Graphene Oxide Promotes Site-Selective Allylic Alkylation of Thiophenes With Alcohols.

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General Methods.

^{1}H-NMR spectra were recorded on Varian 400 (400 MHz) spectrometer or Agilent NMR system, consisting of a 54-mm bore, 500 MHz (11.7 T) Premium Shielded superconducting magnet, a DD2 Performa IV NMR console and the Agilent OneNMR probe. ^{1}H NMR (C_6D_6, 500 MHz); ^{13}C NMR (C_6D_6, 125 MHz). Chemical shifts are reported in ppm from TMS with the solvent resonance as the internal standard (deuterochloroform: 7.26 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = duplet, t = triplet, q = quartet, br = broad, m = multiplet), coupling constants (Hz). ^{13}C-NMR spectra were recorded on a Varian 400 (100 MHz) spectrometer with complete proton decoupling. Chemical shifts are reported in ppm from TMS with the solvent as the internal standard (deuterochloroform: 77.0 ppm). GC-MS spectra were taken by EI ionization at 70 eV on a Hewlett-Packard 5971 with GC injection or by Trace 1300 GC, ISQ Single Quadrupole MS, Thermo Fisher Scientific, Waltham, MA, USA, operating in electron impact (EI) ionization mode at 70 eV. One sample was introduced to the ion source region via a direct exposure probe (DEP). They are reported as: *m/z* (rel. intense). Elemental analyses were carried out by using a EACE 1110 CHNOS analyzer. Graphene oxide is prepared using a modified Hummers method starting from graphite flakes (maximum particle diameter 500 μm).[1]

LC-electrospray ionization mass spectra were obtained with Agilent Technologies MSD1100 single-quadrupole mass spectrometer. Chromatographic purification was done with 240-400 mesh silica gel. Elemental analyses were carried out by using a EACE 1110 CHNOS analyzer.

All anhydrous solvents were supplied by Sigma Aldrich in Sureseal® bottles and used without any further purification. Commercially available chemicals were purchased from Sigma Aldrich, Stream and TCI and used without any further purification. Melting points were measured using open glass capillaries in a Bibby Stuart Scientific Melting Point Apparatus SMP 3 and are calibrated by comparison with literature values (Aldrich). Alcohols **2a** and **2a'** were purchased from Merck-Aldrich and used as received.

Certainly, the cost of styrene oxide cannot be compared with that of GO. However, styrene oxide proved to be poorly effective in the titled transformation, leading to 30% 3aa conversion only when epoxide (100%) was combined with stoichiometric amount of benzoic acid. Therefore, in the present protocol, GO is much more performing with respect to smaller oxiranes. Additionally, I would like to emphasize that with the present work we wish to present a "proof-of-principle", regarding the application of GO to synthetically useful organic reactions. No intent to replace "classic" metal and metal-free catalytic strategies with GO and derivatives.

Computational Details.

All calculations were carried out using the combined quantum mechanical and molecular mechanical (QM/MM) method in the ONIOM formalism, as implemented within the Gaussian 09 program suite.[2] The coupled QM/MM method adopted here is a two-layer ONIOM scheme, where the reactive region is treated at DFT level using the density functional M06-2X (a functional able to account for π-π interactions) and 6-

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[1] a) Park, S.; Ruoff, R. S. *Nat. Nanotechnol.* **2009**, *4*, 217-224; b) Treossi, E.; Melucci, M.; Liscio, A.; Gazzano, M.; Samorì, P.; Palermo, V. *J. Am. Chem. Soc.* **2009**, *131*, 15576-15577.

[2] Gaussian 09, Revision E.01, 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, J. A., Jr.; 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**.

31G* basis set.[3] The remaining region is treated using the UFF force field (see Scheme S1 in SI).[4] The global potential can be referred as M06-2X/6-31G*:UFF potential. ONIOM calculations were performed considering mechanical and electrostatic embedding. In the MM calculations partial atomic (point) charges were used to compute the electrostatic interactions. These charges were calculated using the QEq formalism.[5] The structure of the various critical points (minima and saddle points) was fully optimized. Frequency calculations were carried out at the same level of theory to check the nature of critical points. This approach was recently validated to study similar carbon based nanocatalyst.[6]

X-ray photoelectron spectroscopy (XPS) measurements.

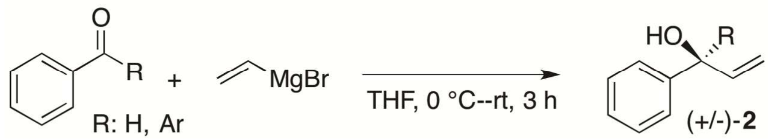
XPS spectra were recorded with a Phoibos 100 hemispherical energy analyzer (Specs) using Mg K_α radiation ($\hbar\omega$ =1253.6 eV). The X-ray power was 125 W. The spectra were recorded in the constant analyzer energy (CAE) mode with analyzer pass energies of 40 eV for the high resolution spectra. Charging effects were corrected by energy calibration on Au 4f $_{7/2}$ level relative to 84.0 eV. The base pressure in the analysis chamber during analysis was 5×10^{-10} mbar. High resolution XPS spectra of C 1s were analyzed by CasaXPS (Casa software, Ltd), the curve fitting was carried out using Gaussian/Lorentzian curves shape (GL(30)) for C-O groups with a full width half-maximum of 1.4 eV and an asymmetric Voigt for the C-C sp2.

For each sample GO were deposited on golden slides purchased from Arrandee (Germany) having the following specifications: Au, 250 nm thick and 2.5 nm of Cr, as adhesive layer. Gold substrates were cleaned using the protocol for silicon substrates. Sample were prepared drop-casting the GO solutions on freshly cleaned golden slice and immediately put in High-Vacuum overnight.

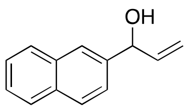
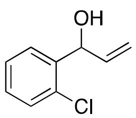
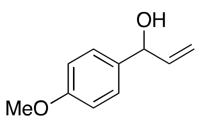
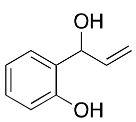
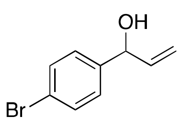
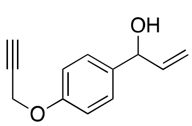
[3] Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215-241.
[4] Rappé, A. K.; Casewit, C. J.; Colwell, K. S.; Goddard, W. A., III; Skiff, W. M. *J. Am. Chem. Soc.* **1992**, *114*, 10024-10035.
[5] Rappé, A. K.; Goddard, W. A., III *J. Phys. Chem.* **1991**, *95*, 3358-3363.

[6] a) Giacinto, P.; Bottoni, A.; Calvaresi, M.; Zerbetto, F. *J. Phys. Chem. C* **2014**, *118*, 5032-5040; b) Spyrou, K.; Calvaresi, M.; Diamanti, E. K.; Tsoufis, T.; Gournis, D.; Rudolf, P.; Zerbetto, F. *Adv. Funct. Mater.* **2015**, *25*, 263-269; c) Giacinto, P.; Zerbetto, F.; Bottoni, A.; Calvaresi, M. *J. Chem. Theory Comput.* **2016**, *12*, 4082-4092; d) Marforio, T. D.; Bottoni, A.; Giacinto, P.; Zerbetto, F.; Calvaresi, M. *J. Phys. Chem. C*, **2017**, *121*, 27674-27682.

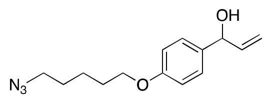
Synthesis of the allylic alcohols: 2b-f,j-l (not optimized protocol).



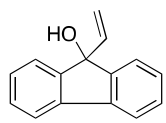
A flame-dried three-necked round bottom flask was charged under nitrogen with anhydrous THF followed by the desired carbonyl compound (3 mmol, 0.2 M) and the mixture was cooled to 0 °C. Therefore, a solution of vinyl-magnesium bromide (1M, 1.5 eq) was added dropwise, followed by stirring at rt for 3 hours. The reaction was quenched with an aqueous NH_4Cl solution (2 M), extracted with Et_2O (3 x 15 mL) and the combined organic phases dried over Na_2SO_4. Solvent was removed by rotary evaporation and the crude was purified by column chromatography to give the desired product.

	**2b**.[7] Yellow oil. Yield = 54% (300 mg). (*c*Hex:Et_2O = 85:15). ***^{1}H-NMR*** (500 MHz, $CDCl_3$) δ: 7.85-7.83 (m, 4H), 7.50-7.48 (m, 3H), 6.17-6.10 (m, 1H), 5.42 (d, J = 17.5 Hz, 1H), 5.38 (d, J = 5.5 Hz, 1H), 5.25 (d, J = 10.0 Hz, 1H), 2.03 (bs, 1H). ***^{13}C-NMR*** (125 MHz, $CDCl_3$) δ: 140.1, 139.9, 133.3, 133.0, 128.4, 128.0, 127.7, 126.2, 126.0, 124.9, 124.5, 115.4, 75.5. ***GC-MS*** (m/z): 128, 184.
	**2c.**[8] Colorless oil. Yield = 44% (222 mg), (*c*Hex:Et_2O = 85:15). ***^{1}H-NMR*** (500 MHz, $CDCl_3$) δ: 7.53 (dd, J = 1.5 Hz, J = 8.0 Hz, 1H), 7.34 (d, J = 8.0 Hz, 1H), 7.28 (t, J = 7.5 Hz, 1H), 7.21 (dt, J = 1.5 Hz, J = 7.5 Hz, 1H), 6.05-5.99 (m, 1H), 5.62 (d, J = 5.5 Hz, 1H), 5.37 (d, J = 17.0 Hz, 1H), 5.21 (d, J = 10.5 Hz, 1H), 2.45 (bs, 1H). ***^{13}C-NMR*** (125 MHz, $CDCl_3$) δ:139.9, 138.3, 132.3, 129.4, 128.7, 127.6, 127.1, 115.5, 71.3. ***GC-MS*** (m/z): 168, 170.
	**2d**.[9] Colorless oil. Yield = 64% (314 mg), (*c*Hex:Et_2O = 80:20). ***^{1}H-NMR*** (400 MHz, $CDCl_3$) δ 7.28 (d, J = 8.0 Hz, 2H), 6.89 (d, J= 8.0 Hz, 2H), 6.08-5.98 (m, 1H), 5.32 (d, J = 18.4 Hz, 1H), 5.18 (d, J = 10.3 Hz, 1H), 5.13 (brs, 1H), 3.78 (s, 3H), 2.16 (brs, 1H). ***^{13}C-NMR*** (100 MHz, $CDCl_3$) δ 159.14, 140.4, 134.9, 127.7(2C), 114.7, 113.9 (2C), 74.8, 55.3. ***GC-MS*** (m/z): 77, 109, 164.
	**2e**.[10] Colorless oil. Yield = 35% (158 mg), (*c*Hex:Et_2O = 80:20). ***^{1}H-NMR*** (400 MHz, $CDCl_3$) δ 7.66 (s, 1H), 7.19 (dt, J = 1.6 Hz, J = 8.4 Hz, 1H), 7.28 (dd, J = 1.2 Hz, J = 7.6 Hz, 1H), 6.89-6.84 (m, 2H), 6.22-6.10 (m, 1H), 5.39 (brs, 1H), 5.35 (d, J = 17.2 Hz, 1H), 5.27 (d, J = 17.2 Hz, 1H), 2.65 (s, 1H). ***^{13}C-NMR*** (100 MHz, $CDCl_3$) δ 155.3, 138.0, 129.3, 127.6, 120.0, 117.1, 116.3, 76.1. ***GC-MS*** (m/z): 150.
	**2f**.[11] Colorless oil. Yield = 54% (343 mg), (*n*-Pent:EtOAc:CH_2Cl_2 = 90:5:5 → 60:20:20). ***^{1}H-NMR*** (500 MHz, $CDCl_3$) δ: 7.48 (dd, J = 3.0 Hz, J = 8.5 Hz, 2H), 7.25 (dd, J = 3.0 Hz, J = 8.5 Hz, 2H), 6.04-5.97 (m, 1H), 5.34 (dd, J = 1.5 Hz, J = 17.0 Hz, 1H), 5.23-5.21 (m, 1H), 5.17 (bs, 1H), 2.01 (bs, 1H). ***^{13}C-NMR*** (125 MHz, $CDCl_3$) δ: 141.5, 139.8, 131.6, 128.0, 121.5, 115.6, 74.7. ***GC-MS*** (m/z): 133, 183-185, 212-214.
	**2g**. Yellow oil. Yield = 96% (541 mg), (*c*Hex:Et_2O = 90:10). ***^{1}H-NMR*** (400 MHz, $CDCl_3$) δ 7.31 (d, J = 8.8 Hz, 2H), 6.97 (d, J = 8.8 Hz, 2H), 6.00-6.09 (m, 1H), 5.34 (dt, J = 1.2, 17.2 Hz, 1H), 5.19 (dt, J = 1.2 Hz, 12.6 Hz, 1H), 5.16 (brs, 1H), 4.69 (d, J = 2.4 Hz, 2H), 2.55 (t, J = 2.8 Hz, 1H). ***^{13}C-NMR*** (100 MHz, $CDCl_3$) δ 157.1, 140.2, 135.8, 127.7(2C), 114.9(2C), 114.8, 78.5, 75.5, 74.8, 55.8. ***GC-MS*** (m/z): 188. ***Anal. Calc.*** for ($C_{12}H_{12}O_2$: 188.08): C, 76.57; H, 6.43; found: C, 77.41, H, 6.55.

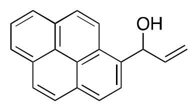
[7] M. Lafrance, M. Roggen, E. M. Carreira, *Angew. Chem. Int. Ed.* **2012**, *51*, 3470-3473.
[8] S. F. Musolino, O. S. Ojo, N. J. Westwood, J. E. Taylor, A. D. Smith, *Chem. Eur. J.* **2016**, *22*, 18916-18922.
[9] F. Wu, H. Li, R. Hong, L. Deng, *Angew. Chem. Int. Ed.* **2006**, *45*, 947-950.
[10] M. Vellakkaran, M. M. S. Andappan, N. Kommu, *Eur. J. Org. Chem.* **2012**, 4694-4698.
[11] J. Štambaský, A. V. Malkov, P. Kočovský, *J. Org. Chem.* **2008**, *73,* 9148-9150.



2h. Pale yellow oil. Yield = 57% (446 mg), (*c*Hex:EtOAc = 80:20). ***^{1}H-NMR*** (400 MHz, $CDCl_3$) δ 7.26 (q, J = 1.6 Hz, J = 6.4 Hz, 2H), 6.86 (q, J = 2.0 Hz, J = 6.8 Hz, 2H), 6.03 (ddd, J = 5.6 Hz, J= 10.0 Hz, J = 16.4 Hz, 1H), 5.33 (d, J = 16.4 Hz, 1H), 5.17 (d, J = 5.6 Hz, 1H), 5.15 (d, J = 5.6 Hz, 1H), 3.95 (t, J = 6.0 Hz, 2H), 3.28 (t, J = 6.8 Hz, 2H), 1.95 (brs, 1H), 1.83-1.76 (m, 2H), 1.68-1.62 (m, 2H), 1.58-1.54 (m, 2H). ***^{13}C-NMR*** (100 MHz, $CDCl_3$) δ 158.6, 140.4, 134.8, 127.7(2C), 114.7, 114.5(2C), 114.9, 74.9, 67.6, 51.3, 28.8, 28.6, 23.4. ***LC-MS***: 206, 248. ***Anal. Calc.*** for ($C_{14}H_{19}N_3O_2$: 261.15): C, 64.35; H, 7.33; found: C, 64.22, H, 7.21.

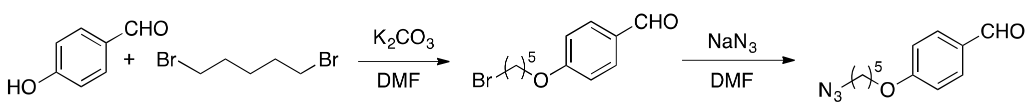


2l. Yellow solid. ***MP*** = 93-95 °C. Yield = 43% (268 mg), (*c*Hex:EtOAc = 90:10). ***^{1}H-NMR*** (500 MHz, $CDCl_3$) δ: 7.64 (d, J = 7.0 Hz, 2H), 7.46 (d, J = 7.0 Hz, 2H), 7.38 (t, J = 7.5 Hz, 2H), 7.31 (t, J = 7.5 Hz, 2H), 5.99 (dd, J = 11.0 Hz, J = 17.5 Hz, 1H), 5.56 (d, J = 17.0 Hz, 1H), 5.22 (d, J = 11.0 Hz, 1H), 2.20 (bs, 1H). ***^{13}C-NMR*** (125 MHz, $CDCl_3$) δ: 148.0, 139.5, 139.1, 129.2, 128.1, 124.5, 120.2, 113.5, 82.5. ***GC-MS*** (m/z): 152, 181, 208.



2m. Pale yellow solid. ***MP*** = 96-97 °C. Yield = 77% (600 mg), (*c*Hex:EtOAc = 80:20). ***^{1}H-NMR*** (500 MHz, $CDCl_3$) δ: 8.40 (d, J = 9.5 Hz, 1H), 8.20-8.15 (m, 4H), 8.11 (d, J = 9.5 Hz, 1H), 8.07-8.00 (m, 3H), 6.39-6.32 (m, 1H), 6.27 (d, J = 4.5 Hz, 1H), 5.48 (d, J = 17.0 Hz, 1H), 5.31 (d, J = 10.0 Hz, 1H), 2.27 (bs, 1H). ***^{13}C-NMR*** (125 MHz, $CDCl_3$) δ: 139.9, 135.6, 131.3, 131.0, 130.7, 128.1, 127.7, 127.5, 127.4, 126.0, 125.3, 125.2, 125.0, 124.8, 124.1, 122.9, 115.6, 72.4. ***GC-MS*** (m/z): 203, 227, 239, 258.

Synthesis of aldehyde, precursor alcohol 2h:



In a 100 mL Schlenk tube, DMF (27 mL) was added followed by 4-hydroxybenzaldehyde (563 mg, 4.6 mmol) and K_2CO_3 (1.27 g, 9.2 mmol). Then 1,5-dibromopentane (1.25 mL, 9.2 mmol) was added at 0 °C. Then the reaction mixture was stirred at room temperature for 12 h. Then the reaction mixture was diluted with EtOAc and washed 3 times with H_2O. The organic phase was dried with Na_2SO_4 and the solvent removed under reduced pressure. The reaction crude was purified via flash chromatography (*c*Hex:AcOEt = 98:2), to give the desired product in 90% yield (1180 mg).[12] Yellow oil. ***^{1}H-NMR*** (400 MHz, $CDCl_3$) δ 9.85 (s, 1H), 7.80 (dd, J = 2.4 Hz, J = 4.8 Hz, 2H), 6.97 (dd, J = 2.8 Hz, J = 5.6 Hz, 2H), 4.04 (t, J = 6.4 Hz, 2H), 3.32 (t, J = 6.4 Hz, 2H), 1.96-1.90 (m, 2H), 1.88-1.79 (m, 2H), 1.64-1.60 (m, 2H). ***^{13}C-NMR*** δ 190.7, 164.0, 131.9(2C), 129.8, 114.7(2C), 67.9, 33.4, 32.3, 28.2, 24.7. ***GC-MS*** (m/z): 69, 121, 149, 151, 270, 272. ***Anal. Calc.*** for ($C_{12}H_{15}BrO_2$: 271.15): C, 53.16; H, 5.58; found: C, 53.01, H, 5.75.

A round bottom flask was charged with the 4-(5-bromopentyloxy) benzaldehyde (250 mg, 0.92 mmol) and 15 mL of reagent grade DMF and 120 mg of NaN_3 (1.84 mmol) was added. The reaction mixture was stirred reflux condition for 16 hours, then the mixture was diluted with E_2O (15 mL) and washed with H_2O (3 x 10 mL). Solvent was removed by rotary evaporation and the crude was purified via flash chromatography (*c*Hex: EtOAc = 98:2). Yield 63% (135 mg). Dark green oil. ***^{1}H-NMR*** (400 MHz, $CDCl_3$) δ 9.87 (s, 1H), 7.80 (dd, J = 2.4 Hz, J = 4.4 Hz, 2H), 6.98 (dd, J = 2.4 Hz, J = 4.4 Hz, 2H), 4.04 (t, J = 6.4 Hz, 2H), 3.30 (t, J = 6.4 Hz 1H), 1.87-1.82 (m, 2H), 1.71-1.65 (m, 2H), 1.60-1.55 (m, 2H). ***^{13}C-NMR*** (100 MHz, $CDCl_3$) δ 190.7, 164.0. 132.0(2C), 129.9, 114.7(2C), 68.0, 51.3. 28.6, 28.5, 23.3. ***LC-MS*** (m/z): 234 $[M+H^+]$. ***Anal. Calc.*** for ($C_{12}H_{15}N_3O_2$: 233.27): C, 61.79; H, 6.48; found: C, 61.59, H, 6.32.

Typical procedure for the GO-assisted Friedel-Crafts reaction.

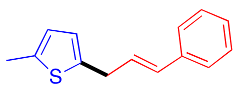
In a typical 2-methylthiophene (29.0 µL, 0.3 mmol) was dissolved in 0.3 mL of reagent grade 1,4-dioxane in which, 3.2 mg of GO (25-50 wt%) were previously suspended. Then, α-vinylbenzyl alcohol (13.0 µL, 0.1 mmol) was added. The mixture was stirred at 90 °C for 8 hours. Then, the catalyst was filtered and washed with EtOAc and CH_2Cl_2. The

[12] A. Alizadeh, M. M. Khodaei, A. Eshghi, *J. Org. Chem.* **2010**, *75*, 8295.

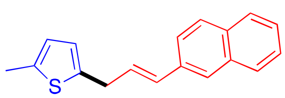
organic phase was evaporated under reduced pressure and the crude purified by column chromatography to give the desired product.

Typical procedure for the GO-assisted Friedel-Crafts reaction on 1mmol scale of 2a.

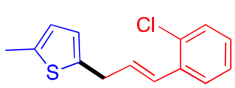
In a typical 2-methylthiophene (290 µL, 3.0 mmol) was dissolved in 2.5 mL of reagent grade 1,4-dioxane in which, 32 mg of GO (25 wt%) were previously suspended. Then, α-vinylbenzyl alcohol (130 µL, 1.0 mmol) was added. The mixture was stirred at 90 °C for 8 hours. Then, the catalyst was filtered and washed with EtOAc and CH_2Cl_2. The organic phase was evaporated under reduced pressure and the crude purified by column chromatography (*c*Hex:Et_2O = 98:2) to give a **3aa+3aa'** mixture (86:14) as an yellow oil.



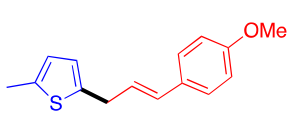
Yield = 90% (192 mg). ***^{1}H-NMR*** (400 MHz, $CDCl_3$) δ 7.42-7.16 (m, 5H), 6.65-6.58 (m, 2H), 6.48 (d, J = 16.0 Hz, 1H), 6.34 (dt, J = 5.3 Hz, J = 14.8 Hz, 1H), 3.64 (d, J = 7.2 Hz, 2H), 2.43 (s, 3H). ***^{13}C-NMR*** (100 MHz, $CDCl_3$) δ 138.2, 137.3, 131.1, 128.5 (2C), 127.2, 126.2 (2C), 124.8, 124.4, 121.1, 33.5, 15.3. ***GC-MS*** (m/z): 214. ***Anal. Calc.*** for ($C_{14}H_{14}S$: 214.08): C, 78.46; H, 6.58; found: C, 78.21, H, 6.33.
3aa' ***^{1}H-NMR*** (400 MHz, $CDCl_3$, *diagnostic signals*) δ 7.01 (d, J = 4.8 Hz, 1H), 6.84 (d, J = 4.8 Hz, 1H), 6.38-6.24 (m, 2H), 3.43 (d, J = 5.6 Hz, 2H), 2.41 (s, 3H). ***^{13}C-NMR*** (100 MHz, $CDCl_3$, *diagnostic signals*) δ 130.5, 129.1, 128.4, 127.0, 126.2, 126.0, 31.8, 12.2.



3ab+3ab'+*b*-3ab (86:11:3). White solid. Yield = 69% (18 mg), (Pent:CH_2Cl_2 = 97:3). ***MP*** = 38-55 °C. ***^{1}H-NMR*** (500 MHz, $CDCl_3$) δ 7.80-7.77 (m, 3H), 7.72 (s, 1H), 7.60 (d, J = 8.5 Hz, 1H), 7.47-7.43 (m, 2H), 6.68-6.61 (m, 3H), 6.54-6.45 (m,1H), 3.72 (d, J = 7.0 Hz, 2H), 2.46 (s, 3H). ***^{13}C-NMR*** (125 MHz, $CDCl_3$) δ 140.7, 138.3, 134.8, 133.6, 132.9, 131.2, 128.9, 128.1, 127.9, 127.6, 126.2, 125.9, 125.7, 124.9, 124.5, 123.6, 33.7, 15.4. ***GC-MS*** (m/z): 165, 249, 264.
3ab' ***^{1}H-NMR*** (500 MHz, $CDCl_3$, *diagnostic signals*) δ 7.69 (s, 1H), 7.05 (d, J = 5.5 Hz, 1H), 6.90 (d, J = 5.5 Hz, 1H), 3.51 (d, J = 6.5 Hz, 2H), 2.43 (s, 3H). ***Anal. Calc.*** for ($C_{18}H_{16}S$: 264.10): C, 81.77; H, 6.10; found: C, 81.62, H, 6.00.
b*-3ab** ***^{1}H-NMR (500 MHz, $CDCl_3$, *diagnostic signals*) δ 6.38-6.32 (m, 1H), 5.26 (d, J = 9.5 Hz, 1H), 5.16 (d, J = 17.0 Hz, 1H), 5.00 (d, J = 7.0 Hz, 1H).

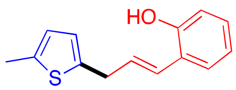


3ac+3ac'+*b*-3ac (60:27:13). Yellow oil. Yield = 69% (17 mg), (*c*Hex:Et_2O = 95:5). ***^{1}H-NMR*** (400 MHz, $CDCl_3$) δ 7.59 (dd, J = 1.6, 7.6 Hz, 1H), 7.37-7.33 (m, 1H), 7.23-7.14 (m, 3H), 6.92-6.89 (m, 1H), 6.65 (d, J = 3.2 Hz, 1H), 6.60 (brs, 1H), 6.4-6.2 (m, 1H), 3.71 (d, J = 7.2 Hz, 2H), 2.43 (s, 3H). ***^{13}C-NMR*** (100 MHz, $CDCl_3$) δ 140.3, 138.3, 135.4, 131.2, 129.6, 128.2, 127.4, 126.8, 126.7, 124.9, 124.5, 121.2, 33.7, 15.3. ***GC-MS*** (m/z): 115, 213, 233, 248.
3ac' ***^{1}H-NMR*** (400 MHz, $CDCl_3$, *diagnostic signals*) δ 7.49 (dd, J = 6.0 Hz, 7.2 Hz, 1H), 7.03 (d, J = 5.2 Hz, 1H), 3.50 (d, J = 6.5 Hz, 2H), 2.40 (s, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$, $CDCl_3$, *diagnostic signals*) δ 138.8, 134.8, 129.5, 32.1, 12.9. ***Anal. Calc.*** for ($C_{14}H_{13}ClS$: 248.04): C, 67.59; H, 5.27; found: C, 67.41, H, 5.15.
b*-3ac'** ***^{1}H-NMR (400 MHz, $CDCl_3$, *diagnostic signals*) δ 5.54 (d, J = 6.6 Hz, 2H), 5.21 (d, J = 10.2 Hz, 2H), 5.03 (d, J = 17.0 Hz, 2H), 2.45 (s, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$, $CDCl_3$, *diagnostic signals*) δ 46.3, 34.1.



3ad+3ad' (98:2). Colourless oil. Yield = 33% (8 mg), (*c*Hex:Et_2O = 98:2). ***^{1}H-NMR*** (500 MHz, $CDCl_3$) δ 7.30 (d, J = 9.0 Hz, 2H), 6.84 (d, J = 9.0 Hz, 2H), 6.62 (d, J = 3.0 Hz, 1H), 6.58 (d, J = 3.0 Hz, 1H), 6.44 (d, J = 15.5 Hz, 1H), 6.20

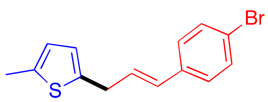
(dt, J = 7.0 Hz, J = 16.0 Hz, 1H), 3.81 (s, 3H), 3.63 (d, J = 6.5 Hz, 2H), 2.44 (s, 3H). ***^{13}C-NMR*** (125 MHz, $CDCl_3$) δ 159.0, 141.2, 138.1, 130.5, 130.1, 127.3, 126.3, 124.8, 124.3, 113.9, 55.3, 33.5, 15.3. ***GC-MS*** (m/z): 145, 229, 244. ***Anal. Calc.*** for ($C_{15}H_{16}OS$: 244.09): C, 73.73; H, 6.60; found: C, 73.54, H, 6.31.



3ae+3ae'+*b*-3ae (76:15:9). Colourless oil. Yield = 39% (9 mg), (*c*Hex:Et_2O = 85:15). ***^{1}H-NMR*** (400 MHz, $CDCl_3$) δ 7.32 (dd, J = 8.0 Hz, J = 2.8 Hz, 1H), 7.19 (dt, J = 8.0 Hz, J = 1.2 Hz, 1H), 6.87 (t, J = 7.3 Hz, 1H), 6.78 (d, J = 8.0 Hz, 1H), 6.70 (d, J = 15.2 Hz 1H), 6.62 (d, J = 4.0 Hz, 1H), 6.57 (d, J = 4.0 Hz, 1H), 6.34 (dt, J = 7.2 Hz, J =16.0 Hz, 1H), 3.68 (d, J = 7.4 Hz, 2H), 2.45 (s, 3H). ***^{13}C-NMR*** (100 MHz, $CDCl_3$) δ 152.6, 140.7, 130.7, 128.3, 127.6, 125.5, 124.8, 124.6, 124.4, 120.9, 115.7, 33.9, 15.3. ***GC-MS*** (m/z): 124, 215, 230. ***Anal. Calc.*** for ($C_{14}H_{14}OS$: 230.08): C, 73.01; H, 6.13; found: C, 72.88, H, 6.25.

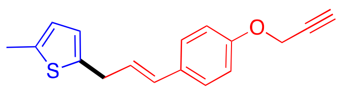
3ae' ***^{1}H-NMR*** (400 MHz, $CDCl_3$, *diagnostic signals*) δ 3.45 (d, J = 6.6 Hz, 2H), 2.41 (s, 3H).

b*-3ae'** ***^{1}H-NMR (400 MHz, $CDCl_3$, *diagnostic signals*) δ 5.25 (d, J = 9.9 Hz, 1H), 5.10 (d, J = 17.0 Hz, 1H), 5.02 (d, J = 6.8 Hz, 1H), 2.39 (s, 3H).



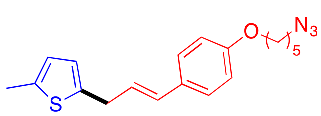
3af+3af' (75:21:4). Colourless oil. Yield = 56% (16 mg), (*n*-Pent). ***^{1}H-NMR*** (500 MHz, $CDCl_3$) δ 7.43-7.40 (m, 2H), 7.23-7.19 (m, 2H), 6.64 (d, J = 12.0 Hz, 2H), 6.43 (d, J = 16.0 Hz, 1H), 6.37-6.33 (m, 1H), 3.64 (d, J = 6.5 Hz, 2H), 2.45 (s, 3H). ***^{13}C-NMR*** (125 MHz, $CDCl_3$) δ 140.3, 138.3, 136.2, 131.6, 131.5, 129.9, 129.3, 127.7, 127.6, 124.9, 124.5, 120.9, 33.5, 15.3. ***GC-MS*** (m/z): 292-294. ***Anal. Calc.*** for ($C_{14}H_{14}BrS$: 291.99): C, 57.35; H, 4.47; found: C, 57.21, H, 4.23.

3af' ***^{1}H-NMR*** (500 MHz, $CDCl_3$, *diagnostic signals*) δ 7.03 (d, J = 5.5 Hz, 1H), 6.84 (d, J = 5.5 Hz, 1H), 3.44 (d, J = 5.0 Hz, 2H), 2.40 (s, 3H

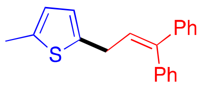


3ag+3ag' (91:9). Pale green oil. Yield = 85% (23 mg), (*c*Hex:Et_2O = 98:2). ***^{1}H-NMR*** (400 MHz, $CDCl_3$) δ 7.29 (d, J = 8.8 Hz, 2H), 6.89 (d, J = 8.8 Hz, 2H), 6.59 (dd, J = 3.3 Hz, J = 15.7 Hz, 1H), 6.56 (d, J = 4.8 Hz, 1H), 6.42 (d, J = 15.7 Hz, 1H), 6.20 (dt, J = 6.8 Hz, J = 15.7 Hz, 1H), 4.68 (d, J = 2.4 Hz, 2H), 3.63 (d, J = 7.2 Hz, 2H), 2.52 (s, 1H), 2.43 (s, 3H). ***^{13}C-NMR*** (100 MHz, $CDCl_3$) δ 156.8, 131.0, 130.4, 127.3(2C), 126.8, 124.8, 124.3, 115.0(2C), 78.5, 75.5, 55.8, 33.5, 29.7, 26.9, 15.3. ***GC-MS*** (m/z): 229, 268. ***Anal. Calc.*** for ($C_{14}H_{14}OS$: 268.09): C, 76.08; H, 6.01; found: C, 75.85, H, 5.78.

3af' ***^{1}H-NMR*** (400 MHz, $CDCl_3$, *diagnostic signals*) δ 3.41 (d, J = 7.2 Hz, 2H).

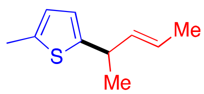


3ah+3ah' (98:2). Yellow oil. Yield = 30% (10 mg) (*c*Hex:EtOAc: 98:2). ***^{1}H-NMR*** (400 MHz, $CDCl_3$) δ 7.28 (dd, J = 1.6 Hz, J = 6.8 Hz, 2H), 6.81 (dd, J = 1.6 Hz, J = 6.4 Hz, 2H), 6.59 (d, J = 2.8 Hz, 1H), 6.55 (dd, J = 1.2 Hz, J = 2.8 Hz, 2H), 6.40 (d, J = 15.6 Hz, 1H), 6.18 (dt, J = 6.8 Hz, J = 15.6 Hz, 1H), 3.94 (t, J = 7.2 Hz, 2H), 3.60 (d, J = 7.2 Hz, 2H), 3.28 (t, J = 7.2 Hz, 2H), 2.44 (s, 3H), 1.80-1.76 (m, 2H), 1.68-1.63 (m, 2H), 1.56-1.52 (m, 2H). ***^{13}C-NMR*** (100 MHz, $CDCl_3$) δ 158.3, 141.2, 130.5, 130.1, 127.3(2C), 126.2, 124.8, 124.2, 114.5(2C), 67.6, 51.3, 33.5, 29.7, 28.8, 28.6, 26.9, 23.4, 15.3. ***DEP*** 313, 341. ***Anal. Calc.*** for ($C_{19}H_{23}N_3OS$: 341.16): C, 66.83; H, 6.79; found: C, 66.95, H, 6.55.

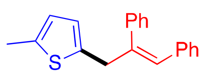


3ai+3ai' (71:29). Colourless oil. Yield = 69% (20 mg), (*c*Hex). ***^{1}H-NMR*** (500 MHz, $CDCl_3$) δ 7.44-7.40 (m, 3H), 7.36-7.34 (m, 1H), 7.32 -7.26 (m, 6H), 6.61 (bs, 1H), 6.59 (bs, 1H) 6.28 (t, J = 7.6 Hz, 1H), 3.56 (d, J = 7.6 Hz, 2H), 2.46 (s, 3H). ***^{13}C-NMR*** (125 MHz, $CDCl_3$) δ 142.6, 142.3, 141.5, 139.5, 137.9, 129.8, 128.3, 128.1, 127.4, 127.2, 127.1, 126.9, 124.8, 123.9, 30.5, 15.3. ***GC-MS*** (m/z): 290. ***Anal. Calc.*** for ($C_{20}H_{18}S$: 290.11): C, 82.71; H, 6.25; found: C, 82.51, H, 6.05.

3ai' ***^{1}H-NMR*** (500 MHz, $CDCl_3$, *diagnostic signals*) δ: 7.02 (d, J = 5.2 Hz, 1H), 6.87 (d, J = 5.2 Hz, 1H), 6.22 (t, J = 7.5 Hz, 1H), 3.36 (d, J = 7.5 Hz, 2H), 2.30 (s, 3H). ***^{13}C-NMR*** (125 MHz, $CDCl_3$, *diagnostic signals*) δ: 129.9, 128.1, 127.1, 121.0, 28.8, 12.9.



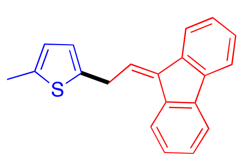
3aj+3aj' (98:2). Colourless oil. Yield = 45% (8 mg), (*c*Hex). ***^{1}H-NMR*** (500 MHz, $CDCl_3$) δ 6.57 (bs, 2H), 5.60-5.50 (m, 2H), 3.60-3.56 (m, 1H), 2.44 (s, 3H),1.69 (d, J = 5.5 Hz, 3H), 1.38 (d, J = 7.0 Hz, 3H). ***^{13}C-NMR*** (125 MHz, $CDCl_3$) δ 148.5, 137.3, 135.8, 124.5, 124.1, 122.3, 38.2, 22.3, 17.7, 15.3. ***GC-MS*** (m/z): 166. ***Anal. Calc.*** for ($C_{10}H_{14}S$: 166.08): C, 72.23; H, 8.49; found: C, 72.39, H, 8.51.



3ak+3ak'+*b*-3ak (75:18:7). Colourless oil. Yield = 62% (18 mg) (*n*-Pent:Et_2O = 98:2). ***^{1}H-NMR*** (500 MHz, $CDCl_3$) δ 7.33 -7.25 (m, 4H), 7.14 (d, J = 6.5 Hz, 2H), 7.10-7.07 (m, 4H), 6.96 (d, J = 6.5 Hz, 2H), 6.56 (s, 1H), 3.90 (s, 2H), 2.42 (s, 3H). ***^{13}C-NMR*** (125 MHz, $CDCl_3$) δ 141.3, 140.6, 139.9, 138.4, 137.1, 129.1, 128.7, 128.4, 128.0, 127.8, 127.1, 126.4, 125.4, 124.7, 41.0, 15.4. ***GC-MS*** (m/z): 111, 178, 275, 290. ***Anal. Calc.*** for ($C_{20}H_{18}S$: 290.11): C, 82.71; H, 6.25; found: C, 82.91, H, 6.15.

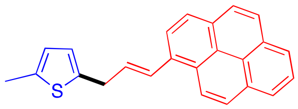
3ak' ***^{1}H-NMR*** (500 MHz, $CDCl_3$, *diagnostic signals*) δ: 6.34 (s, 1H), 3.68 (s, 2H), 2.26 (s, 3H). ***^{13}C-NMR*** (125 MHz, $CDCl_3$, *diagnostic signals*) δ :129.6, 120.9, 39.4.

b*-3ak** ***^{1}H-NMR (500 MHz, $CDCl_3$, *diagnostic signals*) δ: 5.66 (s, 1H), 5.47 (s, 1H), 5.01 (s, 1H). ***^{13}C-NMR*** (125 MHz, $CDCl_3$, *diagnostic signals*) δ: 51.2.



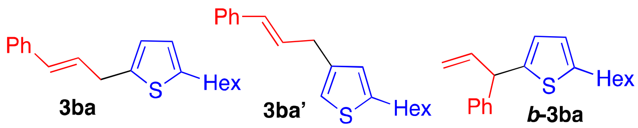
3al+3al' (90:10). Yellow wax. Yield = 56% (16 mg), (*c*Hex:Et_2O = 95:5). ***^{1}H-NMR*** (400 MHz, $CDCl_3$) δ 7.87 (d, J = 7.6 Hz, 1H), 7.77 (d, J = 7.4 Hz, 1H), 7.65 (d, J = 7.6 Hz, 1H), 7.62 (d, J = 7.4 Hz, 1H), 7.42-7.24 (m, 4H), 6.85 (t, *J* = 7.4 Hz, 1H), 6.72 (d, *J* = 3.4 Hz, 1H), 6.60 (dd, J = 1.3 Hz, J = 3.5 Hz, 1H), 4.29 (d, J = 7.5 Hz, 2H), 2.44 (s, 3H). ***^{13}C-NMR*** (100 MHz, $CDCl_3$) δ 141.1, 139.7, 139.2, 138.8, 138.5, 137.1,136.1, 138.1, 127.8, 127.6, 127.1, 127.0, 125.0, 124.9, 124.8, 120.9, 119.9, 119.5, 30.0, 15.3. ***GC-MS*** (m/z): 273, 288. ***Anal. Calc.*** for ($C_{20}H_{16}S$: 288.10): C, 83.29; H, 5.59; found: C, 83.05, H, 5.41.

3al' ***^{1}H-NMR*** (400 MHz, $CDCl_3$, *diagnostic signals*) δ 7.92 (d, J = 7.6 Hz, 1H), 7.05 (d, J = 6.0 Hz, 1H), 6.92 (d, J = 6.0 Hz, 1H), 4.09 (d, J = 7.1 Hz, 1H), 2.46 (s, 3H). ***^{13}C-NMR*** (100 MHz, $CDCl_3$, *diagnostic signals*) δ: 29,7.



3am+3am' (90:10). Pale yellow wax. Yield = 70% (25 mg), (*n*Pent:Et_2O = 97:3).***[1]H-NMR*** (400 MHz, $CDCl_3$) δ: 8.38 (d, J = 9.2 Hz, 1H), 8.16-8.07 (m, 5H), 8.02 (s, 2H), 7.97 (t, J = 7.8 Hz, 1H), 7.52 (d, J = 16.0 Hz, 1H), 6.72 (bs, 1H), 6.62 (bs, 1H), 6.59-6.57 (m, 1H), 3.87 (d, J = 6.4 Hz, 2H), 2.48 (s, 3H). ***[13]C-NMR*** (100 MHz, $CDCl_3$) δ: 140.7, 138.4, 132.1, 132.0, 131.5, 131.0, 130.6, 128.5, 127.4 (2C), 127.4, 125.9, 125.1, 125.0, 124.9 (2C), 124.9, 124.6, 124.1, 123.2, 34.2, 15.4. ***GC-MS*** (m/z): 239, 338. ***Anal. Calc.*** for ($C_{25}H_{20}S$: 352.13): C, 85.19; H, 5.72; found: C, 84.98, H, 5.65.

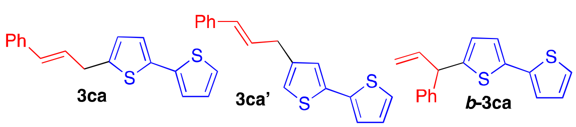
3am' ***[1]H-NMR*** (400 MHz, $CDCl_3$, *diagnostic signals*) δ 8.31 (d, J = 8.0 Hz, 1H), 7.41 (d, J = 16.0 Hz, 1H), 7.07 (d, J = 6.0 Hz, 1H), 6.96 (d, J = 8.0 Hz, 1H), 3.64 (d, J = 8.0 Hz, 1H), 2.48 (s, 3H). ***[13]C-NMR*** (100 MHz, $CDCl_3$, *diagnostic signals*) δ: 36.5.



3ba:3ba':*b*-3ba (77:16:7). Colourless oil (GO = 25 wt%, 90 C°, 6 h). Yield = 51% (8 mg) (*c*Hex). ***[1]H-NMR*** (500 MHz, $CDCl_3$) δ 7.39-7.37 (m, 2H), 7.35-7.28 (m, 2H), 7.24-7.20 (m, 1H), 6.65 (bs,1H), 6.61 (bs,1H), 6.50 (d, J = 16.0 Hz, 1H), 6.39-6.31 (m,1H), 3.67 (d, J = 7.0 Hz, 2H), 2.76 (t, J = 8.0 Hz, 2H), 1.67-1.62 (m, 2H), 1.40-1.27 (m, 6H), 0.91-0.89 (m, 3H). ***[13]C-NMR*** (125 MHz, $CDCl_3$) δ 144.4, 140.4, 137.3, 131.1, 128.5, 128.4, 127.2, 126.2, 124.1, 123.6, 33.6, 31.7, 31.6, 30.2, 28.8, 22.6, 14.1. ***GC-MS*** (m/z): 284. ***Anal. Calc.*** for ($C_{19}H_{22}OS$: 298.14): C, 76.47; H, 7.43; found: C, 76.32, H, 7.22.

3ba' ***[1]H-NMR*** (500 MHz, $CDCl_3$, *diagnostic signals*) δ 7.06 (d, J = 5.0 Hz, 1H), 6.86 (d, J = 5.0 Hz, 1H), 3.46 (d, J = 6.5 Hz, 2H).

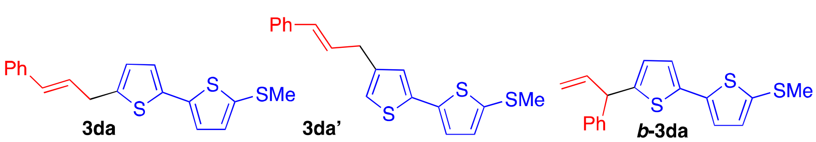
b*-3ba** ***[1]H-NMR (500 MHz, $CDCl_3$, *diagnostic signals*) δ 5.20 (d, J = 10.5 Hz, 1H), 5.10 (d, J = 17.5 Hz, 1H), 4.83 (d, J = 7.5 Hz, 1H).



3ca+3ca'+*b*-3ca (60:33:7). Yellow oil (GO = 50 wt%, 90 C°, 6 h). Yield = 48% (14 mg) (*n*Hex). ***[1]H-NMR*** (400 MHz, $CDCl_3$) δ: 7.40 (d, J = 6.8 Hz, 1H), 7.37-7.30 (m, 3H), 7.26-7.22 (m, 1H), 7.20-7.16 (m, 1H), 7.12-7.07 (m, 1H), 7.04-7.00 (m, 2H), 6.78 (d, J = 3.3 Hz, 1H), 6.55 (d, J = 15.6 Hz, 1H), 6.42-6.38 (m, 1H), 3.72 (d, J = 6.8 Hz, 2H). ***[13]C-NMR*** (100 MHz, $CDCl_3$) δ 142.5, 137.1, 135.8, 131.7, 130.2, 128.5, 128.5, 127.7, 127.4, 126.2, 126.1, 125.4, 123.6, 123.2, 33.5. ***GC-MS*** (m/z): 115, 179, 282. ***Anal. Calc.*** for ($C_{17}H_{14}S_2$: 282.05): C, 72.30; H, 5.00; found: C, 72.45, H, 5.12.

3da' ***[1]H-NMR*** (400 MHz, $CDCl_3$, *diagnostic signals*) δ 3.68 (d, J = 5.0 Hz, 2H). ***[13]C-NMR*** (100 MHz, $CDCl_3$, *diagnostic signals*) δ: 30.3.

b*-3da** ***[1]H-NMR (400 MHz, $CDCl_3$, *diagnostic signals*) δ 5.26 (d, J = 9.6 Hz, 1H), 5.16 (d, J = 17.2 Hz, 1H), 4.88 (d, J = 7.2 Hz,1H).

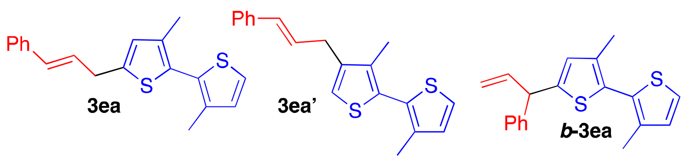


3da+3da'+*b*-3da+3da'' (68:19:13). Yellow oil (GO = 50 wt%, 90 C°, 6 h). Yield = 27% (9 mg), (*c*Hex). ***[1]H-NMR*** (500 MHz, $CDCl_3$) δ 7.39-7.34 (m, 2H), 7.33-7.28 (m, 2H) 7.25 -7.20 (m, 2H), 7.15-7.09 (m, 1H), 7.02-6.95 (m, 2H), 6.47 (d, J = 16.0 Hz, 1H), 6.39-6.29 (m, 1H), 3.60 (d, J = 7.0 Hz, 2H), 2.43 (s, 3H). ***[13]C-NMR*** (125 MHz, $CDCl_3$) δ 144.3, 138.5, 137.3, 131.1, 130.3, 128.5, 128.1, 127.8, 127.2, 126.1, 125.4, 124.6, 123.8, 32.6, 22.2. ***GC-MS*** (m/z): 328. ***Anal. Calc.*** for ($C_{18}H_{16}S_3$: 328.04): C, 65.81; H, 4.91; found: C, 65.61, H, 4.66.

3da' ***^{1}H-NMR*** (500 MHz, $CDCl_3$, *diagnostic signals*) δ 6.93 (d, J = 3.0 Hz ,1H), 6.76 (d, J = 3.0 Hz ,1H), 6.53 (d, J = 16.0 Hz ,1H), 3.79 (d, J = 7.0 Hz, 2H), 2.50 (s, 3H).

b*-3da** ***^{1}H-NMR (500 MHz, $CDCl_3$, *diagnostic signals*): 3.66 (d, J = 5.5 Hz, 2H), 2.52 (s, 3H).

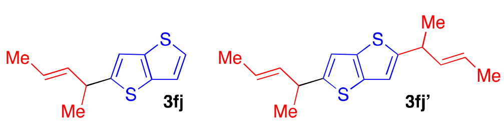
Traces of a forth undefined isomer 3da'' were also detected by NMR. ***^{1}H-NMR*** (500 MHz, $CDCl_3$, *diagnostic signals*): 3.68 (d, J = 6.5 Hz, 2H), 2.51 (s, 3H).



3ea+3ea'+*b*-3ea (63:18:19). Yellow oil (GO = 50 wt%, 90 C°, 6 h). Yield = 60% (19 mg), (*n*Hex:Et_2O = 96:4). ***^{1}H-NMR*** (500 MHz, $CDCl_3$) δ 7.41-7.39 (m, 2H), 7.35-7.30 (m, 3H), 7.26-7.22 (m, 2H), 6.91 (d, J = 5.0 Hz, 1H), 6.54 (d, J = 16.0 Hz, 1H), 6.41-6.35 (m,1H), 3.68 (d, J = 7.0 Hz, 2H), 2.19 (s, 3H), 2.12 (s, 3H). ***^{13}C-NMR*** (125 MHz, $CDCl_3$) δ 142.6, 139.9, 137.2, 136.4, 136.2, 131.6, 129.9, 128.5, 128.2, 127.8, 127.8, 127.3, 126.3, 124.7, 33.5, 14.8, 14.7. ***GC-MS*** (m/z): 310. ***Anal. Calc.*** for ($C_{19}H_{18}S_2$: 310.08): C, 73.50; H, 5.84; found: C, 73.66, H, 5.68.

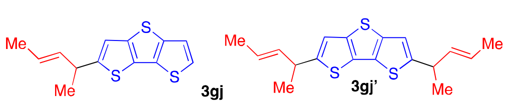
3ea' ***^{1}H-NMR*** (500 MHz, $CDCl_3$, *diagnostic signals*) δ 6.32-6.29 (m, 1H), 3.48 (d, J = 6.0 Hz, 2H).

b*-3ea** ***^{1}H-NMR (500 MHz, $CDCl_3$, *diagnostic signals*) δ 5.23 (d, J = 9.5 Hz, 1H), 5.16 (d, J = 17.0 Hz, 1H), 4.84 (d, J = 7.0 Hz, 1H). ***^{13}C-NMR*** (125 MHz, $CDCl_3$, *diagnostic signals*) δ 51.1.

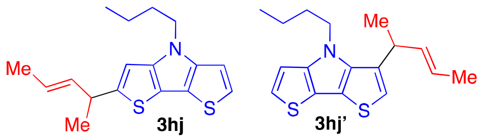


3fj+3fj' (95:5). Colourless oil (GO = 50 wt%, 90 C°, 6 h). Yield = 64% (13 mg) (*n*-Pent:EtOAc:CH_2Cl_2 = 98:1:1). ***^{1}H-NMR*** (500 MHz, $CDCl_3$) δ 7.27 (d, J = 5.5 Hz, 1H), 7.18 (d, J = 5.5 Hz, 1H), 6.99 (s, 1H), 5.66-5.56 (m, 2H), 3.73-3.70 (m, 1H), 1.71 (d, J = 6.0 Hz, 3H), 1.45 (d, J = 6.5 Hz, 3H). ***^{13}C-NMR*** (125 MHz, $CDCl_3$) δ 138.7, 137.4, 135.3, 135.1, 125.4, 125.0, 119.5, 115.0, 39.1, 22.1, 17.8. ***GC-MS*** (m/z): 193, 208. ***Anal. Calc.*** for ($C_{11}H_{12}S_2$: 208.04): C, 63.42; H, 5.81; found: C, 63.31, H, 5.69.

3aq' ***^{1}H-NMR*** (500 MHz, $CDCl_3$, *diagnostic signals*) δ: 3.51-3.47 (m, 1H). ***^{13}C-NMR*** (125 MHz, $CDCl_3$, *diagnostic signals*) δ: 39.0, 22.2.

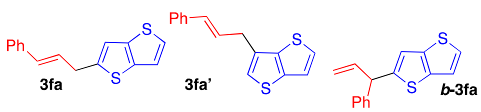


3gj+3gj' (95:5). Colourless oil (GO = 50 wt%, 90 C°, 6 h). Yield = 32% (8 mg) (*c*Hex:Et_2O = 96:4). ***^{1}H-NMR*** (400 MHz, $CDCl_3$) δ: 7.29 (d, J = 5.2 Hz, 1H), 7.26 (d, J = 5.2 Hz, 1H), 7.00 (s, 1H), 5.67-5.56 (m, 2H), 3.76-3.70 (m, 1H), 1.72 (d, J = 5.2 Hz, 3H), 1.47 (d, J = 7.2 Hz, 3H). ***^{13}C-NMR*** (100 MHz, $CDCl_3$) δ: 152.2, 140.8, 140.1, 134.9, 131.3, 129.0, 125.2, 125.0, 120.7, 116.4, 39.1, 22.1, 17.8. ***GC-MS*** (m/z): 249, 264. ***Anal. Calc.*** for ($C_{13}H_{12}S_3$: 264.01): C, 59.05; H, 4.57; found: C, 59.26, H, 4.69.



3hj+3hj' (94:6). Colourless oil (GO = 50 wt%, 90 C°, 6 h). Yield = 28% (9 mg). (*n*-Pent:Et_2O = 95:5). ***[1]H-NMR*** (400 MHz, $CDCl_3$) δ 7.05 (d, J = 5.6 Hz, 1H), 6.97 (d, J = 5.6 Hz, 1H), 6.73 (s, 1H), 5.68-5.54 (m, 2H), 4.15 (t, J = 7.2 Hz, 2H), 3.72-3.68(m, 1H), 1.87-1.80 (m, 2H), 1.72 (d, J = 5.6 Hz, 3H), 1.46 (d, J = 7.2 Hz, 3H), 1.39-1.33 (m, 2H), 0.94 (t, J = 7.6 Hz, 3H). ***[13]C-NMR*** (100 MHz, $CDCl_3$) δ 149.0, 144.0, 143.6, 135.4, 124.6, 121.7, 114.9, 112.5, 110.8, 107.1, 47.0, 39.3, 32.5, 22.2, 20.2, 17.8, 13.7. ***GC-MS*** (m/z): 255, 288, 303. ***Anal. Calc.*** for ($C_{17}H_{21}NS_2$: 303.11): C, 67.28; H, 6.98; found: C, 67.05, H, 6.77.

3hj' ***[1]H-NMR*** (400 MHz, $CDCl_3$) δ: 7.12 (d, J = 5.2 Hz, 1H), 7.01 (d, J = 5.2 Hz, 1H), 6.69 (s,1H).

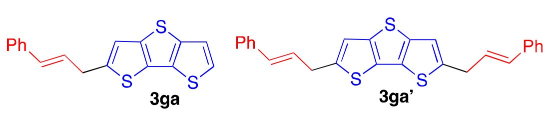


3fa+3fa'+*b*-3fa (85:8:7). White solid. (GO = 50 wt%, 90 C°, 6 h). Yield = 50% (13 mg), (*n*Pent: CH_2Cl_2 = 97:3). ***MP*** = 90-100 °C. ***[1]H-NMR*** (500 MHz, $CDCl_3$) δ: 7.39 (d, J = 7.5 Hz, 2H), 7.32 (d, J = 7.0 Hz, 2H), 7.30 (d, J = 6.0 Hz, 1H), 7.26-7.22 (m, 1H), 7.20 (d, J = 5.5 Hz, 1H), 7.05 (s, 1H), 6.56 (d, J = 15.5 Hz, 1H), 6.40 (dt, J = 6.5 Hz, J = 16.5 Hz, 1H), 3.80 (d, J = 6.5 Hz, 2H). ***[13]C-NMR*** (125 MHz, $CDCl_3$) δ: 145.7, 138.9, 138.0, 137.1, 131.9, 128.6, 127.5, 127.4, 126.3, 125.7, 119.5, 117.0, 34.6. ***GC-MS*** (m/z): 153, 179, 256. ***Anal. Calc.*** for ($C_{15}H_{12}S_2$: 256.04): C, 70.27; H, 4.72; found: C, 70.45, H, 4.51.

3fa' ***[1]H-NMR*** (500 MHz, $CDCl_3$, *diagnostic signals*) δ 6.98 (d, J = 13.5 Hz, 1H), 6.62 (d, J = 16.5 Hz, 1H), 3.66 (d, J = 6.5 Hz, 2H). ***[13]C-NMR*** (125 MHz, $CDCl_3$, *diagnostic signals*) δ: 33.6.

b*-3fa** ***[1]H-NMR (500 MHz, $CDCl_3$, *diagnostic signals*) δ 6.36-6.29 (m, 1H),5.27 (d, J = 10.0 Hz, 1H), 5.18 (d, J = 17.0 Hz, 1H), 4.96 (d, J = 7.5 Hz, 1H). ***[13]C-NMR*** (125 MHz, $CDCl_3$) δ: 51.6.

Traces of a forth undefined isomer 3fa'' were also detected by NMR. ***[1]H-NMR*** (500 MHz, $CDCl_3$, *diagnostic signals*) δ 3.55 (d, J = 7.0 Hz, 2H).

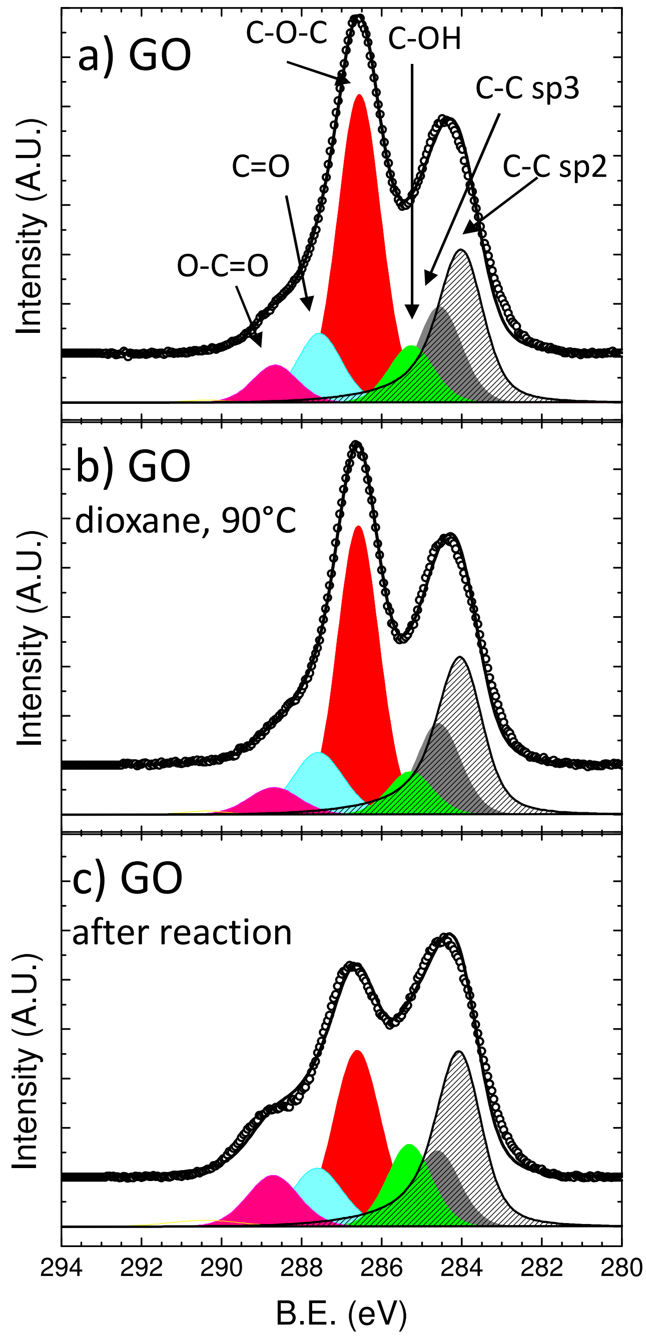


3ga+3ga' (95:5) White solid. (GO = 50 wt%, 90 C°, 6 h). Yield = 32% (10 mg), (*n*Pent:CH_2Cl_2 = 98:2). ***MP*** = 78-110 °C. ***[1]H-NMR*** (500 MHz, $CDCl_3$) δ 7.39 (d, J = 6.0 Hz, 2H), 7.34-7.31 (m, 3H), 7.27-7.23 (m, 2H), 7.07 (s, 1H), 6.57 (d, J = 16.0 Hz, 1H), 6.41 (dt, J = 7.0 Hz, J = 16.0 Hz, 1H), 3.82 (d, J = 7.0 Hz, 2H). ***[13]C-NMR*** (125 MHz, $CDCl_3$) δ: 144.4, 140.9, 140.3, 137.0, 132.1, 131.2, 129.4, 128.6, 127.5, 127.3, 126.3, 125.2, 120.7, 118.3, 34.5. ***GC-MS*** (m/z): 209, 235, 312. ***Anal. Calc.*** for ($C_{17}H_{12}S_3$: 312.01): C, 65.35; H, 3.87; found: C, 65.12, H, 3.71.

3ga' ***[1]H-NMR*** (500 MHz, $CDCl_3$, *diagnostic signals*) δ: 6.25 (dt, J = 6.5 Hz, J = 16.0 Hz, 1H), 3.56 (d, J = 6.5 Hz, 2H).

b*-3ga** ***[1]H-NMR (500 MHz, $CDCl_3$, *diagnostic signals*) δ: 6.35-6.30 (m, 1H), 5.29 (d, J = 6.5 Hz, 1H), 5.19 (d, J = 16.5 Hz, 1H), 4.98 (d, J = 8.0 Hz, 1H).

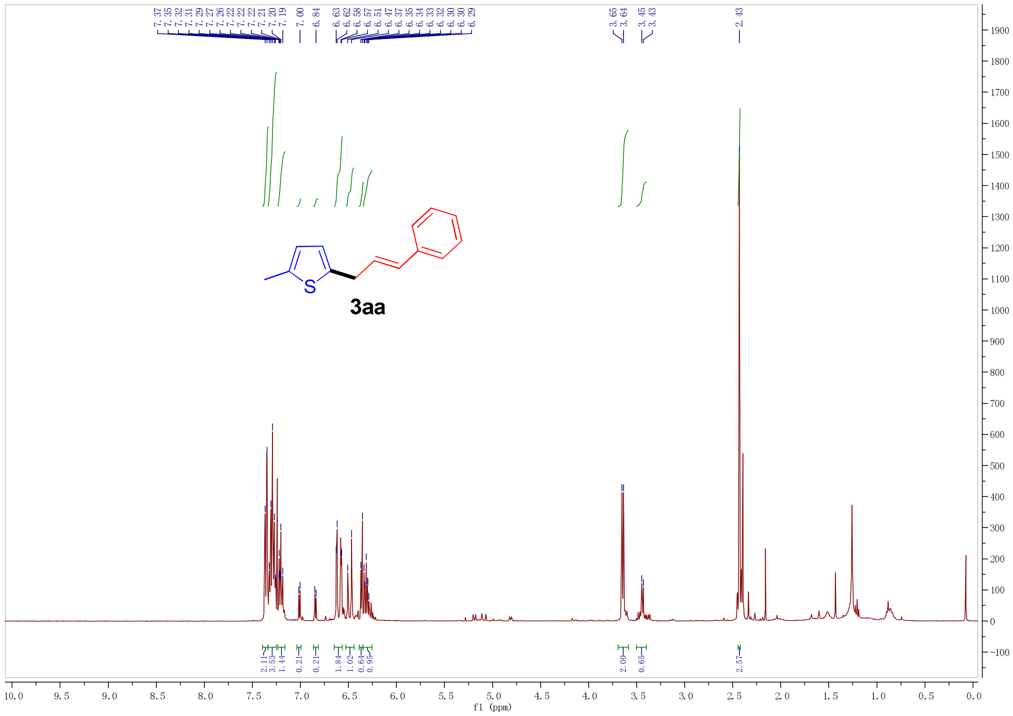
Figure S1

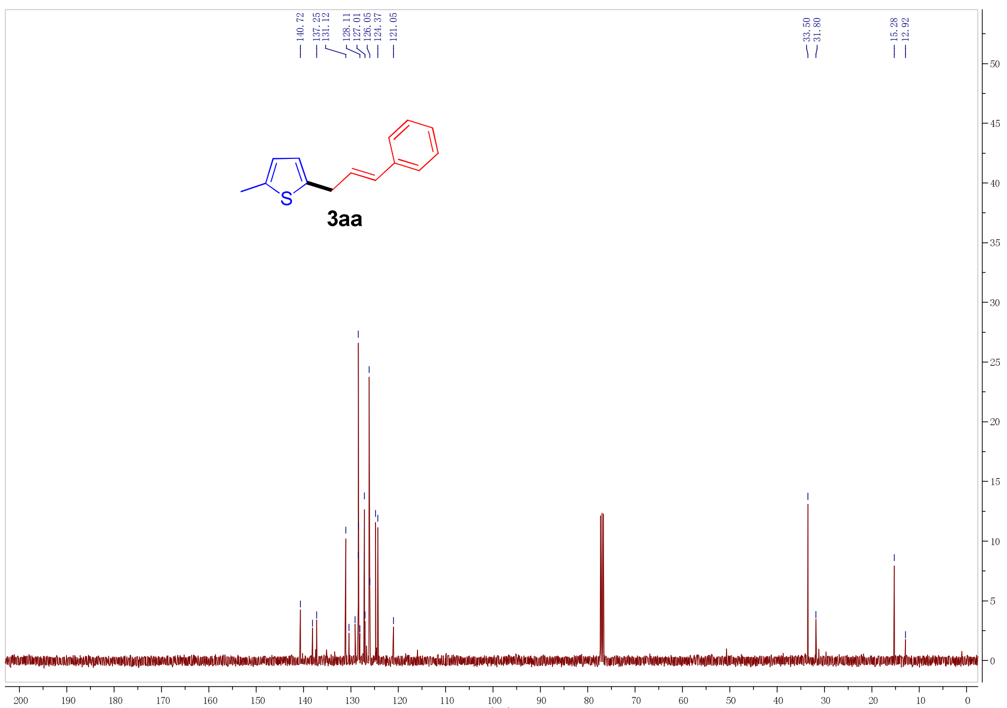


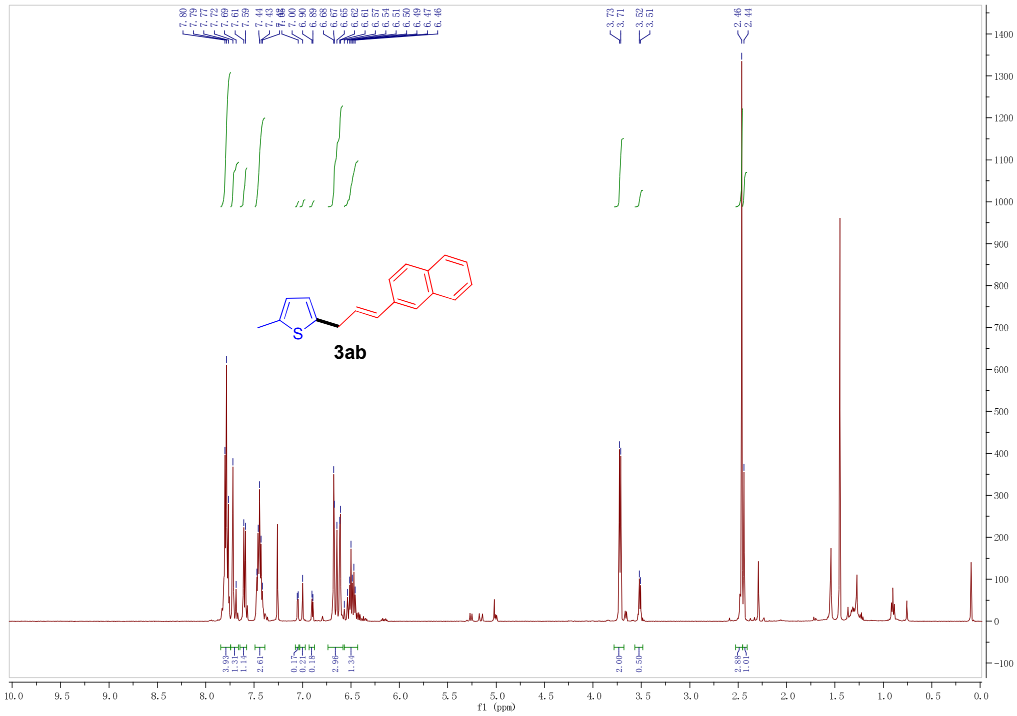
C=C aromatic	C-C defects	C-OH	C-O-C	C=O	O-C=O
284,4	285,0	285,7	286,7	288,0	290,1

Table S1

	GO	GO, 90°C dioxane	GO after reaction
O/C	0.47 ± 0.03	0.44 ± 0,03	0.53 ± 0.03
C-C (sp2)	25.1 ± 0.5	27.7 ± 0.5	31.4 ± 0.6
C-C (sp3)	12.7 ± 0.3	12.9 ± 0.3	10.9 ± 0.3
C-OH	7.6 ± 0.3	6.2 ± 0.3	11.9 ± 0.3
C-O-C	40.3 ± 0.8	38,7 ± 0.8	27.4 ± 0.6
C=O	9.3 ± 0.3	10.1 ± 0.3	9.8 ± 0.3
O-C=O	5.0 ± 0.3	4.4 ± 0.3	8.6 ± 0.3



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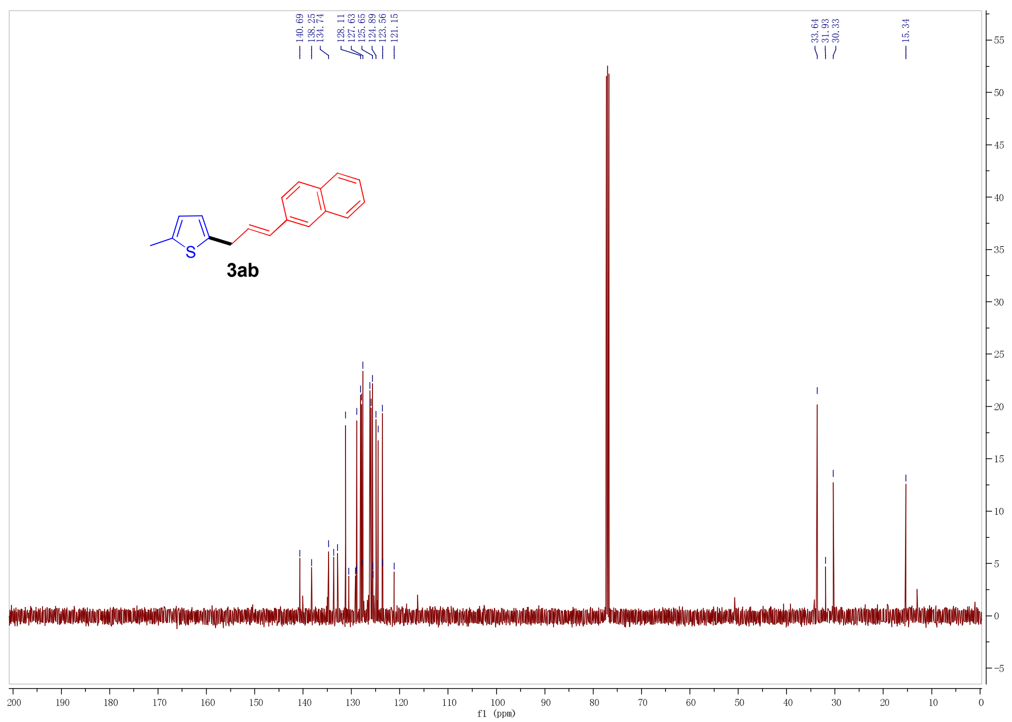
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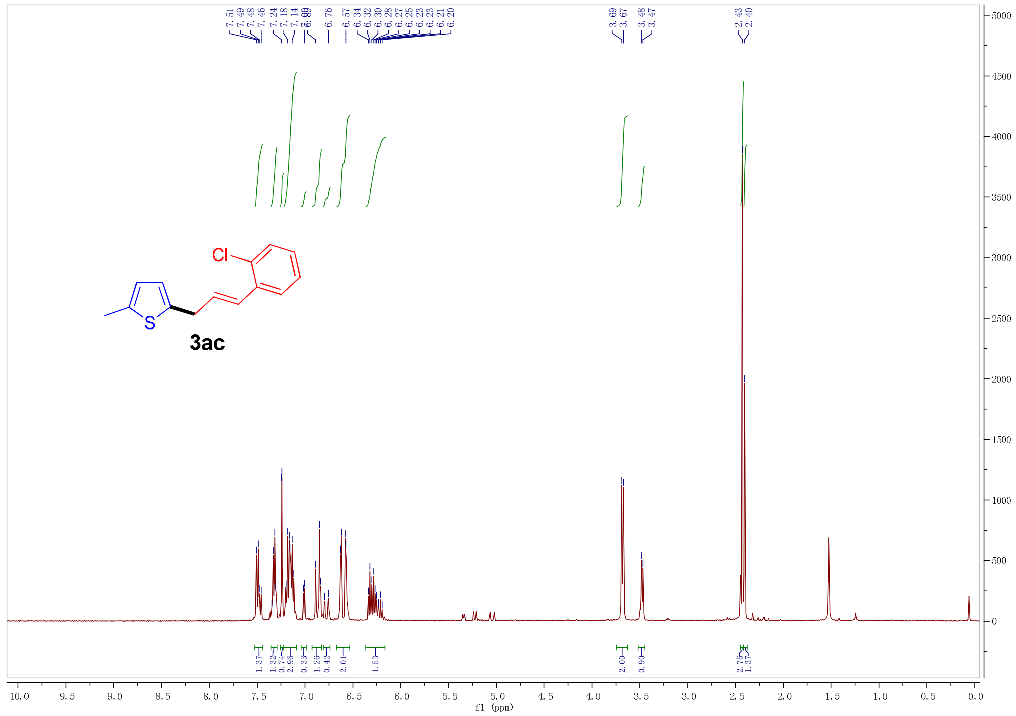

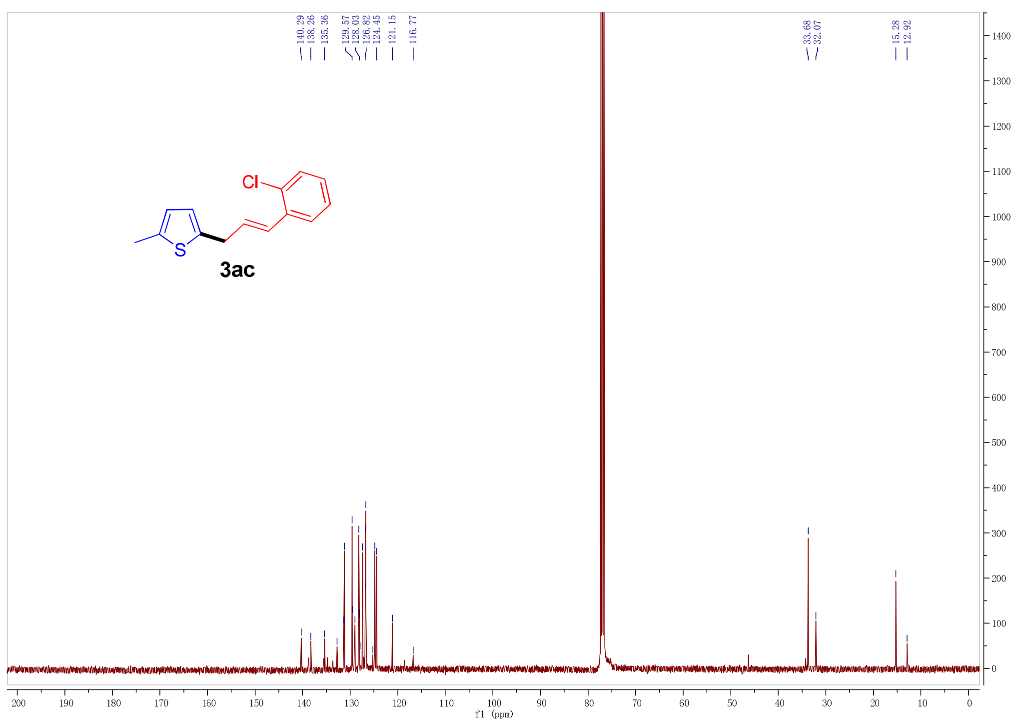

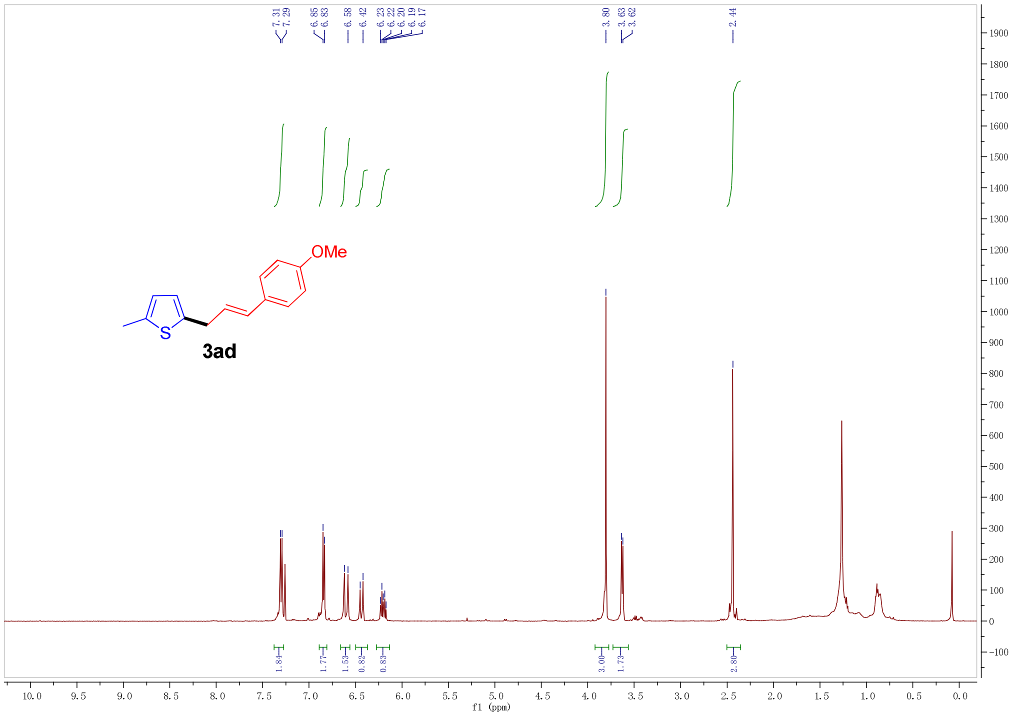
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3.62
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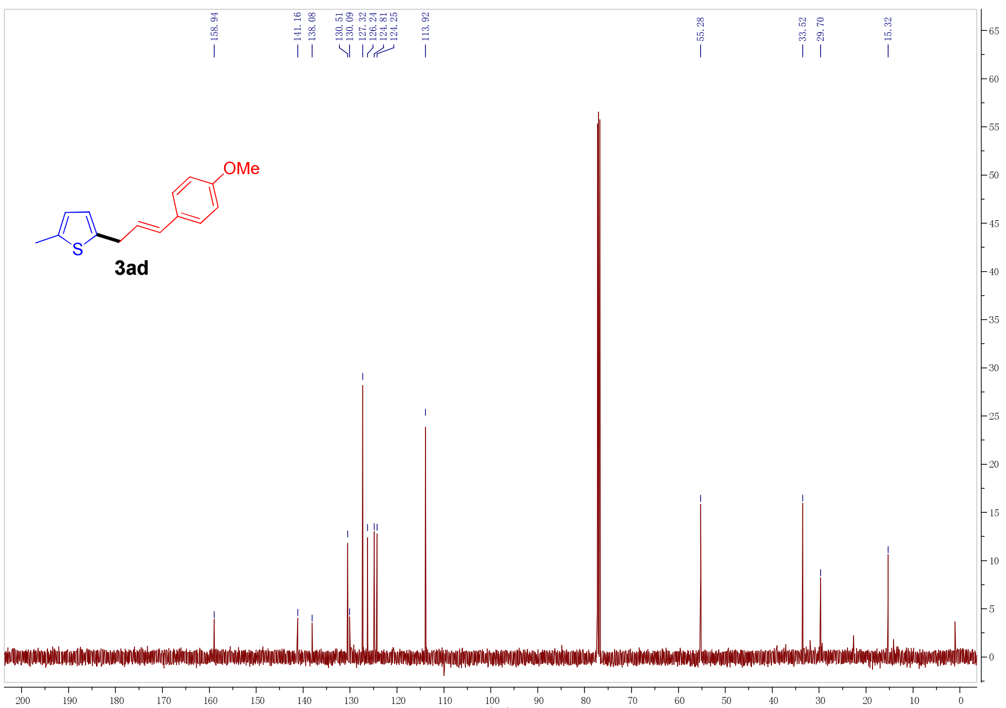
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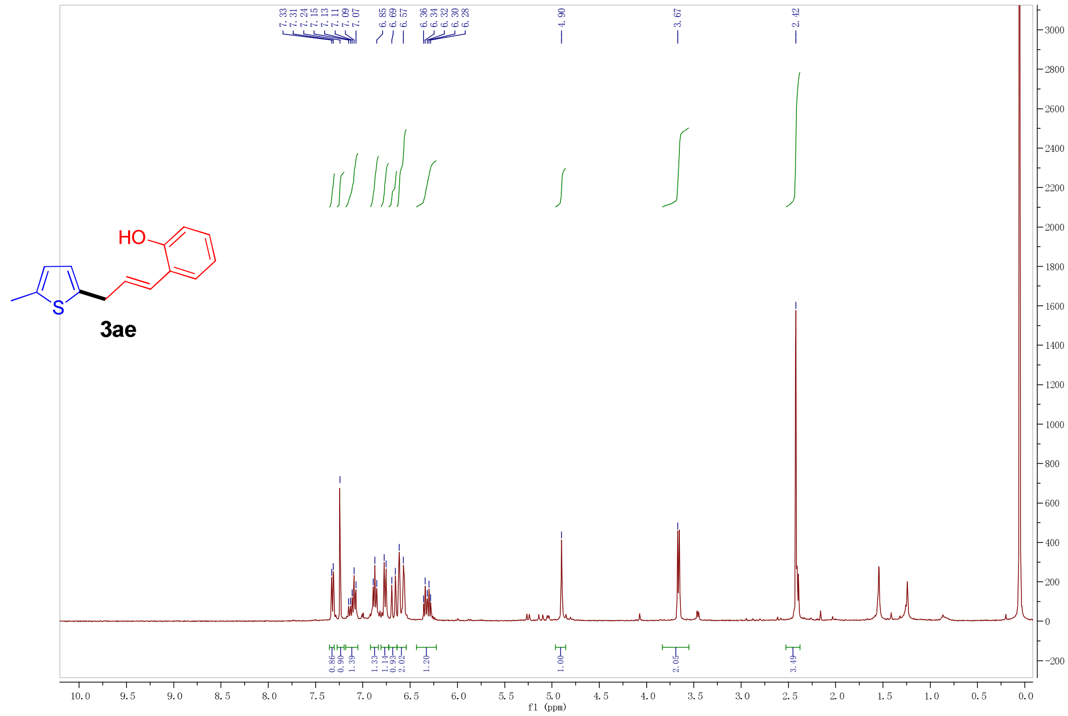
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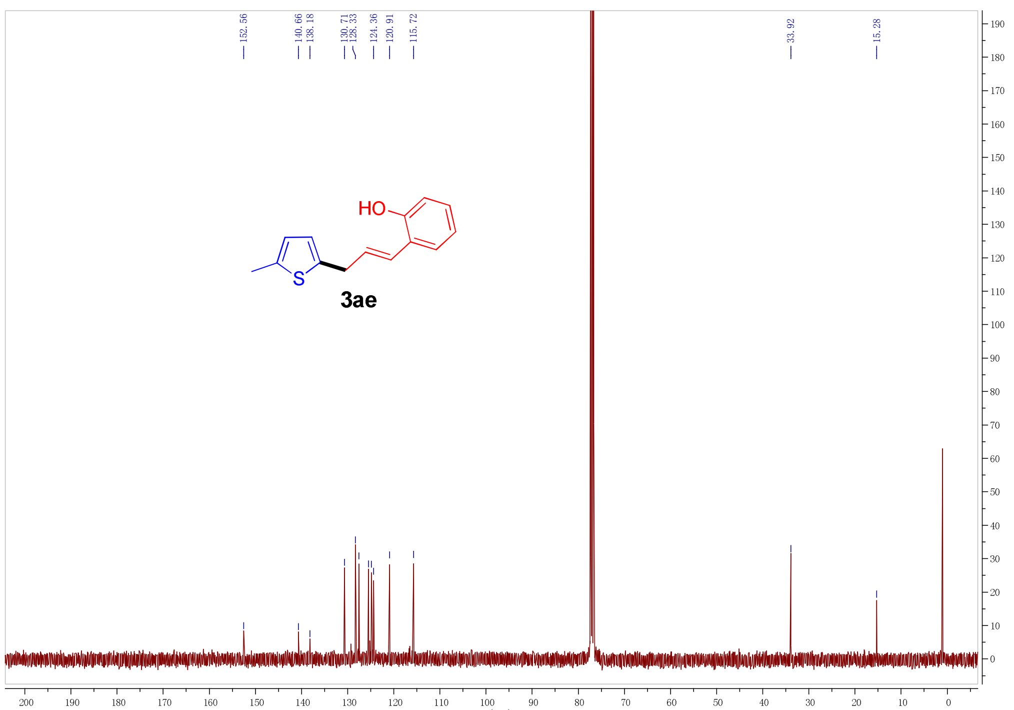
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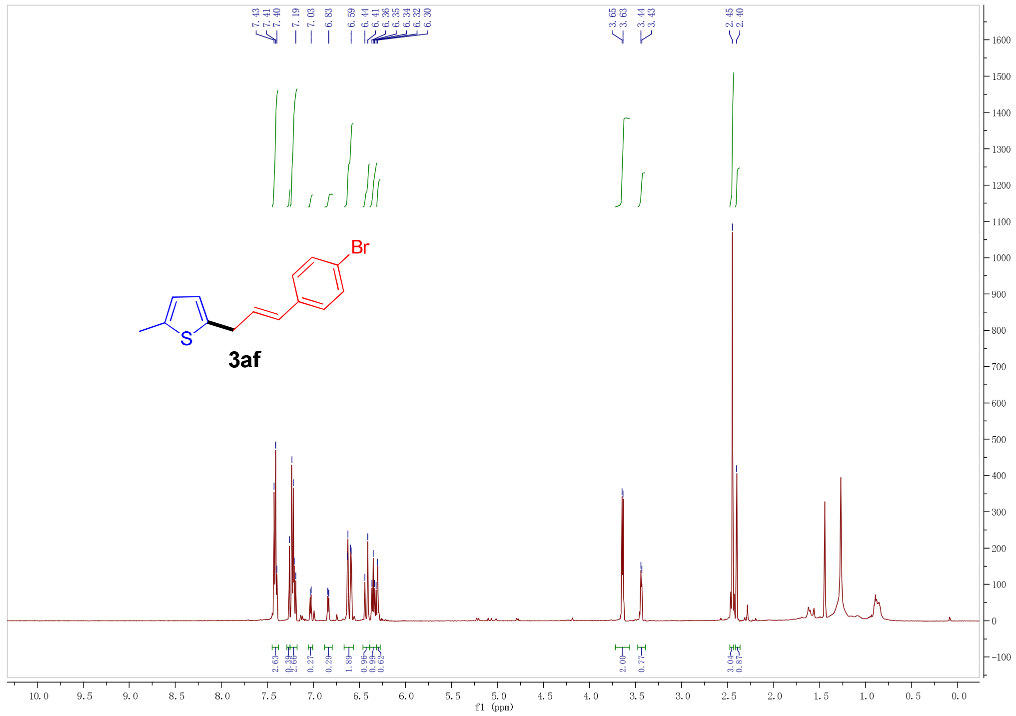

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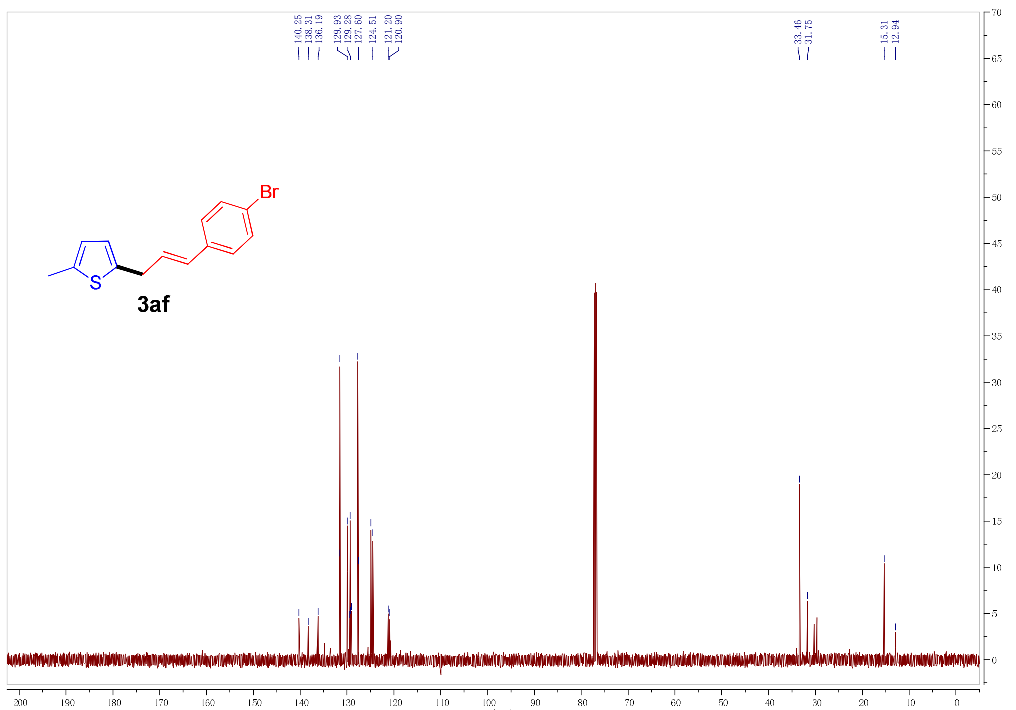

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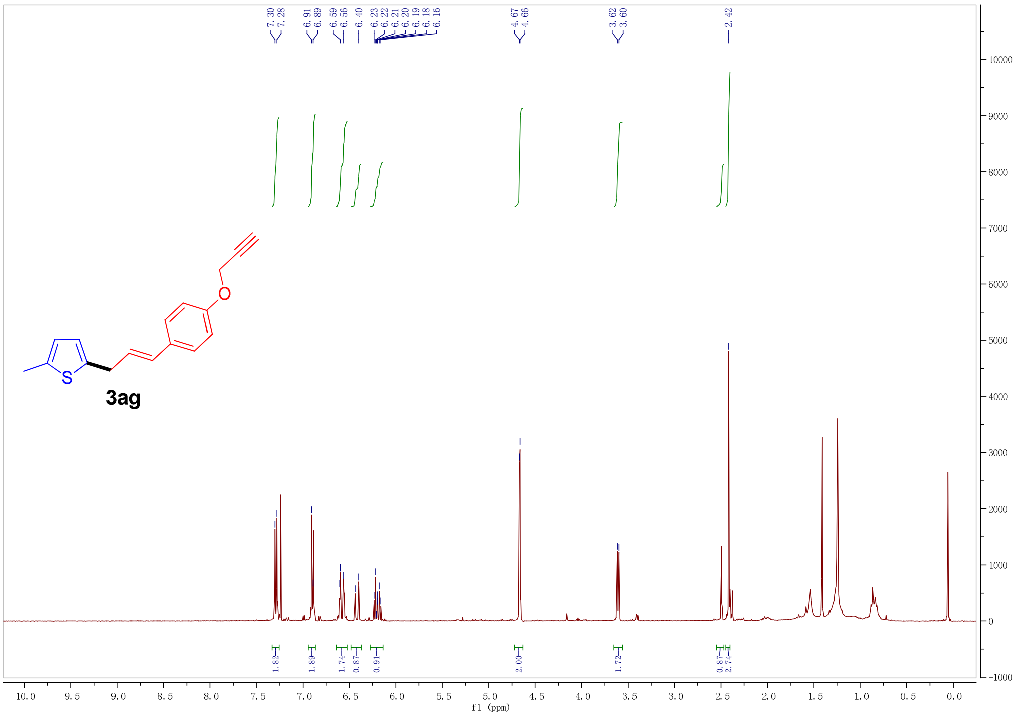
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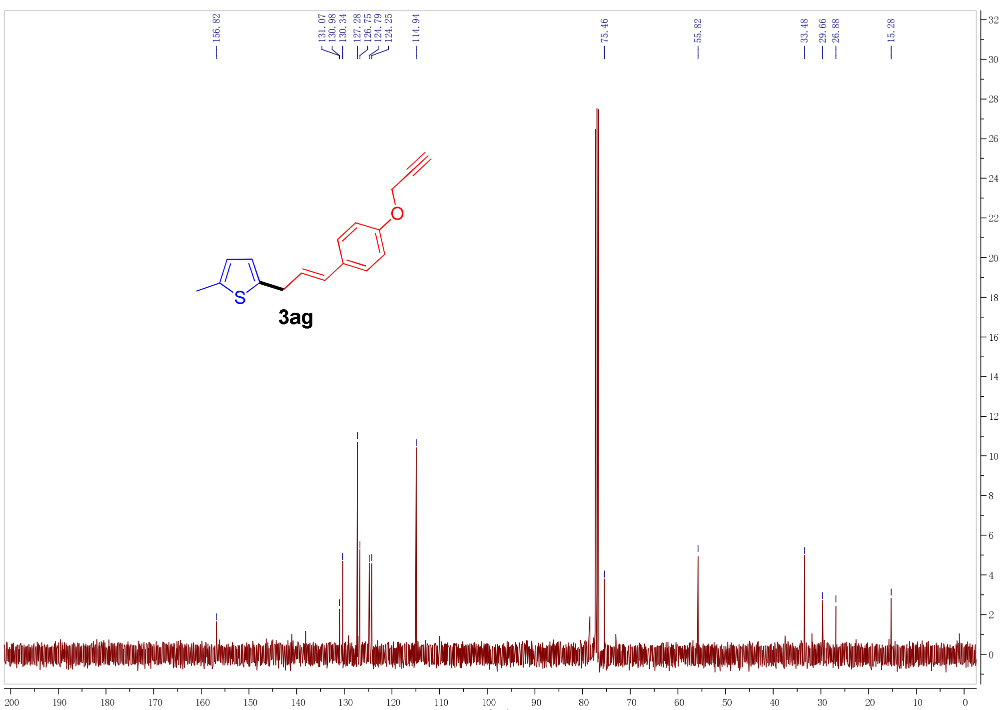
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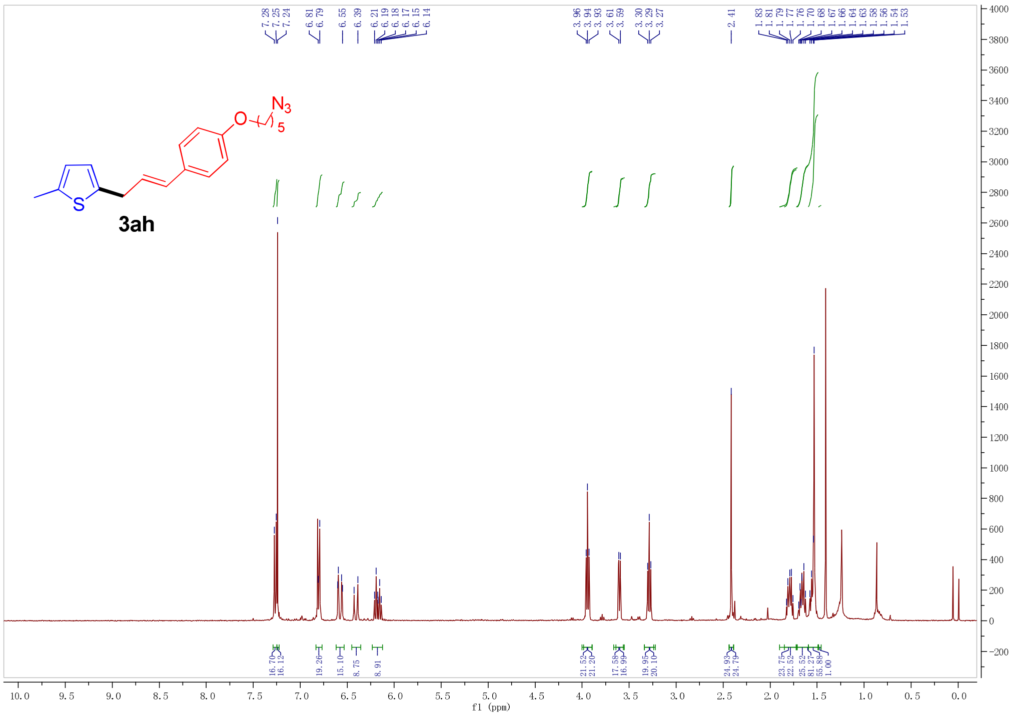
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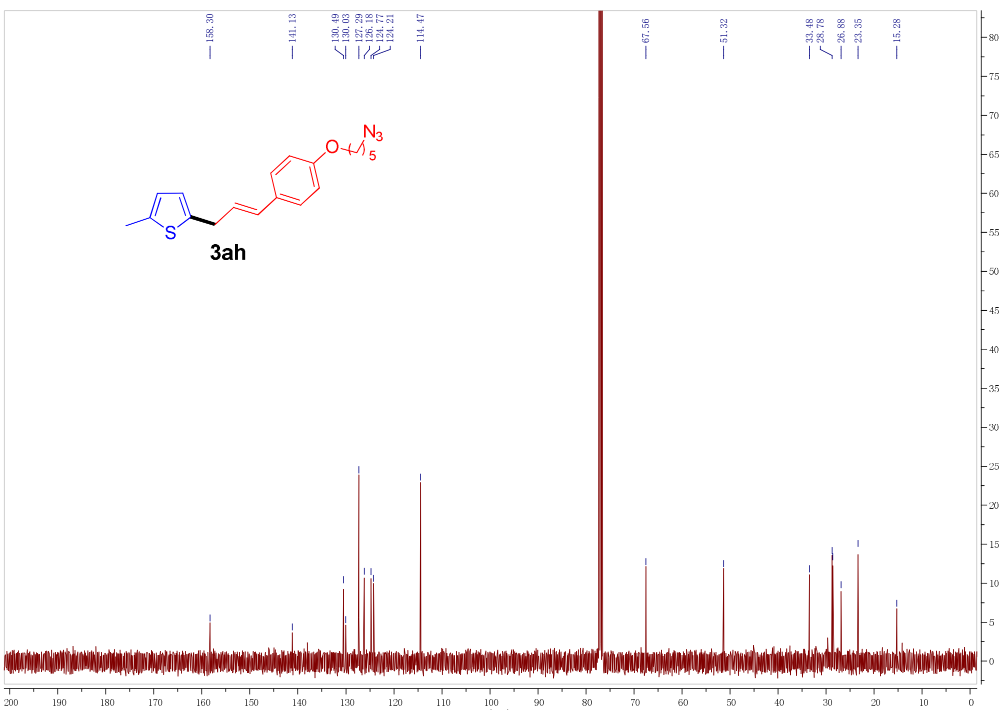
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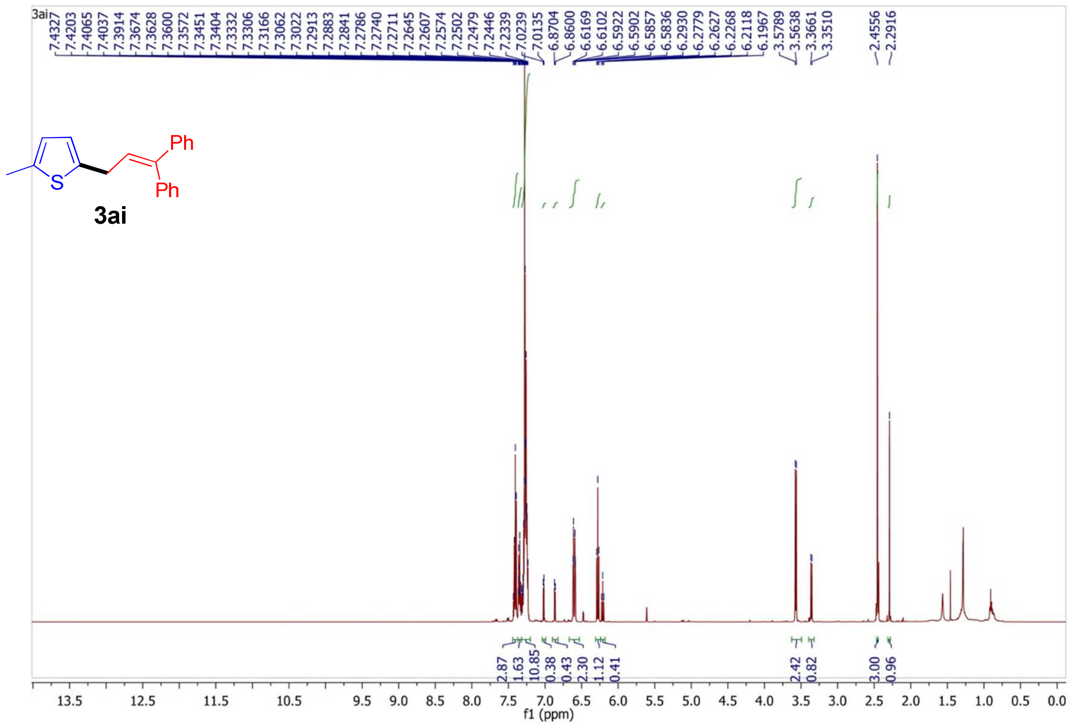
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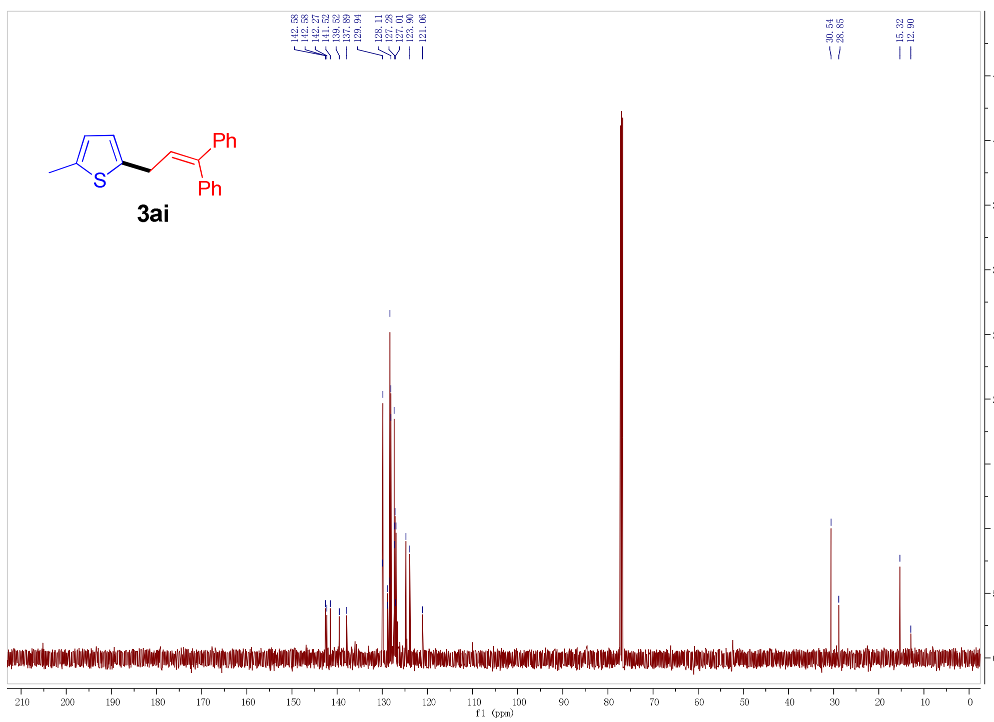
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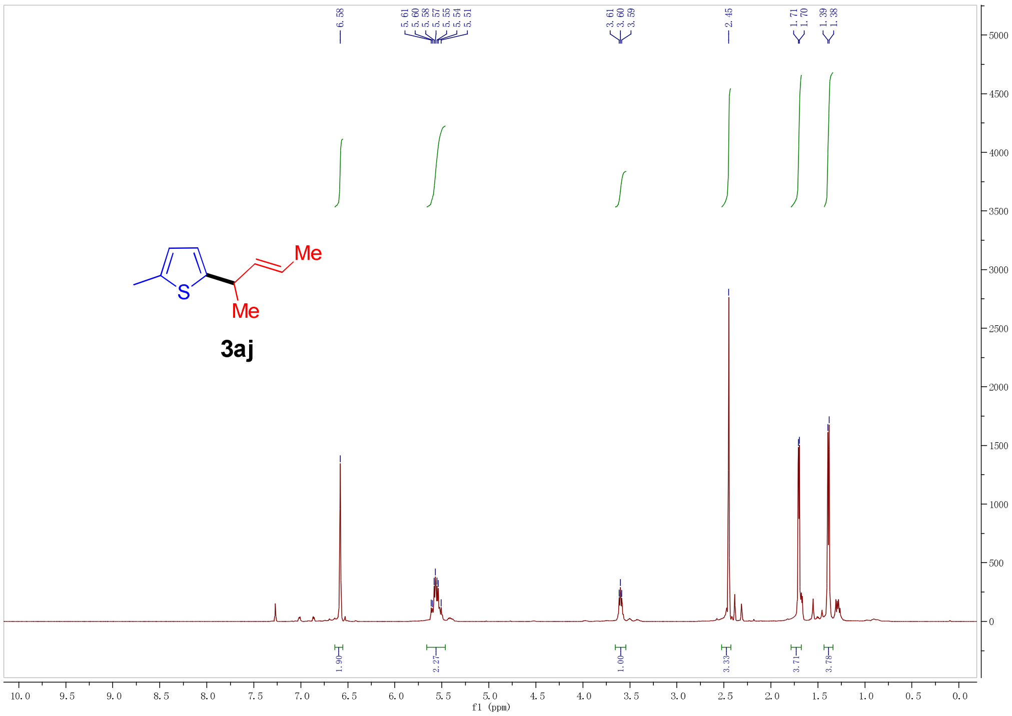
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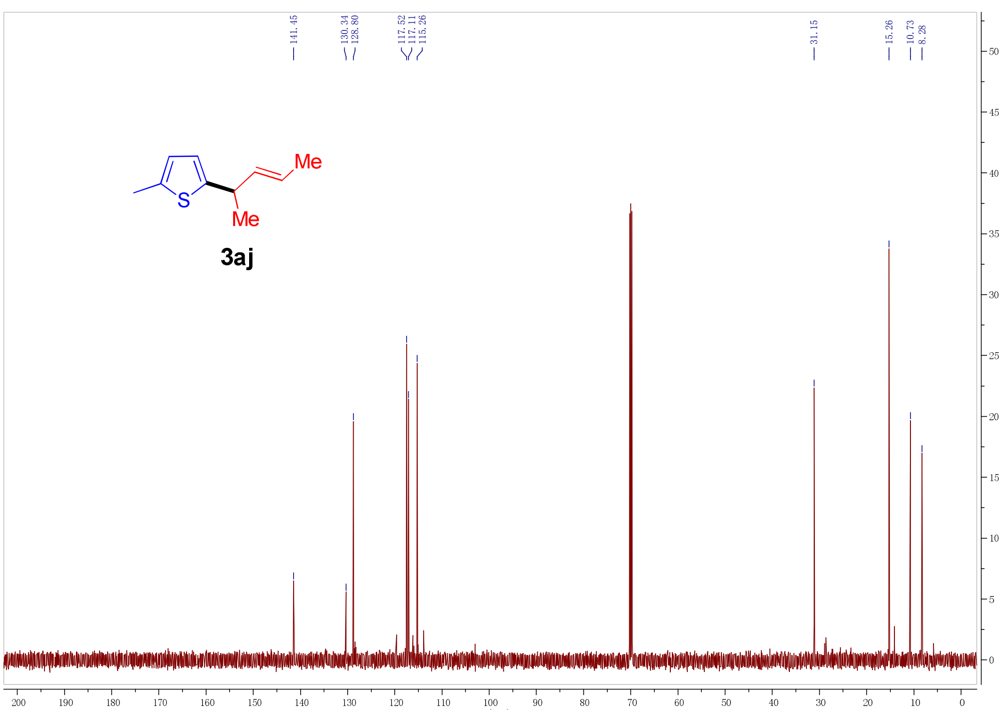
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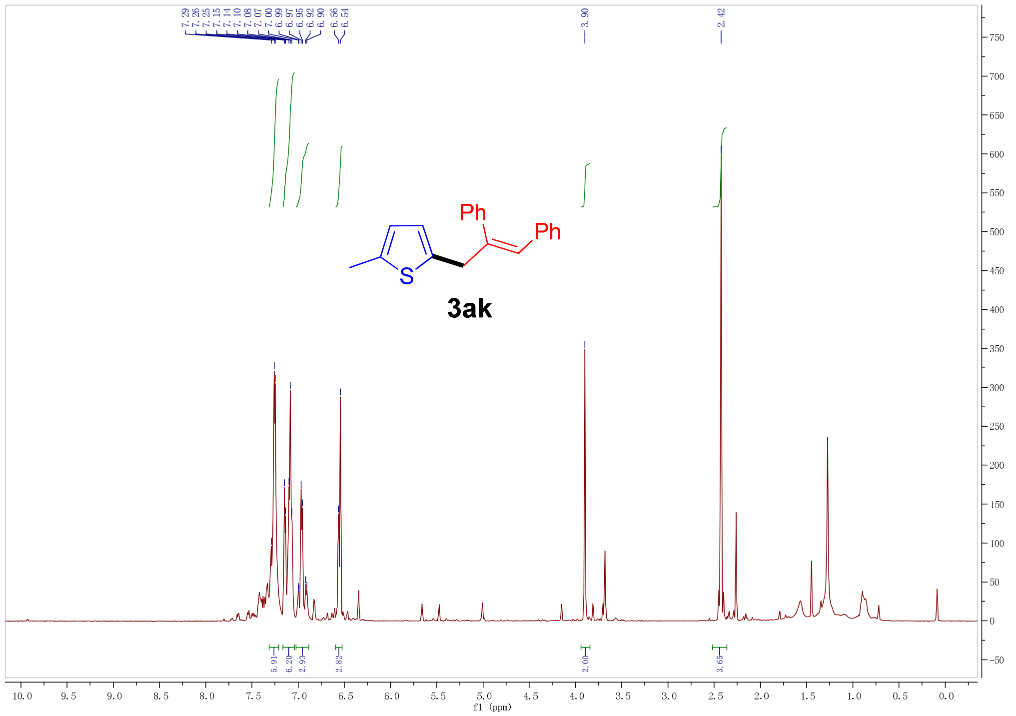
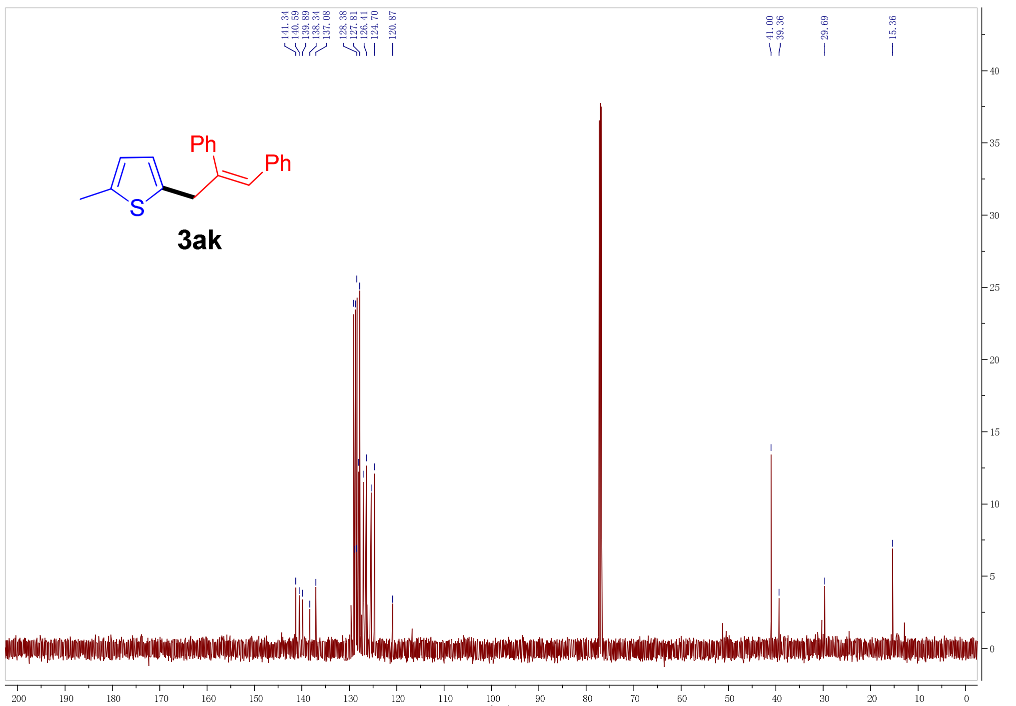
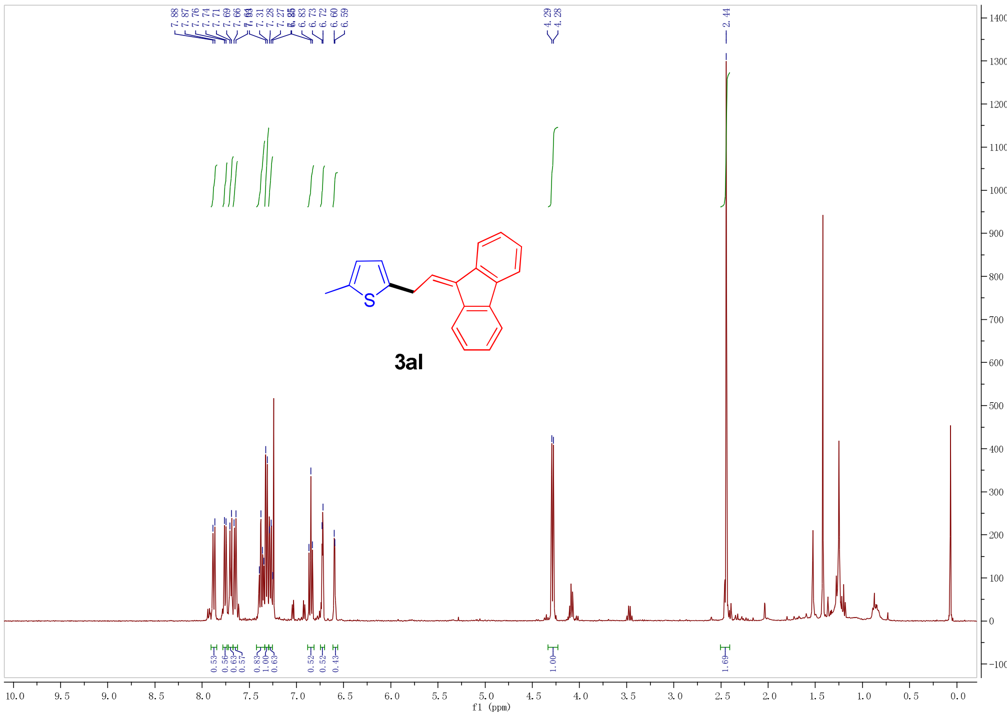
Me
S
Me
3aj
f1 (ppm)



Ph
Ph
S
3ak



Ph
Ph
S
3ak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7.76
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7.69
7.66
7.31
7.29
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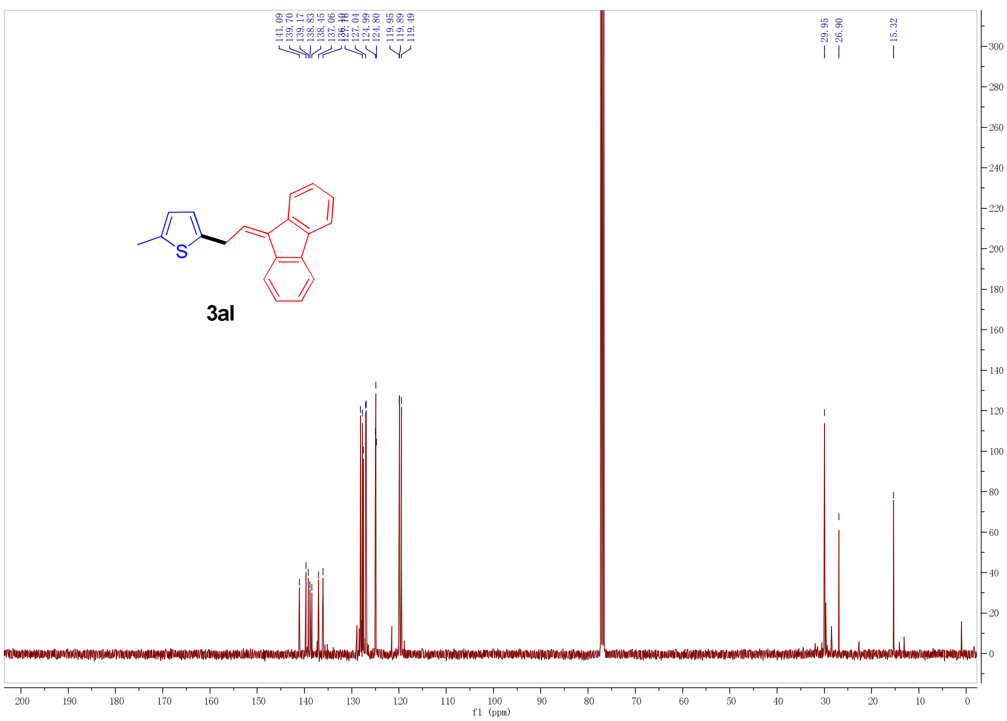
6.83
6.73
6.72
6.60
6.59
4.29
4.28
2.44
3al
f1 (ppm)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139.70
139.17
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138.45
137.06
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124.99
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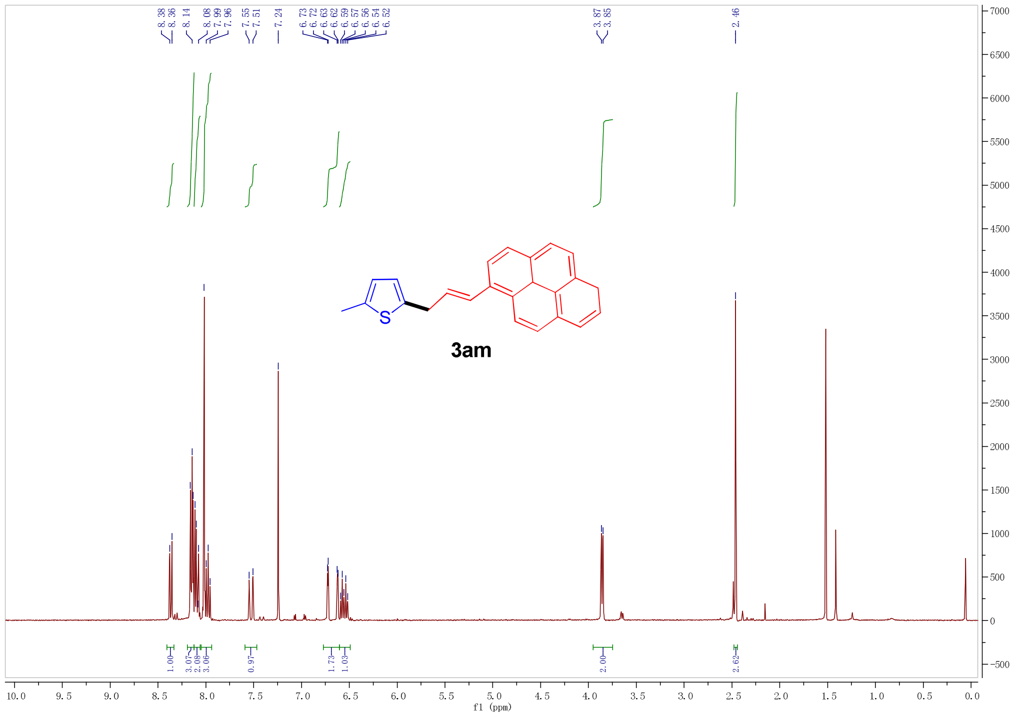
119.95
119.89
119.49
29.95
26.90
15.32
3al
f1 (ppm)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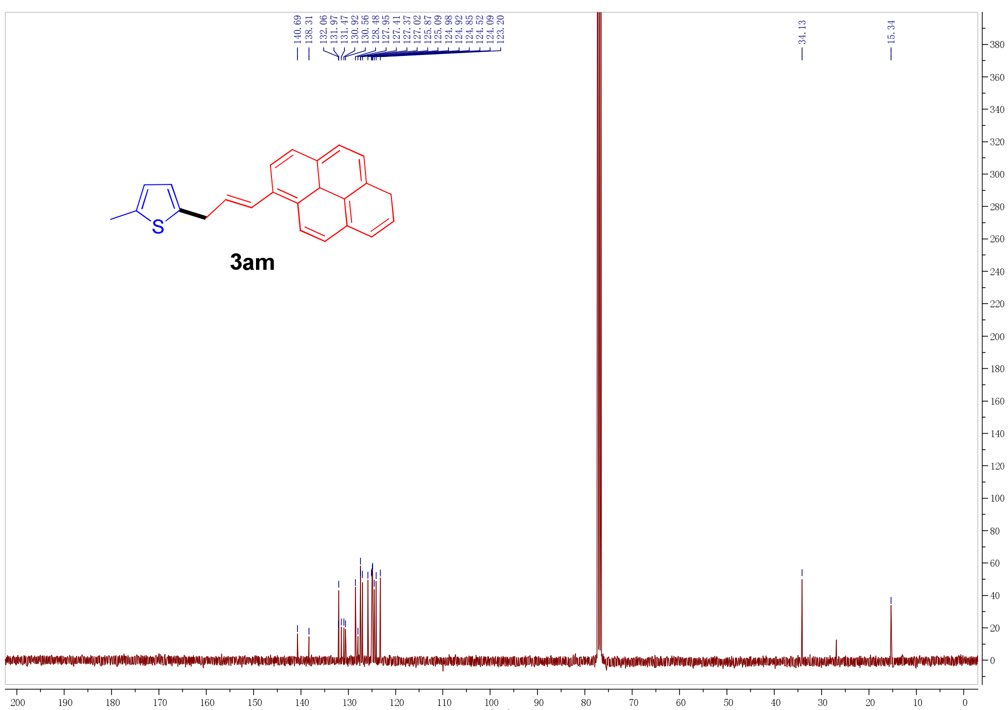
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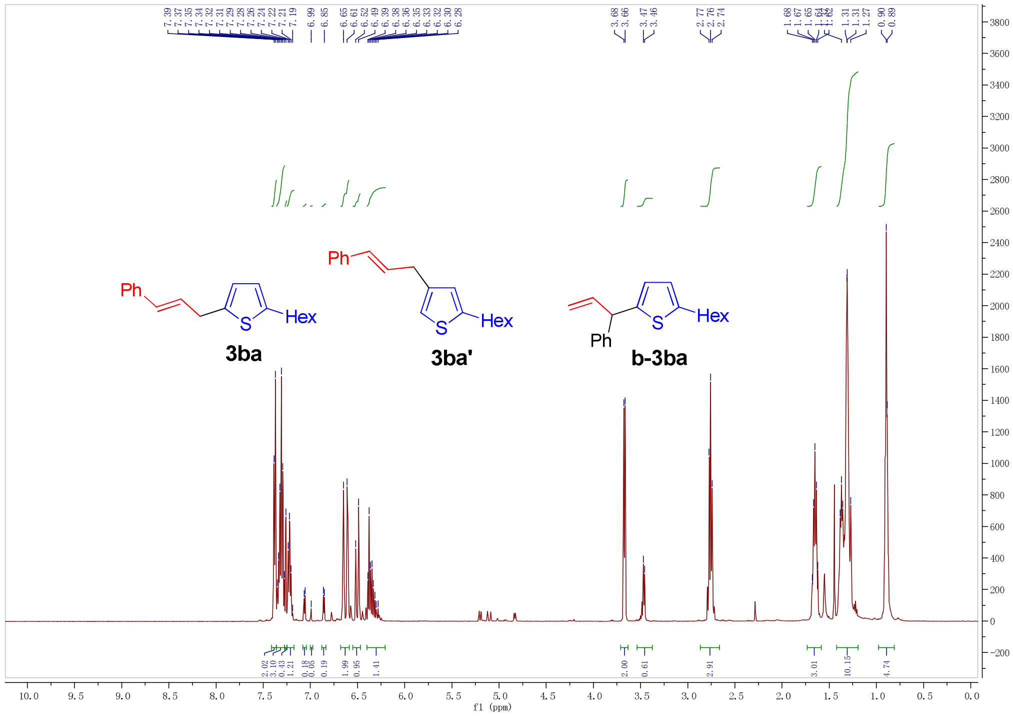
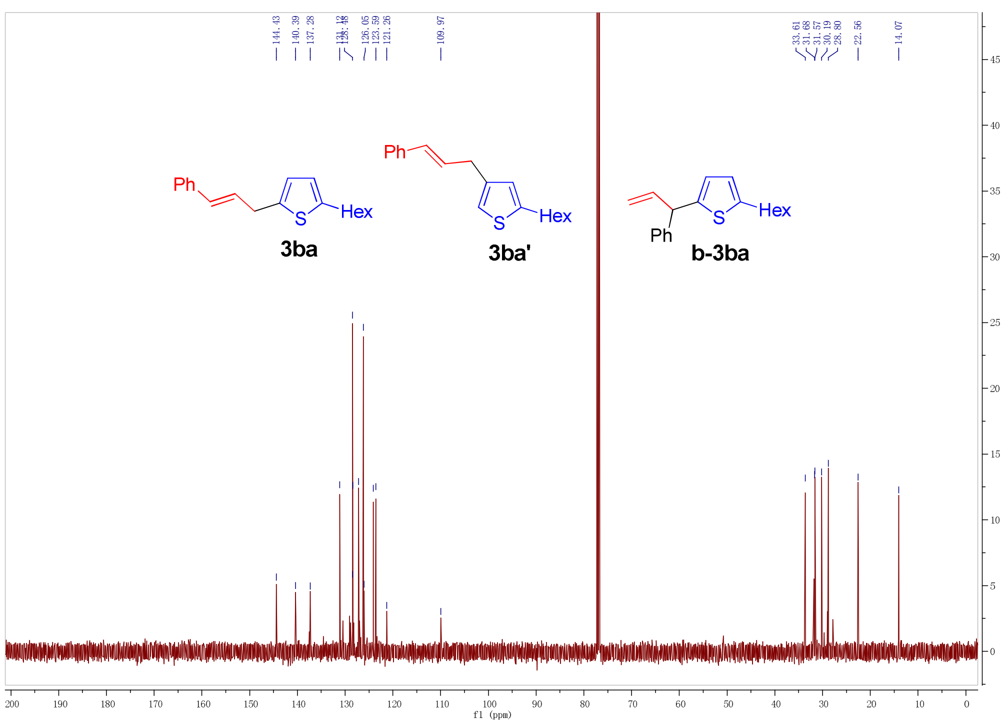
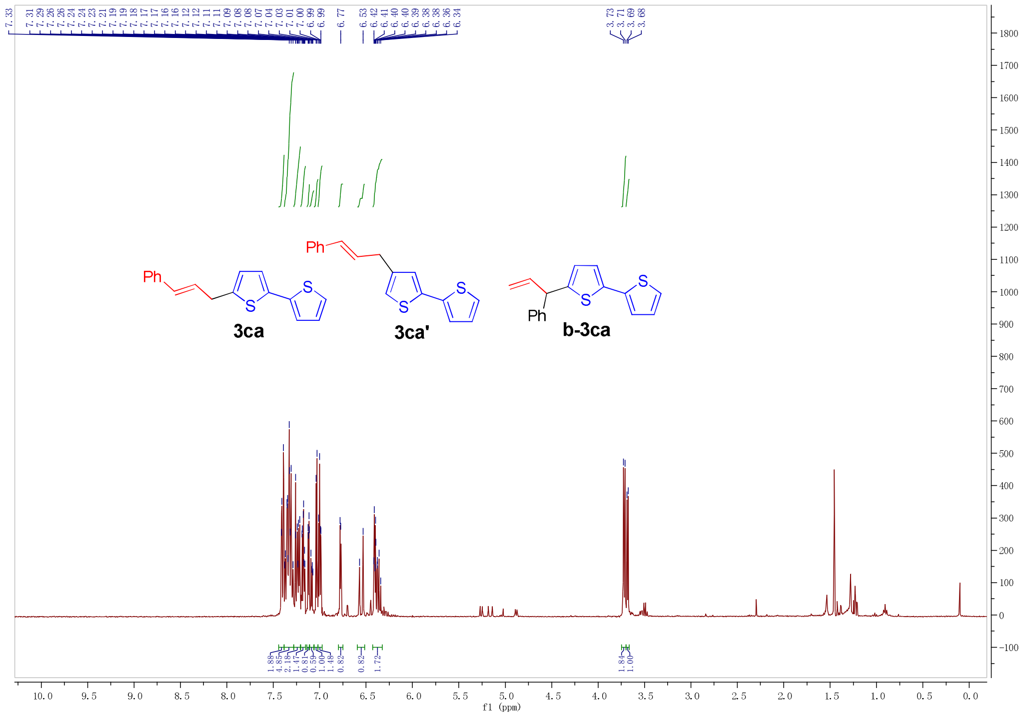
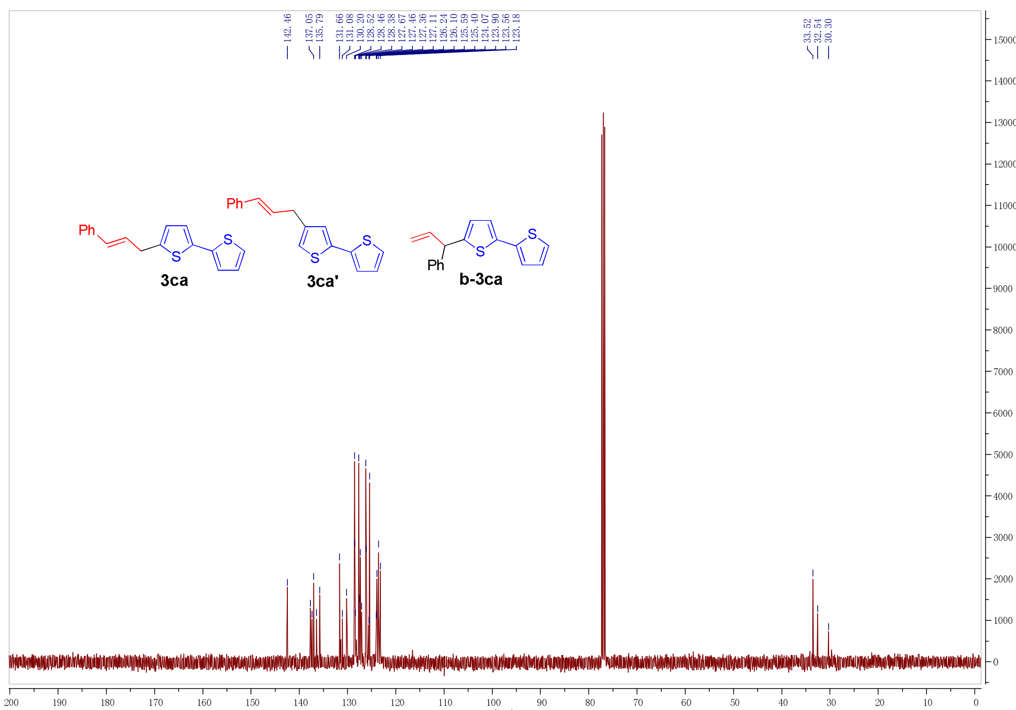
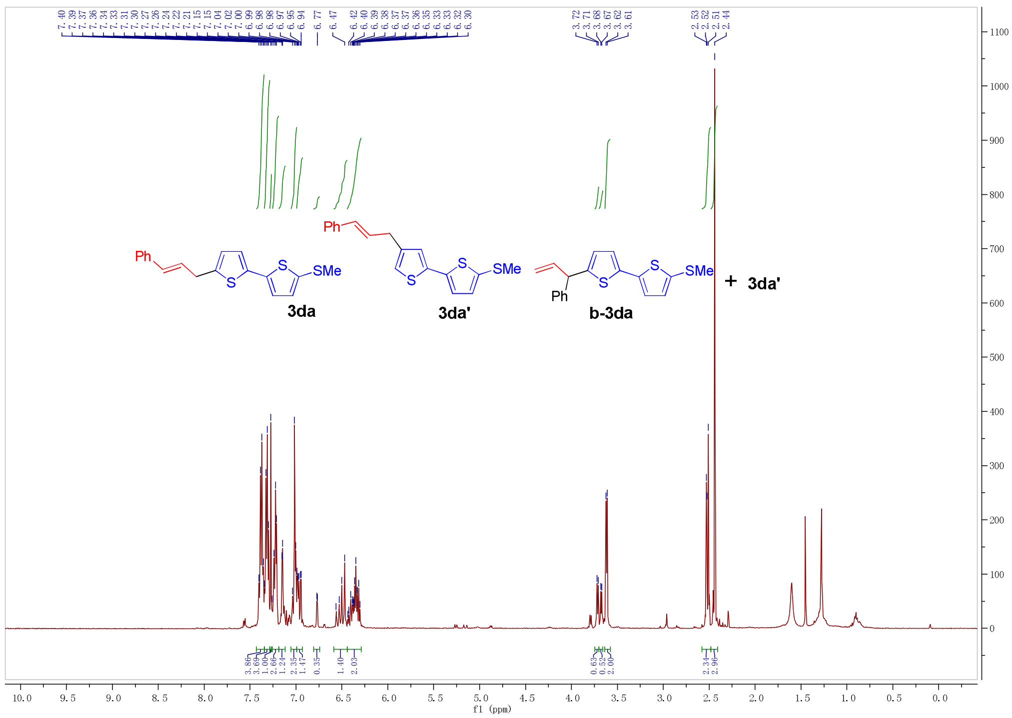

3ba
3ba'
b-3ba
Ph
Hex
S
f1 (ppm)

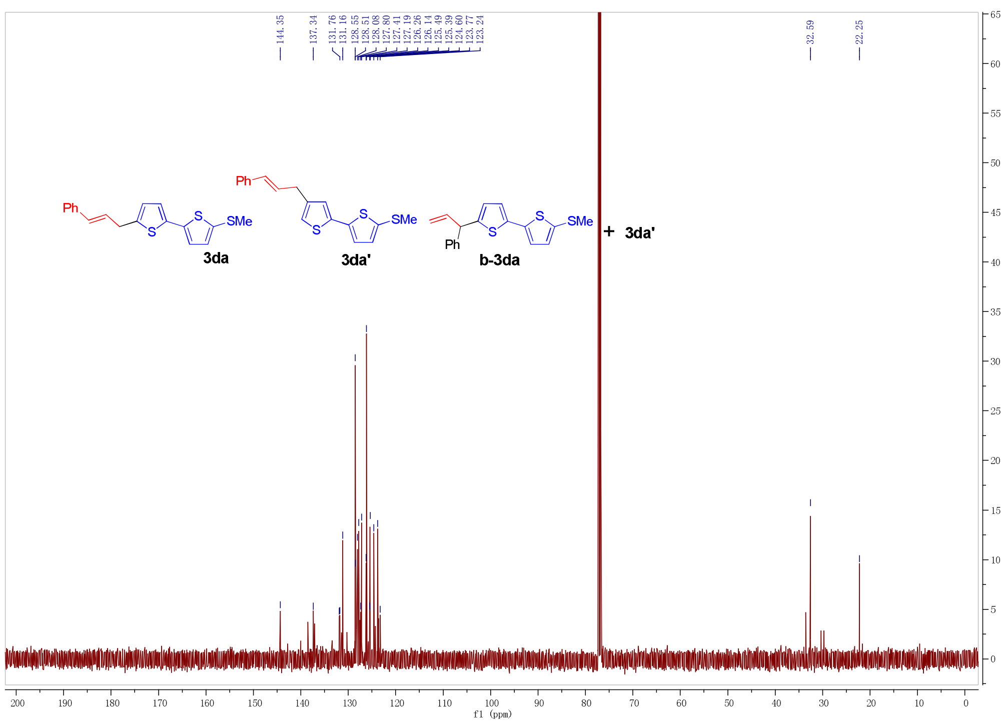

3ba
3ba'
b-3ba
Ph
Hex
S
f1 (ppm)


Ph
S
S
3ca
Ph
S
S
3ca'
Ph
S
S
b-3ca
f1 (ppm)

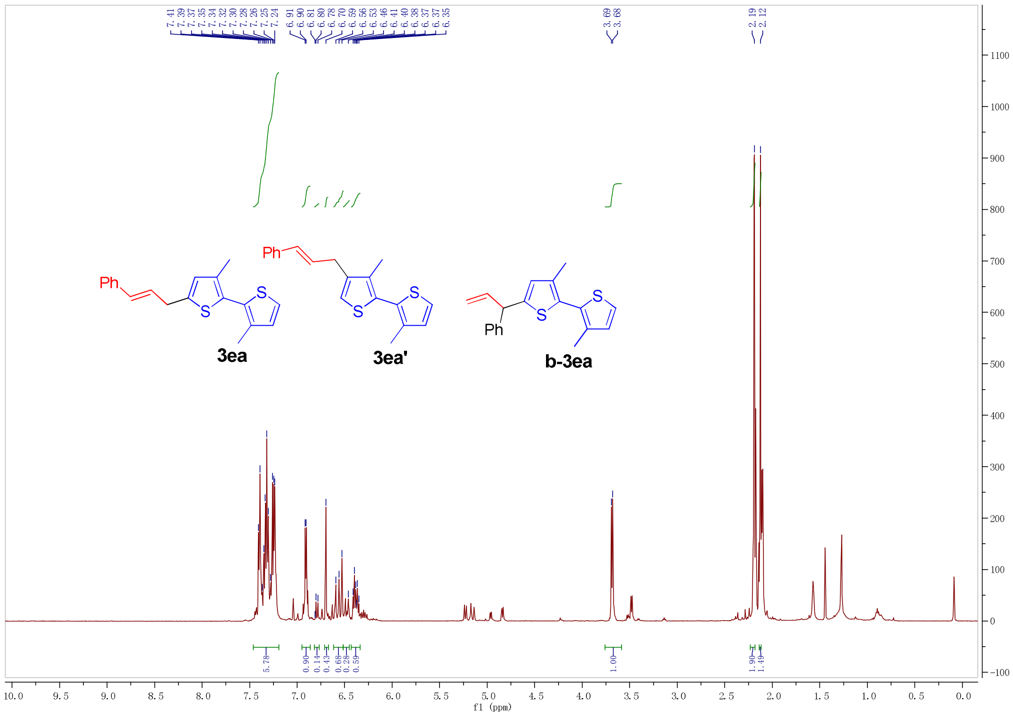

Ph
S
S
3ca
Ph
S
S
3ca'
Ph
S
S
b-3ca
f1 (ppm)

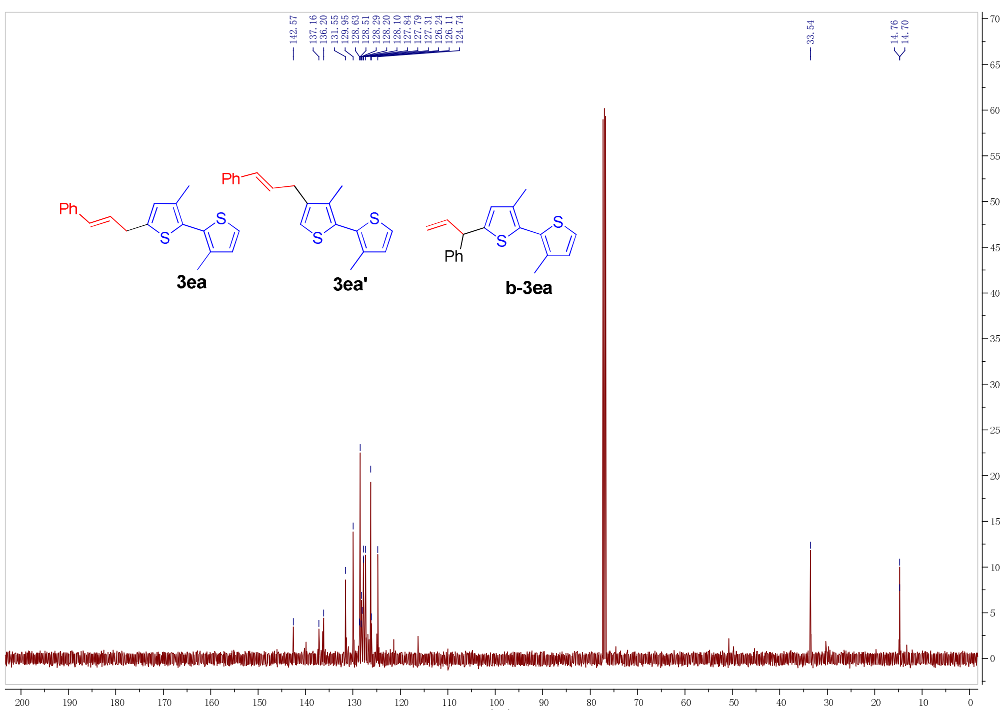


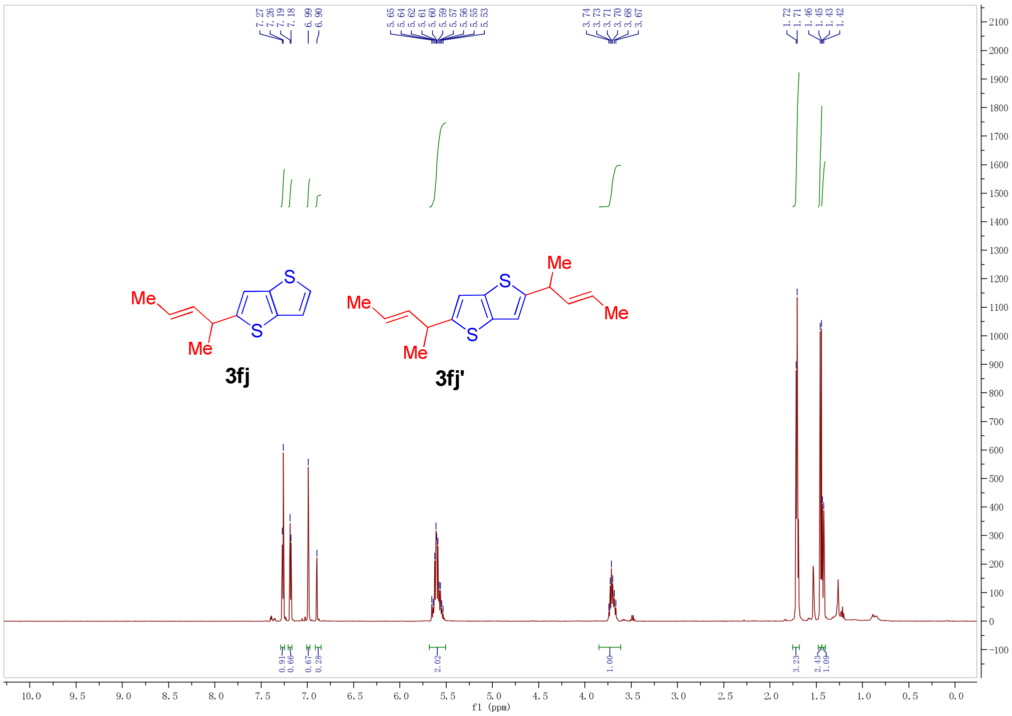
Ph
S
S
SMe
3da
3da'
b-3da
+ 3da'
f1 (ppm)



Ph
S
S
SMe
3da
3da'
b-3da
+ 3da'
f1 (ppm)



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7.19
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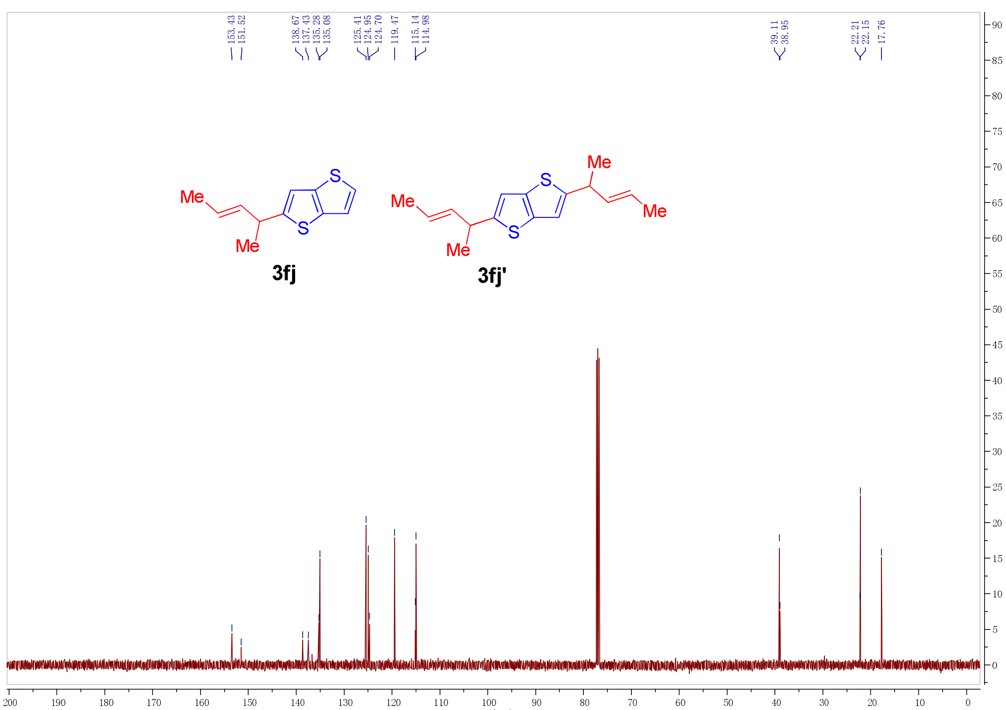
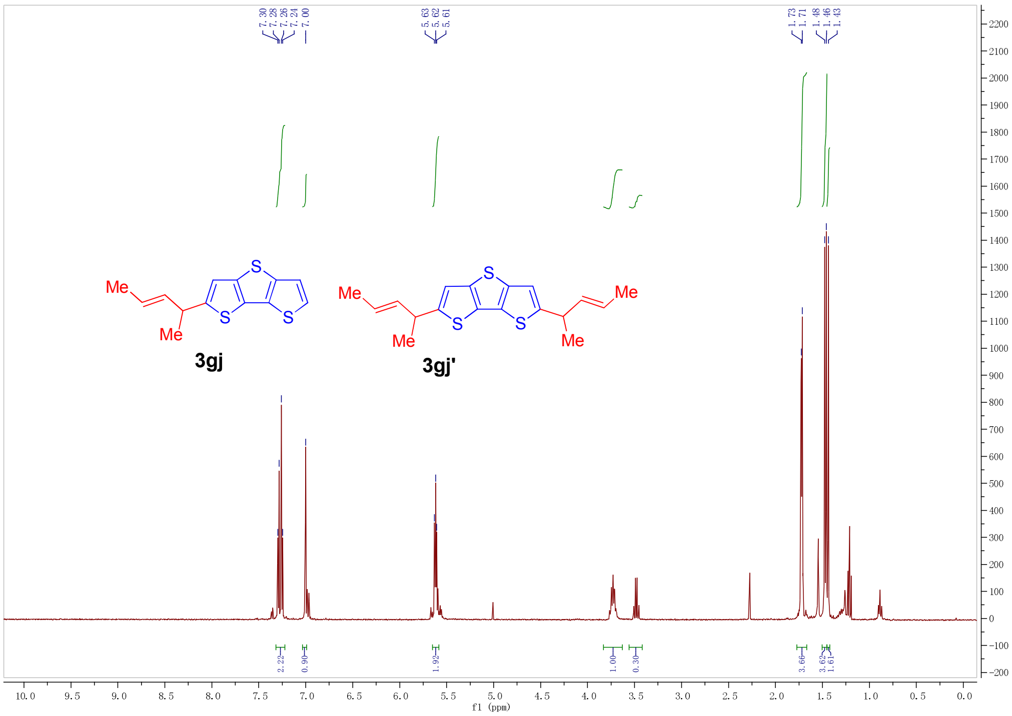
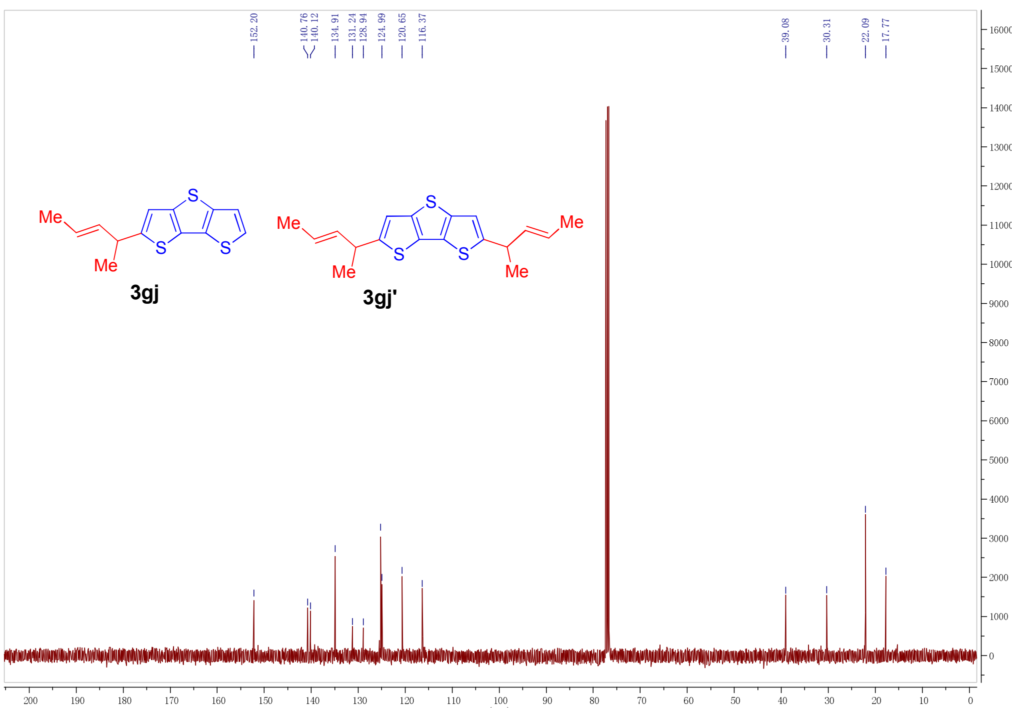
6.90
5.65
5.64
5.62
5.61
5.60
5.59
5.57
5.56
5.55
5.53
3.74
3.73
3.71
3.70
3.68
3.67
1.72
1.71
1.46
1.45
1.43
1.42
Me
S
S
Me
3fj
Me
S
S
Me
Me
Me
3fj'
0.91
0.66
0.67
0.28
2.02
1.00
3.23
2.43
1.09
f1 (ppm)

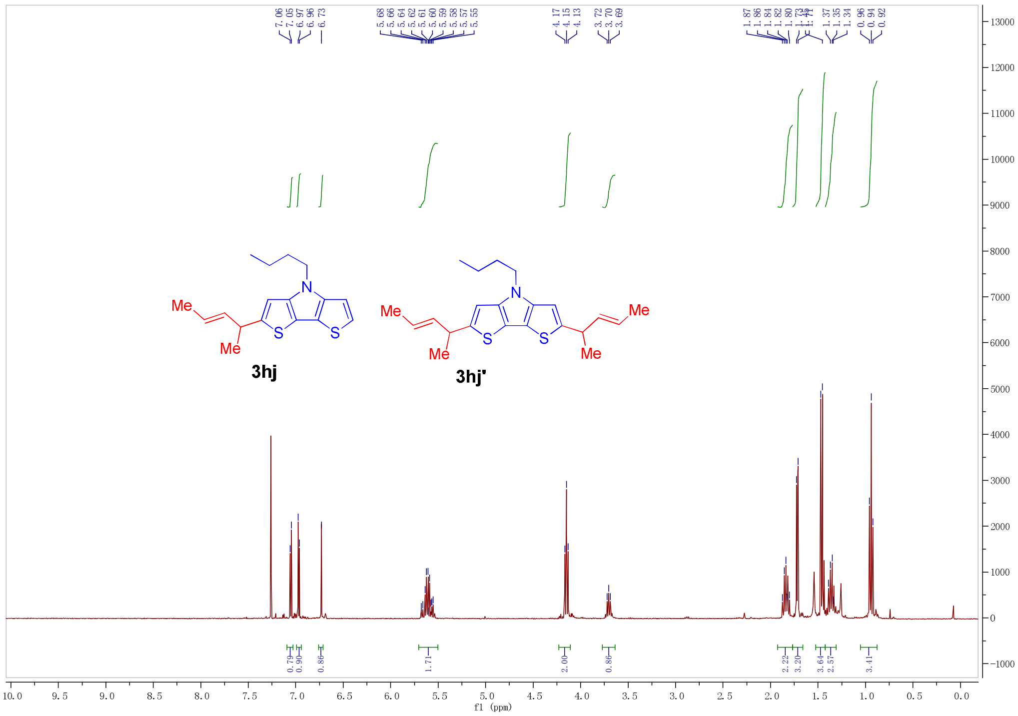

153.43
151.52
138.67
137.43
135.28
135.08
125.41
124.95
124.70
119.47
115.14
114.98
39.11
38.95
22.21
22.15
17.76
Me
S
S
Me
3fj
Me
S
S
Me
Me
Me
3fj'
f1 (ppm)

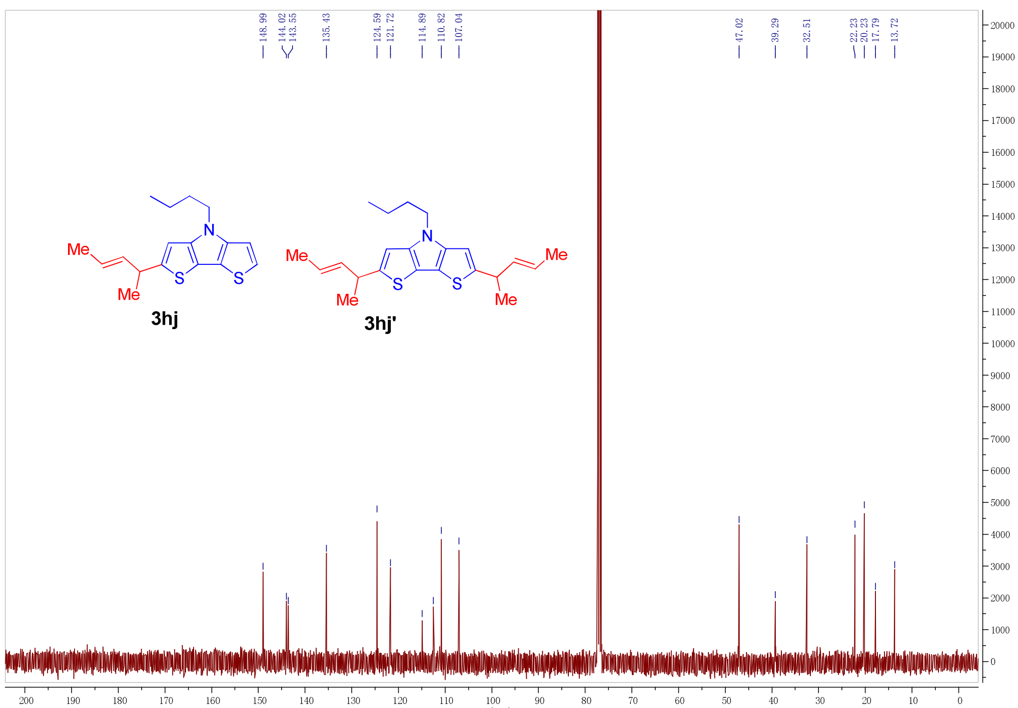


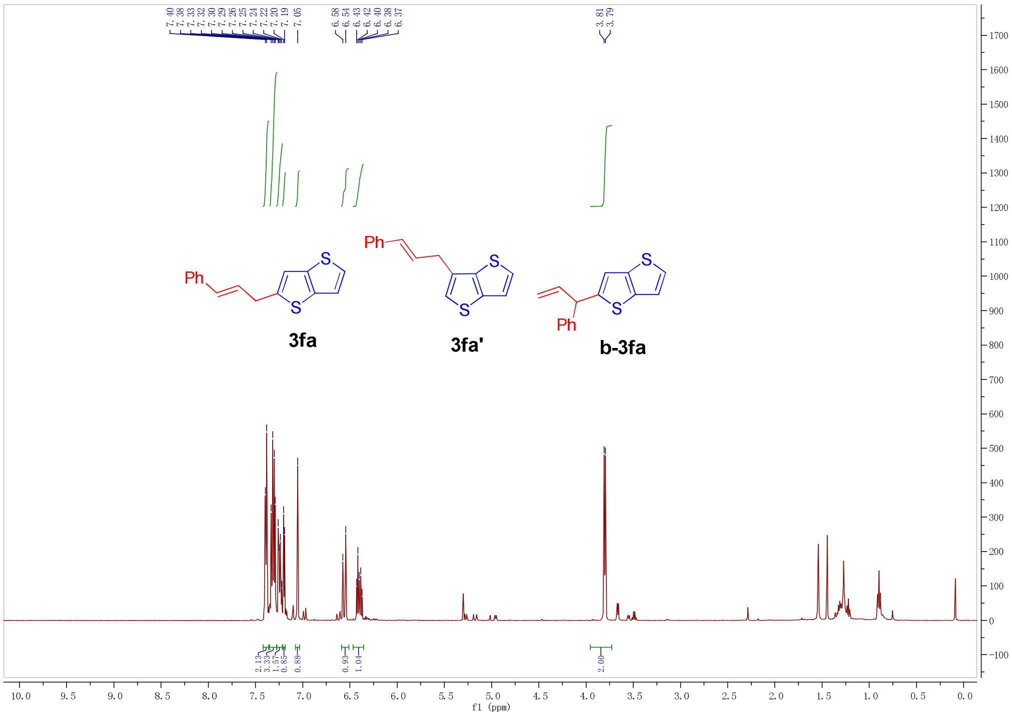
7.30
7.28
7.26
7.24
7.00
5.63
5.62
5.61
1.73
1.71
1.48
1.46
1.43
3gj
3gj'
2.22
0.90
1.92
1.00
0.30
3.66
3.62
1.61
f1 (ppm)



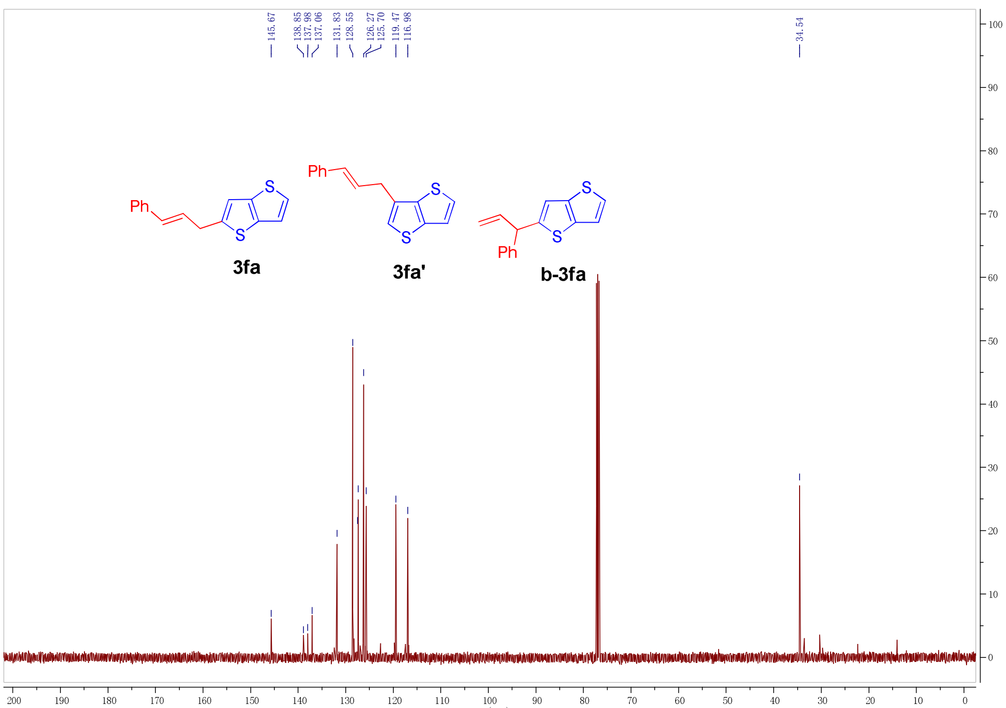
152.20
140.76
140.12
134.91
131.24
128.94
124.99
120.65
116.37
39.08
30.31
22.09
17.77
3gj
3gj'
f1 (ppm)


3hj
3hj'
f1 (ppm)

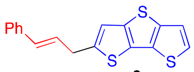

3hj
3hj'
f1 (ppm)



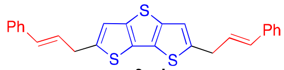
Ph
S
S
3fa
3fa'
b-3fa
f1 (ppm)



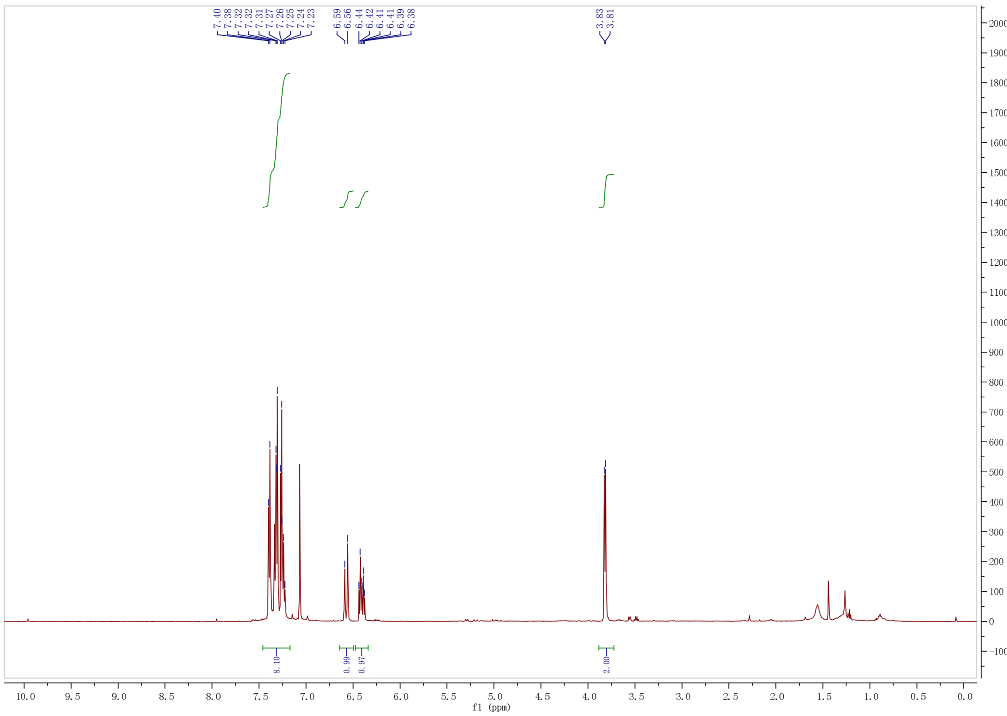
145.67
138.85
137.98
137.06
131.83
128.55
126.27
125.70
119.47
116.98
34.54
Ph
S
3fa
3fa'
b-3fa
f1 (ppm)


Ph
S
S
S

3ga


Ph
S
S
S
Ph

3ga'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7.32
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7.31
7.27
7.26
7.25
7.24
7.23
6.59
6.56
6.44
6.42
6.41
6.41
6.39
6.38
3.83
3.81
8.10
0.99
0.97
2.00
f1 (ppm)

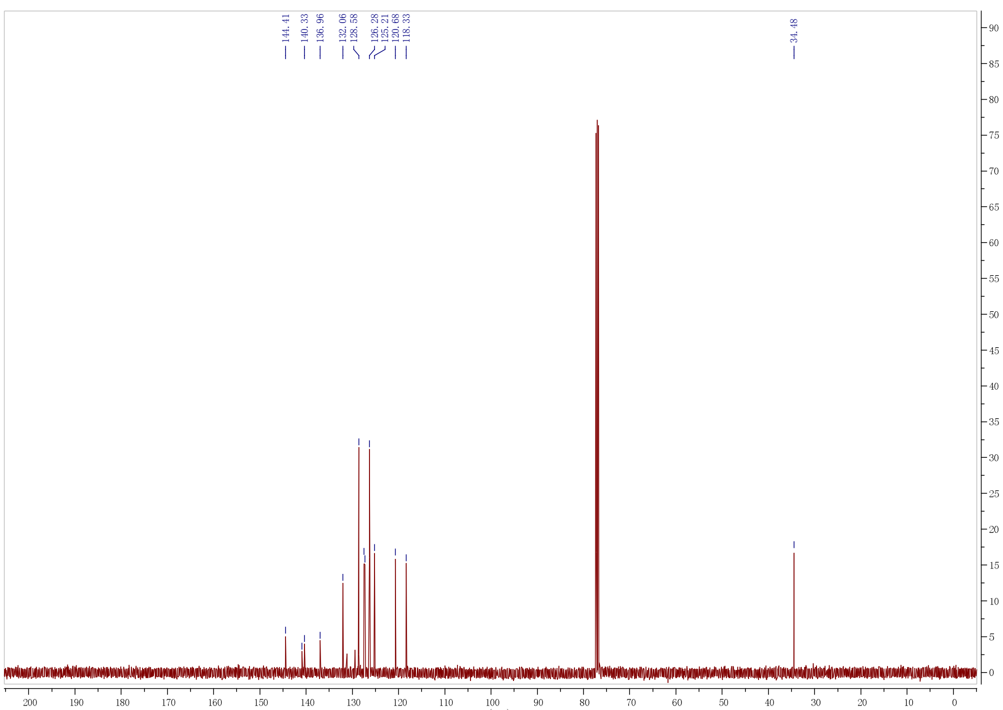
144.41
140.33
136.96
132.06
128.58
126.28
125.21
120.68
118.33
34.48
f1 (ppm)

Figure S2

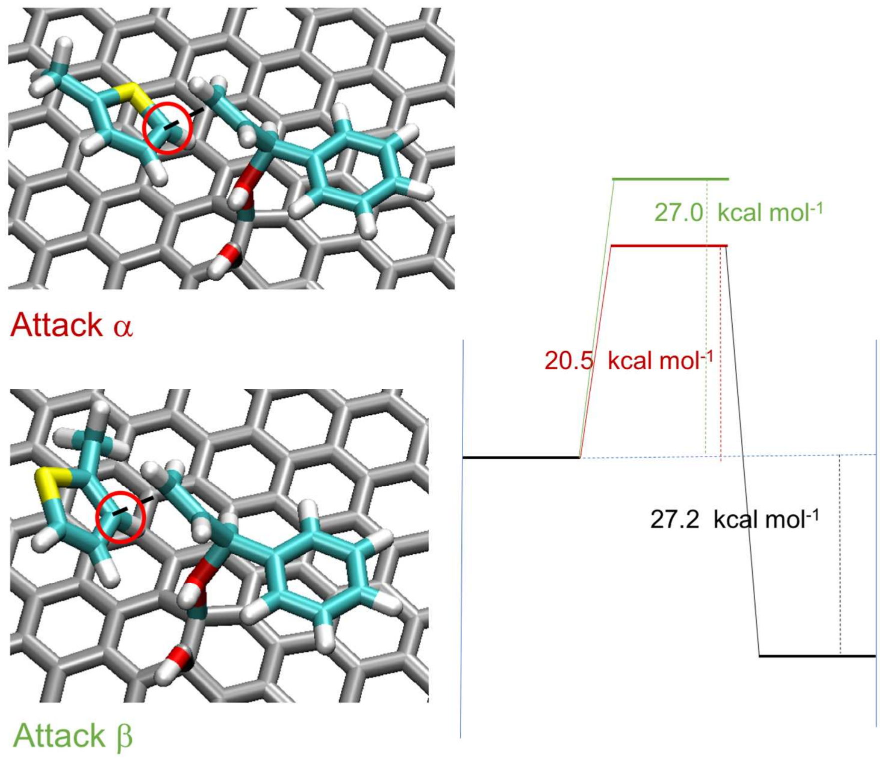

Figure S2. TSs for the Friedel-Crafts-type allylic alkylation of the 2-methyl-thiophene in the α (red path) and β (green path) position.

Table S2. Cartesian coordinates (Ångstroms) for the various computed critical points

RX1-2a

O	1.418715	0.698167	3.706447
C	2.578360	-0.050682	4.025263
H	1.171454	0.477198	2.796047
C	2.856992	0.173192	5.486147
C	2.387158	-1.534243	3.750831
H	3.445104	0.305449	3.445867
C	3.489615	-2.347682	3.486773
C	3.324032	-3.710985	3.268406
C	2.050401	-4.275428	3.314281
C	0.947577	-3.469679	3.582213
C	1.115073	-2.104304	3.801752
H	4.483712	-1.906599	3.454005
H	4.188162	-4.334324	3.058634
H	1.920085	-5.339307	3.141376
H	-0.046871	-3.904237	3.622632

H	0.260275	-1.468524	4.014289
C	4.025871	0.585360	5.962307
H	2.025791	-0.059858	6.150328
H	4.199551	0.703636	7.026895
H	4.854943	0.821850	5.299507

RX1-GO

C	10.314505	9.421254	-0.241179
C	9.080800	10.059696	-0.278548
C	10.386992	8.030645	-0.186472
C	9.213802	7.241255	-0.165262
C	10.459792	5.021157	-0.083343
C	9.248609	5.743398	-0.112653
C	10.484335	3.683629	-0.049397
C	9.300676	2.921051	-0.045311
C	10.497663	0.670935	-0.169399
C	9.310675	1.415515	-0.041498
C	10.491962	-0.666486	-0.172396
C	9.297997	-1.408308	-0.043799
C	10.468343	-3.667075	-0.096701
C	9.283909	-2.907246	-0.053110
C	10.449965	-5.001492	-0.155767
C	9.242356	-5.732794	-0.173897
C	10.388434	-7.944032	-0.402604
C	9.214121	-7.157057	-0.276375
C	10.320700	-9.332325	-0.505278
C	9.093066	-9.980292	-0.491349
C	7.899426	9.309774	-0.258180
C	6.665222	9.966248	-0.297309
C	7.957006	7.892943	-0.198136
C	6.756824	7.144295	-0.168061
C	8.028265	5.026950	-0.083610
C	6.792637	5.727411	-0.101902
C	8.064789	3.604894	-0.036604
C	6.807748	2.828052	0.041570
C	8.088183	0.713361	0.054534
C	6.820266	1.474428	0.108817
C	8.073303	-0.711165	0.059565
C	6.854224	-1.433884	0.146191
C	8.045568	-3.585879	-0.012062
C	6.837541	-2.856934	0.099760
C	8.023106	-5.006655	-0.078255
C	6.788636	-5.692025	-0.052709
C	7.962420	-7.828915	-0.265897
C	6.758541	-7.099063	-0.149827
C	7.911436	-9.242682	-0.374881
C	6.680925	-9.906966	-0.372702
C	5.471846	9.240460	-0.272626
C	4.243312	9.920348	-0.316168
C	5.513421	7.829282	-0.203121
C	4.236576	7.070918	-0.162278
C	5.508584	4.972059	-0.043776
C	4.274075	5.664166	-0.071842
C	5.523032	3.563851	0.049554
C	4.320300	2.846956	0.153561
C	5.552262	0.723504	0.228857
C	4.339496	1.444700	0.260123
C	5.566834	-0.694022	0.268176
C	4.371398	-1.401704	0.383358
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C	4.344202	-5.659568	0.099244
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C	4.311038	-7.062036	-0.021394
C	5.487637	-9.189221	-0.260867
C	4.262462	-9.865241	-0.275650
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C	1.804608	9.911077	-0.332219
C	3.049108	7.738146	-0.201595

C	1.824464	7.040279	-0.154951
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C	1.831408	5.639863	-0.050759
C	3.098113	3.548499	0.118085
C	1.826940	2.814144	0.240848
C	3.079899	0.696474	0.452767
C	1.838640	1.439981	0.459149
C	3.105611	-0.660610	0.546417
C	1.900524	-1.390224	0.692077
C	3.138429	-3.499322	0.377848
C	1.872573	-2.753320	0.566255
C	3.070630	-4.901205	0.247236
C	1.872409	-5.567737	0.232943
C	3.076400	-7.751546	-0.036330
C	1.858463	-7.045576	0.069658
C	3.059649	-9.158170	-0.173738
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C	-0.641840	9.899822	-0.330619
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C	-5.527353	-5.690379	-0.010411
C	-4.259368	-7.780147	-0.123387
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C	-6.737267	9.213922	-0.218510
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C	-6.818078	4.968499	-0.027319
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C	-6.842926	3.547046	0.046866
C	-8.057967	2.827029	0.031407
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C	-6.824151	-0.744934	0.146259
C	-8.033270	-1.474544	0.062948
C	-6.784625	-3.589057	0.050148
C	-8.014649	-2.896501	0.017634
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C	-7.973814	-5.726934	-0.160395
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C	-7.940974	-7.146132	-0.273072
C	-6.658046	-9.225532	-0.378671
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C	-10.392406	-5.800202	-0.342958
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C	-10.358782	-7.184140	-0.449352
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H	11.374792	7.603513	-0.161335
H	11.416246	5.516238	-0.087097
H	11.457017	3.221322	-0.015336
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H	11.449411	-1.143394	-0.295366
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H	11.231292	-9.911163	-0.600830
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H	6.634314	11.049930	-0.346361
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TS1

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C	-7.485630	-5.961437	-0.630983
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C	-6.354575	-6.815365	-0.613983
C	-4.992611	-6.251278	-0.437983
C	-5.961755	-4.005340	-0.298983
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C	3.123415	9.015239	-0.247983
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C	4.282648	-10.318687	-0.723983
C	3.376506	-8.084745	-0.441983
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H	9.777117	-9.519444	-0.742948
H	10.242264	-7.227015	-0.594271
H	10.600857	-5.195255	-0.954877
H	11.019386	-2.936045	-0.868695
H	11.399982	-0.963401	-0.264617
H	11.807628	1.282893	-0.284612
H	12.147784	3.255168	-0.763044
H	12.521395	5.546959	-0.887308
H	12.839901	7.619229	-0.906480
H	12.011546	9.242775	-0.970386
O	-0.396802	1.261801	2.449532
O	-0.808777	-1.019984	2.453415
C	-1.351493	-2.200270	3.179410
H	0.414441	1.785135	2.592455
C	-0.783157	-2.100439	4.564110
C	-2.853787	-2.214169	3.173785
H	-0.934914	-3.054647	2.641612
C	-3.495189	-3.445904	3.043887
C	-4.885575	-3.512494	3.064448
C	-5.634901	-2.347664	3.215013
C	-4.992680	-1.119529	3.361233
C	-3.602648	-1.051362	3.350418
H	-2.906887	-4.347969	2.891176
H	-5.380749	-4.469252	2.936980
H	-6.718687	-2.394768	3.208035
H	-5.574942	-0.209918	3.468253
H	-3.102884	-0.087459	3.424175
C	0.171108	-2.919451	5.000678
H	-1.235798	-1.355023	5.216595
H	0.544752	-2.866376	6.017366
H	0.595324	-3.686077	4.355963
C	2.646354	-0.305200	3.563645
C	3.894009	-0.726405	3.223244
C	4.829379	0.353587	3.109134
C	4.279989	1.574958	3.360394
S	2.607294	1.408331	3.793631
H	1.760521	-0.913383	3.697202
H	4.145290	-1.765860	3.044900
H	5.872872	0.224197	2.844937
H	-0.586163	-0.164327	2.939002
C	4.943759	2.925981	3.350876
H	4.338039	3.640241	2.785272
H	5.079141	3.300617	4.369264
H	5.919476	2.827103	2.870171

TS2 – α attack

C	-10.312108	-9.234875	-0.992999
C	-9.076116	-9.870892	-1.023999
C	-10.388089	-7.849874	-0.860999
C	-9.218078	-7.063890	-0.750999
C	-10.468048	-4.850873	-0.576999
C	-9.256058	-5.570890	-0.619999
C	-10.492030	-3.514873	-0.498999
C	-9.307019	-2.753889	-0.459999
C	-10.494989	-0.509873	-0.648999
C	-9.316999	-1.250889	-0.443999
C	-10.493970	0.826127	-0.639999
C	-9.314960	1.568111	-0.420999
C	-10.506930	3.814128	-0.432999
C	-9.314940	3.065111	-0.403999
C	-10.500911	5.148127	-0.491999
C	-9.298901	5.889111	-0.520999
C	-10.460871	8.083127	-0.814999
C	-9.282882	7.312111	-0.642999
C	-10.405852	9.471126	-0.927999
C	-9.186843	10.134110	-0.881999
C	-7.897106	-9.123908	-0.921999
C	-6.660115	-9.774925	-0.965999

C	-7.960087	-7.712907	-0.781999
C	-6.763077	-6.966924	-0.673999
C	-8.037048	-4.856906	-0.526999
C	-6.803058	-5.556923	-0.535999
C	-8.073029	-3.436906	-0.429999
C	-6.819018	-2.662923	-0.279999
C	-8.100989	-0.547905	-0.282999
C	-6.831999	-1.307923	-0.184999
C	-8.090970	0.877095	-0.269999
C	-6.877960	1.605078	-0.141999
C	-8.083930	3.753094	-0.339999
C	-6.872940	3.033078	-0.197999
C	-8.074911	5.175094	-0.407999
C	-6.847901	5.873078	-0.364999
C	-8.038872	7.997094	-0.610999
C	-6.829882	7.281077	-0.466999
C	-7.999853	9.411093	-0.728999
C	-6.776844	10.089077	-0.700999
C	-5.469105	-9.049941	-0.868999
C	-4.236114	-9.719958	-0.935999
C	-5.517086	-7.645941	-0.713999
C	-4.244076	-6.887958	-0.596999
C	-5.524047	-4.806941	-0.396999
C	-4.287057	-5.491957	-0.422999
C	-5.541028	-3.408940	-0.244999
C	-4.343019	-2.710957	-0.072999
C	-5.570989	-0.548940	-0.004999
C	-4.360999	-1.250956	0.097001
C	-5.590970	0.861060	0.027001
C	-4.389960	1.574044	0.177001
C	-5.655930	3.757061	-0.114999
C	-4.381940	3.039044	0.079001
C	-5.635911	5.165061	-0.215999
C	-4.404901	5.867044	-0.176999
C	-5.597873	7.977060	-0.439999
C	-4.384882	7.269044	-0.300999
C	-5.577853	9.384060	-0.560999
C	-4.358844	10.073044	-0.552999
C	-3.028105	-9.017975	-0.849999
C	-1.798114	-9.690991	-0.944999
C	-3.053085	-7.542974	-0.661999
C	-1.834075	-6.839991	-0.560999
C	-3.082047	-4.772974	-0.281999
C	-1.847056	-5.449991	-0.356999
C	-3.121028	-3.385973	-0.081999
C	-1.864018	-2.637991	0.143001
C	-3.088989	-0.537974	0.352001
C	-1.914999	-1.266990	0.450001
C	-3.106970	0.862026	0.391001
C	-1.939960	1.591011	0.515001
C	-3.161931	3.730027	0.131001
C	-1.900941	2.980010	0.335001
C	-3.119912	5.128027	-0.015999
C	-1.932902	5.799010	-0.028999
C	-3.155873	7.970027	-0.301999
C	-1.932882	7.274010	-0.189999
C	-3.149854	9.377027	-0.432999
C	-1.934844	10.073010	-0.455999
C	-0.586104	-8.990008	-0.871999
C	0.641886	-9.656025	-0.987999
C	-0.602084	-7.518008	-0.670999
C	0.613925	-6.801024	-0.608999
C	-0.633046	-4.744007	-0.257999
C	0.597945	-5.408024	-0.409999
C	-0.652027	-3.293007	0.012001
C	0.559983	-2.582024	0.045001
C	-0.645990	-0.632007	0.936001
C	0.584002	-1.226024	0.308001
C	-0.671969	0.942993	1.028001
C	0.577040	1.608976	0.497001
C	-0.693932	3.658993	0.294001

C	0.538059	2.976977	0.326001
C	-0.695912	5.118994	0.084001
C	0.538098	5.802977	-0.019999
C	-0.709873	7.977994	-0.236999
C	0.519118	7.284977	-0.170999
C	-0.717853	9.384994	-0.368999
C	0.491156	10.087977	-0.425999
C	1.853896	-8.949041	-0.933999
C	3.076887	-9.618058	-1.054999
C	1.845916	-7.472041	-0.746999
C	3.018926	-6.785057	-0.714999
C	1.816954	-4.693041	-0.382999
C	3.033945	-5.386057	-0.544999
C	1.830973	-3.298041	-0.200999
C	3.043983	-2.588058	-0.207999
C	1.771012	-0.479040	0.218001
C	3.044002	-1.190058	-0.039999
C	1.769031	0.896960	0.314001
C	3.028041	1.656943	0.111001
C	1.802069	3.729959	0.116001
C	2.990060	3.065943	0.050001
C	1.734089	5.138960	-0.006999
C	3.003099	5.904943	-0.144999
C	1.734128	7.995960	-0.258999
C	2.968118	7.309943	-0.246999
C	1.713147	9.404961	-0.379999
C	2.915157	10.115944	-0.465999
C	4.291897	-8.916075	-1.014999
C	5.500887	-9.608091	-1.130999
C	4.304916	-7.513075	-0.857999
C	5.531925	-6.807092	-0.831999
C	4.256955	-4.676074	-0.534999
C	5.548945	-5.402092	-0.683999
C	4.252974	-3.280074	-0.379999
C	5.525984	-2.532091	-0.386999
C	4.244012	-0.458074	-0.104999
C	5.521002	-1.185091	-0.273999
C	4.242031	0.951926	-0.042999
C	5.523042	1.701909	-0.173999
C	4.267070	3.814926	-0.112999
C	5.498061	3.118909	-0.190999
C	4.239090	5.220926	-0.181999
C	5.446100	5.944910	-0.296999
C	4.174128	8.033927	-0.356999
C	5.412119	7.352910	-0.375999
C	4.142147	9.441927	-0.457999
C	5.337157	10.159911	-0.559999
C	6.721897	-8.922108	-1.093999
C	7.916887	-9.634124	-1.199999
C	6.744916	-7.518108	-0.950999
C	7.979925	-6.832125	-0.919999
C	6.780954	-4.694109	-0.672999
C	7.996944	-5.414125	-0.794999
C	6.797974	-3.278109	-0.534999
C	8.007984	-2.550125	-0.554999
C	6.786013	-0.418109	-0.322999
C	8.001003	-1.128125	-0.454999
C	6.756032	1.003892	-0.281999
C	7.962042	1.740875	-0.347999
C	6.707071	3.846892	-0.293999
C	7.939062	3.160876	-0.342999
C	6.683090	5.261893	-0.337999
C	7.892100	5.993876	-0.439999
C	6.613129	8.084894	-0.486999
C	7.856120	7.414877	-0.516999
C	6.567148	9.491894	-0.573999
C	7.750158	10.224878	-0.679999
C	9.157896	-8.984141	-1.161999
C	10.300885	-9.788157	-1.284999
C	9.196915	-7.566142	-1.011999
C	10.407925	-6.854158	-0.933999

C	9.231954	-4.726142	-0.781999
C	10.423944	-5.471158	-0.815999
C	9.233974	-3.232142	-0.709999
C	10.414985	-2.476158	-0.840999
C	9.220013	-0.423142	-0.520999
C	10.408003	-1.143158	-0.753999
C	9.202033	1.066858	-0.409999
C	10.385043	1.821842	-0.341999
C	9.159071	3.886859	-0.390999
C	10.367061	3.155842	-0.332999
C	9.134091	5.310859	-0.473999
C	10.310101	6.076843	-0.621999
C	9.058130	8.165860	-0.635999
C	10.273120	7.462844	-0.694999
C	8.999149	9.589861	-0.707999
C	10.130161	10.413846	-0.804999
H	-11.219116	-9.819863	-1.074999
H	-9.042131	-10.948892	-1.130999
H	-11.377083	-7.422861	-0.852999
H	-11.424055	-5.345860	-0.604999
H	-11.464023	-3.050859	-0.455999
H	-11.438995	-0.990860	-0.848999
H	-11.438964	1.304140	-0.835999
H	-11.474936	3.341141	-0.396999
H	-11.468905	5.619141	-0.505999
H	-11.443877	7.650140	-0.882999
H	-11.319844	10.038139	-1.058999
H	-9.170828	11.214109	-0.975999
H	-6.624130	-10.853926	-1.081999
H	-6.757829	11.169076	-0.794999
H	-4.218129	-10.796958	-1.064999
H	-4.349829	11.153043	-0.651999
H	-1.786129	-10.765992	-1.087999
H	-1.934829	11.154010	-0.558999
H	0.654872	-10.731025	-1.129999
H	0.482171	11.167977	-0.524999
H	3.083872	-10.695058	-1.183999
H	2.896171	11.197944	-0.553999
H	5.491872	-10.687091	-1.247999
H	5.308172	11.241912	-0.633999
H	7.877872	-10.713124	-1.313999
H	7.695173	11.306879	-0.740999
H	11.308890	-9.409170	-1.294999
H	10.211870	-10.862155	-1.394999
H	11.368918	-7.341171	-0.953999
H	11.392950	-5.009172	-0.736999
H	11.366978	-2.939171	-1.041999
H	11.355010	-0.647171	-0.895999
H	11.354037	1.352829	-0.279999
H	11.330068	3.632829	-0.262999
H	11.288095	5.637830	-0.715999
H	11.222127	7.958831	-0.814999
H	11.144156	10.052832	-0.816999
H	10.025175	11.491847	-0.860999
O	-0.687965	1.250993	2.455001
O	-0.432996	-1.085010	2.380001
C	-0.997014	-2.340002	3.276001
H	-0.375952	2.166989	2.553001
C	-0.163012	-2.228014	4.465001
C	-2.481012	-2.203982	3.383001
H	-0.703025	-3.165006	2.627001
C	-3.260027	-3.342971	3.171001
C	-4.648026	-3.265952	3.236001
C	-5.262010	-2.043944	3.498001
C	-4.485994	-0.906955	3.720001
C	-3.097995	-0.986974	3.674001
H	-2.777040	-4.287978	2.931001
H	-5.245038	-4.152944	3.052001
H	-6.344009	-1.974929	3.522001
H	-4.962981	0.047052	3.916001
H	-2.505983	-0.083982	3.805001

C	1.028979	-2.889030	4.513001
H	-0.445002	-1.503010	5.224001
H	1.641979	-2.862038	5.408001
H	1.166967	-3.764032	3.884001
C	2.510991	-2.013050	3.264001
C	4.842992	-1.929082	4.183001
H	1.774989	-2.146040	2.484001
H	-0.405985	-0.250010	2.921001
C	6.228987	-2.265101	4.634001
H	6.236975	-3.148101	5.280001
H	6.881985	-2.470110	3.779001
H	6.648999	-1.426107	5.193001
C	2.830007	-0.808055	3.856001
H	2.124019	0.014955	3.915001
S	3.907977	-3.057069	3.265001
C	4.130008	-0.779072	4.415001
H	4.534019	0.051922	4.981001

TS2 – β attack

C	-10.062810	-9.446211	-1.205017
C	-8.812798	-10.056186	-1.210017
C	-10.170837	-8.064213	-1.050017
C	-9.019853	-7.258190	-0.886017
C	-10.320897	-5.080216	-0.653017
C	-9.092883	-5.770192	-0.720017
C	-10.376924	-3.745218	-0.554017
C	-9.209939	-2.957194	-0.517017
C	-10.449984	-0.737219	-0.679017
C	-9.253969	-1.454195	-0.485017
C	-10.479010	0.599780	-0.650017
C	-9.316026	1.365804	-0.421017
C	-10.558070	3.583779	-0.351017
C	-9.349056	2.861803	-0.373017
C	-10.583097	4.920778	-0.384017
C	-9.398112	5.688802	-0.435017
C	-10.612155	7.864778	-0.651017
C	-9.413140	7.114802	-0.530017
C	-10.588183	9.255778	-0.740017
C	-9.380197	9.941802	-0.721017
C	-7.652813	-9.287163	-1.064017
C	-6.401800	-9.913138	-1.088017
C	-7.747841	-7.881165	-0.902017
C	-6.568856	-7.112142	-0.762017
C	-7.890898	-5.030168	-0.610017
C	-6.641885	-5.703143	-0.613017
C	-7.959926	-3.612169	-0.497017
C	-6.723942	-2.812145	-0.341017
C	-8.053984	-0.726171	-0.323017
C	-6.767969	-1.458146	-0.237017
C	-8.076012	0.698828	-0.293017
C	-6.879027	1.452852	-0.173017
C	-8.133070	3.576827	-0.325017
C	-6.905056	2.881852	-0.217017
C	-8.156098	4.998827	-0.369017
C	-6.943113	5.723851	-0.348017
C	-8.182155	7.824826	-0.524017
C	-6.956141	7.131851	-0.428017
C	-8.175183	9.240826	-0.619017
C	-6.965197	9.943851	-0.617017
C	-5.229815	-9.166115	-0.953017
C	-3.982803	-9.811090	-0.998017
C	-5.309843	-7.765116	-0.783017
C	-4.054859	-6.983091	-0.633017
C	-5.380900	-4.929118	-0.451017
C	-4.129887	-5.589093	-0.455017
C	-5.429928	-3.531119	-0.300017
C	-4.248942	-2.808095	-0.115017
C	-5.524985	-0.672121	-0.059017
C	-4.299972	-1.347096	0.042983
C	-5.575013	0.736878	-0.025017

C	-4.389028	1.473902	0.113983
C	-5.703071	3.630876	-0.150017
C	-4.412057	2.938902	0.015983
C	-5.714099	5.038876	-0.238017
C	-4.496114	5.766900	-0.218017
C	-5.737155	7.853875	-0.424017
C	-4.506142	7.169900	-0.325017
C	-5.748183	9.262875	-0.524017
C	-4.543198	9.975899	-0.538017
C	-2.791817	-9.088066	-0.875017
C	-1.547804	-9.737041	-0.949017
C	-2.850846	-7.615067	-0.676017
C	-1.647861	-6.889043	-0.545017
C	-2.941902	-4.847069	-0.289017
C	-1.692889	-5.500044	-0.337017
C	-3.010929	-3.459071	-0.098017
C	-1.772945	-2.682046	0.136983
C	-3.044986	-0.605071	0.293983
C	-1.854972	-1.310047	0.412983
C	-3.091014	0.790928	0.322983
C	-1.939029	1.547951	0.442983
C	-3.207071	3.654926	0.049983
C	-1.931057	2.930951	0.243983
C	-3.193099	5.052926	-0.089017
C	-2.021113	5.747949	-0.115017
C	-3.292156	7.895924	-0.342017
C	-2.053143	7.223949	-0.259017
C	-3.317184	9.303923	-0.455017
C	-2.116199	10.024947	-0.492017
C	-0.351818	-9.013017	-0.844017
C	0.891194	-9.654993	-0.943017
C	-0.400848	-7.544018	-0.634017
C	0.799137	-6.804994	-0.548017
C	-0.491903	-4.772020	-0.212017
C	0.752110	-5.412995	-0.347017
C	-0.542932	-3.319021	0.045983
C	0.652053	-2.585997	0.089983
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H	12.328513	6.132140	-0.843027
H	12.588137	8.211351	-0.814789
H	11.714547	9.811725	-0.841744
O	-0.499397	1.484953	2.491465
O	-0.910399	-0.881878	2.378300
C	-0.590875	-4.336998	3.622030
H	-0.502070	2.456424	2.523261

C	-0.106382	-3.243843	4.221771
C	-2.003501	-4.613725	3.315581
H	0.103995	-5.140987	3.370362
C	-2.407607	-5.942083	3.137645
C	-3.742929	-6.256769	2.906186
C	-4.693978	-5.243081	2.838908
C	-4.298258	-3.913254	2.982676
C	-2.964654	-3.599505	3.211896
H	-1.666286	-6.735720	3.187491
H	-4.037879	-7.291504	2.766012
H	-5.734507	-5.483153	2.645745
H	-5.030646	-3.116516	2.890689
H	-2.652111	-2.561800	3.262570
C	1.356126	-3.076918	4.517084
H	-0.771168	-2.435741	4.514821
H	1.532308	-2.694077	5.527096
H	1.851143	-4.049866	4.436921
C	2.045414	-2.128727	3.490541
C	4.089320	-0.612233	3.620493
C	2.873445	0.116675	3.659653
H	1.705300	-2.453909	2.496433
H	-1.502916	-0.249798	2.821697
S	3.864046	-2.279513	3.515294
C	1.771419	-0.676816	3.585839
H	0.747300	-0.312171	3.524897
C	5.439760	0.005653	3.639703
H	5.545797	0.649614	2.758117
H	5.531512	0.656127	4.516448
H	6.249163	-0.724362	3.641508
H	2.847886	1.200529	3.696624

RX3

C	-11.287711	-7.983352	-1.071278
C	-10.133015	-8.757425	-1.083543
C	-11.204933	-6.599267	-0.927464
C	-9.953528	-5.956269	-0.782257
C	-10.945825	-3.624294	-0.533821
C	-9.821814	-4.472445	-0.622550
C	-10.819781	-2.295159	-0.437729
C	-9.557574	-1.672833	-0.423404
C	-10.485483	0.697473	-0.568021
C	-9.398787	-0.178806	-0.386914
C	-10.327130	2.026555	-0.541816
C	-9.065404	2.620997	-0.326247
C	-9.969812	4.994299	-0.279566
C	-8.878832	4.106186	-0.295444
C	-9.800663	6.318775	-0.339331
C	-8.517521	6.905320	-0.416652
C	-9.409488	9.224466	-0.694319
C	-8.329721	8.314734	-0.549530
C	-9.188796	10.595450	-0.817422
C	-7.895924	11.102740	-0.810991
C	-8.877819	-8.151500	-0.958696
C	-7.725400	-8.941811	-0.990470
C	-8.777886	-6.743989	-0.809141
C	-7.502818	-6.140092	-0.695022
C	-8.529050	-3.901456	-0.537771
C	-7.379578	-4.734158	-0.559496
C	-8.406208	-2.490246	-0.427086
C	-7.071594	-1.865443	-0.291456
C	-8.109215	0.375222	-0.233559
C	-6.934982	-0.525690	-0.170870
C	-7.933849	1.786777	-0.200433
C	-6.643364	2.361058	-0.083536
C	-7.570308	4.637374	-0.264044
C	-6.454899	3.773345	-0.145837
C	-7.386493	6.046014	-0.337368
C	-6.081659	6.587408	-0.332893
C	-7.010489	8.841728	-0.559982
C	-5.894462	7.982937	-0.445795

C	-6.803179	10.239636	-0.688669
C	-5.506558	10.763857	-0.701322
C	-6.461060	-8.359228	-0.879638
C	-5.318067	-9.170993	-0.927880
C	-6.344896	-6.958621	-0.728363
C	-4.992705	-6.353186	-0.607874
C	-6.019910	-4.132534	-0.429209
C	-4.871783	-4.957671	-0.447925
C	-5.877178	-2.737748	-0.279803
C	-4.604559	-2.165770	-0.104352
C	-5.594346	0.070823	0.005436
C	-4.464809	-0.770090	0.083382
C	-5.462587	1.470754	0.066756
C	-4.124718	2.075725	0.217135
C	-5.150257	4.335743	-0.092169
C	-3.961923	3.461349	0.091859
C	-4.961885	5.734809	-0.207953
C	-3.655022	6.287160	-0.201566
C	-4.586438	8.525816	-0.457092
C	-3.464984	7.678648	-0.339868
C	-4.398888	9.920165	-0.589825
C	-3.105607	10.458807	-0.616895
C	-4.037827	-8.618730	-0.828888
C	-2.900220	-9.438320	-0.897455
C	-3.889269	-7.148159	-0.655225
C	-2.595541	-6.597676	-0.547498
C	-3.591730	-4.384616	-0.308047
C	-2.444145	-5.212721	-0.362998
C	-3.464660	-2.996376	-0.123387
C	-2.122445	-2.412685	0.083053
C	-3.120845	-0.188757	0.351276
C	-2.011480	-1.059770	0.391743
C	-2.957599	1.185106	0.427242
C	-1.683421	1.777974	0.533098
C	-2.667028	4.016505	0.111077
C	-1.491207	3.135059	0.300687
C	-2.469655	5.402711	-0.053487
C	-1.216500	5.933664	-0.090248
C	-2.158756	8.231328	-0.369932
C	-1.025872	7.398600	-0.265416
C	-1.985034	9.626598	-0.514977
C	-0.693708	10.175952	-0.562747
C	-1.613284	-8.891138	-0.808599
C	-0.475459	-9.706807	-0.892098
C	-1.453492	-7.426264	-0.625839
C	-0.159634	-6.867664	-0.542558
C	-1.154127	-4.669328	-0.243183
C	-0.007560	-5.483042	-0.356746
C	-0.992997	-3.225631	0.000446
C	0.291111	-2.688566	0.098671
C	-0.695275	-0.569224	0.757976
C	0.477624	-1.346941	0.396205
C	-0.508265	0.982697	0.840694
C	0.819166	1.506333	0.549693
C	-0.211563	3.673541	0.248557
C	0.934888	2.872091	0.321614
C	-0.070664	5.119726	0.040013
C	1.273229	5.686163	-0.075436
C	0.278989	7.958232	-0.326171
C	1.426772	7.137779	-0.247452
C	0.438241	9.352890	-0.477078
C	1.727860	9.907804	-0.546415
C	0.813375	-9.155498	-0.817707
C	1.946787	-9.972706	-0.905499
C	0.984154	-7.687418	-0.645021
C	2.232543	-7.151746	-0.589935
C	1.291874	-4.926964	-0.292421
C	2.417157	-5.765289	-0.424445
C	1.476198	-3.549177	-0.095769
C	2.764934	-2.992635	-0.076109
C	1.759291	-0.744748	0.358835

C	2.938826	-1.609383	0.099483
C	1.922950	0.620798	0.448201
C	3.271931	1.198121	0.241689
C	2.281610	3.474850	0.152768
C	3.414406	2.655782	0.119604
C	2.404975	4.858539	-0.031980
C	3.751090	5.460951	-0.163535
C	2.722262	7.690947	-0.338778
C	3.873364	6.858720	-0.299045
C	2.867639	9.087719	-0.484267
C	4.150581	9.646735	-0.574313
C	3.238667	-9.425888	-0.846517
C	4.355574	-10.262083	-0.934771
C	3.421986	-8.033898	-0.700828
C	4.726526	-7.483129	-0.659333
C	3.717990	-5.212211	-0.390504
C	4.913597	-6.089662	-0.520665
C	3.883331	-3.826701	-0.233304
C	5.239369	-3.238394	-0.236669
C	4.216755	-1.028242	0.021916
C	5.396918	-1.900936	-0.136159
C	4.385306	0.368281	0.072437
C	5.745803	0.969921	-0.069206
C	4.762135	3.233316	-0.051555
C	5.893607	2.385406	-0.109954
C	4.897798	4.631869	-0.161902
C	6.178893	5.202117	-0.283548
C	5.157658	7.429908	-0.408386
C	6.309363	6.603451	-0.396280
C	5.291633	8.829433	-0.538965
C	6.566856	9.395113	-0.641954
C	5.651017	-9.730088	-0.883929
C	6.751560	-10.583847	-0.965400
C	5.844968	-8.337972	-0.753838
C	7.153837	-7.807798	-0.713246
C	6.223204	-5.536749	-0.501258
C	7.342954	-6.401014	-0.603905
C	6.412322	-4.132418	-0.372008
C	7.701115	-3.555432	-0.391354
C	6.745147	-1.289050	-0.187265
C	7.866164	-2.141136	-0.306866
C	6.885866	0.128630	-0.164690
C	8.171566	0.716559	-0.236792
C	7.180194	2.962429	-0.222748
C	8.319975	2.131735	-0.254632
C	7.325259	4.371722	-0.296699
C	8.611435	4.951862	-0.405795
C	7.589100	7.183116	-0.509729
C	8.743806	6.366864	-0.513043
C	7.710771	8.583923	-0.627831
C	8.973820	9.166355	-0.735179
C	8.061703	-10.090419	-0.915828
C	9.098049	-11.030861	-1.016616
C	8.273507	-8.685312	-0.779691
C	9.561482	-8.126092	-0.689814
C	8.652594	-5.867591	-0.584031
C	9.745249	-6.752232	-0.588108
C	8.835972	-4.381820	-0.533510
C	10.099554	-3.775207	-0.675926
C	9.161320	-1.587459	-0.378414
C	10.253729	-2.448484	-0.604459
C	9.321973	-0.102019	-0.284395
C	10.587316	0.507041	-0.216654
C	9.617784	2.706277	-0.307097
C	10.729188	1.835659	-0.227801
C	9.763360	4.123071	-0.416436
C	11.022529	4.741890	-0.573516
C	10.027587	6.966119	-0.636223
C	11.150584	6.122264	-0.673286
C	10.137922	8.386323	-0.736432
C	11.358866	9.070618	-0.833695

H	-12.256066	-8.458952	-1.179653
H	-10.219507	-9.831777	-1.199419
H	-12.134966	-6.056972	-0.944216
H	-11.950327	-4.013543	-0.533614
H	-11.730215	-1.722957	-0.357369
H	-11.478932	0.328868	-0.768199
H	-11.207588	2.620552	-0.725811
H	-10.984953	4.638717	-0.203077
H	-10.701576	6.907853	-0.312395
H	-10.438396	8.911961	-0.735332
H	-10.030458	11.270636	-0.926076
H	-7.748351	12.172134	-0.911053
H	-7.814009	-10.016448	-1.108334
H	-5.359636	11.833640	-0.803209
H	-5.426756	-10.242844	-1.051413
H	-2.971057	11.529564	-0.724740
H	-3.017850	-10.508063	-1.028497
H	-0.569791	11.247175	-0.677158
H	-0.593742	-10.776606	-1.022287
H	1.844486	10.979698	-0.661312
H	1.822956	-11.043278	-1.026069
H	4.261250	10.719989	-0.682828
H	4.216198	-11.332378	-1.043491
H	6.669281	10.470432	-0.740091
H	6.583141	-11.650816	-1.069824
H	9.049773	10.245553	-0.818933
H	10.145202	-10.780512	-1.021017
H	8.879823	-12.087608	-1.116480
H	10.452924	-8.731486	-0.686540
H	10.762329	-6.407241	-0.496192
H	10.985574	-4.355480	-0.878263
H	11.251168	-2.068431	-0.757961
H	11.490890	-0.076921	-0.140267
H	11.740887	2.198015	-0.157280
H	11.940335	4.185454	-0.656337
H	12.150766	6.502878	-0.799747
H	12.323729	8.593231	-0.823316
H	11.383846	10.151100	-0.912203
O	-0.607542	0.143598	1.984353
C	-1.547982	-2.871165	3.525908
C	-0.725797	-2.085074	4.229435
C	-2.995174	-2.658365	3.364349
H	-1.148796	-3.779419	3.070095
C	-3.823512	-3.763321	3.136271
C	-5.201904	-3.608418	3.035234
C	-5.769631	-2.341736	3.153834
C	-4.950084	-1.231383	3.353025
C	-3.572050	-1.385680	3.448956
H	-3.378725	-4.749843	3.032192
H	-5.829983	-4.472470	2.845775
H	-6.842597	-2.214271	3.056306
H	-5.382140	-0.236253	3.396535
H	-2.930788	-0.511346	3.528619
C	0.731791	-2.394581	4.417943
H	-1.116090	-1.193788	4.717055
H	1.026974	-2.327198	5.469557
H	0.934222	-3.414540	4.074635
C	1.610566	-1.443586	3.580015
C	3.879096	-0.310416	3.596174
C	2.821554	0.612851	3.805246
H	1.235070	-1.494206	2.534592
S	3.364755	-1.910006	3.476319
C	1.599362	0.007332	3.840284
H	0.655134	0.536637	3.936922
H	2.991889	1.681104	3.881405
C	5.316833	0.060333	3.478276
H	5.902874	-0.713017	2.979151
H	5.409988	1.001389	2.927699
H	5.725412	0.221849	4.483561

TS3

C	-11.945571	-6.927713	-1.173017
C	-10.868520	-7.805650	-1.179017
C	-11.736651	-5.559701	-1.011017
C	-10.432682	-5.037625	-0.842017
C	-11.208823	-2.628670	-0.586017
C	-10.166767	-3.575609	-0.662017
C	-10.961899	-1.319656	-0.470017
C	-9.648929	-0.817579	-0.420017
C	-10.354072	1.624380	-0.559017
C	-9.354015	0.653439	-0.368017
C	-10.076148	2.931396	-0.532017
C	-8.767176	3.407473	-0.307017
C	-9.453319	5.851433	-0.304017
C	-8.447262	4.868492	-0.290017
C	-9.164396	7.152450	-0.382017
C	-7.833423	7.618528	-0.451017
C	-8.511562	10.002488	-0.771017
C	-7.519504	9.002546	-0.605017
C	-8.167641	11.344508	-0.920017
C	-6.834664	11.733586	-0.917017
C	-9.563548	-7.320574	-1.030017
C	-8.489496	-8.214511	-1.053017
C	-9.335629	-5.930560	-0.863017
C	-8.010658	-5.448483	-0.726017
C	-8.827793	-3.128531	-0.548017
C	-7.759739	-4.062468	-0.569017
C	-8.577875	-1.736516	-0.414017
C	-7.193904	-1.239435	-0.246017
C	-8.022040	1.085517	-0.192017
C	-6.935981	0.081580	-0.111017
C	-7.718122	2.474534	-0.161017
C	-6.382148	2.929613	-0.030017
C	-7.096286	5.278571	-0.250017
C	-6.065229	4.317631	-0.106017
C	-6.785367	6.662589	-0.344017
C	-5.437391	7.082668	-0.337017
C	-6.157528	9.407626	-0.616017
C	-5.124472	8.453686	-0.476017
C	-5.824608	10.777645	-0.771017
C	-4.486631	11.181724	-0.787017
C	-7.177523	-7.752434	-0.921017
C	-6.114469	-8.665372	-0.962017
C	-6.933604	-6.369420	-0.756017
C	-5.531632	-5.892338	-0.622017
C	-6.351766	-3.589386	-0.419017
C	-5.283712	-4.514323	-0.451017
C	-6.083847	-2.217370	-0.236017
C	-4.764873	-1.765293	-0.047017
C	-5.548009	0.551661	0.085983
C	-4.502954	-0.391277	0.162983
C	-5.289090	1.935677	0.141983
C	-3.903118	2.415758	0.291983
C	-4.715255	4.760710	-0.047017
C	-3.612198	3.783775	0.155983
C	-4.400336	6.134729	-0.186017
C	-3.049361	6.566808	-0.183017
C	-3.773496	8.874765	-0.490017
C	-2.733441	7.931826	-0.350017
C	-3.460577	10.243784	-0.652017
C	-2.124601	10.662862	-0.685017
C	-4.789494	-8.235294	-0.845017
C	-3.733440	-9.157232	-0.901017
C	-4.506579	-6.785278	-0.665017
C	-3.168604	-6.356199	-0.545017
C	-3.956739	-4.061245	-0.302017
C	-2.890684	-4.991183	-0.358017
C	-3.706819	-2.692231	-0.085017
C	-2.316846	-2.234149	0.119983
C	-3.108981	0.067804	0.421983

C	-2.083924	-0.902136	0.439983
C	-2.820060	1.422821	0.492983
C	-1.496088	1.900899	0.579983
C	-2.274224	4.221853	0.174983
C	-1.183166	3.235917	0.363983
C	-1.948303	5.580872	-0.017017
C	-0.651328	5.995948	-0.065017
C	-1.383466	8.363905	-0.389017
C	-0.330412	7.433967	-0.269017
C	-1.084547	9.734923	-0.563017
C	0.250428	10.164001	-0.620017
C	-2.401465	-8.733154	-0.797017
C	-1.344411	-9.652092	-0.865017
C	-2.108550	-7.289137	-0.614017
C	-0.769575	-6.853059	-0.520017
C	-1.554709	-4.567105	-0.236017
C	-0.491655	-5.488043	-0.335017
C	-1.263793	-3.144088	0.013983
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PD3

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O	-0.852184	-0.661766	2.256703
C	0.950090	-3.560600	3.328780
C	0.977500	-2.419552	4.026781
C	-0.239712	-4.411104	3.151978
H	1.878671	-3.935756	2.894849
C	-0.088466	-5.794127	2.981374
C	-1.199742	-6.623215	2.867251
C	-2.483994	-6.081905	2.908190
C	-2.647451	-4.704917	3.043736
C	-1.537283	-3.873769	3.154496
H	0.911144	-6.220122	2.948411
H	-1.063762	-7.692130	2.738470
H	-3.351017	-6.727258	2.810868
H	-3.644513	-4.274087	3.044607
H	-1.666052	-2.796117	3.208772
C	2.208290	-1.580314	4.230372
H	0.072413	-2.094034	4.538460
H	2.589319	-1.742496	5.248994
H	2.999938	-1.911780	3.548100
C	1.956425	-0.101653	4.051423
C	2.250816	2.364404	3.652263
C	0.990133	2.032705	4.047418
H	0.019651	-0.393983	2.615656
S	3.251613	0.947326	3.568175
C	0.825345	0.632020	4.297219

H	-0.100678	0.211832	4.682187
C	2.809488	3.737119	3.406919
H	2.050164	4.362391	2.927459
H	3.100824	4.203703	4.352227
H	3.694130	3.709487	2.765688
H	0.196381	2.761557	4.176560