SUPPORTING INFORMATION

Catalytic (4+2) Annulation *via* Regio- and Enantioselective Interception of in-situ Generated Alkylgold Intermediate

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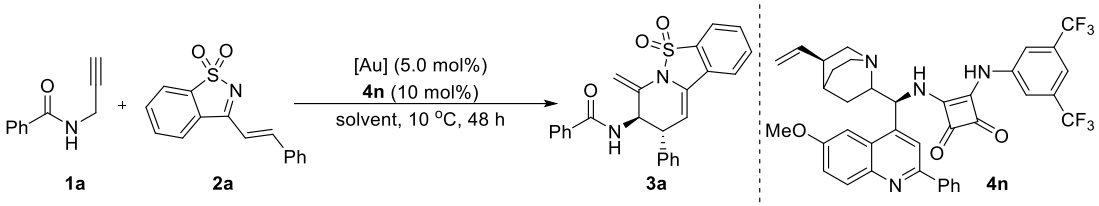
General Information:

All reactions were carried out in oven-dried glassware. Solvents were dried following the standard methods. Flash column chromatography was performed using silica gel (300-400 mesh). Analytical thin-layer chromatography was performed using glass plates pre-coated with 200-300 mesh silica gel impregnated with a fluorescent indicator (254 nm). ^{1}H NMR and ^{13}C NMR spectra were recorded in $CDCl_3$ on a 400 MHz and 500 MHz spectrometer; chemical shifts were reported in ppm with the solvent signal as reference, and coupling constants (*J*) were given in Hertz. The peak information was described as: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, comp = composite. Enantioselectivity was determined on HPLC using Chiralpak IA, IA-3, IC, AD-H, OD-H column. High-resolution mass spectra (HRMS) were recorded on a commercial apparatus (ESI or CI Source). Gold complexes were purchased from Laajoo, and used directly without additional treatment. The racemic products were prepared under the optimal conditions with Et_3N as organocatalyst. Starting materials **1**[1], **2**[2] and **7**[3] were synthesized according to previously published procedure and had physical and spectral properties identical to those earlier reported.

Condition Optimization

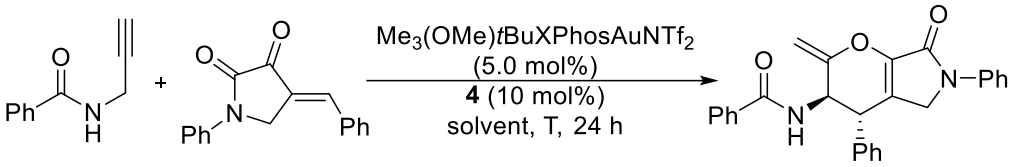
Table S1. Optimization of the reaction conditions for the synthesis of tetrahydropyridine **3a**.[a]



Entry	[Au]	Solvent	Yields [%][b]	*dr*[c]	*ee* [%][d]
1	Me_4*t*BuXPhosAuNTf$_2$	DCE	40	3:1	80/35
2	*t*BuBrettPhosAuNTf$_2$	DCE	72	8:1	96/24
3	IPrAuNTf$_2$	DCE	-/(87)[f]	-	-
4	PMe_3AuCl + AgNTf$_2$	DCE	-/(82)[f]	-	-
5[e]	PMe_3AuCl + AgNTf$_2$	DCE	-/(81)[f]	-	-
6	P(*t*Bu)$_3$AuCl + AgNTf$_2$	DCE	-/(85)[f]	-	-
7	Me_3(OMe)*t*BuXPhosAuNTf$_2$	DCE	93	10:1	96/55
8	Me_3(OMe)*t*BuXPhosAuNTf$_2$	DCM	89	5:1	89/27
9	Me_3(OMe)*t*BuXPhosAuNTf$_2$	$CHCl_3$	90	2:1	77/20
10	Me_3(OMe)*t*BuXPhosAuNTf$_2$	TBME	<5	-	-
11	Me_3(OMe)*t*BuXPhosAuNTf$_2$	toluene	<10	-	-

[a] Unless otherwise noted, the reaction was carried out on a 0.1 mmol scale: **1a** (19.1 mg, 0.12 mmol) in 1.0 mL solvent was added to a solution of catalyst (5.0 mol%), organocatalyst **4n** (7.1 mg, 10 mol%), **2a** (26.9 mg, 0.1 mmol) in solvent (1.0 mL) under argon atmosphere at 10 °C for 48 h. [b] Isolated yields of **3a**. [c] The *dr* ratios were determined by ^{1}H NMR spectroscopy of crude reaction mixture. [d] The *ee* values were determined by chiral HPLC analysis. TBME = methyl *tert*-butyl ether. [e] The reaction was conducted at 60 °C. [f] The yields of compound **5**.

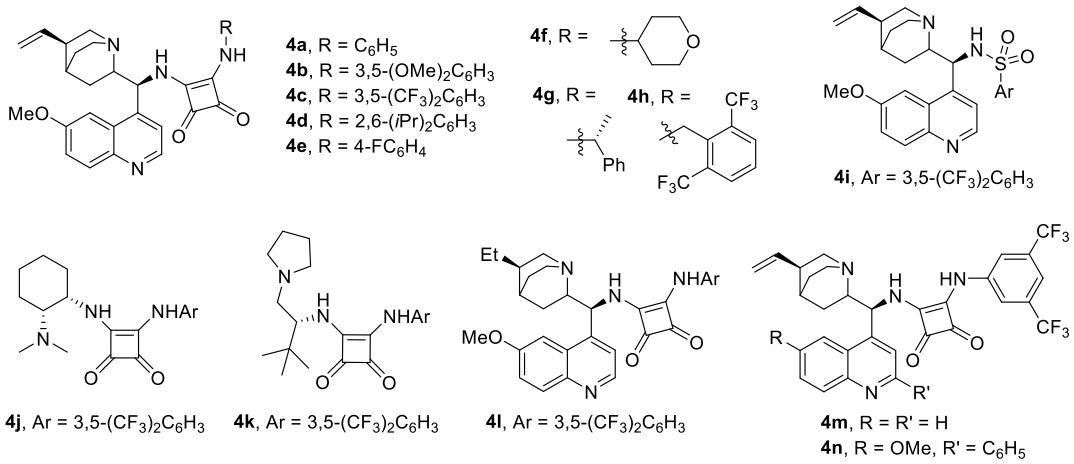
Table S2. Optimization of the reaction conditions for the synthesis of tetrahydropyran **8a**.[a]



1a **7a** **8a**

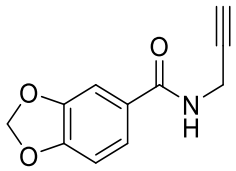
Entry	**4**	T [°C]	Solvent	Yields [%][b]	*dr*[c]	*ee* [%][d]
1	**4c**	10	DCE	79	3:1	70/66
2	**4l**	10	DCE	55	1:1	51/49
3	**4m**	10	DCE	61	2:1	57/49
4	**4n**	10	DCE	65	3:1	55/69
5	**4c**	10	DCM	45	3:1	64/29
6	**4c**	10	DCE:toluene = 9:1	52	3:1	66/46
7	**4c**	10	DCE:TBME = 9:1	34	3:1	71/50
8	**4c**	10	DCE:hexane = 9:1	81	3:1	73/48
9	**4c**	0	DCE:hexane = 9:1	83	4:1	80/57
10	**4c**	0	DCE:hexane = 4:1	76	3:1	79/53
11	**4c**	0	DCE:hexane = 12:1	75	3:1	74/48
12	**4c**	-10	DCE:hexane = 9:1	85	5:1	86/60
13[e]	**4c**	-20	DCE:hexane = 9:1	86	8:1	90

[a] Unless otherwise noted, the reaction was carried out on a 0.1 mmol scale: **1a** (31.8 mg, 0.2 mmol) in 1.0 mL indicated solvent was added to a solution of gold catalyst $Me_3(OMe)$*t*BuXPhosAuNTf$_2$ (5.0 mg, 5.0 mol%), organocatalyst **4** (10 mol%), and **7a** (26.3 mg, 0.1 mmol) in the same solvent (3.0 mL) under argon atmosphere at 10 °C for 24 h. [b] Isolated yields of **8a**. [c] The *dr* ratios were determined by ^{1}H NMR spectroscopy of crude reaction mixture. [d] The *ee* values were determined by chiral HPLC analysis. [e] The reaction was running for 72 h.

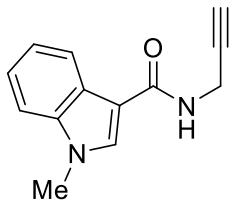


General Procedure for the Preparation of Propargyl Amides 1

Propargyl amides **1** were prepared according to literature procedures.[1] The compounds **1a-1k**, **1u-1v** and **1x** are known compounds and had physical and spectral properties identical to those earlier reported.[1]

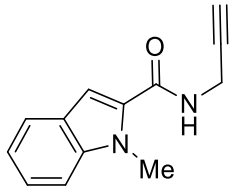


***N*-(Prop-2-yn-1-yl)benzo[*d*][1,3]dioxole-5-carboxamide (1l).** White solid, mp: 105.0-108.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.43 – 7.27 (m, 2H), 6.82 (d, *J* = 8.1 Hz, 1H), 6.27 (s, 1H), 6.02 (d, *J* = 4.2 Hz, 2H), 4.22 – 4.21 (m, 2H), 2.27 (t, *J* = 2.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 166.5, 150.7, 148.2, 128.1, 121.9, 108.2, 107.8, 101.9, 79.7, 72.0, 30.0; HRMS (TOF MS ESI$^+$) calculated for $C_{11}H_9NNaO_3$ $[M+Na]^+$: 226.0475, found 226.0508.

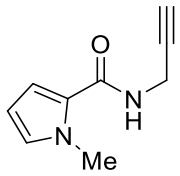


1-Methyl-*N*-(prop-2-yn-1-yl)-1*H*-indole-3-carboxamide (1m). White solid, mp: 112.0-115.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.97 (d, *J* = 7.6 Hz, 1H), 7.67

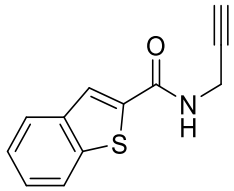
(s, 1H), 7.36 (d, *J* = 7.5 Hz, 1H), 7.33 – 7.27 (m, 2H), 6.06 (s, 1H), 4.31 – 4.29 (m, 2H), 3.82 (s, 3H), 2.28 (t, *J* = 2.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 164.9, 137.4, 132.6, 125.4, 122.8, 121.8, 120.3, 110.31, 110.25, 100.1, 80.3, 71.7, 33.5, 29.4; HRMS (TOF MS ESI$^+$) calculated for $C_{13}H_{12}N_2O$ [M+H]$^+$: 213.1022, found 213.1054.



1-Methyl-*N*-(prop-2-yn-1-yl)-1*H*-indole-2-carboxamide (1n). White solid, mp: 102.0-104.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.60 (d, *J* = 8.0 Hz, 1H), 7.36 – 7.30 (m, 2H), 7.19 – 7.11 (m, 1H), 6.86 (s, 1H), 6.47 (s, 1H), 4.23 – 4.21 (m, 2H), 4.02 (s, 3H), 2.28 (t, *J* = 2.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 162.3, 139.2, 131.2, 126.0, 124.4, 122.0, 120.7, 110.3, 104.5, 79.6, 71.9, 31.7, 29.4; HRMS (TOF MS ESI$^+$) calculated for $C_{13}H_{12}N_2NaO$ [M+Na]$^+$: 235.0842, found 235.0862.

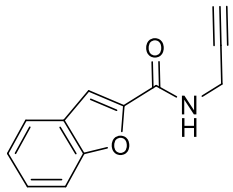


1-Methyl-*N*-(prop-2-yn-1-yl)-1*H*-pyrrole-2-carboxamide (1o). White solid, mp: 101.0-103.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 6.77 – 6.68 (m, 1H), 6.58 – 6.57 (m, 1H), 6.09 – 6.07 (m, 2H), 4.17 – 4.15 (m, 2H), 3.94 (s, 3H), 2.24 (t, *J* = 2.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 161.6, 128.4, 125.1, 112.2, 107.4, 80.0, 71.5, 36.8, 29.0; HRMS (TOF MS ESI$^+$) calculated for $C_9H_{10}N_2NaO$ [M+Na]$^+$: 185.0685, found 185.0725.

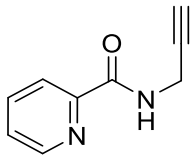


***N*-(Prop-2-yn-1-yl)benzo[*b*]thiophene-2-carboxamide (1p).** White solid, mp: 115.0-118.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.86 (t, *J* = 7.7 Hz, 2H), 7.81 (s,

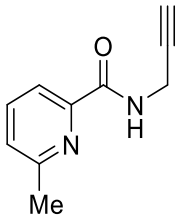
1H), 7.49 – 7.36 (m, 2H), 6.30 (s, 1H), 4.29 – 4.28 (m, 2H), 2.32 (t, *J* = 2.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 162.1, 141.1, 139.1, 137.5, 126.7, 126.0, 125.3, 125.2, 122.9, 79.2, 72.4, 30.0; HRMS (TOF MS ESI$^+$) calculated for $C_{12}H_9NNaOS$ $[M+Na]^+$: 238.0297, found 238.0316.



***N*-(Prop-2-yn-1-yl)benzofuran-2-carboxamide (1q).** White solid, mp: 102.0-104.0 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.67 (d, *J* = 7.8 Hz, 1H), 7.50 (d, *J* = 5.8 Hz, 2H), 7.42 (t, *J* = 7.8 Hz, 1H), 7.30 (t, *J* = 7.5 Hz, 1H), 6.85 (s, 1H), 4.30 – 4.29 (m, 2H), 2.31 (t, *J* = 2.4 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 158.6, 154.9, 148.2, 127.6, 127.2, 123.9, 123.0, 111.9, 111.1, 79.1, 72.2, 29.2; HRMS (TOF MS ESI$^+$) calculated for $C_{12}H_9NNaO_2$ $[M+Na]^+$: 222.0526, found 222.0554.

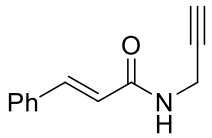


***N*-(Prop-2-yn-1-yl)picolinamide (1r)**. White solid, mp: 101.0-103.0 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 8.50 (d, *J* = 4.7 Hz, 1H), 8.22 (s, 1H), 8.13 (d, *J* = 7.8 Hz, 1H), 7.80 – 7.77 (m, 1H), 7.47 – 7.33 (m, 1H), 4.23 – 4.21 (m, 2H), 2.24 (t, *J* = 2.2 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 164.1, 149.4, 148.2, 137.4, 126.4, 122.3, 79.5, 71.6, 29.1; HRMS (TOF MS ESI$^+$) calculated for $C_9H_8N_2NaO$ $[M+Na]^+$: 183.0529, found 183.0570.

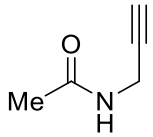


6-Methyl-*N*-(prop-2-yn-1-yl)picolinamide (1s). White solid, mp: 116.0-119.0 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 8.26 (s, 1H), 7.93 (d, *J* = 7.7 Hz, 1H), 7.66 (t, *J* = 7.7 Hz, 1H), 7.23 (d, *J* = 7.7 Hz, 1H), 4.22 – 4.21 (m, 2H), 2.51 (s, 3H), 2.24 (t, *J* =

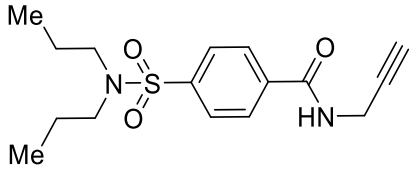
2.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 164.2, 157.3, 148.6, 137.5, 126.1, 119.4, 79.6, 71.5, 29.0, 24.2; HRMS (TOF MS ESI$^+$) calculated for $C_{10}H_{10}N_2NaO$ $[M+Na]^+$: 197.0685, found 197.0726.



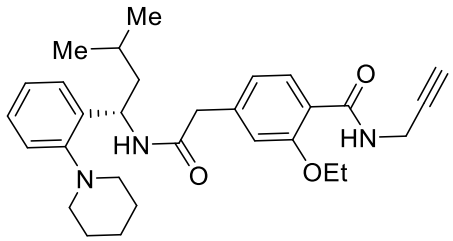
***N*-(Prop-2-yn-1-yl)cinnamamide (1t).** White solid, mp: 106.0-108.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.67 (d, *J* = 15.6 Hz, 1H), 7.54 – 7.46 (m, 2H), 7.37 – 7.31 (comp, 3H), 6.46 (d, *J* = 15.6 Hz, 1H), 6.32 (s, 1H), 4.25 – 4.15 (m, 2H), 2.26 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 165.8, 141.9, 134.7, 130.0, 128.9, 128.0, 120.0, 79.6, 71.8, 29.6.; HRMS (TOF MS ESI$^+$) calculated for $C_{12}H_{11}NNaO$ $[M+Na]^+$: 208.0733, found 208.0740.



***N*-(Prop-2-yn-1-yl)acetamide (1v).** White solid, mp: 95.0-97.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 6.74 (s, 1H), 4.05 – 4.03 (m, 1H), 2.24 (t, *J* = 2.5 Hz, 1H), 2.03 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 170.3, 79.7, 71.3, 29.2, 22.9; HRMS (TOF MS ESI$^+$) calculated for C_5H_7NNaO $[M+Na]^+$: 120.0420, found 120.0422.



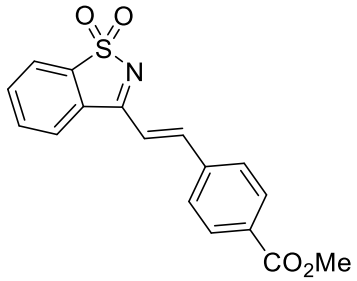
4-(*N*,*N*-Dipropylsulfamoyl)-*N*-(prop-2-yn-1-yl)benzamide (1x). White solid, mp: 105.0-107.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.88 (d, *J* = 8.3 Hz, 2H), 7.76 (d, *J* = 8.4 Hz, 2H), 7.13 (t, *J* = 4.6 Hz, 1H), 4.21 – 4.19 (m, 2H), 3.06 – 3.02 (m, 4H), 2.24 (t, *J* = 2.4 Hz, 1H), 1.52 – 1.47 (m, 4H), 0.82 (t, *J* = 7.4 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 166.1, 143.0, 137.4, 128.1, 127.2, 79.3, 71.9, 50.0, 29.9, 21.9, 11.2; HRMS (TOF MS ESI$^+$) calculated for $C_{16}H_{23}N_2O_3S$ $[M+H]^+$: 323.1424, found 323.1425.



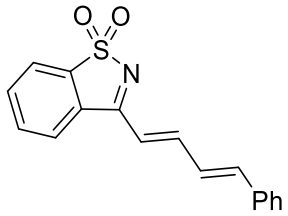
***(S)*-2-Ethoxy-4-(2-((3-methyl-1-(2-(piperidin-1-yl)phenyl)butyl)amino)-2-oxoethyl)-*N*-(prop-2-yn-1-yl)benzamide (1y).** White solid, mp: 112.0-115.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.24 (t, *J* = 4.3 Hz, 1H), 8.14 (d, *J* = 7.9 Hz, 1H), 7.26 – 7.17 (m, 2H), 7.10 – 7.01 (m, 2H), 6.92 – 6.87 (m, 2H), 6.79 (d, *J* = 8.2 Hz, 1H), 5.39 – 5.33 (m, 1H), 4.24 – 4.23 (m, 2H), 4.17 – 3.93 (m, 2H), 3.53 (s, 2H), 2.92 (s, 2H), 2.61 (d, *J* = 8.3 Hz, 2H), 2.26 (t, *J* = 2.5 Hz, 1H), 1.87 – 1.30 (m, 12H), 0.90 (d, *J* = 6.5 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 168.9, 164.9, 157.3, 152.7, 141.0, 138.8, 132.8, 128.0, 127.9, 125.2, 123.0, 122.1, 119.6, 113.1, 79.9, 71.5, 65.0, 50.0, 46.8, 44.2, 29.6, 26.9, 25.5, 24.3, 22.9, 22.7, 14.8; HRMS (TOF MS ESI$^+$) calculated for $C_{30}H_{40}N_3O_3$ $[M+H]^+$: 490.3064, found 490.3026.

General Procedure for the Preparation of Imines 2

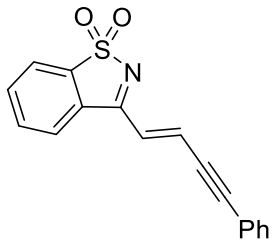
Cyclic 1-Azadine **2** were prepared were prepared according to literature procedures.[2] The compounds **2a-2e** and **2g-2k** are known compounds and had physical and spectral properties identical to those earlier reported.[2]



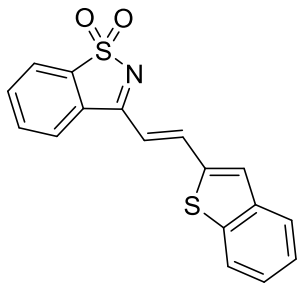
Methyl (*E*)-4-(2-(1,1-Dioxidobenzo[*d*]isothiazol-3-yl)vinyl)benzoate (2f). Yellow solid, mp: 125.0-128.0 °C; ^{1}H NMR (500 MHz, DMSO-d_6) (δ, ppm) 8.52 (d, *J* = 7.1 Hz, 1H), 8.30 (d, *J* = 15.8 Hz, 1H), 8.21 (d, *J* = 6.8 Hz, 1H), 8.15 (d, *J* = 8.3 Hz, 2H), 8.09 – 8.04 (m, 2H), 7.96 – 7.92 (m, 1H), 7.46 (dd, *J* = 20.8, 8.4 Hz, 2H), 3.89 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6) (δ, ppm) 167.7, 165.7, 144.9, 139.4, 138.8, 134.5, 131.6, 130.9, 129.7, 129.1, 125.9, 122.7, 121.0, 118.0, 52.4; HRMS (TOF MS ESI$^+$) calculated for $C_{17}H_{14}NO_4S$ $[M+H]^+$: 328.0638, found 328.0640.



3-((1*E*,3*E*)-4-Phenylbuta-1,3-dien-1-yl)benzo[*d*]isothiazole 1,1-dioxide (2l). Yellow solid, mp: 126.0-129.0 ºC; ^{1}H NMR (500 MHz, DMSO-d_6) (δ, ppm) 8.26 – 8.20 (m, 1H), 8.19 – 8.14 (m, 1H), 8.06 (dd, *J* = 14.9, 10.4 Hz, 1H), 7.96 – 7.87 (m, 2H), 7.66 (d, *J* = 7.3 Hz, 2H), 7.50 – 7.43 (m, 2H), 7.40 (dd, *J* = 13.5, 4.8 Hz, 2H), 7.35 (dd, *J* = 13.2, 5.0 Hz, 2H); ^{13}C NMR (125 MHz, DMSO-d_6) (δ, ppm) 167.2, 147.8, 144.5, 139.6, 135.8, 134.5, 134.3, 130.9, 130.1, 129.2, 127.9, 127.5, 125.2, 122.6, 118.4; HRMS (TOF MS ESI$^+$) calculated for $C_{17}H_{14}NO_2S$ $[M+H]^+$: 296.0740, found 296.0736.

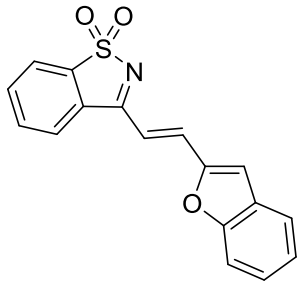


(*E*)-3-(4-Phenylbut-1-en-3-yn-1-yl)benzo[*d*]isothiazole 1,1-dioxide (2m). Yellow solid, mp: 122.0-125.0 ºC; ^{1}H NMR (500 MHz, DMSO-d_6) (δ, ppm) 8.35 (dd, *J* = 5.8, 2.7 Hz, 1H), 8.20 (dd, *J* = 5.9, 2.5 Hz, 1H), 7.94 – 7.91 (m, 2H), 7.74 (d, *J* = 15.5 Hz, 1H), 7.66 – 7.59 (m, 2H), 7.58 – 7.46 (comp, 4H); ^{13}C NMR (125 MHz, DMSO-d_6) (δ, ppm) 166.6, 139.2, 134.62, 134.58, 132.0, 130.40, 130.36, 129.1, 128.1, 126.4, 125.8, 122.7, 121.1, 101.6, 88.7; HRMS (TOF MS ESI$^+$) calculated for $C_{17}H_{12}NO_2S$ $[M+H]^+$: 294.0583, found 294.0580.



(*E*)-3-(2-(Benzo[*b*]thiophen-2-yl)vinyl)benzo[*d*]isothiazole 1,1-dioxide (2n). Yellow solid, mp: 125.0-128.0 ºC; ^{1}H NMR (500 MHz, DMSO-d_6) (δ, ppm) 8.57 (d, *J*

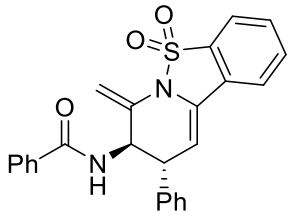
= 15.3 Hz, 1H), 8.51 – 8.42 (m, 1H), 8.19 (dd, *J* = 5.4, 2.5 Hz, 1H), 8.13 (s, 1H), 8.06 (d, *J* = 8.0 Hz, 1H), 7.97 – 7.91 (comp, 3H), 7.59 – 7.40 (comp, 3H); ^{13}C NMR (125 MHz, DMSO-d_6) (δ, ppm) 167.3, 140.9, 140.0, 139.7, 139.5, 139.3, 134.4, 132.6, 130.7, 127.3, 125.9, 125.4, 125.3, 122.9, 122.6, 115.9; HRMS (TOF MS ESI$^+$) calculated for $C_{17}H_{12}NO_2S_2$ $[M+H]^+$: 326.0304, found 326.0310.



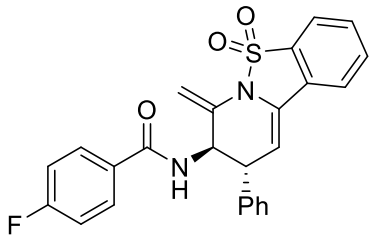
(*E*)-3-(2-(Benzofuran-2-yl)vinyl)benzo[*d*]isothiazole 1,1-dioxide (2o). Yellow solid, mp: 125.0-128.0 ^{o}C; ^{1}H NMR (500 MHz, DMSO-d_6) (δ, ppm) 8.45 (dd, *J* = 5.8, 2.7 Hz, 1H), 8.26 (d, *J* = 15.4 Hz, 1H), 8.20 (dd, *J* = 5.8, 2.7 Hz, 1H), 7.94 – 7.92 (m, 2H), 7.81 (d, *J* = 7.8 Hz, 1H), 7.71 – 7.67 (comp, 3H), 7.51 (t, *J* = 7.7 Hz, 1H), 7.35 (t, *J* = 7.5 Hz, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) (δ, ppm) 167.3, 155.6, 152.5, 139.5, 134.5, 134.4, 132.8, 130.7, 128.2, 128.0, 125.8, 124.0, 122.9, 122.6, 115.7, 114.9, 111.5; HRMS (TOF MS ESI$^+$) calculated for $C_{17}H_{12}NO_3S$ $[M+H]^+$: 310.0532, found 310.0530.

General Procedure for the Synthesis of Tetrahydropyridines 3 and 6

To a 10-mL oven-dried vial containing a magnetic stirring bar, α,β-unsaturated imines **2** (0.1 mmol), **4n** (7.1 mg, 10.0 mol%), and $Me_3(OMe)$*t*BuXPhosAuNTf$_2$ (5.0 mg, 5.0 mol%) in DCE (3.0 mL), was added propargyl amides **1** (0.12 mmol, 1.2 equiv.) in DCE (1.0 mL) at 10 ℃ under argon atmosphere. The resulting reaction mixture was stirred for 48 hours under these conditions. When the reaction was completed (monitored by TLC), the solvent was evaporated *in vacuo* and the residue was purified by flash column chromatography on silica gel (hexanes/ethyl acetate = 8:1 to 5:1) to afford the pure products **3** and **6** in good to high yields with excellent stereoselectivity.

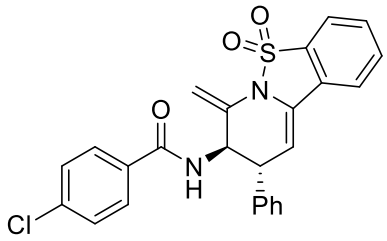


***N*-((8*R*,9*R*)-7-Methylene-5,5-dioxido-9-phenyl-8,9-dihydro-7*H*-benzo[4,5]isothiazolo[2,3-*a*]pyridin-8-yl)benzamide (3a)** 39.8mg, 93% yield, 10:1 *dr*, 96% *ee*, $[\alpha]_D^{20}$ = 218° (c = 0.05, DCM). Yellow solid, mp: 113.5-115.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.86 (d, *J* = 7.7 Hz, 1H), 7.73 – 7.67 (comp, 4H), 7.61 (t, *J* = 7.3 Hz, 1H), 7.43 (t, *J* = 7.0 Hz, 1H), 7.39 – 7.21 (comp, 7H), 6.58 (d, *J* = 6.2 Hz, 1H), 5.84 (d, *J* = 5.5 Hz, 1H), 5.54 (s, 1H), 4.86 – 4.84 (m, 2H), 4.15 – 4.10 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 166.9, 140.0, 133.9, 133.7, 132.7, 132.3, 131.9, 130.6, 130.0, 128.9, 128.7, 128.5, 128.4, 127.7, 127.1, 121.54, 121.45, 104.2, 101.2, 54.8, 44.6; HRMS (TOF MS ESI$^+$) calculated for $C_{25}H_{20}N_2NaO_3S$ $[M+Na]^+$: 451.1087, found 451.1100; HPLC conditions for determination of enantiomeric excess: Chiral AD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{minor} = 20.4 min, t_{major} = 26.6 min.

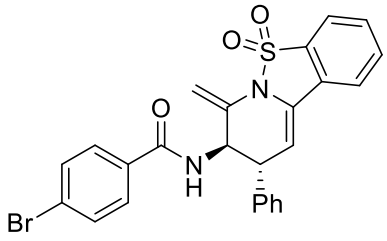


4-Fluoro-*N*-((8*R*,9*R*)-7-methylene-5,5-dioxido-9-phenyl-8,9-dihydro-7*H*-benzo[4,5]isothiazolo[2,3-*a*]pyridin-8-yl)benzamide (3b) 40.2 mg, 90% yield, 11:1 *dr*, 94% *ee*, $[\alpha]_D^{20}$ = 212° (c = 0.05, DCM). Yellow solid, mp: 114.0-116.5 °C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.88 (d, *J* = 7.8 Hz, 1H), 7.80 – 7.66 (comp, 4H), 7.63 (t, *J* = 7.5 Hz, 1H), 7.38 – 7.20 (comp, 5H), 7.03 (t, *J* = 8.5 Hz, 2H), 6.53 (d, *J* = 6.5 Hz, 1H), 5.86 (d, *J* = 5.9 Hz, 1H), 5.55 (d, *J* = 1.1 Hz, 1H), 4.87 (s, 1H), 4.83 (dd, *J* = 6.5, 2.2 Hz, 1H), 4.13 (dd, *J* = 5.7, 2.8 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 165.8, 165.0 (d, *J* = 252.3 Hz),139.9, 133.8, 132.5, 132.3, 130.7, 130.1, 129.6 (d, *J* = 9.0 Hz), 128.9, 128.6, 128.5, 127.8, 121.5 (d, *J* = 6.5 Hz), 115.8 (d, *J* = 21.9 Hz), 104.9, 101.2,

54.9, 44.6; ^{19}F NMR (471 MHz, $CDCl_3$) (δ, ppm) -107.60; HRMS (TOF MS ESI$^+$) calculated for $C_{25}H_{19}FN_2NaO_3S$ $[M+Na]^+$: 469.0993, found 469.0989; HPLC conditions for determination of enantiomeric excess: Chiral AD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{minor} = 20.8 min, t_{major} = 22.8 min.

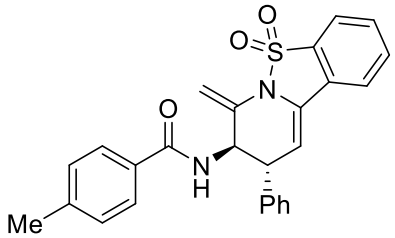


4-Chloro-*N*-((8*R*,9*R*)-7-methylene-5,5-dioxido-9-phenyl-8,9-dihydro-7*H*-benzo[4, 5]isothiazolo[2,3-*a*]pyridin-8-yl)benzamide (3c) 41.2 mg, 89% yield, 10:1 *dr*, 93% *ee*, $[\alpha]_D^{20}$ = 162^o (c = 0.05, DCM). Yellow solid, mp: 110.0-112.0 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.83 (d, *J* = 7.5 Hz, 1H), 7.77 – 7.63 (m, 2H), 7.60 – 7.58 (comp, 3H), 7.37 – 7.06 (comp, 7H), 6.58 (d, *J* = 5.5 Hz, 1H), 5.81 (d, *J* = 5.4 Hz, 1H), 5.51 (s, 1H), 4.83 (s, 1H), 4.80 (d, *J* = 3.9 Hz, 1H), 4.08 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 165.9, 139.8, 138.1, 133.8, 132.5, 132.3, 132.2, 130.7, 130.1, 129.0, 128.9, 128.6, 128.5, 128.4, 127.8, 121.6, 121.5, 104.6, 101.1, 54.9, 44.5; HRMS (TOF MS ESI$^+$) calculated for $C_{25}H_{19}ClN_2NaO_3S$ $[M+Na]^+$: 485.0697, found 485.0703; HPLC conditions for determination of enantiomeric excess: Chiral AD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{minor} = 28.1 min, t_{major} = 35.1 min.

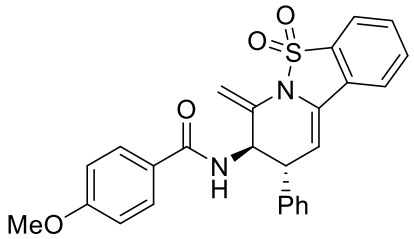


4-Bromo-*N*-((8*R*,9*R*)-7-methylene-5,5-dioxido-9-phenyl-8,9-dihydro-7*H*-benzo[4, 5]isothiazolo[2,3-*a*]pyridin-8-yl)benzamide (3d) 44.0 mg, 87% yield, 12:1 *dr*, 90% *ee*, $[\alpha]_D^{20}$ = 156^o (c = 0.05, DCM). Yellow solid, mp: 111.0-113.0 ^{o}C; ^{1}H NMR (400

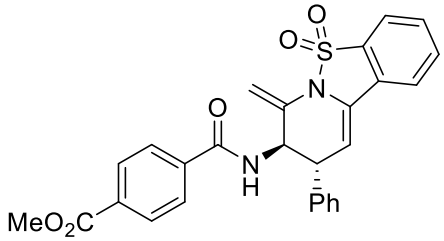
MHz, $CDCl_3$) (δ, ppm) 7.89 (d, *J* = 7.7 Hz, 1H), 7.77 – 7.68 (comp, 3H), 7.58 (d, *J* = 8.6 Hz, 2H), 7.53 – 7.49 (m, 2H), 7.36 – 7.26 (comp, 5H), 6.59 (d, *J* = 6.8 Hz, 1H), 5.87 (d, *J* = 5.9 Hz, 1H), 5.57 (d, *J* = 1.7 Hz, 1H), 4.89 (d, *J* = 1.5 Hz, 1H), 4.87 – 4.80 (m, 1H), 4.14 (dd, *J* = 5.8, 3.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 166.0, 139.8, 133.8, 132.8, 132.5, 132.3, 132.0, 130.7, 130.1, 129.7, 128.9, 128.8, 128.4, 127.8, 126.6, 121.6, 121.5, 104.8, 101.1, 54.9, 44.6; HRMS (TOF MS ESI$^+$) calculated for $C_{25}H_{19}BrN_2NaO_3S$ $[M+Na]^+$: 529.0192, found 529.0195; HPLC conditions for determination of enantiomeric excess: Chiral AD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{minor} = 28.6 min, t_{major} = 41.1 min.



4-Methyl-*N*-((8*R*,9*R*)-7-methylene-5,5-dioxido-9-phenyl-8,9-dihydro-7*H*-benzo[4,5]isothiazolo[2,3-*a*]pyridin-8-yl)benzamide (3e) 37.6 mg, 85% yield, 10:1 *dr*, 96% *ee*, $[\alpha]_D^{20}$ = 126^o (c = 0.05, DCM). Yellow solid, mp: 115.0-118.0 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.90 (d, *J* = 6.8 Hz, 1H), 7.76 – 7.60 (comp, 5H), 7.44 – 7.23 (comp, 5H), 7.18 (d, *J* = 6.7 Hz, 2H), 6.53 (s, 1H), 5.87 (d, *J* = 4.1 Hz, 1H), 5.57 (s, 1H), 4.90 – 4.88 (m, 2H), 4.17 (s, 1H), 2.35 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 166.9, 142.4, 140.0, 133.7, 132.6, 132.3, 131.1, 130.6, 130.0, 129.4, 128.9, 128.5, 127.7, 127.2, 121.6, 121.5, 104.5, 101.2, 54.8, 44.6, 21.6; HRMS (TOF MS ESI$^+$) calculated for $C_{26}H_{22}N_2NaO_3S$ $[M+Na]^+$: 465.1243, found 465.1261; HPLC conditions for determination of enantiomeric excess: Chiral IC, λ = 254 nm, hexane : 2-propanol = 75:25, flow rate = 1.0 mL/min, t_{minor} = 41.1 min, t_{major} = 46.1 min.

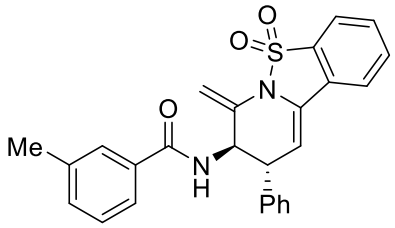


4-Methoxy-*N*-((8*R*,9*R*)-7-methylene-5,5-dioxido-9-phenyl-8,9-dihydro-7*H*-benzo[4,5]isothiazolo[2,3-*a*]pyridin-8-yl)benzamide (3f) 35.8 mg, 78% yield, 10:1 *dr*, 93% *ee*, $[\alpha]_D^{20}$ = 134° (c = 0.05, DCM). Yellow solid, mp: 116.0-119.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.91 (d, *J* = 7.4 Hz, 1H), 7.80 – 7.52 (comp, 5H), 7.43 – 7.16 (comp, 5H), 6.87 (d, *J* = 7.8 Hz, 2H), 6.48 (d, *J* = 5.3 Hz, 1H), 5.88 (d, *J* = 4.9 Hz, 1H), 5.57 (s, 1H), 4.89 (s, 1H), 4.85 (d, *J* = 4.6 Hz, 1H), 4.18 (s, 1H), 3.81 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 166.4, 162.6, 140.0, 133.7, 132.7, 130.6, 130.1, 129.0, 128.9, 128.7, 128.5, 127.7, 126.2, 121.6, 121.5, 114.0, 104.8, 101.3, 100.1, 55.5, 54.9, 44.6; HRMS (TOF MS ESI$^+$) calculated for $C_{26}H_{22}N_2NaO_4S$ $[M+Na]^+$: 481.1192, found 481.1201; HPLC conditions for determination of enantiomeric excess: Chiral IA, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{minor} = 25.5 min, t_{major} = 29.0 min.

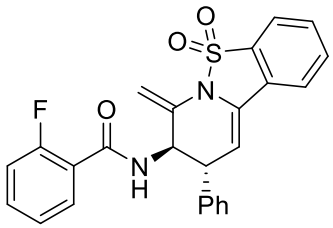


Methyl 4-(((8*R*,9*R*)-7-Methylene-5,5-dioxido-9-phenyl-8,9-dihydro-7*H*-benzo[4,5]isothiazolo[2,3-*a*]pyridin-8-yl)carbamoyl)benzoate (3g) 41.8 mg, 86% yield, >20:1 *dr*, 94% *ee*, $[\alpha]_D^{20}$ = 184° (c = 0.05, DCM). Yellow solid, mp: 118.0-120.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.05 (d, *J* = 6.1 Hz, 2H), 7.91 (d, *J* = 6.2 Hz, 1H), 7.87 – 7.58 (comp, 5H), 7.37 – 7.30 (comp, 5H), 6.69 (s, 1H), 5.90 (s, 1H), 5.60 (s, 1H), 4.93 – 4.90 (m, 2H), 4.17 (s, 1H), 3.92 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 166.3, 166.0, 139.8, 137.8, 133.8, 133.1, 132.5, 132.3, 130.7, 130.1, 130.0, 128.9, 128.5, 128.4, 127.8, 127.2, 121.6, 121.5, 104.6, 101.0, 54.9, 52.5, 44.6; HRMS (TOF MS ESI$^+$) calculated for $C_{27}H_{22}N_2NaO_5S$ $[M+Na]^+$: 509.1142, found 509.1150;

HPLC conditions for determination of enantiomeric excess: Chiral OD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 23.1 min, t_{minor} = 33.6 min.

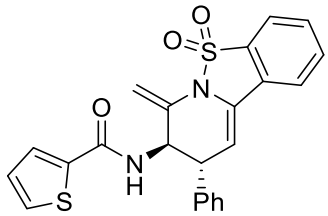


3-Methyl-*N*-((8*R*,9*R*)-7-methylene-5,5-dioxido-9-phenyl-8,9-dihydro-7*H*-benzo[4, 5]isothiazolo[2,3-*a*]pyridin-8-yl)benzamide (3h) 37.6 mg, 85% yield, 10:1 *dr*, 95% *ee*, $[\alpha]_D^{20}$ = 202° (c = 0.05, DCM). Yellow solid, mp: 119.0-121.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.86 (d, *J* = 7.7 Hz, 1H), 7.76 – 7.65 (m, 2H), 7.61 (t, *J* = 7.5 Hz, 1H), 7.53 (s, 1H), 7.45 (d, *J* = 6.4 Hz, 1H), 7.35 – 7.19 (comp, 7H), 6.54 (d, *J* = 6.5 Hz, 1H), 5.84 (d, *J* = 5.7 Hz, 1H), 5.54 (s, 1H), 4.87 – 4.86 (m, 2H), 4.13 (d, *J* = 1.9 Hz, 1H), 2.32 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 167.1, 140.0, 138.6, 133.9, 133.7, 132.7, 132.6, 132.3, 130.6, 130.0, 128.9, 128.6, 128.5, 128.4, 128.0, 127.7, 124.0, 121.53, 121.46, 104.1, 101.2, 54.8, 44.6, 21.4; HRMS (TOF MS ESI$^+$) calculated for $C_{26}H_{22}N_2NaO_3S$ $[M+Na]^+$: 465.1243, found 465.1251; HPLC conditions for determination of enantiomeric excess: Chiral IA, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 11.3 min, t_{minor} = 13.3 min.

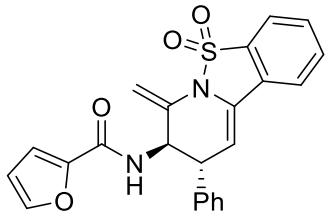


2-Fluoro-*N*-((8*R*,9*R*)-7-methylene-5,5-dioxido-9-phenyl-8,9-dihydro-7*H*-benzo[4, 5]isothiazolo[2,3-*a*]pyridin-8-yl)benzamide (3i) 40.2 mg, 90% yield, 11:1 *dr*, 96% *ee*, $[\alpha]_D^{20}$ = 210° (c = 0.05, DCM). Yellow solid, mp: 115.0-117.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.99 – 7.97 (m, 1H), 7.82 (d, *J* = 6.8 Hz, 1H), 7.69 – 7.57 (comp, 3H), 7.36 (s, 1H), 7.32 – 7.13 (comp, 6H), 6.98 (d, *J* = 8.1 Hz, 2H), 5.81 (d, *J*

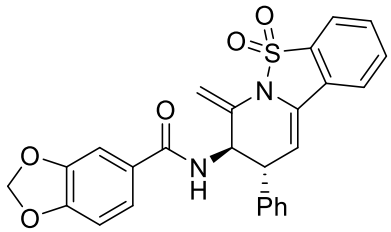
= 3.2 Hz, 1H), 5.50 (s, 1H), 4.89 (s, 1H), 4.82 (d, *J* = 3.2 Hz, 1H), 4.04 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 162.8, 160.7 (d, *J* = 248.0 Hz), 139.9, 133.72, 133.67, 132.6, 132.4, 132.0, 130.7, 130.0, 128.9, 128.4, 128.2, 127.8, 124.9 (d, *J* = 3.1 Hz), 121.49, 121.48, 120.7 (d, *J* = 11.3 Hz), 116.2 (d, *J* = 24.5 Hz), 102.9, 100.4, 54.7, 44.7; ^{19}F NMR (471 MHz, $CDCl_3$) (δ, ppm) -112.81; HRMS (TOF MS ESI$^+$) calculated for $C_{25}H_{19}FN_2NaO_3S$ $[M+Na]^+$: 469.0993, found 469.0996; HPLC conditions for determination of enantiomeric excess: Chiral AD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 25.4 min, t_{minor} = 33.0 min.



***N*-((8*R*,9*R*)-7-Methylene-5,5-dioxido-9-phenyl-8,9-dihydro-7*H*-benzo[4,5]isothiazolo[2,3-*a*]pyridin-8-yl)thiophene-2-carboxamide (3j)** 38.2 mg, 88% yield, 12:1 *dr*, 97% *ee*, $[\alpha]_D^{20}$ = 210^o (c = 0.05, DCM). Yellow solid, mp: 112.0-114.0 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.91 (d, *J* = 7.8 Hz, 1H), 7.77 (d, *J* = 7.7 Hz, 1H), 7.73 (t, *J* = 7.5 Hz, 1H), 7.66 (t, *J* = 7.5 Hz, 1H), 7.46 (d, *J* = 4.8 Hz, 1H), 7.41 (d, *J* = 3.3 Hz, 1H), 7.37 – 7.25 (comp, 5H), 7.01 (t, *J* = 4.2 Hz, 1H), 6.46 (d, *J* = 6.2 Hz, 1H), 5.88 (d, *J* = 5.9 Hz, 1H), 5.58 (s, 1H), 4.90 (s, 1H), 4.82 (d, *J* = 4.3 Hz, 1H), 4.20 (dd, *J* = 5.5, 2.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 161.5, 139.9, 138.5, 133.8, 132.4, 132.3, 130.8, 130.7, 130.1, 128.9, 128.7, 128.5, 128.4, 127.81, 127.78, 121.6, 121.5, 105.1, 101.3, 54.9, 44.6; HRMS (TOF MS ESI$^+$) calculated for $C_{23}H_{18}N_2NaO_3S_2$ $[M+Na]^+$: 457.0651, found 457.0666; HPLC conditions for determination of enantiomeric excess: Chiral IA, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 13.6 min, t_{minor} = 16.1 min.

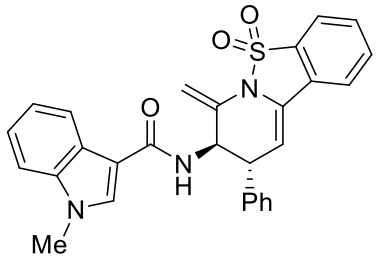


***N*-((8*R*,9*R*)-7-Methylene-5,5-dioxido-9-phenyl-8,9-dihydro-7*H*-benzo[4,5]isothiazolo[2,3-*a*]pyridin-8-yl)furan-2-carboxamide (3k)** 32.2 mg, 77% yield, 10:1 *dr*, 90% *ee*, $[\alpha]_D^{20}$ = 208° (c = 0.05, DCM). Yellow solid, mp: 116.0-118.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.90 (d, *J* = 7.3 Hz, 1H), 7.80 – 7.62 (comp, 3H), 7.43 – 7.22 (comp, 6H), 7.11 (s, 1H), 6.66 (d, *J* = 5.2 Hz, 1H), 6.46 (s, 1H), 5.87 (d, *J* = 4.9 Hz, 1H), 5.54 (s, 1H), 4.87 – 4.85 (m, 2H), 4.08 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 157.8, 147.4, 144.4, 139.9, 133.7, 132.44, 132.42, 130.7, 130.0, 128.9, 128.41, 128.40, 127.8, 121.6, 121.5, 115.0, 112.3, 103.1, 100.7, 54.0, 44.8; HRMS (TOF MS ESI$^+$) calculated for $C_{23}H_{18}N_2NaO_4S$ $[M+Na]^+$: 441.0879, found 441.0891; HPLC conditions for determination of enantiomeric excess: Chiral AD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 14.8 min, t_{minor} = 18.6 min.

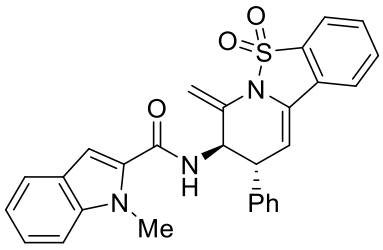


***N*-((8*R*,9*R*)-7-Methylene-5,5-dioxido-9-phenyl-8,9-dihydro-7*H*-benzo[4,5]isothiazolo[2,3-*a*]pyridin-8-yl)benzo[*d*][1,3]dioxole-5-carboxamide (3l)** 41.1 mg, 87% yield, >20:1 *dr*, 96% *ee*, $[\alpha]_D^{20}$ = 160° (c = 0.05, DCM). Yellow solid, mp: 117.0-120.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.90 (d, *J* = 7.8 Hz, 1H), 7.76 (d, *J* = 7.7 Hz, 1H), 7.72 (t, *J* = 7.5 Hz, 1H), 7.65 (t, *J* = 7.5 Hz, 1H), 7.39 – 7.21 (comp, 7H), 6.77 (d, *J* = 8.5 Hz, 1H), 6.41 (d, *J* = 6.5 Hz, 1H), 5.98 (s, 2H), 5.87 (d, *J* = 5.9 Hz, 1H), 5.56 (s, 1H), 4.88 (s, 1H), 4.83 (d, *J* = 4.5 Hz, 1H), 4.15 (dd, *J* = 5.6, 2.6 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 166.1, 150.7, 148.1, 140.0, 133.8, 132.6, 132.3, 130.7, 130.1, 128.9, 128.6, 128.5, 128.1, 127.8, 121.9, 121.6, 121.5,

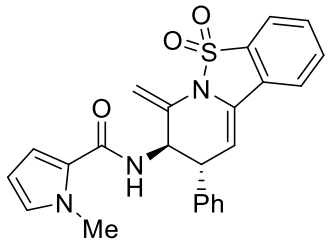
108.2, 107.8, 104.7, 101.8, 101.2, 54.9, 44.6; HRMS (TOF MS ESI$^+$) calculated for $C_{26}H_{20}N_2NaO_5S$ $[M+Na]^+$: 495.0985, found 495.0997; HPLC conditions for determination of enantiomeric excess: Chiral OD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 24.5 min, t_{minor} = 34.3 min.



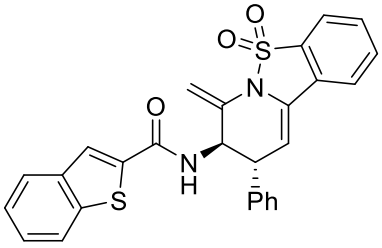
1-Methyl-*N*-((8*R*,9*R*)-7-methylene-5,5-dioxido-9-phenyl-8,9-dihydro-7*H*-benzo[4,5]isothiazolo[2,3-*a*]pyridin-8-yl)-1*H*-indole-3-carboxamide (3m) 42.8 mg, 89% yield, 12:1 *dr*, 97% *ee*, $[\alpha]_D^{20}$ = 145º (c = 0.05, DCM). Yellow solid, mp: 120.0-122.0 ºC; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.93 (d, *J* = 7.9 Hz, 1H), 7.88 (d, *J* = 7.8 Hz, 1H), 7.73 (d, *J* = 7.8 Hz, 1H), 7.68 (t, *J* = 7.4 Hz, 1H), 7.61 (t, *J* = 7.5 Hz, 1H), 7.54 (s, 1H), 7.39 – 7.19 (comp, 7H), 7.16 (t, *J* = 7.3 Hz, 1H), 6.26 (d, *J* = 6.6 Hz, 1H), 5.86 (d, *J* = 5.8 Hz, 1H), 5.55 (d, *J* = 1.4 Hz, 1H), 4.90 – 4.88 (m, 2H), 4.24 (dd, *J* = 5.9, 3.0 Hz, 1H), 3.73 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 164.6, 140.2, 137.3, 133.7, 133.0, 132.31, 132.30, 130.6, 129.9, 128.8, 128.6, 128.5, 127.6, 125.7, 122.8, 121.8, 121.54, 121.47, 120.6, 110.2, 110.0, 104.1, 101.4, 54.6, 44.8, 33.4; HRMS (TOF MS ESI$^+$) calculated for $C_{28}H_{24}N_3O_3S$ $[M+H]^+$: 482.1533, found 482.1527; HPLC conditions for determination of enantiomeric excess: Chiral OD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 26.7 min, t_{minor} = 57.4 min.



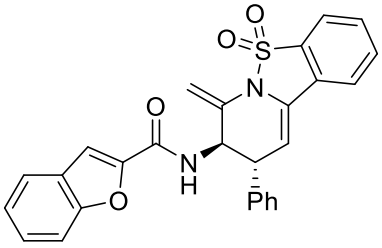
1-Methyl-*N*-((8*R*,9*R*)-7-methylene-5,5-dioxido-9-phenyl-8,9-dihydro-7*H*-benzo[4, 5]isothiazolo[2,3-*a*]pyridin-8-yl)-1*H*-indole-2-carboxamide (3n) Combined in 90% yield, 43.3 mg, 3:1 *dr*, 96(58)% *ee*, $[\alpha]_D^{20}$ = 116º (c = 0.05, DCM). Yellow solid, mp: 119.0-121.0 ºC; composite NMR signals of **3n** and **3n'** ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.86 – 7.83 (comp, 1.3H), 7.71 – 7.64 (comp, 3H), 7.62 – 7.54 (comp, 1.9H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.41 – 7.20 (comp, 11.6H), 7.13 – 7.06 (comp, 1.3H), 6.78 (s, 1H), 6.61 (d, *J* = 7.5 Hz, 1H), 6.53 (d, *J* = 4.8 Hz, 0.3H), 5.90 (d, *J* = 6.0 Hz, 0.3H), 5.83 (d, *J* = 5.5 Hz, 1H), 5.78 (t, *J* = 8.1 Hz, 0.3H), 5.56 (d, *J* = 1.0 Hz, 1H), 5.40 (dd, *J* = 9.3, 6.0 Hz, 0.3H), 4.91 – 4.88 (comp, 2H), 4.81 (d, *J* = 6.9 Hz, 0.3H), 4.12 – 4.02 (m, 1H), 3.98 – 3.96 (comp, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 161.9, 161.6, 140.0, 139.22, 139.17, 137.5, 134.4, 133.7, 133.59, 133.56, 133.0, 132.4, 132.3, 131.4, 131.3, 130.6, 130.0, 129.9, 129.3, 129.1, 128.9, 128.4, 128.3, 127.9, 127.7, 126.0, 125.9, 124.5, 124.3, 122.0, 121.9, 121.5, 121.4, 121.34, 121.32, 120.8, 120.6, 110.3, 110.2, 104.6, 104.0, 103.0, 101.0, 100.9, 96.8, 54.0, 49.2, 44.8, 43.0, 31.62, 31.57, 29.8; HRMS (TOF MS ESI$^+$) calculated for $C_{28}H_{23}N_3NaO_3S$ $[M+Na]^+$: 504.1352, found 504.1356; HPLC conditions for determination of enantiomeric excess of **3n**: Chiral AD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 31.1 min, t_{minor} = 37.3 min; HPLC conditions for determination of enantiomeric excess of **3n'**: Chiral IA, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{minor} = 24.8 min, t_{major} = 43.8 min.



1-Methyl-*N*-((8*R*,9*R*)-7-methylene-5,5-dioxido-9-phenyl-8,9-dihydro-7*H*-benzo[4,5]isothiazolo[2,3-*a*]pyridin-8-yl)-1*H*-pyrrole-2-carboxamide (3o) Combined in 87% yield, 37.5 mg, 3:1 *dr*, 90(64)% *ee*, $[\alpha]_D^{20}$ = 116° (c = 0.05, DCM). Yellow solid, mp: 116.0-119.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.88 (d, *J* = 7.7 Hz, 1H), 7.78 – 7.66 (m, 2H), 7.63 (t, *J* = 7.4 Hz, 1H), 7.39 – 7.32 (comp, 3H), 7.20 (d, *J* = 6.8 Hz, 2H), 6.72 (s, 1H), 6.22 (d, *J* = 2.4 Hz, 1H), 6.10 – 5.98 (m, 1H), 5.94 (d, *J* = 6.3 Hz, 1H), 5.52 (s, 1H), 5.42 (d, *J* = 9.8 Hz, 1H), 5.38 – 5.25 (m, 1H), 4.77 (s, 1H), 3.93 – 3.91 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 160.8, 137.6, 134.7, 133.6, 132.5, 130.6, 130.0, 129.4, 129.0, 128.6, 128.3, 128.1, 125.2, 121.43, 121.39, 111.9, 107.5, 101.0, 96.5, 48.7, 43.2, 36.8; HRMS (TOF MS ESI$^+$) calculated for $C_{24}H_{21}N_3NaO_3S$ $[M+Na]^+$: 454.1196, found 454.1208; HPLC conditions for determination of enantiomeric excess: Chiral AD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 16.1 min, t_{minor} = 19.0 min; NMR signals of **3o'** ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.83 (d, *J* = 7.7 Hz, 1H), 7.74 – 7.63 (m, 2H), 7.58 (t, *J* = 7.5 Hz, 1H), 7.32 – 7.27 (m, 2H), 7.27 – 7.18 (comp, 3H), 6.63 (s, 1H), 6.43 (dd, *J* = 3.9, 1.4 Hz, 1H), 6.19 (d, *J* = 7.1 Hz, 1H), 5.95 (dd, *J* = 3.8, 2.6 Hz, 1H), 5.81 (d, *J* = 5.6 Hz, 1H), 5.47 (d, *J* = 1.5 Hz, 1H), 4.81 (d, *J* = 1.2 Hz, 1H), 4.75 (dd, *J* = 7.1, 3.5 Hz, 1H), 4.02 (dd, *J* = 5.5, 3.7 Hz, 1H), 3.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 161.2, 140.1, 133.7, 133.1, 132.3, 130.6, 130.0, 128.8, 128.5, 128.4, 127.6, 125.2, 124.5, 121.5, 121.4, 112.5, 107.4, 103.3, 101.2, 44.9, 36.7, 31.6; HRMS (TOF MS ESI$^+$) calculated for $C_{24}H_{21}N_3NaO_3S$ $[M+Na]^+$: 454.1196, found 454.1200; HPLC conditions for determination of enantiomeric excess: Chiral IA, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{minor} = 19.0 min, t_{major} = 24.6 min.

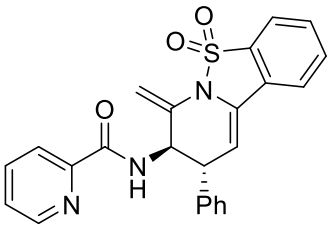


***N*-((8*R*,9*R*)-7-Methylene-5,5-dioxido-9-phenyl-8,9-dihydro-7*H*-benzo[4,5]isothiazolo[2,3-*a*]pyridin-8-yl)benzo[*b*]thiophene-2-carboxamide (3p)** 43.1 mg, 89% yield, 12:1 *dr*, 93% *ee*, $[\alpha]_D^{20}$ = 96° (c = 0.05, DCM). Yellow solid, mp: 118.0-120.0 °C; ^{1}H NMR (500 MHz, DMSO-d_6) (δ, ppm) 9.09 (d, *J* = 8.5 Hz, 1H), 8.19 (d, *J* = 7.9 Hz, 1H), 8.16 – 8.08 (m, 2H), 7.98 (dd, *J* = 19.7, 7.4 Hz, 2H), 7.86 (t, *J* = 7.6 Hz, 1H), 7.76 (t, *J* = 7.6 Hz, 1H), 7.50 – 7.40 (m, 2H), 7.39 – 7.28 (comp, 3H), 7.23 (t, *J* = 7.1 Hz, 1H), 6.21 (d, *J* = 3.0 Hz, 1H), 5.75 (s, 1H), 5.30 (s, 1H), 4.87 – 4.81 (m, 2H), 4.03 (dd, *J* = 8.7, 3.0 Hz, 1H); ^{13}C NMR (125 MHz, DMSO-d_6) (δ, ppm) 161.2, 141.0, 140.2, 139.0, 138.9, 135.2, 134.1, 131.5, 130.9, 128.5, 128.2, 127.4, 127.2, 126.4, 125.29, 125.26, 125.0, 122.8, 122.3, 121.1, 103.3, 95.8, 54.9, 52.8, 43.2; HRMS (TOF MS ESI$^+$) calculated for $C_{27}H_{20}N_2NaO_3S_2$ $[M+Na]^+$: 507.0808, found 507.0825; HPLC conditions for determination of enantiomeric excess: Chiral AD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 54.6 min, t_{minor} = 71.4 min.

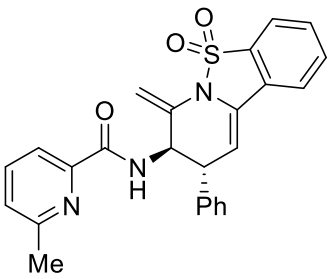


***N*-((8*R*,9*R*)-7-Methylene-5,5-dioxido-9-phenyl-8,9-dihydro-7*H*-benzo[4,5]isothiazolo[2,3-*a*]pyridin-8-yl)benzofuran-2-carboxamide (3q)** 35.1 mg, 75% yield, >20:1 *dr*, 90% *ee*, $[\alpha]_D^{20}$ = 98° (c = 0.05, DCM). Yellow solid, mp: 114.0-117.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.89 (s, 1H), 7.82 – 7.57 (comp, 5H), 7.48 – 7.45 (comp, 3H), 7.36 – 7.25 (comp, 5H), 6.94 (s, 1H), 5.89 (s, 1H), 5.56 (s, 1H), 4.96 – 4.88 (m, 2H), 4.11 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 167.2, 158.4, 154.9, 147.9,

139.9, 133.7, 132.4, 130.7, 129.4, 129.2, 129.0, 128.4, 127.8, 127.2, 123.9, 122.8, 121.6, 121.5, 113.7, 112.1, 111.1, 102.6, 100.7, 54.2, 44.7; HRMS (TOF MS ESI$^+$) calculated for $C_{27}H_{20}N_2NaO_4S$ $[M+Na]^+$: 491.1036, found 491.1034; HPLC conditions for determination of enantiomeric excess: Chiral IA, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 37.1 min, t_{minor} = 46.7 min.

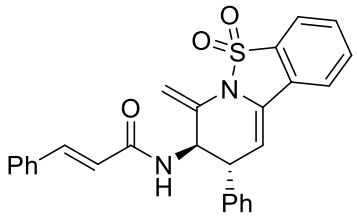


***N*-((8*R*,9*R*)-7-Methylene-5,5-dioxido-9-phenyl-8,9-dihydro-7*H*-benzo[4,5]isothiazolo[2,3-*a*]pyridin-8-yl)picolinamide (3r)** 19.3 mg, 45% yield, >20:1 *dr*, 88% *ee*, $[\alpha]_D^{20}$ = 114^o (c = 0.05, DCM). Yellow solid, mp: 117.0-120.0 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 8.47 (s, 1H), 8.35 – 8.25 (m, 1H), 8.13 (d, *J* = 6.3 Hz, 1H), 7.93 – 7.63 (comp, 6H), 7.52 – 7.27 (comp, 5H), 5.87 (s, 1H), 5.53 (s, 1H), 4.95 (s, 1H), 4.87 (s, 1H), 4.03 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 163.8, 149.3, 148.3, 140.1, 137.4, 133.6, 133.0, 130.6, 129.9, 129.4, 129.2, 128.9, 128.4, 127.7, 126.5, 122.3, 121.5, 121.4, 101.3, 100.6, 54.0, 44.9; HRMS (TOF MS ESI$^+$) calculated for $C_{24}H_{19}N_3NaO_3S$ $[M+Na]^+$: 452.1039, found 452.1043; HPLC conditions for determination of enantiomeric excess: Chiral AD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 22.6 min, t_{minor} = 29.2 min.

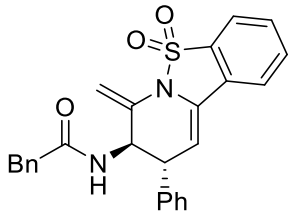


6-Methyl-*N*-((8*R*,9*R*)-7-methylene-5,5-dioxido-9-phenyl-8,9-dihydro-7*H*-benzo[4,5]isothiazolo[2,3-*a*]pyridin-8-yl)picolinamide (3s) 35.5 mg, 80% yield, >20:1 *dr*, 95% *ee*, $[\alpha]_D^{20}$ = 128^o (c = 0.05, DCM). Yellow solid, mp: 118.0-120.0 ^{o}C; ^{1}H NMR

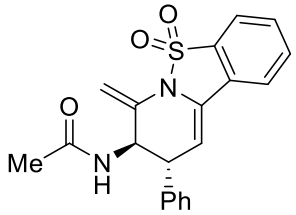
(500 MHz, $CDCl_3$) (δ, ppm) 8.44 (d, *J* = 7.9 Hz, 1H), 7.93 (d, *J* = 7.7 Hz, 1H), 7.88 (d, *J* = 7.8 Hz, 1H), 7.75 (d, *J* = 7.8 Hz, 1H), 7.71 – 7.65 (m, 2H), 7.62 (t, *J* = 7.6 Hz, 1H), 7.35 – 7.28 (comp, 4H), 7.26 – 7.24 (m, 1H), 7.23 (d, *J* = 7.8 Hz, 1H), 5.86 (d, *J* = 5.2 Hz, 1H), 5.54 (d, *J* = 1.9 Hz, 1H), 4.91 (dd, *J* = 8.0, 4.5 Hz, 1H), 4.88 (d, *J* = 1.6 Hz, 1H), 4.07 (t, *J* = 4.9 Hz, 1H), 2.48 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 164.2, 157.5, 148.6, 140.2, 137.5, 133.6, 133.2, 132.5, 130.5, 129.8, 128.8, 128.4, 128.3, 127.7, 126.2, 121.5, 121.4, 119.3, 101.3, 100.9, 54.1, 44.8, 24.3; HRMS (TOF MS ESI$^+$) calculated for $C_{25}H_{21}N_3NaO_3S$ $[M+Na]^+$: 466.1196, found 466.1188; HPLC conditions for determination of enantiomeric excess: Chiral AD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 18.9 min, t_{minor} = 28.0 min.



***N*-((8*R*,9*R*)-7-Methylene-5,5-dioxido-9-phenyl-8,9-dihydro-7*H*-benzo[4,5]isothiazolo[2,3-*a*]pyridin-8-yl)cinnamamide (3t)** 40.4 mg, 89% yield, >20:1 *dr*, 91% *ee*, $[\alpha]_D^{20}$ = 110^o (c = 0.05, DCM). Yellow solid, mp: 118.0-121.0 ^{o}C; ^1H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.89 (d, *J* = 6.0 Hz, 1H), 7.77 – 7.64 (comp, 4H), 7.50 – 7.46 (m, 2H), 7.40 – 7.32 (comp, 8H), 6.38 (d, *J* = 14.9 Hz, 1H), 6.19 (d, *J* = 14.9 Hz, 1H), 5.89 (d, *J* = 0.7 Hz, 1H), 5.54 (s, 1H), 4.87 – 4.83 (m, 2H), 4.12 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 165.3, 142.0, 140.0, 134.8, 133.7, 132.5, 132.3, 130.6, 129.9, 129.4, 129.2, 128.91, 128.89, 128.4, 128.0, 127.7, 121.5, 121.4, 120.2, 103.3, 100.9, 54.7, 44.7; HRMS (TOF MS ESI$^+$) calculated for $C_{27}H_{22}N_2NaO_3S$ $[M+Na]^+$: 477.1243, found 477.1249; HPLC conditions for determination of enantiomeric excess: Chiral AD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 12.5 min, t_{minor} = 15.2 min.

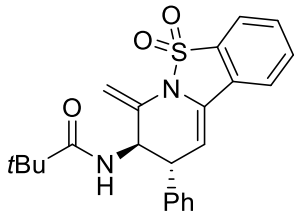


***N*-((8*R*,9*R*)-7-Methylene-5,5-dioxido-9-phenyl-8,9-dihydro-7*H*-benzo[4,5]isothiazolo[2,3-*a*]pyridin-8-yl)-2-phenylacetamide (3u)** Combined in 70% yield, 31.0 mg, 2:1 *dr*, 90(51)% *ee*, $[\alpha]_D^{20}$ = 100º (c = 0.05, DCM). Yellow solid, mp: 115.0-117.0 ºC; composite NMR signals of **3u** and **3u'** ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.82 – 7.79 (comp, 1.5H), 7.70 – 7.52 (comp, 4.5H), 7.30 – 7.08 (comp, 12H), 7.04 (dd, *J* = 6.3, 2.7 Hz, 1H), 6.87 (d, *J* = 6.7 Hz, 2H), 5.86 (d, *J* = 7.7 Hz, 0.5H), 5.77 (d, *J* = 6.1 Hz, 1H), 5.66 (d, *J* = 5.4 Hz, 0.5H), 5.43 – 5.29 (comp, 1.5H), 5.14 – 5.07 (m, 1H), 5.02 (d, *J* = 9.6 Hz, 1H), 4.73 – 4.60 (comp, 1H), 4.45 (s, 1H), 3.78 – 3.73 (comp, 1.5H), 3.48 (s, 2H), 3.44 (d, *J* = 4.6 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 170.4, 170.2, 139.8, 137.2, 134.6, 134.3, 134.2, 133.6, 133.5, 132.93, 132.90, 132.32, 132.26, 130.6, 129.8, 129.7, 129.4, 129.3, 129.1, 128.9, 128.8, 128.7, 128.3, 128.0, 127.9, 127.7, 127.6, 127.2, 121.4, 121.32, 121.30, 121.28, 101.5, 100.8, 100.4, 96.2, 53.7, 49.1, 44.4, 43.8, 43.6, 42.5; HRMS (TOF MS ESI$^+$) calculated for $C_{26}H_{22}N_2NaO_3S$ $[M+Na]^+$: 465.1243, found 465.1245; HPLC conditions for determination of enantiomeric excess of **3u**: Chiral AD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 20.2 min, t_{minor} = 33.9 min; HPLC conditions for determination of enantiomeric excess of **3u'**: Chiral AD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{minor} = 19.0 min, t_{major} = 22.6 min.

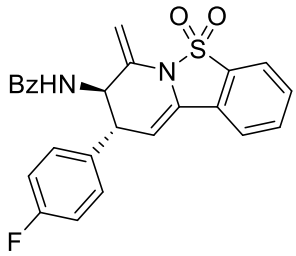


***N*-((8*R*,9*R*)-7-Methylene-5,5-dioxido-9-phenyl-8,9-dihydro-7*H*-benzo[4,5]isothiazolo[2,3-*a*]pyridin-8-yl)acetamide (3v)** 26.0 mg, 71% yield, 9:1 *dr*, 90% *ee*, $[\alpha]_D^{20}$ =

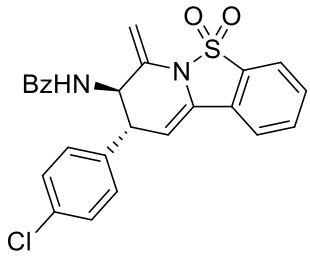
200^{o} (c = 0.05, DCM). Yellow solid, mp: 110.0-113.0 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.88 (d, *J* = 7.8 Hz, 1H), 7.75 (d, *J* = 7.8 Hz, 1H), 7.71 (t, *J* = 7.5 Hz, 1H), 7.64 (t, *J* = 7.4 Hz, 1H), 7.31 (t, *J* = 7.3 Hz, 2H), 7.26 – 7.22 (comp, 3H), 5.89 (d, *J* = 6.8 Hz, 1H), 5.84 (d, *J* = 5.9 Hz, 1H), 5.47 (d, *J* = 1.5 Hz, 1H), 4.78 (d, *J* = 1.3 Hz, 1H), 4.70 (dd, *J* = 7.3, 2.5 Hz, 1H), 3.95 (dd, *J* = 5.8, 2.9 Hz, 1H), 1.95 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 171.3, 139.9, 133.7, 132.5, 132.3, 130.7, 129.9, 128.9, 128.37, 128.36, 127.7, 121.46, 121.45, 102.9, 100.7, 54.3, 44.6, 23.5; HRMS (TOF MS ESI^{+}) calculated for $C_{20}H_{18}N_2NaO_3S$ $[M+Na]^{+}$: 389.0930, found 389.0937; HPLC conditions for determination of enantiomeric excess: Chiral AD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 6.7 min, t_{minor} = 7.8 min.



***N*-((8*R*,9*R*)-7-Methylene-5,5-dioxido-9-phenyl-8,9-dihydro-7*H*-benzo[4,5]isothiazolo[2,3-*a*]pyridin-8-yl)pivalamide (3w)** 36.4 mg, 89% yield, 8:1 *dr*, 90% *ee*, $[\alpha]_D^{20}$ = 90^{o} (c = 0.05, DCM). Yellow solid, mp: 111.0-113.0 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.83 (d, *J* = 7.7 Hz, 1H), 7.71 – 7.65 (m, 2H), 7.63 – 7.56 (m, 1H), 7.35 – 7.29 (comp, 3H), 7.17 – 7.09 (m, 2H), 5.90 (d, *J* = 6.1 Hz, 1H), 5.49 (s, 1H), 5.21 – 5.18 (m, 1H), 4.65 (s, 1H), 3.86 (t, *J* = 5.4 Hz, 1H), 1.08 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 177.5, 137.5, 134.7, 133.6, 132.2, 130.5, 129.7, 129.2, 128.8, 128.1, 127.9, 121.3, 121.2, 100.9, 96.1, 48.6, 42.6, 38.9, 27.4; HRMS (TOF MS ESI^{+}) calculated for $C_{23}H_{24}N_2NaO_3S$ $[M+Na]^{+}$: 431.1400, found 431.1406; HPLC conditions for determination of enantiomeric excess: Chiral AD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 5.9 min, t_{minor} = 7.0 min.

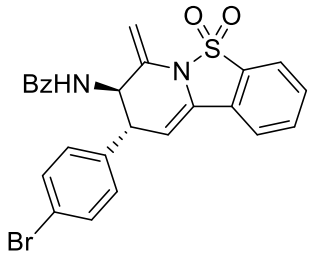


***N*-((8*R*,9*R*)-9-(4-Fluorophenyl)-7-methylene-5,5-dioxido-8,9-dihydro-7*H*-benzo[4,5]isothiazolo[2,3-*a*]pyridin-8-yl)benzamide (6a)** 41.1 mg, 92% yield, 11:1 *dr*, 98% *ee*, $[\alpha]_D^{20}$ = 180° (c = 0.05, DCM). Yellow solid, mp: 121.0-123.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.90 (d, *J* = 7.8 Hz, 1H), 7.80 – 7.69 (comp, 4H), 7.65 (t, *J* = 7.5 Hz, 1H), 7.47 (t, *J* = 7.4 Hz, 1H), 7.38 (t, *J* = 7.6 Hz, 2H), 7.29 (dd, *J* = 8.4, 5.4 Hz, 2H), 7.02 (t, *J* = 8.6 Hz, 2H), 6.58 (d, *J* = 6.6 Hz, 1H), 5.85 (d, *J* = 5.9 Hz, 1H), 5.58 (d, *J* = 1.4 Hz, 1H), 4.90 (d, *J* = 1.3 Hz, 1H), 4.82 (dd, *J* = 6.6, 2.3 Hz, 1H), 4.17 (dd, *J* = 5.8, 2.8 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 166.9, 162.3 (d, *J* = 246.3 Hz), 135.7 (d, *J* = 3.2 Hz), 133.82, 133.77, 132.4, 132.3, 132.0, 130.8, 130.2, 130.1, 130.0, 128.8, 128.5, 127.1, 121.6 (d, *J* = 6.4 Hz), 115.8 (d, *J* = 21.4 Hz), 104.9, 100.9, 55.0, 43.8; ^{19}F NMR (471 MHz, $CDCl_3$) (δ, ppm) -114.73; HRMS (TOF MS ESI$^+$) calculated for $C_{25}H_{19}FN_2NaO_3S$ $[M+Na]^+$: 469.0993, found 469.1003; HPLC conditions for determination of enantiomeric excess: Chiral OD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 11.2 min, t_{minor} = 14.0 min.

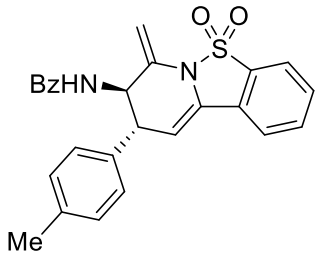


***N*-((8*R*,9*R*)-9-(4-Chlorophenyl)-7-methylene-5,5-dioxido-8,9-dihydro-7*H*-benzo[4,5]isothiazolo[2,3-*a*]pyridin-8-yl)benzamide (6b)** 41.6 mg, 90% yield, 10:1 *dr*, 98% *ee*, $[\alpha]_D^{20}$ = 198° (c = 0.05, DCM). Yellow solid, mp: 120.0-122.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.90 (d, *J* = 7.7 Hz, 1H), 7.78 – 7.64 (comp, 5H), 7.47 (t, *J* =

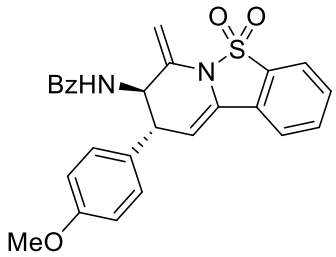
7.2 Hz, 1H), 7.38 (t, *J* = 7.5 Hz, 2H), 7.33 – 7.23 (comp, 4H), 6.58 (d, *J* = 6.2 Hz, 1H), 5.83 (d, *J* = 5.8 Hz, 1H), 5.58 (s, 1H), 4.90 (s, 1H), 4.81 (d, *J* = 4.5 Hz, 1H), 4.17 (d, *J* = 3.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 166.9, 138.5, 133.81, 133.75, 133.6, 132.34, 132.25, 132.0, 130.8, 130.4, 129.8, 129.1, 128.8, 128.5, 127.2, 121.6, 121.5, 105.1, 100.5, 54.9, 43.9; HRMS (TOF MS ESI$^+$) calculated for $C_{25}H_{19}ClN_2NaO_3S$ $[M+Na]^+$: 485.0697, found 485.0692; HPLC conditions for determination of enantiomeric excess: Chiral OD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 15.7 min, t_{minor} = 21.3 min.



***N*-((8*R*,9*R*)-9-(4-Bromophenyl)-7-methylene-5,5-dioxido-8,9-dihydro-7*H*-benzo[4, 5]isothiazolo[2,3-*a*]pyridin-8-yl)benzamide (6c)** 47.1 mg, 93% yield, 10:1 *dr*, 99% *ee*, $[\alpha]_D^{20}$ = 140^o (c = 0.05, DCM). Yellow solid, mp: 119.0-121.0 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.91 (d, *J* = 7.8 Hz, 1H), 7.80 – 7.69 (comp, 4H), 7.66 (t, *J* = 7.4 Hz, 1H), 7.50 – 7.45 (comp, 3H), 7.39 (t, *J* = 7.5 Hz, 2H), 7.21 (d, *J* = 8.1 Hz, 2H), 6.56 (d, *J* = 6.2 Hz, 1H), 5.83 (d, *J* = 5.9 Hz, 1H), 5.59 (s, 1H), 4.91 (s, 1H), 4.80 (d, *J* = 5.0 Hz, 1H), 4.17 (d, *J* = 3.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 166.9, 139.0, 133.8, 133.7, 132.3, 132.1, 132.04, 132.00, 130.8, 130.4, 130.2, 128.8, 128.5, 127.2, 121.8, 121.61, 121.57, 105.4, 100.4, 54.9, 43.9; HRMS (TOF MS ESI$^+$) calculated for $C_{25}H_{19}BrN_2NaO_3S$ $[M+Na]^+$: 529.0192, found 529.0190; HPLC conditions for determination of enantiomeric excess: Chiral OD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 23.7 min, t_{minor} = 26.2 min.

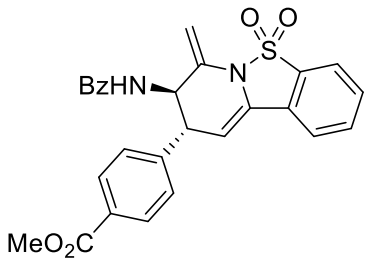


***N*-((8*R*,9*R*)-7-Methylene-5,5-dioxido-9-(*p*-tolyl)-8,9-dihydro-7*H*-benzo[4,5]isothiazolo[2,3-*a*]pyridin-8-yl)benzamide (6d)** 40.3 mg, 91% yield, 10:1 *dr*, 94% *ee*, $[\alpha]_D^{20}$ = 230° (c = 0.05, DCM). Yellow solid, mp: 122.0-125.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.90 (d, *J* = 7.8 Hz, 1H), 7.76 – 7.70 (comp, 4H), 7.64 (t, *J* = 7.5 Hz, 1H), 7.46 (t, *J* = 7.3 Hz, 1H), 7.38 (t, *J* = 7.5 Hz, 2H), 7.21 (d, *J* = 7.8 Hz, 2H), 7.15 (d, *J* = 7.8 Hz, 2H), 6.55 (d, *J* = 6.6 Hz, 1H), 5.86 (d, *J* = 5.8 Hz, 1H), 5.57 (s, 1H), 4.90 (s, 1H), 4.88 – 4.84 (m, 1H), 4.13 (dd, *J* = 5.4, 2.7 Hz, 1H), 2.33 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 166.8, 137.4, 136.9, 133.9, 133.7, 132.7, 132.3, 131.9, 130.6, 129.9, 129.6, 128.7, 128.6, 128.3, 127.2, 121.53, 121.48, 104.4, 101.4, 54.9, 44.2, 21.2; HRMS (TOF MS ESI$^+$) calculated for $C_{26}H_{22}N_2NaO_3S$ $[M+Na]^+$: 465.1243, found 465.1253; HPLC conditions for determination of enantiomeric excess: Chiral AD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{minor} = 20.2 min, t_{major} = 22.4 min.

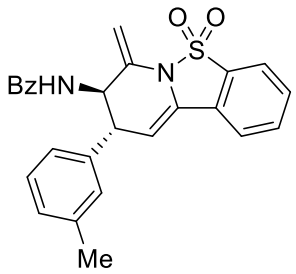


***N*-((8*R*,9*R*)-9-(4-Methoxyphenyl)-7-methylene-5,5-dioxido-8,9-dihydro-7*H*-benzo[4,5]isothiazolo[2,3-*a*]pyridin-8-yl)benzamide (6e)** 39.9 mg, 87% yield, >20:1 *dr*, 91% *ee*, $[\alpha]_D^{20}$ = 180° (c = 0.05, DCM). Yellow solid, mp: 118.0-120.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.90 (d, *J* = 3.6 Hz, 1H), 7.78 – 7.64 (comp, 5H), 7.53 – 7.34 (comp, 3H), 7.27 – 7.25 (m, 2H), 6.89 – 6.87 (m, 2H), 6.54 (s, 1H), 5.86 (d, *J* = 5.8 Hz, 1H), 5.58 (s, 1H), 4.90 (s, 1H), 4.85 – 4.83 (m, 1H), 4.12 (dd, *J* = 5.4, 2.7 Hz,

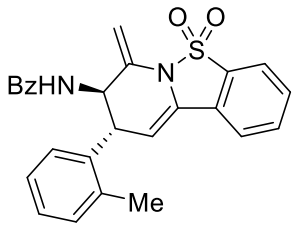
1H), 3.79 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 166.9, 159.2, 133.9, 133.7, 132.6, 132.3, 131.94, 131.91, 130.6, 129.8, 129.5, 128.8, 128.6, 127.2, 121.54, 121.51, 114.3, 104.6, 101.5, 55.4, 55.0, 43.8; HRMS (TOF MS ESI$^+$) calculated for $C_{26}H_{22}N_2NaO_4S$ $[M+Na]^+$: 481.1192, found 481.1202; HPLC conditions for determination of enantiomeric excess: Chiral OD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{minor} = 19.9 min, t_{major} = 26.8 min.



Methyl 4-((8*R*,9*R*)-8-Benzamido-7-methylene-5,5-dioxido-8,9-dihydro-7*H*-benzo [4,5]isothiazolo[2,3-*a*]pyridin-9-yl)benzoate (6f) 41.3 mg, 85% yield, 15:1 *dr*, 98% *ee*, $[\alpha]_D^{20}$ = 184^o (c = 0.05, DCM). Yellow solid, mp: 121.0-123.0 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 8.01 (d, *J* = 8.0 Hz, 2H), 7.91 (d, *J* = 7.8 Hz, 1H), 7.78 (d, *J* = 7.7 Hz, 1H), 7.76 – 7.70 (comp, 3H), 7.67 (t, *J* = 7.5 Hz, 1H), 7.47 (t, *J* = 7.2 Hz, 1H), 7.45 – 7.36 (comp, 4H), 6.62 (d, *J* = 6.3 Hz, 1H), 5.85 (d, *J* = 5.8 Hz, 1H), 5.58 (s, 1H), 4.89 (s, 1H), 4.85 (d, *J* = 4.4 Hz, 1H), 4.27 (d, *J* = 2.9 Hz, 1H), 3.91 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 166.9, 145.1, 133.8, 133.7, 132.3, 132.2, 132.0, 130.9, 130.5, 130.2, 129.6, 128.8, 128.5, 128.4, 127.2, 121.64, 121.55, 105.1, 100.2, 54.7, 52.3, 44.4; HRMS (TOF MS ESI$^+$) calculated for $C_{27}H_{23}N_2O_5S$ $[M+H]^+$: 487.1322, found 487.1334; HPLC conditions for determination of enantiomeric excess: Chiral AD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 23.2 min, t_{minor} = 40.9 min.

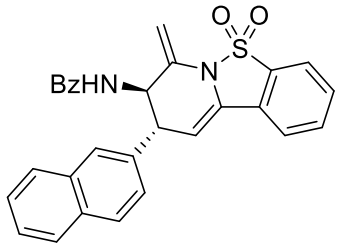


***N*-((8*R*,9*R*)-7-Methylene-5,5-dioxido-9-(*m*-tolyl)-8,9-dihydro-7*H*-benzo[4,5]isothiazolo[2,3-*a*]pyridin-8-yl)benzamide (6g)** 38.5 mg, 87% yield, 10:1 *dr*, 96% *ee*, $[\alpha]_D^{20}$ = 152° (c = 0.05, DCM). Yellow solid, mp: 117.0-119.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.90 (d, *J* = 7.7 Hz, 1H), 7.77 – 7.70 (comp, 4H), 7.64 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.3 Hz, 1H), 7.38 (t, *J* = 7.5 Hz, 2H), 7.22 (t, *J* = 7.6 Hz, 1H), 7.16 (s, 1H), 7.09 (d, *J* = 7.4 Hz, 2H), 6.57 (d, *J* = 6.6 Hz, 1H), 5.86 (d, *J* = 5.8 Hz, 1H), 5.58 (s, 1H), 4.90 (s, 1H), 4.87 (dd, *J* = 6.6, 2.2 Hz, 1H), 4.13 (dd, *J* = 5.6, 2.7 Hz, 1H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 166.9, 139.9, 138.6, 133.9, 133.7, 132.6, 132.3, 131.9, 130.6, 130.0, 129.2, 128.74, 128.72, 128.6, 128.5, 127.2, 125.4, 121.6, 121.5, 104.6, 101.3, 54.9, 44.5, 21.5; HRMS (TOF MS ESI$^+$) calculated for $C_{26}H_{22}N_2NaO_3S$ $[M+Na]^+$: 465.1243, found 465.1262; HPLC conditions for determination of enantiomeric excess: Chiral AD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{minor} = 13.5 min, t_{major} = 17.9 min.

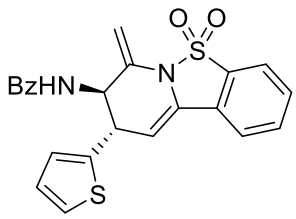


***N*-((8*R*,9*R*)-7-Methylene-5,5-dioxido-9-(*o*-tolyl)-8,9-dihydro-7*H*-benzo[4,5]isothiazolo[2,3-*a*]pyridin-8-yl)benzamide (6h)** 38.9 mg, 88% yield, 10:1 *dr*, 97% *ee*, $[\alpha]_D^{20}$ = 146° (c = 0.05, DCM). Yellow solid, mp: 115.0-118.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.94 (d, *J* = 7.7 Hz, 1H), 7.80 – 7.73 (comp, 4H), 7.68 (t, *J* = 7.3 Hz, 1H), 7.49 (t, *J* = 7.3 Hz, 1H), 7.41 (t, *J* = 7.5 Hz, 2H), 7.28 (d, *J* = 6.1 Hz, 1H), 7.21 (t, *J* = 7.2 Hz, 1H), 7.15 (t, *J* = 7.3 Hz, 1H), 7.04 (d, *J* = 7.5 Hz, 1H), 6.59 (d, *J* = 6.4 Hz, 1H), 5.88 (d, *J* = 6.1 Hz, 1H), 5.60 (s, 1H), 4.90 (s, 1H), 4.82 (d, *J* = 6.2 Hz, 1H), 4.41

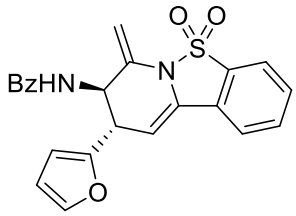
(dd, J = 6.0, 2.0 Hz, 1H), 2.72 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 166.8, 137.5, 136.8, 134.0, 133.8, 132.6, 132.3, 131.9, 131.0, 130.6, 130.3, 128.72, 128.68, 128.6, 127.7, 127.2, 126.1, 121.6, 121.5, 105.2, 101.8, 53.4, 41.1, 19.8; HRMS (TOF MS ESI$^+$) calculated for $C_{26}H_{22}N_2NaO_3S$ $[M+Na]^+$: 465.1243, found 465.1263; HPLC conditions for determination of enantiomeric excess: Chiral AD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{minor} = 9.7 min, t_{major} = 19.0 min.



***N*-((8*R*,9*R*)-7-Methylene-9-(naphthalen-2-yl)-5,5-dioxido-8,9-dihydro-7*H*-benzo[4,5]isothiazolo[2,3-*a*]pyridin-8-yl)benzamide (6i)** 39.7 mg, 83% yield, >20:1 *dr*, 95% *ee*, $[\alpha]_D^{20}$ = 72° (c = 0.05, DCM). Yellow solid, mp: 116.0-118.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 8.92 (d, J = 8.5 Hz, 1H), 7.82 (t, J = 8.7 Hz, 2H), 7.76 – 7.61 (comp, 6H), 7.57 (t, J = 7.6 Hz, 1H), 7.47 (t, J = 7.4 Hz, 1H), 7.38 (t, J = 7.2 Hz, 1H), 7.33 – 7.27 (m, 2H), 7.18 – 7.09 (m, 1H), 6.57 (d, J = 5.4 Hz, 1H), 5.85 (d, J = 6.1 Hz, 1H), 5.43 (s, 1H), 5.04 (d, J = 4.5 Hz, 1H), 4.89 (d, J = 5.0 Hz, 1H), 4.65 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 167.3, 135.0, 134.3, 133.9, 133.8, 132.6, 132.2, 132.0, 131.6, 130.8, 130.7, 129.0, 128.8, 128.7, 128.6, 127.3, 126.6, 126.2, 125.2, 124.1, 121.7, 121.6, 106.1, 101.7, 54.2, 40.1; HRMS (TOF MS ESI$^+$) calculated for $C_{29}H_{22}N_2NaO_3S$ $[M+Na]^+$: 501.1243, found 501.1255; HPLC conditions for determination of enantiomeric excess: Chiral IA, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 10.6 min, t_{minor} = 12.5 min.

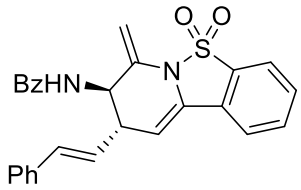


***N*-((8*R*,9*S*)-7-Methylene-5,5-dioxido-9-(thiophen-2-yl)-8,9-dihydro-7*H*-benzo[4,5] isothiazolo[2,3-*a*]pyridin-8-yl)benzamide (6j)** 40.0 mg, 92% yield, 8:1 *dr*, 92% *ee*, $[\alpha]_D^{20}$ = 86° (c = 0.05, DCM). Yellow solid, mp: 112.0-115.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.87 (d, *J* = 7.7 Hz, 1H), 7.78 – 7.67 (comp, 4H), 7.63 (t, *J* = 7.5 Hz, 1H), 7.46 (t, *J* = 7.3 Hz, 1H), 7.40 – 7.35 (comp, 3H), 6.50 (d, *J* = 7.0 Hz, 1H), 6.31 (dd, *J* = 2.9, 1.9 Hz, 1H), 6.16 (d, *J* = 3.1 Hz, 1H), 5.84 (d, *J* = 5.7 Hz, 1H), 5.57 (d, *J* = 1.6 Hz, 1H), 5.12 (dd, *J* = 7.1, 3.4 Hz, 1H), 5.03 (d, *J* = 1.3 Hz, 1H), 4.21 (dd, *J* = 5.5, 3.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 166.9, 152.5, 142.6, 133.9, 133.7, 133.2, 132.3, 131.9, 130.8, 130.3, 128.7, 128.4, 127.2, 121.6, 121.5, 110.5, 107.6, 103.6, 98.3, 51.9, 38.2; HRMS (TOF MS ESI$^+$) calculated for $C_{23}H_{18}N_2NaO_3S_2$ $[M+Na]^+$: 457.0651, found 457.0666; HPLC conditions for determination of enantiomeric excess: Chiral OD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 14.3 min, t_{minor} = 17.7 min.



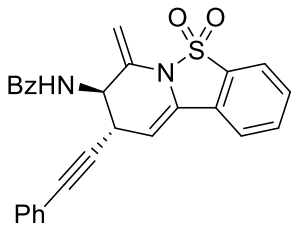
***N*-((8*R*,9*S*)-9-(Furan-2-yl)-7-methylene-5,5-dioxido-8,9-dihydro-7*H*-benzo[4,5]iso thiazolo[2,3-*a*]pyridin-8-yl)benzamide (6k)** Combined in 89% yield, 37.2 mg, 4:1 *dr*, 94(48)% *ee*, $[\alpha]_D^{20}$ = 160° (c = 0.05, DCM). Yellow solid, mp: 113.0-115.0 °C; composite NMR signals of **6k** and **6k'** ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.87 – 7.64 (comp, 7.4H), 7.46 – 7.22 (comp, 5.4H), 6.99 – 6.97 (comp, 2.4H), 6.59 (s, 1H), 5.95 – 5.90 (comp, 1.2H), 5.65 – 5.60 (comp, 1.2H), 5.41 (s, 0.2H), 5.28 (s, 0.2H), 4.98 (d, *J* = 18.5 Hz, 2H), 4.85 (s, 0.2H), 4.40 (s, 1H), 4.27 (s, 0.2H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 166.8, 166.7, 143.0, 140.1, 134.0, 133.8, 133.7, 133.6, 132.5,

132.4, 132.2, 132.0, 131.9, 130.72, 130.70, 129.7, 129.6, 128.8, 128.7, 128.3, 127.7, 127.5, 127.2, 127.1, 127.0, 125.9, 125.7, 125.07, 125.05, 121.54, 121.53, 121.37, 121.35, 104.6, 100.8, 100.7, 96.9, 54.8, 49.6, 39.3, 38.1; HRMS (TOF MS ESI$^+$) calculated for $C_{23}H_{18}N_2NaO_4S$ $[M+Na]^+$: 441.0879, found 441.0886; HPLC conditions for determination of enantiomeric excess of **6k**: Chiral IA, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 17.1 min, t_{minor} = 21.6 min; HPLC conditions for determination of enantiomeric excess of **6k'**: Chiral IA, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{minor} = 19.4 min, t_{major} = 31.1 min.

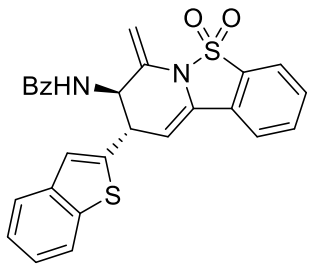


***N*-((8*R*,9*S*)-7-Methylene-5,5-dioxido-9-((*E*)-styryl)-8,9-dihydro-7*H*-benzo[4,5]isothiazolo[2,3-*a*]pyridin-8-yl)benzamide (6l)** Combined in 65% yield, 29.5 mg, 2:1 *dr*, 90(34)% *ee*, $[\alpha]_D^{20}$ = 141° (c = 0.05, DCM). Yellow solid, mp: 117.0-119.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.88 (d, *J* = 7.8 Hz, 1H), 7.81 – 7.67 (comp, 4H), 7.63 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.2 Hz, 1H), 7.40 – 7.34 (comp, 4H), 7.30 (t, *J* = 7.5 Hz, 2H), 7.26 – 7.23 (m, 1H), 6.55 (d, *J* = 15.8 Hz, 1H), 6.46 (d, *J* = 7.0 Hz, 1H), 6.13 (dd, *J* = 15.8, 7.9 Hz, 1H), 5.78 (d, *J* = 5.9 Hz, 1H), 5.63 (s, 1H), 5.11 (s, 1H), 4.90 (dd, *J* = 7.1, 2.5 Hz, 1H), 3.69 (t, *J* = 8.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 166.9, 136.7, 134.0, 133.7, 133.3, 133.1, 132.2, 131.9, 130.6, 129.5, 128.8, 128.7, 128.5, 128.0, 127.5, 127.2, 126.6, 121.52, 121.49, 103.9, 100.7, 52.5, 41.9; HRMS (TOF MS ESI$^+$) calculated for $C_{27}H_{22}N_2NaO_3S$ $[M+Na]^+$: 477.1243, found 477.1245; HPLC conditions for determination of enantiomeric excess: Chiral AD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{minor} = 19.5 min, t_{major} = 22.8 min; NMR signals of **6l'** ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.86 (d, *J* = 7.8 Hz, 1H), 7.75 – 7.68 (comp, 4H), 7.65 – 7.59 (m, 1H), 7.52 – 7.47 (m, 1H), 7.43 – 7.35 (comp, 4H), 7.35 – 7.30 (m, 2H), 7.28 (d, *J* = 7.0 Hz, 1H), 6.62 (d, *J* = 15.8 Hz,

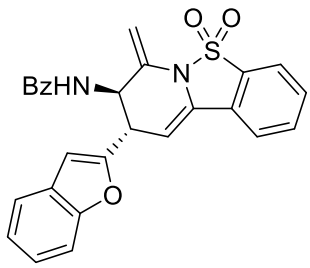
1H), 6.26 (d, *J* = 9.4 Hz, 1H), 6.07 (dd, *J* = 15.7, 9.1 Hz, 1H), 5.81 (d, *J* = 5.9 Hz, 1H), 5.55 (s, 1H), 5.38 – 5.25 (m, 1H), 4.95 (s, 1H), 3.62 – 3.47 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 166.9, 136.2, 134.9, 134.8, 134.1, 133.6, 132.4, 132.1, 130.6, 129.6, 128.90, 128.88, 128.4, 128.0, 127.1, 126.7, 125.1, 121.5, 121.4, 100.2, 96.6, 49.2, 41.3; HRMS (TOF MS ESI$^+$) calculated for $C_{27}H_{22}N_2NaO_3S$ $[M+Na]^+$: 477.1243, found 477.1246; HPLC conditions for determination of enantiomeric excess: Chiral AD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{minor} = 15.2 min, t_{major} = 25.3 min.



***N*-((8*R*,9*R*)-7-Methylene-5,5-dioxido-9-(phenylethynyl)-8,9-dihydro-7*H*-benzo[4, 5]isothiazolo[2,3-*a*]pyridin-8-yl)benzamide (6m)** 36.2 mg, 80% yield, >20:1 *dr*, 93% *ee*, $[\alpha]_D^{20}$ = 300º (c = 0.05, DCM). Yellow solid, mp: 113.0-115.0 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.85 (d, *J* = 7.3 Hz, 1H), 7.75 – 7.60 (comp, 5H), 7.51 – 7.11 (comp, 8H), 6.53 (d, *J* = 5.6 Hz, 1H), 5.80 (d, *J* = 5.1 Hz, 1H), 5.70 (s, 1H), 5.23 (s, 1H), 5.10 (s, 1H), 4.01 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 167.0, 133.7, 132.9, 132.2, 132.0, 131.9, 130.8, 129.6, 128.8, 128.5, 128.4, 127.21, 127.20, 122.8, 121.6, 121.4, 104.1, 98.2, 86.3, 84.6, 52.3, 31.1; HRMS (TOF MS ESI$^+$) calculated for $C_{27}H_{20}N_2NaO_3S$ $[M+Na]^+$: 475.1087, found 475.1078; HPLC conditions for determination of enantiomeric excess: Chiral OD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 18.8 min, t_{minor} = 25.5 min.



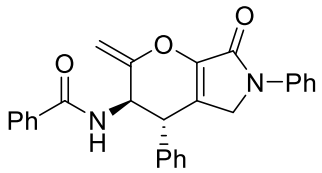
***N*-((8*R*,9*S*)-9-(Benzo[*b*]thiophen-2-yl)-7-methylene-5,5-dioxido-8,9-dihydro-7*H*-benzo[4,5]isothiazolo[2,3-*a*]pyridin-8-yl)benzamide (6n)** Combined in 84% yield, 40.7 mg, 7:1 *dr*, 99(55)% *ee*, $[\alpha]_D^{20}$ = 174° (c = 0.05, DCM). Yellow solid, mp: 118.0-120.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.91 (d, *J* = 7.8 Hz, 1H), 7.78 (d, *J* = 5.5 Hz, 2H), 7.74 – 7.65 (comp, 5H), 7.47 (t, *J* = 7.3 Hz, 1H), 7.39 (t, *J* = 7.6 Hz, 2H), 7.35 – 7.27 (m, 2H), 7.20 (s, 1H), 6.57 (d, *J* = 6.5 Hz, 1H), 5.96 (d, *J* = 6.0 Hz, 1H), 5.63 (s, 1H), 5.07 (dd, *J* = 6.3, 2.0 Hz, 1H), 5.03 (s, 1H), 4.49 (dd, *J* = 5.7, 2.6 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 166.9, 143.8, 139.8, 133.8, 133.7, 132.4, 132.3, 132.0, 130.9, 130.2, 128.8, 128.4, 127.2, 124.5, 124.4, 123.6, 122.6, 122.5, 121.7, 121.6, 105.6, 100.2, 54.7, 40.1; HRMS (TOF MS ESI$^+$) calculated for $C_{27}H_{20}N_2NaO_3S_2$ $[M+Na]^+$: 507.0808, found 507.0810; HPLC conditions for determination of enantiomeric excess: Chiral OD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 18.5 min, t_{minor} = 33.6 min; NMR signals of **6n'** ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.90 (d, *J* = 7.8 Hz, 1H), 7.79 – 7.70 (comp, 6H), 7.66 (t, *J* = 7.5 Hz, 1H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.41 (t, *J* = 7.7 Hz, 2H), 7.37 – 7.31 (m, 2H), 7.16 (s, 1H), 6.14 (d, *J* = 9.7 Hz, 1H), 6.02 (d, *J* = 6.2 Hz, 1H), 5.58 (d, *J* = 2.1 Hz, 1H), 5.56 – 5.44 (m, 1H), 4.99 – 4.79 (m, 1H), 4.34 (t, *J* = 5.9 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 166.9, 141.1, 139.9, 139.7, 134.1, 133.8, 133.7, 132.6, 132.2, 130.9, 130.1, 128.9, 127.8, 127.2, 124.8, 124.7, 123.9, 123.7, 122.5, 121.5, 100.2, 97.0, 49.5, 39.0; HRMS (TOF MS ESI$^+$) calculated for $C_{27}H_{20}N_2NaO_3S_2$ $[M+Na]^+$: 507.0808, found 507.0807; HPLC conditions for determination of enantiomeric excess: Chiral OD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 21.5 min, t_{minor} = 26.7 min.



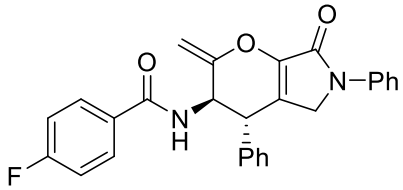
***N*-((8*R*,9*S*)-9-(Benzofuran-2-yl)-7-methylene-5,5-dioxido-8,9-dihydro-7*H*-benzo[4,5]isothiazolo[2,3-*a*]pyridin-8-yl)benzamide (6o)** 40.3 mg, 86% yield, 8:1 *dr*, 94% *ee*, $[\alpha]_D^{20}$ = 172° (c = 0.05, DCM). Yellow solid, mp: 119.0-121.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 8.04 – 7.56 (comp, 7H), 7.50 – 7.35 (comp, 5H), 7.25 – 7.19 (m, 1H), 6.55 – 6.54 (m, 2H), 5.92 – 5.90 (m, 1H), 5.59 (s, 1H), 5.28 (s, 1H), 5.04 (s, 1H), 4.38 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 167.0, 155.5, 155.2, 133.8, 132.8, 132.3, 132.0, 130.9, 130.7, 128.8, 128.31, 128.29, 127.2, 124.3, 122.9, 121.7, 121.5, 121.0, 111.4, 104.7, 104.4, 97.6, 51.6, 38.6; HRMS (TOF MS ESI$^+$) calculated for $C_{27}H_{20}N_2NaO_4S$ $[M+Na]^+$: 491.1036, found 491.1048; HPLC conditions for determination of enantiomeric excess: Chiral OD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 15.3 min, t_{minor} = 22.0 min.

General Procedure for the Synthesis of Dihydropyrans 8

To a 10-mL oven-dried vial containing a magnetic stirring bar, (*E*)-dioxopyrrolidines **7** (0.1 mmol), **4c** (6.31 mg, 10 mol%), and $Me_3(OMe)$*t*BuXPhosAuNTf$_2$ (5.0 mg, 5.0 mol%) in a mixed solvent of DCE and hexane (2.0 mL, 9:1), was added *N*-propargyl amides **1** (0.20 mmol, 2.0 equiv.) in the same solvent (1.0 mL, DCE : hexane = 9:1) at -20 °C under argon atmosphere. The resulting reaction mixture was stirred for 72 hours under these conditions. When the reaction was completed (monitored by TLC), the solvent was evaporated *in vacuo* and the residues was purified by flash column chromatography on silica gel (hexanes/DCM = 1:10 to 1:20) to afford the pure products **8** in good to high yields and stereoselectivity.

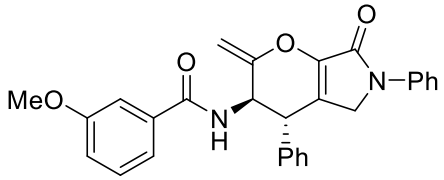


***N*-((3*R*,4*S*)-2-Methylene-7-oxo-4,6-diphenyl-2,3,4,5,6,7-hexahydropyrano[2,3-*c*]pyrrol-3-yl)benzamide (8a)** 36.3 mg, 86% yield, 8:1 *dr*, 90% *ee*. Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.89 – 7.82 (m, 2H), 7.62 – 7.57 (m, 2H), 7.53 – 7.49 (m, 1H), 7.45 – 7.41 (m, 2H), 7.39 – 7.35 (m, 2H), 7.32 – 7.28 (comp, 4H), 7.21 – 7.13 (m, 1H), 7.12 – 7.07 (m, 1H), 5.02 (d, *J* = 6.9 Hz, 1H), 4.92 (d, *J* = 6.9 Hz, 1H), 4.54 (s, 1H), 4.25 – 4.10 (comp, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 167.2, 162.8, 150.7, 144.29, 139.0, 133.7, 132.1, 129.3, 129.1, 128.7, 128.2, 128.1, 127.5, 124.7, 121.5, 118.7, 118.6, 100.3, 53.9, 49.0, 44.7; HRMS (TOF MS ESI$^+$) calculated for $C_{27}H_{22}N_2NaO_3$ $[M+Na]^+$: 445.1523, found 445.1525; HPLC conditions for determination of enantiomeric excess: Chiral OD-H, λ = 254 nm, hexane : 2-propanol = 80:20, flow rate = 1.0 mL/min, t_{minor} = 10.1 min, t_{major} = 15.7 min.

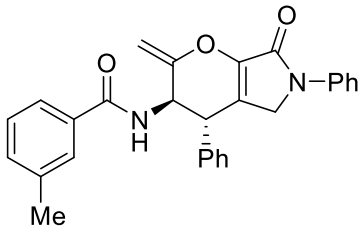


4-Fluoro-*N*-((3*R*,4*S*)-2-methylene-7-oxo-4,6-diphenyl-2,3,4,5,6,7-hexahydropyrano[2,3-*c*]pyrrol-3-yl)benzamide (8b) 34.3 mg, 78% yield, 10:1 *dr*, 88% *ee*. Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.99 – 7.84 (m, 2H), 7.70 (d, *J* = 6.3 Hz, 1H), 7.38 (d, *J* = 8.0 Hz, 2H), 7.27 – 7.25 (m, 2H), 7.23 – 7.18 (m, 1H), 7.17 – 7.15 (m, 2H), 7.12 (t, *J* = 7.7 Hz, 2H), 7.02 – 6.86 (comp, 3H), 4.84 (d, *J* = 6.7 Hz, 1H), 4.79 (s, 1H), 4.41 (s, 1H), 4.06 – 4.04 (comp, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 166.3, 165.0 (d, *J* = 252.1 Hz), 163.0, 150.7, 144.1, 139.0, 138.8, 130.2, 130.13, 130.08 (d, *J* = 3.1 Hz), 129.2, 129.1, 128.0, 124.7, 121.6, 118.6, 115.5 (d, *J* = 21.8 Hz), 100.1, 53.7, 49.2, 44.6; ^{19}F NMR (376 MHz, $CDCl_3$) (δ, ppm) -107.75; HRMS (TOF MS ESI$^+$) calculated for $C_{27}H_{21}FN_2NaO_3$ $[M+Na]^+$: 463.1428, found 463.1426; HPLC conditions for determination of enantiomeric excess: Chiral OD-H, λ = 254 nm,

hexane : 2-propanol = 80:20, flow rate = 1.0 mL/min, t_{minor} = 9.2 min, t_{major} = 14.2 min.

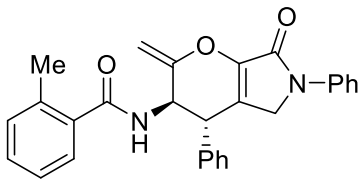


3-Methoxy-*N*-((3*R*,4*S*)-2-methylene-7-oxo-4,6-diphenyl-2,3,4,5,6,7-hexahydropyrano[2,3-*c*]pyrrol-3-yl)benzamide (8c) 38.4 mg, 85% yield, 11:1 *dr*, 90% *ee*. Yellow oil; ^{1}H NMR (500 MHz, DMSO) (δ, ppm) 8.92 (d, *J* = 7.8 Hz, 1H), 7.73 (d, *J* = 7.9 Hz, 2H), 7.38 – 7.33 (comp, 9H), 7.29 – 7.77 (m, 1H), 7.13 – 7.11 (m, 2H), 4.96 – 4.93 (m, 2H), 4.60 (s, 1H), 4.40 (d, *J* = 18.0 Hz, 1H), 4.17 (d, *J* = 6.9 Hz, 1H), 4.10 (d, *J* = 17.9 Hz, 1H), 3.79 (s, 3H); ^{13}C NMR (125 MHz, DMSO) (δ, ppm) 165.9, 162.0, 159.1, 154.0, 143.0, 139.3, 138.7, 135.3, 129.4, 129.0, 128.7, 128.3, 127.5, 123.8, 122.8, 119.7, 118.2, 117.1, 112.8, 95.4, 55.3, 52.1, 47.9, 43.2; HRMS (TOF MS ESI^{+}) calculated for $C_{28}H_{24}N_2NaO_4$ $[M+Na]^{+}$: 475.1628, found 475.1630; HPLC conditions for determination of enantiomeric excess: Chiral OD-H, λ = 254 nm, hexane : 2-propanol = 80:20, flow rate = 1.0 mL/min, t_{minor} = 14.3 min, t_{major} = 27.3 min.

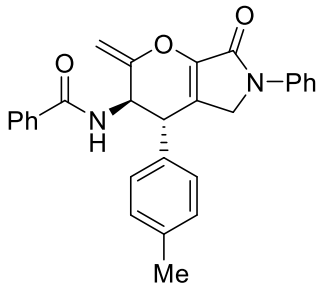


3-Methyl-*N*-((3*R*,4*S*)-2-methylene-7-oxo-4,6-diphenyl-2,3,4,5,6,7-hexahydropyrano[2,3-c]pyrrol-3-yl)benzamide (8d) 29.7 mg, 68% yield, 8:1 *dr*, 91% *ee*. Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.63 – 7.58 (m, 2H), 7.56 – 7.52 (m, 2H), 7.37 – 7.19 (comp, 9H), 7.14 – 7.00 (m, 2H), 4.96 (s, 1H), 4.87 (d, *J* = 6.4 Hz, 1H), 4.49 (s, 1H), 4.21 – 4.06 (comp, 3H), 2.32 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 167.4, 162.8, 150.7, 144.3, 139.0, 138.6, 133.6, 132.8, 129.3, 129.1, 128.6, 128.2, 128.04, 128.03, 124.6, 124.5, 121.5, 118.6, 100.3, 53.9, 49.0, 44.7, 21.4; HRMS (TOF MS ESI^{+}) calculated for $C_{28}H_{24}N_2NaO_3$ $[M+Na]^{+}$: 459.1679, found 459.1677; HPLC

conditions for determination of enantiomeric excess: Chiral OD-H, λ = 254 nm, hexane : 2-propanol = 80:20, flow rate = 1.0 mL/min, t_{minor} = 10.3 min, t_{major} = 14.3 min.

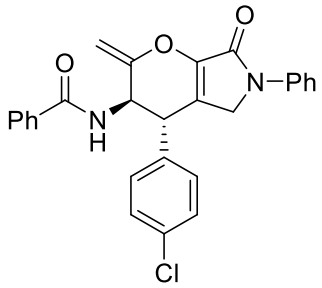


2-Methyl-*N*-((3*R*,4*S*)-2-methylene-7-oxo-4,6-diphenyl-2,3,4,5,6,7-hexahydropyrano[2,3-*c*]pyrrol-3-yl)benzamide (8e) 34.4 mg, 79% yield, 8:1 *dr*, 90% *ee*. Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.69 – 7.62 (m, 2H), 7.61 – 7.55 (m, 2H), 7.39 – 7.34 (m, 2H), 7.32 – 7.26 (comp, 6H), 7.17 – 7.13 (m, 1H), 7.12 – 7.06 (m, 1H), 5.01 (s, 1H), 4.92 (d, *J* = 6.4 Hz, 1H), 4.54 (s, 1H), 4.23 – 4.11 (comp, 3H), 2.37 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 167.4, 162.8, 150.7, 144.3, 139.00, 138.98, 138.6, 133.6, 132.8, 129.3, 129.1, 128.6, 128.2, 128.0, 124.6, 124.5, 121.5, 118.6, 100.3, 53.9, 49.0, 44.7, 21.4; HRMS (TOF MS ESI$^+$) calculated for $C_{28}H_{24}N_2NaO_3$ $[M+Na]^+$: 459.1679, found 459.1680; HPLC conditions for determination of enantiomeric excess: Chiral AD-H, λ = 254 nm, hexane : 2-propanol = 80:20, flow rate = 1.0 mL/min, t_{minor} = 10.7 min, t_{major} = 21.4 min.

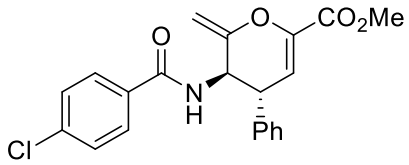


***N*-((3*R*,4*S*)-2-Methylene-7-oxo-6-phenyl-4-(*p*-tolyl)-2,3,4,5,6,7-hexahydropyrano[2,3-c]pyrrol-3-yl)benzamide (8f)** 32.7 mg, 75% yield, 11:1 *dr*, 91% *ee*. Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.83 (d, *J* = 7.6 Hz, 2H), 7.60 (d, *J* = 7.6 Hz, 2H), 7.51 (t, *J* = 7.3 Hz, 1H), 7.45 – 7.41 (m, 2H), 7.32 – 7.26 (m, 2H), 7.22 – 7.13 (comp, 4H), 7.10 (t, *J* = 7.4 Hz, 1H), 7.02 (d, *J* = 6.8 Hz, 1H), 5.02 (d, *J* = 1.7 Hz, 1H),

4.90 (dd, *J* = 6.9, 2.3 Hz, 1H), 4.55 (d, *J* = 1.7 Hz, 1H), 4.23 – 4.16 (m, 2H), 4.14 (d, *J* = 1.7 Hz, 1H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 167.2, 162.8, 150.9, 144.2, 139.1, 137.9, 135.9, 133.8, 132.0, 129.8, 129.3, 128.7, 128.0, 127.4, 124.6, 121.8, 118.6, 100.3, 54.0, 49.0, 44.3, 21.2; HRMS (TOF MS ESI$^+$) calculated for $C_{28}H_{24}N_2NaO_3$ $[M+Na]^+$: 459.1679, found 459.1682; HPLC conditions for determination of enantiomeric excess: Chiral OD-H, λ = 254 nm, hexane : 2-propanol = 80:20, flow rate = 1.0 mL/min, t_{minor} = 8.1 min, t_{major} = 13.2 min.



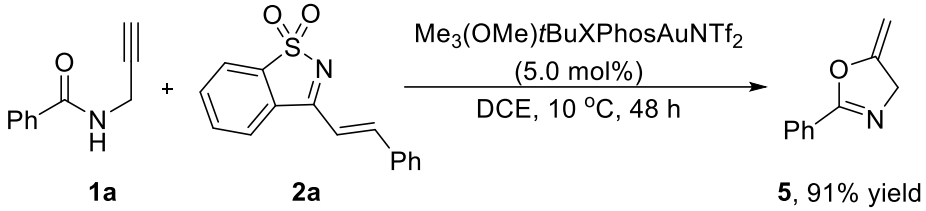
***N*-((3*R*,4*S*)-4-(4-Chlorophenyl)-2-methylene-7-oxo-6-phenyl-2,3,4,5,6,7-hexahydropyrano[2,3-*c*]pyrrol-3-yl)benzamide (8g)** 38.3 mg, 84% yield, 11:1 *dr*, 91% *ee*. Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.82 (d, *J* = 7.6 Hz, 2H), 7.52 – 7.42 (comp, 3H), 7.37 – 7.34 (comp, 3H), 7.27 (d, *J* = 8.2 Hz, 2H), 7.22 – 7.16 (comp, 4H), 7.03 (t, *J* = 7.4 Hz, 1H), 4.93 (s, 1H), 4.80 (d, *J* = 6.7 Hz, 1H), 4.48 (s, 1H), 4.11 – 4.08 (comp, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 167.4, 162.7, 150.3, 144.4, 138.8, 137.5, 134.0, 133.6, 132.1, 129.5, 129.27, 129.25, 128.7, 127.5, 124.8, 120.9, 118.7, 100.6, 53.8, 49.0, 44.0; HRMS (TOF MS ESI$^+$) calculated for $C_{21}H_{21}ClN_2NaO_3$ $[M+Na]^+$: 479.1133, found 479.1134; HPLC conditions for determination of enantiomeric excess: Chiral OD-H, λ = 254 nm, hexane : 2-propanol = 80:20, flow rate = 1.0 mL/min, t_{minor} = 9.8 min, t_{major} = 16.8 min.



Methyl (3*R*,4*R*)-3-(4-chlorobenzamido)-2-methylene-4-phenyl-3,4-dihydro-2*H*-

pyran-6-carboxylate (8h) 23.4 mg, 61% yield, 3:1 *dr*, 73(44)% *ee*. Yellow oil; major isomer: ^{1}H NMR (400 MHz, $CDCl_3$) (δ, ppm) 7.74 (d, *J* = 7.8 Hz, 2H), 7.54 – 7.50 (m, 1H), 7.45 – 7.42 (m, 2H), 7.36 – 7.32 (m, 2H), 7.22 (t, *J* = 7.0 Hz, 1H), 6.48 (d, *J* = 6.7 Hz, 1H), 6.32 (d, *J* = 5.2 Hz, 1H), 4.93 (s, 1H), 4.85 – 4.78 (m, 1H), 4.44 (s, 1H), 3.95 (s, 1H), 3.89 (s, 3H), 3.78 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) (δ, ppm) 167.0, 162.1, 150.7, 142.6, 139.6, 134.0, 132.0, 128.8, 128.8, 128.4, 127.8, 127.2, 111.9, 97.8, 52.8, 52.3, 44.2; minor isomer: ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.57 – 7.52 (m, 2H), 7.42 – 7.34 (comp, 5H), 7.20 – 7.17 (m, 2H), 6.37 (d, *J* = 6.1 Hz, 1H), 5.60 (d, *J* = 9.3 Hz, 1H), 5.45 – 5.33 (m, 1H), 4.99 – 4.91 (m, 1H), 4.36 (t, *J* = 2.0 Hz, 1H), 3.93 (t, *J* = 6.2 Hz, 1H), 3.88 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 166.6, 152.7, 142.4, 136.7, 133.9, 132.1, 129.5, 129.0, 128.8, 128.5, 128.4, 126.9, 111.6, 93.4, 52.8, 47.5, 41.9; HRMS (TOF MS ESI$^+$) calculated for $C_{21}H_{18}ClNNaO_4$ $[M+Na]^+$: 406.0817, found 406.0815; HPLC conditions for determination of enantiomeric excess of the major one: Chiral IA, λ = 254 nm, hexane : 2-propanol = 80:20, flow rate = 1.0 mL/min, t_{minor} = 10.0 min, t_{major} = 10.7 min; HPLC conditions for determination of enantiomeric excess of the minor one: Chiral IA, λ = 254 nm, hexane : 2-propanol = 80:20, flow rate = 1.0 mL/min, t_{major} = 10.8 min, t_{minor} = 14.2 min.

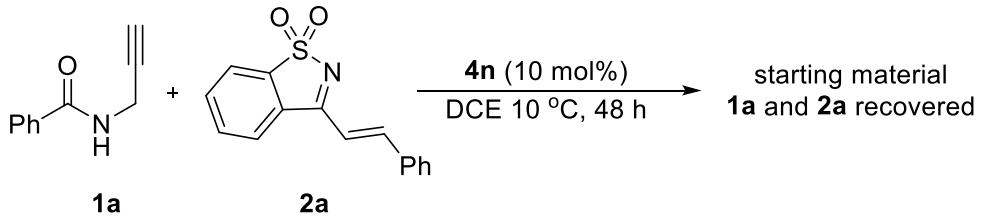
Control Experiments



1a **2a** **5**, 91% yield

To a 10-mL oven-dried vial with a magnetic stirring bar, **1a** (19.1 mg, 0.12 mmol) in 1.0 mL DCE was added to a solution of Me_3(OMe)*t*BuXPhosAuNTf$_2$ (5.0 mg, 5.0 mol%), and **2a** (26.9 mg, 0.1 mmol) in DCE (1.0 mL) under an argon atmosphere, and the reaction mixture was stirred at 10 °C for 48 h. When the reaction was completed (monitored by TLC), the crude reaction mixture was purified by flash column

chromatography on silica gel (Hexanes : EtOAc = 20:1 to 15:1) to give the pure product **5** as colorless oil, 91% yield[1a].



To a 10-mL oven-dried vial with a magnetic stirring bar, **1a** (19.1 mg, 0.12 mmol) in 1.0 mL DCE was added to a solution of **4n** (7.1 mg, 10 mol%) and **2a** (26.9 mg, 0.1 mmol) in DCE (1.0 mL) under an argon atmosphere, and the reaction mixture was stirred at 10 °C for 48 h. Then the reaction mixture was subjected to proton NMR analysis in $CDCl_3$ after the solvent was evaporated, and most of the starting material of **1a** and **2a** remained intact (see Figure S1 for detail).

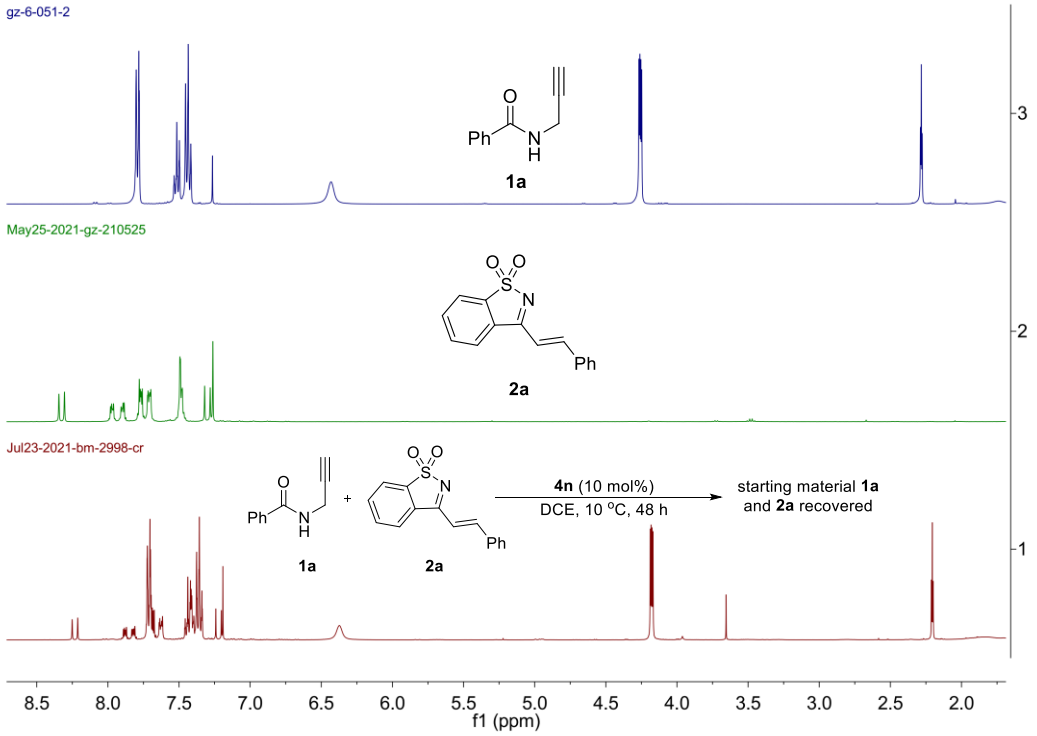
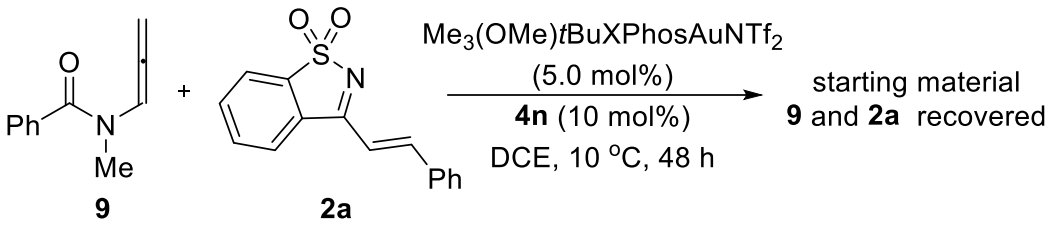


Figure S1. Proton NMR spectrum of crude reaction mixture of **1a** and **2a** in the absence of gold catalyst.



To a 10-mL oven-dried vial with a magnetic stirring bar, **9** (20.8 mg, 0.12 mmol) in 1.0 mL DCE was added to a solution of $Me_3(OMe)$*t*BuXPhosAuNTf$_2$ (5.0 mg, 5.0 mol%), **4n** (7.1 mg, 10 mol%), and **2a** (26.9 mg, 0.1 mmol) in DCE (1.0 mL) under an argon atmosphere, and the reaction mixture was stirred at 10 °C for 48 h. Then the reaction mixture was subjected to proton NMR analysis in $CDCl_3$ after the solvent was evaporated, and most of the starting material of **9** and **2a** remained intact (see Figure S2 for detail).

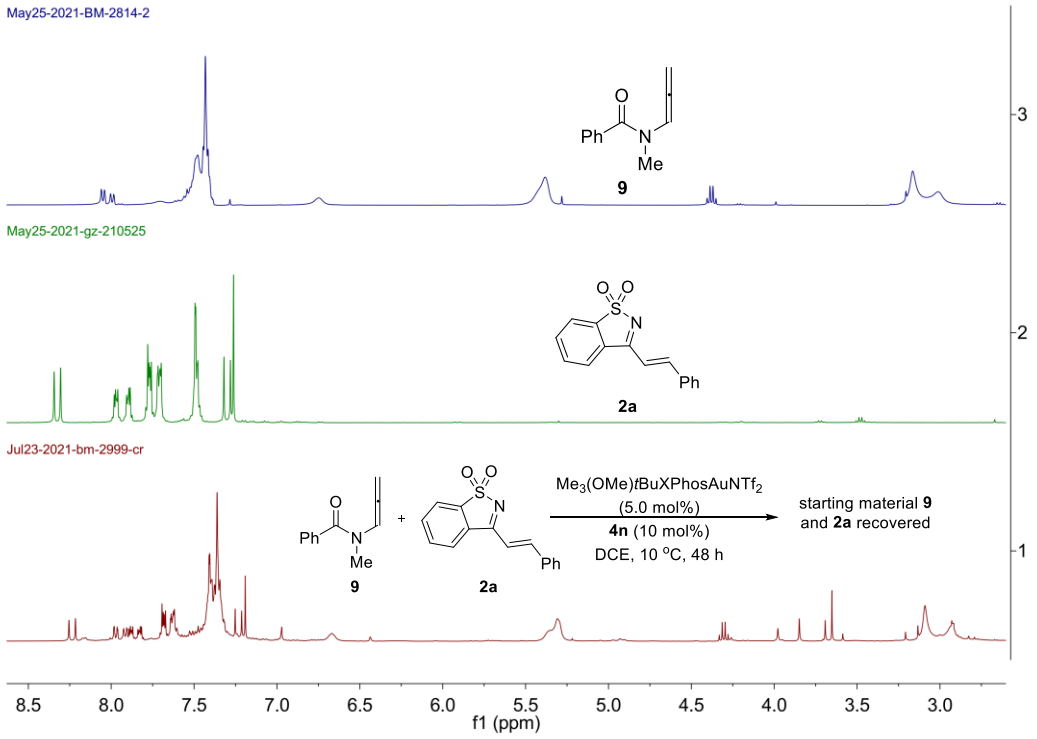
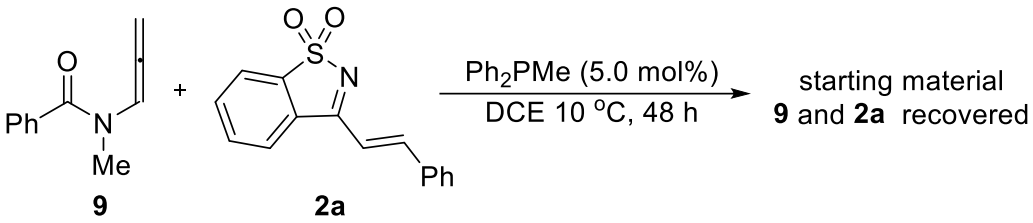


Figure S2. Proton NMR spectrum of crude reaction mixture of **9** and **2a**.



To a 10-mL oven-dried vial with a magnetic stirring bar, **9** (20.8 mg, 0.12 mmol) in 1.0 mL DCE was added to a solution of Ph_2PMe (1.0 mg, 5.0 mol%) and **2a** (26.9 mg, 0.1 mmol) in DCE (1.0 mL) under an argon atmosphere, and the reaction mixture was stirred at 10 °C for 48 h. Then the reaction mixture was subjected to proton NMR analysis in $CDCl_3$ after the solvent was evaporated, and most of the starting material of **9** and **2a** remained intact (see Figure S3 for detail).

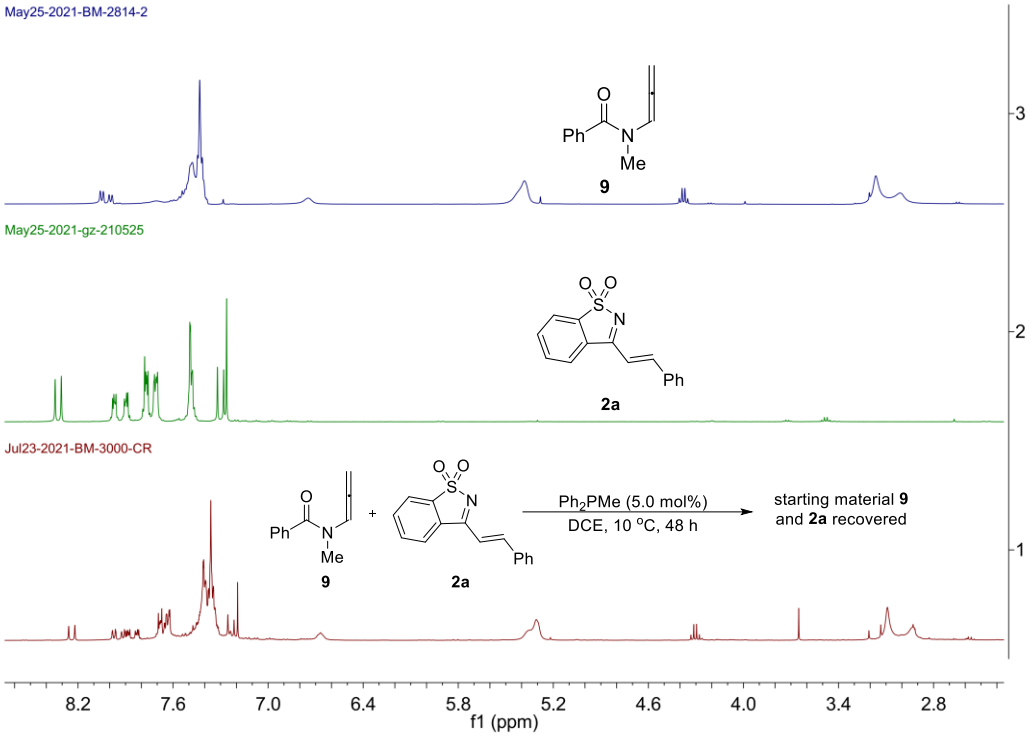
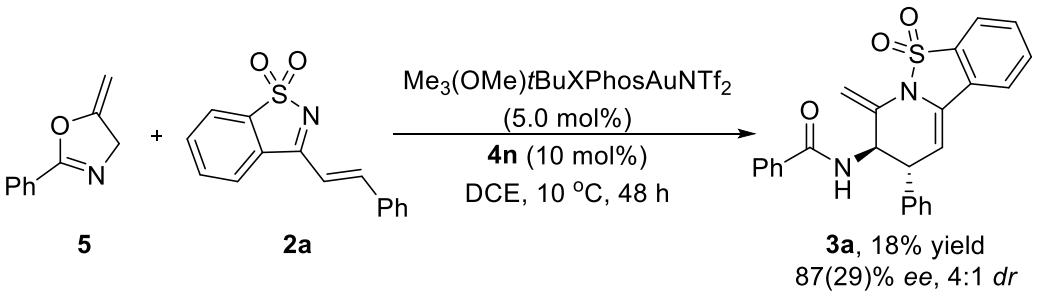
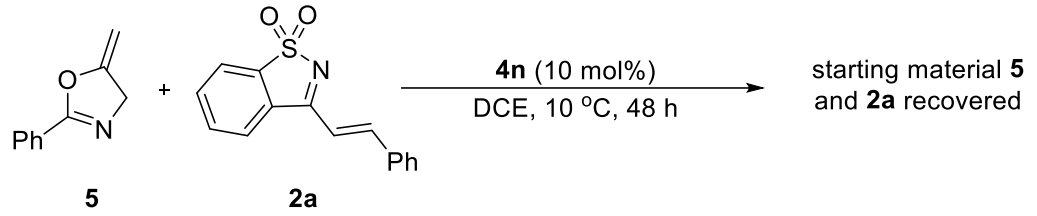


Figure S3. Proton NMR spectrum of crude reaction mixture of **9** and **2a** in the presence of Ph_2PMe.



To a 10-mL oven-dried vial with a magnetic stirring bar, **5** (19.1 mg, 0.12 mmol) in 1.0 mL DCE was added to a solution of $Me_3(OMe)$*t*BuXPhosAuNTf$_2$ (5.0 mg, 5.0 mol%), **4n** (7.1 mg, 10 mol%), and **2a** (26.9 mg, 0.1 mmol) in DCE (1.0 mL) under an argon atmosphere, and the reaction mixture was stirred at 10 °C for 48 h. Then, the crude reaction mixture was purified by flash column chromatography on silica gel (hexanes : EtOAc = 10:1 to 5:1) to give the pure product **3a** as white solid in 18% yield with 4:1 *dr* and 87(29)% *ee*.



To a 10-mL oven-dried vial with a magnetic stirring bar, **5** (19.1 mg, 0.12 mmol) in 1.0 mL DCE was added to a solution of **4n** (1.0 mg, 5.0 mol%) and **2a** (26.9 mg, 0.1 mmol), and DCE (1.0 mL) under an argon atmosphere, and the reaction mixture was stirred at 10 °C for 48 h. Then, the reaction mixture was subjected to proton NMR analysis in $CDCl_3$ after the solvent was evaporated, and most of the starting material of **5** and **2a** remained intact (see Figure S4 for detail).

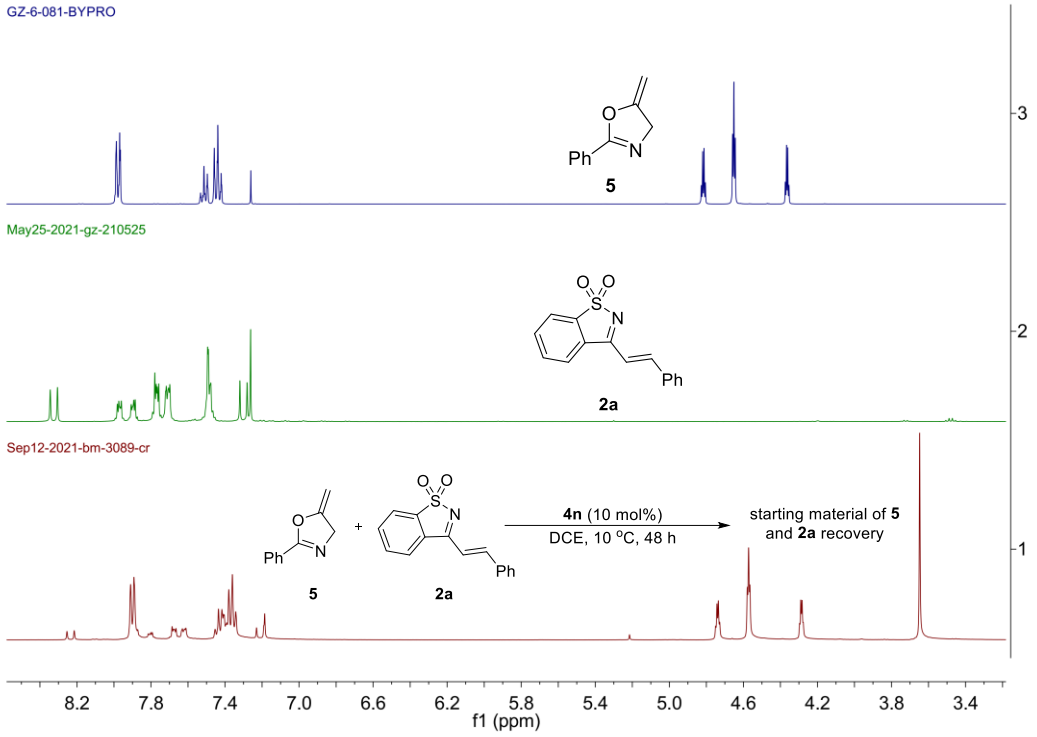
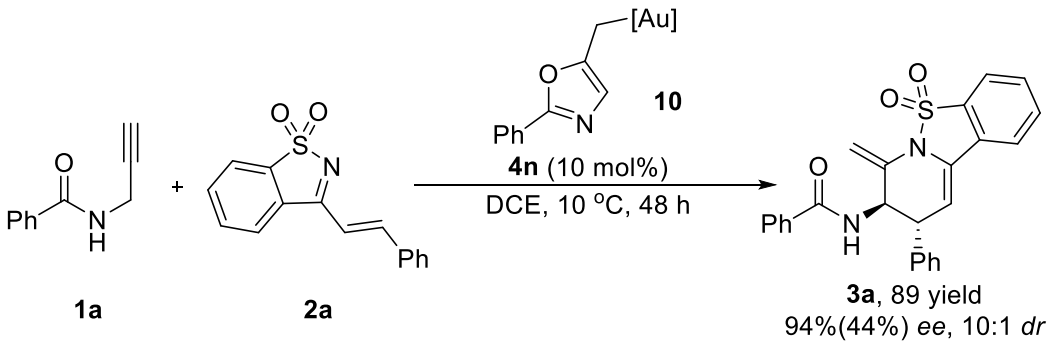
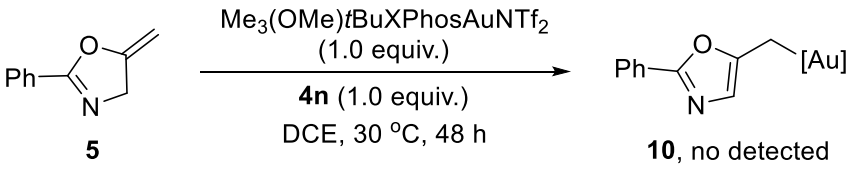


Figure S4. Proton NMR spectrum of crude reaction mixture of **5** and **2a**.



To a 10-mL oven-dried vial with a magnetic stirring bar, **1a** (19.1 mg, 0.12 mmol) in 1.0 mL DCE was added to a solution of **10** (5.8 mg, 5.0 mol%), **4n** (7.1 mg, 10 mol%) and **2a** (26.9 mg, 0.1 mmol) in DCE (1.0 mL) under an argon atmosphere, and the reaction mixture was stirred at 10 °C for 48 h. When the reaction was completed (monitored by TLC), the crude reaction mixture was purified by flash column chromatography on silica gel (hexanes : EtOAc = 10:1 to 5:1) to give the pure product **3a** as white solid, 89% yield with 94(44)% *ee*, 10:1 *dr*.



To a 10-mL oven-dried vial with a magnetic stirring bar, **5** (15.9 mg, 0.1 mmol) in 1.0 mL DCE was added to a solution of Me_3(OMe)*t*BuXPhosAuNTf_2 (100 mg, 1.0 equiv.), and **4n** (71 mg, 1.0 equiv.) in DCE (5.0 mL) under an argon atmosphere, and the reaction mixture was stirred at 30 °C for 48 h. Then, the reaction mixture was subjected to proton NMR analysis in $CDCl_3$ after the solvent was evaporated. Compound **5** remained intact and no alkylgold intermediate **10** was detected (see Figure S5 for detail).

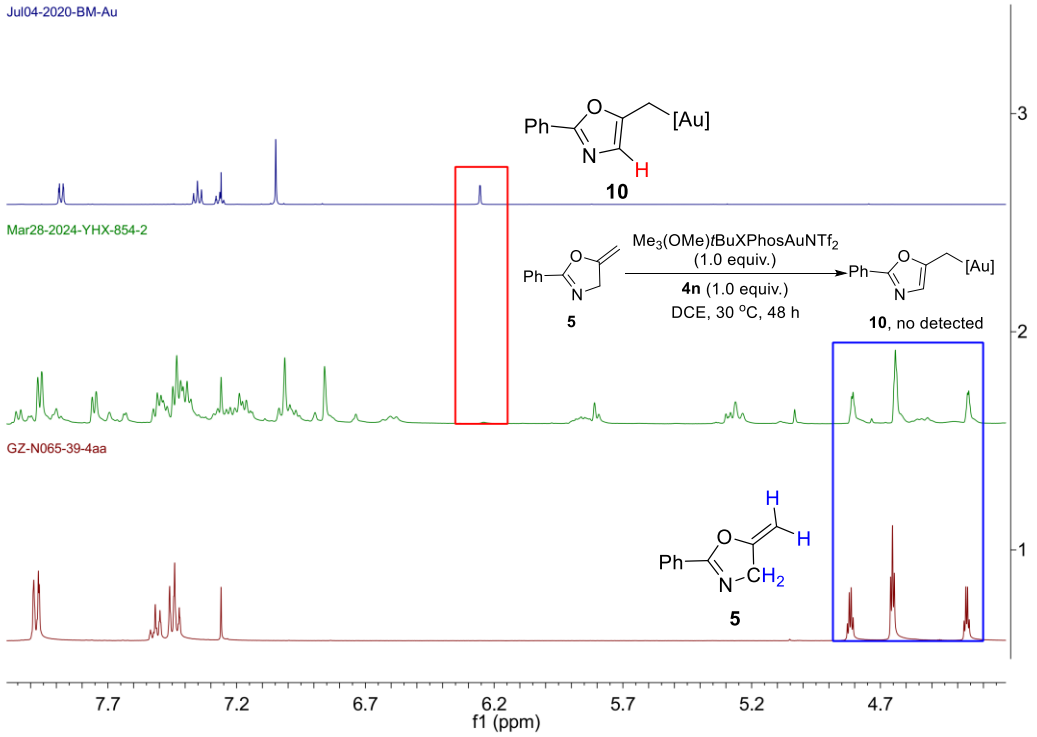
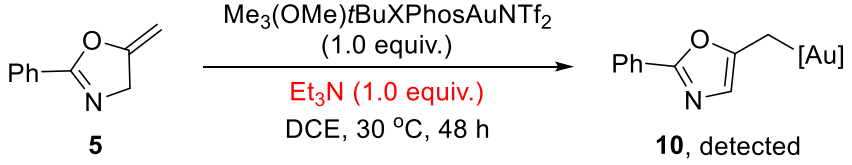


Figure S5. Proton NMR of the crude reaction mixture of **5** under standard conditions.



To a 10-mL oven-dried vial with a magnetic stirring bar, **5** (15.9 mg, 0.1 mmol) in 1.0

mL DCE was added to a solution of Me_3(OMe)*t*BuXPhosAuNTf$_2$ (100 mg, 1.0 equiv.), and Et_3N (10.1 mg, 1.0 equiv.) in DCE (5.0 mL) under an argon atmosphere, and the reaction mixture was stirred at 30 °C for 48 h. Then, the reaction mixture was subjected to proton NMR analysis in $CDCl_3$ after the solvent was evaporated, and the formation of alkylgold intermediate **10** was detected (see Figure S6 for detail).

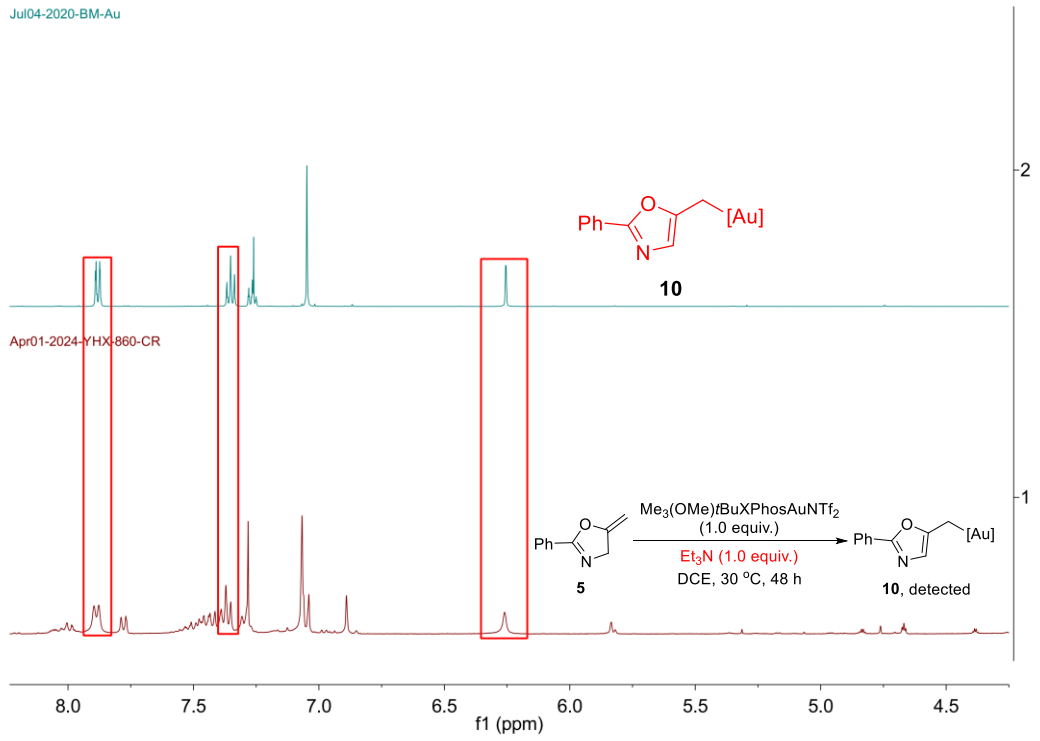
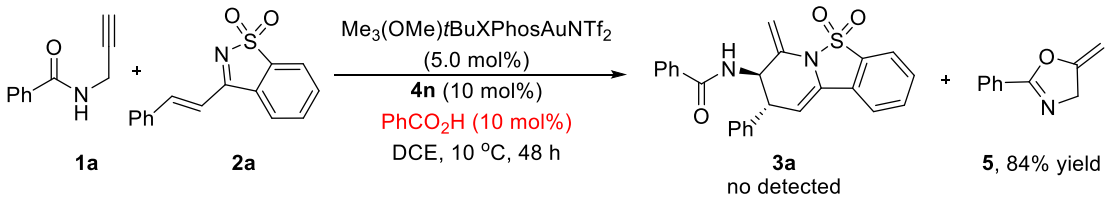
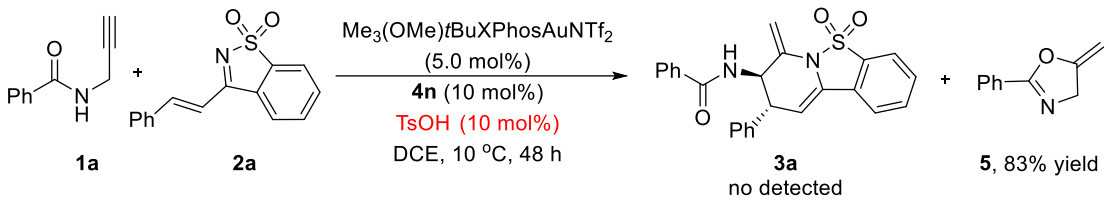


Figure S6. Proton NMR of the crude reaction mixture of **5** under standard conditions in the presence of Et_3N.



To a 10-mL oven-dried vial with a magnetic stirring bar, **1a** (19.1 mg, 0.12 mmol) in 1.0 mL DCE was added to a solution of Me_3(OMe)*t*BuXPhosAuNTf$_2$ (5.0 mg, 5.0 mol%), **4n** (7.1 mg, 10 mol%), $PhCO_2H$ (1.2 mg, 10 mol%), and **2a** (26.9 mg, 0.1 mmol) in DCE (1.0 mL) under an argon atmosphere, and the reaction mixture was stirred at 10 °C for 48 h. Then, the reaction mixture was subjected to proton NMR

analysis in $CDCl_3$ after the solvent was evaporated, and no desired product **3a** was detected, and compound **5** was obtained in 84% yield (see Figure S7 for detail).



To a 10-mL oven-dried vial with a magnetic stirring bar, **1a** (19.1 mg, 0.12 mmol) in 1.0 mL DCE was added to a solution of Me_3(OMe)*t*BuXPhosAuNTf$_2$ (5.0 mg, 5.0 mol%), **4n** (7.1 mg, 10 mol%), TsOH (1.7 mg, 10 mol%), and **2a** (26.9 mg, 0.1 mmol) in DCE (1.0 mL) under an argon atmosphere, and the reaction mixture was stirred at 10 °C for 48 h. Then, the reaction mixture was subjected to proton NMR analysis in $CDCl_3$ after the solvent was evaporated, and no desired product **3a** was detected, and compound **5** was obtained in 83% yield (see Figure S7 for detail).

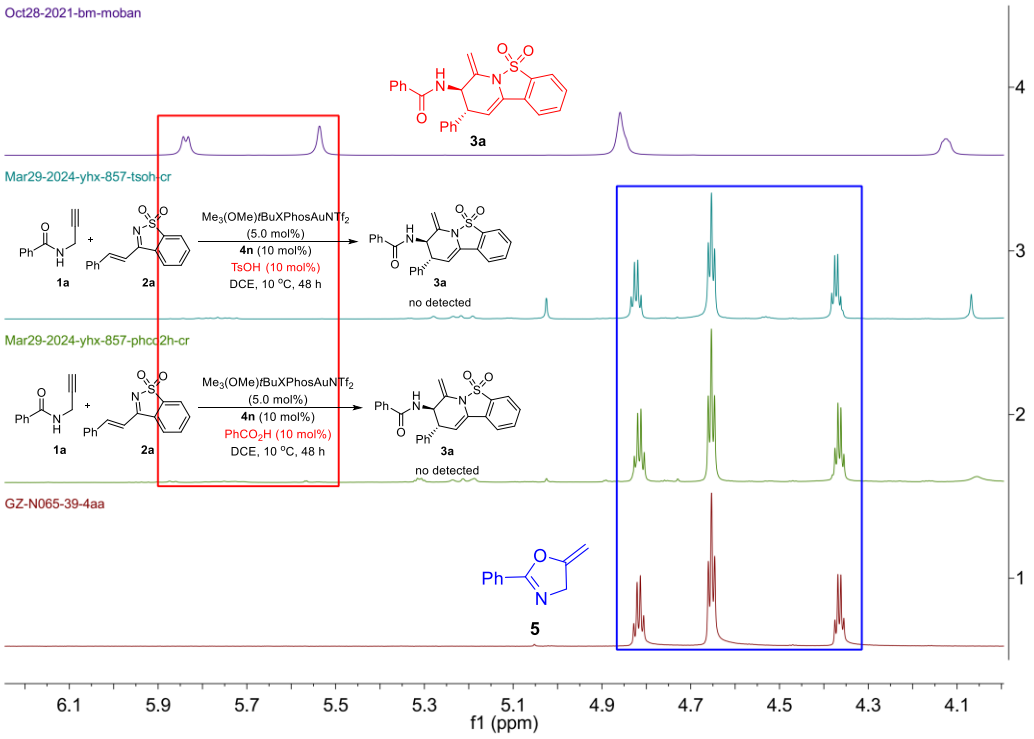
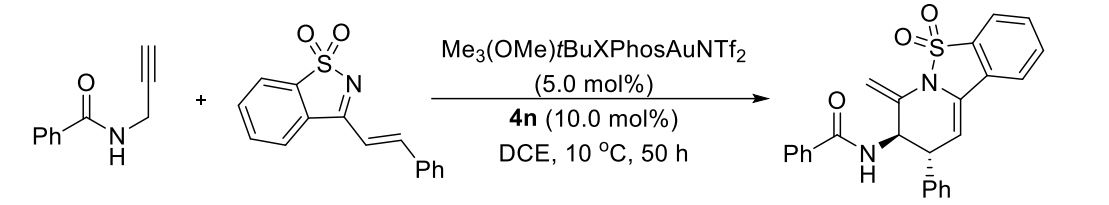


Figure S7. Proton NMR of the crude reaction mixture of **1a** and **2a** under standard conditions in the presence of $PhCO_2H$ and TsOH.

General Procedure for Scale Up



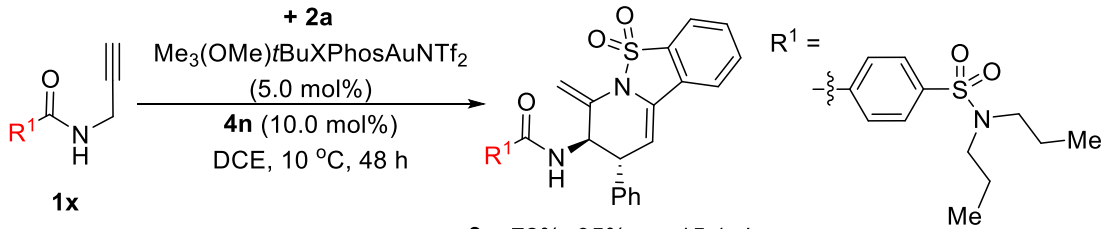
1a
3.6 mmol, 573 mg

2a
3.0 mmol, 807 mg

3a
1.09 g, 85% yield, 93% *ee*, 10:1 *dr*

To a 10-mL oven-dried vial with a magnetic stirring bar, **1a** (573 mg, 3.6 mmol) in 5.0 mL DCE was added to a solution of $Me_3(OMe)tBuXPhosAuNTf_2$ (150 mg, 5.0 mol%), **4n** (213 mg, 10 mol%) and **2a** (807 mg, 3.0 mmol) in DCE (10.0 mL) under an argon atmosphere, and the reaction mixture was stirred at 10 °C for 50 h. When the reaction was completed (monitored by TLC), the crude reaction mixture was purified by flash column chromatography on silica gel (Hexanes : EtOAc = 10:1 to 5:1) to give 1.09 g pure product **3a** as white solid, 85% yield with 93% *ee*, 10:1 *dr*.

Synthetic Applications

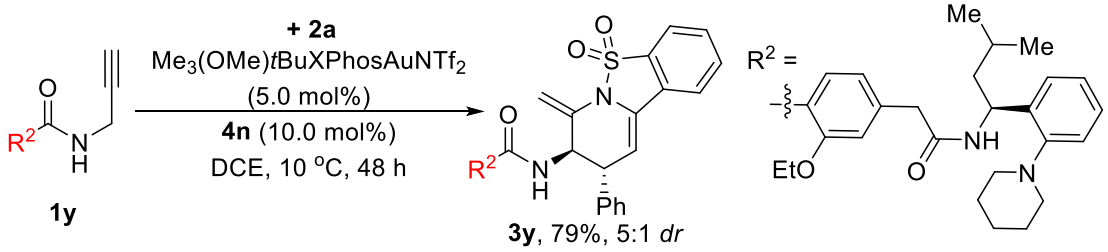


1x

3x, 72%, 95% *ee*, 15:1 *dr*

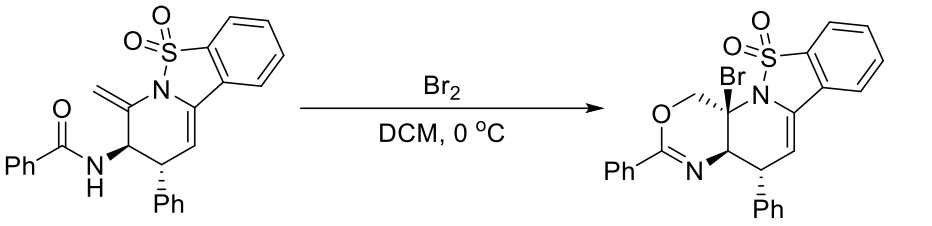
Synthesis of 3x: To a 10-mL oven-dried vial containing a magnetic stirring bar, α,β-unsaturated imine **2a** (26.9 mg, 0.1 mmol), **4n** (7.0 mg, 10.0 mol%), and $Me_3(OMe)tBuXPhosAuNTf_2$ (5.0 mg, 5.0 mol%) in DCE (3.0 mL), was added propargyl amide **1x** (36.7 mg, 0.12 mmol) in DCE (1.0 mL) at 30 °C under argon atmosphere. The resulting reaction mixture was stirred for 48 hours under these conditions. When the reaction was completed (monitored by TLC), the solvent was evaporated *in vacuo* and the residue was purified by flash column chromatography on silica gel (hexanes/ethyl acetate = 8:1 to 5:1) to give 85.1 mg pure product **3x** in 72%

yield with15:1 *dr* and 95% *ee* as yellow solid. mp: 123.0-125.0 °C; $[\alpha]_D^{20}$ = 106° (c = 0.05, DCM); ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 7.91 (d, *J* = 7.7 Hz, 1H), 7.86 – 7.69 (comp, 6H), 7.67 (t, *J* = 7.4 Hz, 1H), 7.37 – 7.28 (comp, 5H), 6.66 (d, *J* = 6.4 Hz, 1H), 5.89 (d, *J* = 5.7 Hz, 1H), 5.58 (s, 1H), 4.91 (s, 1H), 4.88 (d, *J* = 4.9 Hz, 1H), 4.14 (d, *J* = 2.5 Hz, 1H), 3.11 – 2.99 (m, 4H), 1.52 (dd, *J* = 14.8, 7.4 Hz, 4H), 0.85 (t, *J* = 7.3 Hz, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 165.5, 143.3, 139.7, 137.3, 133.9, 132.3, 132.2, 130.8, 130.2, 129.0, 128.6, 128.5, 128.0, 127.9, 127.4, 121.62, 121.55, 105.1, 101.0, 54.9, 50.1, 44.6, 22.1, 11.2; HRMS (TOF MS ESI$^+$) calculated for $C_{31}H_{34}N_3O_5S_2$ $[M+H]^+$: 592.1934, found 592.1938; HPLC conditions for determination of enantiomeric excess: Chiral OD-H, λ = 254 nm, hexane : 2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 16.0 min, t_{minor} = 21.3 min.



Synthesis of 3y: To a 10-mL oven-dried vial containing a magnetic stirring bar, α,β-unsaturated imine **2a** (26.9 mg, 0.1 mmol), **4n** (7.0 mg, 10.0 mol%), and $Me_3(OMe)$*t*BuXPhosAuNTf$_2$ (5.0 mg, 5.0 mol%) in DCE (3.0 mL), was added propargyl amide **1y** (58.7 mg, 0.12 mmol) in DCE (1.0 mL) at 30 °C under argon atmosphere. The resulting reaction mixture was stirred for 48 hours under these conditions. When the reaction was completed (monitored by TLC), the solvent was evaporated *in vacuo* and the residue was purified by flash column chromatography on silica gel (hexanes/ethyl acetate = 8:1 to 5:1) to give 119.8 mg pure product **3y** in 79% yield with 5:1 *dr* as yellow solid. mp: 122.0-124.0 °C; $[\alpha]_D^{20}$ = 74° (c = 0.05, DCM); ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 8.38 (d, *J* = 7.2 Hz, 1H), 8.07 (d, *J* = 7.9 Hz, 1H), 7.84 (d, *J* = 7.7 Hz, 1H), 7.72 (d, *J* = 7.6 Hz, 1H), 7.66 (t, *J* = 7.4 Hz, 1H), 7.59 (t, *J* = 7.4 Hz, 1H), 7.28 – 7.20 (comp, 5H), 7.15 – 7.10 (m, 2H), 7.01 – 6.95 (m, 2H), 6.82 (d, *J* = 7.9 Hz, 1H), 6.75 (s, 1H), 6.69 (s, 1H), 5.85 (d, *J* = 5.7 Hz, 1H), 5.42 (s,

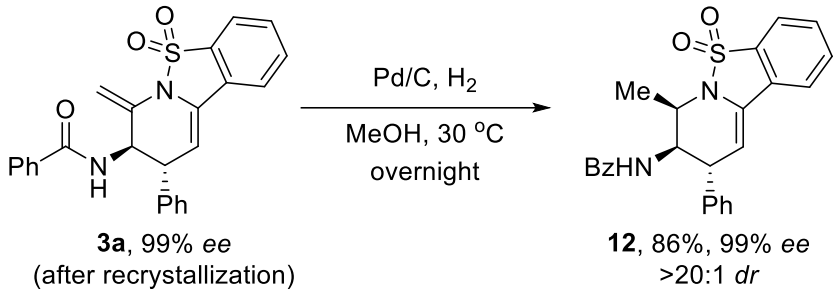
1H), 5.29 (dd, *J* = 15.2, 7.9 Hz, 1H), 4.93 (d, *J* = 6.1 Hz, 1H), 4.75 (s, 1H), 4.02 (d, *J* = 2.9 Hz, 1H), 3.90 – 3.80 (m, 2H), 3.44 (s, 2H), 2.88 – 2.85 (m, 2H), 2.56 – 2.54 (m, 1H), 1.56 – 1.39 (m, 6H), 1.36 – 1.25 (m, 4H), 0.92 (t, *J* = 6.8 Hz, 3H), 0.84 (d, *J* = 6.1 Hz, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 168.9, 164.5, 157.3, 152.6, 141.0, 140.1, 138.7, 133.6, 132.71, 132.68, 132.5, 130.6, 129.8, 128.8, 128.4, 128.3, 128.0, 127.8, 127.6, 125.2, 122.9, 121.9, 121.4, 121.3, 119.8, 112.9, 101.6, 100.8, 64.8, 54.7, 49.9, 46.8, 44.9, 44.2, 26.9, 25.4, 24.2, 22.9, 22.6, 14.0; HRMS (TOF MS ESI$^+$) calculated for $C_{45}H_{51}N_4O_5S$ $[M+H]^+$: 759.3575, found 759.3594; NMR signals of **3y'** ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 8.26 – 8.14 (m, 1H), 7.91 (dd, *J* = 16.3, 8.7 Hz, 2H), 7.77 – 7.66 (m, 2H), 7.63 (t, *J* = 7.4 Hz, 1H), 7.30 – 7.25 (comp, 5H), 7.20 (d, *J* = 7.4 Hz, 2H), 7.16 – 7.11 (m, 2H), 7.10 – 7.02 (m, 2H), 6.92 (d, *J* = 8.0 Hz, 1H), 6.82 (d, *J* = 10.1 Hz, 1H), 6.76 (s, 1H), 5.97 (d, *J* = 6.4 Hz, 1H), 5.61 – 5.53 (m, 1H), 5.52 (s, 1H), 5.39 – 5.23 (m, 1H), 4.83 (s, 1H), 3.99 (t, *J* = 6.1 Hz, 1H), 3.82 – 3.61 (m, 2H), 3.53 (s, 2H), 2.91 (s, 2H), 2.59 (s, 2H), 1.60 – 1,56 (m, 5H), 1.46 – 1.36 (m, 1H), 0.92 (dd, *J* = 6.3, 2.2 Hz, 6H), 0.76 (t, *J* = 7.0 Hz, 3H); HRMS (TOF MS ESI$^+$) calculated for $C_{45}H_{51}N_4O_5S$ $[M+H]^+$: 759.3575, found 759.3592.



3a **11**, 85%, 96% *ee*, >20:1 *dr*

Synthesis of 11: To a 10-mL oven-dried vial with a magnetic stirring bar, **3a** (42.8 mg, 0.1 mmol) in DCM (1.0 mL), was added Br_2 (24 mg, 0.15 mmol, 1.5 equiv.) in DCM (1.0 mL) at 0 °C, and the reaction mixture was stirred for 1 h. When the reaction was completed (monitored by TLC), the crude reaction mixture was purified by column chromatography on silica gel (Hexanes : EtOAc = 10:1) to give 43.0 mg pure product **11** in 85% yield with >20:1 *dr* and 96% *ee* as white solid. mp:112.5-114.0 °C; ^{1}H NMR (500 MHz, $CDCl_3$) (δ, ppm) 8.00 (d, *J* = 7.7 Hz, 2H), 7.84 (d, *J* = 7.8 Hz, 1H), 7.71 (d, *J* = 7.8 Hz, 1H), 7.66 (t, *J* = 7.5 Hz, 1H), 7.59 (t, *J* = 7.5 Hz, 1H), 7.49 (t, *J* =

7.3 Hz, 1H), 7.43 – 7.34 (comp, 6H), 7.35 – 7.30 (m, 1H), 6.02 (d, *J* = 6.2 Hz, 1H), 5.11 (d, *J* = 1.9 Hz, 1H), 4.50 (d, *J* = 11.6 Hz, 1H), 4.33 (dd, *J* = 6.0, 2.2 Hz, 1H), 3.76 (d, *J* = 11.6 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) (δ, ppm) 163.4, 139.9, 133.6, 132.9, 132.6, 132.3, 130.6, 129.3, 128.9, 128.62, 128.60, 128.1, 127.9, 126.4, 121.4, 121.2, 103.5, 95.6, 76.9, 43.0, 34.1; HRMS (TOF MS ESI$^+$) calculated $C_{25}H_{19}BrN_2NaO_3S$ for $[M+Na]^+$: 529.0192, found 529.0190; HPLC conditions for determination of enantiomeric excess: Chiral OD-H, λ = 254 nm, hexane : 2-propanol = 80:20, flow rate = 1.0 mL/min, t_{major} = 13.3 min, t_{minor} = 15.2 min.



Synthesis of 12: To a 10-mL oven-dried vial with a magnetic stirring bar, Pd/C (2.2 mg, 10 mol%) in MeOH (1.0 mL), was added a solution of **3a** (42.8 mg, 0.1 mmol) in MeOH (1.0 mL), and the reaction mixture was stirred under H_2 atmosphere (with a H_2 balloon) at 30 °C overnight. When the reaction was completed (monitored by TLC), the crude reaction mixture was purified by column chromatography on silica gel (Hexanes : EtOAc = 10:1) to give 37.0 mg pure product **12** in 86% yield with >20:1 *dr* and 99% *ee* as white solid. mp:110.5-113.0 °C; ^{1}H NMR (400 MHz, MeOD) (δ, ppm) 7.78 (d, *J* = 7.7 Hz, 1H), 7.72 – 7.68 (m, 1.1 Hz, 1H), 7.61 (t, *J* = 7.5 Hz, 1H), 7.55 (d, *J* = 7.5 Hz, 1H), 7.52 – 7.41 (comp, 3H), 7.37 – 7.32 (comp, 4H), 7.27 – 7.23 (comp, 2H), 7.18 – 7.14 (m, 1H), 4.49 (dd, *J* = 11.5, 2.0 Hz, 1H), 2.74 – 2.53 (m, 1H), 1.95 – 1.83 (m, 1H), 1.71 (d, *J* = 6.5 Hz, 1H); ^{13}C NMR (100 MHz, MeOD) (δ, ppm) 170.5, 156.5, 155.0, 144.3, 143.0, 138.5, 137.2, 135.8, 134.4, 132.5, 130.6, 129.6, 129.4, 128.9, 128.1, 128.0, 124.4, 121.7, 61.7, 38.4, 15.6; HRMS (TOF MS ESI$^+$) calculated $C_{25}H_{22}N_2NaO_3S$ for $[M+Na]^+$: 453.1243, found 453.1245; HPLC conditions for determination of enantiomeric excess: Chiral IC, λ = 254 nm, hexane :

2-propanol = 70:30, flow rate = 1.0 mL/min, t_{major} = 24.7 min, t_{minor} = 42.6 min.

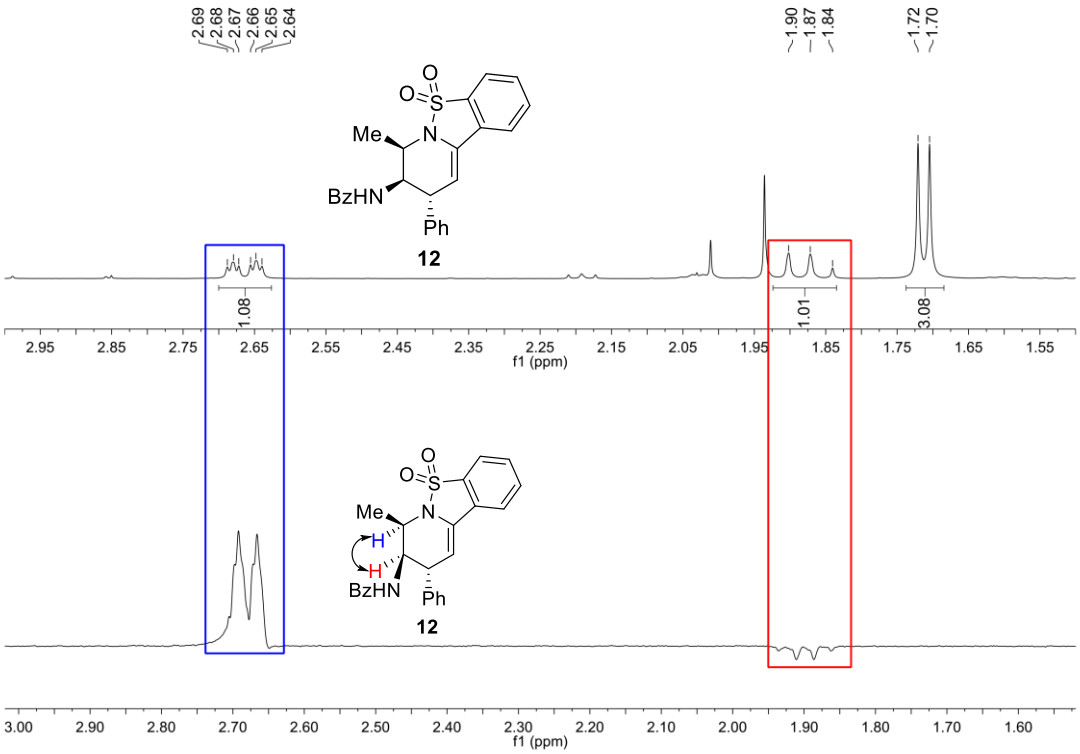
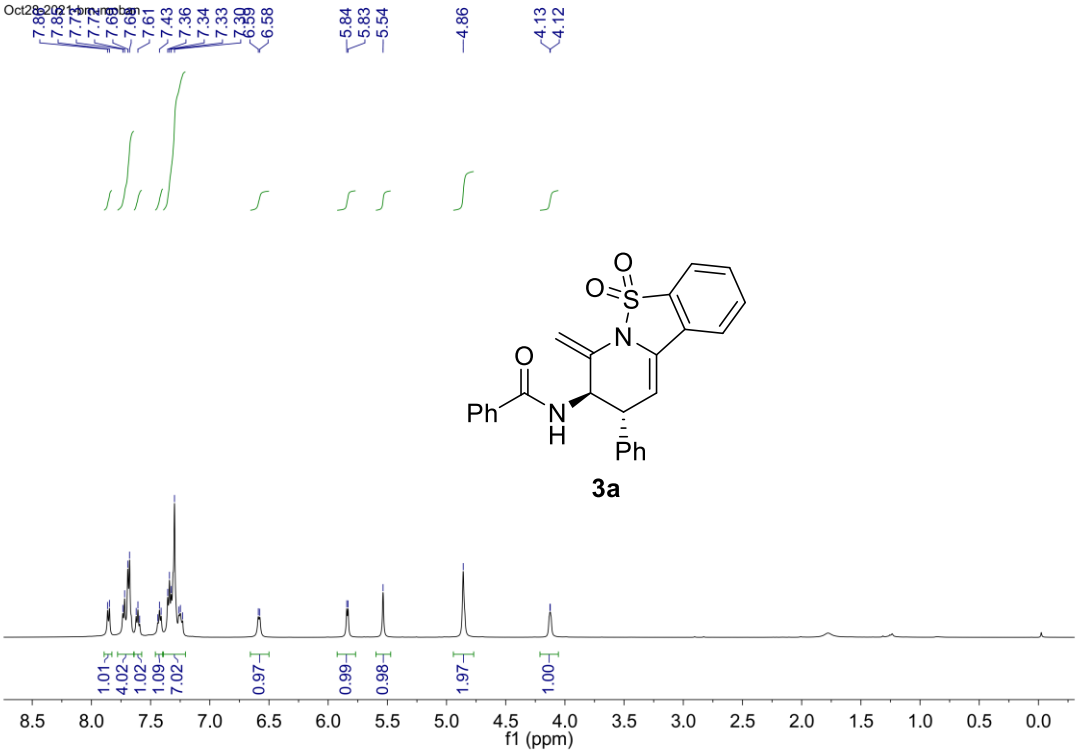


Figure S8. NOE NMR spectra of **12**.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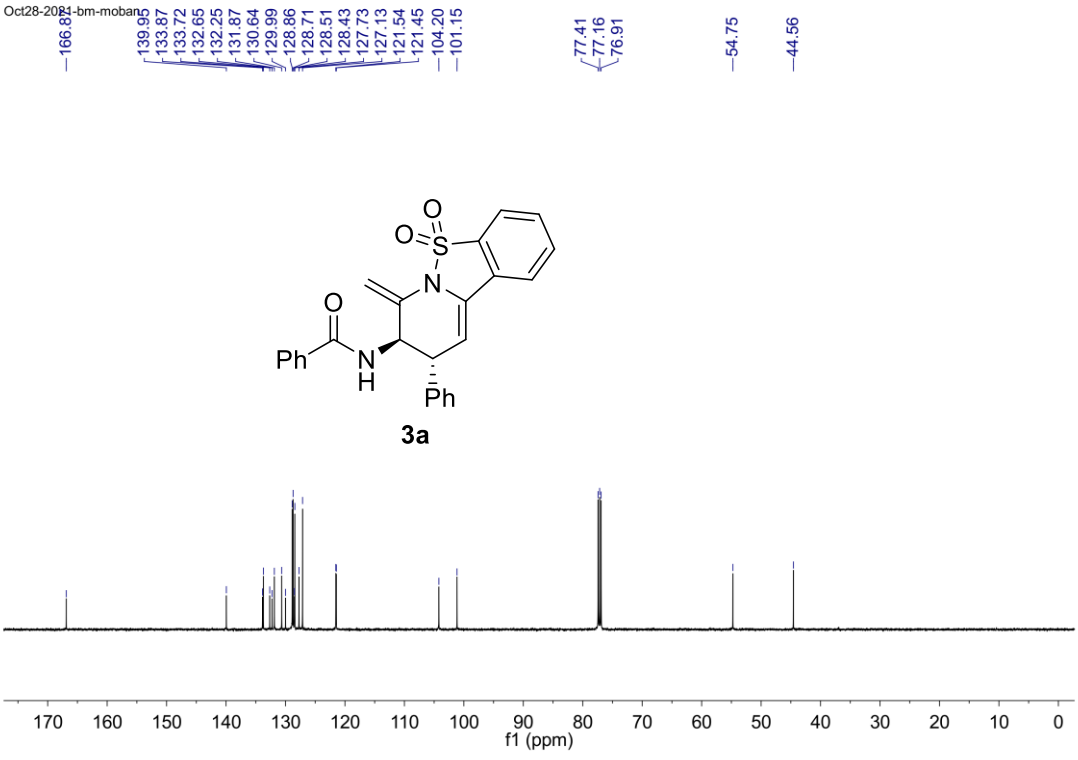
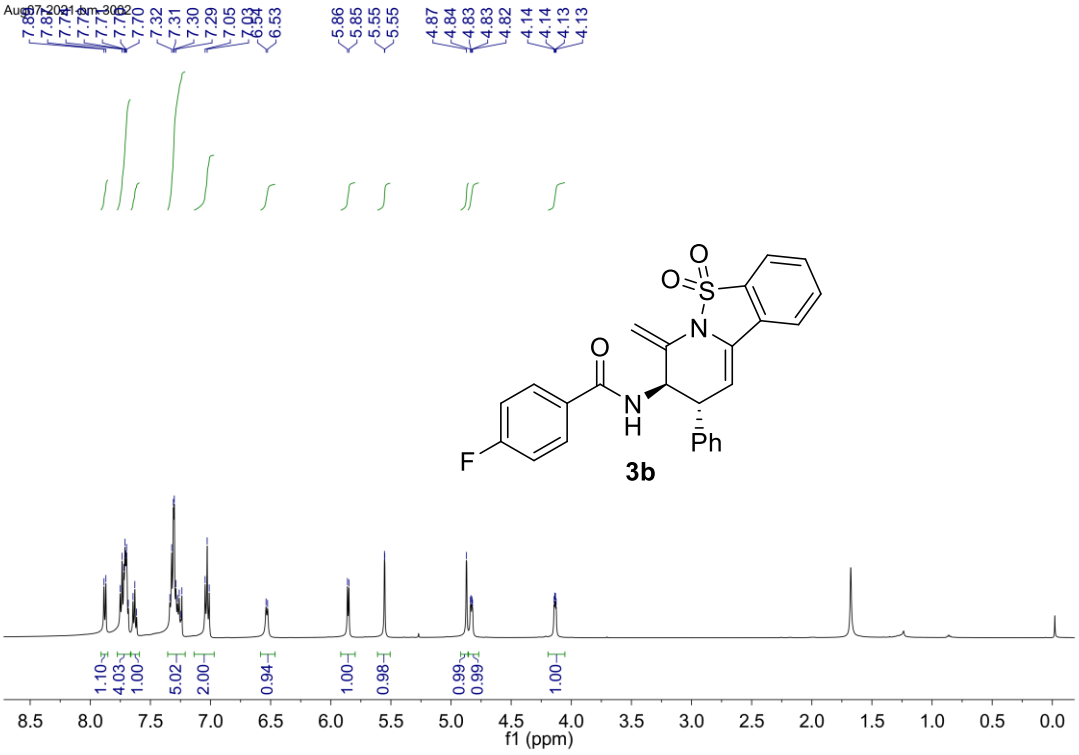
7.85
7.77
7.76
7.68
7.66
7.61
7.43
7.36
7.34
7.33
6.59
6.58
5.84
5.83
5.54
4.86
4.13
4.12
O
O
S
N
O
Ph
N
H
Ph
1.01
4.02
1.02
1.09
7.02
0.97
0.99
0.98
1.97
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

3a


166.83
139.95
133.87
133.72
132.65
132.25
131.87
130.64
129.99
128.86
128.71
128.51
128.43
127.73
127.13
121.54
121.45
104.20
101.15
77.41
77.16
76.91
54.75
44.56
O
O
S
N
O
Ph
N
H
Ph
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

3a


Aug07-2021-bm-3002
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7.84
7.78
7.77
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7.70
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7.31
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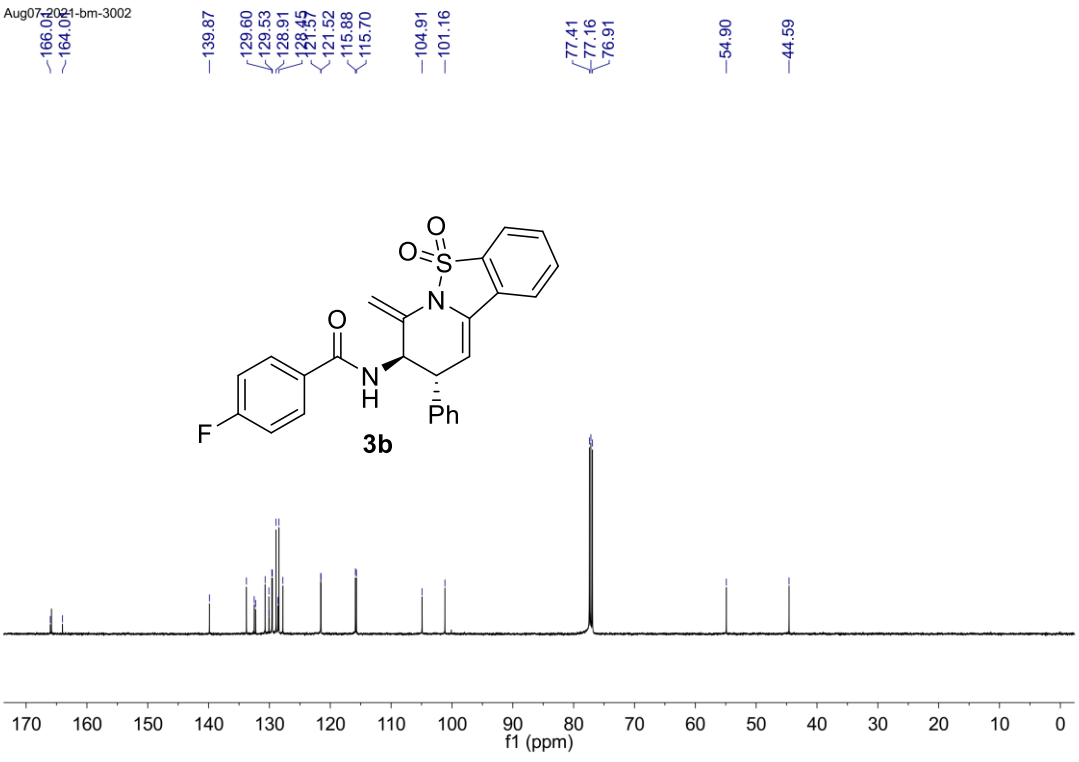
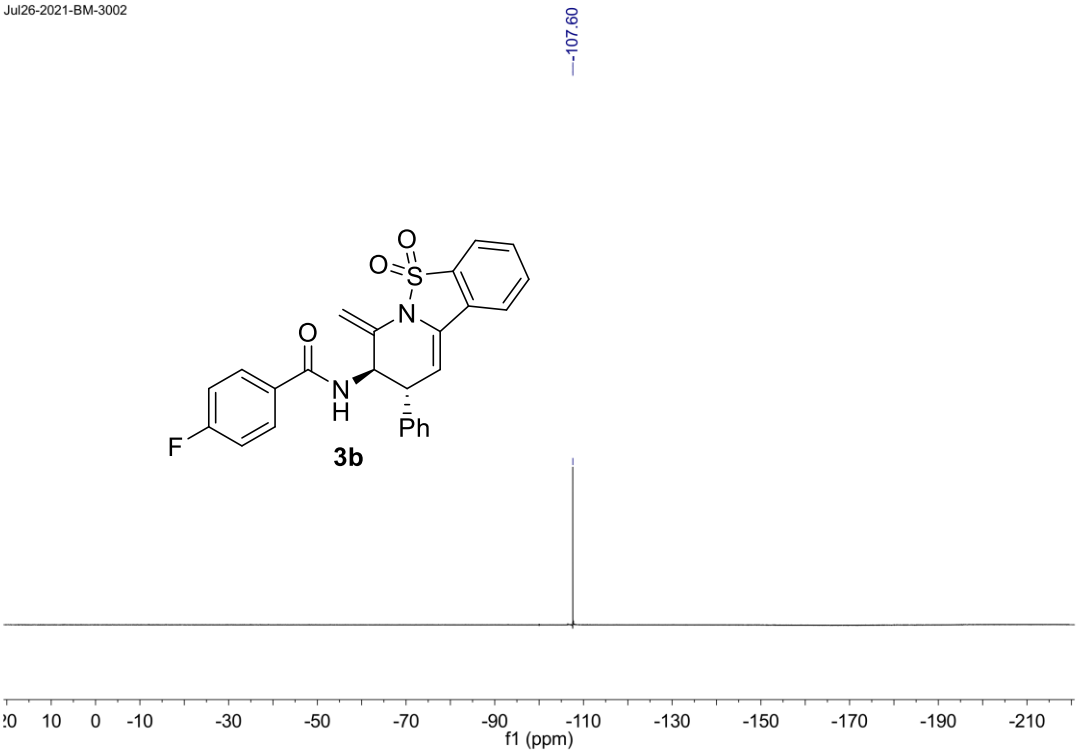
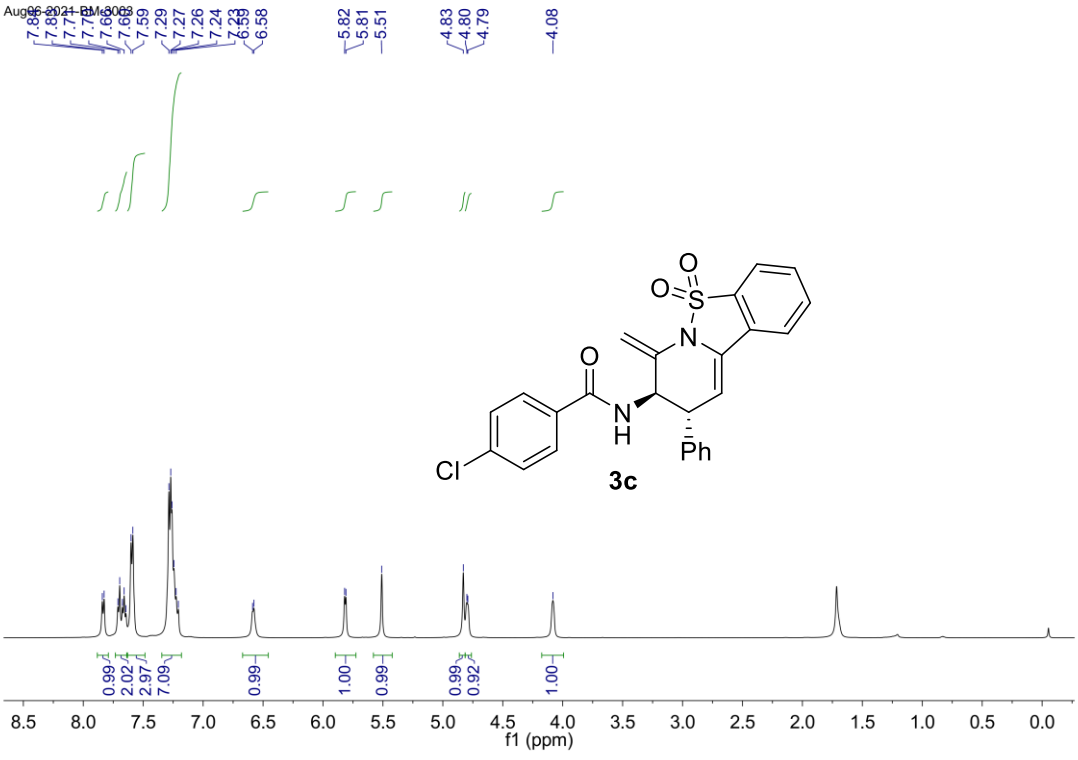
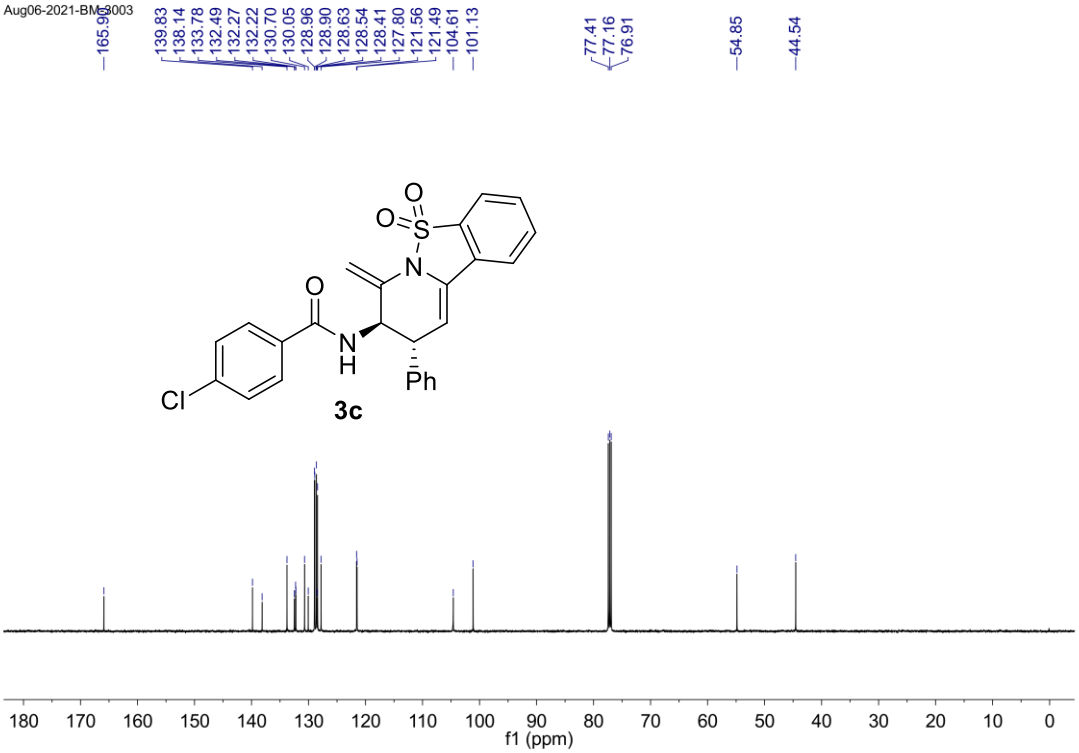
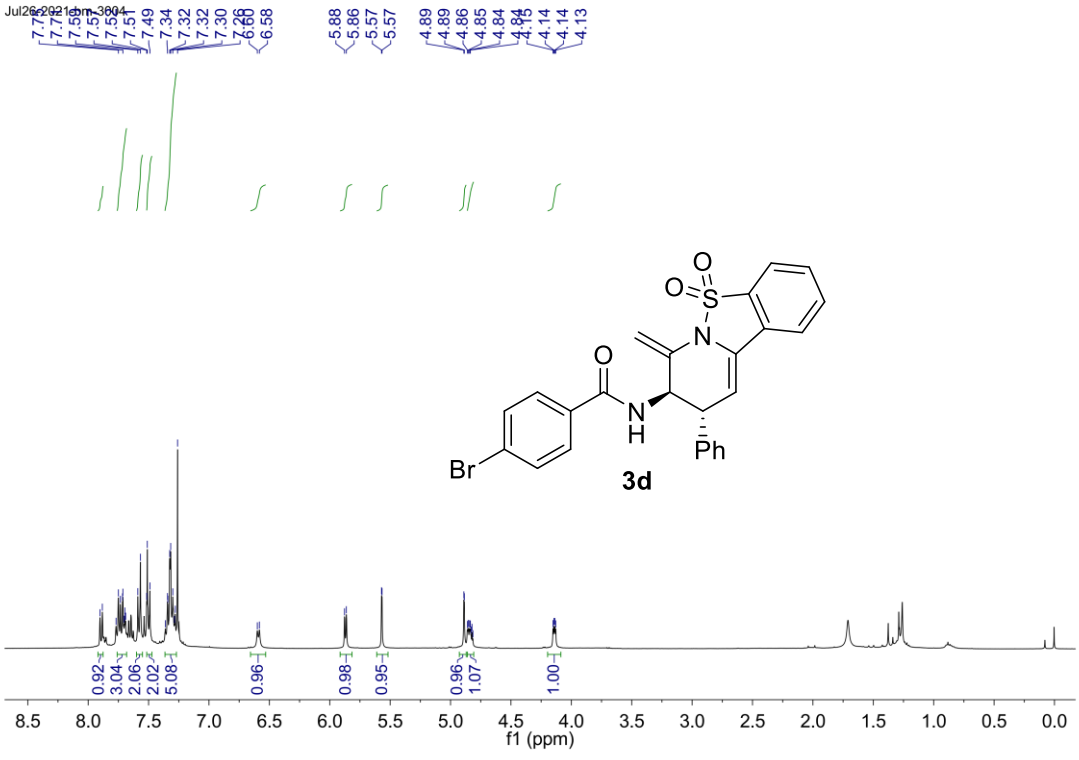
7.05
7.03
6.54
6.53
5.86
5.85
5.55
5.55
4.87
4.84
4.83
4.83
4.82
4.14
4.14
4.13
4.13
O
O
S
N
O
N
H
Ph
F
3b
1.10
4.03
1.00
5.02
2.00
0.94
1.00
0.98
0.99
0.99
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

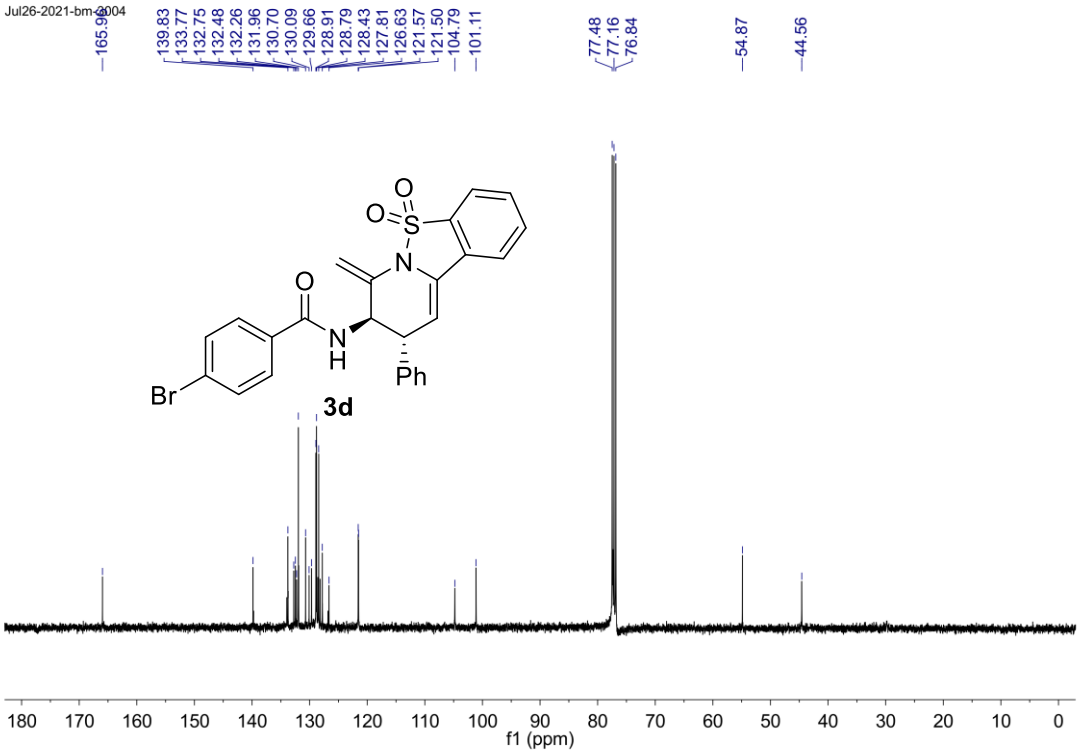

Aug07-2021-bm-3002
166.03
164.05
139.87
129.60
129.53
128.91
128.45
121.57
121.52
115.88
115.70
104.91
101.16
77.41
77.16
76.91
54.90
44.59
O
O
S
N
O
N
H
Ph
F
3b
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

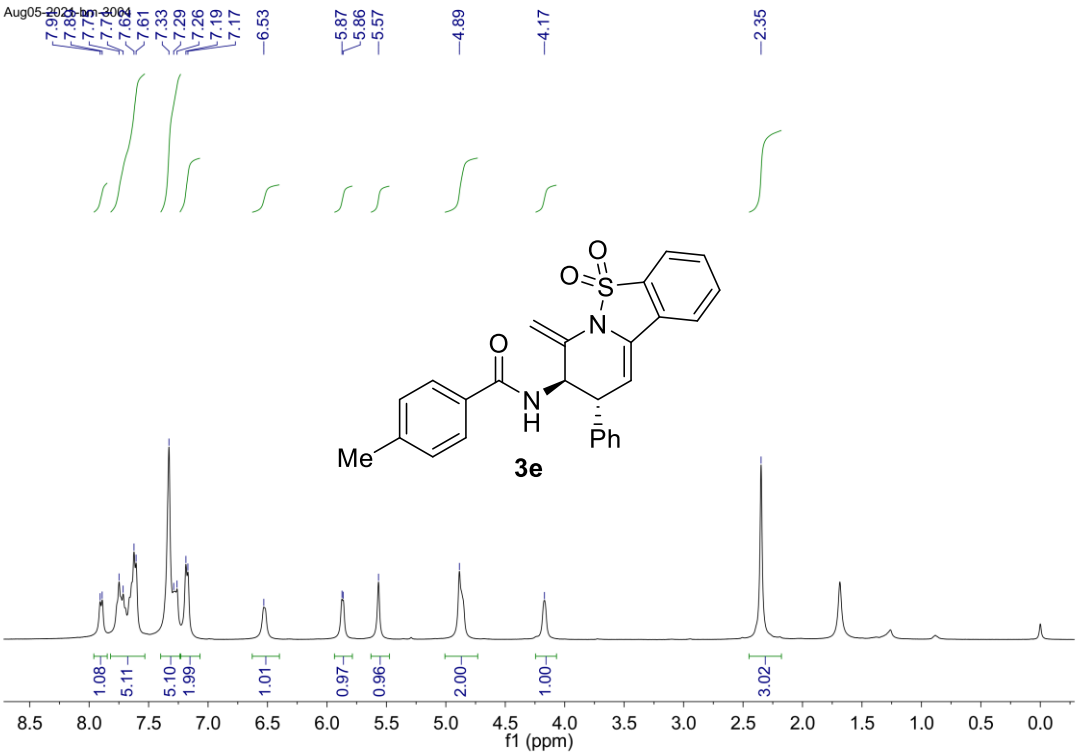

Jul26-2021-BM-3002
-107.60
O
O
S
N
O
N
H
Ph
F
3b
f1 (ppm)

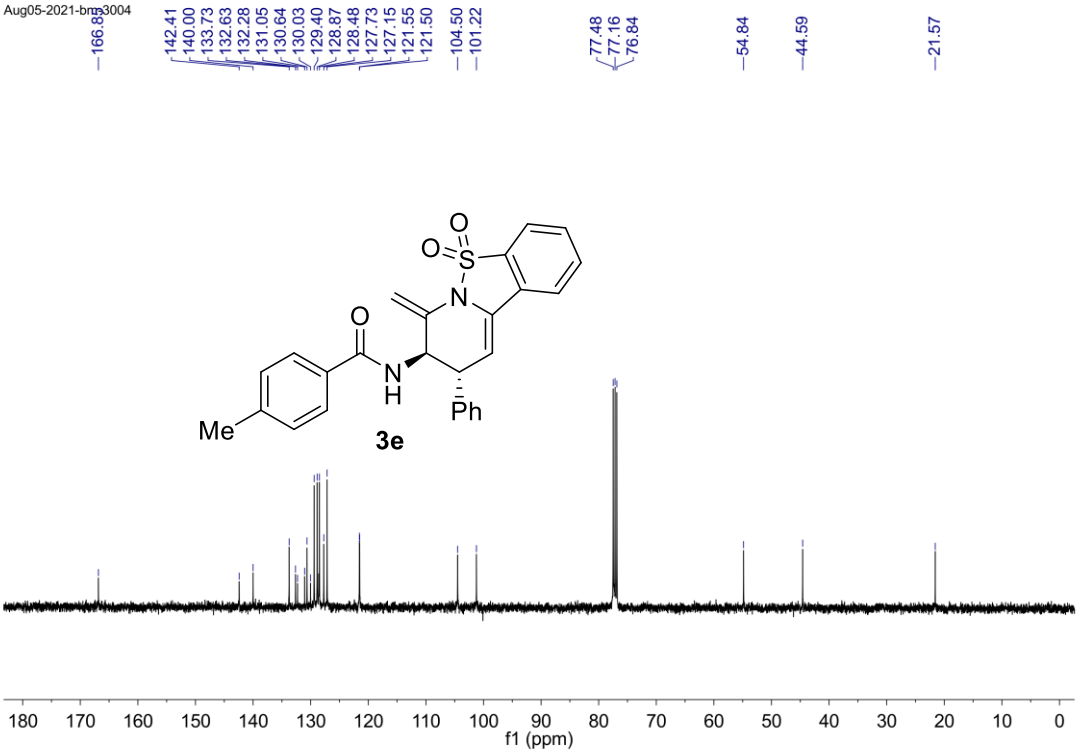

7.85
7.83
7.71
7.70
7.66
7.65
7.59
7.29
7.27
7.26
7.24
6.58
5.82
5.81
5.51
4.83
4.80
4.79
4.08
O
O
S
N
O
N
H
Ph
Cl
3c
0.99
2.02
2.97
7.09
0.99
1.00
0.99
0.99
0.92
1.00
f1 (ppm)

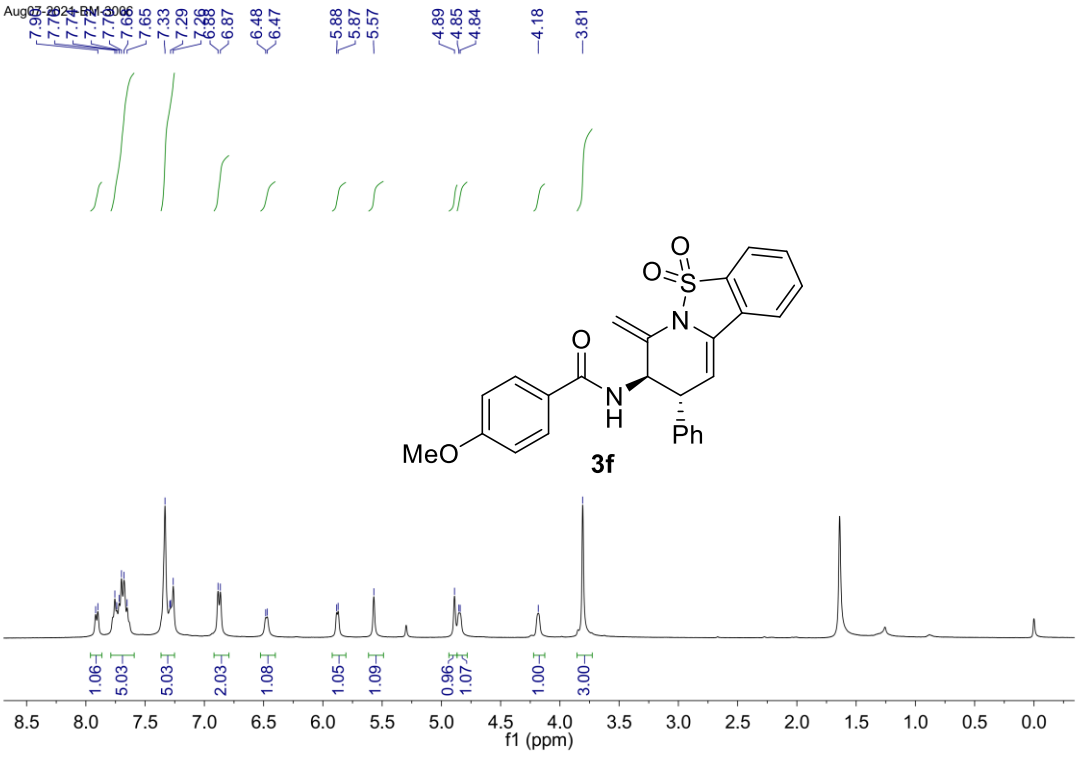

Aug06-2021-BM-3003
165.96
139.83
138.14
133.78
132.49
132.27
132.22
130.70
130.05
128.96
128.90
128.63
128.54
128.41
127.80
121.56
121.49
104.61
101.13
77.41
77.16
76.91
54.85
44.54
O
O
S
N
O
N
H
Ph
Cl
3c
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

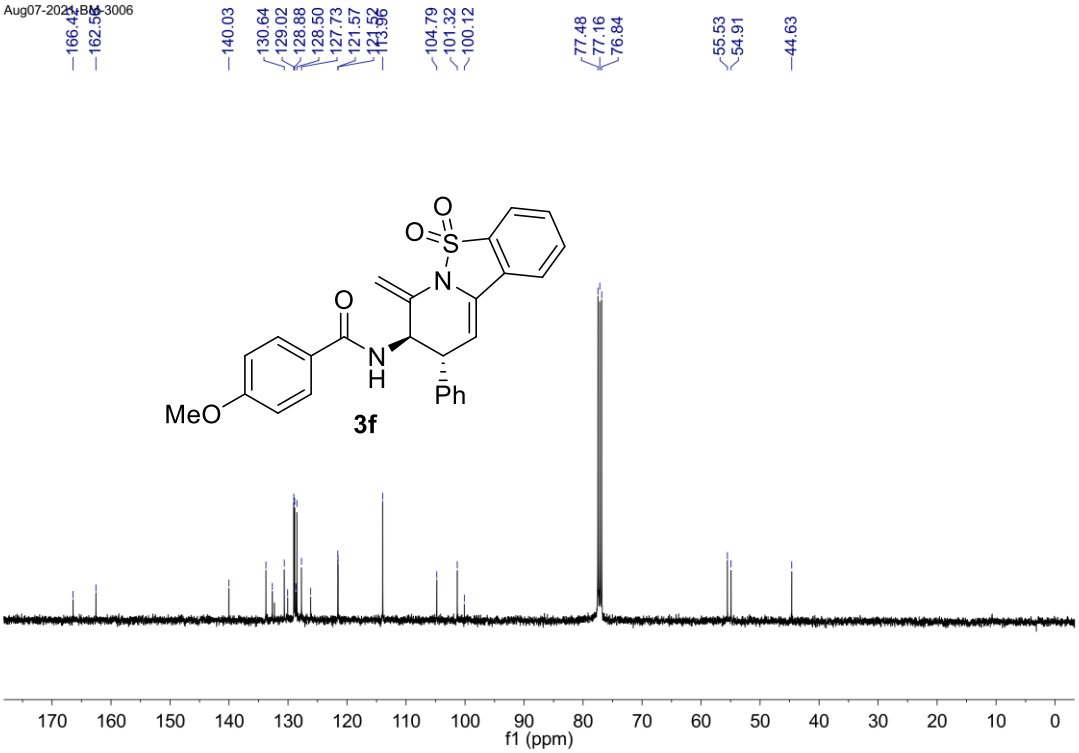

Jul26-2021-bm-3004
7.76
7.74
7.59
7.57
7.52
7.51
7.49
7.34
7.32
7.32
7.30
6.60
6.58
5.88
5.86
5.57
5.57
4.89
4.89
4.86
4.85
4.84
4.14
4.14
4.13
O
O
S
N
O
N
H
Ph
Br
3d
0.92
3.04
2.06
2.02
5.08
0.96
0.98
0.95
0.96
1.07
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

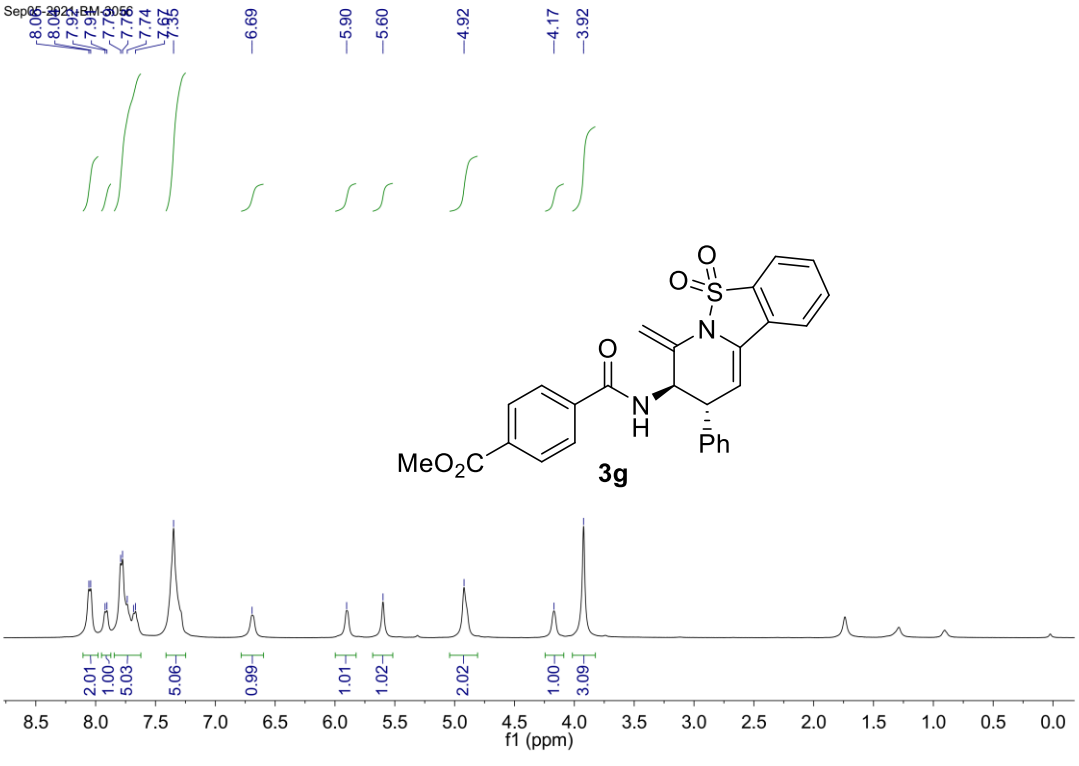

Jul26-2021-bm-3004
165.96
139.83
133.77
132.75
132.48
132.26
131.96
130.70
130.09
129.66
128.91
128.79
128.43
127.81
126.63
121.57
121.50
104.79
101.11
77.48
77.16
76.84
54.87
44.56
O
O
S
N
O
N
H
Ph
Br
3d
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

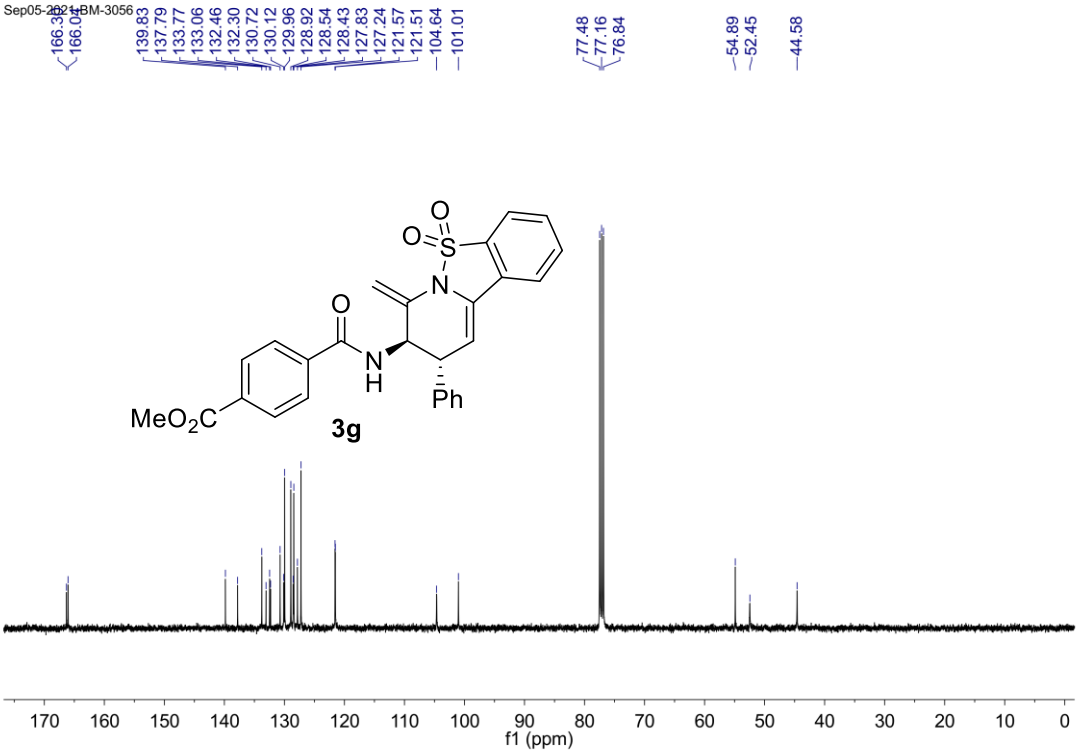

Aug05-2021-bm-3004
7.91
7.85
7.77
7.76
7.64
7.61
7.33
7.29
7.26
7.19
7.17
6.53
5.87
5.86
5.57
4.89
4.17
2.35
O
O
S
N
O
N
H
Ph
Me
3e
1.08
5.11
5.10
1.99
1.01
0.97
0.96
2.00
1.00
3.02
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

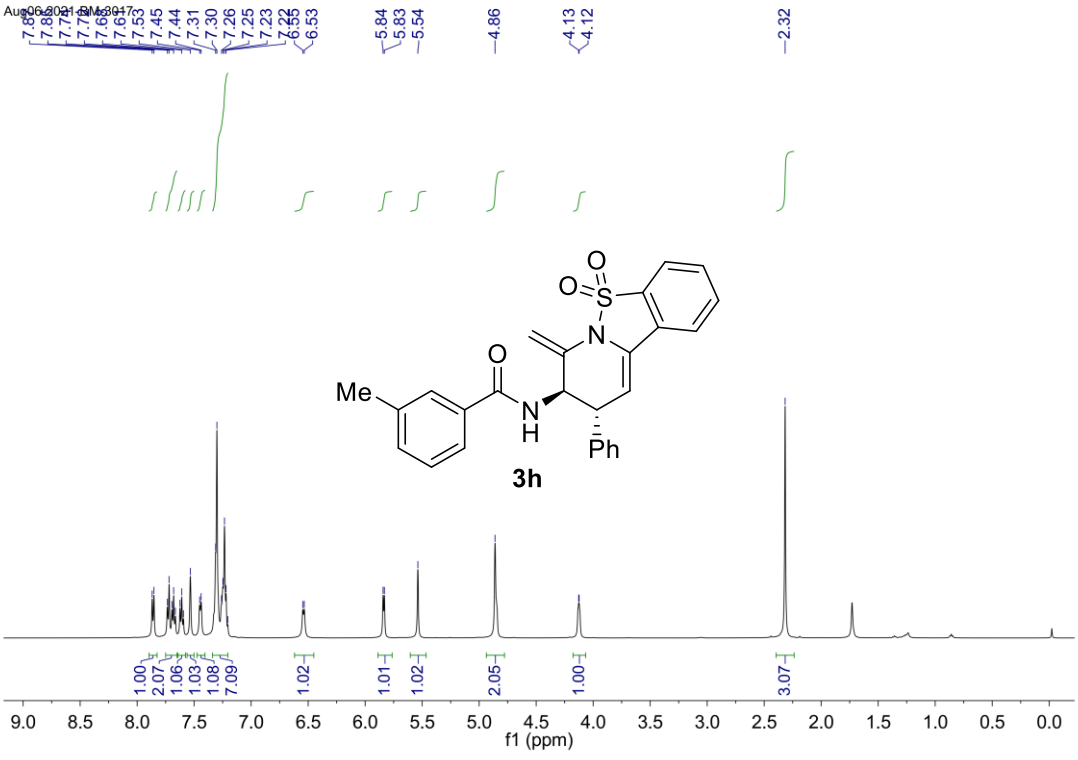

Aug05-2021-bms3004
166.82
142.41
140.00
133.73
132.63
132.28
131.05
130.64
130.03
129.40
128.87
128.48
127.73
127.15
121.55
121.50
104.50
101.22
77.48
77.16
76.84
54.84
44.59
21.57
O
O
S
N
O
N
H
Ph
Me
3e
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

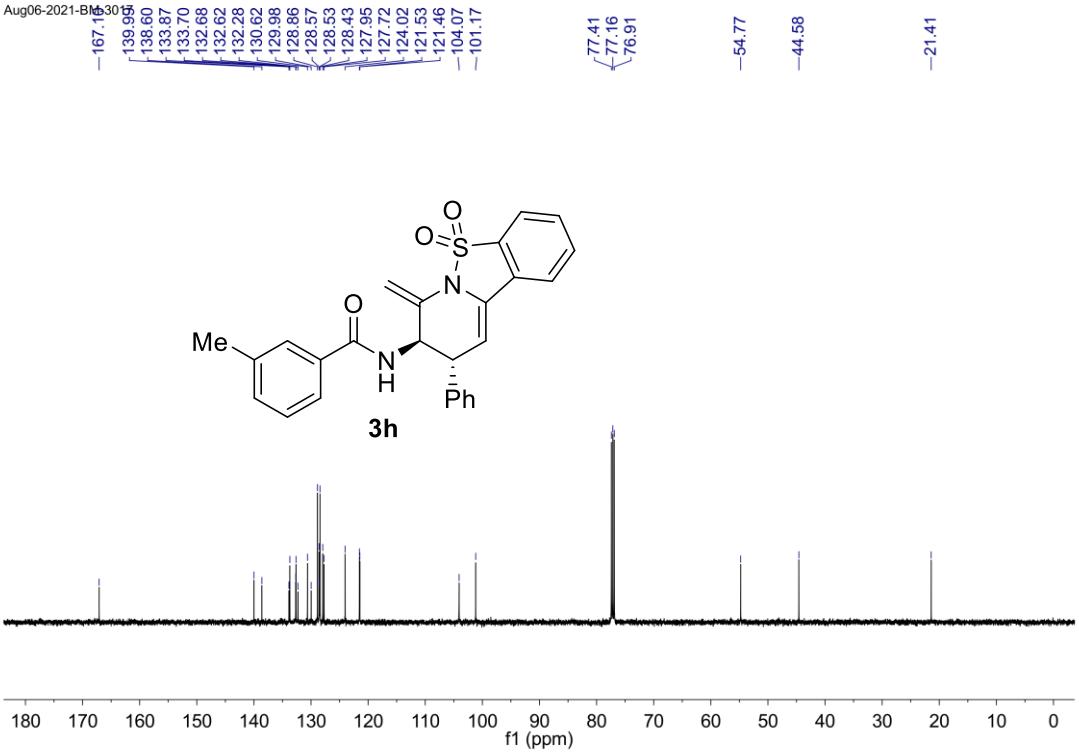

Aug07-2024-BM-3066
7.96
7.78
7.74
7.72
7.70
7.68
7.65
7.33
7.29
7.26
6.88
6.87
6.48
6.47
5.88
5.87
5.57
4.89
4.85
4.84
4.18
3.81
O
O
S
N
O
N
H
Ph
MeO
3f
1.06
5.03
5.03
2.03
1.08
1.05
1.09
0.96
1.07
1.00
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

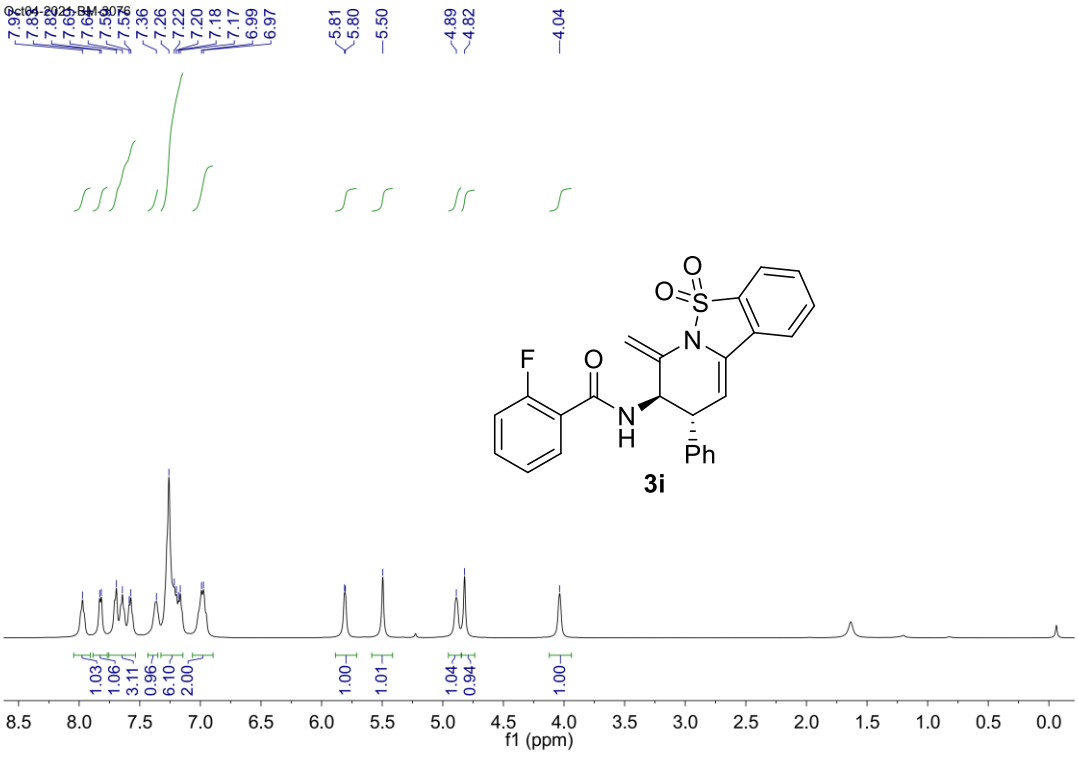

Aug07-2021-BM-3006
166.41
162.56
140.03
130.64
129.02
128.88
128.50
127.73
121.57
104.79
101.32
100.12
77.48
77.16
76.84
55.53
54.91
44.63
O
O
S
N
O
N
H
Ph
MeO
3f
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

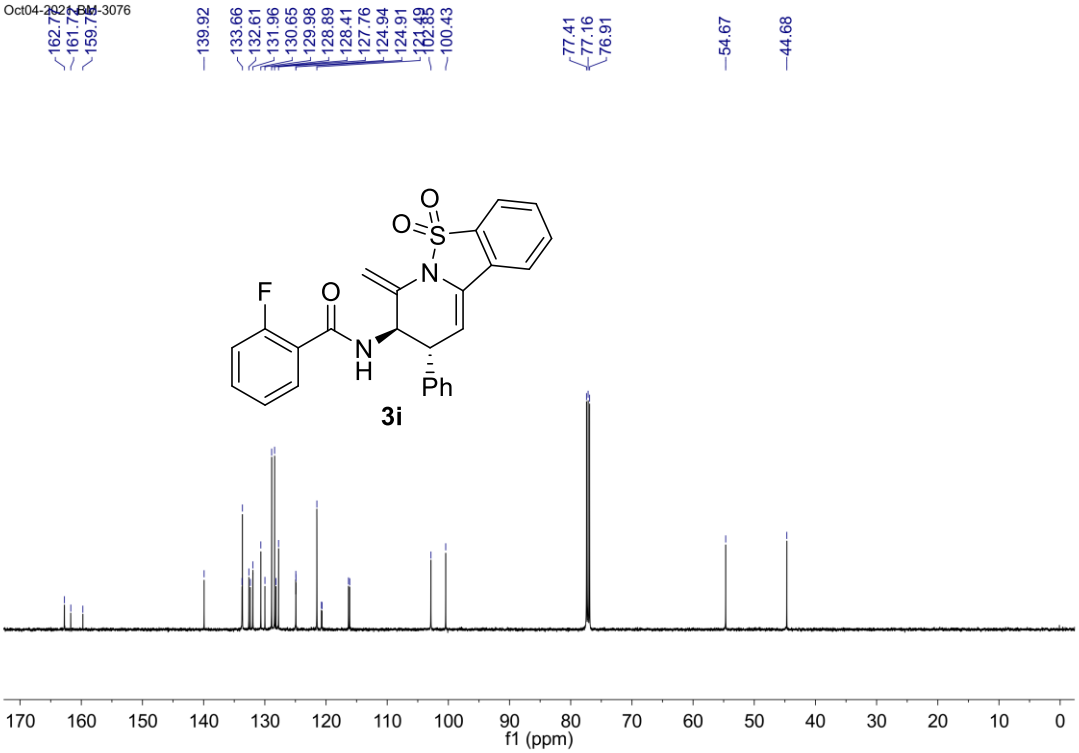

Sep05-2021-BM-3056
8.06
8.05
7.99
7.98
7.79
7.78
7.74
7.67
7.35
6.69
5.90
5.60
4.92
4.17
3.92
O
O
S
N
O
N
H
Ph
MeO2C
3g
2.01
1.00
5.03
5.06
0.99
1.01
1.02
2.02
1.00
3.09
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

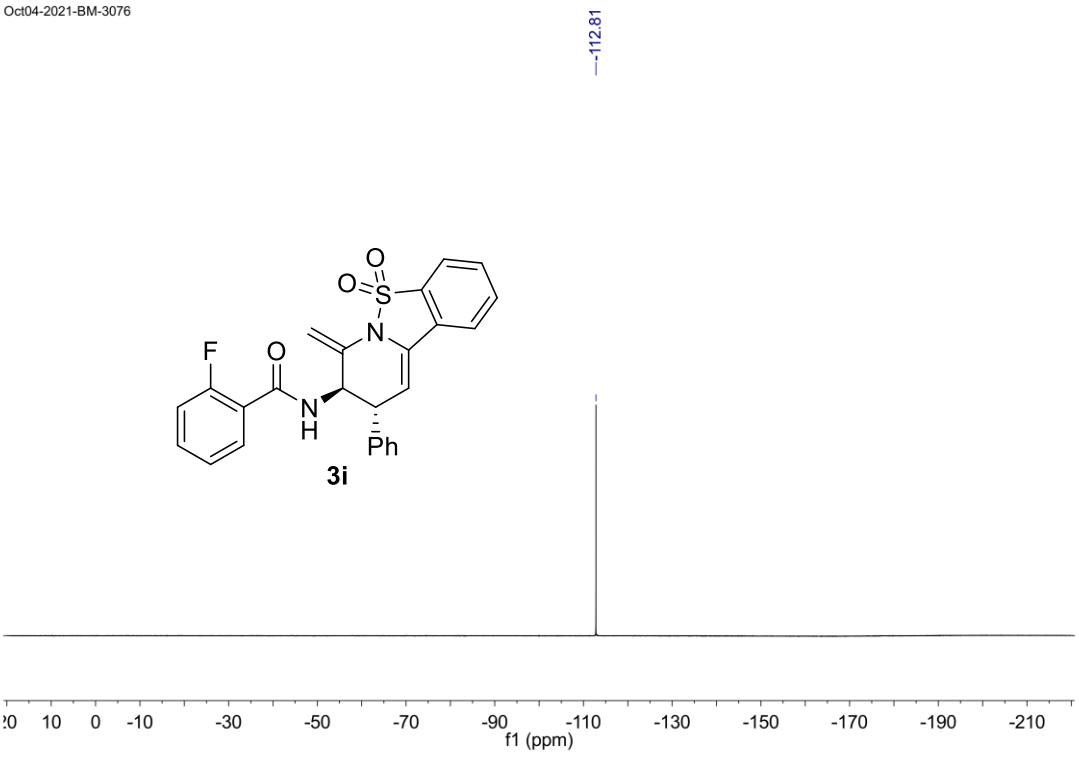

Sep05-2021-BM-3056
166.38
166.04
139.83
137.79
133.77
133.06
132.46
132.30
130.72
130.12
129.96
128.92
128.54
128.43
127.83
127.24
121.57
121.51
104.64
101.01
77.48
77.16
76.84
54.89
52.45
44.58
O
O
S
N
O
N
H
Ph
MeO2C
3g
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

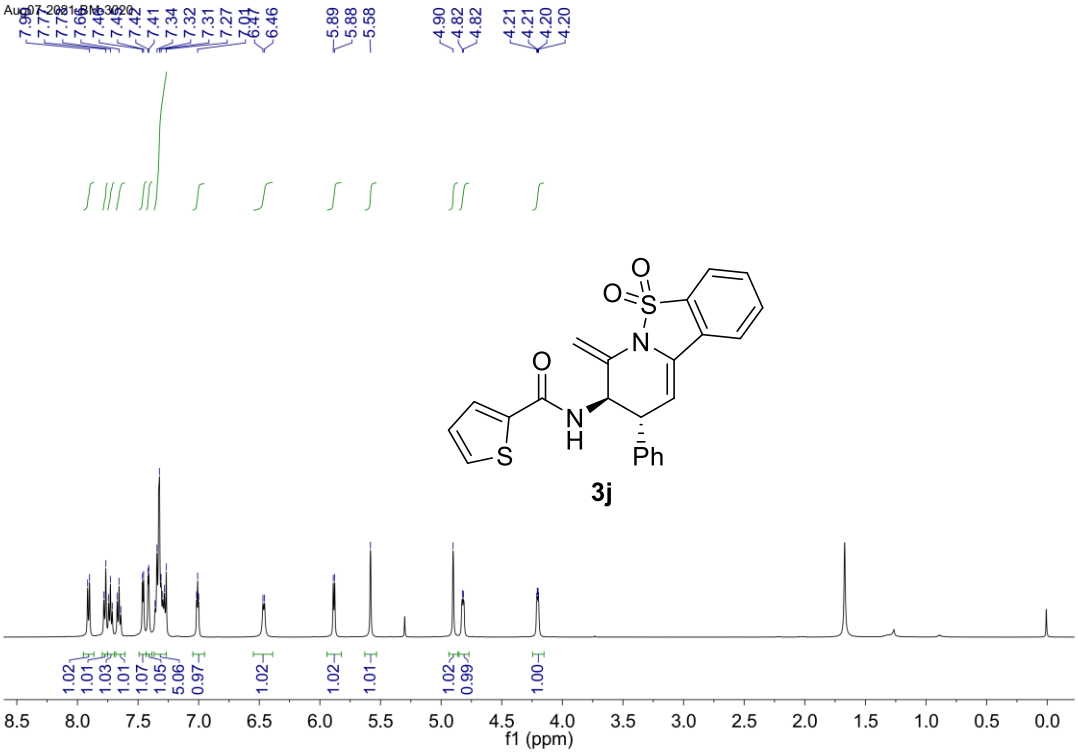

Aug06-2021-BM-3017
7.89
7.88
7.78
7.77
7.68
7.67
7.53
7.45
7.44
7.31
7.30
7.26
7.25
7.23
7.22
6.55
6.53
5.84
5.83
5.54
4.86
4.13
4.12
2.32
O
O
S
N
O
N
H
Ph
Me
3h
1.00
2.07
1.06
1.03
1.08
7.09
1.02
1.01
1.02
2.05
1.00
3.07
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


Aug06-2021-BM-3015
167.16
139.99
138.60
133.87
133.70
132.68
132.62
132.28
130.62
129.98
128.86
128.57
128.53
128.43
127.95
127.72
124.02
121.53
121.46
104.07
101.17
77.41
77.16
76.91
54.77
44.58
21.41
O
O
S
N
O
Me
N
H
Ph
3h
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Oct04-2021-BM-3076
7.93
7.85
7.83
7.69
7.68
7.56
7.55
7.36
7.26
7.22
7.20
7.18
7.17
6.99
6.97
5.81
5.80
5.50
4.89
4.82
4.04
O
O
S
N
F
O
N
H
Ph
3i
1.03
1.06
3.11
0.96
6.10
2.00
1.00
1.01
1.04
0.94
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


Oct04-2021-BM-3076
162.77
161.77
159.78
139.92
133.66
132.61
131.96
130.65
129.98
128.89
128.41
127.76
124.94
124.91
122.85
100.43
77.41
77.16
76.91
54.67
44.68
F
O
O
S
N
N
H
Ph
3i
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Oct04-2021-BM-3076
112.81
F
O
O
S
N
N
H
Ph
3i
20
10
0
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)


Aug07-2021-BM-3020
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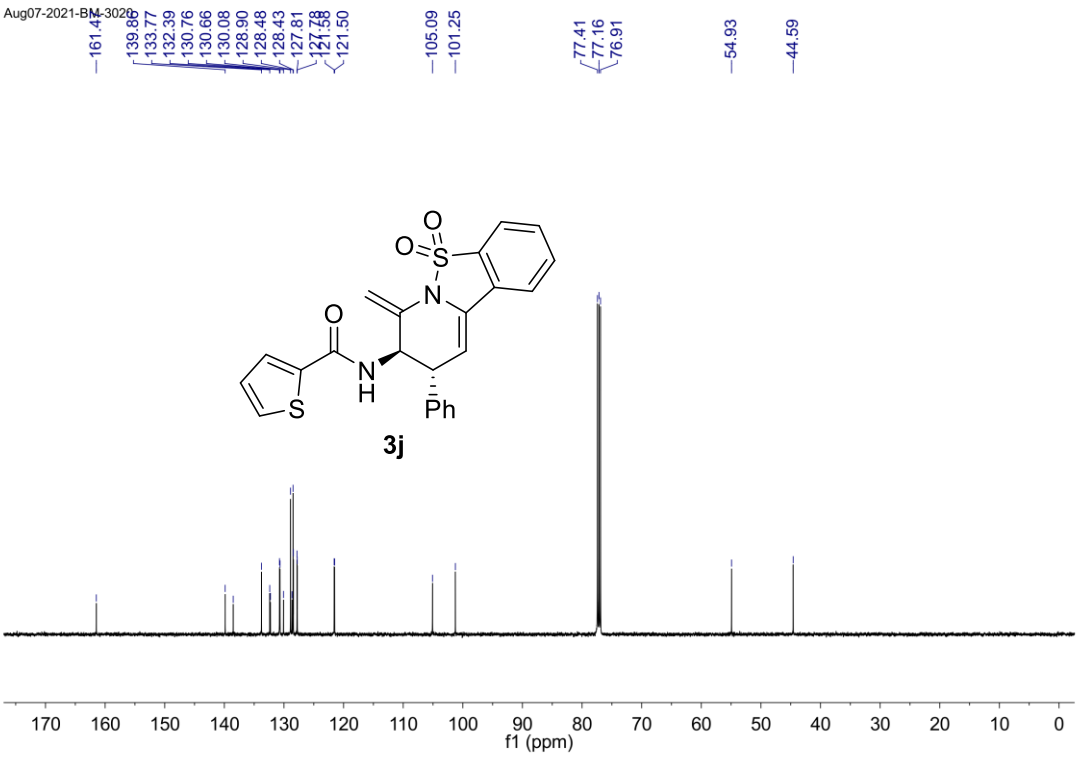
7.77
7.75
7.66
7.46
7.45
7.42
7.41
7.34
7.32
7.31
7.27
7.01
6.47
6.46
5.89
5.88
5.58
4.90
4.82
4.82
4.21
4.21
4.20
4.20
O
O
S
N
O
N
H
S
Ph
3j
1.02
1.01
1.03
1.01
1.07
1.05
5.06
0.97
1.02
1.02
1.01
1.02
0.99
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


Aug07-2021-BM-3020
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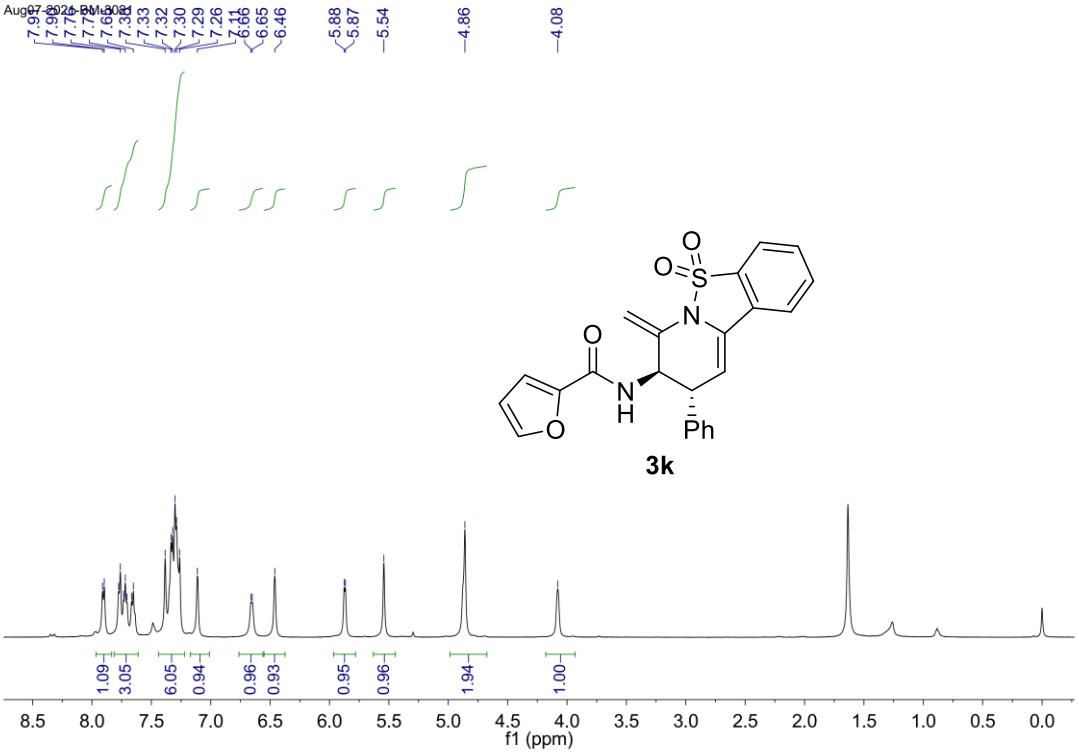
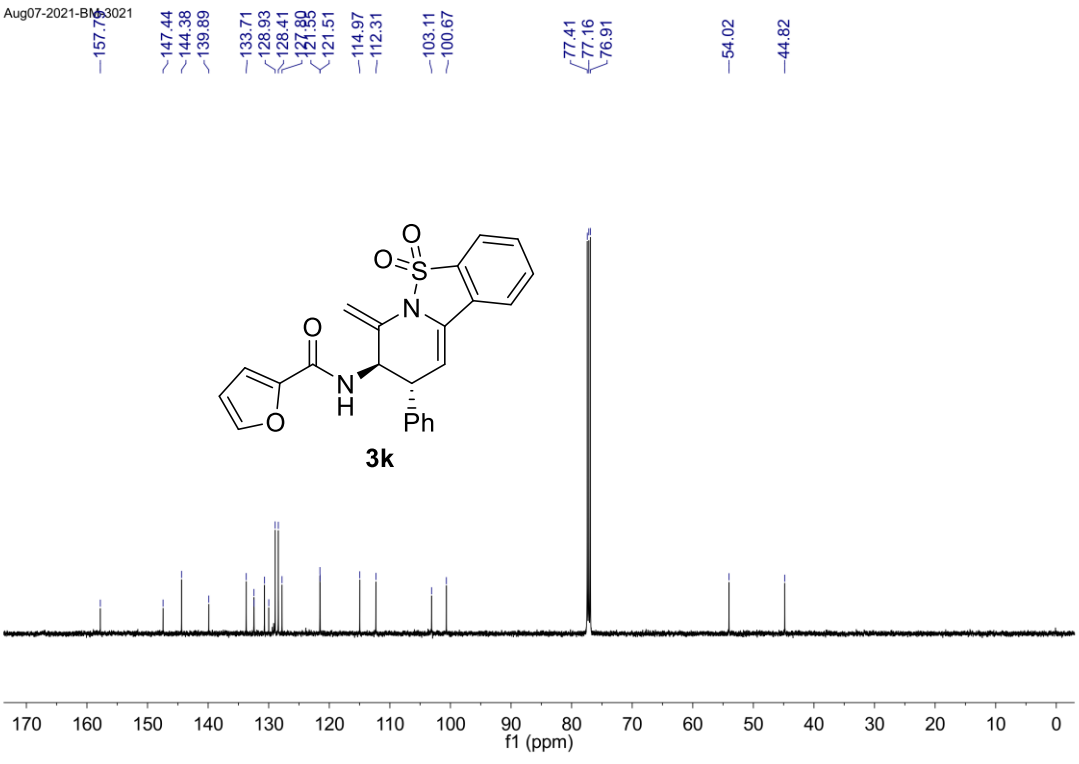
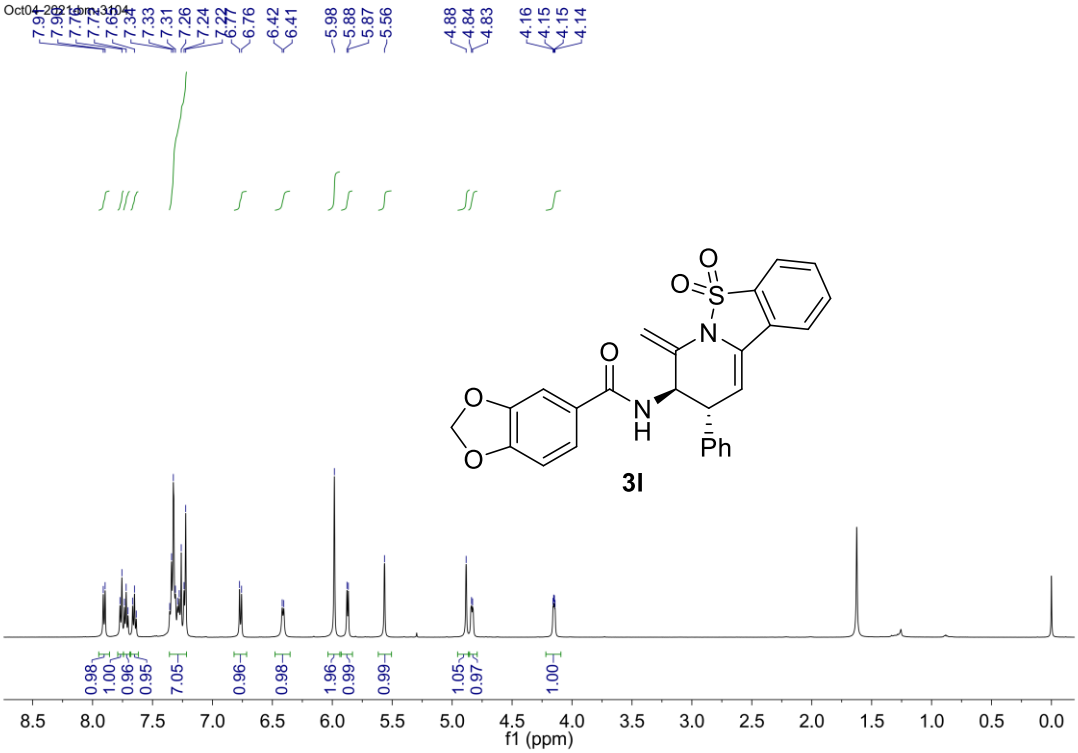
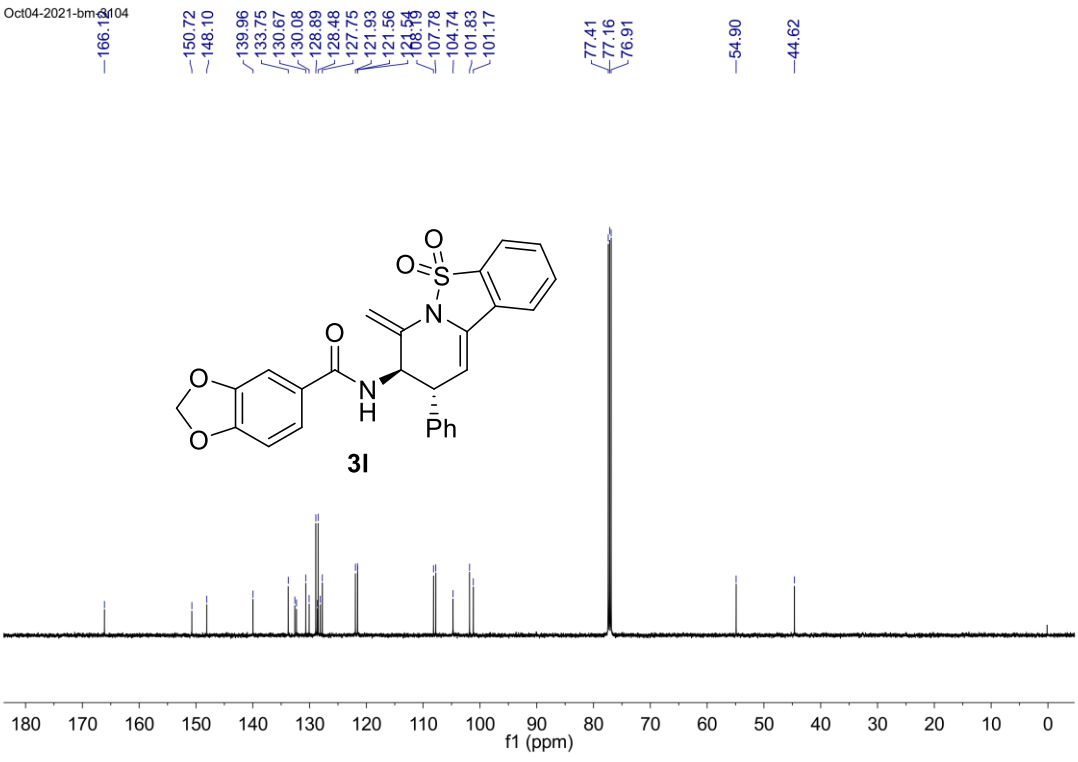
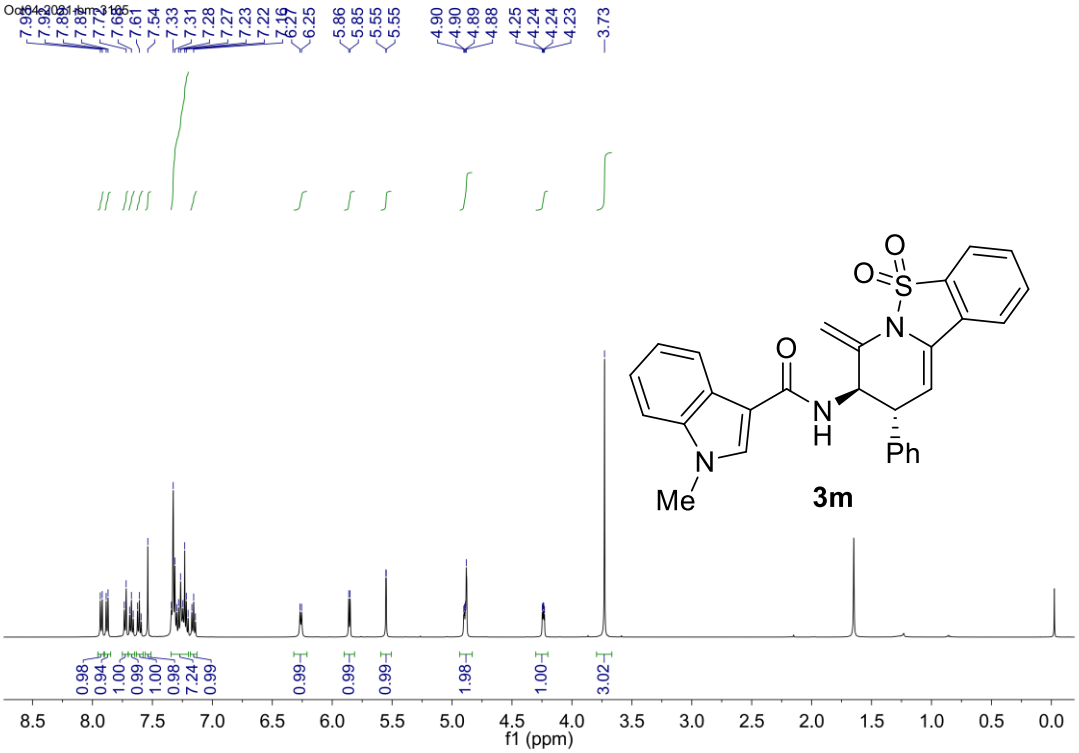
132.39
130.76
130.66
130.08
128.90
128.48
128.43
127.81
121.58
121.50
105.09
101.25
77.41
77.16
76.91
54.93
44.59
O
O
S
N
O
N
H
S
Ph
3j
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

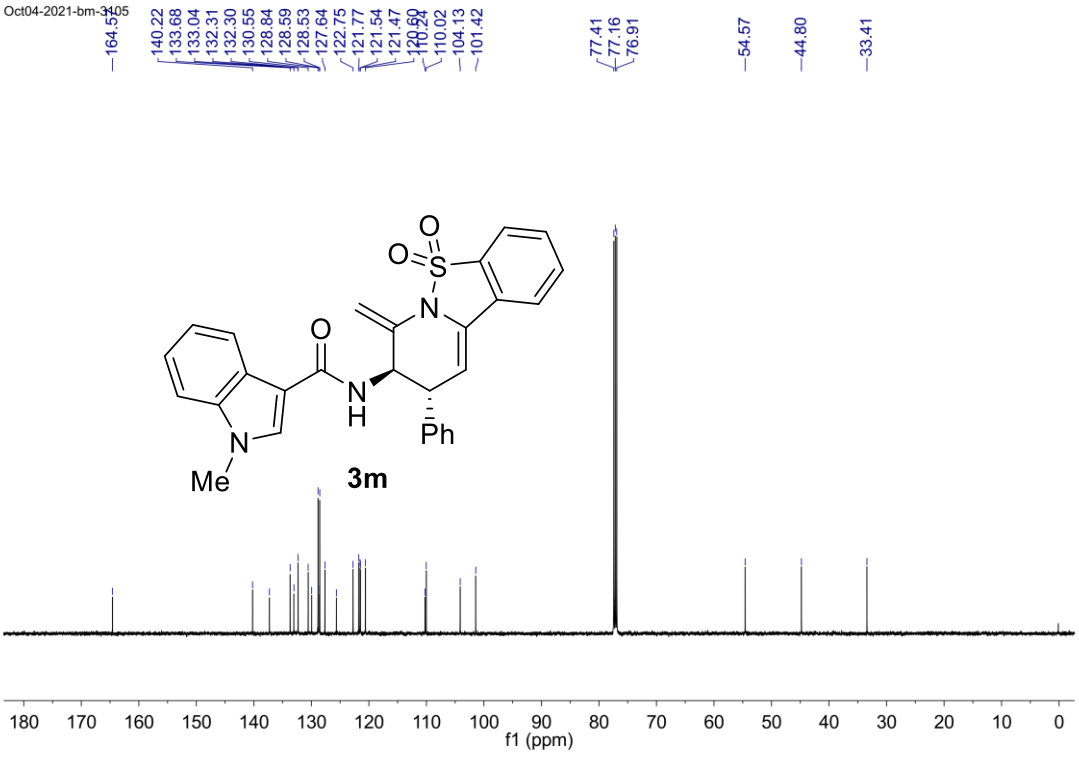

Aug07-2021-BM-3021
7.95
7.90
7.78
7.76
7.66
7.38
7.33
7.32
7.30
7.29
7.26
7.11
6.66
6.65
6.46
5.88
5.87
5.54
4.86
4.08
O
O
S
N
O
N
H
O
Ph
3k
1.09
3.05
6.05
0.94
0.96
0.93
0.95
0.96
1.94
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

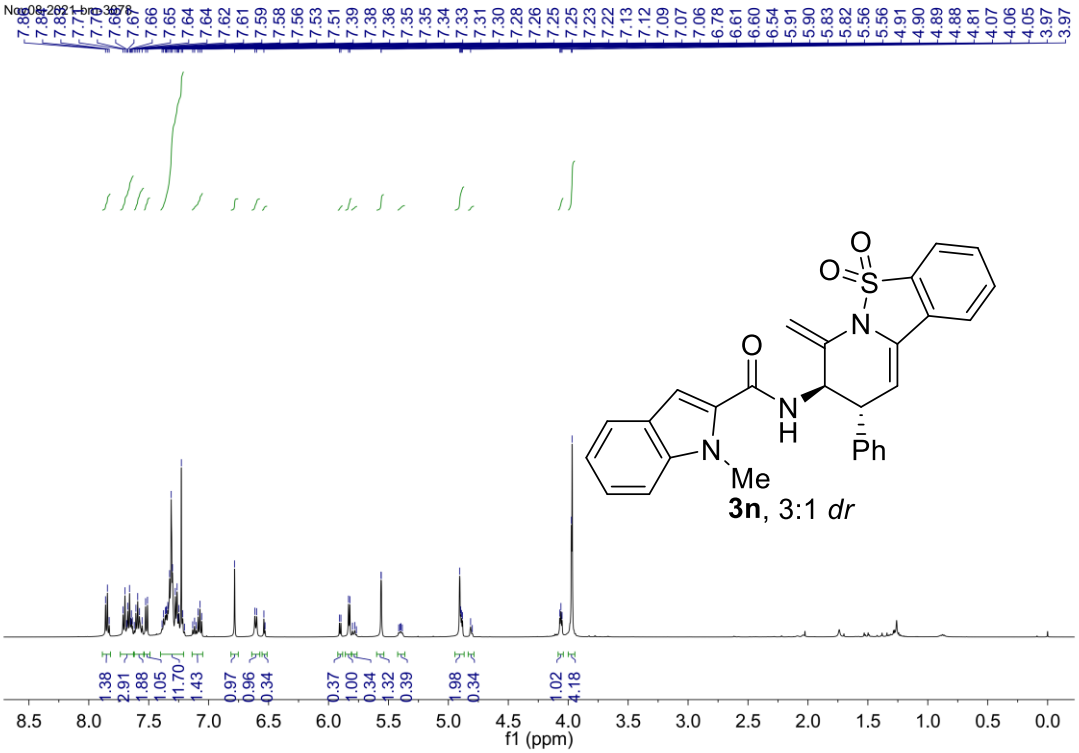

Aug07-2021-BM-3021
157.79
147.44
144.38
139.89
133.71
128.93
128.41
127.80
127.55
121.51
114.97
112.31
103.11
100.67
77.41
77.16
76.91
54.02
44.82
O
O
S
N
O
N
H
O
Ph
3k
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

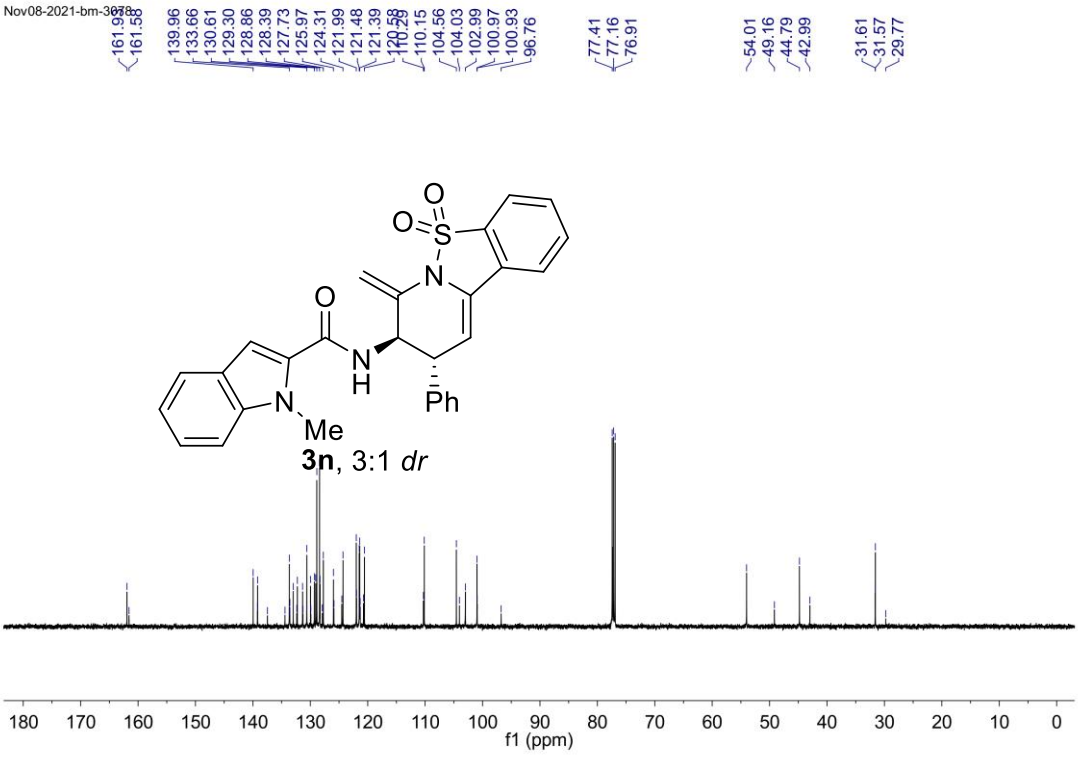

Oct04-2021-bm-3l04
7.98
7.76
7.64
7.34
7.33
7.31
7.26
7.24
6.76
6.42
6.41
5.98
5.88
5.87
5.56
4.88
4.84
4.83
4.16
4.15
4.14
3l
0.98
1.00
0.96
0.95
7.05
0.96
0.98
1.96
0.99
0.99
1.05
0.97
1.00
f1 (ppm)

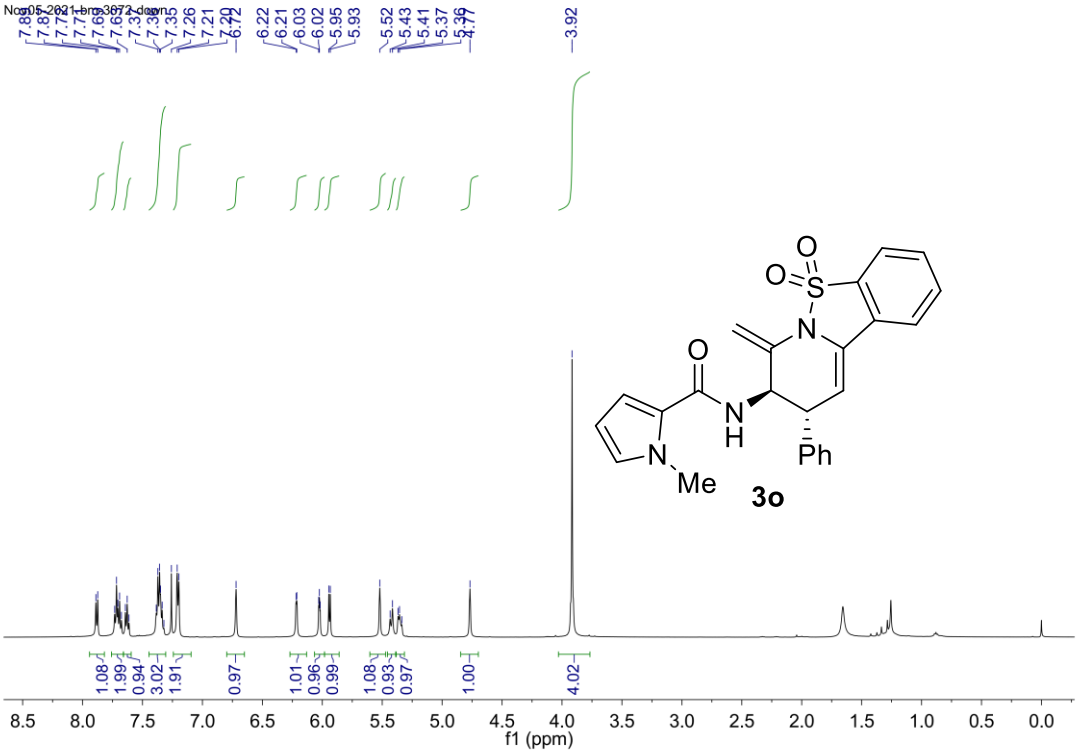

Oct04-2021-bm-3l04
166.12
150.72
148.10
139.96
133.75
130.67
130.08
128.89
128.48
127.75
121.93
121.56
107.78
104.74
101.83
101.17
77.41
77.16
76.91
54.90
44.62
3l
f1 (ppm)

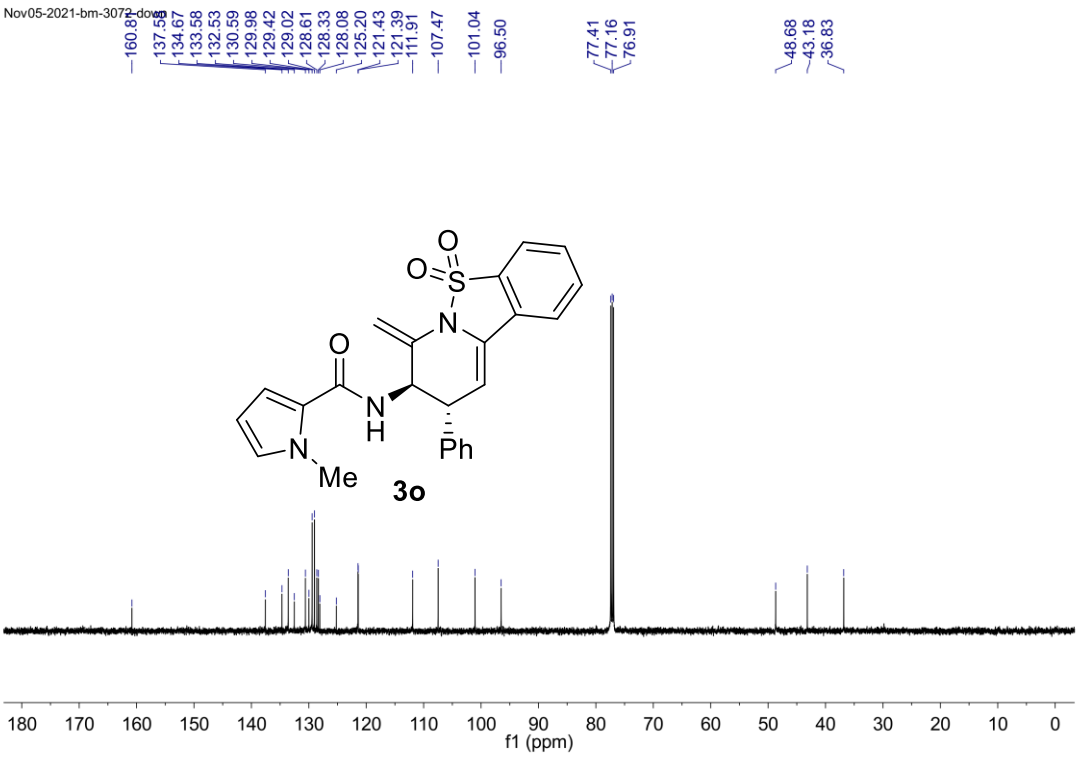

Oct04-2021-bm-3105
7.95
7.92
7.88
7.85
7.72
7.68
7.61
7.54
7.33
7.31
7.28
7.27
7.23
7.22
7.16
6.27
6.25
5.86
5.85
5.55
5.55
4.90
4.90
4.89
4.88
4.25
4.24
4.24
4.23
3.73
0.98
0.94
1.00
0.99
1.00
0.98
7.24
0.99
0.99
0.99
0.99
1.98
1.00
3.02
O
O
S
N
O
N
H
Ph
N
Me
3m
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

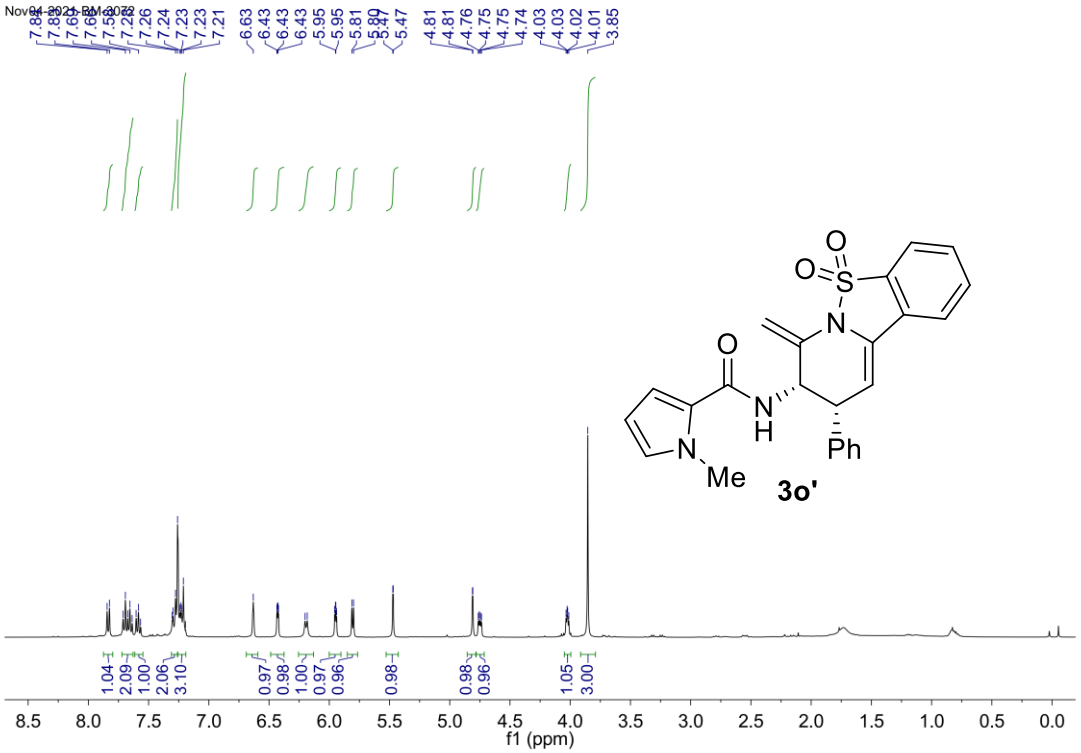

Oct04-2021-bm-3105
164.52
140.22
133.68
133.04
132.31
132.30
130.55
128.84
128.59
128.53
127.64
122.75
121.77
121.54
121.47
120.60
120.24
110.02
104.13
101.42
77.41
77.16
76.91
54.57
44.80
33.41
O
O
S
N
O
N
H
Ph
N
Me
3m
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

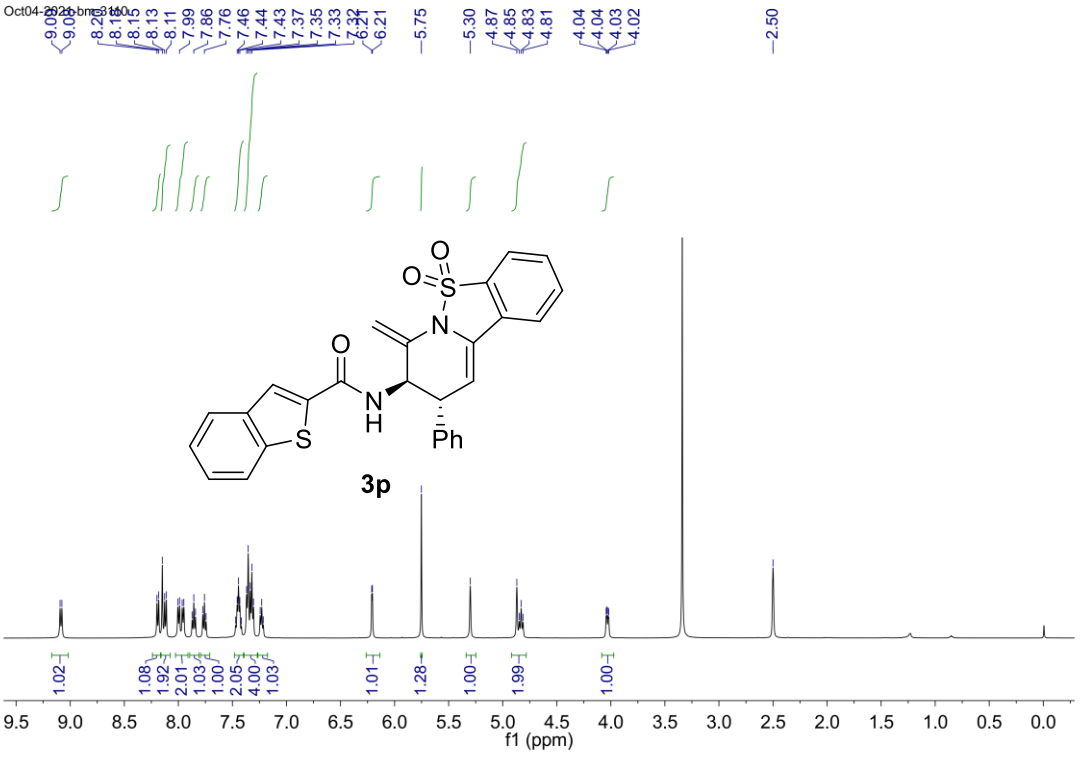

Nov08-2021-bm-3678
7.88 7.84 7.81 7.77 7.76 7.67 7.66 7.65 7.64 7.64 7.62 7.61 7.59 7.58 7.56 7.53 7.51 7.39 7.38 7.36 7.35 7.35 7.34 7.33 7.31 7.30 7.28 7.26 7.25 7.25 7.23 7.22 7.13 7.12 7.09 7.07 7.06 6.78 6.61 6.60 6.54 5.91 5.90 5.83 5.82 5.56 5.56 4.91 4.90 4.89 4.88 4.81 4.07 4.06 4.05 3.97 3.97
O
O
S
N
O
N
H
Ph
N
Me
3n, 3:1 dr
1.38 2.91 1.88 1.05 11.70 1.43 0.97 0.96 0.34 0.37 1.00 0.34 1.32 0.39 1.98 0.34 1.02 4.18
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

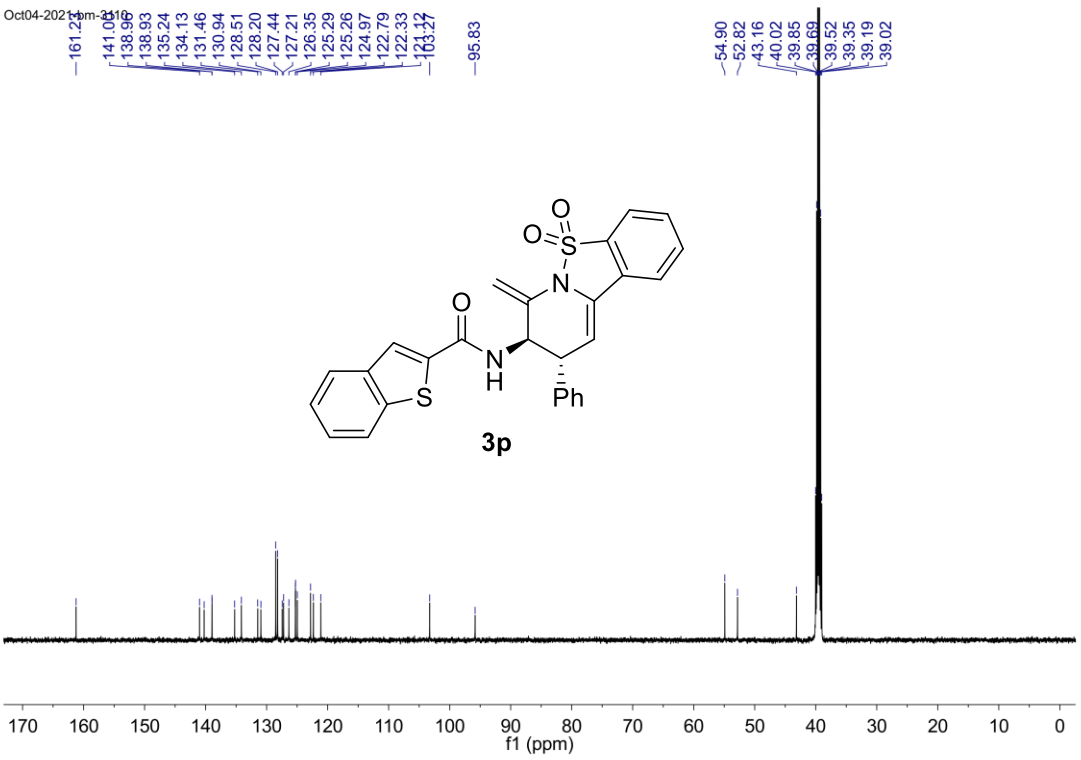

Nov08-2021-bm-3678
161.93 161.58 139.96 133.66 130.61 129.30 128.86 128.39 127.73 125.97 124.31 121.99 121.48 121.39 110.15 104.56 104.03 102.99 100.97 100.93 96.76 77.41 77.16 76.91 54.01 49.16 44.79 42.99 31.61 31.57 29.77
O
O
S
N
O
N
H
Ph
N
Me
3n, 3:1 dr
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

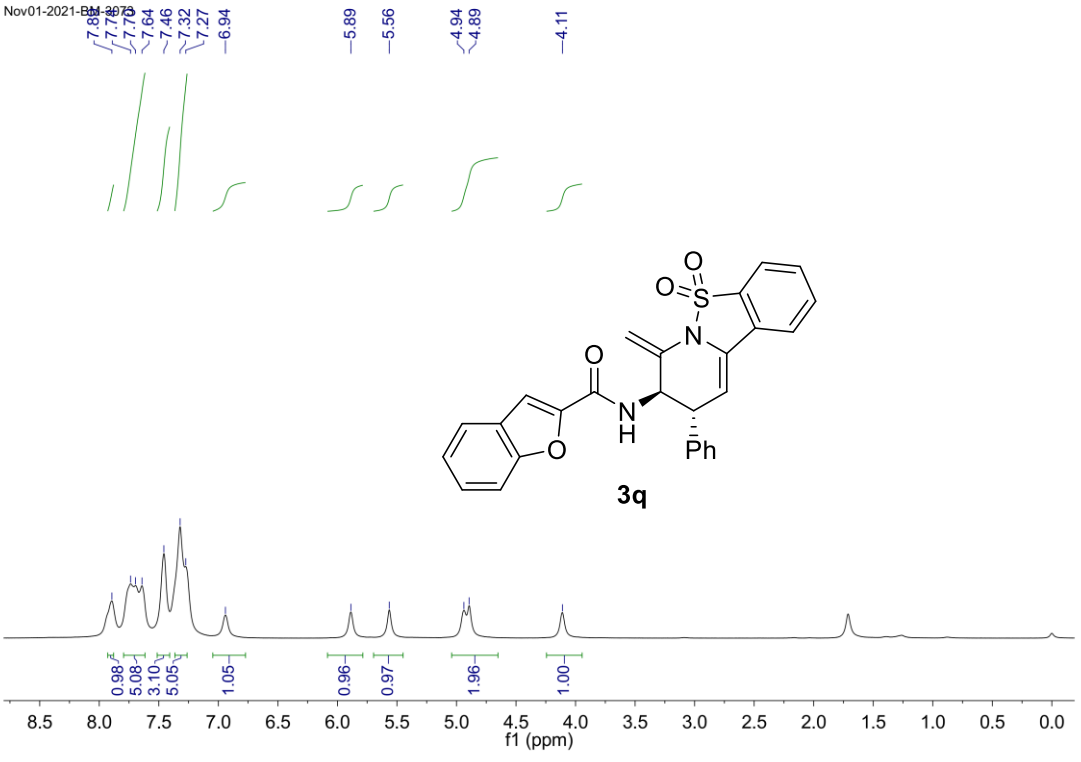

Nov05-2021-bm-3072-down
7.85
7.81
7.79
7.77
7.71
7.69
7.67
7.33
7.30
7.26
7.21
6.22
6.21
6.03
6.02
5.95
5.93
5.52
5.43
5.41
5.37
3.92
O
O
S
N
O
N
H
N
Me
Ph
3o
1.08
1.99
0.94
3.02
1.91
0.97
1.01
0.96
0.99
1.08
0.93
0.97
1.00
4.02
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

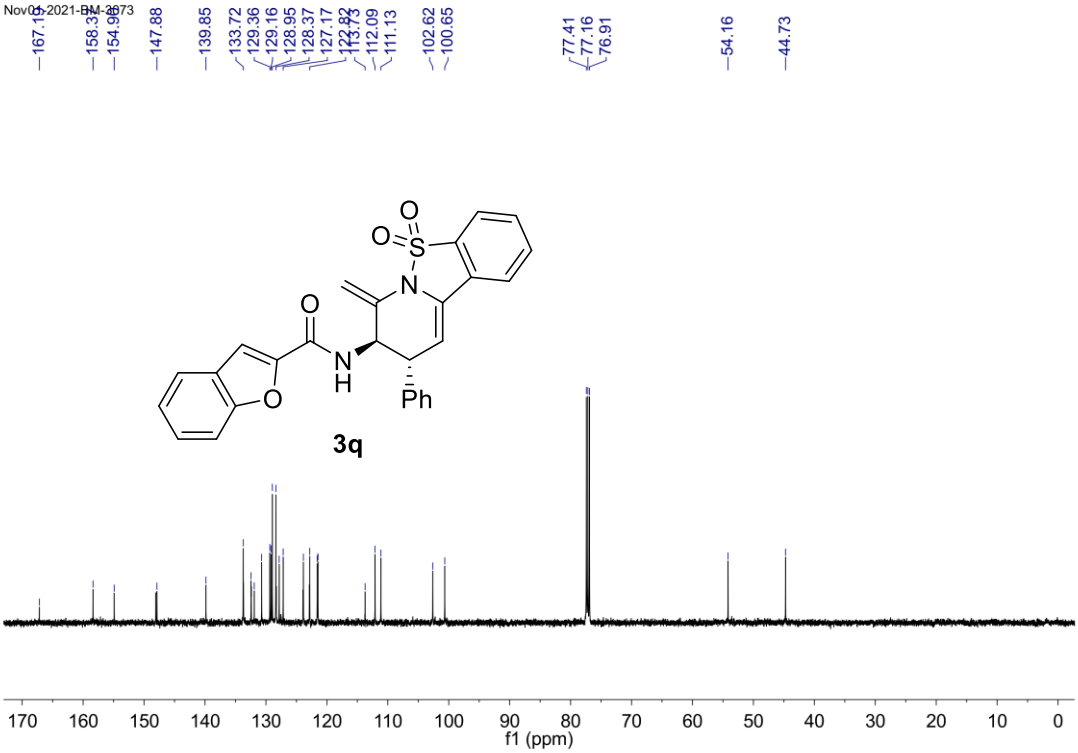

Nov05-2021-bm-3072-down
160.81
137.58
134.67
133.58
132.53
130.59
129.98
129.42
129.02
128.61
128.33
128.08
125.20
121.43
121.39
111.91
107.47
101.04
96.50
77.41
77.16
76.91
48.68
43.18
36.83
O
O
S
N
O
N
H
N
Me
Ph
3o
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

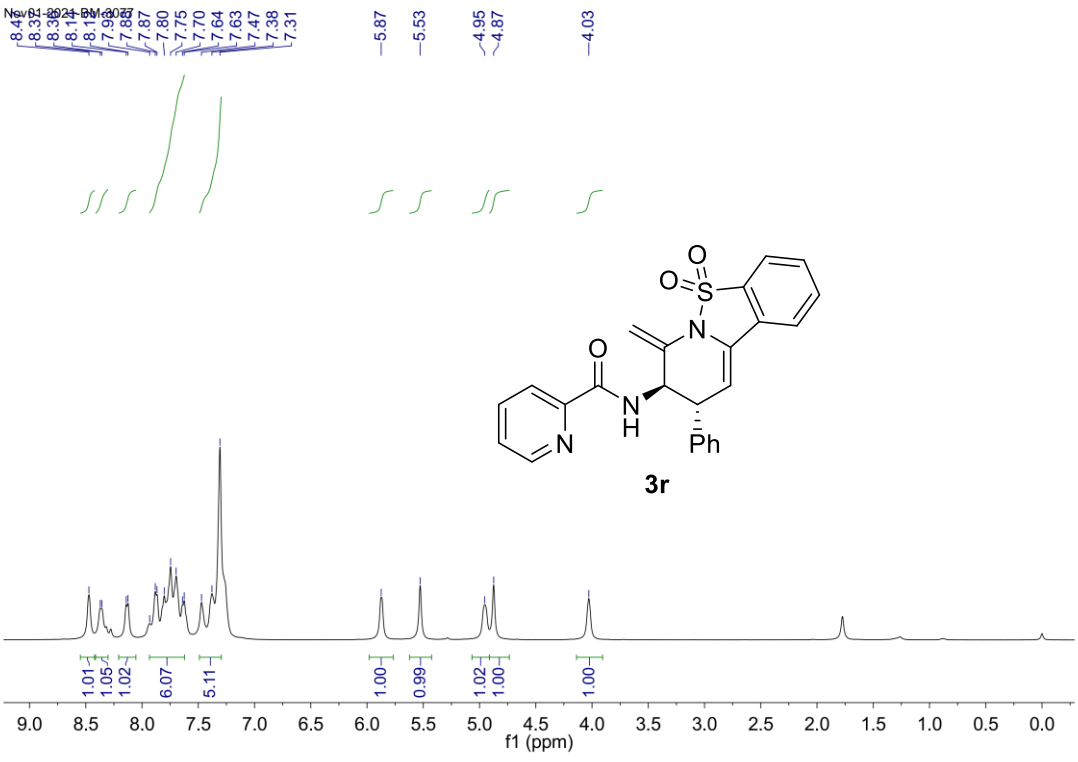

7.84
7.83
7.68
7.68
7.56
7.56
7.26
7.24
7.23
7.23
7.21
6.63
6.43
6.43
6.43
5.95
5.95
5.81
5.80
5.47
4.81
4.81
4.76
4.75
4.75
4.74
4.03
4.03
4.02
4.01
3.85
O
O
S
N
O
N
H
Ph
N
Me
3o'
1.04
2.09
1.00
2.06
3.10
0.97
0.98
1.00
0.97
0.96
0.98
0.98
0.96
1.05
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

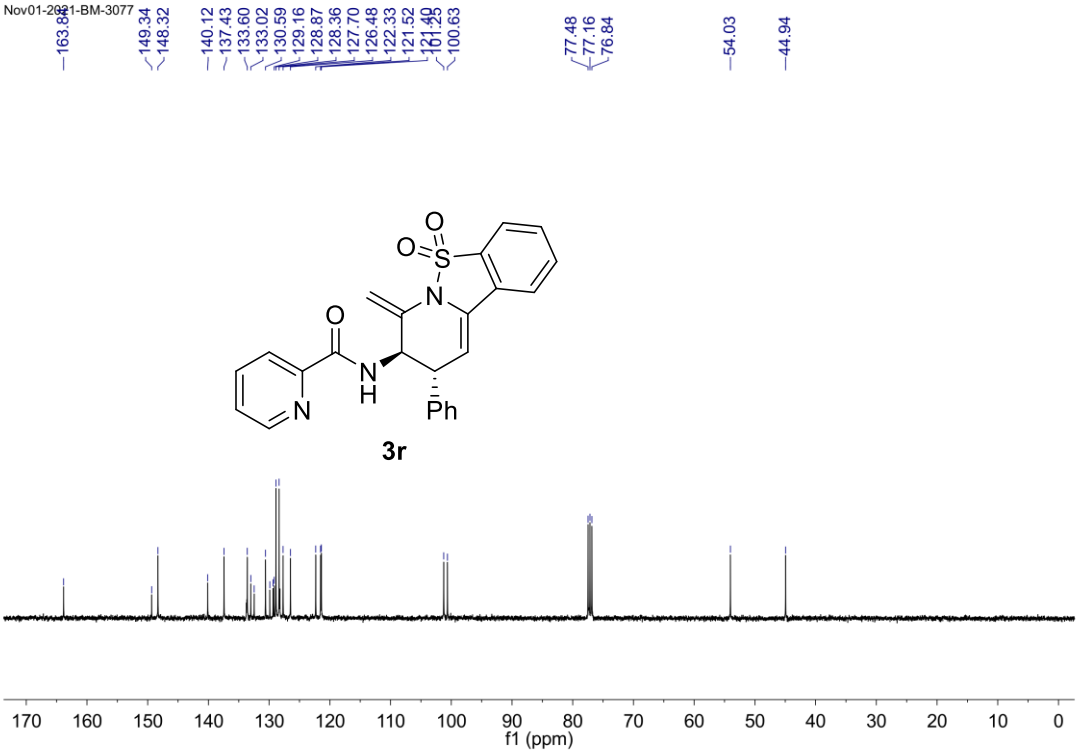

9.09
9.08
8.20
8.19
8.15
8.13
8.11
7.99
7.86
7.76
7.46
7.44
7.43
7.37
7.35
7.33
7.32
6.21
6.21
5.75
5.30
4.87
4.85
4.83
4.81
4.04
4.04
4.03
4.02
2.50
O
O
S
N
O
N
H
Ph
S
3p
1.02
1.08
1.92
2.01
1.03
1.00
2.05
4.00
1.03
1.01
1.28
1.00
1.99
1.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

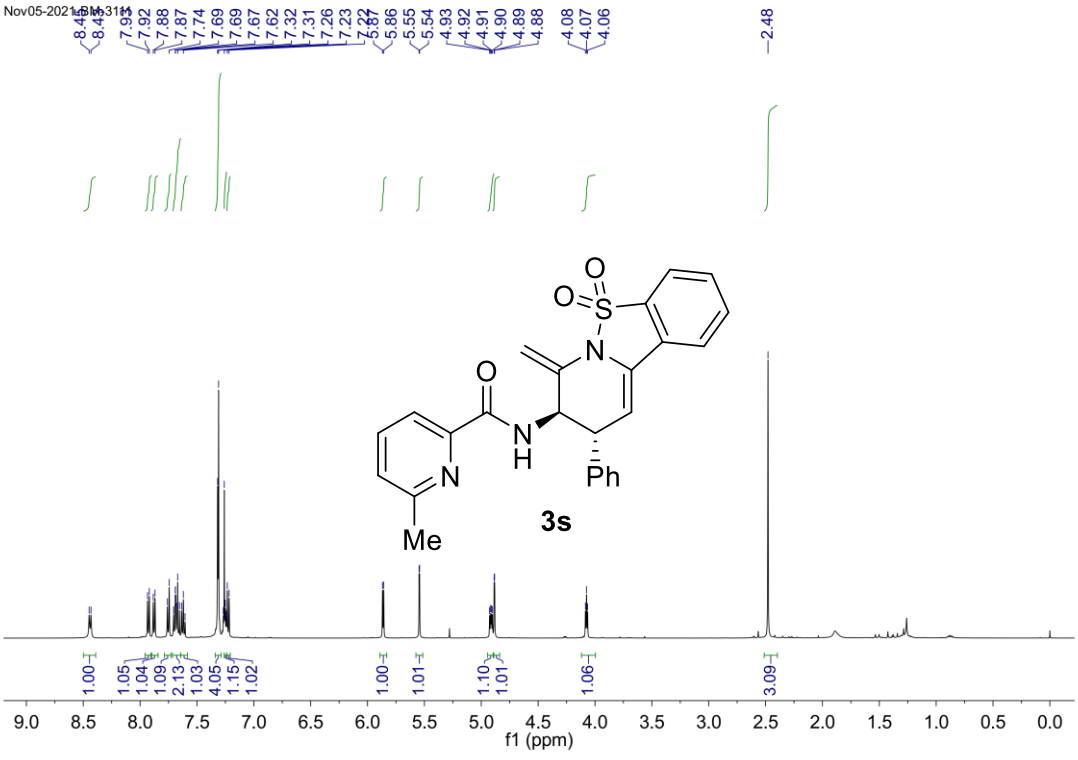

Oct04-2021-bm-3316
161.22
141.06
138.96
138.93
135.24
134.13
131.46
130.94
128.51
128.20
127.44
127.21
126.35
125.29
125.26
124.97
122.79
122.33
95.83
54.90
52.82
43.16
40.02
39.85
39.69
39.52
39.35
39.19
39.02
O
O
S
N
O
N
H
S
Ph
3p
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

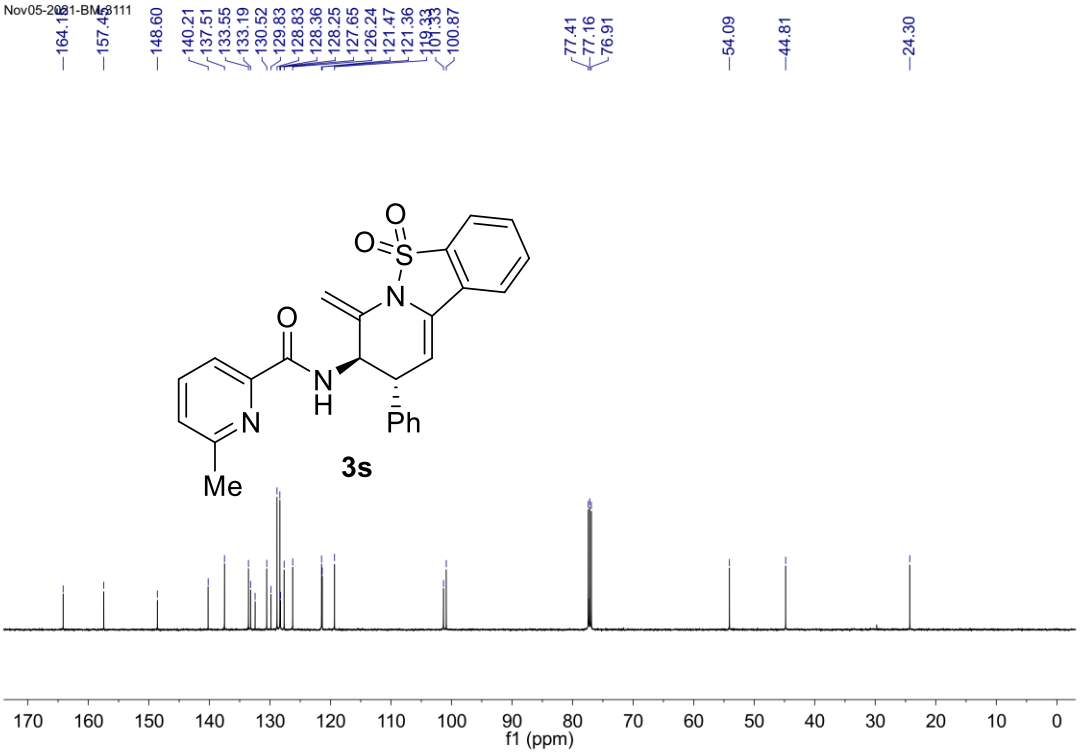

Nov01-2021-BM-3075
7.80
7.78
7.76
7.64
7.46
7.32
7.27
6.94
5.89
5.56
4.94
4.89
4.11
O
O
S
N
O
N
H
O
Ph
3q
0.98
5.08
3.10
5.05
1.05
0.96
0.97
1.96
1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

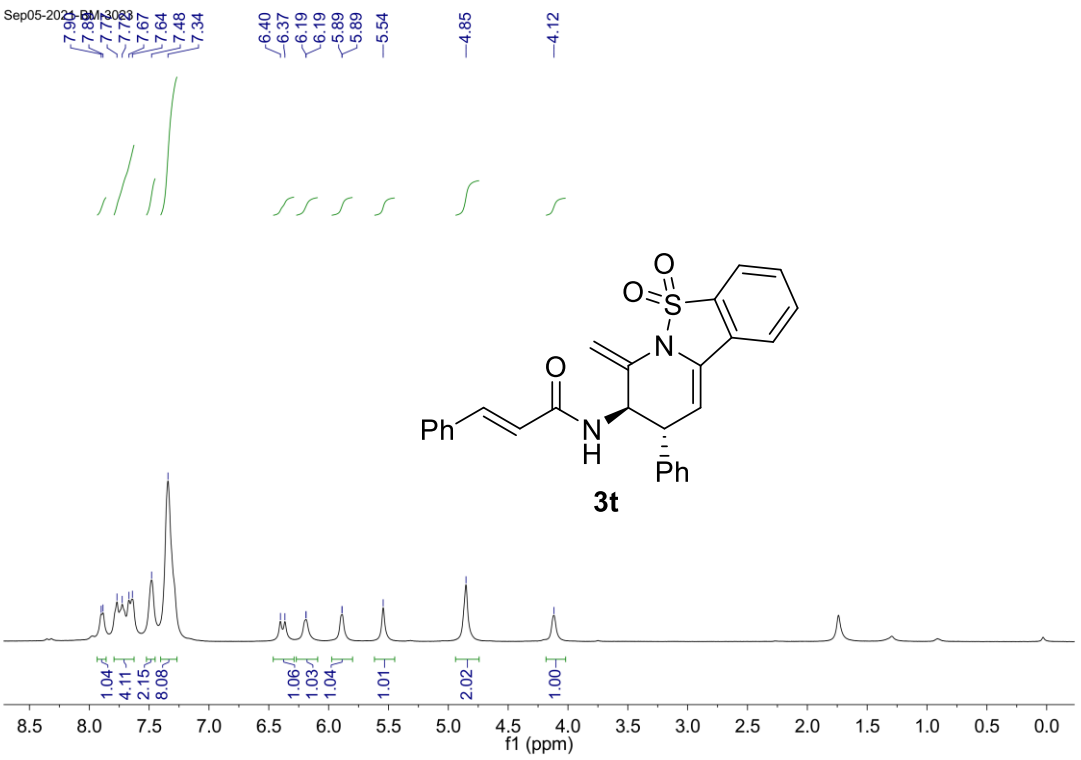

Nov01-2021-BM-3673
167.15
158.33
154.96
147.88
139.85
133.72
129.36
129.16
128.95
128.37
127.17
122.82
113.73
112.09
111.13
102.62
100.65
77.41
77.16
76.91
54.16
44.73
3q
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

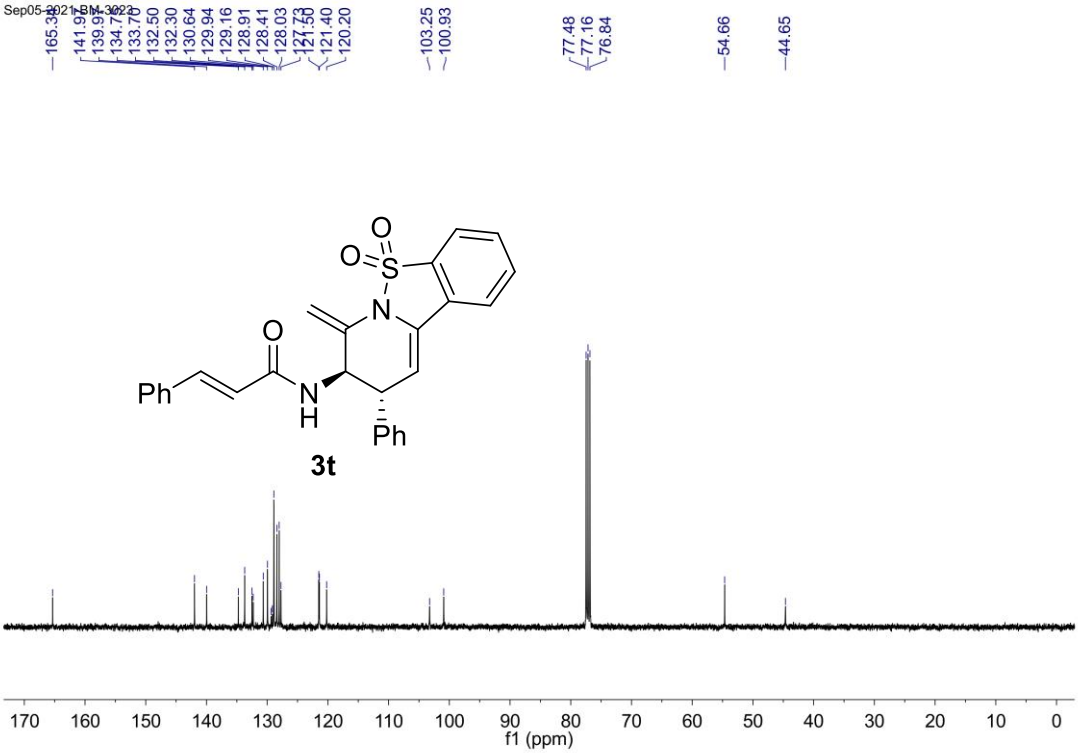

Nov01-2021-BM-3027
8.42
8.33
8.30
8.18
7.99
7.88
7.87
7.80
7.75
7.70
7.64
7.63
7.47
7.38
7.31
5.87
5.53
4.95
4.87
4.03
3r
1.01
1.05
1.02
6.07
5.11
1.00
0.99
1.02
1.00
1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

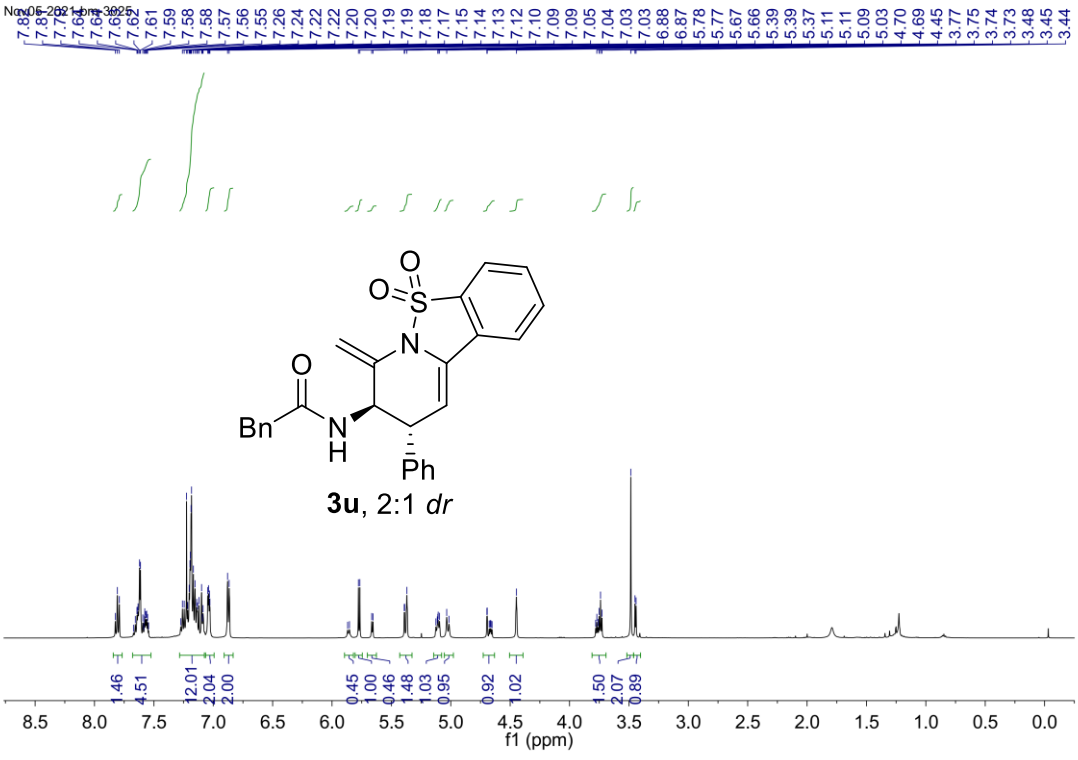

Nov01-2021-BM-3077
163.88
149.34
148.32
140.12
137.43
133.60
133.02
130.59
129.16
128.87
128.36
127.70
126.48
122.33
121.52
121.40
121.25
100.63
77.48
77.16
76.84
54.03
44.94
O
O
S
N
O
N
H
N
Ph
3r
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

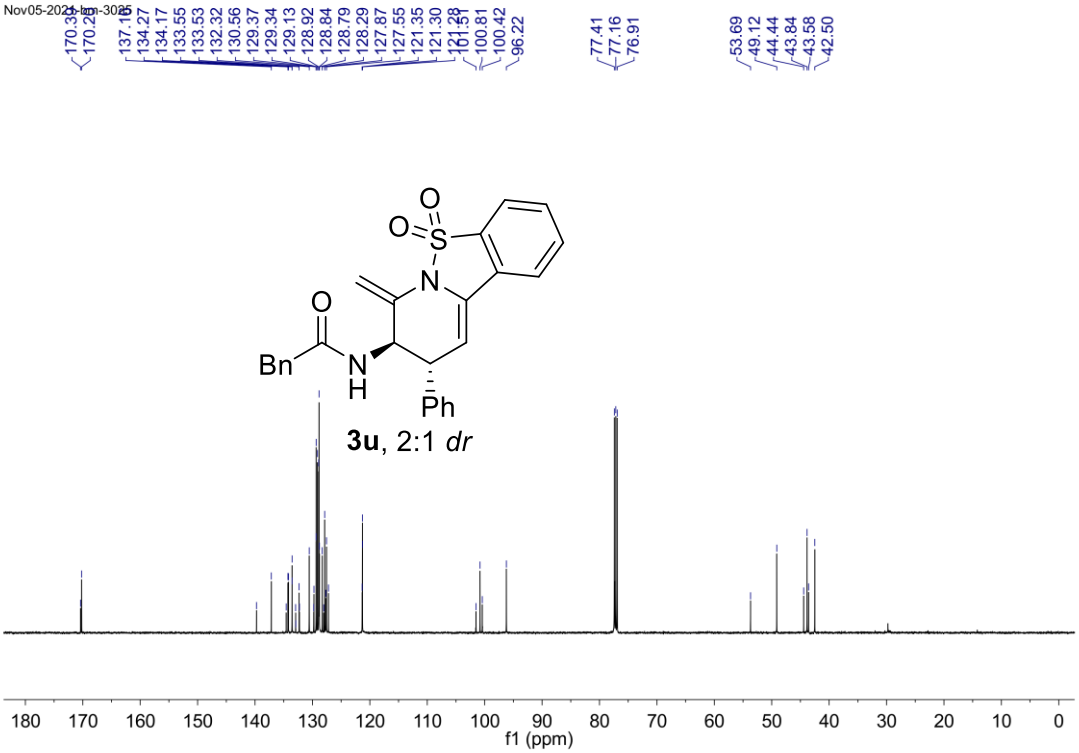

Nov05-2021-BM-3141
8.46
8.45
7.93
7.92
7.88
7.87
7.74
7.69
7.69
7.67
7.62
7.32
7.31
7.26
7.23
5.86
5.55
5.54
4.93
4.92
4.91
4.90
4.89
4.88
4.08
4.07
4.06
2.48
O
O
S
N
O
N
H
N
Ph
Me
3s
1.00
1.05
1.04
1.09
2.13
1.03
4.05
1.15
1.02
1.00
1.01
1.10
1.01
1.06
3.09
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


Nov05-2021-BM-3111
164.18
157.45
148.60
140.21
137.51
133.55
133.19
130.52
129.83
128.83
128.36
128.25
127.65
126.24
121.47
121.36
119.33
101.33
100.87
77.41
77.16
76.91
54.09
44.81
24.30
O
O
S
N
O
N
H
N
Ph
Me
3s
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Sep05-2021-BM-3083
7.91
7.88
7.77
7.76
7.67
7.64
7.48
7.34
6.40
6.37
6.19
6.19
5.89
5.89
5.54
4.85
4.12
O
O
S
N
O
Ph
N
H
Ph
3t
1.04
4.11
2.15
8.08
1.06
1.03
1.04
1.01
2.02
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


Sep05-2021-BM-3023
165.36
141.92
139.99
134.76
133.70
132.50
132.30
130.64
129.94
129.16
128.91
128.41
128.03
121.50
121.40
120.20
103.25
100.93
77.48
77.16
76.84
54.66
44.65
O
O
S
N
O
Ph
N
H
Ph
3t
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Nov06-2021-bm-3025
7.82
7.81
7.79
7.64
7.64
7.63
7.62
7.61
7.59
7.58
7.58
7.57
7.56
7.55
7.26
7.24
7.22
7.22
7.20
7.20
7.19
7.19
7.18
7.17
7.15
7.14
7.13
7.12
7.10
7.09
7.09
7.05
7.04
7.03
7.03
6.88
6.87
5.78
5.77
5.67
5.66
5.39
5.39
5.37
5.11
5.11
5.09
5.03
4.70
4.69
4.45
3.77
3.75
3.74
3.73
3.48
3.45
3.44
O
O
S
N
O
Bn
N
H
Ph
3u, 2:1 dr
1.46
4.51
12.01
2.04
2.00
0.45
1.00
0.46
1.48
1.03
0.95
0.92
1.02
1.50
2.07
0.89
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


Nov05-2021-bm-3085
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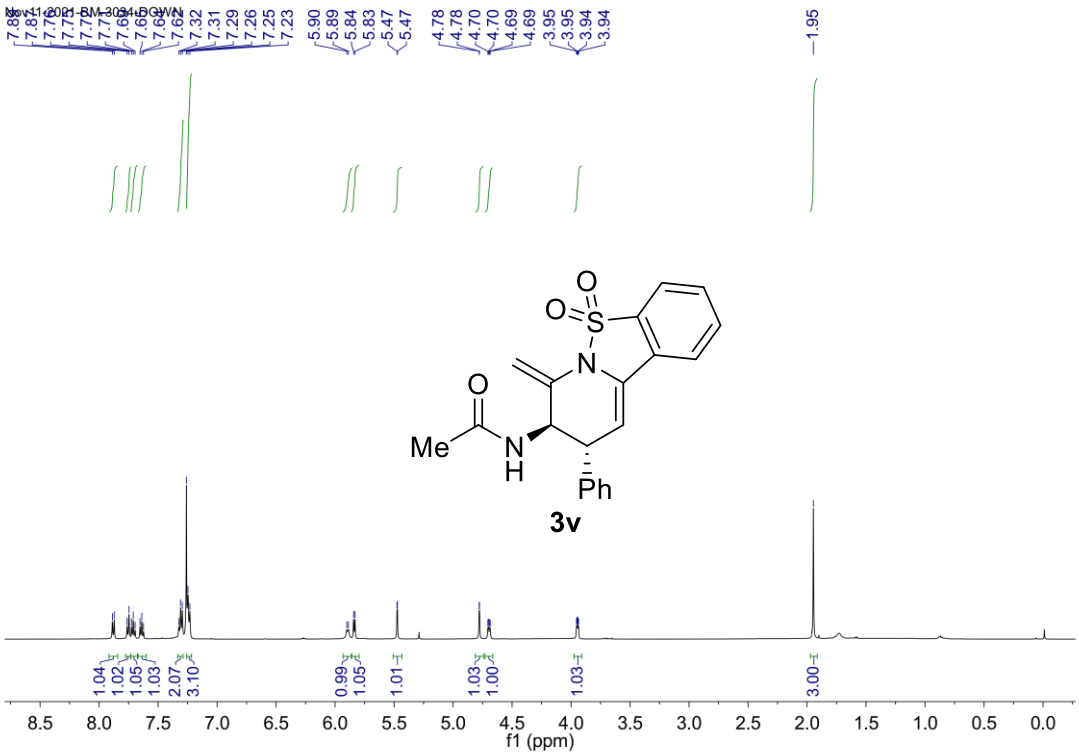
170.20
137.16
134.27
134.17
133.55
133.53
132.32
130.56
129.37
129.34
129.13
128.92
128.84
128.79
128.29
127.87
127.55
121.35
121.30
101.28
101.51
100.81
100.42
96.22
77.41
77.16
76.91
53.69
49.12
44.44
43.84
43.58
42.50
O
O
S
N
O
Bn
N
H
Ph
3u, 2:1 dr
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Nov11-2021-BM-3094-PGWN
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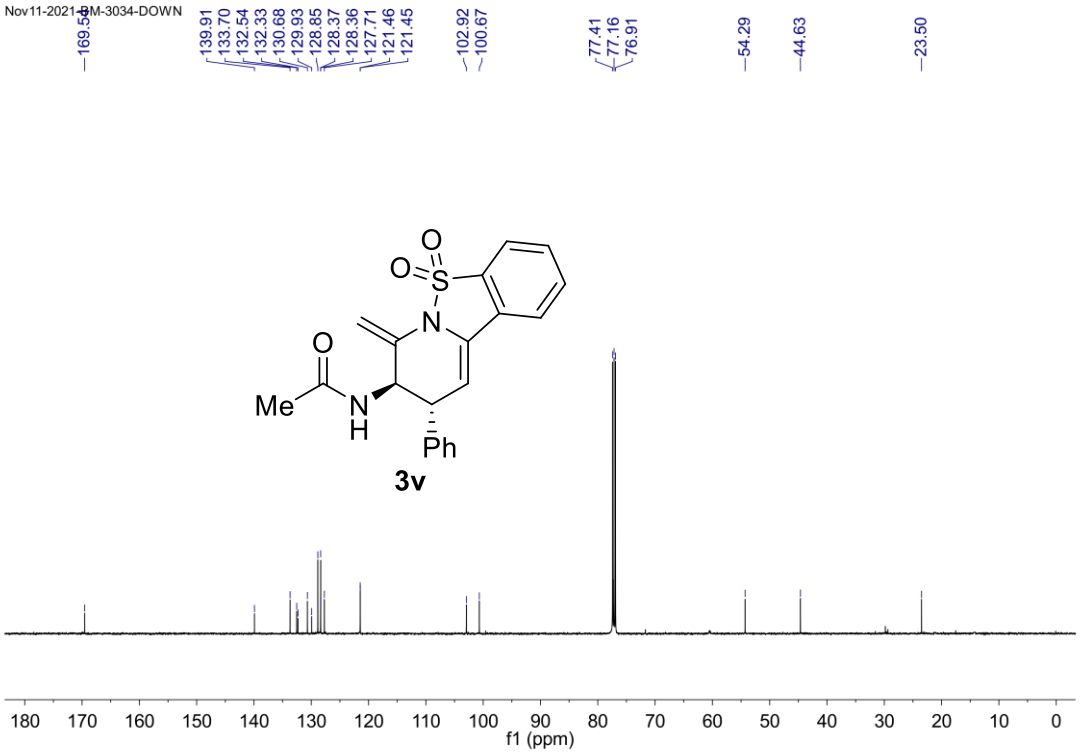
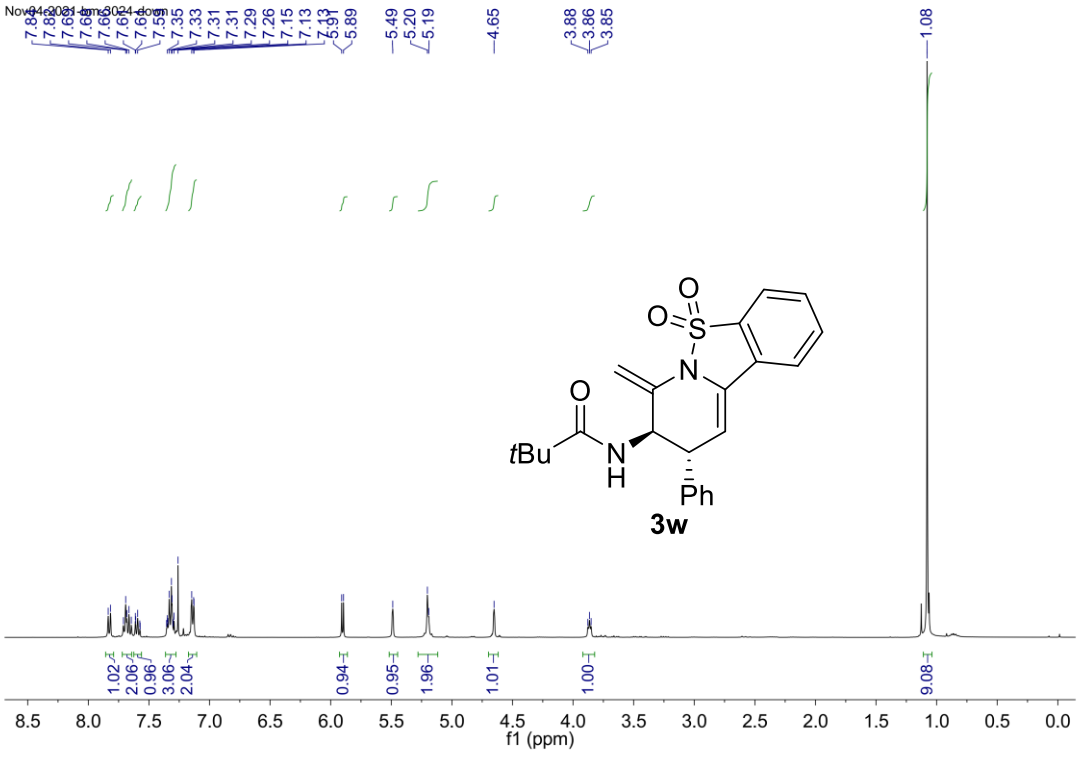
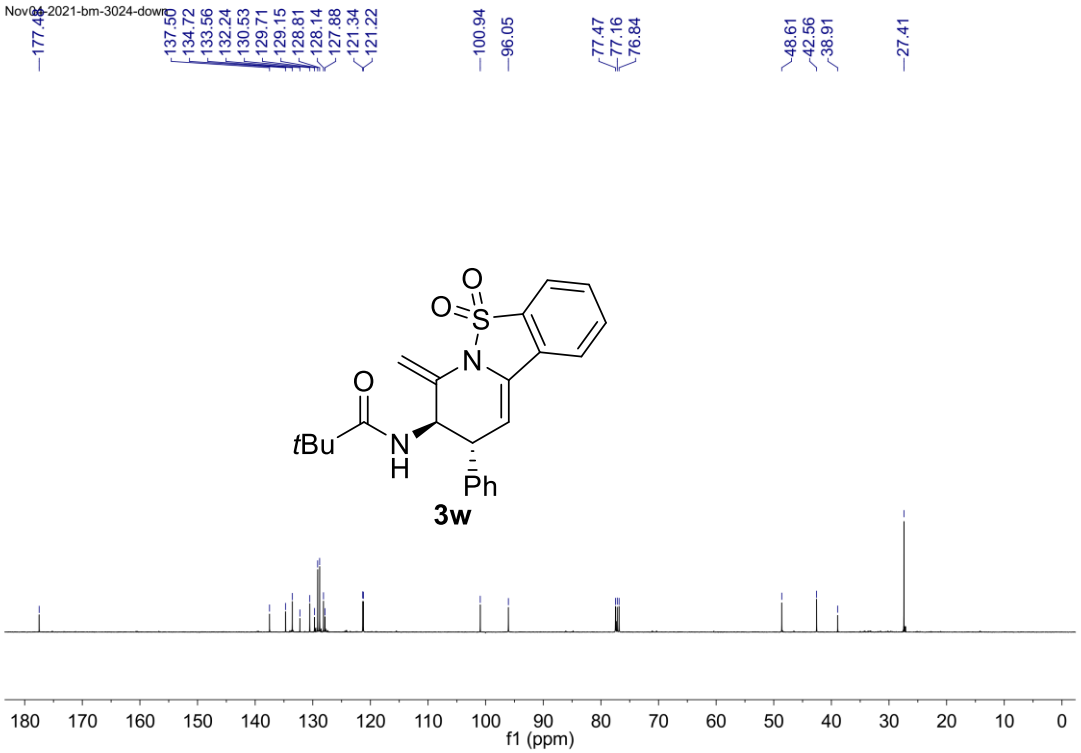
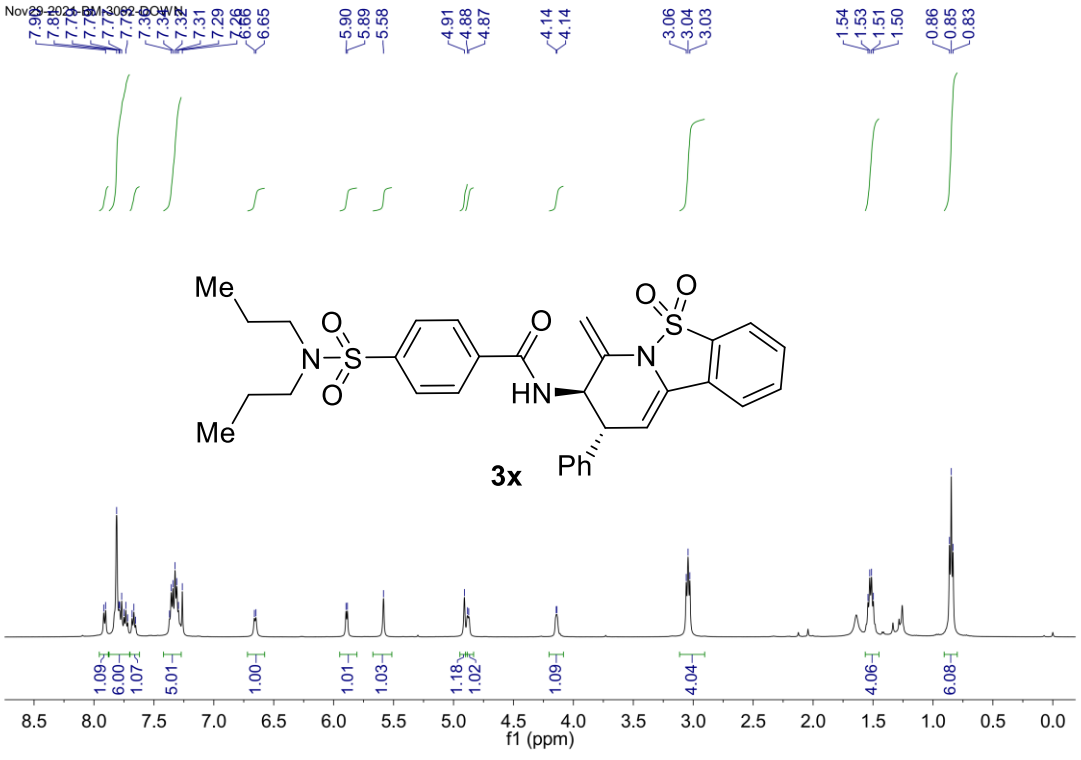
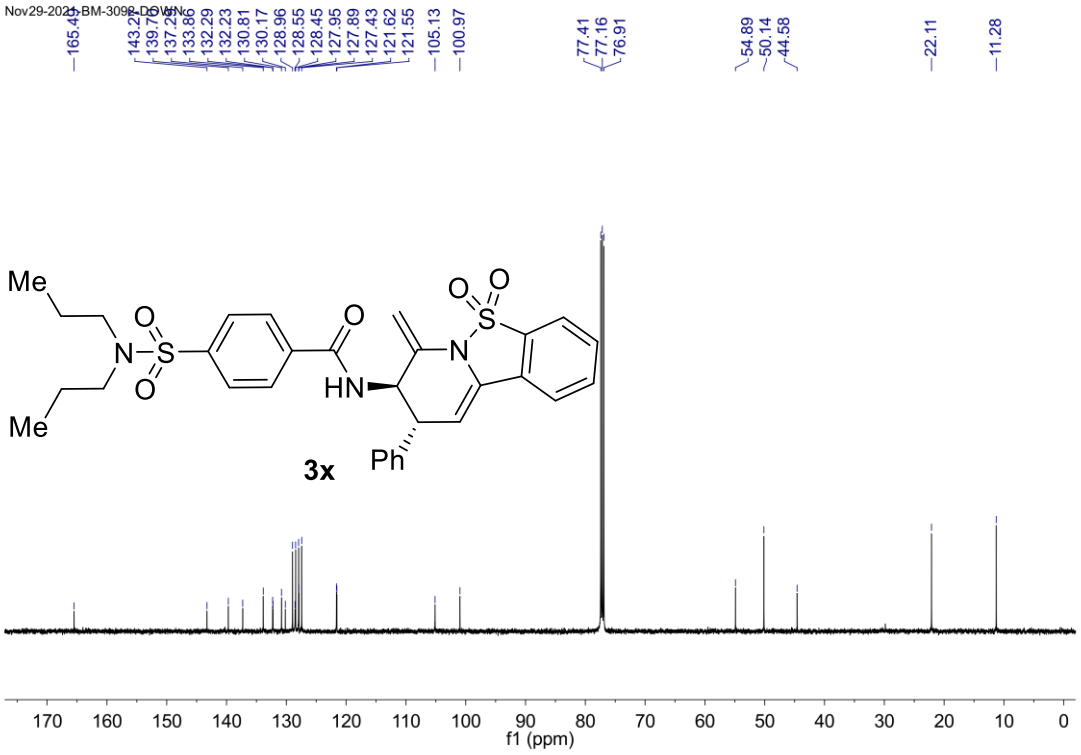
7.77
7.77
7.77
7.77
7.77
7.65
7.64
7.62
7.32
7.31
7.29
7.26
7.25
7.23
5.90
5.89
5.84
5.83
5.47
5.47
4.78
4.78
4.70
4.70
4.69
4.69
3.95
3.95
3.94
3.94
1.95
O
O
S
N
O
Me
N
H
Ph
3v
1.04
1.02
1.05
1.03
2.07
3.10
0.99
1.05
1.01
1.03
1.00
1.03
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

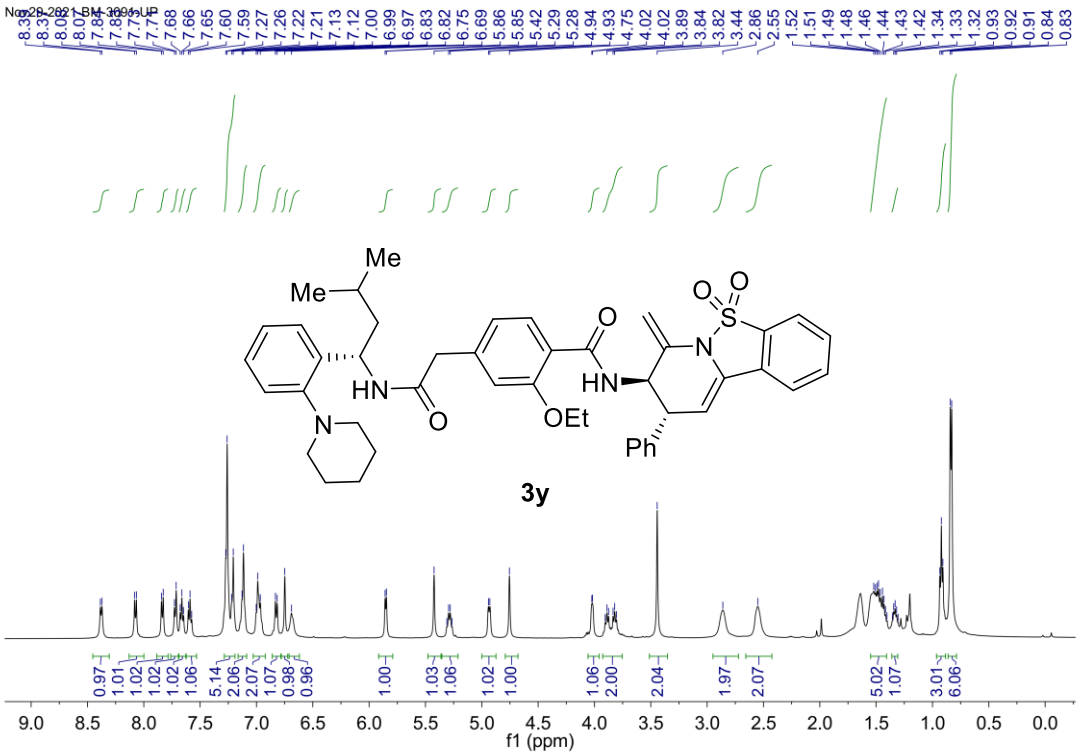

Nov11-2021-BM-3034-DOWN
169.58
139.91
133.70
132.54
132.33
130.68
129.93
128.85
128.37
128.36
127.71
121.46
121.45
102.92
100.67
77.41
77.16
76.91
54.29
44.63
23.50
O
O
S
N
O
Me
N
H
Ph
3v
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

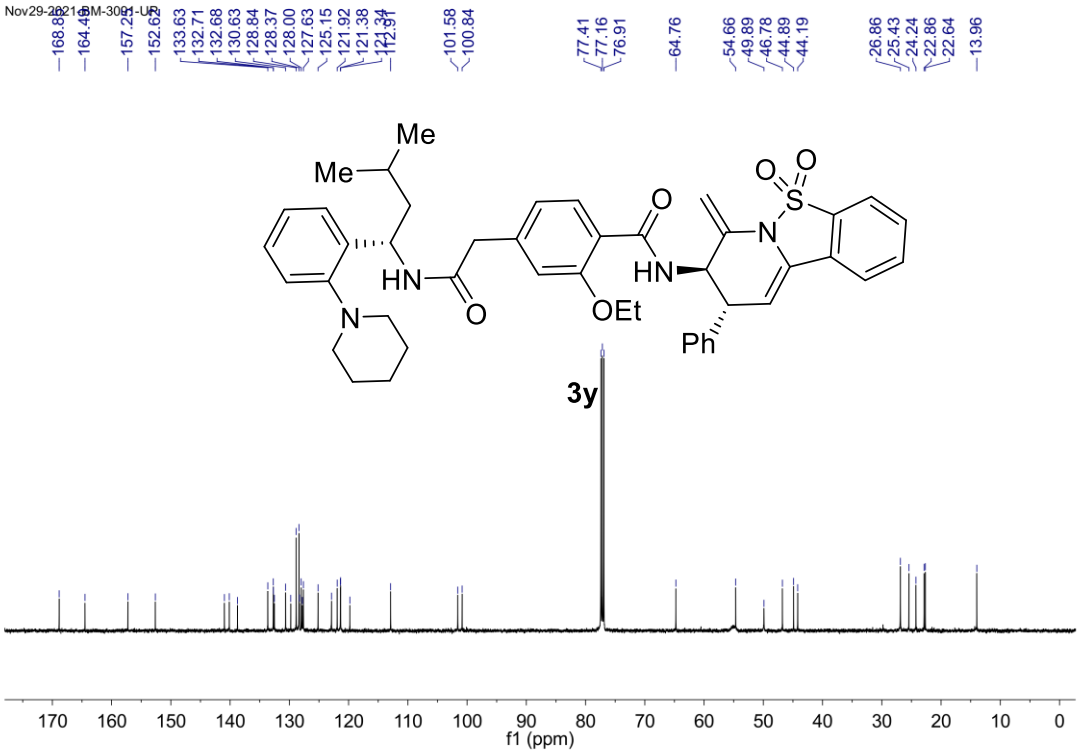

7.84
7.83
7.69
7.68
7.66
7.65
7.63
7.59
7.35
7.33
7.31
7.31
7.29
7.26
7.15
7.13
5.91
5.89
5.49
5.20
5.19
4.65
3.88
3.86
3.85
1.08
O
O
S
N
O
tBu
N
H
Ph
3w
1.02
2.06
0.96
3.06
2.04
0.94
0.95
1.96
1.01
1.00
9.08
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

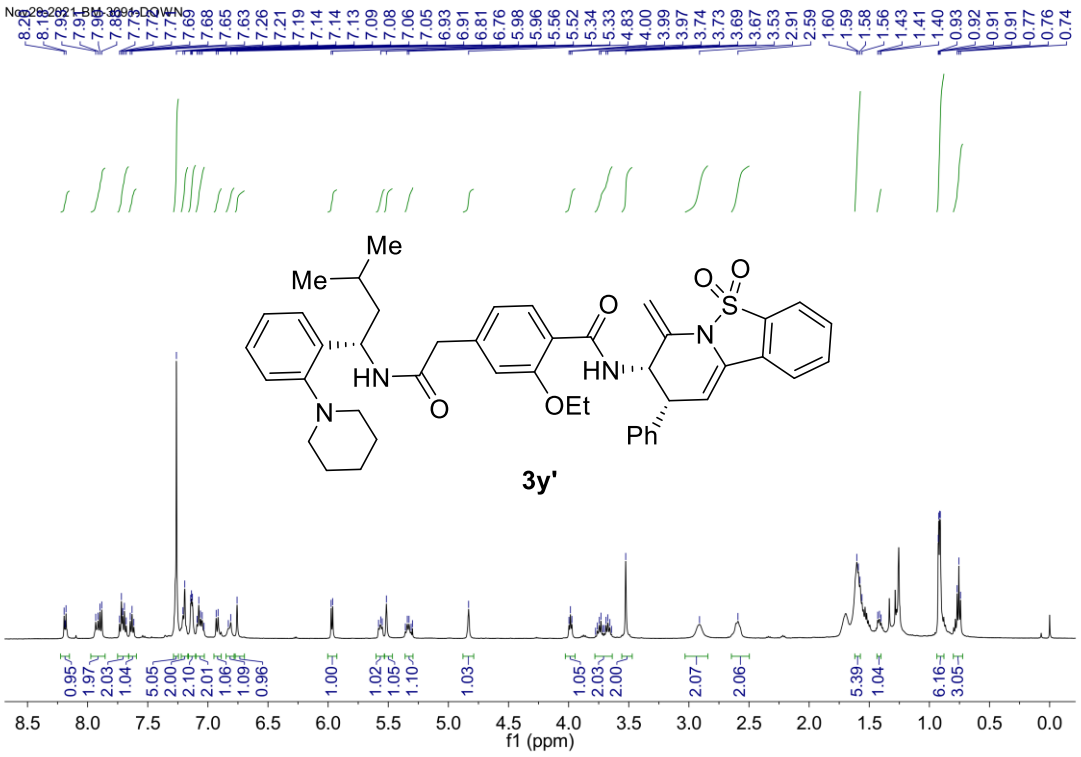

Nov04-2021-bm-3024-down
177.46
137.50
134.72
133.56
132.24
130.53
129.71
129.15
128.81
128.14
127.88
121.34
121.22
100.94
96.05
77.47
77.16
76.84
48.61
42.56
38.91
27.41
O
O
S
N
O
tBu
N
H
Ph
3w
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

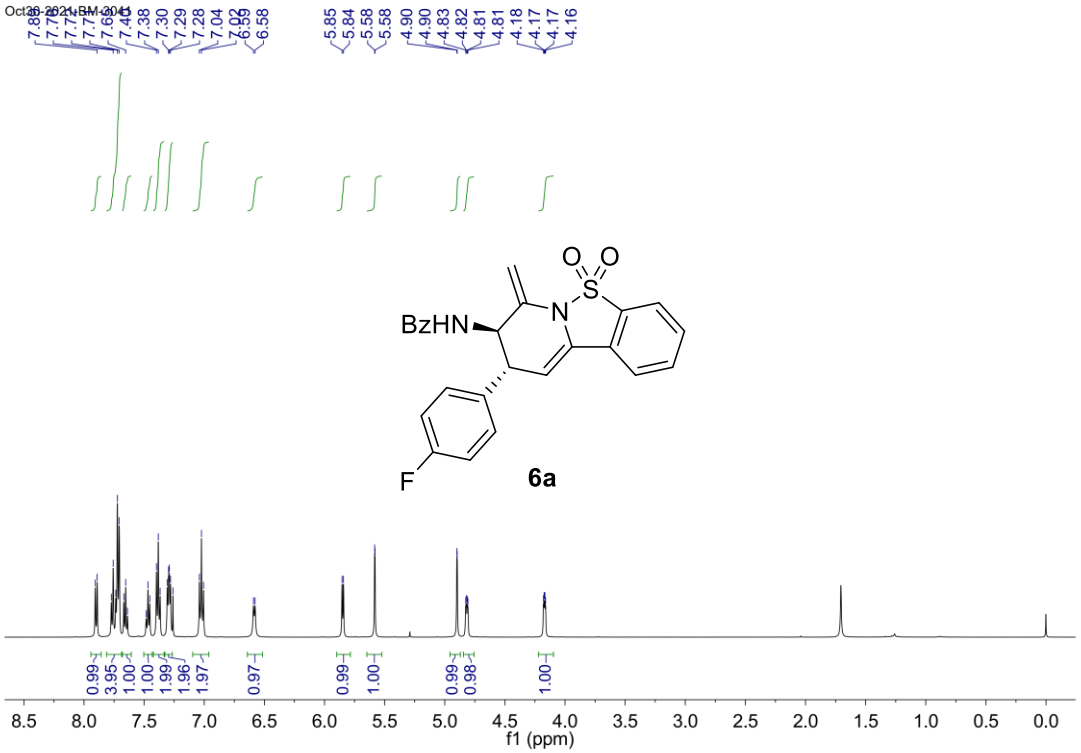

Nov29-2021-BM-3052-DOWN
7.90
7.88
7.76
7.76
7.77
7.75
7.36
7.34
7.32
7.31
7.29
7.26
6.66
6.65
5.90
5.89
5.58
4.91
4.88
4.87
4.14
4.14
3.06
3.04
3.03
1.54
1.53
1.51
1.50
0.86
0.85
0.83
Me
O
O
N
S
O
O
HN
O
O
S
N
Me
Ph
3x
1.09
6.00
1.07
5.01
1.00
1.01
1.03
1.18
1.02
1.09
4.04
4.06
6.08
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

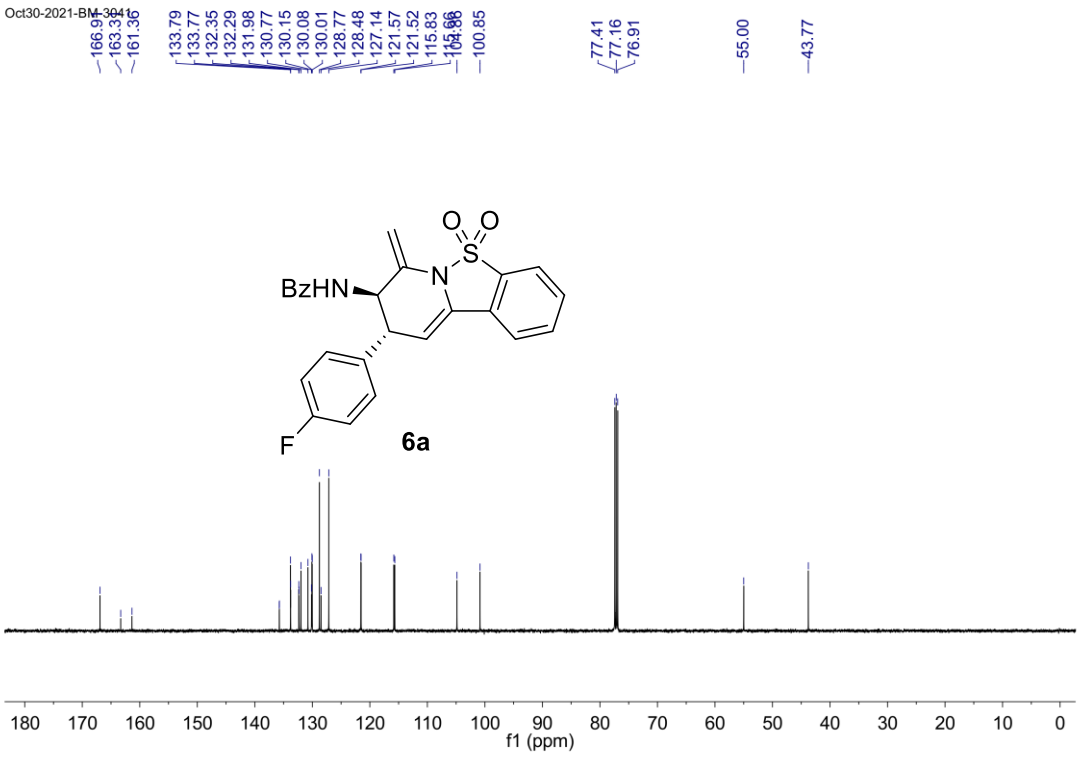

Nov29-2021-BM-3098-DCWIN-c
165.49
143.22
139.76
137.24
133.86
132.29
132.23
130.81
130.17
128.96
128.55
128.45
127.95
127.89
127.43
121.62
121.55
105.13
100.97
77.41
77.16
76.91
54.89
50.14
44.58
22.11
11.28
Me
Me
N
S
O
O
O
O
HN
N
S
O
O
Ph
3x
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

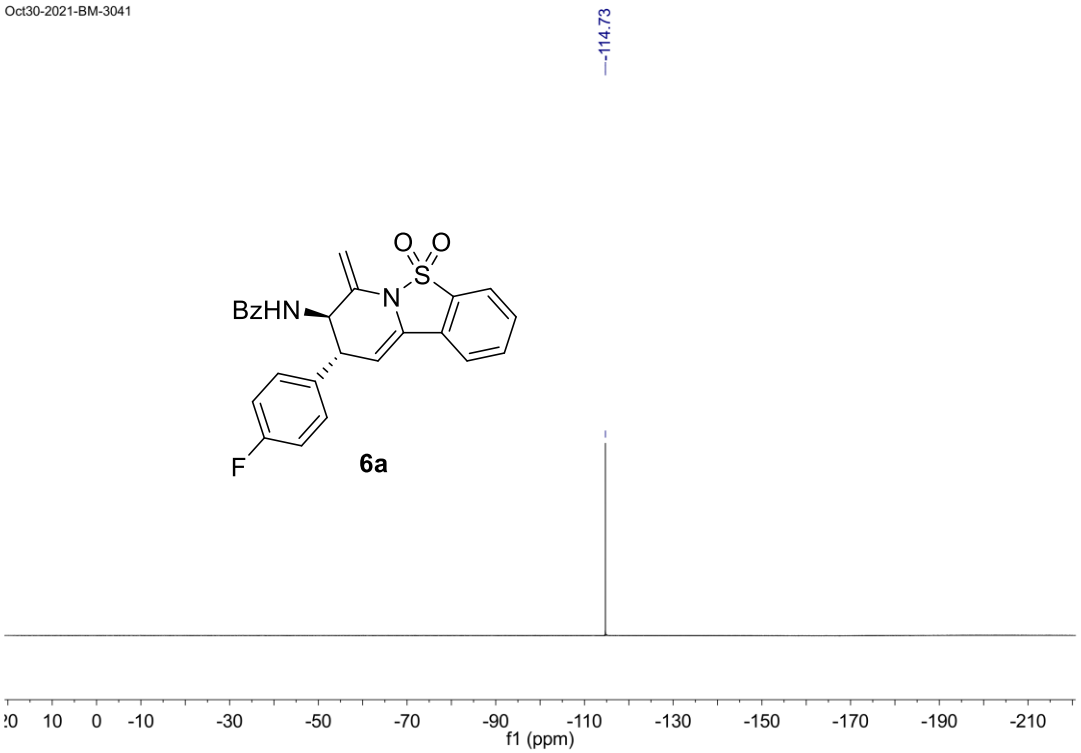

Nov29-2021-BM-3094-UP
8.39
8.38
8.07
8.06
7.84
7.83
7.77
7.76
7.68
7.66
7.65
7.60
7.59
7.27
7.26
7.22
7.21
7.13
7.12
7.00
6.99
6.97
6.83
6.82
6.75
6.69
5.86
5.85
5.42
5.29
5.28
4.94
4.93
4.75
4.02
4.02
3.89
3.84
3.82
3.44
2.86
2.55
1.52
1.51
1.49
1.48
1.46
1.44
1.43
1.42
1.34
1.33
1.32
0.93
0.92
0.91
0.84
0.83
Me
Me
HN
O
N
HN
O
O
O
S
N
OEt
Ph
3y
0.97
1.01
1.02
1.02
1.02
1.06
5.14
2.06
2.07
1.07
0.98
0.96
1.00
1.03
1.06
1.02
1.00
1.06
2.00
2.04
1.97
2.07
5.02
1.07
3.01
6.06
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

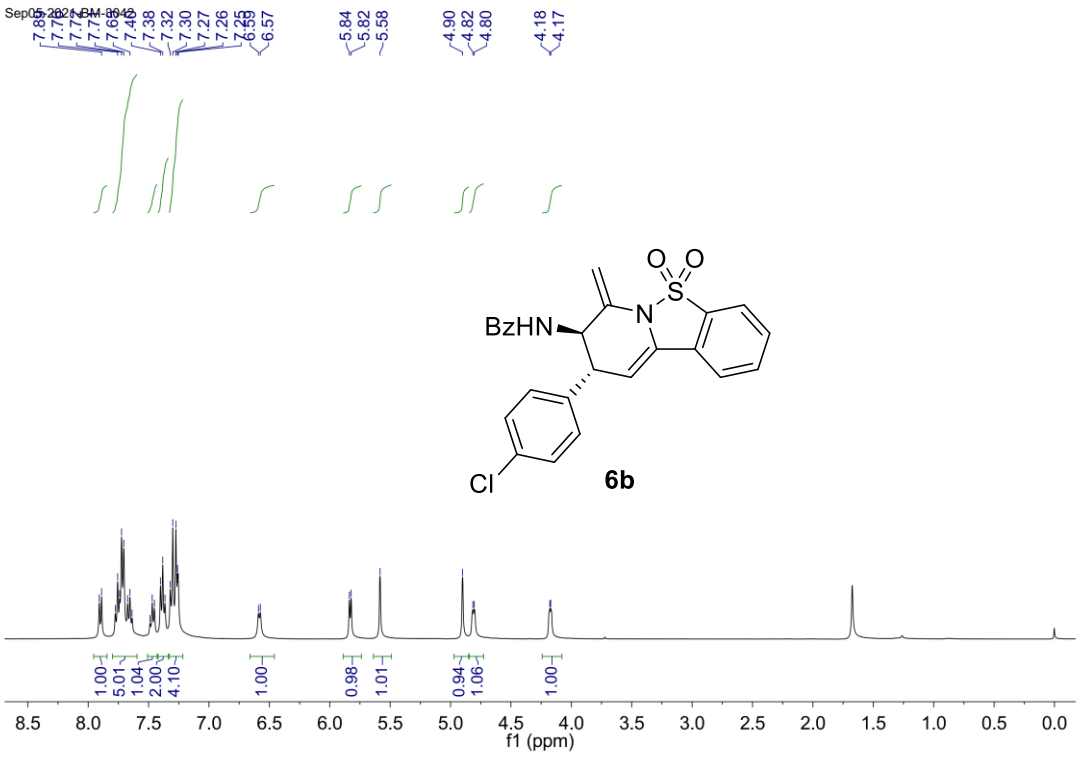

Nov29-2021-BM-3091-UP
168.88
164.46
157.29
152.62
133.63
132.71
132.68
130.63
128.84
128.37
128.00
127.63
125.15
121.92
121.38
101.58
100.84
77.41
77.16
76.91
64.76
54.66
49.89
46.78
44.89
44.19
26.86
25.43
24.24
22.86
22.64
13.96
Me
Me
HN
O
N
O
HN
O
OEt
O
O
S
N
Ph
3y
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

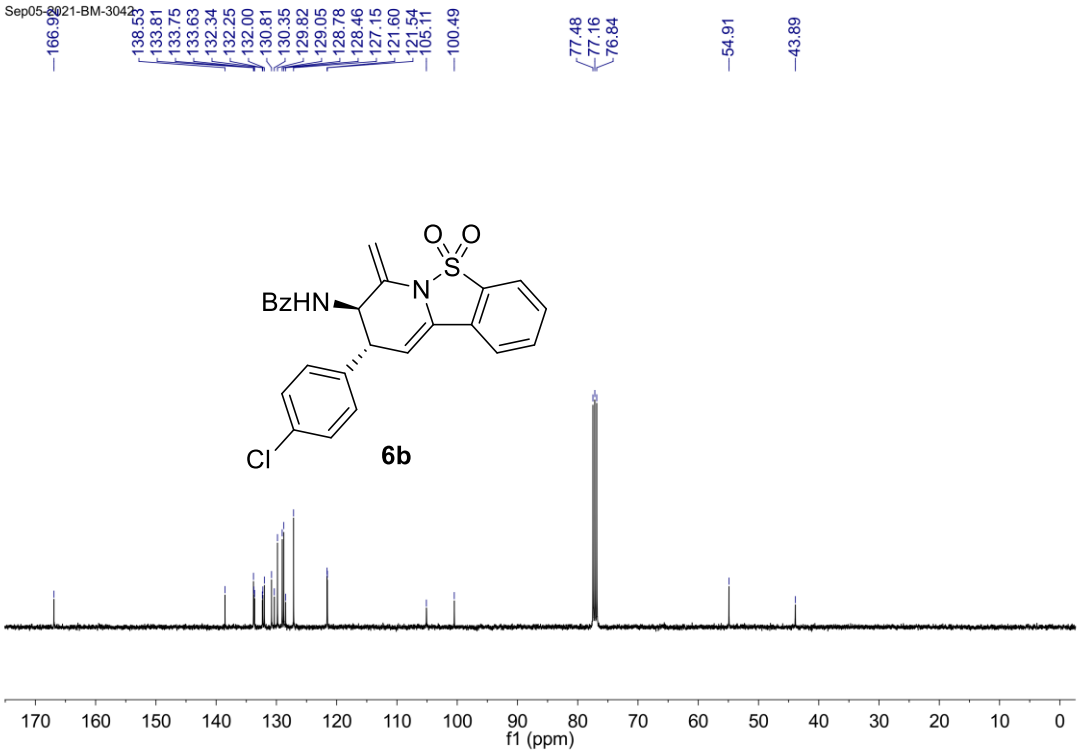

Nov29-2021-BM-3091-DQWN
8.25
8.13
7.92
7.91
7.90
7.88
7.77
7.76
7.69
7.68
7.65
7.63
7.26
7.21
7.19
7.14
7.13
7.09
7.08
7.06
7.05
6.93
6.91
6.81
6.76
5.98
5.96
5.56
5.52
5.34
5.33
4.83
4.00
3.99
3.97
3.74
3.73
3.69
3.67
3.53
2.91
2.59
1.60
1.59
1.58
1.56
1.43
1.41
1.40
0.93
0.92
0.91
0.91
0.77
0.76
0.74
Me
Me
HN
O
N
O
HN
O
OEt
O
O
S
N
Ph
3y'
0.95
1.97
2.03
1.04
5.05
2.00
2.10
2.01
1.06
1.09
0.96
1.00
1.02
1.05
1.10
1.03
1.05
2.03
2.00
2.07
2.06
5.39
1.04
6.16
3.05
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

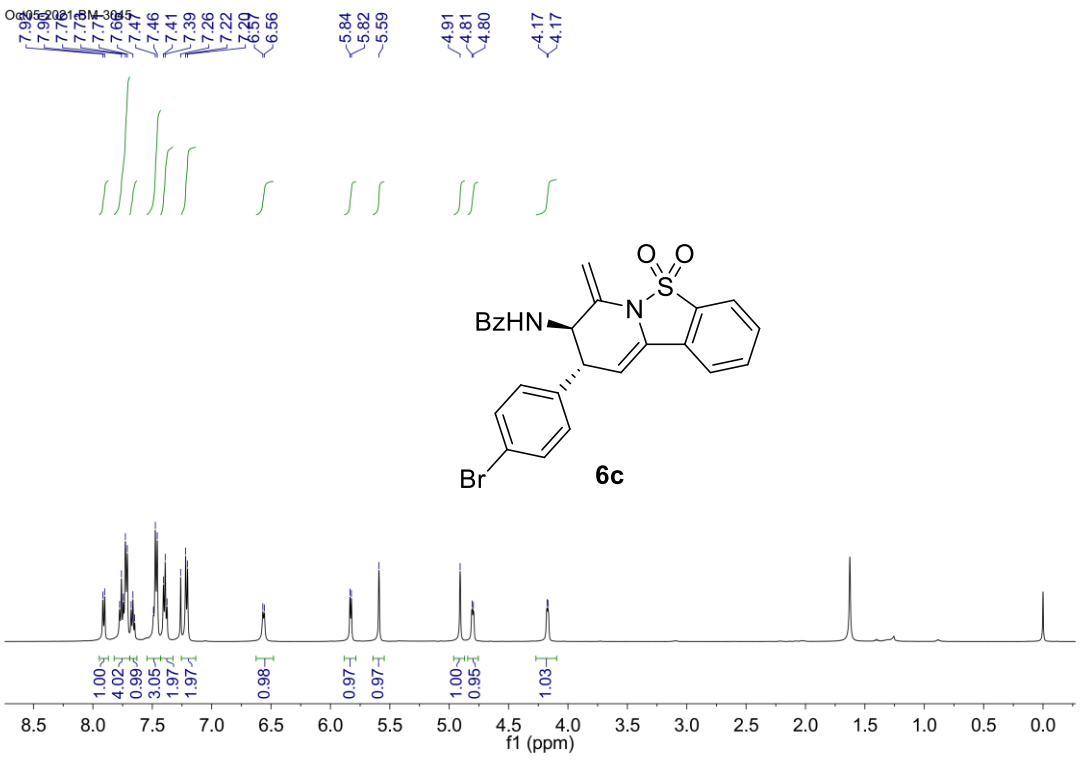

Oct26-2021-BM-3041
7.88
7.78
7.77
7.72
7.71
7.69
7.45
7.38
7.30
7.29
7.28
7.04
7.02
6.59
6.58
5.85
5.84
5.58
5.58
4.90
4.90
4.83
4.82
4.81
4.81
4.18
4.17
4.17
4.16
BzHN
O
O
S
N
F
6a
0.99
3.95
1.00
1.00
1.99
1.96
1.97
0.97
0.99
1.00
0.99
0.98
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

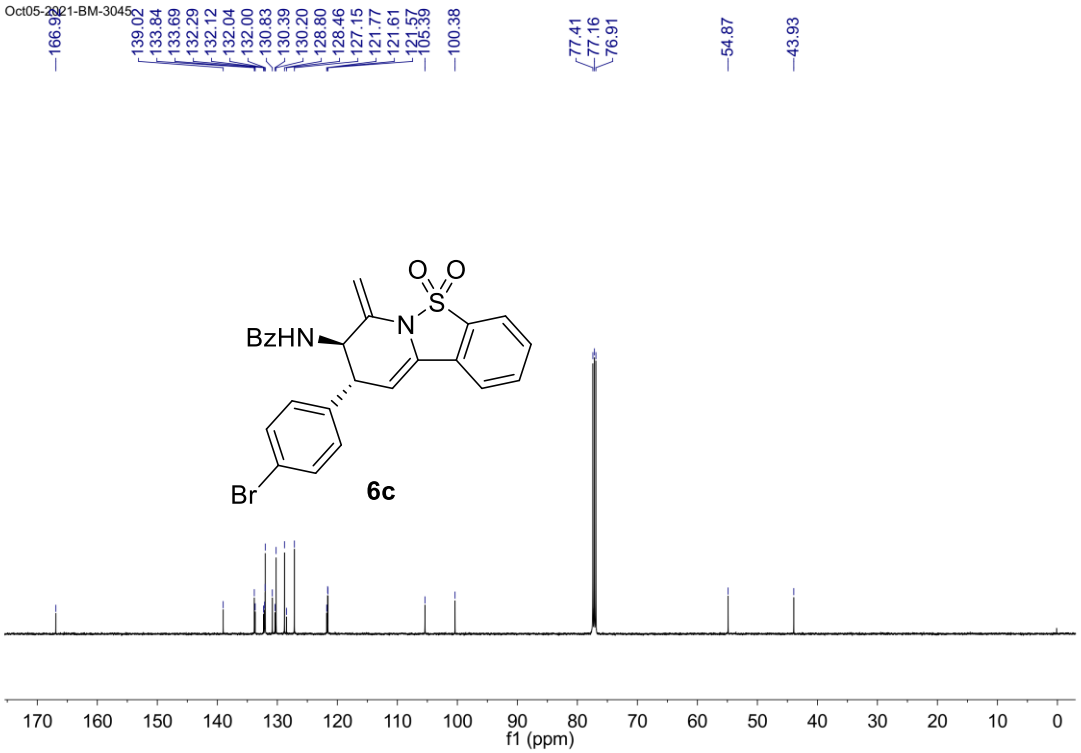

Oct30-2021-BM-3041
166.97
163.31
161.36
133.79
133.77
132.35
132.29
131.98
130.77
130.15
130.08
130.01
128.77
128.48
127.14
121.57
121.52
115.83
100.85
77.41
77.16
76.91
55.00
43.77
BzHN
O
O
S
N
F
6a
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

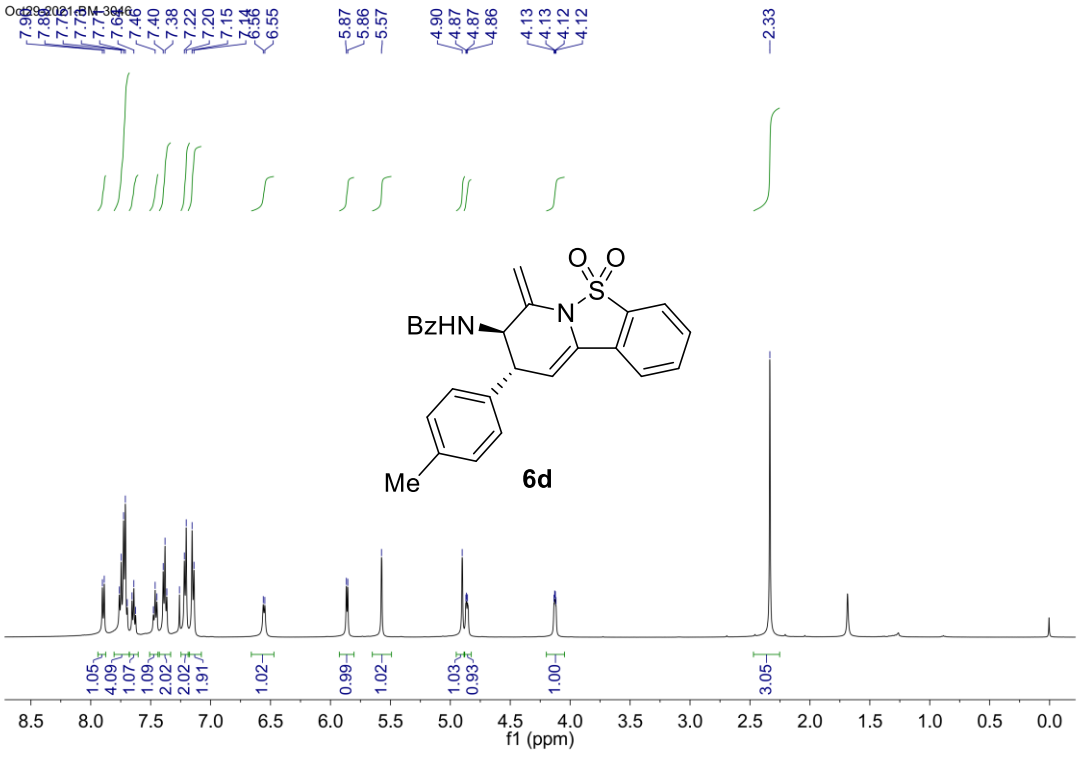

Oct30-2021-BM-3041
-114.73
BzHN
O
O
S
N
F
6a
f1 (ppm)

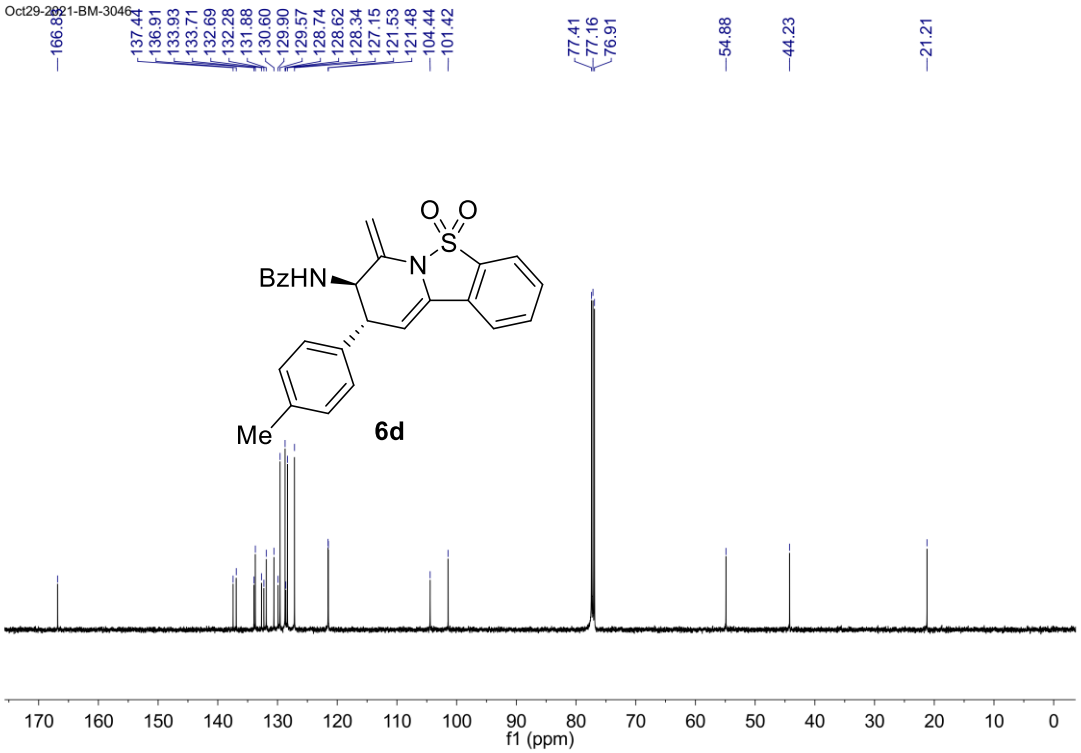

7.84
7.76
7.75
7.73
7.69
7.40
7.38
7.32
7.30
7.27
7.26
6.59
6.57
5.84
5.82
5.58
4.90
4.82
4.80
4.18
4.17
BzHN
O
O
S
N
Cl
6b
1.00
5.01
1.04
2.00
4.10
1.00
0.98
1.01
0.94
1.06
1.00
f1 (ppm)

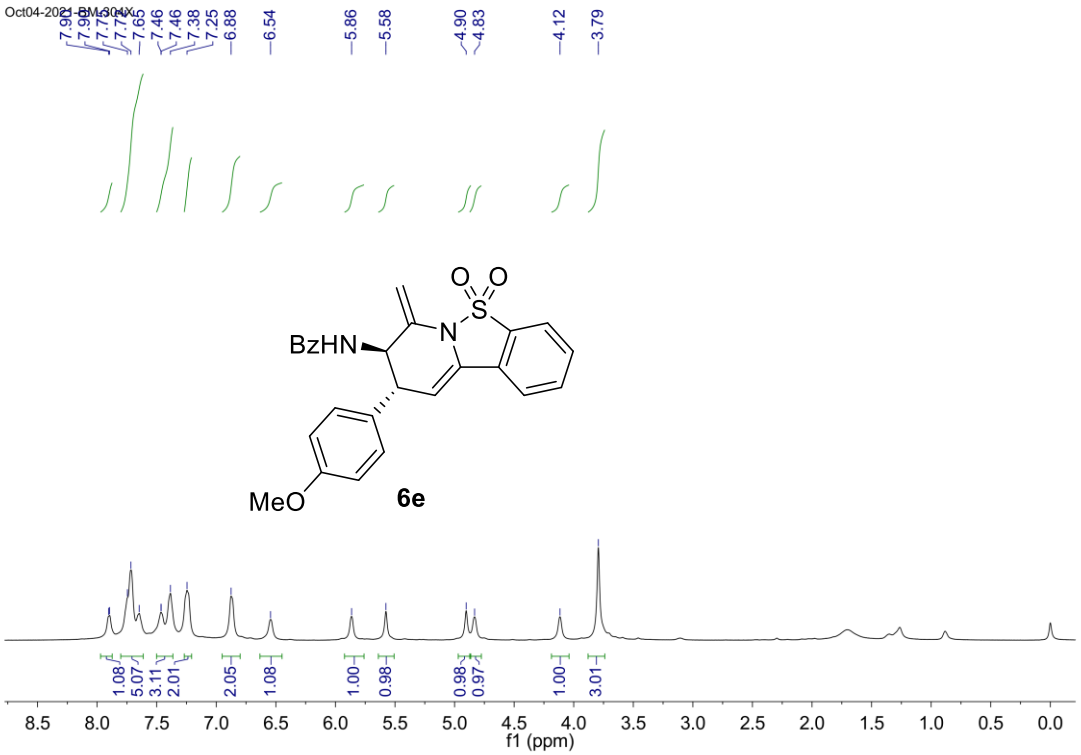

Sep05-2021-BM-3042
166.99
138.53
133.81
133.75
133.63
132.34
132.25
132.00
130.81
130.35
129.82
129.05
128.78
128.46
127.15
121.60
121.54
105.11
100.49
77.48
77.16
76.84
54.91
43.89
O
O
S
N
BzHN
Cl
6b
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

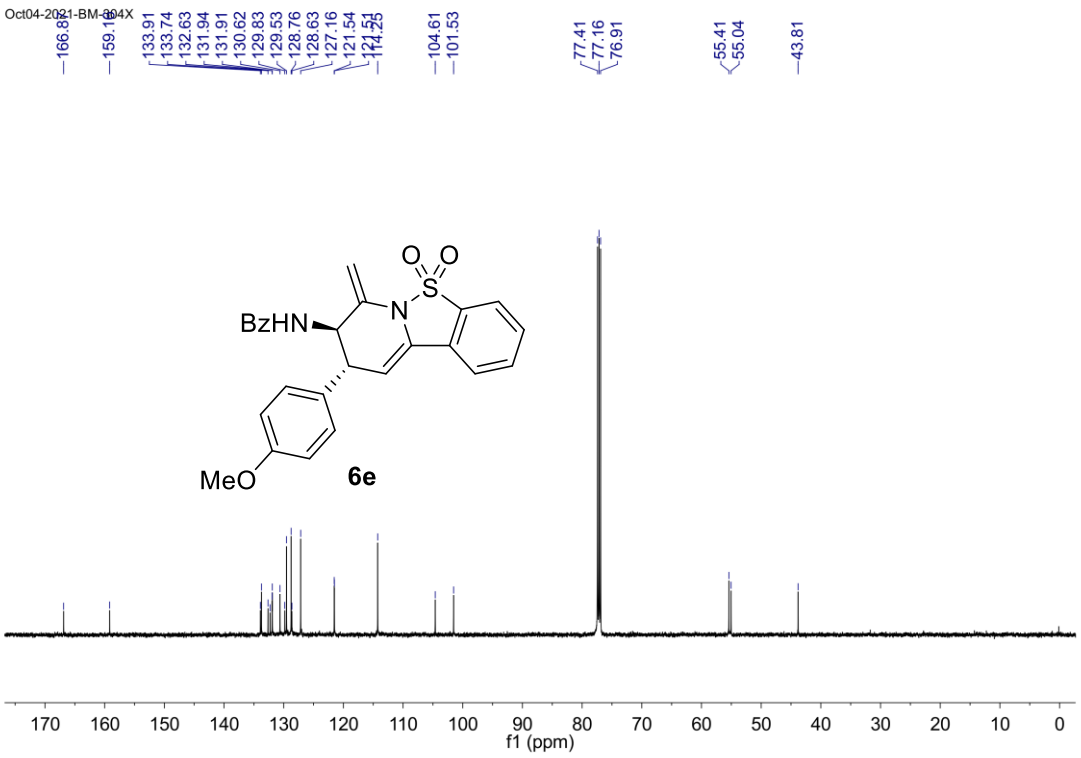

Oct05-2021-BM-3045
7.95
7.90
7.78
7.77
7.77
7.66
7.47
7.46
7.41
7.39
7.26
7.22
7.20
6.57
6.56
5.84
5.82
5.59
4.91
4.81
4.80
4.17
4.17
O
O
S
N
BzHN
Br
6c
1.00
4.02
0.99
3.05
1.97
1.97
0.98
0.97
0.97
1.00
0.95
1.03
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

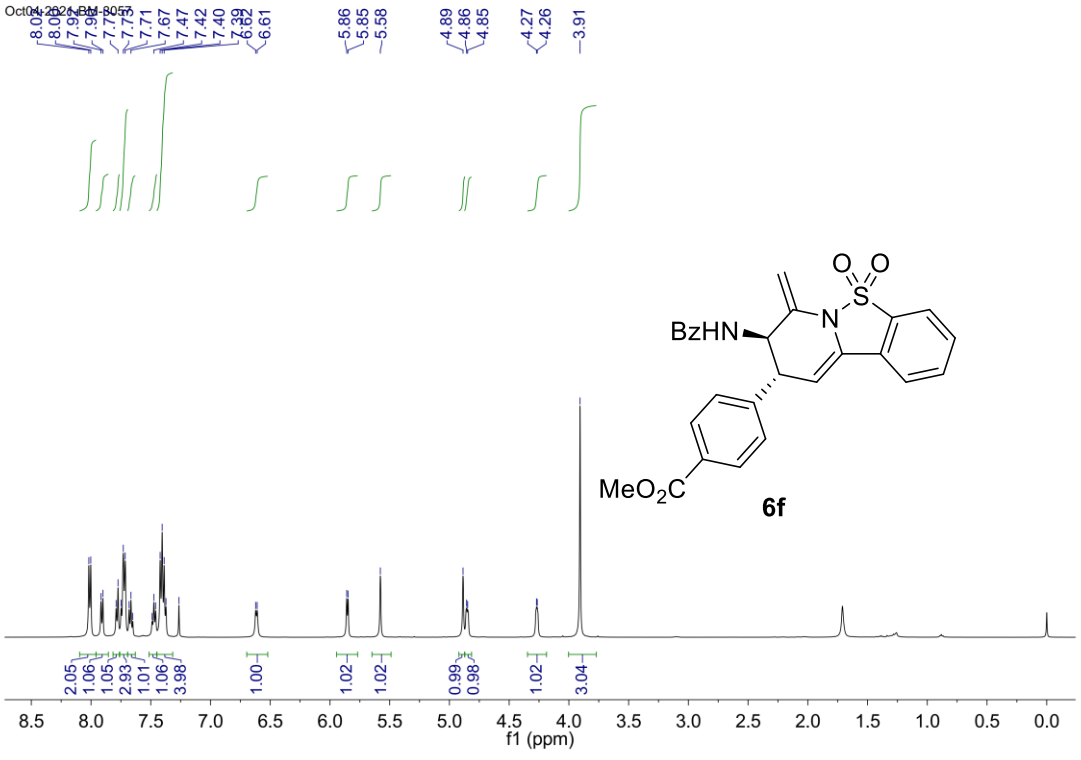

Oct05-2021-BM-3045c
166.99
139.02
133.84
133.69
132.29
132.12
132.04
132.00
130.83
130.39
130.20
128.80
128.46
127.15
121.77
121.61
121.57
105.39
100.38
77.41
77.16
76.91
54.87
43.93
O
O
S
N
BzHN
Br
6c
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

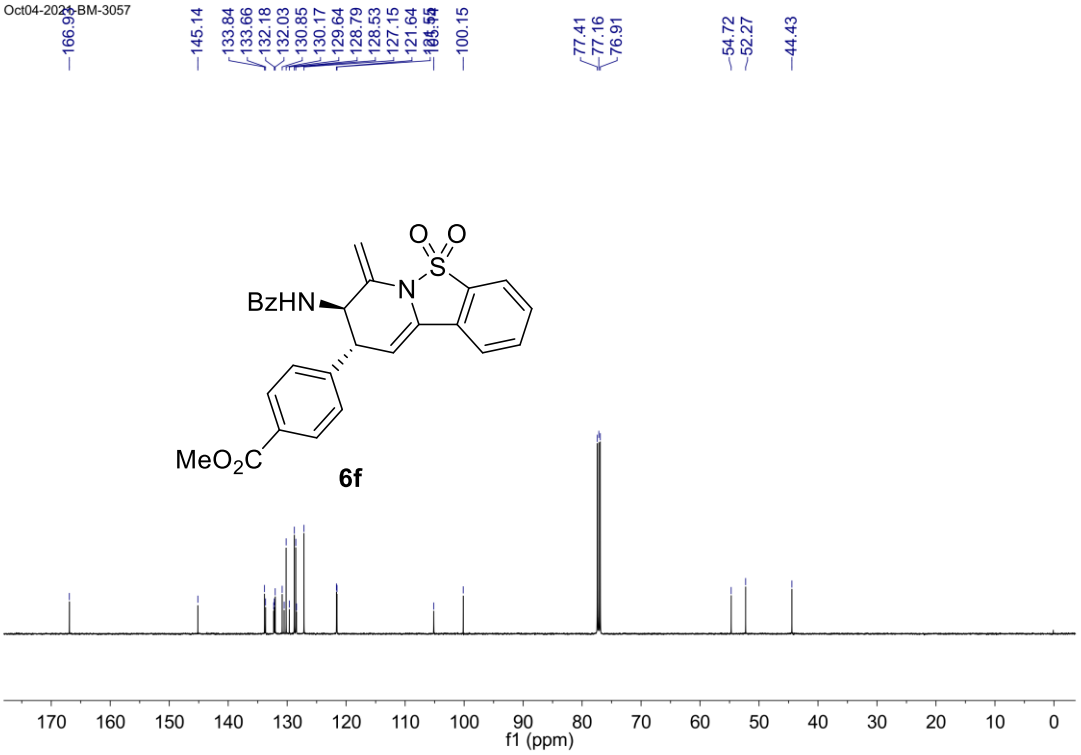

Oct29-2021-BM-3046
7.96
7.88
7.78
7.77
7.77
7.64
7.46
7.40
7.38
7.22
7.20
7.15
7.14
6.56
6.55
5.87
5.86
5.57
4.90
4.87
4.87
4.86
4.13
4.13
4.12
4.12
2.33
O
O
S
N
BzHN
Me
6d
1.05
4.09
1.07
1.09
2.02
2.02
1.91
1.02
0.99
1.02
1.03
0.93
1.00
3.05
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

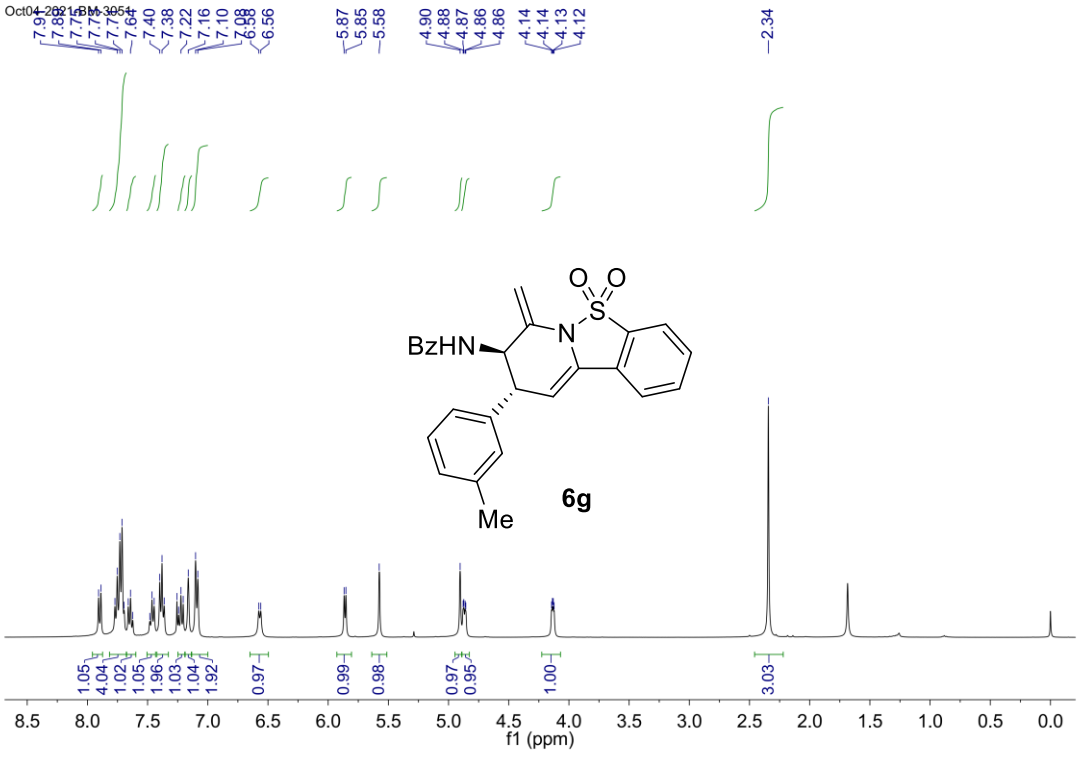

Oct29-2021-BM-3046
166.88
137.44
136.91
133.93
133.71
132.69
132.28
131.88
130.60
129.90
129.57
128.74
128.62
128.34
127.15
121.53
121.48
104.44
101.42
77.41
77.16
76.91
54.88
44.23
21.21
BzHN
N
S
O
O
Me
6d
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

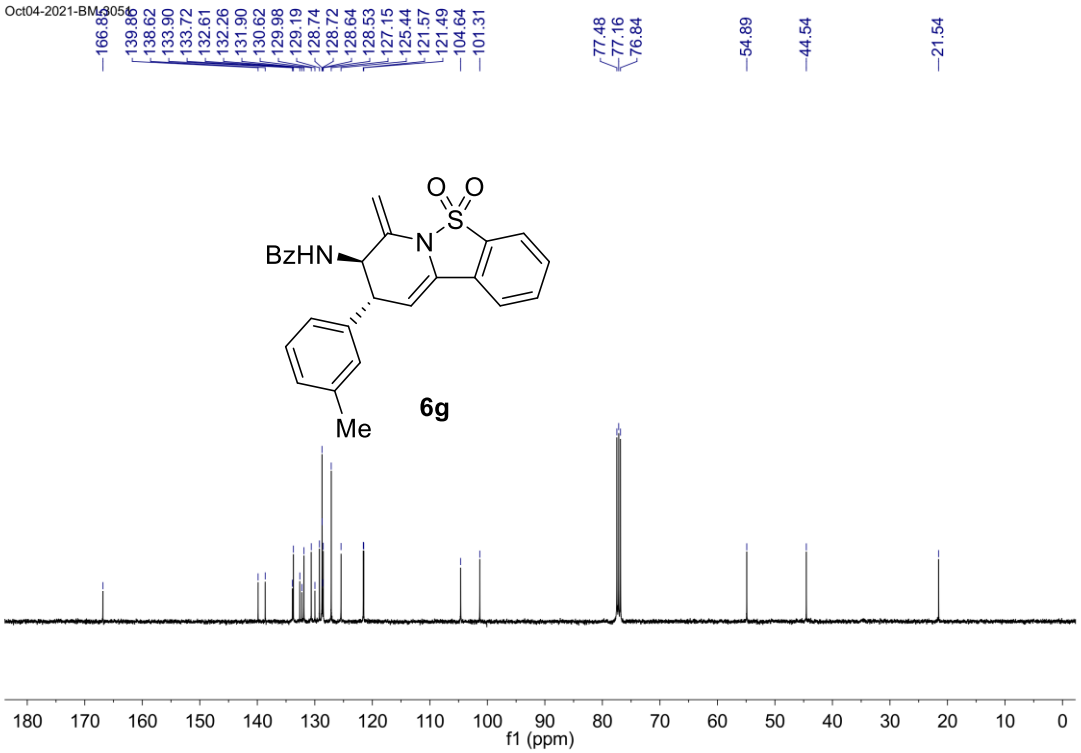

Oct04-2021-BM-304X
7.91
7.90
7.77
7.76
7.65
7.46
7.46
7.38
7.25
6.88
6.54
5.86
5.58
4.90
4.83
4.12
3.79
BzHN
N
S
O
O
MeO
6e
1.08
5.07
3.11
2.01
2.05
1.08
1.00
0.98
0.98
0.97
1.00
3.01
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

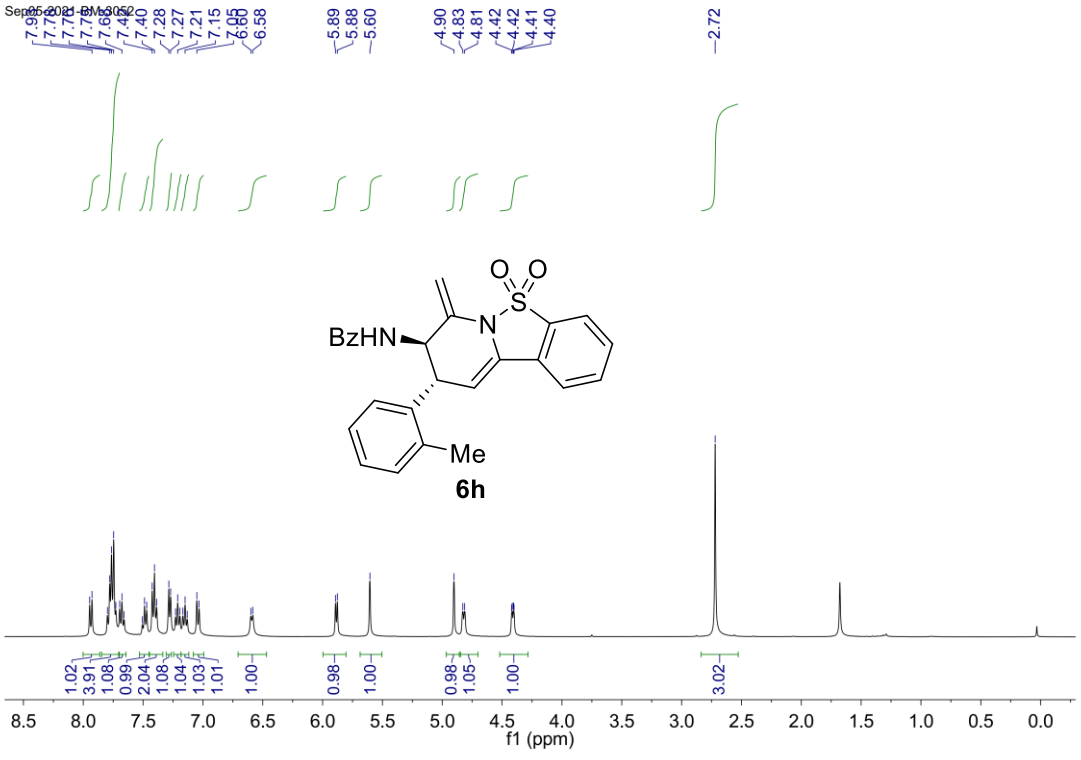

Oct04-2021-BM-304X
166.85
159.16
133.91
133.74
132.63
131.94
131.91
130.62
129.83
129.53
128.76
128.63
127.16
121.54
104.61
101.53
77.41
77.16
76.91
55.41
55.04
43.81
BzHN
N
S
O
O
MeO
6e
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

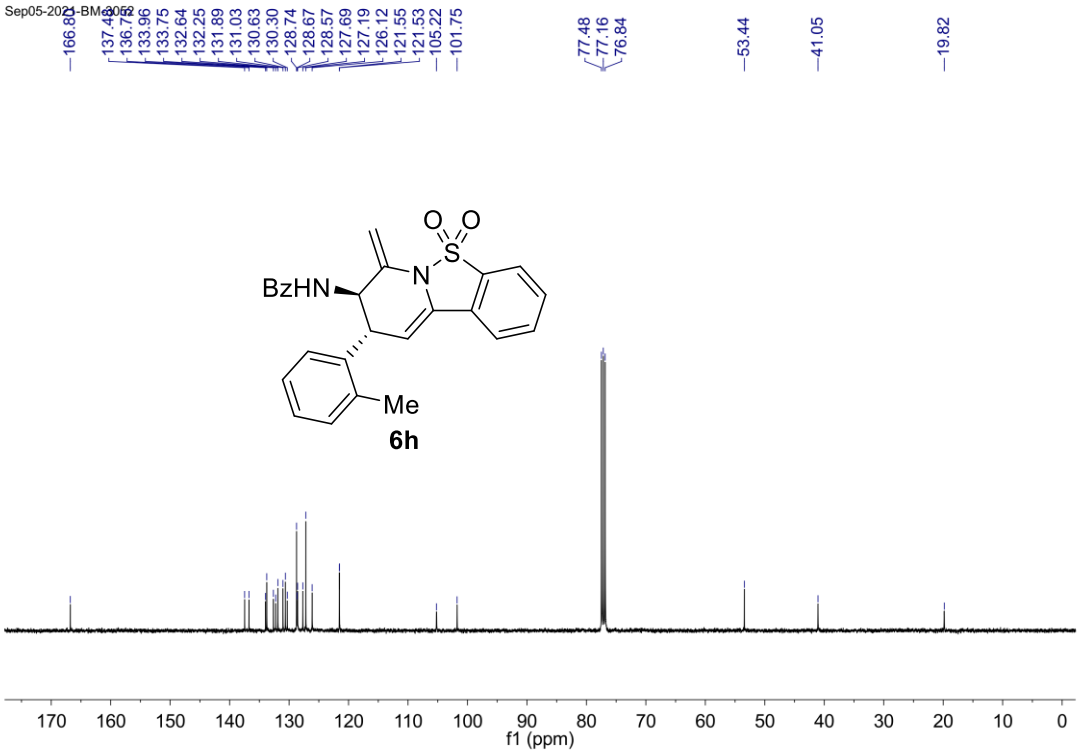

Oct04-2021-BM-305T
8.02
8.00
7.99
7.98
7.77
7.75
7.71
7.67
7.47
7.42
7.40
6.61
5.86
5.85
5.58
4.89
4.86
4.85
4.27
4.26
3.91
BzHN
N
S
O
O
MeO2C
6f
2.05
1.06
1.05
2.93
1.01
1.06
3.98
1.00
1.02
1.02
0.99
0.98
1.02
3.04
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

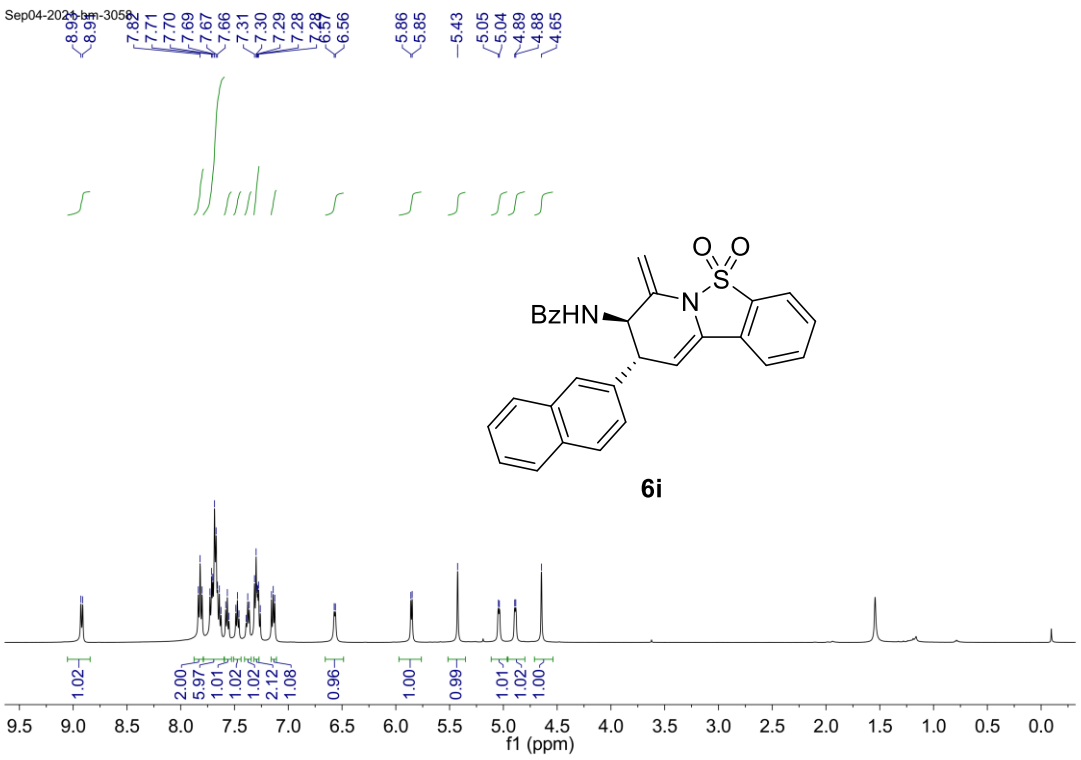

Oct04-2021-BM-3057
166.98
145.14
133.84
133.66
132.18
132.03
130.85
130.17
129.64
128.79
128.53
127.15
121.64
100.15
77.41
77.16
76.91
54.72
52.27
44.43
BzHN
N
S
O
O
MeO2C
6f
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

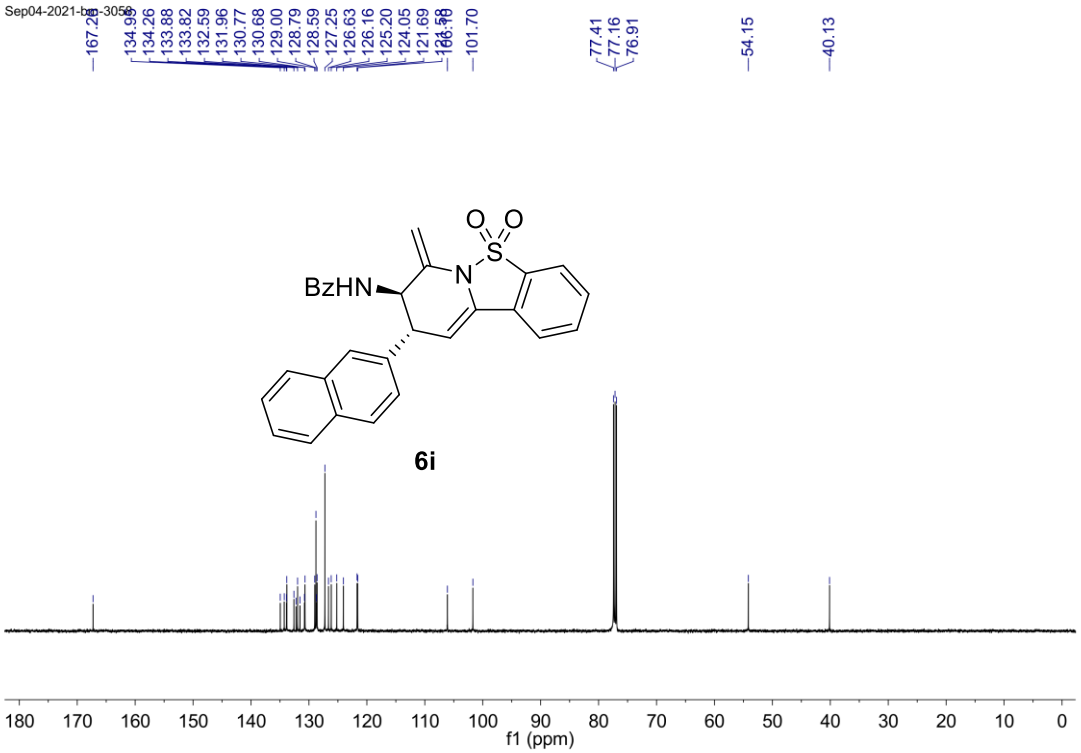

Oct04-2021-BM-3054
7.90
7.88
7.77
7.76
7.64
7.40
7.38
7.22
7.16
7.10
6.58
6.56
5.87
5.85
5.58
4.90
4.88
4.87
4.86
4.86
4.14
4.14
4.13
4.12
2.34
BzHN
N
S
O
O
Me
6g
1.05
4.04
1.02
1.05
1.96
1.03
1.04
1.92
0.97
0.99
0.98
0.97
0.95
1.00
3.03
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

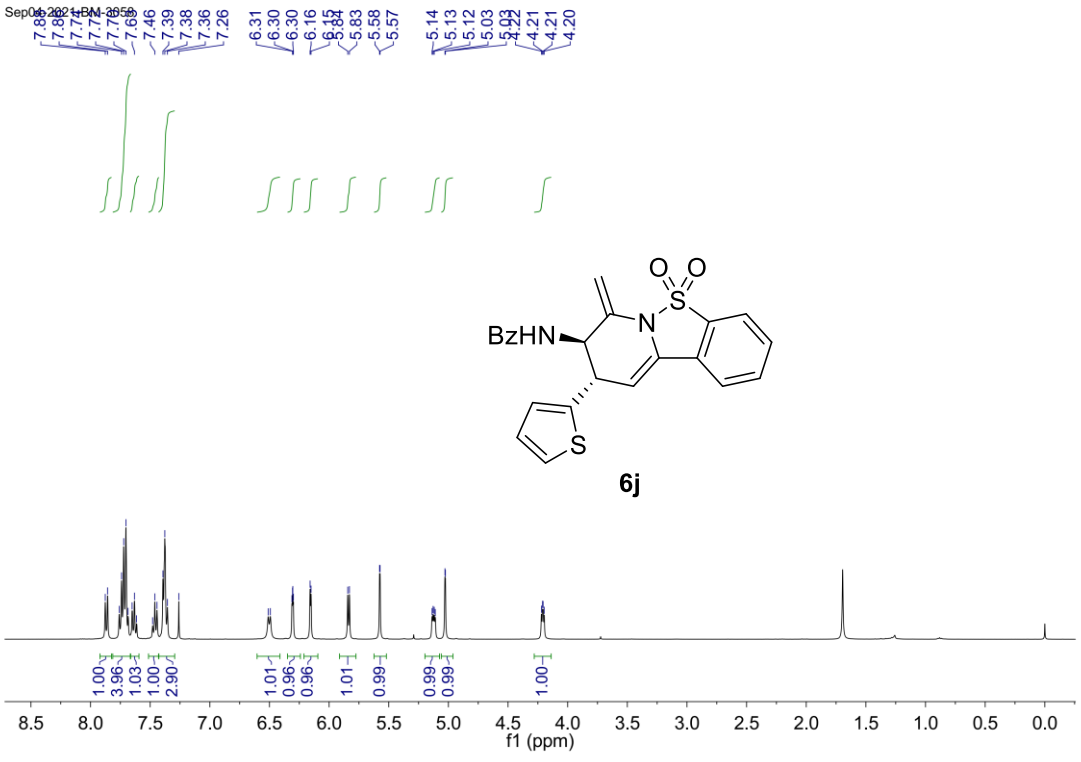

Oct04-2021-BM-3056
166.85
139.86
138.62
133.90
133.72
132.61
132.26
131.90
130.62
129.98
129.19
128.74
128.72
128.64
128.53
127.15
125.44
121.57
121.49
104.64
101.31
77.48
77.16
76.84
54.89
44.54
21.54
O
O
S
N
BzHN
Me
6g
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


Sept05-2021-BM-3052
7.99
7.78
7.76
7.75
7.69
7.45
7.40
7.28
7.27
7.21
7.15
7.05
6.60
6.58
5.89
5.88
5.60
4.90
4.83
4.81
4.42
4.42
4.41
4.40
2.72
O
O
S
N
BzHN
Me
6h
1.02
3.91
1.08
0.99
2.04
1.08
1.04
1.03
1.01
1.00
0.98
1.00
0.98
1.05
1.00
3.02
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

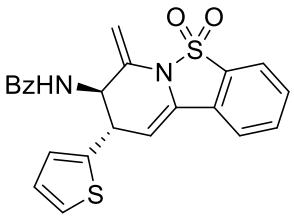

Sep05-2021-BM-3052
166.80
137.48
136.72
133.96
133.75
132.64
132.25
131.89
131.03
130.63
130.30
128.74
128.67
128.57
127.69
127.19
126.12
121.55
121.53
105.22
101.75
77.48
77.16
76.84
53.44
41.05
19.82
O
O
S
N
BzHN
Me
6h
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Sep04-2021-bm-3058
8.99
8.99
7.82
7.71
7.70
7.69
7.67
7.66
7.31
7.30
7.29
7.28
7.28
6.57
6.56
5.86
5.85
5.43
5.05
5.04
4.89
4.88
4.65
O
O
S
N
BzHN
6i
1.02
2.00
5.97
1.01
1.02
1.02
2.12
1.08
0.96
1.00
0.99
1.01
1.02
1.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

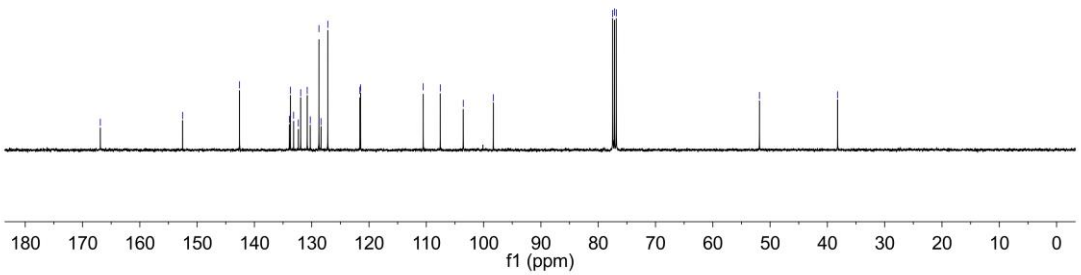

Sep04-2021-bm-3056
167.26
134.99
134.26
133.88
133.82
132.59
131.96
130.77
130.68
129.00
128.79
128.59
127.25
126.63
126.16
125.20
124.05
121.69
101.70
77.41
77.16
76.91
54.15
40.13
O
O
S
N
BzHN
6i
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

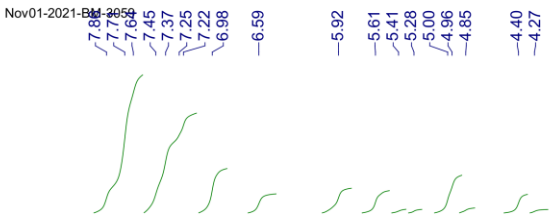

7.80
7.77
7.76
7.66
7.46
7.39
7.38
7.36
7.26
6.31
6.30
6.30
6.16
5.84
5.83
5.58
5.57
5.14
5.13
5.12
5.03
4.22
4.21
4.21
4.20
O
O
S
N
BzHN
S
6j
1.00
3.96
1.03
1.00
2.90
1.01
0.96
0.96
1.01
0.99
0.99
0.99
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

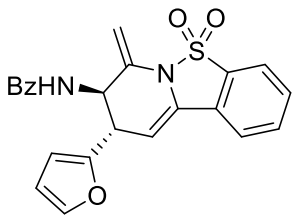

Sep04-2021-BM-3058
166.89
152.53
142.60
133.91
133.72
133.16
131.92
130.79
128.74
127.19
121.59
107.56
103.55
98.30
77.48
77.16
76.84
51.86
38.22


O
O
S
N
BzHN
S

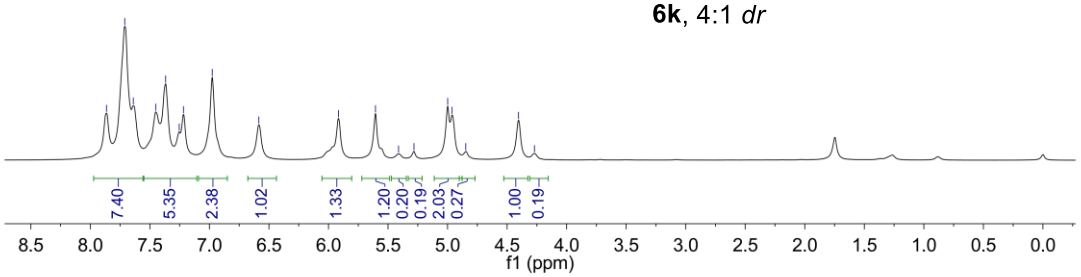
6j

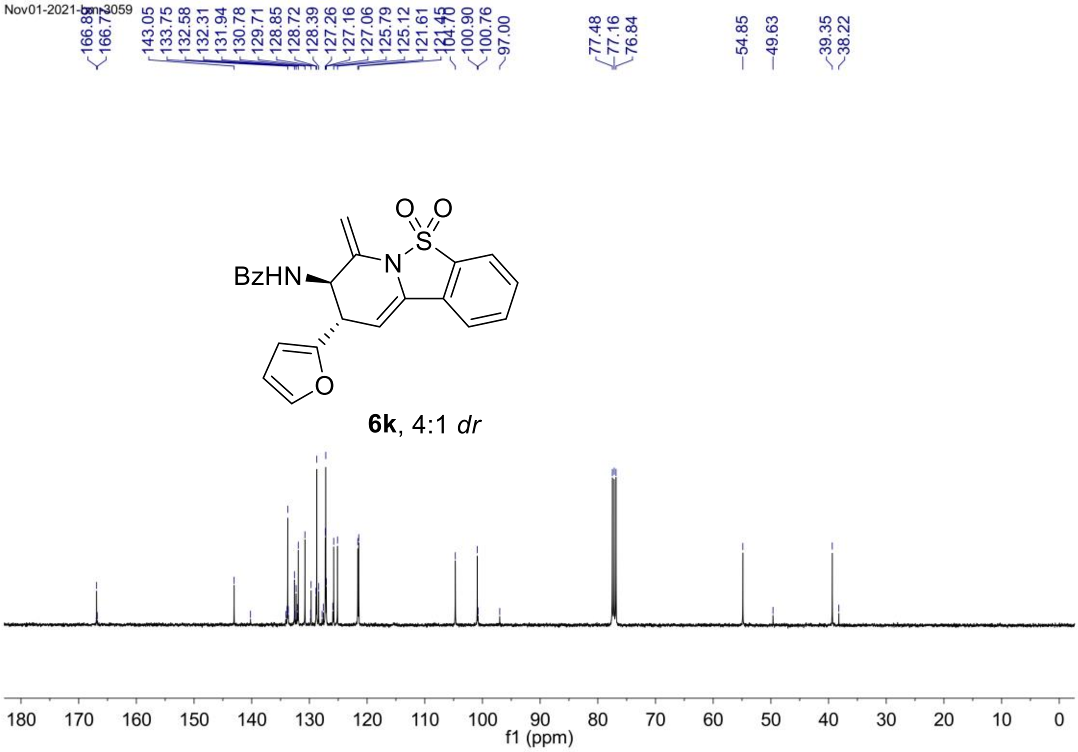

180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

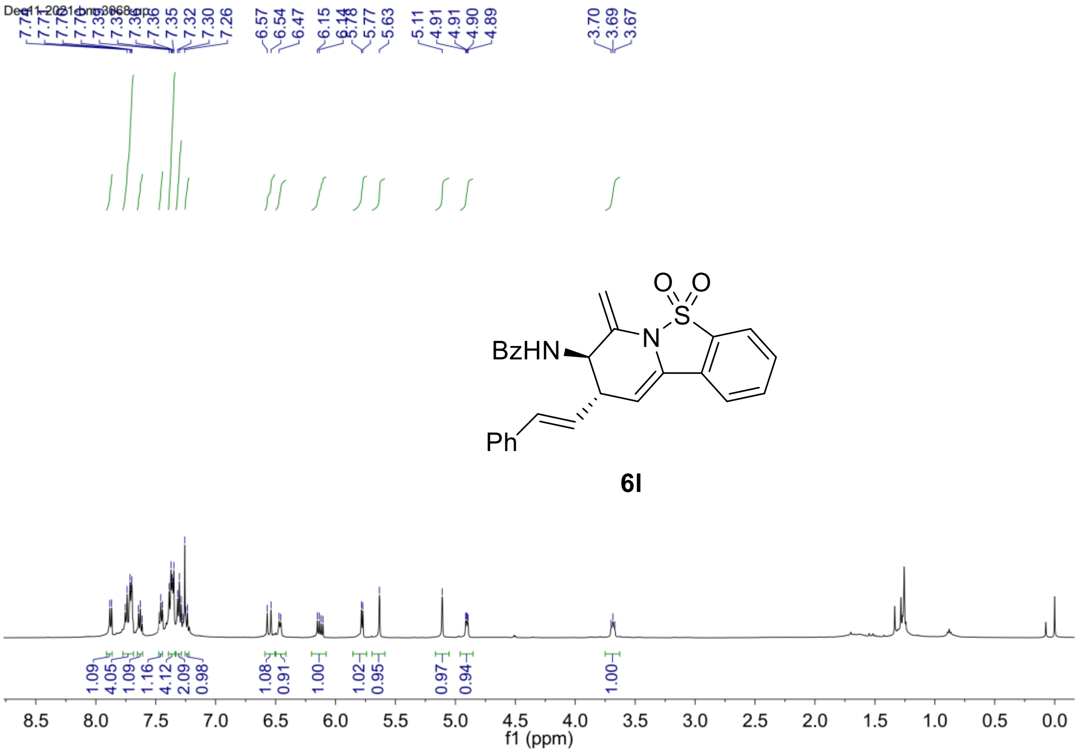

Nov01-2021-BM-3059
7.80
7.79
7.64
7.45
7.37
7.25
7.22
6.98
6.59
5.92
5.61
5.41
5.28
5.00
4.96
4.85
4.40
4.27

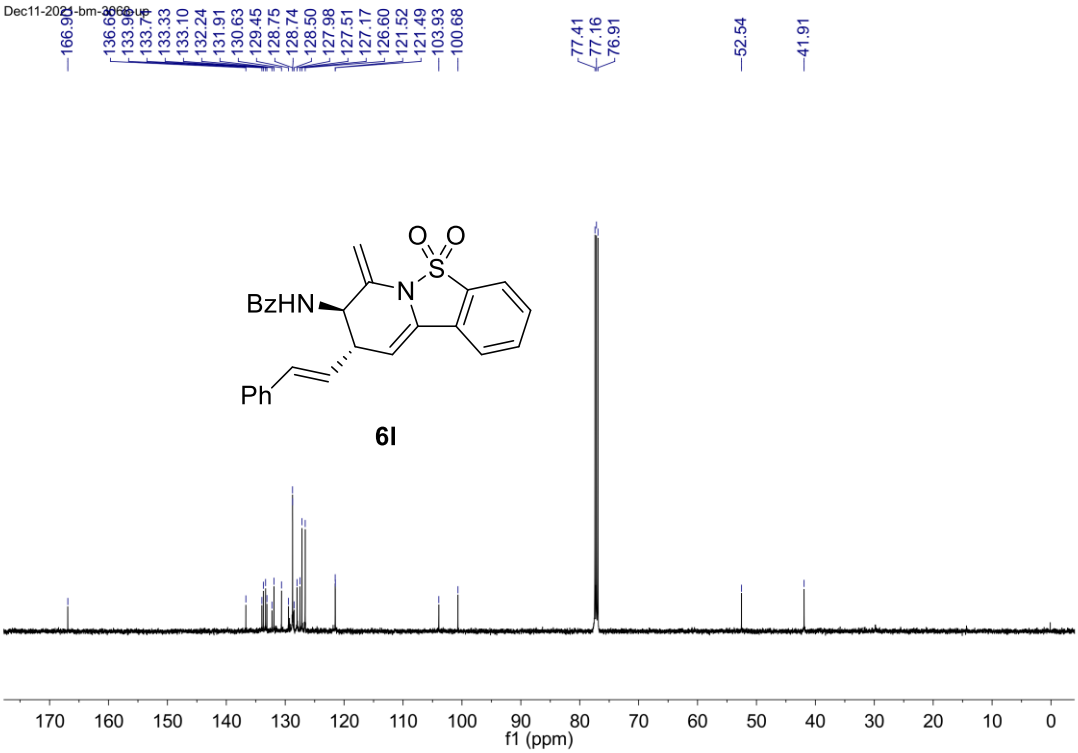

O
O
S
N
BzHN
O

6k, 4:1 *dr*

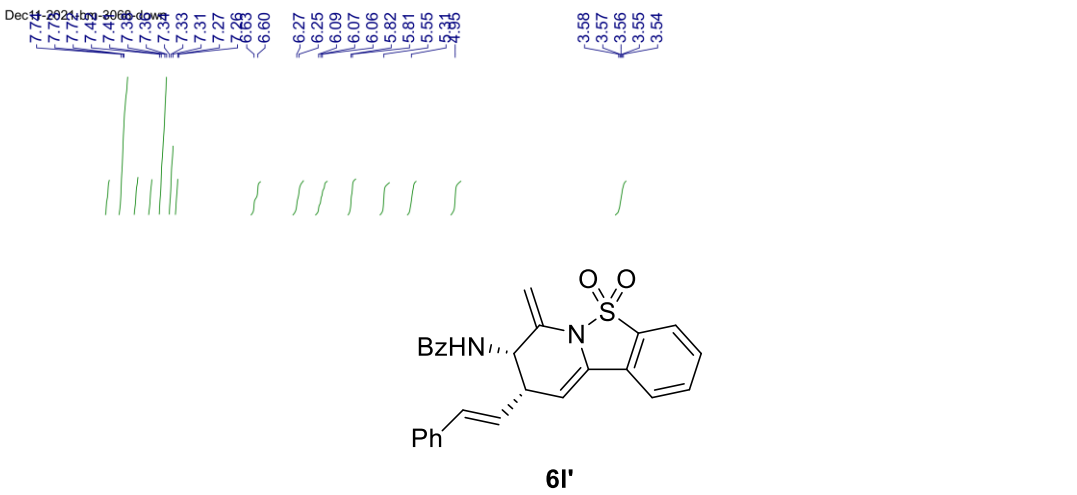

7.40
5.35
2.38
1.02
1.33
1.20
0.20
0.19
2.03
0.27
1.00
0.19
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


Nov01-2021-bmr3059
166.83 166.71 143.05 133.75 132.58 132.31 131.94 130.78 129.71 128.85 128.72 128.39 127.26 127.16 127.06 125.79 125.12 121.61 121.45 104.70 100.90 100.76 97.00 77.48 77.16 76.84 54.85 49.63 39.35 38.22
BzHN
N
S
O
O
O
6k, 4:1 dr
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

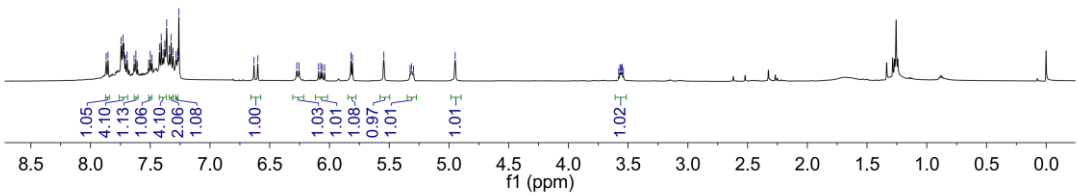

Dec11-2021-bmr3868
7.75 7.71 7.71 7.70 7.39 7.36 7.36 7.35 7.32 7.30 7.26 6.57 6.54 6.47 6.15 6.14 5.78 5.77 5.63 5.11 4.91 4.91 4.90 4.89 3.70 3.69 3.67
BzHN
N
S
O
O
Ph
6l
1.09 4.05 1.09 1.16 4.12 2.09 0.98 1.08 0.91 1.00 1.02 0.95 0.97 0.94 1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

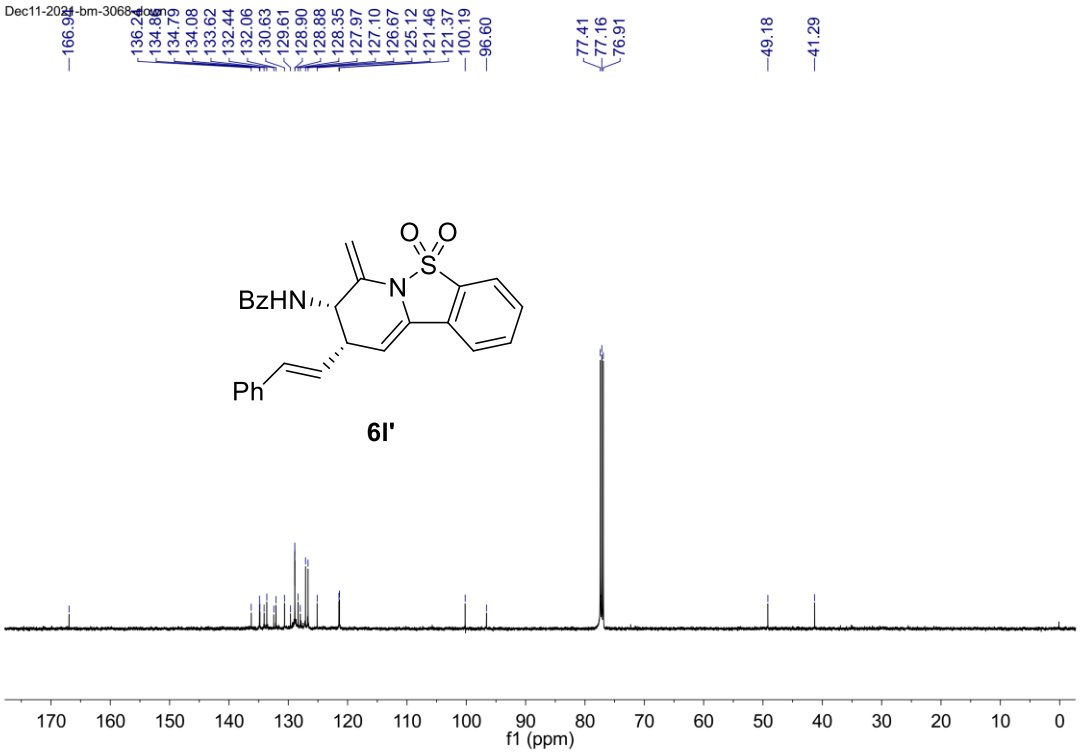

Dec11-2021-bm-3668.up
166.90
136.68
133.96
133.79
133.33
133.10
132.24
131.91
130.63
129.45
128.75
128.74
128.50
127.98
127.51
127.17
126.60
121.52
121.49
103.93
100.68
77.41
77.16
76.91
52.54
41.91
O
O
S
N
BzHN
Ph
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

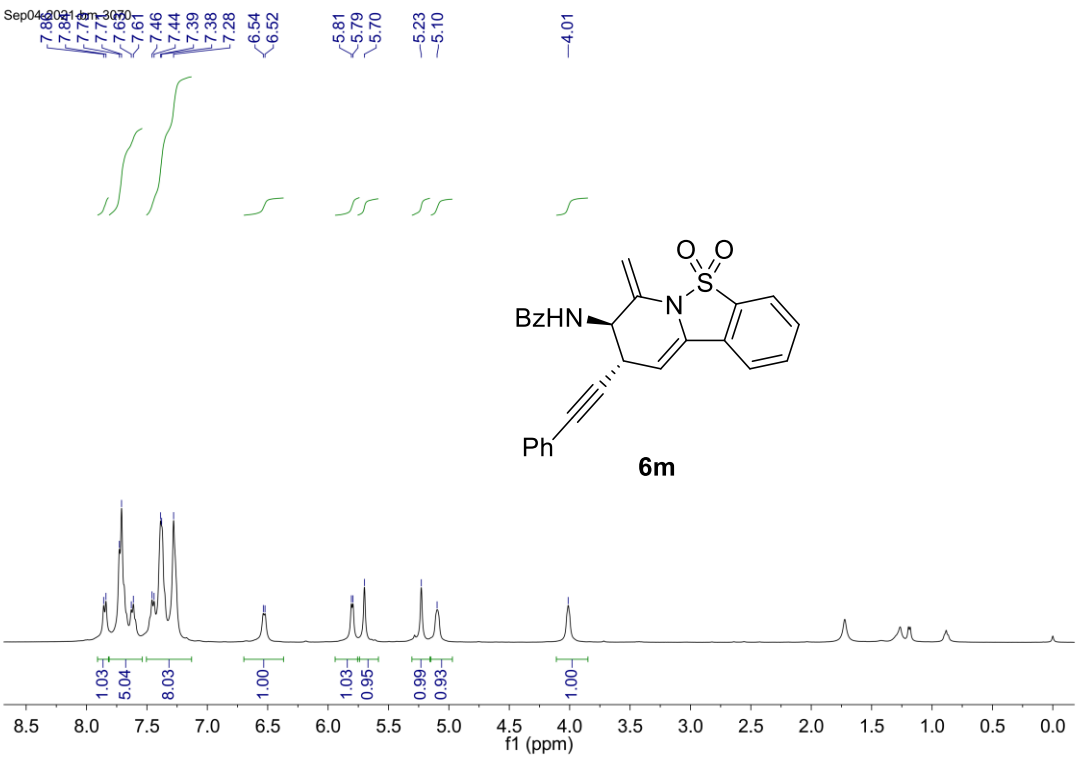
6l

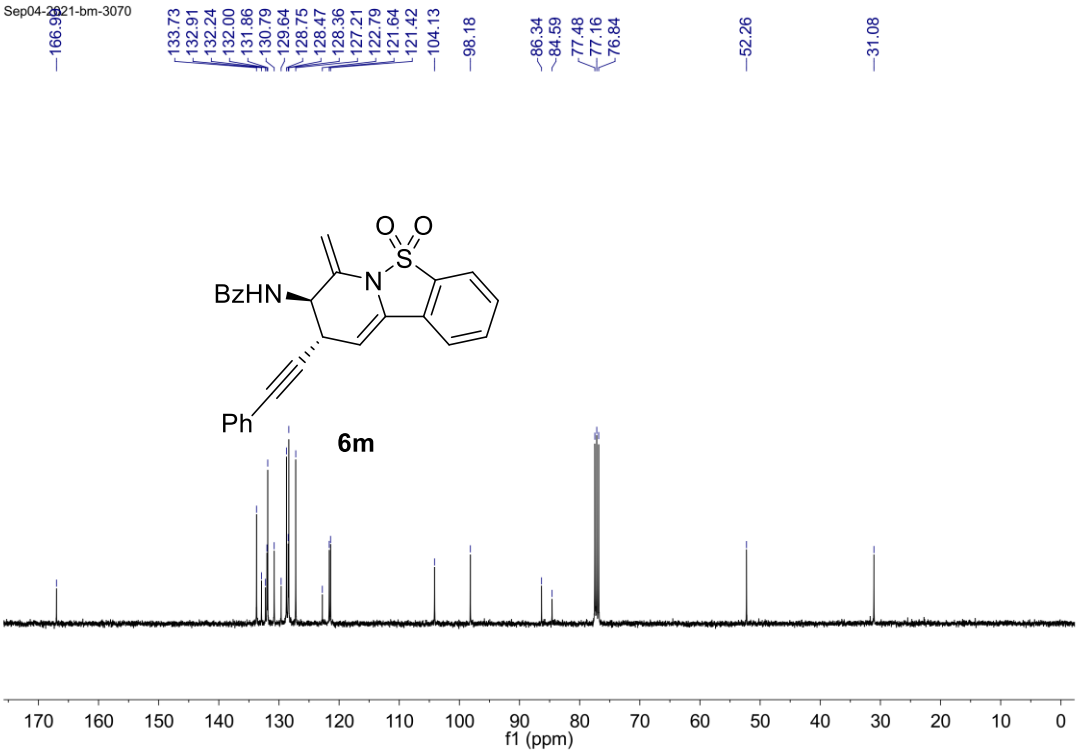

Dec11-2021-bm-3668-down
7.77
7.76
7.75
7.74
7.46
7.45
7.36
7.34
7.33
7.31
7.27
6.63
6.60
6.27
6.25
6.09
6.07
6.06
5.82
5.81
5.55
5.31
4.95
3.58
3.57
3.56
3.55
3.54
O
O
S
N
BzHN
Ph

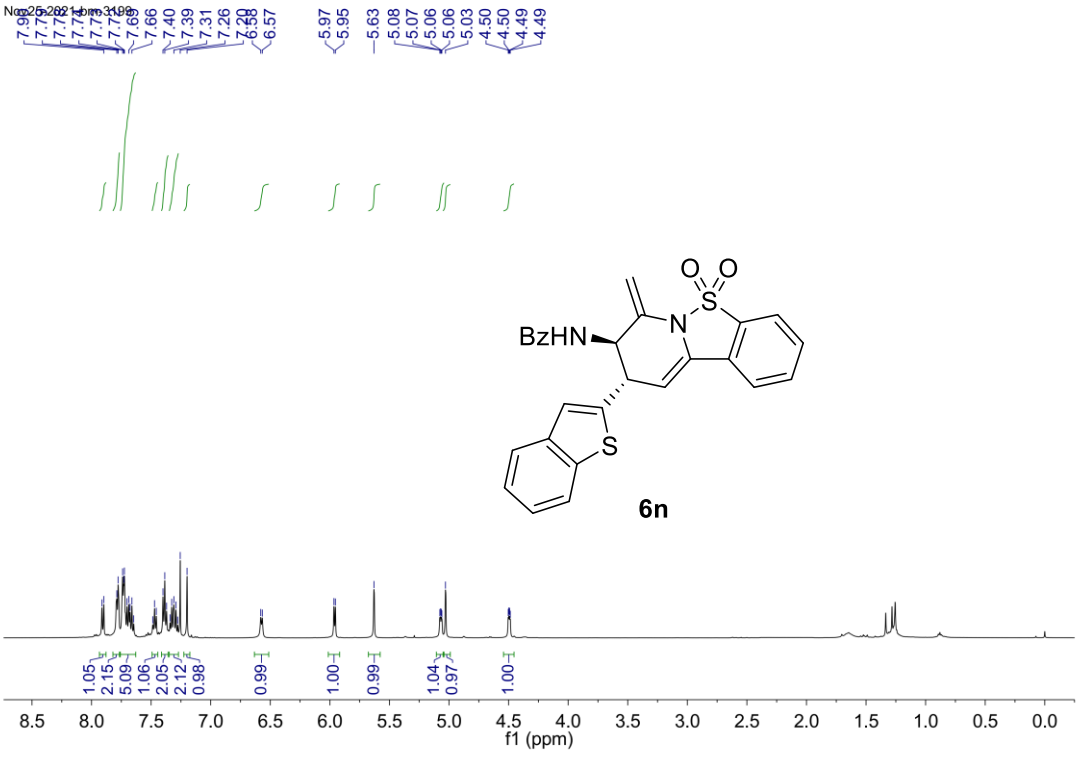
6l'

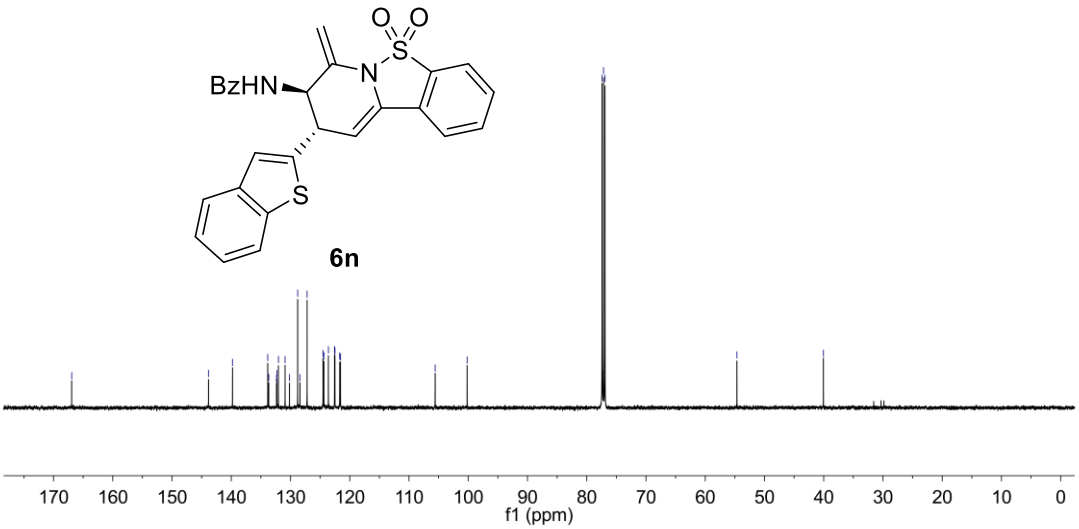

1.05
4.10
1.13
1.06
4.10
2.06
1.08
1.00
1.03
1.01
1.08
0.97
1.01
1.01
1.02
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

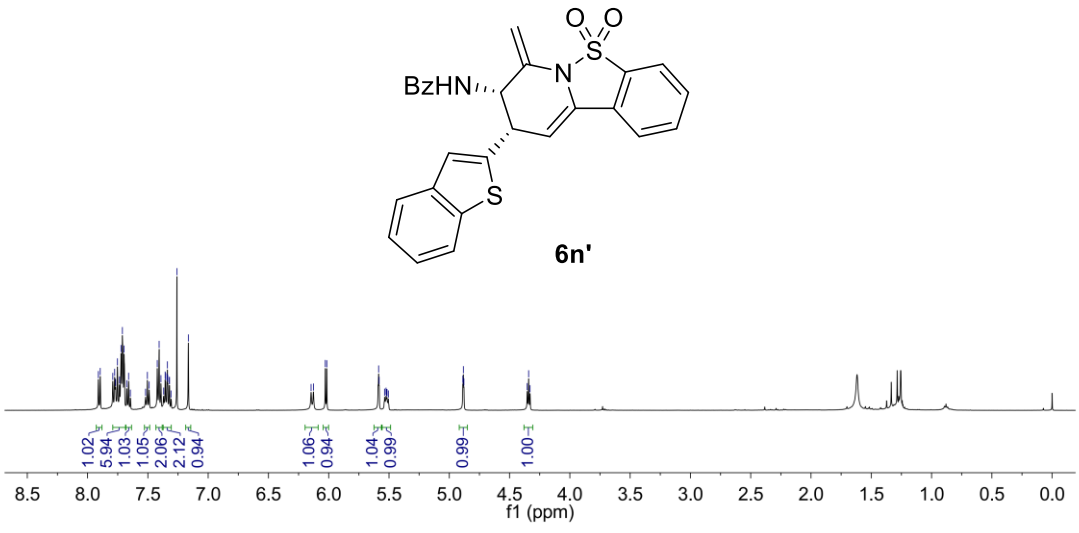

Dec11-2021-bm-3068-down
166.94
136.22
134.88
134.79
134.08
133.62
132.44
132.06
130.63
129.61
128.90
128.88
128.35
127.97
127.10
126.67
125.12
121.46
121.37
100.19
96.60
77.41
77.16
76.91
49.18
41.29
O
O
S
N
BzHN
Ph
6l'
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

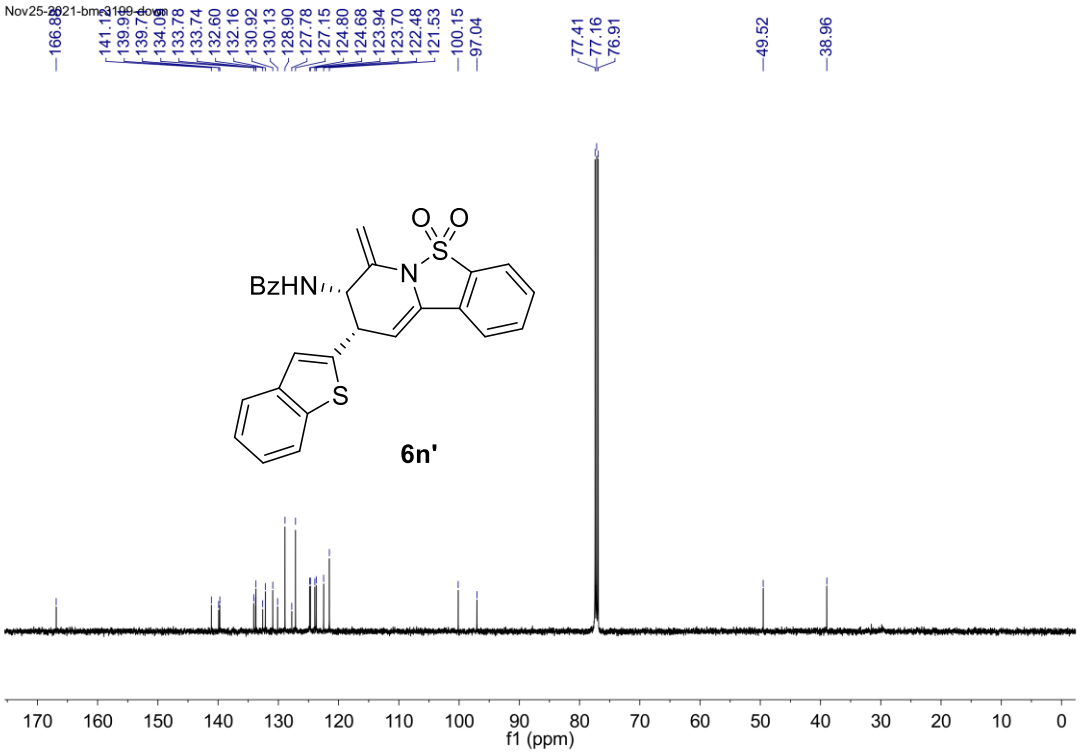

Sep04-2021-bm-3070
7.86
7.84
7.77
7.75
7.61
7.46
7.44
7.39
7.38
7.28
6.54
6.52
5.81
5.79
5.70
5.23
5.10
4.01
O
O
S
N
BzHN
Ph
6m
1.03
5.04
8.03
1.00
1.03
0.95
0.99
0.93
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

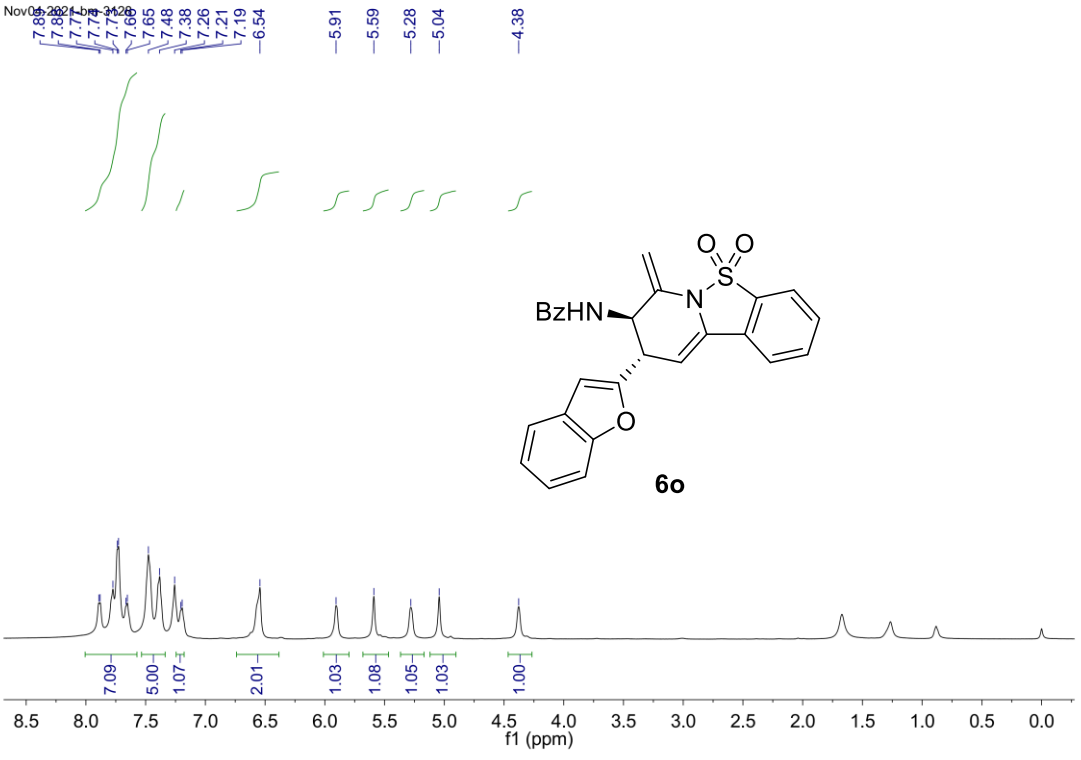

Sep04-2021-bm-3070
166.90
133.73
132.91
132.24
132.00
131.86
130.79
129.64
128.75
128.47
128.36
127.21
122.79
121.64
121.42
104.13
98.18
86.34
84.59
77.48
77.16
76.84
52.26
31.08
BzHN
N
S
O
O
Ph
6m
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

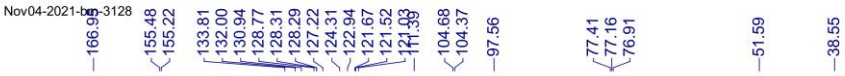

Nov25-2021-bm-3108
7.99
7.78
7.77
7.76
7.75
7.74
7.73
7.69
7.66
7.40
7.39
7.31
7.26
6.58
6.57
5.97
5.95
5.63
5.08
5.07
5.06
5.06
5.03
4.50
4.50
4.49
4.49
BzHN
N
S
O
O
S
6n
1.05
2.15
5.09
1.06
2.05
2.12
0.98
0.99
1.00
0.99
1.04
0.97
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

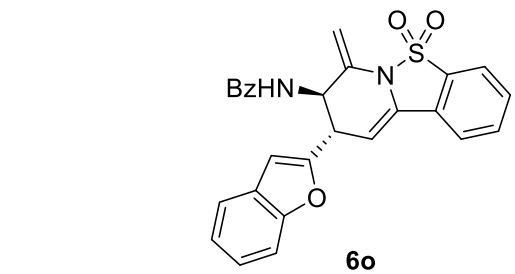

BzHN
O
O
S
N
S
6n
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


BzHN
O
O
S
N
S
6n'
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

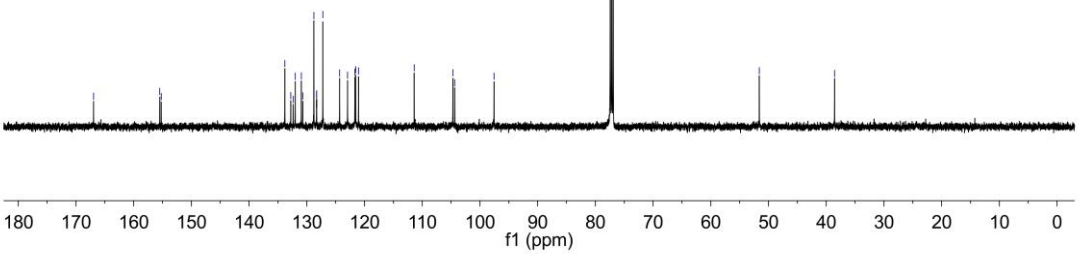

Nov25-2021-bms-3199-down
166.88
141.12
139.99
139.76
134.08
133.78
133.74
132.60
132.16
130.92
130.13
128.90
127.78
127.15
124.80
124.68
123.94
123.70
122.48
121.53
100.15
97.04
77.41
77.16
76.91
49.52
38.96
BzHN
O
O
S
N
S
6n'
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

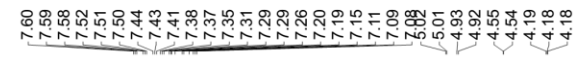

Nov05-2021-bms-3126
7.89
7.88
7.77
7.76
7.75
7.66
7.65
7.48
7.38
7.26
7.21
7.19
6.54
5.91
5.59
5.28
5.04
4.38
BzHN
O
O
S
N
O
6o
7.09
5.00
1.07
2.01
1.03
1.08
1.05
1.03
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

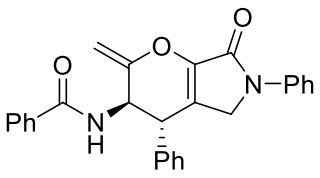

Nov04-2021-bm-3128
166.98
155.48
155.22
133.81
132.00
130.94
128.77
128.31
128.29
127.22
124.31
122.94
121.67
121.52
111.39
104.68
104.37
97.56
77.41
77.16
76.91
51.59
38.55


O
O
S
N
BzHN
O

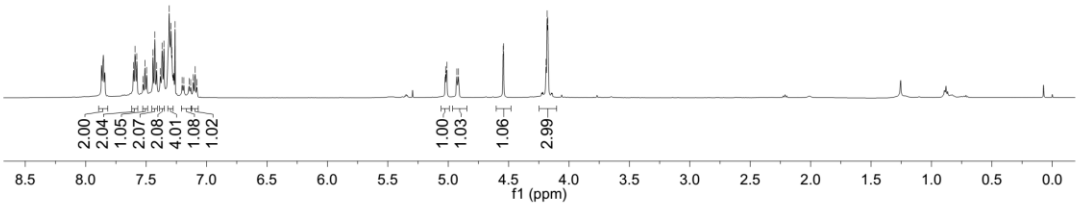
6o

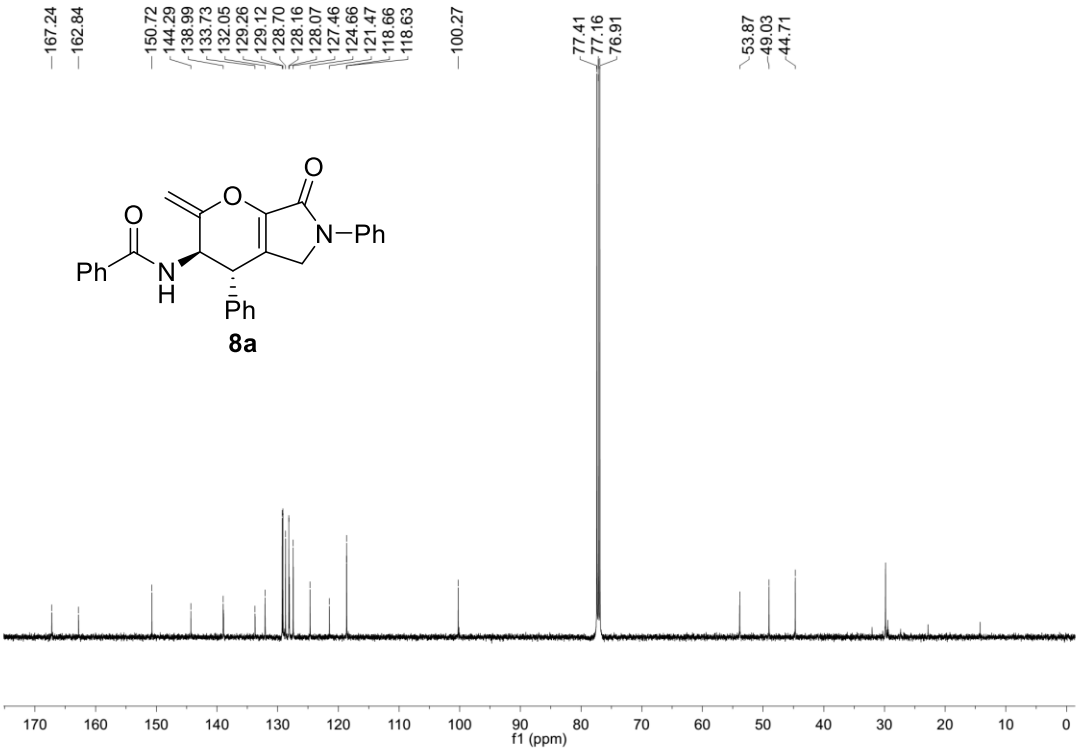

180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

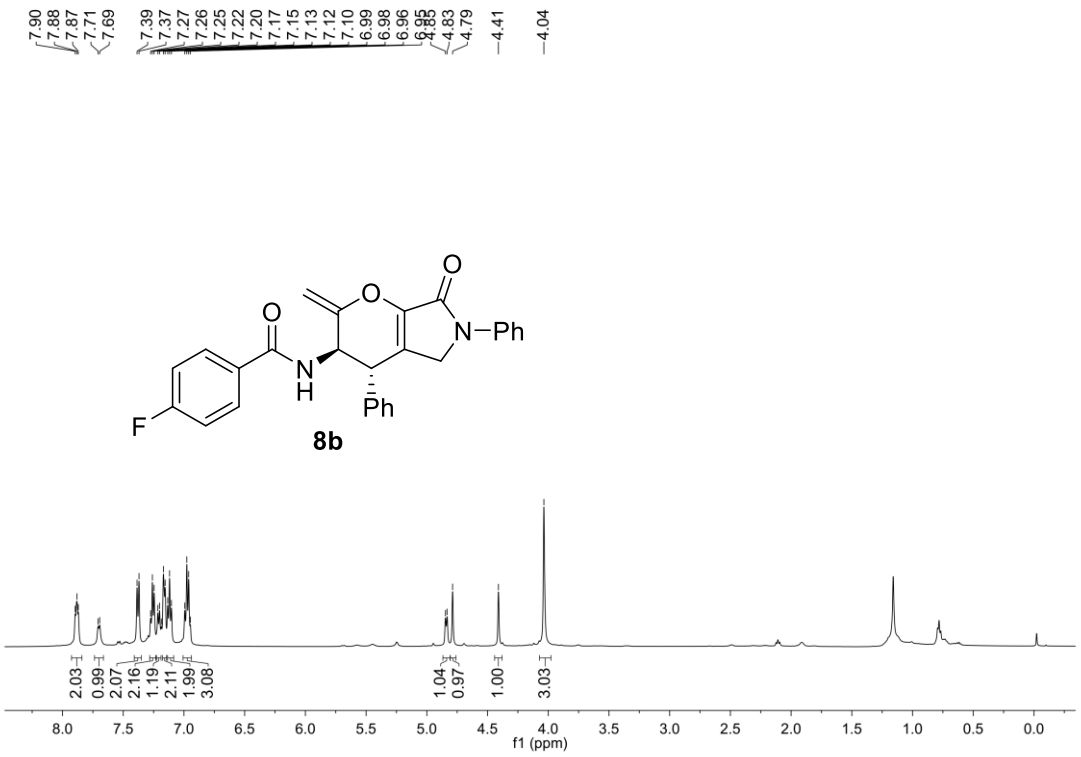

7.60
7.59
7.58
7.52
7.51
7.50
7.44
7.43
7.41
7.38
7.37
7.35
7.31
7.29
7.29
7.26
7.20
7.19
7.15
7.11
7.09
5.01
4.93
4.92
4.55
4.54
4.19
4.18
4.18

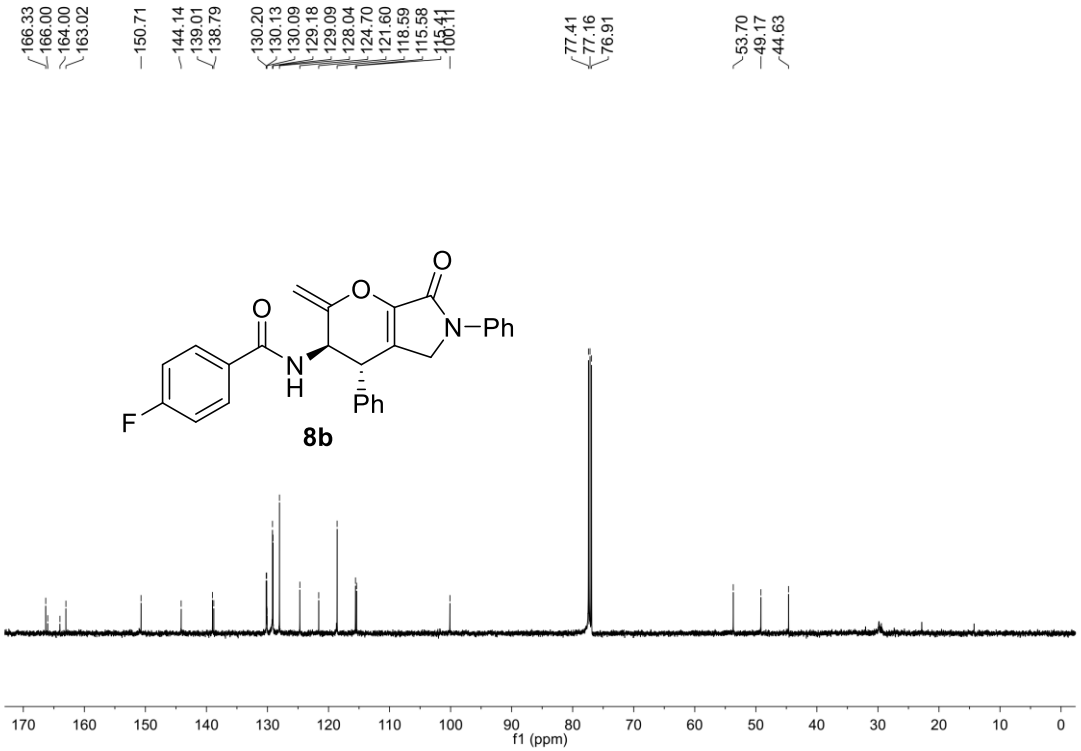

O
O
N—Ph
Ph
N
H
Ph

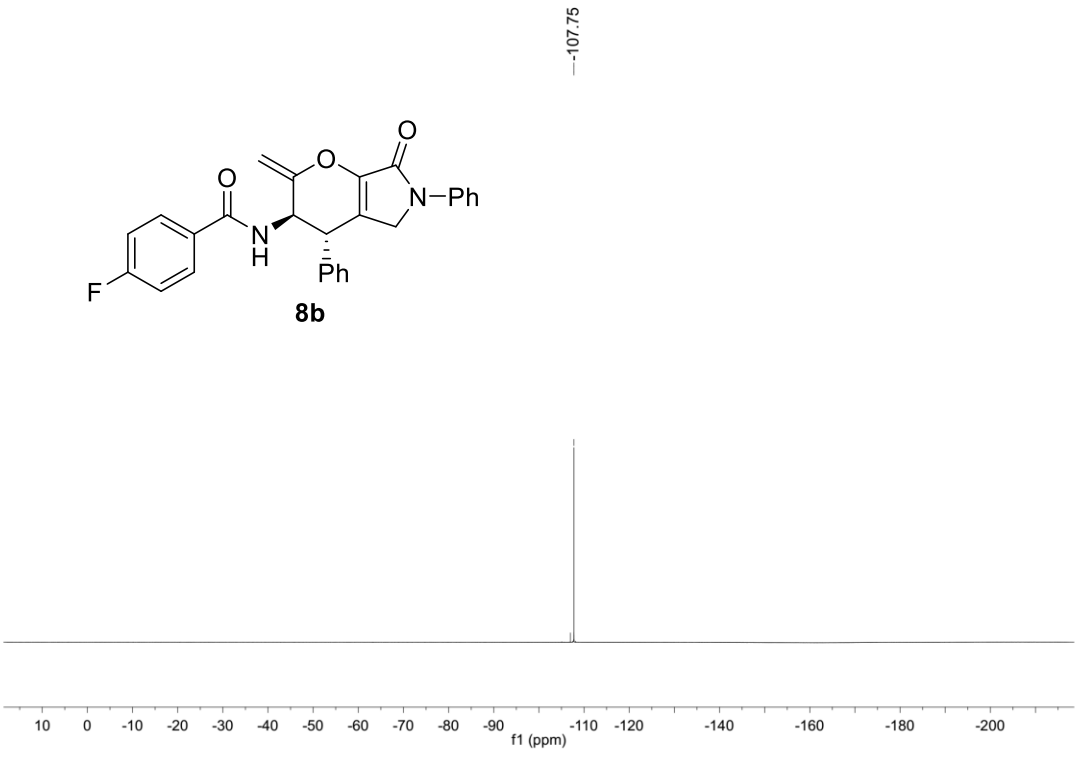
8a

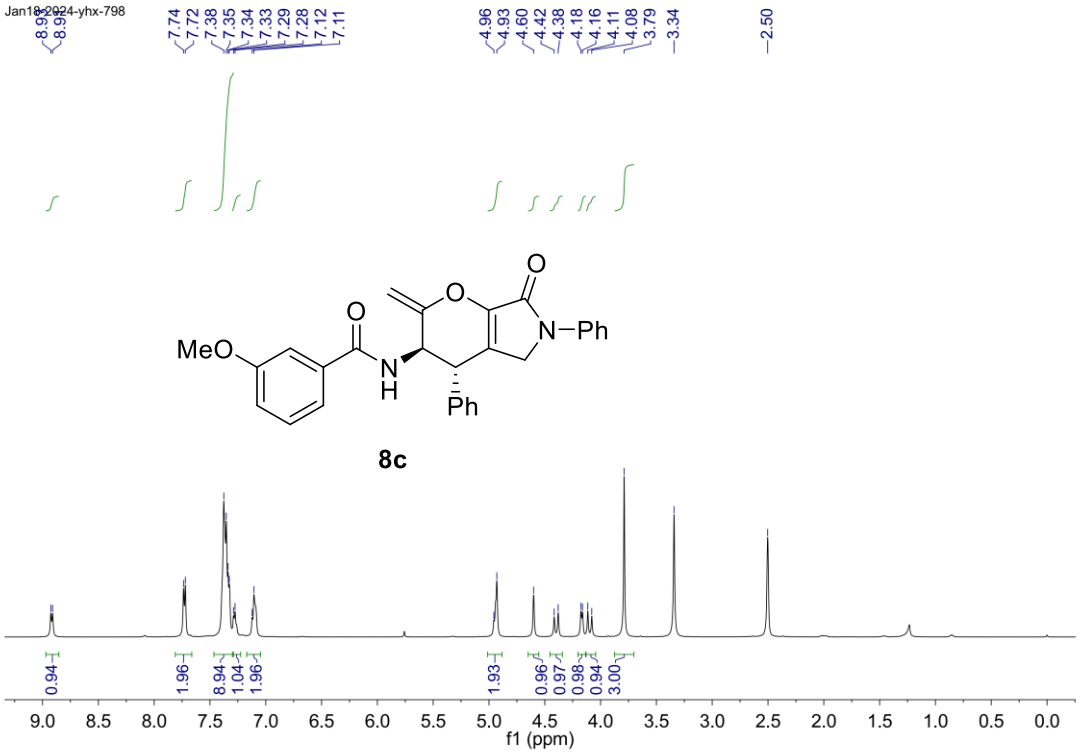

2.00
2.04
1.05
2.07
2.08
4.01
1.08
1.02
1.00
1.03
1.06
2.99
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


167.24
162.84
150.72
144.29
138.99
133.73
132.05
129.26
129.12
128.70
128.16
128.07
127.46
124.66
121.47
118.66
118.63
100.27
77.41
77.16
76.91
53.87
49.03
44.71
O
O
N–Ph
Ph
N
H
Ph
8a
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

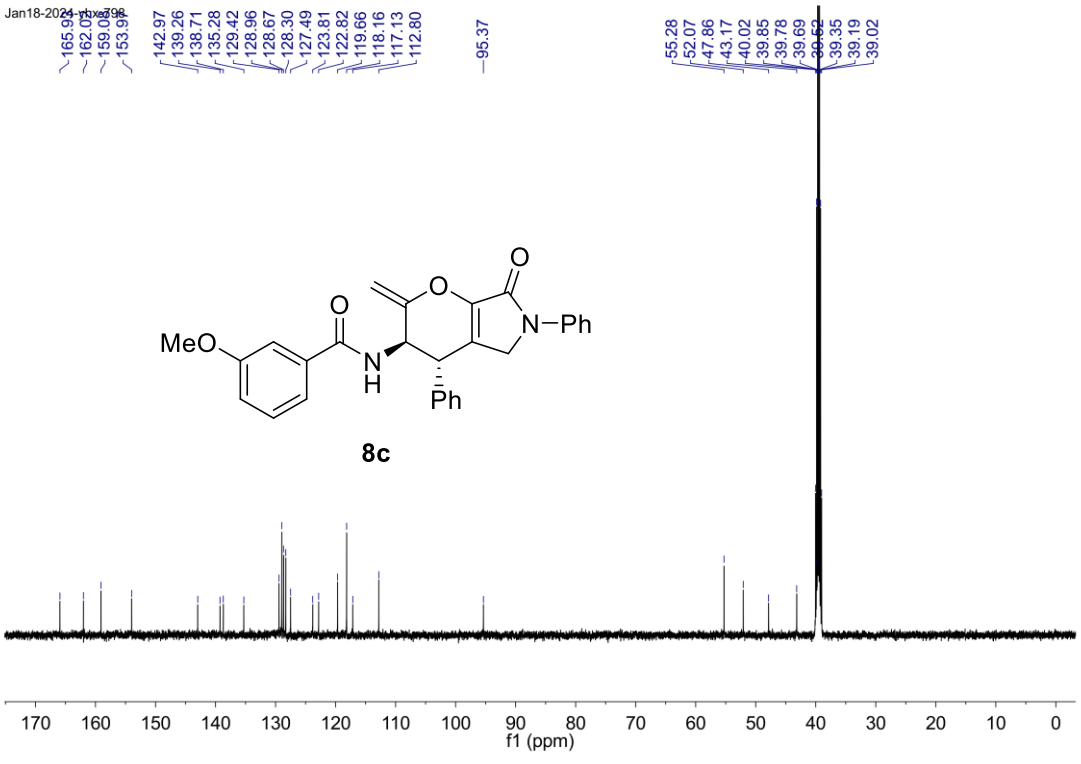

7.90
7.88
7.87
7.71
7.69
7.39
7.37
7.27
7.26
7.25
7.22
7.20
7.17
7.15
7.13
7.12
7.10
6.99
6.98
6.96
4.83
4.79
4.41
4.04
O
O
N–Ph
N
H
Ph
F
8b
2.03
0.99
2.07
2.16
1.19
2.11
1.99
3.08
1.04
0.97
1.00
3.03
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


166.33
166.00
164.00
163.02
150.71
144.14
139.01
138.79
130.20
130.13
130.09
129.18
129.09
128.04
124.70
121.60
118.59
115.58
115.41
100.11
77.41
77.16
76.91
53.70
49.17
44.63
O
O
N
H
F
O
N–Ph
Ph
8b
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

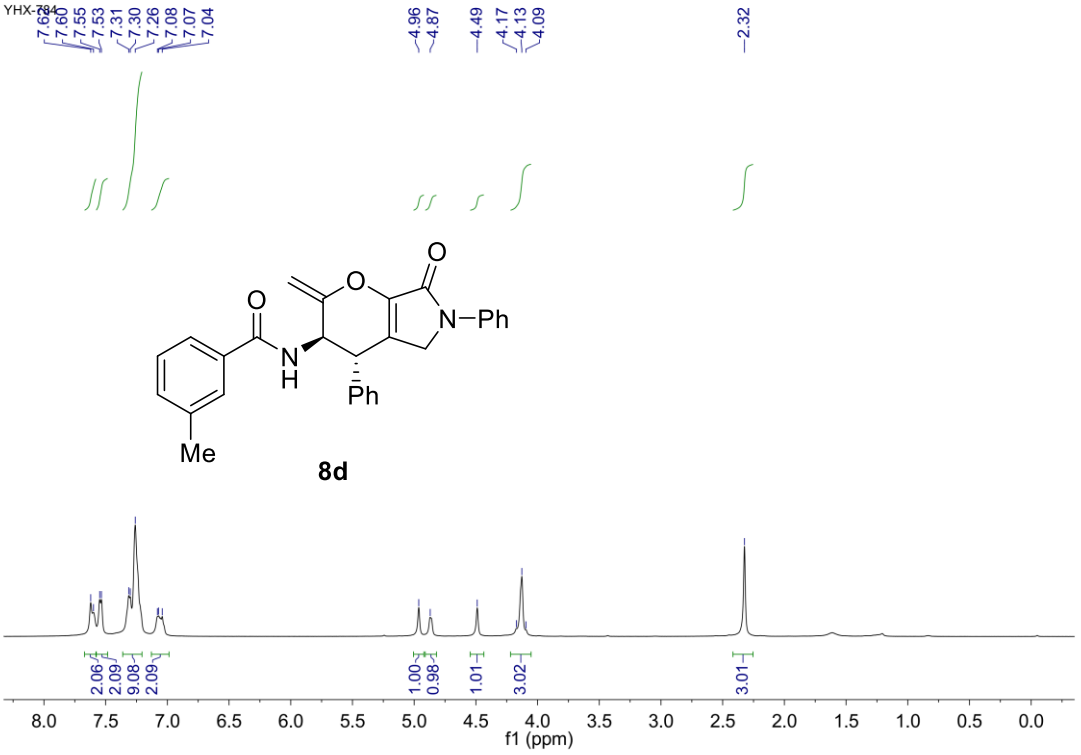

-107.75
O
O
N
H
F
O
N–Ph
Ph
8b
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-120
-140
-160
-180
-200
f1 (ppm)

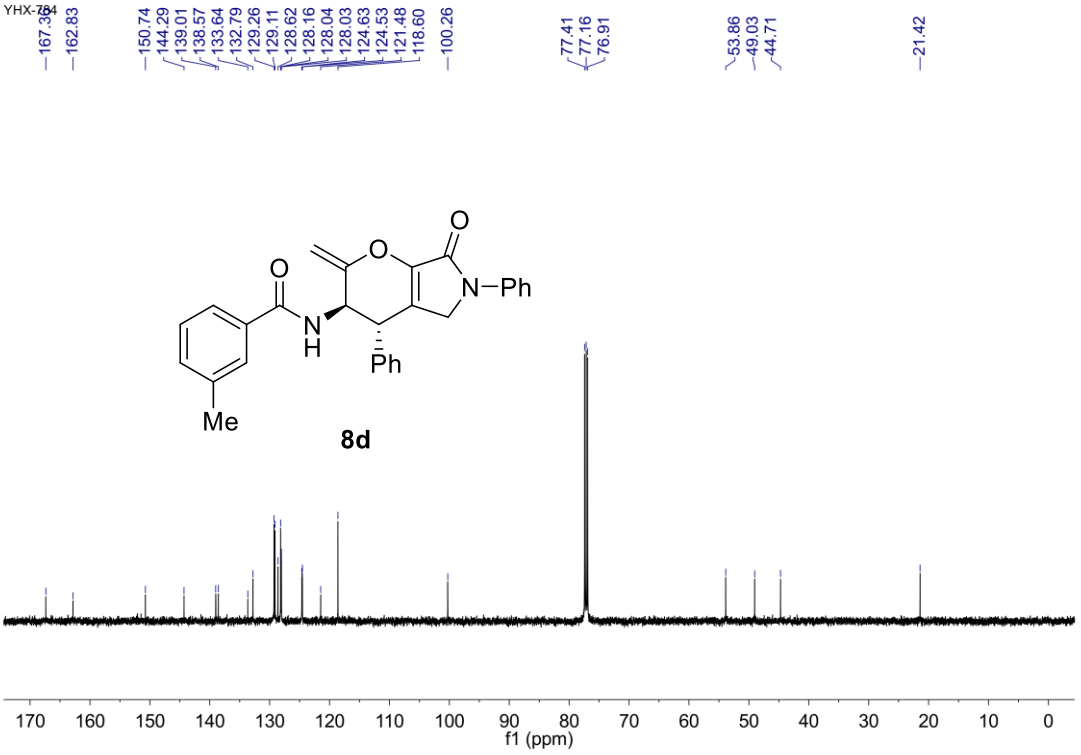

Jan18-2024-yhx-798
8.99
8.98
7.74
7.72
7.38
7.35
7.34
7.33
7.29
7.28
7.12
7.11
4.96
4.93
4.60
4.42
4.38
4.18
4.16
4.11
4.08
3.79
3.34
2.50
MeO
O
O
N
H
O
N–Ph
Ph
0.94
1.96
8.94
1.04
1.96
1.93
0.96
0.97
0.98
0.94
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

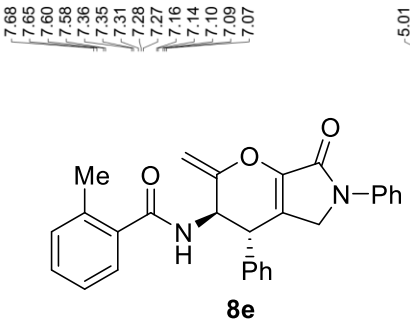
8c


Jan18-2024-yhx-798
165.99
162.05
159.08
153.99
142.97
139.26
138.71
135.28
129.42
128.96
128.67
128.30
127.49
123.81
122.82
119.66
118.16
117.13
112.80
95.37
55.28
52.07
47.86
43.17
40.02
39.85
39.78
39.69
39.52
39.35
39.19
39.02
MeO
O
O
N
H
O
N–Ph
Ph
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

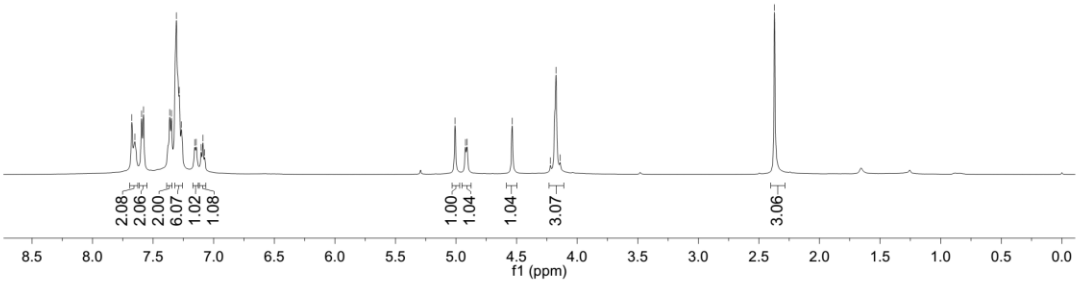
8c

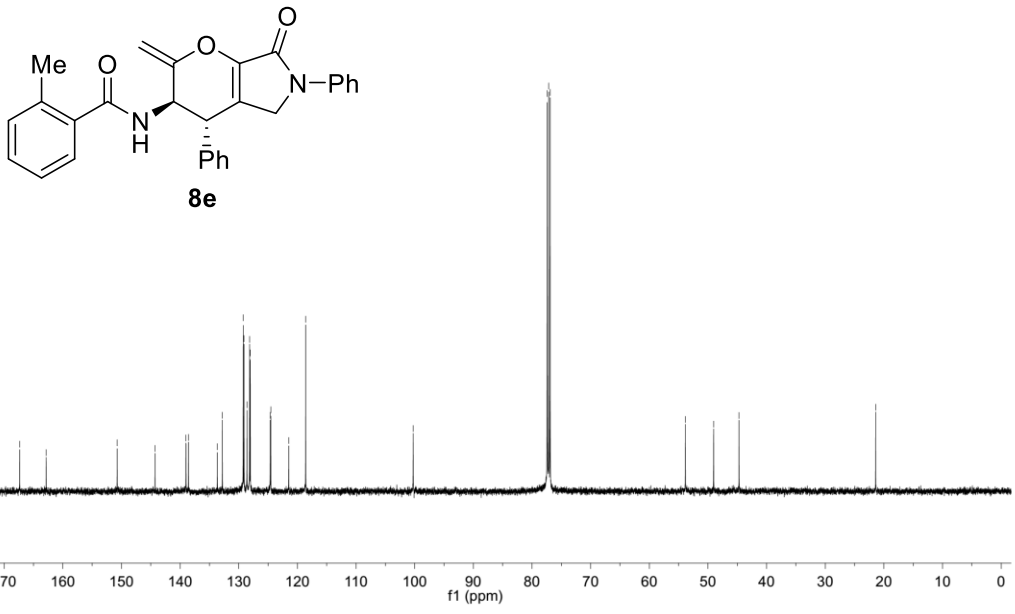

YHX-784
7.62
7.60
7.55
7.53
7.31
7.30
7.26
7.08
7.07
7.04
4.96
4.87
4.49
4.17
4.13
4.09
2.32
O
O
O
N
H
N—Ph
Ph
Me
8d
2.06
2.09
9.08
2.09
1.00
0.98
1.01
3.02
3.01
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


YHX-784
167.36
162.83
150.74
144.29
139.01
138.57
133.64
132.79
129.26
129.11
128.62
128.16
128.04
128.03
124.63
124.53
121.48
118.60
100.26
77.41
77.16
76.91
53.86
49.03
44.71
21.42
O
O
O
N
H
N—Ph
Ph
Me
8d
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

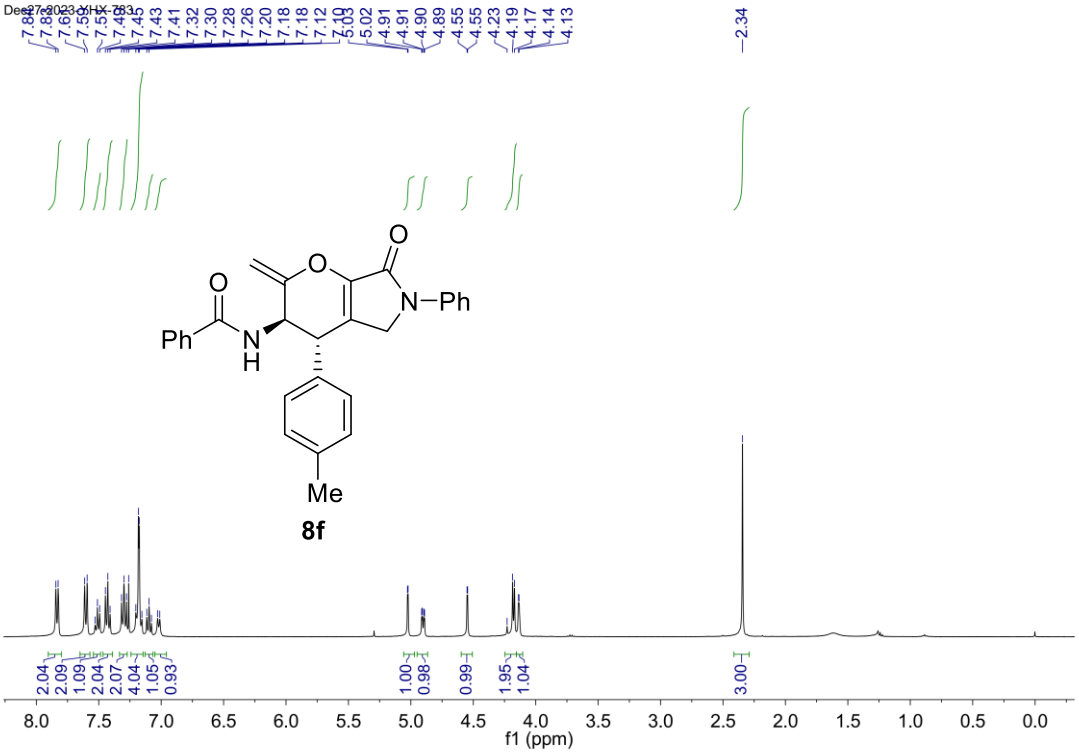


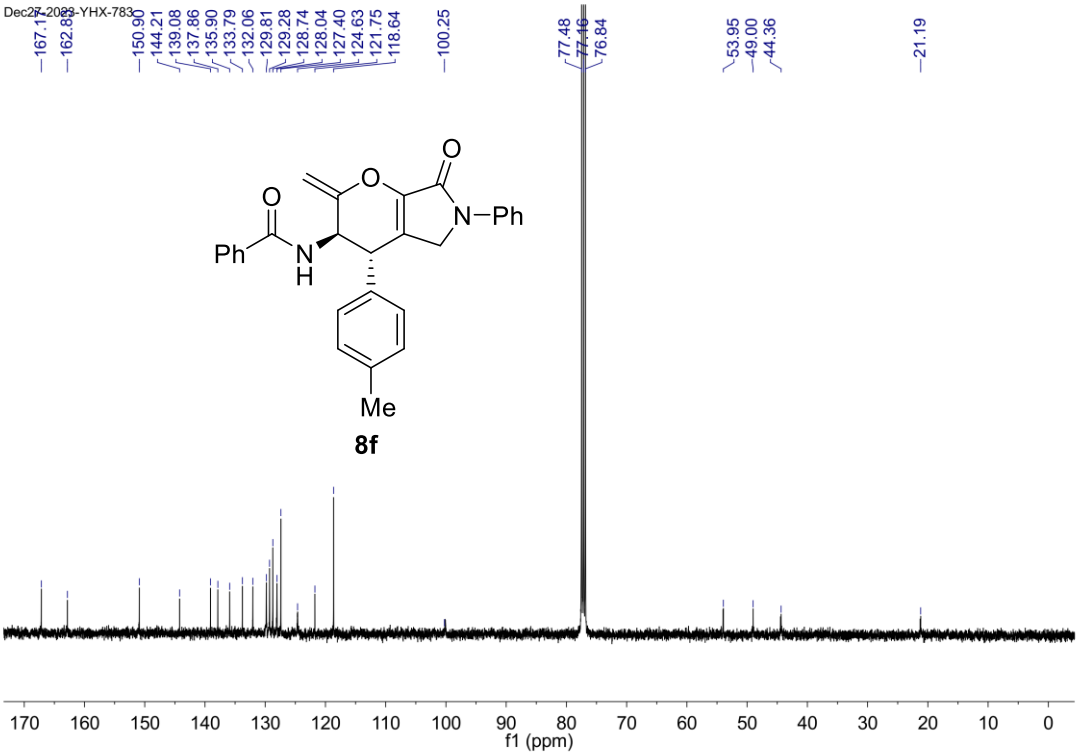
8e

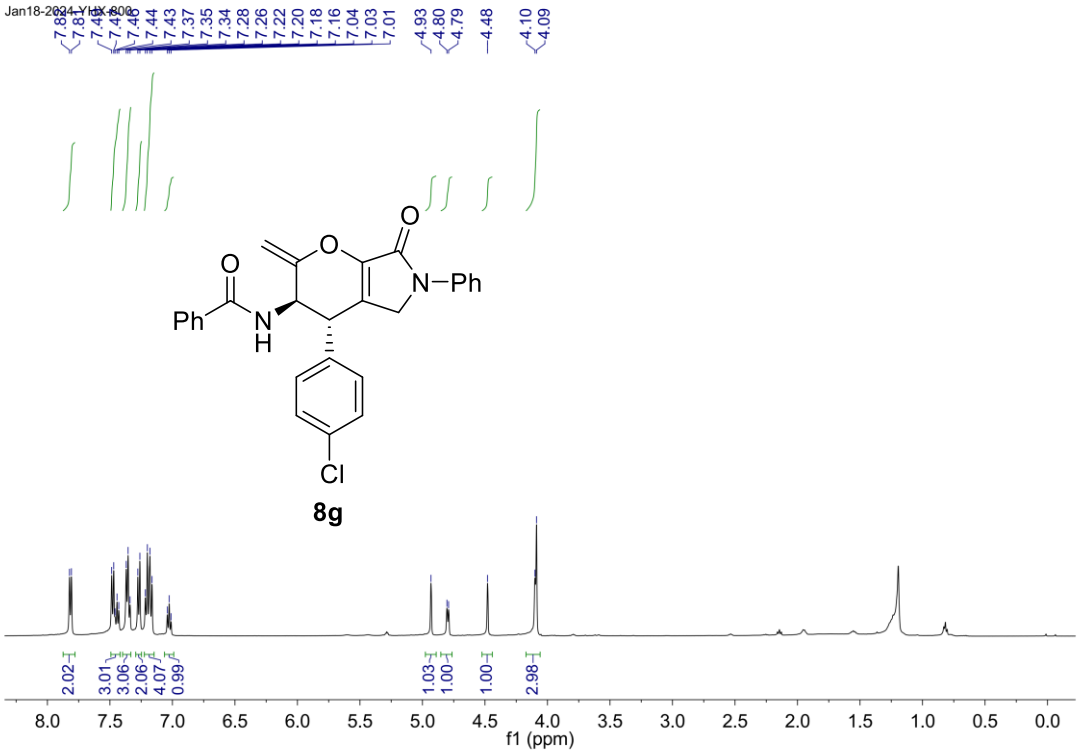


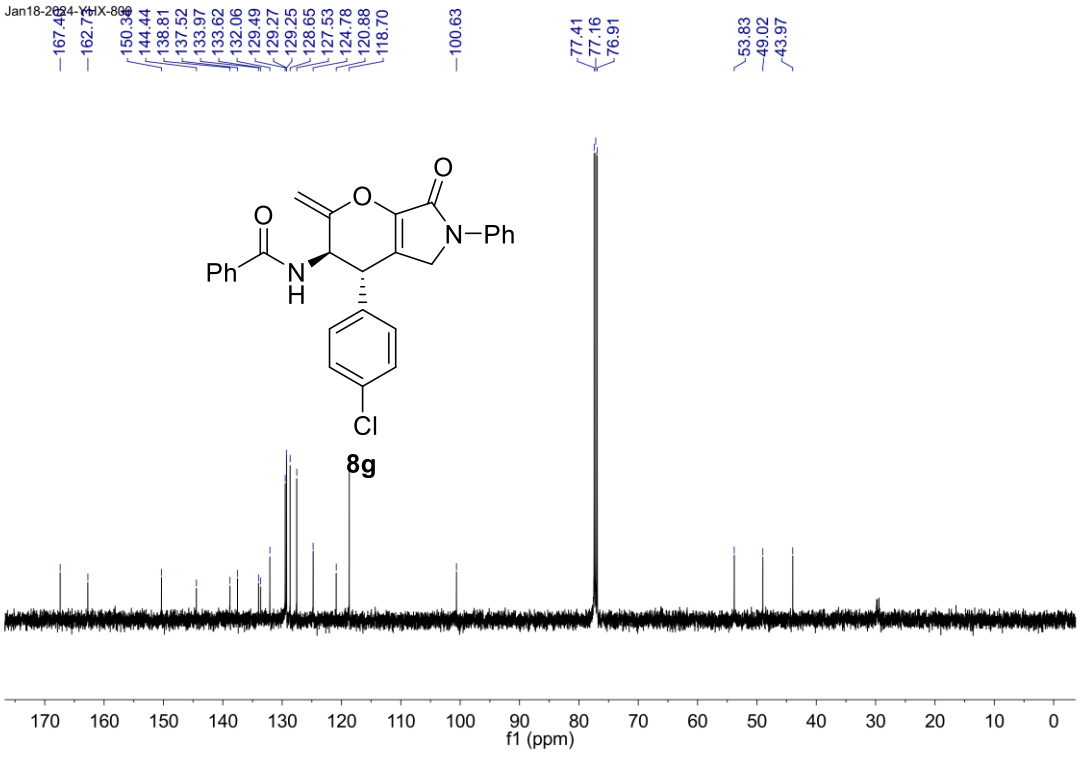


8e

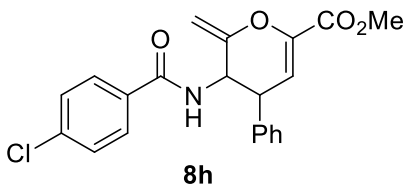

Dec27-2023-YHX-783
7.84
7.82
7.60
7.59
7.51
7.49
7.45
7.43
7.41
7.32
7.30
7.28
7.26
7.20
7.18
7.18
7.12
7.10
7.03
5.02
4.91
4.91
4.90
4.89
4.55
4.55
4.23
4.19
4.17
4.14
4.13
2.34
O
O
O
N−Ph
Ph
N
H
Me
8f
2.04
2.09
1.09
2.04
2.07
4.04
1.05
0.93
1.00
0.98
0.99
1.95
1.04
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


Dec27-2023-YHX-783
167.1
162.8
150.90
144.21
139.08
137.86
135.90
133.79
132.06
129.81
129.28
128.74
128.04
127.40
124.63
121.75
118.64
100.25
77.48
77.16
76.84
53.95
49.00
44.36
21.19
O
O
O
N−Ph
Ph
N
H
Me
8f
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

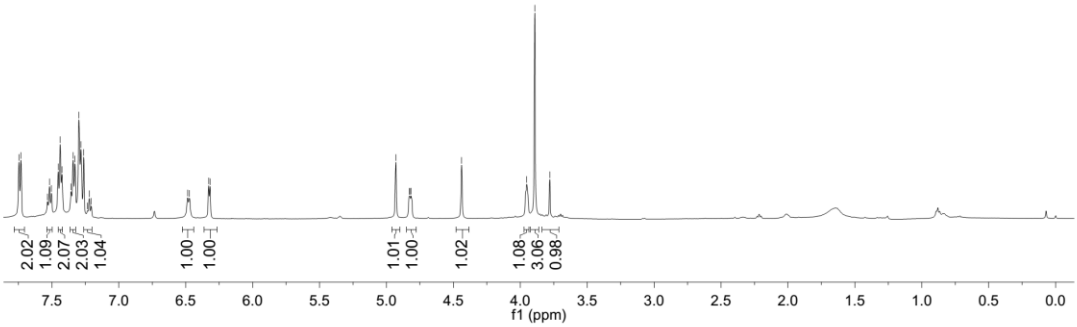

Jan18-2024-YHX-800
7.84
7.81
7.48
7.46
7.44
7.43
7.37
7.35
7.34
7.28
7.26
7.22
7.20
7.18
7.16
7.04
7.03
7.01
4.93
4.80
4.79
4.48
4.10
4.09
O
O
N–Ph
Ph
N
H
Cl
8g
2.02
3.01
3.06
2.06
4.07
0.99
1.03
1.00
1.00
2.98
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

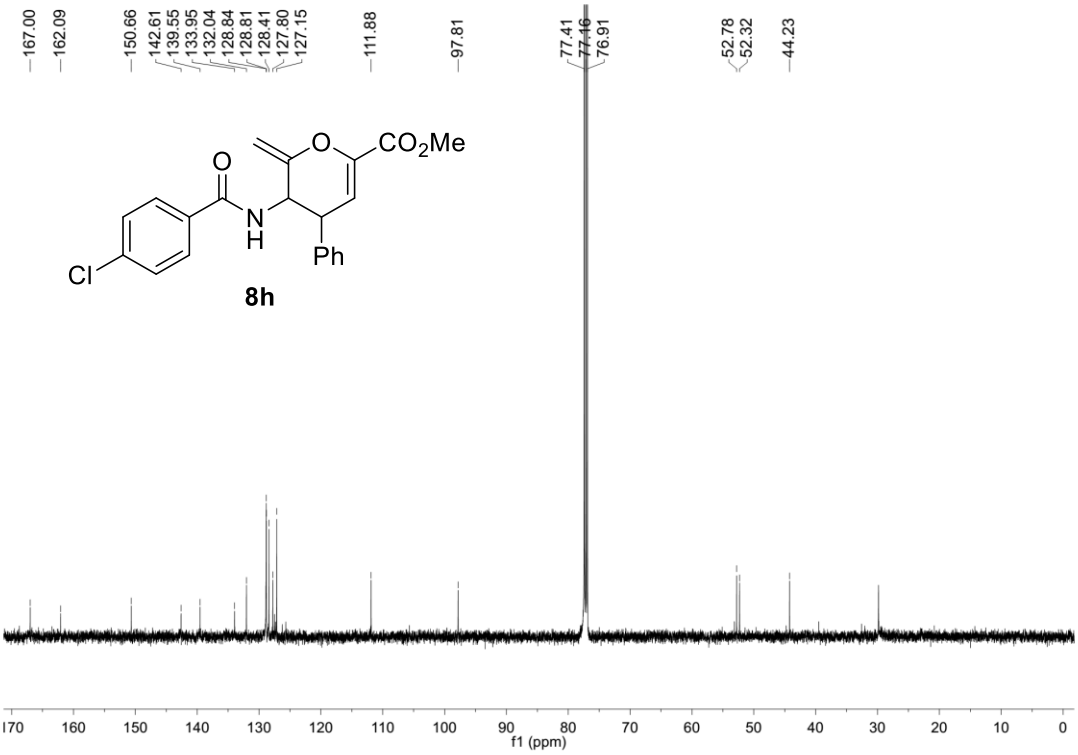

Jan18-2024-YHX-800
167.46
162.75
150.34
144.44
138.81
137.52
133.97
133.62
132.06
129.49
129.27
129.25
128.65
127.53
124.78
120.88
118.70
100.63
77.41
77.16
76.91
53.83
49.02
43.97
O
O
N–Ph
Ph
N
H
Cl
8g
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.75
7.73
7.44
7.34
7.30
7.28
6.47
6.33
6.32
4.93
4.83
4.82
4.82
4.44
3.95
3.89
3.78

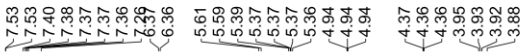

O
CO2Me
O
N
H
Ph
Cl

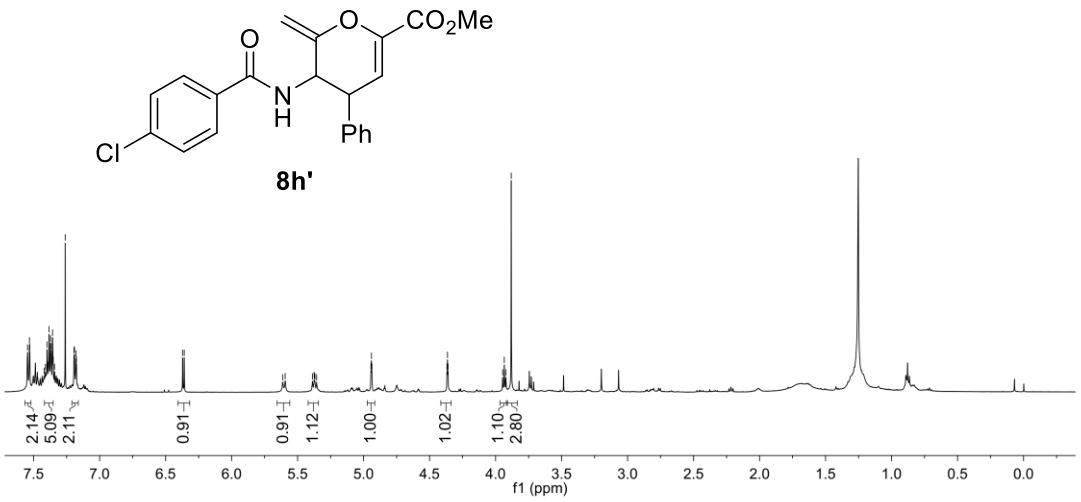
8h

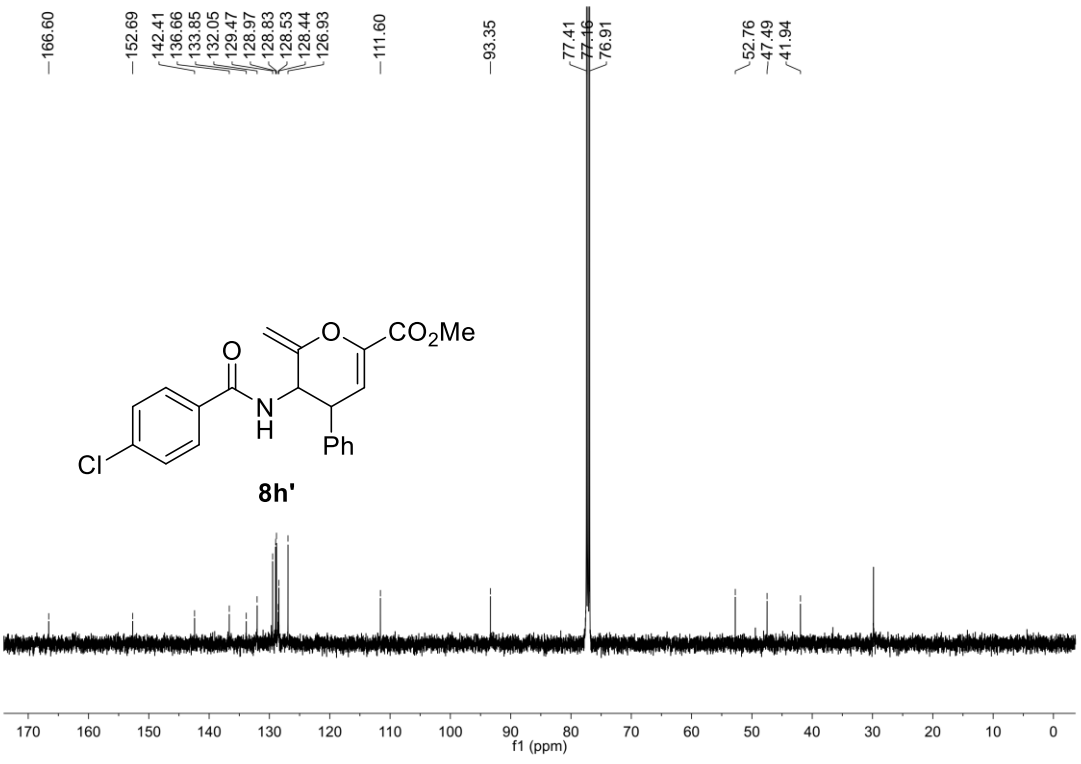

2.02
1.09
2.07
2.03
1.04
1.00
1.00
1.01
1.00
1.02
1.08
3.06
0.98
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


167.00
162.09
150.66
142.61
139.55
133.95
132.04
128.84
128.81
128.41
127.80
127.15
111.88
97.81
77.41
77.16
76.91
52.78
52.32
44.23
O
CO2Me
O
N
H
Ph
Cl
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

8h


7.53
7.53
7.40
7.38
7.37
7.37
7.36
7.26
6.37
6.36
5.61
5.59
5.39
5.37
5.37
5.37
5.36
4.94
4.94
4.94
4.37
4.36
4.36
3.95
3.93
3.92
3.88


O
CO2Me
O
N
H
Ph
Cl
8h'
2.14
5.09
2.11
0.91
0.91
1.12
1.00
1.02
1.10
2.80
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


166.60
152.69
142.41
136.66
133.85
132.05
129.47
128.97
128.83
128.53
128.44
126.93
111.60
93.35
77.41
77.16
76.91
52.76
47.49
41.94
O
CO2Me
O
N
H
Ph
Cl
8h'
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50
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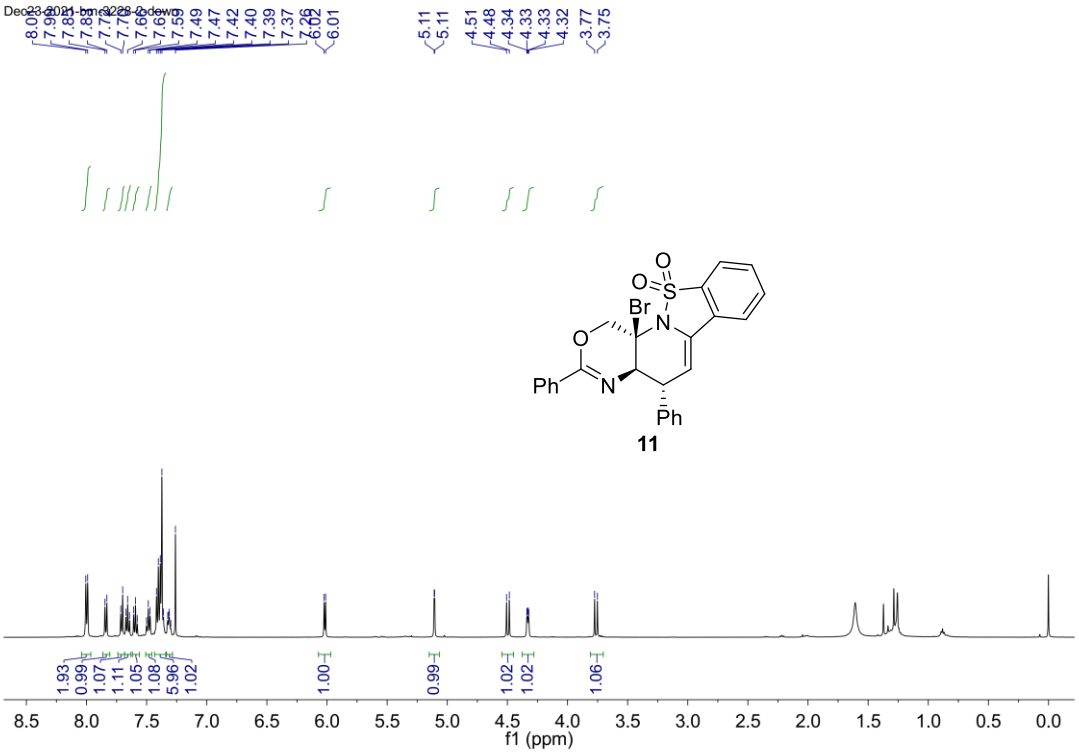
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7.66
7.63
7.59
7.49
7.47
7.42
7.40
7.39
7.37
7.26
6.02
6.01
5.11
5.11
4.51
4.48
4.34
4.33
4.33
4.32
3.77
3.75
O
O
S
Br
N
O
Ph
N
Ph
11
1.93
0.99
1.07
1.11
1.05
1.08
5.96
1.02
1.00
0.99
1.02
1.02
1.06
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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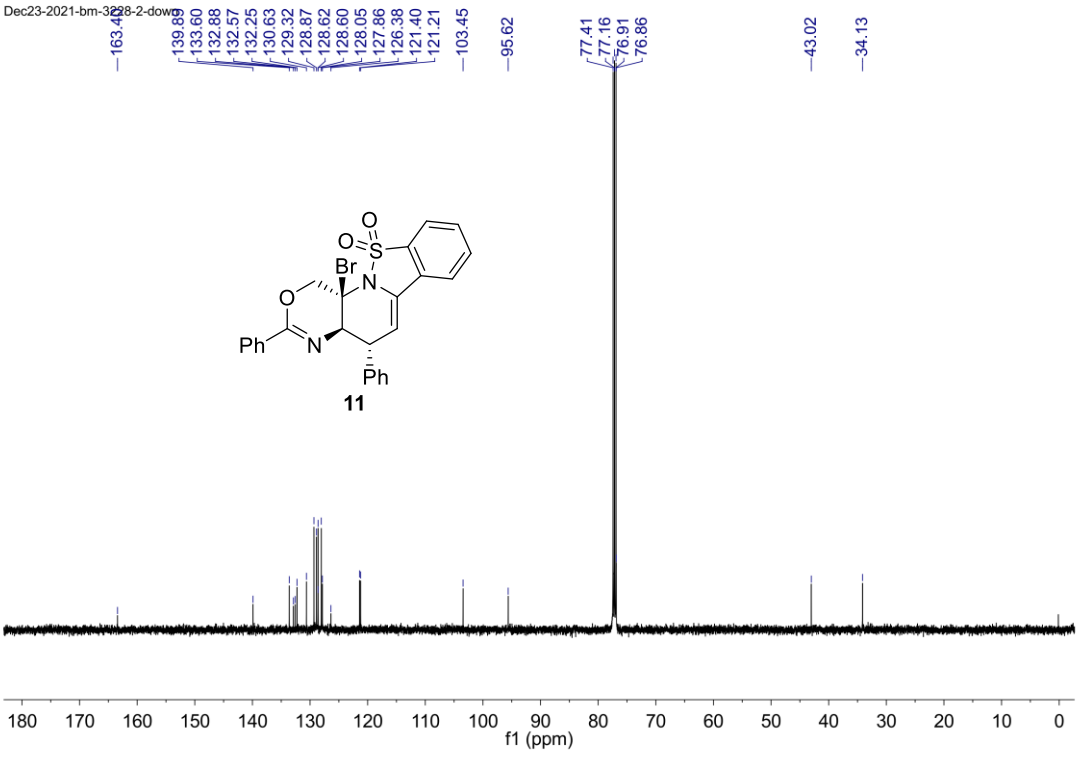
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128.05
127.86
126.38
121.40
121.21
103.45
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77.41
77.16
76.91
76.86
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34.13
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O
S
Br
N
O
Ph
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Ph
11
180
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90
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50
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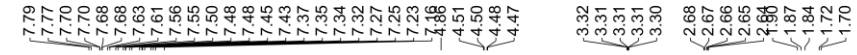
10
0
f1 (ppm)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7.45
7.43
7.37
7.35
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7.32
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7.25
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4.50
4.48
4.47
3.32
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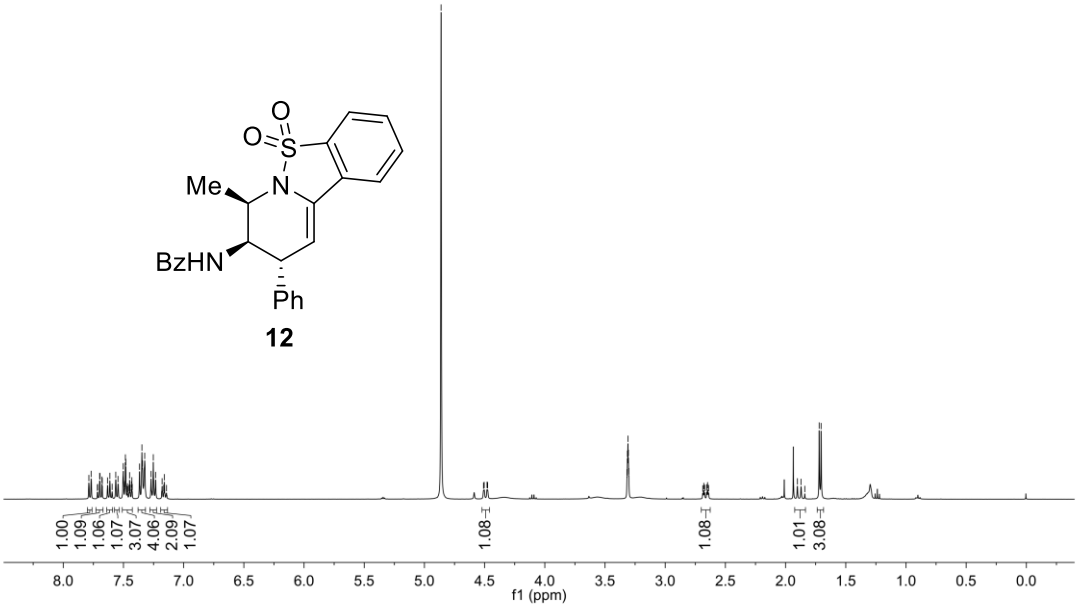
1.70


O
O
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N
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BzHN
Ph
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1.06
1.07
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1.07
1.08
1.08
1.01
3.08
8.0
7.5
7.0
6.5
6.0
5.5
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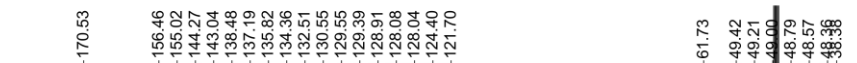
f1 (ppm)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128.91
128.08
128.04
124.40
121.70
61.73
49.42
49.21
49.00
48.79
48.57
15.59

O
O
S
N
Me
BzHN
Ph
12
180
170
160
150
140
130
120
110
100
90
80
70
60
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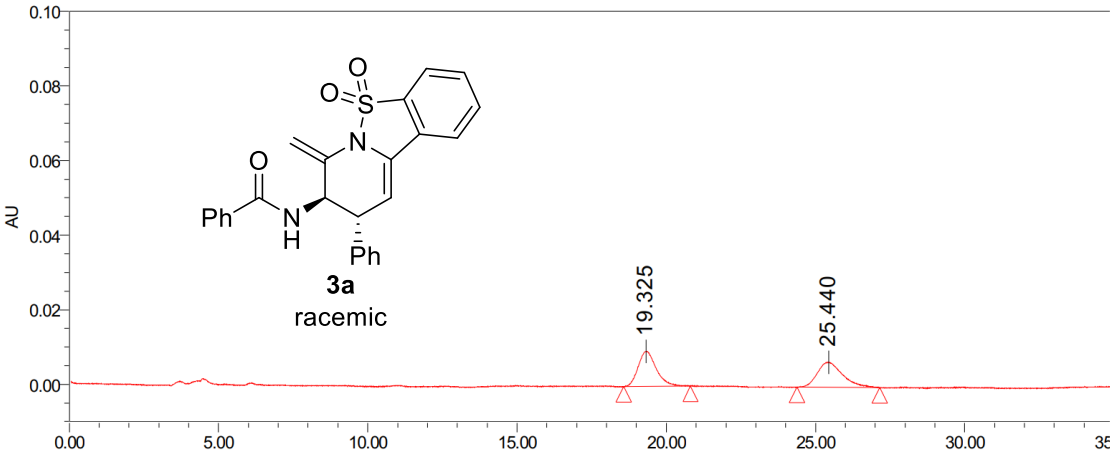
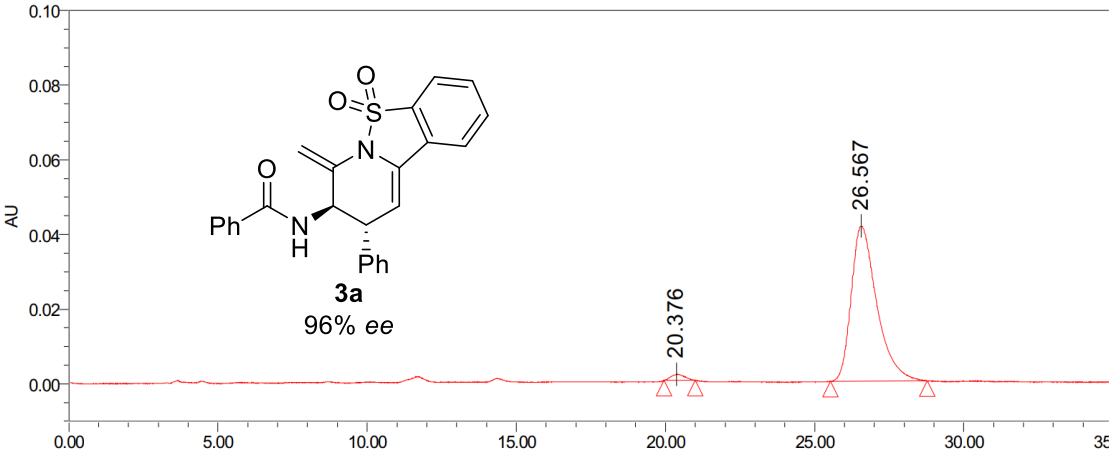
30
20
10
0
f1 (ppm)

Condition: hexane: 2-propanol = 70:30

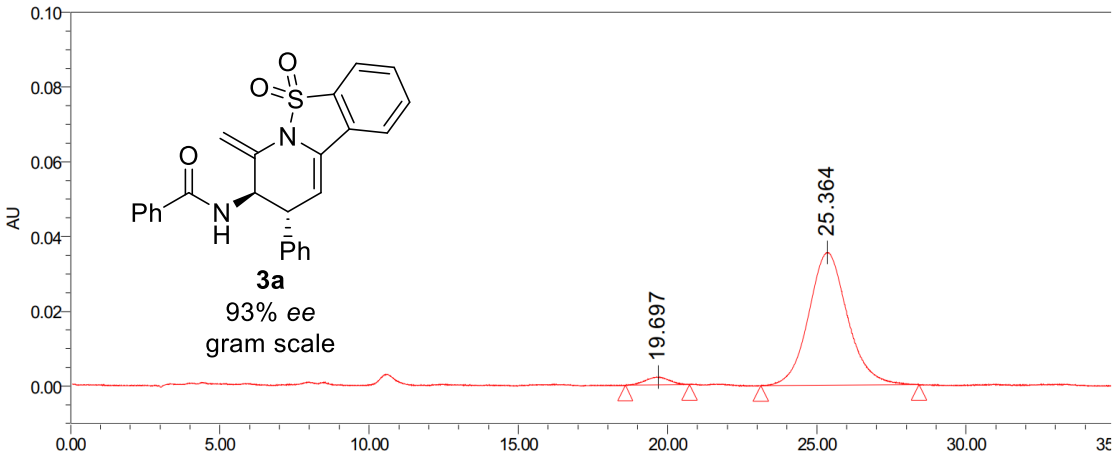
Flow rate = 1.0 mL/min, λ = 254 nm, Chiral AD-H



Entry	Retention Time/min	Area	Height	Area(%)
1	19.325	393482	9427	49.88
2	25.440	395453	6746	50.12



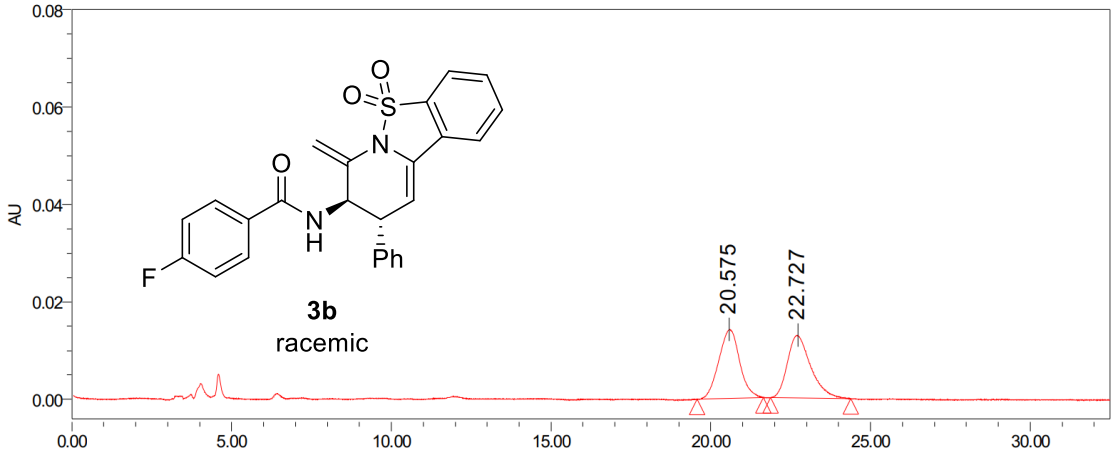
Entry	Retention Time/min	Area	Height	Area(%)
1	20.376	54043	1702	2.15
2	26.567	2460248	41584	97.85



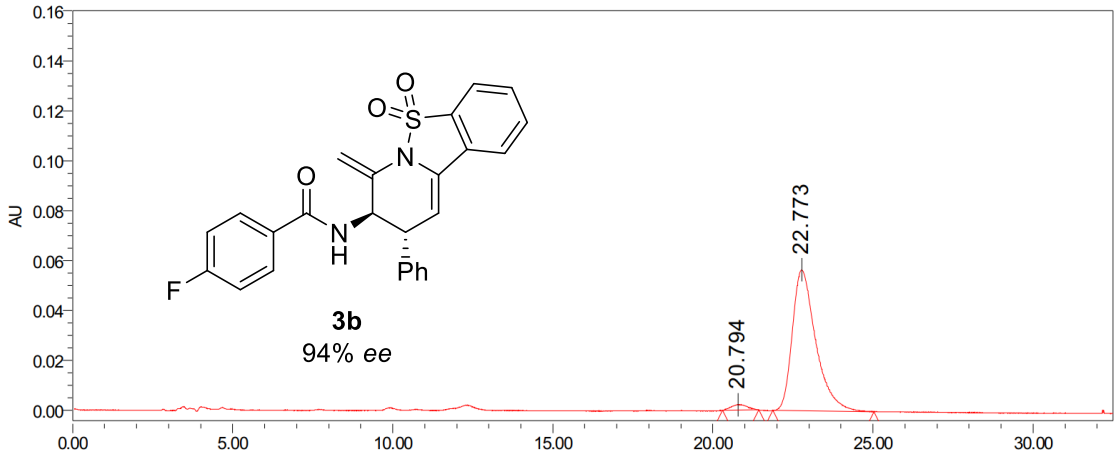
Entry	Retention Time/min	Area	Height	Area(%)
1	19.697	113377	2092	3.40
2	25.364	3219939	35556	96.60

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral AD-H



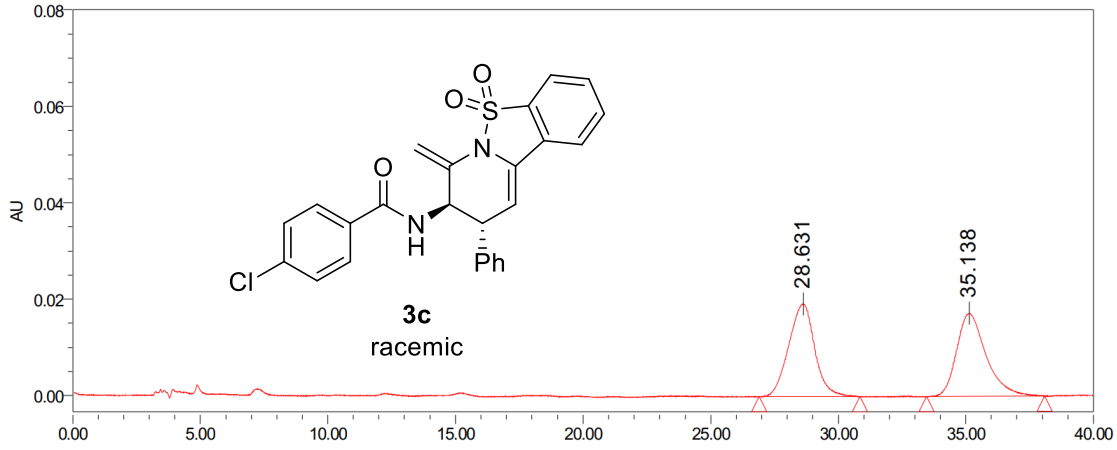
Entry	Retention Time/min	Area	Height	Area(%)
1	20.575	643166	14154	49.69
2	22.727	651097	12866	50.31



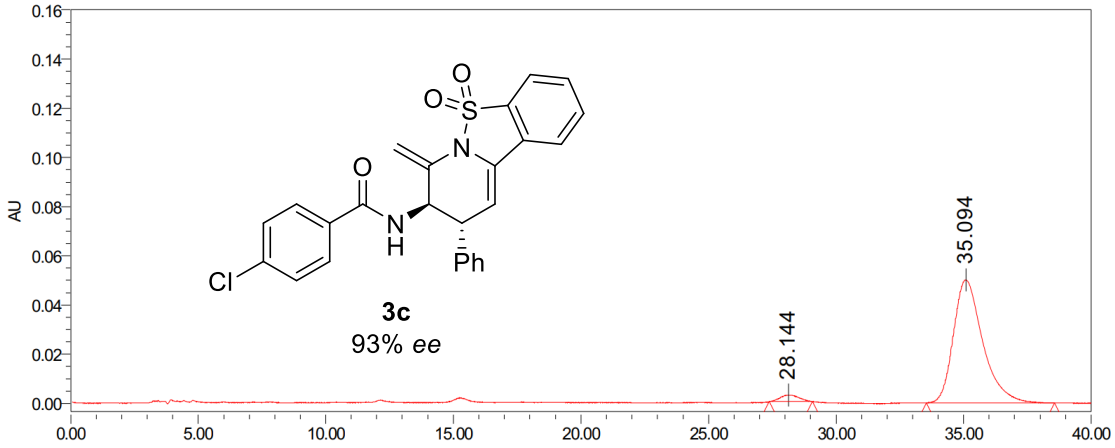
Entry	Retention Time/min	Area	Height	Area(%)
1	20.794	77684	2239	2.63
2	22.773	2872166	56426	97.37

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral AD-H



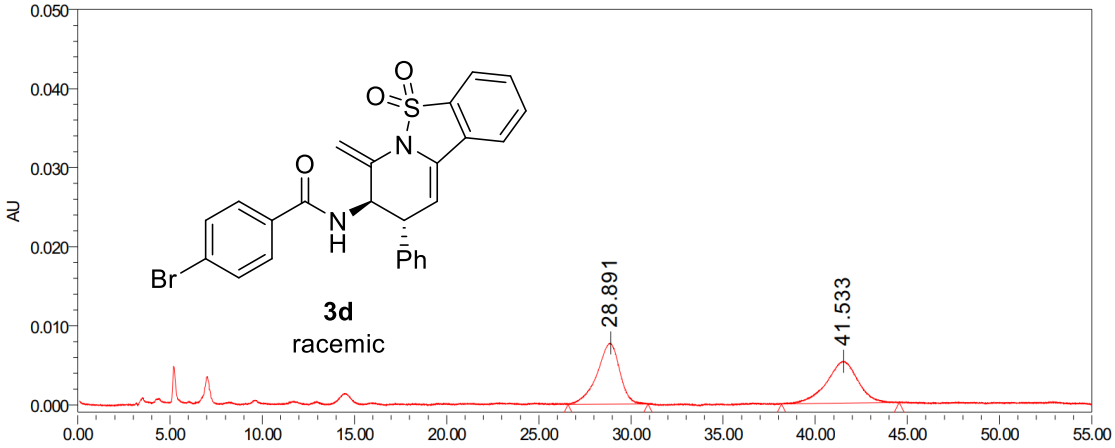
Entry	Retention Time/min	Area	Height	Area(%)
1	28.631	1351412	19184	49.56
2	35.138	1375671	17199	50.44



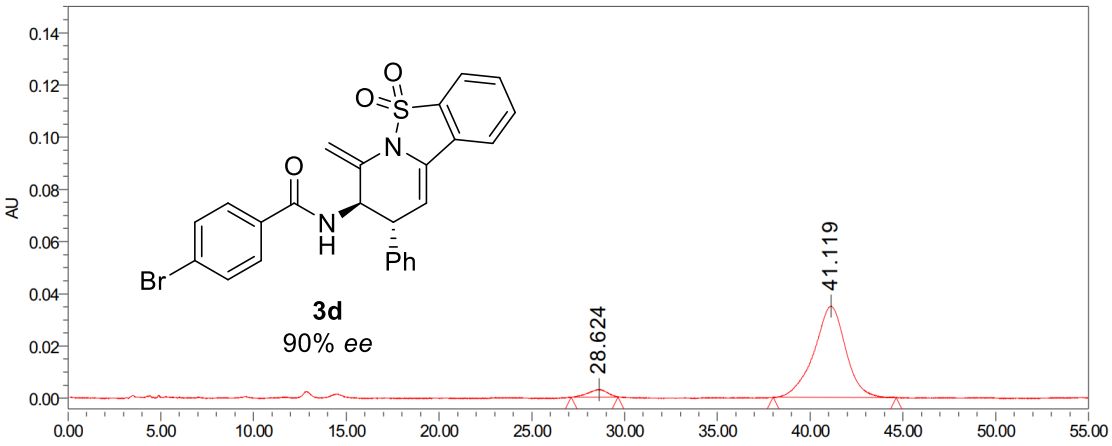
Entry	Retention Time/min	Area	Height	Area(%)
1	28.144	138429	2708	3.35
2	35.094	3997480	50071	96.65

Condition: hexane: 2-propanol = 70:30

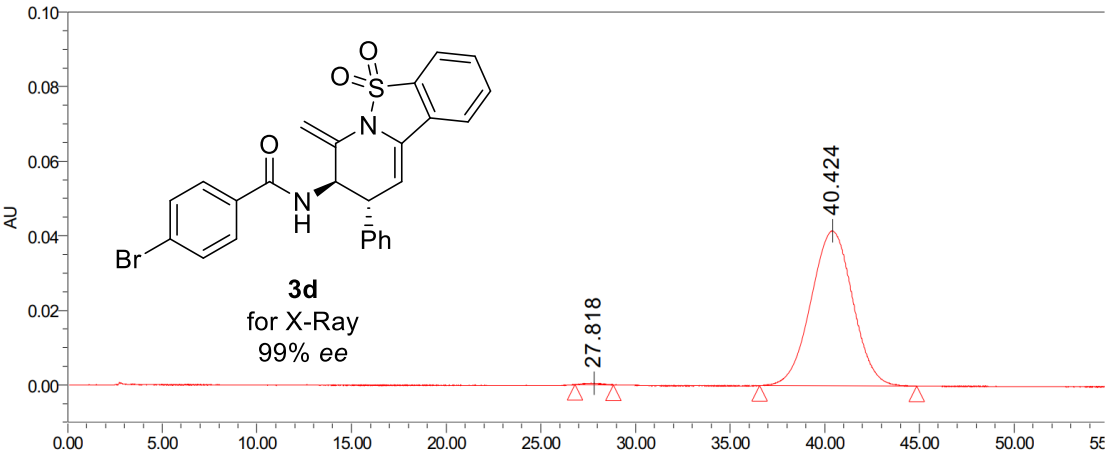
Flow rate = 1.0 mL/min, λ = 254 nm, Chiral AD-H



Entry	Retention Time/min	Area	Height	Area(%)
1	28.891	653293	7710	50.84
2	41.533	631692	5315	49.16



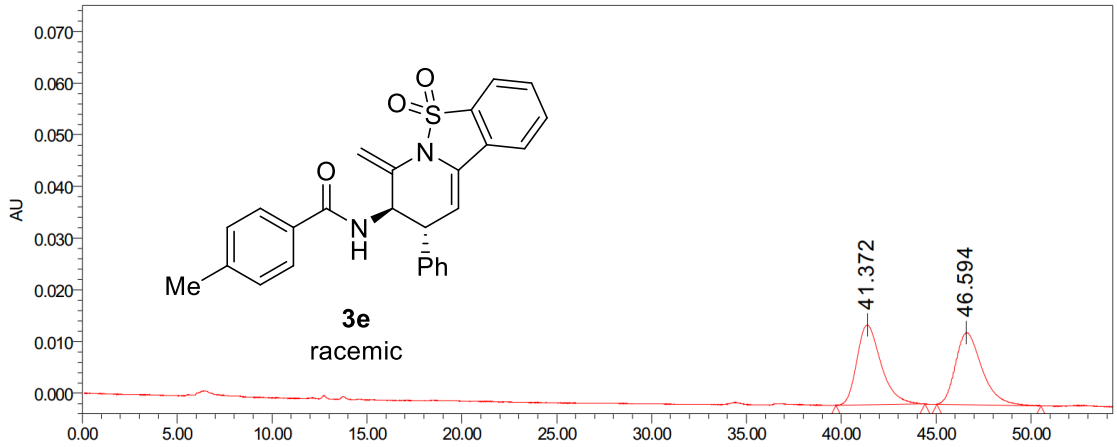
Entry	Retention Time/min	Area	Height	Area(%)
1	28.624	204300	2861	4.70
2	41.119	4145371	34969	95.30



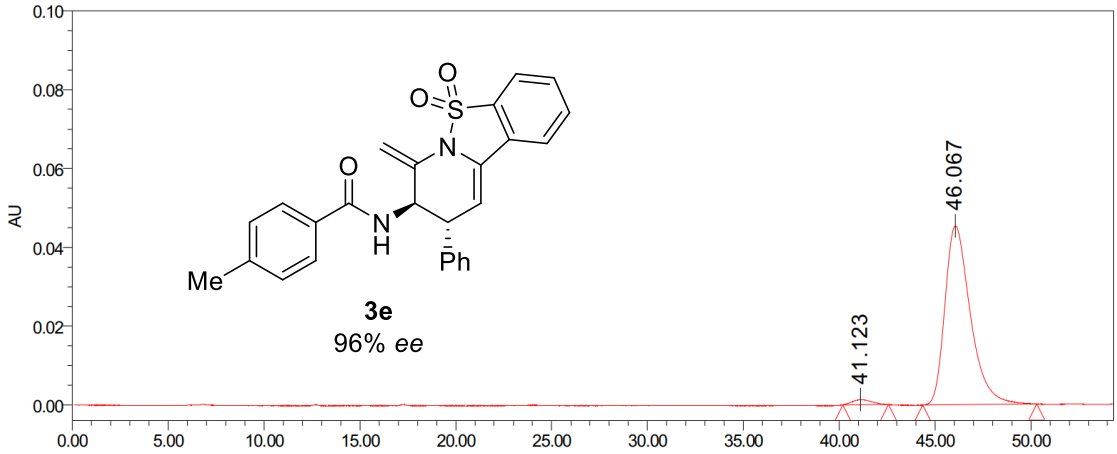
Entry	Retention Time/min	Area	Height	Area(%)
1	27.818	24449	387	0.38
2	40.424	6367331	41523	99.62

Condition: hexane: 2-propanol = 75:25

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral IC



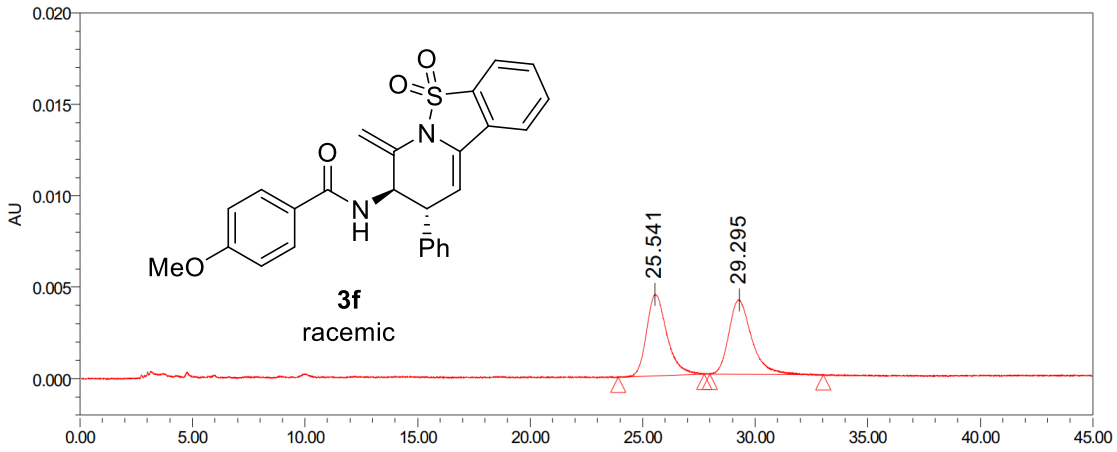
Entry	Retention Time/min	Area	Height	Area(%)
1	41.372	1364934	15431	50.25
2	46.594	1351258	13929	49.75



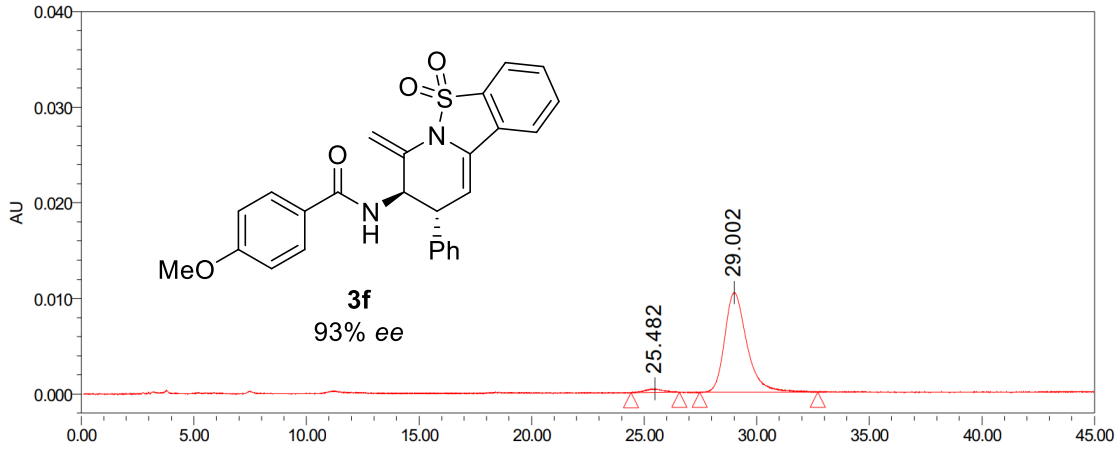
Entry	Retention Time/min	Area	Height	Area(%)
1	41.123	90553	1265	2.10
2	46.067	4217298	45403	97.90

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral IA



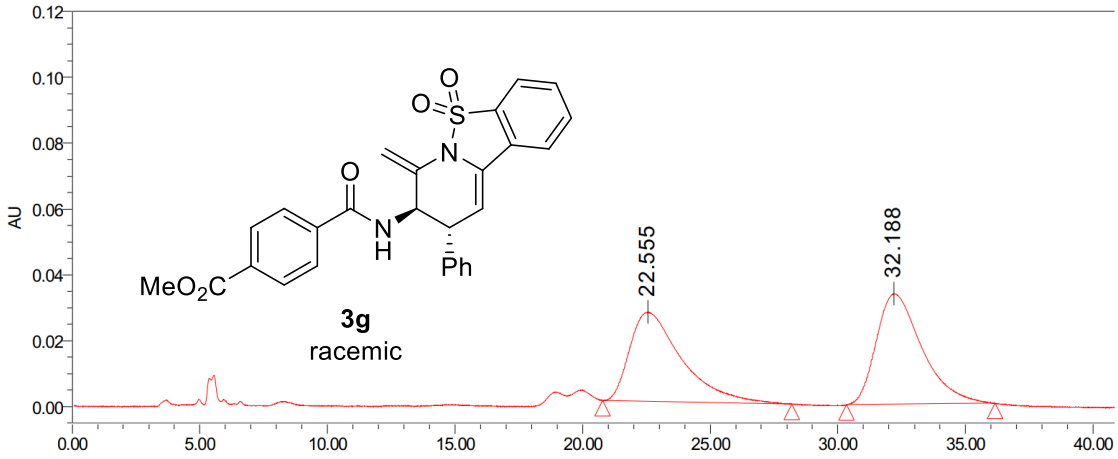
Entry	Retention Time/min	Area	Height	Area(%)
1	25.541	279068	4450	49.63
2	29.295	283172	4058	50.37



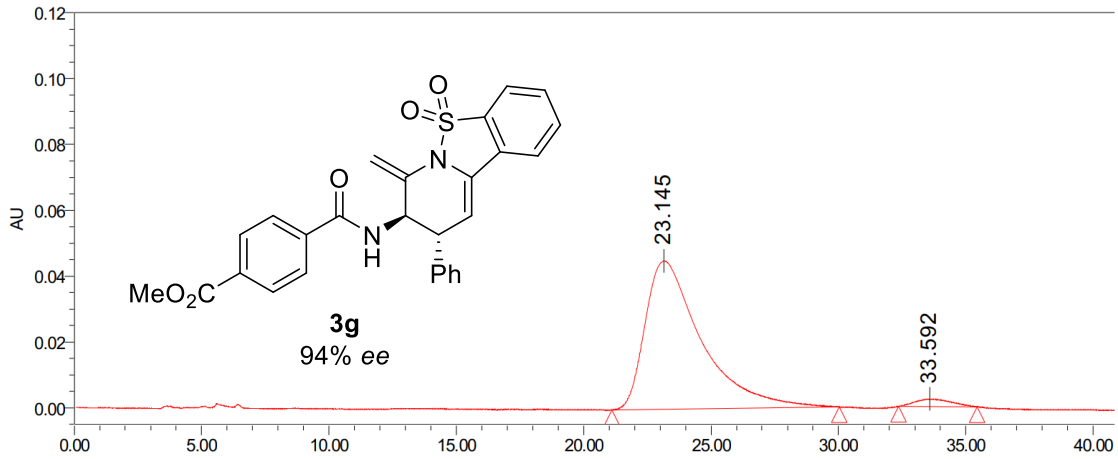
Entry	Retention Time/min	Area	Height	Area(%)
1	25.482	19707	364	2.71
2	29.002	707760	10419	97.29

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral OD-H



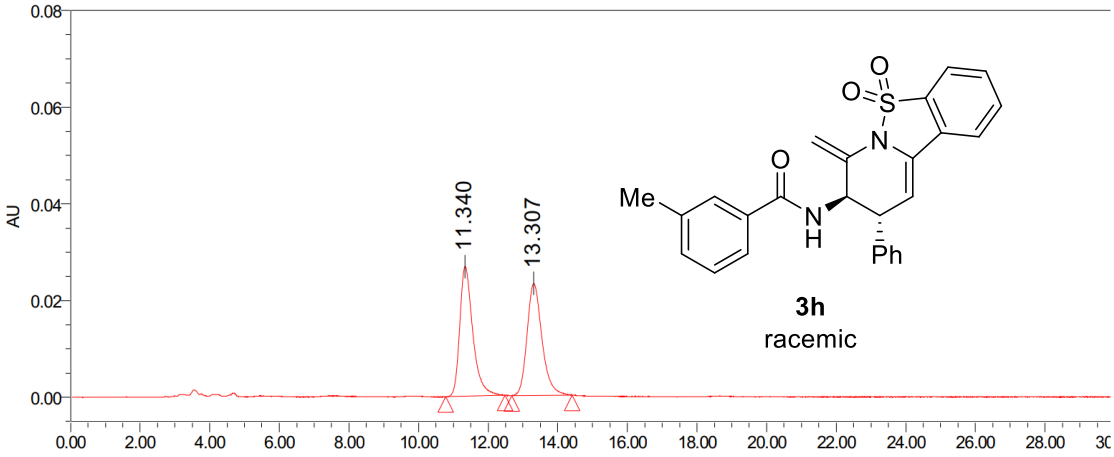
Entry	Retention Time/min	Area	Height	Area(%)
1	22.555	3837414	27109	47.93
2	32.188	4168062	33583	52.07



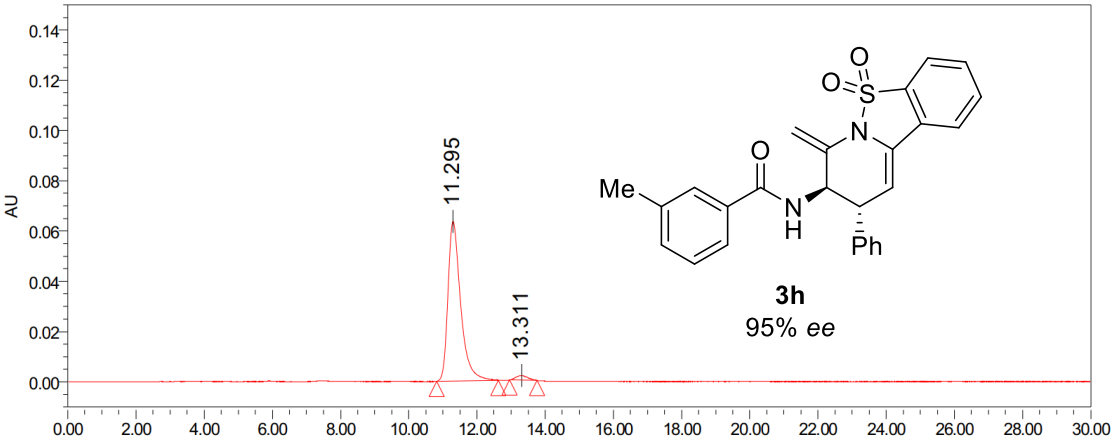
Entry	Retention Time/min	Area	Height	Area(%)
1	23.145	6913636	45077	96.80
2	33.592	228568	2346	3.20

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral IA



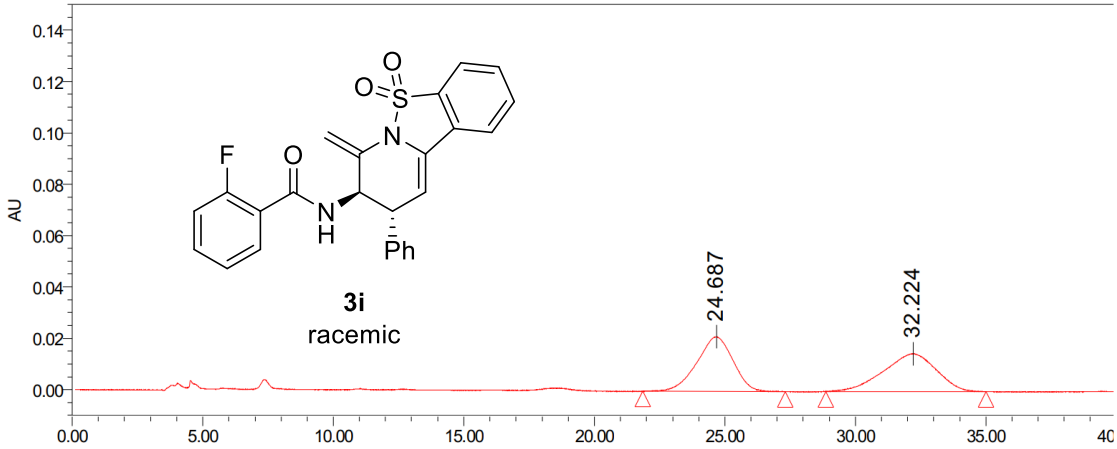
Entry	Retention Time/min	Area	Height	Area(%)
1	11.340	700674	26857	50.40
2	13.307	689607	23135	49.60



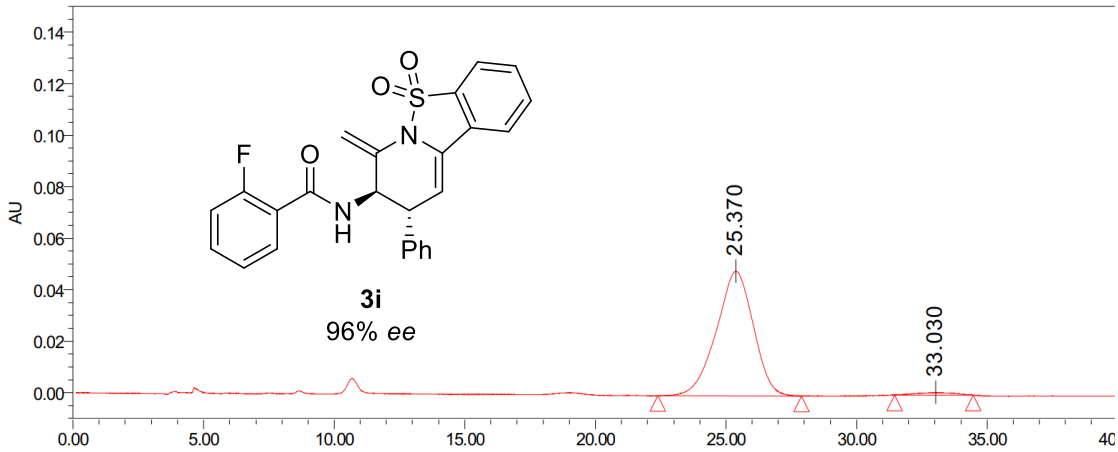
Entry	Retention Time/min	Area	Height	Area(%)
1	11.295	1638160	63494	97.37
2	13.311	44163	1816	2.63

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral AD-H



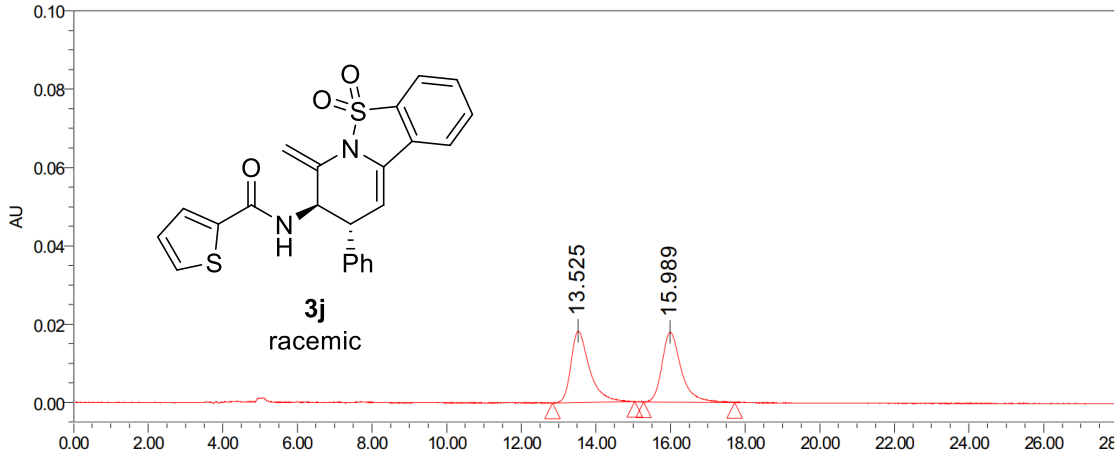
Entry	Retention Time/min	Area	Height	Area(%)
1	24.687	2055758	21287	49.74
2	32.224	2077432	14775	50.26



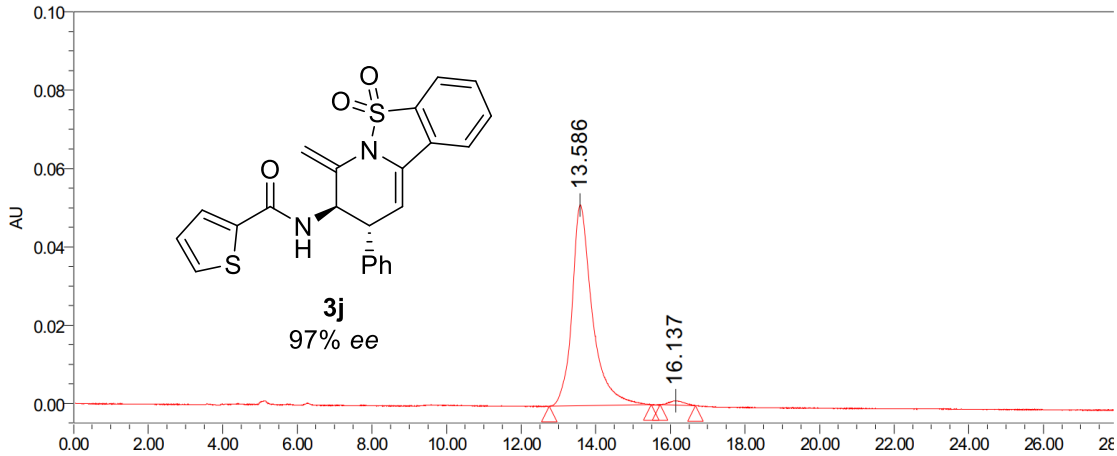
Entry	Retention Time/min	Area	Height	Area(%)
1	25.370	4780106	48360	98.06
2	33.030	94631	980	1.94

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral IA



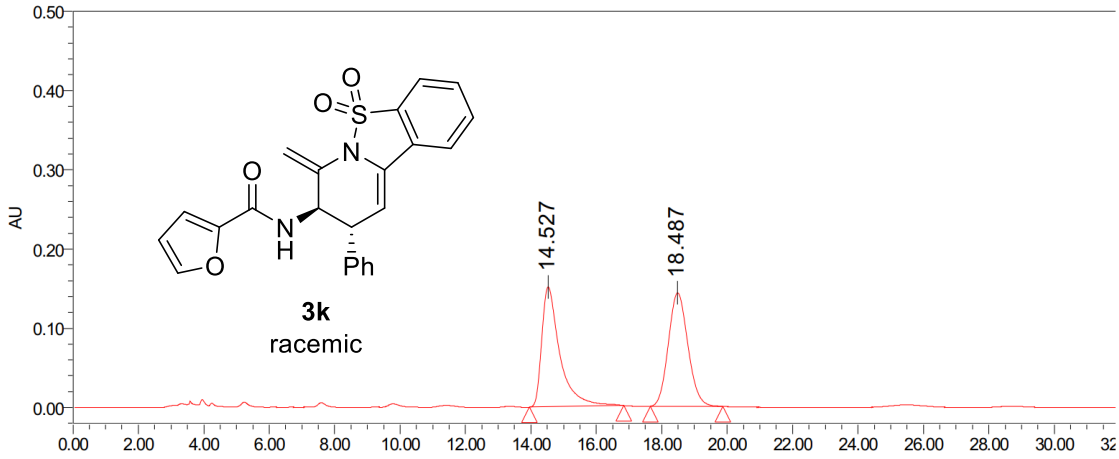
Entry	Retention Time/min	Area	Height	Area(%)
1	13.525	630668	18244	49.72
2	15.989	637658	17858	50.28



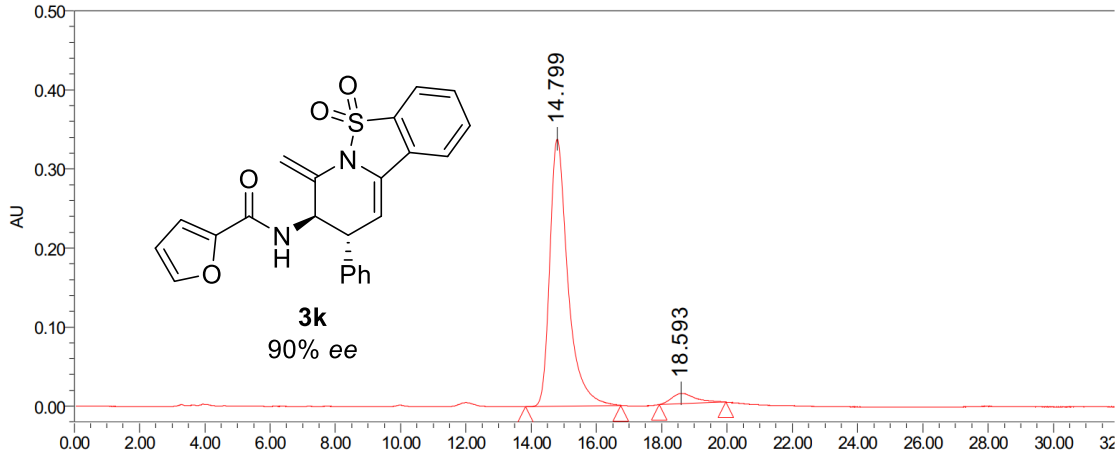
Entry	Retention Time/min	Area	Height	Area(%)
1	13.586	1944092	51316	98.47
2	16.137	30284	1081	1.53

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral AD-H



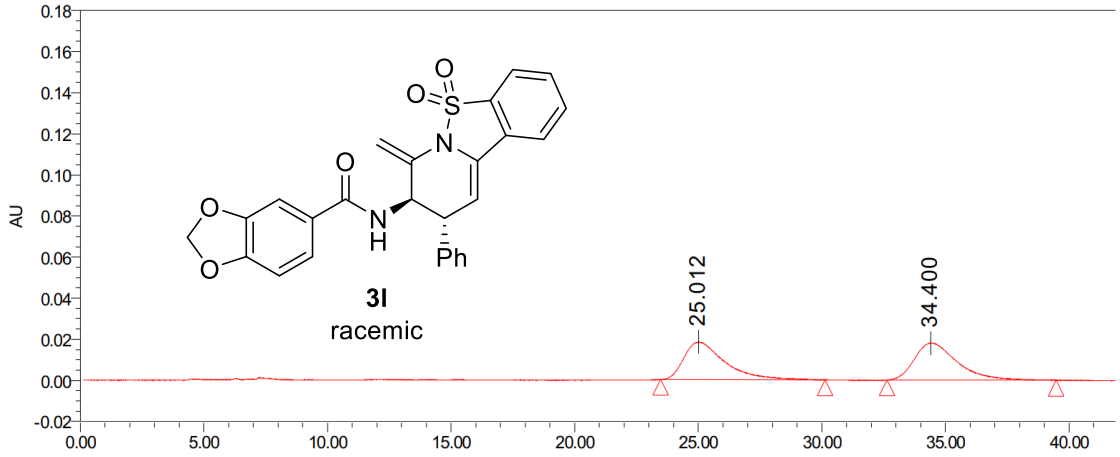
Entry	Retention Time/min	Area	Height	Area(%)
1	14.527	5823444	151177	49.42
2	18.487	5961023	143140	50.58



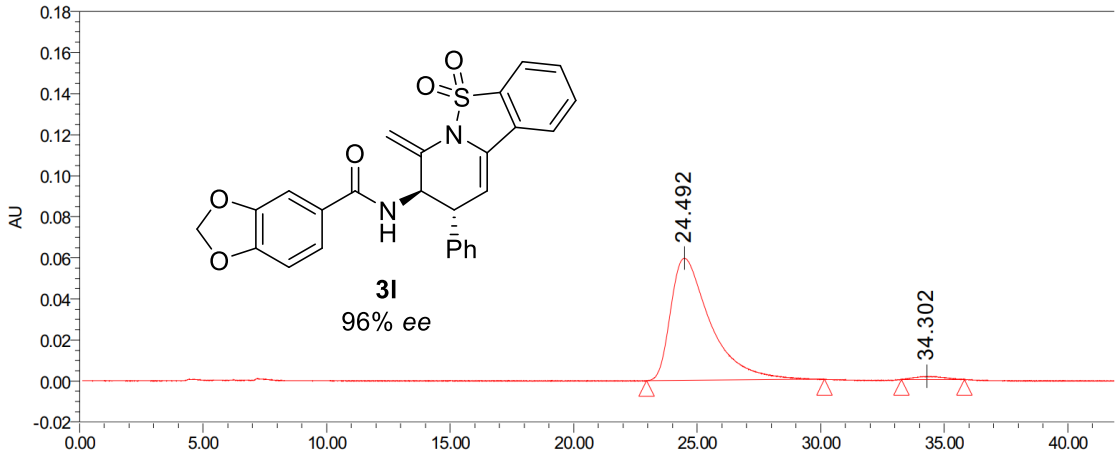
Entry	Retention Time/min	Area	Height	Area(%)
1	14.799	13039599	338212	95.09
2	18.593	672995	13158	4.91

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral OD-H



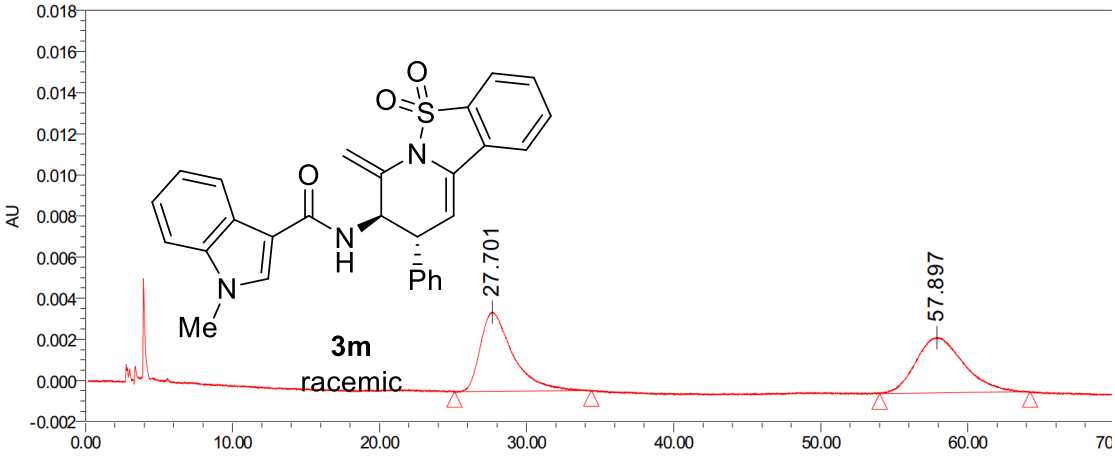
Entry	Retention Time/min	Area	Height	Area(%)
1	25.012	2089263	18335	49.18
2	34.400	2158981	18060	50.82



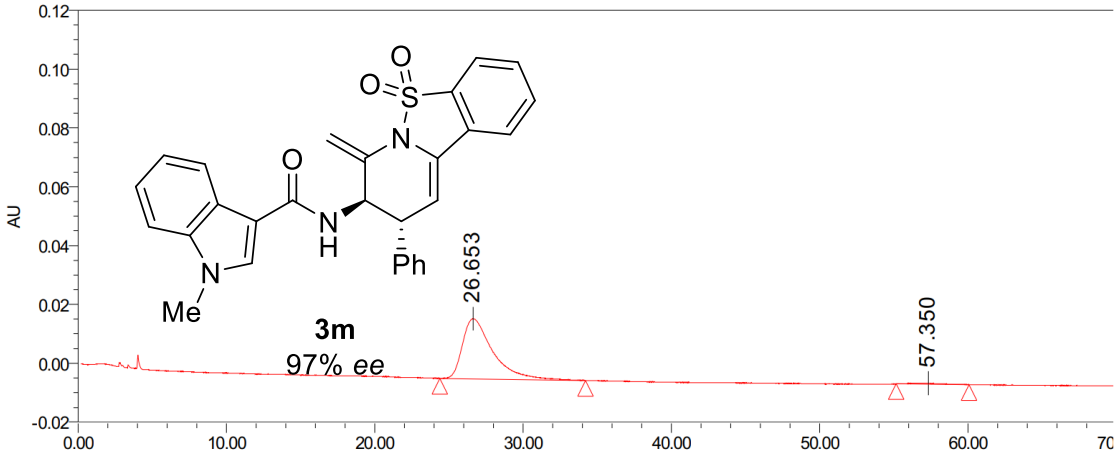
Entry	Retention Time/min	Area	Height	Area(%)
1	24.492	6655154	59563	98.18
2	34.302	123083	1499	1.82

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral OD-H



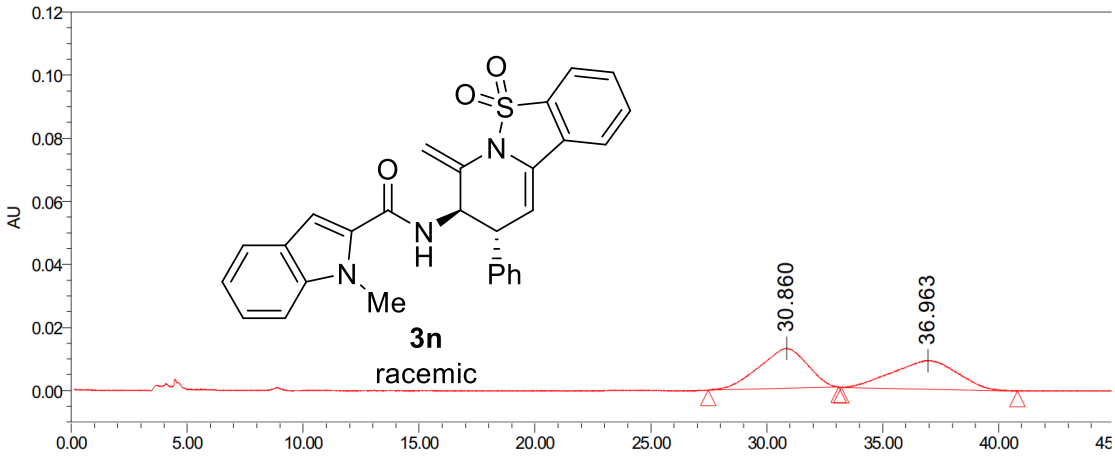
Entry	Retention Time/min	Area	Height	Area(%)
1	27.701	587805	3847	49.14
2	57.897	608299	2688	50.86



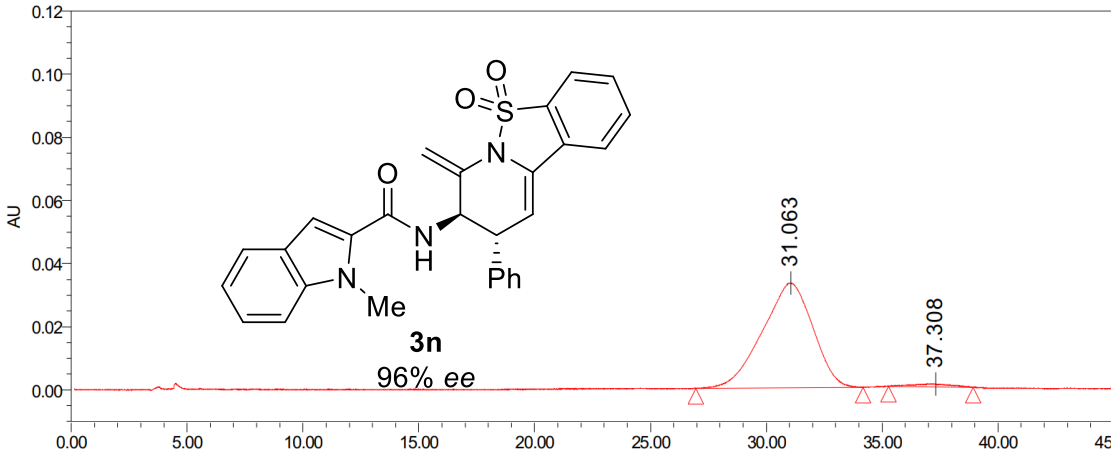
Entry	Retention Time/min	Area	Height	Area(%)
1	26.653	2893185	20468	98.38
2	57.350	47601	322	1.62

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral AD-H



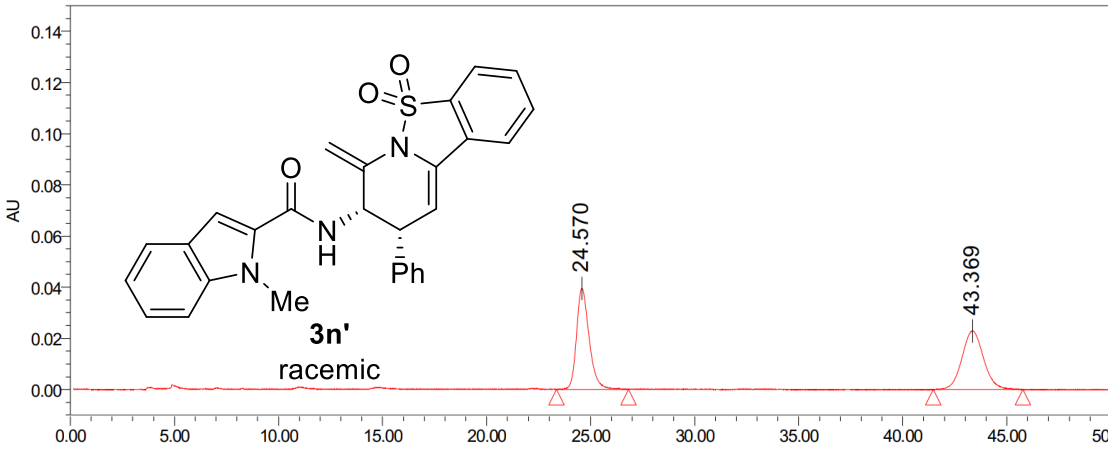
Entry	Retention Time/min	Area	Height	Area(%)
1	30.860	1811472	12666	50.86
2	36.963	1750247	9070	49.14



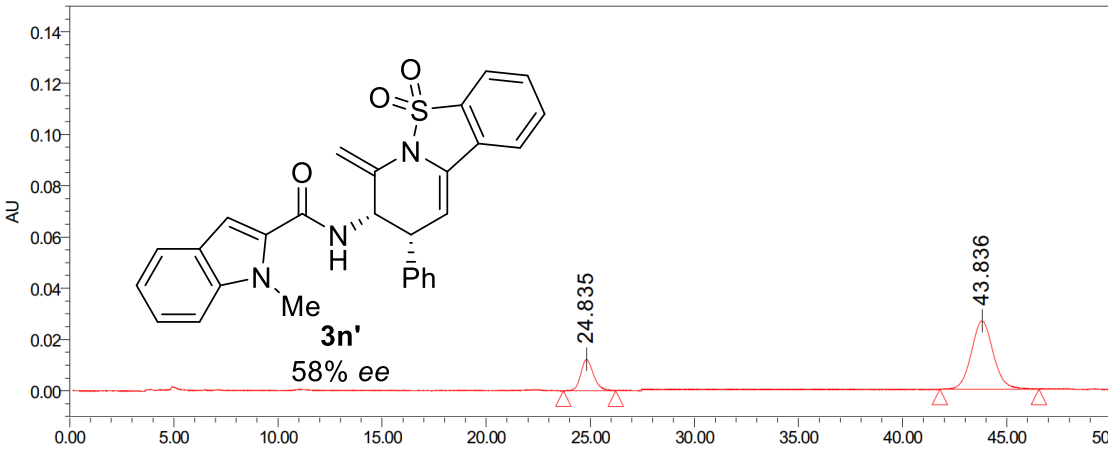
Entry	Retention Time/min	Area	Height	Area(%)
1	31.063	5011799	33215	97.92
2	37.308	106322	938	2.08

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral IA



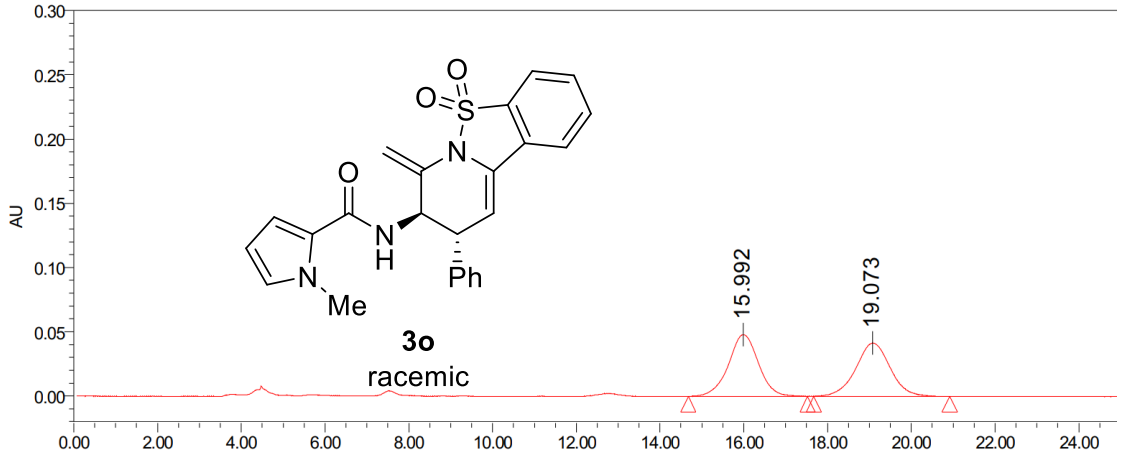
Entry	Retention Time/min	Area	Height	Area(%)
1	24.570	1667533	39485	50.13
2	43.369	1658566	22977	49.87



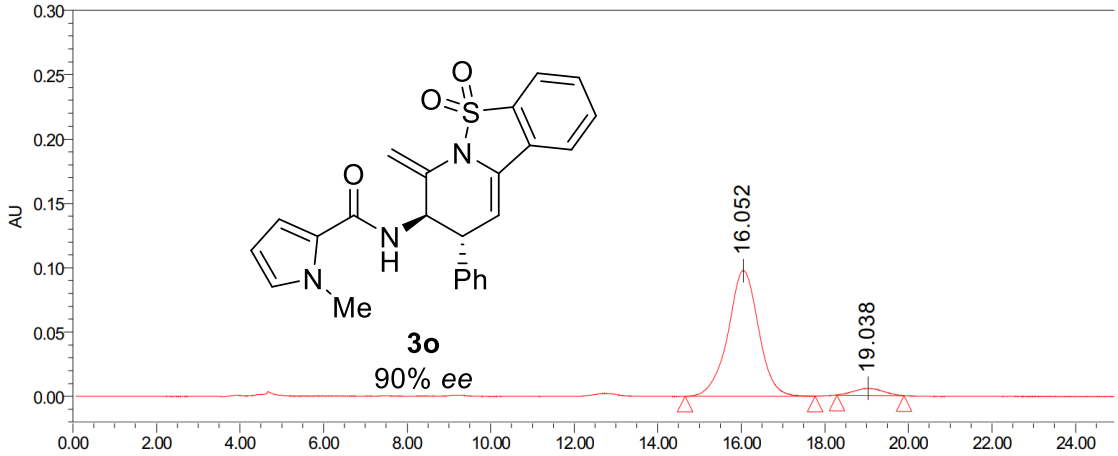
Entry	Retention Time/min	Area	Height	Area(%)
1	24.835	511601	12160	20.78
2	43.836	1950822	26604	79.22

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral AD-H



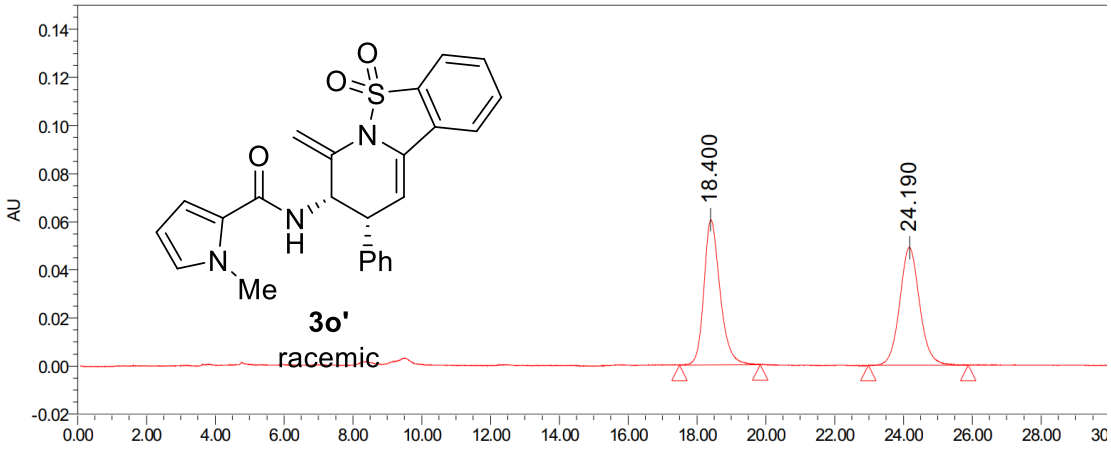
Entry	Retention Time/min	Area	Height	Area(%)
1	15.992	2378613	47864	50.18
2	19.073	2361766	41422	49.82



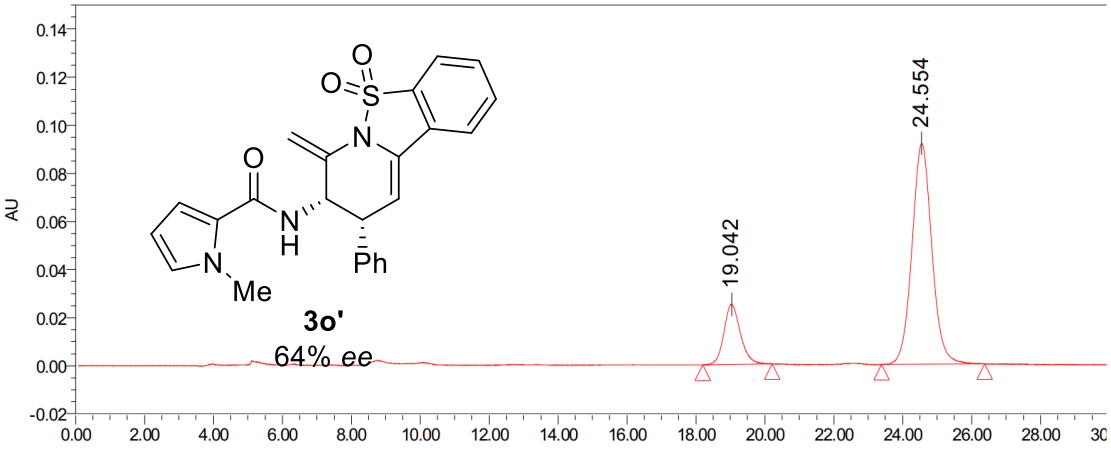
Entry	Retention Time/min	Area	Height	Area(%)
1	16.052	4974116	97681	94.99
2	19.038	262313	5460	5.01

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral IA



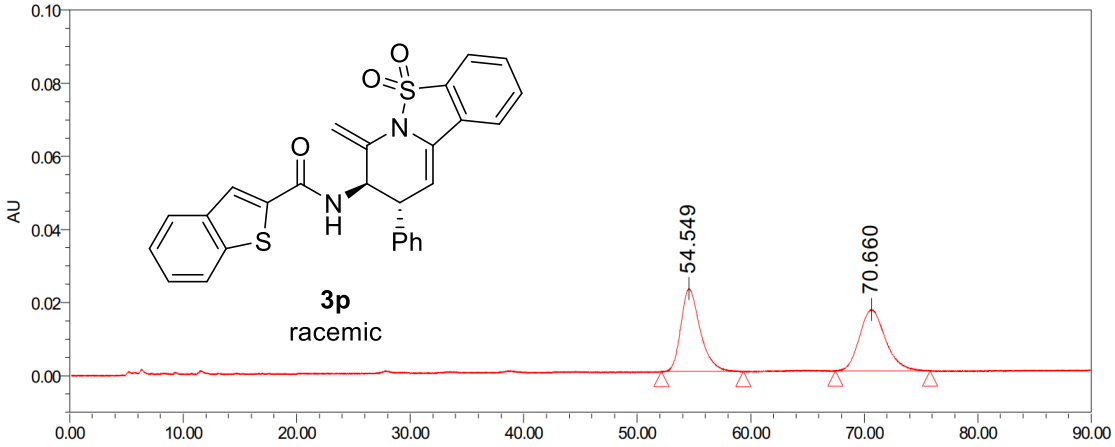
Entry	Retention Time/min	Area	Height	Area(%)
1	18.400	1965780	60421	49.92
2	24.190	1972149	48950	50.08



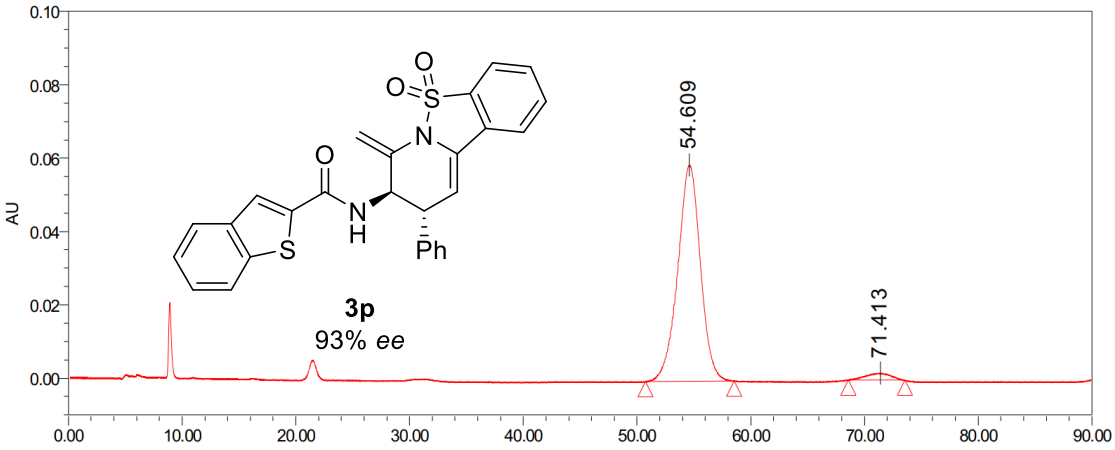
Entry	Retention Time/min	Area	Height	Area(%)
1	19.042	826674	24968	18.30
2	24.554	3690558	91863	81.70

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral AD-H



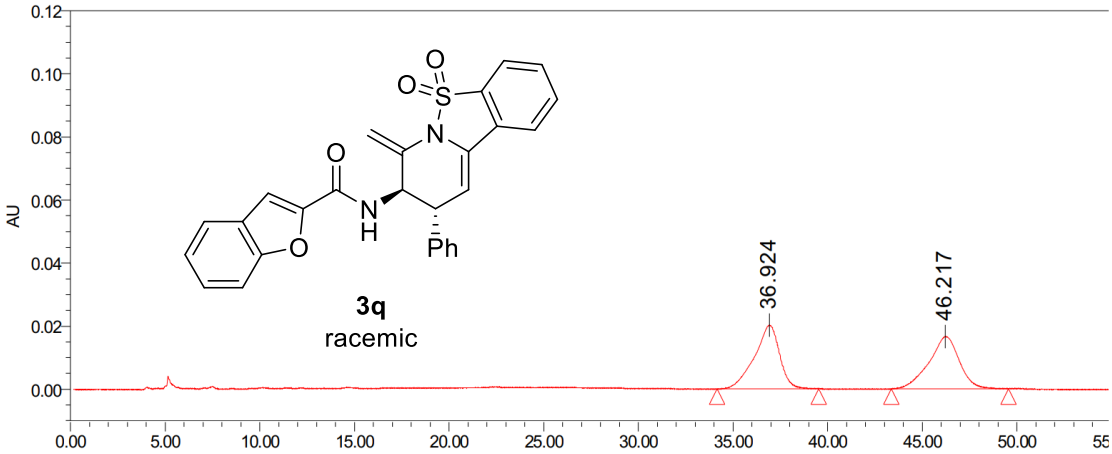
Entry	Retention Time/min	Area	Height	Area(%)
1	54.549	2672626	22668	50.06
2	70.660	2665867	16778	49.94



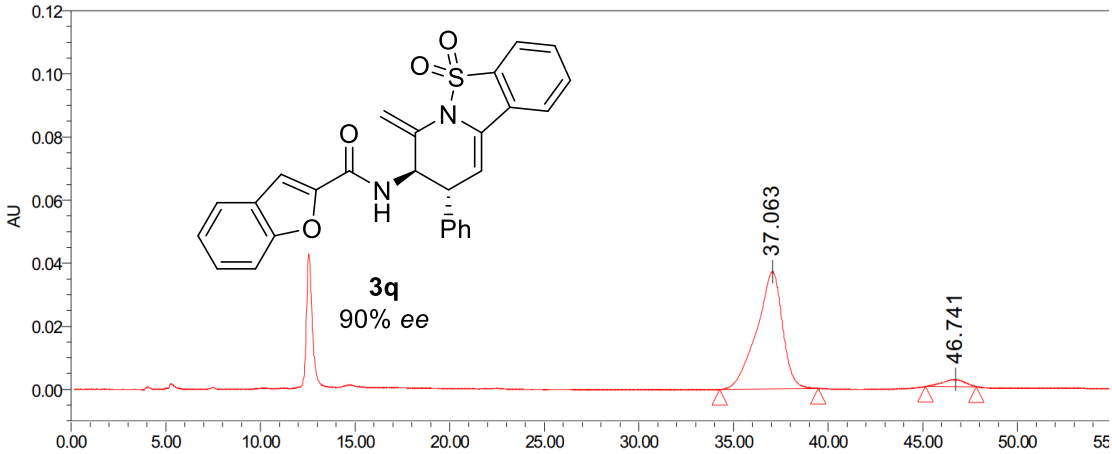
Entry	Retention Time/min	Area	Height	Area(%)
1	54.609	8164785	59055	96.61
2	71.413	286148	1883	3.39

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral IA



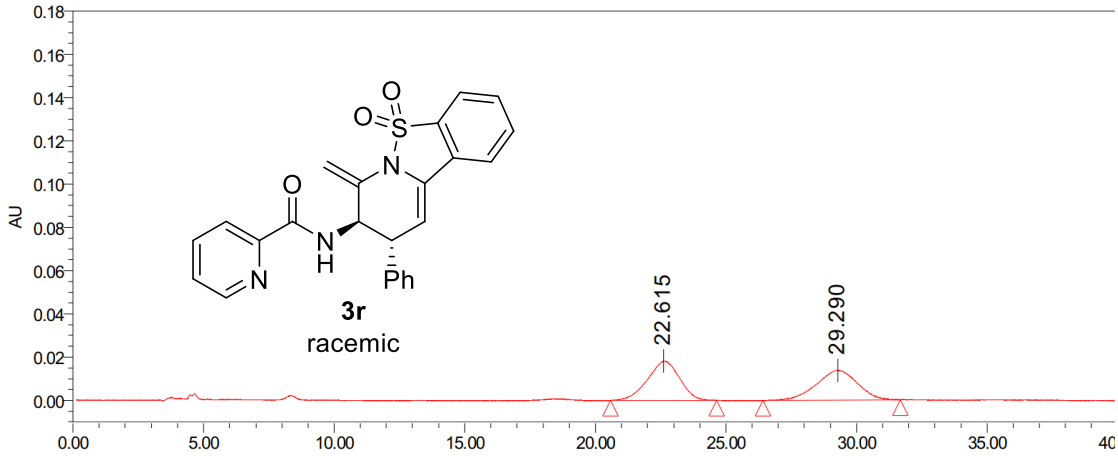
Entry	Retention Time/min	Area	Height	Area(%)
1	36.924	1851737	20174	50.17
2	46.217	1838954	16607	49.83



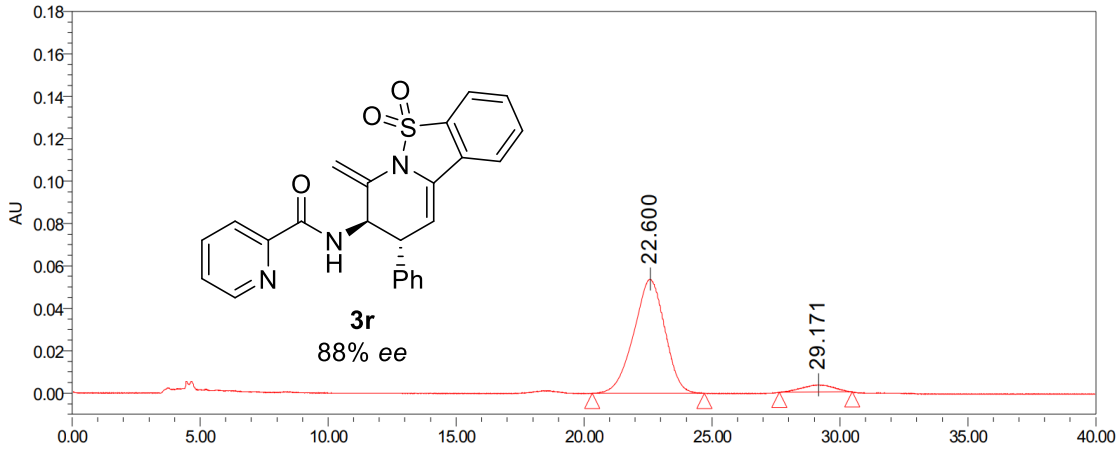
Entry	Retention Time/min	Area	Height	Area(%)
1	37.063	3502223	37191	94.92
2	46.741	187422	2253	5.08

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral AD-H



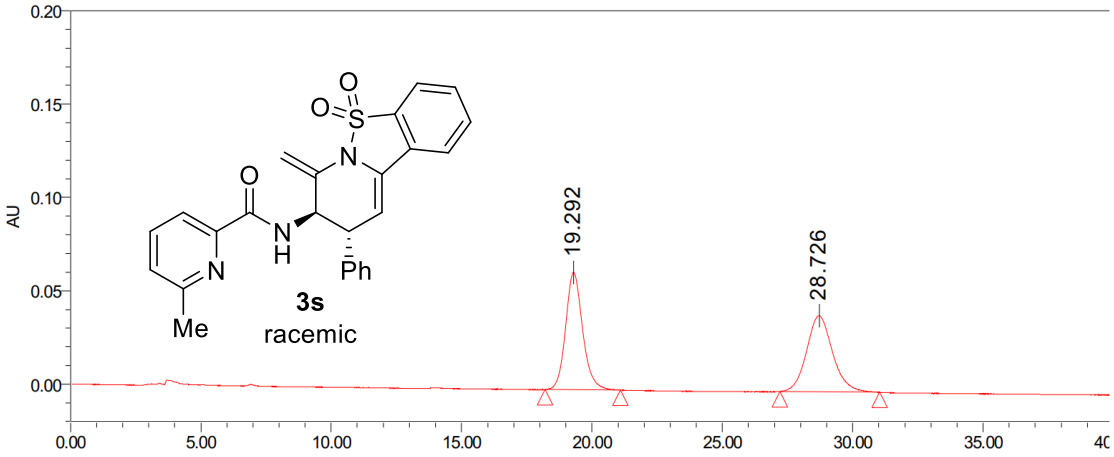
Entry	Retention Time/min	Area	Height	Area(%)
1	22.615	1544837	18158	50.73
2	29.290	1500315	13788	49.27



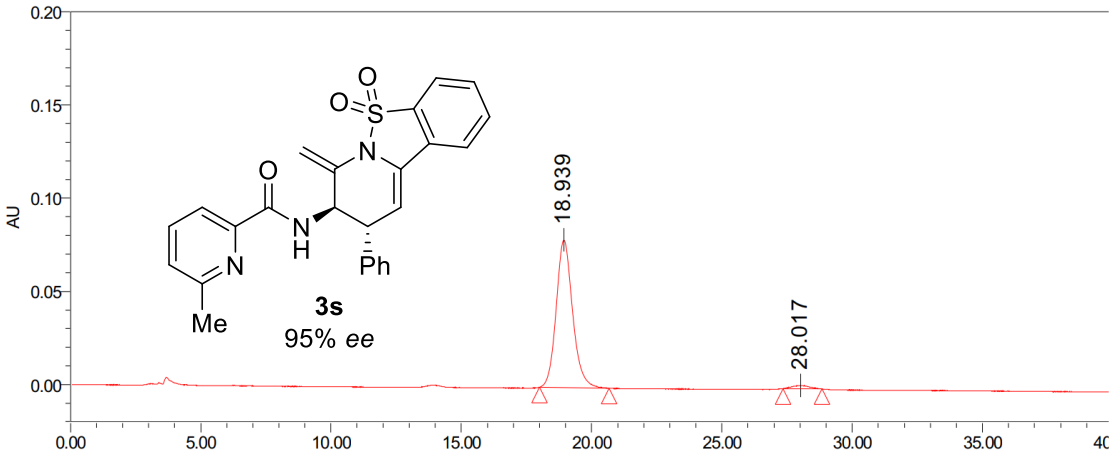
Entry	Retention Time/min	Area	Height	Area(%)
1	22.600	4527381	53830	93.89
2	29.171	294625	3429	6.11

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral AD-H



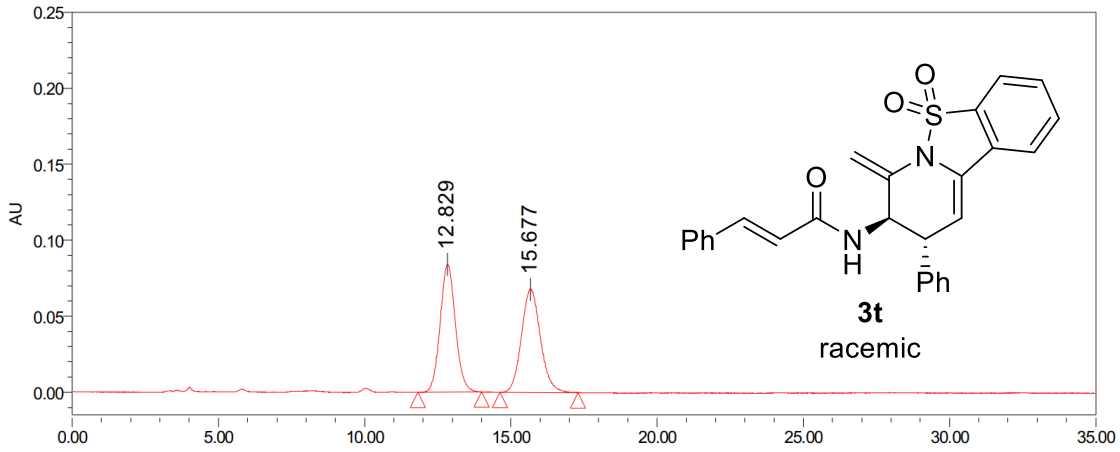
Entry	Retention Time/min	Area	Height	Area(%)
1	19.292	2859517	62867	50.33
2	28.726	2822238	40709	49.67



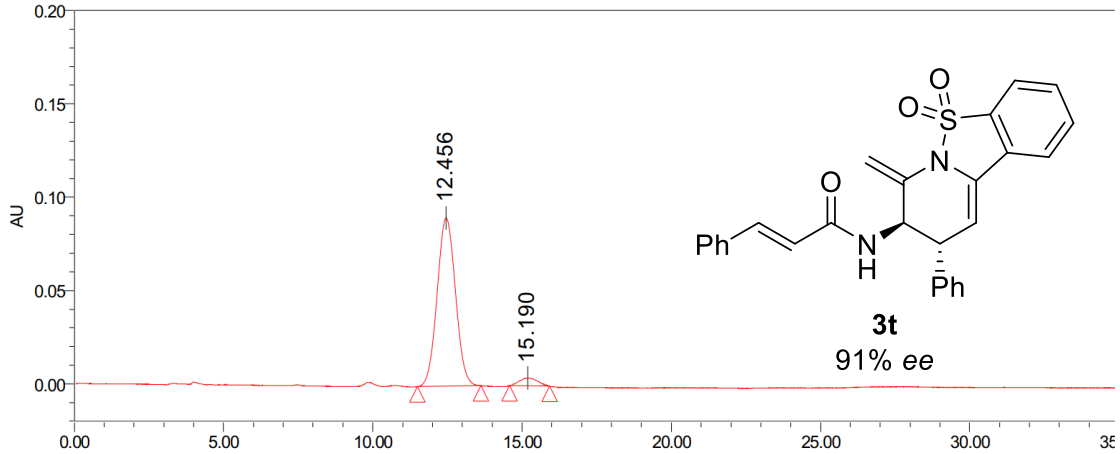
Entry	Retention Time/min	Area	Height	Area(%)
1	18.939	3467569	79138	97.66
2	28.017	83000	1694	2.34

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral AD-H



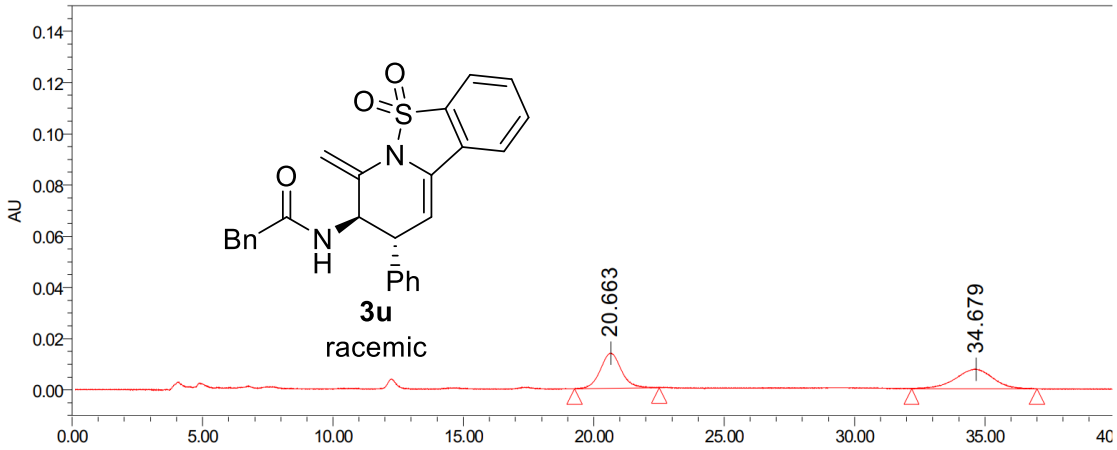
Entry	Retention Time/min	Area	Height	Area(%)
1	12.829	3061233	84004	50.03
2	15.677	3057246	67857	49.97



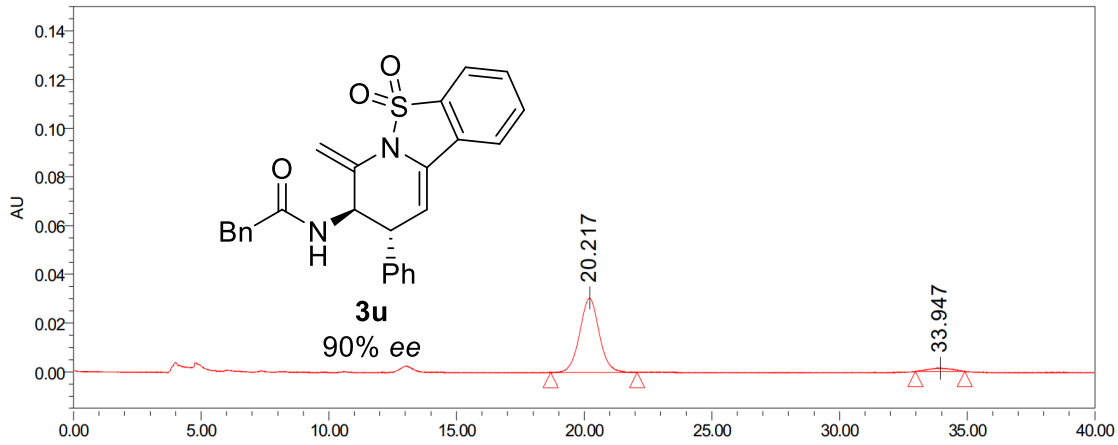
Entry	Retention Time/min	Area	Height	Area(%)
1	12.456	3864828	90173	95.56
2	15.190	179622	4170	4.44

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral AD-H



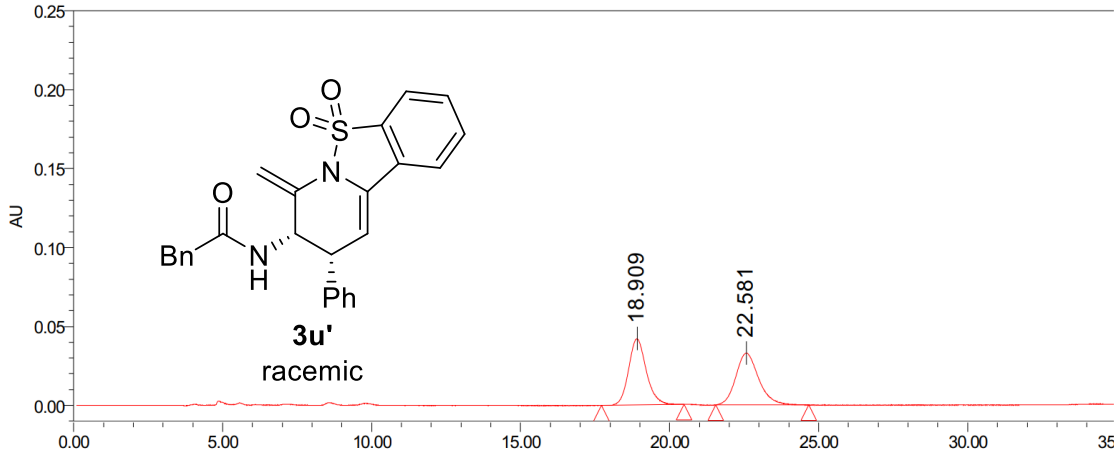
Entry	Retention Time/min	Area	Height	Area(%)
1	20.663	759451	13744	50.53
2	34.679	743439	7542	49.47



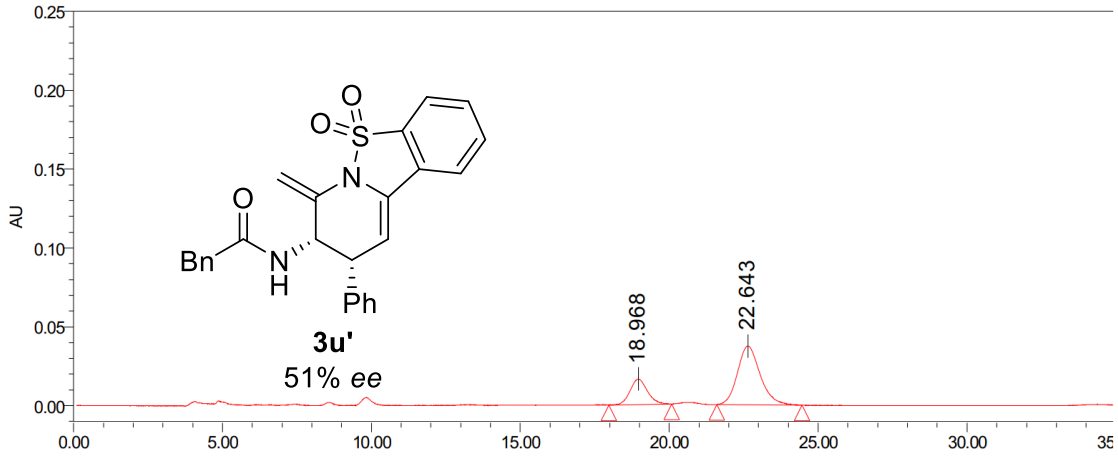
Entry	Retention Time/min	Area	Height	Area(%)
1	20.217	1624722	30519	95.05
2	33.947	84604	1374	4.95

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral AD-H



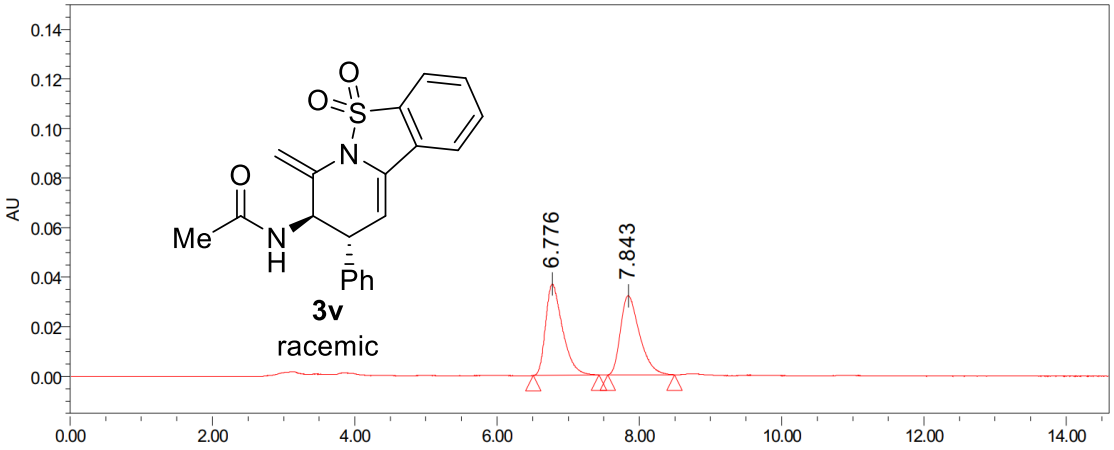
Entry	Retention Time/min	Area	Height	Area(%)
1	18.909	1730540	41968	49.85
2	22.581	1741265	32807	50.15



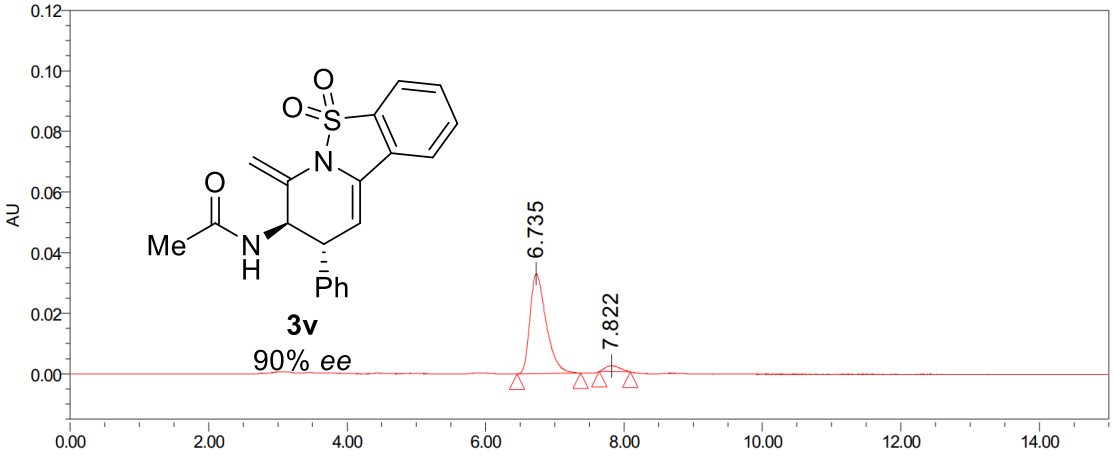
Entry	Retention Time/min	Area	Height	Area(%)
1	18.968	643312	16090	24.51
2	22.643	1980965	37245	75.49

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral AD-H



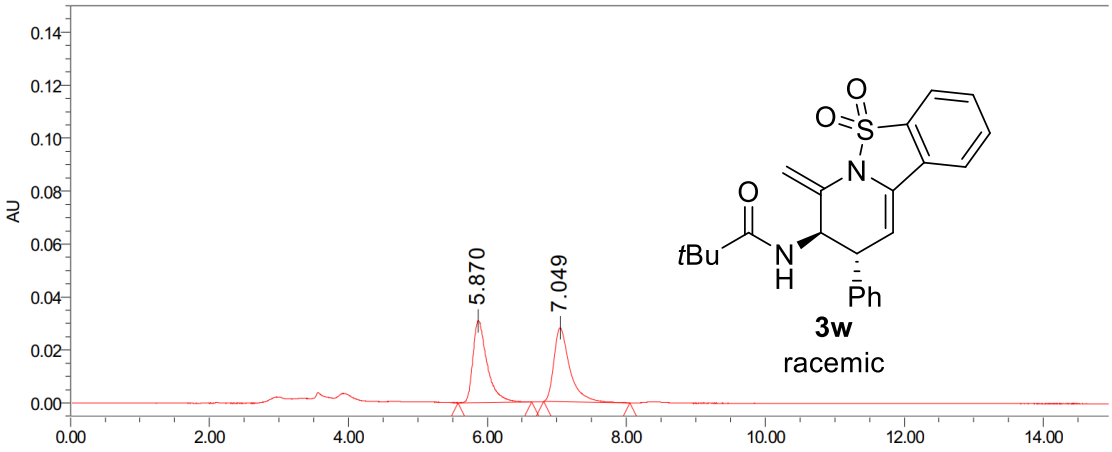
Entry	Retention Time/min	Area	Height	Area(%)
1	6.776	604395	36819	50.52
2	7.843	591871	31869	49.48



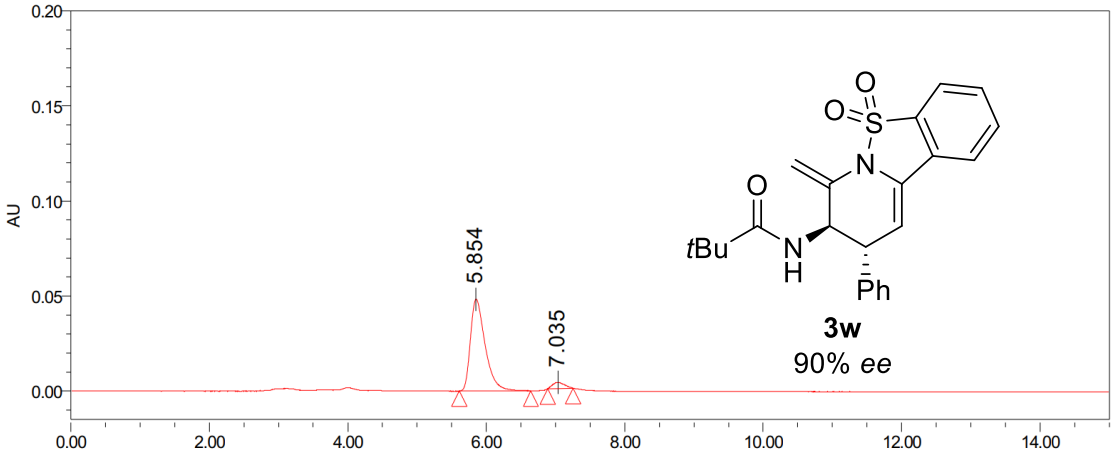
Entry	Retention Time/min	Area	Height	Area(%)
1	6.735	531866	32952	94.77
2	7.822	29329	1977	5.23

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral AD-H



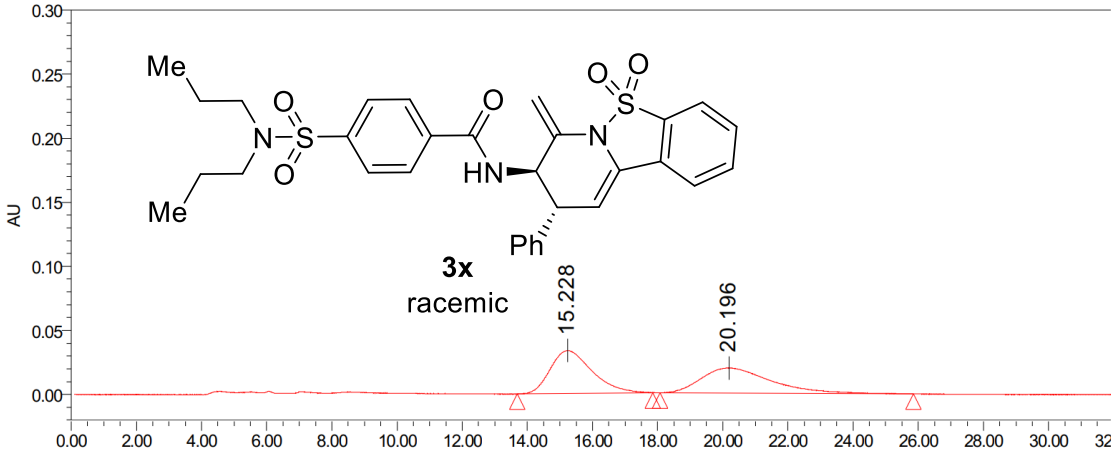
Entry	Retention Time/min	Area	Height	Area(%)
1	5.870	437051	30887	49.64
2	7.049	443371	27865	50.36



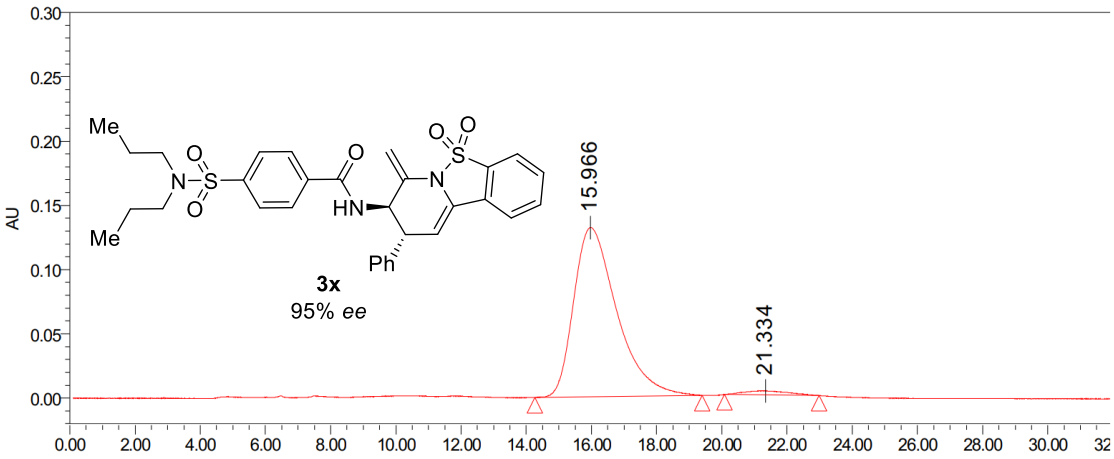
Entry	Retention Time/min	Area	Height	Area(%)
1	5.854	716392	48284	94.87
2	7.035	38730	3220	5.13

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral OD-H



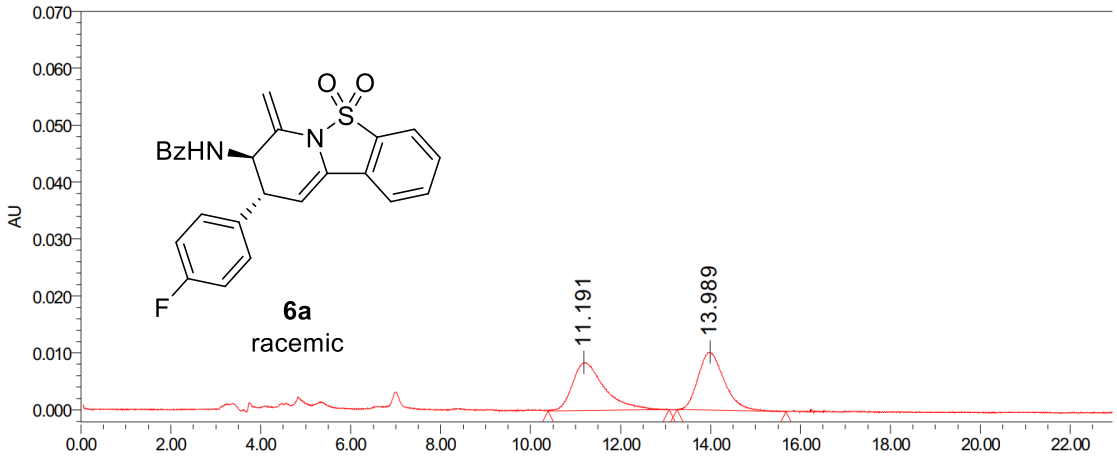
Entry	Retention Time/min	Area	Height	Area(%)
1	15.228	2964594	33390	50.59
2	20.196	2894976	19526	49.41



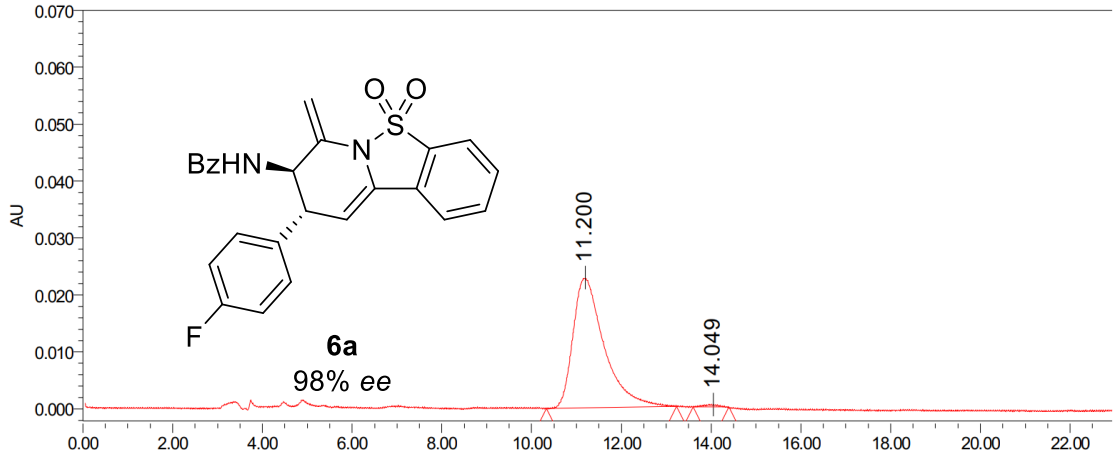
Entry	Retention Time/min	Area	Height	Area(%)
1	15.966	12116279	131602	97.51
2	21.334	309819	3166	2.49

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral OD-H



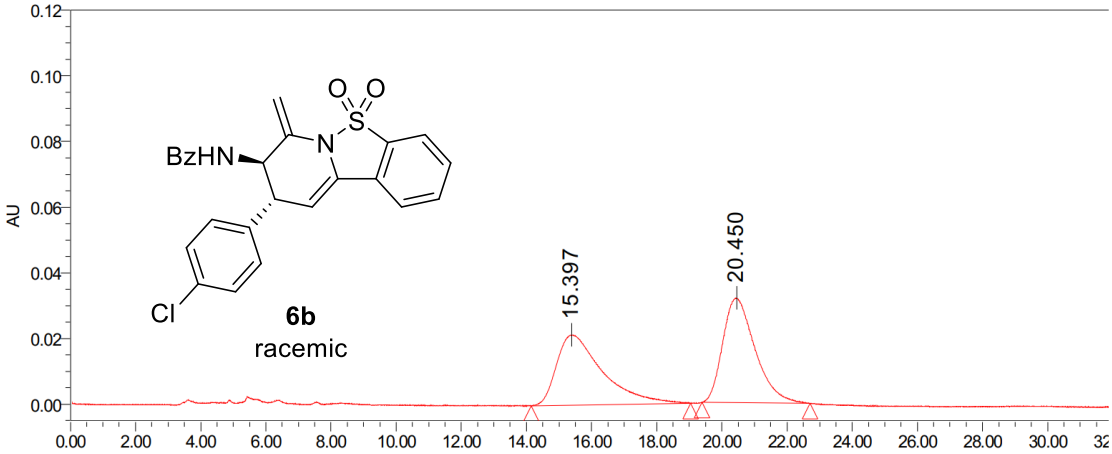
Entry	Retention Time/min	Area	Height	Area(%)
1	11.191	413615	8419	50.26
2	13.989	409373	10166	49.74



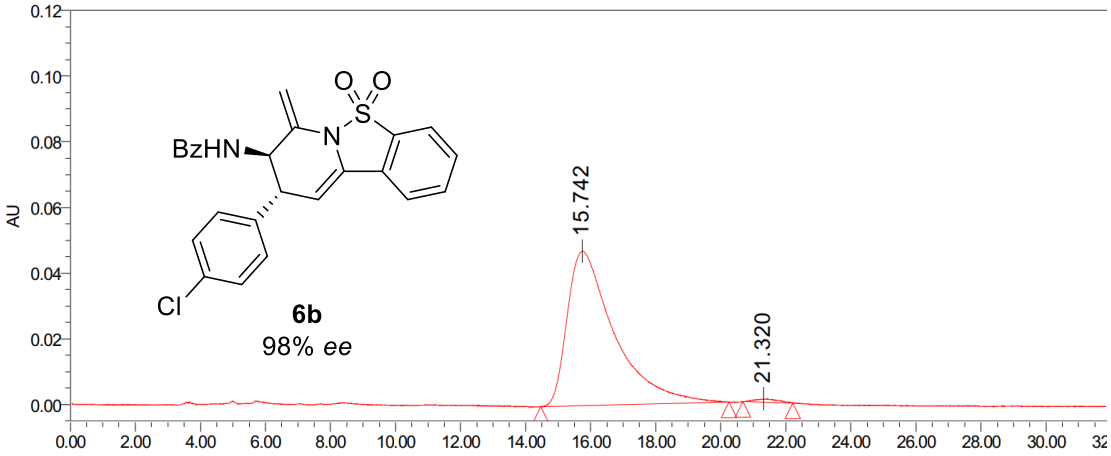
Entry	Retention Time/min	Area	Height	Area(%)
1	11.200	1098795	22825	99.06
2	14.049	10455	479	0.94

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral OD-H



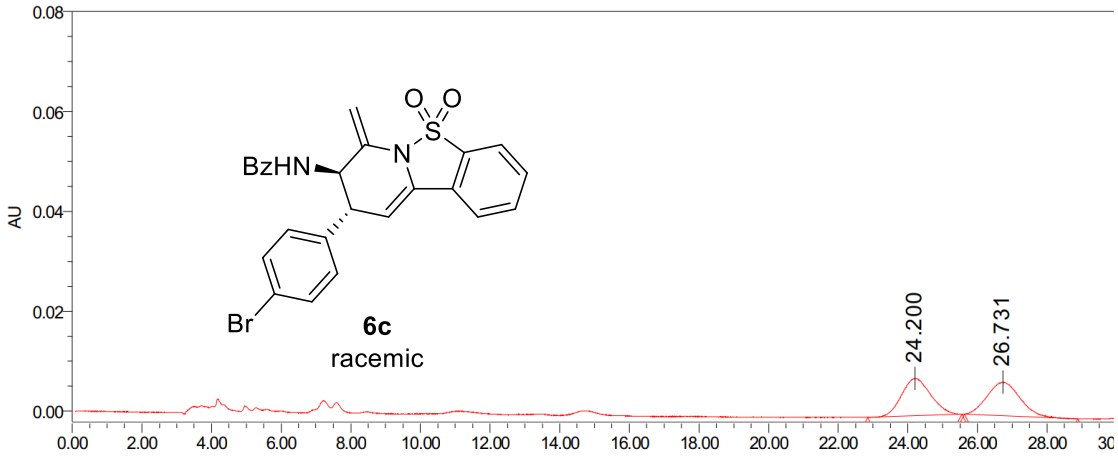
Entry	Retention Time/min	Area	Height	Area(%)
1	15.397	2082411	21446	48.90
2	20.450	2175958	31853	51.10



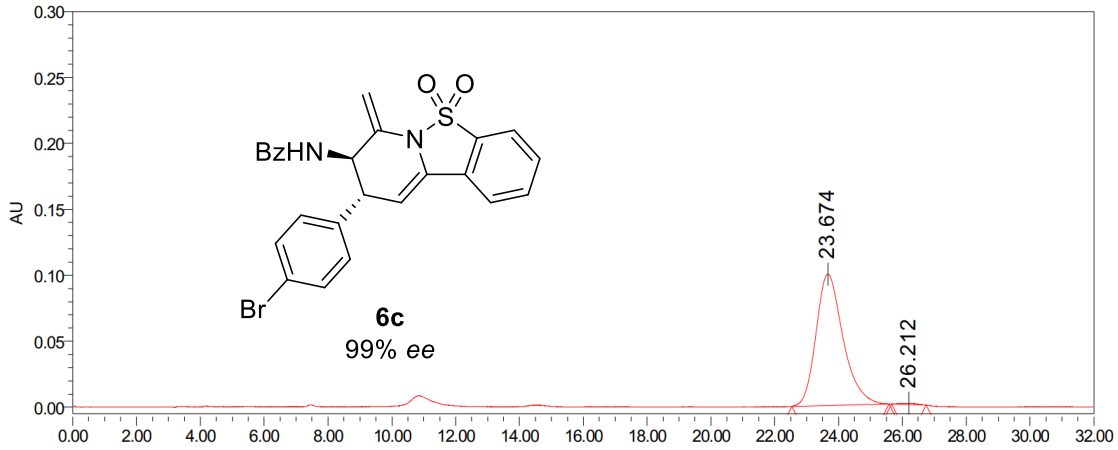
Entry	Retention Time/min	Area	Height	Area(%)
1	15.742	4720911	46988	99.05
2	21.320	45375	994	0.95

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral OD-H



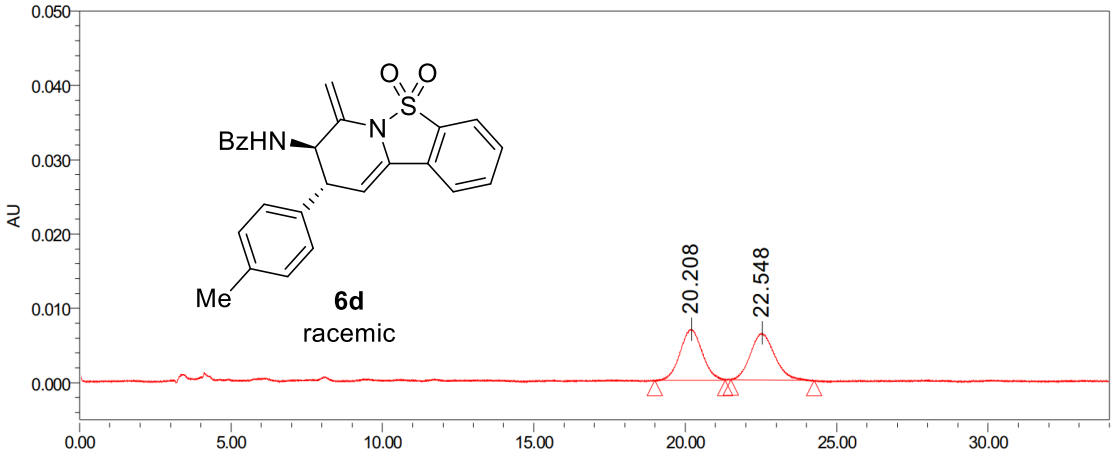
Entry	Retention Time/min	Area	Height	Area(%)
1	24.200	434303	7475	49.82
2	26.731	437386	6691	50.18



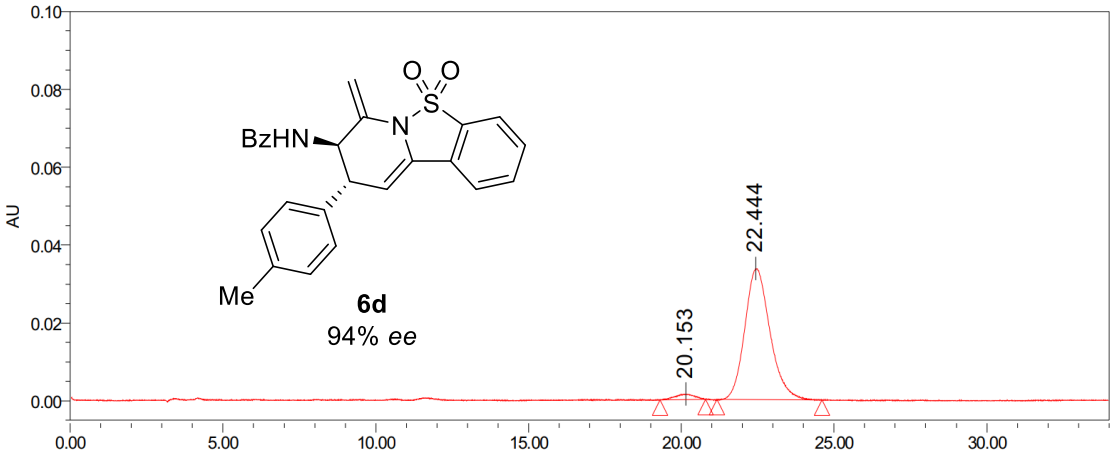
Entry	Retention Time/min	Area	Height	Area(%)
1	23.674	5875284	99555	99.41
2	26.212	35117	1009	0.59

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral AD-H



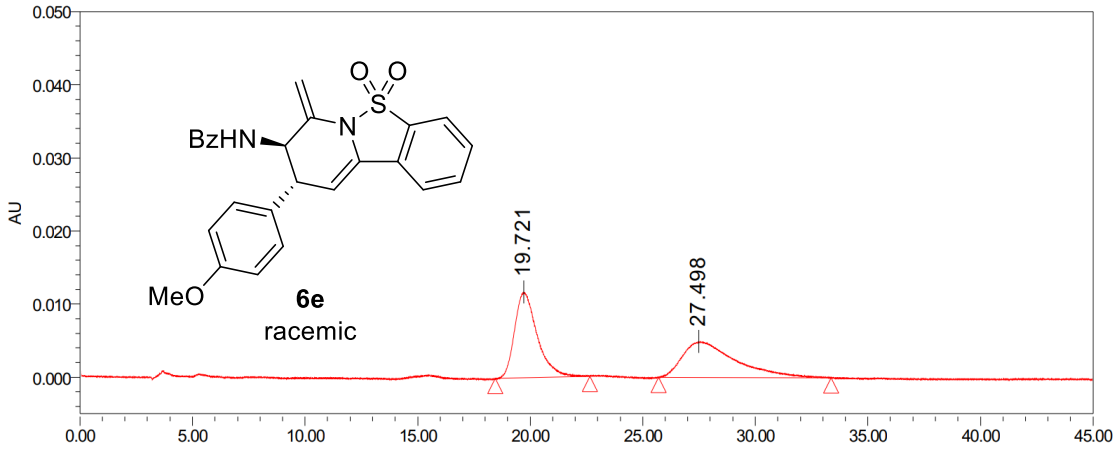
Entry	Retention Time/min	Area	Height	Area(%)
1	20.208	350283	6879	50.06
2	22.548	349440	6335	49.94



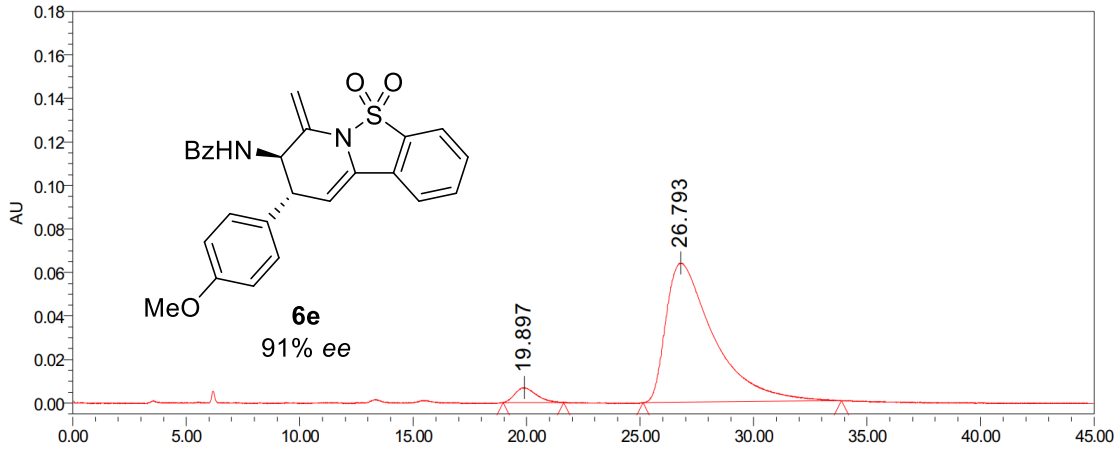
Entry	Retention Time/min	Area	Height	Area(%)
1	20.153	63014	1465	3.14
2	22.444	1941997	33746	96.86

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral OD-H



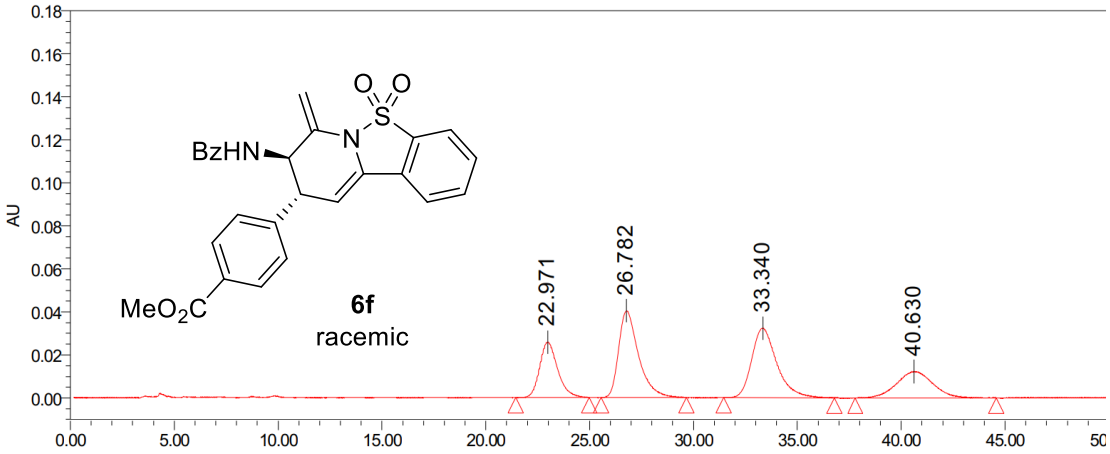
Entry	Retention Time/min	Area	Height	Area(%)
1	19.721	816689	11743	50.31
2	27.498	806769	4942	49.69



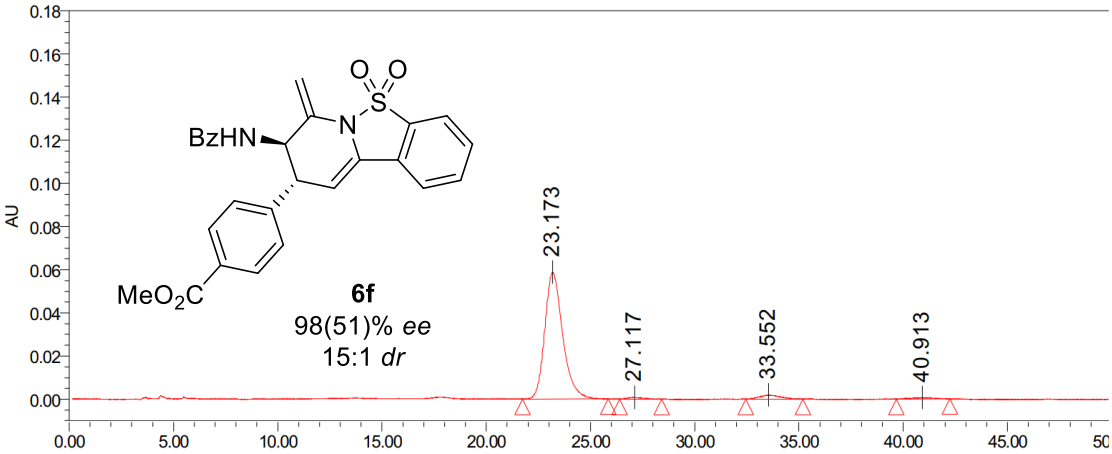
Entry	Retention Time/min	Area	Height	Area(%)
1	19.897	451592	6884	4.59
2	26.793	9391708	64044	95.41

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral AD-H



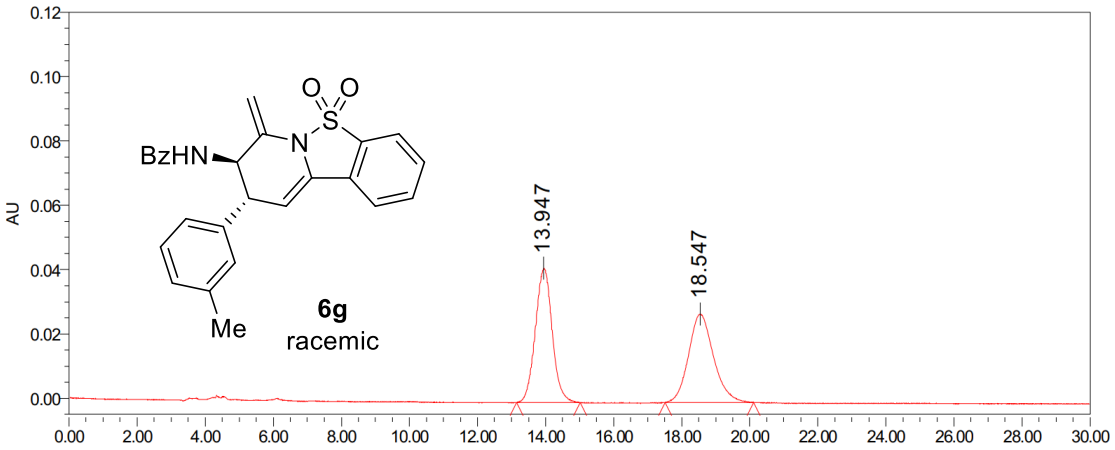
Entry	Retention Time/min	Area	Height	Area(%)
1	22.971	1527762	25720	18.11
2	26.782	2704563	40385	32.06
3	33.340	2710728	32352	32.13
4	40.630	1492572	12309	17.69



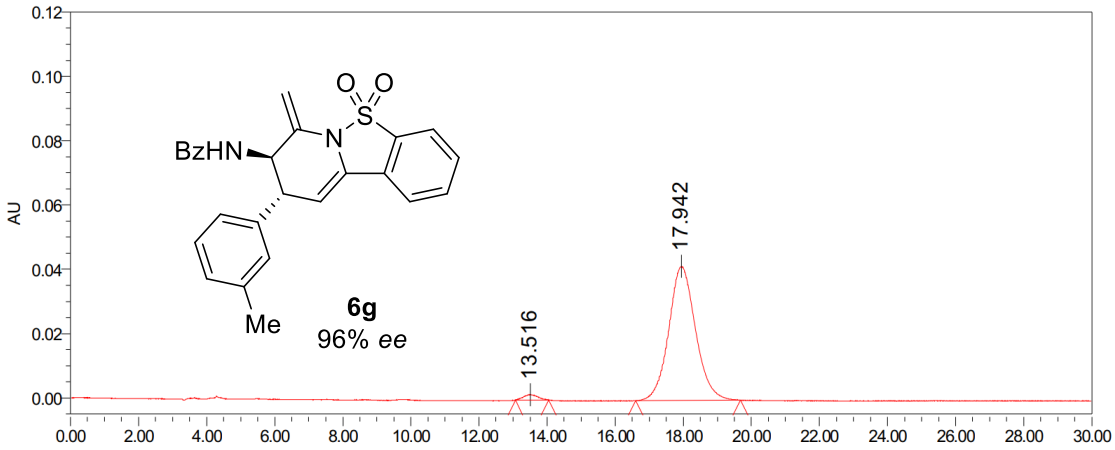
Entry	Retention Time/min	Area	Height	Area(%)
1	23.173	3484863	58792	94.01
2	27.117	42298	793	1.14
3	33.552	132003	1882	3.56
4	40.913	47892	661	1.29

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral AD-H



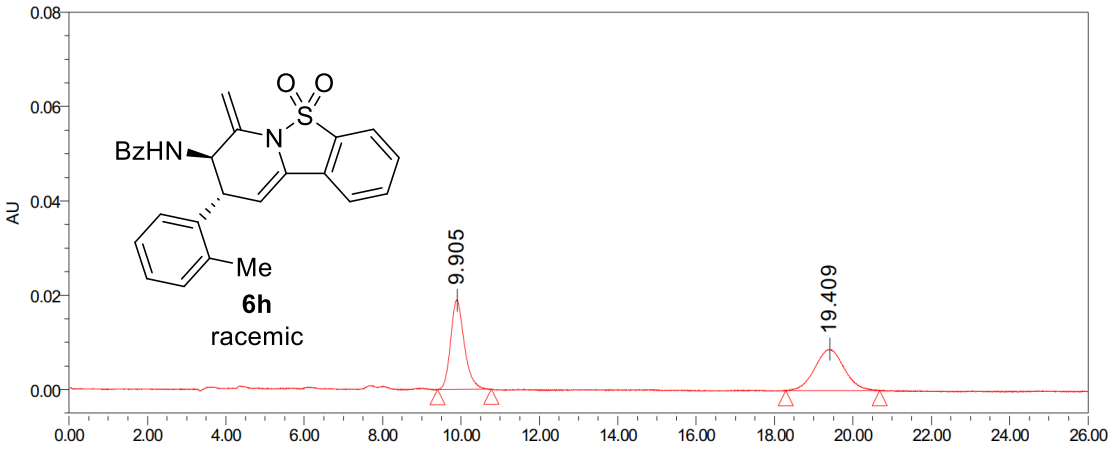
Entry	Retention Time/min	Area	Height	Area(%)
1	13.947	1422552	41693	50.35
2	18.547	1402938	27514	49.65



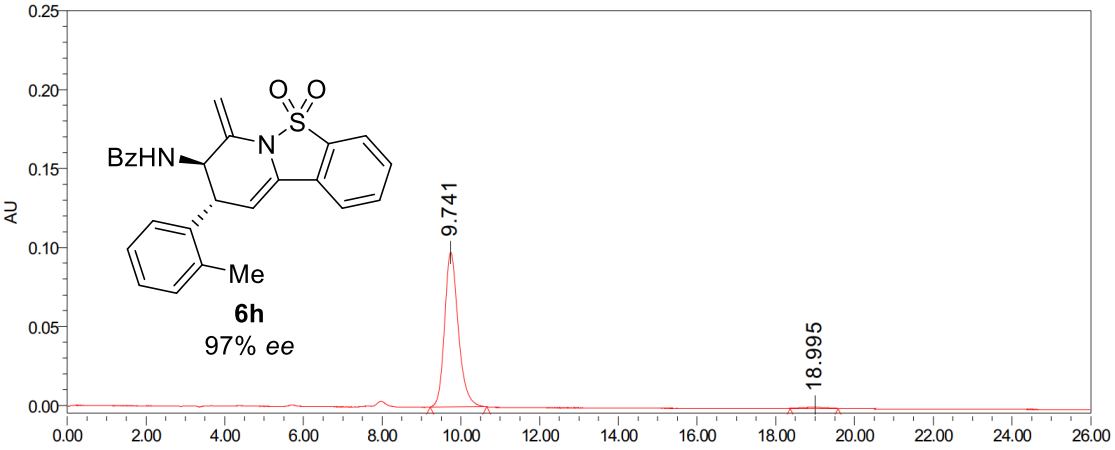
Entry	Retention Time/min	Area	Height	Area(%)
1	13.516	49231	1701	2.11
2	17.942	2279873	41770	97.89

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral AD-H



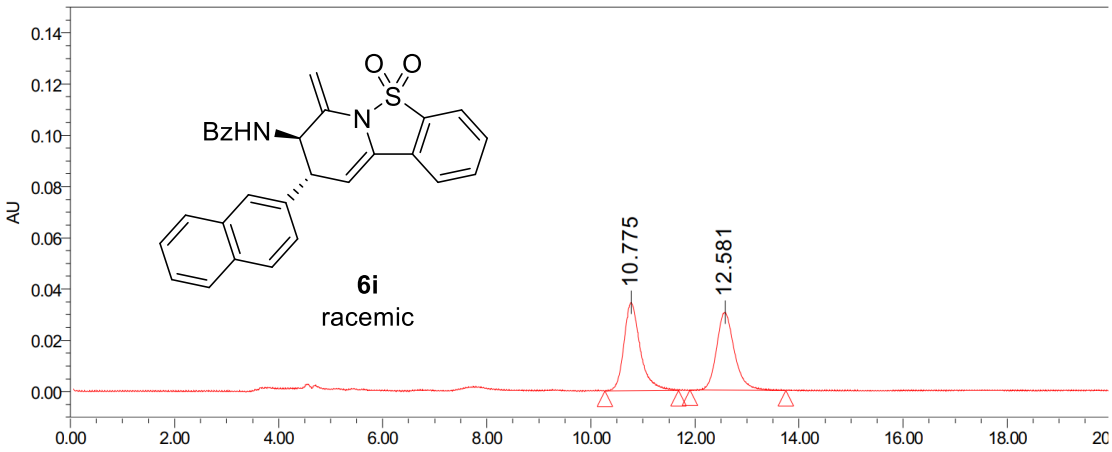
Entry	Retention Time/min	Area	Height	Area(%)
1	9.905	462547	18916	50.29
2	19.409	457133	8797	49.71



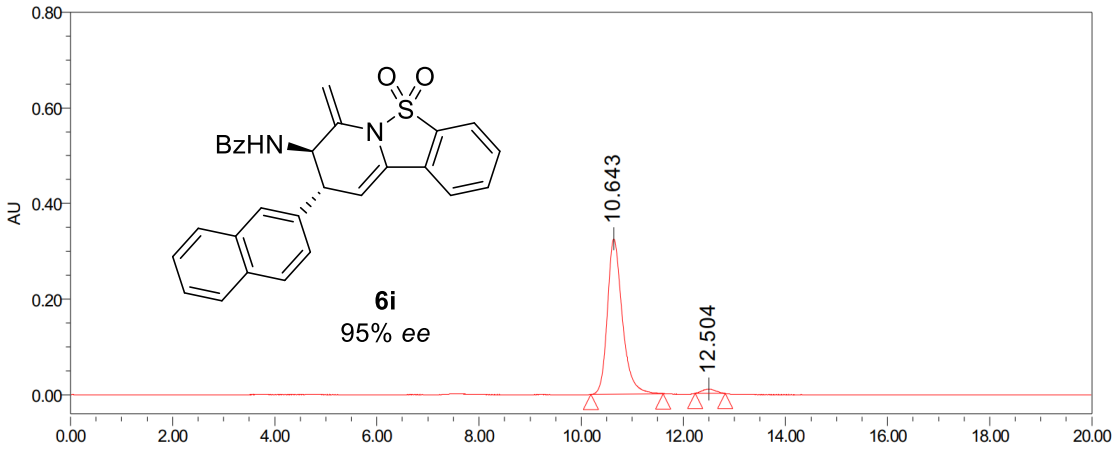
Entry	Retention Time/min	Area	Height	Area(%)
1	9.741	2372275	97811	98.58
2	18.995	34171	854	1.42

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral IA



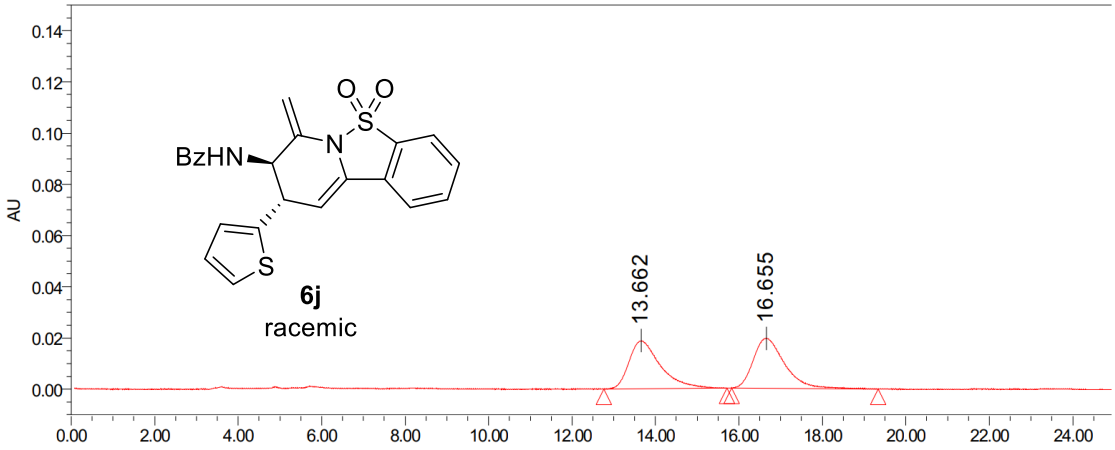
Entry	Retention Time/min	Area	Height	Area(%)
1	10.775	749253	34510	50.81
2	12.581	725355	30384	49.19



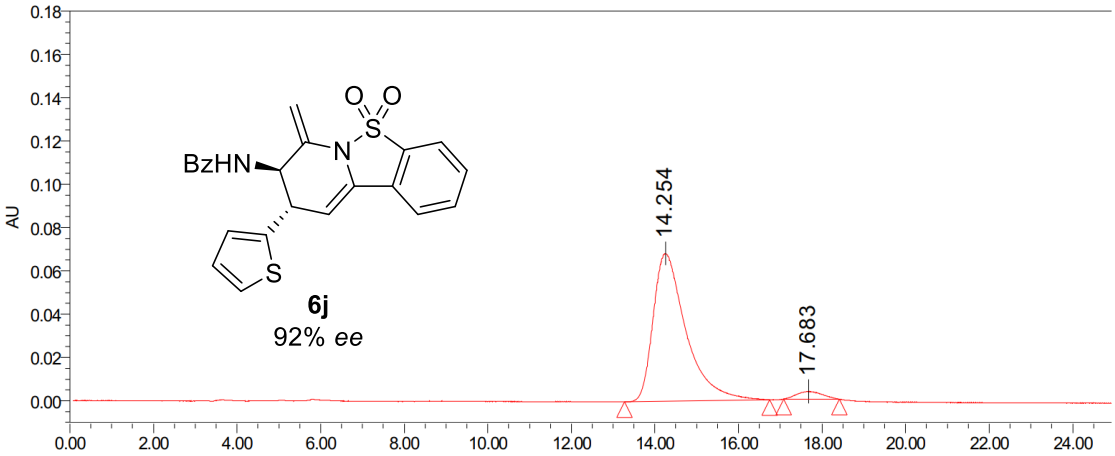
Entry	Retention Time/min	Area	Height	Area(%)
1	10.643	6616418	324684	97.51
2	12.504	169095	9136	2.49

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral OD-H



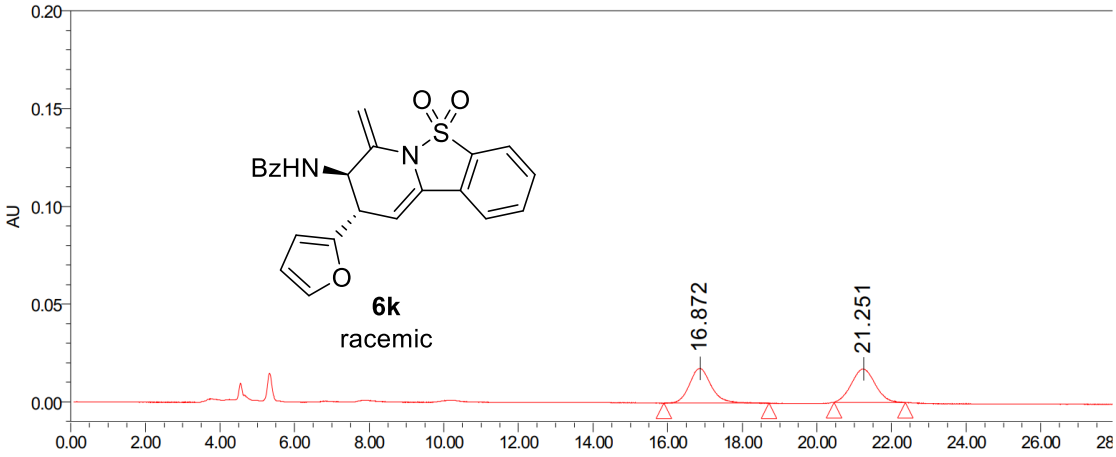
Entry	Retention Time/min	Area	Height	Area(%)
1	13.662	987572	18836	49.43
2	16.655	1010373	19511	50.57



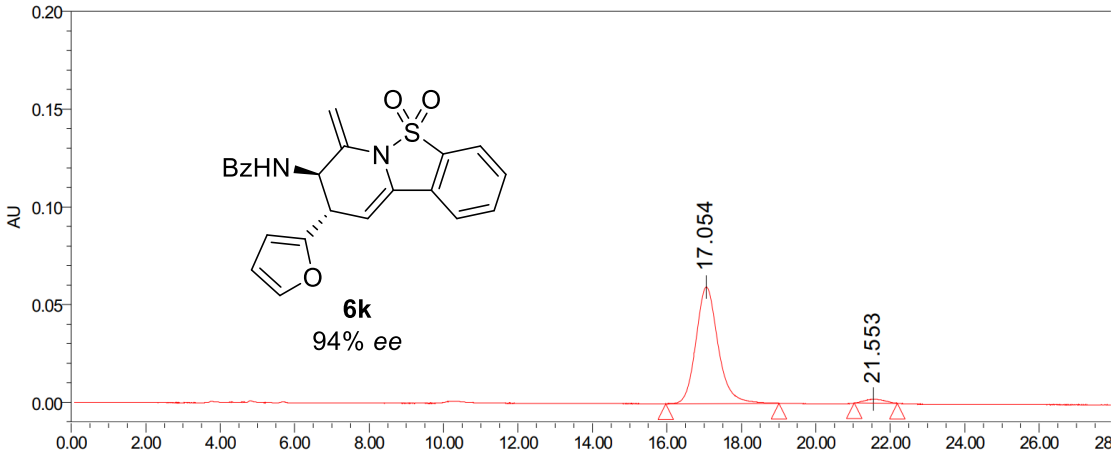
Entry	Retention Time/min	Area	Height	Area(%)
1	14.254	3705347	68203	96.03
2	17.683	153327	3554	3.97

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral IA



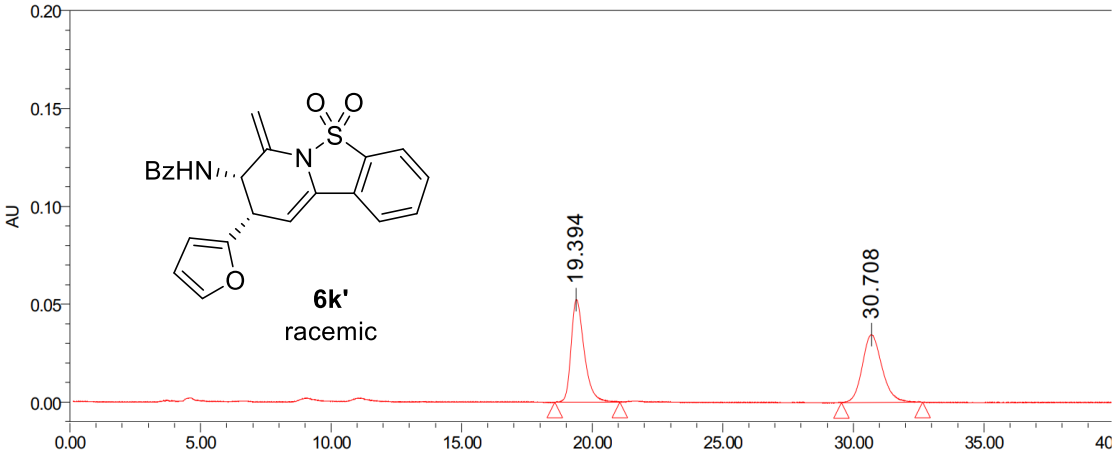
Entry	Retention Time/min	Area	Height	Area(%)
1	16.872	715720	17788	48.75
2	21.251	752291	17001	51.25



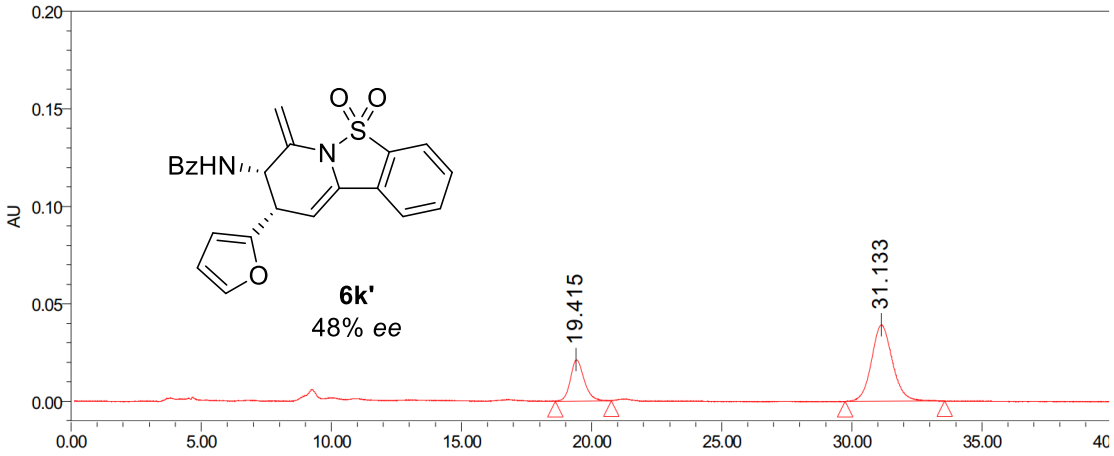
Entry	Retention Time/min	Area	Height	Area(%)
1	17.054	2470484	59640	96.94
2	21.553	77936	2098	3.06

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral IA



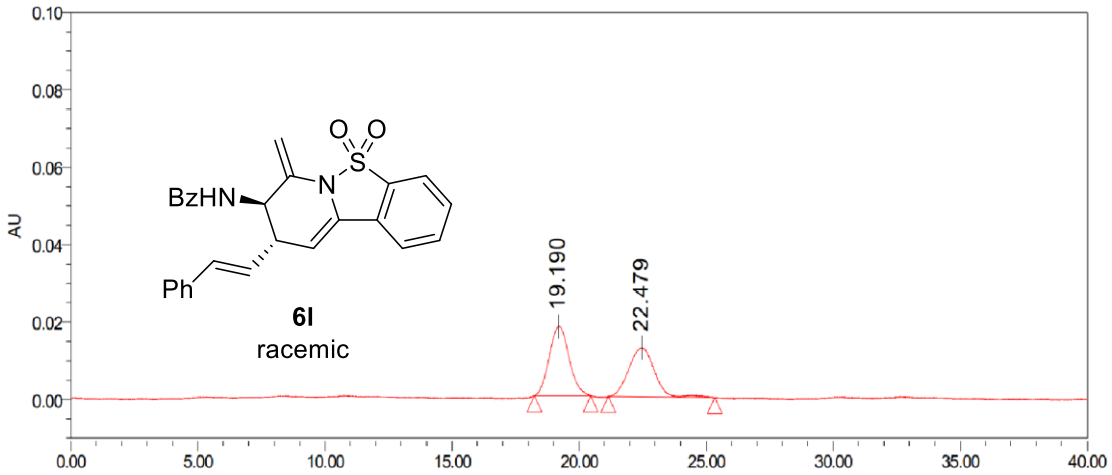
Entry	Retention Time/min	Area	Height	Area(%)
1	19.394	1830032	52362	50.21
2	30.708	1814769	34616	49.79



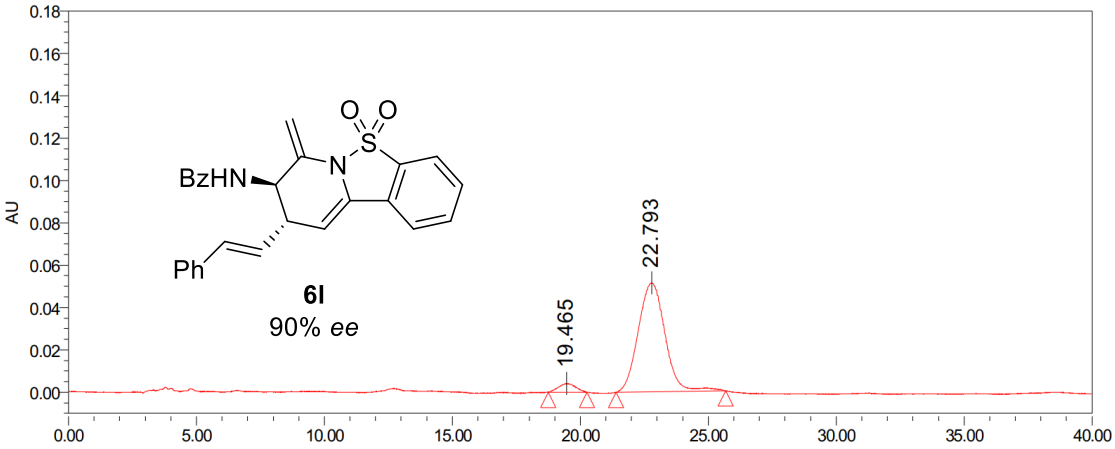
Entry	Retention Time/min	Area	Height	Area(%)
1	19.415	773674	21152	26.13
2	31.133	2186979	39161	73.87

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral AD-H



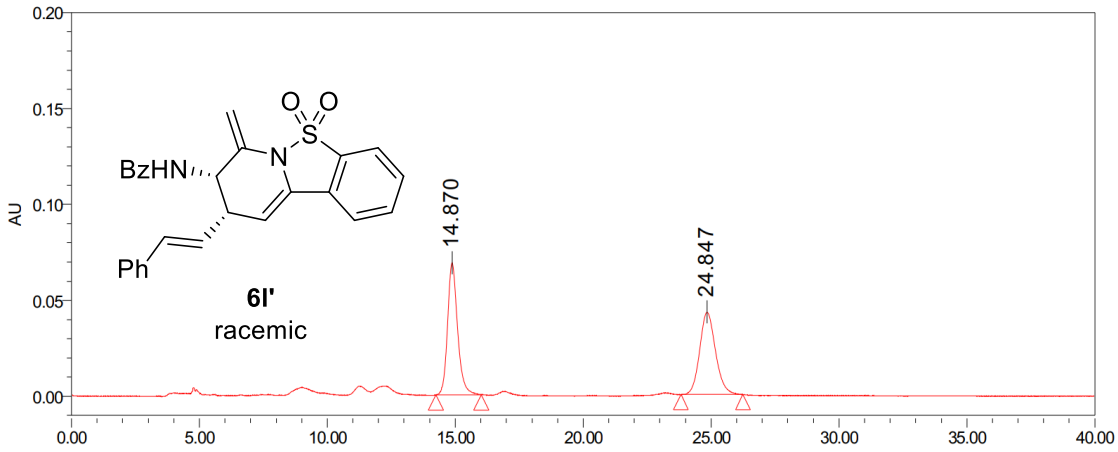
Entry	Retention Time/min	Area	Height	Area(%)
1	19.190	963672	17926	51.88
2	22.479	893786	12728	48.12



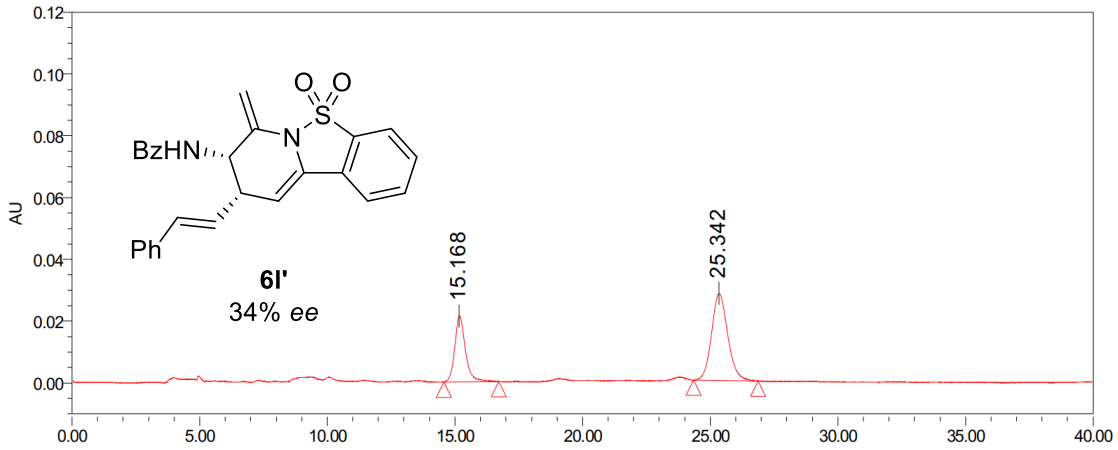
Entry	Retention Time/min	Area	Height	Area(%)
1	19.465	186383	4125	4.79
2	22.793	3702469	51357	95.21

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral AD-H



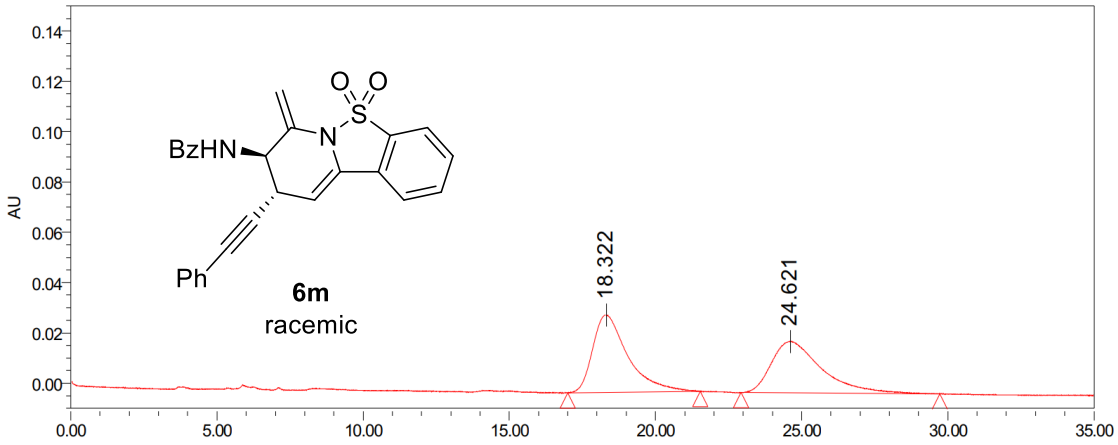
Entry	Retention Time/min	Area	Height	Area(%)
1	14.870	1876459	68837	50.27
2	24.847	1856360	42990	49.73



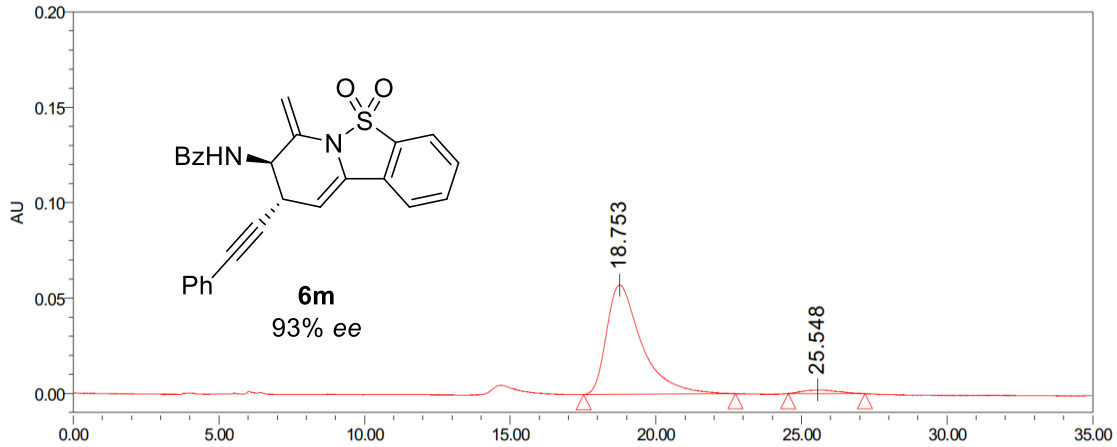
Entry	Retention Time/min	Area	Height	Area(%)
1	15.168	618583	21293	33.07
2	25.342	1251686	28216	66.93

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral OD-H



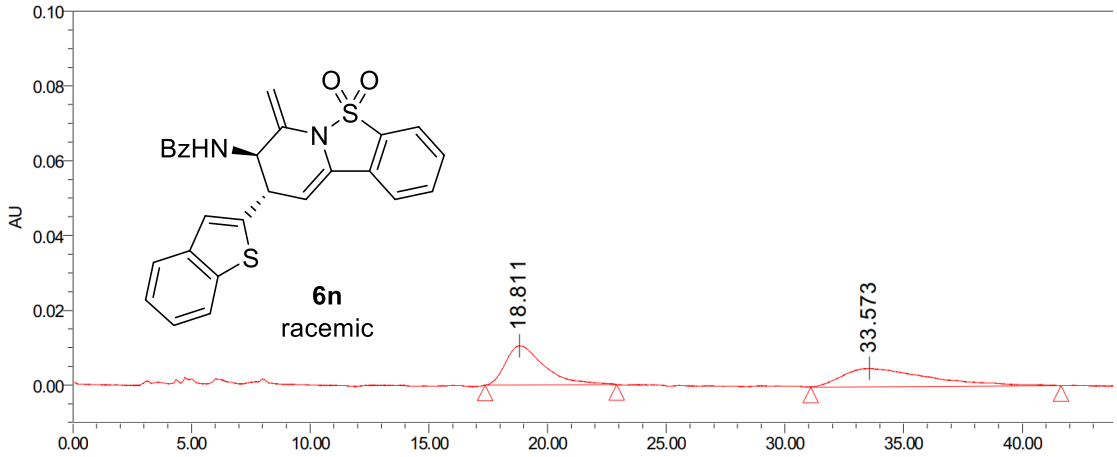
Entry	Retention Time/min	Area	Height	Area(%)
1	18.322	2588324	30866	51.35
2	24.621	2452606	20534	48.65



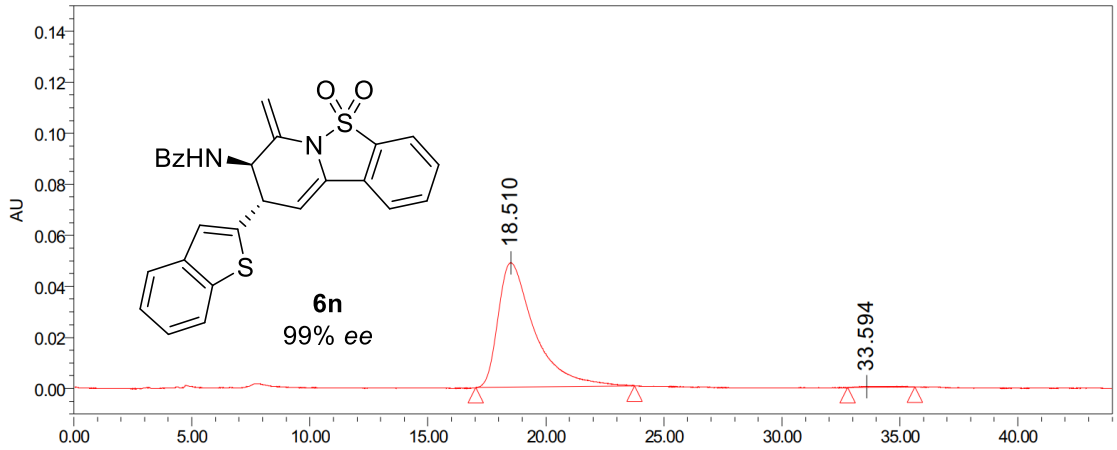
Entry	Retention Time/min	Area	Height	Area(%)
1	18.753	4811259	57345	96.67
2	25.548	165632	1980	3.33

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral OD-H



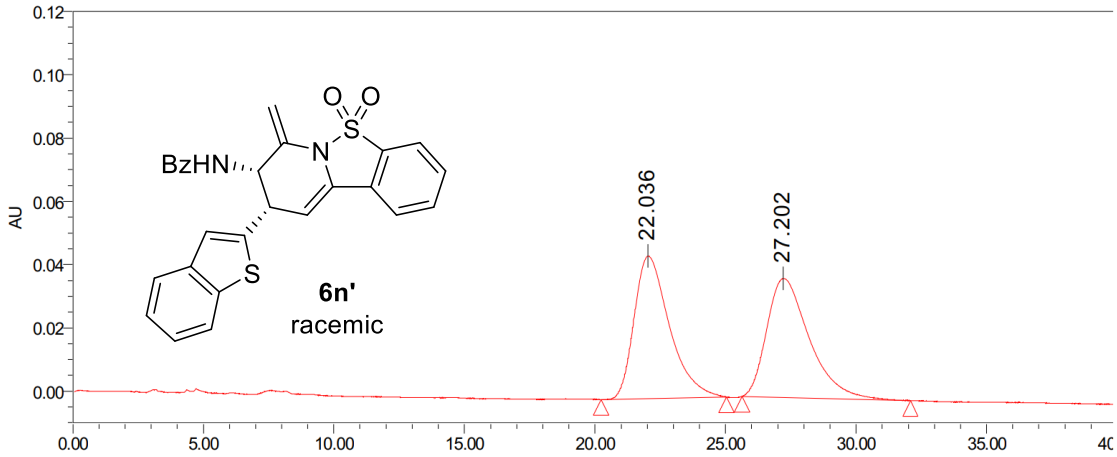
Entry	Retention Time/min	Area	Height	Area(%)
1	18.811	1190463	10475	49.16
2	33.573	1231319	4865	50.84



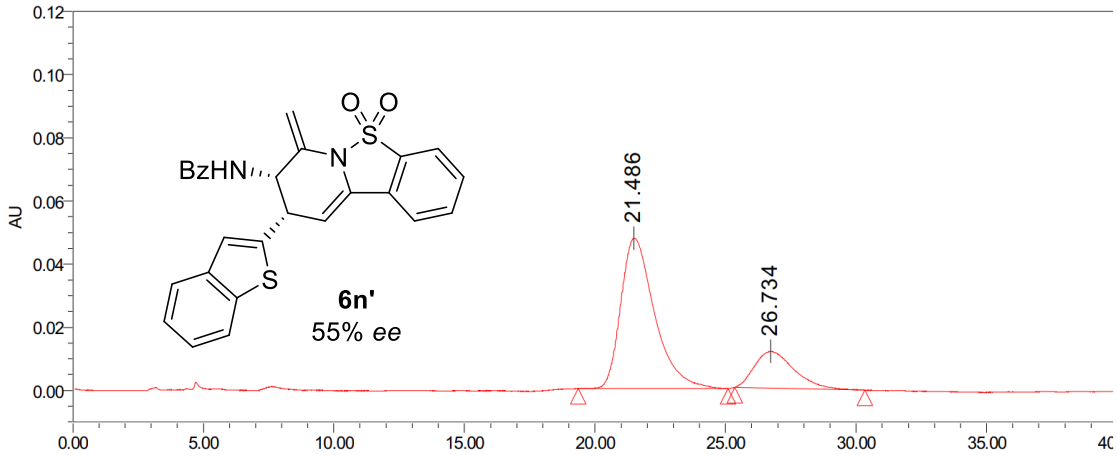
Entry	Retention Time/min	Area	Height	Area(%)
1	18.510	5230015	48741	99.41
2	33.594	31225	340	0.59

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral OD-H



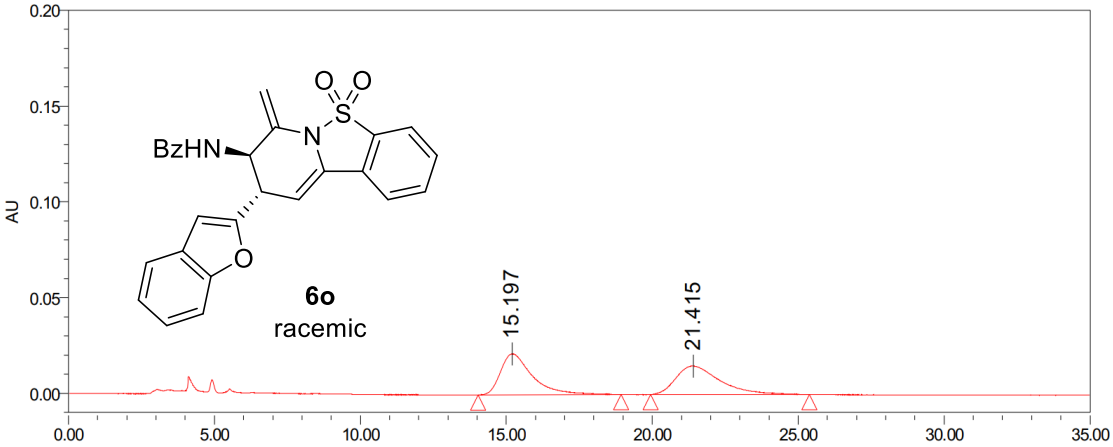
Entry	Retention Time/min	Area	Height	Area(%)
1	22.036	4234982	45054	49.89
2	27.202	4253842	37587	50.11



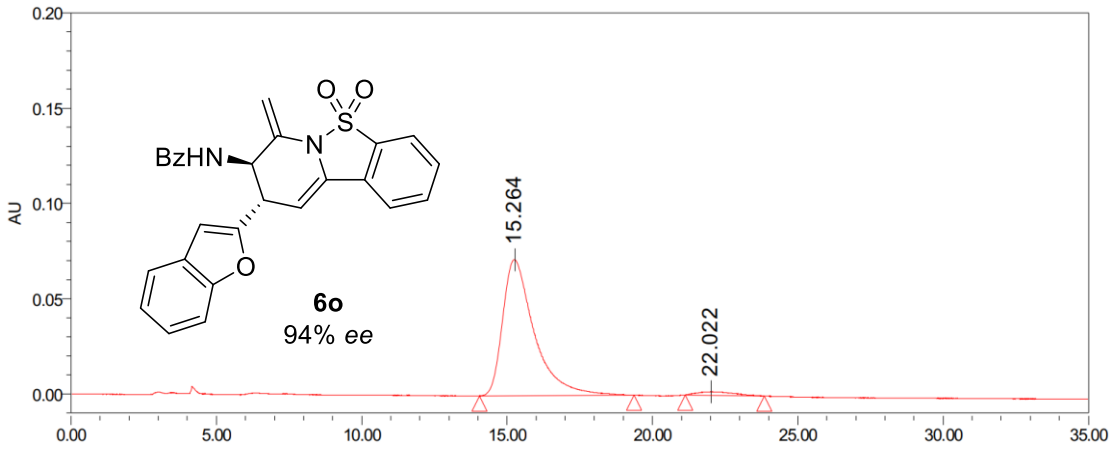
Entry	Retention Time/min	Area	Height	Area(%)
1	21.486	4262622	47549	77.67
2	26.734	1225190	11592	22.33

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral OD-H



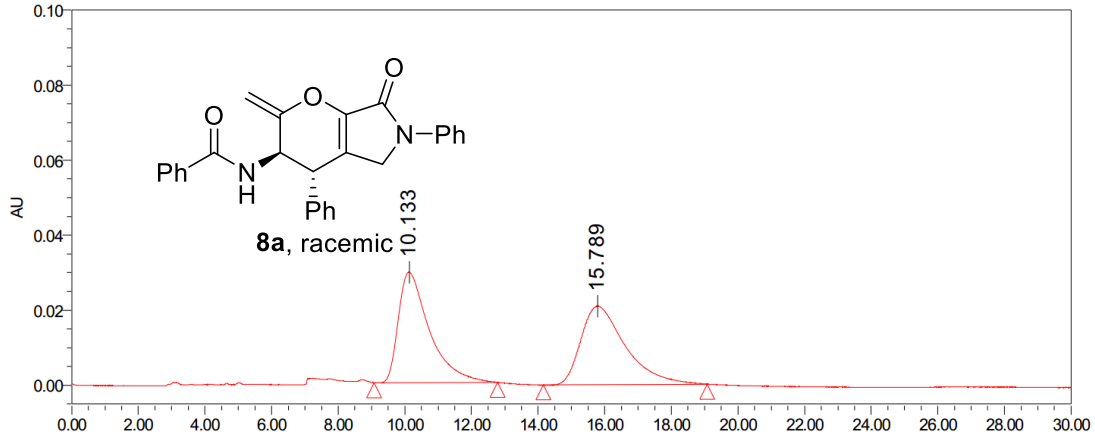
Entry	Retention Time/min	Area	Height	Area(%)
1	15.197	1622250	21450	51.08
2	21.415	1553703	14847	48.92



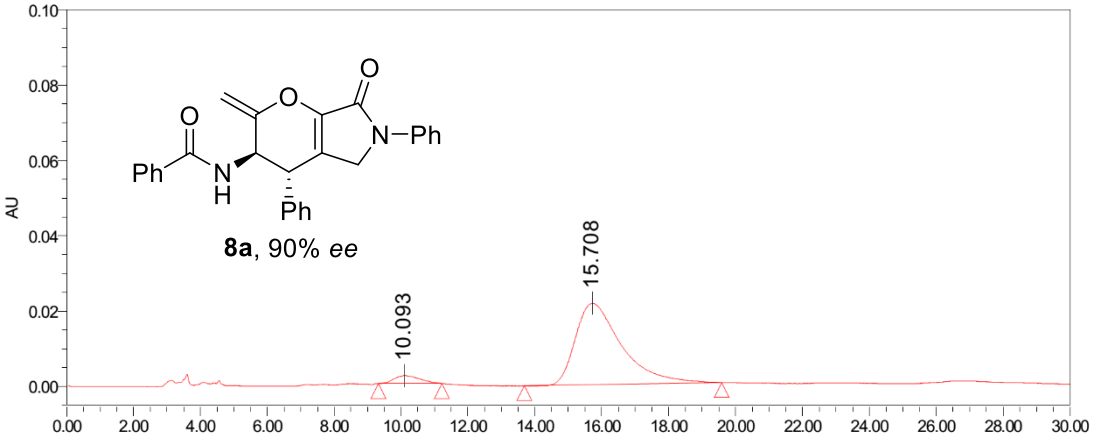
Entry	Retention Time/min	Area	Height	Area(%)
1	15.264	5400946	71381	97.23
2	22.022	153949	1826	2.77

Condition: hexane: 2-propanol = 80:20

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral OD-H



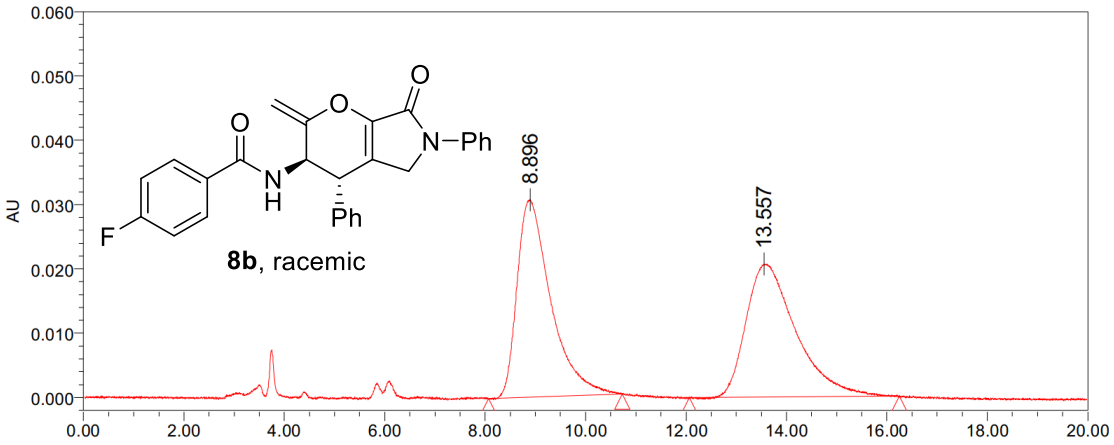
Entry	Retention Time/min	Area	Height	Area(%)
1	10.133	1915406	29481	49.76
2	15.789	1933763	20930	50.24



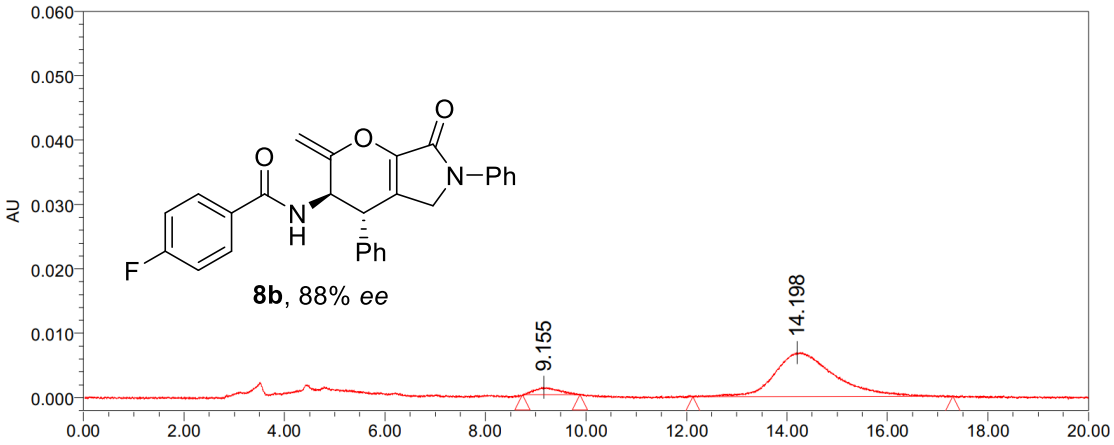
Entry	Retention Time/min	Area	Height	Area(%)
1	10.093	111552	2085	5.11
2	15.708	2069882	21640	94.89

Condition: hexane: 2-propanol = 80:20

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral OD-H



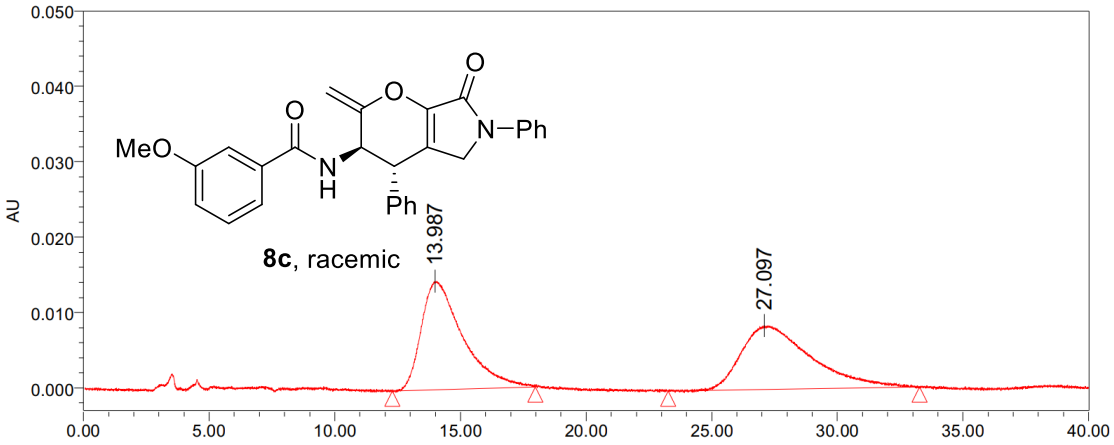
Entry	Retention Time/min	Area	Height	Area(%)
1	8.896	1430806	30736	50.06
2	13.557	1427603	20690	49.94



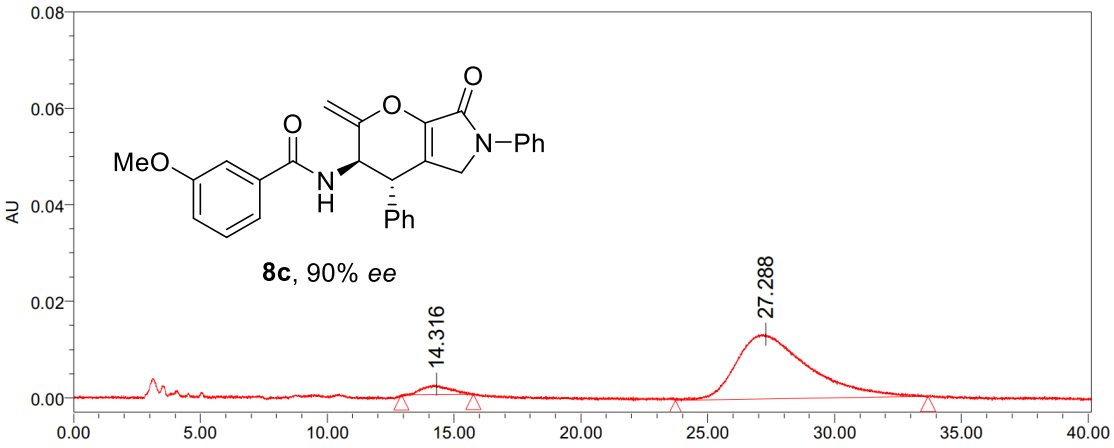
Entry	Retention Time/min	Area	Height	Area(%)
1	9.155	35802	1131	6.01
2	14.198	559799	6845	93.99

Condition: hexane: 2-propanol = 80:20

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral OD-H



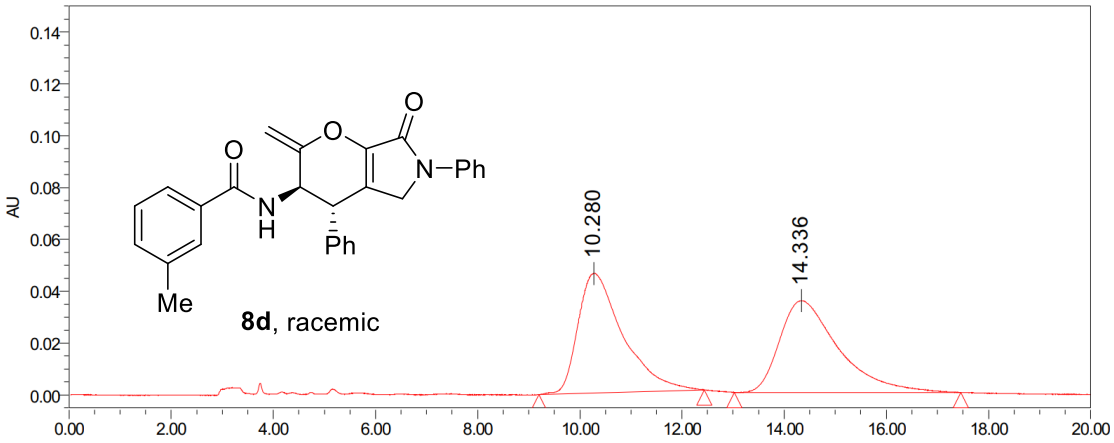
Entry	Retention Time/min	Area	Height	Area(%)
1	13.987	1649933	14445	50.34
2	27.097	1627501	8478	49.66



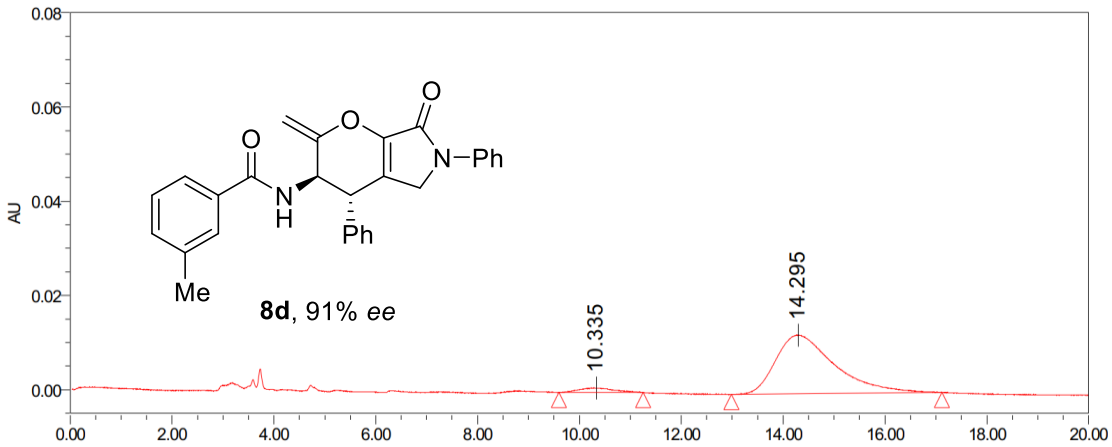
Entry	Retention Time/min	Area	Height	Area(%)
1	14.316	143291	2078	5.15
2	27.288	2637717	13440	94.85

Condition: hexane: 2-propanol = 80:20

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral OD-H



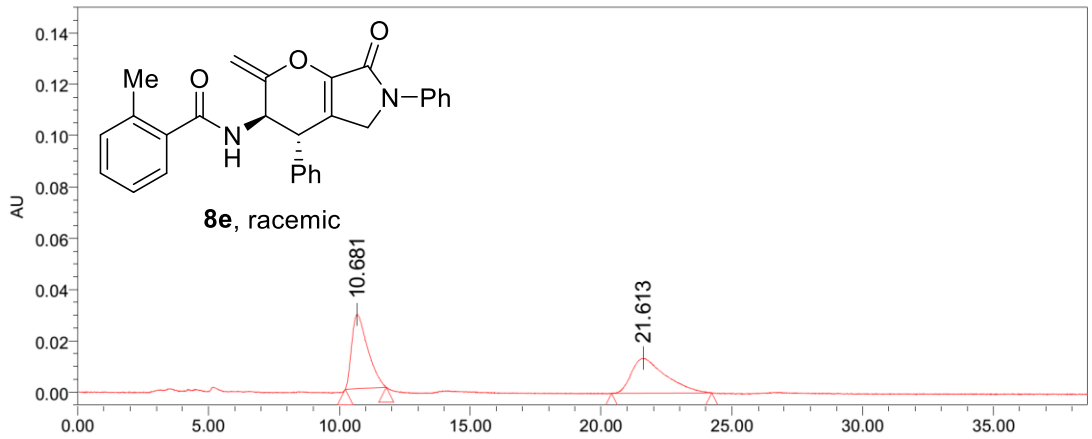
Entry	Retention Time/min	Area	Height	Area(%)
1	10.280	2814490	46178	50.01
2	14.336	2812880	35335	49.99



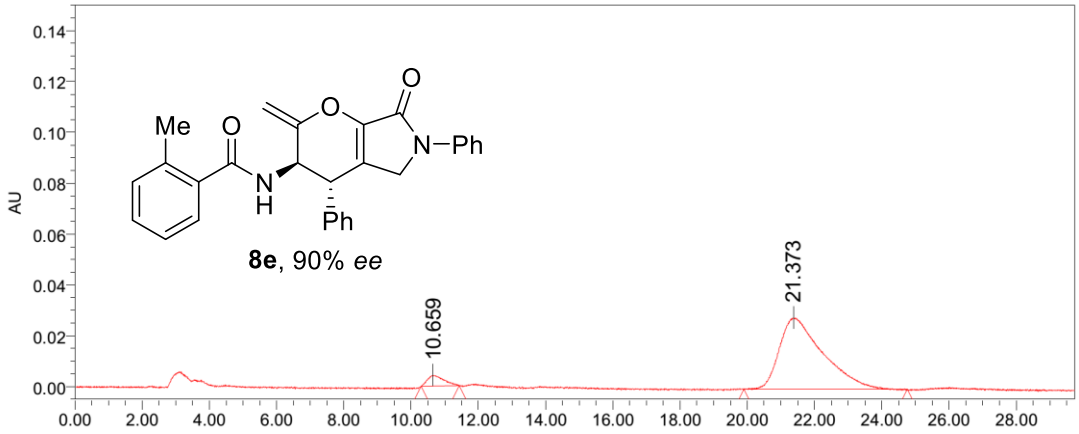
Entry	Retention Time/min	Area	Height	Area(%)
1	10.335	46926	987	4.50
2	14.295	996505	12446	95.50

Condition: hexane: 2-propanol = 80:20

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral AD-H



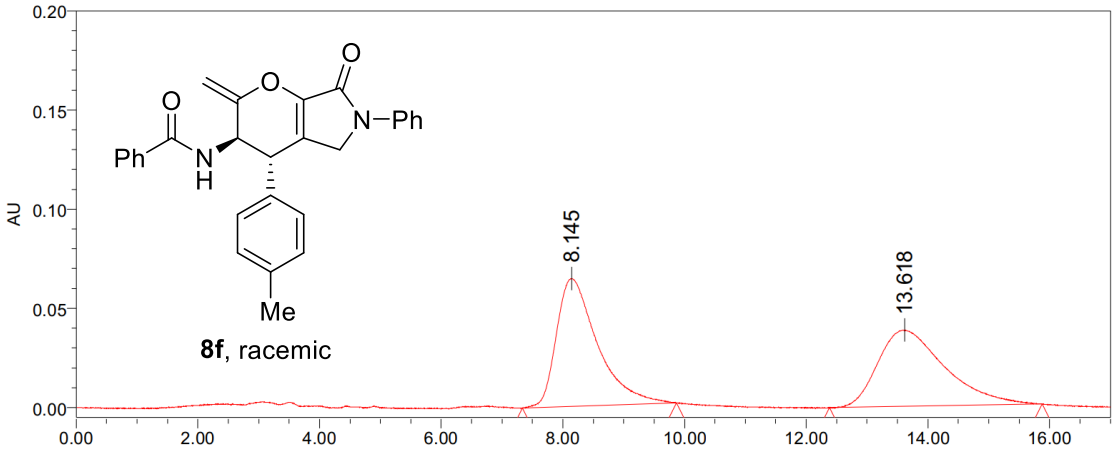
Entry	Retention Time/min	Area	Height	Area(%)
1	10.681	1236128	29033	50.29
2	21.613	1222070	13685	49.71



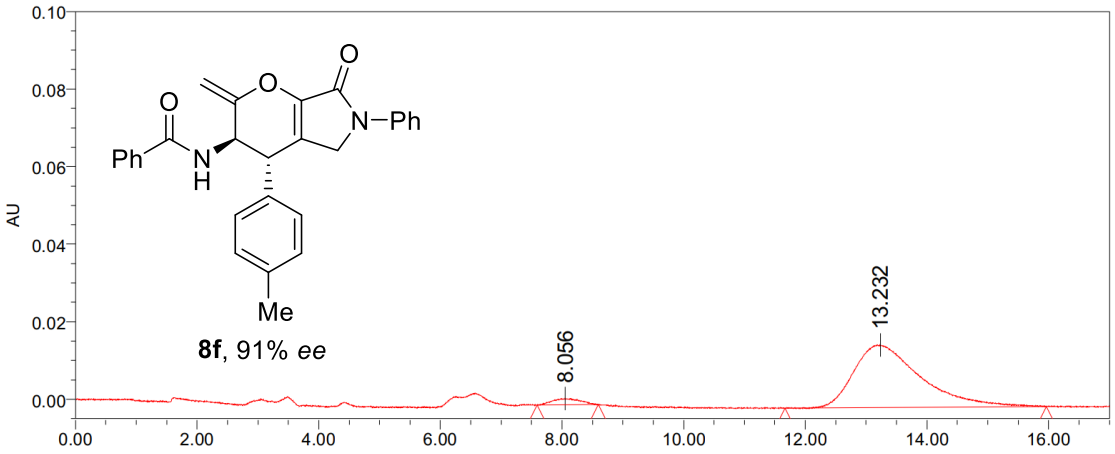
Entry	Retention Time/min	Area	Height	Area(%)
1	10.659	140213	4228	5.22
2	21.373	2544070	28283	94.78

Condition: hexane: 2-propanol = 80:20

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral OD-H



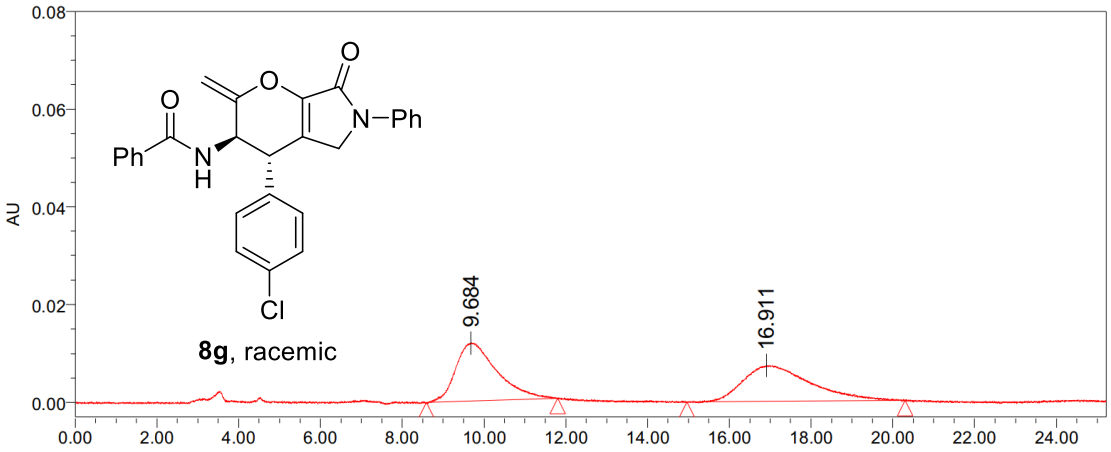
Entry	Retention Time/min	Area	Height	Area(%)
1	8.145	3017962	64524	50.76
2	13.618	2927717	38464	49.24



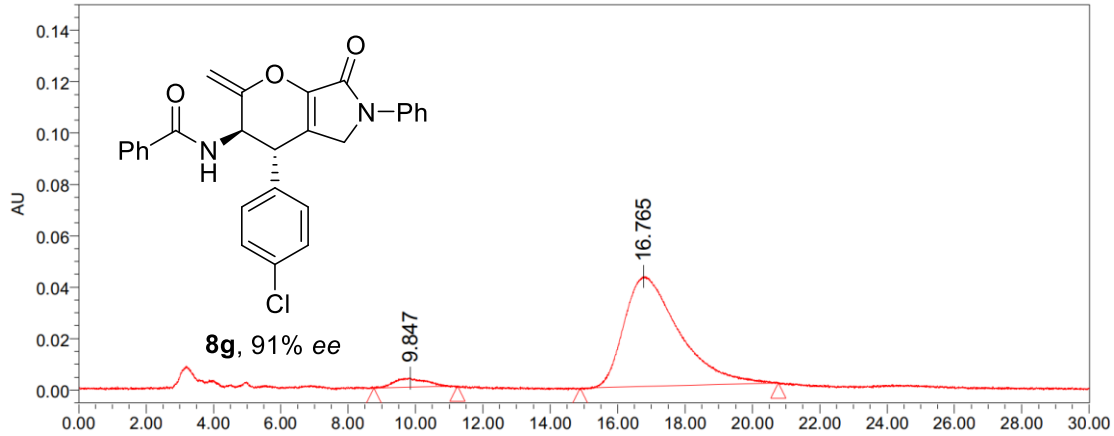
Entry	Retention Time/min	Area	Height	Area(%)
1	8.056	51255	1664	4.02
2	13.232	1222324	16196	95.98

Condition: hexane: 2-propanol = 80:20

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral OD-H



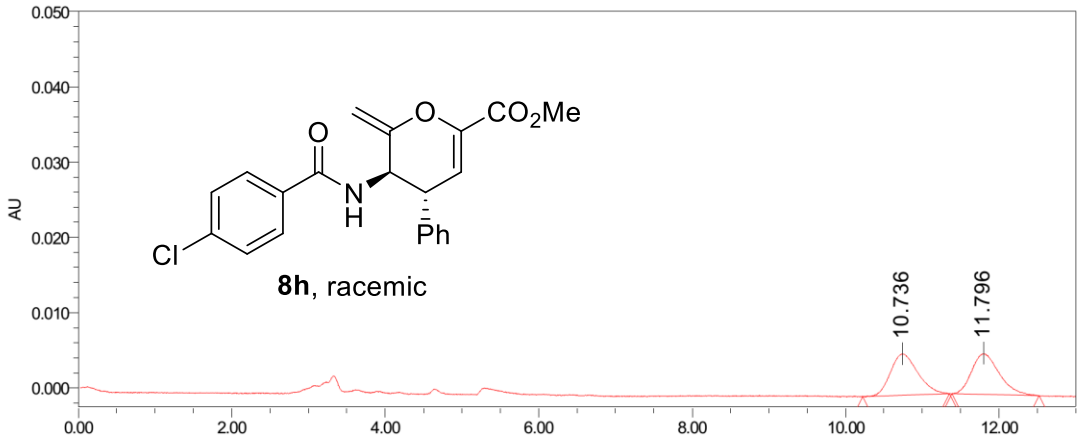
Entry	Retention Time/min	Area	Height	Area(%)
1	9.684	835156	11892	50.23
2	16.911	827660	7298	49.77



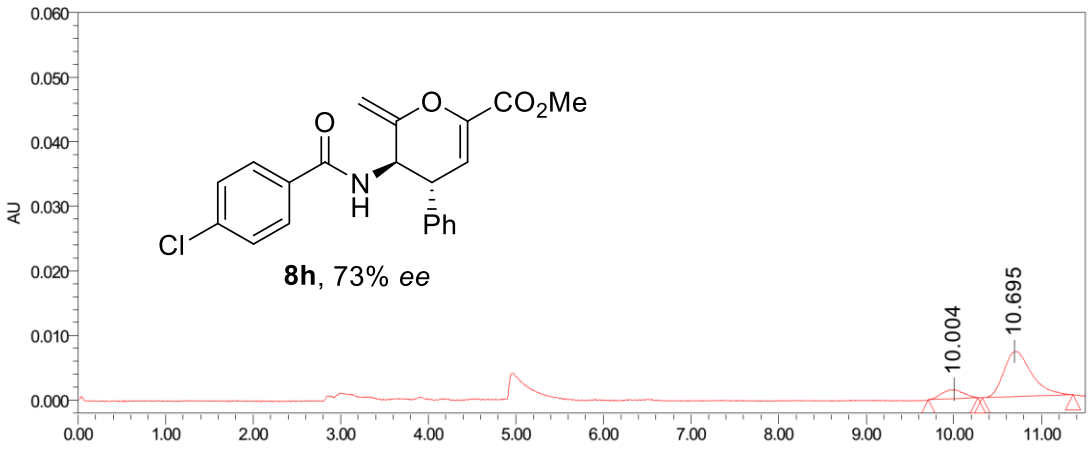
Entry	Retention Time/min	Area	Height	Area(%)
1	9.847	227649	3610	4.05
2	16.765	4829979	42752	95.50

Condition: hexane: 2-propanol = 80:20

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral IA



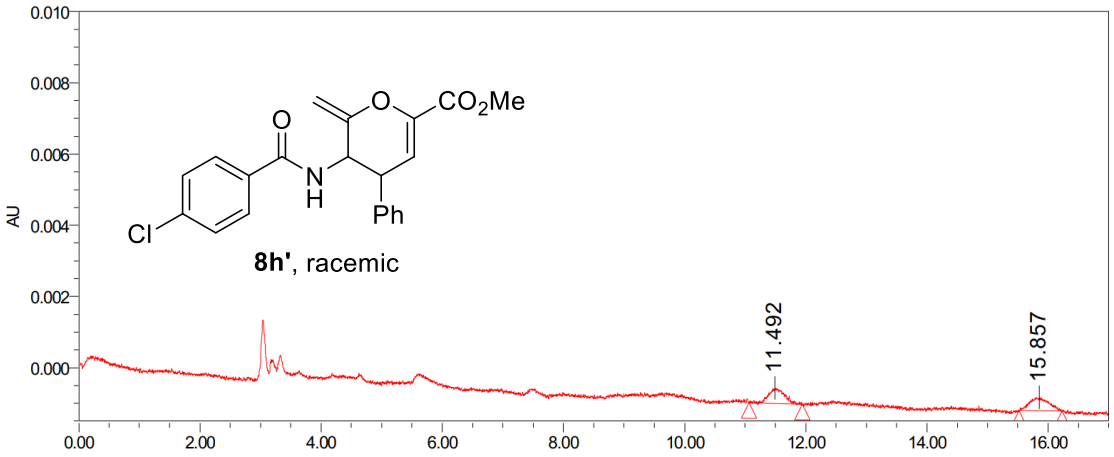
Entry	Retention Time/min	Area	Height	Area(%)
1	10.736	133604	133604	49.80
2	11.796	134653	134653	50.20



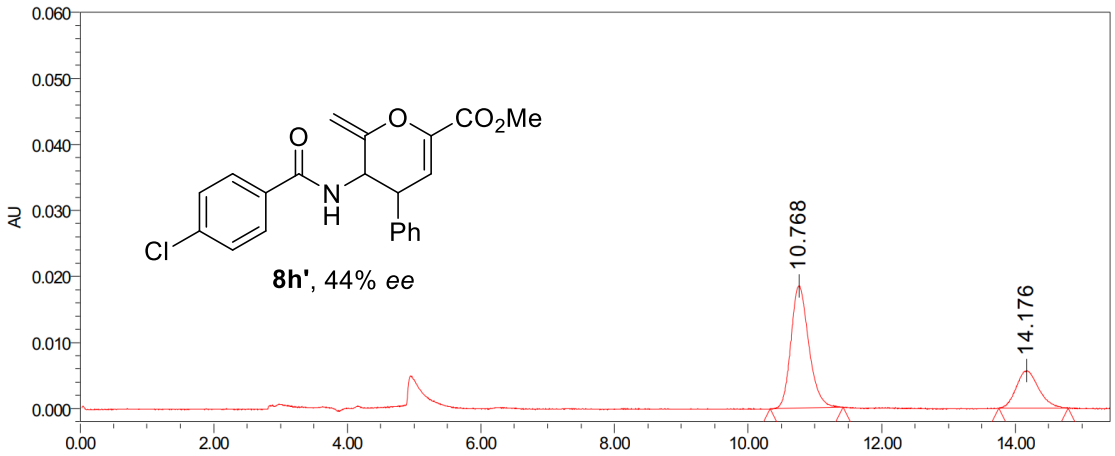
Entry	Retention Time/min	Area	Height	Area(%)
1	10.004	24048	24048	13.41
2	10.695	155265	155265	86.59

Condition: hexane: 2-propanol = 80:20

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral IA



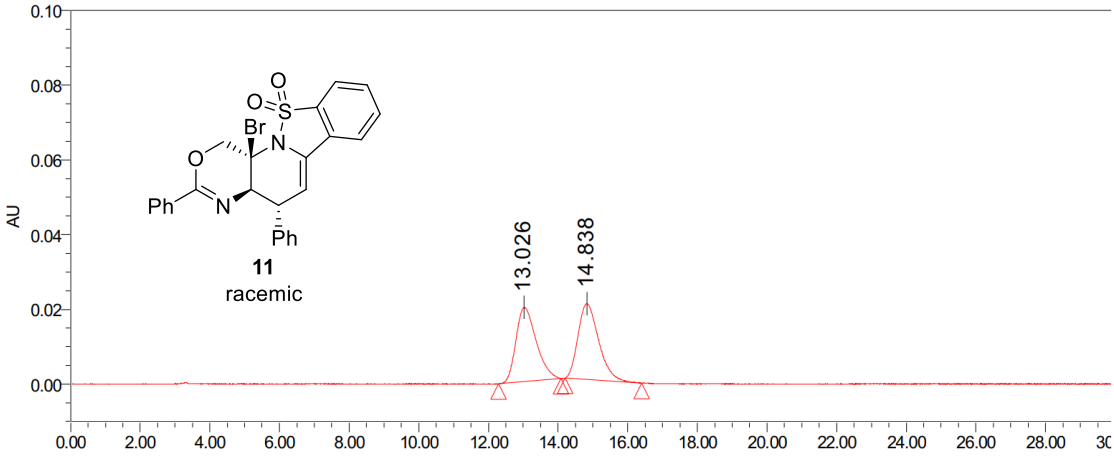
Entry	Retention Time/min	Area	Height	Area(%)
1	11.492	8157	438	50.00
2	15.857	8158	377	50.00



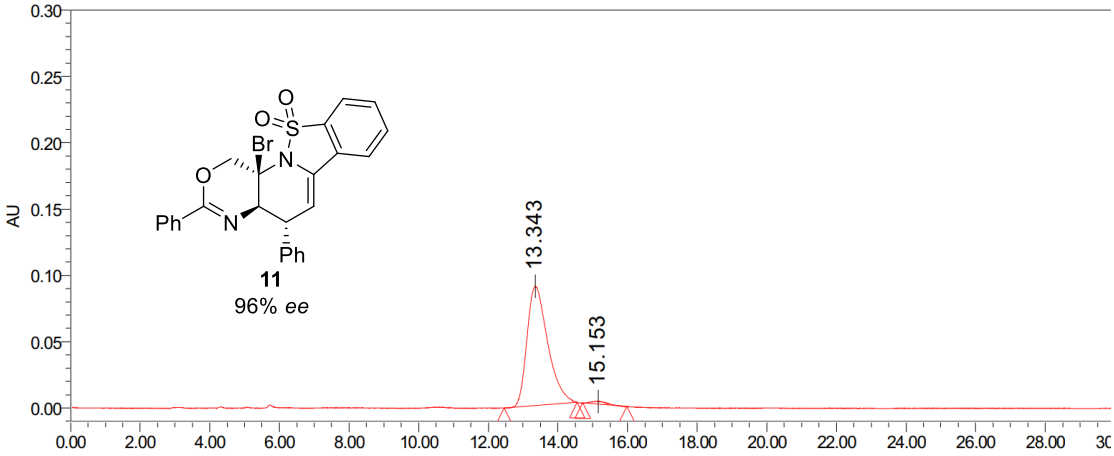
Entry	Retention Time/min	Area	Height	Area(%)
1	10.768	343668	18531	72.15
2	14.176	132663	5673	27.85

Condition: hexane: 2-propanol = 80:20

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral OD-H



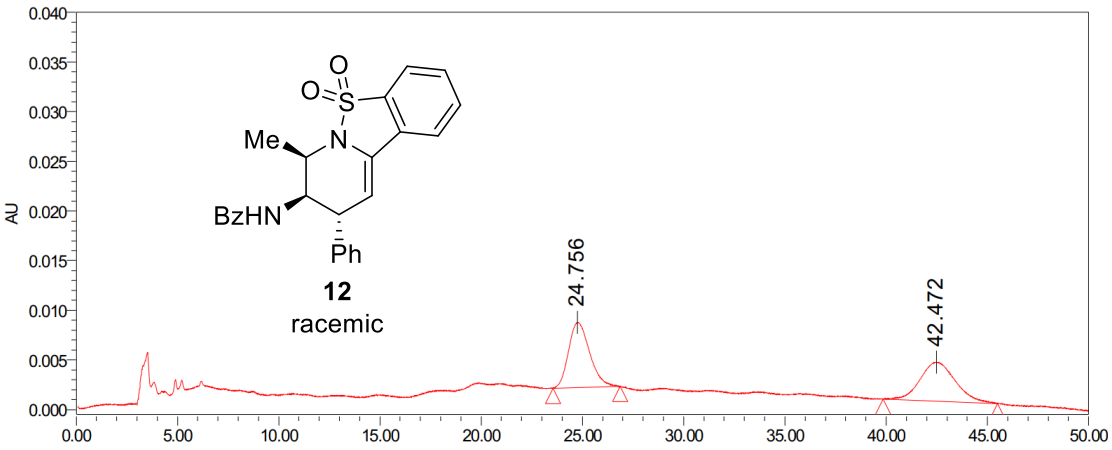
Entry	Retention Time/min	Area	Height	Area(%)
1	13.026	808192	19902	49.22
2	14.838	833734	20299	50.78



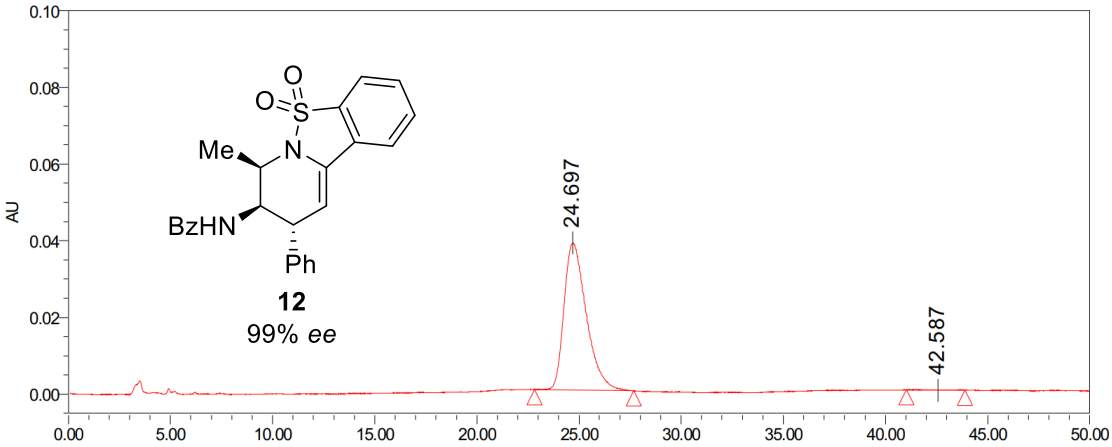
Entry	Retention Time/min	Area	Height	Area(%)
1	13.343	3746693	90076	98.17
2	15.153	70025	2307	1.83

Condition: hexane: 2-propanol = 70:30

Flow rate = 1.0 mL/min, λ = 254 nm, Chiral IC

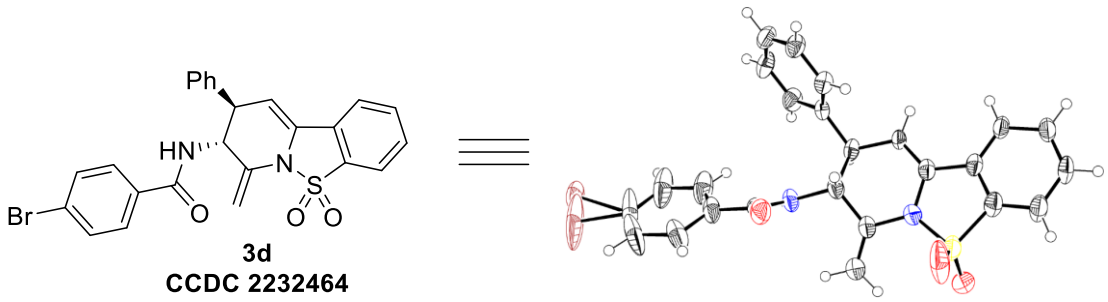


Entry	Retention Time/min	Area	Height	Area(%)
1	24.756	474406	6565	50.07
2	42.472	473062	3928	49.93



Entry	Retention Time/min	Area	Height	Area(%)
1	24.697	2889166	38309	99.75
2	42.587	7286	11	0.25

Crystallographic Data for Compound 3d (2232464)



Bond precision: C-C = 0.0121 A Wavelength=1.54184

Cell: a=8.7505(2) b=13.5024(4) c=19.8631(4)
alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	2346.88(10)	2346.88(10)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C25 H19 Br N2 O3 S	C25 H19 Br N2 O3 S
Sum formula	C25 H19 Br N2 O3 S	C25 H19 Br N2 O3 S
Mr	507.38	507.39
Dx,g cm-3	1.436	1.436
Z	4	4
Mu (mm-1)	3.458	3.458
F000	1032.0	1032.0
F000'	1033.15	
h,k,lmax	11,17,25	11,17,25
Nref	5092[2890]	4965
Tmin,Tmax	0.693,0.708	0.557,1.000
Tmin'	0.567	

Correction method= # Reported T Limits: Tmin=0.557 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.72/0.98 Theta(max)= 79.254

R(reflections)= 0.0811(4648) wR2(reflections)= 0.2264(4965)

S = 1.064 Npar= 299

Computational Studies

All DFT calculations were performed with Gaussian 09[4] software package. Geometry optimizations of all the stationary points were carried out using the PBE0[5] functional and def2-SVP[6] with the corresponding pseudo-potential.[7] The PBE0 was chosen due to its excellent performance on 5d transition metal complexes.[8] Frequency calculations at the same level were performed to validate each structure as either a minimum or a transition state. On the basis of the optimized structures, single-point energy refinements were performed at the BMK-D3(BJ)/def2-TZVPP level[9] under SMD[10] model to account for solvation effects of DCE. The BMK functional was chosen because of its high accuracy in computing the kinetics of gold-catalyzed reactions.[11] Pruned integration grids with 99 radial shells and 590 angular points per shell were used. All discussed energy differences were based on Gibbs energies at 298 K (standard states are the hypothetical states at 1 mol/L) unless otherwise specified. Natural bond analysis was performed with the NBO 3.1 built in Gaussian.[12] 3D structure was prepared with CYLview.[13]

Conformational research was performed for the transition states related to the stereoselectivity of this reaction through a set of workflows. First, Conformer-Rotamer Ensemble Sampling Tool (CREST)[14] based on GFN0-xTB level was used to generate hundreds of low-energy structures of transition states related to different enantiomers and diastereomers. The Au-C bond length and the forming C-C bond were selected as constraints with force constant of 0.5. Then the low energy candidate structures were included in the subsequent constrained geometry optimization step at GFN2-xTB level. Isostat tool in Molclus package[15] was used to sort and distinguish different structures with energy threshold of 1 kcal/mol and geometry threshold of 1 Å. At last, the conformers within an energy window of 3 kcal/mol (~10 candidate structures) were optimized without constrains using Gaussian 09 software package at IEFPCM(DCE)/PBE0/def2-SVP level to account for solvation effect, then single-point energy refinements were performed at SMD(DCE)/BMK-D3(BJ)/def2-TZVPP to find the most stable conformer of the

corresponding transition state. Quasiharmonic corrections were applied with Grimme's quasi-RRHO correction[16] to obtain the thermal correction to Gibbs free energy at 298.15 K and 1 M using Shermo software package.[17] Figure S9 shows selected structures of the stereoselective transition states with different hydrogen bonding modes and conformations.

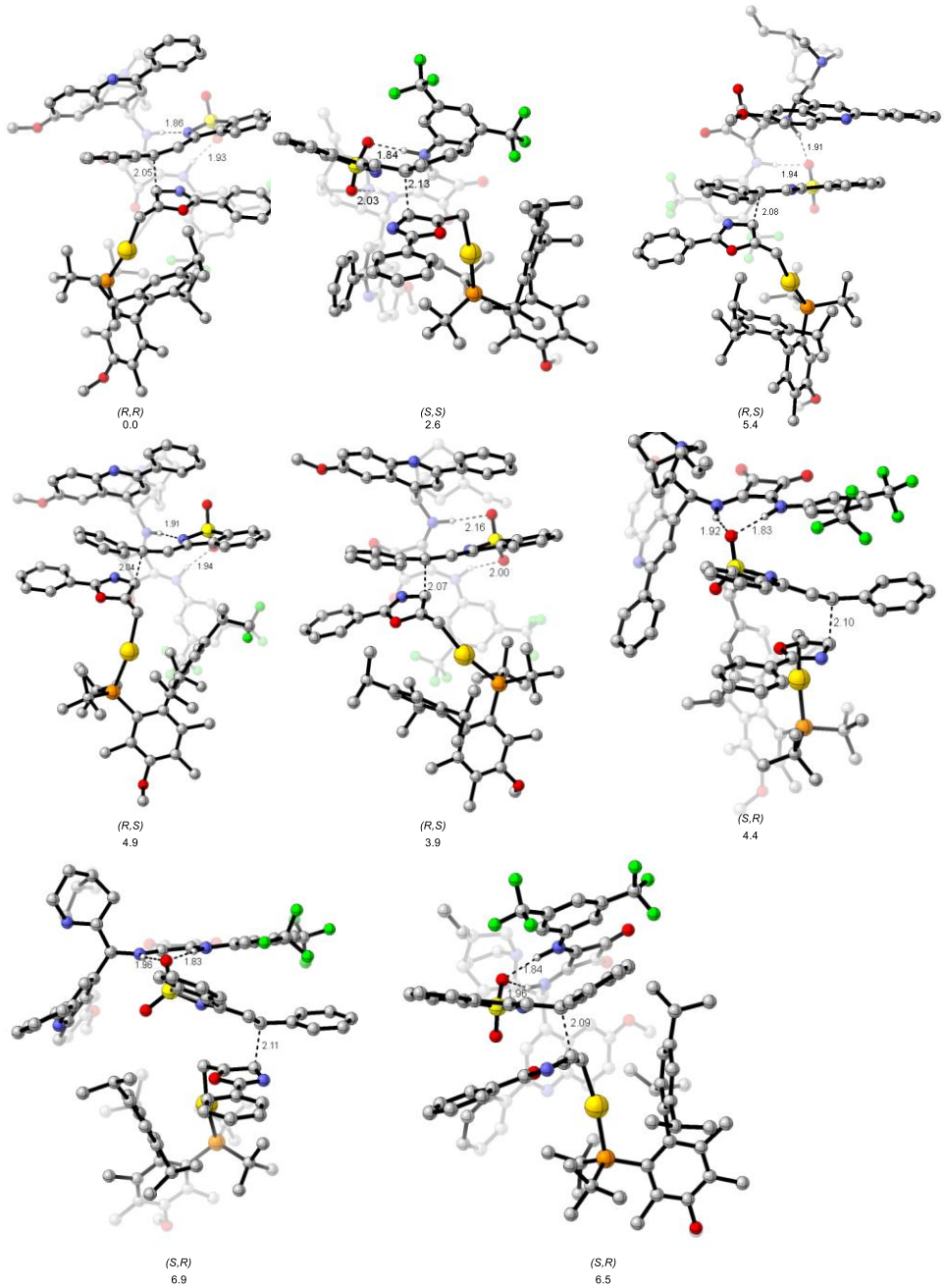


Figure S9. The stereoselective transition states with different hydrogen bonding modes and conformations. Computed at SMD(DCE)/BMK-D3(BJ)/def2-TZVPP// IEFPCM(DCE)/PBE0/def2-SVP.

The activation free energies of the (4+2) annulation of alkylgold species using PMe_3 and $Me_3(OMe)$*t*BuXPhos as ligand and **4n** as catalyst were studied and are shown in Figure S10. According to Figure 1b. The rate-determining step of this (4+2) annulation of alkylgold species is the first nucleophilic addition. Here, we computed the activation free energy of this step using the real catalyst. **2a** first forms a hydrogen-bonding complex **COM1** with **4n**, which is exergonic by 3.2 kcal/mol. Then the alkylgold species undergoes a nucleophilic addition at **COM1** via **TS1-*RR***. DFT calculations found that, using PMe_3 as ligand, the overall activation free energy of this step is 6.5 kcal/mol, while using $Me_3(OMe)$*t*BuXPhos as ligand, the overall activation free energy of this step is 5.1 kcal/mol. These results indicate that if the alkylgold species using PMe_3 and $Me_3(OMe)$*t*BuXPhos as ligands could be obtained, the (4+2) annulations of the alkylgold species would occur fast at room temperature.

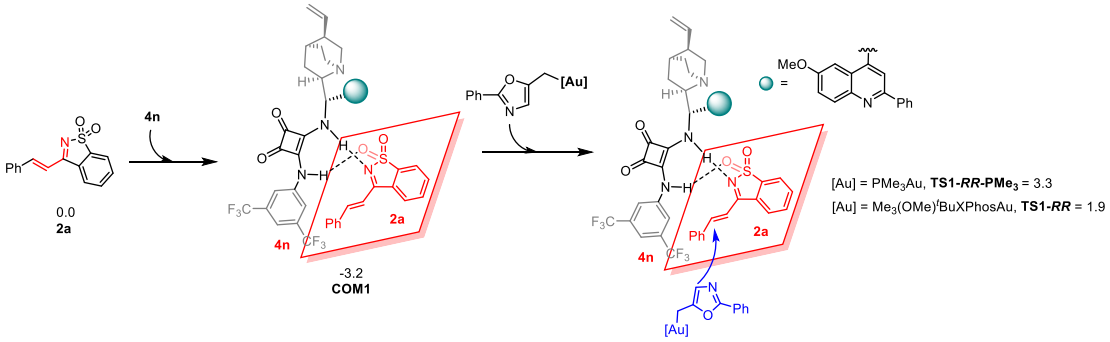


Figure S10. The activation free energies of (4+2) annulation of alkylgold species using PMe_3 and $Me_3(OMe)$*t*BuXPhos as ligands. Computed at SMD(DCE)/BMK-D3(BJ)/def2-TZVPP//IEFPCM(DCE)/PBE0/def2-SVP.

Table S3. Computed energies for the stationary points.

Thermal corrections to Gibbs energies (TCGs), single-point energies (SPEs) in gas phase and solvent.

	Imaginary Frequencies (cm^{-1})	**SPEs (in gas phase)[a] (hartree)**	**TCGs (in gas phase)[b] (hartree)**	**SPEs (under SMD(DCE) model)[c] (hartree)**
A-PMe_3	None	-1111.657258	0.230019	-1112.382995
B-PMe_3	None	-1111.275221	0.220509	-1111.936946

C-PMe$_3$	None	-1111.302541	0.221498	-1111.959881
Int1-PMe$_3$	None	-1111.302541	0.221498	-1111.959881
Int2-PMe$_3$	None	-1111.688272	0.232089	-1112.404857
TS1-PMe$_3$	-117.48	-1111.642221	0.227972	-1112.368394
4n	None	-2506.465985	0.560788	-2510.73746
4n-Proton	None	-2506.856575	0.575545	-2511.19789
Int2'-PMe$_3$	None	-1111.707727	0.234352	-1112.421998
A-XPhos	None	-2354.205154	0.867146	-2357.022709
C-XPhos	None	-2353.836201	0.858443	-2356.590592
Int2-XPhos	None	-2354.242642	0.870303	-2357.048117
Int2'-XPhos	None	-2354.255289	0.874591	-2357.061497
TS2-PMe$_3$	-974.92	-3618.165705	0.815334	-3623.145005
TS3-PMe$_3$	-70.15	-1627.125955	0.384853	-1628.716703
TS2-XPhos	-1095.58	-4860.710998	1.452465	-4867.786636
TS3-XPhos	-70.38	-2869.660228	1.023252	-2873.342983
TS4-PMe$_3$	-36.01	-1627.166412	0.38726	-1628.747138
5	None	-515.46575	0.132903	-516.328239
QN-SQA	None	-930.469777	0.21627	-932.052451
1a	None	-515.429275	0.128606	-516.300868
2a	None	-1179.79213	0.183533	-1181.341017
3a	None	-1695.318964	0.343605	-1697.729972
Int1A	None	-3221.604642	0.674444	-3225.3971
Int2A	None	-3221.629813	0.67182	-3225.412007
Int3A	None	-3221.609041	0.676067	-3225.414139
TS1A	-361.10	-3221.590038	0.670221	-3225.375901
TS2A	-332.89	-3221.590862	0.672528	-3225.374163
TS3A	-498.98	-3221.572582	0.669204	-3225.357934
TS4A	-77.81	-3221.60179	0.67843	-3225.392838
TS5A	-114.73	-3221.607444	0.676913	-3225.4092

[a] Computed at PBE0/def2-SVP

[b] Computed at PBE0/def2-SVP

[c] Computed at SMD(DCE)/BMK-D3(BJ)/def2-TZVPP

Thermal corrections to Gibbs energies (TCGs), single-point energies (SPEs).

	Imaginary Frequencies (cm^{-1})	**SPEs (under IEFPCM(DCE) model)[a] (hartree)**	**TCGs (hartree)[b]**	**SPEs (under SMD(DCE) model)[c] (hartree)**
4n	None	-2506.491094	0.575236	-2510.738062
2a	None	-1179.807745	0.185959	-1181.341132
COM1	None	-3686.323289	0.789304	-3692.109407
C	None	-1111.315191	0.22561	-1111.960089

C-XPhos	None	-2353.84968	0.869081	-2356.59047
TS1-*RR*-PMe$_3$	-363.88	-4797.626958	1.044429	-4804.085679
TS1-*RR*	-361.77	-6040.163471	1.689846	-6048.720234
TS1-*SS*	-351.26	-6040.17044	1.690456	-6048.716726
TS1-*RS*	-379.93	-6040.160713	1.689622	-6048.713831
TS1-*SR*	-351.72	-6040.160948	1.689648	-6048.712976

[a] Computed at IEFPCM(DCE)/PBE0/def2-SVP

[b] Computed at IEFPCM(DCE)/PBE0/def2-SVP after Grimme's quasi-RRHO correction

[c] Computed at SMD(DCE)/BMK-D3(BJ)/def2-TZVPP

Cartesian coordinates for the stationary points

1a

C	0.405513	0.828540	0.009247
C	2.779687	0.517173	-0.497886
C	3.714565	-0.453949	0.065461
O	0.592045	1.961515	0.414385
H	3.102910	0.778655	-1.522482
N	1.413515	0.054727	-0.484136
C	4.491419	-1.269760	0.508611
C	-0.960258	0.207388	0.004250
C	-1.183586	-1.174199	-0.025589
C	-2.055053	1.075994	0.067747
C	-2.482938	-1.677224	-0.014345
H	-0.344022	-1.874848	-0.023342
C	-3.352542	0.573917	0.070557
H	-1.856391	2.148610	0.118024
C	-3.568984	-0.803919	0.026647
H	-2.647487	-2.757281	-0.028340
H	-4.201862	1.260197	0.111551
H	-4.587800	-1.199210	0.033075
H	1.203123	-0.842833	-0.897337
H	2.791182	1.454359	0.081911
H	5.182445	-1.986636	0.912615

2a

S	-2.509442	-1.569014	0.000092
N	-0.835483	-1.342168	0.000027
C	-0.534545	-0.084365	0.000014
O	-2.906746	-2.171193	1.259000
O	-2.906824	-2.171393	-1.258703
C	-2.888333	0.179518	-0.000025
C	-4.117236	0.814193	-0.000033

C	-1.680226	0.870616	-0.000076
C	-4.117027	2.212478	-0.000108
H	-5.049476	0.245495	-0.000011
C	-1.686728	2.264076	-0.000140
C	-2.916305	2.926481	-0.000156
H	-5.066758	2.752517	-0.000130
H	-0.757043	2.836767	-0.000152
H	-2.939460	4.018533	-0.000187
C	0.843128	0.381064	0.000043
H	1.000260	1.461500	0.000252
C	1.886414	-0.476969	-0.000141
H	1.635002	-1.543593	-0.000273
C	3.305536	-0.149893	-0.000100
C	4.237033	-1.202897	-0.000310
C	3.792554	1.170622	0.000248
C	5.605436	-0.949876	-0.000236
H	3.872075	-2.233411	-0.000541
C	5.157816	1.423059	0.000325
H	3.094140	2.010270	0.000430
C	6.069818	0.364105	0.000080
H	6.312837	-1.782348	-0.000426
H	5.518926	2.454234	0.000551
H	7.143498	0.566833	0.000133

3a

C	2.605276	-0.788951	-0.558331
C	0.403590	-0.116949	0.398244
C	-0.534600	-1.282567	0.119926
O	2.237458	-0.756872	-1.719635
H	0.121944	0.262983	1.397054
N	1.785507	-0.513457	0.495465
C	-0.168029	-2.567986	0.101965
S	-3.182731	-1.841138	0.479566
N	-1.868271	-0.871995	-0.040420
C	-2.219148	0.441827	-0.371673
O	-3.108013	-2.036620	1.916991
O	-3.327101	-3.004720	-0.378677
C	-4.332902	-0.570346	0.054670
C	-5.715439	-0.675461	0.138823
C	-3.677914	0.585885	-0.367433
C	-6.467640	0.440095	-0.219389
H	-6.190190	-1.601203	0.470560
C	-4.446525	1.697414	-0.723566

C	-5.833492	1.613974	-0.645471
H	-7.557807	0.397791	-0.170195
H	-3.966681	2.617115	-1.064007
H	-6.438531	2.479371	-0.925546
C	-1.289993	1.373790	-0.645522
H	-1.605484	2.376993	-0.935465
C	0.175903	1.064280	-0.582677
H	0.519613	0.721033	-1.572628
C	1.010023	2.263510	-0.185410
C	2.177296	2.580299	-0.888497
C	0.646259	3.063376	0.905529
C	2.962111	3.669567	-0.511010
H	2.471797	1.958992	-1.738593
C	1.429819	4.151242	1.285640
H	-0.269301	2.835666	1.460679
C	2.591646	4.457747	0.577185
H	3.869574	3.903509	-1.073403
H	1.129174	4.766367	2.137728
H	3.205386	5.312619	0.871894
C	4.018374	-1.147904	-0.197956
C	4.644442	-0.733868	0.983940
C	4.741814	-1.901412	-1.128734
C	5.967330	-1.088977	1.240025
H	4.116645	-0.096872	1.699070
C	6.059523	-2.263683	-0.868059
H	4.243548	-2.188775	-2.057050
C	6.673869	-1.860189	0.318226
H	6.451553	-0.752948	2.160015
H	6.614054	-2.861244	-1.595652
H	7.710370	-2.140697	0.521353
H	0.869864	-2.835855	0.292698
H	-0.888449	-3.363325	-0.092750
H	2.147652	-0.677717	1.423773

A-PMe_3

C	1.986608	-0.552727	-0.543148
C	0.750346	-2.631272	-0.834777
C	-0.409617	-2.549248	0.078997
O	1.019166	0.082096	-0.951933
H	0.437680	-2.274498	-1.828812
N	1.913172	-1.908353	-0.404986
C	-1.352788	-2.689300	0.863737
C	3.276022	0.090705	-0.172874

C	4.485581	-0.614335	-0.099353
C	3.268193	1.467988	0.079667
C	5.661680	0.046451	0.243379
H	4.532221	-1.678562	-0.345164
C	4.442683	2.125649	0.427648
H	2.324667	2.010303	-0.003910
C	5.640286	1.414663	0.512830
H	6.602061	-0.506893	0.289429
H	4.428734	3.198890	0.629837
H	6.564565	1.931165	0.781957
H	2.636197	-2.402364	0.101187
H	1.000700	-3.699146	-0.935828
H	-2.081335	-3.054521	1.574992
Au	-1.518770	-0.572626	0.202486
P	-2.144646	1.632387	-0.136945
C	-3.937407	1.931496	-0.163305
H	-4.140901	2.994966	-0.361379
H	-4.404449	1.320594	-0.948871
H	-4.377175	1.652876	0.804947
C	-1.490858	2.217511	-1.727667
H	-1.676398	3.295826	-1.846513
H	-0.411797	2.006169	-1.760665
H	-1.977281	1.671276	-2.548598
C	-1.467218	2.751618	1.125980
H	-0.371919	2.658352	1.142668
H	-1.741737	3.793215	0.899075
H	-1.857909	2.480508	2.117087

B-PMe$_3$

C	3.343882	0.461320	-0.000280
C	1.372495	1.384901	0.000407
C	1.213201	-0.122108	-0.001079
O	2.520049	-0.616598	-0.001562
H	0.902054	1.852080	0.883888
N	2.803973	1.614601	0.000787
C	0.147081	-0.926302	-0.002071
C	4.785216	0.179731	-0.000026
C	5.692178	1.247564	-0.001104
C	5.260841	-1.136440	0.001565
C	7.059785	0.998052	-0.000602
H	5.295199	2.264832	-0.002329
C	6.632561	-1.380442	0.002192
H	4.545423	-1.960513	0.002414

C	7.532988	-0.316149	0.001092
H	7.764899	1.832953	-0.001522
H	7.000823	-2.409276	0.003569
H	8.608702	-0.509810	0.001557
H	0.902200	1.853807	-0.882260
H	0.381440	-1.999112	-0.003520
Au	-1.798670	-0.342067	0.000038
P	-4.045963	0.275979	0.001136
C	-5.187218	-0.989840	-0.663999
H	-6.231663	-0.641974	-0.641436
H	-4.903240	-1.226714	-1.699580
H	-5.096770	-1.909729	-0.068263
C	-4.440232	1.766025	-0.984349
H	-5.514750	2.003082	-0.943298
H	-3.863918	2.619631	-0.599031
H	-4.142380	1.599650	-2.029702
C	-4.748435	0.657857	1.646772
H	-4.183173	1.484931	2.100265
H	-5.811289	0.936812	1.576457
H	-4.643458	-0.221460	2.298655

C-PMe$_3$

C	-2.943748	-0.858229	0.258862
C	-1.707357	-2.474746	0.841475
C	-1.041074	-1.816432	-0.160577
O	-1.844298	-0.780209	-0.528093
H	-1.384608	-3.359396	1.387411
N	-2.904028	-1.852159	1.092260
C	0.258665	-1.974060	-0.825272
H	0.135413	-1.931806	-1.920506
H	0.671004	-2.962734	-0.572908
Au	1.636728	-0.501857	-0.271411
P	3.156628	1.152514	0.361836
C	2.836841	1.889629	2.004333
H	3.577157	2.667350	2.248240
H	1.828598	2.328442	2.014569
H	2.870454	1.100581	2.769516
C	3.223446	2.599682	-0.754344
H	3.952691	3.346373	-0.403516
H	3.499750	2.267078	-1.765420
H	2.226808	3.061211	-0.808949
C	4.899395	0.607550	0.465298
H	5.219212	0.223480	-0.514232

H	5.562160	1.433158	0.767869
H	4.981025	-0.211358	1.194621
C	-3.997534	0.131295	0.086054
C	-5.135927	0.075581	0.905627
C	-3.899472	1.141068	-0.882699
C	-6.151367	1.013089	0.757116
H	-5.198811	-0.717346	1.653757
C	-4.921164	2.075922	-1.025668
H	-3.015907	1.183150	-1.522557
C	-6.049589	2.017404	-0.208152
H	-7.033681	0.960764	1.400137
H	-4.836107	2.857945	-1.784599
H	-6.850174	2.752362	-0.322855

A-XPhos

Au	0.533920	0.690596	-0.901062
P	-0.008101	-1.607853	-0.917759
C	1.463248	-2.470360	-0.042214
C	-0.181975	-2.187488	-2.761888
C	1.592461	-1.820757	1.336342
H	0.719753	-2.034376	1.970507
H	1.729214	-0.731926	1.273129
H	2.479829	-2.236334	1.840374
C	2.718271	-2.135729	-0.858247
H	2.736757	-2.630716	-1.838377
H	3.599963	-2.487083	-0.298437
H	2.834894	-1.052416	-1.011326
C	1.385082	-3.983492	0.164236
H	0.578760	-4.264683	0.852540
H	2.331232	-4.304168	0.629735
H	1.276525	-4.553178	-0.766485
C	0.570529	-1.160832	-3.623384
H	0.143001	-0.152260	-3.534542
H	0.495316	-1.463203	-4.680383
H	1.638532	-1.103479	-3.368170
C	0.395152	-3.566933	-3.107696
H	-0.138980	-4.404949	-2.644999
H	1.463410	-3.661334	-2.875871
H	0.293705	-3.702373	-4.196471
C	-1.662875	-2.159179	-3.143337
H	-1.753669	-2.377318	-4.219701
H	-2.114041	-1.174786	-2.969327
H	-2.254469	-2.907873	-2.600704

C	-1.603950	-1.790305	0.026734
C	-2.257482	-0.637388	0.570432
C	-2.190291	-3.063213	0.211953
C	-3.473646	-0.794748	1.282131
C	-3.370659	-3.180854	0.960928
C	-4.036053	-2.070934	1.478340
C	-1.711369	-4.341987	-0.403160
H	-0.820974	-4.201003	-1.012827
H	-2.506132	-4.774319	-1.030339
H	-1.480022	-5.101890	0.357187
C	-1.839593	0.814184	0.445460
C	-1.198805	1.457677	1.547071
C	-2.456426	1.629462	-0.550788
C	-1.226162	2.852940	1.636016
C	-2.444232	3.019992	-0.408844
C	-1.865740	3.659008	0.692016
H	-0.755251	3.333347	2.497672
H	-2.948359	3.623744	-1.168603
C	-0.551932	0.679753	2.680790
H	-0.440658	-0.356870	2.333455
C	-1.970091	5.159266	0.888233
H	-1.390380	5.400057	1.795457
C	-3.196880	1.043633	-1.742007
H	-3.097396	-0.050444	-1.680965
C	0.836037	1.218261	3.038186
H	1.345163	0.522658	3.723030
H	0.771407	2.184997	3.561606
H	1.484415	1.367584	2.161422
C	-1.434192	0.641783	3.932600
H	-1.645353	1.658010	4.301927
H	-0.921510	0.095289	4.739302
H	-2.393620	0.141557	3.747908
C	-3.421091	5.573996	1.145148
H	-3.482453	6.650250	1.367687
H	-3.850423	5.025892	1.996980
H	-4.055924	5.379968	0.265793
C	-1.364370	5.953857	-0.269114
H	-0.296043	5.725581	-0.409426
H	-1.443088	7.034521	-0.076350
H	-1.884970	5.754000	-1.219415
C	-2.583797	1.508355	-3.064912
H	-1.503232	1.300958	-3.108629
H	-2.716761	2.591367	-3.213379
H	-3.064373	1.002361	-3.916497

C	-4.694708	1.357897	-1.712809
H	-5.171523	0.991984	-0.793732
H	-5.201088	0.881878	-2.566469
H	-4.882199	2.440967	-1.779977
C	-4.256608	0.365889	1.842932
H	-4.502116	0.195316	2.901944
H	-5.222866	0.467336	1.322769
H	-3.740280	1.327703	1.771111
C	-5.346307	-2.248852	2.183728
H	-5.715223	-3.274432	2.067267
H	-6.109472	-1.566308	1.781532
H	-5.262791	-2.026250	3.260426
O	-3.910479	-4.425378	1.097141
C	-3.611285	-5.098435	2.301908
H	-4.080959	-6.088905	2.243609
H	-4.012064	-4.564058	3.180231
H	-2.522686	-5.224795	2.438376
C	4.386540	1.184829	0.271353
C	3.462312	2.223540	-1.730531
C	2.061690	2.339067	-1.288392
O	3.712157	1.923032	0.967001
H	3.893482	3.229158	-1.561362
N	4.244589	1.199077	-1.091752
C	0.958835	2.809436	-0.975957
C	5.374091	0.221842	0.849744
C	6.089990	-0.722780	0.101293
C	5.583508	0.297814	2.232191
C	7.000639	-1.571314	0.725761
H	5.944338	-0.825041	-0.977644
C	6.493762	-0.549469	2.855337
H	5.018870	1.042211	2.797036
C	7.204488	-1.484865	2.103033
H	7.555768	-2.302909	0.134384
H	6.654802	-0.477650	3.933384
H	7.922919	-2.148359	2.590257
H	4.922446	0.719142	-1.666625
H	3.474693	2.042236	-2.815733
H	0.131747	3.446114	-0.679570

C-XPhos

C	5.364902	0.326766	-0.679355
C	4.213781	1.326688	-2.148315
C	3.478632	1.361457	-0.989107

O	4.229573	0.718558	-0.051782
H	3.947906	1.742342	-3.118517
N	5.396840	0.666258	-1.931442
C	2.154086	1.861560	-0.609300
H	2.213073	2.428722	0.334227
H	1.780916	2.539818	-1.391057
Au	0.784453	0.301631	-0.319964
P	-0.500498	-1.685298	-0.066926
C	-0.153334	-2.627826	-1.711269
C	0.225446	-2.669716	1.450561
C	6.372470	-0.393010	0.085265
C	6.196430	-0.670213	1.449453
C	7.546776	-0.821543	-0.554301
C	7.176289	-1.362600	2.155914
H	5.285790	-0.333881	1.949071
C	8.519870	-1.512536	0.157909
H	7.670847	-0.597114	-1.615731
C	8.340384	-1.787060	1.515697
H	7.030004	-1.571503	3.218859
H	9.430403	-1.840953	-0.349892
H	9.107855	-2.329743	2.073150
C	-0.710620	-1.741449	-2.825661
H	-1.807923	-1.673073	-2.780814
H	-0.291007	-0.727632	-2.785778
H	-0.442577	-2.180921	-3.800890
C	1.374251	-2.691629	-1.863488
H	1.851856	-3.350797	-1.125242
H	1.611286	-3.095820	-2.861544
H	1.838555	-1.696594	-1.782052
C	-0.730731	-4.028766	-1.915520
H	-1.826248	-4.018893	-1.971241
H	-0.364202	-4.403860	-2.885854
H	-0.418953	-4.753460	-1.153806
C	1.580306	-2.017974	1.773143
H	1.478749	-0.955286	2.031253
H	2.027282	-2.538729	2.636810
H	2.290853	-2.082123	0.936394
C	0.501474	-4.167111	1.261592
H	-0.396940	-4.783143	1.135045
H	1.186531	-4.372253	0.428791
H	0.998194	-4.530343	2.176346
C	-0.703858	-2.478823	2.650260
H	-0.224658	-2.912547	3.543836
H	-0.885852	-1.417227	2.858967

H	-1.675624	-2.972603	2.518229
C	-2.350616	-1.400457	0.142658
C	-2.871573	-0.064716	0.189330
C	-3.256473	-2.481345	0.258763
C	-4.265403	0.141664	0.352625
C	-4.632887	-2.233465	0.359963
C	-5.154574	-0.945086	0.433445
C	-2.875852	-3.925376	0.381392
H	-1.799002	-4.065996	0.333298
H	-3.245828	-4.329209	1.336659
H	-3.332416	-4.542004	-0.406253
C	-2.082135	1.222969	0.133611
C	-1.968288	1.939988	-1.083141
C	-1.690532	1.858067	1.338714
C	-1.474027	3.247876	-1.062346
C	-1.199494	3.165365	1.299626
C	-1.089779	3.889378	0.113063
H	-1.392215	3.796846	-2.004393
H	-0.905992	3.640359	2.239942
C	-2.398520	1.359053	-2.421171
H	-2.484048	0.271155	-2.287605
C	-0.604883	5.325676	0.097573
H	-0.526456	5.621310	-0.963104
C	-1.813506	1.189827	2.698777
H	-2.129592	0.149755	2.525892
C	-1.367943	1.618017	-3.522788
H	-1.589684	1.004739	-4.410174
H	-1.378816	2.669930	-3.849215
H	-0.346527	1.386956	-3.185724
C	-3.770981	1.871882	-2.866757
H	-3.770686	2.970209	-2.958025
H	-4.035092	1.454585	-3.851769
H	-4.565026	1.593783	-2.161620
C	-1.620759	6.259205	0.759978
H	-1.293381	7.308837	0.690436
H	-2.610108	6.177498	0.284752
H	-1.743233	6.018656	1.828483
C	0.781677	5.483019	0.721467
H	1.518993	4.830717	0.230992
H	1.131371	6.523734	0.633302
H	0.772171	5.229917	1.793923
C	-0.474085	1.162752	3.438698
H	0.325134	0.743092	2.810137
H	-0.158064	2.174939	3.736095

H	-0.547696	0.562001	4.359244
C	-2.884517	1.846832	3.573651
H	-3.871762	1.836503	3.091910
H	-2.972720	1.320323	4.537357
H	-2.631115	2.896964	3.790735
C	-4.879928	1.512985	0.478996
H	-5.695204	1.648550	-0.248764
H	-5.339245	1.638885	1.473319
H	-4.160633	2.325414	0.338709
C	-6.625830	-0.742027	0.642025
H	-7.124546	-1.695844	0.851352
H	-6.816199	-0.066337	1.489622
H	-7.103735	-0.280845	-0.238325
O	-5.469513	-3.313006	0.472459
C	-6.052798	-3.745346	-0.733478
H	-6.650054	-4.638984	-0.506122
H	-6.714921	-2.975953	-1.168923
H	-5.289566	-4.008221	-1.487899

Int1-PMe$_3$

C	-3.403446	0.422190	0.000841
C	-1.372643	1.492960	-0.000883
C	-1.201919	-0.009241	0.003941
O	-2.542778	-0.542153	0.005728
H	-0.937795	1.967252	-0.895869
N	-2.825441	1.606991	-0.003235
C	-0.147146	-0.809749	0.006646
C	-4.824378	0.138028	-0.000312
C	-5.776945	1.171901	0.003839
C	-5.240782	-1.204148	-0.005863
C	-7.129616	0.862185	0.002077
H	-5.476821	2.222837	0.009482
C	-6.596909	-1.503426	-0.007801
H	-4.494535	-2.000308	-0.008952
C	-7.538872	-0.473747	-0.003889
H	-7.871182	1.663298	0.005604
H	-6.923019	-2.545323	-0.012418
H	-8.604987	-0.712672	-0.005352
H	-3.331927	2.483155	-0.009288
H	-0.940281	1.972841	0.892374
H	-0.396877	-1.879170	0.010703
Au	1.829732	-0.285188	0.002571
P	4.117187	0.189292	-0.003600

C	5.140496	-1.210198	0.564367
H	6.209641	-0.949446	0.541208
H	4.855499	-1.482899	1.590723
H	4.965622	-2.080810	-0.084042
C	4.614452	1.581862	1.065654
H	5.702794	1.740356	1.020787
H	4.102315	2.499048	0.741236
H	4.322061	1.371223	2.104475
C	4.789784	0.611163	-1.646285
H	4.286367	1.508777	-2.033122
H	5.872856	0.798956	-1.589253
H	4.601492	-0.217012	-2.344587

Int1A

C	-4.366180	-0.166357	-1.310119
C	-2.683396	0.616919	-0.166182
C	-2.948460	-0.792141	0.235152
O	-3.987696	-1.223341	-0.464573
H	-1.645822	0.688439	-0.576035
N	-3.668548	0.881103	-1.177392
C	-2.278624	-1.623233	1.132479
H	-2.820895	-2.516736	1.460992
H	-1.690243	-1.108054	1.901261
Au	-0.714951	-2.333844	-0.210949
P	0.983525	-3.187608	-1.534762
C	0.358530	-3.756561	-3.151633
H	1.181438	-4.178841	-3.748818
H	-0.418197	-4.520922	-3.007998
H	-0.080009	-2.905471	-3.692119
C	1.807614	-4.635277	-0.799850
H	2.546513	-5.043361	-1.506866
H	2.333263	-4.347665	0.125956
H	1.063644	-5.409716	-0.564624
C	-0.826720	-0.737643	5.098152
C	-0.209956	1.252196	4.190318
C	0.055937	-1.442017	4.284770
H	-1.450490	-1.274152	5.822923
C	0.707107	0.646905	3.328417
C	0.841001	-0.742710	3.360032
H	0.127462	-2.530244	4.367142
N	-0.974308	0.585888	5.051817
C	1.711375	-1.514640	2.405651
H	2.239355	-2.323665	2.931343

N	2.675250	-0.717150	1.694335
C	3.852642	-1.213042	1.311824
C	4.931830	-0.693235	0.571912
C	4.445967	-2.555260	1.351791
C	5.692645	-1.971949	0.700499
O	6.777550	-2.390890	0.377476
O	4.052593	-3.650562	1.702988
N	5.070302	0.528443	0.035295
C	6.154877	1.092967	-0.639330
C	7.342722	0.398338	-0.905451
C	6.027487	2.428588	-1.053548
C	8.374823	1.043933	-1.581853
H	7.455564	-0.639843	-0.581786
C	7.067889	3.056772	-1.728825
H	5.104664	2.969708	-0.827659
C	8.250313	2.368628	-2.000094
H	9.297010	0.492804	-1.783370
H	6.953235	4.097771	-2.041776
H	9.068583	2.861784	-2.529462
H	-0.338218	2.340462	4.163041
H	1.276323	1.266520	2.632615
H	1.023883	-2.026733	1.695101
S	1.434404	1.933826	-0.679140
N	-0.010065	1.713587	-0.029463
C	-0.727488	2.891404	0.025215
O	1.677356	1.144610	-1.891320
O	2.513999	1.763944	0.350284
C	1.253238	3.665865	-1.025537
C	2.133248	4.539611	-1.648298
C	-0.000453	4.049295	-0.550897
C	1.731646	5.867949	-1.780523
H	3.098763	4.195995	-2.026479
C	-0.389580	5.383587	-0.686812
C	0.483148	6.281357	-1.298620
H	2.393437	6.590597	-2.263404
H	-1.362513	5.720255	-0.322462
H	0.186503	7.327268	-1.408783
C	-1.994565	2.925399	0.512331
H	-2.567148	3.852877	0.511705
C	-2.624680	1.663382	1.011319
H	-1.915519	1.197132	1.717826
C	-3.949213	1.847304	1.711507
C	-4.106752	1.439321	3.041984
C	-5.038505	2.443362	1.059858

C	-5.324659	1.610052	3.700370
H	-3.260389	1.007241	3.584083
C	-6.255442	2.611885	1.717091
H	-4.926550	2.774302	0.024608
C	-6.403769	2.192436	3.039140
H	-5.423734	1.292578	4.741394
H	-7.094353	3.077239	1.193173
H	-7.357677	2.327475	3.555175
H	4.230739	1.120317	0.095818
H	2.413146	0.204217	1.322156
C	2.308581	-2.011435	-1.921906
H	2.874987	-1.799928	-1.004694
H	2.989201	-2.447617	-2.669079
H	1.901502	-1.051830	-2.276612
C	-5.489540	-0.427484	-2.202484
C	-5.880284	0.573039	-3.104492
C	-6.176645	-1.647931	-2.171735
C	-6.949308	0.351136	-3.963517
H	-5.328795	1.515335	-3.116495
C	-7.246976	-1.861751	-3.036161
H	-5.871343	-2.423566	-1.467522
C	-7.634503	-0.865583	-3.931155
H	-7.251845	1.131231	-4.665826
H	-7.783176	-2.813096	-3.009380
H	-8.474921	-1.036965	-4.608135

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C	2.771983	0.789031	-0.380082
C	1.304513	2.229696	-1.101161
C	0.877170	1.723583	0.251284
O	1.811546	0.892289	0.662142
H	1.487120	3.320247	-1.056560
N	2.514040	1.511928	-1.385920
C	-0.239883	2.022226	1.020223
C	3.884609	-0.111226	-0.130695
C	4.864709	-0.255125	-1.125785
C	3.992305	-0.820763	1.074169
C	5.940670	-1.106277	-0.912446
H	4.766442	0.309182	-2.055324
C	5.075022	-1.670167	1.277773
H	3.233388	-0.702617	1.849282
C	6.046816	-1.813626	0.287656
H	6.705189	-1.219057	-1.684043

H	5.163647	-2.221601	2.216145
H	6.896626	-2.480234	0.452347
H	0.536030	2.083091	-1.877852
H	-0.782750	2.932877	0.743821
Au	-1.549647	0.442382	0.274486
P	-3.109887	-1.152259	-0.341600
C	-4.302165	-1.493860	0.989409
H	-5.032048	-2.250494	0.662982
H	-3.771956	-1.862874	1.879059
H	-4.834364	-0.570205	1.258495
C	-2.377172	-2.761271	-0.771607
H	-3.167682	-3.480002	-1.036982
H	-1.693449	-2.644271	-1.624443
H	-1.806531	-3.150564	0.083639
C	-4.107424	-0.662242	-1.782107
H	-3.454130	-0.504208	-2.652068
H	-4.843848	-1.445100	-2.020339
H	-4.635973	0.277311	-1.566248
H	-0.172872	1.802529	2.092194

Int2A

C	1.533588	-0.011442	-1.186594
C	2.097816	1.201038	0.551552
C	0.997862	0.166893	0.972043
O	0.599885	-0.395761	-0.287656
H	2.977353	1.023790	1.189962
N	2.405492	0.839701	-0.816377
C	1.552620	-0.910710	1.885384
H	0.743016	-1.597695	2.171148
H	1.897079	-0.411302	2.809084
Au	3.117126	-2.014820	1.056541
P	4.834032	-3.233715	0.055162
C	5.551460	-2.386219	-1.396432
H	6.345931	-2.988855	-1.863240
H	4.755646	-2.192161	-2.130622
H	5.962020	-1.415638	-1.082422
C	4.338713	-4.868924	-0.595636
H	5.183782	-5.381010	-1.081116
H	3.959468	-5.490843	0.228100
H	3.526135	-4.735618	-1.324618
C	0.461592	3.331831	-3.645571
C	-0.871075	4.016812	-1.936376
C	-0.373187	2.256417	-3.937250

H	1.374674	3.489169	-4.231218
C	-1.770793	2.971957	-2.141400
C	-1.521891	2.056133	-3.166657
H	-0.114208	1.564786	-4.743157
N	0.231024	4.198650	-2.661422
C	-2.436026	0.892374	-3.447053
H	-3.192565	1.171294	-4.200277
N	-3.135469	0.428017	-2.272436
C	-4.414868	0.045197	-2.308714
C	-5.279537	-0.584321	-1.400611
C	-5.442287	0.085585	-3.367213
C	-6.413252	-0.540970	-2.368154
O	-7.577223	-0.858261	-2.375683
O	-5.468757	0.471887	-4.512007
N	-5.032146	-0.995938	-0.140873
C	-5.862556	-1.632693	0.780957
C	-7.228877	-1.854041	0.558061
C	-5.279610	-2.065636	1.985099
C	-7.988171	-2.486425	1.539261
H	-7.687243	-1.539443	-0.383549
C	-6.056252	-2.692045	2.954923
H	-4.204612	-1.934825	2.144047
C	-7.418127	-2.904262	2.741982
H	-9.052237	-2.653603	1.353120
H	-5.584610	-3.028147	3.882089
H	-8.027153	-3.398677	3.501984
H	-1.049874	4.739742	-1.131621
H	-2.645816	2.860621	-1.497689
H	-1.837548	0.079257	-3.897573
S	-1.662559	0.078447	1.745796
N	-0.188521	0.842395	1.513814
C	-0.091998	2.073817	2.185393
O	-1.537742	-1.296568	2.203646
O	-2.519943	0.284965	0.566046
C	-2.136499	1.202600	3.019491
C	-3.295984	1.134987	3.782603
C	-1.194092	2.224046	3.138812
C	-3.499680	2.143816	4.720692
H	-4.018817	0.326385	3.650261
C	-1.421089	3.235557	4.075718
C	-2.568495	3.180996	4.861591
H	-4.394242	2.126636	5.346669
H	-0.705676	4.051697	4.195294
H	-2.746761	3.963474	5.602786

C	0.865229	2.954974	1.856021
H	0.948711	3.899853	2.395251
C	1.726827	2.699028	0.655824
H	1.108867	2.927376	-0.232086
C	2.948261	3.588695	0.599274
C	3.152152	4.449344	-0.483915
C	3.888404	3.574584	1.637313
C	4.278971	5.270765	-0.530304
H	2.410362	4.485464	-1.288490
C	5.014002	4.393811	1.590887
H	3.735706	2.914984	2.497625
C	5.213928	5.243658	0.502789
H	4.423370	5.940462	-1.381954
H	5.738053	4.371028	2.409460
H	6.095692	5.888277	0.464227
H	-4.099777	-0.767606	0.205169
H	-2.608506	0.299706	-1.408457
C	6.283016	-3.605085	1.107058
H	5.961035	-4.198815	1.974838
H	7.051710	-4.162044	0.549023
H	6.713112	-2.663468	1.477943
C	1.453412	-0.637187	-2.513036
C	2.358552	-0.249623	-3.510582
C	0.488980	-1.613781	-2.788496
C	2.293818	-0.832275	-4.771797
H	3.098000	0.517411	-3.270199
C	0.426674	-2.191794	-4.055821
H	-0.207187	-1.913176	-2.002776
C	1.326379	-1.802701	-5.047549
H	2.998617	-0.527291	-5.549337
H	-0.328893	-2.951702	-4.269374
H	1.275008	-2.256717	-6.040344

Int3A

C	0.868980	2.139086	0.306196
C	2.347674	1.424312	-1.267946
C	1.362387	0.409553	-1.842224
O	0.620961	0.922088	0.594112
H	2.861271	1.799057	-2.175970
N	1.676642	2.533238	-0.648513
C	0.291851	0.872769	-2.638803
H	-0.050819	0.185565	-3.420257
H	0.460869	1.903297	-2.977307

Au	-1.509475	1.298561	-1.513582
P	-3.492162	2.076404	-0.631924
C	-3.489431	3.900202	-0.576355
H	-4.442653	4.277310	-0.174726
H	-2.660471	4.241874	0.061940
H	-3.335177	4.298679	-1.589248
C	-3.907135	1.577722	1.067585
H	-4.844654	2.060117	1.383938
H	-4.025032	0.487140	1.109695
H	-3.093785	1.880401	1.741102
C	4.507326	-1.440647	2.932536
C	3.304693	-3.321185	2.501555
C	3.362714	-0.727604	3.291014
H	5.487446	-0.949493	2.960200
C	2.104332	-2.699166	2.830228
C	2.119671	-1.358899	3.227680
H	3.442596	0.318583	3.598520
N	4.489468	-2.709654	2.531248
C	0.839988	-0.636563	3.572615
H	0.442963	-1.020251	4.526595
N	-0.176142	-0.808834	2.554027
C	-1.341916	-1.391390	2.817564
C	-2.463920	-1.790501	2.066721
C	-1.929291	-1.915145	4.071069
C	-3.205883	-2.197949	3.290760
O	-4.322820	-2.563118	3.571547
O	-1.535287	-2.044944	5.205650
N	-2.675411	-1.749656	0.729062
C	-3.849609	-1.996327	0.010969
C	-5.095142	-2.186029	0.629074
C	-3.769460	-2.019622	-1.392957
C	-6.229991	-2.382391	-0.155360
H	-5.168299	-2.218773	1.719581
C	-4.914203	-2.219762	-2.158291
H	-2.797468	-1.898306	-1.874753
C	-6.156671	-2.395479	-1.547975
H	-7.191002	-2.535616	0.342525
H	-4.828038	-2.241743	-3.247830
H	-7.054007	-2.553867	-2.150191
H	3.305350	-4.371052	2.186111
H	1.162687	-3.249510	2.765975
H	1.055646	0.435806	3.708046
S	0.577519	-2.172064	-2.251716
N	1.654293	-0.902284	-1.729356

C	2.821103	-1.414798	-1.098867
O	0.290179	-2.076056	-3.669596
O	-0.534052	-2.220572	-1.310316
C	1.766326	-3.407300	-1.888369
C	1.613233	-4.762338	-2.162008
C	2.879865	-2.866668	-1.247433
C	2.640376	-5.610681	-1.762767
H	0.723846	-5.140059	-2.670313
C	3.896791	-3.737593	-0.839412
C	3.765625	-5.096759	-1.103297
H	2.566034	-6.682006	-1.960165
H	4.769023	-3.361567	-0.301278
H	4.558248	-5.778371	-0.786272
C	3.696151	-0.604518	-0.494315
H	4.580842	-1.046036	-0.030656
C	3.447802	0.853078	-0.324576
H	3.044014	0.951514	0.698397
C	4.702895	1.694878	-0.414180
C	4.795321	2.886937	0.314400
C	5.766391	1.337226	-1.250763
C	5.926433	3.693646	0.216120
H	3.959228	3.186599	0.950371
C	6.901025	2.142402	-1.348553
H	5.707493	0.415839	-1.838134
C	6.984905	3.322995	-0.613351
H	5.981871	4.620317	0.792929
H	7.723149	1.844633	-2.004346
H	7.873429	3.954851	-0.687509
H	-1.846038	-1.623635	0.150317
H	-0.002563	-0.280412	1.678984
C	-4.968519	1.636590	-1.606127
H	-5.088047	0.542676	-1.608899
H	-5.867246	2.102234	-1.173078
H	-4.841764	1.978566	-2.643177
C	0.188726	3.226990	1.088993
C	0.311166	4.570589	0.709945
C	-0.573210	2.908459	2.218607
C	-0.326180	5.570408	1.440532
H	0.921039	4.796953	-0.166953
C	-1.204123	3.910153	2.957142
H	-0.660495	1.859316	2.509136
C	-1.085806	5.244061	2.567020
H	-0.225547	6.615330	1.135033
H	-1.787796	3.648770	3.843994

H	-1.578844	6.030645	3.144133

QN-SQA

C	4.512372	-1.506757	-1.472690
C	5.923814	-1.046062	0.247344
C	3.470970	-0.788100	-0.887386
H	4.359086	-1.999467	-2.440128
C	4.951521	-0.307027	0.920358
C	3.687361	-0.165378	0.344281
H	2.502982	-0.712948	-1.388506
N	5.717195	-1.639923	-0.924419
C	2.616215	0.653370	1.019819
H	2.854232	0.752359	2.093399
N	1.285699	0.109913	0.839489
C	0.254231	0.846855	0.407861
C	-1.107090	0.615508	0.180819
C	0.174549	2.241482	-0.073765
C	-1.325639	2.025098	-0.270082
O	-2.253193	2.698202	-0.635102
O	0.971292	3.133480	-0.223133
N	-1.837284	-0.504291	0.374828
C	-3.201477	-0.750995	0.168264
C	-4.089740	0.224824	-0.300003
C	-3.674568	-2.040941	0.450372
C	-5.430965	-0.105229	-0.478498
H	-3.733244	1.233833	-0.521648
C	-5.017111	-2.353229	0.266433
H	-2.983230	-2.806330	0.816951
C	-5.906167	-1.386280	-0.200245
H	-6.115870	0.663554	-0.844623
H	-5.368311	-3.363313	0.490744
H	-6.960756	-1.629530	-0.345590
H	6.920682	-1.166383	0.687704
H	5.181488	0.150661	1.886435
H	2.604661	1.675123	0.604377
H	-1.325404	-1.312112	0.708768
H	1.129971	-0.841636	1.151408

TS1-PMe_3

C	3.392426	-0.240198	0.561893
C	1.279271	0.422693	1.444831
C	0.630768	-0.656240	0.686982

O	2.976303	-1.384388	0.684961
H	1.381841	0.070008	2.488409
N	2.548148	0.786834	0.880367
C	-0.026496	-1.515729	0.074733
C	4.752657	0.088298	0.070357
C	5.342385	1.349082	0.235343
C	5.468677	-0.933441	-0.565833
C	6.624951	1.587949	-0.248539
H	4.824121	2.148557	0.771874
C	6.748368	-0.690209	-1.052104
H	4.999650	-1.914015	-0.668085
C	7.325831	0.570493	-0.896650
H	7.084752	2.568973	-0.111010
H	7.301728	-1.487881	-1.552482
H	8.332732	0.760444	-1.275801
H	2.766853	1.753711	0.685534
H	0.617529	1.301321	1.463801
H	-0.036988	-2.507105	-0.369052
Au	-1.827501	-0.360808	-0.004938
P	-3.930922	0.564719	-0.280852
C	-4.905124	-0.347340	-1.516738
H	-5.900185	0.110197	-1.627493
H	-4.388195	-0.329402	-2.486910
H	-5.021780	-1.394138	-1.201438
C	-3.902833	2.291843	-0.851915
H	-4.930440	2.660544	-0.993494
H	-3.392418	2.923095	-0.110663
H	-3.359369	2.359637	-1.805204
C	-4.929673	0.558253	1.239161
H	-4.428013	1.148140	2.019463
H	-5.923589	0.988501	1.041921
H	-5.046497	-0.472966	1.602123

TS1A

C	4.490295	-1.414130	0.162907
C	2.617559	-0.492582	0.608968
C	2.470594	-1.197932	-0.617101
O	3.667395	-1.723186	-0.904492
H	1.770435	-0.366083	1.283737
N	3.902470	-0.735615	1.081564
C	1.354246	-1.369762	-1.487740
H	1.618696	-1.777104	-2.470845
H	0.735354	-0.460292	-1.553094

Au	-0.039852	-2.590703	-0.430861
P	-1.653236	-3.714986	0.792456
C	-1.289041	-3.750090	2.577243
H	-2.087166	-4.273296	3.126327
H	-0.327997	-4.252625	2.756511
H	-1.224402	-2.706810	2.921952
C	-1.922850	-5.456953	0.317707
H	-2.707767	-5.914074	0.939764
H	-2.223931	-5.506115	-0.738645
H	-0.987563	-6.022491	0.437322
C	1.374109	5.330587	-1.633069
C	-0.346765	5.431598	-0.156978
C	0.825723	4.226680	-2.279774
H	2.327244	5.747552	-1.979171
C	-0.985884	4.333153	-0.734063
C	-0.388916	3.701852	-1.826116
H	1.347783	3.777327	-3.129233
N	0.808615	5.929198	-0.586244
C	-0.993714	2.502196	-2.510504
H	-1.389535	2.784609	-3.500328
N	-2.063683	1.892775	-1.762664
C	-3.166467	1.416257	-2.343220
C	-4.320459	0.772087	-1.870565
C	-3.659629	1.428393	-3.733974
C	-4.869186	0.632226	-3.249153
O	-5.834650	0.124980	-3.767076
O	-3.247627	1.875056	-4.778476
N	-4.640638	0.427823	-0.605558
C	-5.760596	-0.240868	-0.114083
C	-6.778339	-0.747200	-0.935590
C	-5.848196	-0.413829	1.278347
C	-7.855577	-1.414662	-0.357640
H	-6.724713	-0.611298	-2.019552
C	-6.931192	-1.083908	1.836665
H	-5.054590	-0.014611	1.916322
C	-7.944445	-1.591863	1.023217
H	-8.643697	-1.801761	-1.008788
H	-6.983872	-1.205611	2.921829
H	-8.797035	-2.115290	1.461575
H	-0.804047	5.931885	0.705298
H	-1.929884	3.970520	-0.322348
H	-0.183383	1.773620	-2.708478
S	-1.444766	0.919314	1.911943
N	-0.034352	1.041530	1.119233

C	0.781244	1.945248	1.700838
O	-1.682882	-0.424150	2.447526
O	-2.554173	1.447611	1.079078
C	-1.060868	2.095129	3.188384
C	-1.825414	2.516710	4.264320
C	0.212938	2.590489	2.912518
C	-1.270720	3.488119	5.099223
H	-2.820440	2.107192	4.450571
C	0.754149	3.566331	3.749647
C	0.002984	4.006088	4.839584
H	-1.837510	3.850261	5.959962
H	1.743310	3.985563	3.555050
H	0.415449	4.771145	5.501424
C	2.064316	2.170457	1.225058
H	2.740116	2.815744	1.786005
C	2.504450	1.494815	0.055902
H	1.695056	1.265856	-0.644919
C	3.803857	1.772860	-0.573863
C	3.938670	1.654140	-1.966324
C	4.933905	2.126948	0.180097
C	5.156657	1.908944	-2.590760
H	3.069277	1.366472	-2.564318
C	6.151610	2.379009	-0.443116
H	4.858699	2.183743	1.267882
C	6.266581	2.274291	-1.830027
H	5.240169	1.821445	-3.676666
H	7.022144	2.652205	0.157956
H	7.224346	2.472151	-2.317290
H	-3.975485	0.740728	0.107358
H	-1.934041	1.726940	-0.763127
C	-3.286199	-2.922956	0.684145
H	-3.619148	-2.867947	-0.361772
H	-4.034206	-3.471180	1.276766
H	-3.186462	-1.902742	1.081150
C	5.862598	-1.894103	0.112176
C	6.722848	-1.613837	1.185018
C	6.335729	-2.631199	-0.982465
C	8.035604	-2.067917	1.159611
H	6.337306	-1.039849	2.029926
C	7.652685	-3.081562	-1.000029
H	5.665774	-2.846476	-1.816627
C	8.504646	-2.802350	0.067997
H	8.701377	-1.848943	1.997841
H	8.016986	-3.655267	-1.855479

H	9.537827	-3.157687	0.050943

TS2

C	-1.854184	1.968518	0.143578
C	-1.683735	-0.136513	-0.277778
C	-2.763847	0.040687	0.649284
O	-2.790189	1.333401	0.958774
H	-1.743529	-0.891282	-1.070665
N	-1.229202	1.162729	-0.624195
C	-3.684641	-0.862634	1.246631
C	-1.728307	3.413081	0.282630
C	-0.838100	4.100329	-0.556357
C	-2.480114	4.119456	1.231623
C	-0.704285	5.478538	-0.443046
H	-0.264124	3.538162	-1.295737
C	-2.338416	5.500015	1.338821
H	-3.172554	3.585314	1.884638
C	-1.452714	6.180625	0.504338
H	-0.013317	6.012416	-1.099262
H	-2.923779	6.048738	2.079920
H	-1.344986	7.264378	0.590775
H	-0.692516	-0.614755	0.426075
H	-4.016006	-0.553283	2.247232
Au	-5.445342	-0.810743	0.034449
P	-7.401194	-0.824971	-1.213369
C	-7.942987	-2.497436	-1.694094
H	-8.877367	-2.451512	-2.274142
H	-7.162876	-2.979055	-2.300938
H	-8.105834	-3.106308	-0.793185
C	-7.289188	0.102956	-2.777868
H	-8.243524	0.059116	-3.324748
H	-7.040011	1.152811	-2.567036
H	-6.492656	-0.323294	-3.404371
C	-8.827347	-0.102450	-0.338513
H	-8.609985	0.943080	-0.076937
H	-9.728499	-0.139125	-0.969581
H	-9.012269	-0.660421	0.590621
H	-3.344354	-1.905444	1.211048
C	1.622119	-0.395499	0.400206
C	0.755150	-1.908440	1.915578
C	2.925164	-0.714733	0.761417
H	1.396419	0.351177	-0.368275
C	2.023071	-2.281379	2.333489

C	3.144544	-1.683143	1.743748
H	3.765368	-0.220172	0.271257
N	0.570228	-0.986127	0.968001
C	4.531254	-2.133675	2.135539
H	4.572087	-2.284090	3.226990
N	5.604724	-1.273710	1.706607
C	6.374693	-1.592993	0.646173
C	7.487379	-1.038637	0.006187
C	6.331923	-2.761900	-0.246821
C	7.487846	-2.135236	-1.025057
O	8.108208	-2.406692	-2.014830
O	5.653344	-3.758680	-0.301688
N	8.183258	0.080879	0.275236
C	9.286540	0.655813	-0.381587
C	9.848159	0.115217	-1.543118
C	9.825189	1.824113	0.174534
C	10.939942	0.751373	-2.129111
H	9.439826	-0.796175	-1.985178
C	10.915452	2.446992	-0.423530
H	9.388579	2.247532	1.084727
C	11.480319	1.913662	-1.580823
H	11.374221	0.321739	-3.034952
H	11.325789	3.355944	0.022459
H	12.337233	2.400251	-2.051074
H	-0.142827	-2.359377	2.348321
H	2.135769	-3.043203	3.108712
H	4.692335	-3.122265	1.670144
H	7.906337	0.585549	1.109173
H	5.777743	-0.424039	2.229063

TS2A

C	-4.018892	1.902272	0.264572
C	-2.072979	1.301845	0.944784
C	-1.997562	1.552579	-0.474154
O	-3.230205	1.881395	-0.872218
H	-1.252394	1.611362	1.596594
N	-3.383101	1.616164	1.338319
C	-0.939639	1.397717	-1.390955
H	-1.255547	1.378579	-2.440389
H	-0.307812	0.545455	-1.064245
Au	0.538406	2.885201	-0.996026
P	2.288975	4.285358	-0.449273
C	2.540442	4.347558	1.354060

H	3.440876	4.927790	1.606965
H	1.659337	4.802009	1.829405
H	2.641786	3.317680	1.726602
C	2.120837	6.028640	-0.965806
H	2.992703	6.617043	-0.640474
H	2.036664	6.080822	-2.060844
H	1.207996	6.457399	-0.528188
C	-0.016330	-7.467013	0.709349
C	1.926747	-6.863027	1.716505
C	0.023322	-6.370953	-0.149253
H	-0.850647	-8.176297	0.650709
C	2.066018	-5.737769	0.904466
C	1.093629	-5.476295	-0.061634
H	-0.779116	-6.214760	-0.875868
N	0.911931	-7.718214	1.629811
C	1.188932	-4.299470	-1.001847
H	1.645517	-4.624758	-1.951804
N	1.978589	-3.206891	-0.489616
C	3.005554	-2.689228	-1.162109
C	3.918510	-1.649738	-0.918533
C	3.658781	-3.049075	-2.437881
C	4.611428	-1.878078	-2.215137
O	5.525714	-1.378754	-2.827573
O	3.471582	-3.896249	-3.278975
N	3.978146	-0.801058	0.130731
C	4.885327	0.216869	0.405820
C	5.966011	0.536204	-0.432111
C	4.695558	0.948128	1.593284
C	6.839680	1.558008	-0.065756
H	6.114320	-0.015584	-1.364984
C	5.581297	1.962154	1.942053
H	3.839626	0.713157	2.231095
C	6.663374	2.275948	1.117820
H	7.681155	1.789283	-0.724263
H	5.424270	2.509764	2.875425
H	7.364682	3.065246	1.398131
H	2.683590	-7.079600	2.479980
H	2.920167	-5.068543	1.027300
H	0.166370	-3.956486	-1.240859
S	0.652571	-0.474032	1.829310
N	-0.417074	-0.795472	0.672043
C	-1.690455	-0.597105	1.137682
O	1.143454	0.917809	1.825388
O	1.737066	-1.485081	1.835888

C	-0.468465	-0.675176	3.193677
C	-0.218166	-0.744266	4.555333
C	-1.749958	-0.672323	2.650938
C	-1.323394	-0.831362	5.403245
H	0.802726	-0.748349	4.942964
C	-2.847294	-0.738975	3.505010
C	-2.619933	-0.824812	4.880140
H	-1.174435	-0.907562	6.482787
H	-3.865652	-0.721463	3.114151
H	-3.472333	-0.890787	5.560409
C	-2.785062	-1.231901	0.374640
H	-3.795484	-1.068693	0.759132
C	-2.567112	-1.958122	-0.735592
H	-1.521063	-2.084497	-1.034906
C	-3.566473	-2.615208	-1.578634
C	-3.126293	-3.411340	-2.649175
C	-4.952264	-2.489989	-1.374504
C	-4.030972	-4.067090	-3.480181
H	-2.052257	-3.511869	-2.829236
C	-5.856077	-3.143568	-2.203359
H	-5.329393	-1.867676	-0.559734
C	-5.400534	-3.936749	-3.259180
H	-3.663613	-4.681167	-4.305940
H	-6.928937	-3.032559	-2.027531
H	-6.114248	-4.448716	-3.909074
H	3.258277	-0.949721	0.844818
H	1.681822	-2.745719	0.374734
C	3.887137	3.749402	-1.134861
H	3.825756	3.711983	-2.231848
H	4.691300	4.437534	-0.833521
H	4.127197	2.742017	-0.763124
C	-5.425185	2.237913	0.092253
C	-6.246886	2.333320	1.226140
C	-5.967314	2.462728	-1.180919
C	-7.592307	2.649042	1.083450
H	-5.806487	2.159769	2.210184
C	-7.316705	2.777827	-1.314396
H	-5.326774	2.385428	-2.061110
C	-8.130695	2.871485	-0.186149
H	-8.228605	2.724941	1.968330
H	-7.736056	2.950677	-2.308226
H	-9.189295	3.119428	-0.294988

TS3A

C	3.795846	-1.853232	-1.186586
C	1.805576	-1.130769	-1.055226
C	2.528576	-0.514511	-0.036313
O	3.798563	-1.017186	-0.119898
H	0.755390	-0.979702	-1.302031
N	2.636347	-1.944694	-1.768280
C	2.130571	0.230321	1.131107
H	2.887526	0.695155	1.766955
H	1.097507	0.595452	1.136861
Au	2.587162	1.878337	-0.505464
P	3.009503	3.789501	-1.690056
C	3.090382	5.272595	-0.640465
H	3.341618	6.159303	-1.242691
H	2.095434	5.396253	-0.188114
H	3.840149	5.137250	0.151432
C	1.772223	4.200662	-2.956046
H	2.098565	5.081088	-3.530901
H	1.621207	3.350923	-3.636071
H	0.834045	4.430949	-2.428069
C	-0.846914	5.025370	0.738056
C	-0.887240	3.171680	-0.577661
C	-1.970001	4.610446	1.444422
H	-0.364422	5.976728	0.991446
C	-2.021729	2.670974	0.056672
C	-2.584153	3.398951	1.104254
H	-2.367125	5.232489	2.251239
N	-0.298452	4.323096	-0.256607
C	-3.799001	2.921231	1.864623
H	-3.525797	2.832201	2.931864
N	-4.360525	1.682407	1.393192
C	-5.551540	1.642488	0.786964
C	-6.332795	0.622358	0.224168
C	-6.587749	2.663659	0.553401
C	-7.413674	1.584477	-0.140277
O	-8.477134	1.542608	-0.709069
O	-6.693729	3.841939	0.807582
N	-6.047608	-0.687135	0.091652
C	-6.828420	-1.725337	-0.414316
C	-8.074156	-1.524522	-1.025940
C	-6.323805	-3.031190	-0.292464
C	-8.783201	-2.620630	-1.510456
H	-8.482856	-0.514342	-1.116203
C	-7.044543	-4.113675	-0.786064

H	-5.366040	-3.187789	0.211196
C	-8.280279	-3.917358	-1.401953
H	-9.753003	-2.450149	-1.985144
H	-6.636974	-5.122367	-0.677906
H	-8.848504	-4.766756	-1.787499
H	-0.438413	2.593361	-1.394321
H	-2.434557	1.716603	-0.273721
H	-4.586506	3.690443	1.804950
S	-2.073966	-1.236200	0.196289
N	-0.775136	-1.088034	1.154526
C	-0.054409	-2.221272	1.166116
O	-1.972334	-0.407159	-1.010763
O	-3.320857	-1.040310	0.977724
C	-1.839418	-2.949509	-0.216351
C	-2.595604	-3.783665	-1.025486
C	-0.648658	-3.343569	0.389562
C	-2.132239	-5.088165	-1.204251
H	-3.514030	-3.437525	-1.504644
C	-0.195133	-4.649261	0.202657
C	-0.947181	-5.512747	-0.593462
H	-2.698792	-5.781630	-1.829947
H	0.731634	-4.993332	0.665952
H	-0.602276	-6.537896	-0.747396
C	1.162442	-2.317317	1.834908
H	1.743811	-3.234199	1.732187
C	1.671100	-1.217851	2.562505
H	0.906487	-0.554624	2.978712
C	2.898941	-1.320638	3.372128
C	3.049866	-0.502553	4.504086
C	3.946203	-2.198485	3.046266
C	4.197151	-0.565640	5.289892
H	2.242951	0.184606	4.774627
C	5.093969	-2.261349	3.831105
H	3.867224	-2.831911	2.160377
C	5.225349	-1.446897	4.956496
H	4.287228	0.073466	6.171837
H	5.895408	-2.953549	3.560514
H	6.126486	-1.500124	5.572206
H	-5.111094	-0.956606	0.408106
H	-3.823660	0.814988	1.462578
C	4.607732	3.722259	-2.567567
H	4.794357	4.666316	-3.102544
H	5.419307	3.545123	-1.847454
H	4.597314	2.891811	-3.288037

C	5.034535	-2.521343	-1.548131
C	5.049790	-3.375947	-2.662309
C	6.209604	-2.333939	-0.803824
C	6.222027	-4.029173	-3.022327
H	4.126429	-3.511402	-3.229166
C	7.379104	-2.992704	-1.172443
H	6.195754	-1.672303	0.064730
C	7.390261	-3.840295	-2.280241
H	6.227196	-4.693059	-3.890223
H	8.290873	-2.843710	-0.588871
H	8.310339	-4.355650	-2.566311

TS4A

C	0.678542	0.270716	-1.935554
C	1.456936	-1.637934	-1.222073
C	0.425287	-1.108538	-0.254685
O	0.055140	0.090640	-0.698866
H	1.142402	-2.633955	-1.573629
N	1.430654	-0.682268	-2.298523
C	-0.417532	-1.848870	0.617953
H	-0.785304	-1.242413	1.459087
H	0.046337	-2.791143	0.936064
Au	-2.240695	-2.170049	-0.433458
P	-4.326079	-2.287983	-1.425631
C	-4.857371	-0.670479	-2.076862
H	-5.860061	-0.737194	-2.526599
H	-4.872091	0.058829	-1.252171
H	-4.139320	-0.321500	-2.832888
C	-5.659137	-2.770543	-0.278443
H	-6.632289	-2.787088	-0.792948
H	-5.449452	-3.764441	0.141926
H	-5.692421	-2.039688	0.543154
C	3.783853	2.877295	-1.860620
C	4.751348	1.763593	-0.127576
C	3.081553	3.721514	-1.000974
H	3.672621	2.988723	-2.944959
C	4.098576	2.551257	0.817750
C	3.233722	3.556096	0.378317
H	2.413984	4.492535	-1.396779
N	4.599876	1.910782	-1.442790
C	2.436357	4.389901	1.356047
H	3.022736	4.553483	2.272698
N	1.186566	3.742063	1.725488

C	0.039450	4.037809	1.130673
C	-1.268389	3.504641	1.123345
C	-0.335837	5.111233	0.185232
C	-1.739566	4.537633	0.170479
O	-2.764280	4.795500	-0.426877
O	0.259607	6.003940	-0.373727
N	-1.754359	2.392323	1.717338
C	-3.050586	1.878343	1.716162
C	-4.119396	2.469924	1.023139
C	-3.283545	0.707408	2.461749
C	-5.386460	1.894169	1.088293
H	-3.954716	3.377567	0.435671
C	-4.555552	0.147183	2.514271
H	-2.453478	0.253635	3.008100
C	-5.621311	0.734187	1.829004
H	-6.209379	2.376969	0.553886
H	-4.714947	-0.752733	3.114843
H	-6.625776	0.307728	1.890199
H	5.424438	0.962423	0.199863
H	4.232512	2.356335	1.883811
H	2.198240	5.366821	0.914123
S	1.412537	0.219579	2.811453
N	1.952075	-0.450527	1.447534
C	2.549549	-1.668735	1.698232
O	-0.064965	0.367292	2.819594
O	2.093145	1.479222	3.168559
C	1.919800	-1.082628	3.902494
C	1.774801	-1.177760	5.279319
C	2.542849	-2.057251	3.125758
C	2.282424	-2.319782	5.896592
H	1.284438	-0.387672	5.851993
C	3.054182	-3.193211	3.757313
C	2.915594	-3.313621	5.138637
H	2.190623	-2.439007	6.978580
H	3.557349	-3.972998	3.181449
H	3.311722	-4.198867	5.642097
C	3.021886	-2.400439	0.659511
H	3.469836	-3.382904	0.811087
C	2.944266	-1.787317	-0.695858
H	3.273680	-0.740646	-0.599613
C	3.784276	-2.466875	-1.749862
C	4.665284	-1.715513	-2.535838
C	3.693454	-3.846668	-1.969199
C	5.443938	-2.336460	-3.511987

H	4.739051	-0.633836	-2.380215
C	4.468765	-4.466901	-2.946775
H	3.007558	-4.449236	-1.364928
C	5.349058	-3.711440	-3.721019
H	6.130755	-1.737165	-4.115088
H	4.387269	-5.545638	-3.103582
H	5.960572	-4.195313	-4.486826
H	-1.069471	1.789912	2.190336
H	1.290270	2.909420	2.316198
C	-4.479929	-3.441265	-2.831725
H	-4.249622	-4.462620	-2.496010
H	-5.496832	-3.416139	-3.252847
H	-3.756697	-3.164518	-3.612318
C	0.336148	1.479036	-2.678493
C	1.002209	1.729842	-3.887708
C	-0.651803	2.362575	-2.228113
C	0.686094	2.862693	-4.627114
H	1.765652	1.024504	-4.222424
C	-0.963285	3.499079	-2.972941
H	-1.174868	2.158672	-1.292442
C	-0.291863	3.749562	-4.168691
H	1.208074	3.060823	-5.566410
H	-1.721678	4.193221	-2.602827
H	-0.530909	4.645365	-4.747053

TS5A

C	-0.960355	-2.109050	0.282234
C	-2.460852	-1.409659	-1.209527
C	-1.387168	-0.396520	-1.601600
O	-0.660840	-0.860037	0.392739
H	-2.905042	-1.729896	-2.170852
N	-1.844977	-2.541521	-0.571517
C	-0.316589	-0.841639	-2.456790
H	-0.096863	-0.131143	-3.262720
H	-0.552438	-1.842648	-2.844282
Au	1.579852	-1.267460	-1.569897
P	3.623709	-2.039588	-0.811851
C	3.634895	-3.866325	-0.791741
H	4.608703	-4.249193	-0.449324
H	2.842866	-4.220340	-0.114319
H	3.424774	-4.248963	-1.800716
C	4.124821	-1.587280	0.879001
H	5.074489	-2.078726	1.140536

H	4.249357	-0.498578	0.946360
H	3.343308	-1.904180	1.582913
C	-4.511216	1.372177	3.044870
C	-3.341915	3.210843	2.400207
C	-3.344646	0.677059	3.363587
H	-5.487295	0.890456	3.178056
C	-2.120062	2.602011	2.672571
C	-2.107989	1.294852	3.165872
H	-3.402844	-0.345301	3.747033
N	-4.521957	2.613266	2.563019
C	-0.813343	0.586943	3.480791
H	-0.423752	0.931825	4.453040
N	0.202255	0.828827	2.478588
C	1.414305	1.284339	2.793927
C	2.557379	1.659688	2.067322
C	2.049780	1.627731	4.084092
C	3.339934	1.885921	3.312940
O	4.485616	2.134307	3.604404
O	1.677570	1.667213	5.232511
N	2.743626	1.716568	0.729828
C	3.899046	1.996597	-0.001593
C	5.162560	2.146620	0.590024
C	3.774790	2.100645	-1.398824
C	6.274064	2.384020	-0.216250
H	5.267406	2.102135	1.678094
C	4.896604	2.341522	-2.185641
H	2.788573	2.003082	-1.858824
C	6.157471	2.478820	-1.602859
H	7.251214	2.503451	0.258963
H	4.778693	2.425275	-3.269119
H	7.036844	2.669115	-2.222093
H	-3.363682	4.237995	2.018084
H	-1.183995	3.134306	2.489064
H	-1.008122	-0.495013	3.574999
S	-0.592808	2.198562	-1.917751
N	-1.706271	0.922844	-1.537312
C	-2.928705	1.418808	-1.012081
O	-0.124947	2.129340	-3.289028
O	0.394953	2.267434	-0.846051
C	-1.829021	3.421868	-1.694460
C	-1.665745	4.776971	-1.960067
C	-2.996311	2.869581	-1.171790
C	-2.741161	5.613028	-1.678103
H	-0.732599	5.163722	-2.374555

C	-4.063846	3.726962	-0.883792
C	-3.924126	5.086751	-1.140686
H	-2.660941	6.684220	-1.874040
H	-4.985854	3.338916	-0.447259
H	-4.755947	5.758657	-0.917264
C	-3.847063	0.600663	-0.485769
H	-4.771688	1.034706	-0.099271
C	-3.608121	-0.859617	-0.313334
H	-3.264653	-0.982916	0.729303
C	-4.856263	-1.699107	-0.487852
C	-5.000510	-2.894471	0.226206
C	-5.860351	-1.333333	-1.391533
C	-6.125515	-3.696238	0.049280
H	-4.209240	-3.199706	0.914719
C	-6.988520	-2.133712	-1.568745
H	-5.759174	-0.409393	-1.968875
C	-7.125321	-3.317464	-0.846660
H	-6.222530	-4.625403	0.616467
H	-7.764168	-1.829659	-2.276218
H	-8.009253	-3.945419	-0.982672
H	1.894204	1.665129	0.167144
H	0.010578	0.407679	1.557744
C	5.052305	-1.571784	-1.844290
H	5.169719	-0.477710	-1.821843
H	5.973496	-2.046599	-1.472659
H	4.872287	-1.882952	-2.883244
C	-0.247236	-3.114519	1.125832
C	-0.470531	-4.483785	0.925721
C	0.652768	-2.710003	2.118198
C	0.198561	-5.426813	1.700423
H	-1.178355	-4.775898	0.147397
C	1.314751	-3.655453	2.902303
H	0.825878	-1.643213	2.270230
C	1.092566	-5.016060	2.692530
H	0.019425	-6.492351	1.534532
H	2.004642	-3.327293	3.684448
H	1.610722	-5.757481	3.306178

2a_in solution

S	-2.511557	-1.555757	-0.000049
N	-0.844879	-1.351721	-0.000002
C	-0.532382	-0.090133	0.000029
O	-2.918290	-2.178929	1.252748

O	-2.918226	-2.178873	-1.252895
C	-2.887783	0.185985	-0.000020
C	-4.114558	0.825039	-0.000036
C	-1.673037	0.868358	0.000019
C	-4.102771	2.224288	-0.000009
H	-5.052773	0.266609	-0.000068
C	-1.669882	2.261766	0.000044
C	-2.897093	2.930051	0.000030
H	-5.048858	2.770099	-0.000020
H	-0.737837	2.829989	0.000074
H	-2.913233	4.021934	0.000050
C	0.841052	0.371776	0.000053
H	0.995758	1.451948	0.000104
C	1.887264	-0.486825	0.000006
H	1.646264	-1.555536	-0.000053
C	3.303753	-0.155575	0.000021
C	4.237745	-1.208034	-0.000070
C	3.784521	1.168456	0.000122
C	5.605514	-0.950156	-0.000064
H	3.876467	-2.239842	-0.000147
C	5.149538	1.424188	0.000128
H	3.084610	2.006597	0.000198
C	6.064626	0.366697	0.000035
H	6.316239	-1.779724	-0.000136
H	5.507865	2.456219	0.000207
H	7.137654	0.573004	0.000040

4n-Proton

C	3.721437	1.051505	-2.427656
C	3.956890	2.469710	-0.615771
C	2.942037	0.089154	-1.701270
C	3.209946	1.566327	0.197355
C	2.707758	0.389212	-0.321722
N	4.199781	2.184929	-1.877714
C	1.914493	-0.561420	0.552706
N	0.545951	-0.104985	0.746846
C	-0.492613	-0.892568	0.392309
C	-1.879817	-0.746610	0.269986
C	-0.528817	-2.318007	0.050646
C	-2.036279	-2.189714	-0.134148
O	-2.933892	-2.915602	-0.450204
O	0.314831	-3.185238	-0.037095
N	-2.670507	0.324246	0.445118

C	-4.061759	0.466011	0.301872
C	-4.900019	-0.576947	-0.098855
C	-4.602229	1.726924	0.580155
C	-6.269358	-0.340459	-0.208109
H	-4.497669	-1.567124	-0.329115
C	-5.968803	1.943791	0.455988
H	-3.958381	2.550310	0.899445
C	-6.816960	0.910214	0.063437
H	-7.890784	1.076758	-0.031003
H	3.046782	1.820410	1.247535
H	1.831081	-1.532331	0.048826
H	-2.206682	1.180372	0.727186
H	0.411312	0.896371	0.833902
C	4.504791	3.733180	-0.067400
C	4.072319	4.271772	1.154109
C	5.485190	4.425687	-0.794738
C	4.609902	5.461366	1.638742
H	3.284094	3.784200	1.732901
C	6.024766	5.610907	-0.307942
H	5.809732	4.011091	-1.750434
C	5.591330	6.132773	0.911504
H	4.253490	5.872193	2.586221
H	6.789988	6.134726	-0.885500
H	6.013549	7.065821	1.291774
C	2.471433	-1.063794	-2.363729
C	3.998232	0.800086	-3.795750
H	1.854784	-1.817084	-1.868362
C	3.532631	-0.328289	-4.424537
C	2.754881	-1.277109	-3.706761
H	3.760674	-0.487505	-5.478880
H	4.591718	1.542412	-4.332362
C	2.584384	-0.827240	1.913539
C	1.924683	-1.931194	2.754392
H	2.634102	0.114498	2.481775
C	4.149202	-2.625955	1.188938
C	3.018541	-2.793532	3.392030
H	1.274036	-2.551603	2.121000
H	1.288724	-1.475302	3.525839
C	3.742942	-3.614129	2.300730
H	3.500220	-2.712218	0.306961
H	5.186272	-2.763425	0.854197
H	2.576111	-3.480642	4.126150
N	4.027864	-1.219807	1.703147
C	2.936911	-4.753794	1.743386

H	2.031429	-4.491553	1.180094
C	3.267498	-6.036536	1.894584
H	4.168467	-6.342967	2.436666
H	2.644229	-6.832672	1.480172
C	4.045367	-1.880292	4.071042
H	3.542100	-1.204523	4.778884
H	4.767990	-2.469380	4.653367
C	4.783434	-1.079563	2.988575
H	4.855916	-0.006548	3.214299
H	5.799353	-1.453149	2.798236
C	-6.533475	3.321402	0.700726
C	-7.176706	-1.489529	-0.581734
F	-6.592079	-2.303390	-1.458941
F	-8.316289	-1.053758	-1.117435
F	-7.488625	-2.215155	0.494145
F	-6.691081	3.984237	-0.446177
F	-7.721980	3.259315	1.295390
F	-5.722209	4.049907	1.474235
H	4.654085	-4.035221	2.756649
O	2.260494	-2.392533	-4.250114
C	2.474585	-2.673995	-5.613854
H	1.964138	-3.623250	-5.814913
H	2.044043	-1.893157	-6.262560
H	3.547223	-2.790266	-5.842351
H	4.412676	-0.569432	1.003317

4n

C	3.229782	1.569116	-2.446593
C	4.209481	2.252342	-0.478499
C	2.602754	0.432597	-1.841262
C	3.610374	1.163934	0.219731
C	2.806019	0.261400	-0.432882
N	3.999652	2.442921	-1.762302
C	2.062906	-0.830467	0.312092
N	0.678551	-0.389209	0.502852
C	-0.392628	-1.074320	0.105168
C	-1.774134	-0.841567	0.087252
C	-0.550570	-2.408145	-0.516738
C	-2.059016	-2.177122	-0.507750
O	-3.031645	-2.803319	-0.839746
O	0.212501	-3.275436	-0.864251
N	-2.474339	0.240902	0.504628
C	-3.849229	0.476079	0.508519

C	-4.784718	-0.451317	0.034932
C	-4.293844	1.705414	1.015597
C	-6.140808	-0.134271	0.083435
H	-4.456994	-1.413911	-0.371693
C	-5.650436	2.003532	1.045665
H	-3.576004	2.436716	1.395557
C	-6.590862	1.085147	0.582887
H	-7.655989	1.315237	0.610996
H	3.792502	1.053335	1.286995
H	2.006133	-1.726033	-0.322730
H	-1.923753	1.016214	0.853895
H	0.566500	0.544120	0.883478
C	5.075524	3.230799	0.226771
C	5.668542	2.948556	1.465884
C	5.324092	4.478818	-0.364439
C	6.476093	3.890320	2.100055
H	5.526958	1.971655	1.933480
C	6.125259	5.420399	0.271598
H	4.872340	4.684538	-1.336398
C	6.703369	5.131755	1.508765
H	6.937271	3.648254	3.060779
H	6.302067	6.389716	-0.201433
H	7.334531	5.871048	2.008026
C	1.832425	-0.434728	-2.644010
C	3.041848	1.787359	-3.833699
H	1.354320	-1.327512	-2.238213
C	2.283163	0.933939	-4.599381
C	1.671351	-0.196929	-4.000600
H	2.163095	1.130610	-5.665246
H	3.530111	2.659258	-4.273093
C	2.658878	-1.246078	1.667172
C	1.868515	-2.412196	2.320579
H	2.600423	-0.363929	2.330210
C	4.272227	-2.862590	0.902401
C	2.884102	-3.410246	2.886249
H	1.220749	-2.917003	1.587439
H	1.210198	-2.045206	3.123610
C	3.694875	-4.048480	1.734752
H	3.804021	-2.826559	-0.093524
H	5.349592	-2.999957	0.722852
H	2.363699	-4.199649	3.449401
N	4.075398	-1.581270	1.569274
C	2.911139	-5.010587	0.895120
H	2.072266	-4.595997	0.319095

C	3.176224	-6.314334	0.788425
H	4.008336	-6.776536	1.330952
H	2.572556	-6.968152	0.153448
C	3.862197	-2.657540	3.794402
H	3.306112	-2.143969	4.596067
H	4.547333	-3.364914	4.287828
C	4.638838	-1.647146	2.912302
H	4.624166	-0.636344	3.353511
H	5.698585	-1.931323	2.816844
C	-6.102043	3.354787	1.534422
C	-7.137065	-1.169136	-0.378801
F	-6.722756	-1.788342	-1.483034
F	-8.327826	-0.622721	-0.640182
F	-7.326266	-2.104809	0.555952
F	-6.202720	4.226461	0.525914
F	-7.296863	3.290862	2.122365
F	-5.240563	3.872576	2.416311
H	4.526576	-4.608419	2.196109
O	0.921870	-1.083341	-4.680333
C	0.733605	-0.922746	-6.059708
H	0.107341	-1.761931	-6.387582
H	0.213317	0.021367	-6.299103
H	1.688592	-0.955685	-6.612868

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C	3.426749	1.321639	-2.519399
C	4.268578	2.193911	-0.559954
C	2.731662	0.264027	-1.848665
C	3.596692	1.192154	0.197761
C	2.828954	0.233892	-0.419052
N	4.165417	2.249751	-1.870867
C	2.031139	-0.781985	0.377546
N	0.649937	-0.309626	0.482771
C	-0.410301	-1.010793	0.101469
C	-1.799049	-0.777755	0.057056
C	-0.569187	-2.354321	-0.486906
C	-2.068200	-2.132036	-0.479726
O	-3.034771	-2.791761	-0.791507
O	0.188420	-3.239721	-0.820924
N	-2.501455	0.313619	0.427361
C	-3.875946	0.539108	0.419545
C	-4.328532	1.792998	0.857613
C	-4.806479	-0.419812	0.002825

C	-5.687405	2.078120	0.877485
H	-3.612279	2.549757	1.184029
C	-6.164617	-0.108188	0.026503
H	-4.471519	-1.404822	-0.335609
C	-6.623986	1.132591	0.460221
H	-7.691018	1.358001	0.473916
H	3.686768	1.195693	1.282373
H	1.983879	-1.720458	-0.192110
H	-1.953404	1.105464	0.745954
H	0.523125	0.619092	0.873512
C	5.099852	3.229991	0.106005
C	5.430837	4.402905	-0.591302
C	5.582164	3.073771	1.414494
C	6.207470	5.391955	0.003692
H	5.063429	4.517819	-1.612566
C	6.364651	4.062678	2.008633
H	5.370825	2.161374	1.976019
C	6.677463	5.227192	1.308311
H	6.448679	6.300456	-0.554103
H	6.737358	3.917523	3.025598
H	7.288874	6.002903	1.775912
C	1.998883	-0.667800	-2.614496
C	3.343185	1.398136	-3.932291
H	1.467990	-1.500849	-2.151504
C	2.619174	0.484525	-4.661457
C	1.938151	-0.567999	-3.996826
H	2.578891	0.574116	-5.747367
H	3.879403	2.210521	-4.427068
C	2.572867	-1.104474	1.780569
C	1.735235	-2.202185	2.490368
H	2.511577	-0.176812	2.375467
C	4.173574	-2.808172	1.194511
C	2.708444	-3.176978	3.162511
H	1.096362	-2.744100	1.775309
H	1.061560	-1.760480	3.240405
C	3.541792	-3.916272	2.091209
H	3.739796	-2.837829	0.182687
H	5.252744	-2.983783	1.066848
H	2.151493	-3.909121	3.766748
N	3.985056	-1.475554	1.754817
C	2.763412	-4.918724	1.295831
H	1.953073	-4.524652	0.666711
C	2.998953	-6.233512	1.285084
H	3.802729	-6.675346	1.884609

H	2.399497	-6.916550	0.676540
C	3.674478	-2.380041	4.044823
H	3.104319	-1.798289	4.787262
H	4.328251	-3.064208	4.608164
C	4.502006	-1.451412	3.120543
H	4.491148	-0.411481	3.485435
H	5.557557	-1.763115	3.084536
C	-7.154017	-1.123214	-0.483455
C	-6.171322	3.407530	1.391993
F	-5.186969	4.306099	1.468781
F	-6.698521	3.292802	2.617129
F	-7.123954	3.918666	0.606693
F	-8.350108	-0.981105	0.094709
F	-7.341216	-0.999209	-1.803645
F	-6.745347	-2.374322	-0.262345
H	4.343693	-4.458697	2.620376
O	1.216377	-1.504442	-4.637293
C	1.115965	-1.467786	-6.040596
H	0.634238	-0.540029	-6.392437
H	2.102038	-1.568443	-6.524206
H	0.491330	-2.321973	-6.328976

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C	0.622844	-0.336597	0.000148
C	2.630475	-1.184981	0.000070
C	2.719786	0.325773	0.000042
O	1.419040	0.775769	0.000596
H	3.117114	-1.633068	0.884176
N	1.210058	-1.464162	-0.000396
C	3.758999	1.157111	-0.000496
C	-0.823341	-0.099465	0.000073
C	-1.693368	-1.198067	0.000060
C	-1.341498	1.200899	-0.000012
C	-3.068038	-0.993895	-0.000028
H	-1.265095	-2.202460	0.000129
C	-2.720346	1.398421	-0.000110
H	-0.656391	2.050278	0.000013
C	-3.584002	0.304088	-0.000119
H	-3.744977	-1.851542	-0.000019
H	-3.122969	2.414080	-0.000182
H	-4.665452	0.461737	-0.000195
H	3.117980	-1.633457	-0.883319
H	4.774075	0.759584	-0.000413

H	3.613930	2.238101	0.000030

C-XPhos_in solution

C	5.230992	-0.235889	-0.364998
C	4.538828	0.340546	-2.285771
C	3.563981	0.715575	-1.393427
O	4.023134	0.342438	-0.164314
H	4.537941	0.473341	-3.366414
N	5.577995	-0.260262	-1.616792
C	2.245133	1.340788	-1.498399
H	2.124606	1.742749	-2.515787
H	2.152918	2.180013	-0.788225
Au	0.673677	0.012905	-1.071354
P	-0.976351	-1.677000	-0.742975
C	-0.151202	-3.126803	0.258830
C	-1.372411	-2.233879	-2.545691
C	5.966975	-0.737198	0.786980
C	7.226766	-1.329902	0.598848
C	5.441844	-0.645639	2.085858
C	7.941838	-1.819633	1.686225
H	7.629370	-1.397533	-0.413857
C	6.164243	-1.138217	3.170282
H	4.462959	-0.186583	2.238713
C	7.414693	-1.726693	2.976954
H	8.920813	-2.278769	1.526993
H	5.745596	-1.061786	4.176956
H	7.978424	-2.112365	3.829889
C	-0.395346	-4.555865	-0.243499
H	0.229633	-5.230878	0.363758
H	-0.091577	-4.699490	-1.288269
H	-1.428244	-4.903096	-0.127416
C	-0.586579	-3.030813	1.722030
H	-1.652875	-3.250633	1.863215
H	-0.381757	-2.039037	2.144347
H	-0.011520	-3.765127	2.309909
C	1.366748	-2.892524	0.187894
H	1.874236	-3.690723	0.754764
H	1.657947	-1.927814	0.625622
H	1.745298	-2.920339	-0.843972
C	-1.931795	-0.994349	-3.244366
H	-1.249760	-0.137739	-3.157543
H	-2.913505	-0.708859	-2.838314
H	-2.065693	-1.216615	-4.315855

C	-0.026384	-2.590835	-3.193773
H	0.712933	-1.784131	-3.070785
H	-0.188405	-2.744577	-4.273348
H	0.409192	-3.517710	-2.795670
C	-2.357517	-3.377182	-2.793543
H	-2.392623	-3.552906	-3.881635
H	-3.376807	-3.122966	-2.477378
H	-2.063853	-4.325314	-2.326394
C	-2.522621	-1.068084	0.141114
C	-2.621744	0.294351	0.578439
C	-3.592392	-1.948602	0.430317
C	-3.790463	0.734326	1.252007
C	-4.734802	-1.471113	1.090459
C	-4.869580	-0.140410	1.477965
C	-3.629553	-3.408887	0.101364
H	-2.753382	-3.726266	-0.456954
H	-4.524997	-3.651904	-0.488973
H	-3.688480	-4.019349	1.015804
C	-1.580121	1.380835	0.438323
C	-0.681212	1.628955	1.503717
C	-1.679426	2.335346	-0.607466
C	0.076639	2.804935	1.505900
C	-0.904621	3.497680	-0.550378
C	-0.025482	3.764686	0.500602
H	0.764469	2.990496	2.336609
H	-1.003651	4.229184	-1.356356
C	-0.530725	0.685182	2.685725
H	-1.125688	-0.213315	2.462996
C	0.752036	5.064329	0.584722
H	1.499237	4.933416	1.386555
C	-2.627637	2.164834	-1.784621
H	-2.926794	1.107451	-1.807069
C	0.922771	0.249712	2.883511
H	0.993506	-0.530410	3.657993
H	1.555221	1.091002	3.208090
H	1.352883	-0.145556	1.950822
C	-1.086739	1.285978	3.979321
H	-0.995228	0.566664	4.808735
H	-2.147400	1.556577	3.882166
H	-0.533323	2.195198	4.264449
C	-0.164487	6.219850	0.996062
H	-0.676462	6.006470	1.946780
H	-0.937569	6.400672	0.231417
H	0.410367	7.151627	1.119219

C	1.509395	5.395867	-0.700238
H	2.179450	4.575039	-0.996930
H	2.119815	6.302347	-0.564441
H	0.821261	5.588012	-1.539005
C	-1.955898	2.491134	-3.120805
H	-1.809523	3.575573	-3.246751
H	-2.584410	2.150995	-3.958488
H	-0.970130	2.010850	-3.210642
C	-3.906053	2.994932	-1.637157
H	-3.671259	4.067385	-1.538595
H	-4.494033	2.695481	-0.760085
H	-4.545408	2.872519	-2.526044
C	-3.951319	2.132826	1.793517
H	-4.134677	2.100834	2.879596
H	-4.830770	2.630944	1.356388
H	-3.081356	2.771536	1.615428
C	-6.137885	0.332937	2.122562
H	-5.987212	0.581142	3.186171
H	-6.921330	-0.430865	2.052193
H	-6.508846	1.248823	1.638511
O	-5.756705	-2.354432	1.315904
C	-5.798276	-2.918231	2.610888
H	-4.856405	-3.436163	2.860421
H	-6.618711	-3.648077	2.621256
H	-5.990732	-2.155278	3.384158

COM1

C	-4.468568	0.149911	1.629961
C	-3.907124	1.824185	0.148473
C	-3.660905	-0.828842	0.963004
C	-3.113054	0.914862	-0.604252
C	-2.982265	-0.399199	-0.221183
N	-4.570336	1.433002	1.217130
C	-2.091824	-1.339451	-1.008952
N	-0.694941	-1.068850	-0.687124
C	0.175268	-2.009833	-0.348828
C	1.576944	-2.047979	-0.199935
C	0.054340	-3.442209	-0.023696
C	1.540417	-3.447838	0.280751
O	2.323731	-4.260515	0.724427
O	-0.850768	-4.250795	-0.014933
N	2.487852	-1.084203	-0.448367
C	3.850814	-1.069380	-0.174383

C	4.583641	0.050923	-0.599066
C	4.507958	-2.100314	0.509074
C	5.945153	0.134631	-0.336332
H	4.074794	0.851523	-1.139809
C	5.872894	-1.988686	0.766743
H	3.959960	-2.995539	0.817807
C	6.608123	-0.880114	0.354279
H	7.675712	-0.808718	0.564474
H	-2.613969	1.264948	-1.507517
H	-2.283416	-2.373524	-0.697523
S	0.823901	2.148503	-1.972616
N	0.270290	1.765985	-0.444078
C	0.536095	2.721685	0.410175
O	1.880691	1.187278	-2.311740
O	-0.295473	2.266738	-2.899848
C	1.488296	3.728792	-1.522255
C	2.131554	4.669733	-2.304846
C	1.239059	3.901386	-0.159903
C	2.543781	5.845381	-1.667570
H	2.311560	4.506808	-3.368929
C	1.653319	5.076523	0.463411
C	2.306646	6.043223	-0.305376
H	3.057146	6.617074	-2.245039
H	1.475979	5.250734	1.525913
H	2.636992	6.969829	0.168273
C	0.192945	2.647786	1.805351
H	0.491444	3.492252	2.427752
C	-0.465860	1.585816	2.336933
H	-0.746237	0.778302	1.652139
C	-0.844567	1.390861	3.723220
C	-0.544677	2.320478	4.739837
C	-1.537237	0.214257	4.068102
C	-0.925265	2.075714	6.051717
H	-0.007801	3.241167	4.502609
C	-1.917776	-0.028008	5.384010
H	-1.779969	-0.512841	3.288456
C	-1.612275	0.901364	6.377961
H	-0.686528	2.802967	6.830936
H	-2.455859	-0.945010	5.634102
H	-1.909264	0.713670	7.412616
H	2.158337	-0.282005	-0.992616
H	-0.392458	-0.088296	-0.681264
C	-4.025808	3.250505	-0.252534
C	-5.038626	4.043681	0.309892

C	-3.145378	3.843601	-1.171835
C	-5.174444	5.383173	-0.040507
H	-5.716422	3.580297	1.028787
C	-3.279760	5.187556	-1.517686
H	-2.331443	3.268893	-1.619032
C	-4.294739	5.962357	-0.957511
H	-5.974173	5.981376	0.403716
H	-2.580881	5.631538	-2.231068
H	-4.400075	7.014599	-1.233275
C	-3.582081	-2.134481	1.497566
C	-5.185667	-0.241679	2.788441
H	-2.957878	-2.905589	1.041604
C	-5.108761	-1.521453	3.285602
C	-4.290986	-2.483666	2.637559
H	-5.675174	-1.785478	4.179075
H	-5.801970	0.513492	3.280441
C	-2.299250	-1.256701	-2.532940
C	-1.417173	-2.269234	-3.307177
H	-2.014887	-0.237460	-2.843606
C	-4.134971	-2.802949	-2.762111
C	-2.279751	-2.898627	-4.406442
H	-1.028020	-3.056770	-2.641925
H	-0.539814	-1.769471	-3.745641
C	-3.405792	-3.744814	-3.769745
H	-3.960028	-3.135984	-1.727039
H	-5.224507	-2.847064	-2.914151
H	-1.660448	-3.536915	-5.054994
N	-3.704950	-1.416514	-2.895181
C	-2.930580	-5.009777	-3.124055
H	-2.267467	-4.897925	-2.254545
C	-3.270476	-6.241696	-3.512912
H	-3.938552	-6.408382	-4.365319
H	-2.895651	-7.128585	-2.994095
C	-2.935104	-1.780668	-5.224686
H	-2.155915	-1.125104	-5.646311
H	-3.488835	-2.207309	-6.075856
C	-3.879595	-0.992316	-4.281521
H	-3.694701	0.091800	-4.344832
H	-4.935386	-1.151651	-4.551728
C	6.548537	-3.071105	1.565819
C	6.730698	1.313088	-0.844422
F	5.954807	2.379462	-1.057432
F	7.339588	1.033534	-2.003960
F	7.686360	1.676626	0.016594

F	7.855948	-3.146011	1.299901
F	6.430894	-2.848459	2.882087
F	6.019044	-4.272820	1.326062
H	-4.102912	-4.022926	-4.578423
O	-4.153300	-3.750334	3.068649
C	-4.847237	-4.174427	4.216970
H	-4.549169	-3.601461	5.111390
H	-5.939736	-4.097302	4.086994
H	-4.582444	-5.228064	4.367762

C-PMe$_3$_in solution

C	2.965315	-0.858050	0.256750
C	1.716930	-2.477185	0.823385
C	1.054439	-1.806165	-0.174341
O	1.866818	-0.770567	-0.529762
H	1.387744	-3.364989	1.360842
N	2.917945	-1.860534	1.081576
C	-0.242412	-1.949247	-0.842337
H	-0.113458	-1.886995	-1.936485
H	-0.651827	-2.944463	-0.609879
Au	-1.638089	-0.487242	-0.269390
P	-3.195396	1.136107	0.365414
C	-4.918486	0.539574	0.450804
C	-2.891704	1.862475	2.012148
C	4.023311	0.129050	0.090369
C	5.164245	0.067553	0.907441
C	3.925675	1.145551	-0.872814
C	6.182350	1.003773	0.762164
H	5.233698	-0.725887	1.654414
C	4.949580	2.079289	-1.012904
H	3.041886	1.198248	-1.511579
C	6.080408	2.013718	-0.198011
H	7.065220	0.946218	1.403802
H	4.863175	2.866167	-1.766415
H	6.881880	2.747972	-0.310025
C	-3.276554	2.576336	-0.752965
H	-4.024548	3.303207	-0.401307
H	-2.290120	3.059744	-0.796930
H	-3.543820	2.237681	-1.764281
H	-3.651112	2.622695	2.250492
H	-2.919360	1.067722	2.771451
H	-1.894227	2.324428	2.028310
H	-5.221635	0.156852	-0.534288

H	-4.984447	-0.281316	1.179060
H	-5.597834	1.351458	0.752312

Int2'-XPhos

C	3.801073	-0.601342	-0.546486
C	2.895831	0.379669	-2.330474
C	4.356638	0.724185	-2.226264
O	4.824435	0.050942	-1.105518
H	2.248103	1.269370	-2.300011
N	2.666182	-0.451233	-1.148580
C	5.156620	1.480657	-2.966431
Au	0.673201	-0.939821	-0.651590
P	-1.542929	-1.608435	-0.409179
C	-1.985206	-2.170335	-2.197917
C	-1.601083	-3.092315	0.847175
C	4.119314	-1.389350	0.641453
C	5.214273	-1.021429	1.437939
C	3.375629	-2.532213	0.961432
C	5.533343	-1.772623	2.563914
H	5.808162	-0.145299	1.172043
C	3.708858	-3.285931	2.081238
H	2.555348	-2.841366	0.311099
C	4.781510	-2.902578	2.887457
H	6.379209	-1.479554	3.189297
H	3.136400	-4.184490	2.321620
H	5.041109	-3.495868	3.767400
C	-1.811430	-0.935585	-3.082951
H	-2.550717	-0.157318	-2.845134
H	-0.806311	-0.500441	-2.992787
H	-1.959136	-1.226350	-4.135604
C	-0.947994	-3.225053	-2.608960
H	-1.031386	-4.156976	-2.033056
H	-1.112470	-3.483055	-3.667540
H	0.083032	-2.852175	-2.511383
C	-3.385943	-2.725489	-2.463738
H	-4.166487	-1.969622	-2.316482
H	-3.425947	-3.025928	-3.523258
H	-3.632466	-3.614353	-1.870662
C	-0.164626	-3.616475	0.984359
H	0.505492	-2.859584	1.412164
H	-0.168687	-4.480969	1.668080
H	0.252413	-3.952784	0.023707
C	-2.465671	-4.297932	0.454608

H	-3.542266	-4.097253	0.434314
H	-2.171127	-4.741736	-0.505335
H	-2.313417	-5.074509	1.221141
C	-2.051239	-2.557880	2.208628
H	-1.945528	-3.362800	2.953986
H	-1.432182	-1.714762	2.543765
H	-3.099946	-2.234613	2.215965
C	-2.626454	-0.201544	0.184493
C	-2.076699	1.084457	0.501135
C	-4.010067	-0.417510	0.388656
C	-2.912623	2.085567	1.057406
C	-4.813406	0.620921	0.883265
C	-4.285448	1.852754	1.262708
C	-4.733163	-1.714375	0.197158
H	-4.072453	-2.509935	-0.137523
H	-5.214975	-2.021453	1.137959
H	-5.544163	-1.621484	-0.539923
C	-0.649441	1.540714	0.315112
C	-0.301152	2.284380	-0.844912
C	0.257201	1.505483	1.404573
C	0.920179	2.963310	-0.873571
C	1.475226	2.190155	1.310620
C	1.824519	2.945102	0.192250
H	1.167459	3.566920	-1.752537
H	2.154577	2.159167	2.165501
C	-1.245285	2.446636	-2.028756
H	-1.997071	1.647166	-1.955946
C	3.075666	3.801852	0.134908
H	3.382024	3.843964	-0.925618
C	-0.058821	0.799337	2.714308
H	-1.042905	0.318758	2.599146
C	-0.538812	2.307133	-3.378590
H	-1.277610	2.255869	-4.192936
H	0.108175	3.172304	-3.592282
H	0.083443	1.401745	-3.433810
C	-1.997088	3.780717	-1.986096
H	-1.295633	4.630239	-1.994997
H	-2.652226	3.878910	-2.865747
H	-2.624428	3.870939	-1.090929
C	2.749298	5.233830	0.573699
H	3.632301	5.884506	0.477391
H	1.939746	5.667719	-0.031851
H	2.426436	5.253970	1.626875
C	4.252416	3.247184	0.930807

H	4.495066	2.213962	0.639971
H	5.148903	3.862101	0.761337
H	4.056618	3.259310	2.014641
C	0.969059	-0.286861	3.035344
H	1.091488	-0.990121	2.197648
H	1.960977	0.143786	3.243704
H	0.668381	-0.860688	3.925835
C	-0.168559	1.775675	3.889218
H	-0.919063	2.556473	3.708557
H	-0.453832	1.239357	4.807485
H	0.792378	2.276886	4.085511
C	-2.399684	3.437487	1.484770
H	-3.013802	4.244563	1.057516
H	-2.477790	3.548877	2.578518
H	-1.358351	3.622202	1.204870
C	-5.170134	2.879489	1.902252
H	-6.142217	2.446155	2.165432
H	-4.715823	3.277396	2.821522
H	-5.340360	3.742826	1.237635
O	-6.136370	0.354574	1.080027
C	-7.012415	0.802876	0.067725
H	-8.023105	0.479668	0.349001
H	-7.002399	1.902215	-0.026558
H	-6.756780	0.367540	-0.914448
H	2.656822	-0.184554	-3.248073
H	4.764843	1.994331	-3.844435
H	6.212169	1.591258	-2.715254

Int2'-PMe$_3$

C	-2.199621	-0.525206	-0.065746
C	-1.263517	-2.556076	-0.159829
C	-2.758674	-2.665720	-0.018383
O	-3.233270	-1.357519	0.008337
H	-0.894992	-2.991311	-1.104189
N	-1.041567	-1.108711	-0.139480
C	-3.579898	-3.702424	0.066535
C	-2.512982	0.900528	-0.045796
C	-1.634464	1.852182	-0.585122
C	-3.737555	1.314142	0.502581
C	-1.969331	3.200516	-0.556691
H	-0.702160	1.532507	-1.057524
C	-4.060585	2.665921	0.536266
H	-4.427179	0.571453	0.906780

C	-3.178259	3.608955	0.009611
H	-1.292084	3.938868	-0.991083
H	-5.009345	2.985536	0.972113
H	-3.438497	4.669833	0.030243
H	-0.723749	-3.046713	0.665944
H	-3.183786	-4.717766	0.042217
H	-4.656992	-3.556783	0.157855
Au	0.899285	-0.350406	-0.040462
P	3.056894	0.377703	0.116953
C	3.296398	2.062795	-0.526422
H	2.666775	2.768279	0.034556
H	4.350838	2.362882	-0.428316
H	3.008265	2.099973	-1.586803
C	4.229960	-0.667494	-0.799955
H	5.253328	-0.277176	-0.690942
H	4.192251	-1.695994	-0.413443
H	3.960278	-0.684392	-1.865617
C	3.667215	0.414832	1.830323
H	3.613793	-0.593618	2.264823
H	4.709903	0.766366	1.857430
H	3.041441	1.088004	2.433592

Int2-XPhos

C	4.758609	0.334602	-0.691667
C	3.462656	1.066620	-2.284122
C	2.906360	1.495312	-0.945094
O	3.801362	1.108599	-0.025417
H	2.738688	0.532890	-2.917685
N	4.603871	0.255764	-1.947843
C	1.807201	2.265559	-0.623002
H	1.757939	2.728454	0.366251
H	1.274134	2.767883	-1.434092
Au	0.721352	0.373070	-0.397793
P	-0.253324	-1.758033	-0.144304
C	0.054589	-2.646645	-1.816959
C	0.651182	-2.655670	1.317654
C	5.791198	-0.265126	0.143796
C	5.808834	-0.066231	1.531258
C	6.782885	-1.047118	-0.467844
C	6.812465	-0.649561	2.299192
H	5.041162	0.549715	2.002484
C	7.779555	-1.626252	0.306992
H	6.755571	-1.184459	-1.550683

C	7.795629	-1.428496	1.689801
H	6.830656	-0.491736	3.379742
H	8.553349	-2.233254	-0.168003
H	8.583533	-1.882570	2.295446
C	-0.614658	-1.786600	-2.888931
H	-1.707039	-1.758149	-2.764700
H	-0.235251	-0.755531	-2.890424
H	-0.403836	-2.223119	-3.878644
C	1.570543	-2.646384	-2.057143
H	2.113462	-3.322312	-1.382806
H	1.763021	-2.994139	-3.084805
H	2.009848	-1.642734	-1.954561
C	-0.476223	-4.072404	-1.978667
H	-1.572114	-4.107965	-1.957497
H	-0.161777	-4.434539	-2.971047
H	-0.082142	-4.779581	-1.239462
C	1.995258	-1.936017	1.514789
H	1.865044	-0.876727	1.777371
H	2.539822	-2.420805	2.341046
H	2.633683	-1.990017	0.621123
C	0.975456	-4.142052	1.117725
H	0.095595	-4.793703	1.062062
H	1.608076	-4.330057	0.240966
H	1.548449	-4.474342	1.998043
C	-0.191150	-2.491309	2.583733
H	0.377844	-2.889055	3.439598
H	-0.413963	-1.438697	2.798522
H	-1.141524	-3.038478	2.533387
C	-2.071770	-1.511920	0.190542
C	-2.625148	-0.191003	0.263223
C	-2.923251	-2.623492	0.385714
C	-4.006537	-0.027886	0.535995
C	-4.294629	-2.419449	0.599951
C	-4.847877	-1.144730	0.705054
C	-2.483880	-4.052444	0.477775
H	-1.408311	-4.163112	0.354459
H	-2.773842	-4.469313	1.454508
H	-2.975570	-4.683325	-0.276681
C	-1.890656	1.127032	0.128790
C	-1.954230	1.852180	-1.094881
C	-1.465607	1.813203	1.303606
C	-1.619065	3.210391	-1.104718
C	-1.131957	3.168797	1.227505
C	-1.223046	3.899983	0.041659

H	-1.700335	3.766403	-2.043142
H	-0.829241	3.681993	2.144679
C	-2.440060	1.226938	-2.392642
H	-2.447677	0.138120	-2.243356
C	-0.963586	5.393366	0.003853
H	-1.014321	5.696741	-1.055995
C	-1.422140	1.147033	2.670097
H	-1.678585	0.086506	2.525623
C	-1.509751	1.540540	-3.567098
H	-1.769304	0.923182	-4.440555
H	-1.591893	2.592257	-3.882546
H	-0.453540	1.351709	-3.318855
C	-3.871333	1.645340	-2.741759
H	-3.952357	2.738914	-2.846851
H	-4.177773	1.194782	-3.698575
H	-4.590275	1.325932	-1.976793
C	-2.061843	6.153716	0.752004
H	-1.910319	7.240637	0.665437
H	-3.058884	5.916744	0.351862
H	-2.062041	5.901639	1.824627
C	0.422664	5.770530	0.525694
H	1.222361	5.270265	-0.041496
H	0.583688	6.856009	0.441182
H	0.543361	5.506556	1.588563
C	-0.026087	1.222272	3.291491
H	0.742941	0.818909	2.614650
H	0.254898	2.259956	3.529847
H	0.013826	0.651548	4.232108
C	-2.459152	1.731414	3.633030
H	-3.479496	1.648747	3.235887
H	-2.428946	1.199765	4.596550
H	-2.264416	2.796241	3.836052
C	-4.660759	1.321650	0.692349
H	-5.538666	1.410378	0.034293
H	-5.042849	1.446838	1.718282
H	-3.996122	2.164478	0.480623
C	-6.300655	-0.988128	1.037820
H	-6.742595	-1.951624	1.316849
H	-6.443338	-0.294161	1.879402
H	-6.870392	-0.573429	0.189861
O	-5.073304	-3.520670	0.799331
C	-5.778325	-3.990064	-0.330380
H	-6.322827	-4.891200	-0.019740
H	-6.502897	-3.244392	-0.700065

H	-5.095085	-4.251038	-1.157848
H	3.779806	1.958608	-2.857815

TS1-*RR*-PMe$_3$

C	2.262754	-1.985775	-0.899104
C	1.784324	0.089546	-0.813561
C	2.531226	-0.132627	-2.016348
O	2.704951	-1.457557	-2.101658
H	1.787373	1.048393	-0.294478
N	1.812624	-1.095827	-0.089872
C	3.052352	0.735437	-2.999176
H	3.241676	0.275708	-3.976527
H	2.553494	1.711055	-3.042289
Au	4.951485	1.190546	-2.088864
P	6.988594	1.748464	-1.140301
C	8.359265	1.791926	-2.338388
C	-4.688302	1.354478	-2.859772
C	-5.034779	-0.806241	-2.137705
C	-4.339051	1.825349	-1.552088
C	-4.730927	-0.427997	-0.800759
C	-4.398952	0.868978	-0.489736
N	-5.026698	0.071574	-3.119712
C	-4.046949	1.248294	0.934727
N	-2.668612	0.862257	1.202825
C	-1.767904	1.664096	1.745675
C	-0.455621	1.461112	2.222048
C	-1.736811	3.088643	2.125978
C	-0.299743	2.888703	2.571635
O	0.575163	3.606166	3.013868
O	-2.533396	4.005233	2.095963
N	0.251774	0.316844	2.282447
C	1.500197	0.089806	2.852185
C	1.842060	-1.241377	3.139893
C	2.415384	1.111006	3.126444
C	3.094104	-1.541879	3.656615
H	1.103230	-2.028573	2.971265
C	3.670760	0.783358	3.640839
H	2.140156	2.156235	2.960311
C	4.028911	-0.534730	3.908236
H	5.011470	-0.772347	4.317938
H	-4.775246	-1.174303	-0.007988
H	-4.091302	2.338934	1.046782
S	-1.884832	-2.857391	1.368203

N	-1.287766	-1.621939	0.473649
C	-1.034680	-2.002827	-0.802471
O	-0.977622	-3.181637	2.478641
O	-3.281967	-2.601647	1.753420
C	-1.802458	-4.075304	0.082015
C	-2.130965	-5.421671	0.128201
C	-1.335415	-3.435968	-1.064415
C	-1.974338	-6.155126	-1.048880
H	-2.492763	-5.889435	1.046199
C	-1.185272	-4.180701	-2.235723
C	-1.508646	-5.537084	-2.215453
H	-2.217416	-7.219990	-1.059601
H	-0.820433	-3.719305	-3.155283
H	-1.394943	-6.128442	-3.126703
C	-0.537805	-1.164604	-1.787568
H	-0.417273	-1.580050	-2.788341
C	-0.134754	0.172257	-1.513904
H	-0.465806	0.534501	-0.537475
C	-0.134170	1.232244	-2.544189
C	-0.125421	0.952775	-3.920647
C	-0.143179	2.577465	-2.139949
C	-0.132384	1.983675	-4.857039
H	-0.123319	-0.081404	-4.270484
C	-0.144983	3.609203	-3.075186
H	-0.158402	2.817313	-1.073006
C	-0.139543	3.315120	-4.439597
H	-0.132858	1.744295	-5.923199
H	-0.163371	4.647554	-2.735684
H	-0.144940	4.122236	-5.176285
H	-0.181816	-0.496686	1.824412
H	-2.372743	-0.097927	0.968202
C	6.998052	3.384795	-0.340887
C	2.431205	-3.418534	-0.705568
C	1.865014	-4.032353	0.422415
C	3.155327	-4.191545	-1.626145
C	2.037170	-5.395817	0.632070
H	1.270942	-3.437882	1.117589
C	3.319229	-5.557190	-1.410461
H	3.592219	-3.717328	-2.506740
C	2.765244	-6.161584	-0.281076
H	1.594040	-5.863639	1.514091
H	3.886050	-6.153944	-2.128923
H	2.897526	-7.233340	-0.114179
C	-5.396871	-2.208973	-2.470785

C	-5.993225	-2.492762	-3.709756
C	-5.156647	-3.272044	-1.585631
C	-6.349012	-3.793948	-4.050273
H	-6.170305	-1.663664	-4.396955
C	-5.509633	-4.576070	-1.930225
H	-4.669915	-3.096683	-0.623656
C	-6.110181	-4.843097	-3.160126
H	-6.818706	-3.992486	-5.017178
H	-5.306660	-5.390329	-1.230325
H	-6.389403	-5.865783	-3.425928
C	-3.960733	3.175982	-1.386307
C	-4.665925	2.274791	-3.937454
H	-3.659038	3.571706	-0.414530
C	-4.300219	3.587890	-3.755693
C	-3.930032	4.045733	-2.465010
H	-4.289329	4.265577	-4.609811
H	-4.943243	1.902848	-4.925976
C	-4.974991	0.624620	1.993056
C	-4.607777	1.058060	3.434454
H	-4.855887	-0.468472	1.921389
C	-6.723987	2.285248	2.048236
C	-5.913874	1.330069	4.188522
H	-3.978371	1.962444	3.434844
H	-4.027729	0.271572	3.940955
C	-6.621503	2.562303	3.579819
H	-6.061808	2.965889	1.490101
H	-7.743905	2.491328	1.687835
H	-5.707146	1.511180	5.254400
N	-6.382013	0.908043	1.715178
C	-5.946387	3.865202	3.877554
H	-4.935244	3.998253	3.467682
C	-6.489166	4.866431	4.575735
H	-7.498460	4.789341	4.995407
H	-5.947016	5.799662	4.753110
C	-6.843717	0.123147	4.020936
H	-6.336093	-0.786599	4.380789
H	-7.748104	0.250073	4.636841
C	-7.201865	0.005039	2.517490
H	-7.056729	-1.023863	2.151847
H	-8.258484	0.260578	2.339439
C	7.523169	0.594462	0.163374
C	4.683319	1.878305	3.829100
C	3.477668	-2.973168	3.915004
F	2.417718	-3.783337	3.954119

F	4.130862	-3.107736	5.074486
F	4.293331	-3.439285	2.958185
F	5.596662	1.570509	4.752110
F	5.357663	2.112624	2.684030
F	4.121733	3.034146	4.183279
H	-7.636060	2.604574	4.011880
O	-3.533701	5.308219	-2.212171
C	-3.484531	6.242934	-3.261717
H	-2.772093	5.939038	-4.047416
H	-4.476649	6.401869	-3.716994
H	-3.143217	7.187702	-2.820850
H	8.508833	0.889060	0.554545
H	6.787241	0.612311	0.979597
H	7.579235	-0.424375	-0.244646
H	7.996541	3.604000	0.066756
H	6.723742	4.156588	-1.073633
H	6.262816	3.391315	0.476250
H	8.463106	0.805079	-2.811298
H	8.137972	2.534192	-3.118260
H	9.300917	2.058489	-1.835202

TS2-PMe$_3$

C	3.743660	1.530287	0.483188
C	3.113953	-0.023441	1.841459
C	3.088499	-0.561085	0.508473
O	3.402222	0.443983	-0.310216
H	3.473976	-0.652046	2.665385
N	3.651515	1.289012	1.734508
C	2.805213	-1.847239	-0.020879
C	4.118281	2.761570	-0.199654
C	4.591949	3.843857	0.557492
C	3.988531	2.884932	-1.589755
C	4.928309	5.035258	-0.072890
H	4.693076	3.731247	1.638868
C	4.322495	4.084666	-2.211691
H	3.610652	2.045944	-2.176751
C	4.791597	5.158953	-1.457412
H	5.299302	5.876323	0.517105
H	4.208456	4.183442	-3.293263
H	5.050467	6.099448	-1.949208
H	1.892127	0.210556	2.303213
H	2.440373	-1.816403	-1.057184
Au	4.654946	-2.904337	-0.095734

P	6.598407	-4.166895	-0.212669
C	6.497445	-5.736962	0.708157
H	7.435314	-6.305967	0.616576
H	6.300769	-5.529341	1.769733
H	5.666610	-6.340800	0.315726
C	8.079694	-3.332542	0.446955
H	8.962937	-3.984616	0.366230
H	8.260767	-2.405120	-0.115094
H	7.917383	-3.071026	1.502410
C	7.057061	-4.651650	-1.909588
H	7.214603	-3.751366	-2.520745
H	7.977926	-5.254693	-1.907434
H	6.241704	-5.236530	-2.359032
H	2.149203	-2.440764	0.627411
C	0.413547	2.778409	-2.599686
C	0.102048	4.545271	-1.151330
C	0.259511	1.790392	-1.574896
C	-0.082262	3.637727	-0.064846
C	-0.007980	2.277459	-0.254248
N	0.328081	4.105618	-2.369325
C	-0.298617	1.300283	0.873299
N	-1.710517	0.915031	0.780124
C	-2.119894	-0.338913	0.523941
C	-3.360911	-0.936988	0.265005
C	-1.419209	-1.631909	0.521619
C	-2.742726	-2.298786	0.171759
O	-3.111387	-3.416654	-0.061541
O	-0.275576	-1.974503	0.722810
N	-4.583666	-0.386805	0.145179
C	-5.821172	-0.981990	-0.142673
C	-5.972641	-2.349619	-0.379815
C	-6.940551	-0.140352	-0.187976
C	-7.244293	-2.854451	-0.651650
H	-5.109769	-3.021726	-0.354443
C	-8.196222	-0.662593	-0.467505
H	-6.837381	0.931333	-0.000576
C	-8.362039	-2.028179	-0.698476
H	-9.348282	-2.442254	-0.910763
H	-0.306105	4.042160	0.922844
H	0.273268	0.378838	0.695274
H	-4.637753	0.615895	0.284073
H	-2.346611	1.676310	0.566569
C	0.023427	6.012960	-0.950222
C	0.110567	6.603364	0.319187

C	-0.136158	6.848119	-2.066674
C	0.030737	7.985709	0.469422
H	0.267903	5.988104	1.207974
C	-0.220671	8.227444	-1.915866
H	-0.193176	6.384668	-3.052867
C	-0.139666	8.802668	-0.646845
H	0.107624	8.428338	1.465380
H	-0.352809	8.861656	-2.795771
H	-0.206229	9.886779	-0.528603
C	0.382714	0.426897	-1.910675
C	0.677407	2.343952	-3.922690
H	0.276166	-0.364127	-1.167407
C	0.801694	1.009244	-4.230606
C	0.661131	0.033601	-3.210781
H	1.009092	0.712124	-5.259137
H	0.783789	3.113036	-4.690052
C	0.140117	1.825732	2.271309
C	-0.966752	2.471538	3.136948
H	0.934737	2.559920	2.076724
C	-0.132425	-0.217108	3.596948
C	-0.844815	1.960999	4.574712
H	-1.964311	2.229639	2.744713
H	-0.876185	3.568714	3.122258
C	-1.092790	0.436564	4.627286
H	-0.678155	-0.657501	2.755918
H	0.444169	-1.037675	4.048420
H	-1.576034	2.472133	5.217731
N	0.819390	0.771012	3.066922
C	-2.519768	0.038542	4.394570
H	-2.929126	0.250242	3.397933
C	-3.300825	-0.554748	5.298050
H	-2.933867	-0.797250	6.300794
H	-4.335721	-0.823710	5.072098
C	0.579184	2.228604	5.062492
H	0.806709	3.303434	4.988469
H	0.681454	1.955718	6.123435
C	1.543810	1.401207	4.191905
H	2.361760	2.000457	3.767073
H	2.008738	0.584957	4.765223
C	-9.387161	0.257317	-0.568927
C	-7.384571	-4.342689	-0.867258
F	-6.485086	-4.786865	-1.745708
F	-8.595174	-4.662736	-1.322738
F	-7.190617	-5.009697	0.272406

F	-9.677647	0.525157	-1.843498
F	-10.469864	-0.288602	-0.018656
F	-9.158927	1.423870	0.041960
H	-0.817621	0.101155	5.640921
O	0.795266	-1.288650	-3.419038
C	1.004792	-1.772571	-4.721753
H	1.041266	-2.866077	-4.643883
H	0.180151	-1.493191	-5.399031
H	1.958361	-1.413200	-5.145577

TS2-XPhos

C	0.054767	-2.835490	0.613440
C	0.250724	-0.705814	0.884156
C	1.357673	-1.336848	1.543726
O	1.146896	-2.659434	1.452066
H	0.385599	0.246699	0.359295
N	-0.464665	-1.736335	0.221563
C	2.515358	-0.842678	2.194796
C	-0.346010	-4.206424	0.322393
C	-1.432064	-4.434247	-0.536887
C	0.334548	-5.293788	0.888327
C	-1.828932	-5.735501	-0.819590
H	-1.956230	-3.584427	-0.977916
C	-0.069869	-6.593780	0.597850
H	1.177248	-5.115902	1.558793
C	-1.150946	-6.817216	-0.253858
H	-2.679346	-5.907834	-1.482986
H	0.460268	-7.438682	1.043219
H	-1.469463	-7.838482	-0.475874
H	-0.644033	-0.321154	1.825321
H	2.905156	-1.492487	2.988472
Au	3.957565	-0.975922	0.605239
H	2.467812	0.217684	2.467461
P	5.425355	-1.465797	-1.173966
C	6.250431	-3.116467	-0.640816
C	6.703163	-0.116449	-1.402667
C	4.335863	-1.706217	-2.767983
C	7.024487	-2.807648	0.640836
C	5.112266	-4.091328	-0.306263
C	7.223220	-3.796548	-1.606025
C	6.693738	1.044398	-0.560861
C	7.689651	-0.218575	-2.410977
C	2.887305	-1.902483	-2.290322

C	4.661091	-2.911220	-3.660793
C	4.406195	-0.427282	-3.604470
H	7.868494	-2.128282	0.450265
H	6.383082	-2.363400	1.413519
H	7.437058	-3.746619	1.044530
H	4.541074	-4.403294	-1.191767
H	5.547812	-5.001815	0.136403
H	4.405783	-3.663574	0.422106
H	8.128896	-3.199477	-1.766468
H	7.542267	-4.745399	-1.144262
H	6.783856	-4.045969	-2.578983
C	7.660325	2.062318	-0.762070
C	5.709977	1.376412	0.538944
C	8.661679	0.784719	-2.539431
C	7.762383	-1.287605	-3.458226
H	2.510123	-1.031675	-1.736920
H	2.240025	-2.041777	-3.171671
H	2.771628	-2.789073	-1.649451
H	5.635842	-2.856809	-4.159321
H	4.590485	-3.870204	-3.131083
H	3.906997	-2.938702	-4.464011
H	3.690771	-0.511511	-4.438750
H	4.127728	0.459844	-3.022063
H	5.401430	-0.255738	-4.034423
C	8.651367	1.934653	-1.753582
C	7.679068	3.344647	0.031693
C	6.058749	1.152703	1.896012
C	4.591549	2.202594	0.249490
O	9.585336	0.647472	-3.535912
H	6.973077	-2.028312	-3.350590
H	7.690460	-0.834895	-4.459263
H	8.725469	-1.817803	-3.436174
C	9.651718	3.022006	-2.005739
H	8.674476	3.523602	0.466556
H	7.478682	4.206227	-0.625936
H	6.946732	3.369898	0.843813
C	5.315458	1.774738	2.904814
C	7.257855	0.312898	2.306114
C	3.880140	2.793027	1.298272
C	4.155716	2.519217	-1.171596
C	10.830128	0.111070	-3.145432
H	10.211401	2.831228	-2.928806
H	9.157595	3.999897	-2.105203
H	10.368711	3.117242	-1.173473

C	4.239885	2.619377	2.636072
H	5.609503	1.621264	3.946896
H	7.556874	-0.271407	1.424748
C	6.918031	-0.668778	3.430426
C	8.460473	1.169782	2.711492
H	3.038239	3.447003	1.051391
H	4.794723	1.929778	-1.846477
C	2.700442	2.113825	-1.411691
C	4.359985	3.993235	-1.531640
H	11.442617	0.019980	-4.052143
H	11.352078	0.766173	-2.426635
H	10.718910	-0.887377	-2.686345
C	3.527159	3.352772	3.756039
H	7.731869	-1.397949	3.564620
H	6.788514	-0.153976	4.395261
H	5.989500	-1.223128	3.225143
H	8.207431	1.836885	3.551068
H	9.295726	0.528681	3.034483
H	8.819210	1.792907	1.882278
H	2.522002	1.066688	-1.121225
H	2.007742	2.744761	-0.834489
H	2.423809	2.229181	-2.471098
H	5.404941	4.305751	-1.400483
H	4.083306	4.172097	-2.582320
H	3.730522	4.649508	-0.909868
H	4.032235	3.066624	4.694442
C	3.659479	4.869284	3.605587
C	2.061492	2.936467	3.883133
H	3.208857	5.388795	4.465853
H	4.714763	5.173190	3.541044
H	3.152579	5.226932	2.695021
H	1.969153	1.856419	4.074830
H	1.574568	3.469999	4.715012
H	1.502486	3.169243	2.961666
C	-1.670569	1.230094	-2.432555
C	-1.126408	2.912680	-0.952313
C	-2.387231	0.475166	-1.449718
C	-1.824617	2.237403	0.093005
C	-2.444278	1.029668	-0.129352
N	-1.065508	2.407898	-2.164668
C	-3.276680	0.336064	0.935539
N	-4.675475	0.696229	0.702796
C	-5.642705	-0.222057	0.566430
C	-7.003179	-0.210031	0.232713

C	-5.640071	-1.675046	0.802663
C	-7.109261	-1.695894	0.395895
O	-7.961465	-2.532506	0.276618
O	-4.803745	-2.471119	1.165544
N	-7.806711	0.814365	-0.117111
C	-9.166880	0.826118	-0.453252
C	-9.959651	-0.325427	-0.469515
C	-9.734057	2.063278	-0.783947
C	-11.303635	-0.218430	-0.821576
H	-9.536880	-1.300809	-0.211503
C	-11.078870	2.148535	-1.123055
H	-9.124757	2.970641	-0.782626
C	-11.877755	1.007284	-1.148440
H	-12.932230	1.071639	-1.419009
H	-1.871052	2.708664	1.074267
H	-3.204300	-0.749510	0.781836
H	-7.373054	1.729808	-0.146346
H	-4.851986	1.658667	0.438160
C	-0.449705	4.213545	-0.714737
C	-0.197304	4.709478	0.573423
C	-0.030334	4.977346	-1.815266
C	0.453194	5.928563	0.756029
H	-0.494809	4.140600	1.457040
C	0.615319	6.195215	-1.633343
H	-0.225946	4.586682	-2.815117
C	0.861481	6.677325	-0.346624
H	0.640295	6.296206	1.767978
H	0.926810	6.777979	-2.503610
H	1.366119	7.635762	-0.203903
C	-2.985298	-0.743655	-1.821279
C	-1.590758	0.719499	-3.752326
H	-3.526941	-1.360323	-1.103836
C	-2.180239	-0.473953	-4.095760
C	-2.884509	-1.222642	-3.117533
H	-2.100262	-0.837892	-5.120617
H	-1.043837	1.312158	-4.487888
C	-2.861872	0.606821	2.393942
C	-3.951822	0.297353	3.439423
H	-2.594830	1.669098	2.493027
C	-1.960248	-1.540105	3.161268
C	-3.264673	-0.162152	4.730522
H	-4.630537	-0.490467	3.081539
H	-4.568053	1.192013	3.612314
C	-2.699694	-1.583778	4.516431

H	-2.577795	-1.982103	2.365496
H	-1.018998	-2.108778	3.197772
H	-3.977704	-0.163894	5.566981
N	-1.633710	-0.144472	2.776734
C	-3.724661	-2.678999	4.553845
H	-4.426818	-2.726624	3.711772
C	-3.810426	-3.591096	5.523121
H	-3.115409	-3.598656	6.369750
H	-4.579168	-4.367643	5.506099
C	-2.080302	0.764391	5.027447
H	-2.413834	1.814271	5.049917
H	-1.655781	0.547375	6.019026
C	-1.020285	0.544083	3.930521
H	-0.579673	1.488823	3.578082
H	-0.190490	-0.086846	4.282851
C	-11.690428	3.495353	-1.415621
C	-12.135155	-1.476612	-0.898806
F	-11.983867	-2.074607	-2.083409
F	-13.433658	-1.212230	-0.747743
F	-11.782194	-2.353322	0.039493
F	-12.633553	3.409778	-2.351418
F	-12.256500	4.013586	-0.322889
F	-10.770582	4.368907	-1.837323
H	-1.976806	-1.776200	5.327552
O	-3.467198	-2.408557	-3.363012
C	-3.437694	-2.947035	-4.660495
H	-3.990584	-3.893364	-4.616177
H	-3.930725	-2.282973	-5.390678
H	-2.406695	-3.152784	-4.996018

TS3-PMe$_3$

C	-3.165622	-1.224737	-1.011145
C	-1.174654	-1.641643	-1.799344
C	-1.509901	-0.184457	-2.012764
O	-2.785733	-0.027721	-1.613268
H	-0.215649	-1.800734	-1.283027
N	-2.296981	-2.150895	-1.049874
C	-0.786044	0.835403	-2.565801
C	-4.494232	-1.249495	-0.410324
C	-4.939701	-2.435709	0.193104
C	-5.322946	-0.118531	-0.433629
C	-6.200869	-2.483414	0.772980
H	-4.284441	-3.309131	0.190940

C	-6.585559	-0.176315	0.149848
H	-4.979405	0.798435	-0.915652
C	-7.024158	-1.354868	0.752662
H	-6.549808	-3.406918	1.240094
H	-7.234152	0.702147	0.128753
H	-8.017237	-1.397203	1.206257
H	-1.096089	-2.163006	-2.772492
H	0.148707	0.589420	-3.073834
H	-1.302227	1.758403	-2.842513
Au	-0.016652	1.247600	-0.348085
P	-0.535222	0.562253	1.825820
C	-2.244102	0.986671	2.303702
H	-2.962112	0.514878	1.617206
H	-2.450598	0.643341	3.329132
H	-2.382090	2.076599	2.255808
C	0.496599	1.265089	3.152085
H	0.141100	0.919673	4.135118
H	1.528676	0.922218	2.994094
H	0.459578	2.363375	3.120692
C	-0.394073	-1.237594	2.051758
H	0.651993	-1.516407	1.859088
H	-0.668462	-1.515755	3.080975
H	-1.054476	-1.760762	1.344147
C	3.660079	-0.058177	0.514061
C	3.226035	2.341539	0.397965
C	2.159469	2.583325	-0.587942
O	2.598958	-0.233860	1.100912
H	2.784792	2.230719	1.398373
N	4.041397	1.189973	0.118695
C	1.392721	2.879799	-1.497536
C	4.594357	-1.175227	0.194709
C	5.952367	-0.978719	-0.091754
C	4.080448	-2.477422	0.219051
C	6.775025	-2.066983	-0.369112
H	6.393391	0.021292	-0.064645
C	4.901935	-3.563125	-0.064188
H	3.026550	-2.619900	0.465096
C	6.249846	-3.358932	-0.361103
H	7.834369	-1.906975	-0.581204
H	4.492538	-4.575679	-0.049206
H	6.897250	-4.211617	-0.578788
H	4.819047	1.292385	-0.519896
H	3.862809	3.240807	0.422280
H	0.900976	3.296417	-2.362005

TS3-XPhos

C	4.325802	1.742978	-1.401236
C	3.174883	3.148144	-0.197116
C	2.292499	2.567477	-1.266036
O	3.085577	1.750638	-2.006543
N	4.436228	2.462856	-0.356802
C	0.981391	2.738774	-1.530429
H	0.554163	2.343576	-2.450887
H	0.425541	3.504273	-0.988253
Au	-0.085522	0.693094	-0.123746
P	-0.704168	-1.544174	-0.527424
C	0.244006	-2.444532	0.880345
C	-0.051434	-2.046038	-2.290533
C	5.358892	0.933407	-2.042959
C	5.049849	0.067882	-3.100358
C	6.685671	1.058429	-1.604674
C	6.059796	-0.677124	-3.702832
H	4.019250	-0.012735	-3.449865
C	7.688907	0.314063	-2.214081
H	6.911756	1.754920	-0.794496
C	7.376919	-0.556229	-3.261277
H	5.819642	-1.351430	-4.527765
H	8.723636	0.419921	-1.880099
H	8.168313	-1.136266	-3.741942
C	-0.298929	-1.874540	2.192224
H	-1.335896	-2.194161	2.371727
H	-0.262446	-0.776691	2.213943
H	0.324757	-2.234816	3.025300
C	1.719838	-2.054280	0.730991
H	2.180112	-2.456123	-0.181956
H	2.276571	-2.462989	1.587556
H	1.862606	-0.962266	0.736899
C	0.149716	-3.969146	0.970092
H	-0.866613	-4.311564	1.198706
H	0.790784	-4.285051	1.808714
H	0.512619	-4.490556	0.075630
C	0.977337	-0.982677	-2.701651
H	0.528563	0.015410	-2.778692
H	1.376876	-1.244477	-3.695132
H	1.825834	-0.919158	-2.005450
C	0.660326	-3.401121	-2.407075
H	0.008424	-4.269414	-2.263524

H	1.522079	-3.492367	-1.733240
H	1.051795	-3.478664	-3.434100
C	-1.225422	-1.997258	-3.270741
H	-0.835555	-2.121622	-4.294113
H	-1.754708	-1.035656	-3.233845
H	-1.958611	-2.794807	-3.095285
C	-2.557849	-1.801824	-0.415342
C	-3.464243	-0.716893	-0.177037
C	-3.093423	-3.095865	-0.621407
C	-4.862463	-0.947232	-0.216452
C	-4.482399	-3.292368	-0.586429
C	-5.378994	-2.238212	-0.432670
C	-2.311720	-4.326998	-0.959378
H	-1.243695	-4.135628	-1.017493
H	-2.655073	-4.742068	-1.919301
H	-2.467449	-5.121029	-0.214613
C	-3.106531	0.719086	0.119880
C	-3.110397	1.169991	1.465757
C	-3.074421	1.675956	-0.931447
C	-3.076424	2.546230	1.719382
C	-2.987553	3.036618	-0.615227
C	-3.007956	3.501762	0.702299
H	-3.110108	2.892590	2.756107
H	-2.967120	3.761607	-1.434001
C	-3.226030	0.218448	2.649637
H	-2.957374	-0.783931	2.285038
C	-3.022612	4.984693	1.022168
H	-2.940630	5.072168	2.119140
C	-3.261160	1.292235	-2.393974
H	-3.343670	0.194936	-2.437778
C	-2.275113	0.574597	3.794606
H	-2.247845	-0.242737	4.531097
H	-2.606865	1.476371	4.332757
H	-1.248890	0.753603	3.445565
C	-4.657568	0.136463	3.189443
H	-5.020387	1.128514	3.502835
H	-4.692788	-0.523998	4.069817
H	-5.359841	-0.261558	2.447104
C	-4.352333	5.620258	0.609174
H	-4.387730	6.679140	0.908268
H	-5.204259	5.105687	1.077825
H	-4.493661	5.577056	-0.482657
C	-1.838053	5.732606	0.410211
H	-0.874481	5.320262	0.749822

H	-1.860943	6.794944	0.697152
H	-1.856405	5.692839	-0.690761
C	-2.084510	1.706699	-3.274476
H	-1.149376	1.245747	-2.928685
H	-1.943848	2.799216	-3.279494
H	-2.251708	1.393553	-4.316491
C	-4.559114	1.871738	-2.967026
H	-5.434662	1.603427	-2.362374
H	-4.725132	1.497825	-3.989117
H	-4.517262	2.970982	-3.021887
C	-5.881209	0.154108	-0.066907
H	-6.625856	-0.098158	0.702973
H	-6.449215	0.276579	-1.003279
H	-5.447158	1.124510	0.191998
C	-6.852976	-2.489612	-0.531699
H	-7.050768	-3.503313	-0.899431
H	-7.331450	-1.778939	-1.221558
H	-7.355032	-2.366959	0.442403
O	-4.945708	-4.555656	-0.809525
C	-5.292045	-5.295702	0.342036
H	-5.603337	-6.292630	0.003807
H	-6.126069	-4.829308	0.893731
H	-4.435334	-5.401329	1.030739
H	3.306810	4.237831	-0.328707
C	3.483139	-0.411046	3.127143
C	2.230430	1.659474	3.204185
C	1.138178	2.011721	2.290755
O	2.686261	-0.920346	3.896472
H	1.806286	1.070398	4.035749
N	3.295605	0.863599	2.653546
C	0.179343	2.348272	1.608316
C	4.699991	-1.140123	2.659057
C	5.479821	-0.744433	1.564725
C	5.047693	-2.296126	3.369504
C	6.592020	-1.496405	1.192276
H	5.224380	0.140998	0.976023
C	6.165131	-3.038105	3.002750
H	4.422858	-2.590092	4.215238
C	6.938400	-2.639435	1.912017
H	7.186118	-1.187658	0.329424
H	6.435833	-3.932001	3.569396
H	7.814782	-3.223154	1.620076
H	4.028664	1.316492	2.119849
H	2.622025	2.599437	3.632756

H	-0.726615	2.837704	1.261300
H	2.739109	3.015946	0.805578

TS4-PMe$_3$

C	-3.410285	-0.782064	-0.881982
C	-2.352822	-2.685223	-0.749072
C	-1.470823	-1.662334	-1.427719
O	-2.232402	-0.561073	-1.590844
H	-1.873842	-3.199069	0.096781
N	-3.518750	-1.932118	-0.354554
C	-0.198340	-1.740572	-1.923564
C	-4.350755	0.331922	-0.835340
C	-5.566380	0.163360	-0.155040
C	-4.062276	1.550279	-1.465712
C	-6.479105	1.209270	-0.103069
H	-5.778893	-0.797076	0.318996
C	-4.983786	2.592095	-1.410185
H	-3.121960	1.672979	-2.005763
C	-6.189413	2.423656	-0.729800
H	-7.426954	1.077753	0.423374
H	-4.763402	3.539695	-1.906607
H	-6.912165	3.242143	-0.691556
H	-2.639375	-3.473849	-1.471413
H	0.287971	-2.718855	-1.941777
H	0.155187	-0.976724	-2.619877
Au	0.467692	-0.906283	0.173157
P	-0.160086	-0.511902	2.361832
C	-1.897453	0.002347	2.564432
H	-2.563322	-0.766176	2.144800
H	-2.135026	0.153860	3.628673
H	-2.071816	0.941458	2.019554
C	0.803999	0.782735	3.210830
H	0.450114	0.917090	4.244662
H	1.866493	0.500334	3.222862
H	0.708569	1.733093	2.665675
C	0.010562	-1.983021	3.426457
H	1.054584	-2.327348	3.422588
H	-0.288241	-1.747155	4.459496
H	-0.625831	-2.794312	3.045127
C	3.318102	0.502247	-0.716030
C	3.406823	-1.663811	-1.167097
C	4.770213	-1.039142	-1.334100
O	4.603735	0.308218	-1.045036

H	3.402188	-2.469370	-0.413922
N	2.572929	-0.547788	-0.738797
C	5.948927	-1.539428	-1.680779
C	2.938734	1.872030	-0.368062
C	1.601797	2.288881	-0.443260
C	3.929667	2.782853	0.026395
C	1.259587	3.594385	-0.107326
H	0.834708	1.593813	-0.794267
C	3.579384	4.085156	0.368754
H	4.971860	2.461618	0.065332
C	2.246776	4.491694	0.304849
H	0.220058	3.921291	-0.183162
H	4.352867	4.789822	0.681427
H	1.976755	5.517918	0.565008
H	3.026355	-2.097333	-2.108414
H	6.047868	-2.601831	-1.904169
H	6.830116	-0.900563	-1.751242

TS1-*RR*

C	0.026171	1.790627	1.563436
C	-0.329343	-0.150971	0.762225
C	0.754973	-0.262522	1.695487
O	0.871236	0.945566	2.264228
H	-0.441213	-0.827784	-0.084800
N	-0.604172	1.203435	0.611006
C	1.601828	-1.324398	2.069214
H	2.118924	-1.189943	3.025661
H	1.154906	-2.315516	1.921057
Au	3.078596	-1.370540	0.497845
P	4.437738	-1.776908	-1.385780
C	4.489642	-3.705383	-1.628033
C	-5.051843	-4.235364	1.167499
C	-5.782839	-2.304504	2.194085
C	-4.831555	-3.586077	-0.090956
C	-5.633292	-1.582648	0.977605
C	-5.172908	-2.199350	-0.162305
N	-5.512985	-3.592303	2.262596
C	-5.048568	-1.407994	-1.447963
N	-4.045794	-0.355853	-1.329813
C	-3.156544	-0.121783	-2.284635
C	-2.336161	0.974732	-2.638833
C	-2.685406	-0.901410	-3.442432
C	-1.676071	0.193021	-3.707382

O	-0.736100	0.330660	-4.466827
O	-3.000027	-1.954683	-3.962289
N	-2.312655	2.228544	-2.152502
C	-1.471623	3.280526	-2.494959
C	-1.811606	4.560743	-2.027230
C	-0.314031	3.119789	-3.268147
C	-0.998874	5.649109	-2.317589
H	-2.718956	4.688899	-1.434100
C	0.488271	4.225870	-3.539177
H	-0.060253	2.140978	-3.682925
C	0.164930	5.498021	-3.071299
H	0.803620	6.354147	-3.294295
H	-5.889226	-0.523690	0.946647
H	-4.706993	-2.064786	-2.256804
S	-4.739672	2.524174	0.881578
N	-3.791923	1.224441	1.082939
C	-3.198422	1.208351	2.297952
O	-4.219648	3.363154	-0.223343
O	-6.156556	2.158509	0.741015
C	-4.416624	3.248498	2.467340
C	-4.897281	4.428810	3.013265
C	-3.562281	2.377176	3.144151
C	-4.487177	4.742372	4.310351
H	-5.565927	5.086051	2.453737
C	-3.163004	2.702116	4.441223
C	-3.631922	3.885334	5.012565
H	-4.837961	5.663534	4.780913
H	-2.495690	2.047888	5.005459
H	-3.324913	4.148082	6.027411
C	-2.333019	0.214126	2.724268
H	-1.941270	0.282769	3.739663
C	-1.923637	-0.839892	1.859024
H	-2.517156	-0.901593	0.942311
C	-1.499550	-2.162697	2.361948
C	-1.096941	-2.376152	3.690443
C	-1.483469	-3.256317	1.480149
C	-0.699963	-3.639869	4.121544
H	-1.099277	-1.548708	4.402698
C	-1.079248	-4.518322	1.908181
H	-1.803867	-3.115556	0.443985
C	-0.685781	-4.715309	3.232793
H	-0.397621	-3.785205	5.161534
H	-1.081793	-5.354600	1.205063
H	-0.373351	-5.705660	3.572804

H	-3.030163	2.471193	-1.457602
H	-4.035075	0.232560	-0.476320
C	3.483554	-0.915351	-2.817984
C	0.005662	3.186498	1.977015
C	-0.940047	4.058793	1.417411
C	0.906505	3.668506	2.939201
C	-0.969379	5.394971	1.802080
H	-1.660473	3.671607	0.695563
C	0.869157	5.006827	3.321549
H	1.635575	2.989889	3.385012
C	-0.064351	5.873538	2.752311
H	-1.706247	6.067776	1.358622
H	1.575101	5.375638	4.069428
H	-0.090909	6.923714	3.052903
C	-6.266619	-1.636667	3.432426
C	-6.476249	-2.403766	4.590071
C	-6.522547	-0.257064	3.493024
C	-6.927311	-1.815959	5.767343
H	-6.274884	-3.474962	4.538224
C	-6.972222	0.330965	4.674702
H	-6.372723	0.382738	2.621061
C	-7.177856	-0.443030	5.816115
H	-7.085454	-2.433403	6.655446
H	-7.162353	1.406987	4.699648
H	-7.531992	0.020925	6.740157
C	-4.300746	-4.335098	-1.165220
C	-4.763341	-5.619186	1.273447
H	-4.076437	-3.874360	-2.129100
C	-4.265444	-6.336081	0.210745
C	-4.020045	-5.685649	-1.026234
H	-4.055796	-7.399373	0.330819
H	-4.945426	-6.100541	2.236446
C	-6.396808	-0.785447	-1.869637
C	-6.311895	-0.003513	-3.203348
H	-6.680221	-0.082201	-1.068876
C	-7.343946	-2.617921	-3.119535
C	-7.575426	-0.315808	-4.012601
H	-5.418579	-0.287560	-3.782493
H	-6.230739	1.078304	-3.016614
C	-7.573783	-1.804500	-4.430069
H	-6.349906	-3.091043	-3.131156
H	-8.070698	-3.441859	-3.045241
H	-7.620164	0.320484	-4.909667
N	-7.460301	-1.786171	-1.928499

C	-6.572653	-2.143727	-5.490689
H	-5.513798	-2.027117	-5.220046
C	-6.873356	-2.593269	-6.712145
H	-7.912545	-2.740354	-7.027022
H	-6.094154	-2.832204	-7.441547
C	-8.802900	-0.079349	-3.125031
H	-8.795135	0.957924	-2.752447
H	-9.727052	-0.201247	-3.711940
C	-8.745601	-1.093880	-1.954235
H	-8.897435	-0.594238	-0.984453
H	-9.536623	-1.854696	-2.048449
C	5.796417	-4.238483	-1.038717
H	6.681687	-3.903852	-1.594685
H	5.920288	-3.945344	0.011558
H	5.773686	-5.339911	-1.073524
C	3.319595	-4.287788	-0.818413
H	2.343958	-3.921803	-1.169127
H	3.326698	-5.384526	-0.930492
H	3.402410	-4.057590	0.253053
C	4.330059	-4.227667	-3.061702
H	4.280543	-5.327290	-3.007034
H	3.399467	-3.893806	-3.539003
H	5.170865	-3.988585	-3.722193
C	3.440392	0.567642	-2.454992
H	2.983394	0.732805	-1.470601
H	4.443736	1.018303	-2.460424
H	2.833755	1.099896	-3.203934
C	2.052249	-1.470260	-2.789361
H	1.437138	-0.903403	-3.507052
H	1.998336	-2.529211	-3.077693
H	1.592146	-1.361187	-1.794975
C	4.023852	-1.019193	-4.245685
H	4.988559	-0.510618	-4.363609
H	4.111737	-2.048525	-4.614496
H	3.306109	-0.502873	-4.903701
C	6.167968	-1.086906	-1.172375
C	6.540248	-0.397036	0.028464
C	7.145902	-1.275947	-2.177233
C	7.859304	0.104702	0.168488
C	8.438086	-0.758507	-2.001137
C	8.804916	-0.043606	-0.863480
C	6.938559	-2.011812	-3.464493
H	5.909685	-2.337299	-3.593667
H	7.210503	-1.377498	-4.320574

H	7.585285	-2.901023	-3.522226
C	5.676713	-0.135857	1.241720
C	5.727417	-1.029116	2.344123
C	5.067207	1.132682	1.418299
C	5.180044	-0.641666	3.570964
C	4.550838	1.473175	2.673765
C	4.604925	0.614891	3.770659
H	5.238568	-1.338935	4.411843
H	4.106047	2.463247	2.807528
C	6.419442	-2.381349	2.268590
H	6.708307	-2.541946	1.219036
C	4.085733	1.048119	5.128645
H	3.747753	2.093085	5.017854
C	4.994239	2.175603	0.312715
H	5.245009	1.667964	-0.629324
C	5.493700	-3.525731	2.684726
H	4.547706	-3.504410	2.122680
H	5.976892	-4.499662	2.508761
H	5.243784	-3.474671	3.756109
C	7.706501	-2.413703	3.097200
H	8.415290	-1.636249	2.780787
H	7.494792	-2.259457	4.167523
H	8.205856	-3.390065	2.993416
C	2.879808	0.222008	5.578344
H	2.513075	0.569881	6.557052
H	2.050919	0.301731	4.859265
H	3.140370	-0.843940	5.681195
C	5.190961	1.035687	6.186132
H	6.049270	1.650891	5.875896
H	4.816546	1.430245	7.143794
H	5.559199	0.013791	6.370826
C	3.590916	2.772954	0.175140
H	2.810760	1.997623	0.187407
H	3.368062	3.476335	0.992611
H	3.499297	3.331922	-0.768709
C	6.011403	3.304774	0.500659
H	7.045789	2.938717	0.482206
H	5.904870	4.048961	-0.304515
H	5.852347	3.824886	1.459184
C	8.348455	0.796050	1.416390
H	7.591428	0.866440	2.202872
H	9.220552	0.264351	1.829666
H	8.698716	1.816013	1.194059
C	10.177651	0.548849	-0.756068

H	10.783759	0.039022	0.010822
H	10.706459	0.486890	-1.714422
H	10.127632	1.607643	-0.461072
O	9.339858	-0.938729	-3.014204
C	10.239345	-2.015692	-2.844193
H	10.855630	-2.069814	-3.751322
H	10.899161	-1.863991	-1.973268
H	9.707662	-2.974030	-2.715675
C	1.769271	4.047210	-4.307805
C	-1.381332	7.025610	-1.846697
F	-2.394671	7.001189	-0.974084
F	-1.759930	7.806202	-2.866085
F	-0.356101	7.642876	-1.248855
F	1.973855	5.046984	-5.171016
F	2.832742	4.026209	-3.486670
F	1.793252	2.906646	-5.001267
H	-8.576251	-2.032718	-4.830858
O	-3.515129	-6.311850	-2.106672
C	-3.216792	-7.684424	-2.037726
H	-2.446415	-7.900234	-1.277889
H	-4.113764	-8.289158	-1.822112
H	-2.828820	-7.967904	-3.023877

TS1-*RS*

C	-0.200222	-2.447663	-1.961572
C	-0.510419	-1.111221	-0.323409
C	0.564552	-1.975950	0.028113
O	0.691790	-2.842770	-0.989493
H	-0.657946	-0.099634	0.058858
N	-0.885863	-1.411525	-1.628096
C	1.369938	-2.101472	1.190177
H	0.837017	-1.732242	2.080788
H	1.791587	-3.107284	1.314029
Au	3.001249	-0.717092	1.146557
P	4.548583	1.045580	1.423622
C	3.696817	2.513897	0.521521
C	-6.932526	-2.914866	0.957346
C	-6.063584	-1.446365	2.507115
C	-6.738815	-2.009445	-0.135311
C	-5.802844	-0.489406	1.483840
C	-6.145777	-0.742596	0.176303
N	-6.605262	-2.614774	2.233787
C	-5.969601	0.307851	-0.904385

N	-4.707154	1.026826	-0.810497
C	-3.805395	0.948935	-1.783817
C	-2.604525	1.605691	-2.137021
C	-3.716087	0.065799	-2.963149
C	-2.479235	0.815617	-3.380065
O	-1.725792	0.744623	-4.331029
O	-4.359317	-0.864167	-3.402462
N	-1.929596	2.610555	-1.535313
C	-0.837945	3.338978	-1.996616
C	-0.146764	3.041552	-3.179903
C	-0.423444	4.434465	-1.220924
C	0.929705	3.837272	-3.563988
H	-0.454663	2.193284	-3.798829
C	0.648974	5.218002	-1.631651
H	-0.943334	4.653379	-0.286402
C	1.340156	4.934121	-2.808413
H	2.182321	5.549408	-3.125948
H	-5.320452	0.453536	1.741177
H	-5.941787	-0.192034	-1.878388
S	-2.810401	2.349048	2.000215
N	-2.424683	0.888667	1.426514
C	-2.027691	0.062393	2.415149
O	-2.041820	3.410171	1.323628
O	-4.276589	2.559894	1.932858
C	-2.269783	2.071239	3.666294
C	-2.227442	2.937318	4.747495
C	-1.872774	0.733879	3.733843
C	-1.748318	2.423224	5.954633
H	-2.548668	3.977069	4.659668
C	-1.401600	0.232580	4.946718
C	-1.341632	1.087604	6.048283
H	-1.689694	3.070826	6.832209
H	-1.083505	-0.807720	5.039074
H	-0.970062	0.706422	7.002148
C	-1.785659	-1.285057	2.192344
H	-1.426631	-1.899043	3.018000
C	-2.014102	-1.839915	0.902522
H	-2.704165	-1.258167	0.283943
C	-2.063774	-3.288015	0.652759
C	-1.443664	-4.225215	1.499329
C	-2.749492	-3.760248	-0.480398
C	-1.511366	-5.586301	1.220408
H	-0.903232	-3.888078	2.385890
C	-2.819692	-5.124544	-0.755741

H	-3.239292	-3.044755	-1.145520
C	-2.198599	-6.040954	0.091805
H	-1.027174	-6.301095	1.890335
H	-3.363863	-5.471091	-1.637402
H	-2.252826	-7.111268	-0.122047
H	-2.220179	2.879726	-0.592045
H	-4.536570	1.608109	0.010083
C	4.699305	1.386802	3.334238
C	-0.228904	-3.211804	-3.200476
C	0.497622	-4.405789	-3.325363
C	-0.995221	-2.748551	-4.282466
C	0.457788	-5.126296	-4.516137
H	1.086963	-4.769317	-2.482210
C	-1.027785	-3.475203	-5.467892
H	-1.550928	-1.813291	-4.191046
C	-0.304079	-4.663881	-5.589560
H	1.024006	-6.056479	-4.605107
H	-1.622811	-3.108306	-6.307498
H	-0.334148	-5.229981	-6.523768
C	-5.756218	-1.156071	3.933165
C	-5.858075	-2.186146	4.882722
C	-5.390639	0.124471	4.377045
C	-5.600945	-1.947153	6.228649
H	-6.148637	-3.178580	4.534387
C	-5.137616	0.363631	5.727255
H	-5.302725	0.956005	3.674818
C	-5.239926	-0.668380	6.658798
H	-5.683677	-2.764599	6.949712
H	-4.855122	1.368622	6.050350
H	-5.040164	-0.477913	7.716327
C	-7.124250	-2.411295	-1.432927
C	-7.505537	-4.183902	0.692157
H	-6.973719	-1.766603	-2.299426
C	-7.877214	-4.556227	-0.578512
C	-7.684420	-3.659087	-1.660314
H	-8.315212	-5.541020	-0.743676
H	-7.644718	-4.861398	1.537094
C	-7.208318	1.230991	-0.947886
C	-7.436343	2.134181	0.285049
H	-8.049748	0.521187	-1.008114
C	-6.549363	3.280734	-2.082668
C	-8.149917	3.403373	-0.203221
H	-6.492050	2.404056	0.784636
H	-8.045746	1.612302	1.038373

C	-7.172562	4.257072	-1.039358
H	-5.507993	3.058907	-1.817880
H	-6.523925	3.750245	-3.078577
H	-8.519411	3.986385	0.654098
N	-7.293500	2.025843	-2.179260
C	-6.129682	4.970235	-0.235821
H	-5.474929	4.347379	0.389722
C	-5.932516	6.291690	-0.243893
H	-6.552801	6.958761	-0.853033
H	-5.144558	6.756062	0.356037
C	-9.310659	3.003660	-1.122618
H	-9.979158	2.303858	-0.594657
H	-9.915112	3.887017	-1.382614
C	-8.705234	2.349630	-2.390871
H	-9.248531	1.431728	-2.666580
H	-8.768505	3.028489	-3.256012
C	4.369538	3.887703	0.554969
H	5.322901	3.890791	0.012749
H	3.705430	4.596390	0.035199
H	4.530657	4.282347	1.565173
C	3.582769	2.101737	-0.946395
H	4.571006	2.017704	-1.422404
H	3.050527	1.148985	-1.066623
H	3.016126	2.872657	-1.492317
C	2.284226	2.629832	1.113343
H	1.719871	1.689171	1.017466
H	2.284579	2.920470	2.172668
H	1.734048	3.410287	0.564825
C	4.629625	2.850621	3.790446
H	3.705642	3.354805	3.479156
H	4.634811	2.850313	4.892539
H	5.484175	3.463462	3.480734
C	5.999216	0.763549	3.845354
H	6.062007	-0.304213	3.602574
H	6.894057	1.260340	3.449114
H	6.024738	0.854509	4.943584
C	3.518224	0.668373	4.006780
H	2.545704	1.054898	3.668804
H	3.534494	-0.414914	3.824099
H	3.583011	0.829016	5.095594
C	6.222173	0.671708	0.661991
C	6.467800	-0.586252	0.018966
C	7.263829	1.628794	0.702867
C	7.738191	-0.842558	-0.557709

C	8.486948	1.355287	0.072770
C	8.753043	0.132829	-0.538684
C	7.227366	2.924942	1.452886
H	6.271502	3.088960	1.944394
H	8.021228	2.938122	2.215638
H	7.418631	3.785540	0.796381
C	5.527254	-1.765805	-0.083936
C	4.812044	-2.005636	-1.285193
C	5.597472	-2.797919	0.886709
C	4.224595	-3.258671	-1.492478
C	4.980536	-4.025959	0.632077
C	4.308059	-4.292761	-0.561020
H	3.694273	-3.443199	-2.430844
H	5.058172	-4.814609	1.386156
C	4.701667	-0.971806	-2.395647
H	5.023378	-0.008692	-1.974777
C	3.716447	-5.658840	-0.849378
H	3.263917	-5.600972	-1.854256
C	6.365021	-2.649694	2.190688
H	6.706372	-1.605650	2.252018
C	3.263504	-0.810592	-2.894766
H	2.935114	-1.683862	-3.480065
H	2.555115	-0.686341	-2.061947
H	3.178066	0.071262	-3.547745
C	5.627225	-1.282526	-3.575336
H	6.683926	-1.294679	-3.277595
H	5.388322	-2.263439	-4.017503
H	5.508066	-0.522645	-4.363997
C	4.798474	-6.739378	-0.900492
H	5.288730	-6.862043	0.078680
H	4.363677	-7.712562	-1.178257
H	5.577857	-6.491396	-1.637107
C	2.608141	-6.031099	0.136342
H	2.173810	-7.010764	-0.118563
H	2.994643	-6.098002	1.166229
H	1.796529	-5.288277	0.126264
C	5.474631	-2.929849	3.403344
H	6.002367	-2.688733	4.339563
H	4.547005	-2.338688	3.366745
H	5.187468	-3.991888	3.455323
C	7.612814	-3.534893	2.235925
H	7.345899	-4.602570	2.180717
H	8.298540	-3.317335	1.405651
H	8.161873	-3.377187	3.177772

C	8.101137	-2.160795	-1.194134
H	7.259223	-2.854972	-1.271602
H	8.512169	-2.008360	-2.203824
H	8.896655	-2.660641	-0.617344
C	10.108985	-0.137285	-1.118347
H	10.069492	-0.223330	-2.216688
H	10.811708	0.662941	-0.858342
H	10.518328	-1.087765	-0.744384
O	9.466856	2.308344	0.141840
C	9.548474	3.167142	-0.977561
H	10.330615	3.907596	-0.763707
H	9.818639	2.616314	-1.894715
H	8.595240	3.694218	-1.155854
C	1.036402	6.416632	-0.809942
C	1.718381	3.456862	-4.787444
F	2.737840	2.638035	-4.473173
F	2.257425	4.524479	-5.384523
F	0.974855	2.820666	-5.692310
F	0.345934	7.507236	-1.162351
F	0.815022	6.219378	0.493980
F	2.334047	6.716219	-0.952037
H	-7.767523	5.022397	-1.567027
O	-8.016005	-3.948252	-2.932640
C	-8.570050	-5.204391	-3.237685
H	-8.743851	-5.212586	-4.320735
H	-7.882850	-6.028514	-2.981980
H	-9.532235	-5.364725	-2.722417

TS1-*SR*

C	-1.621244	-3.200583	2.241135
C	-1.756042	-3.672126	0.174832
C	-1.637383	-2.251133	0.279644
O	-1.442199	-2.002112	1.582606
H	-2.201482	-4.171329	-0.683980
N	-1.914948	-4.178603	1.455885
C	-1.712402	-1.204549	-0.668504
H	-1.540181	-1.534845	-1.699777
H	-1.178680	-0.287145	-0.396905
Au	-3.802669	-0.743630	-0.534266
P	-6.144182	-0.506487	-0.365618
C	-6.681929	-1.195480	1.372575
S	2.452244	-0.749081	1.859258
N	1.686175	-1.821247	0.928315

C	1.555456	-3.006468	1.557928
O	1.618754	0.400456	2.224993
O	3.760223	-0.360792	1.247216
C	2.743105	-1.822387	3.240701
C	3.376186	-1.567923	4.447826
C	2.178840	-3.052721	2.910532
C	3.440014	-2.619883	5.363677
H	3.805112	-0.589740	4.674678
C	2.249129	-4.095844	3.834464
C	2.882414	-3.866479	5.056215
H	3.929144	-2.467907	6.328401
H	1.820111	-5.074997	3.614541
H	2.943232	-4.675446	5.787621
C	0.914170	-4.109982	1.013551
H	0.918532	-5.030852	1.596859
C	0.252867	-4.098373	-0.240591
H	0.464722	-3.224184	-0.865172
C	0.068666	-5.353300	-1.002310
C	0.290196	-5.352512	-2.387585
C	-0.303517	-6.556969	-0.381656
C	0.164301	-6.524856	-3.131387
H	0.587851	-4.425491	-2.884776
C	-0.439807	-7.724182	-1.126583
H	-0.510742	-6.568520	0.690947
C	-0.202394	-7.714725	-2.503605
H	0.361942	-6.505209	-4.205837
H	-0.734863	-8.651938	-0.629820
H	-0.305127	-8.634375	-3.084894
C	-6.820699	-1.605891	-1.793346
C	-1.511279	-3.177405	3.692902
C	-1.868558	-4.315662	4.431958
C	-1.036038	-2.036784	4.358434
C	-1.758518	-4.307641	5.818096
H	-2.233695	-5.198354	3.903047
C	-0.925500	-2.039409	5.746605
H	-0.732649	-1.160850	3.781177
C	-1.287966	-3.170187	6.479394
H	-2.041733	-5.194987	6.389275
H	-0.549100	-1.151419	6.259873
H	-1.201191	-3.167598	7.568631
C	-7.907286	-2.117677	1.397216
H	-8.022427	-2.483859	2.430255
H	-7.787558	-3.002699	0.759397
H	-8.849810	-1.621900	1.137590

C	-6.915308	-0.022404	2.326254
H	-7.781362	0.590310	2.045623
H	-6.038494	0.633900	2.393298
H	-7.102665	-0.424091	3.335555
C	-5.499121	-2.021374	1.902875
H	-5.772206	-2.435267	2.887484
H	-4.596775	-1.408443	2.034960
H	-5.244675	-2.864544	1.244388
C	-6.284516	-0.990138	-3.085698
H	-5.190063	-0.903437	-3.072914
H	-6.717704	0.003317	-3.274162
H	-6.561520	-1.640561	-3.931392
C	-6.186875	-2.992999	-1.613314
H	-5.089718	-2.934056	-1.543822
H	-6.439697	-3.609090	-2.491519
H	-6.558638	-3.523276	-0.725616
C	-8.333164	-1.767445	-1.959650
H	-8.499139	-2.473730	-2.789695
H	-8.822568	-0.826320	-2.238599
H	-8.835744	-2.184918	-1.079113
C	-6.661733	1.282635	-0.576552
C	-5.679920	2.301166	-0.810520
C	-8.021814	1.658247	-0.476849
C	-6.094246	3.646519	-0.983545
C	-8.389144	3.000537	-0.653856
C	-7.457557	3.995515	-0.941444
C	-9.159104	0.731780	-0.175018
H	-8.836398	-0.302956	-0.087254
H	-9.927992	0.790798	-0.958949
H	-9.657259	1.010660	0.766367
C	-4.176733	2.137537	-0.848634
C	-3.429201	2.366430	0.334695
C	-3.488411	2.078346	-2.090645
C	-2.044648	2.550461	0.251388
C	-2.104497	2.271311	-2.114972
C	-1.359393	2.529943	-0.962322
H	-1.477901	2.743146	1.167204
H	-1.591073	2.239936	-3.079806
C	-4.082067	2.471741	1.702596
H	-5.137105	2.184874	1.580553
C	0.131393	2.798877	-1.022710
H	0.443256	3.067358	0.000105
C	-4.201855	1.858421	-3.416023
H	-5.214487	1.500039	-3.183813

C	-3.445524	1.512107	2.710145
H	-4.021873	1.496205	3.648790
H	-2.417777	1.816151	2.962202
H	-3.397842	0.485655	2.315301
C	-4.064293	3.903471	2.243956
H	-4.568549	3.949848	3.222465
H	-4.576774	4.601252	1.567131
H	-3.032312	4.263477	2.383080
C	0.457393	3.988454	-1.927099
H	-0.090392	4.890942	-1.615215
H	0.198448	3.781240	-2.978004
H	1.534709	4.214928	-1.890838
C	0.928531	1.559343	-1.429979
H	0.807820	0.743067	-0.702537
H	2.001963	1.796995	-1.480786
H	0.619030	1.187575	-2.420322
C	-3.508948	0.793904	-4.270871
H	-2.561899	1.166118	-4.692163
H	-4.148912	0.505604	-5.119267
H	-3.278128	-0.111594	-3.689414
C	-4.352208	3.149486	-4.225198
H	-3.368984	3.598906	-4.439384
H	-4.958021	3.897694	-3.698403
H	-4.841835	2.939893	-5.189523
C	-5.126661	4.785418	-1.186846
H	-5.248332	5.537251	-0.390491
H	-5.330297	5.314629	-2.130793
H	-4.078443	4.472294	-1.197540
C	-7.911476	5.402156	-1.190836
H	-7.609217	6.078822	-0.374539
H	-9.001938	5.448653	-1.294480
H	-7.462648	5.804196	-2.111451
O	-9.719749	3.311396	-0.576635
C	-10.150335	3.830879	0.665486
H	-9.923637	3.140219	1.495736
H	-11.238183	3.965595	0.601400
H	-9.682676	4.805300	0.885923
C	3.395147	6.421821	-0.015455
C	2.366160	4.932880	1.415719
C	4.321142	5.445669	-0.502618
C	3.228960	3.883603	0.976171
C	4.213155	4.124070	0.044862
N	2.463248	6.149677	0.923275
C	5.230620	3.069384	-0.350789

N	4.676381	1.736152	-0.514281
C	4.716532	1.120994	-1.692934
C	4.522883	-0.208536	-2.117016
C	5.071014	1.555770	-3.058791
C	4.753515	0.149671	-3.532523
O	4.720439	-0.410029	-4.609299
O	5.457517	2.586462	-3.566288
N	4.251754	-1.303007	-1.381448
C	4.154596	-2.630422	-1.775267
C	4.057014	-3.036492	-3.111516
C	4.159552	-3.603795	-0.761809
C	3.944649	-4.395312	-3.406987
H	4.090717	-2.294626	-3.914831
C	4.054624	-4.949471	-1.080359
H	4.254817	-3.294603	0.279419
C	3.940429	-5.364860	-2.408443
H	3.851527	-6.422325	-2.659705
H	3.112731	2.883801	1.396837
H	5.631360	3.331196	-1.336409
H	4.116355	-1.124765	-0.377804
H	4.344628	1.197308	0.291819
C	1.342188	4.717044	2.474188
C	0.629941	5.821720	2.971499
C	1.064075	3.450136	3.008912
C	-0.322065	5.668314	3.973720
H	0.846695	6.804433	2.550141
C	0.108905	3.298844	4.014269
H	1.567625	2.553145	2.645246
C	-0.586484	4.403438	4.504064
H	-0.861199	6.542811	4.347214
H	-0.090308	2.301514	4.414642
H	-1.332454	4.280733	5.293367
C	5.267496	5.829948	-1.477676
C	3.460961	7.739528	-0.533803
H	5.982399	5.120406	-1.895424
C	4.389974	8.094607	-1.483318
C	5.308383	7.127198	-1.965960
H	4.410536	9.117676	-1.860024
H	2.744526	8.469357	-0.151250
C	6.438967	3.131489	0.611957
C	6.193819	2.641606	2.055731
H	6.672223	4.207651	0.656611
C	7.708394	1.073344	0.359826
C	7.536211	2.118926	2.591195

H	5.438877	1.838698	2.098607
H	5.814042	3.460483	2.685171
C	7.896680	0.794751	1.881028
H	6.785733	0.599024	0.001109
H	8.533645	0.628566	-0.218093
H	7.478498	1.960006	3.678684
N	7.648937	2.504770	0.067794
C	7.109146	-0.389460	2.347430
H	6.021438	-0.348416	2.197142
C	7.633899	-1.484779	2.904742
H	8.713241	-1.584943	3.065410
H	7.004811	-2.322563	3.219715
C	8.639654	3.128430	2.250277
H	8.368848	4.124225	2.638148
H	9.584009	2.842252	2.739487
C	8.795548	3.151084	0.708242
H	8.887562	4.181693	0.329941
H	9.704344	2.614559	0.392733
C	3.743643	-4.807343	-4.839588
C	4.106533	-5.992480	0.002546
F	2.448758	-4.725632	-5.191271
F	4.123630	-6.068997	-5.058359
F	4.421483	-4.029338	-5.685936
F	3.092432	-6.858929	-0.095386
F	4.061172	-5.460408	1.226839
F	5.234433	-6.712568	-0.071684
H	8.961593	0.590676	2.086697
O	6.243510	7.390785	-2.896823
C	6.329083	8.681226	-3.450546
H	7.145422	8.651318	-4.182560
H	5.397987	8.967450	-3.967960
H	6.565015	9.440641	-2.686078

TS1-*SS*

C	-1.838783	-3.136583	2.997723
C	-0.269434	-2.500583	1.700433
C	-1.498230	-2.275842	1.023282
O	-2.461678	-2.753603	1.834164
H	0.653159	-1.956282	1.491546
N	-0.564077	-2.957704	2.977412
C	-1.835489	-1.719704	-0.239557
H	-2.761042	-2.120698	-0.674136
H	-0.992812	-1.708537	-0.942903

Au	-2.274311	0.340878	0.147721
P	-2.479825	2.648275	0.623708
C	-0.982512	3.413822	-0.303582
S	4.437459	-2.128502	0.457064
N	2.916270	-2.662392	0.556979
C	2.854451	-3.801627	1.277970
O	4.591706	-0.760520	0.994783
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C	4.148414	-4.211092	1.887347
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C	4.451033	-5.288922	2.719904
C	5.768988	-5.456227	3.146888
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C	-2.456990	-6.129168	-0.607433
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H	2.960181	9.398944	-0.389832
H	4.548011	9.569141	0.433999

References:

[1] a) G. Dong, M. Bao, X. Xie, S. Jia, W. Hu, X. Xu, *Angew. Chem. Int. Ed.* **2021**, *60*, 1992-1999; *Angew. Chem.* **2021**, *133*, 2020-2027; b) Y. Liu, Y. Shi, L. Wei, K. Zhao, J. Zhao, P. Zhang, X. Xu, P. Li, *Chem. Asian J.* **2021**, *16*, 2417-2420.

[2] a) D. Stark, C. Young, T. C. O'Riordan, A. Slawina, A. Smith. *Org. Biomol. Chem.* **2016**, *14*, 8068-8073; b) Z. Liang, D. Wang, C. Zhang, S. Ye, *Org. Biomol. Chem.* **2016**, *14*, 6422-6425; c) J. Izquierdo, M. Pericas, A Recyclable, *ACS Catal.* **2016**, *6*, 348-356; d) Y. Chen, B. Shi, H. Yin, Y. Liu, C. Yu, K. Zhang, T. Li, C. Yao, *Org. Chem. Front.* **2022**, *9*, 5191-5196.

[3] Y. Huang, Y. Li, J. Sun, J. Li, Z. Zha, Z. Wang, *J. Org. Chem.* **2018**, *83*, 8464-8472.

[4] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J Fox, Gaussian 09, Revision E.01; Gaussian, Inc.: Wallingford, CT, **2013**.

[5] C. Adamo, V. Barone, *J. Chem. Phys.* **1999**, *110*, 6158-6170.

[6] F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297-3305.

[7] a) D. Andrae, U. Häußermann, M. Dolg, H. Stoll, H. Preuß, *Theor. Chim. Acta.* **1990**, *77*, 123-141; b) K. A. Peterson, D. Figgen, E. Goll, H. Stoll, M. Dolg, *J. Chem. Phys.* **2003**, *119*, 11113-11123.

[8] a) M. Bühl, C. Reimann, D. A. Pantazis, T. Bredow, F. Neese, *J. Chem. Theory Comput.* **2008**, *4*, 1449-1459; b) R. Kang, H. Chen, S. Shaik, J. Yao, *J. Chem. Theory Comput.* **2011**, *7*, 4002-4011.

[9] a) A. D. Boese, J. M. L Martin, *J. Chem. Phys.* **2004**, *121*, 3405-3416; b) S. Grimme, S. Ehrlich, L. Goerigk, *J. Comput. Chem.* **2011**, *32*, 1456-1465; c) L. Goerigk, S. Grimme, *Phys. Chem. Chem. Phys.* **2011**, *13*, 6670-6688.

[10] A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B* **2009**, *113*, 6378-6396.

[11] R. Kang, W. Lai, J. Yao, S. Shaik, H. Chen, *J. Chem. Theory Comput.* **2012**, *8*, 3119-3127.

[12] NBO Version 3.1, E. D. Glendening, A. E. Reed, J. E. Carpenter, F. Weinhold.

[13] CYLview20; C. Y. Legault, Université de Sherbrooke, **2020** (http://www.cylview.org).

[14] a) P. Pracht, F. Bohle, S. Grimme, *Phys. Chem. Chem. Phys.* **2020**, *22*, 7169-7192; b) S. Grimme, *J. Chem. Theory Comput.* **2019**, *15*, 2847-2862.

[15] T. Lu, Molclus program, Version 1.9.9.9, http://www.keinsci.com/research/molclus.html. (accessed 06 30, 2023).

[16] S. Grimme, *Chem. Eur. J.* **2012**, *18*, 9955-9964.

[17] T. Lu, Q. Chen, *Comput. Theor. Chem.* **2021**, *1200*, 113249.