Supporting information

Solvent-Driven C(sp^3)–H Thiocarbonylation of Benzylamine Derivatives under Catalyst-Free Conditions

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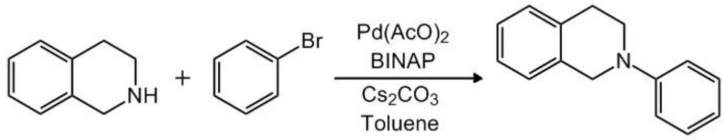
1. General Information

^{1}H NMR and ^{13}C NM1R spectra were recorded on Bruker AVANCE 400 and 500 spectrometer. Chemical shifts of protons were reported in parts per million downfield from tetramethylsilane and were referenced to residual protium in the NMR solvent ($CDCl_3$: δ 7.26), (DMSO-d6: δ 2.50). Chemical shifts of carbon were referenced to the carbon resonances of the solvent ($CDCl_3$: δ 77.0), (DMSO-d6: δ 39.5). Peaks were labeled as singlet (s), doublet (d), triplet (t), quartet (q) and multiplet (m). Melting points were measured on a WRS-2A melting point apparatus and were uncorrected. All products were further characterized by HRMS (high resolution mass spectra). Copies of their ^{1}H NMR and ^{13}C NMR spectra were provided. Substrates of **1c**-**1e** were purchased from *J&K* and used without further purification. DMF was purchased from *J&K* in 99.8% and DMPU was purchased from *J&K* in 98%. Both the grades of DMF and DMPU were analysis pure.

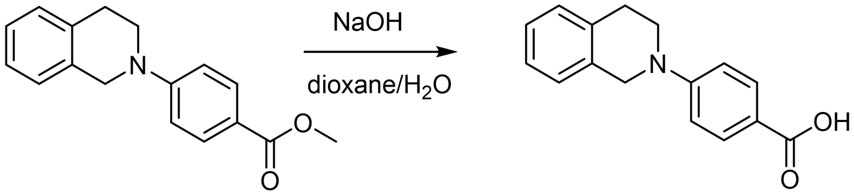
2. General Procedures

(I) Typical procedure for the preparation of substrates 1a, 1b, 1aa–1an, 1ap, 1aq and 1as–1ay.



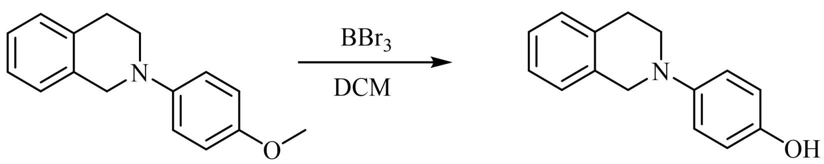
The compound was synthesized according to a known procedure.[1-3] To a solution of cesium carbonate (1.95 g, 6.0 mmol) in toluene (15 mL), bromobenzene (471 mg, 3.0 mmol), $Pd(AcO)_2$ (37 mg, 0.15 mmol), BINAP (186 mg, 0.3 mmol) and 1,2,3,4-tetrahydroisoquinoline (598 mg, 4.5 mmol) were added in sequence. The reaction mixture was stirred at 100 °C for 10 h. After completion of the reaction as shown by TLC, the crude mixture was filtered with celatom. And the filter liquor was heated through vacuum distillation to remove toluene. Then, the crude product was purified by flash chromatography to give a yellow oil **1a** (439 mg, yield: 70%).

(II) Typical procedure for the preparation of substrates 1ao.



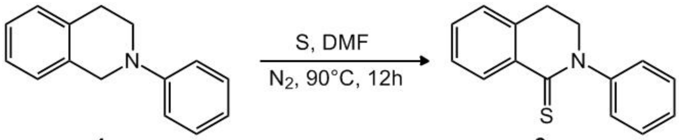
To a solution of NaOH (160 mg, 4.0 mmol) in dioxane (5 mL), H_2O (5 mL), the substrate methyl 4-(3,4-dihydroisoquinolin-2(1H)-yl)benzoatebromobenzene **1am** (534 mg, 2.0 mmol) was added. The reaction mixture was stirred at 90 °C for 2 h. Then, the mixture was acidated with 2 M HCl to pH 3-4. The mixture was extracted with ethyl acetate (5 mL × 3), the combined organic layer was washed with saturated NaCl (5 mL), dried with anhydrous sodium sulfate and concentrated in vacuum, giving a yellow solid **1ao** (455 mg, yield: 90%).

(III) Typical procedure for the preparation of substrates 1ar.



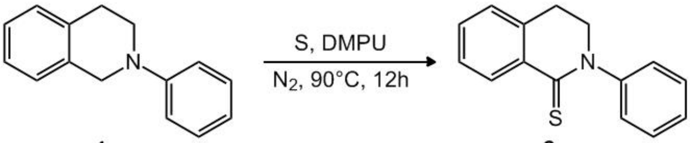
To a solution of the substrate 2-(4-methoxyphenyl)-1, 2, 3, 4-tetrahydroisoquinoline **1ae** (480 mg, 2.0 mmol) in DCM (5 mL), BBr_3 1.0 M (4 mL, 4 mmol) was added dropwise. The mixture was stirred at -78 °C for 2 h. Then, continue to react at room temperature for 10 h. After that, the mixture was quenched with saturated NH_4Cl at 0 °C. The mixture was filted with diatomite, then DCM 10 mL was added for extraction. Then, the combined organic layer was dried with anhydrous sodium sulfate. The crude production was purified by flash chromatography to give a yellow oil **1ar** (90 mg, yield: 20%).

(IV) Typical procedure for catalyst-free C(*sp*^{3})–H thiocarbonylation.



1a 2a

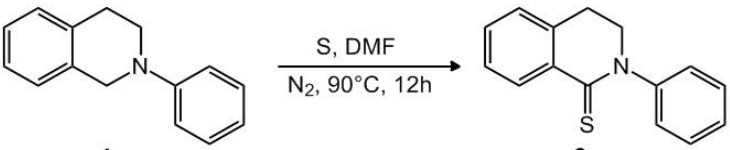
2-phenyl-1, 2, 3, 4-tetrahydroisoquinoline **1a** (62.7 mg, 0.3 mmol) and S (19.2 mg, 0.6 mmol) was added to 10 mL reaction tube containing 2 mL DMF, and the reaction mixture was stirred at 90 °C in nitrogen atmosphere condition for 12 h. Then, DMF was recycled through vacuum distillation at 90 °C in 60 mbar. The rest crude product was purified by flash chromatography to give a yellow solid **2a** (50.2 mg, yield: 70%).



1a 2a

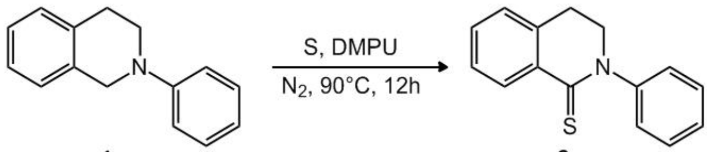
2-phenyl-1, 2, 3, 4-tetrahydroisoquinoline **1a** (62.7 mg, 0.3 mmol) and S (19.2 mg, 0.6 mmol) was added to 10 mL reaction tube containing 2 mL DMPU, and the reaction mixture was stirred at 90°C in nitrogen atmosphere condition for 12 h. Then, most of DMPU was removed through vacuum distillation at 145°C in 60 mbar and the remaining small amount of DMPU was removed by the column chromatography silica gel (200–300 mesh). The rest reaction mixture was further dried on the rotary evaporator and the obtained crude product was purified by flash chromatography to give a yellow solid **2a** (54.5 mg, yield: 76%).

(V) Gram scale reaction



1a 2a

2-phenyl-1, 2, 3, 4-tetrahydroisoquinoline **1a** (1045 mg, 5 mmol) and S (320 mg, 10 mmol) were added to 50 mL reaction tube containing 10 mL DMF, the reaction mixture was stirred at 90°C in nitrogen atmosphere condition for 12 h. Then, about 8 mL DMF was recovered through vacuum distillation at 90°C in 60 mbar (the recovery rate of DMF is about 80%). The rest crude product was further purified by flash chromatography to give a yellow solid **2a** (776 mg, yield: 65%).



1a 2a

2-phenyl-1, 2, 3, 4-tetrahydroisoquinoline 1a (1045 mg, 5 mmol) and S (320 mg, 10 mmol) were added to 50 mL reaction tube containing 10 mL DMPU, the reaction mixture was stirred at 90 °C in nitrogen atmosphere condition for 12 h. Then, about 7.5 mL DMPU was recovered through vacuum distillation at 145 °C in 60 mbar (the recovery of DMPU is about 75%). The rest crude product was further purified by flash chromatography to give a yellow solid **2a** (848 mg, yield: 71%).

3. Computational Method

All the geometry optimization and vibration frequency calculation were carried out in Gaussian09 package.[4] And the density-functional theory (DFT) method[5] were employed for these computations. For geometry optimization, all the structures including the ground states (**1**, **A**, **B**, **C** and **2**) and transition states (**TS1**, **TS2** and **TS3**) were performed at the B3LYP method[6] with 6-31+G(d, p) basis set[7]. For vibration frequency calculation, same computational method and basis set were carried out to make sure that the optimized structures were true energy minima, and obtain the absolute free energies of the optimized molecules. The reaction coordinate driving method (flexible scan) as well as the following restricted geometry optimization and the corresponding vibration frequency were employed to calculate the free energy profiles from **B** state to **C** state for the selected molecules (**1a–1e**) also at the same computational method and basis set. The reaction coordinate from **B** state to **C** state was the attack distance between the S_3•⁻ molecule and the B state. All the above calculations considered the solvation effect (DMPU, DMF, DMA, Acetone and CH_3CN) provided by the PCM solvent continuum models.[8]

4. Figures S1-S2

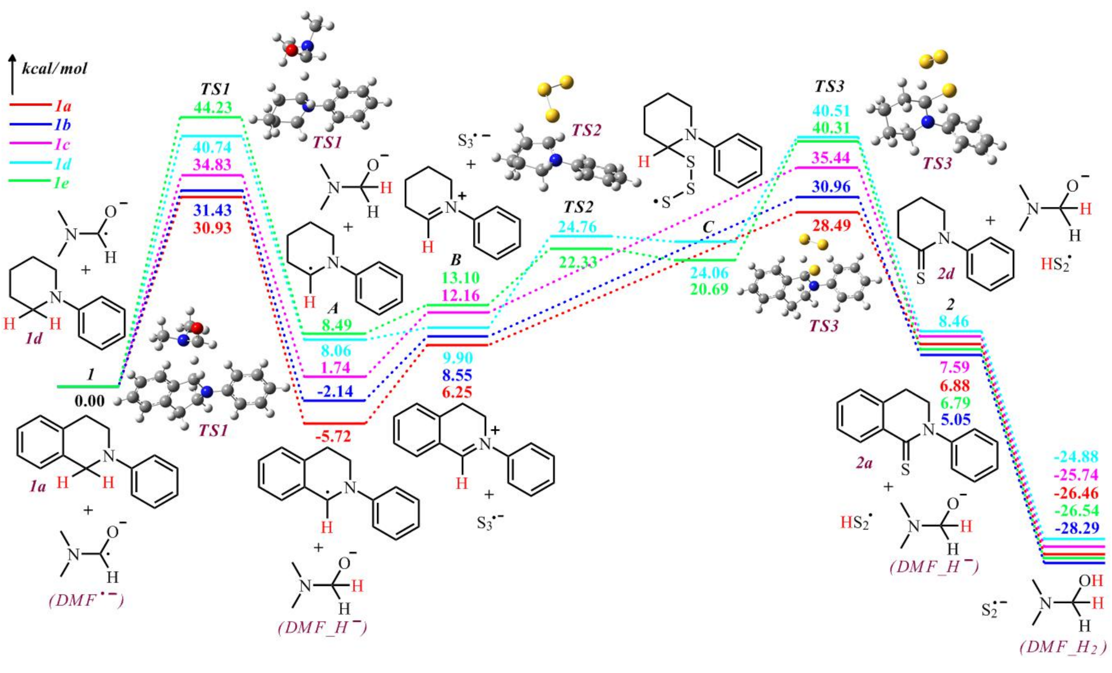


Figure S1. Reaction profiles of **1a–1e** in DMF solvent based on the reaction mechanism in Figure 1 (mechanistic studies).

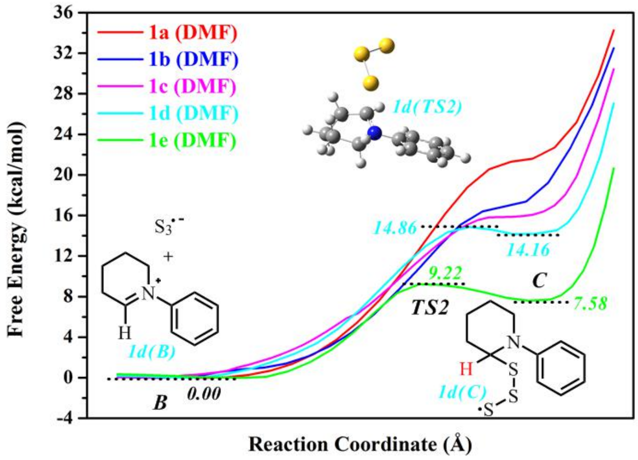
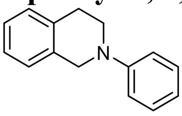


Figure S2. Influence of **C** state on our C(sp^3)–H thiocarbonylation (mechanistic studies).

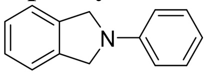
5. Characterization Data

2-phenyl-1, 2, 3, 4-tetrahydroisoquinoline (1a)



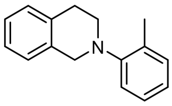
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.31-7.25 (m, 2H), 7.20-7.13 (m, 4H), 6.98 (d, *J* = 8.0 Hz, 2H), 6.82 (t, *J* = 7.2 Hz, 1H), 4.41 (s, 2H), 3.56 (t, *J* = 5.8 Hz, 2H), 2.99 (t, *J* = 5.8 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 150.58, 134.90, 134.49, 129.22, 128.54, 126.56, 126.35, 126.04, 118.68, 115.16, 50.76, 46.54, 29.14. **HRMS** (ESI) calculated for $C_{15}H_{16}N$ $(M+H)^+$: 210.1277, found: 210.1273. Same compound was also reported in previous literature[9] and our characterization data was highly consistent with its data.

2-phenylisoindoline (1b)



White solid. M. p. 171-172 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.49-7.30 (m, 6H), 6.82 (t, *J* = 7.2 Hz, 1H), 6.75 (d, *J* = 8.0 Hz, 2H), 4.71 (s, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 147.20, 137.99, 129.44, 127.21, 122.66, 116.24, 111.65, 53.81. **HRMS** (ESI) calculated for $C_{14}H_{14}N$ $(M+H)^+$: 196.1121, found: 196.1123. Same compound was also reported in previous literature[10] and our characterization data was highly consistent with its data.

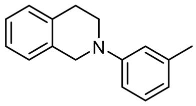
2-(*o*-tolyl)-1, 2, 3, 4-tetrahydroisoquinoline (1aa)



Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.31-7.21 (m, 5H), 7.20-7.13 (m, 2H), 7.08 (t, *J* = 7.2 Hz, 1H), 4.20 (s, 2H), 3.29 (t, *J* = 5.8 Hz, 2H), 3.08 (t, *J* = 5.6 Hz, 2H), 2.42

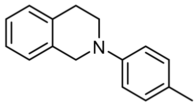
(s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 151.58, 135.53, 134.66, 132.95, 131.20, 128.99, 126.64, 126.46, 126.24, 125.74, 123.27, 119.34, 54.26, 50.36, 29.74, 18.11. **HRMS** (ESI) calculated for $C_{16}H_{18}N$ $(M+H)^+$: 224.1434, found: 224.1433. Same compound was also reported in previous literature[10] and our characterization data was highly consistent with its data.

2-(*m*-tolyl)-1, 2, 3, 4-tetrahydroisoquinoline (1ab)



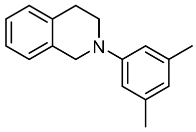
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.22-7.11 (m, 5H), 7.08 (d, J = 8.8 Hz, 2H), 6.99 (t, J = 7.2 Hz, 1H), 4.10 (s, 2H), 3.19 (t, J = 5.6 Hz, 2H), 2.99 (t, J = 5.4 Hz, 2H), 2.34 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 151.63, 135.57, 134.69, 132.99, 131.24, 129.02, 126.68, 126.49, 126.28, 125.78, 123.31, 119.39, 54.31, 50.40, 29.78, 18.15. **HRMS** (ESI) calculated for $C_{16}H_{18}N$ $(M+H)^+$: 224.1434, found: 224.1430. Same compound was also reported in previous literature[9] and our characterization data was highly consistent with its data.

2-(*p*-tolyl)-1, 2, 3, 4-tetrahydroisoquinoline (1ac)



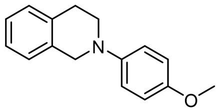
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.48-7.45 (m, 2H), 7.44-7.36 (m, 4H), 7.22 (t, J = 6.6 Hz, 2H), 4.63 (s, 2H), 3.76 (t, J = 5.8 Hz, 2H), 3.24 (t, J = 5.4 Hz, 2H), 2.60 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 148.98, 135.06, 134.90, 130.06, 128.91, 128.51, 126.88, 126.57, 126.26, 116.13, 51.72, 47.52, 29.47, 20.80. **HRMS** (ESI) calculated for $C_{16}H_{18}N$ $(M+H)^+$: 224.1434, found: 224.1432. Same compound was also reported in previous literature[9] and our characterization data was highly consistent with its data.

2-(3, 5-dimethylphenyl)-1, 2, 3, 4-tetrahydroisoquinoline (1ad)



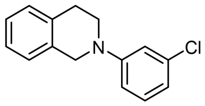
White solid. M. p. 47-48 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.15 (dd, J = 6.4, 4.0 Hz, 4H), 6.62 (s, 2H), 6.50 (s, 1H), 4.37 (s, 2H), 3.52 (t, J = 6.0 Hz, 2H), 2.96 (t, J = 5.8 Hz, 2H), 2.30 (s, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 150.85, 138.77, 134.99, 134.70, 128.56, 126.59, 126.30, 126.02, 120.78, 113.22, 51.00, 46.68, 29.36, 21.81. **HRMS** (ESI) calculated for $C_{17}H_{20}N$ $(M+H)^+$: 238.1590, found: 238.1588. Same compound was also reported in previous literature[9] and our characterization data was highly consistent with its data.

2-(4-methoxyphenyl)-1, 2, 3, 4-tetrahydroisoquinoline (1ae)



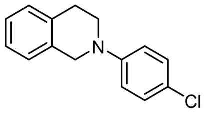
White solid. M. p. 94-95 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.16-7.12 (m, 4H), 6.98 (d, *J* = 8.8 Hz, 2H), 6.86 (d, *J* = 9.2 Hz, 2H), 4.29 (s, 2H), 3.77 (s, 3H), 3.44 (t, *J* = 6.0 Hz, 2H), 2.98 (t, *J* = 5.6 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 158.09, 150.61, 136.09, 129.22, 127.54, 126.68, 118.65, 115.17, 113.21, 112.37, 55.32, 50.22, 46.51, 29.43. **HRMS** (ESI) calculated for $C_{16}H_{18}NO$ $(M+H)^+$: 240.1383, found: 240.1380. Same compound was also reported in previous literature[11] and our characterization data was highly consistent with its data.

2-(3-chlorophenyl)-1, 2, 3, 4-tetrahydroisoquinoline (1af)



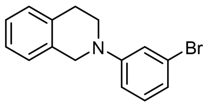
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.24-7.01 (m, 5H), 6.88 (t, *J* = 2.2 Hz, 1H), 6.82-6.66 (m, 2H), 4.34 (s, 2H), 3.48 (t, *J* = 5.8 Hz, 2H), 2.92 (t, *J* = 5.8 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 151.46, 135.16, 134.88, 134.07, 130.21, 128.52, 126.63, 126.30, 118.04, 114.43, 112.67, 50.11, 45.95, 29.12. **HRMS** (ESI) calculated for $C_{15}H_{15}NCl$ $(M+H)^+$: 244.0888, found: 244.0883. Same compound was also reported in previous literature[9] and our characterization data was highly consistent with its data.

2-(4-chlorophenyl)-1, 2, 3, 4-tetrahydroisoquinoline (1ag)



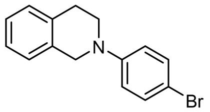
White solid. M. p. 71-72 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.28-7.06 (m, 6H), 6.87 (d, *J* = 9.0 Hz, 2H), 4.36 (s, 2H), 3.51 (t, *J* = 5.8 Hz, 2H), 2.97 (t, *J* = 5.8 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 149.09, 134.71, 134.10, 129.03, 128.55, 126.54, 126.52, 126.17, 123.35, 116.17, 50.66, 46.55, 28.97. **HRMS** (ESI) calculated for $C_{15}H_{15}NCl$ $(M+H)^+$: 244.0888, found: 244.0883. Same compound was also reported in previous literature[9] and our characterization data was highly consistent with its data.

2-(3-bromophenyl)-1, 2, 3, 4-tetrahydroisoquinoline (1ah)



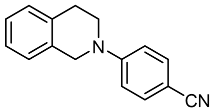
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.39 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.21-7.09 (m, 4H), 7.05 (t, *J* = 2.0 Hz, 1H), 6.89 (d, *J* = 8.0 Hz, 1H), 6.82 (dd, *J* = 8.8, 2.4 Hz, 1H), 4.35 (s, 2H), 3.50 (t, *J* = 5.8 Hz, 2H), 2.93 (t, *J* = 5.8 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 151.57, 134.83, 134.00, 130.45, 130.29, 128.48, 126.57, 126.27, 123.47, 120.94, 117.30, 113.09, 50.08, 45.93, 29.09. **HRMS** (ESI) calculated for $C_{15}H_{15}NBr$ $(M+H)^+$: 288.0383, found: 288.0380. Same compound was also reported in previous literature[12] and our characterization data was highly consistent with its data.

2-(4-bromophenyl)-1, 2, 3, 4-tetrahydroisoquinoline (1ai)



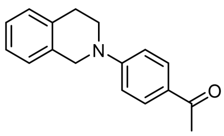
Yellow solid. M. p. 93-94 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.34 (d, *J* = 8.8 Hz, 2H), 7.19-7.15 (m, 4H), 6.82 (d, *J* = 8.8 Hz, 2H), 4.37 (s, 2H), 3.52 (t, *J* = 5.8 Hz, 2H), 2.97 (t, *J* = 5.8 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 149.43, 134.72, 134.05, 131.92, 128.51, 126.53, 126.18, 116.48, 110.47, 50.45, 46.33, 28.95. **HRMS** (ESI) calculated for $C_{15}H_{15}NBr$ $(M+H)^+$: 288.0383, found: 288.0382. Same compound was also reported in previous literature[9] and our characterization data was highly consistent with its data.

4-(3, 4-dihydroisoquinolin-2(*1H*)-yl)benzonitrile (1aj)



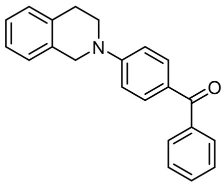
Yellow solid. M. p. 90-91 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.59-7.46 (m, 2H), 7.34-7.11 (m, 4H), 6.95-6.74 (m, 2H), 4.52 (s, 2H), 3.66 (t, *J* = 5.8 Hz, 2H), 3.02 (t, *J* = 5.8 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 152.21, 134.93, 133.58, 133.42, 128.21, 126.97, 126.56, 126.50, 120.45, 112.68, 98.65, 48.79, 44.62, 28.96. **HRMS** (ESI) calculated for $C_{16}H_{15}N_2$ $(M+H)^+$: 235.1230, found: 235.1227. Same compound was also reported in previous literature[9] and our characterization data was highly consistent with its data.

1-(4-(3,4-dihydroisoquinolin-2(*1H*)-yl)phenyl)ethan-1-one (1ak)



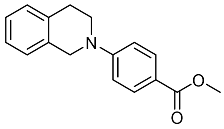
White solid. M. p. 105-106 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.8 Hz, 2H), 7.19-6.98 (m, 4H), 6.75 (d, *J* = 8.8 Hz, 2H), 4.38 (s, 2H), 3.76 (s, 3H), 3.52 (t, *J* = 5.8 Hz, 2H), 2.86 (t, *J* = 5.8 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 167.35, 153.03, 135.06, 133.83, 131.39, 128.25, 126.76, 126.54, 126.41, 118.29, 112.11, 51.61, 49.04, 44.81, 29.08. **HRMS** (ESI) calculated for $C_{17}H_{18}NO$ $(M+H)^+$: 252.1383, found: 252.1380. Same compound was also reported in previous literature[13] and our characterization data was highly consistent with its data.

(4-(3, 4-dihydroisoquinolin-2(*1H*)-yl)phenyl)(phenyl)methanone (1al)



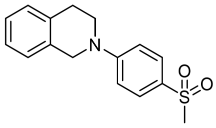
White solid. M. p. 84-85 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.8 Hz, 2H), 7.73-7.71 (m, 2H), 7.51 (t, *J* = 7.4 Hz, 1H), 7.47-7.41 (m, 2H), 7.23-7.11 (m, 4H), 6.87 (d, *J* = 9.0 Hz, 2H), 4.52 (s, 2H), 3.65 (t, *J* = 5.8 Hz, 2H), 2.97 (t, *J* = 5.8 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 195.17, 152.95, 139.14, 135.07, 133.72, 132.81, 131.34, 129.56, 128.25, 128.11, 126.86, 126.55, 126.49, 125.92, 111.85, 48.98, 44.75, 29.06. **HRMS** (ESI) calculated for $C_{22}H_{20}NO$ $(M+H)^+$: 314.1540, found: 314.1537. Same compound was also reported in previous literature[14] and our characterization data was highly consistent with its data.

methyl 4-(3, 4-dihydroisoquinolin-2(*1H*)-yl)benzoate (1am)



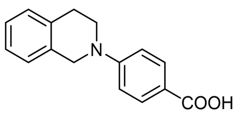
White solid. M. p. 100-101 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.8 Hz, 2H), 7.20-6.97 (m, 4H), 6.75 (d, *J* = 8.8 Hz, 2H), 4.38 (s, 2H), 3.76 (s, 3H), 3.52 (t, *J* = 5.8 Hz, 2H), 2.86 (t, *J* = 5.6 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 167.35, 153.03, 135.06, 133.83, 131.39, 128.25, 126.76, 126.54, 126.41, 118.29, 112.11, 51.61, 49.04, 44.81, 29.08. **HRMS** (ESI) calculated for $C_{17}H_{18}NO_2$ $(M+H)^+$: 268.1332, found: 268.1330.

2-(4-(methylsulfonyl)phenyl)-1, 2, 3, 4-tetrahydroisoquinoline (1an)



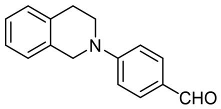
White solid. M. p. 142-143 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 9.2 Hz, 2H), 7.19-7.09 (m, 4H), 6.85 (d, *J* = 9.2 Hz, 2H), 4.45 (s, 2H), 3.59 (t, *J* = 6.0 Hz, 2H), 2.94-2.91 (m, 5H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 153.13, 134.95, 133.44, 129.21, 128.20, 127.12, 126.98, 126.57, 126.52, 112.27, 48.93, 45.09, 44.76, 28.96. **HRMS** (ESI) calculated for $C_{16}H_{18}NO_2S$ $(M+H)^+$: 288.1053, found: 288.1058. Same compound was also reported in previous literature[15] and our characterization data was highly consistent with its data.

4-(3, 4-dihydroisoquinolin-2(1H)-yl)benzoic acid (1ao)



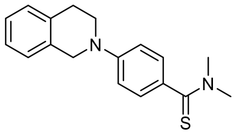
Yellow solid. M. p. 211-213 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.5 Hz, 2H), 7.16-7.04 (m, 4H), 6.81 (d, *J* = 8.5 Hz, 2H), 4.47 (s, 2H), 3.60 (t, *J* = 6.0 Hz, 2H), 2.93 (t, *J* = 6.0 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 172.22, 153.52, 135.08, 133.75, 132.16, 128.21, 126.81, 126.53, 126.46, 117.16, 111.95, 48.96, 44.72, 29.08. **HRMS** (ESI) calculated for $C_{16}H_{14}NO_2$ $(M-H)^-$: 252.1030, found: 252.1023. Same compound was also reported in previous literature[13] and our characterization data was highly consistent with its data.

4-(3, 4-dihydroisoquinolin-2(*1H*)-yl)benzaldehyde (1ap)



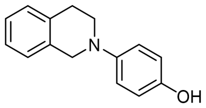
Yellow solid. M. p. 84-85 °C. **^{1}H NMR** (400 MHz, CDCl3) δ 9.76 (s, 1H), 7.77 (d, *J* = 9.0 Hz, 2H), 7.24-7.17 (m, 4H), 6.91 (d, *J* = 9.0 Hz, 2H), 4.55 (s, 2H), 3.68 (t, *J* = 6.0 Hz, 2H), 2.99 (t, *J* = 6.0 Hz, 2H). **^{13}C NMR** (100 MHz, CDCl3) δ 190.40, 153.99, 135.06, 133.51, 132.08, 128.16, 126.97, 126.57, 126.52, 126.07, 112.10, 48.82, 44.65, 29.05. **HRMS** (ESI) calculated for $C_{16}H_{16}NO$ $(M+H)^+$: 238.1227, found: 238.1230.

4-(3, 4-dihydroisoquinolin-2(*1H*)-yl)-*N, N*-dimethylbenzothioamide (1aq)



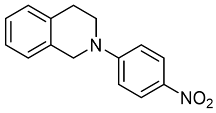
Yellow oil. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.33 (d, *J* = 8.6 Hz, 2H), 7.23-7.13 (m, 4H), 6.87 (d, *J* = 8.4 Hz, 2H), 4.45 (s, 2H), 3.62-3.56 (m, 5H), 3.26 (s, 3H), 2.98 (t, *J* = 5.8 Hz, 2H). **^{13}C NMR (125 MHz, $CDCl_3$)** δ 201.86, 150.67, 134.90, 134.05, 132.51, 128.42, 128.26, 126.56, 126.52, 126.22, 113.11, 49.85, 45.61, 44.54, 43.76, 28.96. **HRMS** (ESI) calculated for $C_{18}H_{20}N_2SNa$ $(M+Na)^+$: 319.0239, found: 319.0242.

4-(3, 4-dihydroisoquinolin-2(*1H*)-yl)phenol (1ar)



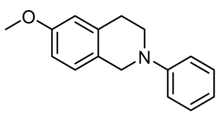
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.20-7.06 (m, 4H), 6.93 (d, *J* = 8.4 Hz, 2H), 6.79 (d, *J* = 8.4 Hz, 2H), 4.53 (s, 1H), 4.29 (s, 2H), 3.44 (t, *J* = 5.6 Hz, 2H), 2.98 (t, *J* = 5.8 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 152.88, 152.71, 134.55, 134.52, 128.69, 126.50, 126.28, 125.93, 118.29, 115.95, 52.76, 48.53, 29.07. **HRMS** (ESI) calculated for $C_{15}H_{16}NO$ $(M+H)^+$: 226.1227, found: 226.1230.

2-(4-nitrophenyl)-1, 2, 3, 4-tetrahydroisoquinoline (1as)



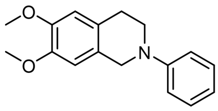
Yellow solid. M. p. 105-106 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.19-8.15 (m, 2H), δ 7.26-7.19 (m, 4H), 6.85-6.81 (m, 2H), 4.58 (s, 2H), 3.70 (t, *J* = 5.8 Hz, 2H), 3.03 (t, *J* = 5.8 Hz, 2H). **^{13}C NMR** (100 MHz, CDCl3) δ 153.82, 134.91, 133.12, 128.10, 127.18, 126.72, 126.50, 126.20, 111.20, 100.00, 48.84, 44.76, 28.99. **HRMS** (ESI) calculated for $C_{15}H_{15}N_2O_2$ $(M+H)^+$: 255.1128, found: 255.1131. Same compound was also reported in previous literature[13] and our characterization data was highly consistent with its data.

6-methoxy-2-phenyl-1, 2, 3, 4-tetrahydroisoquinoline (1at)



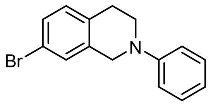
White solid. M. p. 69-70 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.35-7.24 (m, 2H), 7.06 (d, *J* = 8.4 Hz, 1H), 6.96 (d, *J* = 8.0 Hz, 2H), 6.81 (t, *J* = 7.2 Hz, 1H), 6.75 (dd, *J* = 8.4, 2.5 Hz, 1H), 6.69 (s, 1H), 4.34 (s, 2H), 3.78 (s, 3H), 3.53 (t, *J* = 5.8 Hz, 2H), 2.95 (t, *J* = 5.8 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 158.10, 136.06, 129.21, 127.53, 126.65, 118.68, 115.18, 113.21, 112.37, 55.31, 50.23, 46.52, 29.41. **HRMS** (ESI) calculated for $C_{16}H_{18}NO$ $(M+H)^+$: 240.1383, found: 240.1378.

6, 7-dimethoxy-2-phenyl-1, 2, 3, 4-tetrahydroisoquinoline (1au)



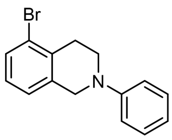
White solid. M. p. 98-99 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.28 (t, *J* = 7.8 Hz, 2H), 6.98 (d, *J* = 8.0 Hz, 2H), 6.82 (t, *J* = 7.2 Hz, 1H), 6.64 (d, *J* = 4.0 Hz, 2H), 4.33 (s, 2H), 3.87 (s, 3H), 3.86 (s, 3H), 3.54 (t, *J* = 5.8 Hz, 2H), 2.89 (t, *J* = 5.4 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 150.63, 147.61, 147.52, 129.20, 126.69, 126.22, 118.77, 115.35, 111.37, 109.40, 56.01, 55.96, 50.53, 46.76, 28.57. **HRMS** (ESI) calculated for $C_{17}H_{20}NO_2$ $(M+H)^+$: 270.1489, found: 270.1483. Same compound was also reported in previous literature[10] and our characterization data was highly consistent with its data.

7-bromo-2-phenyl-1, 2, 3, 4-tetrahydroisoquinoline (1av)



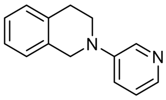
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.42-7.38 (m, 4H), 7.11-7.03 (m, 3H), 6.97 (t, *J* = 7.2 Hz, 1H), 4.43 (s, 2H), 3.61 (t, *J* = 5.8 Hz, 2H), 2.98 (t, *J* = 5.8 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 150.33, 136.83, 133.95, 130.38, 129.49, 129.48, 129.40, 119.61, 119.19, 115.51, 50.49, 46.62, 28.58. **HRMS** (ESI) calculated for $C_{15}H_{15}NBr$ $(M+H)^+$: 288.0383, found: 288.0383. Same compound was also reported in previous literature[16] and our characterization data was highly consistent with its data.

5-bromo-2-phenyl-1, 2, 3, 4-tetrahydroisoquinoline (1aw)



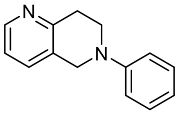
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.40 (d, *J* = 7.6 Hz, 1H), 7.26 (dd, *J* = 8.6, 7.2 Hz, 2H), 7.07-6.99 (m, 2H), 6.96 (d, *J* = 7.8 Hz, 2H), 6.84 (t, *J* = 7.2 Hz, 1H), 4.33 (s, 2H), 3.52 (t, *J* = 5.8 Hz, 2H), 2.93 (t, *J* = 6.0 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 150.37, 137.10, 134.63, 130.44, 129.37, 127.36, 125.79, 125.27, 119.50, 115.96, 51.32, 47.19, 29.82. **HRMS** (ESI) calculated for $C_{15}H_{15}NBr$ $(M+H)^+$: 288.0383, found: 288.0380.

2-(pyridin-3-yl)-1, 2, 3, 4-tetrahydroisoquinoline (1ax)



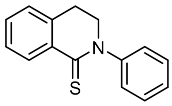
Yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.34 (s, 1H), 8.04 (d, *J* = 4.0 Hz, 1H), 7.23-7.07 (m, 6H), 4.39 (s, 2H), 3.54 (t, *J* = 5.8 Hz, 2H), 2.96 (t, *J* = 5.8 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 146.07, 139.47, 137.26, 134.57, 133.68, 128.53, 126.64, 126.55, 126.27, 123.57, 121.00, 49.76, 45.65, 28.80. **HRMS** (ESI) calculated for $C_{14}H_{15}N_2$ $(M+H)^+$: 211.1230, found: 211.1232. Same compound was also reported in previous literature[17] and our characterization data was highly consistent with its data.

6-phenyl-5, 6, 7, 8-tetrahydro-1, 6-naphthyridine (1ay)



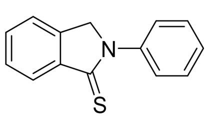
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.43 (d, *J* = 4.4 Hz, 1H), 7.45 (d, *J* = 7.6 Hz, 1H), 7.30 (t, *J* = 8.0 Hz, 2H), 7.12 (dd, *J* = 7.6, 4.8 Hz, 1H), 7.01 (d, *J* = 8.0 Hz, 2H), 6.87 (t, *J* = 7.4 Hz, 1H), 4.39 (s, 2H), 3.65 (t, *J* = 5.8 Hz, 2H), 3.16 (t, *J* = 5.8 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 155.04, 150.27, 147.70, 134.34, 129.67, 129.31, 121.31, 119.49, 115.76, 50.32, 47.02, 32.20. **HRMS** (ESI) calculated for $C_{14}H_{15}N_2$ $(M+H)^+$: 211.1230, found: 211.1235.

2-phenyl-3, 4-dihydroisoquinoline-1(*2H*)-thione (2a)



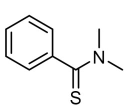
Yellow solid. M. p. 99-100 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.67 (d, *J* = 8.0 Hz, 1H), 7.56-7.45 (m, 3H), 7.42-7.36 (m, 4H), 7.22 (d, *J* = 7.4 Hz, 1H), 4.00 (t, *J* = 6.6 Hz, 2H), 3.19 (t, *J* = 6.6 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 193.95, 147.60, 134.15, 133.04, 132.77, 131.93, 129.77, 127.93, 127.22, 126.70, 126.44, 52.51, 28.55. **HRMS** (ESI) calculated for $C_{15}H_{13}NSNa$ $(M+Na)^+$: 261.9661, found: 261.9663.

2-phenylisoindoline-1-thione (2b)



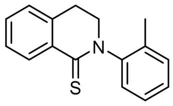
Yellow solid. M. p. 115-116 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.14 (d, *J* = 7.6 Hz, 1H), 7.69-7.63 (m, 2H), 7.60 (td, *J* = 7.4, 1.2 Hz, 1H), 7.56-7.45 (m, 4H), 7.37 (t, *J* = 7.4 Hz, 1H), 5.03 (s, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 193.88, 140.44, 139.98, 139.11, 131.86, 129.25, 128.69, 127.83, 126.30, 125.64, 121.82, 60.31. **HRMS** (ESI) calculated for $C_{14}H_{11}NSNa$ $(M+Na)^+$: 247.9504, found: 247.9507.

***N, N*-dimethylbenzothioamide (2c)**



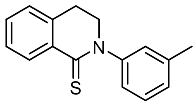
Yellow oil. (25.2 mg). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.35-7.29 (m, 5H), 3.60 (s, 3H), 3.16 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 201.33, 143.41, 128.59, 128.35, 125.75, 44.16, 43.25. **HRMS** (ESI) calculated for $C_9H_{11}NSNa$ $(M+Na)^+$: 187.9504, found: 187.9510.

2-(*o*-tolyl)-3, 4-dihydroisoquinoline-1(*2H*)-thione (2aa)



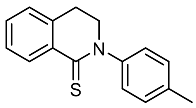
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.62 (d, *J* = 8.0 Hz, 1H), 7.43 (td, *J* = 7.4, 1.2 Hz, 1H), 7.35-7.25 (m, 4H), 7.19-7.13 (m, 2H), 3.93-3.74 (m, 2H), 3.22-3.05 (m, 2H), 2.27 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 192.89, 146.35, 134.08, 134.04, 133.08, 132.53, 131.95, 131.40, 128.30, 127.64, 127.18, 126.80, 126.15, 51.40, 28.61, 18.15. **HRMS** (ESI) calculated for $C_{16}H_{15}NSNa$ $(M+Na)^+$: 275.9817, found: 275.9821.

2-(*m*-tolyl)-3, 4-dihydroisoquinoline-1(*2H*)-thione (2ab)



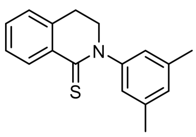
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.64 (d, *J* = 8.0 Hz, 1H), 7.44 (td, *J* = 7.4, 1.4 Hz, 1H), 7.39-7.33 (m, 2H), 7.19 (t, *J* = 5.8 Hz, 2H), 7.15-7.11 (m, 2H), 3.94 (t, *J* = 6.8 Hz, 2H), 3.14 (t, *J* = 6.4 Hz, 2H), 2.40 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 193.76, 147.59, 139.80, 134.21, 133.03, 132.76, 131.83, 129.53, 128.70, 127.17, 126.83, 126.65, 123.39, 52.56, 28.55, 21.42. **HRMS** (ESI) calculated for $C_{16}H_{15}NSNa$ $(M+Na)^+$: 275.9817, found: 275.9819.

2-(*p*-tolyl)-3, 4-dihydroisoquinoline-1(*2H*)-thione (2ac)



Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.67 (d, *J* = 7.6 Hz, 1H), 7.47 (t, *J* = 7.4 Hz, 1H), 7.39 (q, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 9.8 Hz, 1H), 7.24-7.19 (m, 2H), 7.17 (s, 1H), 3.98 (t, *J* = 6.6 Hz, 2H), 3.17 (t, *J* = 6.6 Hz, 2H), 2.43 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 193.90, 145.11, 137.80, 134.19, 133.04, 132.79, 131.86, 130.41, 127.18, 126.66, 126.07, 52.59, 28.54, 21.30. **HRMS** (ESI) calculated for $C_{16}H_{15}NSNa$ $(M+Na)^+$: 275.9817, found: 275.9820.

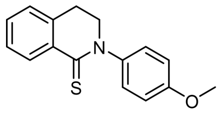
2-(3, 5-dimethylphenyl)-3, 4-dihydroisoquinoline-1(*2H*)-thione (2ad)



Yellow solid. M. p. 95-96 °C. **^{1}H NMR** (400 MHz, CDCl3) δ 8.64 (d, *J* = 8.0 Hz, 1H), 7.45 (t, *J* = 7.4 Hz, 1H), 7.36 (t, *J* = 7.2 Hz, 1H), 7.19 (d, *J* = 7.4 Hz, 1H), 7.01 (s, 1H), 6.94 (s, 2H), 3.93 (t, *J* = 6.6 Hz, 2H), 3.14 (t, *J* = 6.6 Hz, 2H), 2.36 (s, 6H). **^{13}C NMR**

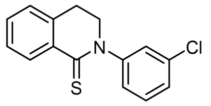
(100 MHz, CDCl3) δ 193.56, 147.54, 139.56, 134.21, 133.05, 132.75, 131.82, 129.69, 127.17, 126.64, 123.80, 52.61, 28.53, 21.37. **HRMS** (ESI) calculated for $C_{17}H_{17}NSNa$ $(M+Na)^+$: 290.0974, found: 290.0979.

2-(4-methoxyphenyl)-3, 4-dihydroisoquinoline-1(*2H*)-thione (2ae)



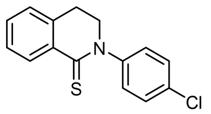
Yellow solid. M. p. 134-135 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.64 (d, *J* = 8.0 Hz, 1H), 7.44 (td, *J* = 7.8, 1.6 Hz, 1H), 7.34 (td, *J* = 8.0, 1.2 Hz, 1H), 7.28-7.22 (m, 2H), 7.18 (d, *J* = 7.4 Hz, 1H), 7.01-6.95 (m, 2H), 3.94 (t, *J* = 6.8 Hz, 2H), 3.84 (s, 3H), 3.14 (t, *J* = 6.4 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 194.15, 158.76, 140.60, 134.25, 133.02, 132.84, 131.80, 127.39, 127.14, 126.62, 114.86, 55.45, 52.74, 28.55. HRMS (ESI) calculated for $C_{16}H_{15}NOSNa$ $(M+Na)^+$: 291.9766, found: 291.9770.

2-(3-chlorophenyl)-3, 4-dihydroisoquinoline-1(*2H*)-thione (2af)



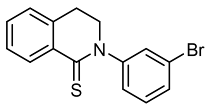
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.60 (d, *J* = 7.8 Hz, 1H), 7.45 (t, *J* = 6.8 Hz, 1H), 7.39 (d, *J* = 8.0 Hz, 1H), 7.36-7.32 (m, 3H), 7.24 (d, *J* = 9.0 Hz, 1H), 7.18 (d, *J* = 7.4 Hz, 1H), 3.93 (t, *J* = 6.6 Hz, 2H), 3.14 (t, *J* = 6.6 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 194.28, 148.38, 135.09, 133.93, 132.99, 132.73, 132.17, 130.74, 128.17, 127.30, 127.07, 126.84, 125.07, 52.41, 28.52. **HRMS** (ESI) calculated for $C_{15}H_{12}NSClNa$ $(M+Na)^+$: 296.6672, found: 296.6676.

2-(4-chlorophenyl)-3, 4-dihydroisoquinoline-1(*2H*)-thione (2ag)



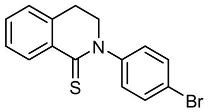
Yellow solid. M. p. 151-153 °C. **^{1}H NMR** (400 MHz, CDCl3) δ 8.65 (d, *J* = 7.8 Hz, 1H), 7.50-7.46 (m, 3H), 7.38 (t, *J* = 7.4 Hz, 1H), 7.31 (d, *J* = 8.6 Hz, 2H), 7.22 (d, *J* = 7.4 Hz, 1H), 3.97 (t, *J* = 6.4 Hz, 2H), 3.18 (t, *J* = 6.6 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 194.33, 145.91, 133.97, 133.57, 132.95, 132.77, 132.13, 130.00, 128.00, 127.30, 126.78, 52.43, 28.51. **HRMS** (ESI) calculated for $C_{15}H_{12}NSClNa$ $(M+Na)^+$: 296.6672, found: 296.6678.

2-(3-bromophenyl)-3, 4-dihydroisoquinoline-1(*2H*)-thione (2ah)



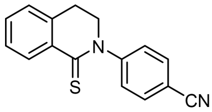
Yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.60 (d, J = 8.0 Hz, 1H), 7.45 (td, *J* = 7.4, 1.4 Hz, 1H), 7.42-7.38 (m, 1H), 7.38-7.31 (m, 3H), 7.24-7.22 (m, 1H), 7.19 (d, *J* = 6.8 Hz, 1H), 3.93 (t, *J* = 6.6 Hz, 2H), 3.14 (t, *J* = 6.6 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 194.28, 148.38, 135.09, 133.92, 133.00, 132.72, 132.17, 130.74, 128.16, 127.29, 127.07, 126.84, 125.07, 52.41, 28.51. **HRMS** (ESI) calculated for $C_{15}H_{12}NSBrNa$ $(M+Na)^+$: 339.8766, found: 339.8770.

2-(4-bromophenyl)-3, 4-dihydroisoquinoline-1(*2H*)-thione (2ai)



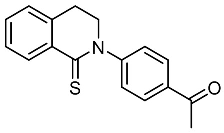
Yellow solid. M. p. 145-146 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.62 (dd, J = 8.0, 1.2 Hz, 1H), 7.64-7.55 (m, 2H), 7.46 (td, *J* = 7.4, 1.4 Hz, 1H), 7.36 (td, *J* = 7.8, 1.4 Hz, 1H), 7.25-7.17 (m, 3H), 3.94 (t, *J* = 6.6 Hz, 2H), 3.16 (t, *J* = 6.6 Hz, 2H). **^{13}C NMR** (100MHz, $CDCl_3$) δ 194.27, 146.42, 133.96, 132.98, 132.93, 132.77, 132.13, 128.34, 127.31, 126.77, 121.61, 52.38, 28.51. **HRMS** (ESI) calculated for $C_{15}H_{12}NSBrNa$ $(M+Na)^+$: 339.8766, found: 339.8772.

4-(1-thioxo-3, 4-dihydroisoquinolin-2(*1H*)-yl)benzonitrile (2aj)



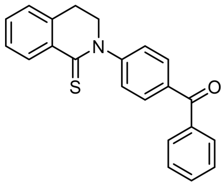
Yellow solid. M. p. 105-106 °C. **^{1}H NMR** (400 MHz, CDCl3) δ 8.61 (d, *J* = 8.0 Hz, 1H), 7.81-7.73 (m, 2H), 7.52-7.48 (m, 3H), 7.38 (t, *J* = 7.8 Hz, 1H), 7.23 (d, *J* = 7.4 Hz, 1H), 3.99 (t, *J* = 6.4 Hz, 2H), 3.20 (t, *J* = 6.4 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 194.54, 151.05, 133.71, 133.67, 132.95, 132.66, 132.46, 128.01, 127.40, 126.95, 118.25, 111.57, 52.12, 28.48. **HRMS** (ESI) calculated for $C_{16}H_{12}N_2SNa$ $(M+Na)^+$: 286.9613, found: 286.9616.

1-(4-(1-thioxo-3, 4-dihydroisoquinolin-2(*1H*)-yl)phenyl)ethan-1-one (2ak)



Yellow solid. M. p. 163-164 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.63 (d, *J* = 8.0 Hz, 1H), 8.09 (d, *J* = 8.4 Hz, 2H), 7.47 (t, *J* = 7.8 Hz, 3H), 7.37 (t, *J* = 7.6 Hz, 1H), 7.21 (d, *J* = 7.4 Hz, 1H), 3.98 (t, *J* = 6.4 Hz, 2H), 3.19 (t, *J* = 6.6 Hz, 2H), 2.63 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 197.00, 194.24, 151.37, 136.19, 133.89, 132.94, 132.70, 132.24, 129.97, 127.36, 126.99, 126.82, 52.21, 28.52, 26.72. **HRMS** (ESI) calculated for $C_{17}H_{15}NOSNa$ $(M+Na)^+$: 303.9766, found: 303.9771.

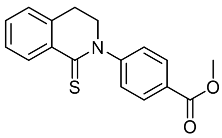
phenyl(4-(1-thioxo-3, 4-dihydroisoquinolin-2(*1H*)-yl)phenyl)methanone (2al)



Yellow solid. M. p. 154-156 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.67 (d, *J* = 7.6 Hz, 1H), 7.97 (d, *J* = 8.4 Hz, 2H), 7.88 (d, *J* = 7.2 Hz, 2H), 7.64 (t, *J* = 7.4 Hz, 1H), 7.58-7.47 (m, 5H), 7.40 (t, *J* = 7.4 Hz, 1H), 7.24 (d, *J* = 7.4 Hz, 1H), 4.03 (t, *J* = 6.6

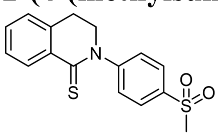
Hz, 2H), 3.22 (t, J = 6.4 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 195.62, 194.23, 150.88, 137.31, 136.67, 133.96, 132.96, 132.74, 132.64, 132.22, 131.68, 130.06, 128.42, 127.36, 126.81, 126.71, 52.33, 28.54. **HRMS** (ESI) calculated for $C_{22}H_{17}NOSNa$ $(M+Na)^+$: 365.9923, found: 365.9925.

methyl 4-(1-thioxo-3, 4-dihydroisoquinolin-2(*1H*)-yl)benzoate (2am)



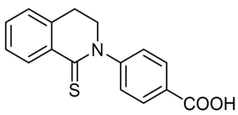
Yellow solid. M. p. 142-144 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.62 (d, J = 8.0 Hz, 1H), 8.16 (d, J = 8.6 Hz, 2H), 7.47 (td, J = 7.4, 1.2 Hz, 1H), 7.43 (d, J = 8.6 Hz, 2H), 7.35 (d, J = 7.8 Hz, 1H), 7.20 (d, J = 7.5 Hz, 1H), 3.97 (t, J = 6.5 Hz, 2H), 3.94 (s, 3H), 3.17 (t, J = 6.5 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 194.20, 166.26, 151.30, 133.93, 132.96, 132.70, 132.18, 131.23, 129.46, 127.32, 126.80, 126.78, 52.32, 52.23, 28.52. **HRMS** (ESI) calculated for $C_{17}H_{15}NO_2SNa$ $(M+Na)^+$: 319.9715, found: 319.9720.

2-(4-(methylsulfonyl)phenyl)-3, 4-dihydroisoquinoline-1(*2H*)-thione (2an)



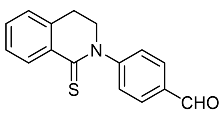
Red solid. M. p. 194-196 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.61 (d, J = 8.0 Hz, 1H), 8.06 (d, J = 8.6 Hz, 2H), 7.58 (d, J = 8.6 Hz, 2H), 7.49 (td, J = 7.5, 1.3 Hz, 1H), 7.38 (t, J = 7.2 Hz, 1H), 7.22 (d, J = 7.5 Hz, 1H), 3.99 (t, J = 6.5 Hz, 2H), 3.20 (t, J = 6.5 Hz, 2H), 3.13 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 194.60, 151.93, 139.58, 133.75, 132.90, 132.72, 132.46, 129.17, 128.00, 127.44, 126.90, 52.25, 44.57, 28.51. **HRMS** (ESI) calculated for $C_{16}H_{15}NO_2S_2Na$ $(M+Na)^+$: 339.9436, found: 339.9440.

4-(1-thioxo-3, 4-dihydroisoquinolin-2(*1H*)-yl)benzoic acid (2ao)



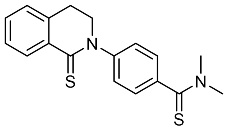
Yellow solid. M. p. 240-242 °C. **^{1}H NMR** (500 MHz, DMSO-d6) δ 12.95 (s, 1H), 8.43 (d, J = 8.0 Hz, 1H), 8.04 (d, J = 8.5 Hz, 2H), 7.57-7.53 (m, 3H), 7.39 (t, J = 7.6 Hz, 1H), 7.35 (d, J = 7.5 Hz, 1H), 3.98 (t, J = 6.5 Hz, 2H), 3.19 (t, J = 6.5 Hz, 2H). **^{13}C NMR** (125 MHz, DMSO-d6) δ 192.84, 167.22, 151.57, 134.50, 133.84, 132.57, 132.18, 130.97, 130.16, 127.68, 127.59, 127.17, 52.43, 27.92. **HRMS** (ESI) calculated for $C_{16}H_{12}NO_2S$ $(M-H)^-$: 282.0594, found: 282.0586.

4-(1-thioxo-3, 4-dihydroisoquinolin-2(*1H*)-yl)benzaldehyde (2ap)



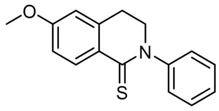
Yellow solid. M. p. 168-170 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.05 (s, 1H), 8.62 (dd, J = 8.0, 1.0 Hz, 1H), 8.05 – 7.99 (m, 2H), 7.58 – 7.52 (m, 2H), 7.49 (td, J = 7.4, 1.2 Hz, 1H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.22 (d, *J* = 7.6 Hz, 1H), 4.00 (t, *J* = 6.6 Hz, 2H), 3.20 (t, *J* = 6.6 Hz, 2H). **^{13}C NMR** (100 MHz, CDCl3) δ 194.37, 191.09, 152.45, 135.37, 133.85, 132.91, 132.71, 132.32, 131.19, 127.62, 127.40, 126.84, 52.17, 28.53. **HRMS** (ESI) calculated for $C_{16}H_{13}NOSNa$ $(M+Na)^+$: 289.9610, found: 289.9612.

***N, N*-dimethyl-4-(1-thioxo-3,4-dihydroisoquinolin-2(*1H*)-yl)benzothioamide (2aq)**



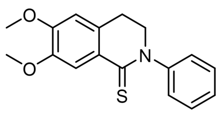
Yellow solid. M. p. 199-201 °C. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.62 (d, *J* = 8.0 Hz, 1H), 7.46 (t, *J* = 7.4 Hz, 1H), 7.43 (d, *J* = 8.4 Hz, 2H), 7.39-7.32 (m, 3H), 7.20 (d, *J* = 7.4 Hz, 1H), 3.96 (t, *J* = 6.8 Hz, 2H), 3.63 (s, 3H), 3.28 (s, 3H), 3.16 (t, *J* = 6.6 Hz, 2H). **^{13}C NMR (125 MHz, $CDCl_3$)** δ 200.13, 194.13, 147.47, 142.58, 134.05, 133.03, 132.74, 132.09, 127.27, 127.25, 126.76, 126.67, 52.41, 44.51, 43.29, 28.51. **HRMS** (ESI) calculated for $C_{18}H_{18}N_2S_2Na$ $(M+Na)^+$: 348.9803, found: 348.9810.

6-methoxy-2-phenyl-3, 4-dihydroisoquinoline-1(*2H*)-thione (2at)



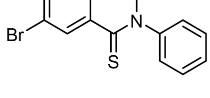
Yellow solid. M. p. 126-127 °C. **^{1}H NMR** (400 MHz, CDCl3) δ 8.62 (d, *J* = 8.8 Hz, 1H), 7.48 (t, *J* = 7.8 Hz, 2H), 7.40-7.31 (m, 3H), 6.86 (dd, *J* = 8.8, 2.6 Hz, 1H), 6.66 (d, *J* = 2.4 Hz, 1H), 3.95 (t, *J* = 6.6 Hz, 2H), 3.87 (s, 3H), 3.11 (t, *J* = 6.6 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 193.34, 162.68, 147.67, 135.37, 135.21, 129.67, 127.80, 127.63, 126.55, 112.71, 111.51, 55.56, 52.37, 28.84. **HRMS** (ESI) calculated for $C_{16}H_{15}NOSNa$ $(M+Na)^+$: 291.9766, found: 291.9771.

6, 7-dimethoxy-2-phenyl-3, 4-dihydroisoquinoline-1(*2H*)-thione (2au)



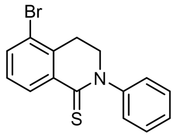
Yellow solid. M. p. 129-130 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.26 (s, 1H), 7.50 (t, *J* = 7.8 Hz, 2H), 7.40-7.34 (m, 3H), 6.65 (s, 1H), 3.98-3.95 (m, 8H), 3.10 (t, *J* = 6.8 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 193.17, 152.39, 147.81, 147.74, 129.68, 127.80, 127.27, 126.89, 126.54, 115.35, 108.70, 56.19, 56.18, 52.55, 28.16. **HRMS** (ESI) calculated for $C_{17}H_{17}NO_2SNa$ $(M+Na)^+$: 321.9872, found: 321.9875.

7-bromo-2-phenyl-3, 4-dihydroisoquinoline-1(*2H*)-thione (2av)



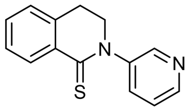
Yellow solid. M. p. 124-125 °C. **^{1}H NMR** (400 MHz, CDCl3) δ 8.81 (d, *J* = 1.6 Hz, 1H), 7.58 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.52 (t, *J* = 7.6 Hz, 2H), 7.44-7.39 (m, 1H), 7.34 (d, *J* = 7.2 Hz, 2H), 7.11 (d, *J* = 8.0 Hz, 1H), 4.10-3.98 (t, *J* = 6.8 Hz, 2H), 3.13 (t, *J* = 6.4 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 192.22, 147.34, 135.30, 134.58, 131.83, 129.85, 128.51, 128.10, 126.31, 120.93, 52.37, 28.09. **HRMS** (ESI) calculated for $C_{15}H_{12}NSBrNa$ (M+Na)$^+$: 339.8766, found: 339.8769.

5-bromo-2-phenyl-3, 4-dihydroisoquinoline-1(*2H*)-thione (2aw)



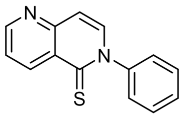
Yellow solid. M. p. 137-138 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.64 (d, *J* = 8.0 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.50 (t, *J* = 7.6 Hz, 2H), 7.40 (d, *J* = 7.6 Hz, 1H), 7.36-7.31 (m, 2H), 7.23 (t, *J* = 8.0 Hz, 1H), 3.97 (t, *J* = 6.8 Hz, 2H), 3.27 (t, *J* = 6.6 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 192.68, 147.34, 136.02, 135.56, 132.99, 132.20, 129.85, 128.10, 128.03, 126.28, 122.54, 51.91, 28.47. **HRMS** (ESI) calculated for $C_{15}H_{12}NSBrNa$ (M+Na)$^+$: 339.8766, found: 339.8771.

2-(pyridin-3-yl)-3, 4-dihydroisoquinoline-1(*2H*)-thione (2ax)



Yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.56-8.54 (m, 2H), 8.53 (s, 1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.40 (t, *J* = 7.5 Hz, 1H), 7.35 (dd, *J* = 8.0, 4.8 Hz, 1H), 7.30 (t, *J* = 7.8 Hz, 1H), 7.14 (d, *J* = 7.5 Hz, 1H), 3.92 (t, *J* = 6.5 Hz, 2H), 3.12 (t, *J* = 6.5 Hz, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 195.13, 148.68, 148.08, 144.02, 134.58, 133.83, 132.96, 132.76, 132.30, 127.36, 126.86, 124.06, 52.40, 28.53. **HRMS** (ESI) calculated for $C_{14}H_{12}N_2SNa$ (M+Na)$^+$: 262.9613, found: 262.9616.

6-phenyl-1, 6-naphthyridine-5(*6H*)-thione (2ay)



Yellow solid. M. p. 141-143 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.32 (d, *J* = 8.5 Hz, 1H), 8.99 (d, *J* = 4.0 Hz, 1H), 7.65-7.55 (m, 3H), 7.51 (dd, *J* = 8.4, 5.2 Hz, 2H), 7.38 (d, *J* = 8.0 Hz, 2H), 7.18 (d, *J* = 7.5 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 186.82, 155.23, 148.90, 145.64, 140.70, 137.46, 130.47, 129.89, 129.14, 126.93, 123.57, 113.29. **HRMS** (ESI) calculated for $C_{14}H_{10}N_2SNa$ (M+Na)$^+$: 260.9457, found: 260.9460.

6. References

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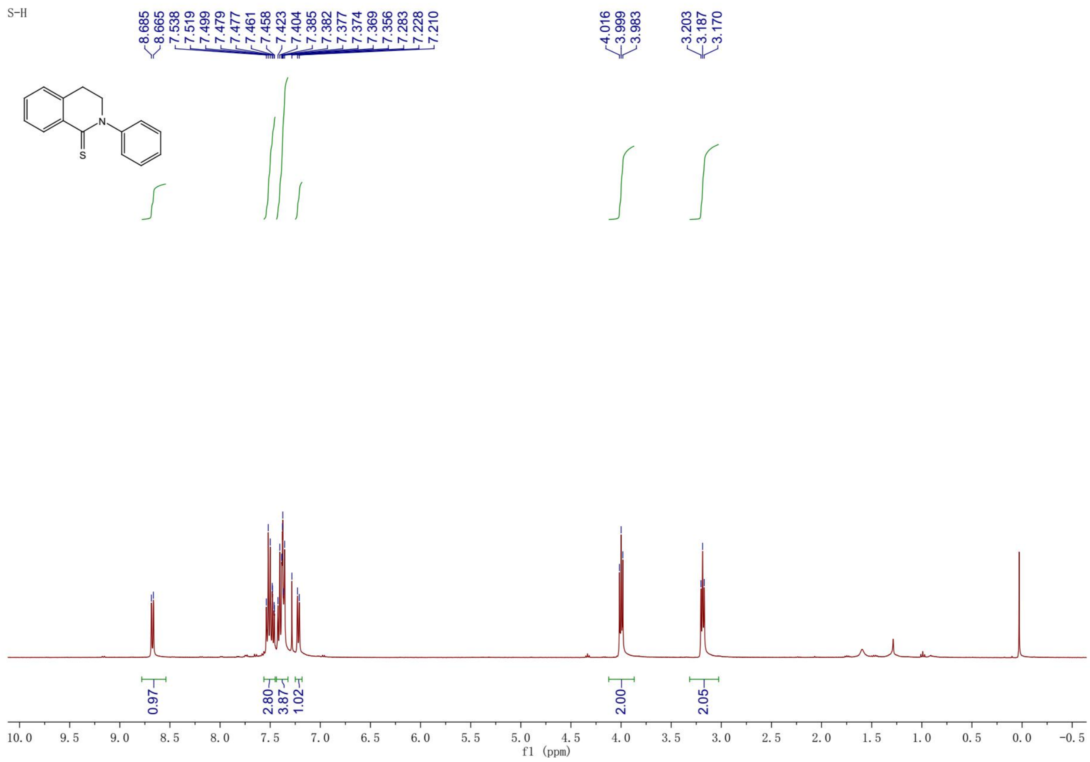
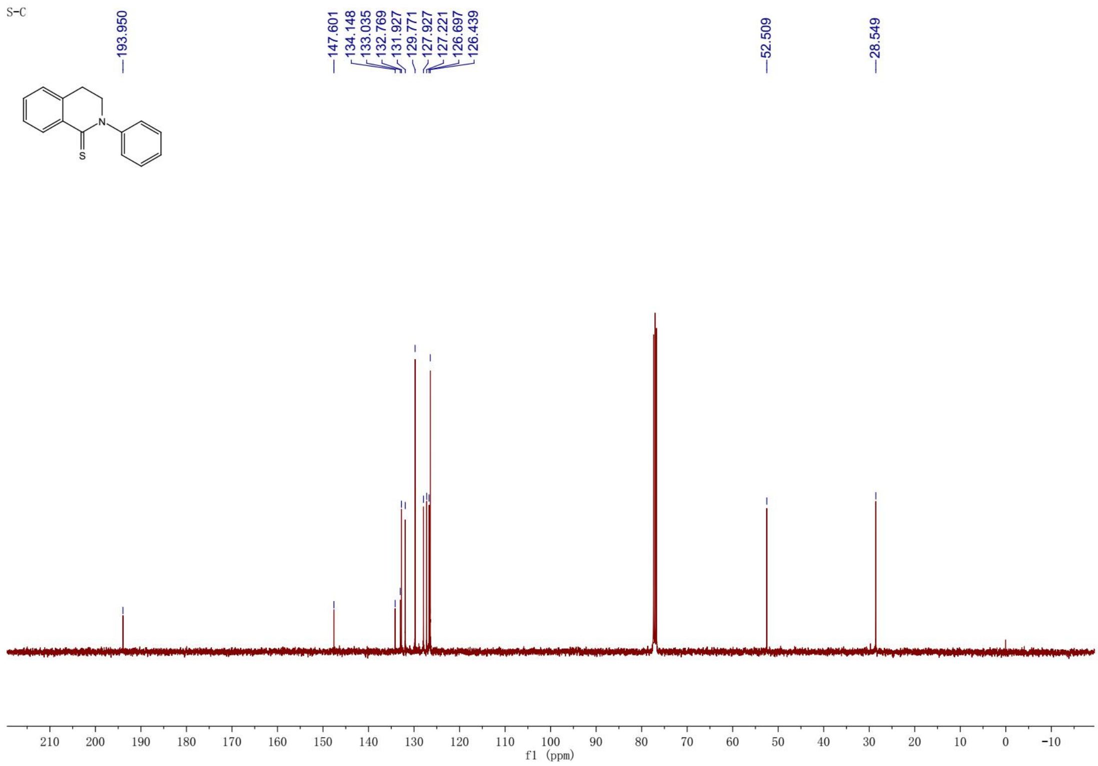
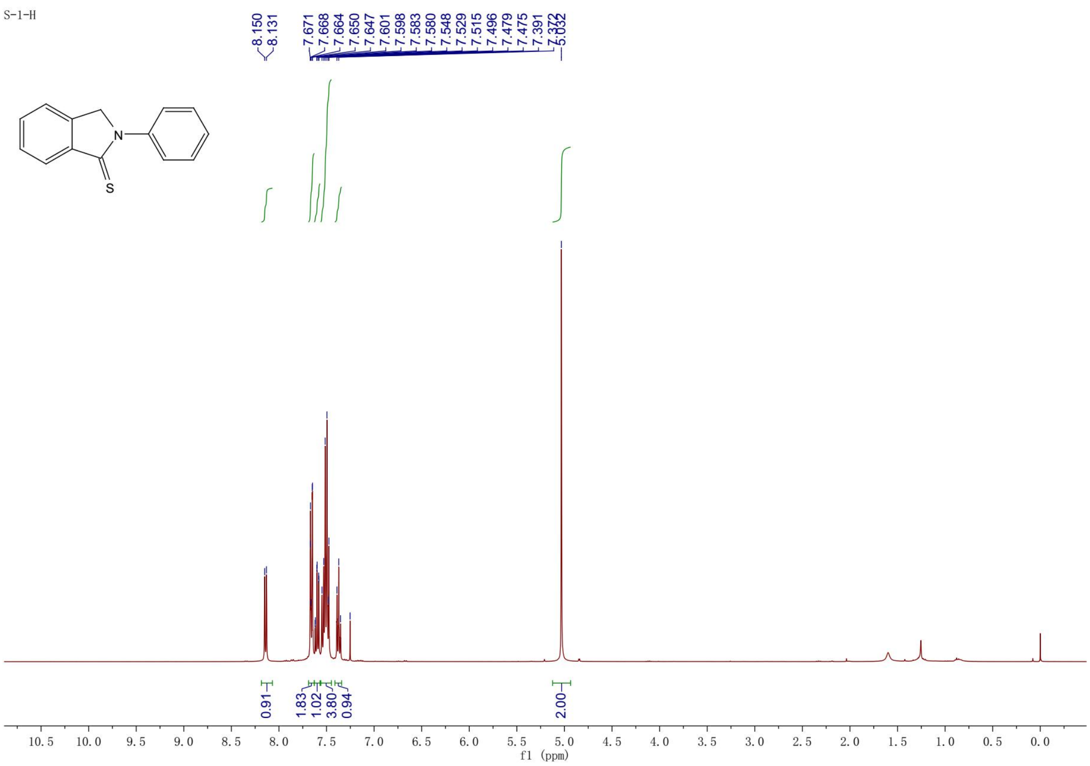
7. [1]H and [13]C NMR Spectra

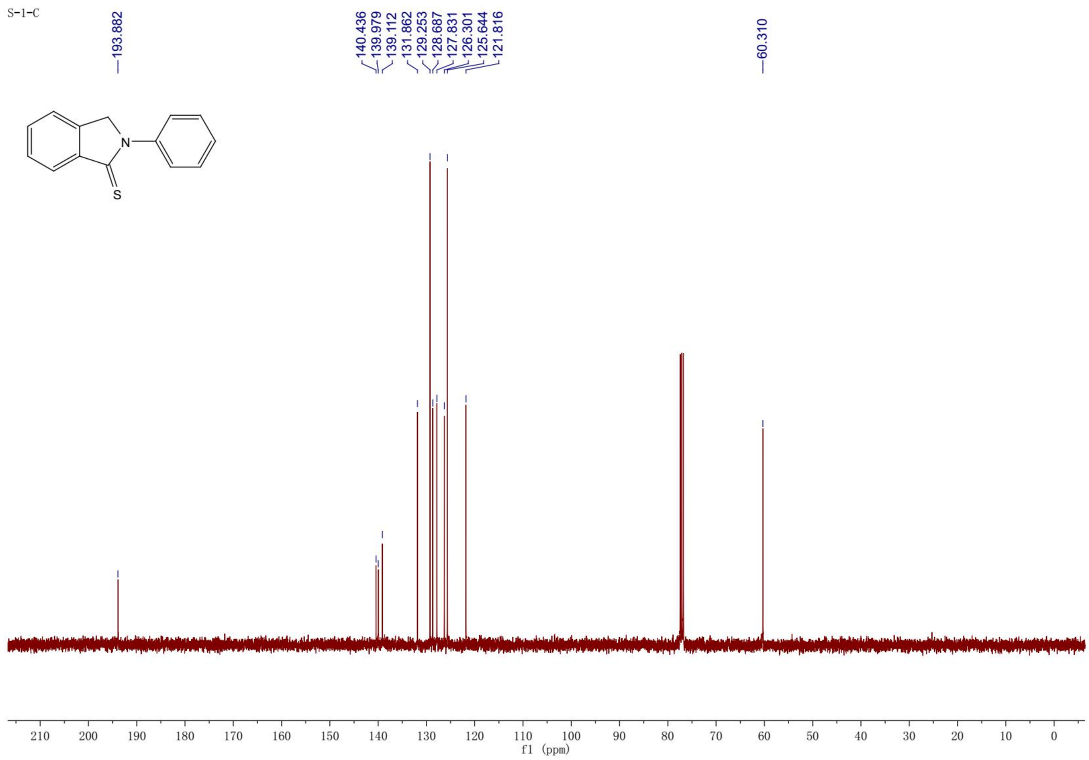
NMR of 2a



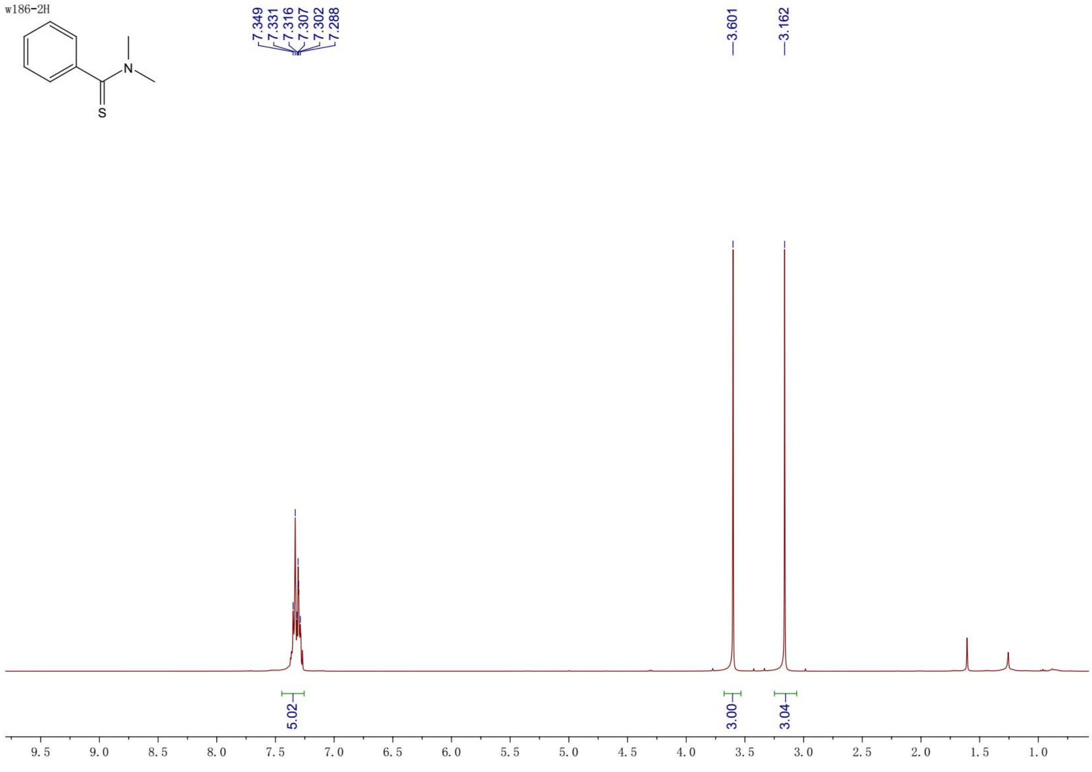


NMR of 2b

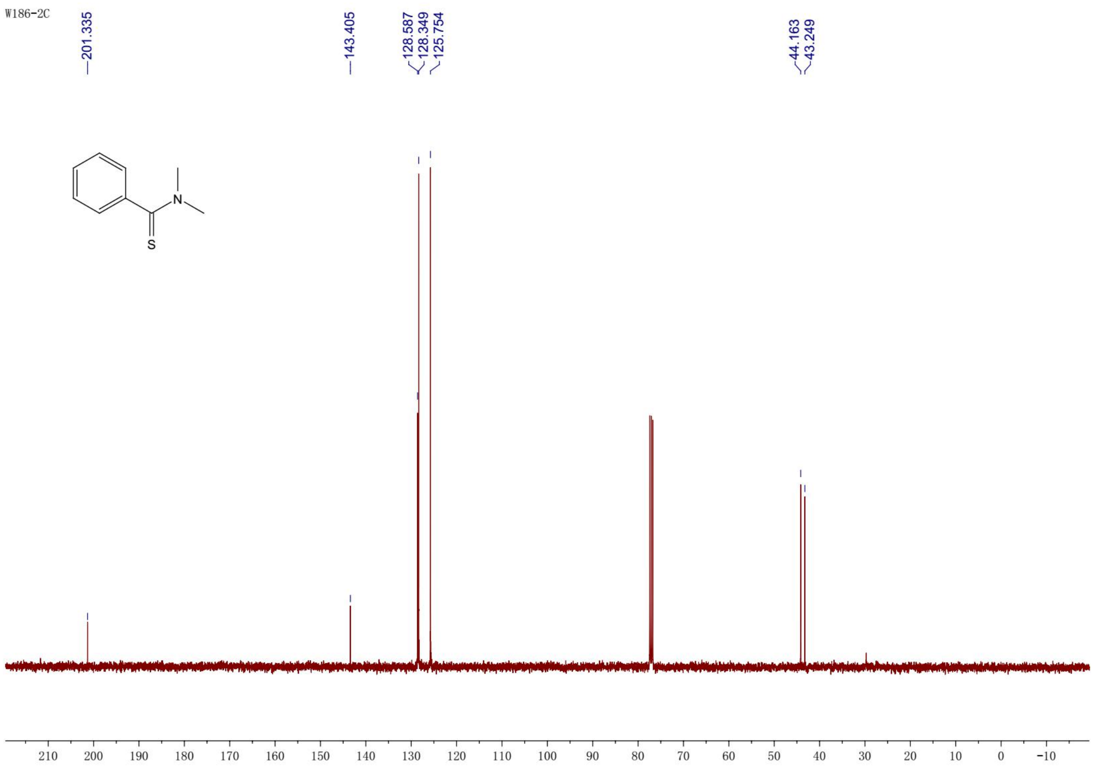

S-1-H
8.150
8.131
7.671
7.668
7.664
7.650
7.647
7.601
7.598
7.583
7.580
7.548
7.529
7.515
7.496
7.479
7.475
7.391
7.372
5.032
N
S
0.91
1.83
1.02
3.80
0.94
2.00
f1 (ppm)


S-1-C
193.882
140.436
139.979
139.112
131.862
129.253
128.687
127.831
126.301
125.644
121.816
60.310
N
S
f1 (ppm)

NMR of 2c

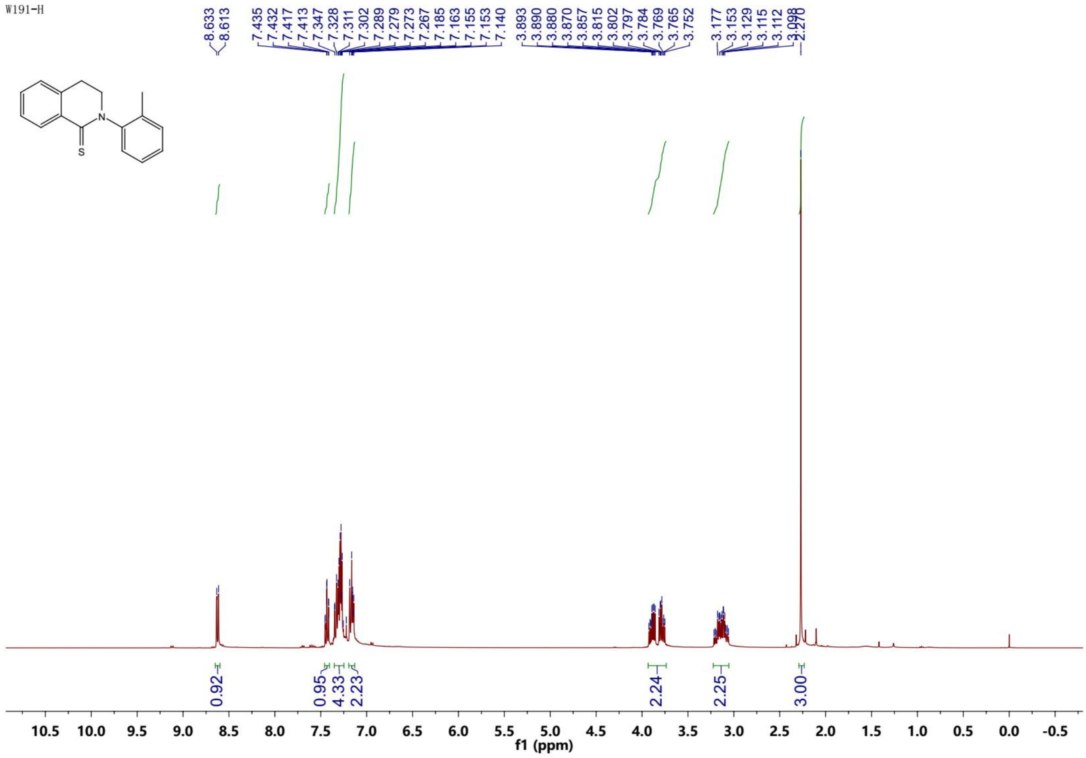


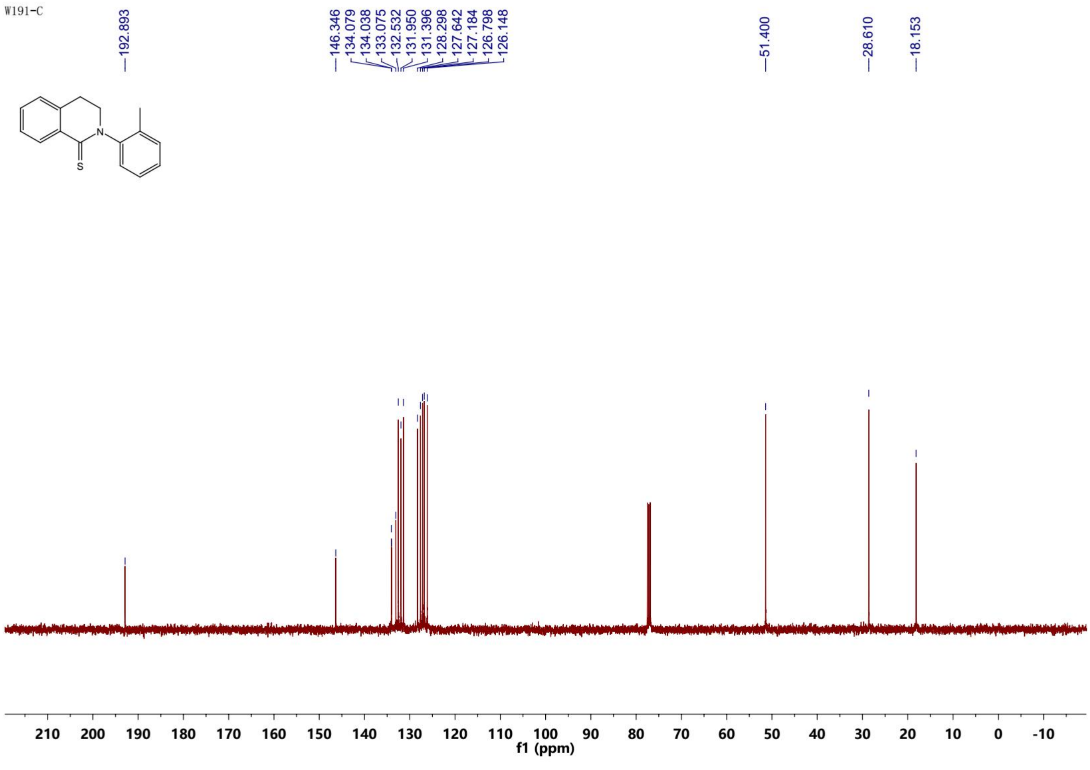
w186-2H
S
N
7.349
7.331
7.316
7.307
7.302
7.288
3.601
3.162
5.02
3.00
3.04
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0



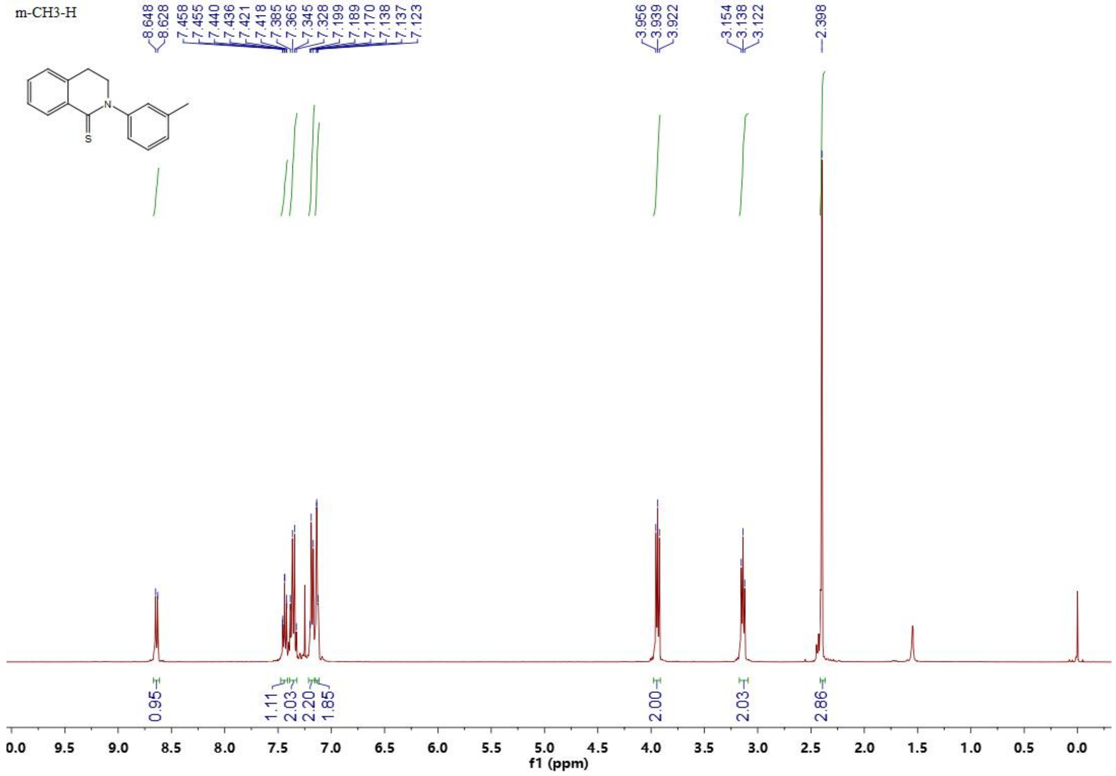
W186-2C
201.335
143.405
128.587
128.349
125.754
44.163
43.249
S
N
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

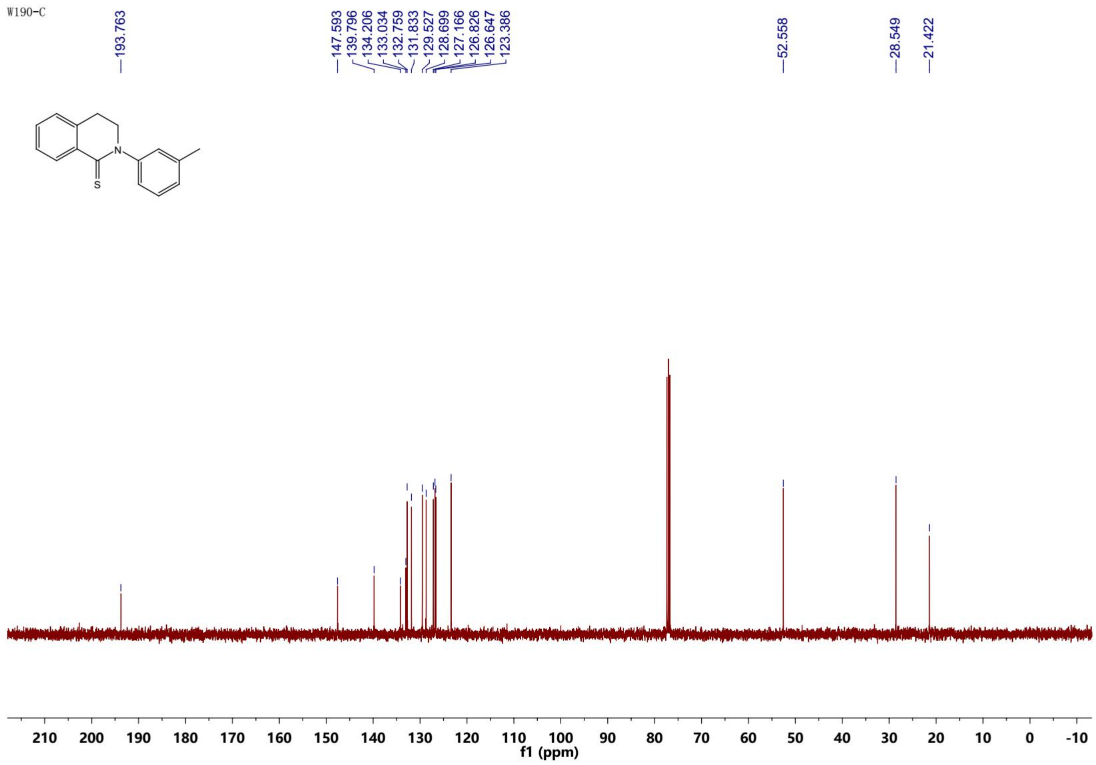
NMR of 2aa


W191-H
8.633
8.613
7.435
7.432
7.417
7.413
7.347
7.328
7.311
7.302
7.289
7.279
7.273
7.267
7.185
7.163
7.155
7.153
7.140
3.893
3.890
3.880
3.870
3.857
3.815
3.802
3.797
3.784
3.769
3.765
3.752
3.177
3.153
3.129
3.115
3.112
N
S
0.92
0.95
4.33
2.23
2.24
2.25
3.00
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)

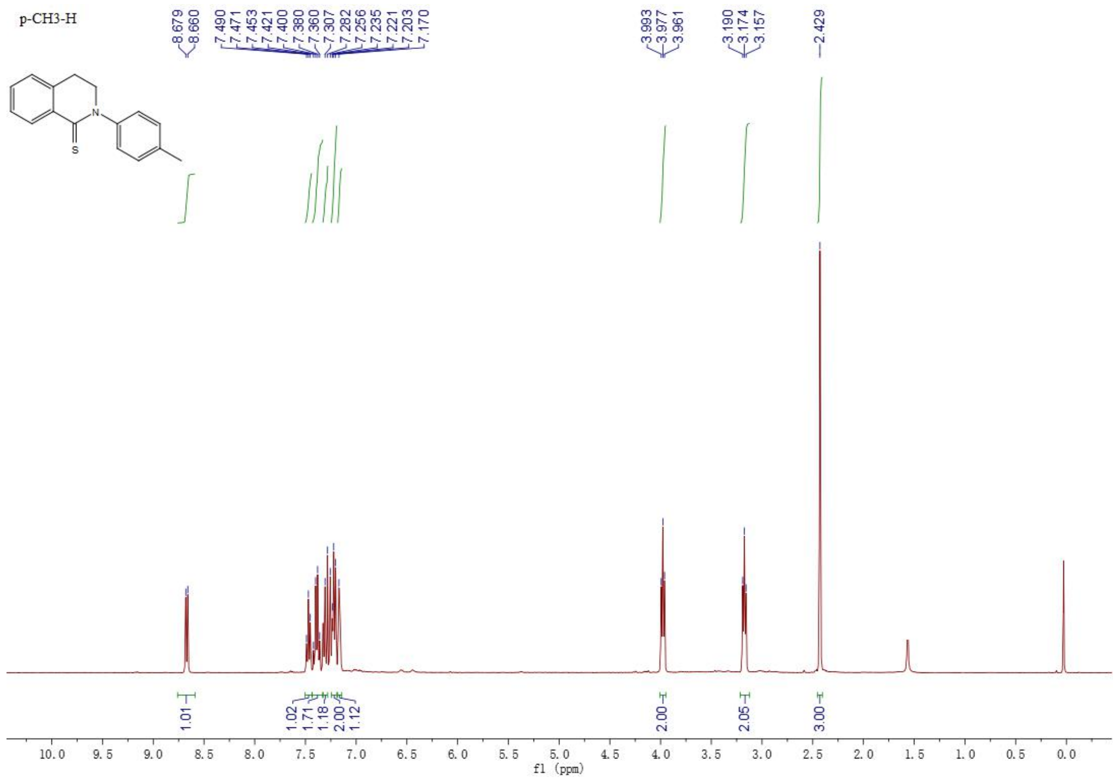

W191-C
192.893
146.346
134.079
134.038
133.075
132.532
131.950
131.396
128.298
127.642
127.184
126.798
126.148
51.400
28.610
18.153
N
S
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

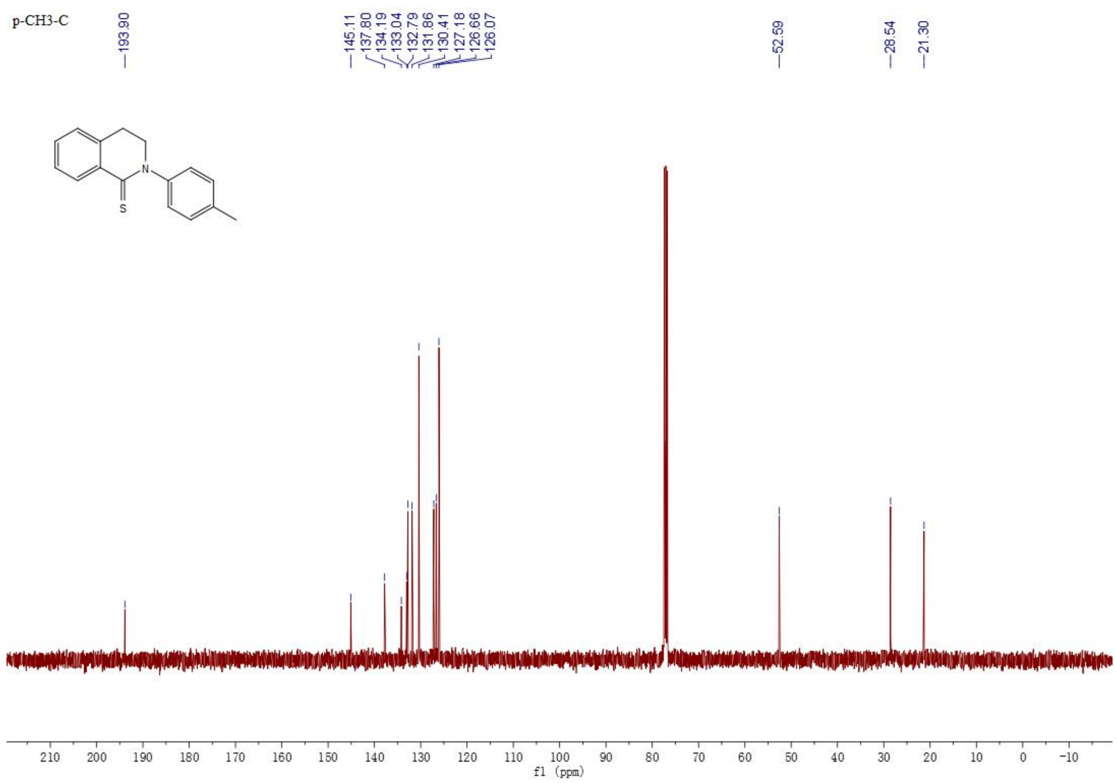
NMR of 2ab


m-CH3-H
8.648
8.628
7.458
7.455
7.440
7.436
7.421
7.418
7.385
7.365
7.345
7.328
7.199
7.189
7.170
7.138
7.137
7.123
3.956
3.939
3.922
3.154
3.138
3.122
2.398
N
S
0.95
1.11
2.03
2.20
1.85
2.00
2.03
2.86
f1 (ppm)

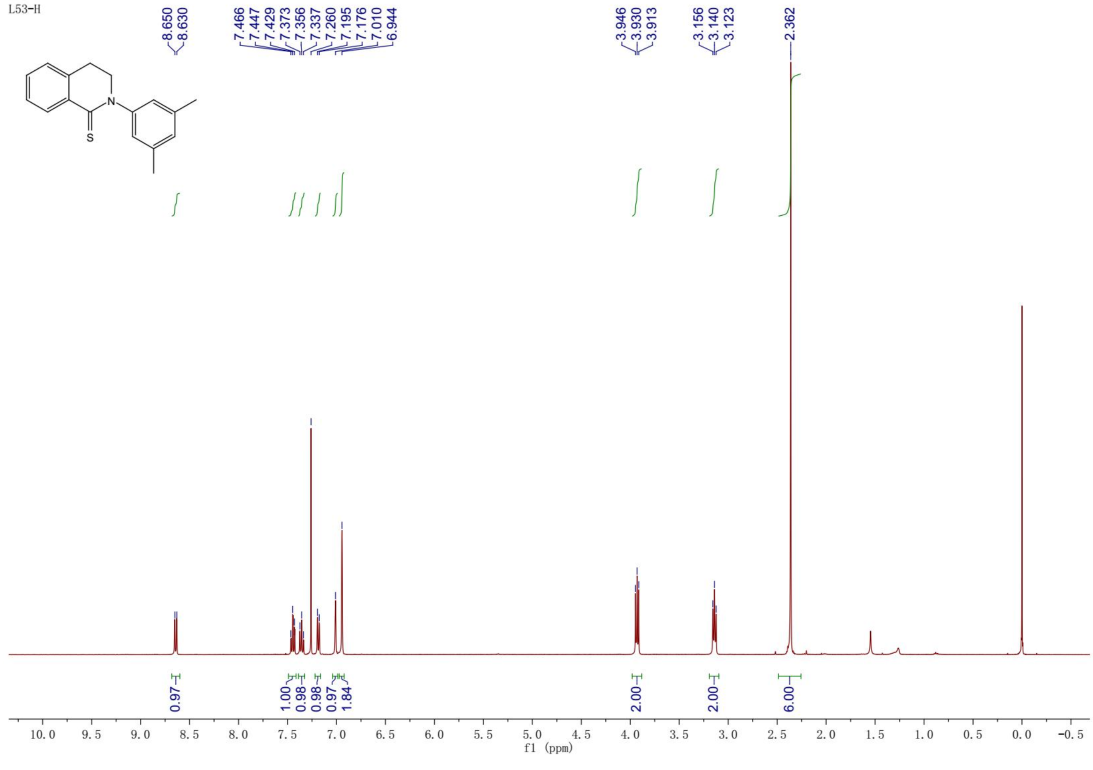

W190-C
193.763
147.593
139.796
134.206
133.034
132.759
131.833
129.527
128.699
127.166
126.826
126.647
123.386
52.558
28.549
21.422
N
S
f1 (ppm)

NMR of 2ac

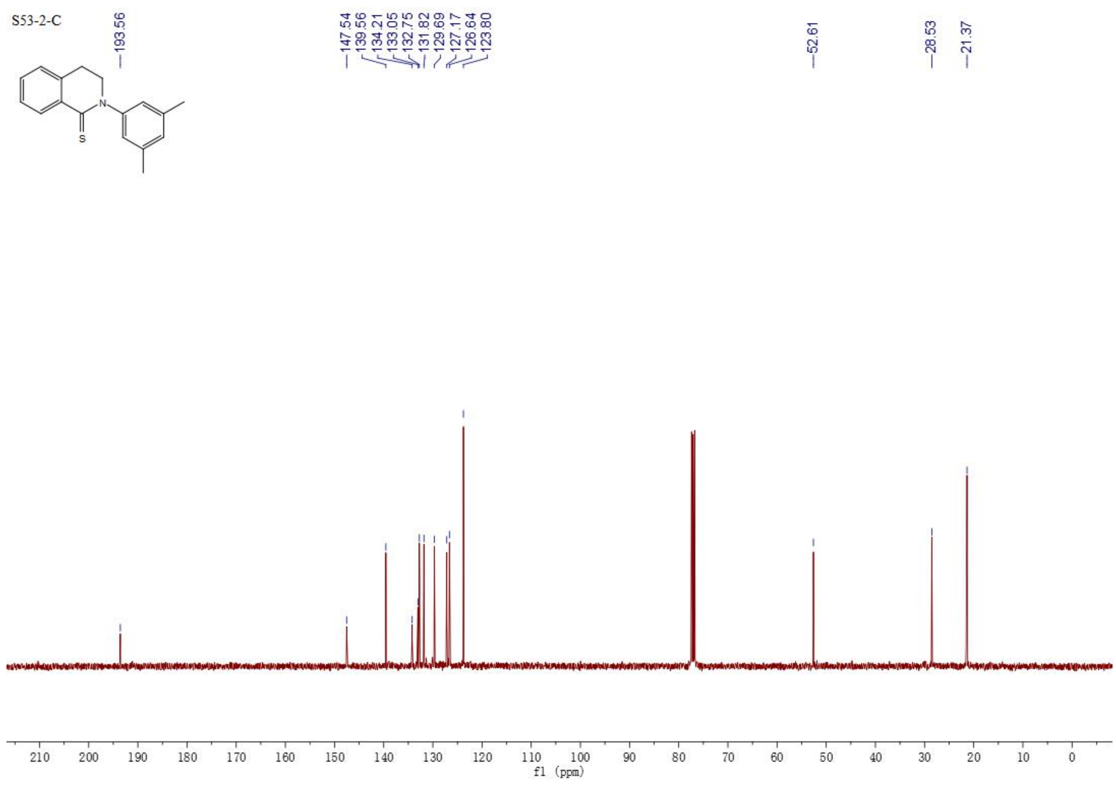

p-CH3-H
8.679
8.660
7.490
7.471
7.453
7.421
7.400
7.380
7.360
7.307
7.282
7.256
7.235
7.221
7.203
7.170
3.993
3.977
3.961
3.190
3.174
3.157
2.429
1.01
1.02
1.71
1.18
2.00
1.12
2.00
2.05
3.00
f1 (ppm)


p-CH3-C
193.90
145.11
137.80
134.19
133.04
132.79
131.86
130.41
127.18
126.66
126.07
52.59
28.54
21.30
f1 (ppm)

NMR of 2ad

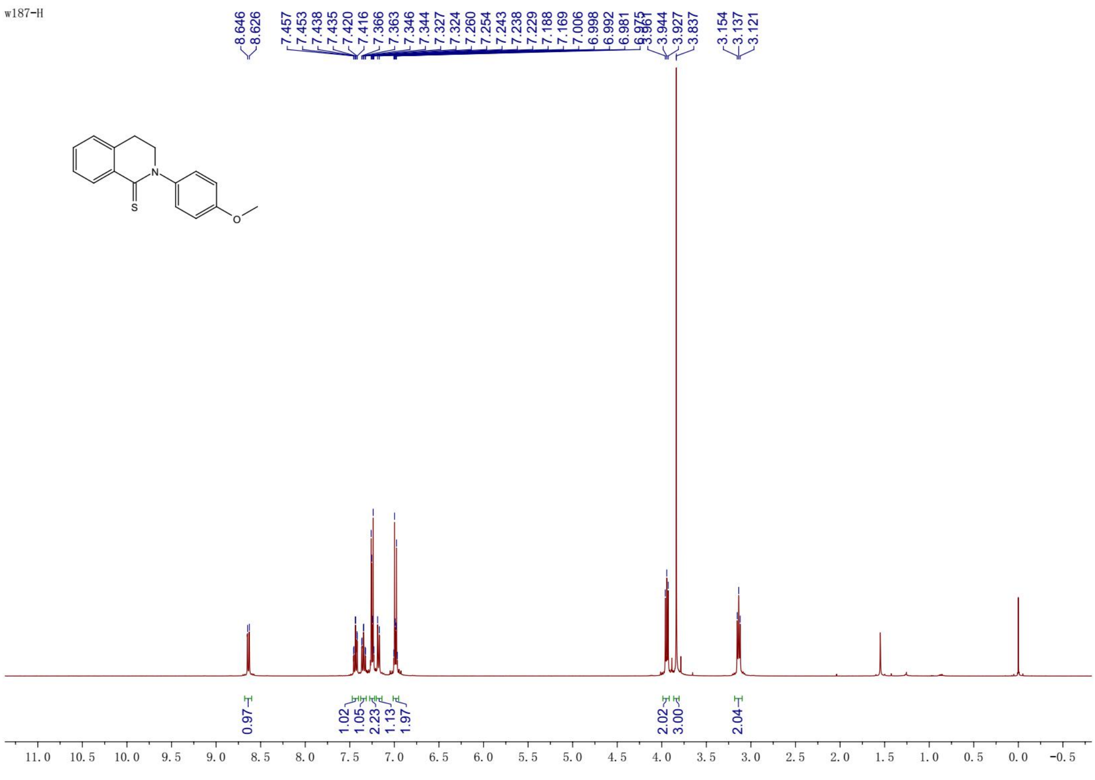


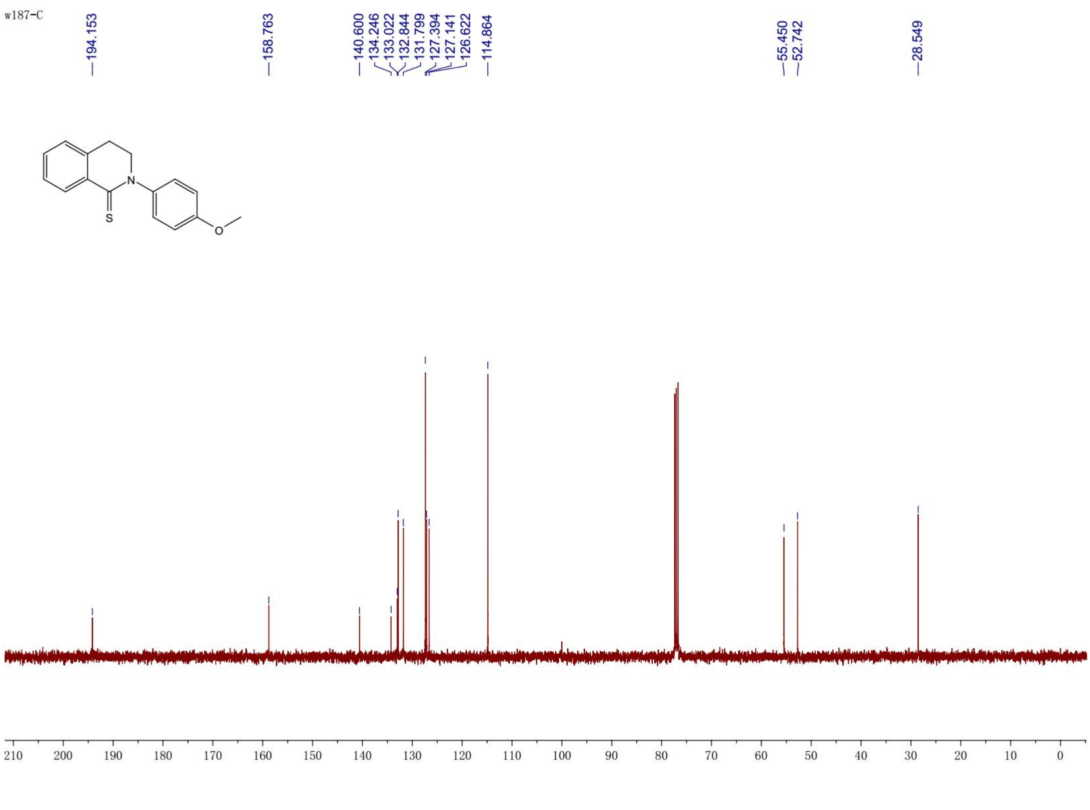
L53-H
8.650
8.630
7.466
7.447
7.429
7.373
7.356
7.337
7.260
7.195
7.176
7.010
6.944
3.946
3.930
3.913
3.156
3.140
3.123
2.362
S
N
0.97
1.00
0.98
0.98
0.97
1.84
2.00
2.00
6.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)



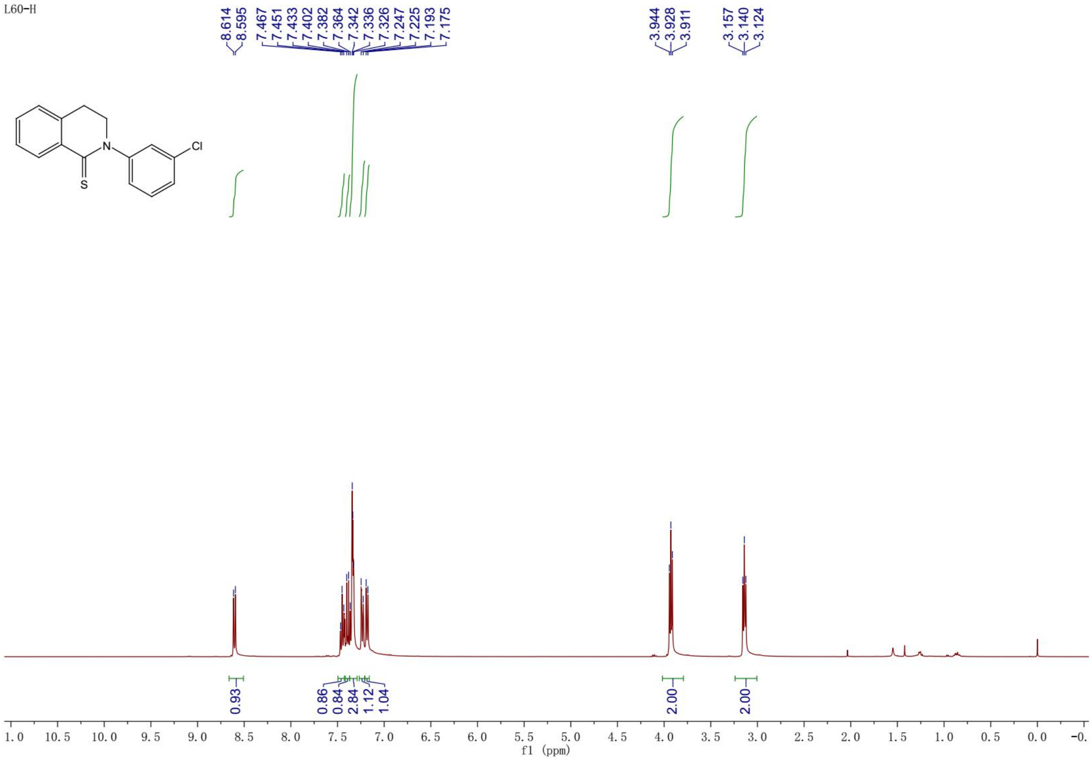
S53-2-C
193.56
147.54
139.56
134.21
133.05
132.75
131.82
129.69
127.17
126.64
123.80
52.61
28.53
21.37
S
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

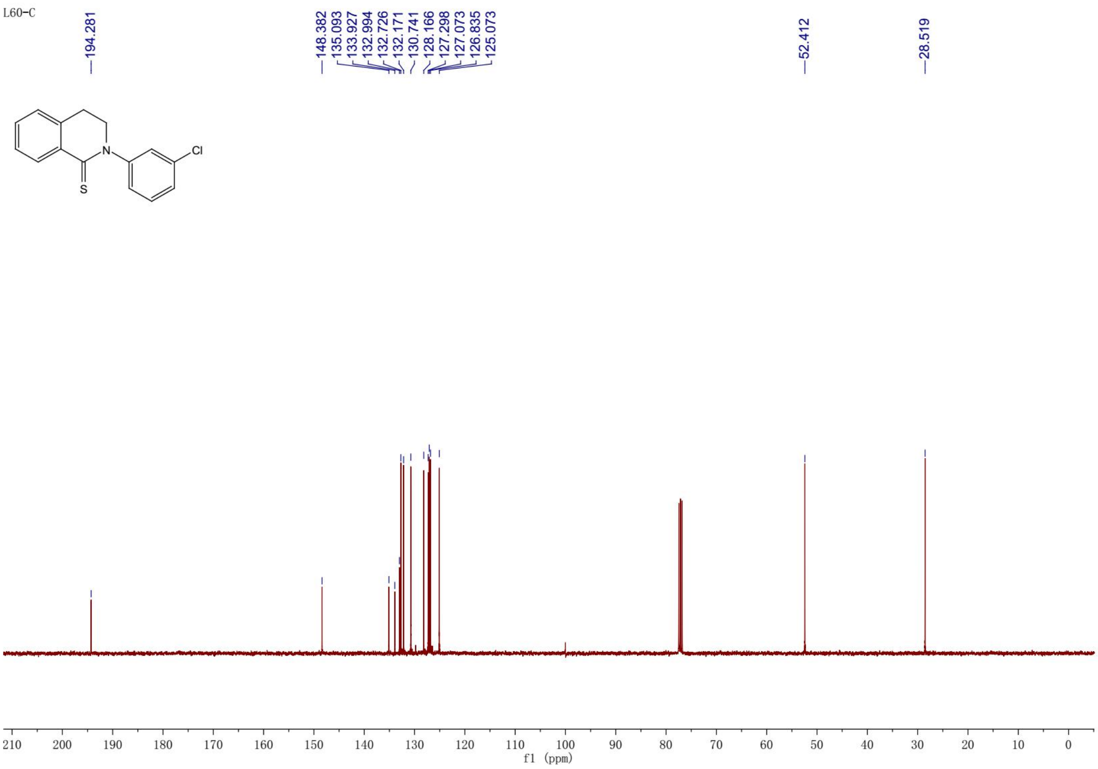
NMR of 2ae


w187-H
8.646
8.626
7.457
7.453
7.438
7.435
7.420
7.416
7.366
7.363
7.346
7.344
7.327
7.324
7.260
7.254
7.243
7.238
7.229
7.188
7.169
7.006
6.998
6.992
6.981
6.975
3.961
3.944
3.927
3.837
3.154
3.137
3.121
N
S
O
0.97
1.02
1.05
2.23
1.13
1.97
2.02
3.00
2.04
11.0 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


w187-C
194.153
158.763
140.600
134.246
133.022
132.844
131.799
127.394
127.141
126.622
114.864
55.450
52.742
28.549
N
S
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

NMR of 2af


L60-H
8.614
8.595
7.467
7.451
7.433
7.402
7.382
7.364
7.342
7.336
7.326
7.247
7.225
7.193
7.175
3.944
3.928
3.911
3.157
3.140
3.124
Cl
N
S
0.93
0.86
0.84
2.84
1.12
1.04
2.00
2.00
f1 (ppm)


L60-C
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135.093
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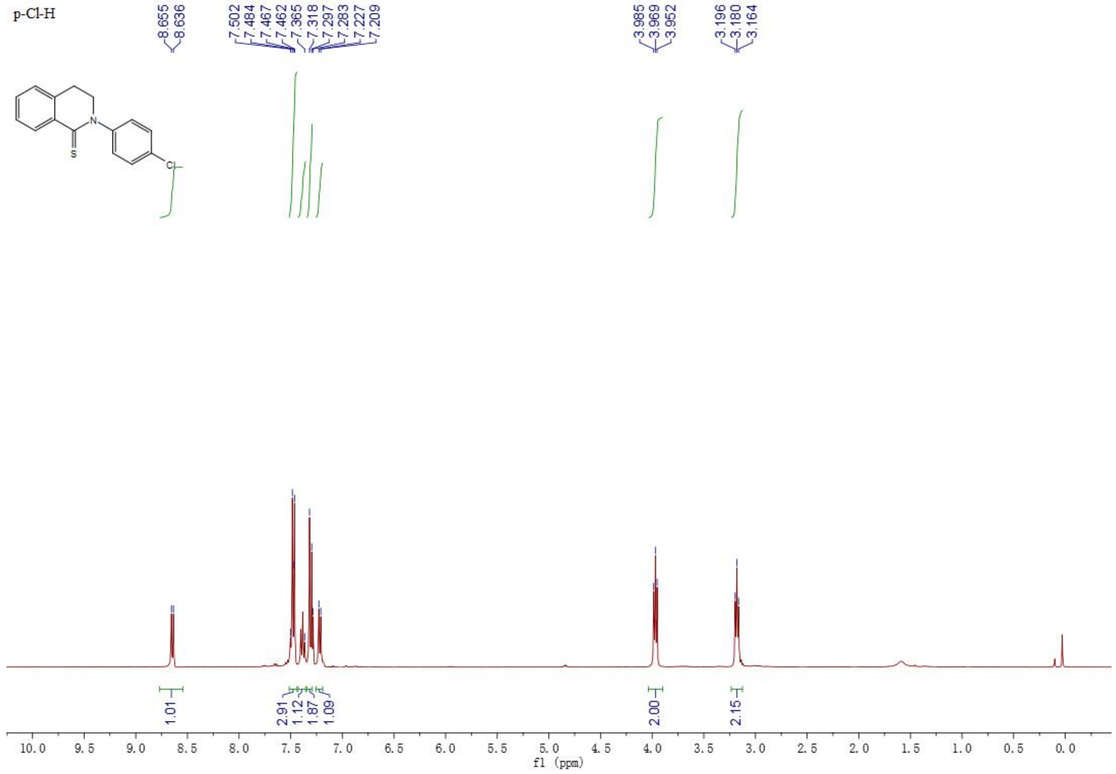
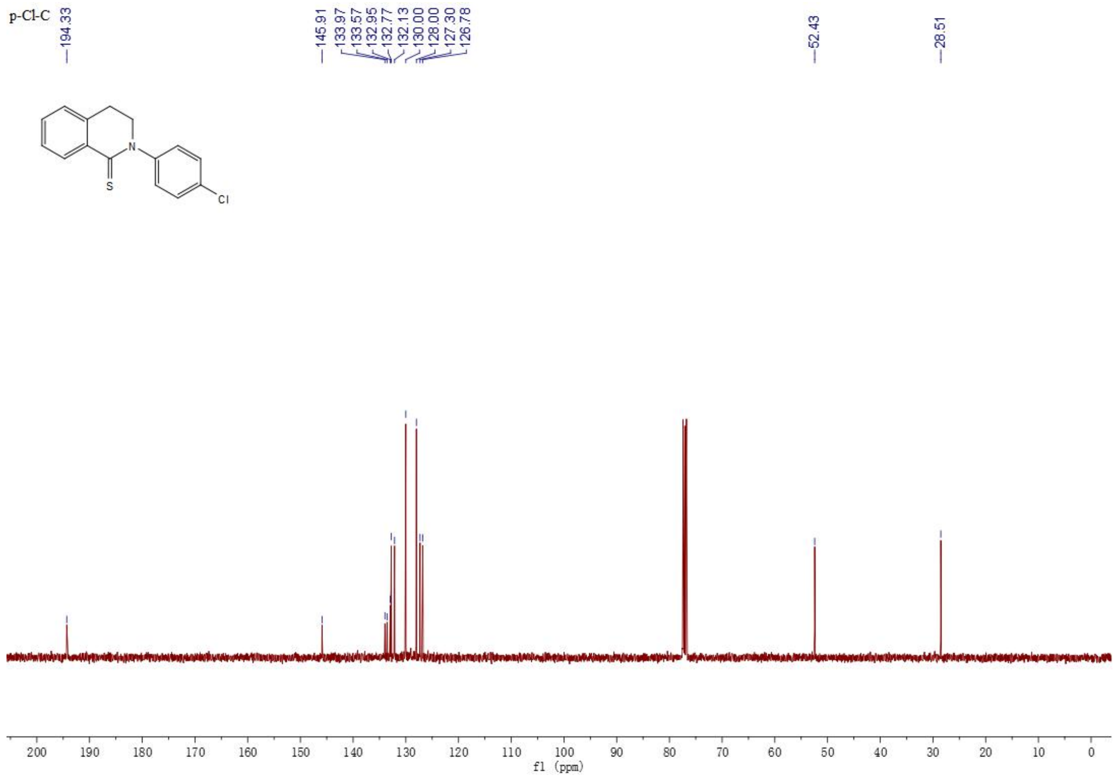
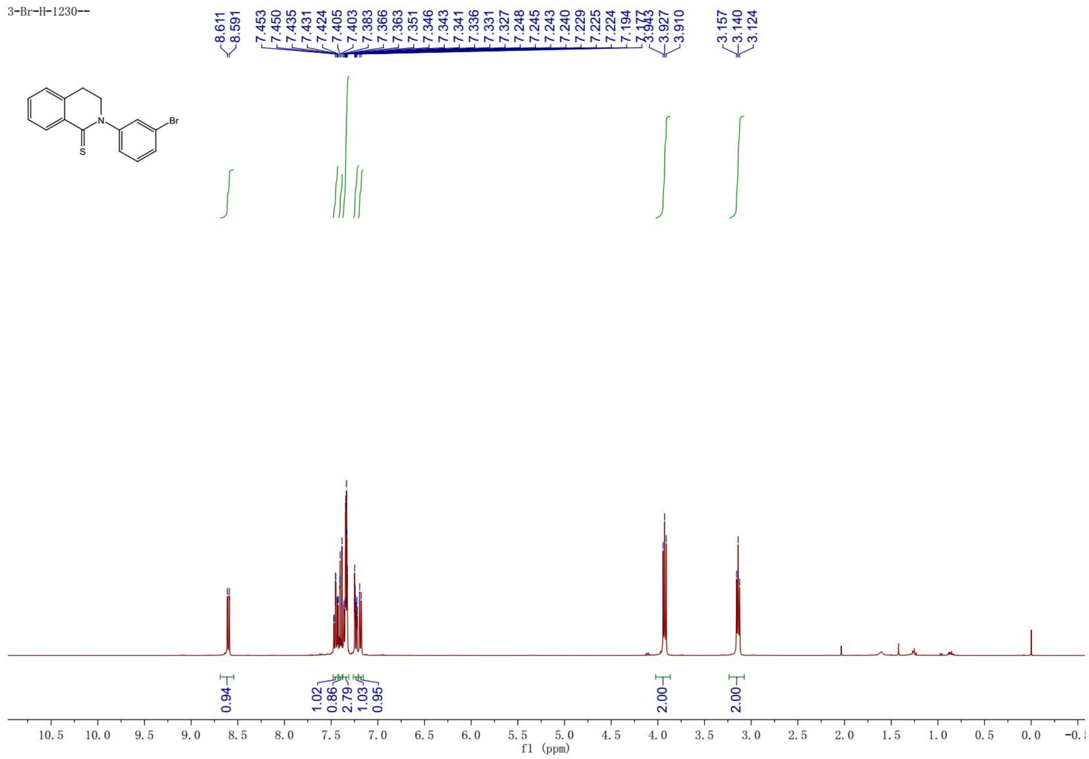
132.994
132.726
132.171
130.741
128.166
127.298
127.073
126.835
125.073
52.412
28.519
Cl
N
S
f1 (ppm)

NMR of 2ag

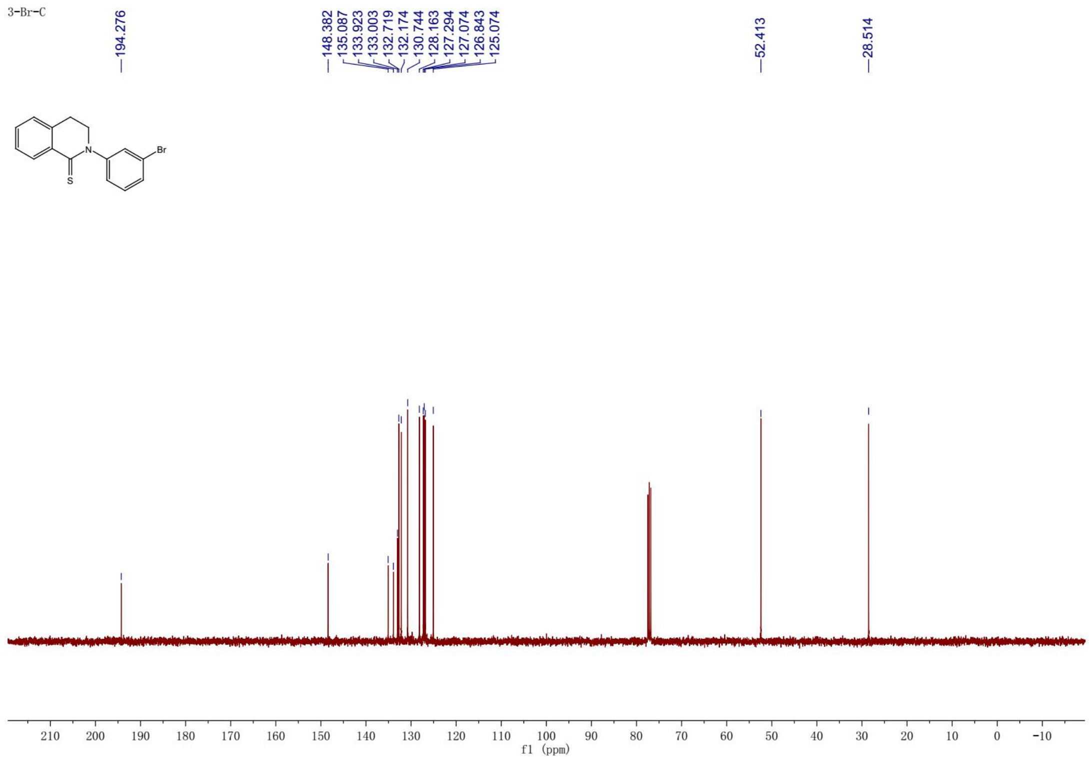

p-Cl-H
8.655
8.636
7.502
7.484
7.467
7.462
7.365
7.318
7.297
7.283
7.227
7.209
3.985
3.969
3.952
3.196
3.180
3.164
N
S
Cl
1.01
2.91
1.12
1.87
1.09
2.00
2.15
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


p-Cl-C
194.33
145.91
133.97
133.57
132.95
132.77
132.13
130.00
128.00
127.30
126.78
52.43
28.51
N
S
Cl
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

NMR of 2ah

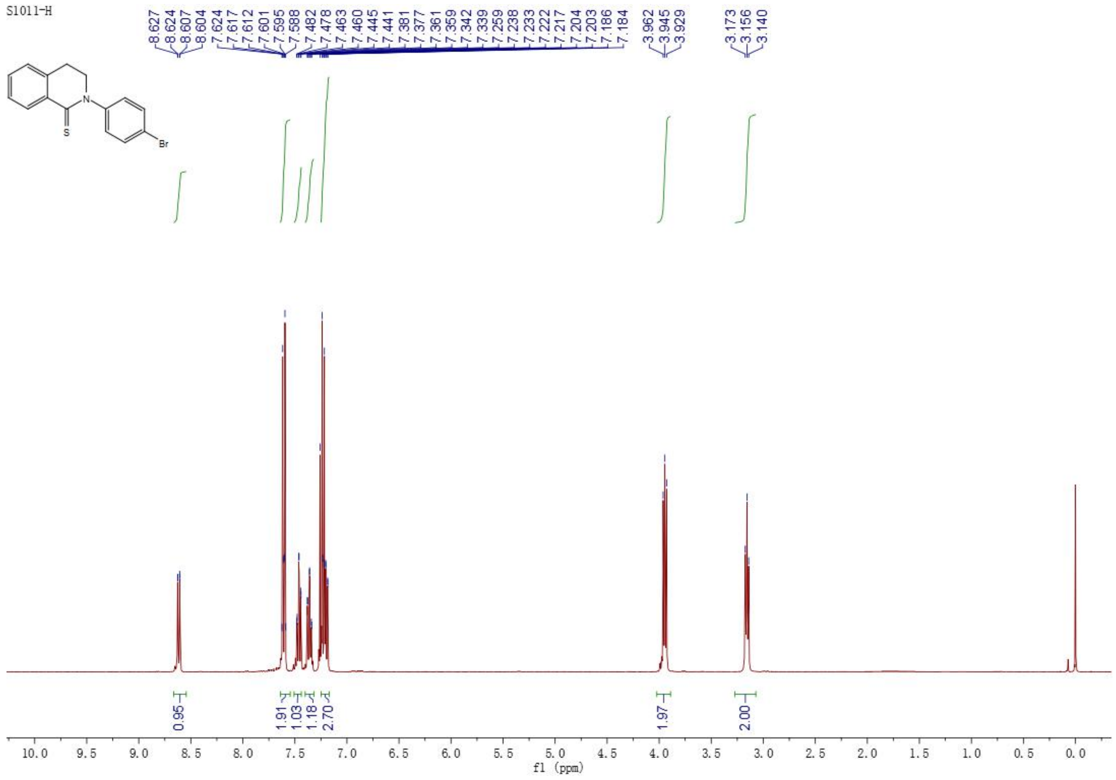


3-Br-H-1230--
8.611
8.591
7.453
7.450
7.435
7.431
7.424
7.405
7.403
7.383
7.366
7.363
7.351
7.346
7.343
7.341
7.336
7.331
7.327
7.248
7.245
7.243
7.240
7.229
7.225
7.224
7.194
7.177
3.943
3.927
3.910
3.157
3.140
3.124
Br
N
S
0.94
1.02
0.86
2.79
1.03
0.95
2.00
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 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
f1 (ppm)



3-Br-C
194.276
148.382
135.087
133.923
133.003
132.719
132.174
130.744
128.163
127.294
127.074
126.843
125.074
52.413
28.514
Br
N
S
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)

NMR of 2ai


S1011-H
8.627
8.624
8.607
8.604
7.624
7.617
7.612
7.601
7.595
7.588
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7.478
7.463
7.460
7.445
7.441
7.381
7.377
7.361
7.359
7.342
7.339
7.259
7.238
7.233
7.222
7.217
7.204
7.203
7.186
7.184
3.962
3.945
3.929
3.173
3.156
3.140
N
S
Br
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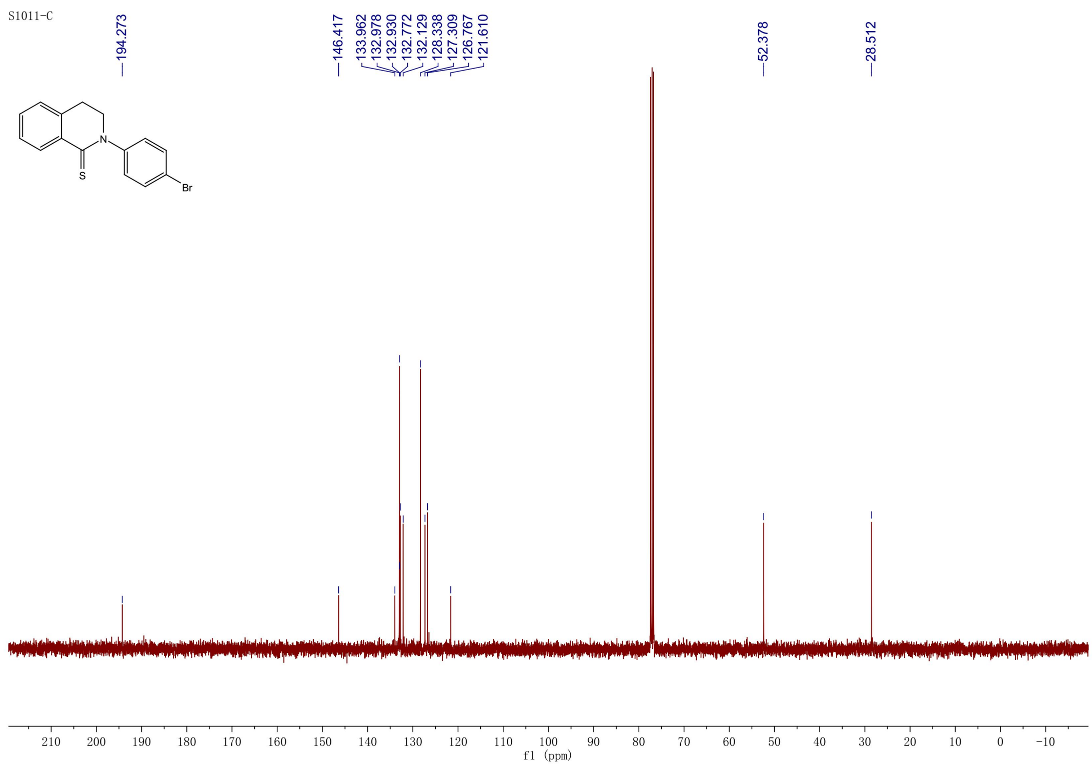
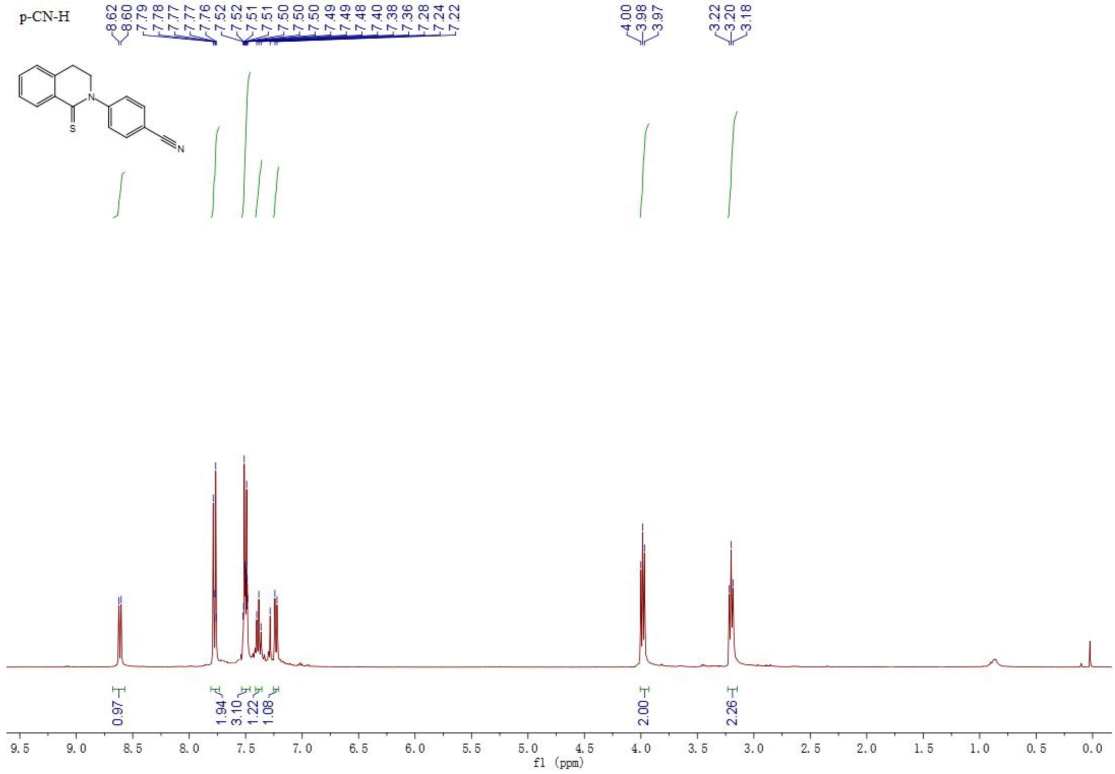
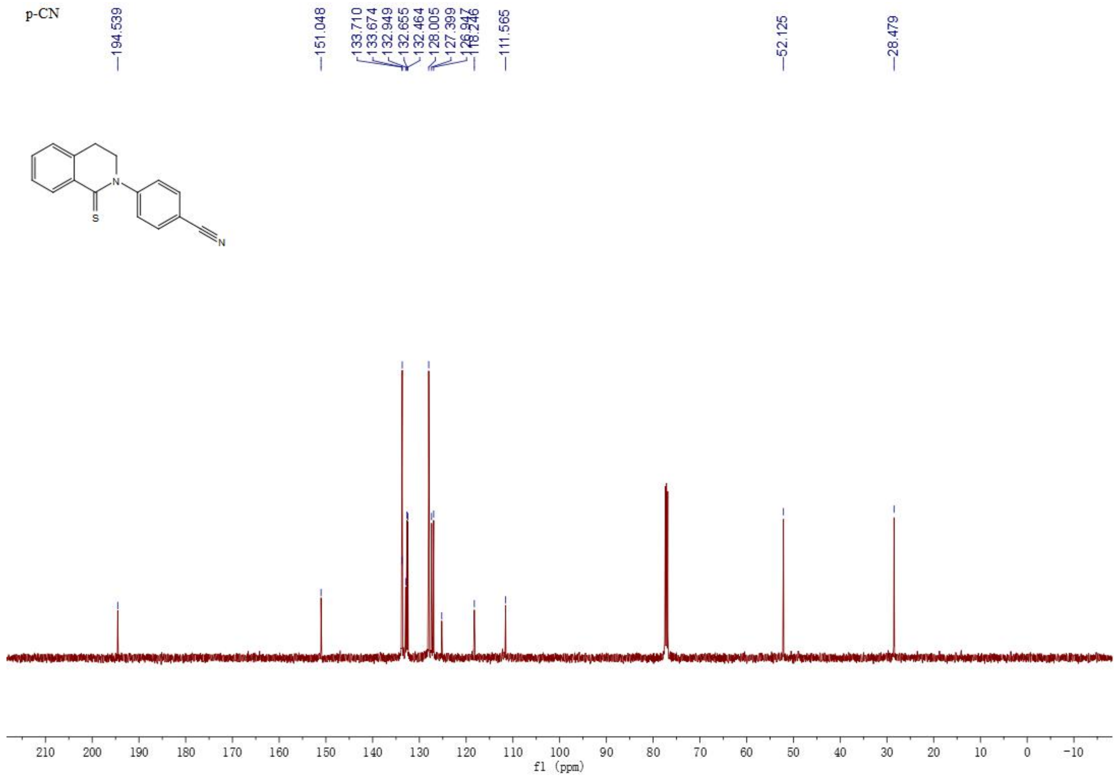
1.03
1.18
2.70
1.97
2.00
f1 (ppm)

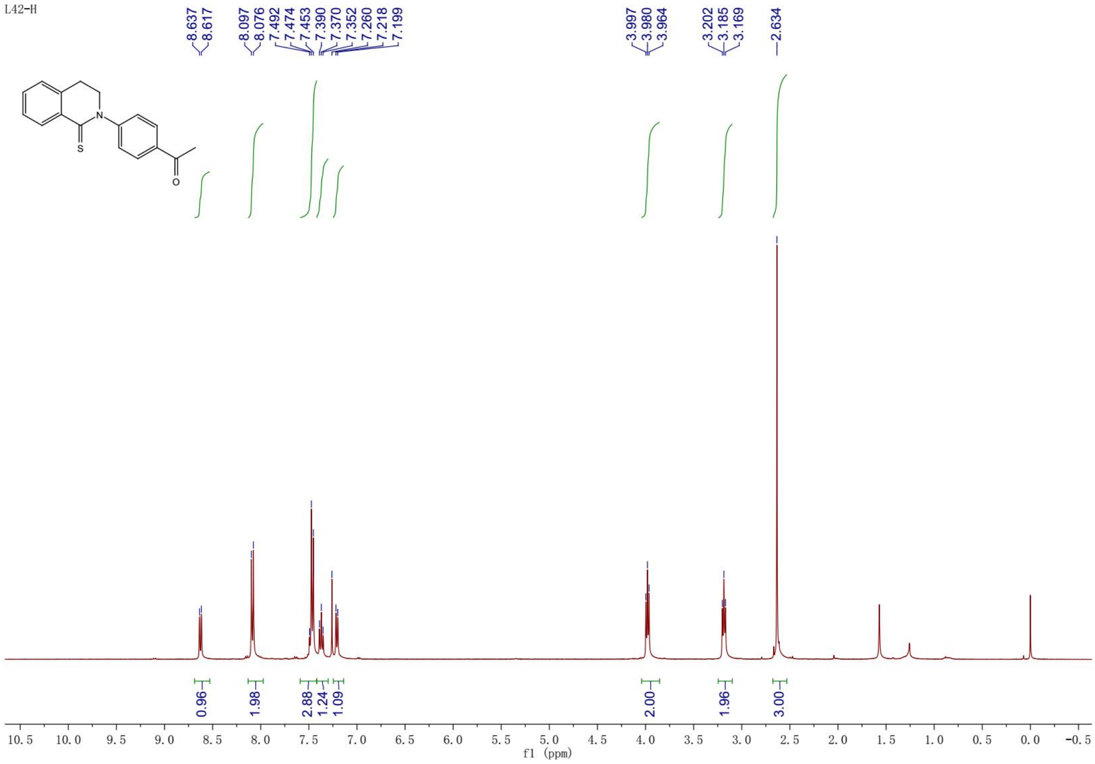

S1011-C
194.273
146.417
133.962
132.978
132.930
132.772
132.129
128.338
127.309
126.767
121.610
52.378
28.512
N
S
Br
f1 (ppm)

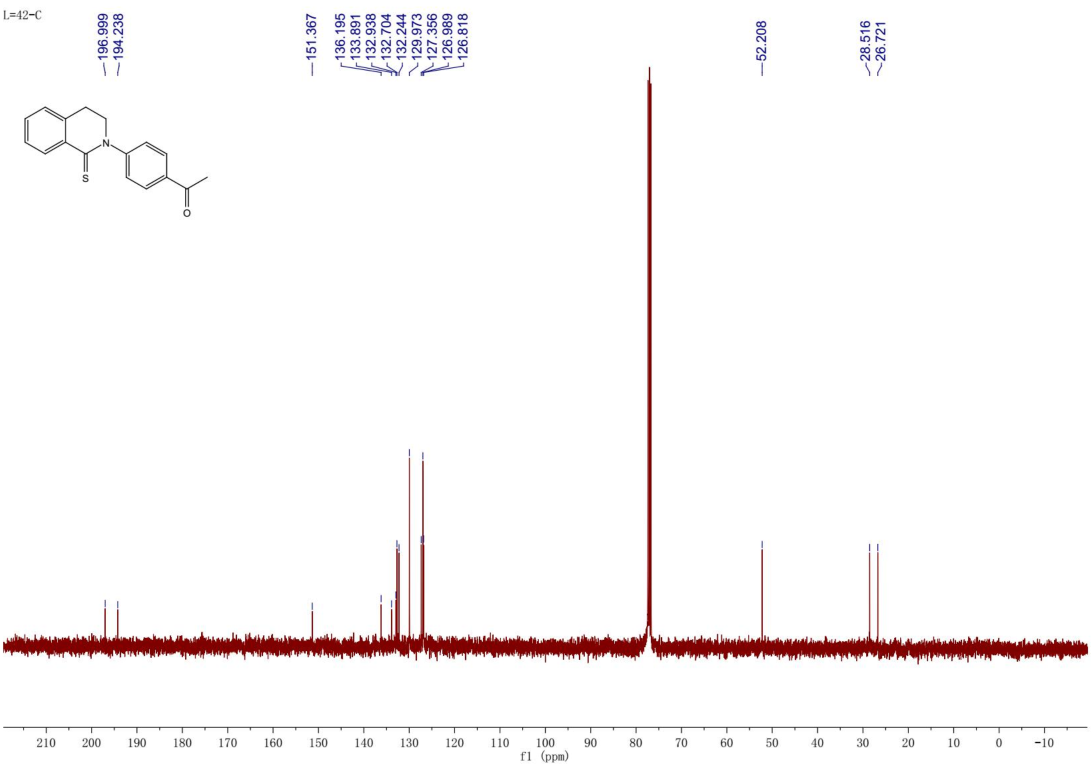
NMR of 2aj


p-CN-H
8.62
8.60
7.79
7.78
7.77
7.77
7.76
7.52
7.52
7.51
7.51
7.50
7.50
7.49
7.49
7.48
7.40
7.38
7.36
7.28
7.24
7.22
4.00
3.98
3.97
3.22
3.20
3.18
0.97
1.94
3.10
1.22
1.08
2.00
2.26
f1 (ppm)

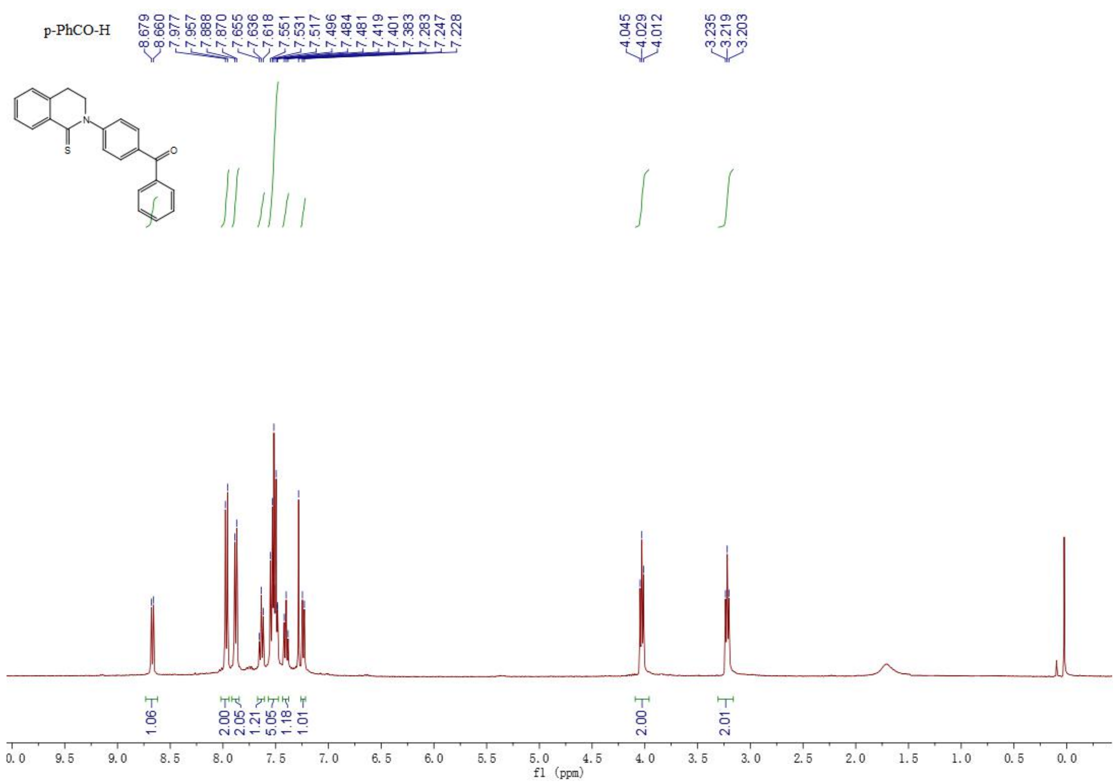

p-CN
194.539
151.048
133.710
133.674
132.949
132.655
132.464
128.005
127.399
111.565
52.125
28.479
f1 (ppm)

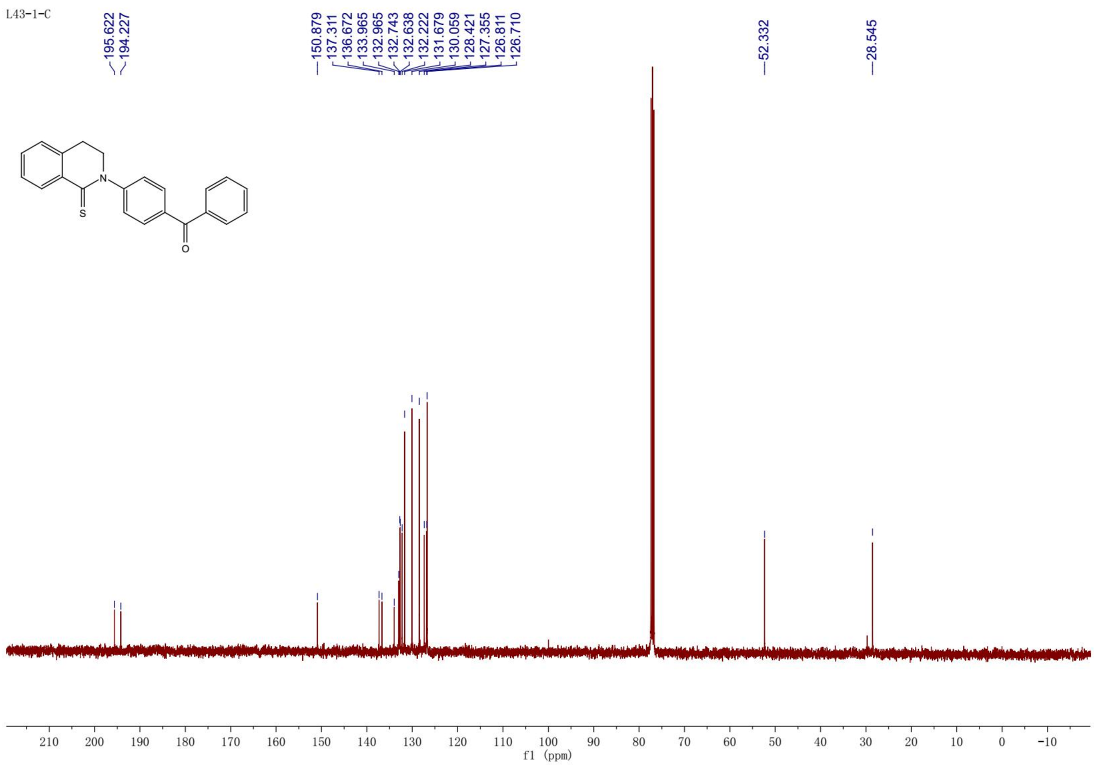
NMR of 2ak


L42-H
8.637
8.617
8.097
8.076
7.492
7.474
7.453
7.390
7.370
7.352
7.260
7.218
7.199
3.997
3.980
3.964
3.202
3.185
3.169
2.634
N
S
O
0.96
1.98
2.88
1.24
1.09
2.00
1.96
3.00
f1 (ppm)

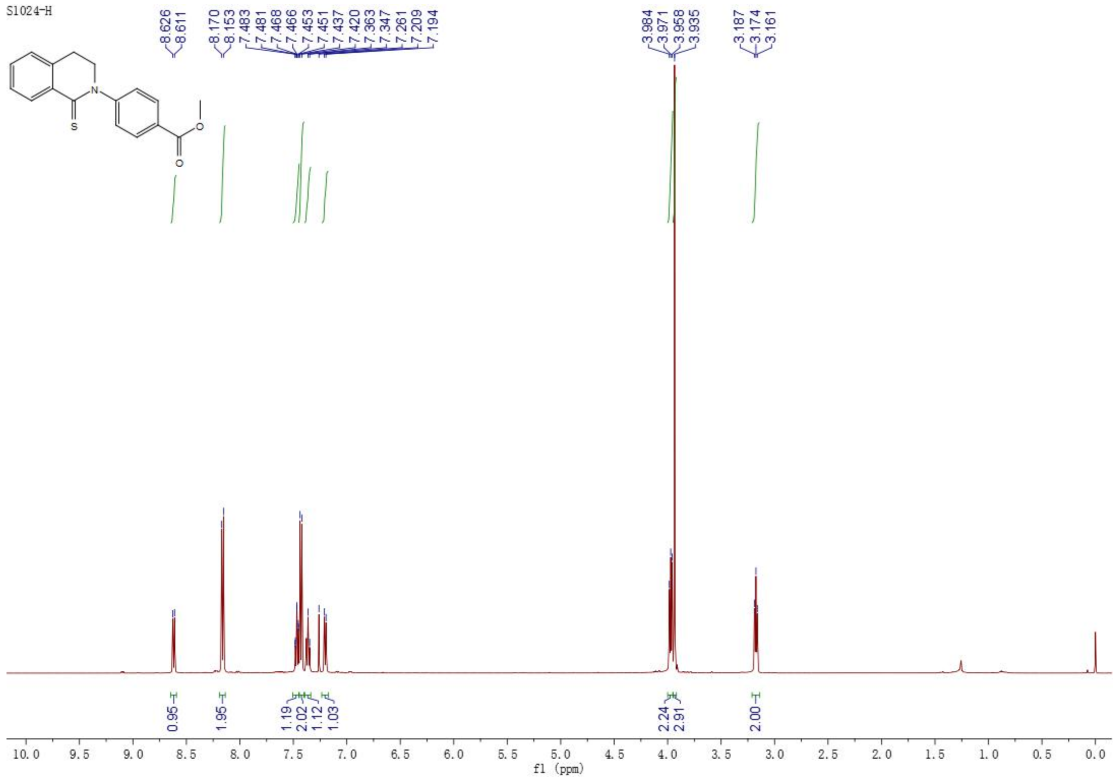

L=42-C
196.999
194.238
151.367
136.195
133.891
132.938
132.704
132.244
129.973
127.356
126.989
126.818
52.208
28.516
26.721
N
S
O
f1 (ppm)

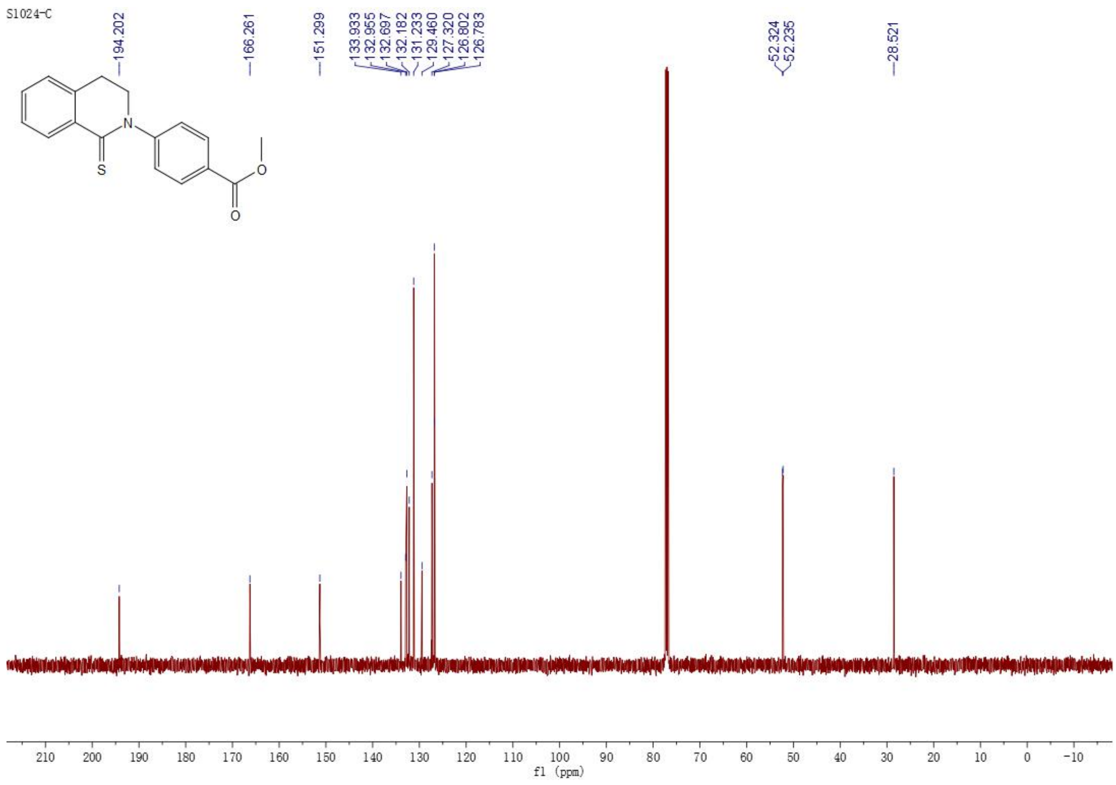
NMR of 2al


p-PhCO-H
8.679
8.660
7.977
7.957
7.888
7.870
7.655
7.636
7.618
7.551
7.531
7.517
7.496
7.484
7.481
7.419
7.401
7.383
7.283
7.247
7.228
4.045
4.029
4.012
3.235
3.219
3.203
N
S
O
1.06
2.00
2.05
1.21
5.05
1.18
1.01
2.00
2.01
f1 (ppm)

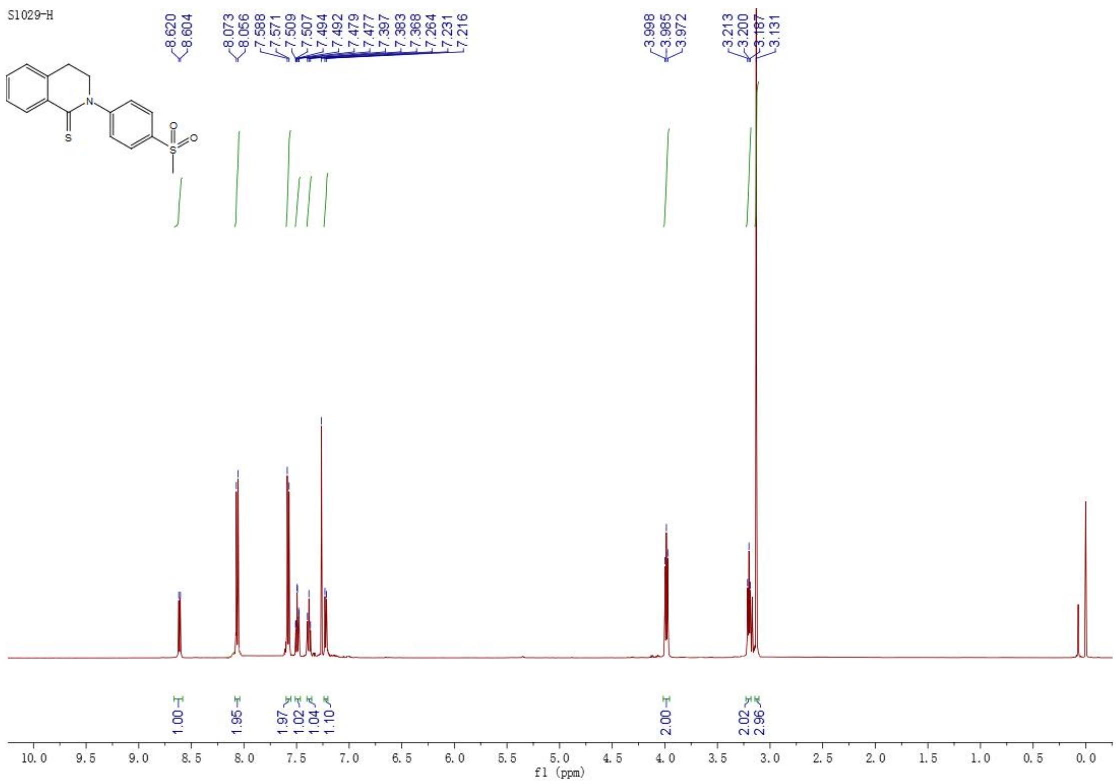

L43-1-C
195.622
194.227
150.879
137.311
136.672
133.965
132.965
132.743
132.638
132.222
131.679
130.059
128.421
127.355
126.811
126.710
52.332
28.545
N
S
O
f1 (ppm)

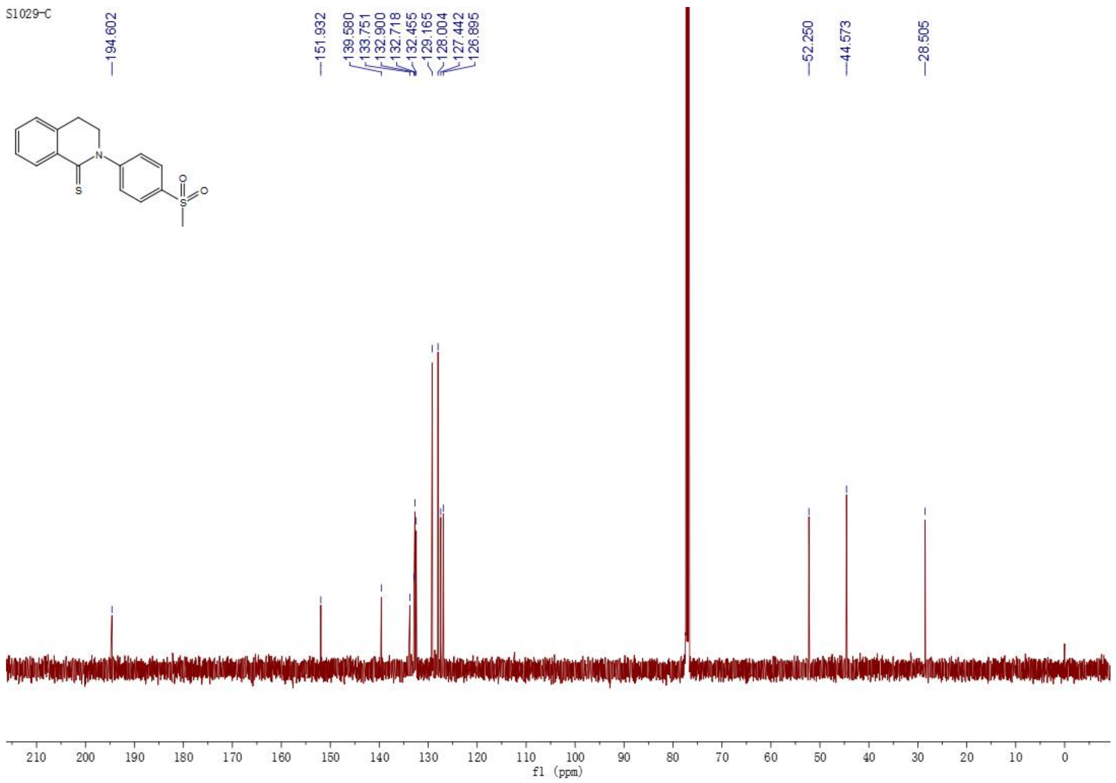
NMR of 2am


S1024-H
8.626
8.611
8.170
8.153
7.483
7.481
7.468
7.466
7.453
7.451
7.437
7.420
7.363
7.347
7.261
7.209
7.194
3.984
3.971
3.958
3.935
3.187
3.174
3.161
0.95
1.95
1.19
2.02
1.12
1.03
2.24
2.91
2.00
f1 (ppm)

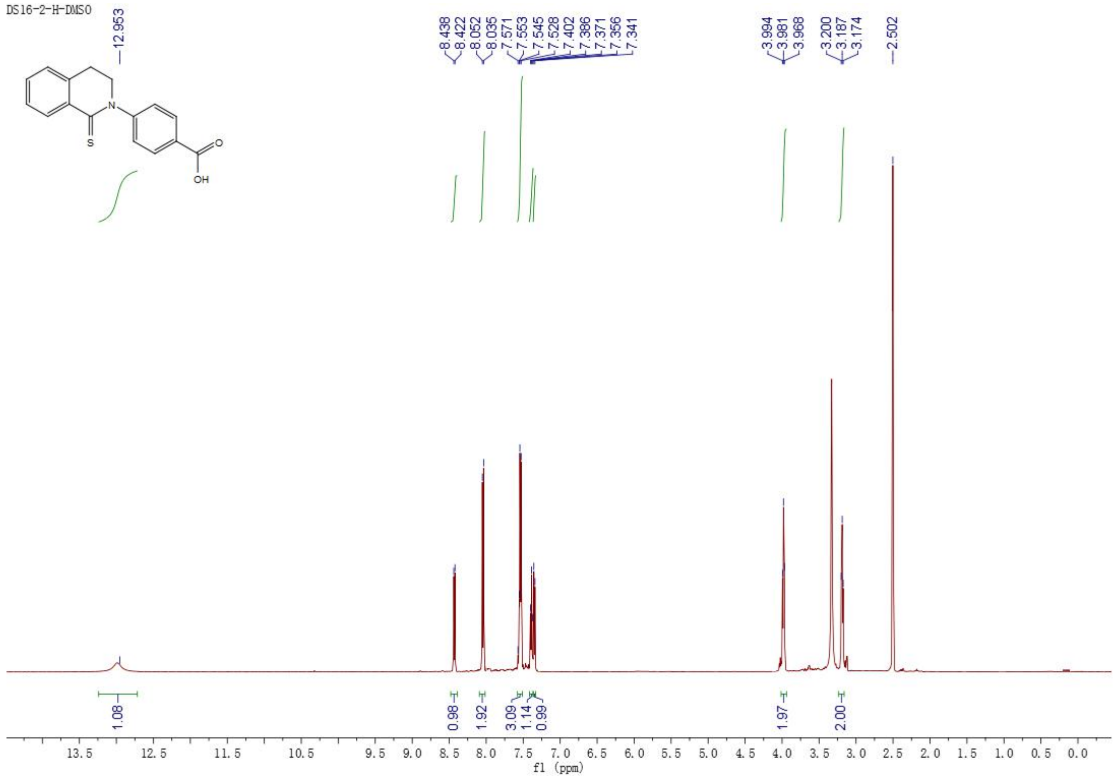

S1024-C
194.202
166.261
151.299
133.933
132.955
132.697
132.182
131.233
129.460
127.320
126.802
126.783
52.324
52.235
28.521
f1 (ppm)

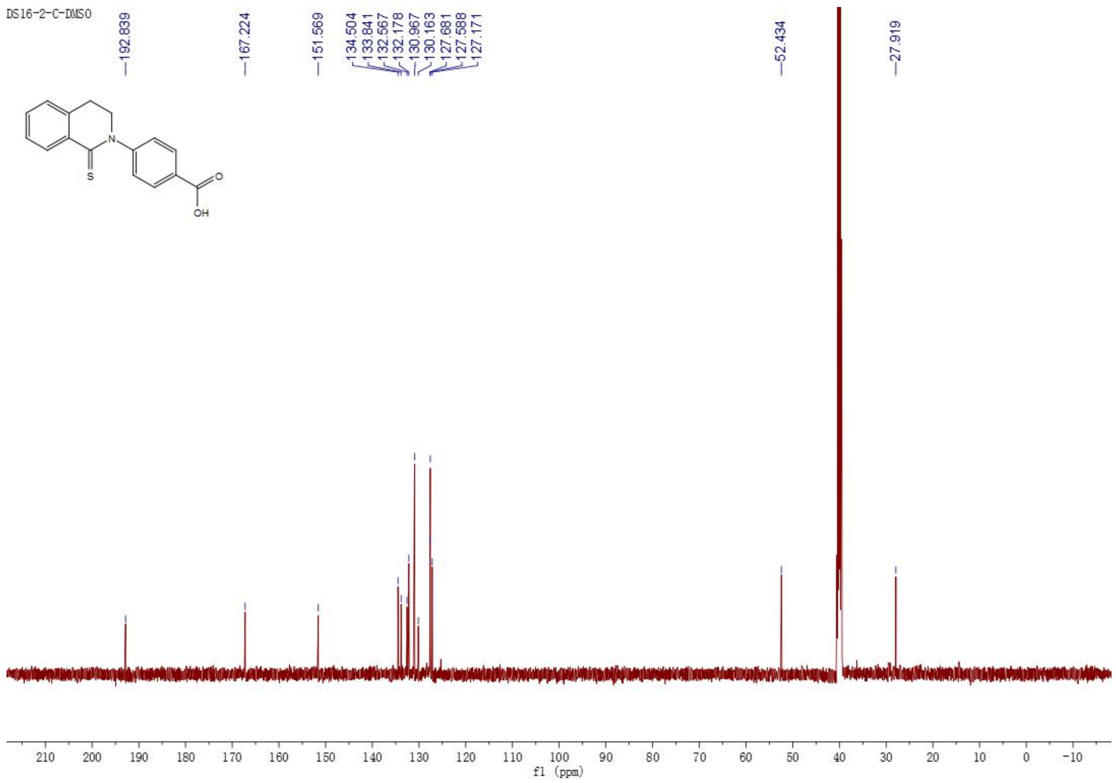
NMR of 2an


S1029-H
8.620
8.604
8.073
8.056
7.588
7.571
7.509
7.507
7.494
7.492
7.479
7.477
7.397
7.383
7.368
7.264
7.231
7.216
3.998
3.985
3.972
3.213
3.200
3.187
3.131
1.00
1.95
1.97
1.02
1.04
1.10
2.00
2.02
2.96
f1 (ppm)

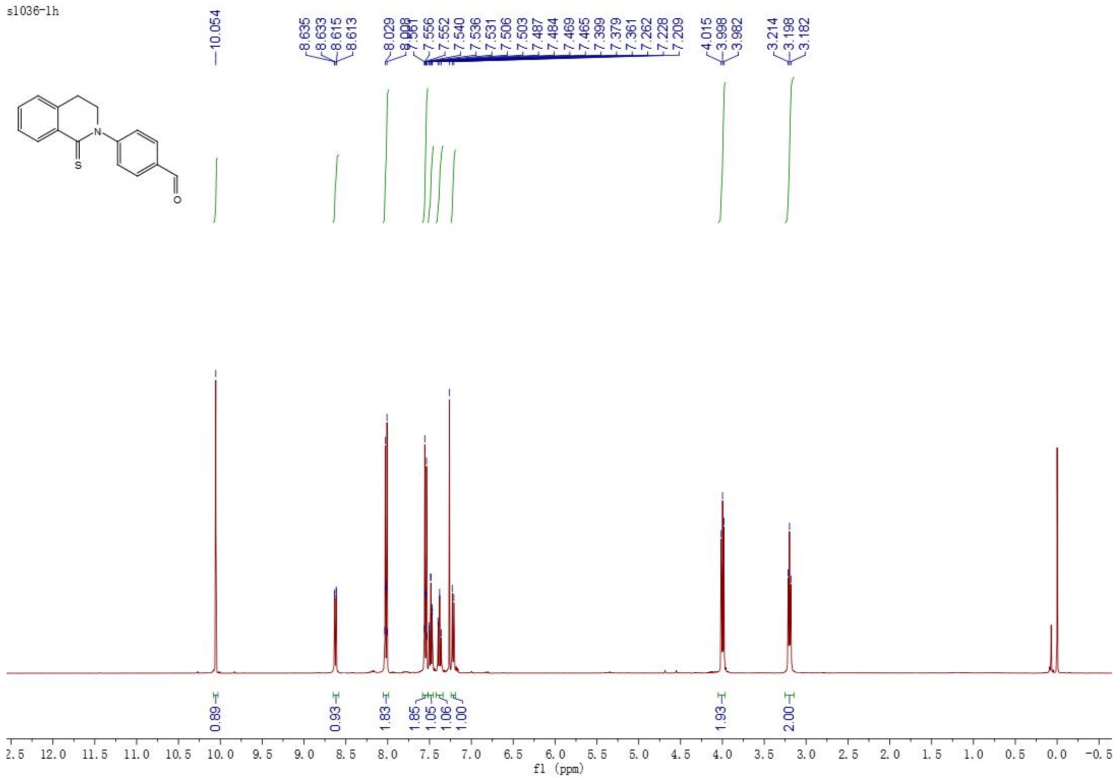

S1029-C
194.602
151.932
139.580
133.751
132.900
132.718
132.455
129.165
128.004
127.442
126.895
52.250
44.573
28.505
f1 (ppm)

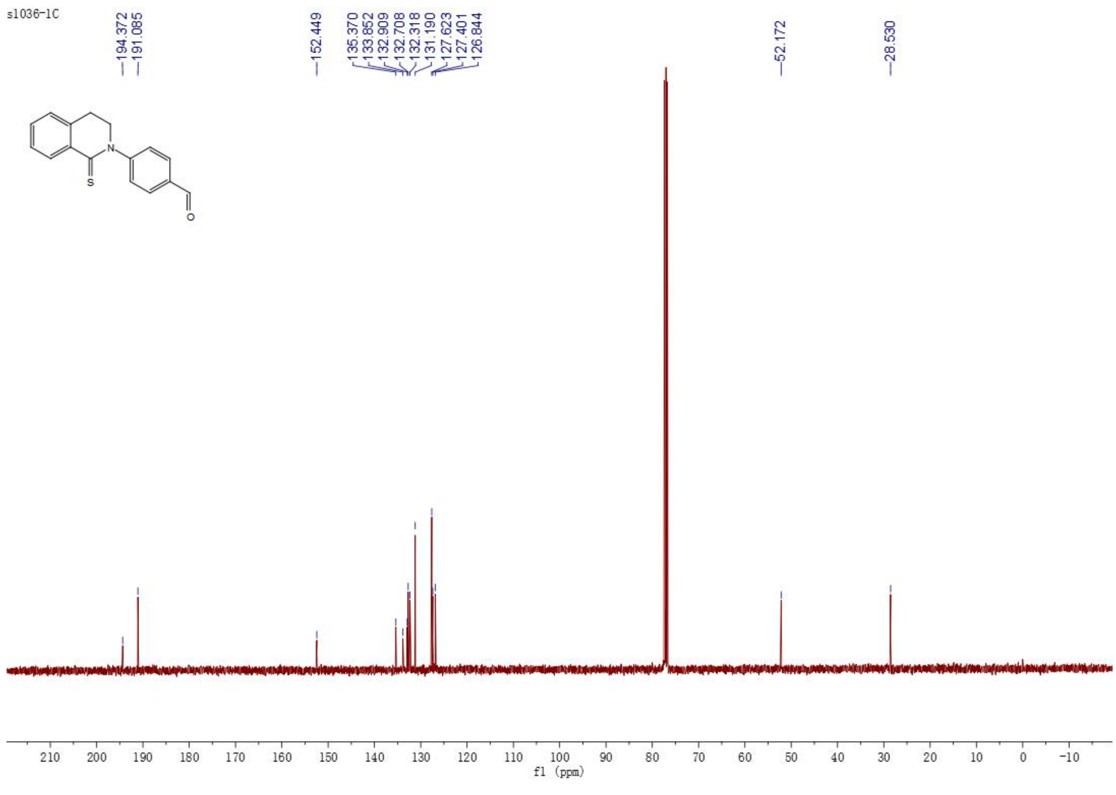
NMR of 2ao



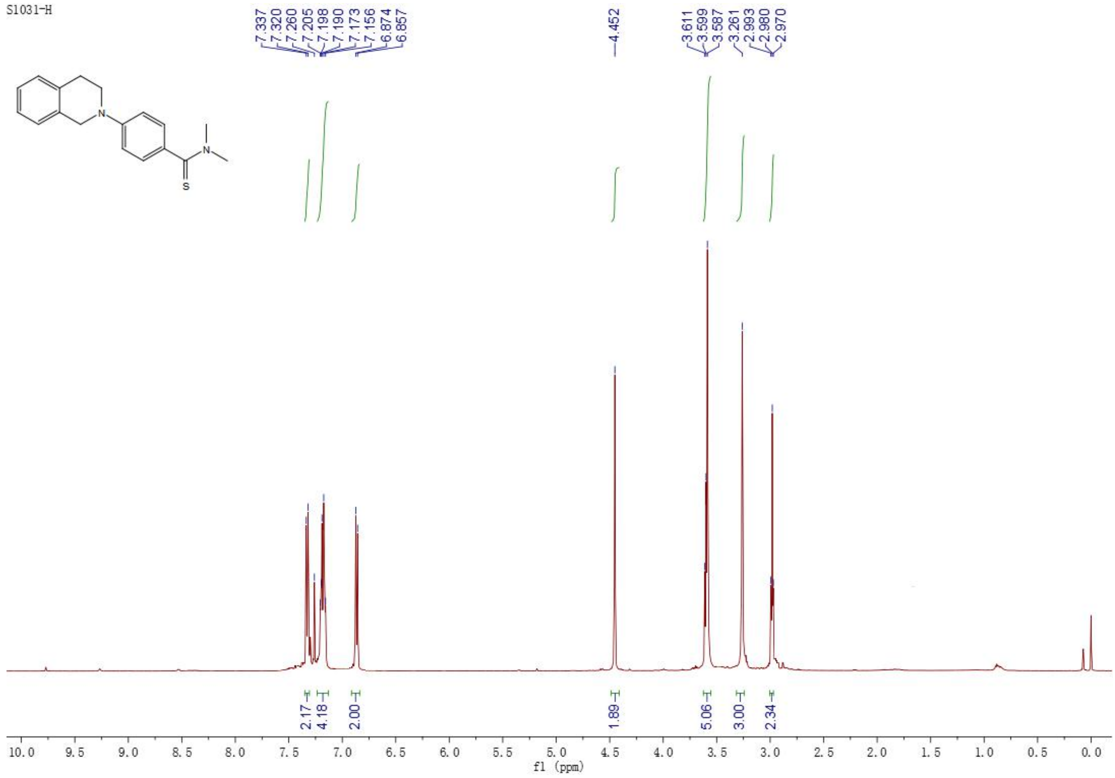


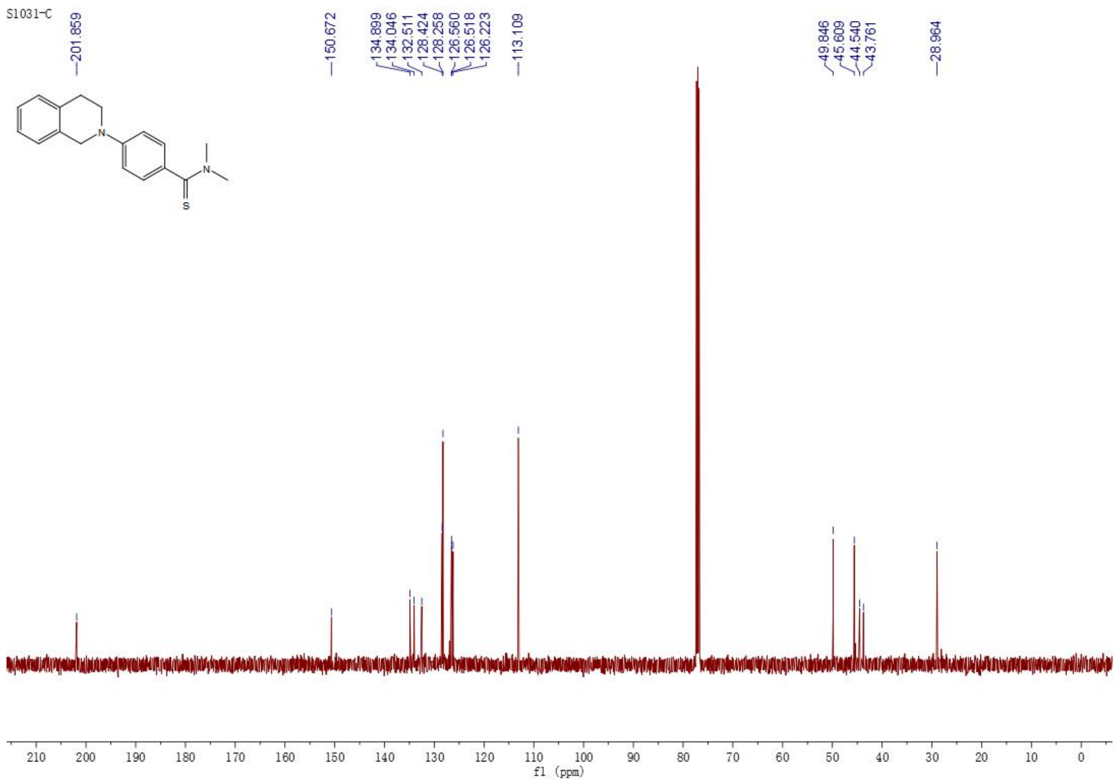
NMR of 2ap


s1036-1h
10.054
8.635
8.633
8.615
8.613
8.029
7.561
7.556
7.552
7.540
7.536
7.531
7.506
7.503
7.487
7.484
7.469
7.465
7.399
7.379
7.361
7.262
7.228
7.209
4.015
3.998
3.982
3.214
3.198
3.182
0.89
0.93
1.83
1.85
1.05
1.06
1.00
1.93
2.00
f1 (ppm)

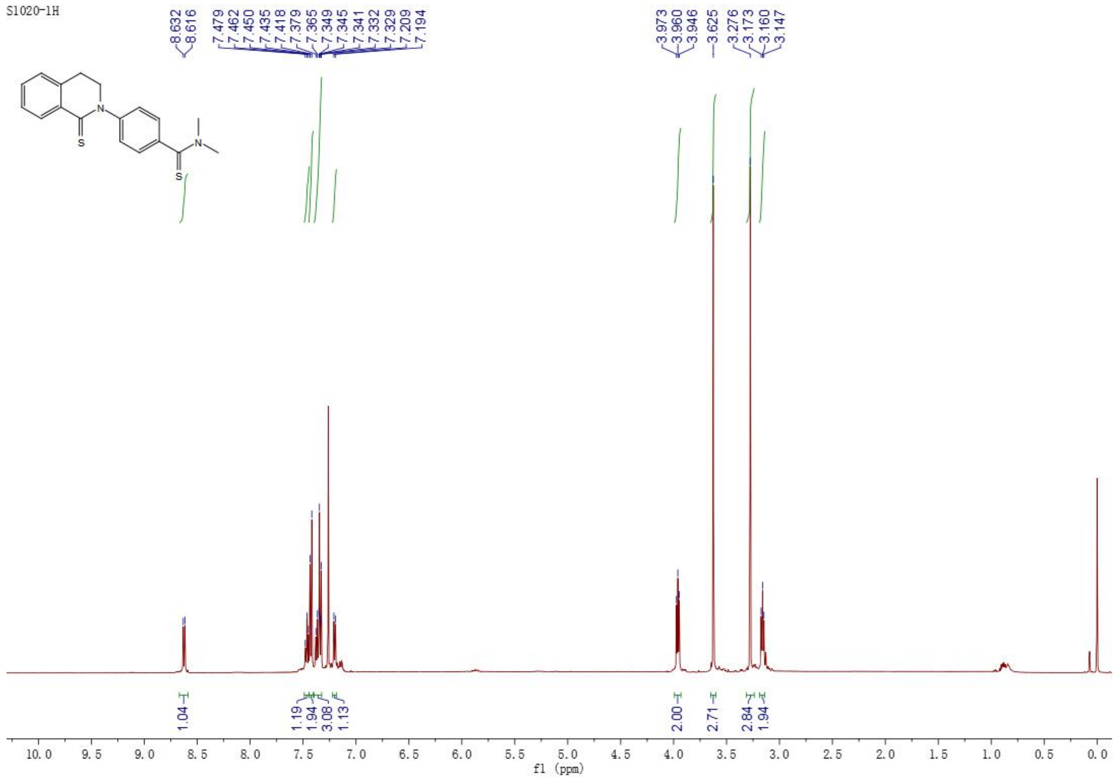

s1036-1C
194.372
191.085
152.449
135.370
133.852
132.909
132.708
132.318
131.190
127.623
127.401
126.844
52.172
28.530
f1 (ppm)

NMR of 1aq

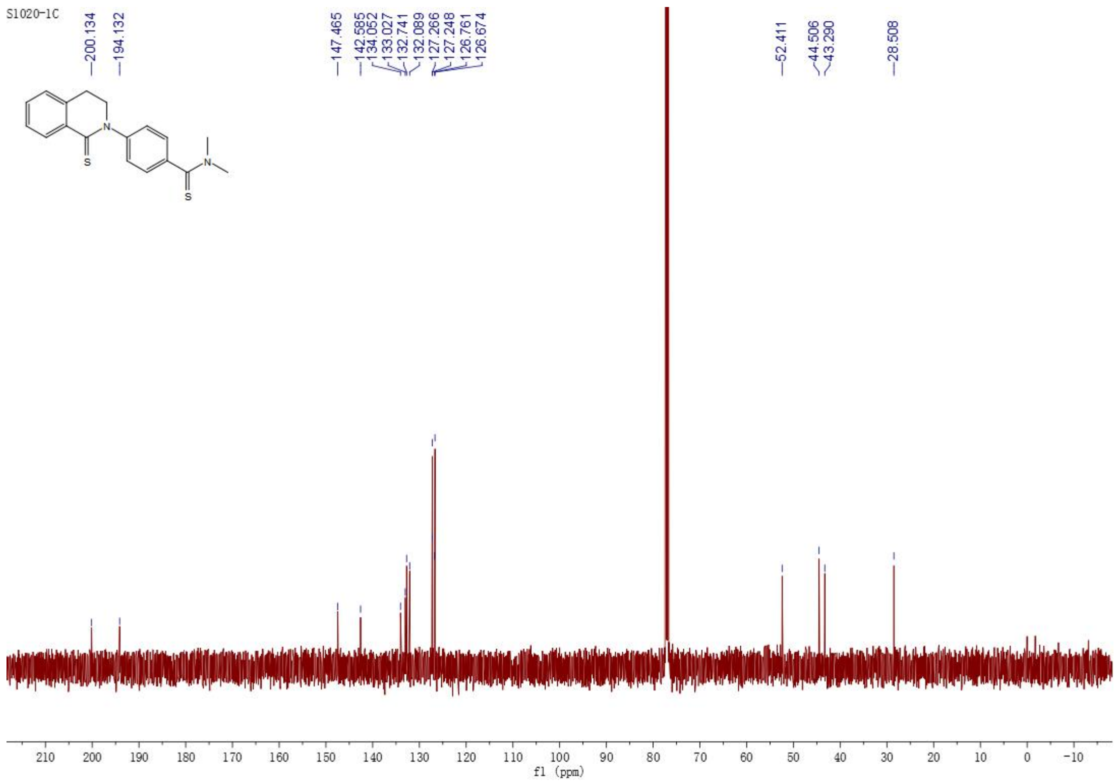

S1031-H
7.337
7.320
7.260
7.205
7.198
7.190
7.173
7.156
6.874
6.857
4.452
3.611
3.599
3.587
3.261
2.993
2.980
2.970
2.17
4.18
2.00
1.89
5.06
3.00
2.34
fl (ppm)


S1031-C
201.859
150.672
134.899
134.046
132.511
128.424
128.258
126.560
126.518
126.223
113.109
49.846
45.609
44.540
43.761
28.964
fl (ppm)

NMR of 2aq

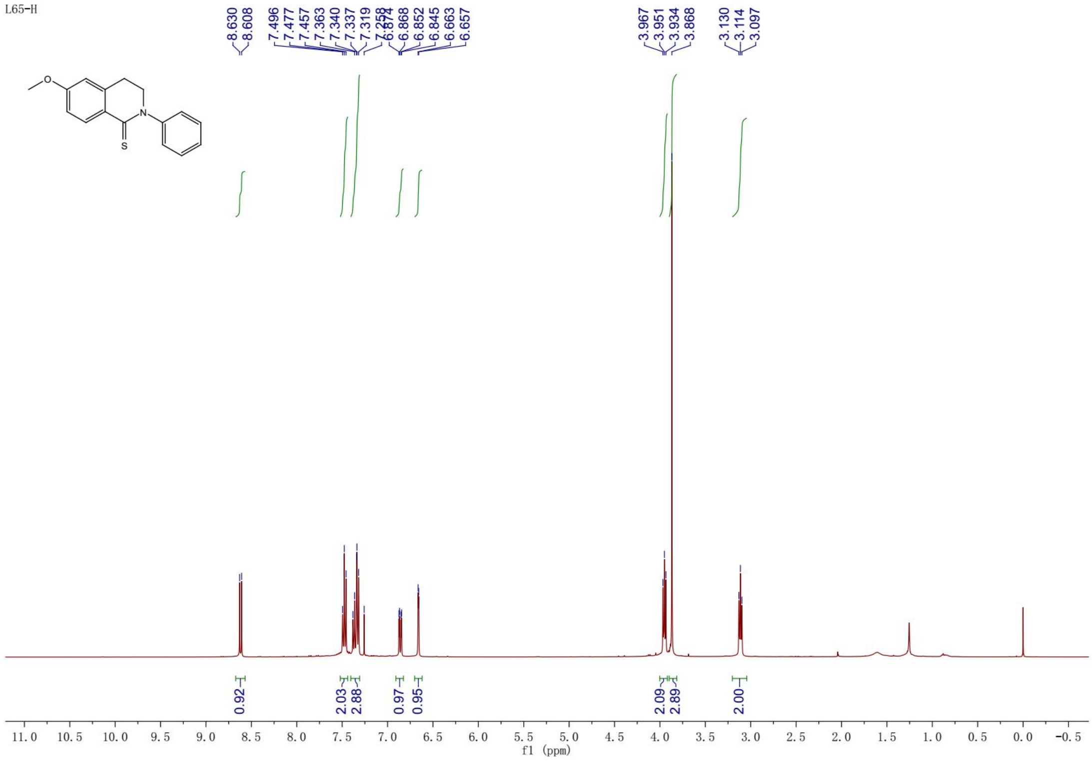


S1020-1H
8.632
8.616
7.479
7.462
7.450
7.435
7.418
7.379
7.365
7.349
7.345
7.341
7.332
7.329
7.209
7.194
3.973
3.960
3.946
3.625
3.276
3.173
3.160
3.147
S
N
S
N
1.04
1.19
1.94
3.08
1.13
2.00
2.71
2.84
1.94
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

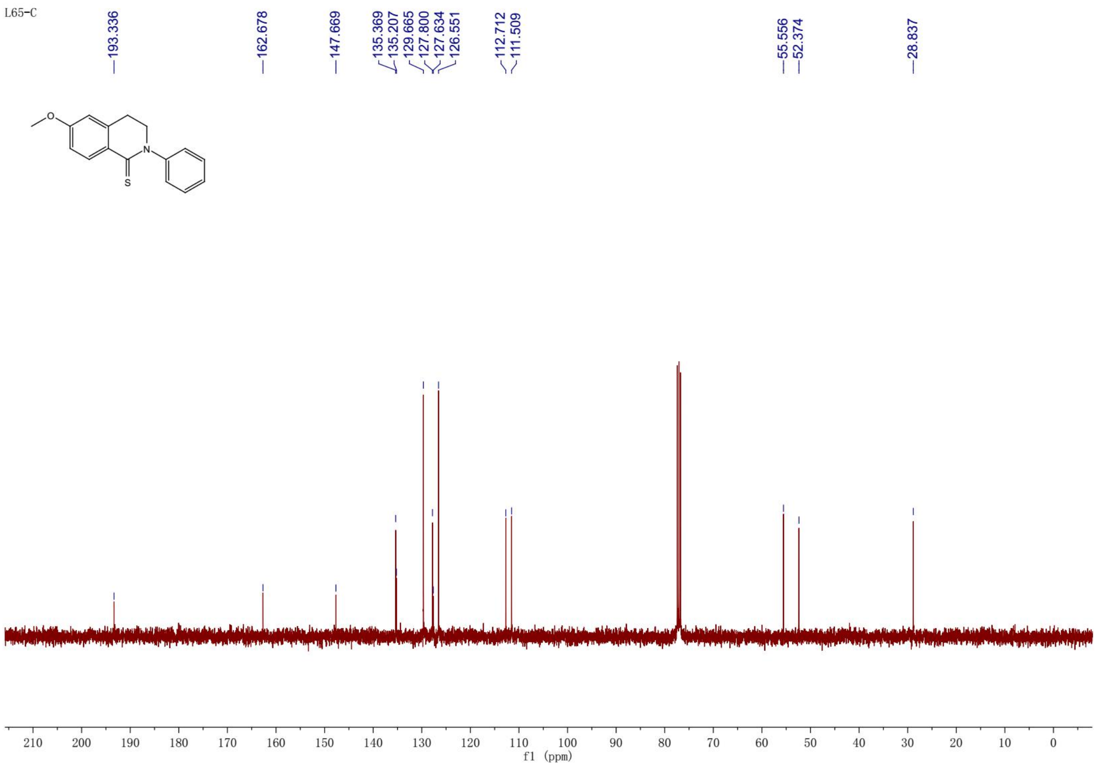


S1020-1C
200.134
194.132
147.465
142.585
134.052
133.027
132.741
132.089
127.266
127.248
126.761
126.674
52.411
44.506
43.290
28.508
S
N
S
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

NMR of 2at

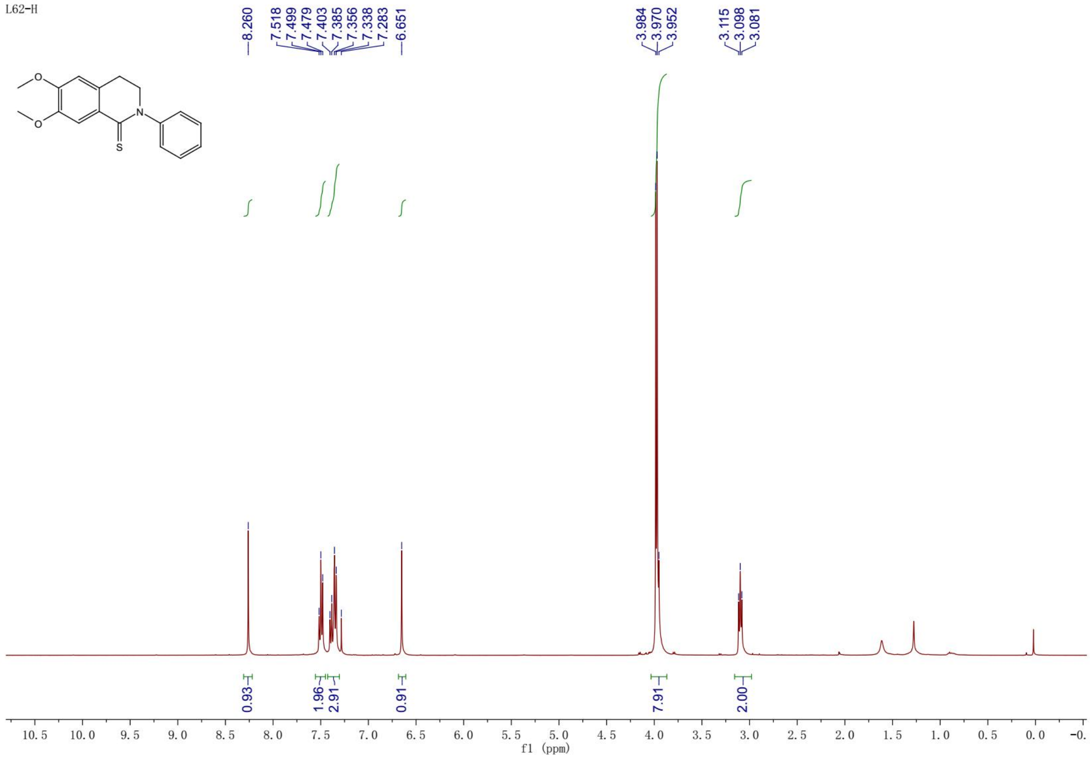


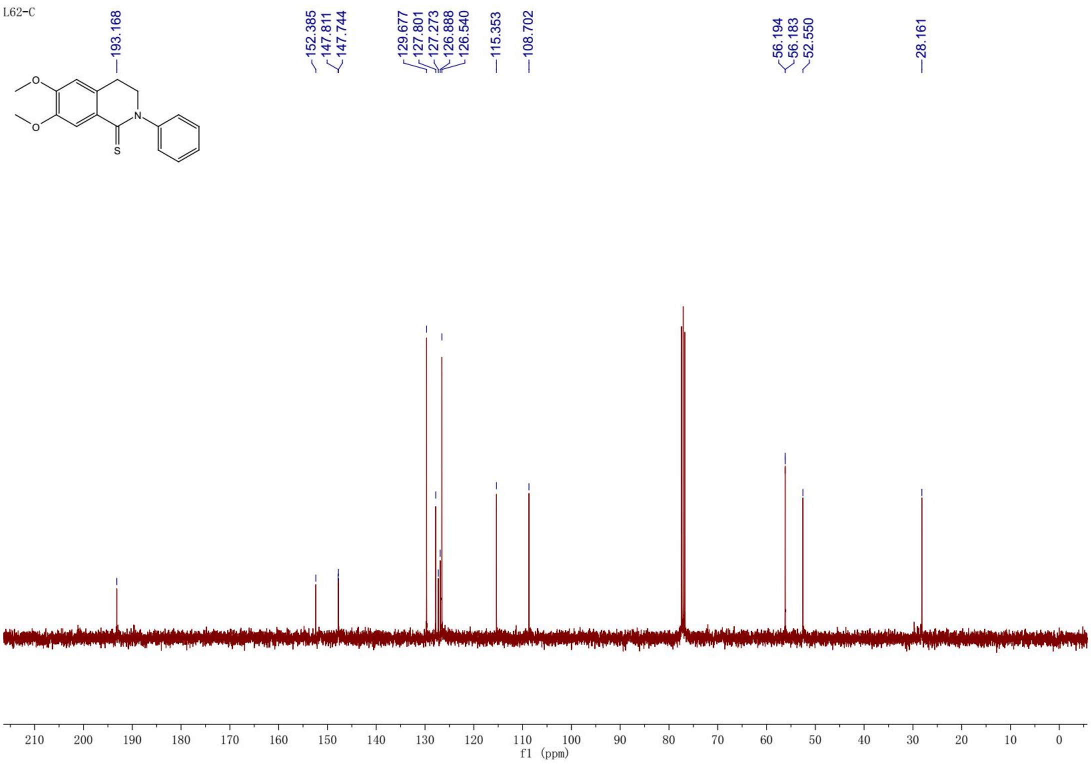
L65-H
8.630
8.608
7.496
7.477
7.457
7.363
7.340
7.337
7.319
7.258
6.874
6.868
6.852
6.845
6.663
6.657
3.967
3.951
3.934
3.868
3.130
3.114
3.097
0.92
2.03
2.88
0.97
0.95
2.09
2.89
2.00
f1 (ppm)



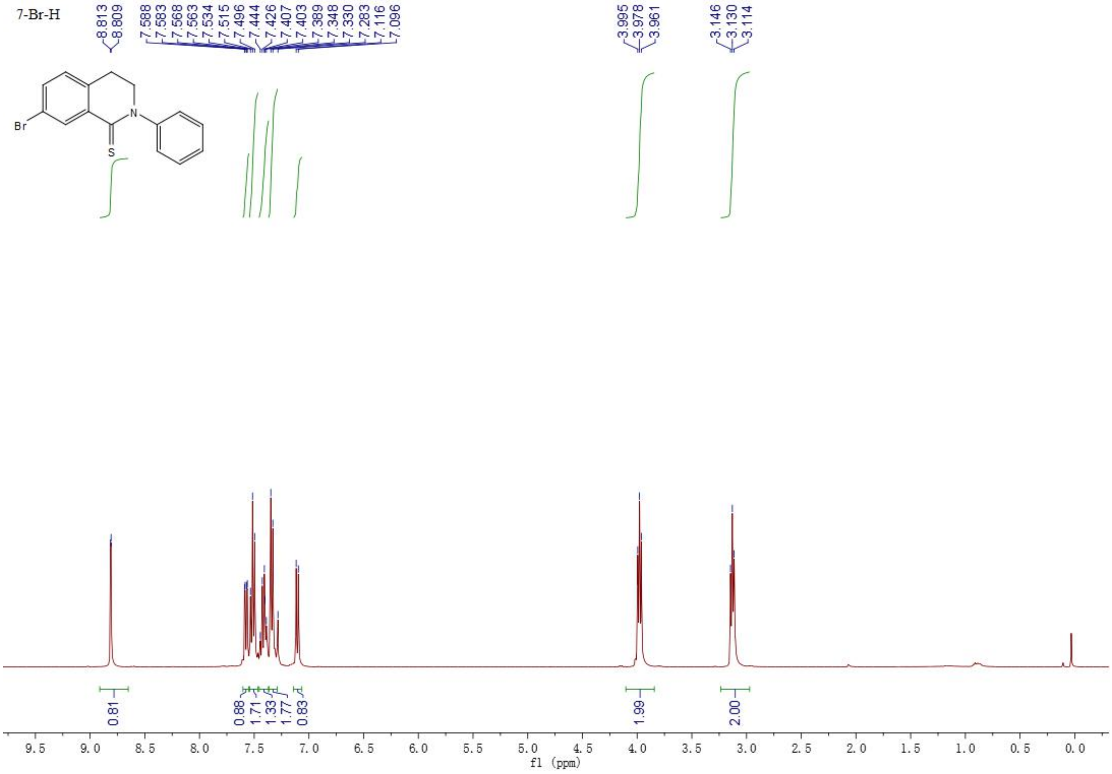
L65-C
193.336
162.678
147.669
135.369
135.207
129.665
127.800
127.634
126.551
112.712
111.509
55.556
52.374
28.837
f1 (ppm)

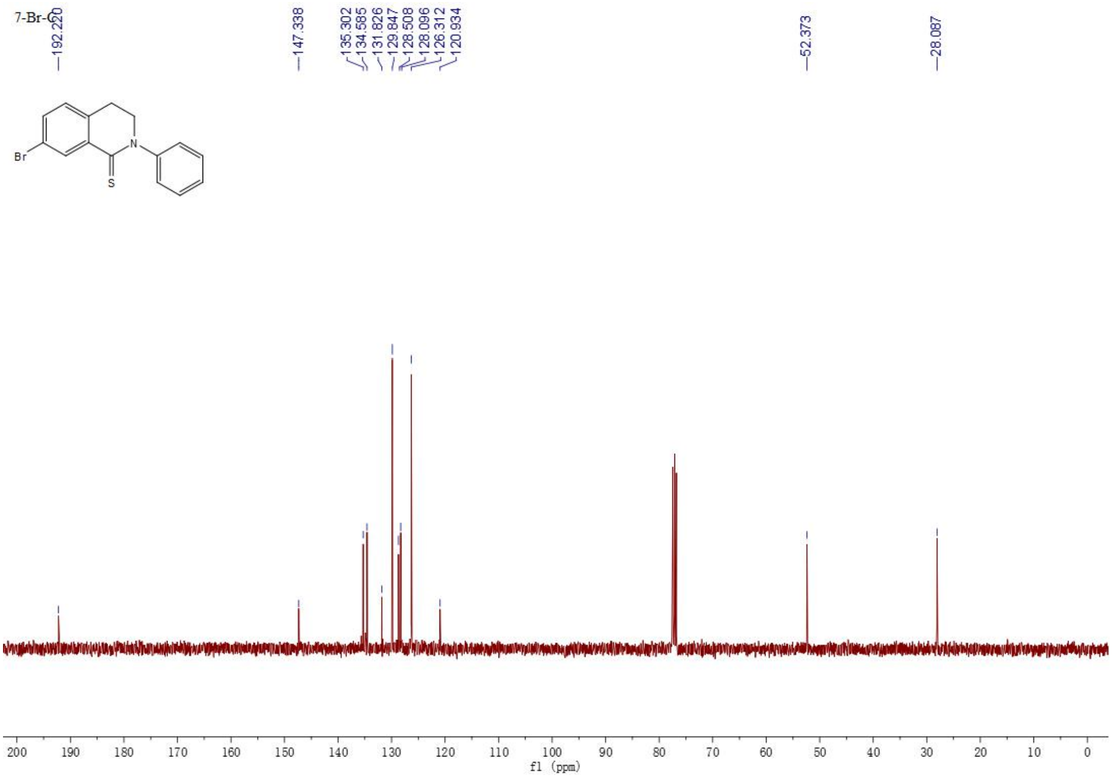
NMR of 2au


L62-H
O
O
N
S
8.260
7.518
7.499
7.479
7.403
7.385
7.356
7.338
7.283
6.651
3.984
3.970
3.952
3.115
3.098
3.081
0.93
1.96
2.91
0.91
7.91
2.00
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.
f1 (ppm)

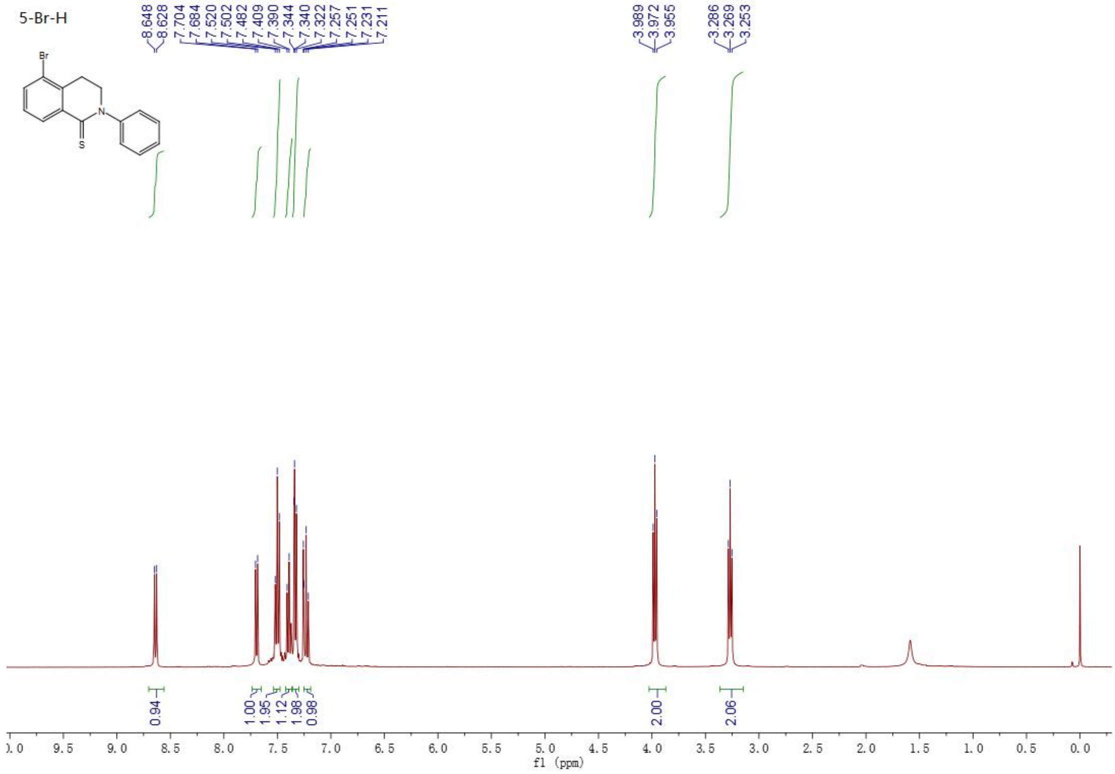

L62-C
O
O
N
S
193.168
152.385
147.811
147.744
129.677
127.801
127.273
126.888
126.540
115.353
108.702
56.194
56.183
52.550
28.161
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

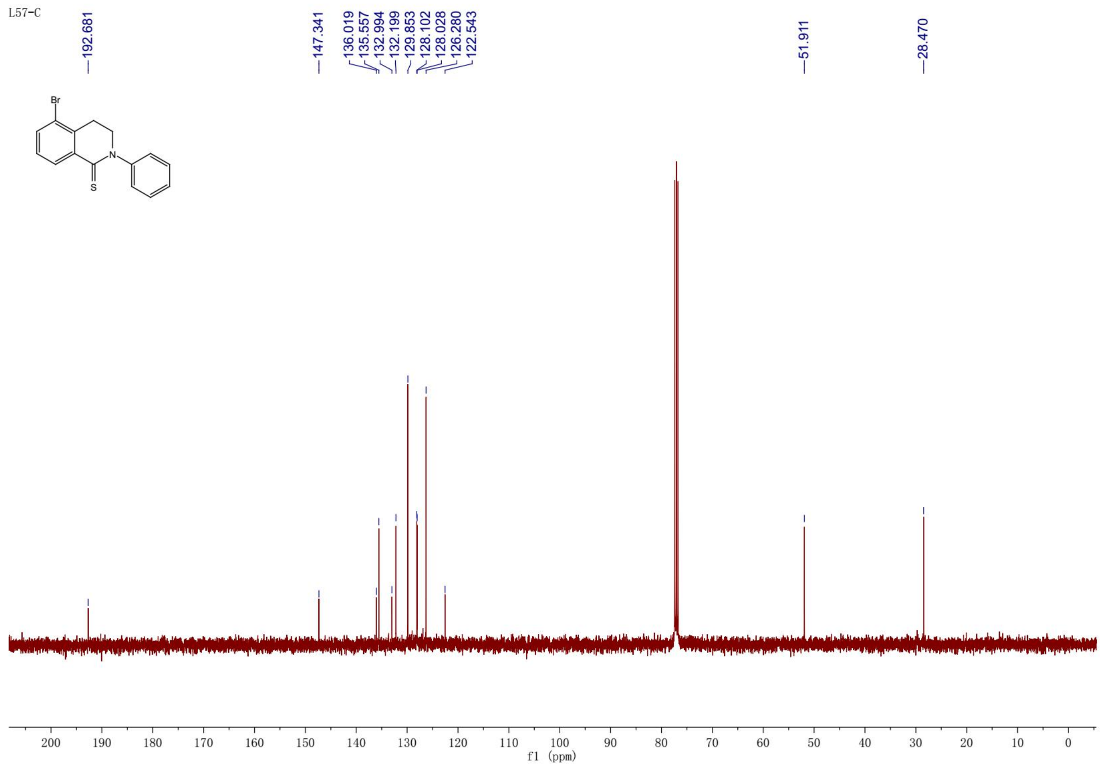
NMR of 2av


7-Br-H
8.813
8.809
7.588
7.583
7.568
7.563
7.534
7.515
7.496
7.444
7.426
7.407
7.403
7.389
7.348
7.330
7.283
7.116
7.096
3.995
3.978
3.961
3.146
3.130
3.114
Br
N
S
0.81
0.88
1.71
1.33
1.77
0.83
1.99
2.00
f1 (ppm)

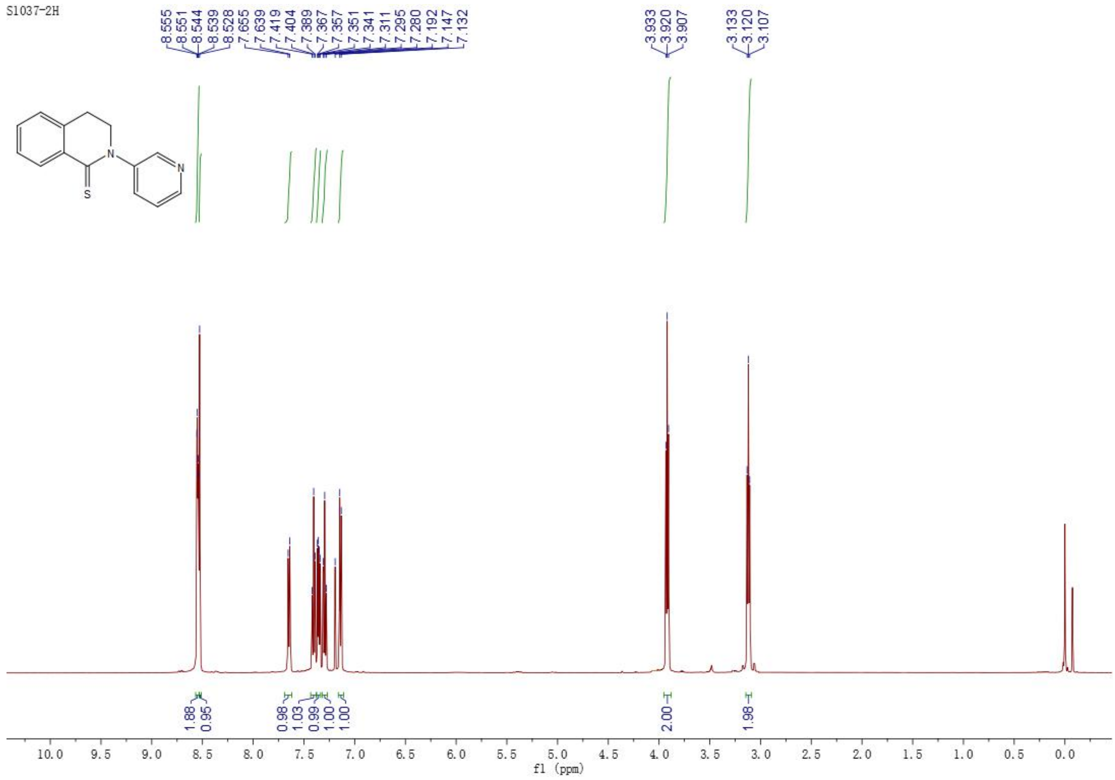

7-Br-C
192.220
147.338
135.302
134.585
131.826
129.847
128.508
128.096
126.312
120.934
52.373
28.087
Br
N
S
f1 (ppm)

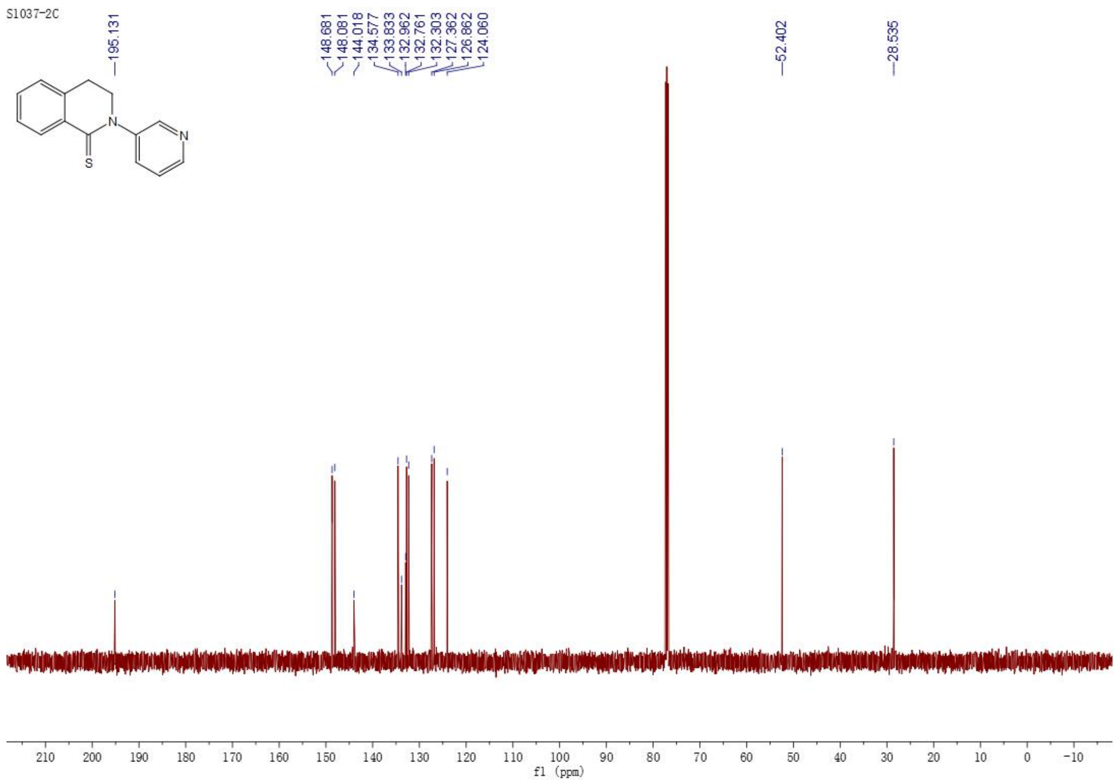
NMR of 2aw


5-Br-H
Br
N
S
8.648
8.628
7.704
7.684
7.520
7.502
7.482
7.409
7.390
7.344
7.340
7.322
7.257
7.251
7.231
7.211
3.989
3.972
3.955
3.286
3.269
3.253
0.94
1.00
1.95
1.12
1.98
0.98
2.00
2.06
f1 (ppm)

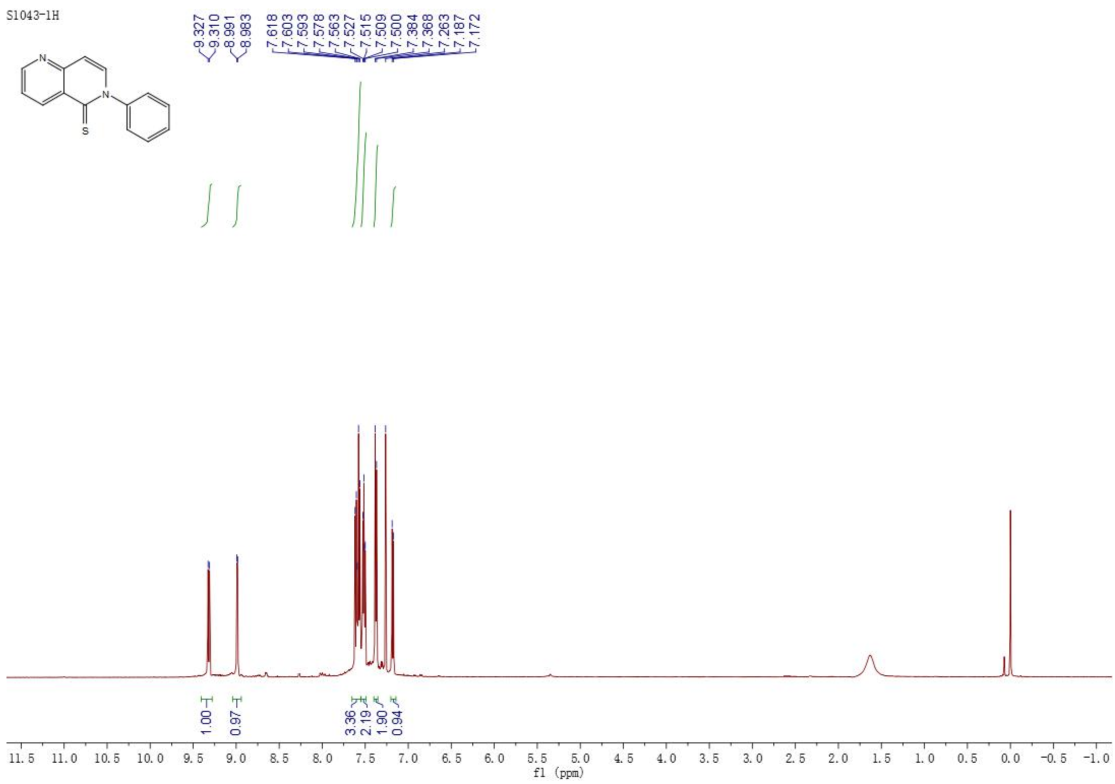

L57-C
192.681
147.341
136.019
135.557
132.994
132.199
129.853
128.102
128.028
126.280
122.543
51.911
28.470
Br
N
S
f1 (ppm)

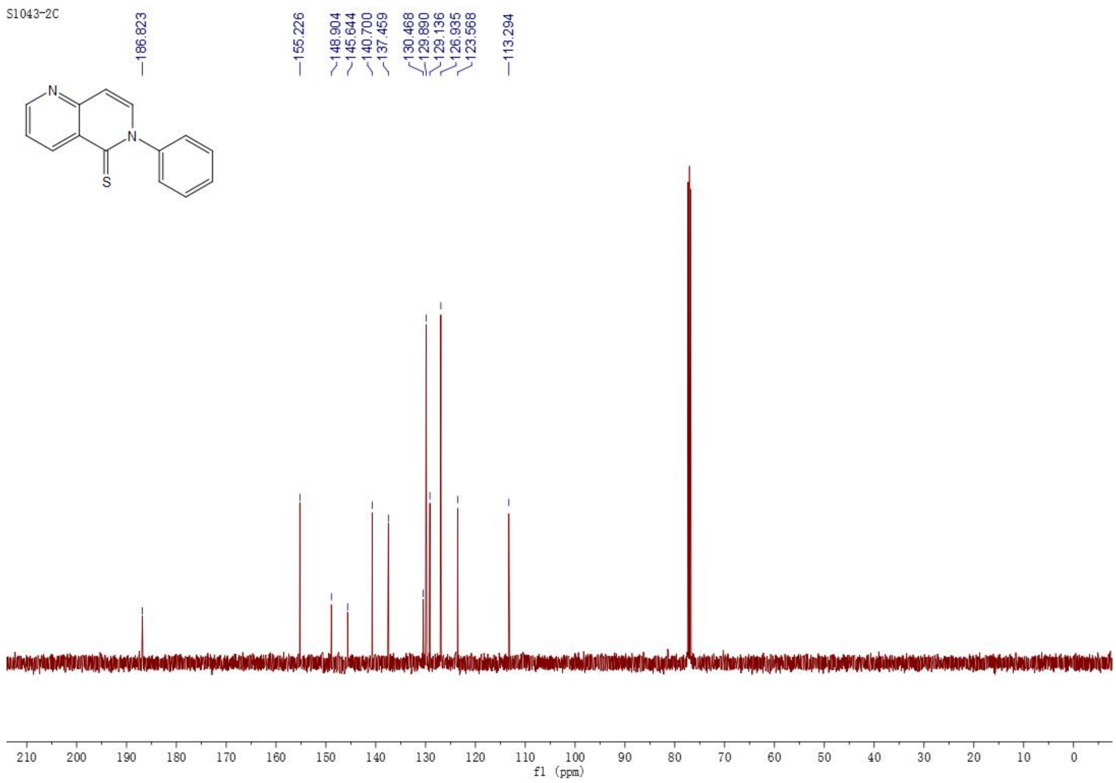
NMR of 2ax


S1037-2H
8.555
8.551
8.544
8.539
8.528
7.655
7.639
7.419
7.404
7.389
7.367
7.357
7.351
7.341
7.311
7.295
7.280
7.192
7.147
7.132
3.933
3.920
3.907
3.133
3.120
3.107
1.88
0.95
0.98
1.03
0.99
1.00
1.00
2.00
1.98
f1 (ppm)


S1037-2C
195.131
148.681
148.081
144.018
134.577
133.833
132.962
132.761
132.303
127.362
126.862
124.060
52.402
28.535
f1 (ppm)

NMR of 2ay


S1043-1H
9.327
9.310
8.991
8.983
7.618
7.603
7.593
7.578
7.563
7.527
7.515
7.509
7.500
7.384
7.368
7.263
7.187
7.172
1.00
0.97
3.36
2.19
1.90
0.94
f1 (ppm)


S1043-2C
186.823
155.226
148.904
145.644
140.700
137.459
130.468
129.890
129.136
126.935
123.568
113.294
f1 (ppm)

8. Molecular Coordinates and Free Energies

1a (1a, DMPU)

ΔG = -635.207575 hartree

C	2.309497	0.706582	0.267491
C	3.664815	0.941671	0.004300
C	4.505241	-0.104909	-0.385629
C	3.986707	-1.396564	-0.527662
C	2.631847	-1.633380	-0.279168
C	1.789825	-0.588631	0.123158
C	1.346785	1.788493	0.680740
C	0.337303	-0.856190	0.453782
N	-0.554078	0.279912	0.188070
C	0.003114	1.614358	-0.034490
C	-4.714281	-0.410882	-0.235545
C	-4.143673	0.800199	-0.641030
C	-2.774516	1.035496	-0.511402
C	-1.913883	0.053716	0.044482
C	-2.504661	-1.170981	0.450444
C	-3.875613	-1.389236	0.308210
H	4.061295	1.949104	0.104674
H	5.555246	0.087589	-0.586461
H	4.630860	-2.213411	-0.839952
H	2.226953	-2.635328	-0.400046
H	1.748880	2.779953	0.450252
H	1.179923	1.753544	1.766649
H	0.264015	-1.153836	1.513897
H	-0.000074	-1.719229	-0.131620
H	0.133994	1.819085	-1.109593
H	-0.701384	2.355353	0.354802
H	-5.780087	-0.587451	-0.341614
H	-4.767647	1.576623	-1.076315
H	-2.374592	1.978259	-0.864238
H	-1.899936	-1.949352	0.899517
H	-4.289954	-2.338744	0.637476

1a (TS1, DMPU)

ΔG = -1055.685229 hartree

C	-2.431627	-1.653696	-0.663572
C	-3.805352	-1.909828	-0.727884
C	-4.643709	-1.693534	0.372638
C	-4.088548	-1.208489	1.567101
C	-2.723920	-0.941839	1.644759
C	-1.867040	-1.155982	0.539978
C	-1.527015	-1.933877	-1.846640
C	-0.444446	-0.792537	0.615589
N	0.383870	-1.342234	-0.425112
C	-0.192301	-1.176879	-1.760308
C	4.352173	-2.703607	0.239722
C	3.954847	-2.240853	-1.019803
C	2.659180	-1.776175	-1.247127
C	1.686987	-1.769661	-0.212349
C	2.107137	-2.238189	1.061763
C	3.408202	-2.690325	1.274015
H	-4.226566	-2.289553	-1.657276
H	-5.707819	-1.899515	0.300821
H	-4.721371	-1.041063	2.435042
H	-2.301107	-0.560409	2.571874
H	-2.031848	-1.670992	-2.784967
H	-1.314329	-3.011251	-1.899726
H	-0.019040	-0.926188	1.605438
H	-0.343107	0.619069	0.546466
H	-0.340068	-0.107319	-1.961031
H	0.486393	-1.572666	-2.513834
H	5.363508	-3.059044	0.410938
H	4.666125	-2.224101	-1.842016
H	2.414135	-1.396095	-2.231620
H	1.402773	-2.276957	1.884672
H	3.681130	-3.049199	2.263475
N	-0.526823	2.367957	-0.845259
C	-1.962507	2.249587	-1.077376
C	-0.163643	2.031664	0.558343
O	-0.895059	2.533643	1.518095
N	1.316519	2.123428	0.690991
C	1.762575	1.767368	2.033870
C	1.852260	3.442026	0.319004
C	1.457840	3.799876	-1.109717
C	-0.055702	3.695809	-1.264921
H	-2.317173	1.268189	-0.755388
H	-2.162683	2.353428	-2.150741
H	-2.551653	3.014777	-0.542456
H	1.365004	0.790460	2.318297
H	1.449119	2.496260	2.801725
H	2.857179	1.707065	2.045322
H	2.944723	3.409201	0.419979
H	1.490400	4.229394	1.011378
H	1.948911	3.113555	-1.811109
H	1.792055	4.816935	-1.347930
H	-0.347256	3.848462	-2.312135
H	-0.544278	4.499202	-0.676796

1a (A, DMPU)

ΔG = -634.588731 hartree

C	2.285372	0.719070	0.242690
C	3.662426	0.913071	0.290069
C	4.555016	-0.134776	0.011320
C	4.047656	-1.403641	-0.320776
C	2.677140	-1.618920	-0.384382
C	1.760574	-0.563338	-0.110230
C	1.286457	1.793659	0.595490
C	0.360672	-0.767979	-0.175979
N	-0.543203	0.270777	-0.073021
C	-0.014412	1.639872	-0.200866
C	-4.710829	-0.472032	0.059224
C	-4.219851	0.718973	-0.485478
C	-2.848231	0.973292	-0.536171

C	-1.928177	0.033012	-0.026271
C	-2.429304	-1.164071	0.529750
C	-3.801796	-1.408994	0.563387
H	4.050334	1.894995	0.553073
H	5.626598	0.035224	0.052185
H	4.730496	-2.221488	-0.534692
H	2.290541	-2.599725	-0.650435
H	1.699182	2.790901	0.410116
H	1.047810	1.742732	1.667842
H	-0.045567	-1.748326	-0.390085
H	0.161014	1.867959	-1.261820
H	-0.760584	2.337605	0.179173
H	-5.778451	-0.665398	0.092143
H	-4.906901	1.457188	-0.889511
H	-2.499601	1.890972	-0.995357
H	-1.747226	-1.886634	0.963784
H	-4.161504	-2.334623	1.004069

1a (B, DMPU)

ΔG = -634.450217 hartree

C	2.288334	0.716761	0.260987
C	3.669958	0.879941	0.293204
C	4.514126	-0.183474	-0.053586
C	3.991198	-1.429889	-0.422707
C	2.613536	-1.615317	-0.447685
C	1.761275	-0.541303	-0.117953
C	1.310555	1.783782	0.687435
C	0.338391	-0.728356	-0.137645
N	-0.515234	0.259944	-0.050933
C	-0.010093	1.667209	-0.066722
C	-4.678116	-0.455005	0.010262
C	-4.155759	0.573986	-0.780027
C	-2.782657	0.821931	-0.800115
C	-1.936174	0.023539	-0.022535
C	-2.447656	-0.999094	0.783804
C	-3.822991	-1.238171	0.790545
H	4.093947	1.835158	0.587401
H	5.589722	-0.037825	-0.032086
H	4.656374	-2.245610	-0.684205
H	2.189272	-2.574531	-0.728316
H	1.718778	2.782507	0.513048
H	1.132401	1.695899	1.767634
H	-0.073627	-1.727268	-0.242793
H	0.107912	1.952590	-1.117646
H	-0.776394	2.294305	0.385262
H	-5.747399	-0.640037	0.023394
H	-4.814951	1.183868	-1.389077
H	-2.381660	1.609005	-1.428828
H	-1.787998	-1.580522	1.419419
H	-4.223289	-2.026391	1.419745

1a (TS3, DMPU)

ΔG = -1829.177645 hartree

C	-2.432778	-1.514398	-0.122316
C	-3.817132	-1.718598	-0.162069
C	-4.707888	-0.659875	0.018239
C	-4.209986	0.628746	0.242464
C	-2.835522	0.846158	0.287387
C	-1.927361	-0.215929	0.106899
C	-1.469262	-2.660396	-0.298633
C	-0.447797	0.042259	0.150967
S	0.096294	1.058120	1.556209
S	1.028342	2.729161	0.448812
S	-0.116263	2.612345	-1.285568
N	0.377926	-1.034892	-0.171284
C	-0.181107	-2.165544	-0.939092
C	4.606403	-0.984999	-0.020945
C	3.933857	-0.099816	-0.866825
C	2.536149	-0.087709	-0.911489
C	1.812223	-0.965984	-0.098267
C	2.482327	-1.863381	0.744308
C	3.877144	-1.868475	0.783685
H	-4.195202	-2.722437	-0.337328
H	-5.778647	-0.836687	-0.017839
H	-4.890611	1.462777	0.383846
H	-2.458147	1.845042	0.471310
H	-1.908600	-3.442018	-0.926018
H	-1.241140	-3.117605	0.673844
H	-0.338924	1.088886	-0.849814
H	-0.364567	-1.834535	-1.972196
H	0.577938	-2.947491	-0.969556
H	5.691688	-0.990099	0.010153
H	4.493523	0.582718	-1.499234
H	2.015339	0.588170	-1.580417
H	1.909528	-2.541188	1.369663
H	4.392764	-2.557674	1.445436

1a (2a, DMPU)

ΔG = -1032.229266 hartree

C	2.283694	-1.007114	-0.122208
C	3.655940	-1.272434	-0.068944
C	4.576052	-0.239801	0.120317
C	4.124762	1.077617	0.258920
C	2.761600	1.355167	0.193185
C	1.825590	0.323495	-0.000833
C	1.267113	-2.101464	-0.316358
C	0.367474	0.629981	-0.103447
S	-0.188752	2.191080	-0.466758
N	-0.478049	-0.404742	0.087461
C	0.005935	-1.757893	0.459873
C	-4.695806	-0.065639	0.080383
C	-4.018296	-0.404061	-1.095663
C	-2.623864	-0.496060	-1.101188
C	-1.912032	-0.239001	0.073356
C	-2.581380	0.090303	1.255138
C	-3.976049	0.178534	1.254729
H	4.002061	-2.297612	-0.168438
H	5.638021	-0.462109	0.167546
H	4.832851	1.885072	0.417764

H	2.403700	2.373243	0.292308
H	1.658550	-3.063224	0.027600
H	1.024855	-2.211410	-1.382433
H	0.193070	-1.783092	1.541552
H	-0.798555	-2.459681	0.238636
H	-5.779427	0.003311	0.082774
H	-4.572969	-0.598251	-2.008702
H	-2.088032	-0.757992	-2.008150
H	-2.014127	0.281218	2.160680
H	-4.498037	0.436669	2.171201

1a (1a, DMF)

ΔG = -635.207599 hartree

C	2.309497	0.706582	0.267491
C	3.664815	0.941671	0.004300
C	4.505241	-0.104909	-0.385629
C	3.986707	-1.396564	-0.527662
C	2.631847	-1.633380	-0.279168
C	1.789825	-0.588631	0.123158
C	1.346785	1.788493	0.680740
C	0.337303	-0.856190	0.453782
N	-0.554078	0.279912	0.188070
C	0.003114	1.614358	-0.034490
C	-4.714281	-0.410882	-0.235545
C	-4.143673	0.800199	-0.641030
C	-2.774516	1.035496	-0.511402
C	-1.913883	0.053716	0.044482
C	-2.504661	-1.170981	0.450444
C	-3.875613	-1.389236	0.308210
H	4.061295	1.949104	0.104674
H	5.555246	0.087589	-0.586461
H	4.630860	-2.213411	-0.839952
H	2.226953	-2.635328	-0.400046
H	1.748880	2.779953	0.450252
H	1.179923	1.753544	1.766649
H	0.264015	-1.153836	1.513897
H	-0.000074	-1.719229	-0.131620
H	0.133994	1.819085	-1.109593
H	-0.701384	2.355353	0.354802
H	-5.780087	-0.587451	-0.341614
H	-4.767647	1.576623	-1.076315
H	-2.374592	1.978259	-0.864238
H	-1.899936	-1.949352	0.899517
H	-4.289954	-2.338744	0.637476

1a (TS1, DMF)

ΔG = -883.669229 hartree

C	1.834459	-1.832918	0.480730
C	3.139312	-2.328895	0.558337
C	4.093528	-2.038084	-0.425145
C	3.724539	-1.230114	-1.512349
C	2.432394	-0.718828	-1.597935
C	1.459372	-1.002079	-0.607965
C	0.789505	-2.194758	1.514015
C	0.129208	-0.390709	-0.699210
N	-0.862755	-0.929106	0.194177
C	-0.339851	-1.163213	1.546844
C	-5.017499	-0.376882	-0.525771
C	-4.567644	-1.159051	0.545942
C	-3.207481	-1.330081	0.795273
C	-2.224041	-0.713579	-0.022251
C	-2.694059	0.080716	-1.099777
C	-4.060823	0.234952	-1.340923
H	3.411462	-2.962027	1.401210
H	5.101865	-2.434242	-0.346985
H	4.447576	-0.999658	-2.290867
H	2.156365	-0.089724	-2.441592
H	1.242442	-2.270377	2.510306
H	0.361613	-3.181721	1.286950
H	-0.232317	-0.323490	-1.724071
H	0.230524	0.997923	-0.428600
H	0.039925	-0.211353	1.949481
H	-1.135213	-1.501717	2.206546
H	-6.078556	-0.249101	-0.716363
H	-5.283980	-1.656012	1.195388
H	-2.913708	-1.971931	1.617524
H	-1.994911	0.603609	-1.739346
H	-4.375155	0.857775	-2.174834
N	1.031855	2.654643	0.872057
C	0.663367	3.864535	1.608854
C	2.438968	2.686110	0.486446
C	0.117335	2.371483	-0.252420
O	0.293043	2.970024	-1.409119
H	-0.386007	3.807958	1.915893
H	0.798326	4.789582	1.015930
H	1.277708	3.953620	2.513467
H	2.698061	3.553028	-0.146804
H	2.691848	1.776732	-0.065562
H	3.062948	2.729579	1.387333
H	-0.912409	2.390967	0.168137

1a (A, DMF)

ΔG = -634.593646 hartree

C	2.285372	0.719070	0.242690
C	3.662426	0.913071	0.290069
C	4.555016	-0.134776	0.011320
C	4.047656	-1.403641	-0.320776
C	2.677140	-1.618920	-0.384382
C	1.760574	-0.563338	-0.110230
C	1.286457	1.793659	0.595490
C	0.360672	-0.767979	-0.175979
N	-0.543203	0.270777	-0.073021
C	-0.014412	1.639872	-0.200866
C	-4.710829	-0.472032	0.059224
C	-4.219851	0.718973	-0.485478
C	-2.848231	0.973292	-0.536171
C	-1.928177	0.033012	-0.026271
C	-2.429304	-1.164071	0.529750
C	-3.801796	-1.408994	0.563387

H	4.050334	1.894995	0.553073
H	5.626598	0.035224	0.052185
H	4.730496	-2.221488	-0.534692
H	2.290541	-2.599725	-0.650435
H	1.699182	2.790901	0.410116
H	1.047810	1.742732	1.667842
H	-0.045567	-1.748326	-0.390085
H	0.161014	1.867959	-1.261820
H	-0.760584	2.337605	0.179173
H	-5.778451	-0.665398	0.092143
H	-4.906901	1.457188	-0.889511
H	-2.499601	1.890972	-0.995357
H	-1.747226	-1.886634	0.963784
H	-4.161504	-2.334623	1.004069

1a (B, DMF)

ΔG = -634.455396 hartree

C	2.288334	0.716761	0.260987
C	3.669958	0.879941	0.293204
C	4.514126	-0.183474	-0.053586
C	3.991198	-1.429889	-0.422707
C	2.613536	-1.615317	-0.447685
C	1.761275	-0.541303	-0.117953
C	1.310555	1.783782	0.687435
C	0.338391	-0.728356	-0.137645
N	-0.515234	0.259944	-0.050933
C	-0.010093	1.667209	-0.066722
C	-4.678116	-0.455005	0.010262
C	-4.155759	0.573986	-0.780027
C	-2.782657	0.821931	-0.800115
C	-1.936174	0.023539	-0.022535
C	-2.447656	-0.999094	0.783804
C	-3.822991	-1.238171	0.790545
H	4.093947	1.835158	0.587401
H	5.589722	-0.037825	-0.032086
H	4.656374	-2.245610	-0.684205
H	2.189272	-2.574531	-0.728316
H	1.718778	2.782507	0.513048
H	1.132401	1.695899	1.767634
H	-0.073627	-1.727268	-0.242793
H	0.107912	1.952590	-1.117646
H	-0.776394	2.294305	0.385262
H	-5.747399	-0.640037	0.023394
H	-4.814951	1.183868	-1.389077
H	-2.381660	1.609005	-1.428828
H	-1.787998	-1.580522	1.419419
H	-4.223289	-2.026391	1.419745

1a (TS3, DMF)

ΔG = -1829.183074 hartree

C	-2.432778	-1.514398	-0.122316
C	-3.817132	-1.718598	-0.162069
C	-4.707888	-0.659875	0.018239
C	-4.209986	0.628746	0.242464
C	-2.835522	0.846158	0.287387
C	-1.927361	-0.215929	0.106899
C	-1.469262	-2.660396	-0.298633
C	-0.447797	0.042259	0.150967
S	0.096294	1.058120	1.556209
S	1.028342	2.729161	0.448812
S	-0.116263	2.612345	-1.285568
N	0.377926	-1.034892	-0.171284
C	-0.181107	-2.165544	-0.939092
C	4.606403	-0.984999	-0.020945
C	3.933857	-0.099816	-0.866825
C	2.536149	-0.087709	-0.911489
C	1.812223	-0.965984	-0.098267
C	2.482327	-1.863381	0.744308
C	3.877144	-1.868475	0.783685
H	-4.195202	-2.722437	-0.337328
H	-5.778647	-0.836687	-0.017839
H	-4.890611	1.462777	0.383846
H	-2.458147	1.845042	0.471310
H	-1.908600	-3.442018	-0.926018
H	-1.241140	-3.117605	0.673844
H	-0.338924	1.088886	-0.849814
H	-0.364567	-1.834535	-1.972196
H	0.577938	-2.947491	-0.969556
H	5.691688	-0.990099	0.010153
H	4.493523	0.582718	-1.499234
H	2.015339	0.588170	-1.580417
H	1.909528	-2.541188	1.369663
H	4.392764	-2.557674	1.445436

1a (2a, DMF)

ΔG = -1032.229317 hartree

C	2.283694	-1.007114	-0.122208
C	3.655940	-1.272434	-0.068944
C	4.576052	-0.239801	0.120317
C	4.124762	1.077617	0.258920
C	2.761600	1.355167	0.193185
C	1.825590	0.323495	-0.000833
C	1.267113	-2.101464	-0.316358
C	0.367474	0.629981	-0.103447
S	-0.188752	2.191080	-0.466758
N	-0.478049	-0.404742	0.087461
C	0.005935	-1.757893	0.459873
C	-4.695806	-0.065639	0.080383
C	-4.018296	-0.404061	-1.095663
C	-2.623864	-0.496060	-1.101188
C	-1.912032	-0.239001	0.073356
C	-2.581380	0.090303	1.255138
C	-3.976049	0.178534	1.254729
H	4.002061	-2.297612	-0.168438
H	5.638021	-0.462109	0.167546
H	4.832851	1.885072	0.417764
H	2.403700	2.373243	0.292308
H	1.658550	-3.063224	0.027600
H	1.024855	-2.211410	-1.382433

H	0.193070	-1.783092	1.541552
H	-0.798555	-2.459681	0.238636
H	-5.779427	0.003311	0.082774
H	-4.572969	-0.598251	-2.008702
H	-2.088032	-0.757992	-2.008150
H	-2.014127	0.281218	2.160680
H	-4.498037	0.436669	2.171201

1a (1a, DMA)

ΔG = -635.207605 hartree

C	2.309497	0.706582	0.267491
C	3.664815	0.941671	0.004300
C	4.505241	-0.104909	-0.385629
C	3.986707	-1.396564	-0.527662
C	2.631847	-1.633380	-0.279168
C	1.789825	-0.588631	0.123158
C	1.346785	1.788493	0.680740
C	0.337303	-0.856190	0.453782
N	-0.554078	0.279912	0.188070
C	0.003114	1.614358	-0.034490
C	-4.714281	-0.410882	-0.235545
C	-4.143673	0.800199	-0.641030
C	-2.774516	1.035496	-0.511402
C	-1.913883	0.053716	0.044482
C	-2.504661	-1.170981	0.450444
C	-3.875613	-1.389236	0.308210
H	4.061295	1.949104	0.104674
H	5.555246	0.087589	-0.586461
H	4.630860	-2.213411	-0.839952
H	2.226953	-2.635328	-0.400046
H	1.748880	2.779953	0.450252
H	1.179923	1.753544	1.766649
H	0.264015	-1.153836	1.513897
H	-0.000074	-1.719229	-0.131620
H	0.133994	1.819085	-1.109593
H	-0.701384	2.355353	0.354802
H	-5.780087	-0.587451	-0.341614
H	-4.767647	1.576623	-1.076315
H	-2.374592	1.978259	-0.864238
H	-1.899936	-1.949352	0.899517
H	-4.289954	-2.338744	0.637476

1a (TS1, DMA)

ΔG = -922.964703 hartree

C	1.989514	-1.708532	0.663298
C	3.309536	-2.156418	0.772865
C	4.218007	-2.026466	-0.285309
C	3.786261	-1.434697	-1.483114
C	2.477664	-0.975023	-1.604670
C	1.551280	-1.096106	-0.540681
C	0.998438	-1.905680	1.789962
C	0.207100	-0.523311	-0.653558
N	-0.742814	-0.958098	0.340485
C	-0.199141	-0.948747	1.699826
C	-4.923888	-0.999866	-0.412576
C	-4.432133	-0.725604	0.867851
C	-3.060404	-0.688177	1.125099
C	-2.113999	-0.944254	0.100620
C	-2.628169	-1.216419	-1.194814
C	-3.999870	-1.240695	-1.437614
H	3.631687	-2.620928	1.703409
H	5.239320	-2.380783	-0.179367
H	4.472669	-1.333485	-2.320106
H	2.154189	-0.512242	-2.534263
H	1.490154	-1.775101	2.762068
H	0.619130	-2.937382	1.769433
H	-0.196345	-0.549448	-1.662231
H	0.314850	0.885274	-0.554239
H	0.101771	0.072064	1.977914
H	-0.962008	-1.279912	2.403242
H	-5.991581	-1.021913	-0.607743
H	-5.121699	-0.519987	1.682894
H	-2.730947	-0.436002	2.125800
H	-1.950735	-1.438950	-2.011250
H	-4.349354	-1.463164	-2.442862
N	0.643236	2.686645	0.738710
C	0.379141	4.098359	1.036237
C	2.034267	2.369569	1.051730
C	0.279010	2.291559	-0.653172
O	1.087462	2.650787	-1.625625
H	-0.676601	4.336416	0.881459
H	0.983058	4.791195	0.419756
H	0.614984	4.298323	2.088487
H	2.756621	2.982868	0.484340
H	2.235693	1.318889	0.828391
H	2.214543	2.536258	2.120815
C	-1.217276	2.507057	-0.919729
H	-1.430492	3.562741	-1.144695
H	-1.511693	1.923856	-1.798810
H	-1.841895	2.195998	-0.075306

1a (A, DMA)

ΔG = -634.593650 hartree

C	2.285347	0.719027	0.242671
C	3.662428	0.912911	0.289971
C	4.554967	-0.134953	0.011139
C	4.047486	-1.403776	-0.320992
C	2.676964	-1.618954	-0.384496
C	1.760456	-0.563353	-0.110241
C	1.286602	1.793786	0.595521
C	0.360522	-0.767880	-0.175855
N	-0.543189	0.270969	-0.072512
C	-0.014405	1.639997	-0.200615
C	-4.710681	-0.472204	0.058972
C	-4.219790	0.718746	-0.485923
C	-2.848198	0.973251	-0.536420
C	-1.928205	0.033201	-0.026041
C	-2.429207	-1.163839	0.530137
C	-3.801655	-1.408967	0.563530

H	4.050395	1.894825	0.552993
H	5.626560	0.034989	0.051959
H	4.730245	-2.221679	-0.535008
H	2.290263	-2.599723	-0.650581
H	1.699413	2.790958	0.409922
H	1.048116	1.743084	1.667931
H	-0.045920	-1.748191	-0.389831
H	0.160997	1.867976	-1.261631
H	-0.760497	2.337867	0.179357
H	-5.778289	-0.665721	0.091716
H	-4.906904	1.456723	-0.890295
H	-2.499502	1.890831	-0.995768
H	-1.746949	-1.886144	0.964354
H	-4.161388	-2.334541	1.004321

1a (B, DMA)

ΔG = -634.455420 hartree

C	2.288312	0.716696	0.261051
C	3.669955	0.879841	0.293250
C	4.514092	-0.183547	-0.053665
C	3.991142	-1.429920	-0.422900
C	2.613475	-1.615327	-0.447834
C	1.761257	-0.541326	-0.117976
C	1.310595	1.783726	0.687634
C	0.338327	-0.728360	-0.137642
N	-0.515200	0.259979	-0.050927
C	-0.010108	1.667257	-0.066456
C	-4.678067	-0.454942	0.010300
C	-4.155565	0.572908	-0.781393
C	-2.782459	0.820835	-0.801550
C	-1.936198	0.023576	-0.022586
C	-2.447772	-0.997917	0.785089
C	-3.823124	-1.236994	0.791888
H	4.093961	1.835029	0.587521
H	5.589690	-0.037916	-0.032177
H	4.656298	-2.245621	-0.684519
H	2.189157	-2.574486	-0.728564
H	1.718848	2.782441	0.513263
H	1.132516	1.695774	1.767837
H	-0.073720	-1.727265	-0.242783
H	0.107844	1.952869	-1.117320
H	-0.776422	2.294230	0.385687
H	-5.747351	-0.639974	0.023459
H	-4.814639	1.181862	-1.391500
H	-2.381251	1.606955	-1.431324
H	-1.788143	-1.578450	1.421544
H	-4.223559	-2.024327	1.422111

1a (TS3, DMA)

ΔG = -1829.179411 hartree

C	-2.433012	-1.514161	-0.122341
C	-3.817385	-1.718197	-0.162148
C	-4.708018	-0.659383	0.018223
C	-4.209962	0.629153	0.242562
C	-2.835473	0.846401	0.287526
C	-1.927427	-0.215773	0.106974
C	-1.469646	-2.660278	-0.298661
C	-0.447831	0.042270	0.151022
S	0.096539	1.058076	1.556188
S	1.028945	2.728774	0.448682
S	-0.115974	2.612214	-1.285496
N	0.377753	-1.035030	-0.171204
C	-0.181386	-2.165587	-0.939048
C	4.606219	-0.985022	-0.021055
C	3.933582	-0.099959	-0.866987
C	2.535874	-0.087933	-0.911562
C	1.812047	-0.966127	-0.098160
C	2.482237	-1.863442	0.744419
C	3.877057	-1.868467	0.783694
H	-4.195575	-2.721978	-0.337488
H	-5.778798	-0.836062	-0.017895
H	-4.890487	1.463258	0.383991
H	-2.457984	1.845233	0.471495
H	-1.909070	-3.441838	-0.926067
H	-1.241620	-3.117526	0.673823
H	-0.338856	1.088804	-0.849843
H	-0.364749	-1.834565	-1.972168
H	0.577551	-2.947643	-0.969461
H	5.691505	-0.990051	0.009994
H	4.493178	0.582550	-1.499485
H	2.014958	0.587826	-1.580540
H	1.909511	-2.541223	1.369866
H	4.392759	-2.557580	1.445473

1a (2a, DMA)

ΔG = -1032.229330 hartree

C	2.283596	-1.007150	-0.122118
C	3.655810	-1.272620	-0.068912
C	4.576066	-0.240064	0.120183
C	4.124946	1.077423	0.258620
C	2.761810	1.355106	0.192977
C	1.825639	0.323502	-0.000743
C	1.266951	-2.101459	-0.316227
C	0.367521	0.630305	-0.103125
S	-0.188581	2.191171	-0.466482
N	-0.478083	-0.404708	0.087357
C	0.005817	-1.757666	0.459998
C	-4.695882	-0.065725	0.080258
C	-4.018321	-0.404053	-1.095790
C	-2.623882	-0.496002	-1.101279
C	-1.912028	-0.238879	0.073248
C	-2.581478	0.090307	1.255029
C	-3.976143	0.178494	1.254615
H	4.001794	-2.297849	-0.168347
H	5.638009	-0.462483	0.167416
H	4.833134	1.884829	0.417312
H	2.403990	2.373228	0.291973
H	1.658323	-3.063230	0.027768
H	1.024677	-2.211410	-1.382303

H	0.193073	-1.782744	1.541681
H	-0.798665	-2.459549	0.238993
H	-5.779523	0.002946	0.082681
H	-4.572974	-0.598391	-2.008811
H	-2.088066	-0.757952	-2.008254
H	-2.014263	0.281227	2.160598
H	-4.498153	0.436491	2.171115

1a (1a, Acetone)

ΔG = -635.207297 hartree

C	2.309497	0.706582	0.267491
C	3.664815	0.941671	0.004300
C	4.505241	-0.104909	-0.385629
C	3.986707	-1.396564	-0.527662
C	2.631847	-1.633380	-0.279168
C	1.789825	-0.588631	0.123158
C	1.346785	1.788493	0.680740
C	0.337303	-0.856190	0.453782
N	-0.554078	0.279912	0.188070
C	0.003114	1.614358	-0.034490
C	-4.714281	-0.410882	-0.235545
C	-4.143673	0.800199	-0.641030
C	-2.774516	1.035496	-0.511402
C	-1.913883	0.053716	0.044482
C	-2.504661	-1.170981	0.450444
C	-3.875613	-1.389236	0.308210
H	4.061295	1.949104	0.104674
H	5.555246	0.087589	-0.586461
H	4.630860	-2.213411	-0.839952
H	2.226953	-2.635328	-0.400046
H	1.748880	2.779953	0.450252
H	1.179923	1.753544	1.766649
H	0.264015	-1.153836	1.513897
H	-0.000074	-1.719229	-0.131620
H	0.133994	1.819085	-1.109593
H	-0.701384	2.355353	0.354802
H	-5.780087	-0.587451	-0.341614
H	-4.767647	1.576623	-1.076315
H	-2.374592	1.978259	-0.864238
H	-1.899936	-1.949352	0.899517
H	-4.289954	-2.338744	0.637476

1a (TS1, Acetone)

ΔG = -828.332790 hartree

C	-2.179325	-1.388959	-0.412084
C	-3.535611	-1.721272	-0.466486
C	-4.462728	-1.165009	0.425068
C	-4.010681	-0.257279	1.396500
C	-2.664660	0.092110	1.457012
C	-1.719194	-0.456632	0.555318
C	-1.171191	-2.038755	-1.333783
C	-0.328652	-0.002093	0.573096
N	0.610496	-0.800027	-0.176363
C	0.110607	-1.209071	-1.488672
C	4.771873	-0.712383	0.684948
C	4.318877	-0.885917	-0.626617
C	2.955450	-0.894320	-0.927541
C	1.978657	-0.745076	0.088929
C	2.453789	-0.563806	1.414318
C	3.817875	-0.548192	1.697263
H	-3.872710	-2.434411	-1.217068
H	-5.512812	-1.436541	0.366563
H	-4.711394	0.176271	2.105821
H	-2.324591	0.798092	2.211257
H	-1.608421	-2.209782	-2.325291
H	-0.895319	-3.027507	-0.940192
H	0.034627	0.263065	1.562140
H	-0.303662	1.314373	0.052424
H	-0.080305	-0.326788	-2.120284
H	0.860318	-1.820277	-1.989681
H	5.833430	-0.700106	0.911904
H	5.033060	-1.000700	-1.438285
H	2.659074	-0.995910	-1.964442
H	1.751745	-0.462365	2.233644
H	4.136607	-0.415643	2.728206
C	-1.343352	2.698344	-1.398210
C	-0.267965	2.663643	-0.300190
O	-0.528910	3.382940	0.779744
C	1.154198	2.811621	-0.863750
H	1.297309	3.833243	-1.254930
H	1.360728	2.106908	-1.678788
H	1.895514	2.652047	-0.072860
H	-1.401025	3.708511	-1.837938
H	-2.325799	2.462182	-0.975290
H	-1.136369	1.990291	-2.211042

1a (A, Acetone)

ΔG = -634.578369 hartree

C	2.285314	0.718915	0.242851
C	3.662304	0.912975	0.290350
C	4.554938	-0.134662	0.011384
C	4.047668	-1.403386	-0.321119
C	2.677239	-1.618704	-0.384790
C	1.760613	-0.563374	-0.110315
C	1.286361	1.793416	0.595749
C	0.360731	-0.768020	-0.176094
N	-0.543189	0.270696	-0.072817
C	-0.014446	1.639649	-0.200742
C	-4.710743	-0.471941	0.059186
C	-4.219743	0.718673	-0.486165
C	-2.848161	0.972965	-0.536807
C	-1.928198	0.033019	-0.026252
C	-2.429358	-1.163689	0.530378
C	-3.801803	-1.408557	0.564007
H	4.050150	1.894876	0.553626
H	5.626498	0.035398	0.052338
H	4.730555	-2.221132	-0.535287
H	2.290683	-2.599432	-0.651199
H	1.699128	2.790703	0.410460

H	1.047614	1.742388	1.668090
H	-0.045571	-1.748256	-0.390583
H	0.161185	1.867695	-1.261730
H	-0.760812	2.337291	0.179199
H	-5.778371	-0.665296	0.092098
H	-4.906795	1.456559	-0.890817
H	-2.499397	1.890289	-0.996622
H	-1.747219	-1.885780	0.965111
H	-4.161624	-2.333850	1.005310

1a (B, Acetone)

ΔG = -634.453850 hartree

C	2.288483	0.716319	0.261567
C	3.670002	0.880022	0.291728
C	4.514062	-0.183152	-0.056135
C	3.991068	-1.429845	-0.424140
C	2.613492	-1.615807	-0.447044
C	1.761203	-0.542014	-0.116435
C	1.310931	1.783183	0.688989
C	0.338384	-0.728905	-0.135498
N	-0.515178	0.259648	-0.049432
C	-0.009996	1.666905	-0.064789
C	-4.678143	-0.454159	0.008656
C	-4.154341	0.570325	-0.786502
C	-2.781183	0.817899	-0.805708
C	-1.936334	0.023649	-0.022164
C	-2.449204	-0.994492	0.788812
C	-3.824598	-1.233255	0.794644
H	4.094068	1.835499	0.584981
H	5.589622	-0.037071	-0.036373
H	4.656186	-2.245323	-0.686499
H	2.189402	-2.575343	-0.726902
H	1.719236	2.781984	0.515137
H	1.133150	1.694893	1.769253
H	-0.074170	-1.727742	-0.240208
H	0.107561	1.953056	-1.115587
H	-0.776322	2.293721	0.387656
H	-5.747469	-0.638897	0.021036
H	-4.812476	1.176807	-1.400054
H	-2.378794	1.601149	-1.438356
H	-1.790495	-1.572402	1.428600
H	-4.226215	-2.017899	1.427446

1a (TS3, Acetone)

ΔG = -1829.156241 hartree

C	-2.433812	-1.513617	-0.121957
C	-3.818195	-1.717048	-0.162874
C	-4.708453	-0.657753	0.016355
C	-4.209906	0.630548	0.240684
C	-2.835403	0.847238	0.286728
C	-1.927661	-0.215384	0.107157
C	-1.470796	-2.660294	-0.296913
C	-0.448124	0.042098	0.151697
S	0.096195	1.058634	1.556500
S	1.032196	2.725696	0.448305
S	-0.115804	2.612787	-1.283731
N	0.377207	-1.035959	-0.169318
C	-0.182010	-2.166432	-0.936946
C	4.605885	-0.984662	-0.023428
C	3.932200	-0.099975	-0.868818
C	2.534465	-0.088347	-0.912127
C	1.811582	-0.966512	-0.097905
C	2.482936	-1.863211	0.744376
C	3.877746	-1.868026	0.782284
H	-4.196762	-2.720732	-0.338108
H	-5.779300	-0.833907	-0.020592
H	-4.890111	1.465055	0.381268
H	-2.457561	1.845920	0.470677
H	-1.910296	-3.442283	-0.923810
H	-1.243314	-3.116785	0.676097
H	-0.339054	1.089657	-0.850026
H	-0.365020	-1.836185	-1.970435
H	0.576632	-2.948866	-0.966721
H	5.691206	-0.989206	0.006777
H	4.490943	0.582931	-1.501633
H	2.012880	0.587528	-1.580457
H	1.910931	-2.540461	1.371081
H	4.394266	-2.556562	1.444048

1a (2a, Acetone)

ΔG = -1032.228691 hartree

C	2.284049	-1.006947	-0.121728
C	3.656328	-1.272036	-0.068194
C	4.576218	-0.239133	0.120406
C	4.124574	1.078236	0.257931
C	2.761372	1.355513	0.191986
C	1.825596	0.323585	-0.001199
C	1.267675	-2.101685	-0.315336
C	0.367352	0.629922	-0.103854
S	-0.189437	2.190262	-0.466477
N	-0.478056	-0.405312	0.087147
C	0.006200	-1.757941	0.460497
C	-4.695738	-0.065606	0.080527
C	-4.018525	-0.405207	-1.095282
C	-2.624145	-0.497229	-1.101003
C	-1.911998	-0.239423	0.073143
C	-2.581101	0.091556	1.254538
C	-3.975715	0.179851	1.254375
H	4.002691	-2.297219	-0.167140
H	5.638256	-0.461160	0.167708
H	4.832486	1.886015	0.415938
H	2.403069	2.373571	0.289810
H	1.659393	-3.063222	0.029120
H	1.025463	-2.212271	-1.381384
H	0.193509	-1.782710	1.542215
H	-0.798139	-2.460142	0.239776
H	-5.779326	0.003964	0.082942
H	-4.573380	-0.599537	-2.008189
H	-2.088450	-0.759003	-2.008083

H	-2.013585	0.284286	2.159523
H	-4.497448	0.439687	2.170519

1a (1a, CH_3CN)

ΔG = -635.207583 hartree

C	2.309497	0.706582	0.267491
C	3.664815	0.941671	0.004300
C	4.505241	-0.104909	-0.385629
C	3.986707	-1.396564	-0.527662
C	2.631847	-1.633380	-0.279168
C	1.789825	-0.588631	0.123158
C	1.346785	1.788493	0.680740
C	0.337303	-0.856190	0.453782
N	-0.554078	0.279912	0.188070
C	0.003114	1.614358	-0.034490
C	-4.714281	-0.410882	-0.235545
C	-4.143673	0.800199	-0.641030
C	-2.774516	1.035496	-0.511402
C	-1.913883	0.053716	0.044482
C	-2.504661	-1.170981	0.450444
C	-3.875613	-1.389236	0.308210
H	4.061295	1.949104	0.104674
H	5.555246	0.087589	-0.586461
H	4.630860	-2.213411	-0.839952
H	2.226953	-2.635328	-0.400046
H	1.748880	2.779953	0.450252
H	1.179923	1.753544	1.766649
H	0.264015	-1.153836	1.513897
H	-0.000074	-1.719229	-0.131620
H	0.133994	1.819085	-1.109593
H	-0.701384	2.355353	0.354802
H	-5.780087	-0.587451	-0.341614
H	-4.767647	1.576623	-1.076315
H	-2.374592	1.978259	-0.864238
H	-1.899936	-1.949352	0.899517
H	-4.289954	-2.338744	0.637476

1a (TS1, CH_3CN)

ΔG = -767.959107 hartree

C	2.282541	-1.179814	0.256565
C	3.659951	-1.395116	0.337598
C	4.568274	-0.625783	-0.404513
C	4.071463	0.383743	-1.245198
C	2.701730	0.618058	-1.330757
C	1.771941	-0.153041	-0.584305
C	1.295811	-2.042354	1.009056
C	0.357036	0.184907	-0.608111
N	-0.552818	-0.741010	0.030194
C	-0.031448	-1.319174	1.269401
C	-4.745602	-0.427918	-0.608440
C	-4.241563	-0.829661	0.632707
C	-2.867149	-0.914204	0.864196
C	-1.929708	-0.611664	-0.156576
C	-2.457217	-0.198115	-1.409238
C	-3.831206	-0.111307	-1.621542
H	4.031107	-2.186097	0.987541
H	5.636117	-0.809571	-0.329368
H	4.757293	0.987848	-1.834521
H	2.329231	1.404568	-1.983960
H	1.717758	-2.368153	1.967651
H	1.082747	-2.955821	0.435222
H	0.000085	0.536418	-1.572927
H	0.191911	1.477525	0.056235
H	0.107104	-0.537973	2.035369
H	-0.748290	-2.042074	1.658608
H	-5.815166	-0.357921	-0.780738
H	-4.922995	-1.067618	1.445782
H	-2.530309	-1.196930	1.853799
H	-1.789832	0.032731	-2.231035
H	-4.190303	0.201613	-2.598896
C	0.310634	2.659904	2.070535
C	-0.013541	2.723578	0.578226
N	-0.368423	3.658094	-0.136294
H	0.230467	3.649018	2.539469
H	1.325368	2.272106	2.221506
H	-0.375290	1.968515	2.575341

1a (A, CH_3CN)

ΔG = -634.593630 hartree

C	2.285347	0.719027	0.242671
C	3.662428	0.912911	0.289971
C	4.554967	-0.134953	0.011139
C	4.047486	-1.403776	-0.320992
C	2.676964	-1.618954	-0.384496
C	1.760456	-0.563353	-0.110241
C	1.286602	1.793786	0.595521
C	0.360522	-0.767880	-0.175855
N	-0.543189	0.270969	-0.072512
C	-0.014405	1.639997	-0.200615
C	-4.710681	-0.472204	0.058972
C	-4.219790	0.718746	-0.485923
C	-2.848198	0.973251	-0.536420
C	-1.928205	0.033201	-0.026041
C	-2.429207	-1.163839	0.530137
C	-3.801655	-1.408967	0.563530
H	4.050395	1.894825	0.552993
H	5.626560	0.034989	0.051959
H	4.730245	-2.221679	-0.535008
H	2.290263	-2.599723	-0.650581
H	1.699413	2.790958	0.409922
H	1.048116	1.743084	1.667931
H	-0.045920	-1.748191	-0.389831
H	0.160997	1.867976	-1.261631
H	-0.760497	2.337867	0.179357
H	-5.778289	-0.665721	0.091716
H	-4.906904	1.456723	-0.890295
H	-2.499502	1.890831	-0.995768
H	-1.746949	-1.886144	0.964354
H	-4.161388	-2.334541	1.004321

1a (B, CH_3CN)

ΔG = -634.461313 hartree

C	2.288312	0.716696	0.261051
C	3.669955	0.879841	0.293250
C	4.514092	-0.183547	-0.053665
C	3.991142	-1.429920	-0.422900
C	2.613475	-1.615327	-0.447834
C	1.761257	-0.541326	-0.117976
C	1.310595	1.783726	0.687634
C	0.338327	-0.728360	-0.137642
N	-0.515200	0.259979	-0.050927
C	-0.010108	1.667257	-0.066456
C	-4.678067	-0.454942	0.010300
C	-4.155565	0.572908	-0.781393
C	-2.782459	0.820835	-0.801550
C	-1.936198	0.023576	-0.022586
C	-2.447772	-0.997917	0.785089
C	-3.823124	-1.236994	0.791888
H	4.093961	1.835029	0.587521
H	5.589690	-0.037916	-0.032177
H	4.656298	-2.245621	-0.684519
H	2.189157	-2.574486	-0.728564
H	1.718848	2.782441	0.513263
H	1.132516	1.695774	1.767837
H	-0.073720	-1.727265	-0.242783
H	0.107844	1.952869	-1.117320
H	-0.776422	2.294230	0.385687
H	-5.747351	-0.639974	0.023459
H	-4.814639	1.181862	-1.391500
H	-2.381251	1.606955	-1.431324
H	-1.788143	-1.578450	1.421544
H	-4.223559	-2.024327	1.422111

1a (TS3, CH_3CN)

ΔG = -1829.170628 hartree

C	-2.433012	-1.514161	-0.122341
C	-3.817385	-1.718197	-0.162148
C	-4.708018	-0.659383	0.018223
C	-4.209962	0.629153	0.242562
C	-2.835473	0.846401	0.287526
C	-1.927427	-0.215773	0.106974
C	-1.469646	-2.660278	-0.298661
C	-0.447831	0.042270	0.151022
S	0.096539	1.058076	1.556188
S	1.028945	2.728774	0.448682
S	-0.115974	2.612214	-1.285496
N	0.377753	-1.035030	-0.171204
C	-0.181386	-2.165587	-0.939048
C	4.606219	-0.985022	-0.021055
C	3.933582	-0.099959	-0.866987
C	2.535874	-0.087933	-0.911562
C	1.812047	-0.966127	-0.098160
C	2.482237	-1.863442	0.744419
C	3.877057	-1.868467	0.783694
H	-4.195575	-2.721978	-0.337488
H	-5.778798	-0.836062	-0.017895
H	-4.890487	1.463258	0.383991
H	-2.457984	1.845233	0.471495
H	-1.909070	-3.441838	-0.926067
H	-1.241620	-3.117526	0.673823
H	-0.338856	1.088804	-0.849843
H	-0.364749	-1.834565	-1.972168
H	0.577551	-2.947643	-0.969461
H	5.691505	-0.990051	0.009994
H	4.493178	0.582550	-1.499485
H	2.014958	0.587826	-1.580540
H	1.909511	-2.541223	1.369866
H	4.392759	-2.557580	1.445473

1a (2a, CH_3CN)

ΔG = -1032.237217 hartree

C	2.283596	-1.007150	-0.122118
C	3.655810	-1.272620	-0.068912
C	4.576066	-0.240064	0.120183
C	4.124946	1.077423	0.258620
C	2.761810	1.355106	0.192977
C	1.825639	0.323502	-0.000743
C	1.266951	-2.101459	-0.316227
C	0.367521	0.630305	-0.103125
S	-0.188581	2.191171	-0.466482
N	-0.478083	-0.404708	0.087357
C	0.005817	-1.757666	0.459998
C	-4.695882	-0.065725	0.080258
C	-4.018321	-0.404053	-1.095790
C	-2.623882	-0.496002	-1.101279
C	-1.912028	-0.238879	0.073248
C	-2.581478	0.090307	1.255029
C	-3.976143	0.178494	1.254615
H	4.001794	-2.297849	-0.168347
H	5.638009	-0.462483	0.167416
H	4.833134	1.884829	0.417312
H	2.403990	2.373228	0.291973
H	1.658323	-3.063230	0.027768
H	1.024677	-2.211410	-1.382303
H	0.193073	-1.782744	1.541681
H	-0.798665	-2.459549	0.238993
H	-5.779523	0.002946	0.082681
H	-4.572974	-0.598391	-2.008811
H	-2.088066	-0.757952	-2.008254
H	-2.014263	0.281227	2.160598
H	-4.498153	0.436491	2.171115

1b (1b, DMPU)

ΔG = -595.921461 hartree

C	1.874074	-0.698599	-0.000007
C	3.073007	-1.411733	0.000013
C	4.279280	-0.700793	0.000051

C	4.279284	0.700784	0.000068
C	3.073014	1.411730	0.000046
C	1.874077	0.698602	0.000008
C	0.461894	-1.225094	-0.000023
C	0.461900	1.225104	-0.000008
N	-0.341879	0.000006	-0.000272
C	-4.561059	-0.000008	0.000124
C	-3.845276	-1.202537	0.000082
C	-2.450303	-1.213625	-0.000032
C	-1.717778	0.000006	-0.000117
C	-2.450316	1.213631	-0.000067
C	-3.845289	1.202528	0.000049
H	3.075953	-2.498361	-0.000002
H	5.222140	-1.239894	0.000063
H	5.222146	1.239881	0.000095
H	3.075965	2.498358	0.000057
H	0.253794	-1.845156	0.885496
H	0.253885	-1.845436	-0.885355
H	0.253907	1.845452	-0.885340
H	0.253792	1.845162	0.885510
H	-5.646561	-0.000013	0.000215
H	-4.376517	-2.150858	0.000144
H	-1.928916	-2.164128	-0.000064
H	-1.928940	2.164139	-0.000127
H	-4.376540	2.150844	0.000083

1b (TS1, DMPU)

ΔG = -1016.395527 hartree

C	-2.908771	0.497373	0.382272
C	-4.200269	0.228333	0.818970
C	-4.885683	-0.874919	0.281952
C	-4.266236	-1.679917	-0.687120
C	-2.965224	-1.411460	-1.123314
C	-2.272181	-0.315621	-0.580139
C	-1.991322	1.631844	0.762998
C	-0.904999	0.154496	-0.812295
N	-0.839095	1.429087	-0.126078
C	2.198155	4.333445	-0.561587
C	1.157007	4.513932	0.356639
C	0.156485	3.554655	0.515305
C	0.161455	2.362551	-0.257332
C	1.228079	2.184590	-1.178548
C	2.217292	3.155560	-1.320354
H	-4.682337	0.865418	1.556905
H	-5.896574	-1.098639	0.609943
H	-4.805977	-2.525322	-1.106031
H	-2.498969	-2.046545	-1.871442
H	-1.695882	1.600346	1.824736
H	-2.452591	2.614912	0.588985
H	-0.552184	0.188993	-1.844466
H	-0.003208	-0.810685	-0.255552
H	2.974128	5.083624	-0.678368
H	1.119621	5.413754	0.965811
H	-0.626235	3.728929	1.244682
H	1.284971	1.279999	-1.771518
H	3.018489	2.984240	-2.035223
N	1.607590	-1.060369	1.267361
C	0.768515	-0.774404	2.424690
C	0.861694	-1.803508	0.215928
O	0.156817	-2.840592	0.585365
N	1.763636	-1.960360	-0.960081
C	1.087780	-2.611259	-2.076795
C	3.006272	-2.673143	-0.630465
C	3.761595	-1.946148	0.478836
C	2.845167	-1.735816	1.681108
H	-0.149648	-0.276284	2.103566
H	1.305204	-0.100394	3.103027
H	0.483201	-1.678229	2.990873
H	0.157278	-2.087128	-2.311021
H	0.836564	-3.667787	-1.878319
H	1.733826	-2.572947	-2.962001
H	3.620924	-2.733059	-1.538020
H	2.796548	-3.715264	-0.315431
H	4.109717	-0.973144	0.109576
H	4.643761	-2.526780	0.774889
H	3.341154	-1.113358	2.437118
H	2.629909	-2.711930	2.161451

1b (A, DMPU)

ΔG = -595.298362 hartree

C	-1.885833	-0.702590	0.004782
C	-3.084115	-1.396184	0.012551
C	-4.290289	-0.668750	0.009610
C	-4.269725	0.737518	-0.001713
C	-3.068552	1.446265	-0.010008
C	-1.855391	0.720825	-0.006636
C	-0.466678	-1.212366	0.003384
C	-0.504506	1.139100	-0.013535
N	0.331953	0.032587	-0.006319
C	4.556244	0.004292	0.003601
C	3.831895	-1.192155	-0.010432
C	2.436724	-1.187828	-0.013409
C	1.723674	0.032359	-0.002297
C	2.460173	1.239920	0.013602
C	3.853580	1.215333	0.015805
H	-3.101214	-2.483028	0.020817
H	-5.239165	-1.196113	0.015981
H	-5.209403	1.283314	-0.003897
H	-3.065728	2.532358	-0.018327
H	-0.235793	-1.822288	-0.880507
H	-0.228375	-1.812281	0.892085
H	-0.116797	2.144592	-0.029299
H	5.641547	-0.005348	0.005616
H	4.353604	-2.145099	-0.019700
H	1.907508	-2.133226	-0.025464
H	1.952590	2.196953	0.026673
H	4.394351	2.157621	0.028438

1b (B, DMPU)

ΔG = -595.161491 hartree

C	1.895061	-0.704118	0.186753
C	3.114645	-1.341329	0.372494
C	4.279464	-0.585742	0.183467
C	4.232475	0.770898	-0.187171
C	3.013190	1.414577	-0.378197
C	1.848081	0.658361	-0.182502
C	0.489854	-1.212760	0.296410
C	0.467893	1.013542	-0.309397
N	-0.313994	-0.010141	-0.045350
C	-4.528350	0.054947	0.015924
C	-3.852936	-1.072144	-0.461831
C	-2.458018	-1.103226	-0.483710
C	-1.744912	0.007774	-0.018768
C	-2.409749	1.136195	0.476715
C	-3.804482	1.156233	0.483437
H	3.172522	-2.386887	0.655563
H	5.245240	-1.060174	0.326315
H	5.158912	1.317963	-0.325492
H	2.963165	2.459179	-0.665975
H	0.213980	-1.547779	1.301036
H	0.270794	-2.017884	-0.410865
H	0.056336	1.973223	-0.598007
H	-5.613326	0.072551	0.029835
H	-4.409163	-1.929138	-0.827130
H	-1.941942	-1.971377	-0.877360
H	-1.849612	1.974352	0.877367
H	-4.322244	2.027714	0.870427

1b (TS3, DMPU)

ΔG = -1789.884316 hartree

C	1.594359	-1.911891	0.190698
C	2.695156	-2.744309	0.374649
C	3.974553	-2.186543	0.266512
C	4.139687	-0.824665	-0.031048
C	3.033683	0.007123	-0.220737
C	1.756907	-0.552883	-0.103922
C	0.133232	-2.242986	0.214571
C	0.428723	0.086857	-0.215107
S	0.101410	1.314802	-1.513747
S	0.869484	3.047459	-0.427892
S	0.302665	2.488903	1.517243
N	-0.517561	-0.939272	-0.047790
C	-4.732808	-0.659538	0.103598
C	-4.107222	-1.872360	-0.199327
C	-2.716604	-1.959862	-0.254431
C	-1.921955	-0.822990	-0.004221
C	-2.554513	0.395452	0.310964
C	-3.945686	0.467772	0.360471
H	0.363667	1.034984	0.931669
H	2.568663	-3.800581	0.593053
H	4.848169	-2.814765	0.410834
H	5.140408	-0.412059	-0.115500
H	3.161600	1.058938	-0.453517
H	-0.214917	-2.642806	1.174058
H	-0.128671	-2.965790	-0.568030
H	-5.815497	-0.595124	0.145367
H	-4.700496	-2.759139	-0.400190
H	-2.260364	-2.909769	-0.504351
H	-1.967104	1.273201	0.542681
H	-4.414567	1.414132	0.612764

1b (2b, DMPU)

ΔG = -992.946077 hartree

C	-1.882548	-1.056587	0.000266
C	-3.081848	-1.764691	0.000451
C	-4.277256	-1.036560	0.000323
C	-4.271527	0.368379	0.000012
C	-3.068208	1.075127	-0.000193
C	-1.876980	0.345303	-0.000065
C	-0.464092	-1.544812	0.000349
C	-0.481420	0.821751	-0.000242
S	0.039458	2.421428	-0.000802
N	0.302565	-0.282933	0.000026
C	4.523347	-0.396670	0.000197
C	3.824573	-0.372210	1.211482
C	2.428005	-0.324203	1.215114
C	1.736886	-0.297832	0.000068
C	2.428032	-0.326585	-1.214905
C	3.824606	-0.374598	-1.211149
H	-3.095785	-2.850456	0.000686
H	-5.225191	-1.566266	0.000466
H	-5.213846	0.907444	-0.000070
H	-3.047822	2.160169	-0.000436
H	-0.211608	-2.137919	-0.886806
H	-0.211556	-2.137472	0.887787
H	5.608505	-0.434075	0.000249
H	4.364123	-0.390752	2.153478
H	1.875124	-0.304346	2.149035
H	1.875190	-0.308521	-2.148888
H	4.364174	-0.394986	-2.153095

1b (1b, DMF)

ΔG = -595.921485 hartree

C	1.874074	-0.698599	-0.000007
C	3.073007	-1.411733	0.000013
C	4.279280	-0.700793	0.000051
C	4.279284	0.700784	0.000068
C	3.073014	1.411730	0.000046
C	1.874077	0.698602	0.000008
C	0.461894	-1.225094	-0.000023
C	0.461900	1.225104	-0.000008
N	-0.341879	0.000006	-0.000272
C	-4.561059	-0.000008	0.000124
C	-3.845276	-1.202537	0.000082
C	-2.450303	-1.213625	-0.000032
C	-1.717778	0.000006	-0.000117
C	-2.450316	1.213631	-0.000067
C	-3.845289	1.202528	0.000049

H	3.075953	-2.498361	-0.000002
H	5.222140	-1.239894	0.000063
H	5.222146	1.239881	0.000095
H	3.075965	2.498358	0.000057
H	0.253794	-1.845156	0.885496
H	0.253885	-1.845436	-0.885355
H	0.253907	1.845452	-0.885340
H	0.253792	1.845162	0.885510
H	-5.646561	-0.000013	0.000215
H	-4.376517	-2.150858	0.000144
H	-1.928916	-2.164128	-0.000064
H	-1.928940	2.164139	-0.000127
H	-4.376540	2.150844	0.000083

1b (TS1, DMF)

ΔG = -844.382308 hartree

N	1.097204	2.837611	0.943713
C	2.487538	2.931815	0.518998
C	0.932518	2.006963	2.128793
C	0.145949	2.521462	-0.130581
O	0.256870	3.187423	-1.253856
H	2.550373	3.577701	-0.358769
H	2.923254	1.948703	0.257946
H	3.089969	3.366647	1.324746
H	1.281779	0.967944	1.984225
H	-0.125246	1.972907	2.411647
H	1.494699	2.435373	2.966254
H	-0.862844	2.493165	0.346321
C	1.374244	-1.843817	0.258319
C	2.461259	-2.601455	0.671488
C	3.717860	-2.376491	0.076437
C	3.853813	-1.396287	-0.919915
C	2.760713	-0.629820	-1.335918
C	1.502379	-0.854658	-0.744601
C	-0.063784	-1.904869	0.711275
C	0.233574	-0.174575	-0.938039
N	-0.726260	-0.944747	-0.184546
C	-4.890336	-0.247277	-0.081417
C	-4.304582	-1.217901	0.740061
C	-2.928600	-1.447443	0.722238
C	-2.078820	-0.702357	-0.138164
C	-2.681170	0.286605	-0.961692
C	-4.057576	0.498722	-0.927345
H	2.347873	-3.367920	1.434892
H	4.578460	-2.962374	0.385502
H	4.825729	-1.231194	-1.378446
H	2.882488	0.123119	-2.110000
H	-0.185412	-1.613460	1.767939
H	-0.496862	-2.909932	0.603613
H	-0.073992	0.088733	-1.951725
H	0.277199	1.196498	-0.409099
H	-5.961588	-0.072692	-0.060086
H	-4.924475	-1.807589	1.411040
H	-2.512601	-2.205440	1.375894
H	-2.065718	0.893524	-1.615185
H	-4.484530	1.265150	-1.569656

1b (A, DMF)

ΔG = -595.301827 hartree

C	-1.885833	-0.702590	0.004782
C	-3.084115	-1.396184	0.012551
C	-4.290289	-0.668750	0.009610
C	-4.269725	0.737518	-0.001713
C	-3.068552	1.446265	-0.010008
C	-1.855391	0.720825	-0.006636
C	-0.466678	-1.212366	0.003384
C	-0.504506	1.139100	-0.013535
N	0.331953	0.032587	-0.006319
C	4.556244	0.004292	0.003601
C	3.831895	-1.192155	-0.010432
C	2.436724	-1.187828	-0.013409
C	1.723674	0.032359	-0.002297
C	2.460173	1.239920	0.013602
C	3.853580	1.215333	0.015805
H	-3.101214	-2.483028	0.020817
H	-5.239165	-1.196113	0.015981
H	-5.209403	1.283314	-0.003897
H	-3.065728	2.532358	-0.018327
H	-0.235793	-1.822288	-0.880507
H	-0.228375	-1.812281	0.892085
H	-0.116797	2.144592	-0.029299
H	5.641547	-0.005348	0.005616
H	4.353604	-2.145099	-0.019700
H	1.907508	-2.133226	-0.025464
H	1.952590	2.196953	0.026673
H	4.394351	2.157621	0.028438

1b (B, DMF)

ΔG = -595.165627 hartree

C	1.895061	-0.704118	0.186753
C	3.114645	-1.341329	0.372494
C	4.279464	-0.585742	0.183467
C	4.232475	0.770898	-0.187171
C	3.013190	1.414577	-0.378197
C	1.848081	0.658361	-0.182502
C	0.489854	-1.212760	0.296410
C	0.467893	1.013542	-0.309397
N	-0.313994	-0.010141	-0.045350
C	-4.528350	0.054947	0.015924
C	-3.852936	-1.072144	-0.461831
C	-2.458018	-1.103226	-0.483710
C	-1.744912	0.007774	-0.018768
C	-2.409749	1.136195	0.476715
C	-3.804482	1.156233	0.483437
H	3.172522	-2.386887	0.655563
H	5.245240	-1.060174	0.326315
H	5.158912	1.317963	-0.325492
H	2.963165	2.459179	-0.665975
H	0.213980	-1.547779	1.301036

H	0.270794	-2.017884	-0.410865
H	0.056336	1.973223	-0.598007
H	-5.613326	0.072551	0.029835
H	-4.409163	-1.929138	-0.827130
H	-1.941942	-1.971377	-0.877360
H	-1.849612	1.974352	0.877367
H	-4.322244	2.027714	0.870427

1b (TS3, DMF)

ΔG = -1789.887326 hartree

C	1.594359	-1.911891	0.190698
C	2.695156	-2.744309	0.374649
C	3.974553	-2.186543	0.266512
C	4.139687	-0.824665	-0.031048
C	3.033683	0.007123	-0.220737
C	1.756907	-0.552883	-0.103922
C	0.133232	-2.242986	0.214571
C	0.428723	0.086857	-0.215107
S	0.101410	1.314802	-1.513747
S	0.869484	3.047459	-0.427892
S	0.302665	2.488903	1.517243
N	-0.517561	-0.939272	-0.047790
C	-4.732808	-0.659538	0.103598
C	-4.107222	-1.872360	-0.199327
C	-2.716604	-1.959862	-0.254431
C	-1.921955	-0.822990	-0.004221
C	-2.554513	0.395452	0.310964
C	-3.945686	0.467772	0.360471
H	0.363667	1.034984	0.931669
H	2.568663	-3.800581	0.593053
H	4.848169	-2.814765	0.410834
H	5.140408	-0.412059	-0.115500
H	3.161600	1.058938	-0.453517
H	-0.214917	-2.642806	1.174058
H	-0.128671	-2.965790	-0.568030
H	-5.815497	-0.595124	0.145367
H	-4.700496	-2.759139	-0.400190
H	-2.260364	-2.909769	-0.504351
H	-1.967104	1.273201	0.542681
H	-4.414567	1.414132	0.612764

1b (2b, DMF)

ΔG = -992.946123 hartree

C	-1.882548	-1.056587	0.000266
C	-3.081848	-1.764691	0.000451
C	-4.277256	-1.036560	0.000323
C	-4.271527	0.368379	0.000012
C	-3.068208	1.075127	-0.000193
C	-1.876980	0.345303	-0.000065
C	-0.464092	-1.544812	0.000349
C	-0.481420	0.821751	-0.000242
S	0.039458	2.421428	-0.000802
N	0.302565	-0.282933	0.000026
C	4.523347	-0.396670	0.000197
C	3.824573	-0.372210	1.211482
C	2.428005	-0.324203	1.215114
C	1.736886	-0.297832	0.000068
C	2.428032	-0.326585	-1.214905
C	3.824606	-0.374598	-1.211149
H	-3.095785	-2.850456	0.000686
H	-5.225191	-1.566266	0.000466
H	-5.213846	0.907444	-0.000070
H	-3.047822	2.160169	-0.000436
H	-0.211608	-2.137919	-0.886806
H	-0.211556	-2.137472	0.887787
H	5.608505	-0.434075	0.000249
H	4.364123	-0.390752	2.153478
H	1.875124	-0.304346	2.149035
H	1.875190	-0.308521	-2.148888
H	4.364174	-0.394986	-2.153095

1c (1c, DMPU)

ΔG = -405.397051 hartree

C	0.903899	1.180241	-0.102646
C	2.247230	1.306324	0.258128
C	3.077213	0.178450	0.286727
C	2.551694	-1.072232	-0.047599
C	1.203460	-1.193280	-0.405726
C	0.364062	-0.071982	-0.438239
C	-2.027062	-0.588270	1.352172
C	-1.089667	-0.195311	-0.854888
N	-2.034274	0.271429	0.169236
C	-3.383775	0.387404	-0.381106
H	0.263466	2.057815	-0.123207
H	2.648717	2.283154	0.513479
H	4.122291	0.275937	0.566536
H	3.186088	-1.953986	-0.027191
H	0.800216	-2.170247	-0.661167
H	-2.703712	-0.177391	2.107502
H	-2.350896	-1.622482	1.124630
H	-1.021922	-0.631892	1.779430
H	-1.298144	-1.243864	-1.143167
H	-1.257172	0.416420	-1.749601
H	-4.059761	0.780513	0.384386
H	-3.382753	1.080472	-1.228063
H	-3.788824	-0.582519	-0.729157

1c (TS1, DMPU)

ΔG = -825.869535 hartree

C	-2.523679	-0.593159	0.784525
C	-3.170281	-1.825701	0.877172
C	-3.149443	-2.730826	-0.193566
C	-2.468021	-2.371659	-1.367153
C	-1.825948	-1.139027	-1.464706
C	-1.827682	-0.212044	-0.391040
C	-2.886597	2.615630	-0.043871
C	-1.091056	1.045296	-0.503222
N	-1.538909	2.157733	0.312502

C	-0.600506	3.279756	0.255884
H	-2.545589	0.093288	1.625165
H	-3.696275	-2.084540	1.793401
H	-3.655974	-3.688851	-0.119069
H	-2.445435	-3.055496	-2.212451
H	-1.309893	-0.875153	-2.385318
H	-3.193127	3.418373	0.636740
H	-2.932169	3.007531	-1.078952
H	-3.605467	1.797882	0.043855
H	-0.885856	1.324466	-1.551303
H	0.304909	0.795842	-0.078635
H	-0.925374	4.064453	0.948435
H	0.402165	2.944863	0.531742
H	-0.553093	3.727175	-0.758413
N	2.067878	0.009891	-1.099936
C	2.240486	1.096028	-2.058825
C	1.596376	0.515799	0.223414
O	2.198257	1.567215	0.718208
N	1.399410	-0.655405	1.119659
C	0.847075	-0.257364	2.408687
C	2.616234	-1.455918	1.296809
C	3.119788	-1.957934	-0.053348
C	3.302708	-0.781318	-1.007437
H	1.330691	1.698942	-2.113142
H	2.432419	0.673052	-3.052275
H	3.077323	1.769195	-1.803090
H	-0.050350	0.346861	2.254065
H	1.553445	0.328963	3.022961
H	0.566073	-1.154434	2.973641
H	2.380324	-2.300588	1.956973
H	3.414892	-0.871674	1.797861
H	2.393323	-2.663589	-0.475395
H	4.070541	-2.490206	0.072157
H	3.557853	-1.138678	-2.013586
H	4.153210	-0.156292	-0.666538

1c (A, DMPU)

ΔG = -404.771201 hartree

C	0.797562	0.975084	-0.350985
C	2.151803	1.299033	-0.327394
C	3.121841	0.334558	-0.018052
C	2.707758	-0.981839	0.252400
C	1.360933	-1.318183	0.233072
C	0.352122	-0.348765	-0.055086
C	-2.265712	1.201653	0.754148
C	-1.010089	-0.765585	-0.070256
N	-2.119973	0.056356	-0.151371
C	-3.391623	-0.609614	-0.422314
H	0.078600	1.733907	-0.640191
H	2.457412	2.314708	-0.565949
H	4.175215	0.596886	0.000402
H	3.446044	-1.746333	0.480336
H	1.058122	-2.340131	0.448568
H	-2.880063	1.973996	0.281660
H	-2.756105	0.891103	1.690709
H	-1.295584	1.626990	1.002403
H	-1.212168	-1.833435	-0.115586
H	-4.120637	0.128497	-0.768222
H	-3.260974	-1.359126	-1.205473
H	-3.797625	-1.099611	0.477737

1c (B, DMPU)

ΔG = -404.634546 hartree

C	-1.298322	-1.334045	0.123704
C	-2.657366	-1.051723	0.215398
C	-3.106292	0.262950	0.052021
C	-2.193300	1.292455	-0.206428
C	-0.829642	1.023995	-0.275090
C	-0.360823	-0.297140	-0.093618
C	2.192333	1.366105	0.430071
C	1.023701	-0.721738	-0.163847
N	2.120703	-0.045284	0.015042
C	3.432602	-0.694358	-0.172956
H	-0.951200	-2.356979	0.233095
H	-3.364594	-1.853283	0.400098
H	-4.167410	0.484184	0.110188
H	-2.546275	2.306593	-0.361080
H	-0.150794	1.831499	-0.512589
H	3.117856	1.502893	0.988308
H	2.210316	2.013005	-0.450538
H	1.345370	1.613450	1.067317
H	1.178633	-1.775181	-0.381605
H	3.962925	-0.700127	0.781833
H	3.297852	-1.712013	-0.534469
H	4.005048	-0.116062	-0.901381

1c (TS3, DMPU)

ΔG = -1599.354737 hartree

C	-1.816386	0.313705	1.080202
C	-3.111184	-0.179235	1.233892
C	-3.710476	-0.913637	0.203602
C	-3.000991	-1.151568	-0.977074
C	-1.702881	-0.659254	-1.132717
C	-1.096568	0.090296	-0.111202
C	-0.584616	2.967908	-0.176104
C	0.299516	0.615458	-0.207620
S	1.446633	-0.139582	-1.426824
S	1.839538	-1.942607	-0.301498
S	1.936011	-1.068767	1.612655
N	0.486846	1.978682	-0.054023
C	1.812214	2.546960	0.188274
H	0.952296	-0.015513	0.951145
H	-1.353329	0.869752	1.890587
H	-3.649163	0.002462	2.159547
H	-4.718076	-1.300240	0.323561
H	-3.456960	-1.721222	-1.781409
H	-1.158482	-0.847688	-2.051626
H	-0.838463	3.392597	0.802083
H	-0.233958	3.779506	-0.822618

H	-1.473312	2.519197	-0.614337
H	1.738239	3.272394	1.005225
H	2.516067	1.764203	0.463987
H	2.180545	3.065269	-0.704805

1c (2c, DMPU)

ΔG = -802.417608 hartree

C	1.176485	0.712691	-0.959318
C	2.567248	0.842246	-0.977624
C	3.349092	0.159870	-0.040349
C	2.733467	-0.662804	0.909255
C	1.345148	-0.812072	0.916107
C	0.554452	-0.118358	-0.012743
C	-1.234017	2.043872	0.684660
C	-0.929866	-0.313042	-0.044525
S	-1.540853	-1.859420	-0.388305
N	-1.712205	0.753733	0.162687
C	-3.167210	0.664121	0.005827
H	0.573797	1.245564	-1.688976
H	3.037493	1.476755	-1.722979
H	4.429719	0.266019	-0.051166
H	3.334199	-1.194667	1.641044
H	0.869134	-1.464717	1.640896
H	-1.349288	2.824208	-0.073954
H	-1.836414	2.310054	1.558039
H	-0.191031	1.978762	0.981362
H	-3.569771	1.675849	-0.053178
H	-3.411181	0.113735	-0.903511
H	-3.616379	0.143880	0.858762

1c (1c, DMF)

ΔG = -405.397065 hartree

C	0.904042	1.180380	-0.101940
C	2.247389	1.306181	0.258885
C	3.077308	0.178230	0.286863
C	2.551697	-1.072241	-0.048133
C	1.203440	-1.193000	-0.406325
C	0.364106	-0.071626	-0.438209
C	-2.027495	-0.589936	1.351432
C	-1.089640	-0.194612	-0.854968
N	-2.034261	0.271226	0.169565
C	-3.383680	0.388279	-0.380780
H	0.263686	2.058029	-0.122087
H	2.648956	2.282853	0.514739
H	4.122399	0.275497	0.566722
H	3.186040	-1.954050	-0.028214
H	0.800140	-2.169799	-0.662339
H	-2.704258	-0.179878	2.107120
H	-2.351475	-1.623792	1.122493
H	-1.022457	-0.634285	1.778880
H	-1.298070	-1.242924	-1.144157
H	-1.257152	0.417886	-1.749155
H	-4.059597	0.781020	0.384981
H	-3.382245	1.082082	-1.227137
H	-3.789136	-0.581143	-0.729750

1c (TS1, DMF)

ΔG = -653.852465 hartree

N	2.470754	-1.188052	-0.301067
C	3.176241	-2.397765	0.123247
C	3.354293	-0.307242	-1.059150
C	1.789750	-0.504115	0.823008
O	2.488435	0.229160	1.660274
H	2.493042	-3.050042	0.677330
H	4.048533	-2.185515	0.770208
H	3.536489	-2.948998	-0.754326
H	4.248335	0.009881	-0.493169
H	2.809316	0.592252	-1.359375
H	3.695299	-0.822304	-1.965327
H	1.107843	-1.259100	1.278672
C	-2.213490	0.073465	0.906726
C	-3.250622	-0.829304	1.142823
C	-3.530916	-1.857765	0.231685
C	-2.747830	-1.962797	-0.928970
C	-1.713755	-1.060900	-1.171101
C	-1.412591	-0.013914	-0.261678
C	-1.338642	3.040068	-0.491954
C	-0.269568	0.861206	-0.495390
N	-0.300551	2.184650	0.092801
C	1.005235	2.838655	0.009824
H	-2.006460	0.861901	1.624029
H	-3.846674	-0.731651	2.047447
H	-4.340734	-2.557212	0.418184
H	-2.951538	-2.749969	-1.651122
H	-1.122403	-1.153928	-2.079639
H	-1.358749	4.004545	0.028515
H	-1.161859	3.233709	-1.567991
H	-2.319854	2.571086	-0.386005
H	0.091551	0.843359	-1.538701
H	0.853130	0.209009	0.179740
H	0.962043	3.810941	0.512965
H	1.759231	2.218527	0.499859
H	1.315931	3.016492	-1.040044

1c (A, DMF)

ΔG = -404.771218 hartree

C	0.797562	0.975084	-0.350985
C	2.151803	1.299033	-0.327394
C	3.121841	0.334558	-0.018052
C	2.707758	-0.981839	0.252400
C	1.360933	-1.318183	0.233072
C	0.352122	-0.348765	-0.055086
C	-2.265712	1.201653	0.754148
C	-1.010089	-0.765585	-0.070256
N	-2.119973	0.056356	-0.151371
C	-3.391623	-0.609614	-0.422314
H	0.078600	1.733907	-0.640191
H	2.457412	2.314708	-0.565949

H	4.175215	0.596886	0.000402
H	3.446044	-1.746333	0.480336
H	1.058122	-2.340131	0.448568
H	-2.880063	1.973996	0.281660
H	-2.756105	0.891103	1.690709
H	-1.295584	1.626990	1.002403
H	-1.212168	-1.833435	-0.115586
H	-4.120637	0.128497	-0.768222
H	-3.260974	-1.359126	-1.205473
H	-3.797625	-1.099611	0.477737

1c (B, DMF)

ΔG = -404.635455 hartree

C	-1.298322	-1.334045	0.123704
C	-2.657366	-1.051723	0.215398
C	-3.106292	0.262950	0.052021
C	-2.193300	1.292455	-0.206428
C	-0.829642	1.023995	-0.275090
C	-0.360823	-0.297140	-0.093618
C	2.192333	1.366105	0.430071
C	1.023701	-0.721738	-0.163847
N	2.120703	-0.045284	0.015042
C	3.432602	-0.694358	-0.172956
H	-0.951200	-2.356979	0.233095
H	-3.364594	-1.853283	0.400098
H	-4.167410	0.484184	0.110188
H	-2.546275	2.306593	-0.361080
H	-0.150794	1.831499	-0.512589
H	3.117856	1.502893	0.988308
H	2.210316	2.013005	-0.450538
H	1.345370	1.613450	1.067317
H	1.178633	-1.775181	-0.381605
H	3.962925	-0.700127	0.781833
H	3.297852	-1.712013	-0.534469
H	4.005048	-0.116062	-0.901381

1c (TS3, DMF)

ΔG = -1599.349580 hartree

C	-1.816184	0.313329	1.080291
C	-3.110970	-0.179649	1.234029
C	-3.710437	-0.913712	0.203598
C	-3.001151	-1.151260	-0.977280
C	-1.703060	-0.658904	-1.132973
C	-1.096570	0.090301	-0.111306
C	-0.584875	2.967742	-0.175333
C	0.299528	0.615460	-0.207785
S	1.446543	-0.139626	-1.426958
S	1.839866	-1.942542	-0.301437
S	1.935870	-1.068634	1.612778
N	0.486873	1.978680	-0.054388
C	1.812214	2.547007	0.187971
H	0.952310	-0.015454	0.951094
H	-1.353019	0.869150	1.890768
H	-3.648807	0.001783	2.159818

H	-4.718029	-1.300326	0.323587
H	-3.457271	-1.720618	-1.781739
H	-1.158833	-0.847018	-2.052050
H	-0.839384	3.390744	0.803412
H	-0.234102	3.780476	-0.820315
H	-1.473181	2.519440	-0.614791
H	1.738426	3.271586	1.005701
H	2.516357	1.764125	0.462562
H	2.179977	3.066314	-0.704748

1c (2c, DMF)

ΔG = -802.417648 hartree

C	1.176485	0.712691	-0.959318
C	2.567248	0.842246	-0.977624
C	3.349092	0.159870	-0.040349
C	2.733467	-0.662804	0.909255
C	1.345148	-0.812072	0.916107
C	0.554452	-0.118358	-0.012743
C	-1.234017	2.043872	0.684660
C	-0.929866	-0.313042	-0.044525
S	-1.540853	-1.859420	-0.388305
N	-1.712205	0.753733	0.162687
C	-3.167210	0.664121	0.005827
H	0.573797	1.245564	-1.688976
H	3.037493	1.476755	-1.722979
H	4.429719	0.266019	-0.051166
H	3.334199	-1.194667	1.641044
H	0.869134	-1.464717	1.640896
H	-1.349288	2.824208	-0.073954
H	-1.836414	2.310054	1.558039
H	-0.191031	1.978762	0.981362
H	-3.569771	1.675849	-0.053178
H	-3.411181	0.113735	-0.903511
H	-3.616379	0.143880	0.858762

1d (1d, DMPU)

ΔG = -482.793072 hartree

N	0.558106	0.022252	-0.151425
C	1.266788	-1.258923	-0.059570
C	2.707003	-1.132972	-0.571071
C	3.472889	-0.021011	0.154995
C	2.684271	1.291920	0.079258
C	1.251436	1.100338	0.581101
C	-3.694070	0.006011	0.008099
C	-2.984189	1.174315	-0.299711
C	-1.591707	1.174561	-0.339632
C	-0.850865	0.001742	-0.062147
C	-1.576426	-1.166590	0.253556
C	-2.975991	-1.159491	0.279182
H	0.733855	-1.995588	-0.666015
H	1.276065	-1.632845	0.981955
H	2.681711	-0.919682	-1.647774
H	3.208994	-2.099458	-0.444250
H	4.473153	0.102168	-0.276157

H	3.612696	-0.300881	1.208990
H	2.654890	1.648516	-0.958924
H	3.167162	2.072816	0.678653
H	0.692296	2.029253	0.470267
H	1.270083	0.858977	1.660790
H	-4.779517	0.007921	0.032360
H	-3.519270	2.092793	-0.526006
H	-1.073556	2.086880	-0.615961
H	-1.058669	-2.087722	0.491587
H	-3.501476	-2.078299	0.526106

1d (TS1, DMPU)

ΔG = -903.252781 hartree

N	-1.872995	-0.460474	0.072974
C	-0.869127	-1.126511	-0.740669
C	-0.837288	-2.640867	-0.647372
C	-2.222263	-3.296862	-0.590469
C	-2.980393	-2.671120	0.578062
C	-3.131934	-1.162606	0.390813
C	-2.101989	3.780091	-0.222412
C	-3.184065	3.040286	0.261725
C	-3.126693	1.647025	0.354612
C	-1.959253	0.932353	-0.023493
C	-0.872951	1.695181	-0.525474
C	-0.950738	3.084521	-0.612924
H	0.528671	-0.835114	-0.319426
H	-0.895527	-0.758798	-1.778025
H	-0.284136	-2.942468	0.254623
H	-0.256335	-3.016716	-1.496505
H	-2.131150	-4.382849	-0.460093
H	-2.770842	-3.125982	-1.528058
H	-2.439057	-2.877661	1.511486
H	-3.984730	-3.096701	0.689214
H	-3.544423	-0.738110	1.311259
H	-3.870689	-0.976555	-0.410564
H	-2.153740	4.862380	-0.296017
H	-4.097228	3.545771	0.566792
H	-4.001830	1.128335	0.722761
H	0.052272	1.202880	-0.800850
H	-0.089762	3.630945	-0.991646
N	1.824707	-0.014216	1.286199
C	1.243227	-0.825879	2.347725
C	1.843686	-0.744986	-0.018832
O	2.401424	-1.934467	-0.026872
N	2.312993	0.231292	-1.056585
C	2.275619	-0.344913	-2.395839
C	3.657562	0.747898	-0.767026
C	3.693647	1.422446	0.602680
C	3.153861	0.473108	1.670537
H	0.256509	-1.183223	2.040049
H	1.121143	-0.212936	3.249445
H	1.857079	-1.705912	2.612760
H	1.279527	-0.744621	-2.604714
H	3.004818	-1.162593	-2.539159
H	2.491990	0.437562	-3.133689
H	3.931069	1.463855	-1.553510
H	4.411633	-0.064266	-0.797886
H	3.079915	2.331840	0.580592
H	4.721346	1.719547	0.846178
H	3.069089	0.991303	2.634945
H	3.864601	-0.365378	1.817024

1d (A, DMPU)

ΔG = -482.150542 hartree

N	-0.563439	0.011392	-0.043272
C	-1.289941	-1.270057	0.031555
C	-2.704845	-1.096110	0.591426
C	-3.484334	-0.019355	-0.168951
C	-2.709265	1.305642	-0.101687
C	-1.269413	1.131047	-0.473137
C	3.677324	0.023683	0.047664
C	2.950167	1.196646	0.286336
C	1.556788	1.194948	0.258807
C	0.839717	0.006396	-0.015530
C	1.580886	-1.172213	-0.261346
C	2.976545	-1.155925	-0.222999
H	-0.723872	-1.946007	0.675584
H	-1.340027	-1.723166	-0.971222
H	-2.640888	-0.822367	1.653096
H	-3.213019	-2.065537	0.538308
H	-4.487772	0.101302	0.254517
H	-3.606118	-0.323696	-1.217276
H	-2.797775	1.704241	0.928200
H	-3.158780	2.059169	-0.757722
H	-0.676090	1.982174	-0.779136
H	4.762568	0.030164	0.072703
H	3.471072	2.123459	0.511428
H	1.019609	2.109600	0.483453
H	1.075662	-2.099809	-0.501992
H	3.517719	-2.077493	-0.419865

1d (B, DMPU)

ΔG = -482.029018 hartree

N	-0.583655	-0.020114	-0.055209
C	-1.284888	1.068391	0.696470
C	-2.748998	1.190376	0.291946
C	-3.428387	-0.182012	0.293063
C	-2.696305	-1.123167	-0.669222
C	-1.220608	-0.970309	-0.659999
C	3.643558	-0.016712	0.031183
C	2.957247	1.068638	-0.524208
C	1.561882	1.080365	-0.552848
C	0.868671	-0.012451	-0.025956
C	1.537892	-1.102221	0.535255
C	2.934793	-1.099020	0.558953
H	-0.731628	1.987390	0.500816
H	-1.166647	0.825918	1.757454
H	-2.818216	1.647345	-0.702357
H	-3.234979	1.871483	0.996043

H	-4.476421	-0.097282	-0.004028
H	-3.411430	-0.603944	1.304189
H	-3.007172	-0.965021	-1.713589
H	-2.911797	-2.180673	-0.471162
H	-0.610255	-1.690510	-1.199186
H	4.728636	-0.016734	0.053300
H	3.505933	1.906507	-0.941612
H	1.029058	1.913635	-0.998546
H	0.978287	-1.929145	0.960285
H	3.463087	-1.939441	0.997035

1d (TS2, DMPU)

ΔG = -1676.760052 hartree

N	0.969602	0.922049	0.165296
C	1.243132	2.209236	-0.517198
C	0.124904	3.235699	-0.305446
C	-0.447677	3.120429	1.106663
C	-1.088771	1.736015	1.283312
C	-0.302124	0.630369	0.584881
S	-1.410876	-0.003907	-1.222885
S	-3.266827	-0.595288	-0.528146
S	-3.206447	-2.354301	0.437642
C	3.947657	-2.099444	0.024477
C	3.903803	-1.107778	-0.957551
C	2.922583	-0.113311	-0.925261
C	1.963656	-0.097969	0.101790
C	2.025484	-1.085611	1.103073
C	3.002347	-2.079055	1.055616
H	-0.378437	-0.338226	1.062647
H	1.375998	2.030914	-1.589920
H	2.192823	2.583551	-0.121183
H	-0.673809	3.078064	-1.038808
H	0.540954	4.230413	-0.492091
H	-1.191571	3.900461	1.293458
H	0.355611	3.259039	1.840599
H	-2.122901	1.736822	0.930385
H	-1.126699	1.464741	2.345825
H	4.711089	-2.870464	-0.005636
H	4.631537	-1.104646	-1.763486
H	2.908239	0.633482	-1.708835
H	1.333281	-1.065167	1.937660
H	3.033102	-2.828877	1.840411

1d (C, DMPU)

ΔG = -1676.761462 hartree

N	0.937498	0.936687	0.146675
C	1.325820	2.337794	-0.113678
C	0.127855	3.178996	-0.556872
C	-1.019659	3.161402	0.471415
C	-1.049541	1.835363	1.260303
C	-0.389023	0.669640	0.534461
S	-1.457596	0.176565	-1.087716
S	-3.176937	-0.705491	-0.280437
S	-2.785501	-2.525079	0.459126
C	3.860143	-2.131937	-0.050289
C	4.235451	-0.785947	-0.024199
C	3.276561	0.226291	0.037072
C	1.900077	-0.086766	0.071346
C	1.527621	-1.449120	0.044590
C	2.499195	-2.449001	-0.014562
H	-0.450711	-0.246079	1.121953
H	2.079263	2.342668	-0.904471
H	1.786903	2.768951	0.786970
H	-0.225987	2.795597	-1.520561
H	0.475355	4.201596	-0.734607
H	-1.971603	3.314807	-0.045700
H	-0.908649	3.988934	1.179668
H	-2.070487	1.554497	1.533253
H	-0.494594	1.944304	2.201701
H	4.610073	-2.915233	-0.097415
H	5.286510	-0.511922	-0.042008
H	3.610074	1.255345	0.082068
H	0.484548	-1.739275	0.040236
H	2.180379	-3.487209	-0.040916

1d (TS3, DMPU)

ΔG = -1676.727438 hartree

N	0.395396	1.071912	-0.065227
C	0.419199	2.356311	0.680499
C	-0.684899	3.316545	0.249339
C	-2.039985	2.607929	0.258117
C	-1.986454	1.403486	-0.685562
C	-0.815395	0.471335	-0.384594
S	-0.680585	-1.002503	-1.426921
S	-2.340790	-2.072225	-0.504555
S	-1.983712	-1.507942	1.495135
C	4.059302	-1.035559	0.193761
C	3.761539	-0.273635	-0.940305
C	2.543821	0.406846	-1.028761
C	1.622539	0.315396	0.019014
C	1.918500	-0.436210	1.161326
C	3.137664	-1.114101	1.243158
H	-1.321146	-0.255638	0.839230
H	1.407906	2.792075	0.521130
H	0.326618	2.130488	1.753371
H	-0.470199	3.697793	-0.756687
H	-0.676631	4.173180	0.931315
H	-2.837741	3.286214	-0.061371
H	-2.285188	2.279357	1.276453
H	-1.881870	1.751603	-1.722767
H	-2.910935	0.821202	-0.638436
H	5.005757	-1.563341	0.261189
H	4.474731	-0.206604	-1.756209
H	2.302968	1.004421	-1.902559
H	1.198931	-0.498301	1.971054
H	3.365414	-1.703181	2.126382

1d (2d, DMPU)

ΔG = -879.812245 hartree

N	0.498162	-0.307619	-0.028769
C	1.033551	-1.698289	0.052147
C	2.507529	-1.798808	-0.312493
C	3.289007	-0.703600	0.408395
C	2.758236	0.661056	-0.036503
C	1.244048	0.807456	-0.039278
S	0.578293	2.367179	-0.101873
C	-3.734493	-0.286282	0.056108
C	-3.058658	-0.351550	-1.166940
C	-1.661710	-0.338833	-1.198679
C	-0.947144	-0.250815	-0.001576
C	-1.613242	-0.197572	1.225288
C	-3.010412	-0.211859	1.250534
H	0.418513	-2.309258	-0.613266
H	0.863675	-2.053535	1.076235
H	2.633143	-1.694744	-1.397403
H	2.860277	-2.798002	-0.037671
H	4.358938	-0.768366	0.186872
H	3.176790	-0.818306	1.494217
H	3.084943	0.868557	-1.064469
H	3.161631	1.470501	0.575912
H	-4.820018	-0.297842	0.078446
H	-3.616596	-0.413490	-2.096359
H	-1.127745	-0.389032	-2.142618
H	-1.042898	-0.137338	2.146988
H	-3.530752	-0.166091	2.202452

1d (1d, DMF)

ΔG = -482.793088 hartree

N	0.558106	0.022252	-0.151425
C	1.266788	-1.258923	-0.059570
C	2.707003	-1.132972	-0.571071
C	3.472889	-0.021011	0.154995
C	2.684271	1.291920	0.079258
C	1.251436	1.100338	0.581101
C	-3.694070	0.006011	0.008099
C	-2.984189	1.174315	-0.299711
C	-1.591707	1.174561	-0.339632
C	-0.850865	0.001742	-0.062147
C	-1.576426	-1.166590	0.253556
C	-2.975991	-1.159491	0.279182
H	0.733855	-1.995588	-0.666015
H	1.276065	-1.632845	0.981955
H	2.681711	-0.919682	-1.647774
H	3.208994	-2.099458	-0.444250
H	4.473153	0.102168	-0.276157
H	3.612696	-0.300881	1.208990
H	2.654890	1.648516	-0.958924
H	3.167162	2.072816	0.678653
H	0.692296	2.029253	0.470267
H	1.270083	0.858977	1.660790
H	-4.779517	0.007921	0.032360
H	-3.519270	2.092793	-0.526006
H	-1.073556	2.086880	-0.615961
H	-1.058669	-2.087722	0.491587
H	-3.501476	-2.078299	0.526106

1d (TS1, DMF)

ΔG = -731.239072 hartree

N	-2.225361	-1.516432	0.627917
C	-2.934239	-2.791916	0.728793
C	-2.700083	-0.584619	1.645804
C	-2.263111	-0.952498	-0.748242
O	-3.398162	-0.446654	-1.203264
H	-2.562220	-3.483721	-0.034701
H	-4.028441	-2.692709	0.596733
H	-2.756734	-3.244091	1.713075
H	-3.782763	-0.373535	1.575644
H	-2.164185	0.364629	1.556436
H	-2.504297	-0.997032	2.643452
H	-1.798443	-1.734073	-1.398203
N	0.805154	0.958068	0.057441
C	-0.269493	1.047451	-0.914882
C	-1.170842	2.263111	-0.808011
C	-0.436359	3.564309	-0.458774
C	0.356727	3.318285	0.822992
C	1.371570	2.191638	0.636677
C	3.415750	-2.393326	-0.220048
C	3.792819	-1.251231	0.492506
C	2.951545	-0.140014	0.583072
C	1.670631	-0.134176	-0.031240
C	1.310674	-1.295035	-0.764743
C	2.164444	-2.394059	-0.847672
H	-1.280878	-0.044136	-0.753786
H	0.099400	0.872266	-1.937752
H	-1.933885	2.094729	-0.032240
H	-1.715252	2.362420	-1.753198
H	-1.150202	4.387082	-0.324704
H	0.245324	3.852516	-1.271786
H	-0.338243	3.061204	1.634205
H	0.904882	4.212450	1.142316
H	1.805219	1.952395	1.612156
H	2.195600	2.554919	-0.004265
H	4.076882	-3.251810	-0.290120
H	4.762406	-1.211270	0.982979
H	3.306805	0.719838	1.135023
H	0.344611	-1.343365	-1.246347
H	1.840968	-3.264443	-1.413704

1d (A, DMF)

ΔG = -482.157181 hartree

N	-0.563439	0.011392	-0.043272
C	-1.289941	-1.270057	0.031555
C	-2.704845	-1.096110	0.591426
C	-3.484334	-0.019355	-0.168951
C	-2.709265	1.305642	-0.101687
C	-1.269413	1.131047	-0.473137
C	3.677324	0.023683	0.047664

C	2.950167	1.196646	0.286336
C	1.556788	1.194948	0.258807
C	0.839717	0.006396	-0.015530
C	1.580886	-1.172213	-0.261346
C	2.976545	-1.155925	-0.222999
H	-0.723872	-1.946007	0.675584
H	-1.340027	-1.723166	-0.971222
H	-2.640888	-0.822367	1.653096
H	-3.213019	-2.065537	0.538308
H	-4.487772	0.101302	0.254517
H	-3.606118	-0.323696	-1.217276
H	-2.797775	1.704241	0.928200
H	-3.158780	2.059169	-0.757722
H	-0.676090	1.982174	-0.779136
H	4.762568	0.030164	0.072703
H	3.471072	2.123459	0.511428
H	1.019609	2.109600	0.483453
H	1.075662	-2.099809	-0.501992
H	3.517719	-2.077493	-0.419865

1d (B, DMF)

ΔG = -482.035076 hartree

N	-0.583655	-0.020114	-0.055209
C	-1.284888	1.068391	0.696470
C	-2.748998	1.190376	0.291946
C	-3.428387	-0.182012	0.293063
C	-2.696305	-1.123167	-0.669222
C	-1.220608	-0.970309	-0.659999
C	3.643558	-0.016712	0.031183
C	2.957247	1.068638	-0.524208
C	1.561882	1.080365	-0.552848
C	0.868671	-0.012451	-0.025956
C	1.537892	-1.102221	0.535255
C	2.934793	-1.099020	0.558953
H	-0.731628	1.987390	0.500816
H	-1.166647	0.825918	1.757454
H	-2.818216	1.647345	-0.702357
H	-3.234979	1.871483	0.996043
H	-4.476421	-0.097282	-0.004028
H	-3.411430	-0.603944	1.304189
H	-3.007172	-0.965021	-1.713589
H	-2.911797	-2.180673	-0.471162
H	-0.610255	-1.690510	-1.199186
H	4.728636	-0.016734	0.053300
H	3.505933	1.906507	-0.941612
H	1.029058	1.913635	-0.998546
H	0.978287	-1.929145	0.960285
H	3.463087	-1.939441	0.997035

1d (TS2, DMF)

ΔG = -1676.765394 hartree

N	0.969604	0.921820	0.165184
C	1.243066	2.208599	-0.518091
C	0.125445	3.235645	-0.305776
C	-0.446474	3.120671	1.106620
C	-1.088264	1.736618	1.283577
C	-0.302482	0.630466	0.584749
S	-1.410459	-0.003160	-1.221650
S	-3.266745	-0.594246	-0.527223
S	-3.207250	-2.354822	0.435728
C	3.947316	-2.100098	0.024642
C	3.904567	-1.107493	-0.956482
C	2.923451	-0.112916	-0.924253
C	1.963418	-0.098329	0.101828
C	2.024197	-1.086944	1.102270
C	3.000975	-2.080471	1.054860
H	-0.378698	-0.337723	1.063364
H	1.375022	2.029869	-1.590875
H	2.193200	2.582732	-0.122977
H	-0.673733	3.078445	-1.038726
H	0.541902	4.230147	-0.492635
H	-1.189830	3.901120	1.293817
H	0.357273	3.258803	1.840140
H	-2.122533	1.738042	0.931045
H	-1.125905	1.465419	2.346107
H	4.710668	-2.871199	-0.005413
H	4.633123	-1.103663	-1.761674
H	2.910097	0.634622	-1.707124
H	1.331299	-1.067225	1.936285
H	3.030851	-2.830980	1.839034

1d (C, DMF)

ΔG = -1676.766518 hartree

N	0.937686	0.936646	0.146753
C	1.326149	2.337671	-0.113921
C	0.128240	3.178924	-0.557137
C	-1.019122	3.161731	0.471329
C	-1.049120	1.835813	1.260392
C	-0.388819	0.669874	0.534705
S	-1.457643	0.176730	-1.087406
S	-3.177068	-0.705082	-0.280117
S	-2.786097	-2.525188	0.458467
C	3.859929	-2.132389	-0.050229
C	4.235387	-0.786427	-0.024510
C	3.276624	0.225935	0.036740
C	1.900107	-0.086958	0.071378
C	1.527501	-1.449287	0.045026
C	2.498950	-2.449297	-0.014121
H	-0.450662	-0.245735	1.122330
H	2.079502	2.342331	-0.904800
H	1.787375	2.768919	0.786598
H	-0.225806	2.795332	-1.520679
H	0.475882	4.201416	-0.735188
H	-1.971112	3.315245	-0.045678
H	-0.907848	3.989325	1.179457
H	-2.070072	1.555119	1.533498
H	-0.494044	1.944818	2.201705
H	4.609767	-2.915773	-0.097350
H	5.286473	-0.512528	-0.042595

H	3.610271	1.254952	0.081438
H	0.484408	-1.739358	0.041100
H	2.180028	-3.487482	-0.040144

1d (TS3, DMF)

ΔG = -1676.727454 hartree

N	0.395170	1.071941	-0.065351
C	0.418626	2.356461	0.680191
C	-0.685539	3.316453	0.248655
C	-2.040524	2.607646	0.257202
C	-1.986626	1.402994	-0.686194
C	-0.815461	0.471109	-0.384826
S	-0.680383	-1.003040	-1.426626
S	-2.340317	-2.072959	-0.503785
S	-1.983417	-1.507692	1.495682
C	4.059457	-1.034804	0.193707
C	3.760491	-0.275021	-0.941487
C	2.542662	0.405259	-1.029973
C	1.622464	0.315705	0.018921
C	1.919638	-0.433713	1.162362
C	3.138923	-1.111399	1.244218
H	-1.321098	-0.255518	0.839266
H	1.407288	2.792346	0.520898
H	0.325871	2.130805	1.753071
H	-0.470654	3.697663	-0.757341
H	-0.677585	4.173128	0.930580
H	-2.838270	3.285760	-0.062672
H	-2.285963	2.279281	1.275545
H	-1.881927	1.750878	-1.723464
H	-2.911022	0.820570	-0.639074
H	5.006017	-1.562396	0.261155
H	4.472863	-0.209455	-1.758226
H	2.300907	1.001248	-1.904602
H	1.200955	-0.494205	1.973007
H	3.367640	-1.698766	2.128332

1d (2d, DMF)

ΔG = -879.812294 hartree

N	0.498162	-0.307619	-0.028769
C	1.033551	-1.698289	0.052147
C	2.507529	-1.798808	-0.312493
C	3.289007	-0.703600	0.408395
C	2.758236	0.661056	-0.036503
C	1.244048	0.807456	-0.039278
S	0.578293	2.367179	-0.101873
C	-3.734493	-0.286282	0.056108
C	-3.058658	-0.351550	-1.166940
C	-1.661710	-0.338833	-1.198679
C	-0.947144	-0.250815	-0.001576
C	-1.613242	-0.197572	1.225288
C	-3.010412	-0.211859	1.250534
H	0.418513	-2.309258	-0.613266
H	0.863675	-2.053535	1.076235
H	2.633143	-1.694744	-1.397403
H	2.860277	-2.798002	-0.037671
H	4.358938	-0.768366	0.186872
H	3.176790	-0.818306	1.494217
H	3.084943	0.868557	-1.064469
H	3.161631	1.470501	0.575912
H	-4.820018	-0.297842	0.078446
H	-3.616596	-0.413490	-2.096359
H	-1.127745	-0.389032	-2.142618
H	-1.042898	-0.137338	2.146988
H	-3.530752	-0.166091	2.202452

1e (1e, DMPU)

ΔG = -443.505290 hartree

N	-0.846490	0.000003	-0.000053
C	-1.659978	1.218742	-0.012979
C	-3.078213	0.705985	-0.304051
C	-3.078203	-0.705989	0.304077
C	-1.659967	-1.218744	0.012992
C	3.375045	-0.000002	0.000017
C	2.658201	1.199165	0.086107
C	1.263398	1.210302	0.088312
C	0.527279	0.000005	-0.000024
C	1.263395	-1.210296	-0.088333
C	2.658197	-1.199167	-0.086091
H	-1.308505	1.918863	-0.780487
H	-1.610994	1.738459	0.957017
H	-3.238504	0.650379	-1.386880
H	-3.848369	1.357152	0.118072
H	-3.848360	-1.357163	-0.118035
H	-3.238485	-0.650382	1.386908
H	-1.611001	-1.738531	-0.956966
H	-1.308460	-1.918805	0.780541
H	4.460610	-0.000005	0.000032
H	3.189349	2.145087	0.157114
H	0.741947	2.157446	0.167239
H	0.741939	-2.157438	-0.167271
H	3.189342	-2.145091	-0.157080

1e (TS1, DMPU)

ΔG = -863.963086 hartree

N	1.747771	1.063684	-0.099690
C	2.289579	2.141867	0.736564
C	1.656158	3.406775	0.142073
C	0.294453	2.912110	-0.385279
C	0.525301	1.451845	-0.763023
C	3.603396	-2.712100	-0.508933
C	4.099028	-1.765599	0.397721
C	3.489162	-0.521092	0.553238
C	2.344056	-0.168911	-0.212268
C	1.842385	-1.142111	-1.119775
C	2.466504	-2.380594	-1.257690
H	3.382806	2.162396	0.681541
H	2.011371	2.005951	1.793781
H	2.277003	3.769277	-0.685686

H	1.571882	4.212119	0.878406
H	-0.068749	3.506426	-1.229885
H	-0.470410	2.970816	0.401296
H	0.542265	1.233053	-1.837611
H	-0.690291	0.789387	-0.262102
H	4.082442	-3.679873	-0.621551
H	4.972512	-1.998470	1.002143
H	3.895683	0.174466	1.278480
H	0.954732	-0.924338	-1.701479
H	2.052487	-3.099160	-1.961251
N	-1.542656	-0.753396	1.091411
C	-0.823493	-0.294560	2.273568
C	-1.898371	0.387954	0.190293
O	-2.537194	1.401238	0.732837
N	-2.495916	-0.210680	-1.048671
C	-2.782945	0.807522	-2.053024
C	-3.706338	-0.991517	-0.758188
C	-3.396058	-2.114209	0.229245
C	-2.716711	-1.547260	1.474247
H	0.055177	0.282066	1.970622
H	-0.480602	-1.162209	2.850351
H	-1.437229	0.339506	2.938112
H	-1.885184	1.397974	-2.255924
H	-3.584172	1.505124	-1.750507
H	-3.090089	0.320321	-2.986595
H	-4.086991	-1.406194	-1.701069
H	-4.507128	-0.346170	-0.344638
H	-2.731380	-2.846704	-0.246559
H	-4.320941	-2.634376	0.507996
H	-2.387007	-2.360625	2.134082
H	-3.441662	-0.938641	2.051369

1e (A, DMPU)

ΔG = -442.862089 hartree

N	-0.869929	0.050094	-0.006362
C	-1.686927	-1.178744	0.023249
C	-3.104053	-0.665817	0.325423
C	-3.105373	0.769054	-0.242603
C	-1.672582	1.182647	-0.078459
C	3.353437	-0.016276	0.005419
C	2.620095	-1.203691	-0.110574
C	1.225664	-1.191437	-0.113517
C	0.516888	0.028775	0.001677
C	1.264121	1.226607	0.125749
C	2.657757	1.193193	0.124078
H	-1.315844	-1.870566	0.784675
H	-1.634462	-1.682816	-0.951698
H	-3.263374	-0.638371	1.408377
H	-3.872141	-1.305894	-0.115174
H	-3.806485	1.429249	0.279230
H	-3.405410	0.763548	-1.304743
H	-1.252955	2.101397	-0.469261
H	4.438792	-0.033222	0.005597
H	3.136729	-2.155045	-0.205429
H	0.689871	-2.127656	-0.218722
H	0.755498	2.176123	0.244064
H	3.205112	2.126727	0.224967

1e (B, DMPU)

ΔG = -442.738774 hartree

N	0.887108	-0.034195	-0.044564
C	1.712032	0.997071	0.667834
C	3.147944	0.669141	0.221769
C	3.065536	-0.774373	-0.333036
C	1.613529	-0.966096	-0.567183
C	-3.330002	0.011355	0.000856
C	-2.622452	1.168965	-0.338974
C	-1.227043	1.165050	-0.348981
C	-0.552622	-0.015298	-0.021751
C	-1.245819	-1.178087	0.329457
C	-2.641467	-1.158435	0.334945
H	1.535570	0.859634	1.738088
H	1.374111	1.991766	0.379365
H	3.851636	0.754752	1.049891
H	3.462469	1.355025	-0.567655
H	3.398945	-1.536694	0.385502
H	3.639443	-0.938603	-1.249536
H	1.153279	-1.791404	-1.100610
H	-4.415153	0.023013	0.010380
H	-3.154284	2.077422	-0.601719
H	-0.680645	2.058208	-0.630311
H	-0.706604	-2.074589	0.617168
H	-3.186332	-2.054931	0.611775

1e (TS2, DMPU)

ΔG = -1637.478107 hartree

N	-0.965335	1.084463	-0.291839
C	-1.370216	2.494578	-0.032551
C	-0.044551	3.268324	-0.109272
C	0.860459	2.355789	-0.955819
C	0.315715	0.990121	-0.651922
S	1.626959	0.317045	1.335157
S	3.280512	-0.489592	0.418418
S	2.806438	-1.988566	-0.845800
C	-3.661903	-2.135152	0.180514
C	-4.117190	-0.815374	0.231431
C	-3.226952	0.249389	0.081011
C	-1.861170	-0.003139	-0.127399
C	-1.398425	-1.329975	-0.174237
C	-2.300382	-2.382643	-0.021446
H	0.666804	0.090128	-1.141199
H	-1.860362	2.568711	0.940534
H	-2.078102	2.800602	-0.809669
H	0.380128	3.386611	0.891393
H	-0.177379	4.259202	-0.546341
H	1.925134	2.452561	-0.743723
H	0.715236	2.531357	-2.032075
H	-4.357141	-2.960177	0.299010
H	-5.170767	-0.605396	0.387460

H	-3.604307	1.263911	0.116794
H	-0.346300	-1.549674	-0.309863
H	-1.930427	-3.402772	-0.055702

1e (C, DMPU)

ΔG = -1637.480874 hartree

N	-0.940191	1.034244	-0.194561
C	-1.298779	2.456587	-0.020043
C	0.043958	3.193653	-0.140107
C	0.908016	2.230228	-0.967775
C	0.423550	0.857982	-0.508916
S	1.376099	0.283224	1.128569
S	3.251834	-0.300169	0.394917
S	3.138475	-2.043046	-0.582747
C	-3.796853	-2.068175	0.074803
C	-4.175885	-0.730954	0.226969
C	-3.234016	0.295311	0.145833
C	-1.874104	0.001775	-0.095758
C	-1.494694	-1.351277	-0.242234
C	-2.450085	-2.364066	-0.159540
H	0.614045	0.040317	-1.204966
H	-1.785125	2.621893	0.946698
H	-1.999297	2.755220	-0.810554
H	0.485810	3.340598	0.850177
H	-0.068003	4.173056	-0.609870
H	1.982217	2.370210	-0.834165
H	0.682864	2.325412	-2.037492
H	-4.533841	-2.862409	0.139516
H	-5.215893	-0.476402	0.410511
H	-3.560572	1.321349	0.264399
H	-0.458545	-1.619338	-0.407930
H	-2.131514	-3.396148	-0.275603

1e (TS3, DMPU)

ΔG = -1637.439202 hartree

N	-0.572983	1.085269	-0.134929
C	-0.768784	2.491062	-0.579742
C	0.556281	3.169705	-0.227951
C	1.579764	2.028497	-0.346086
C	0.774578	0.784745	0.024064
S	1.219827	-0.192778	1.484820
S	2.958296	-1.121819	0.600171
S	2.179828	-1.476649	-1.334957
C	-3.847675	-1.593052	0.049058
C	-4.027887	-0.230588	0.302950
C	-2.948799	0.652419	0.247386
C	-1.660233	0.181213	-0.069122
C	-1.482803	-1.191089	-0.328697
C	-2.568964	-2.063032	-0.267744
H	1.294861	-0.281040	-1.020930
H	-1.618398	2.940350	-0.066258
H	-0.974619	2.495889	-1.657598
H	0.521334	3.542998	0.800487
H	0.774292	4.009185	-0.891636
H	2.453526	2.153502	0.295400
H	1.937562	1.937532	-1.379636
H	-4.689763	-2.276588	0.092852
H	-5.012112	0.153744	0.553009
H	-3.117857	1.699712	0.464775
H	-0.506266	-1.574870	-0.592542
H	-2.411752	-3.116646	-0.478664

1e (2e, DMPU)

ΔG = -840.527112 hartree

N	0.660399	-0.450727	0.029260
C	1.249901	-1.798003	0.228032
C	2.728894	-1.580765	-0.123184
C	2.943718	-0.080160	0.145347
C	1.565756	0.537337	-0.012116
S	1.251300	2.182656	-0.172294
C	-3.542198	-0.025845	-0.000724
C	-2.855260	-0.276980	-1.192804
C	-1.463673	-0.406909	-1.187089
C	-0.765463	-0.279017	0.016920
C	-1.444954	-0.032043	1.213616
C	-2.836349	0.095610	1.200870
H	0.743283	-2.518664	-0.417838
H	1.101782	-2.102538	1.271294
H	2.895449	-1.800982	-1.181892
H	3.388862	-2.219773	0.466675
H	3.666387	0.393917	-0.520976
H	3.275643	0.107946	1.174498
H	-4.623417	0.073554	-0.007647
H	-3.399935	-0.372133	-2.127187
H	-0.920048	-0.600879	-2.106471
H	-0.887296	0.063270	2.139924
H	-3.366531	0.289526	2.128305

1e (1e, DMF)

ΔG = -443.505307 hartree

N	-0.846490	0.000003	-0.000053
C	-1.659978	1.218742	-0.012979
C	-3.078213	0.705985	-0.304051
C	-3.078203	-0.705989	0.304077
C	-1.659967	-1.218744	0.012992
C	3.375045	-0.000002	0.000017
C	2.658201	1.199165	0.086107
C	1.263398	1.210302	0.088312
C	0.527279	0.000005	-0.000024
C	1.263395	-1.210296	-0.088333
C	2.658197	-1.199167	-0.086091
H	-1.308505	1.918863	-0.780487
H	-1.610994	1.738459	0.957017
H	-3.238504	0.650379	-1.386880
H	-3.848369	1.357152	0.118072
H	-3.848360	-1.357163	-0.118035
H	-3.238485	-0.650382	1.386908
H	-1.611001	-1.738531	-0.956966

H	-1.308460	-1.918805	0.780541
H	4.460610	-0.000005	0.000032
H	3.189349	2.145087	0.157114
H	0.741947	2.157446	0.167239
H	0.741939	-2.157438	-0.167271
H	3.189342	-2.145091	-0.157080

1e (TS1, DMF)

ΔG = -691.945735 hartree

N	-3.125707	-1.391916	0.233621
C	-2.912927	-1.975215	-1.083710
C	-4.147335	-0.354247	0.201056
C	-1.858223	-0.960686	0.881841
O	-1.966689	-0.421803	2.083484
H	-2.140439	-2.750239	-1.026336
H	-2.595659	-1.234329	-1.842530
H	-3.837777	-2.442454	-1.441780
H	-3.904415	0.464579	-0.505254
H	-4.250841	0.076613	1.198719
H	-5.108664	-0.785249	-0.102859
H	-1.176015	-1.844044	0.799674
N	0.811223	1.102951	-0.231112
C	0.973298	2.462702	0.300674
C	-0.128921	3.257635	-0.412185
C	-1.238794	2.208631	-0.632972
C	-0.497203	0.888886	-0.795644
C	3.815435	-1.857999	0.023784
C	3.995971	-0.602062	0.619131
C	3.008752	0.380515	0.553488
C	1.783231	0.139015	-0.126320
C	1.606125	-1.143045	-0.717709
C	2.606419	-2.109971	-0.639222
H	1.972994	2.849696	0.075443
H	0.846901	2.480372	1.394370
H	0.246989	3.621024	-1.375713
H	-0.456825	4.123567	0.171545
H	-1.873132	2.439865	-1.494484
H	-1.894191	2.174142	0.249400
H	-0.467199	0.470905	-1.809197
H	-1.263777	-0.134234	0.045882
H	4.588342	-2.618254	0.081551
H	4.918657	-0.381043	1.150515
H	3.182597	1.333288	1.040435
H	0.677381	-1.373146	-1.225335
H	2.435006	-3.078830	-1.102769

1e (A, DMF)

ΔG = -442.868708 hartree

N	-0.869929	0.050094	-0.006362
C	-1.686927	-1.178744	0.023249
C	-3.104053	-0.665817	0.325423
C	-3.105373	0.769054	-0.242603
C	-1.672582	1.182647	-0.078459
C	3.353437	-0.016276	0.005419
C	2.620095	-1.203691	-0.110574
C	1.225664	-1.191437	-0.113517
C	0.516888	0.028775	0.001677
C	1.264121	1.226607	0.125749
C	2.657757	1.193193	0.124078
H	-1.315844	-1.870566	0.784675
H	-1.634462	-1.682816	-0.951698
H	-3.263374	-0.638371	1.408377
H	-3.872141	-1.305894	-0.115174
H	-3.806485	1.429249	0.279230
H	-3.405410	0.763548	-1.304743
H	-1.252955	2.101397	-0.469261
H	4.438792	-0.033222	0.005597
H	3.136729	-2.155045	-0.205429
H	0.689871	-2.127656	-0.218722
H	0.755498	2.176123	0.244064
H	3.205112	2.126727	0.224967

1e (B, DMF)

ΔG = -442.742188 hartree

N	0.887108	-0.034195	-0.044564
C	1.712032	0.997071	0.667834
C	3.147944	0.669141	0.221769
C	3.065536	-0.774373	-0.333036
C	1.613529	-0.966096	-0.567183
C	-3.330002	0.011355	0.000856
C	-2.622452	1.168965	-0.338974
C	-1.227043	1.165050	-0.348981
C	-0.552622	-0.015298	-0.021751
C	-1.245819	-1.178087	0.329457
C	-2.641467	-1.158435	0.334945
H	1.535570	0.859634	1.738088
H	1.374111	1.991766	0.379365
H	3.851636	0.754752	1.049891
H	3.462469	1.355025	-0.567655
H	3.398945	-1.536694	0.385502
H	3.639443	-0.938603	-1.249536
H	1.153279	-1.791404	-1.100610
H	-4.415153	0.023013	0.010380
H	-3.154284	2.077422	-0.601719
H	-0.680645	2.058208	-0.630311
H	-0.706604	-2.074589	0.617168
H	-3.186332	-2.054931	0.611775

1e (TS2, DMF)

ΔG = -1637.481493 hartree

N	-0.965436	1.084267	-0.291610
C	-1.370354	2.494374	-0.032468
C	-0.044765	3.268207	-0.109530
C	0.860108	2.355643	-0.956166
C	0.315809	0.989874	-0.651589
S	1.626063	0.317572	1.334048
S	3.280530	-0.488002	0.417931
S	2.808162	-1.989813	-0.843479

C	-3.662136	-2.135354	0.180009
C	-4.117299	-0.815549	0.231521
C	-3.227017	0.249215	0.081375
C	-1.861258	-0.003281	-0.127368
C	-1.398657	-1.330170	-0.174777
C	-2.300660	-2.382845	-0.022265
H	0.666482	0.090118	-1.141613
H	-1.860356	2.568684	0.940680
H	-2.078365	2.800271	-0.809523
H	0.380100	3.386665	0.891042
H	-0.177753	4.259021	-0.546695
H	1.924859	2.452806	-0.744622
H	0.714290	2.530830	-2.032395
H	-4.357419	-2.960374	0.298267
H	-5.170836	-0.605546	0.387791
H	-3.604309	1.263741	0.117611
H	-0.346582	-1.549901	-0.310700
H	-1.930786	-3.402989	-0.057019

1e (C, DMF)

ΔG = -1637.484102 hartree

N	-0.940247	1.034190	-0.194620
C	-1.298765	2.456524	-0.019897
C	0.044022	3.193527	-0.139999
C	0.907855	2.230061	-0.967885
C	0.423478	0.857892	-0.508877
S	1.376257	0.283331	1.128649
S	3.251834	-0.299874	0.394412
S	3.138607	-2.043256	-0.582399
C	-3.796934	-2.068131	0.074755
C	-4.175984	-0.730892	0.226795
C	-3.234098	0.295360	0.145727
C	-1.874167	0.001767	-0.095716
C	-1.494734	-1.351280	-0.242045
C	-2.450146	-2.364067	-0.159417
H	0.613960	0.040052	-1.204724
H	-1.784962	2.621740	0.946940
H	-1.999428	2.755264	-0.810222
H	0.485972	3.340311	0.850254
H	-0.067824	4.172958	-0.609701
H	1.982092	2.370091	-0.834629
H	0.682335	2.325236	-2.037532
H	-4.533928	-2.862360	0.139418
H	-5.216012	-0.476335	0.410186
H	-3.560620	1.321412	0.264201
H	-0.458571	-1.619321	-0.407693
H	-2.131604	-3.396165	-0.275386

1e (TS3, DMF)

ΔG = -1637.439300 hartree

N	-0.572686	1.085389	-0.135593
C	-0.768212	2.490562	-0.582367
C	0.555911	3.170018	-0.228675
C	1.580091	2.029144	-0.344503
C	0.774763	0.785091	0.024567
S	1.218523	-0.192965	1.485183
S	2.957161	-1.123416	0.601558
S	2.180768	-1.475610	-1.334857
C	-3.847288	-1.592881	0.048775
C	-4.026846	-0.230978	0.306227
C	-2.947727	0.651990	0.250597
C	-1.659962	0.181243	-0.069657
C	-1.483115	-1.190435	-0.332625
C	-2.569288	-2.062389	-0.271566
H	1.295889	-0.279919	-1.020431
H	-1.619241	2.939946	-0.071346
H	-0.971658	2.494003	-1.660692
H	0.519041	3.543841	0.799503
H	0.774703	4.009208	-0.892464
H	2.452534	2.154723	0.298676
H	1.939978	1.938036	-1.377308
H	-4.689403	-2.276383	0.092607
H	-5.010523	0.152846	0.559198
H	-3.115964	1.698814	0.471003
H	-0.507049	-1.573616	-0.599168
H	-2.412697	-3.115549	-0.485196

1e (2e, DMF)

ΔG = -840.527162 hartree

N	0.660399	-0.450727	0.029260
C	1.249901	-1.798003	0.228032
C	2.728894	-1.580765	-0.123184
C	2.943718	-0.080160	0.145347
C	1.565756	0.537337	-0.012116
S	1.251300	2.182656	-0.172294
C	-3.542198	-0.025845	-0.000724
C	-2.855260	-0.276980	-1.192804
C	-1.463673	-0.406909	-1.187089
C	-0.765463	-0.279017	0.016920
C	-1.444954	-0.032043	1.213616
C	-2.836349	0.095610	1.200870
H	0.743283	-2.518664	-0.417838
H	1.101782	-2.102538	1.271294
H	2.895449	-1.800982	-1.181892
H	3.388862	-2.219773	0.466675
H	3.666387	0.393917	-0.520976
H	3.275643	0.107946	1.174498
H	-4.623417	0.073554	-0.007647
H	-3.399935	-0.372133	-2.127187
H	-0.920048	-0.600879	-2.106471
H	-0.887296	0.063270	2.139924
H	-3.366531	0.289526	2.128305

DMPU •⁻

ΔG = -420.523282 hartree

N	-1.194827	-0.102196	-0.471326
C	-2.428466	-0.858910	-0.308922
C	0.000000	-0.897435	-0.148919

O	-0.000001	-1.645325	0.927130
N	1.194827	-0.102198	-0.471326
C	2.428465	-0.858912	-0.308920
C	1.255120	1.169611	0.272418
C	0.000001	1.997308	-0.004758
C	-1.255118	1.169611	0.272421
H	-2.359483	-1.796290	-0.871253
H	-3.269536	-0.276074	-0.704764
H	-2.652833	-1.113274	0.742402
H	2.359477	-1.796298	-0.871240
H	2.652839	-1.113264	0.742405
H	3.269534	-0.276082	-0.704775
H	2.152516	1.720001	-0.039692
H	1.349714	0.990431	1.363179
H	-0.000001	2.315402	-1.055430
H	0.000002	2.900735	0.617268
H	-2.152516	1.720001	-0.039684
H	-1.349708	0.990428	1.363182

DMPU_H ⁻

ΔG = -421.155930 hartree

N	-0.268203	-0.189857	1.216022
C	0.347321	-0.704128	2.435287
O	0.517227	-2.071307	0.000000
N	-0.268203	-0.189857	-1.216022
C	0.347321	-0.704128	-2.435287
C	-0.268203	1.273902	-1.246070
C	-0.936563	1.845680	0.000000
C	-0.268203	1.273902	1.246070
H	0.346011	-1.793897	2.416928
H	-0.217674	-0.356308	3.307918
H	1.397683	-0.363688	2.557127
H	0.346011	-1.793897	-2.416928
H	1.397683	-0.363688	-2.557127
H	-0.217674	-0.356308	-3.307918
H	-0.788310	1.607714	-2.153019
H	0.769346	1.669059	-1.313204
H	-2.003654	1.592167	0.000000
H	-0.855092	2.939752	0.000000
H	-0.788310	1.607714	2.153019
H	0.769346	1.669059	1.313204
C	0.443421	-0.748733	0.000000
H	1.471082	-0.248203	0.000000

DMPU_H$_2$

ΔG = -421.642128 hartree

N	-1.205763	-0.062410	-0.274020
C	-2.417895	-0.763689	0.158786
N	1.205763	-0.062421	-0.274020
C	2.417892	-0.763703	0.158792
C	1.241980	1.340832	0.163285
C	0.000005	2.083670	-0.312567
C	-1.241971	1.340841	0.163293
H	-2.427019	-1.780523	-0.234631
H	-3.289688	-0.232727	-0.233080
H	-2.510804	-0.809774	1.260126
H	2.427000	-1.780545	-0.234601
H	2.510807	-0.809763	1.260133
H	3.289687	-0.232756	-0.233091
H	2.151003	1.795226	-0.243550
H	1.313224	1.408148	1.267513
H	0.000001	2.148132	-1.406472
H	0.000011	3.104188	0.085899
H	-2.150994	1.795241	-0.243534
H	-1.313207	1.408154	1.267522
C	-0.000002	-0.755554	0.173673
H	-0.000004	-0.855810	1.286524
O	0.000005	-2.058151	-0.389353
H	-0.000119	-2.712552	0.320766

DMF •⁻

ΔG = -248.510913 hartree

N	-0.362581	-0.017934	-0.312967
C	-0.480359	1.386172	0.057061
C	-1.561349	-0.763989	0.040095
C	0.859665	-0.646780	0.163508
O	2.001557	-0.044064	-0.026778
H	0.427725	1.916803	-0.232630
H	-0.616792	1.512833	1.153043
H	-1.338620	1.837505	-0.452398
H	-1.771158	-0.736907	1.128934
H	-1.447295	-1.812790	-0.253984
H	-2.429553	-0.353165	-0.486026
H	0.793554	-1.738648	-0.015928

DMF_H ⁻

ΔG = -249.133982 hartree

N	-0.389458	0.006588	-0.369713
C	-0.549167	1.381577	0.086903
C	-1.560837	-0.785110	-0.015786
O	2.012505	0.008780	-0.142903
H	0.347418	1.951308	-0.165029
H	-0.698364	1.444903	1.186569
H	-1.415383	1.847179	-0.397453
H	-1.732483	-0.833225	1.080349
H	-1.444995	-1.811454	-0.381698
H	-2.460973	-0.358238	-0.472228
C	0.865373	-0.605986	0.207325
H	0.798033	-1.673978	-0.118880
H	0.700694	-0.625733	1.328930

DMF_H$_2$

ΔG = -249.625339 hartree

N	-0.416395	-0.000378	-0.304225
C	-0.605554	1.395687	0.092013
C	-1.616341	-0.799582	-0.058667
H	0.300519	1.964845	-0.125235

H	-0.835637	1.497885	1.169480
H	-1.432185	1.829229	-0.478262
H	-1.893378	-0.844116	1.011116
H	-1.464843	-1.821869	-0.417954
H	-2.458224	-0.364878	-0.605105
O	1.922025	-0.026635	-0.294539
H	2.620436	0.022281	0.371573
C	0.753586	-0.591697	0.306158
H	0.722334	-1.672729	0.123571
H	0.789395	-0.421370	1.399679

DMA •⁻

ΔG = -287.804456 hartree

N	0.608883	0.084588	-0.292067
C	1.596305	-0.953120	-0.007718
C	1.126119	1.396253	0.088968
C	-0.725006	-0.242853	0.202090
O	-1.119566	-1.476235	0.033223
H	1.213474	-1.921316	-0.328058
H	1.827657	-1.017207	1.076681
H	2.526019	-0.734091	-0.543099
H	1.218898	1.507009	1.189551
H	0.483633	2.197430	-0.280219
H	2.119110	1.536412	-0.350142
C	-1.757069	0.849163	-0.049805
H	-1.508365	1.823023	0.381781
H	-1.915261	0.999984	-1.142667
H	-2.712908	0.529865	0.373649

DMA_H⁻

ΔG = -288.426681 hartree

N	0.630704	0.078939	-0.348374
C	1.571586	-0.993688	-0.034829
C	1.200052	1.354910	0.079853
O	-1.181816	-1.444019	-0.029539
H	1.147333	-1.949226	-0.342807
H	1.797236	-1.053459	1.052004
H	2.517689	-0.827271	-0.563046
H	1.286857	1.434262	1.184477
H	0.598559	2.196198	-0.271506
H	2.206887	1.469503	-0.337253
C	-0.723654	-0.213003	0.281622
H	-0.544876	-0.092951	1.396213
C	-1.717000	0.905696	-0.121336
H	-1.447076	1.905182	0.241260
H	-1.812848	0.941477	-1.214536
H	-2.696068	0.652379	0.298270

DMA_H₂

ΔG = -288.918299 hartree

N	0.655697	0.017634	-0.310802
C	1.534429	-1.082793	0.101706
C	1.301611	1.306160	-0.048204
H	1.065809	-2.039602	-0.129673
H	1.759592	-1.054280	1.184771
H	2.479015	-1.014691	-0.445271
H	1.430739	1.510403	1.031356
H	0.736608	2.127205	-0.492114
H	2.293667	1.297795	-0.507551
O	-1.238085	-1.303306	-0.265694
H	-1.933896	-1.610771	0.331379
C	-0.666729	-0.106219	0.290179
H	-0.580074	-0.245715	1.387626
C	-1.580476	1.084847	0.008860
H	-1.264502	1.983594	0.545420
H	-1.612808	1.297979	-1.064630
H	-2.592359	0.839125	0.344606

Acetone •⁻

ΔG = -193.181295 hartree

C	1.273429	-0.624623	0.025787
C	0.000000	0.157086	-0.251186
O	0.000001	1.440061	0.061381
C	-1.273430	-0.624622	0.025788
H	-1.414143	-0.782924	1.121346
H	-1.271338	-1.618833	-0.440121
H	-2.158285	-0.082011	-0.327918
H	1.414151	-0.782900	1.121348
H	2.158289	-0.082029	-0.327936
H	1.271325	-1.618843	-0.440102

Acetone_H⁻

ΔG = -193.804116 hartree

C	1.259543	-0.639840	-0.087553
C	0.000000	0.159455	0.333812
O	-0.000001	1.447064	-0.149911
C	-1.259543	-0.639840	-0.087553
H	0.000000	0.138213	1.457914
H	-1.283407	-1.650042	0.347911
H	-1.291543	-0.736336	-1.182180
H	-2.166718	-0.110311	0.228839
H	1.283408	-1.650042	0.347910
H	2.166718	-0.110310	0.228840
H	1.291544	-0.736334	-1.182180

Acetone_H₂

ΔG = -194.305930 hartree

C	1.183955	-0.807332	-0.103166
C	-0.002124	0.036360	0.362636
O	0.078025	1.378042	-0.166826
C	-1.342482	-0.529087	-0.088700
H	0.009155	0.094351	1.461408
H	0.916305	1.770178	0.114745
H	-1.488741	-1.534414	0.318807
H	-1.384668	-0.590103	-1.182100
H	-2.165646	0.104812	0.255464

H	1.125487	-1.817663	0.316516
H	2.133425	-0.365919	0.221287
H	1.194384	-0.885222	-1.196143

CH_3CN •⁻

ΔG = -132.804567 hartree

C	1.139243	0.091597	0.000000
C	-0.305447	-0.425321	0.000000
N	-1.361741	0.196206	0.000000
H	1.182256	1.196421	-0.000003
H	1.673579	-0.283762	-0.880759
H	1.673575	-0.283757	0.880764

CH_3CN_H⁻

ΔG = -133.414304 hartree

C	-1.155468	-0.147637	-0.000001
C	0.291444	0.375834	0.000002
N	1.355878	-0.296012	-0.000001
H	0.270724	1.513178	-0.000003
H	-1.702957	0.216827	0.882753
H	-1.171785	-1.243998	-0.000039
H	-1.702981	0.216893	-0.882713

CH_3CN_H_2

ΔG = -133.922204 hartree

C	-1.183124	-0.165994	-0.000057
C	0.188795	0.444749	-0.000073
N	1.314605	-0.160275	0.000050
H	0.218933	1.539852	-0.000068
H	1.172851	-1.176591	-0.000179
H	-1.741449	0.169418	0.882277
H	-1.141688	-1.259253	-0.004010
H	-1.744911	0.175974	-0.877588

S_3 •⁻ (DMPU)

ΔG = -1194.753853 hartree

S	1.712620	-0.367441	0.000000
S	0.000000	0.734404	0.000000
S	-1.712620	-0.366963	0.000000

S_3 •⁻ (DMF)

ΔG = -1194.754001 hartree

S	1.712560	-0.367470	0.000000
S	0.000000	0.734463	0.000000
S	-1.712560	-0.366993	0.000000

S_3 •⁻ (DMA)

ΔG = -1194.754035 hartree

S	1.712546	-0.367477	0.000000
S	0.000000	0.734477	0.000000
S	-1.712546	-0.367000	0.000000

S_3 •⁻ (Acetone)

ΔG = -1194.752102 hartree

S	1.713298	-0.367104	0.000000
S	0.000000	0.733729	0.000000
S	-1.713298	-0.366625	0.000000

S_3 •⁻ (CH_3CN)

ΔG = -1194.753901 hartree

S	1.712600	-0.367450	0.000000
S	0.000000	0.734423	0.000000
S	-1.712600	-0.366973	0.000000

HS_2 • (DMPU)

ΔG = -796.979074 hartree

S	0.040243	-0.966128	0.000000
S	0.040243	1.044086	0.000000
H	-1.287774	-1.247328	0.000000

HS_2 • (DMF)

ΔG = -796.979085 hartree

S	0.040243	-0.966127	0.000000
S	0.040243	1.044085	0.000000
H	-1.287768	-1.247319	0.000000

HS_2 • (DMA)

ΔG = -796.979087 hartree

S	0.040243	-0.966127	0.000000
S	0.040243	1.044085	0.000000
H	-1.287767	-1.247317	0.000000

HS_2 • (Acetone)

ΔG = -796.978955 hartree

S	0.040245	-0.966132	0.000000
S	0.040245	1.044097	0.000000
H	-1.287844	-1.247442	0.000000

HS_2 • (CH_3CN)

ΔG = -796.979078 hartree

S	0.040243	-0.966128	0.000000
S	0.040243	1.044086	0.000000
H	-1.287772	-1.247325	0.000000

S_2 •⁻ (DMPU)

ΔG = -796.540689 hartree

S	0.000000	0.000000	1.022522
S	0.000000	0.000000	-1.022522

S_2 •$^-$ (DMF)

ΔG = -796.540851 hartree

S	0.000000	0.000000	1.022523
S	0.000000	0.000000	-1.022523

S_2 •$^-$ (DMA)

ΔG = -796.540889 hartree

S	0.000000	0.000000	1.022524
S	0.000000	0.000000	-1.022524

S_2 •$^-$ (Acetone)

ΔG = -796.538768 hartree

S	0.000000	0.000000	1.022507
S	0.000000	0.000000	-1.022507

S_2 •$^-$ (CH_3CN)

ΔG = -796.540741 hartree

S	0.000000	0.000000	1.022522
S	0.000000	0.000000	-1.022522

S_2^{2-} (DMPU)

ΔG = -796.659387 hartree

S	0.000000	0.000000	1.103023
S	0.000000	0.000000	-1.103023

S_2^{2-} (DMF)

ΔG = -796.660017 hartree

S	0.000000	0.000000	1.103040
S	0.000000	0.000000	-1.103040

S_2^{2-} (DMA)

ΔG = -796.660165 hartree

S	0.000000	0.000000	1.103045
S	0.000000	0.000000	-1.103045

S_2^{2-} (Acetone)

ΔG = -796.651913 hartree

S	0.000000	0.000000	1.102835
S	0.000000	0.000000	-1.102835

S_2^{2-} (CH_3CN)

ΔG = -796.659590 hartree

S	0.000000	0.000000	1.103029
S	0.000000	0.000000	-1.103029