Angewandte Chemie
Eine Zeitschrift der Gesellschaft Deutscher Chemiker

Supporting Information

© Wiley-VCH 2013

69451 Weinheim, Germany

Gold(I)-Catalyzed *endo*-Selective Intramolecular α-Alkenylation of β-Yne-Furans: Synthesis of Seven-Membered-Ring-Fused Furans and DFT Calculations**

*Zhe Dong, Cheng-Hang Liu, Yi Wang, Mu Lin, and Zhi-Xiang Yu**

anie_201306965_sm_miscellaneous_information.pdf

Supporting Information

Contents

1. General

Air and moisture sensitive reactions were carried out in oven-dried glassware sealed with rubber septa under a positive pressure of dry argon. Similarly sensitive liquids and solutions were transferred via syringe. Reactions were stirred using Teflon-coated magnetic stir bars. Elevated temperatures were maintained using Thermostat-controlled silicone oil baths. Organic solutions were concentrated using a Büchi rotary evaporator with a desktop vacuum pump. Tetrahydrofuran, diethyl ether, 1,2-dimethoxyethane and toluene were distilled from sodium and benzophenone prior to use. Dichloromethane, 1,2-dichloroethane and acetonitrile were distilled from CaH_2 prior to use. Synthetic reagents were purchased from Acros, Aldrich, and Alfa Aesar and used without further purification, unless otherwise indicated. Analytical TLC was performed with 0.25 mm silica gel G plates with a 254 nm fluorescent indicator. The TLC plates were visualized by ultraviolet light and treatment with phosphomolybdic acid stain followed by gentle heating. Purification of products was accomplished by flash chromatography on silica gel and the purified compounds showed a single spot by analytical TLC.

NMR spectra were measured on Bruker ARX 400 (^{1}H at 400 MHz, ^{13}C at 100 MHz) and Bruker AVANCE 600 (^{1}H at 600 MHz, ^{13}C at 150 MHz) nuclear magnetic resonance spectrometers. ^{1}H-NMR spectra are reported relative to Me_4Si (0 ppm) or residual solvent signals (C_6D_6: 7.16 ppm, CD_2Cl_2: 5.32 ppm). Data for ^{1}H-NMR spectra are reported as follows: chemical shift (ppm, s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, dt = doublet of triplets, dm = doublet of multiplet, ddd = doublet of doublet of doublets, tdd = triplet of doublet of doublets, m = multiplet), coupling constant (Hz), and integration. Data for ^{13}C-NMR are reported in terms of chemical shift (ppm) relative to residual solvent peak ($CDCl_3$: 77.0 ppm, C_6D_6: 128.0 ppm, CD_2Cl_2: 53.8 ppm). 2D NMR experiments were conducted on a Bruker AVANCE 600 nuclear magnetic resonance spectrometer. Infrared spectra were recorded on Mettler-Toledo ReactIR iC10 system with an SiComp probe and are reported in wavenumbers (cm^{-1}). High-resolution mass spectra (HRMS) were recorded on a Bruker Apex IV FTMS mass spectrometer (ESI).

Abbreviations:

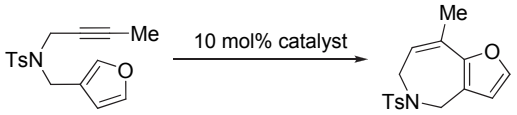
Boc = *t*-butoxycarbonyl
DCE = 1,2-dichloroethane
DCM = dichloromethane
DEAD = diethyl azodicarboxylate
DME = 1,2-dimethoxyethane
DMF = *N*,*N*-dimethylformamide
DMP = Dess–Martin periodinane
DMPU = 1,3-dimethylpropyleneurea
EA = ethyl acetate
IPr = 1,3-bis(2,6-diisopropylphenyl) imidazole-2-ylidene
JohnPhos = 2-(di-*tert*-butylphosphino)biphenyl
LDA = lithium diisopropylamide
MS = molecular sieve
PDC = pyridinium dichromate
PE = petroleum ether
TBAF = tetrabutylammonium fluoride
Tf = trifluoromethanesulfonyl
THF = tetrahydrofuran
TLC = thin layer chromatography
TMS = trimethylsilyl
Ts = *p*-toluenesulfonyl

2. Experimental Procedures and Characterization Data

2.1 Screening Reaction Conditions

Table S1 shows the results of screening reaction conditions for the alkenylation reaction. To verify whether gold(I) catalyst plays a decisive role in the reaction, we first tried some Brønsted acid (Table S1, entry 1) and Lewis acids (Table S1, entries 2–3) as catalysts. When TfOH was used, the reaction gave complex mixture. Lewis acid didn't work either, because the substrate slowly decomposed and no desired cyclization product was observed. The alkenylation reaction under $PtCl_2$ catalysis (Table S1, entry 4) gave product **2a** with 28% yield. $AuCl_3$–catalyzed alkenylation reaction (Table S1, entry 5) had a very low conversion. Various ligands were screened for the gold(I)-catalyzed reaction (Table S1, entries 6–9), showing that the reaction yields were not improved. Under the catalysis of gold catalyst **4**, [JohnPhosAu(NCMe)]SbF_6, various solvents (Table S1, entries 10–14) were screened, showing that generation of byproducts can be avoided and the reaction yields can be improved in these solvents. When the catalyst loading was reduced from 10 mol% to 5 mol%, the reaction yields didn't change obviously. Though the cyclization reaction in toluene (Table S1, entry 12) gave a relatively high yield, the reaction rate was very slow. Furthermore, we found that some less reactive substrates cannot be used in the alkenylation reaction in toluene. Finally, we found that DME gave the highest yield of the alkenylation product. Therefore, we used 5 mol% gold catalyst **4** as the standard catalyst and DME as the solvent for the investigation of the substrate scope of the target reaction. For all reactions reported in Table S1, we did not observe any six-membered ring product.

Table S1: Optimization studies on the cyclization to give the seven-membered ring.



1a **2a**

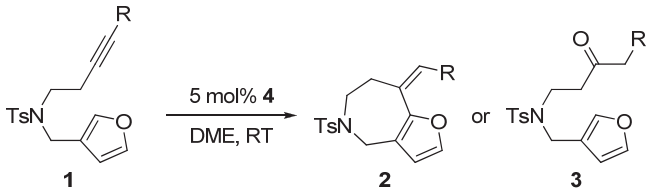
entry	solvent	catalyst	*T*	*t* [h]	yield[a]
1	DCM	TfOH	RT	12	mixture
2	DCM	$AgSbF_6$	RT	24	decomposed
3	DCM	BF_3•Et_2O	RT	24	decomposed
4	toluene	$PtCl_2$	70 °C	24	28%
5	DCM	$AuCl_3$	RT	10	low conversion
6	DCM	$Au(PPh_3)Cl+AgSbF_6$[b]	RT	1	trace
7	DCM	$Au(IPr)Cl+AgSbF_6$[b]	RT	0.3	69%
8	DCM	$Au[P(OPh\text{-}t\text{-}Bu\text{-}2,4)_3]Cl+AgSbF_6$[b]	RT	0.5	35%
9	DCE	**4**	RT	0.3	74%
10	DCM	**4**	RT	1	60%
11	MeCN	**4**	70 °C	24	trace
12	toluene	**4**[c]	RT	4	87%
13	THF	**4**[c]	RT	6	79%
14	DME	**4**[c]	RT	3	90%

[a] Isolated yield. [b] Gold and silver salts were added at ratio:1:1.3. [c] 5 mol% catalyst is used.

2.2 Test of the Elongated-Tethered Substrates

Table S2 shows how we tested the influence of the tether length. Only elongated-tethered substrate with the terminal alkyne (**1t**) can give the fused-cycloheptafuran product **2t** via 7-*exo-dig* cyclization (Table S2, entry 1). Substrates with internal alkynes (R = Me, CO_2Me and COMe) did not react or gave hydration products (Table S2, entries 2–4). DFT calculations of model substrates show that the regioselective α-alkenylation of elongated-tethered substrates is easy when R = H, but are difficult when R = Me and CO_2Me (activation energies are 12.2, 15.1, 16.8 kcal/mol, respectively, see Figure S5 for details). Consequently, cyclization of **1t** can be realized while the competing hydration reaction become favored for **1u**–**w**. The lower activity of methyl substrate **1u** compared to the terminal alkyne substrate **1t** may be due to the fact that Me is better in stabilizing the substrate–catalyst complex and lowing the electrophilicity of the gold-coordinated alkyne moiety, leading to higher activation energy of α-alkenylation. The lower activity of ynoate ester substrate **1v** compared to **1t** may be explained by the coordination of the carbonyl oxygen atom to the gold cation in the substrate–catalyst complex, which leads to higher activation energy in this case.

Table S2: Test of the elongated-tethered substrates.

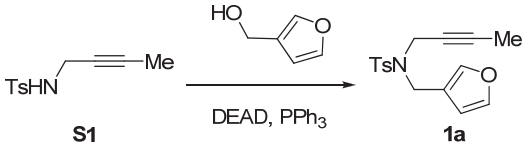


Entry	Substrate	*t* [h]	Product, yield[%][a]
1	**1t** R = H	20	**2t**, 47
2[b]	**1u** R = Me	48	no reaction
3[c]	**1v** R = CO_2Me	24	**3v**, 78
4	**1w** R = COMe	24	**3w**, 20

[a] Yield of isolated products. [b] A trace amount of hydration product can be observed when the reaction time is longer. [c] When 4 Å MS was added, no hydration product was observes. DME = 1,2-dimethoxyethane, Ts = *p*-toluenesulfonyl.

2.3 Synthesis of Substrates

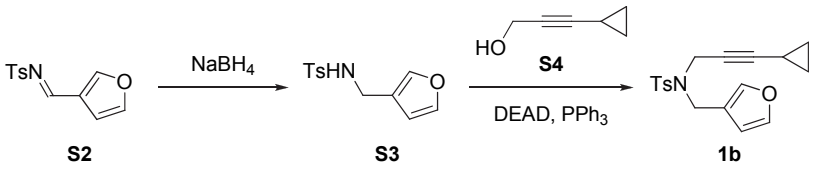
β-Yne-Furan (1a)



S1[1] to **1a**: To a stirred solution of 3-furanmethanol (0.26 g, 2.65 mmol), tosylamide **S1** (0.55 g, 2.46 mmol), and PPh_3 (1.32 g, 5 mmol) in anhydrous THF (35 mL) was added DEAD (0.91 g, 5.22 mmol) at 0 ºC. The mixture was then stirred overnight at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 10:1) to afford β-yne-furan **1a** (0.62 g, 83%).

1a: Colorless oil: TLC R_f (PE/EA 10:1) = 0.28. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.77 (d, J = 8.0 Hz, 2H), 7.37-7.38 (m, 2H), 7.31 (d, J = 8.0 Hz, 2H), 6.39-6.40 (m, 1H), 4.20 (s, 2H), 3.93 (dd, J = 4.5 and 2.1 Hz, 2H), 2.43 (s, 3H), 1.55 (t, J = 2.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.5, 143.3, 141.5, 136.1, 129.3, 127.9, 119.5, 110.7, 81.7, 71.5, 40.7, 36.0, 21.5, 3.2. IR (neat): ν 3371, 2928, 2857, 1739, 1665, 1639, 1605, 1505, 1352, 1162 cm^{-1}. HRMS (ESI): Calcd for $C_{16}H_{17}NNaO_3S$ (M + Na^+): 326.0821; found: 326.0814.

β-Yne-Furan (1b)



S2[2] to **S3**: To a stirred solution of imine **S2** (0.80 g, 3.21 mmol) in anhydrous MeOH (20 mL) was added $NaBH_4$ (0.26 g, 6.88 mmol) at 0 ºC carefully. After 1 h, the temperature was raised to room temperature and the mixture was stirred for 0.5 h. The resulting mixture was quenched with water (60 mL), extracted 3 times with ether (120 mL) and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 5:1) to afford tosylamide **S3** (0.73 g, 91%).

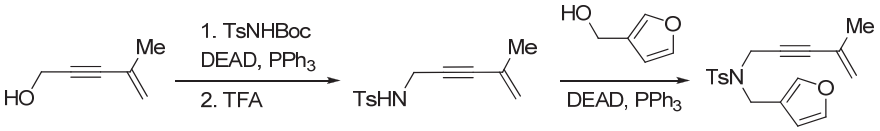
S3 to **1b**: To a stirred solution of tosylamide **S3** (401 mg, 1.60 mmol), alcohol **S4**[3] (198 mg, 2.06 mmol), and PPh_3 (854 mg, 3.26 mmol) in anhydrous THF (40 mL) was added DEAD (607 mg, 3.48 mmol) at 0 ºC. The mixture was then stirred for 40 h at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 10:1) to afford β-yne-furan **1b** (395 mg, 75%).

1b: White solid: TLC R_f (PE/EA 10:1) = 0.35, m.p. = 52-54 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.75 (d, J = 8.0 Hz, 2H), 7.37-7.38 (m, 2H), 7.32 (d, J = 8.0 Hz, 2H), 6.40-6.41 (m, 1H), 4.20 (s, 2H), 3.93 (d, J = 1.8 Hz, 2H), 2.45 (s, 3H), 0.94-1.02 (m, 1H), 0.60-0.65 (m, 2H), 0.30-0.34 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.5, 143.4, 141.5, 136.1, 129.4, 127.8, 119.4, 110.8, 89.5, 67.5, 40.7, 36.0, 21.5, 7.9, -0.9. IR (neat): ν 1341, 1170, 1099, 1028, 909, 879, 816 cm^{-1}. HRMS (ESI): Calcd for $C_{18}H_{20}NO_3S$ (M + H^+): 330.1158; found: 330.1161.

---

[1] Jiao, L.; Lin, M.; Zhuo, L.-G.; Yu, Z.-X. *Org. Lett.* **2010**, *12*, 2528.
[2] Chen, X.; Dong, S.; Qiao, Z.; Zhu, Y.; Xie, M.; Lin, L.; Liu, X.; Feng, X. *Chem. Eur. J.* **2011**, *17*, 2583.
[3] Schelper, M.; De Meijere, A. *Eur. J. Org. Chem.* **2005**, *3*, 582.

β-Yne-Furan (1c)



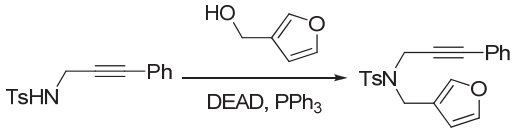
S5 **S6** **1c**

S5[4] to **S6**: To a stirred solution of alcohol **S5** (2.4 g, 25.0 mmol), TsNHBoc (6.8 g, 25.1 mmol), and PPh_3 (14.1 g, 53.8 mmol) in anhydrous THF (125 mL) was added DEAD (10.6 g, 60.8 mmol) at 0 ºC. The mixture was then stirred for 2 h at room temperature. The reaction mixture was concentrated and the crude product was dissolved in anhydrous DCM (100 mL). To the stirred solution of crude product was added TFA (18 g, 158 mmol). The mixture was stirred for 16 h at room temperature. Then saturated $NaHCO_3$ solution was added to quench the reaction. The resulting mixture was extracted twice with ether (100 mL) and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 10:1) to afford tosylamide **S6** (5.3 g, 85%).

S6 to **1c**: To a stirred solution of 3-furanmethanol (0.26 g, 2.65 mmol), tosylamide **S6** (0.60 g, 2.41 mmol), and PPh_3 (1.30 g, 4.96 mmol) in anhydrous THF (35 mL) was added DEAD (0.98 g, 5.62 mmol) at 0 ºC. The mixture was then stirred overnight at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 10:1) to afford β-yne-furan **1c** (0.73 g, 92%).

1c: Colorless oil: TLC R_f (PE/EA 10:1) = 0.24. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.77 (d, J = 8.3 Hz, 2H), 7.38-7.39 (m, 2H), 7.31 (d, J = 8.3 Hz, 2H), 6.41-6.42 (m, 1H), 5.10-5.13 (m, 1H), 4.97 (s, 1H), 4.22 (s, 2H), 4.10 (s, 2H), 2.42 (s, 3H), 1.65 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.6, 143.5, 141.6, 135.9, 129.5, 127.8, 125.8, 122.1, 119.3, 110.7, 87.1, 80.6, 40.9, 36.2, 23.0, 21.5. IR (neat): ν 2965, 2928, 2857, 1464, 1352, 1162, 1095 cm^{-1}. HRMS (ESI): Calcd for $C_{18}H_{20}NO_3S$ (M + H^+): 330.1158; found: 330.1159.

β-Yne-Furan (1d)



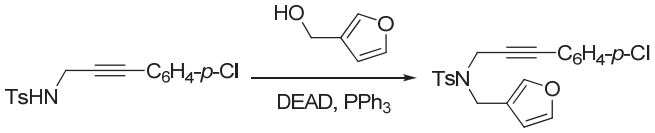
S7 **1d**

S7[5] to **1d**: To a stirred solution of 3-furanmethanol (171 mg, 1.74 mmol), tosylamide **S7** (335 mg, 1.17 mmol), and PPh_3 (665 mg, 2.54 mmol) in anhydrous THF (30 mL) was added DEAD (505 mg, 2.90 mmol) at 0 ºC. The mixture was then stirred for 6 h at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 10:1) to afford β-yne-furan **1d** (339 mg, 79%).

1d: White solid: TLC R_f (PE/EA 10:1) = 0.61, m.p. = 51-52 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81 (d, J = 8.1 Hz, 2H), 7.40-7.41 (m, 2H), 7.23-7.30 (m, 5H), 7.06 (dd, J = 8.1 and 1.5 Hz, 2H), 6.45-6.46 (m, 1H), 4.30 (s, 2H), 4.21 (s, 2H), 2.35 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.7, 143.6, 141.6, 135.8, 131.4, 129.6, 128.4, 128.1, 127.8, 122.1, 119.3, 110.8, 85.9, 81.5, 41.0, 36.4, 21.4. IR (neat): ν 2935, 1356, 1166, 1093, 1024, 905, 760, 689 cm^{-1}. HRMS (ESI): Calcd for $C_{21}H_{20}NO_3S$ (M + H^+): 366.1158; found: 366.1163.

[4] Kern, N.; Blanc, A.; Miaskiewicz, S.; Robinette, M.; Weibel, J.-M.; Pale, P. *J. Org. Chem.* **2012**, *77*, 4323.
[5] Park, J.; Cho, Y.; Chung, Y. *Angew. Chem. Int. Ed*. **2010**, *49*, 5138.

β-Yne-Furan (1e)

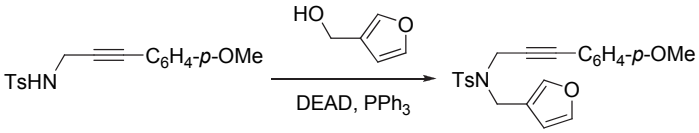


S8 **1e**

S8[6] to **1e**: To a stirred solution of 3-furanmethanol (177 mg, 1.80 mmol), tosylamide **S8** (570 mg, 1.78 mmol), and PPh_3 (944 mg, 3.60 mmol) in anhydrous THF (30 mL) was added DEAD (680 mg, 3.90 mmol) at 0 ºC. The mixture was then stirred overnight at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 10:1) to afford β-yne-furan **1e** (478 mg, 67%).

1e: Light yellow solid: TLC R_f (PE/EA 10:1) = 0.24, m.p. = 88-90 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.80 (d, J = 7.8 Hz, 2H), 7.40 (s, 2H), 7.28-7.29 (m, 2H), 7.22 (d, J = 7.9 Hz, 2H), 6.98 (d, J = 7.8 Hz, 2H), 6.44 (s, 1H), 4.28 (s, 2H), 4.19 (s, 2H), 2.36 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.7, 143.6, 141.6, 135.8, 134.5, 132.7, 129.5, 128.5, 127.9, 120.6, 119.2, 110.7, 84.7, 82.6, 41.1, 36.3, 21.4. IR (neat): ν 2965, 2928, 2861, 1743, 1602, 1468, 1348, 1266, 1166, 1158, 1091, 1021 cm^{-1}. HRMS (ESI): Calcd for $C_{21}H_{19}ClNO_3S$ (M + H$^+$): 400.0769*;* found: 400.0774.

β-Yne-Furan (1f)

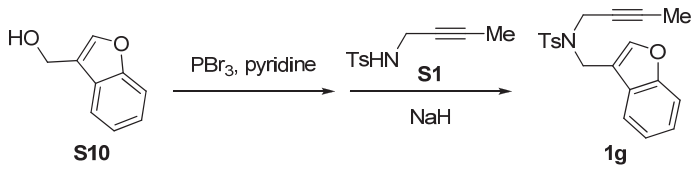


S9 **1f**

S9[6] to **1f**: To a stirred solution of 3-furanmethanol (183 mg, 1.86 mmol), tosylamide **S9** (490 mg, 1.55 mmol), and PPh_3 (820 mg, 3.13 mmol) in anhydrous THF (30 mL) was added DEAD (679 mg, 3.90 mmol) at 0 ºC. The mixture was then stirred overnight at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 30:1) to afford β-yne-furan **1f** (320 mg, 52%).

1f: Yellow solid: TLC R_f (PE/EA 5:1) = 0.43, m.p. = 92-94 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.80 (d, J = 8.1 Hz, 2H), 7.40-7.41 (m, 2H), 7.28 (d, J = 8.1 Hz, 2H), 7.01 (d, J = 8.8 Hz, 2H), 6.77 (d, J = 8.8 Hz, 2H), 6.44-6.45 (m, 1H), 4.29 (s, 2H), 4.19 (s, 2H), 3.80 (s, 3H), 2.37 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.7, 143.7, 143.5, 141.6, 136.0, 133.0, 129.6, 127.9, 119.4, 114.3, 113.8, 110.8, 85.9, 80.1, 55.3, 41.0, 36.5, 21.5. IR (neat): ν 3289, 2931, 1345, 1170, 1099, 1021 cm^{-1}. HRMS (ESI): Calcd for $C_{22}H_{22}NO_4S$ (M + H$^+$): 396.1264; found: 396.1261.

β-Yne-Furan (1g)



S10 **1g**

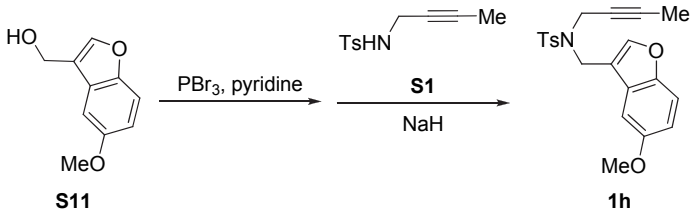
S10[7] to **1g**: To a stirred solution of alcohol **S10** (2.52 g, 17.0 mmol), pyridine (0.12 mL, 1.5 mmol) in anhydrous Et_2O (100 mL) was added PBr_3 (0.6 mL, 6 mmol) in anhydrous Et_2O (30 mL) at 0 ºC. The mixture was then stirred overnight at room temperature. Then saturated $NaHCO_3$

[6] Shintani, R.; Nakatsu, H.; Takatsu, K.; Hayashi, T. *Chem. Eur. J.* **2009**, *15*, 8692.
[7] Podea, P. V.; Tosa, M. I.; Paizs C.; Irimie F. D. *Tetrahedron: Asymmetry* **2008**, *4*, 500.

solution (20 mL) was added to quench the reaction. The resulting mixture was extracted twice with ether (120 mL) and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 5:1) to afford bromide. The bromide was used in the next step. Then to a suspension of NaH (60% purity, 150 mg, 3.75 mmol) in DMF (15mL) was added tosylamide **S1** (444 mg, 1.99 mmol) at 0 ºC. After stirred for 20 min, a solution of bromide (440mg, 2.08 mmol) in DMF (9 mL) was added and the reaction mixture was allowed to warm to room temperature and stirred for 30 min. Then saturated NH_4Cl solution (10 mL) was added to quench the reaction. The resulting mixture was extracted four times with ether (80 mL) and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 10:1) to afford β-yne-furan **1g** (670 mg, 50% for two steps).

1g: White solid: TLC R_f (PE/EA 10:1) = 0.18, m.p. = 132-134 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81-7.85 (m, 3H), 7.56 (s, 1H), 7.47 (d, J = 8.0 Hz, 1H), 7.28-7.34 (m, 4H), 4.47 (s, 2H), 3.92 (s, 2H), 2.45 (s, 3H), 1.53 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.6, 143.9, 143.4, 135.9, 129.3, 128.0, 126.8, 124.8, 123.0, 120.6, 114.6, 111.4, 82.1, 71.3, 40.0, 36.1, 21.5, 3.2. IR (neat): ν 2928, 2862, 1598, 1460, 1352, 1162, 1099 cm^{-1}. HRMS (ESI): Calcd for $C_{20}H_{20}NO_3S$ (M + H^+): 354.1158; found: 354.1160.

β-Yne-Furan (1h)

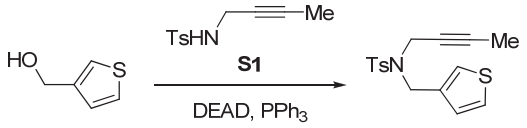


S11[8] to **1h**: To a stirred solution of alcohol **S11** (0.98 g, 5.5 mmol), pyridine (0.05 mL, 0.6 mmol) in anhydrous THF (40 mL) was added PBr_3 (0.25 mL, 2.5 mmol) in anhydrous THF (15 mL) at 0 ºC. The mixture was then stirred overnight at room temperature. Then saturated $NaHCO_3$ solution (10 mL) was added to quench the reaction. The resulting mixture was extracted three times with ether (60 mL) and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 10:1) to afford bromide. The bromide was used in the next step. Then to a suspension of NaH (90 mg, 3.75 mmol) in DMF (15 mL) was added tosylamide **S1** (329 mg, 1.48 mmol) at 0 ºC. After stirred for 15 min, a solution of bromide (395 mg, 1.64 mmol) in DMF (10 mL) was added and the reaction mixture was allowed to warm to room temperature and stirred for 2 h. Then saturated NH_4Cl solution (10 mL) was added to quench the reaction. The resulting mixture was extracted four times with ether (80 mL) and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 5:1) to afford β-yne-furan **1h** (524 mg, 60% for two steps).

[8] Paul, N. M.; Taylor, M.; Kumar, R.; Deschamps, J. R.; Luedtke, R. R.; Newman, A. H. *J. Med. Chem*. **2008**, *51*, 6095.

1h: Light yellow solid: TLC R_f (PE/EA 5:1) = 0.83, m.p. = 118-122 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.83 (d, J = 8.5 Hz, 2H), 7.53 (s, 1H), 7.32-7.36 (m, 4H), 6.91 (dd, J = 8.5 and 2.6 Hz, 1H), 4.43 (s, 2H), 3.93 (d, J = 2.3 Hz, 2H), 3.87 (s, 3H), 2.45 (s, 3H), 1.55 (t, J = 2.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.1, 150.5, 144.7, 143.4, 135.9, 129.3, 128.0, 127.3, 114.6, 114.1, 111.9, 102.3, 82.0, 71.4, 55.9, 40.0, 36.0, 21.5, 3.2. IR (neat): ν 2913, 1598, 1479, 1341, 1233, 1158, 1099 cm^{-1}. HRMS (ESI): Calcd for $C_{21}H_{22}NO_4S$ ($M + H^+$): 384.1264; found: 384.1259.

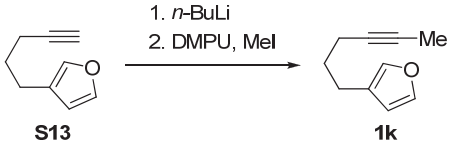
β-Yne-Furan (1i)



S12[9] to **1i**: To a stirred solution of 3-thiophenmethanol (240 mg, 2.14 mmol), tosylamide **S1** (478 mg, 2.14 mmol), and PPh_3 (1.12 g, 4.28 mmol) in anhydrous THF (20 mL) was added DEAD (784 mg, 4.50 mmol) at 0 ºC. The mixture was then stirred overnight at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1) to afford β-yne-furan **1i** (384 mg, 59%).

1i: Light yellow oil: TLC R_f (PE/EA 10:1) = 0.29. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.77 (d, J = 7.7 Hz, 2H), 7.31 (d, J = 7.7 Hz, 2H), 7.28-7.29 (m, 1H), 7.19 (s, 1H), 7.07 (d, J = 4.6 Hz, 1H), 4.34 (s, 2H), 3.90 (s, 2H), 2.44 (s, 3H), 1.55 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.3, 136.2, 129.3, 128.0, 127.9, 126.3, 124.1, 81.8, 71.6, 44.9, 36.2, 21.5, 3.2. IR (neat): ν 2928, 2857, 1661, 1635, 1602, 1356, 1341, 1170, 1095 cm^{-1}. HRMS (ESI): Calcd for $C_{16}H_{17}NNaO_2S_2$ ($M + Na^+$): 342.0593; found: 342.0597.

β-Yne–Furan (1k)

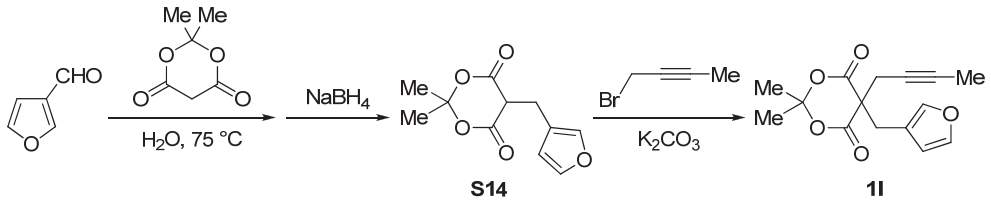


S13[10] to **1k**: To a stirred solution of alkyne **S13** (37.5 mg, 0.28 mmol) in anhydrous THF (2 mL) was added *n*-BuLi (2.4 M, 0.14 ml, 0.34 mmol) at -78 ºC. After stirred for 1 h, DMPU (36 mg, 0.28 mmol) was added and the reaction mixture was stirred at -78 ºC for 5 min. Then MeI (0.17ml, 2.73 mmol) was added and the reaction mixture was allowed to warm to room temperature and stirred for 4 h. Then water was added to quench the reaction. The resulting mixture was extracted three times with ether and the combined organic phase was dried over $MgSO_4$ and concentrated in ice bath. The crude product was purified by flash column chromatography on silica gel (eluted with pentane) to afford alkyne **1k** (36.4 mg, 88%).

1k: Colorless oil: TLC R_f (pentane) = 0.31. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.35 (t, J = 1.4 Hz, 1H), 7.22-7.23 (m, 1H), 6.26-6.27 (m, 1H), 2.51 (t, J = 7.5 Hz, 2H), 2.16 (tq, J = 7.1 and 2.5 Hz, 2H), 1.79 (t, J = 2.5 Hz, 3H), 1.69-1.76 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 142.7, 139.0, 124.4, 111.0, 78.7, 75.9, 29.3, 23.8, 18.2, 3.5. IR (neat): ν 2936, 2865, 2257, 1543, 1503, 1166, 1030, 918, 722 cm^{-1}. HRMS (EI): Calcd for $C_{10}H_{13}O$ ($M + H^+$): 149.0966; found: 149.0961.

[9] Dowle, M. D.; Hayes, R.; Judd, D. B.; Williams, C. N. *Synthesis*, **1983**, 73.
[10] Yamamoto, H.; Sasaki, I.; Imagawa, H.; Nishizawa, M. *Org. Lett.* **2007**, *9*, 1399.

β-Yne-Furan (1l)

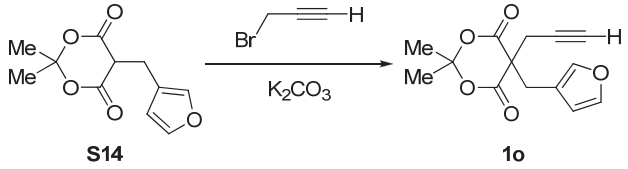


S14 **1l**

S14 to **1l**: 3-Furancarbaldehyde (600 mg, 6.24 mmol) and Meldrum's acid (990 mg, 6.87 mmol) was dissolved in H_2O (12mL) and heated to 75℃. After 2 h, the mixture was filtered. The solid was kept and washed twice with cold water (3mL). To a stirred solution of crude product in anhydrous MeOH (25 mL) was added $NaBH_4$ (0.49 g, 12.95 mmol) carefully. After 1 h, the resulting mixture was quenched with water (25 mL), acidized to pH = 2 with HCl (3 M), extracted 3 times with DCM (120 mL) and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 5:1) to afford **S14** (1.12 g, 80%). To a suspension of K_2CO_3 (540 mg, 5.09 mmol) and **S14** (520 mg, 2.32 mmol) in DMF (15 mL) was added 1-bromo-2-butyne (280 mg, 2.10 mmol). The mixture was then stirred at room temperature for 1 day. Then water (10 mL) was added to quench the reaction. The resulting mixture was extracted with ether (80 mL) and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1) to afford β-yne-furan **1l** (490 mg, 88%).

1l: White solid: TLC R_f (PE/EA 10:1) = 0.30, m.p. = 114-116 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.33 (s, 1H), 7.29 (s, 1H), 6.27 (s, 1H), 3.09 (s, 2H), 2.92 (d, J = 2.2 Hz, 2H), 1.75 (s, 3H), 1.72 (s, 3H), 1.18 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.3, 143.1, 141.5, 118.1, 111.7, 106.3, 80.7, 73.0, 56.5, 33.8, 29.8, 29.0, 28.9, 3.5. IR (neat): ν 2928, 2958, 1773, 1732, 1371, 1278, 1207, 1106, 1054 cm^{-1}. HRMS (ESI): Calcd for $C_{15}H_{16}NaO_5$ (M + Na^+): 299.0890; found: 299.0889.

β-Yne-Furan (1o)

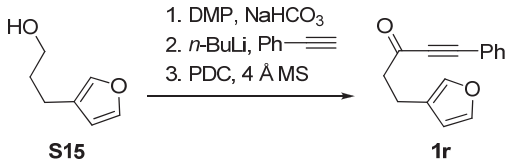


S14 **1o**

S14 to **1o**: To a suspension of K_2CO_3 (345 mg, 3.25 mmol) and **S14** (318 mg, 1.42 mmol) in DMF (10 mL) was added 3-bromo-1-propyne (80% in toluene, 195 mg, 1.31 mmol). The mixture was then stirred for 2 h at room temperature. Then water (10 mL) was added to quench the reaction. The resulting mixture was extracted with ether (80 mL) and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 5:1) to afford β-yne-furan **1o** (184 mg, 54%).

1o: White solid: TLC R_f (PE/EA 3:1) = 0.63, m.p. = 96-98 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34-7.35 (m, 1H), 7.30 (s, 1H), 6.27-6.28 (m, 1H), 3.12 (s, 2H), 2.97-2.98 (m, 2H), 2.17-2.18 (m, 1H), 1.73 (s, 3H), 1.18 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.9, 143.2, 141.6, 117.9, 111.7, 106.6, 78.0, 73.2, 56.0, 34.1, 30.1, 29.0, 28.2. IR (neat): ν 1745, 1363, 1285, 1104, 1056, 957 cm^{-1}. HRMS (ESI): Calcd for $C_{14}H_{14}NaO_5$ (M + Na^+): 285.0733; found: 285.0737.

β-Yne–Furan (1r)



S15 **1r**

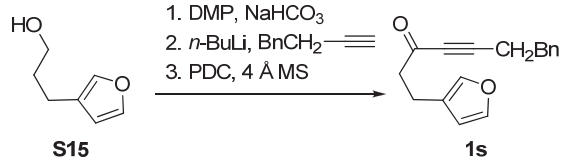
S15[11] to **1r**: To a solution of **S15** (170 mg, 1.35 mmol) in DCM (5 mL) was added DMP (860 mg, 2.03 mmol) and $NaHCO_3$ (450 mg, 5.36 mmol). The mixture was then stirred for 30 min at room temperature. Then saturated $Na_2S_2O_3$ solution was added to quench the reaction. The resulting mixture was extracted three times with ether (30 mL) and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 5:1) to afford aldehyde. The aldehyde was used in the next step.

Then to a solution of phenylacetylene (150 mg, 1.47 mmol) in anhydrous THF (10 mL) was added *n*-BuLi (2.4 M, 0.55 mL, 1.32 mmol) at -78 ℃. After stirred for 30 min, a solution of aldehyde in anhydrous THF (2 mL) was added and the reaction mixture was allowed to warm to room temperature and stirred for 3 h. Then water (10 mL) was added to quench the reaction. The resulting mixture was extracted with ether (60 mL) and the combined organic phase was dried over $MgSO_4$ and concentrated to afford alcohol. The crude product was used in the next step.

To a solution of alcohol in DCM (5 mL) was added PDC (346 mg, 0.92 mmol) and 4 Å MS (300 mg). The mixture was then stirred for 1 h at room temperature. The resulting mixture was filtrated and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 10:1) to afford product **1r** (74.4 mg, 25% for 3 steps).

1r: Light yellow oil: TLC R_f (PE/EA 5:1) = 0.58. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.55-7.59 (m, 2H), 7.44-7.48 (m, 1H), 7.35-7.40 (m, 3H), 7.26-7.27 (m, 1H), 7.30-7.31 (m, 1H), 2.92-2.96 (m, 2H), 2.85-2.89 (m, 2H).^{13}C NMR (100 MHz, $CDCl_3$): δ 186.8, 143.0, 139.2, 133.0, 130.8, 128.6, 123.2, 119.9, 110.8, 91.2, 87.7, 45.7, 19.4. IR (neat): ν 1670, 1093, 913, 873, 758, 689, 600 cm^{-1}. HRMS (ESI): Calcd for $C_{15}H_{13}O_2$ ($M + H^+$): 225.0910; found: 225.0910.

β-Yne–Furan (1s)



S15 **1s**

S15[11] to **1s**: To a solution of **S15** (459 mg, 3.64 mmol) in DCM (15 mL) was added DMP (2.31 g, 5.46 mmol) and $NaHCO_3$ (1.22 g, 14.5mmol). The mixture was then stirred for 30 min at room temperature. Then saturated $Na_2S_2O_3$ solution was added to quench the reaction. The resulting mixture was extracted three times with ether (60 mL) and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 10:1) to afford aldehyde. The aldehyde was used in the next step.

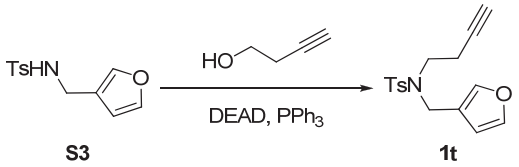
[11] Menon, R. S.; Banwell, M. G. *Org. Biomol. Chem.* **2010**, *8*, 5483.

Then to a solution of 4-phenyl-1-butyne (233.4mg, 1.6 mmol) in anhydrous THF (3 mL) was added *n*-BuLi (2.4 M, 0.6 mL, 1.44 mmol) at -78 ℃. After stirred for 30 min, aldehyde was added and the reaction mixture was allowed to warm to room temperature and stirred for 4 h. Then water (3 mL) was added to quench the reaction. The resulting mixture was extracted with ether (15 mL) and the combined organic phase was dried over $MgSO_4$ and concentrated to afford alcohol. The crude product was used in the next step.

To a solution of alcohol in DCM (5 mL) was added PDC (564 mg, 1.50 mmol) and 4 Å MS (280 mg). The mixture was then stirred for 1 h at room temperature. The resulting mixture was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1) to afford product **1s** (96.8 mg, 10% for 3 steps).

1s: Colorless oil: TLC R_f (PE/EA 5:1) = 0.53. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.29-7.34 (m, 3H), 7.19-7.23 (m, 4H), 6.23-6.24 (m, 1H), 2.89 (t, J = 7.4, 2H), 2.74 (s, 4H), 2.67 (t, J = 7.4, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 186.9, 142.9, 139.6, 139.1, 128.5, 128.4, 126.7, 123.3, 110.8, 93.6, 81.3, 45.6, 33.9, 21.1, 19.2. IR (neat): ν 1718, 1562, 1335, 1164, 1093, 1028 cm^{-1}. HRMS (ESI): Calcd for $C_{17}H_{17}O_2$ ($M + H^+$): 256.1223; found: 256.1225.

β-Yne-Furan (1t)

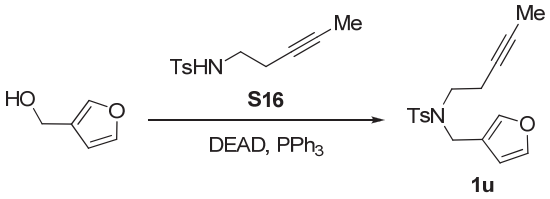


S3 **1t**

S3 to **1t**: To a stirred solution of 3-butyn-1-ol (136 mg, 1.94 mmol), tosylamide **S3** (285 mg, 1.14 mmol), and PPh_3 (602 mg, 2.30 mmol) in anhydrous THF (30 mL) was added DEAD (440 mg, 2.52 mmol) at 0 ºC. The mixture was then stirred for 48 h at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 10:1) to afford β-yne-furan **1t** (185 mg, 54%).

1t: White solid: TLC R_f (PE/EA 5:1) = 0.50, m.p. = 58-60 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72 (d, J = 8.3 Hz, 2H), 7.30-7.35 (m, 4H), 6.23-6.24 (m, 1H), 4.26 (s, 2H), 3.26-3.30 (m, 2H), 2.44 (s, 3H), 2.34-2.38 (m, 2H), 1.94 (t, J = 2.7 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.7, 143.5, 141.1, 136.9, 129.8, 127.2, 120.4, 110.5, 81.0, 70.2, 45.9, 43.0, 21.5, 19.2. IR (neat): ν 1348, 1170, 1102, 1017, 797 cm^{-1}. HRMS (ESI): Calcd for $C_{16}H_{18}NO_3S$ ($M + H^+$): 304.1002; found: 304.0998.

β-Yne-Furan (1u)

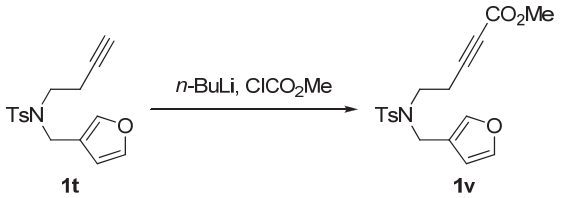


1u

S16[12] to **1u**: To a stirred solution of 3-furanmethanol (0.34 g, 3.4 mmol), tosylamide **S16** (0.80 g, 3.37 mmol), and PPh_3 (1.78 g, 6.8 mmol) in anhydrous THF (40 mL) was added DEAD (1.22 g, 7.0 mmol) at 0 ºC. The mixture was then stirred overnight at room temperature. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 5:1) to afford β-yne-furan **1u** (0.68 g, 64%).

1u: Light yellow oil: TLC R_f (PE/EA 10:1) = 0.29. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72 (d, J = 8.3 Hz, 2H), 7.34-7.35 (m, 1H), 7.32-7.33 (m, 1H), 7.28-7.31 (m, 2H), 6.24-6.25 (m, 1H), 4.25 (s, 2H), 3.21-3.25 (m, 2H), 2.43 (s, 3H), 2.26-2.31 (m, 2H), 1.71 (t, J = 2.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.6, 143.3, 141.0, 137.1, 129.7, 127.2, 120.5, 110.6, 77.5, 75.7, 46.3, 42.7, 21.5, 19.3, 3.4. IR (neat): ν 3363, 2961, 2928, 2861, 1665, 1639, 1464, 1341, 1166, 1099 cm^{-1}. HRMS (ESI): Calcd for $C_{17}H_{19}NNaO_3S$ ($M + Na^+$): 340.0978; found: 340.0979.

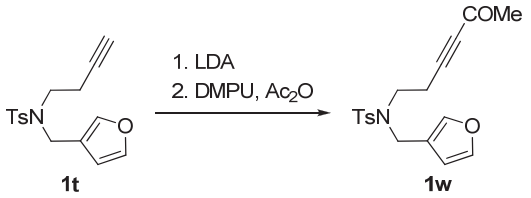
β-Yne–Furan (1v)



1t to **1v**: To a solution of **1t** (107 mg, 0.35 mmol) in anhydrous THF (5 mL) was added *n*-BuLi (1.6 M, 0.26 mL, 0.42 mmol) at -78 ºC. After stirred for 1 h, $ClCO_2Me$ (87 mg, 0.92 mmol) was added and the reaction mixture was allowed to warm to room temperature and stirred overnight. Then water (5 mL) was added to quench the reaction. The resulting mixture was extracted with EtOAc (30 mL) and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 10:1) to afford β-yne-furan **1v** (78 mg, 61%).

1v: White solid: TLC R_f (PE/EA 5:1) = 0.11, m.p. = 71-73 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72 (d, J = 8.5 Hz, 2H), 7.32-7.36 (m, 4H), 6.23-6.24 (m, 1H), 4.25 (s, 2H), 3.75 (s, 3H), 3.30 (t, J = 7.4 Hz, 2H), 2.52 (t, J = 7.4 Hz, 2H), 2.45 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.8, 143.9, 143.7, 141.2, 136.5, 129.9, 127.2, 120.1, 110.4, 85.8, 74.3, 52.7, 45.0, 43.3, 21.5, 19.7. IR (neat): ν 2245, 1720, 1653, 1460, 1342, 1251, 1151, 1076, 1022 cm^{-1}. HRMS (ESI): Calcd for $C_{18}H_{20}NO_5S$ ($M + H^+$): 362.1057; found: 362.1063.

β-Yne–Furan (1w)

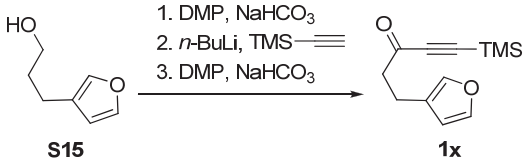


[12] Yin, Y.; Ma, W.; Chai, Z.; Zhao, G. *J. Org. Chem.* **2007**, *72*, 5731.

1t to **1w**: To a solution of **1t** (60.0 mg, 0.20 mmol) in anhydrous THF (2 mL) was added LDA (2.4 M, 0.12 mL, 0.24 mmol) at -78 ℃. After stirred for 45 min, DMPU (26 mg, 0.20 mmol) was added and the reaction mixture was stirred at -78 ºC for 10 min. Then Ac_2O (40 mg, 0.40 mmol) was added and the reaction mixture was allowed to warm to room temperature and stirred for 6 hours. Then water (2 mL) was added to quench the reaction. The resulting mixture was extracted with ether (20 mL) and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 5:1) to afford β-yne-furan **1w** (16.5 mg, 25%).

1w: Colorless oil: TLC R_f (PE/EA 3:1) = 0.45. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72 (d, J = 8.2, 2H), 7.36-7.37 (m, 1H), 7.33 (d, J = 8.2, 2H), 7.31 (s, 1H), 6.21-6.22 (m, 1H), 4.24 (s, 2H), 3.28-3.32 (m, 2H), 2.53-2.57 (m, 2H), 2.45 (s, 3H), 2.29 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 184.4, 143.9, 143.7, 141.1, 136.5, 129.9, 127.2, 120.2, 110.4, 89.5, 82.5, 45.3, 43.3, 32.6, 21.5, 20.0. IR (neat): ν 2221, 1674, 1460, 1344, 1234, 1164, 1098, 1022, 806 cm^{-1}. HRMS (ESI): Calcd for $C_{18}H_{19}NNaO_4S$ ($M + Na^+$): 368.0927; found: 368.0928.

β-Yne–Furan (1x)



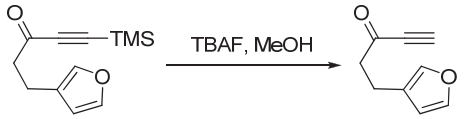
S15[11] to **1x**: To a solution of **S15** (305 mg, 2.42 mmol) in DCM (8 mL) was added DMP (1.5 g, 3.54mmol) and $NaHCO_3$ (0.82 g, 9.76mmol). The mixture was then stirred for 30 min at room temperature. Then saturated $Na_2S_2O_3$ solution was added to quench the reaction. The resulting mixture was extracted three times with ether (45 mL) and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 5:1) to afford aldehyde. The aldehyde was used in the next step.

Then to a solution of Trimethyl silyl acetylene (253 mg, 2.58 mmol) in anhydrous THF (10 mL) was added *n*-BuLi (2.4 M, 1.08 mL, 3.01mmol) at -78 ℃. After stirred for 30 min, a solution of aldehyde in anhydrous THF (2 mL) was added and the reaction mixture was allowed to warm to room temperature and stirred for 3 h. Then water (10 mL) was added to quench the reaction. The resulting mixture was extracted with ether (60 mL) and the combined organic phase was dried over $MgSO_4$ and concentrated to afford alcohol. The crude product was used in the next step.

To a solution of alcohol in DCM (10 mL) was added DMP (937 mg, 2.21 mmol) and $NaHCO_3$ (495 mg, 5.89 mmol). The mixture was then stirred for 1 h at room temperature. Then saturated $Na_2S_2O_3$ solution was added to quench the reaction. The resulting mixture was extracted three times with ether (45 mL) and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 5:1) to afford product **1x** (207.9 mg, 39% for 3 steps).

1x: Light yellow oil: TLC R_f (PE/EA 10:1) = 0.64. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.33-7.35 (m, 1H), 7.23 (s, 1H), 6.26-6.27 (m, 1H), 2.75-2.85 (m, 4H), 0.23-0.26 (m, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 186.5, 143.0, 139.1, 123.2, 110.8, 101.8, 98.3, 45.5, 19.1, -0.8. IR (neat): ν 2962, 2360, 1678, 1253, 1109, 913, 847, 744, 600 cm^{-1}. HRMS (ESI): Calcd for $C_{12}H_{17}O_2Si$ ($M + H^+$): 221.0992; found: 221.0991.

β-Yne–Furan (1y)



1x **1y**

1x to **1y**: To a solution of **1x** (155 mg, 0.70mmol) in THF (10.6 mL) and MeOH (0.28 mL) at -78 °C was added TBAF (1 M THF solution, 0.28 mL, 0.28 mmol). After the reaction mixture was stirred at -78 °C for 20 min, saturated NH_4Cl solution was added to quench the reaction. The reaction mixture was diluted by water and extracted three times with ether (45 mL). Then the combined organic layers were dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1) to afford product **1y** (83.6 mg, 80%).

1y: Light yellow oil: TLC R_f (PE/EA 10:1) = 0.52. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34 (t, J = 1.6 Hz, 1H), 7.24 (s, 1H), 6.26-6.27 (m, 1H), 3.25 (s, 1H), 2.84-2.89 (m, 2H), 2.79-2.82 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 186.1, 143.0, 139.1, 122.9, 110.7, 81.2, 78.8, 45.6, 18.9. IR (neat): ν 3275, 2094, 1681, 1104, 1023, 913, 874, 744, 600 cm^{-1}. HRMS (EI): Calcd for $C_9H_8O_2$ (M^+): 148.0526; found: 148.0524.

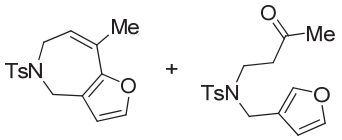
2.4 Experimental Details for Gold(I)-Catalyzed Intramolecular α-Alkenylation of Furans

General procedure for gold(I)-catalyzed intramolecular α-alkenylation of furans: A solution of β-yne-furan substrate and [JohnPhosAu(NCMe)]SbF_6 (5 mol%) in anhydrous DME (or toluene) was stirred under Ar atmosphere at room temperature. When TLC indicated the disappearance of the starting material, the reaction mixture was concentrated. The crude mixture was submitted to flash column chromatography on silica gel to afford the corresponding product.

Note: Two regioisomers could be formed from the alkyne hydration reaction, but we only observed one regioisomer (**3a**,**i**,**l** in Table 1 and **3v**,**w** in Table S2). Similar regioselectivity has been observed by Zhang and co-workers in the transfromation of alkynes to enones (Lu, B.; Li, C.; Zhang, L. *J. Am. Chem. Soc.* **2010**, *132*, 14070). In other cases (substrates **1b-h**,**j-k**,**m-t**), no hydration products were observed.

Experimental Data for Gold(I)-Catalyzed Intramolecular α-Alkenylation of Furans:

Product (2a) + Product (3a)



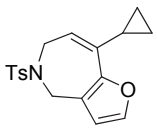
2a **3a**

Following the general procedure, β-yne-furan **1a** (20.2 mg, 0.07 mmol) was converted to product **2a** (18.2 mg, 90%) and product **3a** (0.3 mg, 1%). Volume of DME: 1 mL, room temperature, reaction time: 3 h.

2a: White solid: TLC R_f (PE/EA 5:1) = 0.52, m.p. = 68-70 ºC. ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.53 (d, J = 8.2 Hz, 2H), 7.28-7.29 (m, 1H), 7.17 (d, J = 8.2 Hz, 2H), 6.28-6.29 (m, 1H), 5.43 (t, J = 4.9 Hz, 1H), 4.53 (s, 2H), 4.00 (d, J = 4.9 Hz, 2H), 2.36 (s, 3H), 1.78 (s, 3H). ^{13}C NMR (100 MHz, CD_2Cl_2): δ 149.9, 143.7, 141.8, 137.2, 130.3, 129.3, 127.7, 120.8, 120.7, 111.6, 48.2, 47.4, 21.5, 19.4. IR (neat): ν 2983, 2928, 2861, 1737, 1602, 1501, 1448, 1244, 1166, 1095, 1021 cm^{-1}. HRMS (ESI): Calcd for $C_{16}H_{18}NO_3S$ (M + H^+): 304.1002, found: 304.1006.

3a: Colorless oil: TLC R_f (PE/EA 5:1) = 0.15. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.69 (d, J = 8.2 Hz, 2H), 7.34-7.35 (m, 1H), 7.31 (d, J = 8.2 Hz, 2H), 7.27 (s, 1H), 6.24-6,25 (m, 1H), 4.17 (s, 2H), 3.32 (t, J = 7.2, 2H), 2.70 (t, J = 7.2 Hz, 2H), 2.44 (s, 3H), 2.06 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 206.8, 143.6, 143.5, 141.0, 136.3, 129.8, 127.2, 120.6, 110.5, 43.8, 43.6, 42.5, 30.1, 21.5. IR (neat): ν 1714, 1336, 1158, 1022, 912, 874, 743, 655, 549 cm^{-1}. HRMS (ESI): Calcd for $C_{16}H_{20}NO_4S$ (M + H^+): 322.1108; found: 322.1112.

Product (2b)

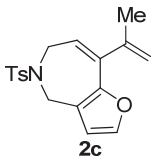


2b

Following the general procedure, β-yne-furan **1b** (40.3 mg, 0.12 mmol) was converted to product **2b** (36.7 mg, 91%). Volume of DME: 2 mL, room temperature, reaction time: 3 h.

2b: Colorless oil: TLC R_f (PE/EA 10:1) = 0.21. ^{1}H NMR (400 MHz, C_6D_6): δ 7.58 (d, J = 8.2 Hz, 2H), 6.85 (d, J = 1.7 Hz, 1H), 6.68 (d, J = 8.2 Hz, 2H), 5.76 (d, J = 1.7 Hz, 1H), 5.02 (t, J = 5.4 Hz, 1H), 4.35 (s, 2H), 3.74 (d, J = 5.4 Hz, 2H), 1.86 (s, 3H), 1.47-1.54 (m, 1H), 0.45-0.50 (m, 2H), 0.13-0.17 (m, 2H). ^{13}C NMR (100 MHz, C_6D_6): δ 149.8, 142.5, 141.3, 138.2, 135.5, 129.0, 127.7, 121.0, 118.9, 111.4, 47.1, 46.8, 21.0, 13.4, 6.0. IR (neat): ν 2287, 1605, 1356, 1173, 1102 cm^{-1}. HRMS (ESI): Calcd for $C_{18}H_{20}NO_3S$ (M + H$^+$): 330.1158; found: 330.1158.

Product (2c)

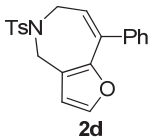


2c

Following the general procedure, β-yne-furan **1c** (44.7 mg, 0.14 mmol) was converted to product **2c** (39.2 mg, 88%). Volume of DME: 2 mL, room temperature, reaction time: 3 h.

2c: Colorless oil: TLC R_f (PE/EA 10:1) = 0.41. ^{1}H NMR (400 MHz, C_6D_6): δ 7.62 (d, J = 8.2 Hz, 2H), 6.80-6.81 (m, 1H), 6.71 (d, J = 8.2 Hz, 2H), 5.76-5.77 (m, 1H), 5.46 (t, J = 6.0 Hz, 1H), 4.94-4.95 (m, 1H), 4.89-4.90 (m, 1H), 4.32 (s, 2H), 3.70 (d, J = 6.0 Hz, 2H), 1.87 (s, 3H), 1.68 (s, 3H). ^{13}C NMR (100 MHz, C_6D_6): δ 148.1, 143.2, 142.7, 141.7, 138.1, 129.3, 129.3, 127.7, 122.7, 122.3, 115.4, 111.4, 46.4, 46.1, 22.0, 21.0. IR (neat): ν 2983, 2928, 2864, 1602, 1497, 1448, 1445, 1348, 1166, 1099 cm^{-1}. HRMS (ESI): Calcd for $C_{18}H_{19}NNaO_3S$ (M + Na$^+$): 352.0978; found: 352.0982.

Product (2d)

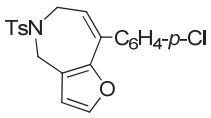


2d

Following the general procedure, β-yne-furan **1d** (46.6 mg, 0.13 mmol) was converted to product **2d** (35.2 mg, 76%). Volume of DME: 2 mL, room temperature, reaction time: 4 h.

2d: White solid: TLC R_f (PE/EA 10:1) = 0.18, m.p. = 153-154 ºC. ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.58 (d, J = 8.2 Hz, 2H), 7.30-7.31 (m, 3H), 7.28 (d, J = 1.6 Hz, 1H), 7.16 (d, J = 8.2 Hz, 2H), 7.02-7.04 (m, 2H), 6.38 (d, J = 1.6 Hz, 1H), 5.73 (t, J = 5.8 Hz, 1H), 4.65 (s, 2H), 4.14 (d, J = 5.8 Hz, 2H), 2.35 (s, 3H). ^{13}C NMR (100 MHz, CD_2Cl_2): δ 148.1, 143.8, 142.5, 139.0, 137.4, 136.6, 129.7, 128.8, 128.2, 128.1, 127.7, 124.3, 123.2, 111.8, 47.6, 47.1, 21.6. IR (neat): ν 2939, 1803, 1594, 1352, 1155, 1102, 935 cm^{-1}. HRMS (ESI): Calcd for $C_{21}H_{20}NO_3S$ (M + H$^+$): 366.1185; found: 366.1161.

Product (2e)

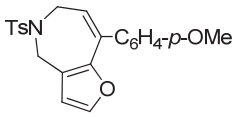


2e

Following the general procedure, β-yne-furan **1e** (39.3 mg, 0.10 mmol) was converted to product **2e** (35.6 mg, 90%). Volume of DME: 2 mL, room temperature, reaction time: 3 h.

2e: White solid: TLC R_f (PE/EA 10:1) = 0.18, m.p. = 120-121 ºC. ^{1}H NMR (400 MHz, C_6D_6): δ 7.57 (d, J = 8.2 Hz, 2H), 7.09 (dt, J = 1.8 and 1.3 Hz, 2H), 6.71 (d, J = 1.7 Hz, 1H), 6.68 (dt, J = 1.8 and 1.3 Hz, 2H), 6.59 (d, J = 8.2 Hz, 2H), 5.77 (d, J = 1.7 Hz, 1H), 5.26 (t, J = 5.8 Hz, 1H), 4.41 (s, 2H), 3.78 (d, J = 5.8 Hz, 2H), 1.80 (s, 3H). ^{13}C NMR (100 MHz, C_6D_6): δ 147.4, 142.7, 141.9, 138.2, 137.5, 135.1, 133.7, 130.2, 129.2, 128.1, 127.7, 124.7, 123.3, 111.5, 47.0, 46.7, 21.0. IR (neat): ν 2931, 2857, 2283, 1598, 1494, 1345, 1166, 1088, 1017 cm^{-1}. HRMS (ESI): Calcd for $C_{21}H_{19}ClNO_3S$ (M + H$^+$): 400.0769*;* found: 400.0763.

Product (2f)

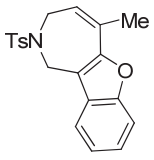


2f

Following the general procedure, β-yne-furan **1f** (42.5 mg, 0.11 mmol) was converted to product **2f** (41.6 mg, 98%). Volume of DME: 2 mL, room temperature, reaction time: 3 h.

2f: White solid: TLC R_f (PE/EA 5:1) = 0.14, m.p. = 138-140 ºC. ^{1}H NMR (400 MHz, C_6D_6): δ 7.63 (d, J = 7.9 Hz, 2H), 6.93-6.95 (m, 2H), 6.77 (d, J = 7.9 Hz, 2H), 6.74-6.75 (m, 1H), 6.65 (d, J = 7.9 Hz, 2H), 5.81-5.82 (m, 1H), 5.47 (t, J = 5.8 Hz, 1H), 4.45 (s, 2H), 3.85 (d, J = 5.8 Hz, 2H), 3.33 (s, 3H), 1.84 (s, 3H). ^{13}C NMR (100 MHz, C_6D_6): δ 159.8, 148.4, 142.6, 141.8, 138.2, 136.2, 131.5, 130.0, 129.2, 127.7, 123.4, 123.0, 113.5, 111.5, 54.8, 47.0, 46.7, 21.0. IR (neat): ν 2916, 1512, 1348, 1255, 1170, 1095, 842 cm^{-1}. HRMS (ESI): Calcd for $C_{22}H_{22}NO_4S$ (M + H$^+$): 396.1264; found: 396.1267.

Product (2g)

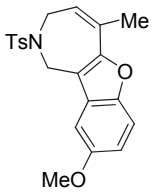


2g

Following the general procedure, β-yne-furan **1g** (41.2 mg, 0.12 mmol) was converted to product **2g** (29.3 mg, 71%). Volume of DME: 2 mL, room temperature, reaction time: 2 h.

2g: Colorless oil: TLC R_f (PE/EA 10:1) = 0.43. ^{1}H NMR (400 MHz, C_6D_6): δ 7.56 (d, J = 8.2 Hz, 2H), 7.17-7.21 (m, 1H), 7.07-7.09 (m, 1H), 7.00-7.04 (m, 2H), 6.55 (d, J = 8.0 Hz, 2H), 5.24 (td, J = 5.4 and 1.2 Hz, 1H), 4.61 (s, 2H), 3.82 (dd, J = 5.4 and 1.2 Hz, 2H), 1.79 (s, 3H), 1.74 (d, J = 1.2 Hz, 3H). ^{13}C NMR (100 MHz, C_6D_6): δ 153.6, 151.1, 142.6, 138.0, 129.9, 128.9, 128.3, 127.7, 125.2, 125.1, 123.1, 119.1, 115.6, 111.2, 47.7, 45.5, 21.0, 19.6. IR (neat): ν 2928, 2857, 2283, 1598, 1460, 1345, 1251, 1166 cm^{-1}. HRMS (ESI): Calcd for $C_{20}H_{20}NO_3S$ (M + H$^+$): 354.1158; found: 354.1151.

Product (2h)

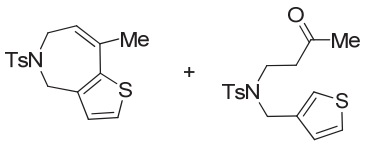


2h

Following the general procedure, β-yne-furan **1h** (51.8 mg, 0.14 mmol) was converted to product **2h** (38.6 mg, 74%). Volume of DME: 2 mL, room temperature, reaction time: 6 h.

2h: White solid: TLC R_f (PE/EA 10:1) = 0.26, m.p. = 192-193 ºC. ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.44 (d, J = 8.0 Hz, 2H), 7.18-7.20 (m, 1H), 7.01 (d, J = 8.0 Hz, 2H), 6.79-6.81 (m, 2H), 5.59 (t, J = 5.4 Hz, 1H), 4.66 (s, 2H), 4.00 (d, J = 5.4 Hz, 2H), 3.76 (s, 3H), 2.24 (s, 3H), 1.79 (s, 3H). ^{13}C NMR (100 MHz, CD_2Cl_2): δ 156.5, 152.1, 148.5, 143.8, 137.0, 130.8, 129.4, 128.7, 127.6, 124.8, 115.5, 114.3, 112.0, 101.1, 56.2, 48.1, 45.9, 21.5, 19.6. IR (neat): ν 2931, 1605, 1486, 1330, 1211, 1155, 1095, 1032, 942 cm^{-1}. HRMS (ESI): Calcd for $C_{21}H_{22}NO_4S$ (M + H$^+$): 406.1084; found: 406.1075.

Product (2i) + Product (3i)



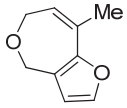
2i **3i**

Following the general procedure, β-yne-furan **1i** (42.0 mg, 0.13 mmol) was converted to product **2i** (19.3 mg, 46%) and product **3i** (17.4 mg, 39%). Volume of DME: 2 mL, room temperature, reaction time: 20 h.

2i: White solid: TLC R_f (PE/EA 5:1) = 0.45, m.p. = 84-86 ºC. ^{1}H NMR (400 MHz, C_6D_6): δ 7.52 (d, J = 8.2 Hz, 2H), 6.65 (d, J = 8.2 Hz, 2H), 6.60 (d, J = 5.1 Hz, 1H), 6.43 (d, J = 5.1 Hz, 1H), 4.99 (t, J = 4.9 Hz, 1H), 4.34 (s, 2H), 3.85 (d, J = 4.9 Hz, 2H), 1.87 (s, 3H), 1.61 (d, J = 1.1 Hz, 3H). ^{13}C NMR (100 MHz, C_6D_6): δ 142.2, 140.2, 137.9, 135.8, 131.3, 128.9, 128.8, 127.7, 123.8, 122.8, 48.6, 48.5, 24.2, 21.0. IR (neat): ν 2928, 2857, 1669, 1602, 1497, 1445, 1337, 1218, 1170, 1102, 1035 cm^{-1}. HRMS (ESI): Calcd for $C_{16}H_{17}NNaO_2S_2$ (M + H$^+$): 342.0593; found: 342.0596.

3i: Light yellow oil: TLC R_f (PE/EA 5:1) = 0.24. ^{1}H NMR (400 MHz, C_6D_6): δ 7.66 (d, J = 8.2 Hz, 2H), 6.90-6.91 (m, 1H), 6.80-6.82 (m, 2H), 6.79 (s, 1H), 6.70-6.71 (m, 1H), 4.07 (s, 2H), 3.32 (t, J = 7.3 Hz, 2H), 2.30 (t, J = 7.3 Hz, 2H), 1.92 (s, 3H), 1.44 (s, 3H). ^{13}C NMR (100 MHz, C_6D_6): δ 205.1, 143.0, 138.2, 137.5, 129.8, 128.1, 127.5, 126.4, 123.6, 48.4, 43.6, 43.5, 29.3, 21.1. IR (neat): ν 2287, 1714, 1335, 1157, 912, 814, 748, 655, 548, 496 cm^{-1}. HRMS (ESI): Calcd for $C_{16}H_{20}NO_3S_2$ (M + H$^+$): 338.0879; found: 338.0874.

Product (2j)

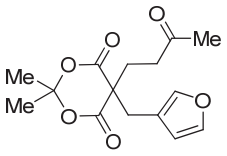


2j

Following the general procedure, β-yne-furan **1j**[13] (42.2 mg, 0.28 mmol) was converted to product **2j** (25.5 mg, 60%). Volume of toluene: 3.5 mL, room temperature, reaction time: 20 h.

2j: Yellow oil: TLC R_f (PE/EA 10:1) = 0.52. ^{1}H NMR (400 MHz, C_6D_6): δ 6.94 (s, 1H), 5.80 (s, 1H), 5.31-5.32 (m, 1H), 4.53 (s, 2H), 4.02 (d, J = 4.4 Hz, 2H), 2.04 (s, 3H). ^{13}C NMR (100 MHz, C_6D_6): δ 149.9, 141.2, 129.7, 125.0, 124.9, 110.4, 69.3, 68.1, 19.2. IR (neat): ν 2931, 2853, 1736, 1464, 1278, 1132, 1080 cm^{-1}. HRMS (ESI): Calcd for $C_9H_{11}O_2$ (M + H$^+$): 151.0754; found: 151.0750.

Product (3l)

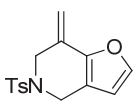


3l

Following the general procedure, β-yne-furan **1l** (16.4 mg, 0.06mmol) was converted to product **3l** (13.2 mg, 76%). Volume of DME: 1.2 mL, room temperature, reaction time: 4 d.

3l: Colorless oil: TLC R_f (PE/EA 3:1) = 0.39. ^{1}H NMR (400 MHz, C_6D_6): δ 7.19 (s, 1H), 6.92-6.93 (m, 1H), 6.24 (s, 1H), 2.95 (s, 2H), 2.28 (t, J = 7.4 Hz, 2H), 2.13 (t, J = 7.4 Hz, 2H), 1.54 (s, 3H), 1.23 (s, 3H), 0.79 (s, 3H). ^{13}C NMR (100 MHz, C_6D_6): δ 203.9, 168.7, 143.1, 142.0, 119.4, 112.4, 105.3, 55.4, 38.1, 32.4, 29.1, 29.0, 28.7. IR (neat): ν 1740, 1345, 1284, 1204, 948, 603 cm^{-1}. HRMS (ESI): Calcd for $C_{15}H_{18}NaO_6$ (M + Na$^+$): 317.0996; found: 317.0996.

Product (2m)



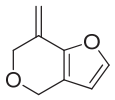
2m

[13] Pastine, S. J.; Youn, S. W.; Sames, D. *Tetrahedron* **2003**, *59*, 8859.

Following the general procedure, β-yne-furan **1m**[14] (59.8 mg, 0.21 mmol) was converted to product **2m** (30.1 mg, 50%). Volume of DME: 2 mL, room temperature, reaction time: 1 h.

2m: Colorless oil: TLC R_f (PE/EA 10:1) = 0.34. ^{1}H NMR (400 MHz, C_6D_6): δ 7.62 (d, J = 8.2, 2H), 6.75-6.77 (m, 2H), 6.74 (s, 1H), 5.64-5.66 (m, 1H), 5.21 (s, 1H), 4.55 (s, 1H), 4.03 (s, 2H), 3.84 (s, 2H), 1.87 (s, 3H). ^{13}C NMR (100 MHz, C_6D_6): δ 147.9, 143.0, 142.6, 135.6, 129.8, 129.4, 127.9, 117.8, 109.0, 104.6, 49.3, 43.9, 21.0. IR (neat): ν 3375, 2928, 2853, 1662, 1602, 1497, 1345, 1162, 1091, 1039 cm^{-1}. HRMS (ESI): Calcd for $C_{15}H_{16}NO_3S$ (M + H^+): 290.0845; found: 290.0849.

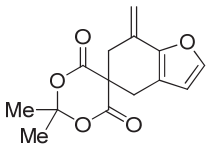
Product (2n)



2n

Following the general procedure, β-yne-furan **1n**[13] (42.3 mg, 0.31 mmol) was converted to product **2n**[13] (10.5 mg, 25%). Volume of toluene: 5 mL, room temperature, reaction time: 20 min.

Product (2o)

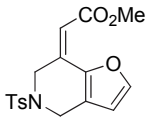


2o

Following the general procedure, β-yne-furan **1o** (44.1 mg, 0.17 mmol) was converted to product **2o** (18.8 mg, 43%). Volume of DME: 2 mL, room temperature, reaction time: 7 h.

2o: Colorless oil: TLC R_f (PE/EA 5:1) = 0.29. ^{1}H NMR (400 MHz, C_6D_6): δ 6.97-6.98 (m, 1H), 5.85-5.86 (m, 1H), 5.52 (s, 1H), 4.63 (s, 1H), 2.90 (s, 2H), 2.78 (s, 2H), 1.15-1.16 (m, 3H), 1.09-1.10 (m, 3H). ^{13}C NMR (100 MHz, C_6D_6): δ 168.1, 148.6, 142.4, 129.6, 116.7, 110.7, 106.6, 104.3, 50.2, 39.5, 30.4, 28.7, 28.0. IR (neat): ν 1737, 1655, 1389, 1318, 1285, 1195, 1169, 1098, 1043, 950, 894 cm^{-1}. HRMS (ESI): Calcd for $C_{14}H_{15}O_5$ (M + H^+): 263.0914; found: 263.0912.

Product (2p)



2p

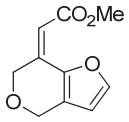
Following the general procedure, β-yne-furan **1p**[15] (40.1 mg, 0.12 mmol) was converted to product **2p** (36.8 mg, 92%). Volume of DME: 2 mL, room temperature, reaction time: 4 h.

[14] Hashmi, A. S. K.; Weyrauch, J. P.; Kurpejović, E.; Frost, T. M.; Miehlich, B.; Frey, W.; Bats, J. W. *Chem. Eur. J.* **2006**, 12, 5806.

[15] Yamamoto, Y.; Kuwabara, S.; Ando, Y.; Nagata, H.; Nishiyama, H.; Itoh, K. *J. Org. Chem.* **2004**, *69*, 6697.

2o: White solid: TLC R_f (PE/EA 5:1) = 0.15, m.p. = 131-133 ºC. ^{1}H NMR (400 MHz, C_6D_6): δ 7.56 (d, J = 8.2 Hz, 2H), 6.79 (d, J = 1.5 Hz, 1H), 6.73 (d, J = 8.0 Hz, 2H), 5.52 (d, J = 1.5 Hz, 1H), 5.28 (s, 1H), 3.96 (s, 2H), 3.65 (s, 2H), 3.47 (s, 3H), 1.86 (s, 3H). ^{13}C NMR (100 MHz, C_6D_6): δ 165.2, 145.6, 144.7, 143.3, 135.5, 131.1, 129.5, 128.3, 123.7, 111.5, 108.8, 51.0, 50.4, 44.0, 21.0. IR (neat): ν 1717, 1637, 1447, 1339, 1257, 1158, 1089, 1041, 950, 899, 830 cm^{-1}. HRMS (ESI): Calcd for $C_{17}H_{18}NO_5S$ ($M + H^+$): 348.0900; found: 348.0896.

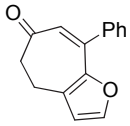
Product (2q)



2q

Following the general procedure, β-yne-furan **1q**[13] (32.5 mg, 0.17 mmol) was converted to product **2q**[13] (24.8 mg, 76%). Volume of DME: 2 mL, room temperature, reaction time: 1 h.

Product (2r)

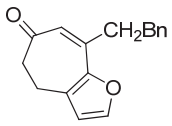


2r

Following the general procedure, β-yne-furan **1r** (30.4 mg, 0.14mmol) was converted to product **2r** (28.4 mg, 93%). Volume of DME: 2mL, room temperature, reaction time: 2 h.

2r: Light yellow oil: TLC R_f (PE/EA 5:1) = 0.48. ^{1}H NMR (400 MHz, C_6D_6): δ 7.24-7.27 (m, 2H), 7.10-7.12 (m, 3H), 6.78 (d, J = 1.5 Hz, 1H), 6.30 (s, 1H), 5.83 (d, J = 1.5 Hz, 1H), 2.50-2.53 (m, 2H), 2.23-2.26 (m, 2H). ^{13}C NMR (100 MHz, C_6D_6): δ 197.6, 148.6, 142.8, 142.7, 139.1, 130.1, 129.1, 128.9, 128.3, 127.3, 113.4, 41.6, 19.7. IR (neat): ν 1634, 1481, 1335, 1272, 1087, 753, 699 cm^{-1}. HRMS (ESI): Calcd for $C_{15}H_{13}O_2$ ($M + H^+$): 225.0910; found: 225.0912.

Product (2s)

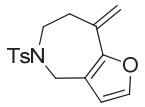


2s

Following the general procedure, β-yne-furan **1s** (36.9 mg, 0.15 mmol) was converted toproduct **2s** (21.8 mg, 59%). Volume of DME: 2 mL, room temperature, reaction time: 2 h.

2s: Colorless oil: TLC R_f (PE/EA 5:1) = 0.34. ^{1}H NMR (400 MHz, C_6D_6): δ 7.13 (d, J = 7.5, 2H), 7.06-7.07 (m, 1H), 7.01-7.03 (m, 2H), 6.83 (d, J = 1.4, 1H), 6.03 (s, 1H), 5.80 (d, J = 1.4, 1H), 2.68-2.69 (m, 4H), 2.47-2.50 (m, 2H), 2.16-2.19 (m, 2H). ^{13}C NMR (100 MHz, C_6D_6): δ 197.6, 149.6, 142.6, 142.0, 141.3, 128.9, 128.6, 126.4, 125.9, 113.4, 41.0, 37.0, 35.8, 19.8. IR (neat): ν 1648, 1562, 1486, 1281, 1117, 704 cm^{-1}. HRMS (ESI): Calcd for $C_{17}H_{17}O_2$ ($M + H^+$): 256.1223; found: 256.1227.

Product (2t)

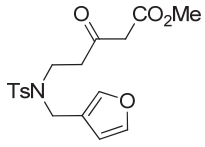


2t

Following the general procedure, β-yne-furan **1t** (40.7 mg, 0.13 mmol) was converted to product **2t** (19.1 mg, 47%). Volume of DME: 2 mL, room temperature, reaction time: 20 h.

2t: White solid: TLC R_f (PE/EA 30:1) = 0.11, m.p. = 60-62 ºC. ^{1}H NMR (400 MHz, C_6D_6): δ 7.62 (d, J = 8.1 Hz, 2H), 6.79-6.80 (m, 1H), 6.77 (d, J = 7.5 Hz, 2H), 5.73-5.74 (m, 1H), 5.42 (s, 1H), 4.65 (s, 1H), 4.14 (s, 2H), 3.16-3.19 (m, 2H), 2.31-2.33 (m, 2H), 1.89 (s, 3H). ^{13}C NMR (100 MHz, C_6D_6): δ 150.3, 142.7, 141.5, 137.2, 135.9, 129.5, 127.5, 119.5, 111.8, 110.8, 47.7, 44.7, 35.0, 21.0. IR (neat): ν 1605, 1497, 1095, 1024, 1088, 950, 801 cm^{-1}. HRMS (ESI): Calcd for $C_{16}H_{18}NO_3S$ (M + H$^+$): 304.1002; found: 304.0997.

Product (3v)

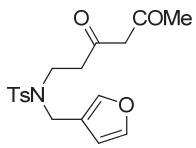


3v

Following the general procedure, β-yne-furan **1v** (42.3 mg, 0.12 mmol) was converted to product **3v** (34.7 mg, 78%). Volume of DME: 2 mL, room temperature, reaction time: 24 h.

3v: Colorless oil: TLC R_f (PE/EA 5:1) = 0.13. ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.68 (d, J = 8.1 Hz, 2H), 7.36 (d, J = 8.1 Hz, 2H), 7.34 (s, 1H), 7.30 (s, 1H), 6.25 (s, 1H), 4.17-4.20 (m, 2H), 3.67-3.71 (m, 3H), 3.36 (s, 2H), 3.32-3.35 (m, 2H), 2.77 (t, J = 8.1 Hz, 2H), 2.43-2.44 (m, 3H). ^{13}C NMR (100 MHz, CD_2Cl_2): δ 201.3, 167.6, 144.2, 144.1, 141.6, 136.8, 130.2, 127.5, 121.2, 110.9, 52.6, 49.5, 44.0, 43.1, 42.6, 21.6. IR (neat): ν 1753, 1720, 1322, 1151, 1095, 1024, 814 cm^{-1}. HRMS (ESI): Calcd for $C_{18}H_{21}NaNO_6S$ (M + Na$^+$): 402.0982; found: 402.0993.

Product (3w)



3w

Following the general procedure but adding 3 μL water. β-yne-furan **1w** (28.6 mg, 0.083 mmol) was converted to product **3w** (5.9 mg, 20%). Volume of DME: 2mL, room temperature, reaction time: 24 h.

3w: Colorless oil: TLC R_f (PE/EA 3:1) = 0.30. ^{1}H NMR (400 MHz, C_6D_6): δ 15.70-16.0 (bs, 0.9H), 7.66 (d, J = 8.1, 2H), 7.00 (s, 0.1H), 6.97 (s, 0.9H), 6.96 (s, 0.1H), 6.94 (s, 0.9H), 6.77 (d, J = 8.1, 2H), 6.17-6.18 (m, 0.9H), 6.16-6.17 (m, 0.1H), 4.92 (s, 0.9H), 3.97 (s, 1.8H), 3.95 (s, 0.2H), 3.33-3.36 (m, 1.8H), 3.30-3.32 (m, 0.2H), 2.78 (s, 0.2H), 2.51-2.54 (m, 0.2H), 2.36-2.39 (m, 1.8H), 1.90 (s, 3H), 1.59 (s, 0.3H), 1.53 (s, 2.7H). ^{13}C NMR (100 MHz, C_6D_6): δ 192.7, 189.8, 143.7, 142.9, 141.4, 137.9, 129.7, 127.6, 121.2, 110.9, 100.5, 44.0, 43.5, 38.9, 23.8, 21.0. IR (neat): v 1764, 1730, 1334, 1158, 1099, 1055, 827 cm^{-1}. HRMS (ESI): Calcd for $C_{18}H_{22}NO_5S$ ($M + H^+$): 364.1213; found: 364.1213.

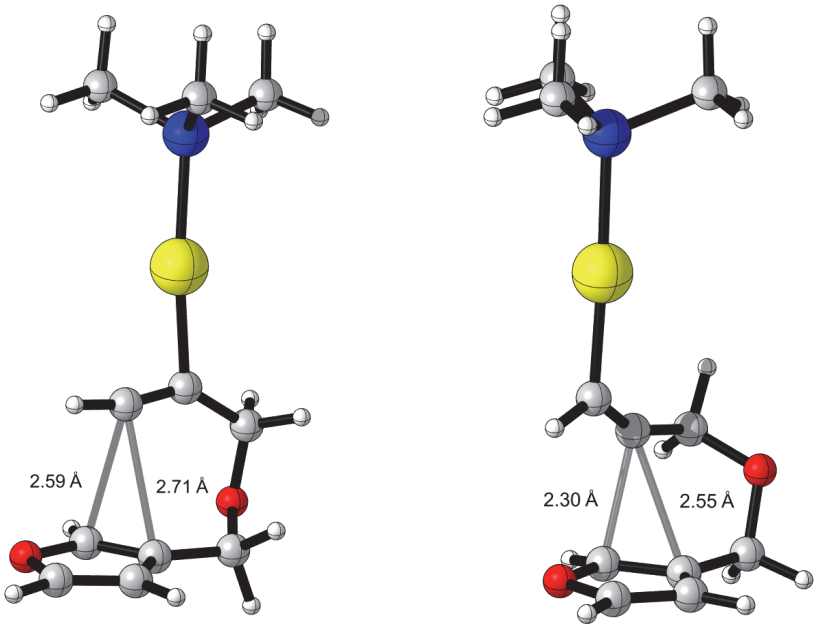
About 87% of **3w** exists as its enol form, based on the integral of ^{1}H NMR of 4.92 ppm.

3. DFT Study

3.1 Computational Details and Discussion

All DFT calculations were performed with the Gaussian 09 software package.[16] Geometry optimization of all the minima and transition states involved was carried out at the B3LYP level of theory.[17] The SDD basis set (Stuttgart/Dresden ECP)[18] was used for gold and the 6-31G(d) basis set[19] for the other atoms. The key word "5D" was used to specify that five d-type orbitals were used for all elements in the calculations. Frequency calculations at the same level were performed to validate each structure as either a minimum or a transition state and to evaluate its zero-point energy and the thermal corrections at 298 K. In the paper and the Supporting Information, all discussed energies are Gibbs free energies in gas phase (ΔG_{gas}) at 298 K unless specified. We found that the conclusions in both the gas phase and toluene are the same (see computed solvent effects in Figure S2).

The DFT-calculated structures[20] of transition states **TS1-H**, **TS2-H**, **TS1-Me**, and **TS2-Me** shown in Figure 2 of the paper are provided in Figure S1.



TS1-H **TS2-H**

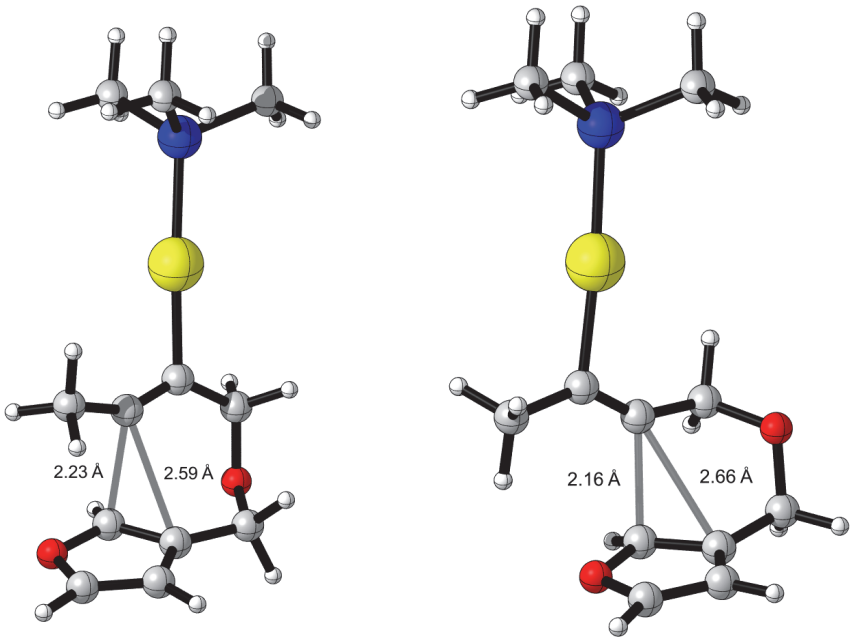
[16] Gaussian 09, Revision A.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2009**.

[17] a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648; (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785.

[18] a) Szentpaly, L. V.; Fuentealba, P.; Preuss, H.; Stoll, H. *Chem. Phys. Lett.* **1982**, *93*, 555; b) Dolg, M.; Wedig, U.; Stoll, H.; Preuss, H. *J. Chem. Phys.* **1987**, *86*, 866; c) Schwerdtfeger, P.; Dolg, M.; Schwarz, W. H. E.; Bowmaker, G. A.; Boyd, P. D. W. *J. Chem. Phys.* **1989**, *91*, 1762.

[19] Hehre, W. J.; Radom, L.; Schleyer, P. v. R.; Pople, J. A. *Ab Initio Molecular Orbital Theory*; Wiley: New York, **1986**.

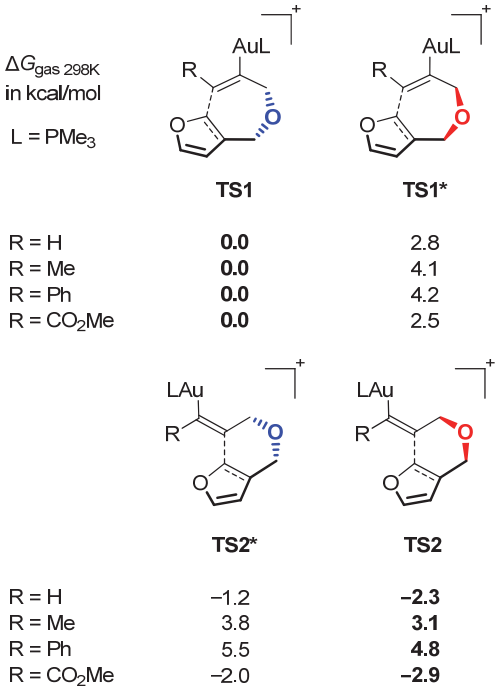
[20] Figures created with: CYLview, 1.0b; Legault, C. Y., Université de Sherbrooke, **2009**. http://www.cylview.org.



TS1-Me **TS2-Me**

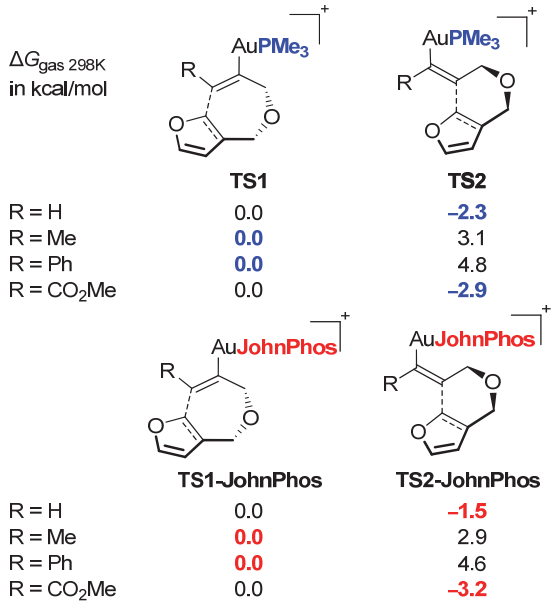
Figure S1. DFT-calculated structures of transition states **TS1-H**, **TS2-H**, **TS1-Me**, and **TS2-Me** (C gray; H white; O red; P blue; Au yellow).

The relative Gibbs free energies of different conformers for transition states shown in Figure 2 of the paper are provided in Scheme S1.



Scheme S1. Relative Gibbs free energies at 298 K of different conformers for **TS1** and **TS2**.

We have tested whether using PMe_3 to model the bulky JohnPhos ligand is appropriate or not. Calculations found that regioselectivity of the alkenylation reaction is the same for PMe_3 and JohnPhos (Scheme S2). These results further support that the regioselectivity is mainly controlled by the electronic effect.



Scheme S2. Relative Gibbs free energies at 298 K of **TS1** and **TS2** with PMe_3 and JohnPhos.

Solvation energies in toluene were evaluated by IEFPCM calculations with radii and non-electrostatic terms for SMD solvation model.[21] The results shown in Figure S2 are very similar to those given in Figure 2 of the paper.

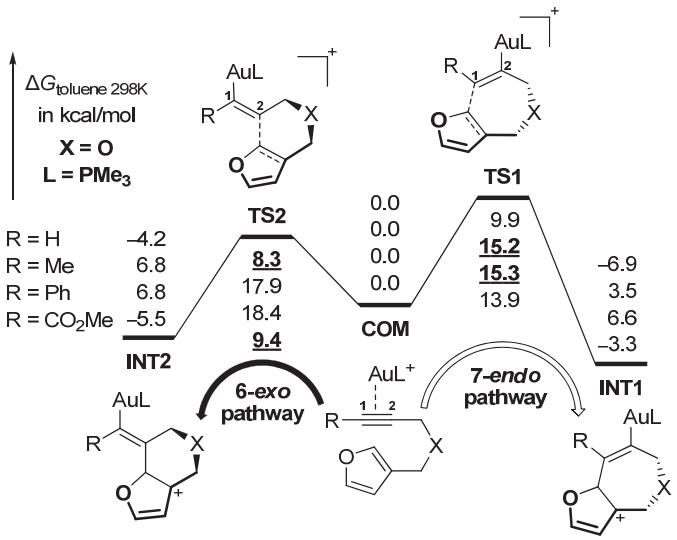


Figure S2. Relative Gibbs free energies in toluene at 298 K.

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

In Figure S3, different cyclization pathways for *O*- and *CH*$_2$-tethered methyl substrates were compared (Note [17] of the paper). 7-*Endo* cyclization is favored over 6-*exo* cyclization when X = O, as mentioned in both Figure 2 and Figure S2 (see Table 1, entry 12 in the paper). However, if X = CH_2, formation of six-membered ring is favored. If we take ligand exchange step into account, the overall activation energies are 16.7 and 17.7 kcal/mol for substrates with X = O and CH_2, respectively. This suggests that the *CH*$_2$-tethered substrate is less reactive than the *O*-tethered substrate (by about 1 kcal/mol). We speculate that in this case, some unknown side reactions become favored over the alkenylation of *CH*$_2$-tethered substrate. Consequently, these unknown side reactions lead to the decomposition of *CH*$_2$-tethered substrate (see Table 1, entry 13 in the paper).

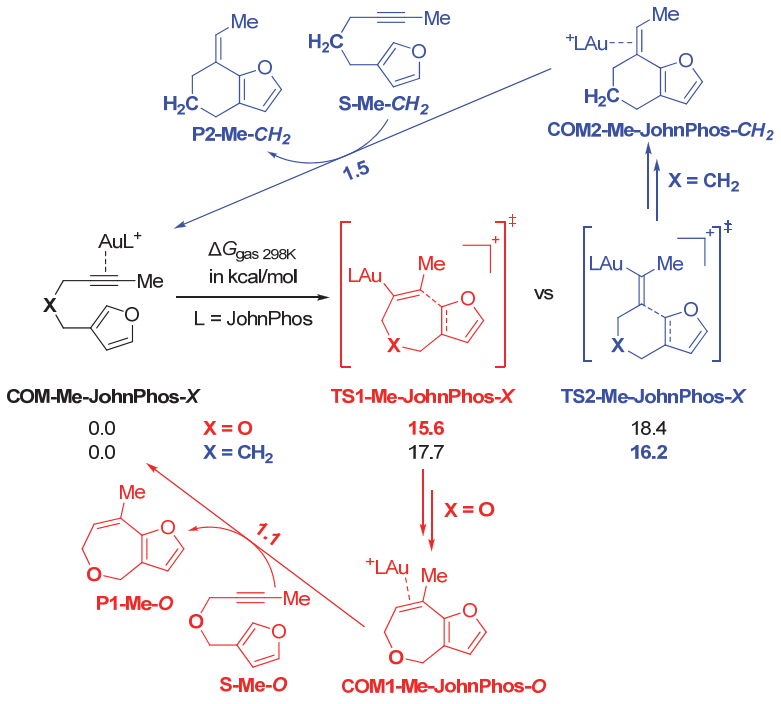


Figure S3. Different α-alkenylation pathways for *O*- and *CH*$_2$-tethered methyl substrates.

In Figure S4, three different cyclization pathways A, B, and C for **COM-CO$_2$Me** were compared. Generation of **P2-CO$_2$Me** is favored with respect to **P1-CO$_2$Me**, because **TS2-CO$_2$Me** is favored over **TS1-CO$_2$Me** by 2.9 kcal/mol. Futhermore, the *syn*-attack transition state **TS3-CO$_2$Me**, which leads to *E*-isomer **P3-CO$_2$Me**, is disfavored with respect to the *anti*-attack transition state **TS2-CO$_2$Me** by 5.8 kcal/mol owing to the repulsion between furan and AuL^+ moiety in **TS3-CO$_2$Me**. Therefore, generation of *Z*-isomer **P2-CO$_2$Me** is favored over **P1-CO$_2$Me** and **P2-CO$_2$Me**. This DFT-predicted regio- and stereoselectivity is in good agreement with the experiment (see Scheme 3a of the paper).

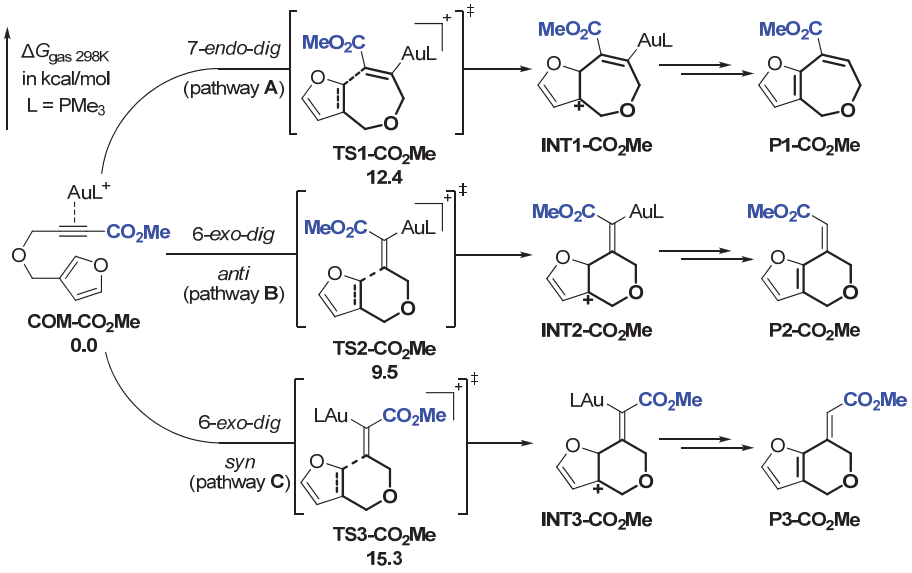


Figure S4. Three different α-alkenylation pathways for **COM-CO$_2$Me**.

In Figure S5, different cyclization pathways for elongated-tethered substrates were compared. It is very interesting to note that formations of eight-membered rings are disfavored compared to the formations of seven-membered rings when R = H and CO$_2$Me. However, if R = Me, formation of eight-membered ring is favored. The ligand exchange steps were also tested. The overall activation energies are 12.2, 15.1, and 16.8 kcal/mol when R = H, CO$_2$Me, and Me, respectively. This implies that CO$_2$Me and Me are not good terminal substituents compared to H for the alkenylation of elongated-tethered substrates.

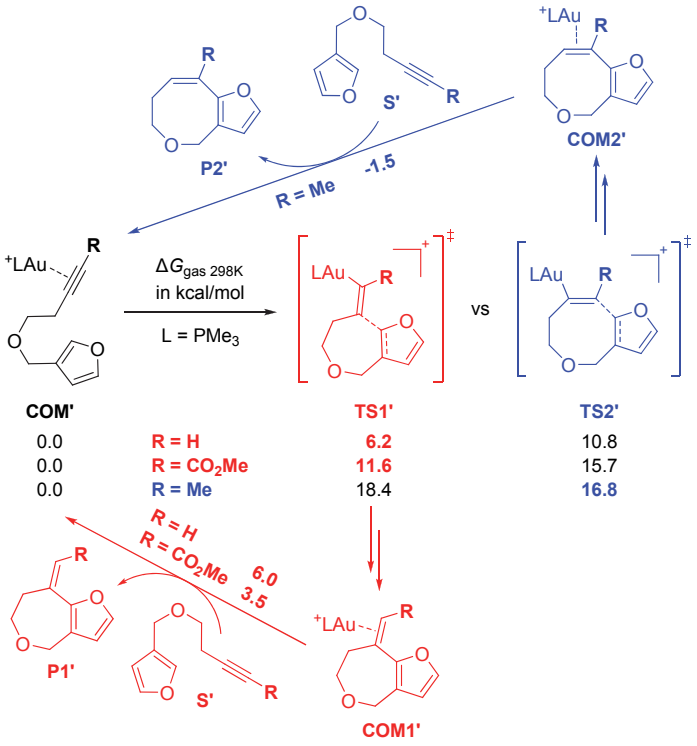


Figure S5. Different α-alkenylation pathways for elongated-tethered substrates.

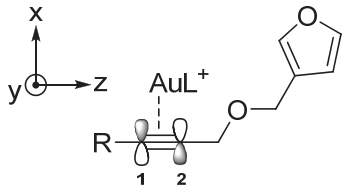
3.2 In-Depth Analyses of Substituent Effects on Regioselectivity

In the paper, we used the NPA charges to evaluate which carbon of the triple bond is more eletrophilic. Such method has been used in previous reports to explain the observed regioselectivity of alkyne cyclizations (see Ref. [21] of the paper). Analysis of charges can be easily understood by chemists, however, it is not the only approach to explain the regioselectivity of a nucleophilic addition. Herein we report in-depth analyses of substituent effects on the observed regioselectivity using two methods concerning the gold–substrate complexes, and the transition states, respectively.

3.2.1 Analysis of the Gold–Substrate Complexes

Analysis of the gold–substrate complexes (**COM**s in Figure 2 of the paper) are carried out to understand the regiochemistry (Table S3). In the paper, we used the NPA charges to evaluate which carbon of the triple bond is more eletrophilic and therefore more reactive towards nucleophilic attack of the furan ring (Figure 2). Here we use FMO interaction and reorganization energy to explain the regioselectivity, respectively.

Table S3: Analysis of orbital coefficients and bond lengths of **COM**s (L = PMe_3).



COM

R	coefficients (NAO basis)		energy [eV] (orbital)	bond lengths [Å]	
	C1	C2		C1–Au	C2–Au
H	–0.44 (p_x)	**+0.50** (p_x)	–4.97 (LUMO)	2.29	**2.35**
Me	**–0.47** (p_x)	+0.40 (p_x)	–4.60 (LUMO)	**2.38**	2.28
Ph	**+0.49** (p_x)	–0.29 (p_x)	–5.14 (LUMO)	**2.51**	2.22
CO_2Me	–0.38 (p_y) **–0.50** (p_x)	**+0.54** (p_y) +0.46 (p_x)	–4.78 (LUMO) –4.74 (LUMO+1)	2.33	2.32

FMO analysis of substituent effect on regioselectivity. During the course of the reaction, there exists a significant FMO interaction between the HOMO of furan and the LUMO of the gold–alkyne moiety (the orbital shown in Table S3), which can be easily understood as the electron flow from furan to the gold–alkyne moiety. The LUMO coefficient at the C2 atom in **COM-H** is larger than that at C1 (+0.50 at C2 versus –0.44 at C1), which suggests that C2 matchs HOMO of the furan moiety better than C1, according to FMO theory. Therefore, the *exo* pathway is favored over the *endo* pathway caused by the polarization of the triple bond. In contrast, when R = Me or Ph, the LUMO coefficient at the C1 atom is larger than that at C2 (Table S3), which indicates that seven-membered ring will be formed dominantly.

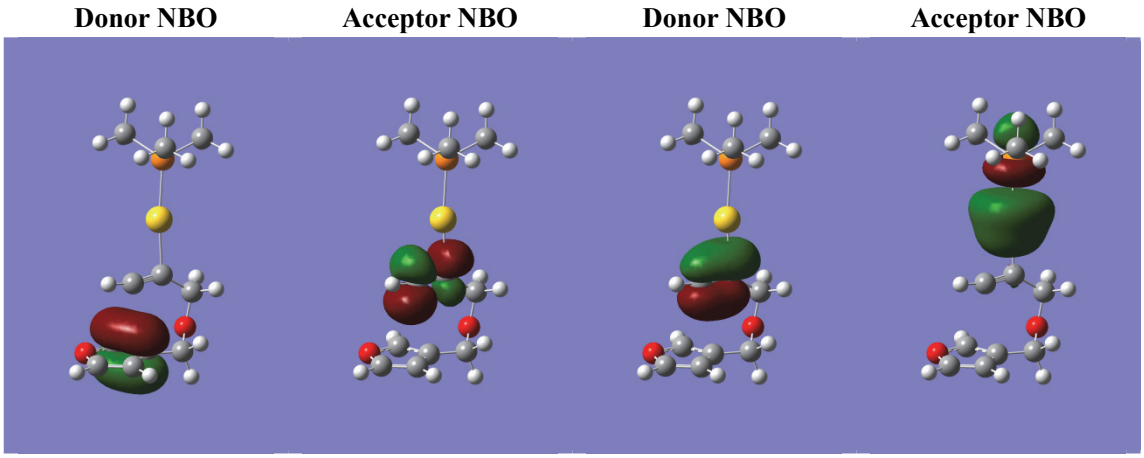
When R = CO_2Me, the LUMO of the gold–substrate complex is consisted of the out-of-plane π_y^* orbital, which is in conjugation with the in-plane carbonyl group, but this orbital is perpendicular to the xz-plane and cannot interact with the HOMO of furan. We find that the LUMO+1, which involves the in-plane π_x^* orbital, could interact with the HOMO of furan. The p_x coefficient at C1 is larger than that at C2 in LUMO+1 (–0.50 at C1 versus +0.46 at C2), which suggests that seven-membered ring will be formed dominantly. However, it is not in accordance with the observed regioselectivity. We reason that in the transition state, the ester group rotates to the yz-plane and forms a conjugation system with the π_x^* orbital. Therefore, analysis of orbital coefficient of π_x^* in **COM-CO_2Me** (which is not in conjugation with the carbonyl group) is not reasonable. In this case, the regioselectivity of the alkenylation reaction of ynoate ester substrate could be understood using the NBO analysis of transition states (see Section 3.2.2 for details).

FMO analysis of substituent effect on relative reactivities. The FMO interaction can also be used to understand the relative reactivities of yne-furan substrates. According to FMO theory, the lower the LUMO energy of the gold–substrate complex is, the faster the reaction will be. The LUMO energy of **COM-Me** is higher than that of **COM-H** (–4.60 eV when R = Me versus –4.97 eV when R = H), therefore, the reaction of methyl substrate is slower than that of terminal alkyne substrate. Similarly, the LUMO or LUMO+1 energy of **COM-CO_2Me** is higher than LUMO energy of **COM-H** (Table S3), therefore, the ynoate ester substrate is less reactive than terminal alkyne substrate. The LUMO energy of **COM-Ph** is lower than that of **COM-H** (–5.14 eV when R = Ph versus –4.97 eV when R = H). Due to this, phenyl substrate should be more reactive than terminal alkyne substrate. But it is not the case. We attribute this to the loss of conjugation energy when R = Ph: phenyl group is not in an optimal position to form conjugated system. In addition, the phenyl group in the transition states is experiencing steric repulsions with furan and the AuL^+ moiety.

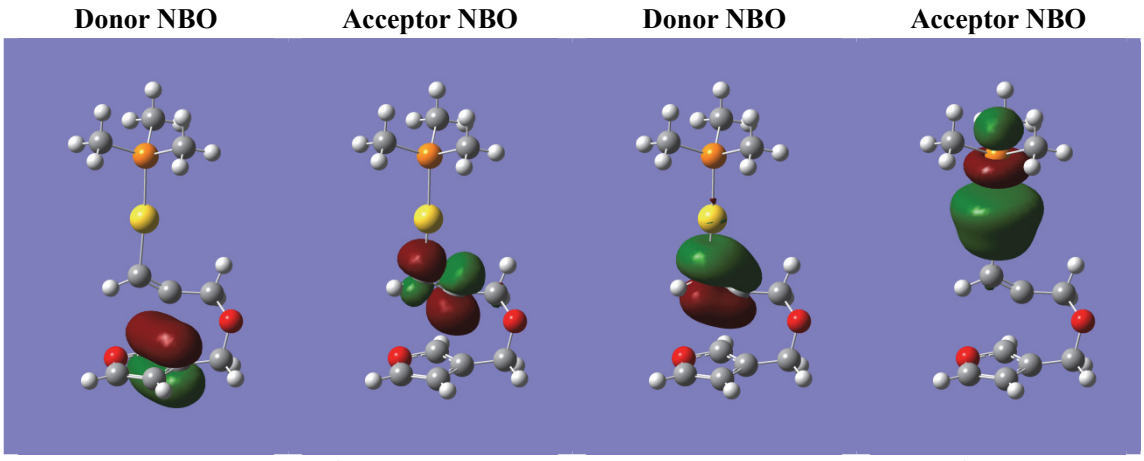
Analysis of substituent effect on regioselectivity based on reorganization energy. Analysis of the C–Au bond lengths can also provide explanation for the observed regioselectivity. During the reaction, there exists reorganization energy to weaken one C–Au bond (simultaneously strengthen another C–Au bond). Formation of **TS1** leads to the weakening of the C1–Au bond while the C2–Au bond is weakened from **COM** to **TS2**. When R = H, the reorganization energy of **TS1** is expected to be larger than that of **TS2**, because C1–Au is stronger than C2–Au in **COM-H** (2.29 Å for C1–Au versus 2.35 Å for C2–Au). Therefore, the *exo* pathway will be favored when R = H. However, when R = Me or Ph, C2–Au is much stronger than C1–Au in **COM** (Table S3), so **TS1** will be favored over **TS2**. Reorganization energy cannot be used to explain the regioselectivity of ynoate ester substrate: when R = CO_2Me, the bond lengths of C1–Au and C2–Au are nearly the same in **COM-CO_2Me** (2.33 Å for C1–Au versus 2.32 Å for C2–Au), but six-membered ring product is formed exclusively experimentally. In this case, the regioselectivity of the alkenylation reaction of ynoate ester substrate could be understood using the NBO analysis of transition states (see Section 3.2.2 for details).

3.2.2 NBO Analysis of Substituent Effects on the Regioselectivity

Here we give the natural bond orbital (NBO) analysis of the α-alkenylation transition states to gain more insights into the substituent effects on the observed regioselectivity.[22] There are significant π(furan)→π*(alkyne, in plane) and π(alkyne, in plane)→σ*(Au–P) interactions in the α-alkenylation transition states (Figure S6). These donor–acceptor interactions can be easily understood as the electron flow from furan to alkyne, and finally to the $Au(PMe_3)^+$ moiety.



TS1-H



TS2-H

Figure S6. NBO analysis of α-alkenylation transition states **TS1-H** and **TS2-H** calculated at B3LYP/SDD–6-31G(d) level (isovalue = 0.040).

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

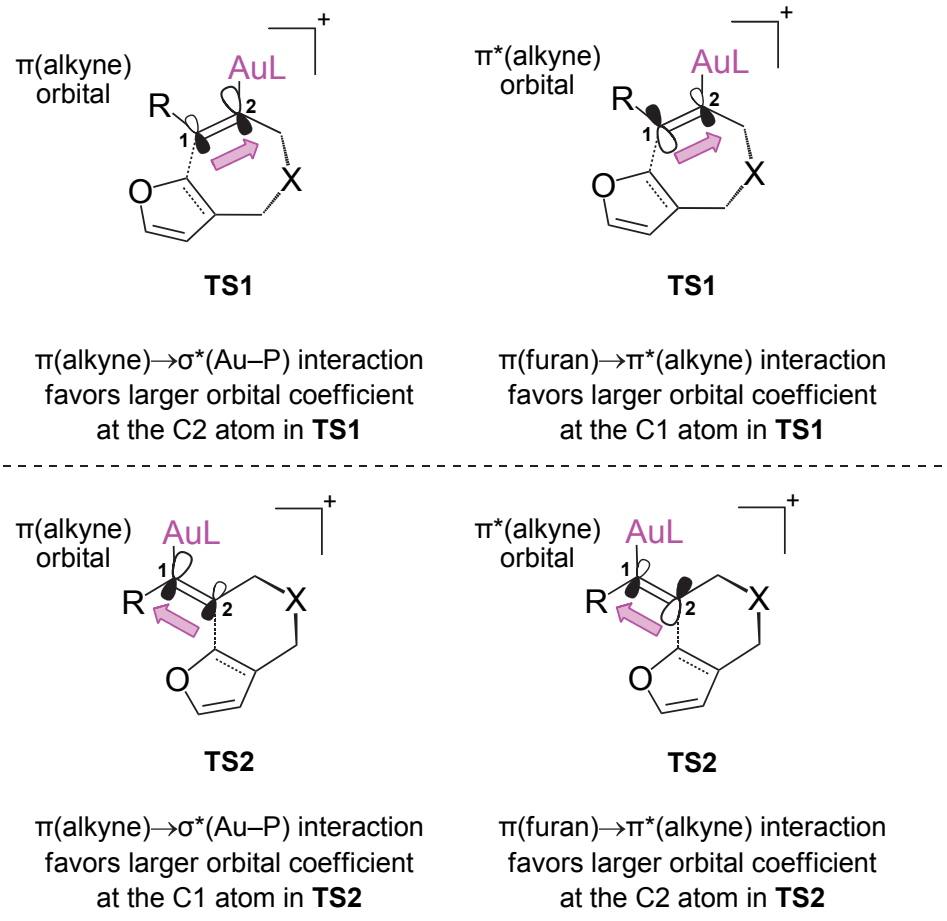
Second-order perturbation energy of electron delocalization $E(2)$ has been determined to evaluate the relative magnitude of the stabilizing effects induced by different substituents in the competing 7-*endo* and 6-*exo* cyclization transition states (Table S4). It is noteworthy that **TS1** and **TS2** differ in the stabilization energies significantly. When R = Me and Ph, **TS1** is stabilized more effectively than **TS2**. In contrast, when R = H and CO_2Me, **TS2** is stabilized more effectively than **TS1**. These results are in accordance with the experimentally observed regioselectivity and DFT-calculated potential energy surface (Figure 2 of the paper). The difference in energies of **TS1** and **TS2** can be devided into two parts: (1) the difference in intrinsic barriers for **TS1** and **TS2** due to the different ring strains and intrinsic difference in the stabilization energies of donor–acceptor interactions; (2) substituent effect on the stabilization energies of donor–acceptor interactions in **TS1** and **TS2**.

Table S4: Second-order perturbation energies $E(2)$, off-diagonal NBO Fock matrix element F, the ratio of natural bond orbital population $P\pi^*$(alkyne)/$P\pi$(alkyne), and bond length d(C≡C) in **TS1** and **TS2** calculated at B3LYP/SDD–6-31G(d) level.

	$E(2)$ [kcal/mol] / F		$P\pi^*$(alkyne)	d(C≡C)
	π(furan)→π*(alkyne)	π(alkyne)→σ*(Au–P)	$P\pi$(alkyne)	[Å]
TS1-H	12.76/0.053	75.30/0.179	0.114	1.252
TS2-H	**34.76/0.089**	**92.52/0.194**	**0.192**	**1.275**
TS1-Me	43.73/0.098	**92.33/0.193**	**0.223**	**1.287**
TS2-Me	43.79/0.101	82.24/0.183	0.214	1.284
TS1-Ph	**63.74/0.119**	**104.62/0.203**	**0.299**	**1.301**
TS2-Ph	42.43/0.099	78.79/0.178	0.215	1.282
TS1-CO_2Me	18.01/0.063	72.67/0.176	0.173	1.270
TS2-CO_2Me	**29.49/0.081**	**79.86/0.183**	**0.192**	**1.274**

Analysis of intrinsic barriers for TS1 and TS2. In the 7-*endo* cyclization transition state **TS1**, the π(alkyne)→σ*(Au–P) interaction favors larger orbital coefficient at C2 than at C1 in the π(alkyne) orbital to gain maximum overlap (the off-diagonal NBO Fock matrix element F in Table S4 corresponds to the magnitude of overlap) between the π(alkyne) and σ*(Au–P) orbitals, while the π(furan)→π*(alkyne) interaction favors larger orbital coefficient at C1 than at C2 in the π*(alkyne) orbital (see Scheme S3 and Figure S6). In contrast, in the 6-*exo* cyclization transition state **TS2**, the π(alkyne)→σ*(Au–P) interaction favors larger orbital coefficient at C1 than at C2 in the π(alkyne) orbital, while the π(furan)→π*(alkyne) interaction favors larger orbital coefficient at C2 than at C1 in the π*(alkyne) orbital (see Scheme S3 and Figure S6).

Intrinsic barriers for **TS1** and **TS2** are proposed to be similar. To evaluate this hypothesis, we perform some DFT calculations on the cyclization reactions of bis-(3-furanylmethoxymethyl) acetylene, which is a symmetric alkyne (Figure S7). The difference in energies of the 7-*endo* and 6-*exo* cyclizations is found to be only 0.2 kcal/mol for **TS1-symm** and **TS2-symm** (14.1 kcal/mol for **TS1-symm** versus 14.3 kcal/mol for **TS2-symm**). The poor regioselectivity can be easily understood considering the nonpolar nature of the symmetric alkyne (this also suggests that the ring strains in **TS1** and **TS2** are very similar in the present case). Therefore, the intrinsic reaction barriers for the 7-*endo* and 6-*exo* cyclizations are very similar.



Scheme S3. The polarization of the triple bond in **TS1** and **TS2**.

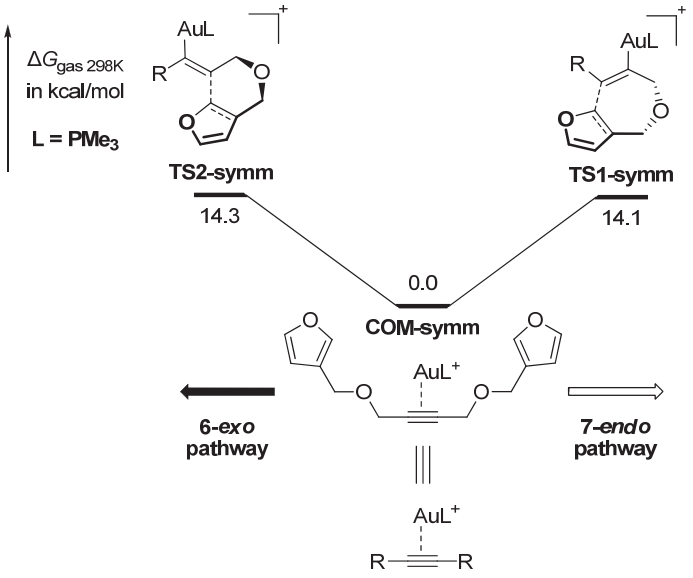


Figure S7. Different alkenylation pathways for bis-(3-furanylmethoxymethyl) acetylene at 298 K.

Analysis of substituent effect on the relative magnitude of stabilizing donor–acceptor interactions. We reasoned that the substituent effect on the polarization of the triple bond plays a vital role in determining the relative magnitude of the stabilizing donor–acceptor interactions. The length of the triple bond correlates with the ratio of natural bond orbital population $P\pi^*$(alkyne)/$P\pi$(alkyne) with coefficient of determination (R^2) equals to 0.97 (Figure S8). The growth of the population of π^*(alkyne) reflects the increase in the electron-donating abilities of the substituents while the decrease of population of π(alkyne) corresponds to the increase in the electron-withdrawing abilities of the substituents.[23] Therefore, the larger the ratio of natural bond orbital population $P\pi^*$(alkyne)/$P\pi$(alkyne) is, the longer and more polar the triple bond will be.

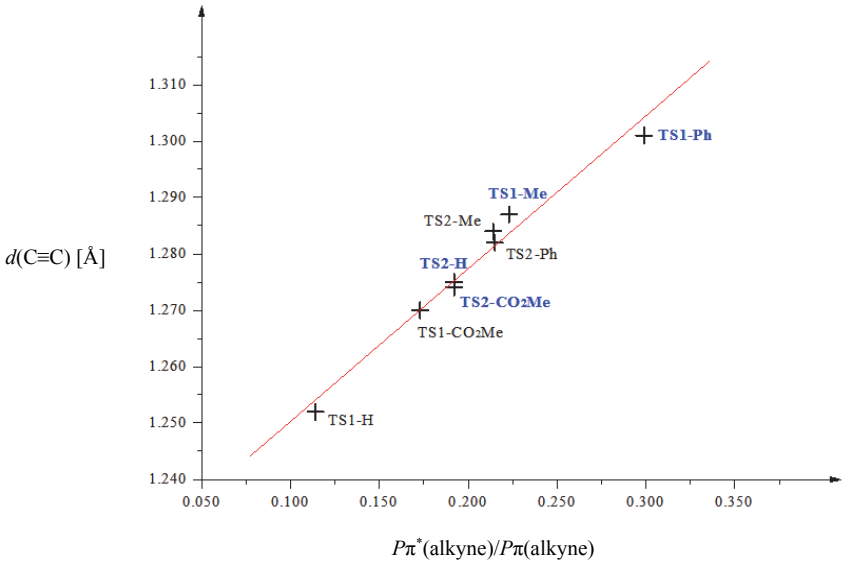
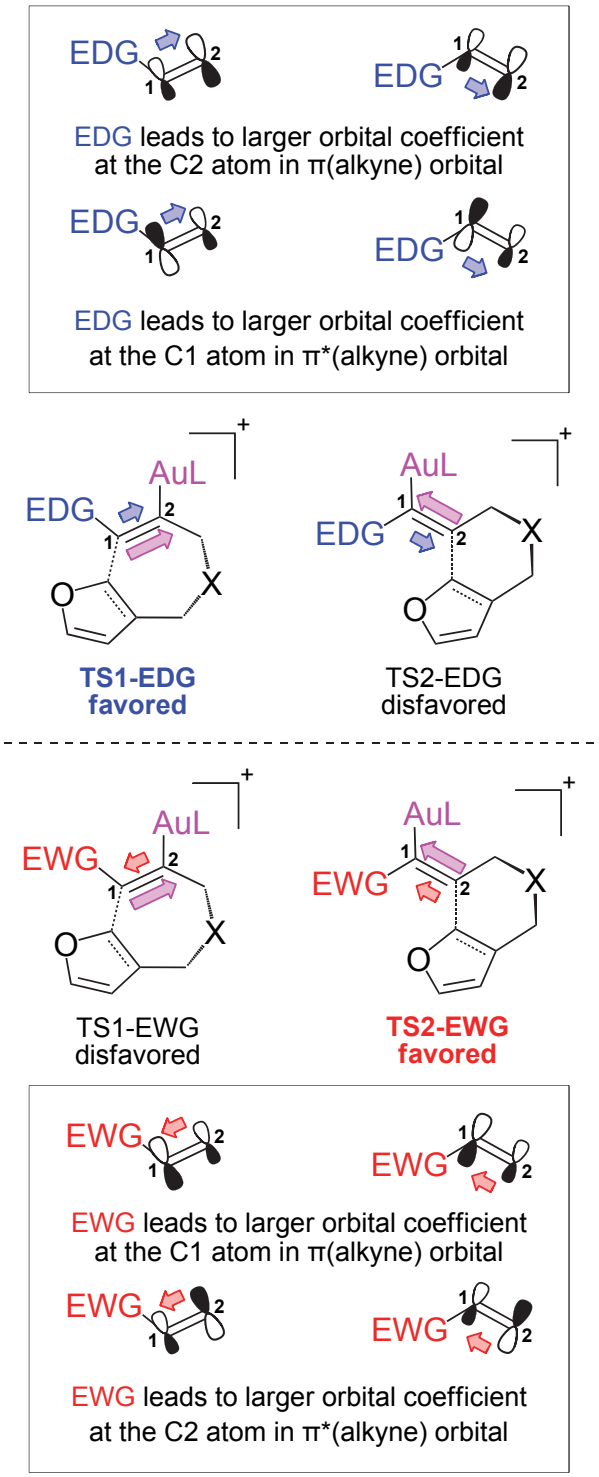


Figure S8. Relationship between the length of the triple bond and the ratio of natural bond orbital population $P\pi^*$(alkyne)/$P\pi$(alkyne). d(C≡C)/Å=1.223+0.27$P\pi^*$(alkyne)/$P\pi$(alkyne), R^2=0.97.

It is known that electron-donating group (EDG) polarizes the alkyne in such a way that the orbital coefficient at C2 is larger than that at C1 (the carbon atom which EDG is attached to) in the π(alkyne) orbital while the orbital coefficient at C1 is larger than that at C2 in the π^*(alkyne) orbital (Scheme S4, top). Due to this, when an EDG is used as the terminal substituent, both the stabilizing π(alkyne)→σ^*(Au–P) and π(furan)→π^*(alkyne) interactions in **TS1** can be further enhanced, while these two interactions become weakened in **TS2** (see Scheme S4 and Table S4). Consequently, EDG favors **TS1** and the *endo*-selective alkenylation product was formed.

In contrast, the alkyne polarization induced by electron-withdrawing group (EWG) has opposite effect to that of EDG. For EWG substituted alkyne, the orbital coefficient at C1 (the carbon atom which EWG is attached to) is larger than that at C2 in the π(alkyne) orbital while the orbital coefficient at C2 is larger than that at C1 in the π^*(alkyne) orbital (Scheme S4, bottom). Due to this, when an EWG is used as the terminal substituent, both the π(alkyne)→σ^*(Au–P) and π(furan)→π^*(alkyne) interactions in **TS1** become weakened, while these two interactions are further enhanced in **TS2** (see Scheme S4 and Table S4). Consequently, EWG favors **TS2** and the *exo*-selective alkenylation product was obtained.

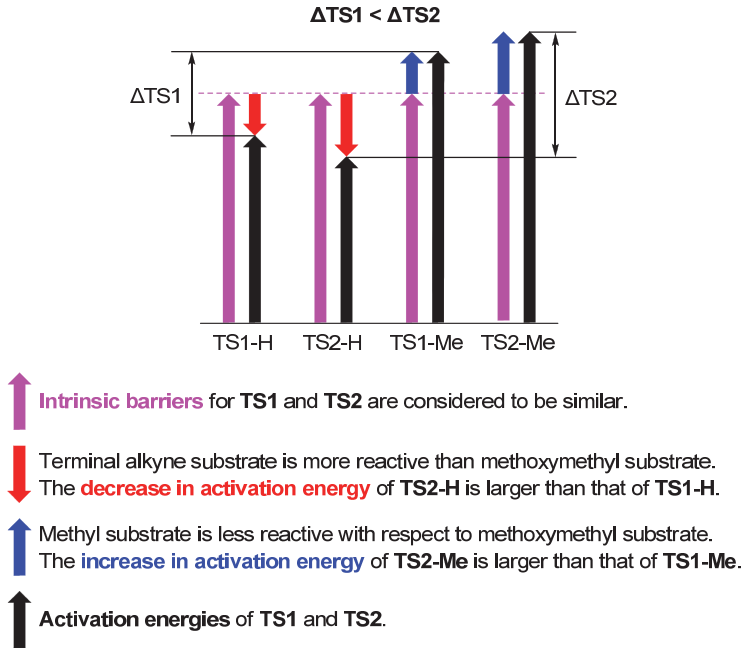
[23] Keiko, N. A.; Aksamentova, T. N.; Chipanina, N. N.; Verochkina, E. A.; Vchislo, N. V. *Tetrahedron* **2013**, *69*, 2022.



Scheme S4. Substituent effects on the alkyne polarization and regioselectivity.

Why variation in the energy of TS1 is smaller than that of TS2 when the R group changes from H to Me? Interestingly, when the terminal substituent changes from H to Me, both the 7-*endo* and 6-*exo* cyclizations require higher activation energies, however, the activation energy variations are quite different: 4.2 kcal/mol for **TS1** versus 9.6 kcal/mol for **TS2**.

To understand these results, we provide an energy decomposition model shown in Scheme S5. The activation energy (in black) can be divided into two parts: the intrinsic barrier (in pink) and increase (in blue) or decrease (in red) of activation energy induced by the substituent. Intrinsic barriers for **TS1** and **TS2** are considered to be similar, as indicated by the computed energies of the model reactions shown in Figure S7.



Scheme S5. Energy decomposition model for alkenylation transition states **TS1** and **TS2**.

When the R group changes from 3-furanylmethoxymethyl to a more electron-donating methyl group, the reactivity is expected to be reduced because the LUMO energy of **COM** increases, according to FMO theory. However, calculations indicate that these two substrates have very similar reactivities (14.1 kcal/mol for the symmetric alkyne substrate versus 13.4 kcal/mol for methyl substrate). This discrepancy is due to the additional coordination of the oxygen (sp^3) atom of the 3-furanylmethoxymethyl group to the gold atom in **COM-symm**, making the reaction barrier for the alkenylation more higher. Here we do not consider this additional stabilization effect caused by the O–Au coordination, but concentrate on how the activation energy increases when the R group changes from 3-furanylmethoxymethyl to Me. Analysis of substituent effect on stabilization energies based on the NBO analysis has shown that there exists stronger stabilization effect on **TS1** than on **TS2** when R = EDG (relative to the tether). As a result, the activation energy increase of **TS1** is smaller than that of **TS2** when the R group changes from 3-furanylmethoxymethyl to Me (Scheme S5).

In contrast, when the R group changes from 3-furanylmethoxymethyl to H, the LUMO energy of **COM** decreases, as a result, the reaction barriers of the substrate decreases. Analysis of substituent effect on stabilization energies based on the NBO analysis has shown that there exists stronger stabilization effect on **TS2** than on **TS1** when R = EWG (relative to the tether). Therefore,

the activation energy decrease of **TS1** is smaller than that of **TS2** when the R group changes from 3-furanylmethoxymethyl to H (Scheme S5).

Consequently, we reason that the smaller variation in the energy of **TS1** with respect to that of **TS2** when the R group changes from H to Me is due to the different electronic-donating/ withdrawing properties of H and Me relative to the tether, which is 3-furanylmethoxymethyl group.

3.3 Computed Energies of All Stationary Points

Table S5: Sum of electronic and thermal enthalpies (***H***, in Hartree), sum of electronic and thermal free energies (***G***, in Hartree), thermal correction to Gibbs free energy (***TCG***, in Hartree), and total energy in toluene with non-electrostatic terms ($E_{toluene}$, in Hartree).

Figure 2, S2 and S4 X = O, L = PMe_3	***H***	***G***	***TCG***	$E_{toluene}$
COM-H	-1056.441555	-1056.515275	0.204637	-1056.771000
TS1-H	-1056.429881	-1056.500593	0.206673	-1056.757222
INT1-H	-1056.458368	-1056.526144	0.211996	-1056.789394
TS2-H	-1056.435125	-1056.504335	0.208311	-1056.761406
INT2-H	-1056.453274	-1056.521369	0.211985	-1056.785066
COM-Me	-1095.741166	-1095.819193	0.230867	-1096.101055
TS1-Me	-1095.726315	-1095.797874	0.236291	-1096.082269
INT1-Me	-1095.742518	-1095.813760	0.238114	-1096.102647
TS2-Me	-1095.720420	-1095.792904	0.235550	-1096.077278
INT2-Me	-1095.734993	-1095.807522	0.237040	-1096.096381
COM-Ph	-1287.425189	-1287.511736	0.278686	-1287.843750
TS1-Ph	-1287.410312	-1287.489892	0.284541	-1287.825153
INT1-Ph	-1287.420813	-1287.500383	0.285860	-1287.840382
TS2-Ph	-1287.399797	-1287.482277	0.281520	-1287.817295
INT2-Ph	-1287.417062	-1287.497515	0.285193	-1287.839361
COM-CO_2Me	-1284.264306	-1284.350992	0.239959	-1284.643299
TS1-CO_2Me	-1284.250421	-1284.331203	0.244858	-1284.626063
INT1-CO_2Me	-1284.277379	-1284.355821	0.248845	-1284.657521
TS2-CO_2Me	-1284.254931	-1284.335776	0.244880	-1284.633216
INT2-CO_2Me	-1284.277263	-1284.356798	0.248372	-1284.660439
TS3-CO_2Me	-1284.245477	-1284.326668	0.244055	

Table S6: Sum of electronic and thermal enthalpies (***H***, in Hartree), sum of electronic and thermal free energies (***G***, in Hartree), and thermal correction to Gibbs free energy (***TCG***, in Hartree).

Scheme S2 X = O, L = JohnPhos	***H***	***G***	***TCG***
TS1-H-JohnPhos	-1714.744419	-1714.849694	0.493262
TS2-H-JohnPhos	-1714.748132	-1714.852073	0.494858
TS1-Me-JohnPhos	-1754.037557	-1754.143701	0.522823
TS2-Me-JohnPhos	-1754.031518	-1754.139157	0.521539
TS1-Ph-JohnPhos	-1945.720083	-1945.834111	0.571195
TS2-Ph-JohnPhos	-1945.710983	-1945.826735	0.569346
TS1-CO_2Me-JohnPhos	-1942.564241	-1942.679490	0.531514
TS2-CO_2Me-JohnPhos	-1942.568468	-1942.684540	0.530815

Table S7: Sum of electronic and thermal enthalpies (***H***, in Hartree), sum of electronic and thermal free energies (***G***, in Hartree), and thermal correction to Gibbs free energy (***TCG***, in Hartree).

Figure S3 L = JohnPhos, R = Me	***H***	***G***	***TCG***
COM-Me-JohnPhos-*O*	-1754.055994	-1754.168520	0.517511
TS1-Me-JohnPhos-*O*	-1754.037557	-1754.143701	0.522823
COM1-Me-JohnPhos-*O*	-1754.116788	-1754.222441	0.526336
TS2-Me-JohnPhos-*O*	-1754.031518	-1754.139157	0.521539
S-Me-*O*	-499.120496	-499.174104	0.128112
P1-Me-*O*	-499.181327	-499.226316	0.138359
COM-Me-JohnPhos-CH_2	-1718.144136	-1718.259922	0.538831
TS1-Me-JohnPhos-CH_2	-1718.123979	-1718.231718	0.545741
TS2-Me-JohnPhos-CH_2	-1718.125989	-1718.234074	0.545526
COM2-Me-JohnPhos-CH_2	-1718.206864	-1718.313131	0.550198
S-Me-CH_2	-463.213014	-463.266969	0.152487
P2-Me-CH_2	-463.272391	-463.317822	0.162437

Table S8: Sum of electronic and thermal enthalpies (***H***, in Hartree), sum of electronic and thermal free energies (***G***, in Hartree), and thermal correction to Gibbs free energy (***TCG***, in Hartree).

Figure S5 X = OCH_2, L = PMe_3	***H***	***G***	***TCG***
COM′-H	-1095.724903	-1095.805318	0.227990
TS1′-H	-1095.723960	-1095.795499	0.235990
COM1′-H	-1095.798737	-1095.870625	0.239137
TS2′-H	-1095.715673	-1095.788109	0.235121
S′-H	-499.115056	-499.165891	0.130525
P1′-H	-499.177818	-499.221716	0.139822
COM′-CO_2Me	-1323.547993	-1323.641612	0.263159
TS1′-CO_2Me	-1323.537921	-1323.623198	0.270348
COM1′-CO_2Me	-1323.613507	-1323.697056	0.275146
TS2′-CO_2Me	-1323.533047	-1323.616594	0.272272
S′-CO_2Me	-726.939230	-727.003754	0.165506
P1′-CO_2Me	-726.998338	-727.053542	0.176449
COM′-Me	-1135.022841	-1135.107415	0.254399
TS1′-Me	-1135.001716	-1135.07804	0.261628
TS2′-Me	-1135.005886	-1135.080634	0.263124
COM2′-Me	-1135.072474	-1135.146852	0.266534
S′-Me	-538.409694	-538.466983	0.154718
P2′-Me	-538.462008	-538.508884	0.16679

Table S9: Sum of electronic and thermal enthalpies (***H***, in Hartree), sum of electronic and thermal free energies (***G***, in Hartree), and thermal correction to Gibbs free energy (***TCG***, in Hartree).

Figure S7 X = O, L = PMe_3, R = 3-furanylmethoxymethyl	***H***	***G***	***TCG***
COM-symm	-1438.981894	-1439.077145	0.304136
TS1-symm	-1438.964896	-1439.054666	0.308359
TS2-symm	-1438.965355	-1439.054376	0.309317

3.4 Coordinates of All Stationary Points

COM-H

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.999151	0.377651	-1.014279
2	6	0	-3.438646	-0.333835	0.008039
3	6	0	-3.479433	0.536100	1.156569
4	6	0	-4.059500	1.692403	0.734926
5	8	0	-4.381802	1.607277	-0.589114
6	6	0	-2.899837	-1.720013	-0.065343
7	6	0	1.841093	-2.717693	0.080702
8	8	0	-1.456926	-1.659028	0.000961
9	6	0	-0.848810	-2.932247	-0.019100
10	6	0	0.614209	-2.739978	0.034580
11	1	0	-3.143972	0.308799	2.159395
12	1	0	-4.329187	2.616455	1.223257
13	1	0	-3.263544	-2.334316	0.771277
14	1	0	-3.199843	-2.208280	-1.002967
15	1	0	-1.096301	-3.491657	-0.935863
16	1	0	-1.153653	-3.548456	0.842392
17	1	0	-4.202973	0.149497	-2.050222
18	79	0	1.302869	-0.489195	0.002767
19	15	0	1.390876	1.834247	-0.040712
20	6	0	2.633962	2.493914	-1.219125
21	6	0	-0.215496	2.569933	-0.535875
22	6	0	1.804431	2.572299	1.588205
23	1	0	2.619174	3.589099	-1.207091
24	1	0	2.410373	2.143054	-2.230648
25	1	0	3.633491	2.146305	-0.942570
26	1	0	-0.477632	2.239303	-1.544889
27	1	0	-0.145587	3.663125	-0.522223
28	1	0	-1.005295	2.245929	0.148616
29	1	0	1.059805	2.272850	2.331279
30	1	0	1.819110	3.665046	1.513948
31	1	0	2.786585	2.222347	1.918750
32	1	0	2.892563	-2.923618	0.129047

TS1-H

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.033406	-0.472046	-0.949361
2	6	0	4.113064	0.131319	0.285648
3	6	0	4.576163	-0.884584	1.187790
4	6	0	4.744220	-2.010403	0.439057
5	8	0	4.413925	-1.777020	-0.862351
6	6	0	3.820784	1.577733	0.591492
7	6	0	1.537953	-0.525687	-0.266166
8	8	0	2.960287	2.168639	-0.385826
9	6	0	1.586372	2.064432	-0.126328
10	6	0	1.087859	0.638423	-0.172176
11	1	0	4.761985	-0.782801	2.248083
12	1	0	5.072214	-3.013449	0.667030
13	1	0	3.390540	1.681900	1.598560
14	1	0	4.743920	2.166370	0.567753
15	1	0	1.078854	2.654429	-0.893687
16	1	0	1.326686	2.487961	0.856520
17	79	0	-0.993417	0.062732	-0.046297
18	15	0	-3.304363	-0.283040	0.088663
19	6	0	-3.987421	-1.214962	-1.339354
20	6	0	-3.821107	-1.218736	1.582543
21	6	0	-4.250321	1.290483	0.144331
22	1	0	-5.070662	-1.334743	-1.229570
23	1	0	-3.522107	-2.203202	-1.397386
24	1	0	-3.778398	-0.677438	-2.268793
25	1	0	-3.351375	-2.206587	1.585273
26	1	0	-4.909685	-1.339656	1.595667
27	1	0	-3.509000	-0.682975	2.483669
28	1	0	-3.949189	1.877132	1.017104
29	1	0	-5.324073	1.083300	0.205670
30	1	0	-4.050667	1.878271	-0.756340
31	1	0	3.815061	-0.099691	-1.937778
32	1	0	1.681761	-1.587794	-0.293655

INT1-H

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.437783	-0.535024	-0.752389
2	6	0	4.088849	0.193883	0.359924
3	6	0	4.885347	-0.683312	1.066685
4	6	0	4.783054	-1.908836	0.396465
5	8	0	4.000307	-1.885053	-0.641329
6	6	0	3.793614	1.645493	0.555746
7	6	0	1.910877	-0.629412	-0.516629
8	8	0	2.927402	2.112956	-0.440671
9	6	0	1.534839	1.842123	-0.192686
10	6	0	1.088251	0.405149	-0.280031
11	1	0	5.469295	-0.498397	1.958216
12	1	0	5.251438	-2.861864	0.623987
13	1	0	3.398858	1.814980	1.573669
14	1	0	4.733948	2.210440	0.484840
15	1	0	1.005616	2.436625	-0.943112
16	1	0	1.261429	2.253068	0.793138
17	79	0	-0.956440	0.081461	-0.069465
18	15	0	-3.285494	-0.256751	0.148266
19	6	0	-4.118408	-0.769696	-1.411375
20	6	0	-3.759484	-1.551846	1.368158
21	6	0	-4.209849	1.240599	0.689281
22	1	0	-5.193877	-0.902648	-1.251992
23	1	0	-3.690191	-1.711254	-1.767831
24	1	0	-3.961875	-0.008514	-2.181449
25	1	0	-3.322627	-2.511962	1.077722
26	1	0	-4.848554	-1.655800	1.421071
27	1	0	-3.377074	-1.285444	2.357987
28	1	0	-3.838963	1.573289	1.663311
29	1	0	-5.281492	1.028168	0.767670
30	1	0	-4.057647	2.049820	-0.031116
31	1	0	3.703260	-0.177683	-1.753217
32	1	0	1.558701	-1.654945	-0.572044

TS2-H

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.954659	-0.461491	-0.907331
2	6	0	4.263464	0.247927	0.249910
3	6	0	4.360259	-0.726723	1.288935
4	6	0	4.147214	-1.936164	0.695320
5	8	0	3.916025	-1.791674	-0.640219
6	6	0	1.837420	0.367307	-0.541620
7	6	0	2.143562	1.819191	-0.612709
8	8	0	2.955959	2.257673	0.447656
9	6	0	4.294542	1.744847	0.346421
10	6	0	1.053918	-0.622805	-0.362166
11	1	0	3.974710	-0.192984	-1.953912
12	1	0	4.556530	-0.544911	2.336142
13	1	0	4.134282	-2.951475	1.063333
14	1	0	2.578910	2.076724	-1.591549
15	1	0	1.189321	2.349114	-0.516861
16	1	0	4.810167	2.079647	1.247368
17	1	0	4.792154	2.183396	-0.530180
18	79	0	-1.001331	-0.207801	-0.118417
19	15	0	-3.304734	0.100587	0.178826
20	6	0	-4.171605	-1.436002	0.693847
21	1	0	-3.758946	-1.796355	1.640656
22	1	0	-5.242952	-1.245568	0.818976
23	1	0	-4.032230	-2.213298	-0.063130
24	6	0	-3.727883	1.344684	1.464111
25	1	0	-3.312097	2.318862	1.190780
26	1	0	-4.814876	1.434575	1.564735
27	1	0	-3.302384	1.044216	2.425991
28	6	0	-4.178148	0.658586	-1.339262
29	1	0	-4.036315	-0.073717	-2.139381
30	1	0	-5.249687	0.772576	-1.142821
31	1	0	-3.771099	1.617907	-1.671834
32	1	0	1.320384	-1.675333	-0.317981

INT2-H

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.476433	-0.391379	-0.736289
2	6	0	4.364500	0.414305	0.132690
3	6	0	5.014812	-0.434381	1.001504
4	6	0	4.573672	-1.724397	0.673083
5	8	0	3.717763	-1.758891	-0.307815
6	6	0	2.003970	0.070988	-0.539233
7	6	0	1.973143	1.590315	-0.565865
8	8	0	2.864754	2.158245	0.400825
9	6	0	4.230844	1.907128	0.104096
10	6	0	0.973520	-0.761853	-0.373454
11	1	0	3.749860	-0.359034	-1.799932
12	1	0	5.700025	-0.184782	1.800389
13	1	0	4.831570	-2.680641	1.117521
14	1	0	2.232314	1.983744	-1.564238
15	1	0	0.973511	1.931553	-0.297092
16	1	0	4.832834	2.391083	0.875019
17	1	0	4.512970	2.311479	-0.881501
18	79	0	-1.013118	-0.276997	-0.113555
19	15	0	-3.313176	0.171216	0.198008
20	6	0	-4.286867	-1.296057	0.735521
21	1	0	-3.894139	-1.673264	1.684426
22	1	0	-5.343312	-1.036278	0.862662
23	1	0	-4.201196	-2.090697	-0.011598
24	6	0	-3.678890	1.451357	1.470031
25	1	0	-3.211344	2.399266	1.187347
26	1	0	-4.759148	1.601527	1.571081
27	1	0	-3.268811	1.140609	2.435542
28	6	0	-4.182195	0.766145	-1.312347
29	1	0	-4.092210	0.020511	-2.107871
30	1	0	-5.243097	0.943937	-1.105915
31	1	0	-3.724639	1.696759	-1.661028
32	1	0	1.200992	-1.829132	-0.386564

COM-Me

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.198540	-0.364314	-0.992820
2	6	0	-3.467542	-0.920783	0.017257
3	6	0	-3.667840	-0.065156	1.159806
4	6	0	-4.499667	0.929419	0.746966
5	8	0	-4.831615	0.757313	-0.565832
6	6	0	-2.637516	-2.155732	-0.060441
7	6	0	2.247178	-2.264114	0.049310
8	8	0	-1.245525	-1.782042	-0.008375
9	6	0	-0.372577	-2.892378	-0.031181
10	6	0	1.022048	-2.395845	0.011768
11	1	0	-3.263128	-0.199347	2.153830
12	1	0	-4.951880	1.778753	1.236091
13	1	0	-2.852861	-2.832674	0.779772
14	1	0	-2.835464	-2.700953	-0.994218
15	1	0	-0.506008	-3.492816	-0.945495
16	1	0	-0.538681	-3.556369	0.832461
17	1	0	-4.374162	-0.645119	-2.020911
18	79	0	1.209115	-0.123291	-0.009188
19	15	0	0.835680	2.170350	-0.040392
20	6	0	1.935312	3.086092	-1.190953
21	6	0	-0.878186	2.565680	-0.563847
22	6	0	1.055832	2.970527	1.597436
23	1	0	1.691664	4.153898	-1.175657
24	1	0	1.809394	2.704073	-2.208059
25	1	0	2.980050	2.953133	-0.895568
26	1	0	-1.047322	2.198779	-1.580236
27	1	0	-1.036647	3.649410	-0.541534
28	1	0	-1.596874	2.077535	0.101469
29	1	0	0.376051	2.518507	2.325360
30	1	0	0.843798	4.042763	1.525345
31	1	0	2.082804	2.830954	1.947028
32	6	0	3.711784	-2.328375	0.098471
33	1	0	4.163115	-1.865944	-0.784592
34	1	0	4.104236	-1.839421	0.995293
35	1	0	4.012032	-3.382720	0.124359

TS1-Me

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.800991	-0.233877	0.874389
2	6	0	-4.035457	0.428156	-0.329839
3	6	0	-4.815446	-0.455775	-1.126823
4	6	0	-5.048437	-1.556791	-0.347028
5	8	0	-4.464754	-1.433937	0.867785
6	6	0	-3.567201	1.827750	-0.606014
7	6	0	-1.711620	-0.584623	0.180945
8	8	0	-2.724989	2.268307	0.446169
9	6	0	-1.355596	1.960874	0.272935
10	6	0	-1.007248	0.492190	0.178335
11	6	0	-1.791864	-2.037315	-0.039792
12	1	0	-5.168328	-0.296906	-2.136248
13	1	0	-5.590932	-2.475818	-0.517690
14	1	0	-3.063514	1.897767	-1.582428
15	1	0	-4.428448	2.505348	-0.632896
16	1	0	-0.846831	2.401940	1.134599
17	1	0	-0.967252	2.460292	-0.629092
18	1	0	-0.842792	-2.374495	-0.470254
19	1	0	-1.984872	-2.590133	0.884352
20	1	0	-2.577454	-2.285539	-0.763697
21	79	0	1.080290	0.079878	0.036525
22	15	0	3.402922	-0.213723	-0.089414
23	6	0	4.174934	-0.685330	1.511204
24	6	0	3.932658	-1.514076	-1.276786
25	6	0	4.293529	1.304761	-0.619037
26	1	0	5.258433	-0.796544	1.395320
27	1	0	3.753297	-1.631243	1.863489
28	1	0	3.971998	0.083976	2.261953
29	1	0	3.509759	-2.479810	-0.984808
30	1	0	5.025005	-1.593090	-1.294561
31	1	0	3.575212	-1.268280	-2.281009
32	1	0	3.946403	1.613167	-1.609518
33	1	0	5.372585	1.120971	-0.658481
34	1	0	4.094869	2.117353	0.085901
35	1	0	-3.509506	0.135873	1.844243

INT1-Me

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.438337	-0.337459	-0.711771
2	6	0	3.955411	0.444932	0.427403
3	6	0	4.812633	-0.354808	1.164438
4	6	0	4.920220	-1.546847	0.446310
5	8	0	4.198041	-1.580319	-0.641739
6	6	0	3.536915	1.870797	0.582294
7	6	0	1.914435	-0.605832	-0.391477
8	8	0	2.750585	2.255699	-0.512710
9	6	0	1.368221	1.880096	-0.385194
10	6	0	1.033601	0.410924	-0.297282
11	6	0	1.587584	-2.068224	-0.196278
12	1	0	5.325244	-0.123217	2.088131
13	1	0	5.508699	-2.434086	0.657911
14	1	0	3.028350	2.030094	1.549346
15	1	0	4.438581	2.498892	0.590710
16	1	0	0.882986	2.319583	-1.262539
17	1	0	0.951255	2.390499	0.498873
18	1	0	0.510042	-2.179302	-0.060944
19	1	0	1.902080	-2.674977	-1.053843
20	1	0	2.075398	-2.488471	0.694251
21	79	0	-1.021811	0.092437	-0.067510
22	15	0	-3.357910	-0.186964	0.160475
23	6	0	-4.212085	-0.658237	-1.400970
24	6	0	-3.861046	-1.483960	1.366672
25	6	0	-4.238866	1.327732	0.724918
26	1	0	-5.289792	-0.765302	-1.237163
27	1	0	-3.810500	-1.605974	-1.771775
28	1	0	-4.039976	0.108383	-2.162277
29	1	0	-3.454780	-2.452745	1.060866
30	1	0	-4.952332	-1.557026	1.425350
31	1	0	-3.465124	-1.242036	2.357481
32	1	0	-3.854693	1.637671	1.701305
33	1	0	-5.315477	1.143188	0.805810
34	1	0	-4.068243	2.141726	0.014092
35	1	0	3.598798	0.077325	-1.708229

TS2-Me

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.833400	-0.256090	-0.753181
2	6	0	4.199993	0.715414	0.188792
3	6	0	4.676235	0.015306	1.323510
4	6	0	4.645809	-1.314100	0.990574
5	8	0	4.169890	-1.496741	-0.257371
6	6	0	1.716420	0.142739	-0.570892
7	6	0	1.763729	1.620433	-0.820433
8	8	0	2.468595	2.353594	0.152968
9	6	0	3.885356	2.173803	0.047687
10	6	0	0.976506	-0.891007	-0.389312
11	1	0	3.792438	-0.206378	-1.833213
12	1	0	4.998454	0.437480	2.265003
13	1	0	4.915210	-2.212223	1.527799
14	1	0	2.169573	1.816608	-1.826791
15	1	0	0.735694	1.990112	-0.796969
16	1	0	4.329215	2.761238	0.852563
17	1	0	4.240782	2.567414	-0.916053
18	79	0	-1.056173	-0.247974	-0.113909
19	15	0	-3.316043	0.252729	0.235110
20	6	0	-4.284815	-1.191450	0.830577
21	1	0	-3.871833	-1.551423	1.777397
22	1	0	-5.333389	-0.912237	0.979919
23	1	0	-4.231308	-2.002606	0.098587
24	6	0	-3.602839	1.569223	1.485861
25	1	0	-3.121097	2.497981	1.166535
26	1	0	-4.676031	1.747665	1.613545
27	1	0	-3.172376	1.268948	2.445596
28	6	0	-4.193158	0.825341	-1.275673
29	1	0	-4.133727	0.057559	-2.052568
30	1	0	-5.245930	1.029178	-1.052177
31	1	0	-3.724709	1.738160	-1.655059
32	6	0	1.176472	-2.376250	-0.301469
33	1	0	2.197425	-2.663541	-0.562962
34	1	0	0.959903	-2.728340	0.713474
35	1	0	0.483501	-2.891575	-0.973480

INT2-Me

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.453802	-0.274708	-0.648686
2	6	0	4.255425	0.747683	0.066927
3	6	0	5.055729	0.116720	0.993511
4	6	0	4.803279	-1.252301	0.846744
5	8	0	3.925261	-1.529393	-0.075030
6	6	0	1.921702	0.016827	-0.476430
7	6	0	1.727588	1.521442	-0.643629
8	8	0	2.556727	2.296408	0.226665
9	6	0	3.929421	2.196946	-0.115477
10	6	0	0.938206	-0.878388	-0.310589
11	1	0	3.694930	-0.343304	-1.719017
12	1	0	5.732188	0.563365	1.709577
13	1	0	5.224528	-2.100184	1.377269
14	1	0	1.926167	1.832614	-1.684879
15	1	0	0.699867	1.779247	-0.392182
16	1	0	4.493261	2.835217	0.567104
17	1	0	4.114086	2.524099	-1.151577
18	79	0	-1.054586	-0.268624	-0.086399
19	15	0	-3.332234	0.297002	0.199058
20	6	0	-4.370146	-1.096951	0.806715
21	1	0	-3.993236	-1.445083	1.772991
22	1	0	-5.413537	-0.783689	0.920709
23	1	0	-4.322068	-1.929911	0.099003
24	6	0	-3.637496	1.652899	1.406872
25	1	0	-3.128015	2.563890	1.078853
26	1	0	-4.709714	1.856606	1.499794
27	1	0	-3.240367	1.371239	2.386615
28	6	0	-4.175261	0.855978	-1.339521
29	1	0	-4.120048	0.069028	-2.097541
30	1	0	-5.226826	1.091466	-1.143160
31	1	0	-3.676661	1.746832	-1.732922
32	6	0	1.103940	-2.381137	-0.270388
33	1	0	2.104728	-2.741035	-0.524942
34	1	0	0.849493	-2.762135	0.726975
35	1	0	0.394015	-2.848188	-0.962373

COM-Ph

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.793697	-1.622657	-0.964042
2	6	0	-3.896946	-1.850306	0.039409
3	6	0	-4.339052	-1.040917	1.147029
4	6	0	-5.460288	-0.397534	0.722561
5	8	0	-5.749702	-0.745330	-0.564916
6	6	0	-2.707490	-2.747570	-0.013123
7	6	0	2.035981	-1.465422	0.007361
8	8	0	-1.518113	-1.938061	-0.006116
9	6	0	-0.327168	-2.698214	-0.004753
10	6	0	0.831960	-1.769904	-0.000180
11	1	0	-3.887640	-0.976247	2.127787
12	1	0	-6.152365	0.287286	1.188541
13	1	0	-2.682760	-3.423724	0.855280
14	1	0	-2.727557	-3.367274	-0.921396
15	1	0	-0.260898	-3.342904	-0.896079
16	1	0	-0.265920	-3.347859	0.883422
17	1	0	-4.890810	-2.003161	-1.970180
18	79	0	0.345757	0.393537	-0.021531
19	15	0	-0.624480	2.503746	-0.036951
20	6	0	0.180724	3.700247	-1.174655
21	6	0	-2.382345	2.427355	-0.560800
22	6	0	-0.633422	3.321806	1.607674
23	1	0	-0.344334	4.661236	-1.148016
24	1	0	0.162668	3.309703	-2.196160
25	1	0	1.222762	3.852152	-0.878889
26	1	0	-2.444760	2.045608	-1.583967
27	1	0	-2.833143	3.424949	-0.520872
28	1	0	-2.939398	1.748106	0.091645
29	1	0	-1.164467	2.694943	2.329747
30	1	0	-1.129661	4.296295	1.544317
31	1	0	0.392607	3.463613	1.959166
32	6	0	3.422880	-1.149712	0.017063
33	6	0	4.125864	-1.017092	-1.200732
34	6	0	4.106910	-1.009658	1.244785
35	6	0	5.490249	-0.750252	-1.183308
36	1	0	3.594934	-1.131652	-2.140605
37	6	0	5.471428	-0.742929	1.246896
38	1	0	3.561519	-1.118614	2.177009
39	6	0	6.161600	-0.612920	0.036668
40	1	0	6.033352	-0.651939	-2.118004
41	1	0	5.999994	-0.638987	2.189287
42	1	0	7.227687	-0.405948	0.044306

TS1-Ph

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.430940	-0.884098	-0.886785
2	6	0	-3.586647	-1.502574	0.361037
3	6	0	-4.453458	-0.672987	1.115359
4	6	0	-4.819543	0.346633	0.273067
5	8	0	-4.256652	0.212832	-0.943983
6	6	0	-2.932813	-2.810081	0.697300
7	6	0	-1.497281	-0.199422	-0.300002
8	8	0	-2.053803	-3.182329	-0.348613
9	6	0	-0.743862	-2.651144	-0.228611
10	6	0	-0.609480	-1.146642	-0.214460
11	1	0	-4.771801	-0.804937	2.139931
12	1	0	-5.458419	1.208231	0.404980
13	1	0	-2.413054	-2.763868	1.667204
14	1	0	-3.695808	-3.593955	0.772991
15	1	0	-0.188453	-3.057898	-1.078864
16	1	0	-0.268018	-3.040859	0.685832
17	79	0	1.372894	-0.420237	-0.055088
18	15	0	3.607130	0.281897	0.100355
19	6	0	4.266864	1.013091	-1.453414
20	6	0	3.906004	1.563374	1.386053
21	6	0	4.775905	-1.077020	0.512356
22	1	0	5.311990	1.314308	-1.323971
23	1	0	3.673277	1.888594	-1.732533
24	1	0	4.202809	0.280785	-2.263571
25	1	0	3.303643	2.451064	1.171692
26	1	0	4.964220	1.845104	1.410351
27	1	0	3.615532	1.177866	2.367773
28	1	0	4.504608	-1.520867	1.474726
29	1	0	5.802135	-0.698380	0.568723
30	1	0	4.723566	-1.856191	-0.253757
31	1	0	-3.151389	-1.305300	-1.839362
32	6	0	-1.711478	1.220448	-0.138413
33	6	0	-1.795188	2.069373	-1.262689
34	6	0	-1.825937	1.774912	1.153318
35	6	0	-1.944366	3.441085	-1.093338
36	1	0	-1.729035	1.642543	-2.258853
37	6	0	-1.981696	3.151296	1.314992
38	1	0	-1.766767	1.121838	2.018356
39	6	0	-2.038337	3.983559	0.194711
40	1	0	-1.991386	4.090856	-1.961982
41	1	0	-2.057120	3.572970	2.312865
42	1	0	-2.158896	5.055502	0.321978

INT1-Ph

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.255443	-0.532747	-0.753856
2	6	0	-3.675959	-1.287355	0.438711
3	6	0	-4.559945	-0.502738	1.165372
4	6	0	-4.781229	0.629002	0.382780
5	8	0	-4.113841	0.633849	-0.743218
6	6	0	-3.160290	-2.673921	0.653477
7	6	0	-1.751775	-0.127509	-0.404784
8	8	0	-2.347979	-3.051854	-0.426249
9	6	0	-1.001860	-2.560389	-0.322542
10	6	0	-0.791917	-1.068805	-0.271509
11	1	0	-5.014922	-0.710636	2.124052
12	1	0	-5.418645	1.487963	0.563975
13	1	0	-2.644539	-2.763101	1.625280
14	1	0	-4.018466	-3.359547	0.684720
15	1	0	-0.484763	-2.978985	-1.192052
16	1	0	-0.535159	-3.008323	0.570657
17	79	0	1.211651	-0.514587	-0.067270
18	15	0	3.494391	0.057837	0.098719
19	6	0	4.104302	1.098772	-1.292044
20	6	0	3.937068	1.011788	1.610163
21	6	0	4.634061	-1.387688	0.121577
22	1	0	5.166608	1.333854	-1.165485
23	1	0	3.532885	2.030780	-1.334252
24	1	0	3.965247	0.568176	-2.238651
25	1	0	3.366140	1.944654	1.637746
26	1	0	5.007052	1.245666	1.623137
27	1	0	3.687681	0.428995	2.501892
28	1	0	4.402986	-2.028027	0.978067
29	1	0	5.676865	-1.059727	0.190371
30	1	0	4.503382	-1.975747	-0.791680
31	1	0	-3.356216	-1.014613	-1.725565
32	6	0	-1.530903	1.331117	-0.187075
33	6	0	-1.133280	1.806992	1.073692
34	6	0	-1.698808	2.253887	-1.235226
35	6	0	-0.890281	3.167684	1.277583
36	1	0	-1.008383	1.102888	1.891507
37	6	0	-1.444534	3.608956	-1.033850
38	1	0	-2.011070	1.905125	-2.215945
39	6	0	-1.042120	4.070346	0.224145
40	1	0	-0.586574	3.519883	2.259494
41	1	0	-1.560590	4.306656	-1.858239
42	1	0	-0.853730	5.128588	0.380563

TS2-Ph

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.580540	-0.876595	-0.731215
2	6	0	-3.784287	-1.893102	0.210172
3	6	0	-4.322106	-1.265789	1.361526
4	6	0	-4.476700	0.056655	1.035119
5	8	0	-4.060873	0.303367	-0.223464
6	6	0	-1.408538	-0.979675	-0.535489
7	6	0	-1.238778	-2.442669	-0.808901
8	8	0	-1.840375	-3.280037	0.149784
9	6	0	-3.270306	-3.291178	0.048861
10	6	0	-0.853471	0.151043	-0.296673
11	1	0	-3.530339	-0.914609	-1.811028
12	1	0	-4.558974	-1.729394	2.308820
13	1	0	-4.844142	0.911753	1.583683
14	1	0	-1.605439	-2.677492	-1.822021
15	1	0	-0.169432	-2.665523	-0.779995
16	1	0	-3.625302	-3.946348	0.845540
17	1	0	-3.570347	-3.717123	-0.919916
18	79	0	1.273154	-0.133522	-0.089508
19	15	0	3.592197	-0.224167	0.171673
20	6	0	4.331240	1.413013	0.561187
21	1	0	3.905883	1.800641	1.491438
22	1	0	5.417446	1.325372	0.672083
23	1	0	4.108311	2.121317	-0.242045
24	6	0	4.146196	-1.335776	1.526784
25	1	0	3.811057	-2.358266	1.329818
26	1	0	5.238560	-1.325364	1.607339
27	1	0	3.713296	-1.007279	2.476114
28	6	0	4.485848	-0.807969	-1.324931
29	1	0	4.266287	-0.147406	-2.168740
30	1	0	5.566525	-0.815114	-1.146143
31	1	0	4.159142	-1.819552	-1.582934
32	6	0	-1.239640	1.566972	-0.178122
33	6	0	-1.752006	2.251745	-1.293115
34	6	0	-1.063714	2.258014	1.033590
35	6	0	-2.099738	3.598072	-1.188578
36	1	0	-1.873498	1.728152	-2.236779
37	6	0	-1.428121	3.599895	1.133450
38	1	0	-0.657078	1.735676	1.895243
39	6	0	-1.943658	4.274488	0.023353
40	1	0	-2.495581	4.117786	-2.056257
41	1	0	-1.302070	4.121362	2.077960
42	1	0	-2.216482	5.322681	0.101144

INT2-Ph

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.183918	-0.803932	0.641227
2	6	0	3.830397	-1.905424	-0.111816
3	6	0	4.688406	-1.357468	-1.037755
4	6	0	4.617396	0.030928	-0.850257
5	8	0	3.794569	0.393707	0.092211
6	6	0	1.630737	-0.897452	0.493693
7	6	0	1.239007	-2.354961	0.694813
8	8	0	1.924678	-3.232637	-0.203758
9	6	0	3.316861	-3.302237	0.061288
10	6	0	0.798796	0.124035	0.260417
11	1	0	3.443179	-0.797692	1.709342
12	1	0	5.288880	-1.865912	-1.779995
13	1	0	5.135366	0.832754	-1.365929
14	1	0	1.436563	-2.682081	1.731211
15	1	0	0.176832	-2.474612	0.485846
16	1	0	3.757799	-3.994055	-0.658676
17	1	0	3.514955	-3.672179	1.080914
18	79	0	-1.271659	-0.119852	0.070191
19	15	0	-3.614522	-0.259910	-0.167861
20	6	0	-4.374645	1.251671	-0.893251
21	1	0	-3.955496	1.435532	-1.886938
22	1	0	-5.460945	1.138796	-0.977194
23	1	0	-4.151569	2.116661	-0.261647
24	6	0	-4.192788	-1.629866	-1.253266
25	1	0	-3.860322	-2.590008	-0.847542
26	1	0	-5.285608	-1.631927	-1.327457
27	1	0	-3.766132	-1.513694	-2.253956
28	6	0	-4.521096	-0.514238	1.414158
29	1	0	-4.303966	0.309660	2.100409
30	1	0	-5.601468	-0.560477	1.239594
31	1	0	-4.193993	-1.446981	1.883114
32	6	0	1.217214	1.545580	0.155494
33	6	0	1.230488	2.203620	-1.088248
34	6	0	1.555292	2.277282	1.308316
35	6	0	1.608672	3.542709	-1.178124
36	1	0	0.943940	1.656909	-1.983363
37	6	0	1.922508	3.619933	1.215276
38	1	0	1.522063	1.790089	2.279833
39	6	0	1.956075	4.256666	-0.027466
40	1	0	1.621848	4.033789	-2.147465
41	1	0	2.180704	4.169868	2.116124
42	1	0	2.238831	5.302892	-0.098042

COM-CO_2Me

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.499552	-1.507006	-0.979424
2	6	0	-3.633356	-1.792326	0.036949
3	6	0	-4.059406	-0.982985	1.150951
4	6	0	-5.142008	-0.282373	0.717144
5	8	0	-5.421182	-0.594863	-0.582018
6	6	0	-2.487602	-2.742354	-0.011915
7	6	0	2.194697	-1.386031	0.008639
8	8	0	-1.258862	-1.982301	-0.007614
9	6	0	-0.106495	-2.792589	-0.002834
10	6	0	1.084817	-1.920885	0.002595
11	1	0	-3.625737	-0.956055	2.141432
12	1	0	-5.812711	0.423713	1.182570
13	1	0	-2.488372	-3.413939	0.859417
14	1	0	-2.530193	-3.361366	-0.919019
15	1	0	-0.053231	-3.442350	-0.892423
16	1	0	-0.061627	-3.443918	0.886158
17	1	0	-4.595033	-1.866563	-1.993458
18	79	0	0.653573	0.359554	-0.018931
19	15	0	-0.292918	2.479867	-0.032230
20	6	0	0.562672	3.633163	-1.174603
21	6	0	-2.052331	2.454718	-0.552562
22	6	0	-0.260908	3.289393	1.614537
23	1	0	0.086412	4.619048	-1.142571
24	1	0	0.517898	3.244867	-2.196113
25	1	0	1.613099	3.729852	-0.885422
26	1	0	-2.128283	2.072940	-1.574727
27	1	0	-2.469975	3.466725	-0.514623
28	1	0	-2.629253	1.796490	0.104051
29	1	0	-0.814580	2.683350	2.337330
30	1	0	-0.715859	4.284072	1.555257
31	1	0	0.772325	3.386697	1.960016
32	6	0	3.593291	-0.923160	0.020202
33	8	0	3.898930	0.249389	0.019573
34	8	0	4.411737	-1.967862	0.031209
35	6	0	5.831691	-1.658203	0.043861
36	1	0	6.076488	-1.082747	0.938700
37	1	0	6.328466	-2.626403	0.051600
38	1	0	6.093612	-1.088262	-0.849656

TS1-CO_2Me

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.656124	-0.431828	-1.005063
2	6	0	-3.893114	-1.062859	0.206196
3	6	0	-4.884961	-0.281456	0.870387
4	6	0	-5.192782	0.738813	0.017229
5	8	0	-4.465694	0.658699	-1.125533
6	6	0	-3.287078	-2.367832	0.641567
7	6	0	-1.387017	0.111290	-0.138643
8	8	0	-2.304579	-2.810114	-0.290092
9	6	0	-0.980951	-2.443545	0.007065
10	6	0	-0.713672	-0.960875	-0.044342
11	1	0	-5.316486	-0.456926	1.845898
12	1	0	-5.881403	1.568555	0.078372
13	1	0	-2.861804	-2.291575	1.653858
14	1	0	-4.060887	-3.143167	0.672147
15	1	0	-0.352766	-2.951190	-0.729623
16	1	0	-0.679643	-2.803663	1.004236
17	79	0	1.340832	-0.290078	0.005462
18	15	0	3.612808	0.238038	0.032943
19	6	0	4.123192	1.254034	-1.409717
20	6	0	4.118016	1.200700	1.513935
21	6	0	4.709998	-1.234802	0.010091
22	1	0	5.191074	1.490671	-1.349885
23	1	0	3.547404	2.183820	-1.429319
24	1	0	3.927670	0.706946	-2.336502
25	1	0	3.552647	2.136060	1.558067
26	1	0	5.188394	1.429570	1.471329
27	1	0	3.909902	0.625345	2.420639
28	1	0	4.513853	-1.859344	0.886436
29	1	0	5.760756	-0.925646	0.017929
30	1	0	4.518119	-1.827523	-0.889013
31	1	0	-3.157799	-0.755118	-1.904539
32	6	0	-1.453539	1.584106	-0.125697
33	8	0	-2.523063	2.043760	0.511763
34	8	0	-0.572077	2.254751	-0.623547
35	6	0	-2.653090	3.487717	0.556762
36	1	0	-2.726321	3.886591	-0.457139
37	1	0	-3.568749	3.670456	1.116313
38	1	0	-1.791813	3.924194	1.065828

INT1-CO_2Me

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.231613	-0.314838	-0.769349
2	6	0	-3.816657	-1.024421	0.388215
3	6	0	-4.845224	-0.261799	0.899559
4	6	0	-4.961539	0.834200	0.033695
5	8	0	-4.103415	0.836704	-0.943726
6	6	0	-3.253733	-2.360333	0.755515
7	6	0	-1.750914	0.087560	-0.438886
8	8	0	-2.395637	-2.804526	-0.264060
9	6	0	-1.042756	-2.326248	-0.150558
10	6	0	-0.792808	-0.843351	-0.238248
11	1	0	-5.466337	-0.451258	1.764489
12	1	0	-5.665445	1.660060	0.055878
13	1	0	-2.754679	-2.311754	1.739453
14	1	0	-4.075020	-3.082765	0.851111
15	1	0	-0.497559	-2.838136	-0.950347
16	1	0	-0.623641	-2.689644	0.801502
17	79	0	1.228336	-0.335296	-0.043291
18	15	0	3.516280	0.184791	0.125323
19	6	0	4.208910	0.926058	-1.410227
20	6	0	3.913465	1.406899	1.443547
21	6	0	4.613377	-1.249135	0.482372
22	1	0	5.268720	1.170677	-1.280730
23	1	0	3.656072	1.836411	-1.660116
24	1	0	4.102395	0.221936	-2.240765
25	1	0	3.363827	2.335160	1.261503
26	1	0	4.987048	1.623331	1.461996
27	1	0	3.611024	1.012329	2.418122
28	1	0	4.327533	-1.706070	1.434426
29	1	0	5.660755	-0.933172	0.536409
30	1	0	4.506660	-2.000891	-0.305268
31	1	0	-3.272592	-0.871617	-1.708527
32	6	0	-1.423511	1.549032	-0.315262
33	8	0	-0.429335	2.072973	-0.769349
34	8	0	-2.336408	2.214775	0.426759
35	6	0	-2.072718	3.624335	0.613495
36	1	0	-1.123238	3.764099	1.134232
37	1	0	-2.036004	4.134451	-0.351690
38	1	0	-2.899567	3.996246	1.218211

TS2-CO_2Me

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.815029	-0.211140	-0.556099
2	6	0	-3.947947	-1.339200	0.248543
3	6	0	-4.161454	-0.856905	1.572528
4	6	0	-4.190894	0.504439	1.480193
5	8	0	-4.000576	0.910628	0.197936
6	6	0	-1.534565	-0.670740	-0.638508
7	6	0	-1.621777	-2.072336	-1.130981
8	8	0	-2.262260	-2.963045	-0.257470
9	6	0	-3.681732	-2.742440	-0.201530
10	6	0	-0.871644	0.370119	-0.323522
11	1	0	-3.869565	-0.066718	-1.625800
12	1	0	-4.269377	-1.446721	2.471751
13	1	0	-4.312556	1.293639	2.207012
14	1	0	-2.086244	-2.081480	-2.130907
15	1	0	-0.591279	-2.428390	-1.239297
16	1	0	-4.068544	-3.474894	0.508019
17	1	0	-4.123938	-2.936808	-1.188939
18	79	0	1.224359	-0.010909	-0.108673
19	15	0	3.519842	-0.255127	0.234412
20	6	0	4.275207	1.235501	0.997123
21	1	0	3.798146	1.442032	1.959543
22	1	0	5.348320	1.080709	1.152874
23	1	0	4.128523	2.101537	0.345220
24	6	0	3.949915	-1.646080	1.355222
25	1	0	3.596321	-2.590189	0.930789
26	1	0	5.034954	-1.699732	1.495492
27	1	0	3.469020	-1.501025	2.326902
28	6	0	4.476781	-0.553908	-1.305303
29	1	0	4.326984	0.275769	-2.002199
30	1	0	5.544529	-0.643931	-1.078060
31	1	0	4.133604	-1.475413	-1.784438
32	6	0	-1.248362	1.770098	0.047502
33	8	0	-1.148976	2.215846	1.167279
34	8	0	-1.662165	2.437566	-1.034124
35	6	0	-2.052168	3.813941	-0.806771
36	1	0	-2.941595	3.845618	-0.173820
37	1	0	-1.238521	4.362989	-0.328697
38	1	0	-2.266927	4.215673	-1.795795

INT2-CO_2Me

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.337367	-0.367621	-0.792738
2	6	0	-3.996678	-1.309002	0.146218
3	6	0	-4.750508	-0.576873	1.032417
4	6	0	-4.608847	0.764699	0.636777
5	8	0	-3.857560	0.927641	-0.410655
6	6	0	-1.802798	-0.557016	-0.619457
7	6	0	-1.537634	-2.040215	-0.831292
8	8	0	-2.192680	-2.818953	0.176340
9	6	0	-3.608307	-2.757545	0.099629
10	6	0	-0.898019	0.354220	-0.245102
11	1	0	-3.614303	-0.507247	-1.845546
12	1	0	-5.315423	-0.926110	1.886076
13	1	0	-5.019363	1.666790	1.077469
14	1	0	-1.869348	-2.379835	-1.828012
15	1	0	-0.472126	-2.239485	-0.722446
16	1	0	-4.007814	-3.316116	0.948006
17	1	0	-3.979803	-3.214377	-0.833747
18	79	0	1.149181	-0.023408	-0.064022
19	15	0	3.464890	-0.369695	0.176631
20	6	0	4.313071	0.963685	1.119654
21	1	0	3.883018	1.038167	2.122829
22	1	0	5.385520	0.757261	1.203165
23	1	0	4.171275	1.922642	0.612520
24	6	0	3.912393	-1.918898	1.063510
25	1	0	3.521711	-2.784068	0.519616
26	1	0	4.999897	-2.013920	1.152917
27	1	0	3.469740	-1.913031	2.063935
28	6	0	4.382930	-0.465177	-1.415662
29	1	0	4.241399	0.461562	-1.979545
30	1	0	5.452918	-0.617365	-1.237654
31	1	0	3.998355	-1.294722	-2.016362
32	6	0	-1.259441	1.745173	0.157136
33	8	0	-1.886668	2.027797	1.163566
34	8	0	-0.746074	2.660023	-0.684235
35	6	0	-0.982337	4.039425	-0.333712
36	1	0	-2.054522	4.248847	-0.305906
37	1	0	-0.546055	4.262059	0.643003
38	1	0	-0.498601	4.622415	-1.116418

TS3-CO_2Me

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.072659	-2.047821	-0.640969
2	6	0	3.151103	-1.958445	0.228621
3	6	0	2.635372	-2.271549	1.523623
4	6	0	1.317671	-2.568160	1.345583
5	8	0	0.966337	-2.456839	0.030744
6	6	0	2.189087	0.401895	-0.560849
7	6	0	3.593535	0.518770	-0.993239
8	8	0	4.534121	-0.030730	-0.118645
9	6	0	4.516732	-1.467838	-0.141759
10	6	0	1.075583	0.955123	-0.272568
11	1	0	2.001266	-2.058224	-1.718996
12	1	0	3.180173	-2.276886	2.457209
13	1	0	0.530019	-2.877950	2.015277
14	1	0	3.715808	0.152501	-2.025672
15	1	0	3.747334	1.611880	-1.008545
16	1	0	5.269376	-1.784692	0.581307
17	1	0	4.810024	-1.825562	-1.138715
18	79	0	-0.856985	0.124129	-0.124070
19	15	0	-3.072003	-0.627809	-0.087528
20	6	0	-4.246646	0.617062	0.582728
21	1	0	-4.204746	1.528052	-0.021385
22	1	0	-5.269302	0.225012	0.570440
23	1	0	-3.971633	0.871281	1.610539
24	6	0	-3.723606	-1.050870	-1.753699
25	1	0	-3.121835	-1.850107	-2.196105
26	1	0	-4.765416	-1.381927	-1.684701
27	1	0	-3.668334	-0.174926	-2.406572
28	6	0	-3.351303	-2.136563	0.926179
29	1	0	-3.065820	-1.944871	1.964757
30	1	0	-4.406708	-2.427917	0.894933
31	1	0	-2.742670	-2.960144	0.541416
32	6	0	1.107728	2.475247	-0.094384
33	8	0	0.327838	2.843356	0.926723
34	8	0	1.761122	3.222358	-0.782708
35	6	0	0.335625	4.262322	1.231886
36	1	0	-0.030183	4.829871	0.373833
37	1	0	-0.330012	4.370322	2.086620
38	1	0	1.347905	4.585071	1.482967

TS1-H-JohnPhos

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.216968	0.431579	-0.833284
2	6	0	5.378652	-0.415524	0.246685
3	6	0	5.878572	-1.645746	-0.292229
4	6	0	5.992760	-1.452438	-1.636799
5	8	0	5.598938	-0.195235	-1.982093
6	6	0	5.108735	-0.057533	1.685226
7	6	0	2.945962	-0.247123	-0.553437
8	8	0	4.259531	1.081452	1.788710
9	6	0	2.877627	0.799433	1.781909
10	6	0	2.391648	0.167024	0.502550
11	1	0	6.117245	-2.549397	0.251108
12	1	0	6.318533	-2.081593	-2.451735
13	1	0	4.681058	-0.916324	2.224316
14	1	0	6.044348	0.211458	2.187683
15	1	0	2.368390	1.754561	1.928492
16	1	0	2.608565	0.138061	2.620701
17	79	0	0.320194	-0.280080	0.159717
18	1	0	4.987916	1.482084	-0.911023
19	1	0	3.039805	-0.747079	-1.498768
20	15	0	-1.954278	-0.926737	-0.000741
21	6	0	-3.153582	0.473646	-0.165858
22	6	0	-2.132848	-1.994777	-1.586092
23	6	0	-2.384282	-1.850000	1.635648
24	6	0	-2.776327	1.837627	-0.255147
25	6	0	-4.529006	0.158963	-0.167516
26	6	0	-3.576378	-2.400765	-1.944195
27	6	0	-1.267290	-3.262621	-1.437082
28	6	0	-1.577696	-1.133734	-2.742455
29	6	0	-3.618524	-2.771268	1.569953
30	6	0	-1.167967	-2.705563	2.057515
31	6	0	-2.609187	-0.761076	2.707192
32	6	0	-3.788441	2.811518	-0.338730
33	6	0	-1.379362	2.385236	-0.270753

34	6	0	-5.513103	1.139293	-0.252852
35	1	0	-4.846071	-0.872967	-0.101152
36	1	0	-3.540794	-3.030997	-2.841248
37	1	0	-4.199314	-1.535132	-2.181956
38	1	0	-4.066930	-2.982910	-1.160350
39	1	0	-1.682889	-3.965627	-0.709068
40	1	0	-0.236999	-3.029740	-1.145518
41	1	0	-1.231529	-3.780265	-2.403343
42	1	0	-0.524230	-0.873239	-2.593466
43	1	0	-2.148015	-0.207864	-2.871402
44	1	0	-1.655536	-1.703149	-3.676638
45	1	0	-3.764960	-3.220440	2.559833
46	1	0	-4.540201	-2.238465	1.326129
47	1	0	-3.488156	-3.593538	0.860748
48	1	0	-0.930413	-3.490892	1.335458
49	1	0	-0.270633	-2.095480	2.203789
50	1	0	-1.400297	-3.194270	3.011594
51	1	0	-1.754179	-0.078715	2.782719
52	1	0	-3.506447	-0.167152	2.514279
53	1	0	-2.730119	-1.247321	3.682687
54	6	0	-5.139527	2.478903	-0.338594
55	1	0	-3.492568	3.854014	-0.408211
56	6	0	-0.677824	2.531043	-1.478745
57	6	0	-0.831819	2.941866	0.897414
58	1	0	-6.560836	0.854086	-0.250560
59	1	0	-5.891307	3.259757	-0.405187
60	6	0	0.543735	3.207885	-1.516096
61	1	0	-1.106755	2.140544	-2.397317
62	6	0	0.388911	3.621440	0.858712
63	1	0	-1.382806	2.869952	1.831478
64	6	0	1.078947	3.757686	-0.348607
65	1	0	1.062742	3.327587	-2.463136
66	1	0	0.782998	4.070764	1.766636
67	1	0	2.015294	4.307498	-0.383026

TS2-H-JohnPhos

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.169523	0.370031	-0.820266
2	6	0	-5.602304	-0.402417	0.261449
3	6	0	-5.708690	0.489655	1.363731
4	6	0	-5.400138	1.729879	0.877419
5	8	0	-5.100273	1.680914	-0.443811
6	6	0	-3.204001	-0.507603	-0.592099
7	6	0	-3.548945	-1.947140	-0.768666
8	8	0	-4.359039	-2.449007	0.270779
9	6	0	-5.683487	-1.900250	0.235402
10	6	0	-2.319676	0.385046	-0.346891
11	1	0	-5.225502	0.200610	-1.886526
12	1	0	-5.969499	0.240758	2.382657
13	1	0	-5.353844	2.708656	1.332210
14	1	0	-4.014860	-2.121214	-1.752189
15	1	0	-2.610436	-2.507576	-0.729703
16	1	0	-6.197386	-2.291583	1.114439
17	1	0	-6.207042	-2.249292	-0.666598
18	79	0	-0.304695	-0.201854	-0.175895
19	1	0	-2.471363	1.453281	-0.215696
20	15	0	1.945010	-0.900826	0.079243
21	6	0	3.174116	0.485145	0.088939
22	6	0	2.093694	-1.768010	1.784407
23	6	0	2.375174	-2.027784	-1.424829
24	6	0	2.821615	1.857548	0.034326
25	6	0	4.543579	0.149276	0.131141
26	6	0	3.525517	-2.159923	2.199515
27	6	0	1.196902	-3.022833	1.786625
28	6	0	1.552402	-0.759290	2.822168
29	6	0	3.577843	-2.971821	-1.228721
30	6	0	1.137141	-2.890760	-1.759914
31	6	0	2.646140	-1.085031	-2.617372
32	6	0	3.850455	2.817490	0.025896
33	6	0	1.435306	2.431821	-0.020768

34	6	0	5.545091	1.115610	0.120462
35	1	0	4.841648	-0.889598	0.174855
36	1	0	3.473410	-2.669755	3.169354
37	1	0	4.168802	-1.285956	2.327817
38	1	0	4.003670	-2.847947	1.498204
39	1	0	1.591891	-3.817191	1.146092
40	1	0	0.171655	-2.797509	1.472414
41	1	0	1.150978	-3.422017	2.807143
42	1	0	0.507197	-0.493357	2.631592
43	1	0	2.146629	0.160388	2.844223
44	1	0	1.609001	-1.213383	3.819068
45	1	0	3.725287	-3.538471	-2.156353
46	1	0	4.512618	-2.442752	-1.030642
47	1	0	3.410197	-3.700470	-0.430632
48	1	0	0.864624	-3.572239	-0.949562
49	1	0	0.265562	-2.271592	-1.996320
50	1	0	1.365125	-3.501586	-2.642106
51	1	0	1.813903	-0.391631	-2.786374
52	1	0	3.559941	-0.499805	-2.484844
53	1	0	2.761865	-1.689560	-3.525139
54	6	0	5.195402	2.463272	0.067742
55	1	0	3.573361	3.866705	-0.014688
56	6	0	0.754789	2.773254	1.159743
57	6	0	0.883241	2.822336	-1.252882
58	1	0	6.587570	0.813342	0.152899
59	1	0	5.960733	3.233719	0.058746
60	6	0	-0.446985	3.483896	1.109448
61	1	0	1.185625	2.508581	2.121182
62	6	0	-0.319167	3.531291	-1.303135
63	1	0	1.415111	2.592918	-2.172243
64	6	0	-0.984925	3.868942	-0.121595
65	1	0	-0.946104	3.758970	2.034715
66	1	0	-0.721141	3.840134	-2.264136
67	1	0	-1.902333	4.450272	-0.160209

TS1-Me-JohnPhos (in Scheme S2)

TS1-Me-JohnPhos-*O* (in Figure S3)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.039395	0.524619	-0.524152
2	6	0	5.349190	-0.299471	0.560987
3	6	0	6.177954	-1.336622	0.054970
4	6	0	6.373458	-1.047116	-1.270057
5	8	0	5.723334	0.079824	-1.632626
6	6	0	4.880064	-0.019603	1.959162
7	6	0	3.049090	-0.296346	-0.568266
8	8	0	4.000824	1.090445	1.956593
9	6	0	2.638750	0.760221	1.732152
10	6	0	2.316324	0.083912	0.423017
11	6	0	3.119706	-1.090110	-1.810120
12	1	0	6.585830	-2.179466	0.595263
13	1	0	6.929147	-1.543273	-2.053262
14	1	0	4.408765	-0.907558	2.409045
15	1	0	5.738331	0.247663	2.587118
16	1	0	2.095251	1.706386	1.792051
17	1	0	2.273771	0.116328	2.548545
18	1	0	2.174964	-1.630334	-1.925108
19	1	0	3.289592	-0.469074	-2.694967
20	1	0	3.916511	-1.842122	-1.759322
21	79	0	0.236856	-0.306958	0.141282
22	1	0	4.731042	1.557121	-0.555313
23	15	0	-2.057232	-0.906782	0.015613
24	6	0	-3.250342	0.504028	-0.133984
25	6	0	-2.288922	-1.986368	-1.555494
26	6	0	-2.478107	-1.813085	1.665940
27	6	0	-2.866192	1.866574	-0.219924
28	6	0	-4.628093	0.200666	-0.106537
29	6	0	-3.743730	-2.375946	-1.885357
30	6	0	-1.440389	-3.266406	-1.412230
31	6	0	-1.743636	-1.145960	-2.731528
32	6	0	-3.734687	-2.705269	1.637778
33	6	0	-1.274436	-2.695360	2.069098
34	6	0	-2.652175	-0.711240	2.734006

35	6	0	-3.873396	2.848724	-0.262259
36	6	0	-1.467977	2.406077	-0.279827
37	6	0	-5.607271	1.188410	-0.155873
38	1	0	-4.951394	-0.829251	-0.043427
39	1	0	-3.732844	-3.016034	-2.776199
40	1	0	-4.358426	-1.504054	-2.121608
41	1	0	-4.229108	-2.942556	-1.087006
42	1	0	-1.855944	-3.958456	-0.673774
43	1	0	-0.403289	-3.046826	-1.134573
44	1	0	-1.425754	-3.790764	-2.375568
45	1	0	-0.686975	-0.889667	-2.599404
46	1	0	-2.309858	-0.218178	-2.864996
47	1	0	-1.838473	-1.726961	-3.657136
48	1	0	-3.865221	-3.146556	2.633551
49	1	0	-4.649939	-2.152379	1.415970
50	1	0	-3.642360	-3.533823	0.929832
51	1	0	-1.078948	-3.498108	1.353504
52	1	0	-0.357040	-2.108671	2.180155
53	1	0	-1.494713	-3.163184	3.036572
54	1	0	-1.779988	-0.048655	2.783022
55	1	0	-3.539776	-0.098042	2.556990
56	1	0	-2.761604	-1.186875	3.716190
57	6	0	-5.226428	2.526467	-0.231145
58	1	0	-3.571440	3.889659	-0.328970
59	6	0	-0.770833	2.470433	-1.497242
60	6	0	-0.913884	3.036123	0.846784
61	1	0	-6.656620	0.909986	-0.132338
62	1	0	-5.973718	3.313636	-0.267867
63	6	0	0.451667	3.140800	-1.583775
64	1	0	-1.205118	2.023722	-2.387021
65	6	0	0.309242	3.705951	0.760163
66	1	0	-1.459668	3.023871	1.786546
67	6	0	0.994046	3.762324	-0.456431
68	1	0	0.965661	3.199084	-2.539411
69	1	0	0.710948	4.207778	1.636594
70	1	0	1.931664	4.306330	-0.529996

TS2-Me-JohnPhos (in Scheme S2)

TS2-Me-JohnPhos-*O* (in Figure S3)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.078477	0.668174	0.030714
2	6	0	5.509668	-0.509779	0.666929
3	6	0	6.056510	-1.336233	-0.340403
4	6	0	6.010183	-0.603845	-1.500124
5	8	0	5.462105	0.607694	-1.295811
6	6	0	3.036661	0.314082	0.280341
7	6	0	3.027410	0.083677	1.763202
8	8	0	3.755530	-1.051399	2.180208
9	6	0	5.168511	-0.851955	2.085489
10	6	0	2.293588	0.433351	-0.763483
11	1	0	5.018545	1.676427	0.420210
12	1	0	6.432817	-2.343421	-0.228723
13	1	0	6.314831	-0.818470	-2.514638
14	1	0	3.388882	0.984317	2.287577
15	1	0	1.992933	-0.088463	2.064551
16	1	0	5.635076	-1.787358	2.397927
17	1	0	5.481148	-0.052539	2.774222
18	79	0	0.267194	-0.128038	-0.301762
19	6	0	2.505227	0.822178	-2.196847
20	1	0	3.518726	1.189247	-2.377501
21	1	0	2.319891	-0.034748	-2.854837
22	1	0	1.792323	1.602606	-2.479113
23	15	0	-1.930094	-0.976483	-0.036836
24	6	0	-3.258442	0.300801	0.163315
25	6	0	-1.959917	-2.040123	1.561119
26	6	0	-2.330811	-1.957645	-1.648266
27	6	0	-3.012520	1.694242	0.254553
28	6	0	-4.596485	-0.144484	0.207908
29	6	0	-3.345374	-2.583034	1.964718
30	6	0	-0.976539	-3.217073	1.397425
31	6	0	-1.461341	-1.117951	2.695578
32	6	0	-3.472308	-2.987781	-1.538089
33	6	0	-1.056153	-2.705059	-2.102992
34	6	0	-2.686998	-0.906083	-2.721655

35	6	0	-4.109839	2.565149	0.386188
36	6	0	-1.675205	2.374235	0.223534
37	6	0	-5.667162	0.735303	0.336849
38	1	0	-4.814652	-1.201733	0.143327
39	1	0	-3.222653	-3.198124	2.864664
40	1	0	-4.044100	-1.780724	2.213810
41	1	0	-3.797805	-3.217710	1.199087
42	1	0	-1.341587	-3.965946	0.688100
43	1	0	0.016243	-2.885724	1.073307
44	1	0	-0.860929	-3.717902	2.366397
45	1	0	-0.442924	-0.758757	2.513676
46	1	0	-2.114691	-0.250071	2.833686
47	1	0	-1.456361	-1.682979	3.635652
48	1	0	-3.605731	-3.458401	-2.519932
49	1	0	-4.432113	-2.541019	-1.270100
50	1	0	-3.244780	-3.787435	-0.827686
51	1	0	-0.726628	-3.457918	-1.382468
52	1	0	-0.222469	-2.018573	-2.281546
53	1	0	-1.273971	-3.222817	-3.045283
54	1	0	-1.899198	-0.151356	-2.830242
55	1	0	-3.627436	-0.392618	-2.504325
56	1	0	-2.794998	-1.412289	-3.688597
57	6	0	-5.421885	2.103850	0.427325
58	1	0	-3.913195	3.630803	0.456783
59	6	0	-0.984331	2.645364	1.415246
60	6	0	-1.189982	2.921109	-0.975912
61	1	0	-6.681994	0.349947	0.365871
62	1	0	-6.242689	2.807730	0.528714
63	6	0	0.168960	3.433690	1.406142
64	1	0	-1.370195	2.262247	2.355995
65	6	0	-0.037205	3.710253	-0.984198
66	1	0	-1.736913	2.750401	-1.899439
67	6	0	0.644602	3.969668	0.207055
68	1	0	0.677555	3.652277	2.341451
69	1	0	0.310936	4.144032	-1.917861
70	1	0	1.526333	4.604484	0.203857

TS1-Ph-JohnPhos

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.641523	-1.203195	-0.246683
2	6	0	-4.906626	-0.994663	1.116677
3	6	0	-5.856749	0.052388	1.187935
4	6	0	-6.166955	0.362932	-0.113144
5	8	0	-5.494008	-0.410134	-0.984771
6	6	0	-4.256314	-1.814334	2.191303
7	6	0	-2.822047	-0.212427	-0.084713
8	8	0	-3.295796	-2.676822	1.612866
9	6	0	-2.008928	-2.091738	1.451706
10	6	0	-1.912124	-0.862417	0.584004
11	1	0	-6.264631	0.518799	2.073700
12	1	0	-6.833687	1.094204	-0.547795
13	1	0	-3.811420	-1.176092	2.971432
14	1	0	-5.010489	-2.444952	2.677653
15	1	0	-1.381498	-2.880508	1.028385
16	1	0	-1.595428	-1.840477	2.442013
17	79	0	0.052424	-0.086319	0.403281
18	1	0	-4.297463	-2.094037	-0.747747
19	6	0	-3.063496	1.036209	-0.782567
20	6	0	-3.084445	1.082597	-2.191677
21	6	0	-3.276871	2.223784	-0.054700
22	6	0	-3.270682	2.292747	-2.851498
23	1	0	-2.942275	0.165917	-2.755957
24	6	0	-3.470951	3.433622	-0.721990
25	1	0	-3.264725	2.189532	1.030256
26	6	0	-3.465502	3.469653	-2.117982
27	1	0	-3.269387	2.322318	-3.937045
28	1	0	-3.624393	4.345786	-0.152838
29	1	0	-3.616136	4.411954	-2.636908
30	15	0	2.237684	0.854356	0.434030
31	6	0	3.568326	-0.103629	-0.434058
32	6	0	2.769813	0.918475	2.279026
33	6	0	2.137467	2.581639	-0.416785
34	6	0	3.378427	-1.382410	-1.016564
35	6	0	4.858906	0.464182	-0.483089
36	6	0	4.214106	1.386556	2.544449
37	6	0	1.790998	1.829142	3.048727
38	6	0	2.632940	-0.528827	2.803881

39	6	0	3.256710	3.577111	-0.052560
40	6	0	0.783714	3.231101	-0.049914
41	6	0	2.154310	2.321441	-1.938613
42	6	0	4.487232	-2.034641	-1.587899
43	6	0	2.088601	-2.139660	-1.124036
44	6	0	5.938210	-0.191546	-1.068042
45	1	0	5.034710	1.438131	-0.047398
46	1	0	4.372862	1.407036	3.629754
47	1	0	4.952380	0.700363	2.122786
48	1	0	4.416433	2.393020	2.169935
49	1	0	1.925841	2.886288	2.799842
50	1	0	0.745217	1.558839	2.865021
51	1	0	1.980412	1.722417	4.123930
52	1	0	1.604897	-0.898178	2.725270
53	1	0	3.290014	-1.221322	2.267138
54	1	0	2.920930	-0.551022	3.862188
55	1	0	3.083149	4.507882	-0.606822
56	1	0	4.253204	3.226884	-0.330216
57	1	0	3.257349	3.832370	1.010843
58	1	0	0.689288	3.431860	1.020656
59	1	0	-0.064663	2.611620	-0.356208
60	1	0	0.704954	4.191958	-0.573870
61	1	0	1.364869	1.623059	-2.239927
62	1	0	3.114061	1.925791	-2.281940
63	1	0	1.973935	3.268850	-2.461225
64	6	0	5.752756	-1.457741	-1.618831
65	1	0	4.333642	-3.015091	-2.028777
66	6	0	1.854977	-3.254069	-0.303059
67	6	0	1.189935	-1.873601	-2.170254
68	1	0	6.914117	0.284477	-1.085703
69	1	0	6.582305	-1.990568	-2.074295
70	6	0	0.747918	-4.078914	-0.518051
71	1	0	2.559344	-3.489679	0.490236
72	6	0	0.085992	-2.701114	-2.388196
73	1	0	1.379088	-1.036488	-2.836706
74	6	0	-0.136918	-3.807491	-1.564796
75	1	0	0.593973	-4.948496	0.115364
76	1	0	-0.584697	-2.494475	-3.217926
77	1	0	-0.981639	-4.465460	-1.749550

TS2-Ph-JohnPhos

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.740496	-0.243137	1.243428
2	6	0	4.967945	-1.613897	1.045391
3	6	0	5.556734	-1.740381	-0.235022
4	6	0	5.722276	-0.461229	-0.703764
5	8	0	5.268179	0.448345	0.178145
6	6	0	2.634199	-0.373203	1.104062
7	6	0	2.389916	-1.453436	2.116170
8	8	0	2.983513	-2.694845	1.799264
9	6	0	4.408566	-2.675032	1.942117
10	6	0	2.089067	0.473052	0.307153
11	1	0	4.697526	0.325986	2.162900
12	1	0	5.820741	-2.654725	-0.747660
13	1	0	6.123605	-0.062799	-1.624426
14	1	0	2.717411	-1.115963	3.113801
15	1	0	1.314224	-1.634711	2.153443
16	1	0	4.758703	-3.669416	1.660970
17	1	0	4.674652	-2.490718	2.993688
18	79	0	-0.067091	0.314462	0.366945
19	6	0	2.521903	1.582920	-0.557473
20	6	0	3.056268	2.752889	0.009325
21	6	0	2.370954	1.502778	-1.953147
22	6	0	3.450500	3.812078	-0.807768
23	6	0	2.781819	2.560187	-2.763559
24	6	0	3.319378	3.718517	-2.195103
25	15	0	-2.418006	0.564650	0.461776
26	6	0	-3.414571	-0.750990	-0.382534
27	6	0	-2.829376	2.202977	-0.449684
28	6	0	-2.912458	0.553155	2.326913
29	6	0	-2.857844	-1.787712	-1.173523
30	6	0	-4.817767	-0.695867	-0.247304
31	6	0	-4.333440	2.495025	-0.617598
32	6	0	-2.157613	3.375184	0.294390
33	6	0	-2.204220	2.073368	-1.856875
34	6	0	-4.257969	1.226137	2.666426
35	6	0	-1.807146	1.272453	3.133856
36	6	0	-2.950933	-0.926844	2.764482
37	6	0	-3.728305	-2.700999	-1.796817
38	6	0	-1.401097	-2.038808	-1.425346

39	6	0	-5.659468	-1.617176	-0.863464
40	1	0	-4.439138	3.461503	-1.125462
41	1	0	-4.830269	1.746145	-1.239236
42	1	0	-4.865693	2.570326	0.333711
43	1	0	-2.634859	3.585109	1.256477
44	1	0	-1.089885	3.198843	0.464829
45	1	0	-2.250832	4.280217	-0.318130
46	1	0	-1.116740	1.952929	-1.814933
47	1	0	-2.626083	1.230861	-2.415074
48	1	0	-2.420047	2.987576	-2.423369
49	1	0	-4.420014	1.141849	3.748094
50	1	0	-5.114100	0.751547	2.182349
51	1	0	-4.263365	2.292198	2.423341
52	1	0	-1.704055	2.326555	2.863565
53	1	0	-0.831232	0.793639	3.005288
54	1	0	-2.067876	1.228118	4.198554
55	1	0	-2.010341	-1.443006	2.538448
56	1	0	-3.766536	-1.479819	2.291104
57	1	0	-3.099250	-0.970643	3.850313
58	6	0	-5.109837	-2.627531	-1.649860
59	6	0	-0.823895	-1.663503	-2.648153
60	6	0	-0.641653	-2.810686	-0.529893
61	6	0	0.484069	-2.040228	-2.963538
62	1	0	-1.411288	-1.095209	-3.364237
63	6	0	0.665553	-3.188766	-0.845582
64	1	0	-1.091724	-3.142567	0.402247
65	6	0	1.230361	-2.804140	-2.063896
66	1	0	0.908161	-1.756812	-3.923265
67	1	0	1.239947	-3.784340	-0.142401
68	1	0	2.240962	-3.112002	-2.317086
69	1	0	1.942107	0.606551	-2.392065
70	1	0	2.674222	2.483003	-3.841956
71	1	0	3.628559	4.544424	-2.828907
72	1	0	3.863705	4.710558	-0.358307
73	1	0	3.159492	2.828341	1.088051
74	1	0	-5.271419	0.087513	0.344459
75	1	0	-6.734415	-1.539334	-0.730610
76	1	0	-5.748540	-3.354374	-2.143034
77	1	0	-3.294013	-3.490498	-2.402881

TS1-CO_2Me-JohnPhos

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.958196	0.652366	-0.278722
2	6	0	5.132510	0.194021	1.024650
3	6	0	5.903110	-0.995297	0.929685
4	6	0	6.174314	-1.164796	-0.401123
5	8	0	5.636023	-0.169547	-1.143369
6	6	0	4.597001	0.883446	2.248489
7	6	0	2.763857	-0.033515	-0.188986
8	8	0	3.700493	1.927910	1.893815
9	6	0	2.344484	1.541790	1.790796
10	6	0	2.054350	0.568591	0.677942
11	1	0	6.205539	-1.650889	1.733994
12	1	0	6.707917	-1.926692	-0.949711
13	1	0	4.114583	0.159962	2.923484
14	1	0	5.421311	1.347079	2.802812
15	1	0	1.779938	2.461006	1.616933
16	1	0	1.993979	1.104849	2.739089
17	79	0	0.035286	-0.074503	0.365830
18	1	0	4.672357	1.616067	-0.668624
19	6	0	2.971062	-1.078594	-1.207166
20	8	0	2.703777	-0.621153	-2.436649
21	8	0	3.365198	-2.193832	-0.937206
22	6	0	2.936399	-1.559491	-3.512794
23	1	0	2.321504	-2.452101	-3.377629
24	1	0	2.657124	-1.027299	-4.420704
25	1	0	3.991218	-1.841798	-3.537075
26	15	0	-2.185294	-0.902498	0.313585
27	6	0	-3.443101	0.253852	-0.401305
28	6	0	-2.708724	-1.193651	2.136066
29	6	0	-2.172735	-2.496016	-0.771983
30	6	0	-3.169266	1.593903	-0.775757
31	6	0	-4.759947	-0.227564	-0.557482
32	6	0	-4.183042	-1.597623	2.333898
33	6	0	-1.793543	-2.268317	2.757795
34	6	0	-2.477011	0.150287	2.862449
35	6	0	-3.340318	-3.473805	-0.530211

36	6	0	-0.852237	-3.257226	-0.513493
37	6	0	-2.187087	-2.026491	-2.242646
38	6	0	-4.224383	2.383995	-1.268238
39	6	0	-1.840817	2.288827	-0.719860
40	6	0	-5.785807	0.568649	-1.057972
41	1	0	-4.998618	-1.244486	-0.276545
42	1	0	-4.352683	-1.759067	3.405450
43	1	0	-4.870741	-0.812062	2.011427
44	1	0	-4.446098	-2.526222	1.821648
45	1	0	-1.994277	-3.266947	2.358376
46	1	0	-0.731354	-2.042657	2.611415
47	1	0	-1.980141	-2.307908	3.837861
48	1	0	-1.426056	0.457868	2.830946
49	1	0	-3.085467	0.955462	2.437540
50	1	0	-2.763838	0.037720	3.915111
51	1	0	-3.221969	-4.324283	-1.212802
52	1	0	-4.319826	-3.037592	-0.737671
53	1	0	-3.342875	-3.876703	0.486349
54	1	0	-0.755678	-3.600714	0.519522
55	1	0	0.026798	-2.649492	-0.749995
56	1	0	-0.829686	-4.144247	-1.158525
57	1	0	-1.370544	-1.326199	-2.454814
58	1	0	-3.130290	-1.546697	-2.517214
59	1	0	-2.051792	-2.899708	-2.892408
60	6	0	-5.516798	1.889106	-1.412220
61	1	0	-4.008001	3.410026	-1.550451
62	6	0	-1.555262	3.184367	0.323149
63	6	0	-0.945530	2.204291	-1.799557
64	1	0	-6.785283	0.157713	-1.164376
65	1	0	-6.303627	2.529065	-1.800477
66	6	0	-0.400436	3.970871	0.291154
67	1	0	-2.255877	3.285787	1.147591
68	6	0	0.207827	2.991973	-1.832076
69	1	0	-1.172233	1.542389	-2.631052
70	6	0	0.481975	3.879490	-0.788467
71	1	0	-0.207358	4.675016	1.096210
72	1	0	0.879645	2.925368	-2.683173
73	1	0	1.366052	4.509937	-0.825686

TS2-CO_2Me-JohnPhos

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.991892	0.482374	-0.319300
2	6	0	-5.158507	-0.280688	-1.477473
3	6	0	-5.479930	-1.595308	-1.044076
4	6	0	-5.546665	-1.538880	0.320525
5	8	0	-5.282503	-0.290539	0.772928
6	6	0	-2.797303	0.491732	-0.620024
7	6	0	-2.753989	1.029562	-2.010072
8	8	0	-3.361948	0.203975	-2.972921
9	6	0	-4.791924	0.190387	-2.851364
10	6	0	-2.164692	0.110796	0.422148
11	1	0	-5.034783	1.549227	-0.149520
12	1	0	-5.628421	-2.469102	-1.662601
13	1	0	-5.742578	-2.280690	1.080669
14	1	0	-3.183864	2.044482	-2.029591
15	1	0	-1.697901	1.107697	-2.283811
16	1	0	-5.154413	-0.490446	-3.622628
17	1	0	-5.190484	1.196062	-3.048938
18	79	0	-0.070020	-0.208520	0.096057
19	6	0	-2.599943	-0.293291	1.788529
20	8	0	-2.554089	-1.428002	2.210040
21	8	0	-3.007910	0.777646	2.485572
22	6	0	-3.448196	0.507055	3.836116
23	1	0	-4.342183	-0.120349	3.818197
24	1	0	-2.658965	0.004352	4.399197
25	1	0	-3.671677	1.482962	4.265107
26	15	0	2.158921	-0.953193	-0.126240
27	6	0	3.450250	0.370369	-0.011326
28	6	0	2.341418	-1.721418	-1.874620
29	6	0	2.450861	-2.190119	1.323542
30	6	0	3.164750	1.758828	0.033395
31	6	0	4.801361	-0.034398	0.007722
32	6	0	3.775228	-2.147963	-2.247009
33	6	0	1.394992	-2.933179	-1.994601
34	6	0	1.890908	-0.628814	-2.869372
35	6	0	3.620693	-3.175412	1.128298

36	6	0	1.160834	-3.016178	1.536363
37	6	0	2.697437	-1.335726	2.585725
38	6	0	4.239218	2.665993	0.080117
39	6	0	1.806039	2.394600	0.047503
40	6	0	5.848539	0.880594	0.065544
41	1	0	5.048667	-1.086692	-0.030834
42	1	0	3.750594	-2.592173	-3.249607
43	1	0	4.459838	-1.297077	-2.285544
44	1	0	4.188307	-2.899915	-1.570474
45	1	0	1.730831	-3.783780	-1.394102
46	1	0	0.367872	-2.686003	-1.704140
47	1	0	1.375500	-3.261975	-3.040810
48	1	0	0.845460	-0.341428	-2.714407
49	1	0	2.512281	0.270127	-2.799643
50	1	0	1.984746	-1.019267	-3.890039
51	1	0	3.684061	-3.811302	2.019728
52	1	0	4.589844	-2.682756	1.023658
53	1	0	3.468320	-3.838495	0.272112
54	1	0	0.906867	-3.633531	0.671005
55	1	0	0.295676	-2.387770	1.769444
56	1	0	1.319936	-3.691349	2.386186
57	1	0	1.880898	-0.625683	2.761836
58	1	0	3.635872	-0.776869	2.534892
59	1	0	2.747597	-2.001196	3.455931
60	6	0	5.565163	2.244391	0.097747
61	1	0	4.013094	3.727649	0.112032
62	6	0	1.277850	2.957684	-1.124708
63	6	0	1.125419	2.600081	1.259768
64	1	0	6.874830	0.526140	0.081360
65	1	0	6.367308	2.975324	0.139116
66	6	0	0.093061	3.698067	-1.088578
67	1	0	1.812983	2.838177	-2.062941
68	6	0	-0.056821	3.343258	1.295961
69	1	0	1.542748	2.201780	2.180684
70	6	0	-0.575510	3.894947	0.122111
71	1	0	-0.287791	4.146374	-2.002666
72	1	0	-0.561945	3.504211	2.244008
73	1	0	-1.481661	4.493561	0.155762

COM-Me-JohnPhos-*O*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.550969	-1.280593	1.900757
2	6	0	4.643447	-0.413001	0.850737
3	6	0	5.175998	-1.182414	-0.244297
4	6	0	5.359031	-2.442640	0.231328
5	8	0	4.980860	-2.517257	1.542303
6	6	0	4.263418	1.027912	0.852896
7	6	0	0.513579	3.082654	-1.506382
8	8	0	3.050884	1.199710	0.094235
9	6	0	2.647427	2.551197	0.037003
10	6	0	1.423855	2.675396	-0.782305
11	6	0	-0.424968	3.764503	-2.404509
12	1	0	5.395864	-0.829465	-1.242456
13	1	0	5.743101	-3.355935	-0.196681
14	1	0	5.054285	1.645226	0.400258
15	1	0	4.106725	1.385807	1.881397
16	1	0	3.427355	3.184543	-0.417521
17	1	0	2.441167	2.947803	1.044499
18	1	0	-1.390283	3.931019	-1.917252
19	1	0	-0.586948	3.189228	-3.321464
20	1	0	-0.003845	4.737775	-2.683180
21	1	0	4.230931	-1.169896	2.926439
22	79	0	-0.043036	0.919481	-0.754636
23	15	0	-1.078473	-1.189040	-0.596051
24	6	0	-2.124387	-1.412709	0.913743
25	6	0	-2.251416	-1.363561	-2.103970
26	6	0	0.344736	-2.486350	-0.528239
27	6	0	-2.399170	-0.388122	1.854731
28	6	0	-2.673381	-2.692699	1.138046
29	6	0	-3.124490	-2.634590	-2.094614
30	6	0	-1.416774	-1.323430	-3.400135
31	6	0	-3.189655	-0.137144	-2.065045
32	6	0	-0.059040	-3.921434	-0.919913
33	6	0	1.475988	-2.024400	-1.475026

34	6	0	0.882718	-2.473533	0.918983
35	6	0	-3.210518	-0.692987	2.962814
36	6	0	-1.904369	1.028122	1.810157
37	6	0	-3.470446	-2.972528	2.244033
38	1	0	-2.480029	-3.492693	0.435998
39	1	0	-3.725528	-2.642007	-3.011989
40	1	0	-3.819797	-2.649023	-1.251780
41	1	0	-2.539535	-3.557316	-2.084203
42	1	0	-0.814871	-2.226768	-3.535064
43	1	0	-0.749972	-0.454684	-3.437628
44	1	0	-2.099242	-1.257235	-4.256056
45	1	0	-2.637765	0.805391	-2.147966
46	1	0	-3.787398	-0.108474	-1.148106
47	1	0	-3.884176	-0.196626	-2.911768
48	1	0	0.826243	-4.561552	-0.823688
49	1	0	-0.827943	-4.347586	-0.271486
50	1	0	-0.394508	-3.992228	-1.958392
51	1	0	1.160130	-1.979857	-2.520697
52	1	0	1.878330	-1.048022	-1.189768
53	1	0	2.298391	-2.746511	-1.407701
54	1	0	1.181260	-1.467303	1.233189
55	1	0	0.155735	-2.863681	1.636598
56	1	0	1.777898	-3.105014	0.965054
57	6	0	-3.743418	-1.962639	3.164394
58	1	0	-3.419180	0.096319	3.678835
59	6	0	-2.685618	2.039727	1.228434
60	6	0	-0.745778	1.393928	2.516068
61	1	0	-3.872674	-3.971811	2.380638
62	1	0	-4.364365	-2.159367	4.033316
63	6	0	-2.310559	3.381411	1.337046
64	1	0	-3.606189	1.775741	0.715268
65	6	0	-0.373928	2.736389	2.627756
66	1	0	-0.153698	0.624339	3.004130
67	6	0	-1.154547	3.733847	2.038153
68	1	0	-2.939801	4.152604	0.900603
69	1	0	0.509523	3.003361	3.201890
70	1	0	-0.878434	4.779018	2.145590

COM1-Me-JohnPhos-*O*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.831736	-0.116946	-0.575165
2	6	0	-4.400444	-0.570424	0.605351
3	6	0	-5.365511	-1.548808	0.232654
4	6	0	-5.321649	-1.634471	-1.131297
5	8	0	-4.402946	-0.787298	-1.637332
6	6	0	-4.077045	-0.144800	2.011980
7	6	0	-2.856381	0.889055	-0.905065
8	8	0	-2.814332	0.480047	2.154929
9	6	0	-2.683716	1.745903	1.517255
10	6	0	-2.234531	1.677786	0.067949
11	6	0	-2.644486	1.181643	-2.374514
12	1	0	-6.006619	-2.117107	0.892461
13	1	0	-5.863681	-2.229724	-1.851256
14	1	0	-4.876553	0.506785	2.400362
15	1	0	-4.039966	-1.026584	2.659386
16	1	0	-1.940228	2.302148	2.093621
17	1	0	-3.635111	2.299862	1.581468
18	1	0	-1.833643	1.898821	-2.516806
19	1	0	-2.430944	0.276300	-2.948877
20	1	0	-3.566640	1.608913	-2.788302
21	1	0	-1.738468	2.581345	-0.289348
22	79	0	-0.468812	0.265408	-0.076716
23	15	0	1.393809	-1.178577	0.057411
24	6	0	3.030040	-0.316517	-0.011591
25	6	0	1.297801	-2.055055	1.761109
26	6	0	1.315639	-2.367573	-1.459248
27	6	0	3.188437	1.090800	-0.085313
28	6	0	4.188670	-1.121427	-0.033723
29	6	0	2.521363	-2.923287	2.114938
30	6	0	0.021036	-2.919055	1.809446
31	6	0	1.183784	-0.930120	2.814182
32	6	0	2.116195	-3.676947	-1.311996
33	6	0	-0.162255	-2.735145	-1.722527

34	6	0	1.843816	-1.571380	-2.671976
35	6	0	4.490243	1.616324	-0.184598
36	6	0	2.103550	2.128314	-0.063478
37	6	0	5.466748	-0.579205	-0.128744
38	1	0	4.097933	-2.197659	0.023995
39	1	0	2.335428	-3.394819	3.087572
40	1	0	3.432398	-2.327834	2.213120
41	1	0	2.701720	-3.726157	1.396007
42	1	0	0.088188	-3.797607	1.160728
43	1	0	-0.873175	-2.347827	1.537341
44	1	0	-0.116820	-3.282925	2.834859
45	1	0	0.278421	-0.329217	2.678204
46	1	0	2.054430	-0.265896	2.797266
47	1	0	1.136184	-1.385297	3.811000
48	1	0	2.005577	-4.252693	-2.239066
49	1	0	3.186422	-3.513165	-1.168741
50	1	0	1.743679	-4.304692	-0.497722
51	1	0	-0.618261	-3.280975	-0.892563
52	1	0	-0.772183	-1.848496	-1.922731
53	1	0	-0.208149	-3.380930	-2.607989
54	1	0	1.305699	-0.625504	-2.805151
55	1	0	2.911366	-1.350633	-2.591010
56	1	0	1.691153	-2.169125	-3.578712
57	6	0	5.619224	0.803459	-0.207207
58	1	0	4.605412	2.694691	-0.239383
59	6	0	1.619130	2.634506	1.154905
60	6	0	1.715752	2.762194	-1.256522
61	1	0	6.331972	-1.235136	-0.142771
62	1	0	6.607095	1.247969	-0.283527
63	6	0	0.771431	3.745217	1.178812
64	1	0	1.941198	2.181852	2.088321
65	6	0	0.863890	3.869162	-1.232505
66	1	0	2.110852	2.403246	-2.203163
67	6	0	0.393872	4.367862	-0.014064
68	1	0	0.432580	4.141390	2.132389
69	1	0	0.593340	4.359947	-2.163533
70	1	0	-0.240519	5.249754	0.006870

S-Me

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.832548	1.037560	-0.000001
2	6	0	1.845770	-0.324225	-0.000004
3	6	0	3.234454	-0.702600	0.000000
4	6	0	3.944130	0.458173	0.000004
5	8	0	3.105875	1.531213	0.000003
6	6	0	0.657040	-1.234294	-0.000005
7	6	0	-3.878381	0.292229	0.000003
8	8	0	-0.520605	-0.449262	-0.000012
9	6	0	-1.696758	-1.245290	0.000009
10	6	0	-2.881514	-0.391100	0.000004
11	6	0	-5.074608	1.129960	-0.000001
12	1	0	3.640384	-1.705390	-0.000003
13	1	0	4.999377	0.685504	0.000006
14	1	0	0.677149	-1.896248	-0.885034
15	1	0	0.677144	-1.896238	0.885033
16	1	0	-1.707193	-1.905437	0.885407
17	1	0	-1.707206	-1.905464	-0.885369
18	1	0	-5.694002	0.943819	-0.885796
19	1	0	-5.693484	0.944579	0.886314
20	1	0	-4.806393	2.193407	-0.000538
21	1	0	1.035975	1.763376	0.000001

P1-Me

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.554334	0.335814	0.004173
2	6	0	-0.570750	-1.041002	-0.002446
3	6	0	-1.949769	-1.427132	0.060168
4	6	0	-2.672315	-0.273964	0.095823
5	8	0	-1.849311	0.804791	0.059820
6	6	0	0.603360	-1.978234	-0.099687
7	6	0	0.499653	1.340363	-0.006291
8	8	0	1.810065	-1.370721	-0.509413
9	6	0	2.324999	-0.386721	0.388089
10	6	0	1.794983	1.008070	0.163025
11	6	0	0.072297	2.776248	-0.207374
12	1	0	-2.343620	-2.434868	0.066215
13	1	0	-3.729407	-0.058943	0.138860
14	1	0	0.741917	-2.510093	0.858954
15	1	0	0.399084	-2.742898	-0.858608
16	1	0	3.408893	-0.390152	0.232991
17	1	0	2.145856	-0.705829	1.429621
18	1	0	0.940045	3.441731	-0.196530
19	1	0	-0.453006	2.906497	-1.161296
20	1	0	-0.620982	3.097292	0.578821
21	1	0	2.536450	1.804041	0.134831

COM-Me-JohnPhos-*CH_2*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.412655	-0.099465	0.259229
2	6	0	-6.788599	-0.351593	-0.928305
3	6	0	-7.849528	-0.489016	-1.894213
4	6	0	-9.013831	-0.310151	-1.215784
5	8	0	-8.765979	-0.070872	0.101444
6	6	0	-5.314174	-0.468611	-1.204601
7	6	0	-1.627752	0.059634	2.000091
8	6	0	-2.931392	-0.374542	-0.314499
9	6	0	-2.083584	-0.161472	0.874424
10	6	0	-1.381240	0.360557	3.418250
11	1	0	-7.744542	-0.694339	-2.951029
12	1	0	-10.054051	-0.319952	-1.503565
13	1	0	-5.099478	-1.460384	-1.629440
14	1	0	-5.030208	0.255866	-1.982280
15	1	0	-2.661351	0.358584	-1.084678
16	1	0	-2.727003	-1.366684	-0.736256
17	1	0	-0.861883	-0.462625	3.918740
18	1	0	-0.784444	1.270821	3.529215
19	1	0	-2.342818	0.513918	3.921613
20	1	0	-7.062245	0.075020	1.264922
21	79	0	0.209505	-0.340876	0.635150
22	15	0	2.365891	-0.867912	-0.157776
23	6	0	3.304514	0.567957	-0.849491
24	6	0	3.364985	-1.512176	1.348639
25	6	0	2.138081	-2.149016	-1.579743
26	6	0	2.827722	1.903473	-0.857636
27	6	0	4.567582	0.303703	-1.420274
28	6	0	4.858334	-1.776353	1.070334
29	6	0	2.705376	-2.802457	1.876667
30	6	0	3.267160	-0.411232	2.428149
31	6	0	3.385412	-2.996683	-1.899774
32	6	0	0.985784	-3.109163	-1.206940
33	6	0	1.722586	-1.347634	-2.832462
34	6	0	3.637033	2.902413	-1.428721
35	6	0	1.515683	2.391206	-0.316864

36	6	0	5.349885	1.308319	-1.981934
37	1	0	4.956318	-0.705702	-1.428079
38	1	0	5.310633	-2.171075	1.988141
39	1	0	5.396337	-0.861085	0.812213
40	1	0	5.025020	-2.516707	0.284392
41	1	0	2.847733	-3.649487	1.199093
42	1	0	1.631560	-2.677427	2.055529
43	1	0	3.172530	-3.070308	2.831950
44	1	0	2.232633	-0.230016	2.739730
45	1	0	3.697258	0.536089	2.086635
46	1	0	3.832010	-0.732083	3.311702
47	1	0	3.138848	-3.668370	-2.730935
48	1	0	4.241040	-2.398723	-2.220919
49	1	0	3.689771	-3.625476	-1.058551
50	1	0	1.193898	-3.695263	-0.308367
51	1	0	0.042329	-2.574911	-1.053629
52	1	0	0.839323	-3.814327	-2.034030
53	1	0	0.839468	-0.724870	-2.646441
54	1	0	2.525863	-0.703196	-3.199025
55	1	0	1.465785	-2.053624	-3.631267
56	6	0	4.881052	2.620498	-1.985023
57	1	0	3.267435	3.923454	-1.430325
58	6	0	1.416755	2.862630	1.002482
59	6	0	0.418663	2.563060	-1.177964
60	1	0	6.316295	1.063036	-2.411878
61	1	0	5.476276	3.419281	-2.417343
62	6	0	0.245860	3.478976	1.452416
63	1	0	2.272156	2.776115	1.666923
64	6	0	-0.751860	3.178297	-0.726603
65	1	0	0.497742	2.241205	-2.213080
66	6	0	-0.841418	3.638263	0.589614
67	1	0	0.196531	3.862576	2.468146
68	1	0	-1.582041	3.324101	-1.412534
69	1	0	-1.742174	4.139063	0.932824
70	6	0	-4.432410	-0.250273	0.032131
71	1	0	-4.685093	-0.985571	0.805117
72	1	0	-4.623043	0.743069	0.455430

TS1-Me-JohnPhos-CH_2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.023302	-0.221123	-0.544464
2	6	0	4.978754	0.548942	-0.521318
3	6	0	5.387697	-0.368350	0.458914
4	6	0	6.278291	-0.910507	-1.517745
5	8	0	5.594714	0.235005	-1.716532
6	6	0	5.069117	-0.294905	1.922377
7	6	0	6.182611	-1.333005	-0.218639
8	6	0	2.627836	0.561494	1.892930
9	6	0	2.320043	0.049311	0.506320
10	6	0	3.009388	-0.898577	-1.860975
11	1	0	6.636727	-2.218072	0.204814
12	1	0	6.778301	-1.317756	-2.385320
13	1	0	4.677124	-1.261818	2.267417
14	1	0	6.016734	-0.150618	2.459197
15	1	0	2.033838	1.467107	2.063126
16	1	0	2.224010	-0.181221	2.595372
17	1	0	2.052294	-1.414366	-1.976082
18	1	0	3.143775	-0.199453	-2.692208
19	1	0	3.795763	-1.660388	-1.925250
20	79	0	0.237745	-0.314667	0.166810
21	1	0	4.692537	1.585686	-0.441033
22	6	0	4.093713	0.839097	2.273590
23	1	0	4.120759	1.002102	3.356789
24	1	0	4.442183	1.776558	1.823373
25	15	0	-2.057998	-0.898922	-0.004494
26	6	0	-3.246878	0.519028	-0.126705
27	6	0	-2.283282	-1.929271	-1.609032
28	6	0	-2.501031	-1.855839	1.611785
29	6	0	-2.856337	1.880639	-0.193494
30	6	0	-4.626108	0.222211	-0.108705
31	6	0	-3.737207	-2.303362	-1.959749
32	6	0	-1.439210	-3.215614	-1.499742
33	6	0	-1.728087	-1.055119	-2.755414
34	6	0	-3.755034	-2.749600	1.541955
35	6	0	-1.301089	-2.749148	2.002127

36	6	0	-2.689397	-0.788441	2.711845
37	6	0	-3.858448	2.868221	-0.228867
38	6	0	-1.454922	2.414279	-0.238213
39	6	0	-5.600488	1.215107	-0.149103
40	1	0	-4.954182	-0.807070	-0.061512
41	1	0	-3.723578	-2.912136	-2.872293
42	1	0	-4.348625	-1.422100	-2.168291
43	1	0	-4.228159	-2.895918	-1.184021
44	1	0	-1.860622	-3.928012	-0.784218
45	1	0	-0.403186	-3.007101	-1.210055
46	1	0	-1.420893	-3.711398	-2.478081
47	1	0	-0.672545	-0.803652	-2.607255
48	1	0	-2.292389	-0.123095	-2.865338
49	1	0	-1.816299	-1.608300	-3.698595
50	1	0	-3.896212	-3.220796	2.522514
51	1	0	-4.669552	-2.193335	1.325597
52	1	0	-3.651844	-3.556475	0.810842
53	1	0	-1.094408	-3.527437	1.262959
54	1	0	-0.386518	-2.164820	2.143889
55	1	0	-1.533302	-3.248919	2.950728
56	1	0	-1.818233	-0.127560	2.792060
57	1	0	-3.575176	-0.170168	2.543403
58	1	0	-2.810471	-1.294717	3.677262
59	6	0	-5.213137	2.552168	-0.207051
60	1	0	-3.551135	3.908458	-0.280907
61	6	0	-0.767188	2.529207	-1.456936
62	6	0	-0.888608	2.990126	0.910878
63	1	0	-6.651244	0.941402	-0.132986
64	1	0	-5.956599	3.343259	-0.237253
65	6	0	0.458584	3.195388	-1.523339
66	1	0	-1.210606	2.124183	-2.362042
67	6	0	0.337788	3.655807	0.844441
68	1	0	-1.427561	2.939312	1.853267
69	6	0	1.013207	3.762719	-0.373721
70	1	0	0.965472	3.293465	-2.479539
71	1	0	0.748521	4.116194	1.739265
72	1	0	1.952437	4.306144	-0.431641

TS2-Me-JohnPhos-*CH*$_2$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.034724	0.208335	0.325316
2	6	0	5.076183	0.699422	0.057031
3	6	0	5.614156	-0.500761	0.556266
4	6	0	6.067289	-0.319780	-1.620031
5	8	0	5.432792	0.814556	-1.276648
6	6	0	6.199669	-1.164964	-0.548333
7	6	0	3.050756	-0.083762	1.789671
8	6	0	5.423802	-0.995995	1.951280
9	6	0	2.288955	0.343780	-0.715576
10	1	0	4.956242	1.652984	0.553637
11	1	0	6.665267	-2.140604	-0.551386
12	1	0	6.361651	-0.400899	-2.656861
13	1	0	3.363275	0.813625	2.344021
14	1	0	2.012014	-0.271609	2.078235
15	1	0	6.016837	-1.898976	2.123240
16	1	0	5.768168	-0.238428	2.666961
17	79	0	0.248970	-0.181105	-0.273343
18	6	0	2.489651	0.754548	-2.146161
19	1	0	3.473086	1.200373	-2.310237
20	1	0	2.382536	-0.112391	-2.809172
21	1	0	1.724905	1.479172	-2.439700
22	6	0	3.922964	-1.277337	2.203621
23	1	0	3.611030	-2.168588	1.646871
24	1	0	3.773354	-1.483300	3.268957
25	15	0	-1.984329	-0.948560	-0.050628
26	6	0	-3.269466	0.373496	0.146254
27	6	0	-2.084844	-2.032192	1.530921
28	6	0	-2.400281	-1.894315	-1.680197
29	6	0	-2.975798	1.756284	0.256648
30	6	0	-4.623380	-0.023454	0.159847
31	6	0	-3.496275	-2.524795	1.908057
32	6	0	-1.147812	-3.245935	1.365082
33	6	0	-1.566664	-1.145981	2.685115
34	6	0	-3.577941	-2.885667	-1.598327
35	6	0	-1.146832	-2.679760	-2.129956

36	6	0	-2.706091	-0.817804	-2.744372
37	6	0	-4.044076	2.664997	0.372085
38	6	0	-1.614942	2.388374	0.265150
39	6	0	-5.664453	0.892945	0.275056
40	1	0	-4.877852	-1.071511	0.080434
41	1	0	-3.411642	-3.154597	2.802296
42	1	0	-4.166483	-1.698362	2.156545
43	1	0	-3.961941	-3.132171	1.128342
44	1	0	-1.532816	-3.970408	0.641207
45	1	0	-0.139379	-2.949604	1.055543
46	1	0	-1.065051	-3.763611	2.328704
47	1	0	-0.535080	-0.818140	2.518448
48	1	0	-2.191121	-0.258004	2.828865
49	1	0	-1.592937	-1.724403	3.616830
50	1	0	-3.713836	-3.339696	-2.587650
51	1	0	-4.525563	-2.409438	-1.337862
52	1	0	-3.388271	-3.701392	-0.894974
53	1	0	-0.853601	-3.454209	-1.416480
54	1	0	-0.287338	-2.020734	-2.287811
55	1	0	-1.370503	-3.176321	-3.082256
56	1	0	-1.891405	-0.089680	-2.834038
57	1	0	-3.630864	-0.274668	-2.532206
58	1	0	-2.819298	-1.308199	-3.718862
59	6	0	-5.372362	2.251123	0.381655
60	1	0	-3.810742	3.722154	0.457161
61	6	0	-0.927826	2.590696	1.472567
62	6	0	-1.098464	2.962263	-0.908227
63	1	0	-6.692780	0.543976	0.280174
64	1	0	-6.169376	2.983315	0.471888
65	6	0	0.251745	3.338212	1.503719
66	1	0	-1.336648	2.187086	2.394797
67	6	0	0.081341	3.709468	-0.876442
68	1	0	-1.640946	2.844714	-1.842627
69	6	0	0.758730	3.900639	0.329997
70	1	0	0.758060	3.503410	2.451106
71	1	0	0.455674	4.163098	-1.790250
72	1	0	1.662630	4.502766	0.358511

COM2-Me-JohnPhos-*CH_2*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.810695	-0.109653	-0.239359
2	6	0	4.639312	-0.700271	0.698271
3	6	0	5.348416	-1.726670	0.011439
4	6	0	4.899266	-1.697709	-1.279983
5	8	0	3.968184	-0.728614	-1.457500
6	6	0	2.921564	0.991097	-0.018850
7	6	0	3.062097	1.572106	1.387344
8	6	0	4.689405	-0.245768	2.125859
9	6	0	2.115419	1.639195	-0.963132
10	1	0	6.090995	-2.399403	0.417396
11	1	0	5.141717	-2.279122	-2.157277
12	1	0	3.873643	2.315039	1.333718
13	1	0	2.154304	2.122905	1.650023
14	1	0	4.819187	-1.098924	2.801386
15	1	0	5.569526	0.397575	2.273908
16	6	0	2.253767	1.536314	-2.471799
17	1	0	2.438603	0.519722	-2.820408
18	1	0	1.353464	1.918239	-2.961608
19	1	0	3.096261	2.158714	-2.805931
20	1	0	1.696940	2.585513	-0.614304
21	79	0	0.439761	0.272456	-0.296548
22	6	0	3.405156	0.532680	2.466838
23	1	0	2.569959	-0.173225	2.565598
24	1	0	3.515959	1.035393	3.433171
25	15	0	-1.400449	-1.175055	0.044876
26	6	0	-3.032120	-0.314486	0.199574
27	6	0	-1.118083	-2.119740	1.691719
28	6	0	-1.501408	-2.305388	-1.514216
29	6	0	-3.193810	1.094329	0.199597
30	6	0	-4.187655	-1.119810	0.284269
31	6	0	-2.294293	-3.006510	2.147162
32	6	0	0.153310	-2.983116	1.562368
33	6	0	-0.890679	-1.037641	2.770077
34	6	0	-2.293832	-3.615115	-1.332379
35	6	0	-0.065338	-2.670007	-1.954850

36	6	0	-2.152789	-1.457600	-2.628443
37	6	0	-4.496317	1.621409	0.278943
38	6	0	-2.109975	2.130342	0.125828
39	6	0	-5.466143	-0.576147	0.364516
40	1	0	-4.094219	-2.197297	0.287899
41	1	0	-1.999916	-3.514572	3.073663
42	1	0	-3.188299	-2.419309	2.370357
43	1	0	-2.554513	-3.781756	1.422602
44	1	0	0.007834	-3.837996	0.895221
45	1	0	1.012287	-2.405349	1.203425
46	1	0	0.409168	-3.383800	2.550851
47	1	0	-0.020119	-0.411761	2.547281
48	1	0	-1.764207	-0.387402	2.885127
49	1	0	-0.715869	-1.529954	3.734553
50	1	0	-2.289525	-4.153916	-2.287745
51	1	0	-3.340690	-3.451643	-1.067763
52	1	0	-1.841158	-4.277133	-0.588846
53	1	0	0.471383	-3.257537	-1.205528
54	1	0	0.531154	-1.780444	-2.181332
55	1	0	-0.125071	-3.274993	-2.867857
56	1	0	-1.622127	-0.511097	-2.785467
57	1	0	-3.202142	-1.232944	-2.420007
58	1	0	-2.108833	-2.019861	-3.568967
59	6	0	-5.622443	0.808343	0.360341
60	1	0	-4.613575	2.700936	0.279689
61	6	0	-1.489144	2.603580	1.294329
62	6	0	-1.855110	2.793208	-1.086886
63	1	0	-6.328970	-1.232351	0.427717
64	1	0	-6.610938	1.253922	0.420735
65	6	0	-0.635622	3.708902	1.250134
66	1	0	-1.707878	2.128153	2.246356
67	6	0	-0.999318	3.896686	-1.131037
68	1	0	-2.356659	2.460460	-1.991780
69	6	0	-0.390879	4.360816	0.038128
70	1	0	-0.187578	4.078945	2.168522
71	1	0	-0.830523	4.408961	-2.074251
72	1	0	0.249861	5.237781	0.009190

S-Me-*CH*$_2$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.089875	1.061229	-0.000007
2	6	0	1.962486	-0.297133	0.000002
3	6	0	3.313449	-0.801949	0.000004
4	6	0	4.134157	0.281717	-0.000004
5	8	0	3.405044	1.432070	-0.000011
6	6	0	0.700771	-1.117622	0.000010
7	6	0	-4.118286	0.236963	-0.000002
8	6	0	-1.852236	-1.183200	0.000008
9	6	0	-3.099721	-0.415711	0.000000
10	6	0	-5.353281	1.018598	-0.000002
11	1	0	3.616831	-1.840494	0.000011
12	1	0	5.206558	0.406108	-0.000006
13	1	0	0.703594	-1.784256	-0.875464
14	1	0	0.703592	-1.784239	0.875496
15	1	0	-1.826425	-1.845563	0.877656
16	1	0	-1.826424	-1.845579	-0.877627
17	1	0	-5.964581	0.800985	-0.884648
18	1	0	-5.964105	0.801739	0.885157
19	1	0	-5.144219	2.095609	-0.000518
20	1	0	1.379999	1.873772	-0.000011
21	6	0	-0.592183	-0.292586	0.000000
22	1	0	-0.617680	0.361757	-0.880033
23	1	0	-0.617682	0.361774	0.880021

P2-Me-*CH*$_2$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.026999	0.391814	-0.071142
2	6	0	-1.397341	0.290677	-0.024140
3	6	0	-1.899173	1.632134	0.011167
4	6	0	-0.807638	2.446388	-0.014773
5	8	0	0.342020	1.714800	-0.064564
6	6	0	0.920580	-0.708291	-0.129551
7	6	0	0.204574	-2.036467	-0.364316
8	6	0	-2.109733	-1.031465	0.001277
9	6	0	2.262801	-0.654877	-0.015002
10	1	0	-2.933609	1.945560	0.055685
11	1	0	-0.677801	3.518012	-0.001649
12	1	0	-0.007422	-2.145343	-1.439433
13	1	0	0.869078	-2.863059	-0.089563
14	1	0	-2.960370	-1.003027	0.694495
15	1	0	-2.533089	-1.253330	-0.990508
16	6	0	3.147590	0.541219	0.189162
17	1	0	2.584580	1.461762	0.343277
18	1	0	3.806855	0.385906	1.054509
19	1	0	3.807771	0.688275	-0.678166
20	1	0	2.788303	-1.608225	-0.084616
21	6	0	-1.124955	-2.145218	0.407006
22	1	0	-1.577152	-3.128525	0.231006
23	1	0	-0.921543	-2.071894	1.483346

COM′-H

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.753493	1.403201	-0.000489
2	6	0	-5.985928	0.060733	0.000394
3	6	0	-7.417044	-0.091178	0.000729
4	6	0	-7.929502	1.168886	0.000023
5	8	0	-6.928901	2.091997	-0.000737
6	6	0	-4.970469	-1.036998	0.000947
7	8	0	-3.663470	-0.460849	-0.000099
8	6	0	-2.637511	-1.414123	0.000441
9	6	0	-1.324798	-0.596834	-0.001066
10	6	0	-0.150938	-1.470386	-0.000653
11	6	0	0.749833	-2.310987	-0.000293
12	1	0	-4.854350	1.997299	-0.001034
13	1	0	-7.979602	-1.014885	0.001403
14	1	0	-8.934092	1.563242	-0.000061
15	1	0	-5.089647	-1.683028	-0.884810
16	1	0	-5.088908	-1.681459	0.887947
17	1	0	-2.679329	-2.059576	0.892474
18	1	0	-2.680182	-2.061493	-0.890161
19	1	0	-1.317779	0.048718	-0.886748
20	1	0	-1.317012	0.050657	0.883191
21	1	0	1.284193	-3.242017	-0.000052
22	79	0	2.043136	-0.476987	-0.000129
23	15	0	3.785280	1.072685	0.000265
24	6	0	3.770765	2.176135	1.466767
25	6	0	5.430636	0.258841	0.000065
26	6	0	3.770726	2.176868	-1.465686
27	1	0	4.616140	2.871191	1.421433
28	1	0	3.844163	1.581197	2.381668
29	1	0	2.838792	2.747957	1.496179
30	1	0	5.537720	-0.369986	0.888608
31	1	0	6.221653	1.016517	0.000140
32	1	0	5.537651	-0.369743	-0.888657
33	1	0	3.844024	1.582389	-2.380892
34	1	0	4.616137	2.871861	-1.420065
35	1	0	2.838777	2.748751	-1.494736

TS1′-H

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.760365	-0.639833	-0.921655
2	6	0	-4.111158	-0.378175	0.395937
3	6	0	-3.932063	-1.605764	1.095569
4	6	0	-3.519288	-2.518974	0.163465
5	8	0	-3.439462	-1.955353	-1.068491
6	6	0	-1.689077	0.407072	-0.467107
7	6	0	-2.033380	1.783578	-0.844472
8	6	0	-3.008837	2.517598	0.107795
9	8	0	-4.330875	2.020021	0.060567
10	6	0	-4.609798	0.937792	0.929660
11	6	0	-0.914502	-0.526344	-0.080563
12	1	0	-3.918167	-0.087168	-1.834323
13	1	0	-4.082031	-1.787771	2.150770
14	1	0	-3.281131	-3.571568	0.215152
15	1	0	-1.084616	2.340607	-0.851871
16	1	0	-2.429890	1.821874	-1.865660
17	1	0	-3.066973	3.559177	-0.220348
18	1	0	-2.617682	2.498282	1.135180
19	1	0	-4.196480	1.123063	1.932949
20	1	0	-5.700852	0.902468	1.028789
21	1	0	-1.199325	-1.541052	0.200276
22	79	0	1.161642	-0.157062	-0.011604
23	15	0	3.486271	0.109392	0.092196
24	6	0	4.219850	0.827014	-1.433206
25	6	0	4.050393	1.204286	1.457024
26	6	0	4.379086	-1.476225	0.351288
27	1	0	5.306840	0.913979	-1.329840
28	1	0	3.797632	1.818990	-1.618543
29	1	0	3.991426	0.187793	-2.290993
30	1	0	3.623990	2.203966	1.332787
31	1	0	5.143194	1.278690	1.460106
32	1	0	3.715961	0.802268	2.417813
33	1	0	4.055199	-1.936587	1.289260
34	1	0	5.459928	-1.303375	0.391235
35	1	0	4.156738	-2.166137	-0.467969

COM1′-H

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.483876	0.590588	-0.262109
2	6	0	-3.532230	0.664248	0.657489
3	6	0	-3.866530	2.040042	0.773568
4	6	0	-3.011494	2.716572	-0.053101
5	8	0	-2.177045	1.874219	-0.684285
6	6	0	-1.741171	-0.466398	-0.859944
7	6	0	-2.025773	-1.909737	-0.486959
8	6	0	-3.424152	-2.234809	0.045662
9	8	0	-3.614704	-1.695661	1.345188
10	6	0	-4.250895	-0.442980	1.378457
11	6	0	-0.743575	-0.196611	-1.820254
12	1	0	-4.638016	2.472338	1.395632
13	1	0	-2.888385	3.765518	-0.281880
14	1	0	-1.816343	-2.534214	-1.363505
15	1	0	-1.310139	-2.214241	0.287141
16	1	0	-3.510590	-3.321015	0.142727
17	1	0	-4.210384	-1.895918	-0.644312
18	1	0	-5.274393	-0.512389	0.969414
19	1	0	-4.349683	-0.180051	2.436994
20	1	0	-0.732076	0.788851	-2.282435
21	1	0	-0.470831	-1.018322	-2.482015
22	79	0	1.022525	-0.080289	-0.499970
23	15	0	3.025459	0.083371	0.696528
24	6	0	4.036440	-1.449980	0.632989
25	6	0	4.127911	1.413314	0.069568
26	6	0	2.804736	0.442779	2.485844
27	1	0	4.967842	-1.315621	1.193610
28	1	0	4.275950	-1.694194	-0.406046
29	1	0	3.475683	-2.284180	1.064499
30	1	0	4.372149	1.229368	-0.980741
31	1	0	5.054574	1.446009	0.652701
32	1	0	3.623543	2.381163	0.143291
33	1	0	2.272137	1.389879	2.611730
34	1	0	3.778412	0.510001	2.983233
35	1	0	2.216875	-0.351344	2.955237

TS2′-H

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.677416	-0.772744	-0.909574
2	6	0	-4.059199	-0.398907	0.368583
3	6	0	-4.257758	-1.617575	1.089322
4	6	0	-4.008218	-2.628064	0.204648
5	8	0	-3.675198	-2.135022	-1.017041
6	6	0	-1.504888	-0.460112	-0.213369
7	6	0	-0.972159	0.682405	-0.331647
8	6	0	-1.352740	2.102420	-0.616896
9	6	0	-2.534916	2.607346	0.234358
10	8	0	-3.754657	1.958941	-0.082687
11	6	0	-4.264908	1.012881	0.840610
12	1	0	-3.588159	-0.219510	-1.830511
13	1	0	-4.543981	-1.727741	2.126109
14	1	0	-4.025679	-3.704870	0.287769
15	1	0	-1.489567	-1.510238	0.021669
16	1	0	-1.617176	2.181344	-1.679567
17	1	0	-0.503691	2.773689	-0.453465
18	1	0	-2.301983	2.506632	1.302729
19	1	0	-2.670350	3.672697	0.015577
20	1	0	-3.831989	1.152461	1.841188
21	1	0	-5.343276	1.201414	0.929072
22	79	0	1.091743	0.098356	-0.074984
23	15	0	3.386412	-0.298306	0.148748
24	6	0	4.398808	1.212873	-0.112505
25	6	0	3.873342	-0.924338	1.806551
26	6	0	4.040975	-1.529929	-1.047959
27	1	0	5.463535	0.980547	-0.002828
28	1	0	4.122657	1.977786	0.619122
29	1	0	4.221382	1.611398	-1.115658
30	1	0	3.581777	-0.203750	2.576149
31	1	0	4.956744	-1.079195	1.851765
32	1	0	3.367425	-1.872599	2.009997
33	1	0	3.539055	-2.491349	-0.905533
34	1	0	5.118783	-1.663487	-0.905419
35	1	0	3.853870	-1.189633	-2.070572

S′-H

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.070476	-0.971015	-0.000048
2	6	0	1.790390	0.361724	0.000080
3	6	0	3.065517	1.029384	0.000087
4	6	0	4.008025	0.048268	-0.000051
5	8	0	3.420039	-1.179827	-0.000138
6	6	0	0.434743	0.997748	0.000228
7	8	0	-0.552533	-0.016440	-0.000112
8	6	0	-1.871241	0.491369	-0.000387
9	6	0	-2.825283	-0.709274	0.000413
10	6	0	-4.229191	-0.300903	0.000095
11	6	0	-5.382135	0.057931	-0.000182
12	1	0	1.450060	-1.852111	-0.000131
13	1	0	3.246383	2.095970	0.000178
14	1	0	5.087460	0.053000	-0.000104
15	1	0	0.313614	1.648249	-0.884408
16	1	0	0.313518	1.647683	0.885267
17	1	0	-2.050301	1.118162	0.888048
18	1	0	-2.050315	1.117079	-0.889578
19	1	0	-2.607924	-1.328775	-0.879244
20	1	0	-2.607939	-1.327519	0.880956
21	1	0	-6.402405	0.367000	-0.000394

P1′-H

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.600817	0.427262	-0.046153
2	6	0	0.651888	-0.946911	0.025495
3	6	0	2.044262	-1.297241	0.019140
4	6	0	2.735386	-0.128820	-0.058182
5	8	0	1.882477	0.926380	-0.100426
6	6	0	-0.487399	1.398851	-0.024115
7	6	0	-1.881900	0.905136	-0.355556
8	6	0	-2.316535	-0.415908	0.293789
9	8	0	-1.724973	-1.548845	-0.326478
10	6	0	-0.472030	-1.934989	0.200014
11	6	0	-0.257965	2.696380	0.243578
12	1	0	2.461720	-2.294432	0.061447
13	1	0	3.786286	0.113403	-0.109658
14	1	0	-2.601627	1.684768	-0.078539
15	1	0	-1.968284	0.760887	-1.441569
16	1	0	-3.396787	-0.535929	0.156365
17	1	0	-2.113737	-0.414490	1.376904
18	1	0	-0.579237	-2.175518	1.273958
19	1	0	-0.215972	-2.869827	-0.310568
20	1	0	0.738452	3.070739	0.452258
21	1	0	-1.069994	3.417555	0.246576

COM′-CO_2Me

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.109464	-1.522948	-0.000818
2	6	0	-6.227470	-0.165625	0.000557
3	6	0	-7.640614	0.106777	0.001497
4	6	0	-8.257883	-1.105406	0.000616
5	8	0	-7.338993	-2.109831	-0.000789
6	6	0	-5.122586	0.842109	0.000939
7	8	0	-3.869342	0.157974	0.000494
8	6	0	-2.765431	1.020553	0.000406
9	6	0	-1.528179	0.097282	0.000136
10	6	0	-0.279089	0.864071	-0.000116
11	6	0	0.641728	1.686347	-0.000321
12	1	0	-5.263818	-2.191006	-0.001846
13	1	0	-8.123046	1.074758	0.002668
14	1	0	-9.292235	-1.413373	0.000817
15	1	0	-5.186552	1.494851	0.887579
16	1	0	-5.186702	1.495690	-0.885077
17	1	0	-2.753187	1.668841	-0.890551
18	1	0	-2.752907	1.668667	0.891485
19	1	0	-1.570066	-0.552163	0.882462
20	1	0	-1.570508	-0.552162	-0.882172
21	79	0	1.779445	-0.295078	-0.000887
22	15	0	3.473311	-1.889611	0.002336
23	6	0	2.924914	-3.544625	-0.571062
24	6	0	4.862553	-1.405550	-1.094041
25	6	0	4.205992	-2.145409	1.664956
26	1	0	3.768376	-4.243352	-0.557818
27	1	0	2.532828	-3.475512	-1.589770
28	1	0	2.135062	-3.924938	0.083036
29	1	0	4.508160	-1.310111	-2.124393
30	1	0	5.653942	-2.161795	-1.053813
31	1	0	5.268278	-0.441137	-0.775090
32	1	0	4.609626	-1.201044	2.041453
33	1	0	5.012230	-2.884936	1.611110
34	1	0	3.439824	-2.499464	2.360652
35	6	0	1.552982	2.844171	-0.000002
36	8	0	0.857165	3.973853	0.001023
37	8	0	2.760674	2.728804	-0.000476
38	6	0	1.639993	5.198468	0.001705
39	1	0	0.904188	6.000264	0.002824
40	1	0	2.265498	5.236958	0.895602
41	1	0	2.264506	5.238568	-0.892817

TS1′-CO_2Me

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.706866	-0.066247	-0.838219
2	6	0	4.229576	-0.600933	0.331006
3	6	0	4.629839	0.506666	1.131899
4	6	0	4.362227	1.623461	0.394174
5	8	0	3.813235	1.302816	-0.801274
6	6	0	1.386483	-0.692579	-0.472191
7	6	0	1.505180	-2.090394	-0.916982
8	6	0	2.340926	-3.053273	-0.044089
9	8	0	3.732728	-2.919309	-0.239614
10	6	0	4.403294	-2.056436	0.658169
11	6	0	0.722360	0.334442	-0.131689
12	1	0	3.570642	-0.489921	-1.820702
13	1	0	5.052921	0.479179	2.126197
14	1	0	4.473083	2.678323	0.595711
15	1	0	0.473877	-2.471506	-0.952430
16	1	0	1.881880	-2.133035	-1.945981
17	1	0	2.087399	-4.071244	-0.355865
18	1	0	2.072936	-2.941114	1.015964
19	1	0	4.088735	-2.251296	1.695416
20	1	0	5.466025	-2.317757	0.590826
21	79	0	-1.387448	-0.071034	-0.027470
22	15	0	-3.700602	-0.328214	0.142124
23	6	0	-4.576358	-0.159053	-1.464195
24	6	0	-4.221130	-1.958579	0.811353
25	6	0	-4.470996	0.918230	1.250221
26	1	0	-5.656680	-0.271685	-1.322558
27	1	0	-4.224521	-0.923857	-2.162616
28	1	0	-4.371560	0.824635	-1.896501
29	1	0	-3.866273	-2.760603	0.157589
30	1	0	-5.313162	-2.009863	0.879928
31	1	0	-3.792286	-2.105556	1.806826
32	1	0	-4.048422	0.833738	2.255599
33	1	0	-5.554197	0.763730	1.301145
34	1	0	-4.270042	1.925297	0.873434
35	6	0	1.031889	1.748283	0.243784
36	8	0	1.455419	2.079959	1.325514
37	8	0	0.720657	2.570190	-0.765588
38	6	0	0.977111	3.974536	-0.533361
39	1	0	0.471158	4.306684	0.375669
40	1	0	2.051661	4.147550	-0.439787
41	1	0	0.584318	4.485144	-1.411156

COM1′-CO_2Me

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.309635	-0.224658	0.560763
2	6	0	-3.495161	-0.858964	0.949481
3	6	0	-3.624842	-0.632801	2.342307
4	6	0	-2.514458	0.074944	2.724709
5	8	0	-1.717859	0.329567	1.678837
6	6	0	-1.693999	-0.007253	-0.700125
7	6	0	-2.061291	-0.923862	-1.849921
8	6	0	-3.568495	-1.184121	-2.045738
9	8	0	-4.077084	-2.106495	-1.100833
10	6	0	-4.536206	-1.546583	0.105221
11	6	0	-0.745924	1.020590	-0.944317
12	1	0	-4.429041	-0.965708	2.983663
13	1	0	-2.166383	0.429916	3.684017
14	1	0	-1.653172	-0.508220	-2.776439
15	1	0	-1.593297	-1.904234	-1.696816
16	1	0	-3.702679	-1.650688	-3.025565
17	1	0	-4.141782	-0.245166	-2.036016
18	1	0	-5.351208	-0.826256	-0.086379
19	1	0	-4.968635	-2.374190	0.675616
20	6	0	-0.782694	2.362720	-0.251323
21	8	0	-1.655725	2.770268	0.479530
22	8	0	0.281592	3.097369	-0.641980
23	6	0	0.303719	4.460306	-0.164898
24	1	0	-0.581861	4.996884	-0.512931
25	1	0	0.331932	4.479630	0.927129
26	1	0	1.208710	4.897632	-0.584726
27	1	0	-0.477442	1.135082	-1.996387
28	79	0	1.084679	-0.050136	-0.280088
29	15	0	3.117477	-1.022153	0.323008
30	6	0	4.392851	-0.884612	-0.992276
31	6	0	3.873677	-0.255558	1.811848
32	6	0	3.006184	-2.816604	0.704513
33	1	0	5.331349	-1.342899	-0.662083
34	1	0	4.571177	0.168631	-1.227754
35	1	0	4.047642	-1.388447	-1.899749
36	1	0	4.043024	0.810498	1.634589
37	1	0	4.829760	-0.737075	2.044003
38	1	0	3.201125	-0.361992	2.667900
39	1	0	2.313043	-2.978443	1.535062
40	1	0	3.991783	-3.208844	0.977815
41	1	0	2.634461	-3.360016	-0.169010

TS2′-CO_2Me

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.678542	0.447343	-0.039365
2	6	0	4.132884	-0.834674	0.245619
3	6	0	4.594602	-0.804608	1.589156
4	6	0	4.416018	0.484319	2.024603
5	8	0	3.888337	1.257243	1.055690
6	6	0	1.314083	0.486216	-0.160498
7	6	0	0.786747	-0.665868	-0.026775
8	6	0	1.252619	-2.078647	0.103479
9	6	0	1.909898	-2.640676	-1.178482
10	8	0	3.044345	-1.929971	-1.628401
11	6	0	4.157812	-1.969184	-0.746315
12	1	0	3.574067	0.955922	-0.983360
13	1	0	5.002670	-1.624422	2.164497
14	1	0	4.595391	0.969733	2.973086
15	1	0	1.973505	-2.102213	0.931352
16	1	0	0.431670	-2.746518	0.379409
17	1	0	1.200218	-2.619634	-2.009734
18	1	0	2.170092	-3.691476	-0.975776
19	1	0	5.046215	-1.877563	-1.382472
20	1	0	4.226274	-2.938096	-0.230418
21	79	0	-1.347142	-0.274182	0.056560
22	15	0	-3.665203	-0.068814	0.162526
23	6	0	-4.394407	0.665551	-1.355870
24	6	0	-4.549003	-1.661064	0.404270
25	6	0	-4.221811	1.012109	1.540015
26	1	0	-5.481094	0.756155	-1.251598
27	1	0	-4.167970	0.034350	-2.220033
28	1	0	-3.965965	1.657080	-1.528480
29	1	0	-4.325202	-2.340078	-0.423591
30	1	0	-5.630558	-1.493541	0.448404
31	1	0	-4.221021	-2.130123	1.336438
32	1	0	-3.894557	0.593026	2.495929
33	1	0	-5.313813	1.098853	1.540051
34	1	0	-3.780044	2.006598	1.429301
35	6	0	1.076440	1.937847	-0.329103
36	8	0	0.040289	2.447921	0.052386
37	8	0	2.062755	2.580467	-0.946312
38	6	0	1.871914	4.006436	-1.127172
39	1	0	1.745315	4.489739	-0.156530
40	1	0	2.778927	4.351204	-1.620395
41	1	0	0.994293	4.187740	-1.750482

S′-CO_2Me

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.219594	-0.967276	-0.000503
2	6	0	3.907223	0.358314	-0.000461
3	6	0	5.165617	1.056965	-0.000688
4	6	0	6.131597	0.099012	-0.000842
5	8	0	5.573613	-1.142999	-0.000701
6	6	0	2.537311	0.962489	-0.000216
7	8	0	1.573272	-0.075742	-0.000312
8	6	0	0.244214	0.400485	-0.000006
9	6	0	-0.675340	-0.827881	-0.000167
10	6	0	-2.089741	-0.469922	0.000124
11	6	0	-3.258217	-0.152720	0.000367
12	1	0	3.621237	-1.863509	-0.000403
13	1	0	5.320371	2.127617	-0.000735
14	1	0	7.210571	0.129985	-0.001029
15	1	0	2.399619	1.608931	-0.885007
16	1	0	2.399786	1.608600	0.884844
17	1	0	0.047429	1.020846	0.888915
18	1	0	0.047173	1.021267	-0.888576
19	1	0	-0.444810	-1.443138	-0.879681
20	1	0	-0.444553	-1.443561	0.878985
21	6	0	-4.631606	0.297347	0.000663
22	8	0	-5.487062	-0.747531	0.000663
23	8	0	-4.974138	1.462213	0.000887
24	6	0	-6.879158	-0.388943	0.000951
25	1	0	-7.420780	-1.335086	0.000908
26	1	0	-7.125093	0.196522	0.890965
27	1	0	-7.125395	0.196777	-0.888813

P1′-CO_2Me

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.672255	0.497848	-0.284741
2	6	0	1.900400	0.924420	0.175781
3	6	0	1.895456	2.349630	0.054161
4	6	0	0.688812	2.682999	-0.486826
5	8	0	-0.057789	1.577695	-0.705412
6	6	0	0.095981	-0.833168	-0.405471
7	6	0	1.075905	-1.946349	-0.727978
8	6	0	2.239002	-2.113781	0.269395
9	8	0	3.258414	-1.138554	0.131139
10	6	0	3.004059	0.095191	0.779428
11	6	0	-1.221001	-1.130208	-0.290716
12	1	0	2.692330	3.027607	0.328436
13	1	0	0.240541	3.619092	-0.783858
14	1	0	0.531293	-2.896494	-0.771287
15	1	0	1.521183	-1.774924	-1.716836
16	1	0	2.727070	-3.073792	0.070692
17	1	0	1.859997	-2.135430	1.304310
18	1	0	2.791419	-0.085042	1.848162
19	1	0	3.944717	0.652267	0.727030
20	6	0	-2.310306	-0.250410	0.185578
21	8	0	-2.215649	0.770869	0.836198
22	8	0	-3.510726	-0.797921	-0.154966
23	6	0	-4.658482	-0.073339	0.302074
24	1	0	-4.664287	-0.004466	1.393907
25	1	0	-4.667953	0.939023	-0.112151
26	1	0	-5.522793	-0.638213	-0.050010
27	1	0	-1.540010	-2.143329	-0.518179

COM′-Me

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.773308	-1.456497	0.000037
2	6	0	-5.978997	-0.109728	0.000015
3	6	0	-7.406877	0.070242	-0.000006
4	6	0	-7.944331	-1.179393	0.000004
5	8	0	-6.962264	-2.122219	0.000030
6	6	0	-4.940759	0.966789	0.000018
7	8	0	-3.647208	0.365364	-0.000033
8	6	0	-2.600047	1.297448	0.000048
9	6	0	-1.302606	0.464862	-0.000120
10	6	0	-0.107175	1.327654	-0.000046
11	6	0	0.703888	2.259451	0.000047
12	1	0	-4.885843	-2.067876	0.000056
13	1	0	-7.951096	1.004904	-0.000026
14	1	0	-8.956558	-1.553759	-0.000005
15	1	0	-5.047926	1.614799	0.886235
16	1	0	-5.047973	1.614854	-0.886153
17	1	0	-2.633430	1.945551	-0.890990
18	1	0	-2.633355	1.945314	0.891262
19	1	0	-1.303435	-0.184739	0.882332
20	1	0	-1.303505	-0.184492	-0.882754
21	79	0	1.947627	0.289369	-0.000051
22	15	0	3.669614	-1.281395	0.000030
23	6	0	3.633273	-2.387682	-1.464331
24	6	0	5.334561	-0.507133	-0.000764
25	6	0	3.634056	-2.386437	1.465355
26	1	0	4.462771	-3.101463	-1.417252
27	1	0	3.720107	-1.796590	-2.380563
28	1	0	2.688742	-2.938598	-1.493589
29	1	0	5.456086	0.118450	-0.889733
30	1	0	6.107828	-1.282936	-0.000642
31	1	0	5.456581	0.119223	0.887591
32	1	0	3.721364	-1.794553	2.381030
33	1	0	4.463521	-3.100269	1.418471
34	1	0	2.689533	-2.937315	1.495576
35	6	0	1.436095	3.534999	0.000127
36	1	0	2.064875	3.636210	-0.889742
37	1	0	0.709103	4.355384	0.000246
38	1	0	2.064995	3.636043	0.889927

TS1′-Me

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.661068	-0.277227	0.849080
2	6	0	4.211876	0.161900	-0.360874
3	6	0	4.692913	-0.993908	-1.028260
4	6	0	4.477677	-2.041847	-0.172217
5	8	0	3.878545	-1.640156	0.962400
6	6	0	1.554043	0.177508	0.484915
7	6	0	1.556835	1.612250	0.883640
8	6	0	2.291064	2.595786	-0.047783
9	8	0	3.703055	2.510613	0.035844
10	6	0	4.310968	1.583867	-0.834488
11	6	0	0.838994	-0.825416	0.114210
12	1	0	3.608725	0.236047	1.797474
13	1	0	5.153046	-1.046417	-2.005294
14	1	0	4.674266	-3.101845	-0.253654
15	1	0	0.504793	1.920321	0.931514
16	1	0	1.957435	1.729966	1.897849
17	1	0	2.036410	3.610431	0.272747
18	1	0	1.952562	2.466746	-1.086256
19	1	0	3.901742	1.671232	-1.854262
20	1	0	5.370565	1.862024	-0.891132
21	79	0	-1.223271	-0.231874	0.029041
22	15	0	-3.522076	0.190778	-0.111730
23	6	0	-4.291471	0.657980	1.491610
24	6	0	-3.968306	1.548324	-1.269101
25	6	0	-4.483779	-1.263903	-0.693890
26	1	0	-5.366747	0.824848	1.365980
27	1	0	-3.829611	1.572970	1.873889
28	1	0	-4.135502	-0.139569	2.223856
29	1	0	-3.500137	2.482602	-0.945625
30	1	0	-5.054830	1.684167	-1.298774
31	1	0	-3.609315	1.311315	-2.274869
32	1	0	-4.138906	-1.564305	-1.687609
33	1	0	-5.550932	-1.021928	-0.742848
34	1	0	-4.338543	-2.103822	-0.008240
35	6	0	1.095360	-2.266748	-0.238083
36	1	0	1.636217	-2.338104	-1.188421
37	1	0	1.695455	-2.745785	0.540588
38	1	0	0.166586	-2.829559	-0.343702

TS2′-Me

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.633470	-0.414477	-0.796277
2	6	0	-4.118783	0.033959	0.434762
3	6	0	-4.847437	-1.049417	0.992796
4	6	0	-4.812198	-2.053655	0.058777
5	8	0	-4.115971	-1.685209	-1.033553
6	6	0	-1.537015	-0.656182	-0.173788
7	6	0	-0.874033	0.418756	-0.414178
8	6	0	-1.228162	1.803763	-0.902763
9	6	0	-2.073913	2.658188	0.063461
10	8	0	-3.454474	2.331535	0.061660
11	6	0	-3.922203	1.404610	1.016249
12	1	0	-3.373821	0.140469	-1.684070
13	1	0	-5.346264	-1.083548	1.951612
14	1	0	-5.219663	-3.054807	0.044784
15	1	0	-1.767069	1.728032	-1.857808
16	1	0	-0.314277	2.365652	-1.117132
17	1	0	-1.662485	2.613250	1.081776
18	1	0	-2.022457	3.696697	-0.278352
19	1	0	-3.259251	1.359009	1.893888
20	1	0	-4.894752	1.770216	1.370662
21	79	0	1.210110	0.036488	-0.099198
22	15	0	3.523085	-0.208365	0.175334
23	6	0	4.448991	1.362535	-0.059340
24	6	0	4.021917	-0.808375	1.840517
25	6	0	4.287890	-1.391243	-1.006581
26	1	0	5.523421	1.196823	0.074293
27	1	0	4.108757	2.106831	0.666563
28	1	0	4.269941	1.752795	-1.065487
29	1	0	3.667853	-0.113012	2.607150
30	1	0	5.112165	-0.890683	1.906864
31	1	0	3.577274	-1.789502	2.031278
32	1	0	3.846663	-2.383885	-0.877614
33	1	0	5.368587	-1.454745	-0.839570
34	1	0	4.102502	-1.061738	-2.033073
35	6	0	-1.543842	-2.063864	0.267285
36	1	0	-2.362400	-2.265731	0.966282
37	1	0	-1.634618	-2.751618	-0.579553
38	1	0	-0.608000	-2.275770	0.793715

COM2′-Me

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.134941	0.945887	0.256902
2	6	0	3.345680	0.786282	-0.388268
3	6	0	3.645361	2.059501	-0.969331
4	6	0	2.622887	2.895460	-0.635707
5	8	0	1.703236	2.245318	0.123210
6	6	0	1.372211	0.083097	1.146114
7	6	0	1.128835	-1.257159	0.842105
8	6	0	1.537644	-2.013668	-0.407895
9	6	0	3.024982	-2.454357	-0.498010
10	8	0	3.851147	-1.512213	-1.142286
11	6	0	4.274264	-0.403749	-0.363581
12	1	0	4.524610	2.311830	-1.545968
13	1	0	2.406726	3.930989	-0.851485
14	1	0	1.343050	-1.428407	-1.313828
15	1	0	0.915117	-2.913733	-0.461449
16	1	0	3.421064	-2.710806	0.497408
17	1	0	3.074006	-3.349182	-1.124316
18	1	0	4.451737	-0.721424	0.675834
19	1	0	5.237815	-0.098549	-0.780564
20	6	0	1.064367	0.645362	2.523447
21	1	0	2.006541	0.768231	3.073081
22	1	0	0.604332	1.635432	2.457271
23	1	0	0.411305	-0.016518	3.099021
24	1	0	0.820838	-1.880771	1.683418
25	79	0	-0.896658	-0.277712	0.253451
26	15	0	-3.058980	0.204040	-0.472298
27	6	0	-3.637213	-0.920225	-1.804266
28	6	0	-4.312662	0.073698	0.863016
29	6	0	-3.231641	1.902277	-1.150318
30	1	0	-4.654533	-0.651550	-2.108759
31	1	0	-3.631703	-1.954645	-1.448677
32	1	0	-2.972826	-0.846070	-2.670036
33	1	0	-4.317253	-0.940516	1.272713
34	1	0	-5.308347	0.306109	0.470062
35	1	0	-4.073360	0.773265	1.669129
36	1	0	-2.970703	2.637896	-0.384066
37	1	0	-4.262753	2.074424	-1.477626
38	1	0	-2.557976	2.033345	-2.001986

S′-Me

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.732431	-0.949150	0.000058
2	6	0	-2.416282	0.375462	0.000010
3	6	0	-3.672955	1.077300	-0.000029
4	6	0	-4.641765	0.122122	-0.000015
5	8	0	-4.087325	-1.121506	0.000019
6	6	0	-1.043365	0.973724	0.000017
7	8	0	-0.084952	-0.066557	-0.000023
8	6	0	1.248377	0.404801	0.000014
9	6	0	2.173209	-0.817903	-0.000078
10	6	0	3.587896	-0.443520	-0.000019
11	6	0	4.751027	-0.111647	0.000000
12	1	0	-2.135789	-1.846504	0.000097
13	1	0	-3.824856	2.148413	-0.000067
14	1	0	-5.720689	0.156127	-0.000038
15	1	0	-0.905037	1.620929	0.884764
16	1	0	-0.905049	1.620988	-0.884689
17	1	0	1.442663	1.026884	-0.888690
18	1	0	1.442665	1.026746	0.888814
19	1	0	1.936813	-1.431293	0.879455
20	1	0	1.936858	-1.431141	-0.879728
21	6	0	6.159378	0.278344	0.000037
22	1	0	6.680925	-0.107628	-0.884508
23	1	0	6.270775	1.369698	-0.000988
24	1	0	6.680410	-0.105911	0.885633

P2′-Me

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.902752	0.207881	-0.022328
2	6	0	0.461149	-1.058329	0.285236
3	6	0	1.540567	-1.945568	-0.047119
4	6	0	2.554937	-1.165694	-0.508020
5	8	0	2.191878	0.147414	-0.493677
6	6	0	0.285948	1.519348	0.132245
7	6	0	-1.006785	1.722720	-0.197861
8	6	0	-1.925433	0.781785	-0.937936
9	6	0	-2.674128	-0.294617	-0.112216
10	8	0	-1.962738	-1.501498	0.075087
11	6	0	-0.837193	-1.425373	0.948189
12	1	0	1.550373	-3.021719	0.063274
13	1	0	3.551028	-1.371920	-0.869689
14	1	0	-1.375346	0.247644	-1.722354
15	1	0	-2.687840	1.390187	-1.441224
16	1	0	-2.988953	0.122609	0.858890
17	1	0	-3.574556	-0.592485	-0.659216
18	1	0	-1.052506	-0.718241	1.764213
19	1	0	-0.742613	-2.423951	1.387762
20	6	0	1.155539	2.621795	0.695506
21	1	0	1.542783	2.361883	1.688962
22	1	0	2.026845	2.793079	0.051795
23	1	0	0.599009	3.560731	0.773546
24	1	0	-1.425450	2.701166	0.038585

COM-symm

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.410698	0.390127	-0.484095
2	6	0	4.700993	-0.354910	0.413382
3	6	0	4.615257	0.449460	1.606248
4	6	0	5.278499	1.605171	1.331783
5	8	0	5.770564	1.581139	0.058673
6	6	0	4.131591	-1.713938	0.190113
7	6	0	-0.644062	-2.583194	-0.089907
8	8	0	2.695258	-1.603134	0.149462
9	6	0	2.044867	-2.837259	-0.065212
10	6	0	0.586124	-2.593753	-0.092606
11	6	0	-2.104888	-2.810666	-0.055773
12	1	0	4.140021	0.181765	2.540065
13	1	0	5.504080	2.492533	1.903403
14	1	0	4.411015	-2.402857	1.001278
15	1	0	4.496163	-2.138859	-0.756178
16	1	0	2.350846	-3.295069	-1.019968
17	1	0	2.263671	-3.560315	0.737509
18	1	0	-2.330088	-3.517577	0.759539
19	1	0	-2.416572	-3.282158	-1.002073
20	1	0	5.743390	0.210926	-1.495999
21	79	0	-0.010620	-0.348067	-0.295232
22	15	0	0.074957	1.963396	-0.452181
23	6	0	-1.587436	2.735585	-0.549261
24	6	0	0.993140	2.559912	-1.925915
25	6	0	0.910752	2.733495	0.989833
26	1	0	-1.497093	3.826973	-0.574875
27	1	0	-2.098204	2.395288	-1.454579
28	1	0	-2.190104	2.438525	0.314026
29	1	0	0.515233	2.189071	-2.837155
30	1	0	1.007386	3.655014	-1.946861
31	1	0	2.021009	2.187231	-1.894078
32	1	0	1.929959	2.344288	1.077273
33	1	0	0.946336	3.821902	0.870534
34	1	0	0.364731	2.490429	1.906016
35	8	0	-2.743129	-1.567036	0.138700
36	6	0	-4.180082	-1.670568	0.194328
37	1	0	-4.453303	-2.349928	1.015713
38	1	0	-4.554546	-2.105287	-0.743596
39	6	0	-4.745755	-0.308850	0.408068
40	6	0	-5.463915	0.425906	-0.491128
41	6	0	-5.318256	1.659606	1.310895
42	6	0	-4.651389	0.507762	1.591768
43	8	0	-5.821035	1.621625	0.042075
44	1	0	-4.166727	0.251101	2.523843
45	1	0	-5.539611	2.552971	1.874732
46	1	0	-5.803064	0.236329	-1.498964

TS1-symm

Standard orientation:

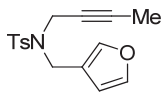
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.669165	-2.258134	-0.591032
2	6	0	-2.209205	-3.390481	0.075609
3	6	0	-3.049505	-3.550821	1.215434
4	6	0	-3.978915	-2.550440	1.139136
5	8	0	-3.775295	-1.772183	0.048274
6	6	0	-1.093889	-4.268569	-0.416498
7	6	0	-0.813311	-1.211397	0.229761
8	8	0	-0.437786	-3.662047	-1.518017
9	6	0	0.632546	-2.809863	-1.169617
10	6	0	0.272285	-1.609170	-0.327357
11	6	0	-1.506342	-0.252850	1.104723
12	1	0	-2.982607	-4.310625	1.981564
13	1	0	-4.818618	-2.276801	1.761687
14	1	0	-0.385123	-4.503839	0.392367
15	1	0	-1.506688	-5.218390	-0.775410
16	1	0	1.060070	-2.470751	-2.117203
17	1	0	1.415928	-3.374209	-0.638444
18	1	0	-0.753190	0.164279	1.794959
19	1	0	-2.241947	-0.780031	1.736315
20	79	0	1.826811	-0.179746	-0.017771
21	15	0	3.610127	1.324711	0.185437
22	6	0	3.476256	2.769086	-0.943443
23	6	0	3.795839	2.044810	1.866935
24	6	0	5.242196	0.568675	-0.192907
25	1	0	4.334933	3.436729	-0.814141
26	1	0	2.556195	3.321806	-0.732172
27	1	0	3.441831	2.426214	-1.981654
28	1	0	2.888393	2.591609	2.139439
29	1	0	4.649054	2.731081	1.896169
30	1	0	3.953261	1.246486	2.598042
31	1	0	5.436188	-0.260657	0.493555
32	1	0	6.040101	1.312181	-0.091706
33	1	0	5.243808	0.179601	-1.215307
34	1	0	-2.501853	-1.890050	-1.589977
35	8	0	-2.111329	0.751829	0.329212
36	6	0	-2.952161	1.615059	1.096542
37	1	0	-3.769480	1.024553	1.543527
38	1	0	-2.378179	2.053953	1.929793
39	6	0	-3.490379	2.688109	0.205637
40	6	0	-3.341618	2.795338	-1.144969
41	1	0	-2.835570	2.194747	-1.883189
42	6	0	-4.552455	4.513444	-0.533087
43	1	0	-5.104170	5.417333	-0.741270
44	6	0	-4.286710	3.818279	0.605638
45	1	0	-4.613475	4.071445	1.605105
46	8	0	-3.982048	3.904422	-1.608556

TS2-symm

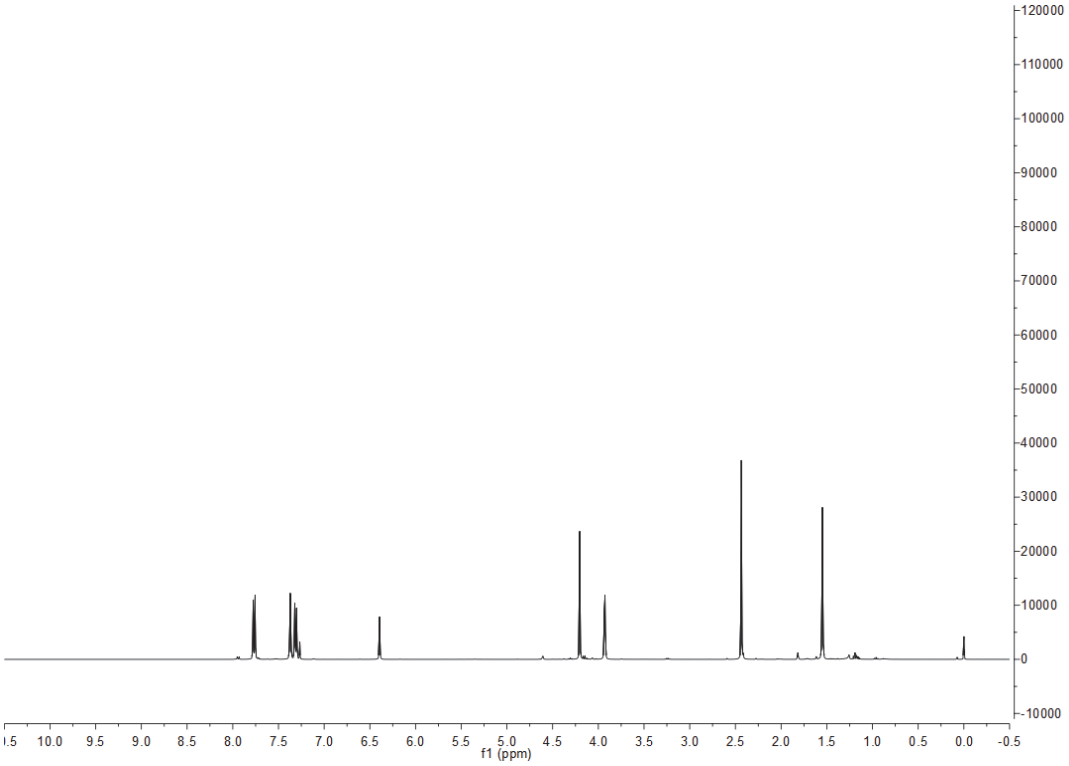
Standard orientation:

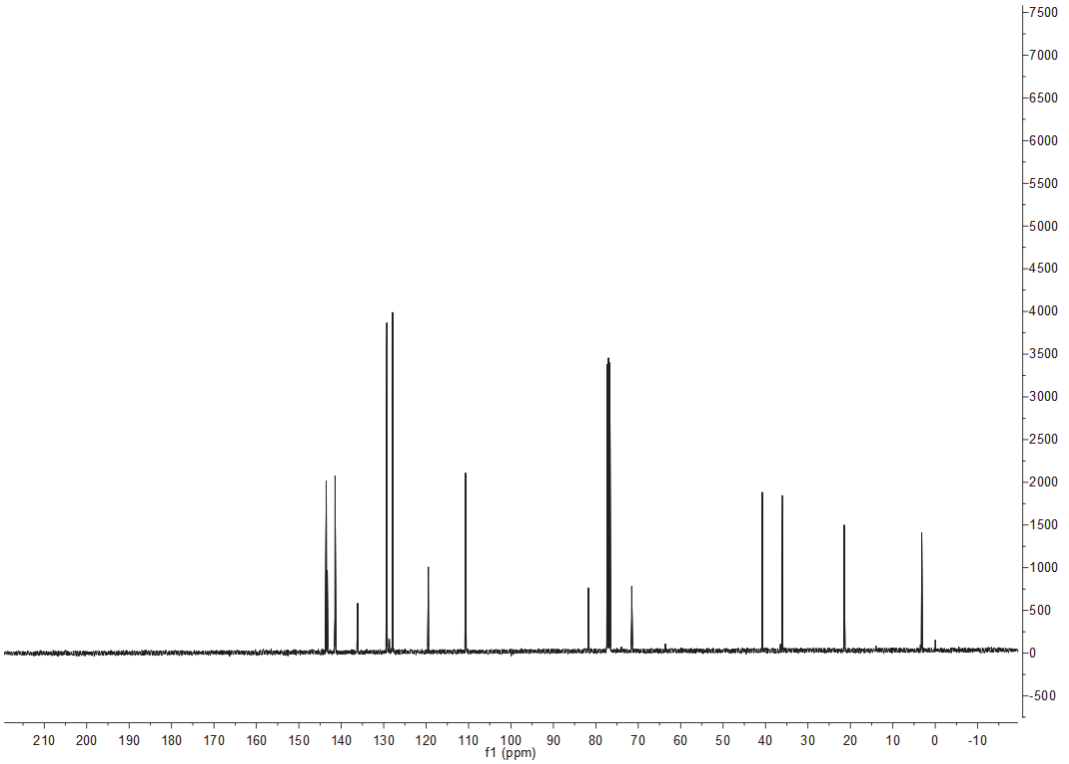
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.061154	1.223373	-0.847259
2	6	0	-4.847982	0.598258	0.128321
3	6	0	-4.932168	1.505651	1.215438
4	6	0	-4.267025	2.634985	0.819634
5	8	0	-3.756399	2.495842	-0.423847
6	6	0	-2.409844	-0.116867	-0.517713
7	6	0	-3.134846	-1.409724	-0.739258
8	8	0	-4.129551	-1.675587	0.221884
9	6	0	-5.278005	-0.836347	0.058152
10	6	0	-1.290838	0.450678	-0.254784
11	1	0	-4.030176	1.089338	-1.920093
12	1	0	-5.419926	1.343048	2.166269
13	1	0	-4.074211	3.581769	1.303564
14	1	0	-3.556869	-1.441550	-1.757204
15	1	0	-2.397803	-2.211655	-0.651002
16	1	0	-5.962010	-1.091722	0.868625
17	1	0	-5.767505	-1.056461	-0.902070
18	79	0	0.291654	-1.000896	-0.052773
19	15	0	2.161484	-2.368288	0.200452
20	6	0	2.863071	-2.316426	1.898707
21	1	0	2.121382	-2.674750	2.618457
22	1	0	3.759018	-2.943409	1.962874
23	1	0	3.126258	-1.286349	2.156047
24	6	0	1.896312	-4.153155	-0.152065
25	1	0	1.546967	-4.280083	-1.180877
26	1	0	2.828429	-4.712839	-0.018483
27	1	0	1.136809	-4.555871	0.524432
28	6	0	3.541557	-1.858346	-0.901622
29	1	0	3.784269	-0.805672	-0.726919
30	1	0	4.429205	-2.472792	-0.715683
31	1	0	3.238831	-1.972834	-1.946729
32	6	0	-0.805496	1.859028	-0.072330
33	1	0	-1.231445	2.512321	-0.848416
34	1	0	-1.146392	2.237946	0.905464
35	8	0	0.608297	1.855748	-0.133422
36	6	0	1.191620	3.154097	0.039046
37	1	0	0.817864	3.823431	-0.751908
38	1	0	0.883052	3.577226	1.007327
39	6	0	2.676744	3.024905	-0.024243
40	6	0	3.559898	3.241458	0.993220
41	1	0	3.443228	3.551042	2.021371
42	6	0	4.770288	2.664098	-0.736051
43	1	0	5.718254	2.474392	-1.216087
44	6	0	3.477824	2.644109	-1.159980
45	1	0	3.125926	2.405910	-2.154362
46	8	0	4.835677	3.029746	0.577187

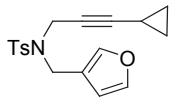
4. ^{1}H and ^{13}C-NMR Spectra for New Compounds



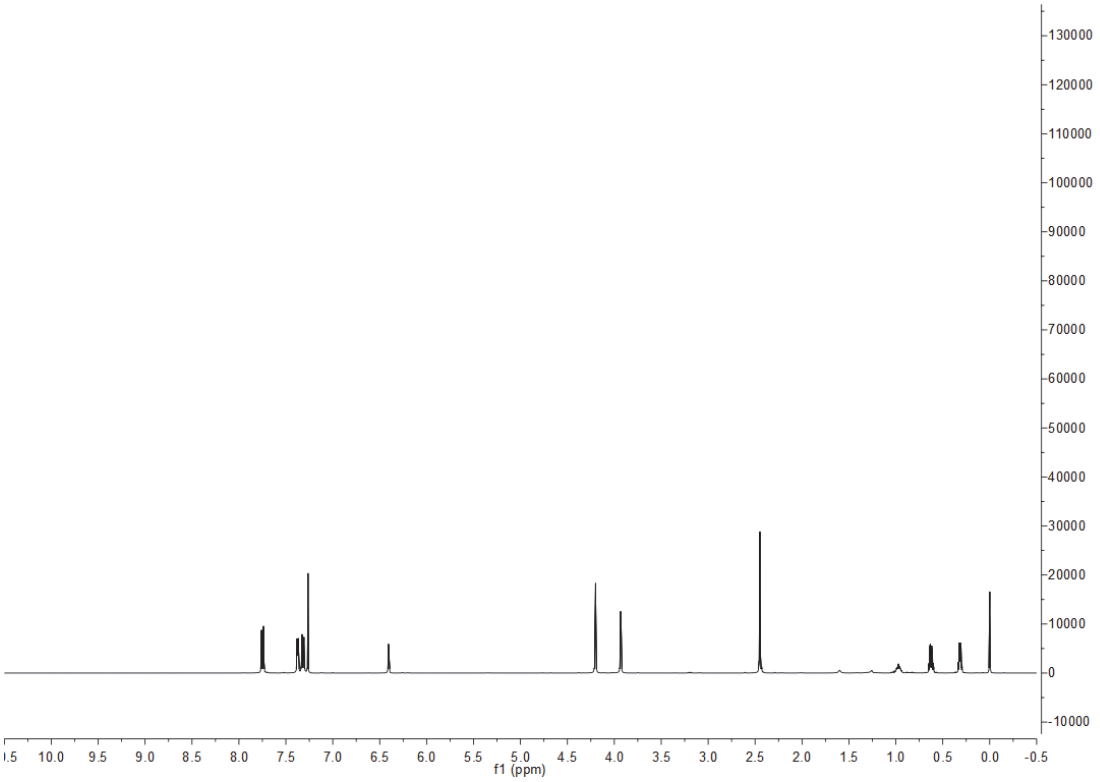
1a

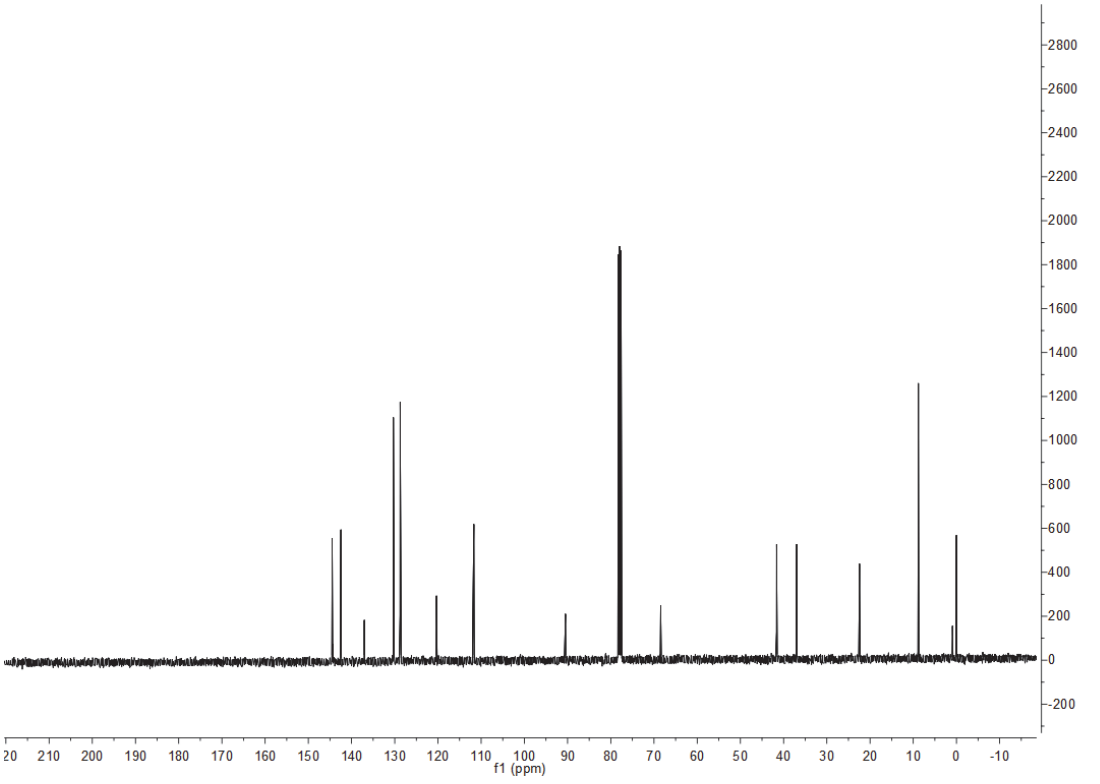


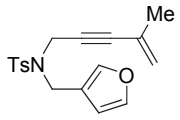



TsN
O

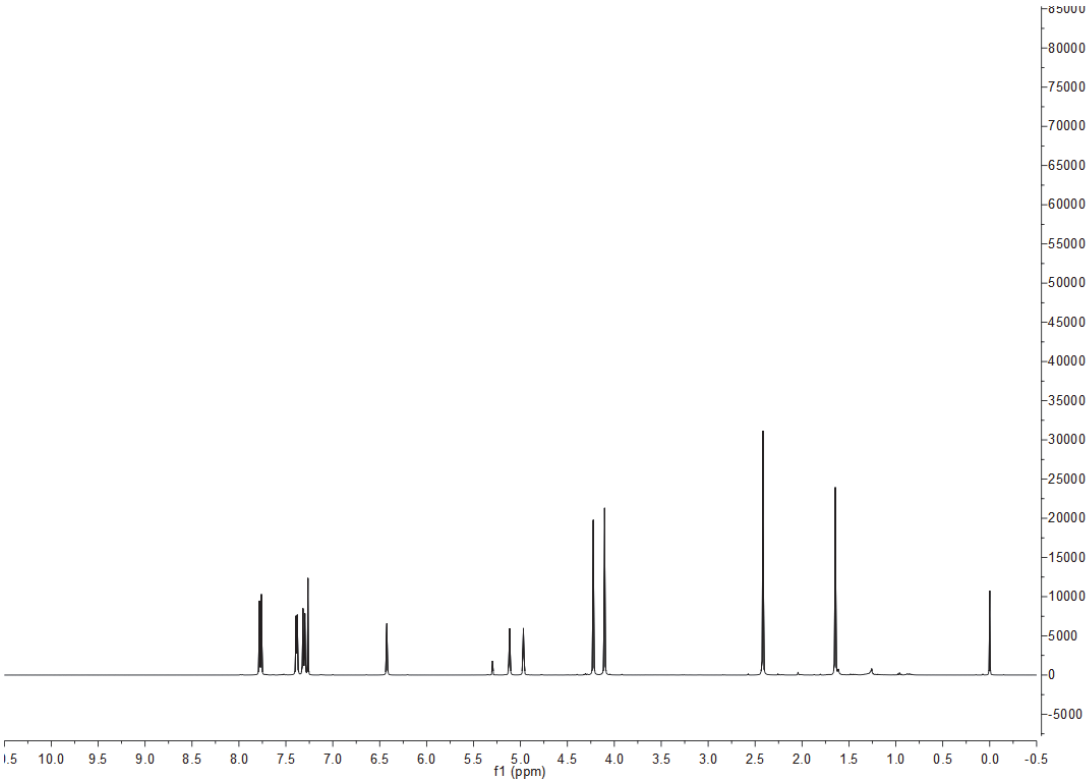
1b

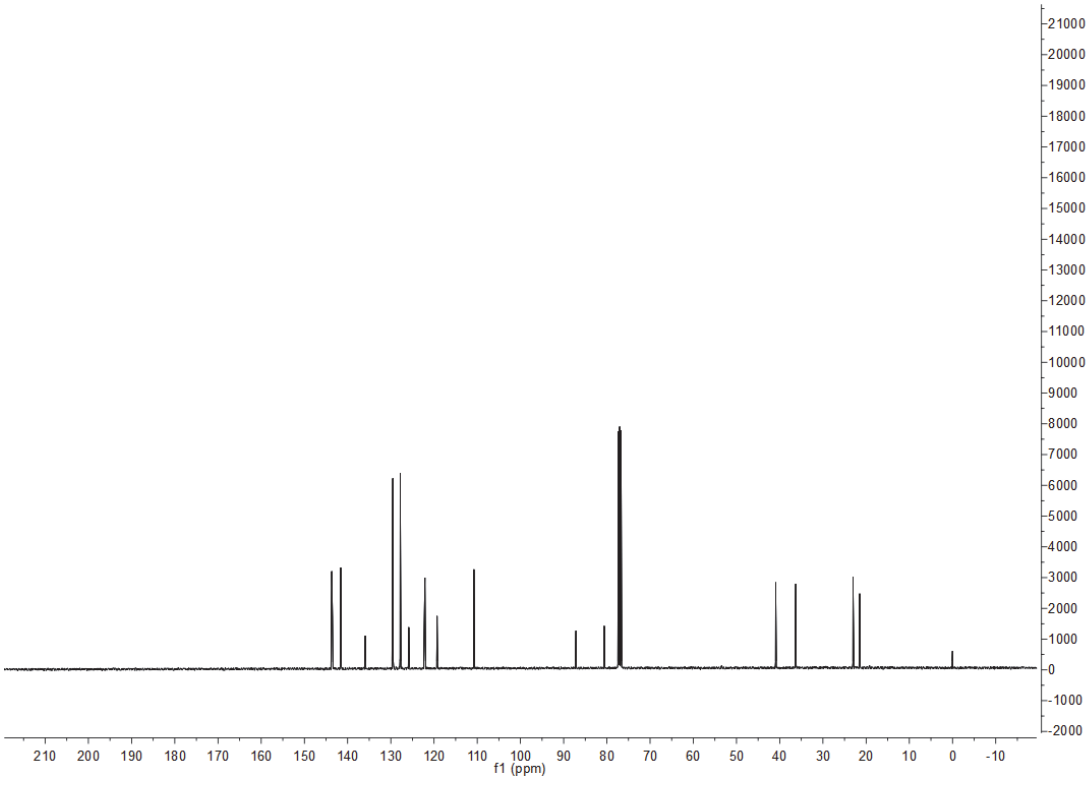

130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

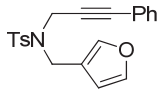

2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



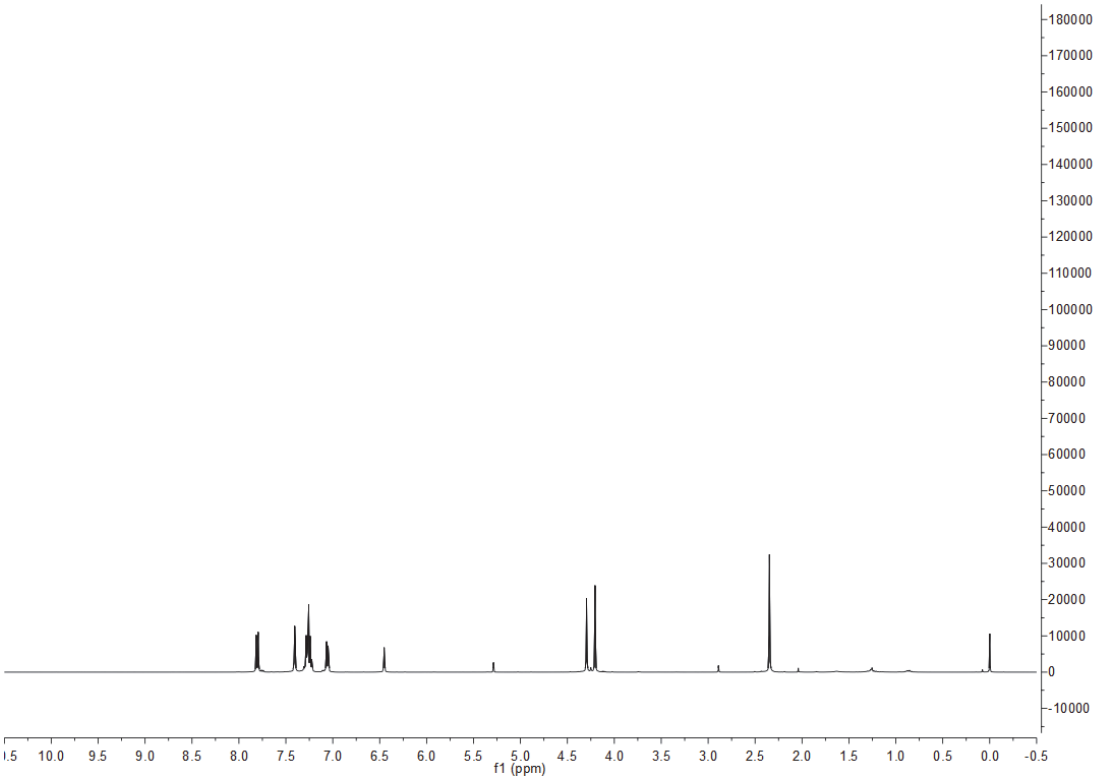
1c

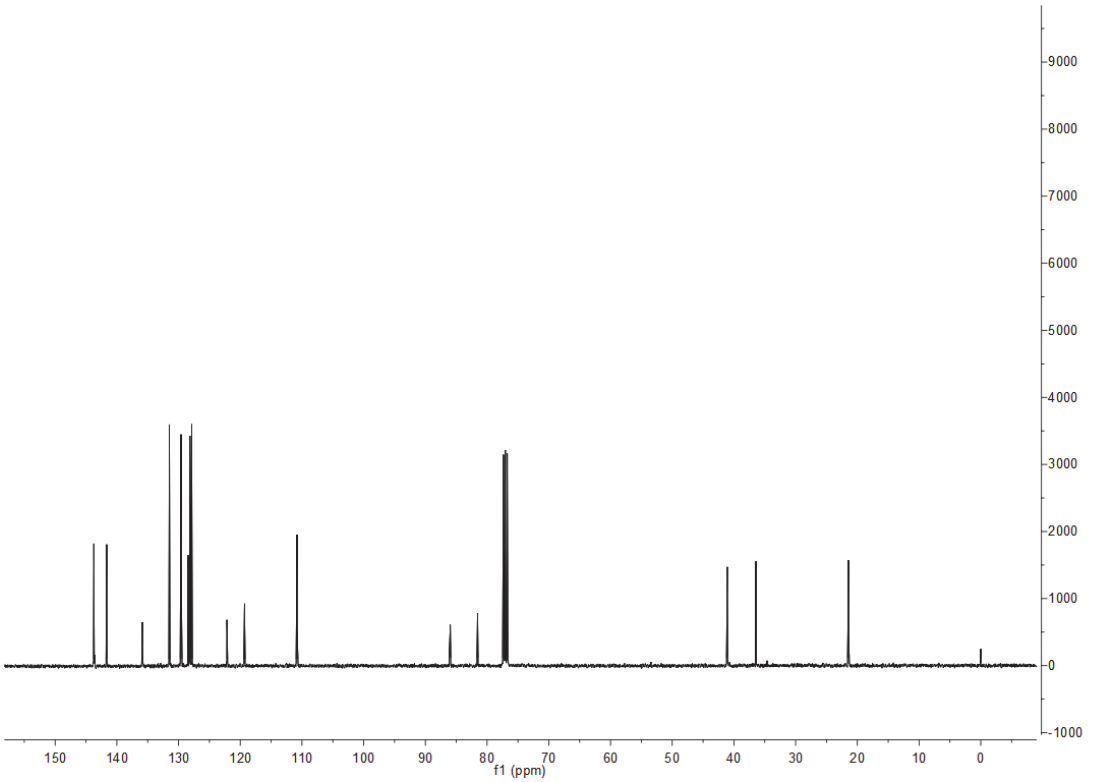


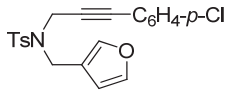



Ph
TsN
O

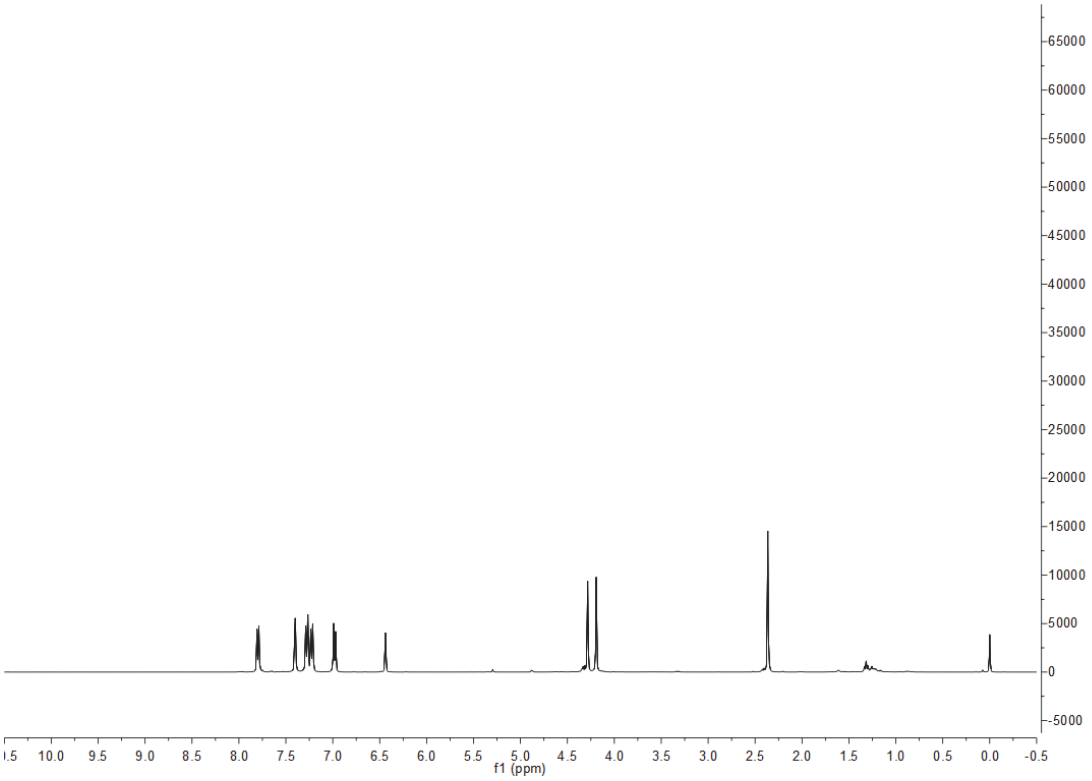
1d

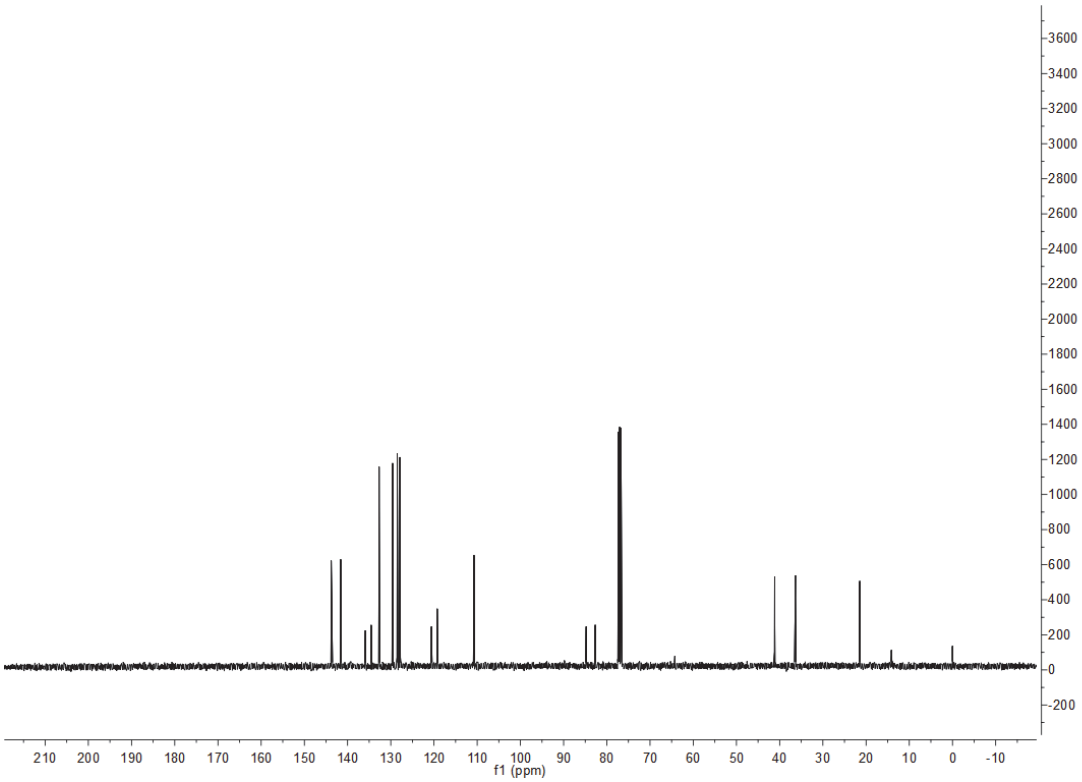

180000
170000
160000
150000
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

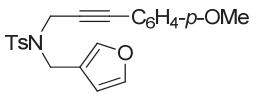

9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



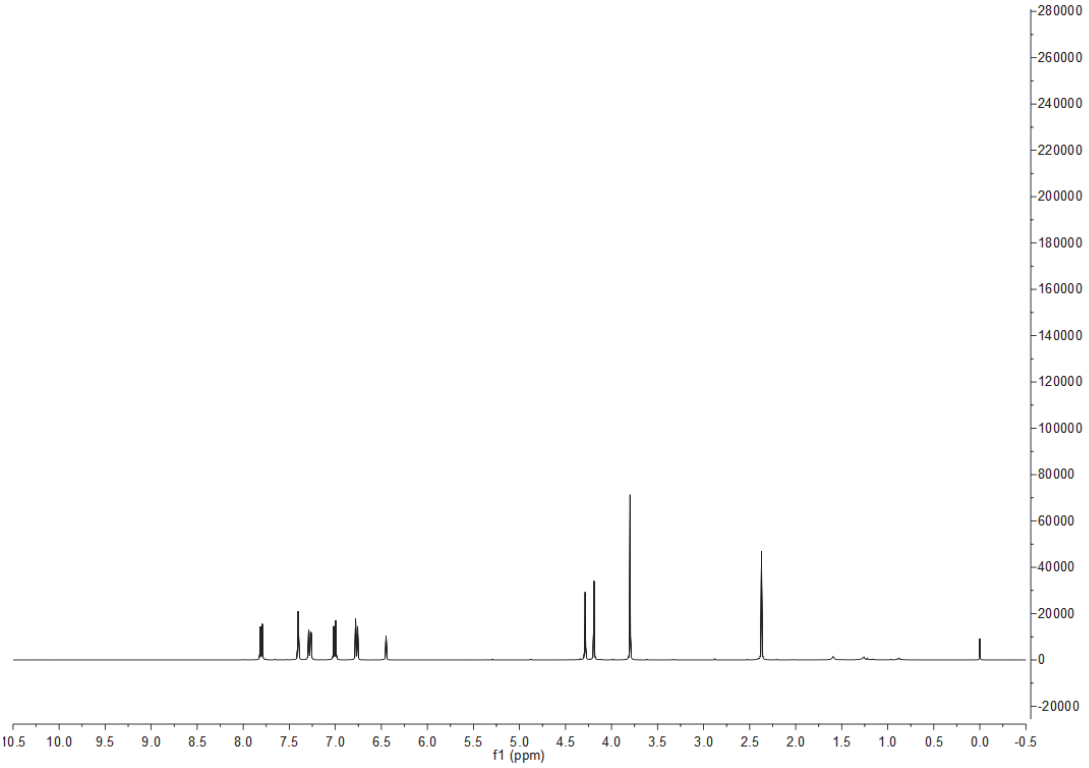
1e

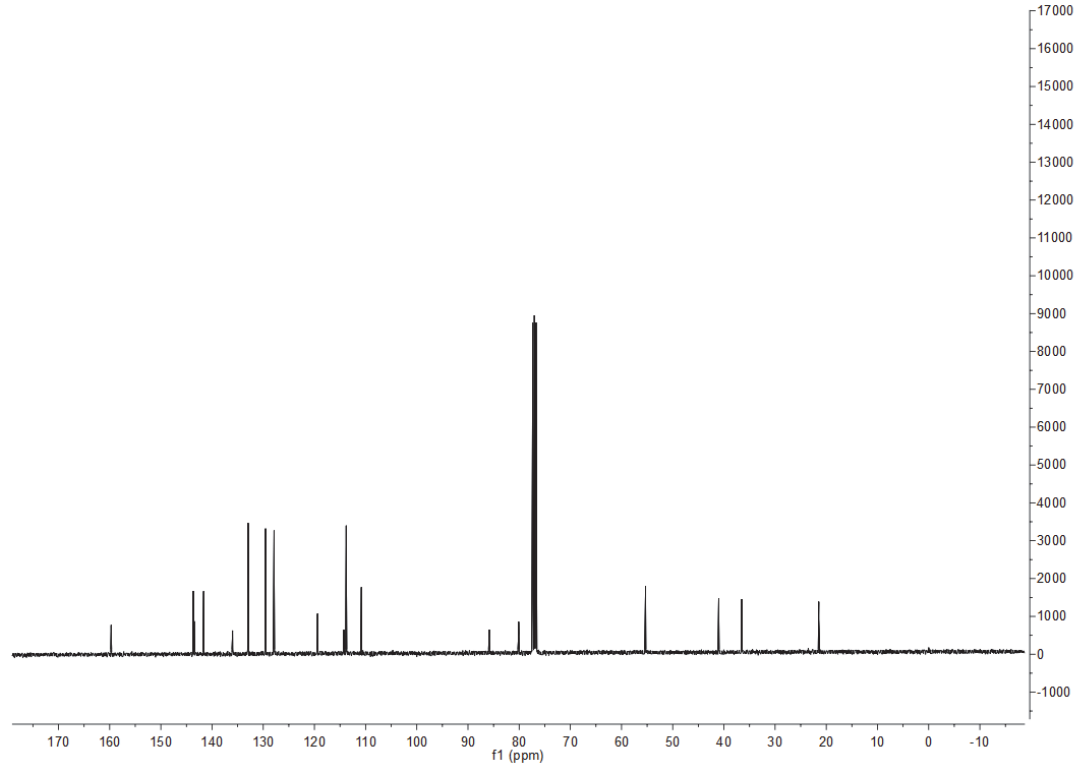


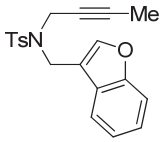



C6H4-p-OMe
TsN
O

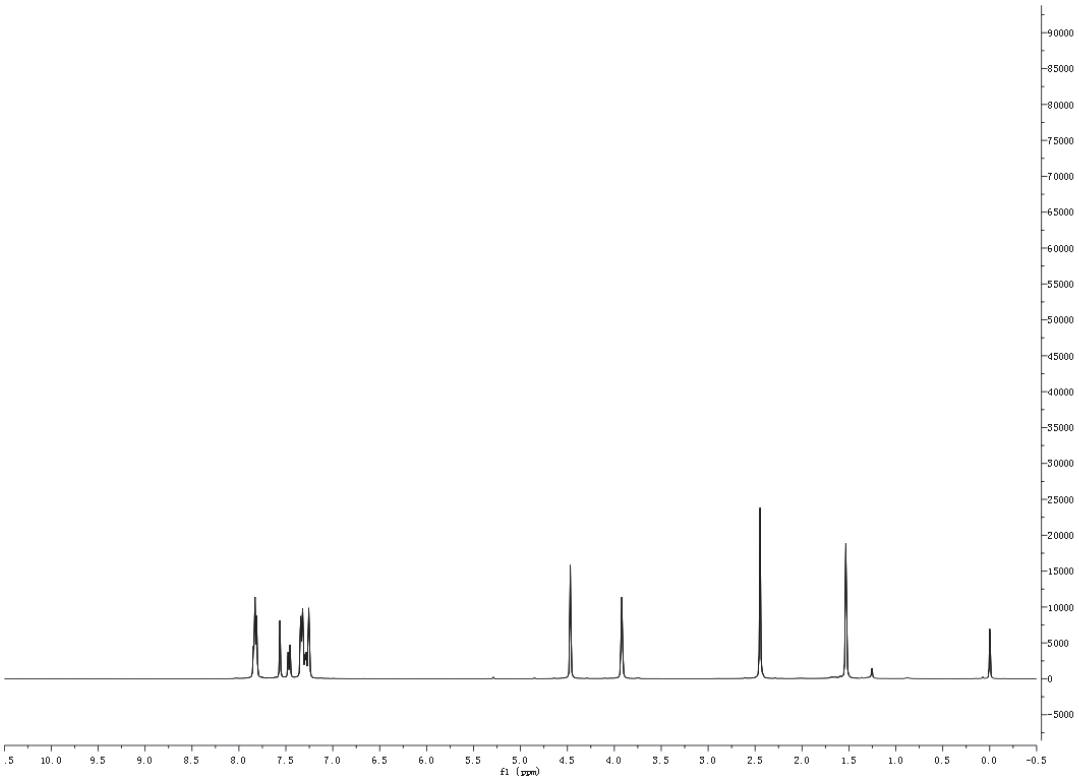
1f

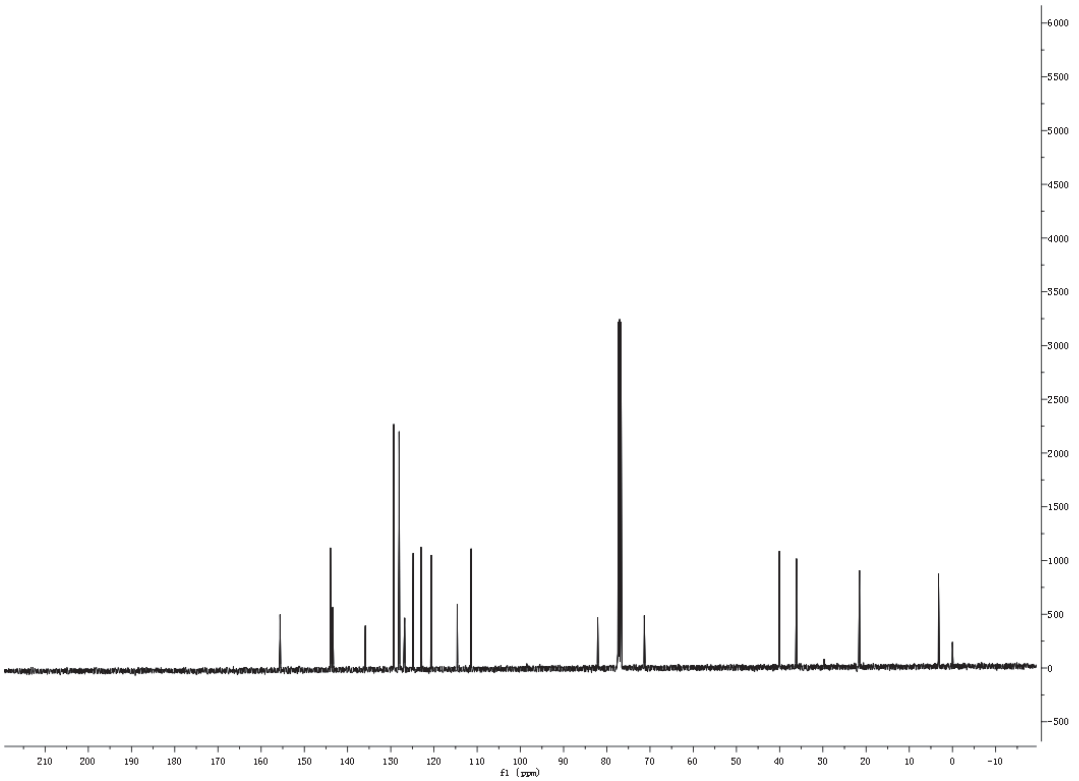

280000
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
-20000
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

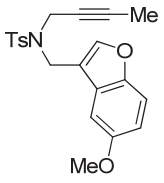

17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



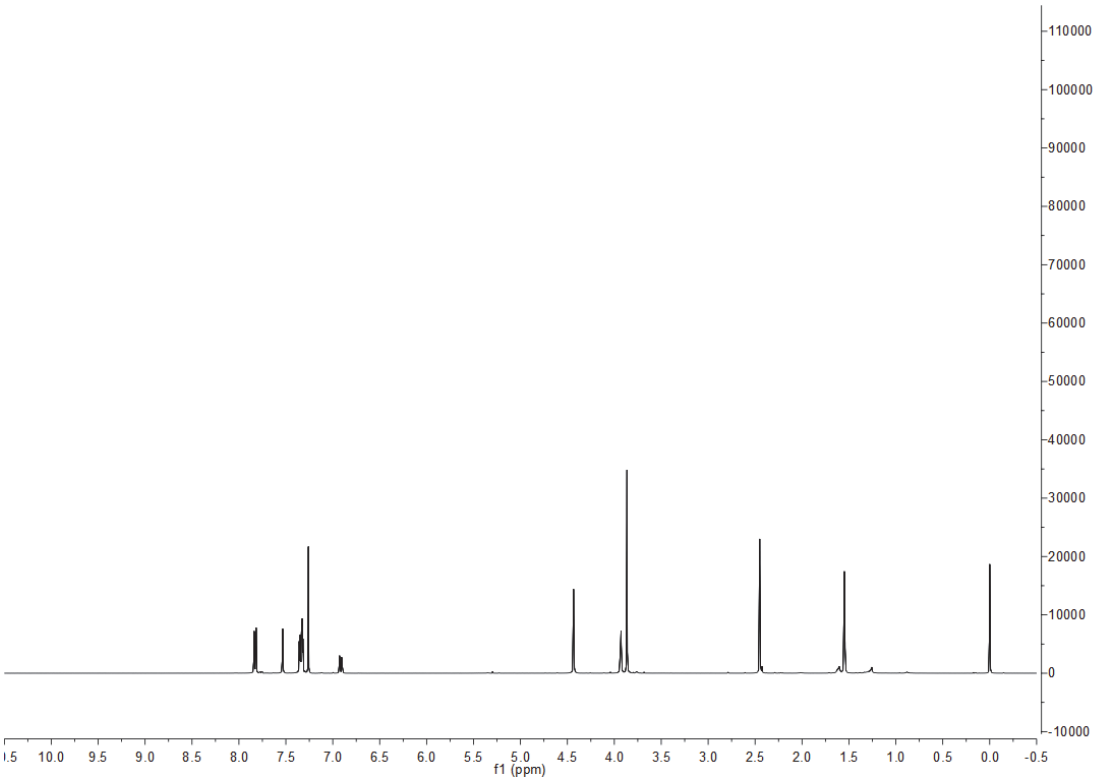
1g

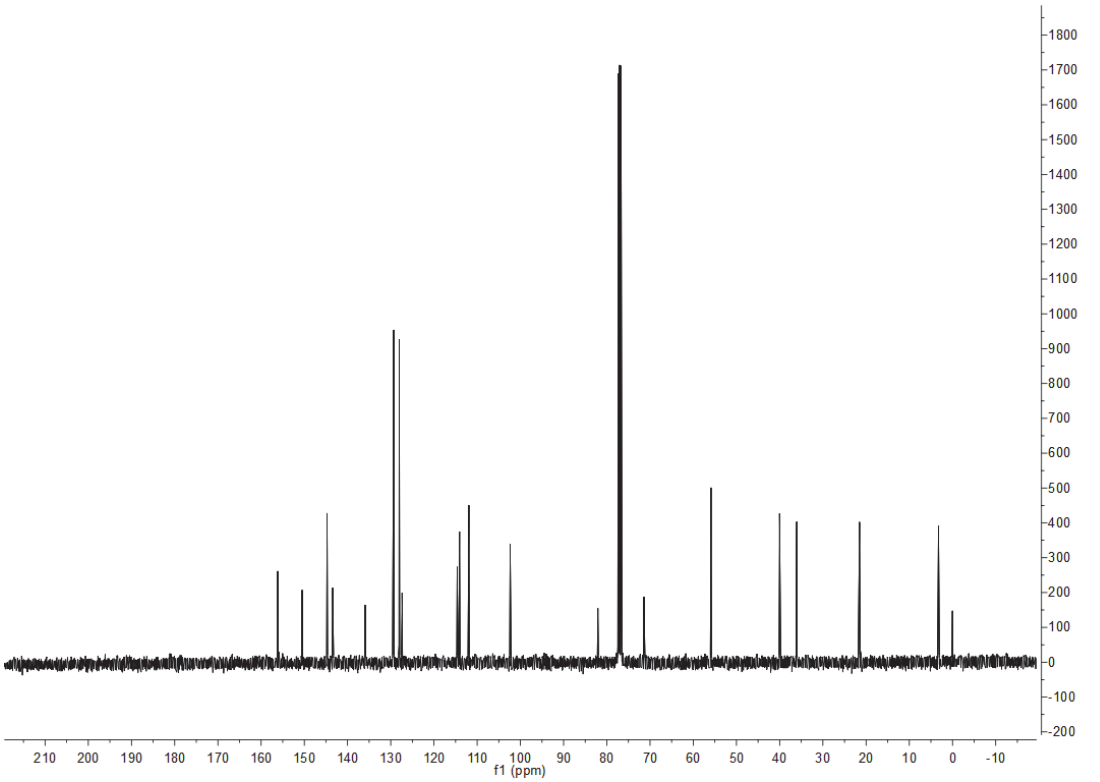


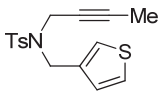




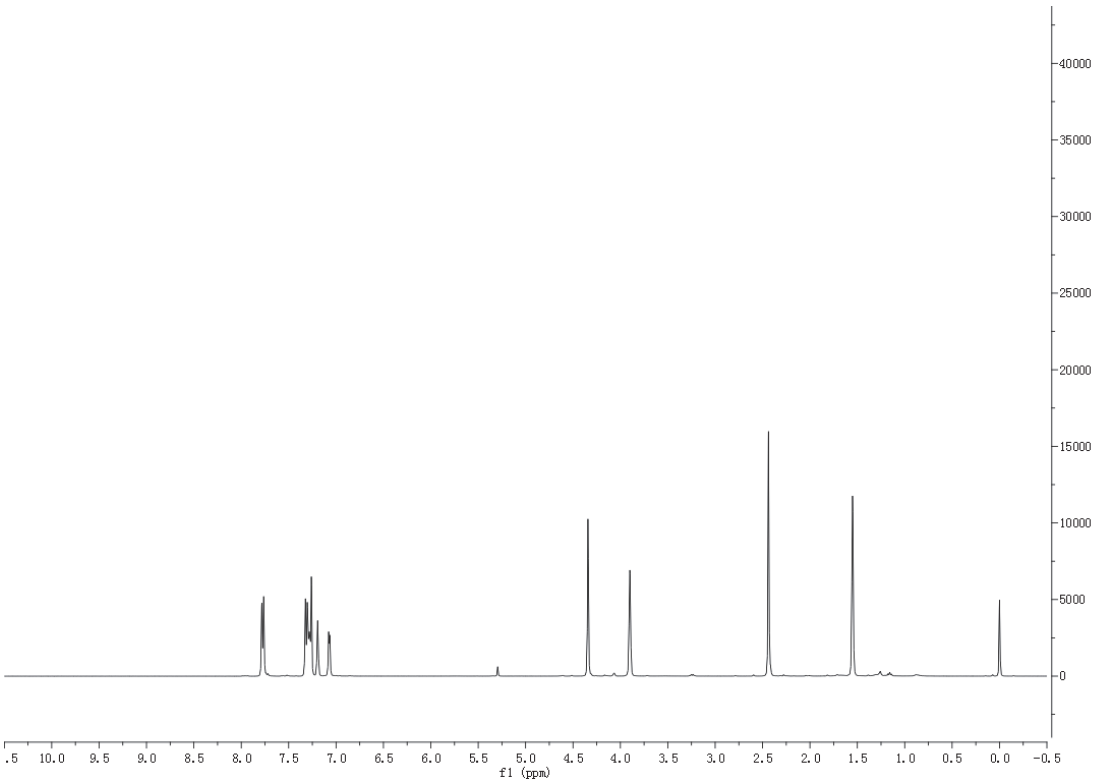
1h

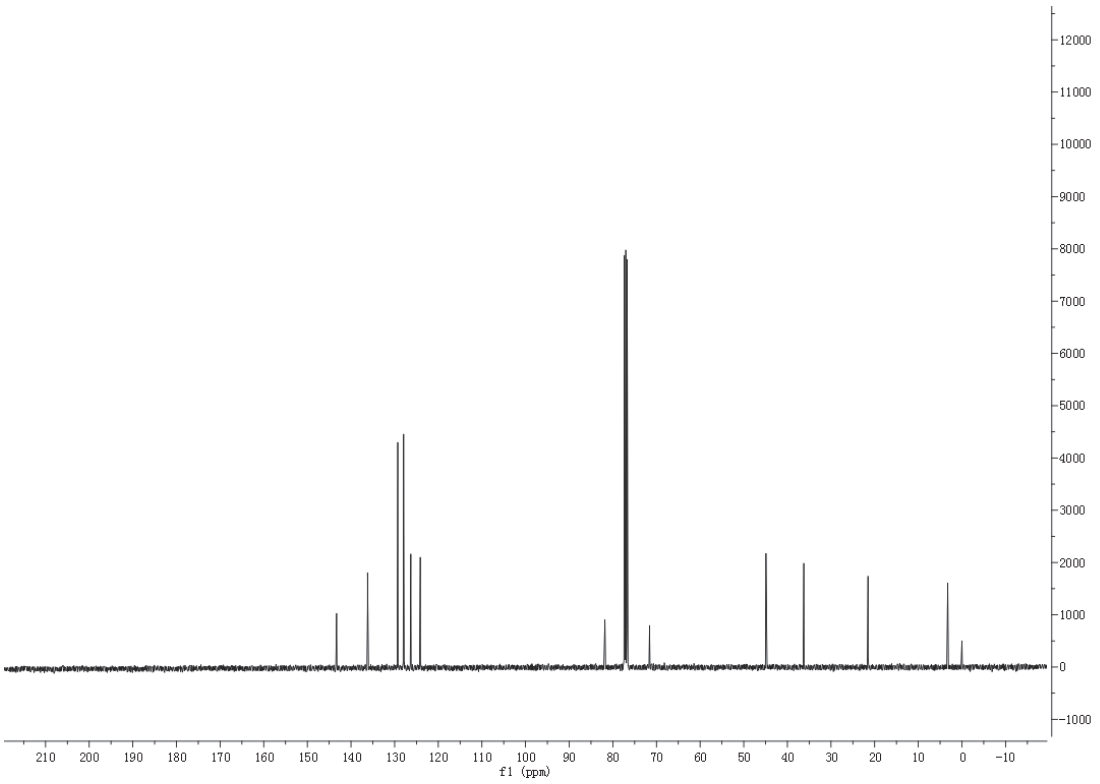


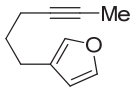



Me
TsN
S

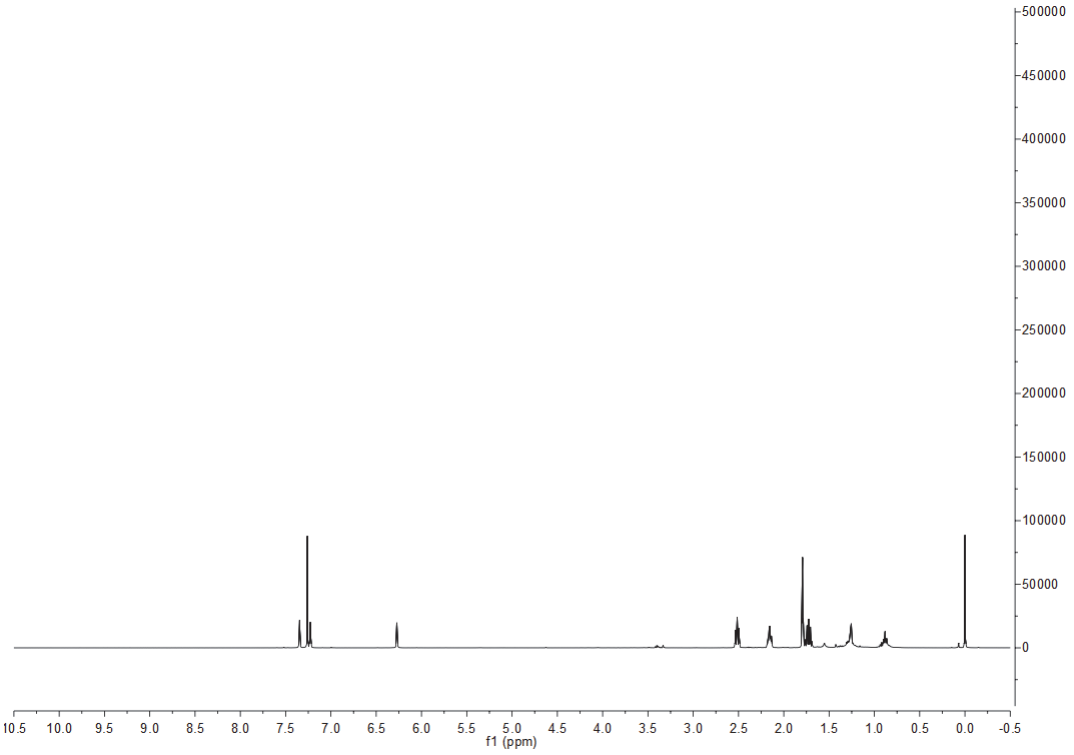
1i

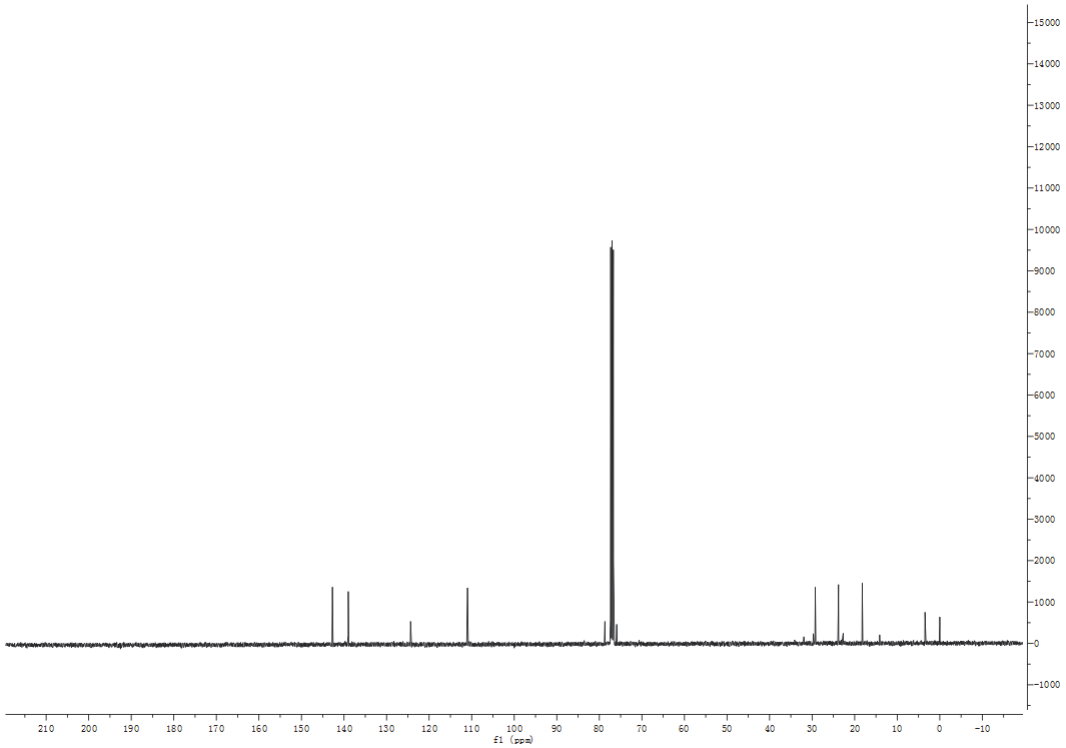

40000
35000
30000
25000
20000
15000
10000
5000
0
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

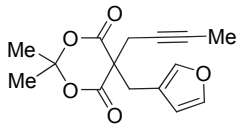

12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


Me
O

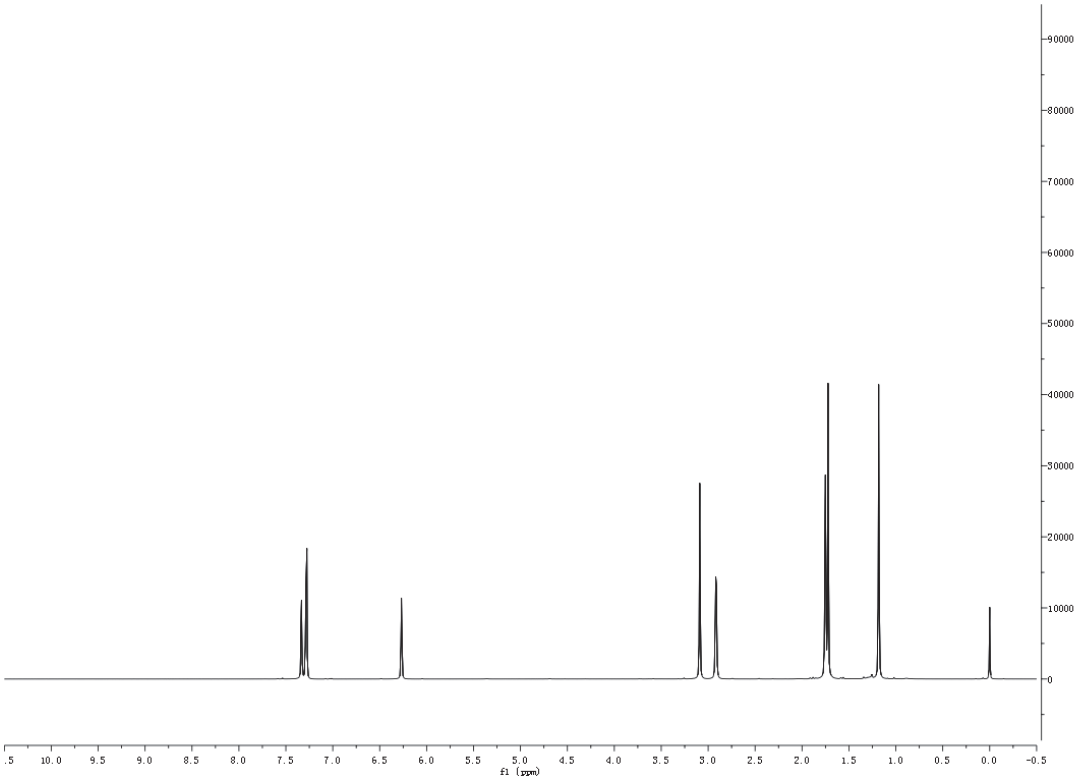
1k

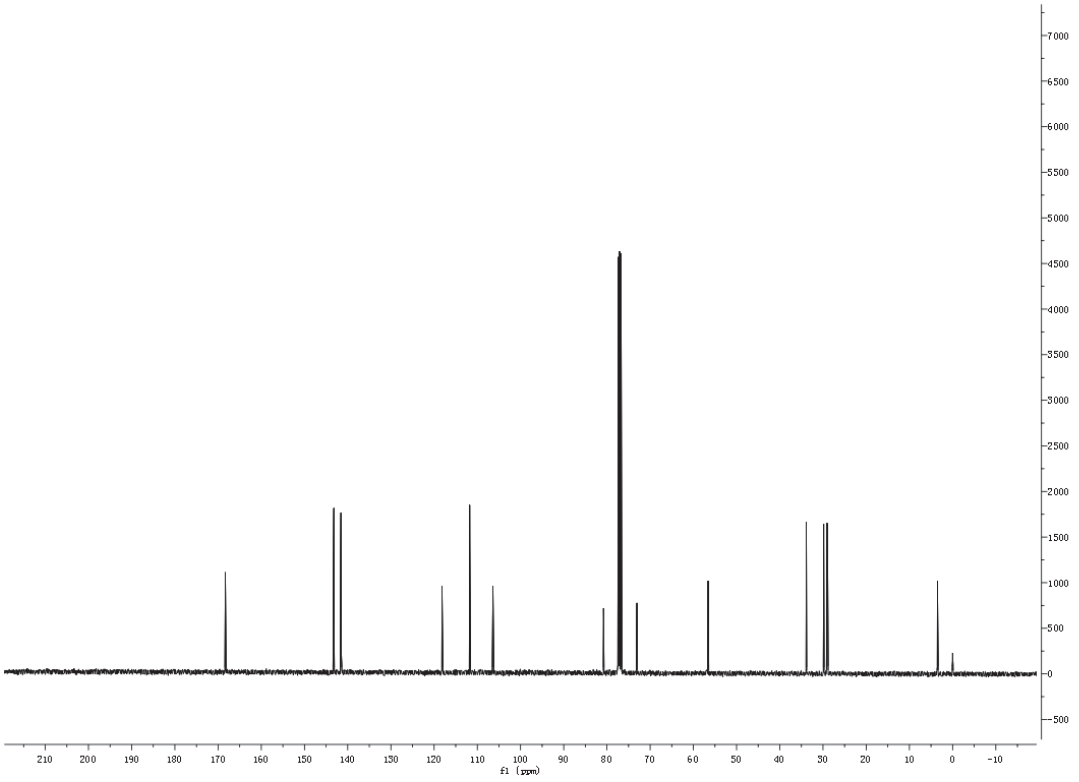

500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

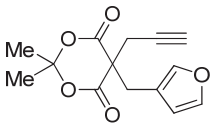

15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



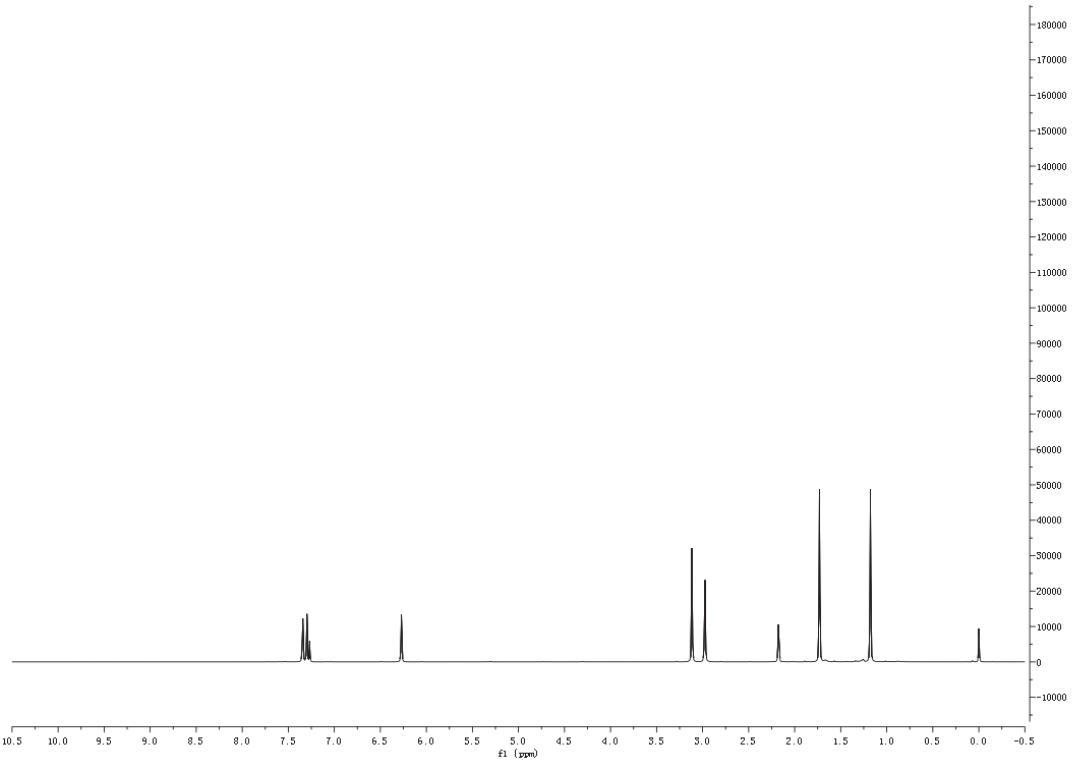
1l

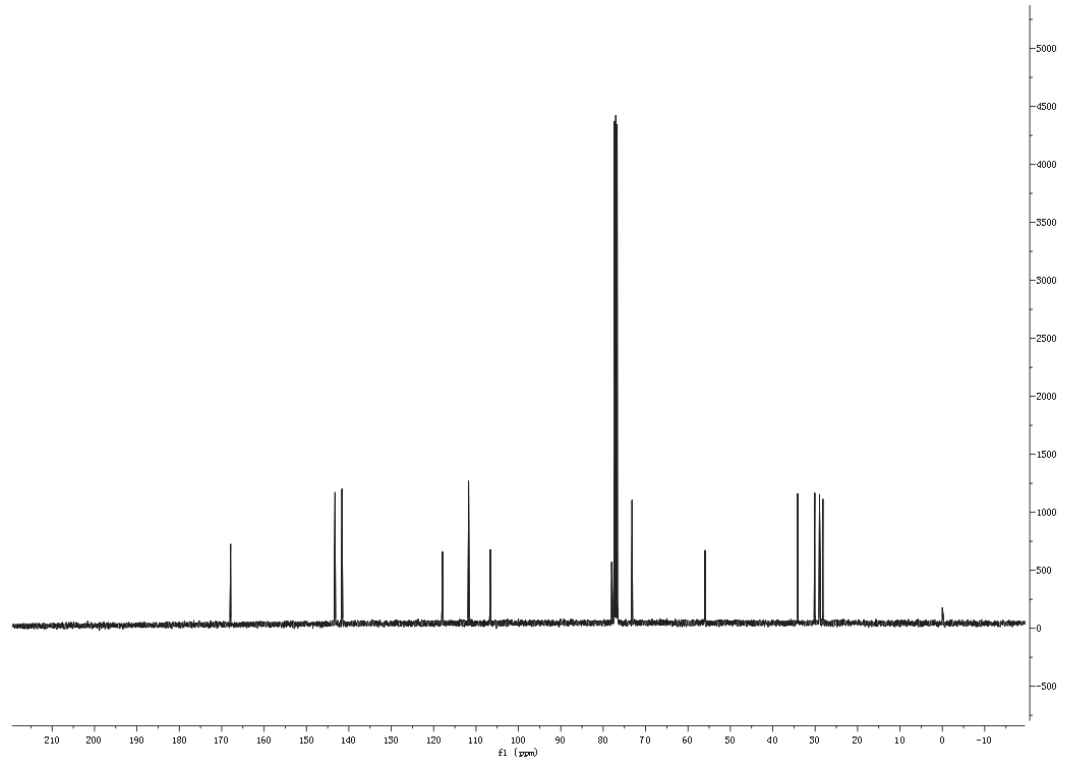


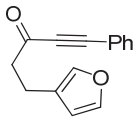




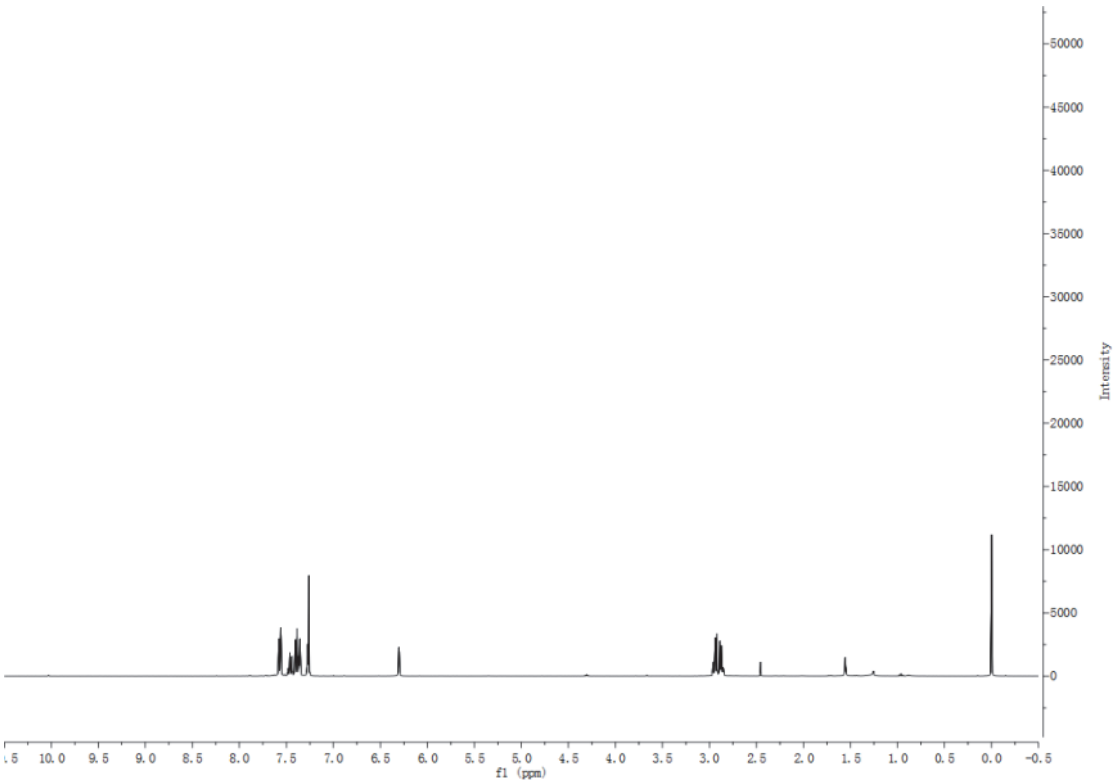
1o

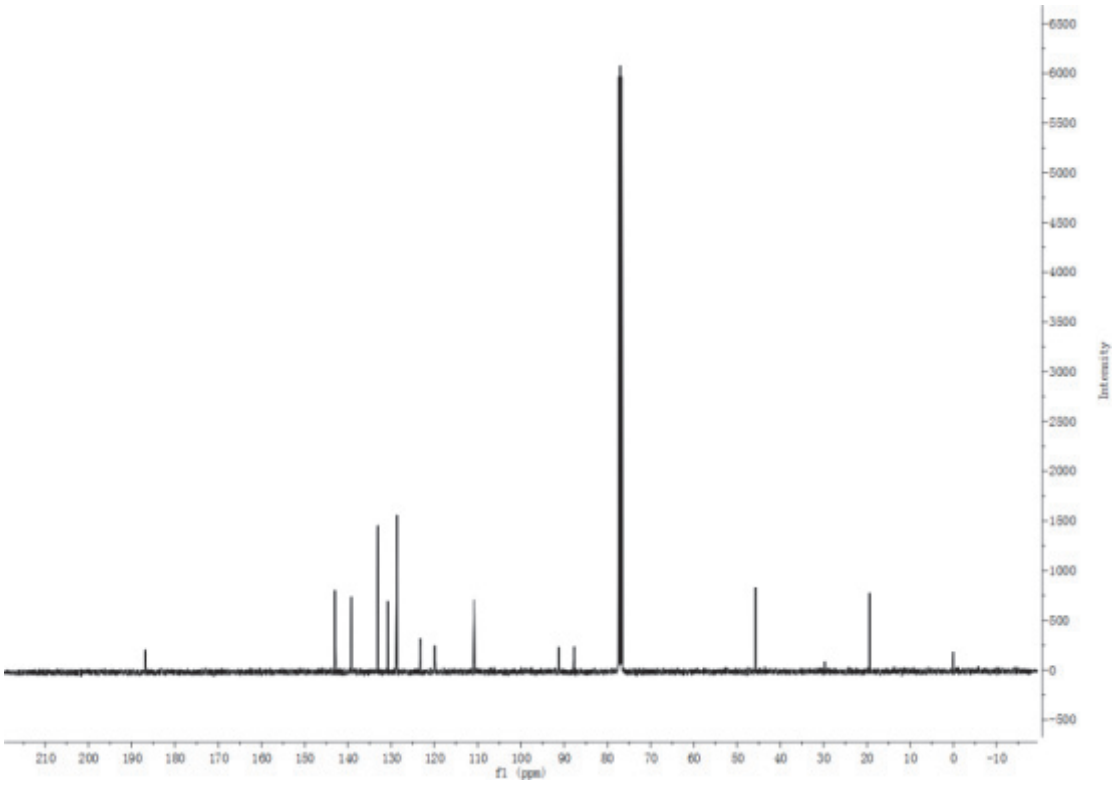


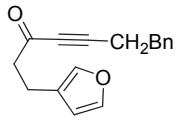




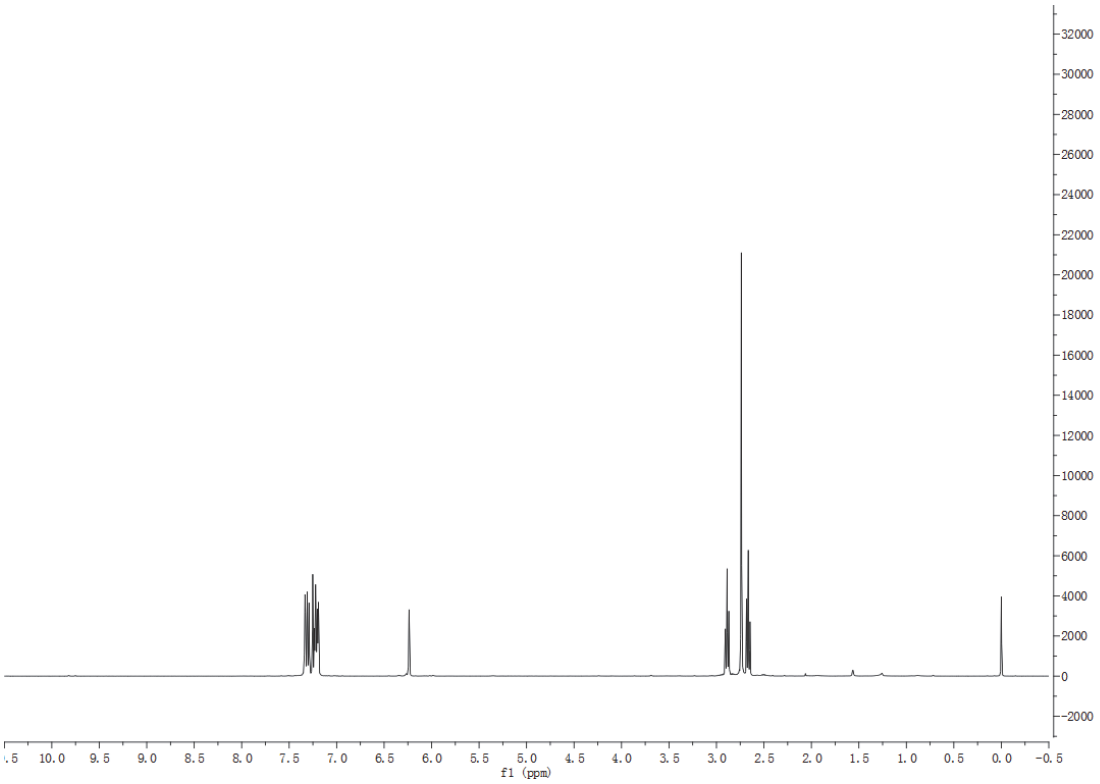
1r

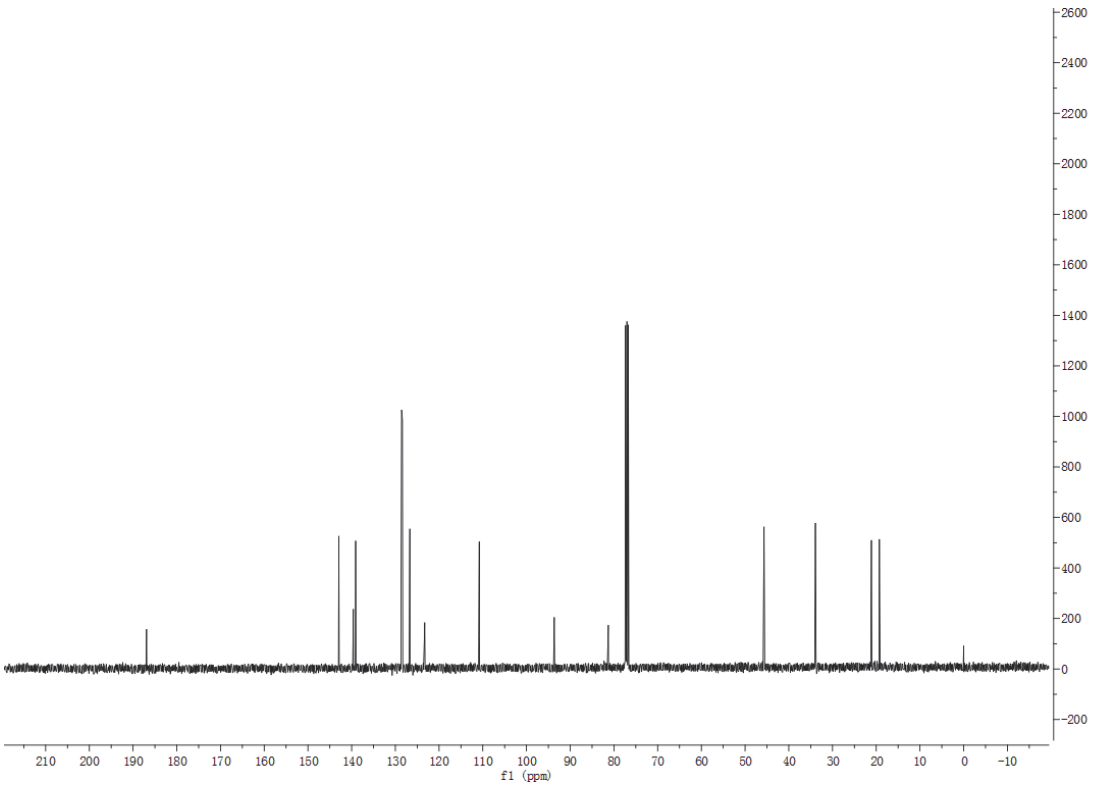


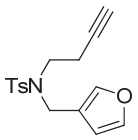




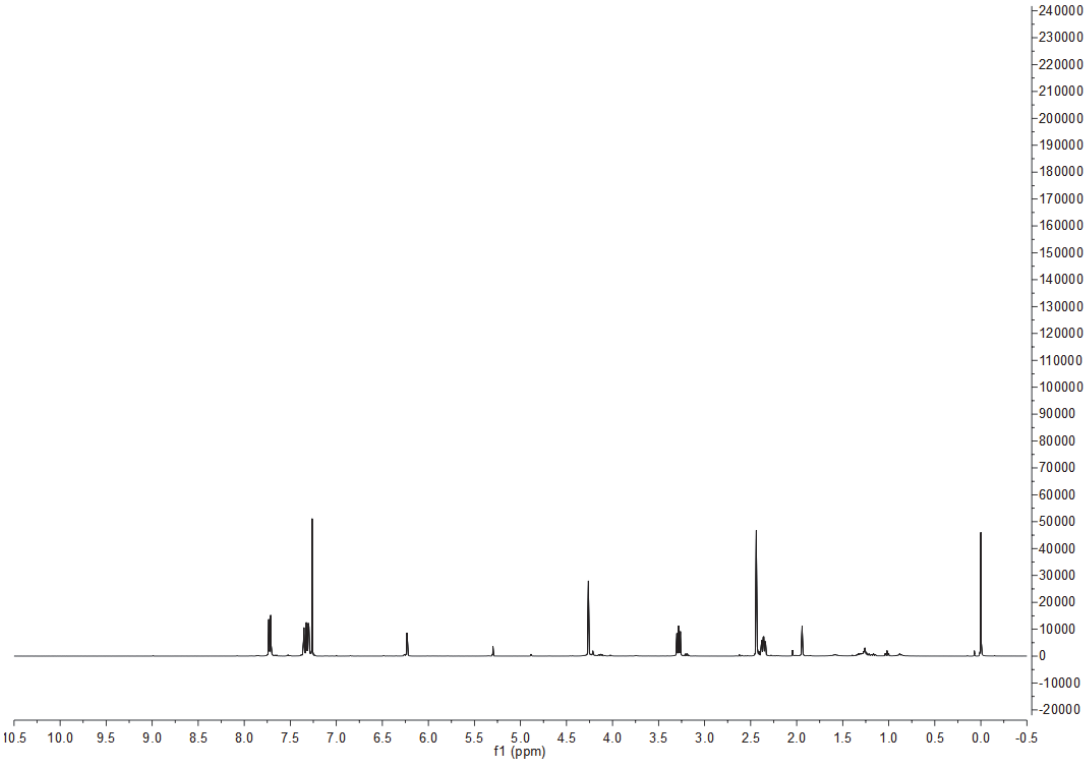
1s

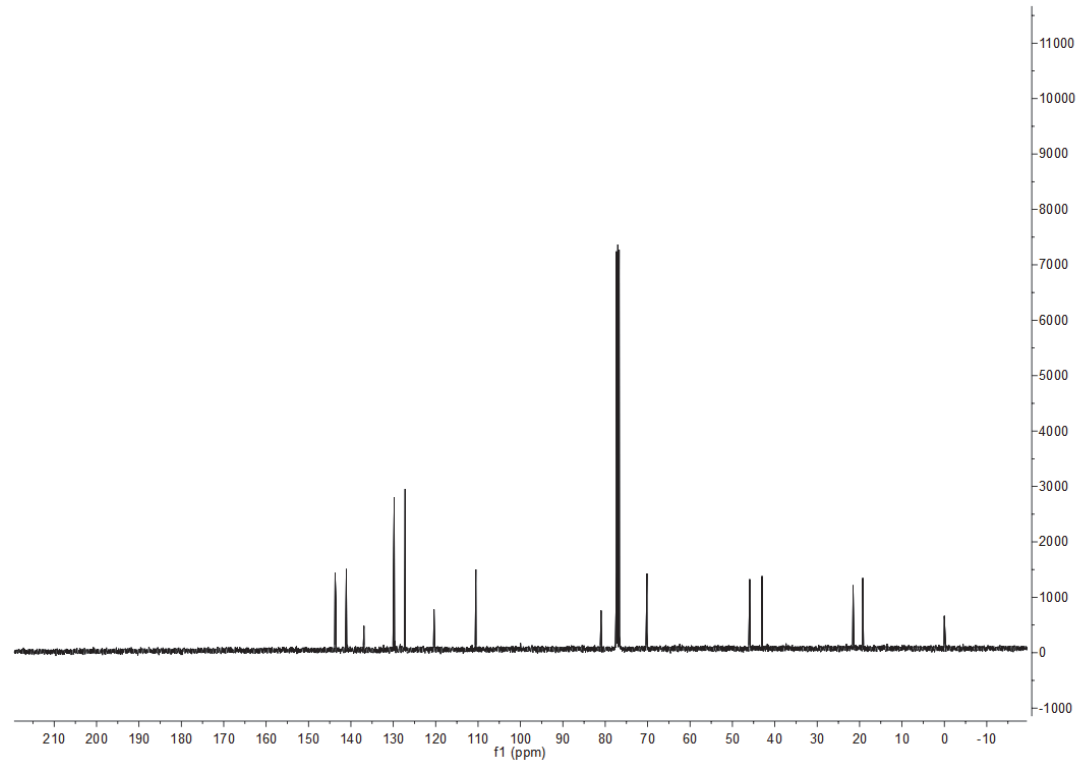


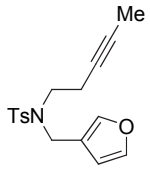




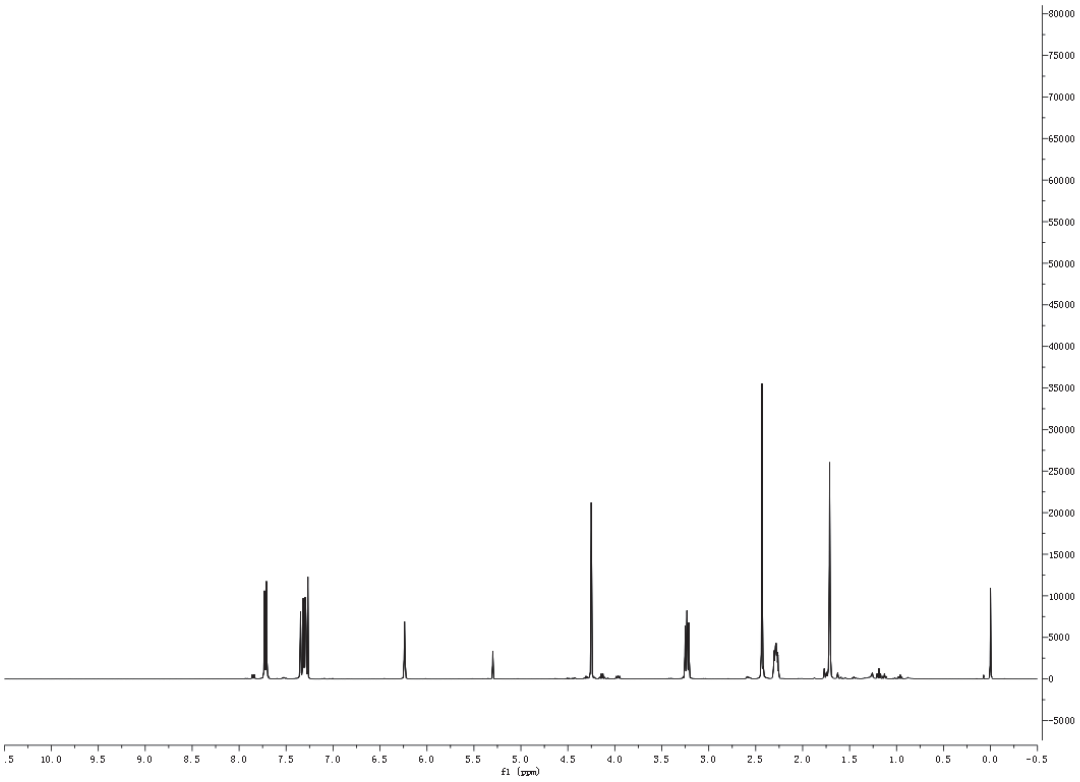
1t

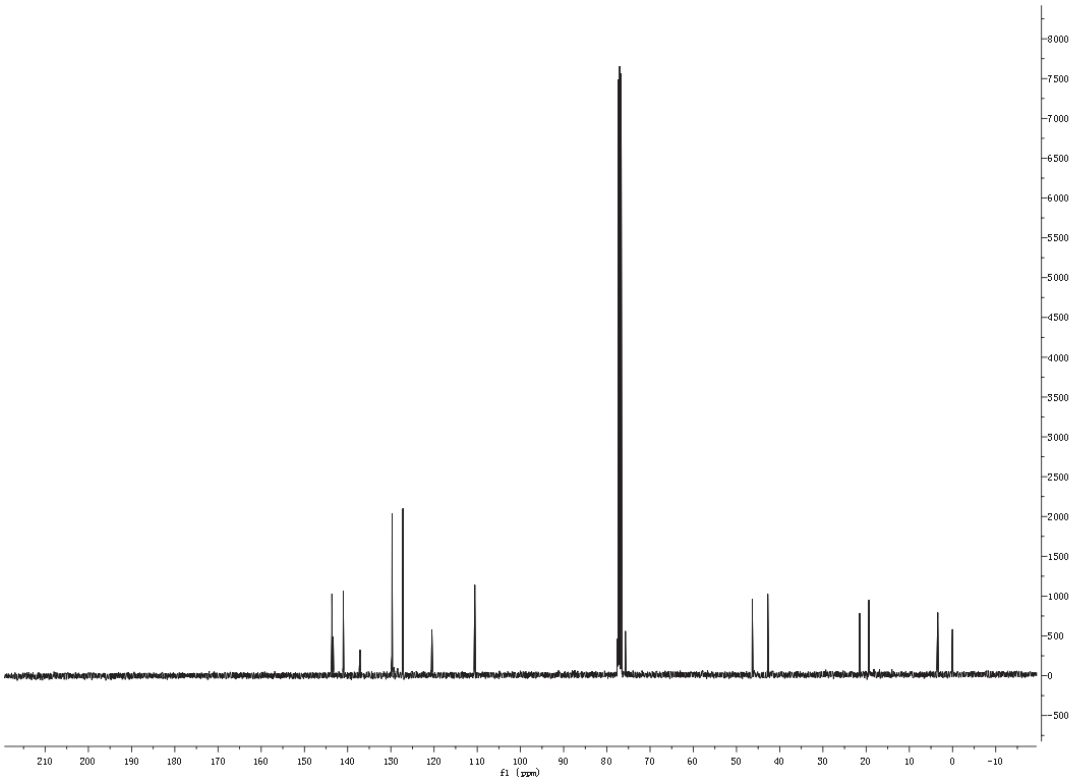


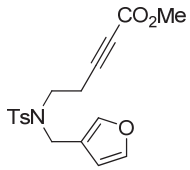




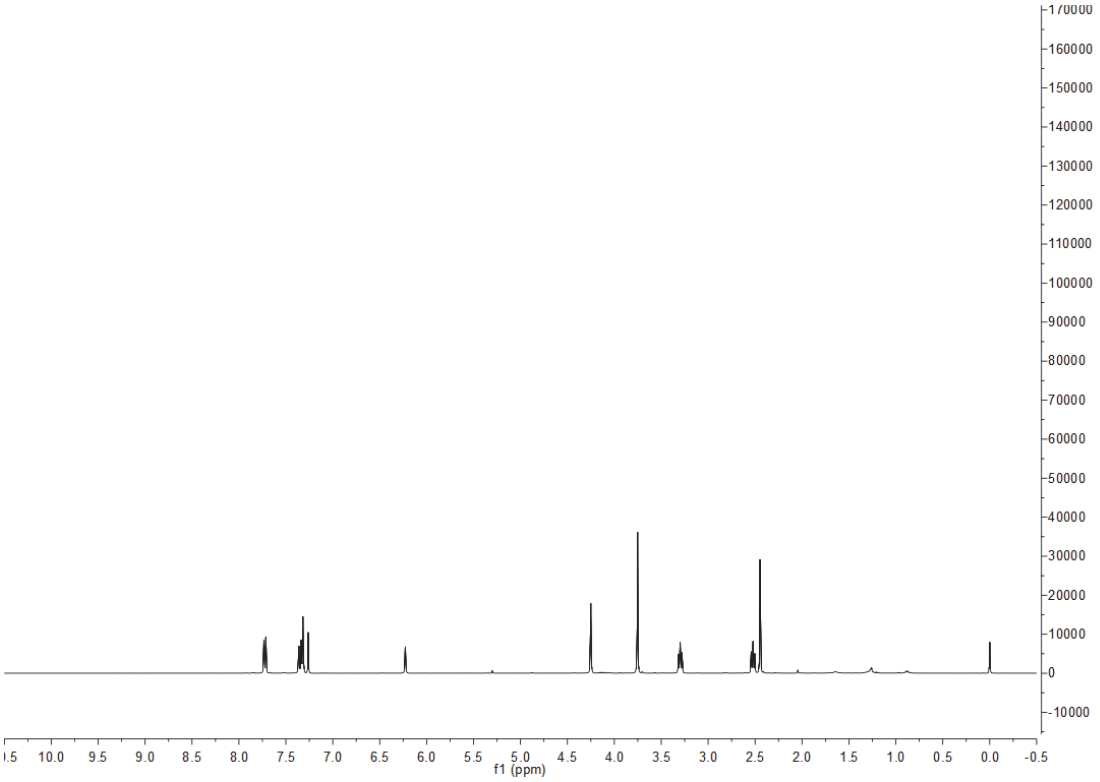
1u

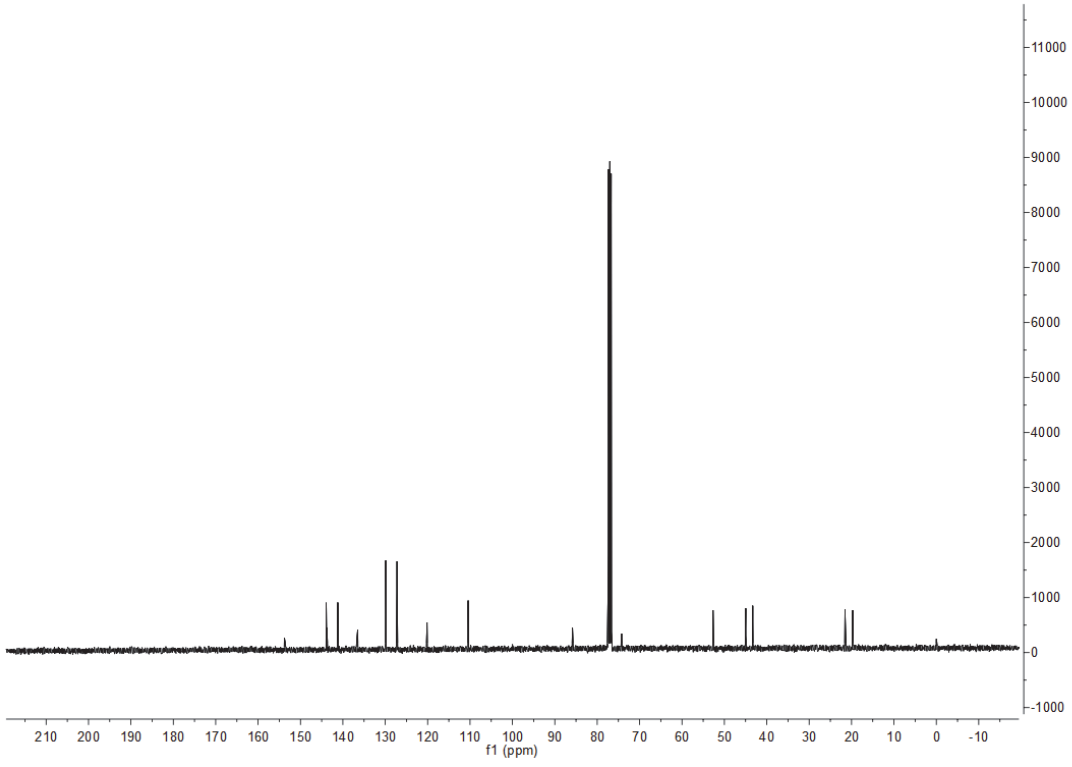


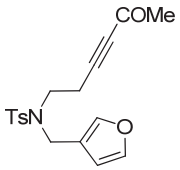




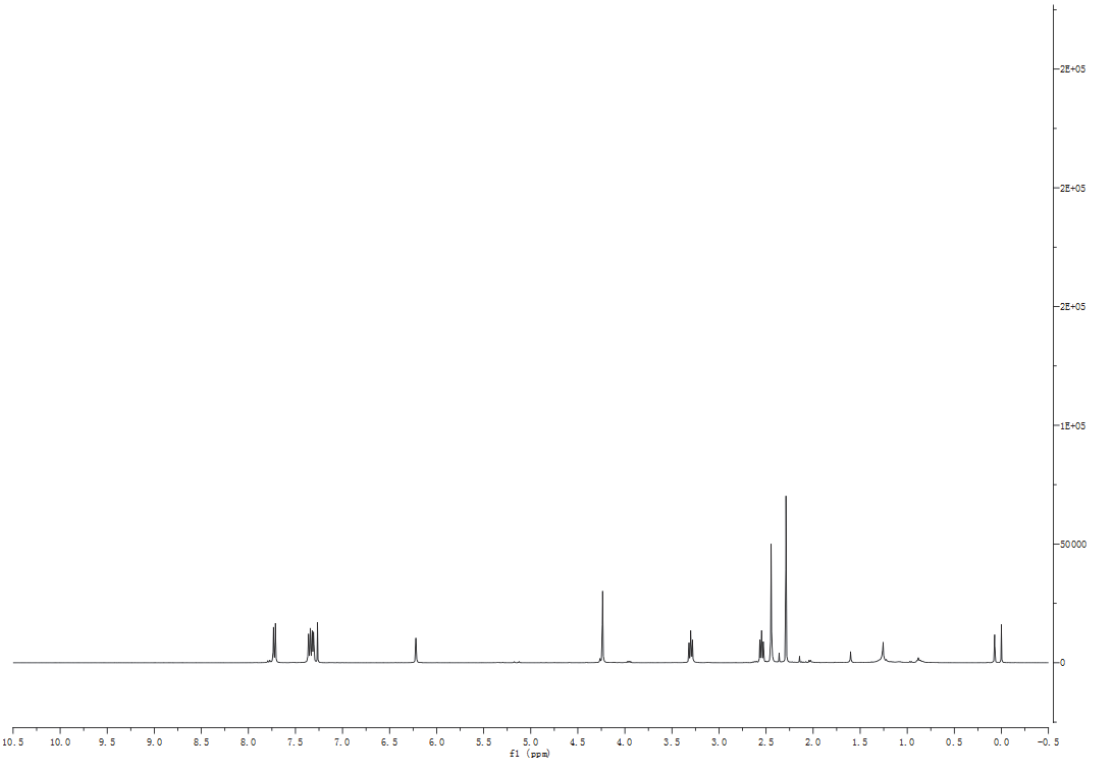
1v

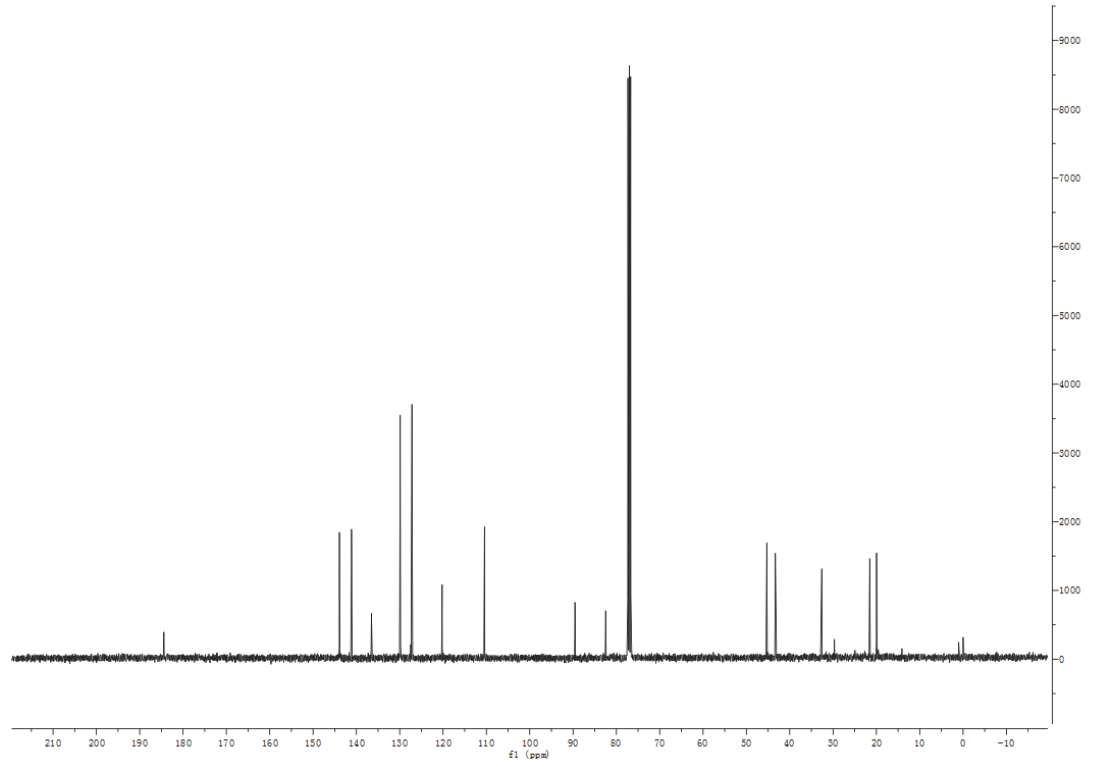


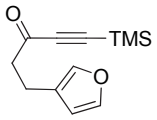



COMe
TsN
O

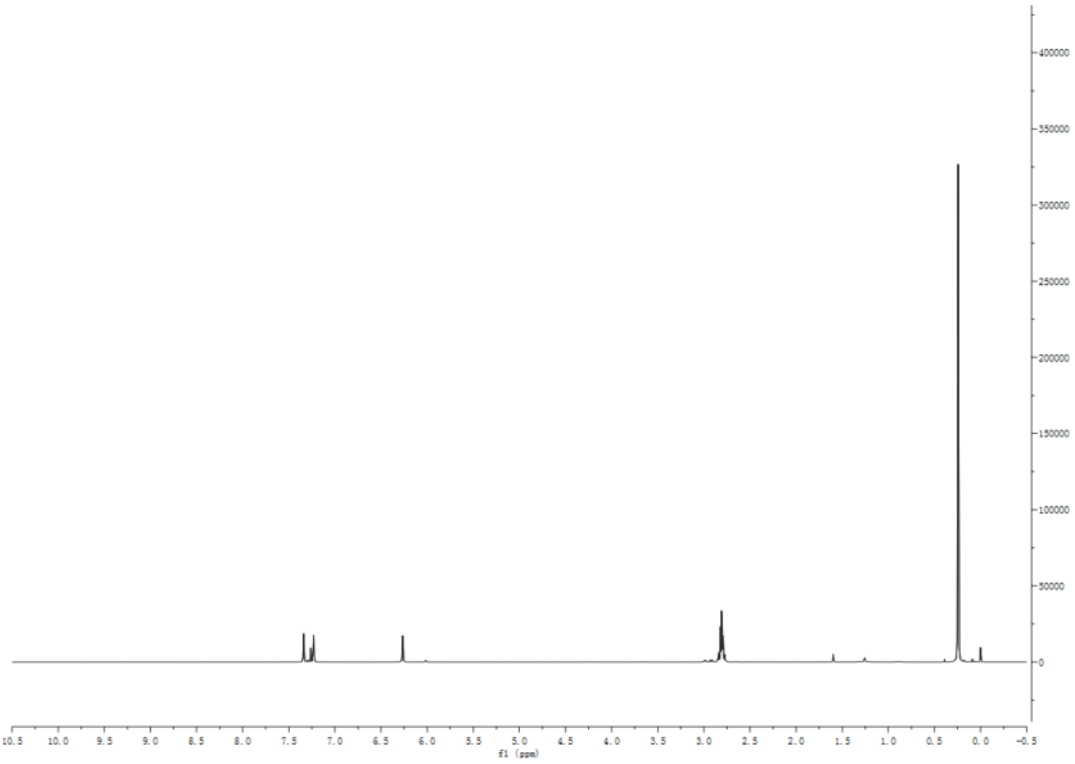
1w

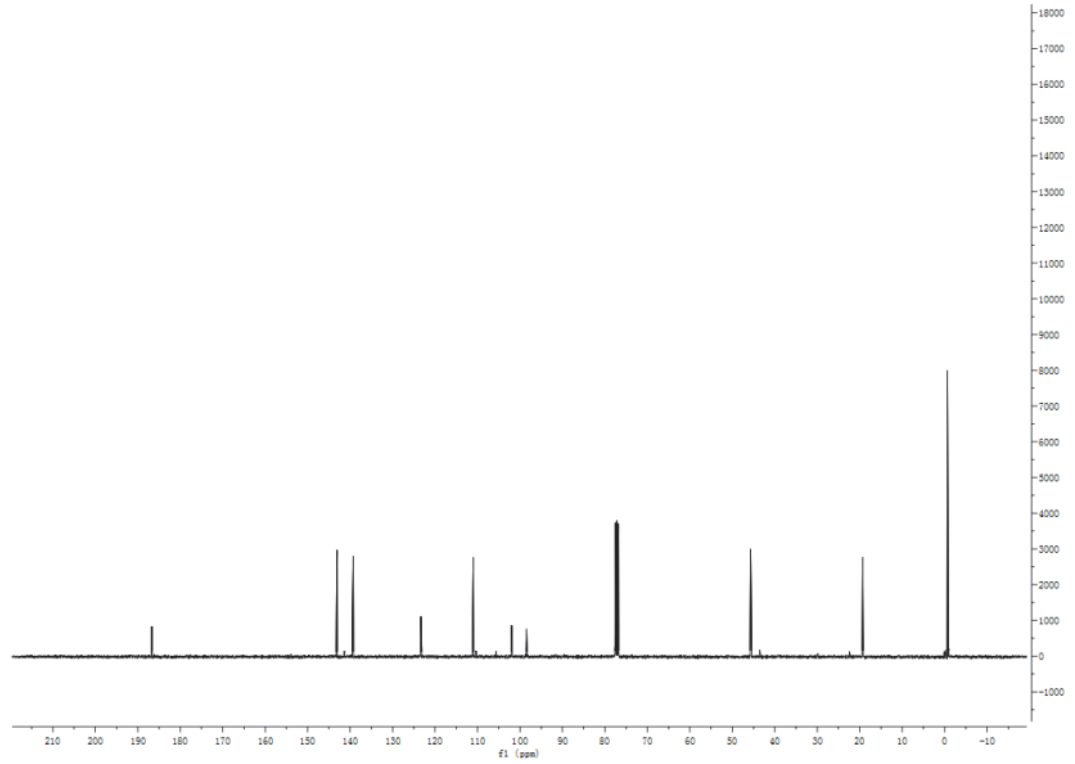

2E+05
2E+05
2E+05
1E+05
50000
0
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

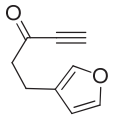

9000
8000
7000
6000
5000
4000
3000
2000
1000
0
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


O
TMS
O

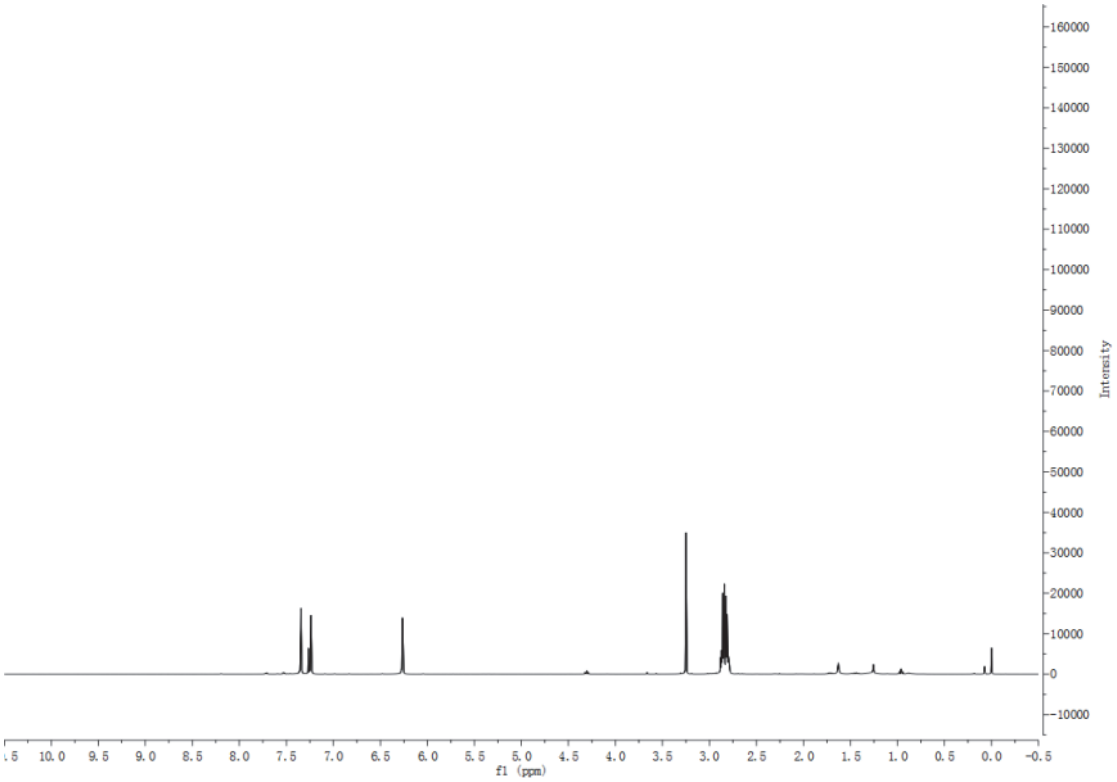
1x

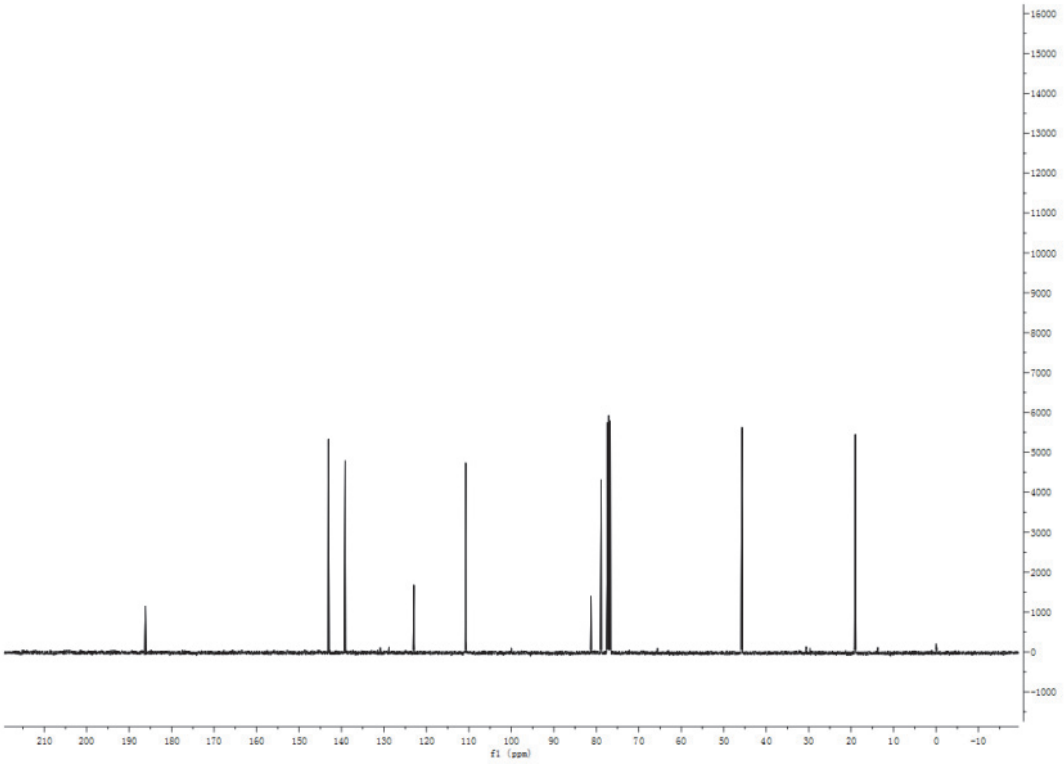

400000
350000
300000
250000
200000
150000
100000
50000
0
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

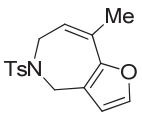

18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



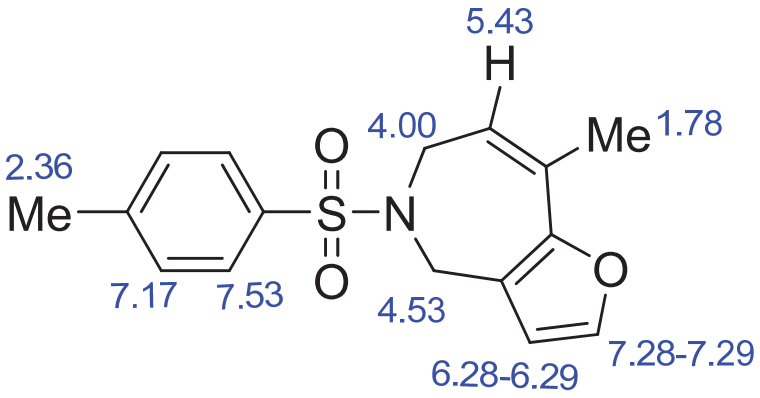
1y

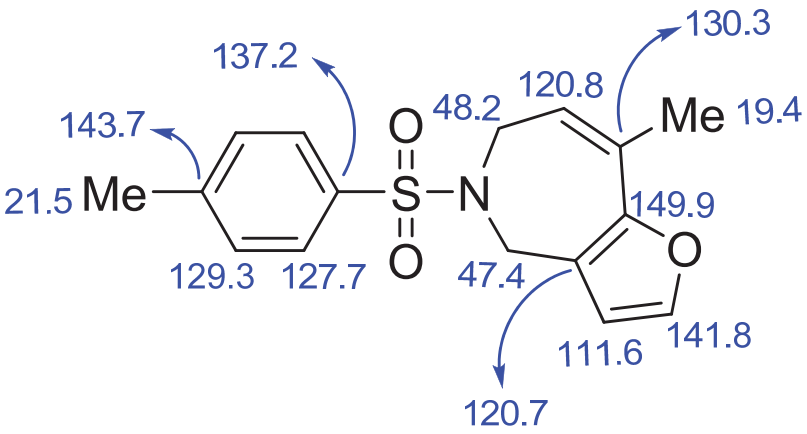


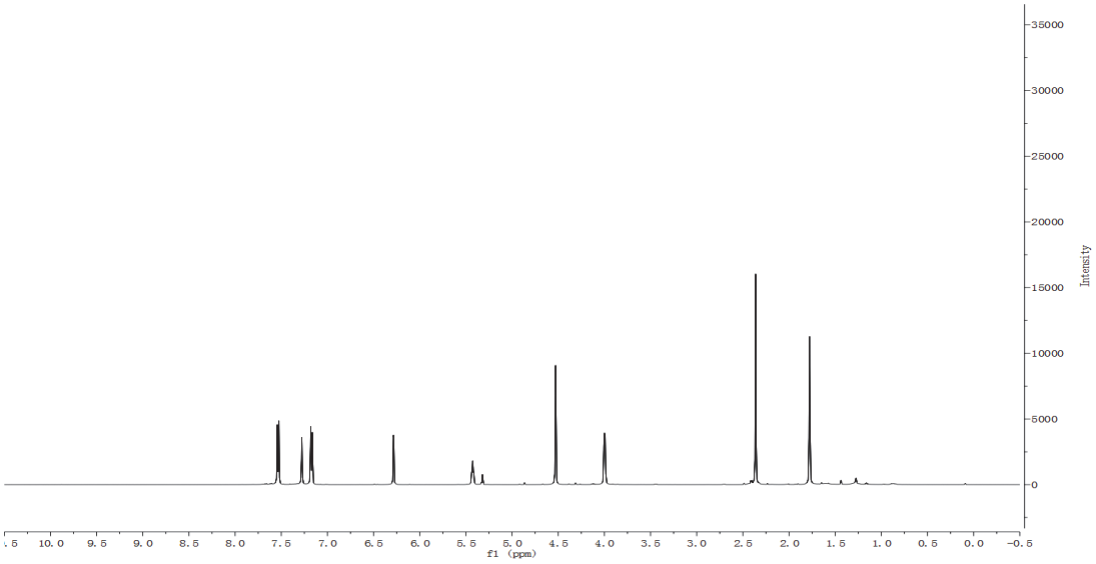


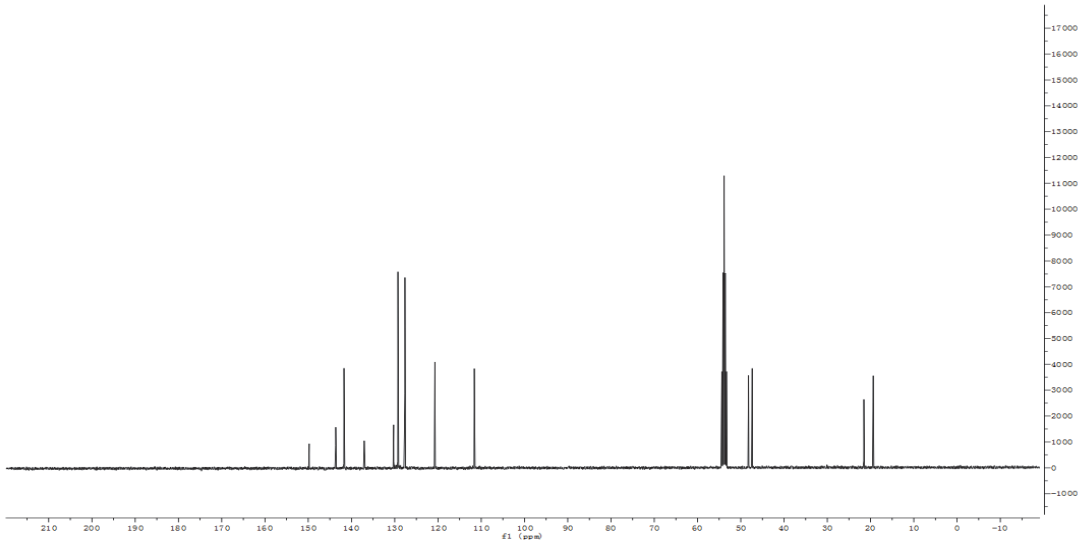

Me
TsN
O

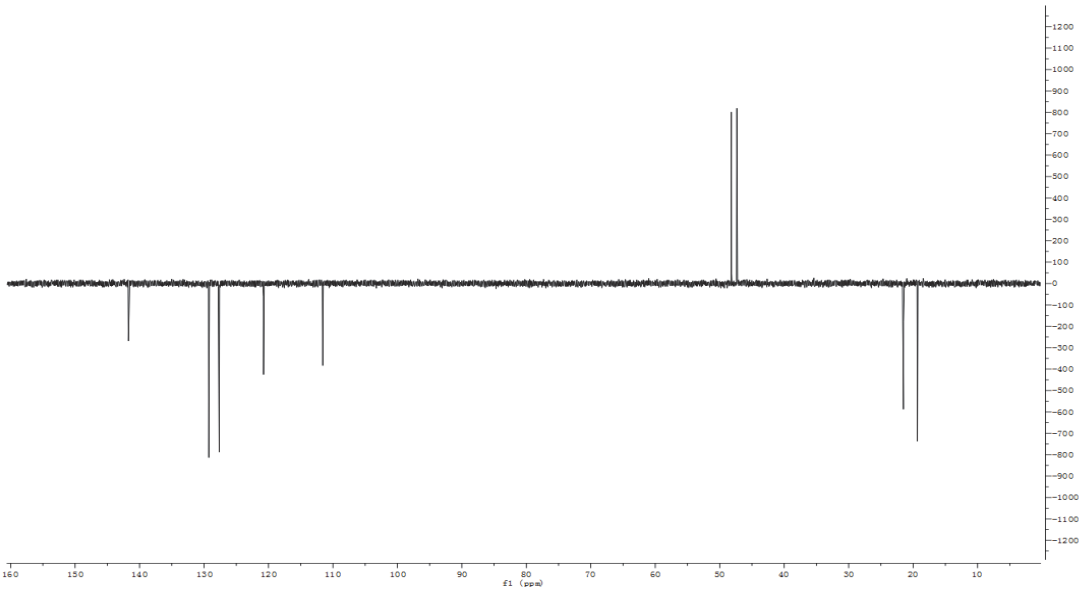
2a

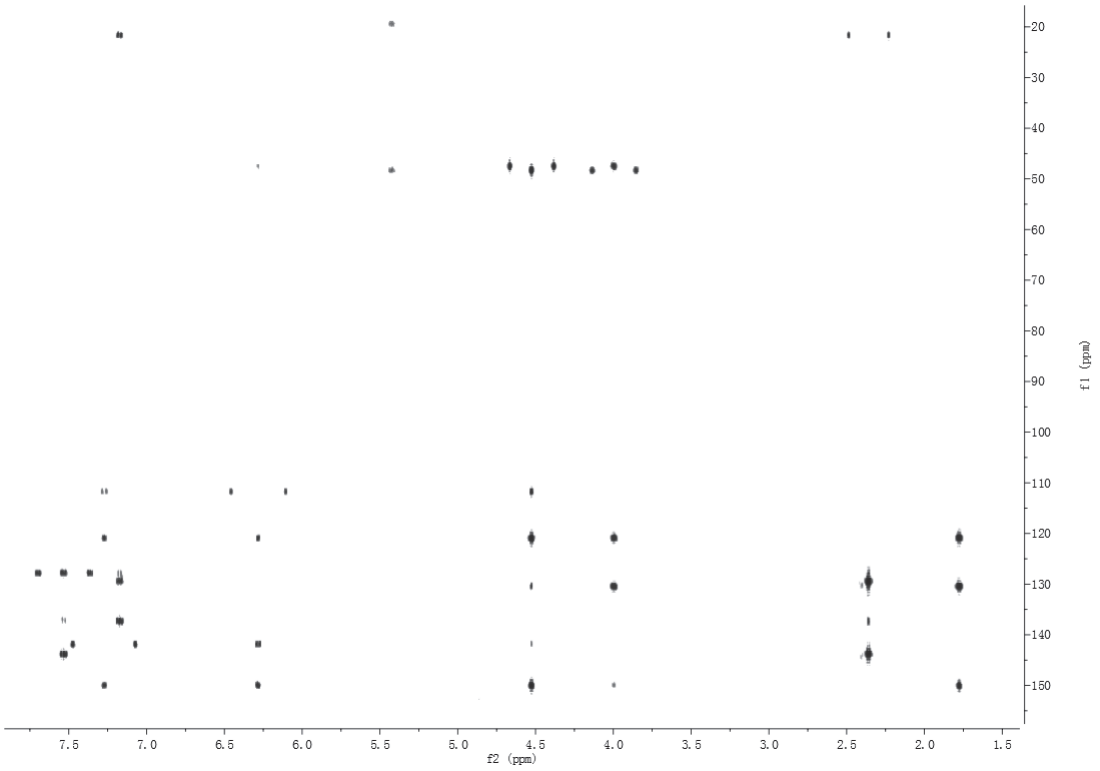

5.43
H
4.00
Me
1.78
2.36
Me
O
S
N
O
O
7.17
7.53
4.53
6.28-6.29
7.28-7.29

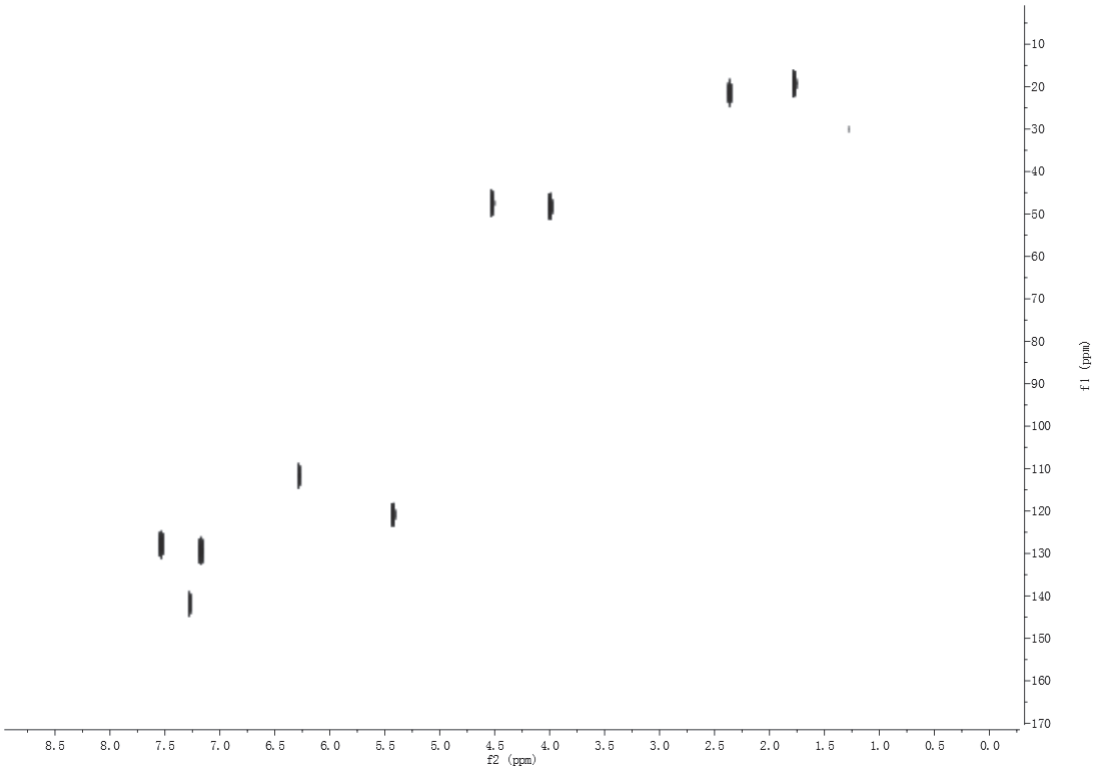

137.2
130.3
120.8
48.2
Me
19.4
143.7
O
21.5
Me
S
N
149.9
O
O
129.3
127.7
47.4
111.6
141.8
120.7

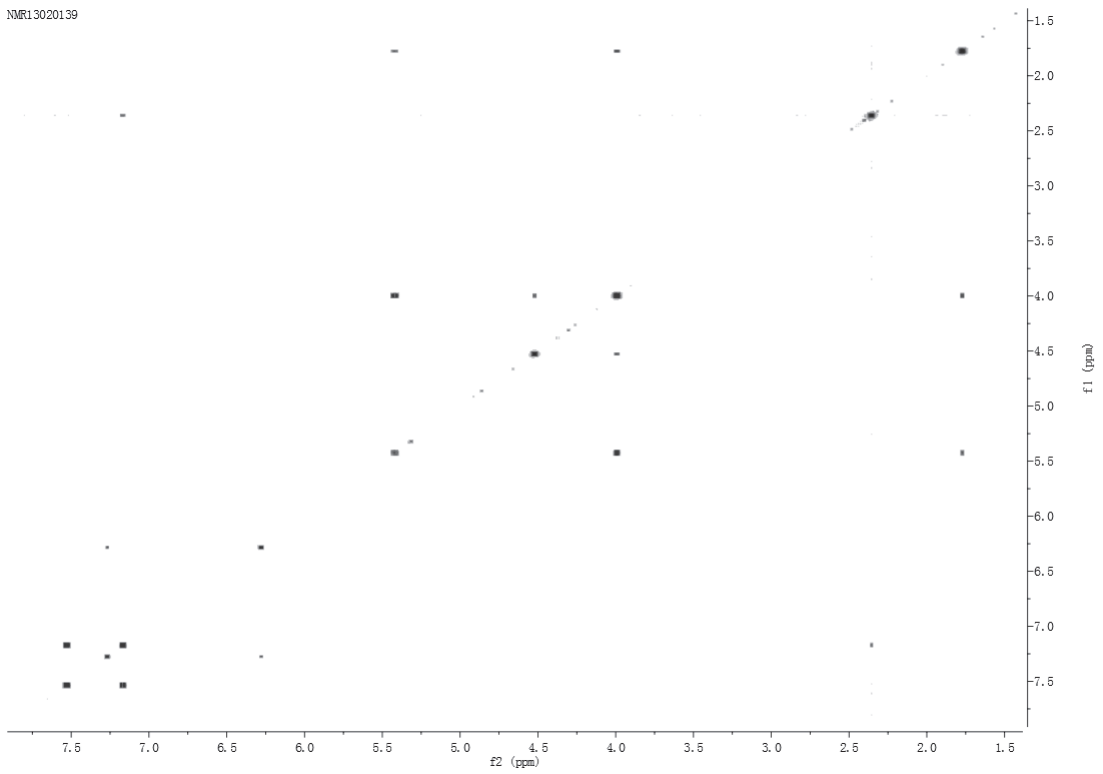

Intensity
f1 (ppm)

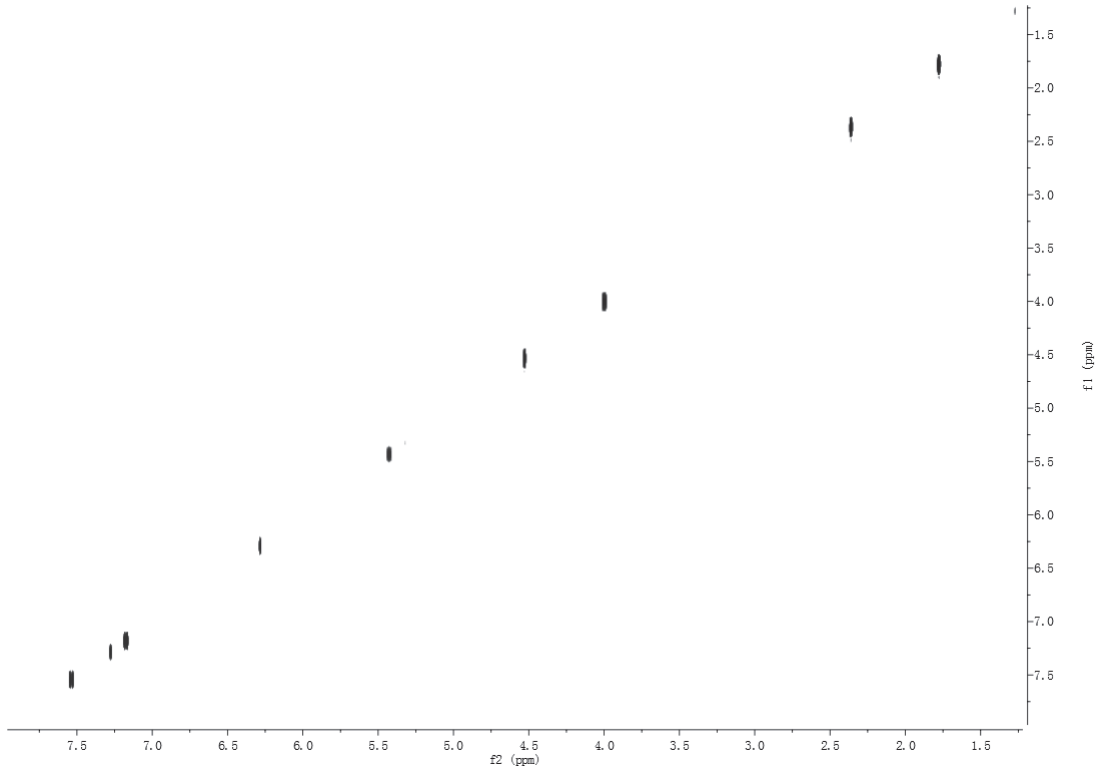

f1 (ppm)

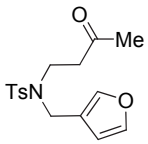

f1 (ppm)


f2 (ppm)
f1 (ppm)

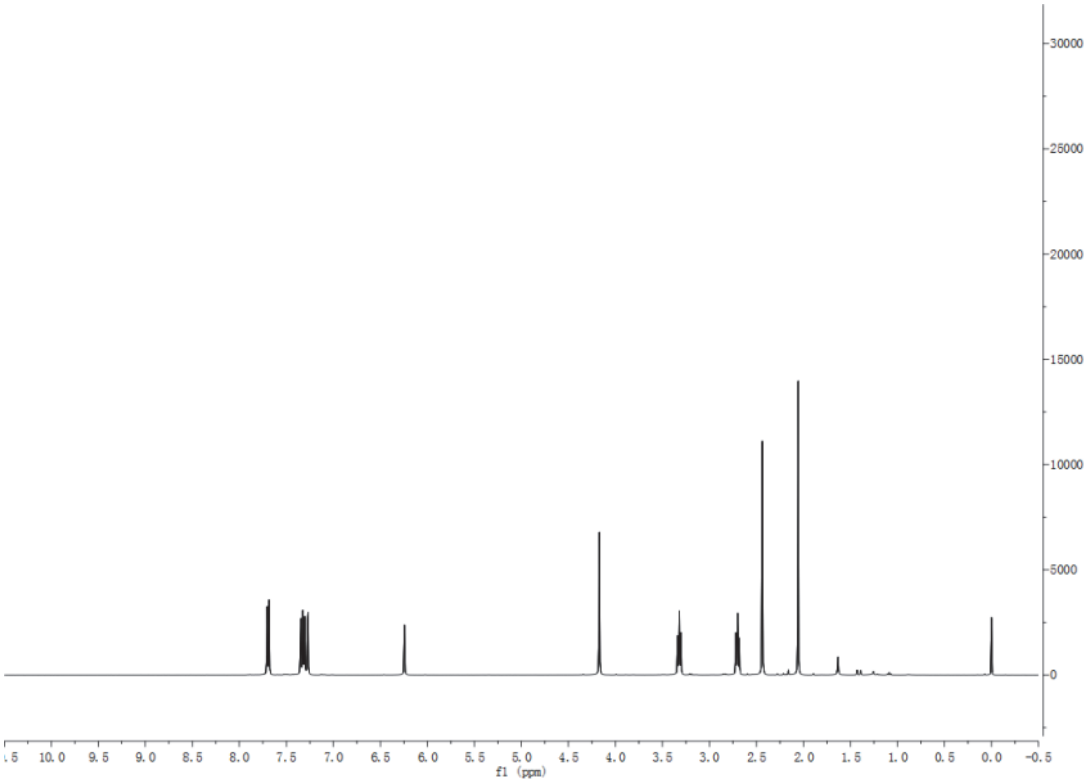

f2 (ppm)
f1 (ppm)

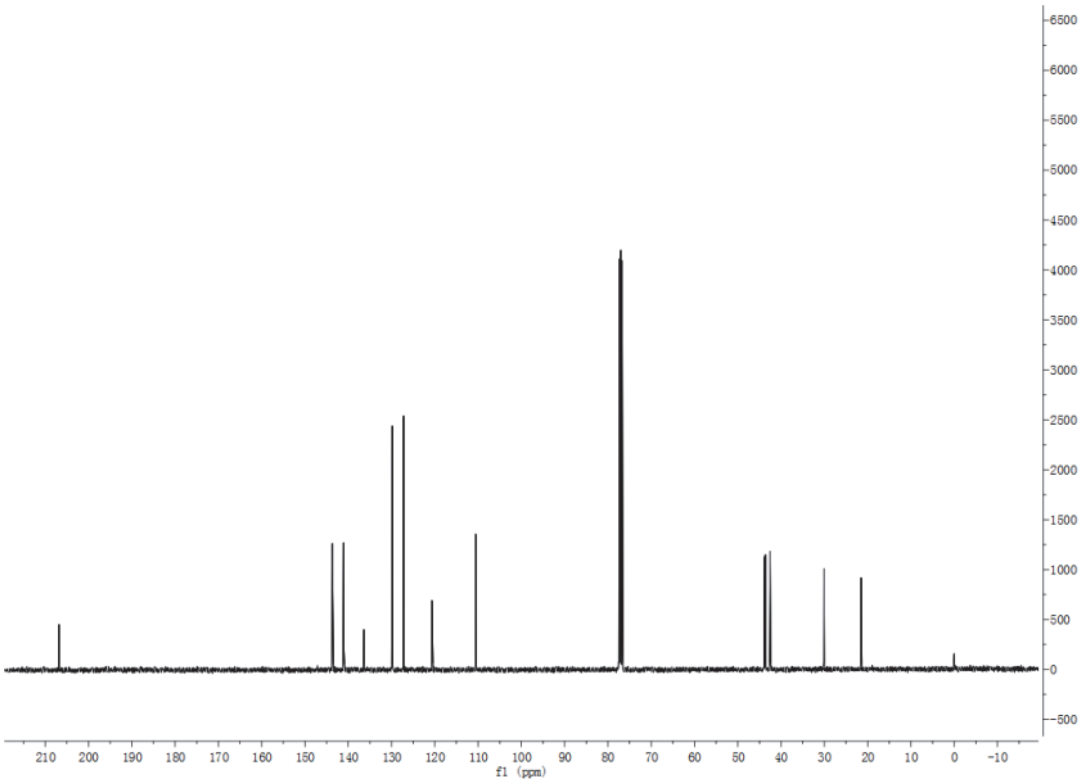

NMR13020139
f2 (ppm)
f1 (ppm)

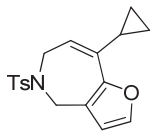

f2 (ppm)
f1 (ppm)


O
Me
TsN
O

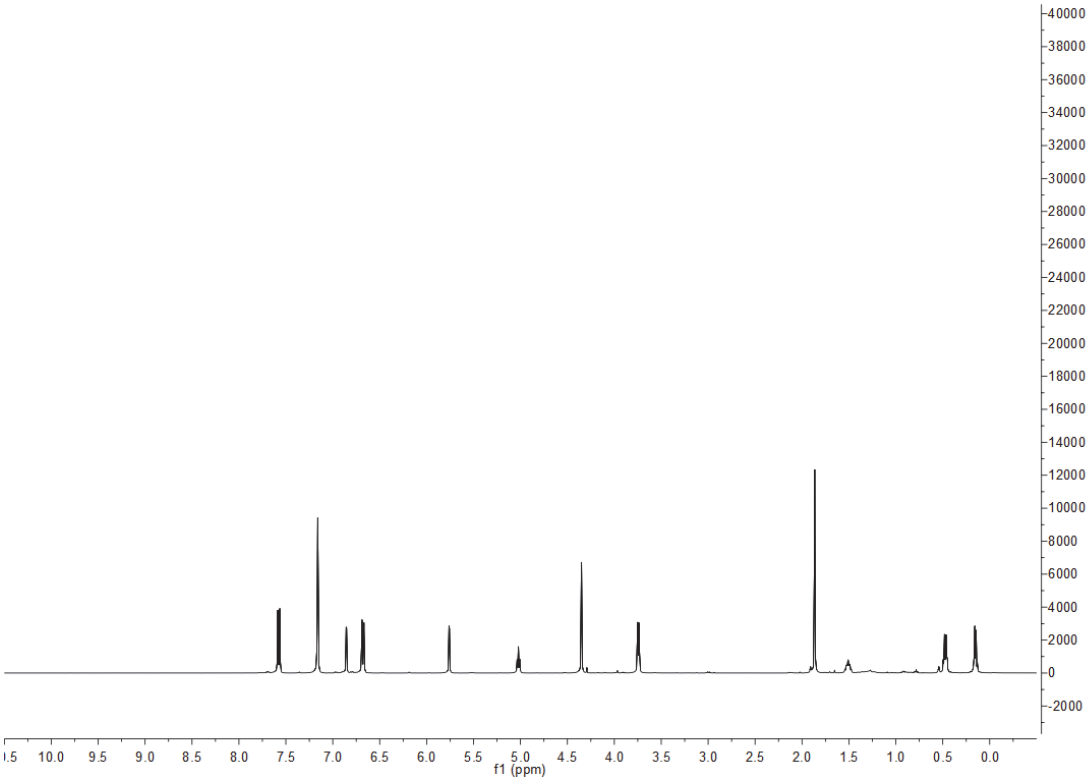
3a

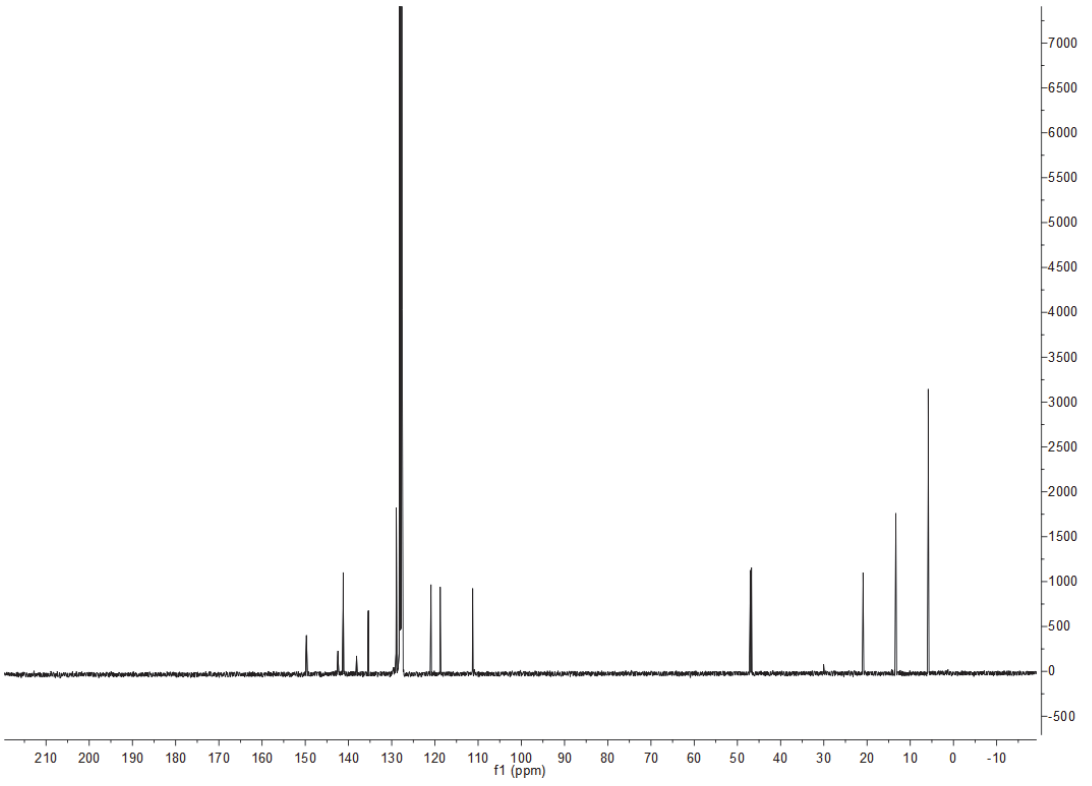

30000
25000
20000
15000
10000
5000
0
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

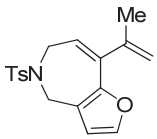

6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


TsN
O

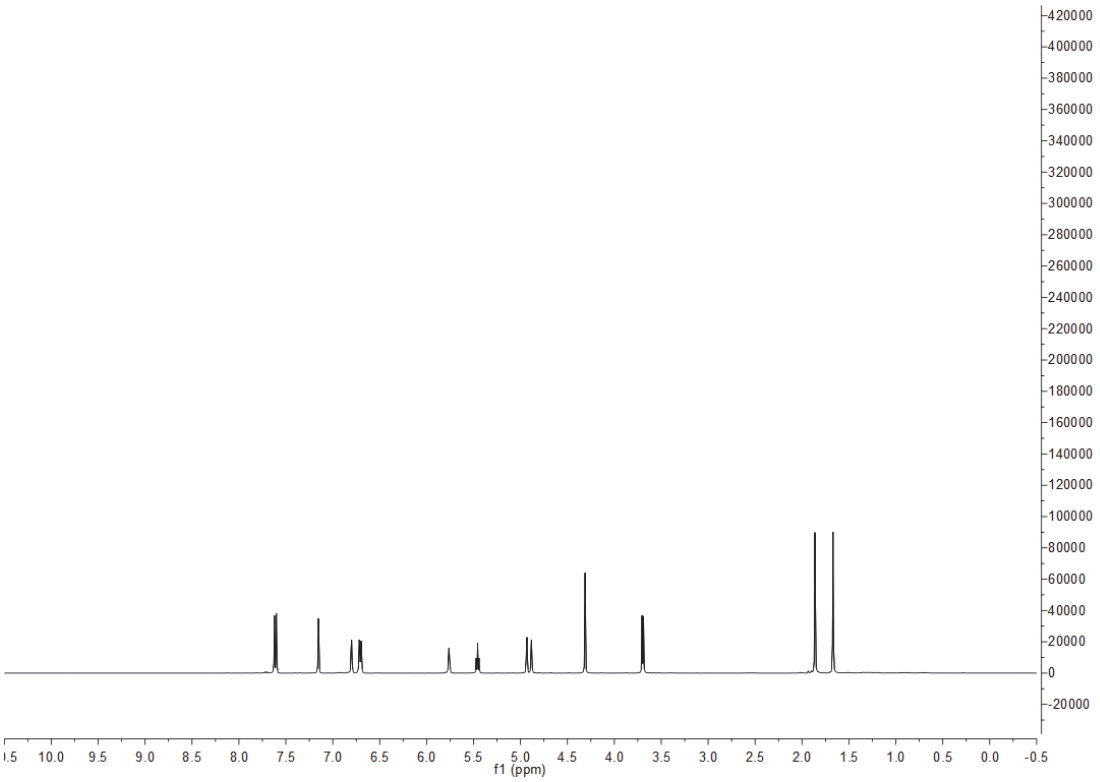
2b

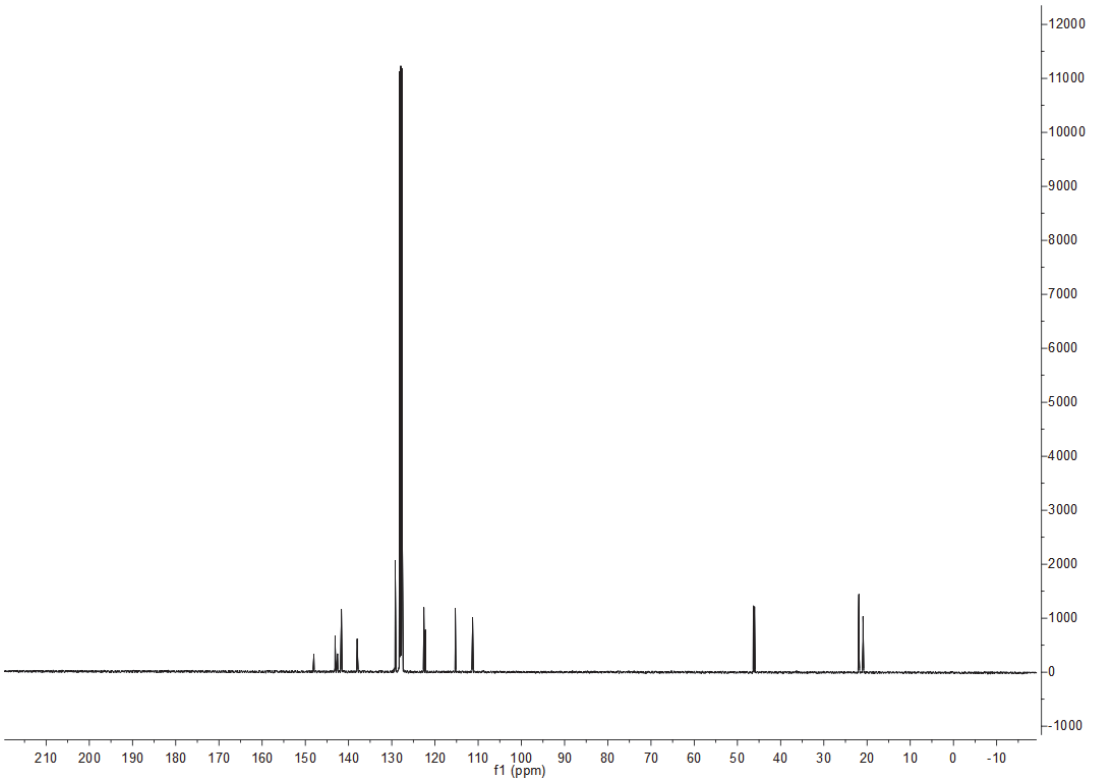

40000
38000
36000
34000
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

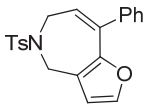

7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



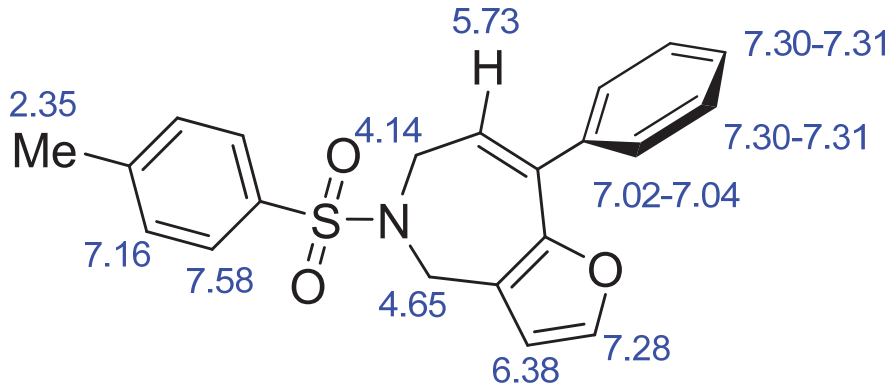
2c

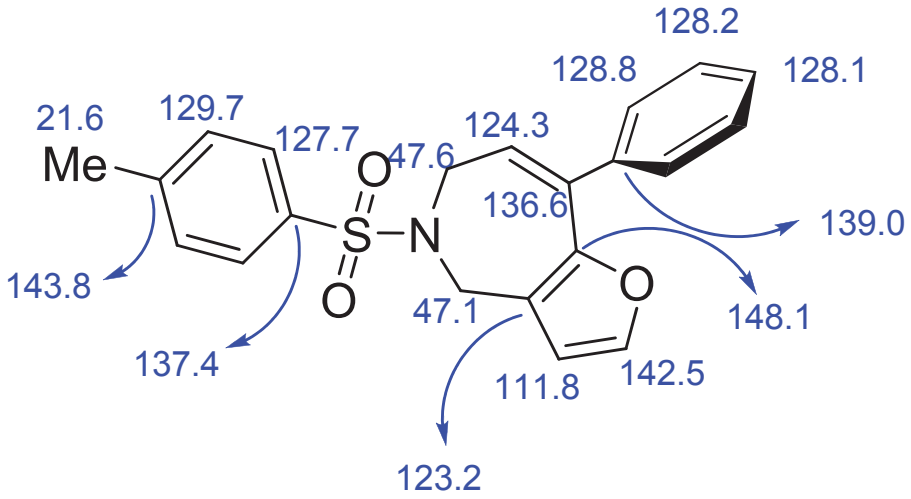


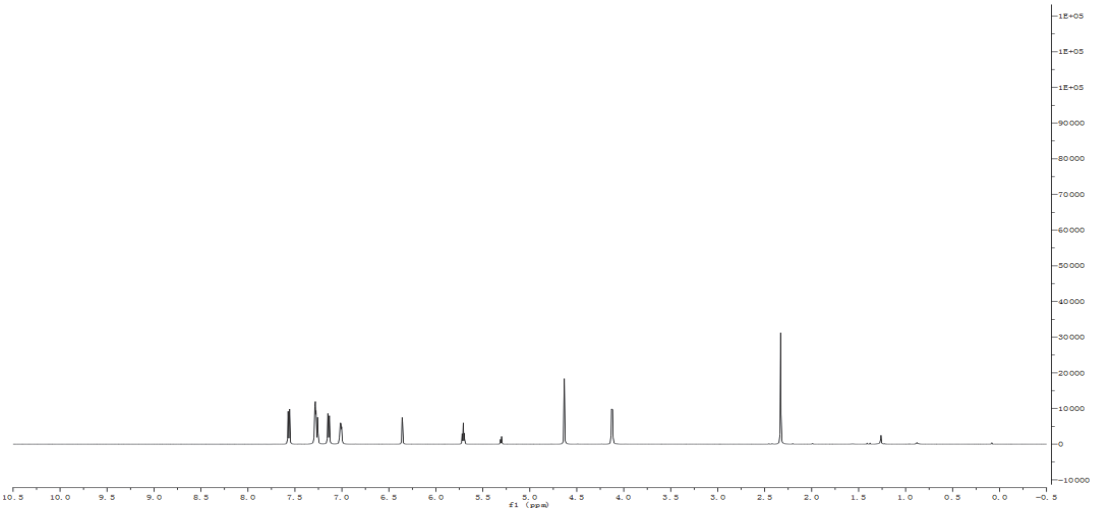


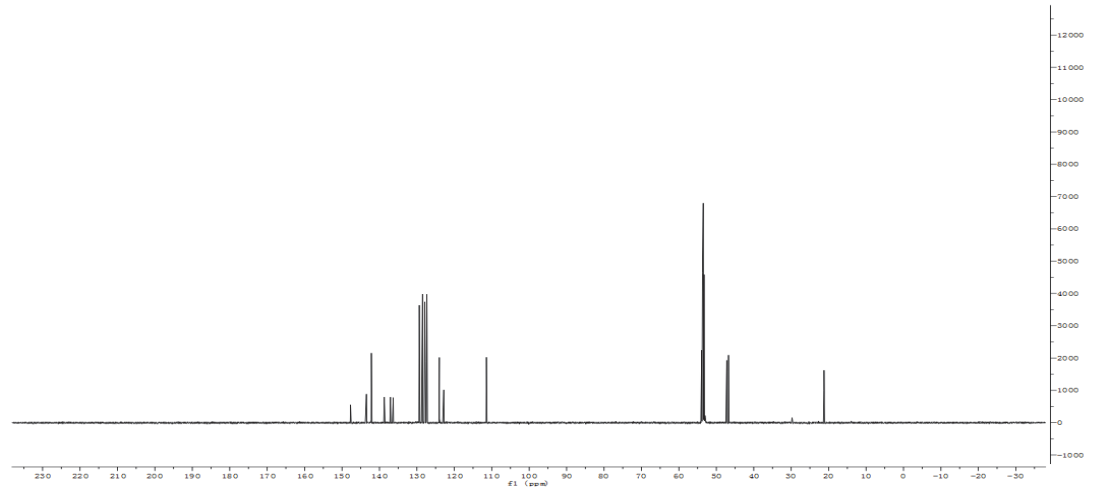

Ph
TsN
O

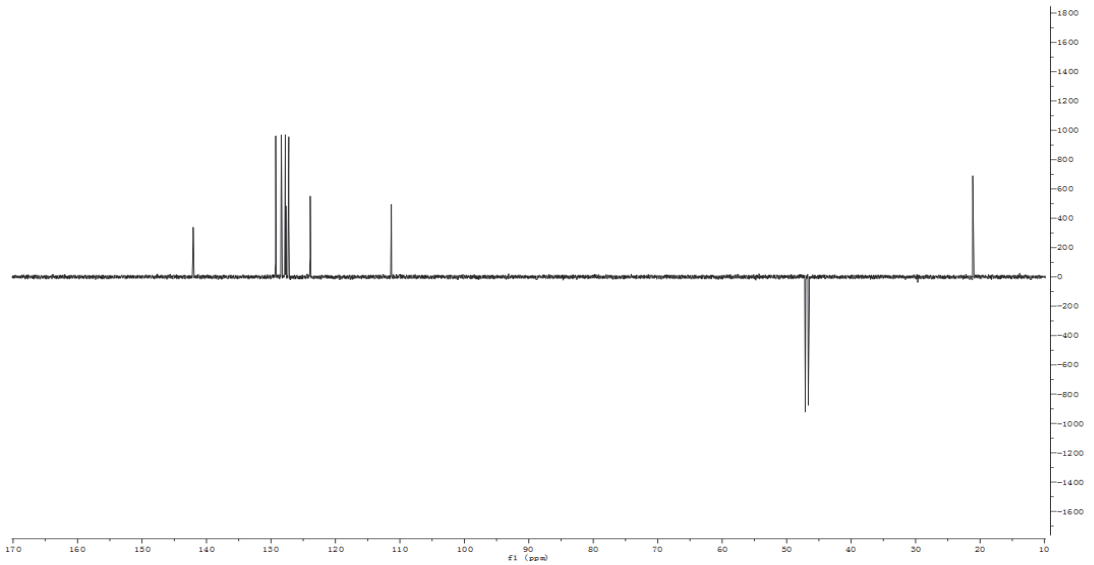
2d

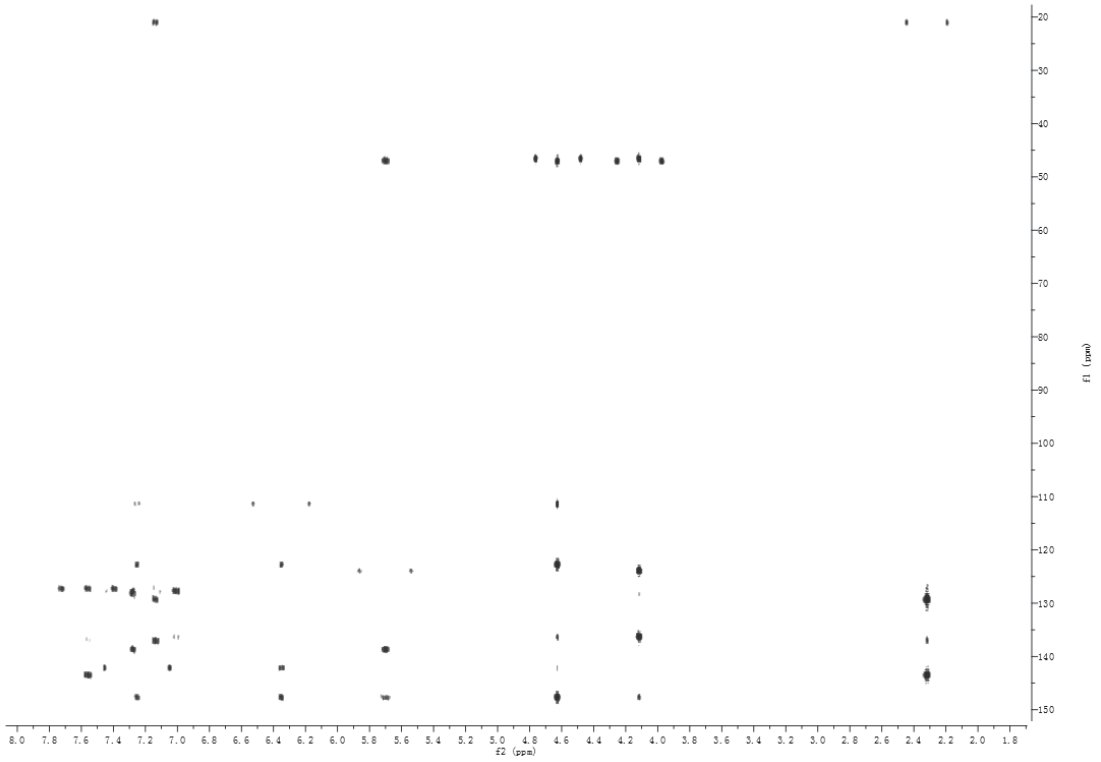

5.73
H
7.30-7.31
2.35
Me
4.14
O
7.30-7.31
7.02-7.04
S
N
7.16
7.58
O
O
4.65
7.28
6.38

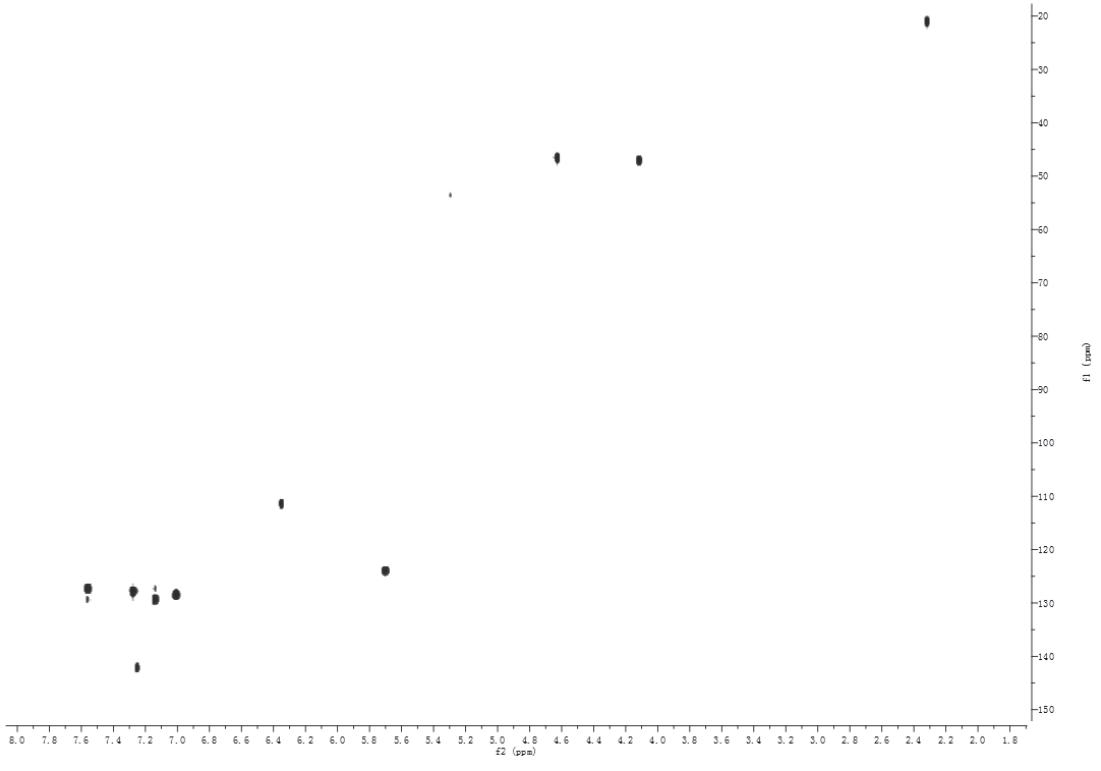

128.2
128.8
128.1
21.6
129.7
127.7
124.3
Me
47.6
O
136.6
139.0
S
N
143.8
O
47.1
O
148.1
137.4
111.8
142.5
123.2

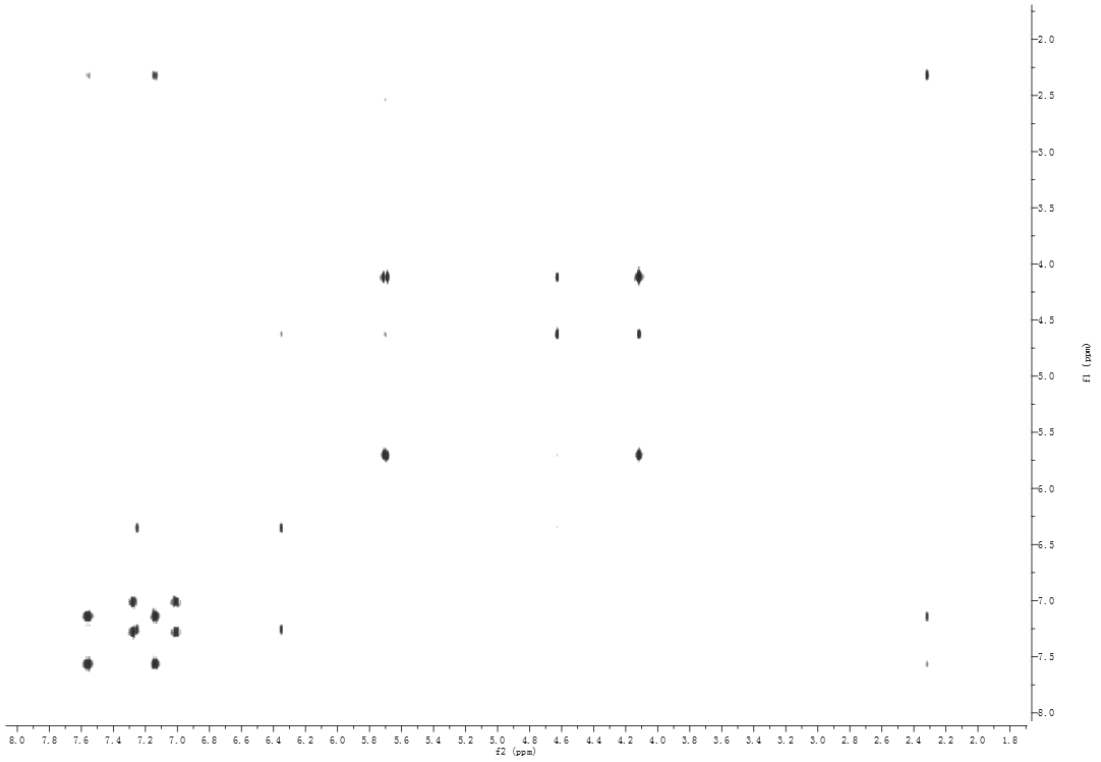


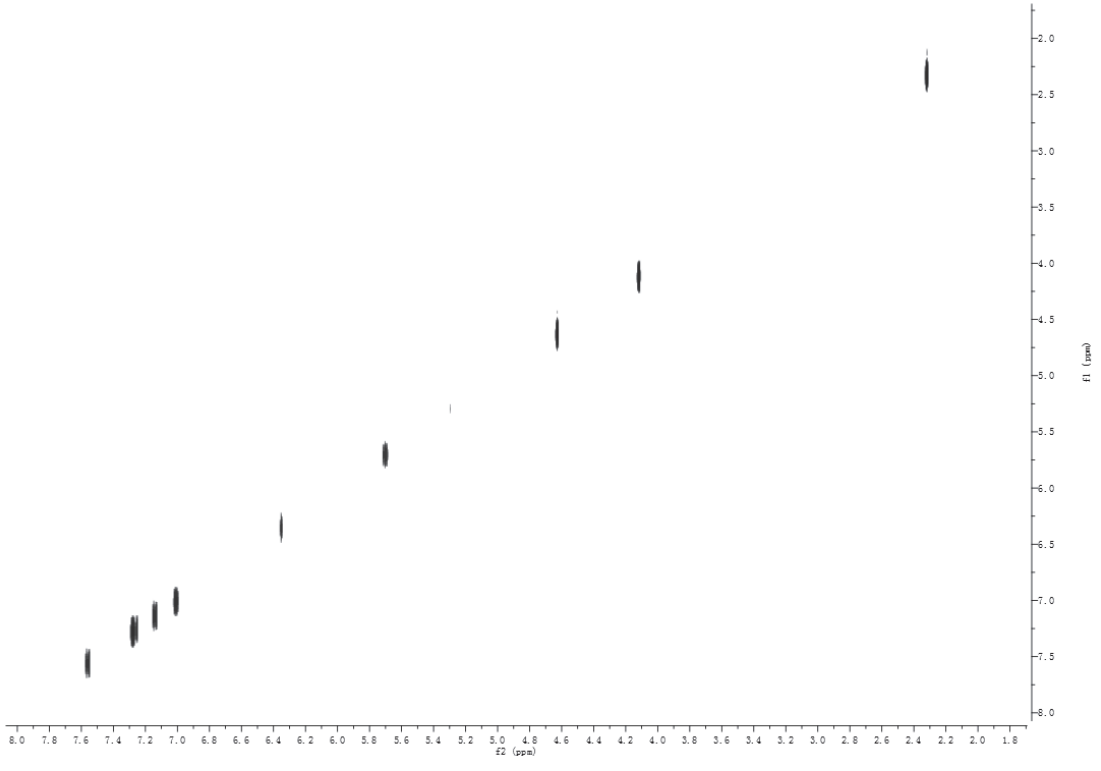


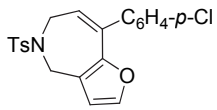



f1 (ppm)
f2 (ppm)

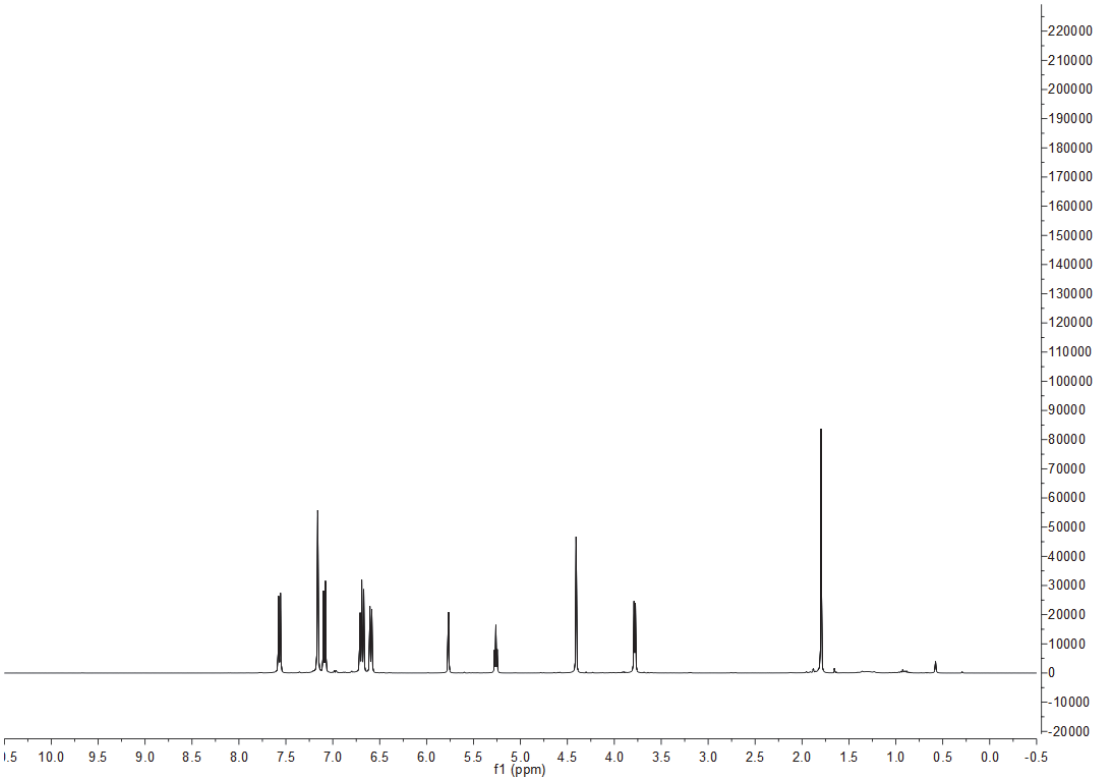

f1 (ppm)
f2 (ppm)

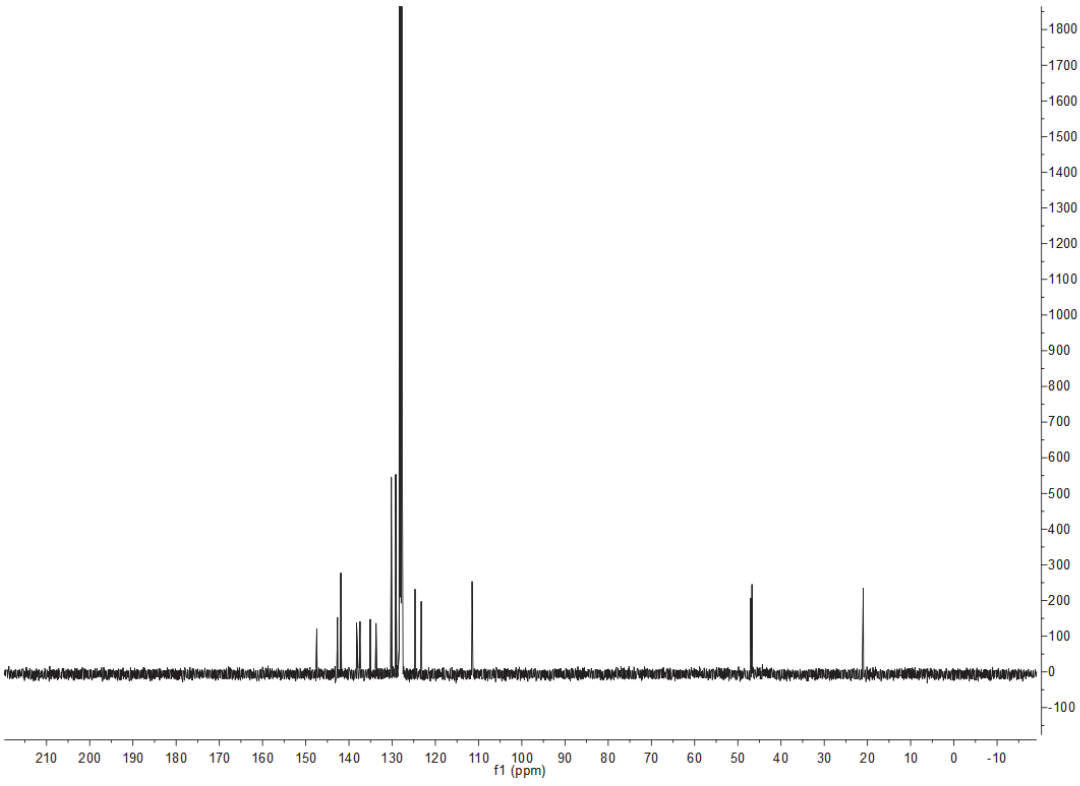

f2 (ppm)
f1 (ppm)

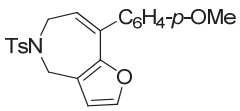

f2 (ppm)
f1 (ppm)



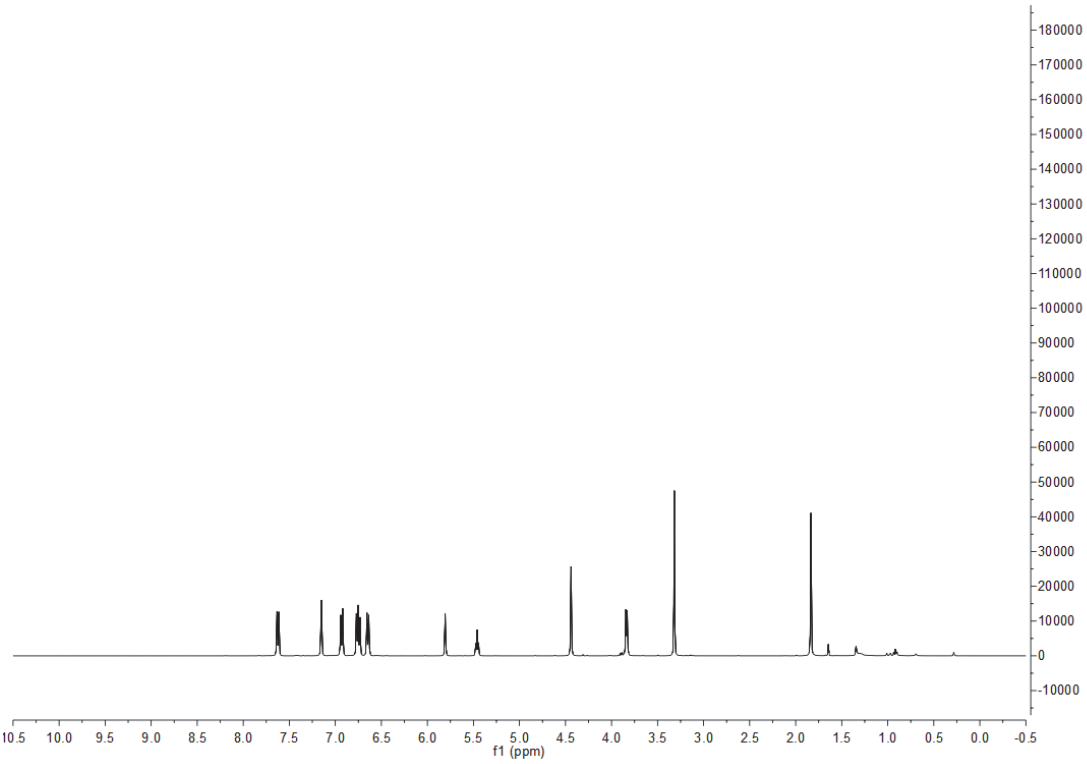
2e

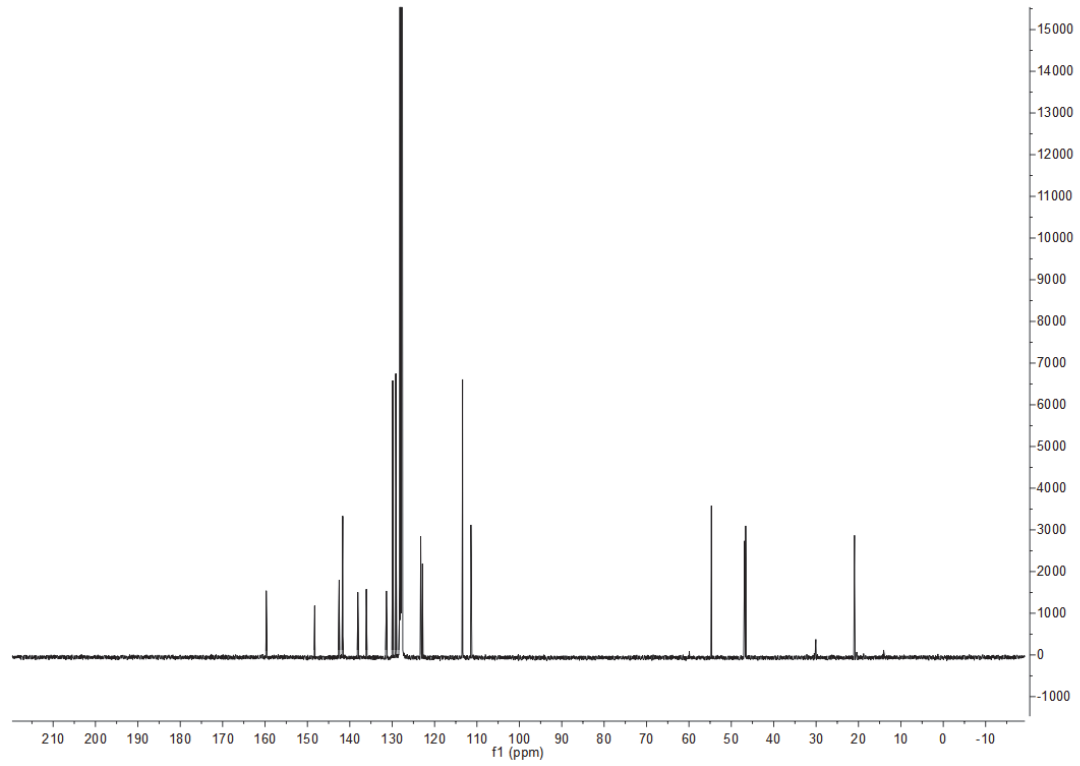


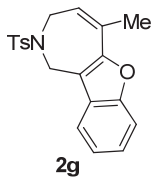




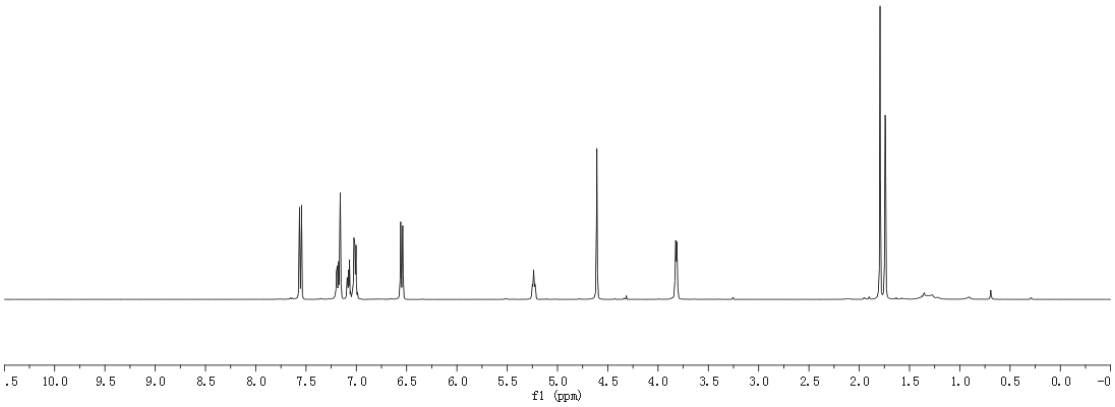
2f

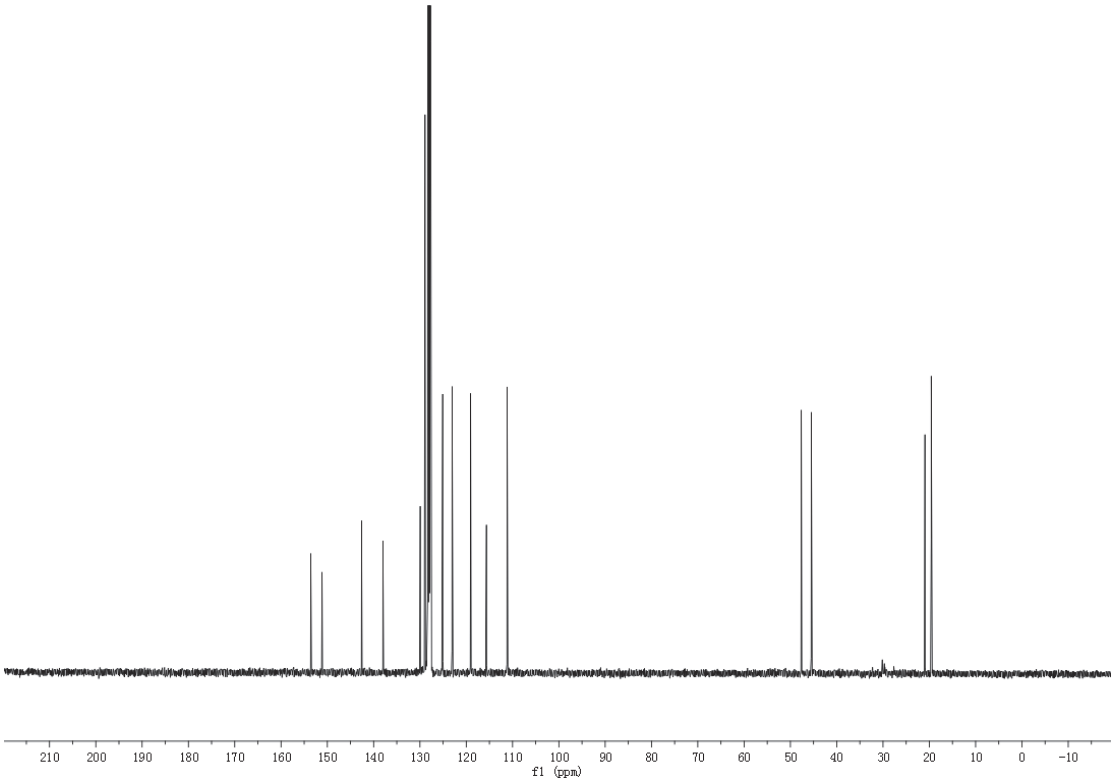


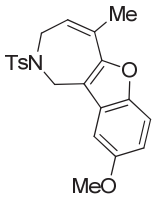



Me
TsN
O

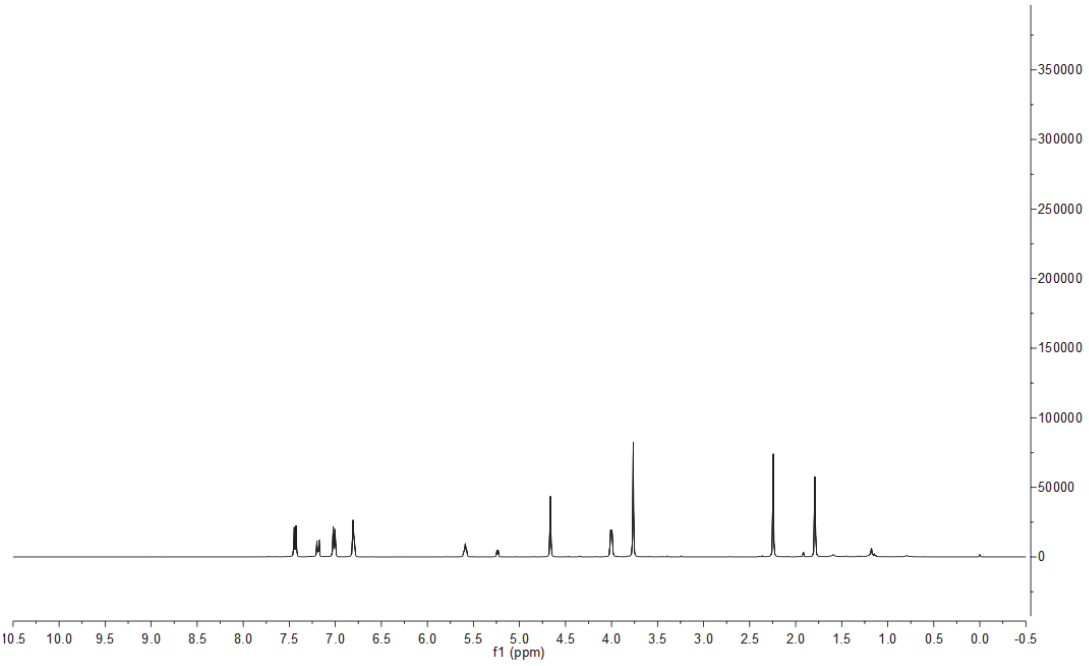
2g

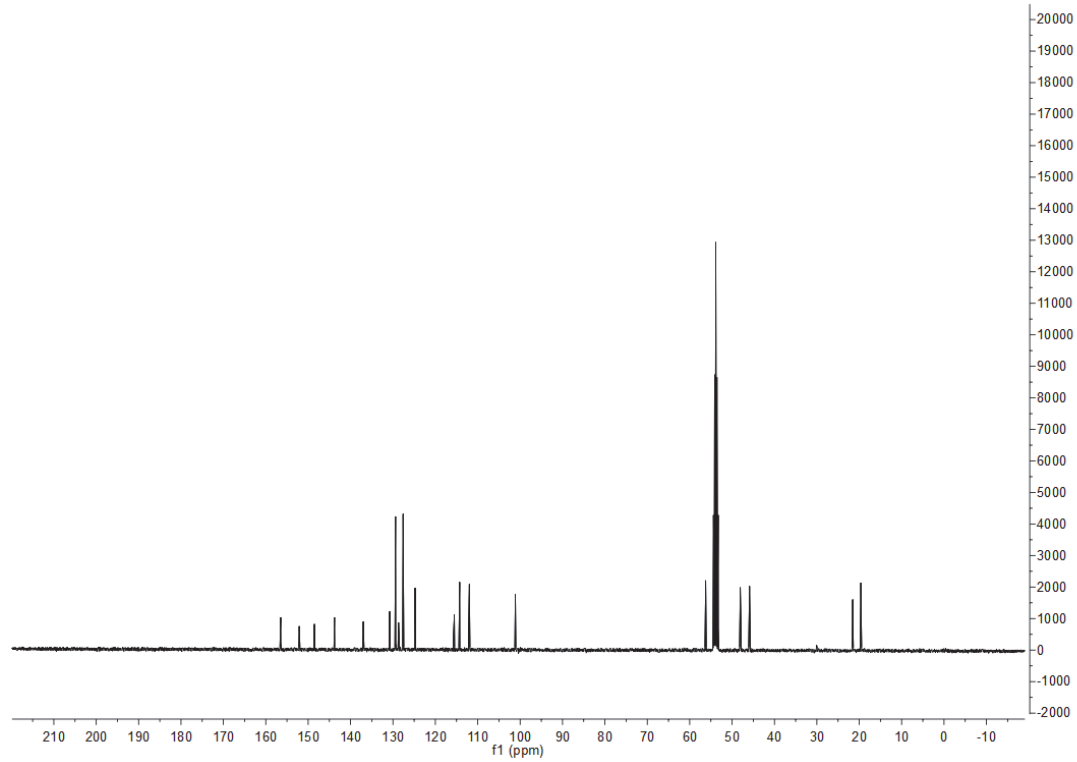

.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)

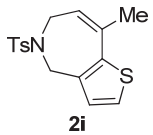

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


Me
TsN
O
MeO

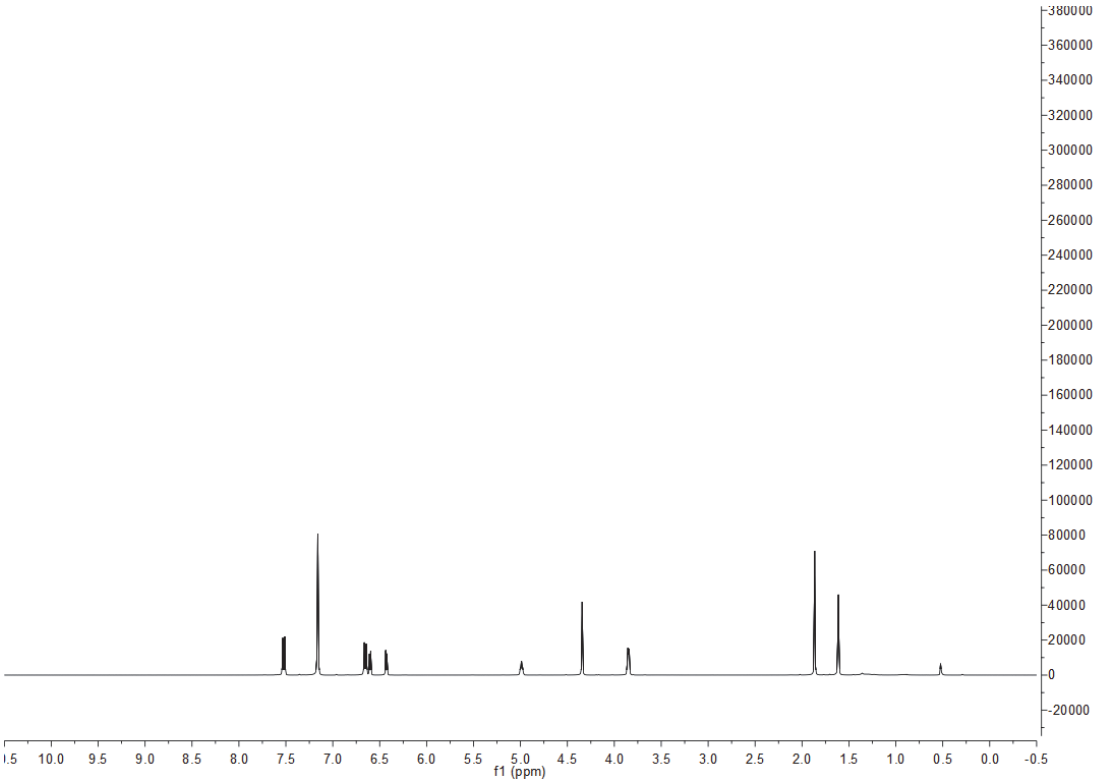
2h

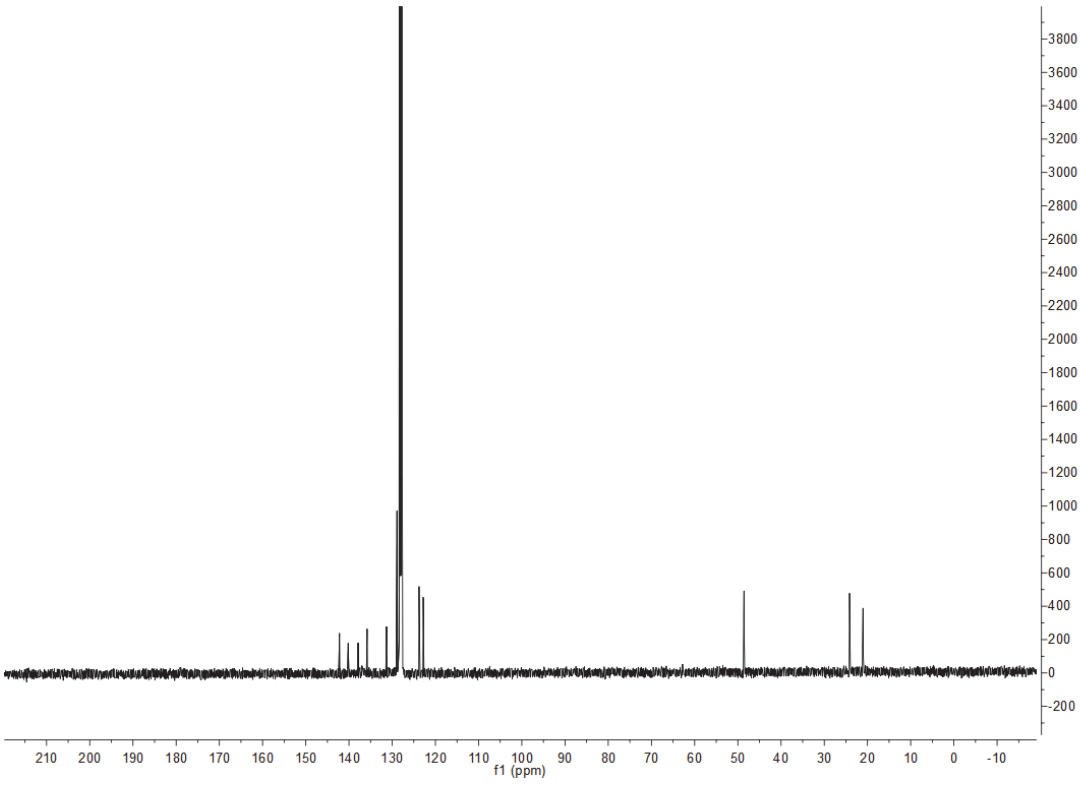

350000
300000
250000
200000
150000
100000
50000
0
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

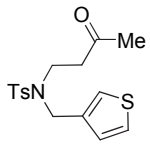

20000
19000
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



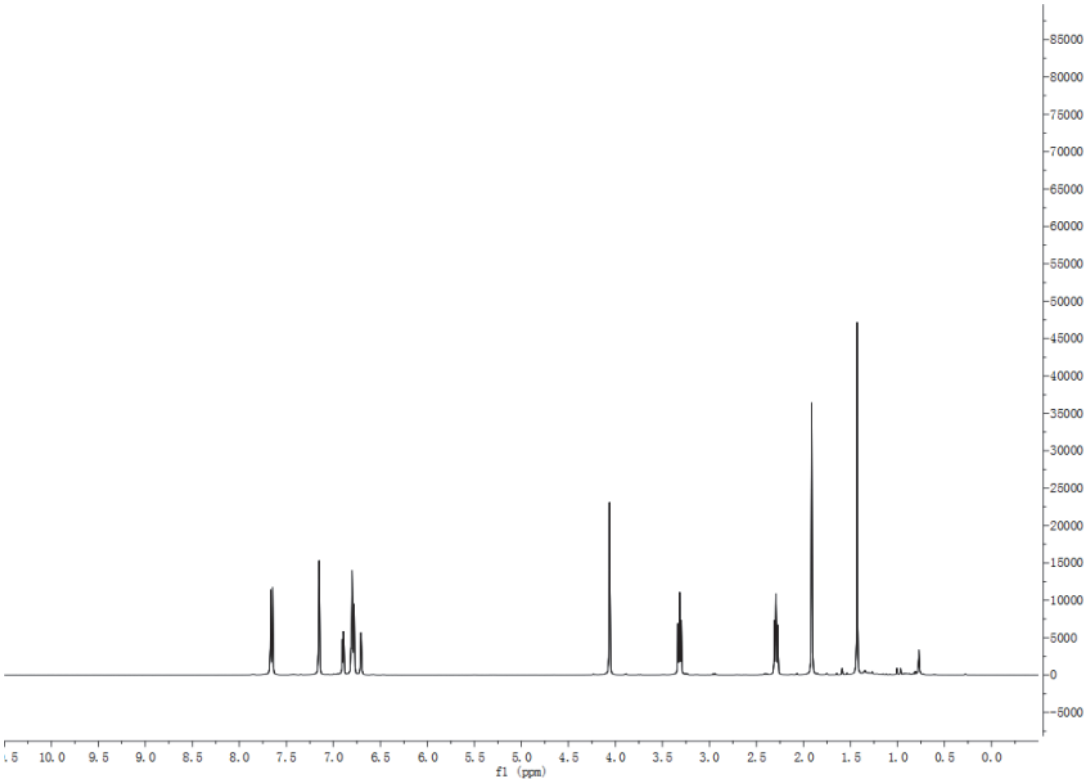
2i

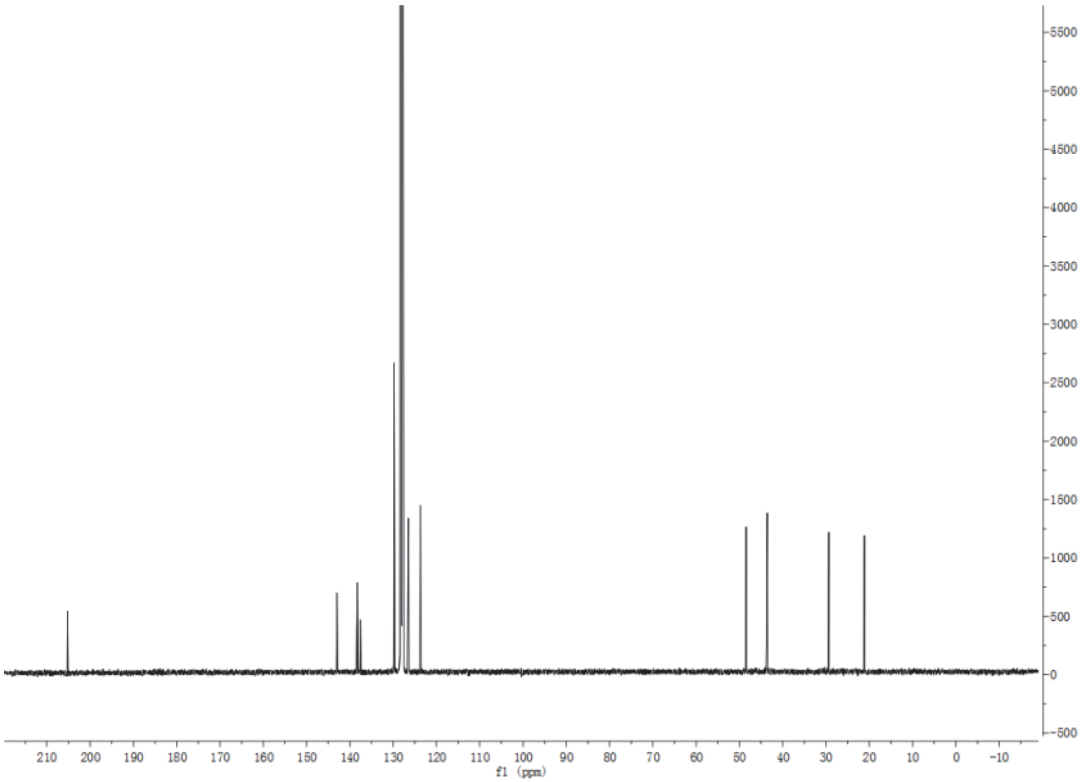


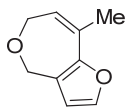




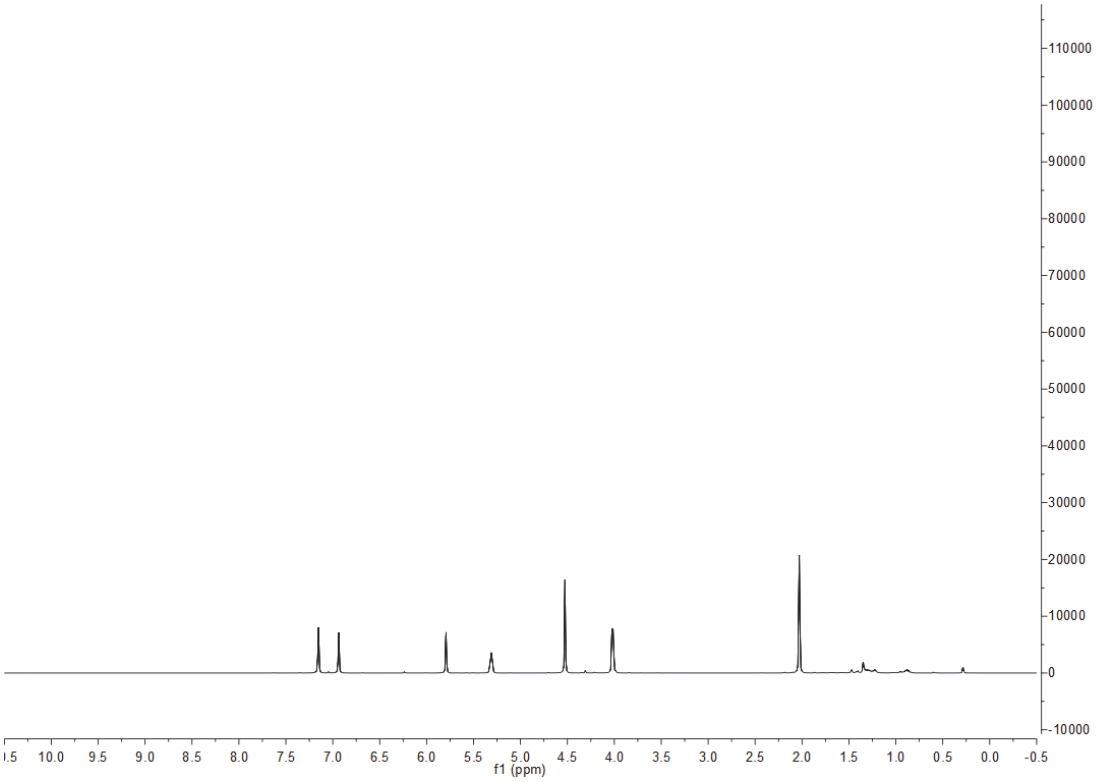
3i

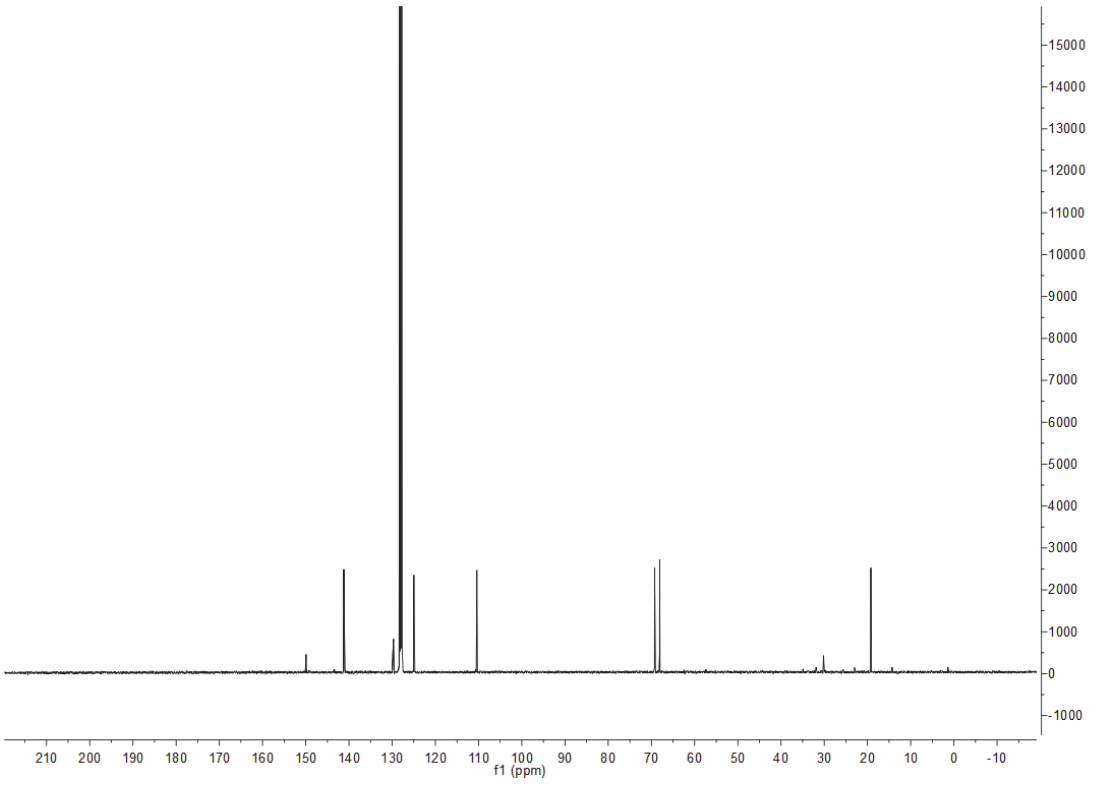


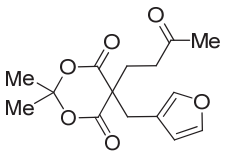



Me
O
O

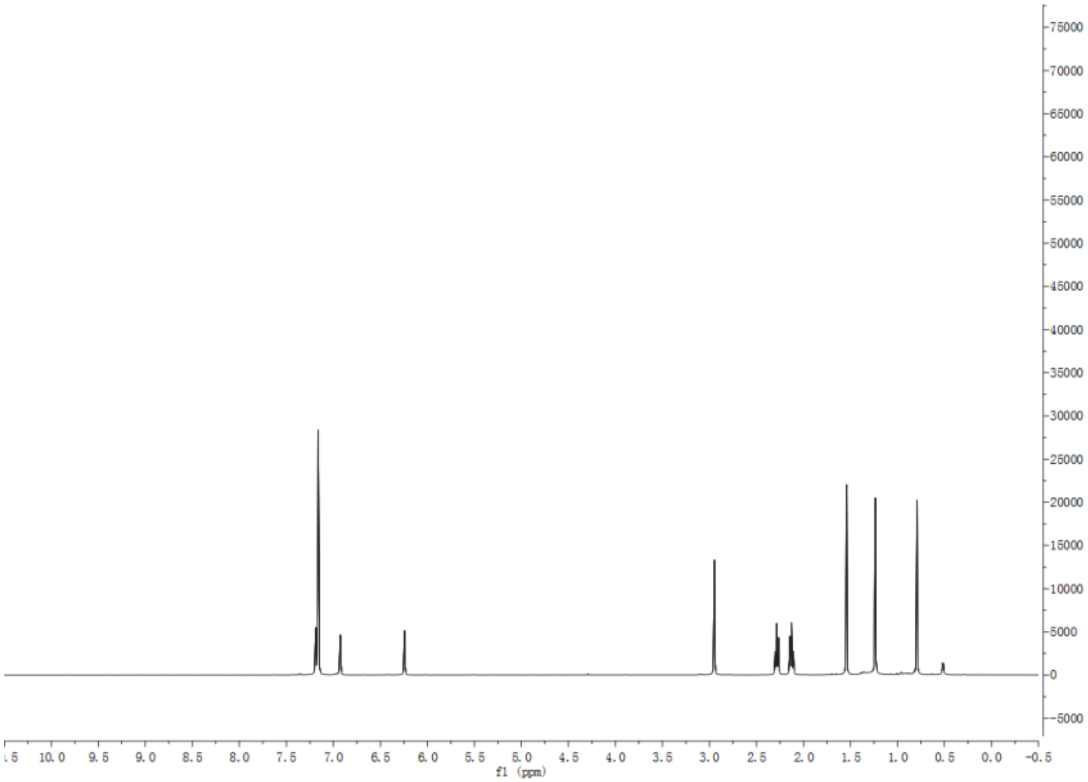
2j

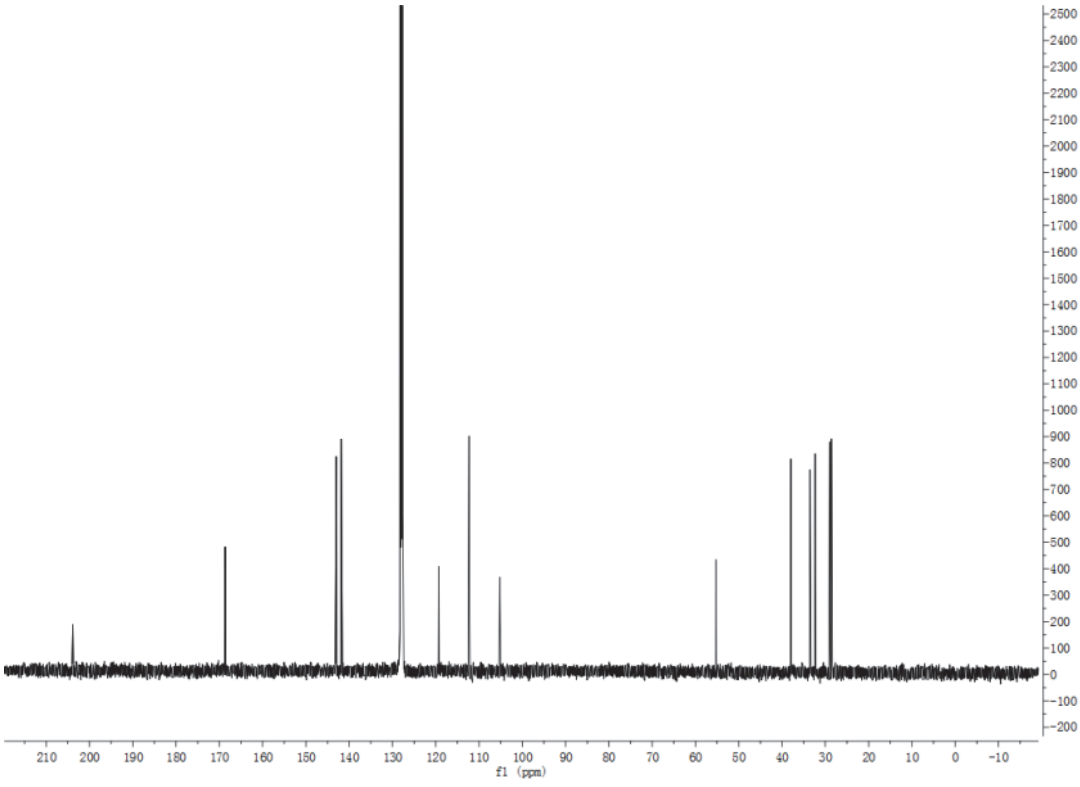

110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

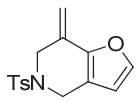

15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



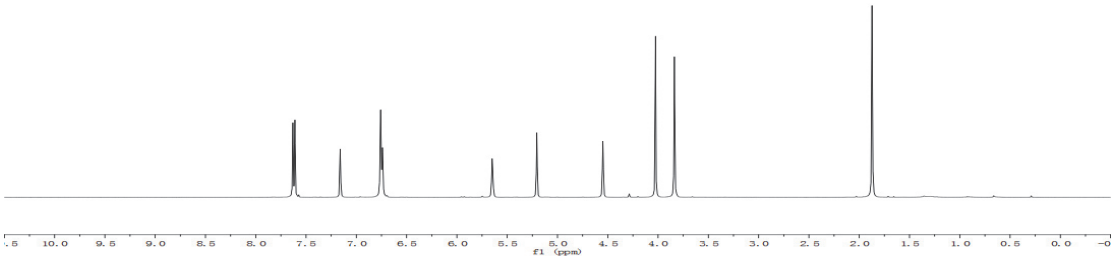
3l

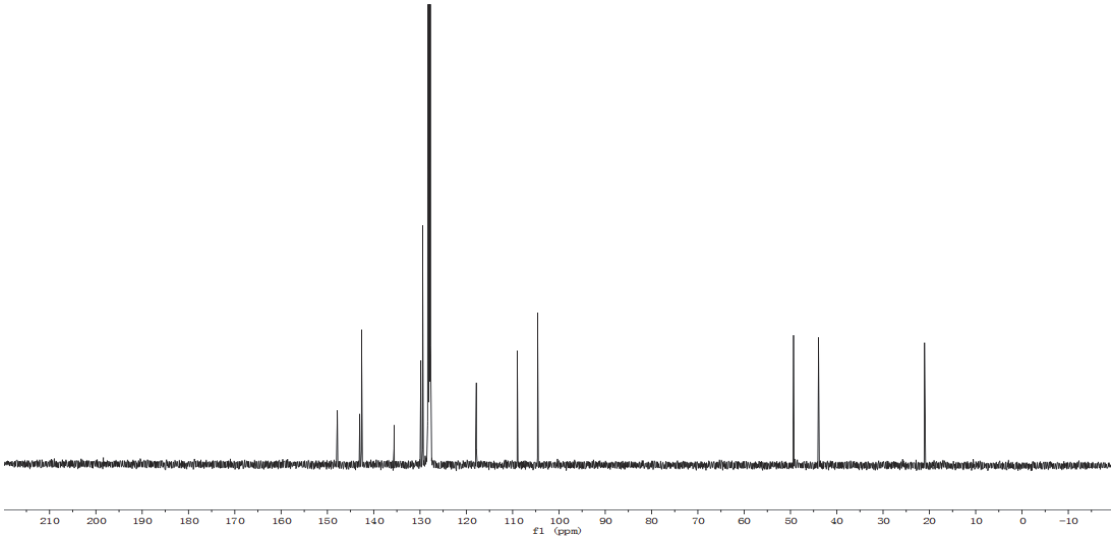


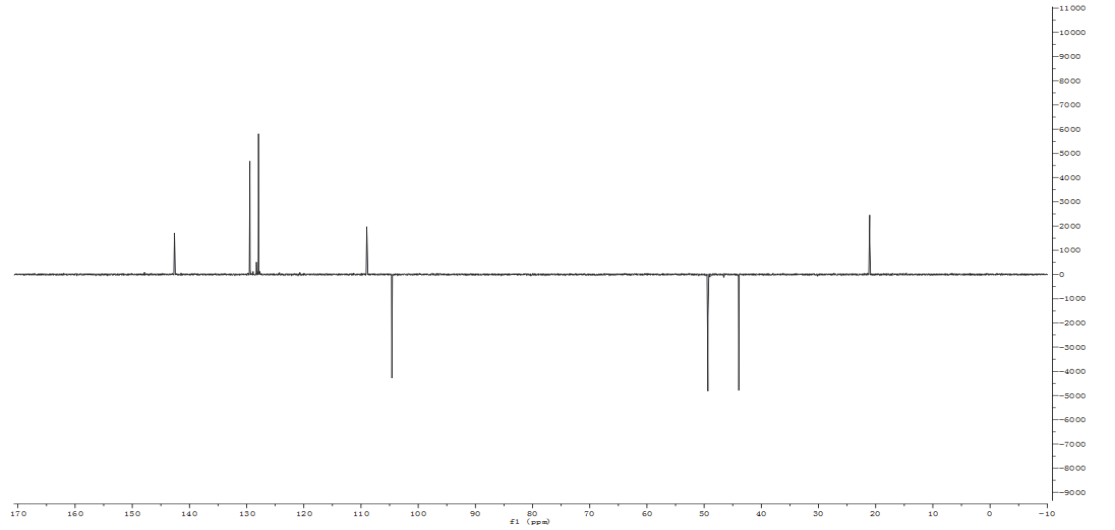


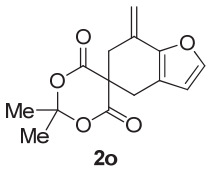


2m

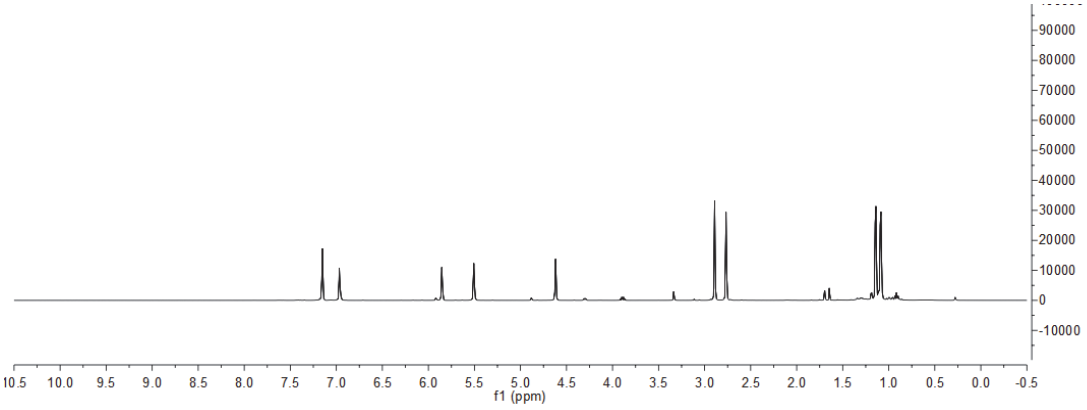


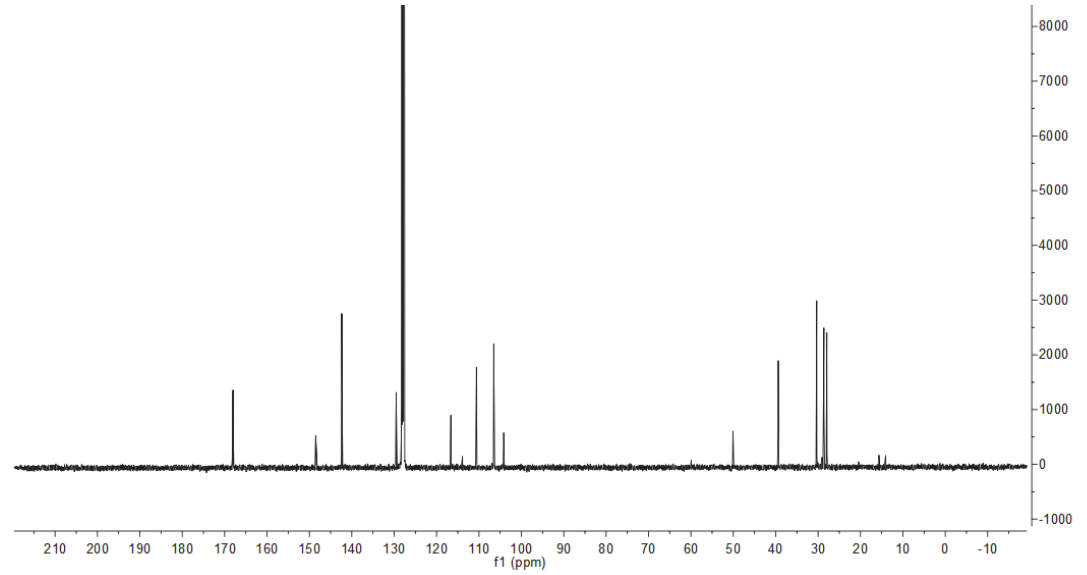


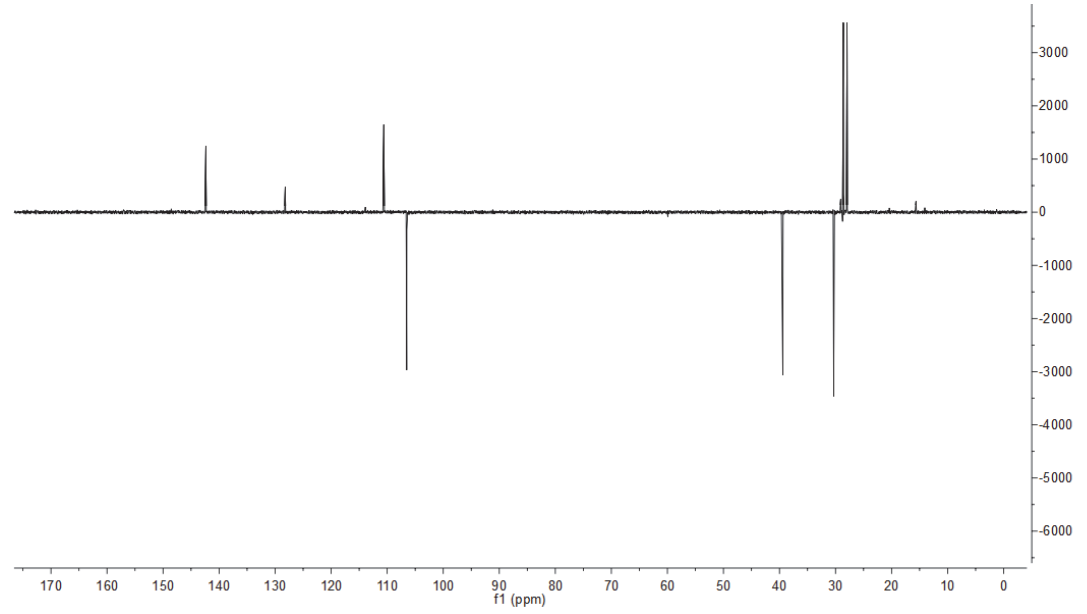


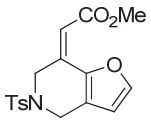


2o

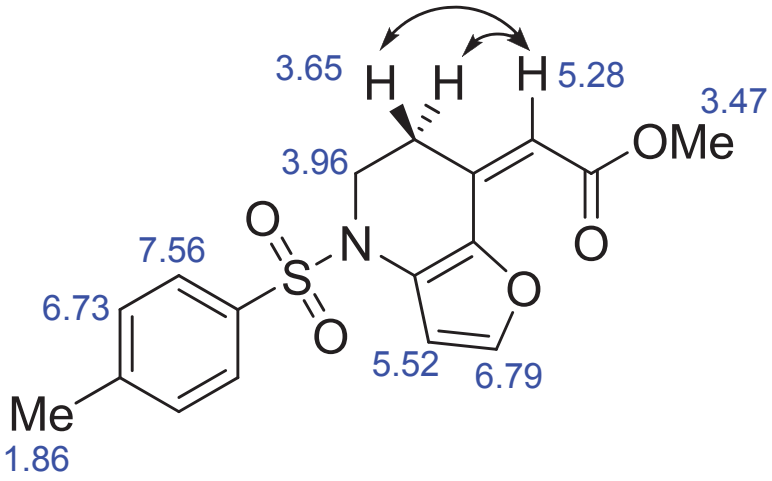


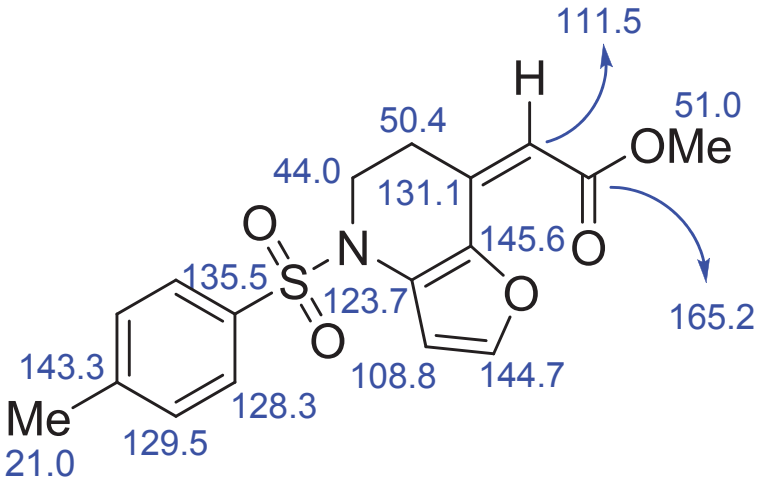


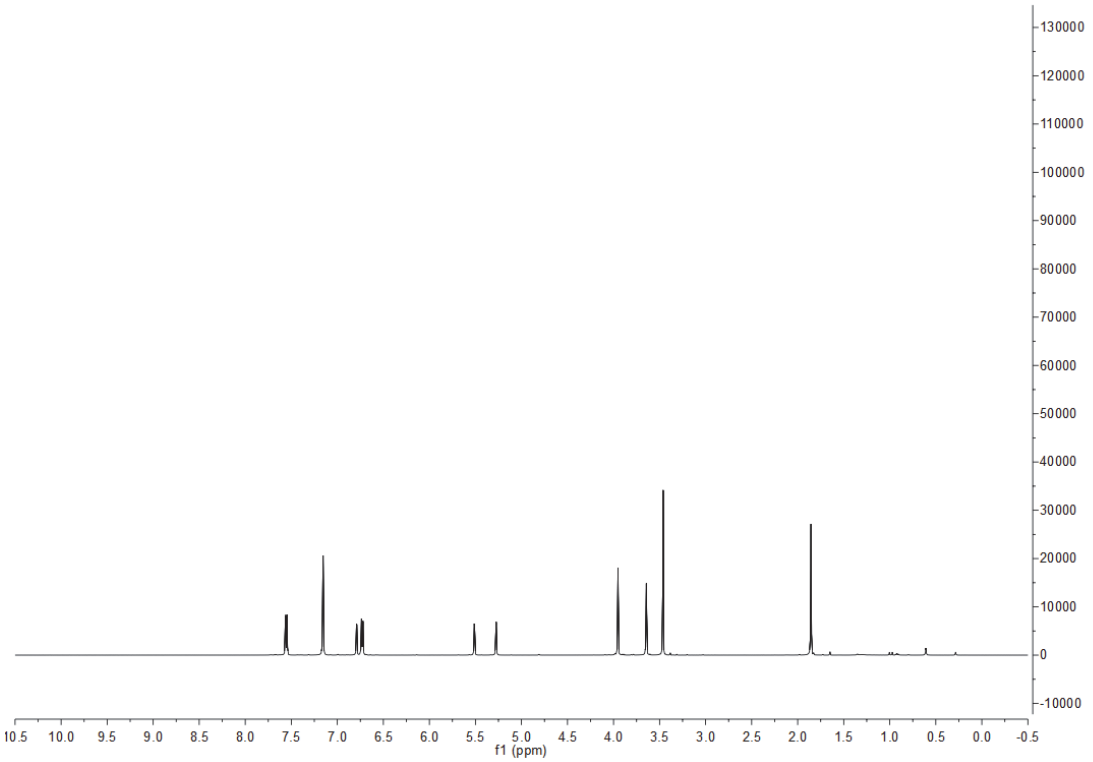


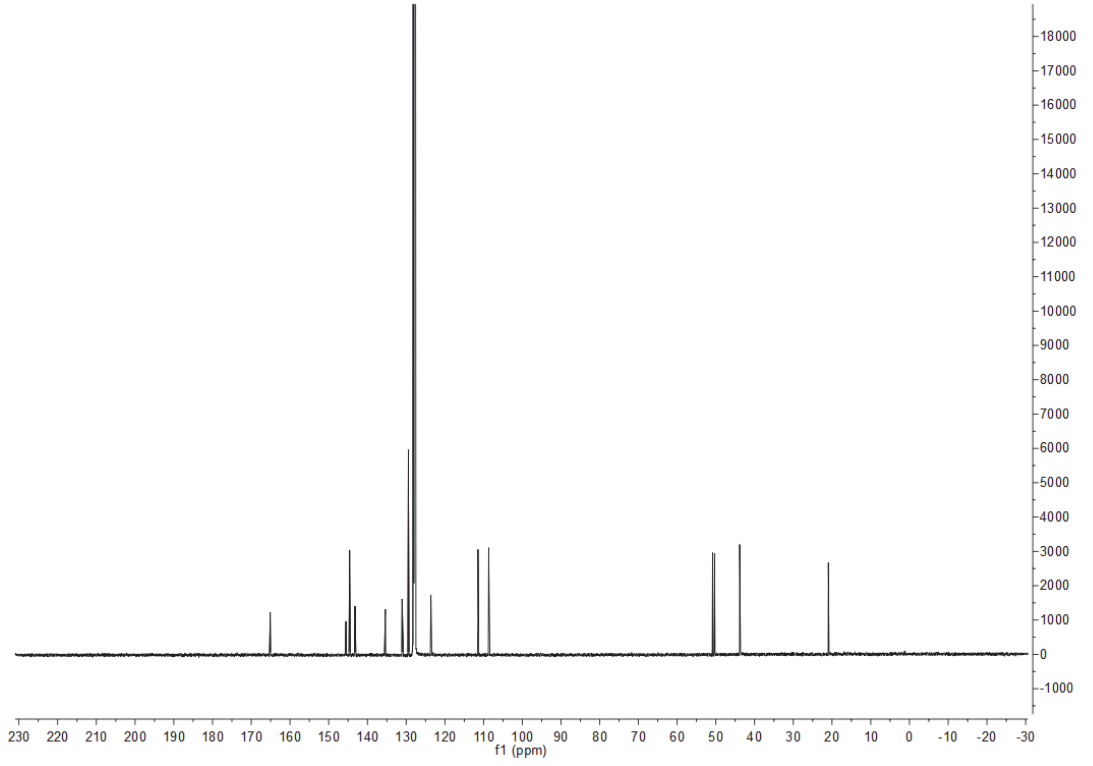

CO2Me
O
TsN

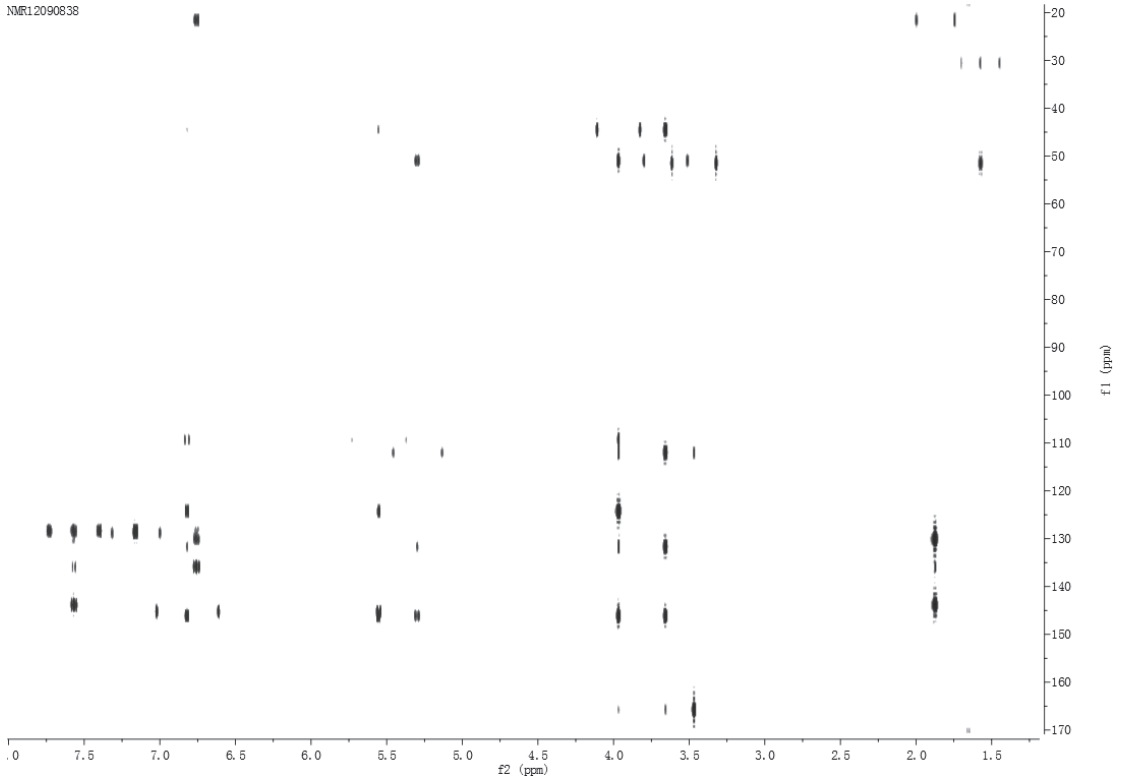
2p

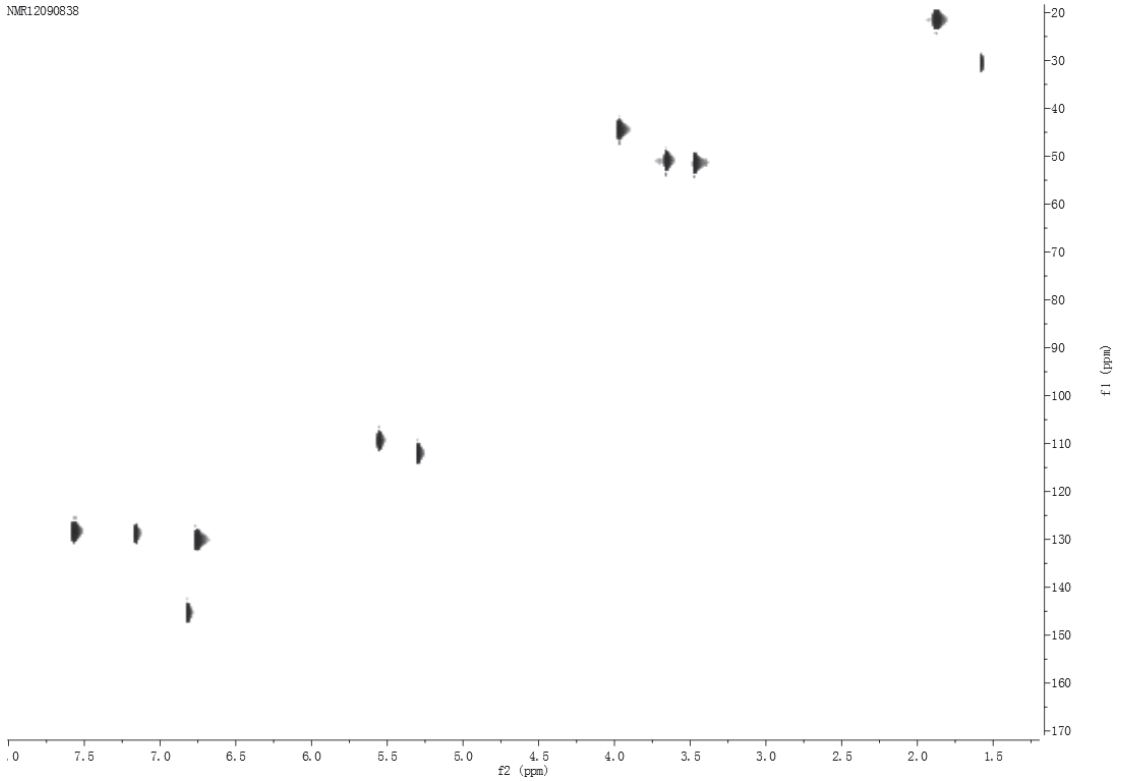

3.65
H
H
H
5.28
3.47
OMe
3.96
O
N
O
7.56
S
O
6.73
O
5.52
6.79
Me
1.86

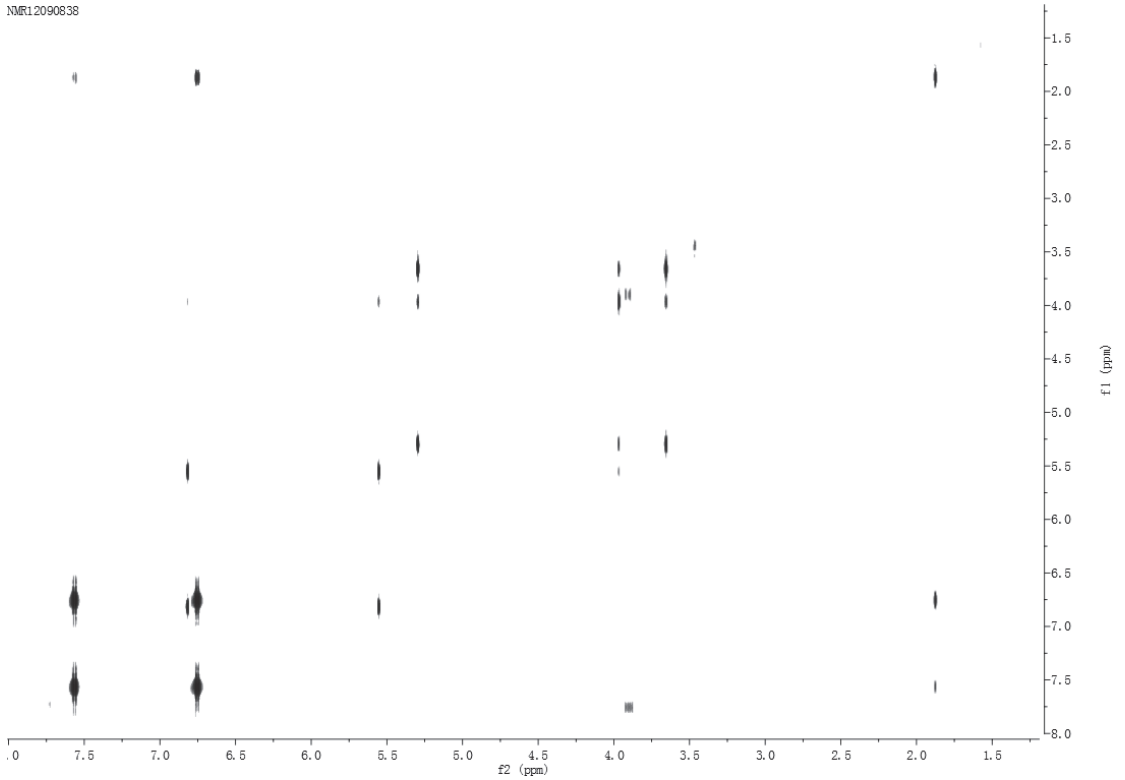

111.5
H
51.0
50.4
OMe
44.0
131.1
O
N
145.6
O
135.5
S
123.7
O
165.2
143.3
O
108.8
144.7
128.3
Me
129.5
21.0

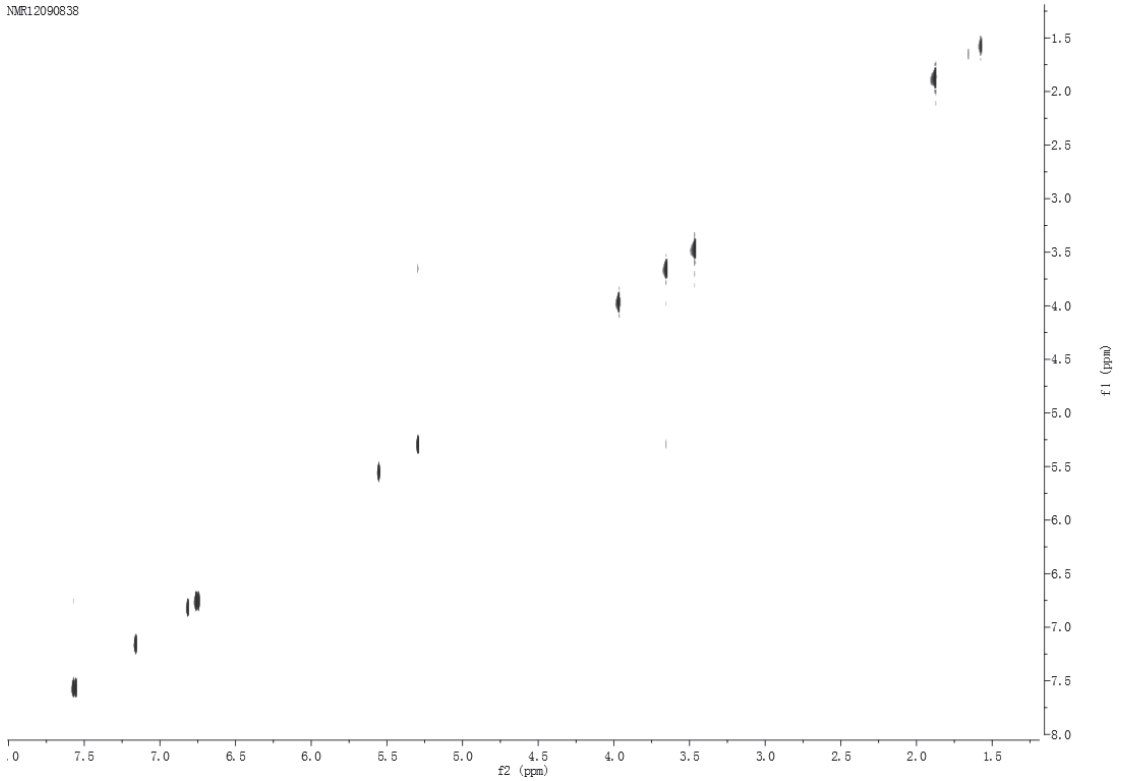

130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

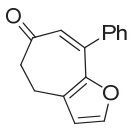

18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30
f1 (ppm)


NMR12090838
f2 (ppm)
f1 (ppm)

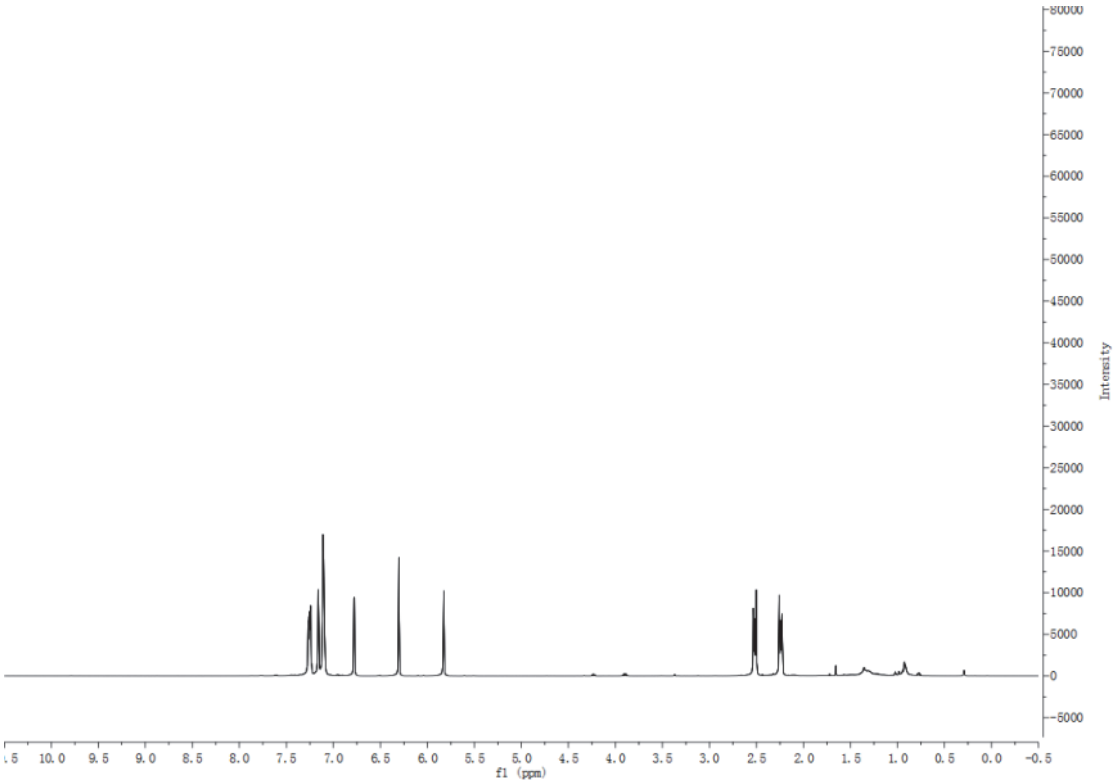

NMR12090838
f2 (ppm)
f1 (ppm)

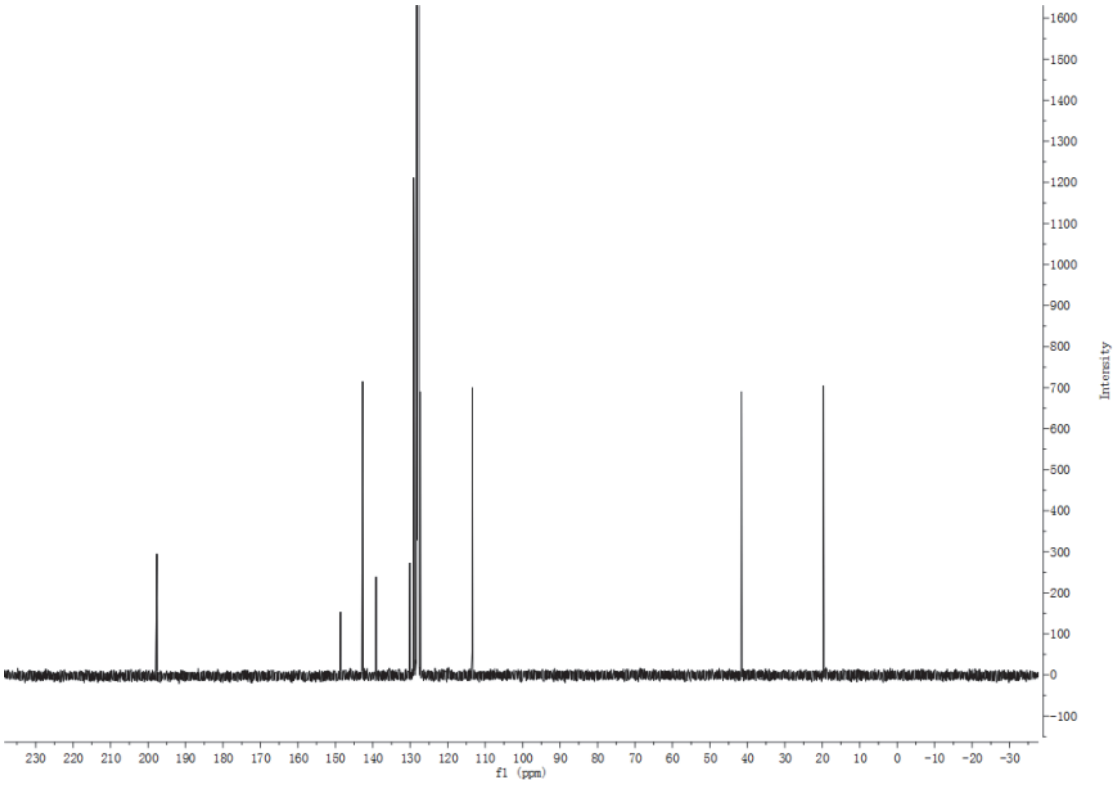

NMR12090838
f2 (ppm)
f1 (ppm)

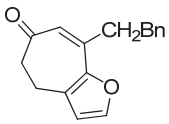

NMR12090838
f2 (ppm)
f1 (ppm)



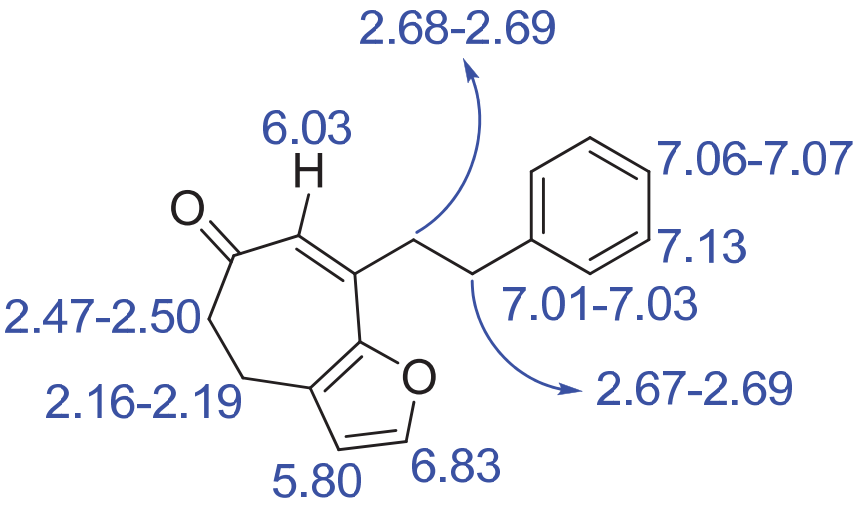
2r

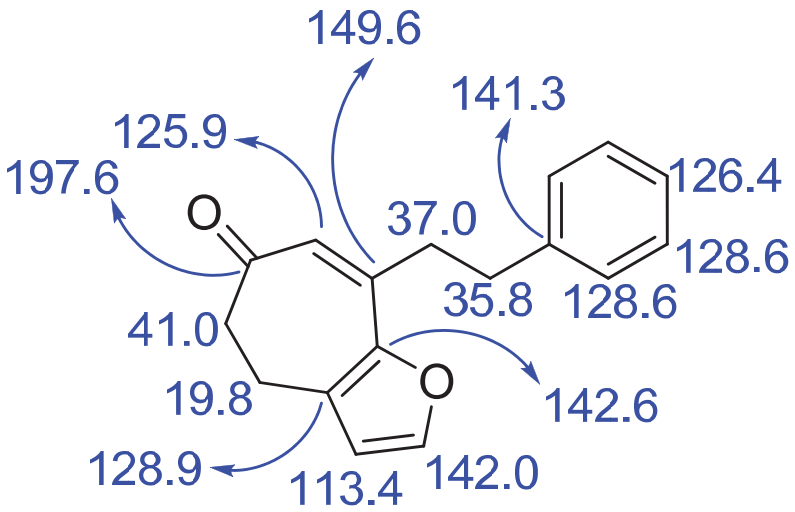


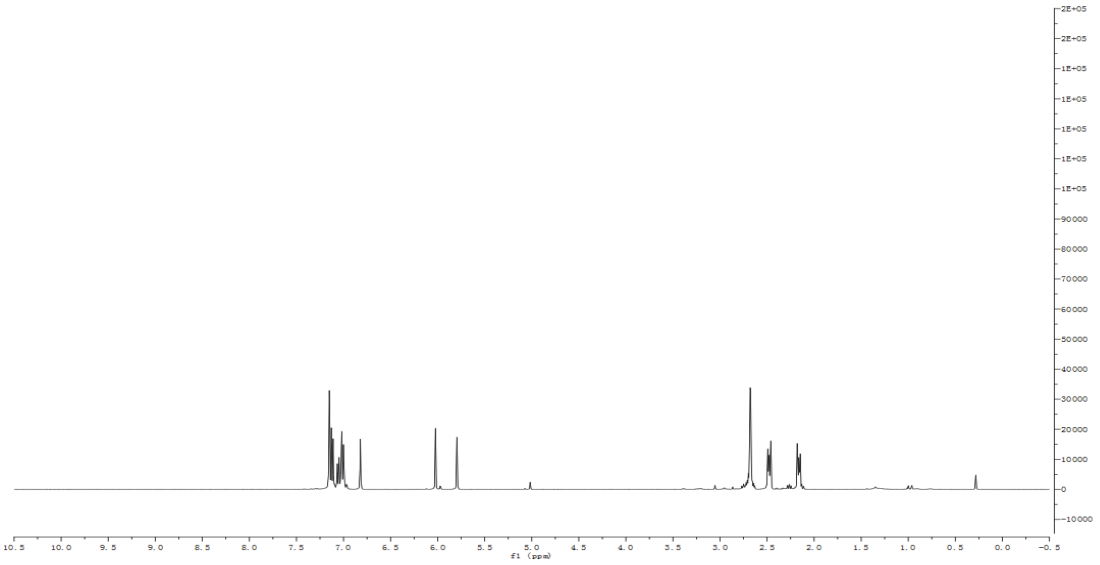


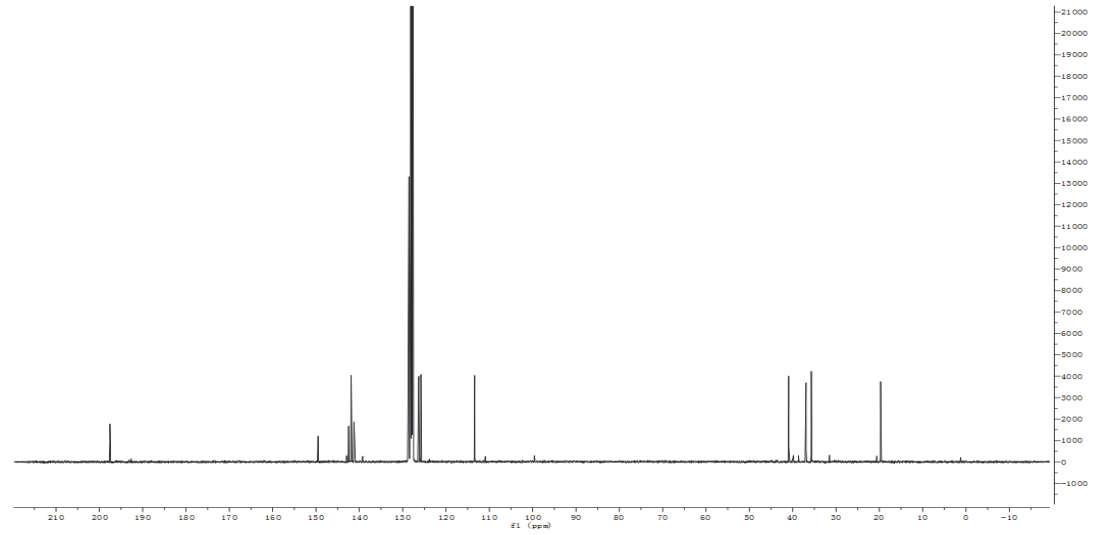

O
CH2Bn
O

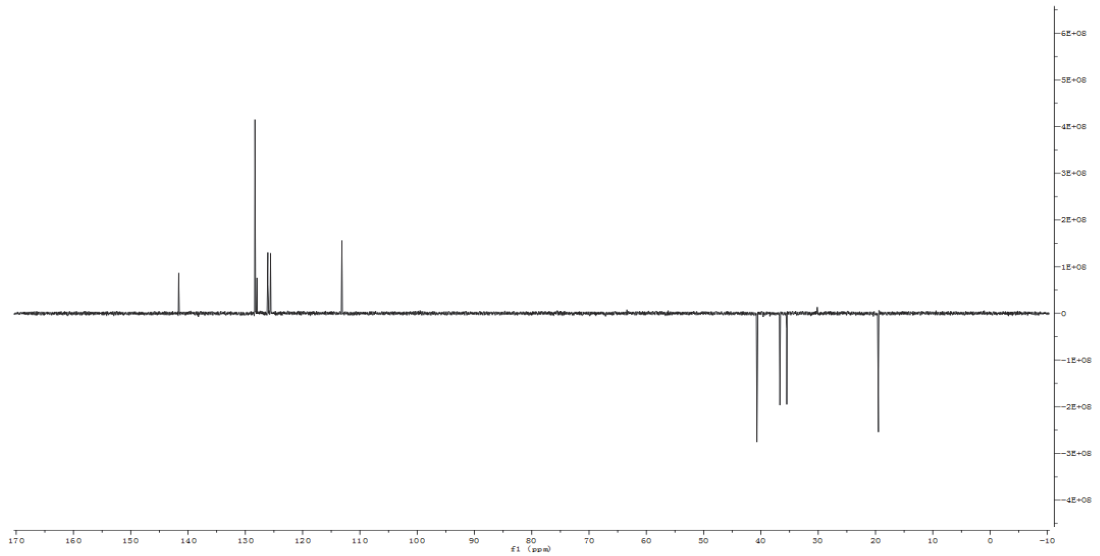
2s

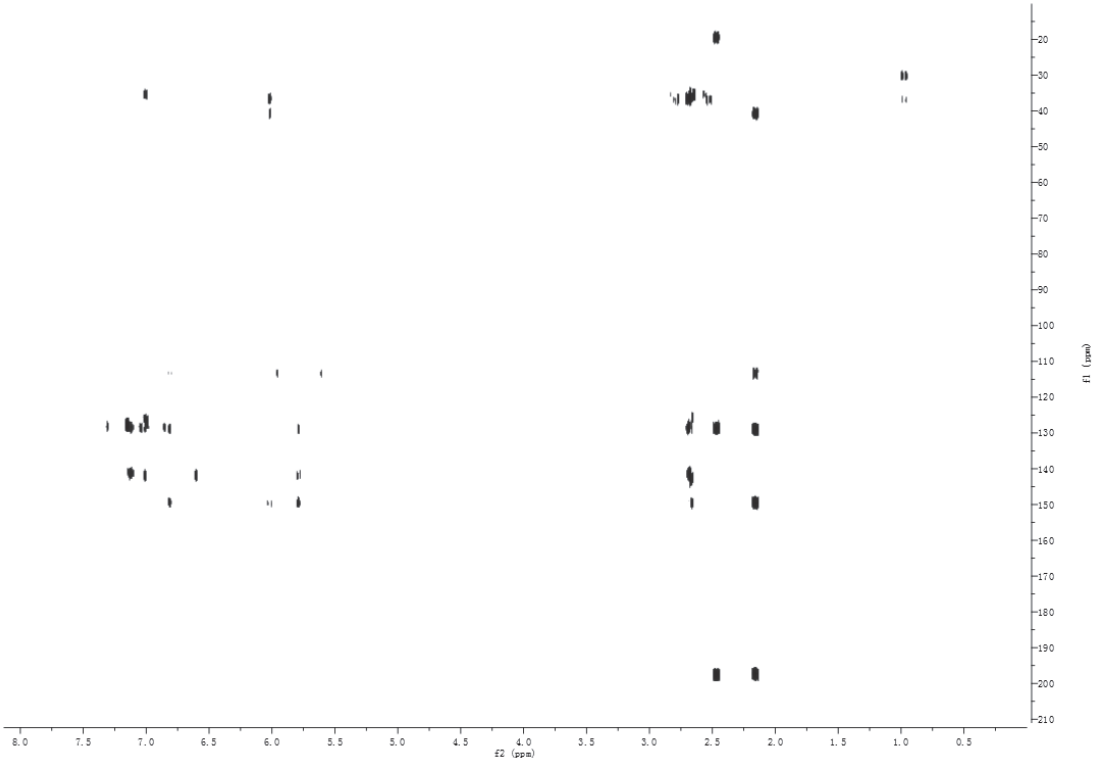

2.68-2.69
6.03
H
O
7.06-7.07
7.13
7.01-7.03
2.67-2.69
2.47-2.50
2.16-2.19
O
5.80
6.83

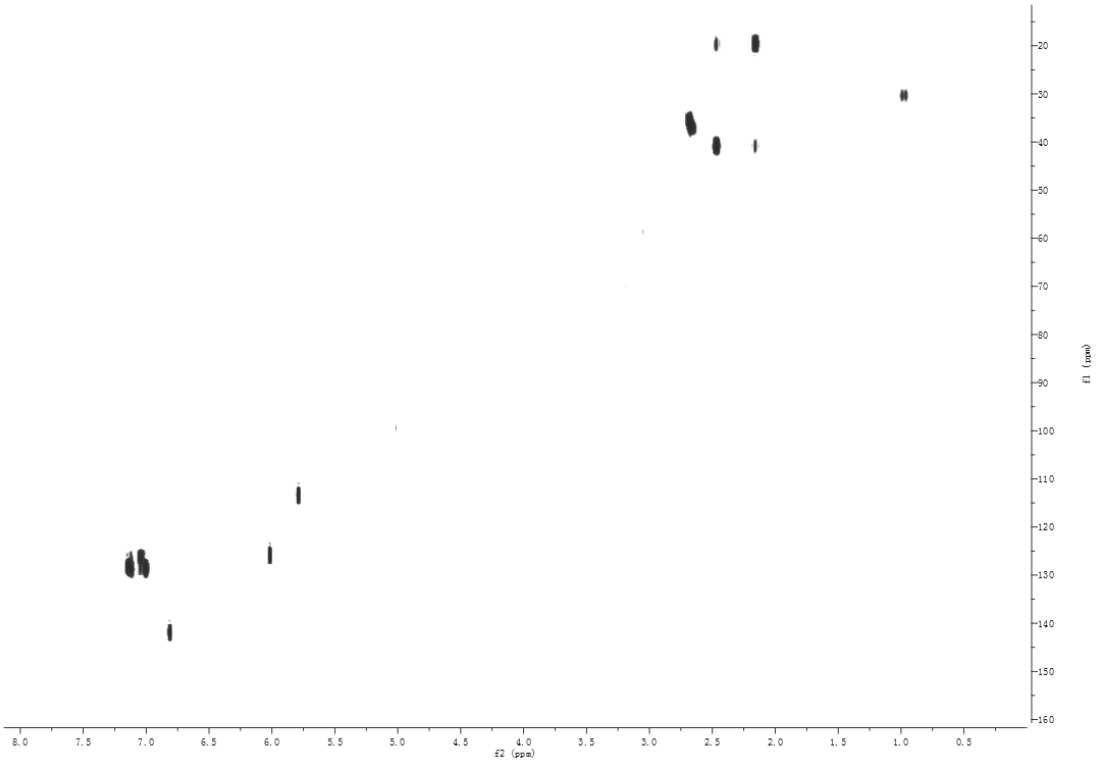

149.6
141.3
125.9
197.6
126.4
O
37.0
128.6
35.8
128.6
41.0
19.8
O
142.6
128.9
113.4
142.0

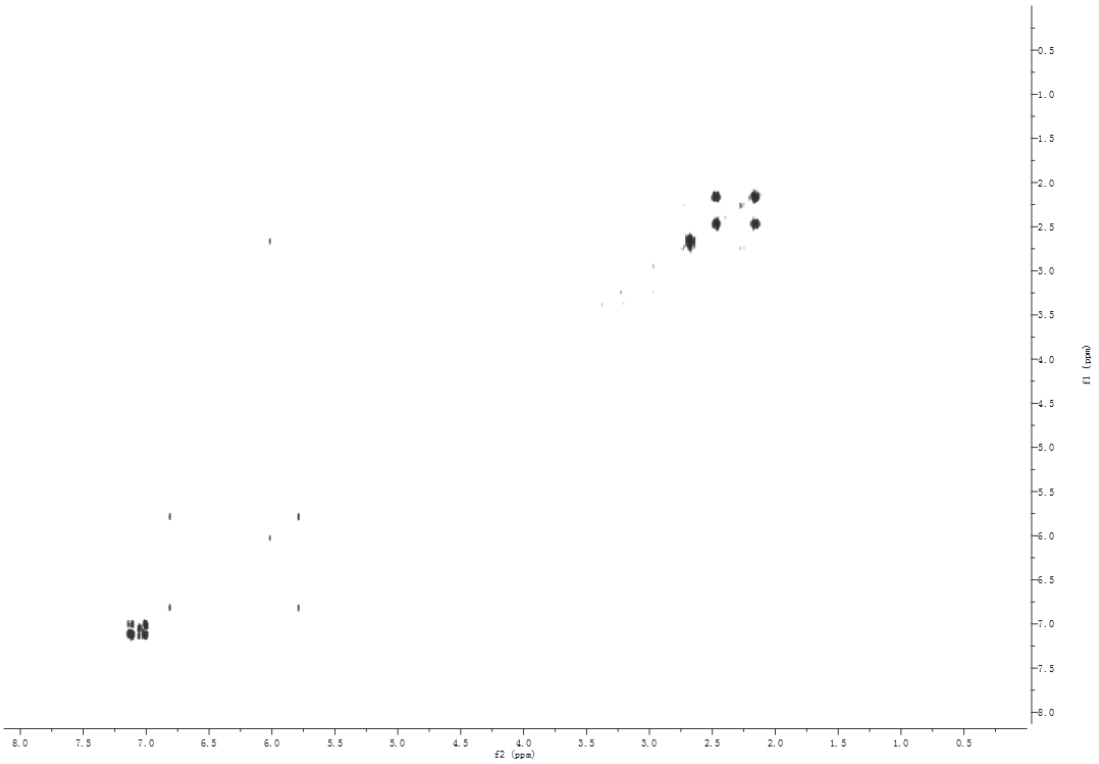

f1 (ppm)

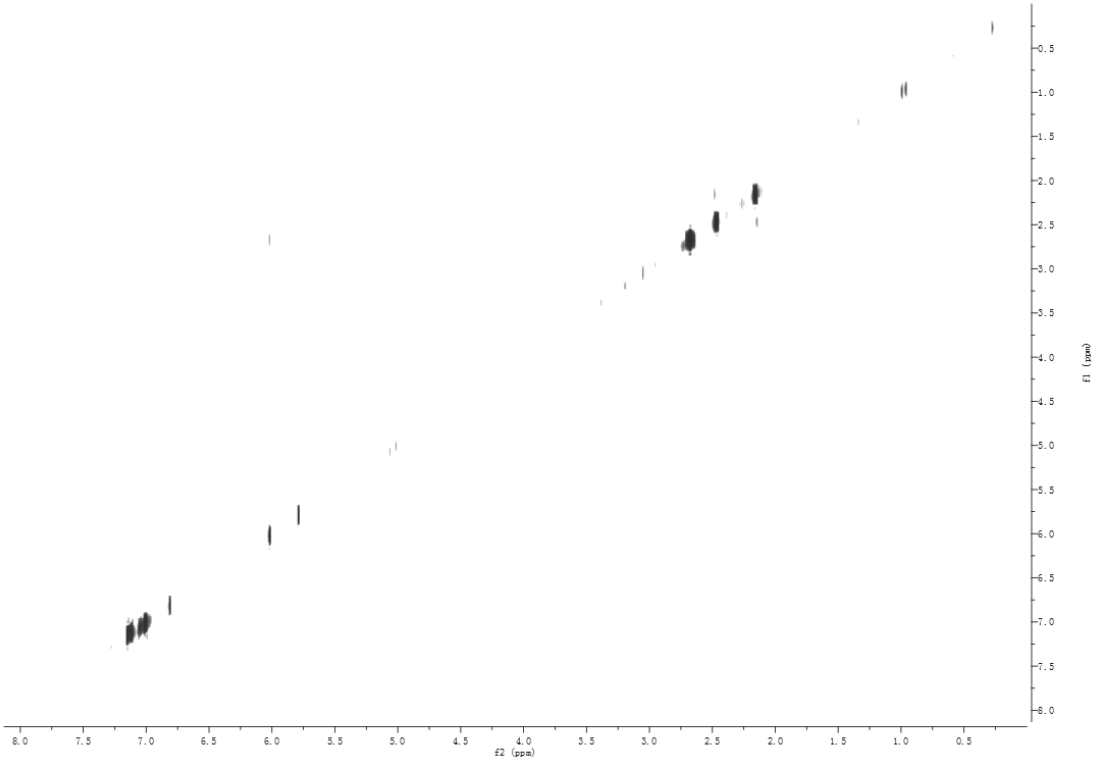

f1 (ppm)

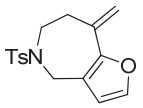

f1 (ppm)


f2 (ppm)
f1 (ppm)

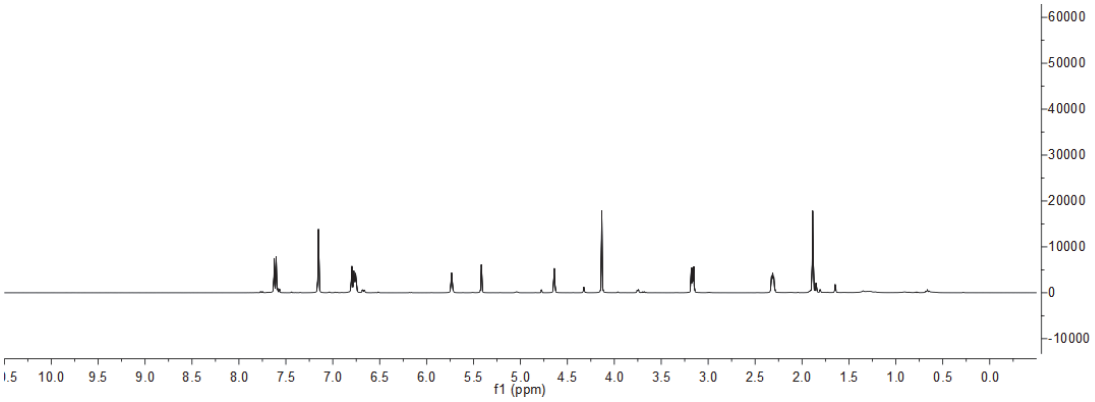

f2 (ppm)
f1 (ppm)

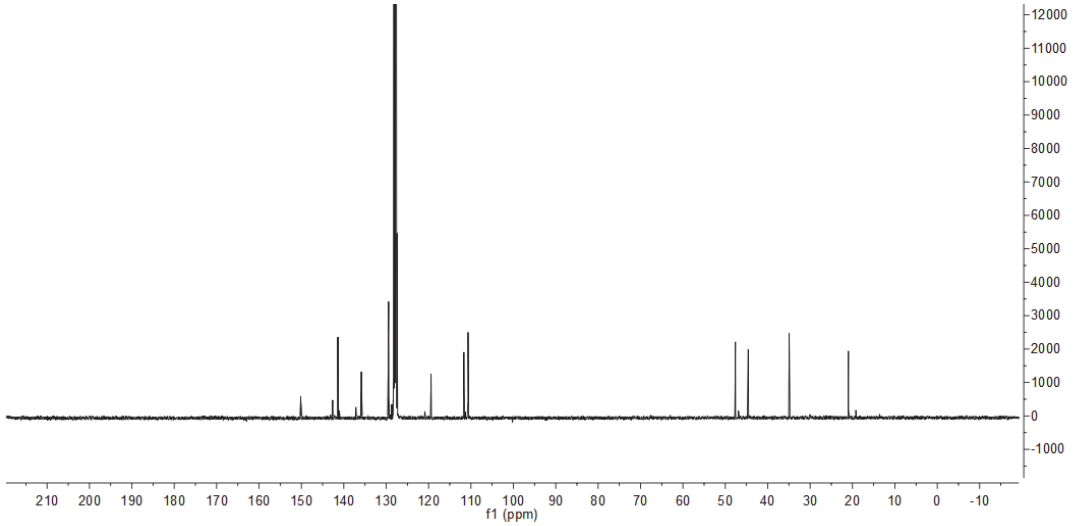

f2 (ppm)
f1 (ppm)

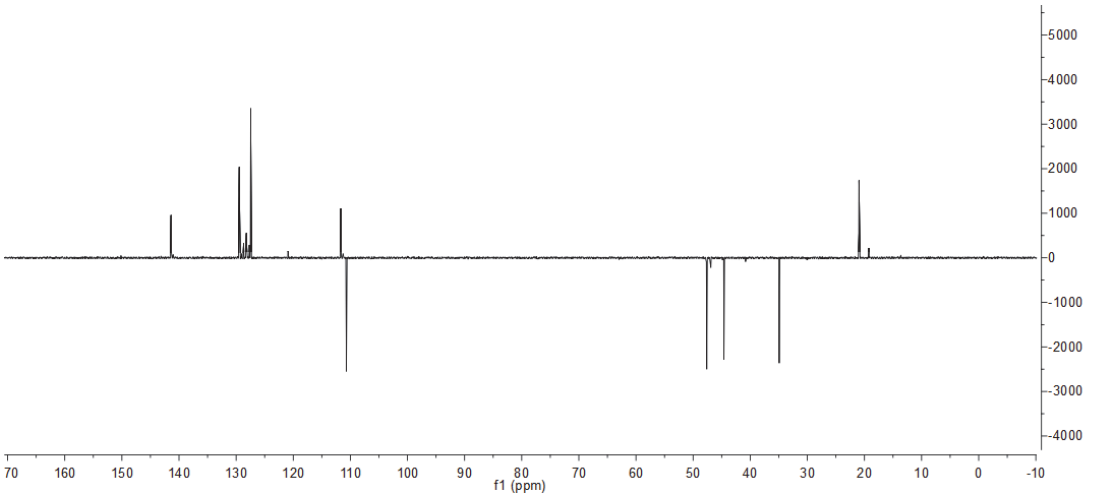

f2 (ppm)
f1 (ppm)

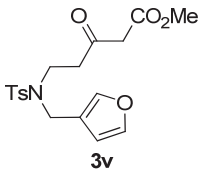

TsN
O

2t

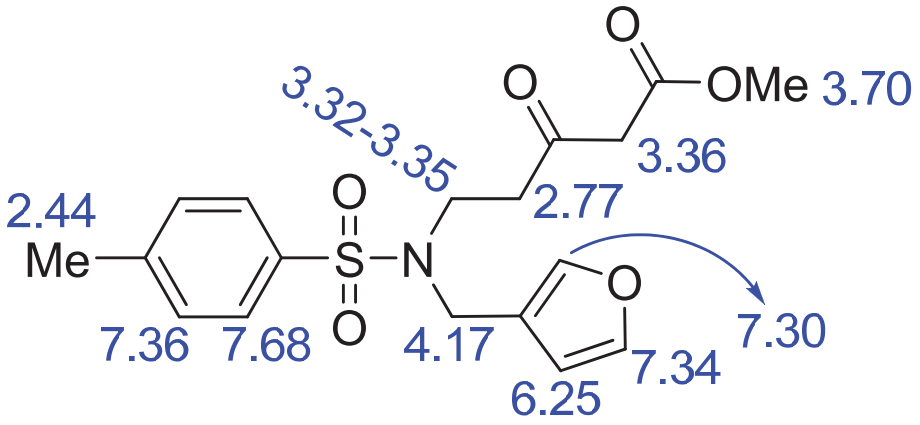

60000
50000
40000
30000
20000
10000
0
-10000
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

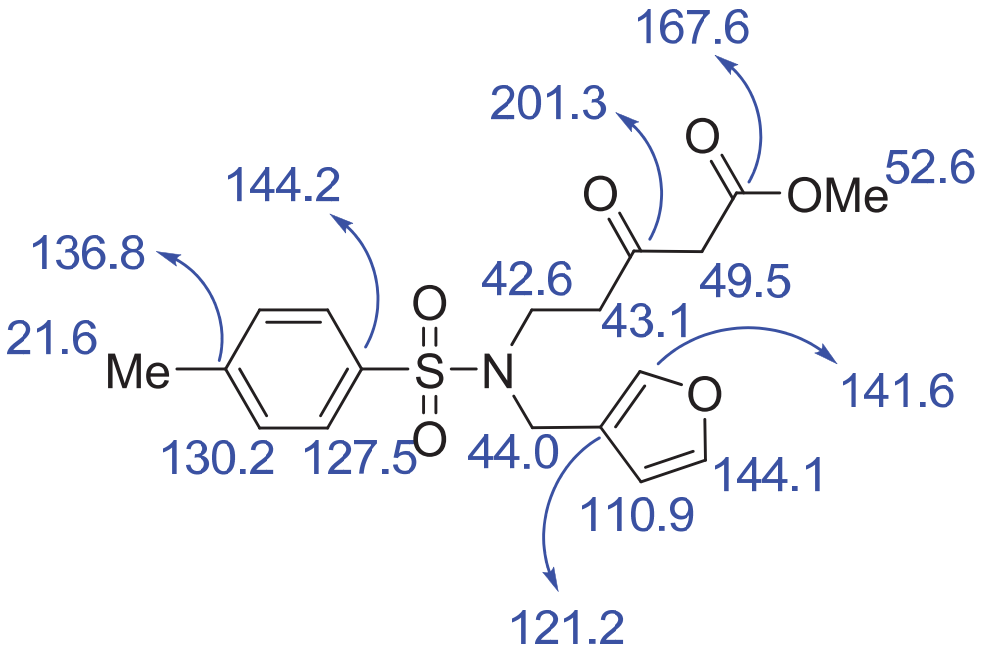

12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

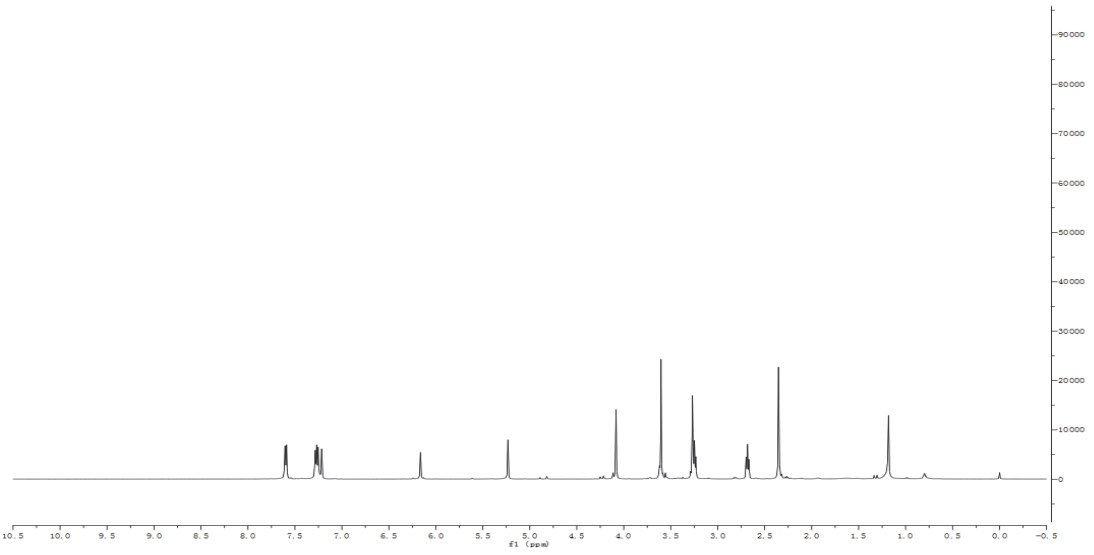

5000
4000
3000
2000
1000
0
-1000
-2000
-3000
-4000
70 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

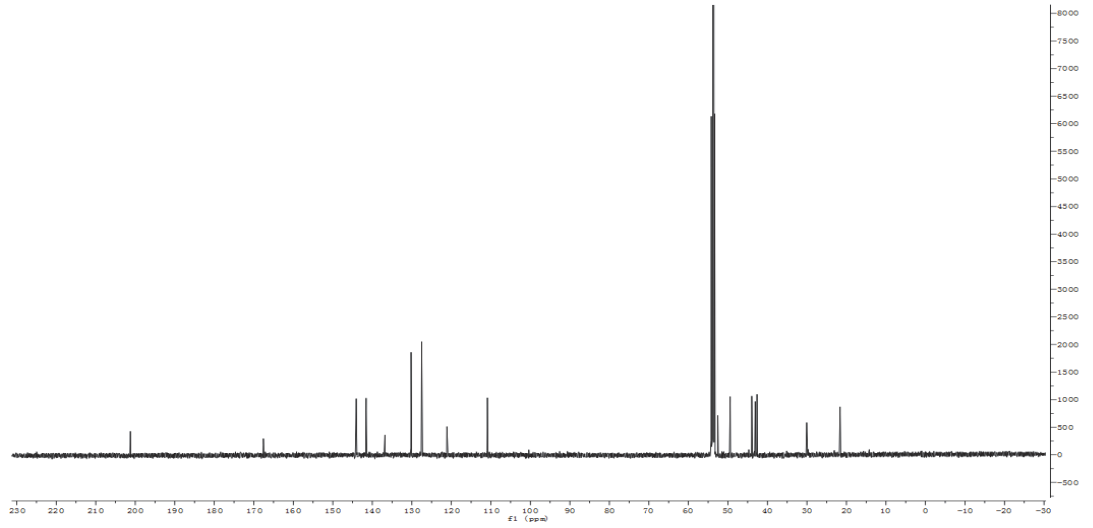

O
CO2Me
TsN
O

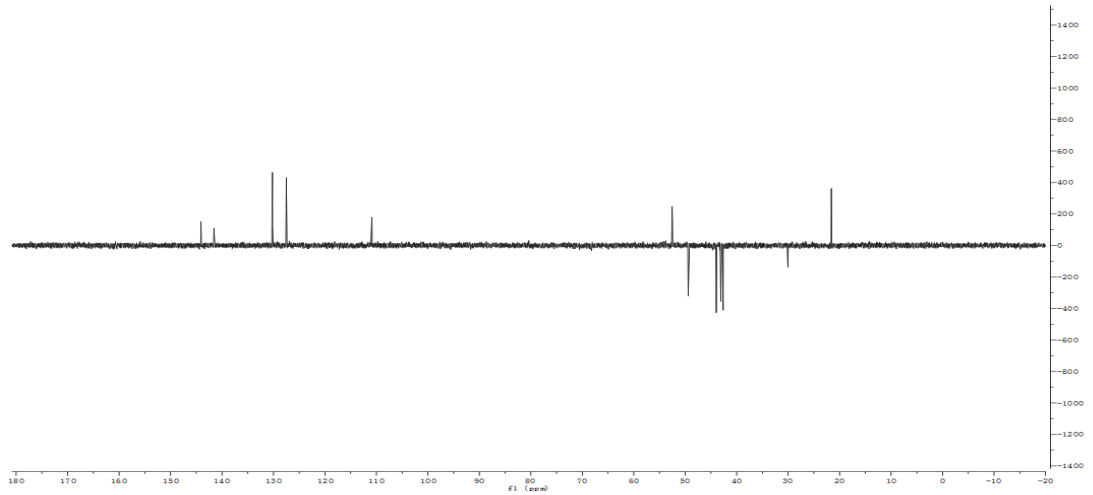
3v

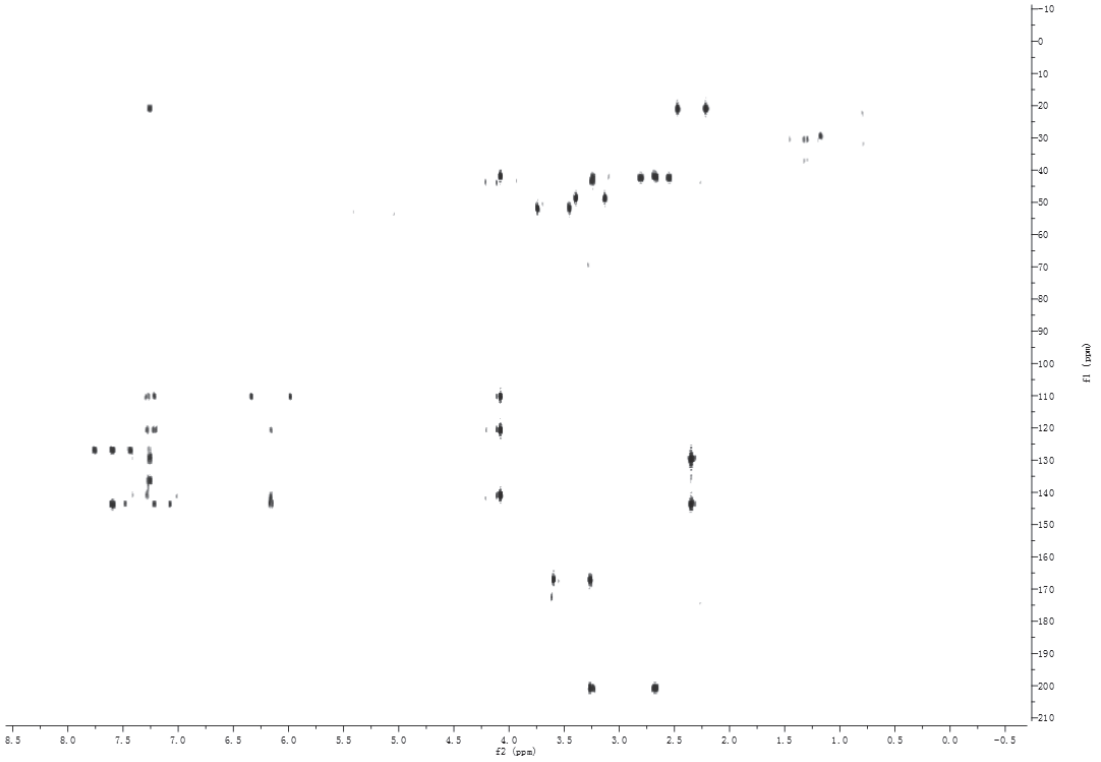

O
O
OMe 3.70
3.32-3.35
3.36
2.77
2.44
Me
O
S
N
O
7.36
7.68
4.17
O
7.30
7.34
6.25

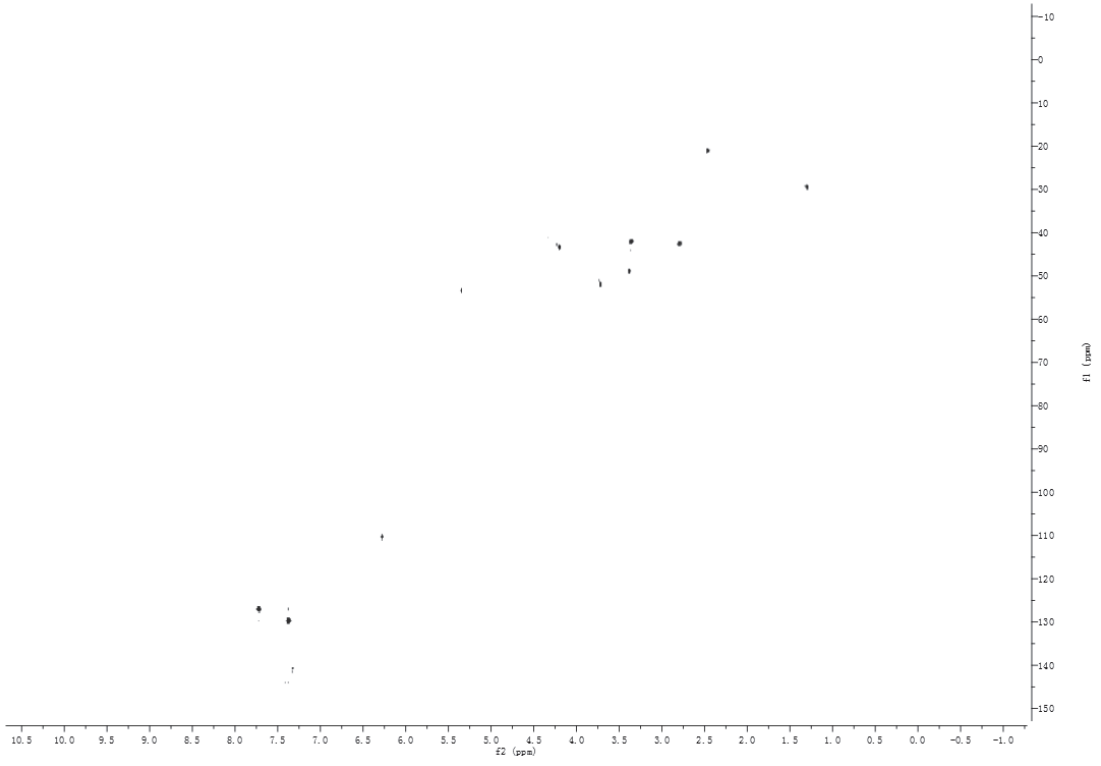

167.6
201.3
O
144.2
O
OMe 52.6
136.8
42.6
49.5
43.1
21.6
O
Me
S
N
141.6
O
130.2
127.5
O
44.0
144.1
110.9
121.2

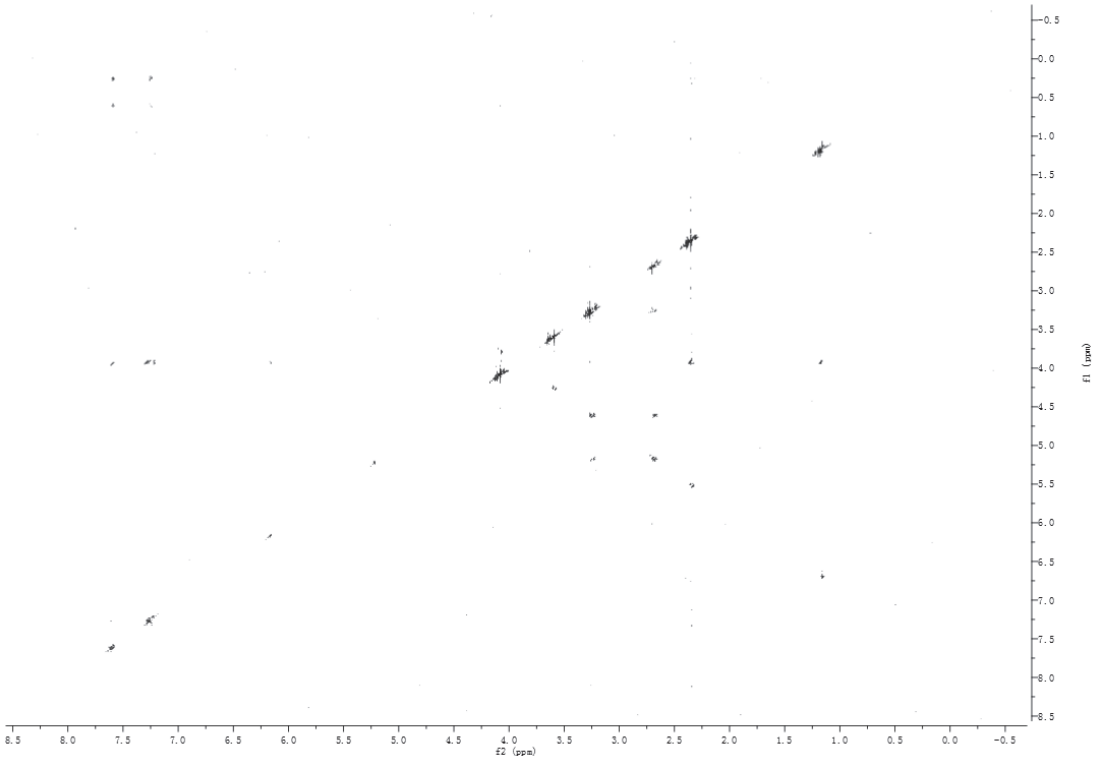


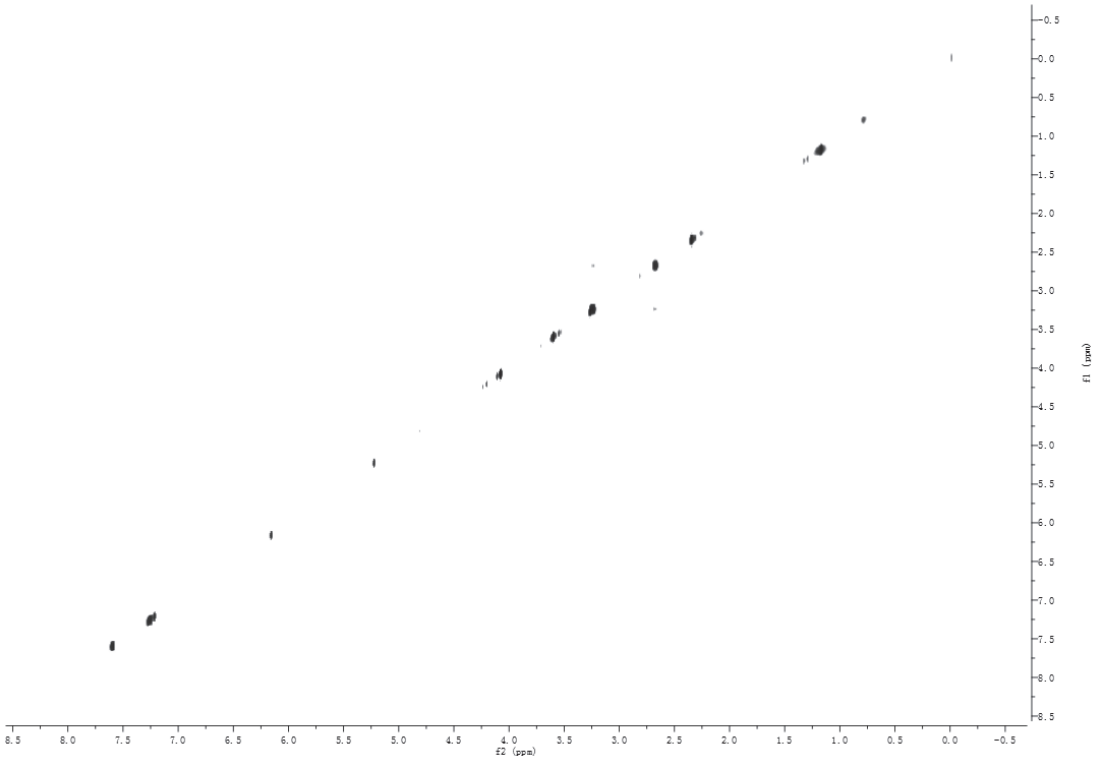


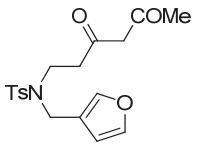



f2 (ppm)
f1 (ppm)


f2 (ppm)
f1 (ppm)


f2 (ppm)
f1 (ppm)


f2 (ppm)
f1 (ppm)



3w