

**Experimental and theoretical researches on
cyclic(alkyl)(amino)carbene-copper (CAAC-Cu) catalyzed
Friedel-Crafts reaction of N, N-dialkylanilines with styrenes**

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1. General information

The manipulations which are sensitive to moisture or air were performed in a nitrogen-filled glove box (JMS-1X) or using standard Schlenk techniques unless stated otherwise. NMR spectra were recorded on a Bruker AV 500 (or Bruker AV 400) spectrometer. The NMR multiplicities are abbreviated as follows: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. All the solvents used for the reactions were distilled after drying over an appropriate drying agent. Commercially available reagents were purchased from TCI Chemical. Mass spectroscopy (MS) measurements were performed on a Shimadzu GCMS-TQ8040 NX. A Shimadzu GC-2014 system was used to monitor the reaction conversion.

2. Friedel-Crafts Reaction

(**Caution:** Sealed ampoules containing toluene at high temperature are under high pressure and explosion may happen. Only new ampoules can be used and the reaction should be performed behind a blast shield).

Procedure for the reactions listed in Table 1: Catalysts as mentioned in Table 1 were loaded in a dried brown ampoule (2 mL) equipped with magnetic stirrer bar. Toluene (0.8 mL), N, N-dimethylaniline (0.8 mmol) and α -methylstyrene (3.2 mmol) were added. The ampoule was sealed, placed in an oil bath, and heated at the specified temperature for 24 h. The conversions were determined by GC.

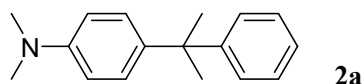
For 2a-p: (CAAC)CuCl (0.04 mmol) and $\text{KB}(\text{C}_6\text{F}_5)_4$ (0.04 mmol) were loaded in a dried brown ampoule (2 mL) equipped with magnetic stirrer bar. Toluene (0.8 mL), N,N-dialkylaniline (0.8 mmol) and styrenes (3.2 mmol) were added. The ampoule was sealed, placed in an oil bath, and heated at the indicated temperature for 24 h. The volatiles were removed under vacuum and the products were isolated by flash chromatography on silica gel (eluent: 2/98 ethyl acetate/ petroleum ether). In cases in which the aromatic amine cannot be separated from the products, the aromatic amines were removed under vacuum at 100 °C. Isolated yields are calculated in respect to N,N-dialkylaniline.

For 2q: (CAAC)CuCl (0.06 mmol) and $\text{KB}(\text{C}_6\text{F}_5)_4$ (0.06 mmol) were loaded in a dried brown ampoule (2 mL) equipped with magnetic stirrer bar. Toluene (0.6 mL), N,N-diethylaniline (0.6 mmol) and indene (2.4 mmol) were added. The ampoule was sealed, placed in an oil bath, and heated at the specified temperature for 72 h. The volatiles were removed under vacuum and the products were isolated by flash chromatography on silica gel (eluent: 1/99 ethyl acetate/ petroleum ether). Isolated yields are calculated in respect to N,N-diethylaniline.

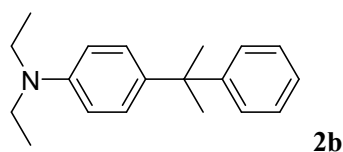


Figure S1. The photograph of the ampoule used in the experiment. It can be sealed using blowlamp after all samples are loaded.

3. ^{13}C NMR, ^1H NMR data and MS data for the hydroarylation products

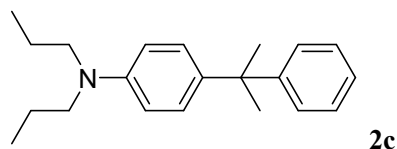


^{13}C NMR (100 MHz, Chloroform-*d*) δ 151.39 (C_{qaro}), 148.59 (C_{qaro}), 138.84 (C_{qaro}), 127.94 (CH_{aro}), 127.48 (CH_{aro}), 126.83 (CH_{aro}), 125.43 (CH_{aro}), 112.36 (CH_{aro}), 42.09 (C), 40.76 (CH_3), 30.95 (CH_3); ^1H NMR (400 MHz, Chloroform-*d*) δ 7.24 (d, J = 4.4 Hz, 4H), 7.21 – 7.12 (m, 1H), 7.10 (d, J = 8.9 Hz, 2H), 6.66 (d, J = 8.9 Hz, 2H), 2.89 (s, 6H), 1.65 (s, 6H); MS calculated m/e for $\text{C}_{17}\text{H}_{21}\text{N}$: 239.2, found: 239.2 (Relative abundance: 45%)

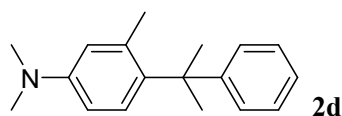


^{13}C NMR (100 MHz, Chloroform-*d*) δ 151.51 (C_{qaro}), 145.81 (C_{qaro}), 137.54 (C_{qaro}), 127.94 (CH_{aro}), 127.68 (CH_{aro}), 126.90 (CH_{aro}), 125.41 (CH_{aro}), 111.44 (CH_{aro}), 44.36 (CH_2), 42.03 (C),

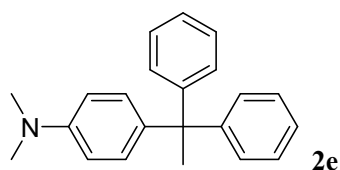
31.02 (CH₃), 12.81 (CH₃); ¹H NMR (400 MHz, Chloroform-*d*) δ 7.30 – 7.20 (m, 4H), 7.14 (d, *J* = 6.7 Hz, 1H), 7.06 (d, *J* = 8.9 Hz, 2H), 6.58 (d, *J* = 8.9 Hz, 2H), 3.29 (q, *J* = 7.0 Hz, 4H), 1.64 (s, 6H), 1.12 (t, *J* = 7.0 Hz, 6H); MS calculated m/e for C₁₉H₂₅N: 267.2, found: 267.2 (Relative abundance: 37%).



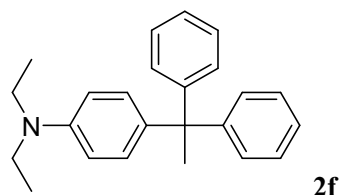
¹³C NMR (100 MHz, Chloroform-*d*) δ 151.48 (C_{q,aro}), 146.20 (C_{q,aro}), 137.27 (C_{q,aro}), 127.91 (CH_{aro}), 127.56 (CH_{aro}), 126.88 (CH_{aro}), 125.38 (CH_{aro}), 111.24 (CH_{aro}), 53.04 (CH₂), 41.98 (C), 30.98 (CH₃), 20.61 (CH₂), 11.58 (CH₃); ¹H NMR (400 MHz, Chloroform-*d*) δ 7.23 – 7.12 (m, 4H), 7.05 (q, *J* = 7.1 Hz, 1H), 6.96 (d, *J* = 8.5 Hz, 2H), 6.46 (d, *J* = 8.7 Hz, 2H), 3.12 – 3.07 (m, 4H), 1.56 (s, 6H), 1.50 (q, *J* = 7.5 Hz, 4H), 0.81 (t, *J* = 7.4 Hz, 6H); MS calculated m/e for C₂₁H₂₉N: 295.2, found: 295.2 (Relative abundance: 33%). HRMS (m/z): [M+H]⁺ calcd for [C₂₁H₂₉N H]⁺: 295.2379; found: 295.2387.



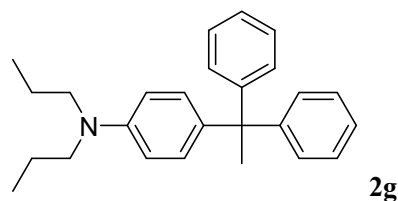
¹³C NMR (100 MHz, Chloroform-*d*) δ 151.80 (C_{q,aro}), 148.96 (C_{q,aro}), 137.55 (C_{q,aro}), 135.92 (C_{q,aro}), 128.07 (CH_{aro}), 126.88 (CH_{aro}), 125.91 (CH_{aro}), 125.04 (CH_{aro}), 116.81 (CH_{aro}), 109.52 (CH_{aro}), 42.66 (CH₃), 40.61 (C), 31.10 (CH₃), 22.13 (CH₃). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.44 (d, *J* = 8.7 Hz, 1H), 7.27 – 7.17 (m, 4H), 7.13 (t, *J* = 6.9 Hz, 1H), 6.61 (dd, *J* = 8.7, 2.9 Hz, 1H), 6.47 (d, *J* = 2.9 Hz, 1H), 2.92 (s, 6H), 1.75 (s, 3H), 1.65 (s, 6H); MS calculated m/e for C₁₈H₂₃N: 253.2, found: 253.2 (Relative abundance: 46%).



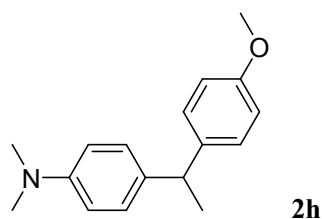
^{13}C NMR (100 MHz, Chloroform-*d*) δ 149.96 (C_qaro), 148.77 (C_qaro), 137.15 (C_qaro), 129.54 (CH_{aro}), 128.91 (CH_{aro}), 127.93 (CH_{aro}), 125.91 (CH_{aro}), 112.14 (CH_{aro}), 51.87 (C), 40.77 (CH₃), 30.71 (CH₃); ^1H NMR (400 MHz, Chloroform-*d*) δ 7.25 – 7.17 (m, 4H), 7.15 (d, J = 6.5 Hz, 2H), 7.10 (d, J = 8.2 Hz, 4H), 6.94 (d, J = 8.2 Hz, 2H), 6.61 (d, J = 8.5 Hz, 2H), 2.86 (s, 6H), 2.13 (s, 3H); MS calculated m/e for C₂₂H₂₃N: 301.2, found: 301.2 (Relative abundance: 44%).



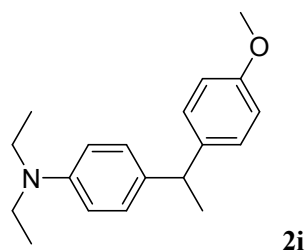
^{13}C NMR (100 MHz, Chloroform-*d*) δ 150.00 (C_qaro), 145.93 (C_qaro), 135.73 (C_qaro), 129.60 (CH_{aro}), 128.84 (CH_{aro}), 127.77 (CH_{aro}), 125.73 (CH_{aro}), 111.12 (CH_{aro}), 51.70 (C), 44.31 (CH₂), 30.58 (CH₃), 12.79 (CH₃); ^1H NMR (400 MHz, Chloroform-*d*) δ 7.22 (d, J = 7.7 Hz, 4H), 7.17 (d, J = 7.1 Hz, 2H), 7.12 (d, J = 7.1 Hz, 4H), 6.90 (d, J = 8.9 Hz, 2H), 6.57 (d, J = 8.9 Hz, 2H), 3.30 (q, J = 7.0 Hz, 4H), 2.14 (s, 3H), 1.13 (t, J = 7.0 Hz, 6H); MS calculated m/e for C₂₄H₂₇N: 329.2, found: 329.2 (Relative abundance: 41%).



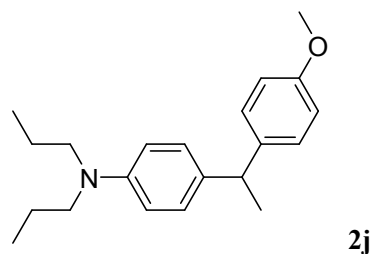
^{13}C NMR (100 MHz, Chloroform-*d*) δ 149.98 (C_qaro), 146.29 (C_qaro), 135.43 (C_qaro), 129.46 (CH_{aro}), 128.81 (CH_{aro}), 127.73 (CH_{aro}), 125.68 (CH_{aro}), 110.93 (CH_{aro}), 52.96 (CH₂), 51.65 (C), 30.52 (CH₂), 20.56 (CH₃), 11.53 (CH₃); ^1H NMR (400 MHz, Chloroform-*d*) δ 7.18 – 7.12 (m, 4H), 7.08 (t, J = 7.2 Hz, 2H), 7.04 (d, J = 7.0 Hz, 4H), 6.81 (d, J = 8.9 Hz, 2H), 6.44 (d, J = 8.9 Hz, 2H), 3.14 – 3.08 (m, 4H), 2.06 (s, 3H), 1.56 – 1.46 (m, 4H), 0.82 (t, J = 7.4 Hz, 6H); MS calculated m/e for C₂₆H₃₁N: 357.3, found: 357.3 (Relative abundance: 42%). HRMS (m/z): [M+H]⁺ calcd for [C₂₆H₃₁N H]⁺: 358.2536; found: 358.2543.



^{13}C NMR (100 MHz, Chloroform-*d*) δ 157.68 (C_{qaro}), 149.04 (C_{qaro}), 139.48 (C_{qaro}), 135.01 (C_{qaro}), 128.46 (CH_{aro}), 128.12 (CH_{aro}), 113.67 (CH_{aro}), 112.85 (CH_{aro}), 55.26 (CH_3), 42.97 (CH), 40.85 (CH_3), 22.31 (CH_3); ^1H NMR (400 MHz, Chloroform-*d*) δ 7.12 (d, J = 8.5 Hz, 2H), 7.07 (d, J = 8.5 Hz, 2H), 6.80 (d, J = 8.7 Hz, 2H), 6.67 (d, J = 8.8 Hz, 2H), 4.01 (q, J = 7.2 Hz, 1H), 3.75 (s, 3H), 2.89 (s, 6H), 1.57 (d, J = 7.2 Hz, 3H); MS calculated m/e for $\text{C}_{17}\text{H}_{21}\text{NO}$: 255.2, found: 255.2 (Relative abundance: 39%).

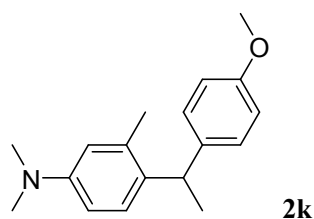


^{13}C NMR (100 MHz, Chloroform-*d*) δ 157.65 (C_{qaro}), 146.14 (C_{qaro}), 139.64 (C_{qaro}), 133.65 (C_{qaro}), 128.28 (CH_{aro}), 113.64 (CH_{aro}), 111.91 (CH_{aro}), 55.26 (CH_3), 44.39 (CH_2), 42.94 (CH), 22.37 (CH_3), 12.69 (CH_3); ^1H NMR (400 MHz, Chloroform-*d*) δ 7.14 (d, J = 8.4 Hz, 2H), 7.04 (d, J = 8.5 Hz, 2H), 6.81 (d, J = 8.7 Hz, 2H), 6.60 (d, J = 8.8 Hz, 2H), 3.99 (q, J = 7.2 Hz, 1H), 3.76 (s, 3H), 3.30 (q, J = 7.1 Hz, 4H), 1.57 (d, J = 7.2 Hz, 3H), 1.12 (t, J = 7.0 Hz, 6H). MS calculated m/e for $\text{C}_{19}\text{H}_{25}\text{NO}$: 283.2, found: 283.2 (Relative abundance: 36%).

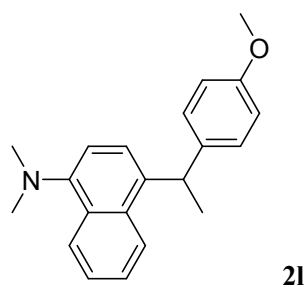


^{13}C NMR (100 MHz, Chloroform-*d*) δ 157.65 (C_{qaro}), 146.54 (C_{qaro}), 139.65 (C_{qaro}), 133.36 (C_{qaro}), 128.48 (CH_{aro}), 128.19 (CH_{aro}), 113.64 (CH_{aro}), 111.66 (CH_{aro}), 55.26

(CH₂), 53.04 (CH₃), 42.93 (CH₁), 22.37 (CH₂), 20.52 (CH₃), 11.54 (CH₃). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.14 (d, *J* = 8.7 Hz, 2H), 7.02 (d, *J* = 8.7 Hz, 2H), 6.80 (d, *J* = 8.7 Hz, 2H), 6.55 (d, *J* = 8.8 Hz, 2H), 3.99 (q, *J* = 7.2 Hz, 1H), 3.75 (s, 3H), 3.21 – 3.15 (m, 4H), 1.61 – 1.54 (m, 7H), 0.89 (t, *J* = 7.4 Hz, 6H). MS calculated m/e for C₂₁H₂₉NO: 311.2, found: 311.2 (Relative abundance: 32%). HRMS (m/z): [M+H]⁺ calcd for [C₂₁H₂₉NO H]⁺: 312.2328; found: 312.2331.

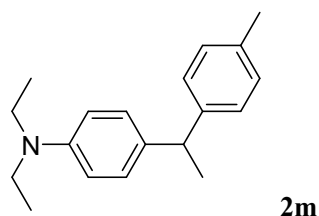


¹³C NMR (100 MHz, Chloroform-*d*) δ 157.51 (C_{q,aro}), 148.99 (C_{q,aro}), 139.35 (C_{q,aro}), 136.63 (C_{q,aro}), 132.77 (C_{q,aro}), 128.48 (CH_{aro}), 127.24 (CH_{aro}), 115.01 (CH_{aro}), 113.60 (CH_{aro}), 110.50 (CH_{aro}), 55.23 (CH₃), 40.81 (CH₃), 39.41 (CH), 22.49 (CH₃), 20.25 (CH₃); ¹H NMR (400 MHz, Chloroform-*d*) δ 7.11 (d, *J* = 8.5 Hz, 1H), 7.06 (d, *J* = 8.5 Hz, 2H), 6.78 (d, *J* = 8.7 Hz, 2H), 6.60 (dd, *J* = 8.5, 2.8 Hz, 1H), 6.54 (d, *J* = 2.7 Hz, 1H), 4.17 (q, *J* = 7.2 Hz, 1H), 3.75 (s, 3H), 2.90 (s, 6H), 2.19 (s, 3H), 1.54 (d, *J* = 7.2 Hz, 3H). MS calculated m/e for C₁₈H₂₃NO: 269.2, found: 269.2 (Relative abundance: 36%).

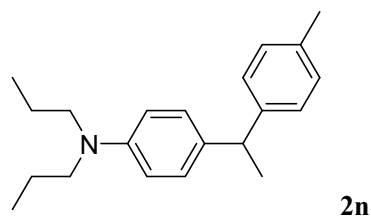


¹³C NMR (100 MHz, Chloroform-*d*) δ 157.74 (C_{q,aro}), 149.58 (C_{q,aro}), 139.22 (C_{q,aro}), 136.49 (C_{q,aro}), 132.87 (C_{q,aro}), 129.31 (C_{q,aro}), 128.57 (CH_{aro}), 125.71 (CH_{aro}), 124.77 (CH_{aro}), 124.68 (CH_{aro}), 124.45 (CH_{aro}), 124.11 (CH_{aro}), 113.80 (CH_{aro}), 113.62 (CH_{aro}), 55.23 (CH₃), 45.42 (CH₃), 39.54 (CH), 22.85 (CH₃); ¹H NMR (400 MHz, Chloroform-*d*) δ 8.28 (d, *J* = 7.8 Hz, 1H), 8.01 (d, *J* = 8.1 Hz, 1H), 7.40 (dt, *J* = 15.0, 6.7 Hz, 2H), 7.30 (d, *J* = 7.8 Hz, 1H), 7.13 (d, *J* = 8.6 Hz, 2H),

7.04 (d, $J = 7.8$ Hz, 1H), 6.77 (d, $J = 8.7$ Hz, 2H), 4.78 (q, $J = 7.1$ Hz, 1H), 3.72 (d, $J = 0.9$ Hz, 3H), 2.86 (s, 6H), 1.70 (d, $J = 7.1$ Hz, 3H). MS calculated m/e for $C_{21}H_{23}NO$: 305.2, found: 305.2 (Relative abundance: 53%).

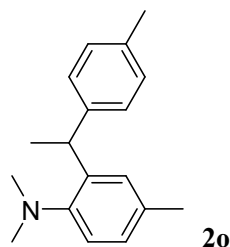


^{13}C NMR (100 MHz, Chloroform- d) δ 146.19 (C_{qaro}), 144.51 (C_{qaro}), 135.16 (C_{qaro}), 133.56 (C_{qaro}), 129.01 (CH_{aro}), 128.36 (CH_{aro}), 127.52 (CH_{aro}), 111.99 (CH_{aro}), 44.44 (CH_2), 43.43 (CH), 22.28 (CH_3), 21.07 (CH_3), 12.74 (CH_3). 1H NMR (400 MHz, Chloroform- d) δ 7.11 (d, $J = 8.1$ Hz, 2H), 7.07 – 7.03 (m, 4H), 6.60 (d, $J = 8.8$ Hz, 2H), 4.00 (q, $J = 7.1$ Hz, 1H), 3.29 (q, $J = 7.1$ Hz, 4H), 2.28 (s, 3H), 1.57 (d, $J = 7.2$ Hz, 3H), 1.11 (t, $J = 7.1$ Hz, 6H). MS calculated m/e for $C_{19}H_{25}N$: 267.2, found: 267.2 (Relative abundance: 36%). HRMS (m/z): $[M+H]^+$ calcd for $[C_{19}H_{25}N H]^+$: 268.2066; found: 268.2062.

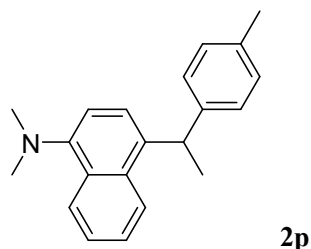


^{13}C NMR (100 MHz, Chloroform- d) δ 146.53 (C_{qaro}), 144.46 (C_{qaro}), 135.12 (C_{qaro}), 133.20 (C_{qaro}), 128.95 (CH_{aro}), 128.21 (CH_{aro}), 127.46 (CH_{aro}), 111.67 (CH_{aro}), 53.03 (CH_2), 43.35 (CH), 22.21 (CH_2), 21.01 (CH_3), 20.51 (CH_3), 11.52 (CH_3). 1H NMR (400 MHz, Chloroform- d) δ 7.04 (d, $J = 8.2$ Hz, 2H), 7.01 – 6.95 (m, 4H), 6.48 (d, $J = 8.7$ Hz, 2H), 3.93 (q, $J = 7.2$ Hz, 1H), 3.13 – 3.08 (m, 4H), 2.22 (s, 3H), 1.50 (q, $J = 8.3$, 7.7 Hz, 7H), 0.82 (t, $J = 7.4$ Hz, 6H). MS calculated m/e for $C_{21}H_{29}N$: 295.2,

found: 295.2 (Relative abundance: 31%). HRMS (m/z): $[M+H]^+$ calcd for $[C_{21}H_{29}N H]^+$: 296.2379; found: 295.296.2391.

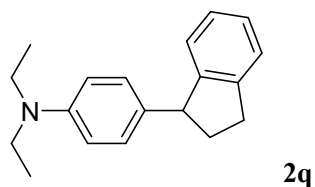


^{13}C NMR (100 MHz, Chloroform-*d*) δ 149.91 (C_{q,aro}), 144.02 (C_{q,aro}), 142.21 (C_{q,aro}), 134.91 (C_{q,aro}), 133.51 (C_{q,aro}), 128.93 (CH_{aro}), 128.83 (CH_{aro}), 127.51 (CH_{aro}), 127.29 (CH_{aro}), 120.32 (CH_{aro}), 46.08 (CH₃), 36.79 (CH), 22.41 (CH₃), 21.00 (CH₃). 1H NMR (400 MHz, Chloroform-*d*) δ 7.08 (d, J = 8.1 Hz, 2H), 7.00 (d, J = 7.4 Hz, 3H), 6.90 (d, J = 8.3 Hz, 2H), 4.74 (q, J = 7.3 Hz, 1H), 2.52 (s, 6H), 2.22 (s, 3H), 2.18 (s, 3H), 1.48 (d, J = 7.3 Hz, 3H). MS calculated m/e for C₁₈H₂₃N: 253.2, found: 253.2 (Relative abundance: 100%). HRMS (m/z): $[M+H]^+$ calcd for $[C_{18}H_{23}N H]^+$: 254.1909; found: 254.1914.



^{13}C NMR (100 MHz, Chloroform-*d*) δ 149.53 (C_{q,aro}), 144.04 (C_{q,aro}), 136.31 (C_{q,aro}), 135.29 (C_{q,aro}), 132.86 (C_{q,aro}), 129.09 (CH_{aro}), 127.49 (CH_{aro}), 125.68 (CH_{aro}), 124.70 (CH_{aro}), 124.63 (CH_{aro}), 124.40 (CH_{aro}), 124.08 (CH_{aro}), 113.57 (CH_{aro}), 45.39 (CH₃), 39.92 (CH), 22.75 (CH₃), 21.01 (CH₃). 1H NMR (400 MHz, Chloroform-*d*) δ 8.20 (d, J = 7.9 Hz, 1H), 7.94 (d, J = 8.0 Hz, 1H), 7.39 – 7.28 (m, 2H), 7.25 (d, J = 7.8 Hz, 1H), 7.05 (d, J = 8.1 Hz, 2H), 6.99 (d, J = 2.2 Hz, 2H), 6.97 (d, J = 2.3 Hz, 1H), 4.73 (q, J = 7.1 Hz, 1H), 2.80 (s, 6H), 2.20 (s, 3H), 1.64 (d, J = 7.1 Hz, 3H). MS calculated

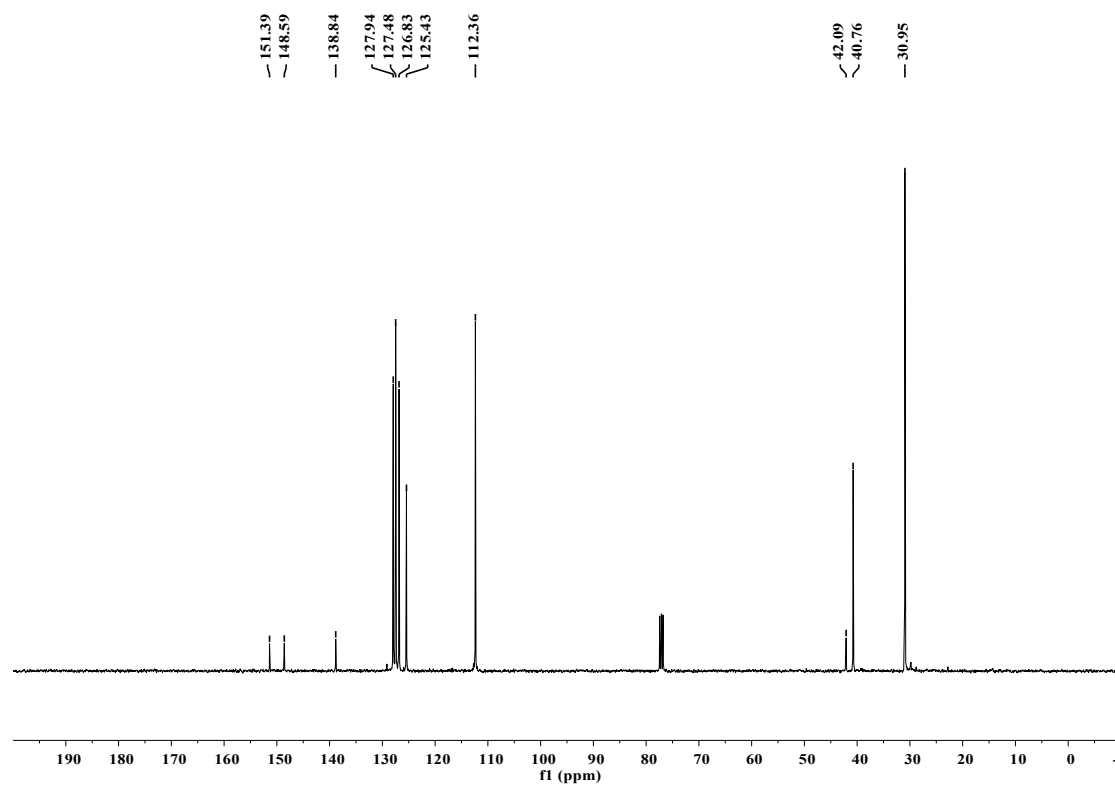
m/e for C₂₁H₂₃N: 289.2, found: 289.2 (Relative abundance: 55%). HRMS (m/z): [M+H]⁺
calcd for [C₂₁H₂₃N H]⁺: 290.1909; found: 290.1902.



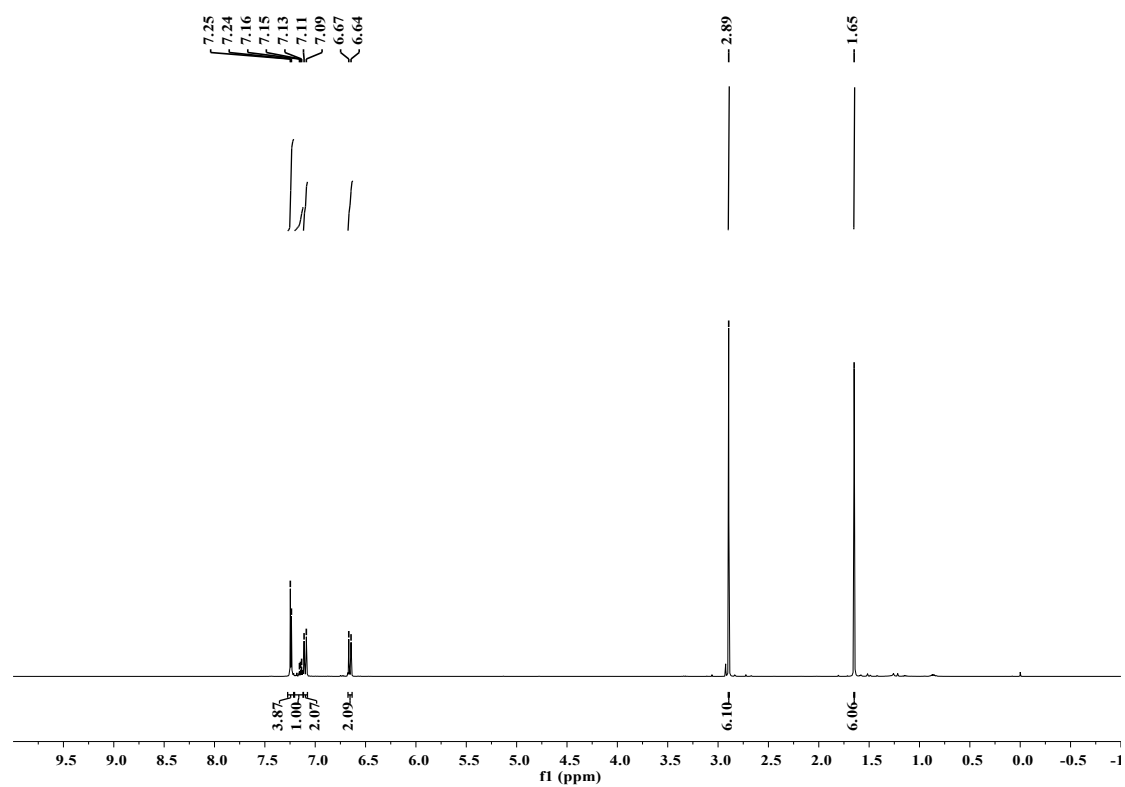
¹³C NMR (101 MHz, Chloroform-*d*) δ 147.68 (C_qaro), 146.47 (C_qaro), 144.28 (C_qaro), 132.00 (C_qaro), 128.90 (CH_{aro}), 126.19 (CH_{aro}), 124.96 (CH_{aro}), 124.23 (CH_{aro}), 111.95 (CH_{aro}), 50.71 (CH), 44.37 (CH₂), 36.78 (CH₂), 31.78 (CH₂), 12.69 (CH₃). ¹H NMR (400 MHz, Chloroform-*d*) δ 7.26 (d, *J* = 7.0 Hz, 1H), 7.17 (d, *J* = 7.3 Hz, 2H), 7.01 (dd, *J* = 13.0, 8.0 Hz, 3H), 6.63 (d, *J* = 8.8 Hz, 2H), 4.22 (t, *J* = 8.3 Hz, 1H), 3.33 (q, *J* = 7.1 Hz, 4H), 3.01 – 2.89 (m, 2H), 2.52 (dq, *J* = 12.2, 4.3 Hz, 1H), 2.07 – 1.95 (m, 1H), 1.15 (t, *J* = 7.1 Hz, 6H). MS calculated m/e for C₁₉H₂₃N: 265.2, found: 265.2 (Relative abundance: 42%).

4. Original NMR spectra

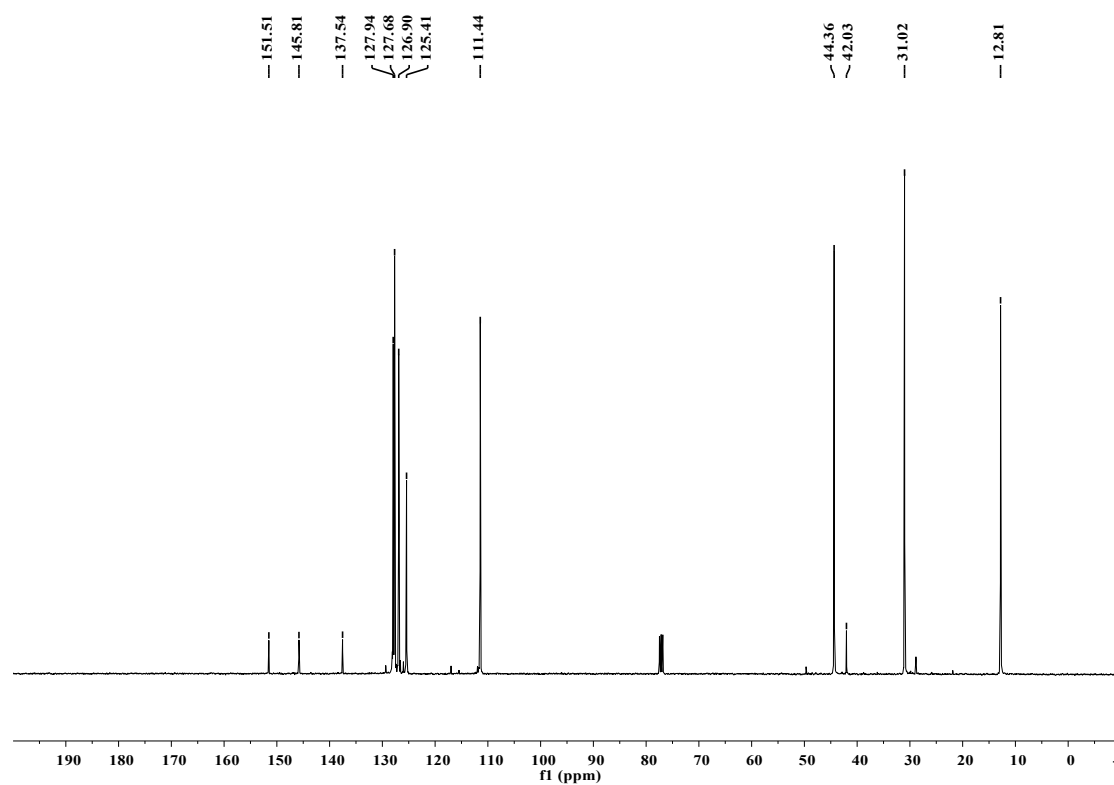
2a (^{13}C NMR)



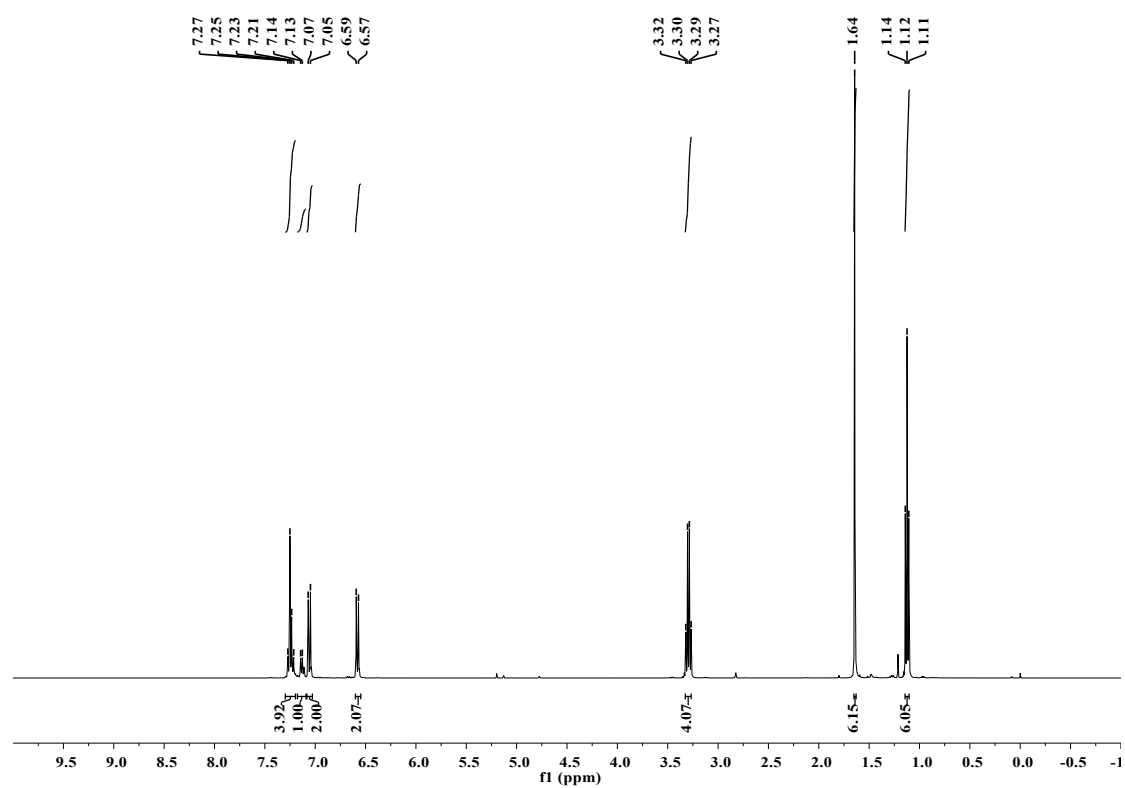
2a (^1H NMR)



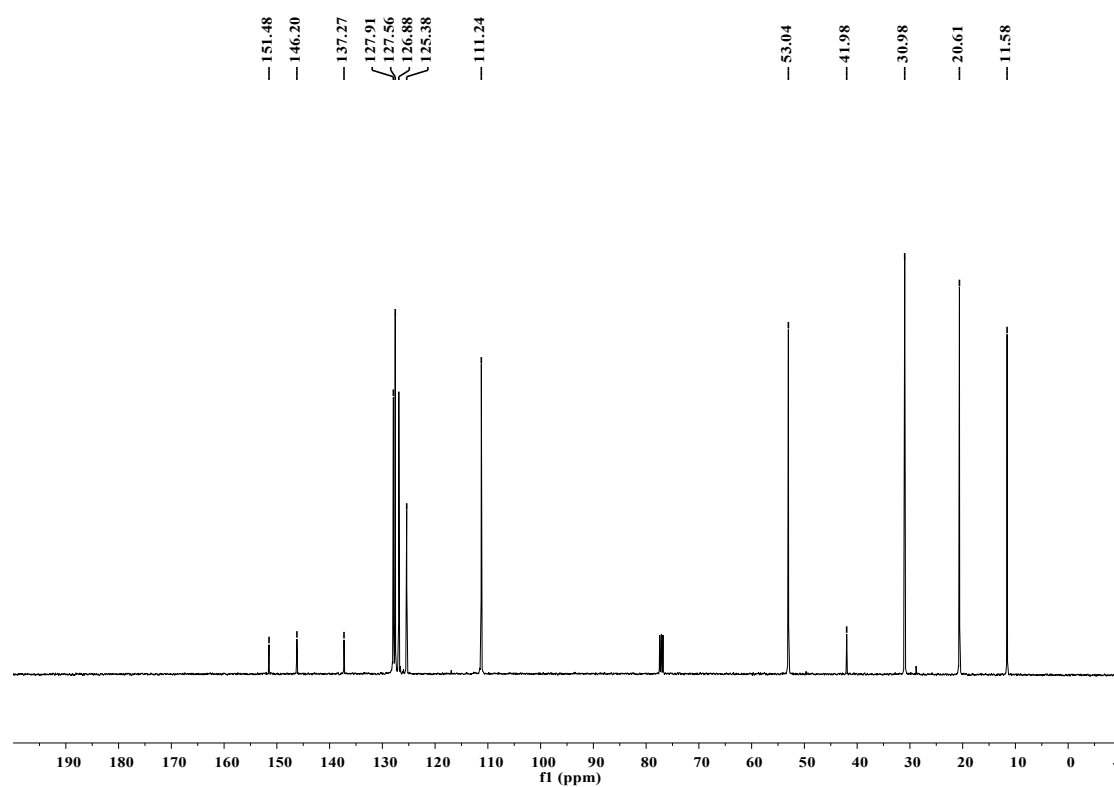
2b (^{13}C NMR)



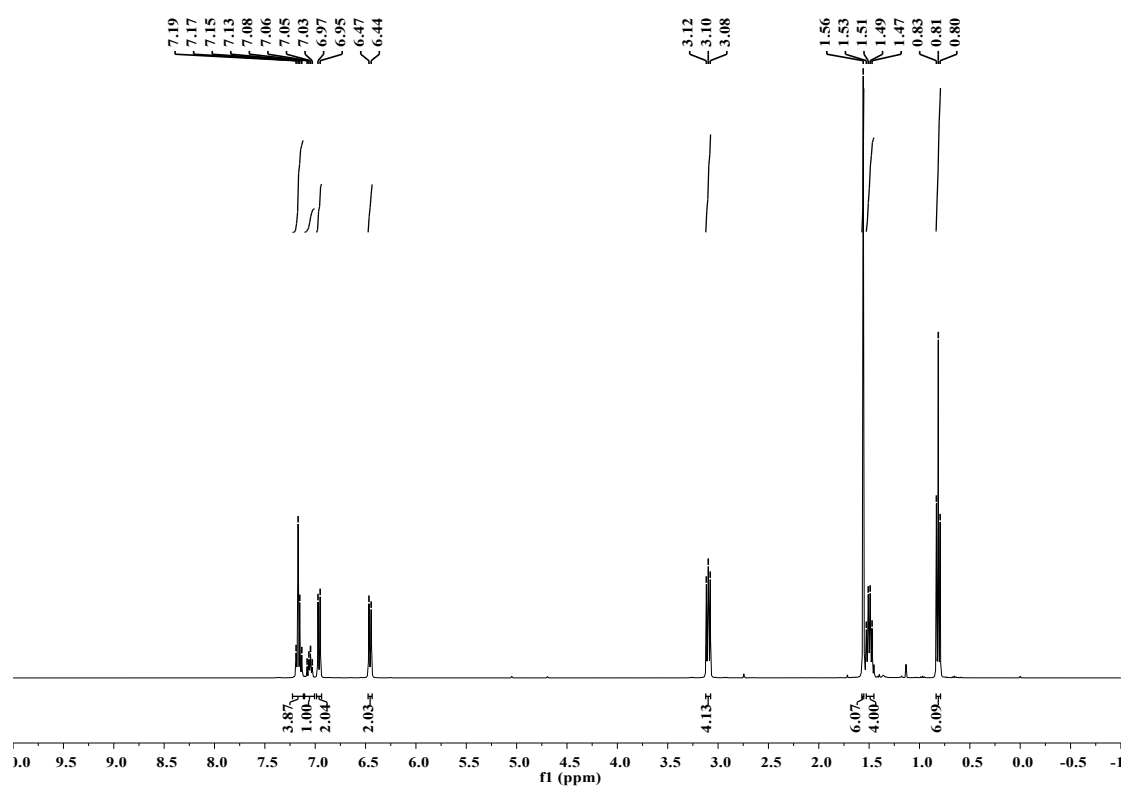
2b (^1H NMR)



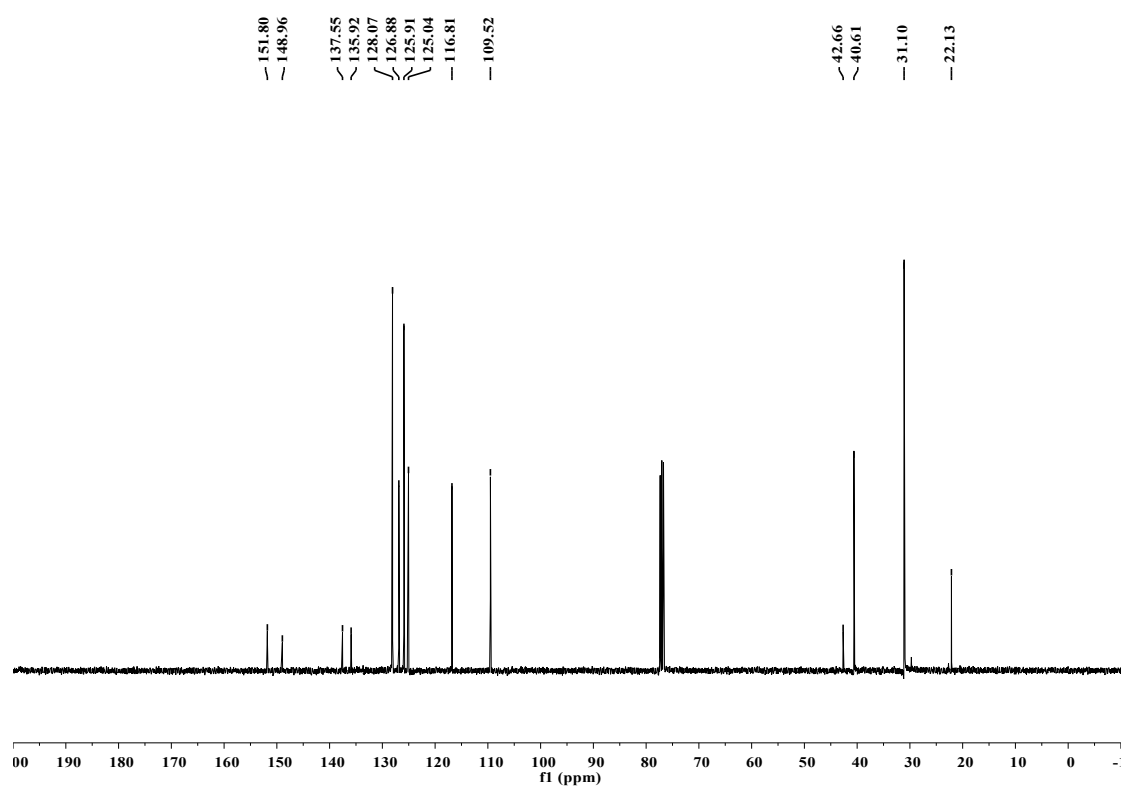
2c (^{13}C NMR)



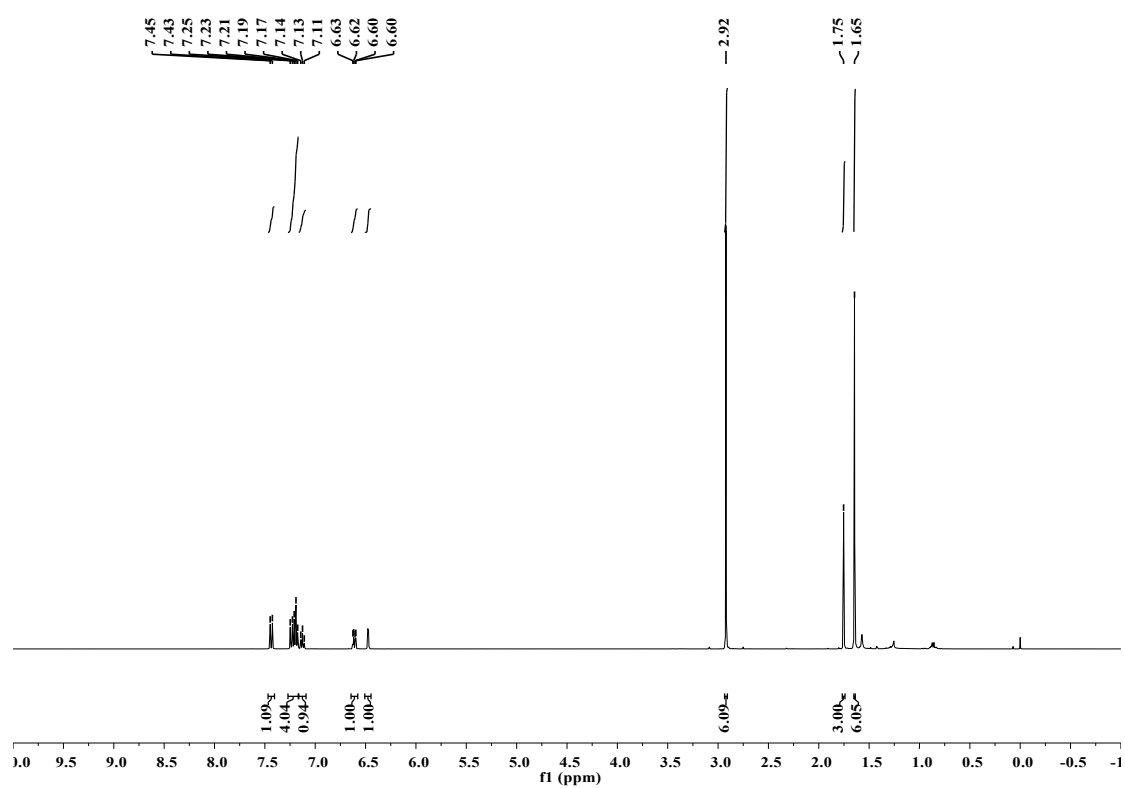
2c (^1H NMR)



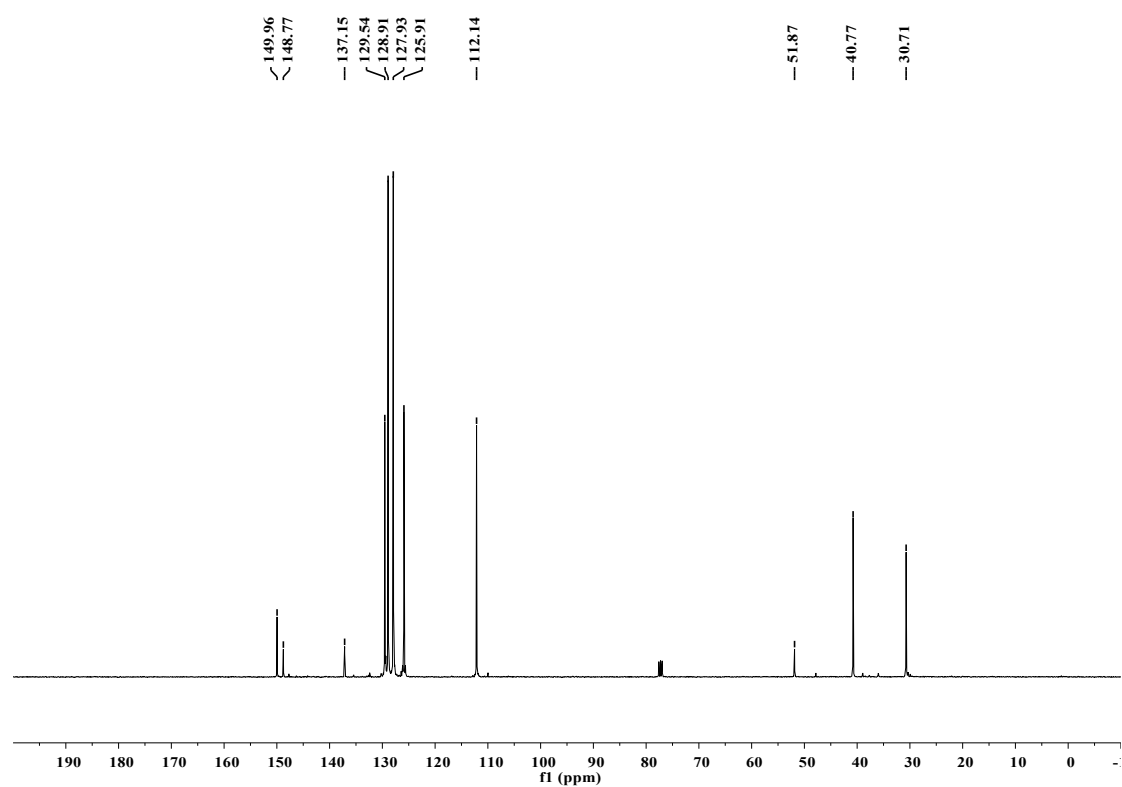
2d (^{13}C NMR)



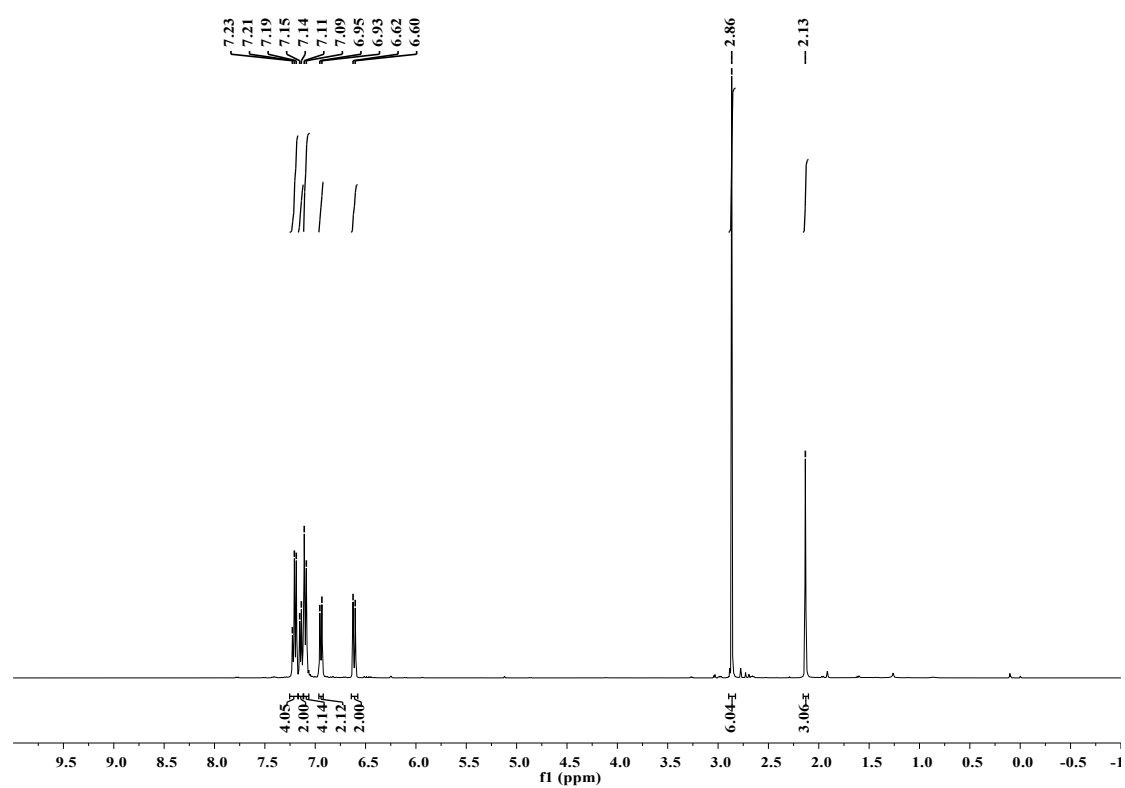
2d (^1H NMR)



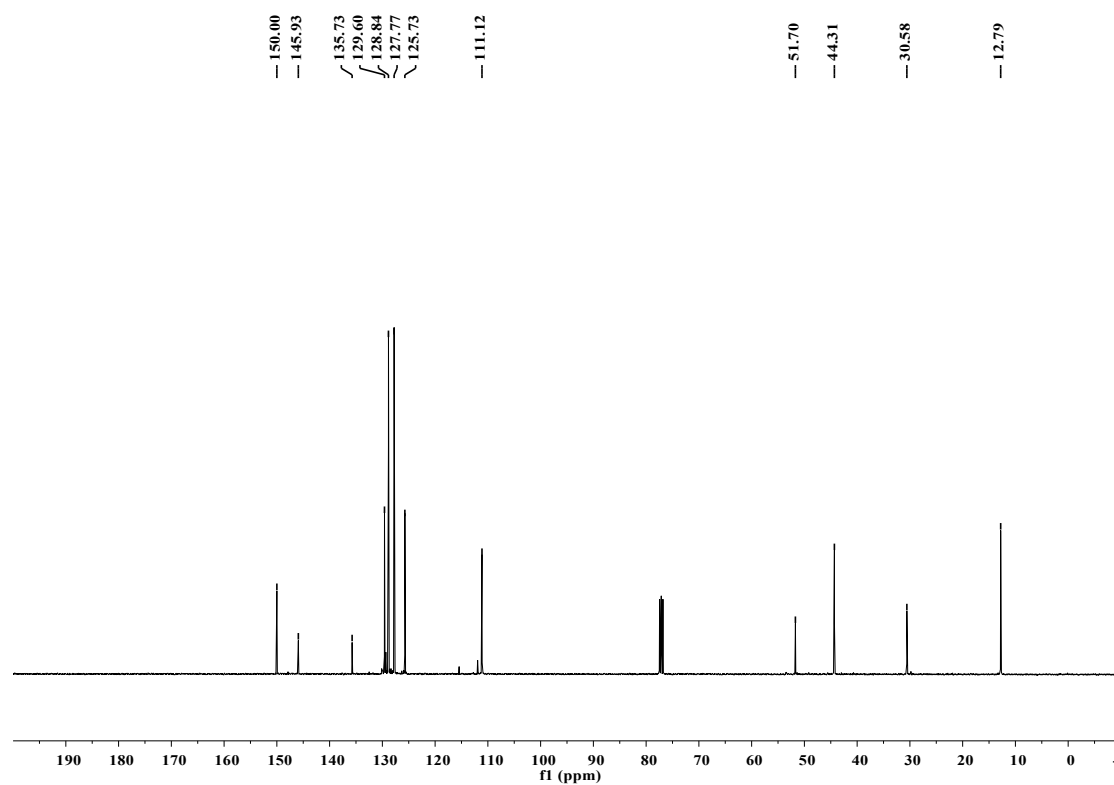
2e (^{13}C NMR)



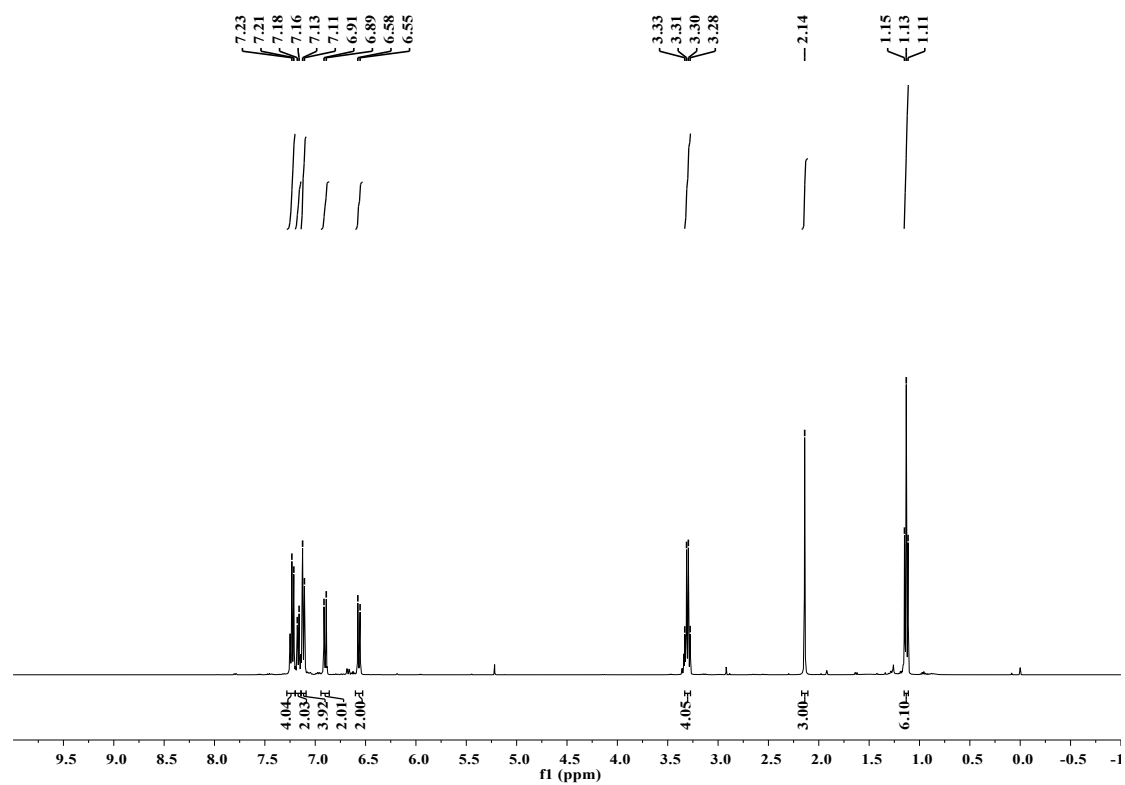
2e (^1H NMR)



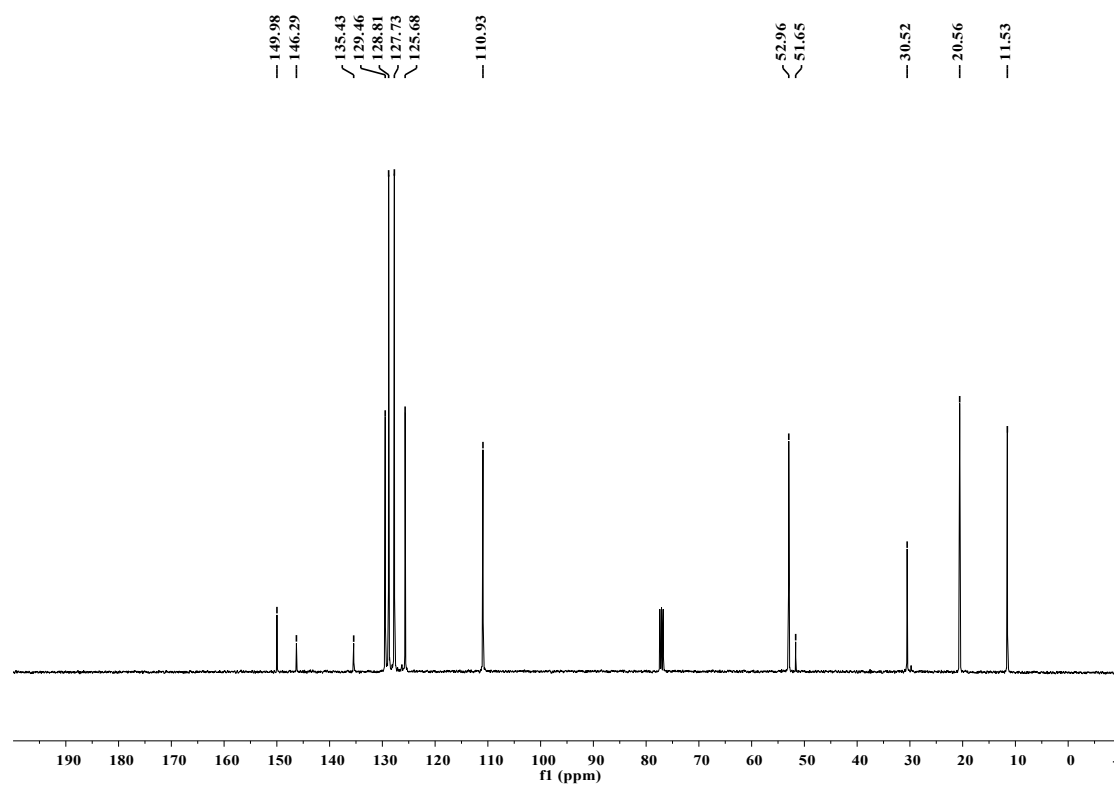
2f (^{13}C NMR)



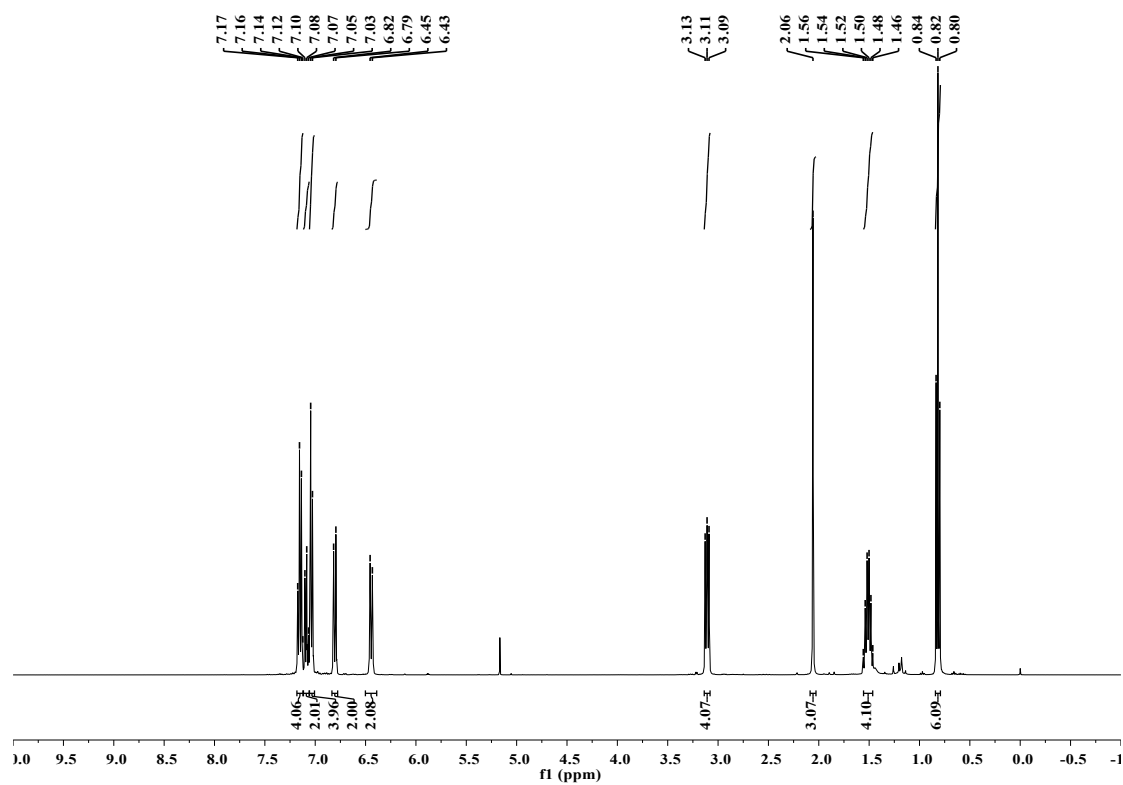
2f (^1H NMR)



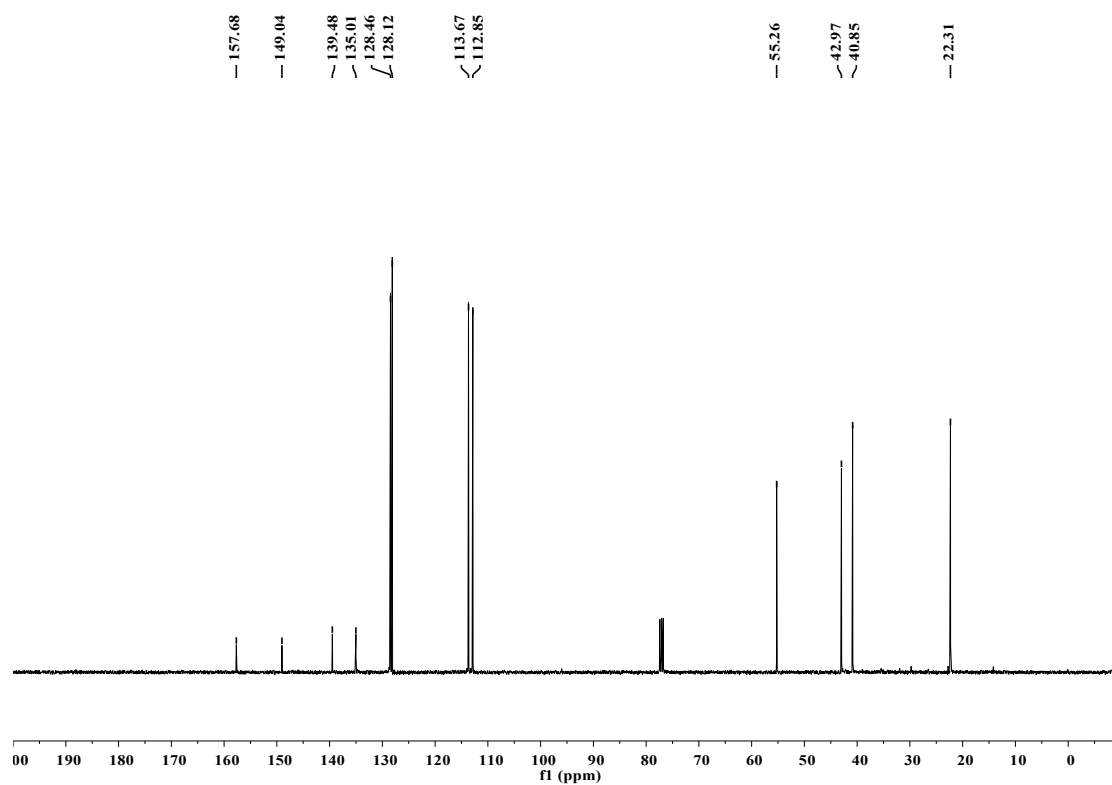
2g (^{13}C NMR)



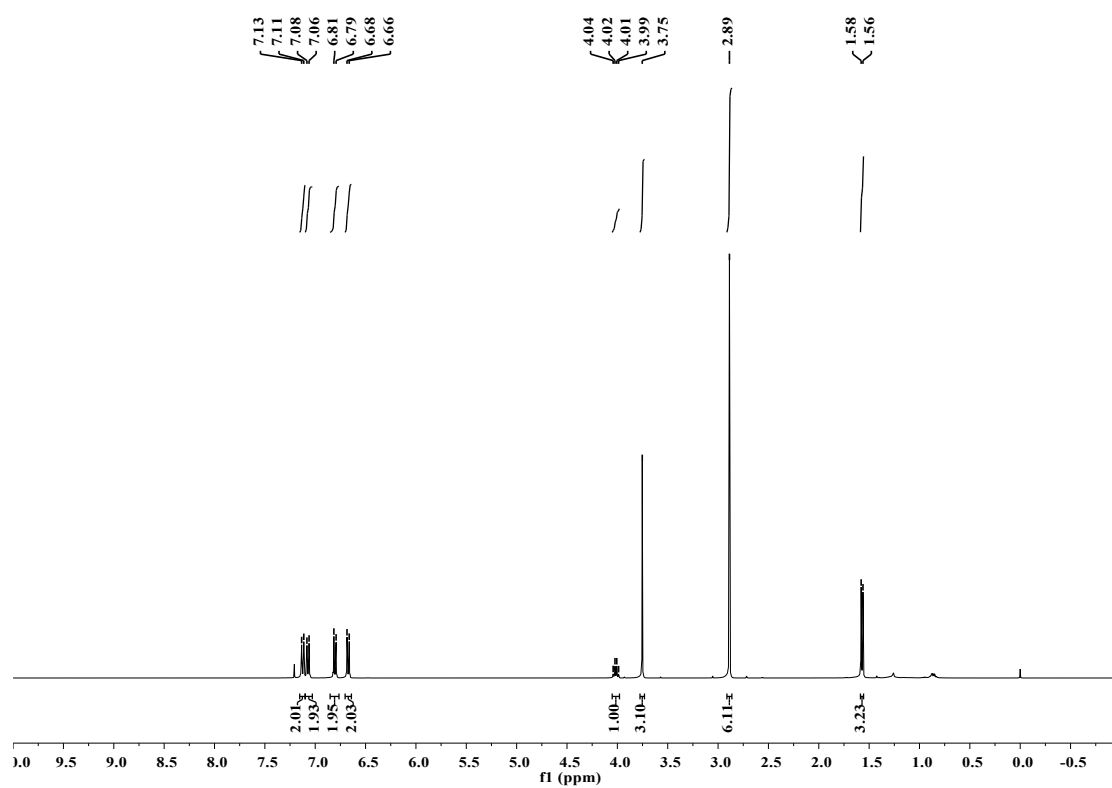
2g (^1H NMR)



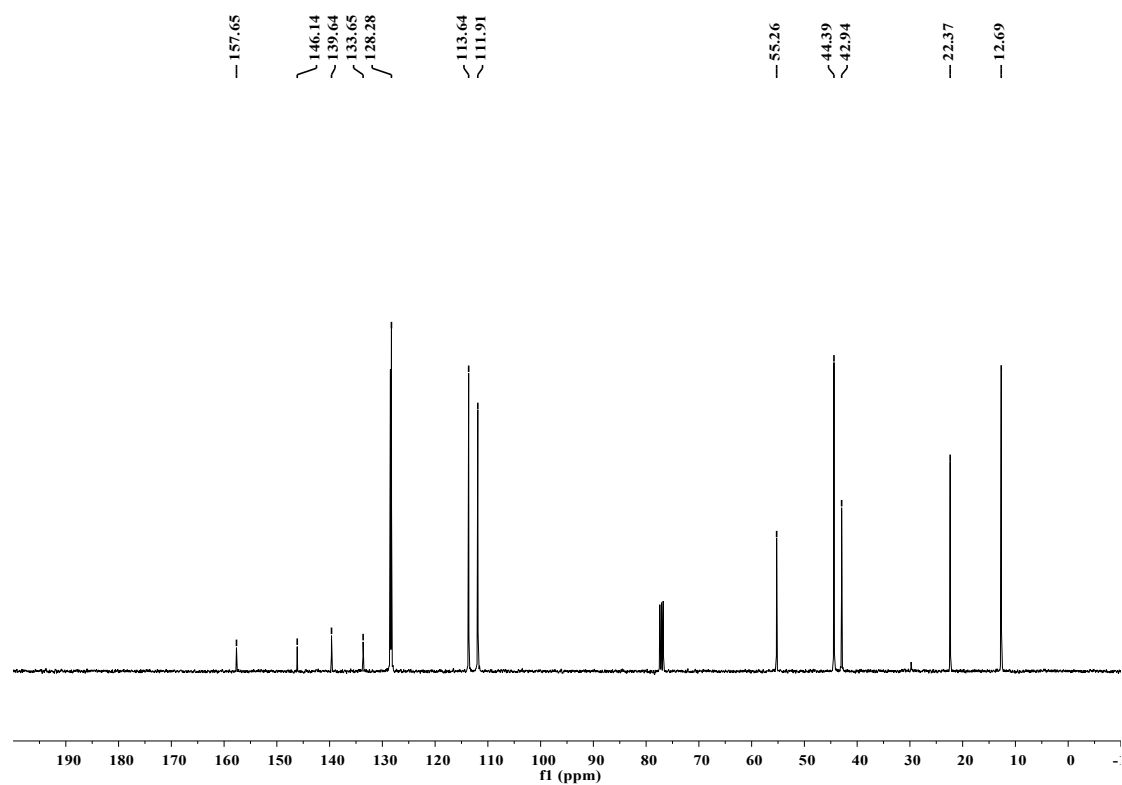
2h (^{13}C NMR)



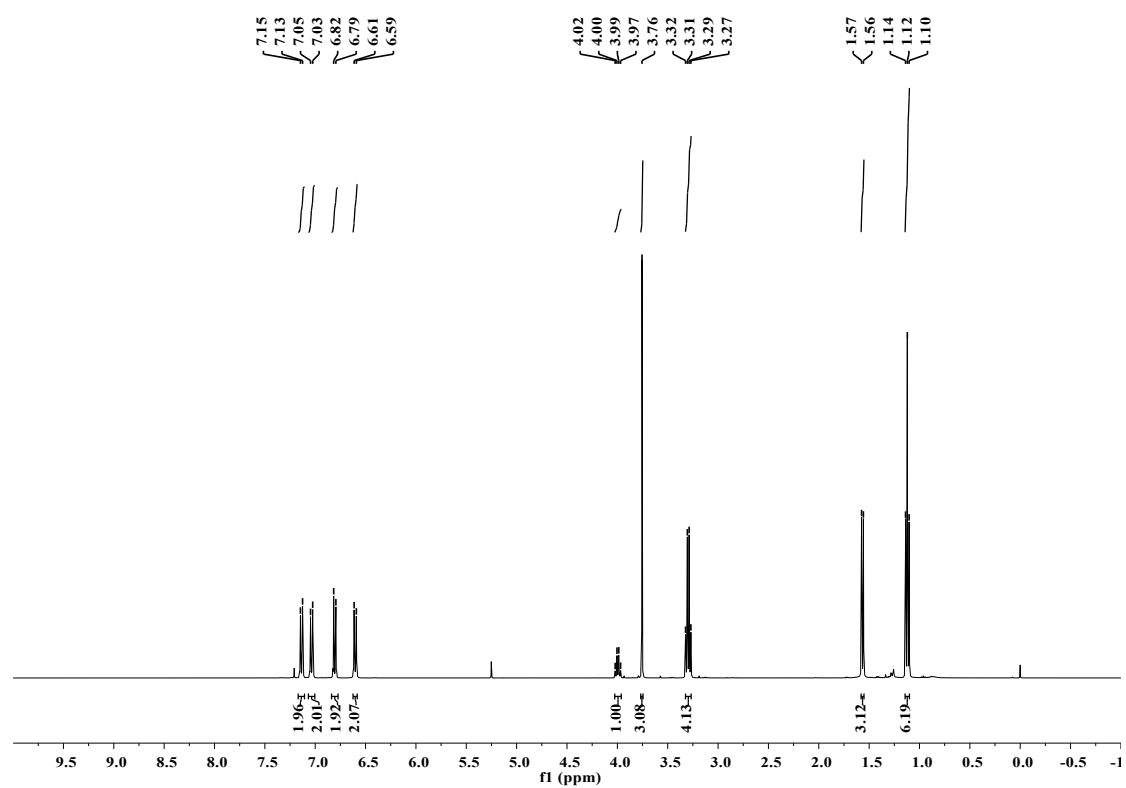
2h (^1H NMR)



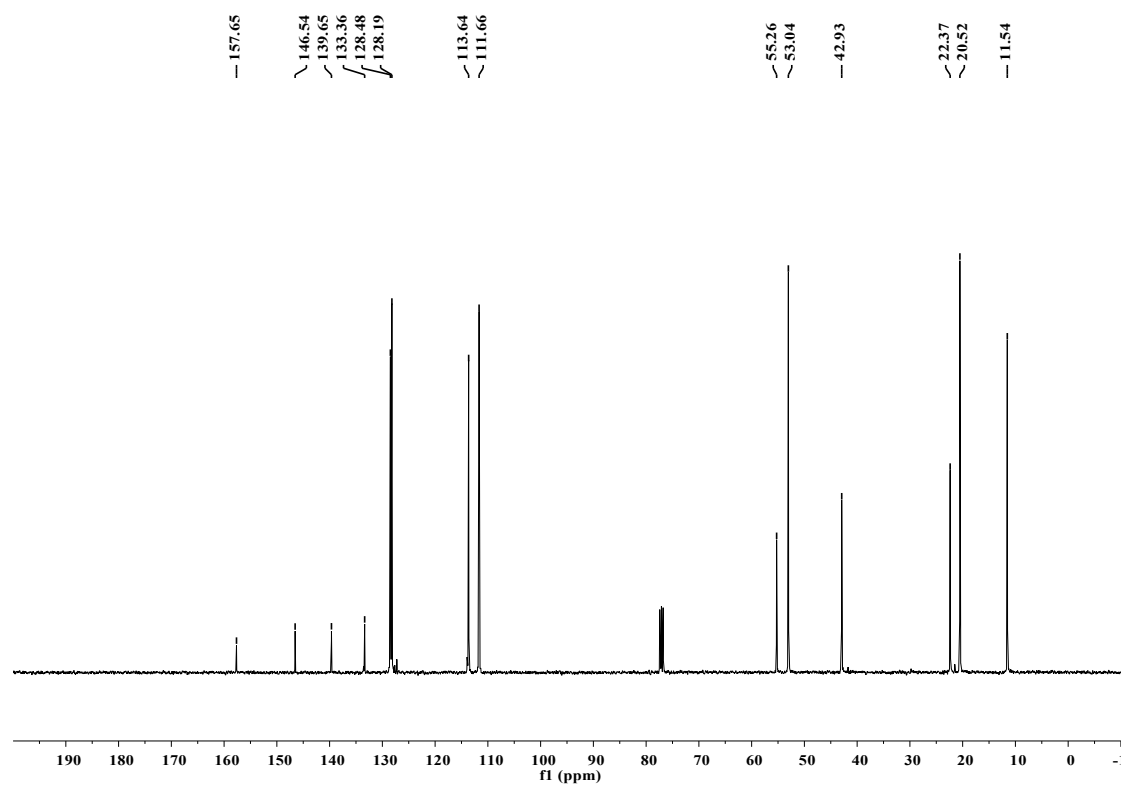
2i (^{13}C NMR)



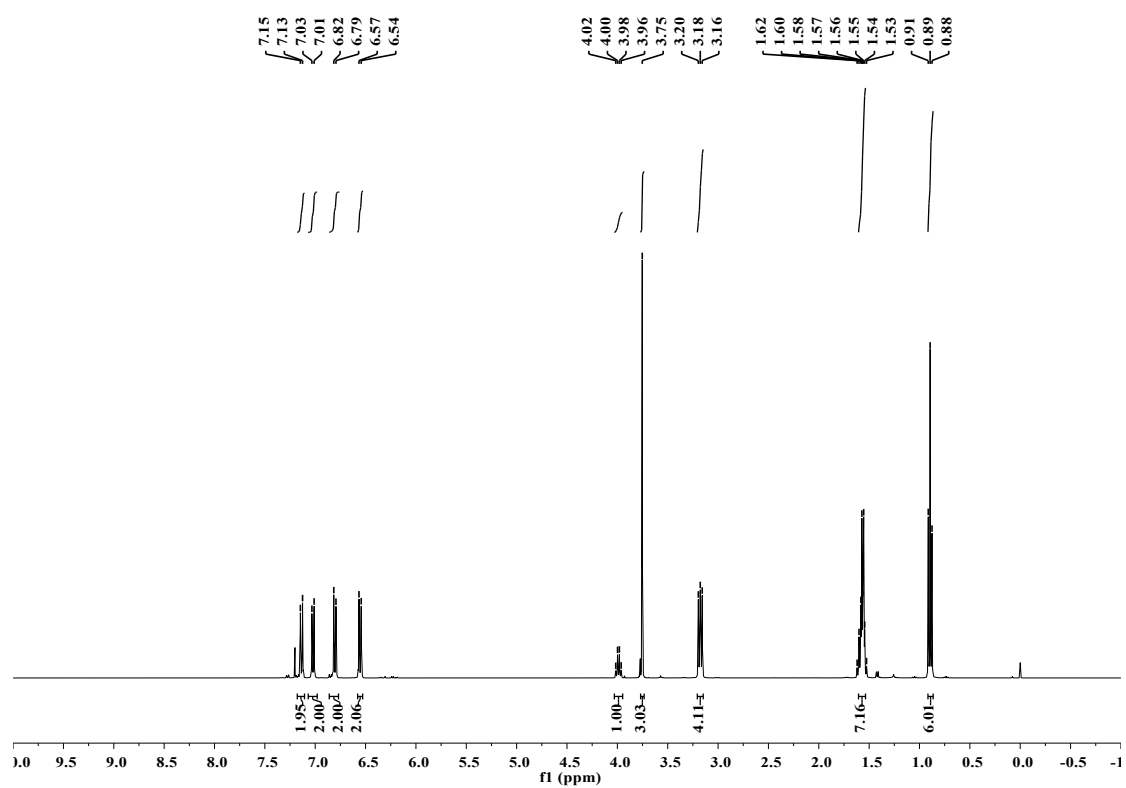
2i (^1H NMR)



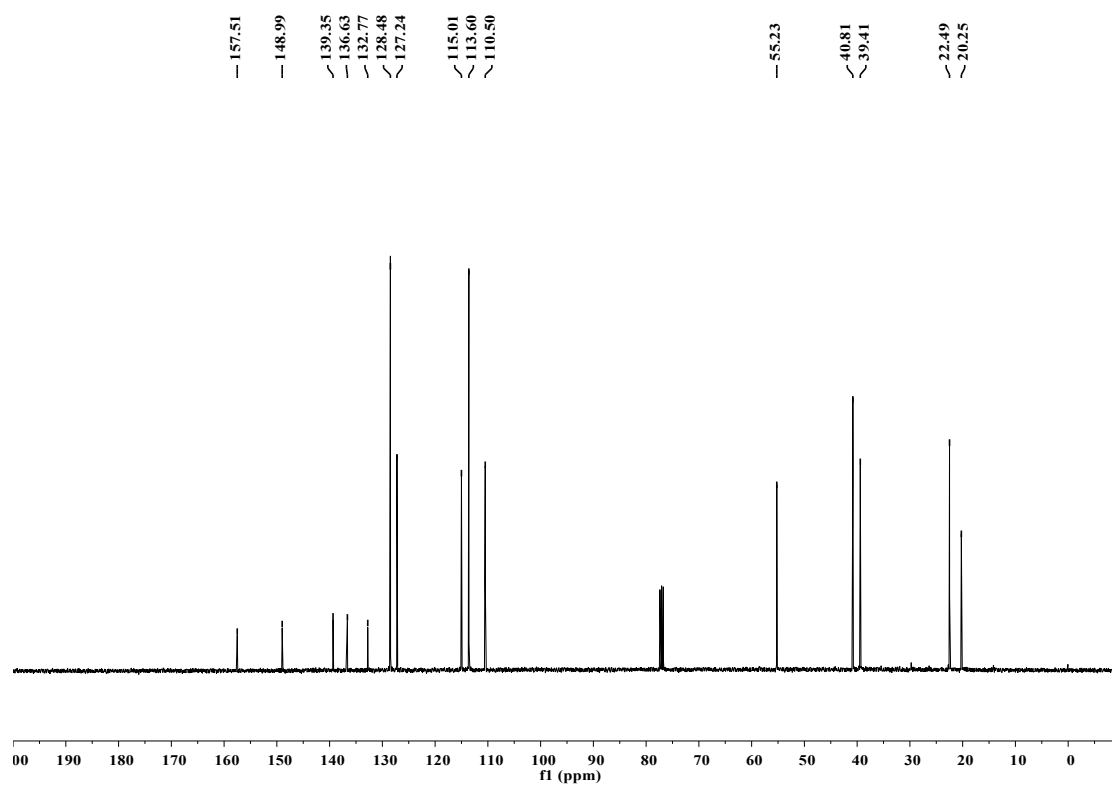
2j (^{13}C NMR)



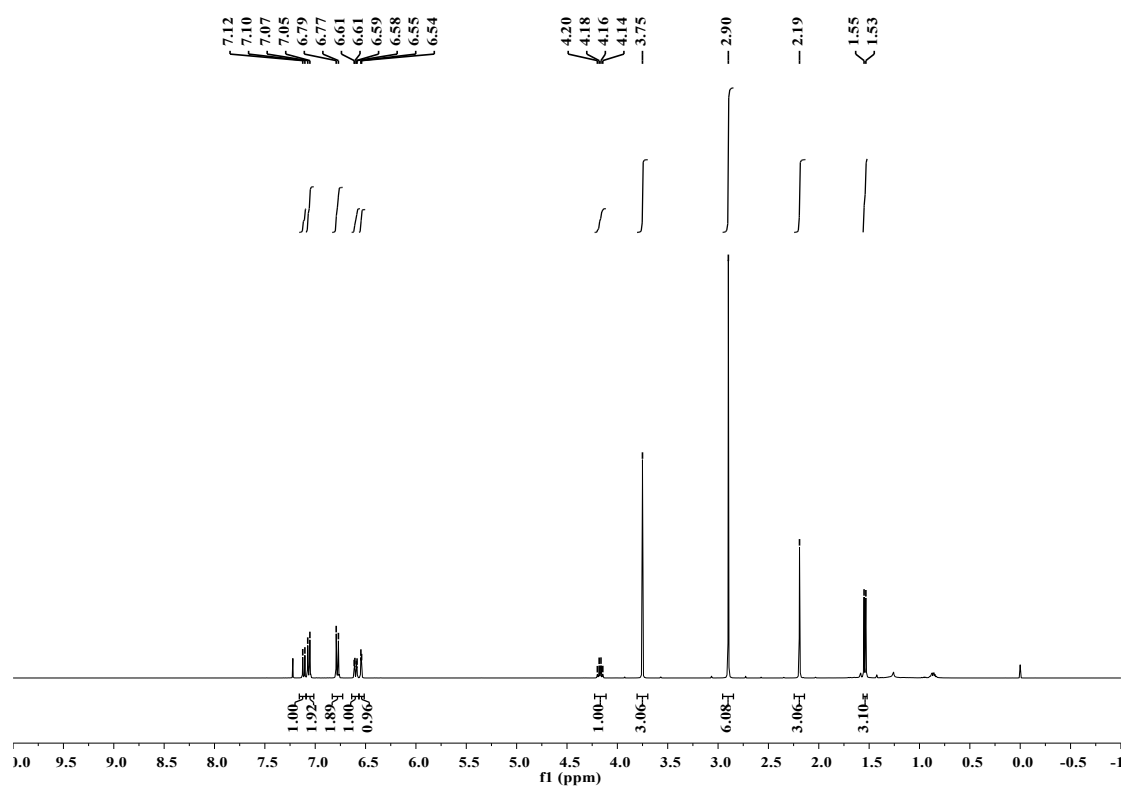
2j (^1H NMR)



2k (^{13}C NMR)



2k (^1H NMR)

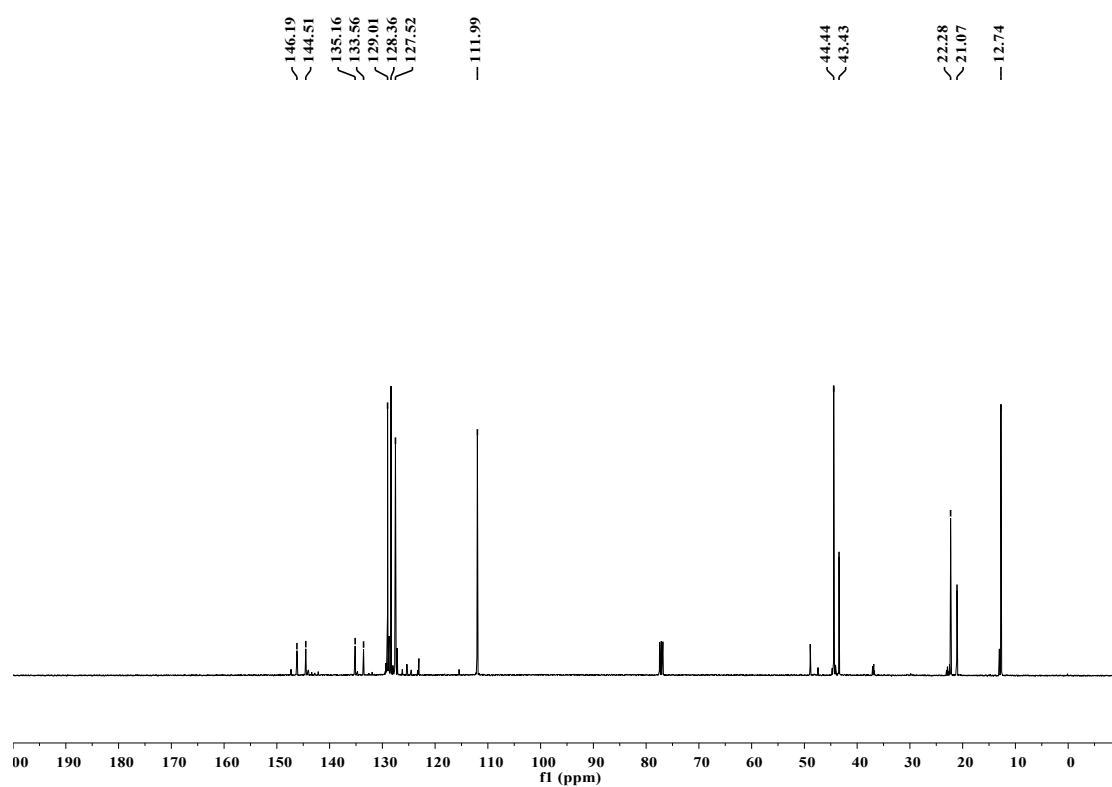


157.74
149.58
139.22
136.49
132.87
129.31
128.57
125.71
124.77
124.68
124.45
124.11
113.80
113.62
55.23
45.42
39.54
22.85

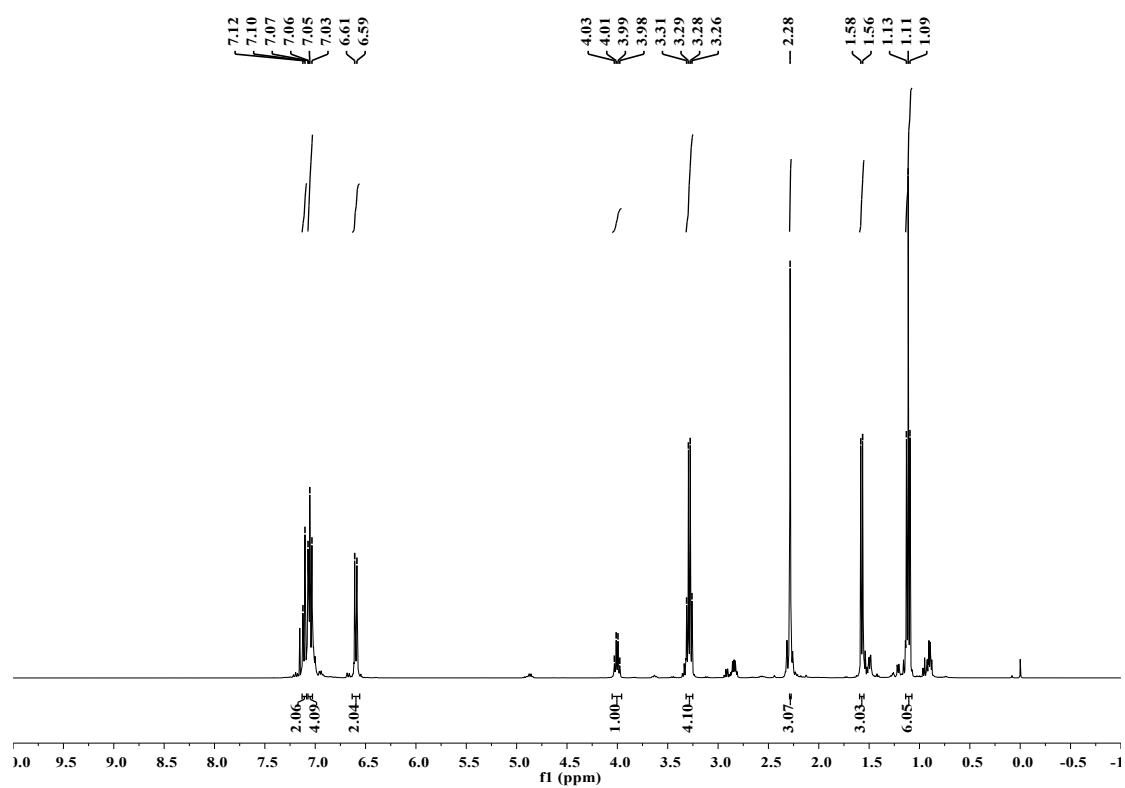
f1 (ppm)

¹H NMR spectrum of compound **1** in CDCl₃. The x-axis is chemical shift in ppm, ranging from 1.0 to -1.0. The spectrum shows several peaks with integration values and chemical shift labels. Integration values are: 0.91, 1.01, 1.92, 1.01, 1.97, 1.00, 1.86, 1.03, 3.04, 6.13, 3.12. Chemical shift labels are: 8.29, 8.27, 8.02, 8.00, 7.44, 7.43, 7.40, 7.38, 7.36, 7.31, 7.29, 7.14, 7.12, 7.05, 7.03, 6.79, 6.76, 4.81, 4.79, 4.78, 4.76, 2.86, 1.70, 1.69.

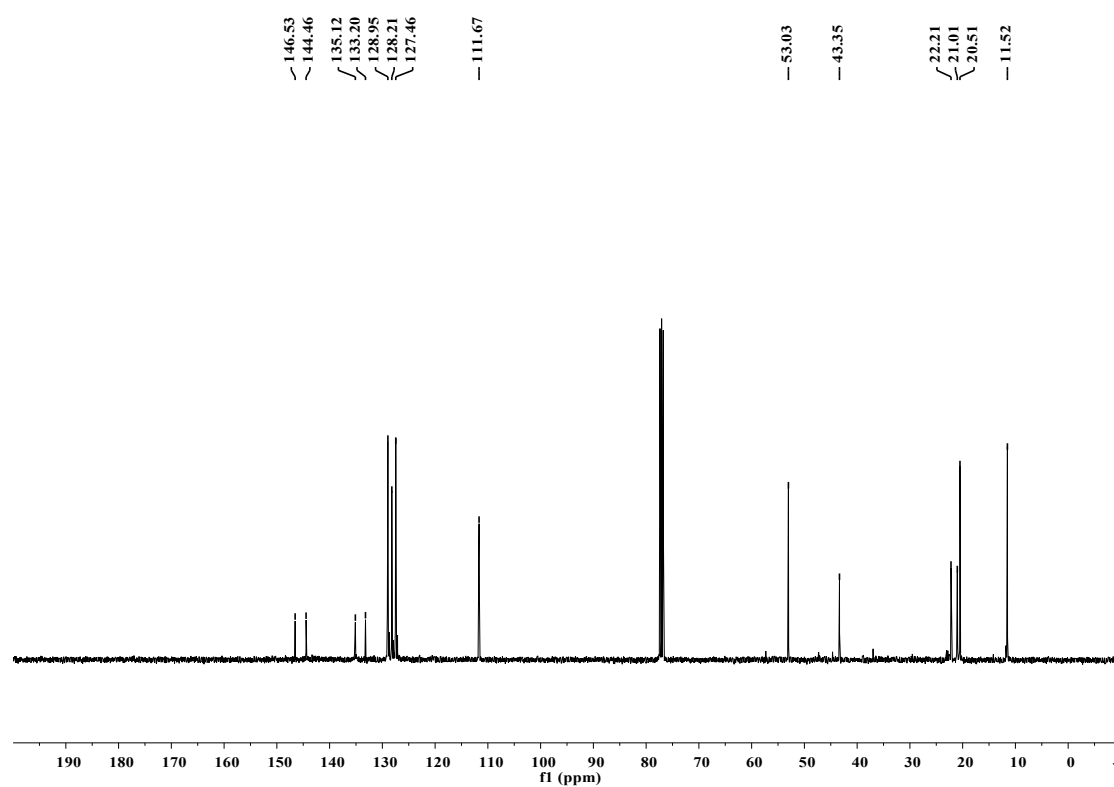
2m (^{13}C NMR)



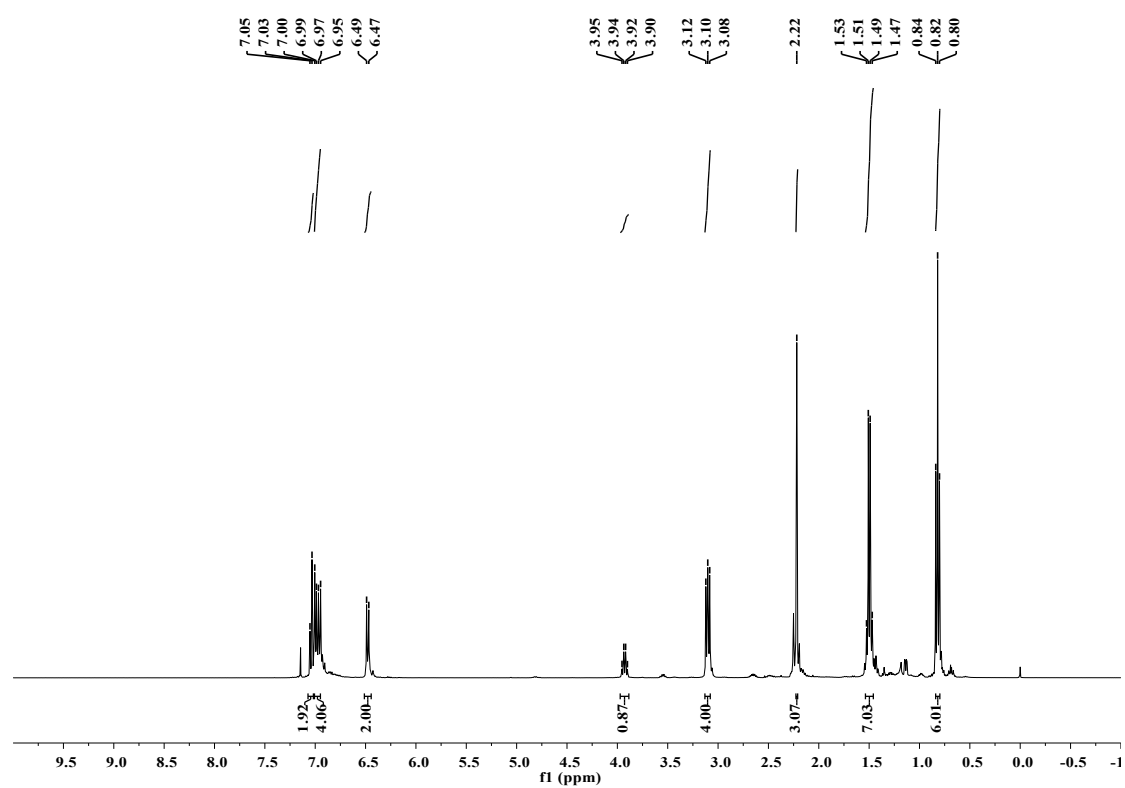
2m (^1H NMR)



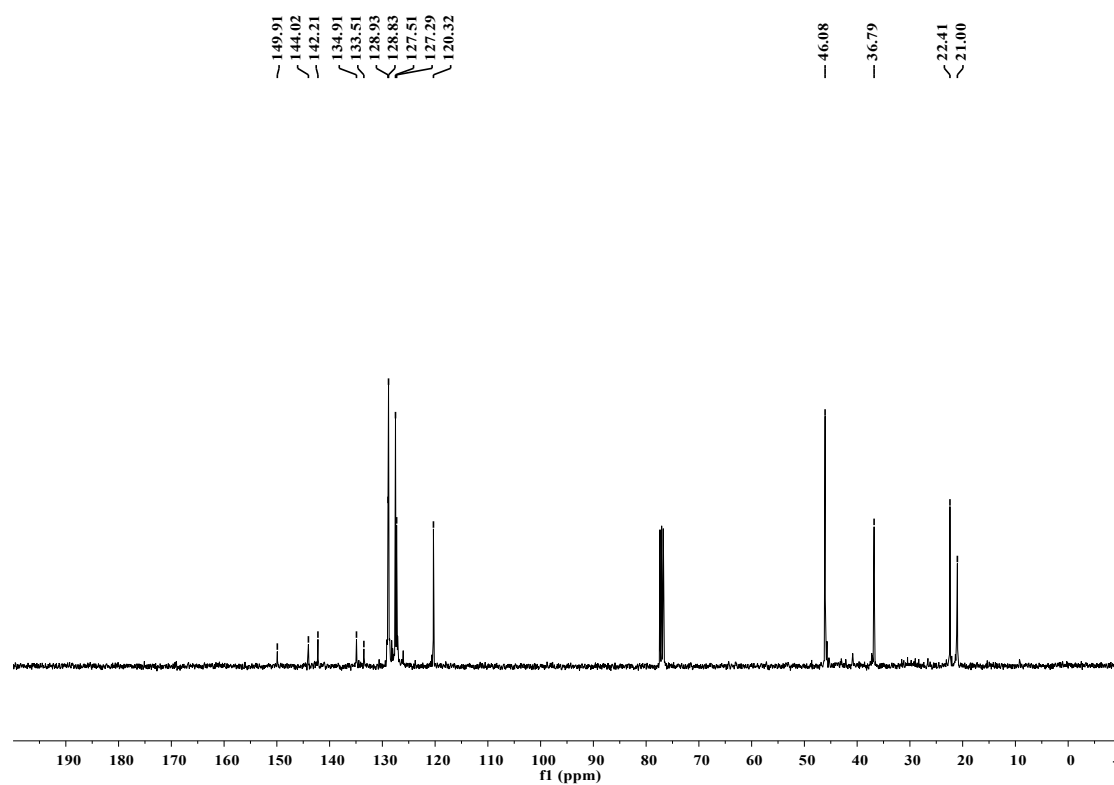
2n (^{13}C NMR)



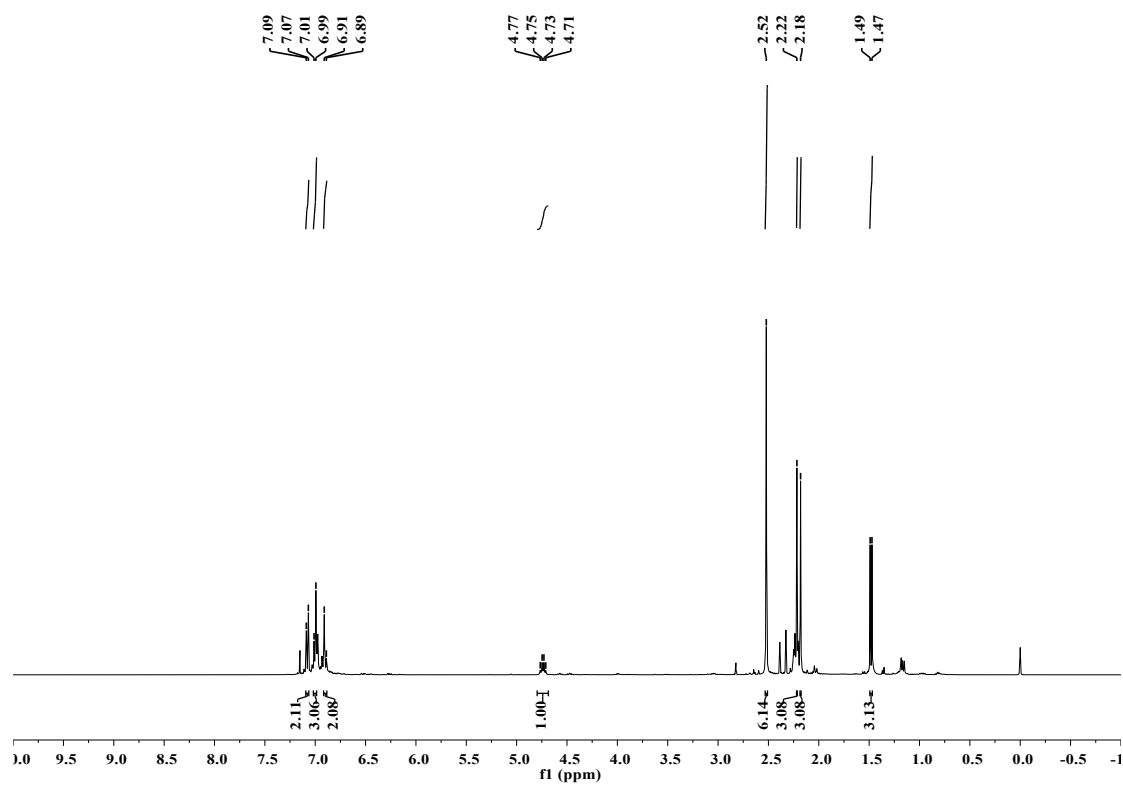
2n (^1H NMR)



2o (^{13}C NMR)



2o (^1H NMR)



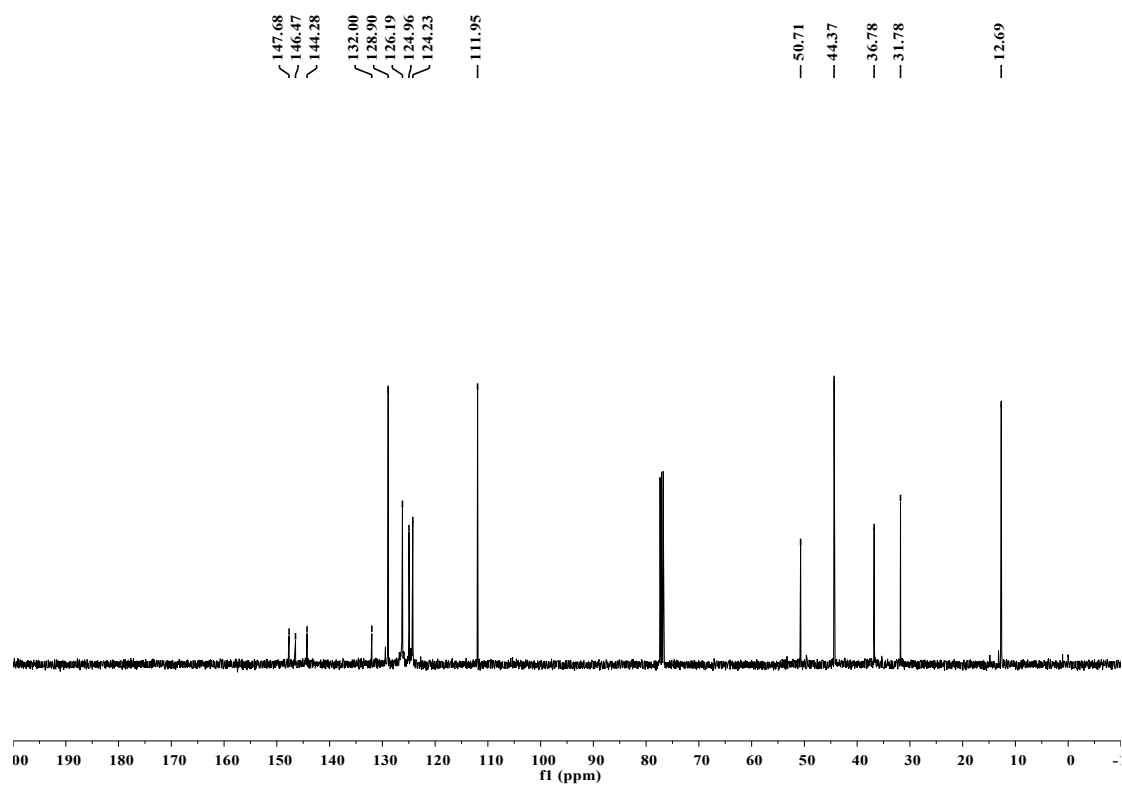
149.53
144.04
136.31
135.29
132.86
129.09
127.49
125.68
124.70
124.63
124.40
124.08
113.57
— 45.39
— 39.92
— 22.75
— 21.01

f1 (ppm)

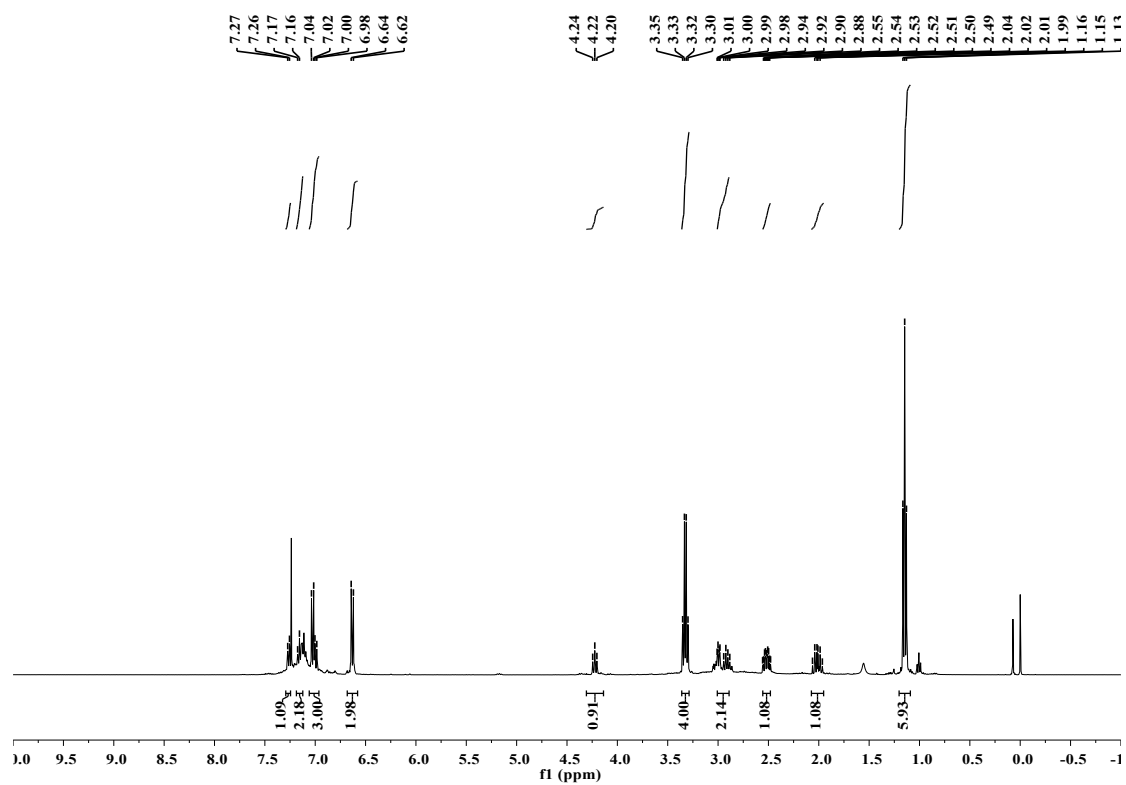
¹H NMR spectrum (CDCl₃) of compound 10a. The x-axis represents chemical shift in ppm, ranging from -1 to 9.5. The spectrum shows several peaks with corresponding integration values below the baseline. The peaks are labeled with their chemical shifts (ppm) above the baseline.

Chemical Shift (ppm)	Integration
8.21	0.91
8.19	0.93
7.95	2.00
7.93	1.02
7.37	2.01
7.35	1.82
7.33	1.00
7.31	1.00
7.26	
7.24	
7.06	
7.04	
6.99	
6.97	
4.75	1.00
4.74	
4.72	
4.70	
3.80	6.01
3.02	3.02
1.63	3.01

2q (^{13}C NMR)



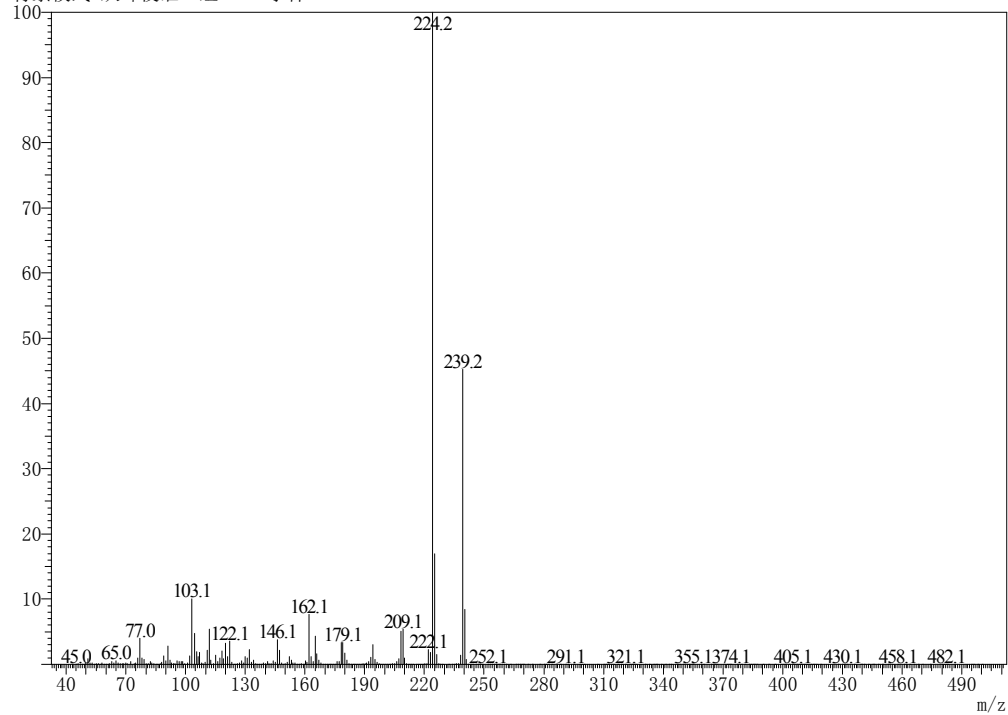
2q (^1H NMR)



5. Original low resolution MS spectra

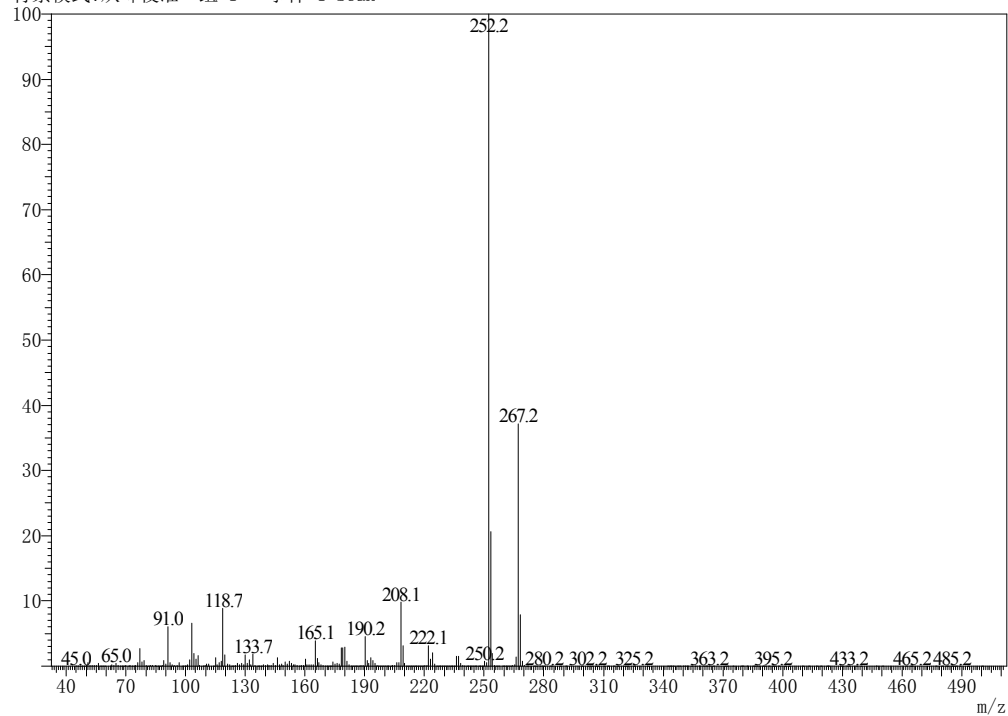
2a

流路号:1 保留时间:20.495(扫描数:3400)
质量峰:324
原始模式:平均 20.490-20.500(3399-3401) 基峰:224(3767580)
背景模式:从峰校准 组 1 - 事件 1 Scan



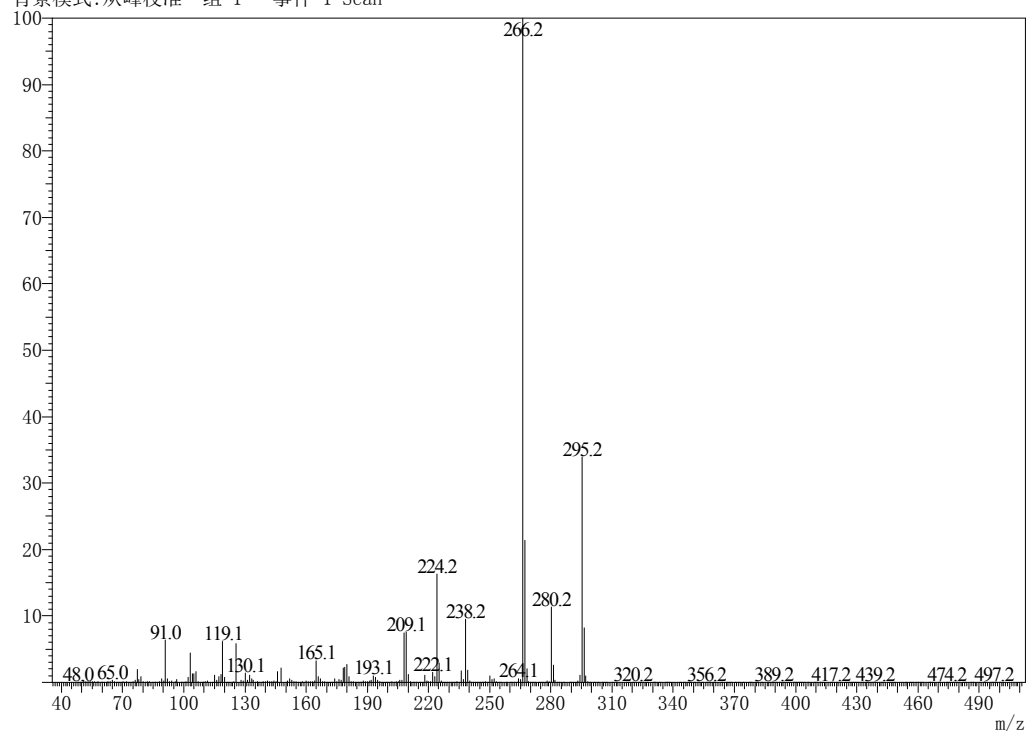
2b

流路号:1 保留时间:21.415(扫描数:3584)
质量峰:308
原始模式:平均 21.410-21.420(3583-3585) 基峰:252(2977382)
背景模式:从峰校准 组 1 - 事件 1 Scan



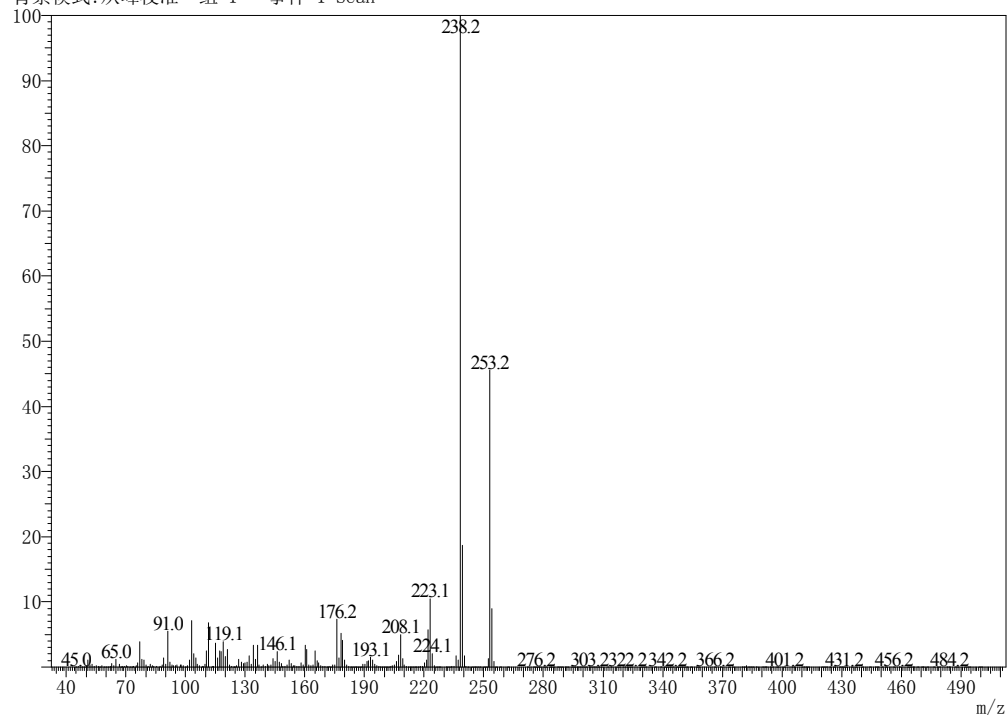
2c

流路号:1 保留时间:22.765(扫描数:3854)
质量峰:350
原始模式:平均 22.760-22.770(3853-3855) 基峰:266(4055107)
背景模式:从峰校准 组 1 - 事件 1 Scan



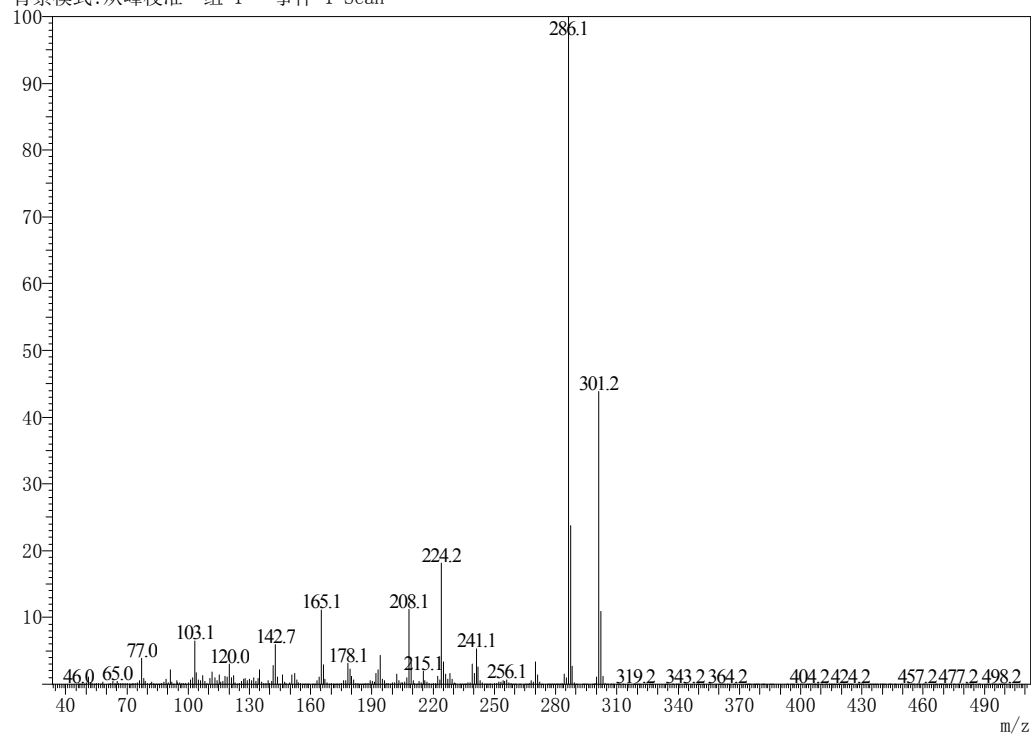
2d

流路号:1 保留时间:21.140(扫描数:3529)
质量峰:331
原始模式:平均 21.135-21.145(3528-3530) 基峰:238(244984)
背景模式:从峰校准 组 1 - 事件 1 Scan



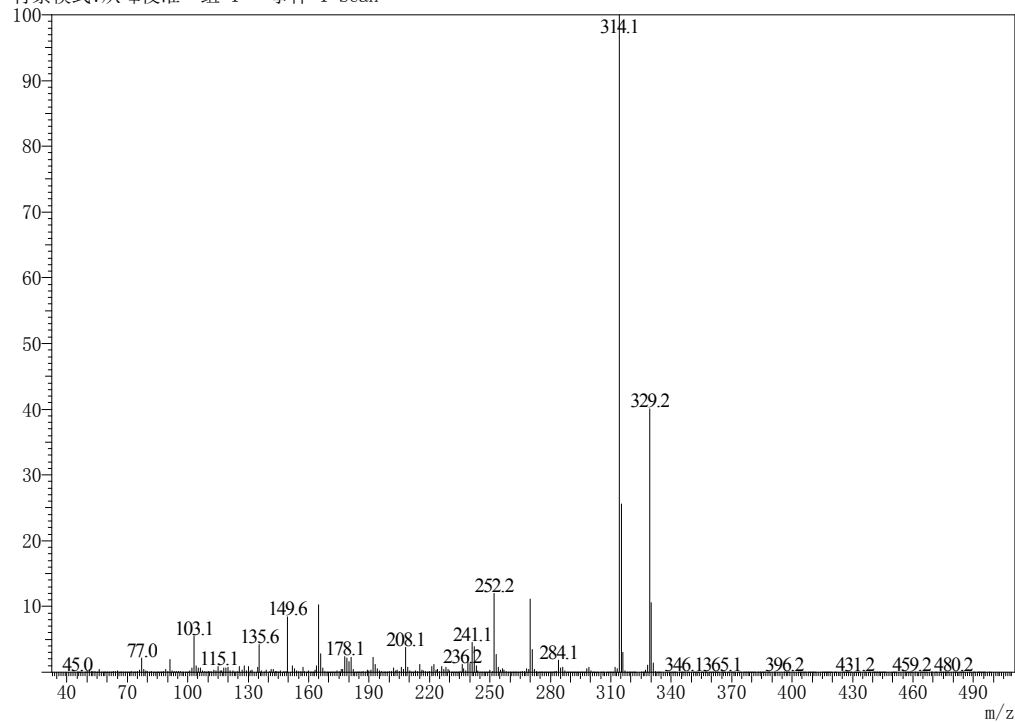
2e

流路号:1 保留时间:26.120(扫描数:4525)
质量峰:346
原始模式:平均 26.115-26.125(4524-4526) 基峰:286(156311)
背景模式:从峰校准 组 1 - 事件 1 Scan



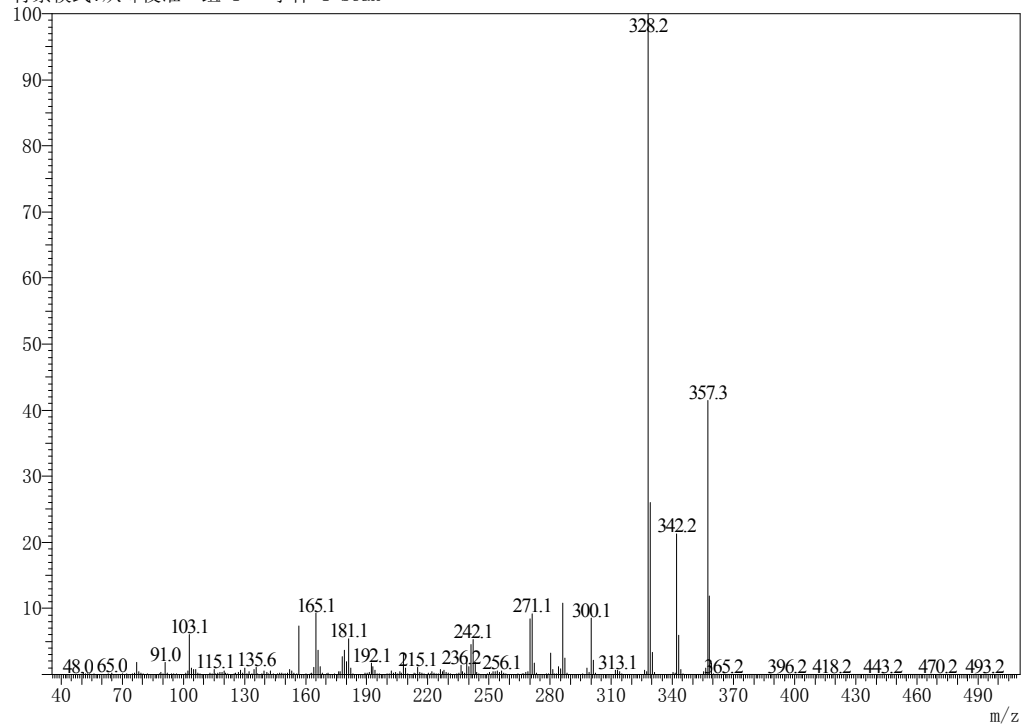
2f

流路号:1 保留时间:27.430(扫描数:4787)
质量峰:378
原始模式:平均 27.425-27.435(4786-4788) 基峰:314(1403258)
背景模式:从峰校准 组 1 - 事件 1 Scan



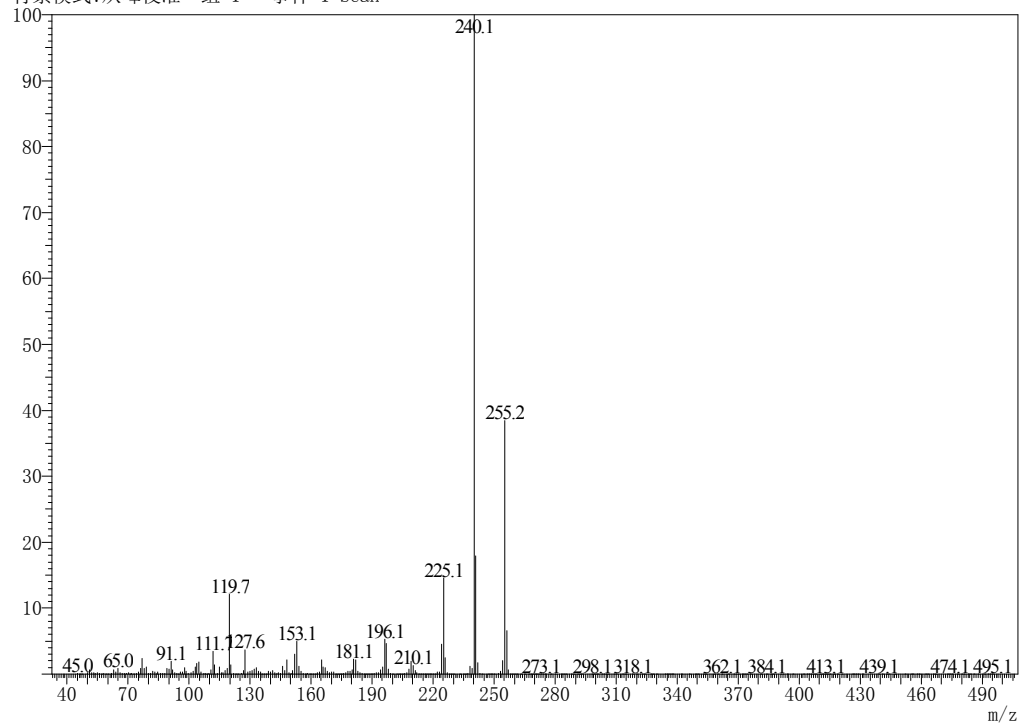
2g

流路号:1 保留时间:30.270(扫描数:5355)
质量峰:345
原始模式:平均 30.265-30.275(5354-5356) 基峰:328(1207408)
背景模式:从峰校准 组 1 - 事件 1 Scan



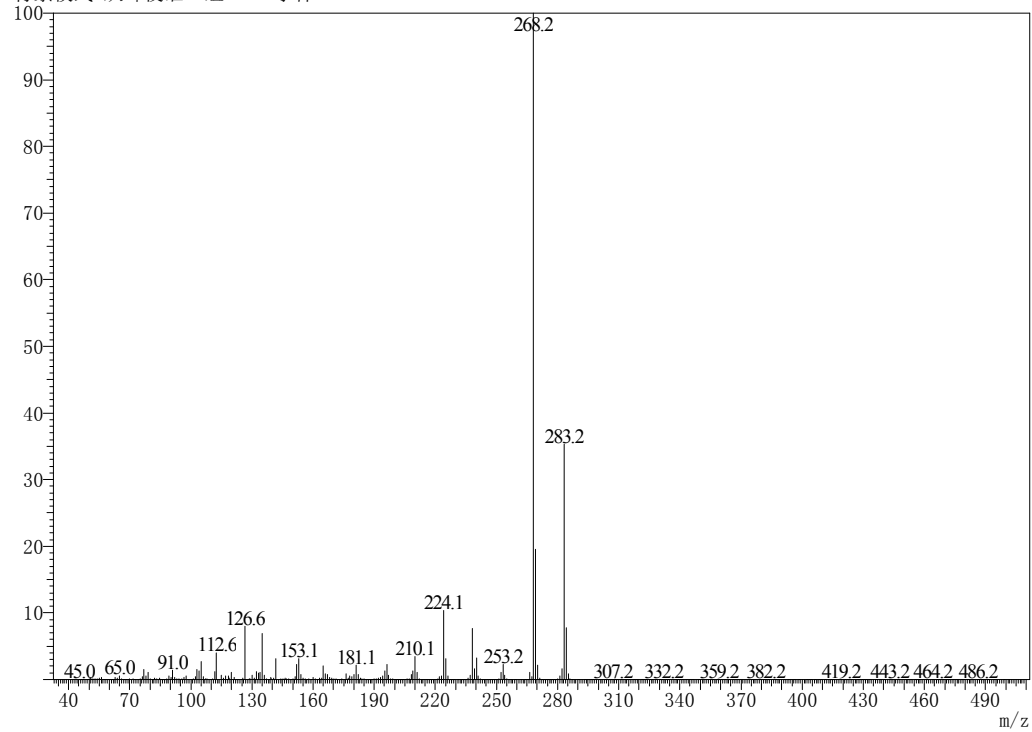
2h

流路号:1 保留时间:22.570(扫描数:3815)
质量峰:325
原始模式:平均 22.565-22.575(3814-3816) 基峰:240(504651)
背景模式:从峰校准 组 1 - 事件 1 Scan



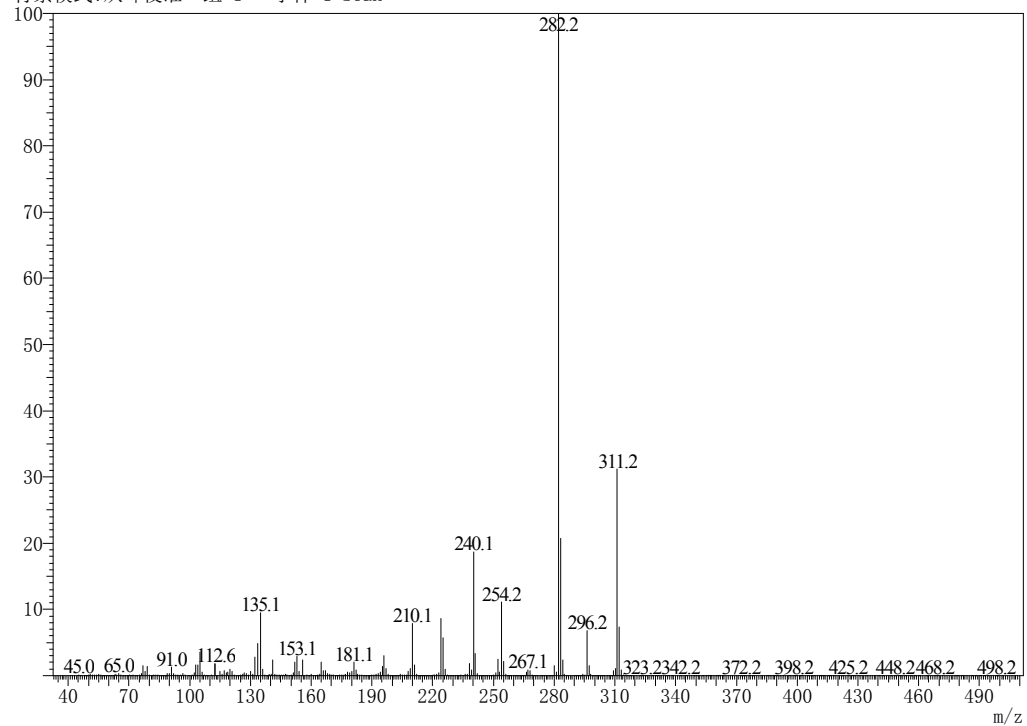
2i

流路号:1 保留时间:23.410(扫描数:3983)
质量峰:350
原始模式:平均 23.405-23.415(3982-3984) 基峰:268(1757302)
背景模式:从峰校准 组 1 - 事件 1 Scan



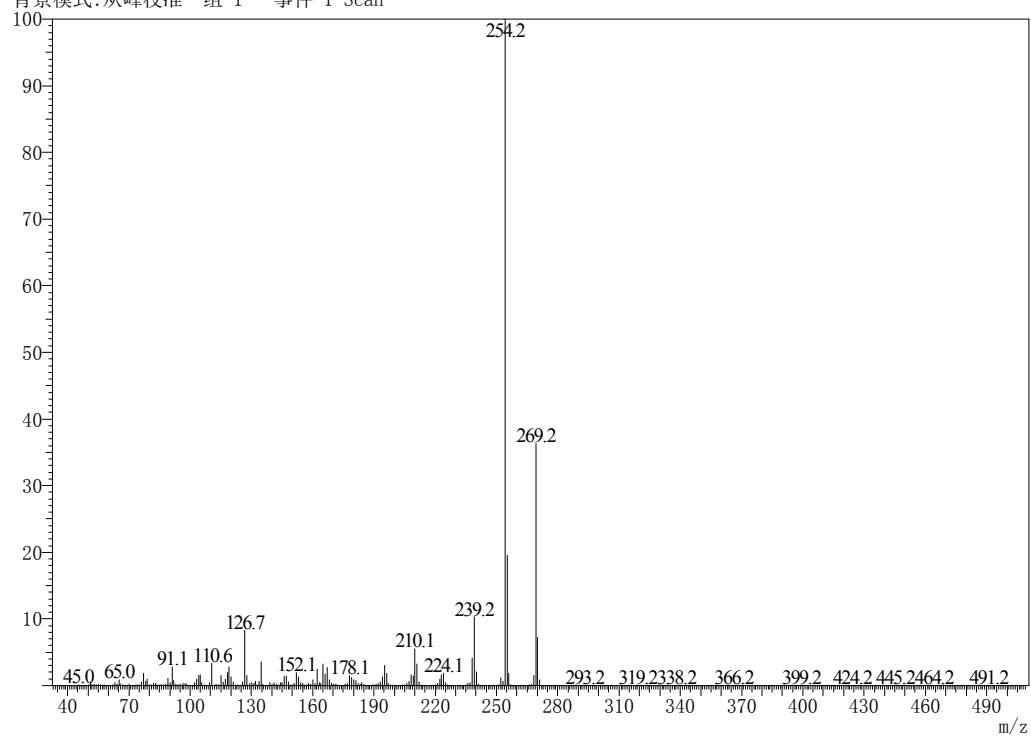
2j

流路号:1 保留时间:24.960(扫描数:4293)
质量峰:337
原始模式:平均 24.955-24.965(4292-4294) 基峰:282(934796)
背景模式:从峰校准 组 1 - 事件 1 Scan



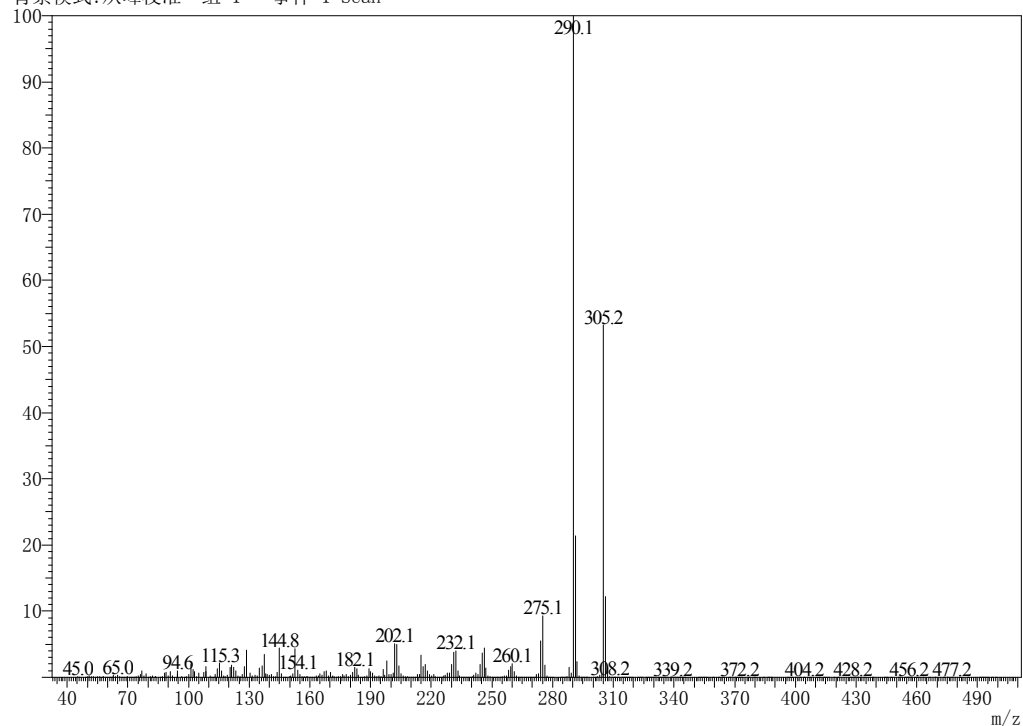
2k

流路号:1 保留时间:23.135(扫描数:3928)
质量峰:323
原始模式:平均 23.130-23.140(3927-3929) 基峰:254(165419)
背景模式:从峰校准 组 1 - 事件 1 Scan



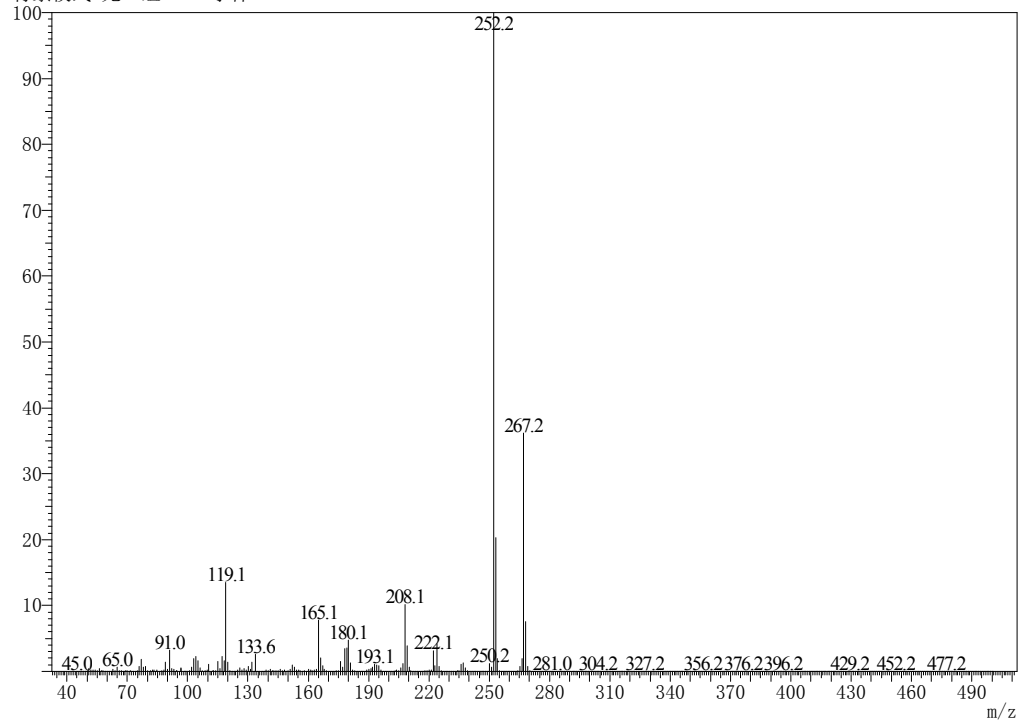
2l

流路号:1 保留时间:26.905(扫描数:4682)
质量峰:350
原始模式:平均 26.900-26.910(4681-4683) 基峰:290(1327438)
背景模式:从峰校准 组 1 - 事件 1 Scan



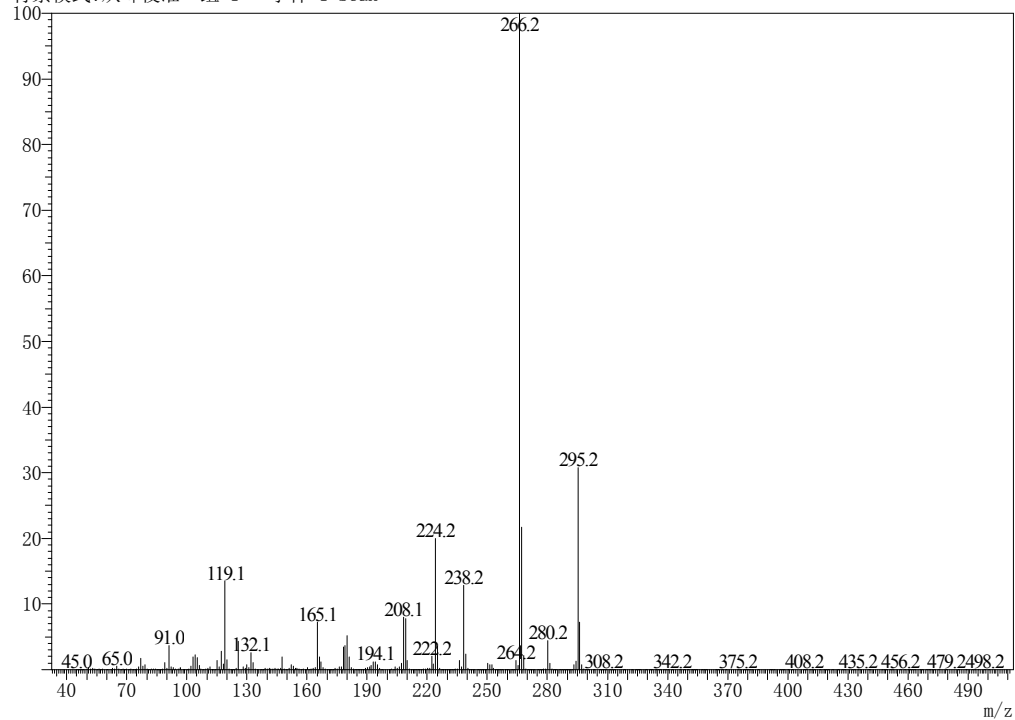
2m

流路号:1 保留时间:21.980(扫描数:3697)
质量峰:456
原始模式:平均 21.920-22.040(3685-3709) 基峰:252(278230)
背景模式:无 组 1 - 事件 1 Scan



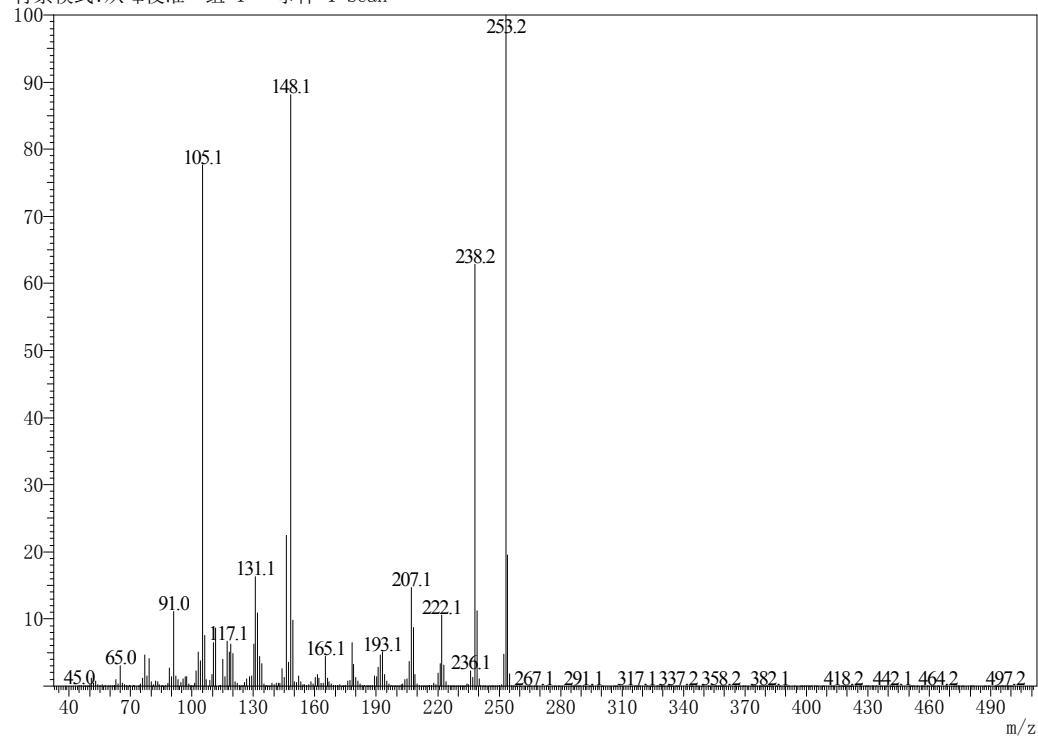
2n

流路号:1 保留时间:23.295(扫描数:3960)
质量峰:340
原始模式:平均 23.290-23.300(3959-3961) 基峰:266(213868)
背景模式:从峰校准 组 1 - 事件 1 Scan



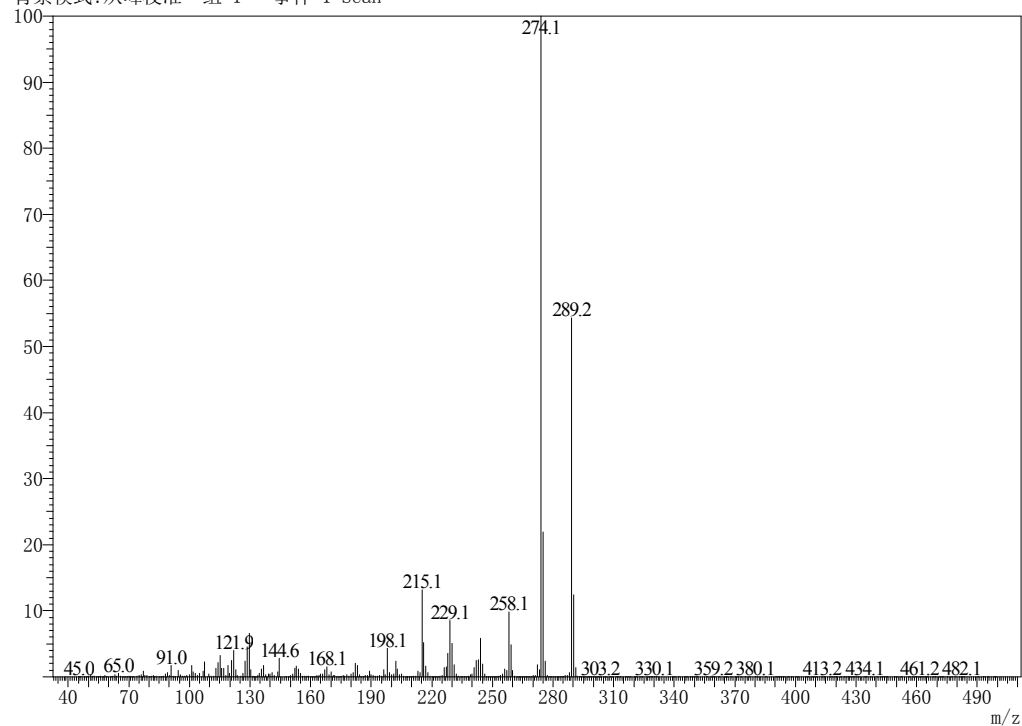
2o

流路号:1 保留时间:19.165(扫描数:3134)
质量峰:334
原始模式:平均 19.160-19.170(3133-3135) 基峰:253(1160420)
背景模式:从峰校准 组 1 - 事件 1 Scan



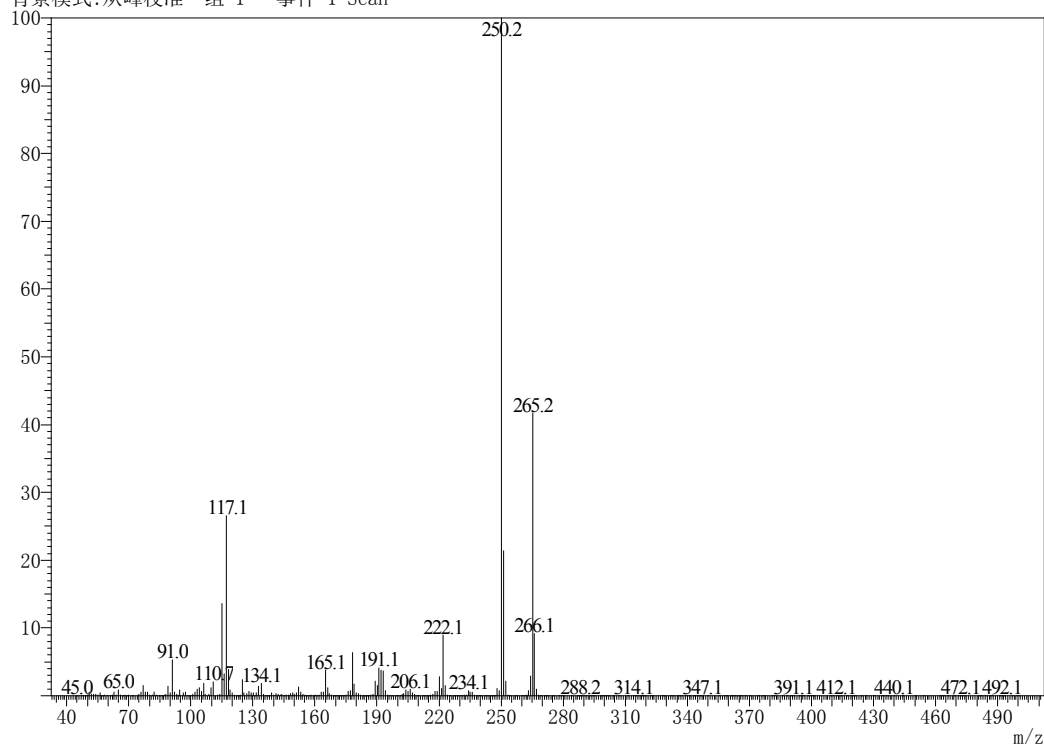
2p

流路号:1 保留时间:24.665(扫描数:4234)
质量峰:359
原始模式:平均 24.660-24.670(4233-4235) 基峰:274(1025735)
背景模式:从峰校准 组 1 - 事件 1 Scan



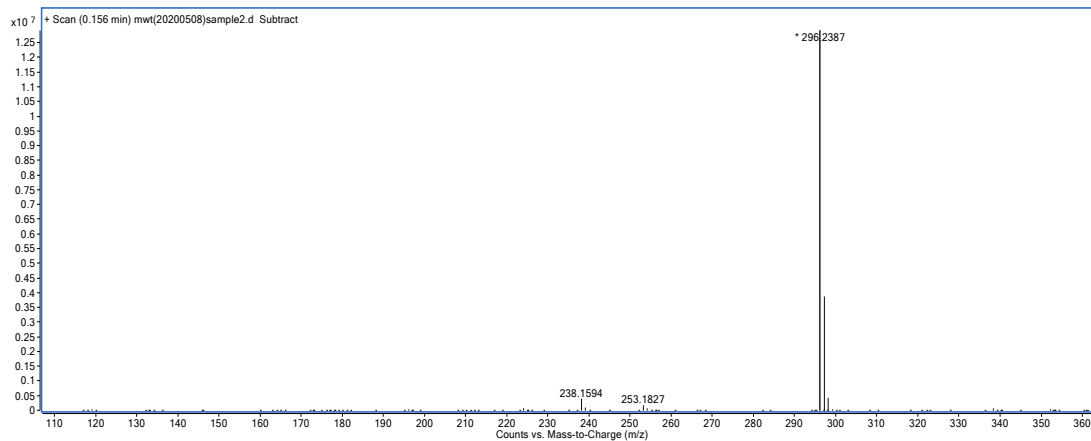
2q

流路号:1 保留时间:22.665(扫描数:3834)
质量峰:326
原始模式:平均 22.660-22.670(3833-3835) 基峰:250(406373)
背景模式:从峰校准 组 1 - 事件 1 Scan

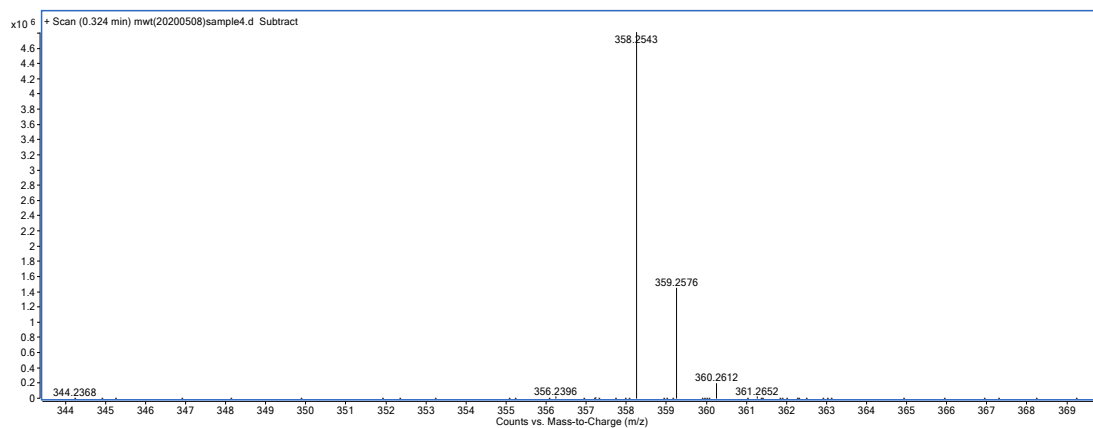


6. Original high resolution MS spectra for the new products

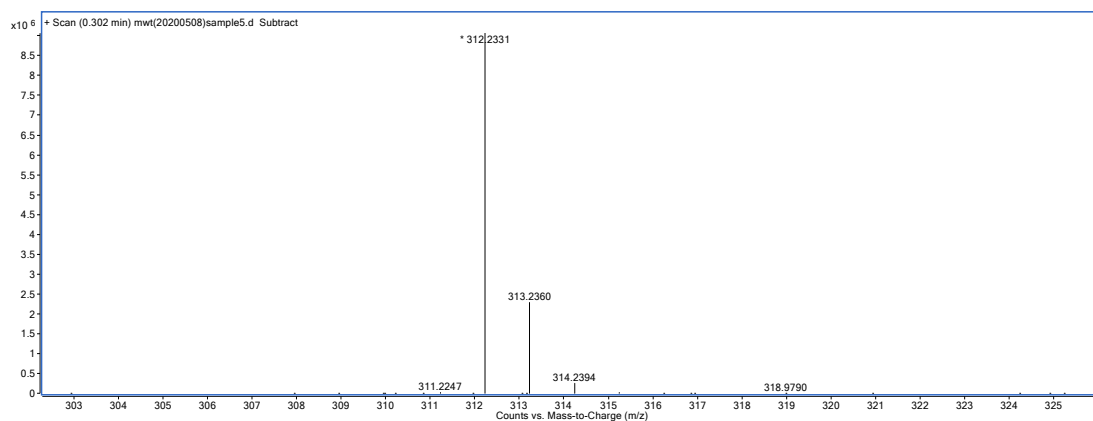
2c



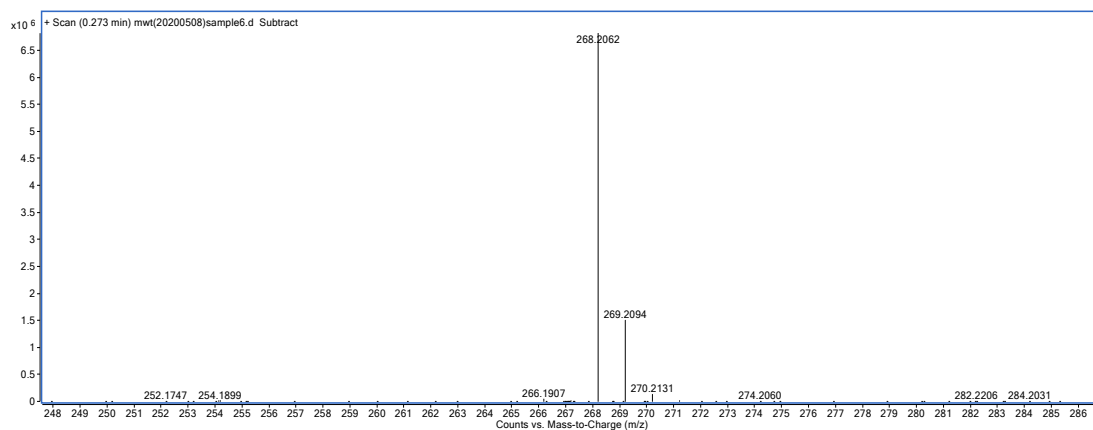
2g



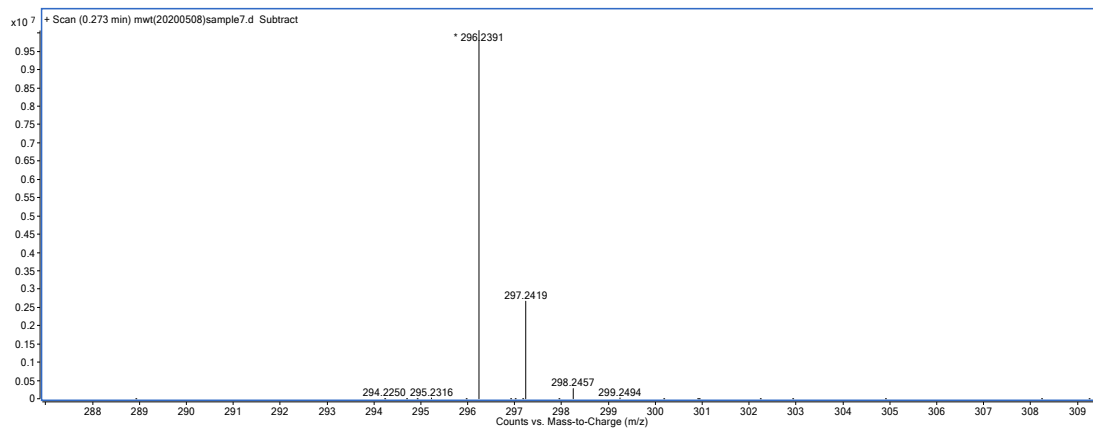
2j



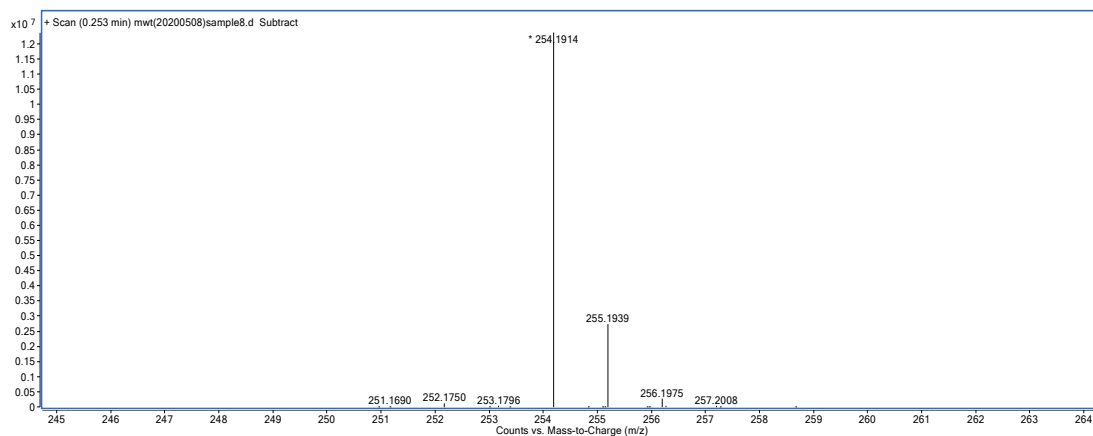
2m



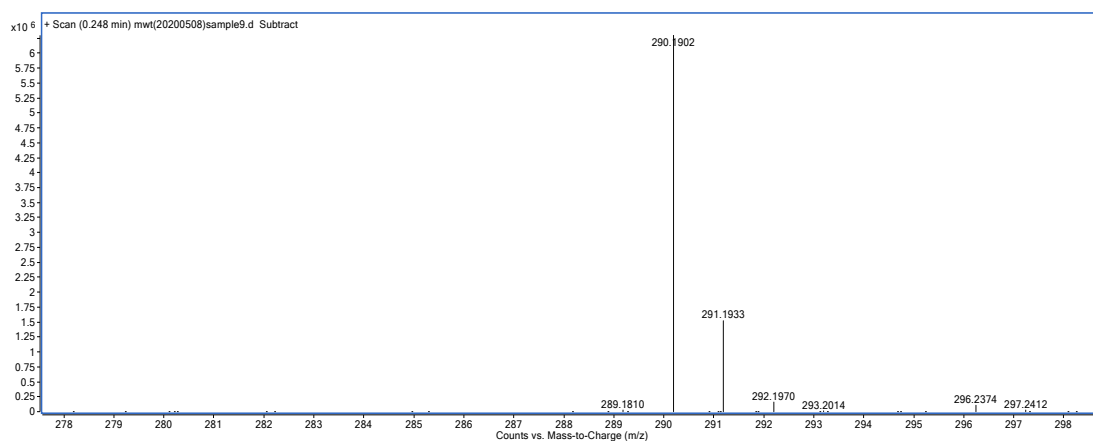
2n



2o



2p



7. Theoretical calculation method

All the calculations were performed with the B3LYP and M06-2X method based on density functional theory. LANL2DZ basis set was used for Cu and Au atom and 6-311+G* basis set was used for the other atoms (abbreviation as B3LYP/6-311+G*/LANL2DZ or M062X/6-311+G*/LANL2DZ). All of the structures were fully optimized with B3LYP/6-311+G*/LANL2DZ method. Energy calculations have been done by using M062X/6-311+G*/LANL2DZ method. The influence of solvent was performed in condensed phase with the Polarizable Continuum Model (PCM) using aniline as solvent. This method creates the solute cavity via a set of overlapping spheres.

The computed stationary points have been characterized as minima or transition states by diagonalizing the Hessian matrix and analyzing the vibrational normal modes. In this way, the stationary points can be classified as minima if no imaginary frequencies are shown or as transition states if only one imaginary frequency is obtained. The particular nature of the transition states has been determined by analyzing the motion described by the eigenvector associated with the imaginary frequency. All calculations were performed with the Gaussian 09 suite of programs ^{S1}.

References

(S1) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I.

Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. G. Johnson, W. Chen, M. W. Wong, C. Gonzalez, J. A. Pople, GAUSSIAN 03, Gaussian, Inc., Pittsburgh, PA, 2009.

8. Cartesians coordinates of the optimized structures

Rea (CAAC-Cu⁺)

6	0	1.868503	-1.778537	-1.860629
6	0	2.854752	-0.826168	-1.864097
6	0	3.865696	-0.730926	-0.777577
6	0	4.501126	0.488334	-0.485971
6	0	4.242154	-1.868617	-0.041942
6	0	5.457015	0.572463	0.521772
6	0	5.203632	-1.784860	0.958442
6	0	5.810382	-0.562914	1.248412
6	0	3.020291	0.078529	-3.063079
29	0	0.818098	-0.238905	-0.841727
7	0	-1.622205	0.558217	0.476206
6	0	-2.113763	-0.803574	0.256507
6	0	-2.457815	1.631483	1.208870
6	0	-1.839698	-1.802839	1.217771
6	0	-2.829593	-1.086353	-0.929099
6	0	-0.439077	0.942427	0.089187
6	0	-0.185145	2.381885	0.499191
6	0	-3.005188	-0.094500	-2.077493
6	0	-3.125798	-3.364190	-0.132570
6	0	-3.332050	-2.381235	-1.090284
6	0	-2.371749	-3.077476	0.996159
6	0	-0.931390	-1.603407	2.430106
6	0	-1.569865	2.878002	0.996260

6	0	-1.582445	-2.049171	3.751632
6	0	-2.114902	-0.490952	-3.271667
6	0	-4.468451	0.052296	-2.530970
6	0	0.410872	-2.333404	2.229113
6	0	0.874174	2.329226	1.646752
6	0	0.371043	3.214189	-0.684119
6	0	-3.845948	1.785998	0.585318
6	0	-2.625030	1.274360	2.690301
6	0	-0.450426	3.202636	-1.976499
6	0	1.324384	3.685623	2.198785
1	0	1.267336	-1.950593	-2.747853
1	0	1.814888	-2.543413	-1.092137
1	0	4.249425	1.384096	-1.041642
1	0	3.813408	-2.835325	-0.279798
1	0	5.933045	1.523918	0.732663
1	0	5.492989	-2.678382	1.500846
1	0	6.564996	-0.500224	2.024890
1	0	3.023335	1.137672	-2.797039
1	0	3.986051	-0.124889	-3.535935
1	0	2.235300	-0.083210	-3.802103
1	0	-2.664696	0.885469	-1.743566
1	0	-3.535034	-4.358620	-0.275994
1	0	-3.889298	-2.626350	-1.987204
1	0	-2.184694	-3.862789	1.719542
1	0	-0.699844	-0.542962	2.519906
1	0	-1.488917	3.456095	1.917401
1	0	-2.029424	3.535188	0.256725
1	0	-2.551496	-1.574042	3.916295
1	0	-1.738231	-3.130165	3.785377

1	0	-0.936489	-1.792326	4.595479
1	0	-1.060574	-0.545772	-2.982823
1	0	-2.204435	0.241330	-4.078873
1	0	-2.396842	-1.466640	-3.675666
1	0	-4.846452	-0.863224	-2.992241
1	0	-4.553497	0.845578	-3.278548
1	0	-5.133123	0.300655	-1.701404
1	0	0.270947	-3.413083	2.130331
1	0	1.073387	-2.160375	3.081534
1	0	0.927919	-1.980965	1.331307
1	0	0.472281	1.727777	2.468630
1	0	1.752641	1.784724	1.282899
1	0	0.482939	4.248420	-0.346978
1	0	1.386834	2.860859	-0.900214
1	0	-3.803174	2.100724	-0.456741
1	0	-4.389940	2.556843	1.136340
1	0	-4.427191	0.864626	0.653347
1	0	-3.162327	0.334375	2.820673
1	0	-3.217776	2.056046	3.170783
1	0	-1.674211	1.213907	3.219862
1	0	-1.454214	3.612379	-1.837525
1	0	-0.557533	2.196377	-2.390849
1	0	0.035561	3.817605	-2.737760
1	0	0.486962	4.294438	2.549448
1	0	1.876007	4.271831	1.461677
1	0	1.989608	3.533175	3.052083

TS1 (CAAC-Cu⁺)

6	0	1.143478	1.221999	-0.123546
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6	0	2.373176	1.064654	-0.971070
6	0	2.030415	1.242409	-2.450665
6	0	3.629149	1.790699	-0.529268
6	0	3.922399	1.992030	0.830117
6	0	4.530955	2.328682	-1.463147
6	0	5.047038	2.705187	1.235702
6	0	5.652573	3.051812	-1.062022
6	0	5.918488	3.244233	0.291108
6	0	2.838990	-0.799724	-0.899674
6	0	4.026518	-1.052823	-1.681975
6	0	5.230444	-1.329261	-1.113860
6	0	5.348255	-1.480463	0.310455
6	0	4.141880	-1.430821	1.087776
6	0	2.951962	-1.133454	0.498531
7	0	6.542771	-1.679035	0.890105
6	0	6.649529	-1.900736	2.336646
6	0	7.777304	-1.684386	0.095996
29	0	-0.477784	0.063764	-0.219571
7	0	-3.316228	-0.501242	0.079576
6	0	-3.512317	0.898837	0.457789
6	0	-4.494616	-1.490204	0.003889
6	0	-3.767935	1.860633	-0.545674
6	0	-3.419640	1.258428	1.821272
6	0	-2.142594	-0.984297	-0.234482
6	0	-2.282742	-2.444437	-0.641177
6	0	-2.959688	0.308036	2.925044
6	0	-3.995923	3.537051	1.201072
6	0	-3.677889	2.589273	2.163244
6	0	-4.018443	3.174950	-0.137842

6	0	-3.688572	1.578010	-2.045000
6	0	-3.745854	-2.811771	-0.275415
6	0	-4.940035	2.033525	-2.816050
6	0	-1.534509	0.671634	3.387409
6	0	-3.916353	0.271077	4.129819
6	0	-2.428123	2.229052	-2.648471
6	0	-2.033205	-2.490785	-2.181879
6	0	-1.236664	-3.331483	0.079905
6	0	-5.280802	-1.531674	1.315894
6	0	-5.457569	-1.113893	-1.128169
6	0	-1.200442	-3.236473	1.607776
6	0	-2.067879	-3.881697	-2.823396
1	0	1.391033	1.373361	0.929653
1	0	0.683677	2.168256	-0.453201
1	0	2.817068	0.943619	-3.142409
1	0	1.127699	0.681944	-2.695734
1	0	1.819836	2.299737	-2.637295
1	0	3.255069	1.607897	1.590555
1	0	4.356301	2.211720	-2.525035
1	0	5.231342	2.856432	2.294701
1	0	6.312191	3.474296	-1.813139
1	0	6.785380	3.815966	0.605425
1	0	1.904319	-1.090257	-1.367433
1	0	3.966105	-0.985043	-2.762741
1	0	6.098462	-1.462356	-1.744610
1	0	4.176987	-1.614787	2.152717
1	0	2.054335	-1.077163	1.104122
1	0	6.090099	-2.787837	2.642217
1	0	7.692999	-2.054596	2.596272

1	0	6.281465	-1.035872	2.893740
1	0	7.836107	-2.568812	-0.544382
1	0	7.843456	-0.788149	-0.522692
1	0	8.630942	-1.692924	0.767980
1	0	-2.907483	-0.699952	2.514001
1	0	-4.201548	4.561855	1.492219
1	0	-3.618328	2.891990	3.202584
1	0	-4.223152	3.932617	-0.885728
1	0	-3.584455	0.503199	-2.188475
1	0	-4.238107	-3.371023	-1.072107
1	0	-3.773823	-3.447357	0.611087
1	0	-5.858217	1.609510	-2.404841
1	0	-5.049153	3.120844	-2.808479
1	0	-4.870173	1.726508	-3.863399
1	0	-0.827822	0.658576	2.553084
1	0	-1.185259	-0.039719	4.142076
1	0	-1.501010	1.669604	3.832877
1	0	-3.931587	1.222466	4.667311
1	0	-3.595721	-0.493946	4.842713
1	0	-4.942777	0.044622	3.834906
1	0	-2.461810	3.318780	-2.566028
1	0	-2.341571	1.980104	-3.710372
1	0	-1.521106	1.885786	-2.144563
1	0	-2.773168	-1.853445	-2.677655
1	0	-1.061591	-2.026962	-2.385209
1	0	-1.417818	-4.371871	-0.206436
1	0	-0.245544	-3.078390	-0.314587
1	0	-4.664879	-1.844065	2.158618
1	0	-6.090910	-2.258129	1.214752

1	0	-5.733815	-0.566438	1.549294
1	0	-5.906590	-0.133355	-0.965550
1	0	-6.270059	-1.843990	-1.154490
1	0	-4.978245	-1.121900	-2.107438
1	0	-2.148810	-3.526052	2.068175
1	0	-0.959934	-2.225851	1.948312
1	0	-0.438368	-3.908993	2.010440
1	0	-3.007188	-4.408135	-2.632687
1	0	-1.253547	-4.520346	-2.475303
1	0	-1.965910	-3.792156	-3.907983
Int1				
29	0	1.738306	0.011698	-0.126376
7	0	4.615086	-0.448217	-0.039869
6	0	4.812019	1.001628	-0.047103
6	0	5.809667	-1.416893	0.018451
6	0	4.848041	1.703869	1.178740
6	0	4.951142	1.667990	-1.285313
6	0	3.428328	-0.998828	-0.053953
6	0	3.573621	-2.513367	0.025557
6	0	4.720659	1.003542	-2.641100
6	0	5.329814	3.736545	-0.065962
6	0	5.220909	3.039701	-1.260851
6	0	5.122262	3.074760	1.135425
6	0	4.501640	1.084682	2.531659
6	0	5.091792	-2.771139	-0.167175
6	0	5.566888	1.343929	3.611477
6	0	3.380424	1.471182	-3.243164
6	0	5.866705	1.245593	-3.639243

6	0	3.125521	1.586921	3.012185
6	0	3.082608	-2.921168	1.449897
6	0	2.701886	-3.216617	-1.044663
6	0	6.820423	-1.138173	-1.096597
6	0	6.533384	-1.315503	1.366702
6	0	2.894378	-2.752507	-2.491374
6	0	3.074643	-4.423737	1.750197
6	0	0.156837	1.198356	-0.260771
6	0	-1.227731	0.951807	0.398536
6	0	-2.106605	-0.034009	-0.534542
6	0	-1.419331	-1.291720	-0.893355
6	0	-1.967801	-2.516625	-0.733245
6	0	-3.303543	-2.669770	-0.202403
6	0	-4.036280	-1.475233	0.143679
6	0	-3.473503	-0.257869	-0.012843
7	0	-3.838730	-3.879523	-0.045117
6	0	-3.054014	-5.105081	-0.258976
6	0	-5.234356	-4.075706	0.378934
6	0	-2.008912	2.278919	0.504010
6	0	-2.276468	3.031942	-0.651338
6	0	-2.438058	2.810565	1.726618
6	0	-2.939865	4.253036	-0.591201
6	0	-3.096150	4.041414	1.795046
6	0	-3.354674	4.767697	0.637925
6	0	-1.050893	0.277384	1.769134
1	0	4.638362	-0.072692	-2.488985
1	0	5.549350	4.799143	-0.072346
1	0	5.336572	3.574119	-2.196900
1	0	5.160459	3.636786	2.061705

1	0	4.414637	0.005970	2.405573
1	0	5.476423	-3.511749	0.535544
1	0	5.293133	-3.159054	-1.167138
1	0	6.561657	1.018030	3.301122
1	0	5.635245	2.403587	3.869692
1	0	5.310822	0.807444	4.529598
1	0	2.545421	1.271746	-2.566403
1	0	3.185159	0.955087	-4.188299
1	0	3.389539	2.545118	-3.448656
1	0	5.934865	2.295452	-3.934924
1	0	5.699764	0.667037	-4.552322
1	0	6.837424	0.955969	-3.231810
1	0	3.134246	2.665336	3.192489
1	0	2.847737	1.096117	3.949910
1	0	2.345887	1.380060	2.275120
1	0	3.706306	-2.415665	2.194299
1	0	2.073172	-2.519735	1.590884
1	0	2.894781	-4.292525	-0.987764
1	0	1.650255	-3.080767	-0.763831
1	0	6.382495	-1.245424	-2.088607
1	0	7.636456	-1.860946	-1.018091
1	0	7.256337	-0.141225	-1.010752
1	0	6.956591	-0.322160	1.521002
1	0	7.361771	-2.027984	1.376216
1	0	5.885562	-1.553343	2.210756
1	0	3.919269	-2.897052	-2.843145
1	0	2.645183	-1.695753	-2.616111
1	0	2.249350	-3.324253	-3.164268
1	0	4.054003	-4.885917	1.600062

1	0	2.356010	-4.966821	1.132295
1	0	2.796863	-4.592950	2.793813
1	0	0.006937	1.469063	-1.316635
1	0	0.538341	2.127022	0.188673
1	0	-2.205558	0.540190	-1.469873
1	0	-0.424474	-1.198623	-1.312582
1	0	-1.411751	-3.391273	-1.042980
1	0	-5.032773	-1.541965	0.559221
1	0	-4.047615	0.616572	0.272954
1	0	-3.587856	-5.941163	0.185680
1	0	-2.919039	-5.306251	-1.324898
1	0	-2.079909	-5.033578	0.223284
1	0	-5.312771	-4.075680	1.469246
1	0	-5.882180	-3.302437	-0.024602
1	0	-5.577457	-5.036975	0.001382
1	0	-1.938461	2.676587	-1.620009
1	0	-2.252493	2.278535	2.651250
1	0	-3.121190	4.811246	-1.504395
1	0	-3.402189	4.429622	2.761455
1	0	-3.862529	5.725027	0.690139
1	0	-0.545604	-0.682548	1.649197
1	0	-0.415966	0.891070	2.411588
1	0	-1.994328	0.101542	2.295165
6	0	-7.660413	-1.189606	1.884146
6	0	-7.076012	0.074135	1.973182
6	0	-7.035533	0.929529	0.876578
6	0	-7.579464	0.543716	-0.371521
6	0	-8.177498	-0.736701	-0.445384
6	0	-8.214806	-1.576422	0.663896

7	0	-7.526617	1.383327	-1.474060
6	0	-7.188159	2.787532	-1.279377
6	0	-8.306841	1.046866	-2.656359
1	0	-7.718539	-1.836891	2.752572
1	0	-6.662324	0.415078	2.917539
1	0	-6.599146	1.911635	1.003709
1	0	-8.644291	-1.071116	-1.362376
1	0	-8.712854	-2.537858	0.574252
1	0	-6.184771	2.901984	-0.862229
1	0	-7.194965	3.291240	-2.244533
1	0	-7.896931	3.304737	-0.617961
1	0	-8.001047	0.081399	-3.067529
1	0	-9.386921	1.009044	-2.457066
1	0	-8.129596	1.796034	-3.426122

TS2

6	0	1.05794	1.34088	-1.78599
6	0	2.56423	1.64878	-1.58528
6	0	3.06325	0.27565	-1.00196
6	0	3.23664	-0.84464	-1.88039
6	0	3.8563	-2.00597	-1.49561
6	0	4.42075	-2.14281	-0.19321
6	0	4.31282	-1.02038	0.67765
6	0	3.70149	0.14077	0.27276
7	0	5.04081	-3.28611	0.1938
6	0	5.66575	-3.38271	1.51194
6	0	5.19869	-4.3993	-0.74099
6	0	3.22105	2.01145	-2.93755
6	0	2.82189	2.79083	-0.59137

6	0	1.7952	3.45421	0.0871
6	0	4.13768	3.22326	-0.35571
6	0	2.06564	4.50926	0.96273
6	0	4.41308	4.27203	0.51521
6	0	3.37406	4.92451	1.18017
1	0	0.94072	0.66548	-2.63904
1	0	0.44262	2.22669	-1.99179
1	0	2.84197	-0.79194	-2.88865
1	0	3.93018	-2.81498	-2.20965
1	0	4.74318	-1.05774	1.66934
1	0	3.67429	0.97527	0.96244
1	0	4.9405	-3.19762	2.30878
1	0	6.06	-4.38657	1.64723
1	0	6.49378	-2.67498	1.62028
1	0	4.22969	-4.75635	-1.10026
1	0	5.81131	-4.1193	-1.60369
1	0	5.69014	-5.22497	-0.23291
1	0	4.30204	2.13861	-2.86258
1	0	3.02706	1.25065	-3.69658
1	0	2.80393	2.9527	-3.30325
1	0	0.76406	3.16354	-0.06693
1	0	4.96709	2.73153	-0.85352
1	0	1.2449	5.00972	1.46668
1	0	5.44046	4.58479	0.67099
1	0	3.58551	5.74798	1.85393
1	0	1.68603	0.17184	-0.70116
29	0	-0.08182	0.46644	-0.35163
7	0	-2.6448	-0.54347	0.63837
6	0	-3.20609	-0.35047	-0.69996

6	0	-3.48646	-1.12549	1.79352
6	0	-3.10223	-1.38982	-1.65233
6	0	-3.82774	0.88055	-1.00946
6	0	-1.40392	-0.26569	0.92857
6	0	-1.11115	-0.62675	2.37461
6	0	-3.79523	2.10534	-0.09745
6	0	-4.39309	-0.02246	-3.19453
6	0	-4.42438	1.00959	-2.26762
6	0	-3.71888	-1.19697	-2.89289
6	0	-2.28037	-2.66175	-1.44855
6	0	-2.49886	-0.98156	2.97311
6	0	-3.06807	-3.94836	-1.75246
6	0	-2.81869	3.15911	-0.65599
6	0	-5.18189	2.73303	0.12818
6	0	-0.99513	-2.61346	-2.29862
6	0	-0.15717	-1.86249	2.33101
6	0	-0.40971	0.54604	3.10712
6	0	-4.77362	-0.32802	2.01018
6	0	-3.85636	-2.5864	1.51217
6	0	-1.12616	1.89856	3.07153
6	0	0.32688	-2.37654	3.69086
1	0	-3.40827	1.80351	0.8755
1	0	-4.87169	0.0983	-4.16068
1	0	-4.91403	1.94041	-2.53014
1	0	-3.66197	-1.97959	-3.64094
1	0	-1.96471	-2.70713	-0.4069
1	0	-2.46556	-1.90056	3.55977
1	0	-2.84071	-0.19605	3.64858
1	0	-4.00168	-4.00427	-1.18954

1	0	-3.31883	-4.03149	-2.81272
1	0	-2.4695	-4.82672	-1.49526
1	0	-1.81424	2.74597	-0.78572
1	0	-2.74778	4.01472	0.02161
1	0	-3.14627	3.53351	-1.62928
1	0	-5.58526	3.17068	-0.78813
1	0	-5.11552	3.53858	0.8646
1	0	-5.90928	2.00514	0.49279
1	0	-1.22289	-2.57316	-3.3671
1	0	-0.38757	-3.50583	-2.12152
1	0	-0.38675	-1.73802	-2.05534
1	0	-0.66414	-2.67803	1.80369
1	0	0.71273	-1.60595	1.71642
1	0	-0.26079	0.25346	4.15062
1	0	0.59292	0.66433	2.67987
1	0	-4.57792	0.71348	2.2628
1	0	-5.32045	-0.77063	2.84628
1	0	-5.42767	-0.3624	1.137
1	0	-4.47045	-2.68135	0.61572
1	0	-4.44394	-2.96632	2.35113
1	0	-2.9818	-3.22918	1.40702
1	0	-2.11866	1.85911	3.52806
1	0	-1.24291	2.27587	2.05227
1	0	-0.5518	2.64277	3.62825
1	0	-0.49858	-2.61323	4.36733
1	0	0.97525	-1.65925	4.1975
1	0	0.90322	-3.29551	3.55582

Int2

6	0	-0.27496	1.64753	0.19391
6	0	1.07036	1.54478	-0.58017
6	0	1.86039	0.26716	-0.22427
6	0	1.65932	-0.43269	0.97339
6	0	2.37792	-1.57674	1.31084
6	0	3.35601	-2.11577	0.44883
6	0	3.55021	-1.43242	-0.77488
6	0	2.82271	-0.27663	-1.08395
7	0	4.09368	-3.24832	0.78398
6	0	3.64939	-4.0641	1.90793
6	0	4.82	-3.94474	-0.26982
6	0	1.95466	2.76683	-0.21434
6	0	2.33672	2.97991	1.12344
6	0	2.3649	3.72715	-1.14871
6	0	3.07512	4.09515	1.50888
6	0	3.10831	4.84988	-0.76894
6	0	3.46884	5.04295	0.56069
6	0	0.73313	1.53383	-2.08654
1	0	-0.08052	1.75393	1.26905
1	0	-0.71839	2.61435	-0.08474
1	0	0.8955	-0.09328	1.6616
1	0	2.14487	-2.06583	2.24787
1	0	4.20343	-1.84565	-1.53397
1	0	2.99968	0.17794	-2.05342
1	0	4.35269	-4.88262	2.0526
1	0	3.63428	-3.48352	2.83265
1	0	2.64882	-4.49225	1.75466
1	0	4.1612	-4.31923	-1.06617
1	0	5.57284	-3.29566	-0.72385

1	0	5.34833	-4.79317	0.16201
1	0	2.01916	2.27541	1.88521
1	0	2.08995	3.62545	-2.19115
1	0	3.32727	4.23761	2.55592
1	0	3.39106	5.58081	-1.52048
1	0	4.02944	5.92275	0.8592
1	0	0.18169	0.62371	-2.32881
1	0	0.09116	2.38145	-2.33614
1	0	1.60545	1.58104	-2.74397
6	0	9.54756	-1.06419	-0.83105
6	0	8.46593	-1.08035	-1.70989
6	0	7.24733	-0.52475	-1.32808
6	0	7.12346	0.04119	-0.06236
6	0	8.1939	0.06932	0.82346
6	0	9.40977	-0.4898	0.42998
7	0	5.81873	0.66521	0.28741
6	0	5.7233	2.07421	-0.24882
6	0	5.46449	0.62071	1.74671
1	0	10.49581	-1.49673	-1.12939
1	0	8.56702	-1.52346	-2.69413
1	0	6.40805	-0.53149	-2.0158
1	0	8.10543	0.51025	1.80829
1	0	10.24837	-0.47317	1.11673
1	0	5.07842	0.10965	-0.17999
1	0	5.90452	2.04958	-1.32054
1	0	4.73051	2.46424	-0.0378
1	0	6.48627	2.67569	0.24133
1	0	5.58237	-0.39913	2.10404
1	0	6.10677	1.30262	2.29857

1	0	4.42851	0.93682	1.84029
29	0	-1.69668	0.29402	-0.06309
7	0	-4.43651	-0.74869	-0.10102
6	0	-4.93799	0.58234	0.23889
6	0	-5.39661	-1.93172	-0.31721
6	0	-5.24262	1.49535	-0.79587
6	0	-5.09509	0.92959	1.59931
6	0	-3.16305	-1.00209	-0.26709
6	0	-2.98741	-2.45755	-0.67878
6	0	-4.58644	0.07553	2.75893
6	0	-6.03411	3.05686	0.89146
6	0	-5.65873	2.17467	1.89451
6	0	-5.80438	2.72458	-0.43571
6	0	-4.89673	1.26673	-2.26611
6	0	-4.39202	-3.09163	-0.49448
6	0	-6.08494	1.49758	-3.21616
6	0	-3.32254	0.71115	3.37209
6	0	-5.64568	-0.16454	3.84853
6	0	-3.70547	2.15476	-2.67793
6	0	-2.54592	-2.43346	-2.17543
6	0	-1.89388	-3.14918	0.17412
6	0	-6.31809	-2.13885	0.88694
6	0	-6.26458	-1.71464	-1.56266
6	0	-2.06174	-3.05183	1.69301
6	0	-2.24623	-3.79761	-2.80525
1	0	-4.28934	-0.89696	2.36686
1	0	-6.47776	4.01417	1.14503
1	0	-5.79437	2.4646	2.93042
1	0	-6.05297	3.44161	-1.21009

1	0	-4.57283	0.23384	-2.38752
1	0	-4.67311	-3.71842	-1.34236
1	0	-4.41159	-3.73737	0.3854
1	0	-6.95931	0.90425	-2.94066
1	0	-6.39276	2.54604	-3.23617
1	0	-5.80663	1.22751	-4.23891
1	0	-2.54081	0.85093	2.62102
1	0	-2.92361	0.07427	4.16781
1	0	-3.54063	1.68981	3.80866
1	0	-5.91527	0.75983	4.36554
1	0	-5.25842	-0.85272	4.60557
1	0	-6.56434	-0.59416	3.44373
1	0	-3.95493	3.21683	-2.60248
1	0	-3.42144	1.95342	-3.71545
1	0	-2.83341	1.97174	-2.04559
1	0	-3.3249	-1.93559	-2.76294
1	0	-1.6596	-1.79599	-2.2591
1	0	-1.85548	-4.20486	-0.11286
1	0	-0.92403	-2.71991	-0.1005
1	0	-5.7631	-2.34679	1.80132
1	0	-6.9631	-2.99923	0.69132
1	0	-6.96424	-1.27585	1.05803
1	0	-6.89843	-0.83271	-1.46146
1	0	-6.92266	-2.5779	-1.68851
1	0	-5.67343	-1.61658	-2.4736
1	0	-3.00441	-3.48403	2.0402
1	0	-2.02112	-2.01541	2.03681
1	0	-1.26006	-3.5969	2.19893
1	0	-3.08631	-4.49269	-2.71937

1	0	-1.37273	-4.27698	-2.35818
1	0	-2.03735	-3.67695	-3.87155
TS3				
6	0	-0.96781	-1.12181	-0.12709
6	0	-1.91592	-0.8697	-1.36207
6	0	-3.01109	0.18899	-1.09193
6	0	-2.66738	1.47163	-0.64873
6	0	-3.5979	2.49371	-0.49341
6	0	-4.9655	2.28632	-0.78552
6	0	-5.31183	1.00472	-1.2641
6	0	-4.36043	0.00002	-1.41183
7	0	-5.91064	3.28373	-0.61021
6	0	-5.47004	4.6468	-0.36089
6	0	-7.25175	3.09361	-1.14371
6	0	-2.53823	-2.23151	-1.75026
6	0	-2.38021	-2.8062	-3.0161
6	0	-3.29389	-2.95168	-0.80958
6	0	-2.93856	-4.04886	-3.32777
6	0	-3.8547	-4.18739	-1.11476
6	0	-3.67623	-4.74785	-2.37984
6	0	-1.0706	-0.30816	-2.52891
29	0	0.74252	0.04715	0.0666
7	0	3.65403	0.72457	-0.13523
6	0	4.11659	-0.66448	-0.03876
6	0	4.689	1.85063	-0.37589
6	0	4.2122	-1.45218	-1.21071
6	0	4.52155	-1.16856	1.21982
6	0	2.40528	1.11082	-0.08608

6	0	2.3254	2.62224	-0.30105
6	0	4.27721	-0.46237	2.55237
6	0	5.25938	-3.20426	0.11417
6	0	5.09707	-2.44217	1.26136
6	0	4.79896	-2.71746	-1.0992
6	0	3.63718	-1.06515	-2.57257
6	0	3.79722	3.10331	-0.28415
6	0	4.66385	-1.13561	-3.71855
6	0	3.18468	-1.21151	3.3407
6	0	5.53958	-0.32843	3.42322
6	0	2.43554	-1.96973	-2.90887
6	0	1.66382	2.83775	-1.69902
6	0	1.46304	3.30221	0.79162
6	0	5.79044	1.85062	0.68373
6	0	5.33784	1.69931	-1.75511
6	0	1.88833	3.06339	2.24324
6	0	1.44992	4.29496	-2.1226
1	0	-1.42539	-1.8921	0.50184
1	0	-0.11672	-1.72378	-0.51704
1	0	-1.62974	1.69882	-0.42218
1	0	-3.24921	3.46403	-0.16247
1	0	-6.33306	0.78215	-1.54434
1	0	-4.69493	-0.95494	-1.79741
1	0	-4.88329	4.71106	0.56
1	0	-4.86529	5.0557	-1.18288
1	0	-6.34128	5.28647	-0.23148
1	0	-7.72905	2.2142	-0.70385
1	0	-7.26128	2.97895	-2.23646
1	0	-7.86424	3.9561	-0.88662

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1	0	-3.47057	-2.5338	0.17572
1	0	-2.79387	-4.46401	-4.32019
1	0	-4.436	-4.71301	-0.36365
1	0	-4.11066	-5.71229	-2.62104
1	0	-1.69018	-0.08465	-3.39989
1	0	-0.59523	0.62867	-2.23249
1	0	-0.2842	-1.00029	-2.83395
1	0	3.89862	0.5409	2.35142
1	0	5.72087	-4.18453	0.16981
1	0	5.41926	-2.84774	2.21362
1	0	4.88908	-3.33737	-1.98382
1	0	3.26459	-0.04142	-2.51705
1	0	4.01139	3.78446	-1.10816
1	0	4.01849	3.65154	0.63259
1	0	5.55638	-0.53996	-3.52422
1	0	4.98898	-2.16201	-3.90461
1	0	4.21442	-0.77047	-4.64621
1	0	2.29227	-1.36527	2.73193
1	0	2.90457	-0.65361	4.23956
1	0	3.53305	-2.19653	3.66133
1	0	5.89812	-1.30222	3.76527
1	0	5.31978	0.26242	4.31702
1	0	6.36253	0.15592	2.8966
1	0	2.7452	-3.00867	-3.04668
1	0	1.95917	-1.64263	-3.83701
1	0	1.68572	-1.9553	-2.11617
1	0	2.27504	2.33413	-2.4555
1	0	0.69739	2.32487	-1.70957

1	0	1.46204	4.37894	0.60006
1	0	0.42477	2.97628	0.65851
1	0	5.39721	1.9943	1.68949
1	0	6.46862	2.68182	0.47543
1	0	6.3811	0.93383	0.66119
1	0	5.91253	0.77619	-1.82906
1	0	6.03268	2.52875	-1.90601
1	0	4.61062	1.72768	-2.56679
1	0	2.88833	3.45004	2.45383
1	0	1.88677	2.00162	2.50583
1	0	1.2077	3.57458	2.92912
1	0	2.37396	4.87833	-2.10251
1	0	0.71914	4.80715	-1.49373
1	0	1.07089	4.32817	-3.14681
1	0	-1.21196	-0.35789	1.20601
6	0	-5.21981	-2.29878	3.18995
6	0	-5.21846	-1.15267	2.39738
6	0	-4.03758	-0.45758	2.15653
6	0	-2.83646	-0.90254	2.71732
6	0	-2.83397	-2.05508	3.5073
6	0	-4.02344	-2.74704	3.73858
7	0	-1.59634	-0.15814	2.43674
6	0	-1.74409	1.30242	2.68556
6	0	-0.41977	-0.65418	3.1839
1	0	-6.14318	-2.8361	3.37573
1	0	-6.13938	-0.79439	1.95118
1	0	-4.06618	0.41103	1.51345
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1	0	-4.00398	-3.63776	4.35702

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1	0	-0.57509	-0.58411	4.26174
1	0	-0.20767	-1.68471	2.90588
1	0	0.43484	-0.03991	2.90838
Pro				
6	0	3.76654	3.14042	0.38613
6	0	2.23648	2.8788	0.36268
6	0	1.90314	1.66924	-0.53656
6	0	0.77181	1.61896	-1.35189
6	0	0.49984	0.52412	-2.2167
6	0	1.42274	-0.56551	-2.31778
6	0	2.51873	-0.54123	-1.42044
6	0	2.74027	0.53818	-0.58037
7	0	1.27599	-1.56007	-3.24956
6	0	0.31387	-1.3979	-4.33215
6	0	2.31895	-2.57126	-3.40137
6	0	1.55891	4.15909	-0.1623
6	0	0.6749	4.9218	0.60632
6	0	1.8637	4.62253	-1.45265
6	0	0.11705	6.10318	0.10989
6	0	1.30953	5.79625	-1.95266
6	0	0.43058	6.54603	-1.17007
6	0	1.80971	2.53659	1.80737
1	0	4.31281	2.32094	0.85881
1	0	4.17274	3.28274	-0.61681
1	0	3.97292	4.04709	0.95913

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1	0	-0.25871	0.66622	-2.9789
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1	0	3.62603	0.49453	0.04347
1	0	-0.70654	-1.32207	-3.94956
1	0	0.52234	-0.51028	-4.94239
1	0	0.35475	-2.27	-4.98098
1	0	3.26648	-2.14158	-3.74796
1	0	2.5043	-3.0924	-2.46028
1	0	1.99111	-3.31042	-4.12951
1	0	0.41338	4.61306	1.61089
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1	0	-0.55955	6.67802	0.7343
1	0	1.56879	6.13027	-2.95224
1	0	0.0019	7.46558	-1.55429
1	0	0.73456	2.36746	1.89039
1	0	2.31397	1.6249	2.136
1	0	2.0865	3.33326	2.50279
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6	0	5.98132	-2.81228	-1.13981
6	0	6.29132	-1.64366	-0.45054
6	0	5.82557	-1.42831	0.86537
6	0	5.05207	-2.45461	1.45166
6	0	4.74936	-3.61686	0.74849
7	0	6.10493	-0.24276	1.55146
6	0	7.1867	0.60192	1.05545
6	0	5.90443	-0.22009	2.99548
1	0	4.98844	-4.73053	-1.08732
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1	0	4.69839	-2.36249	2.47002
1	0	4.16754	-4.39025	1.24117
1	0	6.97628	0.95737	0.04499
1	0	7.27305	1.48011	1.69379
1	0	8.1576	0.08686	1.04416
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1	0	6.15773	0.76912	3.37433
29	0	-0.7563	-0.17462	-0.63652
7	0	-3.15973	-1.07811	0.82963
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6	0	-3.75419	-2.11384	1.8122
6	0	-4.64288	-0.334	-1.02341
6	0	-4.17436	1.18276	0.86469
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6	0	-1.32325	-2.40227	1.34833
6	0	-3.39321	1.60734	2.10576
6	0	-5.73199	1.8364	-0.88388
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6	0	-4.37238	-1.57242	-1.87579
6	0	-2.47264	-2.82255	2.29937
6	0	-5.65112	-2.31629	-2.29969
6	0	-2.3384	2.66525	1.73166
6	0	-4.29234	2.13435	3.23833
6	0	-3.55368	-1.18485	-3.12195
6	0	-1.01937	-3.49273	0.27144
6	0	-0.0183	-2.03307	2.09813

6	0	-4.51449	-1.4396	2.95558
6	0	-4.71116	-3.06545	1.08614
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1	0	-6.01766	0.44461	-2.47851
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1	0	-2.61392	-3.90387	2.31779
1	0	-2.25248	-2.52051	3.324
1	0	-6.27831	-2.5842	-1.4477
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1	0	-5.39303	-3.23895	-2.82698
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1	0	-1.74393	2.93782	2.6084
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1	0	-3.69511	2.32549	4.1342
1	0	-5.07923	1.42642	3.50474
1	0	-4.11317	-0.51137	-3.77623
1	0	-3.2946	-2.07422	-3.70377
1	0	-2.62713	-0.67714	-2.84154
1	0	-1.94869	-3.73333	-0.25556
1	0	-0.35375	-3.05828	-0.48285
1	0	0.31719	-2.91674	2.64871
1	0	0.76056	-1.83088	1.35341
1	0	-3.87944	-0.77937	3.54511
1	0	-4.88839	-2.21693	3.62633

1	0	-5.37699	-0.87508	2.5972
1	0	-5.56406	-2.53245	0.66537
1	0	-5.1021	-3.785	1.80928
1	0	-4.22267	-3.6318	0.29292
1	0	-0.80704	-1.0281	3.88552
1	0	-0.4017	0.07224	2.56466
1	0	0.87106	-0.66923	3.52623
1	0	-0.99343	-5.25263	1.58598
1	0	0.61141	-4.63675	1.18555
1	0	-0.3206	-5.51845	-0.01617

Rea (pryNHC-Au⁺)

79	0	0.515550	-0.408982	-0.120302
6	0	-2.401422	0.111788	2.576800
6	0	-3.535273	-1.861141	1.515810
6	0	-3.800771	-2.090115	-0.853313
6	0	-4.011152	-2.598416	0.432328
6	0	-2.685419	-0.165807	0.048466
6	0	-2.944206	-0.368521	-2.478913
6	0	-2.874857	-0.638893	1.355058
6	0	-3.145495	-0.879504	-1.072607
7	0	-0.242135	2.374745	-0.890650
7	0	-2.034138	1.113684	-0.173530
6	0	-2.892559	2.320857	0.034531
6	0	0.757003	3.042998	-0.026031
6	0	0.018490	3.547840	1.228463
6	0	-1.234393	3.335809	-1.402494
6	0	-2.162875	3.646041	-0.235001
6	0	-0.729265	1.192711	-0.409876

6	0	-4.750176	-3.896968	0.634610
6	0	-1.312936	4.267465	0.905597
6	0	1.591726	-2.311948	0.494617
6	0	2.535236	-1.903775	-0.426976
6	0	3.729376	-1.114085	-0.032867
6	0	4.347769	-0.237578	-0.940477
6	0	4.294930	-1.259466	1.245478
6	0	5.476099	0.488010	-0.572900
6	0	5.430526	-0.542997	1.606762
6	0	6.021338	0.337634	0.701330
6	0	2.460579	-2.403179	-1.848842
1	0	-3.161447	0.813214	2.937852
1	0	-1.488537	0.679990	2.392283
1	0	-2.200436	-0.578614	3.397571
1	0	-3.680493	-2.243278	2.522220
1	0	-4.160948	-2.651475	-1.710747
1	0	-3.394242	-1.047847	-3.203430
1	0	-1.884833	-0.270067	-2.732688
1	0	-3.402932	0.613713	-2.628833
1	0	-3.274383	2.262108	1.055646
1	0	-3.749747	2.227458	-0.636014
1	0	1.207672	3.854043	-0.601633
1	0	1.544371	2.333150	0.233941
1	0	-0.172002	2.684009	1.874772
1	0	0.665100	4.220181	1.799609
1	0	-1.760558	2.885481	-2.247165
1	0	-0.698856	4.212179	-1.768435
1	0	-2.926931	4.376456	-0.517229
1	0	-4.595131	-4.298256	1.637666

1	0	-4.434616	-4.655720	-0.085714
1	0	-5.827772	-3.756785	0.501281
1	0	-1.089853	5.294829	0.596541
1	0	-1.909630	4.355744	1.818106
1	0	0.876205	-3.084291	0.231814
1	0	1.731165	-2.132969	1.555368
1	0	3.940419	-0.103705	-1.935722
1	0	3.871171	-1.965358	1.950644
1	0	5.935268	1.165004	-1.285121
1	0	5.863314	-0.683149	2.591314
1	0	6.909269	0.893315	0.982823
1	0	2.520777	-1.595949	-2.580826
1	0	3.315587	-3.060597	-2.037150
1	0	1.544819	-2.964833	-2.032968

TS1 (pryNHC-Au⁺)

79	0	0.889976	-0.461882	-0.974320
6	0	2.169821	0.374262	2.764697
6	0	2.199124	2.808888	2.129441
6	0	3.157918	3.594695	0.081072
6	0	2.506665	3.875849	1.284498
6	0	3.205065	1.251191	0.604979
6	0	4.206989	2.035881	-1.597090
6	0	2.539016	1.489373	1.816283
6	0	3.518507	2.295959	-0.279933
7	0	3.453051	-2.040448	-0.946189
7	0	3.633216	-0.092257	0.264970
6	0	4.912548	-0.520708	0.905834
6	0	2.862836	-3.302707	-0.458887

6	0	3.221916	-3.442932	1.033867
6	0	4.921980	-2.097165	-0.919951
6	0	5.330729	-1.951845	0.540237
6	0	2.854147	-0.904367	-0.453077
6	0	2.169702	5.296213	1.664840
6	0	4.707709	-3.129153	1.336781
6	0	-1.053082	-0.021525	-1.714766
6	0	-2.025401	0.854415	-0.974422
6	0	-1.441932	2.237156	-0.711587
6	0	-3.463942	0.832568	-1.413691
6	0	-4.045219	-0.315470	-1.982205
6	0	-4.274270	1.979162	-1.319281
6	0	-5.355634	-0.312112	-2.450803
6	0	-5.582812	1.988200	-1.794239
6	0	-6.132095	0.841584	-2.363691
1	0	3.037971	-0.011571	3.308841
1	0	1.713295	-0.467825	2.239768
1	0	1.460925	0.727067	3.515557
1	0	1.684226	3.005331	3.065988
1	0	3.396282	4.409929	-0.596386
1	0	4.417665	2.972026	-2.115580
1	0	3.589215	1.420847	-2.257675
1	0	5.158858	1.512435	-1.468219
1	0	4.790551	-0.392732	1.983389
1	0	5.690874	0.178357	0.588357
1	0	3.265004	-4.120725	-1.061512
1	0	1.781921	-3.271736	-0.604857
1	0	2.577553	-2.759334	1.597151
1	0	2.986145	-4.451327	1.387773

1	0	5.319019	-1.292673	-1.543592
1	0	5.234750	-3.045395	-1.359415
1	0	6.417192	-2.006198	0.661553
1	0	1.416836	5.335489	2.454812
1	0	1.793545	5.864211	0.810271
1	0	3.056097	5.822547	2.033875
1	0	5.308565	-4.013852	1.096130
1	0	4.834881	-2.968477	2.411816
1	0	-1.516394	-0.945290	-2.061306
1	0	-0.815559	0.547291	-2.628277
1	0	-2.015486	2.848316	-0.016815
1	0	-0.420397	2.155702	-0.341831
1	0	-1.401904	2.778942	-1.662738
1	0	-3.465588	-1.223090	-2.084221
1	0	-3.881929	2.893487	-0.893620
1	0	-5.764515	-1.210704	-2.901591
1	0	-6.169228	2.898808	-1.727977
1	0	-7.148201	0.850004	-2.743909
6	0	-2.067100	0.110388	0.899800
6	0	-2.997805	0.885038	1.671038
6	0	-4.226299	0.409009	2.018351
6	0	-4.603505	-0.938750	1.699074
6	0	-3.613850	-1.780177	1.091387
6	0	-2.395578	-1.276496	0.742165
7	0	-5.835186	-1.400607	1.981412
6	0	-6.193426	-2.796849	1.712624
6	0	-6.846760	-0.528850	2.587929
1	0	-1.014843	0.343939	1.012120
1	0	-2.731978	1.897378	1.955746

1	0	-4.909777	1.048421	2.559622
1	0	-3.830951	-2.822876	0.904511
1	0	-1.660141	-1.925186	0.279465
1	0	-5.567226	-3.484385	2.286738
1	0	-7.227463	-2.960524	2.002580
1	0	-6.095930	-3.029822	0.649559
1	0	-6.582422	-0.263987	3.615610
1	0	-6.973082	0.384859	2.004572
1	0	-7.799781	-1.050175	2.606000

Rea (pryNHC-Cu⁺)

29	0	0.563970	-0.580486	-0.146569
6	0	-2.169400	0.189778	2.548647
6	0	-3.420855	-1.722142	1.508383
6	0	-3.719503	-1.947174	-0.857074
6	0	-3.949992	-2.434807	0.433275
6	0	-2.480562	-0.086854	0.023640
6	0	-2.782448	-0.284818	-2.499641
6	0	-2.689045	-0.542590	1.334500
6	0	-2.994072	-0.779389	-1.088630
7	0	0.164846	2.228221	-0.908380
7	0	-1.741464	1.139299	-0.213498
6	0	-2.497004	2.412939	-0.017956
6	0	1.208616	2.790328	-0.026089
6	0	0.507204	3.352462	1.226131
6	0	-0.727954	3.283030	-1.418249
6	0	-1.641777	3.666837	-0.259939
6	0	-0.428431	1.088273	-0.428519
6	0	-4.769265	-3.682060	0.648954

6	0	-0.751885	4.191859	0.899546
6	0	1.316797	-2.480781	0.399876
6	0	2.284834	-2.119563	-0.500622
6	0	3.518423	-1.399618	-0.084360
6	0	4.193713	-0.547319	-0.974598
6	0	4.061294	-1.587033	1.198899
6	0	5.352982	0.116758	-0.584849
6	0	5.224990	-0.930472	1.583074
6	0	5.871891	-0.071368	0.694851
6	0	2.179302	-2.566011	-1.940218
1	0	-2.886760	0.937760	2.903125
1	0	-1.227650	0.705642	2.355749
1	0	-2.006678	-0.502362	3.376473
1	0	-3.582929	-2.087988	2.518318
1	0	-4.123058	-2.488770	-1.707942
1	0	-3.269384	-0.946156	-3.216929
1	0	-1.722789	-0.231933	-2.764940
1	0	-3.197825	0.716497	-2.648460
1	0	-2.906700	2.384622	0.994020
1	0	-3.345057	2.406110	-0.707297
1	0	1.746403	3.560469	-0.583520
1	0	1.921531	2.006104	0.239520
1	0	0.232174	2.504944	1.863282
1	0	1.205602	3.959860	1.809139
1	0	-1.283570	2.890868	-2.273227
1	0	-0.112538	4.111920	-1.769789
1	0	-2.328764	4.470176	-0.541842
1	0	-4.645989	-4.077419	1.658726
1	0	-4.497648	-4.469731	-0.058228

1	0	-5.835038	-3.476786	0.505779
1	0	-0.434656	5.199668	0.608692
1	0	-1.348178	4.320332	1.807626
1	0	0.518208	-3.157296	0.111321
1	0	1.434091	-2.302124	1.464991
1	0	3.812626	-0.388007	-1.976647
1	0	3.595236	-2.281462	1.888738
1	0	5.856775	0.773630	-1.285667
1	0	5.637616	-1.103220	2.571128
1	0	6.783239	0.435249	0.993360
1	0	2.257920	-1.736477	-2.646177
1	0	3.006132	-3.246029	-2.167550
1	0	1.241743	-3.088240	-2.132337

TS1 (pyrNHC-Cu⁺)

29	0	1.115239	-0.853146	-1.067160
6	0	2.096683	0.614438	2.571402
6	0	1.714803	2.898445	1.595161
6	0	2.574429	3.553093	-0.541049
6	0	1.855901	3.878153	0.612888
6	0	3.003280	1.340500	0.296941
6	0	3.921200	1.990507	-1.985748
6	0	2.280345	1.625247	1.464983
6	0	3.156800	2.298497	-0.721481
7	0	3.784933	-2.009213	-0.876460
7	0	3.642245	0.051707	0.127971
6	0	4.930074	-0.127708	0.861148
6	0	3.341957	-3.291240	-0.299270
6	0	3.633556	-3.244468	1.214116

6	0	5.245070	-1.861766	-0.786821
6	0	5.549431	-1.520693	0.666170
6	0	3.005663	-0.931513	-0.518655
6	0	1.275154	5.258536	0.795028
6	0	5.042008	-2.693079	1.549876
6	0	-0.732430	-0.875648	-1.797591
6	0	-1.772655	0.169856	-1.512312
6	0	-1.318556	1.529613	-2.047486
6	0	-3.216746	-0.175210	-1.830986
6	0	-3.707378	-1.483888	-1.689560
6	0	-4.112600	0.793681	-2.313514
6	0	-5.018602	-1.811913	-2.023459
6	0	-5.423117	0.468090	-2.658346
6	0	-5.885390	-0.837313	-2.514078
1	0	2.939935	0.620065	3.270360
1	0	1.995577	-0.401584	2.186710
1	0	1.204400	0.841972	3.157584
1	0	1.154448	3.128565	2.497427
1	0	2.690836	4.299834	-1.321651
1	0	3.988896	2.873371	-2.622587
1	0	3.441318	1.197168	-2.565673
1	0	4.942065	1.658713	-1.775955
1	0	4.734858	0.088742	1.913796
1	0	5.629512	0.632914	0.503177
1	0	3.879192	-4.099367	-0.801797
1	0	2.274800	-3.422124	-0.491058
1	0	2.870074	-2.610841	1.678550
1	0	3.520451	-4.239362	1.655920
1	0	5.564313	-1.074102	-1.473638

1	0	5.705650	-2.795603	-1.112563
1	0	6.625015	-1.416730	0.840043
1	0	0.534995	5.283113	1.597494
1	0	0.796323	5.619010	-0.119125
1	0	2.056867	5.980802	1.051702
1	0	5.771205	-3.502483	1.428711
1	0	5.081373	-2.415860	2.607821
1	0	-1.130388	-1.888780	-1.707021
1	0	-0.478539	-0.753507	-2.863557
1	0	-1.914511	2.376194	-1.708110
1	0	-0.279445	1.712673	-1.772433
1	0	-1.372480	1.512394	-3.140108
1	0	-3.055226	-2.271079	-1.334012
1	0	-3.791382	1.818280	-2.451281
1	0	-5.356831	-2.838001	-1.918328
1	0	-6.078788	1.238274	-3.051772
1	0	-6.902172	-1.094532	-2.791909
6	0	-1.747840	0.461171	0.370140
6	0	-2.745933	1.437284	0.745305
6	0	-3.879224	1.104585	1.418142
6	0	-4.088258	-0.241180	1.876886
6	0	-3.023043	-1.184318	1.683370
6	0	-1.907218	-0.833068	0.988433
7	0	-5.233651	-0.597724	2.479654
6	0	-5.415336	-1.953491	3.010792
6	0	-6.338253	0.357145	2.630826
1	0	-0.728493	0.834237	0.348099
1	0	-2.603997	2.470133	0.446250
1	0	-4.615709	1.867438	1.629821

1	0	-3.113654	-2.189225	2.072353
1	0	-1.124377	-1.565863	0.826096
1	0	-4.661079	-2.186060	3.765813
1	0	-6.392739	-2.022748	3.479669
1	0	-5.364569	-2.698162	2.212796
1	0	-6.092886	1.140289	3.353526
1	0	-6.586442	0.817529	1.673410
1	0	-7.217653	-0.171944	2.987427

Rea (CAAC-Au⁺)

6	0	2.054142	-2.393815	-0.012029
6	0	2.984652	-1.675240	-0.737062
6	0	4.059404	-0.887468	-0.083706
6	0	4.646070	0.212099	-0.733343
6	0	4.549292	-1.251801	1.182678
6	0	5.666428	0.937001	-0.126997
6	0	5.576989	-0.533322	1.782363
6	0	6.135213	0.567129	1.132603
6	0	3.027568	-1.815871	-2.238787
79	0	0.774574	-0.524542	-0.213855
7	0	-1.881154	0.795035	0.065488
6	0	-2.477047	-0.504988	0.387783
6	0	-2.725635	2.087775	0.029738
6	0	-2.519904	-0.929304	1.735507
6	0	-2.989692	-1.298289	-0.663648
6	0	-0.617109	0.970607	-0.188480
6	0	-0.290835	2.435060	-0.417066
6	0	-2.808107	-0.983261	-2.147553
6	0	-3.741119	-2.901175	1.002857

6	0	-3.628245	-2.493372	-0.318542
6	0	-3.173696	-2.134921	2.010553
6	0	-1.822191	-0.212479	2.890675
6	0	-1.688107	3.105042	-0.496104
6	0	-2.753546	0.063966	4.084972
6	0	-1.799299	-1.959696	-2.784901
6	0	-4.129622	-1.003397	-2.936994
6	0	-0.592666	-1.015739	3.360126
6	0	0.521182	2.907438	0.833179
6	0	0.554698	2.643576	-1.699105
6	0	-3.923553	1.941024	-0.909081
6	0	-3.238622	2.440677	1.429350
6	0	-0.010414	2.057388	-2.995901
6	0	0.987897	4.366482	0.804568
1	0	1.453895	-3.151127	-0.505527
1	0	2.125902	-2.476483	1.066940
1	0	4.299092	0.517326	-1.713404
1	0	4.155808	-2.126128	1.688027
1	0	6.102295	1.786040	-0.642241
1	0	5.953265	-0.841613	2.751675
1	0	6.939903	1.124647	1.599510
1	0	3.015531	-0.852973	-2.752257
1	0	3.963443	-2.309060	-2.520517
1	0	2.196102	-2.413029	-2.612747
1	0	-2.381015	0.015619	-2.241867
1	0	-4.251751	-3.827174	1.245197
1	0	-4.038046	-3.120762	-1.101838
1	0	-3.231013	-2.484537	3.034982
1	0	-1.452432	0.747939	2.531831

1	0	-1.727062	4.026995	0.084439
1	0	-1.926355	3.375231	-1.525441
1	0	-3.656803	0.603002	3.793522
1	0	-3.067942	-0.859545	4.576782
1	0	-2.233438	0.664657	4.835960
1	0	-0.835887	-1.932468	-2.268115
1	0	-1.629073	-1.702440	-3.834193
1	0	-2.164082	-2.989610	-2.752114
1	0	-4.554964	-2.008303	-2.989809
1	0	-3.958392	-0.674642	-3.965670
1	0	-4.885665	-0.350174	-2.497947
1	0	-0.880986	-1.992071	3.758472
1	0	-0.064724	-0.477271	4.152195
1	0	0.111067	-1.185103	2.540665
1	0	-0.087880	2.747742	1.729120
1	0	1.393206	2.255108	0.945324
1	0	0.696842	3.719888	-1.829454
1	0	1.552718	2.228335	-1.519911
1	0	-3.623983	1.735753	-1.935955
1	0	-4.476948	2.883118	-0.911659
1	0	-4.608674	1.159410	-0.576709
1	0	-3.892136	1.663651	1.826423
1	0	-3.828027	3.357665	1.359093
1	0	-2.433644	2.622613	2.141218
1	0	-0.984313	2.479222	-3.257105
1	0	-0.119657	0.970756	-2.944606
1	0	0.659403	2.277683	-3.830613
1	0	0.162931	5.068854	0.659093
1	0	1.725892	4.551597	0.022078

1	0	1.459559	4.618513	1.757335
TS1 (CAAC-Au ⁺)				
6	0	1.357707	1.348924	-0.072297
6	0	2.567377	1.133725	-0.937794
6	0	2.223422	1.248137	-2.417179
6	0	3.855708	1.783652	-0.519408
6	0	4.169339	1.998094	0.835373
6	0	4.779922	2.250944	-1.472205
6	0	5.332176	2.660691	1.216617
6	0	5.939322	2.922094	-1.094074
6	0	6.222971	3.131079	0.253769
6	0	2.958850	-0.855388	-0.812181
6	0	4.130539	-1.134066	-1.592367
6	0	5.338860	-1.395492	-1.019044
6	0	5.463813	-1.493067	0.407568
6	0	4.265040	-1.394117	1.188299
6	0	3.069382	-1.120045	0.591799
7	0	6.661365	-1.690987	0.988477
6	0	6.773288	-1.845806	2.442089
6	0	7.884614	-1.775343	0.183690
79	0	-0.393881	0.141761	-0.196582
7	0	-3.325201	-0.534760	0.079622
6	0	-3.573989	0.832728	0.540859
6	0	-4.472987	-1.551806	-0.066413
6	0	-3.859560	1.843251	-0.405268
6	0	-3.514336	1.109214	1.925412
6	0	-2.141427	-0.973143	-0.260171
6	0	-2.235096	-2.406953	-0.759457

6	0	-3.031001	0.113369	2.978398
6	0	-4.185197	3.394600	1.439179
6	0	-3.837416	2.403168	2.345220
6	0	-4.174289	3.116692	0.080303
6	0	-3.754084	1.662798	-1.919149
6	0	-3.687790	-2.833080	-0.422746
6	0	-5.023050	2.101742	-2.671881
6	0	-1.639969	0.518474	3.506482
6	0	-4.014235	-0.049766	4.151283
6	0	-2.528423	2.420319	-2.467614
6	0	-1.984374	-2.350752	-2.300397
6	0	-1.171587	-3.314763	-0.091975
6	0	-5.262676	-1.699003	1.235217
6	0	-5.440551	-1.130232	-1.177492
6	0	-1.136055	-3.308910	1.438602
6	0	-1.976588	-3.701233	-3.023919
1	0	1.625548	1.459710	0.978762
1	0	0.977092	2.335454	-0.381461
1	0	3.004066	0.906864	-3.094872
1	0	1.308107	0.699029	-2.635744
1	0	2.033000	2.302151	-2.646352
1	0	3.491741	1.662185	1.608881
1	0	4.590863	2.119302	-2.529613
1	0	5.533194	2.824869	2.270418
1	0	6.616067	3.291712	-1.857475
1	0	7.121143	3.662903	0.549650
1	0	1.997651	-1.062851	-1.267003
1	0	4.064085	-1.102452	-2.674563
1	0	6.202458	-1.554189	-1.649879

1	0	4.303523	-1.536893	2.259450
1	0	2.173050	-1.044747	1.197295
1	0	6.221097	-2.721968	2.791275
1	0	7.818614	-1.978309	2.706422
1	0	6.400018	-0.959619	2.960933
1	0	7.891628	-2.673688	-0.439876
1	0	7.991766	-0.896366	-0.454775
1	0	8.744058	-1.816264	0.847049
1	0	-2.914649	-0.861447	2.504233
1	0	-4.441221	4.388849	1.790304
1	0	-3.805825	2.641240	3.402417
1	0	-4.403434	3.909735	-0.622549
1	0	-3.590406	0.606509	-2.131349
1	0	-4.161946	-3.355672	-1.254420
1	0	-3.700425	-3.521573	0.423463
1	0	-5.922549	1.610422	-2.296165
1	0	-5.184530	3.180097	-2.599514
1	0	-4.931746	1.863087	-3.735285
1	0	-0.912681	0.599721	2.694720
1	0	-1.274031	-0.224997	4.221306
1	0	-1.673580	1.482533	4.021310
1	0	-4.090135	0.863302	4.747093
1	0	-3.672275	-0.842275	4.823135
1	0	-5.021004	-0.306171	3.816323
1	0	-2.624584	3.498683	-2.314655
1	0	-2.424165	2.246542	-3.542870
1	0	-1.607600	2.093265	-1.979057
1	0	-2.745303	-1.708950	-2.757264
1	0	-1.029329	-1.843674	-2.471917

1	0	-1.338639	-4.338661	-0.439699
1	0	-0.186519	-3.021363	-0.470935
1	0	-4.640264	-2.041151	2.061304
1	0	-6.047349	-2.444579	1.083910
1	0	-5.749125	-0.765608	1.523649
1	0	-5.915797	-0.174623	-0.954262
1	0	-6.232598	-1.878985	-1.254127
1	0	-4.958166	-1.062289	-2.152668
1	0	-2.078938	-3.640612	1.881860
1	0	-0.909751	-2.315836	1.834985
1	0	-0.362501	-3.991513	1.800266
1	0	-2.895187	-4.270814	-2.858883
1	0	-1.137372	-4.330596	-2.720933
1	0	-1.887591	-3.542661	-4.101723