Hofmann reaction-involving annulation of *o*-(pyridin-2-yl)aryl amides selectively and rapidly leads to potential potocatalytic active 6*H*-pyrido[1,2-*c*]quinazolin-6-one derivatives

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Supporting Information

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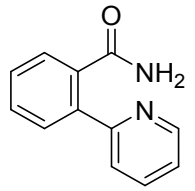
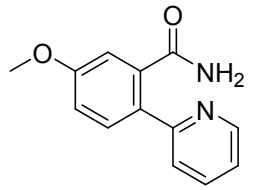
I. Analytical data of compounds

All the compounds of **1** were synthesized by following the procedure described in literature.[1]



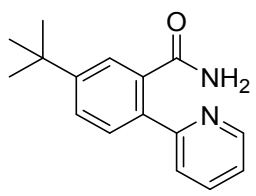
2-(pyridin-2-yl) benzamide (1a).

The product was isolated by flash chromatography (eluent: EA) as a white solid (158.4 mg, 80%); mp: 134-136 ^{o}C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.38 (s, 1H), 7.52 (t, J = 7.5, 1H), 7.44 (d, J = 7.2 Hz, 1H), 7.28 (t, J = 6.6, 3H), 7.21 (t, J = 6.9, 1H), 7.05 (t, J = 6.0 Hz, 1H), 6.20 (s, 1H), 5.87 (s, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 172.0, 158.2, 149.0, 138.7, 136.7, 135.3, 130.3, 130.1, 128.5, 123.9, 122.4. HRMS (ESI), *m/z* calcd. for $C_{12}H_{10}N_2NaO$ ($[M+Na]^+$) 221.0685, found: 221.0683.



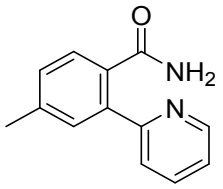
5-methoxy-2-(pyridin-2-yl)benzamide (1b).

The product was isolated by flash chromatography (eluent: EA) as a white solid (193.8 mg, 85%); mp: 142-144 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, J = 4.4 Hz, 1H), 7.68 (td, J = 7.8, 2.0 Hz, 1H), 7.44 (d, J = 8.0 Hz, 1H), 7.40 (d, J = 8.4 Hz, 1H), 7.21-7.17 (m, 1H), 7.15 (d, J = 2.8 Hz, 1H), 6.97 (dd, J = 8.4, 2.8 Hz, 1H), 6.67 (s, 1H), 6.14 (s, 1H), 3.82 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.8, 159.6, 157.9, 148.9, 136.6, 131.6, 131.0, 123.9, 122.0, 116.3, 113.5, 55.5. HRMS (ESI), *m/z* calcd. for $C_{13}H_{12}N_2NaO_2$ ($[M+Na]^+$) 251.0791, found: 251.0786.



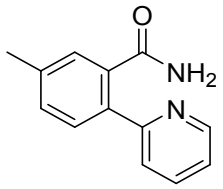
5-(tert-butyl)-2-(pyridin-2-yl)benzamide (1c).

The product was isolated by flash chromatography (eluent: EA) as a white solid (216.0 mg, 85%); mp: 130-132 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.63 (d, J = 3.6 Hz, 1H), 7.75-7.72 (m, 2H), 7.54-7.51 (m, 2H), 7.45 (d, J = 8.4 Hz, 1H), 7.26 (t, J = 6.0 Hz, 1H), 6.30 (s, 1H), 5.79 (s, 1H), 1.36 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 172.3, 158.4, 151.9, 149.1, 136.7, 135.8, 134.8, 130.0, 127.5, 125.7, 124.0, 122.3, 34.8, 31.2. HRMS (ESI), *m/z* calcd. for $C_{16}H_{19}N_2O$ ($[M+H]^+$) 255.1492, found: 255.1490.



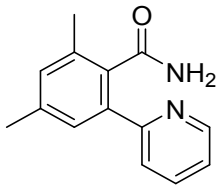
4-methyl-2-(pyridin-2-yl)benzamide (1d).

The product was isolated by flash chromatography (eluent: EA) as a white solid (184.5 mg, 87%); mp: 135-137 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.62 (d, J = 4.8 Hz, 1H), 7.73 (m, 1H), 7.60 (d, J = 7.8 Hz, 1H), 7.49 (d, J = 7.8 Hz, 1H), 7.32 (s, 1H), 7.28-7.23 (m, 2H), 6.29 (s, 1H), 5.90 (s, 1H), 2.41 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 171.8, 158.6, 149.0, 140.6, 138.7, 136.6, 132.4, 130.9, 129.2, 128.8, 124.1, 122.4, 21.3. HRMS (ESI), *m/z* calcd. for $C_{13}H_{12}N_2NaO$ ($[M+Na]^+$) 235.0842, found: 235.0835.



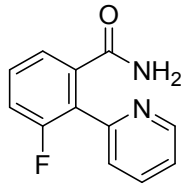
5-methyl-2-(pyridin-2-yl)benzamide (1e).

The product was isolated by flash chromatography (eluent: EA) as a white solid (173.9 mg, 82%); mp: 150-152 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 (d, J = 4.8 Hz, 1H), 7.70 (td, J = 7.8, 1.6 Hz, 1H), 7.47 (d, J = 6.8 Hz, 2H), 7.38 (d, J = 7.6 Hz, 1H), 7.27 (d, J = 6.8 Hz, 1H), 7.22 (m, 1H), 6.51 (s, 1H), 6.13 (s, 1H), 2.39 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.2, 158.3, 148.9, 138.6, 136.6, 135.8, 135.2, 130.9, 130.1, 129.2, 124.0, 122.2, 21.1. HRMS (ESI), *m/z* calcd. for $C_{13}H_{12}N_2NaO$ ($[M+Na]^+$) 235.0842, found: 235.0840.



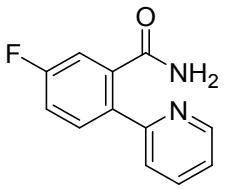
2,4-dimethyl-6-(pyridin-2-yl)benzamide (1f).

The product was isolated by flash chromatography (eluent: EA) as a white solid (180.9 mg, 80%); mp: 168-170 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60-8.58 (m, 1H), 7.69 (td, J = 7.8, 1.7 Hz, 1H), 7.57 (m, 1H), 7.25-7.19 (m, 2H), 7.08 (s, 1H), 5.77 (s, 2H), 2.41 (s, 3H), 2.35 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.3, 158.3, 149.2, 139.0, 137.8, 136.5, 135.3, 132.9, 131.3, 127.7, 123.7, 122.2, 21.2, 19.8. HRMS (ESI), *m/z* calcd. for $C_{14}H_{14}N_2NaO$ ($[M+Na]^+$) 249.0998, found: 249.0992.



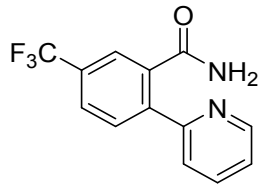
3-fluoro-2-(pyridin-2-yl)benzamide (1g).

The product was isolated by flash chromatography (eluent: EA) as a white solid (179.3 mg, 83%); mp: 155-157 ^{o}C; ^{1}H NMR (600 MHz, CDCl3) δ 8.63 (d, J = 4.8 Hz, 1H), 7.77 (td, J = 7.8, 1.8 Hz, 1H), 7.48 (d, J = 7.8 Hz, 1H), 7.46 (d, J = 7.8 Hz, 1H), 7.39-7.38 (m, 1H), 7.31-7.29 (m, 1H), 7.22-7.19 (m, 1H), 6.59 (s, 1H), 6.02 (s, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.2 (d, $J_{C\text{-}F}$ = 3.0 Hz), 159.8 (d, $J_{C\text{-}F}$ = 246.6 Hz), 152.7, 149.2, 137.9 (d, $J_{C\text{-}F}$ = 2.0 Hz), 136.6, 130.0 (d, $J_{C\text{-}F}$ = 8.6 Hz), 126.7 (d, $J_{C\text{-}F}$ = 16.5 Hz), 125.8 (d, $J_{C\text{-}F}$ = 2.3 Hz), 124.3 (d, $J_{C\text{-}F}$ = 3.5 Hz), 123.0, 117.8 (d, $J_{C\text{-}F}$ = 22.8 Hz). HRMS (ESI), *m/z* calcd. for $C_{12}H_9FN_2NaO$ ($[M+Na]^+$) 239.0591, found: 239.0590.



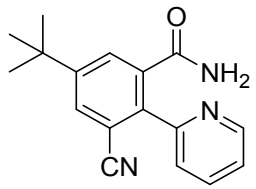
5-fluoro-2-(pyridin-2-yl)benzamide (1h).

The product was isolated by flash chromatography (eluent: EA) as a white solid (170.7 mg, 79%); mp: 149-151 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.61-8.59 (m, 1H), 7.75 (td, J = 7.8, 1.7 Hz, 1H), 7.51-7.47 (m, 2H), 7.38 (dd, J = 8.8, 2.4 Hz, 1H), 7.30-7.26 (m, 1H), 7.21-7.16 (m, 1H), 6.53 (s, 1H), 5.95 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.3, 162.4 (d, $J_{C\text{-}F}$ = 248.4 Hz), 157.4, 149.1, 137.3 (d, $J_{C\text{-}F}$ = 6.9 Hz), 136.9, 134.8 (d, $J_{C\text{-}F}$ = 3.5 Hz), 132.2 (d, $J_{C\text{-}F}$ = 8.0 Hz), 124.0, 122.6, 117.3 (d, $J_{C\text{-}F}$ = 21.3 Hz), 115.8 (d, $J_{C\text{-}F}$ = 23.1 Hz). HRMS (ESI), *m/z* calcd. for $C_{12}H_9FN_2NaO$ ($[M+Na]^+$) 239.0591, found: 239.0584.



2-(pyridin-2-yl)-5-(trifluoromethyl)benzamide (1i).

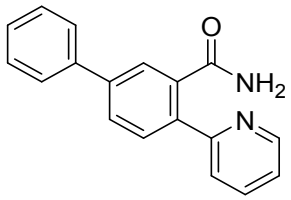
The product was isolated by flash chromatography (eluent: EA) as a white solid (226.1 mg, 85%); mp: 168-170 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.65 (d, J = 4.2 Hz, 1H), 7.94 (s, 1H), 7.80 (t, J = 7.5 Hz, 1H), 7.74 (d, J = 7.8 Hz, 1H), 7.63 (d, J = 8.4 Hz, 1H), 7.54 (d, J = 7.8 Hz, 1H), 7.35-7.33 (m, 1H), 6.55 (s, 1H), 5.96 (s, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.3, 156.9, 149.3, 141.9, 137.08, 136.0, 130.8, 130.7 (d, $J_{C\text{-}F}$ = 3.0 Hz), 126.9 (q, $J_{C\text{-}F}$ = 3.6 Hz), 125.8 (q, $J_{C\text{-}F}$ = 3.7 Hz), 124.0, 123.6 (d, $J_{C\text{-}F}$ = 270.9), 123.2. HRMS (ESI), *m/z* calcd. for $C_{13}H_9F_3N_2NaO$ ($[M+Na]^+$) 289.0559, found: 289.0553.



5-(tert-butyl)-3-cyano-2-(pyridin-2-yl)benzamide (1j).

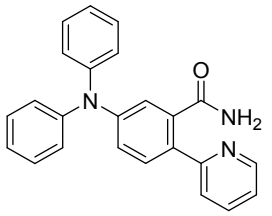
The product was isolated by flash chromatography (eluent: EA) as a white solid (217.7 mg, 78%); mp: 110-112 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66-8.64 (m, 1H), 7.93 (d, J = 2.0 Hz, 1H), 7.85-7.81 (m, 2H), 7.52 (d, J = 8.0 Hz, 1H), 7.52-7.32 (m, 1H), 6.40 (s, 1H), 6.04 (s, 1H), 1.36 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.0, 154.8, 152.8, 149.4, 138.9, 137.2, 136.7, 132.1, 130.1, 125.1, 123.8, 117.8, 113.2,

35.1, 30.9. HRMS (ESI), *m/z* calcd. for $C_{17}H_{18}N_3O$ ($[M+H]^+$) 280.1444, found: 280.1442.



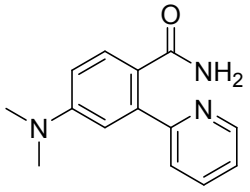
4-(pyridin-2-yl)-[1,1'-biphenyl]-3-carboxamide (1k).

The product was isolated by flash chromatography (eluent: EA) as a white solid (235.7 mg, 86%); mp: 196-198 ^oC; ^1H NMR (600 MHz, $CDCl_3$) δ 8.67 (d, J = 4.2 Hz, 1H), 7.95 (d, J = 1.8 Hz, 1H), 7.79-7.74 (m, 2H), 7.66-7.64 (m, 2H), 7.62 (d, J = 8.4 Hz, 1H), 7.58 (d, J = 7.8 Hz, 1H), 7.47 (t, J = 7.5 Hz, 2H), 7.39 (t, J = 7.5 Hz, 1H), 7.31-7.29 (m, 1H), 6.35 (s, 1H), 5.67 (s, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 171.7, 158.0, 149.2, 141.5, 139.6, 137.4, 136.8, 135.7, 130.8, 129.0, 128.4, 128.0, 127.4, 127.2, 124.0, 122.5. HRMS (ESI), *m/z* calcd. for $C_{18}H_{14}N_2NaO$ ($[M+Na]^+$) 297.0998, found: 297.0992.



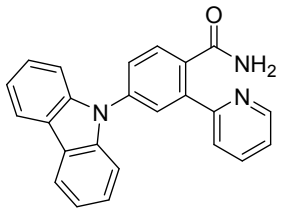
5-(diphenylamino)-2-(pyridin-2-yl)benzamide (1l).

The product was isolated by flash chromatography (eluent: EA) as a white solid (281.1 mg, 77%); mp: 230-232 ^oC; ^1H NMR (600 MHz, $CDCl_3$) δ 8.63-8.61 (m, 1H), 7.73 (td, J = 7.8, 1.8 Hz, 1H), 7.52 (d, J = 7.8 Hz, 1H), 7.40 (d, J = 9.0 Hz, 1H), 7.35 (d, J = 2.4 Hz, 1H), 7.30-7.26 (m, 4H), 7.25-7.23 (m, 1H), 7.18 (dd, J = 8.4, 2.4 Hz, 1H), 7.14-7.12 (m, 4H), 7.09-7.06 (m, 2H), 6.15 (s, 1H), 5.60 (s, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 171.6, 158.0, 149.1, 148.3, 147.1, 136.7, 136.3, 131.9, 131.3, 129.5, 125.0, 124.0, 123.7, 123.7, 122.1, 122.0. HRMS (ESI), *m/z* calcd. For $C_{24}H_{20}N_3O$ ($[M+H]^+$) 366.1601, found: 366.1603.



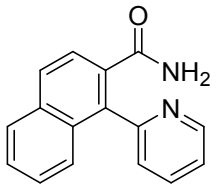
4-(dimethylamino)-2-(pyridin-2-yl)benzamide (1m).

The product was isolated by flash chromatography (eluent: EA) as a white solid (144.6 mg, 60%); mp: 146-148 ^{o}C; ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.57 (d, J = 4.8 Hz, 1H), 7.76 (t, J = 8.7 Hz, 1H), 7.46-7.36 (m, 3H), 7.32-7.25 (m, 1H), 6.93 (s, 1H), 6.77 (s, 1H), 6.73 (d, J = 9.0 HZ, 1H), 2.96 (s, 6H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 171.2, 159.7, 151.2, 149.1, 141.0, 136.4, 129.8, 124.8, 123.9, 122.3, 113.8, 111.2, 40.4. HRMS (ESI), *m/z* calcd. for $C_{14}H_{15}N_3NaO$ ([M+Na]$^+$) 264.1107, found: 264.1112.



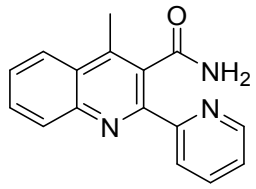
4-(9*H*-carbazol-9-yl)-2-(pyridin-2-yl)benzamide (1n).

The product was isolated by flash chromatography (eluent: EA) as a white solid (315.8 mg, 87%); mp: 193-195 ^{o}C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.65 (d, J = 4.8 Hz, 1H), 8.14 (d, J = 7.8 Hz, 2H), 7.98 (d, J = 7.8 Hz, 1H), 7.78-7.75 (m, 2H), 7.70 (d, J = 7.8 Hz, 1H), 7.61 (d, J = 7.8 Hz, 1H), 7.49-7.38 (m, 4H), 7.31 (t, J = 6.9 Hz, 3H), 6.58 (s, 1H), 5.96 (s, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 171.1, 157.4, 149.2, 140.8, 140.5, 139.6, 137.1, 134.1, 130.7, 128.5, 126.8, 126.2, 124.1, 123.7, 123.0, 120.5, 109.7. HRMS (ESI), *m/z* calcd. for $C_{24}H_{18}N_3O$ ([M+H]$^+$) 364.1444, found: 364.1443.



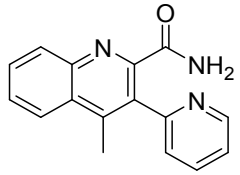
1-(pyridin-2-yl)-2-naphthamide (1o).

The product was isolated by flash chromatography (eluent: EA) as a white solid (213.4 mg, 86%); mp: 193-195 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.76 (d, J = 4.2 Hz, 1H), 7.95 (d, J = 8.4 Hz, 1H), 7.90 (d, J = 8.4 Hz, 1H), 7.84 (t, J = 7.8 Hz, 1H), 7.79 (d, J = 9.0 Hz, 1H), 7.53 (t, J = 7.5 Hz, 1H), 7.48-7.38 (m, 4H), 6.00 (s, 1H), 5.70 (s, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 171.3, 157.8, 149.4, 137.0, 136.2, 134.3, 132.5, 131.8, 129.0, 128.2, 127.1, 127.1, 126.6, 126.1, 124.8, 122.9. HRMS (ESI), *m/z* calcd. for $C_{16}H_{12}N_2NaO$ ($[M+Na]^+$) 271.0842, found: 271.0840.



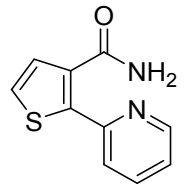
4-methyl-2-(pyridin-2-yl)quinoline-3-carboxamide (1p).

The product was isolated by flash chromatography (eluent: EA) as a white solid (131.5 mg, 50%); mp: 154-156 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.67 (d, J = 4.8 Hz, 1H), 8.20 (d, J = 7.8 Hz, 1H), 8.17 (d, J = 8.4 Hz, 1H), 8.09 (d, J = 8.4 Hz, 1H), 7.85 (t, J = 7.8 Hz, 1H), 7.78 (t, J = 7.5 Hz, 1H), 7.64 (t, J = 7.5 Hz, 1H), 7.36-7.34 (m, 1H), 5.86 (s, 2H), 2.85 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.6, 156.1, 152.3, 147.5, 145.9, 141.9, 135.9, 129.4, 129.1, 128.3, 126.39, 126.0, 123.2, 122.7, 122.7, 14.58. HRMS (ESI), *m/z* calcd. for $C_{16}H_{14}N_3O$ ($[M+H]^+$) 264.1131, found: 264.1125.



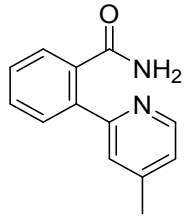
4-methyl-3-(pyridin-2-yl)quinoline-2-carboxamide (1q).

The product was isolated by flash chromatography (eluent: EA) as a white solid (105.2 mg, 40%); mp: 164-166 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.71-8.70 (m, 1H), 8.14 (d, J = 8.4 Hz, 1H), 8.10 (d, J = 8.4 Hz, 1H), 7.83 (s, 1H), 7.80-7.77 (m, 2H), 7.70-7.67 (m, 1H), 7.35 (d, J = 7.8 Hz, 1H), 7.33-7.31 (m, 1H), 5.43 (s, 1H), 2.47 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.5, 158.1, 149.2, 147.9, 145.6, 144.7, 135.8, 133.0, 130.4, 129.9, 128.8, 128.3, 124.7, 124.3, 122.0, 15.6. HRMS (ESI), *m/z* calcd. for $C_{16}H_{14}N_3O$ ($[M+H]^+$) 264.1131, found: 264.1126.



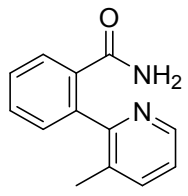
2-(pyridin-2-yl)thiophene-3-carboxamide (1r).

The product was isolated by flash chromatography (eluent: EA) as a white solid (185.6 mg, 91%); mp: 178-180 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.57 (d, J = 4.8 Hz, 1H), 8.05 (s, 1H), 7.83 (d, J = 3.6 Hz, 2H), 7.63 (d, J = 5.2 Hz, 1H), 7.52 (s, 1H), 7.34-7.31 (m, 1H), 7.23 (d, J = 5.2 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 167.1, 150.9, 149.1, 142.5, 137.0, 135.0, 129.2, 127.3, 122.9, 121.8. HRMS (ESI), *m/z* calcd. for $C_{10}H_8N_2NaOS$ ([M+Na]$^+$) 227.0250, found: 227.0247.



2-(4-methylpyridin-2-yl)benzamide (1s).

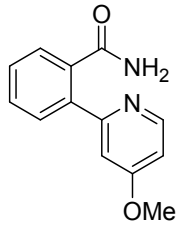
The product was isolated by flash chromatography (eluent: EA) as a white solid (190.9 mg, 90%); mp: 167-169 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.46 (d, J = 4.8 Hz, 1H), 7.70-7.68 (m, 1H), 7.49-7.43 (m, 3H), 7.32 (s, 1H), 7.10-7.09 (m, 1H), 6.46 (s, 1H), 5.90 (s, 1H), 2.39 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 171.8, 158.3, 148.8, 148.1, 138.9, 135.2, 130.3, 130.1, 128.7, 128.5, 124.9, 123.6, 21.2. HRMS (ESI), *m/z* calcd. for $C_{13}H_{12}N_2NaO$ ([M+Na]$^+$) 235.0842, found: 235.0841.



2-(3-methylpyridin-2-yl)benzamide (1t).

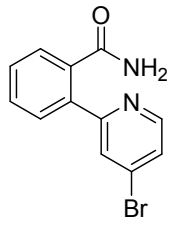
The product was isolated by flash chromatography (eluent: EA) as a white solid (190.9 mg, 90%); mp: 146-148 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.48 (d, J = 4.8 Hz, 1H), 7.84-7.83 (m, 1H), 7.61 (d, J = 7.8 Hz, 1H), 7.54-7.53 (m, 1H), 7.50-7.49 (m,

1H), 7.29-7.24 (m, 2H), 6.11 (s, 1H), 5.95 (s, 1H), 2.13 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.8, 158.7, 146.4, 138.5, 138.5, 134.4, 132.5, 130.7, 129.6, 129.0, 128.4, 123.0, 19.4. HRMS (ESI), *m/z* calcd. for $C_{13}H_{12}N_2NaO$ ($[M+Na]^+$) 235.0842, found: 235.0839.



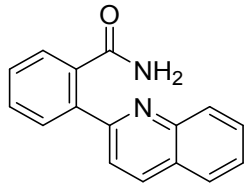
2-(4-methoxypyridin-2-yl)benzamide (1u).

The product was isolated by flash chromatography (eluent: EA) as a white solid (205.2 mg, 90%); mp: 138-140 ^{o}C; ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.42 (d, J = 6.0 Hz, 1H), 7.73 (s, 1H), 7.63 (d, J = 7.8 Hz, 1H), 7.53-7.43 (m, 3H), 7.29 (s, 1H), 7.15 (s, 1H), 6.94 (d, J = 6.0 Hz, 1H), 3.86 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 171.6, 165.8, 159.8, 150.8, 138.8, 138.0, 130.2, 129.5, 128.5, 128.0, 109.7, 108.8, 55.71. HRMS (ESI), *m/z* calcd. for $C_{13}H_{13}N_2O_2$ ($[M+H]^+$) 229.0972, found: 229.0980.



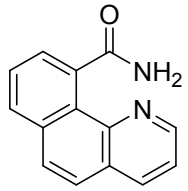
2-(4-bromopyridin-2-yl)benzamide (1v).

The product was isolated by flash chromatography (eluent: EA) as a white solid (231.8 mg, 84%); mp: 160-162 ^{o}C; ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.51 (d, J = 5.3 Hz, 1H), 7.84 (s, 1H), 7.82 (s, 1H), 7.66-7.61 (m, 2H), 7.56-7.49 (m, 3H), 7.40 (s, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 171.3, 160.0, 150.7, 137.9, 137.7, 132.4, 130.4, 129.9, 129.1, 128.3, 126.4, 125.6. HRMS (ESI), *m/z* calcd. for $C_{14}H_{10}N_2NaO$ ($[M+Na]^+$) 298.9790, found: 298.9784.



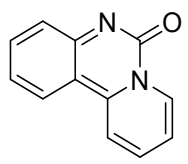
2-(quinolin-2-yl)benzamide (1w).

The product was isolated by flash chromatography (eluent: EA) as a white solid (205.9 mg, 83%); mp: 199-201 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (d, J = 8.4 Hz, 1H), 8.08 (d, J = 8.4 Hz, 1H), 7.86 (d, J = 8.0 Hz, 1H), 7.78-7.73 (m, 2H), 7.65-7.62 (m, 2H), 7.59-7.54 (m, 2H), 7.52-7.48 (m, 1H), 6.35 (s, 1H), 5.79 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.5, 158.6, 147.6, 139.0, 136.7, 135.3, 130.5, 130.4, 130.0, 129.4, 128.9, 128.9, 127.7, 127.1, 126.9, 122.1. HRMS (ESI), *m/z* calcd. for $C_{16}H_{12}N_2NaO$ ($[M+Na]^+$) 271.0842, found: 271.0837.



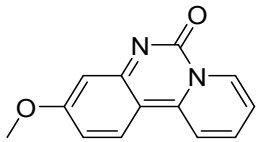
benzo[*h*]quinoline-10-carboxamide (1x).

The product was isolated by flash chromatography (eluent: EA) as a white solid (204.2 mg, 92%); mp: 298-300 ^{o}C; ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.90 (dd, J = 4.2, 1.8 Hz, 1H), 8.42 (dd, J = 7.8, 1.8 Hz, 1H), 8.06 (d, J = 7.2 Hz, 1H), 7.99 (d, J = 9.0 Hz, 1H), 7.91 (d, J = 9.0 Hz, 1H), 7.74 (t, J = 7.5 Hz, 1H), 7.66 (dd, J = 8.4, 4.2 Hz, 1H), 7.60 (s, 1H), 7.57-7.56 (m, 1H), 7.30 (s, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 173.9, 148.3, 145.5, 137.7, 136.2, 134.3, 128.9, 128.3, 128.0, 127.3, 127.2, 127.0, 126.5, 122.6. HRMS (ESI), *m/z* calcd. for $C_{14}H_{10}N_2NaO$ ($[M+Na]^+$) 245.0685, found: 245.0684.



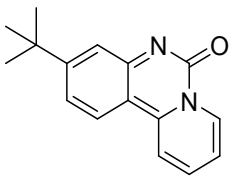
6*H*-pyrido[1,2-*c*]quinazolin-6-one (2a).

Yellow solid (35.6 mg, 91%); mp: 214-216 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.70 (d, J = 6.8 Hz, 1H), 9.20 (d, J = 8.4 Hz, 1H), 8.85 (t, J = 8.0 Hz, 1H), 8.70 (d, J = 8.0 Hz, 1H), 8.20 (t, J = 7.0 Hz, 1H), 7.91 (t, J = 7.8 Hz 1H), 7.56 (t, J = 7.6 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 148.0, 147.3, 143.8, 137.4, 136.0, 135.9, 125.9, 124.8, 124.7, 122.6, 117.2, 112.5. HRMS (ESI), *m/z* calcd. for $C_{12}H_9N_2O$ ([M+H]$^+$) 197.0709, found: 197.0703.



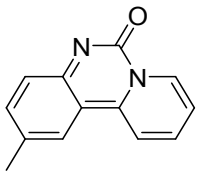
3-methoxy-6*H*-pyrido[1,2-*c*]quinazolin-6-one (2b).

Yellow solid (44.3 mg, 98%); mp: ＞300 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.50 (d, J = 6.8 Hz, 1H), 8.86 (d, J = 8.8 Hz, 1H), 8.43-8.38 (m, 2H), 7.81 (t, J = 6.8 Hz, 1H), 6.85 (dd, J = 9.2, 2.4 Hz, 1H), 6.78 (d, J = 2.4 Hz, 1H), 3.89 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 164.7, 153.0, 147.9, 147.0, 141.6, 133.5, 126.9, 121.4, 113.0, 106.7, 105.2, 56.0. HRMS (ESI), *m/z* calcd. for $C_{13}H_{11}N_2O_2$ ([M+H]$^+$) 227.0815, found: 227.0815.



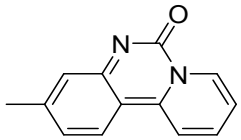
3-(tert-butyl)-6*H*-pyrido[1,2-*c*]quinazolin-6-one (2c).

Yellow solid (48.3 mg, 96%); mp: 156-158 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.80 (d, J = 6.6 Hz, 1H), 8.56 (d, J = 8.4 Hz, 1H), 8.26 (t, J = 7.5 Hz, 1H), 8.08 (d, J = 9.0 Hz, 1H), 7.69 (t, J = 6.6 Hz, 1H), 7.63 (s, 1H), 7.33 (d, J = 9.0 Hz, 1H), 1.39 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.3, 148.0, 140.3, 134.2, 123.0, 122.2, 122.2, 122.2, 120.9, 120.6, 120.4, 35.5, 30.8. HRMS (ESI), *m/z* calcd. for $C_{16}H_{17}N_2O$ ([M+H]$^+$) 253.1335, found: 253.1328.



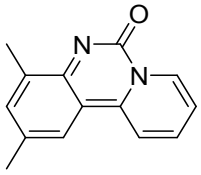
2-methyl-6*H*-pyrido[1,2-*c*]quinazolin-6-one (2d).

Yellow solid (37.8 mg, 90%); mp: 216-218 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.83 (d, J = 6.0 Hz, 1H), 8.57 (d, J = 8.4 Hz, 1H), 8.26-8.23 (m, 1H), 7.90 (s, 1H), 7.70 (t, J = 6.9 Hz, 1H), 7.53-7.49 (m, 2H), 2.47 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 149.0, 147.9, 147.0, 139.9, 137.0, 134.3, 131.5, 126.6, 122.2, 120.8, 120.4, 111.4, 21.3. HRMS (ESI), *m/z* calcd. for $C_{14}H_{15}N_2O_2^+$ ([M+MeOH+H]$^+$) 243.1128, found: 243.1127.



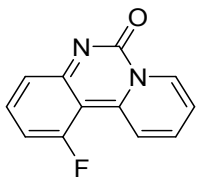
3-methyl-6*H*-pyrido[1,2-*c*]quinazolin-6-one (2e).

Yellow solid (41.2 mg, 98%); mp: 220-222 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.77 (d, J = 6.8 Hz, 1H), 8.51 (d, J = 8.4 Hz, 1H), 8.21 (t, J = 7.8 Hz, 1H), 8.00 (d, J = 8.4 Hz, 1H), 7.65 (t, J = 7.0 Hz, 1H), 7.36 (s, 1H), 7.04 (d, J = 8.4 Hz, 1H), 2.47 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.9, 148.1, 147.2, 146.2, 140.0, 134.1, 125.9, 124.1, 123.1, 120.4, 120.3, 109.6, 22.1. HRMS (ESI), *m/z* calcd. for $C_{14}H_{15}N_2O_2^+$ ([M+MeOH+H]$^+$) 243.1128, found: 243.1128.



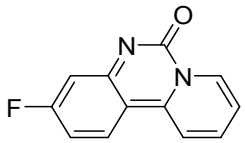
2,4-dimethyl-6*H*-pyrido[1,2-*c*]quinazolin-6-one (2f).

Yellow solid (43.5 mg, 97%); mp: 232-234 °C; ^{1}H NMR (600 MHz, DMSO-d_6) δ 9.74-9.72 (m, 1H), 9.25 (d, J = 8.4 Hz, 1H), 8.88-8.85 (m, 1H), 8.46 (s, 1H), 8.21-8.18 (m, 1H), 7.65 (s, 1H), 2.52 (s, 3H), 2.46 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 148.6, 147.7, 144.7, 139.0, 136.3, 134.6, 126.2, 125.0, 123.7, 123.2, 113.0, 20.9, 17.7. HRMS (ESI), *m/z* calcd. for $C_{14}H_{13}N_2O$ ([M+H]$^+$) 225.1022, found: 225.1017.



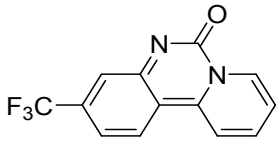
1-fluoro-6*H*-pyrido[1,2-*c*]quinazolin-6-one (2g).

Yellow solid (41.5 mg, 97%); mp: 236-238 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.97 (d, J = 6.6 Hz, 1H), 9.03 (dd, J = 8.4, 5.4 Hz, 1H), 8.36-8.33 (m, 1H), 7.82 (t, J = 6.6 Hz, 1H), 7.61-7.57 (m, 1H), 7.41 (d, J = 8.4 Hz, 1H), 6.92 (dd, J = 13.2, 7.8 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 160.5 (d, $J_{C\text{-}F}$ = 255.5 Hz), 151.8, 146.6, 141.3, 134.8, 134.4 (d, $J_{C\text{-}F}$ = 12.0 Hz), 125.2 (d, $J_{C\text{-}F}$ = 25.5 Hz), 122.6 (d, $J_{C\text{-}F}$ = 3.3 Hz), 121.8, 107.7 (d, $J_{C\text{-}F}$ = 23.3 Hz), 102.4 (d, $J_{C\text{-}F}$ = 8.6 Hz), 100.0. HRMS (ESI), *m/z* calcd. for $C_{13}H_{12}FN_2O_2$ ($[M+MeOH+H]^+$) 247.0877, found: 247.0875.



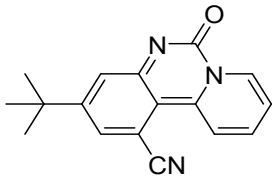
3-fluoro-6*H*-pyrido[1,2-*c*]quinazolin-6-one (2h).

Yellow solid (41.1 mg, 96%); mp: 191-193 °C; ^{1}H NMR (600 MHz, DMSO-d_6) δ 9.71 (d, J = 6.6 Hz, 1H), 9.24 (d, J = 7.8 Hz, 1H), 8.91-8.87 (m, 2H), 8.20 (t, J = 6.9 Hz, 1H), 7.50 (s, 1H), 7.37-7.35 (m, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 164.3 (d, $J_{C\text{-}F}$ = 253.8 Hz), 145.8 (d, $J_{C\text{-}F}$ = 5.3 Hz), 142.3, 138.0, 134.2, 127.9 (d, $J_{C\text{-}F}$ = 11.1 Hz), 123.0, 120.9, 116.5, 111.6 (d, $J_{C\text{-}F}$ = 23.6 Hz), 108.1, 101.8 (d, $J_{C\text{-}F}$ = 25.8 Hz). HRMS (ESI), *m/z* calcd. for $C_{12}H_8FN_2O$ ($[M+H]^+$) 215.0615, found: 215.0616.



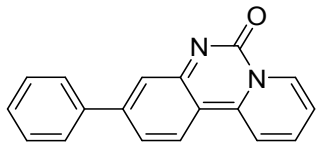
3-(trifluoromethyl)-6*H*-pyrido[1,2-*c*]quinazolin-6-one (2i).

Yellow solid (48.5 mg, 92%); mp: 244-246 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.93 (d, J = 6.6 Hz, 1H), 8.67 (d, J = 8.4 Hz, 1H), 8.41 (t, J = 7.8 Hz, 1H), 8.26 (d, J = 9.0 Hz, 1H), 7.88 (t, J = 6.8 Hz, 1H), 7.86 (s, 1H), 7.40 (d, J = 9.0 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 153.3, 150.4, 147.8, 146.5, 141.4, 136.2, 135.0, 124.4, 124.3, 124.2 (q, $J_{C\text{-}F}$ = 3.0 Hz), 121.7 (d, $J_{C\text{-}F}$ = 221.3 Hz), 117.5 (q, $J_{C\text{-}F}$ = 2.4 Hz), 113.3. HRMS (ESI), *m/z* calcd. for $C_{13}H_8F_3N_2O$ ($[M+H]^+$) 265.0583, found: 265.0585.



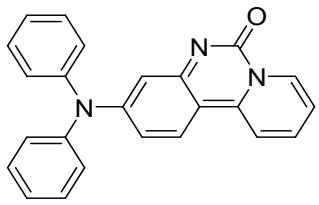
3-(tert-butyl)-6-oxo-6*H*-pyrido[1,2-*c*]quinazoline-1-carbonitrile (2j).

Yellow solid (52.6 mg, 95%); mp: 155-157 °C; ^{1}H NMR (600 MHz, DMSO-d_6) δ 9.89 (d, J = 6.6 Hz, 1H), 9.61 (d, J = 8.4 Hz, 1H), 9.06-9.04 (m, 1H), 8.34 (t, J = 6.9 Hz, 1H), 8.26 (d, J = 1.8 Hz, 1H), 7.81 (d, J = 28.8 Hz, 1H), 1.39 (s, 9H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 158.9, 148.4, 145.7, 144.2, 137.7, 131.9, 126.1, 123.1, 120.4, 119.1, 109.7, 108.3, 36.0, 30.5. HRMS (ESI), *m/z* calcd. for $C_{17}H_{16}N_3O$ ([M+H]$^+$) 278.1288, found: 278.1289.



3-phenyl-6*H*-pyrido[1,2-*c*]quinazolin-6-one (2k).

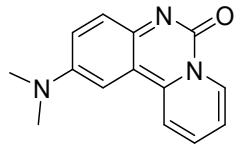
Yellow solid (53.9 mg, 99%); mp: 235-237 °C; ^{1}H NMR (600 MHz, DMSO-d_6) δ 9.74-9.73 (m, 1H), 9.31 (d, J = 8.4 Hz, 1H), 8.92-8.89 (m, 1H), 8.85 (d, J = 8.4 Hz, 1H), 8.21 (t, J = 6.9 Hz, 1H), 7.93 (dd, J = 8.4, 1.2 Hz, 1H), 7.85-7.78 (m, 3H), 7.60 (t, J = 7.5 Hz, 2H), 7.54 (t, J = 7.5 Hz, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 148.3, 148.0, 147.8, 144.4, 138.2, 138.1, 136.5, 130.0, 129.9, 127.7, 127.3, 125.2, 124.0, 123.2, 114.5, 112.2. HRMS (ESI), *m/z* calcd. for $C_{18}H_{13}N_2O$ ([M+H]$^+$) 273.1022, found: 273.1023.



3-(diphenylamino)-6*H*-pyrido[1,2-*c*]quinazolin-6-one (2l).

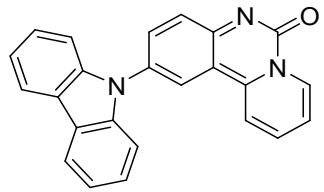
Yellow solid (68.9 mg, 95%); mp: 122-124 °C; ^{1}H NMR (600 MHz, DMSO-d_6) δ 9.41 (d, J = 6.6 Hz, 1H), 8.88-8.86 (m, 1H), 8.64-8.61 (m, 1H), 8.47 (d, J = 9.0 Hz,

1H), 7.90 (t, *J* = 6.9 Hz, 1H), 7.52 (t, *J* = 7.8 Hz, 4H), 7.40-7.31 (m, 6H), 6.82 (dd, *J* = 9.3, 2.1 Hz, 1H), 6.71 (d, *J* = 2.4 Hz, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 154.5, 148.2, 146.3, 144.8, 144.5, 139.4, 135.1, 130.9, 128.1, 127.7, 127.4, 122.5, 121.9, 115.5, 105.0, 101.4. HRMS (ESI), *m/z* calcd. for $C_{24}H_{18}N_3O$ ($[M+H]^+$) 364.1444, found: 364.1444.



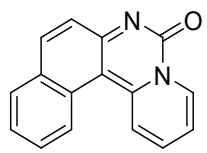
2-(dimethylamino)-6*H*-pyrido[1,2-*c*]quinazolin-6-one (2m).

Black solid (43.0 mg, 90%); mp: 194-196 ^{o}C; ^{1}H NMR (600 MHz, DMSO-d_6) δ 9.62 (d, *J* = 7.2 Hz, 1H), 9.07 (d, *J* = 8.4 Hz, 1H), 8.45 (t, *J* = 1.8 Hz 1H), 7.92 (t, *J* = 6.8 Hz, 1H), 7.48 (s, 1H), 7.44-7.42 (m, 1H), 7.28 (d, *J* = 9.0 Hz, 1H), 2.98 (s, 6H).^{13}C NMR (150 MHz, DMSO-d_6) δ 147.1, 146.3, 146.1, 143.3, 141.1, 133.8, 126.4, 124.7, 122.4, 122.2, 112.7, 104.1, 41.4. HRMS (ESI), *m/z* calcd. for $C_{15}H_{18}N_3O_2$ ($[M+MeOH+H]^+$) 272.1394, found: 272.1385.



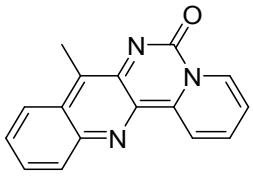
2-(9*H*-carbazol-9-yl)-6*H*-pyrido[1,2-*c*]quinazolin-6-one (2n).

Brown solid (68.6 mg, 95%); mp: 268-270 ^{o}C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.92 (d, *J* = 6.6 Hz, 1H), 8.56 (d, *J* = 8.4 Hz, 1H), 8.34 (s, 1H), 8.31 (t, *J* = 7.5 Hz, 1H), 8.17 (d, *J* = 7.8 Hz, 2H), 7.86-7.78 (m, 3H), 7.43 (t, *J* = 7.5 Hz, 2H), 7.38 (d, *J* = 8.4 Hz, 2H), 7.32 (t, *J* = 7.8 Hz, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 150.0, 147.8, 146.9, 141.1, 140.9, 134.7, 134.5, 131.5, 131.5, 128.6, 126.2, 123.4, 121.8, 121.7, 120.8, 120.5, 120.3, 112.2, 109.5. HRMS (ESI), *m/z* calcd. for $C_{25}H_{20}N_3O_2$ ($[M+MeOH+H]^+$) 394.1550, found: 394.1552.



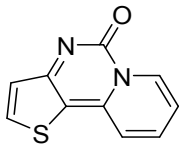
6*H*-benzo[*f*]pyrido[1,2-*c*]quinazolin-6-one (2o).

Yellow solid (48.2 mg, 98%); mp: 189-191 °C; ^{1}H NMR (600 MHz, DMSO-d_6) δ 9.77 (d, J = 6.6 Hz, 1H), 9.29 (d, J = 8.4 Hz, 1H), 8.81 (t, J = 7.8 Hz, 1H), 8.73 (dd, J = 8.4, 3.3 Hz, 1H), 8.44 (d, J = 9.0 Hz, 1H), 8.22-8.13 (m, 2H), 7.88 (t, J = 7.8 Hz, 1H), 7.74 (t, J = 7.5 Hz, 1H), 7.62 (t, J = 8.7 Hz, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 147.6, 146.7, 144.8, 140.5, 138.4, 136.1, 131.1, 130.6, 130.5, 128.4, 127.1, 126.7, 125.0, 124.0, 117.4, 107.2. HRMS (ESI), *m/z* calcd. for $C_{16}H_{11}N_2O$ ([M+H]$^+$) 247.0866, found: 247.0868.



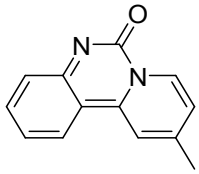
8-methyl-6*H*-pyrido[1',2':1,6]pyrimido[5,4-*b*]quinolin-6-one (2p).

Red solid (45.4 mg, 87%); mp: 258-260 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.95 (d, J = 6.0 Hz, 1H), 9.65 (d, J = 7.8 Hz, 1H), 8.51 (t, J = 7.5 Hz, 1H), 8.11 (t, J = 8.7 Hz, 2H), 7.99 (t, J = 6.6 Hz, 1H), 7.66-7.62 (m, 1H), 7.61-7.55 (m, 1H), 3.02 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 148.9, 144.8, 144.3, 141.9, 139.7, 137.7, 135.0, 131.1, 130.9, 130.6, 128.0, 127.9, 124.5, 124.0, 123.3, 12.1. HRMS (ESI), *m/z* calcd. for $C_{17}H_{16}N_3O_2$ ([M+MeOH+H]$^+$) 294.1237, found: 294.1234.



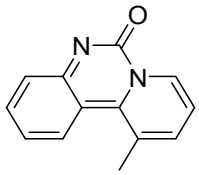
5*H*-pyrido[1,2-*c*]thieno[2,3-*e*]pyrimidin-5-one (2r).

Yellow solid (36.4 mg, 90%); mp: 200-202 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.50 (d, J = 7.2 Hz, 1H), 8.01-7.99 (m, 1H), 7.82 (d, J = 5.4 Hz, 1H), 7.79 (d, J = 8.4 Hz, 1H), 7.43 (td, J = 6.9, 1.2 Hz, 1H), 7.21 (d, J = 5.4 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.3, 150.1, 144.3, 138.7, 135.8, 133.2, 125.3, 121.4, 118.3, 109.4. HRMS (ESI), *m/z* calcd. for $C_{10}H_7N_2OS$ ([M+H]$^+$) 203.0274, found: 203.0275.



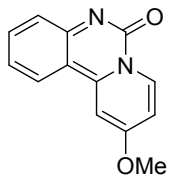
10-methyl-6*H*-pyrido[1,2-*c*]quinazolin-6-one (2s).

Yellow solid (38.2 mg, 91%); mp: 188-190 °C; ^{1}H NMR (600 MHz, DMSO-d_6) δ 9.59 (d, J = 6.6 Hz, 1H), 9.17 (s, 1H), 8.73 (d, J = 7.8 Hz, 1H), 8.07 (d, J = 6.6 Hz, 1H), 7.92 (t, J = 7.5 Hz, 1H), 7.59-7.55 (m, 2H), 2.81 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 162.3, 147.4, 144.2, 137.2, 136.3, 135.7, 126.4, 126.3, 125.3, 122.7, 117.2, 112.8, 22.6. HRMS (ESI), *m/z* calcd. for $C_{13}H_{11}N_2O$ ($[M+H]^+$) 211.0866, found: 211.0866.



11-methyl-6*H*-pyrido[1,2-*c*]quinazolin-6-one (2t).

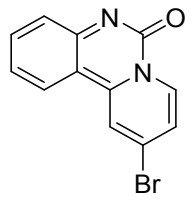
Yellow solid (39.1 mg, 93%); mp: 170-172 °C; ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.91 (d, J = 6.0 Hz, 1H), 8.28 (d, J = 8.4 Hz, 1H), 8.13 (d, J = 7.2 Hz, 1H), 7.66-7.58 (m, 3H), 7.19-7.17 (m, 1H), 3.08 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 150.80, 148.0, 146.9, 144.3, 134.4, 133.7, 133.7, 127.1, 126.7, 121.1, 120.5, 113.5, 25.7. HRMS (ESI), *m/z* calcd. for $C_{14}H_{15}N_2O_2$ ($[M+MeOH+H]^+$) 243.1128, found: 243.1126.



10-methoxy-6*H*-pyrido[1,2-*c*]quinazolin-6-one (2u).

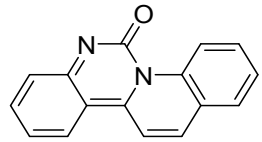
Yellow solid (42.0 mg, 93%); mp: 238-240 °C; ^{1}H NMR (600 MHz, DMSO-d_6) δ 9.46 (d, J = 7.2 Hz, 1H), 8.49 (d, J = 8.4 Hz, 1H), 8.25-8.23 (m, 1H), 7.60 (t, J = 7.8 Hz, 1H), 7.53-7.51 (m, 1H), 7.26 (d, J = 7.8 Hz, 1H), 7.19-7.07 (m, 1H), 4.19 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 169.0, 150.4, 150.3, 146.4, 136.5, 134.5, 125.5,

125.4, 120.9, 112.9, 112.4, 102.6, 58.3. HRMS (ESI), *m/z* calcd. for $C_{14}H_{15}N_2O_3$ ($[M+MeOH+H]^+$) 259.1077, found: 259.1076.



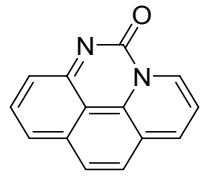
10-bromo-6*H*-pyrido[1,2-*c*]quinazolin-6-one (2v).

Yellow solid (42.7 mg, 78%); mp: 260-262 ^oC; ^1H NMR (600 MHz, $CDCl_3$) δ 9.67 (d, J = 7.2Hz, 1H), 8.72 (s, 1H), 8.07 (d, J = 8.4 Hz, 1H), 7.82 (d, J = 7.2 Hz, 1H), 7.70 (t, J = 7.5 Hz, 1H), 7.60 (d, J = 8.4 Hz, 1H), 7.24 (s, 1H). ^{13}C NMR (150MHz, $CDCl_3$) δ 151.6, 148.5, 146.6, 138.0, 135.7, 135.0, 126.9, 124.8, 123.3, 123.3, 122.4, 110.7. HRMS (ESI), *m/z* calcd. for $C_{13}H_{12}BrN_2O_2$ ($[M+MeOH+H]^+$) 307.0077, found: 307.0069.



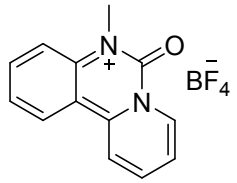
6*H*-quinolino[1,2-*c*]quinazolin-6-one (2w).

Red solid (43.8 mg, 89%); mp: 162-164 ^oC; ^1H NMR (600 MHz, $CDCl_3$) δ 9.46 (d, J = 9.0 Hz, 1H), 8.28 (d, J = 9.0 Hz, 1H), 8.09 (d, J = 8.4 Hz, 1H), 7.93 (d, J = 7.8 Hz, 1H), 7.86 (d, J = 7.8 Hz, 1H), 7.79 (t, J = 7.5 Hz, 1H), 7.64 (t, J = 7.2 Hz, 1H), 7.55 (t, J = 7.5 Hz, 1H), 7.43 (d, J = 8.3 Hz, 1H), 7.19 (t, J = 7.5 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.5, 153.4, 146.1, 139.6, 137.3, 130.4, 129.8, 129.3, 128.7, 127.4, 126.7, 126.4, 124.8, 122.1, 121.7, 120.8. HRMS (ESI), *m/z* calcd. for $C_{16}H_{11}N_2O$ ($[M+H]^+$) 247.0866, found: 247.0858.



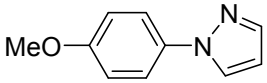
5*H*-pyrido[1,2,3-*cd*]perimidin-5-one (2x).

Red solid (40.5 mg, 92%); mp: ＞300 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.17-10.16 (m, 1H), 9.63 (d, J = 7.6 Hz, 1H), 8.62 (t, J = 7.2 Hz, 1H), 8.50 (q, J = 10.7 Hz, 1H), 8.34 (t, J = 7.8 Hz, 1H), 8.27 (d, J = 7.6 Hz, 1H), 7.91 (d, J = 7.6 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 147.6, 144.5, 137.1, 136.8, 135.4, 134.9, 133.3, 130.8, 128.2, 126.1, 123.7, 123.6, 114.4, 108.4. HRMS (ESI), *m/z* calcd. for $C_{14}H_9N_2O$ ([M+H]$^+$) 221.0709, found: 221.0710.



3a

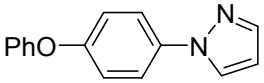
Yellow solid; mp: > 300 °C; ^{1}H NMR (400 MHz, DMSO) δ 9.82 (d, J = 6.0 Hz, 1H), 9.34 (d, J = 8.4 Hz, 1H), 8.98 -8.87 (m, 2H), 8.25 (t, J = 6.6 Hz, 1H), 8.08 (t, J = 7.4 Hz, 1H), 7.91 (d, J = 8.4 Hz, 1H), 7.71 (t, J = 7.6 Hz, 1H), 3.94 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 148.4, 147.6, 145.3, 137.9, 137.12, 137.08, 127.0, 125.8, 125.7, 123.0, 116.8, 113.4. ^{19}F NMR (376 MHz, DMSO) δ -148.3. HRMS (ESI), *m/z* calcd. for $C_{13}H_{11}N_2O$ ([M]$^+$) 211.0866, found: 211.0843.



1-(4-methoxyphenyl)-1*H*-pyrazole (4a). [2]

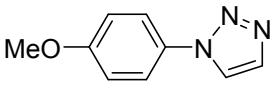
The title compound was prepared in 60% as an inseparable mixture. The para:ortho ratio of the inseparable mixture was 6:1 as determined by ^{1} H NMR of the isolated product mixture. The NMR and HRMS data of only the major isomer **4a** are given.

Yellow oil (21 mg, 60%); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.83 (d, J = 2.4 Hz, 1H), 7.69 (s, 1H), 7.59 (d, J = 8.4 Hz, 2H), 6.97 (d, J = 9.0 Hz, 2H), 6.44 (s, 1H), 3.85 (s, 3H).



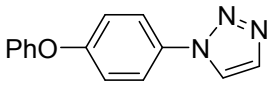
1-(4-phenoxyphenyl)-1*H*-pyrazole (4b). [3]

Yellow solid (26 mg, 55%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, J = 2.4 Hz, 1H), 7.71 (s, 1H), 7.66-7.62 (m, 2H), 7.38 – 7.33 (m, 2H), 7.15-7.07 (m, 3H), 7.03 (d, J = 7.6 Hz, 2H), 6.46 (t, J = 2.5 Hz, 2H).



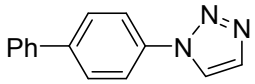
1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (4c). [3]

White solid (25 mg, 71%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (s 1H), 7.83 (s, 1H), 7.65-7.61 (m, 2H), 7.05-6.98 (m, 2H), 3.86 (s, 3H).



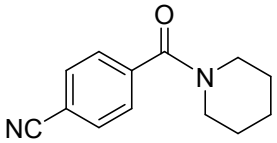
1-(4-phenoxyphenyl)-1*H*-1,2,3-triazole (4d).

White solid; mp: 91-92 ^{o}C ; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (s, 1H), 7.83 (s, 1H), 7.70-7.64 (m, 2H), 7.41-7.35 (m, 2H), 7.20-7.10 (m, 3H), 7.08-7.04 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.9, 156.3, 134.4, 132.2, 130.1, 124.2, 122.4, 121.9, 119.5, 119.3. HRMS (ESI), *m/z* calcd. for $C_{14}H_{11}N_3NaO$ ([M+Na]$^+$) 260.0794, found: 260.0793.



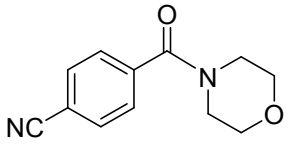
1-([1,1'-biphenyl]-4-yl)-1*H*-1,2,3-triazole (4e).

White solid; mp: 182-184 ^{o}C ; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, J = 2.2 Hz, 1H), 7.77 (t, J = 6.5 Hz, 3H), 7.69 (d, J = 8.5 Hz, 2H), 7.62 (d, J = 7.6 Hz, 2H), 7.46 (t, J = 7.6 Hz, 2H), 7.37 (t, J = 7.3 Hz, 1H), 6.49 (s, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 141.8, 139.6, 136.2, 134.5, 129.0, 128.40 (s), 128.0, 127.1, 121.7, 121.0. HRMS (ESI), *m/z* calcd. for $C_{14}H_{12}N_3$ ([M+H]$^+$) 222.1026, found: 222.1027.



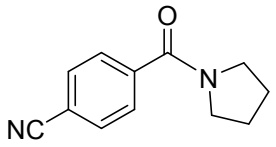
4-(piperidine-1-carbonyl)benzonitrile (5a). [4]

Yellow solid (39 mg, 90%); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.69 (d, J = 7.8 Hz, 2H), 7.48 (d, J = 7.8 Hz, 2H), 3.70 (s, 2H), 3.27 (s, 2H), 1.68 (s, 4H), 1.51 (s, 2H).



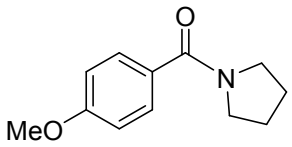
4-(morpholine-4-carbonyl)benzonitrile (5b). [5]

Brown solid (38 mg, 89%); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.72 (d, J = 7.8 Hz, 2H), 7.51 (d, J = 7.8 Hz, 2H), 3.79 (s, 4H), 3.62 (s, 2H), 3.38 (s, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 168.3, 139.7, 132.5, 127.8, 118.0, 113.8, 66.8, 48.0, 42.7.



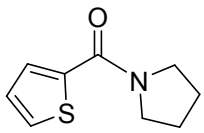
4-(pyrrolidine-1-carbonyl)benzonitrile (5c). [4]

Yellow oil (35 mg, 88%); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.70 (d, J = 7.8 Hz, 2H), 7.61 (d, J = 7.2 Hz, 2H), 3.65 (t, J = 6.9 Hz, 2H), 3.37 (t, J = 6.6 Hz, 2H), 2.02-1.95 (m, 2H), 1.94-1.88 (m, 2H).



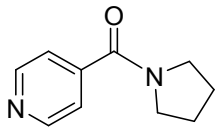
(4-methoxyphenyl)(pyrrolidin-1-yl)methanone (5d). [4]

Yellow oil (36 mg, 88%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, J = 8.8 Hz, 2H), 6.90 (d, J = 8.8 Hz, 2H), 3.83 (s, 3H), 3.63 (t, J = 6.6 Hz, 2H), 3.48 (t, J = 6.2 Hz, 2H), 1.97-1.85 (m, 4H).



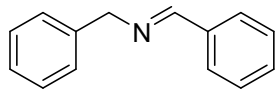
pyrrolidin-1-yl(thiophen-2-yl)methanone (5e). [4]

Yellow oil (30 mg, 81%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, J = 4.4, 1.1 Hz, 1H), 7.46 (d, J = 5.0, 1H), 7.07 (dd, J = 5.0, 3.8 Hz, 1H), 3.81-3.62 (m, 4H), 2.04-1.91 (m, 4H).



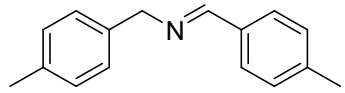
pyridin-4-yl(pyrrolidin-1-yl)methanone (5f). [4]

Yellow oil (28 mg, 80%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, J = 6.0 Hz, 2H), 7.38 (d, J = 6.0 Hz, 2H), 3.65 (t, J = 7.0 Hz, 2H), 3.38 (t, J = 6.6 Hz, 2H), 2.02-1.80 (m, 4H).



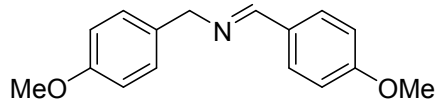
(*E*)-*N*-benzyl-1-phenylmethanimine (6a). [6]

Orange oil (29 mg, 74%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (s, 1H), 7.81 – 7.76 (m, 2H), 7.44 – 7.42 (m, 2H), 7.35 (d, J = 4.5 Hz, 4H), 7.32 (s, 1H), 4.84 (d, J = 1.0 Hz, 2H).



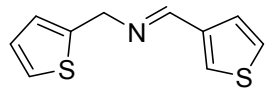
(*E*)-*N*-(4-methylbenzyl)-1-(p-tolyl)methanimine (6b). [6]

White solid (30 mg, 66%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (s, 1H), 7.67 (d, J = 8.0 Hz, 2H), 7.22 (dd, J = 7.8, 2.2 Hz, 4H), 7.15 (d, J = 8.0 Hz, 2H), 4.77 (s, 2H), 2.39 (s, 3H), 2.34 (s, 3H).



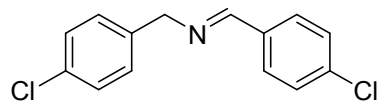
(*E*)-*N*-(4-methoxybenzyl)-1-(4-methoxyphenyl)methanimine (6c). [6]

Yellow oil (40 mg, 78%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (s, 1H), 7.71 (d, J = 8.8 Hz, 2H), 7.23 (s, 2H), 6.90 (q, J = 8.8 Hz, 4H), 4.73 (s, 2H), 3.84 (s, 3H), 3.80 (s, 3H).



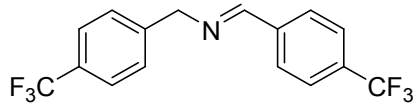
(*E*)-*N*-(thiophen-2-ylmethyl)-1-(thiophen-3-yl)methanimine (6d). [7]

Yellow oil (15 mg, 36%); ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.42 (s, 1H), 7.42 (d, J = 4.8 Hz, 1H), 7.33 (d, J = 3.6 Hz, 1H), 7.24 (d, J = 4.8 Hz, 1H), 7.08 (t, J = 4.2 Hz, 1H), 7.01-6.95 (m, 2H), 4.95 (s, 2H).



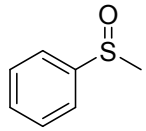
(*E*)-*N*-(4-chlorobenzyl)-1-(4-chlorophenyl)methanimine (6e). [6]

White solid (21 mg, 40%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (s, 1H), 7.71 (d, J = 8.4 Hz, 2H), 7.40 (d, J = 8.4 Hz, 2H), 7.32 (d, J = 8.4 Hz, 2H), 7.26 (d, J = 8.4 Hz, 2H), 4.77 (s, 2H).



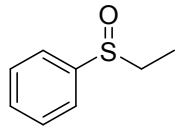
(*E*)-*N*-(4-(trifluoromethyl)benzyl)-1-(4(trifluoromethyl)phenyl)methanimine (6f). [6]

Yellow oil (25 mg, 37%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (s, 1H), 7.91 (d, J = 8.0 Hz, 2H), 7.69 (d, J = 8.0 Hz, 2H), 7.62 (d, J = 8.0 Hz, 2H), 7.47 (d, J = 8.0 Hz, 2H), 4.90 (s, 2H).



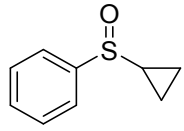
(methylsulfinyl)benzene (7a). [8]

White solid (24 mg, 84%); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.65 (d, J = 7.4 Hz, 2H), 7.56-7.48 (m, 3H), 2.73 (s, 3H).



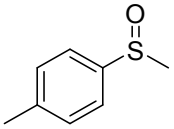
(ethylsulfinyl)benzene (7b). [8]

Colorless oil (25 mg, 80%); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.60 (d, J = 7.2 Hz, 2H), 7.54-7.47 (m, 3H), 2.93-2.85 (m, 1H), 2.80-2.70 (m, 1H), 1.19 (t, J = 7.5 Hz, 3H).



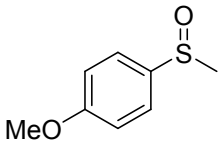
(cyclopropylsulfinyl)benzene (7c). [8]

Colorless oil (29 mg, 86%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70-7.64 (m, 2H), 7.56-7.48 (m, 3H), 2.29-2.24 m, 1H), 1.29 – 1.22 (m, 1H), 1.07-0.90 (m, 3H).



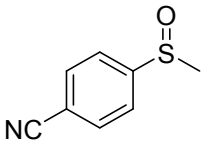
1-methyl-4-(methylsulfinyl)benzene (7d). [8]

White solid (26 mg, 84%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, J = 8.4 Hz, 2H), 7.33 (d, J = 8.0 Hz, 2H), 2.70 (s, 3H), 2.41 (s, 3H).



1-methoxy-4-(methylsulfinyl)benzene (7e). [8]

White solid (30 mg, 86%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, J = 8.8 Hz, 2H), 7.1 (d, J = 8.8 Hz, 2H), 3.83 (s, 3H), 2.68 (s, 3H).

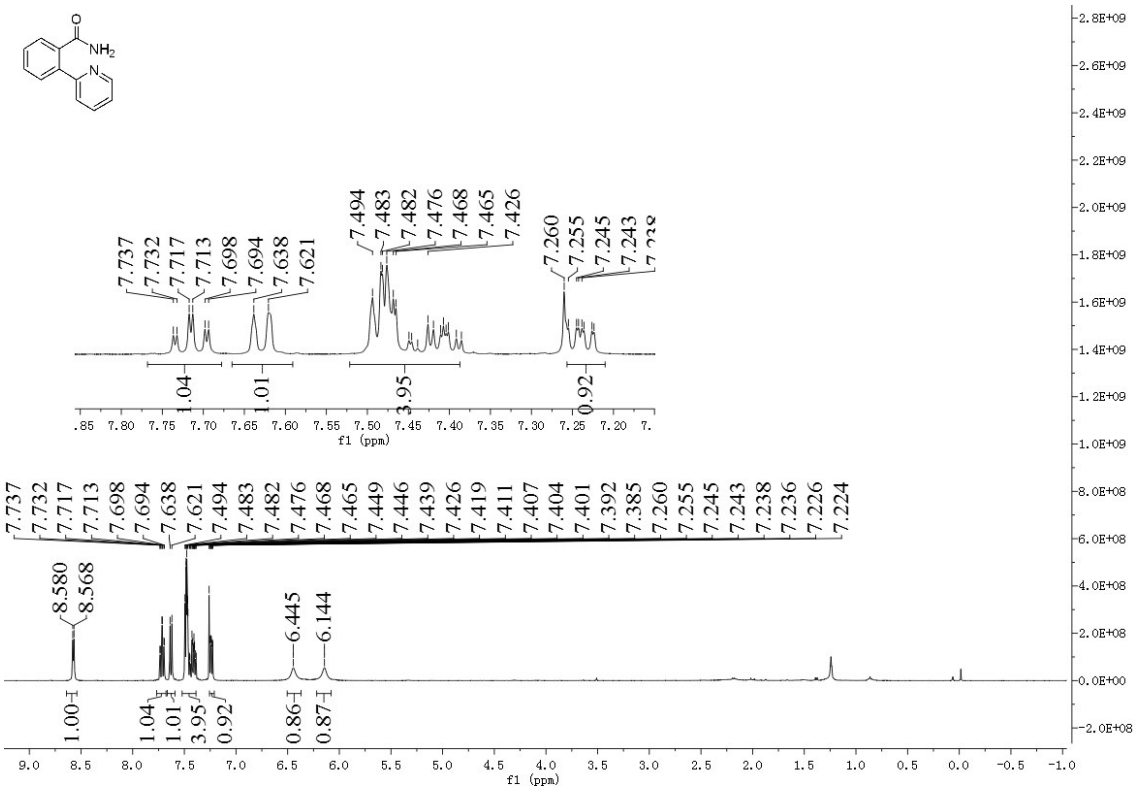


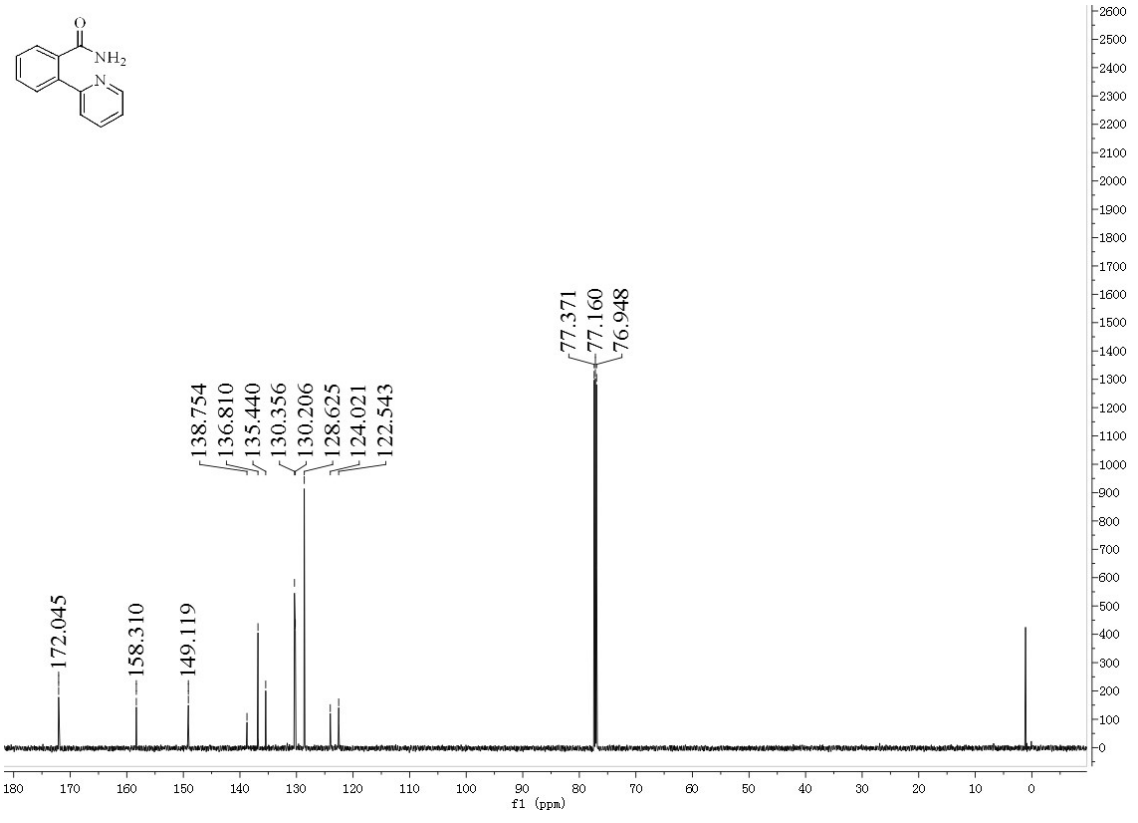
4-(methylsulfinyl)benzonitrile (7f). [8]

White solid (13 mg, 40%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, J = 8.4 Hz, 2H), 7.77 (d, J = 8.4 Hz, 2H), 2.76 (s, 3H).

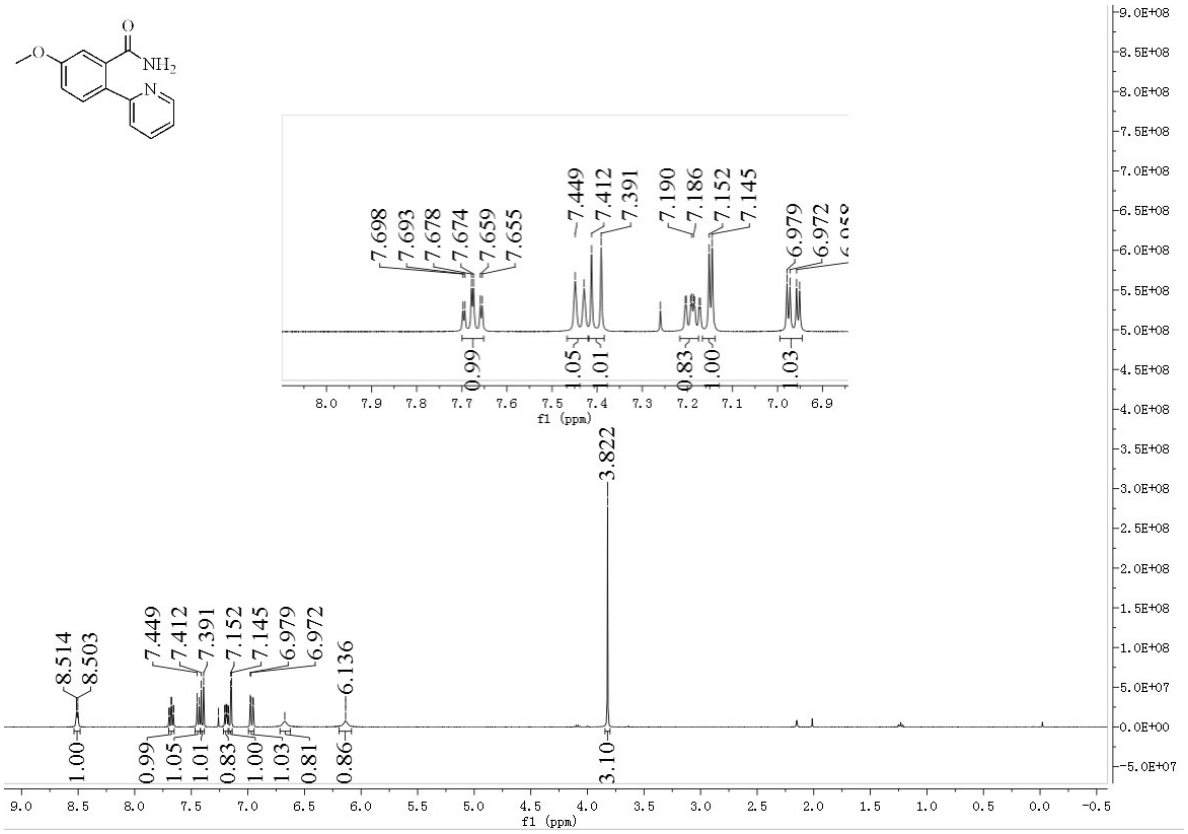
II. NMR spectra copies of synthesized compounds

Compound **1a**





Compound **1b**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7.674
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7.655
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7.412
7.391
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7.152
7.145
6.979
6.972
f1 (ppm)
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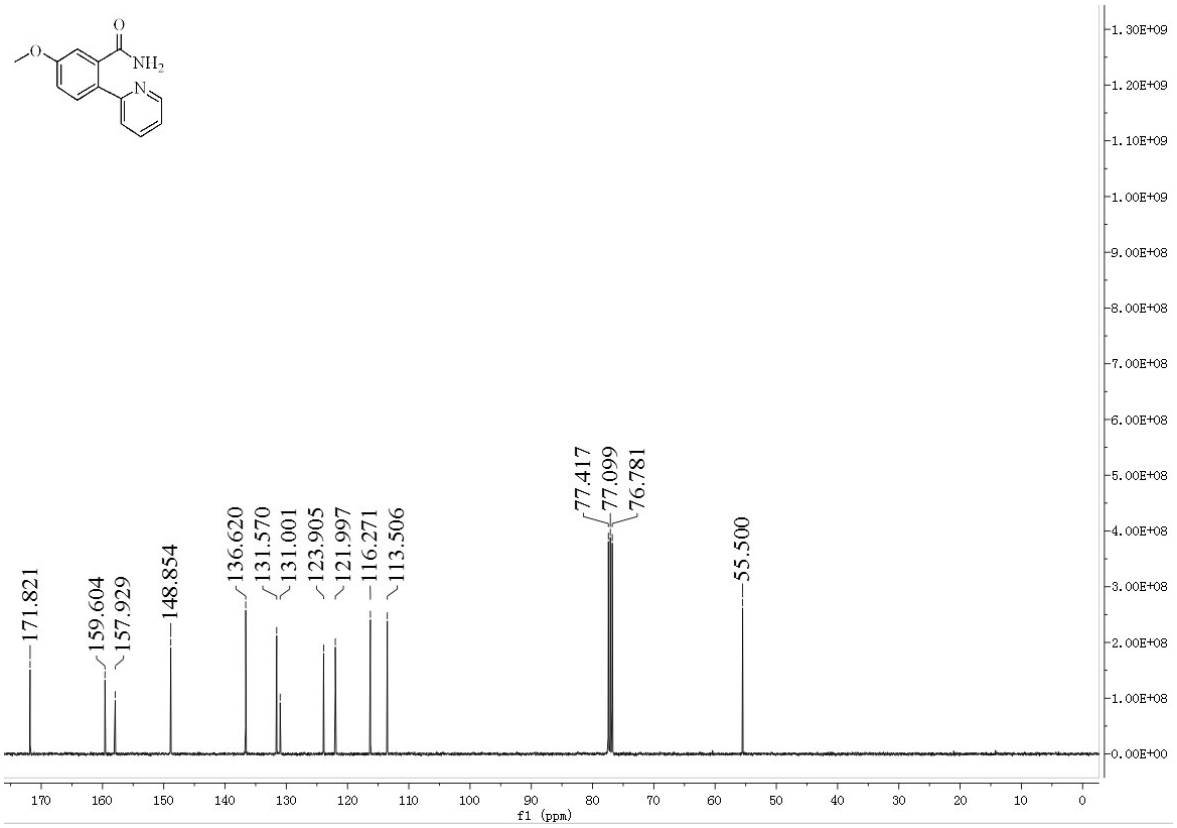
7.412
7.391
7.152
7.145
6.979
6.972
6.136
3.822
f1 (ppm)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159.604
157.929
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136.620
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131.001
123.905
121.997
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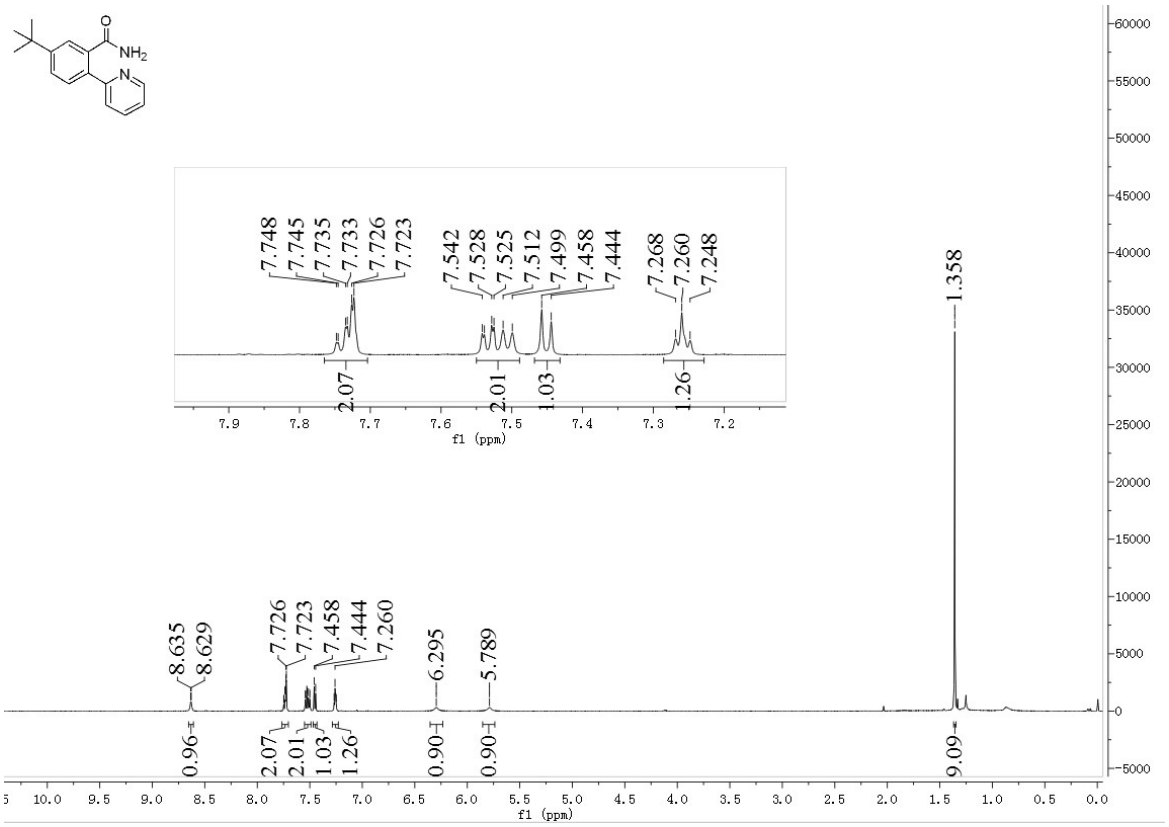
113.506
77.417
77.099
76.781
55.500
f1 (ppm)

Compound **1c**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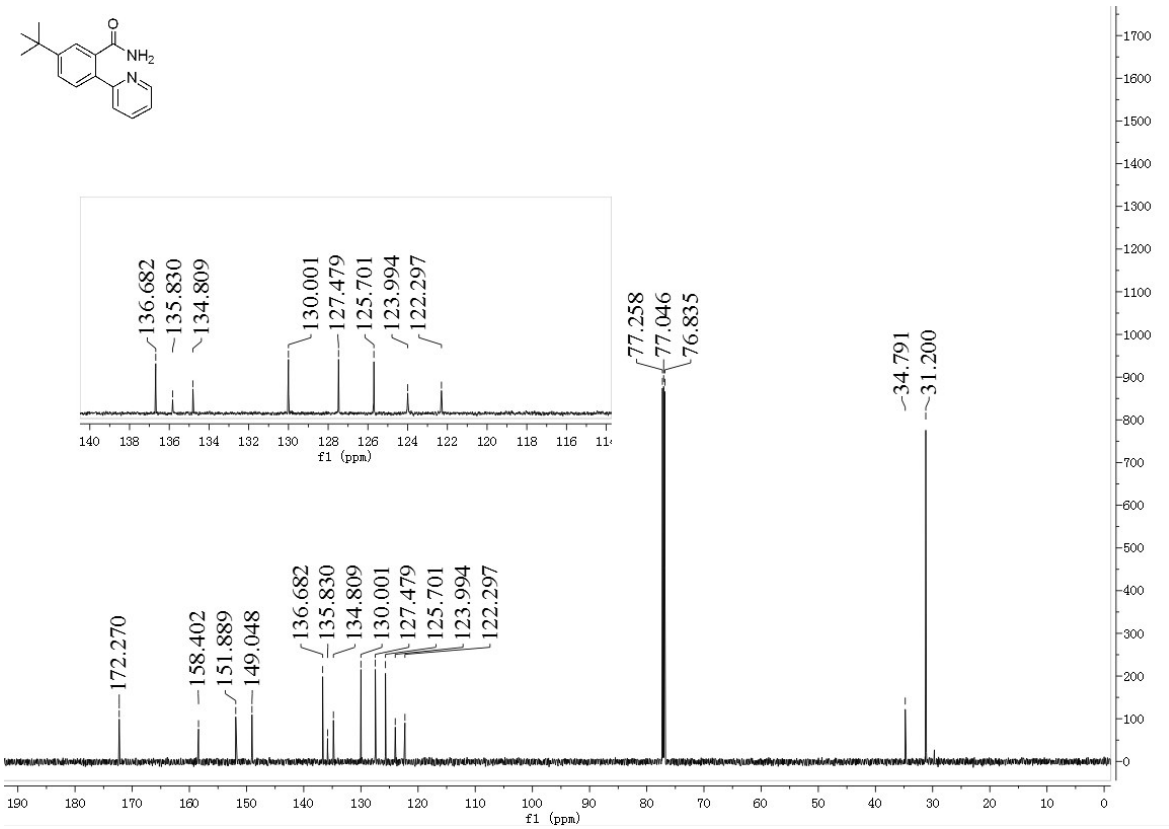
7.735
7.733
7.726
7.723
7.542
7.528
7.525
7.512
7.499
7.458
7.444
7.268
7.260
7.248
2.07
2.01
1.03
1.26
f1 (ppm)
1.358
8.635
8.629
7.726
7.723
7.458
7.444
7.260
6.295
5.789
0.96
2.07
2.01
1.03
1.26
0.90
0.90
9.09
f1 (ppm)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O
N
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134.809
130.001
127.479
125.701
123.994
122.297
f1 (ppm)
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77.046
76.835
34.791
31.200
172.270
158.402
151.889
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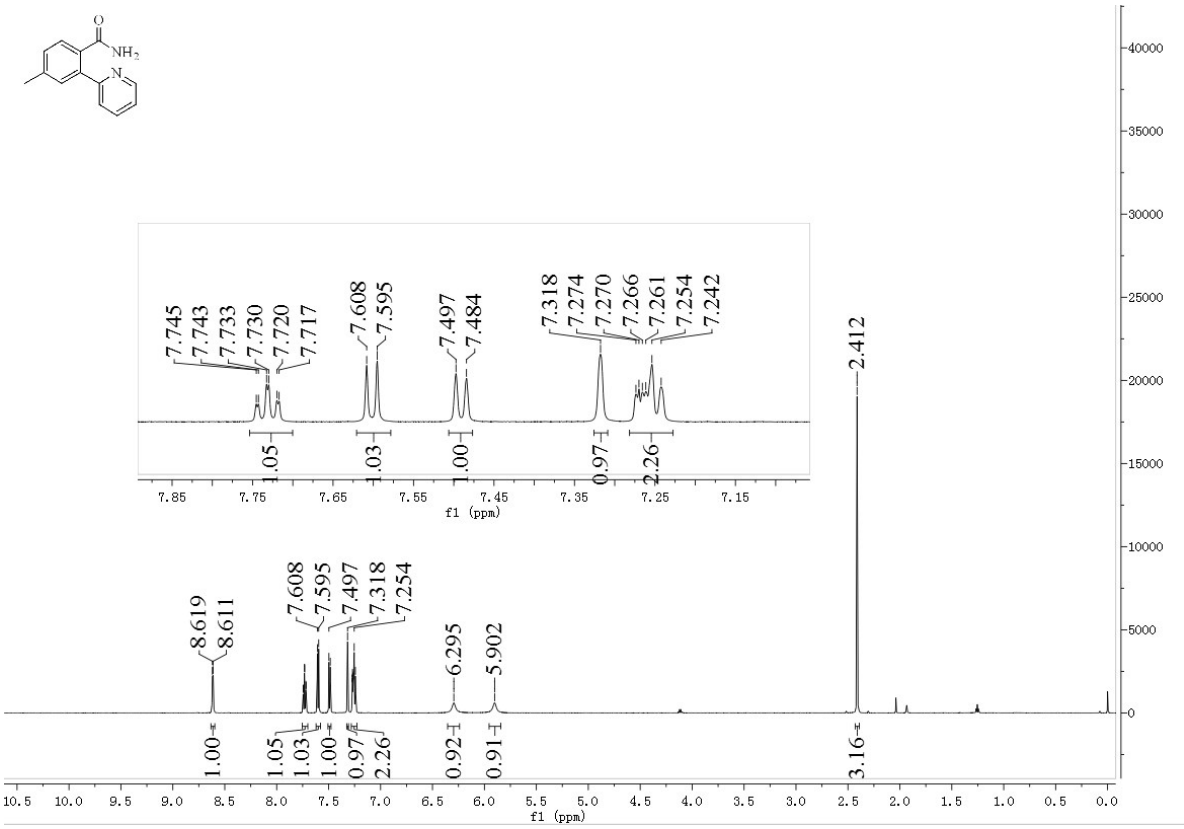
135.830
134.809
130.001
127.479
125.701
123.994
122.297
f1 (ppm)

Compound **1d**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7.733
7.730
7.720
7.717
7.608
7.595
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7.484
7.318
7.274
7.270
7.266
7.261
7.254
7.242
2.412
1.05
1.03
1.00
0.97
2.26
f1 (ppm)
8.619
8.611
7.608
7.595
7.497
7.318
7.254
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5.902
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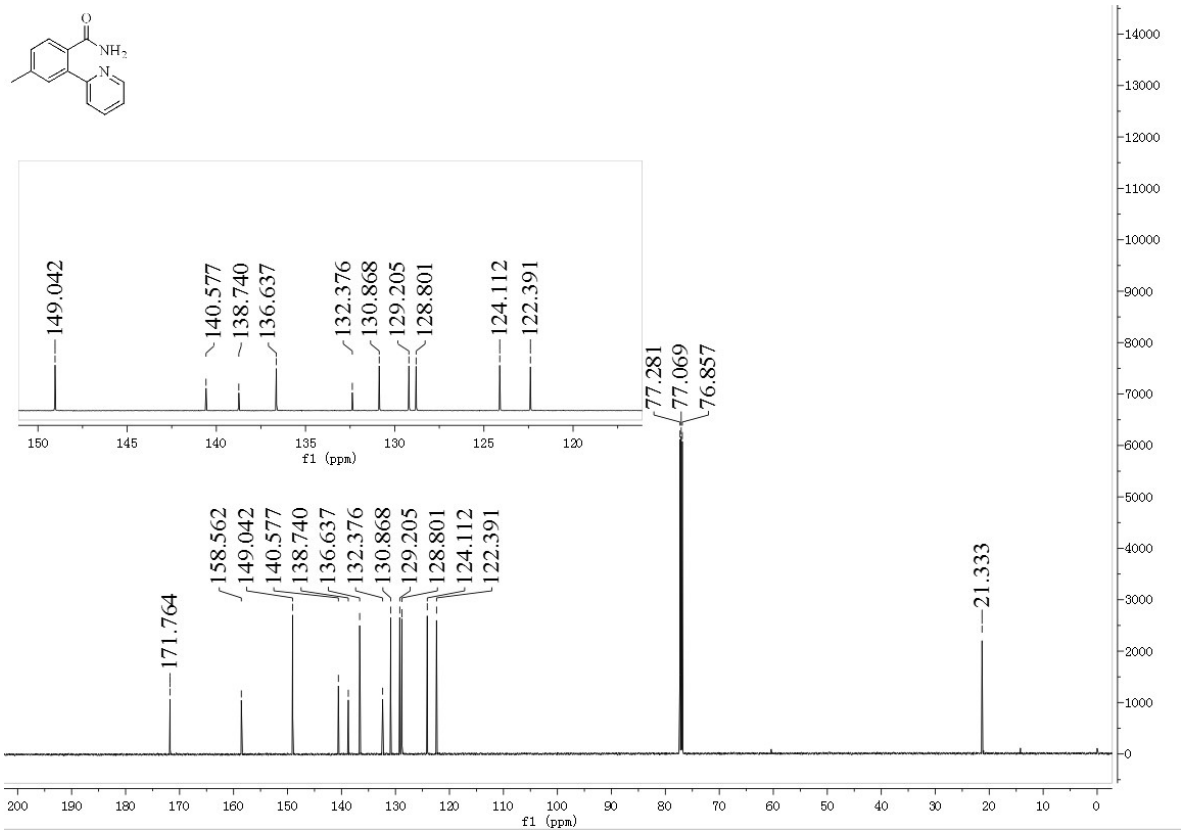
1.05
1.03
1.00
0.97
2.26
0.92
0.91
3.16
f1 (ppm)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136.637
132.376
130.868
129.205
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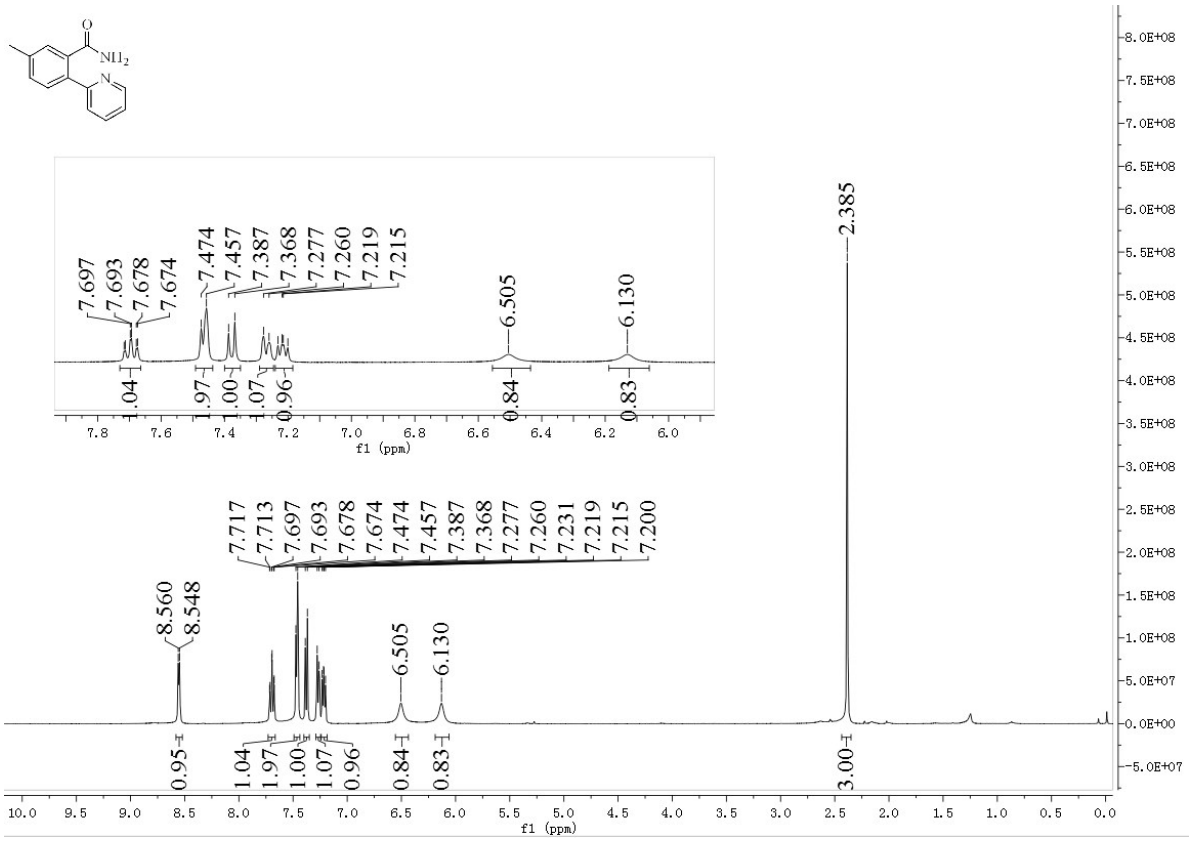
77.069
76.857
f1 (ppm)
171.764
158.562
149.042
140.577
138.740
136.637
132.376
130.868
129.205
128.801
124.112
122.391
21.333
f1 (ppm)

Compound **1e**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7.693
7.678
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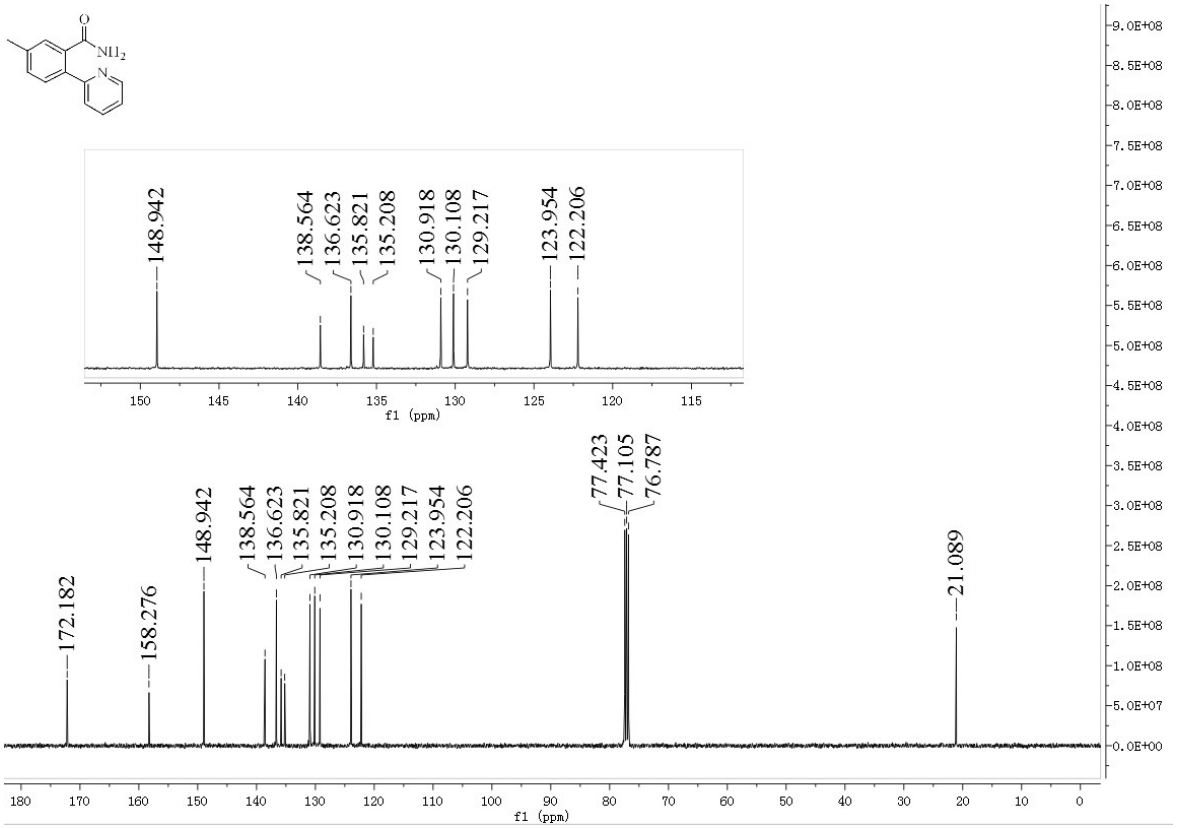
7.474
7.457
7.387
7.368
7.277
7.260
7.219
7.215
6.505
6.130
2.385
8.560
8.548
7.717
7.713
7.231
7.200
0.95
1.04
1.97
1.00
1.07
0.96
0.84
0.83
3.00
f1 (ppm)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136.623
135.821
135.208
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130.108
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123.954
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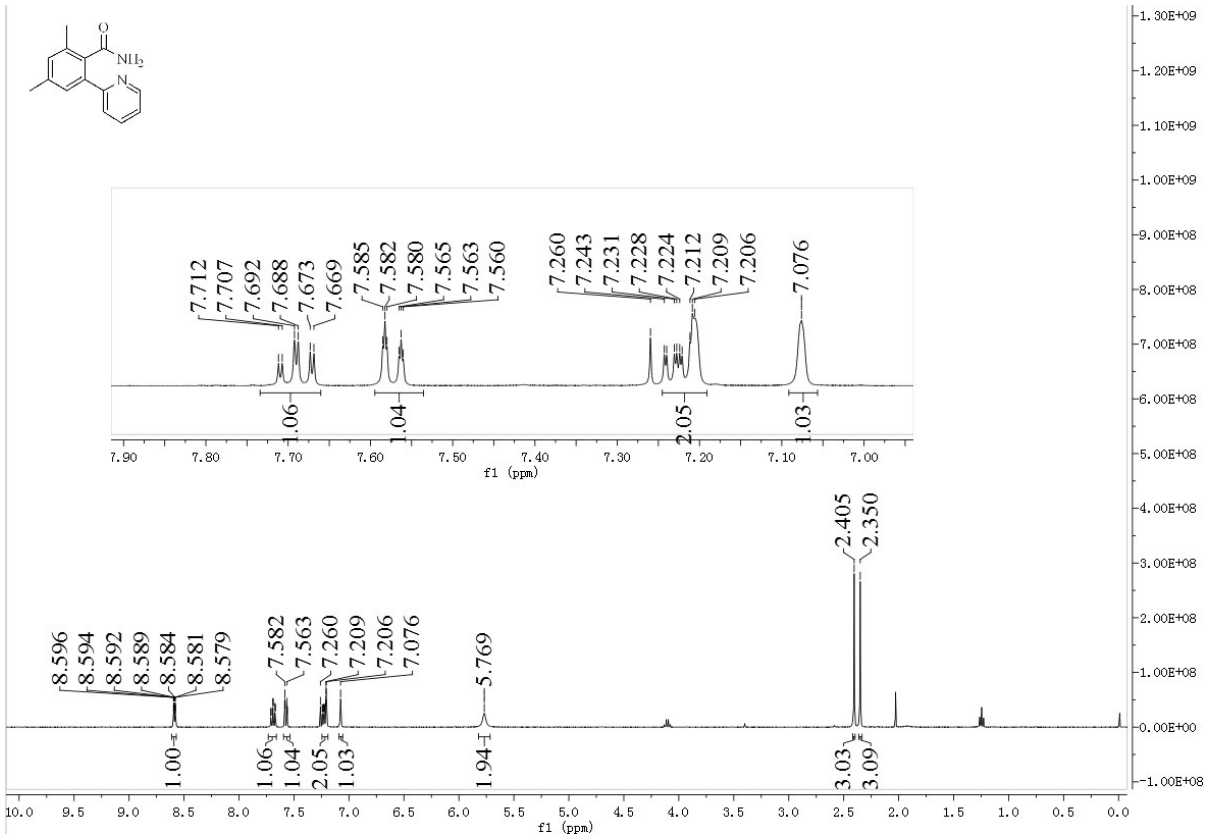
77.105
76.787
172.182
158.276
21.089
f1 (ppm)

Compound **1f**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7.707
7.692
7.688
7.673
7.669
7.585
7.582
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7.565
7.563
7.560
7.260
7.243
7.231
7.228
7.224
7.212
7.209
7.206
7.076
1.06
1.04
2.05
1.03
f1 (ppm)
2.405
2.350
8.596
8.594
8.592
8.589
8.584
8.581
8.579
7.582
7.563
7.260
7.209
7.206
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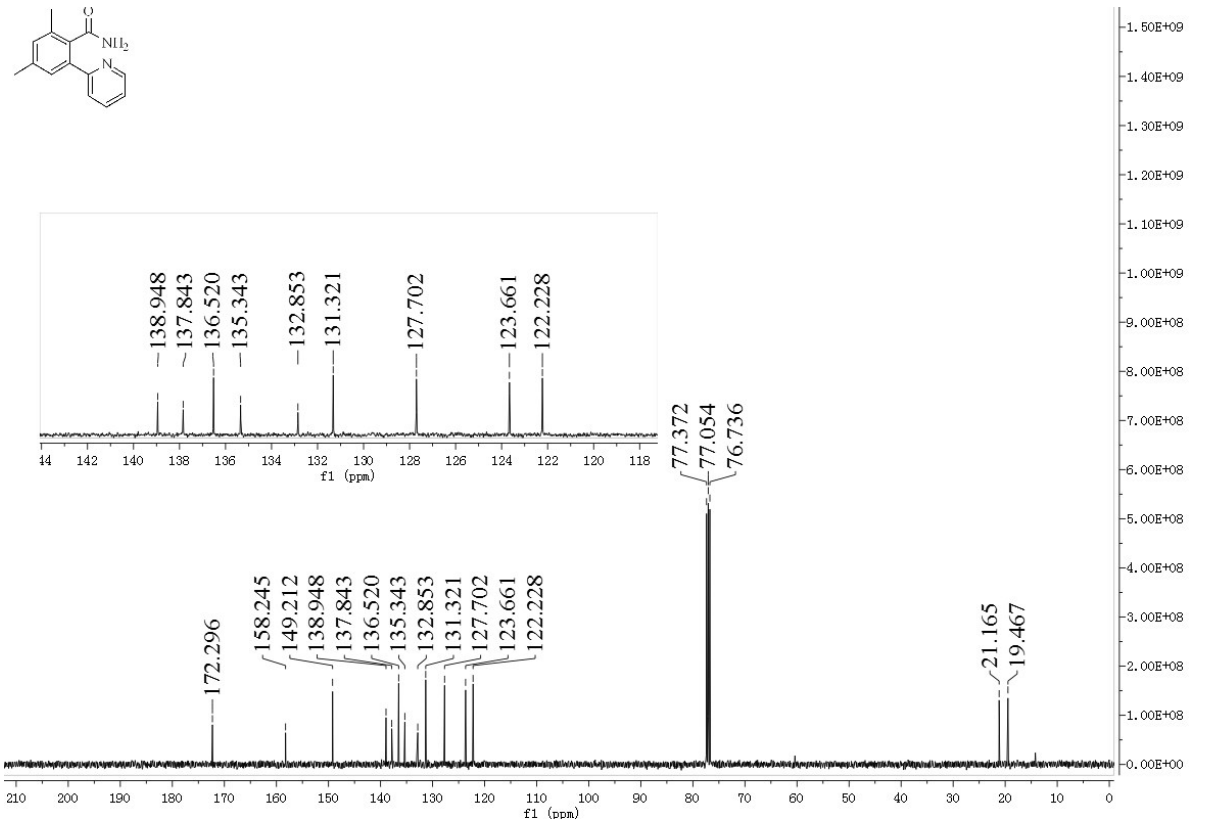
1.04
2.05
1.03
1.94
3.03
3.09
f1 (ppm)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135.343
132.853
131.321
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123.661
122.228
f1 (ppm)
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77.054
76.736
172.296
158.245
149.212
138.948
137.843
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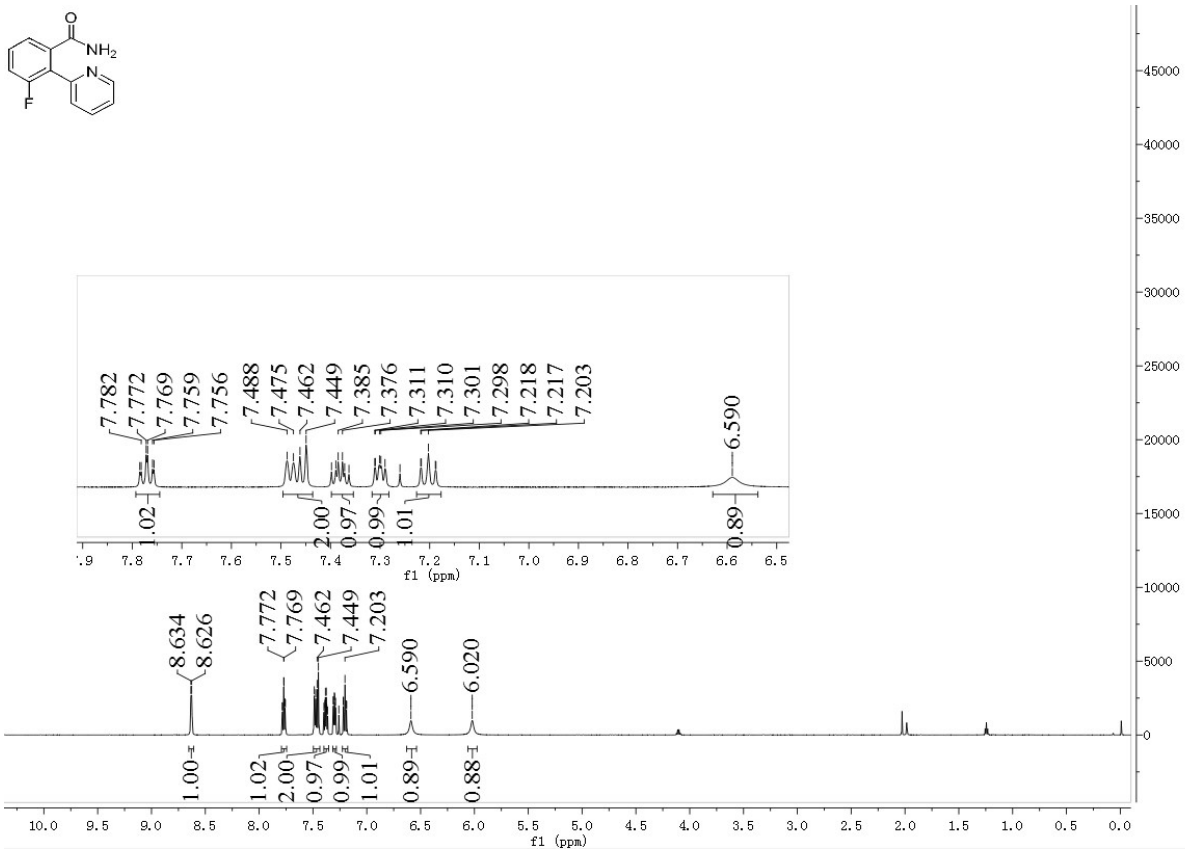
132.853
131.321
127.702
123.661
122.228
21.165
19.467
f1 (ppm)

Compound **1g**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7.488
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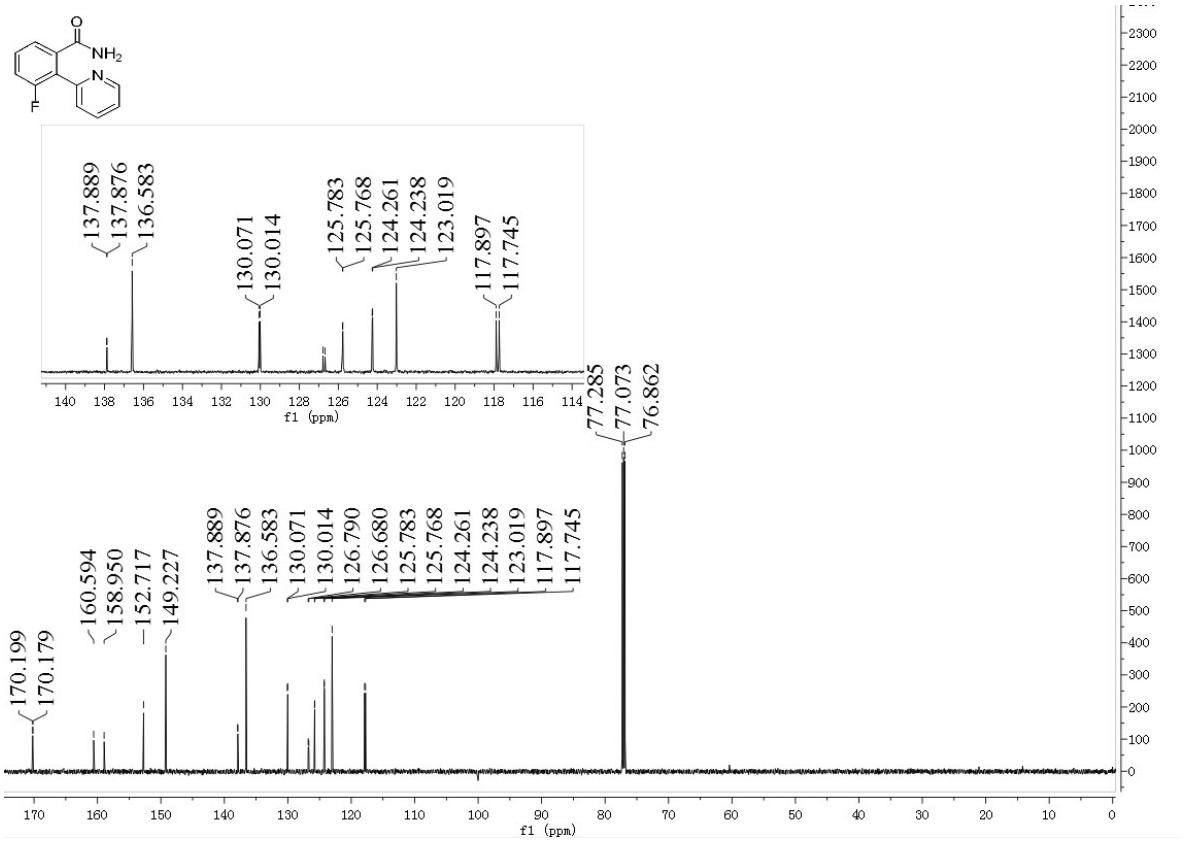
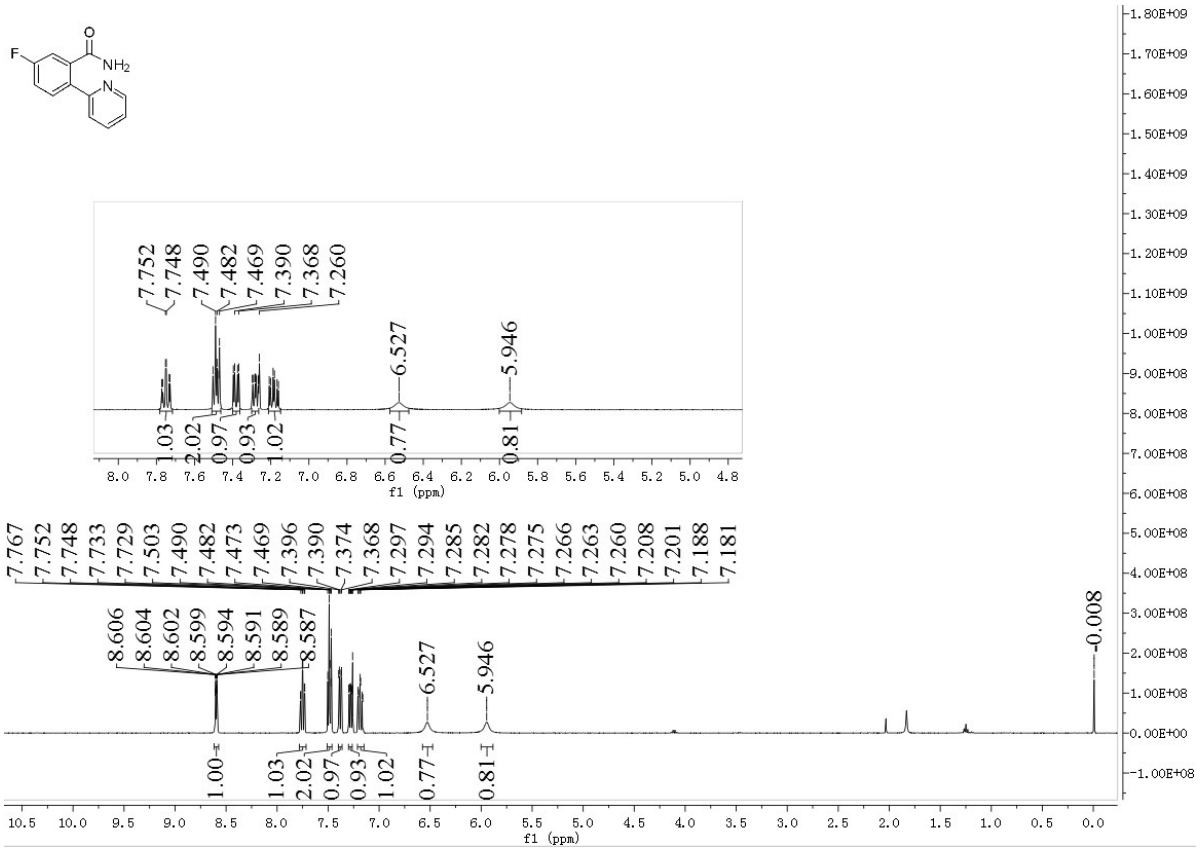
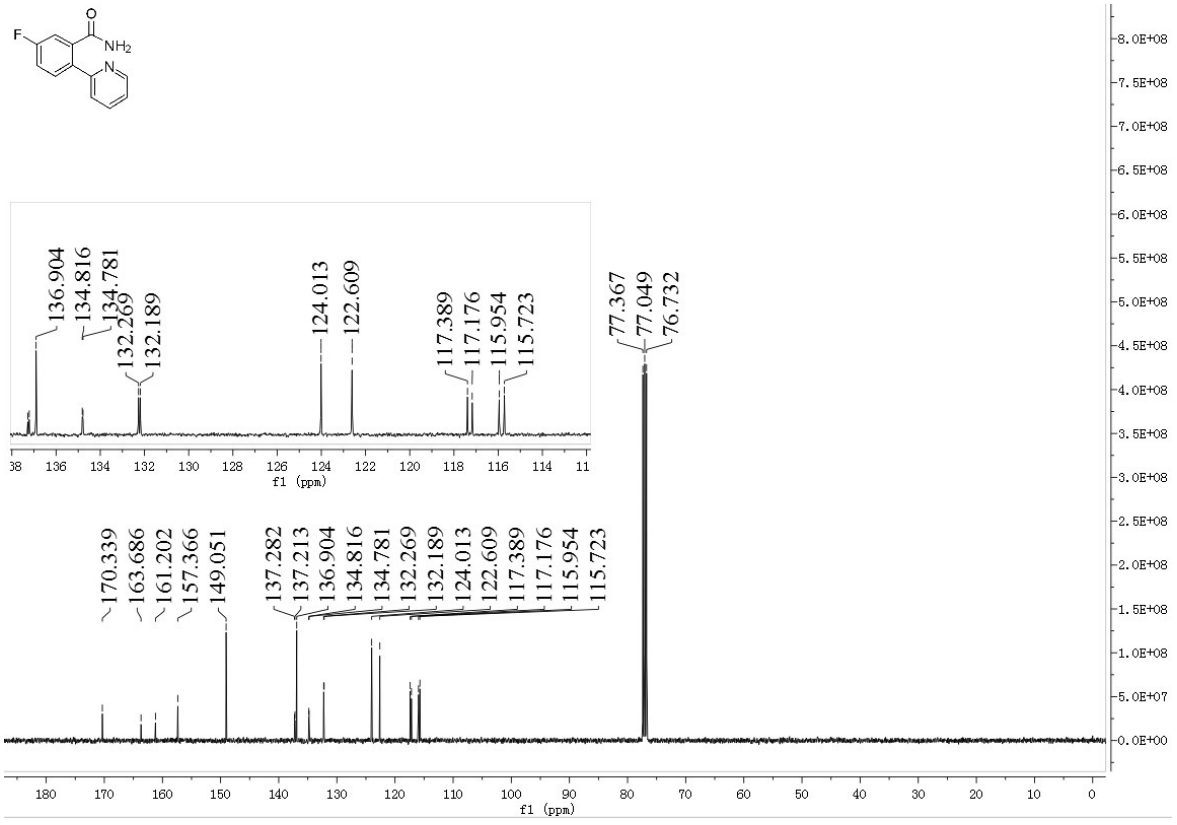
7.462
7.449
7.385
7.376
7.311
7.310
7.301
7.298
7.218
7.217
7.203
6.590
1.02
2.00
0.97
0.99
1.01
0.89
f1 (ppm)
8.634
8.626
7.772
7.769
7.462
7.449
7.203
6.590
6.020
1.00
1.02
2.00
0.97
0.99
1.01
0.89
0.88
f1 (ppm)

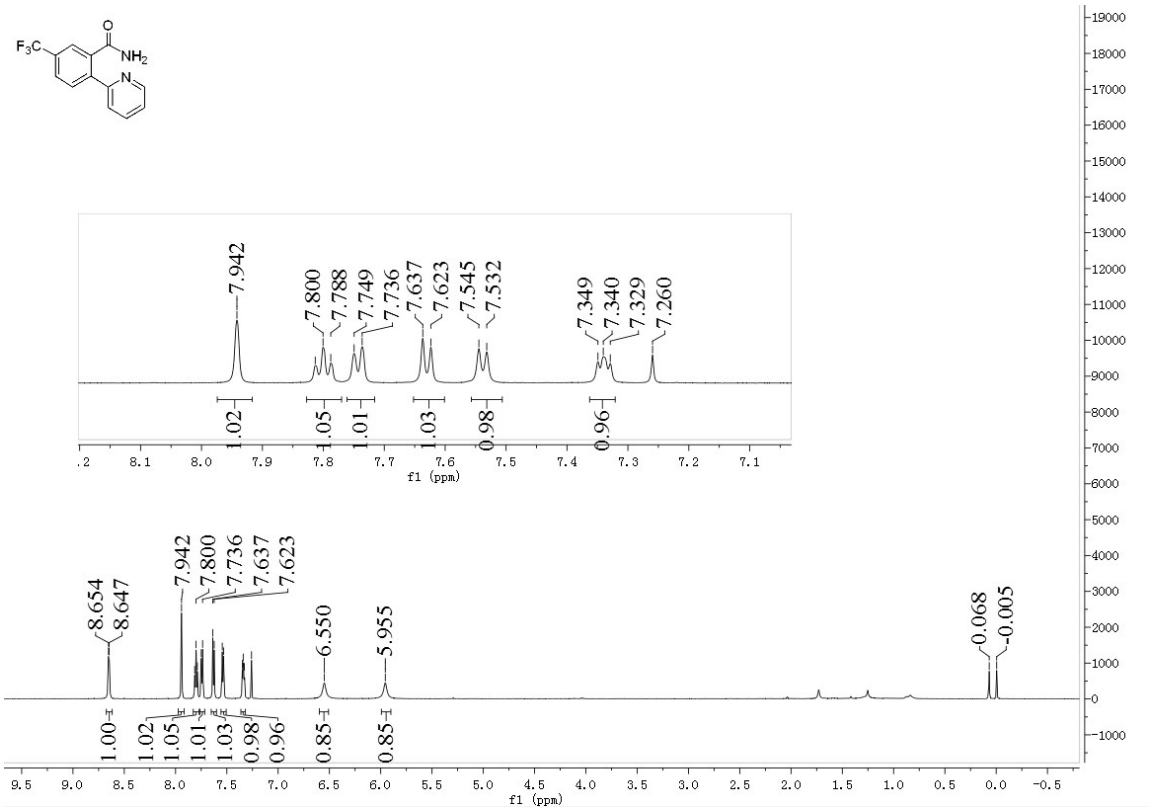

137.889
137.876
136.583
130.071
130.014
125.783
125.768
124.261
124.238
123.019
117.897
117.745
f1 (ppm)
77.285
77.073
76.862
170.199
170.179
160.594
158.950
152.717
149.227
137.889
137.876
136.583
130.071
130.014
126.790
126.680
125.783
125.768
124.261
124.238
123.019
117.897
117.745
f1 (ppm)

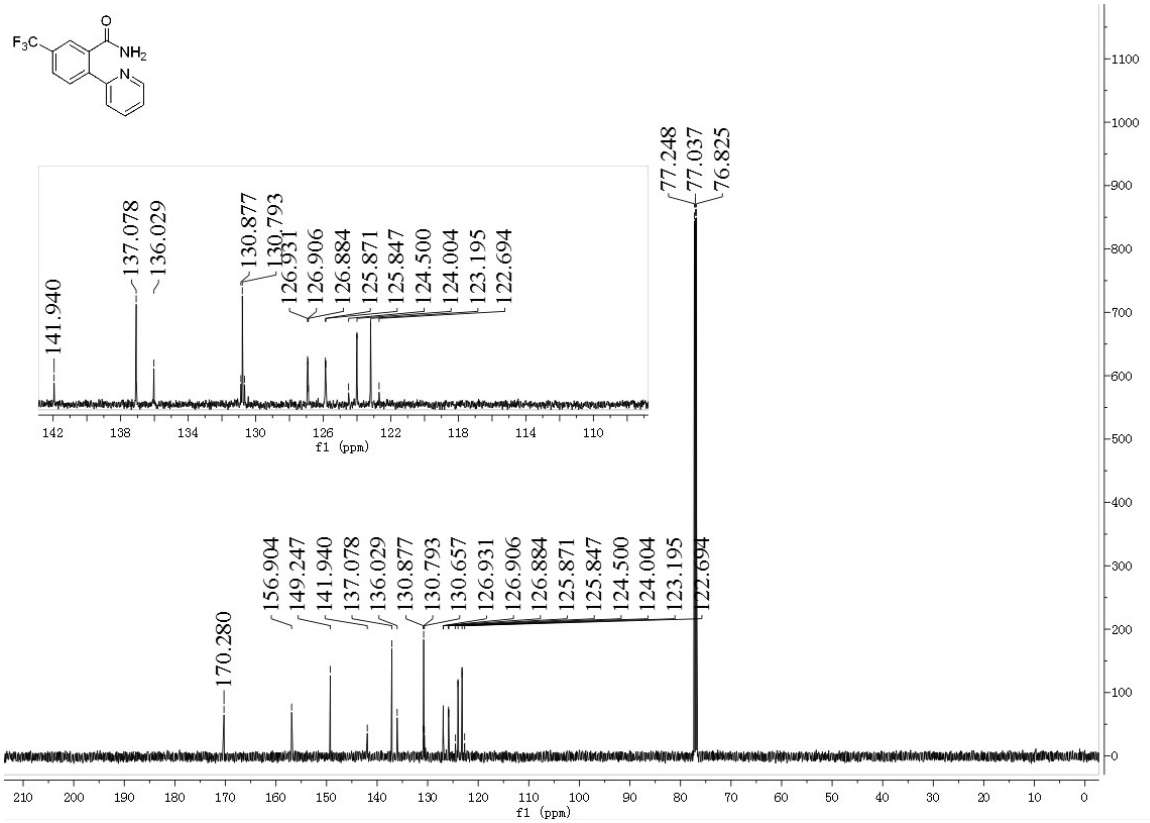
Compound **1h**


F
O
NH2
N
7.752
7.748
7.490
7.482
7.469
7.390
7.368
7.260
6.527
5.946
1.03
2.02
0.97
0.93
1.02
0.77
0.81
f1 (ppm)
7.767
7.752
7.748
7.733
7.729
7.503
7.490
7.482
7.473
7.469
7.396
7.390
7.374
7.368
7.297
7.294
7.285
7.282
7.278
7.275
7.266
7.263
7.260
7.208
7.201
7.188
7.181
8.606
8.604
8.602
8.599
8.594
8.591
8.589
8.587
0.008
6.527
5.946
1.00
1.03
2.02
0.97
0.93
1.02
0.77
0.81
f1 (ppm)

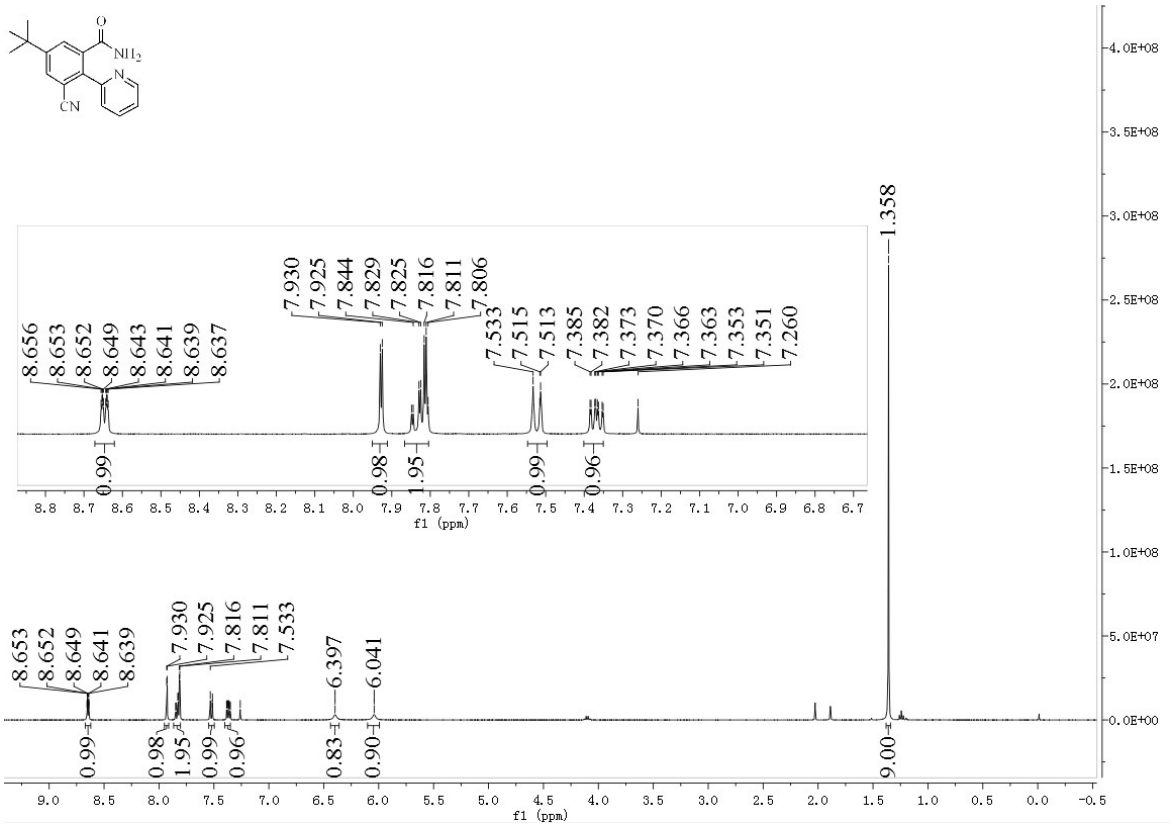

F
O
NH2
N
136.904
134.816
134.781
132.269
132.189
124.013
122.609
117.389
117.176
115.954
115.723
77.367
77.049
76.732
f1 (ppm)
170.339
163.686
161.202
157.366
149.051
137.282
137.213
136.904
134.816
134.781
132.269
132.189
124.013
122.609
117.389
117.176
115.954
115.723
f1 (ppm)

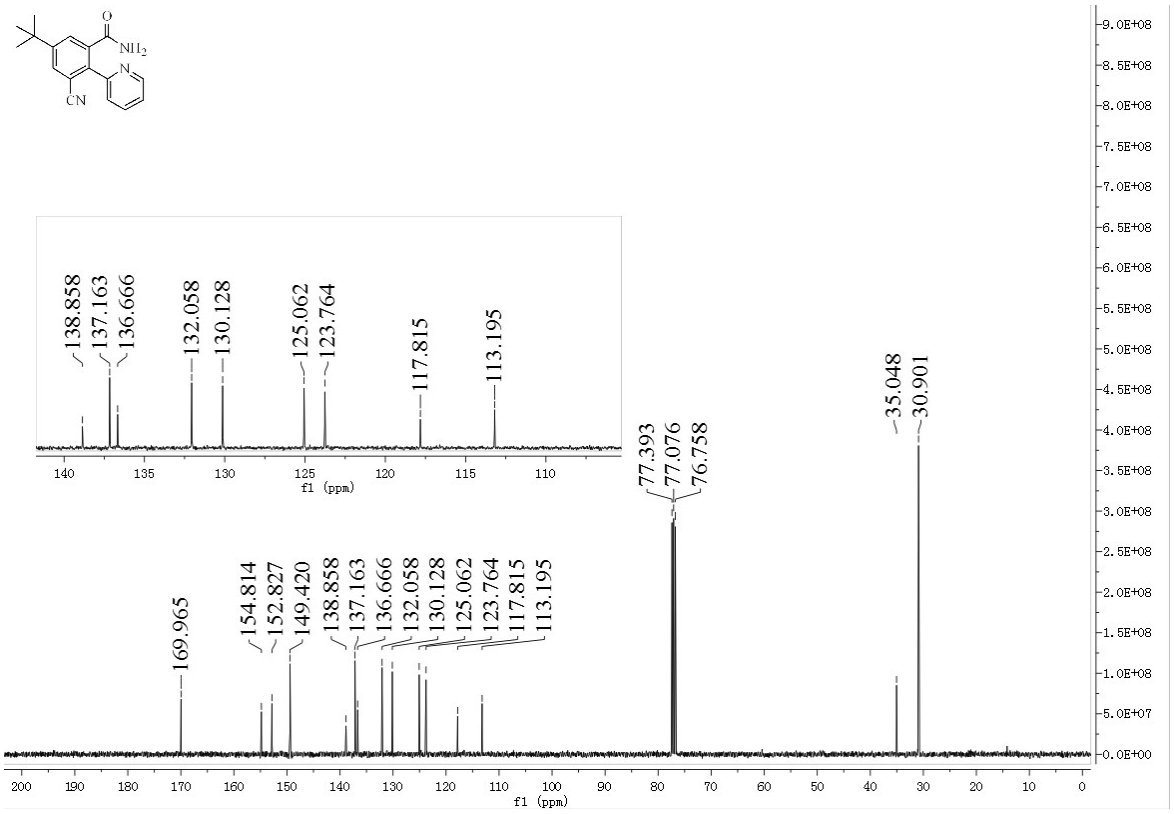
Compound **1i**


F3C
O
NH2
N
7.942
7.800
7.788
7.749
7.736
7.637
7.623
7.545
7.532
7.349
7.340
7.329
7.260
1.02
1.05
1.01
1.03
0.98
0.96
f1 (ppm)
8.654
8.647
7.942
7.800
7.736
7.637
7.623
6.550
5.955
0.068
-0.005
1.00
1.02
1.05
1.01
1.03
0.98
0.96
0.85
0.85
f1 (ppm)

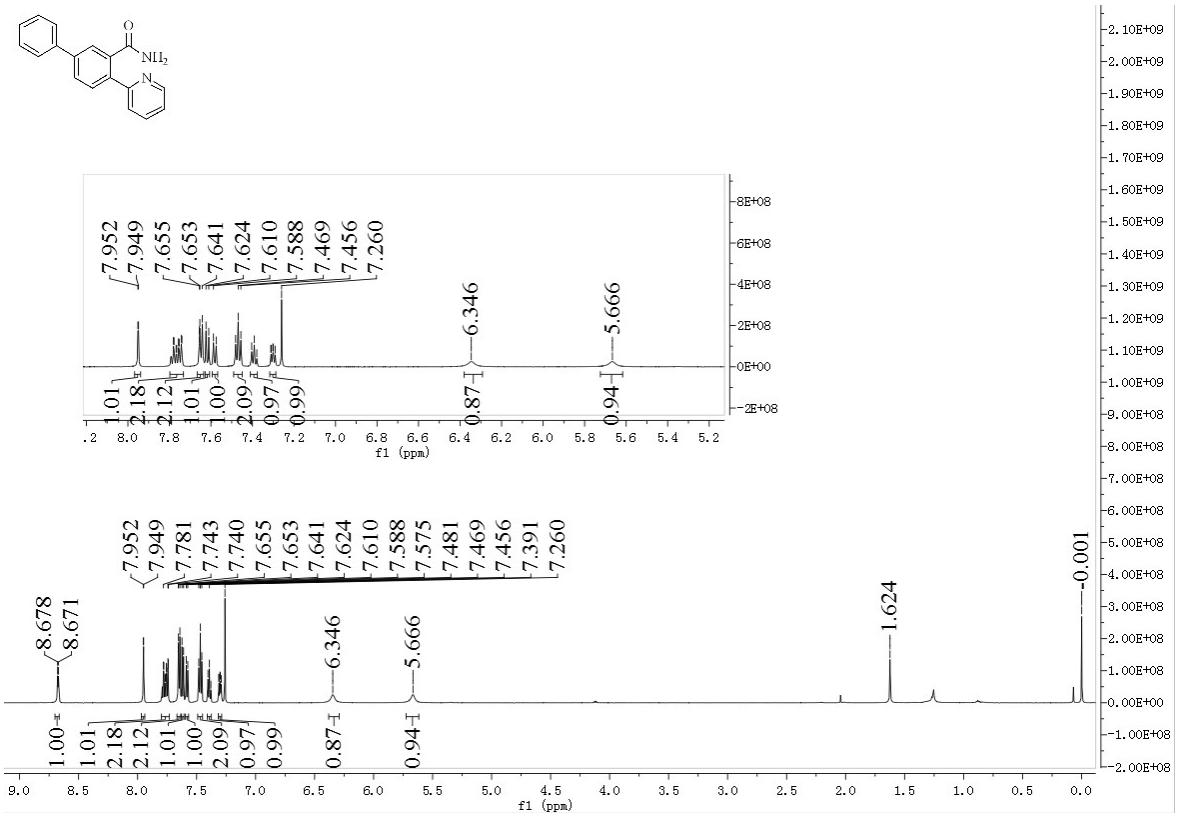

F3C
O
NH2
N
141.940
137.078
136.029
130.877
130.793
126.931
126.906
126.884
125.871
125.847
124.500
124.004
123.195
122.694
77.248
77.037
76.825
f1 (ppm)
170.280
156.904
149.247
141.940
137.078
136.029
130.877
130.793
130.657
126.931
126.906
126.884
125.871
125.847
124.500
124.004
123.195
122.694
f1 (ppm)

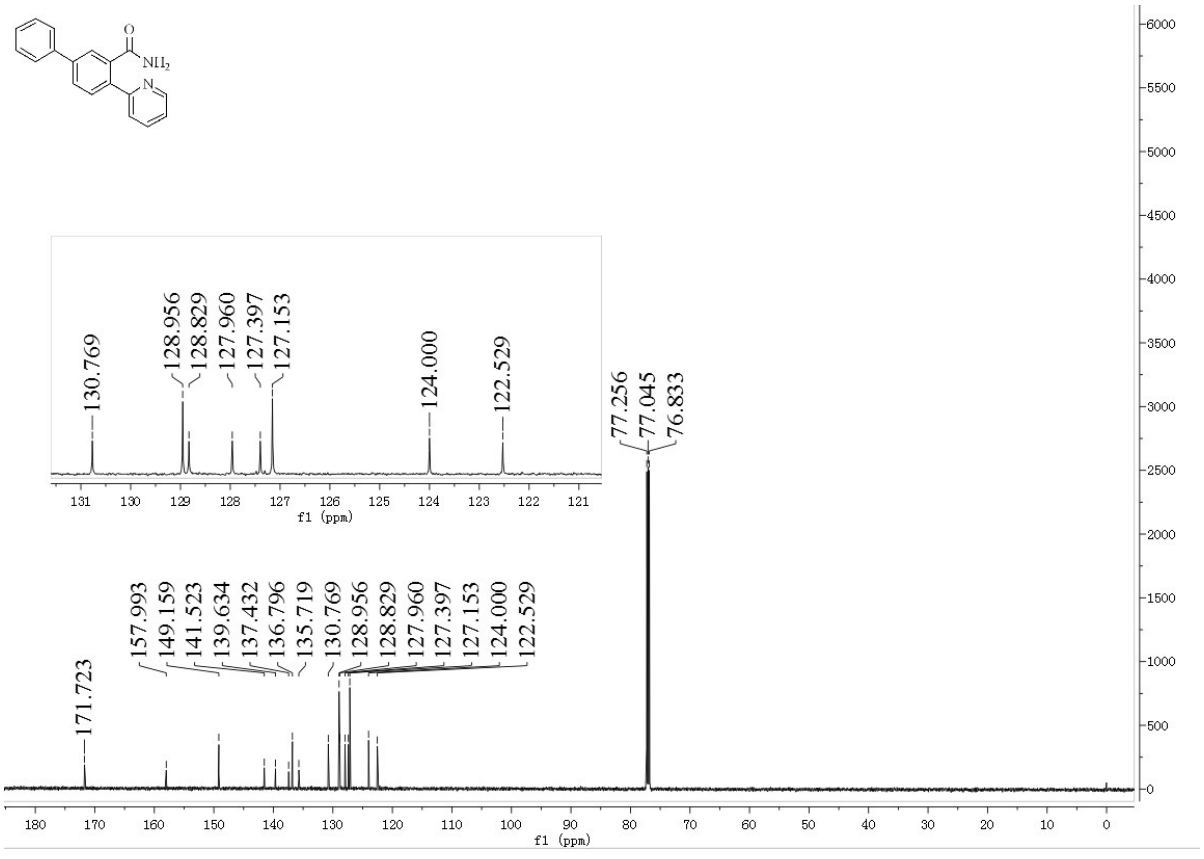
Compound **1j**


8.656
8.653
8.652
8.649
8.643
8.641
8.639
8.637
7.930
7.925
7.844
7.829
7.825
7.816
7.811
7.806
7.533
7.515
7.513
7.385
7.382
7.373
7.370
7.366
7.363
7.353
7.351
7.260
1.358
0.99
0.98
1.95
0.99
0.96
9.00
0.83
0.90
6.397
6.041
f1 (ppm)

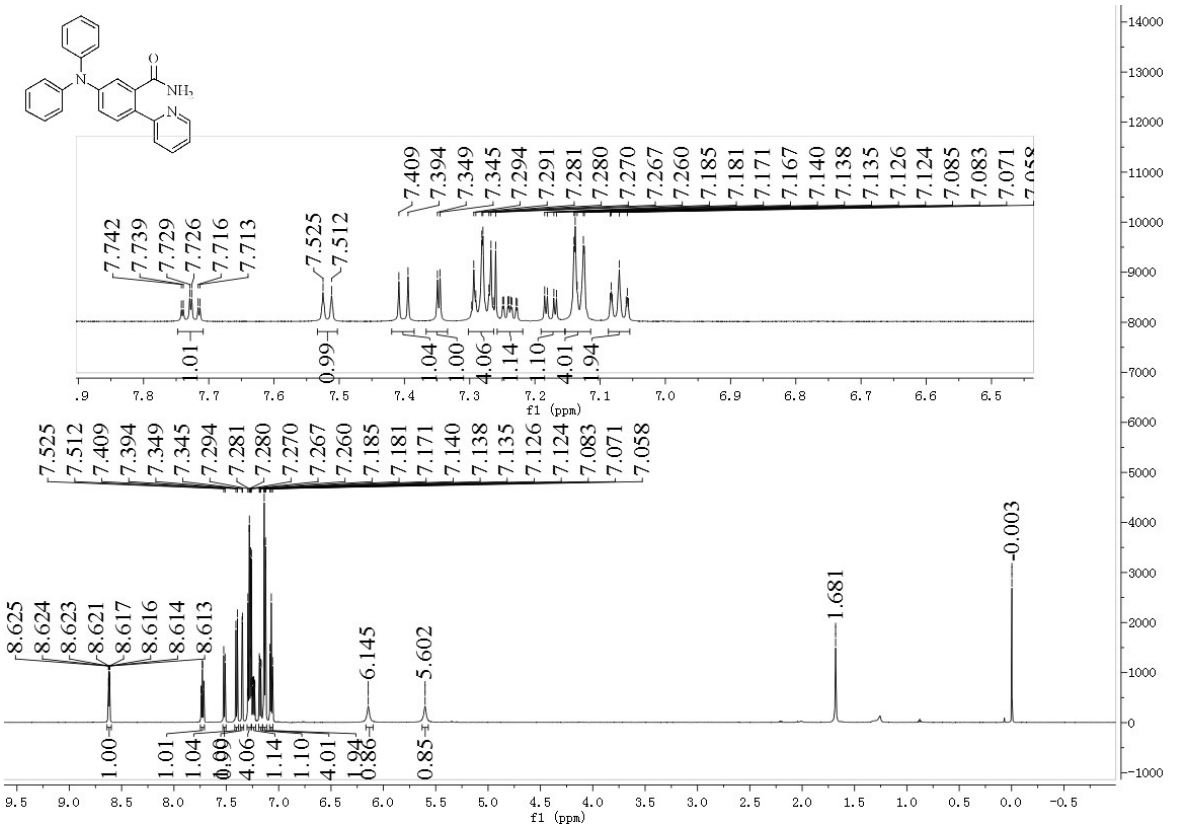

138.858
137.163
136.666
132.058
130.128
125.062
123.764
117.815
113.195
77.393
77.076
76.758
35.048
30.901
169.965
154.814
152.827
149.420
f1 (ppm)

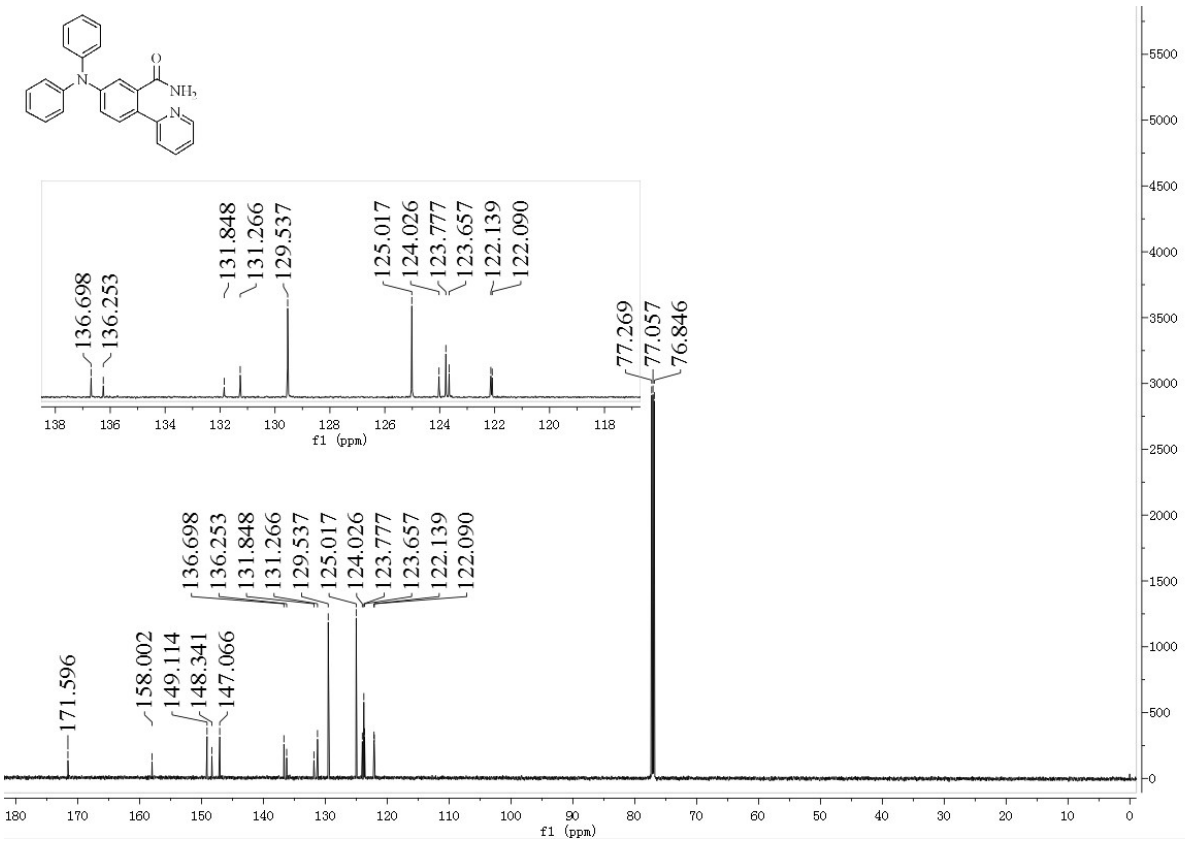
Compound **1k**


7.952
7.949
7.655
7.653
7.641
7.624
7.610
7.588
7.469
7.456
7.260
6.346
5.666
1.01
2.18
2.12
1.01
1.00
2.09
0.97
0.99
0.87
0.94
f1 (ppm)
8.678
8.671
7.952
7.949
7.781
7.743
7.740
7.655
7.653
7.641
7.624
7.610
7.588
7.575
7.481
7.469
7.456
7.391
7.260
6.346
5.666
1.624
0.001
1.00
1.01
2.18
2.12
1.01
1.00
2.09
0.97
0.99
0.87
0.94
f1 (ppm)

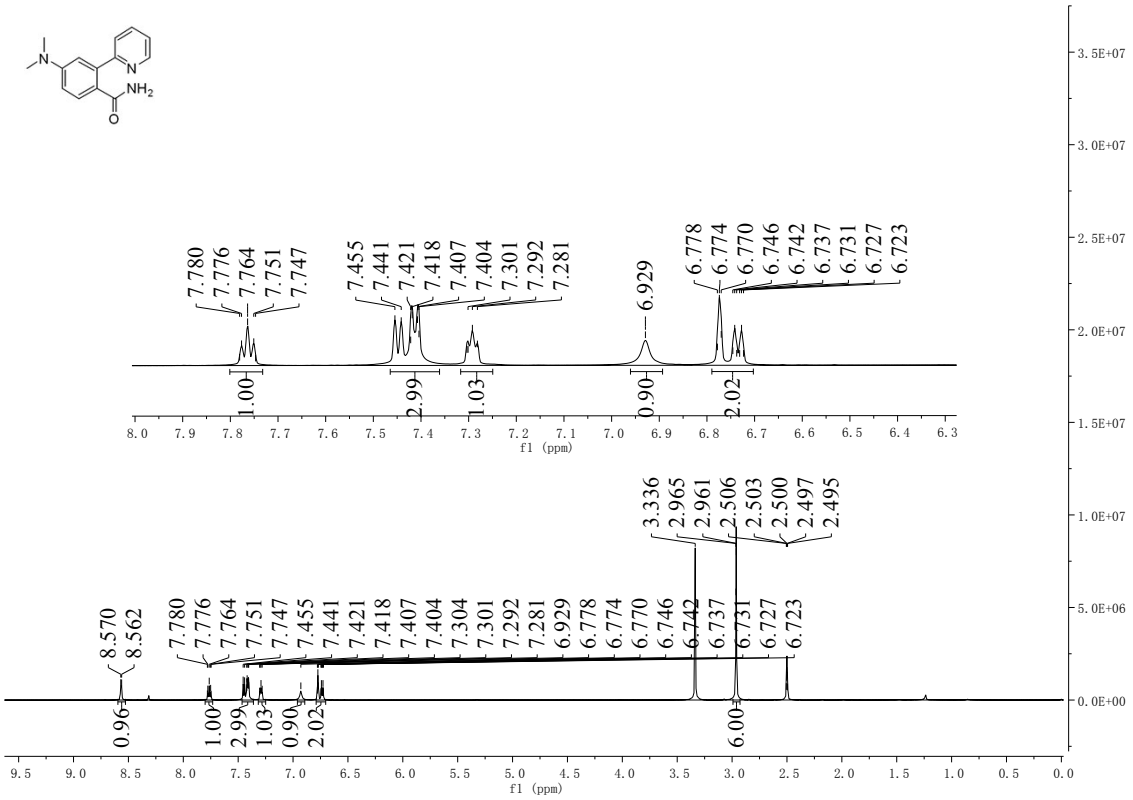

130.769
128.956
128.829
127.960
127.397
127.153
124.000
122.529
77.256
77.045
76.833
f1 (ppm)
171.723
157.993
149.159
141.523
139.634
137.432
136.796
135.719
130.769
128.956
128.829
127.960
127.397
127.153
124.000
122.529
f1 (ppm)

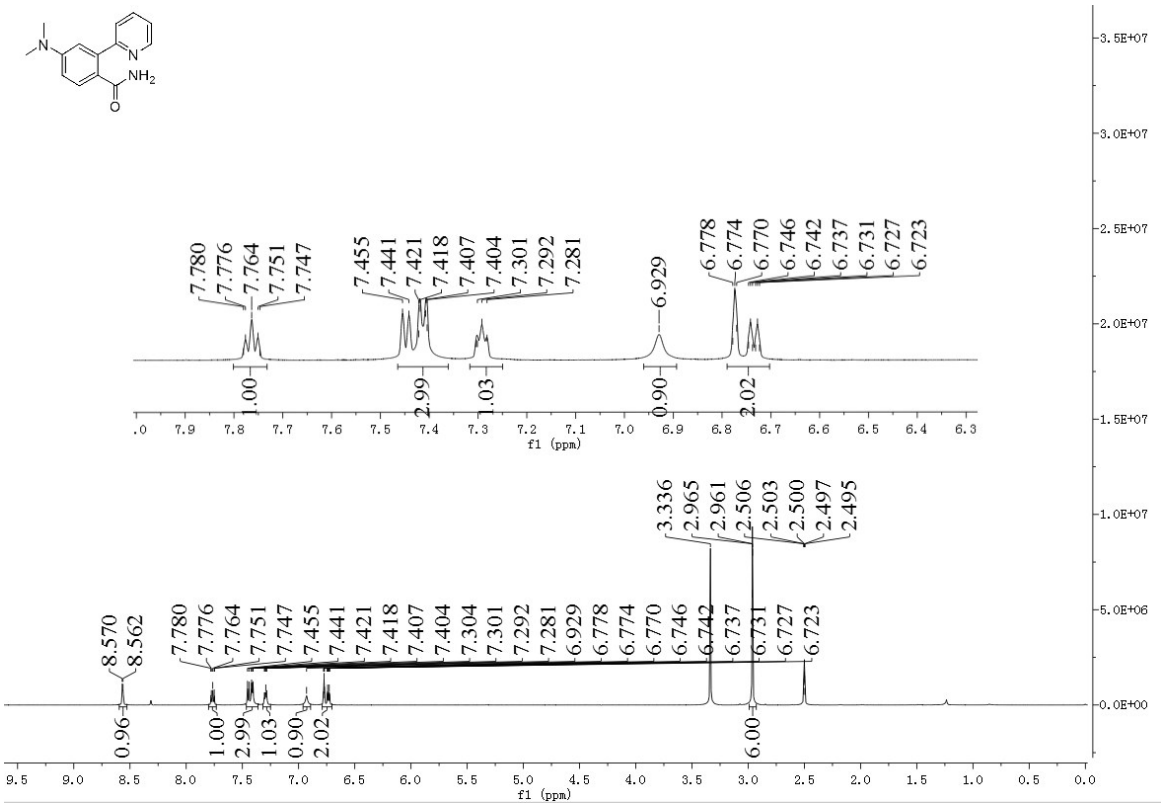
Compound **1l**


7.742
7.739
7.729
7.726
7.716
7.713
7.525
7.512
7.409
7.394
7.349
7.345
7.294
7.291
7.281
7.280
7.270
7.267
7.260
7.185
7.181
7.171
7.167
7.140
7.138
7.135
7.126
7.124
7.085
7.083
7.071
8.625
8.624
8.623
8.621
8.617
8.616
8.614
8.613
6.145
5.602
1.681
-0.003
f1 (ppm)

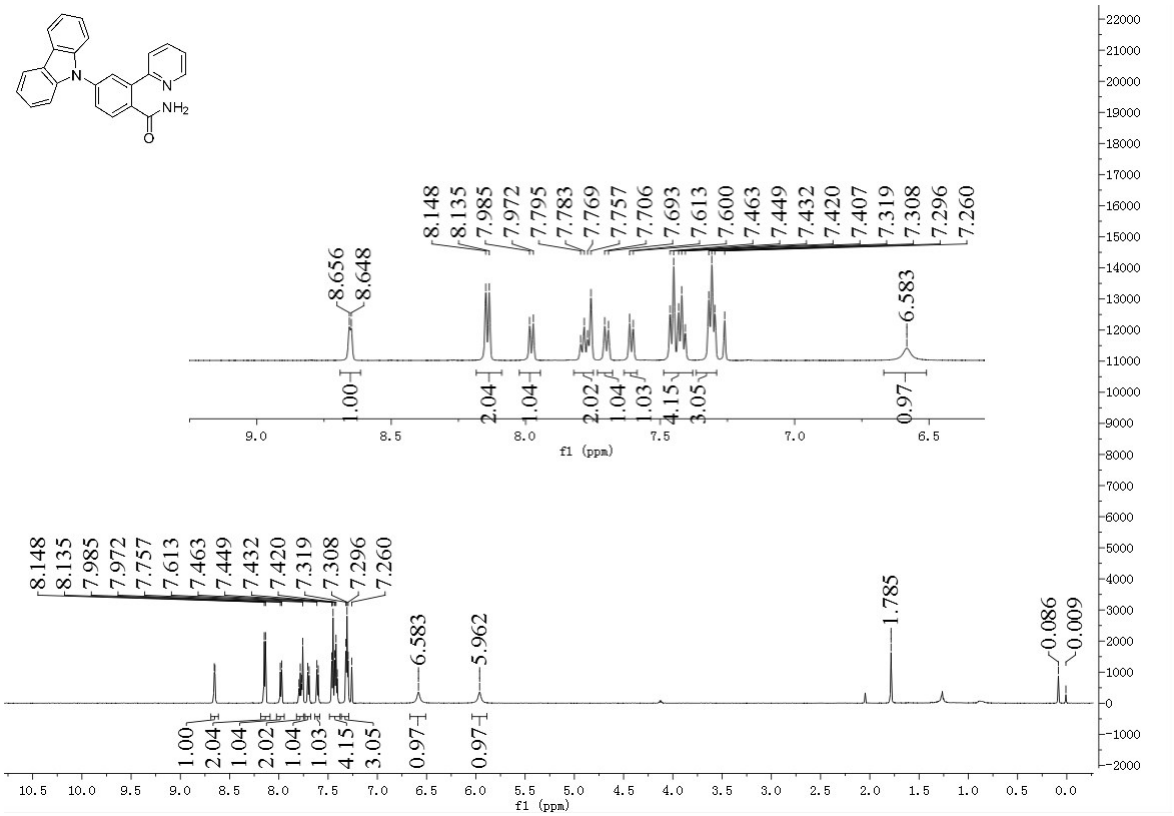

136.698
136.253
131.848
131.266
129.537
125.017
124.026
123.777
123.657
122.139
122.090
77.269
77.057
76.846
171.596
158.002
149.114
148.341
147.066
f1 (ppm)

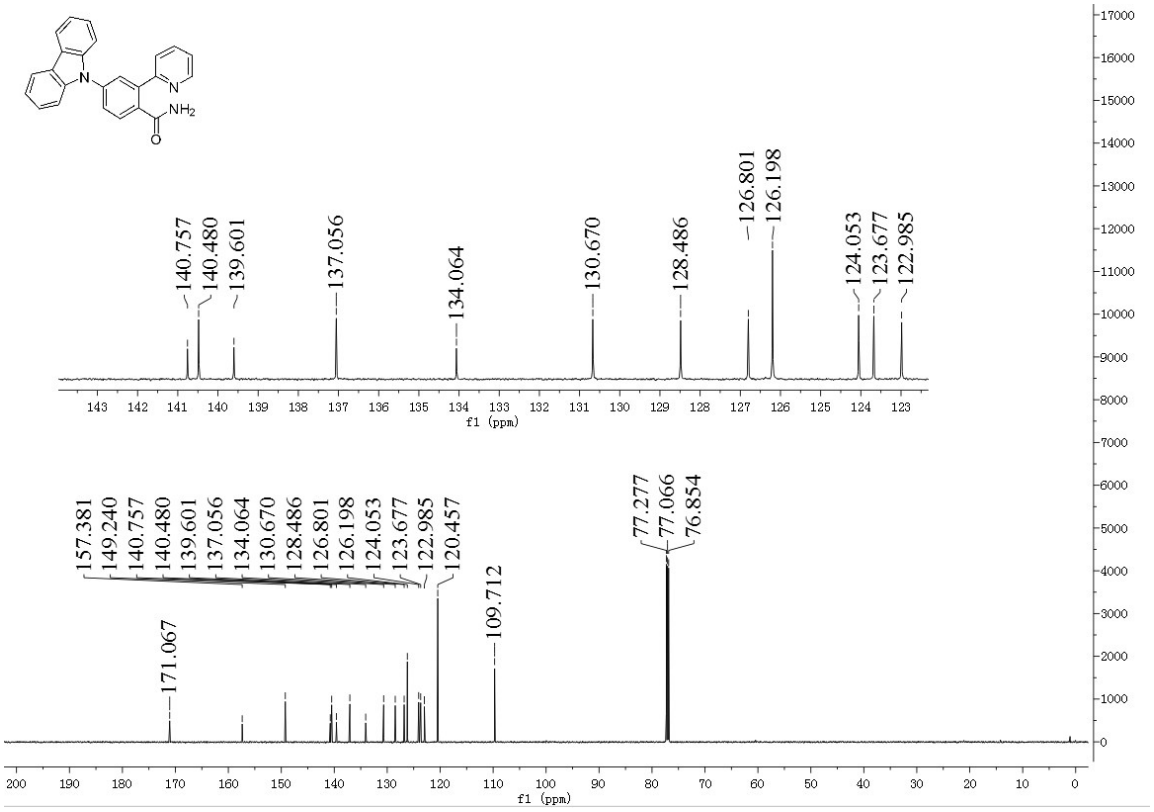
Compound **1m**


7.780
7.776
7.764
7.751
7.747
7.455
7.441
7.421
7.418
7.407
7.404
7.301
7.292
7.281
6.929
6.778
6.774
6.770
6.746
6.742
6.737
6.731
6.727
6.723
1.00
2.99
1.03
0.90
2.02
f1 (ppm)
3.336
2.965
2.961
2.506
2.503
2.500
2.497
2.495
8.570
8.562
0.96
6.00

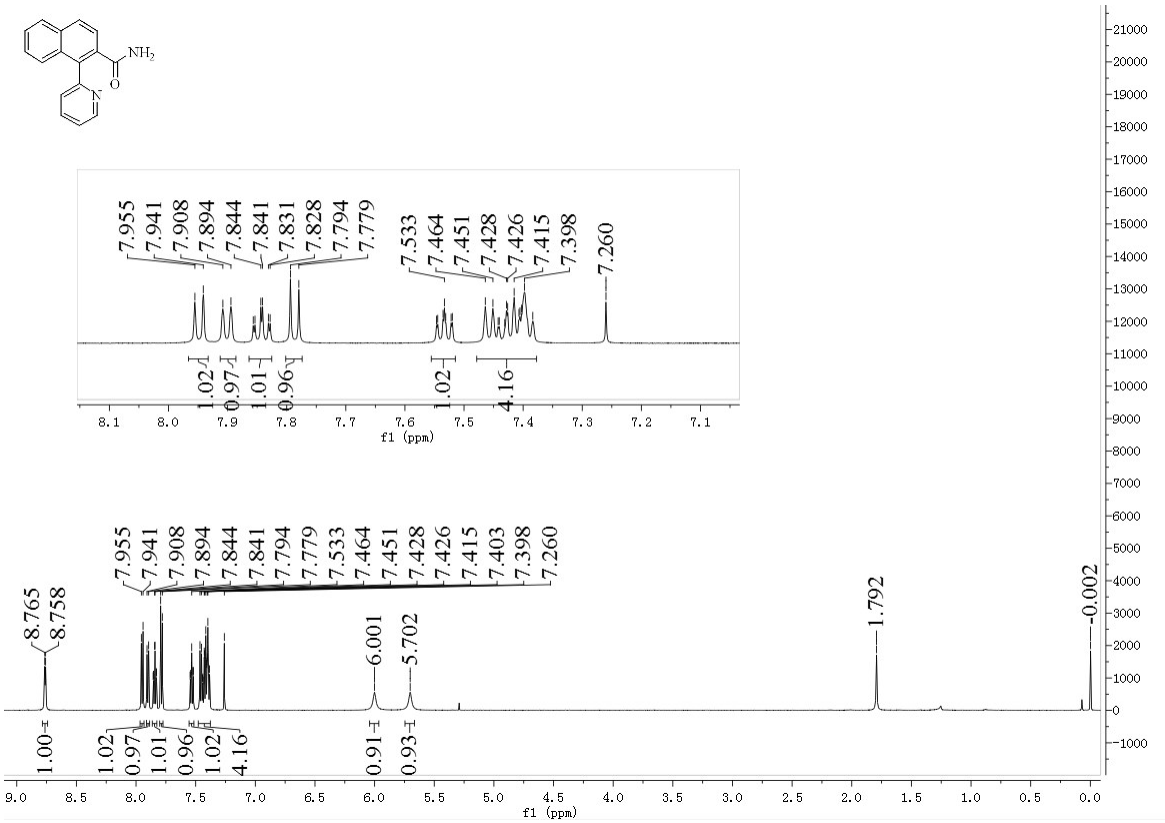

7.780
7.776
7.764
7.751
7.747
7.455
7.441
7.421
7.418
7.407
7.404
7.301
7.292
7.281
6.929
6.778
6.774
6.770
6.746
6.742
6.737
6.731
6.727
6.723
1.00
2.99
1.03
0.90
2.02
f1 (ppm)
3.336
2.965
2.961
2.506
2.503
2.500
2.497
2.495
8.570
8.562
0.96
6.00

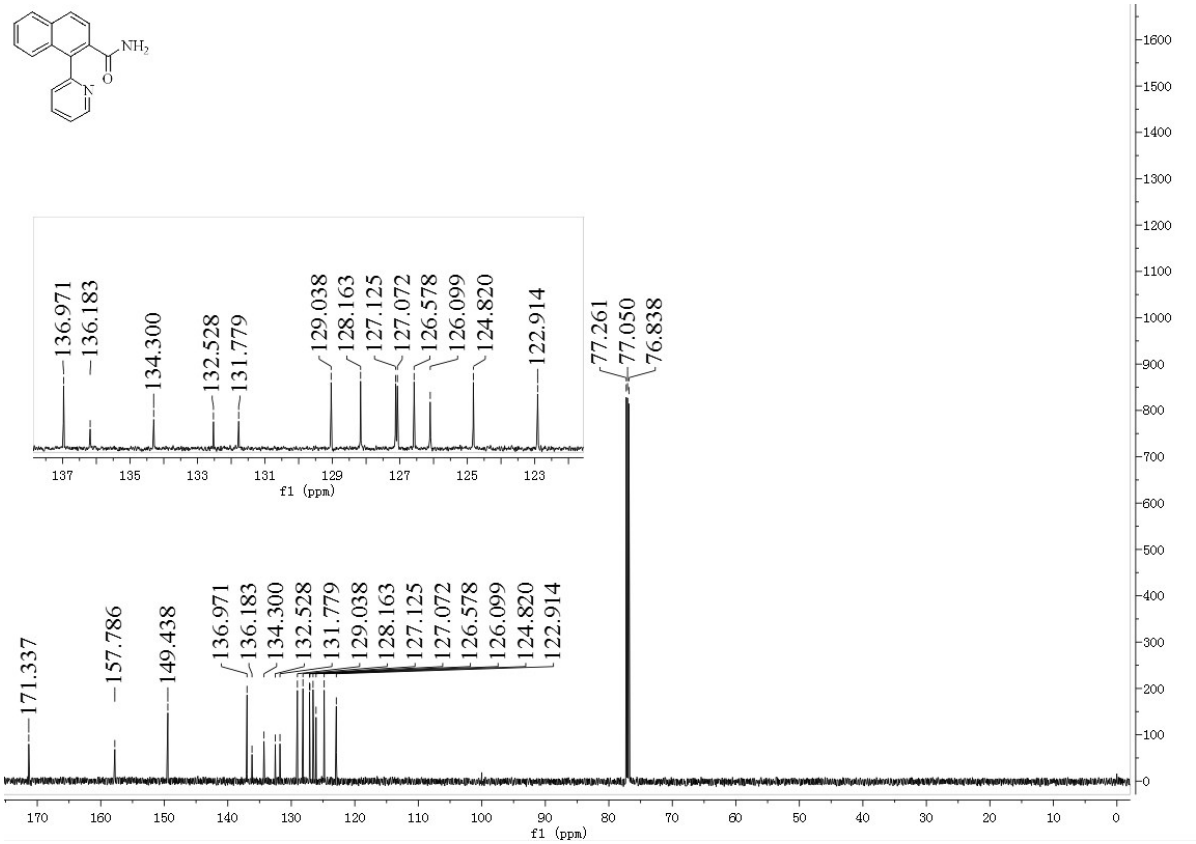
Compound **1n**


8.148
8.135
7.985
7.972
7.795
7.783
7.769
7.757
7.706
7.693
7.613
7.600
7.463
7.449
7.432
7.420
7.407
7.319
7.308
7.296
7.260
8.656
8.648
6.583
1.00
2.04
1.04
2.02
1.04
1.03
4.15
3.05
0.97
f1 (ppm)
8.148
8.135
7.985
7.972
7.757
7.613
7.463
7.449
7.432
7.420
7.319
7.308
7.296
7.260
6.583
5.962
1.785
0.086
0.009
1.00
2.04
1.04
2.02
1.04
1.03
4.15
3.05
0.97
0.97
f1 (ppm)

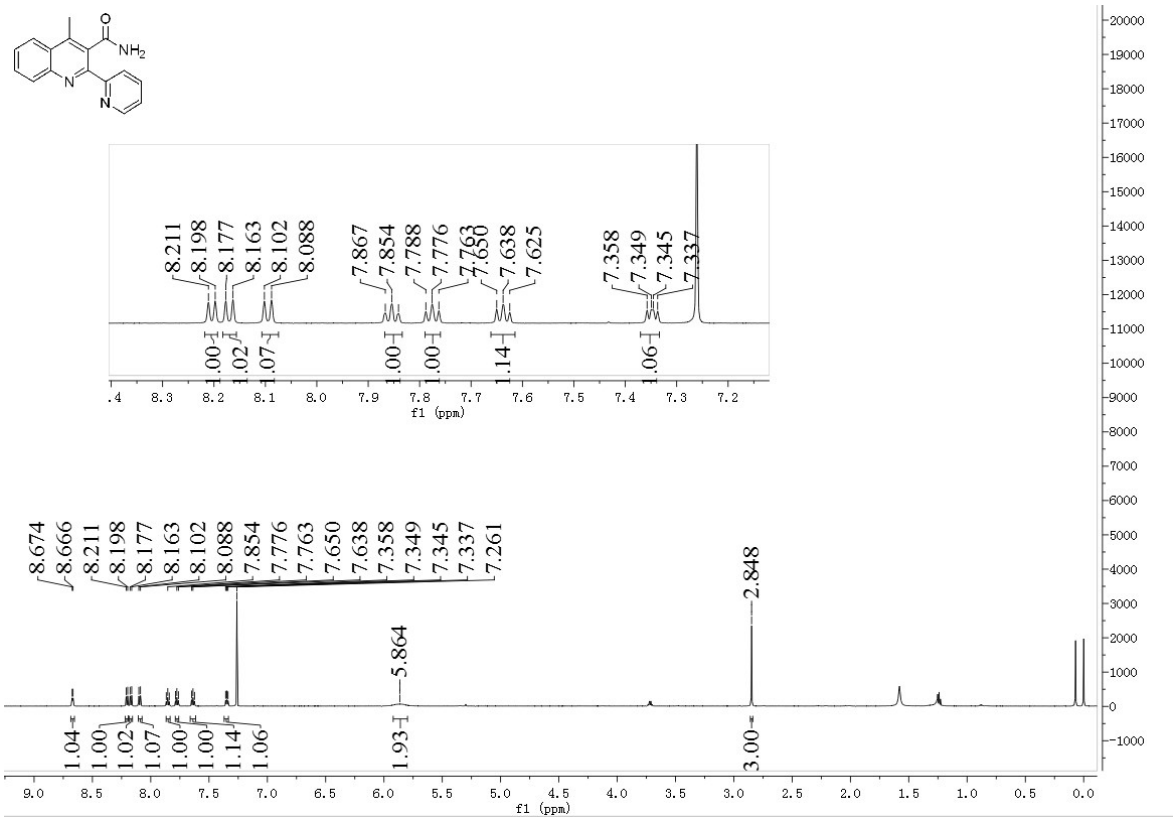

140.757
140.480
139.601
137.056
134.064
130.670
128.486
126.801
126.198
124.053
123.677
122.985
f1 (ppm)
157.381
149.240
140.757
140.480
139.601
137.056
134.064
130.670
128.486
126.801
126.198
124.053
123.677
122.985
120.457
109.712
171.067
77.277
77.066
76.854
f1 (ppm)

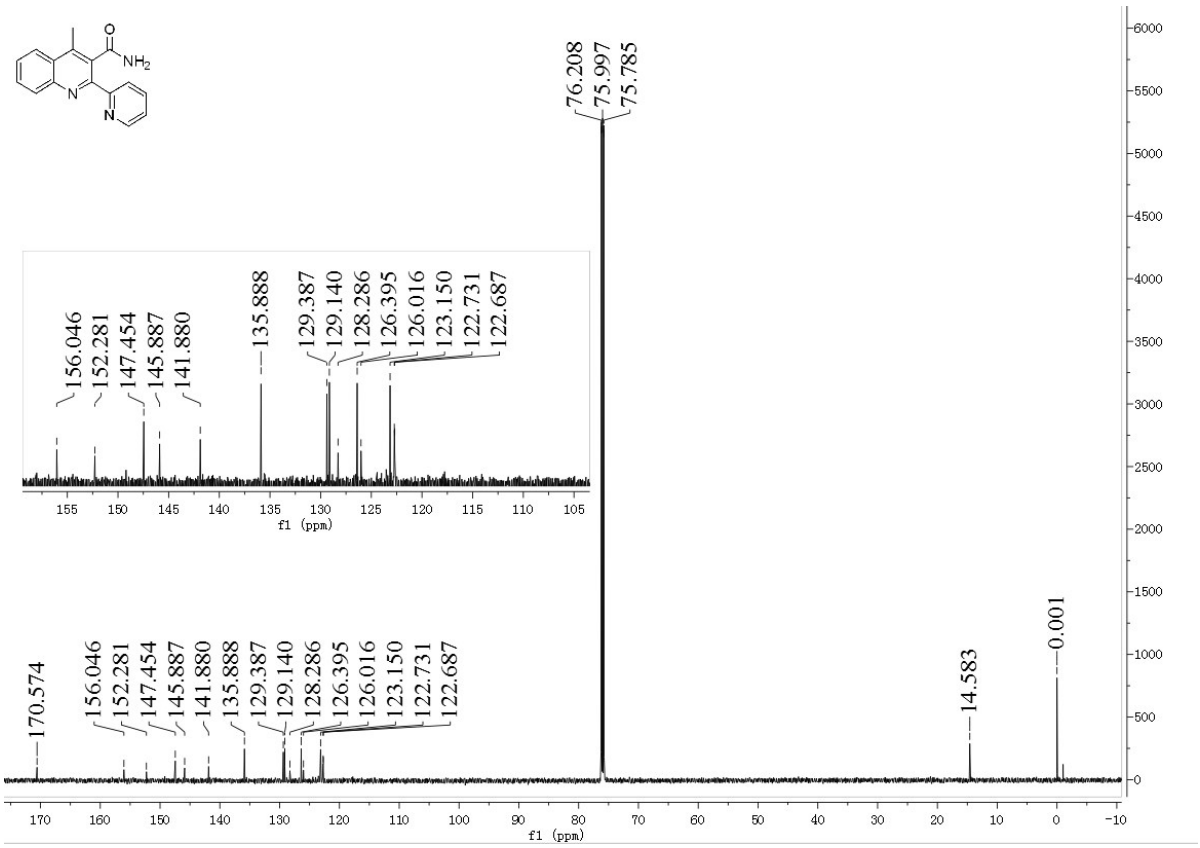
Compound **1o**


NH2
O
N
7.955
7.941
7.908
7.894
7.844
7.841
7.831
7.828
7.794
7.779
7.533
7.464
7.451
7.428
7.426
7.415
7.398
7.260
1.02
0.97
1.01
0.96
1.02
4.16
f1 (ppm)
8.765
8.758
7.955
7.941
7.908
7.894
7.844
7.841
7.794
7.779
7.533
7.464
7.451
7.428
7.426
7.415
7.403
7.398
7.260
6.001
5.702
1.792
-0.002
1.00
1.02
0.97
1.01
0.96
1.02
4.16
0.91
0.93
f1 (ppm)

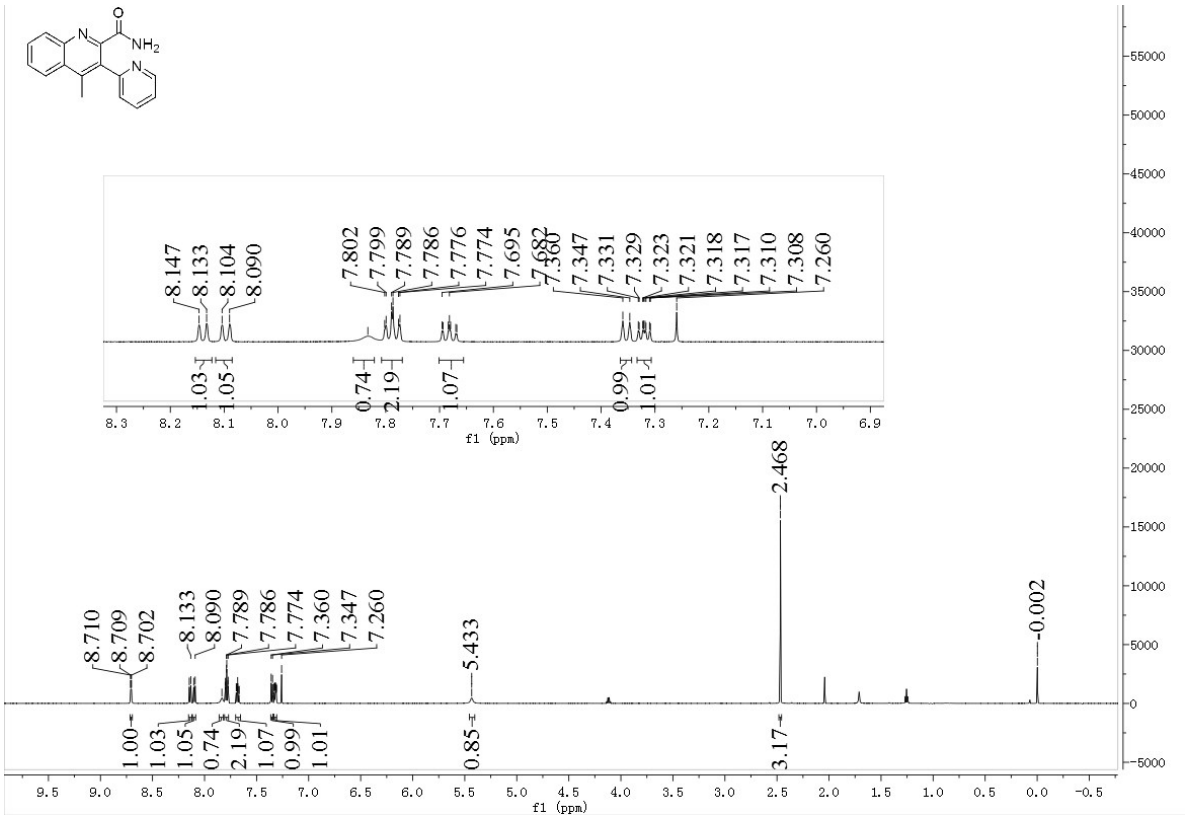

NH2
O
N
136.971
136.183
134.300
132.528
131.779
129.038
128.163
127.125
127.072
126.578
126.099
124.820
122.914
77.261
77.050
76.838
f1 (ppm)
171.337
157.786
149.438
136.971
136.183
134.300
132.528
131.779
129.038
128.163
127.125
127.072
126.578
126.099
124.820
122.914
f1 (ppm)

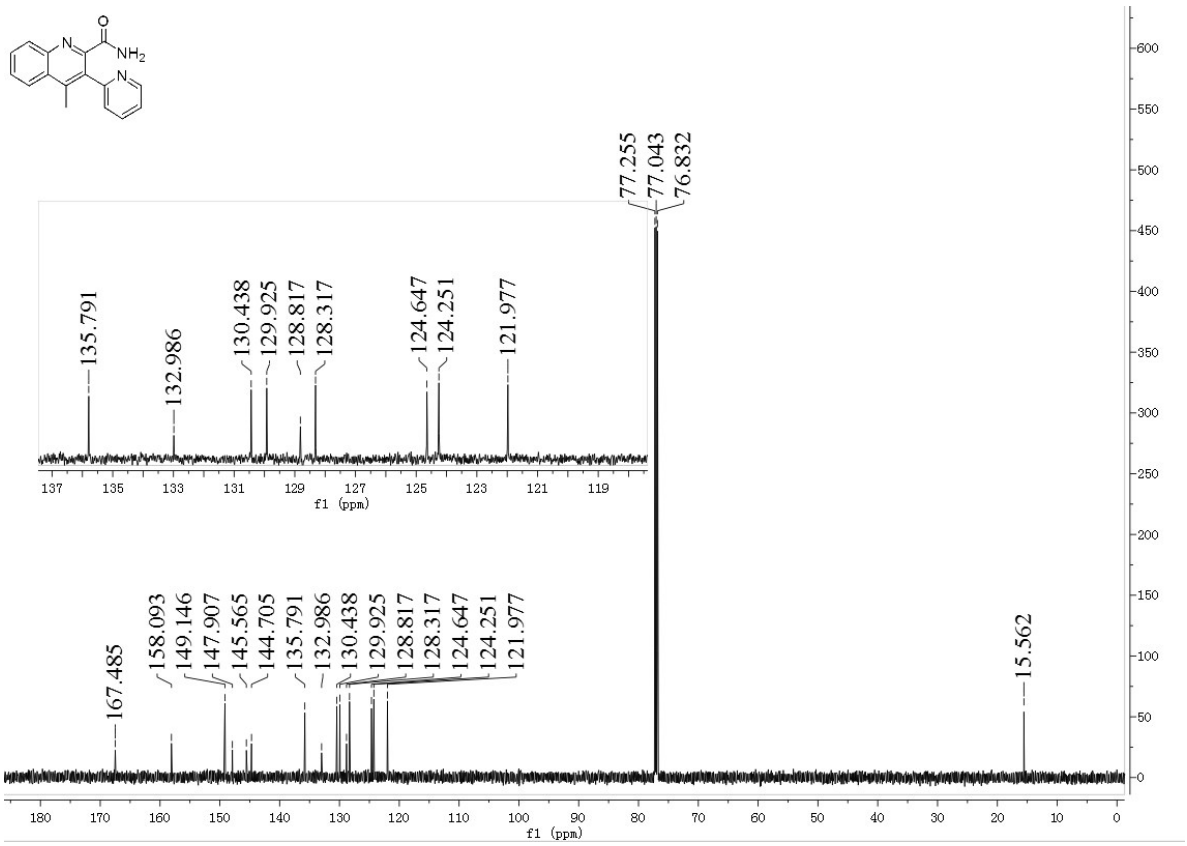
Compound **1p**


8.211
8.198
8.177
8.163
8.102
8.088
7.867
7.854
7.788
7.776
7.763
7.650
7.638
7.625
7.358
7.349
7.345
7.337
1.00
1.02
1.07
1.00
1.00
1.14
1.06
f1 (ppm)
8.674
8.666
8.211
8.198
8.177
8.163
8.102
8.088
7.854
7.776
7.763
7.650
7.638
7.358
7.349
7.345
7.337
7.261
5.864
2.848
1.04
1.00
1.02
1.07
1.00
1.00
1.14
1.06
1.93
3.00
f1 (ppm)

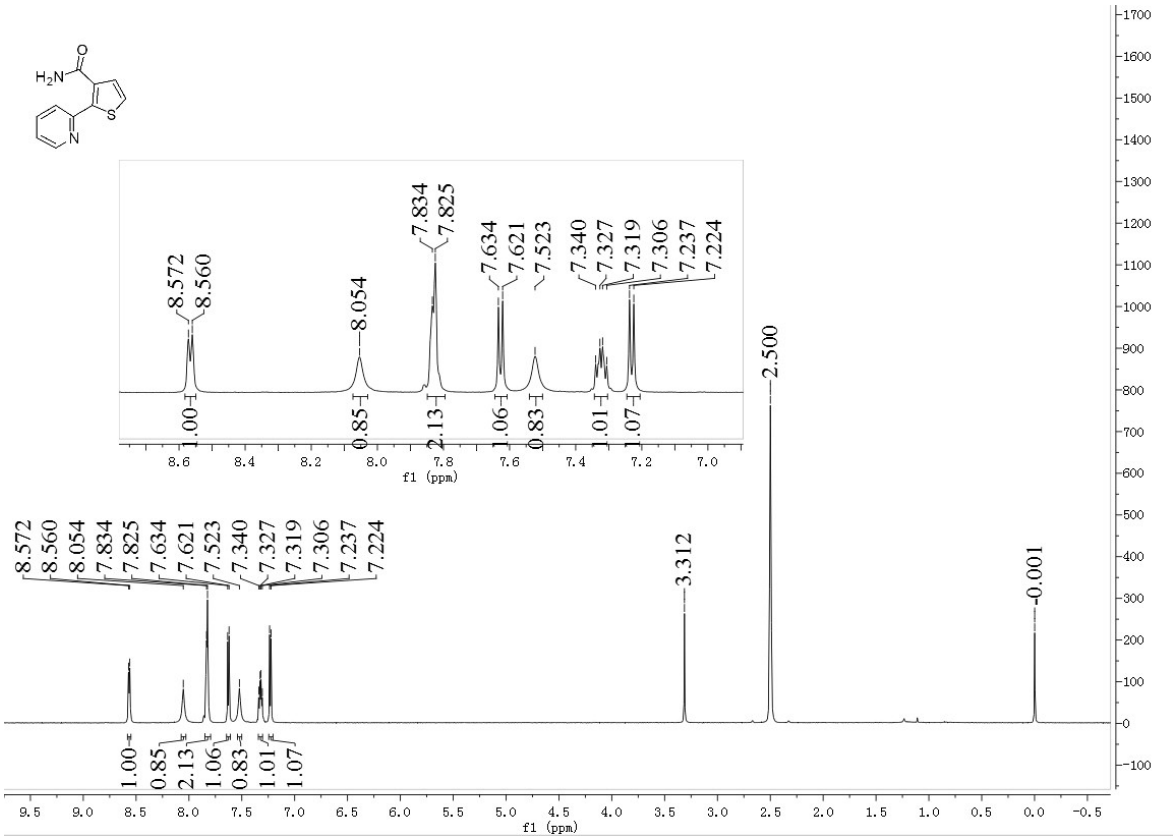

76.208
75.997
75.785
156.046
152.281
147.454
145.887
141.880
135.888
129.387
129.140
128.286
126.395
126.016
123.150
122.731
122.687
f1 (ppm)
170.574
156.046
152.281
147.454
145.887
141.880
135.888
129.387
129.140
128.286
126.395
126.016
123.150
122.731
122.687
14.583
0.001
f1 (ppm)

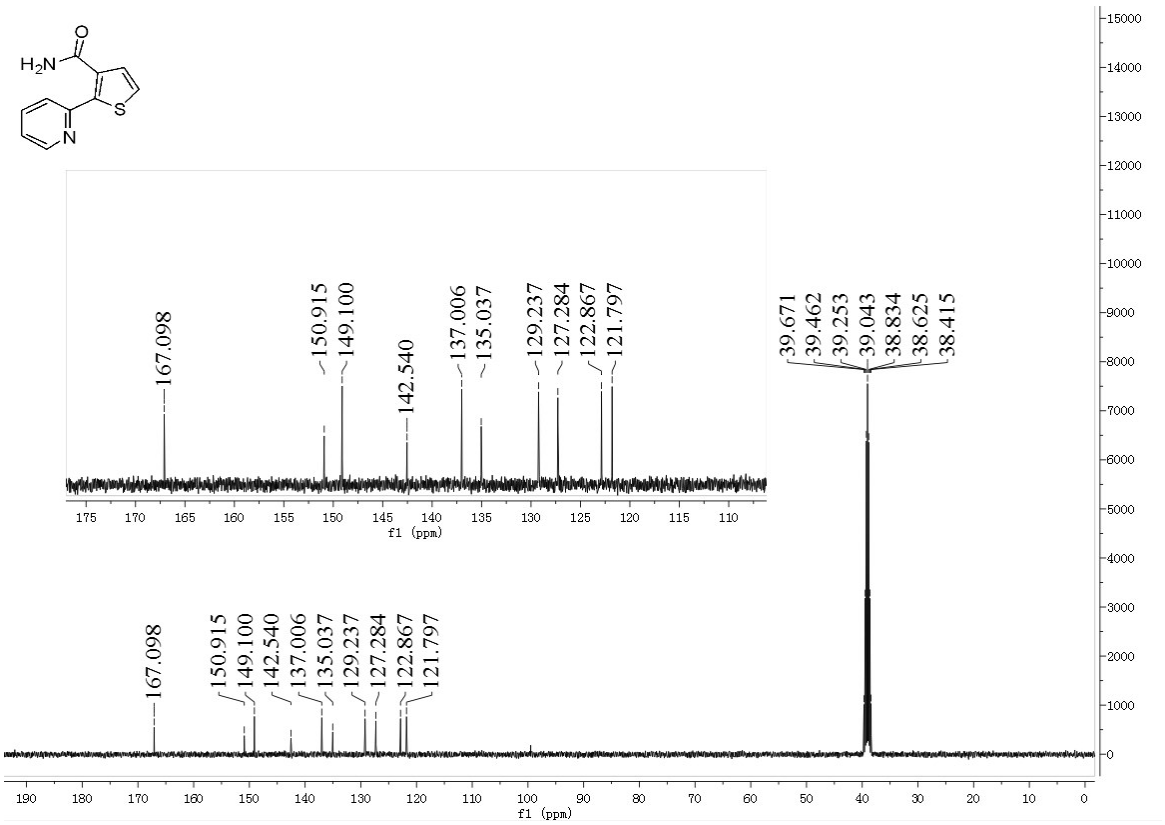
Compound **1q**


8.147
8.133
8.104
8.090
7.802
7.799
7.789
7.786
7.776
7.774
7.695
7.682
7.360
7.347
7.331
7.329
7.323
7.321
7.318
7.317
7.310
7.308
7.260
1.03
1.05
0.74
2.19
1.07
0.99
1.01
f1 (ppm)
2.468
8.710
8.709
8.702
8.133
8.090
7.789
7.786
7.774
7.360
7.347
7.260
5.433
-0.002
1.00
1.03
1.05
0.74
2.19
1.07
0.99
1.01
0.85
3.17
f1 (ppm)

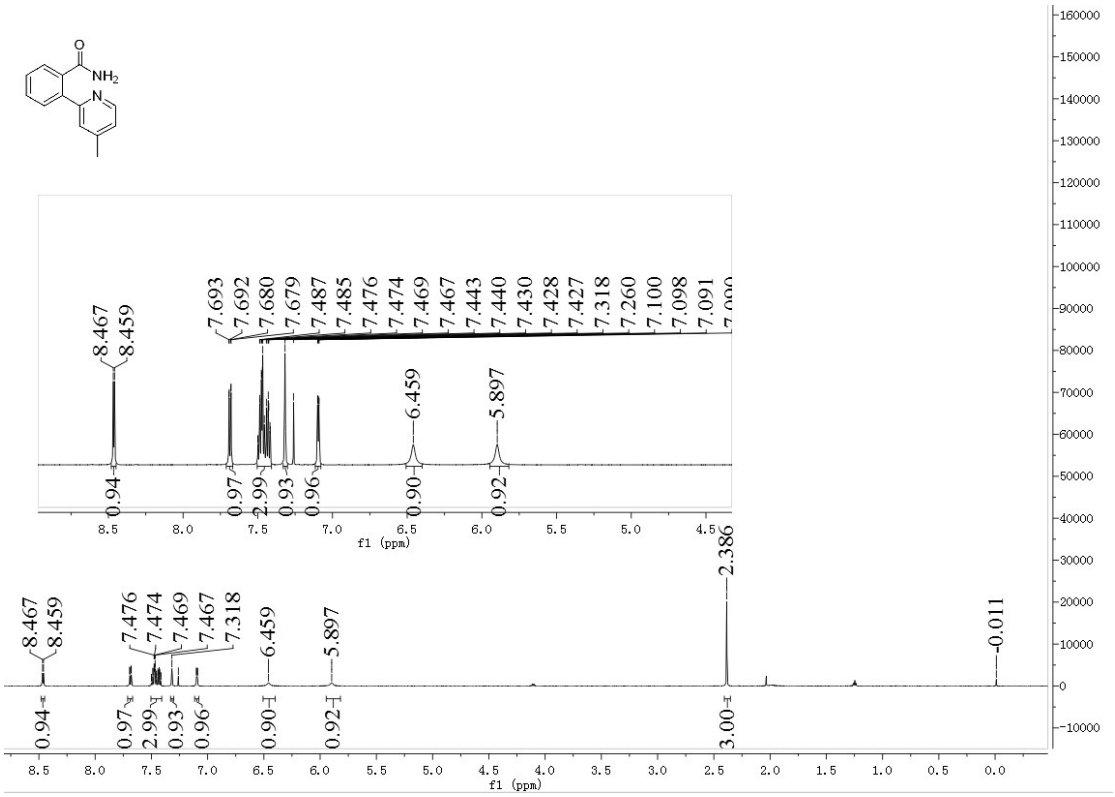

77.255
77.043
76.832
135.791
132.986
130.438
129.925
128.817
128.317
124.647
124.251
121.977
f1 (ppm)
167.485
158.093
149.146
147.907
145.565
144.705
135.791
132.986
130.438
129.925
128.817
128.317
124.647
124.251
121.977
15.562
f1 (ppm)

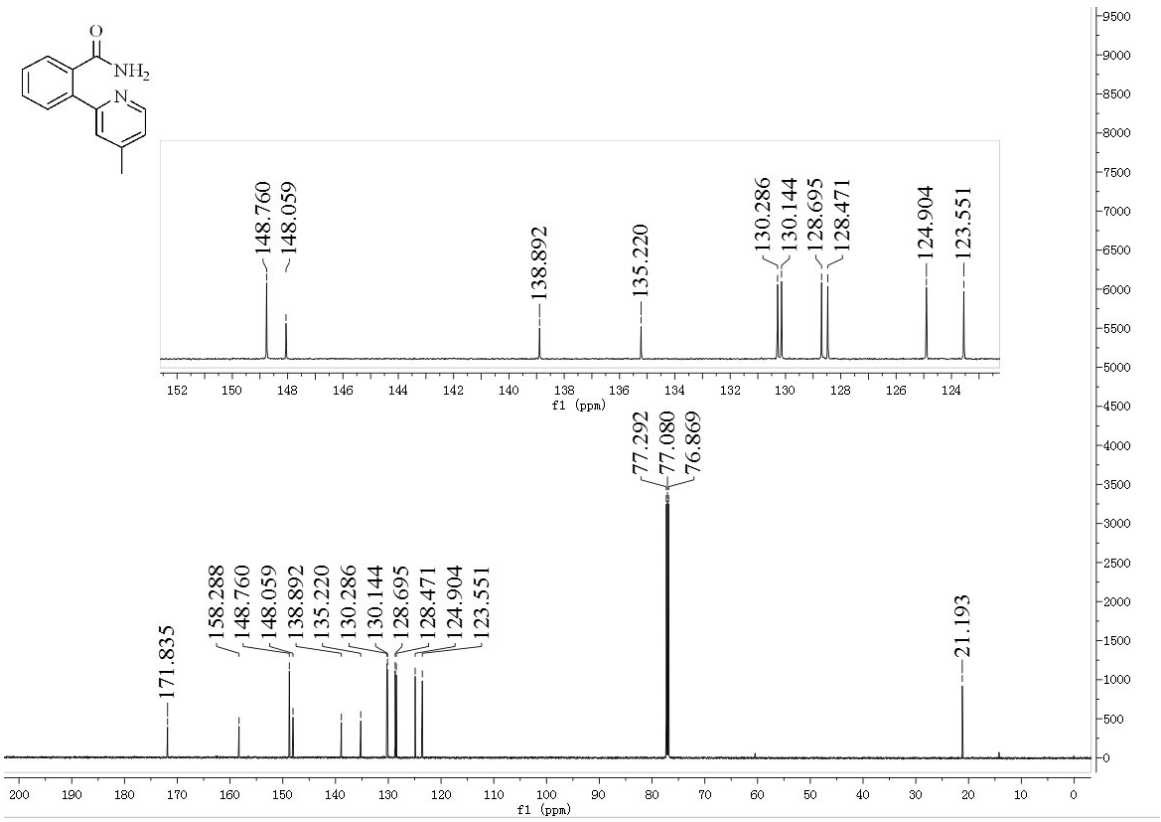
Compound **1r**


8.572
8.560
8.054
7.834
7.825
7.634
7.621
7.523
7.340
7.327
7.319
7.306
7.237
7.224
3.312
2.500
-0.001
1.00
0.85
2.13
1.06
0.83
1.01
1.07
f1 (ppm)

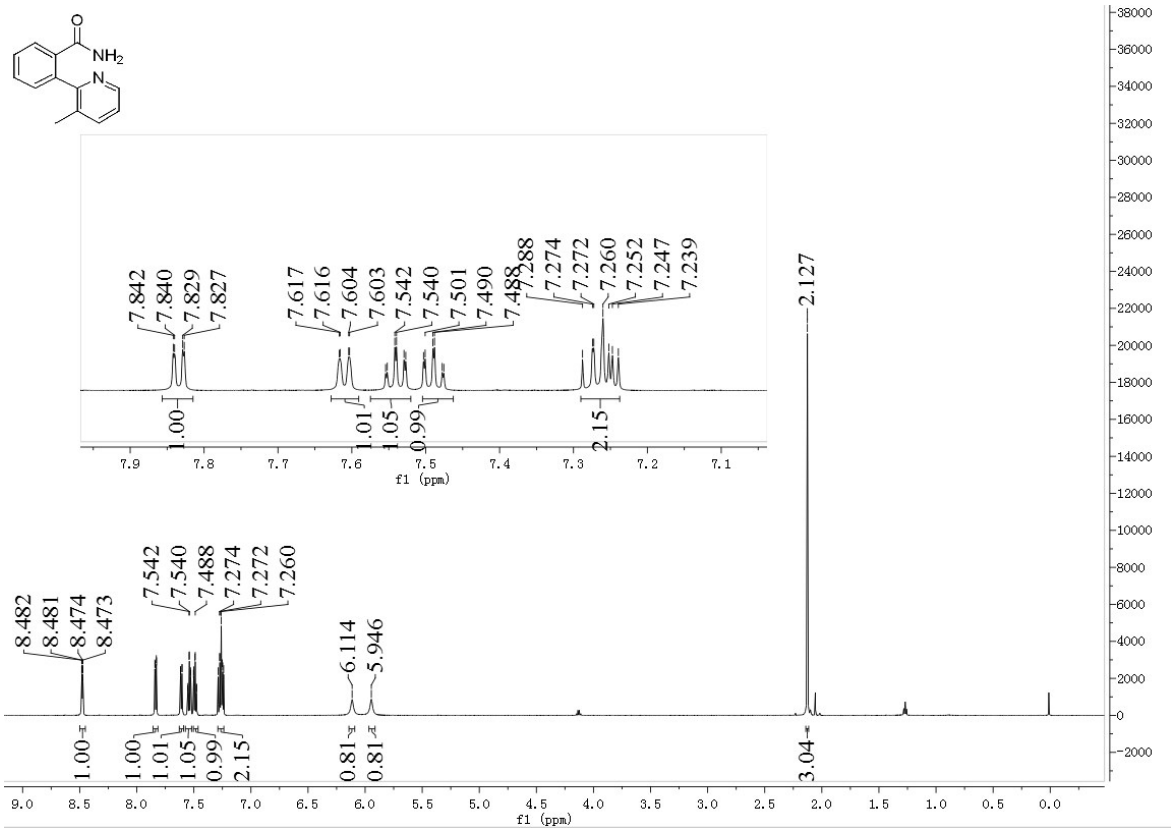

167.098
150.915
149.100
142.540
137.006
135.037
129.237
127.284
122.867
121.797
39.671
39.462
39.253
39.043
38.834
38.625
38.415
f1 (ppm)

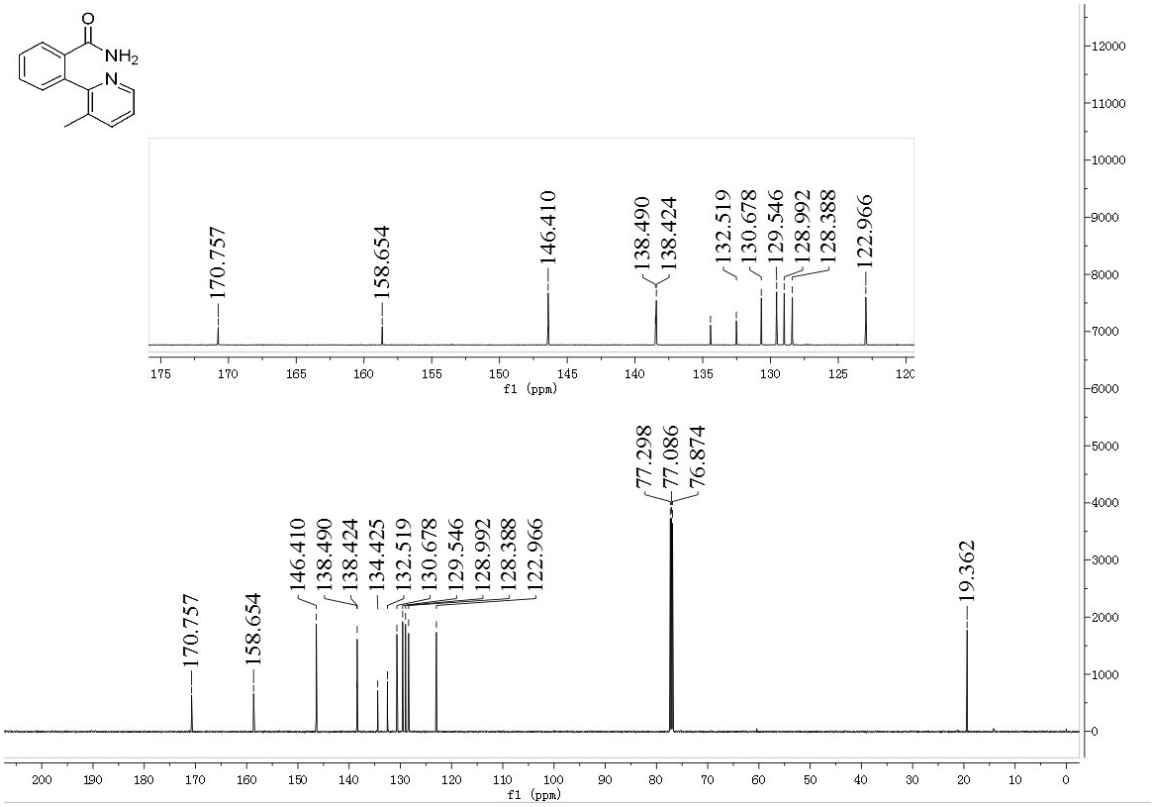
Compound **1s**


8.467
8.459
7.693
7.692
7.680
7.679
7.487
7.485
7.476
7.474
7.469
7.467
7.443
7.440
7.430
7.428
7.427
7.318
7.260
7.100
7.098
7.091
6.459
5.897
0.94
0.97
2.99
0.93
0.96
0.90
0.92
f1 (ppm)
2.386
0.011
3.00
f1 (ppm)

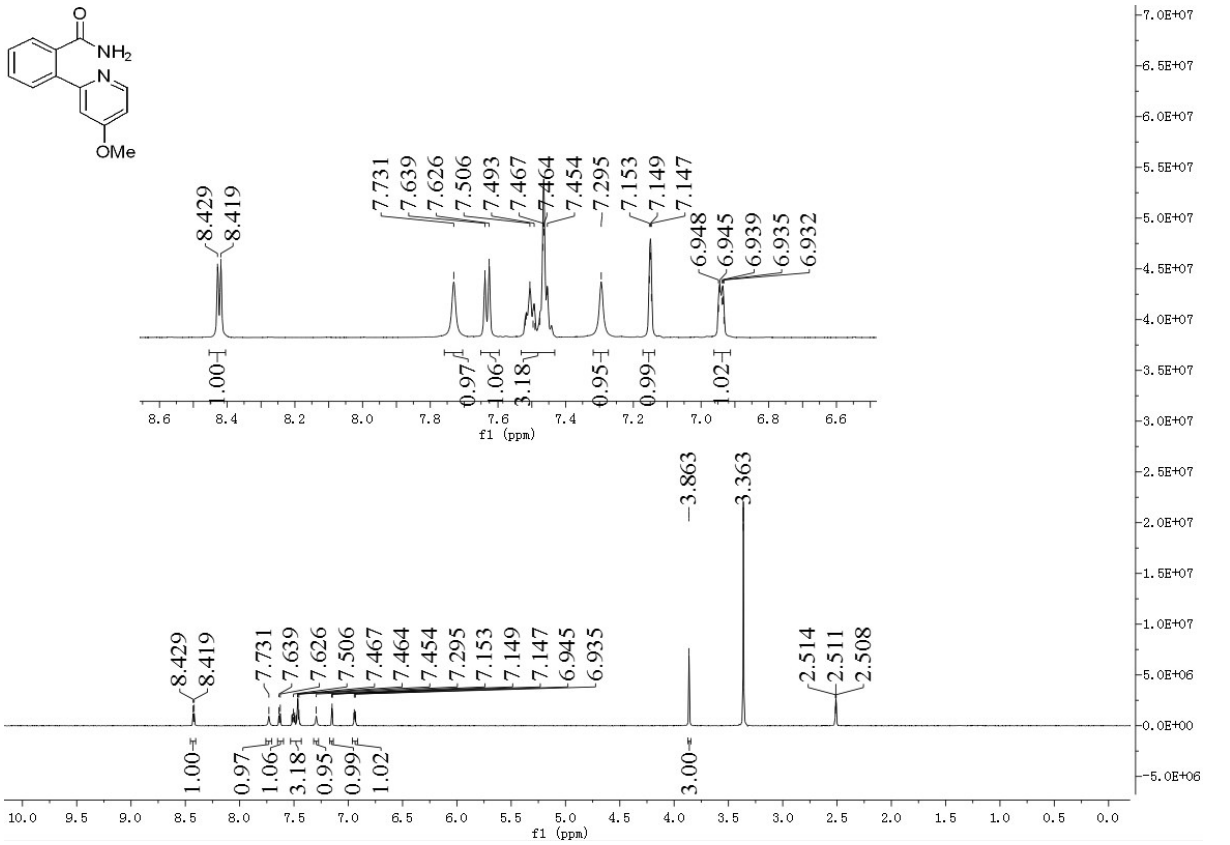

148.760
148.059
138.892
135.220
130.286
130.144
128.695
128.471
124.904
123.551
f1 (ppm)
77.292
77.080
76.869
171.835
158.288
148.760
148.059
138.892
135.220
130.286
130.144
128.695
128.471
124.904
123.551
21.193
f1 (ppm)

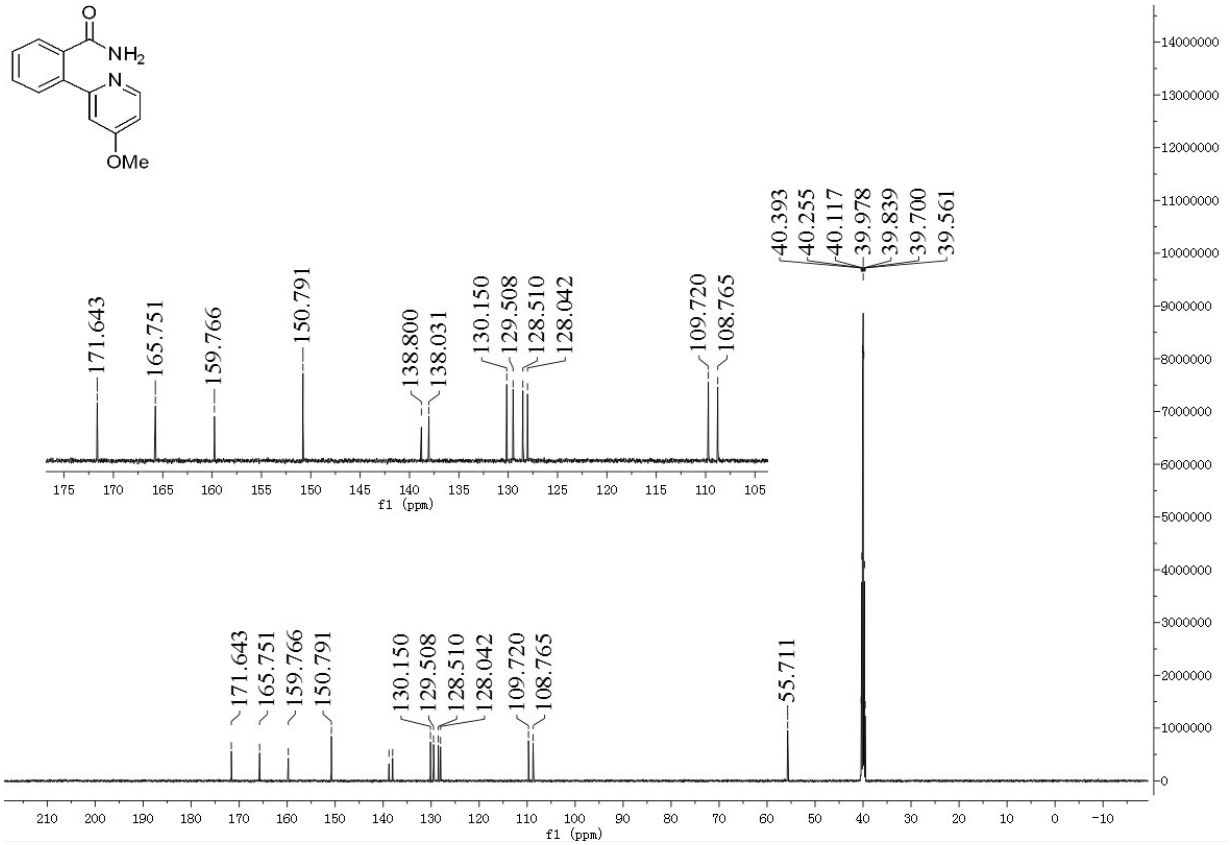
Compound **1t**


7.842
7.840
7.829
7.827
7.617
7.616
7.604
7.603
7.542
7.540
7.501
7.490
7.488
7.288
7.274
7.272
7.260
7.252
7.247
7.239
2.127
1.00
1.01
1.05
0.99
2.15
f1 (ppm)
8.482
8.481
8.474
8.473
7.542
7.540
7.488
7.274
7.272
7.260
6.114
5.946
1.00
1.00
1.01
1.05
0.99
2.15
0.81
0.81
3.04
f1 (ppm)

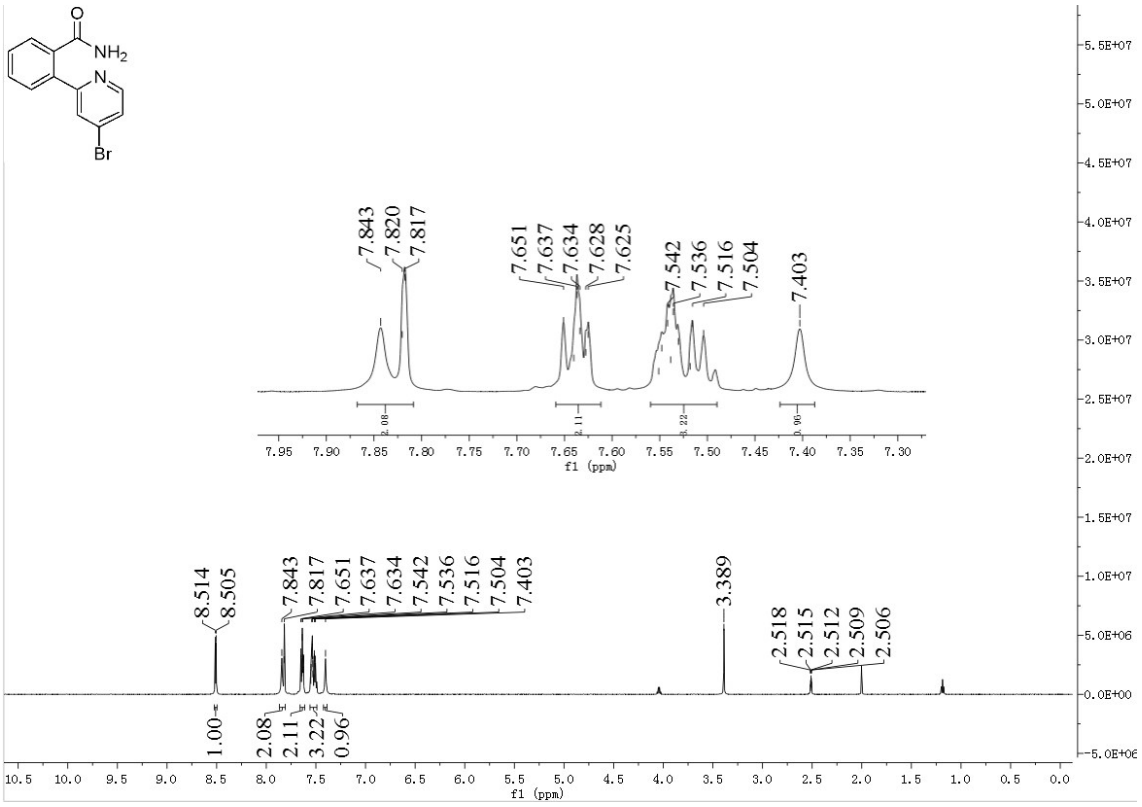

170.757
158.654
146.410
138.490
138.424
132.519
130.678
129.546
128.992
128.388
122.966
f1 (ppm)
77.298
77.086
76.874
170.757
158.654
146.410
138.490
138.424
134.425
132.519
130.678
129.546
128.992
128.388
122.966
19.362
f1 (ppm)

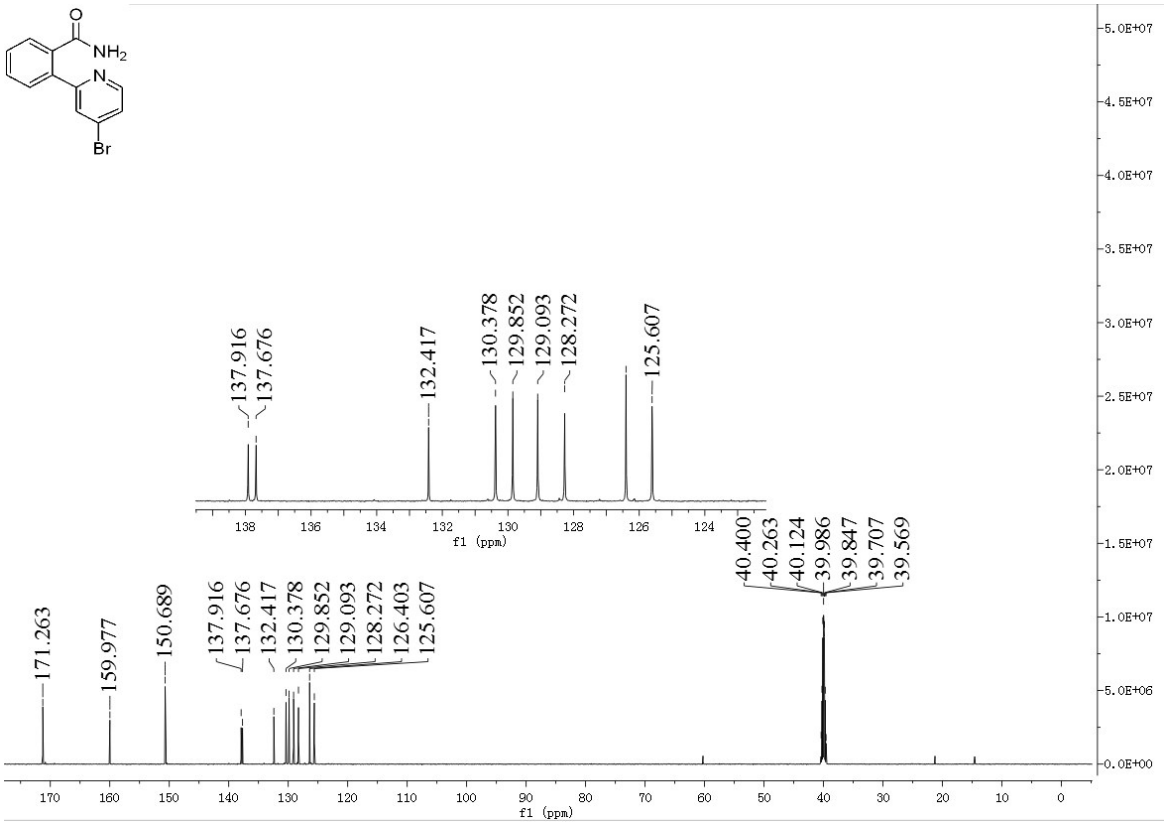
Compound **1u**


NH2
N
OMe
8.429
8.419
7.731
7.639
7.626
7.506
7.493
7.467
7.464
7.454
7.295
7.153
7.149
7.147
6.948
6.945
6.939
6.935
6.932
1.00
0.97
1.06
3.18
0.95
0.99
1.02
3.863
3.363
2.514
2.511
2.508
3.00
f1 (ppm)

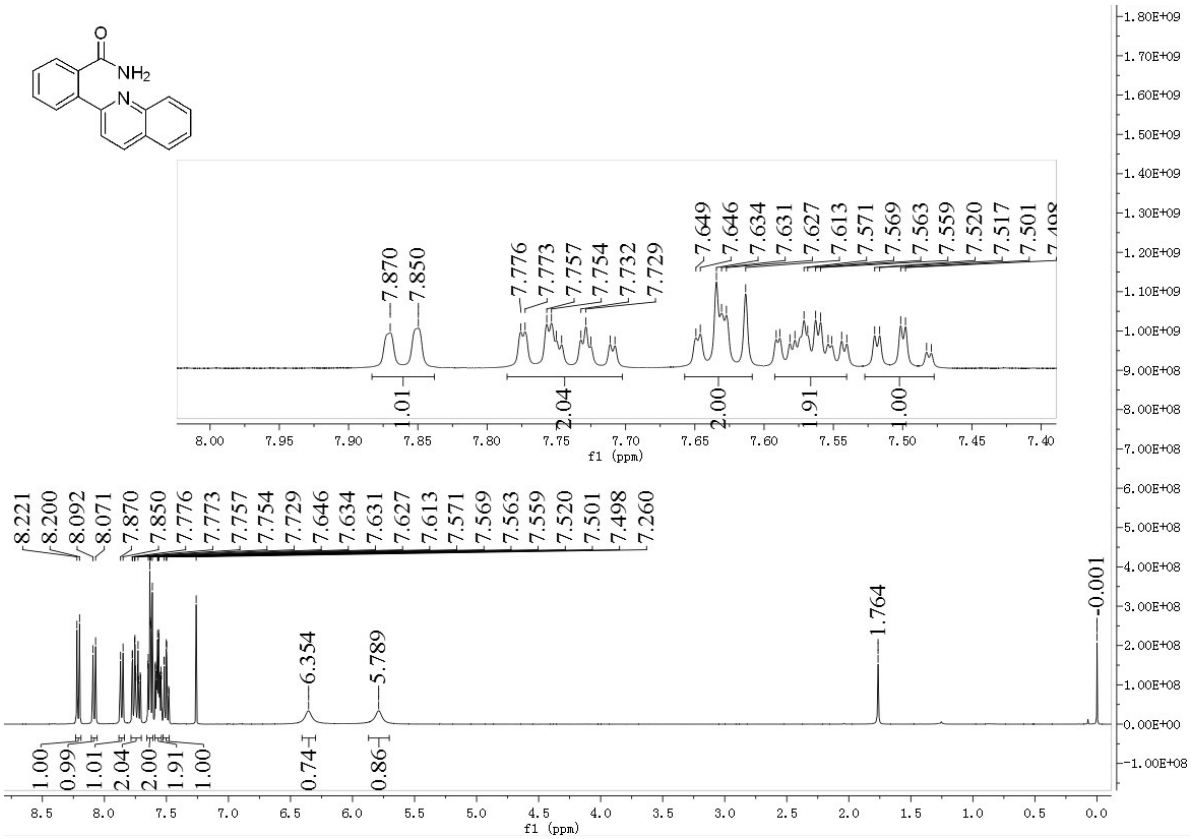

NH2
N
OMe
171.643
165.751
159.766
150.791
138.800
138.031
130.150
129.508
128.510
128.042
109.720
108.765
40.393
40.255
40.117
39.978
39.839
39.700
39.561
55.711
f1 (ppm)

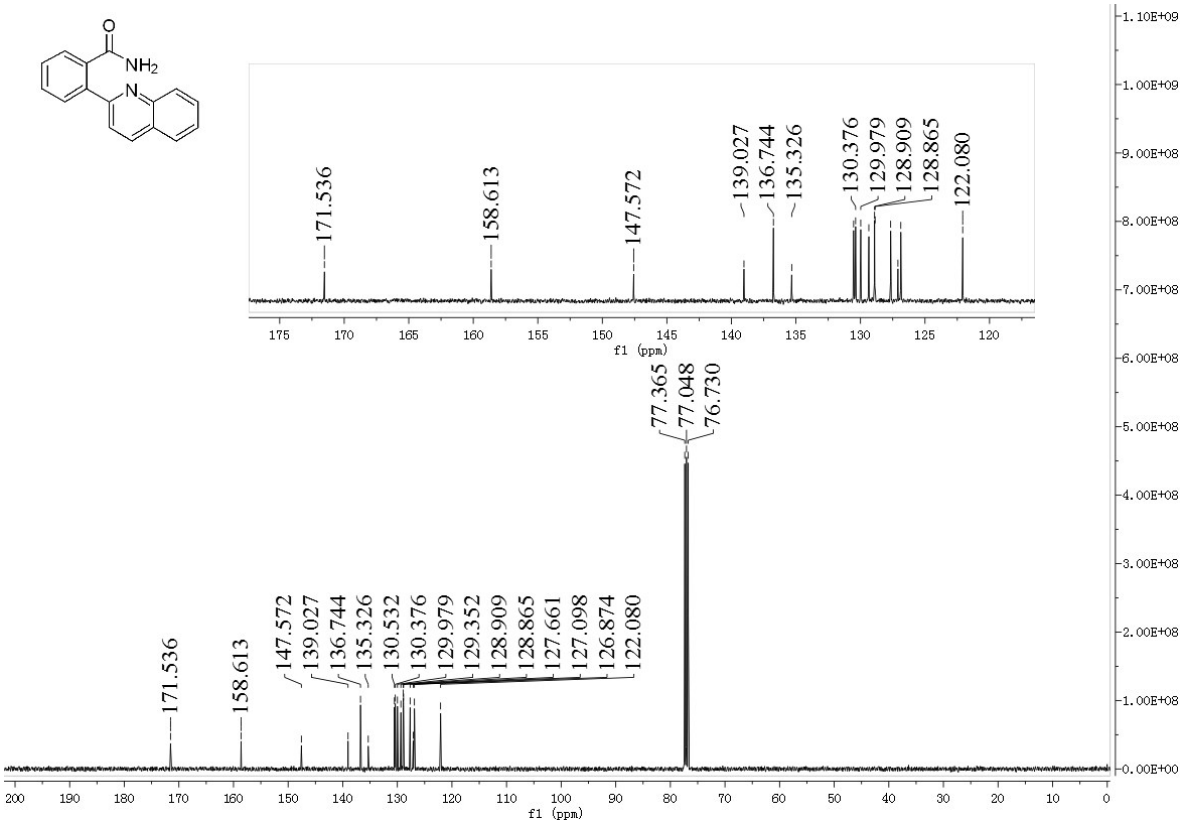
Compound **1v**


O
NH2
N
Br
7.843
7.820
7.817
7.651
7.637
7.634
7.628
7.625
7.542
7.536
7.516
7.504
7.403
f1 (ppm)
8.514
8.505
7.843
7.817
7.651
7.637
7.634
7.542
7.536
7.516
7.504
7.403
3.389
2.518
2.515
2.512
2.509
2.506
1.00
2.08
2.11
3.22
0.96
f1 (ppm)

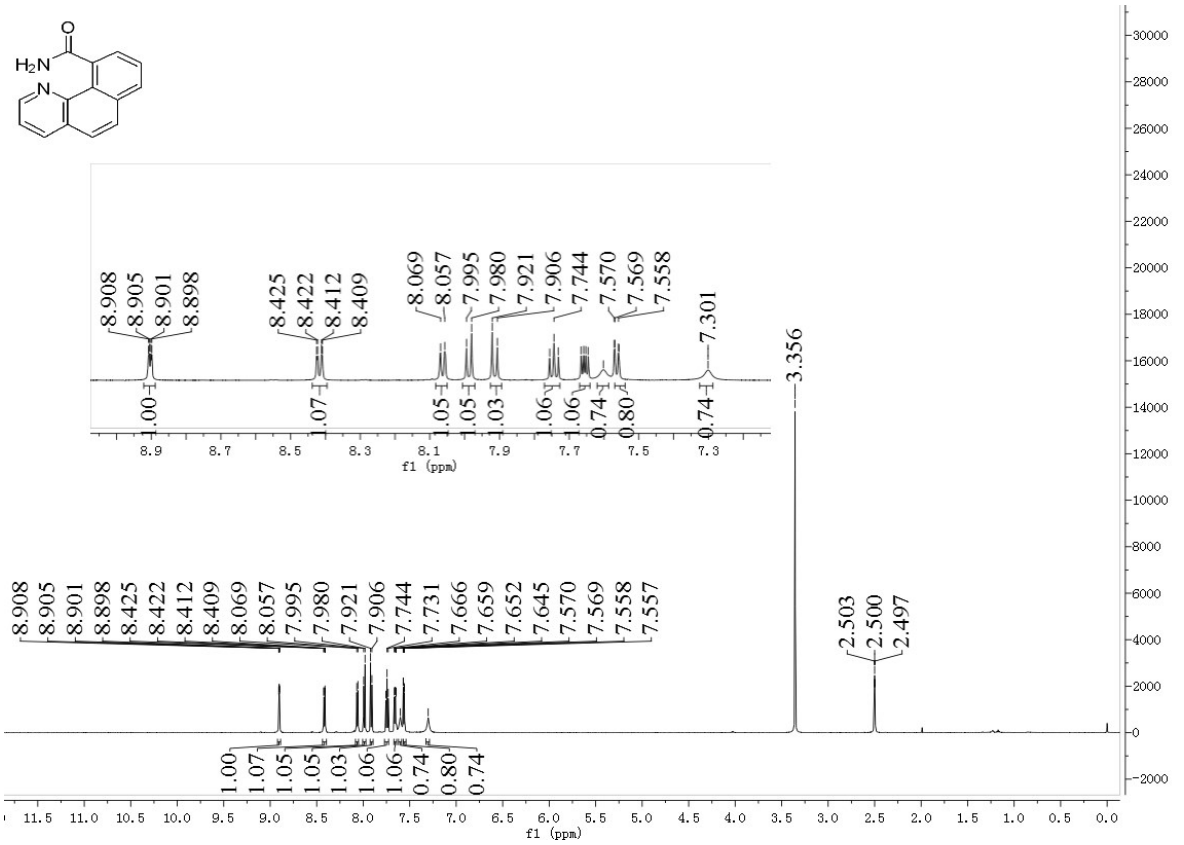

O
NH2
N
Br
137.916
137.676
132.417
130.378
129.852
129.093
128.272
125.607
f1 (ppm)
40.400
40.263
40.124
39.986
39.847
39.707
39.569
171.263
159.977
150.689
137.916
137.676
132.417
130.378
129.852
129.093
128.272
126.403
125.607
f1 (ppm)

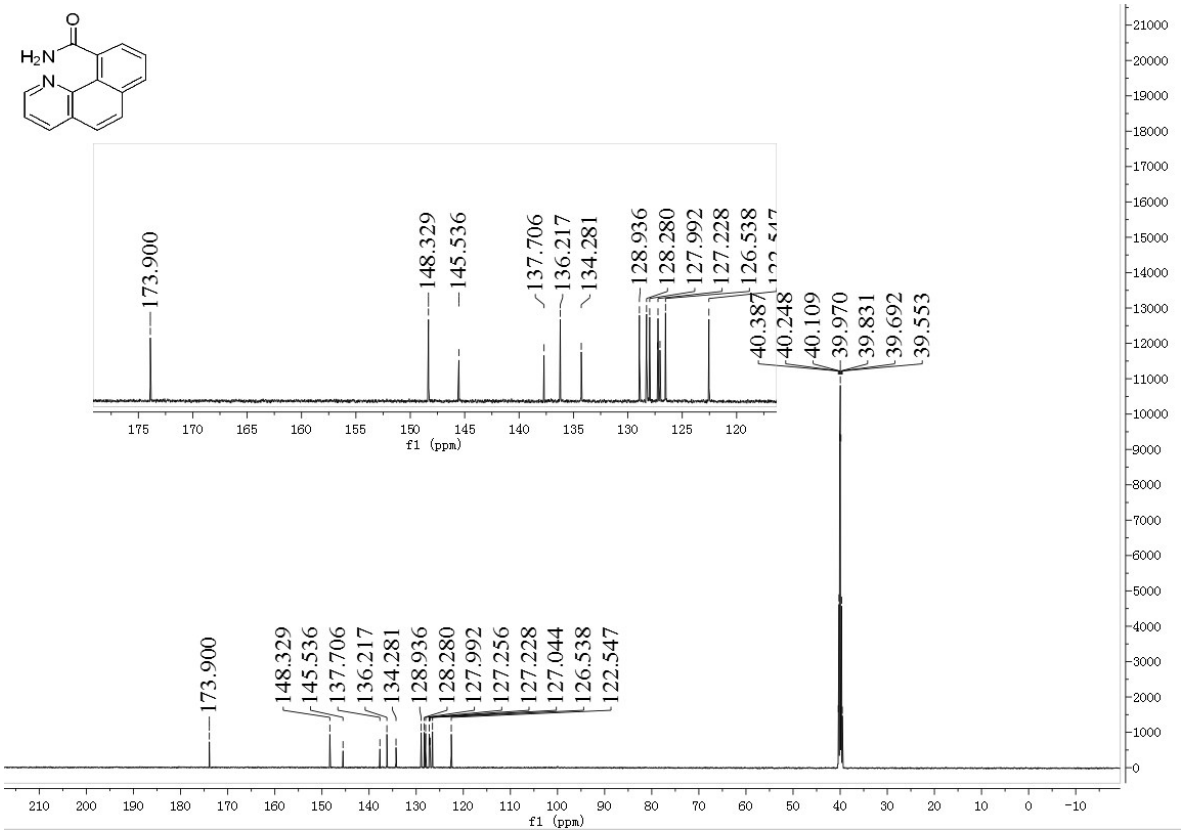
Compound **1w**


NH2
O
N
7.870
7.850
7.776
7.773
7.757
7.754
7.732
7.729
7.649
7.646
7.634
7.631
7.627
7.613
7.571
7.569
7.563
7.559
7.520
7.517
7.501
1.01
2.04
2.00
1.91
1.00
f1 (ppm)
8.221
8.200
8.092
8.071
7.498
7.260
6.354
5.789
1.764
-0.001
0.74
0.86
f1 (ppm)

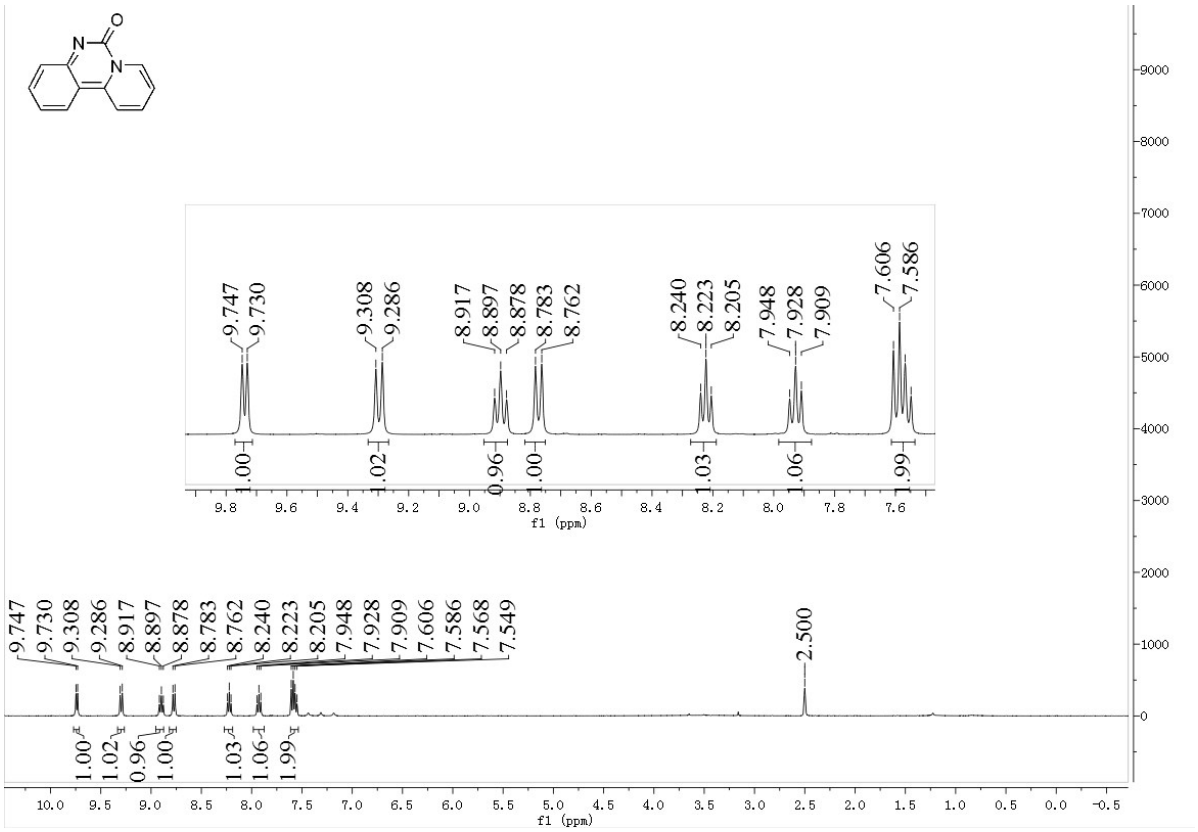

NH2
O
N
171.536
158.613
147.572
139.027
136.744
135.326
130.376
129.979
128.909
128.865
122.080
f1 (ppm)
77.365
77.048
76.730
147.572
139.027
136.744
135.326
130.532
130.376
129.979
129.352
128.909
128.865
127.661
127.098
126.874
122.080
171.536
158.613
f1 (ppm)

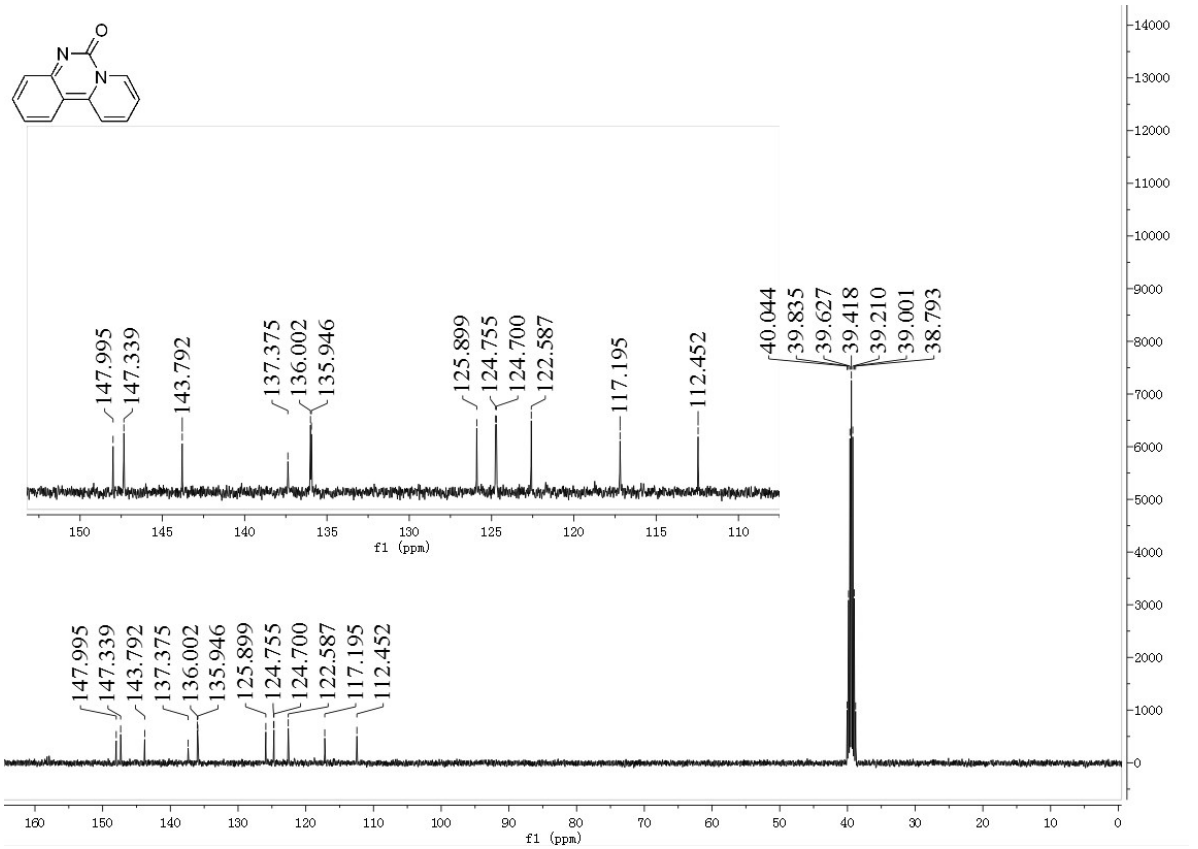
Compound **1x**


8.908
8.905
8.901
8.898
8.425
8.422
8.412
8.409
8.069
8.057
7.995
7.980
7.921
7.906
7.744
7.731
7.666
7.659
7.652
7.645
7.570
7.569
7.558
7.557
7.301
3.356
2.503
2.500
2.497
1.00
1.07
1.05
1.05
1.03
1.06
1.06
0.74
0.80
0.74
f1 (ppm)

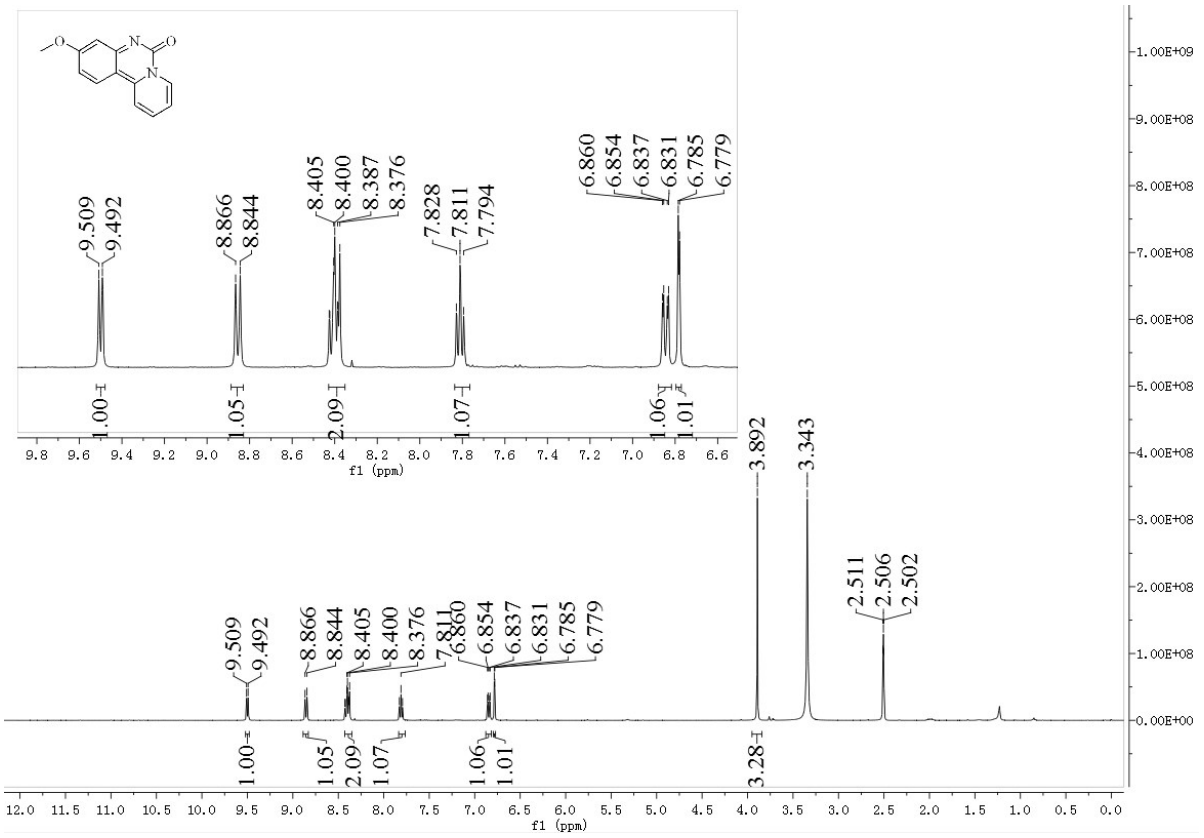

173.900
148.329
145.536
137.706
136.217
134.281
128.936
128.280
127.992
127.228
126.538
40.387
40.248
40.109
39.970
39.831
39.692
39.553
173.900
148.329
145.536
137.706
136.217
134.281
128.936
128.280
127.992
127.256
127.228
127.044
126.538
122.547
f1 (ppm)

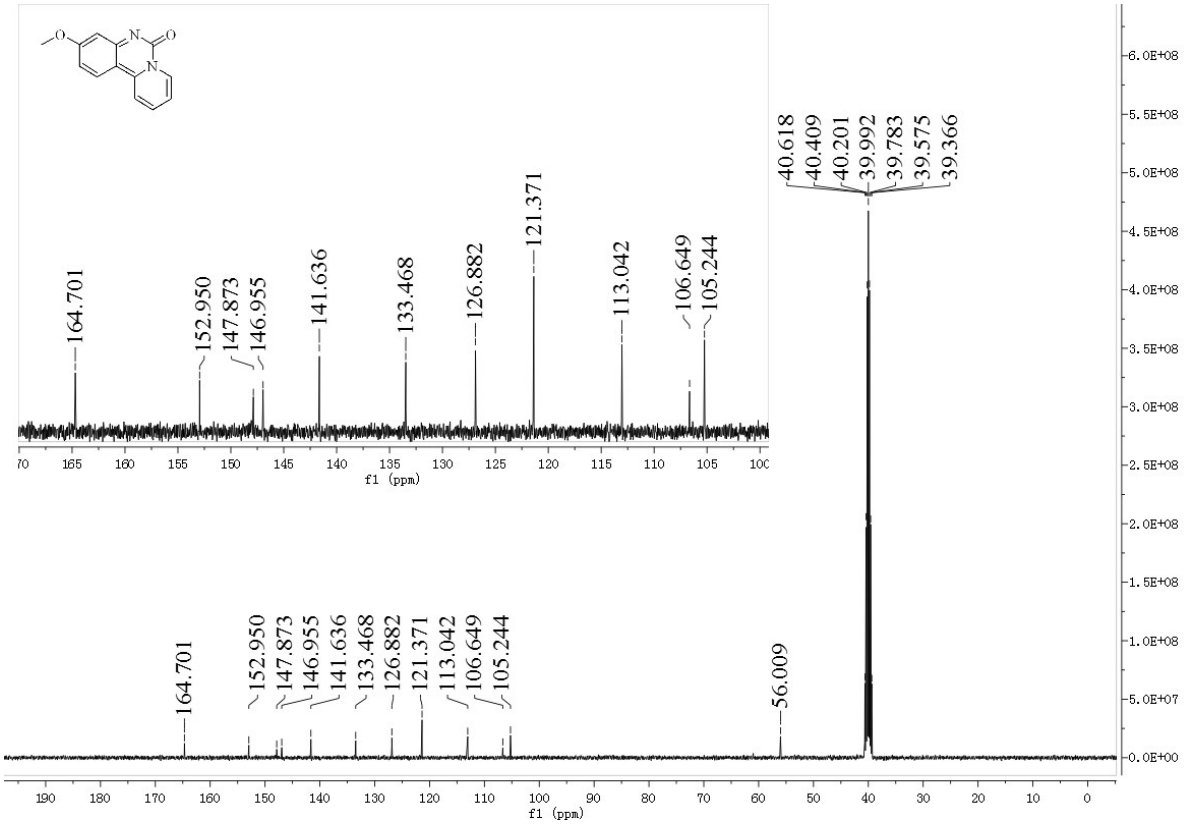
Compound **2a**


9.747
9.730
9.308
9.286
8.917
8.897
8.878
8.783
8.762
8.240
8.223
8.205
7.948
7.928
7.909
7.606
7.586
7.568
7.549
2.500
1.00
1.02
0.96
1.00
1.03
1.06
1.99
f1 (ppm)

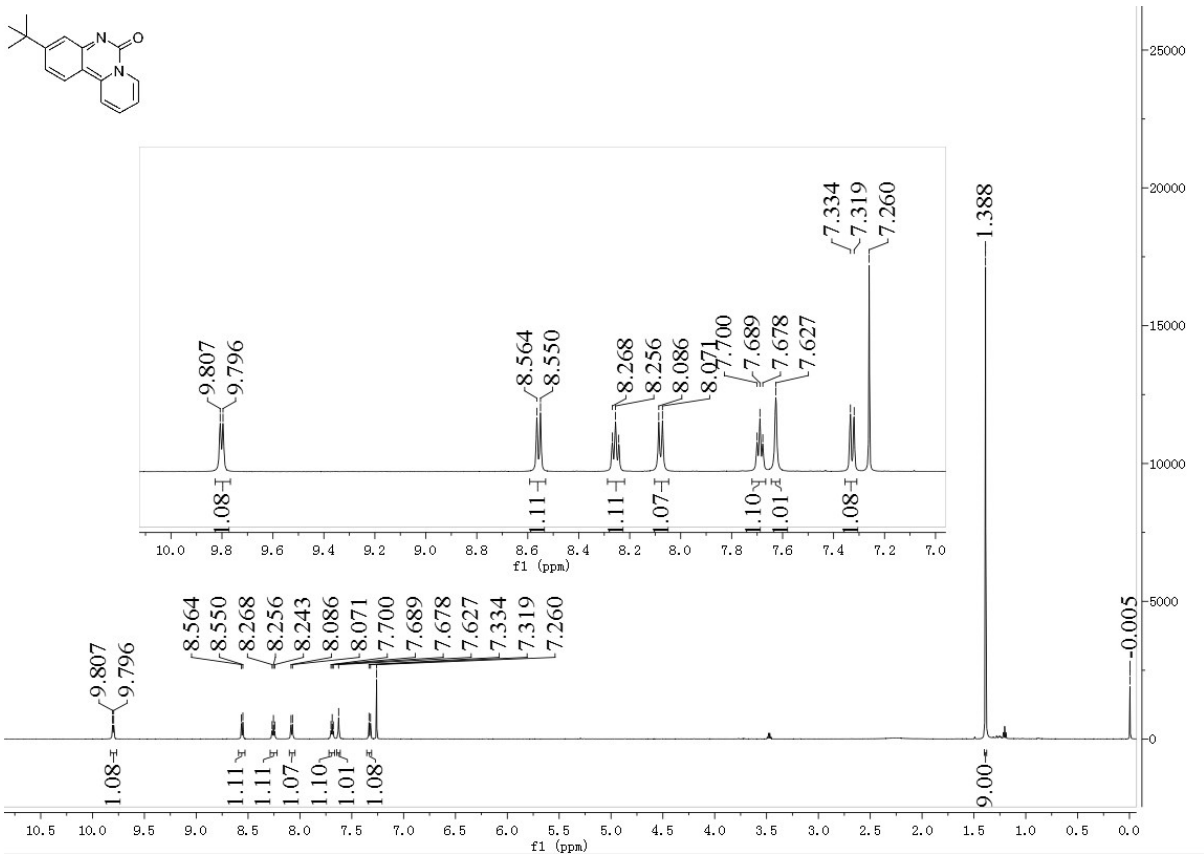

147.995
147.339
143.792
137.375
136.002
135.946
125.899
124.755
124.700
122.587
117.195
112.452
40.044
39.835
39.627
39.418
39.210
39.001
38.793
f1 (ppm)

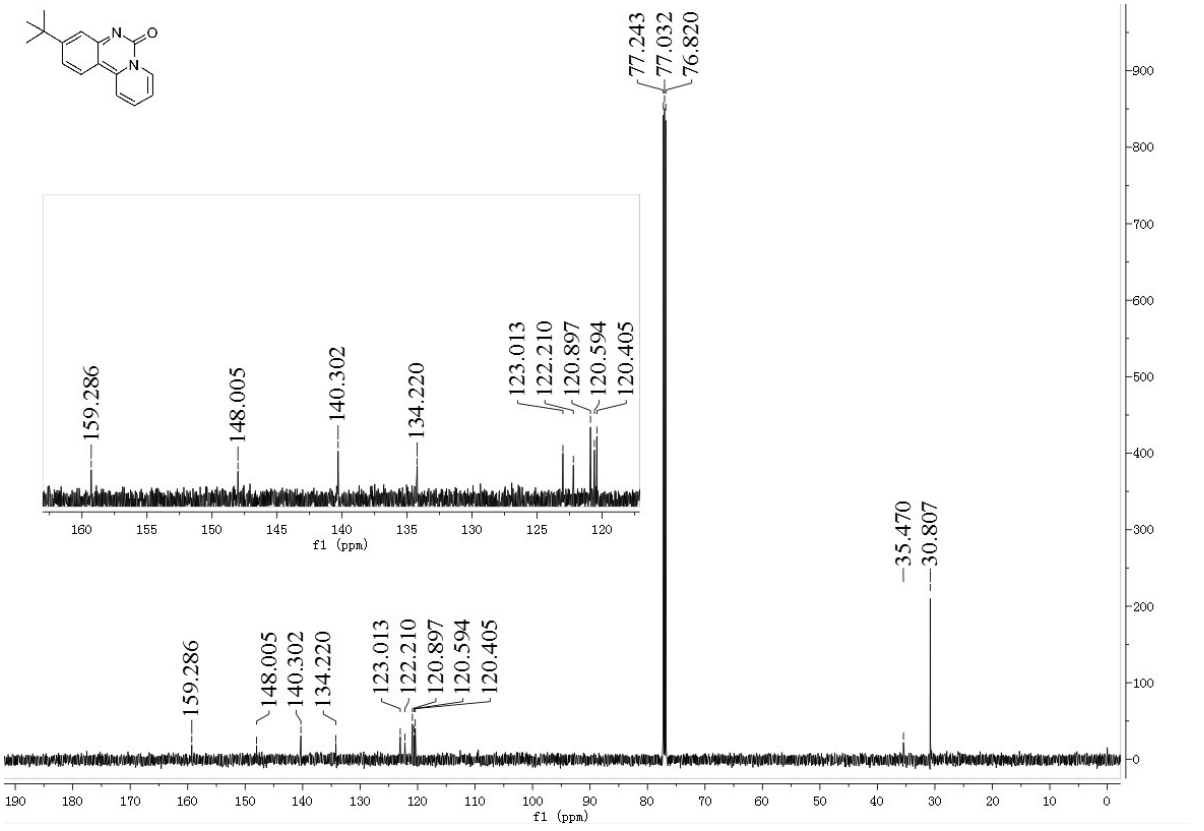
Compound **2b**


9.509
9.492
8.866
8.844
8.405
8.400
8.387
8.376
7.828
7.811
7.794
6.860
6.854
6.837
6.831
6.785
6.779
3.892
3.343
2.511
2.506
2.502
f1 (ppm)

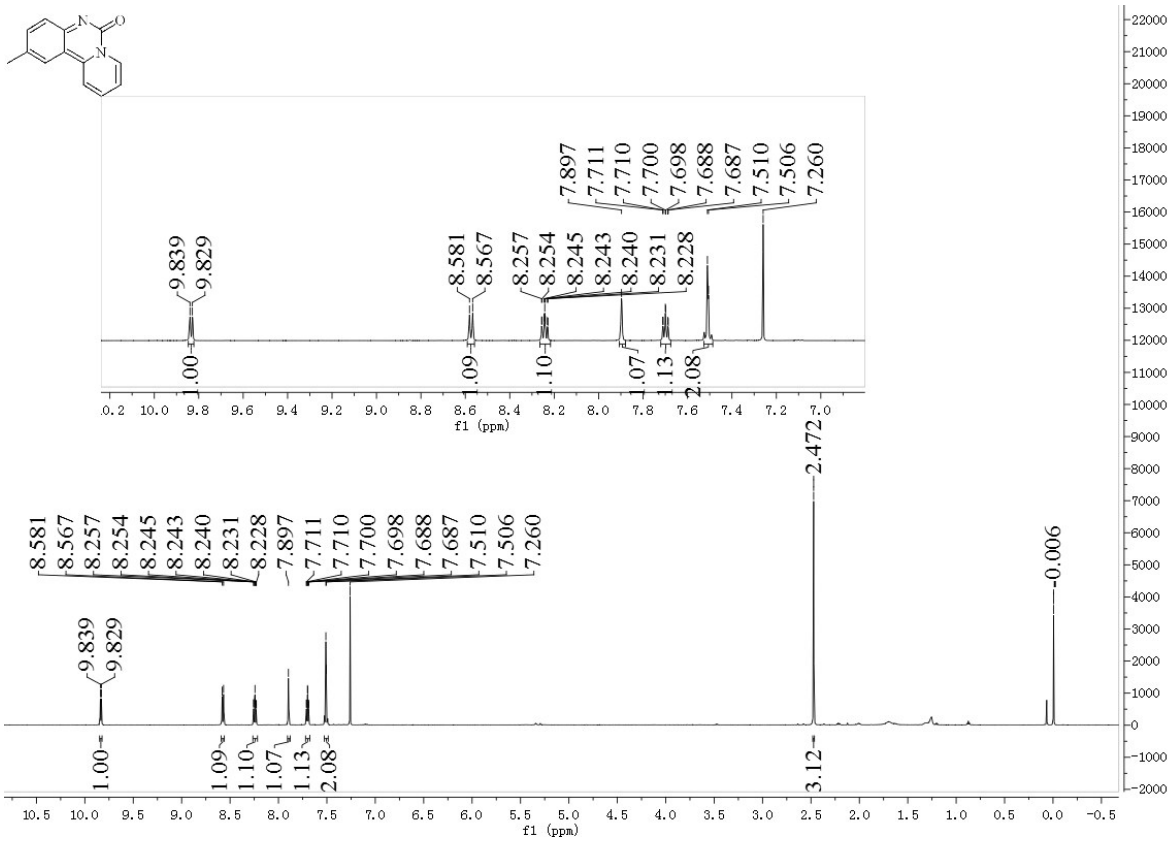

164.701
152.950
147.873
146.955
141.636
133.468
126.882
121.371
113.042
106.649
105.244
40.618
40.409
40.201
39.992
39.783
39.575
39.366
56.009
f1 (ppm)

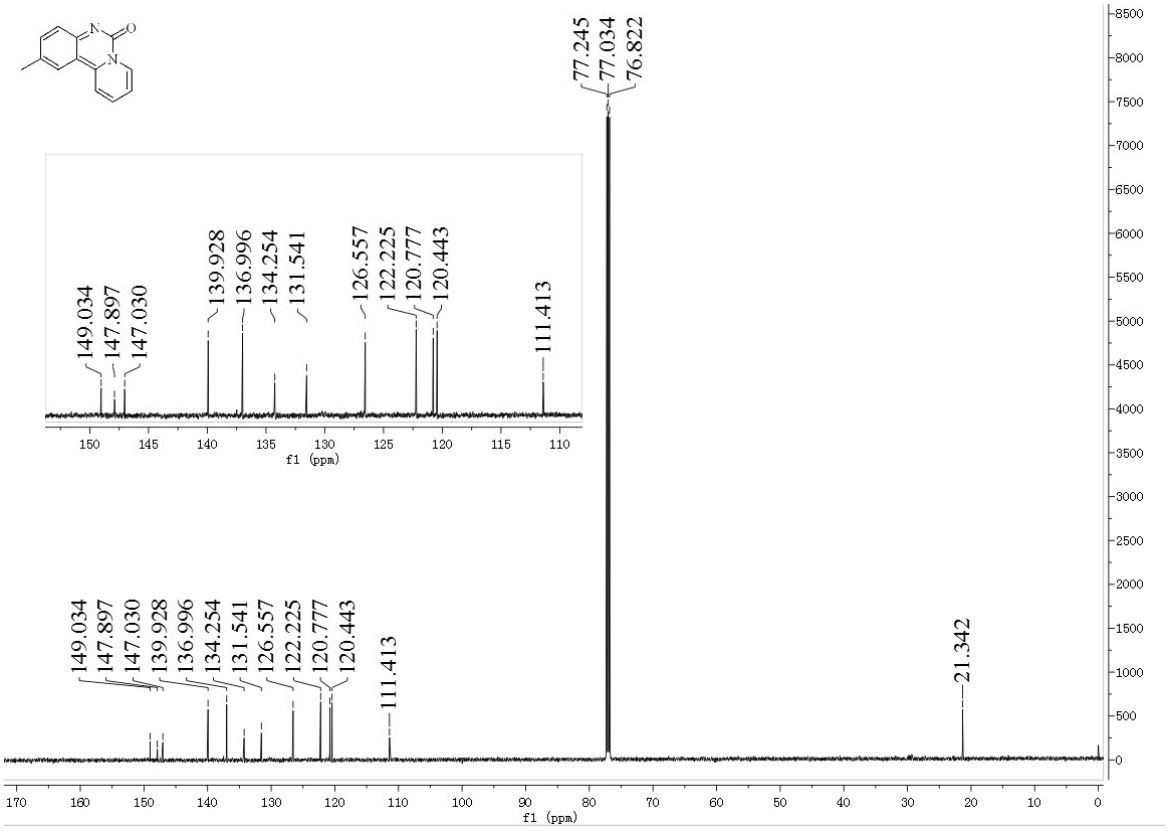
Compound **2c**


9.807
9.796
8.564
8.550
8.268
8.256
8.243
8.086
8.071
7.700
7.689
7.678
7.627
7.334
7.319
7.260
1.388
-0.005
1.08
1.11
1.11
1.07
1.10
1.01
1.08
9.00
f1 (ppm)

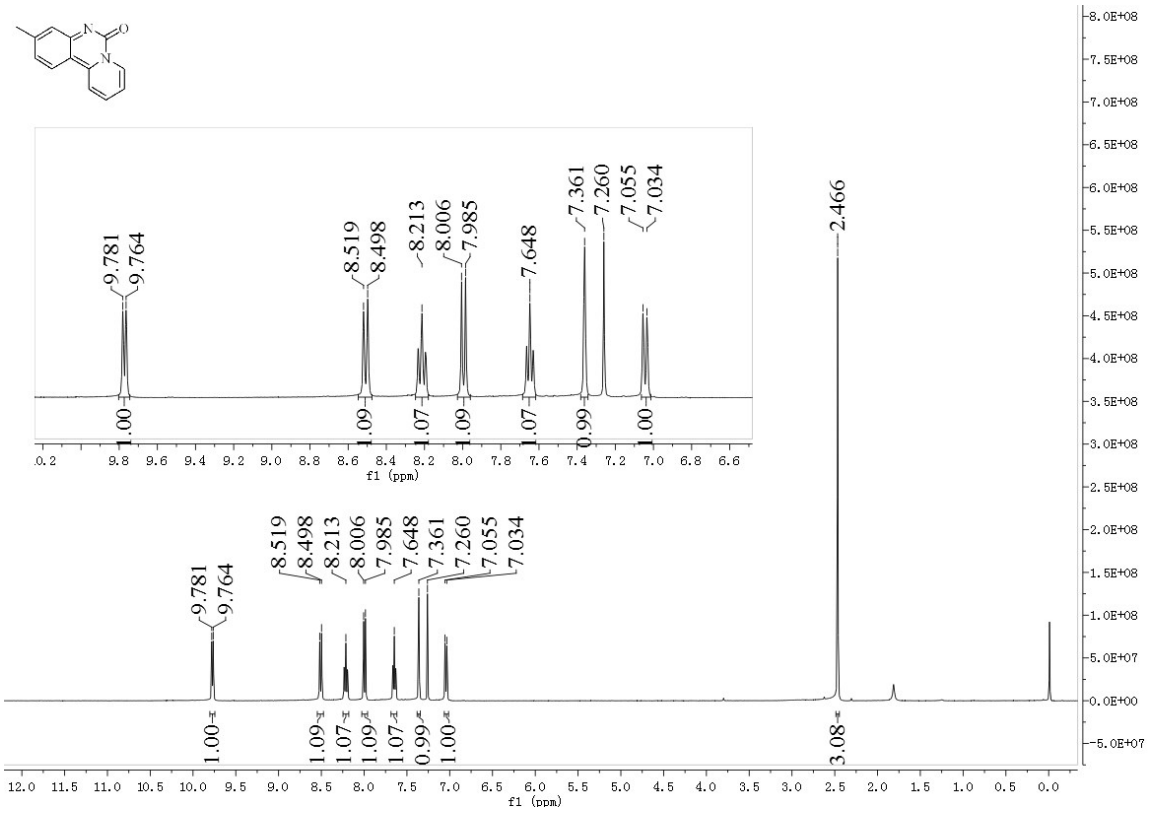

77.243
77.032
76.820
159.286
148.005
140.302
134.220
123.013
122.210
120.897
120.594
120.405
35.470
30.807
f1 (ppm)

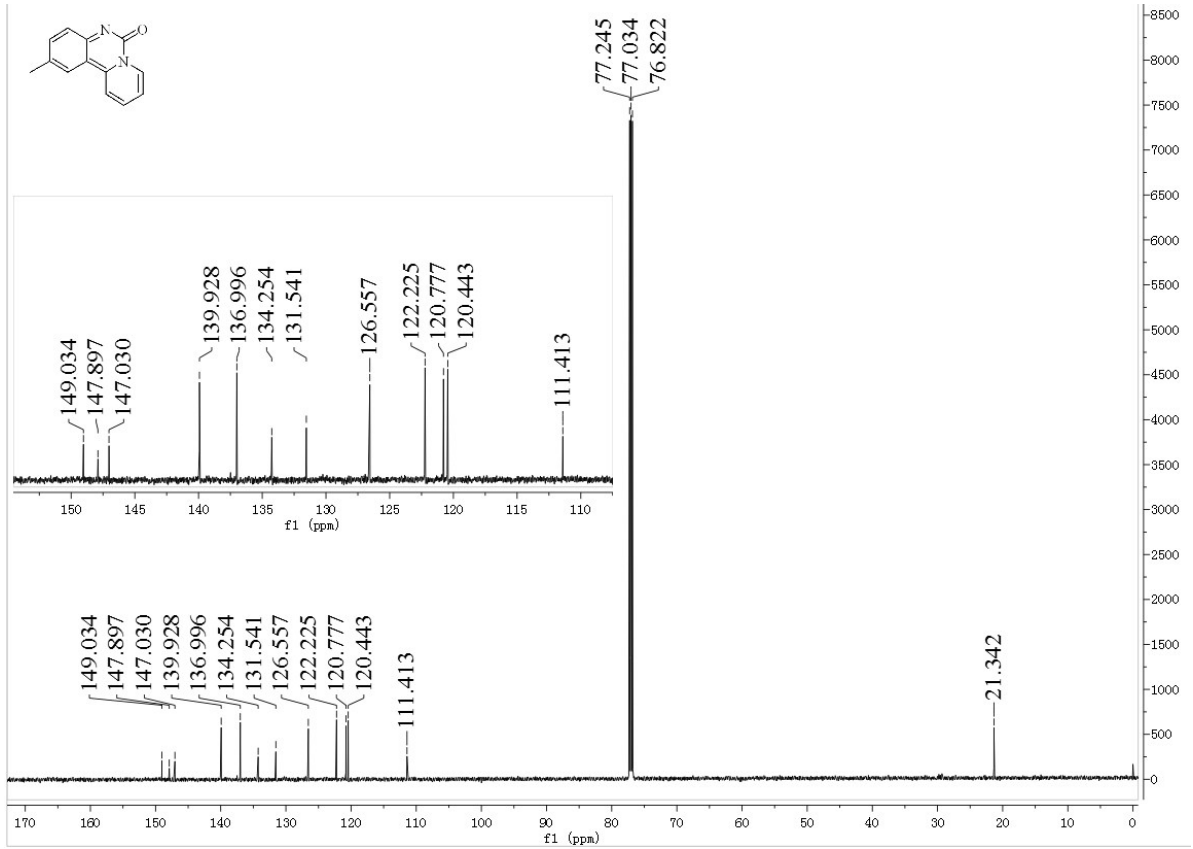
Compound **2d**


9.839
9.829
8.581
8.567
8.257
8.254
8.245
8.243
8.240
8.231
8.228
7.897
7.711
7.710
7.700
7.698
7.688
7.687
7.510
7.506
7.260
2.472
0.006
1.00
1.09
1.10
1.07
1.13
2.08
3.12
f1 (ppm)

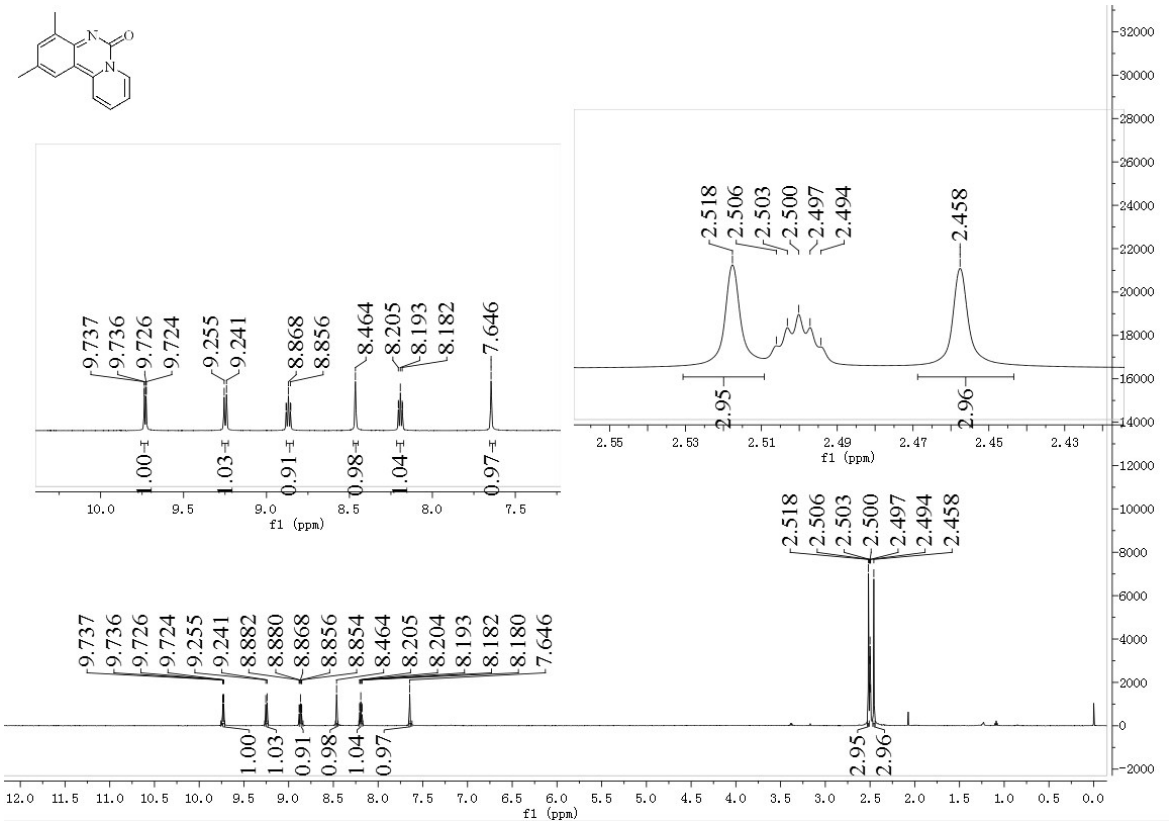

77.245
77.034
76.822
149.034
147.897
147.030
139.928
136.996
134.254
131.541
126.557
122.225
120.777
120.443
111.413
21.342
f1 (ppm)

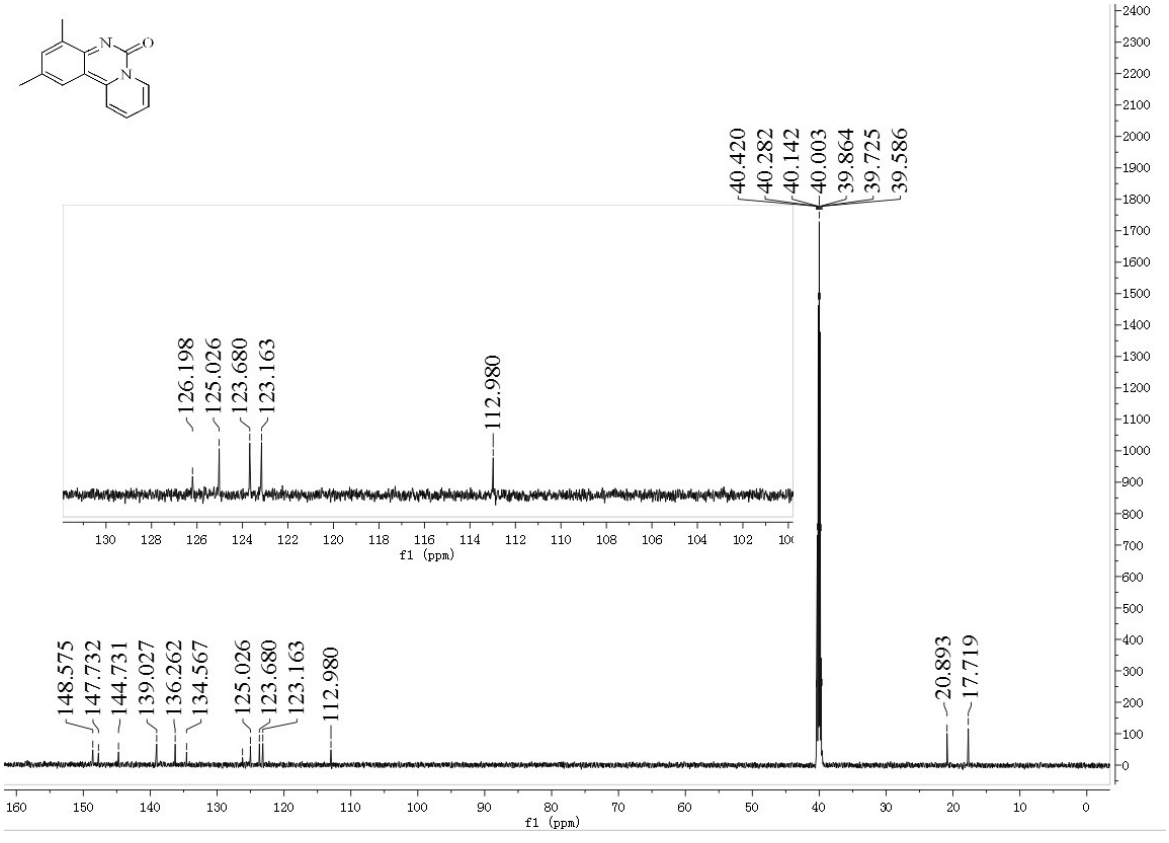
Compound **2e**


9.781
9.764
8.519
8.498
8.213
8.006
7.985
7.648
7.361
7.260
7.055
7.034
2.466
1.00
1.09
1.07
1.09
1.07
0.99
1.00
3.08
f1 (ppm)

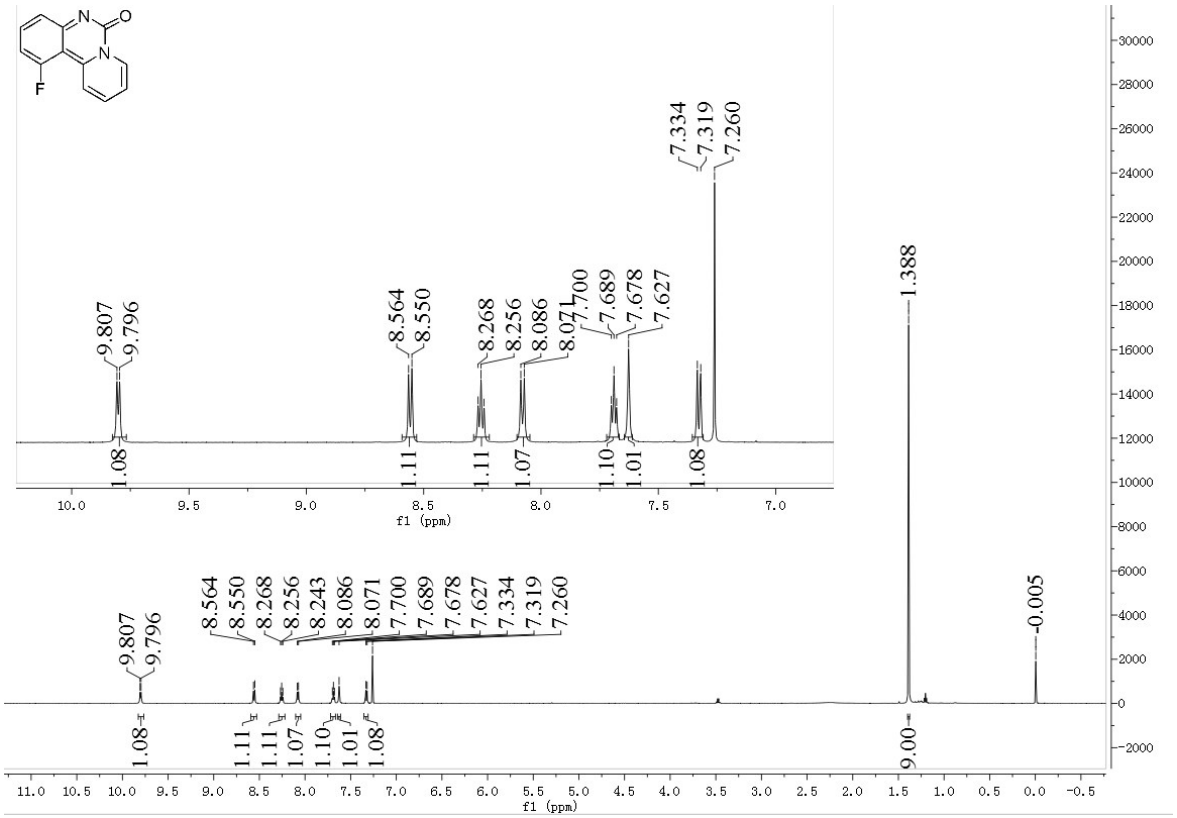

77.245
77.034
76.822
149.034
147.897
147.030
139.928
136.996
134.254
131.541
126.557
122.225
120.777
120.443
111.413
21.342
f1 (ppm)

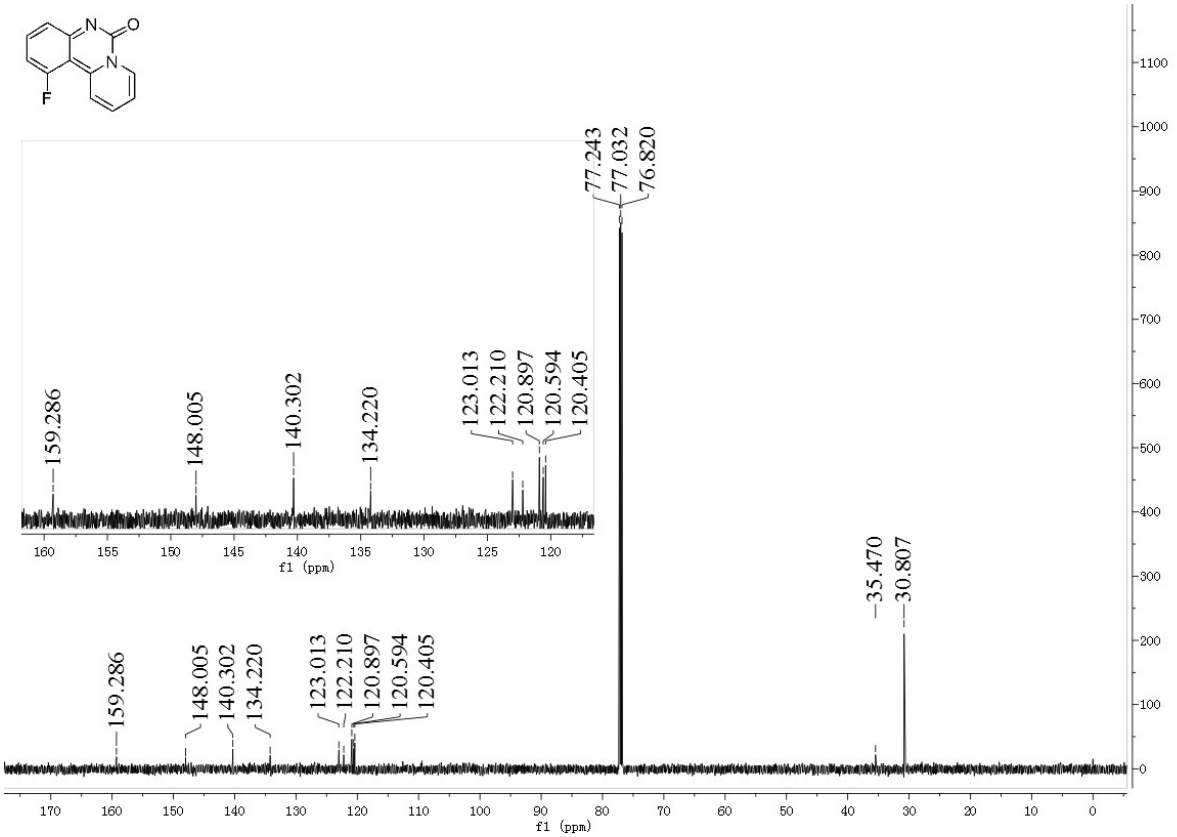
Compound **2f**


9.737
9.736
9.726
9.724
9.255
9.241
8.868
8.856
8.464
8.205
8.193
8.182
7.646
1.00
1.03
0.91
0.98
1.04
0.97
2.518
2.506
2.503
2.500
2.497
2.494
2.458
2.95
2.96
f1 (ppm)

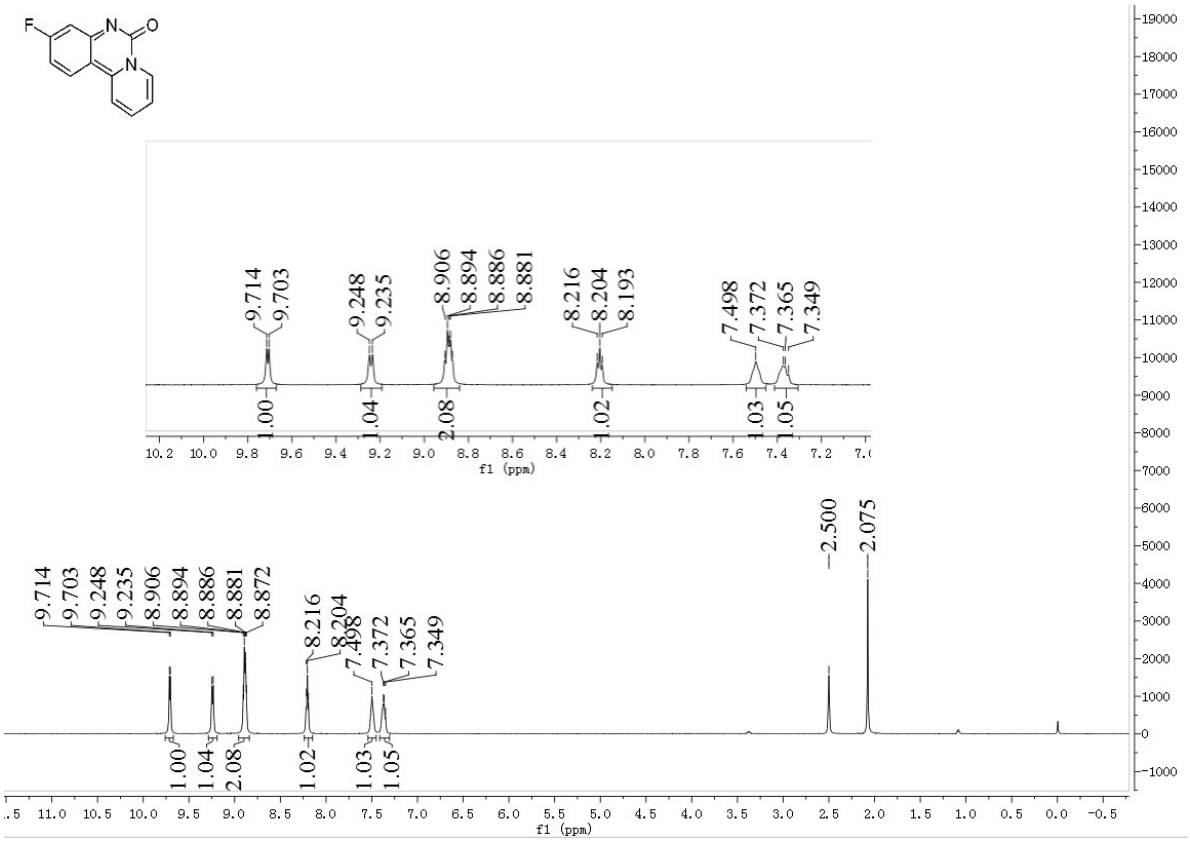

40.420
40.282
40.142
40.003
39.864
39.725
39.586
126.198
125.026
123.680
123.163
112.980
148.575
147.732
144.731
139.027
136.262
134.567
20.893
17.719
f1 (ppm)

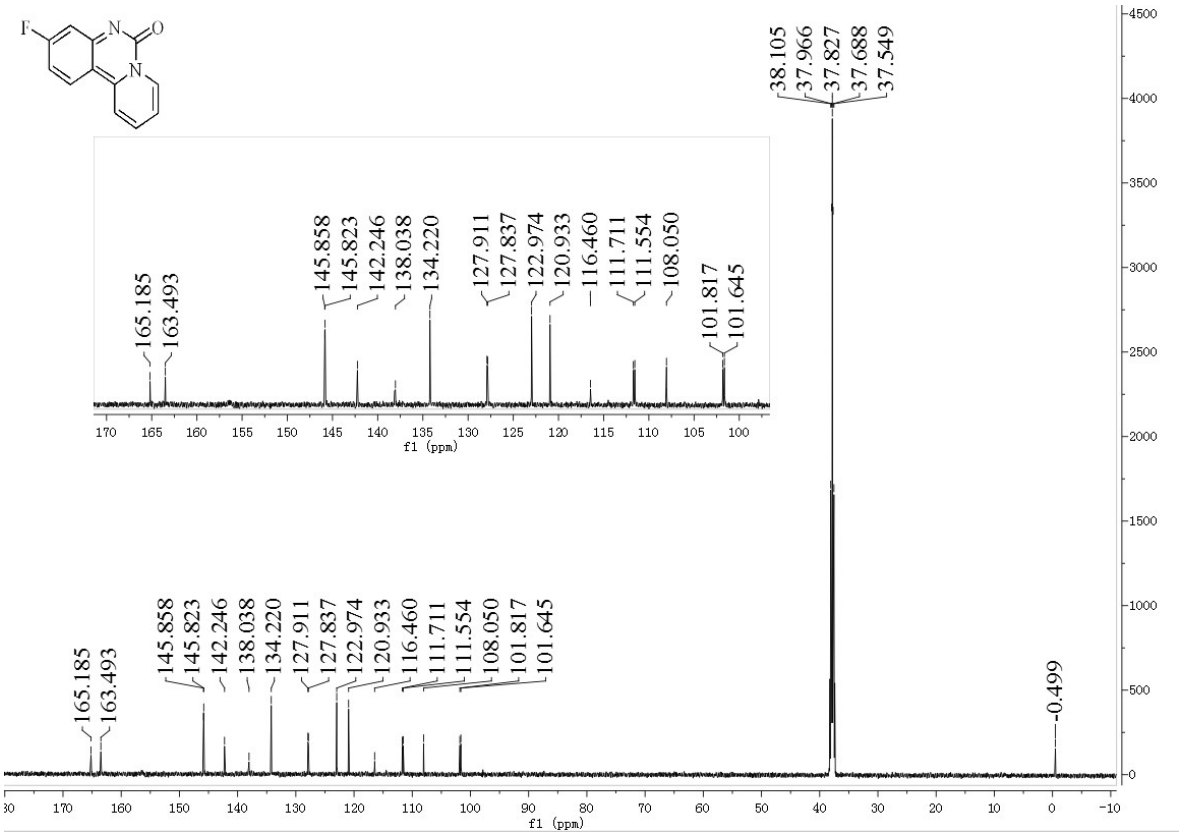
Compound **2g**


9.807
9.796
8.564
8.550
8.268
8.256
8.243
8.086
8.071
7.700
7.689
7.678
7.627
7.334
7.319
7.260
1.388
-0.005
1.08
1.11
1.11
1.07
1.10
1.01
1.08
9.00
f1 (ppm)

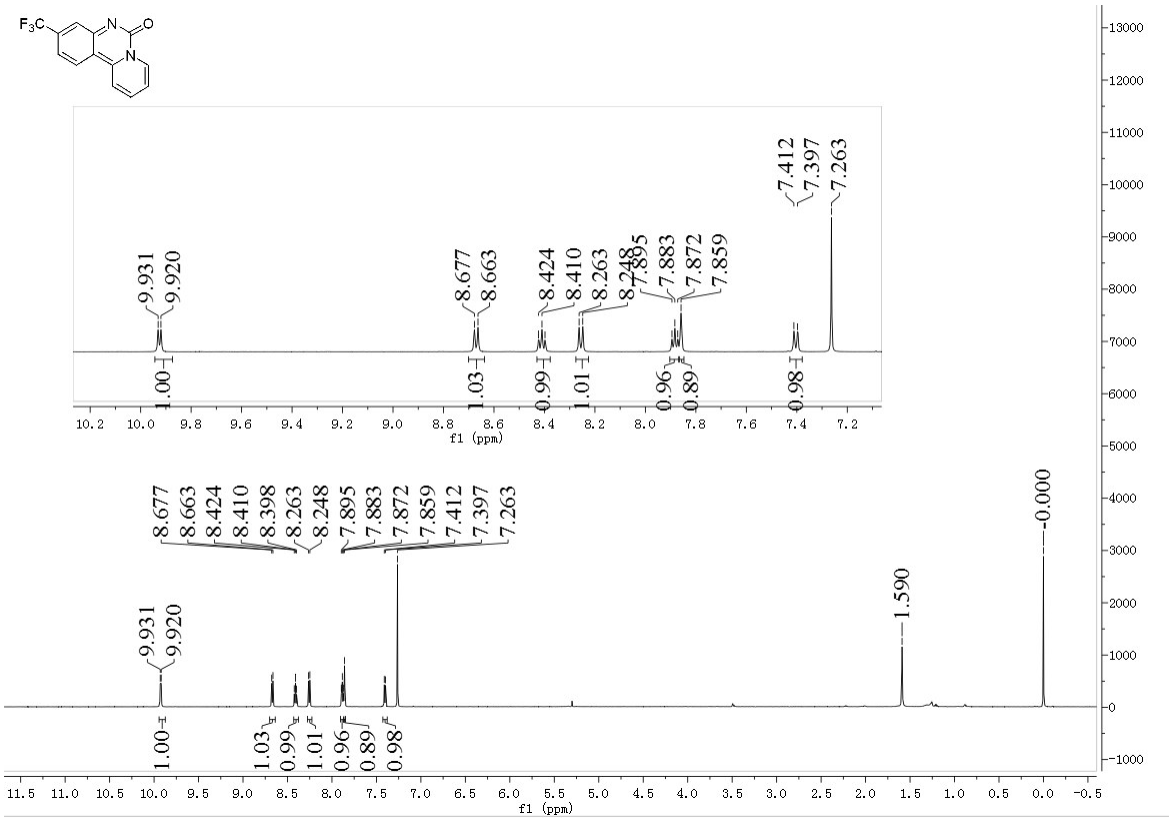

77.243
77.032
76.820
159.286
148.005
140.302
134.220
123.013
122.210
120.897
120.594
120.405
35.470
30.807
f1 (ppm)

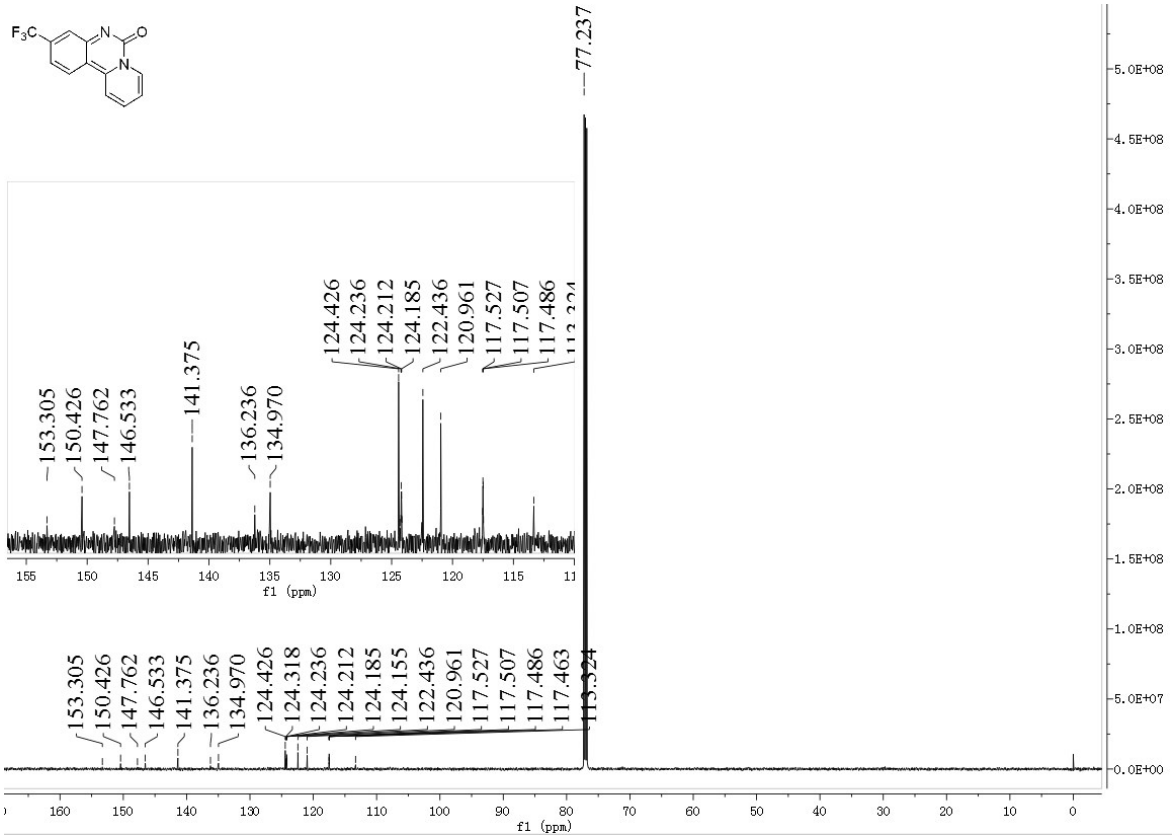
Compound **2h**


F
N
O
N
9.714
9.703
9.248
9.235
8.906
8.894
8.886
8.881
8.872
8.216
8.204
8.193
7.498
7.372
7.365
7.349
2.500
2.075
1.00
1.04
2.08
1.02
1.03
1.05
f1 (ppm)

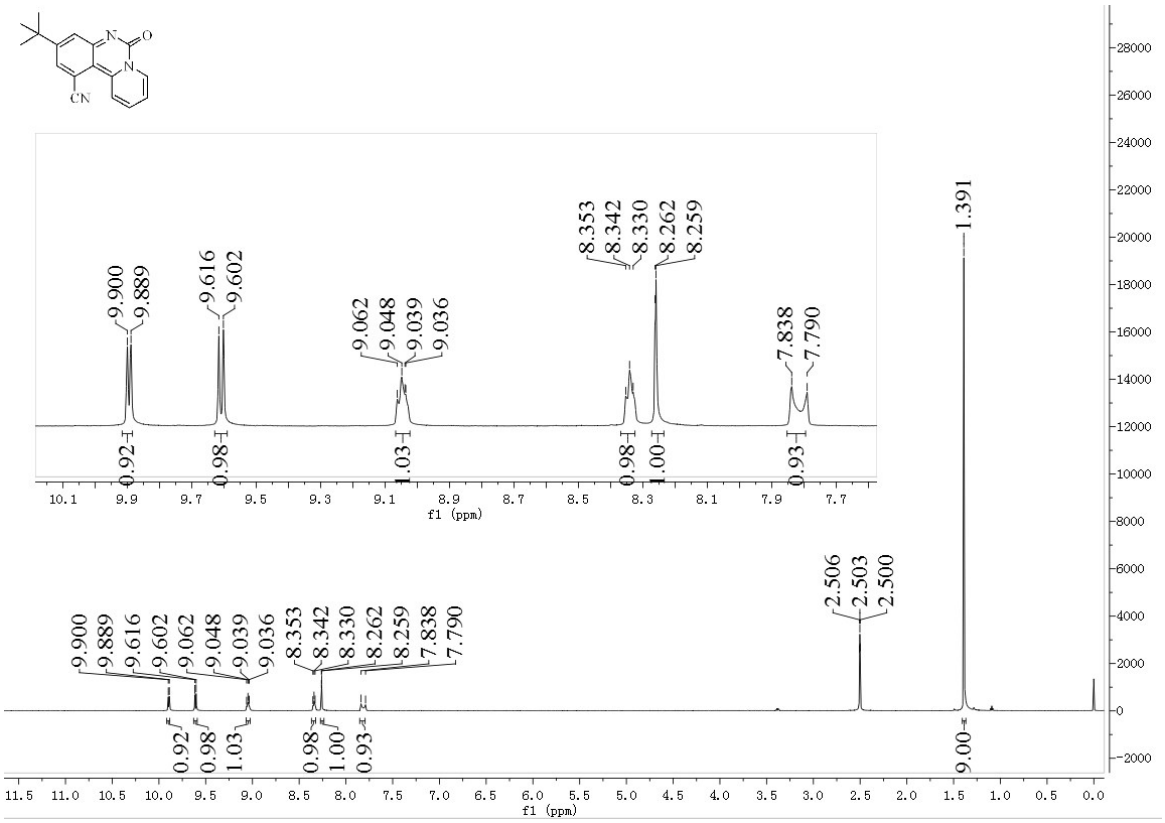

F
N
O
N
38.105
37.966
37.827
37.688
37.549
165.185
163.493
145.858
145.823
142.246
138.038
134.220
127.911
127.837
122.974
120.933
116.460
111.711
111.554
108.050
101.817
101.645
-0.499
f1 (ppm)

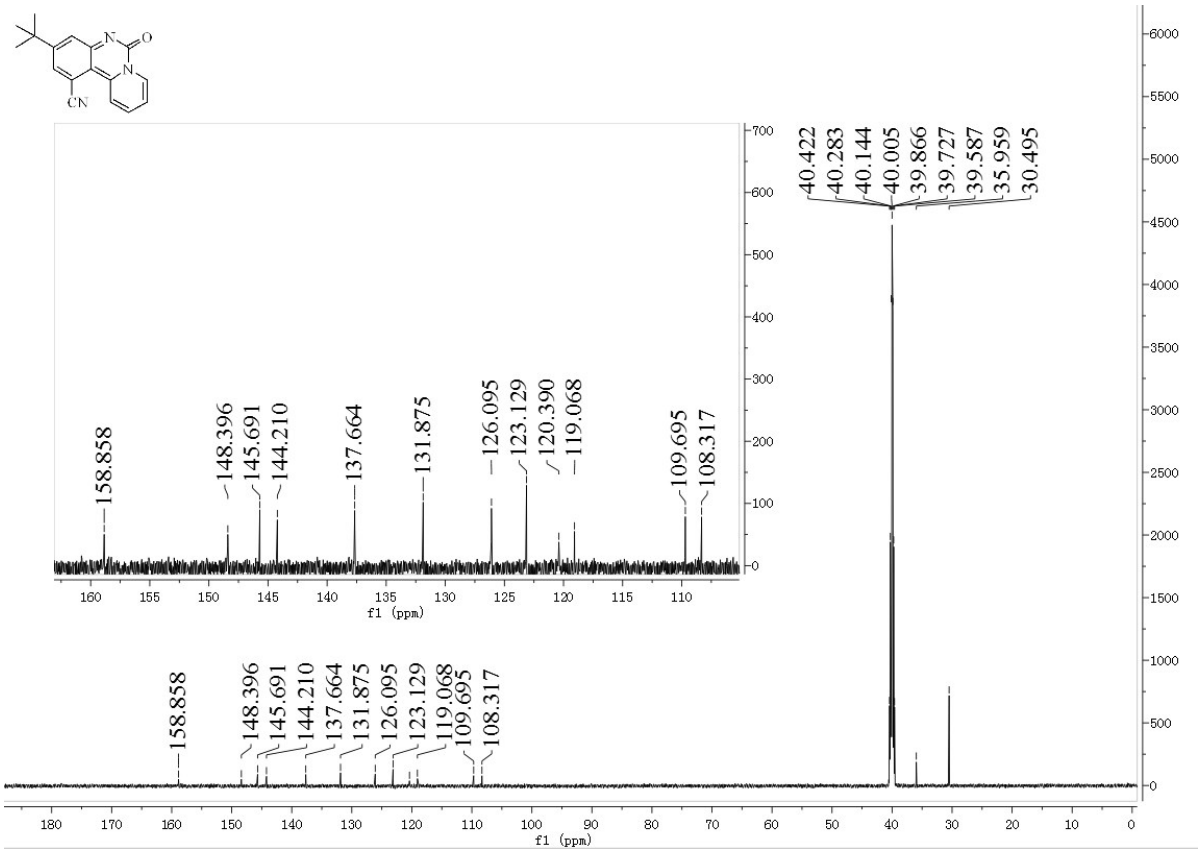
Compound **2i**


F3C
N
O
9.931
9.920
8.677
8.663
8.424
8.410
8.263
8.248
7.895
7.883
7.872
7.859
7.412
7.397
7.263
1.590
0.000
f1 (ppm)

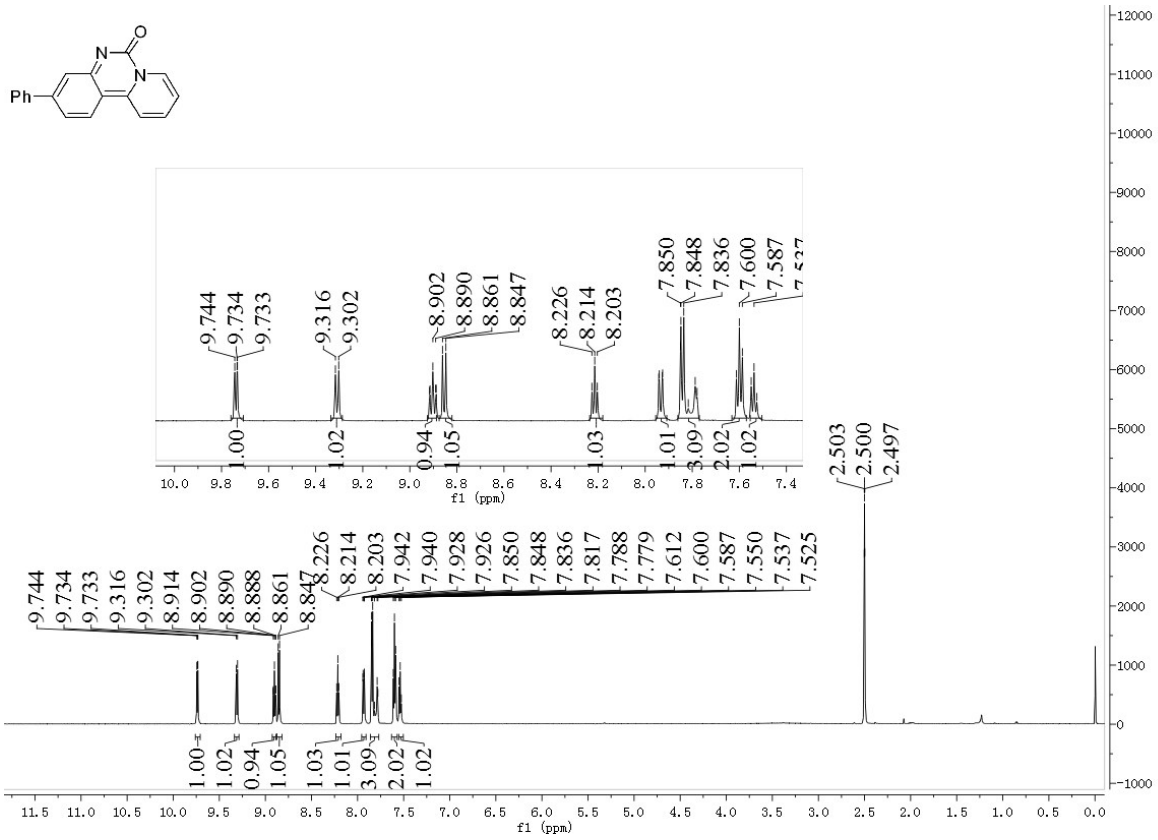

F3C
N
O
77.237
153.305
150.426
147.762
146.533
141.375
136.236
134.970
124.426
124.236
124.212
124.185
122.436
120.961
117.527
117.507
117.486
124.318
124.155
117.463
113.324
f1 (ppm)

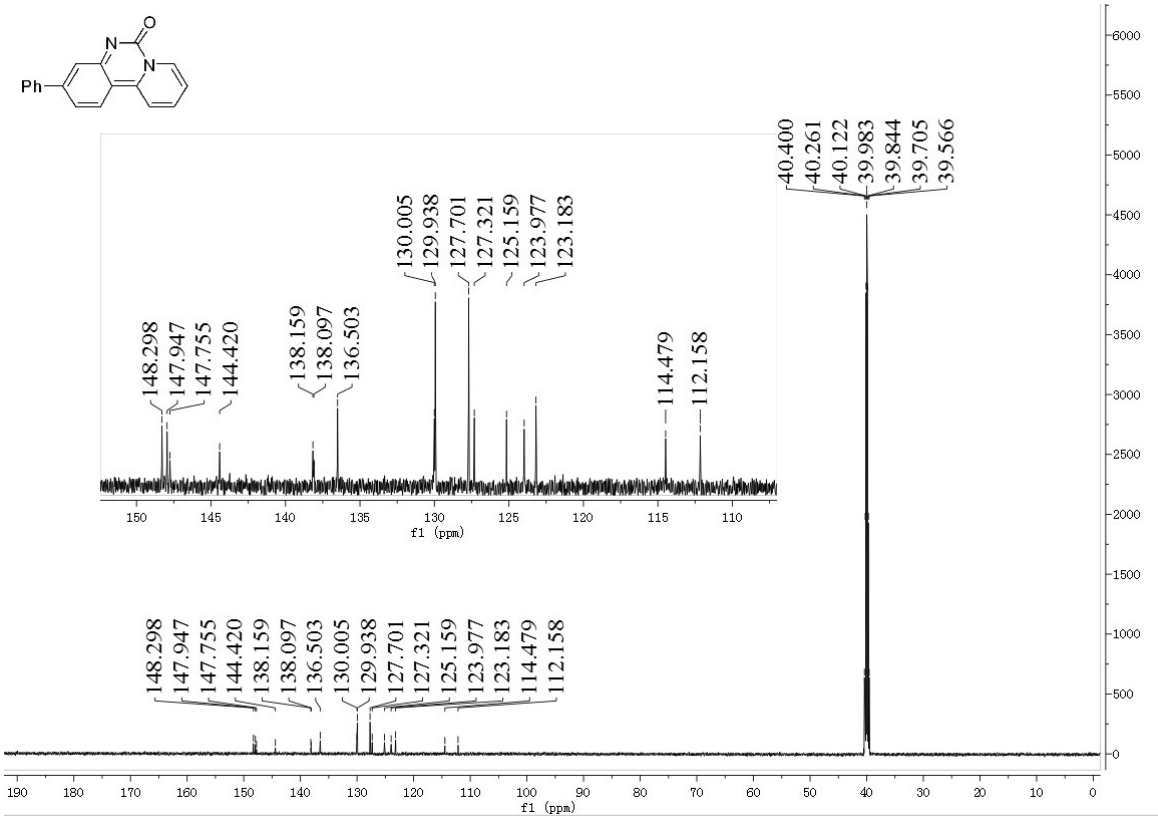
Compound **2j**


9.900
9.889
9.616
9.602
9.062
9.048
9.039
9.036
8.353
8.342
8.330
8.262
8.259
7.838
7.790
1.391
2.506
2.503
2.500
f1 (ppm)

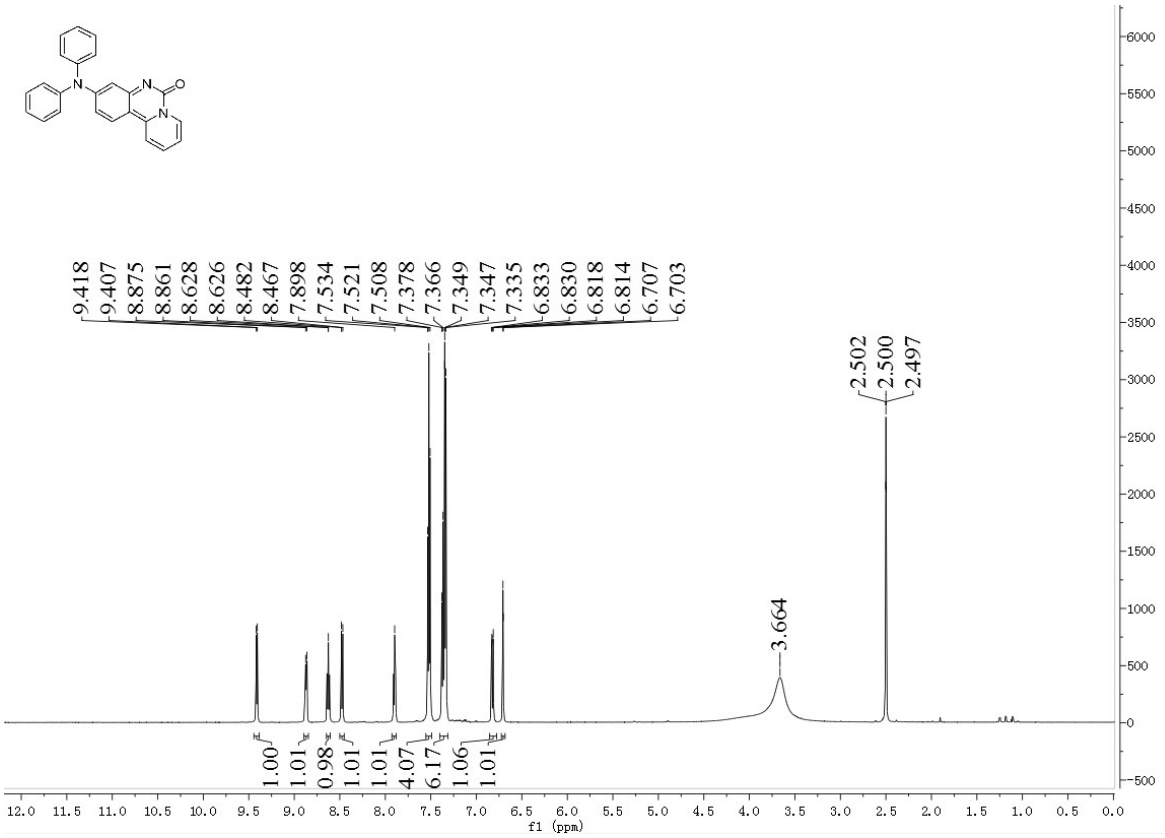

158.858
148.396
145.691
144.210
137.664
131.875
126.095
123.129
120.390
119.068
109.695
108.317
40.422
40.283
40.144
40.005
39.866
39.727
39.587
35.959
30.495
f1 (ppm)

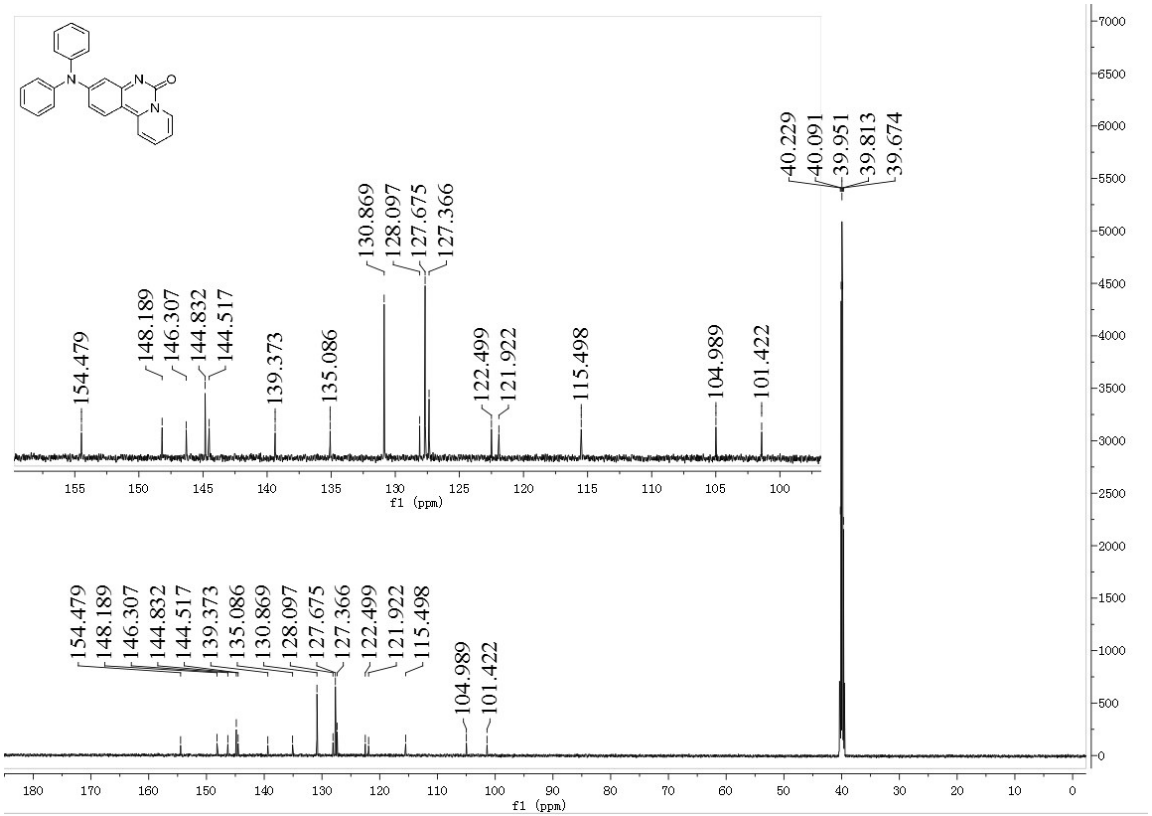
Compound **2k**


Ph
9.744
9.734
9.733
9.316
9.302
8.902
8.890
8.861
8.847
8.226
8.214
8.203
7.850
7.848
7.836
7.600
7.587
2.503
2.500
2.497
f1 (ppm)

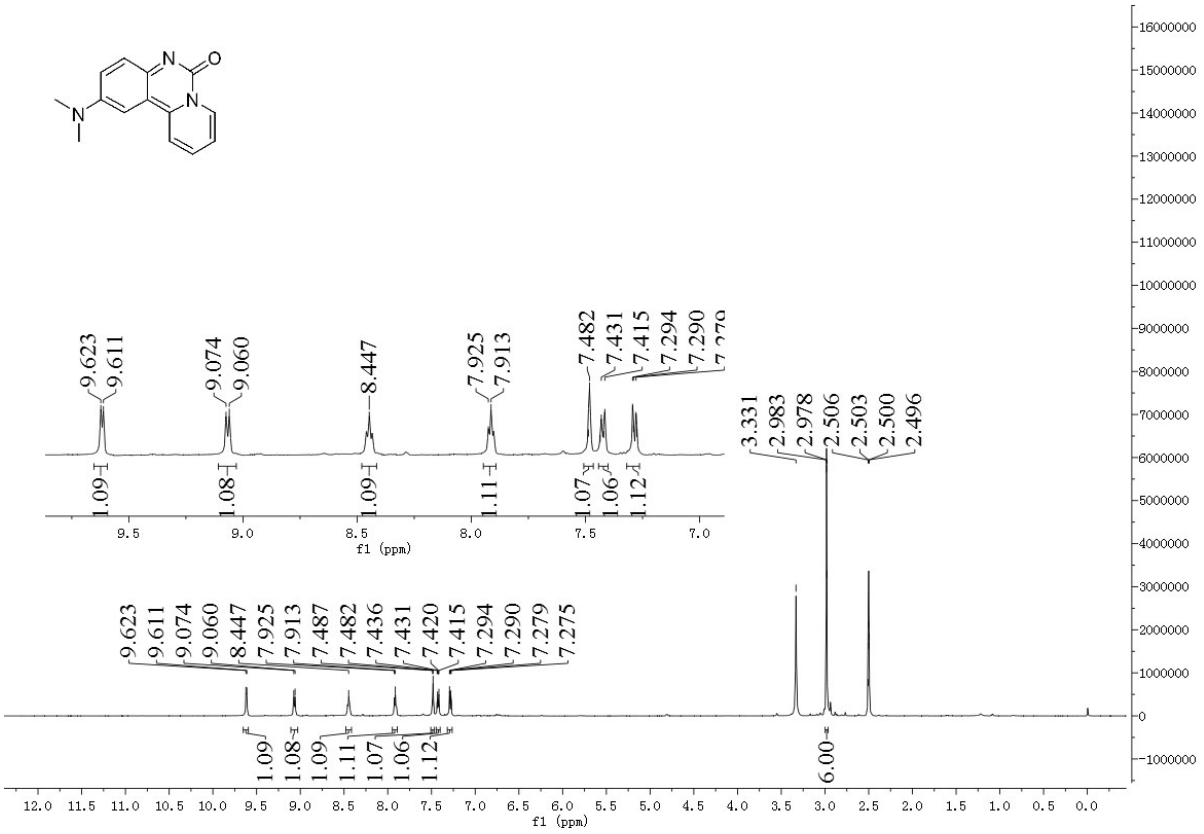

Ph
40.400
40.261
40.122
39.983
39.844
39.705
39.566
130.005
129.938
127.701
127.321
125.159
123.977
123.183
148.298
147.947
147.755
144.420
138.159
138.097
136.503
114.479
112.158
f1 (ppm)

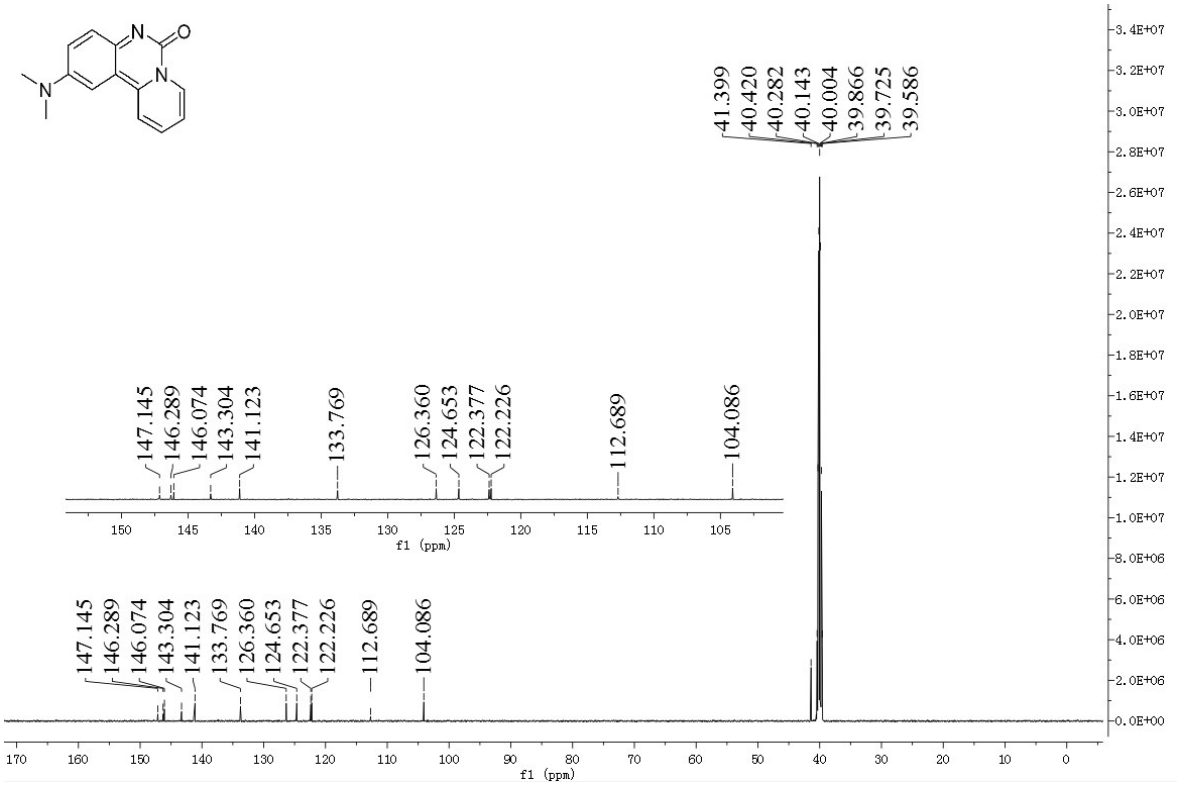
Compound **2l**


9.418
9.407
8.875
8.861
8.628
8.626
8.482
8.467
7.898
7.534
7.521
7.508
7.378
7.366
7.349
7.347
7.335
6.833
6.830
6.818
6.814
6.707
6.703
2.502
2.500
2.497
3.664
1.00
1.01
0.98
1.01
1.01
4.07
6.17
1.06
1.01
f1 (ppm)

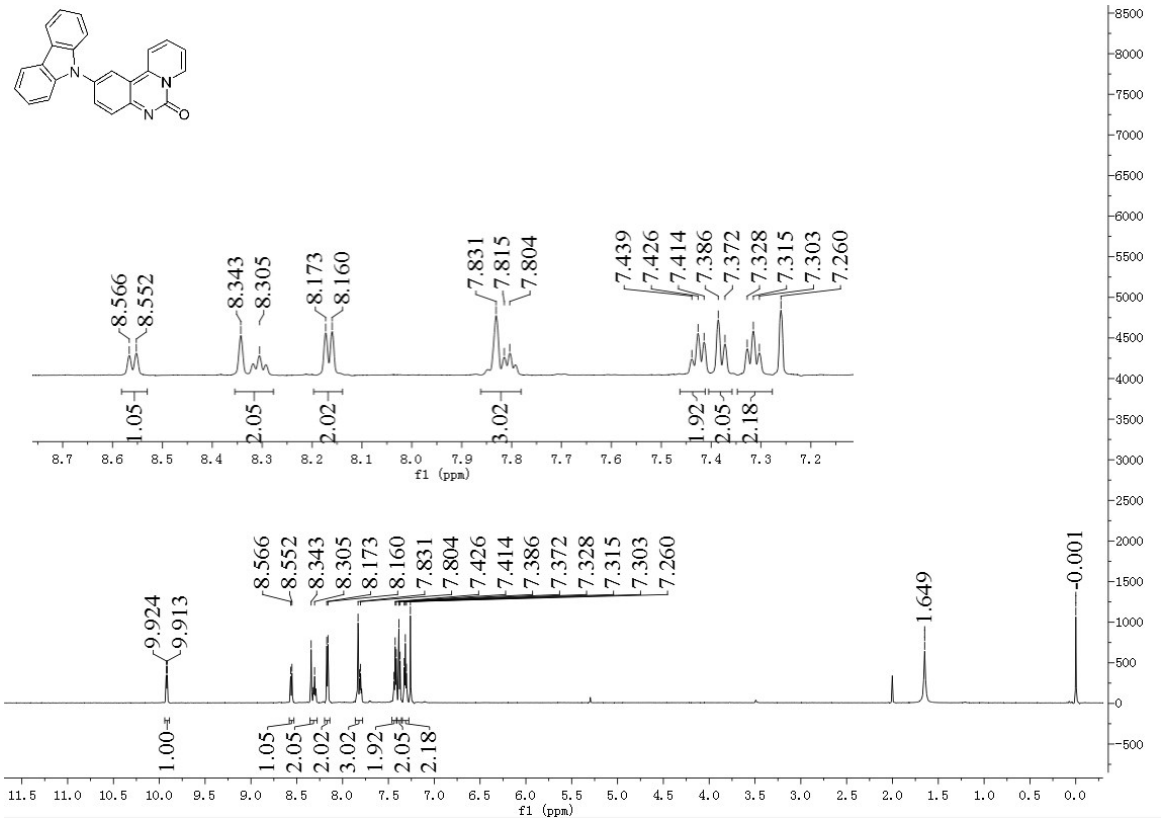

154.479
148.189
146.307
144.832
144.517
139.373
135.086
130.869
128.097
127.675
127.366
122.499
121.922
115.498
104.989
101.422
40.229
40.091
39.951
39.813
39.674
f1 (ppm)

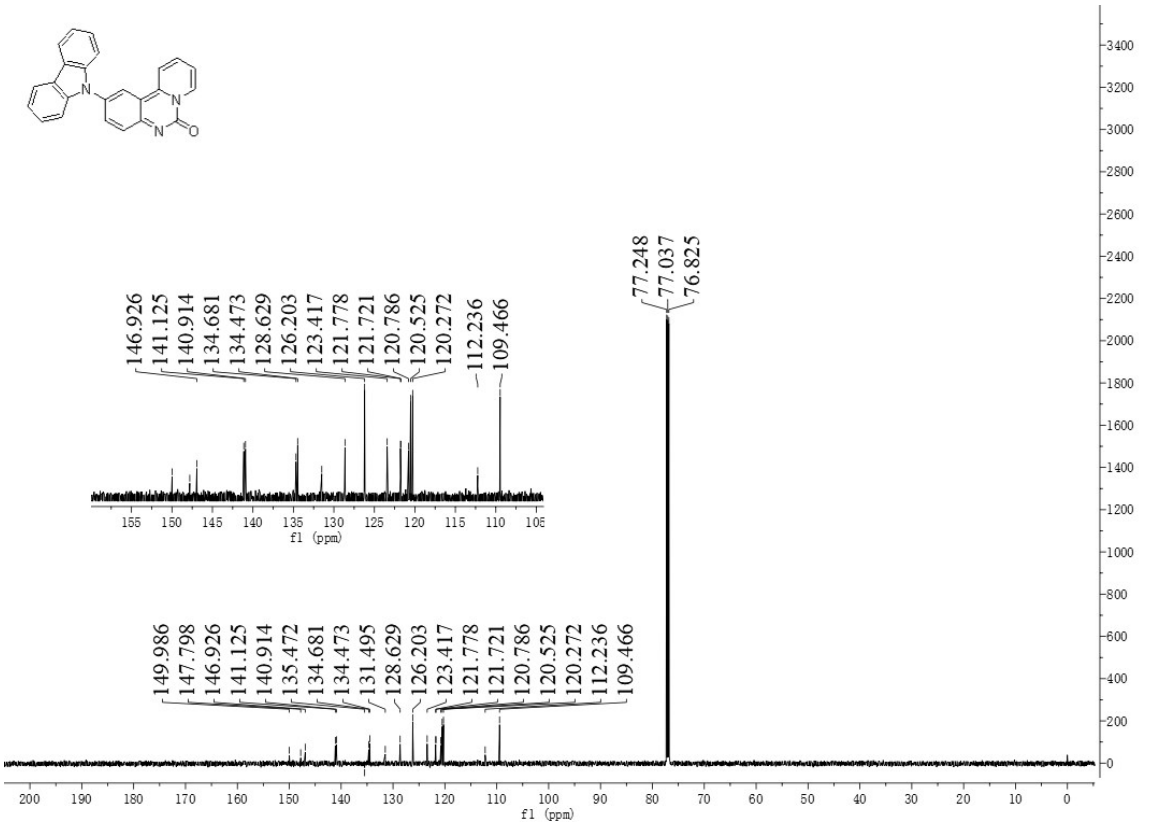
Compound **2m**


9.623
9.611
9.074
9.060
8.447
7.925
7.913
7.482
7.431
7.415
7.294
7.290
3.331
2.983
2.978
2.506
2.503
2.500
2.496
1.09
1.08
1.09
1.11
1.07
1.06
1.12
6.00
f1 (ppm)

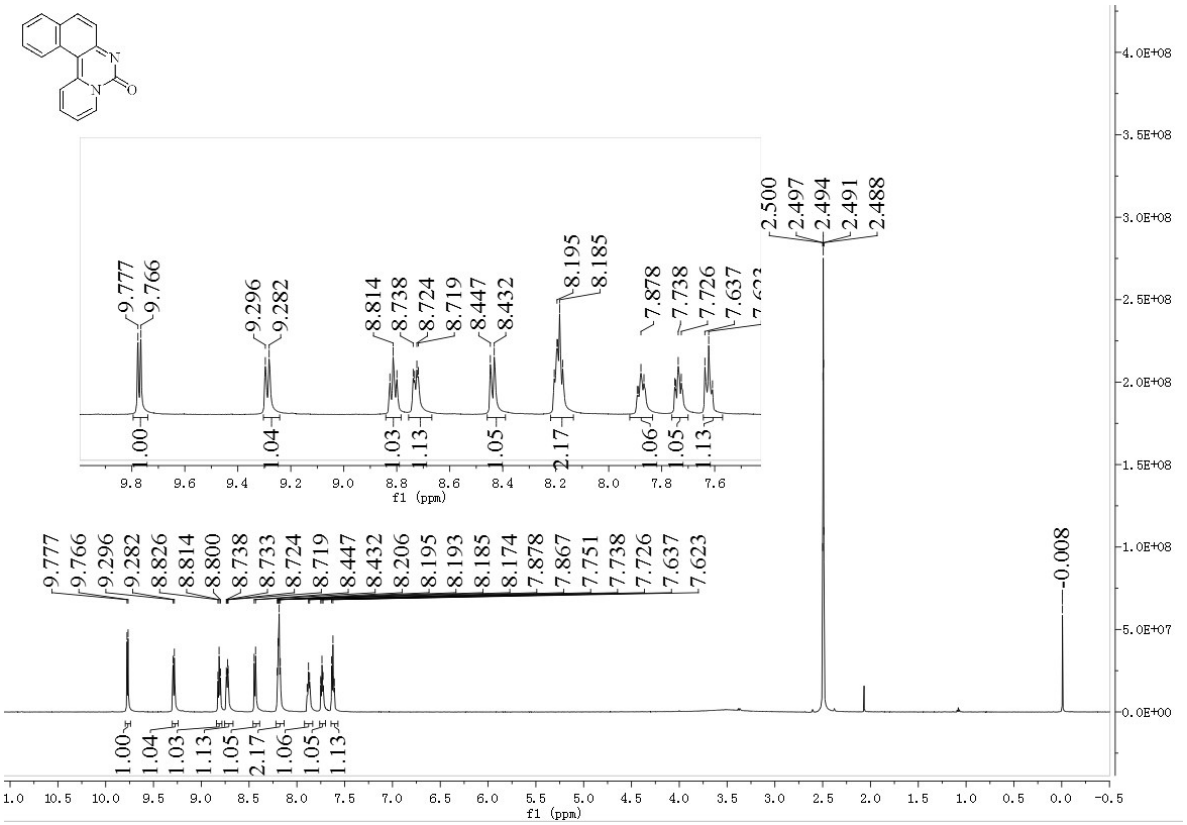

41.399
40.420
40.282
40.143
40.004
39.866
39.725
39.586
147.145
146.289
146.074
143.304
141.123
133.769
126.360
124.653
122.377
122.226
112.689
104.086
f1 (ppm)

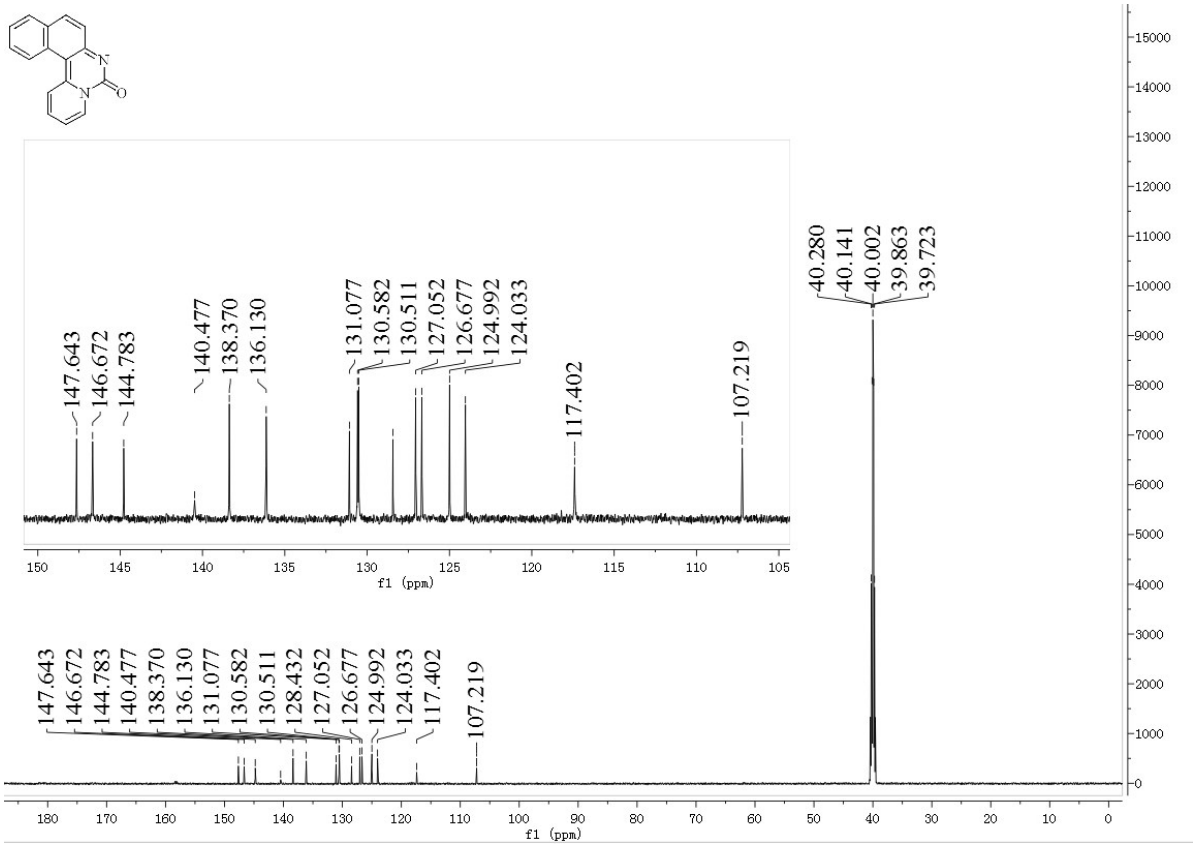
Compound **2n**


8.566
8.552
8.343
8.305
8.173
8.160
7.831
7.815
7.804
7.439
7.426
7.414
7.386
7.372
7.328
7.315
7.303
7.260
1.05
2.05
2.02
3.02
1.92
2.05
2.18
f1 (ppm)
9.924
9.913
1.649
-0.001
1.00

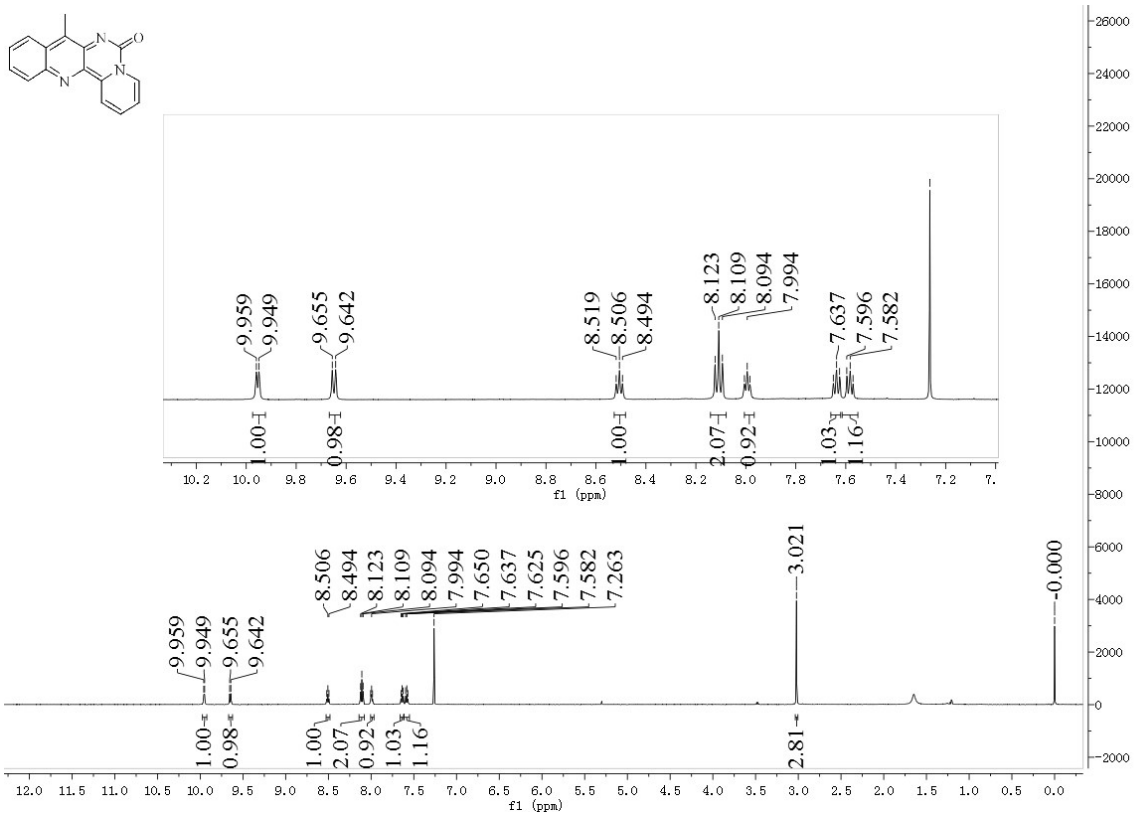

146.926
141.125
140.914
134.681
134.473
128.629
126.203
123.417
121.778
121.721
120.786
120.525
120.272
112.236
109.466
77.248
77.037
76.825
149.986
147.798
146.926
141.125
140.914
135.472
134.681
134.473
131.495
128.629
126.203
123.417
121.778
121.721
120.786
120.525
120.272
112.236
109.466
f1 (ppm)

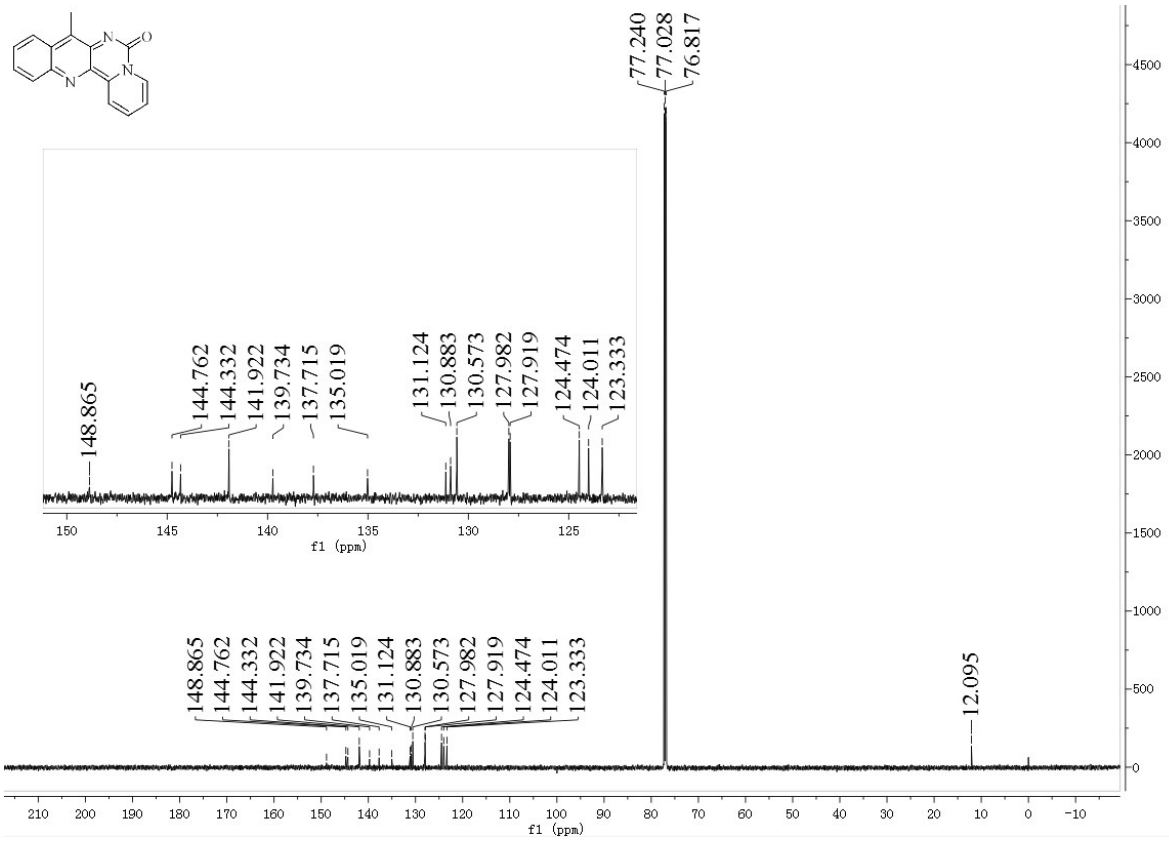
Compound **2o**


9.777
9.766
9.296
9.282
8.814
8.738
8.724
8.719
8.447
8.432
8.195
8.185
7.878
7.738
7.726
7.637
2.500
2.497
2.494
2.491
2.488
-0.008
f1 (ppm)

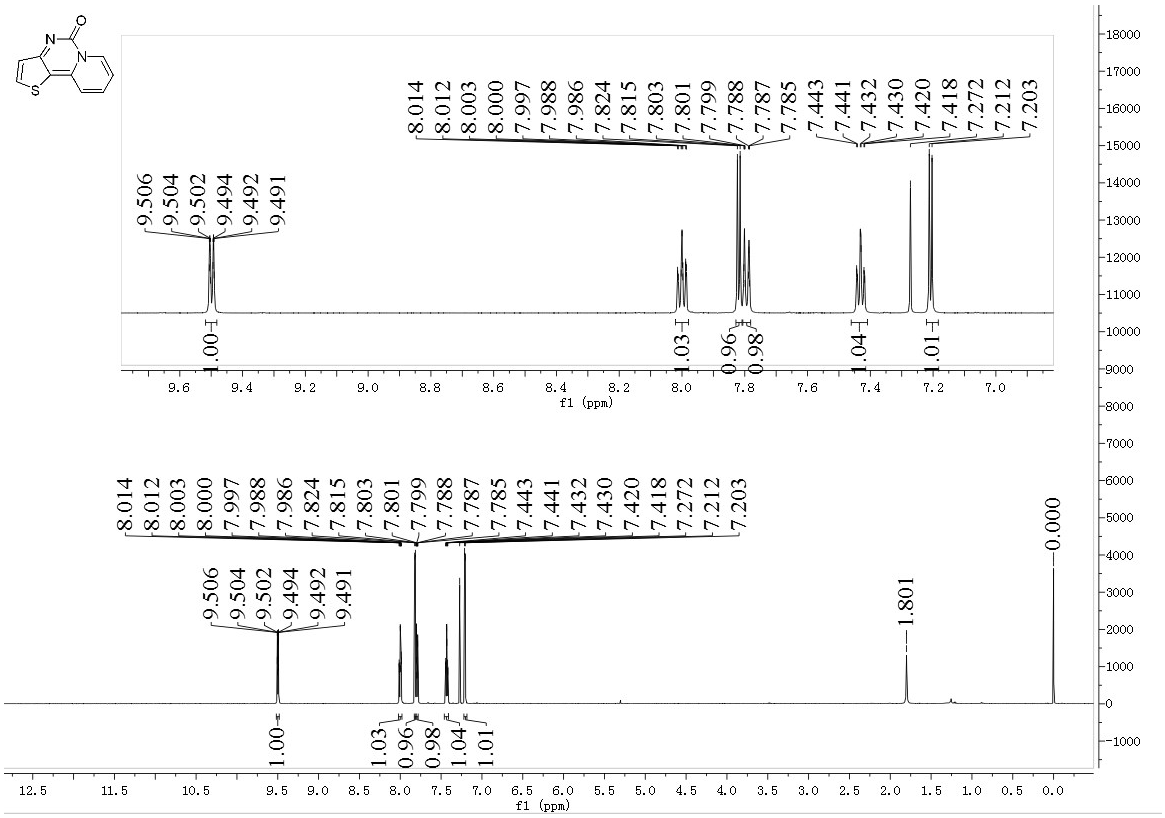

147.643
146.672
144.783
140.477
138.370
136.130
131.077
130.582
130.511
128.432
127.052
126.677
124.992
124.033
117.402
107.219
40.280
40.141
40.002
39.863
39.723
f1 (ppm)

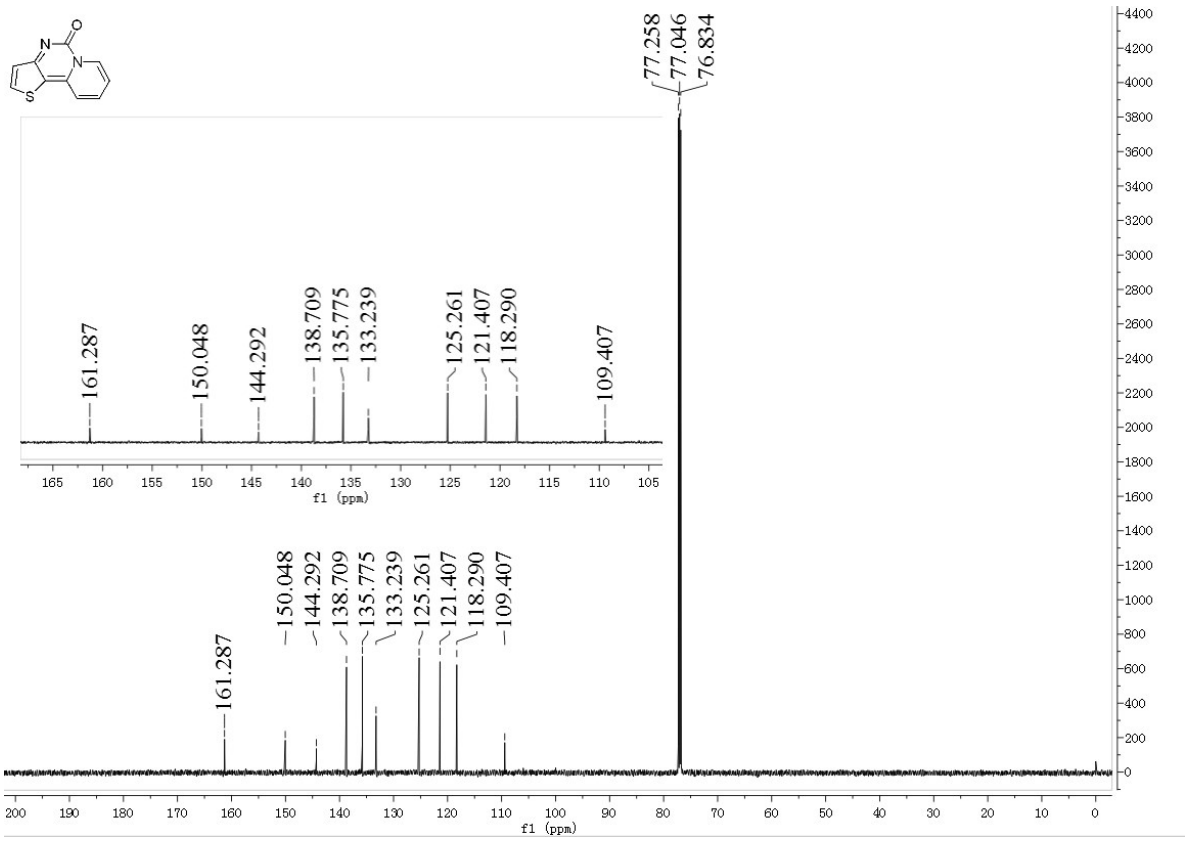
Compound **2p**


9.959
9.949
9.655
9.642
8.519
8.506
8.494
8.123
8.109
8.094
7.994
7.637
7.596
7.582
1.00
0.98
1.00
2.07
0.92
1.03
1.16
f1 (ppm)
8.506
8.494
8.123
8.109
8.094
7.994
7.650
7.637
7.625
7.596
7.582
7.263
3.021
-0.000
2.81
f1 (ppm)

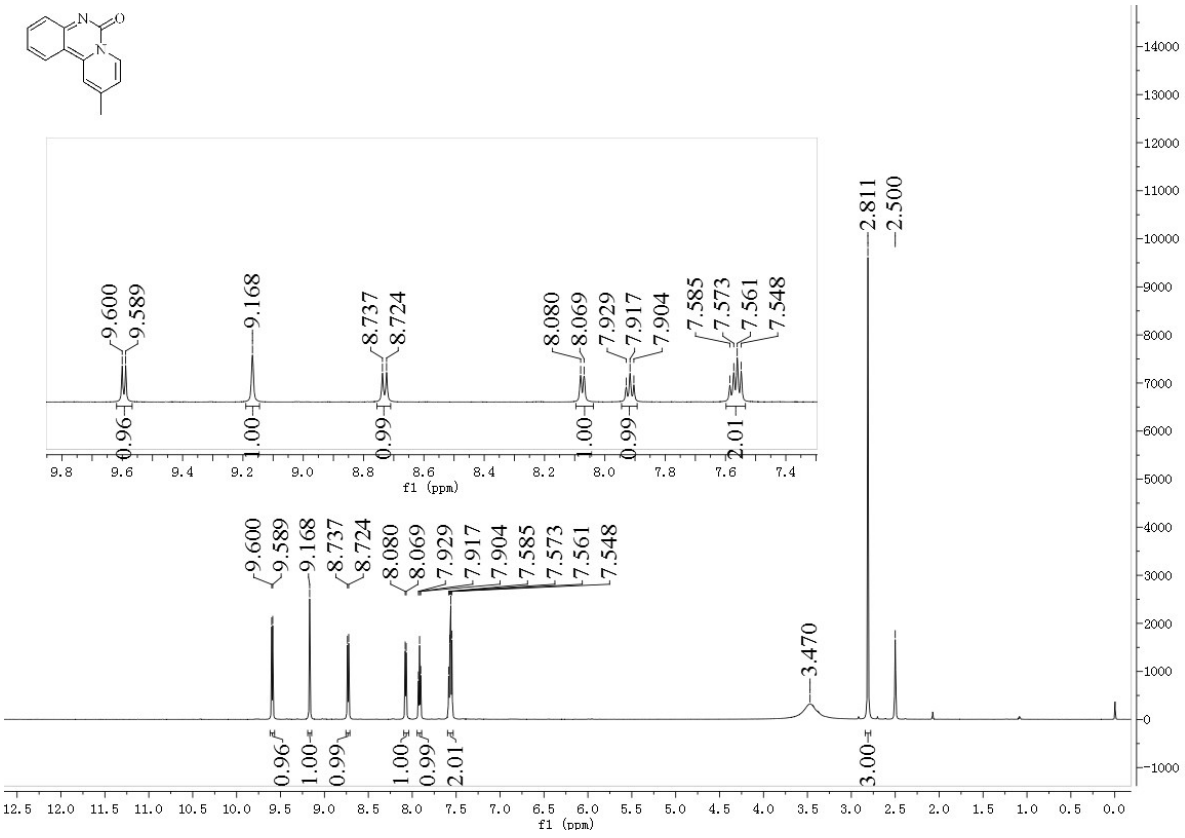

77.240
77.028
76.817
148.865
144.762
144.332
141.922
139.734
137.715
135.019
131.124
130.883
130.573
127.982
127.919
124.474
124.011
123.333
f1 (ppm)
12.095
f1 (ppm)

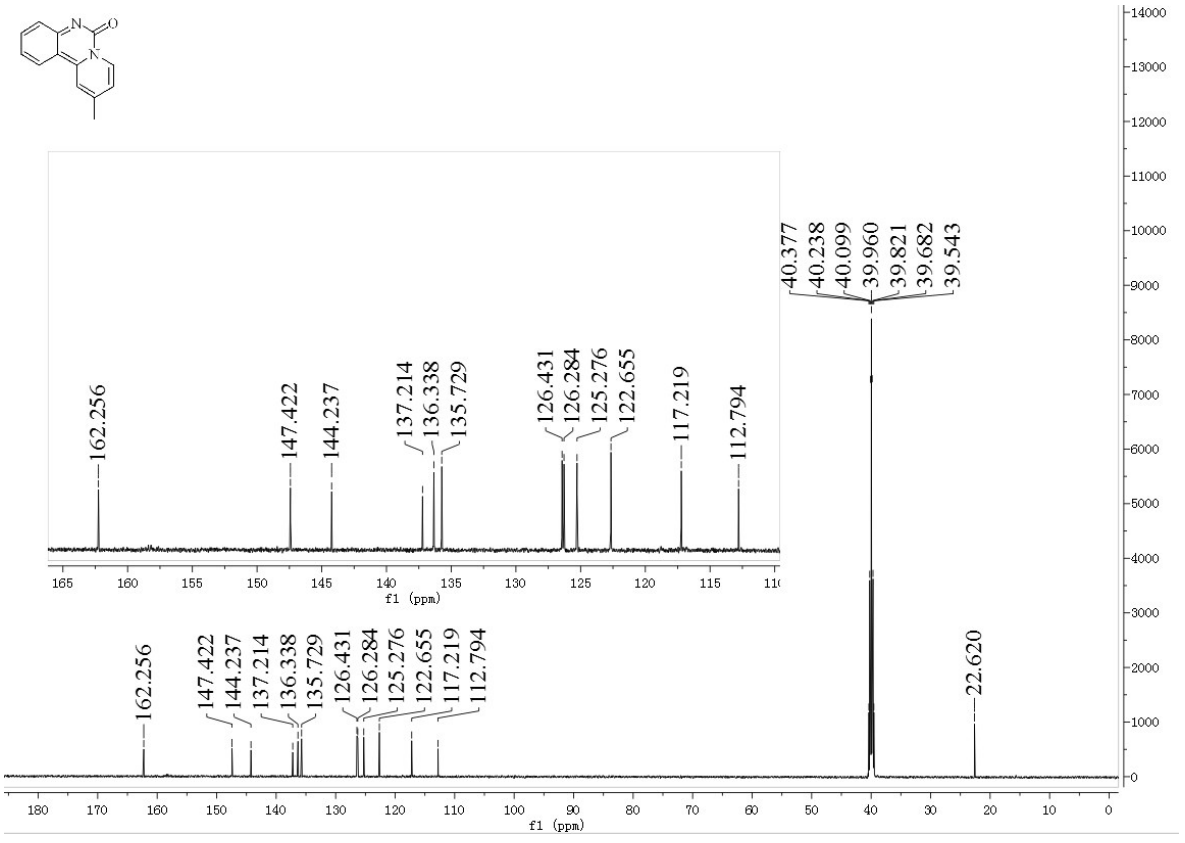
Compound **2r**


8.014
8.012
8.003
8.000
7.997
7.988
7.986
7.824
7.815
7.803
7.801
7.799
7.788
7.787
7.785
7.443
7.441
7.432
7.430
7.420
7.418
7.272
7.212
7.203
9.506
9.504
9.502
9.494
9.492
9.491
1.00
1.03
0.96
0.98
1.04
1.01
f1 (ppm)
0.000
1.801

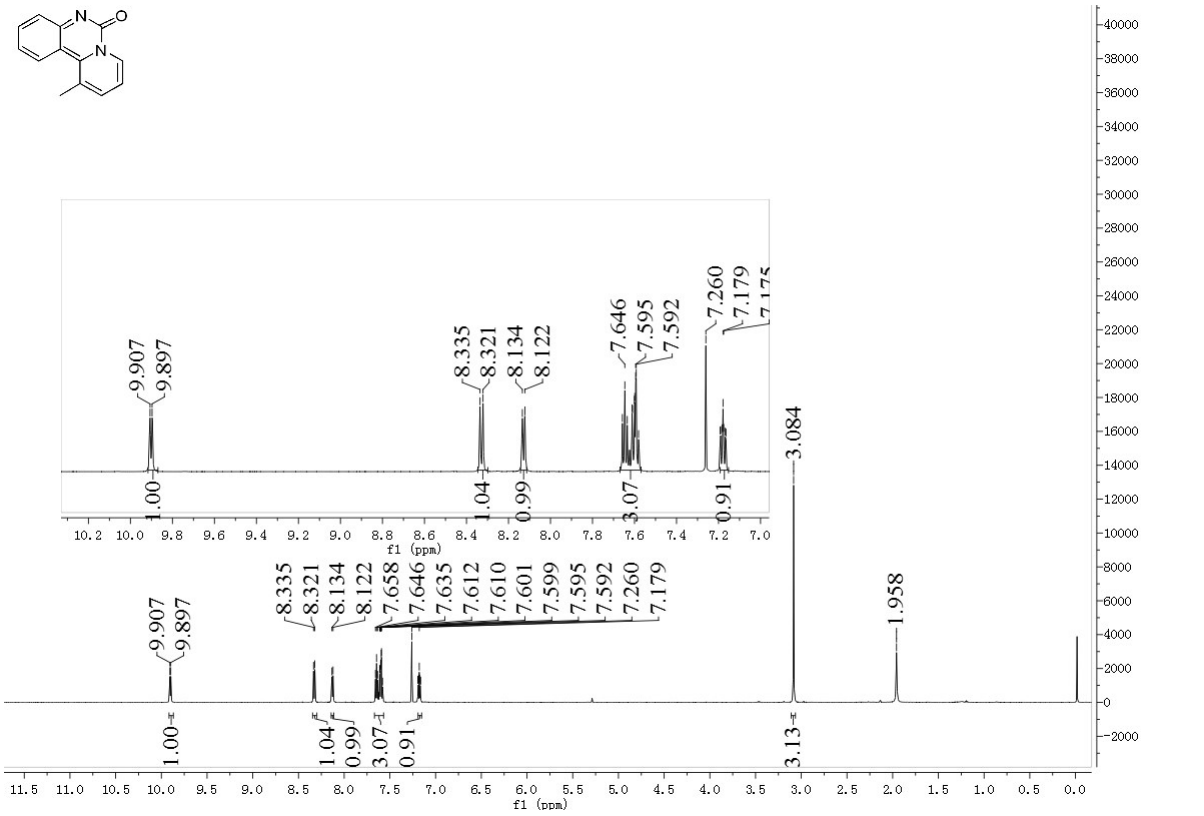

77.258
77.046
76.834
161.287
150.048
144.292
138.709
135.775
133.239
125.261
121.407
118.290
109.407
f1 (ppm)

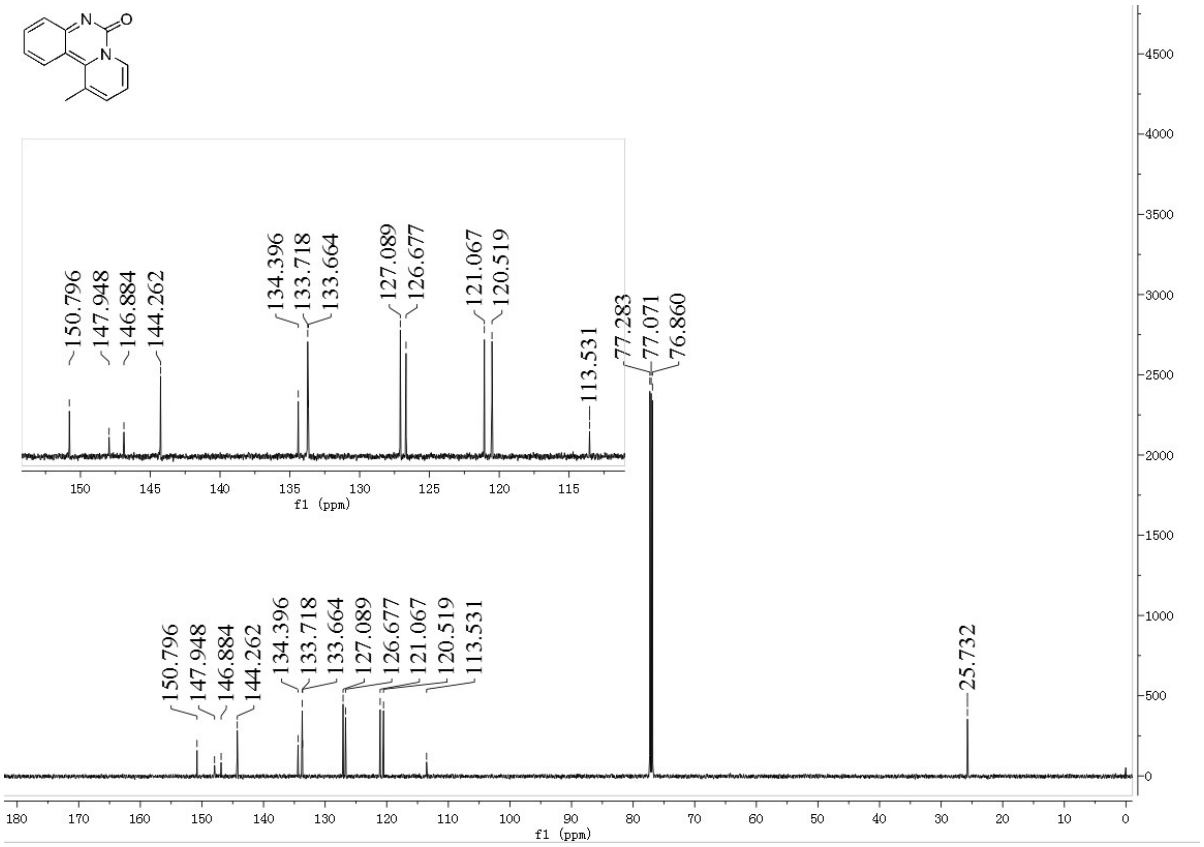
Compound **2s**


9.600
9.589
9.168
8.737
8.724
8.080
8.069
7.929
7.917
7.904
7.585
7.573
7.561
7.548
2.811
2.500
3.470
0.96
1.00
0.99
1.00
0.99
2.01
3.00
f1 (ppm)

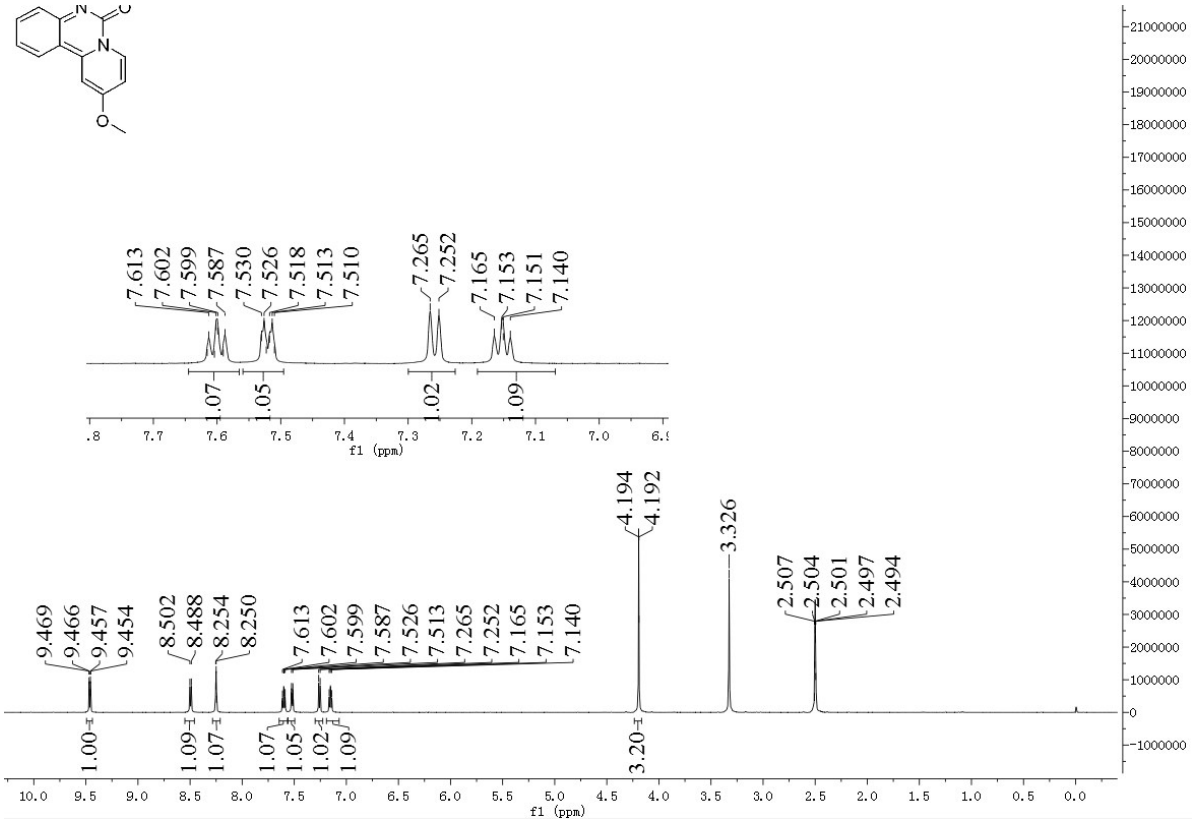

162.256
147.422
144.237
137.214
136.338
135.729
126.431
126.284
125.276
122.655
117.219
112.794
40.377
40.238
40.099
39.960
39.821
39.682
39.543
22.620
f1 (ppm)

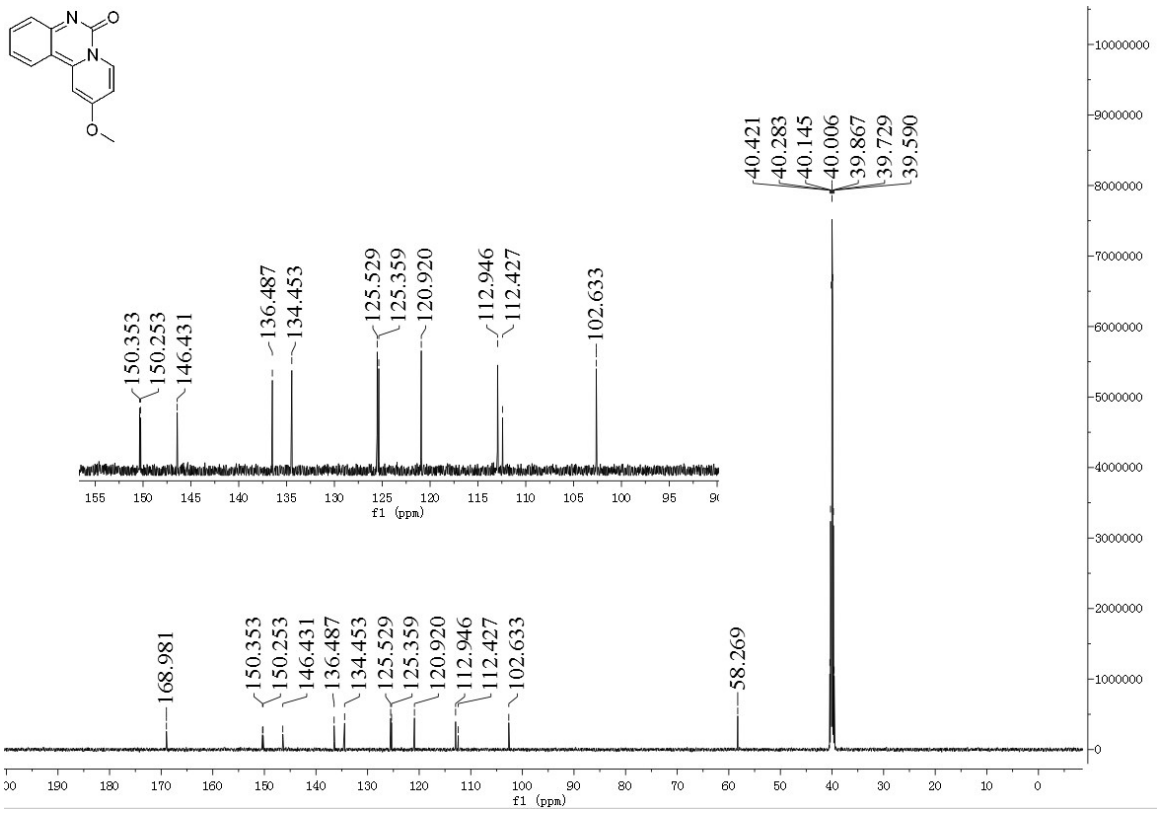
Compound **2t**


9.907
9.897
8.335
8.321
8.134
8.122
7.658
7.646
7.635
7.612
7.610
7.601
7.599
7.595
7.592
7.260
7.179
3.084
1.958
1.00
1.04
0.99
3.07
0.91
3.13
f1 (ppm)

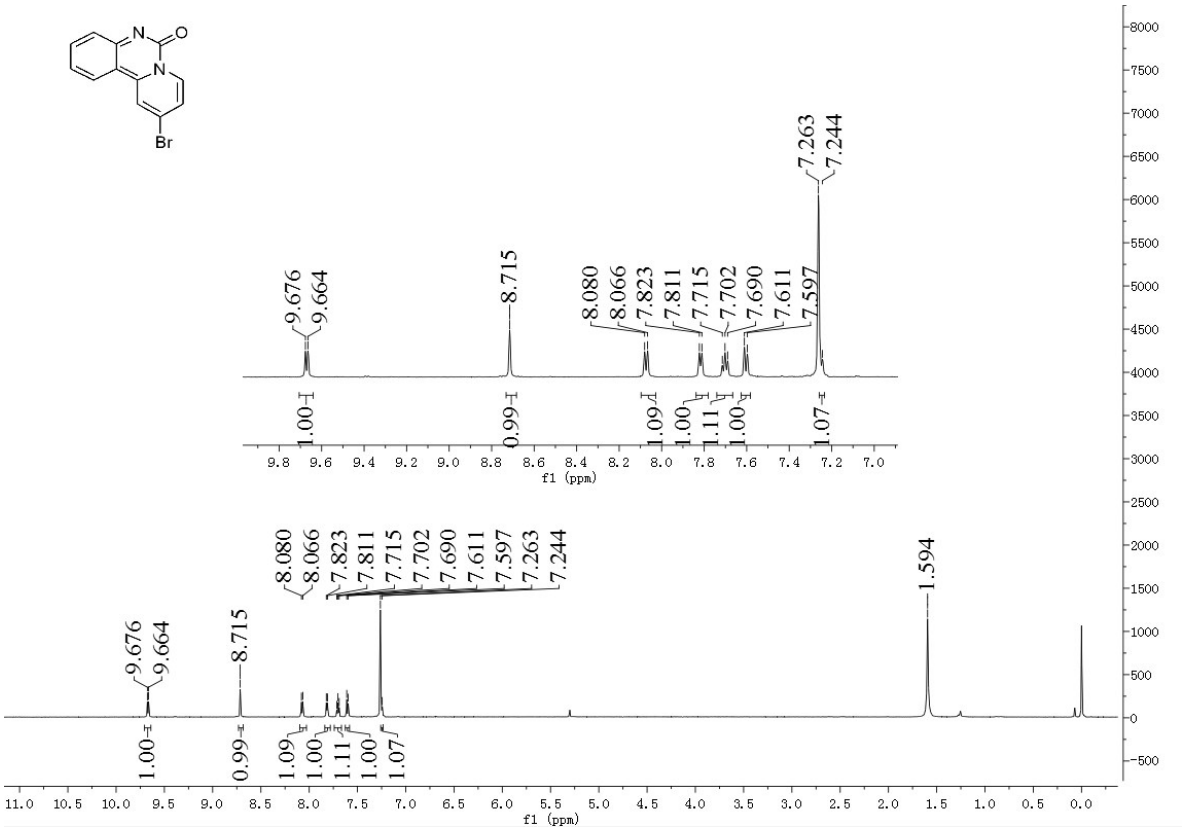

150.796
147.948
146.884
144.262
134.396
133.718
133.664
127.089
126.677
121.067
120.519
113.531
77.283
77.071
76.860
25.732
f1 (ppm)

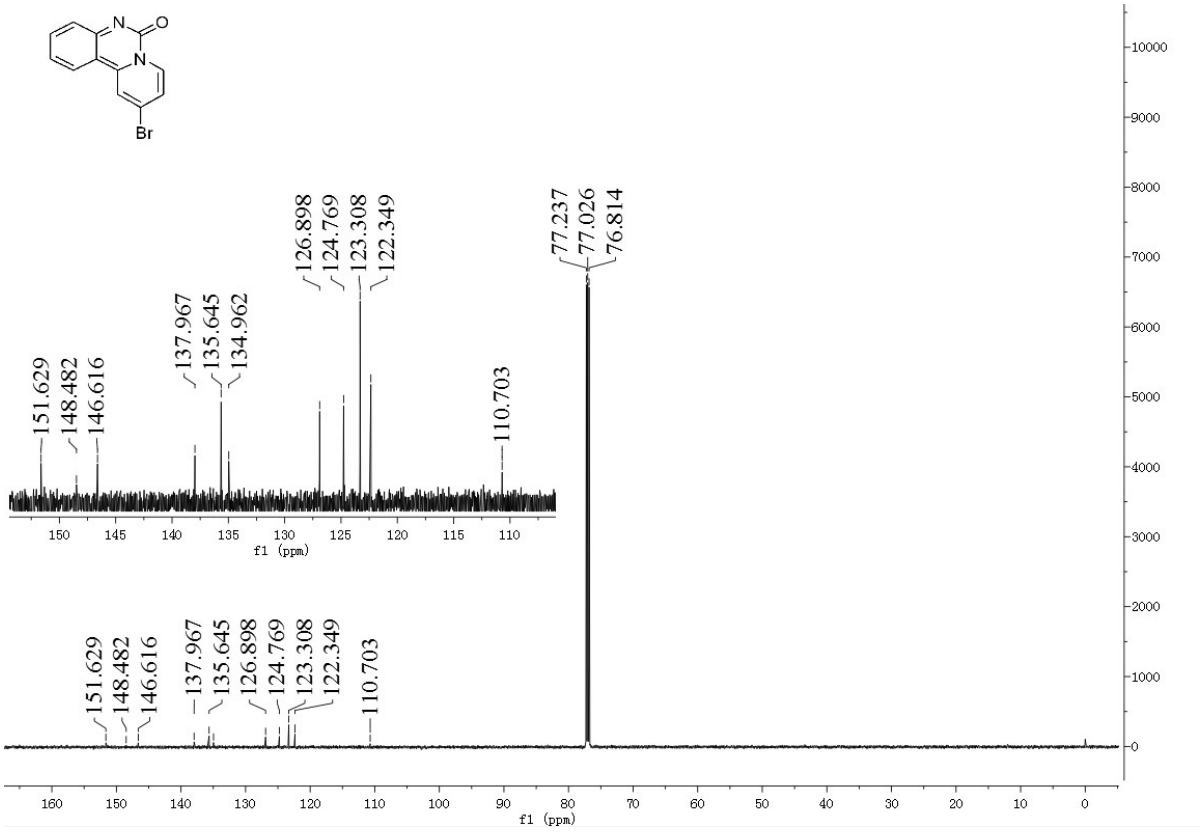
Compound **2u**


7.613
7.602
7.599
7.587
7.530
7.526
7.518
7.513
7.510
7.265
7.252
7.165
7.153
7.151
7.140
1.07
1.05
1.02
1.09
f1 (ppm)
4.194
4.192
3.326
2.507
2.504
2.501
2.497
2.494
9.469
9.466
9.457
9.454
8.502
8.488
8.254
8.250
1.00
1.09
1.07
1.07
1.05
1.02
1.09
3.20
f1 (ppm)

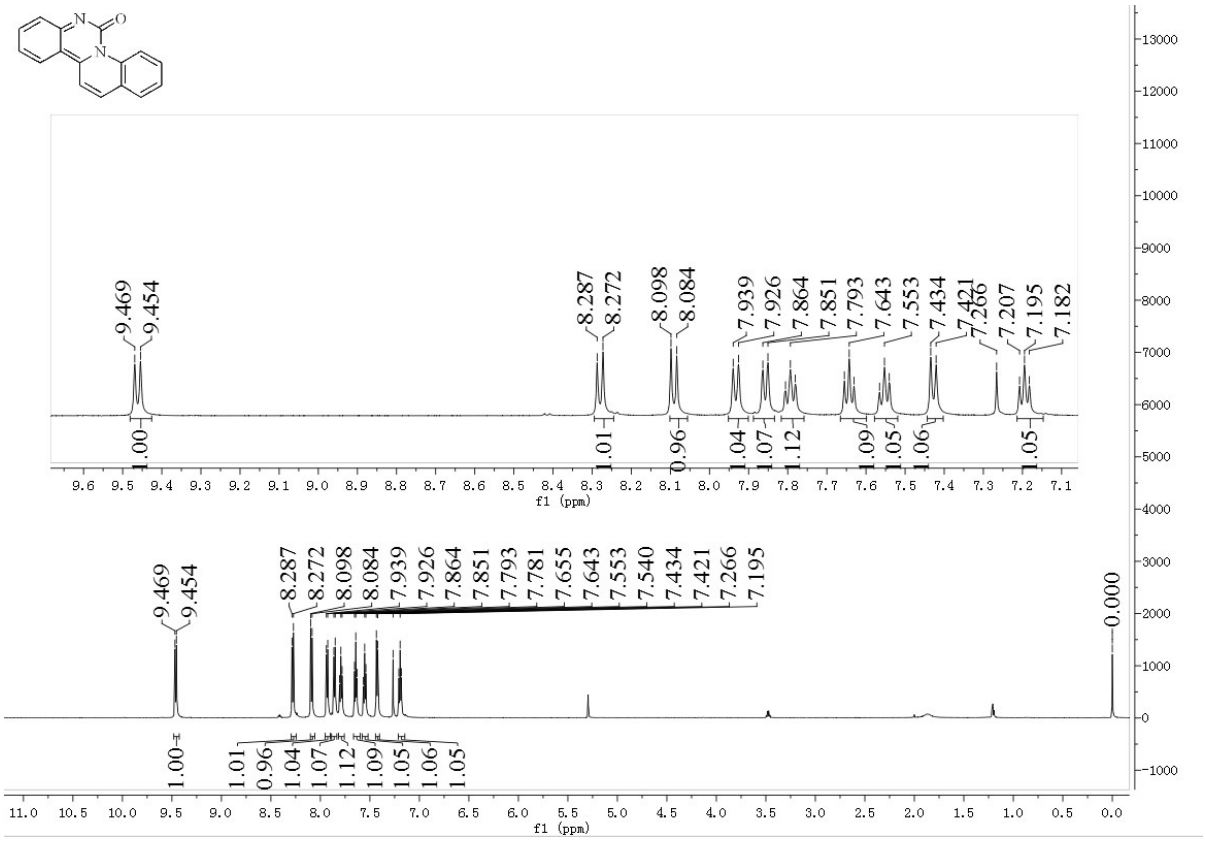

150.353
150.253
146.431
136.487
134.453
125.529
125.359
120.920
112.946
112.427
102.633
f1 (ppm)
40.421
40.283
40.145
40.006
39.867
39.729
39.590
168.981
150.353
150.253
146.431
136.487
134.453
125.529
125.359
120.920
112.946
112.427
102.633
58.269
f1 (ppm)

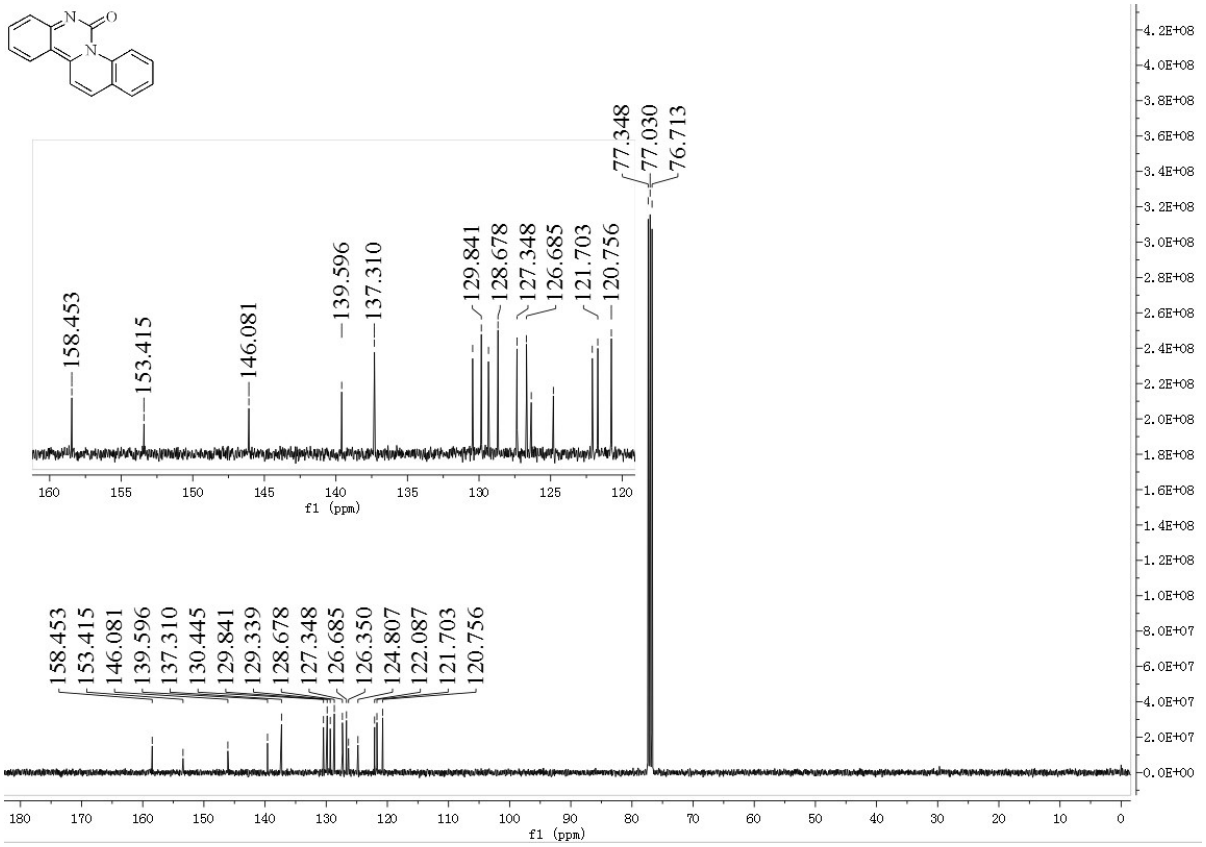
Compound **2v**


9.676
9.664
8.715
8.080
8.066
7.823
7.811
7.715
7.702
7.690
7.611
7.597
7.263
7.244
1.594
1.00
0.99
1.09
1.00
1.11
1.00
1.07
f1 (ppm)

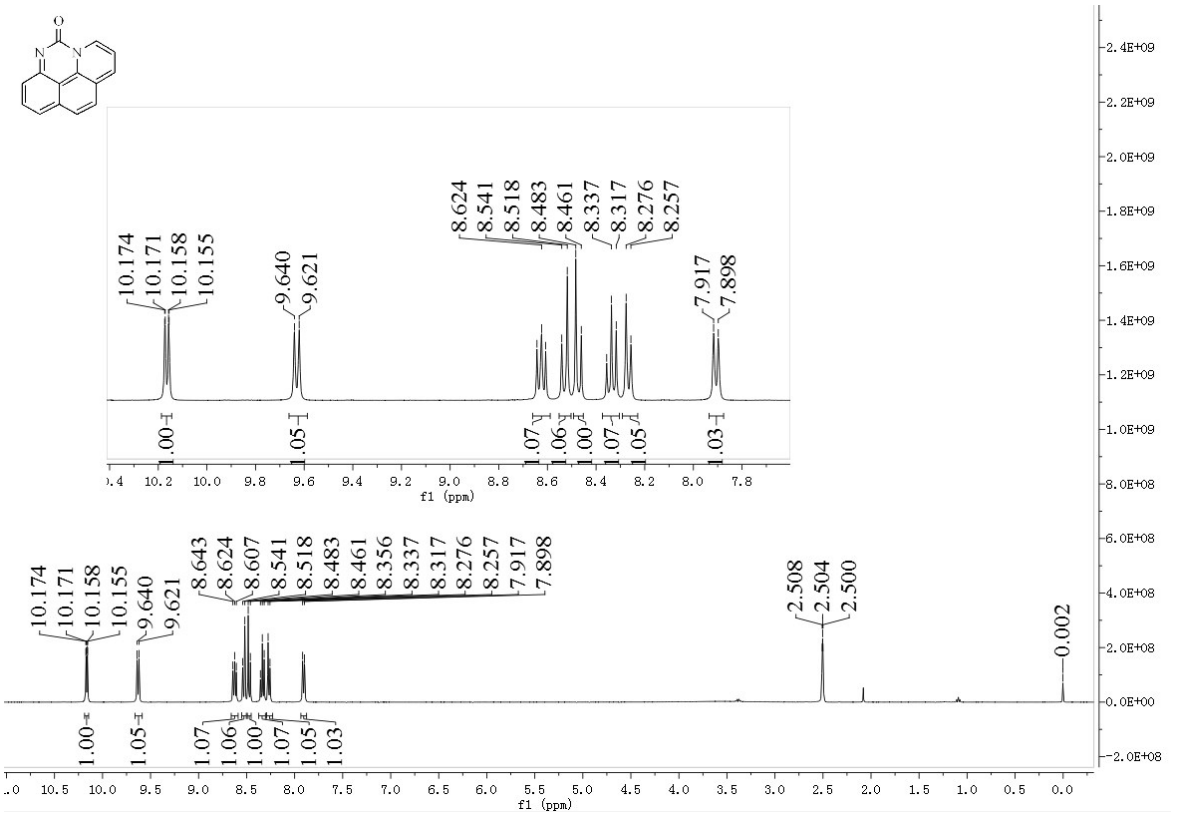

151.629
148.482
146.616
137.967
135.645
134.962
126.898
124.769
123.308
122.349
110.703
77.237
77.026
76.814
f1 (ppm)

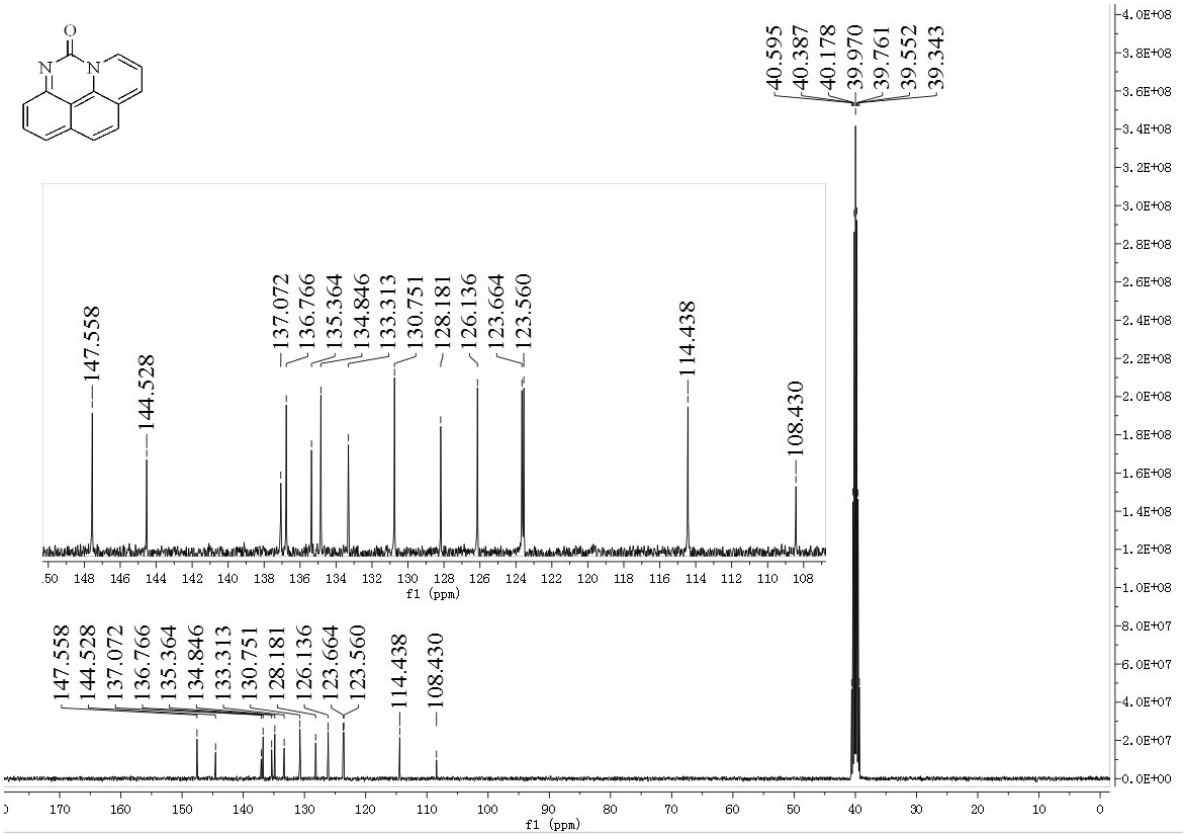
Compound **2w**


9.469
9.454
8.287
8.272
8.098
8.084
7.939
7.926
7.864
7.851
7.793
7.643
7.553
7.434
7.421
7.266
7.207
7.195
7.182
1.00
1.01
0.96
1.04
1.07
1.12
1.09
1.05
1.06
1.05
f1 (ppm)
9.469
9.454
8.287
8.272
8.098
8.084
7.939
7.926
7.864
7.851
7.793
7.781
7.655
7.643
7.553
7.540
7.434
7.421
7.266
7.195
0.000
1.00
1.01
0.96
1.04
1.07
1.12
1.09
1.05
1.06
1.05
f1 (ppm)

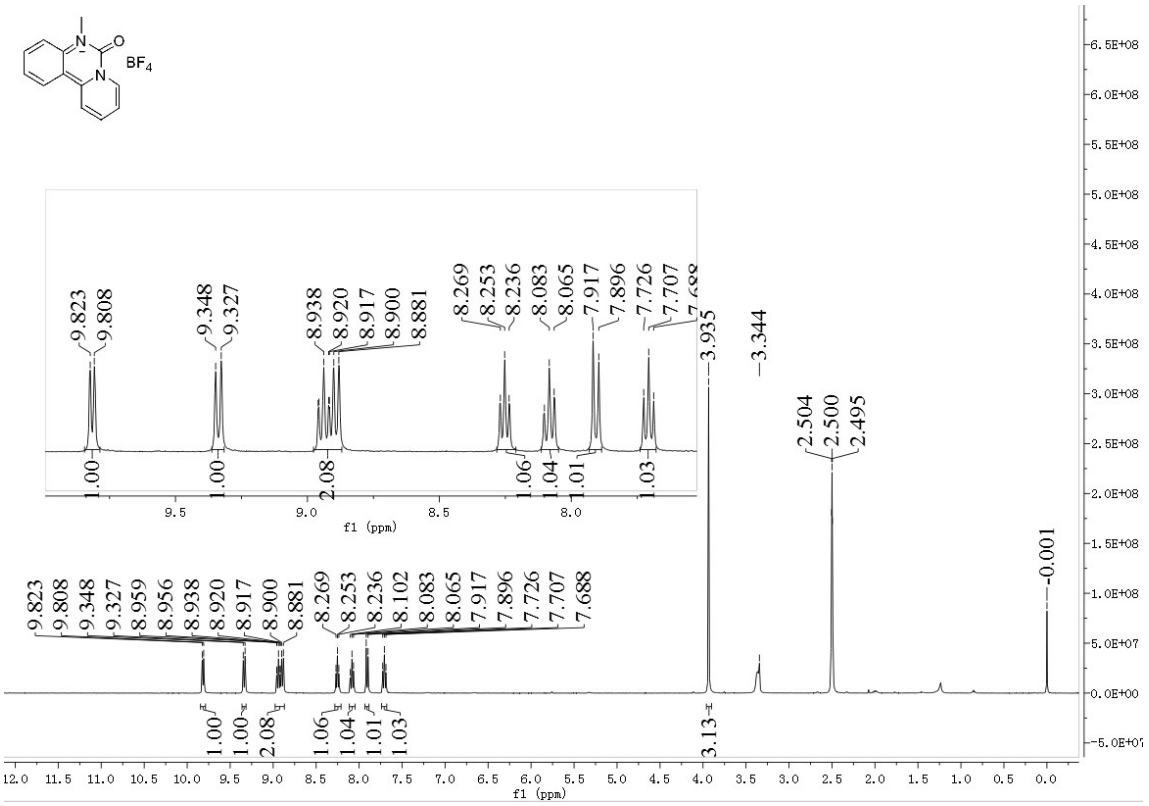

77.348
77.030
76.713
158.453
153.415
146.081
139.596
137.310
129.841
128.678
127.348
126.685
121.703
120.756
f1 (ppm)
158.453
153.415
146.081
139.596
137.310
130.445
129.841
129.339
128.678
127.348
126.685
126.350
124.807
122.087
121.703
120.756
f1 (ppm)

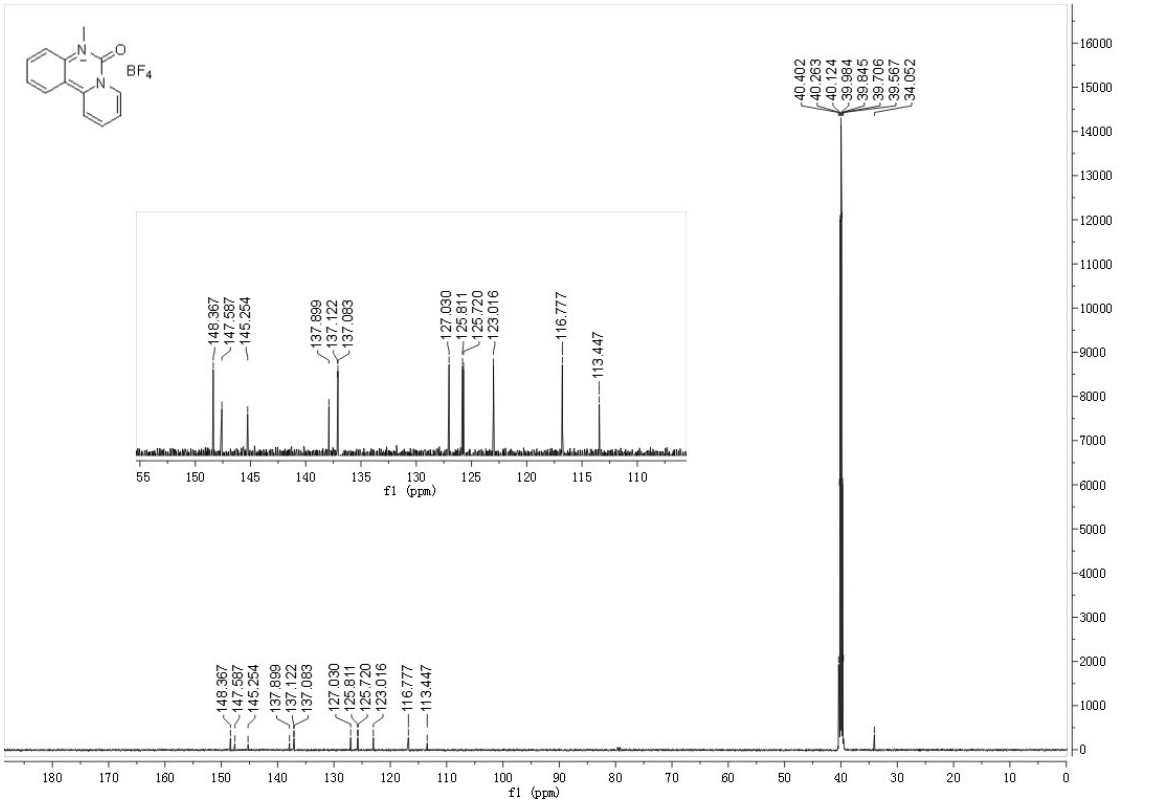
Compound **2x**

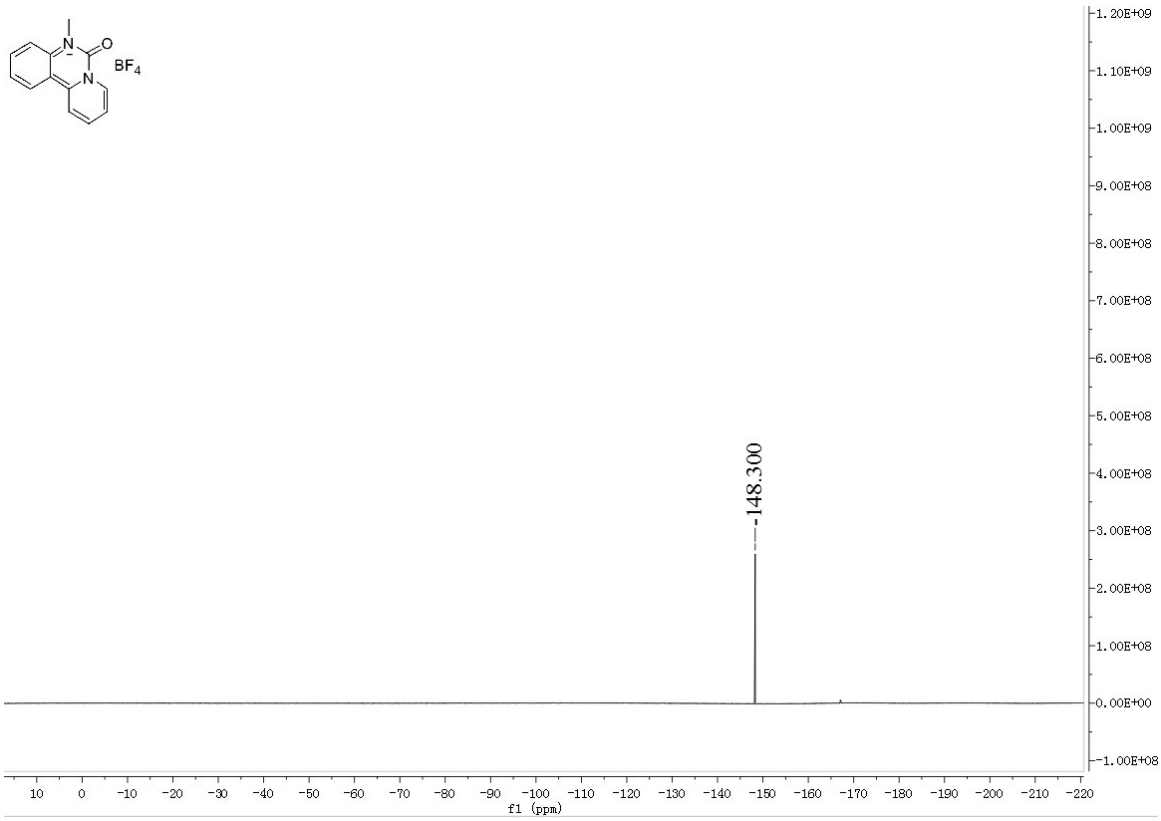

10.174
10.171
10.158
10.155
9.640
9.621
8.643
8.624
8.607
8.541
8.518
8.483
8.461
8.356
8.337
8.317
8.276
8.257
7.917
7.898
2.508
2.504
2.500
0.002
f1 (ppm)


147.558
144.528
137.072
136.766
135.364
134.846
133.313
130.751
128.181
126.136
123.664
123.560
114.438
108.430
40.595
40.387
40.178
39.970
39.761
39.552
39.343
f1 (ppm)

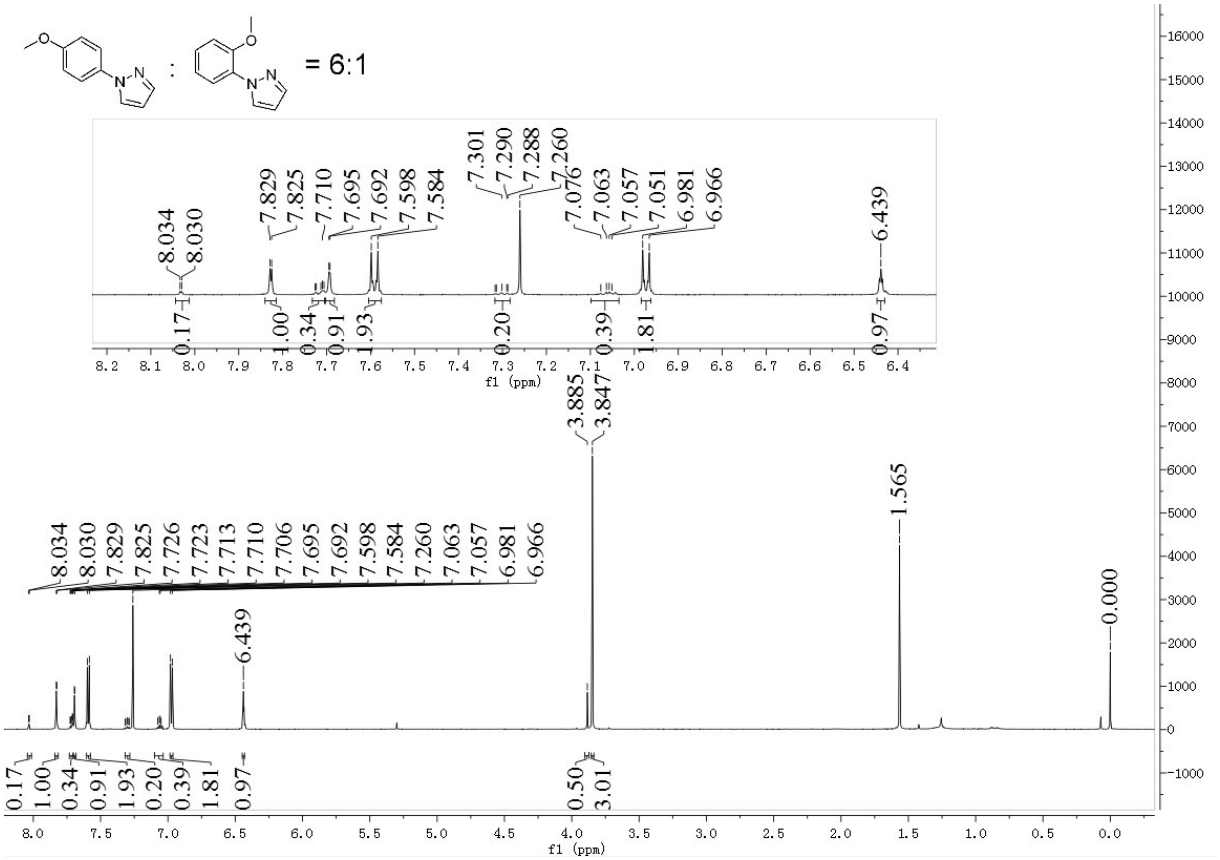
Compound **3a**


BF4
9.823
9.808
9.348
9.327
8.938
8.920
8.917
8.900
8.881
8.269
8.253
8.236
8.083
8.065
7.917
7.896
7.726
7.707
3.935
3.344
2.504
2.500
2.495
-0.001
1.00
1.00
2.08
1.06
1.04
1.01
1.03
3.13
f1 (ppm)

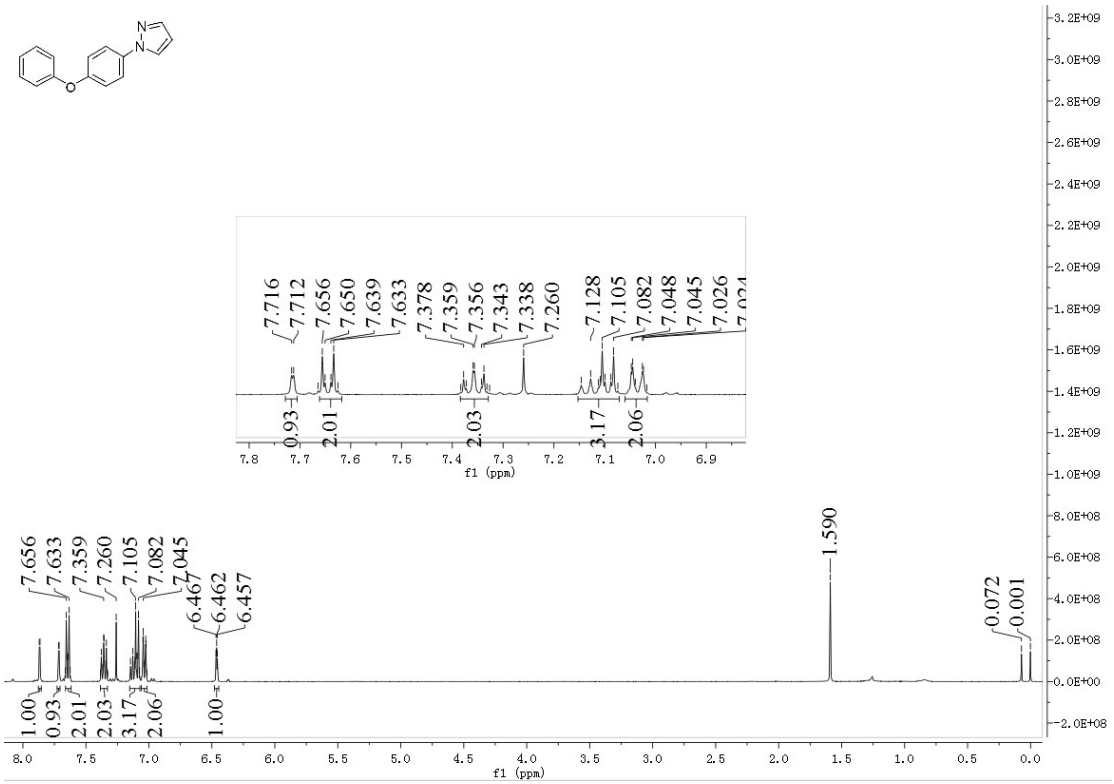

BF4
40.402
40.263
40.124
39.984
39.845
39.706
39.567
34.052
148.367
147.587
145.254
137.899
137.122
137.083
127.030
125.811
125.720
123.016
116.777
113.447
f1 (ppm)


BF4
-148.300
f1 (ppm)

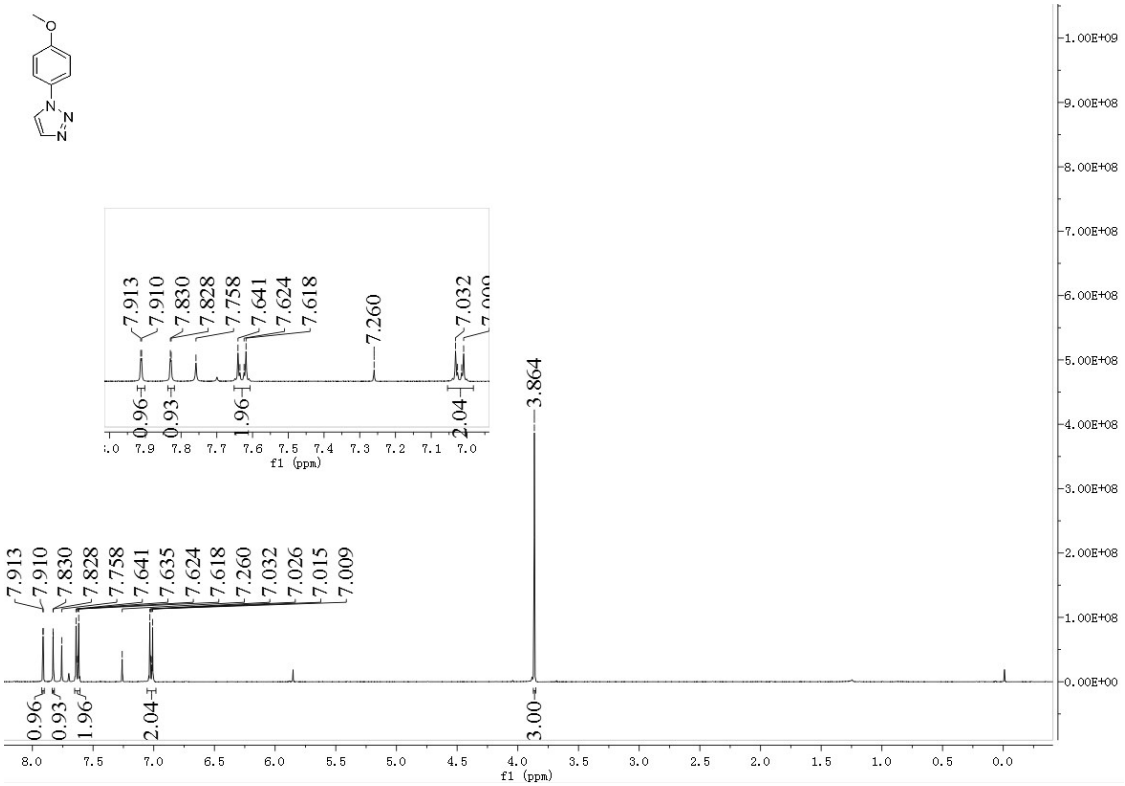
Compound **4a**


= 6:1
8.034
8.030
7.829
7.825
7.710
7.695
7.692
7.598
7.584
7.301
7.290
7.288
7.260
7.076
7.063
7.057
7.051
6.981
6.966
6.439
3.885
3.847
1.565
0.000
f1 (ppm)

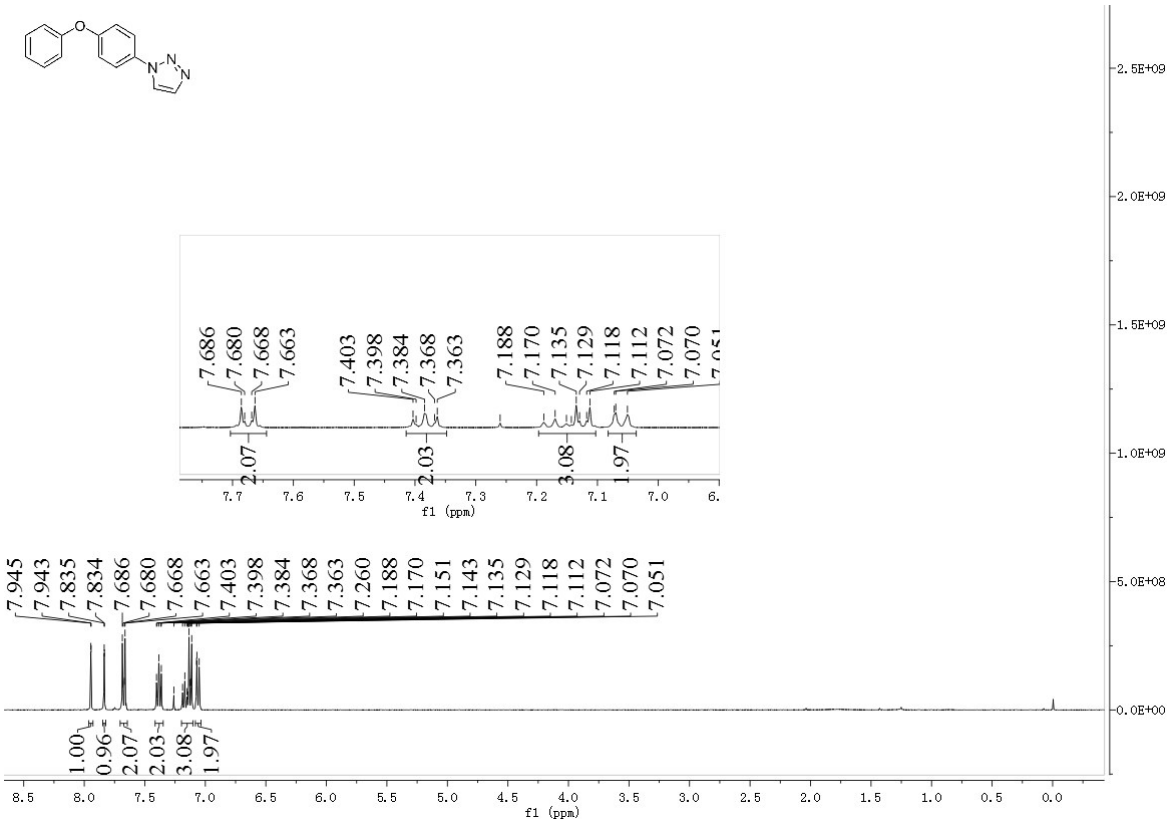
Compound **4b**

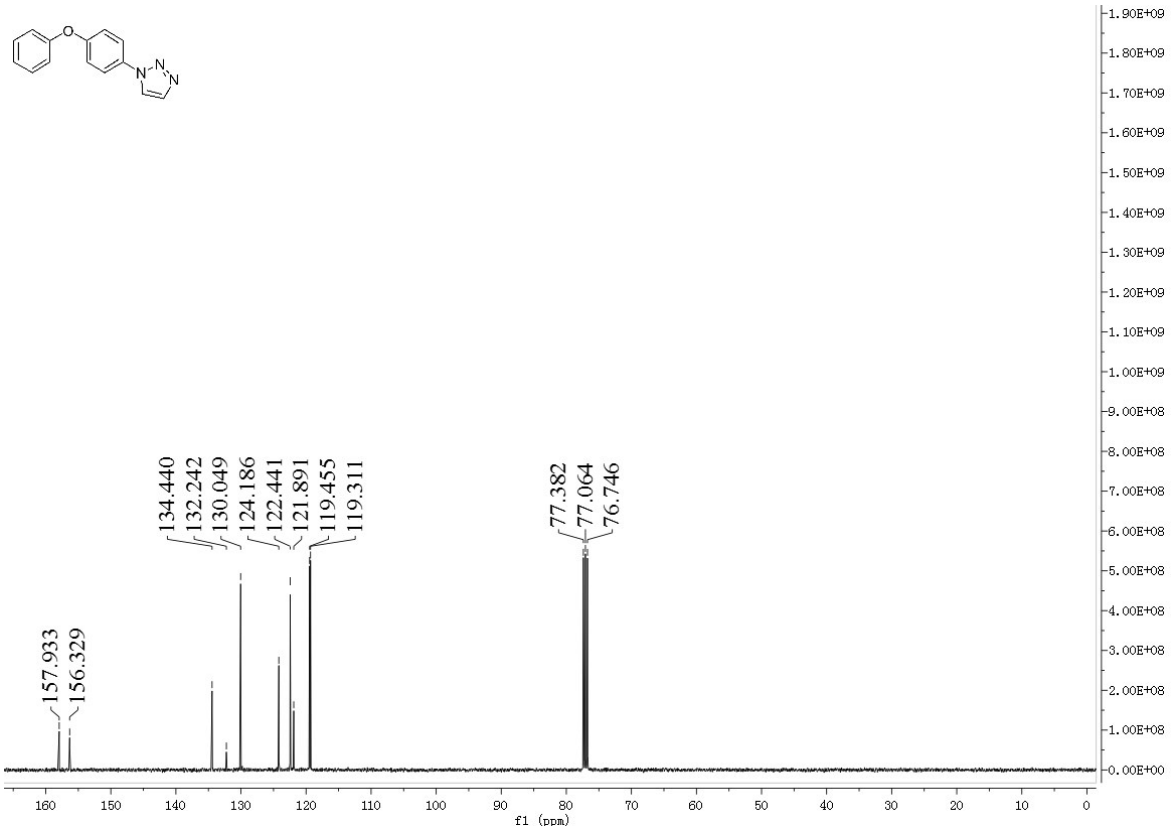


Compound **4c**

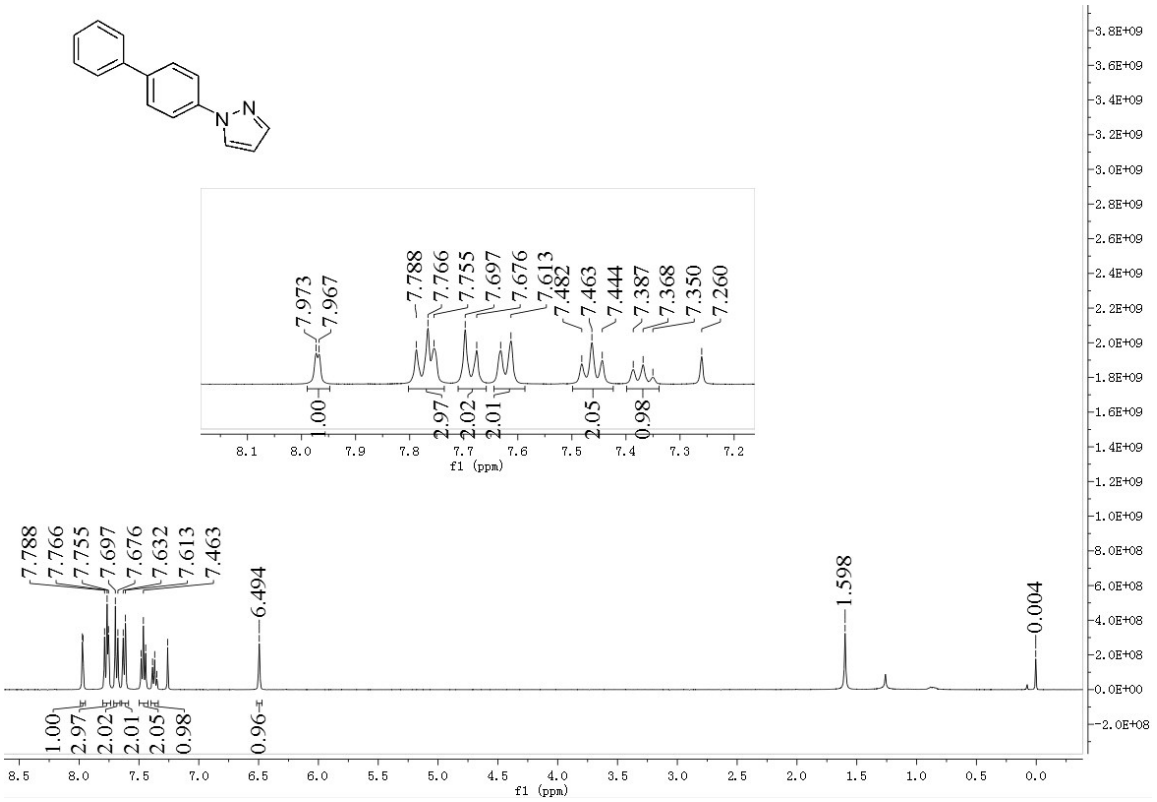


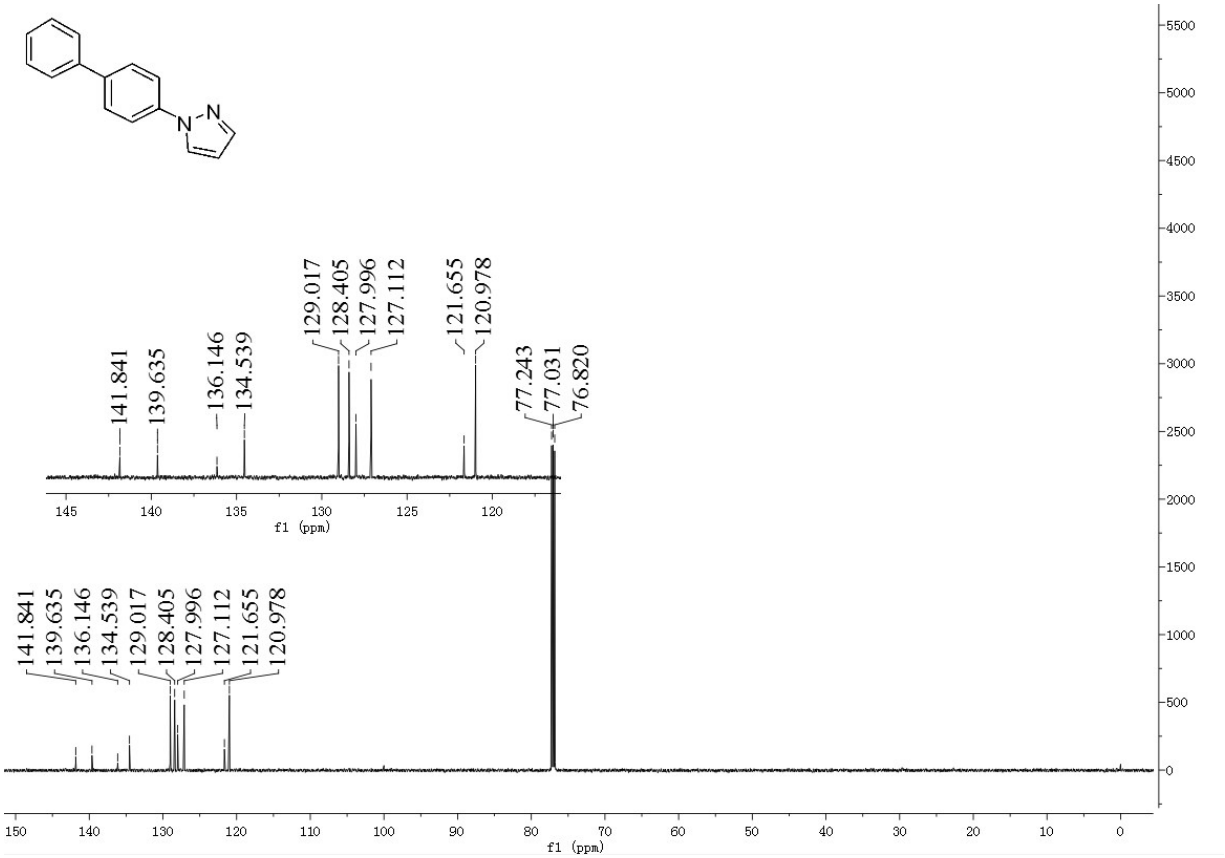
Compound **4d**


7.945
7.943
7.835
7.834
7.686
7.680
7.668
7.663
7.403
7.398
7.384
7.368
7.363
7.260
7.188
7.170
7.151
7.143
7.135
7.129
7.118
7.112
7.072
7.070
7.051
1.00
0.96
2.07
2.03
3.08
1.97
f1 (ppm)

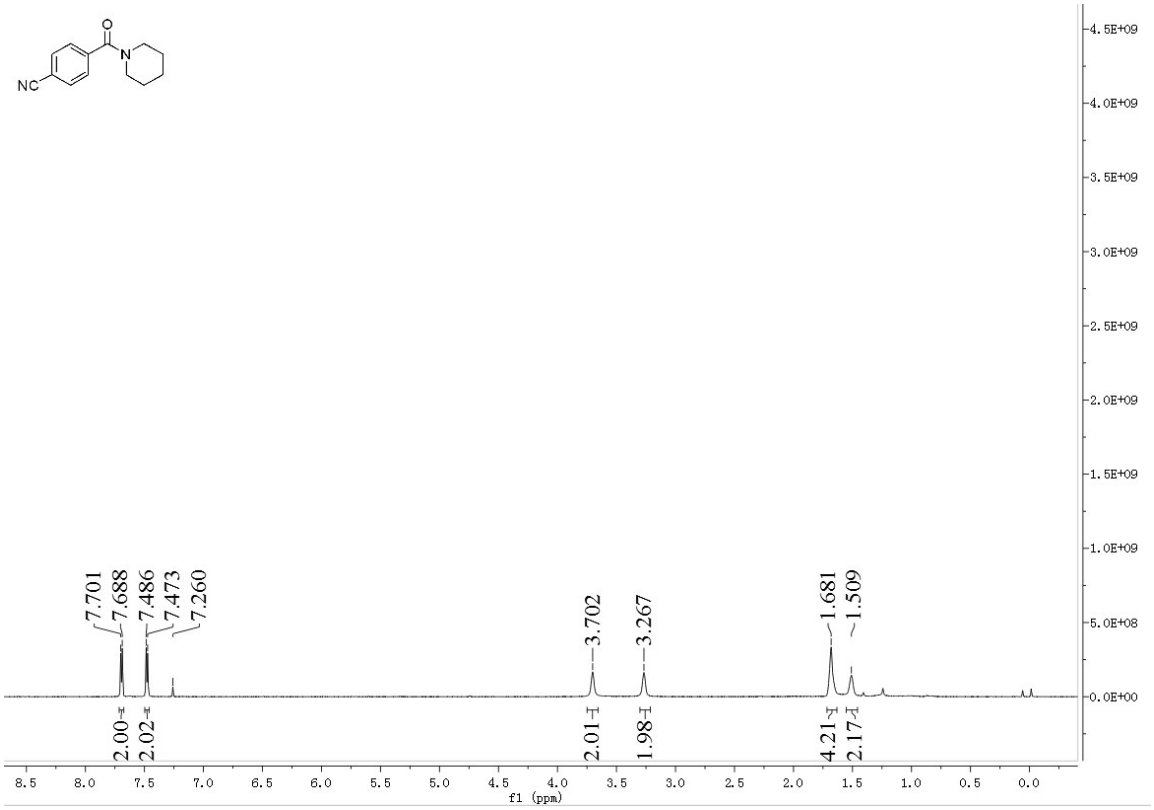

157.933
156.329
134.440
132.242
130.049
124.186
122.441
121.891
119.455
119.311
77.382
77.064
76.746
f1 (ppm)

Compound **4e**

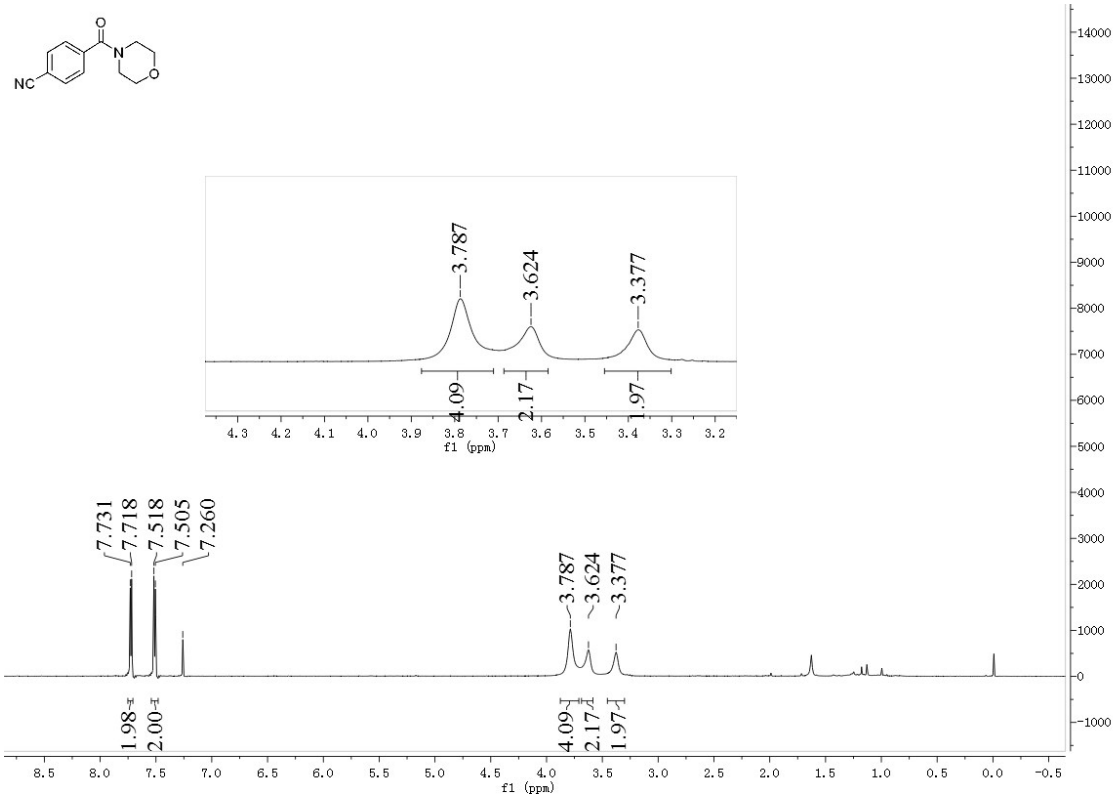

7.973
7.967
7.788
7.766
7.755
7.697
7.676
7.613
7.482
7.463
7.444
7.387
7.368
7.350
7.260
1.00
2.97
2.02
2.01
2.05
0.98
f1 (ppm)
7.788
7.766
7.755
7.697
7.676
7.632
7.613
7.463
6.494
1.598
0.004
1.00
2.97
2.02
2.01
2.05
0.98
0.96
f1 (ppm)

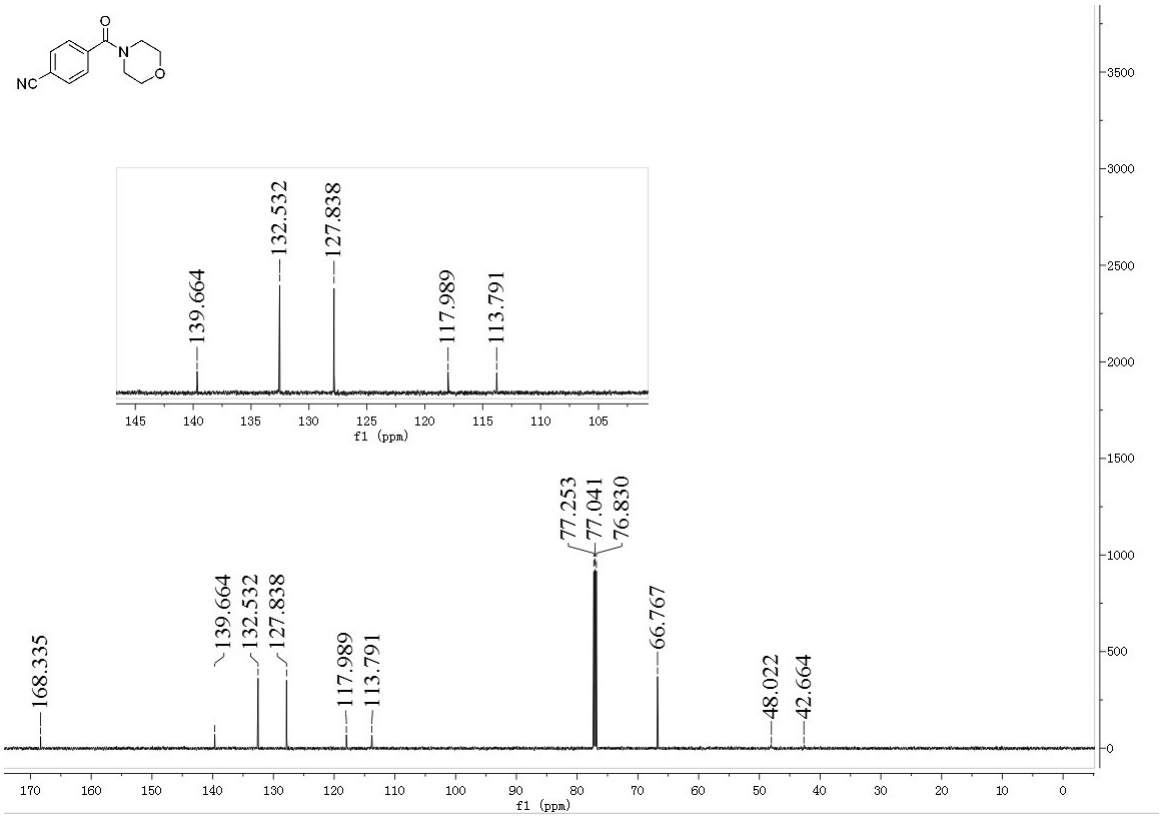

141.841
139.635
136.146
134.539
129.017
128.405
127.996
127.112
121.655
120.978
77.243
77.031
76.820
f1 (ppm)
141.841
139.635
136.146
134.539
129.017
128.405
127.996
127.112
121.655
120.978
f1 (ppm)

Compound **5a**

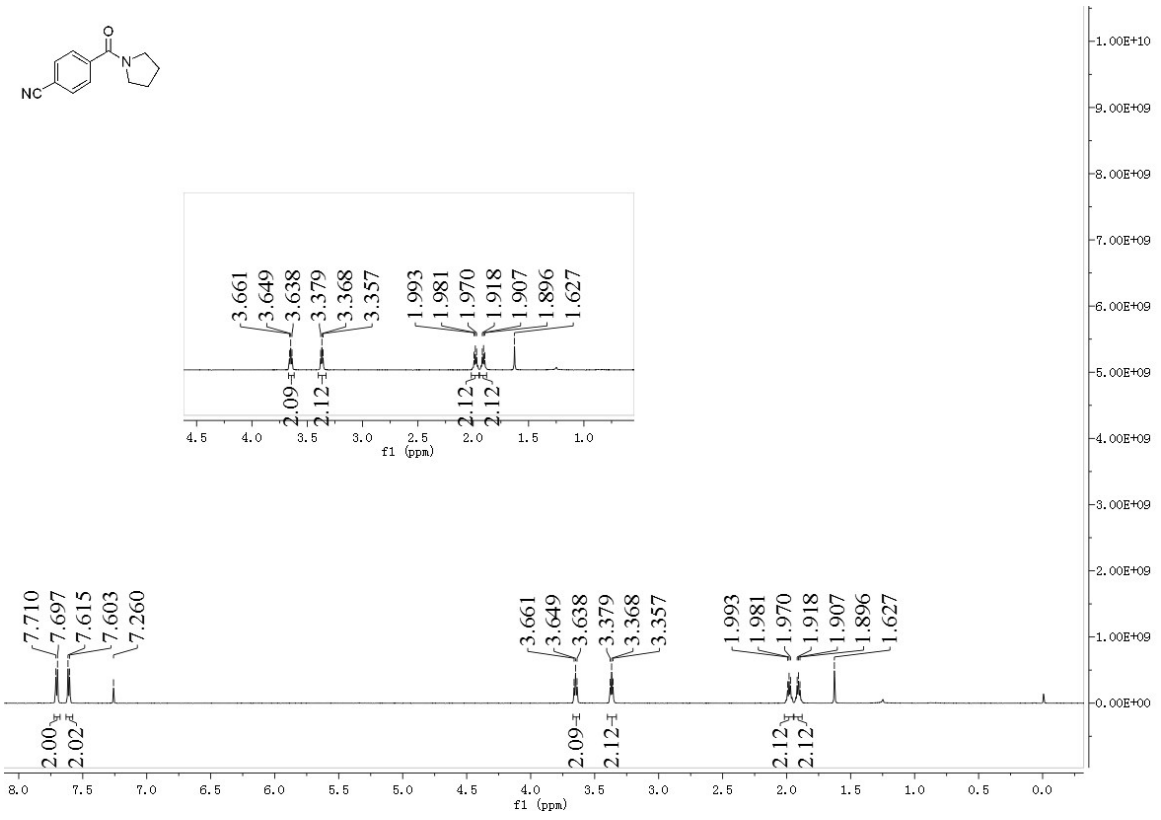


Compound **5b**

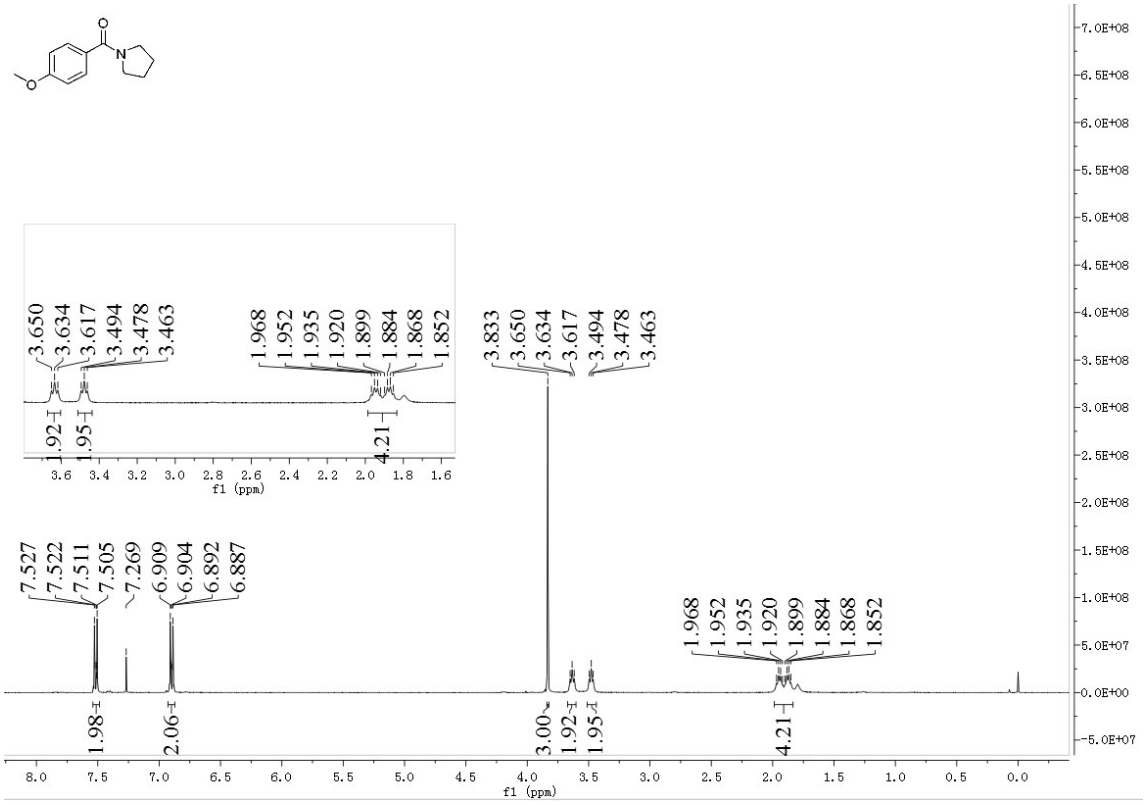



NC
O
N
O
139.664
132.532
127.838
117.989
113.791
f1 (ppm)
77.253
77.041
76.830
66.767
48.022
42.664
168.335

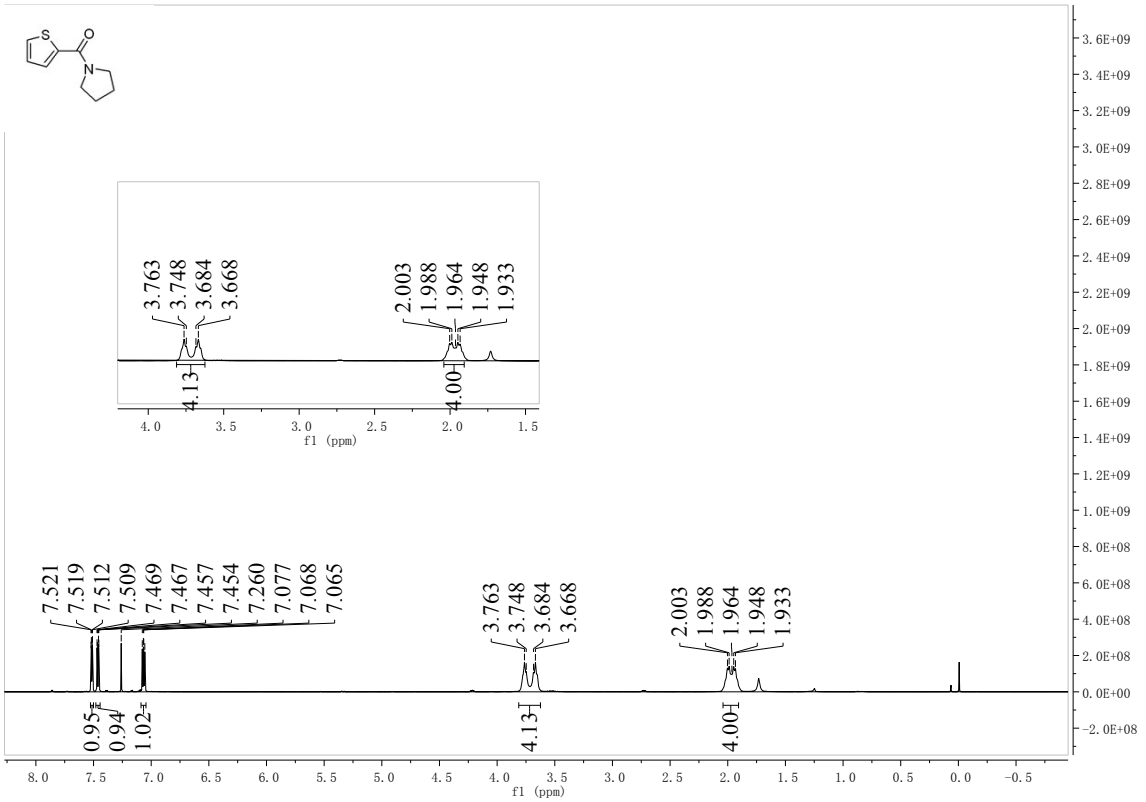
Compound **5c**


NC
O
N
3.661
3.649
3.638
3.379
3.368
3.357
1.993
1.981
1.970
1.918
1.907
1.896
1.627
2.09
2.12
2.12
2.12
f1 (ppm)
7.710
7.697
7.615
7.603
7.260
2.00
2.02

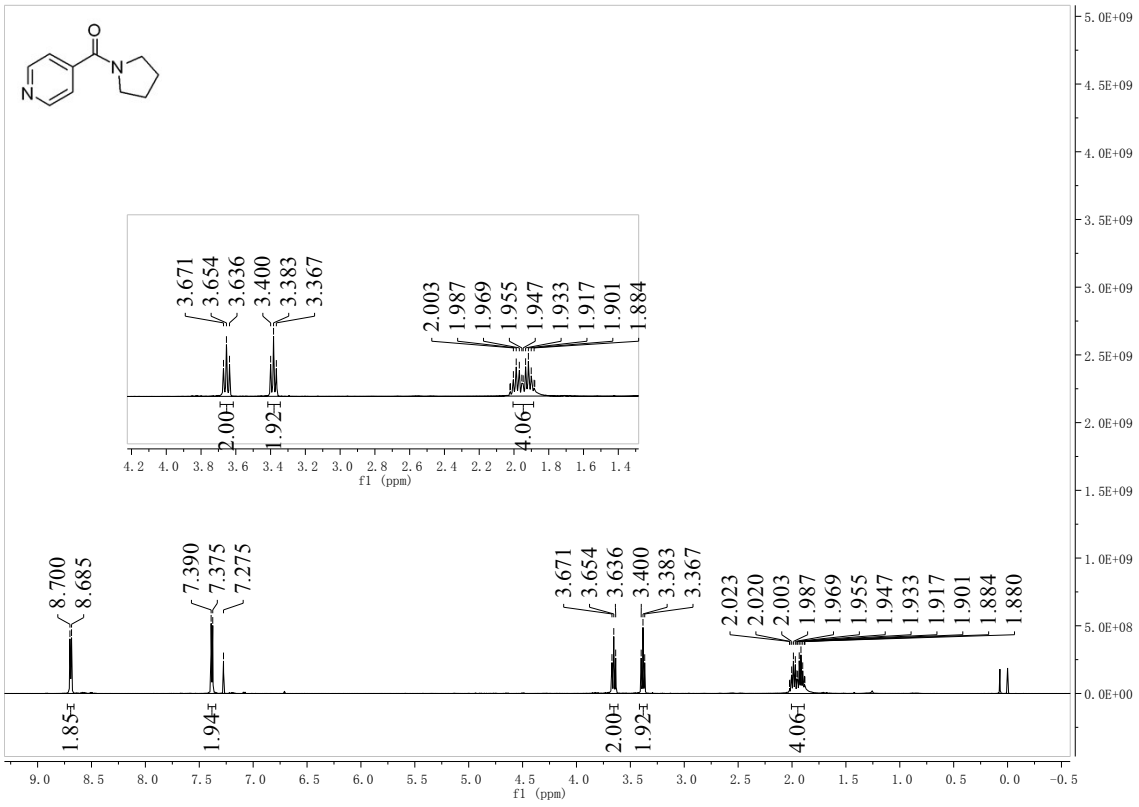
Compound **5d**



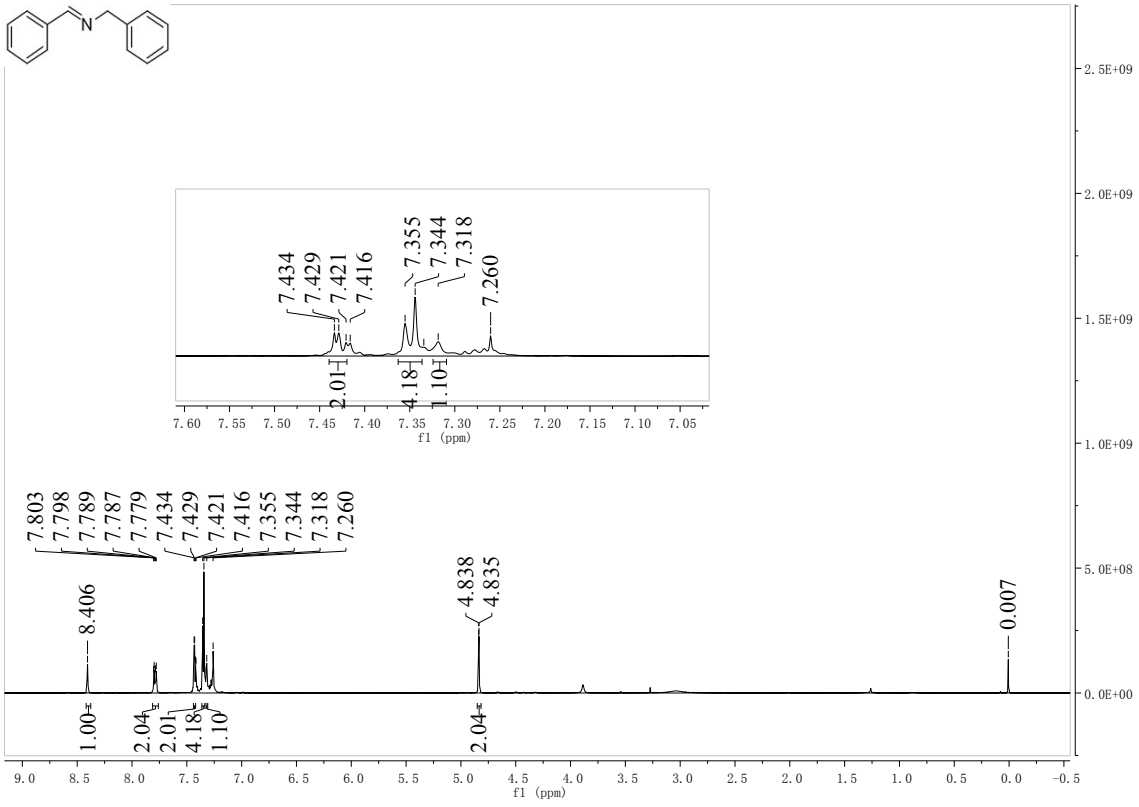
Compound **5e**



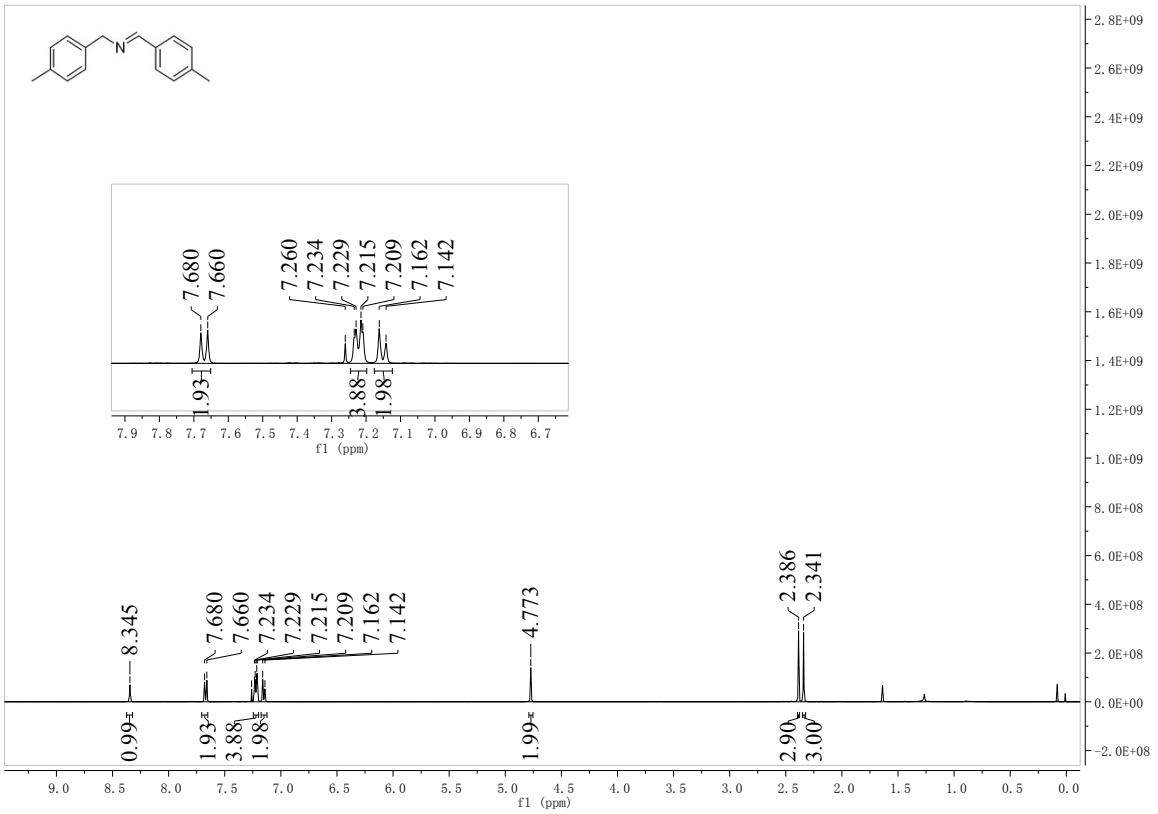
Compound **5f**



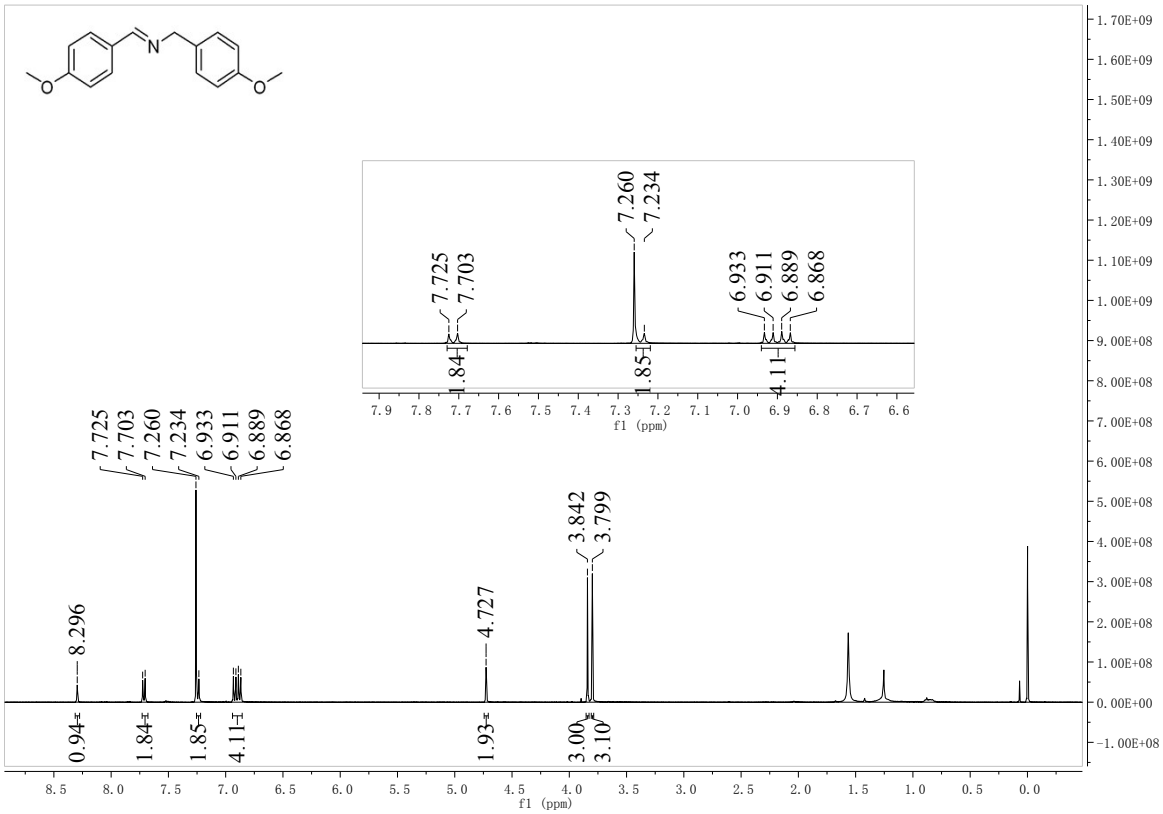
Compound **6a**



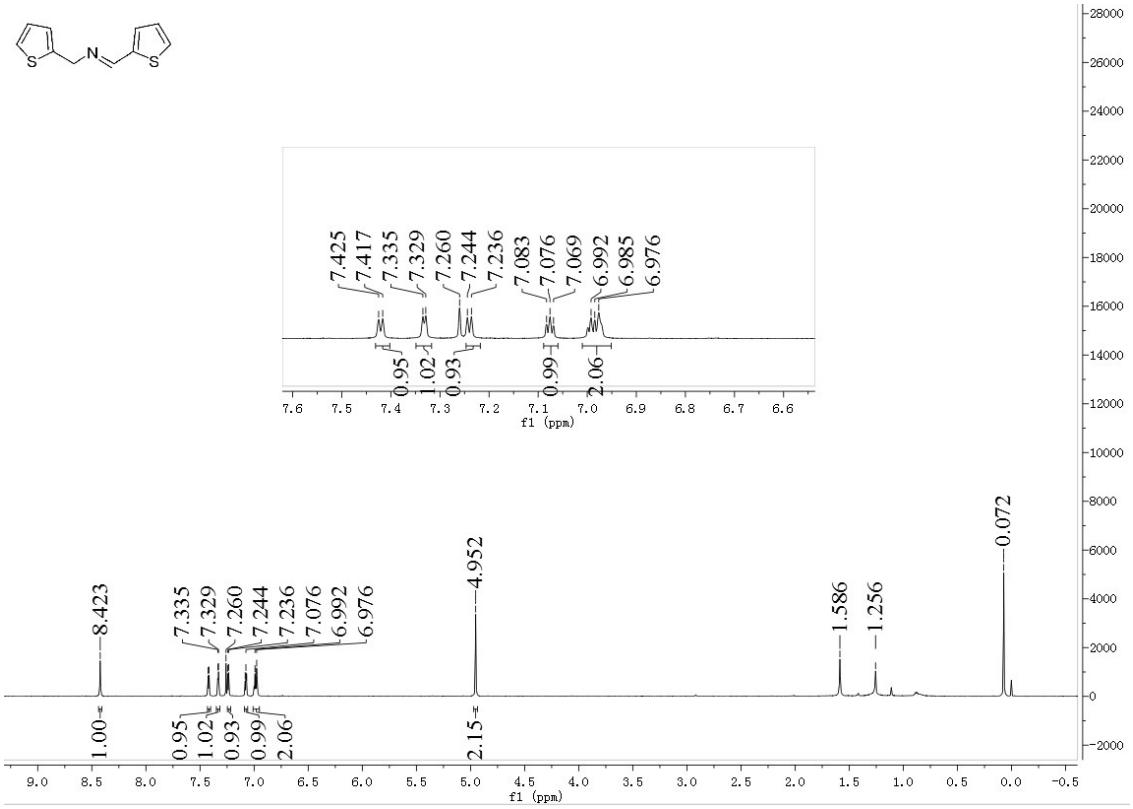
Compound **6b**



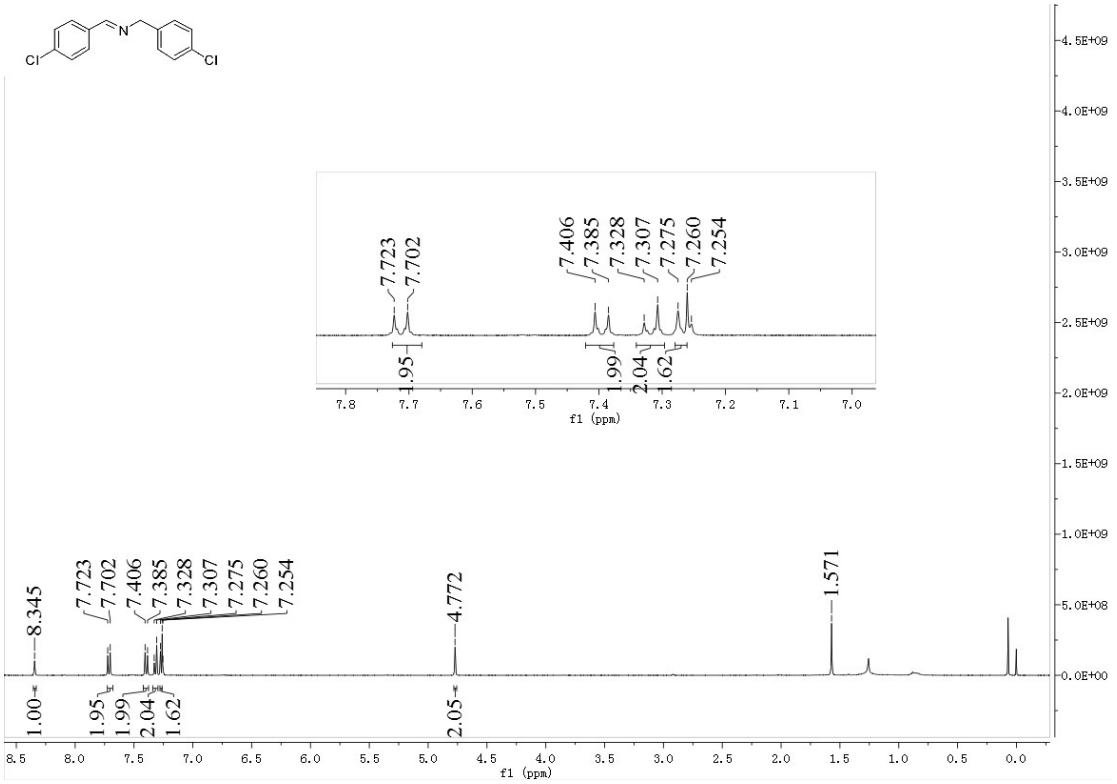
Compound **6c**



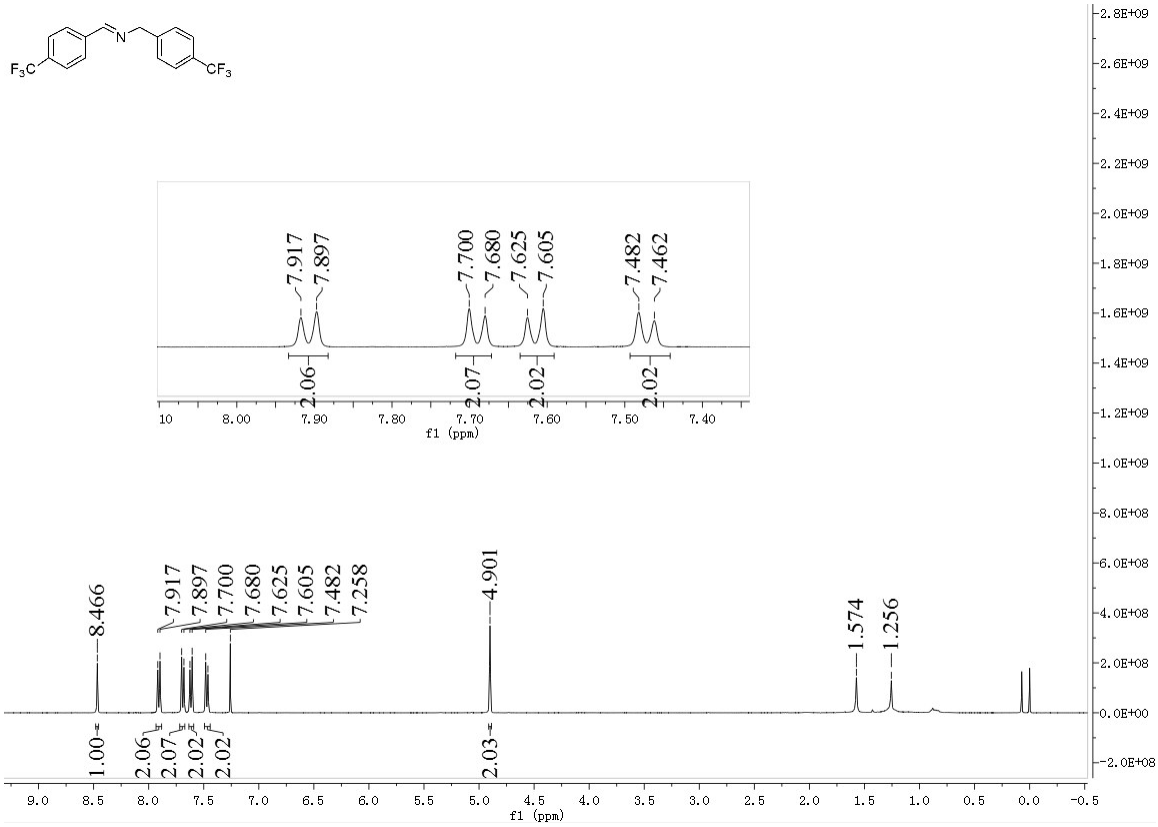
Compound **6d**



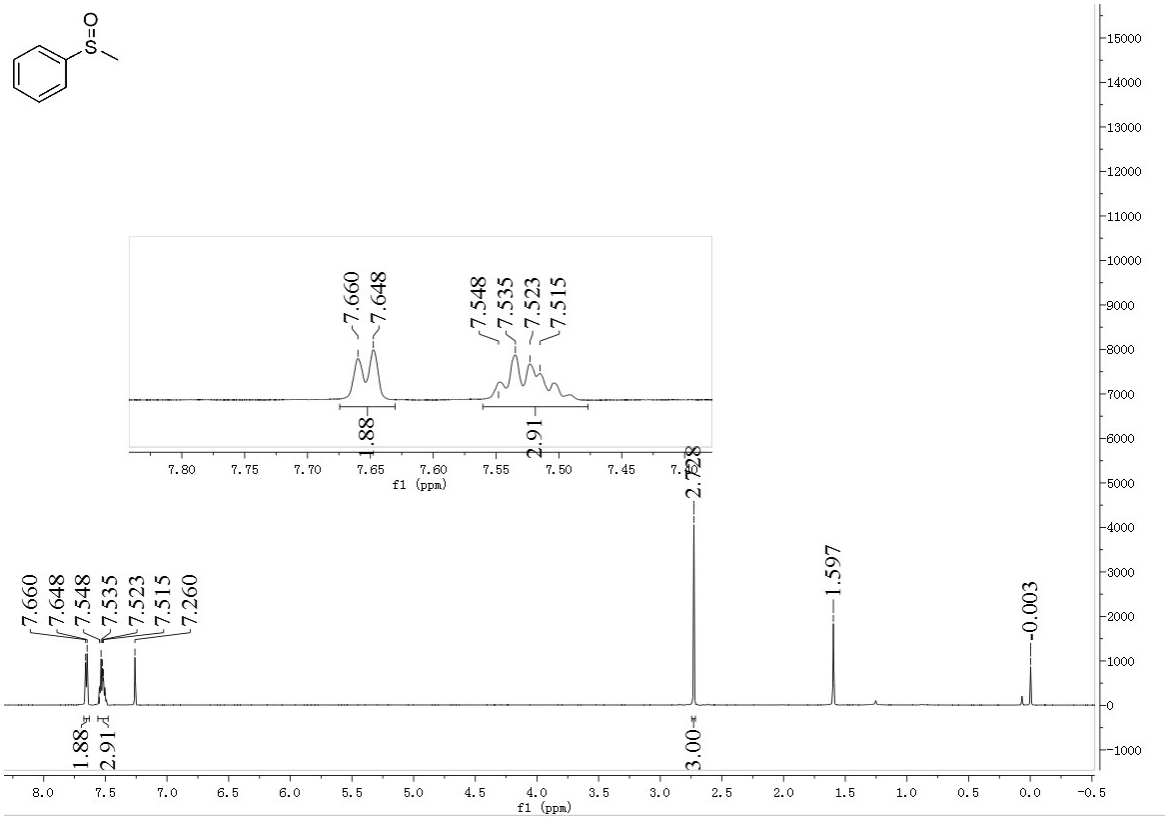
Compound **6e**



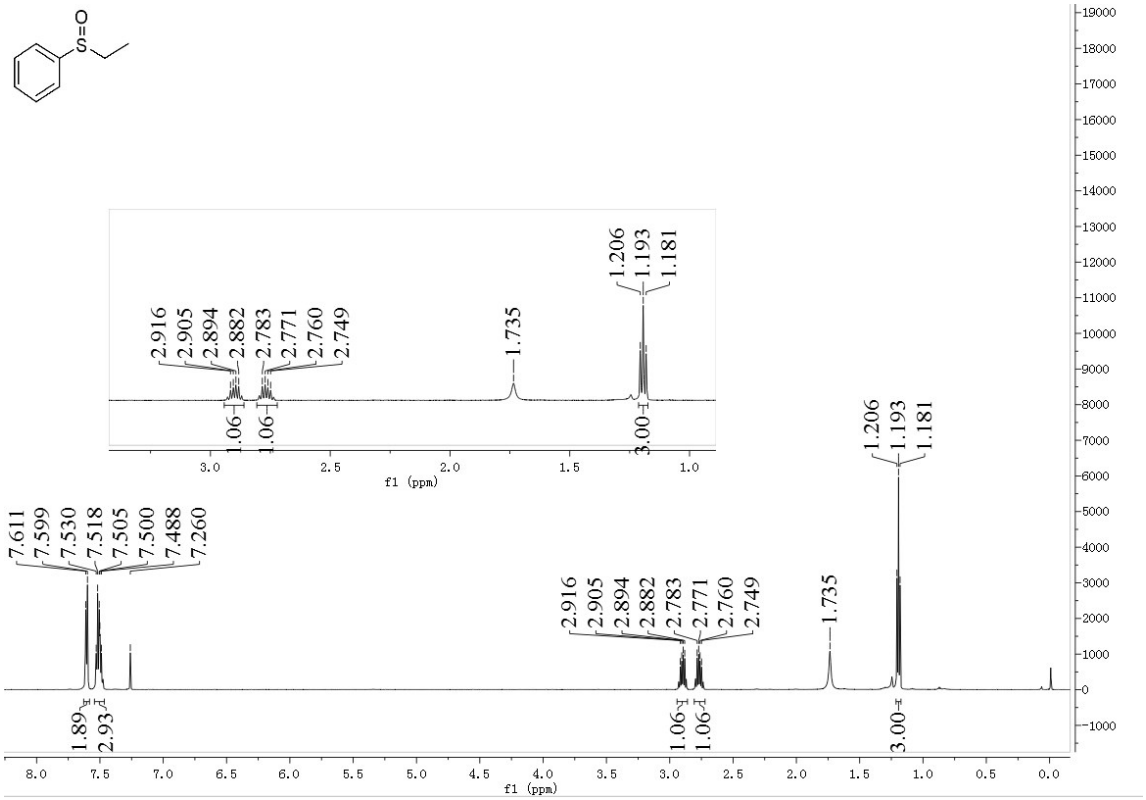
Compound **6f**



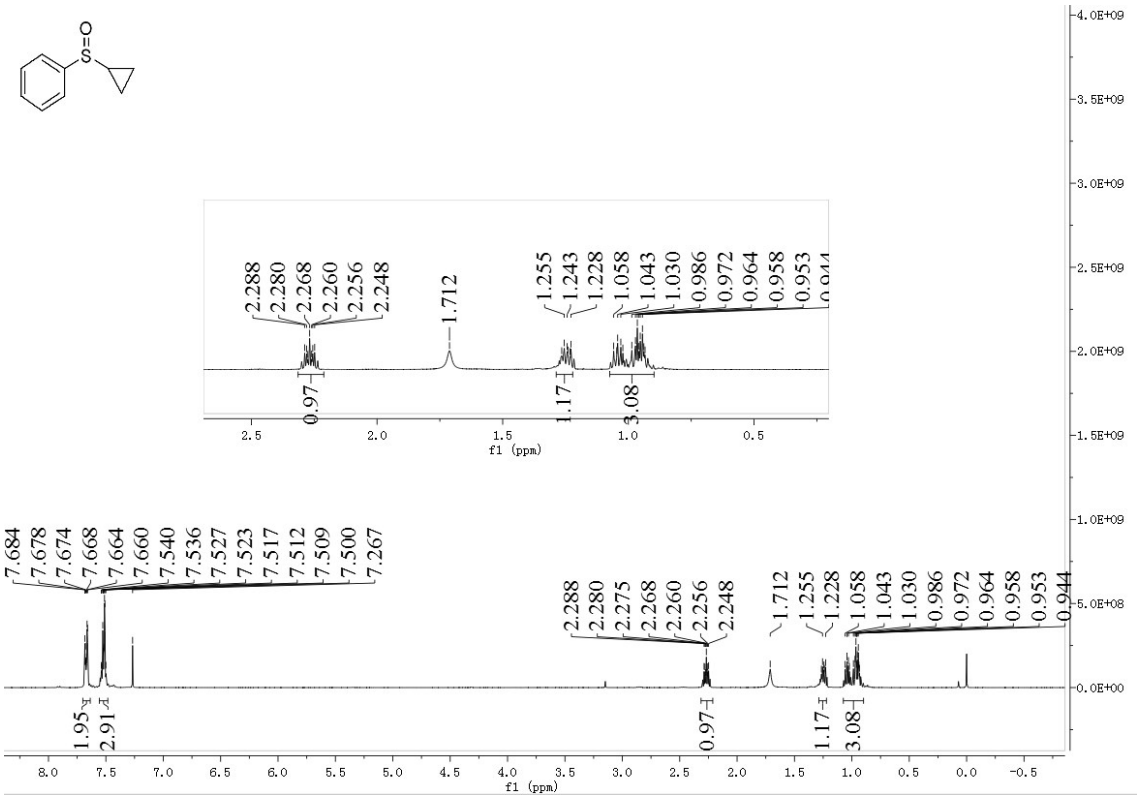
Compound **7a**



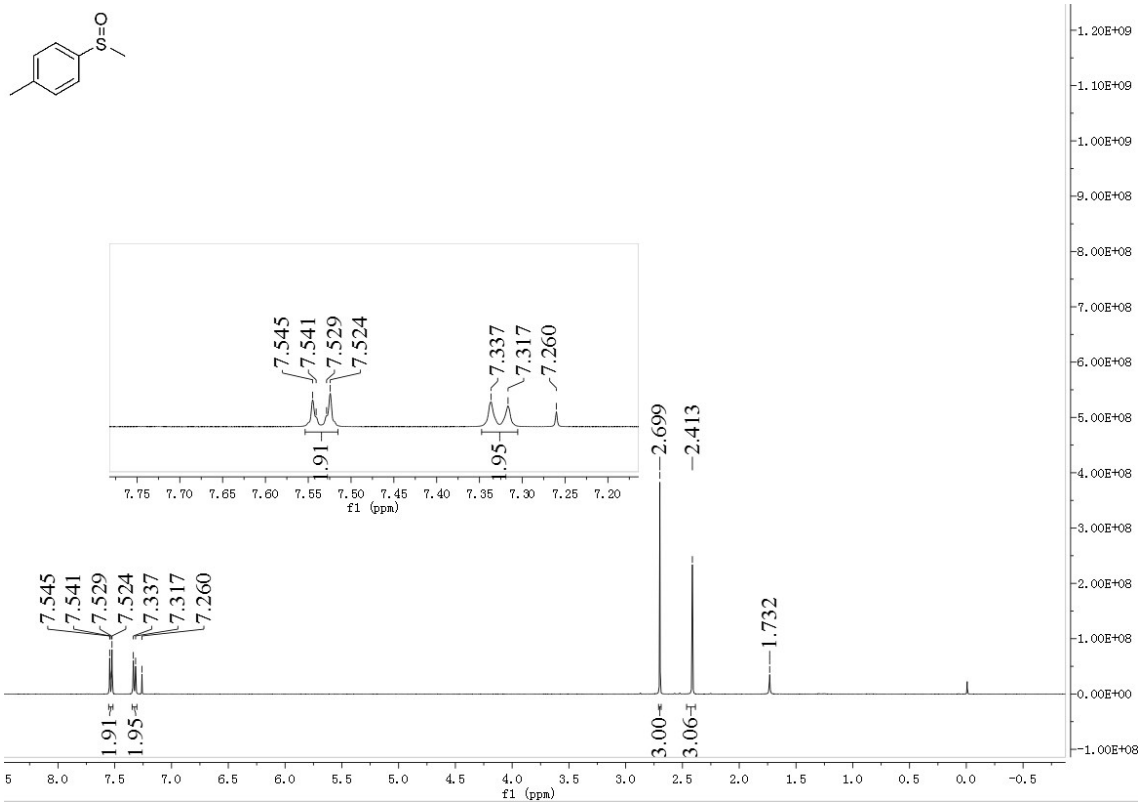
Compound **7b**



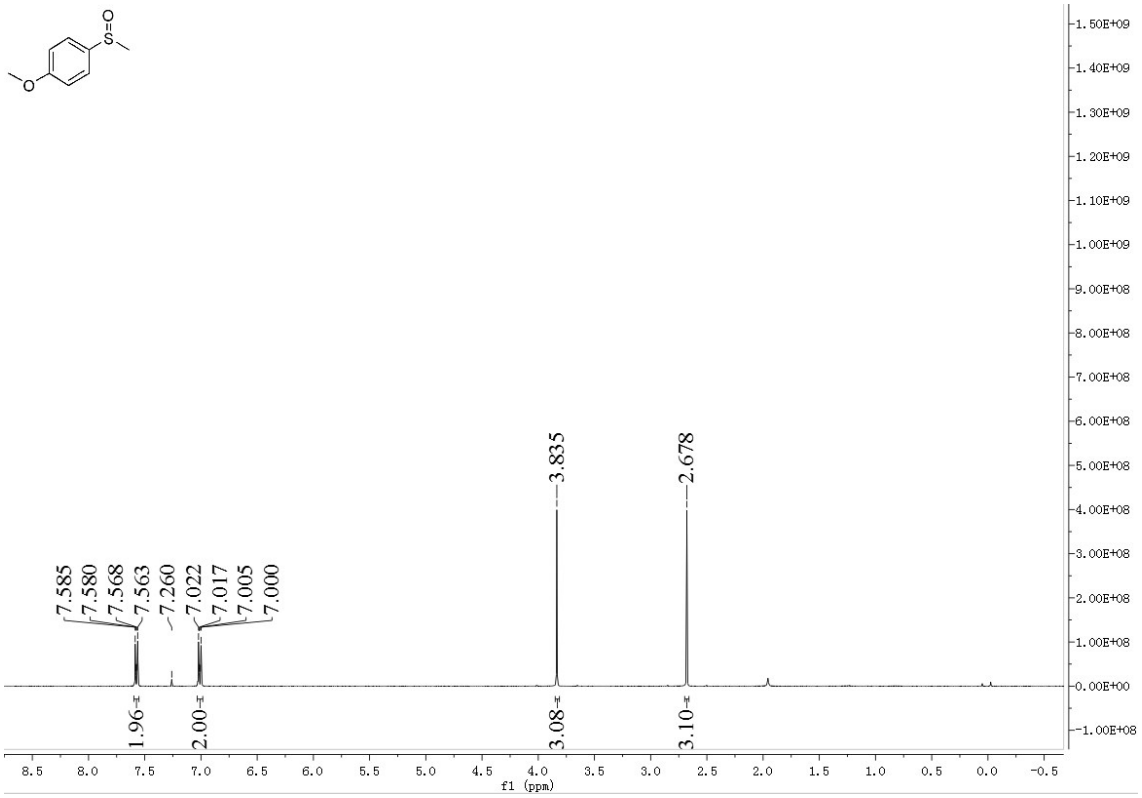
Compound **7c**



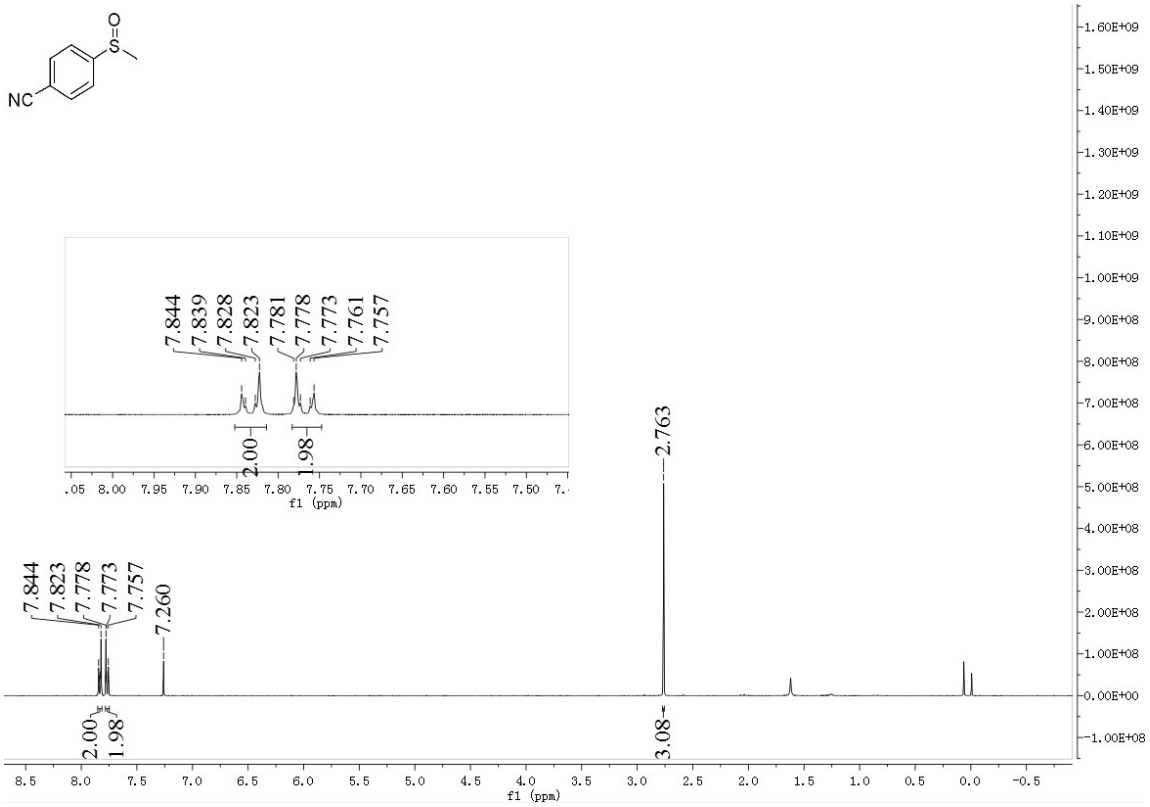
Compound **7d**



Compound **7e**



Compound **7f**


NC
O
S
7.844
7.839
7.828
7.823
7.781
7.778
7.773
7.761
7.757
2.00
1.98
f1 (ppm)
7.844
7.823
7.778
7.773
7.757
7.260
2.763
2.00
1.98
3.08
f1 (ppm)

III. X-ray single crystal diffraction data of 3a

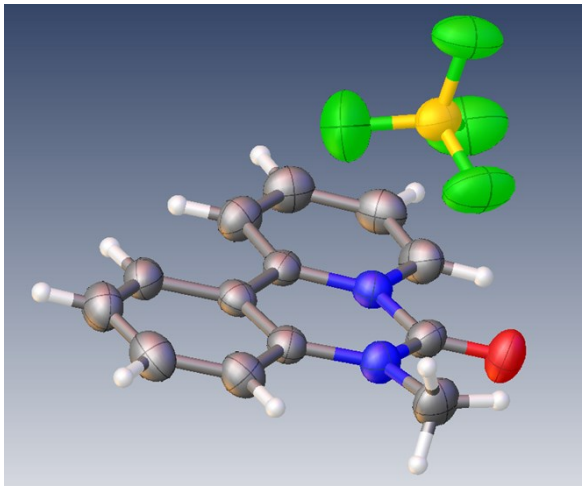


Figure S1 Crystal structure for 3a

Table 1 Crystal data and structure refinement for 3a.

Identification code	**3a**
Empirical formula	$C_{13}H_{11}BF_4N_2O$
Formula weight	298.05
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	$Pna2_1$
a/Å	10.3539(5)
b/Å	10.9951(6)
c/Å	11.0590(7)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1258.98(12)
Z	4
ρ_{calc}g/cm^3	1.572
μ/mm^{-1}	0.140
F(000)	608.0
Crystal size/mm^3	0.33 × 0.28 × 0.24
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.542 to 50.23
Index ranges	$-8 \le h \le 12$, $-13 \le k \le 11$, $-12 \le l \le 13$
Reflections collected	4515
Independent reflections	1997 [R_{int} = 0.0202, R_{sigma} = 0.0264]
Data/restraints/parameters	1997/1/191
Goodness-of-fit on F^2	0.870
Final R indexes [I>=2σ (I)]	R_1 = 0.0443, wR_2 = 0.1253
Final R indexes [all data]	R_1 = 0.0505, wR_2 = 0.1345
Largest diff. peak/hole / e Å^{-3}	0.40/-0.27

Flack parameter -0.3(5)

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 3a. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
F1	2038(3)	5103(3)	2053(3)	76.6(10)
O20	6112(3)	6166(3)	4663(3)	56.4(9)
N7	5059(3)	4567(3)	5571(3)	35.2(7)
N19	4317(3)	6602(3)	5755(3)	38.9(8)
F3	3110(3)	6471(3)	3163(4)	85.7(11)
C18	3324(4)	6210(4)	6517(4)	36.8(9)
F4	3802(3)	4569(4)	3084(5)	100.4(13)
F5	1994(6)	4985(5)	4072(5)	123.0(18)
C13	3198(4)	4975(4)	6792(4)	35.7(9)
C12	4102(3)	4111(4)	6276(4)	34.8(8)
C14	2177(4)	4591(4)	7532(4)	43.1(10)
C17	2462(4)	7048(4)	7025(4)	44.5(10)
C6	5221(4)	5848(4)	5281(4)	39.7(9)
C15	1320(4)	5425(4)	7990(5)	49.8(11)
C10	4914(4)	2099(4)	5898(5)	50.9(12)
C16	1498(4)	6642(5)	7750(4)	51.4(12)
C8	5937(4)	3808(4)	5021(5)	46.5(11)
C21	4367(4)	7880(4)	5353(5)	51.3(12)
C11	4043(4)	2868(4)	6457(4)	45.2(10)
C9	5869(4)	2591(4)	5173(5)	49.6(11)
B2	2713(5)	5285(5)	3096(5)	46.8(12)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 3a. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F1	98(2)	59.1(19)	72(2)	-5.8(16)	-42.1(19)	0.5(16)
O20	50.8(17)	52.1(18)	66(2)	5.3(17)	16.9(17)	-8.8(14)
N7	35.6(15)	35.0(17)	35.0(18)	-0.9(14)	-2.2(14)	0.8(13)
N19	42.8(16)	32.7(17)	41(2)	4.1(14)	0.8(15)	0.8(13)
F3	114(2)	46.1(16)	97(3)	5.7(16)	-40(2)	-18.3(17)
C18	35.3(18)	42(2)	33(2)	1.7(17)	-4.6(17)	-0.5(15)
F4	88(2)	77(2)	137(4)	-7(2)	-42(3)	18.7(17)
F5	142(4)	149(4)	78(3)	13(3)	27(3)	-49(3)
C13	35.3(19)	42(2)	30(2)	-0.8(16)	-5.1(16)	1.2(15)

C12	34.5(18)	40(2)	30(2)	3.1(16)	-6.4(16)	-3.3(15)
C14	43(2)	49(2)	37(2)	3.8(18)	-0.4(18)	-6.0(18)
C17	51(2)	42(2)	41(2)	2.7(19)	-2(2)	7.7(18)
C6	39(2)	37(2)	42(2)	1.5(18)	-3.0(19)	-6.0(16)
C15	43(2)	60(3)	46(3)	5(2)	5(2)	1.9(18)
C10	55(2)	40(2)	58(3)	2(2)	-7(2)	4.1(18)
C16	46(2)	64(3)	44(3)	0(2)	0(2)	13(2)
C8	39(2)	49(2)	51(3)	-7(2)	4(2)	4.0(18)
C21	61(3)	34(2)	59(3)	8(2)	3(2)	-5.4(18)
C11	47(2)	39(2)	50(3)	7(2)	-3(2)	-0.8(17)
C9	47(2)	48(3)	54(3)	-9(2)	-4(2)	10.6(18)
B2	53(3)	41(3)	47(3)	9(2)	-10(3)	-6(2)

Table 4 Bond Lengths for 3a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
F1	B2	1.364(6)	F4	B2	1.375(6)
O20	C6	1.202(5)	F5	B2	1.352(7)
N7	C12	1.357(5)	C13	C12	1.450(5)
N7	C6	1.454(5)	C13	C14	1.402(6)
N7	C8	1.375(5)	C12	C11	1.383(6)
N19	C18	1.397(5)	C14	C15	1.372(6)
N19	C6	1.356(5)	C17	C16	1.356(6)
N19	C21	1.475(5)	C15	C16	1.376(7)
F3	B2	1.369(6)	C10	C11	1.383(7)
C18	C13	1.397(5)	C10	C9	1.383(7)
C18	C17	1.401(6)	C8	C9	1.351(6)

Table 5 Bond Angles for 3a.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C12	N7	C6	124.6(3)	C16	C17	C18	119.3(4)
C12	N7	C8	120.9(3)	O20	C6	N7	119.8(4)
C8	N7	C6	114.4(3)	O20	C6	N19	124.9(4)
C18	N19	C21	120.1(3)	N19	C6	N7	115.3(3)
C6	N19	C18	123.5(3)	C14	C15	C16	119.5(4)
C6	N19	C21	116.2(3)	C11	C10	C9	119.1(4)
N19	C18	C17	120.5(4)	C17	C16	C15	122.2(4)
C13	C18	N19	120.0(3)	C9	C8	N7	120.7(4)
C13	C18	C17	119.5(4)	C12	C11	C10	120.8(4)
C18	C13	C12	119.4(4)	C8	C9	C10	119.8(4)
C18	C13	C14	119.3(4)	F1	B2	F3	109.8(4)
C14	C13	C12	121.3(4)	F1	B2	F4	109.1(5)

N7	C12	C13	117.1(3)	F3	B2	F4	107.5(4)
N7	C12	C11	118.7(4)	F5	B2	F1	110.9(4)
C11	C12	C13	124.2(4)	F5	B2	F3	110.8(5)
C15	C14	C13	120.1(4)	F5	B2	F4	108.6(5)

Table 6 Torsion Angles for 3a.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N7	C12	C11	C10	-2.1(6)	C14	C13	C12	C11	0.2(6)
N7	C8	C9	C10	-0.6(7)	C14	C15	C16	C17	3.1(7)
N19	C18	C13	C12	-0.2(6)	C17	C18	C13	C12	-179.2(4)
N19	C18	C13	C14	-178.3(4)	C17	C18	C13	C14	2.6(6)
N19	C18	C17	C16	179.2(4)	C6	N7	C12	C13	-1.3(5)
C18	N19	C6	O20	-177.0(4)	C6	N7	C12	C11	178.5(4)
C18	N19	C6	N7	2.9(6)	C6	N7	C8	C9	-177.5(4)
C18	C13	C12	N7	1.9(5)	C6	N19	C18	C13	-2.3(6)
C18	C13	C12	C11	-177.9(4)	C6	N19	C18	C17	176.7(4)
C18	C13	C14	C15	-0.7(6)	C8	N7	C12	C13	-178.3(4)
C18	C17	C16	C15	-1.2(7)	C8	N7	C12	C11	1.5(6)
C13	C18	C17	C16	-1.7(6)	C8	N7	C6	O20	-4.0(6)
C13	C12	C11	C10	177.7(4)	C8	N7	C6	N19	176.1(4)
C13	C14	C15	C16	-2.2(7)	C21	N19	C18	C13	173.1(4)
C12	N7	C6	O20	178.8(4)	C21	N19	C18	C17	-7.9(6)
C12	N7	C6	N19	-1.1(6)	C21	N19	C6	O20	7.4(6)
C12	N7	C8	C9	-0.2(6)	C21	N19	C6	N7	-172.7(3)
C12	C13	C14	C15	-178.8(4)	C11	C10	C9	C8	0.0(7)
C14	C13	C12	N7	180.0(4)	C9	C10	C11	C12	1.3(7)

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 3a.

Atom	*x*	*y*	*z*	U(eq)
H14	2079.74	3770.27	7712.87	52
H17	2549.78	7874.26	6866.88	53
H15	625.33	5169.82	8458.86	60
H10	4859.84	1261.68	6009.52	61
H16	938.05	7204.06	8096.59	62
H8	6584.46	4137.35	4538.51	56
H21A	3541.93	8111.29	5029.25	77
H21B	5016.11	7967.63	4739.21	77
H21C	4574.5	8393.45	6027.34	77
H11	3409.19	2546.16	6959.16	54
H9	6462.22	2084.99	4790.67	60

IV Photophysical and Redox Properties of 2a and 3a

All photophysical and redox properties of **2a** and **3a** were tested following the procedure described in literature.[9]

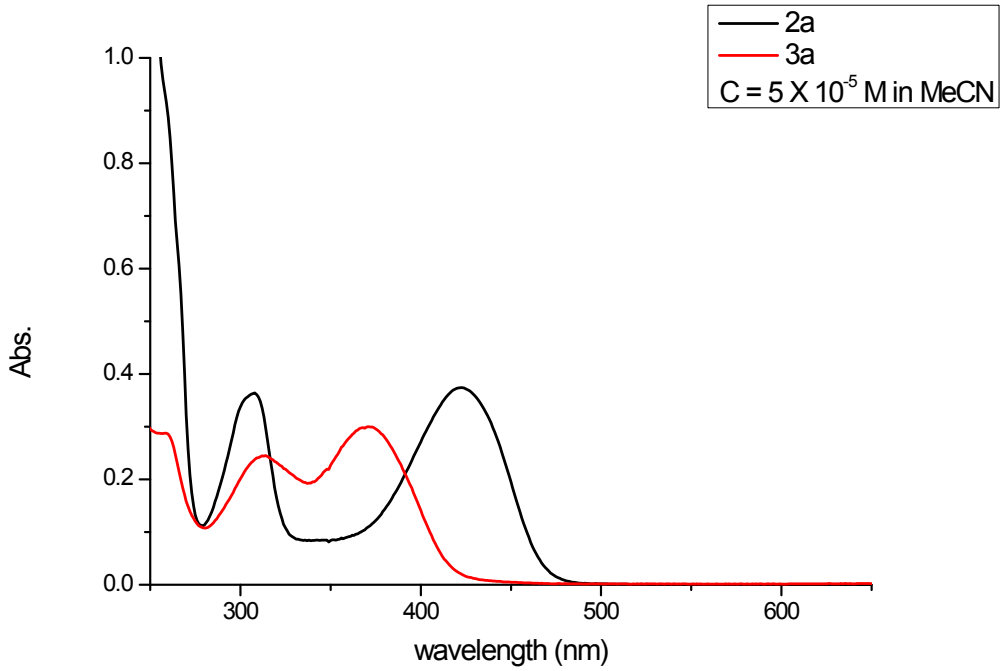


Figure S2 Absorption spectrum for 2a and 3a

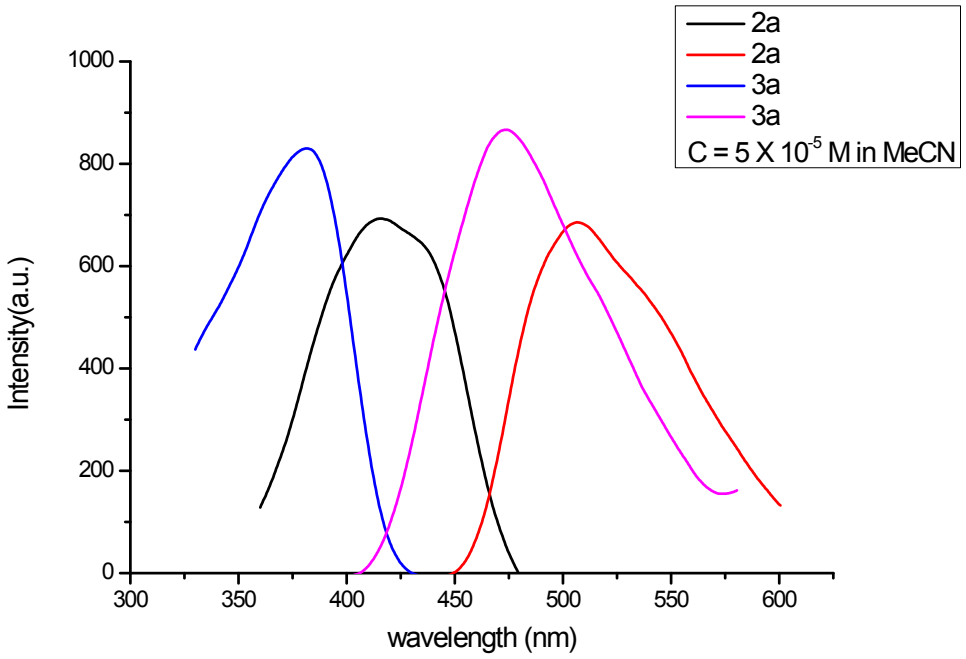


Figure S3 Excitation and emission spectrum for 2a and 3a

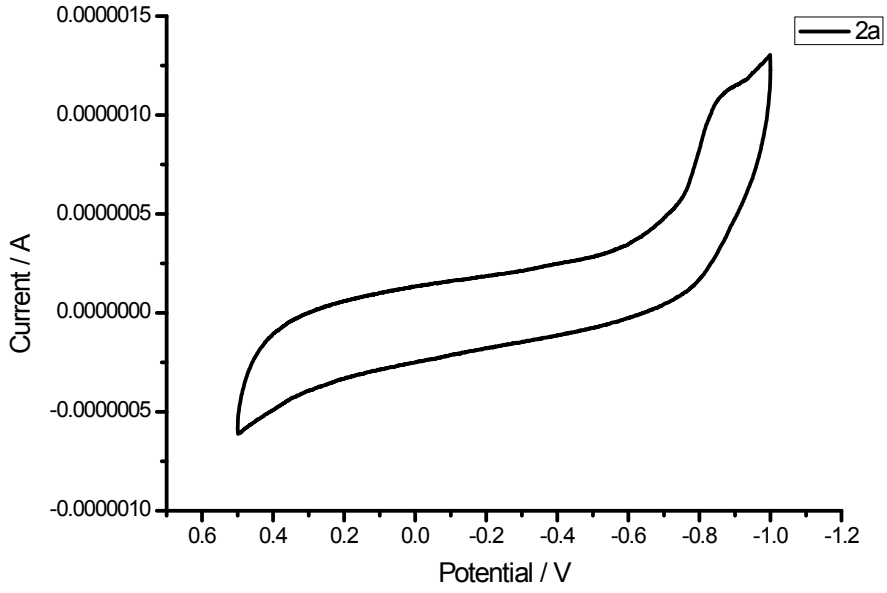


Figure S4 Cyclic voltammogram for 2a

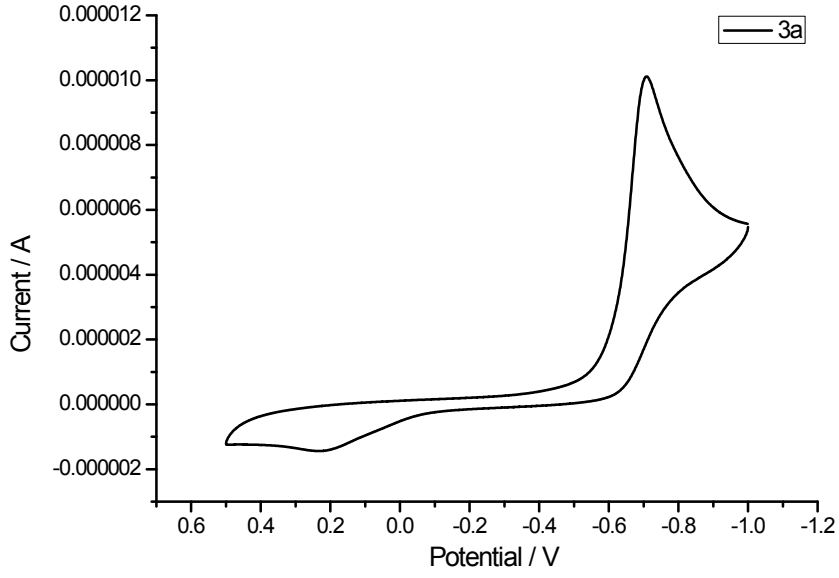


Figure S4 Cyclic voltammogram for 3a

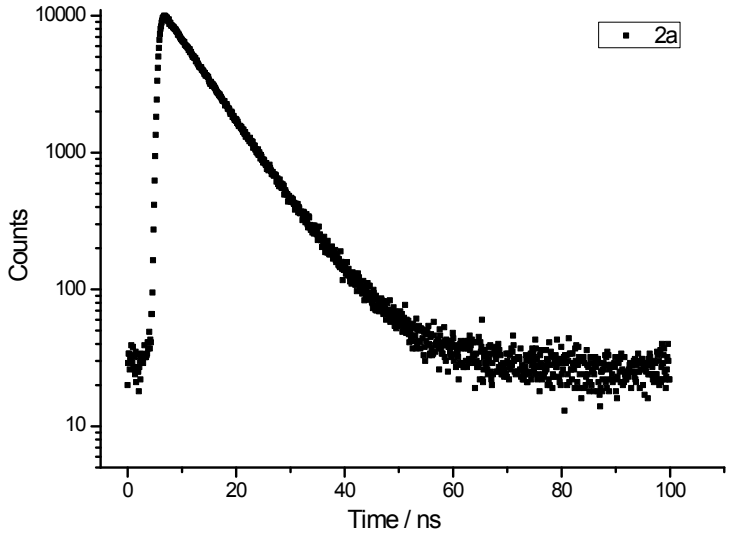


Figure S5 Fluorescence lifetime for 2a

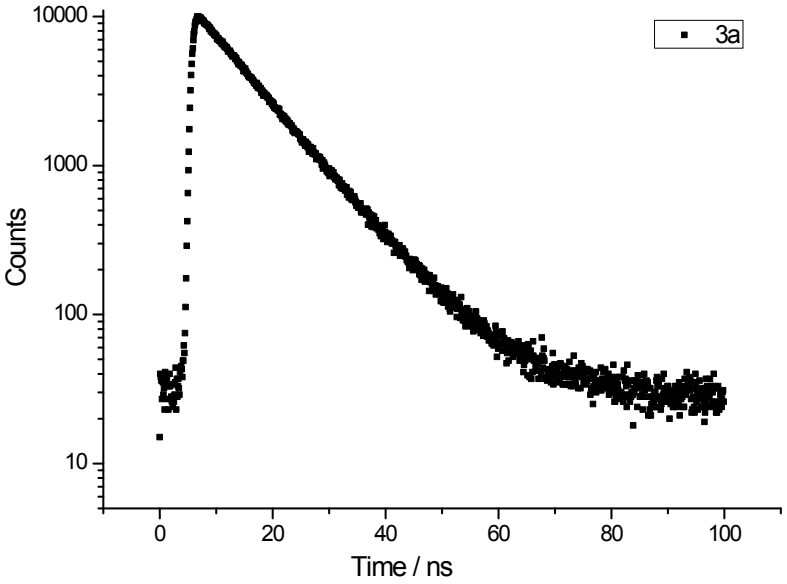


Figure S6 Fluorescence lifetime for 3a

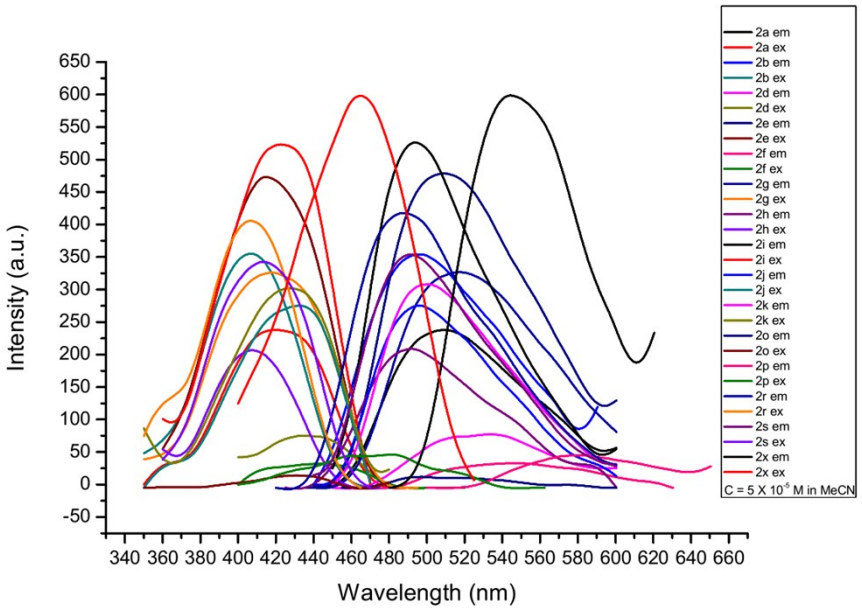


Figure S7 Excitation and emission spectrum for 2

V. References

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