Supporting Information

A Desymmetric Dearomatization Cyclopropanation of [2.2]Paracyclophane

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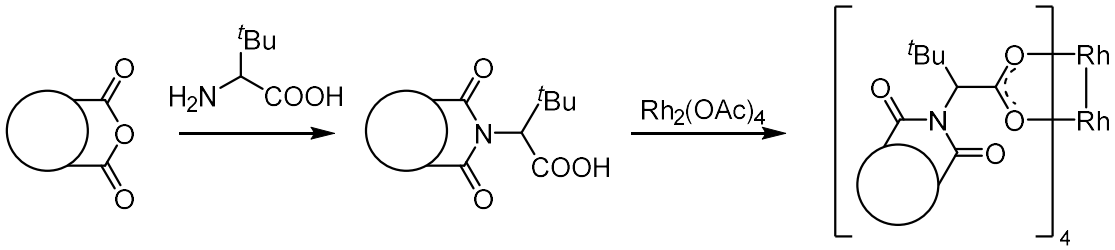
Context

1. General Information

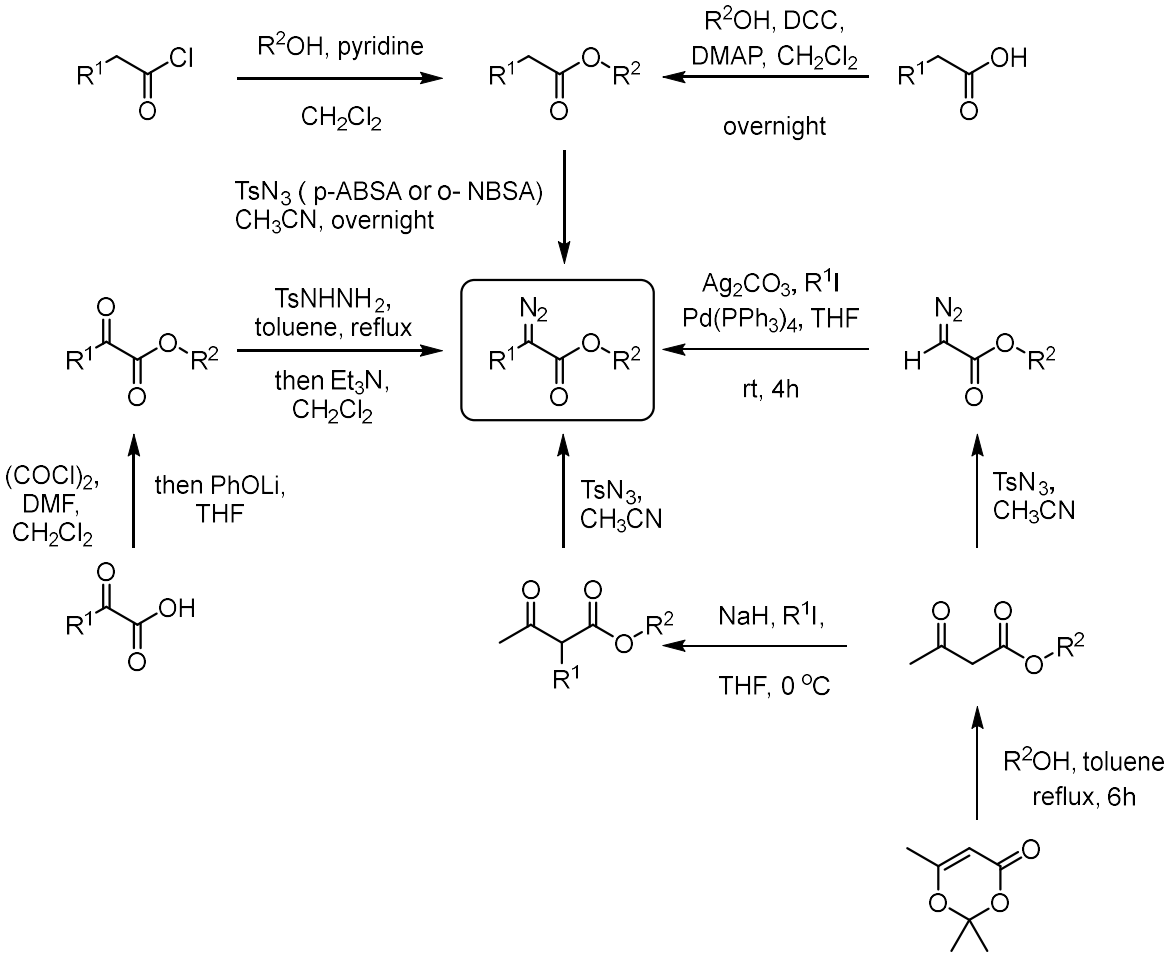
Unless otherwise noted, analytic grade solvents were used for the chromatography, and all the reagents were obtained commercially and used without further purification. All reactions were performed under a nitrogen atmosphere and in flame-dried or oven-dried glassware with magnetic stirring. Reactions were monitored by TLC. Solvents were dried with CaH_2. All NMR spectra were recorded on Bruker-500 MHz spectrometer. The chemical shifts (δ) and coupling constants (*J*) were expressed in ppm and Hz respectively. Solvent resonances and Trimethylsilane (TMS) were used for internal chemical shift calibration (^{1}H NMR: TMS at δ = 0 ppm; ^{13}C NMR: $CDCl_3$ at δ = 77.0 ppm). HRMS were measured on the Q-TOF6510 instruments.

2. Preparation of Starting Materials

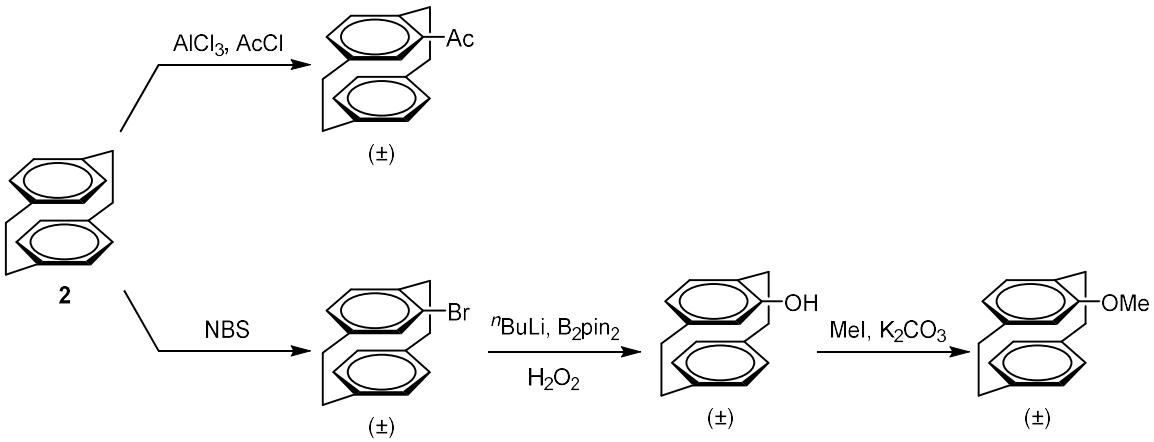
Rh_2(*S*-DOSP)$_4$, Rh_2(*S*-PTAD)$_4$ and Rh_2(*S*-TCPTAD)$_4$ were purchased from Sigma-Aldrich. Other Rhodium(II) complexes were synthesized according to reported procedures.[1-4]



Diazo compounds were synthesized according to reported procedures.[5]

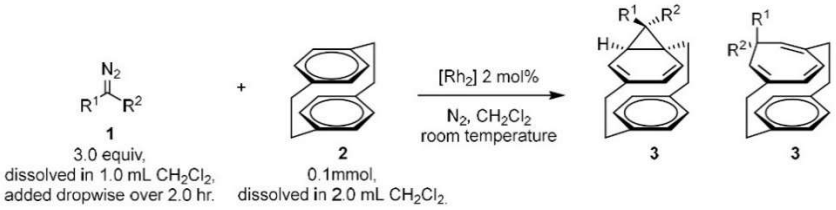


Monosubstituted [2.2]Paracyclophanes were synthesized according to reported procedures.[6,7]

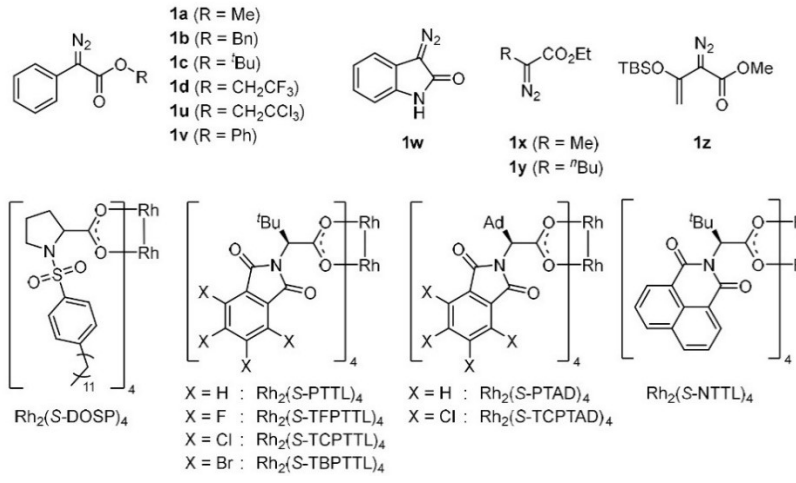


3. Optimization of Conditions

Table S1. Optimization of Conditions.

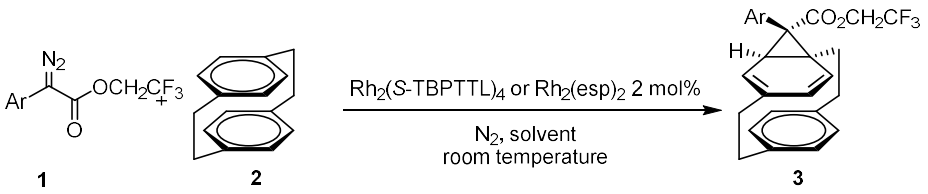


entry	catalyst	1	changes of standard conditions	yield (%)	ee (%)	3 : 4
1	Fe(TPP)Cl	**1a**	none	0	--	--
2	CoTPP	**1a**	none	0	--	--
3	$Cu(CN)_4PF_6$	**1a**	none	< 10	--	--
4	$Rh_2(OAc)_4$	**1a**	none	43	--	2 : 1
5	$Rh_2(esp)_2$	**1a**	none	53	--	2 : 1
6	Rh_2(S-DOSP)$_4$	**1a**	none	16	-4	--
7	Rh_2(S-TCPTTL)$_4$	**1a**	none	32	54	5 : 1
8	Rh_2(S-TCPTTL)$_4$	**1b**	none	trace	--	--
9	Rh_2(S-TCPTTL)$_4$	**1c**	none	--	--	--
10	Rh_2(S-TCPTTL)$_4$	**1d**	none	20	81	5 : 1
11	Rh_2(S-PTTL)$_4$	**1d**	none	8	10	4 : 1
12	Rh_2(S-NTTL)$_4$	**1d**	none	61	67	3 : 1
13	Rh_2(S-TFPTTL)$_4$	**1d**	none	33	69	2 : 1
14	Rh_2(S-TCPTAD)$_4$	**1d**	none	50	90	10 : 1
15	Rh_2(S-PTAD)$_4$	**1d**	none	37	81	1 : 1
16	Rh_2(S-TBPTTL)$_4$	**1d**	none	63	94	> 20 : 1
17	Rh_2(S-TBPTTL)$_4$	**1d**	cool down to -15 °C	< 10	--	--
18	Rh_2(S-TBPTTL)$_4$	**1d**	heat to 39 °C	34	93	12 : 1
19	Rh_2(S-TBPTTL)$_4$	**1d**	2 was dissolved in 1.0 mL CH_2Cl_2	62	93	> 20 : 1
20	Rh_2(S-TBPTTL)$_4$	**1d**	n-hexane as solvent	15	--	--
21	Rh_2(S-TBPTTL)$_4$	**1d**	toluene as solvent	0	--	--
22	Rh_2(S-TBPTTL)$_4$	**1d**	DME as solvent	0	--	--
23	Rh_2(S-TBPTTL)$_4$	**1d**	1,2-DCE as solvent	0	--	--
24	Rh_2(S-TBPTTL)$_4$	**1d**	1 mol% of [Rh_2]	59	93	> 20 : 1
25	Rh_2(S-TBPTTL)$_4$	**1d**	1 was added in 10.0 hr	62	94	> 20 : 1
26	Rh_2(S-TBPTTL)$_4$	**1d**	6.0 equiv of 1	68	94	> 20 : 1
27	Rh_2(S-TBPTTL)$_4$	**1d**	0.1 mmol of 1 (0.1 M); 5.0 equiv of 2	0	--	--
28	Rh_2(S-TBPTTL)$_4$	**1d**	0.1 mmol of 1 (0.3 M); 5.0 equiv of 2	0	--	--
29	Rh_2(S-TBPTTL)$_4$	**1u**	none	0	--	--
30	Rh_2(S-TBPTTL)$_4$	**1v**	none	0	--	--
31	Rh_2(S-TBPTTL)$_4$	**1w**	none	0	--	--
32	Rh_2(S-TBPTTL)$_4$	**1x**	none	0	--	--
33	Rh_2(S-TBPTTL)$_4$	**1y**	none	0	--	--
34	Rh_2(S-TBPTTL)$_4$	**1z**	none	0	--	--



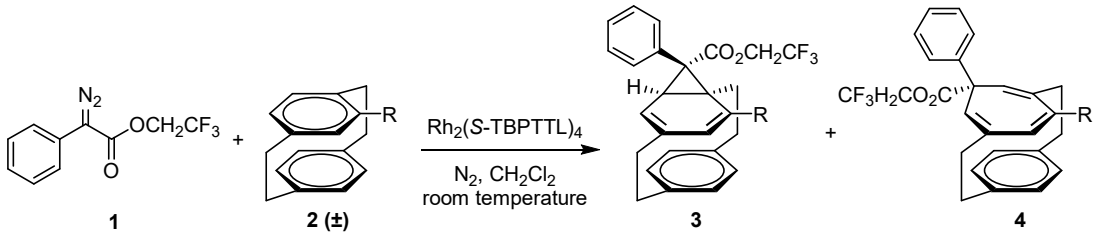
4. Dearomatization Cyclopropanation of [2.2]Paracyclophane

(1) Genera procedure of enantioselective dearomatization cyclopropanation [2.2]Paracyclophane



[2.2]Paracyclophane (1.0 equiv., 20.8 mg, 0.1 mmol) and Rh_2(*S*-TBPTTL)$_4$ (2 mol%, 5.0 mg, 0.002 mmol) (for racemic reaction, a same equivalent of $Rh_2(esp)_2$ instead) were charged to a Schlenk tube equipped with a magnetic stirring bar. The tube was then charged with nitrogen 3 times. Under a nitrogen atmosphere, CH_2Cl_2 (1.0 mL) or a mixed solvent (n-hexane : CH_2Cl_2 = 1 : 1) was added as solvent with a syringe. The suspension was vigorously stirred and a CH_2Cl_2 solution of diazo (3.0 equiv. or 5.0 equiv., 0.1M) was dropwise added diazo via a pump over 2 hours at room temperature. After the full injection of diazo, the solution was allowed to continue stirring for 15 minutes. When no diazo remained determined by TLC, the solvent was evaporated *in vacuo*, and the residue was roughly purified by silicon chromatography (EtOAc/hexane/DCM) to remove most of the unreacted [2.2]Paracyclophane and dimer of diazo. The regioselectivity of the reaction was determined by ^{1}H NMR. The corresponding product was then separated by silicon chromatography (EtOAc/hexane). Enantiomeric excess (ee) values were determined by chiral HPLC analysis.

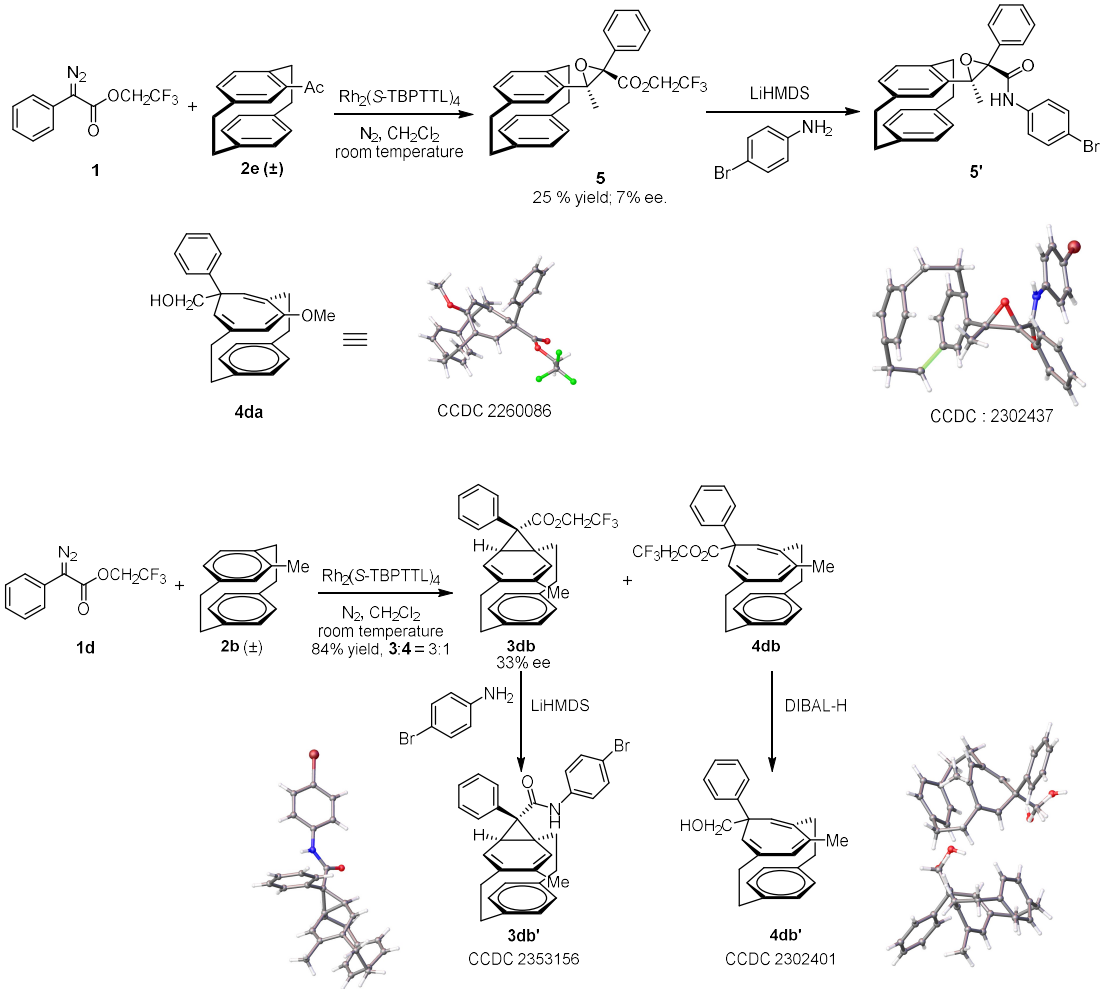
(2) Attempt of kinetic resolution of monosubstituted cyclopropanation [2.2]Paracyclophane



Monosubstituted [2.2]paracyclophane (1.0 equiv., 0.1 mmol) and Rh_2(*S*-TBPTTL)$_4$ (2 mol%, 5.0 mg, 0.002 mmol) were charged to a Schlenk tube equipped with a magnetic stirring bar. The tube was then charged with nitrogen three times. Under a nitrogen atmosphere, CH_2Cl_2 (1.0 mL) was added as solvent with a syringe. The suspension was vigorously stirred and a solution of diazo (x equiv., 0.1 M in CH_2Cl_2) was dropwise added diazo via a pump over 2 hours at room temperature. After the full injection of diazo, the solution was allowed to continue stirring for 15 minutes. When no diazo remained determined by TLC, the solvent was evaporated *in vacuo*, and the residue was roughly purified by silicon chromatography to remove most of the unreacted [2.2]Paracyclophane and dimer of diazo. The regioselectivity of the reaction was determined by ^{1}H NMR. The corresponding product was then separated by silicon chromatography. Enantiomeric excess (ee) values were determined by chiral HPLC analysis. The results are listed below

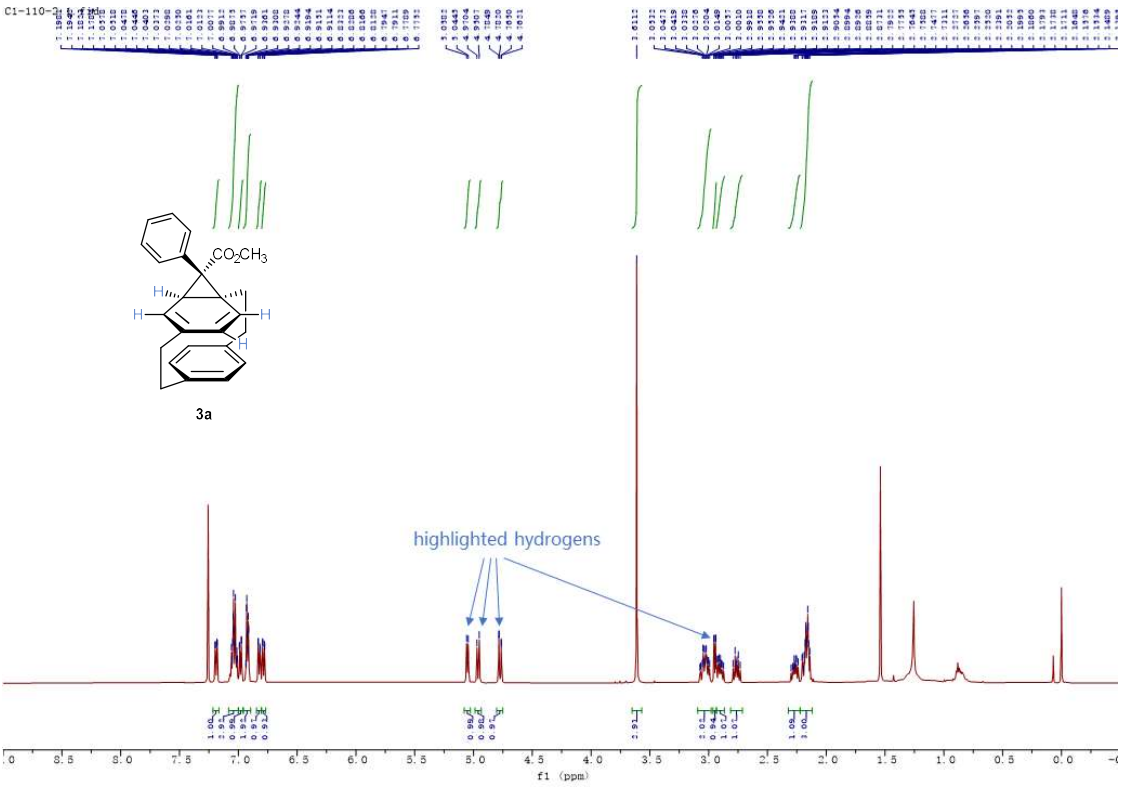
entry	**2**	R	x	product	yield (%)	**3** : **4**	ee (**3**/**4**%)
1	**2a**	OMe	0.5	--	trace	--	--
2	**2a**	OMe	3.0	**3db**/**4db**	65	< 1 : 20	-- / 10
3	**2b**	Me	3.0	**3da**/**4da**	84	3 : 1	33 / --
4	**2b**	Me	0.5	--	trace	--	--
5	**2c**	NHboc	3.0	**3dc**/**4dc**	29	< 1 : 20	-- / 27
6	**2d**	Br	3.0	--	0	--	--

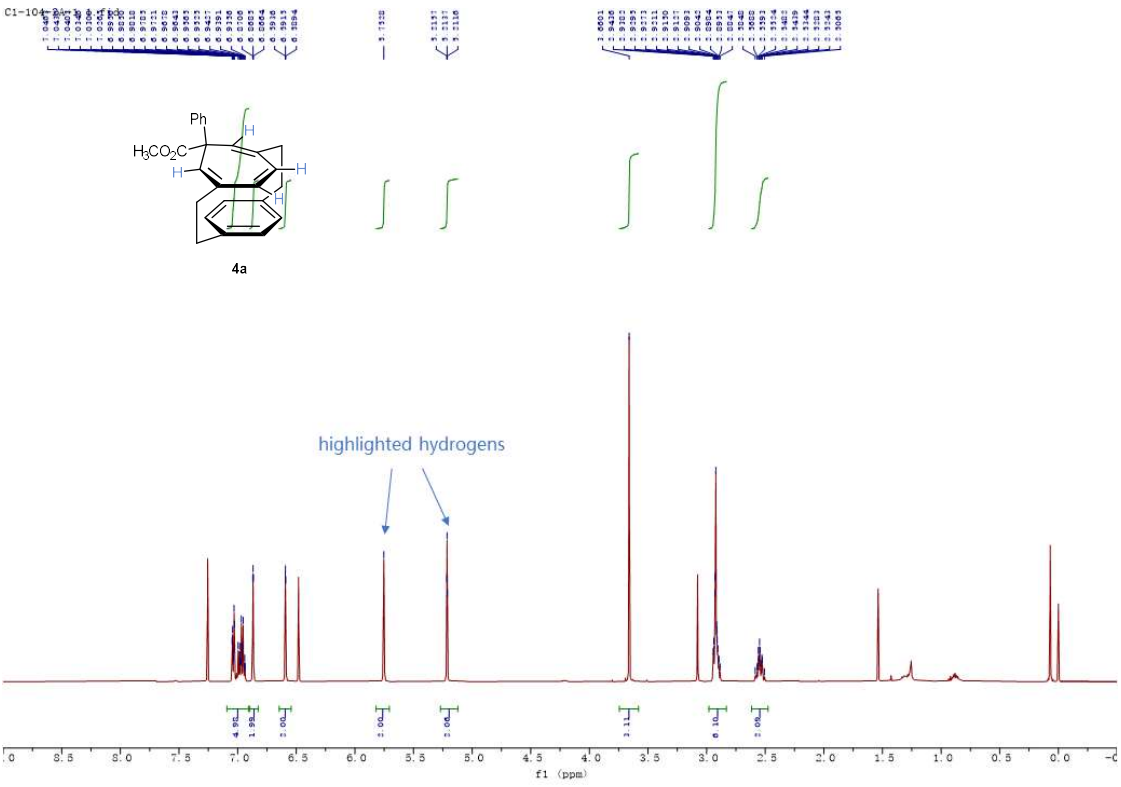
Essential structures of the products above were confirmed via X-ray single crystal diffraction by itself or derivate (single crystal of **5** has been shown in the text).



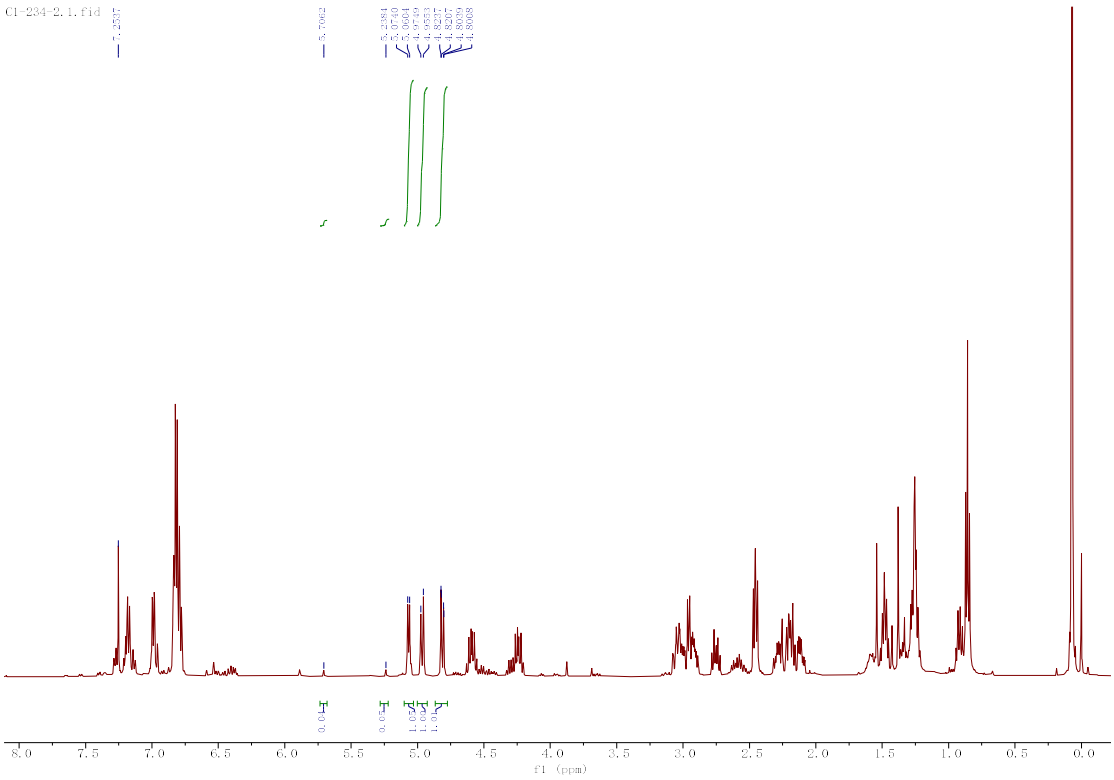
(3) Calculation of the Ratio of Regioisomers

In this reaction, two possible regioisomers (**3** and **4**) were detected with confirmed structures. The regioselectivity was measured by crude ^{1}H NMR analysis. The outstanding difference of these regioisomers in ^{1}H NMR is the chemical shift of hydrogens located in the dearomatized ring of [2.2]Paracyclophane. corresponding hydrogen atoms in 6π electrocyclic ring expansion product **3'**, an achiral substance, generate two single peak signals and those in cyclopropanation product **3** generate two doublet peak singles and two doublet of doublets peaks (one of their signals overlaps with ethylene's in [2.2]paracyclophane at around 3.0 ppm and wasn't used as reference). Such as the ^{1}H NMR spectra of **3a** and **3a'** shown below.





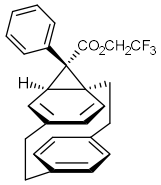
For example, through the preparation procedures detailed in Chapter 4, ^{1}H NMR spectra of the cured product **3h** is shown below.



The ratio of **3h** and **4h** was calculated as follow:

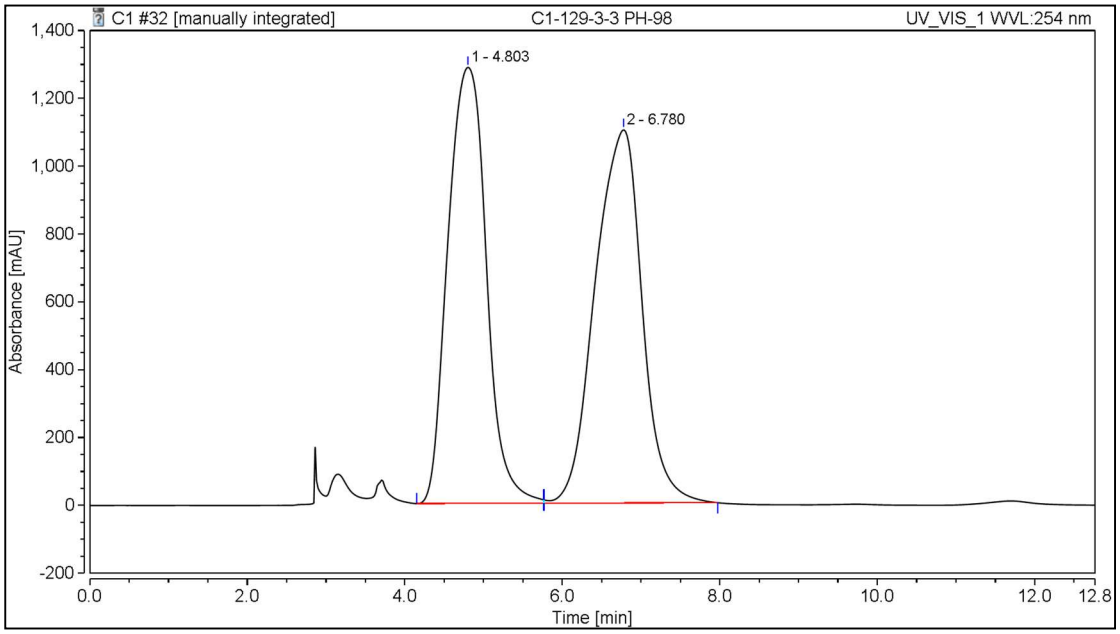
$$\mathrm{rr}(\mathbf{3h}:\mathbf{4h}) = \frac{1.01+1.00+1.01}{3} : \frac{0.04+0.05}{2} \times \frac{1}{2} = 1.007 : 0.023 \approx 44 : 1 > 20 : 1$$

In this text, all the ratios of **3** and **4** are calculated as > 20 : 1 and not repeated any more.

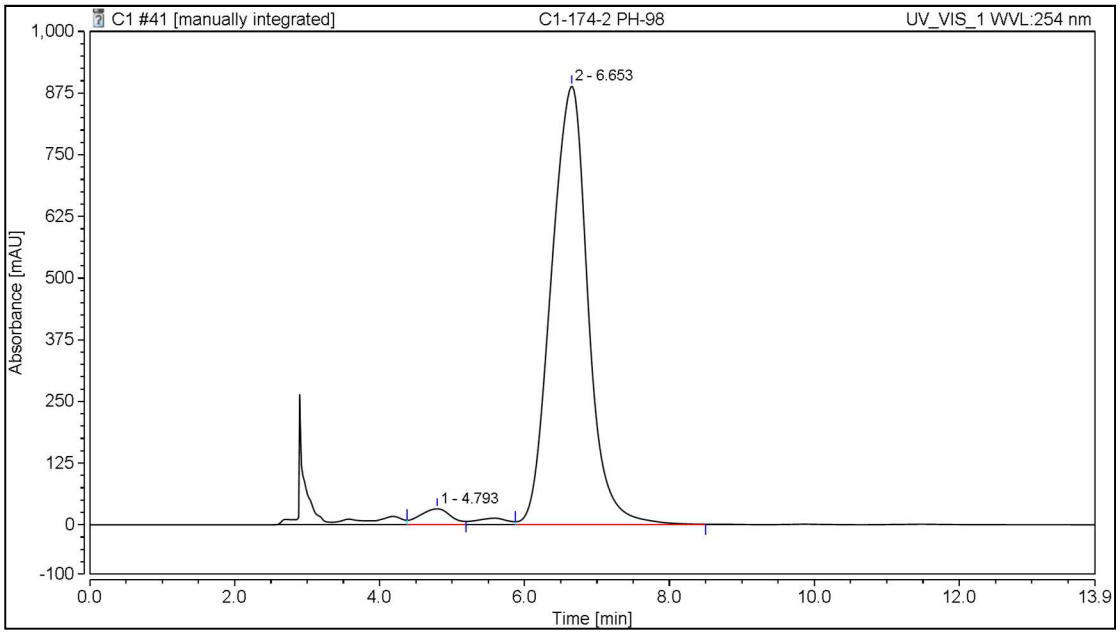


3d

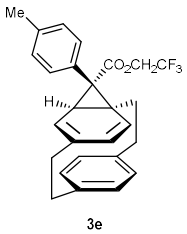
Colorless oil. 63% yield. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.18 (dd, *J* = 7.9, 1.9 Hz, 1H), 7.07 – 7.01 (m, 3H), 6.99 (dd, *J* = 7.8, 1.8 Hz, 1H), 6.94 – 6.90 (m, 2H), 6.83 (dd, *J* = 7.8, 1.9 Hz, 1H), 6.79 (dd, *J* = 7.9, 1.8 Hz, 1H), 5.08 (d, *J* = 6.8 Hz, 1H), 4.98 (d, *J* = 9.8 Hz, 1H), 4.81 (dd, *J* = 9.9, 1.4 Hz, 1H), 4.59 (dq, *J* = 12.6, 8.5 Hz, 1H), 4.24 (dq, *J* = 12.6, 8.4 Hz, 1H), 3.08 – 3.00 (m, 2H), 2.99 (dd, *J* = 6.9, 1.6 Hz, 1H), 2.92 (ddd, *J* = 13.2, 9.8, 6.3 Hz, 1H), 2.76 (dt, *J* = 13.9, 8.3 Hz, 1H), 2.28 (ddd, *J* = 13.3, 10.4, 6.4 Hz, 1H), 2.23 – 2.11 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.36, 139.67, 139.34, 134.74, 133.96, 133.06, 132.58, 132.40, 132.07, 131.86, 130.88, 128.31, 127.94, 126.68, 126.64, 61.11 (q, *J* = 37.3 Hz, CF_3), 41.90, 41.02, 35.03, 34.79, 34.41, 32.91, 32.33. ^{19}F NMR (471 MHz, $CDCl_3$) δ -73.93. HRMS (ESI, m/z) calcd for $C_{26}H_{23}F_3O_2$ $[M+H]^+$ 425.1723, found 425.1704. $[\alpha]^{20}_D$ = 4.7° (c 0.71, $CHCl_3$); 94% ee; Chiral HPLC analysis of the product: Phenomenex 00G-4457-E0 250X4.6 mm 5u column; hexane/2-propanol = 98/2, detected at 254 nm, Flow rate = 1.0 mL/min, Retention times: 4.8 min(minor), 6.7 min (major).



Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	4.803	726.435	1285.956	48.90	53.89
2	6.780	758.995	1100.273	51.10	46.11
Total:		**1485.430**	**2386.229**	**100.00**	**100.00**

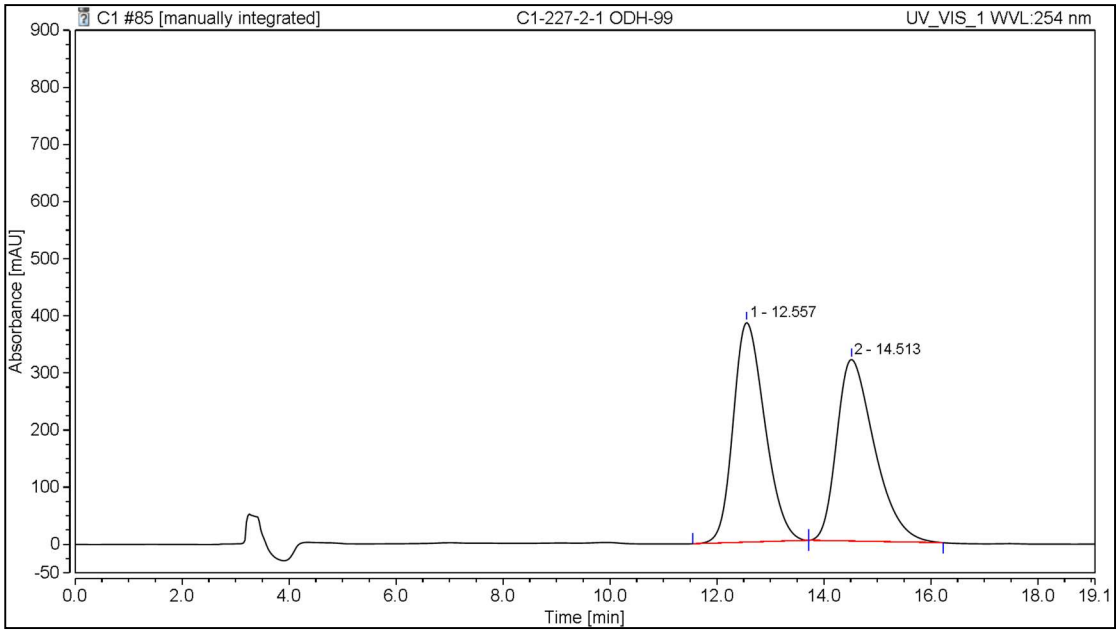


Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	4.793	16.000	32.210	2.98	3.50
2	6.653	521.120	888.948	97.02	96.50
Total:		**537.120**	**921.158**	**100.00**	**100.00**

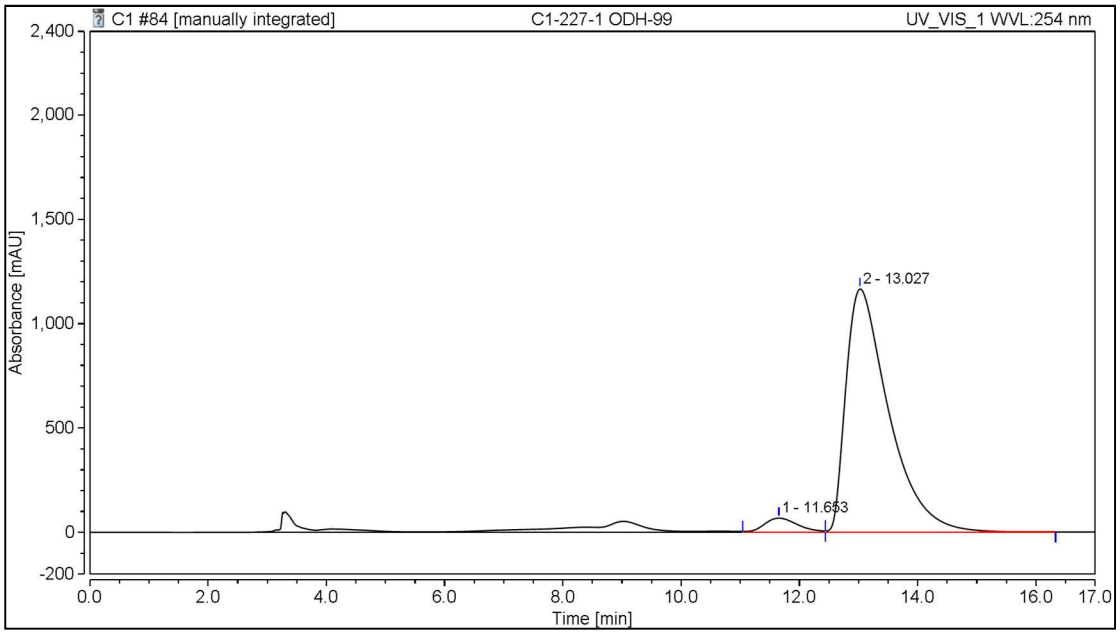


3e

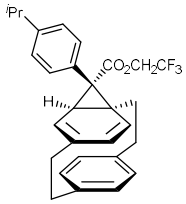
Colorless oil. 55% yield. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.18 (dd, *J* = 7.8, 1.9 Hz, 1H), 6.99 (dd, *J* = 7.8, 1.8 Hz, 1H), 6.95 – 6.76 (m, 6H), 5.07 (d, *J* = 6.8 Hz, 1H), 4.97 (d, *J* = 9.8 Hz, 1H), 4.83 (dd, *J* = 9.8, 1.4 Hz, 1H), 4.62 (dq, *J* = 12.6, 8.5 Hz, 1H), 4.23 (dq, *J* = 12.6, 8.5 Hz, 1H), 3.03 (dddd, *J* = 18.1, 11.6, 9.0, 3.5 Hz, 2H), 2.96 (dd, *J* = 6.9, 1.6 Hz, 1H), 2.94 – 2.88 (m, 1H), 2.75 (dt, *J* = 13.9, 8.3 Hz, 1H), 2.29 (ddd, *J* = 16.6, 12.2, 7.2 Hz, 1H), 2.25 – 2.15 (m, 5H), 2.11 (ddd, *J* = 14.8, 7.8, 3.8 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.53, 139.70, 139.33, 136.14, 134.61, 133.04, 132.55, 132.40, 131.99, 131.63, 130.88, 128.33, 128.00, 127.49, 60.59 (q, *J* = 36.5 Hz, CF_3), 41.80, 40.85, 35.11, 34.81, 34.43, 32.58, 32.34, 21.23. ^{19}F NMR (471 MHz, $CDCl_3$) δ -73.86. HRMS (ESI, m/z) calcd for $C_{27}H_{25}F_3O_2$ $[M+H]^+$ 439.1879, found 439.1859. $[\alpha]^{22}_D$ = 13.9° (c 0.39, $CHCl_3$); 91% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 99/1, detected at 254 nm, Flow rate = 1.0 mL/min, Retention times: 11.7 min (minor), 13.0 min (major).



Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	12.557	262.664	384.307	50.26	54.73
2	14.513	259.954	317.834	49.74	45.27
Total:		**522.618**	**70.141**	**100.00**	**100.00**

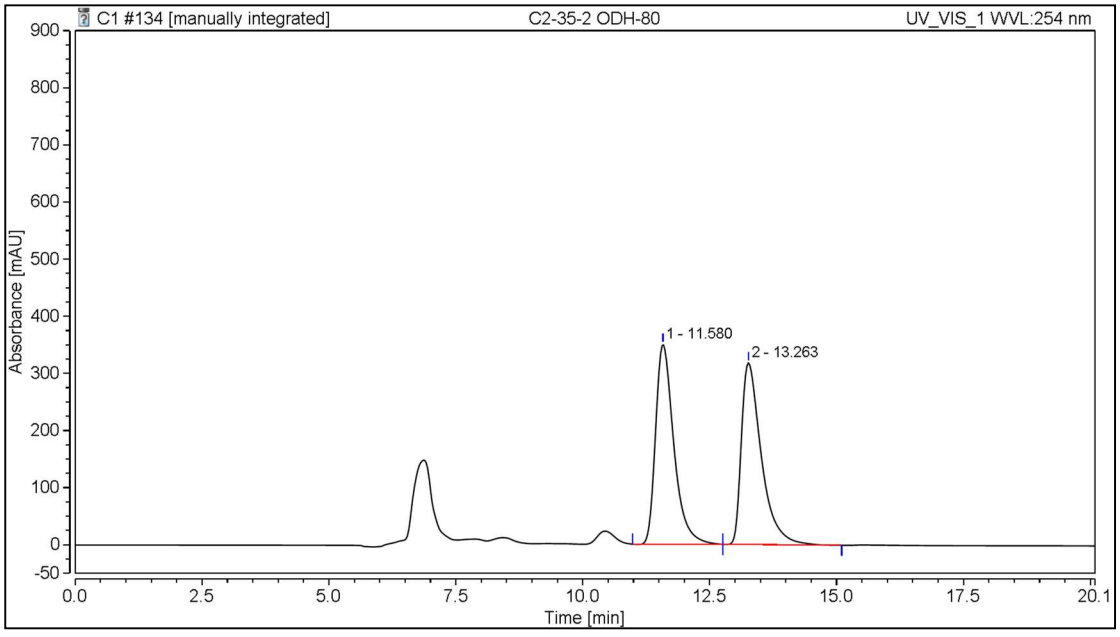


Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	11.653	43.724	67.307	4.28	5.46
2	13.027	976.707	1165.299	95.72	94.54
Total:		**1020.431**	**1232.606**	**100.00**	**100.00**

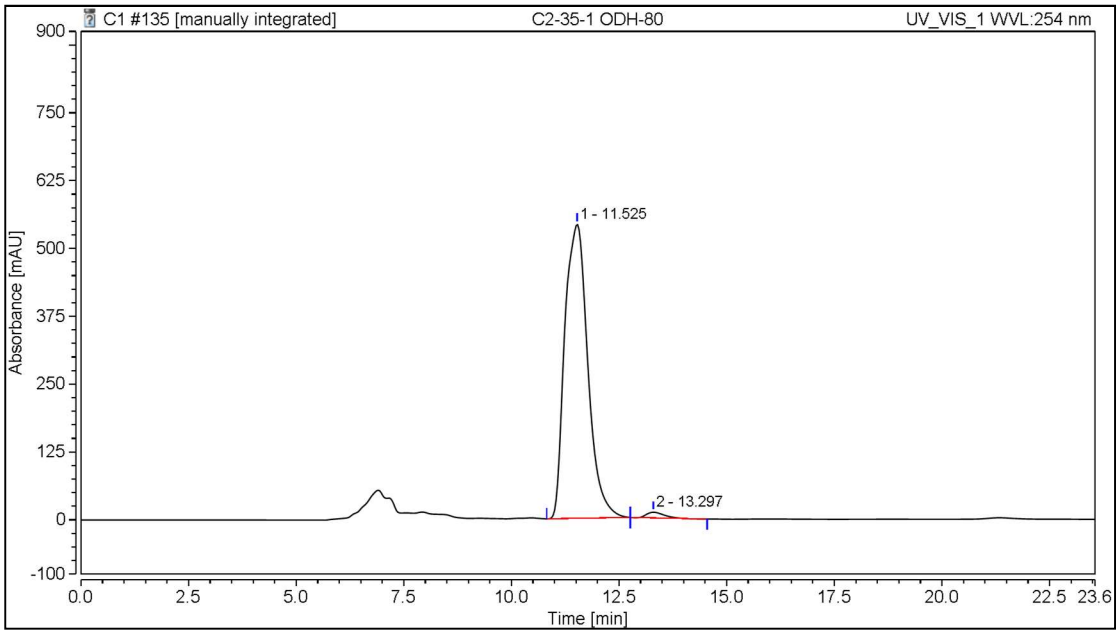


3f

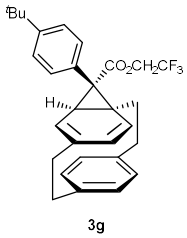
Light yellow oil. 52% yield. The mixture of hexane and DCM was used as solvent. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.11 (dd, *J* = 7.9, 1.9 Hz, 1H), 6.92 (dd, *J* = 7.8, 1.9 Hz, 1H), 6.80 (d, *J* = 8.0 Hz, 2H), 6.78 – 6.73 (m, 3H), 6.72 (dd, *J* = 7.9, 1.8 Hz, 1H), 5.00 (d, *J* = 6.8 Hz, 1H), 4.89 (d, *J* = 9.8 Hz, 1H), 4.74 (dd, *J* = 9.9, 1.4 Hz, 1H), 4.53 (dq, *J* = 12.7, 8.5 Hz, 1H), 4.17 (dq, *J* = 12.6, 8.4 Hz, 1H), 2.96 (dddd, *J* = 21.2, 11.6, 9.0, 3.4 Hz, 2H), 2.89 (dd, *J* = 6.9, 1.7 Hz, 1H), 2.85 (ddd, *J* = 13.3, 8.2, 4.8 Hz, 1H), 2.68 (dt, *J* = 13.9, 8.2 Hz, 2H), 2.22 (ddd, *J* = 13.3, 10.3, 6.3 Hz, 1H), 2.17 – 2.08 (m, 2H), 2.03 (ddd, *J* = 14.8, 7.9, 3.8 Hz, 1H), 1.06 (d, *J* = 6.9 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.55, 146.95, 139.70, 139.34, 134.59, 133.04, 132.57, 132.40, 131.90, 131.55, 131.12, 130.86, 128.34, 127.91, 124.70, 60.60 (q, *J* = 36.5 Hz, CF_3), 41.63, 40.69, 35.15, 34.86, 34.43, 33.57, 32.66, 32.33, 23.83, 23.79. ^{19}F NMR (471 MHz, $CDCl_3$) δ -73.88. HRMS (ESI, m/z) calcd for $C_{29}H_{29}F_3O_2$ $[M+H]^+$ 467.2192, found 467.2164. $[\alpha]^{21}_D$ = 21.0° (c 0.74, $CHCl_3$); 97% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 80/20, detected at 254 nm, Flow rate = 0.5 mL/min, Retention times: 11.5 min (major), 13.3 min (minor).



Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	11.580	145.742	349.909	50.13	52.38
2	13.263	145.012	318.075	49.87	47.62
Total:		**290.754**	**667.984**	**100.00**	**100.00**

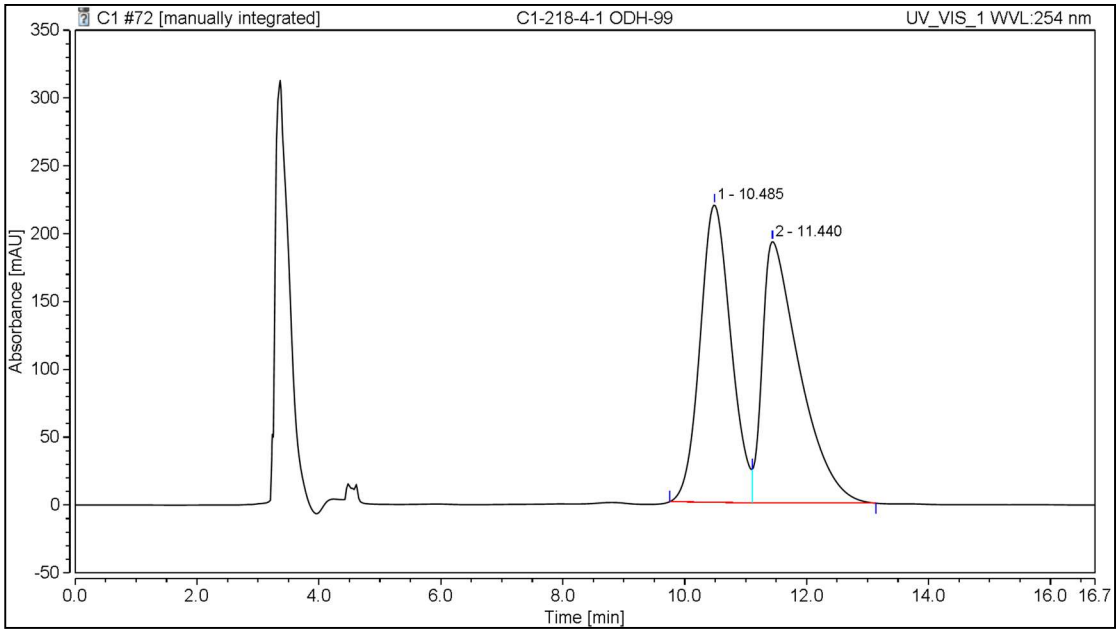


Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	11.525	335.984	541.952	98.57	98.11
2	13.297	4.887	10.425	1.43	1.89
Total:		**340.871**	**552.376**	**100.00**	**100.00**

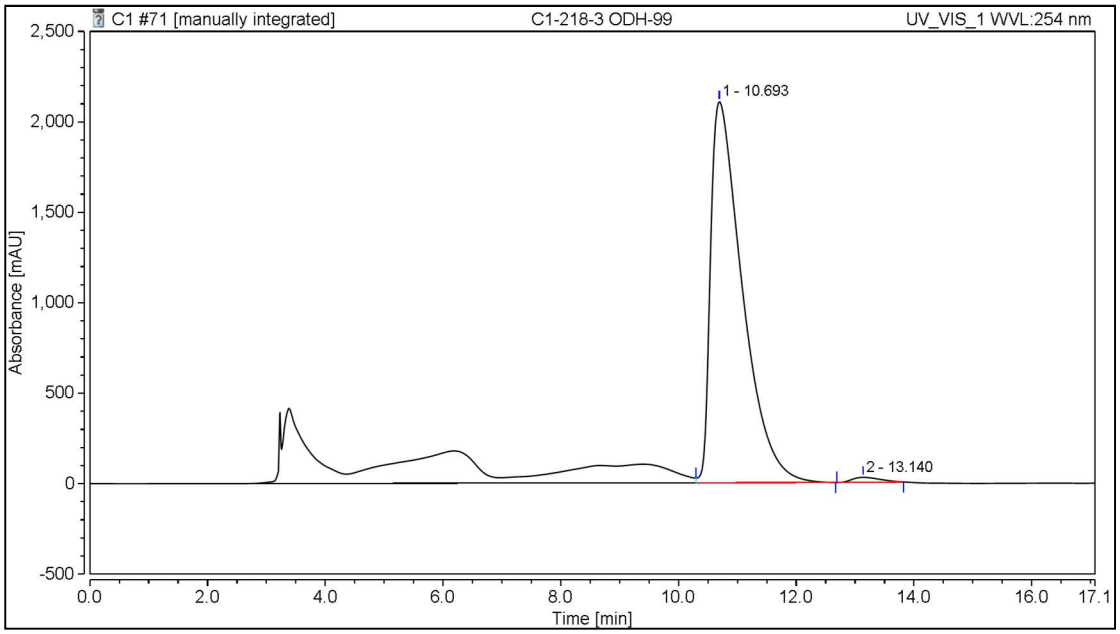


3g

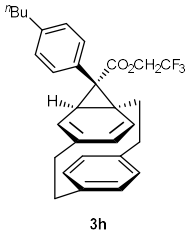
Light yellow oil. 70% yield. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.18 (dd, *J* = 7.9, 2.0 Hz, 1H), 7.02 (d, *J* = 8.4 Hz, 1H), 6.99 (dd, *J* = 7.8, 1.8 Hz, 1H), 6.82 (m, 3H), 6.79 (dd, *J* = 7.9, 1.8 Hz, 1H), 5.07 (d, *J* = 6.9 Hz, 1H), 4.96 (d, *J* = 9.9, 1H), 4.80 (dd, *J* = 9.9, 1.4 Hz, 1H), 4.60 (dq, *J* = 12.7, 8.5 Hz, 1H), 4.24 (dq, *J* = 12.7, 8.5 Hz, 1H), 3.09 – 2.98 (m, 2H), 2.96 (dd, *J* = 6.9, 1.7 Hz, 1H), 2.95 – 2.89 (m, 1H), 2.76 (dt, *J* = 13.9, 8.2 Hz, 1H), 2.30 (ddd, *J* = 13.3, 10.3, 6.3 Hz, 1H), 2.25 – 2.16 (m, 2H), 2.10 (ddd, *J* = 14.9, 7.8, 3.9 Hz, 1H), 3.09 – 2.98 (m, 2H), 2.96 (dd, *J* = 6.9, 1.7 Hz, 1H), 2.95 – 2.89 (m, 1H), 1.20 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.54, 149.22, 139.70, 139.34, 134.58, 133.04, 132.57, 132.40, 131.86, 131.24, 130.91, 130.86, 130.75, 128.82, 128.35, 127.87, 127.73, 125.70, 123.55, 60.52 (q, *J* = 36.5 Hz, CF_3), 41.56, 40.62, 35.17, 34.88, 34.43, 34.34, 32.58, 32.33, 31.27. ^{19}F NMR (471 MHz, $CDCl_3$) δ -73.87. HRMS (ESI, m/z) calcd for $C_{30}H_{31}F_3O_2$ $[M+H]^+$ 481.2349, found 481.2333. $[\alpha]^{20}_D$ = 15.4° (c 1.01, $CHCl_3$); 98% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 99/1, detected at 254 nm, Flow rate = 1.0 mL/min, Retention times: 10.7 min (major), 13.1 min (minor).



Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	10.485	128.722	219.238	48.53	53.22
2	11.440	136.541	192.733	51.47	46.78
Total:		**265.262**	**411.971**	**100.00**	**100.00**

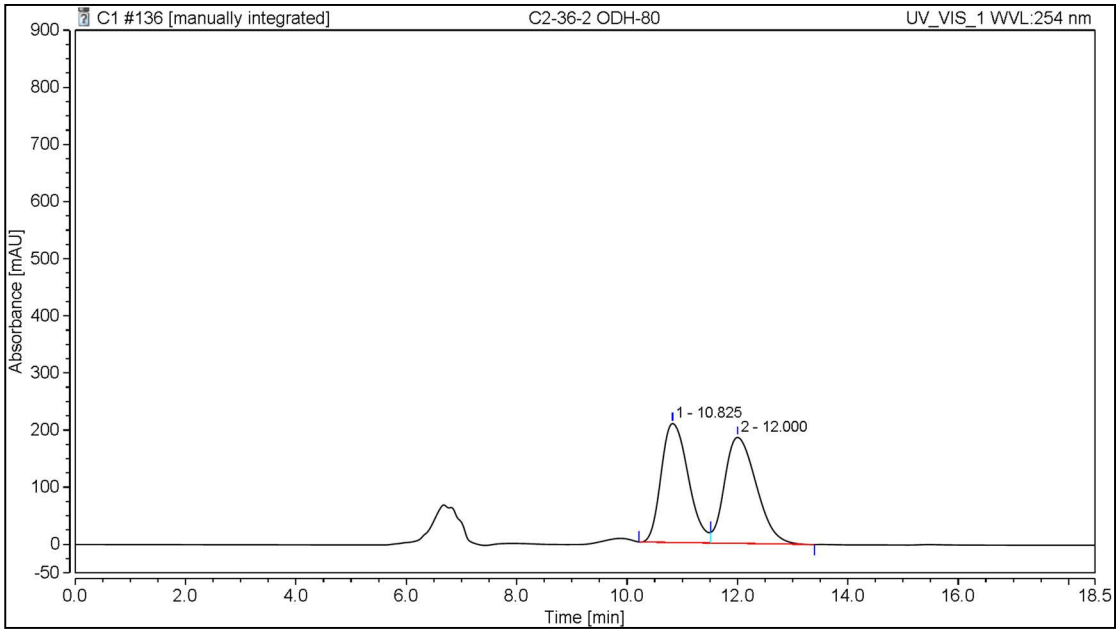


Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	10.693	1315.811	2107.271	98.88	98.72
2	13.140	14.897	27.403	1.12	1.28
Total:		**1330.708**	**2134.679**	**100.00**	**100.00**

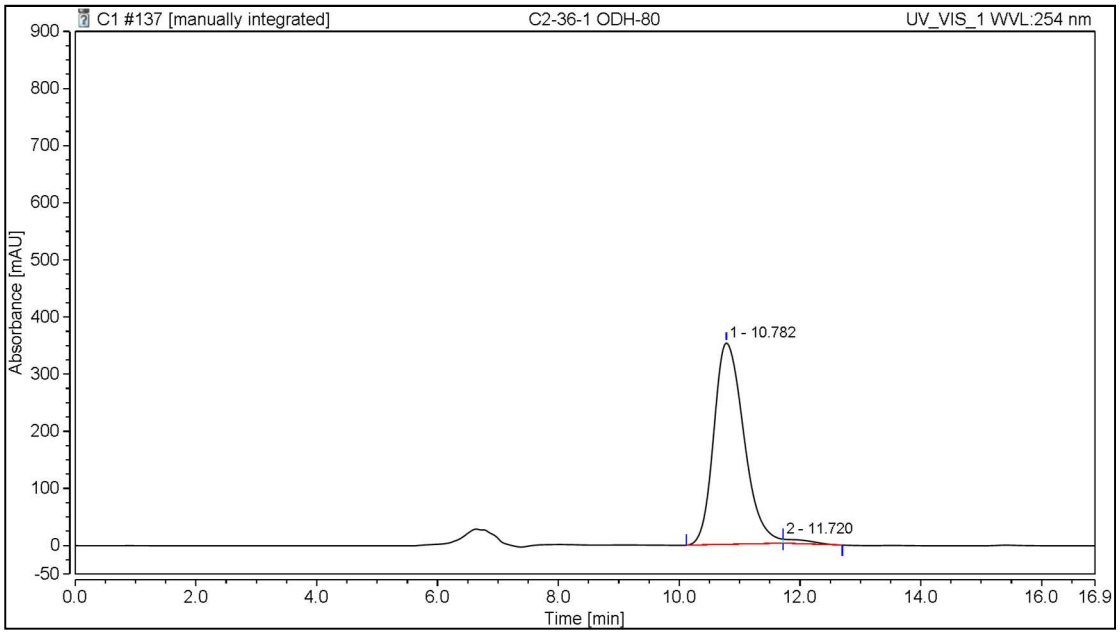


3h

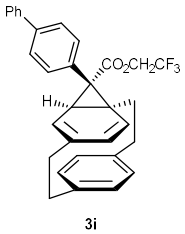
Colorless oil. 49% yield. The mixture of hexane and DCM was used as solvent. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.17 (dd, *J* = 7.9, 1.9 Hz, 1H), 6.99 (dd, *J* = 7.8, 1.8 Hz, 1H), 6.85 – 6.75 (m, 6H), 5.07 (d, *J* = 6.8 Hz, 1H), 4.96 (dt, *J* = 9.8, 1.2 Hz, 1H), 4.81 (dd, *J* = 9.9, 1.4 Hz, 1H), 4.58 (dq, *J* = 12.6, 8.5 Hz, 1H), 4.24 (dq, *J* = 12.6, 8.4 Hz, 1H), 3.02 (m, 2H), 2.96 (dd, *J* = 6.9, 1.6 Hz, 1H), 2.94 – 2.88 (m, 1H), 2.46 (t, *J* = 7.9 Hz, 2H), 2.29 (ddd, *J* = 13.3, 10.2, 6.2 Hz, 1H), 2.23 – 2.16 (m, 2H), 2.11 (ddd, *J* = 14.8, 7.9, 3.9 Hz, 1H), 1.52 – 1.45 (m, 2H), 1.29 – 1.21 (m, 2H), 0.86 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.54, 141.08, 139.69, 139.33, 134.60, 133.05, 132.58, 132.38, 131.99, 131.56, 131.07, 130.86, 128.32, 127.93, 126.69, 60.63 (q, *J* = 36.5 Hz, CF_3), 41.71, 40.84, 35.31, 35.09, 34.83, 34.43, 33.24, 32.66, 32.33, 22.32, 13.92. ^{19}F NMR (471 MHz, $CDCl_3$) δ -73.92. HRMS (ESI, m/z) calcd for $C_{30}H_{31}F_3O_2$ $[M+H]^+$ 481.2349, found 481.2333. $[\alpha]^{21}_D$ = 26.4° (c 0.71, $CHCl_3$); 96% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 80/20, detected at 254 nm, Flow rate = 0.5 mL/min, Retention times: 10.8 min (major), 11.7 min (minor).



Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	10.825	118.791	208.331	48.99	52.87
2	12.000	123.669	185.707	51.01	47.13
Total:		**242.460**	**394.038**	**100.00**	**100.00**

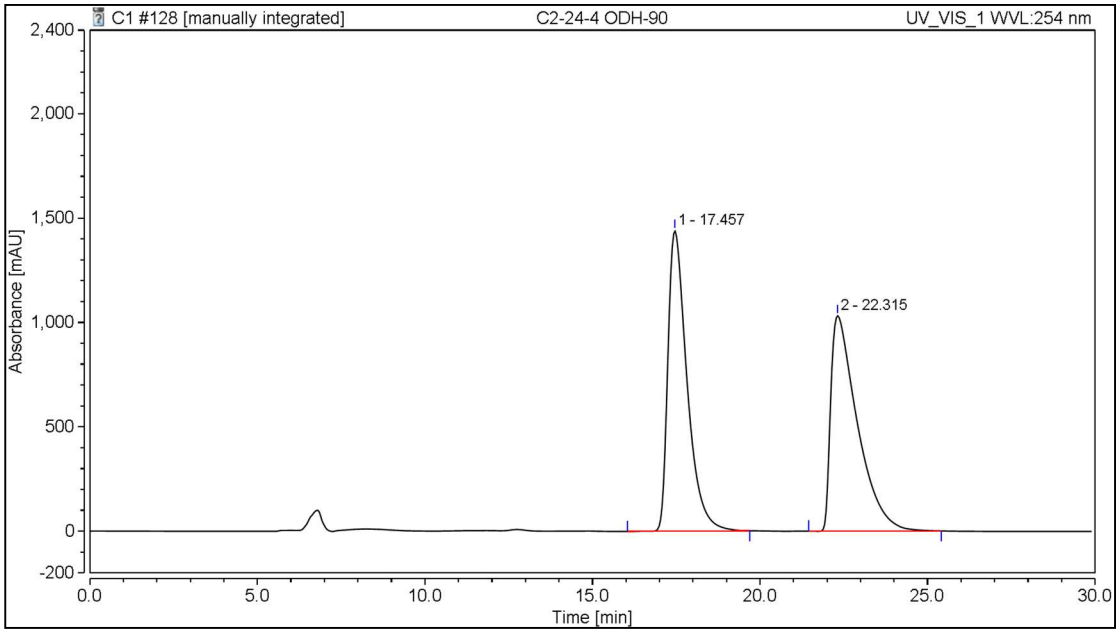


Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	10.782	203.280	352.545	98.20	98.06
2	11.720	3.727	6.982	1.80	1.94
Total:		**207.007**	**359.528**	**100.00**	**100.00**

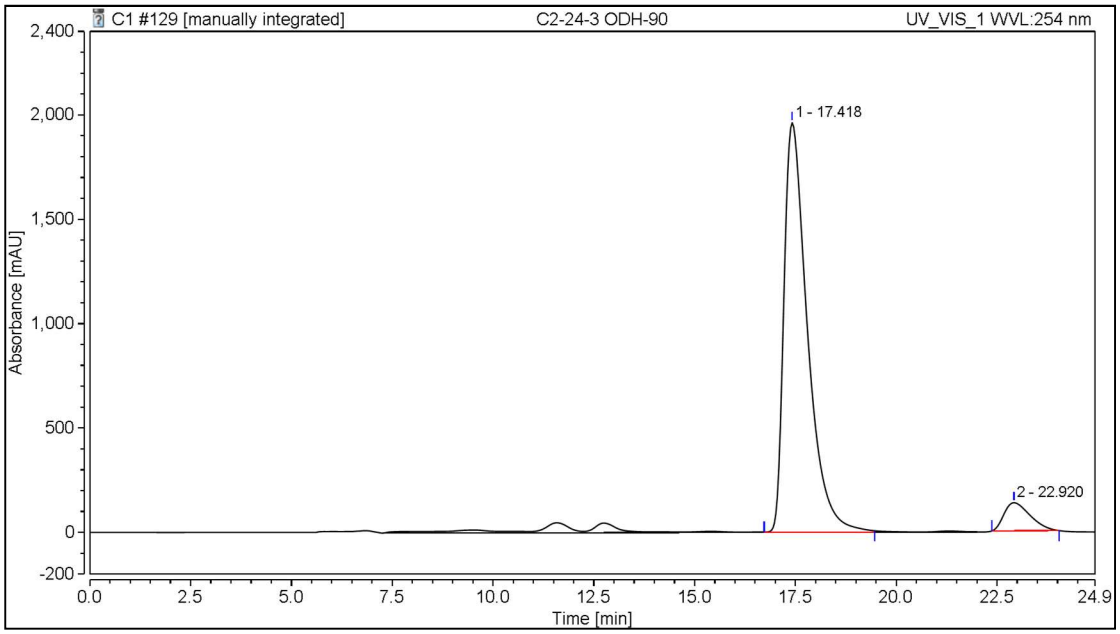


3i

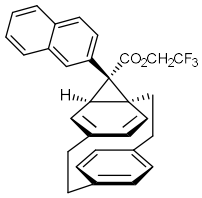
Colorless solid. 46% yield. 5.0 equiv. of diazo compound was used. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.52 – 7.48 (m, 2H), 7.36 (dd, *J* = 8.4, 6.9 Hz, 2H), 7.27 (dd, *J* = 11.2, 8.3 Hz, 3H), 7.19 (dd, *J* = 7.9, 1.9 Hz, 1H), 7.02 – 6.95 (m, 3H), 6.84 (dd, *J* = 7.8, 1.9 Hz, 1H), 6.80 (dd, *J* = 7.9, 1.8 Hz, 1H), 5.10 (d, *J* = 6.8 Hz, 1H), 5.00 (d, *J* = 9.8 Hz, 1H), 4.84 (dd, *J* = 9.9, 1.4 Hz, 1H), 4.63 (dq, *J* = 12.6, 8.5 Hz, 1H), 4.26 (dq, *J* = 12.7, 8.4 Hz, 1H), 3.10 – 2.98 (m, 3H), 2.93 (ddd, *J* = 13.2, 9.7, 6.3 Hz, 1H), 2.78 (dt, *J* = 13.9, 8.2 Hz, 1H), 2.30 (ddd, *J* = 13.3, 10.3, 6.3 Hz, 1H), 2.26 – 2.18 (m, 2H), 2.15 (ddd, *J* = 14.8, 7.9, 3.9 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.33, 140.82, 139.67, 139.37, 139.09, 134.85, 133.08, 132.60, 132.43, 132.20, 131.94, 130.90, 128.61, 128.55, 127.89, 127.04, 126.90, 125.36, 60.68 (q, *J* = 36.5 Hz, CF_3), 42.01, 41.00, 35.06, 34.83, 34.42, 32.61, 32.34. ^{19}F NMR (471 MHz, $CDCl_3$) δ -73.84. HRMS (ESI, m/z) calcd for $C_{32}H_{27}F_3O_2$ $[M+H]^+$ 501.2036, found 501.2042. $[\alpha]^{22}_D$ = 15.4° (c 0.24, $CHCl_3$); 86% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 90/10, detected at 254 nm, Flow rate = 0.5 mL/min, Retention times: 17.4 min (major), 22.9 min (minor).



Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	17.457	951.848	1440.127	50.17	58.26
2	22.315	945.504	1031.805	49.83	41.74
Total:		**1897.352**	**2471.932**	**100.00**	**100.00**

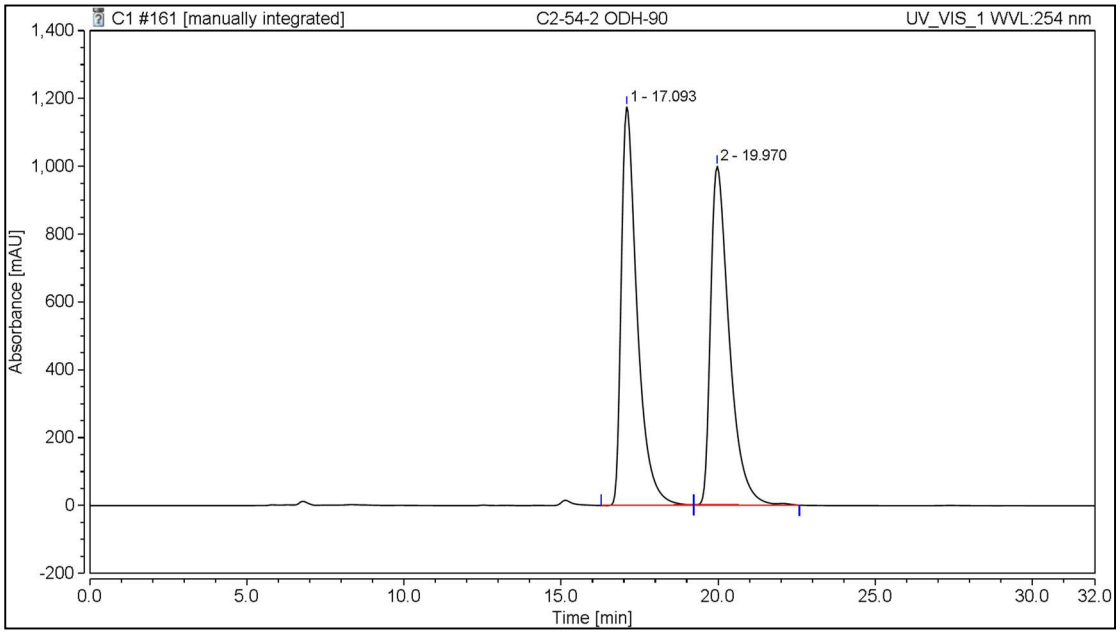


Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	17.418	1322.450	1962.351	92.92	93.58
2	22.920	100.819	134.587	7.08	6.42
Total:		**1423.268**	**2096.938**	**100.00**	**100.00**

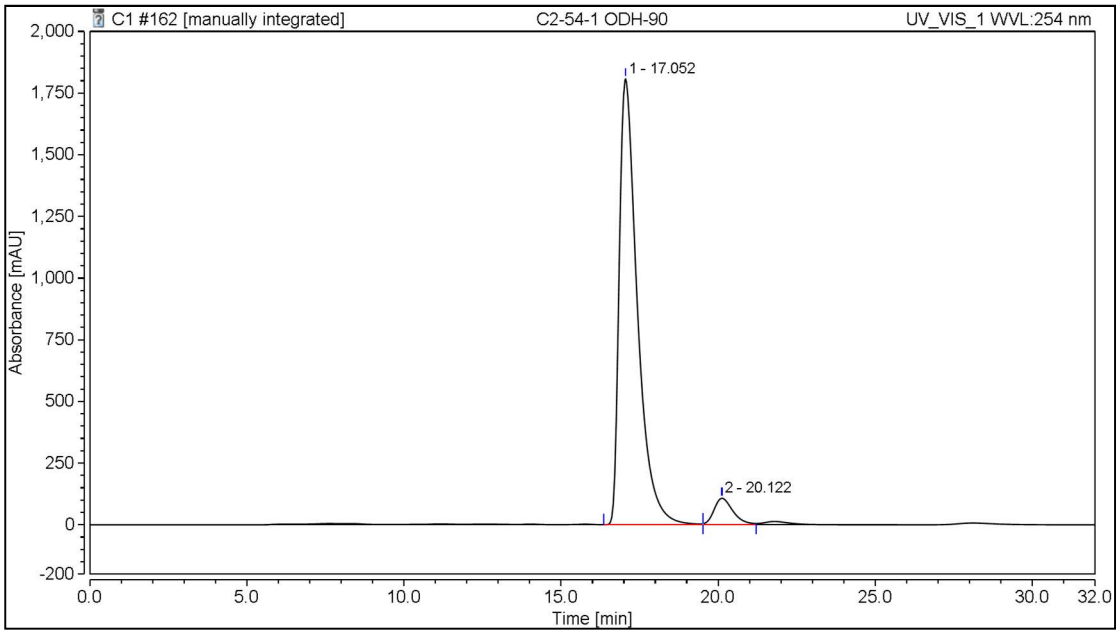


3j

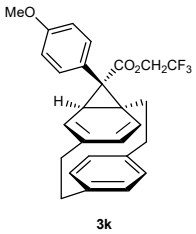
Colorless solid. 50% yield. The mixture of hexane and DCM was used as solvent. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.69 (d, *J* = 7.7 Hz, 1H), 7.60 (d, *J* = 7.7 Hz, 1H), 7.54 (d, *J* = 8.5 Hz, 1H), 7.33 (td, *J* = 16.3, 14.8, 8.4 Hz, 3H), 7.21 (d, *J* = 7.9 Hz, 1H), 7.11 (d, *J* = 8.5 Hz, 1H), 6.97 (d, *J* = 8.0 Hz, 1H), 6.84 (d, *J* = 7.8 Hz, 1H), 6.80 (d, *J* = 7.8 Hz, 1H), 5.17 (d, *J* = 6.9 Hz, 1H), 5.03 (d, *J* = 9.9 Hz, 1H), 4.73 (d, *J* = 9.8 Hz, 1H), 4.64 (dq, *J* = 12.5, 8.5 Hz, 1H), 4.19 (dq, *J* = 12.5, 8.5 Hz, 1H), 3.05 (dt, *J* = 22.7, 8.2 Hz, 3H), 2.89 (ddd, *J* = 13.2, 9.8, 6.2 Hz, 1H), 2.80 (dt, *J* = 14.0, 8.2 Hz, 1H), 2.32 – 2.15 (m, 3H), 2.10 (ddd, *J* = 13.2, 9.8, 2.9 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.37, 139.64, 139.38, 134.91, 133.07, 132.62, 132.37, 132.33, 132.27, 131.79, 131.26, 130.89, 130.40, 130.36, 128.68, 127.87, 127.72, 127.41, 126.32, 125.53, 125.21, 60.61 (q, *J* = 36.5 Hz, CF_3), 42.08, 41.22, 34.99, 34.78, 34.39, 32.93, 32.33. ^{19}F NMR (471 MHz, $CDCl_3$) δ -73.88. HRMS (ESI, m/z) calcd for $C_{30}H_{25}F_3O_2$ $[M+H]^+$ 475.1879, found 475.1881. $[\alpha]^{20}_D$ = -3.9° (c 0.35, $CHCl_3$); 88% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 90/10, detected at 254 nm, Flow rate = 0.5 mL/min, Retention times: 17.1 min (major), 20.1 min (minor).



Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	17.093	687.023	1174.658	49.99	54.05
2	19.970	687.375	998.699	50.01	45.95
Total:		**1374.399**	**2173.357**	**100.00**	**100.00**

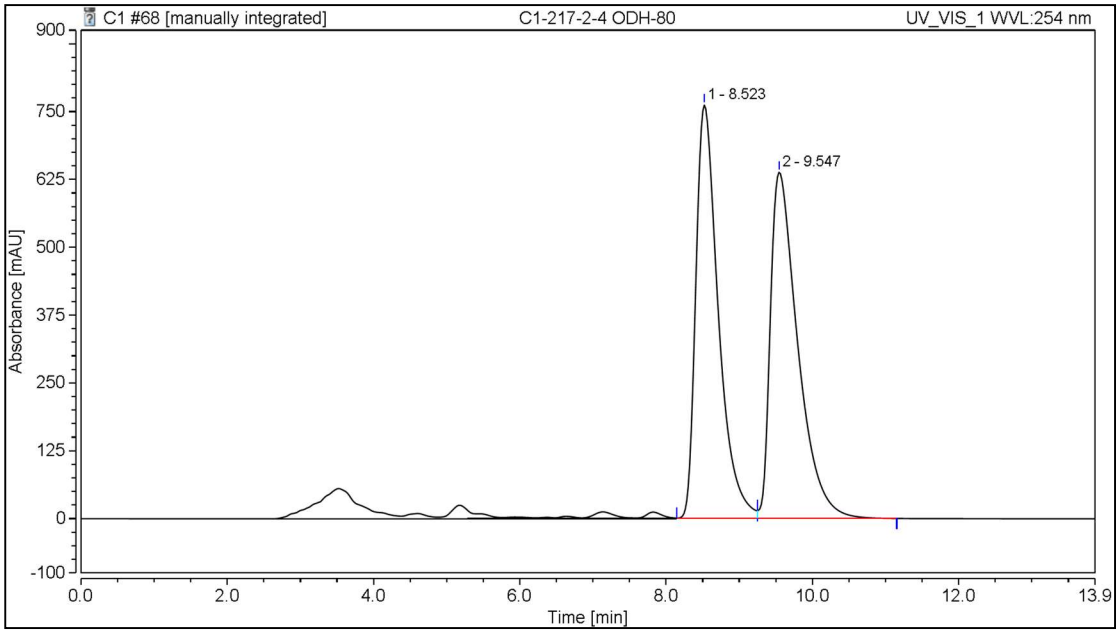


Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	17.052	1209.923	1808.105	94.07	94.37
2	20.122	76.251	107.878	5.93	5.63
Total:		**1286.175**	**1915.983**	**100.00**	**100.00**

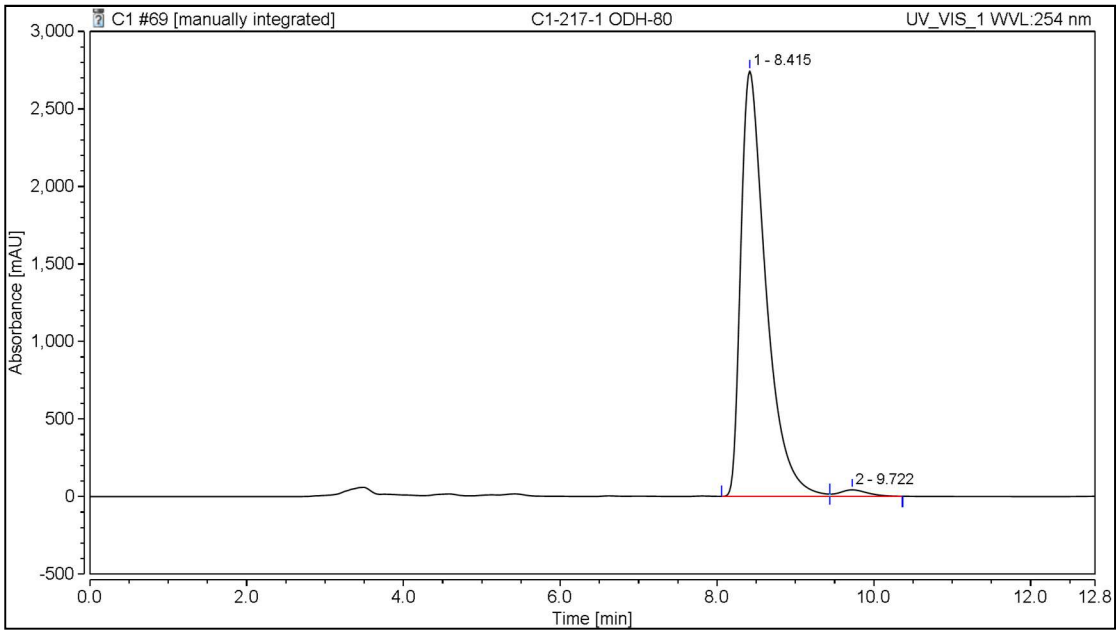


3k

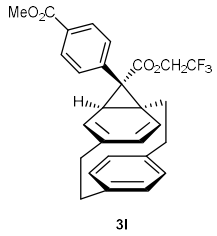
Light yellow oil. 33% yield.^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.17 (dd, *J* = 7.9, 1.9 Hz, 1H), 6.99 (dd, *J* = 7.8, 1.8 Hz, 1H), 6.85 – 6.81 (m, 2H), 6.78 (dd, *J* = 8.0, 1.8 Hz, 1H), 6.56 (d, *J* = 8.7 Hz, 2H), 5.06 (d, *J* = 6.8 Hz, 1H), 4.96 (d, *J* = 9.9 Hz, 0H), 4.83 (dd, *J* = 9.9, 1.5 Hz, 1H), 4.60 (dq, *J* = 12.7, 8.5 Hz, 1H), 4.25 (dq, *J* = 12.6, 8.4 Hz, 1H), 3.68 (s, 3H), 3.08 – 2.97 (m, 2H), 2.97 – 2.89 (m, 2H), 2.75 (dt, *J* = 13.9, 8.3 Hz, 1H), 2.29 (ddd, *J* = 13.3, 10.2, 6.2 Hz, 1H), 2.24 – 2.15 (m, 2H), 2.10 (ddd, *J* = 14.9, 7.9, 3.9 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.60, 158.07, 139.67, 139.32, 134.71, 133.06, 132.86, 132.57, 132.39, 131.99, 130.86, 128.43, 127.92, 126.11, 112.16, 60.64 (q, *J* = 36.5 Hz, CF_3), 54.94, 41.90, 40.98, 35.04, 34.81, 34.42, 32.31, 32.22. ^{19}F NMR (471 MHz, $CDCl_3$) δ -73.89. HRMS (ESI, m/z) calcd for $C_{27}H_{25}F_3O_3$ $[M+H]^+$ 455.1829, found 47455.1892. $[\alpha]^{22}_D$ = 16.5° (c 0.37, $CHCl_3$); 97% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 80/20, detected at 254 nm, Flow rate = 1.0 mL/min, Retention times: 8.4 min (major), 9.7 min (minor).



Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	8.523	271.512	762.151	49.56	54.42
2	9.547	276.360	638.370	50.44	45.58
Total:		**547.871**	**1440.521**	**100.00**	**100.00**

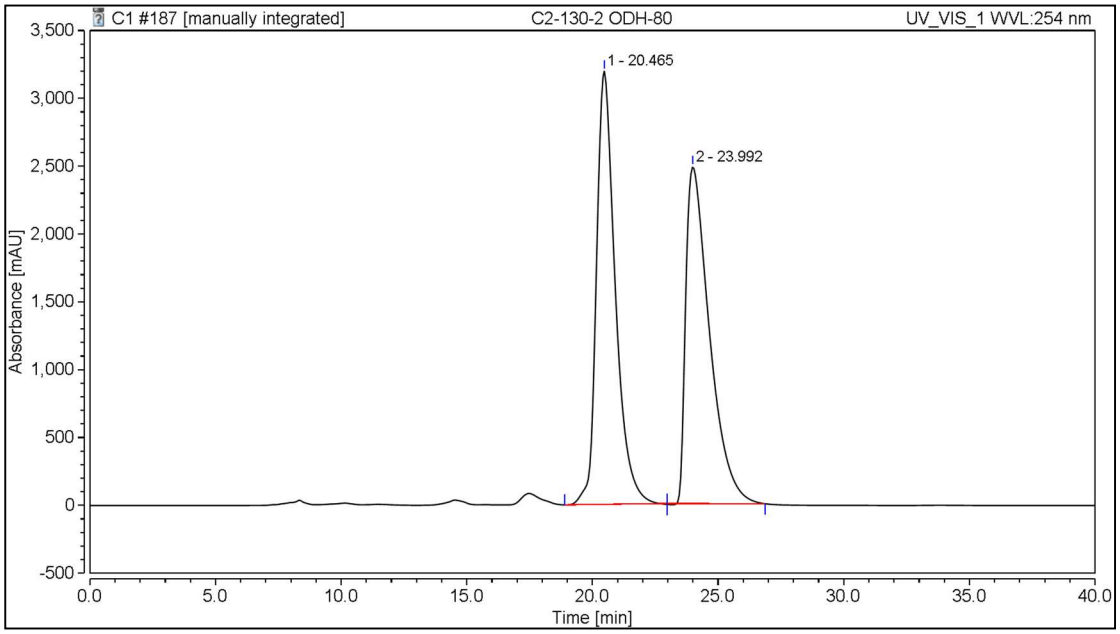


Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	8.415	1018.632	2743.707	98.33	98.50
2	9.722	17.249	41.645	1.67	1.50
Total:		**1035.881**	**2785.352**	**100.00**	**100.00**

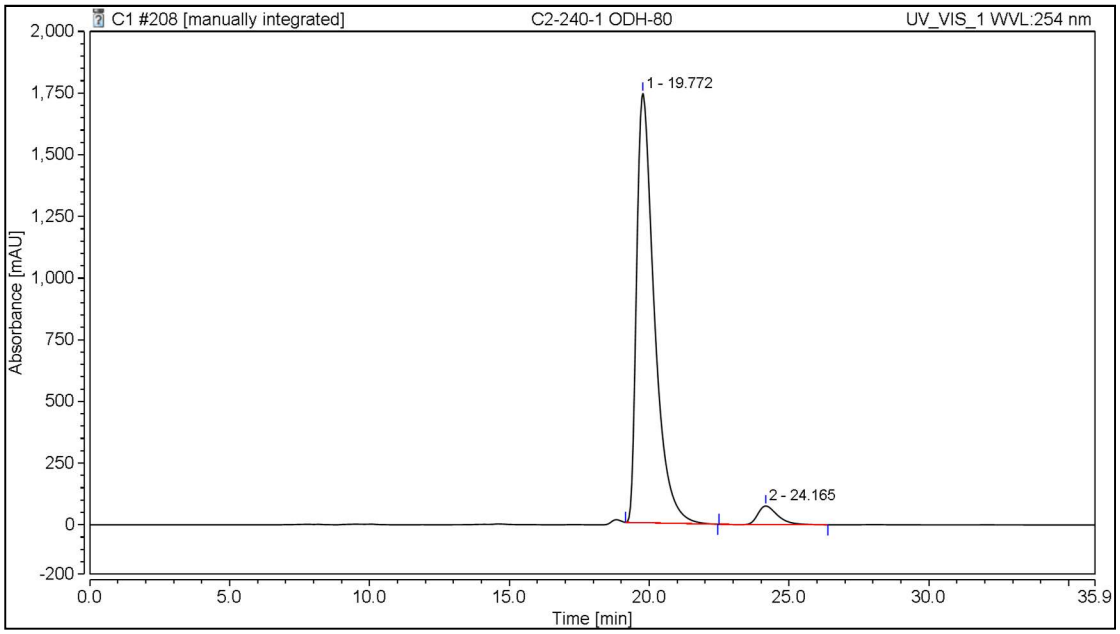


31

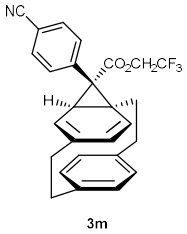
Colorless oil. 46% yield. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.71 (d, *J* = 8.5 Hz, 2H), 7.18 (dd, *J* = 7.9, 1.9 Hz, 1H), 6.98 (d, *J* = 8.3 Hz, 3H), 6.82 (dd, *J* = 7.8, 2.0 Hz, 1H), 6.78 (dd, *J* = 7.9, 1.8 Hz, 1H), 5.10 (d, *J* = 6.8 Hz, 1H), 4.97 (dd, *J* = 9.9, 1.5 Hz, 1H), 4.78 (dd, *J* = 9.8, 1.4 Hz, 1H), 4.56 (dq, *J* = 12.6, 8.5 Hz, 1H), 4.26 (dq, *J* = 12.7, 8.4 Hz, 1H), 3.83 (s, 3H), 3.06 – 2.99 (m, 3H), 2.92 (ddd, *J* = 13.1, 9.8, 6.3 Hz, 1H), 2.78 (dt, *J* = 13.9, 8.3 Hz, 1H), 2.29 (ddd, *J* = 13.2, 10.2, 6.0 Hz, 1H), 2.21 – 2.14 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.66, 167.07, 139.55, 139.34, 139.22, 135.11, 133.06, 132.61, 132.38, 131.87, 130.87, 128.57, 128.42, 128.09, 127.70, 60.77 (q, *J* = 36.5 Hz, CF_3), 51.90, 42.34, 41.36, 34.80, 34.74, 34.35, 32.58, 32.25. ^{19}F NMR (471 MHz, $CDCl_3$) δ -73.99. HRMS (ESI, m/z) calcd for $C_{28}H_{25}F_3O_4$ $[M+H]^+$ 483.1778, found 483.1777. $[\alpha]^{21}_D$ = 18.9° (c 0.37, $CHCl_3$); 92% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 80/20, detected at 254 nm, Flow rate = 0.4 mL/min, Retention times: 19.8 min (major), 24.2 min (minor).



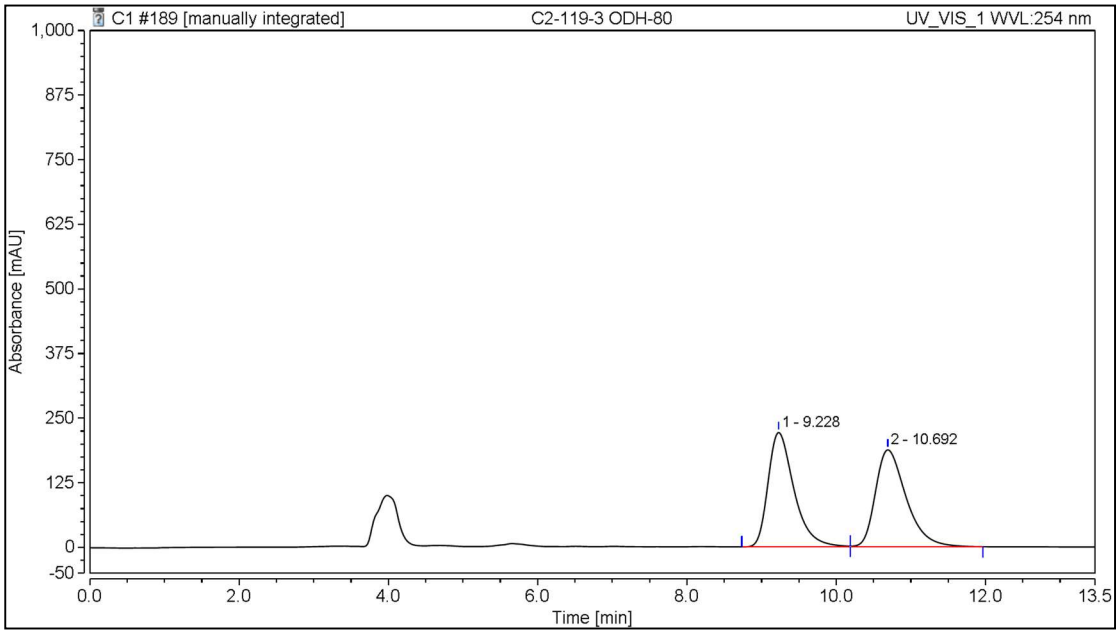
Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	20.465	2773.500	3193.010	50.59	56.27
2	23.992	2709.099	2481.630	49.41	43.73
Total:		**5482.599**	**5674.640**	**100.00**	**100.00**



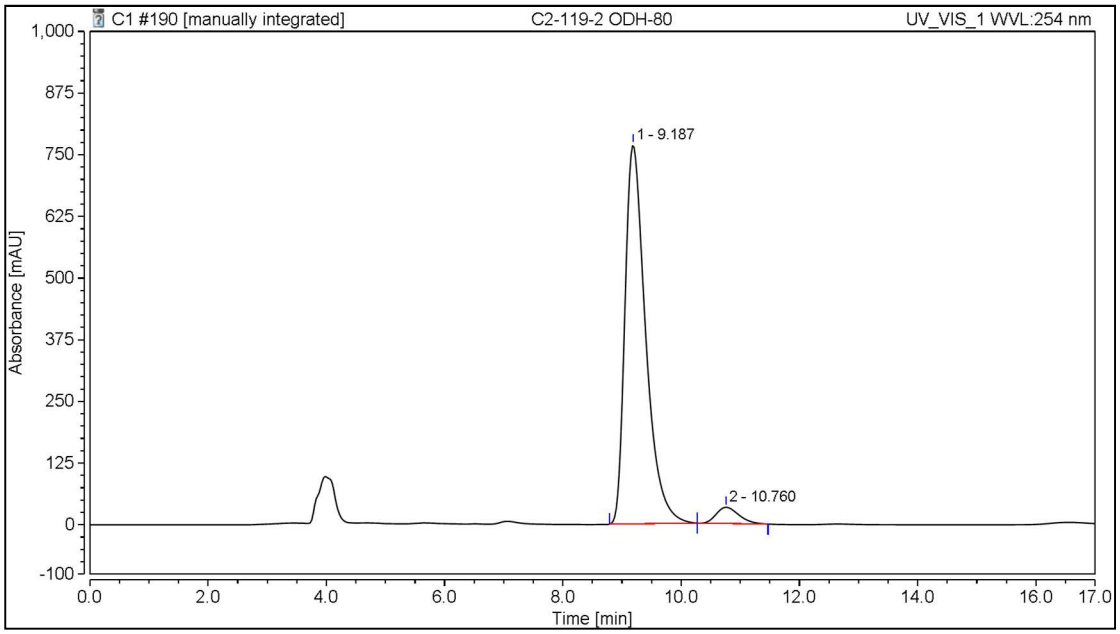
Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	19.772	1274.024	1740.137	95.47	95.86
2	24.165	60.509	75.179	4.53	4.14
Total:		**1334.533**	**1815.316**	**100.00**	**100.00**



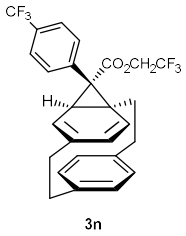
Colorless oil. 39% yield. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.32 (d, *J* = 8.4 Hz, 2H), 7.17 (dd, *J* = 7.9, 1.9 Hz, 1H), 7.01 (d, *J* = 8.3 Hz, 1H), 6.99 (dd, *J* = 7.8, 1.9 Hz, 1H), 6.83 (dd, *J* = 7.9, 1.9 Hz, 1H), 6.78 (dd, *J* = 7.9, 1.8 Hz, 1H), 5.10 (d, *J* = 6.9 Hz, 1H), 4.97 (d, *J* = 9.8 Hz, 1H), 4.82 (dd, *J* = 9.9, 1.4 Hz, 1H), 4.55 (dq, *J* = 12.6, 8.4 Hz, 1H), 4.28 (dq, *J* = 12.6, 8.4 Hz, 1H), 3.10 – 3.00 (m, 3H), 2.94 (ddd, *J* = 13.2, 9.7, 6.2 Hz, 1H), 2.78 (dt, *J* = 13.9, 8.3 Hz, 1H), 2.30 (ddd, *J* = 13.2, 10.1, 6.0 Hz, 1H), 2.20 (ddd, *J* = 14.2, 9.0, 4.4 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.15, 139.46, 139.33, 135.49, 133.05, 132.63, 132.55, 132.41, 131.75, 130.88, 130.69, 128.76, 127.55, 118.93, 110.51, 60.86 (q, *J* = 36.5 Hz, CF_3), 42.66, 41.46, 34.73, 34.69, 34.32, 32.46, 32.19. ^{19}F NMR (471 MHz, $CDCl_3$) δ -74.03. HRMS (ESI, m/z) calcd for $C_{27}H_{22}F_3NO_2$ $[M+H]^+$450.1675, found 450.1675. HRMS (ESI, m/z) calcd for $C_{28}H_{25}F_3O_4$ $[M+H]^+$ 483.1778, found 483.1777. $[\alpha]^{22}_D$ = 22.1° (c 0.42, $CHCl_3$); 91% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 80/20, detected at 254 nm, Flow rate = 1.0 mL/min, Retention times: 9.2 min (major), 10.8 min (minor).



Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	9.228	89.251	221.415	49.93	54.13
2	10.692	89.499	187.626	50.07	45.87
Total:		**178.749**	**409.041**	**100.00**	**100.00**

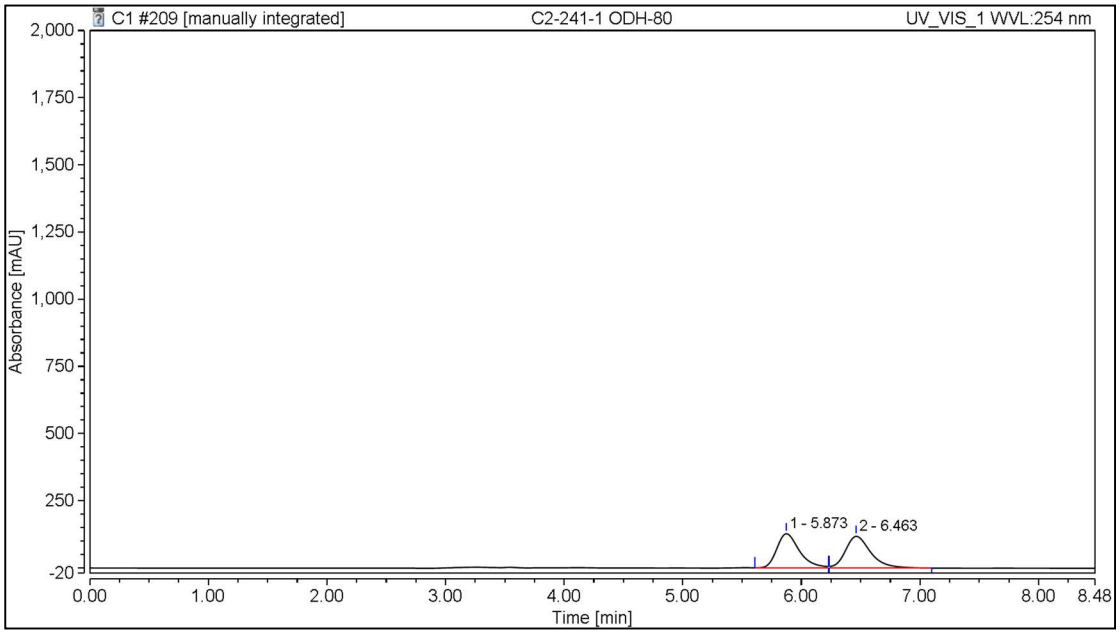


Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	9.187	310.666	768.011	95.51	95.89
2	10.760	14.591	32.886	4.49	4.11
Total:		**178.749**	**409.041**	**100.00**	**100.00**

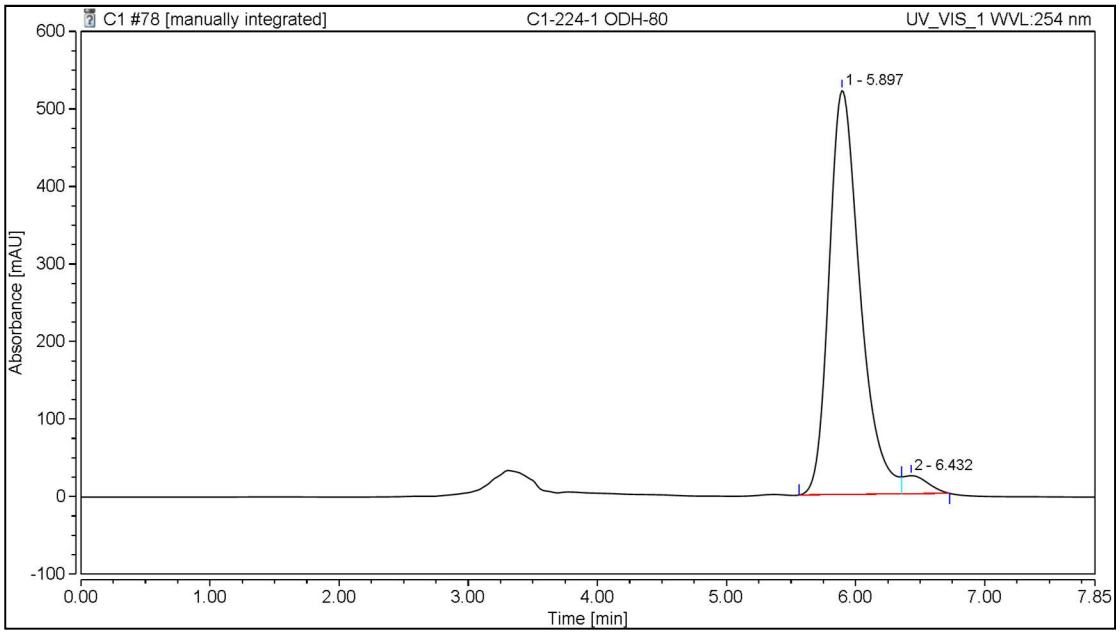


3n

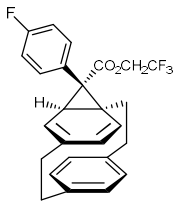
Colorless oil. 41% yield. 5.0 equiv. of diazo compound was used. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.28 (d, *J* = 8.1 Hz, 2H), 7.18 (dd, *J* = 7.9, 1.9 Hz, 1H), 7.02 (d, *J* = 8.0 Hz, 2H), 6.99 (dd, *J* = 7.8, 1.8 Hz, 1H), 6.83 (dd, *J* = 7.9, 1.9 Hz, 1H), 6.79 (dd, *J* = 8.0, 1.8 Hz, 1H), 5.10 (d, *J* = 6.9 Hz, 1H), 4.97 (d, *J* = 9.9 Hz, 1H), 4.82 (dd, *J* = 9.8, 1.4 Hz, 1H), 4.59 (dq, *J* = 12.4, 8.4 Hz, 1H), 4.26 (dq, *J* = 12.4, 8.4 Hz, 1H), 3.09 – 3.01 (m, 3H), 2.93 (ddd, *J* = 13.2, 9.8, 6.4 Hz, 1H), 2.77 (dt, *J* = 13.9, 8.3 Hz, 1H), 2.30 (ddd, *J* = 13.3, 10.3, 6.3 Hz, 1H), 2.26 – 2.16 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.61, 139.55, 139.35, 135.26, 133.05, 132.60, 132.44, 132.09, 131.74, 130.89, 128.92, 128.86, 128.68, 127.65, 123.74 (q, *J* = 36.5 Hz, CF_3), 60.75 (q, *J* = 36.5 Hz, CF_3), 42.33, 41.21, 34.83, 34.76, 34.35, 32.39, 32.25. ^{19}F NMR (471 MHz, $CDCl_3$) δ -62.41, -73.99. HRMS (ESI, m/z) calcd for $C_{27}H_{22}F_6O_2$ $[M+H]^+$ 493.1597, found 493.1562. $[\alpha]^{20}_D$ = 20.5° (c 2.00, $CHCl_3$); 93% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 80/20, detected at 254 nm, Flow rate = 1.0 mL/min, Retention times: 5.9 min (major), 6.4 min (minor).



Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	5.873	28.128	127.263	49.12	51.91
2	6.463	29.131	117.891	50.88	48.09
Total:		**57.259**	**245.154**	**100.00**	**100.00**

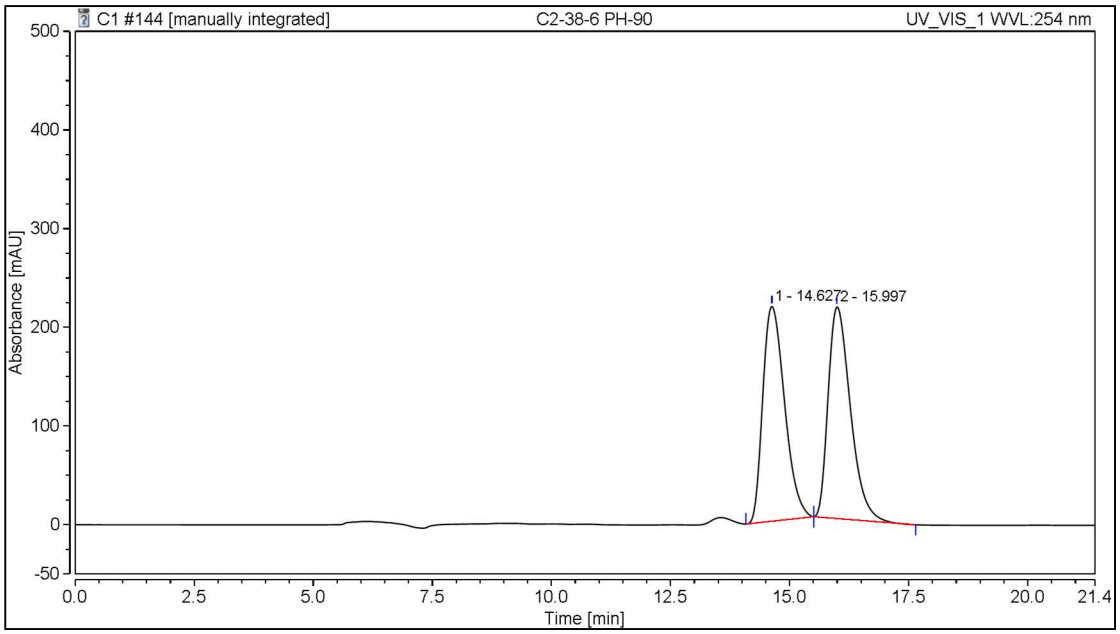


Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	5.897	145.049	521.251	96.54	95.72
2	6.432	5.201	23.290	3.46	4.28
Total:		**312.136**	**1044.378**	**100.00**	**100.00**

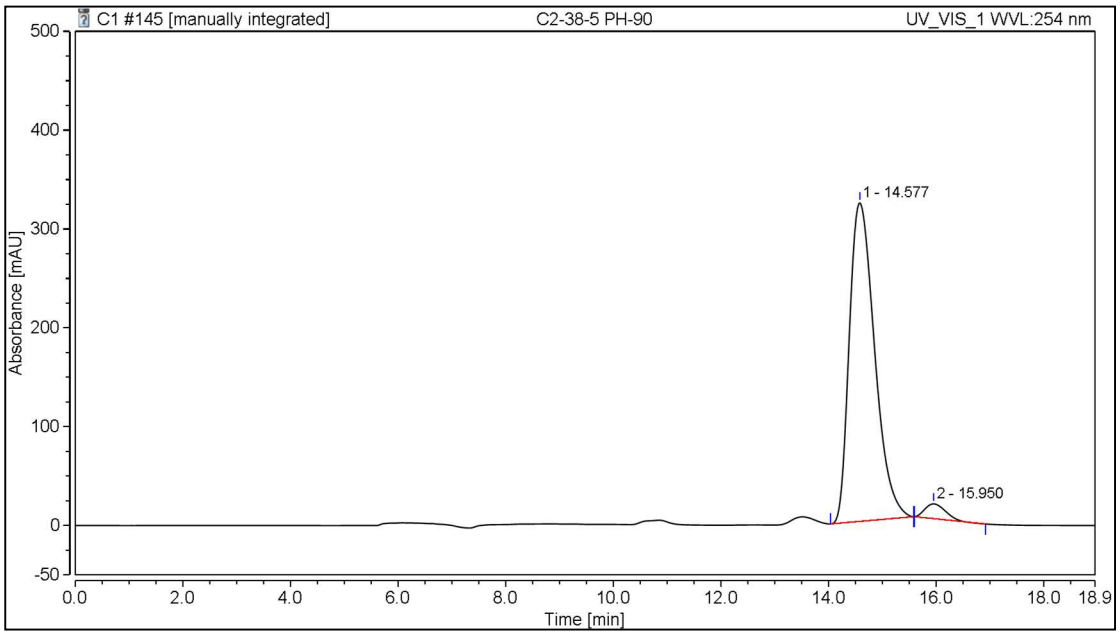


3o

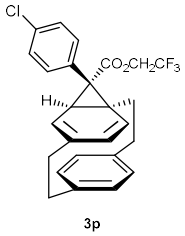
Colorless oil. 48% yield. The mixture of hexane and DCM was used as solvent. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.17 (dd, *J* = 7.9, 1.9 Hz, 1H), 7.00 (dd, *J* = 7.8, 1.8 Hz, 1H), 6.90 – 6.85 (m, 2H), 6.83 (dd, *J* = 7.8, 2.0 Hz, 1H), 6.79 (dd, *J* = 7.9, 1.8 Hz, 1H), 5.07 (d, *J* = 6.8 Hz, 1H), 4.97 (d, *J* = 9.8 Hz, 1H), 4.83 (dd, *J* = 9.9, 1.4 Hz, 1H), 4.57 (dq, *J* = 12.6, 8.5 Hz, 1H), 4.26 (dq, *J* = 12.6, 8.6 Hz, 1H), 3.09 – 2.99 (m, 2H), 2.98 (dd, *J* = 6.9, 1.6 Hz, 1H), 2.93 (ddd, *J* = 13.3, 9.7, 6.3 Hz, 1H), 2.75 (dt, *J* = 14.0, 8.3 Hz, 1H), 2.29 (ddd, *J* = 13.3, 10.3, 6.4 Hz, 1H), 2.24 – 2.17 (m, 2H), 2.13 (ddd, *J* = 14.8, 8.0, 4.2 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.19, 161.50 (d, *J* = 245.7 Hz) , 139.48 (d, *J* = 36.5 Hz), 135.01, 133.38 (d, *J* = 8.19 Hz), 133.04, 132.58, 132.44, 131.97, 130.89, 129.65 (d, *J* = 3.2 Hz), 128.52, 127.81, 113.81, 113.64, 60.73(q, *J* = 36.5 Hz, CF_3), 42.19, 41.18, 34.91, 34.77, 34.38, 32.28, 32.06.^{19}F NMR (471 MHz, $CDCl_3$) δ -73.98, -115.45. HRMS (ESI, m/z) calcd for $C_{26}H_{22}F_4O_2$ $[M+H]^+$ 443.1629, found 443.1614. $[\alpha]^{22}_D$ = 19.34° (c 0.66, $CHCl_3$); 93% ee; Chiral HPLC analysis of the product: Phenomenex 00G-4457-E0 250X4.6 mm 5u column; hexane/2-propanol = 90/10, detected at 254 nm, Flow rate = 0.5 mL/min, Retention times: 14.6 min (major), 16.0 min (minor).



Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	14.627	115.673	217.922	49.88	50.37
2	15.997	116.239	214.721	50.12	49.63
Total:		**231.991**	**432.643**	**100.00**	**100.00**

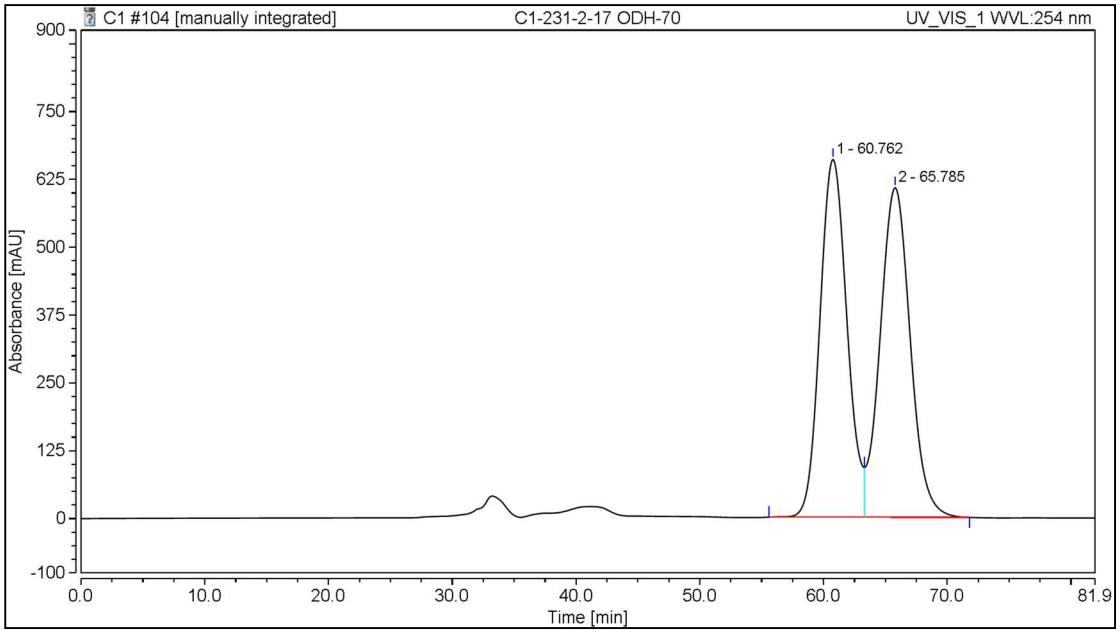


Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	14.577	175.325	322.531	96.34	95.55
2	15.950	6.655	15.004	3.66	4.45
Total:		**181.981**	**337.535**	**100.00**	**100.00**

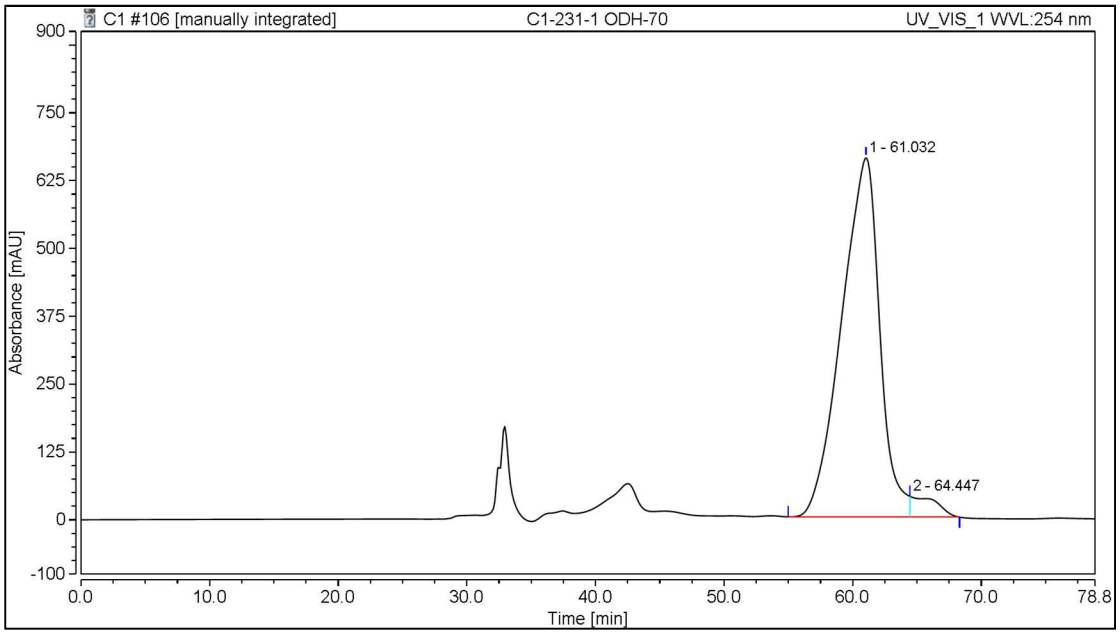


3p

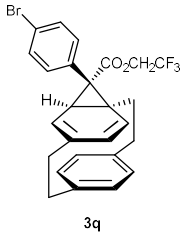
Colorless oil. 40% yield. 5.0 equiv. of diazo compound was used. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.17 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.02 – 6.96 (m, 3H), 6.87 – 6.80 (m, 3H), 6.78 (dd, *J* = 7.9, 1.8 Hz, 1H), 5.07 (d, *J* = 6.8 Hz, 1H), 4.96 (d, *J* = 9.9 Hz, 1H), 4.83 (dd, *J* = 9.9, 1.4 Hz, 1H), 4.58 (dq, *J* = 12.7, 8.5 Hz, 1H), 4.26 (dq, *J* = 12.6, 8.4 Hz, 1H), 3.09 – 2.99 (m, 2H), 2.98 (dd, *J* = 6.9, 1.6 Hz, 1H), 2.93 (ddd, *J* = 13.2, 9.7, 6.3 Hz, 1H), 2.76 (dt, *J* = 13.9, 8.3 Hz, 1H), 2.29 (ddd, *J* = 13.2, 10.3, 6.4 Hz, 1H), 2.24 – 2.09 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.91, 139.57, 139.33, 135.10, 133.15, 133.05, 132.59, 132.45, 132.43, 132.41, 131.83, 130.87, 128.66, 127.71, 127.06, 60.73 (q, *J* = 36.5 Hz, CF_3), 42.21, 41.17, 34.86, 34.77, 34.37, 32.25. ^{19}F NMR (471 MHz, $CDCl_3$) δ -73.95. HRMS (ESI, m/z) calcd for $C_{26}H_{22}ClF_3O_2$ $[M+H]^+$ 459.1333, found 459.1335. $[\alpha]^{21}_D$ = 13.0° (c 0.47, $CHCl_3$); 92% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 70/30, detected at 254 nm, Flow rate = 0.1 mL/min, Retention times: 61.0 min (major), 64.4 min (minor).



Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	60.762	1663.818	659.675	49.29	52.05
2	65.785	1712.066	607.646	50.71	47.95
Total:		**3375.885**	**1267.321**	**100.00**	**100.00**

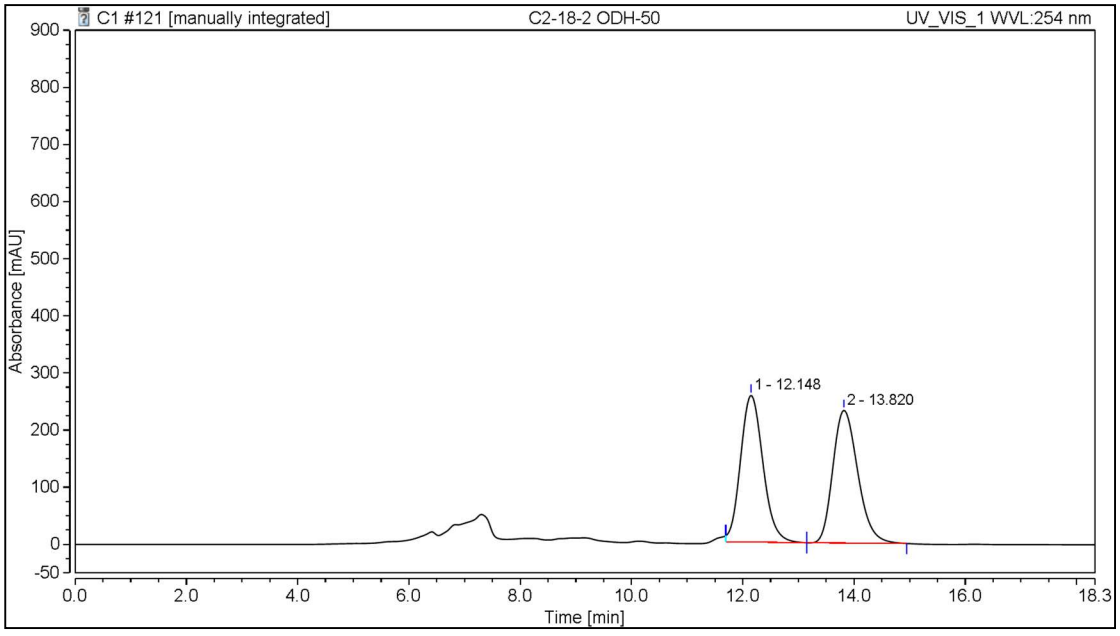


Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	61.032	2269.112	661.978	96.23	94.56
2	64.447	88.802	38.093	3.77	5.44
Total:		**2357.914**	**700.071**	**100.00**	**100.00**

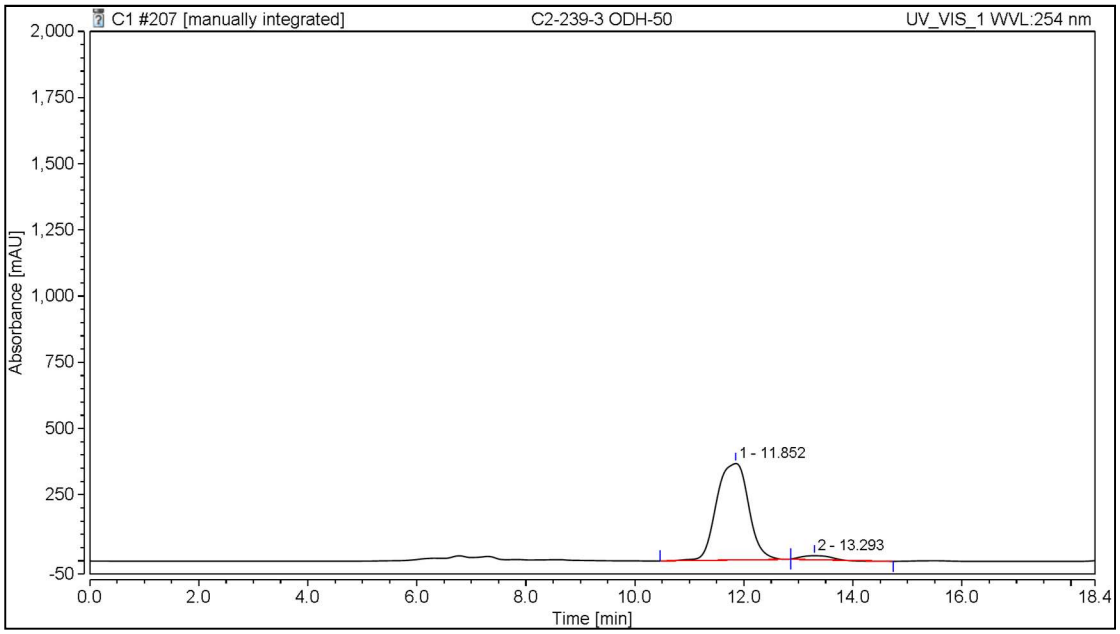


3q

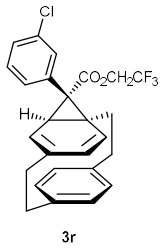
Colorless oil. 49% yield. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.19 – 7.12 (m, 3H), 6.99 (dd, *J* = 7.8, 1.8 Hz, 1H), 6.82 (dd, *J* = 7.9, 1.9 Hz, 1H), 6.78 (dd, *J* = 8.9, 2.3 Hz, 3H), 5.06 (d, *J* = 6.8 Hz, 1H), 4.95 (dt, *J* = 9.9, 1.2 Hz, 1H), 4.83 (dd, *J* = 9.9, 1.4 Hz, 1H), 4.59 (dq, *J* = 12.6, 8.4 Hz, 1H), 4.25 (dq, *J* = 12.6, 8.4 Hz, 1H), 3.09 – 2.99 (m, 2H), 2.98 (dd, *J* = 6.9, 1.6 Hz, 1H), 2.93 (ddd, *J* = 13.2, 9.7, 6.3 Hz, 1H), 2.76 (dt, *J* = 14.0, 8.3 Hz, 1H), 2.29 (ddd, *J* = 13.3, 10.2, 6.3 Hz, 1H), 2.25 – 2.10 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.83, 139.57, 139.34, 135.13, 133.54, 133.06, 132.97, 132.59, 132.42, 131.81, 130.87, 130.02, 128.69, 127.70, 120.74, 60.72 (q, *J* = 36.5 Hz, CF_3), 42.20, 41.14, 34.86, 34.78, 34.38, 32.26, 32.19. ^{19}F NMR (471 MHz, $CDCl_3$) δ -73.93. HRMS (ESI, m/z) calcd for $C_{26}H_{22}BrF_3O_2$ $[M+H]^+$ 503.0828, found 503.0835. $[\alpha]^{21}_D$ = 12.2° (c 0.36, $CHCl_3$); 92% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 50/50, detected at 254 nm, Flow rate = 0.5 mL/min, Retention times: 11.9 min (major), 13.3 min (minor).



Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	12.148	120.482	256.852	50.00	52.50
2	13.820	120.501	232.346	50.00	47.50
Total:		**240.983**	**489.198**	**100.00**	**100.00**

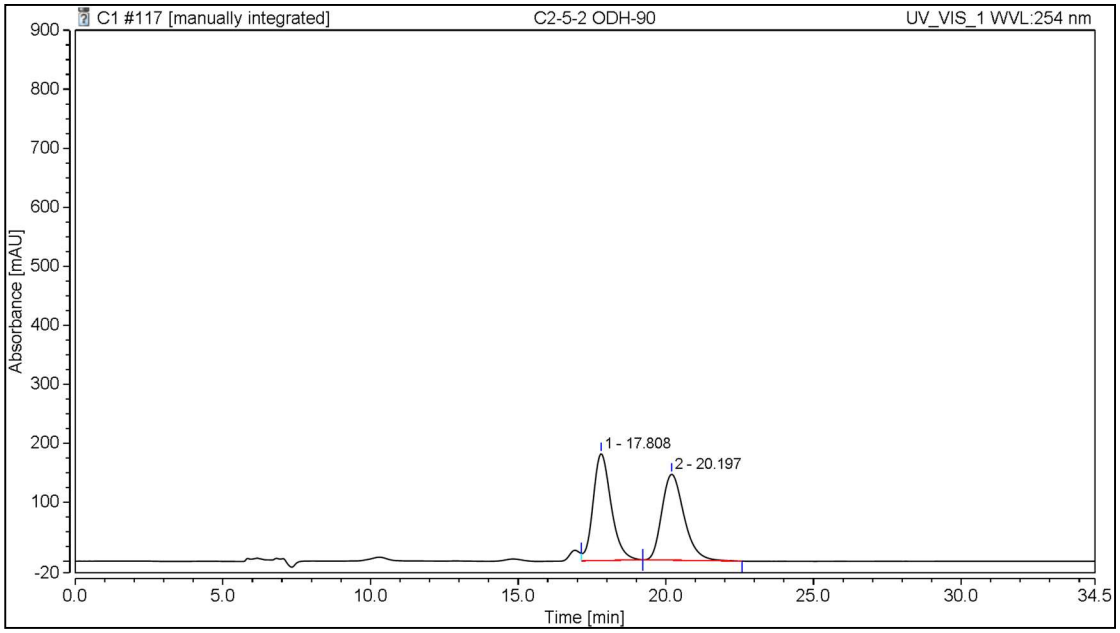


Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	11.852	247.963	364.795	96.46	95.96
2	13.293	9.113	15.363	3.54	4.04
Total:		**257.076**	**380.158**	**100.00**	**100.00**

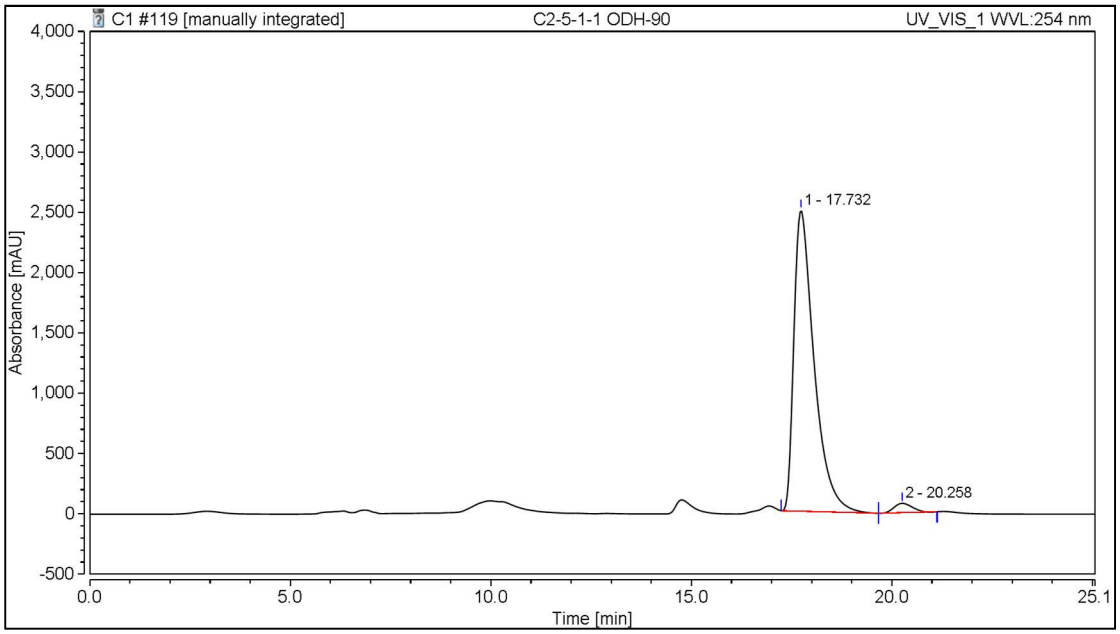


3r

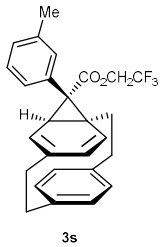
Colorless solid. 44% yield.^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.17 (dd, *J* = 7.9, 1.9 Hz, 1H), 7.04 (ddd, *J* = 8.0, 2.1, 1.1 Hz, 1H), 6.99 (dd, *J* = 7.8, 1.8 Hz, 1H), 6.96 (t, *J* = 7.8 Hz, 1H), 6.89 (t, *J* = 1.9 Hz, 1H), 6.83 (dd, *J* = 7.9, 1.9 Hz, 1H), 6.79 (ddd, *J* = 9.1, 7.0, 1.6 Hz, 2H), 5.09 (d, *J* = 6.9 Hz, 1H), 4.99 (d, *J* = 9.9 Hz, 1H), 4.85 (dd, *J* = 9.8, 1.4 Hz, 1H), 4.58 (dq, *J* = 12.6, 8.4 Hz, 1H), 4.27 (dq, *J* = 12.6, 8.4 Hz, 1H), 3.09 – 3.00 (m, 2H), 2.99 (dd, *J* = 6.9, 1.6 Hz, 1H), 2.94 (ddd, *J* = 13.2, 9.8, 6.3 Hz, 1H), 2.77 (dt, *J* = 14.0, 8.2 Hz, 1H), 2.32 (ddd, *J* = 13.4, 10.4, 6.3 Hz, 1H), 2.25 – 2.11 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.75, 139.55, 139.35, 135.80, 135.19, 133.07, 132.61, 132.39, 132.15, 131.91, 131.78, 130.86, 130.09, 128.62, 127.97, 127.57, 126.92, 60.76 (q, *J* = 36.5 Hz, CF_3), 45.86, 42.18, 41.22, 34.84, 34.76, 34.37, 32.24. ^{19}F NMR (471 MHz, $CDCl_3$) δ -73.96. HRMS (ESI, m/z) calcd for $C_{26}H_{22}ClF_3O_2$ $[M+H]^+$ 459.1333, found 459.1333. $[\alpha]^{20}_D$ = 13.6° (c 0.56, $CHCl_3$); 95% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 90/10, detected at 254 nm, Flow rate = 0.5 mL/min, Retention times: 17.7 min (major), 20.3 min (minor).



Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	17.808	128.692	181.191	50.38	55.43
2	20.197	126.771	145.702	49.62	44.57
Total:		**255.463**	**326.893**	**100.00**	**100.00**

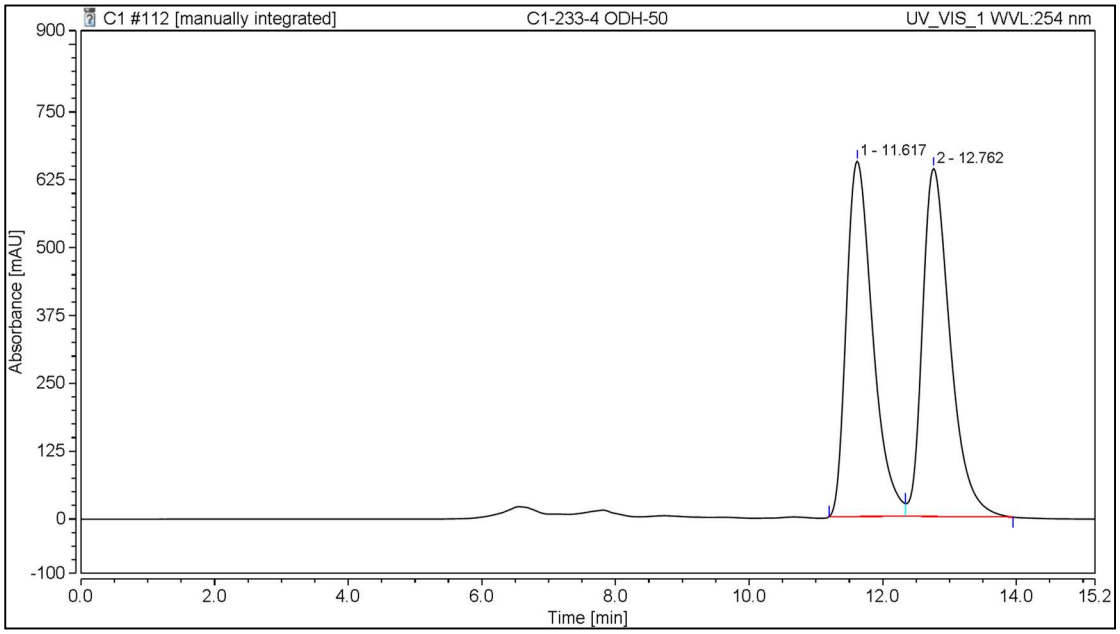


Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	17.732	1457.106	2496.716	97.31	96.99
2	20.258	40.264	77.509	2.69	3.01
Total:		**1497.371**	**2574.225**	**100.00**	**100.00**

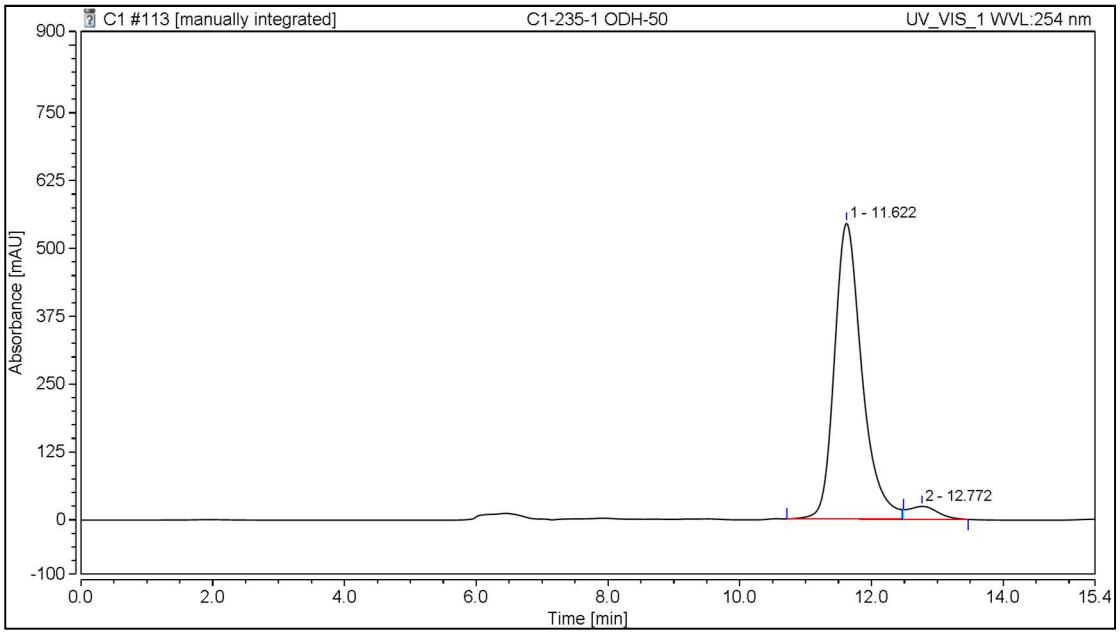


3s

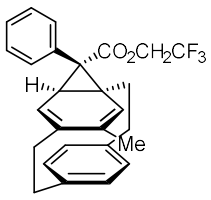
Colorless oil. 60% yield. 5.0 equiv. of diazo compound was used. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.18 (dd, *J* = 7.9, 2.0 Hz, 1H), 6.99 (dd, *J* = 7.8, 1.8 Hz, 1H), 6.92 (t, *J* = 7.7 Hz, 1H), 6.87 (d, *J* = 7.5 Hz, 1H), 6.83 (dd, *J* = 7.8, 1.9 Hz, 1H), 6.78 (dd, *J* = 7.8, 1.8 Hz, 1H), 6.74 – 6.69 (m, 2H), 5.07 (d, *J* = 6.8 Hz, 1H), 4.98 (d, *J* = 9.8 Hz, 1H), 4.82 (dd, *J* = 9.9, 1.4 Hz, 1H), 4.61 (dq, *J* = 12.6, 8.5 Hz, 1H), 4.24 (dq, *J* = 12.6, 8.5 Hz, 1H), 3.08 – 2.98 (m, 2H), 2.97 (dd, *J* = 6.9, 1.6 Hz, 1H), 2.92 (ddd, *J* = 13.2, 9.7, 6.2 Hz, 1H), 2.76 (dt, *J* = 13.9, 8.2 Hz, 1H), 2.29 (ddd, *J* = 13.2, 10.3, 6.2 Hz, 1H), 2.24 – 2.17 (m, 2H), 2.16 (s, 3H), 2.13 (ddd, *J* = 10.9, 7.8, 3.9 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.42, 139.66, 139.34, 135.98, 134.62, 133.83, 133.06, 132.65, 132.59, 132.36, 132.01, 130.85, 128.85, 128.25, 127.90, 127.41, 126.46, 60.61 (q, *J* = 36.5 Hz , CF_3), 41.69, 40.89, 35.10, 34.78, 34.42, 32.87, 32.32, 21.19. ^{19}F NMR (471 MHz, $CDCl_3$) δ -73.91. HRMS (ESI, m/z) calcd for $C_{27}H_{25}F_3O_2$ $[M+H]^+$ 439.1879, found 439.1875. $[\alpha]^{22}_D$ = 40.36° (c 0.37, $CHCl_3$); 91% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 50/50, detected at 254 nm, Flow rate = 0.5 mL/min, Retention times: 11.6 min (major), 12.8 min (minor).



Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	11.617	298.741	655.159	49.27	50.52
2	12.762	307.623	641.573	50.73	49.48
Total:		**606.364**	**1296.732**	**100.00**	**100.00**



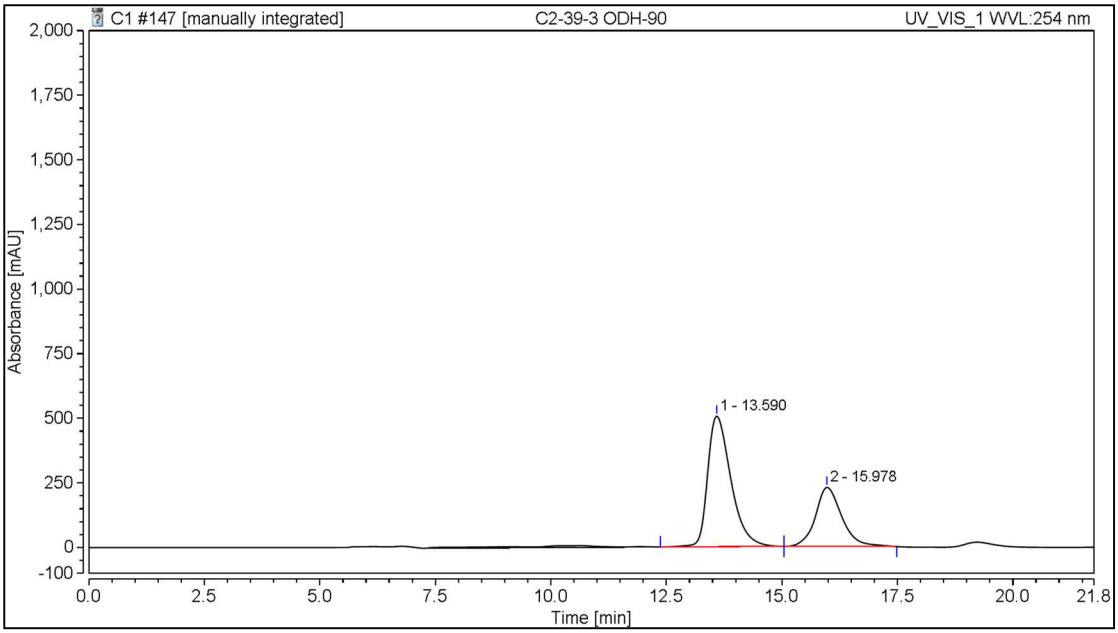
Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	11.622	264.137	545.209	95.48	95.82
2	12.772	12.516	23.797	4.52	4.18
Total:		**276.653**	**569.007**	**100.00**	**100.00**



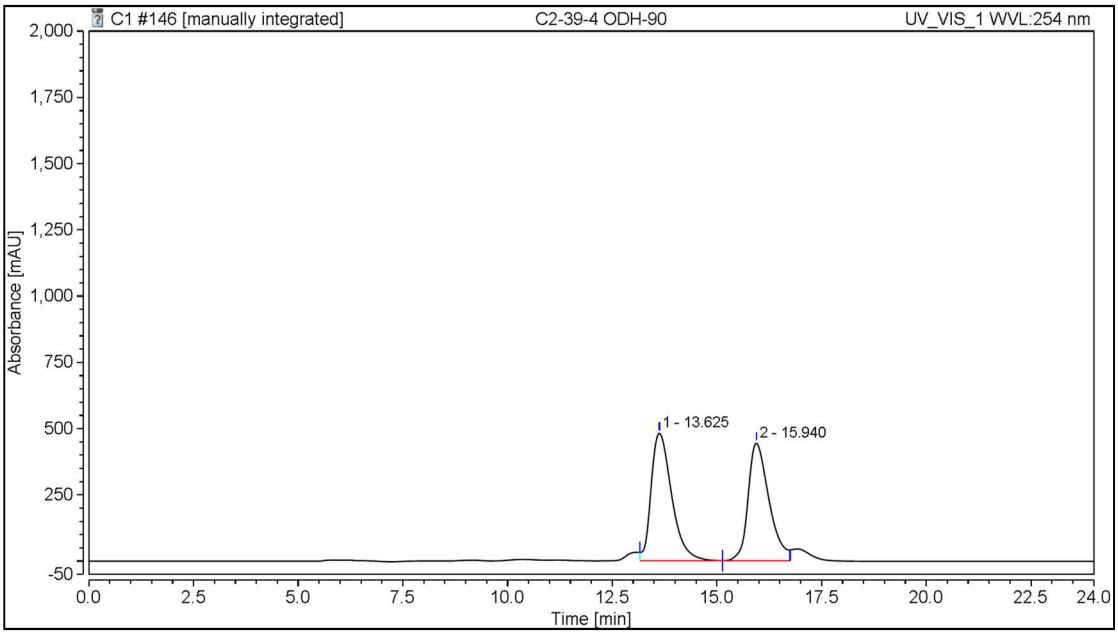
3db

Colorless oil. 84% yield. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.19 (dd, *J* = 7.9, 2.0 Hz, 1H), 7.05 – 6.98 (m, 4H), 6.90 – 6.84 (m, 2H), 6.82 – 6.74 (m, 2H), 5.04 (d, *J* = 6.9 Hz, 1H), 4.64 (s, 1H), 4.59 (dq, *J* = 12.6, 8.5 Hz, 2H), 4.25 (dq, *J* = 12.7, 8.4 Hz, 1H), 3.15 – 3.03 (m, 2H), 2.95 (dd, *J* = 6.9, 1.8 Hz, 1H), 2.84 (ddd, *J* = 13.2, 9.5, 7.5 Hz, 1H), 2.69 (ddd, *J* = 13.9, 9.8, 7.7 Hz,

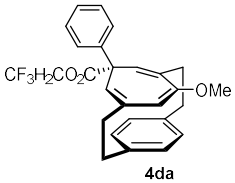
1H), 2.40 (dd, J = 13.4, 9.5 Hz, 1H), 2.19 – 2.05 (m, 3H), 1.15 (d, J = 1.5 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.50, 139.26, 138.79, 136.12, 134.01, 132.78, 132.22, 132.03, 131.91, 131.15, 130.10, 129.97, 129.45, 126.49, 126.33, 60.55 (q, J = 37 Hz, CF_3), 42.95, 40.34, 34.23, 34.06, 32.93, 32.15, 19.49.^{19}F NMR (471 MHz, $CDCl_3$) δ -73.94.. 32% ee; Daicel Chiralpak AD-H 250X4.6 mm 5u column; hexane/2-propanol = 90/10, detected at 254 nm, Flow rate = 0.5 mL/min, Retention times: 13.6 min (major), 15.9 min (minor).



Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	13.590	294.673	505.273	66.07	68.86
2	15.978	151.314	228.448	33.93	31.14
Total:		**445.988**	**733.721**	**100.00**	**100.00**



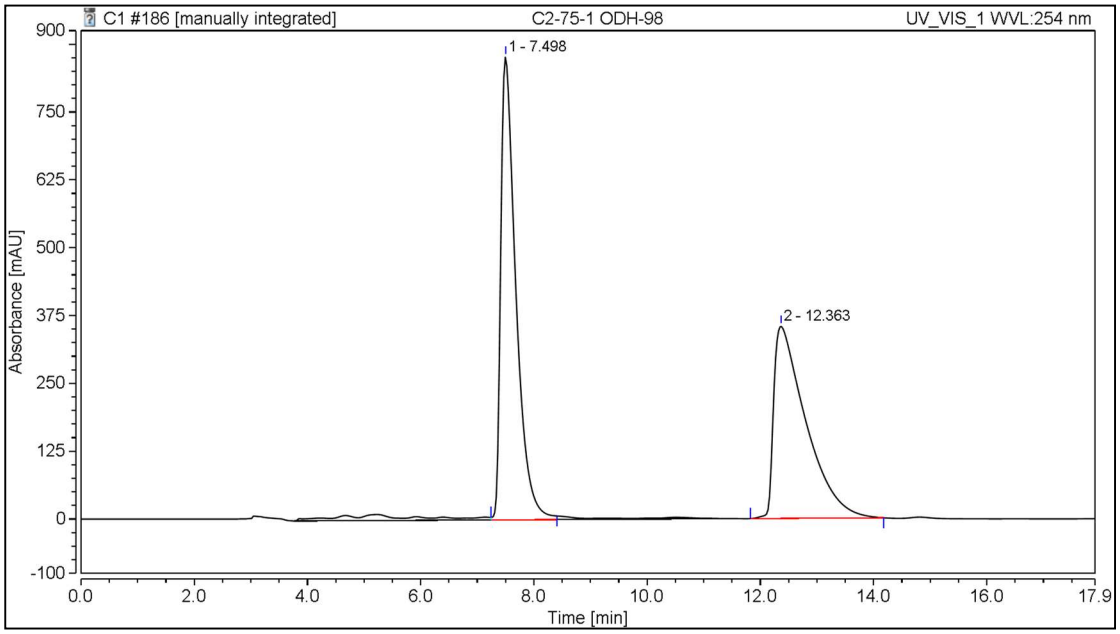
Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	13.625	274.432	481.361	51.61	52.00
2	15.940	257.325	444.271	48.39	48.00
Total:		**531.757**	**925.632**	**100.00**	**100.00**



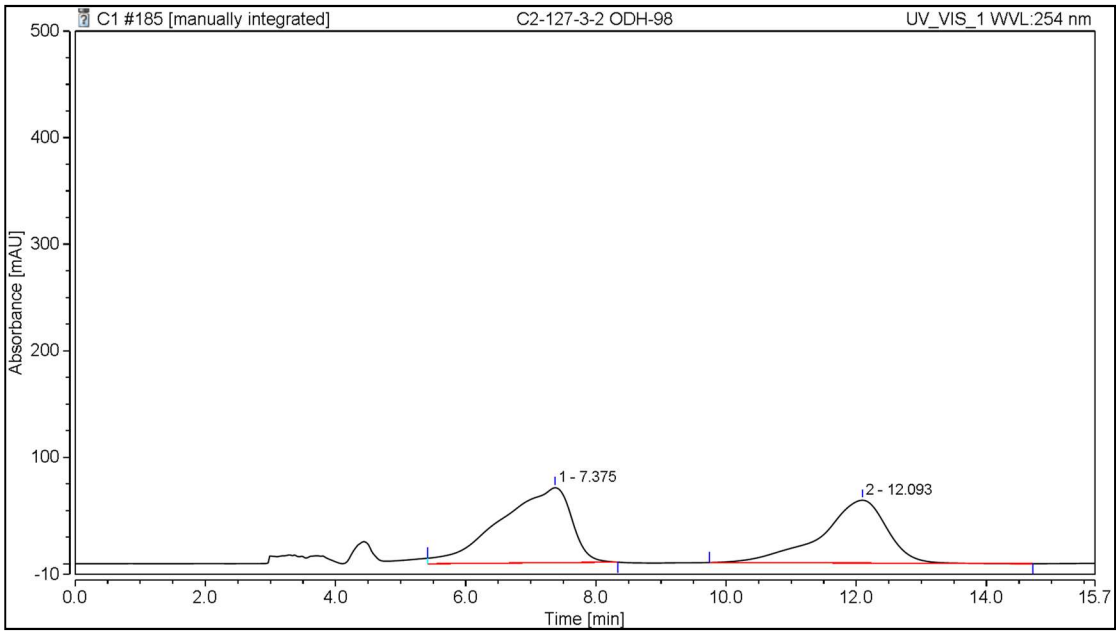
4da

Colorless crystal. 65% yield. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.08 – 7.04 (m, 2H), 6.97 (m, 3H), 6.85 – 6.76 (m, 2H), 6.62 (qd, *J* = 7.9, 1.7 Hz, 2H), 5.74 (s, 1H), 5.56 (s, 1H), 4.40 (q, *J* = 8.4 Hz, 2H), 4.28 (s, 1H), 3.13 (dddd, *J* = 14.1, 9.3, 3.3, 1.6 Hz, 1H), 3.05 (s, 3H), 3.04 – 2.78 (m, 5H), 2.67 (ddd, *J* = 14.2, 9.8, 7.0 Hz, 1H), 2.35 (ddd, *J* = 13.0, 9.0, 6.8 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.22, 155.88, 138.83, 138.58, 137.52, 135.24, 132.03, 131.99, 131.72, 131.05, 127.79, 127.67, 126.53, 125.69, 125.63, 124.94, 119.43, 108.43, 59.97 (q, *J* = 40.0 Hz, CF_3), 54.76, 52.50, 36.82, 33.59, 32.56, 30.83. ^{19}F NMR (471 MHz, $CDCl_3$) δ -73.74. HRMS (ESI, m/z) calcd for $C_{27}H_{25}F_3O_3$

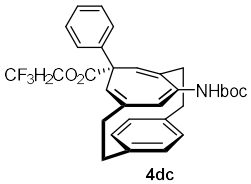
$[M+H]^+$ 455.1829, found 455.1825. 13% ee; Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 98/2, detected at 254 nm, Flow rate = 1.0 mL/min, Retention times: 7.4 min (major), 12.1 min (minor).



Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	7.498	264.623	853.086	53.17	70.66
2	12.363	233.058	354.163	46.83	29.34
Total:		**497.682**	**1207.249**	**100.00**	**100.00**



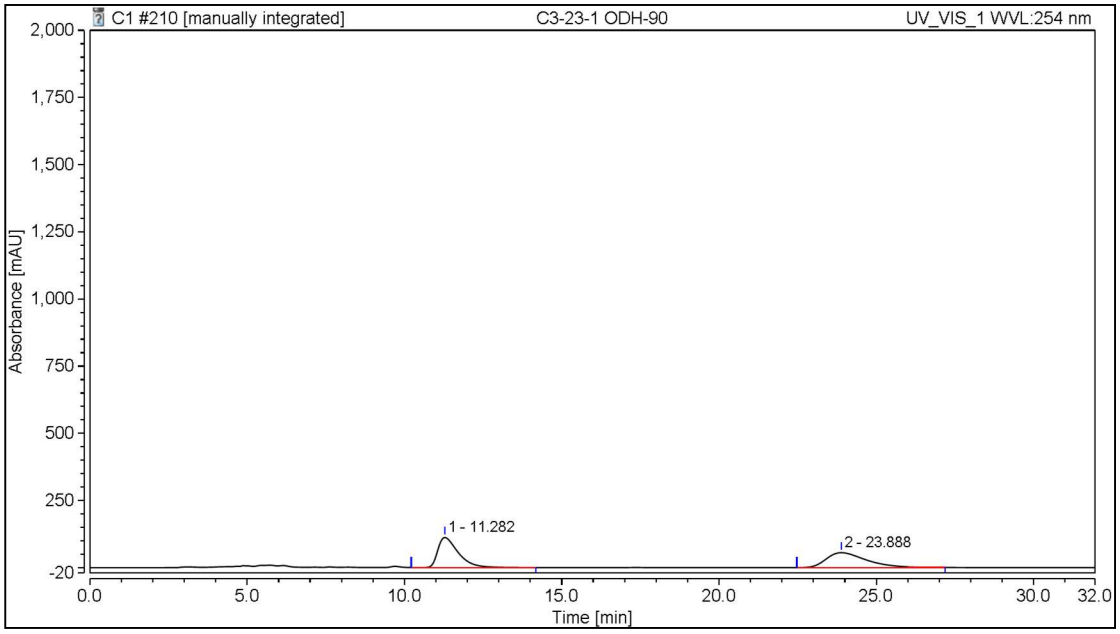
Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	7.375	893254	70.403	56.47	54.39
2	12.093	68.790	59.040	43.53	45.61
Total:		**158.045**	**129.443**	**100.00**	**100.00**



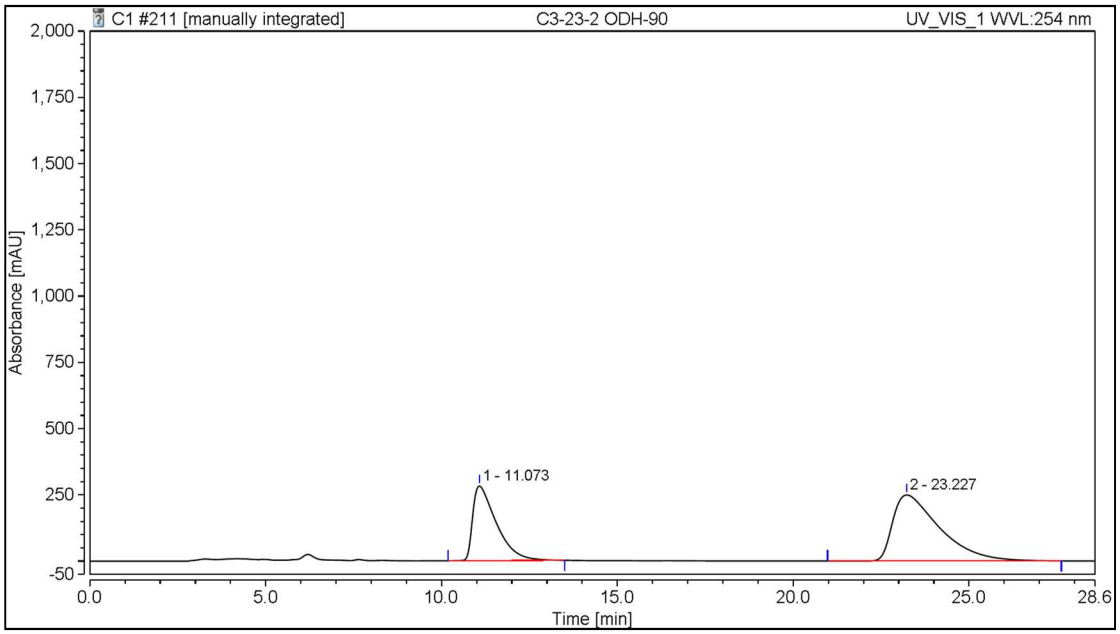
4dc

Colorless solid. 25% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.49 – 7.39 (m, 5H), 6.83 – 6.76 (m, 2H), 6.54 (dd, *J* = 7.8, 1.9 Hz, 1H), 6.47 (dd, *J* = 7.9, 2.0 Hz, 1H), 6.24 (s, 1H), 6.04 (dd, *J* = 7.9, 1.9 Hz, 1H), 5.80 (s, 1H), 4.98 (s, 1H), 4.55 (dq, *J* = 12.7, 8.4 Hz, 1H), 4.34 (dq, *J* = 12.7, 8.4 Hz, 1H), 3.24 – 3.06 (m, 4H), 3.03 – 2.82 (m, 3H), 2.47 (ddd, *J* = 14.3, 10.2, 7.4 Hz, 1H), 1.55 (s, 10H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.54, 152.61, 139.19, 138.78, 138.73, 136.74, 135.61, 134.34, 132.41, 132.13, 131.93, 129.73, 129.58, 129.09, 128.75, 128.12, 126.59, 124.20, 121.44, 80.55, 60.62 (q, *J* = 36.5 Hz, CF_3), 54.63, 34.02, 33.01, 32.80, 32.52, 28.40. ^{19}F NMR (376 MHz,

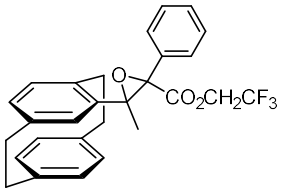
$CDCl_3$) δ -73.54. HRMS (ESI, m/z) calcd for $C_{31}H_{32}F_3NO_4$ $[M+NH_4]^+$ 557.2622, found 557.2621. 27% ee; Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 90/10, detected at 254 nm, Flow rate = 1.0 mL/min, Retention times: 11.1 min (minor), 23.2 min (major).



Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	11.282	84.252	111.967	50.66	66.82
2	23.888	55.605	49.34	33.18	41.35
Total:		**166.308**	**167.572**	**100.00**	**100.00**



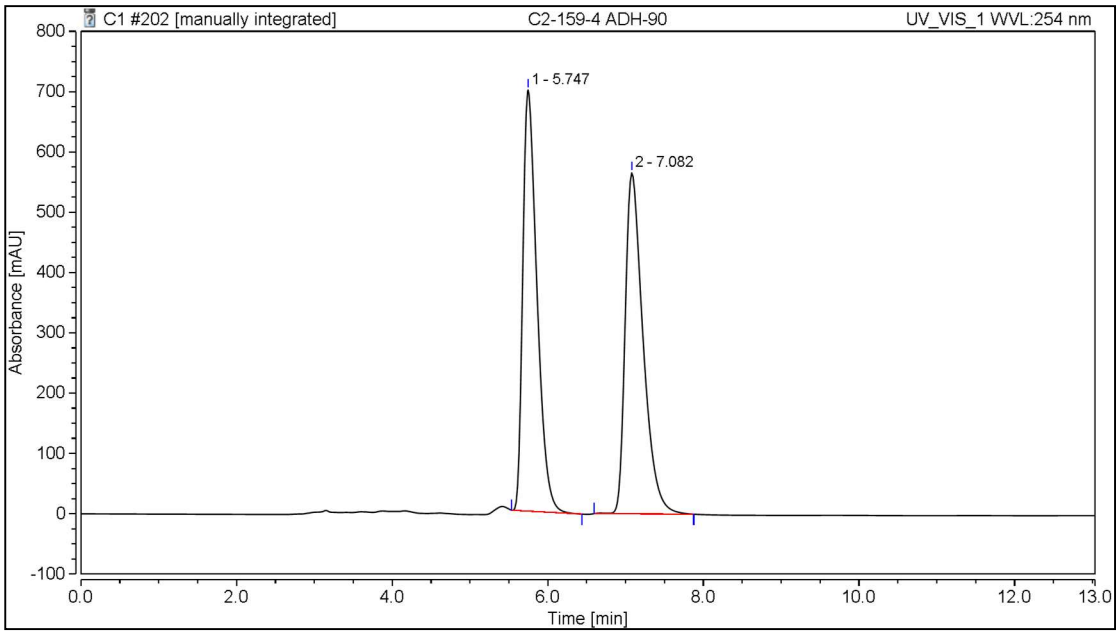
Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	11.073	219.497	282.062	36.37	53.09
2	23.227	384.046	249.199	63.63	46.91
Total:		**603.544**	**531.261**	**100.00**	**100.00**



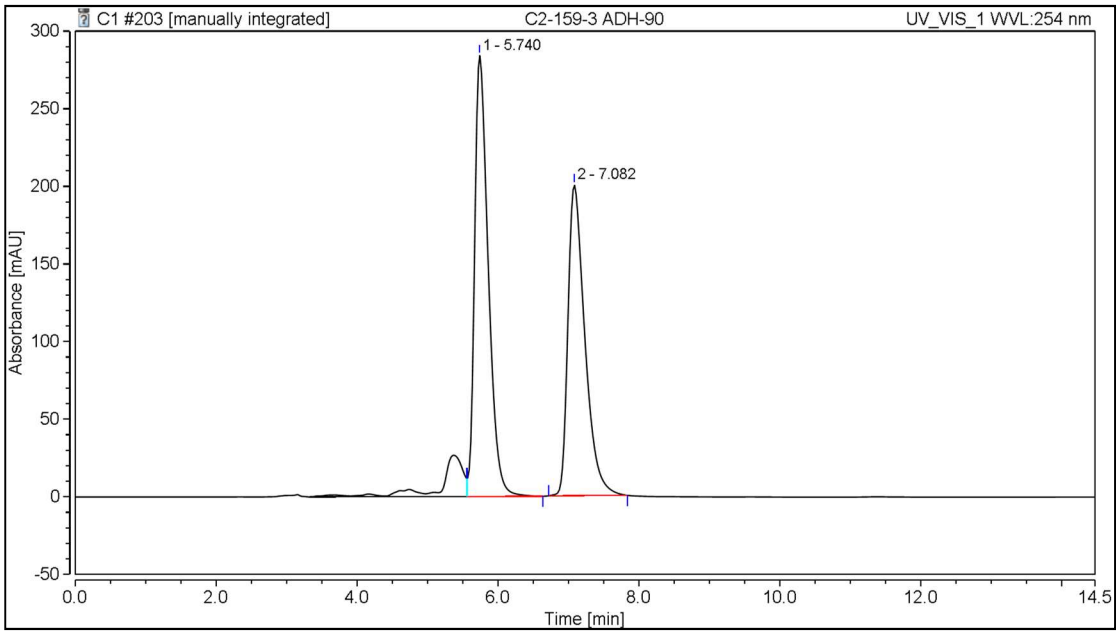
5

Colorless solid. 25% yield. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.65 – 7.59 (m, 2H), 7.47 – 7.29 (m, 3H), 6.64 (d, *J* = 1.4 Hz, 2H), 6.60 – 6.52 (m, 1H), 6.47 (s, 1H), 6.38 (d, *J* = 1.1 Hz, 2H), 6.33 (d, *J* = 7.8 Hz, 1H), 3.84 – 3.71 (m, 2H), 3.66 (dq, *J* = 12.5, 8.4 Hz, 1H), 3.20 – 3.04 (m, 5H), 3.03 (ddd, *J* = 13.1, 10.7, 4.8 Hz, 1H), 2.92 (ddd, *J* = 13.1, 10.3, 4.8 Hz, 1H), 1.64 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.24, 138.79, 138.32, 137.79, 137.60, 134.82, 134.22, 132.37, 131.73, 131.67, 130.84, 130.72, 128.84, 127.68, 127.35, 126.71, 68.35, 67.74, 59.67 (q, *J* = 37 Hz, CF_3), 34.84, 34.26, 34.04, 32.87, 19.42. ^{19}F NMR (471 MHz, $CDCl_3$) δ -73.51. HRMS (ESI, m/z) calcd for $C_{28}H_{25}F_3O_3$ $[M+H]^+$ 467.1829, found 467.1827. 7% ee; Daicel Chiralpak AD-H

250X4.6 mm 5u column; hexane/2-propanol = 90/10, detected at 254 nm, Flow rate = 1.0 mL/min, Retention times: 5.7 min (major), 7.1 min (minor).



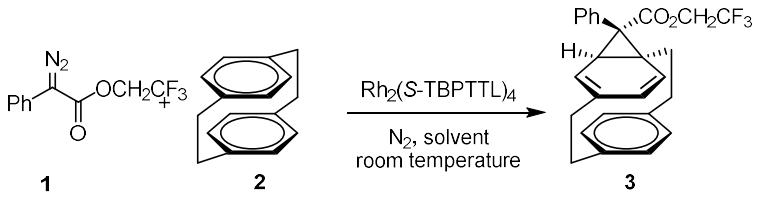
Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	5.747	147.631	698.589	49.47	55.25
2	7.082	150.812	565.794	50.53	44.75
Total:		**298.443**	**1264.382**	**100.00**	**100.00**



Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	5.740	63.636	284.034	53.33	58.65
2	7.082	55.679	200.248	46.67	41.35
Total:		**119.316**	**484.282**	**100.00**	**100.00**

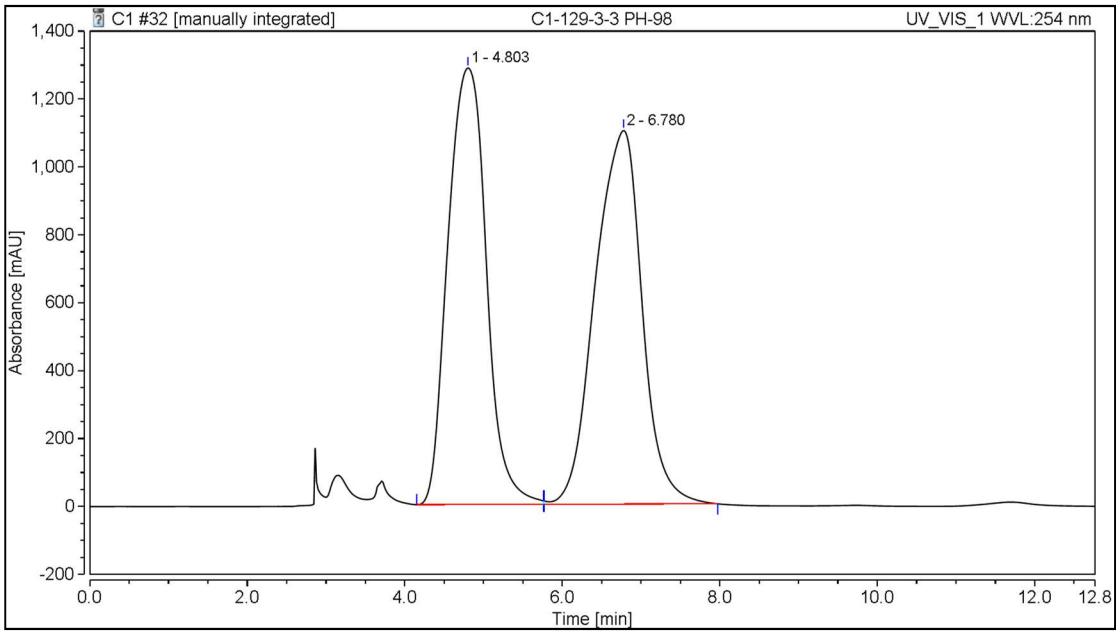
5. Synthetic Applications

(1) Gram Scale experiment

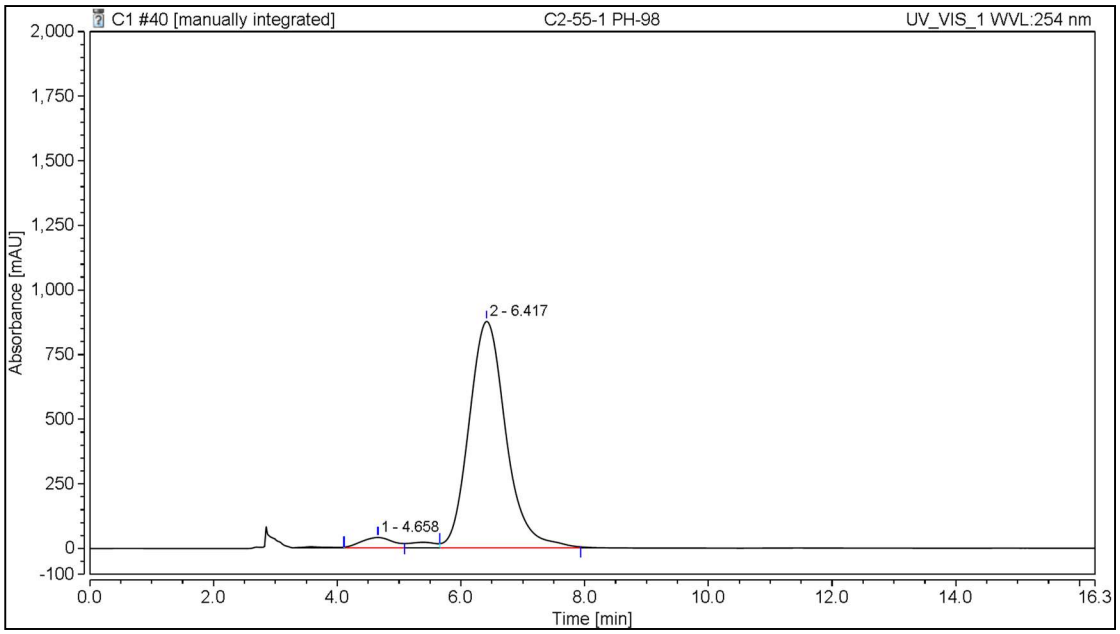


[2.2]Paracyclophane (1.0 equiv., 832 mg, 4.0 mmol) and Rh_2(*S*-TBPTTL)$_4$ (0.1 %, 10.0 mg, 0.004 mmol) were charged to a Schlenk tube equipped with a magnetic stirring bar. The tube was then charged with nitrogen 3 times. Under a nitrogen atmosphere, CH_2Cl_2 (20.0 mL) was added as solvent with a syringe. The suspension was vigorously stirred and a solution of **3d** (2.5 equiv., 10.0 mmol, 2.4 g, 1.0 M in DCM,) was dropwise added diazo via a pump over 20 hours at room temperature. After the full injection of diazo, the solution was allowed to continue stirring for 15 minutes. When no diazo remained determined by TLC, the solvent was evaporated *in vacuo*, and the residue was purified by silicon chromatography (EtOAc/hexane/DCM) to obtain the desired product. Enantiomeric excess (ee) values were determined by chiral HPLC analysis.

Colorless oil. 58% yield. 92% ee; Chiral HPLC analysis of the product: Phenomenex 00G-4457-E0 250X4.6 mm 5u column; hexane/2-propanol = 98/2, detected at 254 nm, Flow rate = 1.0 mL/min, Retention times: 4.7 min (minor), 6.4 min (major).

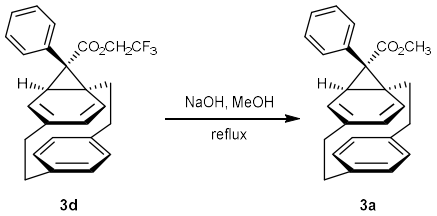


Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	4.803	726.435	1285.956	48.90	53.89
2	6.780	758.995	1100.273	51.10	46.11
Total:		**1485.430**	**2386.229**	**100.00**	**100.00**



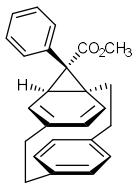
Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	4.658	24.029	39.797	3.82	4.34
2	6.417	604.837	876.597	96.18	95.66
Total:		**628.865**	**916.394**	**100.00**	**100.00**

(2) Synthesis of 3a



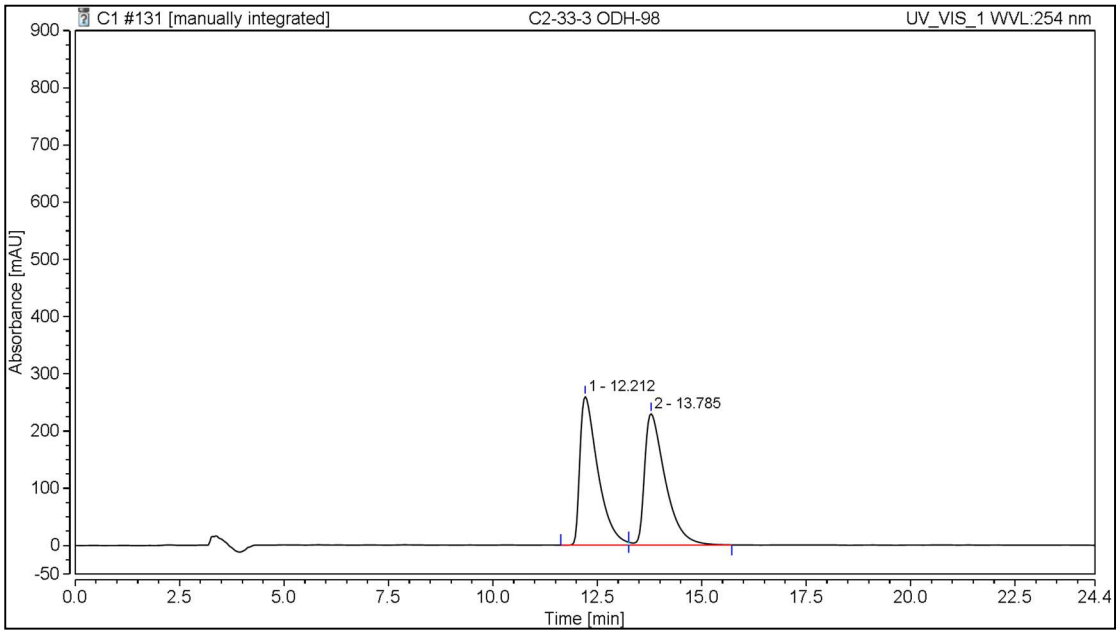
3d 3a

NaOH (10.0 equiv., 0.5g, 12.6 mmol) and **3d** (1.0 equiv., 537 mg, 1.26 mmol) were dissolved in MeOH (10.0 mL) under a nitrogen atmosphere. The solution was heated to reflux and stirred overnight. After no **3d** remained, the reaction was allowed to cold down to room temperature. The solution was dissolved in water and extracted with CH_2Cl_2 three times. The organic phase was collected and dried over anhydrous Na_2SO_4. Then, the solvent was evaporated *in vacuo*. The residue was purified by a silica gel column chromatography (EtOAc/hexane) to give the desired product **3a**. Enantiomeric excess (ee) values were determined by chiral HPLC analysis.



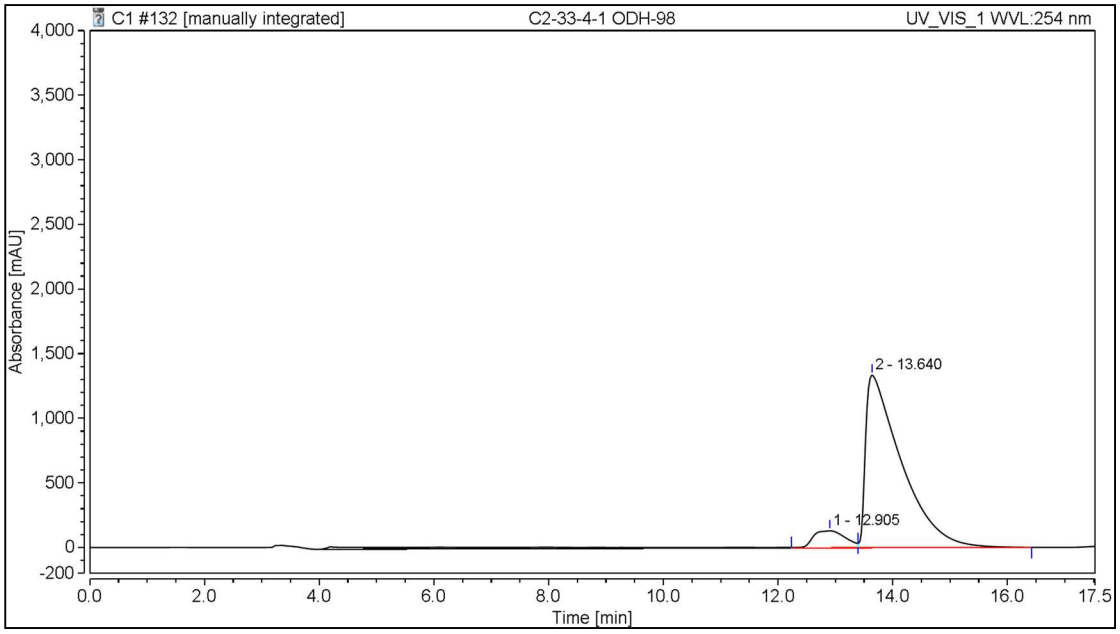
3a

Colorless solid. 85% yield. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.19 (dd, *J* = 7.9, 2.0 Hz, 1H), 7.07 – 7.00 (m, 3H), 6.98 (dd, *J* = 7.8, 1.9 Hz, 1H), 6.95 – 6.89 (m, 2H), 6.82 (dd, *J* = 7.9, 1.9 Hz, 1H), 6.78 (dd, *J* = 7.9, 1.8 Hz, 1H), 5.05 (d, *J* = 6.9 Hz, 1H), 4.96 (d, *J* = 9.9 Hz, 1H), 4.77 (dd, *J* = 9.9, 1.4 Hz, 1H), 3.61 (s, 3H), 3.03 (dddd, *J* = 14.3, 11.5, 8.6, 3.7 Hz, 2H), 2.95 (dd, *J* = 6.9, 1.6 Hz, 1H), 2.90 (ddd, *J* = 13.2, 9.7, 6.4 Hz, 1H), 2.76 (dt, *J* = 13.9, 8.4 Hz, 1H), 2.27 (ddd, *J* = 13.3, 10.3, 6.4 Hz, 1H), 2.21 – 2.12 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 174.18, 139.87, 139.28, 135.06, 134.15, 132.95, 132.50, 132.48, 132.44, 131.94, 130.93, 128.32, 127.77, 126.55, 126.30, 52.57, 40.78, 40.46, 35.23, 34.81, 34.44, 33.11, 32.44. HRMS (ESI, m/z) calcd for $C_{25}H_{24}O_2$ $[M+H]^+$ 357.1849, found 357.1864. $[\alpha]^{21}_D$ = 31.9° (c 0.44, $CHCl_3$); 83% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 98/2, detected at 254 nm, Flow rate = 1.0 mL/min, Retention times: 12.9 min (minor), 13.6 min (major).



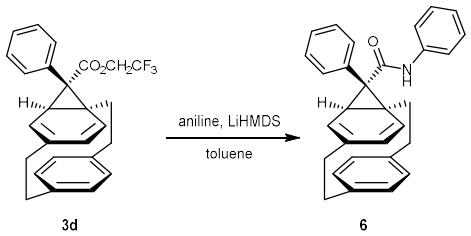
Integration Result					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%

1	12.212	129.418	259.713	49.52	53.08
2	13.785	131.922	229.578	50.48	46.92
Total:		**231.991**	**432.643**	**100.00**	**100.00**



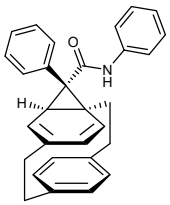
Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	12.905	85.491	131.959	8.14	8.99
2	13.640	964.944	1336.156	91.86	91.01
Total:		**1050.435**	**1468.115**	**100.00**	**100.00**

(3) Synthesis of 6



3d 6

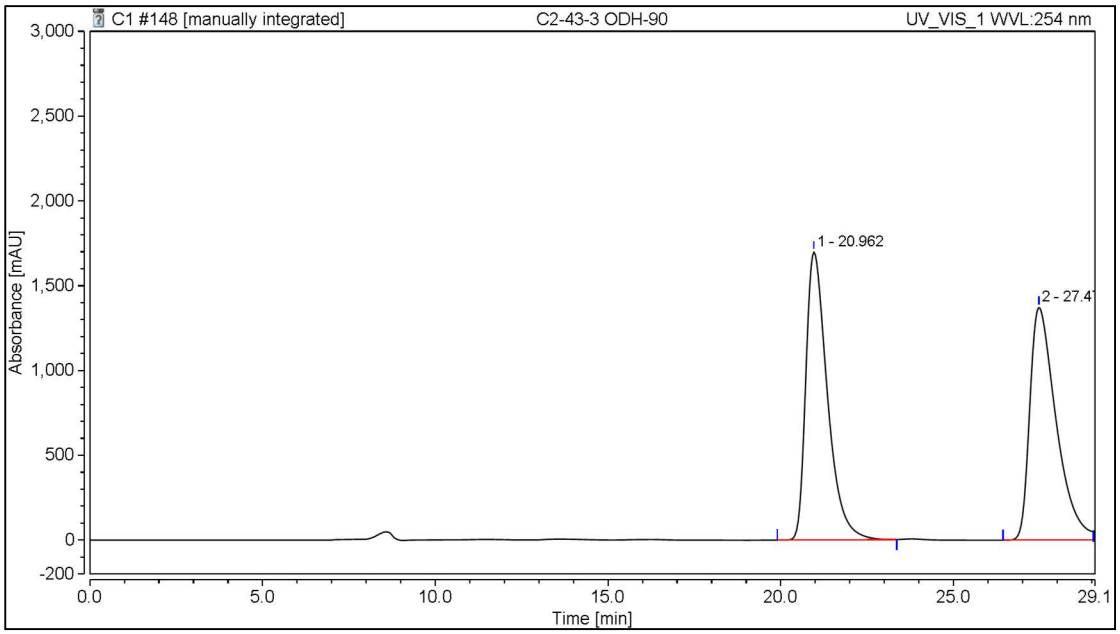
To a toluene solution (0.1 M) of **3a** (1.0 equiv., 40.2 mg, 0.095 mmol) and aniline (2.0 equiv., 17.7 mg, 0.19 mmol) was dropwise added LiHMDS (1.0 M in THF, 2.1 equiv., 0.2 mmol) over 5 minutes at room temperature under nitrogen atmosphere. The solution was stirred overnight. Then the solution was quenched with saturate ammonium chloride solution and extracted with ethyl acetate three times. The organic phase was collected and dried over anhydrous Na_2SO_4. Then, the solvent was evaporated *in vacuo*. The residue was purified by a silica gel column chromatography (EtOAc/hexane) to give the desired product **6**. Enantiomeric excess (ee) values were determined by chiral HPLC analysis.



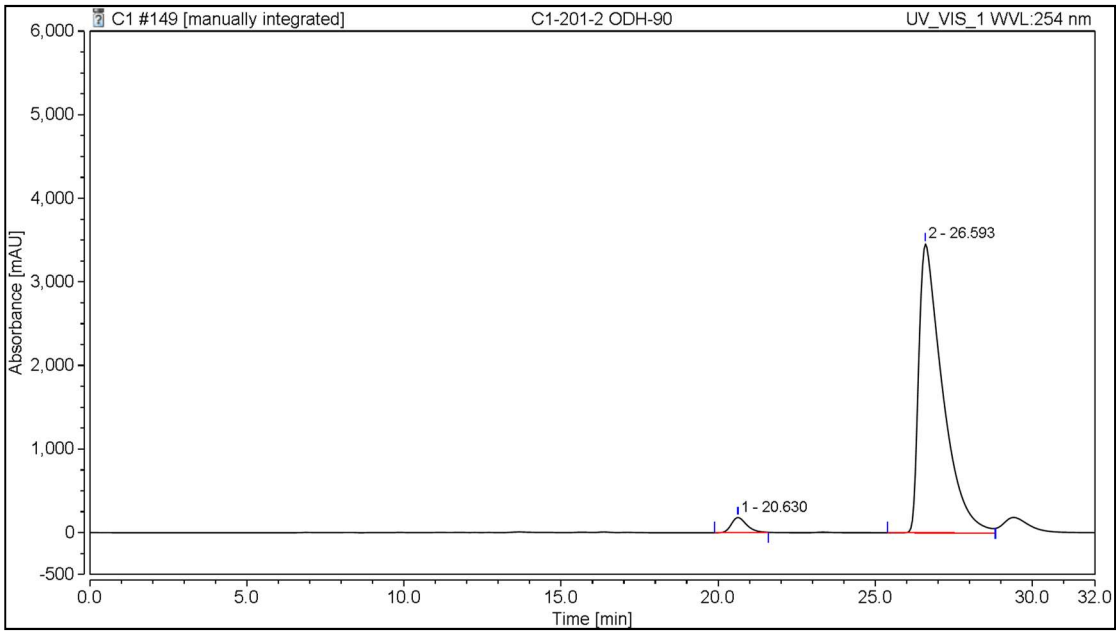
6

Colorless crystal. 66% yield. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.29 – 7.20 (m, 5H), 7.16 (dd, *J* = 4.7, 1.9 Hz, 3H), 7.06 – 7.02 (m, 2H), 6.99 (dd, *J* = 7.8, 1.9 Hz, 1H), 6.84 (dd, *J* = 7.8, 1.9 Hz, 1H), 6.80 (dd, *J* = 7.9, 1.8 Hz, 1H), 5.07 (d, *J* = 6.9 Hz, 1H), 5.03 (d, *J* = 9.8 Hz, 1H), 4.80 (dd, *J* = 9.9, 1.5 Hz, 1H), 3.15 (dd, *J* = 6.9, 1.7 Hz, 1H), 3.06 (tdd, *J* = 10.7, 9.0, 2.9 Hz, 2H), 2.94 – 2.86 (m, 1H), 2.82 (ddd, *J* = 13.9, 9.5, 7.6 Hz, 1H), 2.53 (ddd, *J* = 14.6, 7.6, 3.0 Hz, 1H), 2.27 (ddd, *J* = 13.3, 10.2, 6.7 Hz, 1H), 2.20 (ddd, *J* = 13.0, 9.7, 2.7 Hz, 1H), 2.07 (ddd, *J* = 14.6, 9.6, 7.8 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.18, 139.35, 138.08, 137.08, 134.38, 133.04, 132.68, 131.75, 131.56, 131.31, 131.20, 130.13, 127.88, 127.80, 126.97, 126.41, 126.34, 122.97, 118.57, 40.21, 39.27, 33.85, 33.57, 33.43, 31.61. HRMS (ESI, m/z) calcd for $C_{24}H_{22}O_2$ $[M+H]^+$ 418.2165, found 418.2170. $[\alpha]^{22}_D$ = 18.5° (c 0.49, $CHCl_3$); 93% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 90/10, detected

at 254 nm, Flow rate = 0.5 mL/min, Retention times: 20.6 min (minor), 26.6 min (major).

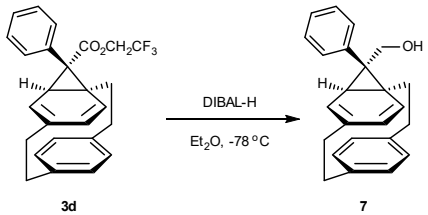


Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	20.962	1223.451	1698.078	50.29	55.32
2	27.477	1209.485	1371.711	49.71	44.68
Total:		**2432.937**	**3069.789**	**100.00**	**100.00**



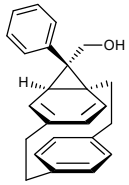
Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	20.630	105.354	181.887	3.36	5.00
2	26.593	3034.275	3457.671	96.64	95.00
Total:		**3139.629**	**3639.558**	**100.00**	**100.00**

(4) Synthesis of 7



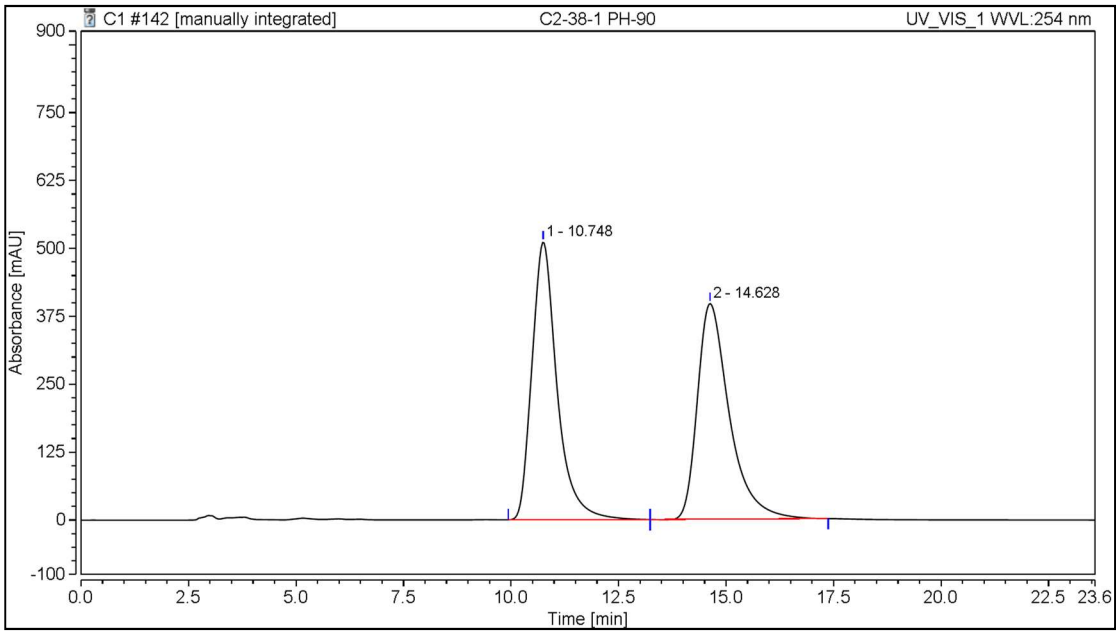
To an ethyl ether solution of **3d** (1.0 equiv., 45.0 mg, 0.11 mmol) was dropwise add DIBAL-H (1.0 M in hexane, 2.0 equiv., 0.2 mL) at -78 ºC under nitrogen atmosphere. The solution was stirred at -78 ºC overnight. Then the reaction was allowed to warm up to room temperature and quenched with saturate ammonium chloride

solution. The mixture was acidified to pH = 4 with 10% hydrochloric acid. The mixture was extracted with ethyl ether three times. The organic phase was collected, washed with saturate sodium biscarbonate solution 3 times, and dried over anhydrous Na_2SO_4. The solvent was evaporated *in vacuo*. The residue was purified by a silica gel column chromatography (EtOAc/hexane) to give the desired product **7**. Enantiomeric excess (ee) values were determined by chiral HPLC analysis.

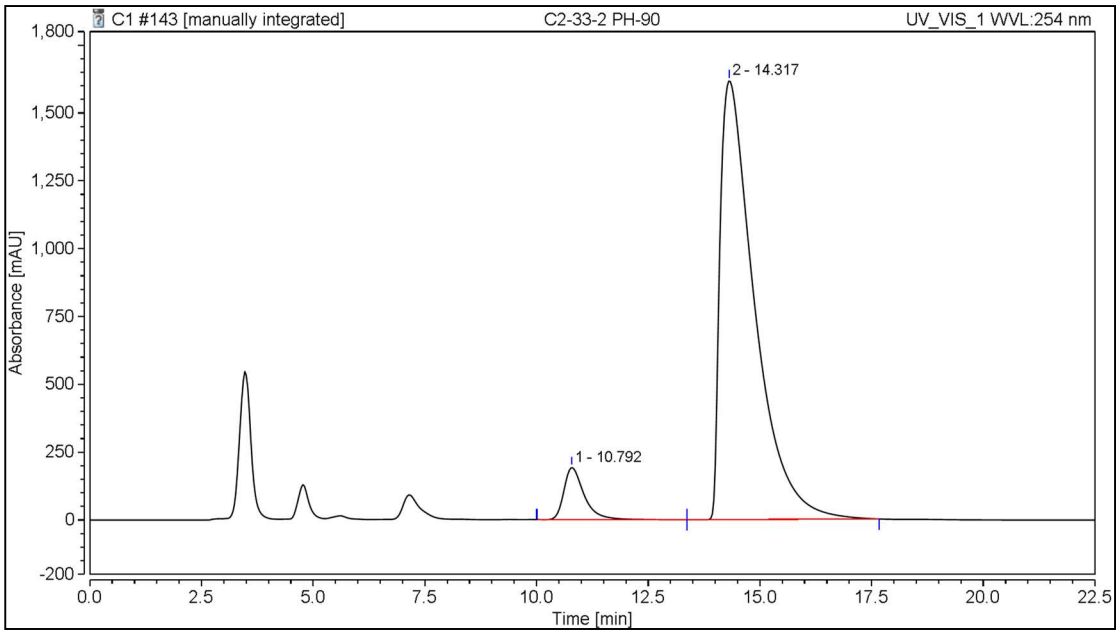


7

Colorless solid. 66% yield. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.13 – 7.04 (m, 4H), 7.01 (dd, *J* = 7.8, 1.8 Hz, 1H), 6.95 (dd, *J* = 7.4, 2.2 Hz, 2H), 6.82 (dd, *J* = 7.8, 1.9 Hz, 1H), 6.77 (dd, *J* = 8.0, 1.8 Hz, 1H), 4.92 (m, 2H), 4.67 (dd, *J* = 10.0, 1.5 Hz, 1H), 3.82 (dd, *J* = 11.4, 4.7 Hz, 1H), 3.68 (dd, *J* = 11.7, 5.3 Hz, 1H), 3.05 (dtd, *J* = 12.8, 10.1, 8.9, 3.3 Hz, 2H), 2.90 (ddd, *J* = 13.1, 9.6, 6.5 Hz, 1H), 2.63 (dt, *J* = 14.0, 8.3 Hz, 1H), 2.36 – 2.10 (m, 4H), 1.88 (dd, *J* = 6.7, 1.5 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 139.56, 139.42, 138.34, 134.14, 132.96, 132.65, 132.44, 132.13, 130.88, 130.58, 128.11, 127.34, 126.12, 125.56, 70.03, 38.94, 35.75, 35.17, 34.96, 34.70, 32.64, 31.97. HRMS (ESI, m/z) calcd for $C_{24}H_{22}O$ $[M+H]^+$ 329.1900, found 329.1899. $[\alpha]^{22}_D$ = -11.7° (c 0.93, $CHCl_3$); 87% ee; Chiral HPLC analysis of the product: Phenomenex 00G-4457-E0 250X4.6 mm 5u column; hexane/2-propanol = 90/10, detected at 254 nm, Flow rate = 1.0 mL/min, Retention times: 10.8 min (minor), 14.3 min (major).

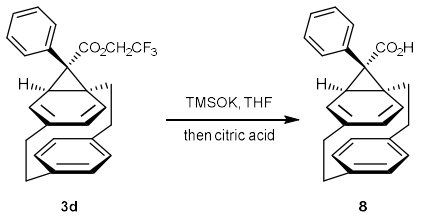


Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	10.748	345.714	511.441	50.31	56.30
2	14.628	341.505	397.023	49.69	43.70
Total:		**687.219**	**908.464**	**100.00**	**100.00**



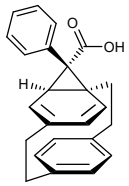
Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	10.792	100.658	191.785	6.51	10.60
2	14.317	1446.437	1617.798	93.49	43.70
Total:		**687.219**	**908.464**	**100.00**	**100.00**

(5) Synthesis of 8



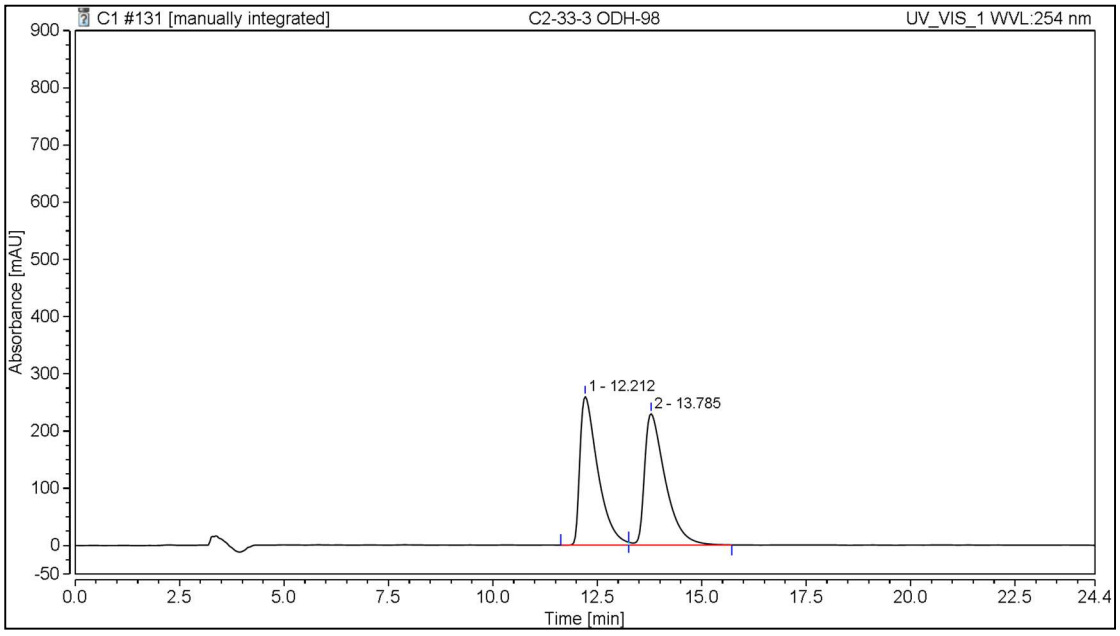
3d 8

To a THF (9.0 mL) solution of **3d** (1.0 equiv., 386.0 mg, 0.91 mmol) was add TMSOK (10.0 equiv., 1.17g, 9.1 mmol) at room temperature under nitrogen atmosphere. The solution was stirred overnight. Then the reaction was quenched with 0.5M citric acid solution. The mixture was extracted with ethyl acetate three times. The organic phase was collected and washed with saturate sodium chloride solution 3 times. Then the organic phase was dried over anhydrous Na_2SO_4. The solvent was evaporated *in vacuo*. The residue was purified by a silica gel column chromatography (EtOAc/hexane) to give the desired product **8**. To evaluate the Enantiomeric excess (ee) value, **8** was esterificated to correspond methyl ester **3a** with dicyclohexylcarbodiimide (DCC) and methanol. Enantiomeric excess (ee) values were determined by chiral HPLC analysis.

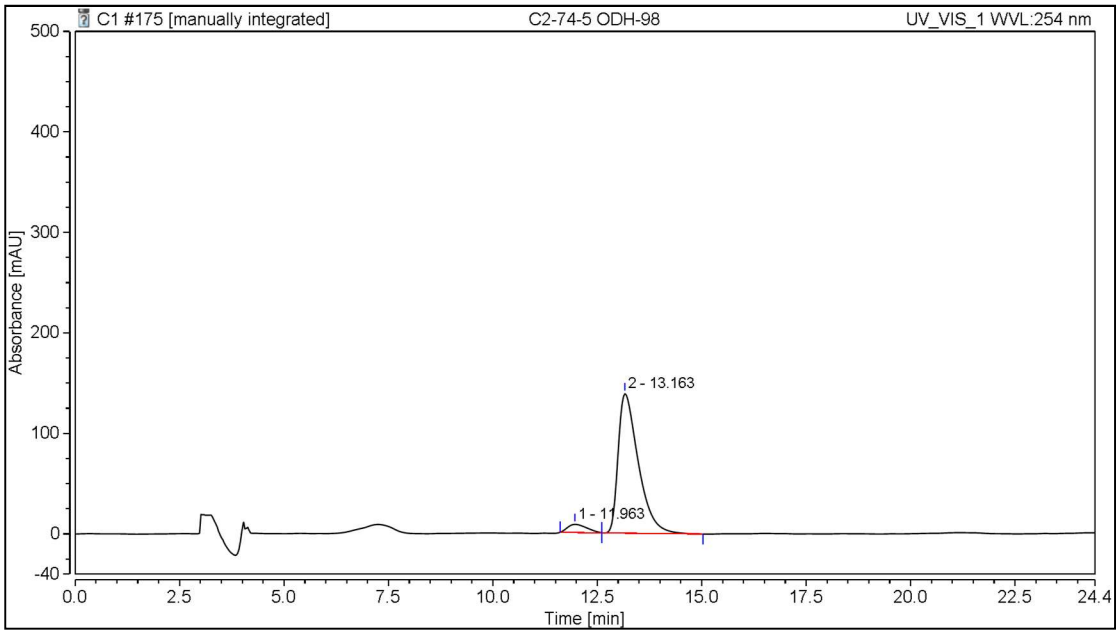


8

Colorless solid. 66% yield. ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.13 (dd, *J* = 8.0, 2.0 Hz, 1H), 6.99 – 6.95 (m, 1H), 6.95 – 6.90 (m, 2H), 6.82 (dd, *J* = 7.8, 2.0 Hz, 1H), 6.77 (dd, *J* = 7.9, 1.8 Hz, 1H), 5.06 (d, *J* = 6.8 Hz, 1H), 4.98 (d, *J* = 9.9 Hz, 1H), 4.81 (dd, *J* = 9.9, 1.4 Hz, 1H), 3.03 (tdd, *J* = 14.2, 6.6, 3.1 Hz, 2H), 2.94 (dd, *J* = 6.9, 1.6 Hz, 1H), 2.91 – 2.85 (m, 1H), 2.70 (ddd, *J* = 13.8, 9.2, 7.5 Hz, 1H), 2.38 (ddd, *J* = 14.7, 7.6, 3.3 Hz, 1H), 2.30 – 2.22 (m, 1H), 2.16 (tdd, *J* = 17.1, 9.5, 5.3 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 179.47, 138.84, 138.20, 133.66, 131.86, 131.55, 131.48, 131.36, 131.05, 130.68, 129.90, 127.63, 127.52, 127.33, 126.95, 41.38, 40.56, 36.18, 34.00, 33.72, 33.34, 31.42. HRMS (ESI, m/z) calcd for $C_{24}H_{22}O_2$ $[M+H]^+$ 343.1693, found 343.1697. $[\alpha]^{21}_D$ = 20.7° (c 0.53, $CHCl_3$); 87% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OD-H 250X4.6 mm 5u column; hexane/2-propanol = 98/2, detected at 254 nm, Flow rate = 1.0 mL/min, Retention times: 10.8 min (minor), 14.3 min (major).

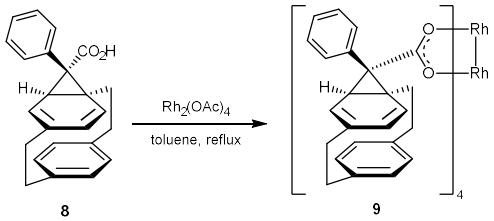


Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	12.212	129.418	259.713	49.52	53.08
2	13.785	131.922	229.578	50.48	46.92
Total:		**231.991**	**432.643**	**100.00**	**100.00**



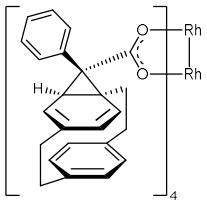
Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	11.963	4.380	8.157	5.33	5.55
2	13.163	77.800	138.885	94.67	94.45
Total:		**82.180**	**147.042**	**100.00**	**100.00**

(6) Synthesis of 9



8 9

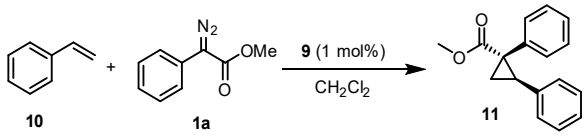
$Rh_2(OAc)_4$ (1.0 equiv., 110.5 mg, 0.25 mmol) and **8** (8.0 equiv., 0.68 g, 2.0 mmol) were dissolved in toluene (10 mL) under nitrogen atmosphere. The solution was heated to reflux for 3 hours. then the reaction was allowed to cold down to room temperature. The solution was washed with saturate sodium bicarbonate solution and saturate sodium chloride solution each 3 times. The organic phase was dried over anhydrous Na_2SO_4. Solvent was removed *in vacuo* and residue was purified by a silica gel column chromatography (EtOAc/hexane). Then, the product **9** was obtained by recrystallization from toluene and acetonitrile.



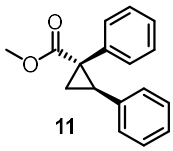
9

Green Crystal. 39% yield.^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.18 (dd, *J* = 7.9, 1.9 Hz, 1H), 7.11 – 7.06 (m, 1H), 7.04 (t, *J* = 7.3 Hz, 2H), 7.01 (dd, *J* = 7.8, 1.8 Hz, 1H), 6.87 (dd, *J* = 7.9, 1.9 Hz, 1H), 6.81 (dd, *J* = 7.9, 1.8 Hz, 1H), 6.76 – 6.69 (m, 2H), 4.95 (d, *J* = 6.9 Hz, 1H), 4.89 (d, *J* = 9.8 Hz, 1H), 4.76 (dd, *J* = 9.9, 1.3 Hz, 1H), 3.07 (tdd, *J* = 16.5, 8.4, 3.1 Hz, 2H), 2.92 – 2.81 (m, 2H), 2.68 (dt, *J* = 13.7, 8.6 Hz, 1H), 2.22 (m, 2H), 2.01 – 1.89 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 191.12, 139.98, 139.14, 135.81, 133.74, 132.93, 132.79, 132.74, 132.39, 131.67, 131.01, 128.79, 127.09, 126.48, 126.07, 40.55, 39.55, 35.84, 35.35, 34.81, 34.45, 32.72.

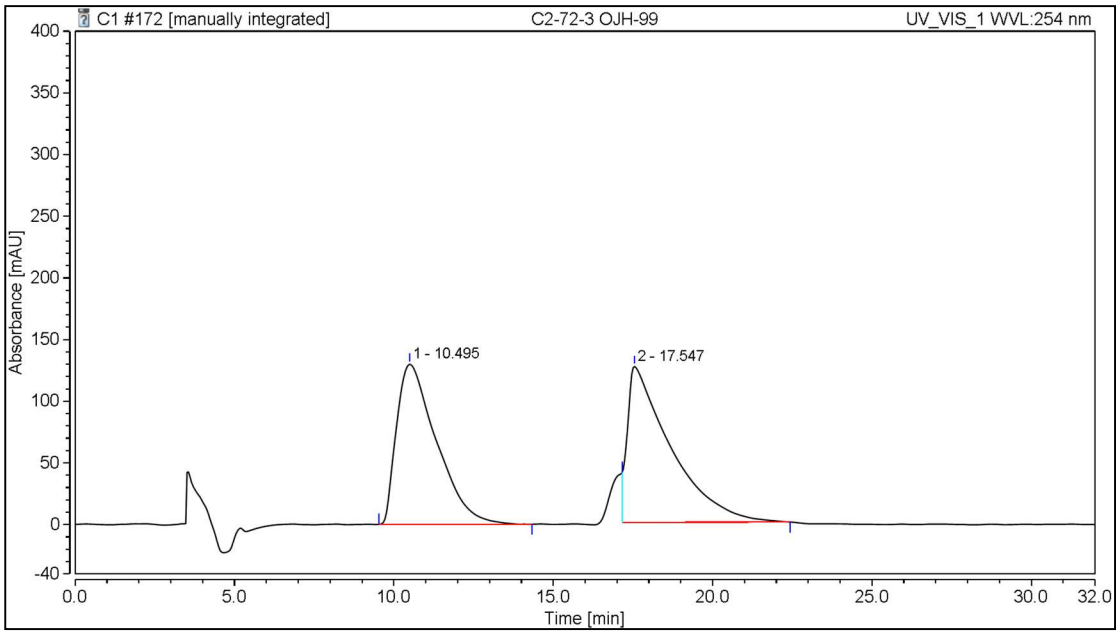
(7) Rhodium(II) complex 9 catalyzed cyclopropanation of styrene



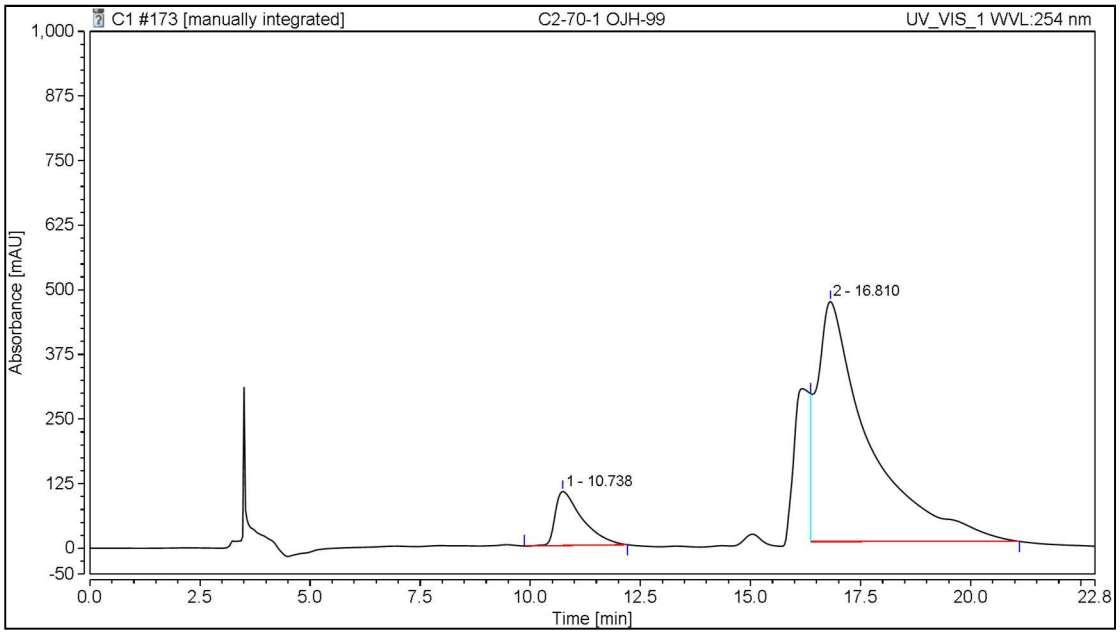
To a solution of styrene **10** (5.0 equiv., 52.1 mg, 0.5 mmol) and **9** (1 mol%, 1.5 mg, 0.001 mmol) in DCM (1.0 mL) was dropwise added **1a** (1.0 equiv., 17.6 mg, 0.1 mmol, 0.1M in CH_2Cl_2) over 2 hours under nitrogen atmosphere at room temperature. Then the solution was evaporated and residue was purified by a silica gel column chromatography (EtOAc/hexane) to obtain the desired product **11**.



Colorless liquid. 71% yield. The NMR spectra is consistent with the reported data.[8] 79% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OJ-H 250X4.6 mm 5u column; hexane/2-propanol = 99/1, detected at 254 nm, Flow rate = 1.0 mL/min, Retention times: 10.7 min (minor), 16.8 min (major).

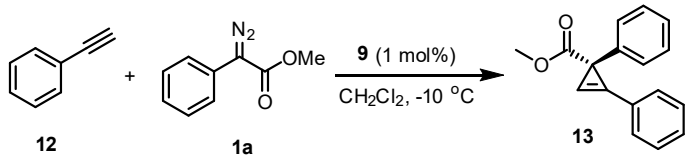


Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	10.495	188.150	129.737	48.60	50.65
2	17.547	199.020	126.414	51.40	49.35
Total:		**387.171**	**256.151**	**100.00**	**100.00**

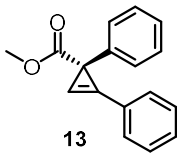


Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	10.738	74.219	104.499	10.31	18.37
2	16.810	645.796	464.497	89.69	81.63
Total:		**720.016**	**568.997**	**100.00**	**100.00**

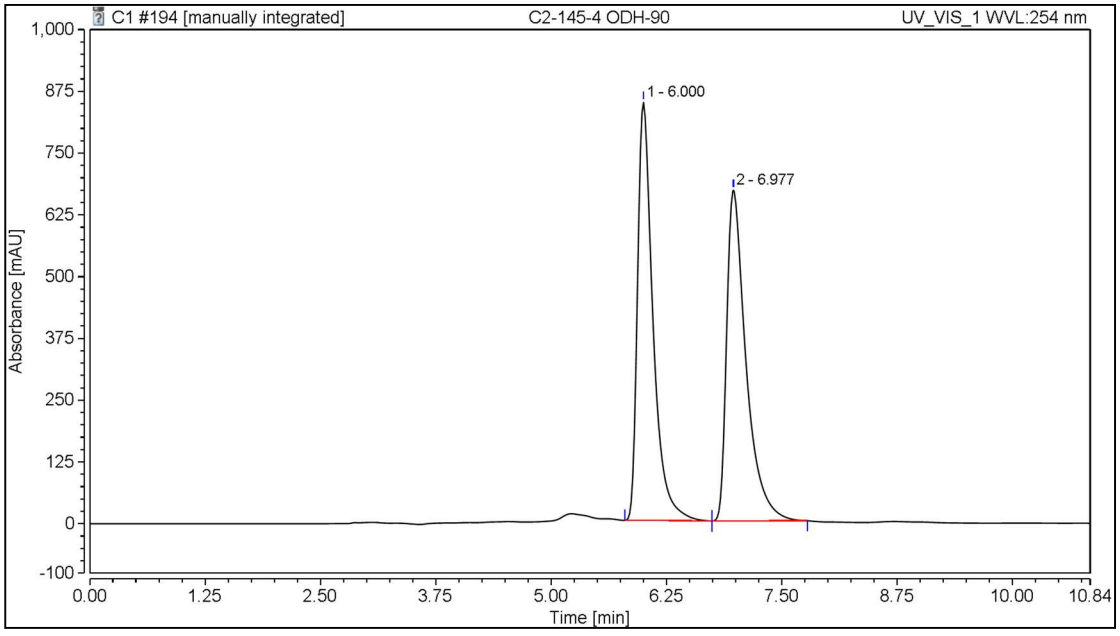
(8) Rhodium(II) complex 9 catalyzed cyclopropenation of Phenylacetylene



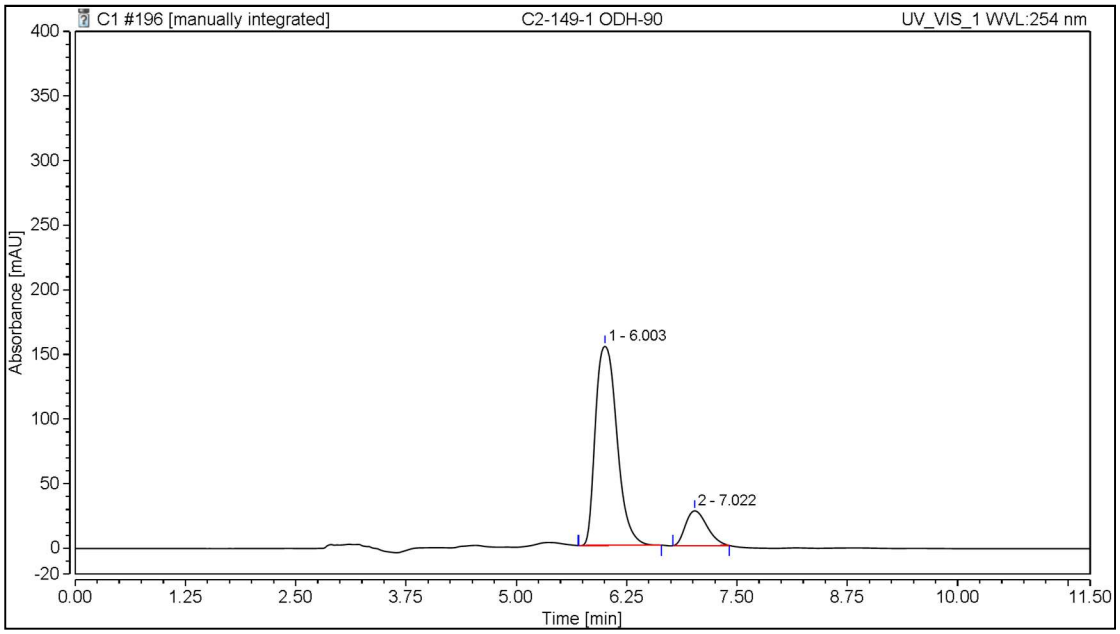
To a solution of phenylacetylene **12** (5.0 equiv., 51.1 mg, 0.5 mmol) and **9** (1 mol%, 1.5 mg, 0.001 mmol) in DCM (1.0 mL) was dropwise added **1a** (1.0 equiv., 17.6 mg, 0.1 mmol, 0.1M in CH_2Cl_2) over 2 hours under nitrogen atmosphere at -10 °C. Then the solution was evaporated and residue was purified by a silica gel column chromatography (EtOAc/hexane) to obtain the desired product **13**.



Colorless oil. 57% yield. The NMR spectra is consistent with reported data.[9] 70% ee; Chiral HPLC analysis of the product: Daicel Chiralpak OJ-H 250X4.6 mm 5u column; hexane/2-propanol = 99/1, detected at 254 nm, Flow rate = 1.0 mL/min, Retention times: 10.7 min (minor), 16.8 min (major).



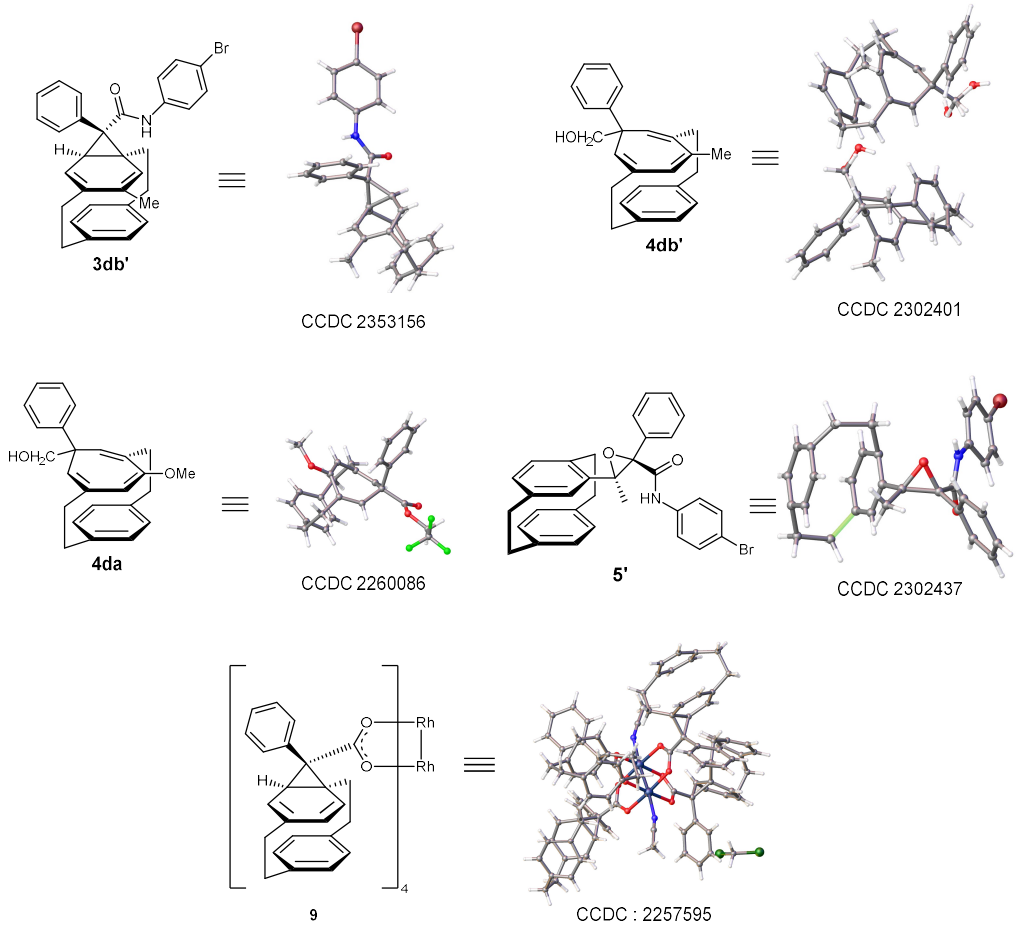
Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	6.000	164.215	846.309	50.27	55.84
2	6.977	162.454	669.224	49.73	44.16
Total:		**82.180**	**147.042**	**100.00**	**100.00**



Integration Results					
No.	Retention Time	Area	Height	Relative Area	Relative Height
	min	mAU*min	mAU	%	%
1	6.003	43.678	154.125	85.09	85.12
2	7.022	7.652	26.944	14.91	14.88
Total:		**51.330**	**181.069**	**100.00**	**100.00**

6. X-Ray Crystallography

CCDC 2257595, CCDC 2260086, CCDC 2302437, CCDC 2353156, and CCDC 2302401 contain supplementary crystallographic data for this paper.



These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/ci

7. DFT Calculations

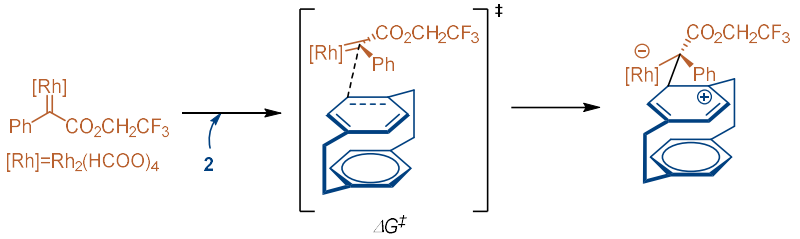
(1) Computational Method

DFT calculations were performed with Gaussian 09[10] software package. For the free energy surface of $Rh_2(HCOO)_4$, geometry optimizations of all the stationary points were carried out using the B3LYP[11-12] functional and def2-SVP[15,16] with Grimme's D3(BJ) dispersion correction[15,16]. Frequency calculations at the same level were performed to validate each structure as either a minimum or a transition state. Pruned integration grids with 99 radial shells and 590 angular points per shell were used. On the basis of the optimized structures, single-point energy refinements at the SMD(DCM)/ωB97M-V/def2-TZVPP level[17,18] were performed with ORCA 4.2.1 program package[19,20] and the default RIJCOSX approximation[21] along with the def2/J auxiliary basis set[22]. ωB97M-V has been shown as a good functional for both main-group chemistry and organometallic reactions[23-26] (also see benchmark study below). For all the transition states with Rh_2(*S*-TBPTTL)$_4$, the geometry optimizations were carried out at B3LYP-D3(BJ)/def2-SVP under SMD(DCM) model and the energies computed at this level are in good agreement with the experiments (also see benchmark study below). 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. Noncovalent interactions[27] were analyzed by Multiwfn[28] using fchk file which was generated from Gaussian 09 at SMD(DCM)/B3LYP-D3(BJ)/def2-SVP. 3D structure was prepared with CYLview[29].

(2) Benchmark Study

A benchmark study was performed to evaluate the accuracy in computing kinetics of the key nucleophilic steps in this reaction. The state-of-the-art method DLPNO-CCSD(T)[30] was used as reference (DLPNO-CCSD(T) were performed with ORCA 4.2.1[19,20] using the def2-TZVP/C auxiliary basis set and tight thresholds), different functionals including B3LYP-D3(BJ)[11,12,15,16], BMK[32], BMK-D3(BJ), M06[33], M06L[34], M06-D3, M06L-D3, PBE0-D3(BJ)[35], ωB97X-D[36], ωB97M-V[18], PWPB95-D3(BJ)[37], ωB97X-V[38], TPSSh[39], MN15L[40], MN15[41], SCAN-D3(BJ)[42] were tested. All the single point energies were computed with def2-TZVP basis set in gas phase based on the optimized structures at B3LYP-D3(BJ)/def2-SVP. The results are shown in **Table S1**. Using DLPNO-CCSD(T) as reference, different functionals give very different activation free energies of this reaction, suggesting that it's difficult to accurately computed both the organic part and transition-metal complex. Nevertheless, the ωB97M-V functional, which has been shown as a good functional for both main-group chemistry and organometallic reactions[19], performs best among these functionals. It's interesting to find that B3LYP-D3(BJ) with a small def2-SVP basis set gives a better result for this reaction, which is a coincidence, probably due to the error offsetting effect of the density functional and basis set. Therefore, we choose the ωB97M-V functional to study the mechanism of this reaction. While for the selectivity study in the real system, the results at B3LYP-D3(BJ)/def2-SVP under SMD(DCM) model are given in the main text, which is consistent well with the experiments. The results of ωB97M-V for the key transition states are also given in **Table S2**, which is slightly overestimated the *ee* value.

Table S3. Benchmark Study of the key nucleophilic step



Method [a]	DLPNO-CCSD(T)	B3LYP-D3(BJ)	B3LYP-D3(BJ) [b]	BMK-D3(BJ)	BMK	M06-D3	M06L-D3	PBE0-D3(BJ)	ωB97X-D	M06L	M06	ωB97M-V	PWPB95-D3	ωB97X-V	TPSSh	MN15L	MN15	SCAN-D3(BJ)
$\Delta G^{\ddagger}$	**3.3**	10.1	**2.8**	-3.3	15.7	7.3	13.9	8.7	9.1	17.4	13.6	**4.9**	5.7	7.5	28.7	12.8	9.2	11.3

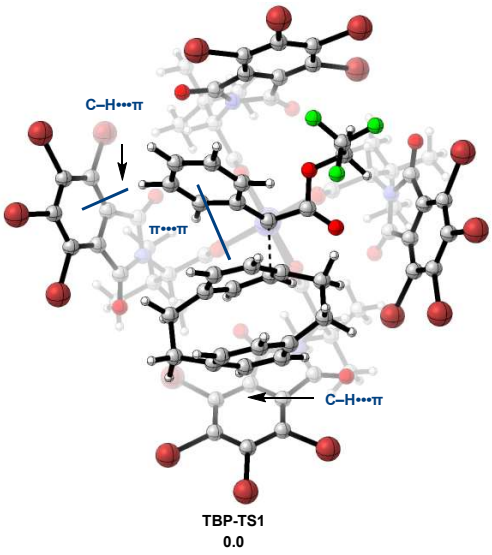
[a]computed with TZVP basis set in gas phase based on the optimized structure at B3LYP-D3/def2SVP. [b]computed with def2-SVP basis set.

Table S4. The relative Gibbs free energy of the selective transition states computed at different level.

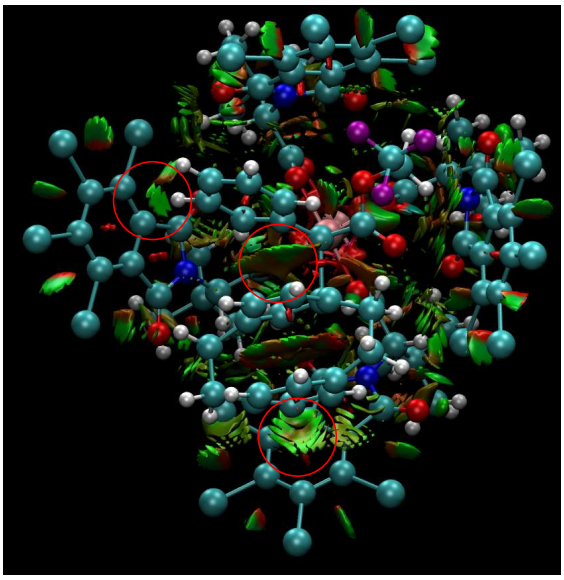
Transition state	$\Delta\Delta G^{\ddagger}$ Relative Gibbs free energy at SMD(DCM)/B3LYP-D3(BJ)/def2-SVP	$\Delta\Delta G^{\ddagger}$ Relative Gibbs free energy at SMD(DCM)/ωB97M-V/def2-TZVPP//SMD(DCM)/B3LYP-D3(BJ)/def2-SVP
TBP-TS1	**0.0**	**0.0**
TBP-TS2	2.8	3.5
TBP-TS3	2.6	4.5
TBP-TS4	3.8	4.8
TBP-TS1-OMe	**0.0**	**0.0**
TBP-TS4-OMe	-2.1	-1.1

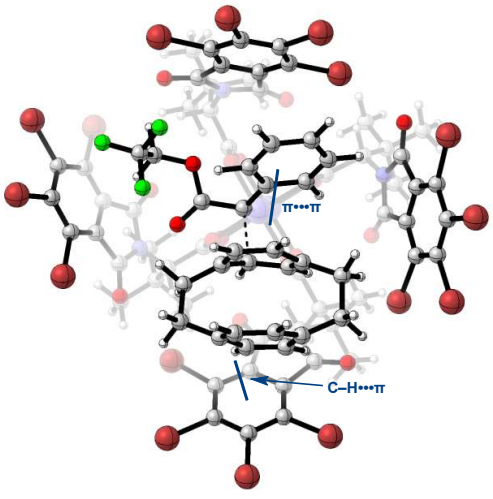
(3) NCI Analysis for the Enantio- and Regioselective Transition States of Cyclopropanation of PCP Using Rh_2(*S*-TBPTTL)$_4$

NCI analysis was carried out for the key selectivity-determined transition states (Figure S1), finding that **TBP-TS1** satisfies well with the cavity formed by the ligands and has additional C-H•••π interactions among other transition states. That's why the reaction could afford good regio- and enantioselectivities

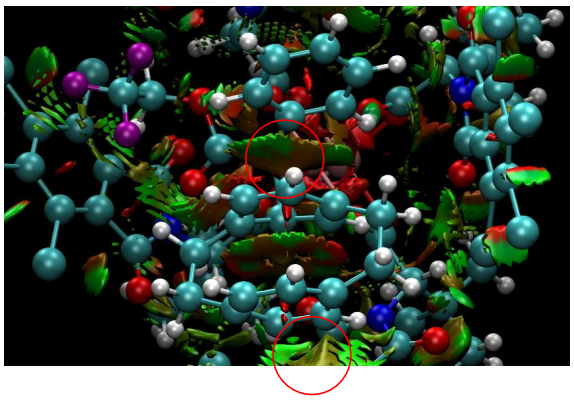


TBP-TS1
0.0





TBP-TS2



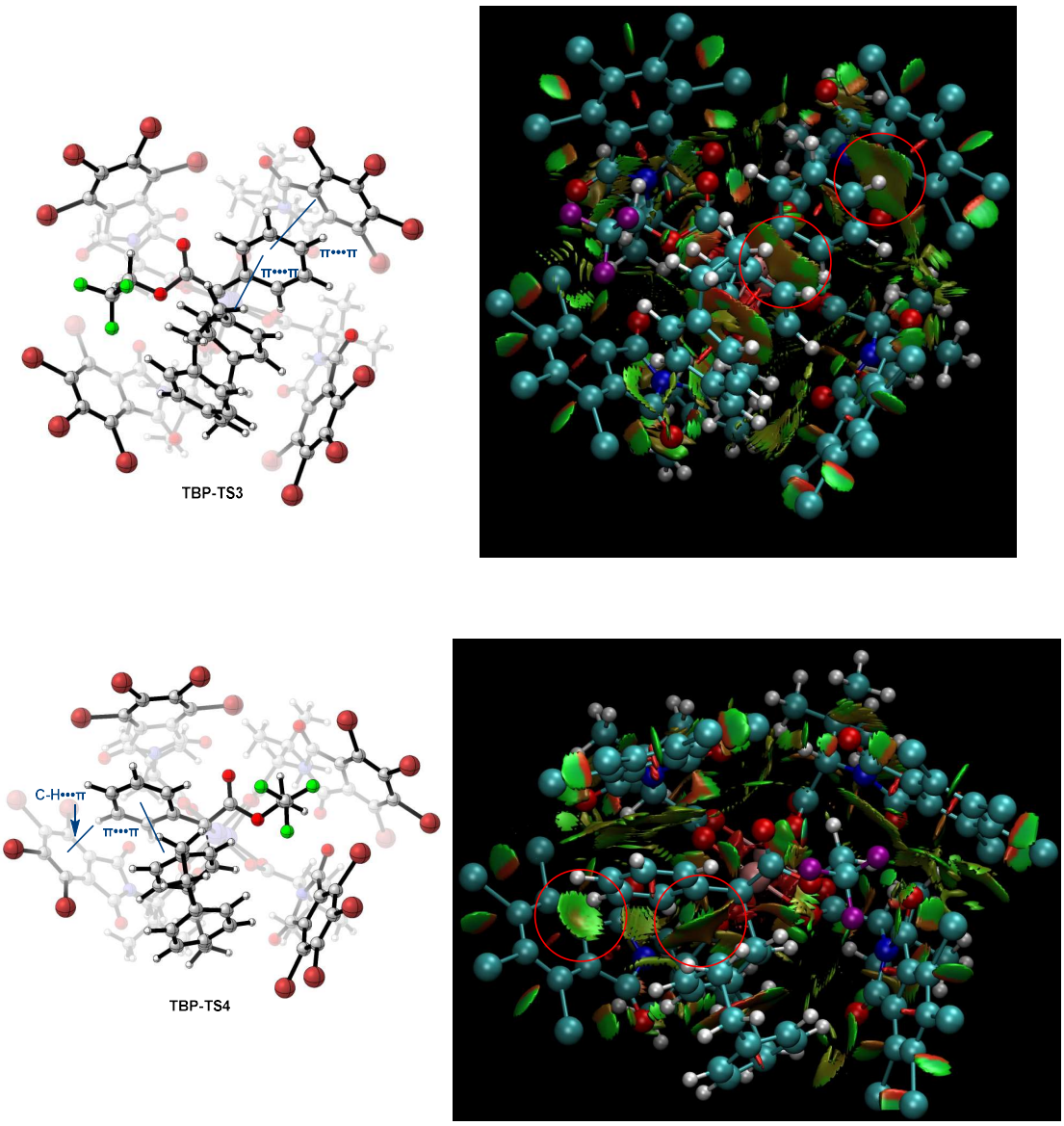


Figure S2. NCI analysis for the enantio- and regioselective transition states of cyclopropanation of PCP using Rh_2(*S*-TBPTTL)$_4$.

(4) The Regioselective Transition States of Cyclopropanation of Methoxy-Substituted PCP 2' Using Rh_2(*S*-TBPTTL)$_4$

The regioselective transition states of methoxy-substituted PCP **2'** using Rh_2(*S*-TBPTTL)$_4$ were shown in Figure S2, computed at SMD(DCM)/B3LYP-D3(BJ)/def2-SVP. Among these transition states, **TBP-TS4-OMe** is the most favored one than others by more than 1.0 kcal/mol. Thus, for methoxy-substituted PCP **2a**, **4da** is the major product.

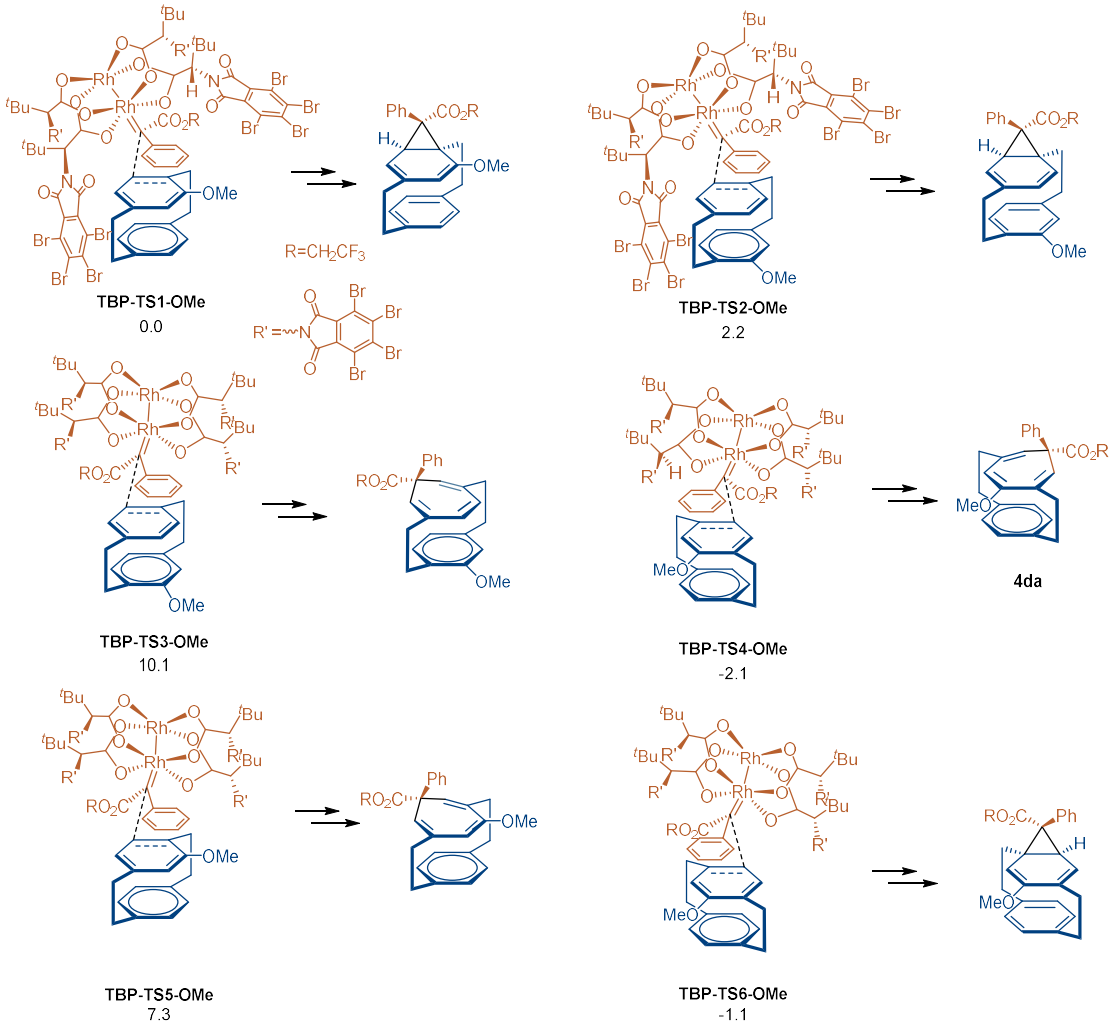


Figure S3. The regioselective transition states of cyclopropanation of methoxy-substituted PCP **2'** using Rh_2(*S*-TBPTTL)$_4$.

(5) The Selective Transition States of Cyclopropanation of PCP 2' Using Methyl α-diazophenylacetate 1a

The enantio- and regioselective transition states of PCP **2** using methyl α-diazophenylacetate **1a** under Rh_2(*S*-TBPTTL)$_4$ catalyst were shown in Figure S3, computed at SMD(DCM)/B3LYP-D3(BJ)/def2-SVP. DFT calculations predicted that using Rh_2(*S*-TBPTTL)$_4$ as catalyst, the methyl ester **1a** gives an energy difference of 2.4 kcal/mol ($\Delta\Delta G^{\ddagger}$) between the enantioselective transition states (**TBP-TS1-Me** and **TBP-TS2-Me**), indicating a smaller *ee* value than the trifluoroethyl ester **1d (**$\Delta\Delta G^{\ddagger}$ = 2.8 kcal/mol). While **TBP-TS1-Me** is favored over **TBP-TS3-Me** and **TBP-TS4-Me** by more than 5 kcal/mol, predicting that only **4c'** could be obtained under Rh_2(*S*-TBPTTL)$_4$. This is consistent with experiments, which gave the sole product **3d'** with a lower *ee* (47%).

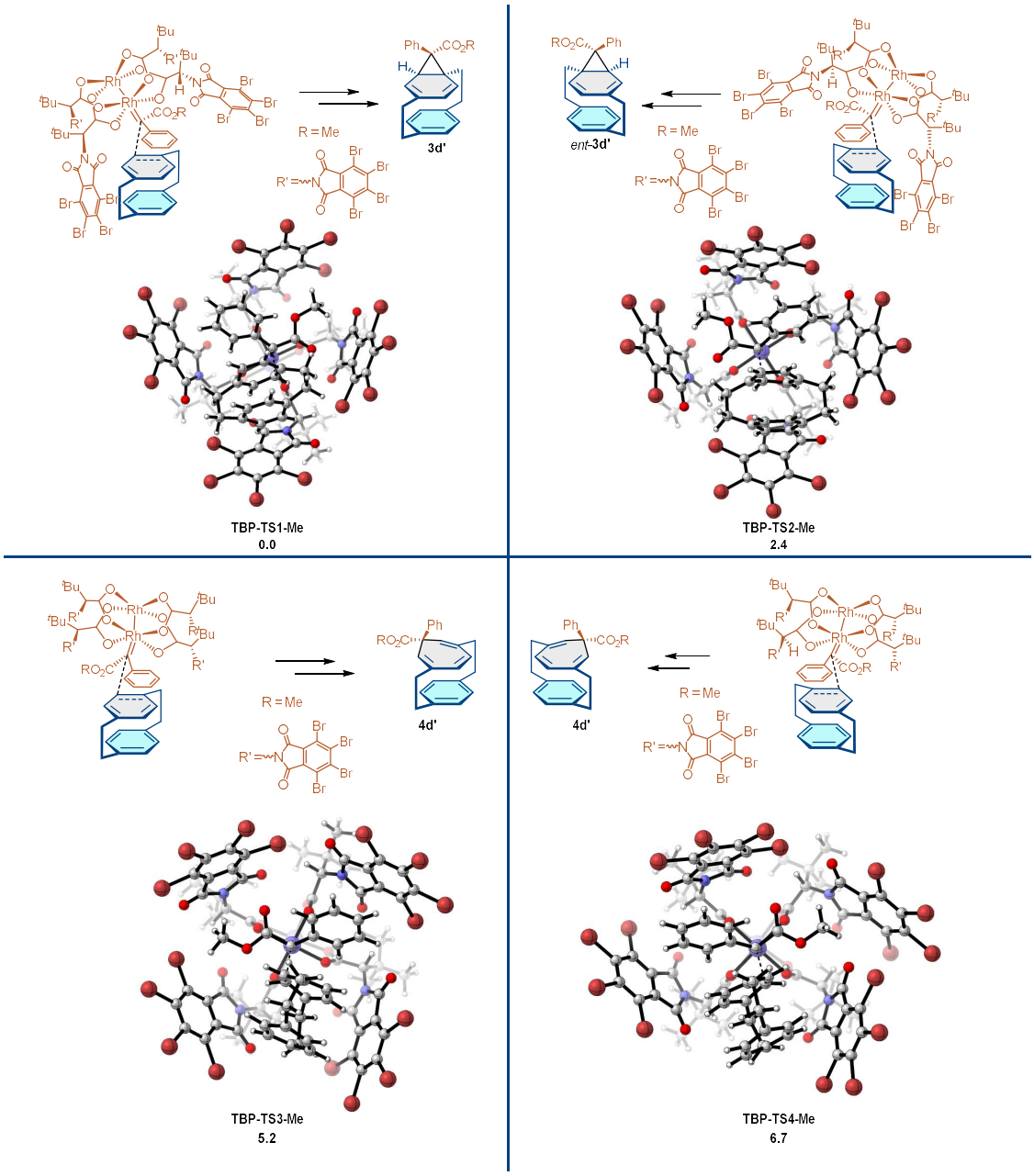


Figure S4. The selective transition states of cyclopropanation of PCP **2** using methyl α-diazophenylacetate **1a**.

Table S5. Computed Energies for the Stationary Points.

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)[a] (hartree)	SPEs (under SMD model)[b] (hartree)
$Rh_2(HCOO)_4$	None	-977.469276	0.061691	-977.959406
2	None	-618.942882	0.235474	-619.290269
1d	None	-944.073731	0.119094	-944.858709
N_2	None	-109.439974	-0.01277	-109.546485
Com1	None	-1921.579262	0.20401	-1922.84425
Int1	None	-1812.136007	0.196583	-1813.30376
Int2A	None	-2431.103115	0.458913	-2432.61062
Int2B	None	-2431.102268	0.459589	-2432.60911
Int3A	None	-1453.61018	0.375286	-1454.64441
Int3B	None	-1453.623939	0.37413	-1454.66376
3d	None	-1453.619724	0.375888	-1454.66058
4d	None	-1453.627262	0.373967	-1454.66576
TS1	-435.40	-1921.556696	0.202598	-1922.82773
TS2A	-373.48	-2431.098003	0.4586	-2432.60255
TS2B	-375.77	-2431.097389	0.458698	-2432.60278
TS2C	-336.27	-2431.082234	0.459415	-2432.5906
TS3A	-213.95	-2431.10183	0.461012	-2432.60936
TS3B	-26.47	-2431.082267	0.458768	-2432.58606
TS3C	-27.87	-2431.091091	0.460551	-2432.60303
TS3D	-151.44	-2431.103434	0.460662	-2432.60708
TS4A	-474.83	-1453.601325	0.374443	-1454.63764
TS4B	-449.59	-1453.613518	0.374131	-1454.65189
	Imaginary Frequencies (cm^{-1})	**SPEs[c] (under SMD model) (hartree)**	**TCGs[c] (hartree)**	**G[c] (under SMD model) (hartree)**
TBP-TS1	-330.70	-46435.6799	1.140206	-46434.5397
TBP-TS2	-326.25	-46435.6764	1.141085	-46434.5353
TBP-TS3	-329.38	-46435.6748	1.139144	-46434.53561
TBP-TS4	-365.27	-46435.6734	1.139722	-46434.53368
TBP-TS1-OMe	-346.42	-46550.133	1.170739	-46548.96227
TBP-TS2-OMe	-345.78	-46550.1279	1.169042	-46548.95885
TBP-TS3-OMe	-278.17	-46550.1175	1.171368	-46548.94617

TBP-TS4-OMe	-204.18	-46550.1363	1.170676	-46548.96564
TBP-TS5-OMe	-268.70	-46550.1242	1.173677	-46548.95057
TBP-TS6-OMe	-86.49	-46550.1368	1.172746	-46548.96404
TBP-TS1-Me	-355.46	-46098.8777	1.171618	-46097.74048
TBP-TS2-Me	-348.24	-46098.8735	1.136916	-46097.73663
TBP-TS3-Me	-375.86	-46098.8697	1.137518	-46097.73223
TBP-TS4-Me	-378.60	-46098.8696	1.139786	-46097.72985

[a]Computed at B3LYP-D3(BJ)/def2-SVP.

[b]Computed at SMD(DCM)/ωB97M-V/def2-TZVPP//B3LYP-D3(BJ)/def2-SVP.

[c]Computed at SMD(DCM)/B3LYP-D3(BJ)/def2-SVP.

Cartesian coordinates for the stationary points

1d

C	0.829224	0.514400	-0.285680
C	2.220042	0.069345	-0.055856
C	2.560961	-1.296107	-0.092640
C	3.235071	1.010550	0.206501
C	3.880230	-1.695153	0.127433
H	1.788584	-2.035151	-0.293127
C	4.548818	0.600393	0.425318
H	3.004112	2.077457	0.241271
C	4.881055	-0.756505	0.387135
H	4.124113	-2.759779	0.095010
H	5.317801	1.349828	0.626961
H	5.910737	-1.077787	0.558696
C	-0.323290	-0.335289	-0.592158
O	-0.316382	-1.537949	-0.690891
O	-1.447626	0.425589	-0.776907
C	-2.667569	-0.261004	-0.971715
H	-2.488371	-1.306315	-1.257379
H	-3.234450	0.259328	-1.755840
C	-3.481127	-0.237580	0.311617
F	-3.799019	1.012236	0.675425
F	-4.622434	-0.920410	0.132498
F	-2.808399	-0.798939	1.325271
N	0.571260	1.806122	-0.209825
N	0.379843	2.919166	-0.137559

2

C	0.697234	-1.542932	1.195524
C	-0.697529	-1.542960	1.195325
C	-1.414848	-1.394445	-0.001040
C	-0.697168	-1.540373	-1.197520
C	0.697586	-1.540365	-1.197323
C	1.414908	-1.394421	-0.000630
H	1.230735	-1.509669	2.149728
H	-1.231297	-1.509675	2.149380
H	-1.230653	-1.505070	-2.151659
H	1.231335	-1.505001	-2.151313
C	2.804720	-0.802317	0.000284
H	3.363674	-1.146500	-0.883217
H	3.361821	-1.145930	0.885164
C	-2.804683	-0.802384	-0.000617
H	-3.362674	-1.147019	0.883305
H	-3.362718	-1.145620	-0.885066
C	-2.804716	0.802324	0.000610
C	2.804677	0.802393	-0.000318
C	1.414824	1.394438	0.000624
C	0.697549	1.540367	1.197328
C	0.697166	1.542957	-1.195513
C	-0.697200	1.540294	1.197548
H	1.231346	1.505015	2.151286
C	-0.697627	1.542975	-1.195309
H	1.230628	1.509700	-2.149734
C	-1.414899	1.394453	0.001052
H	-1.230676	1.504959	2.151686

H	-1.231376	1.509690	-2.149370
H	-3.362686	1.146926	-0.883333
H	-3.362778	1.145537	0.885051
H	3.361716	1.146017	-0.885229
H	3.363643	1.146618	0.883159

3d

C	0.410187	1.171580	-0.166445
C	-0.214079	2.526399	-0.012917
C	-0.084096	3.232090	1.191356
C	-0.901173	3.119279	-1.076701
C	-0.641547	4.501945	1.333383
H	0.464068	2.777568	2.019255
C	-1.463940	4.391731	-0.937449
H	-1.000626	2.578348	-2.019212
C	-1.338819	5.083603	0.268696
H	-0.531405	5.042583	2.276596
H	-2.000382	4.843286	-1.775618
H	-1.778964	6.077709	0.379496
C	1.886539	1.236429	-0.381364
O	2.582937	2.184662	-0.125806
O	2.396666	0.082439	-0.923236
C	3.790853	0.019850	-1.134859
H	4.256226	0.997977	-0.950546
H	3.977682	-0.302269	-2.169472
C	4.414165	-1.000973	-0.201145
F	3.887941	-2.225071	-0.370765
F	5.731319	-1.083203	-0.437966
F	4.243057	-0.663683	1.087537
C	-0.339336	0.011702	-0.812644
C	-1.723817	0.029192	-1.326579
C	-2.807159	0.161280	-0.526504
C	-2.587295	0.438585	0.888815
C	-1.367596	0.335734	1.455337
C	-0.139186	-0.012834	0.695066
H	0.326531	-0.631920	-1.386958
H	-1.859714	-0.275661	-2.366965
H	-3.455663	0.651177	1.518383
H	-1.260704	0.447041	2.537829
C	0.774035	-1.036577	1.389660
H	0.484756	-1.041583	2.452738
H	1.825738	-0.725783	1.372439
C	-4.186438	-0.228710	-1.014989
H	-4.194035	-0.167074	-2.113374
H	-4.946110	0.483466	-0.653263
C	-4.631547	-1.694579	-0.589575
C	0.688509	-2.496988	0.852492
C	-0.735981	-2.891142	0.535298
C	-1.149712	-3.076218	-0.793596
C	-1.734610	-2.816207	1.514185
C	-2.486047	-2.911299	-1.155938
H	-0.395697	-3.222153	-1.572436
C	-3.066443	-2.623661	1.150040
H	-1.455457	-2.743318	2.568908
C	-3.436364	-2.528425	-0.198040
H	-2.759148	-2.919465	-2.215104
H	-3.803765	-2.395476	1.924778
H	-5.329246	-1.631871	0.259331
H	-5.188253	-2.138721	-1.430197
H	1.146981	-3.158649	1.606846
H	1.304883	-2.585103	-0.053882

4d

C	1.017709	-0.650921	-0.203494
C	2.534013	-0.836709	-0.032795
C	3.397602	-0.692584	-1.123654
C	3.067069	-1.229043	1.199850
C	4.769142	-0.918621	-0.983445
H	2.995354	-0.387958	-2.091304
C	4.436713	-1.454542	1.345431
H	2.402541	-1.353611	2.055986
C	5.295108	-1.296563	0.253935
H	5.429269	-0.795391	-1.845702
H	4.835567	-1.756471	2.317067
H	6.368155	-1.469274	0.367238
C	0.392544	-2.032208	-0.446110
O	0.860065	-3.089546	-0.128197
O	-0.846311	-1.909337	-1.008219
C	-1.682052	-3.047253	-1.027133
H	-1.145427	-3.934263	-0.662423
H	-2.043879	-3.218762	-2.051078
C	-2.874810	-2.774376	-0.129293
F	-3.600335	-1.731555	-0.564682
F	-3.676752	-3.846459	-0.089161

F	-2.484525	-2.495423	1.127265
C	0.319845	-0.141097	1.060731
C	0.640064	0.313245	-1.317343
C	0.996139	1.617547	-1.343784
C	1.690048	2.260910	-0.240137
C	1.523943	2.001308	1.085185
C	0.608985	1.033004	1.666327
H	-0.473123	-0.766877	1.478439
H	0.020218	-0.078619	-2.124558
H	2.299643	3.133462	-0.498833
H	2.013467	2.684195	1.787630
C	-0.102094	1.444212	2.956077
H	0.374776	2.364937	3.324326
H	0.055303	0.682873	3.737371
C	0.583288	2.510969	-2.513332
H	0.971473	2.107061	-3.462883
H	1.062511	3.492356	-2.378803
C	-0.961676	2.728926	-2.661340
C	-1.643300	1.704095	2.820986
C	-1.974610	2.211671	1.441710
C	-2.476925	1.323013	0.484635
C	-1.503962	3.457083	1.000233
C	-2.302900	1.571355	-0.874791
H	-2.890371	0.363838	0.802516
C	-1.336419	3.708469	-0.360074
H	-1.149895	4.191158	1.730021
C	-1.630179	2.718890	-1.310306
H	-2.575461	0.794268	-1.592974
H	-0.854591	4.637416	-0.678999
H	-1.125990	3.673830	-3.205345
H	-1.389300	1.926601	-3.282389
H	-1.943538	2.409239	3.613422
H	-2.191936	0.767312	3.003402

Com1

Rh	-0.289196	0.312957	0.079161
Rh	0.056446	2.687542	-0.171864
O	1.081715	0.046601	-1.433645
O	1.399275	2.272126	-1.665354
O	1.214775	0.314038	1.473245
O	1.575584	2.528539	1.204685
O	-1.620859	0.729067	1.584471
O	-1.306747	2.955538	1.343872
O	-1.778020	0.466402	-1.325231
O	-1.472589	2.697445	-1.538717
C	1.614964	1.067637	-1.952108
C	1.814494	1.401433	1.708057
C	-1.829296	1.942632	1.872969
C	-2.034943	1.603184	-1.808429
C	-0.711915	-2.083981	0.375071
C	-2.169864	-2.259405	0.112637
C	-2.633886	-2.584488	-1.172524
C	-3.103058	-2.050680	1.143023
C	-4.003463	-2.712611	-1.406496
H	-1.921522	-2.728980	-1.980359
C	-4.468711	-2.181938	0.898432
H	-2.770671	-1.757971	2.139520
C	-4.927437	-2.516238	-0.378324
H	-4.348312	-2.966899	-2.411528
H	-5.177764	-2.015752	1.712668
H	-5.997992	-2.617859	-0.570181
C	0.379374	-2.538112	-0.532582
O	0.245877	-2.873554	-1.679139
O	1.572661	-2.490699	0.106163
C	2.731683	-2.636673	-0.690935
H	2.550540	-2.268656	-1.708940
H	3.041888	-3.692294	-0.735898
C	3.854734	-1.839567	-0.053606
F	4.045784	-2.181124	1.225610
F	4.991711	-2.085980	-0.726801
F	3.637328	-0.516748	-0.095772
H	2.642169	1.348926	2.442226
H	-2.557223	2.128487	2.687660
H	2.356890	0.874908	-2.752023
H	-2.851636	1.638943	-2.556589
N	-0.350995	-2.078734	1.673883
N	-0.068353	-2.027237	2.758095

Int1

Rh	0.322297	-0.394787	-0.069914
Rh	2.742014	0.077114	0.048981
O	0.077071	1.233255	1.151403
O	2.291689	1.691856	1.237964
O	0.278417	0.838739	-1.705734

O	2.498747	1.269631	-1.608482
O	0.803963	-1.997197	-1.271731
O	3.024353	-1.567073	-1.163422
O	0.587620	-1.581090	1.597102
O	2.806180	-1.141194	1.711877
C	1.086475	1.909124	1.507478
C	1.349503	1.390685	-2.094581
C	2.023791	-2.216057	-1.542904
C	1.746687	-1.679475	2.103793
C	-1.635531	-0.748218	-0.192145
C	-2.322893	-1.988502	-0.018740
C	-3.742390	-2.059436	-0.124382
C	-1.606599	-3.182985	0.268146
C	-4.409145	-3.261343	0.057153
H	-4.309303	-1.157235	-0.359085
C	-2.283857	-4.383035	0.445781
H	-0.524627	-3.139133	0.344335
C	-3.679399	-4.424901	0.343242
H	-5.497058	-3.303518	-0.025570
H	-1.725434	-5.295434	0.664647
H	-4.206047	-5.372117	0.484441
C	-2.422869	0.434070	-0.609991
O	-2.746128	0.623243	-1.756013
O	-2.687590	1.269521	0.418556
C	-3.199530	2.551834	0.105313
H	-4.006633	2.782284	0.813790
H	-3.575927	2.583031	-0.926282
C	-2.117584	3.610703	0.256212
F	-1.077574	3.384174	-0.554368
F	-2.640355	4.808595	-0.061612
F	-1.656644	3.688486	1.511965
H	1.242516	2.056275	-2.974390
H	2.211500	-3.093082	-2.195328
H	0.858836	2.796299	2.130447
H	1.814819	-2.325677	3.002710

Int2A

Rh	-1.415203	-0.416694	0.001193
Rh	-3.509517	-1.659712	-0.334729
O	-2.260512	1.041915	-1.197122
O	-4.170871	-0.124892	-1.518717
O	-0.679300	-1.386193	-1.670789
O	-2.611535	-2.524767	-1.982654
O	-0.811681	-2.032878	1.155557
O	-2.755140	-3.150092	0.865425
O	-2.302352	0.443066	1.639966
O	-4.237268	-0.695823	1.328552
C	-3.412212	0.862432	-1.680170
C	-1.436587	-2.199985	-2.276970
C	-1.602677	-3.005232	1.332800
C	-3.488320	0.119845	1.926762
C	0.578732	0.785237	0.336659
C	0.787002	1.115799	1.779109
C	1.190601	2.401291	2.198091
C	0.668780	0.120966	2.765884
C	1.438889	2.681624	3.539412
H	1.311427	3.197298	1.465276
C	0.923154	0.399963	4.111925
H	0.352688	-0.877463	2.477407
C	1.306914	1.680489	4.508312
H	1.742626	3.690420	3.830124
H	0.810245	-0.394008	4.854708
H	1.502392	1.900788	5.560691
C	0.235123	1.859724	-0.611824
O	0.497717	1.873520	-1.800608
O	-0.504090	2.845214	-0.029066
C	-1.006845	3.850182	-0.874864
H	-1.023436	3.515833	-1.919929
H	-2.019885	4.105981	-0.536208
C	-0.135775	5.089484	-0.769451
F	-0.127343	5.591459	0.475670
F	-0.590504	6.044807	-1.595396
F	1.143400	4.830844	-1.098674
H	-0.999746	-2.683392	-3.175173
H	-1.220931	-3.823372	1.978012
H	-3.796127	1.680105	-2.324259
H	-3.918031	0.618989	2.819105
C	1.844962	-1.526598	0.239631
C	1.691700	-0.184372	-0.355160
C	2.874568	0.681049	-0.209652
C	3.639205	0.504122	0.951843
C	3.607174	-0.714921	1.611468
C	2.822944	-1.819924	1.141703
H	1.158865	-2.293864	-0.110366
H	1.332373	-0.270335	-1.383278

H	4.380604	1.252380	1.239786
H	4.293427	-0.878021	2.448163
C	3.192903	-3.249818	1.463006
H	3.480147	-3.352464	2.521221
H	2.300603	-3.875196	1.314414
C	3.360192	1.593852	-1.294879
H	2.591762	2.319213	-1.597732
H	4.228145	2.150501	-0.910401
C	3.779725	0.778511	-2.576567
C	4.372374	-3.818749	0.556076
C	4.595290	-2.943573	-0.652181
C	3.642718	-2.895539	-1.679437
C	5.549109	-1.916530	-0.607518
C	3.478176	-1.734036	-2.435886
H	2.921211	-3.710092	-1.788218
C	5.405430	-0.768902	-1.389012
H	6.346611	-1.957804	0.139977
C	4.281714	-0.603465	-2.209946
H	2.631235	-1.659728	-3.123292
H	6.093561	0.067952	-1.239221
H	4.537661	1.369656	-3.115056
H	2.903848	0.690719	-3.234819
H	5.295122	-3.869020	1.153405
H	4.116498	-4.850910	0.271044

Int2B

Rh	1.541757	-0.229253	0.007218
Rh	3.857847	-1.020556	-0.140167
O	2.105830	1.226074	-1.350546
O	4.242166	0.492545	-1.464220
O	1.112105	-1.499985	-1.567768
O	3.255555	-2.211765	-1.713670
O	1.228507	-1.779199	1.339586
O	3.364107	-2.506054	1.195771
O	2.161460	0.980942	1.544911
O	4.296817	0.234107	1.424488
C	3.294555	1.258286	-1.771220
C	2.054450	-2.177159	-2.073867
C	2.190821	-2.547530	1.633069
C	3.371416	0.942438	1.900646
C	-0.706041	0.545608	0.214475
C	-0.980896	1.024066	1.600976
C	-0.592261	0.273179	2.723508
C	-1.686959	2.223814	1.833712
C	-0.864731	0.715419	4.020622
H	-0.054111	-0.658347	2.574853
C	-1.955714	2.669088	3.125074
H	-2.033334	2.818791	0.989464
C	-1.541847	1.916622	4.229918
H	-0.536822	0.114374	4.872546
H	-2.495283	3.608252	3.269549
H	-1.751113	2.265187	5.244360
C	-0.557019	1.547213	-0.866888
O	-0.822293	1.377298	-2.040182
O	-0.010839	2.705127	-0.403042
C	0.272888	3.704651	-1.350271
H	0.260184	3.296814	-2.369250
H	1.257921	4.132178	-1.119048
C	-0.771967	4.800844	-1.246317
F	-0.750905	5.404981	-0.048901
F	-0.555382	5.737043	-2.183732
F	-2.014759	4.314592	-1.423954
H	1.776184	-2.819689	-2.934255
H	1.958817	-3.351919	2.360810
H	3.526797	2.062337	-2.499232
H	3.647572	1.616049	2.737053
C	-1.530656	-0.742988	-0.351487
C	-2.772291	0.047230	-0.420926
C	-3.756024	-0.009912	0.564271
C	-3.502139	-0.861978	1.642612
C	-2.492784	-1.858451	1.578377
C	-1.646205	-1.941857	0.502681
H	-1.094104	-0.943155	-1.331286
H	-2.859009	0.729688	-1.264654
H	-4.202305	-0.883543	2.482410
H	-2.537403	-2.676248	2.302011
C	-1.093354	-3.261692	0.048184
H	-1.181104	-3.980062	0.876781
H	-0.033273	-3.170023	-0.209889
C	-5.106064	0.631627	0.331804
H	-4.972683	1.513126	-0.311973
H	-5.526289	0.994382	1.282015
C	-6.157799	-0.349698	-0.354947
C	-1.856151	-3.828473	-1.218517
C	-3.265686	-3.293739	-1.336372

C	-3.560581	-2.277030	-2.258452
C	-4.237344	-3.583502	-0.368184
C	-4.655284	-1.429305	-2.071176
H	-2.857218	-2.067550	-3.068935
C	-5.312328	-2.717716	-0.160860
H	-4.075697	-4.410763	0.328710
C	-5.463881	-1.557241	-0.933868
H	-4.786999	-0.572552	-2.737850
H	-5.970921	-2.879153	0.697306
H	-6.895758	-0.667685	0.396671
H	-6.703760	0.215153	-1.126069
H	-1.838553	-4.928070	-1.152721
H	-1.290603	-3.549298	-2.119453

Int3A

C	-0.073978	1.118010	-0.187169
C	-0.780323	2.479181	-0.021375
C	-0.678282	3.171439	1.192844
C	-1.486391	3.068678	-1.073159
C	-1.273836	4.421182	1.353637
H	-0.128408	2.723955	2.022004
C	-2.089164	4.321321	-0.914793
H	-1.578937	2.541903	-2.023485
C	-1.986504	5.001501	0.298661
H	-1.182492	4.946241	2.307683
H	-2.645181	4.761880	-1.746138
H	-2.459481	5.978438	0.425285
C	1.431833	1.400955	-0.334604
O	2.007763	2.374043	0.065985
O	2.076041	0.377915	-0.970759
C	3.462628	0.523340	-1.212442
H	3.803187	1.529692	-0.933050
H	3.653117	0.336035	-2.278920
C	4.243950	-0.496511	-0.406853
F	3.864746	-1.754109	-0.689987
F	5.549554	-0.387097	-0.689814
F	4.087128	-0.314000	0.913574
C	-0.571381	0.336994	-1.385473
C	-1.787155	-0.235067	-1.558472
C	-2.871542	-0.406298	-0.627120
C	-2.767020	-0.137024	0.715520
C	-1.554580	-0.021186	1.466807
C	-0.280802	0.244701	1.068577
H	0.143972	0.203248	-2.197471
H	-1.942229	-0.703645	-2.535169
H	-3.653829	-0.353309	1.318987
H	-1.656116	-0.410093	2.484549
C	0.840810	-0.352757	1.893485
H	0.527351	-0.265297	2.945331
H	1.776677	0.216495	1.810995
C	-4.033505	-1.269714	-1.081328
H	-4.366075	-0.991948	-2.094009
H	-4.886728	-1.103767	-0.407951
C	-3.684499	-2.830112	-1.080417
C	1.177621	-1.883285	1.632081
C	0.040971	-2.646375	1.002649
C	0.015625	-2.809124	-0.386999
C	-1.120874	-2.990993	1.712955
C	-1.179864	-3.071337	-1.053752
H	0.921182	-2.603205	-0.963049
C	-2.324312	-3.220035	1.042939
H	-1.115751	-2.953033	2.806218
C	-2.393579	-3.139457	-0.357330
H	-1.188214	-3.084564	-2.146557
H	-3.244185	-3.347020	1.621275
H	-4.531255	-3.368359	-0.627072
H	-3.610169	-3.174617	-2.123151
H	1.472102	-2.320259	2.599382
H	2.053071	-1.945719	0.975339

Int3B

C	0.682847	-1.082877	-0.324377
C	2.071267	-1.570035	-0.051446
C	3.028069	-1.586897	-1.072267
C	2.412846	-2.067907	1.210972
C	4.308290	-2.092557	-0.836890
H	2.765635	-1.196082	-2.057657
C	3.691032	-2.574161	1.451359
H	1.666706	-2.058572	2.007909
C	4.643118	-2.584221	0.427714
H	5.046739	-2.101994	-1.642278
H	3.945430	-2.963190	2.440236
H	5.645260	-2.977772	0.615098
C	-0.288702	-2.172100	-0.639705

O	-0.120435	-3.347078	-0.447909
O	-1.461508	-1.668868	-1.148259
C	-2.600113	-2.498268	-1.131685
H	-2.332712	-3.528229	-0.855269
H	-3.077138	-2.486465	-2.122236
C	-3.577555	-1.937584	-0.113387
F	-3.966183	-0.690632	-0.429848
F	-4.671409	-2.706934	-0.044204
F	-3.023099	-1.882993	1.110687
C	0.031443	0.022310	0.530737
C	0.406424	0.283679	-0.946580
C	1.472546	1.259373	-1.190492
C	2.304693	1.593261	-0.162479
C	1.960274	1.333018	1.212395
C	0.777812	0.746408	1.557594
H	-1.025953	-0.145006	0.730412
H	-0.426018	0.288152	-1.647661
H	3.129218	2.286941	-0.349352
H	2.547967	1.841061	1.981976
C	0.092291	1.030806	2.873080
H	0.835793	1.458389	3.561716
H	-0.274457	0.100951	3.338689
C	1.444848	2.043111	-2.481157
H	1.370233	1.369717	-3.350963
H	2.400190	2.579586	-2.577627
C	0.256075	3.102403	-2.575038
C	-1.135529	2.037700	2.755882
C	-1.137862	2.772013	1.436620
C	-1.957503	2.342131	0.385102
C	-0.119082	3.688187	1.131055
C	-1.609543	2.607224	-0.941701
H	-2.798518	1.673958	0.589929
C	0.228757	3.949497	-0.191930
H	0.498813	4.093942	1.936879
C	-0.433969	3.304423	-1.247963
H	-2.190667	2.146331	-1.745570
H	1.113255	4.556748	-0.403161
H	0.678090	4.046789	-2.953024
H	-0.476135	2.760601	-3.321759
H	-1.079885	2.734750	3.606956
H	-2.076718	1.478343	2.863900

N_2

N	0.000000	0.000000	0.550196
N	0.000000	0.000000	-0.550196

$Rh_2(HCOO)_4$

Rh	0.000005	0.000032	1.193905
Rh	-0.000018	-0.000042	-1.193857
O	-1.482006	1.412926	1.129875
O	-1.479149	1.416018	-1.130105
O	-1.413046	-1.481949	1.130024
O	-1.416198	-1.478919	-1.129951
O	1.482125	-1.412838	1.129994
O	1.479058	-1.416073	-1.129987
O	1.412834	1.482107	1.129921
O	1.416370	1.478757	-1.130056
C	-1.885787	1.801673	-0.000039
C	-1.801735	-1.885736	0.000078
C	1.885841	-1.801622	0.000070
C	1.801736	1.885704	-0.000051
H	-2.566916	-2.686468	-0.000017
H	2.686436	-2.566952	-0.000023
H	-2.686212	2.567180	-0.000114
H	2.567040	2.686322	-0.000073

TBP-TS1-Me

Rh	-0.341392	0.010773	1.548099
Rh	-0.287291	0.185413	4.008895
N	-4.057631	2.732623	1.599670
O	-4.542596	0.729151	2.657332
O	-3.783994	4.335042	-0.048417
C	-4.692717	1.497283	1.736905
C	-5.529690	1.328193	0.502497
C	-6.430629	0.330147	0.154456
C	-7.013055	0.384766	-1.135044
C	-6.702752	1.443317	-2.018597
C	-5.820009	2.477576	-1.621103
C	-5.245921	2.394365	-0.358492
C	-4.283163	3.310035	0.344494
N	2.421711	3.863080	1.604803
O	0.281590	4.271071	2.386060

O	4.318587	3.824968	0.281798	C	-4.320683	3.050704	4.732855
C	1.185804	4.513903	1.623246	C	-2.385942	4.640794	4.480386
C	1.230021	5.503298	0.494579	C	1.671687	1.811601	2.657048
C	0.285649	6.428871	0.066691	C	2.826075	2.818579	2.541895
C	0.567748	7.170046	-1.107690	C	3.449613	3.378556	3.858472
C	1.774811	6.964785	-1.813930	C	2.437576	4.153424	4.716904
C	2.731579	6.030536	-1.346417	C	4.597507	4.332368	3.479743
C	2.438168	5.320529	-0.188953	C	4.047452	2.209611	4.662284
C	3.222868	4.265543	0.535686	C	1.433987	-1.855195	2.876328
N	3.577233	-2.650443	2.024258	C	2.463872	-2.996532	2.910037
O	3.810630	-0.406759	2.546480	C	2.934232	-3.501532	4.311203
O	3.786096	-4.697346	0.954389	C	1.714576	-4.072274	5.058221
C	4.178948	-1.391717	1.952017	C	3.941790	-4.648828	4.112519
C	5.330733	-1.539625	0.997844	C	3.612864	-2.400992	5.142028
C	6.260924	-0.610375	0.546012	C	-2.221347	-1.685021	3.010440
C	7.257341	-1.055050	-0.358663	C	-3.248525	-2.831151	3.064440
C	7.273889	-2.393874	-0.810692	C	-3.547156	-3.477455	4.452826
C	6.293560	-3.314604	-0.364345	C	-4.225175	-2.424725	5.348382
C	5.344628	-2.864351	0.545093	C	-4.539771	-4.634874	4.243190
C	4.172601	-3.570895	1.158972	C	-2.284477	-4.025858	5.134740
N	-2.902879	-3.791026	2.017936	H	1.950693	-3.833089	2.415240
O	-0.628181	-3.988211	2.395641	H	3.525774	-5.455790	3.491674
O	-5.016376	-3.985816	1.100129	H	4.209423	-5.072666	5.092809
C	-1.604566	-4.221394	1.725113	H	4.875956	-4.302176	3.644092
C	-1.711710	-5.005846	0.449084	H	3.912417	-2.812592	6.119433
C	-0.723442	-5.573907	-0.344036	H	4.526168	-2.030003	4.652135
C	-1.119825	-6.176025	-1.562249	H	2.943484	-1.549727	5.313736
C	-2.474524	-6.173684	-1.962852	H	2.042460	-4.527265	6.006286
C	-3.461310	-5.579882	-1.140244	H	0.973827	-3.296609	5.283688
C	-3.054677	-5.013360	0.061071	H	1.219283	-4.853664	4.460752
C	-3.833576	-4.231063	1.075838	H	3.270114	1.525752	5.023096
O	-1.676312	1.548609	1.594781	H	4.595182	2.605374	5.532193
O	-1.605383	1.767358	3.837011	H	4.752740	1.626299	4.051315
O	1.226357	1.377729	1.550873	H	5.355902	3.835339	2.856418
O	1.278307	1.478305	3.798741	H	5.093946	4.691728	4.394322
O	1.062519	-1.497001	1.720384	H	4.235662	5.216868	2.933475
O	1.020054	-1.390671	3.967917	H	1.571805	3.534419	4.981533
O	-1.870094	-1.340153	1.846539	H	2.072646	5.053727	4.200513
O	-1.827753	-1.168015	4.085268	H	2.927530	4.485312	5.646548
C	-2.017320	2.079905	2.693421	H	3.618120	2.262894	2.020629
C	-3.022979	3.225725	2.507275	H	-1.696254	3.897237	4.899207
C	-3.568628	3.969627	3.758739	H	-2.763299	5.268852	5.303003
C	-4.527900	5.067374	3.265274	H	-1.810548	5.281614	3.795603

H	-5.223132	2.621071	4.274750
H	-4.639589	3.633913	5.612125
H	-3.685112	2.224447	5.076211
H	-4.036167	5.746662	2.551370
H	-4.880976	5.668485	4.117587
H	-5.412417	4.640778	2.767574
H	-2.471140	3.968712	1.912552
H	-1.825028	-4.831105	4.543675
H	-1.532875	-3.240843	5.283830
H	-2.550555	-4.443652	6.119262
H	-4.553617	-2.893587	6.289572
H	-3.545621	-1.598730	5.590573
H	-5.115827	-2.001167	4.855410
H	-4.099955	-5.447001	3.644178
H	-5.456638	-4.297022	3.737621
H	-4.821402	-5.059457	5.219432
H	-4.190931	-2.376417	2.719746
Br	8.557547	0.171078	-0.977682
Br	6.133504	1.202933	1.058531
Br	8.583283	-2.961439	-2.048428
Br	6.247671	-5.094401	-0.995207
Br	4.358569	5.733887	-2.264570
Br	2.123530	7.935067	-3.399135
Br	-0.701942	8.419296	-1.741134
Br	-1.330058	6.659388	1.012556
Br	-5.421453	3.932971	-2.760909
Br	-7.463157	1.486571	-3.750926
Br	-8.187234	-0.995843	-1.677905
Br	-6.851017	-1.052629	1.372210
Br	-5.278387	-5.503440	-1.667450
Br	-2.981396	-6.948034	-3.614518
Br	0.192778	-6.982594	-2.664795
Br	1.092233	-5.463340	0.165384
C	-0.620410	-0.149518	-0.622379
C	-0.846726	1.072386	-1.421307
C	-0.208656	2.283346	-1.081230
C	-1.676801	1.079883	-2.569509
C	-0.427652	3.445283	-1.823079
H	0.457562	2.300183	-0.221468
C	-1.916152	2.245654	-3.292421
H	-2.151353	0.157035	-2.898254
C	-1.293889	3.439993	-2.917556
H	0.079555	4.366351	-1.545377
H	-2.584153	2.218980	-4.156295
H	-1.476710	4.360351	-3.477560
C	-1.622912	-1.248091	-0.781202
O	-1.404934	-2.442470	-0.792165
O	-2.871615	-0.742791	-0.838919
C	-3.960753	-1.650954	-0.963562
H	-4.405873	-1.840049	0.018757
H	-3.631332	-2.597036	-1.409412
C	1.666675	0.709704	-3.347199
C	0.831316	-0.375788	-3.580190
C	0.701692	-1.374841	-2.612712
C	1.071303	-1.015109	-1.267702
C	2.066286	0.017920	-1.104308
C	2.436755	0.825197	-2.155925
H	1.829173	1.435524	-4.148214
H	0.410288	-0.517661	-4.577414
H	1.077560	-1.803638	-0.514751
H	2.514821	0.140598	-0.118147
C	3.711622	1.628736	-2.175875
H	4.031428	1.850108	-1.150620
H	3.539294	2.595341	-2.671390
C	0.369772	-2.791162	-3.017886
H	-0.632191	-2.846577	-3.472711
H	0.337550	-3.410939	-2.116989
C	1.421118	-3.384210	-4.041711
C	4.899726	0.881299	-2.935987
C	4.490994	-0.486325	-3.426424
C	4.002634	-0.699911	-4.722076
C	4.290064	-1.512351	-2.490948
C	3.142773	-1.773674	-4.992880
H	4.182030	0.049673	-5.498236
C	3.433731	-2.576216	-2.753550
H	4.690290	-1.392770	-1.488676
C	2.741290	-2.647802	-3.975202
H	2.659224	-1.833126	-5.972081
H	3.198056	-3.284494	-1.954948
H	1.534975	-4.453330	-3.805730
H	1.022029	-3.319986	-5.064444
H	5.746390	0.803497	-2.238832
H	5.232414	1.503848	-3.778983
H	-4.700149	-1.171161	-1.617058

TBP-TS1-OMe

Rh	-0.191982	0.047612	1.701568
Rh	-0.063716	0.226483	4.155203
N	-3.552642	3.199528	1.789394
O	-4.255484	1.238360	2.800348
O	-3.123320	4.818554	0.192159
C	-4.320238	2.039197	1.897734
C	-5.177517	2.000465	0.665822
C	-6.183502	1.117742	0.292887
C	-6.799223	1.305152	-0.967547
C	-6.400578	2.368077	-1.808987
C	-5.391588	3.271249	-1.396698
C	-4.799366	3.067702	-0.156143
C	-3.729817	3.842950	0.559018
N	2.977098	3.586731	1.681597
O	0.906541	4.231112	2.489029
O	4.845891	3.344525	0.339713
C	1.821669	4.370485	1.713226
C	1.959421	5.345953	0.579918
C	1.119616	6.373051	0.165094
C	1.465245	7.074887	-1.016568
C	2.632495	6.736272	-1.738347
C	3.487187	5.703444	-1.280079
C	3.129999	5.028895	-0.119000
C	3.805182	3.898545	0.602286
N	3.404922	-3.019588	2.072652
O	3.905800	-0.821658	2.602354
O	3.336764	-5.059924	0.973074
C	4.140273	-1.834588	1.987448
C	5.230596	-2.097313	0.987210
C	6.245162	-1.273202	0.512762
C	7.147043	-1.812149	-0.438573
C	6.988213	-3.133600	-0.913581
C	5.924188	-3.942687	-0.443222
C	5.071321	-3.404760	0.512877
C	3.854983	-3.986444	1.171143
N	-3.189910	-3.426497	2.276310
O	-0.945461	-3.887132	2.605632
O	-5.328427	-3.363452	1.397474
C	-1.959004	-4.015338	1.963165
C	-2.193465	-4.806305	0.708318
C	-1.297445	-5.480995	-0.111193
C	-1.800288	-6.060408	-1.300932
C	-3.169320	-5.956108	-1.635282
C	-4.061685	-5.260544	-0.784894
C	-3.546436	-4.691000	0.373921
C	-4.192500	-3.775579	1.372182
O	-1.355207	1.716852	1.769895
O	-1.197596	1.942432	4.006130
O	1.508725	1.247822	1.668025
O	1.628546	1.336476	3.912794
O	1.038526	-1.599189	1.843905
O	1.057280	-1.492837	4.091272
O	-1.856788	-1.125141	2.036423
O	-1.752532	-0.930479	4.272485
C	-1.603101	2.292917	2.870597
C	-2.467247	3.550806	2.702345
C	-2.920076	4.332917	3.968108
C	-3.770967	5.527049	3.500466
C	-3.748136	3.481411	4.941889
C	-1.666497	4.874516	4.678886
C	2.025960	1.630832	2.761486
C	3.278507	2.509884	2.620975
C	3.977198	3.005158	3.926471
C	3.060605	3.869641	4.806584
C	5.203398	3.846781	3.527721
C	4.475760	1.780852	4.715699
C	1.392771	-1.998974	2.991685
C	2.289656	-3.247140	2.993905
C	2.743651	-3.809633	4.377305
C	1.491152	-4.242109	5.161695
C	3.606952	-5.062826	4.142278
C	3.567697	-2.796818	5.187524
C	-2.227846	-1.406412	3.211875
C	-3.391159	-2.409391	3.305283
C	-3.742382	-2.986607	4.712023
C	-4.271085	-1.840218	5.592897
C	-4.872654	-4.017890	4.543863
C	-2.544834	-3.673832	5.386327
H	1.671577	-4.018594	2.513201
H	3.080918	-5.812866	3.533390
H	3.856138	-5.521318	5.111768
H	4.558777	-4.822378	3.643813
H	3.848676	-3.243625	6.154875
H	4.501222	-2.528855	4.669346
H	3.004303	-1.876012	5.380637

H	1.794837	-4.737353	6.097540
H	0.850902	-3.388690	5.412915
H	0.891318	-4.958369	4.578552
H	3.643898	1.170480	5.086523
H	5.071892	2.118260	5.578300
H	5.114166	1.137767	4.091060
H	5.896525	3.284763	2.883954
H	5.751671	4.148785	4.433368
H	4.915980	4.766799	2.995985
H	2.148899	3.332082	5.093843
H	2.766301	4.799177	4.297232
H	3.601200	4.155569	5.723325
H	4.000024	1.869890	2.093760
H	-1.043209	4.061237	5.071284
H	-1.967345	5.519969	5.519377
H	-1.045533	5.471503	3.993869
H	-4.689959	3.141964	4.487482
H	-4.004312	4.084466	5.828210
H	-3.190905	2.596131	5.274237
H	-3.225054	6.160105	2.783606
H	-4.046301	6.151885	4.364298
H	-4.703008	5.197466	3.016047
H	-1.829975	4.232884	2.119701
H	-2.191777	-4.534296	4.799731
H	-1.703325	-2.982702	5.518770
H	-2.846845	-4.047064	6.378313
H	-4.631000	-2.243946	6.552557
H	-3.494077	-1.094419	5.799615
H	-5.116743	-1.327018	5.105822
H	-4.544628	-4.893011	3.962089
H	-5.749063	-3.582697	4.040973
H	-5.189702	-4.380218	5.534174
H	-4.273276	-1.844076	2.964731
Br	8.550696	-0.730147	-1.098178
Br	6.344233	0.534555	1.050334
Br	8.167645	-3.820548	-2.219067
Br	5.641718	-5.688611	-1.105999
Br	5.065012	5.235742	-2.213261
Br	3.064743	7.660048	-3.330745
Br	0.333102	8.456634	-1.635867
Br	-0.445324	6.784014	1.134457
Br	-4.851049	4.718705	-2.487143
Br	-7.199079	2.580361	-3.509583
Br	-8.141425	0.098170	-1.530010
Br	-6.684814	-0.302557	1.438532
Br	-5.896194	-5.075283	-1.207842
Br	-3.821404	-6.727139	-3.235828
Br	-0.609885	-6.970305	-2.459374
Br	0.540005	-5.535817	0.321597
C	-0.501321	-0.093142	-0.470247
C	-0.654383	1.146409	-1.256687
C	0.002769	2.331532	-0.865026
C	-1.447153	1.201989	-2.427829
C	-0.183380	3.521162	-1.568423
H	0.651330	2.307355	0.007502
C	-1.653719	2.395719	-3.114877
H	-1.901431	0.295316	-2.816898
C	-1.028277	3.567597	-2.679551
H	0.322261	4.425664	-1.238226
H	-2.301997	2.406159	-3.993924
H	-1.190018	4.511277	-3.205655
C	-1.562459	-1.125790	-0.608503
O	-1.430467	-2.327752	-0.565045
O	-2.803494	-0.550709	-0.702022
C	-3.888463	-1.409954	-0.969177
H	-4.721917	-1.173154	-0.298899
H	-3.597433	-2.457653	-0.843429
C	-4.329541	-1.225435	-2.407298
F	-3.361080	-1.601759	-3.271568
F	-5.412702	-1.969488	-2.663745
F	-4.628956	0.052546	-2.695546
C	1.776743	0.576205	-3.256771
C	0.842296	-0.439106	-3.449658
C	0.678100	-1.424353	-2.458243
C	1.121084	-1.076299	-1.135778
C	2.186337	-0.111430	-1.003386
C	2.573997	0.648795	-2.081463
H	2.001339	1.261189	-4.073924
H	1.090624	-1.860299	-0.378823
H	2.671393	-0.010914	-0.033379
C	3.907637	1.346087	-2.164473
H	4.298844	1.526817	-1.156609
H	3.793539	2.329287	-2.643610
C	0.194915	-2.800632	-2.844030
H	-0.825214	-2.759025	-3.255151
H	0.149352	-3.409684	-1.936781

C	1.142529	-3.493032	-3.903744
C	4.983890	0.508238	-2.993783
C	4.442692	-0.825665	-3.448584
C	3.884605	-1.013530	-4.720774
C	4.198723	-1.820497	-2.490978
C	2.938053	-2.023915	-4.947629
H	4.094335	-0.289888	-5.513781
C	3.253493	-2.817745	-2.707662
H	4.645318	-1.720506	-1.506378
C	2.513658	-2.853427	-3.902527
H	2.417664	-2.062233	-5.907941
H	2.994571	-3.497476	-1.891741
H	1.190171	-4.562350	-3.645925
H	0.702344	-3.414141	-4.906652
H	5.864975	0.368245	-2.350345
H	5.309658	1.100450	-3.861007
O	0.180671	-0.645865	-4.610079
C	0.317215	0.298038	-5.659442
H	-0.339683	-0.044123	-6.469669
H	0.000855	1.302820	-5.334003
H	1.353759	0.345584	-6.030878

TBP-TS1

Rh	-0.194551	0.050467	1.633566
Rh	-0.059375	0.226037	4.086826
N	-3.551633	3.204463	1.738109
O	-4.248421	1.239716	2.746274
O	-3.130571	4.829583	0.144878
C	-4.315886	2.041761	1.844920
C	-5.173358	2.002349	0.613234
C	-6.175150	1.115791	0.238273
C	-6.790034	1.301748	-1.022747
C	-6.396751	2.368774	-1.861578
C	-5.394274	3.277682	-1.445877
C	-4.800468	3.073412	-0.206170
C	-3.733110	3.850850	0.509890
N	2.978972	3.586874	1.612177
O	0.909503	4.230149	2.423440
O	4.845435	3.345888	0.267237
C	1.824136	4.371691	1.647494
C	1.962129	5.350892	0.517559
C	1.122652	6.379714	0.106498
C	1.468332	7.085440	-1.072832
C	2.635668	6.749356	-1.795706
C	3.490008	5.714431	-1.341357
C	3.132333	5.035604	-0.182910
C	3.806369	3.901694	0.533466
N	3.407152	-3.020685	2.002662
O	3.904118	-0.821041	2.528591
O	3.345795	-5.064240	0.908627
C	4.142761	-1.835748	1.918310
C	5.238899	-2.101069	0.925181
C	6.251612	-1.275704	0.448780
C	7.157311	-1.815854	-0.498188
C	7.003427	-3.139773	-0.967886
C	5.940362	-3.949769	-0.496955
C	5.083692	-3.410533	0.454998
C	3.863253	-3.990443	1.107352
N	-3.187910	-3.426532	2.215593
O	-0.941929	-3.881339	2.542701
O	-5.328313	-3.372238	1.340538
C	-1.956200	-4.013564	1.902287
C	-2.190641	-4.808597	0.650071
C	-1.294566	-5.484922	-0.168077
C	-1.798241	-6.069839	-1.354785
C	-3.168270	-5.970497	-1.686705
C	-4.060938	-5.274328	-0.837078
C	-3.544626	-4.698264	0.318049
C	-4.191338	-3.781337	1.314636
O	-1.353812	1.722301	1.710016
O	-1.191257	1.943686	3.946223
O	1.510659	1.245799	1.595713
O	1.632837	1.334427	3.840511
O	1.036160	-1.599091	1.770097
O	1.058826	-1.493257	4.017482
O	-1.858877	-1.121956	1.970551
O	-1.749648	-0.928345	4.206483
C	-1.599147	2.296515	2.812355
C	-2.463818	3.554668	2.648634
C	-2.913374	4.334144	3.917143
C	-3.765477	5.529238	3.454172
C	-3.739080	3.480498	4.891034
C	-1.658005	4.874297	4.625851
C	2.029262	1.628650	2.689034
C	3.281518	2.507881	2.548599

C	3.981787	3.000757	3.854321
C	3.066680	3.864710	4.736512
C	5.208139	3.842246	3.455629
C	4.480470	1.775244	4.641580
C	1.392517	-1.999172	2.917365
C	2.289517	-3.247317	2.921152
C	2.741071	-3.808620	4.306197
C	1.487404	-4.239736	5.089475
C	3.604128	-5.062646	4.074420
C	3.564891	-2.795567	5.116426
C	-2.227301	-1.403829	3.146874
C	-3.389847	-2.407495	3.242666
C	-3.739578	-2.982408	4.650734
C	-4.267416	-1.834574	5.530250
C	-4.869958	-4.014075	4.485711
C	-2.541295	-3.668591	5.324799
H	1.672408	-4.019132	2.439969
H	3.079084	-5.813222	3.465383
H	3.850851	-5.519940	5.045094
H	4.557353	-4.823525	3.578003
H	3.844332	-3.241745	6.084506
H	4.499401	-2.529015	4.599248
H	3.002117	-1.874113	5.308027
H	1.789912	-4.734785	6.025804
H	0.847506	-3.385830	5.339693
H	0.887653	-4.955792	4.506049
H	3.648683	1.165286	5.013228
H	5.078191	2.111435	5.503549
H	5.117390	1.132206	4.015415
H	5.900551	3.280737	2.810654
H	5.757243	4.142690	4.361281
H	4.920887	4.763245	2.925499
H	2.154736	3.327605	5.023811
H	2.772843	4.795355	4.228928
H	3.608391	4.148731	5.653179
H	4.002420	1.869101	2.019182
H	-1.033824	4.060296	5.015339
H	-1.956689	5.518325	5.468197
H	-1.038694	5.472508	3.940356
H	-4.681597	3.141434	4.437754
H	-3.993866	4.081836	5.778916
H	-3.180834	2.594870	5.220726
H	-3.221467	6.163795	2.737209
H	-4.038578	6.152227	4.320043
H	-4.698787	5.200620	2.971546
H	-1.828336	4.237983	2.065474
H	-2.188596	-4.529705	4.738908
H	-1.699828	-2.977194	5.455864
H	-2.842486	-4.040840	6.317393
H	-4.625848	-2.236751	6.491108
H	-3.490446	-1.088099	5.734628
H	-5.113974	-1.322585	5.043502
H	-4.542504	-4.890292	3.905266
H	-5.747000	-3.579946	3.983040
H	-5.185750	-4.374589	5.477077
H	-4.272597	-1.843647	2.901402
Br	8.556782	-0.731296	-1.162022
Br	6.337533	0.537338	0.970195
Br	8.188188	-3.828933	-2.267301
Br	5.664512	-5.699120	-1.153426
Br	5.068102	5.250195	-2.275554
Br	3.068632	7.679339	-3.384176
Br	0.336153	8.469166	-1.687468
Br	-0.442384	6.787238	1.077257
Br	-4.865604	4.734279	-2.529902
Br	-7.194430	2.579826	-3.562731
Br	-8.124512	0.087985	-1.589262
Br	-6.672709	-0.307112	1.382500
Br	-5.897158	-5.097530	-1.255726
Br	-3.821611	-6.749550	-3.282862
Br	-0.607831	-6.980684	-2.512499
Br	0.543341	-5.537624	0.263509
C	-0.517389	-0.083034	-0.535073
C	-0.671970	1.158071	-1.315902
C	-0.005299	2.339700	-0.926560
C	-1.474765	1.222933	-2.480169
C	-0.192588	3.532464	-1.623028
H	0.651133	2.310079	-0.060013
C	-1.681943	2.420612	-3.160922
H	-1.946089	0.321640	-2.861024
C	-1.047152	3.587024	-2.727000
H	0.320141	4.433400	-1.294031
H	-2.338164	2.438061	-4.034064
H	-1.208986	4.533557	-3.247917
C	-1.571110	-1.123062	-0.677575
O	-1.429345	-2.324463	-0.644354

O	-2.817393	-0.557986	-0.763013
C	-3.895362	-1.426516	-1.029552
H	-4.732030	-1.192594	-0.362354
H	-3.596683	-2.471338	-0.898489
C	-4.334424	-1.252946	-2.469623
F	-3.356177	-1.617684	-3.329118
F	-5.404754	-2.014017	-2.728275
F	-4.651318	0.019288	-2.763685
C	1.731017	0.570657	-3.359861
C	0.823913	-0.466818	-3.540202
C	0.664206	-1.433030	-2.545462
C	1.104228	-1.069533	-1.222072
C	2.159167	-0.091802	-1.113128
C	2.543696	0.667184	-2.195803
H	1.913056	1.264812	-4.184432
H	0.362414	-0.605136	-4.519838
H	1.086557	-1.839403	-0.450110
H	2.644837	0.025937	-0.144086
C	3.868990	1.380002	-2.276056
H	4.235219	1.606489	-1.267871
H	3.749505	2.340704	-2.797559
C	0.223887	-2.832854	-2.904615
H	-0.796521	-2.827566	-3.319159
H	0.187351	-3.430812	-1.989034
C	1.193622	-3.518359	-3.950255
C	4.980180	0.528848	-3.044152
C	4.462839	-0.817362	-3.489414
C	3.926711	-1.028131	-4.766636
C	4.217644	-1.804429	-2.523324
C	2.990979	-2.048644	-4.988968
H	4.134909	-0.310871	-5.565735
C	3.289346	-2.817133	-2.739003
H	4.647303	-1.685137	-1.533164
C	2.561997	-2.872032	-3.940728
H	2.477691	-2.097799	-5.953457
H	3.028528	-3.489679	-1.917902
H	1.242238	-4.588415	-3.694804
H	0.765041	-3.446259	-4.960359
H	5.836465	0.406763	-2.364710
H	5.335786	1.104950	-3.910413

TBP-TS2-Me

Rh	0.355391	0.119734	1.655927
Rh	0.390162	-0.000746	4.118233
N	4.582589	1.827596	1.757741
O	2.908763	3.313916	2.349845
O	6.219888	0.697948	0.580800
C	3.733227	2.921372	1.559624
C	4.067057	3.456364	0.195635
C	3.550254	4.543929	-0.500414
C	4.047320	4.790679	-1.803786
C	5.017972	3.941100	-2.377981
C	5.543387	2.852556	-1.641274
C	5.058460	2.637525	-0.357078
C	5.407126	1.587779	0.657166
N	1.953790	-4.234427	1.666685
O	3.508634	-2.833290	2.658971
O	0.818119	-5.470185	0.071527
C	3.192606	-3.601430	1.781655
C	3.986733	-4.034306	0.582951
C	5.305598	-3.779235	0.230735
C	5.748763	-4.213366	-1.041575
C	4.868980	-4.897111	-1.911570
C	3.540540	-5.182962	-1.511887
C	3.129438	-4.748215	-0.259143
C	1.811144	-4.891688	0.443663
N	-4.102838	-1.580232	2.005065
O	-2.358216	-3.048232	2.403638
O	-5.984161	-0.580012	1.088058
C	-3.379477	-2.763693	1.825912
C	-4.139444	-3.557567	0.802130
C	-3.836099	-4.767542	0.187871
C	-4.763244	-5.284301	-0.750013
C	-5.939624	-4.569869	-1.068920
C	-6.199481	-3.312990	-0.470618
C	-5.286832	-2.833267	0.460953
C	-5.234045	-1.522807	1.188985
N	-1.403414	4.421632	2.163600
O	-2.817817	2.652030	2.642707
O	-0.459549	6.294469	1.181025
C	-2.532570	3.618757	1.977478
C	-3.264127	4.204672	0.802138
C	-4.427382	3.793244	0.161622
C	-4.863335	4.538817	-0.961475
C	-4.120733	5.648256	-1.423846

C	-2.936396	6.045534	-0.757064	H	-3.159098	0.740740	5.418777
C	-2.538298	5.314239	0.355505	H	-4.610238	1.424987	4.652080
C	-1.333981	5.462833	1.237697	H	-0.581090	-3.829569	5.006572
O	2.379260	0.391049	1.802792	H	-0.483214	-5.560344	5.423953
O	2.426018	0.285043	4.049095	H	-1.302567	-5.042665	3.927282
O	0.559149	-1.906438	1.699568	H	0.209291	-6.699187	2.663664
O	0.606715	-2.039965	3.945279	H	0.996741	-7.113216	4.206094
O	-1.709134	-0.166049	1.770972	H	1.979551	-6.584372	2.823913
O	-1.628616	-0.235216	4.017993	H	2.016160	-3.615843	5.139648
O	0.074869	2.159848	1.912824	H	3.028181	-4.816351	4.301811
O	0.141952	2.026767	4.156423	H	2.008089	-5.322284	5.663742
C	2.952657	0.483937	2.926934	H	-0.050724	-4.337213	2.017002
C	4.442908	0.857033	2.841613	H	4.238316	-0.284885	5.414399
C	5.188523	1.241701	4.154027	H	5.862515	0.220837	5.951348
C	6.632119	1.623269	3.781417	H	5.682422	-0.858270	4.547400
C	4.533523	2.419120	4.892184	H	4.565454	3.340609	4.293664
C	5.238468	0.005027	5.069616	H	5.076478	2.610575	5.831982
C	0.658277	-2.534379	2.791374	H	3.484010	2.209075	5.135707
C	0.838091	-4.046610	2.593279	H	7.135745	0.812560	3.232782
C	0.886877	-4.971476	3.842678	H	7.209861	1.829374	4.696017
C	2.055049	-4.654489	4.788065	H	6.665256	2.528623	3.156009
C	1.025466	-6.422569	3.348878	H	4.935383	-0.050772	2.458434
C	-0.450442	-4.837668	4.593171	H	-2.693184	4.239244	4.758939
C	-2.229455	-0.303138	2.917902	H	-1.559069	3.060329	5.458726
C	-3.752031	-0.528520	2.958905	H	-1.855760	4.616585	6.278052
C	-4.403699	-0.736384	4.366395	H	0.605234	5.240680	6.296474
C	-4.214187	0.550144	5.192082	H	0.995484	3.663732	5.562111
C	-5.918081	-0.955405	4.190638	H	1.558711	5.169216	4.795468
C	-3.829547	-1.952316	5.111276	H	-1.872363	6.422741	3.806951
C	-0.020326	2.646381	3.074292	H	-0.132903	6.806067	3.770140
C	-0.338367	4.151824	3.130502	H	-1.013820	6.768629	5.320096
C	-0.582887	4.793023	4.531516	H	0.555392	4.632287	2.704280
C	0.722900	4.702900	5.342312	Br	-4.378726	-6.919012	-1.618653
C	-0.917310	6.282950	4.336551	Br	-2.154034	-5.572992	0.470461
C	-1.739364	4.129868	5.296151	Br	-7.156857	-5.262436	-2.337678
H	-4.171809	0.396664	2.539413	Br	-7.714588	-2.286107	-0.941309
H	-6.391158	-0.132735	3.635127	Br	2.338865	-6.103285	-2.648210
H	-6.391929	-1.016086	5.182546	Br	5.460399	-5.438265	-3.625863
H	-6.143286	-1.897662	3.667554	Br	7.523274	-3.840577	-1.582150
H	-4.320318	-2.043936	6.093702	Br	6.454392	-2.861704	1.419557
H	-4.020907	-2.887454	4.563087	Br	6.865069	1.709928	-2.373240
H	-2.748734	-1.861610	5.270268	Br	5.619802	4.244308	-4.146847
H	-4.764765	0.462398	6.142101	Br	3.409246	6.288616	-2.768307

Br	2.208912	5.620316	0.267411
Br	-1.887123	7.492927	-1.374549
Br	-4.689321	6.601908	-2.954759
Br	-6.446237	4.017697	-1.857624
Br	-5.333816	2.234471	0.727000
C	0.603125	0.113334	-0.587860
C	0.652235	1.371925	-1.362246
C	1.419910	1.511496	-2.544039
C	-0.132384	2.481690	-0.976744
C	1.457028	2.711582	-3.257888
H	2.009451	0.672229	-2.905945
C	-0.107355	3.672657	-1.694723
H	-0.750339	2.402755	-0.087544
C	0.691996	3.798769	-2.835609
H	2.080120	2.789293	-4.152110
H	-0.706336	4.518541	-1.362150
H	0.712861	4.740079	-3.387499
C	1.744933	-0.837063	-0.782283
O	1.710171	-2.051286	-0.750153
O	2.915739	-0.175496	-0.924254
C	4.091470	-0.977805	-0.969289
H	3.925266	-1.882056	-1.568894
H	4.388729	-1.256158	0.048044
C	-0.587266	-0.632710	-3.537461
C	-1.423213	0.475812	-3.546505
C	-2.292131	0.769042	-2.456074
C	-2.034829	0.125294	-1.268525
C	-1.012048	-0.894187	-1.172958
C	-0.546087	-1.464406	-2.415830
H	-0.092881	-0.935104	-4.463007
H	-1.510224	1.068127	-4.460677
H	-2.581903	0.368199	-0.356892
H	-1.081726	-1.567469	-0.317895
C	-0.223275	-2.929229	-2.567160
H	-0.243883	-3.405721	-1.581800
H	0.798199	-3.064267	-2.951190
C	-3.538355	1.582055	-2.702433
H	-3.297835	2.462365	-3.316906
H	-3.919910	1.948567	-1.743747
C	-4.696182	0.755135	-3.425673
C	-1.230781	-3.664023	-3.544539
C	-2.527177	-2.898752	-3.708159
C	-2.832097	-2.204411	-4.885383
C	-3.309734	-2.617352	-2.576272
C	-3.690611	-1.096029	-4.861044
H	-2.277184	-2.428006	-5.800920
C	-4.183349	-1.534902	-2.559409
H	-3.130666	-3.169592	-1.655425
C	-4.286294	-0.676472	-3.663619
H	-3.791048	-0.479014	-5.758698
H	-4.678356	-1.256578	-1.628827
H	-5.588933	0.796438	-2.784325
H	-4.949587	1.248636	-4.374792
H	-1.402410	-4.672368	-3.135891
H	-0.760987	-3.792822	-4.530431
H	4.877868	-0.363847	-1.419597

TBP-TS2-OMe

Rh	-0.276548	0.053835	1.699526
Rh	-0.199913	0.224710	4.156630
N	-3.629427	3.216372	1.734329
O	-4.345871	1.247859	2.721058
O	-3.182683	4.852488	0.159367
C	-4.393920	2.052090	1.820517
C	-5.222973	2.014389	0.569685
C	-6.212593	1.125569	0.168952
C	-6.798675	1.313398	-1.105403
C	-6.389095	2.383978	-1.931878
C	-5.400125	3.295255	-1.489967
C	-4.834832	3.089253	-0.237363
C	-3.787325	3.868344	0.505830
N	2.910334	3.583379	1.763534
O	0.822778	4.233159	2.521536
O	4.809378	3.335977	0.466618
C	1.756557	4.370873	1.768191
C	1.924204	5.346574	0.639272
C	1.096668	6.374976	0.203786
C	1.471443	7.074522	-0.970417
C	2.655394	6.733722	-1.663368
C	3.497586	5.700107	-1.183748
C	3.110504	5.026667	-0.031528
C	3.764741	3.894477	0.705496
N	3.304899	-3.031078	2.151139
O	3.792149	-0.831490	2.686444
O	3.266793	-5.075253	1.056802

C	4.043157	-1.846795	2.082101	C	3.449185	-5.071289	4.227702
C	5.161876	-2.114591	1.115690	C	3.387250	-2.804778	5.268724
C	6.183222	-1.288897	0.659300	C	-2.346367	-1.401054	3.161795
C	7.116507	-1.833383	-0.257836	C	-3.512006	-2.403432	3.228954
C	6.979622	-3.161561	-0.720930	C	-3.895620	-2.979304	4.627814
C	5.904949	-3.970550	-0.275127	C	-4.443963	-1.831686	5.495025
C	5.021115	-3.427009	0.649200	C	-5.022163	-4.010434	4.435372
C	3.782267	-4.003127	1.269373	C	-2.714140	-3.666587	5.329762
N	-3.287808	-3.421750	2.205751	H	1.556697	-4.023732	2.547311
O	-1.049454	-3.878518	2.580628	H	2.939677	-5.820339	3.603806
O	-5.409401	-3.367478	1.285955	H	3.669407	-5.530234	5.203968
C	-2.049811	-4.009149	1.918438	H	4.415659	-4.832517	3.757352
C	-2.257936	-4.803368	0.661091	H	3.645463	-3.252951	6.241779
C	-1.344714	-5.479106	-0.138435	H	4.332771	-2.536761	4.772693
C	-1.823586	-6.064523	-1.335089	H	2.819914	-1.883999	5.449682
C	-3.186966	-5.967661	-1.694093	H	1.586883	-4.738902	6.135124
C	-4.097399	-5.272285	-0.862908	H	0.662641	-3.391377	5.421765
C	-3.604951	-4.694254	0.301678	H	0.724243	-4.963393	4.593075
C	-4.272257	-3.776942	1.284287	H	3.480338	1.148370	5.174337
O	-1.434022	1.728671	1.751957	H	4.903596	2.083950	5.701644
O	-1.324059	1.945070	3.991592	H	4.972341	1.108622	4.211978
O	1.432632	1.245608	1.703610	H	5.800064	3.255550	3.036349
O	1.497893	1.332014	3.950826	H	5.621716	4.114701	4.584778
O	0.945778	-1.599705	1.863219	H	4.826968	4.744035	3.129342
O	0.915402	-1.496314	4.110753	H	1.999484	3.318834	5.153573
O	-1.951688	-1.115383	1.995072	H	2.644986	4.785025	4.377686
O	-1.891952	-0.930103	4.233538	H	3.441409	4.130733	5.820877
C	-1.703534	2.301593	2.849138	H	3.914312	1.859273	2.191171
C	-2.560488	3.562914	2.668297	H	-1.180021	4.060302	5.065161
C	-3.035150	4.341385	3.928219	H	-2.108604	5.519570	5.502045
C	-3.873836	5.539799	3.449652	H	-1.158769	5.475146	3.993769
C	-3.884026	3.487871	4.882093	H	-4.817177	3.152019	4.407415
C	-1.793792	4.876793	4.664618	H	-4.156996	4.088086	5.765321
C	1.924448	1.625814	2.810138	H	-3.335207	2.600291	5.222115
C	3.183637	2.500199	2.704225	H	-3.312459	6.174724	2.746606
C	3.853183	2.984941	4.028922	H	-4.164409	6.161157	4.311005
C	2.921108	3.851712	4.890368	H	-4.797085	5.214885	2.945619
C	5.094526	3.819926	3.664343	H	-1.910774	4.245380	2.100013
C	4.324663	1.754014	4.824565	H	-2.347279	-4.526637	4.751000
C	1.273174	-2.002319	3.018070	H	-1.876099	-2.975425	5.482061
C	2.165123	-3.253993	3.042675	H	-3.039186	-4.040557	6.314153
C	2.581984	-3.816381	4.438275	H	-4.824913	-2.233941	6.447140
C	1.308667	-4.245941	5.190184	H	-3.672063	-1.085134	5.717602

H	-5.278789	-1.319752	4.988358
H	-4.680939	-4.886759	3.863044
H	-5.886678	-3.576062	3.911676
H	-5.361836	-4.370962	5.418806
H	-4.385497	-1.837738	2.867718
Br	8.529148	-0.748767	-0.892083
Br	6.240510	0.530956	1.160482
Br	8.203880	-3.857567	-1.979493
Br	5.651813	-5.725259	-0.926936
Br	5.097316	5.230894	-2.076923
Br	3.127469	7.655518	-3.245482
Br	0.354986	8.455229	-1.619923
Br	-0.490891	6.789083	1.134332
Br	-4.850829	4.757269	-2.556257
Br	-7.146548	2.596994	-3.651148
Br	-8.116452	0.097699	-1.705829
Br	-6.731178	-0.302537	1.297331
Br	-5.925424	-5.099853	-1.317376
Br	-3.807404	-6.749109	-3.302242
Br	-0.608414	-6.972281	-2.469334
Br	0.483371	-5.531353	0.332055
C	-0.548507	-0.075037	-0.479017
C	-0.694159	1.170623	-1.255228
C	-0.036666	2.351268	-0.847790
C	-1.474203	1.240603	-2.434453
C	-0.210497	3.546669	-1.542833
H	0.603462	2.318431	0.030811
C	-1.669379	2.441383	-3.113736
H	-1.937087	0.340926	-2.828693
C	-1.043664	3.606042	-2.662953
H	0.296462	4.445827	-1.200518
H	-2.308951	2.462051	-3.999101
H	-1.195551	4.554793	-3.182811
C	-1.595550	-1.118032	-0.645673
O	-1.450688	-2.318953	-0.605712
O	-2.841444	-0.557809	-0.765242
C	-3.909597	-1.429646	-1.058247
H	-4.762267	-1.201142	-0.409475
H	-3.609785	-2.473782	-0.923631
C	-4.317456	-1.253427	-2.507016
F	-3.319016	-1.611325	-3.346204
F	-5.378434	-2.018436	-2.791320
F	-4.633353	0.018360	-2.804440
C	1.724312	0.589690	-3.272774
C	0.824924	-0.453501	-3.458122
C	0.665999	-1.419002	-2.463215
C	1.088094	-1.046458	-1.135350
C	2.134888	-0.059678	-1.018747
C	2.524332	0.698043	-2.101111
H	1.916737	1.277476	-4.100347
H	1.069426	-1.815099	-0.362055
H	2.607397	0.067381	-0.044337
C	3.841899	1.424820	-2.179866
H	4.158486	1.759858	-1.185210
H	3.731571	2.321568	-2.806248
C	0.244553	-2.823577	-2.826082
H	-0.774877	-2.831296	-3.243357
H	0.214424	-3.424110	-1.911872
C	1.225834	-3.494103	-3.869543
C	5.002284	0.517070	-2.792184
C	4.488878	-0.811816	-3.287707
C	3.941305	-0.961988	-4.579859
C	4.228273	-1.828053	-2.366691
C	3.012174	-1.985356	-4.839923
C	3.308010	-2.845306	-2.612855
H	4.648601	-1.729713	-1.370409
C	2.596182	-2.852139	-3.820018
H	2.469552	-1.992667	-5.785246
H	3.040222	-3.539894	-1.813575
H	1.266098	-4.568555	-3.632425
H	0.813319	-3.401425	-4.884683
H	5.748085	0.348082	-2.003441
H	5.499444	1.073156	-3.596882
H	0.372734	-0.597358	-4.441066
O	4.242574	0.014142	-5.473405
C	3.678522	-0.030948	-6.770098
H	4.091548	0.826180	-7.318899
H	3.948459	-0.960835	-7.299787
H	2.578617	0.058914	-6.742111

TBP-TS2

Rh	0.168556	0.155590	1.724596
Rh	0.183213	0.054059	4.184220
N	4.110785	2.427801	1.850950
O	2.256620	3.676016	2.456850

O	5.798134	1.450618	0.613714
C	3.126656	3.407436	1.664408
C	3.392545	4.000057	0.309754
C	2.749381	5.028198	-0.370523
C	3.228828	5.365820	-1.660537
C	4.322006	4.675340	-2.228703
C	4.980344	3.652129	-1.504179
C	4.488450	3.329224	-0.245378
C	4.931353	2.286641	0.734801
N	2.455424	-3.891947	1.848076
O	3.713109	-2.243099	2.880220
O	1.626933	-5.343197	0.244015
C	3.569188	-3.065355	2.006969
C	4.478700	-3.377402	0.853750
C	5.750353	-2.906176	0.548967
C	6.315759	-3.276069	-0.695693
C	5.590907	-4.089002	-1.597290
C	4.309302	-4.582908	-1.250348
C	3.785844	-4.227468	-0.014233
C	2.483347	-4.588479	0.638463
N	-3.952876	-2.209042	1.979053
O	-2.004392	-3.378509	2.419830
O	-5.935974	-1.508364	1.001544
C	-3.036385	-3.251567	1.806463
C	-3.615036	-4.134261	0.737949
C	-3.092068	-5.261617	0.112974
C	-3.890548	-5.905615	-0.864295
C	-5.160981	-5.392652	-1.210061
C	-5.649855	-4.213411	-0.596339
C	-4.857840	-3.605673	0.370575
C	-5.047601	-2.319985	1.119893
N	-2.213660	4.152832	2.189741
O	-3.358275	2.196564	2.667238
O	-1.537475	6.132748	1.196050
C	-3.215087	3.195017	2.003107
C	-4.023999	3.671067	0.829229
C	-5.119270	3.099859	0.191955
C	-5.665363	3.781651	-0.923580
C	-5.086653	4.983331	-1.389249
C	-3.961747	5.538255	-0.732122
C	-3.462178	4.871135	0.379631
C	-2.289261	5.189220	1.258492
O	2.124776	0.711878	1.883450
O	2.161023	0.626579	4.131616
O	0.690458	-1.816176	1.793518
O	0.697709	-1.928138	4.041407
O	-1.825863	-0.436479	1.807301
O	-1.781302	-0.481859	4.056701
O	-0.422280	2.130396	1.970970
O	-0.353709	2.024298	4.214535
C	2.669760	0.882538	3.013069
C	4.099896	1.436808	2.925650
C	4.803846	1.898880	4.234764
C	6.187695	2.455509	3.855570
C	4.017422	2.982830	4.987032
C	5.006281	0.668594	5.137667
C	0.857681	-2.414749	2.893920
C	1.283893	-3.880142	2.723196
C	1.427369	-4.775630	3.986806
C	2.499315	-4.275751	4.966806
C	1.804246	-6.192678	3.518965
C	0.059305	-4.842318	4.689436
C	-2.340416	-0.650963	2.945048
C	-3.805273	-1.124227	2.949124
C	-4.447976	-1.449502	4.337144
C	-4.494121	-0.156982	5.173604
C	-5.900021	-1.914310	4.119084
C	-3.697020	-2.559671	5.089674
C	-0.596490	2.606675	3.127518
C	-1.131310	4.048856	3.168441
C	-1.483060	4.656040	4.561681
C	-0.189355	4.756545	5.390431
C	-2.022770	6.082443	4.351932
C	-2.543893	3.838193	5.315041
H	-4.362576	-0.277733	2.523404
H	-6.487471	-1.176195	3.553865
H	-6.383984	-2.060591	5.097056
H	-5.951755	-2.876262	3.586202
H	-4.187736	-2.740620	6.059610
H	-3.716810	-3.508016	4.531373
H	-2.650145	-2.291719	5.274803
H	-5.049570	-0.342032	6.106634
H	-3.490781	0.199958	5.432513
H	-5.012324	0.646949	4.626638
H	-0.238119	-3.863535	5.086555
H	0.107642	-5.556493	5.526727

H	-0.727563	-5.179394	3.997538
H	1.062851	-6.599599	2.814248
H	1.855858	-6.870177	4.385551
H	2.788016	-6.210217	3.024907
H	2.295369	-3.249551	5.296644
H	3.503640	-4.299673	4.518961
H	2.518072	-4.931217	5.852732
H	0.479186	-4.313584	2.114533
H	4.048836	0.254547	5.477536
H	5.598352	0.950250	6.022776
H	5.552294	-0.128546	4.607678
H	3.922732	3.901597	4.390836
H	4.547403	3.240695	5.918275
H	3.007551	2.640601	5.247745
H	6.782720	1.717158	3.296108
H	6.744321	2.721581	4.767650
H	6.106229	3.363505	3.238533
H	4.693390	0.598891	2.526919
H	-3.499189	3.817363	4.769658
H	-2.219795	2.802924	5.477179
H	-2.734409	4.301425	6.296653
H	-0.393695	5.287625	6.333600
H	0.218505	3.767644	5.631346
H	0.583669	5.323888	4.846643
H	-2.979602	6.083715	3.807302
H	-1.311576	6.709391	3.794197
H	-2.202442	6.553581	5.330808
H	-0.313290	4.652821	2.747289
Br	-3.212965	-7.436548	-1.743260
Br	-1.311471	-5.789742	0.446321
Br	-6.199798	-6.246132	-2.537407
Br	-7.311625	-3.458644	-1.085793
Br	3.308810	-5.668169	-2.433371
Br	6.325614	-4.522380	-3.283647
Br	8.034888	-2.641417	-1.158186
Br	6.676636	-1.798088	1.766302
Br	6.510199	2.776841	-2.191468
Br	4.917299	5.106453	-3.972396
Br	2.405257	6.780443	-2.610255
Br	1.268380	5.902951	0.397636
Br	-3.122662	7.113350	-1.358346
Br	-5.792743	5.850595	-2.914082
Br	-7.168169	3.048574	-1.808593
Br	-5.777064	1.415012	0.739430
C	0.438455	0.201272	-0.528453
C	0.347043	1.463844	-1.290908
C	1.089535	1.697288	-2.474118
C	-0.559604	2.475961	-0.901399
C	0.998144	2.900587	-3.176572
H	1.754052	0.930021	-2.856054
C	-0.665278	3.668241	-1.610013
H	-1.168853	2.323287	-0.016645
C	0.119380	3.893882	-2.745926
H	1.611006	3.050226	-4.068518
H	-1.356380	4.439792	-1.273888
H	0.038319	4.837299	-3.288553
C	1.666006	-0.624302	-0.725171
O	1.762346	-1.829816	-0.686778
O	2.788321	0.158269	-0.884224
C	3.985925	-0.526492	-1.187880
H	3.944124	-1.558513	-0.831669
H	4.824764	0.005415	-0.724243
C	4.205972	-0.567384	-2.686741
F	4.221479	0.658902	-3.238166
F	5.380459	-1.156532	-2.963894
F	3.242127	-1.263623	-3.326102
C	-0.625317	-0.626962	-3.494356
C	-1.583092	0.377166	-3.499395
C	-2.499775	0.545544	-2.420104
C	-2.188394	-0.083513	-1.238268
C	-1.054683	-0.978663	-1.141829
C	-0.506656	-1.468910	-2.386304
H	-0.078970	-0.850122	-4.412858
H	-1.721913	0.974808	-4.403501
H	-2.776543	0.076051	-0.333597
H	-1.058113	-1.667973	-0.296763
C	-0.006559	-2.880688	-2.557771
H	-0.004296	-3.379802	-1.582996
H	1.036147	-2.880183	-2.907102
C	-3.828849	1.208579	-2.680847
H	-3.682193	2.138647	-3.250054
H	-4.281627	1.482334	-1.722613
C	-4.850087	0.277771	-3.478741
C	-0.888640	-3.701623	-3.585232
C	-2.262902	-3.091540	-3.769858
C	-2.618358	-2.413634	-4.941882

C	-3.101215	-2.927430	-2.654364
C	-3.599597	-1.412041	-4.918507
H	-2.018896	-2.550836	-5.846239
C	-4.097422	-1.956986	-2.640009
H	-2.878410	-3.476139	-1.741003
C	-4.269987	-1.091281	-3.730175
H	-3.749053	-0.790897	-5.806370
H	-4.649924	-1.761426	-1.719803
H	-5.771067	0.202864	-2.882186
H	-5.113173	0.765382	-4.428249
H	-0.948575	-4.735549	-3.210128
H	-0.378804	-3.742757	-4.558591

TBP-TS3-Me

Rh	-0.138494	-0.154094	1.638669
Rh	0.005993	-0.212828	4.093409
N	1.779005	-4.473043	1.684460
O	3.259206	-2.851079	2.407905
O	0.746277	-6.107409	0.406167
C	2.976533	-3.758492	1.661646
C	3.775707	-4.327876	0.525680
C	5.060938	-4.037803	0.086238
C	5.521660	-4.682781	-1.086656
C	4.695181	-5.600600	-1.773505
C	3.401503	-5.906388	-1.286819
C	2.972726	-5.264177	-0.132383
C	1.683235	-5.377994	0.625400
N	-4.358177	-2.163432	2.049684
O	-2.526793	-3.566629	2.234951
O	-6.339271	-1.193672	1.354489
C	-3.513894	-3.206338	1.642788
C	-4.118390	-3.743476	0.376894
C	-3.649500	-4.709544	-0.505327
C	-4.407878	-4.953197	-1.676262
C	-5.588839	-4.223187	-1.941032
C	-6.035428	-3.234031	-1.033394
C	-5.291272	-3.026941	0.121697
C	-5.457773	-2.010304	1.209264
N	-2.212812	4.004527	1.995588
O	-3.571852	2.223220	2.583803
O	-1.265001	5.777149	0.851895
C	-3.315500	3.154556	1.859820
C	-4.055640	3.641123	0.645553
C	-5.225713	3.176075	0.055261
C	-5.660102	3.809357	-1.136304
C	-4.947061	4.904732	-1.673272
C	-3.784959	5.392347	-1.025750
C	-3.350925	4.729691	0.116901
C	-2.147095	4.961164	0.981231
N	4.329781	1.543664	1.752134
O	3.134423	3.196514	2.844346
O	5.413542	0.353492	0.089155
C	3.866219	2.842873	1.950766
C	4.406068	3.649489	0.802626
C	4.278756	5.001038	0.509025
C	4.805466	5.466471	-0.721346
C	5.424220	4.568959	-1.621354
C	5.562446	3.198875	-1.289904
C	5.054710	2.768765	-0.070322
C	4.998359	1.395145	0.534334
O	0.399028	-2.130662	1.686942
O	0.340376	-2.237254	3.932927
O	-2.131255	-0.677253	1.892036
O	-1.992602	-0.600063	4.133503
O	-0.703014	1.813982	1.812937
O	-0.396818	1.804261	4.042708
O	1.856038	0.421696	1.715462
O	2.026033	0.108806	3.935104
C	0.475271	-2.744141	2.788569
C	0.705929	-4.258792	2.654264
C	0.873034	-5.092958	3.961212
C	1.111270	-6.563802	3.574132
C	2.050301	-4.616484	4.826304
C	-0.443407	-5.018287	4.755724
C	-2.604984	-0.813182	3.055457
C	-4.080316	-1.241284	3.145623
C	-4.605555	-1.727555	4.536404
C	-3.772244	-2.882557	5.113663
C	-6.058385	-2.208435	4.369638
C	-4.614885	-0.532791	5.507766
C	-0.723254	2.351453	2.960439
C	-1.143839	3.830925	2.974627
C	-1.428578	4.502305	4.353832
C	-0.111418	4.562425	5.148957
C	-1.897205	5.945510	4.095171

C	-2.507746	3.766696	5.163118
C	2.510319	0.324823	2.798622
C	4.035312	0.419748	2.634246
C	4.943797	0.367800	3.903241
C	4.782327	-1.008867	4.572571
C	6.404116	0.507581	3.435409
C	4.642584	1.475991	4.924177
H	-0.285668	4.368041	2.538841
H	-1.162343	6.511287	3.502495
H	-2.035191	6.465732	5.055653
H	-2.860650	5.973728	3.563145
H	-2.638082	4.265230	6.137187
H	-3.479931	3.781770	4.649525
H	-2.234766	2.719434	5.346027
H	-0.260804	5.147422	6.070214
H	0.242103	3.562149	5.426744
H	0.682359	5.054883	4.563122
H	-3.601375	-0.175304	5.724503
H	-5.090295	-0.829621	6.456189
H	-5.193793	0.308105	5.091312
H	-6.700589	-1.424463	3.942483
H	-6.465463	-2.488490	5.353699
H	-6.124846	-3.095850	3.721717
H	-2.718974	-2.602420	5.237231
H	-3.814406	-3.771160	4.467729
H	-4.173210	-3.166802	6.100087
H	-4.644885	-0.329298	2.893693
H	-0.655789	-3.997689	5.095076
H	-0.381238	-5.673705	5.638988
H	-1.292305	-5.356307	4.141009
H	3.010403	-4.724545	4.299775
H	2.105829	-5.230365	5.739974
H	1.937430	-3.565861	5.121080
H	0.310098	-6.948241	2.925695
H	1.143886	-7.182827	4.484285
H	2.070056	-6.700352	3.050323
H	-0.206415	-4.615729	2.153188
H	4.850563	2.476723	4.520978
H	3.595082	1.448186	5.250713
H	5.284714	1.335375	5.808810
H	5.477253	-1.084287	5.423984
H	3.761184	-1.158604	4.943869
H	5.006262	-1.823715	3.870104
H	6.603637	1.498520	2.999342
H	6.663927	-0.251408	2.681292
H	7.083774	0.378751	4.291756
H	4.281750	-0.471516	2.036794
Br	-7.207973	3.161986	-2.011251
Br	-6.171262	1.732075	0.814923
Br	-5.533777	5.730180	-3.270552
Br	-2.850748	6.902305	-1.676563
Br	-7.562022	-2.171542	-1.389209
Br	-6.576658	-4.546920	-3.523801
Br	-3.803921	-6.258876	-2.908122
Br	-2.015889	-5.583021	-0.168806
Br	2.262927	-7.117822	-2.187364
Br	5.303922	-6.416532	-3.368250
Br	7.246069	-4.275229	-1.749813
Br	6.146913	-2.823421	1.038944
Br	6.365028	1.965117	-2.477737
Br	6.050142	5.184511	-3.296016
Br	4.631461	7.293430	-1.171209
Br	3.397228	6.159874	1.713736
C	-0.251782	-0.393597	-0.568537
C	0.800504	-1.239204	-1.186886
C	0.510641	-2.237038	-2.149018
C	2.158534	-1.011643	-0.885725
C	1.526111	-2.954191	-2.774593
H	-0.524254	-2.456052	-2.404003
C	3.180849	-1.721198	-1.525801
H	2.409377	-0.274600	-0.130629
C	2.870327	-2.687707	-2.479899
H	1.269394	-3.722591	-3.508025
H	4.218325	-1.494950	-1.272637
H	3.663302	-3.233583	-2.994675
C	-1.660640	-0.836931	-0.786269
O	-2.012610	-1.997089	-0.707843
O	-2.540652	0.160618	-1.011958
C	-3.901012	-0.206906	-1.214610
H	-4.398899	-0.338383	-0.249301
H	-3.976115	-1.131200	-1.802841
C	1.957668	1.144806	-3.115911
C	2.132482	1.829825	-1.899915
C	1.045470	2.144125	-1.107261
C	-0.180362	1.425820	-1.366870
C	-0.369538	0.927732	-2.704554

C	0.680249	0.821635	-3.606620
H	2.826633	0.995824	-3.761837
H	3.105391	2.272786	-1.692105
H	-1.065986	1.793475	-0.855315
H	-1.374337	0.627005	-2.999372
C	0.442410	0.618643	-5.084806
H	-0.335351	-0.142719	-5.243727
H	1.365908	0.240974	-5.546617
C	1.026255	3.380139	-0.246691
H	1.822209	3.363460	0.507189
H	0.085846	3.394638	0.308953
C	1.163089	4.709385	-1.093826
C	0.003449	1.954747	-5.839901
C	0.165921	3.161831	-4.951539
C	1.424304	3.743891	-4.743548
C	-0.856200	3.493054	-4.047549
C	1.708081	4.419671	-3.552141
H	2.233677	3.551972	-5.453978
C	-0.567032	4.154108	-2.853610
H	-1.866262	3.108605	-4.213798
C	0.749312	4.519830	-2.533725
H	2.732246	4.750853	-3.360928
H	-1.351777	4.269701	-2.104233
H	0.560453	5.476422	-0.587833
H	2.205866	5.046979	-1.072133
H	-1.048084	1.853750	-6.146663
H	0.607202	2.047599	-6.754886
H	-4.372156	0.623510	-1.754691

TBP-TS3-OMe

Rh	0.172221	0.062478	1.732625
Rh	0.387249	0.033292	4.180909
N	3.753327	2.960208	1.573691
O	1.932166	4.021907	2.532615
O	5.218037	2.136189	-0.015739
C	2.734575	3.913860	1.635737
C	2.848626	4.712682	0.371389
C	2.154232	5.840463	-0.046079
C	2.480337	6.387949	-1.309626
C	3.473492	5.790648	-2.116219
C	4.172695	4.643800	-1.667427
C	3.844460	4.127801	-0.419764
C	4.396787	2.949929	0.333618
N	3.278089	-3.548578	1.829478
O	4.261743	-1.661027	2.738734
O	2.734058	-5.266074	0.371695
C	4.265096	-2.568972	1.941186
C	5.253483	-2.855405	0.847398
C	6.428345	-2.202660	0.496691
C	7.091797	-2.615812	-0.683957
C	6.568617	-3.667077	-1.470432
C	5.379404	-4.331784	-1.082860
C	4.746244	-3.910308	0.079989
C	3.466915	-4.370807	0.716960
N	-3.347595	-3.059727	2.276976
O	-1.168828	-3.837124	2.386957
O	-5.553606	-2.742987	1.650636
C	-2.249461	-3.813329	1.849539
C	-2.716653	-4.556644	0.631256
C	-2.009982	-5.354039	-0.263399
C	-2.730534	-5.924330	-1.343041
C	-4.118000	-5.698156	-1.488190
C	-4.809232	-4.865772	-0.573390
C	-4.082483	-4.295493	0.464617
C	-4.488098	-3.292934	1.504184
N	-2.909630	3.526710	2.309403
O	-3.758830	1.576122	3.226631
O	-2.466718	5.257342	0.838902
C	-3.809930	2.463612	2.408917
C	-4.775980	2.635956	1.269838
C	-5.909179	1.907150	0.925496
C	-6.584306	2.258378	-0.270054
C	-6.090737	3.293953	-1.095867
C	-4.948645	4.038336	-0.711283
C	-4.326572	3.704844	0.486300
C	-3.131302	4.305216	1.169621
O	1.911044	1.109655	1.746086
O	2.244570	0.894402	3.961392
O	1.255994	-1.689605	1.755726
O	1.208419	-1.832338	4.000104
O	-1.586501	-1.023213	1.998870
O	-1.452495	-0.840807	4.235566
O	-0.930680	1.772010	2.025137
O	-0.481170	1.900596	4.221891
C	2.582590	1.258186	2.807704

C	3.948861	1.910363	2.567375
C	4.807402	2.347179	3.790590
C	6.106490	2.968994	3.247301
C	4.096525	3.370975	4.688158
C	5.171864	1.097190	4.612275
C	1.484946	-2.271803	2.854221
C	2.121659	-3.664025	2.714976
C	2.416957	-4.482351	4.009390
C	3.396957	-3.775461	4.958304
C	3.023770	-5.834418	3.591435
C	1.084906	-4.759211	4.728526
C	-1.996676	-1.242427	3.176062
C	-3.305684	-2.042464	3.322734
C	-3.651602	-2.590166	4.747830
C	-3.962795	-1.403341	5.678323
C	-4.923036	-3.452973	4.651650
C	-2.522494	-3.453562	5.330984
C	-0.986518	2.333264	3.158177
C	-1.717359	3.685347	3.141827
C	-1.967733	4.417036	4.492162
C	-0.602499	4.785034	5.102008
C	-2.729803	5.719285	4.189314
C	-2.784292	3.578650	5.486992
H	-4.100997	-1.329250	3.052248
H	-5.764865	-2.893787	4.218625
H	-5.213291	-3.784684	5.660559
H	-4.762586	-4.356457	4.043538
H	-2.816764	-3.818683	6.328125
H	-2.322396	-4.332315	4.700745
H	-1.589272	-2.886973	5.432811
H	-4.306451	-1.780538	6.654612
H	-3.084481	-0.768025	5.840644
H	-4.766653	-0.775364	5.260713
H	0.621787	-3.834675	5.092257
H	1.261692	-5.422403	5.590203
H	0.369532	-5.255587	4.055512
H	2.371041	-6.372618	2.887600
H	3.163025	-6.467252	4.481729
H	4.010470	-5.712660	3.118271
H	3.024391	-2.790248	5.265126
H	4.385714	-3.640398	4.495293
H	3.539041	-4.391389	5.861169
H	1.378216	-4.231096	2.136872
H	4.289255	0.664455	5.098713
H	5.902494	1.368701	5.390724
H	5.618086	0.316067	3.979083
H	3.914806	4.319799	4.163404
H	4.729116	3.591187	5.563386
H	3.131602	2.989186	5.047215
H	6.641149	2.273860	2.581080
H	6.777332	3.223899	4.082311
H	5.911433	3.893338	2.682095
H	4.523938	1.133419	2.040149
H	-3.795385	3.369476	5.108639
H	-2.295103	2.620311	5.704437
H	-2.891804	4.135005	6.432164
H	-0.753053	5.406930	5.998546
H	-0.033593	3.892547	5.390614
H	0.009490	5.359737	4.388947
H	-3.732036	5.519931	3.779632
H	-2.186419	6.348424	3.467645
H	-2.859497	6.298208	5.116863
H	-1.056766	4.337171	2.548442
Br	-1.802763	-6.975781	-2.613059
Br	-0.147311	-5.587073	-0.062528
Br	-5.058665	-6.460185	-2.939487
Br	-6.654313	-4.501380	-0.765454
Br	4.642521	-5.731360	-2.118081
Br	7.444791	-4.187349	-3.061527
Br	8.673358	-1.728801	-1.215692
Br	7.097905	-0.792926	1.563978
Br	5.516918	3.830756	-2.716416
Br	3.858458	6.500611	-3.827307
Br	1.543515	7.911951	-1.926113
Br	0.802305	6.590056	1.038146
Br	-4.252635	5.418349	-1.800487
Br	-6.947090	3.688382	-2.737067
Br	-8.148186	1.315750	-0.763549
Br	-6.488346	0.467124	1.999450
C	0.321077	0.257792	-0.558680
C	0.377392	1.594652	-1.191815
C	1.151242	1.841784	-2.354580
C	-0.401511	2.667882	-0.711152
C	1.191242	3.095203	-2.957824
H	1.720376	1.035377	-2.808369
C	-0.377130	3.924105	-1.322179

H	-1.015730	2.508657	0.168534
C	0.419843	4.143772	-2.445763
H	1.813520	3.246103	-3.842931
H	-0.986534	4.728944	-0.910948
H	0.430379	5.122563	-2.929480
C	1.454443	-0.662524	-0.858310
O	1.415955	-1.854862	-1.065285
O	2.641276	0.021103	-0.803337
C	3.817374	-0.686303	-1.115286
H	3.700963	-1.756456	-0.918353
H	4.632143	-0.252443	-0.523970
C	4.163760	-0.517556	-2.582766
F	4.353211	0.765041	-2.920003
F	5.293904	-1.188552	-2.870045
F	3.194626	-0.995860	-3.391491
C	-1.960742	1.184619	-3.188632
C	-2.650097	1.101754	-1.965273
C	-2.452853	0.020246	-1.125532
C	-1.244510	-0.742375	-1.329695
C	-0.709789	-0.763347	-2.665871
C	-1.103051	0.158104	-3.625690
H	-2.206701	1.997827	-3.876071
H	-1.113307	-1.649973	-0.742085
H	0.030928	-1.525949	-2.902577
C	-0.813153	-0.039780	-5.095237
H	0.238758	-0.326056	-5.245592
H	-0.972974	0.913094	-5.619216
C	-3.562665	-0.504317	-0.254923
H	-3.859018	0.223861	0.511393
H	-3.187964	-1.374602	0.288881
C	-4.831766	-0.896753	-1.103475
C	-1.734055	-1.154811	-5.757243
C	-2.929508	-1.451497	-4.887134
C	-3.961537	-0.498282	-4.750590
C	-2.845555	-2.449528	-3.912328
C	-4.730165	-0.448507	-3.578615
C	-3.593377	-2.389356	-2.732795
H	-2.069832	-3.214039	-4.009574
C	-4.463344	-1.316558	-2.509378
H	-5.421757	0.378149	-3.419080
H	-3.376802	-3.093239	-1.931529
H	-5.375828	-1.676443	-0.554462
H	-5.505727	-0.033404	-1.163761
H	-1.144029	-2.074657	-5.878593
H	-2.025541	-0.809882	-6.758894
H	-3.475398	1.793532	-1.785988
O	-4.029687	0.444844	-5.726188
C	-4.933873	1.523673	-5.584501
H	-4.696722	2.140664	-4.700573
H	-4.826816	2.141263	-6.486457
H	-5.978688	1.176247	-5.509679

TBP-TS3

Rh	0.093599	-0.190249	1.685924
Rh	0.278231	-0.240699	4.134831
N	3.208614	-3.725848	1.671690
O	4.110205	-1.736949	2.436517
O	2.726021	-5.565615	0.347539
C	4.119824	-2.668145	1.666487
C	5.045590	-2.928225	0.513340
C	6.166604	-2.234444	0.075443
C	6.800047	-2.678711	-1.110137
C	6.307159	-3.802797	-1.810285
C	5.182963	-4.514085	-1.326838
C	4.577841	-4.059488	-0.162278
C	3.393110	-4.588416	0.589734
N	-3.366263	-3.325902	2.099571
O	-1.206359	-4.125503	2.333055
O	-5.518905	-2.958410	1.337693
C	-2.251887	-4.094433	1.732404
C	-2.665582	-4.838307	0.495077
C	-1.926529	-5.651483	-0.356079
C	-2.583022	-6.176400	-1.496576
C	-3.938126	-5.871810	-1.758942
C	-4.662372	-5.023675	-0.887257
C	-4.003223	-4.525274	0.230792
C	-4.453223	-3.526358	1.253532
N	-3.039254	3.255068	2.198042
O	-3.811510	1.144696	2.759170
O	-2.700930	5.270172	1.116116
C	-3.863636	2.133419	2.067698
C	-4.770961	2.430149	0.906544
C	-5.787494	1.673619	0.336427
C	-6.452198	2.201150	-0.798125
C	-6.095878	3.466259	-1.316540

C	-5.078953	4.235850	-0.699086
C	-4.428647	3.691107	0.401926
C	-3.302365	4.228718	1.232011
N	3.756900	2.812119	1.776444
O	2.021095	3.908745	2.845009
O	5.218117	2.096341	0.130988
C	2.835961	3.844047	1.955772
C	3.036234	4.777298	0.793673
C	2.413113	5.979456	0.480689
C	2.729507	6.588243	-0.758817
C	3.636626	5.971128	-1.650430
C	4.280399	4.760076	-1.297649
C	3.971776	4.192816	-0.067148
C	4.436761	2.909892	0.559524
O	1.163965	-1.936968	1.699927
O	1.154043	-2.088514	3.943614
O	-1.670138	-1.248841	1.929266
O	-1.545569	-1.156887	4.170705
O	-0.979232	1.556507	1.906563
O	-0.645313	1.591241	4.132335
O	1.835099	0.922490	1.752470
O	2.121556	0.645436	3.964897
C	1.430307	-2.513598	2.792491
C	2.119398	-3.877888	2.635231
C	2.530656	-4.645023	3.928603
C	3.211640	-5.962867	3.516764
C	3.501711	-3.847332	4.812946
C	1.251684	-4.994950	4.711121
C	-2.081947	-1.519459	3.093345
C	-3.382161	-2.337030	3.173187
C	-3.782740	-2.921789	4.566463
C	-2.678849	-3.796830	5.180875
C	-5.047323	-3.782154	4.391224
C	-4.133928	-1.754649	5.507333
C	-1.120432	2.051476	3.064827
C	-1.918733	3.364899	3.126551
C	-2.312082	3.916481	4.532720
C	-1.026420	4.301785	5.287404
C	-3.145663	5.195208	4.332990
C	-3.137010	2.912804	5.352733
C	2.492077	1.034132	2.831333
C	3.885778	1.655849	2.658370
C	4.757903	1.925760	3.922817
C	5.074962	0.581172	4.602457
C	6.082800	2.552143	3.450730
C	4.091951	2.874581	4.931145
H	-1.256672	4.117495	2.669275
H	-2.606255	5.942968	3.732515
H	-3.372820	5.641822	5.313369
H	-4.105812	4.986106	3.836727
H	-3.361588	3.344476	6.341420
H	-4.096209	2.684987	4.865165
H	-2.597221	1.969236	5.502641
H	-1.288413	4.806766	6.230594
H	-0.411846	3.424615	5.522158
H	-0.413237	4.998471	4.692961
H	-3.262589	-1.123297	5.717944
H	-4.516258	-2.149937	6.461848
H	-4.920586	-1.118890	5.068708
H	-5.868498	-3.212142	3.932582
H	-5.385427	-4.139076	5.376427
H	-4.856702	-4.669779	3.768441
H	-1.748793	-3.234361	5.328659
H	-2.454768	-4.666399	4.546305
H	-3.014113	-4.175648	6.159919
H	-4.171485	-1.623998	2.887354
H	0.734574	-4.096299	5.068044
H	1.509370	-5.617827	5.582429
H	0.549820	-5.564140	4.081719
H	4.446252	-3.636707	4.289297
H	3.748072	-4.437028	5.710859
H	3.067593	-2.892367	5.134084
H	2.571539	-6.561334	2.851607
H	3.427669	-6.561379	4.415466
H	4.169238	-5.786805	3.002640
H	1.366110	-4.491103	2.119153
H	3.946818	3.881308	4.514404
H	3.115398	2.494696	5.257924
H	4.739079	2.973460	5.817737
H	5.784284	0.747409	5.428697
H	4.171137	0.112086	5.009964
H	5.529808	-0.127124	3.894846
H	5.930028	3.543381	2.996865
H	6.592673	1.916835	2.709956
H	6.760529	2.680694	4.308631
H	4.426256	0.909742	2.055891

Br	-7.810848	1.182830	-1.626990
Br	-6.219723	-0.026336	1.037721
Br	-6.964710	4.142071	-2.853805
Br	-4.605720	5.950240	-1.342284
Br	-6.462433	-4.550607	-1.227938
Br	-4.795979	-6.580736	-3.289957
Br	-1.613063	-7.283038	-2.687741
Br	-0.094357	-5.944799	-0.034724
Br	4.490948	-6.017003	-2.241741
Br	7.131648	-4.354143	-3.421090
Br	8.292955	-1.725547	-1.774496
Br	6.812582	-0.747954	1.041692
Br	5.482637	3.894562	-2.473554
Br	3.977807	6.745266	-3.341498
Br	1.897013	8.218524	-1.230120
Br	1.155053	6.742222	1.665938
C	0.049614	-0.468317	-0.527646
C	1.316863	-0.907420	-1.159462
C	1.379737	-1.968554	-2.095526
C	2.512394	-0.206638	-0.899290
C	2.571034	-2.295669	-2.736014
H	0.484466	-2.544532	-2.320025
C	3.707778	-0.527791	-1.551946
H	2.499738	0.590765	-0.164621
C	3.739763	-1.564816	-2.481589
H	2.588154	-3.123226	-3.449400
H	4.605068	0.052153	-1.327034
H	4.664140	-1.808470	-3.008706
C	-1.129933	-1.354958	-0.715386
O	-1.097877	-2.565821	-0.684067
O	-2.309797	-0.679286	-0.840774
C	-3.480235	-1.417616	-1.093589
H	-4.170773	-1.328867	-0.246101
H	-3.251599	-2.473323	-1.283531
C	-4.151753	-0.834980	-2.319166
F	-3.407278	-1.010675	-3.431719
F	-5.336433	-1.417431	-2.525944
F	-4.355890	0.493222	-2.198664
C	1.529886	1.701959	-3.171495
C	1.472132	2.443451	-1.975098
C	0.359676	2.372228	-1.159157
C	-0.537309	1.263994	-1.372867
C	-0.554922	0.678836	-2.684670
C	0.446662	0.924630	-3.614672
H	2.379291	1.858758	-3.841450
H	2.223427	3.214457	-1.808841
H	-1.485558	1.310264	-0.846611
H	-1.387257	0.032780	-2.953404
C	0.253381	0.601913	-5.079148
H	-0.068121	-0.442752	-5.207558
H	1.218730	0.709853	-5.594348
C	-0.104279	3.542232	-0.333307
H	0.655265	3.859983	0.390613
H	-0.969027	3.220503	0.253272
C	-0.492207	4.785809	-1.229727
C	-0.816016	1.545833	-5.786105
C	-1.074281	2.781283	-4.959340
C	-0.107945	3.792446	-4.858169
C	-2.097325	2.767173	-3.998084
C	-0.024366	4.581475	-3.707569
H	0.677434	3.868897	-5.615905
C	-2.011700	3.557226	-2.849236
H	-2.897429	2.026241	-4.073275
C	-0.900208	4.384774	-2.628383
H	0.820331	5.266645	-3.592844
H	-2.749364	3.414509	-2.056894
H	-1.283917	5.332314	-0.699498
H	0.371462	5.458579	-1.300869
H	-1.753695	0.985245	-5.914831
H	-0.439334	1.795424	-6.789725

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Rh	-0.493380	0.016322	1.585630
Rh	-0.574307	-0.179137	4.042177
N	-3.851857	-3.071319	1.265814
O	-1.760078	-3.940932	1.745314
O	-5.755268	-2.392465	0.139134
C	-2.667780	-3.757421	0.970372
C	-2.786123	-4.184346	-0.462305
C	-1.879476	-4.851163	-1.280483
C	-2.258820	-5.074343	-2.627346
C	-3.530498	-4.676315	-3.097199
C	-4.445541	-4.029150	-2.233912
C	-4.035946	-3.766187	-0.933175
C	-4.709773	-2.994957	0.164487

N	-3.921512	3.201151	2.150308
O	-4.666610	1.219355	3.088196
O	-3.536960	4.893462	0.620354
C	-4.791227	2.114780	2.287854
C	-5.823137	2.280884	1.210117
C	-6.961455	1.535882	0.925161
C	-7.701400	1.874109	-0.235498
C	-7.275730	2.927963	-1.076890
C	-6.123680	3.686295	-0.753216
C	-5.428098	3.354430	0.402806
C	-4.196026	3.957671	1.009584
N	3.735502	2.136282	1.827209
O	2.984718	4.316904	2.110489
O	4.446742	0.197090	0.786172
C	3.598173	3.482009	1.489802
C	4.319474	3.654131	0.180743
C	4.606008	4.798373	-0.553943
C	5.224745	4.637152	-1.818576
C	5.551818	3.348123	-2.298411
C	5.297232	2.199557	-1.508833
C	4.683058	2.382470	-0.275751
C	4.303499	1.395524	0.785220
N	2.815171	-3.488407	2.000571
O	3.568418	-1.775473	3.358748
O	2.645667	-5.033041	0.280927
C	3.748951	-2.554868	2.453298
C	4.941611	-2.690449	1.551110
C	6.157973	-2.019683	1.547446
C	7.014329	-2.201574	0.437197
C	6.643016	-3.064082	-0.619924
C	5.433297	-3.796105	-0.558802
C	4.607022	-3.597118	0.540921
C	3.254567	-4.166577	0.861034
O	-2.205187	-1.081849	1.596136
O	-2.379523	-1.159299	3.836017
O	-1.652740	1.702291	1.813315
O	-1.521838	1.648595	4.060008
O	1.261755	1.116048	1.816374
O	1.260788	0.736542	4.036991
O	0.677723	-1.698596	1.656674
O	0.345112	-2.001306	3.860204
C	-2.764121	-1.439297	2.674096
C	-4.050026	-2.253308	2.460113
C	-4.651655	-3.020173	3.675248
C	-5.881230	-3.801878	3.179978
C	-3.653514	-4.001051	4.306170
C	-5.119277	-1.996079	4.725368
C	-1.906769	2.145441	2.975377
C	-2.740022	3.435588	2.976121
C	-3.033080	4.142146	4.330997
C	-3.830856	3.277249	5.317965
C	-3.833346	5.420570	4.024026
C	-1.684748	4.549157	4.952721
C	1.799250	1.114591	2.964734
C	3.285092	1.474456	3.047432
C	3.807770	2.092759	4.396049
C	3.966872	0.942530	5.410583
C	5.197345	2.710474	4.158032
C	2.868705	3.153103	4.996607
C	0.785628	-2.351735	2.735646
C	1.497054	-3.711383	2.596368
C	1.530518	-4.665563	3.830003
C	0.082756	-5.004880	4.224293
C	2.228980	-5.969392	3.401858
C	2.280703	-4.081108	5.036860
H	3.749761	0.477742	2.975211
H	5.873015	2.007998	3.645488
H	5.653398	2.965602	5.126968
H	5.152741	3.636756	3.567144
H	3.320035	3.558219	5.916771
H	2.697406	3.982712	4.300729
H	1.897269	2.715561	5.264075
H	4.354564	1.340434	6.361736
H	3.006708	0.449162	5.605242
H	4.668944	0.178795	5.044912
H	-1.087175	3.672998	5.235649
H	-1.858546	5.154004	5.856462
H	-1.091827	5.158811	4.250778
H	-3.301062	6.070514	3.311949
H	-3.995048	5.991180	4.951635
H	-4.823144	5.189657	3.600587
H	-3.315810	2.333294	5.535348
H	-4.833694	3.041163	4.933818
H	-3.960513	3.829682	6.262675
H	-2.141270	4.145751	2.389315
H	-4.272494	-1.461112	5.171789

H	-5.668725	-2.513509	5.527836
H	-5.792338	-1.246723	4.280504
H	-3.351169	-4.784228	3.596632
H	-4.119971	-4.494795	5.174116
H	-2.747714	-3.485050	4.649340
H	-6.615004	-3.140320	2.694736
H	-6.375081	-4.295686	4.031346
H	-5.602325	-4.583870	2.457305
H	-4.799597	-1.504252	2.158015
H	3.345621	-3.917597	4.816272
H	1.845958	-3.126996	5.358969
H	2.225218	-4.792518	5.876953
H	0.087021	-5.756609	5.029579
H	-0.455242	-4.118787	4.581066
H	-0.474277	-5.416342	3.370271
H	3.288589	-5.804903	3.151797
H	1.739082	-6.426024	2.528664
H	2.196482	-6.694426	4.230057
H	0.920346	-4.220894	1.811915
Br	5.571247	6.159925	-2.880809
Br	4.174968	6.509266	0.123015
Br	6.322575	3.140836	-4.012329
Br	5.775282	0.466565	-2.100007
Br	-5.515613	5.089990	-1.866161
Br	-8.236430	3.328452	-2.654989
Br	-9.255195	0.887370	-0.663630
Br	-7.491111	0.123081	2.058637
Br	-6.183689	-3.552054	-2.809214
Br	-4.019473	-4.987312	-4.900454
Br	-1.035735	-5.916468	-3.802538
Br	-0.201837	-5.393545	-0.620281
Br	4.904865	-4.962526	-1.950993
Br	7.753776	-3.230373	-2.143352
Br	8.648296	-1.253374	0.360131
Br	6.644247	-0.909095	2.996114
C	-0.576389	-0.008456	-0.613425
C	-1.901598	-0.139223	-1.262201
C	-3.041811	0.473424	-0.704657
C	-2.077031	-0.844310	-2.477592
C	-4.294605	0.349396	-1.306771
H	-2.933313	1.041847	0.215168
C	-3.327459	-0.967232	-3.077615
H	-1.219387	-1.312683	-2.955925
C	-4.447455	-0.370162	-2.490914
H	-5.163057	0.808482	-0.842638
H	-3.426902	-1.529981	-4.008558
H	-5.432993	-0.467137	-2.949631
C	0.415339	-1.056683	-0.999203
O	0.104444	-2.207279	-1.231020
O	1.698322	-0.647148	-0.978418
C	2.690237	-1.627051	-1.277992
H	2.342932	-2.622266	-0.981617
H	3.590104	-1.328566	-0.734369
C	-1.699016	3.045400	-1.688656
C	-1.721540	2.501335	-2.982498
C	-0.634109	1.767611	-3.494518
C	0.312268	1.345740	-2.572131
C	0.243375	1.712700	-1.180878
C	-0.621240	2.818164	-0.847267
H	-2.450042	3.789361	-1.418176
H	-2.543331	2.771700	-3.651056
H	1.138676	0.710019	-2.890046
H	1.155329	1.603185	-0.596659
C	-0.241046	3.830882	0.192517
H	0.298715	3.350302	1.017470
H	-1.152929	4.288000	0.592076
C	-0.395637	1.653435	-4.982388
H	-1.328733	1.382564	-5.499363
H	0.322982	0.841241	-5.164025
C	0.170943	2.994047	-5.632798
C	0.660459	5.001800	-0.409482
C	0.833168	4.923162	-1.907714
C	-0.121646	5.452503	-2.786763
C	1.824035	4.096163	-2.462427
C	-0.236442	4.960950	-4.091793
H	-0.878839	6.144059	-2.406531
C	1.739626	3.642145	-3.777397
H	2.604078	3.694639	-1.819347
C	0.623943	3.958927	-4.565390
H	-1.088891	5.268556	-4.704455
H	2.464594	2.906666	-4.136982
H	0.996443	2.720771	-6.307859
H	-0.616099	3.457137	-6.245678
H	1.636225	4.966477	0.087736
H	0.195930	5.959291	-0.132233
H	2.892524	-1.636752	-2.361841

TBP-TS4-OMe

Rh	0.029150	-0.290814	1.795094
Rh	0.158416	-0.341439	4.256528
N	-3.084512	-3.753152	2.017293
O	-0.851475	-4.359702	2.131346
O	-5.293662	-3.581537	1.353629
C	-1.900400	-4.325487	1.534787
C	-2.241011	-4.874384	0.177839
C	-1.426079	-5.442833	-0.795588
C	-2.035280	-5.831902	-2.013880
C	-3.421828	-5.659143	-2.218719
C	-4.227402	-5.074697	-1.213480
C	-3.610177	-4.682468	-0.033188
C	-4.159887	-3.949910	1.152191
N	-3.625608	2.674795	2.303970
O	-4.091922	0.456991	2.781009
O	-3.611598	4.768830	1.316159
C	-4.305362	1.463022	2.148673
C	-5.296230	1.691630	1.039826
C	-6.229986	0.832543	0.470114
C	-6.975327	1.307493	-0.638258
C	-6.794679	2.624001	-1.118091
C	-5.861512	3.491158	-0.499241
C	-5.125637	2.999428	0.571969
C	-4.054649	3.648058	1.397576
N	3.416129	2.969707	1.854089
O	1.594311	3.980518	2.864711
O	4.894795	2.258866	0.222777
C	2.424901	3.942187	1.988922
C	2.586249	4.852697	0.805814
C	1.949077	6.046304	0.493475
C	2.260455	6.660978	-0.743699
C	3.216380	6.083079	-1.610404
C	3.890346	4.890060	-1.247607
C	3.556067	4.295491	-0.036312
C	4.079260	3.052326	0.628397
N	3.493317	-3.516871	1.855601
O	4.277350	-1.525609	2.731412
O	3.122801	-5.304981	0.430439
C	4.354901	-2.425011	1.927483
C	5.317144	-2.581227	0.785388
C	6.394035	-1.795799	0.394263
C	7.020627	-2.095134	-0.839518
C	6.563000	-3.171171	-1.634437
C	5.488139	-3.983276	-1.196138
C	4.890166	-3.670572	0.018498
C	3.730244	-4.305667	0.727729
O	-1.565259	-1.590082	2.010436
O	-1.539817	-1.487449	4.255754
O	-1.305629	1.288487	1.999486
O	-1.002382	1.349232	4.228420
O	1.637093	0.980813	1.850850
O	1.891527	0.755322	4.078331
O	1.327705	-1.874949	1.859108
O	1.251512	-2.076654	4.095692
C	-1.983565	-1.913100	3.158042
C	-3.175001	-2.887673	3.189102
C	-3.454377	-3.643849	4.528712
C	-4.576383	-4.669536	4.288333
C	-2.215513	-4.383128	5.055158
C	-3.957238	-2.629385	5.571947
C	-1.539313	1.736940	3.161781
C	-2.539178	2.907479	3.252153
C	-3.029630	3.334459	4.674578
C	-3.673284	2.178570	5.456369
C	-4.069899	4.457693	4.510957
C	-1.833044	3.910087	5.454645
C	2.255755	1.151446	2.944326
C	3.606675	1.863161	2.785107
C	4.423854	2.249001	4.056495
C	4.832470	0.960261	4.792617
C	5.703582	2.963875	3.585603
C	3.661557	3.171954	5.019393
C	1.601877	-2.453262	2.948473
C	2.390488	-3.763094	2.781741
C	2.816872	-4.538136	4.065008
C	1.544102	-4.993231	4.800668
C	3.594291	-5.794515	3.632668
C	3.705150	-3.705701	5.002533
H	4.217838	1.135637	2.229631
H	6.271985	2.348621	2.870681
H	6.355670	3.169995	4.448353
H	5.481489	3.926167	3.099144
H	4.278985	3.349951	5.914821

H	3.443570	4.150025	4.568490
H	2.712489	2.722317	5.338962
H	5.494449	1.215078	5.635478
H	3.957801	0.427872	5.186309
H	5.370472	0.271282	4.126352
H	-1.081780	3.142462	5.674212
H	-2.183710	4.337541	6.407305
H	-1.341792	4.716881	4.885666
H	-3.666665	5.307515	3.940339
H	-4.370641	4.824710	5.504379
H	-4.980595	4.104247	4.003305
H	-2.981047	1.336679	5.582019
H	-4.579460	1.806068	4.956710
H	-3.969613	2.534883	6.456132
H	-1.996458	3.774812	2.843720
H	-3.187168	-1.890852	5.824779
H	-4.250444	-3.157737	6.493110
H	-4.842681	-2.088464	5.198853
H	-1.870986	-5.146842	4.343774
H	-2.462884	-4.890805	6.001485
H	-1.383390	-3.693423	5.242462
H	-5.483051	-4.194188	3.886372
H	-4.836847	-5.156634	5.240976
H	-4.265803	-5.459868	3.587844
H	-4.051834	-2.249047	2.995405
H	4.655380	-3.428250	4.522888
H	3.202543	-2.785086	5.324860
H	3.949931	-4.299998	5.897894
H	1.817529	-5.629660	5.657240
H	0.966097	-4.139981	5.174126
H	0.893902	-5.581557	4.134605
H	4.548306	-5.539201	3.145779
H	3.009899	-6.413147	2.935079
H	3.830402	-6.405175	4.518106
H	1.696588	-4.411255	2.225558
Br	1.361416	8.246527	-1.241444
Br	0.736511	6.826900	1.719788
Br	3.583835	6.882262	-3.282401
Br	5.191354	4.106292	-2.370750
Br	-5.598914	5.262529	-1.111303
Br	-7.785394	3.236646	-2.608387
Br	-8.191509	0.141218	-1.496559
Br	-6.441531	-0.917760	1.133549
Br	-6.079708	-4.777985	-1.466533
Br	-4.210379	-6.158557	-3.865427
Br	-0.953852	-6.555087	-3.388698
Br	0.423446	-5.613049	-0.491610
Br	4.843947	-5.427160	-2.232706
Br	7.380413	-3.534513	-3.299221
Br	8.462547	-1.024680	-1.427892
Br	6.986674	-0.372796	1.487627
C	0.039612	-0.444949	-0.393257
C	-1.124447	-1.084848	-1.025583
C	-2.426953	-0.777722	-0.573234
C	-1.012482	-1.938735	-2.151193
C	-3.554593	-1.301363	-1.209593
H	-2.541080	-0.131069	0.293318
C	-2.137072	-2.459615	-2.782114
H	-0.026334	-2.197208	-2.531159
C	-3.417285	-2.131345	-2.321639
H	-4.548015	-1.065280	-0.831957
H	-2.015223	-3.115105	-3.647200
H	-4.302897	-2.527052	-2.822433
C	1.379036	-1.002058	-0.748152
O	1.626599	-2.175930	-0.906854
O	2.367154	-0.053911	-0.793069
C	3.668598	-0.466634	-1.135765
H	3.796257	-1.542186	-0.981530
H	4.378128	0.112139	-0.531368
C	3.943020	-0.170496	-2.596353
F	3.761288	1.127778	-2.896307
F	5.209550	-0.489983	-2.908160
F	3.132826	-0.874454	-3.414276
C	-2.141041	1.989493	-1.688519
C	-2.046410	1.279398	-2.912667
C	-0.772794	0.909442	-3.447233
C	0.288164	0.974062	-2.580007
C	0.159693	1.441570	-1.223522
C	-1.008965	2.235476	-0.941237
H	-3.064619	2.516742	-1.458977
H	1.268443	0.659377	-2.928646
H	1.076396	1.726055	-0.714428
C	-0.893834	3.475809	-0.091093
H	0.107105	3.497491	0.356449
H	-1.598662	3.456223	0.741407
C	-0.584764	0.694706	-4.929266

H	-1.463753	0.188955	-5.349399
H	0.278902	0.031928	-5.079508
C	-0.331401	2.049576	-5.733933
C	-1.144433	4.794793	-0.917751
C	-0.819518	4.621720	-2.382374
C	-1.841389	4.539571	-3.338172
C	0.467673	4.230577	-2.780201
C	-1.642272	3.855684	-4.542019
H	-2.844801	4.889654	-3.081363
C	0.673832	3.564468	-3.987962
H	1.293852	4.320175	-2.074415
C	-0.409446	3.250419	-4.825317
H	-2.495165	3.673909	-5.202034
H	1.663419	3.154171	-4.207120
H	0.661421	1.987906	-6.203678
H	-1.075270	2.126102	-6.540339
H	-0.551867	5.594129	-0.454120
H	-2.196622	5.089452	-0.807311
O	-3.091518	1.059893	-3.699153
C	-4.397210	1.456944	-3.289706
H	-4.475149	2.554563	-3.271337
H	-5.088864	1.052292	-4.038107
H	-4.638152	1.044113	-2.301507

TBP-TS4

Rh	-0.639123	0.154706	1.650456
Rh	-0.711010	-0.049406	4.103652
N	-4.003524	-2.927198	1.314311
O	-1.904266	-3.809029	1.734147
O	-5.913543	-2.196803	0.230499
C	-2.824033	-3.602400	0.979461
C	-2.961277	-3.980122	-0.464882
C	-2.062364	-4.609958	-1.320082
C	-2.459304	-4.781803	-2.669770
C	-3.742074	-4.379000	-3.104685
C	-4.649059	-3.771913	-2.204390
C	-4.219407	-3.550823	-0.902672
C	-4.874391	-2.810709	0.226472
N	-4.196367	3.165170	2.214524
O	-4.877545	1.179735	3.193322
O	-3.852237	4.828536	0.643000
C	-5.019075	2.045116	2.362937
C	-6.016775	2.118698	1.244002
C	-7.106839	1.307281	0.950704
C	-7.775857	1.518533	-0.280775
C	-7.356343	2.545081	-1.158670
C	-6.281739	3.398972	-0.807199
C	-5.634596	3.168548	0.400664
C	-4.468615	3.866176	1.036725
N	3.636259	2.162975	1.841220
O	2.752822	4.306773	1.937708
O	4.537415	0.215072	0.983432
C	3.459419	3.479498	1.413408
C	4.289576	3.620152	0.165387
C	4.576992	4.733300	-0.615172
C	5.337002	4.537476	-1.795089
C	5.842785	3.257883	-2.120234
C	5.607999	2.152250	-1.265918
C	4.803507	2.357758	-0.151251
C	4.352554	1.407670	0.911835
N	2.671462	-3.359191	2.028629
O	3.446072	-1.701794	3.442094
O	2.481931	-4.835657	0.251478
C	3.628894	-2.476847	2.533374
C	4.853159	-2.667701	1.686081
C	6.115658	-2.095871	1.773500
C	7.037017	-2.361028	0.733709
C	6.673931	-3.189374	-0.353176
C	5.406271	-3.818693	-0.386206
C	4.519641	-3.545335	0.648990
C	3.118742	-4.030897	0.888066
O	-2.343421	-0.958460	1.663681
O	-2.499397	-1.057540	3.903654
O	-1.845823	1.807474	1.882242
O	-1.707061	1.755260	4.128263
O	1.111380	1.254293	1.866696
O	1.118154	0.888345	4.088468
O	0.545525	-1.544423	1.707020
O	0.229264	-1.863643	3.909853
C	-2.892939	-1.329083	2.742601
C	-4.179125	-2.143335	2.534272
C	-4.754728	-2.945456	3.739896
C	-5.985037	-3.724901	3.242758
C	-3.738245	-3.931738	4.330992
C	-5.214530	-1.954002	4.824376

C	-2.123332	2.232511	3.045844
C	-3.036598	3.468914	3.050238
C	-3.373844	4.155852	4.404563
C	-4.101442	3.244207	5.403705
C	-4.263451	5.372955	4.094939
C	-2.052967	4.658111	5.015870
C	1.658530	1.246409	3.009685
C	3.152930	1.562963	3.079040
C	3.692085	2.228651	4.398494
C	3.814497	1.126381	5.468976
C	5.099510	2.790319	4.130775
C	2.785335	3.349436	4.933983
C	0.655440	-2.209947	2.778969
C	1.346246	-3.575374	2.609339
C	1.360438	-4.563256	3.817256
C	-0.093770	-4.881999	4.202829
C	2.031821	-5.869089	3.353500
C	2.120179	-4.027795	5.040829
H	3.589743	0.551124	3.052245
H	5.758443	2.035894	3.672443
H	5.556717	3.098986	5.083407
H	5.084109	3.674677	3.476443
H	3.229464	3.771178	5.850064
H	2.665797	4.158691	4.203309
H	1.788183	2.965625	5.191173
H	4.227219	1.554643	6.396109
H	2.837553	0.681837	5.695499
H	4.482716	0.318246	5.135454
H	-1.390183	3.826518	5.289284
H	-2.261825	5.244355	5.924394
H	-1.512932	5.312566	4.311683
H	-3.782597	6.053366	3.374454
H	-4.458343	5.938186	5.019471
H	-5.237153	5.069301	3.679871
H	-3.521411	2.338349	5.619664
H	-5.090007	2.938905	5.032799
H	-4.256215	3.792240	6.347223
H	-2.481890	4.217529	2.468253
H	-4.365111	-1.424048	5.271934
H	-5.745682	-2.498792	5.621029
H	-5.900347	-1.198948	4.410842
H	-3.439884	-4.695292	3.598918
H	-4.185641	-4.449287	5.195059
H	-2.832292	-3.414224	4.671059
H	-6.729811	-3.057421	2.783120
H	-6.463963	-4.242154	4.088673
H	-5.710264	-4.487376	2.498063
H	-4.937054	-1.389092	2.269816
H	3.190564	-3.888080	4.830852
H	1.708942	-3.070627	5.384154
H	2.040959	-4.757621	5.862949
H	-0.105571	-5.650764	4.991701
H	-0.612694	-3.992921	4.579509
H	-0.658649	-5.262200	3.340103
H	3.095630	-5.721592	3.110564
H	1.533921	-6.290319	2.467020
H	1.981482	-6.616423	4.160648
H	0.765871	-4.054742	1.808588
Br	5.662652	6.005157	-2.939461
Br	3.976623	6.449564	-0.101932
Br	6.848720	3.007034	-3.701061
Br	6.411344	0.470361	-1.580035
Br	-5.698100	4.782450	-1.957670
Br	-8.216508	2.775732	-2.826212
Br	-9.209626	0.386105	-0.758188
Br	-7.684660	-0.001672	2.179343
Br	-6.403203	-3.292174	-2.727810
Br	-4.255833	-4.624783	-4.910699
Br	-1.241885	-5.555532	-3.895860
Br	-0.373733	-5.168568	-0.700317
Br	4.911318	-4.985174	-1.788789
Br	7.878217	-3.452472	-1.788753
Br	8.759947	-1.583673	0.800350
Br	6.577385	-1.011664	3.249738
C	-0.673088	0.158163	-0.550808
C	-1.967541	-0.010009	-1.244852
C	-3.154113	0.515476	-0.695967
C	-2.065288	-0.664890	-2.497073
C	-4.377221	0.355914	-1.346364
H	-3.105615	1.044286	0.252072
C	-3.286264	-0.812974	-3.149836
H	-1.168371	-1.065074	-2.966177
C	-4.452229	-0.298543	-2.575034
H	-5.283779	0.735570	-0.886441
H	-3.326128	-1.328275	-4.112083
H	-5.414821	-0.409094	-3.076432

C	0.359699	-0.845076	-0.920051
O	0.118469	-2.001422	-1.180159
O	1.642865	-0.380541	-0.844147
C	2.671002	-1.289456	-1.172600
H	2.331240	-2.327253	-1.065596
H	3.524837	-1.080114	-0.518182
C	3.098270	-1.074535	-2.610987
F	3.425971	0.214764	-2.848838
F	4.167352	-1.828713	-2.900711
F	2.124110	-1.385072	-3.486838
C	-1.881770	3.169312	-1.633055
C	-1.825453	2.643387	-2.934038
C	-0.682606	1.971866	-3.410827
C	0.245737	1.587921	-2.456693
C	0.103676	1.928665	-1.065579
C	-0.827137	2.985465	-0.751957
H	-2.680408	3.869505	-1.383610
H	-2.633898	2.879755	-3.631214
H	1.118614	1.013044	-2.754259
H	0.994808	1.852851	-0.444971
C	-0.534031	3.997449	0.316576
H	0.055245	3.540219	1.120523
H	-1.478635	4.357334	0.736282
C	-0.373486	1.878059	-4.886354
H	-1.282994	1.618819	-5.448740
H	0.350150	1.065263	-5.044069
C	0.229994	3.226368	-5.489914
C	0.249497	5.267800	-0.250150
C	0.522190	5.192387	-1.733262
C	-0.399081	5.662740	-2.678498
C	1.591809	4.419149	-2.212776
C	-0.394621	5.164110	-3.986411
H	-1.218324	6.311534	-2.355856
C	1.622453	3.953751	-3.526094
H	2.348078	4.067856	-1.513662
C	0.550546	4.210931	-4.393648
H	-1.217060	5.424548	-4.659040
H	2.407852	3.254541	-3.827058
H	1.128910	2.966781	-6.069343
H	-0.498523	3.663227	-6.188415
H	1.191011	5.352522	0.307454
H	-0.349549	6.162193	-0.025391

TBP-TS5-OMe

Rh	0.173331	0.067505	1.737671
Rh	0.292530	0.041714	4.195197
N	3.779063	2.901210	1.689435
O	1.849790	3.925969	2.461403
O	5.432242	2.112976	0.278842
C	2.708730	3.799602	1.621702
C	2.861513	4.516568	0.312621
C	2.118942	5.553523	-0.238134
C	2.499910	6.031989	-1.515357
C	3.591389	5.457998	-2.202864
C	4.344870	4.413329	-1.613711
C	3.957554	3.961575	-0.358082
C	4.526190	2.879461	0.511452
N	3.132309	-3.581381	1.926910
O	4.109518	-1.733032	2.921958
O	2.580315	-5.210600	0.374382
C	4.114236	-2.602859	2.083047
C	5.102952	-2.832897	0.976843
C	6.286231	-2.172528	0.669647
C	6.947393	-2.518677	-0.533278
C	6.411242	-3.510049	-1.386574
C	5.215778	-4.186745	-1.040760
C	4.587364	-3.835016	0.147477
C	3.311554	-4.332617	0.764148
N	-3.481845	-2.923077	2.171796
O	-1.325042	-3.746826	2.353070
O	-5.670307	-2.585783	1.489059
C	-2.393850	-3.716394	1.793055
C	-2.855566	-4.494682	0.594702
C	-2.145767	-5.320884	-0.270673
C	-2.861712	-5.923842	-1.335236
C	-4.244083	-5.683918	-1.506153
C	-4.934007	-4.807272	-0.632750
C	-4.214587	-4.219297	0.400332
C	-4.613463	-3.161876	1.387155
N	-2.839762	3.617190	2.232303
O	-3.697346	1.627959	3.052763
O	-2.419844	5.446365	0.877120
C	-3.740200	2.548729	2.272326
C	-4.700272	2.779580	1.138513
C	-5.812981	2.051503	0.730905

C	-6.495963	2.482799	-0.433143
C	-6.048728	3.613754	-1.152111
C	-4.919680	4.345346	-0.711655
C	-4.273102	3.913671	0.439721
C	-3.074890	4.469487	1.151419
O	1.977271	0.999838	1.807235
O	2.168517	0.879192	4.045967
O	1.116372	-1.744716	1.822453
O	1.072137	-1.852890	4.069166
O	-1.662492	-0.910654	1.941840
O	-1.565364	-0.786172	4.184735
O	-0.816270	1.862120	1.971169
O	-0.528912	1.921987	4.198723
C	2.574439	1.204506	2.903546
C	3.937293	1.887572	2.729058
C	4.698210	2.384196	3.992562
C	6.011767	3.034331	3.522418
C	3.894949	3.407587	4.808337
C	5.044484	1.167434	4.869999
C	1.333027	-2.314179	2.928069
C	1.953693	-3.712087	2.781770
C	2.201197	-4.563284	4.061035
C	3.173827	-3.901590	5.048868
C	2.784832	-5.918499	3.622044
C	0.844415	-4.818355	4.740878
C	-2.102724	-1.142294	3.105986
C	-3.441648	-1.898899	3.211923
C	-3.848787	-2.428019	4.628559
C	-4.137441	-1.226203	5.547449
C	-5.151417	-3.239278	4.503120
C	-2.773329	-3.336883	5.244383
C	-0.947505	2.391173	3.111740
C	-1.664519	3.750556	3.093002
C	-1.946254	4.460025	4.449821
C	-0.596189	4.788875	5.113009
C	-2.672852	5.784544	4.155248
C	-2.815407	3.617067	5.395516
H	-4.201408	-1.159951	2.912589
H	-5.958831	-2.650224	4.045161
H	-5.480613	-3.551997	5.506112
H	-5.012446	-4.153485	3.905886
H	-3.110696	-3.686431	6.233438
H	-2.595286	-4.225695	4.621461
H	-1.819461	-2.811333	5.370548
H	-4.525936	-1.586097	6.513404
H	-3.238667	-0.627907	5.735590
H	-4.901326	-0.566448	5.104673
H	0.394708	-3.887278	5.106531
H	0.980411	-5.498332	5.596866
H	0.134678	-5.286080	4.041553
H	2.132398	-6.424162	2.893863
H	2.895643	-6.576816	4.497867
H	3.780766	-5.805473	3.166111
H	2.814848	-2.915631	5.369258
H	4.175603	-3.777326	4.611525
H	3.281317	-4.541254	5.940022
H	1.221914	-4.256703	2.169291
H	4.144771	0.712763	5.302030
H	5.706879	1.481298	5.692245
H	5.565806	0.390367	4.289985
H	3.704614	4.326294	4.235031
H	4.465426	3.688411	5.708519
H	2.927740	2.997169	5.126636
H	6.612436	2.341499	2.912727
H	6.614533	3.330981	4.394774
H	5.827316	3.938514	2.922105
H	4.568030	1.113862	2.264563
H	-3.812827	3.431127	4.970663
H	-2.351011	2.647378	5.615300
H	-2.955641	4.158845	6.344913
H	-0.765070	5.395198	6.016994
H	-0.054338	3.880007	5.401769
H	0.048726	5.367442	4.432413
H	-3.665665	5.616165	3.710168
H	-2.094857	6.420804	3.468022
H	-2.821649	6.341513	5.093370
H	-0.981179	4.402314	2.527462
Br	-1.931600	-7.030562	-2.555655
Br	-0.279819	-5.523239	-0.068229
Br	-5.174856	-6.479885	-2.945060
Br	-6.761873	-4.396812	-0.880248
Br	4.465537	-5.510202	-2.163231
Br	7.280585	-3.934544	-3.009466
Br	8.539473	-1.617429	-1.006338
Br	6.966865	-0.840012	1.824251
Br	5.847035	3.663549	-2.482020

Br	4.046753	6.066680	-3.935426
Br	1.527669	7.456445	-2.294748
Br	0.627800	6.254332	0.676645
Br	-4.285711	5.857420	-1.655698
Br	-6.959316	4.162516	-2.718085
Br	-8.010259	1.518527	-1.029206
Br	-6.349528	0.506810	1.670585
C	0.426445	0.186553	-0.566798
C	0.362406	1.479353	-1.284678
C	1.099073	1.720923	-2.469566
C	-0.516028	2.502003	-0.863567
C	1.022642	2.939099	-3.147859
H	1.739048	0.945150	-2.876798
C	-0.608526	3.711611	-1.546462
H	-1.119492	2.341423	0.024018
C	0.167622	3.940848	-2.688665
H	1.627551	3.093387	-4.044589
H	-1.283767	4.485729	-1.181403
H	0.097346	4.892484	-3.219312
C	1.668375	-0.620264	-0.763728
O	1.783689	-1.824708	-0.799882
O	2.772857	0.198001	-0.829170
C	4.008431	-0.414443	-1.122016
H	4.017823	-1.459548	-0.800407
H	4.798616	0.161057	-0.624334
C	4.271186	-0.388042	-2.615496
F	4.242419	0.855794	-3.120098
F	5.482891	-0.906855	-2.880227
F	3.363354	-1.108411	-3.306896
C	-1.449079	0.492799	-3.645123
C	-2.273765	0.742924	-2.532350
C	-2.232896	-0.112992	-1.431098
C	-1.060775	-0.938202	-1.293613
C	-0.366200	-1.298905	-2.509456
C	-0.601892	-0.630279	-3.696033
H	-1.575123	1.087602	-4.548759
H	-1.076859	-1.689122	-0.504226
H	0.341914	-2.122545	-2.465072
C	-0.191713	-1.191674	-5.035308
H	0.727459	-1.783873	-4.922923
H	0.033497	-0.366500	-5.727052
C	-3.453428	-0.261432	-0.568404
H	-3.708074	0.694906	-0.093556
H	-3.223394	-0.960888	0.239321
C	-4.701055	-0.756102	-1.403785
C	-1.323823	-2.108900	-5.693801
C	-2.573908	-2.138561	-4.850212
C	-3.596226	-1.190714	-5.003750
C	-2.572776	-2.898219	-3.669920
C	-4.445606	-0.862120	-3.935781
H	-3.657648	-0.613026	-5.930734
C	-3.388272	-2.541657	-2.599659
H	-1.826081	-3.684589	-3.534535
C	-4.263788	-1.447101	-2.677206
H	-5.152842	-0.036062	-4.047970
H	-3.239405	-3.029769	-1.639888
H	-5.298736	-1.414050	-0.757822
H	-5.334096	0.100975	-1.662626
H	-0.916403	-3.124794	-5.804281
H	-1.543457	-1.729434	-6.702334
O	-3.263621	1.667485	-2.546163
C	-3.382579	2.534784	-3.660588
H	-3.594970	1.979416	-4.588485
H	-4.226829	3.199727	-3.448464
H	-2.471735	3.140218	-3.794211

TBP-TS6-OMe

Rh	0.256999	-0.353423	1.751091
Rh	0.221908	-0.378519	4.218378
N	-3.410230	-3.124826	1.456134
O	-2.153486	-5.077743	1.321077
O	-4.430338	-1.155498	0.790173
C	-2.879009	-4.252067	0.823507
C	-3.381876	-4.200263	-0.594977
C	-3.277112	-5.119343	-1.630643
C	-3.808026	-4.759548	-2.892584
C	-4.436297	-3.507531	-3.079916
C	-4.565103	-2.601535	-2.000918
C	-4.029993	-2.976035	-0.774856
C	-4.015579	-2.259780	0.537127
N	-3.707536	2.387593	2.392074
O	-4.121396	0.428334	3.550222
O	-3.834384	4.114541	0.853492
C	-4.445242	1.245451	2.723267
C	-5.643397	1.253483	1.817260

C	-6.706817	0.366461	1.711487
C	-7.607348	0.533247	0.634028
C	-7.441635	1.597611	-0.281919
C	-6.389279	2.529126	-0.116579
C	-5.505042	2.332401	0.938922
C	-4.275729	3.096954	1.335135
N	2.897382	3.428579	1.924987
O	0.639533	3.687377	2.367262
O	4.975434	3.519276	0.906920
C	1.597170	3.882150	1.661004
C	1.680302	4.629689	0.363285
C	0.683573	5.221693	-0.403152
C	1.060095	5.790754	-1.644196
C	2.414837	5.815590	-2.047589
C	3.415458	5.233409	-1.233846
C	3.016506	4.621165	-0.051766
C	3.803012	3.815444	0.939190
N	4.209219	-2.992374	2.201642
O	4.400340	-0.776838	2.844797
O	4.449832	-4.983248	1.044855
C	4.780530	-1.717811	2.189372
C	5.925776	-1.797197	1.218653
C	6.812848	-0.818919	0.785016
C	7.851463	-1.210600	-0.096228
C	7.947479	-2.545862	-0.547283
C	6.993217	-3.510619	-0.140904
C	5.996953	-3.111049	0.740855
C	4.830858	-3.868057	1.305815
O	-1.237987	-1.752917	1.818259
O	-1.403667	-1.646509	4.061008
O	-1.212680	1.118724	1.941145
O	-1.044413	1.222339	4.180857
O	1.752531	1.037511	1.899634
O	1.790178	0.954403	4.148446
O	1.719601	-1.827766	1.883270
O	1.518634	-1.950727	4.120235
C	-1.807763	-1.996757	2.923016
C	-3.175014	-2.676829	2.826639
C	-3.562566	-3.678347	3.969783
C	-4.756119	-4.529683	3.505440
C	-2.403952	-4.594874	4.397525
C	-4.007591	-2.843075	5.186519
C	-1.497489	1.608128	3.075722
C	-2.467446	2.804520	3.046818
C	-2.708845	3.597980	4.370470
C	-3.343700	2.755494	5.488021
C	-3.649931	4.775037	4.052874
C	-1.365836	4.176194	4.848023
C	2.164221	1.407993	3.039019
C	3.247431	2.498646	2.997745
C	3.642192	3.187527	4.340245
C	4.319412	2.141134	5.244358
C	4.668928	4.293533	4.037837
C	2.438203	3.815588	5.057376
C	2.026622	-2.289075	3.025771
C	3.087139	-3.402559	3.038522
C	3.530882	-3.949556	4.435768
C	2.319016	-4.617506	5.111066
C	4.605205	-5.032291	4.224077
C	4.121582	-2.855781	5.340178
H	4.142784	1.972651	2.632676
H	5.544693	3.901980	3.499481
H	5.018864	4.737464	4.982759
H	4.231882	5.104253	3.434762
H	2.773253	4.284794	5.996506
H	1.966381	4.596904	4.444198
H	1.676573	3.064365	5.299205
H	4.686163	2.626632	6.162623
H	3.626097	1.340141	5.528336
H	5.184031	1.681797	4.738506
H	-0.657482	3.383952	5.116326
H	-1.532600	4.808259	5.734681
H	-0.900567	4.794654	4.066975
H	-3.251438	5.411568	3.248679
H	-3.774412	5.399041	4.951534
H	-4.651887	4.431640	3.752115
H	-2.730469	1.880241	5.733501
H	-4.350167	2.406007	5.215947
H	-3.446268	3.376288	6.392961
H	-1.997689	3.500626	2.339025
H	-3.195644	-2.194687	5.539947
H	-4.304514	-3.511857	6.009760
H	-4.867338	-2.201423	4.939568
H	-2.040465	-5.200887	3.559275
H	-2.748810	-5.272374	5.195273
H	-1.562493	-4.010427	4.796090

H	-5.575930	-3.902865	3.120342
H	-5.147335	-5.108025	4.356859
H	-4.476880	-5.247914	2.720973
H	-3.857930	-1.818079	2.928235
H	5.030555	-2.417322	4.901440
H	3.405130	-2.046843	5.527401
H	4.406409	-3.298538	6.308170
H	2.640228	-5.113664	6.040410
H	1.536385	-3.891406	5.360781
H	1.879662	-5.388361	4.456276
H	5.532073	-4.616239	3.800142
H	4.253992	-5.835780	3.560234
H	4.865715	-5.479892	5.195526
H	2.627579	-4.244018	2.495892
Br	-0.279896	6.502714	-2.774575
Br	-1.107186	5.228421	0.188469
Br	2.902898	6.610622	-3.693891
Br	5.243253	5.261958	-1.726499
Br	-6.149476	3.977884	-1.307801
Br	-8.616183	1.776152	-1.754575
Br	-9.018393	-0.703460	0.403417
Br	-6.926784	-1.021778	2.973581
Br	-5.441645	-0.936511	-2.199896
Br	-5.097396	-3.018968	-4.783661
Br	-3.628620	-5.955122	-4.347858
Br	-2.445795	-6.793281	-1.345065
Br	7.053628	-5.293166	-0.768216
Br	9.324873	-3.048513	-1.739828
Br	9.081892	0.088754	-0.703634
Br	6.523326	0.990614	1.233988
C	0.098119	-0.302496	-0.351332
C	-0.189047	-1.480957	-1.144636
C	-0.824320	-1.433840	-2.414975
C	0.239127	-2.753605	-0.683471
C	-1.052968	-2.594236	-3.152694
H	-1.165825	-0.484202	-2.814962
C	0.036999	-3.903347	-1.435293
H	0.753036	-2.814126	0.272368
C	-0.604383	-3.827433	-2.678166
H	-1.565511	-2.528497	-4.114477
H	0.379487	-4.866594	-1.052693
H	-0.758994	-4.731750	-3.269949
C	-0.527928	1.005693	-0.694911
O	-0.033196	2.103045	-0.612208
O	-1.844341	0.826857	-1.022152
C	-2.609782	1.981164	-1.289847
H	-2.220727	2.857935	-0.760451
H	-3.638602	1.765753	-0.980229
C	-2.620480	2.277684	-2.779382
F	-3.216099	1.297770	-3.483990
F	-3.286113	3.415650	-3.022201
F	-1.379833	2.414320	-3.283212
C	1.686293	-0.172676	-3.436790
C	2.150220	-1.491581	-3.311017
C	2.891429	-1.899675	-2.157605
C	2.834885	-1.069572	-1.059574
C	2.232979	0.216491	-1.122649
C	1.890675	0.735667	-2.405682
H	1.325520	0.181049	-4.401102
H	3.290860	-1.382735	-0.121867
H	2.391622	0.900259	-0.290262
C	1.971884	2.211235	-2.719192
H	2.105474	2.756879	-1.780506
H	1.032060	2.573549	-3.158201
C	3.868064	-3.039775	-2.287589
H	3.387247	-3.915711	-2.744153
H	4.192679	-3.339102	-1.284043
C	5.145892	-2.653796	-3.159813
C	3.157361	2.557008	-3.715075
C	4.185493	1.451473	-3.793435
C	4.218003	0.577905	-4.889642
C	4.909227	1.075947	-2.649624
C	4.705953	-0.726864	-4.754179
H	3.719411	0.867484	-5.819080
C	5.398223	-0.222008	-2.519685
H	4.971007	1.755669	-1.795767
C	5.180465	-1.185743	-3.517438
H	4.582703	-1.433729	-5.579214
H	5.826823	-0.531750	-1.568353
H	6.040070	-2.934913	-2.587262
H	5.149131	-3.259433	-4.076794
H	3.609671	3.500861	-3.382097
H	2.747134	2.740438	-4.718703
O	2.071031	-2.397407	-4.287786
C	1.441250	-2.064228	-5.519031
H	2.003509	-1.277635	-6.045864

H	1.442215	-2.981599	-6.120829
H	0.405586	-1.730677	-5.358653

TS1

Rh	0.084289	-0.486632	0.039820
Rh	-1.653563	-2.197798	-0.195106
O	-0.701894	0.376579	-1.646487
O	-2.296920	-1.211387	-1.875287
O	-1.235199	0.555315	1.216953
O	-2.868320	-0.985728	0.945339
O	0.710549	-1.486909	1.733191
O	-0.895378	-3.065526	1.516953
O	1.275278	-1.681792	-1.139838
O	-0.322031	-3.275636	-1.333331
C	-1.696729	-0.161340	-2.211177
C	-2.402947	0.094162	1.381577
C	0.083853	-2.533196	2.085501
C	0.812384	-2.784250	-1.552289
C	1.588316	1.022154	0.170145
C	3.011183	0.678397	-0.003223
C	3.905015	1.523626	-0.694101
C	3.494228	-0.536321	0.527343
C	5.237168	1.151757	-0.862252
H	3.545853	2.455329	-1.127976
C	4.832398	-0.888207	0.378522
H	2.807588	-1.190775	1.062092
C	5.705827	-0.049988	-0.322609
H	5.915304	1.806627	-1.413841
H	5.195130	-1.828247	0.800068
H	6.753142	-0.334425	-0.450221
C	1.047345	2.256476	-0.467056
O	1.256940	2.531970	-1.620882
O	0.225720	2.962353	0.345894
C	-0.575313	3.969259	-0.239256
H	-0.377513	4.046399	-1.317130
H	-0.359109	4.929699	0.250839
C	-2.046627	3.654373	-0.021480
F	-2.339235	3.491247	1.275377
F	-2.778152	4.683404	-0.483969
F	-2.434147	2.550645	-0.672875
H	-3.083108	0.729272	1.982844
H	0.457675	-3.024793	3.006502
H	-2.075196	0.364536	-3.110261
H	1.500529	-3.384898	-2.181192
N	1.447476	1.391093	1.917553
N	1.285992	1.118570	2.976943

TS2A

Rh	-1.396057	-0.432521	0.096825
Rh	-3.498638	-0.649298	-1.181485
O	-2.314323	1.153871	1.048729
O	-4.234071	0.949354	-0.128819
O	-0.737471	0.829986	-1.401051
O	-2.679147	0.662726	-2.552919
O	-0.719740	-2.052474	-1.016564
O	-2.652629	-2.241831	-2.176418
O	-2.217065	-1.719146	1.469764
O	-4.147841	-1.923124	0.299460
C	-3.491653	1.483237	0.727734
C	-1.523022	1.103311	-2.356863
C	-1.487857	-2.582320	-1.874589
C	-3.384222	-2.161002	1.268412
C	0.397841	-0.210909	1.336637
C	0.866183	-1.358803	2.134898
C	1.432885	-1.205906	3.421975
C	0.787586	-2.664125	1.607497
C	1.864249	-2.307022	4.154329
H	1.514329	-0.212127	3.858326
C	1.228651	-3.767708	2.340524
H	0.364932	-2.805133	0.616149
C	1.763759	-3.596414	3.617323
H	2.283136	-2.160865	5.152959
H	1.145150	-4.768286	1.909388
H	2.103173	-4.460221	4.194506
C	0.136365	1.059729	2.068921
O	-0.285438	1.140247	3.198510
O	0.285709	2.168271	1.288026
C	-0.298218	3.359056	1.757767
H	-1.257967	3.156997	2.250494
H	0.363632	3.884760	2.465702
C	-0.516736	4.251803	0.553940
F	0.628332	4.458820	-0.125067
F	-0.972018	5.448121	0.959096
F	-1.407759	3.744402	-0.308080

H	-1.127845	1.817208	-3.108488
H	-1.064846	-3.451124	-2.420810
H	-3.910455	2.351812	1.275945
H	-3.773532	-2.846175	2.049009
C	1.911046	-0.862966	-0.868280
C	1.792910	0.260483	0.018258
C	2.905354	0.529174	0.889124
C	3.706556	-0.560339	1.233255
C	3.684088	-1.719605	0.456230
C	2.898161	-1.810945	-0.720896
H	1.200165	-0.922987	-1.688363
H	1.249735	1.104304	-0.399962
H	4.465055	-0.457736	2.012224
H	4.389319	-2.523197	0.687333
C	3.257699	-2.730490	-1.863059
H	3.619539	-3.699618	-1.486703
H	2.347877	-2.933529	-2.446628
C	3.340395	1.930936	1.222261
H	2.538935	2.507730	1.702192
H	4.180807	1.874757	1.930027
C	3.793860	2.720458	-0.072877
C	4.364302	-2.115470	-2.836787
C	4.580699	-0.644567	-2.575650
C	3.630416	0.304182	-2.978127
C	5.545250	-0.233601	-1.643351
C	3.478251	1.497680	-2.268768
H	2.901157	0.046565	-3.751283
C	5.409887	0.971727	-0.954060
H	6.343154	-0.925128	-1.357895
C	4.288111	1.787524	-1.158724
H	2.631234	2.150174	-2.497600
H	6.104332	1.201533	-0.140802
H	4.563810	3.447592	0.231332
H	2.935233	3.294520	-0.448455
H	5.308319	-2.661296	-2.689985
H	4.045276	-2.296464	-3.874562

TS2B

Rh	-1.472481	-0.386047	-0.053552
Rh	-3.728464	-0.203263	0.929965
O	-2.146049	0.957913	-1.471007
O	-4.220594	1.092843	-0.580639
O	-0.934514	1.199099	1.162258
O	-3.017632	1.397844	2.024124
O	-1.049246	-1.712339	1.480265
O	-3.108872	-1.513706	2.395258
O	-2.206426	-1.936880	-1.180804
O	-4.270796	-1.793422	-0.256866
C	-3.334200	1.384466	-1.417926
C	-1.821091	1.742163	1.886885
C	-1.946420	-1.972769	2.336870
C	-3.412983	-2.283141	-1.033333
C	0.471264	-0.580439	-1.063198
C	0.911574	-1.915229	-1.506215
C	1.645431	-2.109949	-2.699356
C	0.619605	-3.053915	-0.727144
C	2.027183	-3.383061	-3.112429
H	1.899752	-1.251814	-3.319091
C	1.007614	-4.329214	-1.138125
H	0.074867	-2.924421	0.204148
C	1.706378	-4.501190	-2.334389
H	2.578635	-3.505223	-4.047746
H	0.756190	-5.194396	-0.519940
H	2.004507	-5.500941	-2.660312
C	0.385371	0.478424	-2.110834
O	0.075359	0.298560	-3.264043
O	0.571660	1.732370	-1.607223
C	0.160660	2.814270	-2.406452
H	-0.752147	2.567152	-2.964005
H	0.947002	3.112800	-3.119203
C	-0.104970	3.977704	-1.472658
F	0.956091	4.233367	-0.687378
F	-0.359526	5.082672	-2.193131
F	-1.157718	3.762005	-0.671184
H	-1.484689	2.622704	2.471554
H	-1.653991	-2.692777	3.129060
H	-3.619492	2.103955	-2.212325
H	-3.746257	-3.127339	-1.670816
C	1.719723	0.137495	0.287362
C	2.811847	0.228084	-0.640140
C	3.821214	-0.723540	-0.696484
C	3.655937	-1.849287	0.127803
C	2.722966	-1.857163	1.181809
C	1.883113	-0.776695	1.389398
H	1.170905	1.054927	0.485622

H	2.834321	1.092592	-1.302357
H	4.366587	-2.676837	0.049698
H	2.789564	-2.648707	1.932029
C	1.386258	-0.416497	2.761210
H	1.508218	-1.287526	3.421809
H	0.321808	-0.163840	2.729418
C	5.119598	-0.424360	-1.409024
H	4.914092	0.249606	-2.253773
H	5.549056	-1.344166	-1.834238
C	6.209176	0.260942	-0.464862
C	2.167782	0.822649	3.368339
C	3.532287	1.014598	2.743724
C	3.734661	2.002592	1.766669
C	4.539918	0.052187	2.900546
C	4.761191	1.884194	0.826594
H	3.001472	2.806257	1.653974
C	5.545909	-0.083990	1.943604
H	4.453394	-0.695414	3.694219
C	5.591950	0.755389	0.820431
H	4.813696	2.600756	0.001947
H	6.227808	-0.937110	2.003008
H	6.996692	-0.473893	-0.240188
H	6.683262	1.079980	-1.027235
H	2.234274	0.675355	4.458067
H	1.566590	1.728314	3.200713

TS2C

Rh	-1.419766	-0.474653	-0.034801
Rh	-3.629111	-0.932005	-1.038652
O	-2.182926	1.367465	0.488125
O	-4.197918	0.954552	-0.452605
O	-0.882441	0.260066	-1.908055
O	-2.917380	-0.152108	-2.808446
O	-0.858862	-2.332372	-0.785975
O	-2.925885	-2.785974	-1.587170
O	-2.152624	-1.322558	1.678308
O	-4.202643	-1.680372	0.784860
C	-3.365625	1.667157	0.156300
C	-1.733129	0.253460	-2.845303
C	-1.724117	-3.055765	-1.362048
C	-3.352161	-1.713652	1.710541
C	0.445471	-0.040619	1.182849
C	0.954803	-1.163346	2.040854
C	1.509285	-0.912467	3.315303
C	0.920141	-2.500130	1.610598
C	1.990327	-1.941426	4.119855
H	1.558590	0.109088	3.692184
C	1.404790	-3.536125	2.413407
H	0.491189	-2.733390	0.641361
C	1.942205	-3.265498	3.671453
H	2.404629	-1.708539	5.103924
H	1.351354	-4.565314	2.049238
H	2.317147	-4.076198	4.301242
C	0.007509	1.130516	1.995142
O	-0.655013	1.027729	3.000349
O	0.329047	2.350805	1.487193
C	-0.376263	3.452729	2.010407
H	-1.400017	3.167162	2.284518
H	0.126905	3.869716	2.897669
C	-0.417780	4.521239	0.938330
F	0.818690	4.882512	0.545579
F	-1.028404	5.615939	1.419610
F	-1.085023	4.124689	-0.154443
H	-1.377560	0.656514	-3.816721
H	-1.365000	-4.046953	-1.708841
H	-3.696231	2.687085	0.439881
H	-3.687524	-2.140073	2.677613
C	2.954014	-1.621385	-0.579943
C	1.927206	-0.747089	-0.817493
C	1.795552	0.496578	-0.088290
C	2.814434	0.722040	0.908199
C	3.843769	-0.172415	1.144295
C	4.001784	-1.295593	0.316053
H	3.030867	-2.533632	-1.173495
H	1.176151	-0.969539	-1.574164
H	2.768233	1.658054	1.467367
H	4.608068	0.064021	1.887161
C	5.311526	-2.042915	0.226194
H	5.812026	-2.046871	1.205469
H	5.105318	-3.090394	-0.038370
C	1.402239	1.746026	-0.922517
H	0.319003	1.854603	-0.991137
H	1.771159	2.622588	-0.381036
C	1.988070	1.765069	-2.368120
C	6.297829	-1.421101	-0.861996

C	5.595414	-0.382727	-1.708139
C	4.788505	-0.742691	-2.797259
C	5.474057	0.926640	-1.218921
C	3.699250	0.053041	-3.156550
H	4.912426	-1.724854	-3.262477
C	4.389364	1.720346	-1.578422
H	6.148484	1.268632	-0.429089
C	3.396365	1.221801	-2.438128
H	2.987796	-0.315982	-3.900496
H	4.235010	2.677646	-1.073587
H	1.934004	2.810974	-2.715338
H	1.337708	1.174864	-3.029294
H	7.151312	-0.965470	-0.338307
H	6.695182	-2.240466	-1.479240

TS3A

Rh	-1.397679	-0.409782	0.007857
Rh	-3.485892	-0.515375	-1.224344
O	-0.711193	-1.888373	-1.263470
O	-2.654021	-1.967132	-2.413254
O	-0.760988	0.994394	-1.363525
O	-2.735363	0.946469	-2.464243
O	-2.294651	1.043929	1.155981
O	-4.235366	0.934879	0.005986
O	-2.170506	-1.825528	1.271243
O	-4.102966	-1.955067	0.099367
C	-1.477482	-2.328447	-2.166738
C	-1.568743	1.367568	-2.260827
C	-3.482120	1.385940	0.905906
C	-3.325413	-2.274412	1.039158
C	0.847173	-0.271794	1.333677
C	0.949265	-1.589859	2.013463
C	1.185573	-1.685130	3.400423
C	0.857358	-2.785160	1.279666
C	1.315277	-2.924853	4.022300
H	1.258817	-0.776399	3.994096
C	0.990891	-4.026959	1.904819
H	0.651577	-2.746559	0.214393
C	1.220824	-4.105791	3.278259
H	1.494855	-2.969228	5.099510
H	0.905032	-4.939215	1.308865
H	1.323876	-5.077200	3.768263
C	0.315249	0.877248	2.091899
O	-0.141397	0.872691	3.211490
O	0.360479	2.037162	1.354158
C	-0.257649	3.166544	1.916029
H	0.419073	3.693110	2.610085
H	-1.170894	2.887980	2.456676
C	-0.602108	4.119215	0.789611
F	-1.539728	3.633547	-0.037904
F	-1.073218	5.265631	1.307665
F	0.473887	4.422043	0.039819
H	-1.200632	2.155506	-2.947765
H	-3.908232	2.176096	1.555609
H	-1.056921	-3.123658	-2.815052
H	-3.697501	-3.042611	1.745984
C	1.716725	0.094127	0.063200
C	2.013823	-0.888620	-1.007015
C	3.068213	-1.736267	-0.937278
C	3.803254	-1.778879	0.311678
C	3.678496	-0.797052	1.257574
C	2.804646	0.313284	1.036156
H	1.294967	1.000404	-0.368809
H	1.414952	-0.816541	-1.912629
H	4.549457	-2.565661	0.454352
H	4.339474	-0.790141	2.127300
C	3.235722	1.674462	1.541610
H	4.137902	1.512838	2.151171
H	2.498881	2.145068	2.205586
C	3.578863	-2.447404	-2.171065
H	2.734073	-2.581477	-2.862435
H	3.944018	-3.455432	-1.917813
C	4.736059	-1.664720	-2.934118
C	3.572384	2.674593	0.384111
C	4.207107	1.946551	-0.781239
C	3.493549	1.748525	-1.974385
C	5.384792	1.208499	-0.603523
C	3.801100	0.683838	-2.822847
H	2.606857	2.356449	-2.174355
C	5.671871	0.125014	-1.432722
H	6.003929	1.381152	0.281336
C	4.808671	-0.228624	-2.479029
H	3.148132	0.473185	-3.674441
H	6.507883	-0.533876	-1.181569
H	5.698122	-2.162911	-2.741354

H	4.545043	-1.741437	-4.015818
H	4.229280	3.457897	0.797460
H	2.647727	3.167734	0.054646

TS3B

Rh	-1.441611	-0.010491	0.002232
Rh	-3.652740	-0.565050	0.921073
O	-1.938277	-1.210514	-1.598120
O	-4.027025	-1.595211	-0.815639
O	-0.792161	-1.772935	0.932979
O	-2.845511	-2.266582	1.742339
O	-1.128472	1.091701	1.727920
O	-3.133407	0.507773	2.602359
O	-2.365246	1.588389	-0.883261
O	-4.374300	1.144129	0.051954
C	-3.100603	-1.699995	-1.658178
C	-1.625756	-2.489563	1.554797
C	-2.023795	1.091708	2.621133
C	-3.585246	1.814606	-0.662958
C	0.587937	0.969301	-1.130410
C	0.249293	2.408280	-1.327723
C	0.148688	2.983306	-2.611380
C	0.064279	3.259021	-0.218365
C	-0.070783	4.352450	-2.767720
H	0.243601	2.348873	-3.489175
C	-0.160899	4.626441	-0.379139
H	0.025666	2.824570	0.776087
C	-0.220452	5.187205	-1.656181
H	-0.122441	4.771181	-3.776275
H	-0.309978	5.253428	0.504044
H	-0.395941	6.257909	-1.786098
C	0.463670	0.047364	-2.261424
O	-0.133013	0.189810	-3.305390
O	1.161171	-1.118883	-2.011817
C	0.956026	-2.192993	-2.890292
H	-0.093694	-2.522140	-2.871242
H	1.231626	-1.941899	-3.926358
C	1.850144	-3.306433	-2.390701
F	3.149447	-2.947336	-2.407110
F	1.716795	-4.395456	-3.159075
F	1.557456	-3.656338	-1.123949
H	-1.224290	-3.427867	1.991718
H	-1.791935	1.681263	3.532544
H	-3.323847	-2.297218	-2.565661
H	-4.003672	2.712818	-1.159846
C	1.567317	-0.310480	0.684998
C	1.921160	0.709695	-0.333471
C	2.587609	1.921487	0.231845
C	2.444445	2.197812	1.566911
C	1.986469	1.202070	2.460761
C	1.665665	-0.098362	2.049606
H	1.269011	-1.280480	0.299316
H	2.616404	0.246673	-1.042752
H	2.868141	3.115305	1.981097
H	2.012117	1.422715	3.532229
C	1.686852	-1.264030	3.009342
H	1.241531	-0.976136	3.973714
H	1.065191	-2.064504	2.591511
C	3.626826	2.606063	-0.597716
H	3.253591	2.768609	-1.620315
H	3.850552	3.590895	-0.164349
C	4.975028	1.745003	-0.673339
C	3.159793	-1.825909	3.269604
C	4.158263	-1.195454	2.331968
C	4.193855	-1.573133	0.982000
C	4.810208	-0.005490	2.686504
C	4.627582	-0.672019	0.006693
H	3.754064	-2.522445	0.664831
C	5.251055	0.891666	1.709095
H	4.862574	0.284340	3.739830
C	5.038263	0.628484	0.349060
H	4.527016	-0.952894	-1.045047
H	5.637449	1.867802	2.015915
H	5.816027	2.443525	-0.548468
H	5.058459	1.318765	-1.683341
H	3.441747	-1.622659	4.313375
H	3.136104	-2.918969	3.146651

TS3C

Rh	1.085024	-0.596809	0.072747
Rh	2.950748	-2.210602	-0.108279
O	1.790399	0.198170	-1.696390
O	3.500155	-1.275634	-1.850720
O	-0.040239	-1.952205	-1.036317

O	1.665957	-3.433524	-1.175232
O	0.523424	-1.632657	1.787149
O	2.282037	-3.051597	1.654309
O	2.355762	0.585772	1.158337
O	4.086168	-0.862092	0.948718
C	2.816000	-0.300727	-2.241392
C	0.500017	-3.041816	-1.399803
C	1.245089	-2.597788	2.184621
C	3.549326	0.209313	1.328078
C	-0.546697	0.938574	0.230331
C	-0.609011	1.738601	1.515129
C	-0.183621	1.232565	2.751597
C	-1.173350	3.028946	1.492722
C	-0.334372	1.980766	3.922033
H	0.276688	0.249700	2.793359
C	-1.323067	3.779440	2.657766
H	-1.516910	3.447786	0.543569
C	-0.906940	3.253918	3.884631
H	0.012153	1.565697	4.872026
H	-1.764400	4.778203	2.608248
H	-1.018271	3.837712	4.801656
C	-0.188775	1.820963	-0.913707
O	-0.693419	1.888680	-2.018959
O	0.883394	2.581882	-0.589724
C	1.523184	3.265026	-1.639025
H	1.029599	4.228311	-1.848829
H	1.532109	2.662330	-2.556393
C	2.949231	3.548641	-1.210335
F	3.668160	2.428487	-1.037687
F	3.555244	4.272963	-2.171212
F	3.004762	4.248162	-0.071907
H	-0.150883	-3.725210	-1.984809
H	0.904017	-3.094520	3.116985
H	3.142338	0.188527	-3.181827
H	4.195132	0.916993	1.886057
C	-1.942218	0.063586	-0.066946
C	-2.654851	0.580883	-1.251867
C	-3.823756	1.316751	-1.164612
C	-4.266164	1.634101	0.135403
C	-3.750034	1.011897	1.287056
C	-2.757903	0.063683	1.164164
H	-1.577451	-0.936337	-0.307838
H	-2.274042	0.283417	-2.223759
H	-5.147928	2.273623	0.246988
H	-4.274468	1.140917	2.235926
C	-2.605066	-1.042258	2.156721
H	-3.140456	-0.776830	3.079311
H	-1.545149	-1.202418	2.396776
C	-4.716170	1.498077	-2.372699
H	-4.086381	1.496068	-3.273619
H	-5.217382	2.477708	-2.340913
C	-5.828192	0.363667	-2.514746
C	-3.177703	-2.405488	1.575473
C	-4.173766	-2.182804	0.455992
C	-3.768057	-2.318881	-0.882866
C	-5.415434	-1.576486	0.689335
C	-4.441424	-1.655789	-1.910618
H	-2.837953	-2.846131	-1.108607
C	-6.071902	-0.886609	-0.333229
H	-5.800986	-1.510003	1.710716
C	-5.524079	-0.813432	-1.622195
H	-4.029174	-1.682610	-2.923059
H	-6.960103	-0.294893	-0.093717
H	-6.808990	0.786957	-2.251223
H	-5.879423	0.066628	-3.573441
H	-3.622206	-2.963535	2.414010
H	-2.333580	-2.999394	1.197159

TS3D

Rh	1.650589	-0.062732	0.070641
Rh	3.929902	0.321091	-0.701293
O	1.928877	1.577925	1.293205
O	4.059315	1.890327	0.605353
O	1.021385	1.201787	-1.442112
O	3.142441	1.577803	-2.133705
O	1.597165	-1.643820	-1.258443
O	3.708111	-1.275205	-1.974768
O	2.447785	-1.274405	1.515452
O	4.563175	-0.947155	0.779241
C	3.046406	2.162376	1.298693
C	1.897901	1.735409	-2.182226
C	2.616489	-1.893057	-1.964284
C	3.696932	-1.443560	1.548170
C	-0.649500	-0.557365	0.931195
C	-0.639300	-1.903321	1.565745

C	-0.102207	-3.017714	0.899389
C	-1.200697	-2.110221	2.842480
C	-0.104148	-4.282673	1.490895
H	0.341665	-2.886246	-0.082571
C	-1.201905	-3.371552	3.433441
H	-1.632637	-1.268584	3.380696
C	-0.651441	-4.467400	2.760821
H	0.331698	-5.127971	0.952300
H	-1.638490	-3.500237	4.426969
H	-0.652089	-5.456940	3.224807
C	-0.581434	0.619924	1.828624
O	-0.302506	0.632419	3.003006
O	-0.856718	1.778066	1.136335
C	-0.851773	2.990772	1.837791
H	0.029680	3.587914	1.559265
H	-0.846353	2.820142	2.923920
C	-2.105999	3.741774	1.440865
F	-3.217706	3.044781	1.764573
F	-2.166610	4.923495	2.067275
F	-2.159962	3.970810	0.117824
H	1.515841	2.419485	-2.967165
H	2.527277	-2.756430	-2.654240
H	3.141557	3.019471	1.995746
H	4.072778	-2.111175	2.348919
C	-1.427974	-0.287457	-0.445471
C	-2.634693	-0.239406	0.403222
C	-3.518182	-1.326830	0.518479
C	-3.197474	-2.470835	-0.199232
C	-2.227986	-2.439197	-1.247989
C	-1.485984	-1.319267	-1.501588
H	-1.108126	0.684728	-0.814173
H	-2.852719	0.695522	0.909850
H	-3.829463	-3.357937	-0.104031
H	-2.243151	-3.256105	-1.974412
C	-1.006156	-0.977899	-2.884782
H	-1.087021	-1.877027	-3.513851
H	0.047625	-0.674925	-2.865278
C	-4.863795	-1.111035	1.174907
H	-4.741294	-0.437224	2.035572
H	-5.246154	-2.063749	1.570294
C	-5.956126	-0.486586	0.191276
C	-1.837972	0.198498	-3.542894
C	-3.233814	0.309335	-2.970595
C	-3.553130	1.330874	-2.063576
C	-4.146509	-0.749127	-3.094200
C	-4.596462	1.177377	-1.145005
H	-2.897759	2.201458	-1.974345
C	-5.172445	-0.913989	-2.164801
H	-3.966877	-1.532507	-3.835961
C	-5.330298	-0.015896	-1.098215
H	-4.730193	1.932516	-0.365640
H	-5.777706	-1.824537	-2.192135
H	-6.718039	-1.251849	-0.019662
H	-6.462048	0.338928	0.714349
H	-1.851322	0.027097	-4.631338
H	-1.304473	1.144592	-3.370925

TS4A

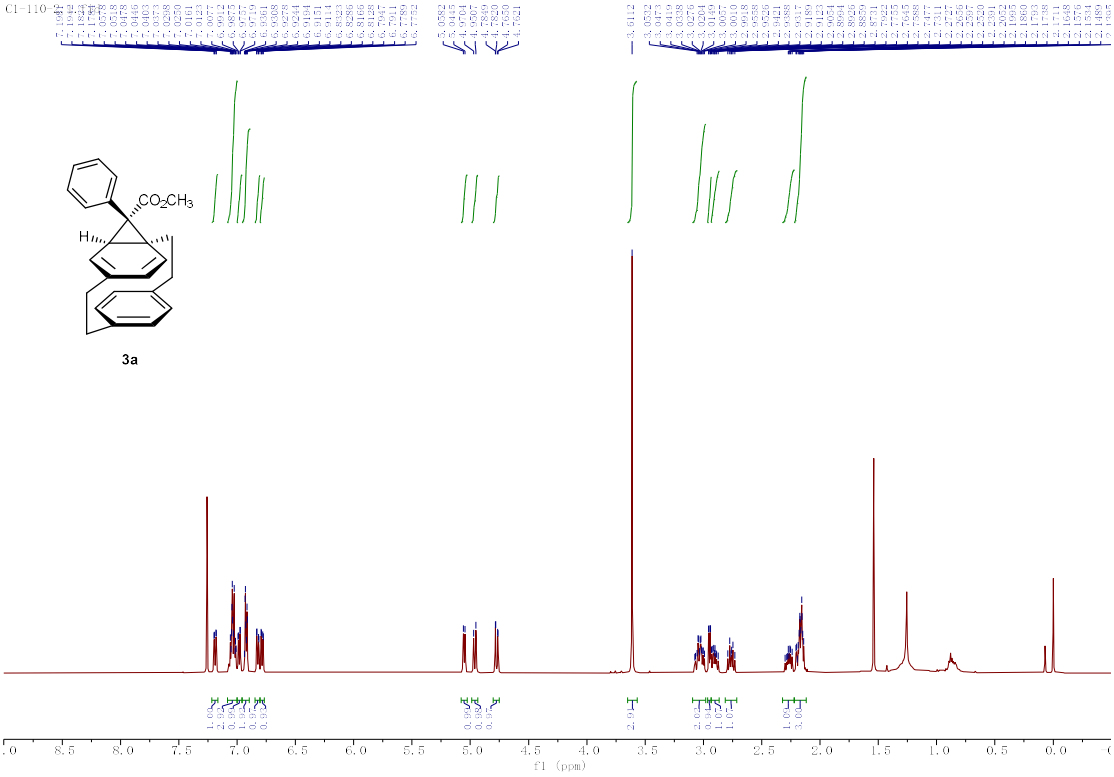
C	0.271374	1.114316	-0.043559
C	-0.369210	2.488810	0.019342
C	-0.427915	3.189279	1.230134
C	-0.845775	3.096327	-1.145327
C	-0.963773	4.475708	1.276198
H	-0.050981	2.718590	2.139164
C	-1.385113	4.385675	-1.101972
H	-0.806118	2.551972	-2.090298
C	-1.447973	5.076984	0.109206
H	-1.004452	5.013321	2.226654
H	-1.759747	4.848313	-2.018346
H	-1.872824	6.083143	0.146104
C	1.788139	1.273171	-0.032801
O	2.384876	2.040163	0.672855
O	2.413079	0.427108	-0.897830
C	3.827239	0.424518	-0.921038
H	4.230529	1.242014	-0.307817
H	4.160084	0.527264	-1.963508
C	4.339813	-0.899779	-0.384842
F	3.825327	-1.941125	-1.057238
F	5.673960	-0.947738	-0.500970
F	4.029072	-1.064572	0.911612
C	-0.264230	0.113097	-1.002528
C	-1.595612	-0.069499	-1.417038
C	-2.748621	0.123512	-0.670433
C	-2.661744	0.373995	0.721020
C	-1.507432	0.183056	1.458073

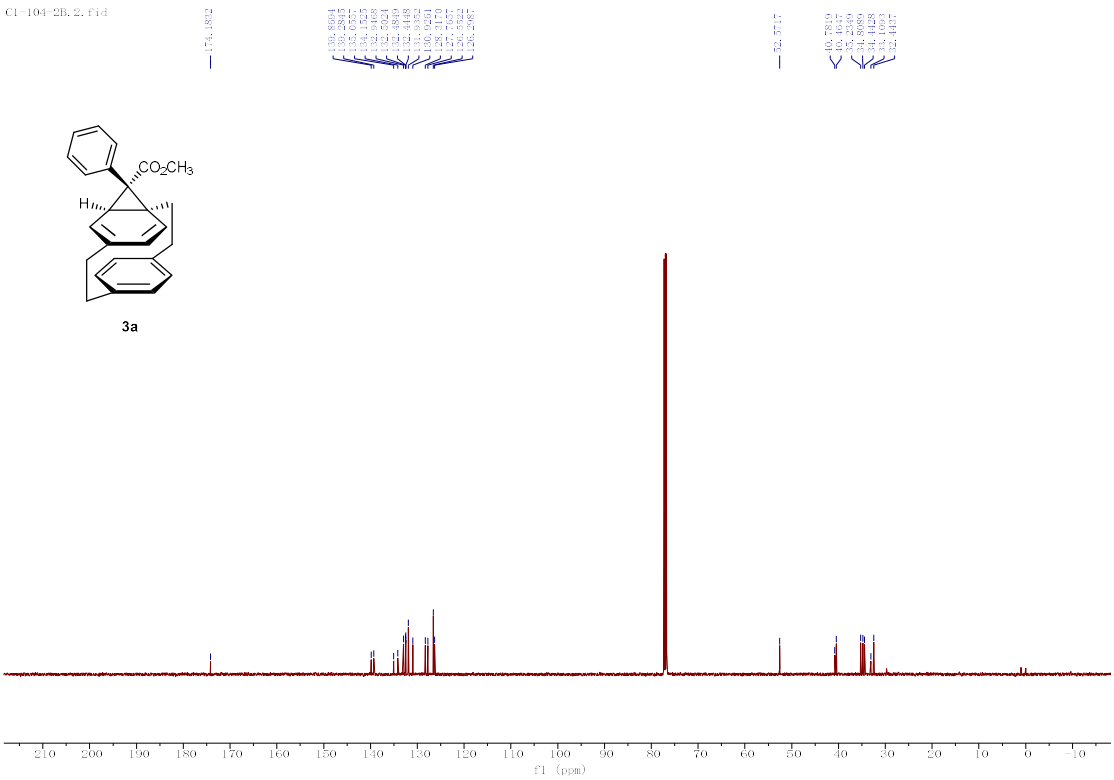
C	-0.178702	0.080095	0.974740
H	0.493409	-0.478568	-1.515773
H	-1.706341	-0.603020	-2.363955
H	-3.601251	0.422296	1.279570
H	-1.644655	-0.070506	2.513622
C	0.761505	-0.889892	1.669668
H	0.430201	-0.925622	2.720518
H	1.795589	-0.519312	1.695567
C	-4.062136	-0.402014	-1.228442
H	-4.023841	-0.353843	-2.326706
H	-4.898428	0.244294	-0.918238
C	-4.412613	-1.898380	-0.801823
C	0.792635	-2.366873	1.135192
C	-0.570158	-2.859145	0.706262
C	-0.848932	-3.080151	-0.650404
C	-1.660502	-2.846095	1.587460
C	-2.153096	-2.996046	-1.137027
H	-0.019833	-3.184845	-1.356005
C	-2.960172	-2.720709	1.097513
H	-1.487464	-2.764820	2.664147
C	-3.206668	-2.644042	-0.281189
H	-2.325447	-3.039859	-2.216238
H	-3.778554	-2.533300	1.798486
H	-5.188200	-1.874728	-0.021186
H	-4.855443	-2.404067	-1.674996
H	1.233018	-2.989855	1.932010
H	1.479894	-2.421621	0.278093

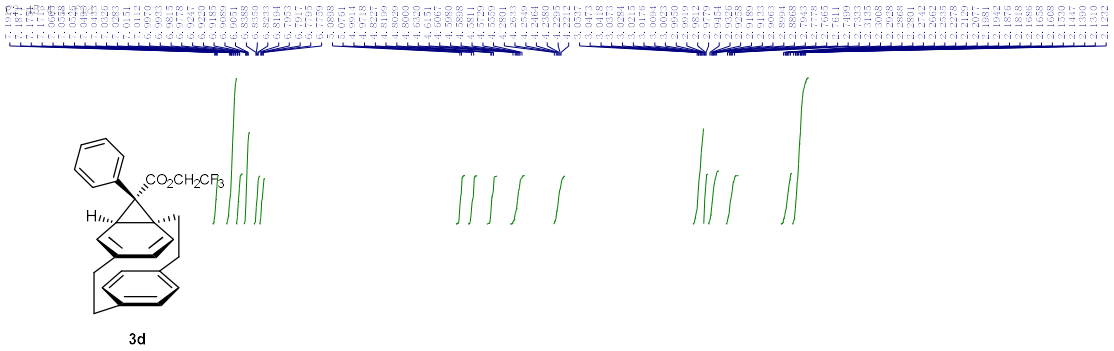
TS4B

C	0.931360	-0.855735	-0.230021
C	2.412763	-1.091508	-0.051064
C	3.275571	-1.006580	-1.147874
C	2.925082	-1.469337	1.193661
C	4.635899	-1.287480	-1.002690
H	2.879219	-0.707643	-2.120390
C	4.284080	-1.749735	1.343637
H	2.252337	-1.540596	2.050013
C	5.144256	-1.655795	0.245721
H	5.301246	-1.216056	-1.866584
H	4.673695	-2.043833	2.321237
H	6.209109	-1.871579	0.362761
C	0.192530	-2.167365	-0.433076
O	0.575849	-3.250056	-0.086097
O	-1.032280	-1.961557	-1.001590
C	-1.990097	-2.994757	-0.929039
H	-1.567623	-3.889962	-0.451118
H	-2.345242	-3.242713	-1.939812
C	-3.162683	-2.483000	-0.111217
F	-3.728103	-1.401992	-0.671196
F	-4.100101	-3.432801	-0.002310
F	-2.773348	-2.134012	1.128823
C	0.171390	-0.050128	0.795879
C	0.451510	0.274852	-1.087350
C	1.153748	1.476451	-1.285162
C	1.969485	2.004749	-0.279705
C	1.774159	1.756839	1.089327
C	0.736984	0.962154	1.587810
H	-0.822606	-0.422020	1.045401
H	-0.412700	0.057850	-1.711976
H	2.616899	2.848579	-0.536640
H	2.288570	2.424342	1.787055
C	0.072583	1.331615	2.909306
H	0.672638	2.132291	3.366418
H	0.100879	0.484141	3.614761
C	0.848735	2.315256	-2.520933
H	1.109308	1.770235	-3.444067
H	1.503846	3.198436	-2.490843
C	-0.643549	2.801527	-2.651872
C	-1.420225	1.822127	2.801338
C	-1.691141	2.437537	1.451031
C	-2.426167	1.733894	0.490456
C	-0.955910	3.553658	1.022628
C	-2.229675	1.975602	-0.870111
H	-3.048394	0.888432	0.795444
C	-0.762027	3.795640	-0.333772
H	-0.415029	4.157609	1.756599
C	-1.297161	2.927374	-1.297965
H	-2.702847	1.311801	-1.599133
H	-0.072951	4.586540	-0.643030
H	-0.639794	3.754335	-3.206662
H	-1.216279	2.086328	-3.262265
H	-1.604391	2.526058	3.629608
H	-2.103457	0.972455	2.953231

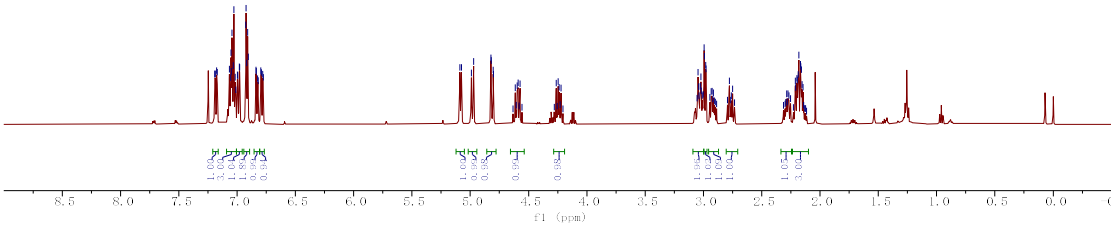
8. NMR Spectra of All Products







3d



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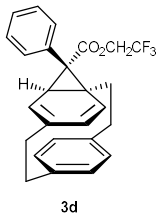

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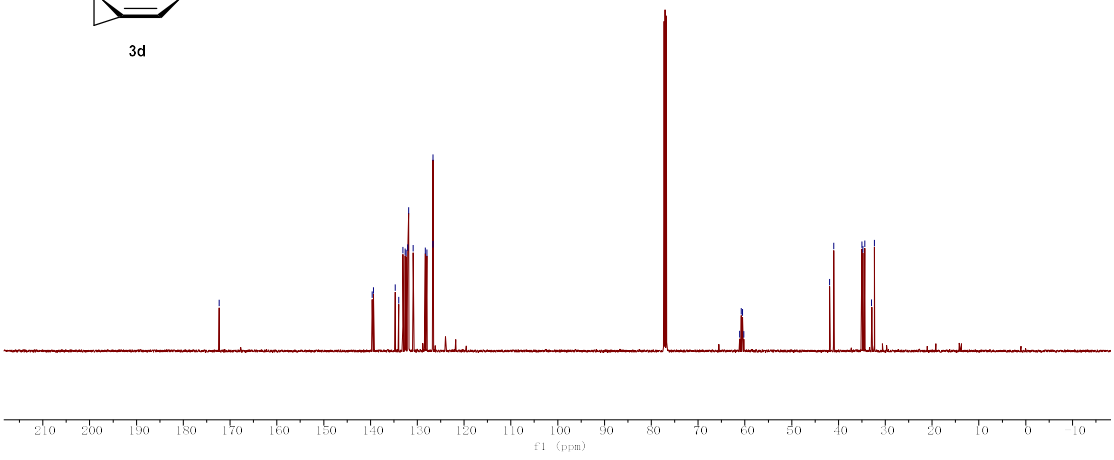
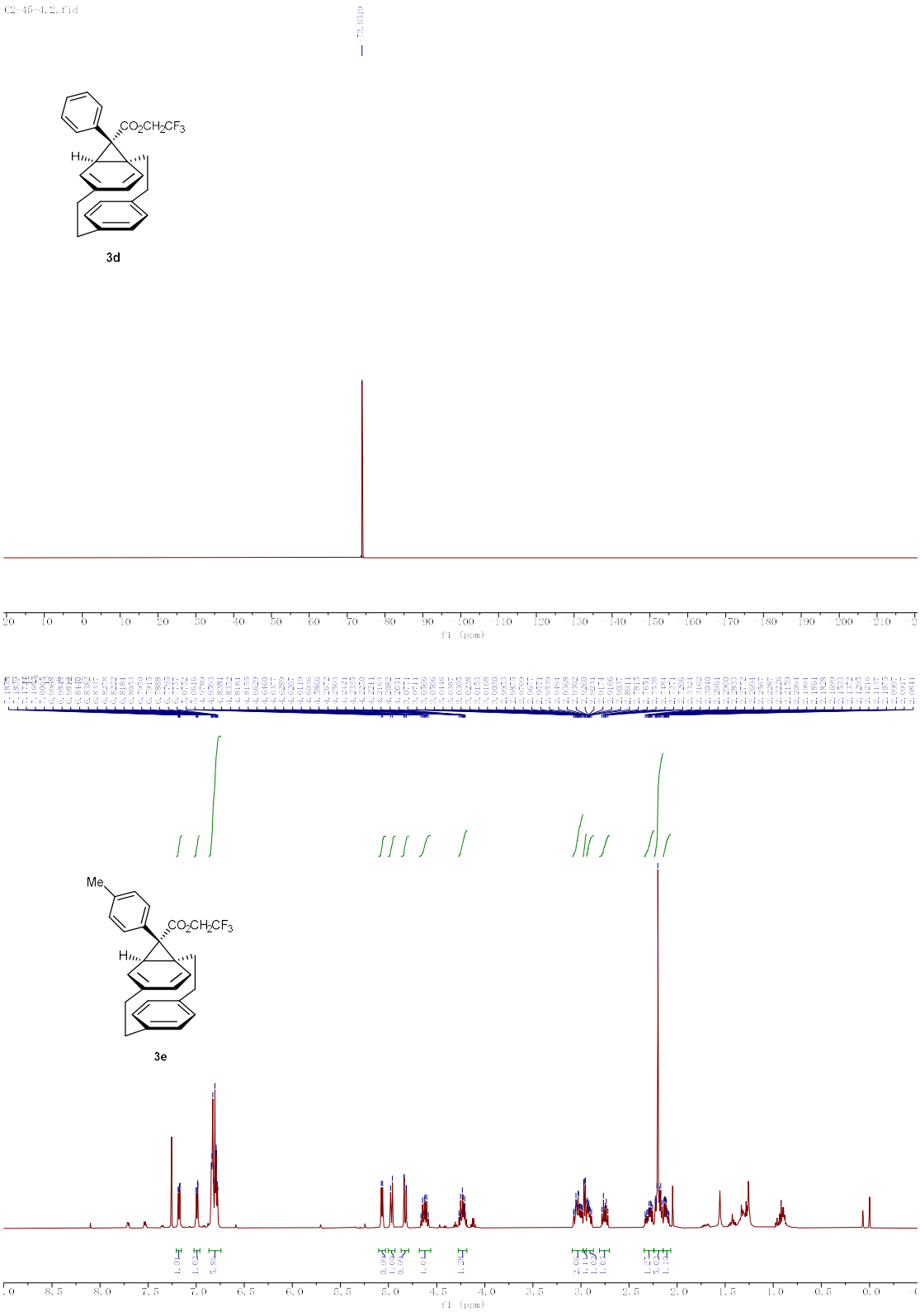
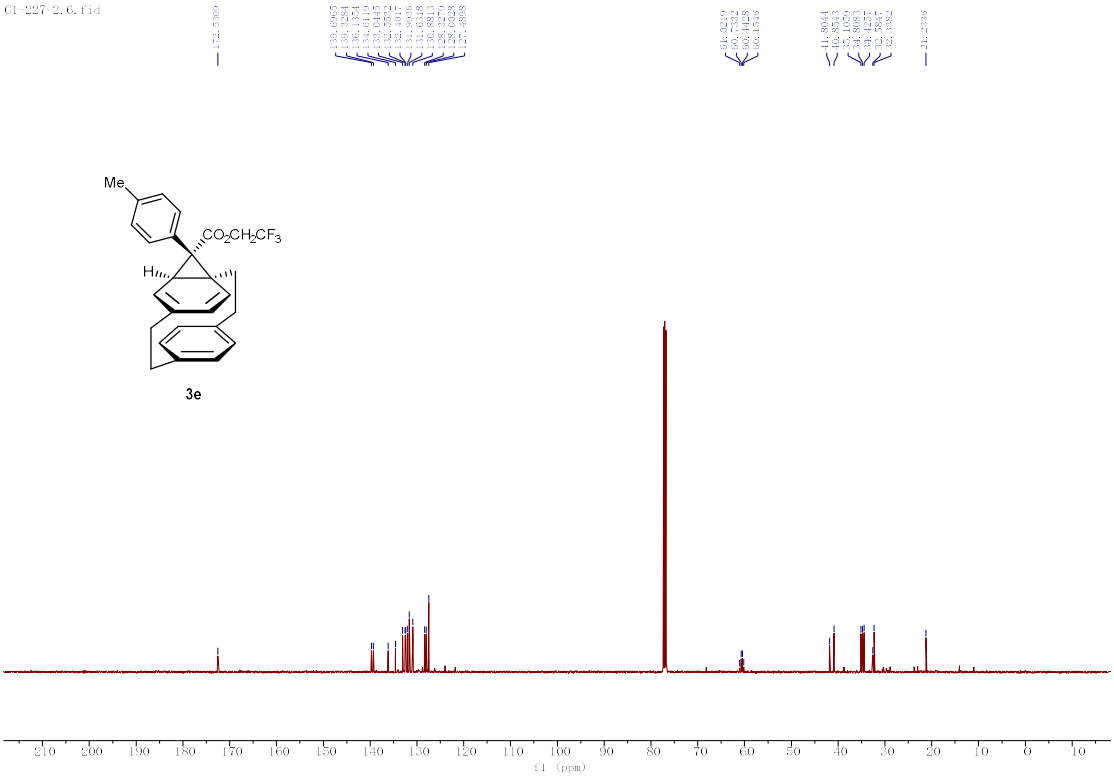



C2-45-4.2.fid
CO2CH2CF3
H
3d
Me
CO2CH2CF3
H
3e
f1 (ppm)

C1-227-2.6.fid



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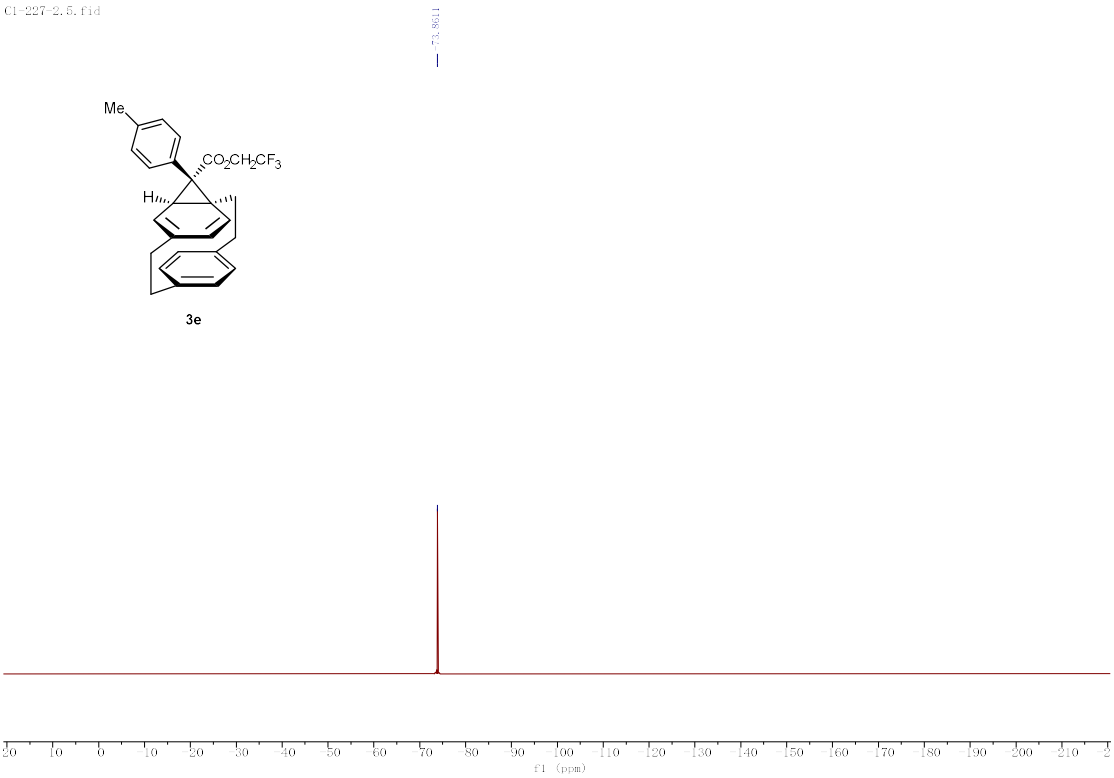

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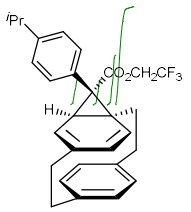

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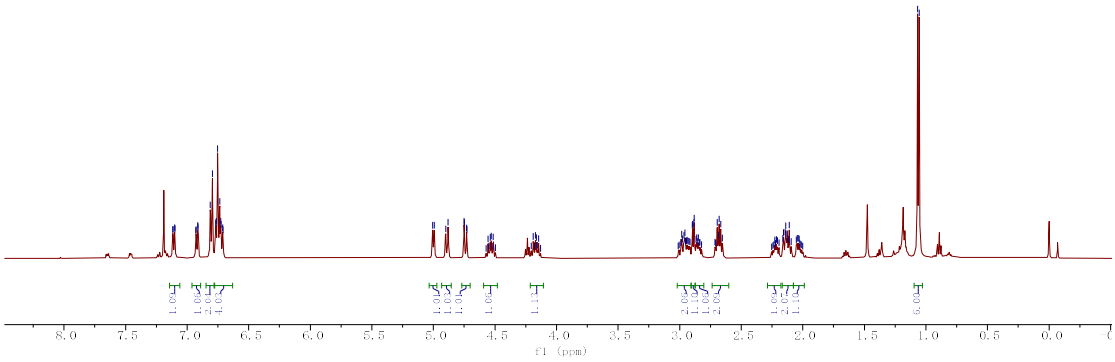

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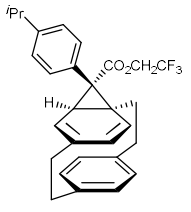

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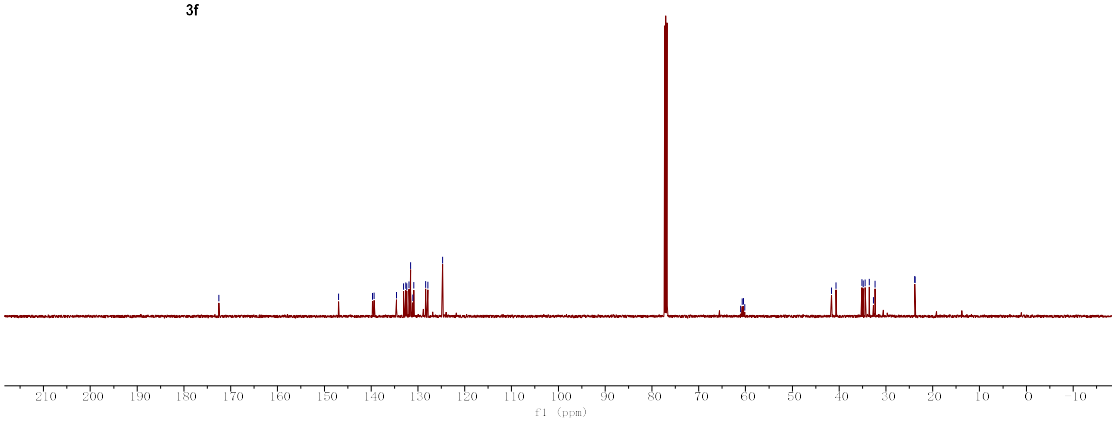

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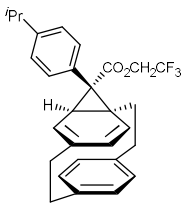

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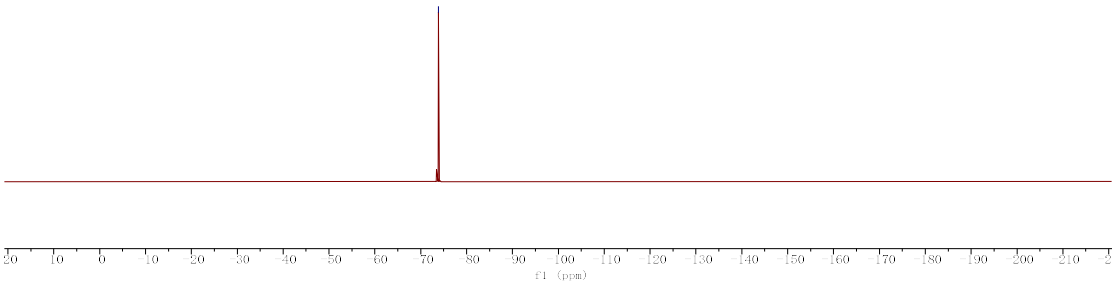

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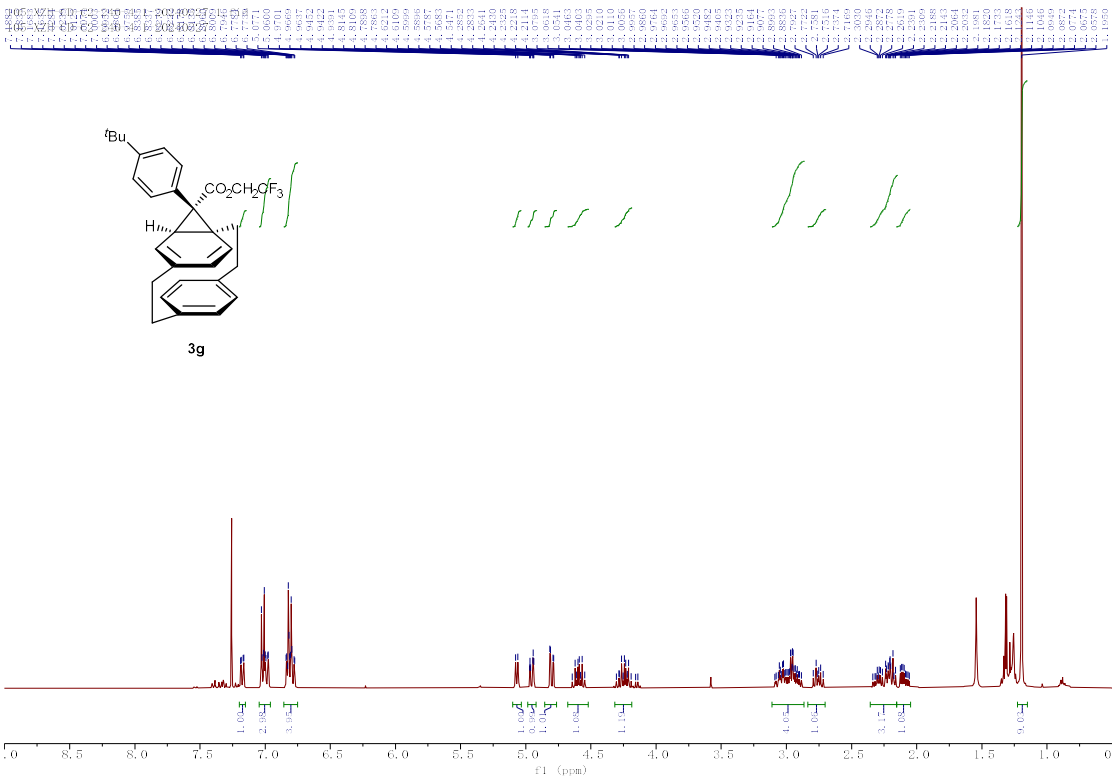

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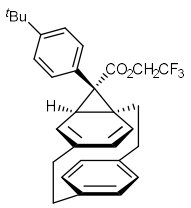

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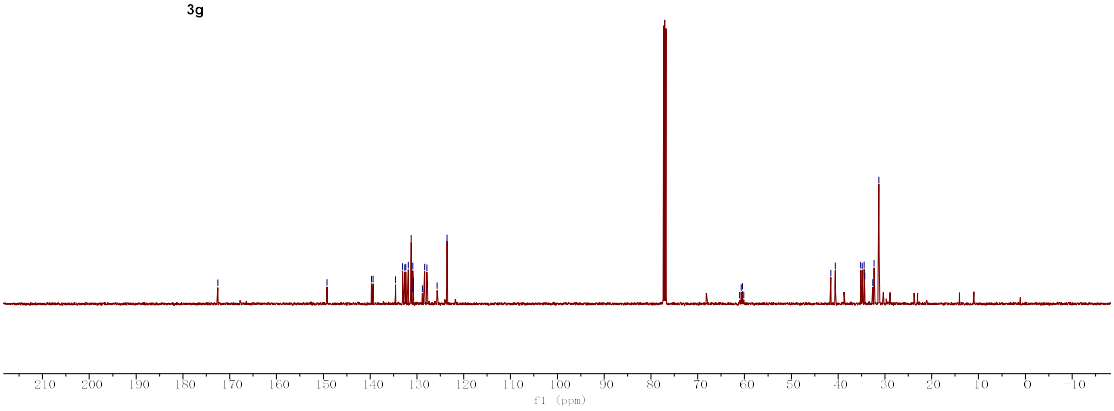

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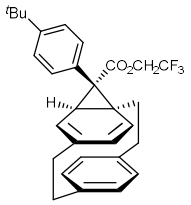

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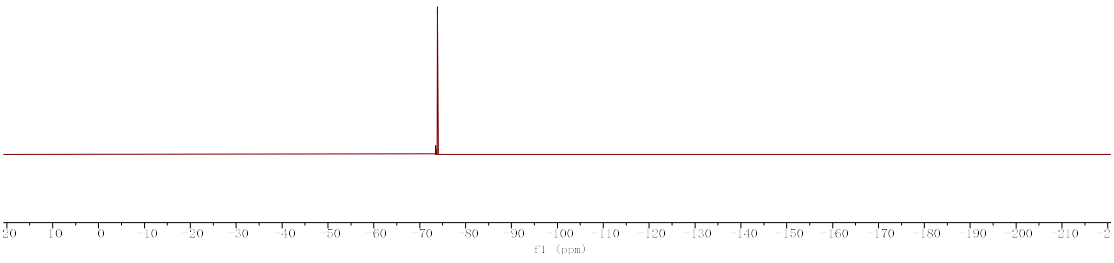
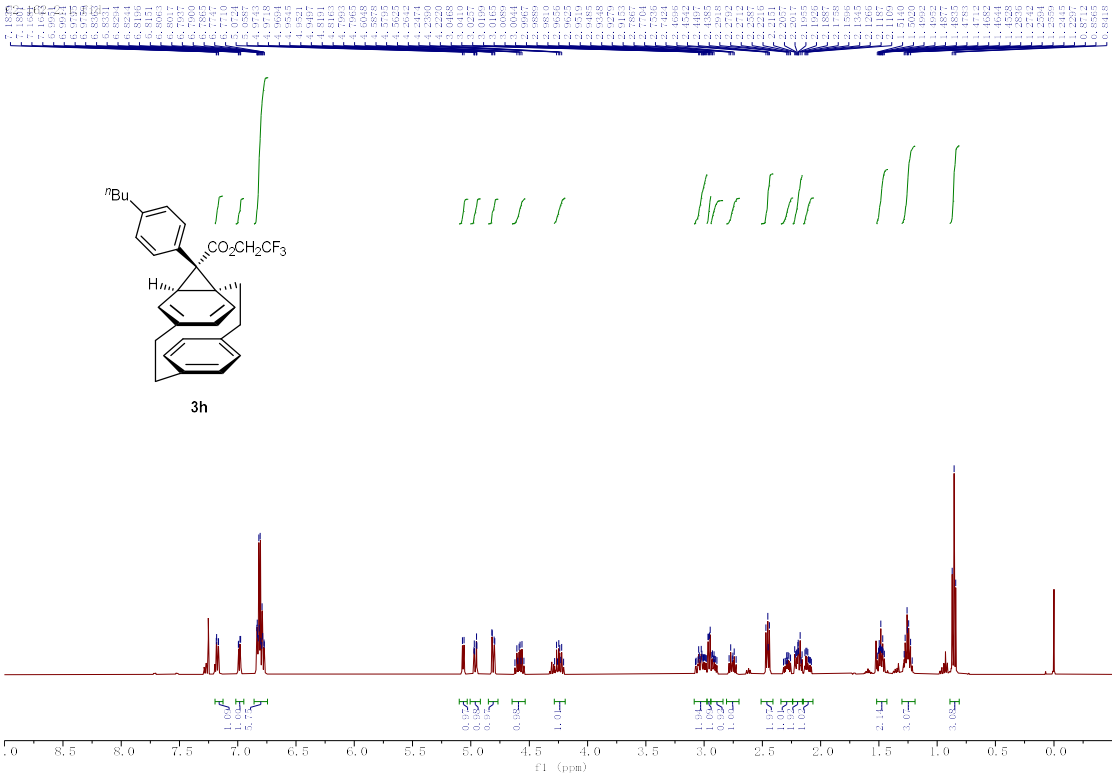
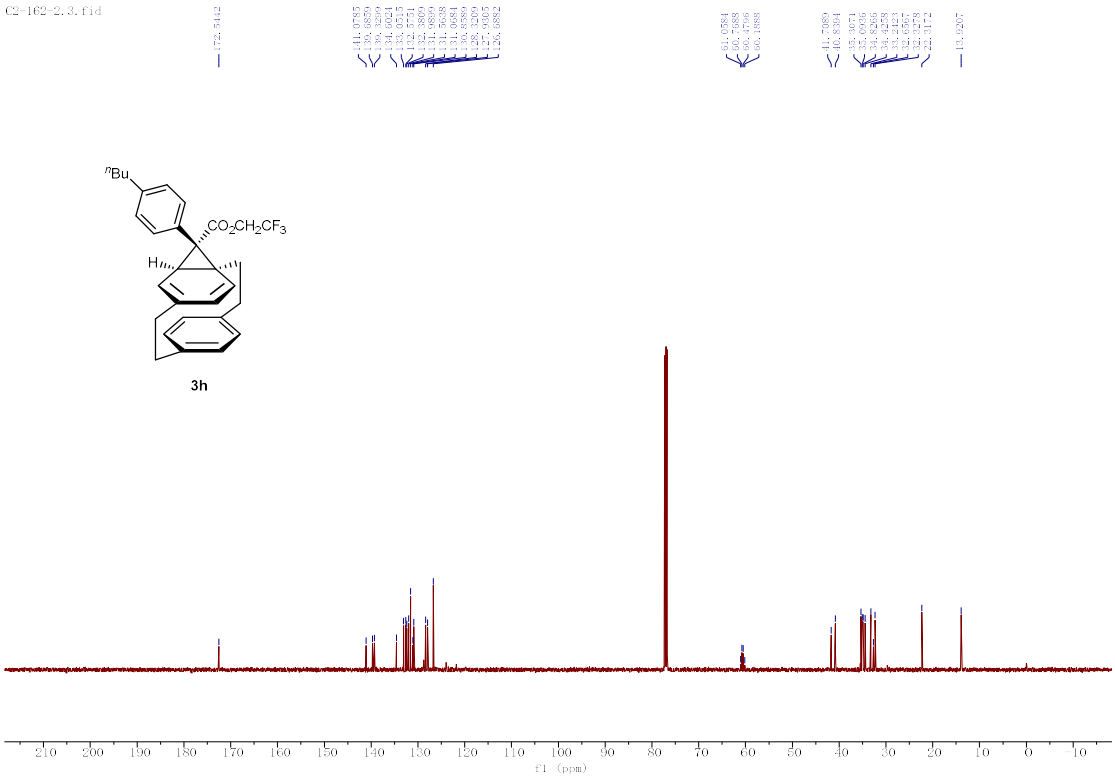



nBu
CO2CH2CF3
H
3h
f1 (ppm)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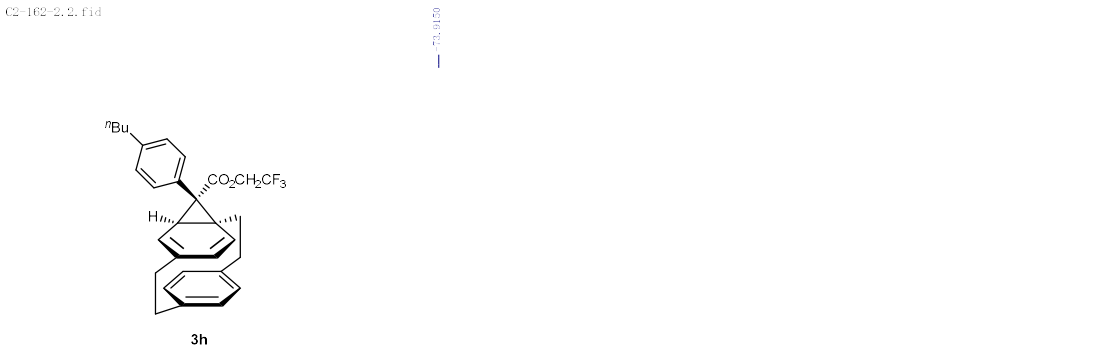
nBu
CO2CH2CF3
H
3h
f1 (ppm)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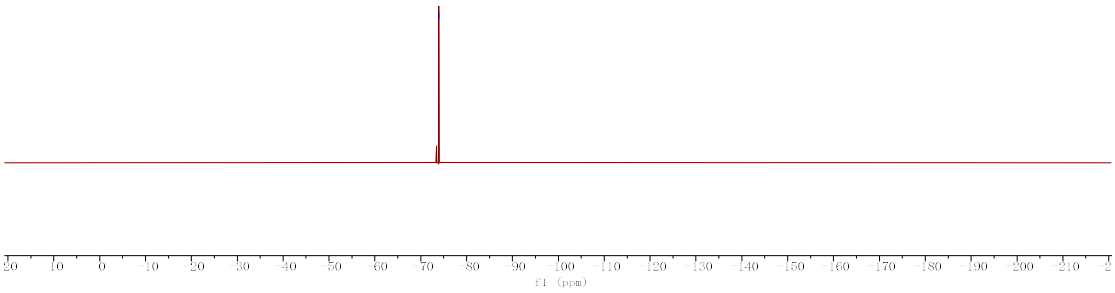
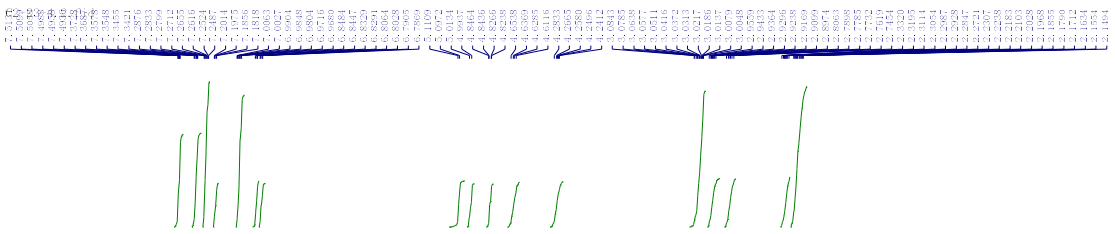
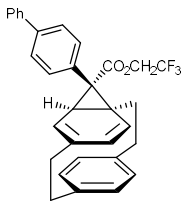
nBu
CO2CH2CF3
H

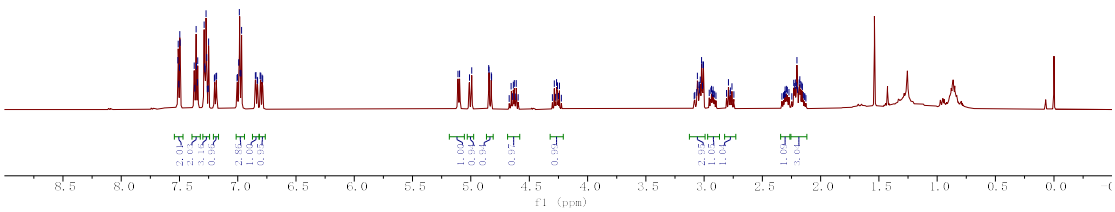
3h


f1 (ppm)

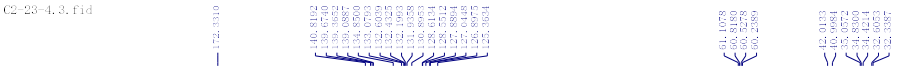


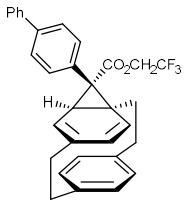

Ph
CO2CH2CF3
H

3i

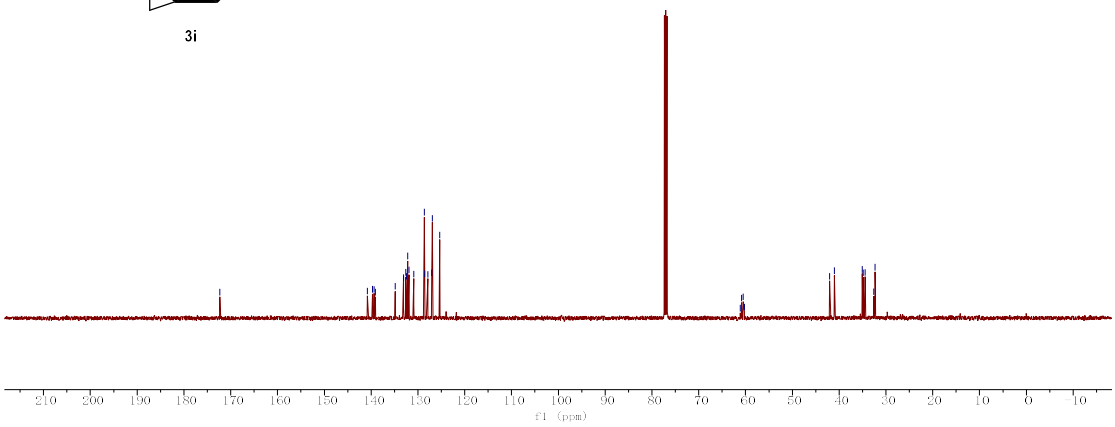

f1 (ppm)

C2-23-4.3.fid

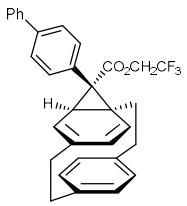




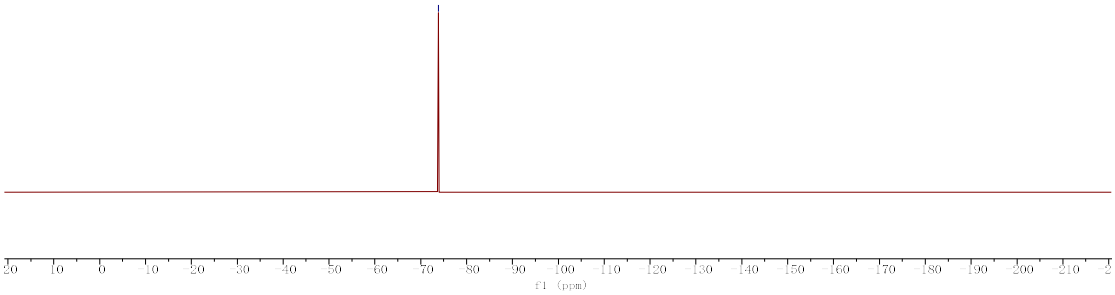
3i



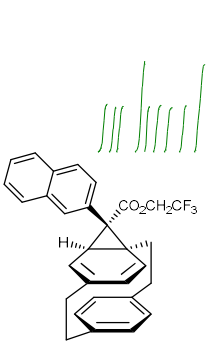
C2-23-4.1.fid



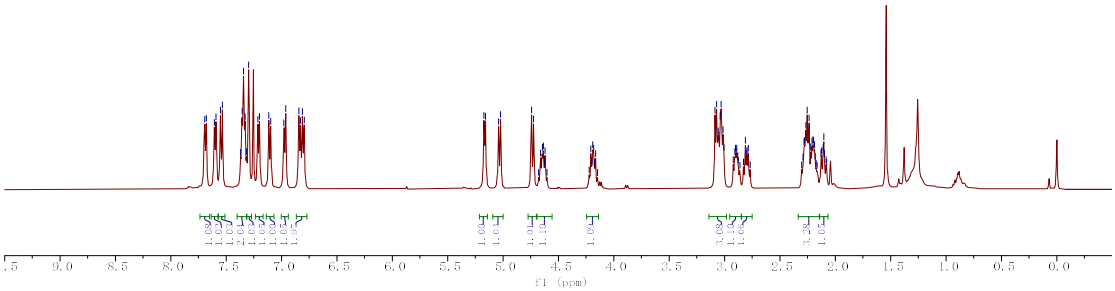
3i



C2-54-2.1.fid

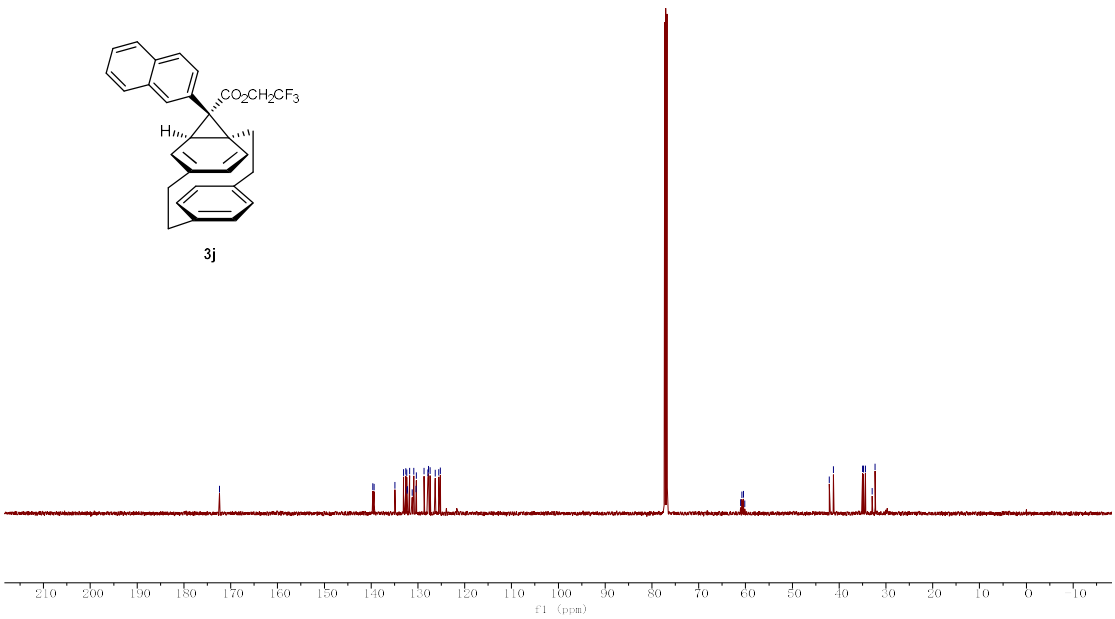


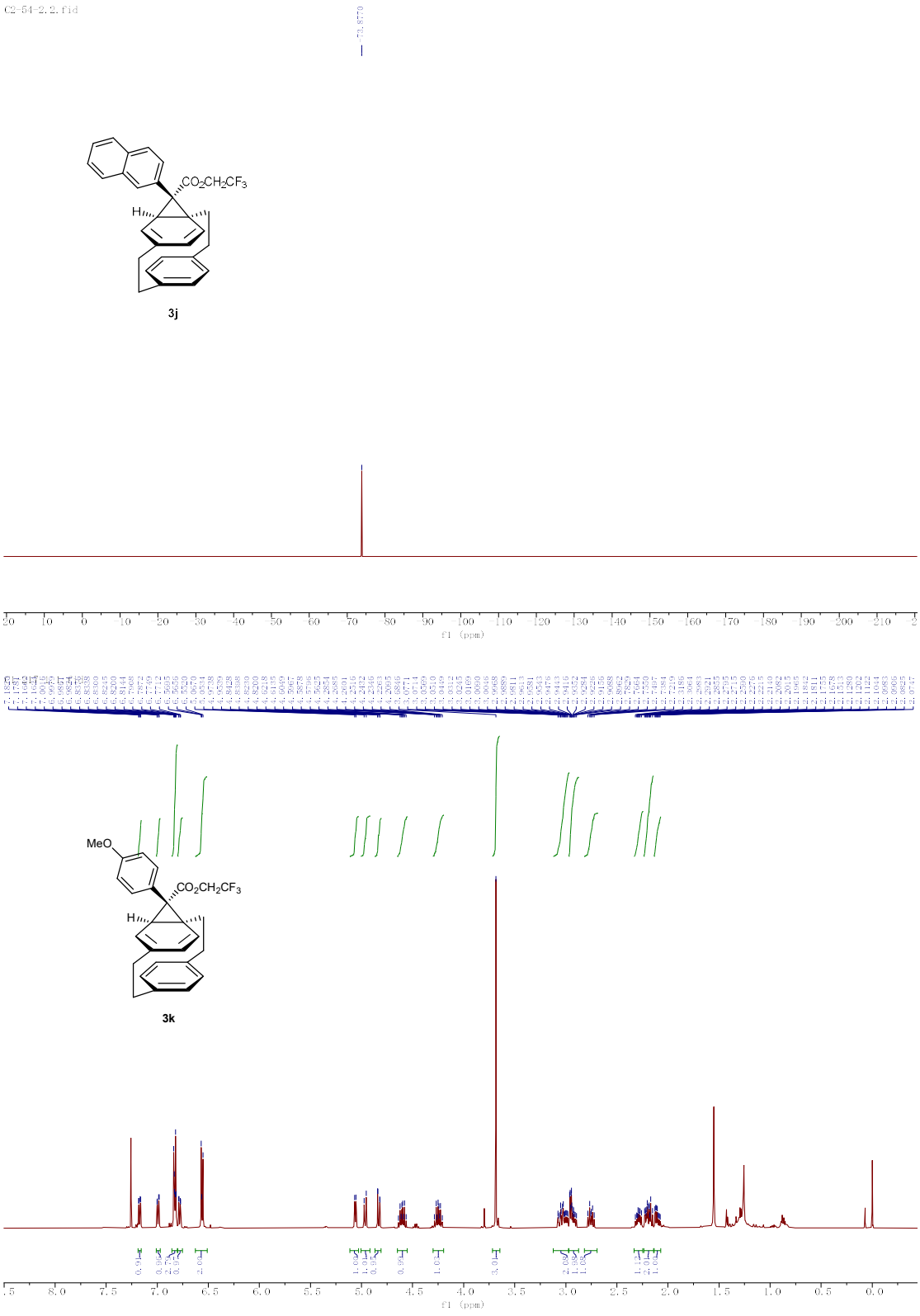
3j

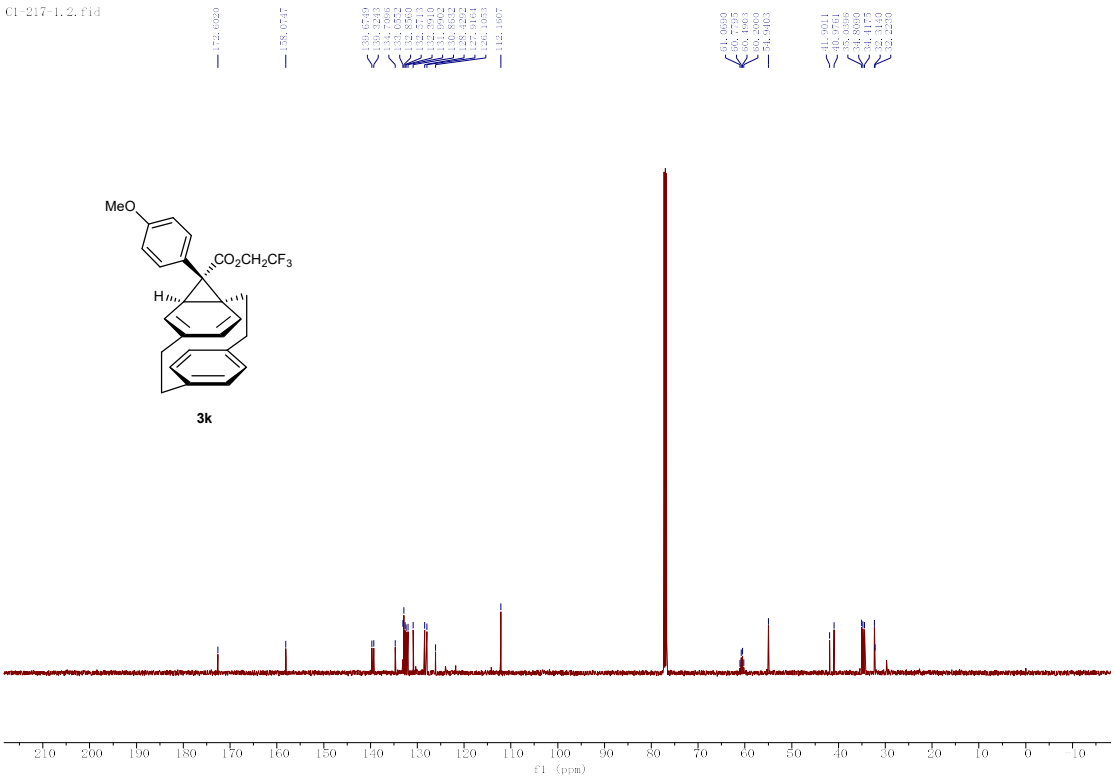


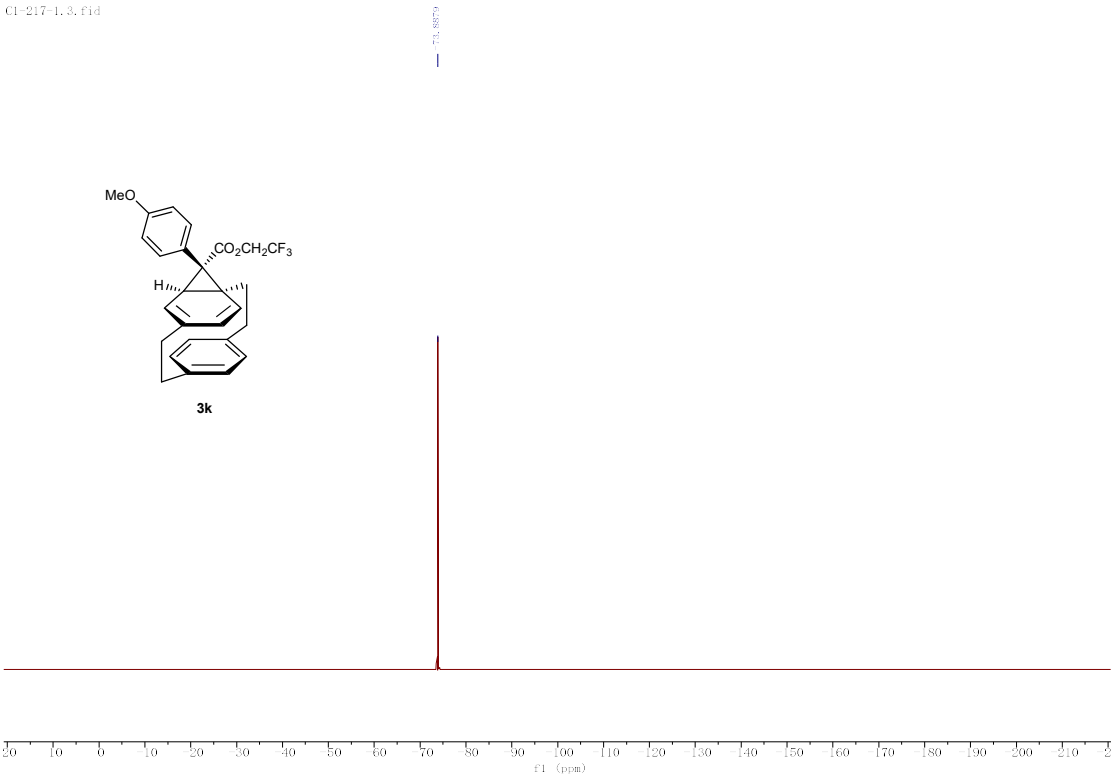
C2-54-2.3.fid

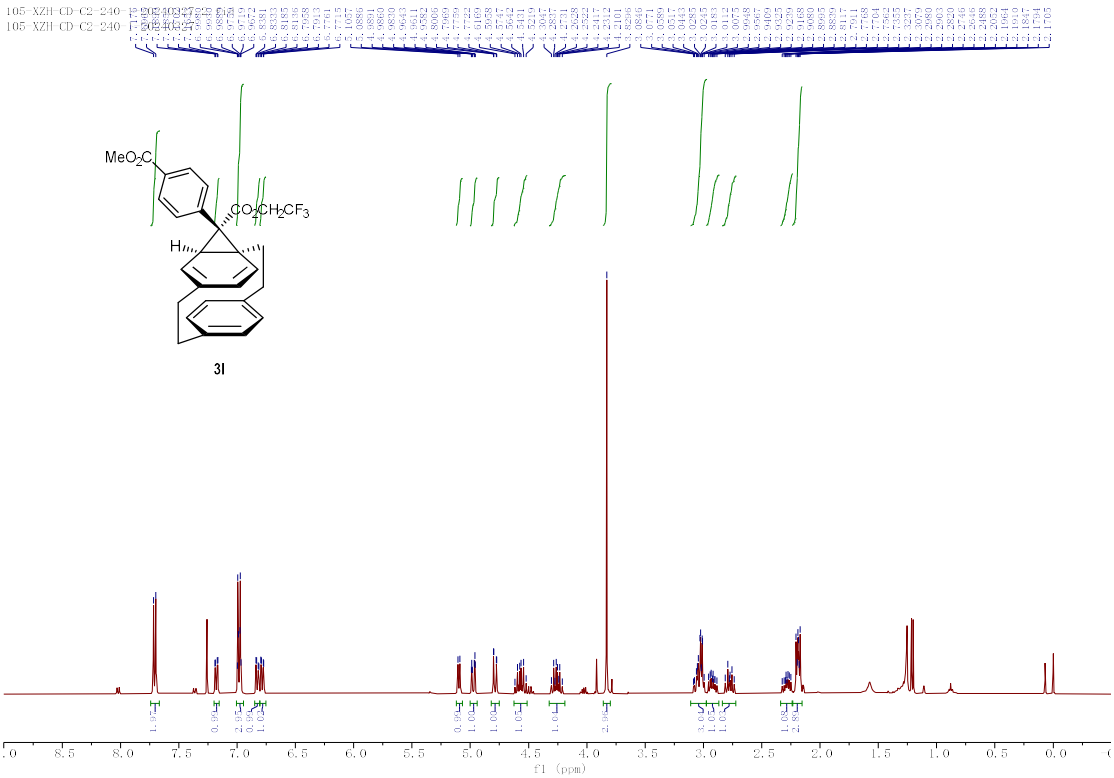
3j

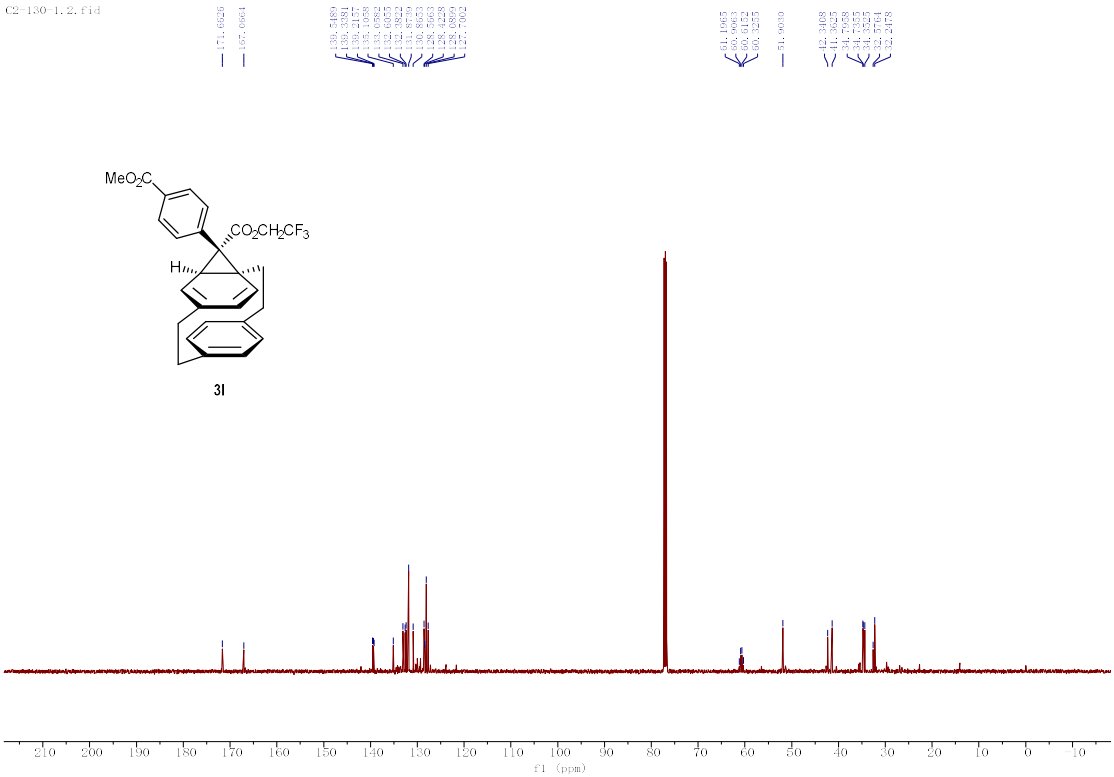



C2-54-2.2.fid
CO2CH2CF3
H
3j
MeO
CO2CH2CF3
H
3k
f1 (ppm)

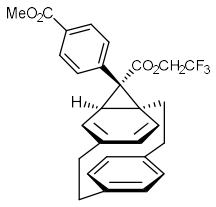

C1-217-1.2.fid
MeO
CO2CH2CF3
H
3k
f1 (ppm)


C1-217-1.3.fid
MeO
CO2CH2CF3
H
3k
f1 (ppm)

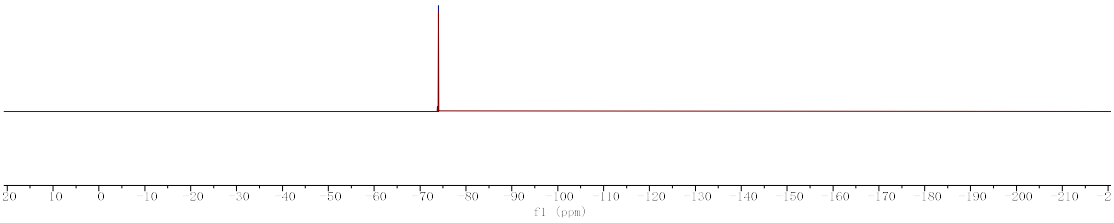

MeO2C
CO2CH2CF3
H
3l
f1 (ppm)


MeO2C
CO2CH2CF3
H
3l
f1 (ppm)

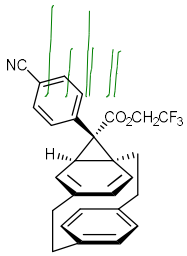
105-XZH-CD-C2-240-1-20240327.3.fid
105-XZH-CD-C2-240-1-20240327



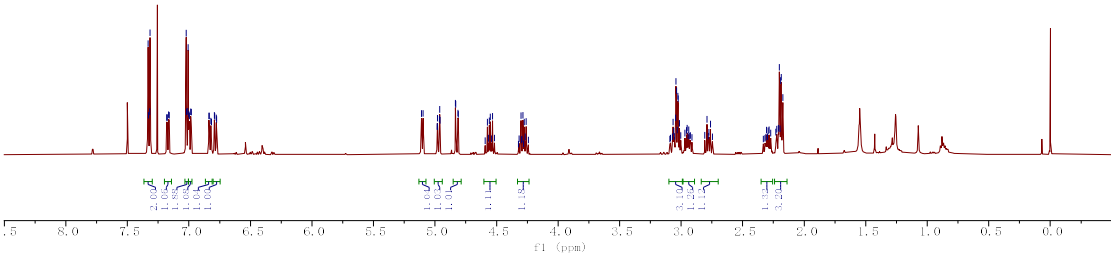
3l



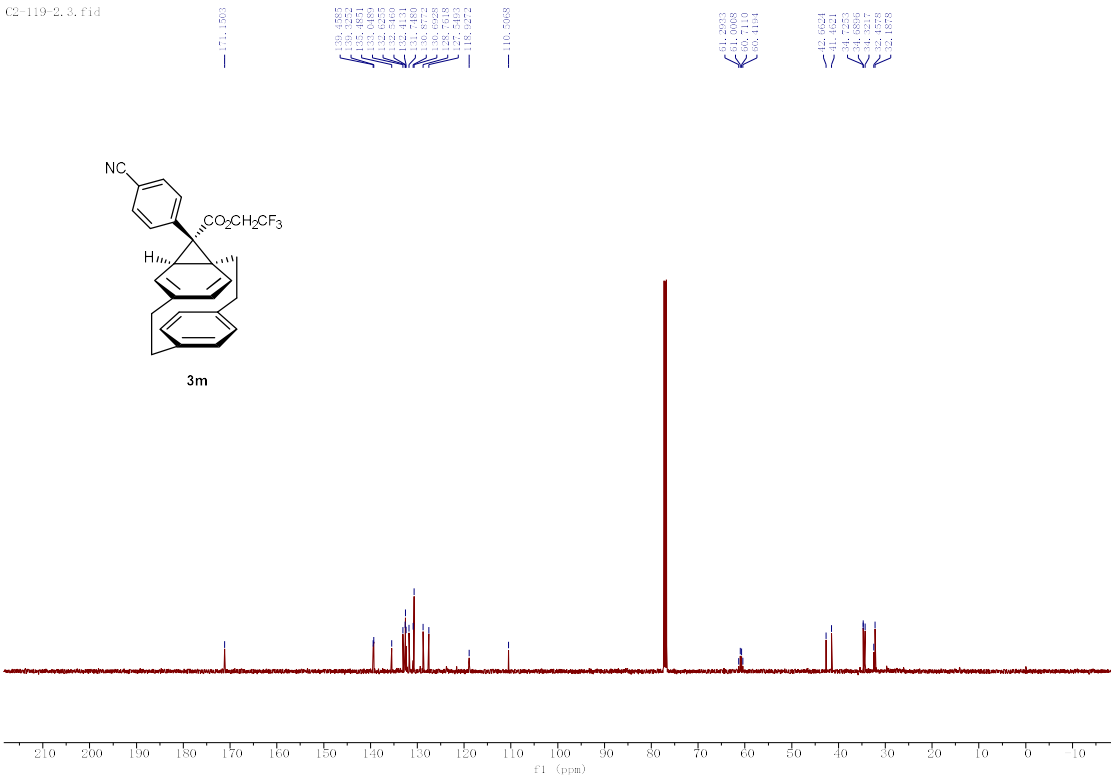
C2-119



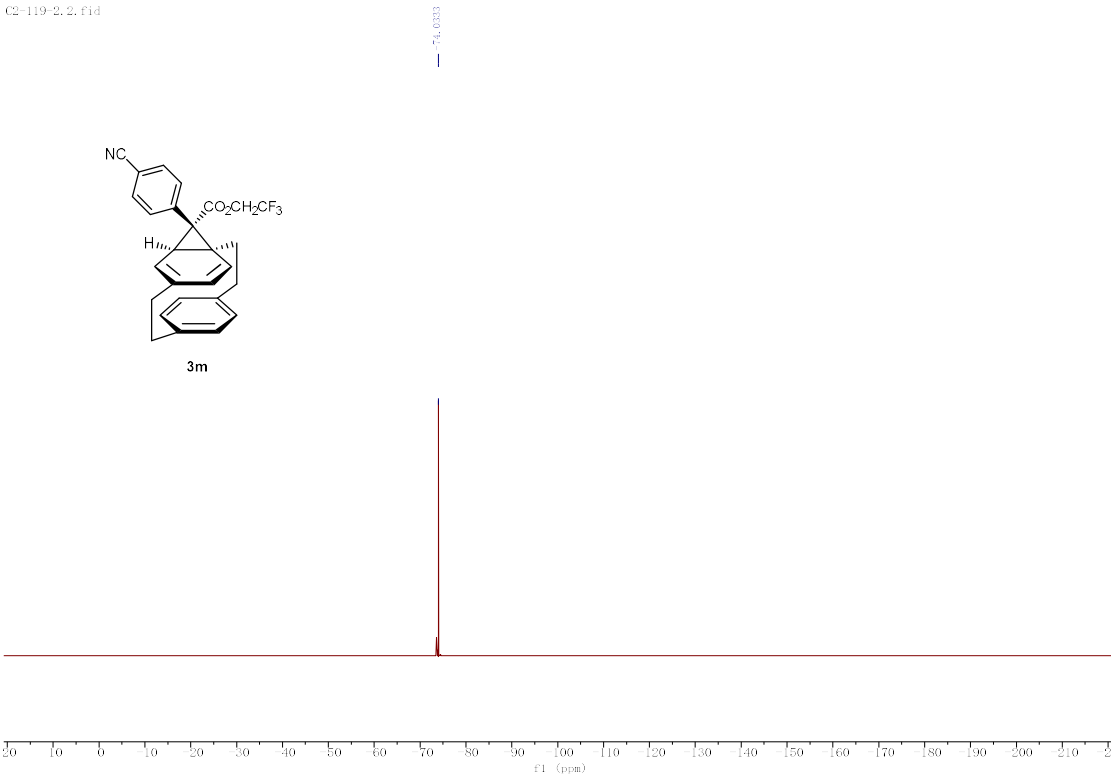
3m

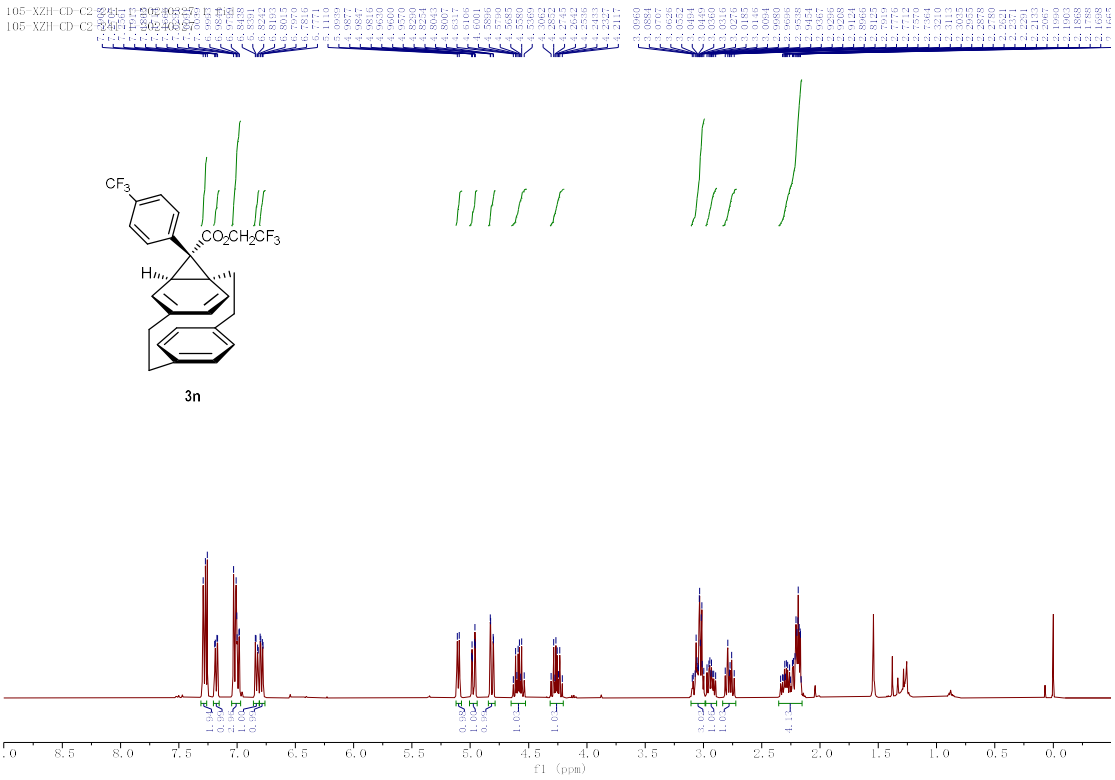


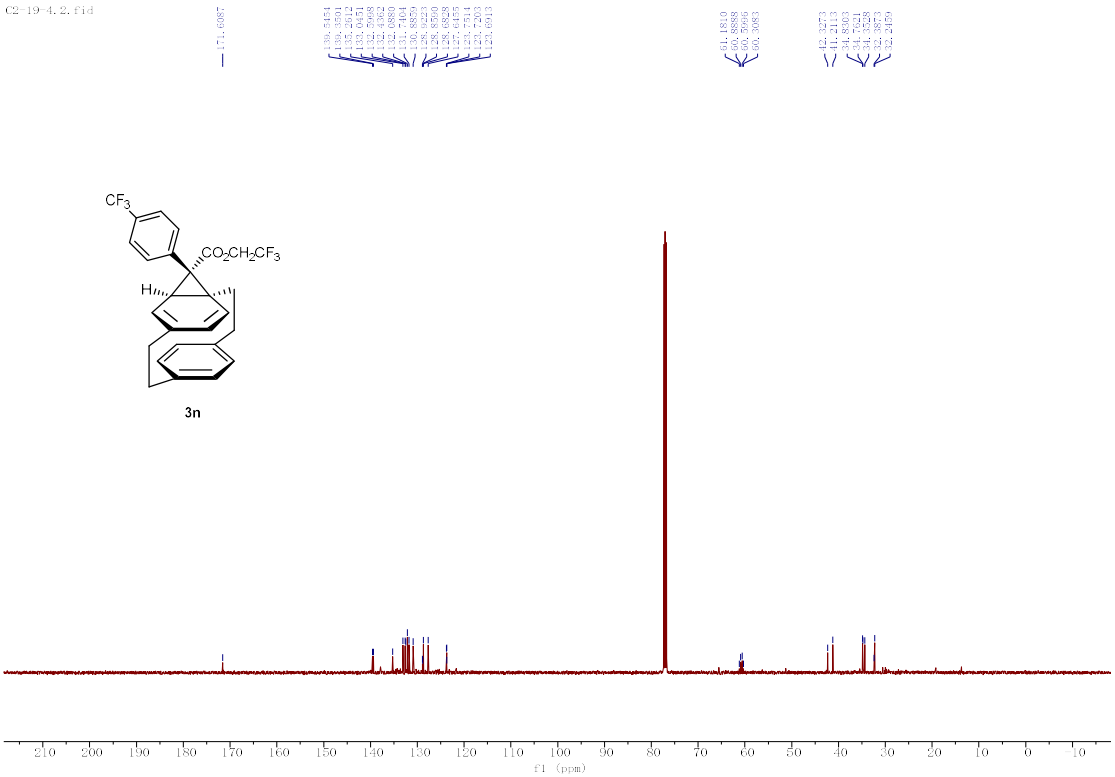
C2-119-2.3.fid

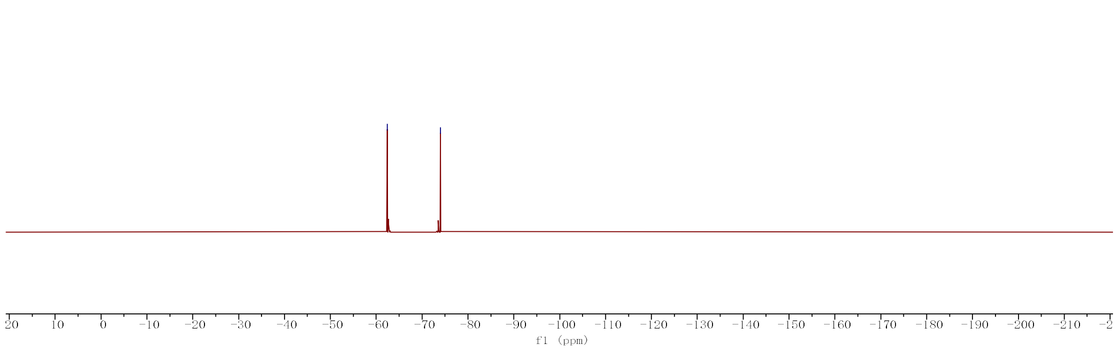


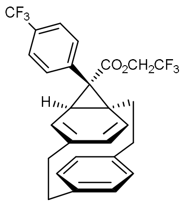
C2-119-2.2.fid



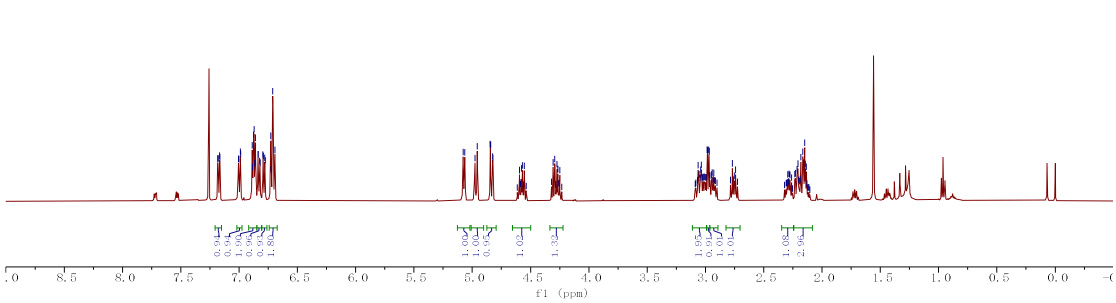

105-XZH-CD-C2
105-XZH-CD-C2
CF3
CO2CH2CF3
H
3n
f1 (ppm)

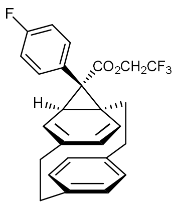

C2-19-4.2.fid
CF3
CO2CH2CF3
H
3n
f1 (ppm)





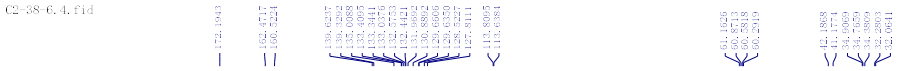
3n

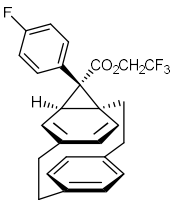




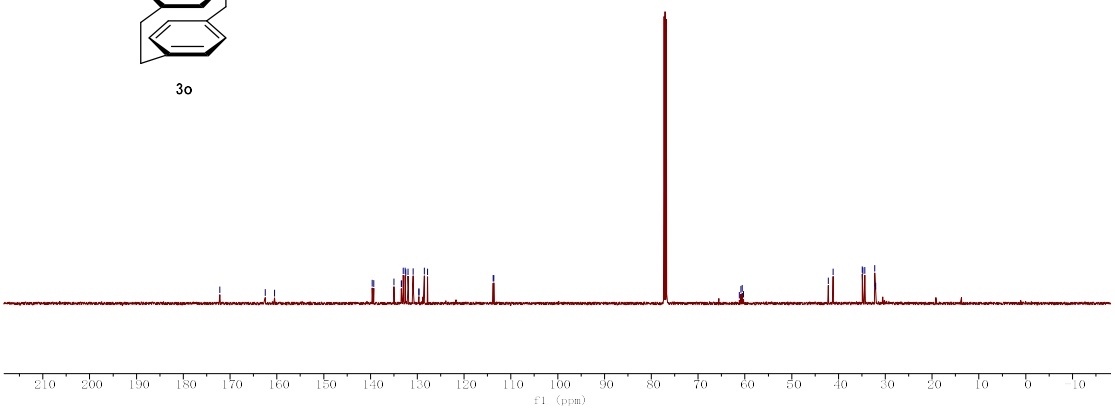
3o

C2-38-6.4.fid

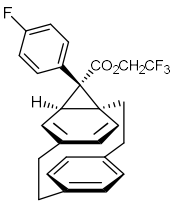




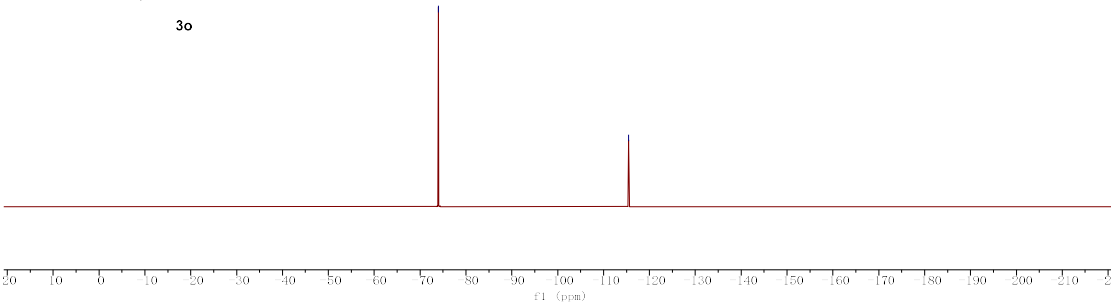
3o

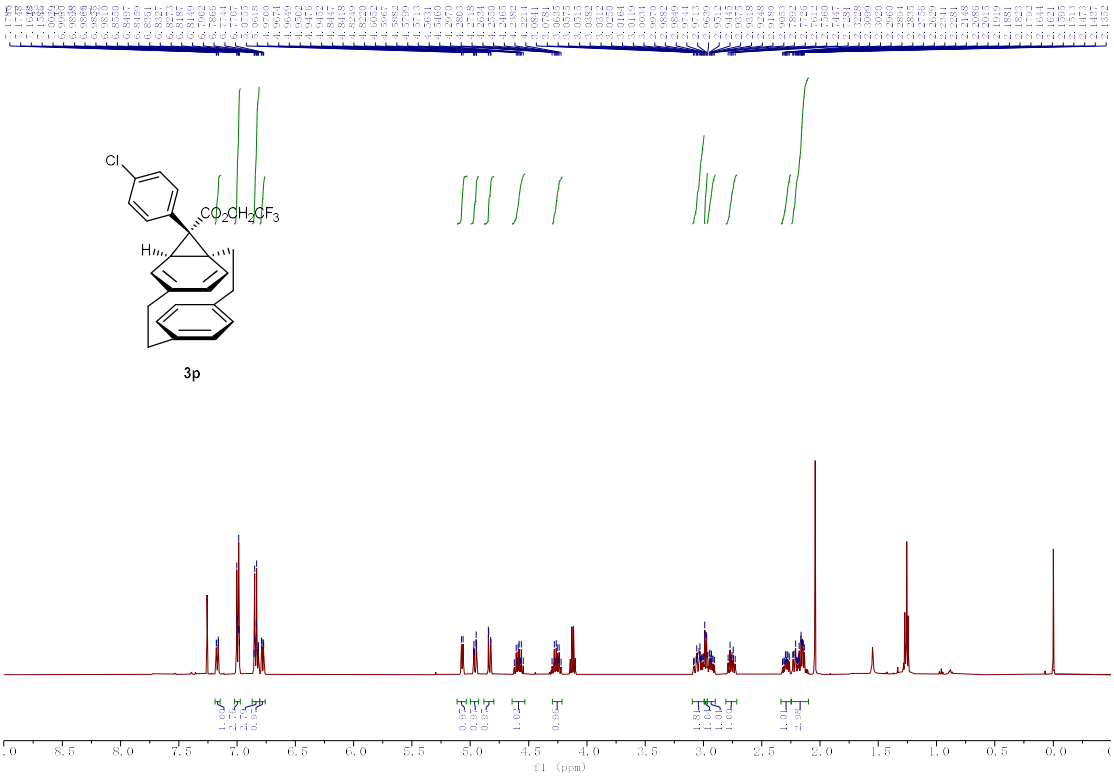


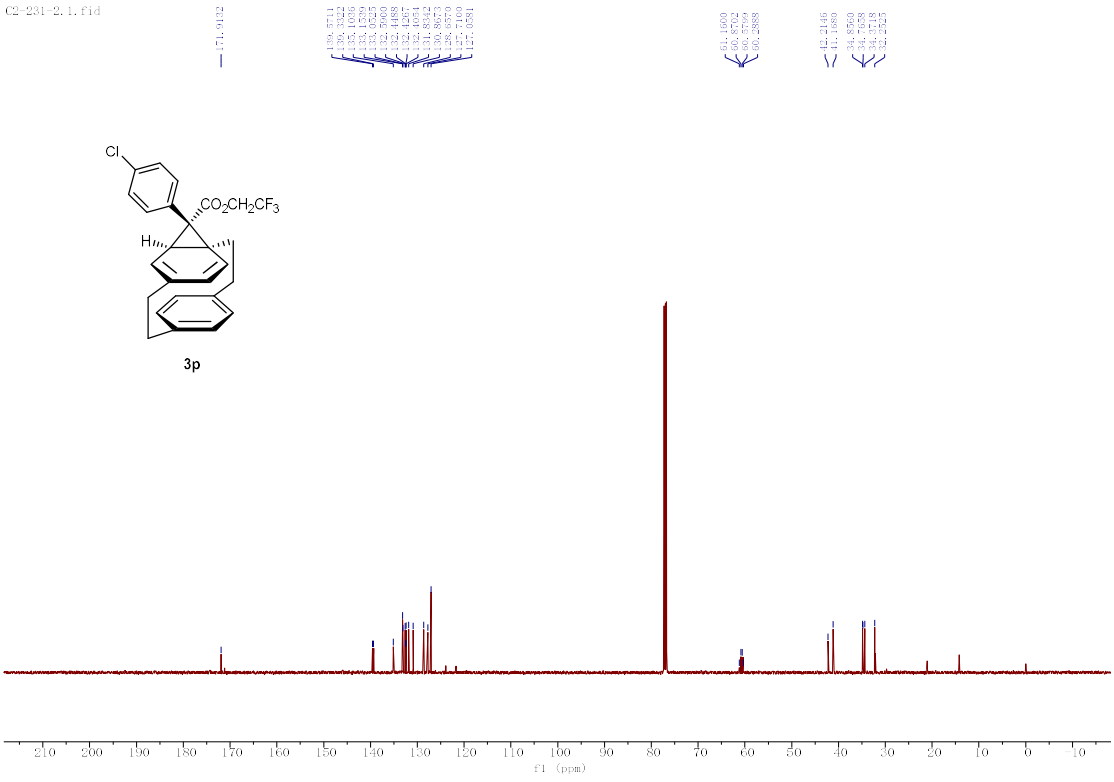
C2-38-6.5.fid

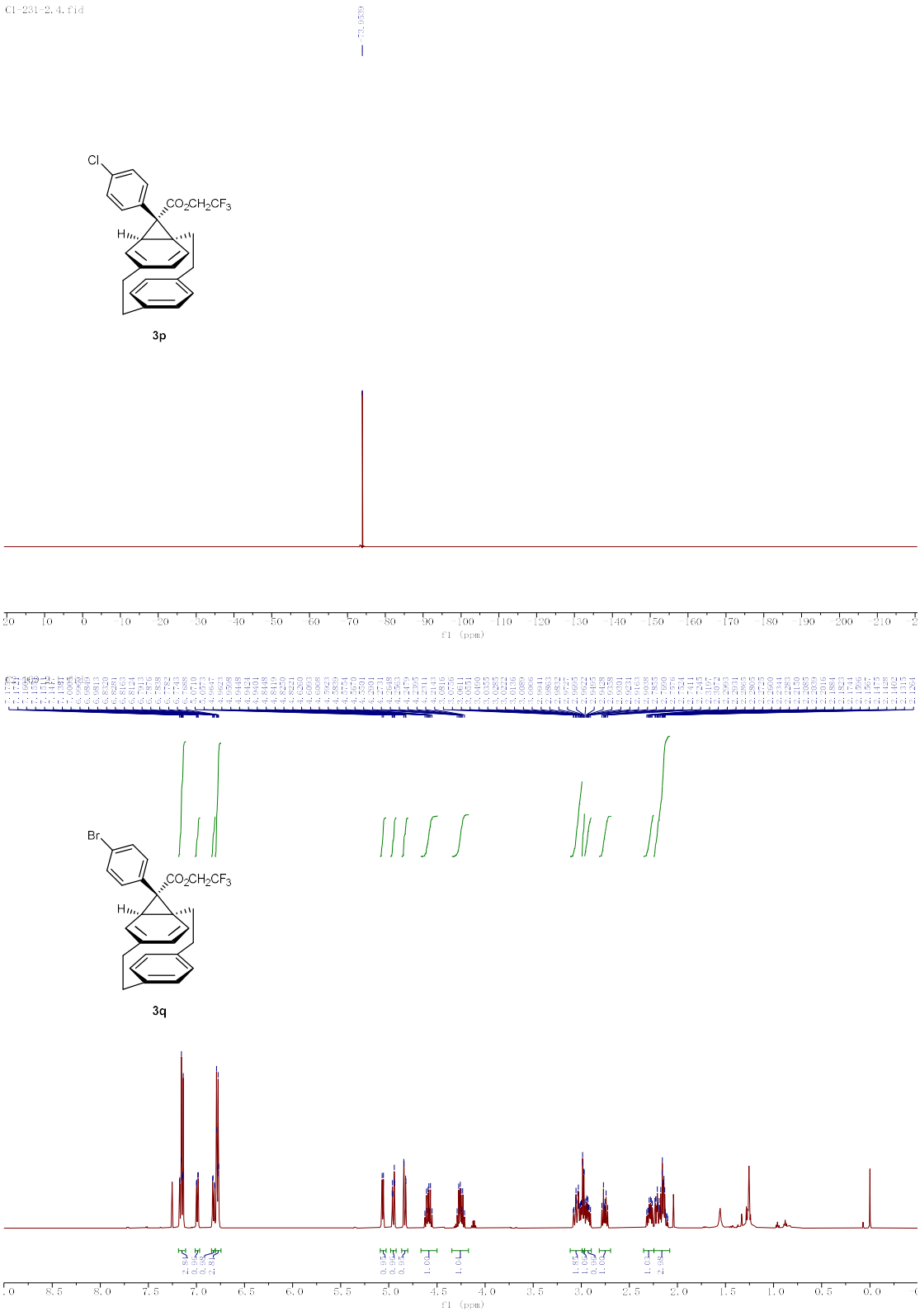


3o

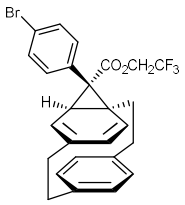



Cl
CO2CH2CF3
H
3p
f1 (ppm)

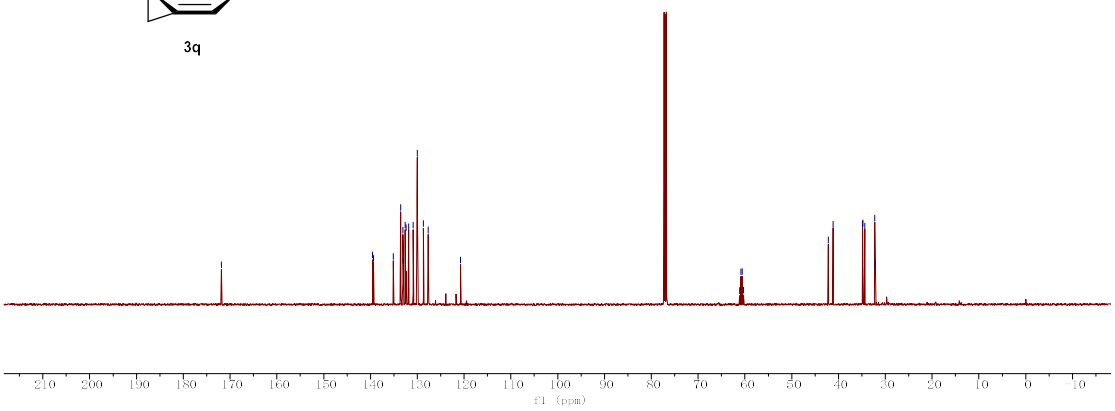

C2-231-2.1.fid
Cl
CO2CH2CF3
H
3p
f1 (ppm)


Cl
CO2CH2CF3
H
3p
Br
CO2CH2CF3
H
3q
f1 (ppm)

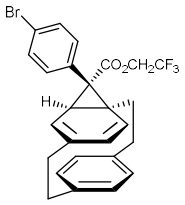
C2-169-2.2.fid



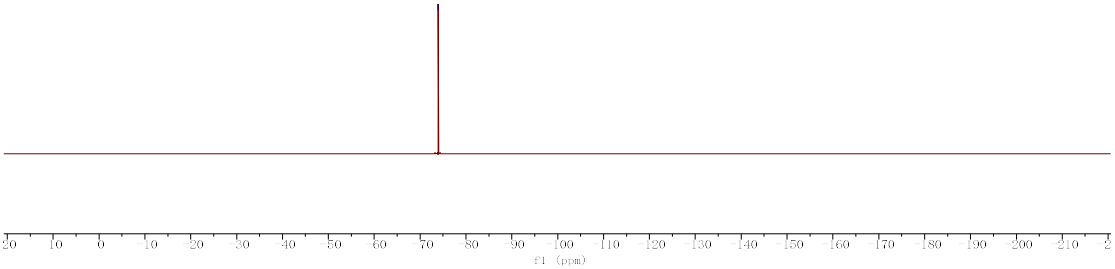
3q

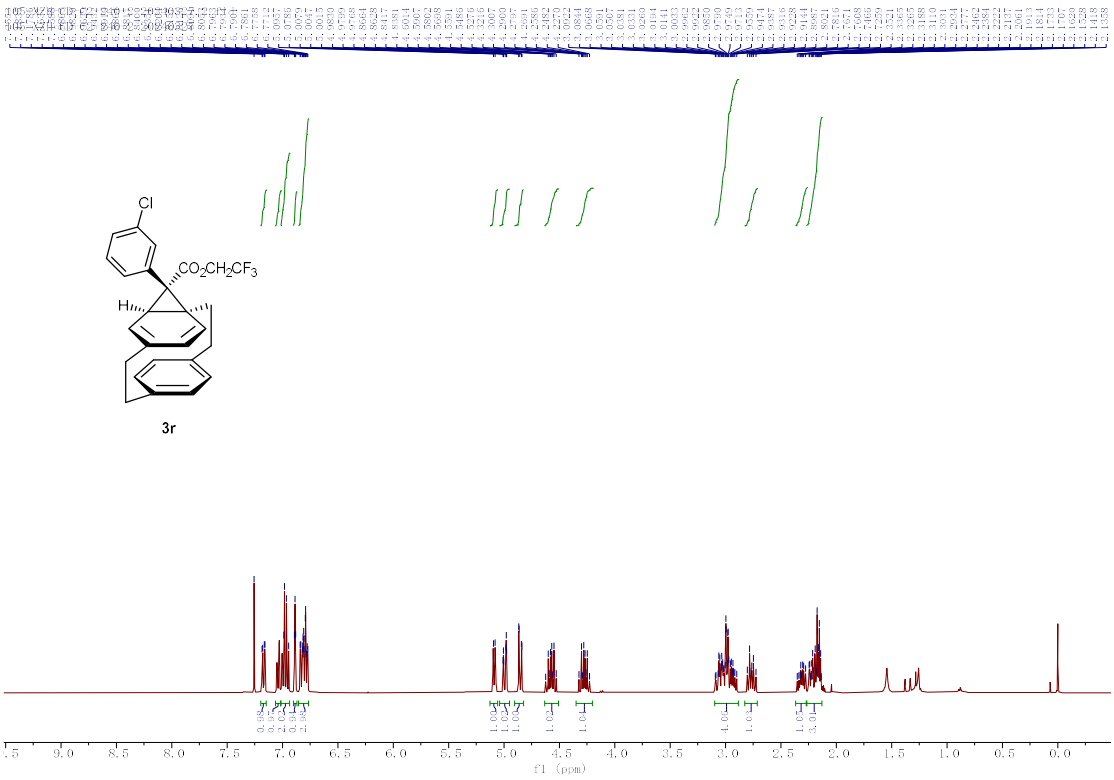


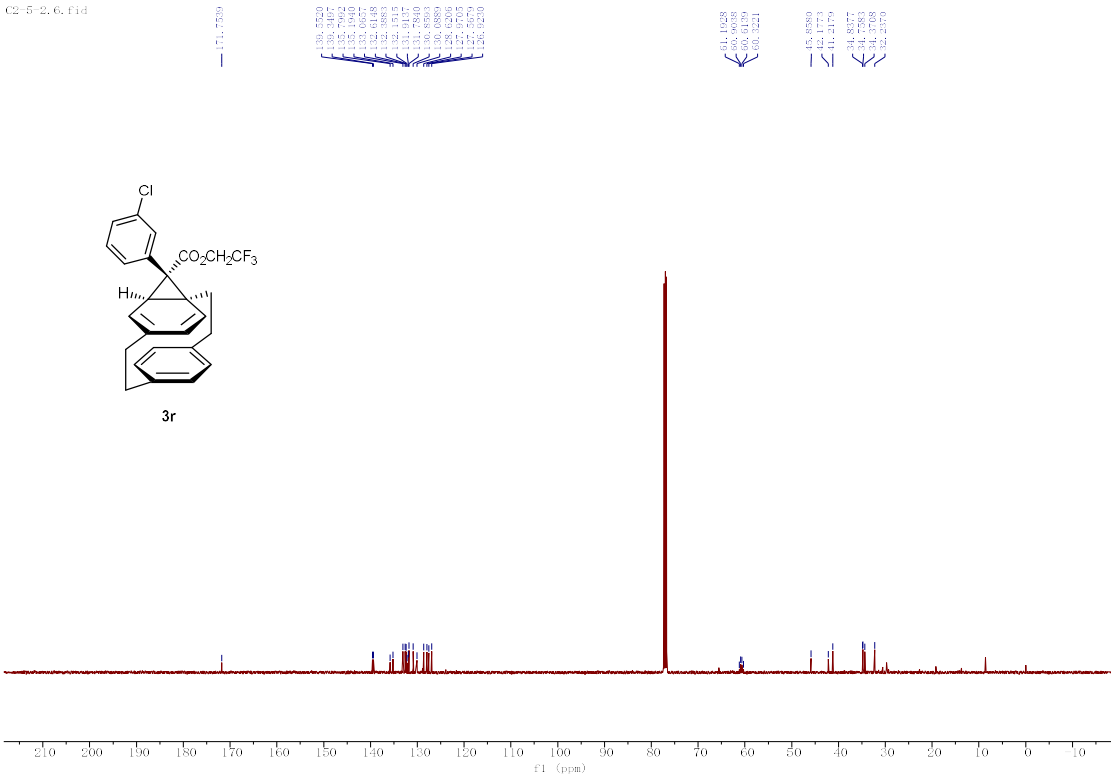
C2-169-2.3.fid



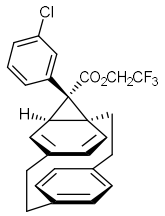
3q



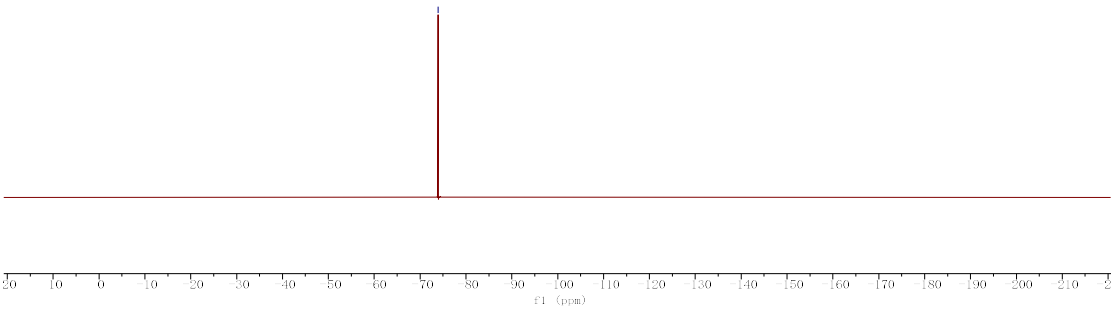

Cl
CO2CH2CF3
H
3r
f1 (ppm)


C2-5-2.6.fid
Cl
CO2CH2CF3
H
3r
f1 (ppm)

C2-5-2.5.fid

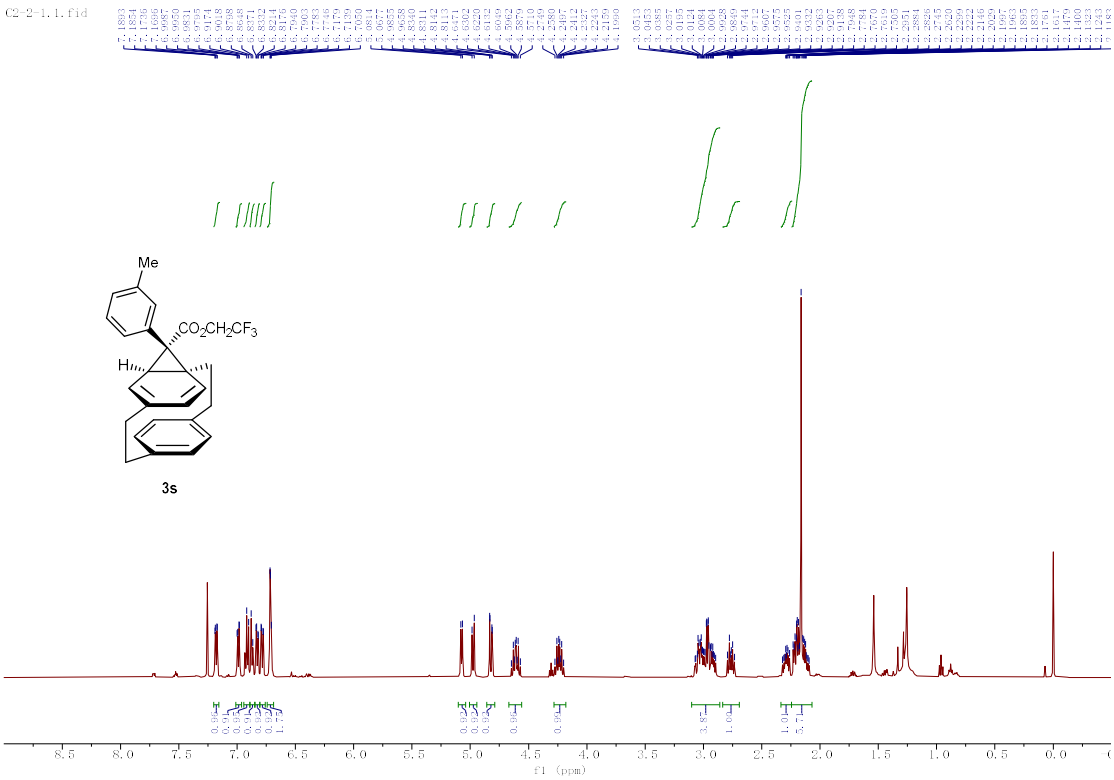


3r

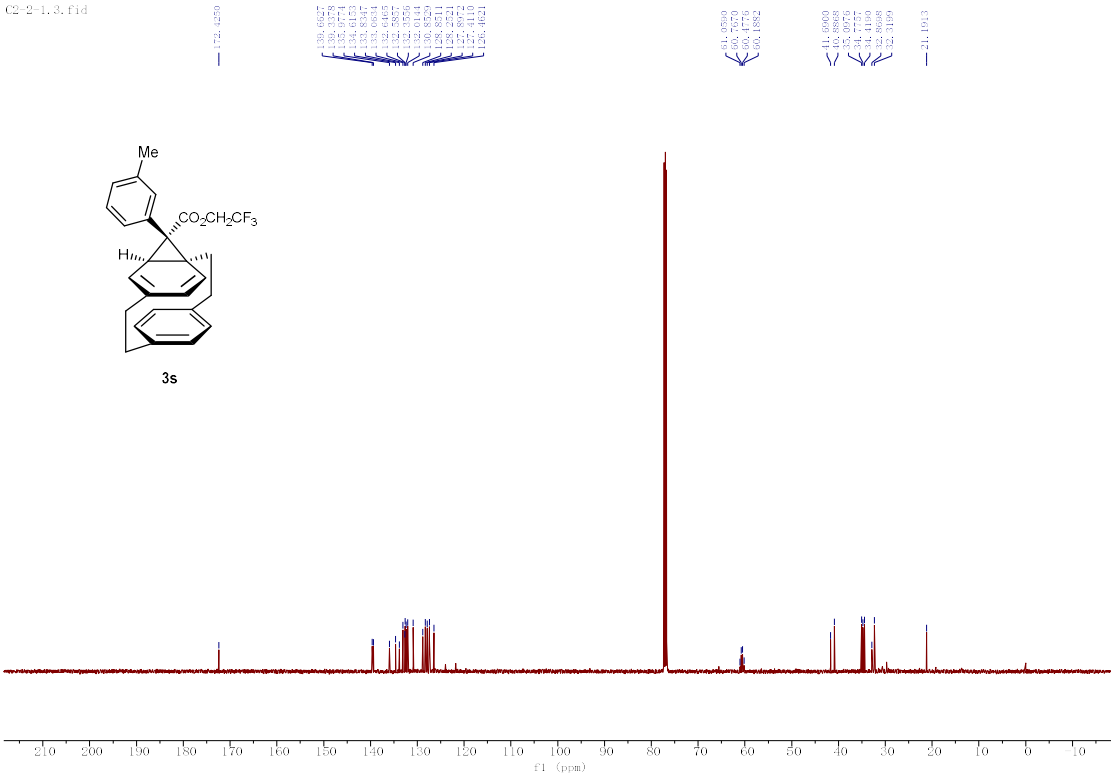


C2-2-1.1.fid

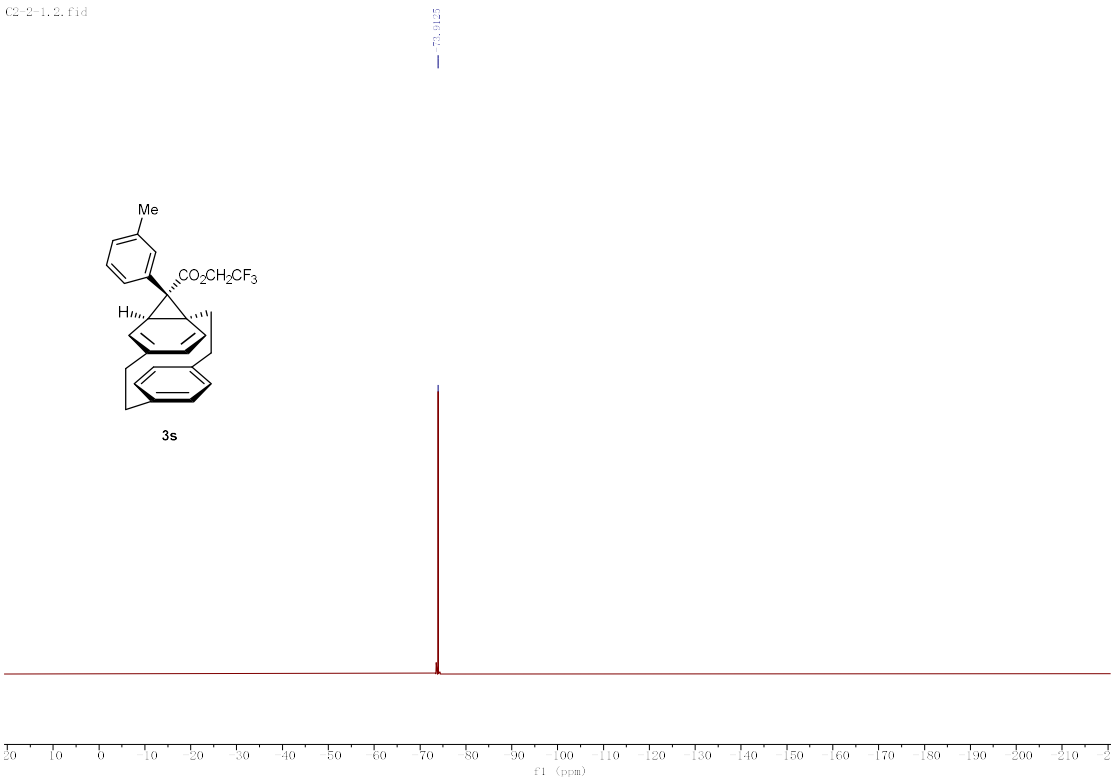
3s

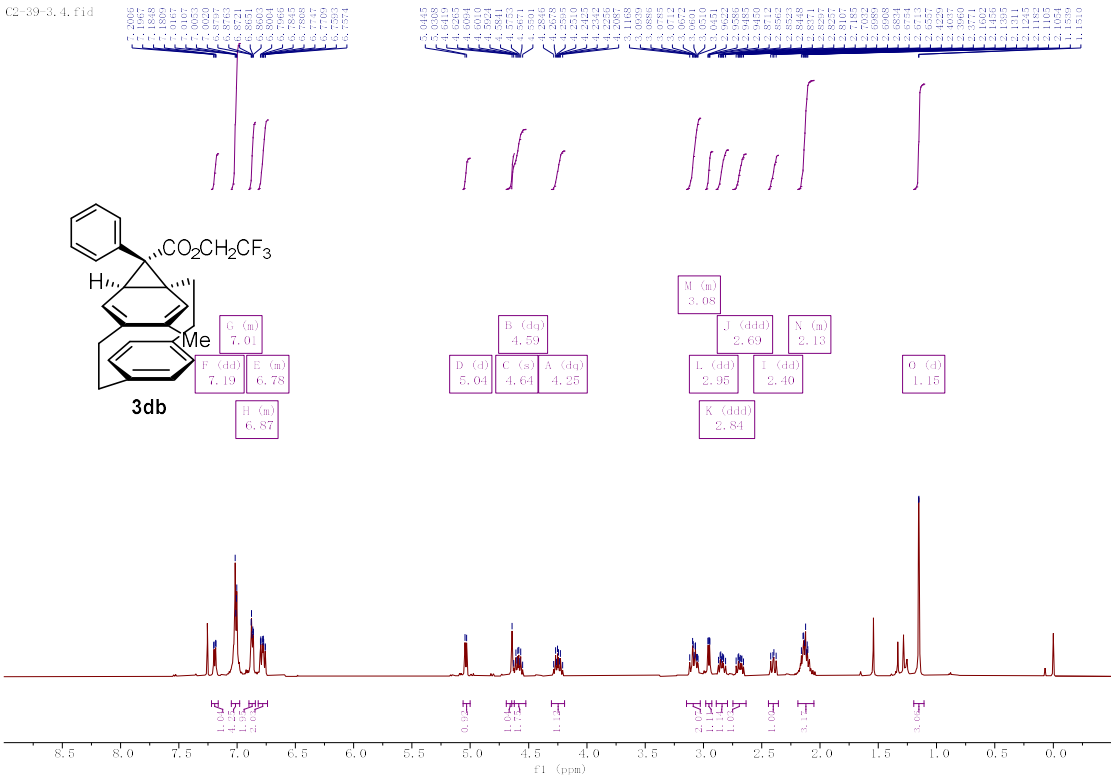


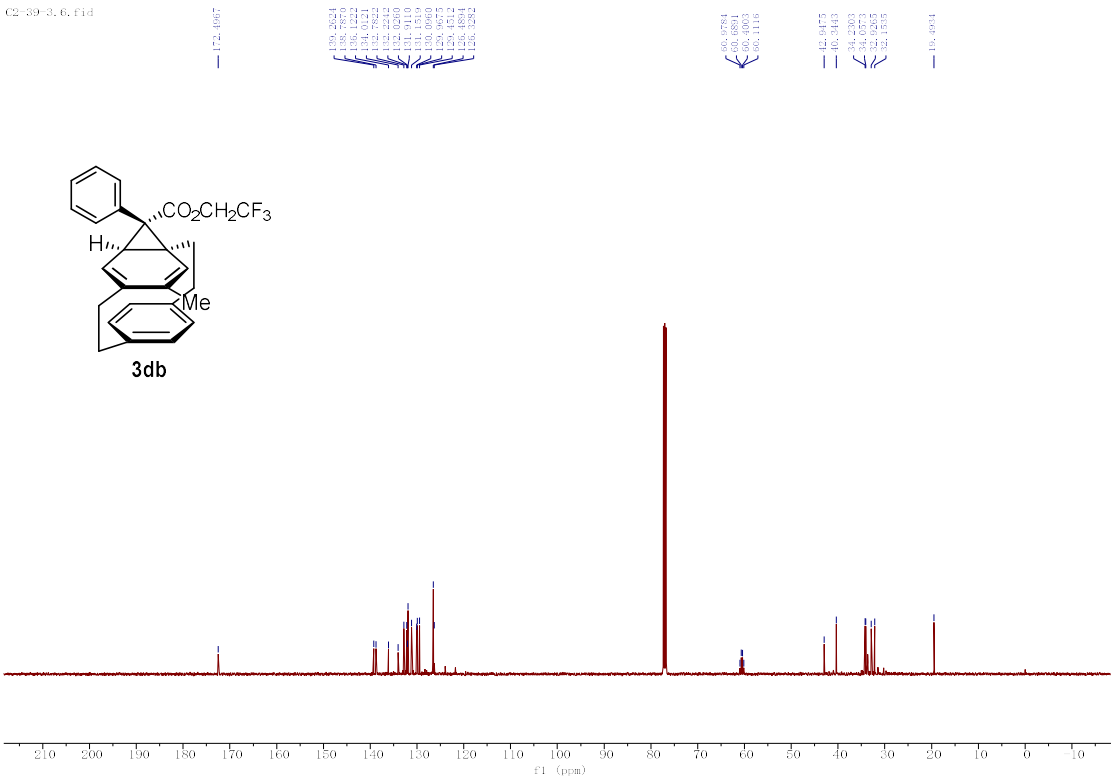
C2-2-1.3.fid

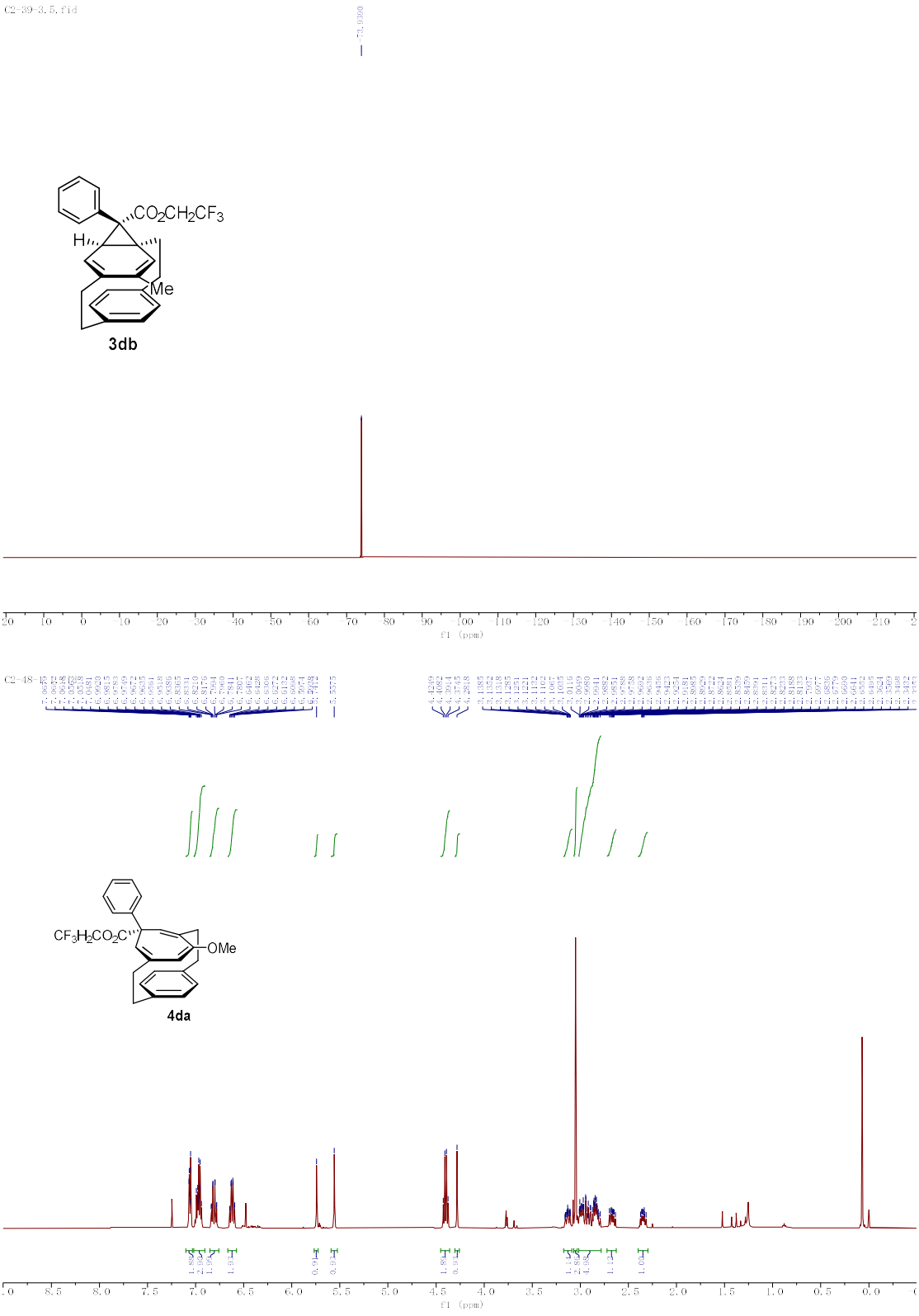


C2-2-1.2.fid

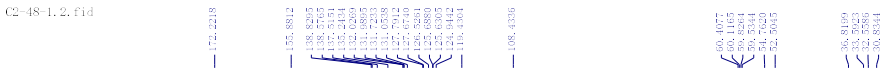


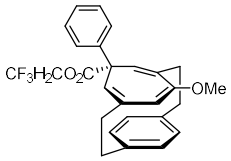

C2-39-3.4.fid
CO2CH2CF3
H
Me
3db
G (m) 7.01
F (dd) 7.19
E (m) 6.78
H (m) 6.87
B (dq) 4.59
D (d) 5.04
C (s) 4.64
A (dq) 4.25
M (m) 3.08
J (ddd) 2.69
N (m) 2.13
L (dd) 2.95
I (dd) 2.40
K (ddd) 2.84
O (d) 1.15
f1 (ppm)


C2-39-3.6.fid
CO2CH2CF3
H
Me
3db
f1 (ppm)


C2-39-3.5.fid
CO2CH2CF3
H
Me
3db
f1 (ppm)
C2-48-
CF3H2CO2C
OMe
4da
f1 (ppm)

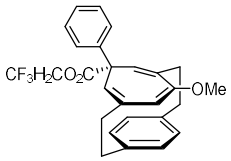
C2-48-1.2.fid



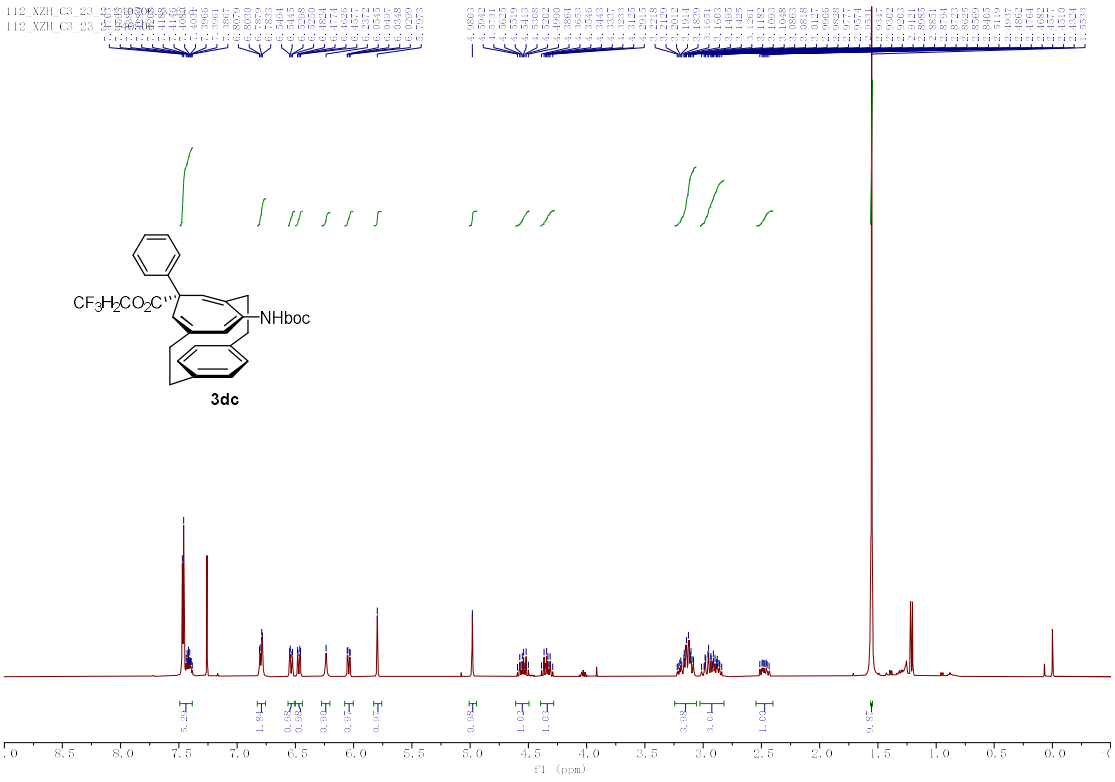


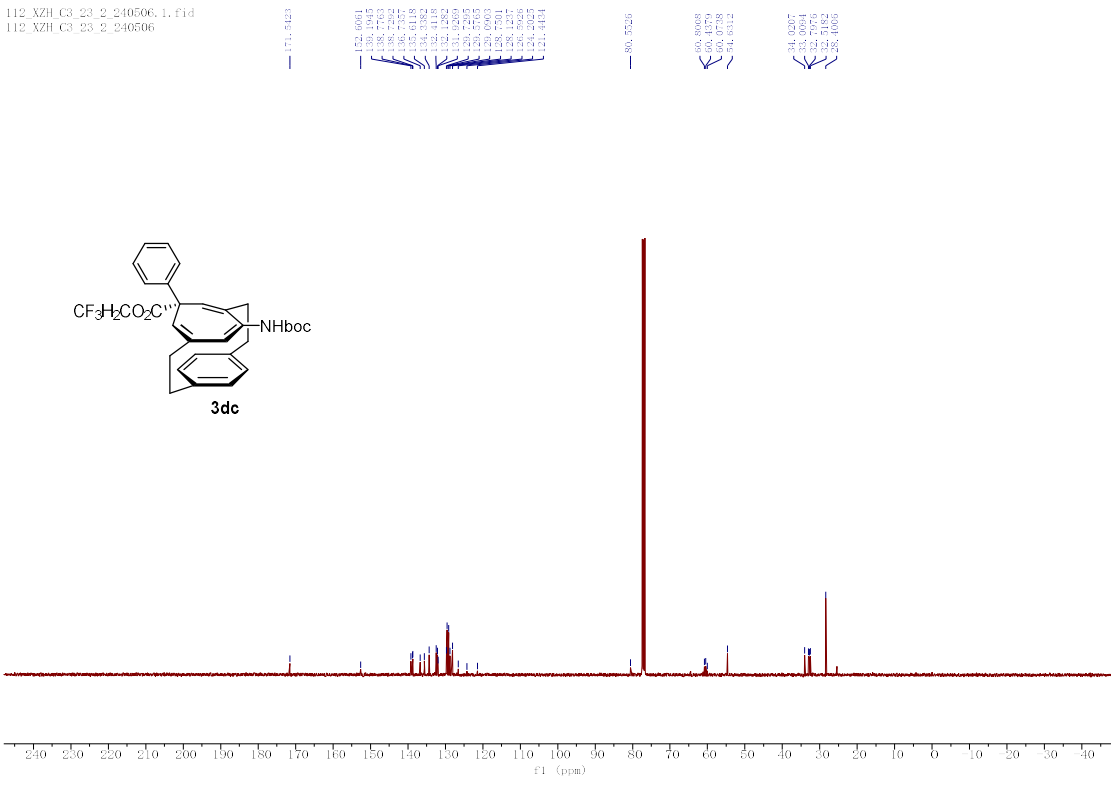
4da

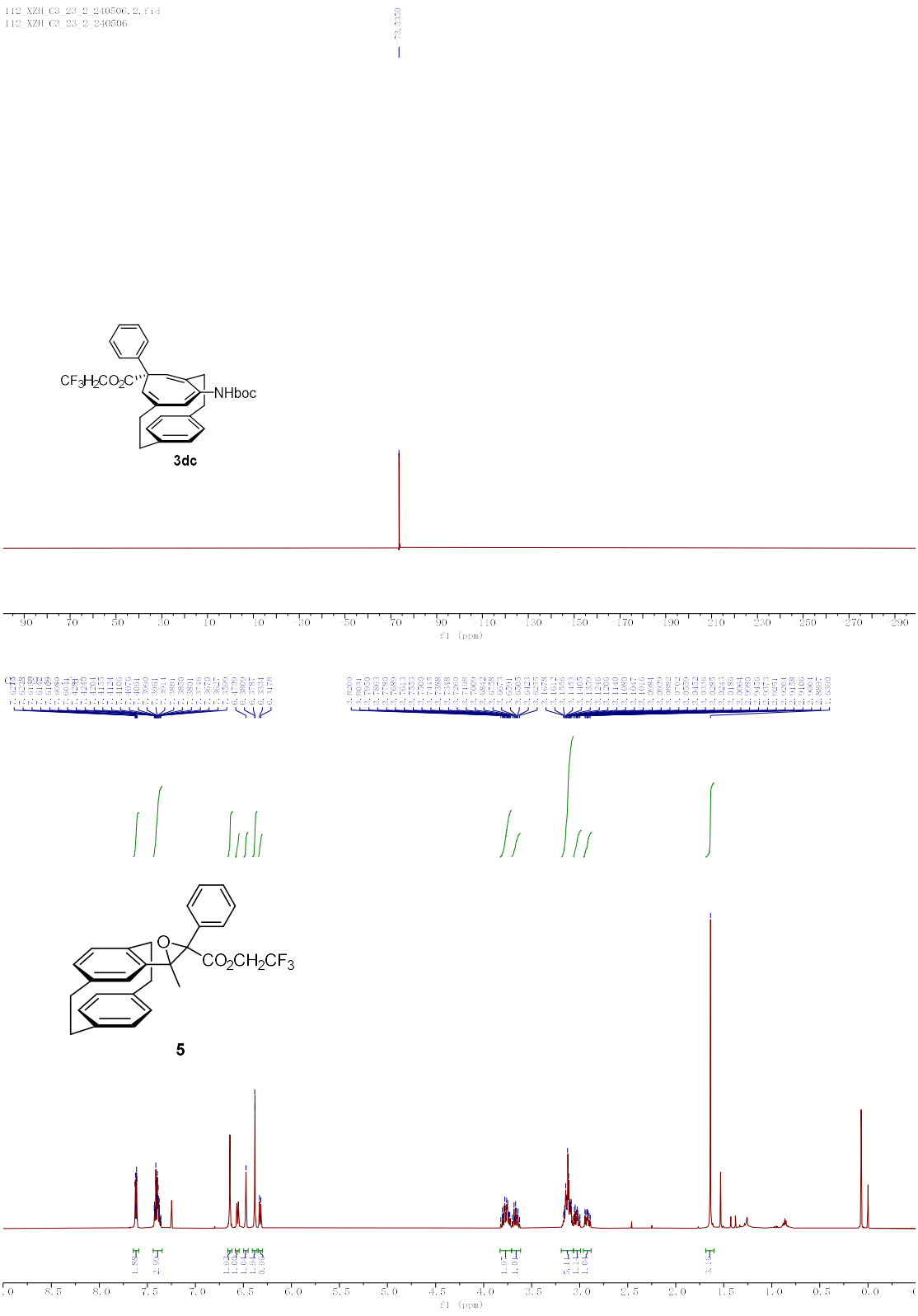
C2-48-1.3.fid



4da


112_XZH_C3_23_2_240506
112_XZH_C3_23_2_240506
CF3H2CO2C
NHboc
3dc
f1 (ppm)


112_XZH_C3_23_2_240506.1.fid
112_XZH_C3_23_2_240506
CF3H2CO2C
NHboc
3dc
f1 (ppm)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NHboc
3dc
f1 (ppm)
O
CO2CH2CF3
5
f1 (ppm)

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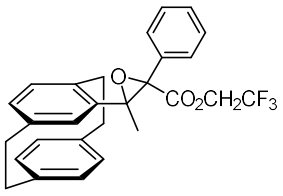

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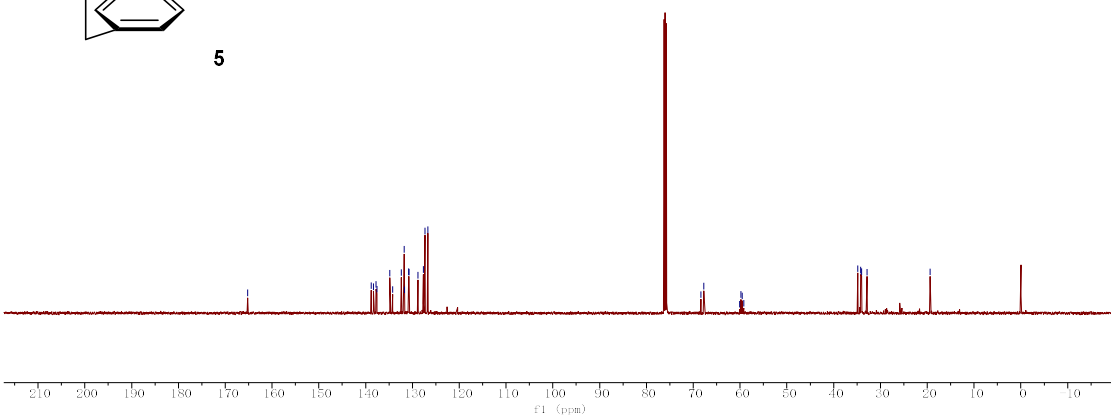

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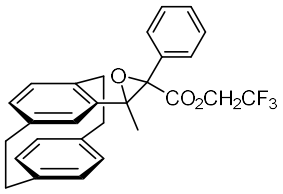

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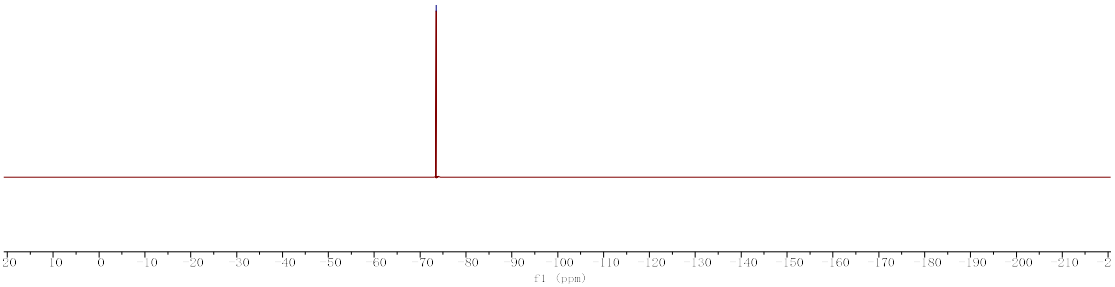

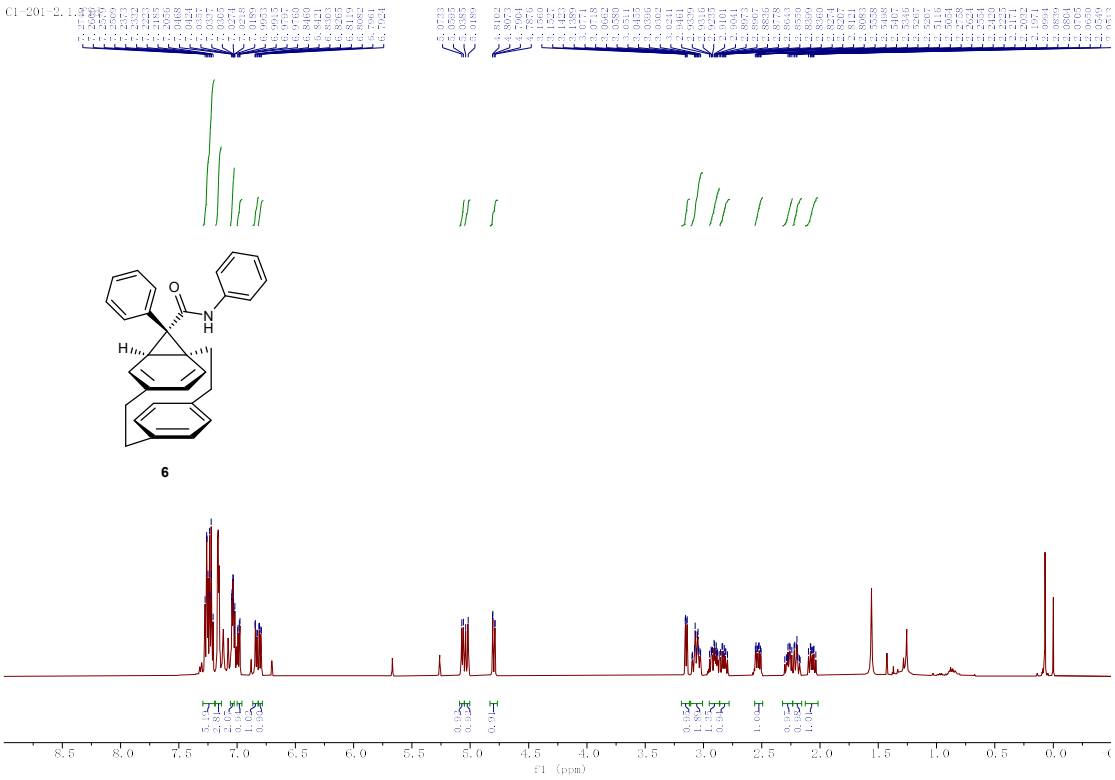
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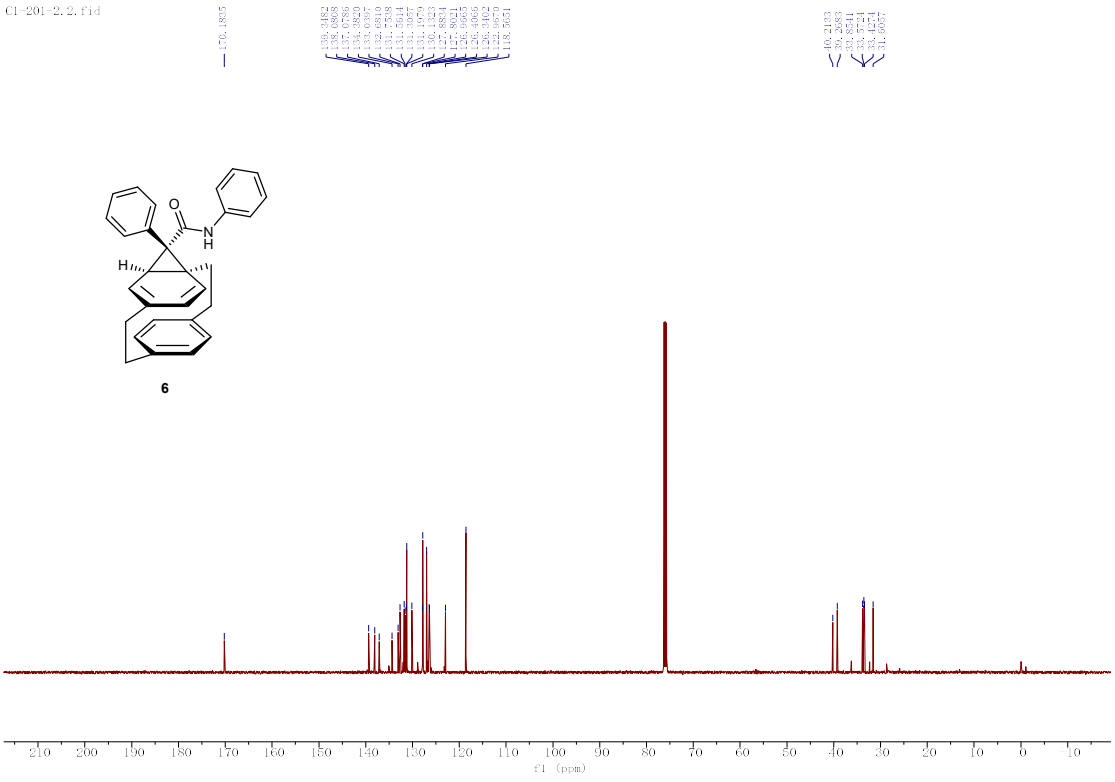
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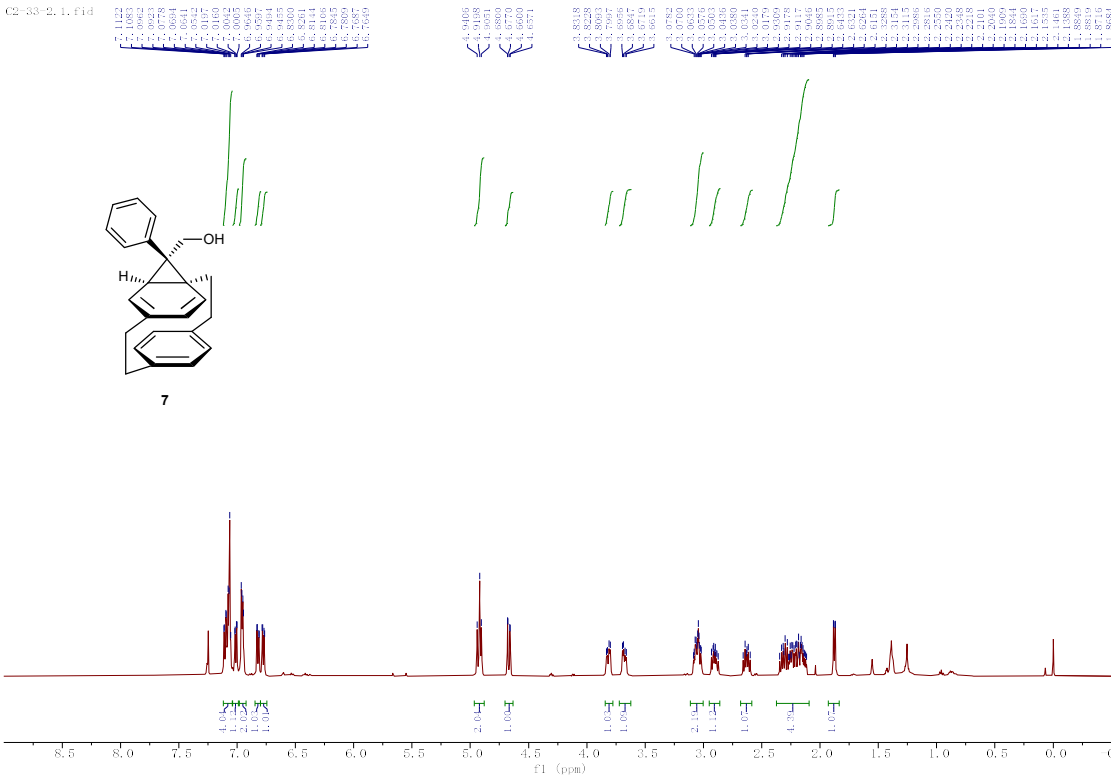
f1 (ppm)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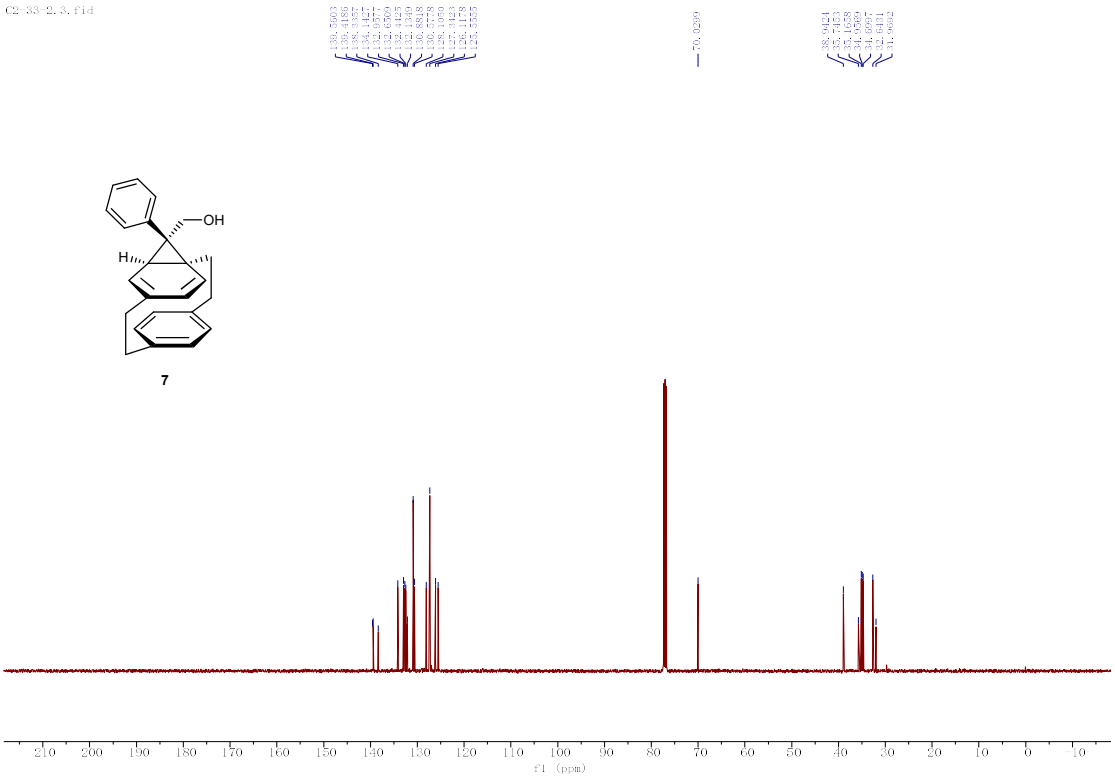
H
7
f1 (ppm)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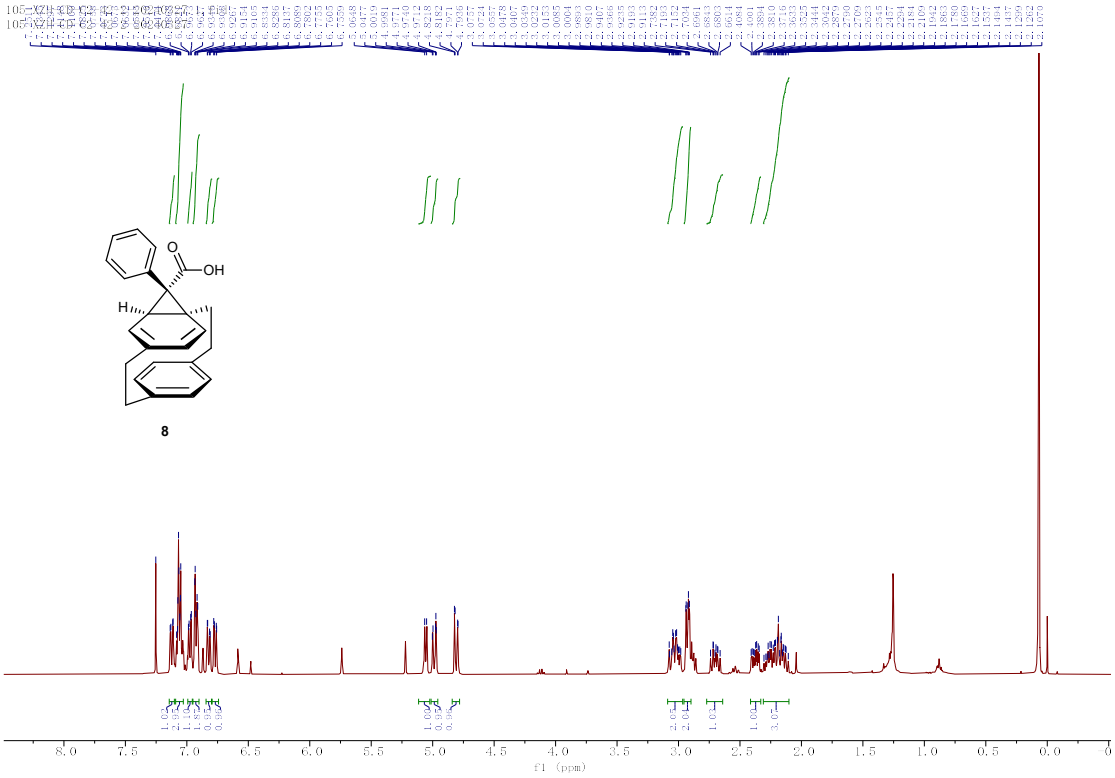
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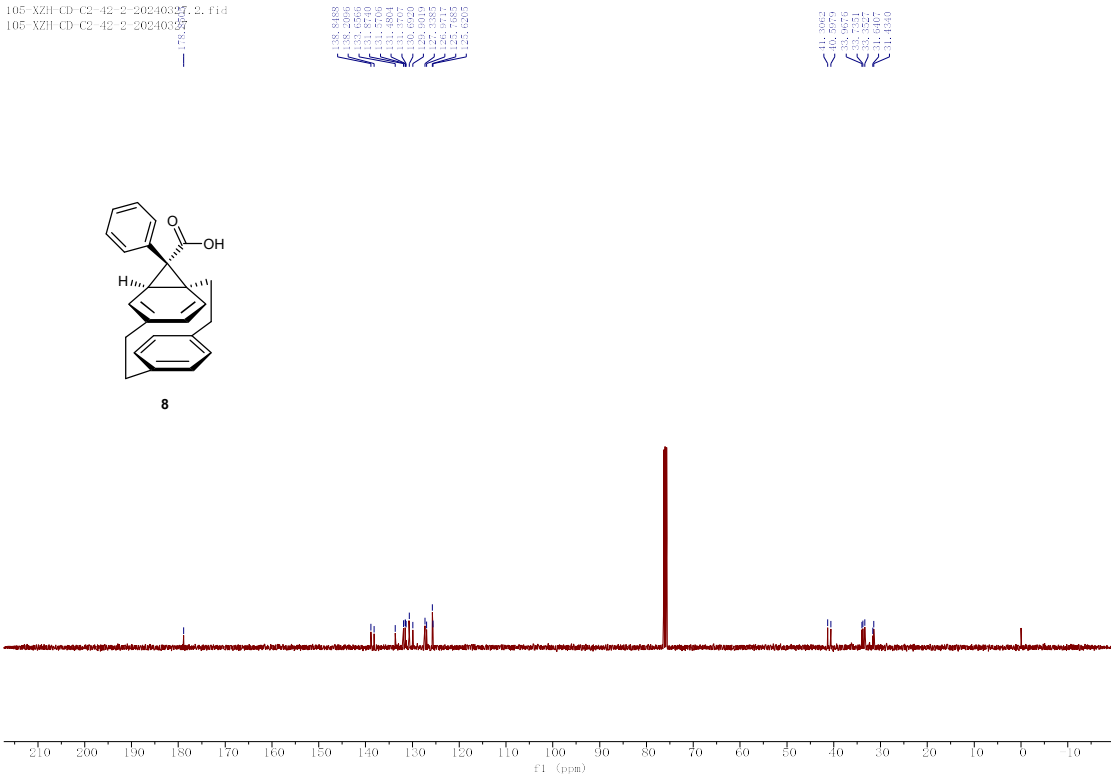
OH
H
8
f1 (ppm)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H
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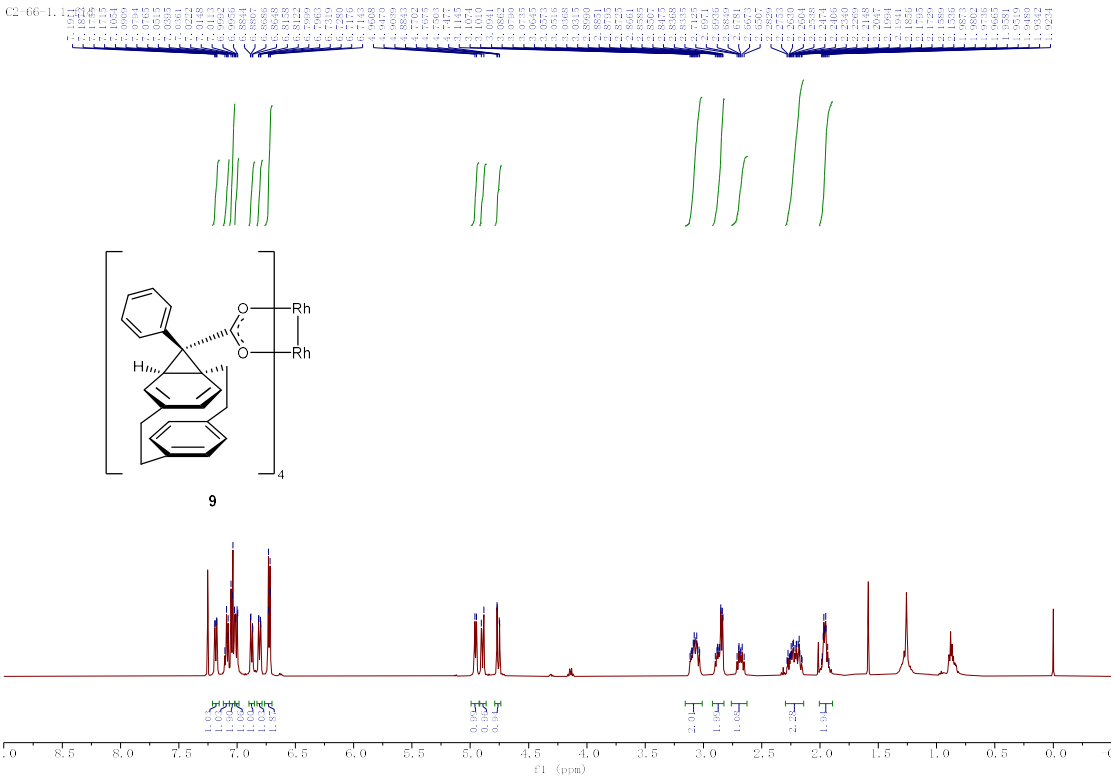
f1 (ppm)



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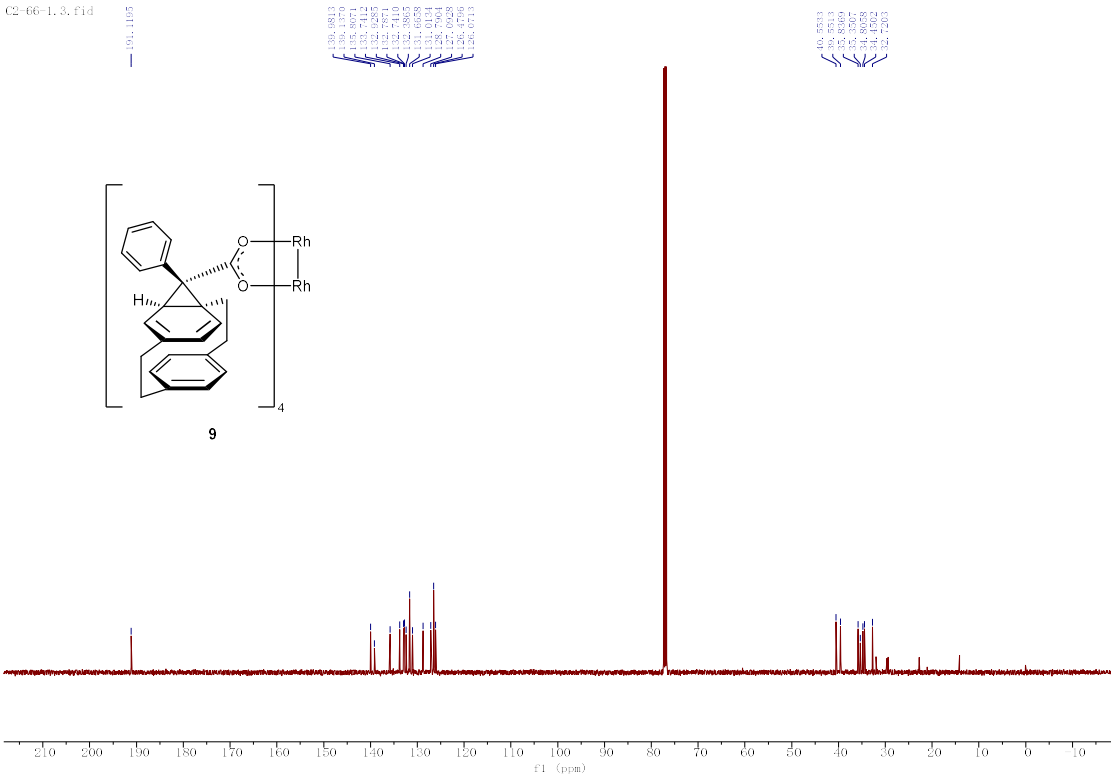

9

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