Supporting Information

N-Methylation of *ortho*-Substituted Aromatic Amines with Methanol Catalyzed by 2-Arylbenzo[*d*]oxazole NHC-Ir(III) Complexes

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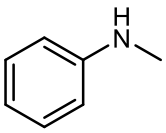
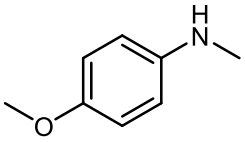
1. Characterization data of substrates



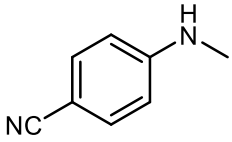
N-methylaniline

Followed the general procedure, purification by column chromatography (PE/EtOAc 50:1) gave product (99%) *N*-methylaniline as yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (td, *J* = 7.4, 1.8 Hz, 2H), 6.84 (t, *J* = 7.3 Hz, 1H), 6.71 (d, *J* = 7.7 Hz, 2H), 3.57 (s, 1H), 2.91 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.45 (s), 129.28 (s), 117.28 (s), 112.50 (s), 30.76 (s) ppm. GC-MS (m/z): 107.07 (calc. 107.10).



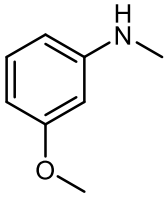
4-Methoxy-*N*-methylaniline

Followed the general procedure, purification by column chromatography (PE/EtOAc 50:1) gave product (89%) 4-methoxy-*N*-methylaniline as a oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.82 (d, *J* = 8.7 Hz, 2H), 6.60 (d, *J* = 8.6 Hz, 2H), 3.77 (s, 3H), 2.81 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.13 (s), 143.75 (s), 114.96 (s), 113.67 (s), 55.89 (s), 31.63 (s). GC-MS (m/z): 137.08 (calc. 137.10).



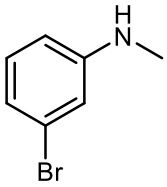
4-(Methylamino)benzonitrile

Followed the general procedure, purification by column chromatography (PE/EtOAc 10:1) gave product (98%), 4-(methylamino)benzonitrile as a colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (s, 2H), 6.46 (s, 2H), 4.34 (s, 1H), 2.78 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.30 (s), 133.66 (s), 120.63 (s), 111.84 (s), 98.37 (s), 29.95 (s). GC-MS (m/z): 132.07 (calc. 132.02).



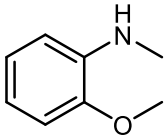
3-Methoxy-N-methylaniline

Followed the general procedure, purification by column chromatography (PE/EtOAc 50:1) gave product (92%) 3-methoxy-*N*-methylaniline as a oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.12 (t, *J* = 8.1 Hz, 1H), 6.31 (dd, *J* = 8.1, 2.3 Hz, 1H), 6.26 (dd, *J* = 8.0, 2.1 Hz, 1H), 6.19 (t, *J* = 2.2 Hz, 1H), 3.81 (s, 4H), 2.85 (s, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 129.79 (s), 105.58 (s), 102.21 (s), 98.23 (s), 54.96 (s), 30.60 (s), 29.58 (s). GC-MS (m/z): 137.08 (calc. 137.14).



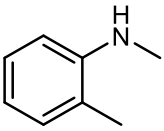
3-Bromo-*N*-methylaniline

Followed the general procedure, purification by column chromatography (PE/EtOAc 50:1) gave 89 mg (96%), 3-bromo-*N*-methylaniline as a colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.07 (t, *J* = 8.0 Hz, 1H), 6.87 (d, *J* = 7.8 Hz, 1H), 6.77 (t, *J* = 1.9 Hz, 1H), 6.55 (dd, *J* = 8.2, 1.8 Hz, 1H), 3.80 (s, 1H), 2.83 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.50 (s), 130.36 (s), 123.20 (s), 119.74 (s), 114.67 (s), 111.16 (s), 30.42 (s). GC-MS (m/z): 184.98(calc. 184.99).



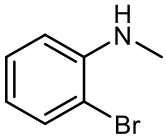
2-Methoxy-*N*-methylaniline

Followed the general procedure, purification by column chromatography (PE/EtOAc 50:1) gave product (86%) 2-methoxy-*N*-methylaniline as a oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.95 (t, *J* = 7.6 Hz, 1H), 6.82 (d, *J* = 7.4 Hz, 1H), 6.72 (t, *J* = 7.7 Hz, 1H), 6.66 (d, *J* = 7.7 Hz, 1H), 4.28 (s, 1H), 3.89 (s, 3H), 2.91 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.80 (s), 139.29 (s), 121.25 (s), 116.19 (s), 109.18 (d, *J* = 8.7 Hz), 55.28 (s), 30.26 (s). GC-MS (m/z): 137.08 (calc. 137.11).



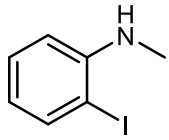
N,2-dimethylaniline

Followed the general procedure, purification by column chromatography (PE/EtOAc 50:1) gave product (73 %), *N*,2-dimethylaniline as a colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.20 (m, 1H), 7.13 (d, *J* = 7.2 Hz, 1H), 6.75 (t, *J* = 7.4 Hz, 1H), 6.69 (d, *J* = 8.0 Hz, 1H), 2.96 (s, 3H), 2.21 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.17 (s), 129.82 (s), 127.11 (s), 121.82 (s), 116.77 (s), 109.05 (s), 30.68 (s), 17.29 (s). GC-MS (m/z): 121.08 (calc. 121.15).



2-Bromo-*N*-methylaniline

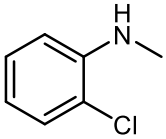
Followed the general procedure, purification by column chromatography (PE/EtOAc 50:1) gave product (83 %), 2-bromo-*N*-methylaniline as a colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.25 (s, 1H), 6.67 (dd, *J* = 8.1, 1.1 Hz, 1H), 6.64 – 6.57 (m, 1H), 4.39 (s, 1H), 2.93 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.97 (s), 132.28 (s), 128.56 (s), 117.60 (s), 110.74 (s), 109.62 (s), 30.61 (s). GC-MS (m/z): 184.98(calc. 185.15).



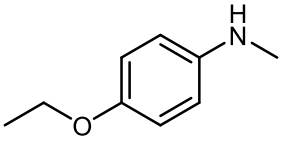
2-Iodo-*N*-methylaniline

Followed the general procedure, purification by column chromatography (PE/EtOAc 50:1) gave product (78 %), 2-iodo-*N*-methylaniline as a brown oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.31 – 7.18 (m, 1H), 6.57 (dd, *J* = 8.1, 1.2 Hz, 1H), 6.46 (td, *J* = 7.6, 1.4 Hz, 1H), 4.21 (s, 1H), 2.90 (d, *J* = 3.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.16 (s), 138.86 (s), 129.47 (s), 118.47 (s), 109.99 (s), 30.97 (s). GC-MS (m/z): 232.97 (calc. 233.06).

2-Chloro-*N*-methylaniline

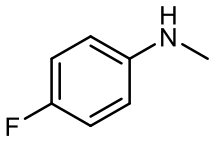


Followed the general procedure, purification by column chromatography (PE/EtOAc 50:1) gave product (75%), 2-chloro-*N*-methylaniline as a colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (d, *J* = 7.2 Hz, 1H), 7.24 – 7.16 (m, 1H), 6.67 (t, *J* = 7.4 Hz, 2H), 4.37 (s, 1H), 2.92 (d, *J* = 4.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.01 (s), 128.95 (s), 127.84 (s), 119.04 (s), 117.00 (s), 110.61 (s), 30.35 (s). GC-MS (m/z): 141.03 (calc. 141.23).



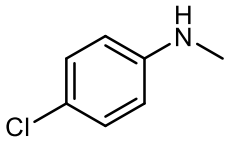
4-Ethoxy-*N*-methylaniline

Followed the general procedure, purification by column chromatography (PE/EtOAc 10:1) gave product (88%) 4-ethoxy-*N*-methylaniline as a brown oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.84 (dd, *J* = 11.0, 6.6 Hz, 2H), 6.60 (d, *J* = 7.8 Hz, 2H), 3.99 (dt, *J* = 11.2, 4.7 Hz, 2H), 3.29 (s, 1H), 2.81 (d, *J* = 3.9 Hz, 3H), 1.41 (td, *J* = 6.9, 4.7 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.36 (s), 143.82 (s), 115.88 (s), 113.66 (s), 64.22 (s), 31.59 (s), 15.09 (s). GC-MS (m/z): 151.09 (calc. 151.11).



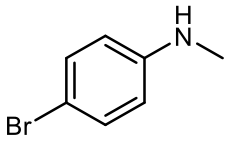
4-Fluoro-*N*-methylaniline

Followed the general procedure, purification by column chromatography (PE/EtOAc 50:1) gave product (95%), 4-fluoro-*N*-methylaniline as a colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.01 – 6.87 (m, 2H), 6.56 (ddd, *J* = 6.8, 5.1, 3.0 Hz, 2H), 3.40 (dd, *J* = 57.2, 12.0 Hz, 1H), 2.81 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.93 (s), 154.60 (s), 145.73 (s), 115.66 (s), 115.44 (s), 113.11 (d, *J* = 7.4 Hz), 31.25 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -128.56 (s). GC-MS (m/z): 125.06 (calc. 125.36).



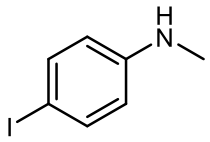
4-Chloro-*N*-methylaniline

Followed the general procedure, purification by column chromatography (PE/EtOAc 50:1) gave product (99%), 4-chloro-*N*-methylaniline as a colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.11 (s, 2H), 5.50 (s, 2H), 2.70 (s, 1H), 1.79 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.91 (s), 129.01 (s), 121.81 (s), 113.44 (s), 30.79 (s). GC-MS (m/z): 141.03 (calc. 141.23).



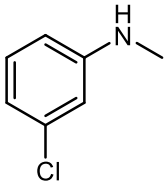
4-Bromo-*N*-methylaniline

Followed the general procedure, purification by column chromatography (PE/EtOAc 50:1) gave product (96%), 4-bromo-*N*-methylaniline as a colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.13 (d, *J* = 7.9 Hz, 2H), 6.34 (d, *J* = 8.0 Hz, 2H), 3.59 (s, 1H), 2.65 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.34 (s), 131.88 (s), 113.98 (s), 108.76 (s), 30.72 (s). GC-MS (m/z): 184.98(calc. 185.02).



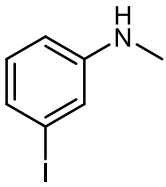
4-Iodo-*N*-methylaniline

Followed the general procedure, purification by column chromatography (PE/EtOAc 50:1) gave product (91%), 4-iodo-*N*-methylaniline as a colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 8.8 Hz, 2H), 6.39 (d, *J* = 8.8 Hz, 2H), 3.52 (s, 1H), 2.80 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.92 (s), 137.76 (s), 129.30 (s), 114.74 (s), 30.67 (s). GC-MS (m/z): 232.97(calc. 232.99).



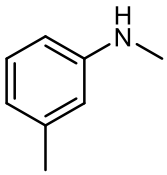
3-Chloro-*N*-methylaniline

Followed the general procedure, purification by column chromatography (PE/EtOAc 50:1) gave product (95%), 3-chloro-*N*-methylaniline as a colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.12 (t, *J* = 8.0 Hz, 1H), 6.70 (dt, *J* = 19.9, 10.0 Hz, 1H), 6.65 – 6.55 (m, 1H), 6.50 (dd, *J* = 8.1, 2.0 Hz, 1H), 3.82 (s, 1H), 2.84 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.33 (s), 134.90 (s), 130.02 (s), 116.86 (s), 111.76 (s), 110.73 (s), 30.41 (s). GC-MS (m/z): 141.03 (calc. 141.53).



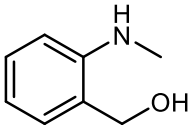
3-Iodo-*N*-methylaniline

Followed the general procedure, purification by column chromatography (PE/EtOAc 50:1) gave product (95%), 3-iodo-*N*-methylaniline as a brown oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.07 (d, *J* = 6.9 Hz, 1H), 7.01 – 6.88 (m, 2H), 6.63 – 6.55 (m, 1H), 3.75 (s, 1H), 2.82 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.41 (s), 130.58 (s), 125.88 (s), 120.69 (s), 111.77 (s), 95.31 (s), 30.44 (s). GC-MS (m/z): 232.97 (calc. 233.03).



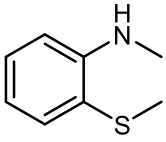
N,3-Dimethylaniline

Followed the general procedure, purification by column chromatography (PE/EtOAc 50:1) gave product (98%), *N*,3-dimethylaniline as a colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.16 (s, 1H), 6.62 (d, *J* = 7.4 Hz, 1H), 6.50 (d, *J* = 6.5 Hz, 2H), 3.68 (s, 1H), 2.88 (s, 3H), 2.37 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.34 (s), 138.88 (s), 129.00 (s), 118.12 (s), 113.10 (s), 109.56 (s), 30.69 (s), 21.56 (s). GC-MS (m/z): 121.08 (calc. 121. 12).



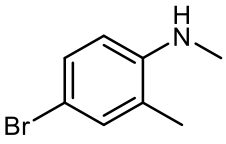
(2-(Methylamino)phenyl)methanol

Followed the general procedure, purification by column chromatography (PE/EtOAc 10:1) gave product (90 %), (2-(methylamino)phenyl)methanol as a colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (t, *J* = 7.7 Hz, 1H), 7.08 (d, *J* = 7.6 Hz, 1H), 6.70 (t, *J* = 7.0 Hz, 2H), 4.65 (s, 2H), 2.89 (d, *J* = 0.7 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.46 (s), 129.59 (s), 128.84 (s), 124.23 (s), 116.26 (s), 109.99 (s), 64.59 (s), 30.20 (s). GC-MS (m/z): 137.08 (calc. 137.10).



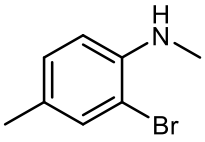
N-Methyl-2-(methylthio)aniline

Followed the general procedure, purification by column chromatography (PE/EtOAc 10:1) gave product (85 %), *N*-Methyl-2-(methylthio)aniline as a colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.40 (m, 1H), 7.25 (ddd, *J* = 8.1, 7.4, 1.6 Hz, 1H), 6.69 (td, *J* = 7.5, 1.3 Hz, 1H), 6.64 (dd, *J* = 8.1, 1.0 Hz, 1H), 2.93 (s, 3H), 2.35 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.13 (s), 133.64 (s), 129.32 (s), 119.55 (s), 116.72 (s), 109.39 (s), 30.48 (s), 17.88 (s). GC-MS (m/z): 153.06 (calc. 153.08).



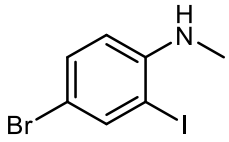
4-Bromo-*N*,2-dimethylaniline

Followed the general procedure, purification by column chromatography (PE/EtOAc 50:1) gave product (77 %), 4-bromo-*N*,2-dimethylanilineas as a colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 – 7.23 (m, 1H), 7.18 (d, *J* = 2.3 Hz, 1H), 6.49 (d, *J* = 8.6 Hz, 1H), 2.89 (s, 3H), 2.12 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.14 (s), 132.15 (s), 129.56 (s), 123.87 (s), 110.46 (s), 108.31 (s), 30.64 (s), 17.04 (s). GC-MS (m/z): 198.99 (calc. 199.01).



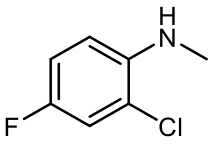
2-Bromo-*N*,4-dimethylaniline

Followed the general procedure, purification by column chromatography (PE/EtOAc 50:1) gave product (78 %), 2-bromo-*N*,4-dimethylaniline as a colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (t, *J* = 4.1 Hz, 1H), 7.08 – 7.03 (m, 1H), 6.61 – 6.56 (m, 1H), 2.91 (s, 3H), 2.27 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.67 (s), 132.53 (s), 128.93 (s), 127.02 (s), 110.65 (s), 109.41 (s), 30.73 (s), 19.89 (s). GC-MS (m/z): 198.99 (calc. 199.04).



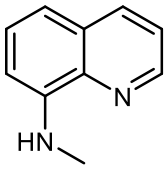
4-Bromo-2-iodo-*N*-methylaniline

Followed the general procedure, purification by column chromatography (PE/EtOAc 50:1) gave product (76 %), 4-bromo-2-iodo-*N*-methylaniline as a colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 2.0 Hz, 1H), 7.39 – 7.31 (m, 1H), 6.40 (t, *J* = 19.1 Hz, 1H), 4.24 (s, 1H), 2.88 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.23 (s), 140.12 (s), 132.00 (s), 110.71 (s), 108.34 (s), 84.80 (s), 30.93 (s). GC-MS (m/z): 310.88 (calc. 310.95).



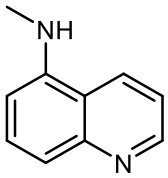
2-Chloro-4-fluoro-*N*-methylaniline

Followed the general procedure, purification by column chromatography (PE/EtOAc 50:1) gave product (83 %), 2-chloro-4-fluoro-*N*-methylaniline as a colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21 – 7.12 (m, 1H), 6.39 – 6.28 (m, 2H), 4.45 (s, 1H), 2.89 (d, *J* = 5.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 129.49 (s), 129.49 (s), 103.26 (s), 103.03 (s), 98.04 (s), 97.76 (s), 30.22 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -113.52 – -113.79 (m). GC-MS (m/z): 159.02 (calc. 159.11).



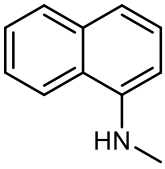
N-Methylquinolin-8-amine

Followed the general procedure, purification by column chromatography (PE/EtOAc 50:1) gave product (92 %), *N*-methylquinolin-8-amine as a colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73 (dd, *J* = 4.1, 1.6 Hz, 1H), 8.08 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.44 (d, *J* = 8.0 Hz, 1H), 7.42 – 7.37 (m, 2H), 7.07 (d, *J* = 8.2 Hz, 1H), 6.68 (d, *J* = 7.6 Hz, 1H), 6.16 (s, 1H), 3.07 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.81 (s), 135.99 (s), 127.86 (s), 121.38 (s), 113.69 (s), 104.13 (s), 30.07 (s). GC-MS (m/z): 158.08 (calc. 158.15).



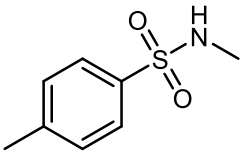
N-Methylquinolin-5-amine

Followed the general procedure, purification by column chromatography (PE/EtOAc 50:1) gave product (89 %), *N*-methylquinolin-5-amine as a colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.79 (s, 1H), 8.07 (d, *J* = 7.9 Hz, 1H), 7.52 (t, *J* = 7.6 Hz, 1H), 7.42 (d, *J* = 7.6 Hz, 1H), 7.21 (d, *J* = 18.1 Hz, 1H), 6.55 (d, *J* = 6.9 Hz, 1H), 4.43 (s, 1H), 2.94 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.91 (s), 144.71 (s), 130.46 (s), 128.64 (s), 119.27 (s), 118.38 (s), 104.13 (s), 30.98 (s). GC-MS (m/z): 158.08 (calc. 158.14).



N-methylnaphthalen-1-amine

Followed the general procedure, purification by column chromatography (PE/EtOAc 50:1) gave product (82 %), *N*-methylnaphthalen-1-amine as a colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (s, 2H), 7.45 – 7.22 (m, 3H), 7.17 (s, 1H), 6.53 (s, 1H), 4.43 (d, *J* = 67.7 Hz, 1H), 2.93 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.57 (s), 134.28 (s), 128.67 (s), 126.69 (s), 125.70 (s), 124.68 (s), 123.51 (s), 119.80 (s), 117.33 (s), 103.81 (s), 31.02 (s). GC-MS (m/z): 157.08 (calc. 157.12).



N,4-dimethylbenzenesulfonamide

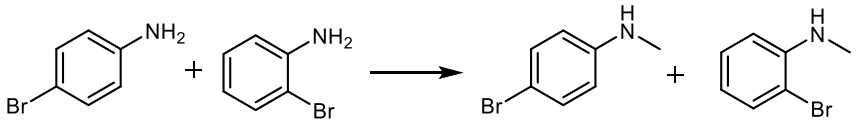
Followed the general procedure, purification by column chromatography (PE/EtOAc 10:1) gave product (94 %), *N*,4-dimethylbenzenesulfonamide as white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.6 Hz, 2H), 7.24 (d, *J* = 7.6 Hz, 2H), 5.17 (s, 1H), 2.53 (d, *J* = 4.2 Hz, 3H), 2.35 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.46 (s), 135.75 (s), 129.72 (s), 127.25 (s), 29.22 (s), 21.47 (s). GC-MS (m/z): 185.05 (calc. 185.08).

2. Control experiments and kinetic experiments

2.1 Control experiments

Reaction under optimized conditions

A mixture of 2-bromoaniline (42.5 mg, 0.25 mmol), 4-bromoaniline (42.5 mg, 0.25 mmol), **7** (0.5 mol%) KO^{t}Bu (56 mg, 1.0 equiv.), methanol (1 mL), in a 15 mL pressure tube with magnetic bar was stirred at130 °C for 12 h. After cooling to the room temperature, the solvents were removed under vacuum, and the yields were determined by 1H NMR with 1,3,5-trimethoxybenzene as the internal standard.



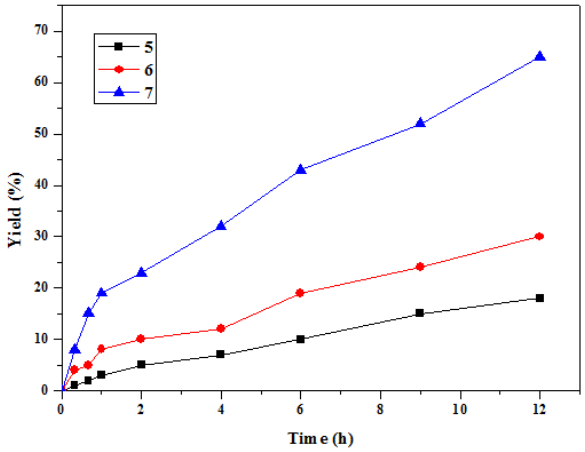
1.935 : 1

2.2 Kinetic experiments

Reaction under optimized conditions
A mixture of 2-bromoaniline (85mg, 0. 5 mmol), **5,** and **6,** or **7** (0.5 mol%) as catalyst, respectively, KO*t*Bu (56 mg, 1.0 equiv.), methanol (1 mL), in a 15 mL pressure tube with magnetic bar was stirred at 130 °C. After specific time, the reaction mixture was cooled to room temperature. The solvents were removed under vacuum, and the yields were determined by ^{1}H NMR with 1,3,5-trimethoxybenzene as the internal standard.

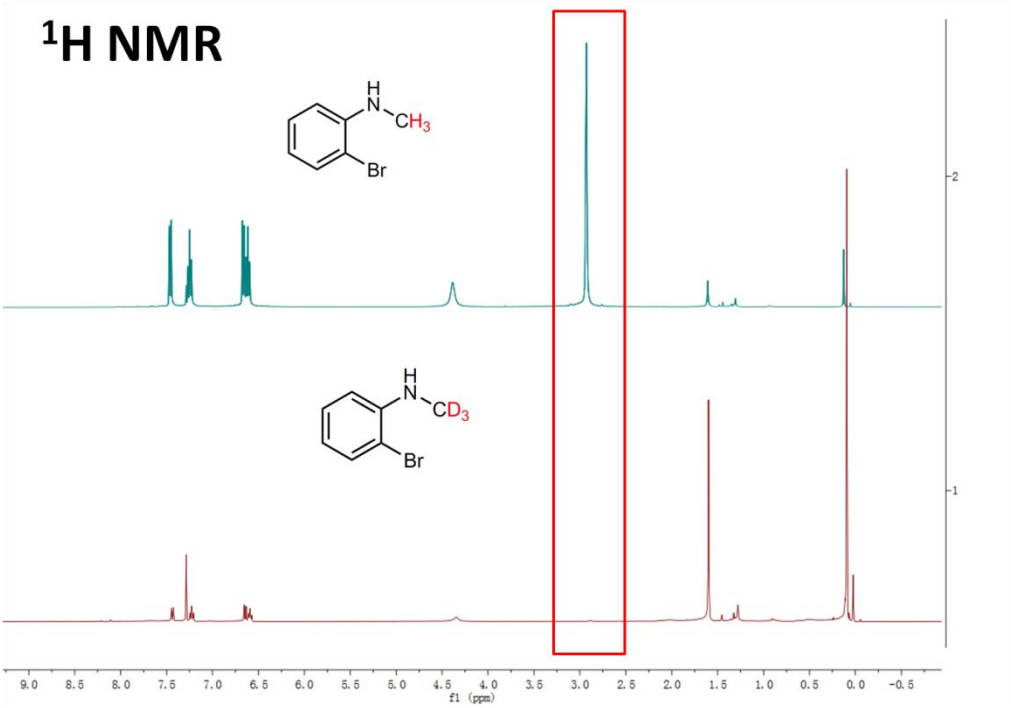
The results are as following table.

Entry	Time(h)	Yield$_5$(%)	Yield$_6$(%)	Yield$_7$(%)
1	0	0	0	0
2	0.33	1	4	8
3	0.67	2	5	15
4	1	3	8	19
5	2	5	10	23
6	4	7	12	32
7	6	10	19	43
8	9	15	24	52
9	12	18	30	65

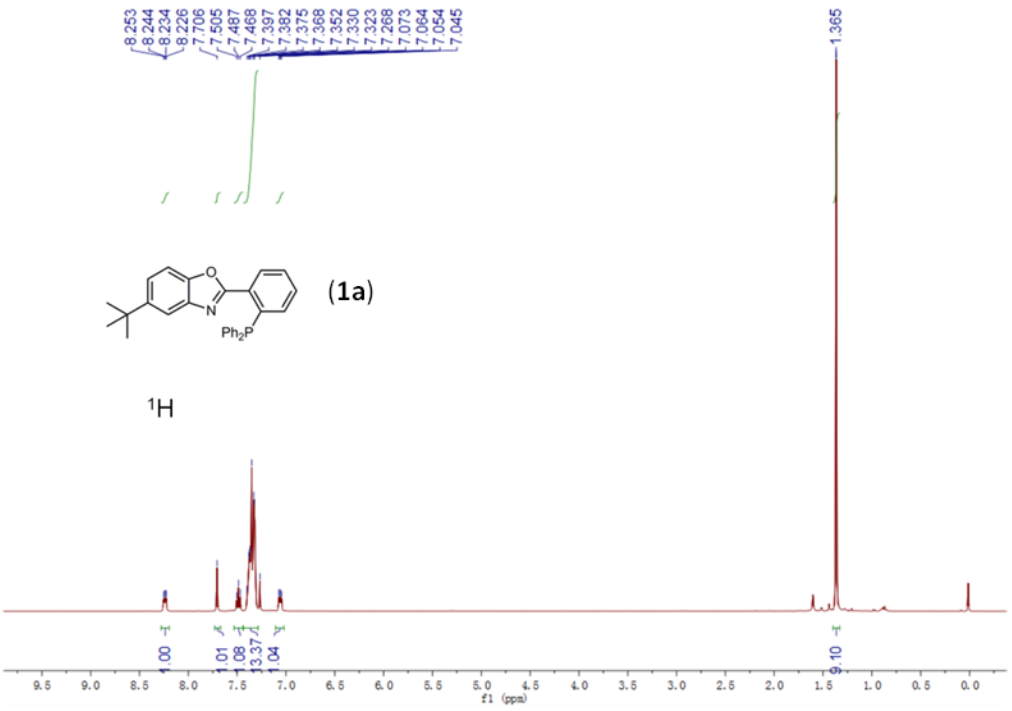


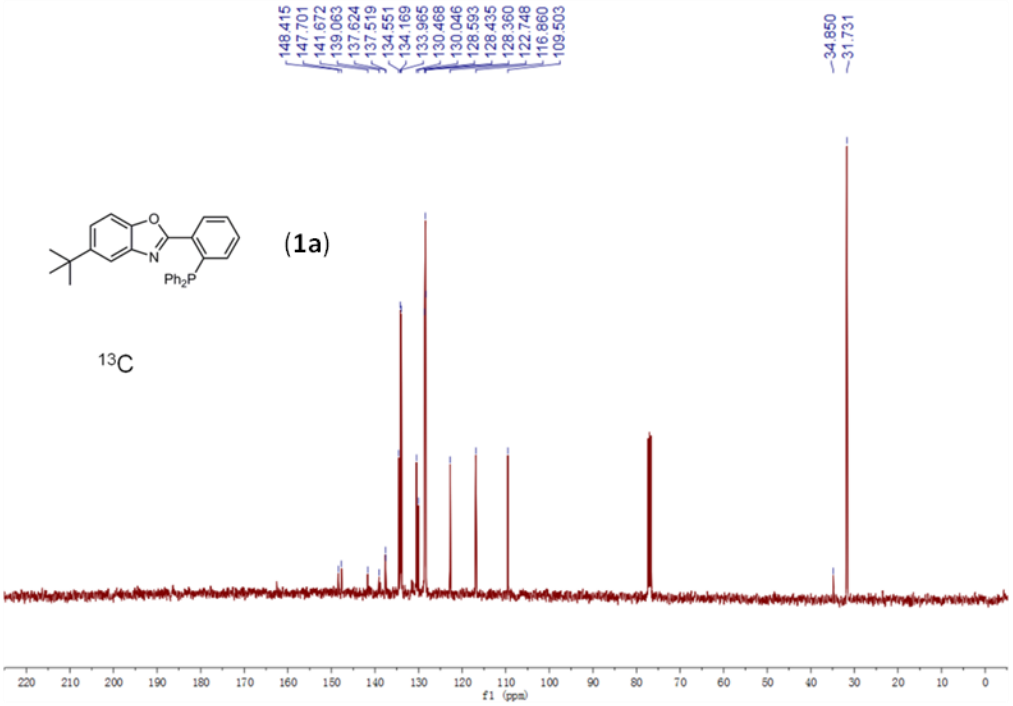
3. Deuteration experiments.

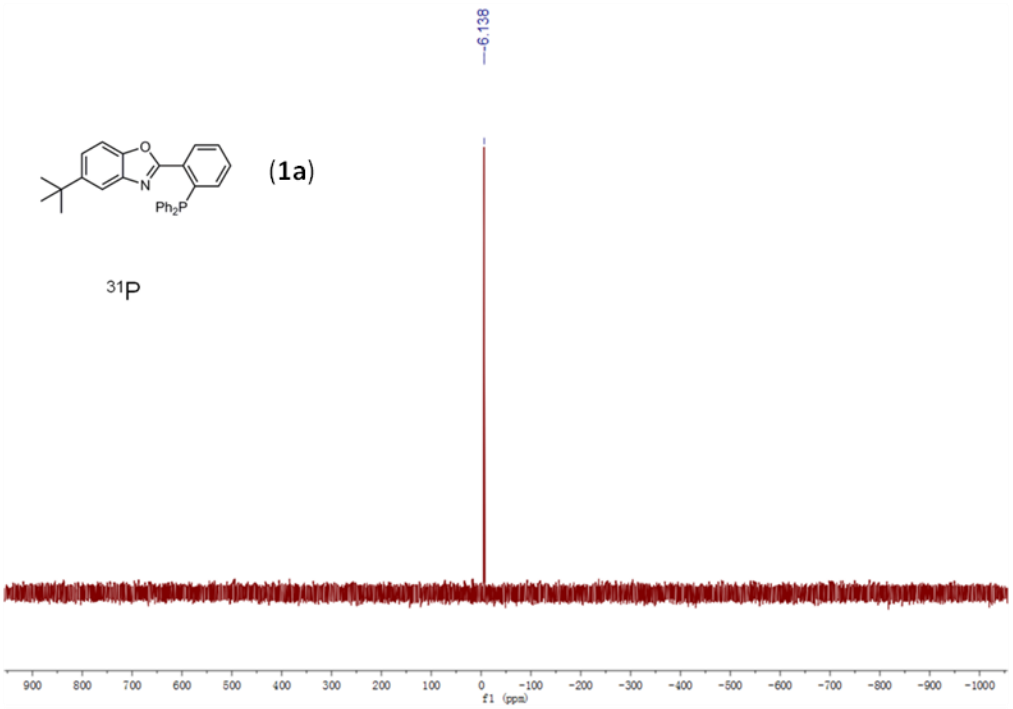
A mixture of 2-bromoaniline (85mg, 0. 5 mmol), **7** (4.2 mg, 0.5 mol%) KO^{t}Bu (56 mg, 1.0 equiv.), CD_3OD (1 mL), in a 15 mL pressure tube with magnetic bar was stirred at 130 °C for 12 h. the reaction mixture was cooled to room temperature. The solvents were removed under vacuum, and the yields were determined by ^{1}H NMR with 1,3,5-trimethoxybenzene as the internal standard.

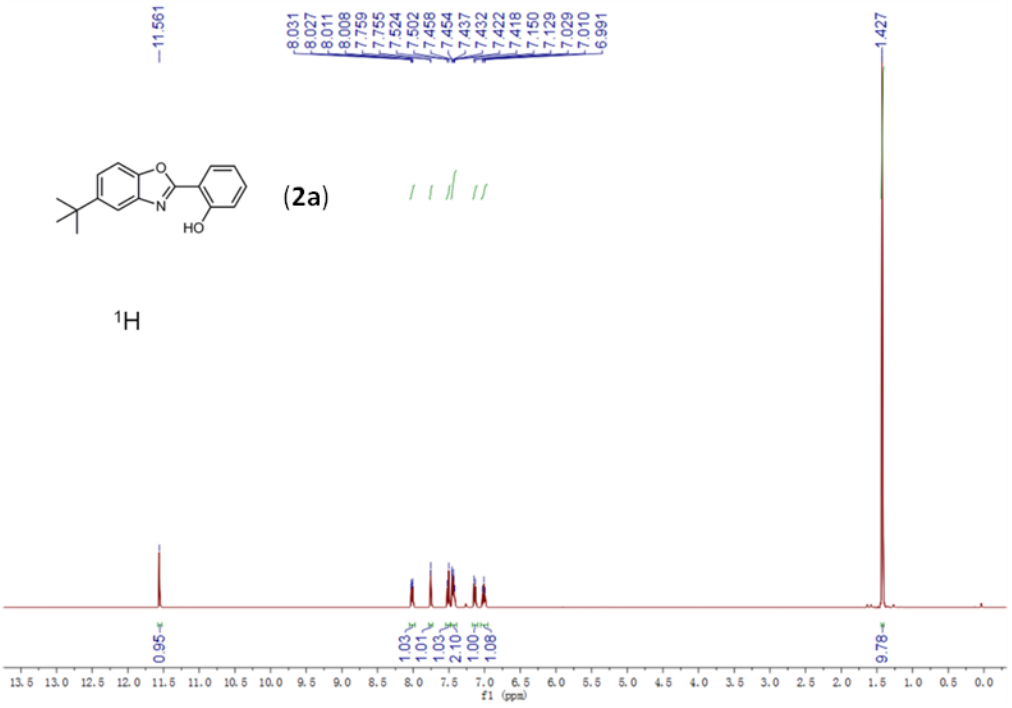


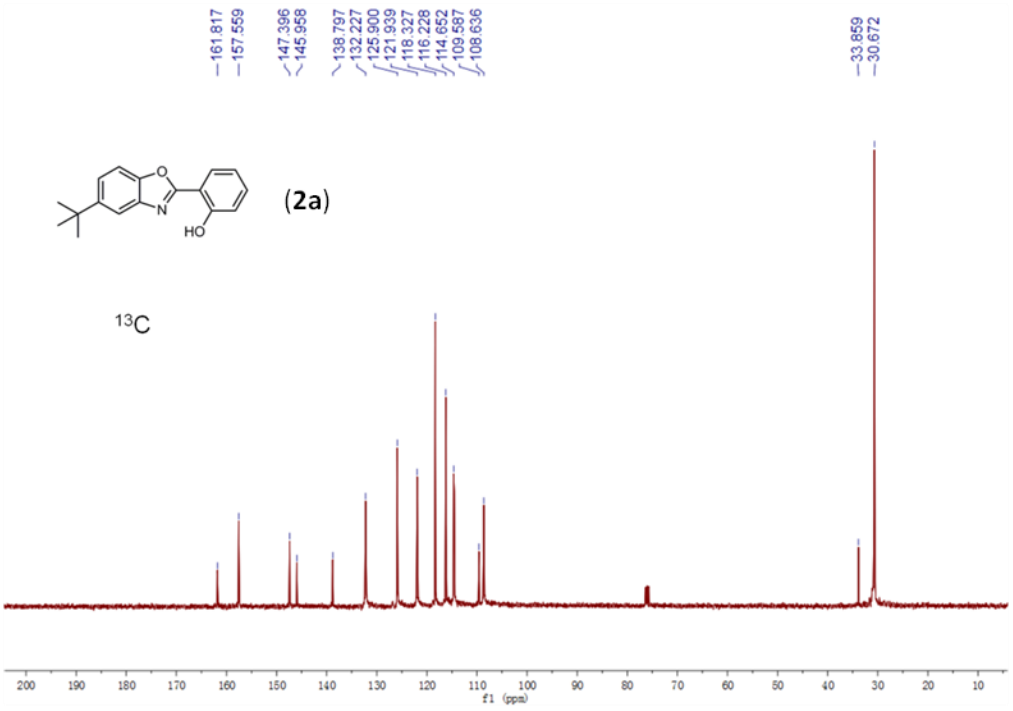
4. NMR spectra of compounds and substrates

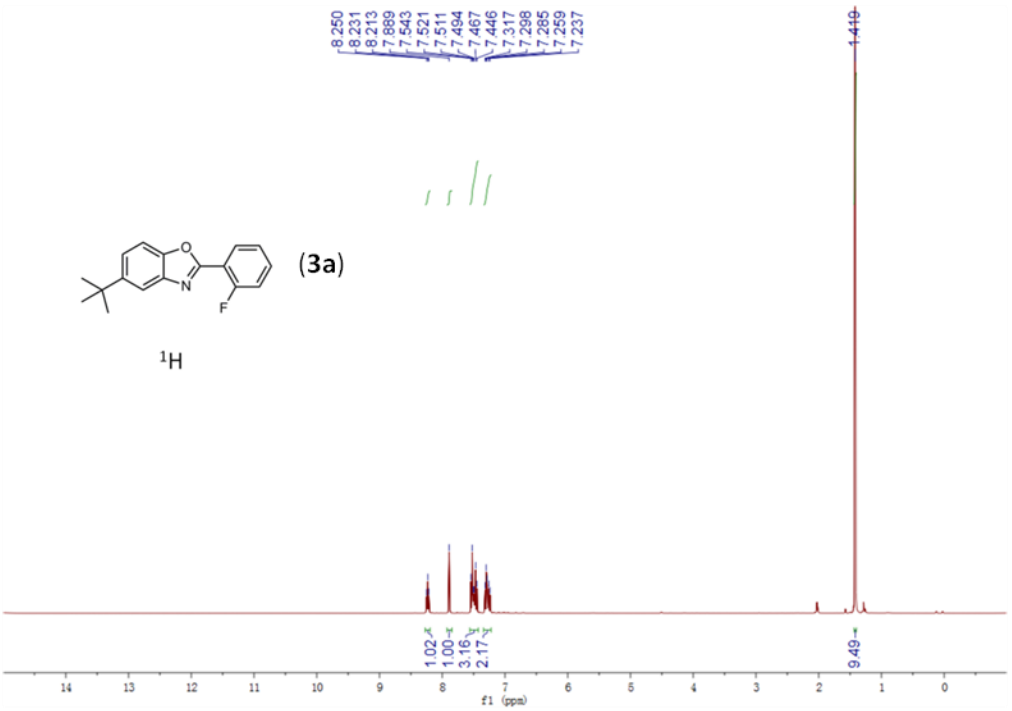

8.253
8.244
8.234
8.226
7.706
7.505
7.487
7.468
7.397
7.382
7.375
7.368
7.352
7.330
7.323
7.268
7.073
7.064
7.054
7.045
1.365
(1a)
Ph2P
1H
1.00
1.01
1.08
13.37
1.04
9.10
f1 (ppm)

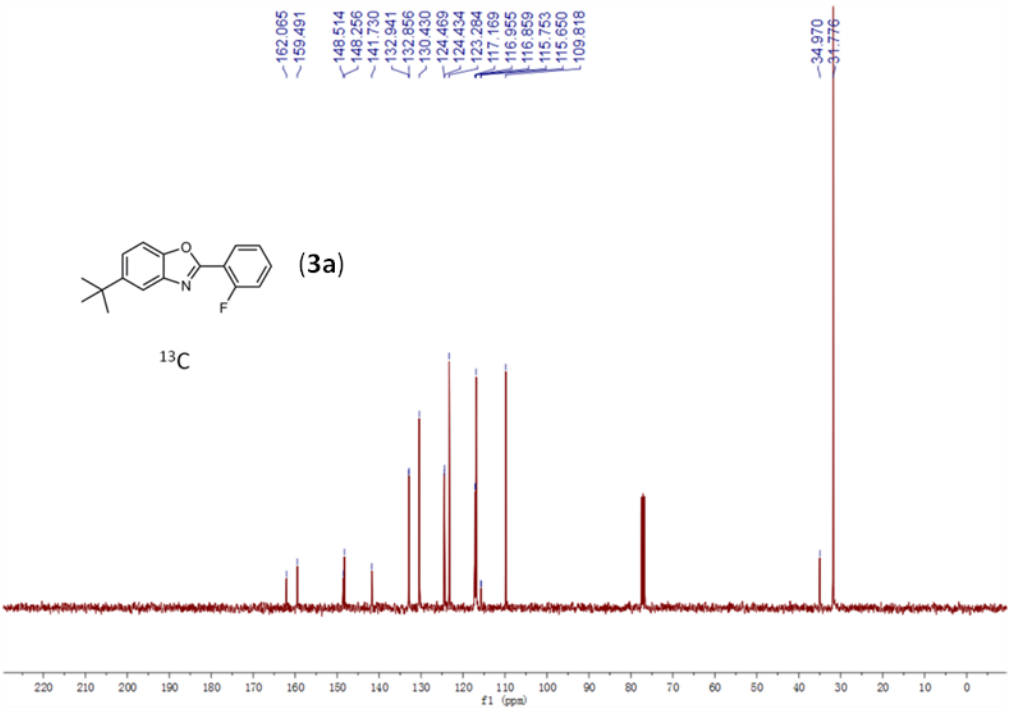

148.415
147.701
141.672
139.063
137.624
137.519
134.551
134.169
133.965
130.468
130.046
128.593
128.435
128.360
122.748
116.860
109.503
34.850
31.731
(1a)
Ph2P
13C
f1 (ppm)

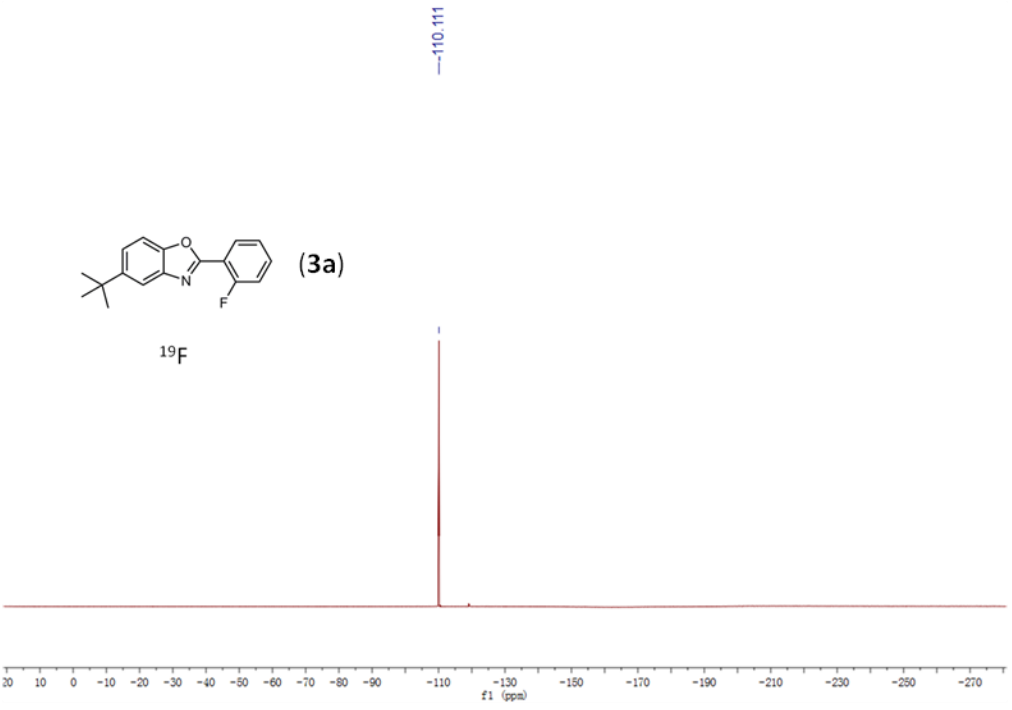

-6.138
(1a)
Ph2P
31P
f1 (ppm)

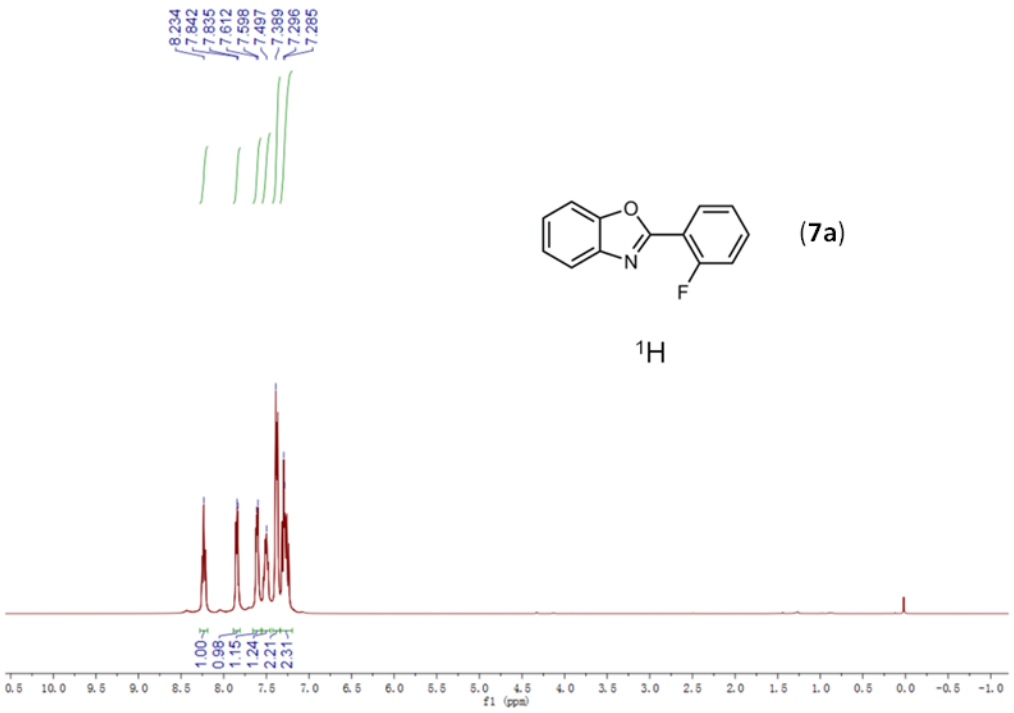

-11.561
8.031
8.027
8.011
8.008
7.759
7.755
7.524
7.502
7.458
7.454
7.437
7.432
7.422
7.418
7.150
7.129
7.029
7.010
6.991
-1.427
(2a)
HO
1H
0.95
1.03
1.01
1.03
2.10
1.00
1.08
9.78
f1 (ppm)

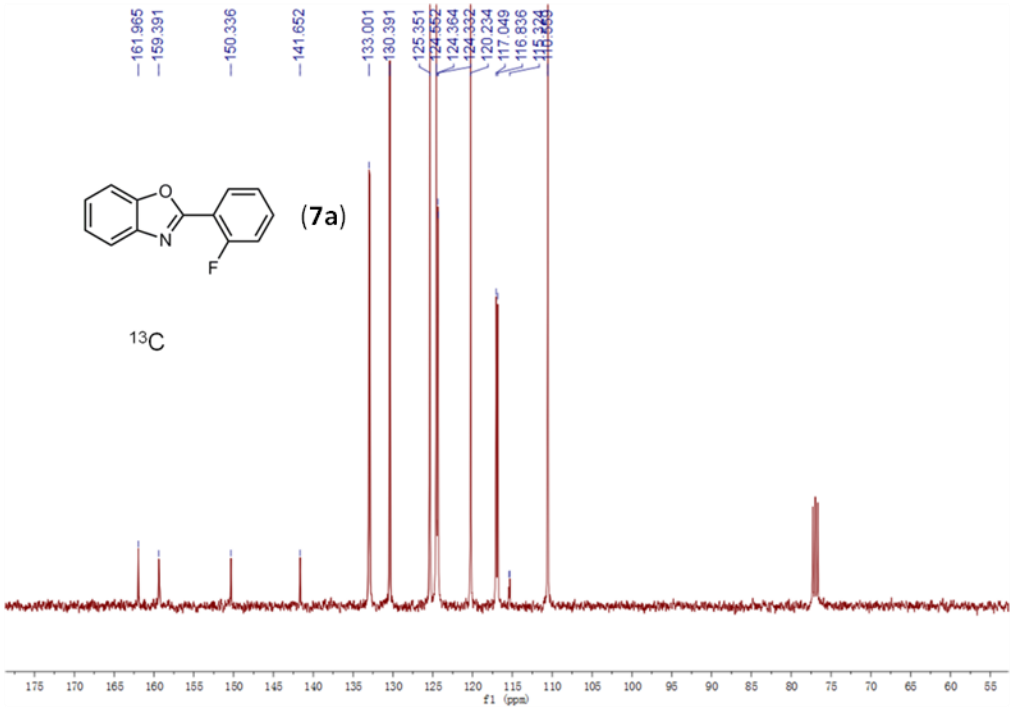

161.817
157.559
147.396
145.958
138.797
132.227
125.900
121.939
118.327
116.228
114.652
109.587
108.636
33.859
30.672
(2a)
HO
13C
f1 (ppm)

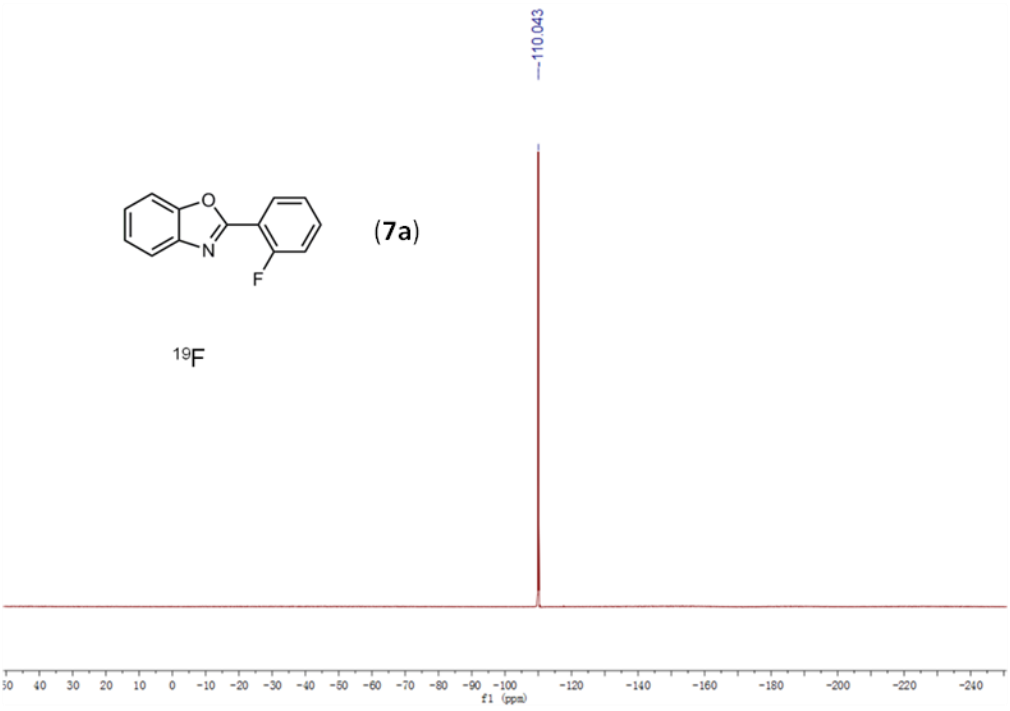

8.250
8.231
8.213
7.889
7.543
7.521
7.511
7.494
7.467
7.446
7.317
7.298
7.285
7.259
7.237
1.410
(3a)
F
1H
1.02
1.00
3.16
2.17
9.49
f1 (ppm)

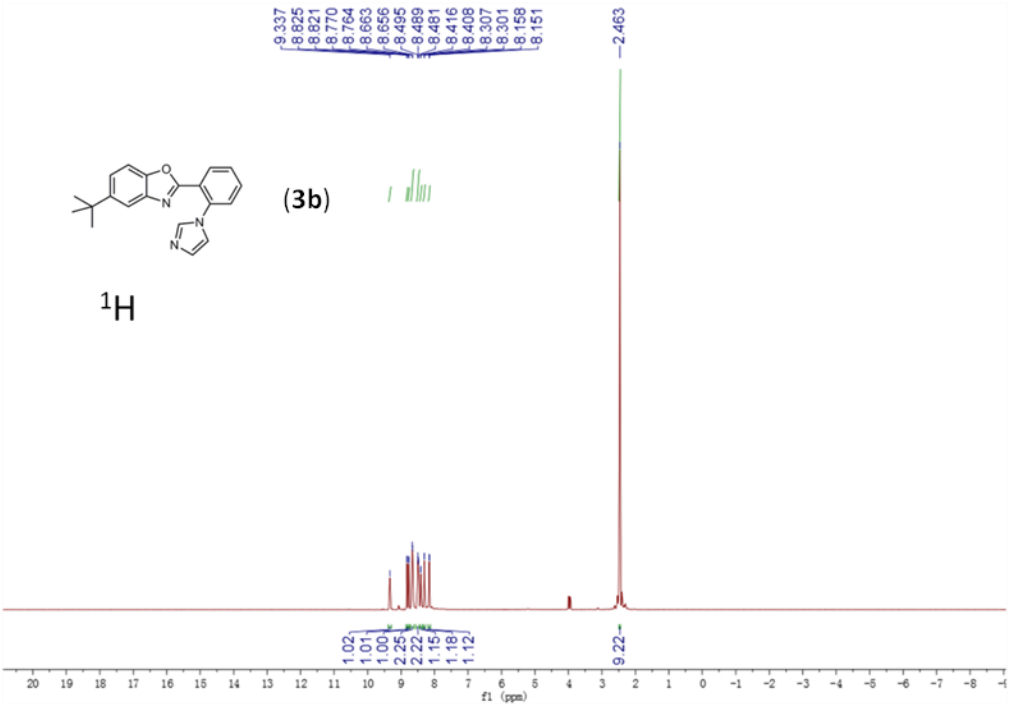

162.065
159.491
148.514
148.256
141.730
132.941
132.856
130.430
124.469
124.434
123.284
117.169
116.955
116.859
115.753
115.650
109.818
34.970
31.776
(3a)
13C
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

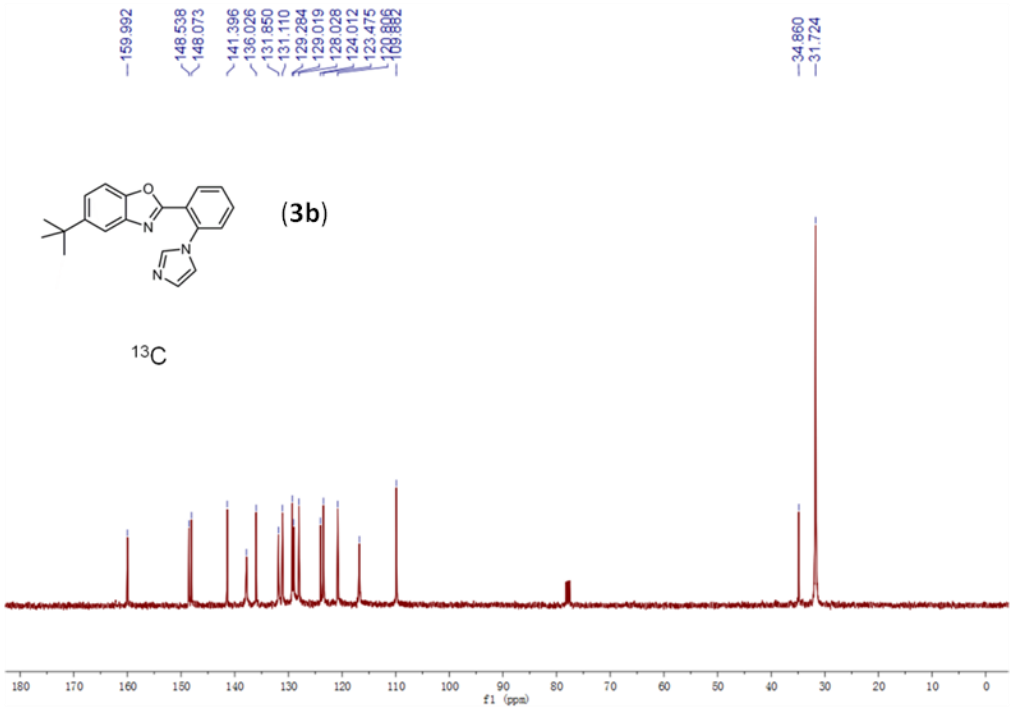

110.111
(3a)
19F
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270
f1 (ppm)

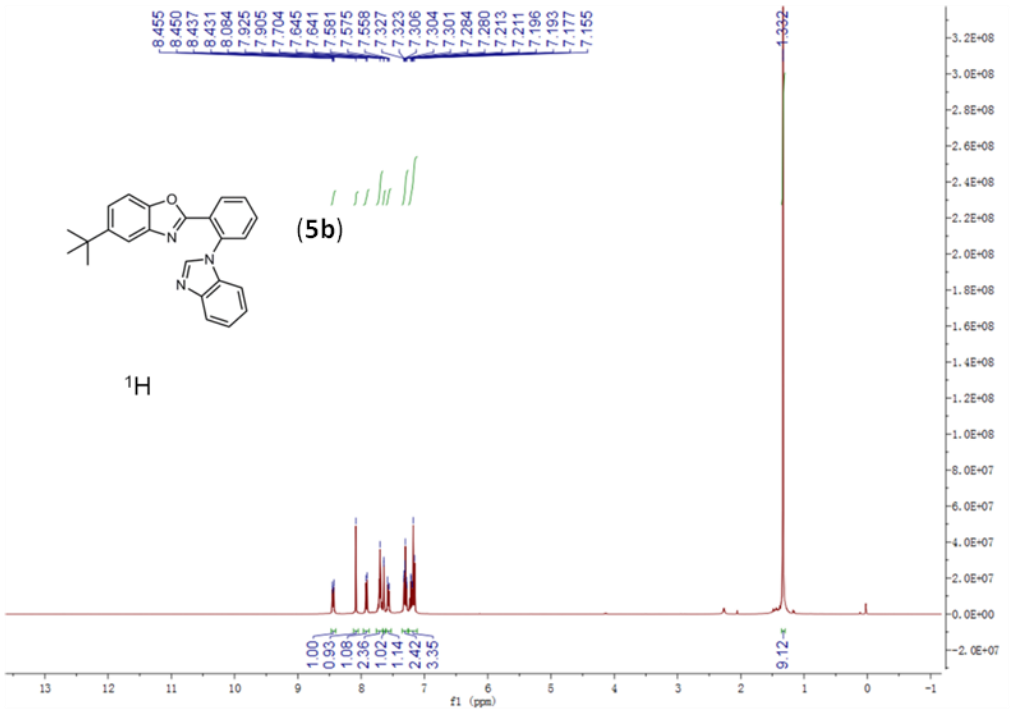

8.234
7.842
7.835
7.612
7.598
7.497
7.389
7.296
7.285
(7a)
^{1}H
1.00
0.98
1.15
1.24
2.21
2.31
f1 (ppm)


161.965
159.391
150.336
141.652
133.001
130.391
125.351
124.552
124.364
124.332
120.234
117.049
116.836
115.324
(7a)
^{13}C
f1 (ppm)


110.043
(7a)
19F
f1 (ppm)


9.337
8.825
8.821
8.770
8.764
8.663
8.656
8.495
8.489
8.481
8.416
8.408
8.307
8.301
8.158
8.151
2.463
(3b)
1H
1.02
1.01
1.00
2.25
2.22
1.15
1.18
1.12
9.22
f1 (ppm)


159.992
148.538
148.073
141.396
136.026
131.850
131.110
129.284
129.019
128.028
124.012
123.475
120.806
109.882
34.860
31.724
(3b)
13C
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.455
8.450
8.437
8.431
8.084
7.925
7.905
7.704
7.645
7.641
7.581
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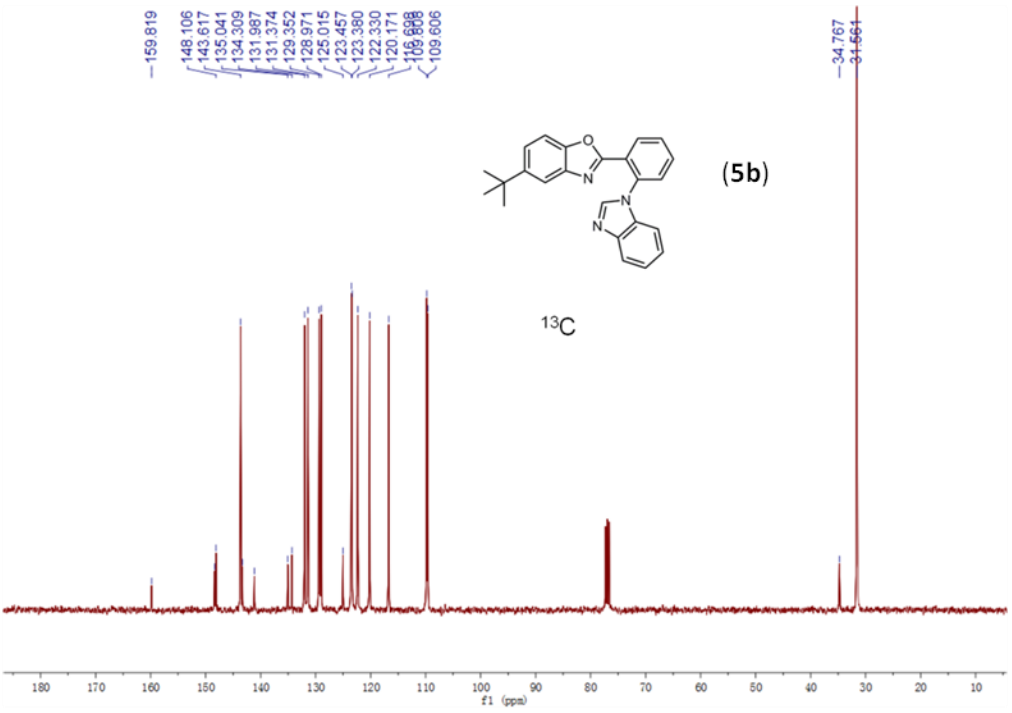
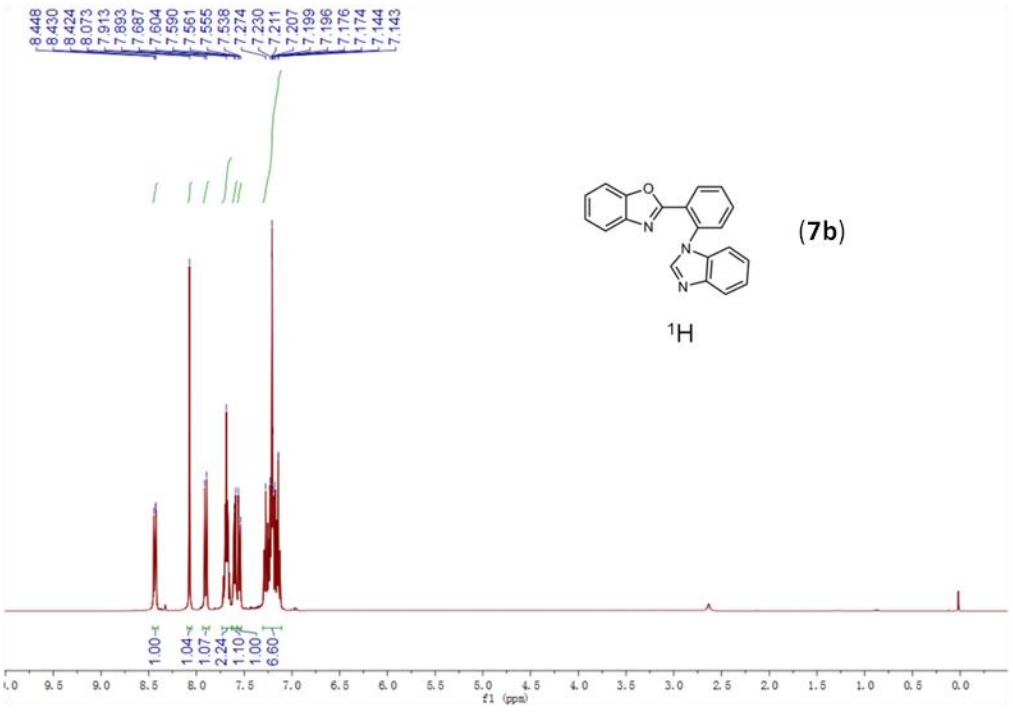
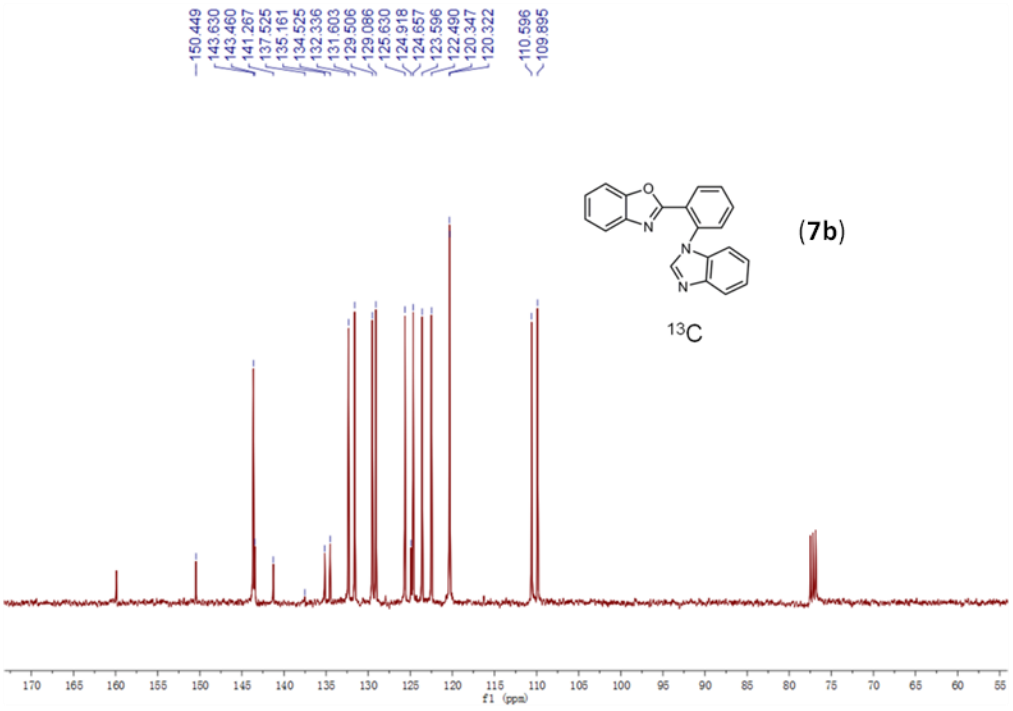
7.558
7.327
7.323
7.306
7.304
7.301
7.284
7.280
7.213
7.211
7.196
7.193
7.177
7.155
1.332
(5b)
1H
1.00
0.93
1.08
2.36
1.02
1.14
2.42
3.35
9.12
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)
3.2E+08
3.0E+08
2.8E+08
2.6E+08
2.4E+08
2.2E+08
2.0E+08
1.8E+08
1.6E+08
1.4E+08
1.2E+08
1.0E+08
8.0E+07
6.0E+07
4.0E+07
2.0E+07
0.0E+00
-2.0E+07


159.819
148.106
143.617
135.041
134.309
131.987
131.374
129.352
128.971
125.015
123.457
123.380
122.330
120.171
116.698
109.808
109.606
34.767
31.561
(5b)
13C
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


8.448
8.430
8.424
8.073
7.913
7.893
7.687
7.604
7.590
7.561
7.555
7.538
7.274
7.230
7.211
7.207
7.199
7.196
7.176
7.174
7.144
7.143
(7b)
1H
1.00
1.04
1.07
2.24
1.10
1.00
6.60
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


150.449
143.630
143.460
141.267
137.525
135.161
134.525
132.336
131.603
129.506
129.086
125.630
124.918
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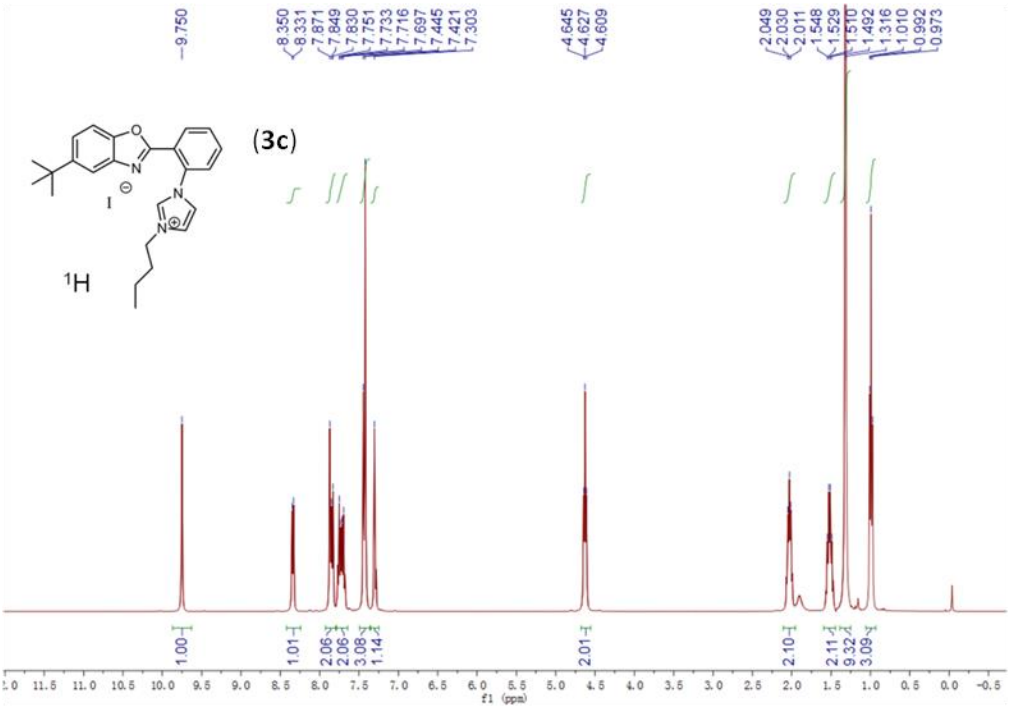
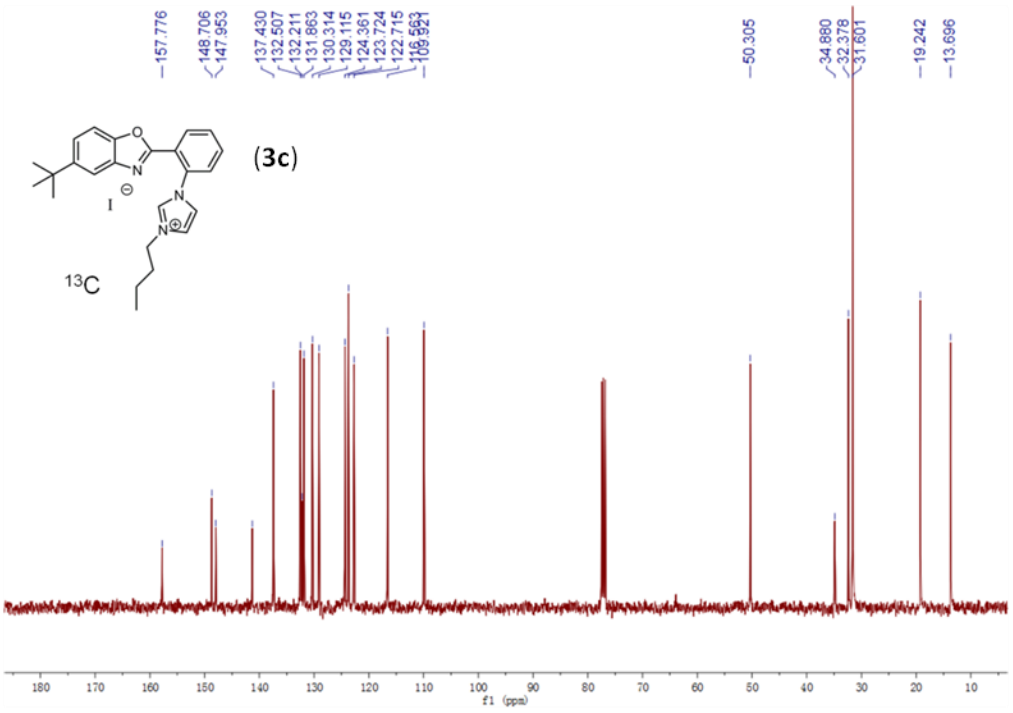
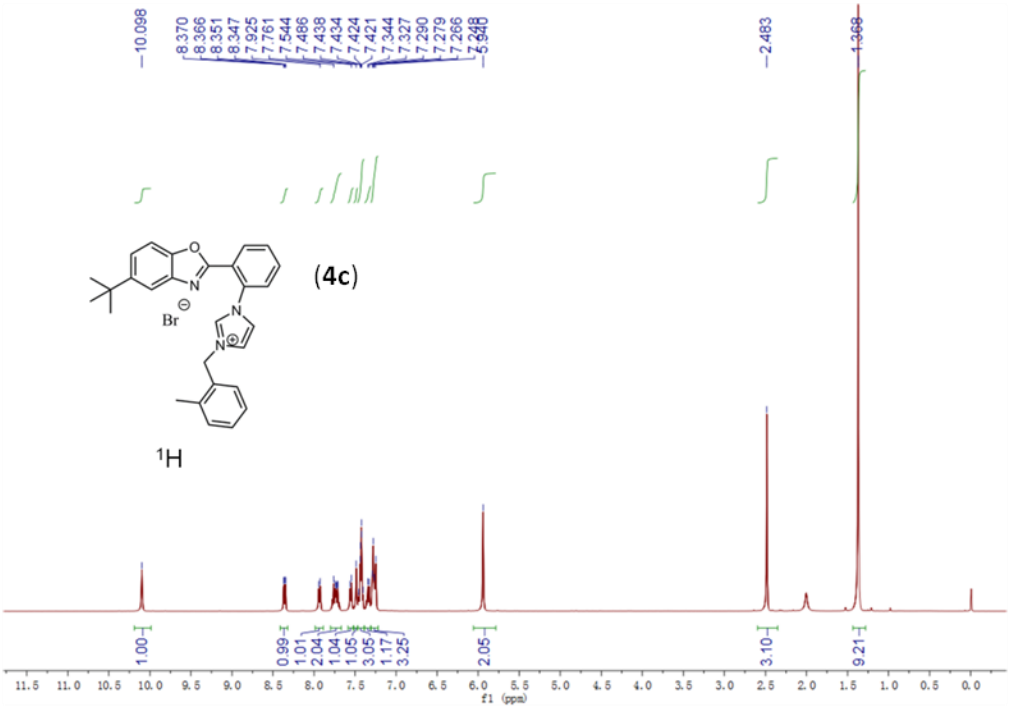
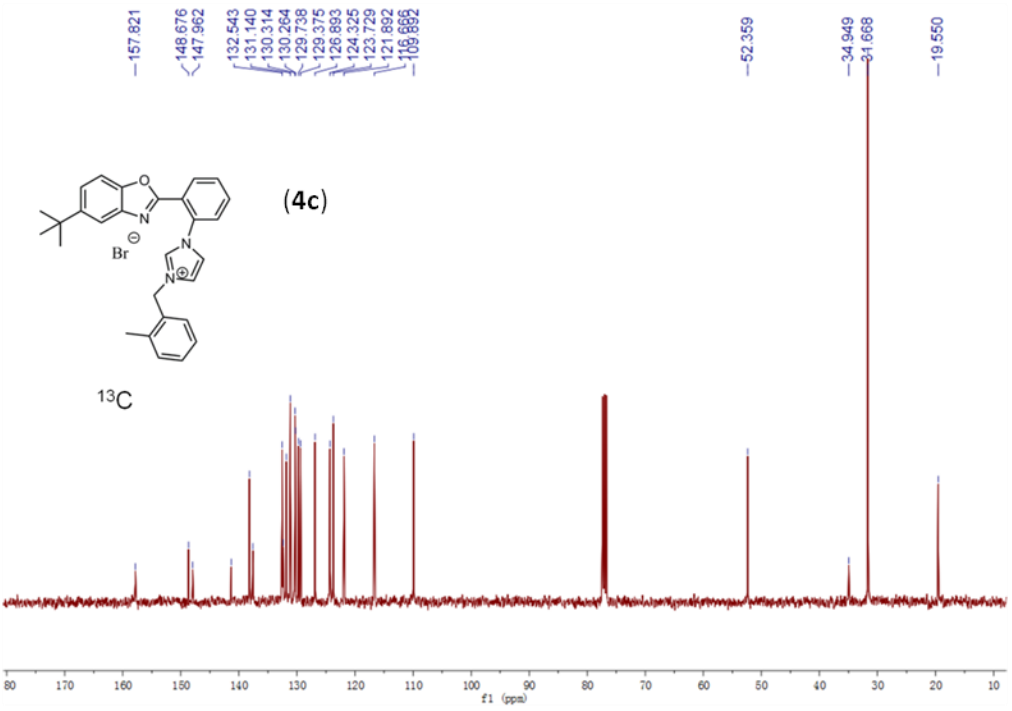
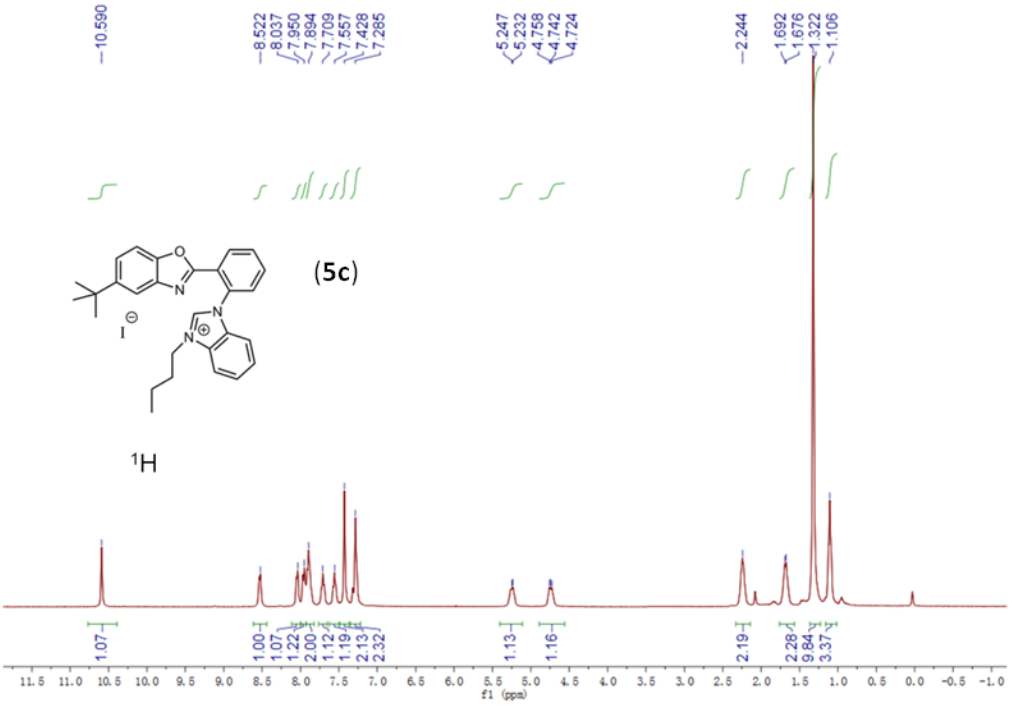
123.596
122.490
120.347
120.322
110.596
109.895
(7b)
13C
f1 (ppm)

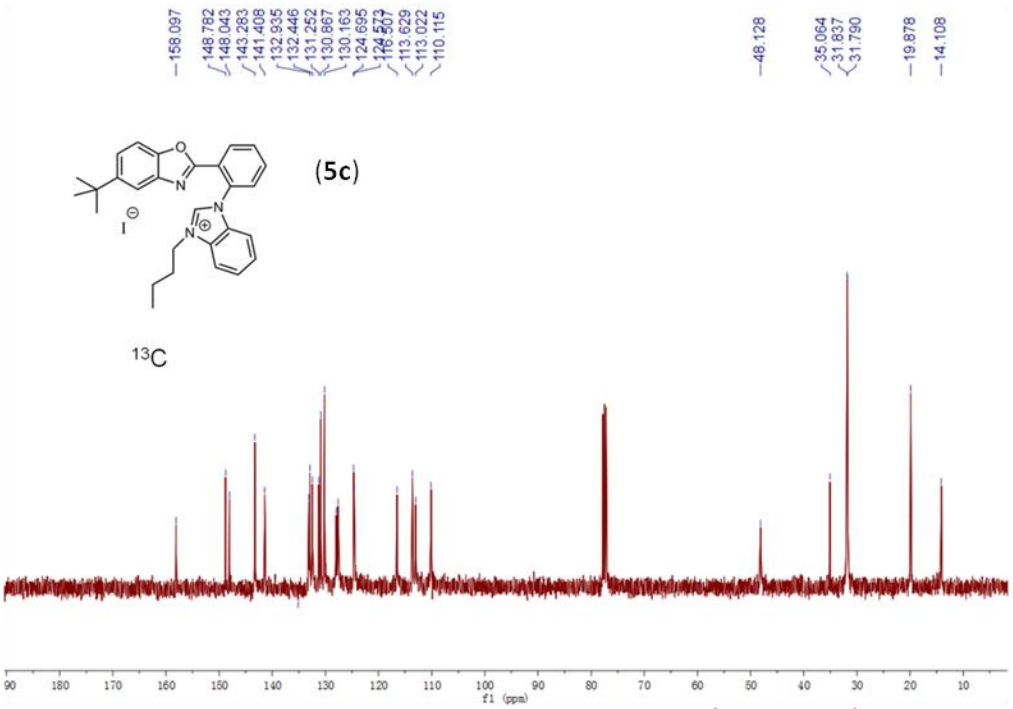

9.750
8.350
8.331
7.871
7.849
7.830
7.751
7.733
7.716
7.697
7.445
7.421
7.303
4.645
4.627
4.609
2.049
2.030
2.011
1.548
1.529
1.510
1.492
1.316
1.010
0.992
0.973
(3c)
I
1H
1.00
1.01
2.06
2.06
3.08
1.14
2.01
2.10
2.11
9.32
3.09
f1 (ppm)

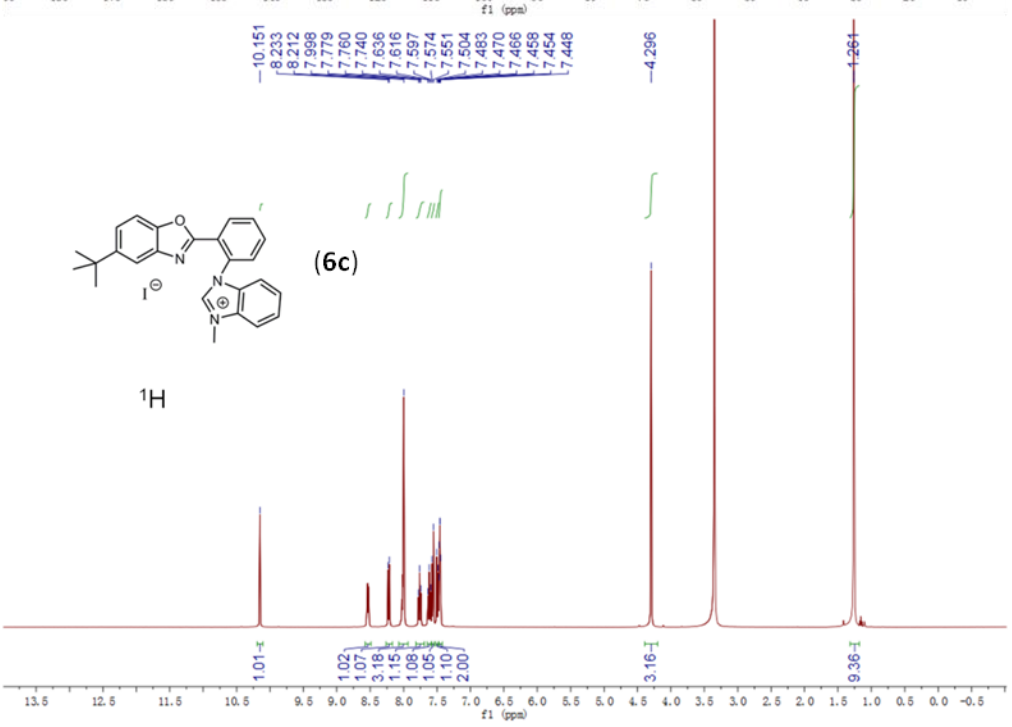

157.776
148.706
147.953
137.430
132.507
132.211
131.863
130.314
129.115
124.361
123.724
122.715
116.563
109.921
50.305
34.880
32.378
31.601
19.242
13.696
(3c)
I
13C
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

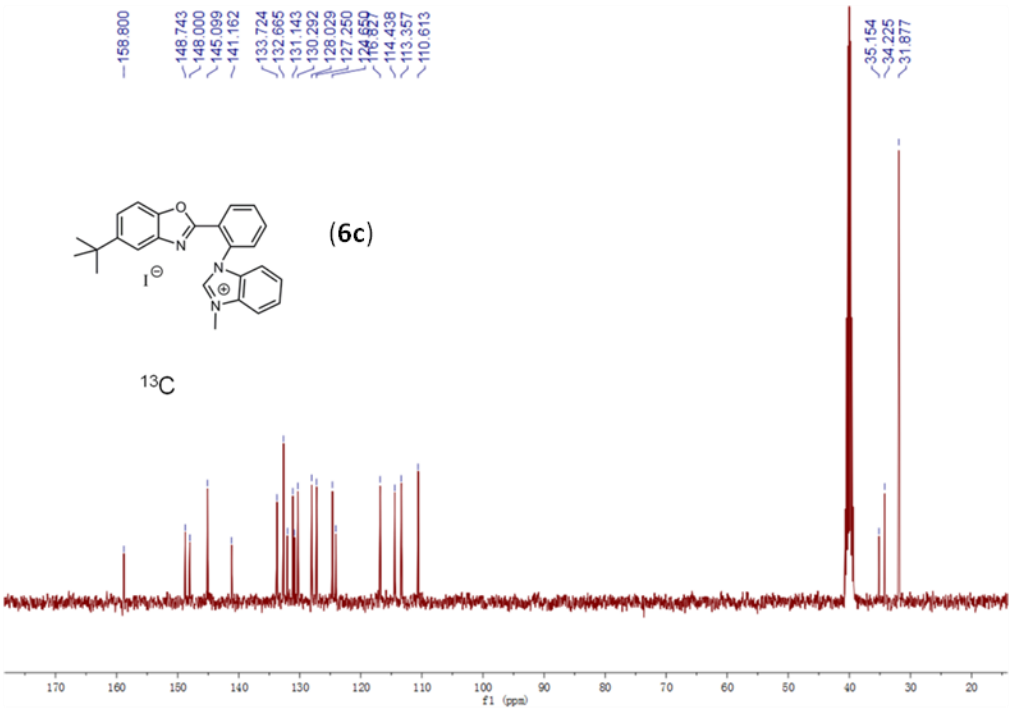

10.098
8.370
8.366
8.351
8.347
7.925
7.761
7.544
7.486
7.438
7.434
7.424
7.421
7.344
7.327
7.290
7.279
7.266
5.940
2.483
1.368
(4c)
Br
1H
1.00
0.99
1.01
2.04
1.04
1.05
3.05
1.17
3.25
2.05
3.10
9.21
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

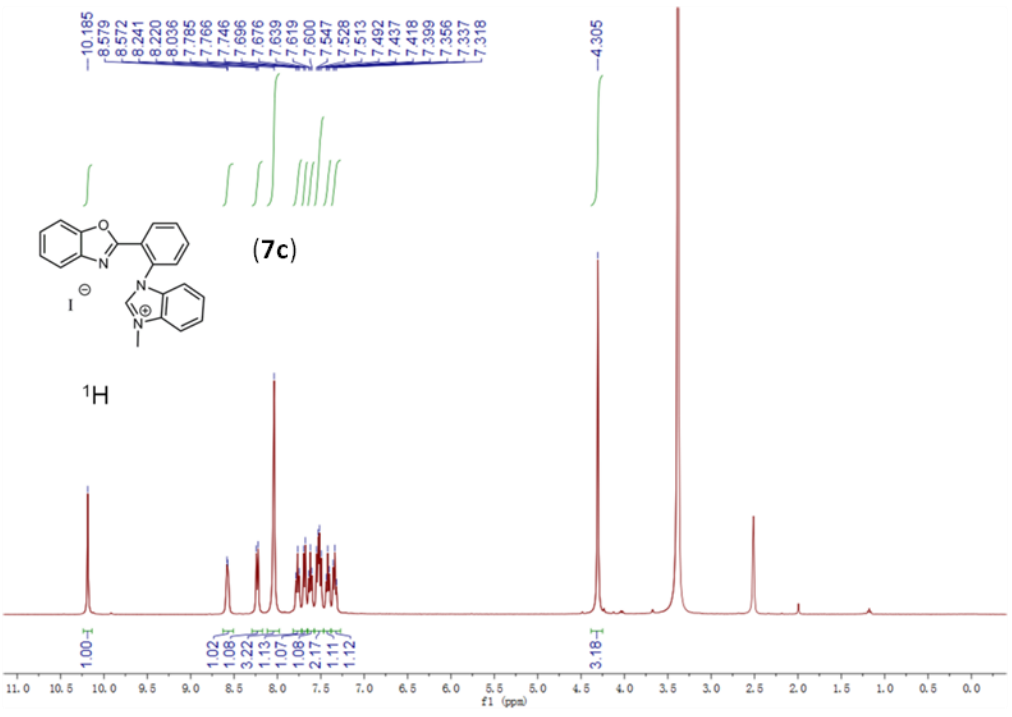

157.821
148.676
147.962
132.543
131.140
130.314
130.264
129.738
129.375
126.893
124.325
123.729
121.892
52.359
34.949
31.668
19.550
(4c)
Br
13C
f1 (ppm)

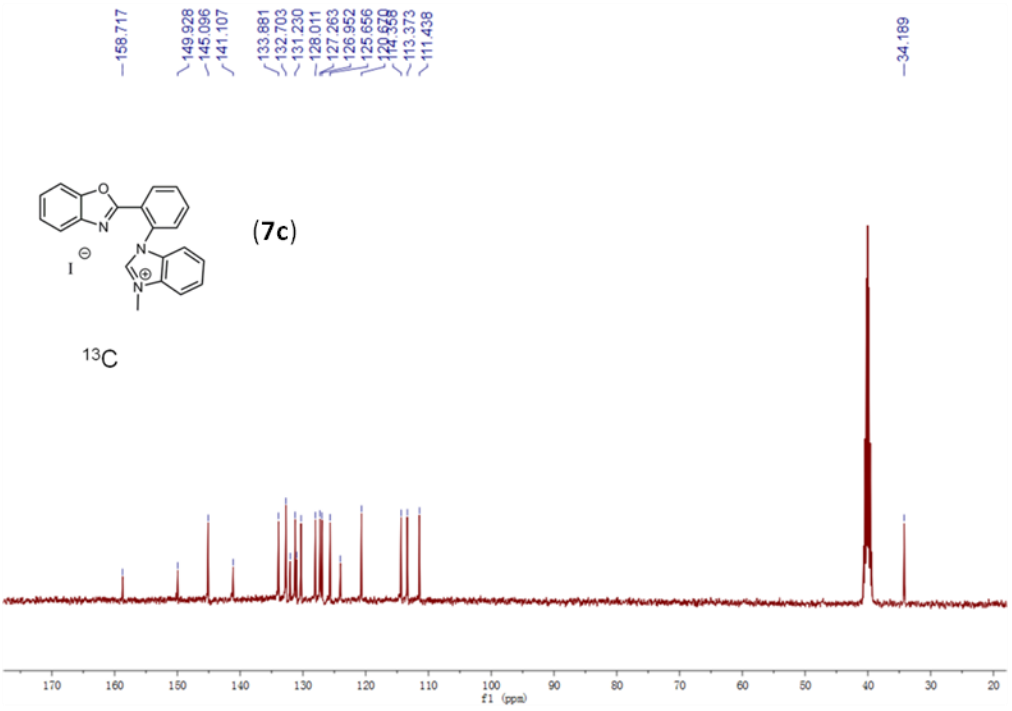

10.590
8.522
8.037
7.950
7.894
7.709
7.557
7.428
7.285
5.247
5.232
4.758
4.742
4.724
2.244
1.692
1.676
1.322
1.106
(5c)
I
1H
1.07
1.00
1.07
1.22
2.00
1.12
1.19
2.13
2.32
1.13
1.16
2.19
2.28
9.84
3.37
f1 (ppm)

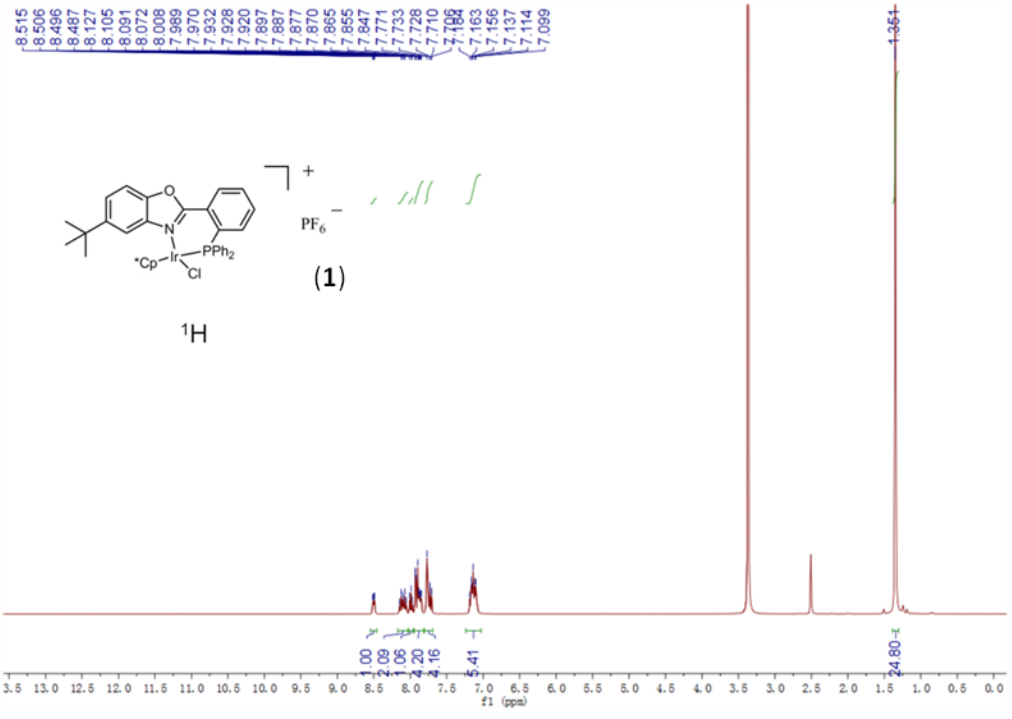

158.097
148.782
148.043
143.283
141.408
132.935
132.446
131.252
130.867
130.163
124.695
124.573
116.507
113.629
113.022
110.115
48.128
35.064
31.837
31.790
19.878
14.108
(5c)
13C
f1 (ppm)

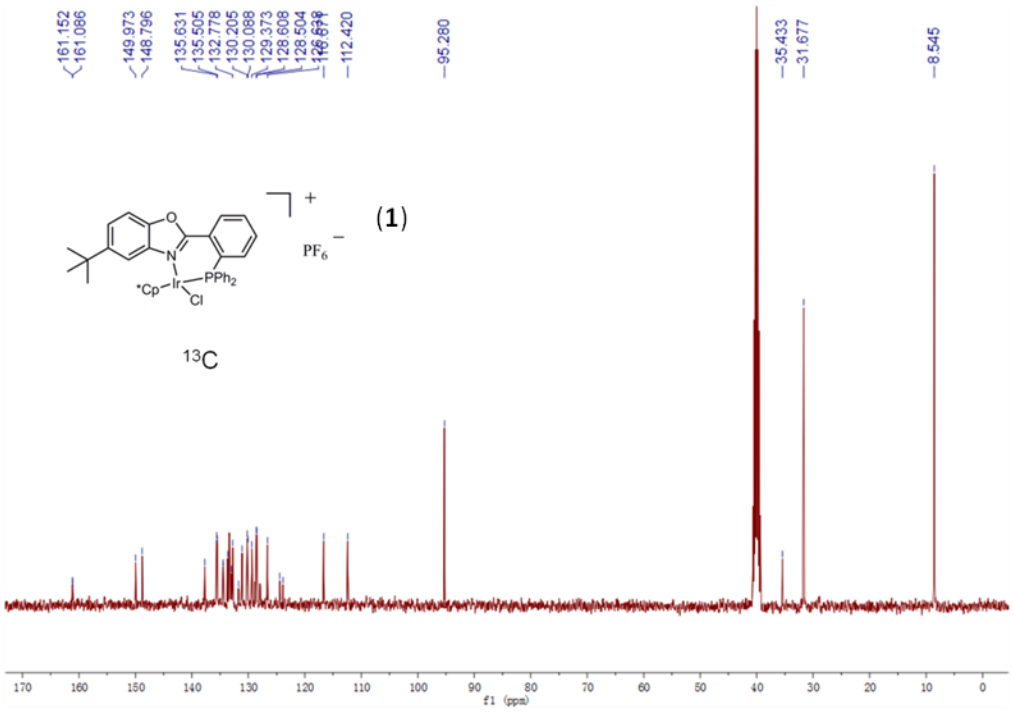

10.151
8.233
8.212
7.998
7.779
7.760
7.740
7.636
7.616
7.597
7.574
7.551
7.504
7.483
7.470
7.466
7.458
7.454
7.448
4.296
1.261
(6c)
1H
1.01
1.02
1.07
3.18
1.15
1.08
1.05
1.10
2.00
3.16
9.36
f1 (ppm)

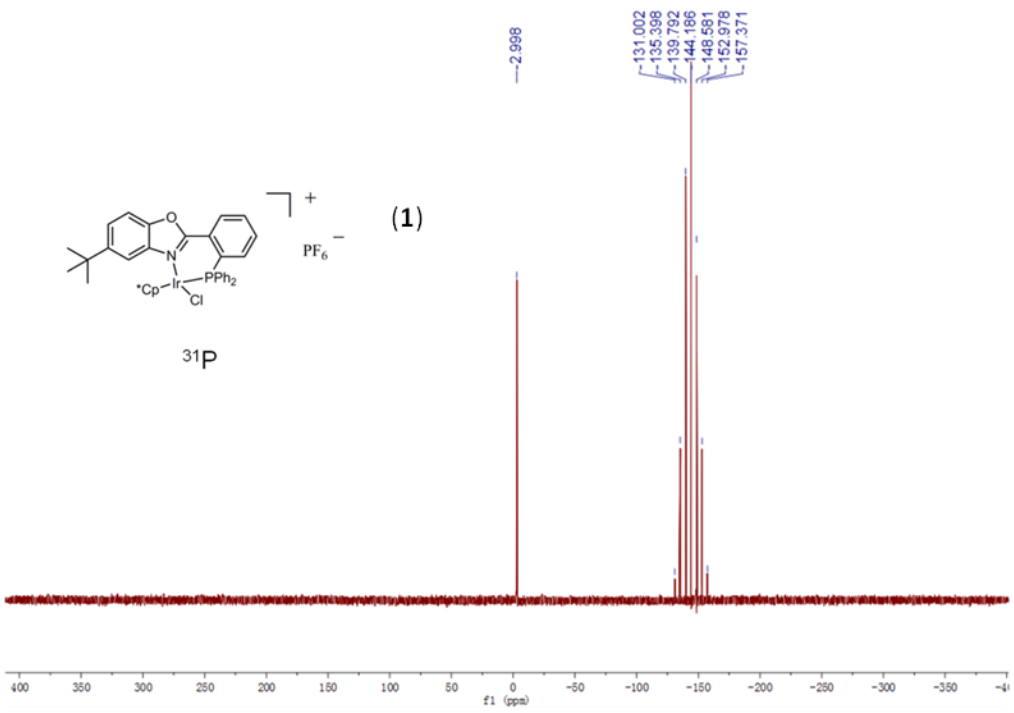

158.800
148.743
148.000
145.099
141.162
133.724
132.665
131.143
130.292
128.029
127.250
124.650
116.527
114.438
113.357
110.613
35.154
34.225
31.877
(6c)
13C
f1 (ppm)

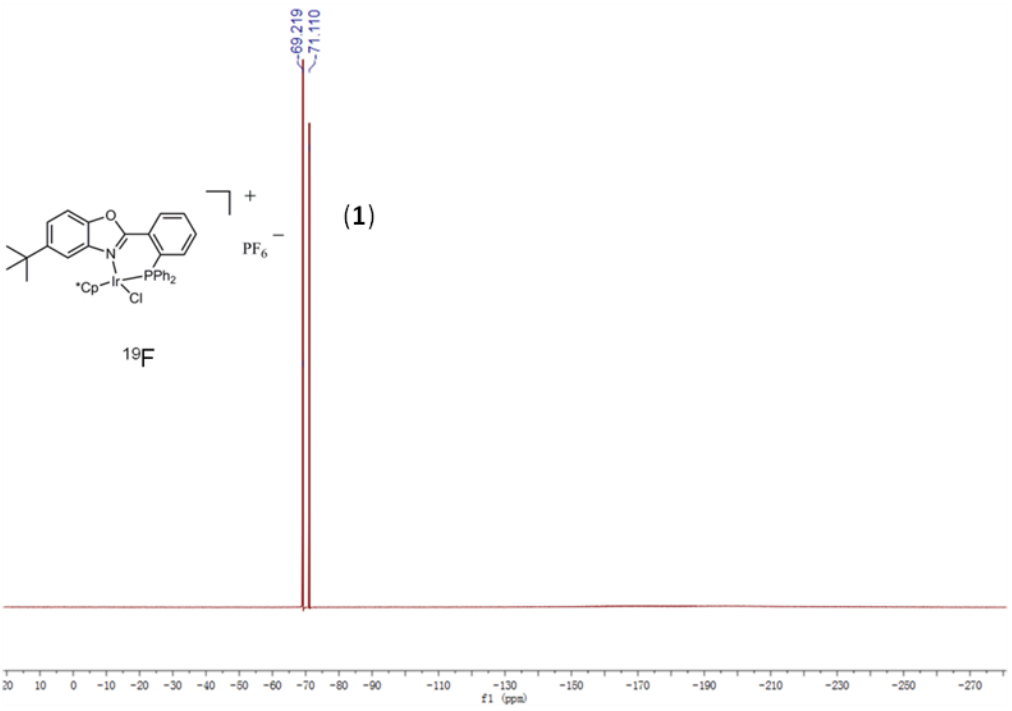

10.185
8.579
8.572
8.241
8.220
8.036
7.785
7.766
7.746
7.696
7.676
7.639
7.619
7.600
7.547
7.528
7.513
7.492
7.437
7.418
7.399
7.356
7.337
7.318
4.305
(7c)
1H
1.00
1.02
1.08
3.22
1.13
1.07
1.08
2.17
1.11
1.12
3.18
f1 (ppm)

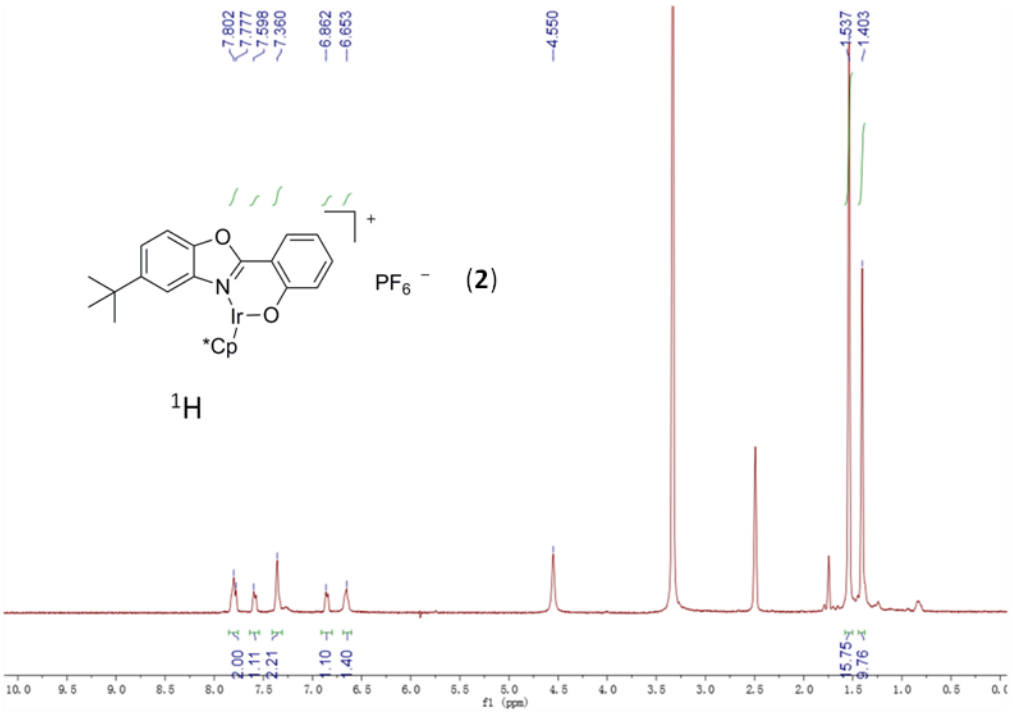

158.717
149.928
145.096
141.107
133.881
132.703
131.230
128.011
127.263
126.952
125.656
120.670
114.358
113.373
111.438
34.189
(7c)
^{13}C
f1 (ppm)

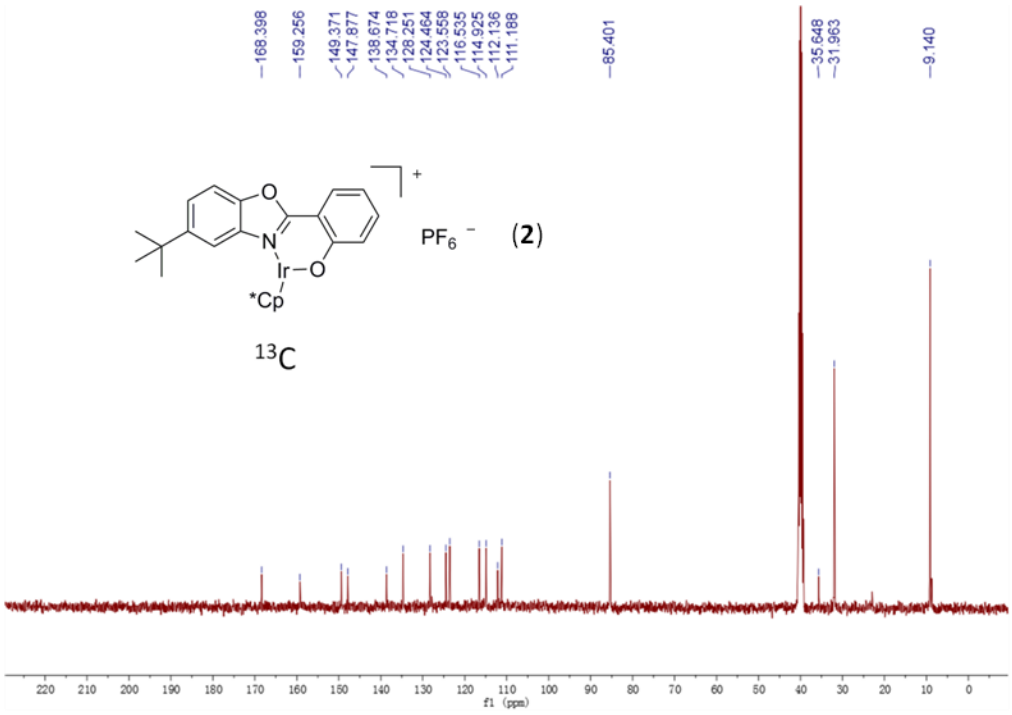

8.515
8.506
8.496
8.487
8.127
8.105
8.091
8.072
8.008
7.989
7.970
7.932
7.928
7.920
7.897
7.887
7.877
7.870
7.865
7.855
7.847
7.771
7.733
7.728
7.710
7.163
7.156
7.137
7.114
7.099
1.351
PF6
(1)
^{1}H
1.00
2.09
1.08
4.20
4.16
5.41
24.80
f1 (ppm)

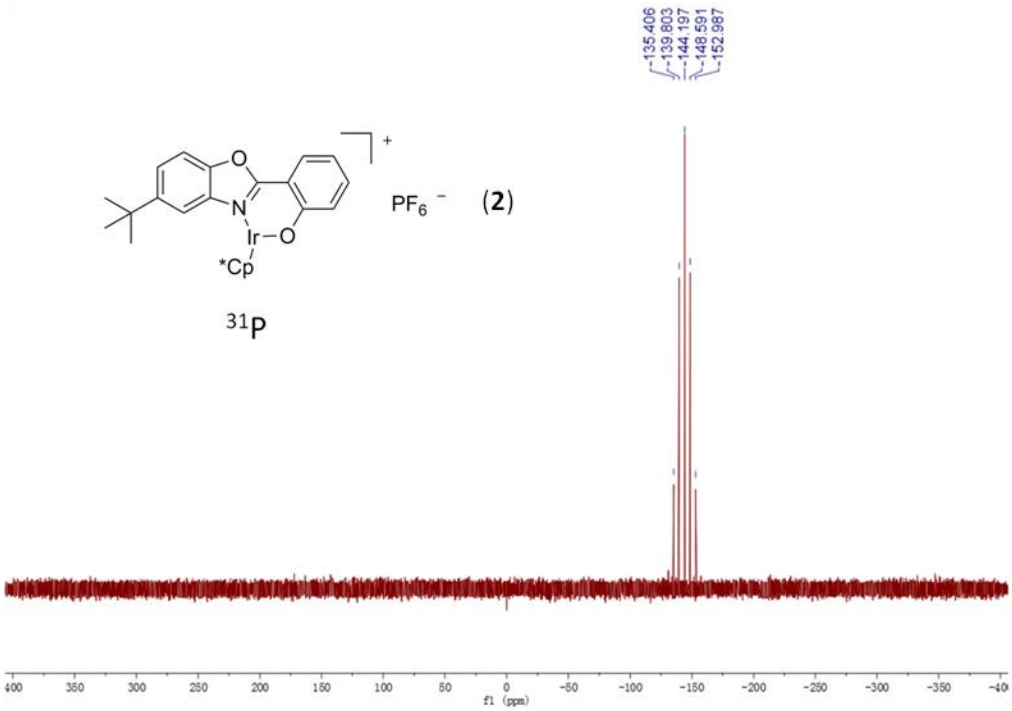

161.152
161.086
149.973
148.796
135.631
135.505
132.778
130.205
130.088
129.373
128.608
128.504
112.420
95.280
35.433
31.677
8.545
(1)
PF6
*Cp
Ir
PPh2
Cl
13C
f1 (ppm)

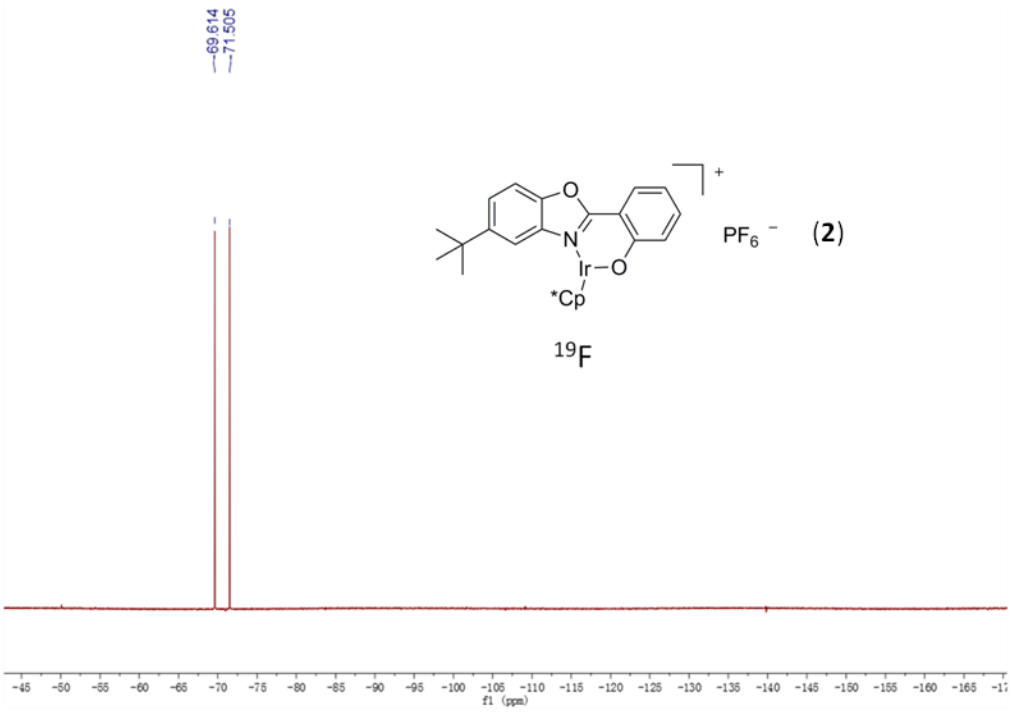

2.998
131.002
135.398
139.792
144.186
148.581
152.978
157.371
(1)
PF6
*Cp
Ir
PPh2
Cl
31P
f1 (ppm)

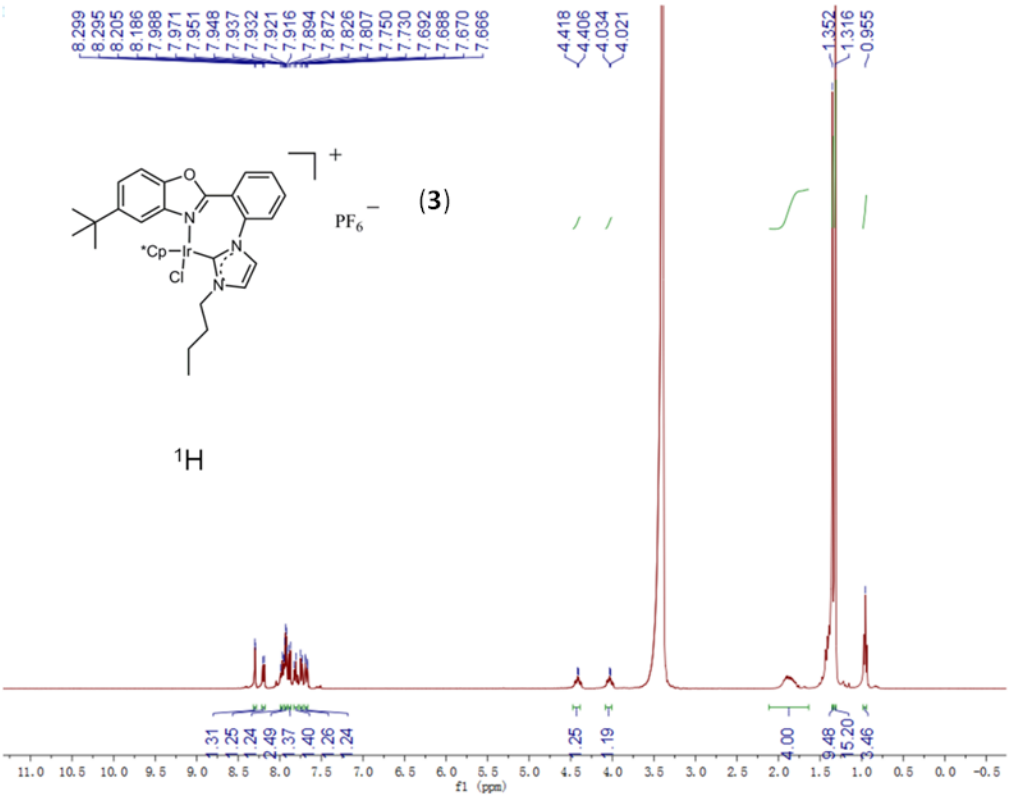

-69.219
-71.110
PF6 −
(1)
19F
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270
f1 (ppm)

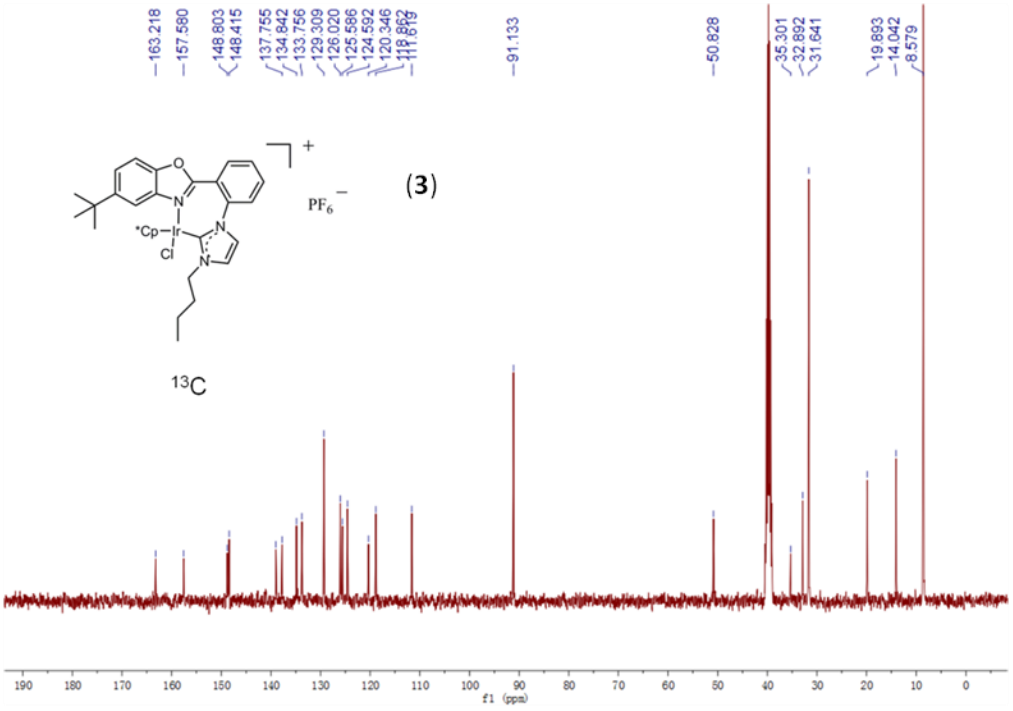

7.802
7.777
7.598
7.360
6.862
6.653
4.550
1.537
1.403
PF6 −
(2)
1H
2.00
1.11
2.21
1.10
1.40
15.75
9.76
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

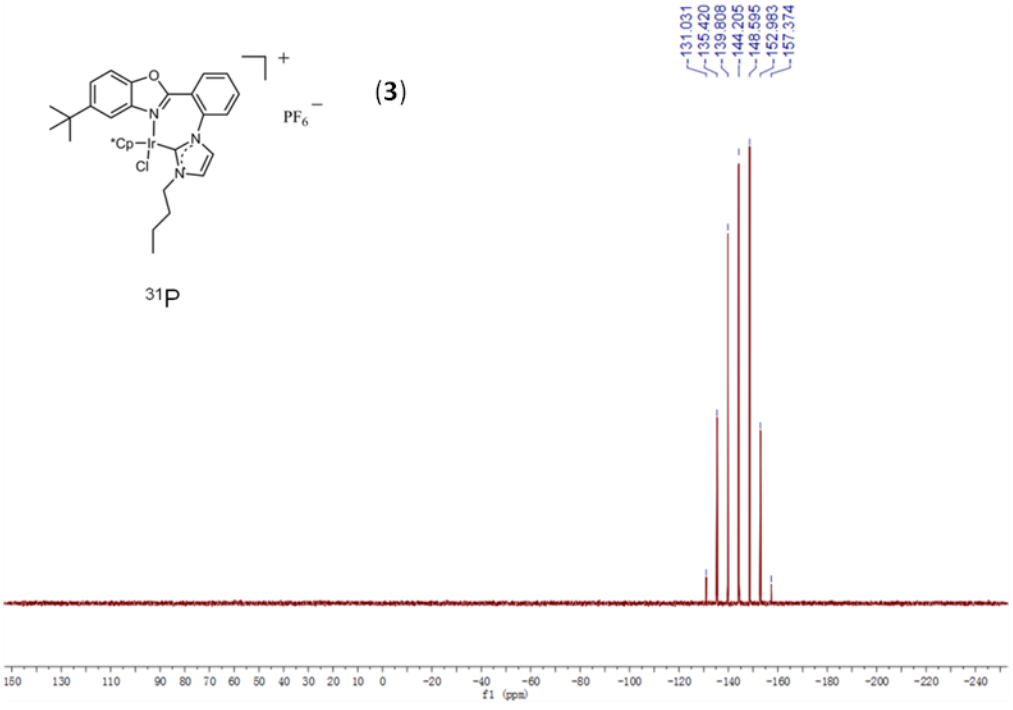

168.398
159.256
149.371
147.877
138.674
134.718
128.251
124.464
123.558
116.535
114.925
112.136
111.188
85.401
35.648
31.963
9.140
PF6 −
(2)
*Cp
13C
f1 (ppm)

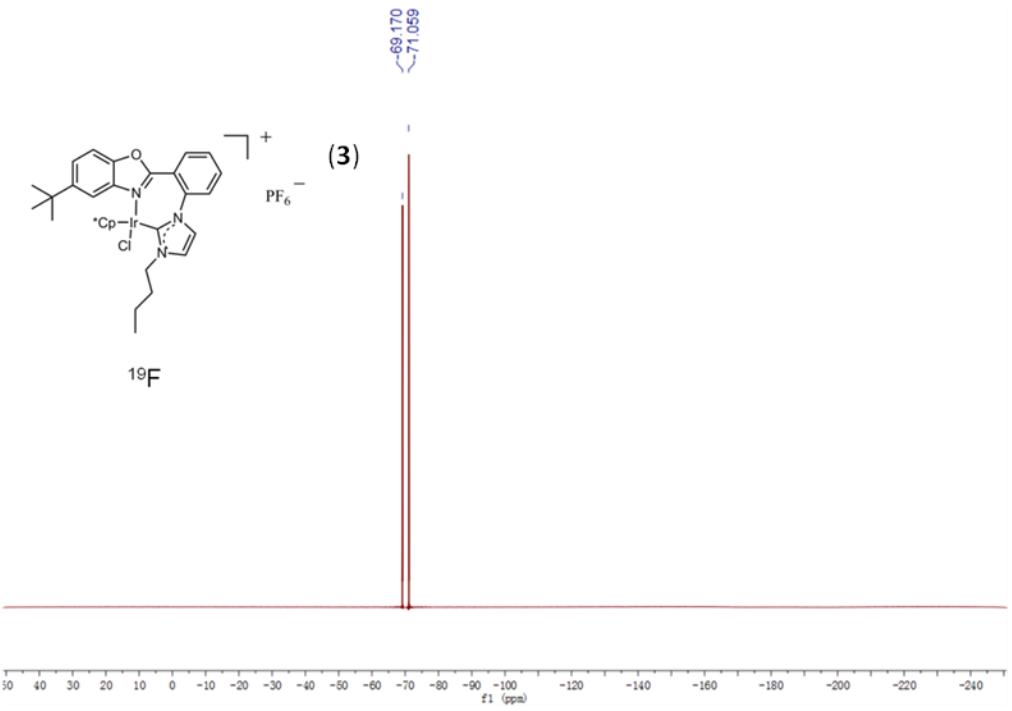

135.406
139.803
144.197
148.591
152.987
PF6 −
(2)
*Cp
31P
f1 (ppm)

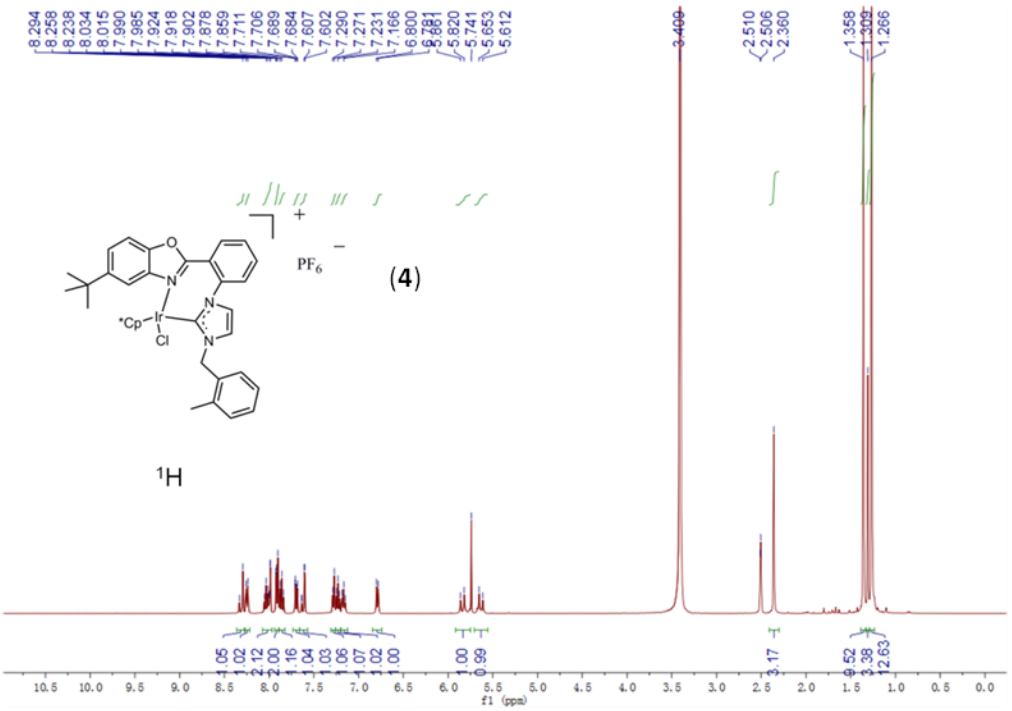

-69.614
-71.505
PF6 −
(2)
*Cp
19F
f1 (ppm)

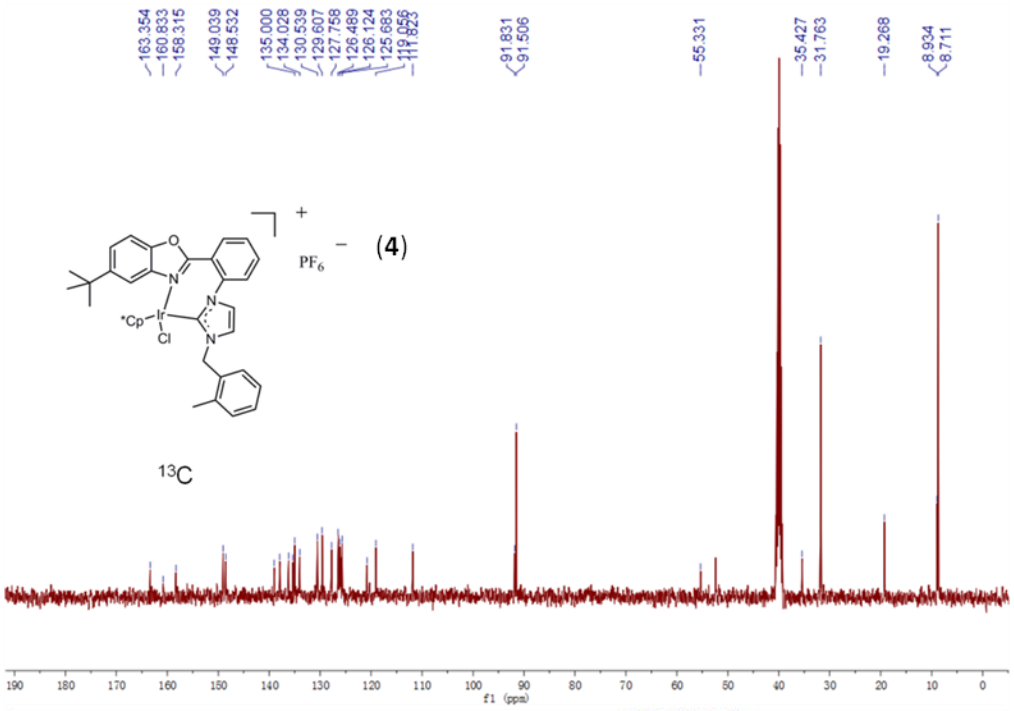

8.299
8.295
8.205
8.186
7.988
7.971
7.951
7.948
7.937
7.932
7.921
7.916
7.894
7.872
7.826
7.807
7.750
7.730
7.692
7.688
7.670
7.666
4.418
4.406
4.034
4.021
1.352
1.316
0.955
PF6 −
(3)
*Cp
Ir
Cl
1H
1.31
1.25
1.24
2.49
1.37
1.40
1.26
1.24
1.25
1.19
4.00
9.48
15.20
3.46
f1 (ppm)

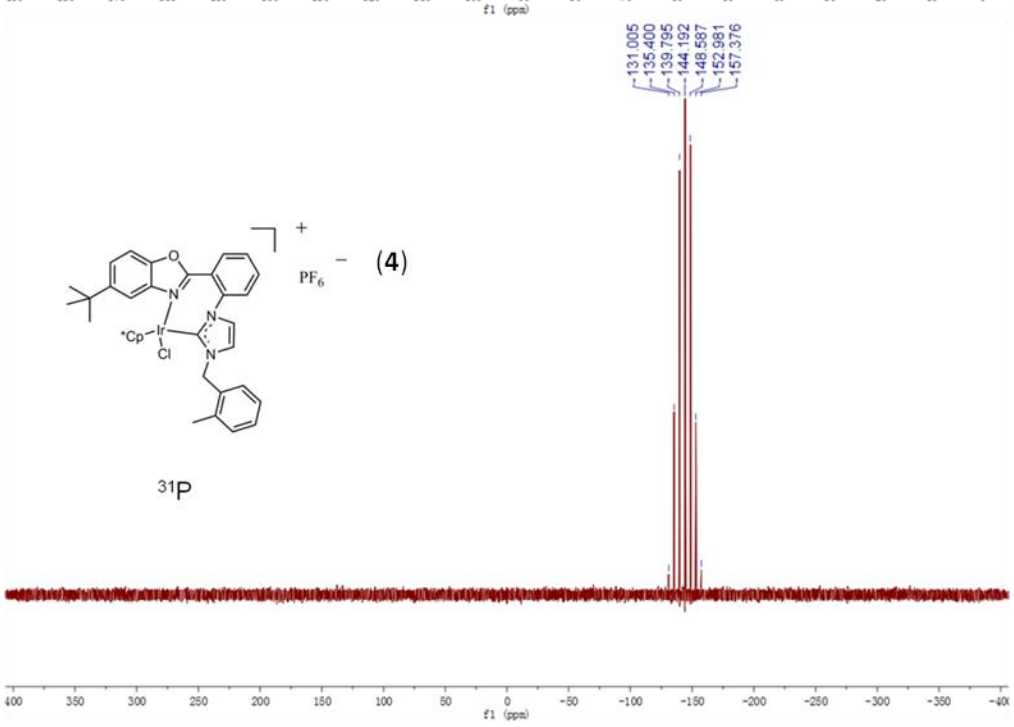

163.218
157.580
148.803
148.415
137.755
134.842
133.756
129.309
126.020
125.586
124.592
120.346
91.133
50.828
35.301
32.892
31.641
19.893
14.042
8.579
(3)
PF6
*Cp
Ir
Cl
13C
f1 (ppm)

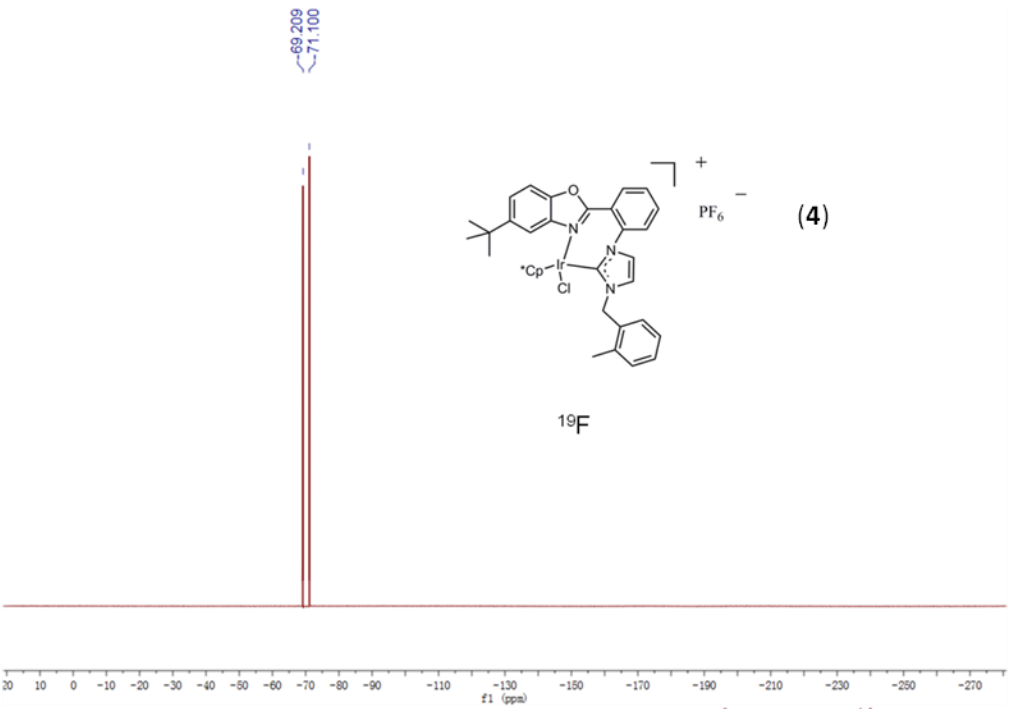

131.031
135.420
139.808
144.205
148.595
152.983
157.374
(3)
PF6
*Cp
Ir
Cl
31P
f1 (ppm)

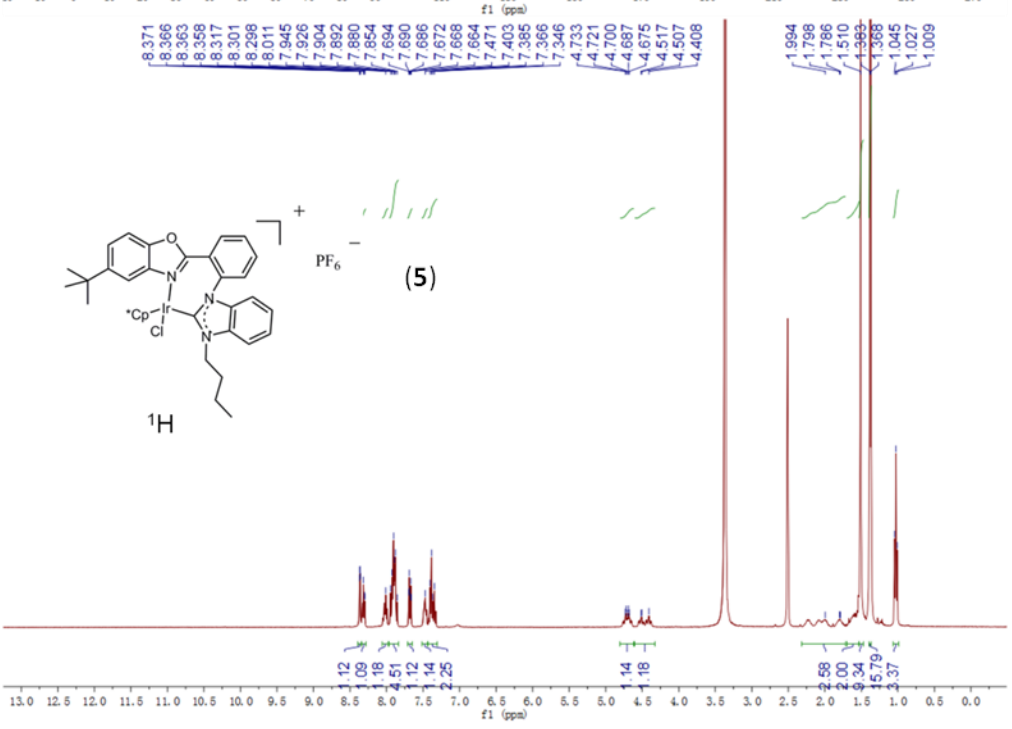

69.170
71.059
(3)
PF6
*Cp
Ir
Cl
19F
f1 (ppm)

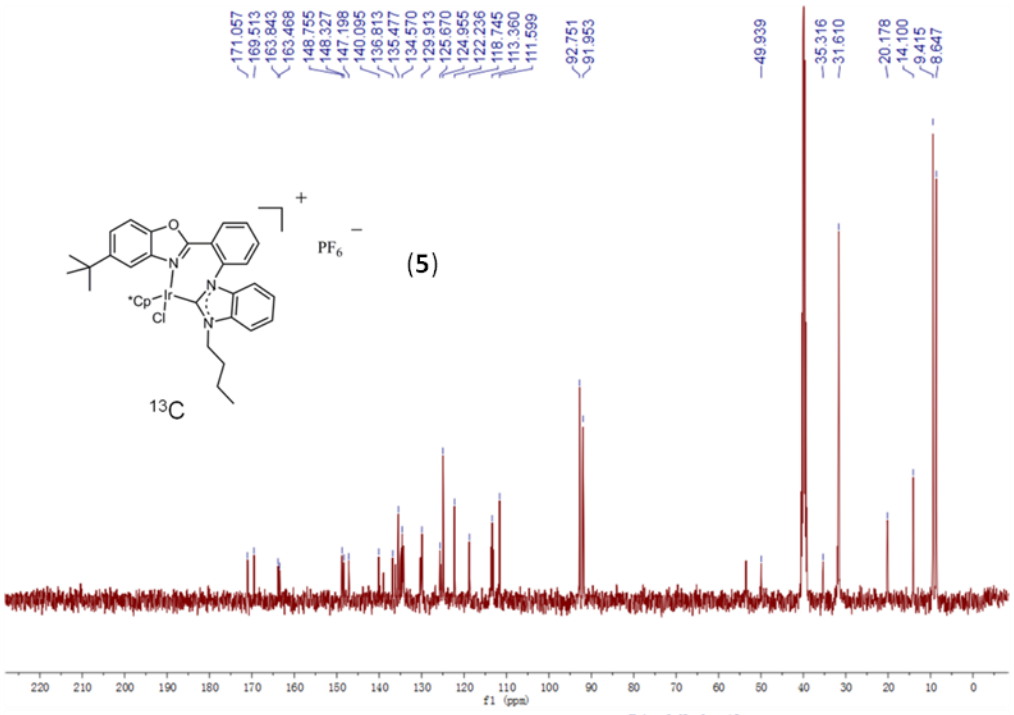

8.294
8.258
8.238
8.034
8.015
7.990
7.985
7.924
7.918
7.902
7.878
7.859
7.711
7.706
7.689
7.684
7.607
7.602
7.290
7.271
7.231
7.166
6.800
6.781
5.820
5.741
5.653
5.612
3.409
2.510
2.506
2.360
1.358
1.309
1.266
(4)
PF6
*Cp
Ir
Cl
1H
1.05
1.02
2.12
2.00
1.16
1.04
1.03
1.06
1.07
1.02
1.00
1.00
0.99
3.17
9.52
3.38
12.63
f1 (ppm)

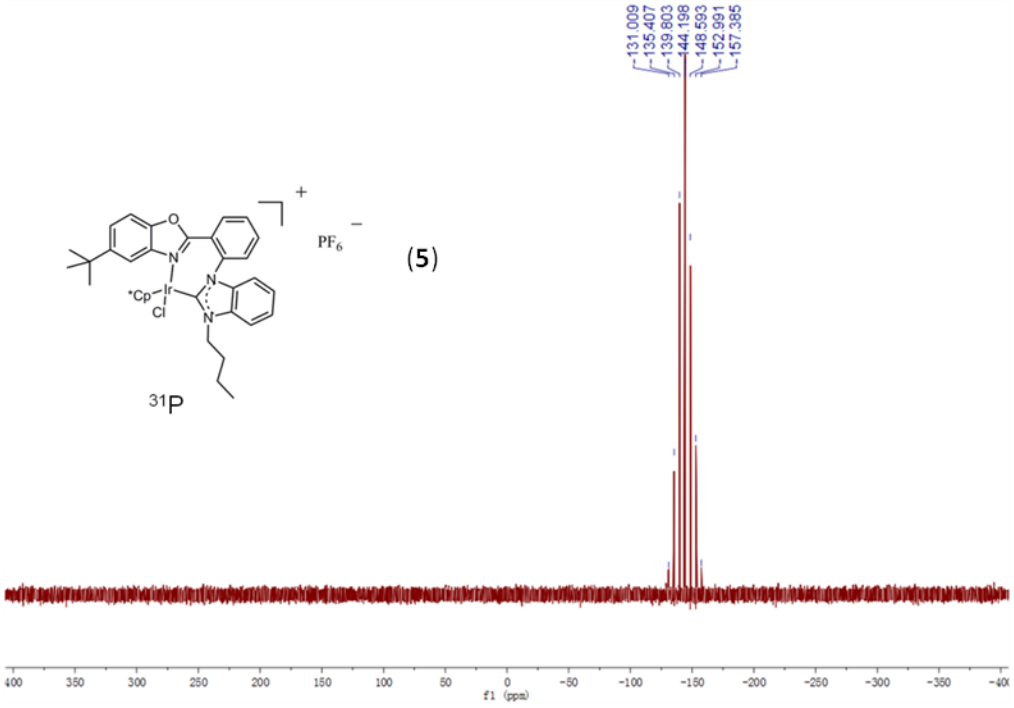

163.354
160.833
158.315
149.039
148.532
135.000
134.028
130.539
129.607
127.758
126.489
126.124
125.683
91.831
91.506
55.331
35.427
31.763
19.268
8.934
8.711
(4)
PF6
*Cp
Ir
Cl
13C
f1 (ppm)

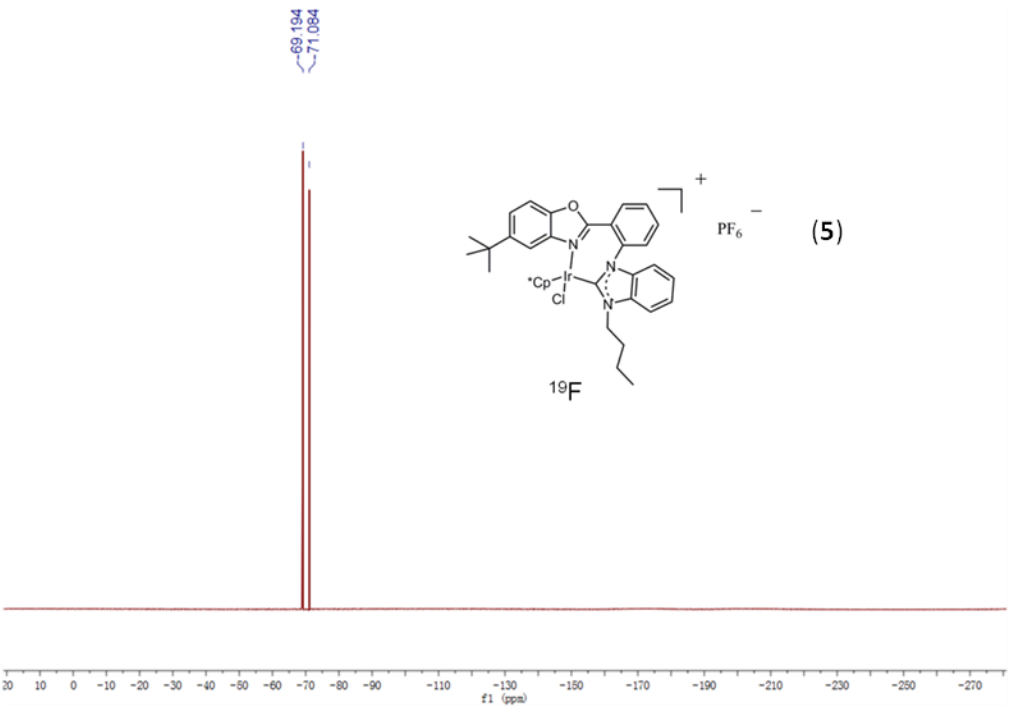

131.005
135.400
139.795
144.192
148.587
152.981
157.376
(4)
PF6
*Cp
Ir
Cl
31P
f1 (ppm)

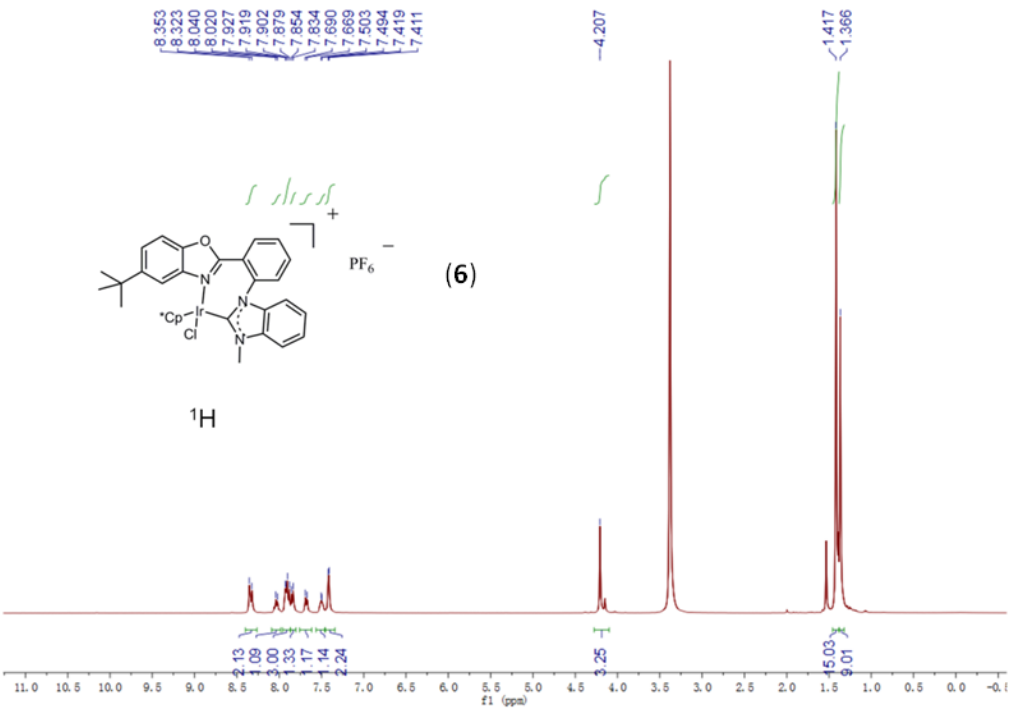

-69.209
-71.100
PF6
(4)
*Cp
Ir
Cl
19F
f1 (ppm)

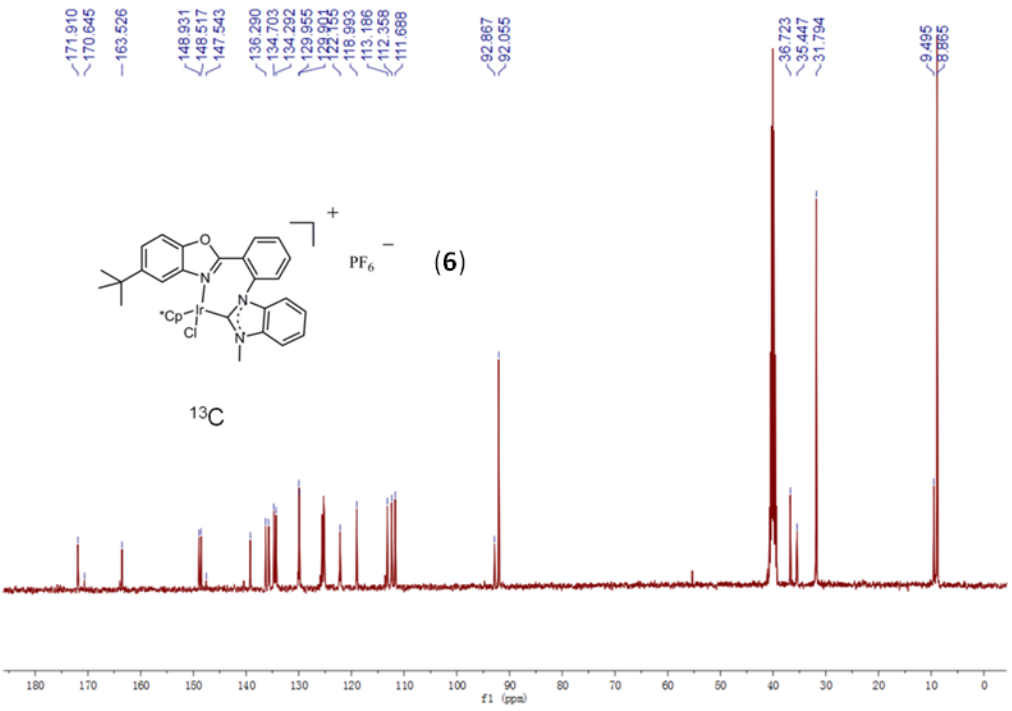

8.371
8.366
8.363
8.358
8.317
8.301
8.298
8.011
7.945
7.926
7.904
7.892
7.880
7.854
7.694
7.690
7.686
7.672
7.668
7.664
7.471
7.403
7.385
7.366
7.346
4.733
4.721
4.700
4.687
4.675
4.517
4.507
4.408
1.994
1.798
1.786
1.510
1.383
1.368
1.045
1.027
1.009
PF6
(5)
*Cp
Ir
Cl
1H
1.12
1.09
1.18
4.51
1.12
1.14
2.25
1.14
1.18
2.58
2.00
3.34
15.79
3.37
f1 (ppm)

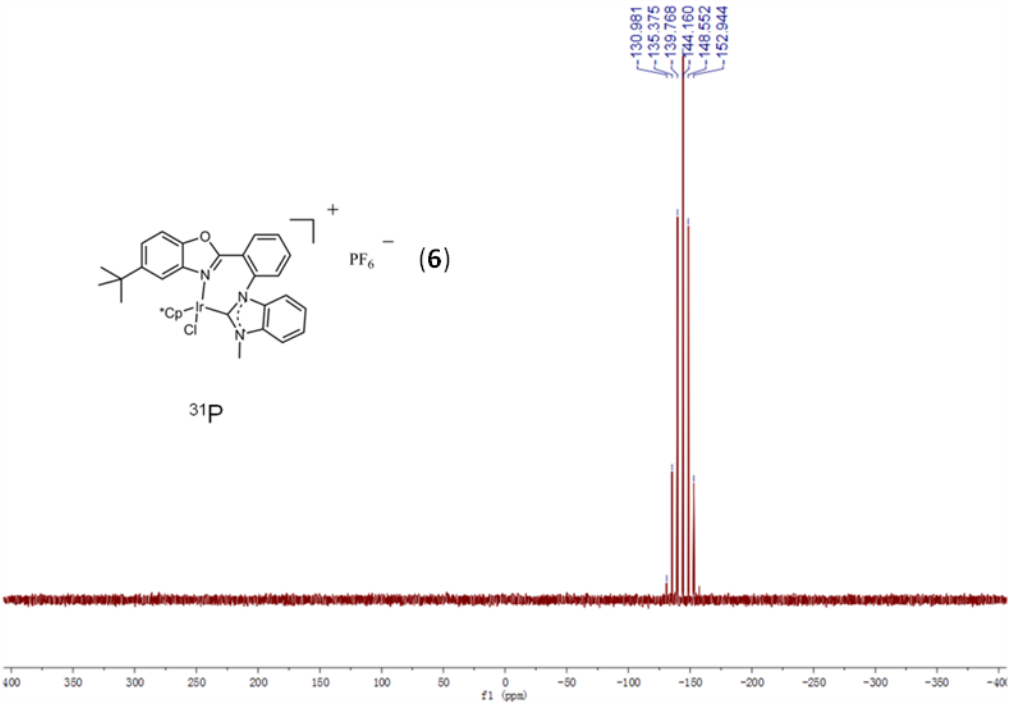

171.057
169.513
163.843
163.468
148.755
148.327
147.198
140.095
136.813
135.477
134.570
129.913
125.670
124.955
122.236
118.745
113.360
111.599
92.751
91.953
49.939
35.316
31.610
20.178
14.100
9.415
8.647
PF6
(5)
13C
f1 (ppm)

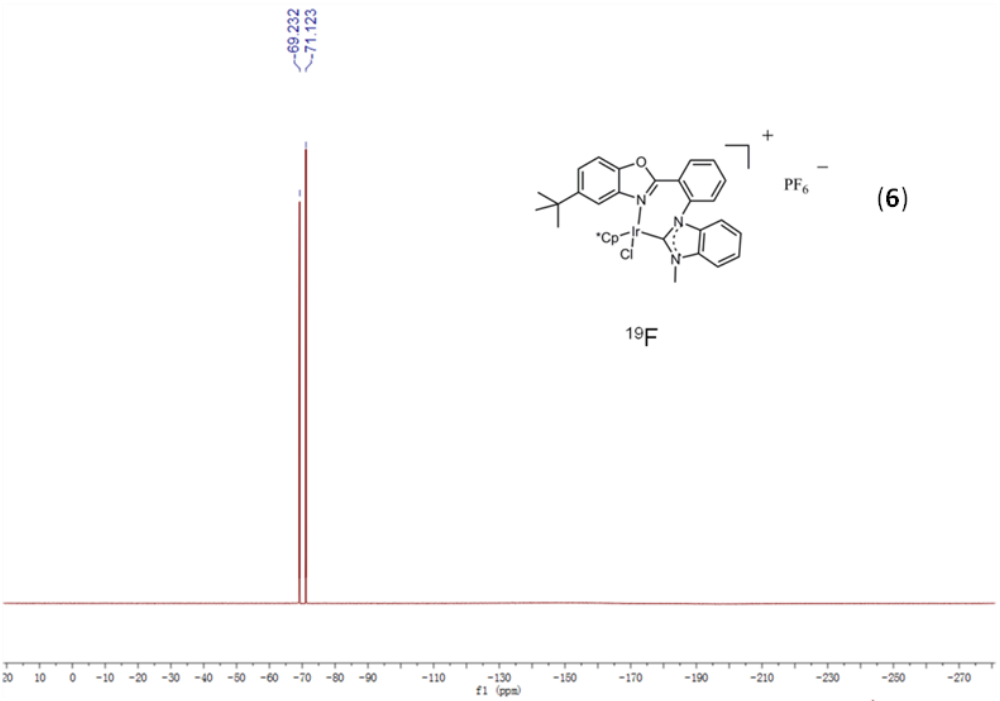

131.009
135.407
139.803
144.198
148.593
152.991
157.385
PF6
(5)
31P
f1 (ppm)

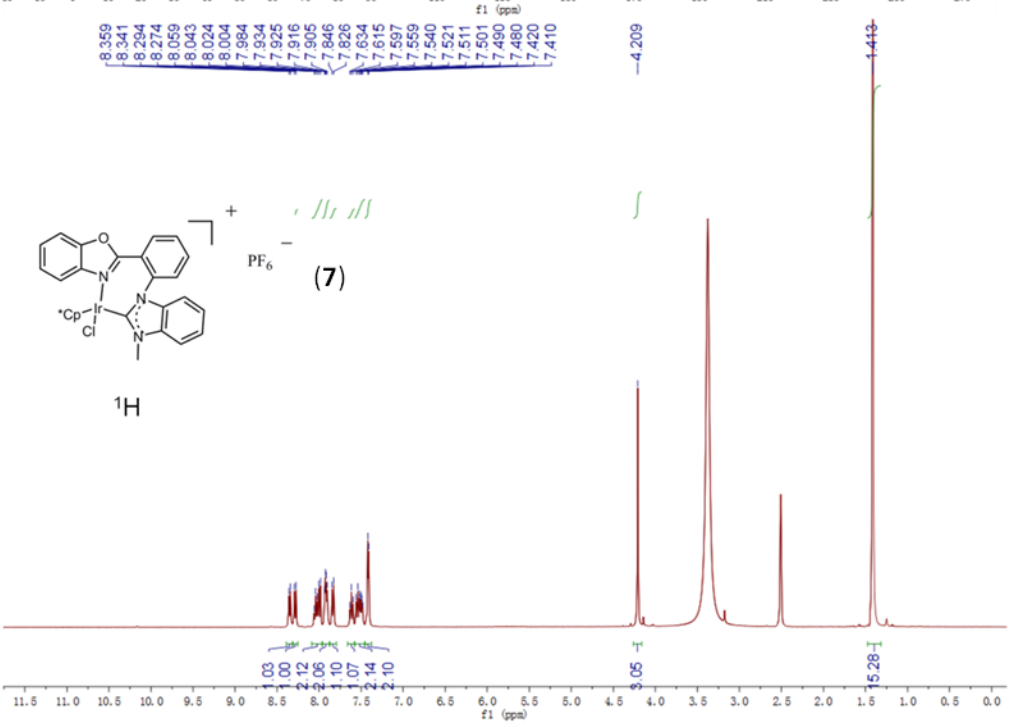

-69.194
-71.084
PF6
(5)
*Cp
Ir
Cl
19F
f1 (ppm)

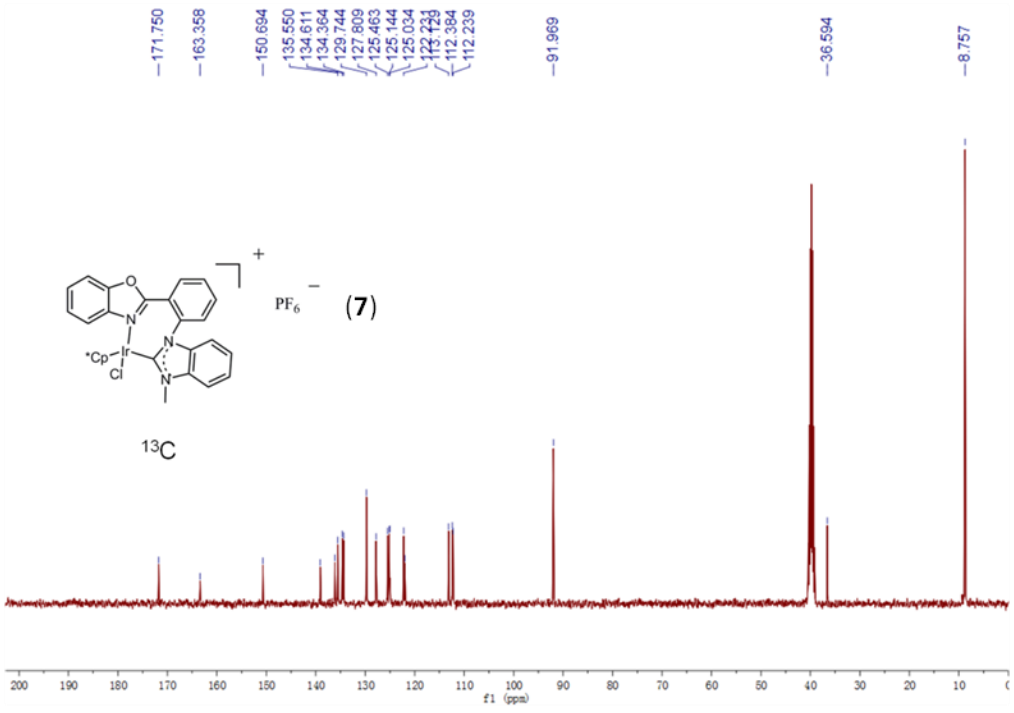

8.353
8.323
8.040
8.020
7.927
7.919
7.902
7.879
7.854
7.834
7.690
7.669
7.503
7.494
7.419
7.411
4.207
1.417
1.366
PF6
(6)
*Cp
Ir
Cl
1H
2.13
1.09
3.00
1.33
1.17
1.14
2.24
3.25
15.03
9.01
f1 (ppm)

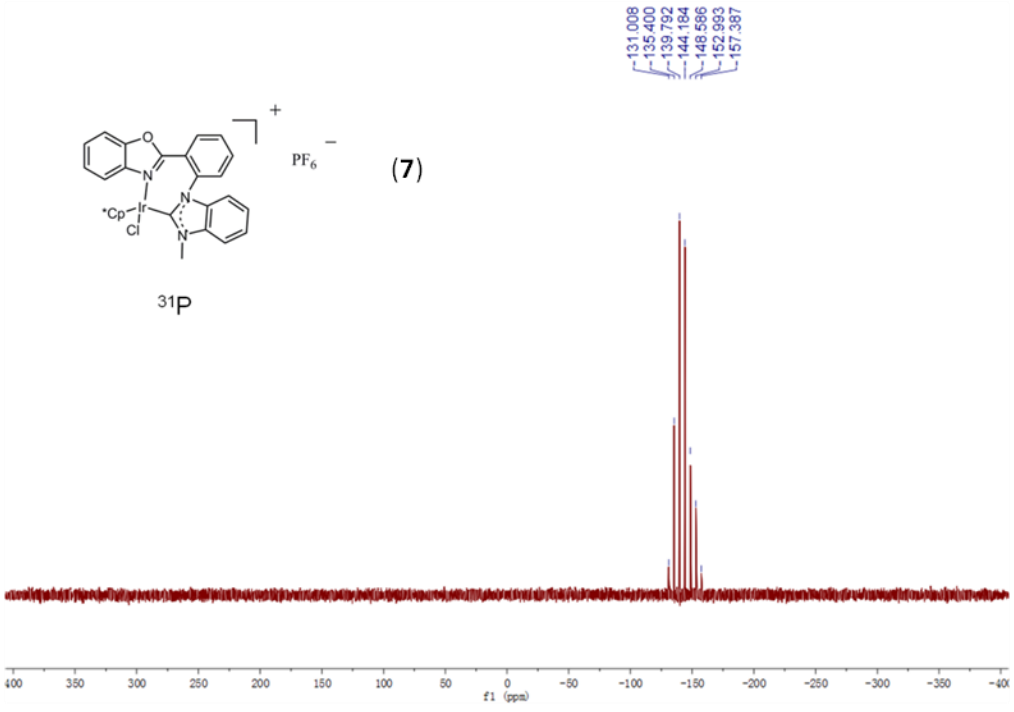

171.910
170.645
163.526
148.931
148.517
147.543
136.290
134.703
134.292
129.955
129.901
122.155
118.993
113.186
112.358
111.688
92.867
92.055
36.723
35.447
31.794
9.495
8.865
PF6
(6)
13C
f1 (ppm)

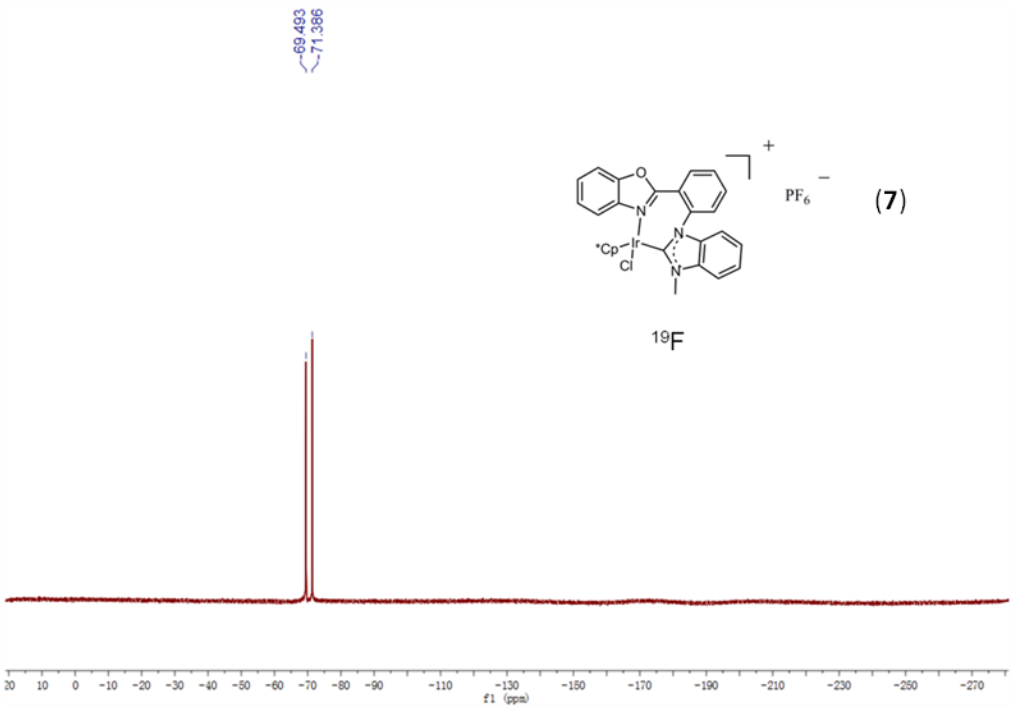

130.981
135.375
139.768
144.160
148.552
152.944
PF6
(6)
31P
f1 (ppm)

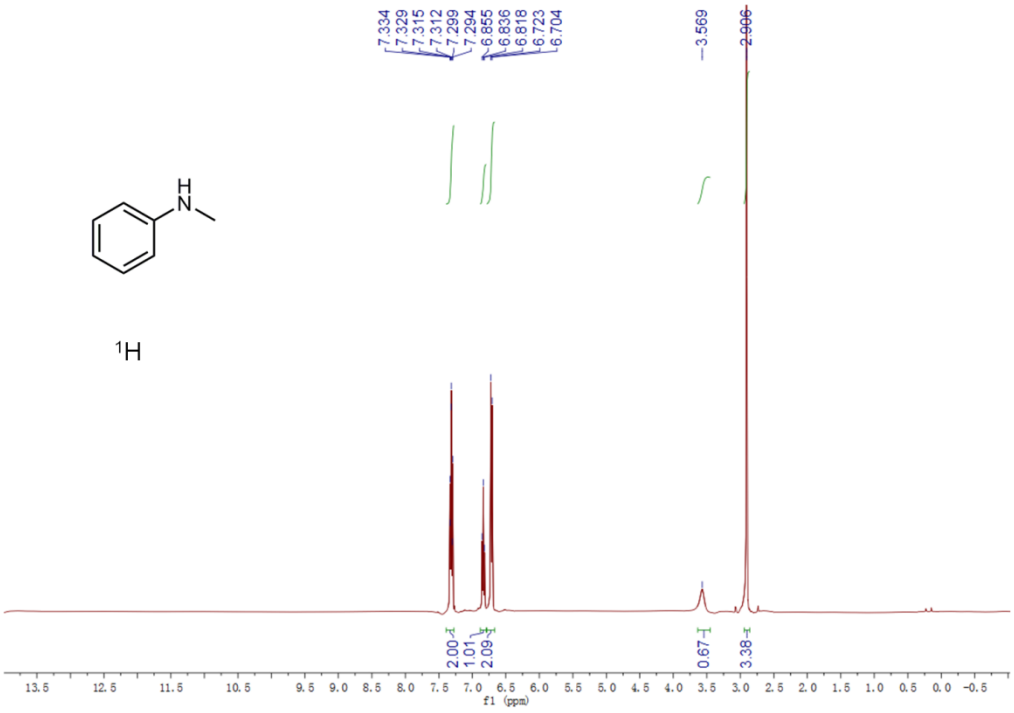

-69.232
-71.123
PF6
(6)
19F
f1 (ppm)

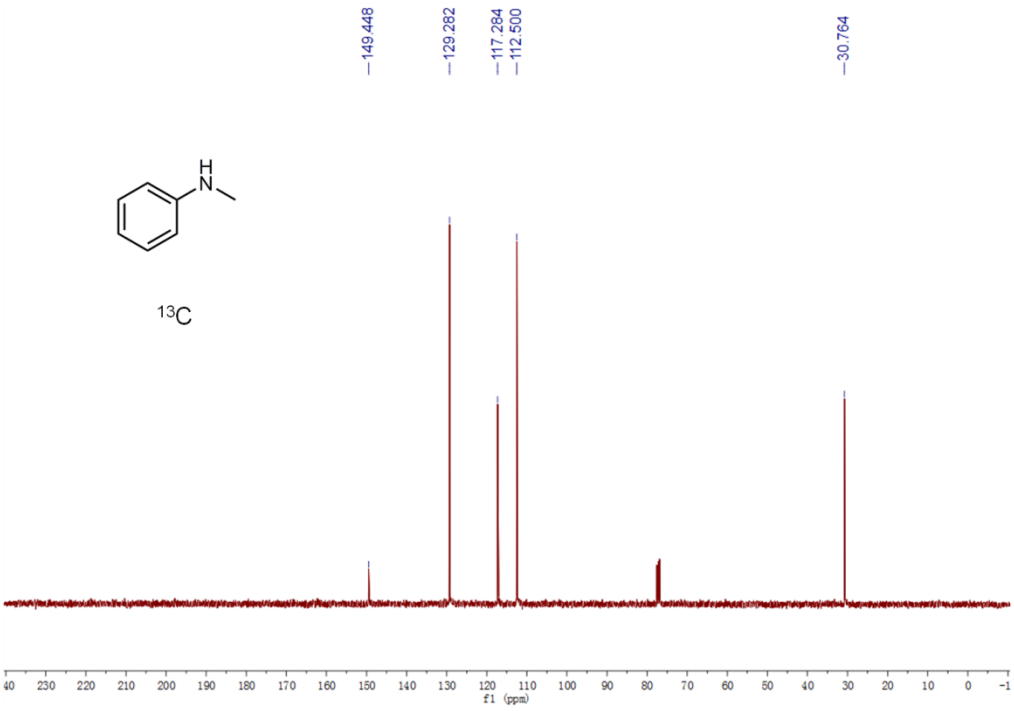

8.359
8.341
8.294
8.274
8.059
8.043
8.024
8.004
7.984
7.934
7.925
7.916
7.905
7.846
7.826
7.634
7.615
7.597
7.559
7.540
7.521
7.511
7.501
7.490
7.480
7.420
7.410
4.209
1.413
PF6
(7)
1H
1.03
1.00
2.12
2.06
1.10
1.07
2.14
2.10
3.05
15.28
f1 (ppm)

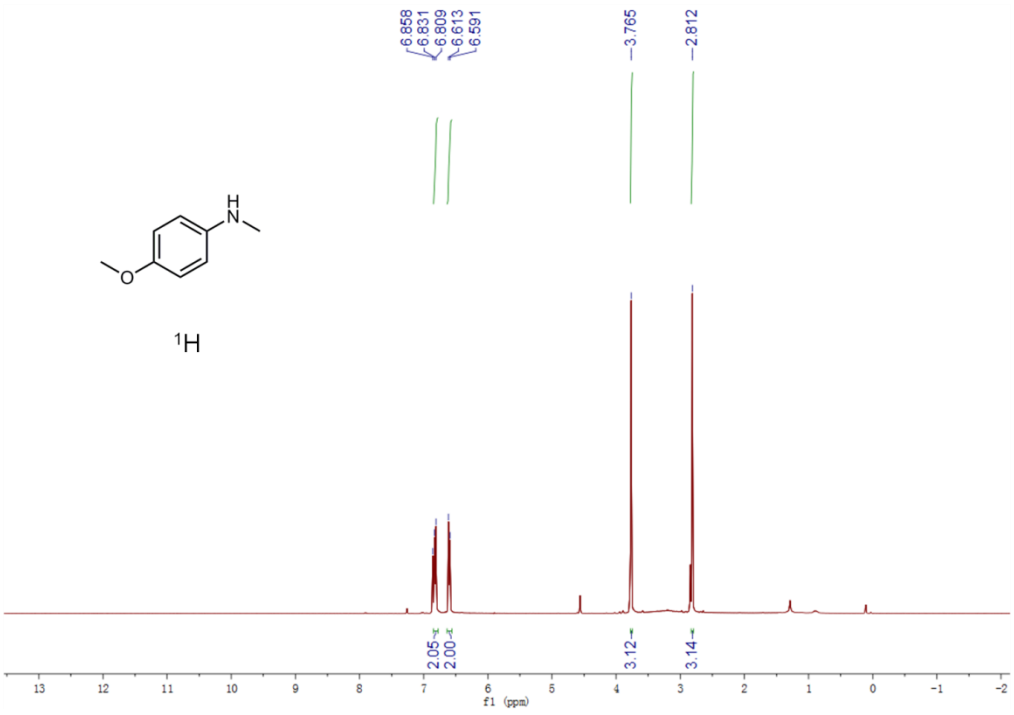

171.750
163.358
150.694
135.550
134.611
134.364
129.744
127.809
125.463
125.144
125.034
122.231
113.129
112.384
112.239
91.969
36.594
8.757
PF6
(7)
13C
f1 (ppm)

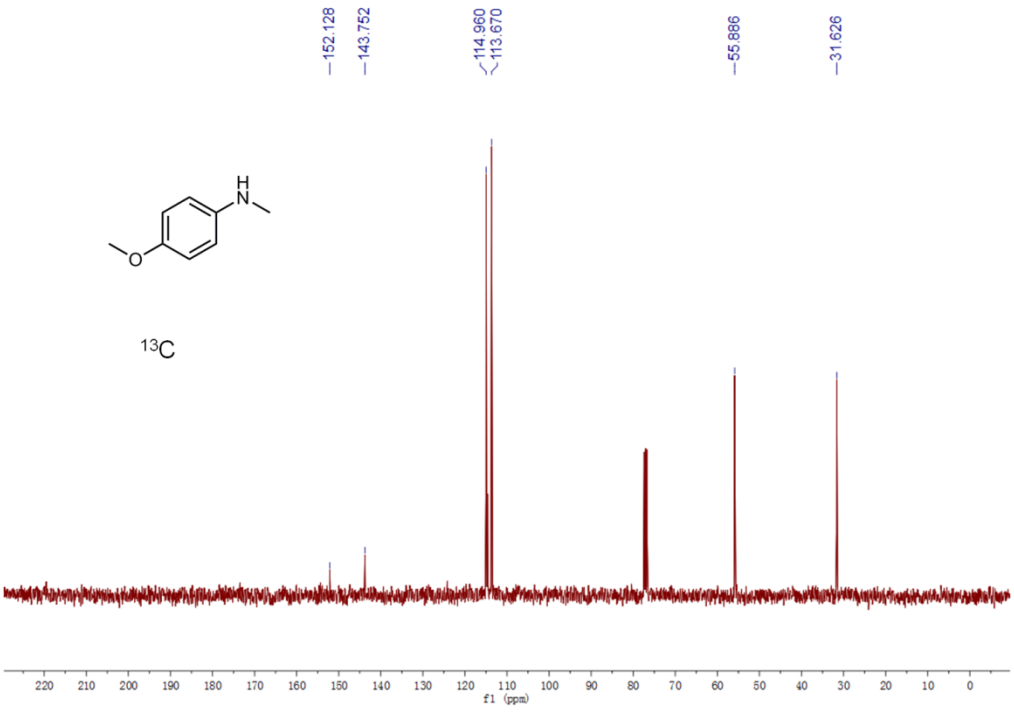

131.008
135.400
139.792
144.184
148.586
152.993
157.387
PF6
(7)
31P
f1 (ppm)

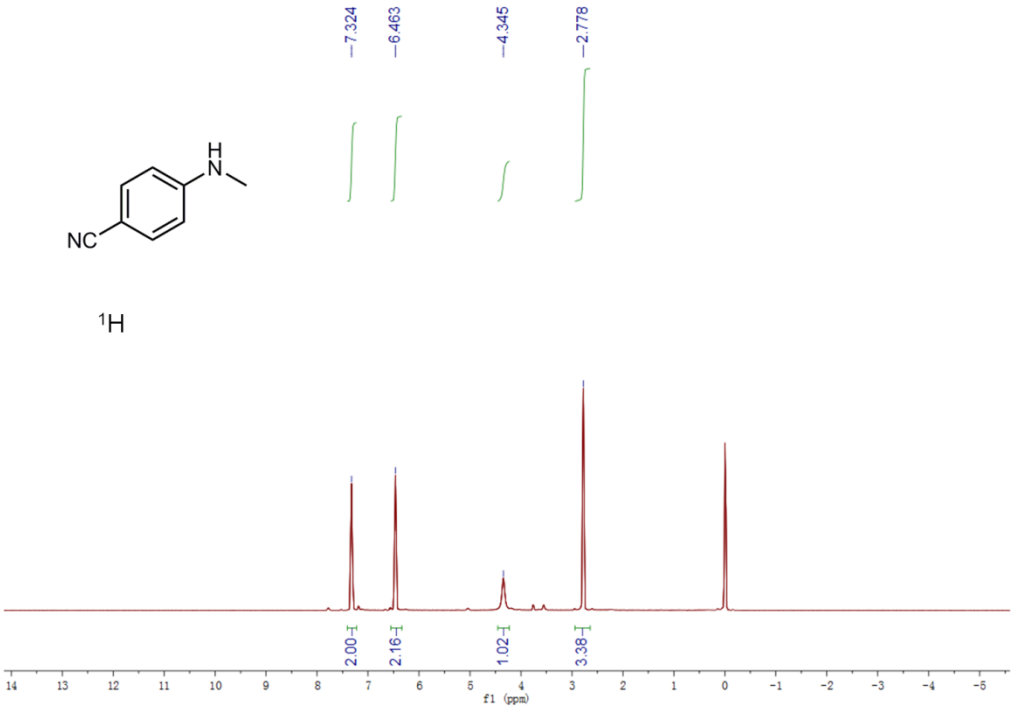

-69.493
-71.386
PF6
(7)
19F
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270
f1 (ppm)

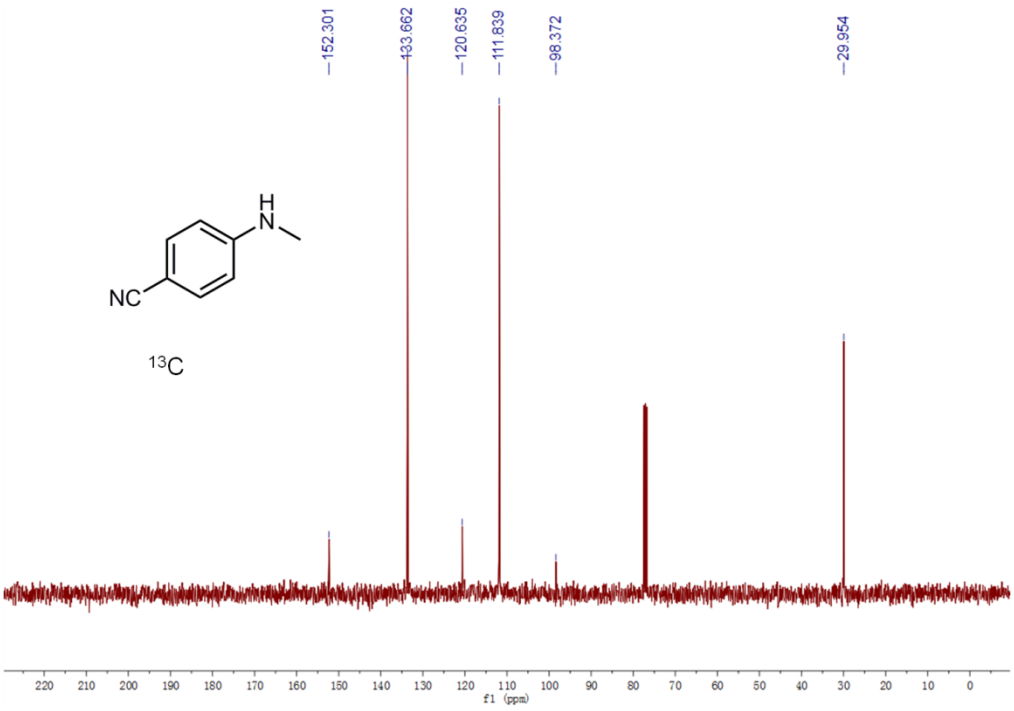

7.334
7.329
7.315
7.312
7.299
7.294
6.855
6.836
6.818
6.723
6.704
3.569
2.906
1H
2.00
1.01
2.09
0.67
3.38
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

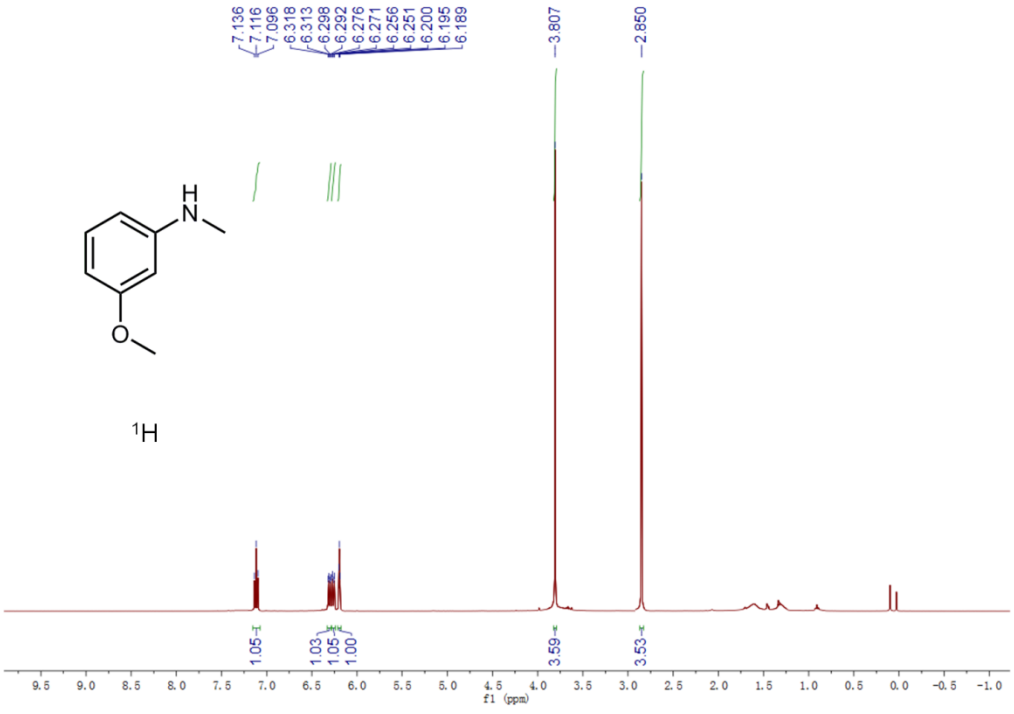

149.448
129.282
117.284
112.500
30.764
H
N
13C
40 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

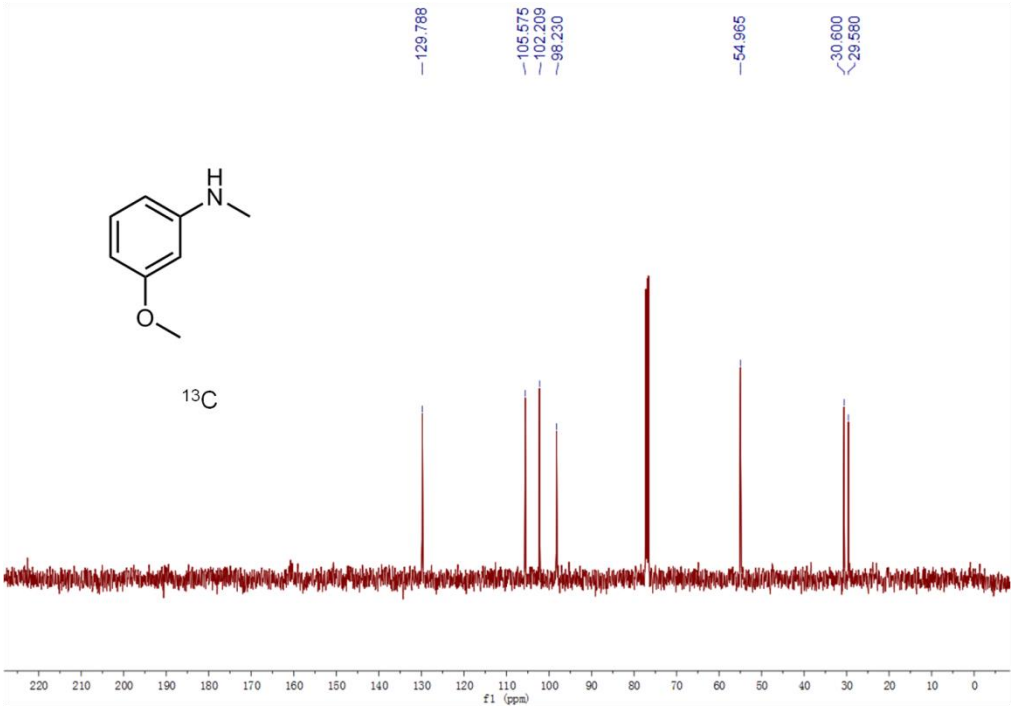

6.858
6.831
6.809
6.613
6.591
3.765
2.812
H
N
O
1H
2.05
2.00
3.12
3.14
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)

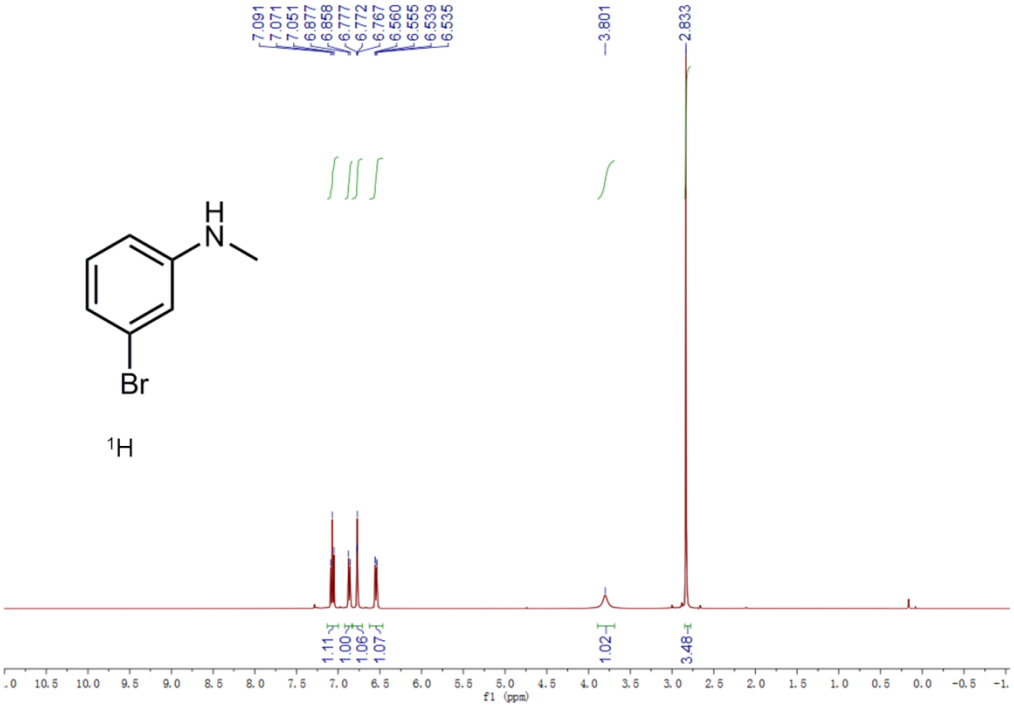

152.128
143.752
114.960
113.670
55.886
31.626
H
N
O
13C
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

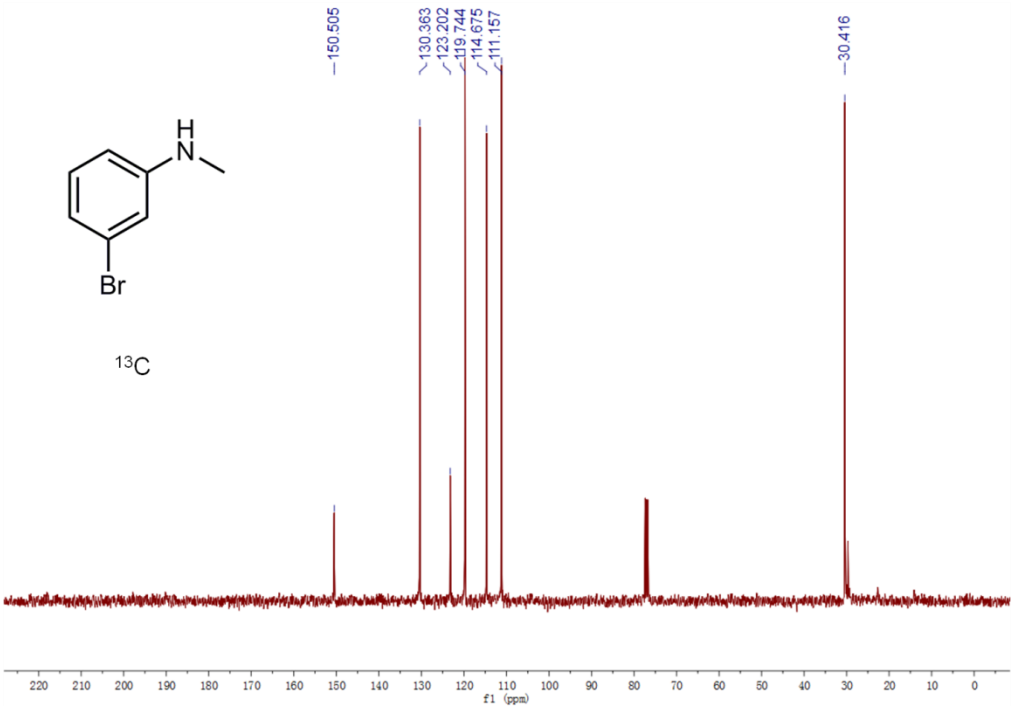

7.324
6.463
4.345
2.778
H
N
NC
1H
2.00
2.16
1.02
3.38
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5
f1 (ppm)

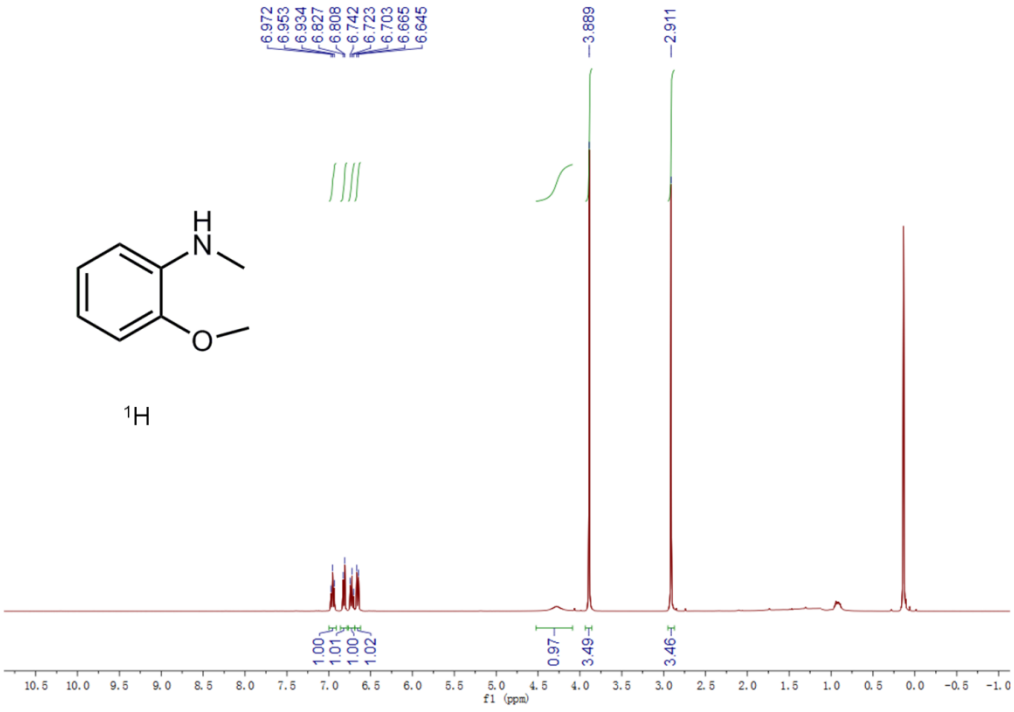

152.301
133.662
120.635
111.839
98.372
29.954
NC
H
N
13C
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

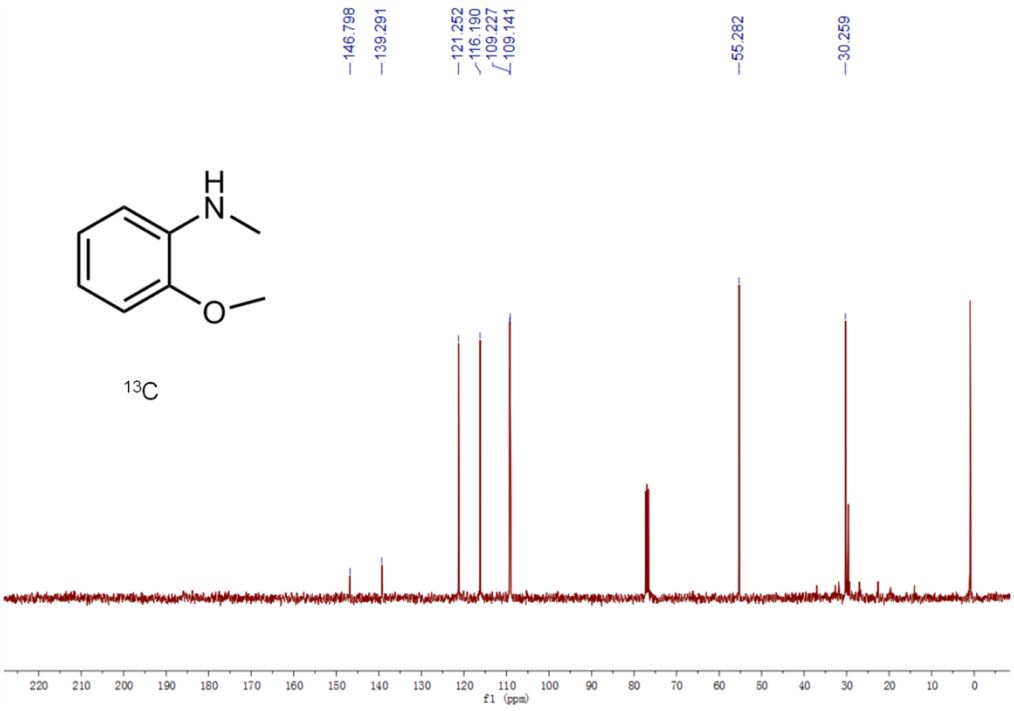

7.136
7.116
7.096
6.318
6.313
6.298
6.292
6.276
6.271
6.256
6.251
6.200
6.195
6.189
3.807
2.850
H
N
O
1H
1.05
1.03
1.05
1.00
3.59
3.53
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

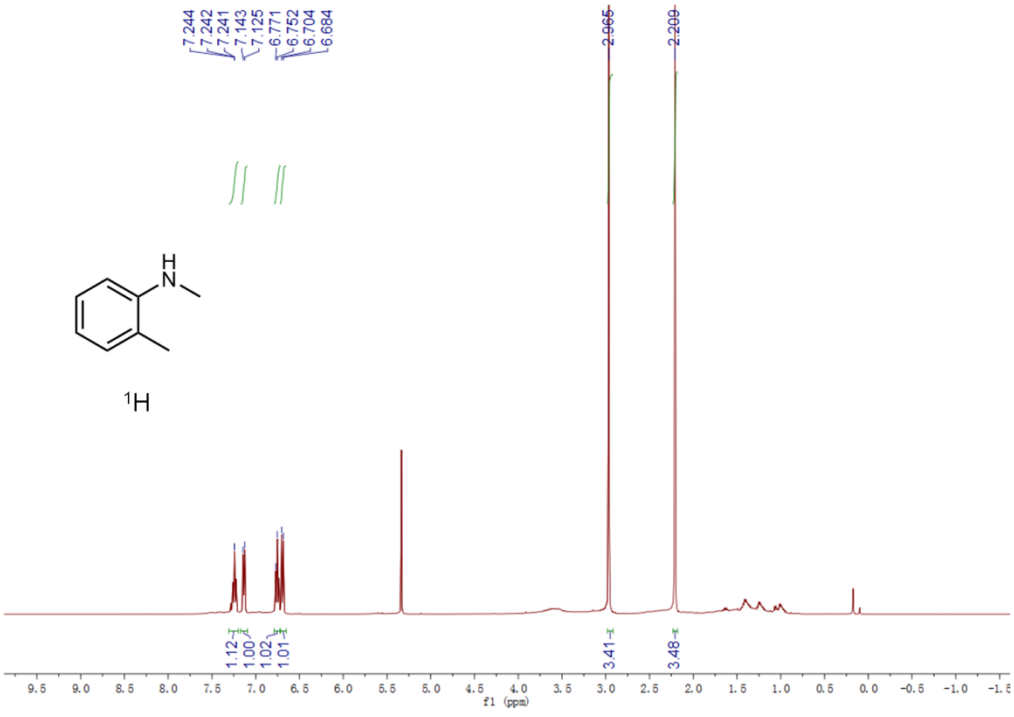

129.788
105.575
102.209
96.230
54.965
30.600
29.580
H
N
O
13C
f1 (ppm)

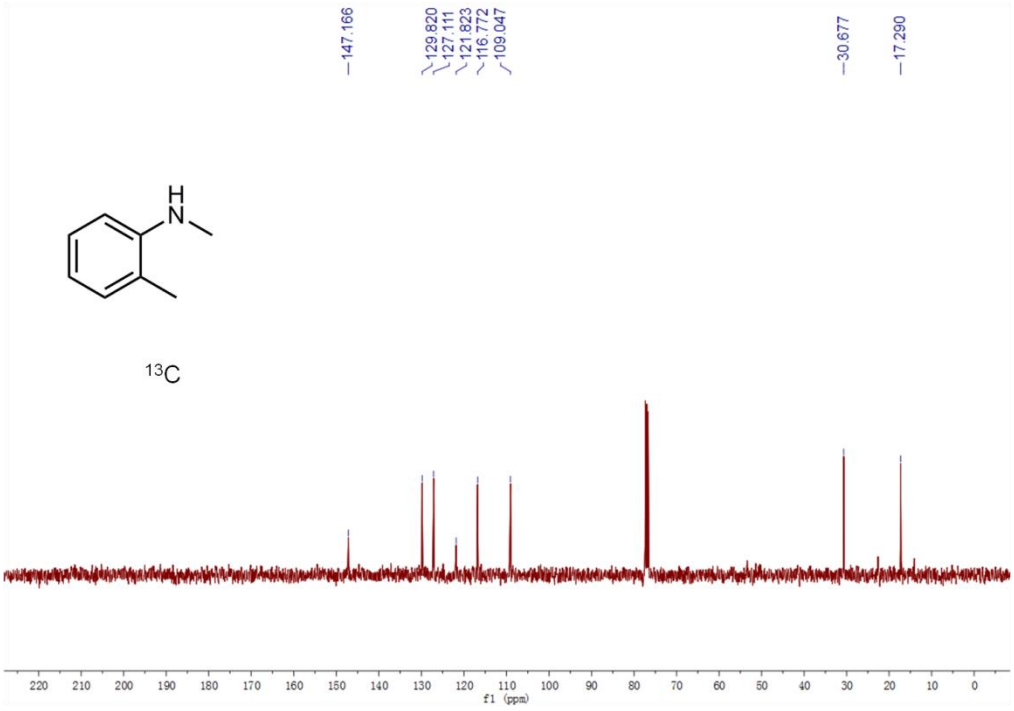

7.091
7.071
7.051
6.877
6.858
6.777
6.772
6.767
6.560
6.555
6.539
6.535
3.801
2.833
H
N
Br
1H
1.11
1.00
1.06
1.07
1.02
3.48
f1 (ppm)

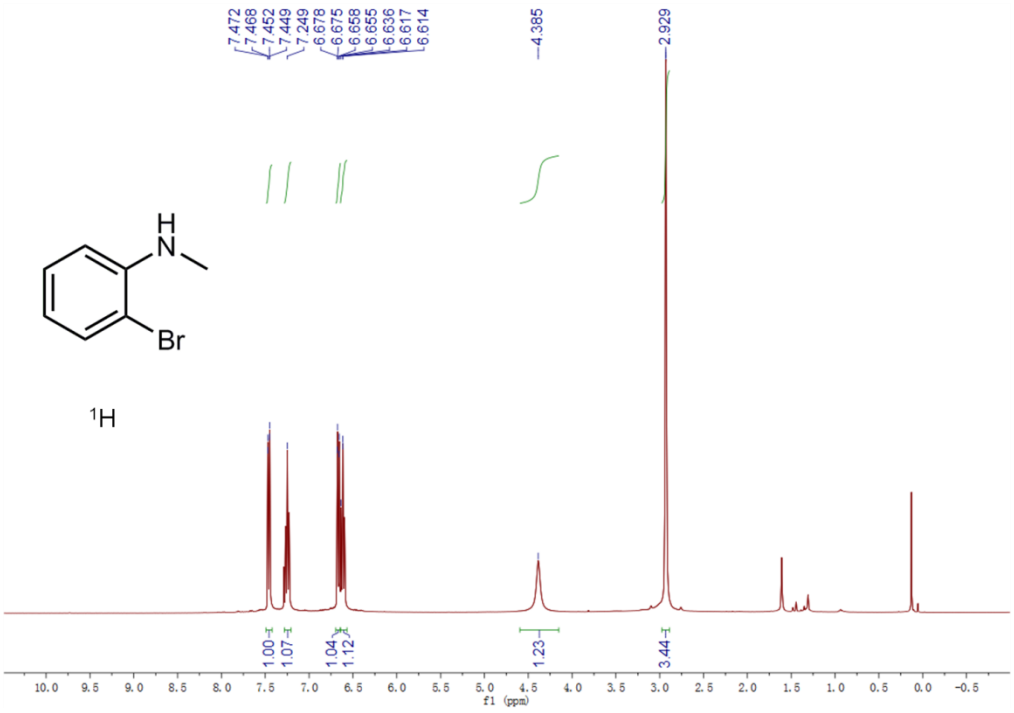

150.505
130.363
123.202
119.744
114.675
111.157
30.416
H
N
Br
13C
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

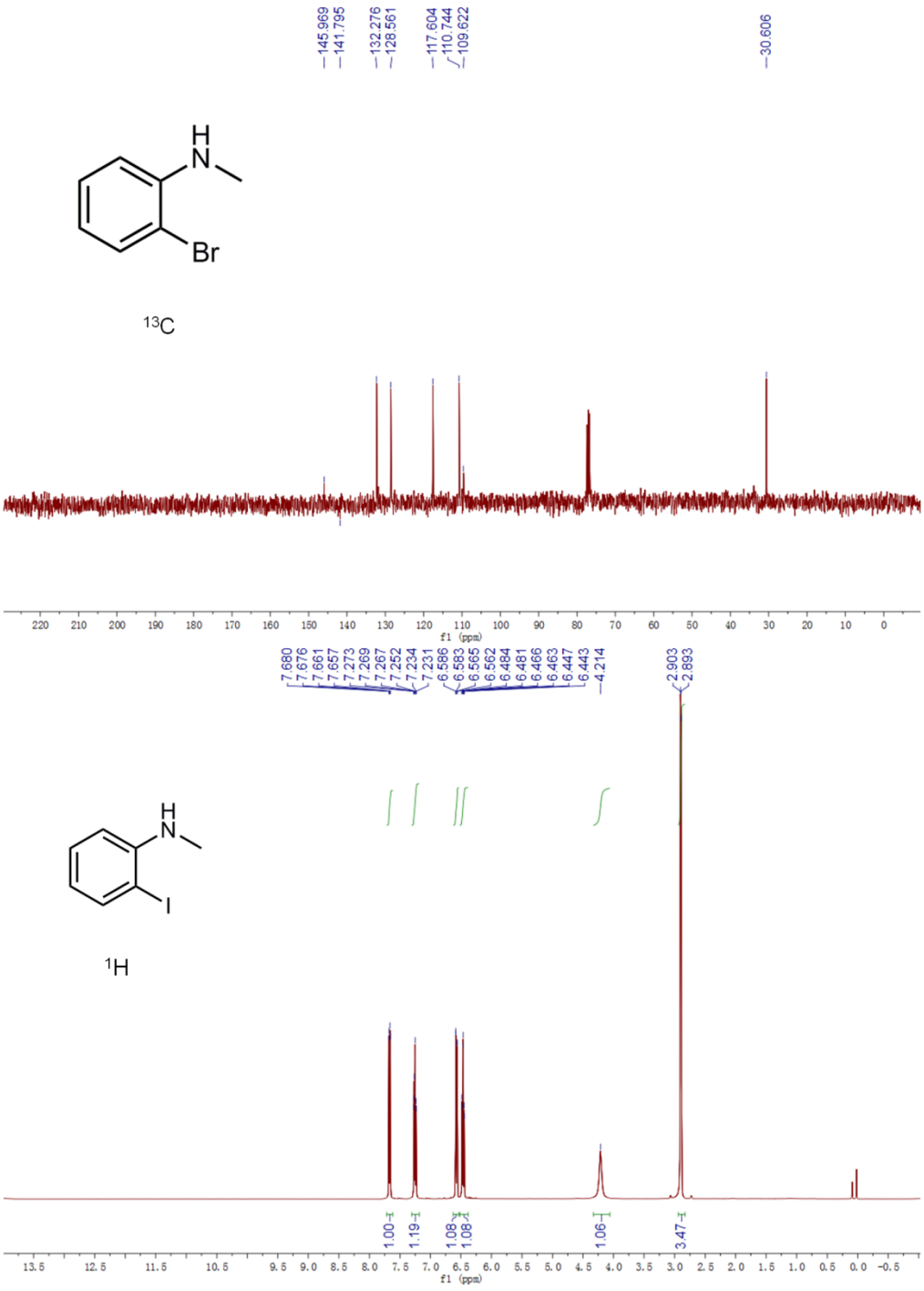

6.972
6.953
6.934
6.827
6.808
6.742
6.723
6.703
6.665
6.645
3.889
2.911
H
N
O
1H
1.00
1.01
1.00
1.02
0.97
3.49
3.46
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

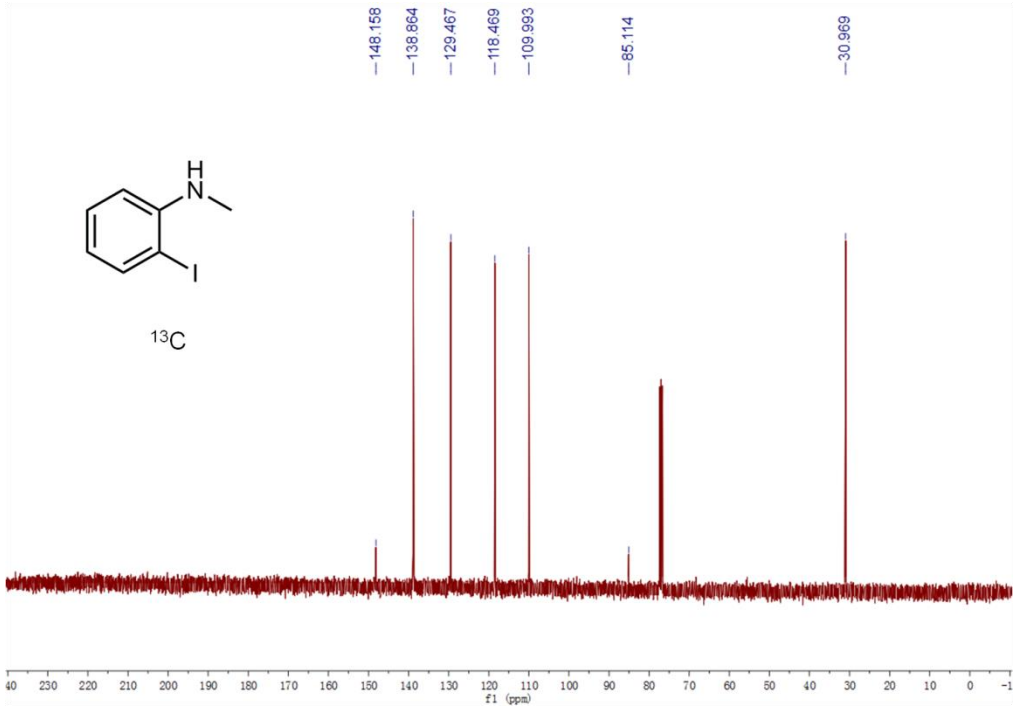

146.798
139.291
121.252
116.190
109.227
109.141
55.282
30.259
13C
f1 (ppm)

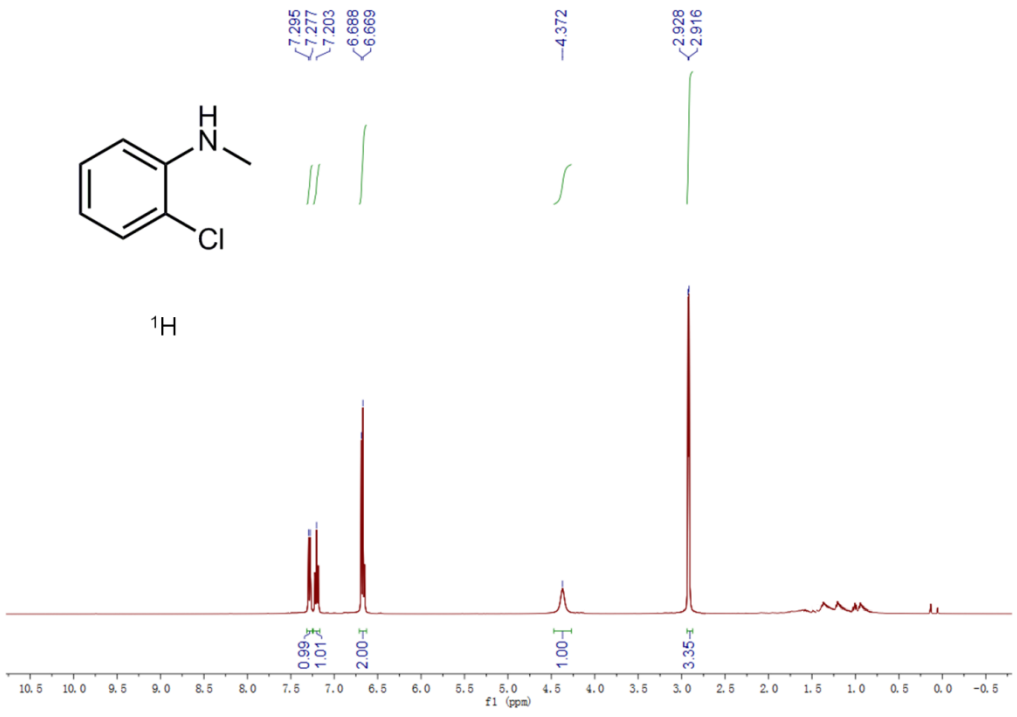

7.244
7.242
7.241
7.143
7.125
6.771
6.752
6.704
6.684
2.965
2.209
1.12
1.00
1.02
1.01
3.41
3.48
1H
f1 (ppm)

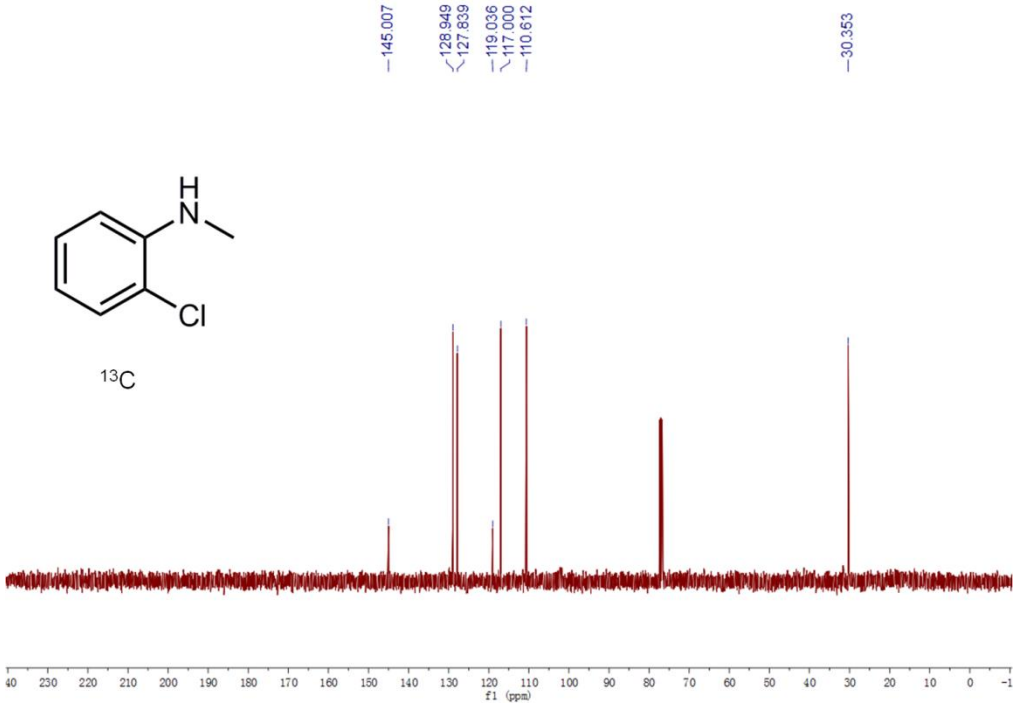

147.166
129.820
127.111
121.823
116.772
109.047
30.677
17.290
13C
f1 (ppm)

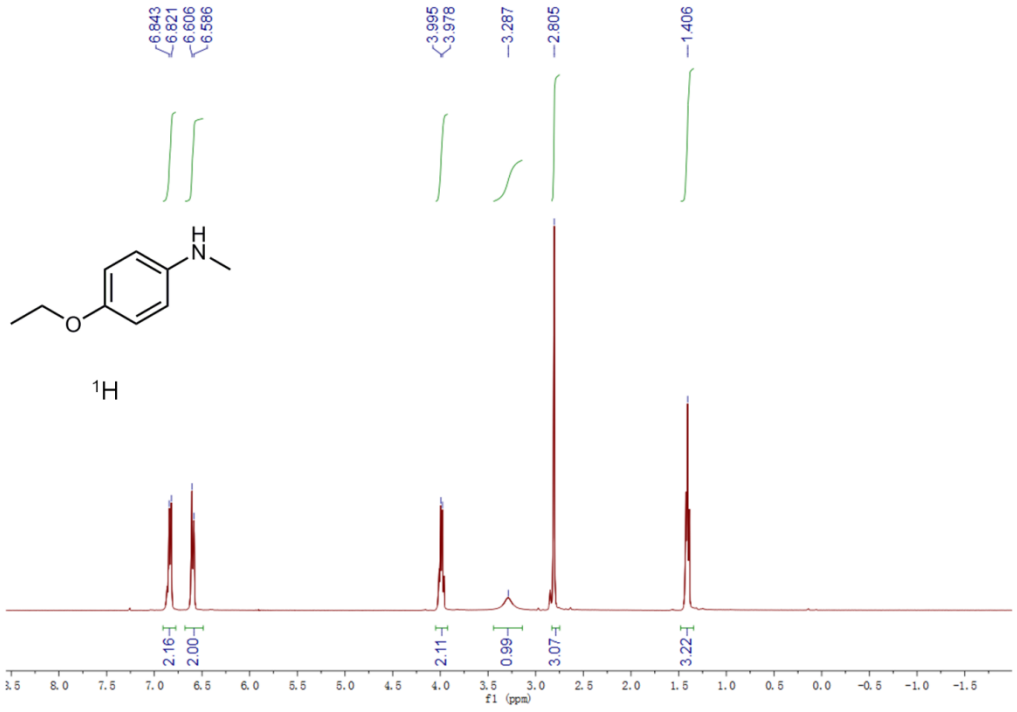

7.472
7.468
7.452
7.449
7.249
6.678
6.675
6.658
6.655
6.636
6.617
6.614
4.385
2.929
Br
1H
1.00
1.07
1.04
1.12
1.23
3.44
f1 (ppm)

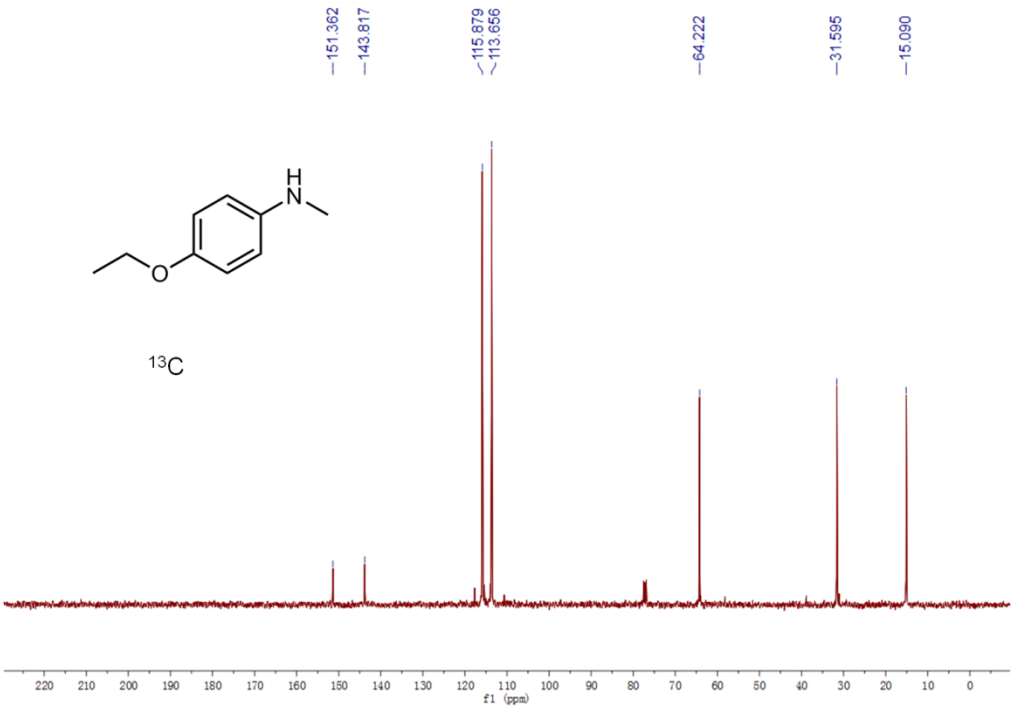

145.969
141.795
132.276
128.561
117.604
110.744
109.622
30.606
H
N
Br
13C
f1 (ppm)
7.680
7.676
7.661
7.657
7.273
7.269
7.267
7.252
7.234
7.231
6.586
6.583
6.565
6.562
6.484
6.481
6.466
6.463
6.447
6.443
4.214
2.903
2.893
H
N
I
1H
1.00
1.19
1.08
1.08
1.06
3.47
f1 (ppm)

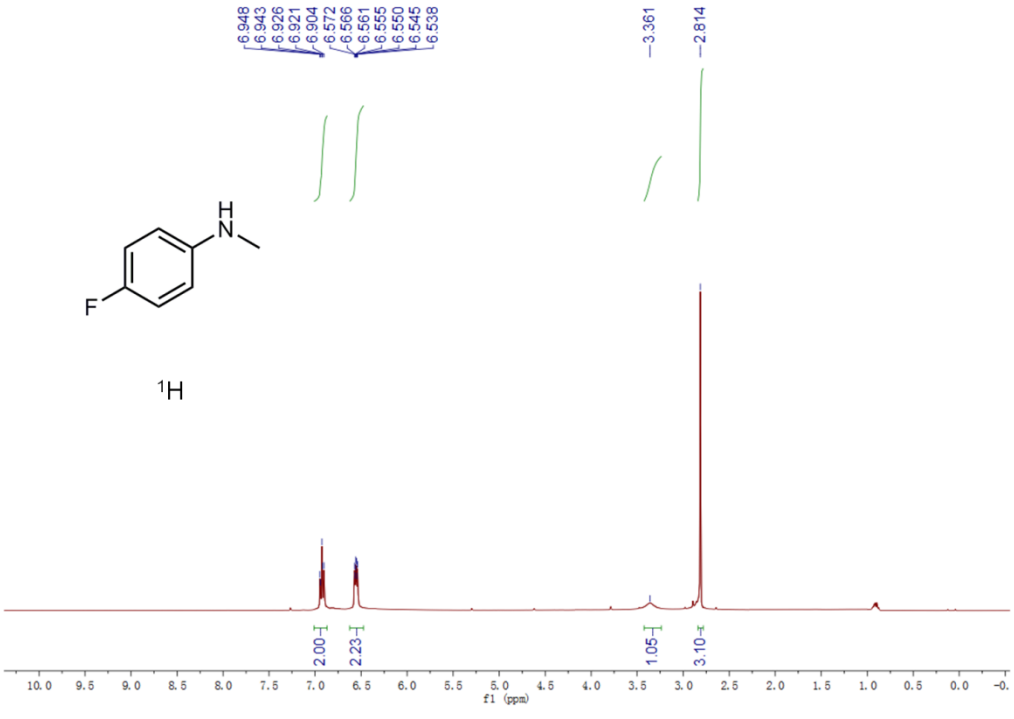

148.158
138.864
129.467
118.469
109.993
85.114
30.969
H
N
I
13C
f1 (ppm)

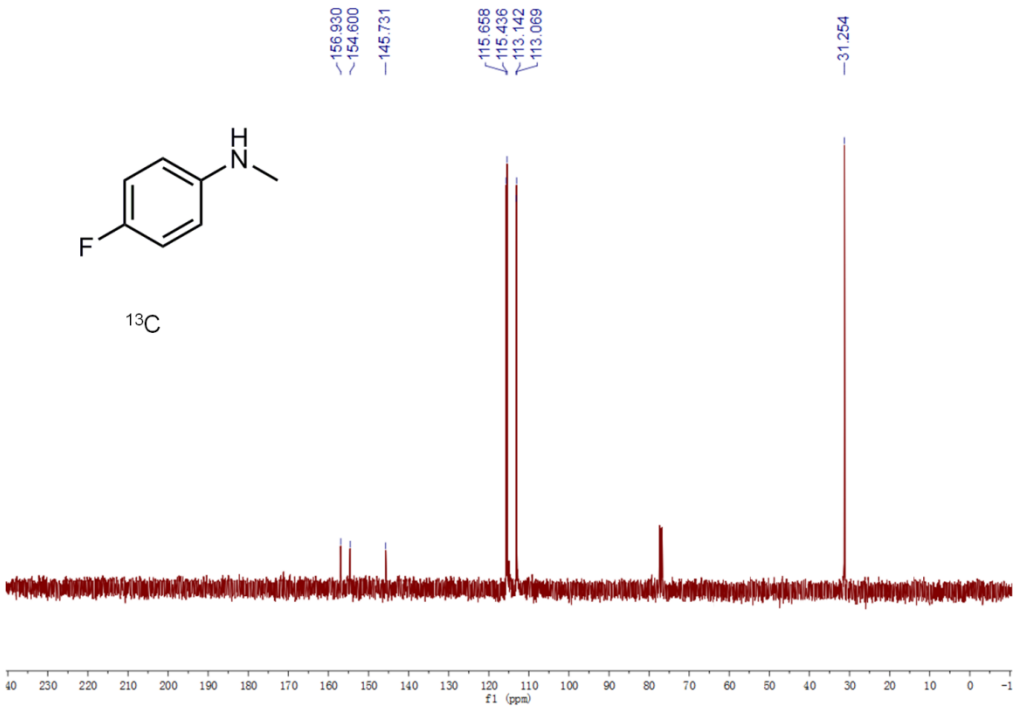

7.295
7.277
7.203
6.688
6.669
4.372
2.928
2.916
H
N
Cl
1H
0.99
1.01
2.00
1.00
3.35
f1 (ppm)

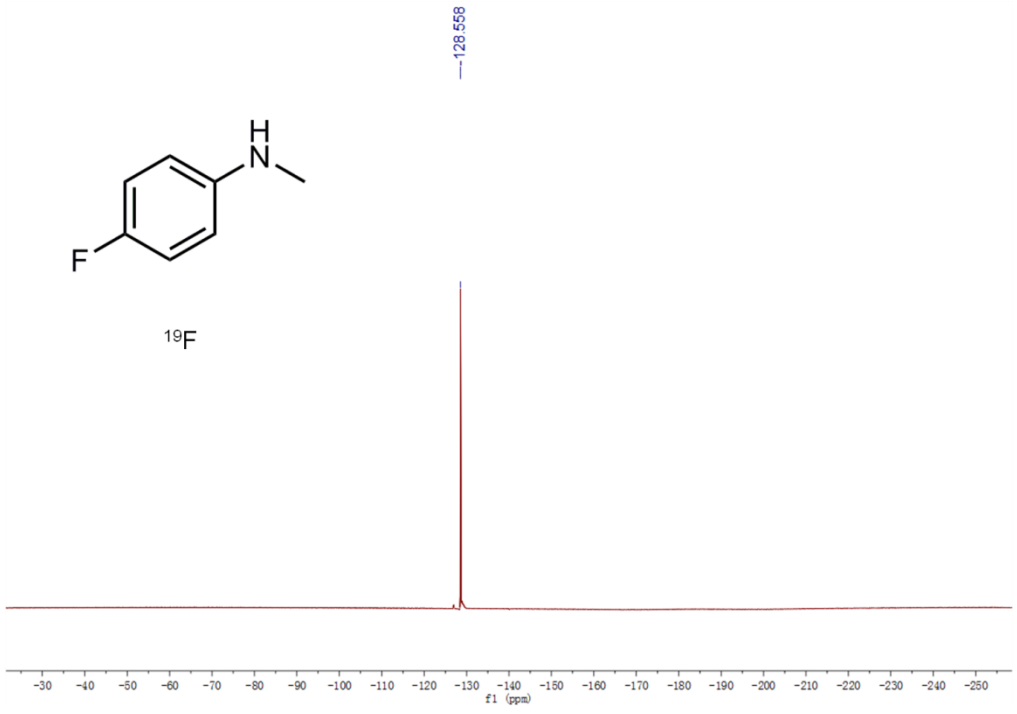

145.007
128.949
127.839
119.036
117.000
110.612
30.353
H
N
Cl
13C
f1 (ppm)

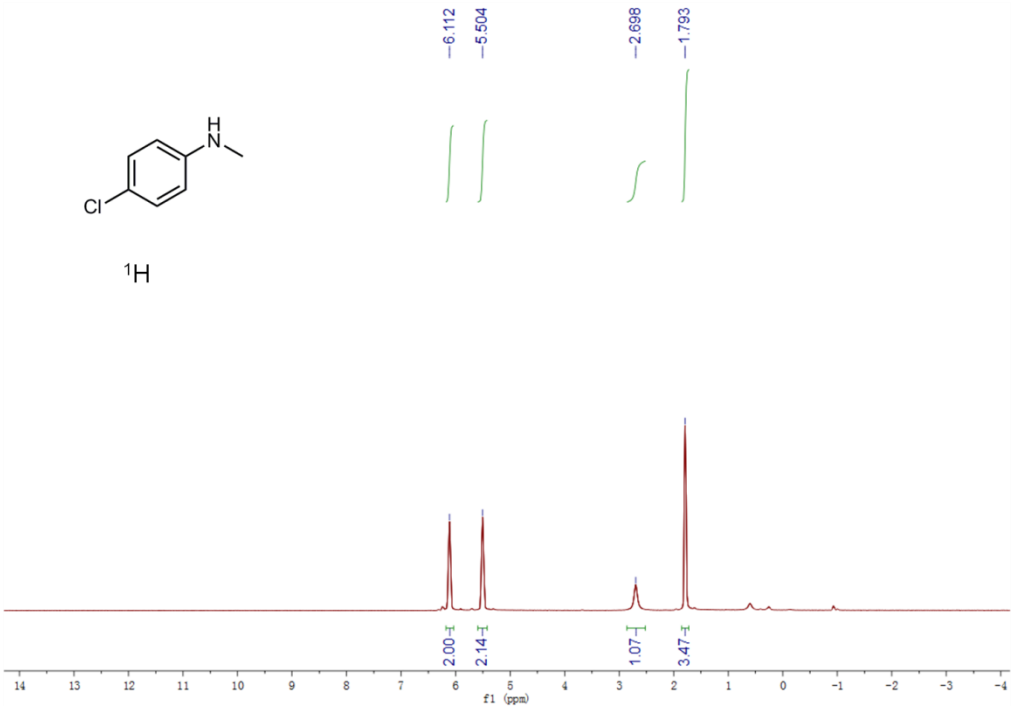

6.843
6.821
6.606
6.586
3.995
3.978
3.287
2.805
1.406
H
N
O
1H
2.16
2.00
2.11
0.99
3.07
3.22
f1 (ppm)


151.362
143.817
115.879
113.656
64.222
31.595
15.090
H
N
O
13C
f1 (ppm)

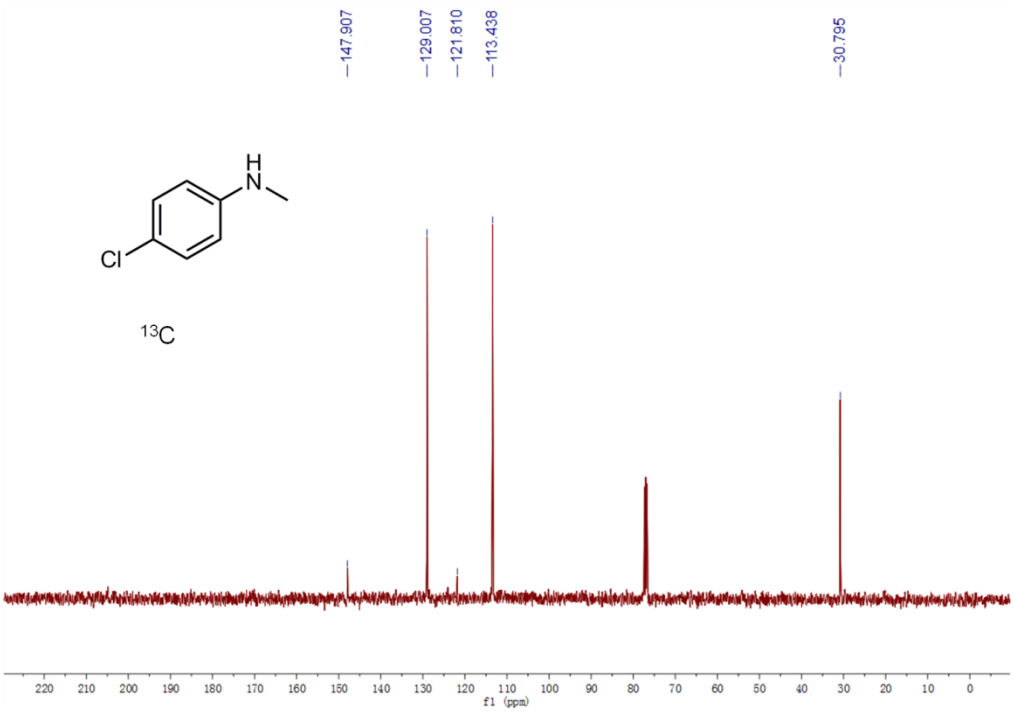

6.948
6.943
6.926
6.921
6.904
6.572
6.566
6.561
6.555
6.550
6.545
6.538
3.361
2.814
H
N
F
1H
2.00
2.23
1.05
3.10
f1 (ppm)


156.930
154.600
145.731
115.658
115.436
113.142
113.069
31.254
H
N
F
13C
f1 (ppm)

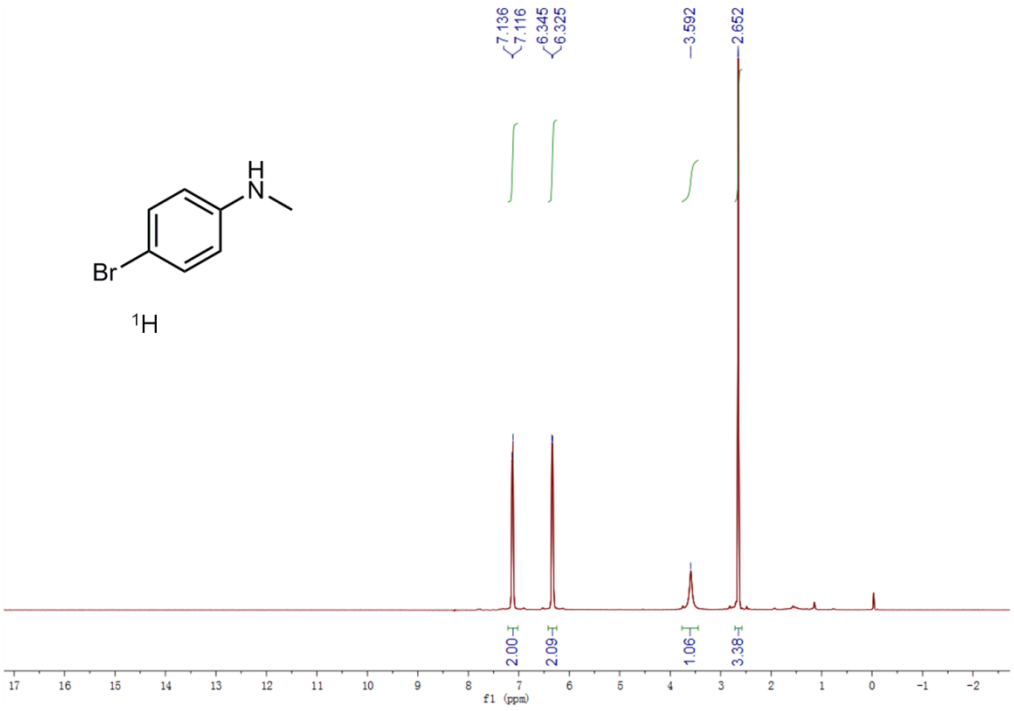

128.558
H
N
F
19F
f1 (ppm)


6.112
5.504
2.698
1.793
Cl
H
N
2.00
2.14
1.07
3.47
f1 (ppm)

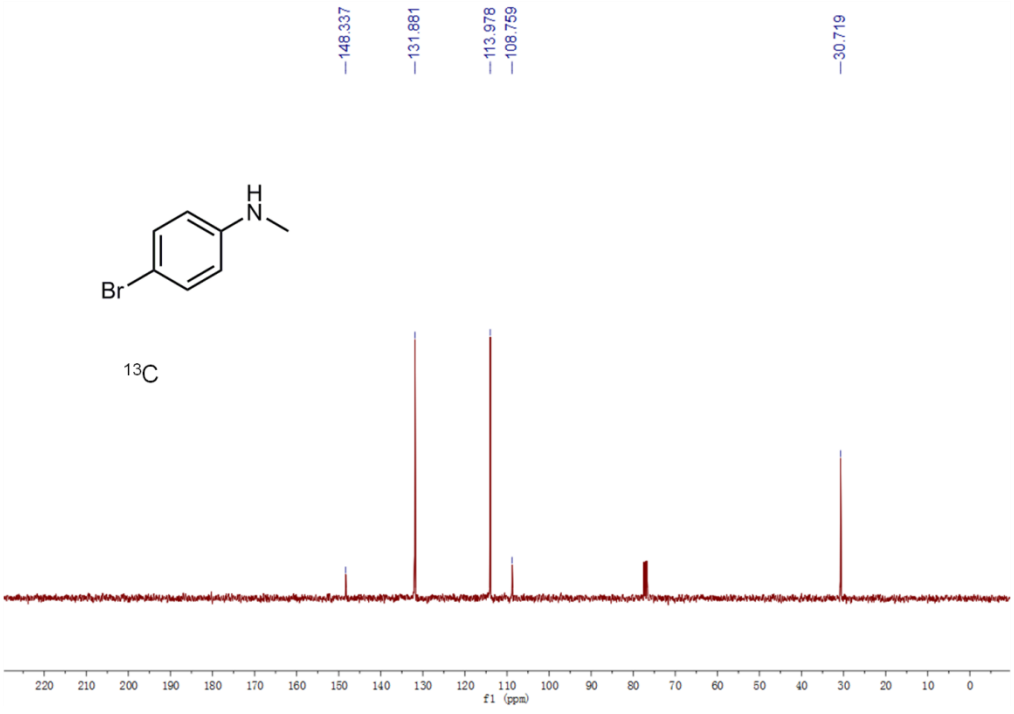
^{1}H


147.907
129.007
121.810
113.438
30.795
Cl
H
N
f1 (ppm)

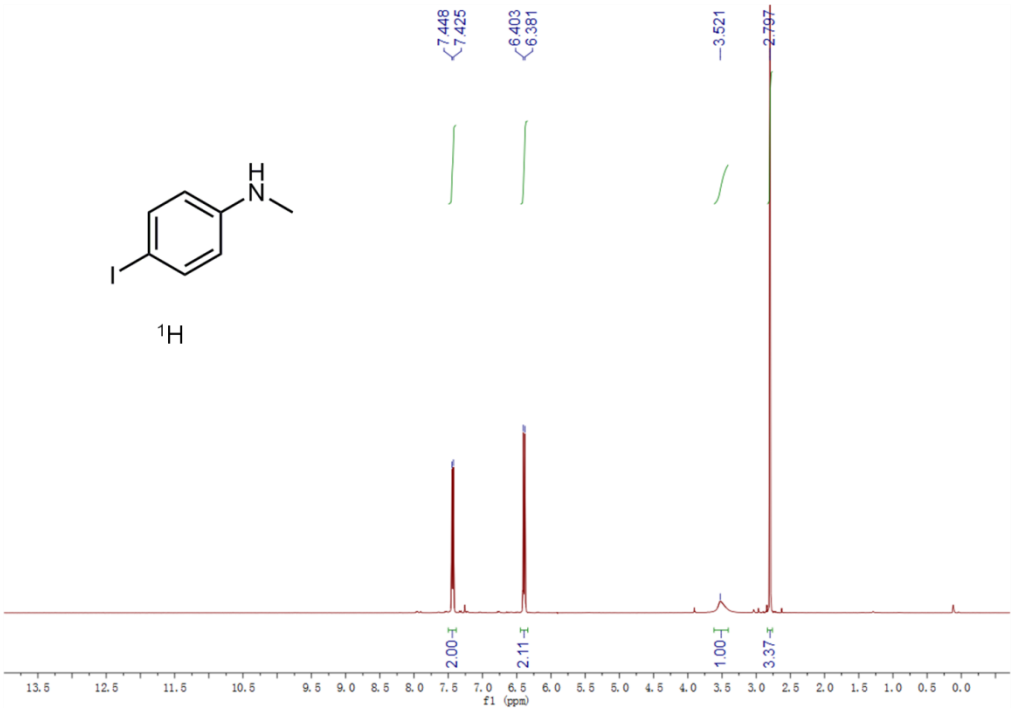
^{13}C


7.136
7.116
6.345
6.325
3.592
2.652
Br
H
N
2.00
2.09
1.06
3.38
f1 (ppm)

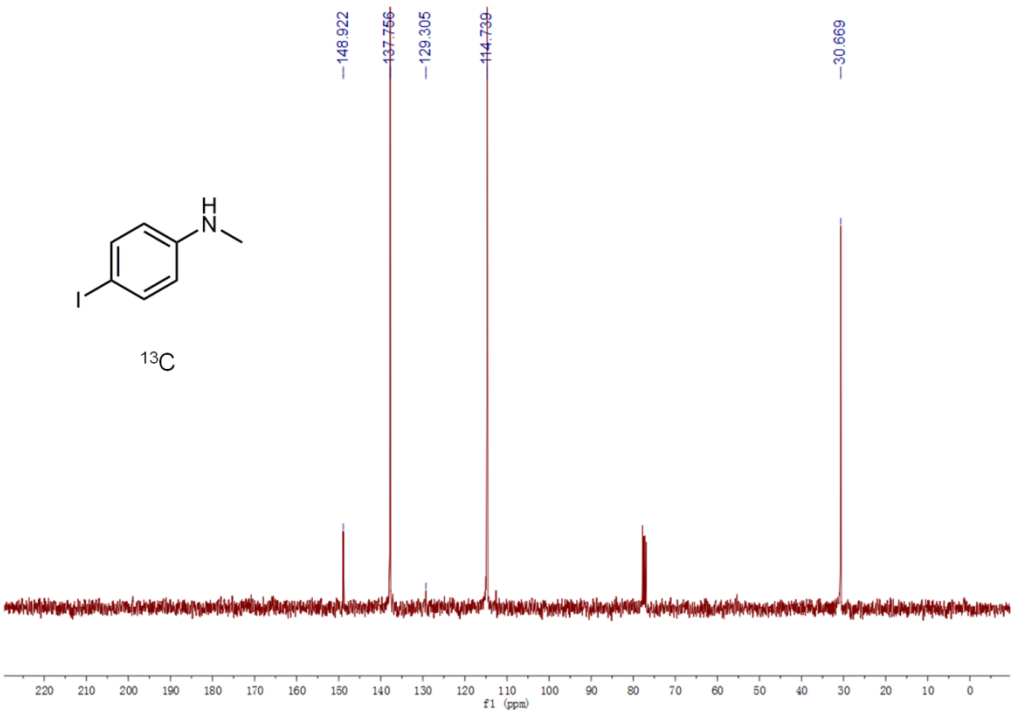
^{1}H


148.337
131.881
113.978
108.759
30.719
Br
H
N
f1 (ppm)

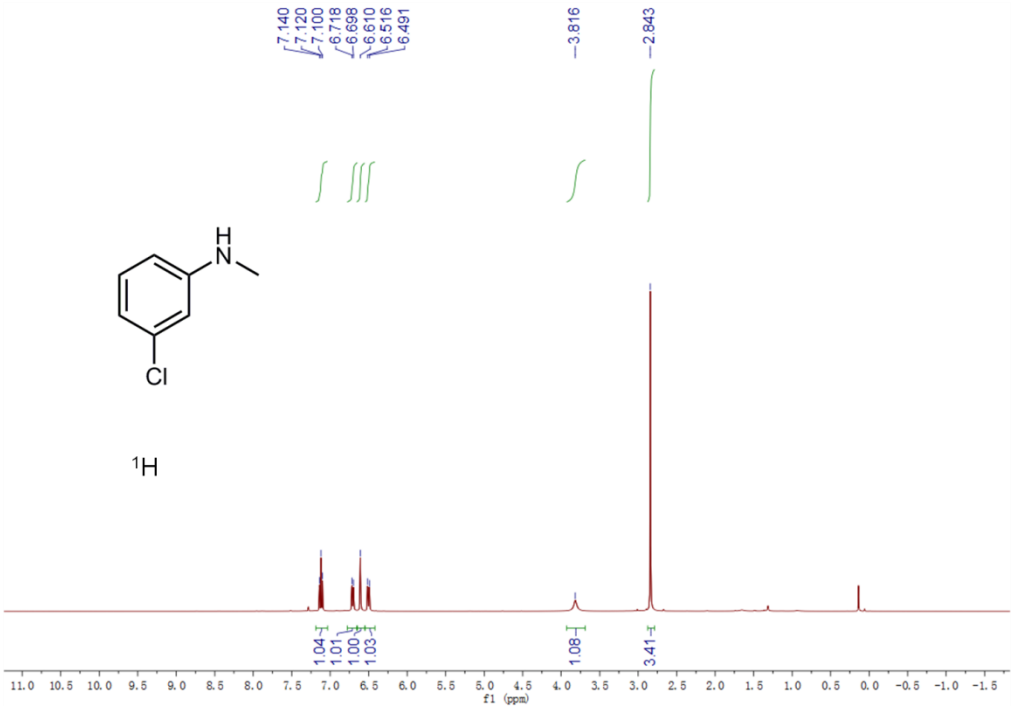
^{13}C

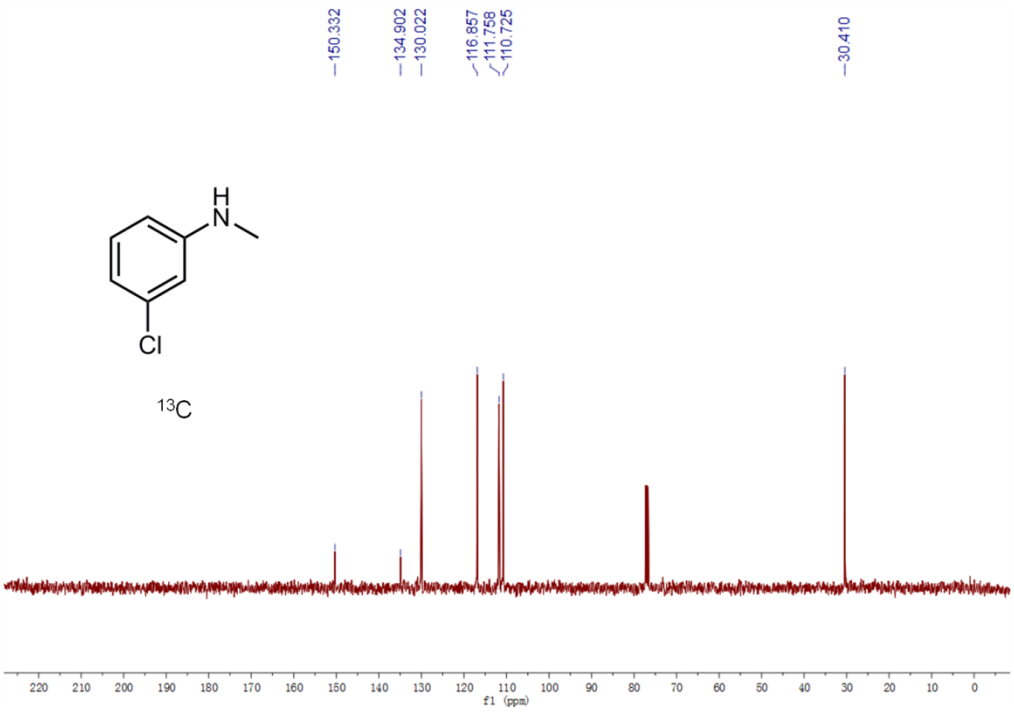

7.448
7.425
6.403
6.381
3.521
2.787
2.00
2.11
1.00
3.37
f1 (ppm)

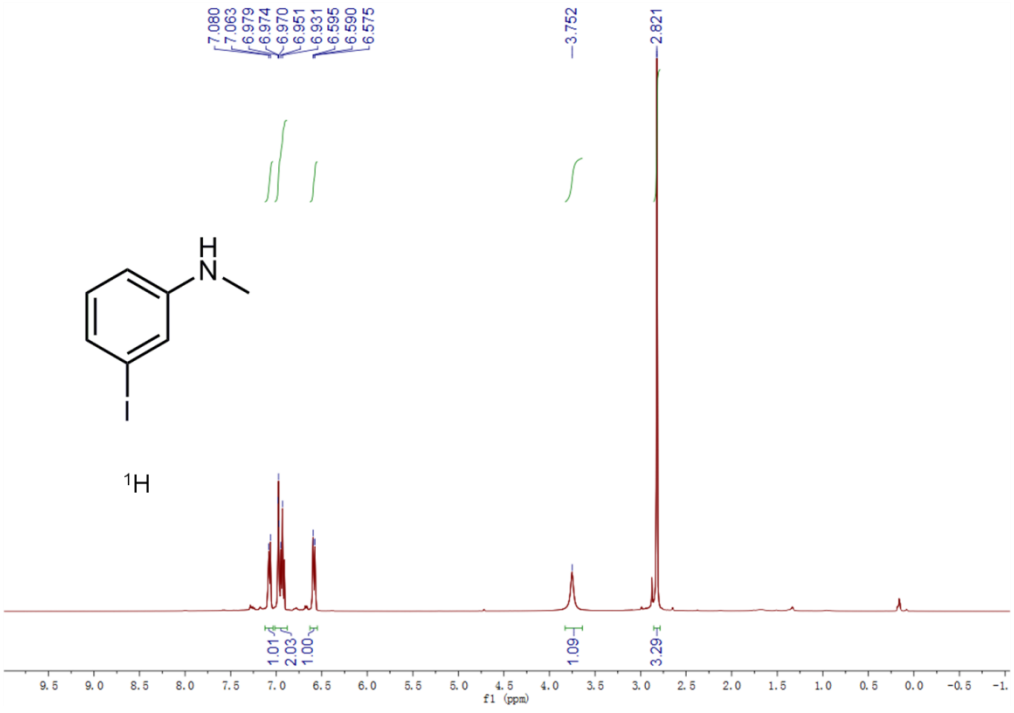
^{1}H

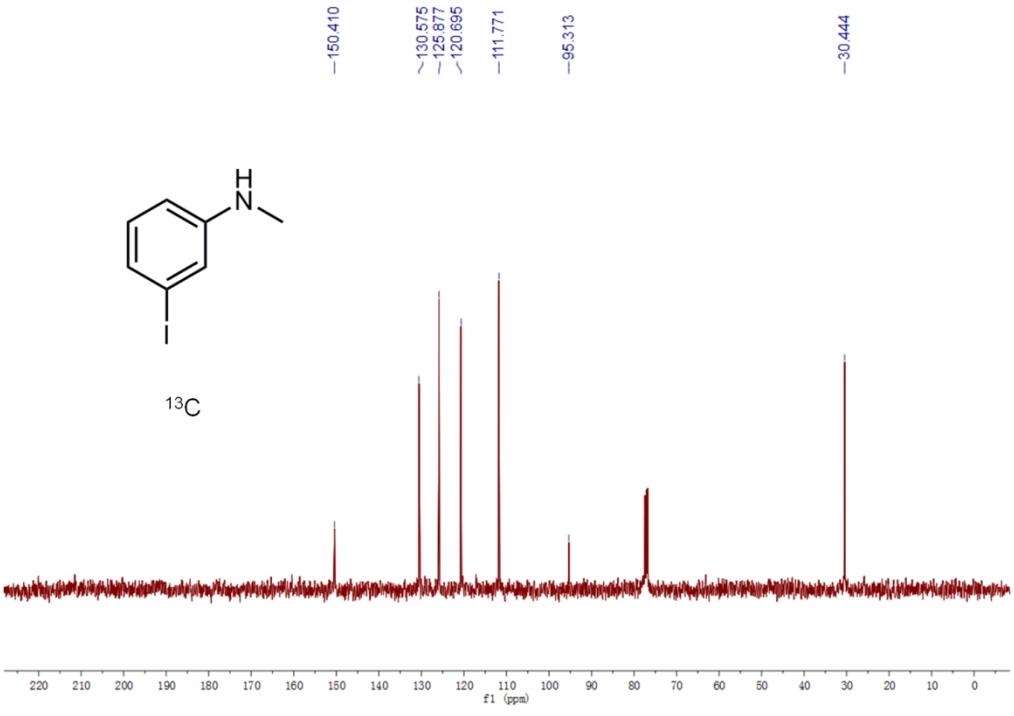

148.922
137.756
129.305
114.739
30.669
f1 (ppm)

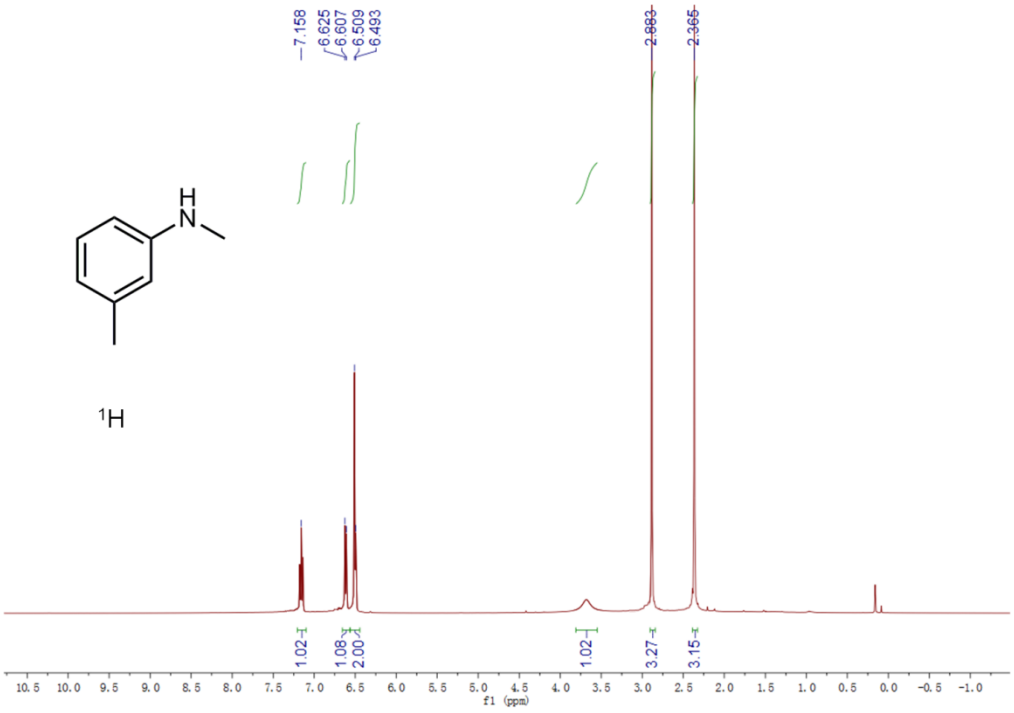
^{13}C

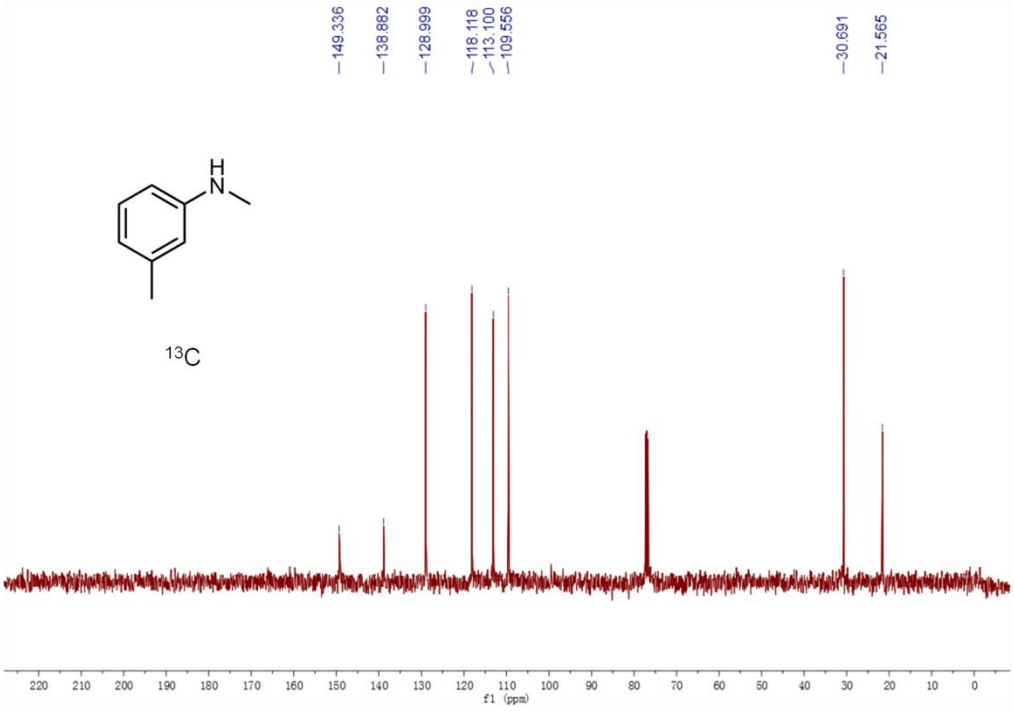

7.140
7.120
7.100
6.718
6.698
6.610
6.516
6.491
3.816
2.843
H
N
Cl
1H
1.04
1.01
1.00
1.03
1.08
3.41
f1 (ppm)

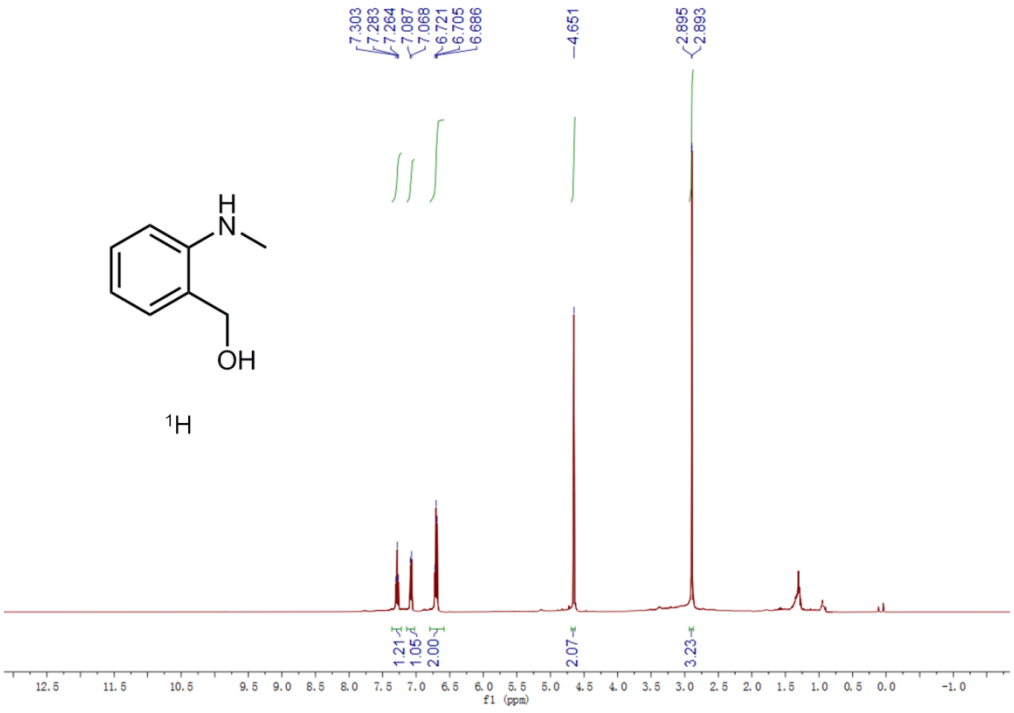

150.332
134.902
130.022
116.857
111.758
110.725
30.410
H
N
Cl
13C
f1 (ppm)

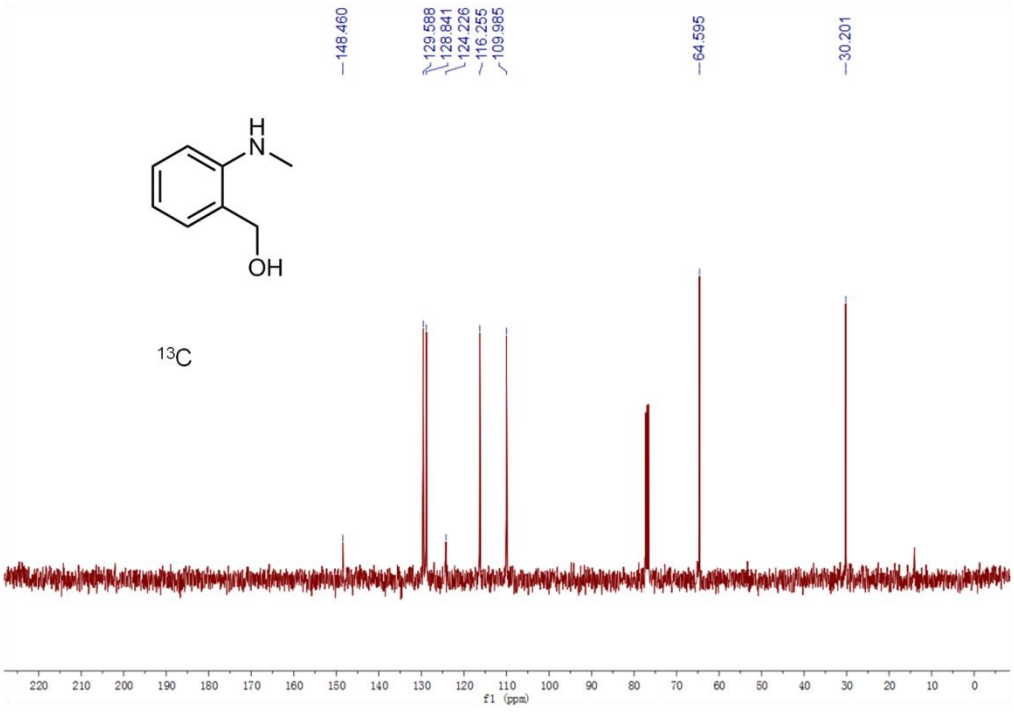

7.080
7.063
6.979
6.974
6.970
6.951
6.931
6.595
6.590
6.575
3.752
2.821
H
N
I
1H
1.01
2.03
1.00
1.09
3.29
f1 (ppm)

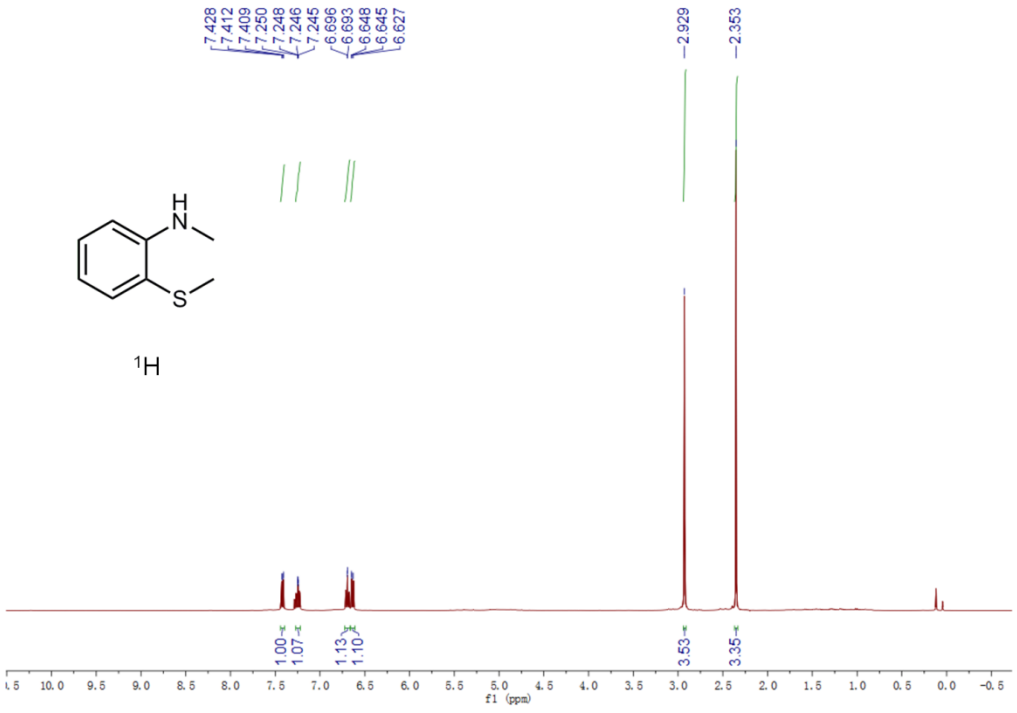

150.410
130.575
125.877
120.695
111.771
95.313
30.444
H
N
I
13C
f1 (ppm)


7.158
6.625
6.607
6.509
6.493
2.883
2.365
H
N
1H
1.02
1.08
2.00
1.02
3.27
3.15
f1 (ppm)

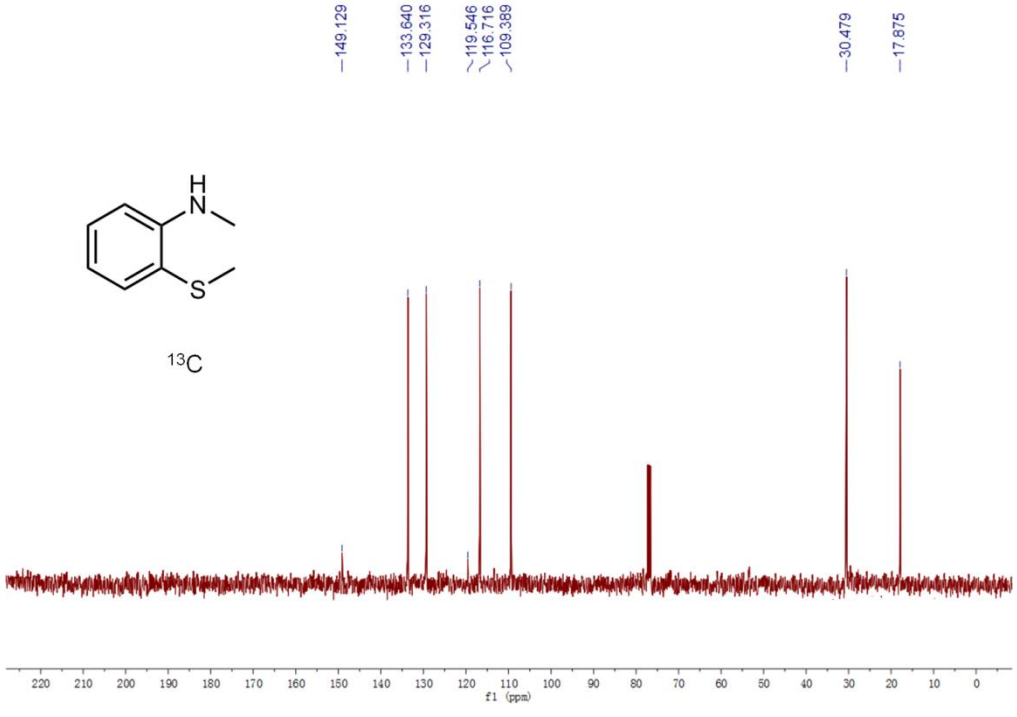

149.336
138.882
128.999
118.118
113.100
109.556
30.691
21.565
H
N
13C
f1 (ppm)


7.303
7.283
7.264
7.087
7.068
6.721
6.705
6.686
4.651
2.895
2.893
H
N
OH
1H
1.21
1.05
2.00
2.07
3.23
f1 (ppm)

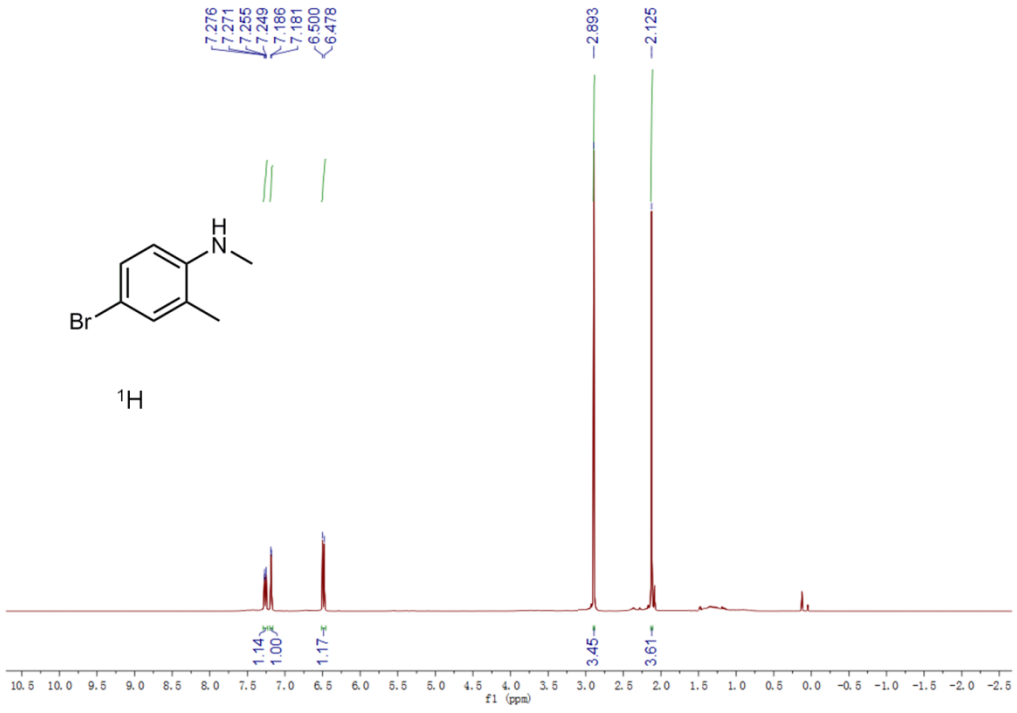

148.460
129.588
128.841
124.226
116.255
109.985
64.595
30.201
H
N
OH
13C
f1 (ppm)

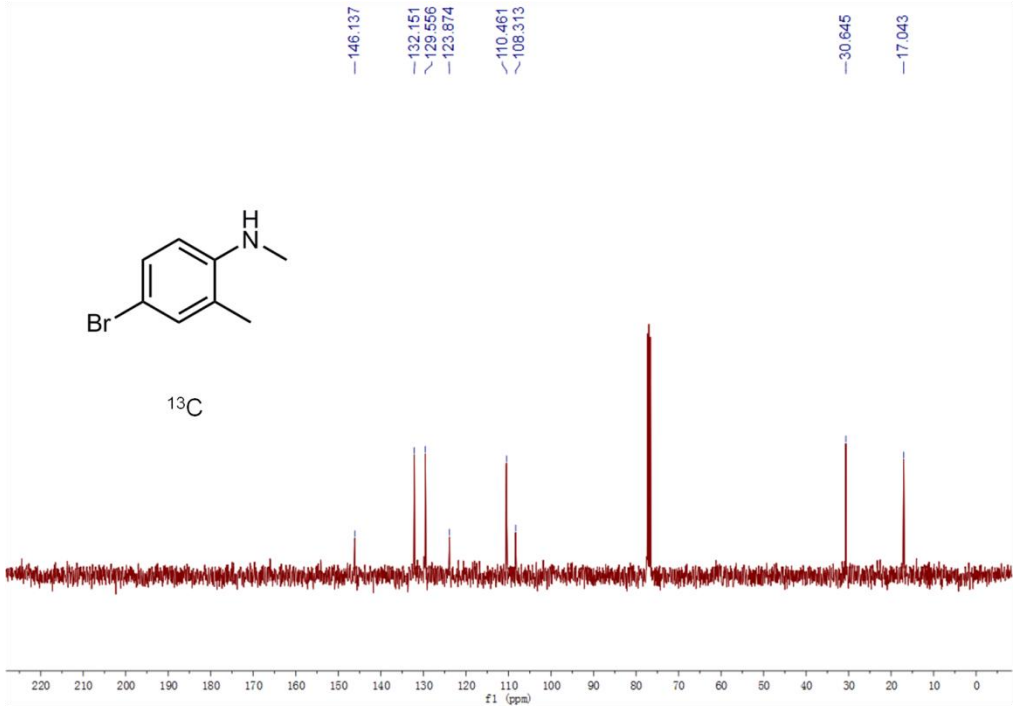

7.428
7.412
7.409
7.250
7.248
7.246
7.245
6.696
6.693
6.648
6.645
6.627
2.929
2.353
1.00
1.07
1.13
1.10
3.53
3.35
f1 (ppm)

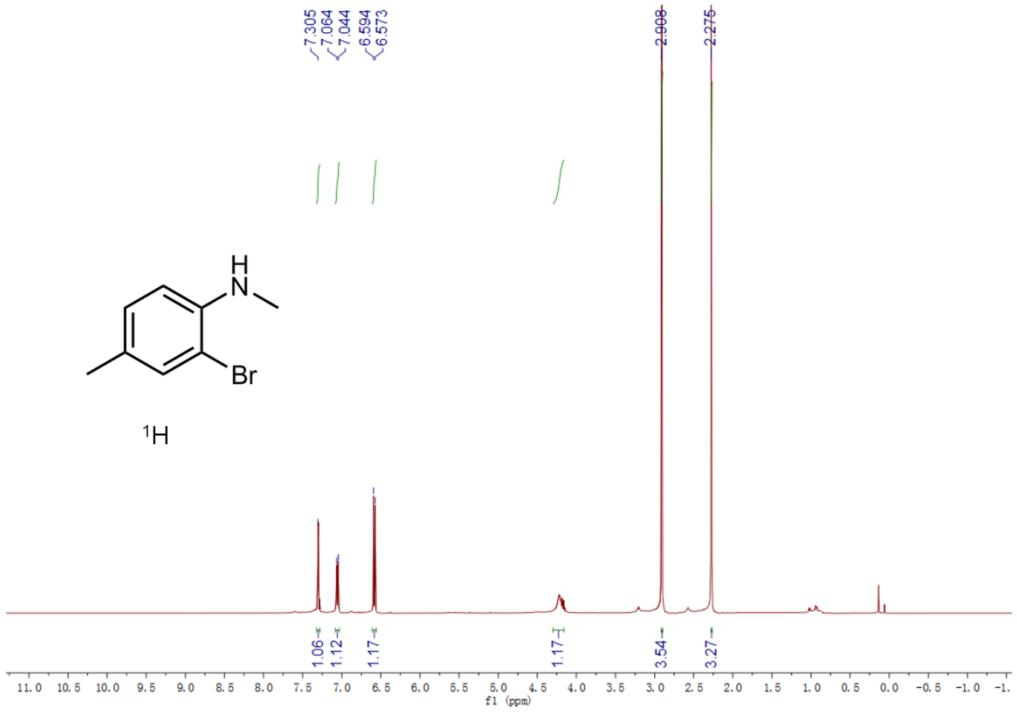
^{1}H

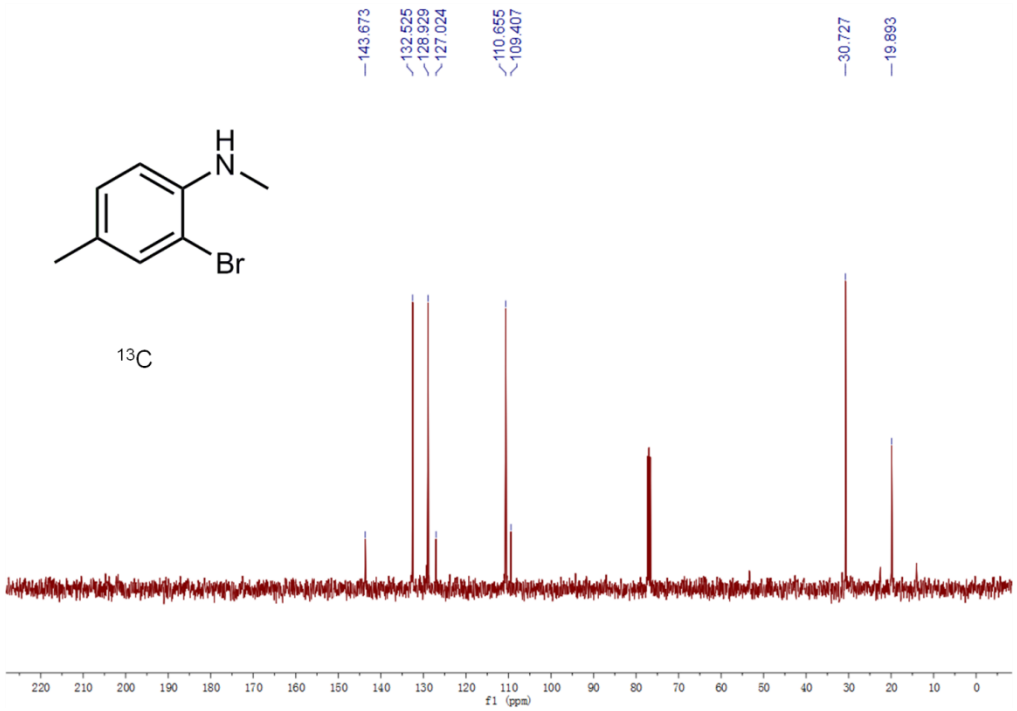

149.129
133.640
129.316
119.546
116.716
109.389
30.479
17.875
f1 (ppm)

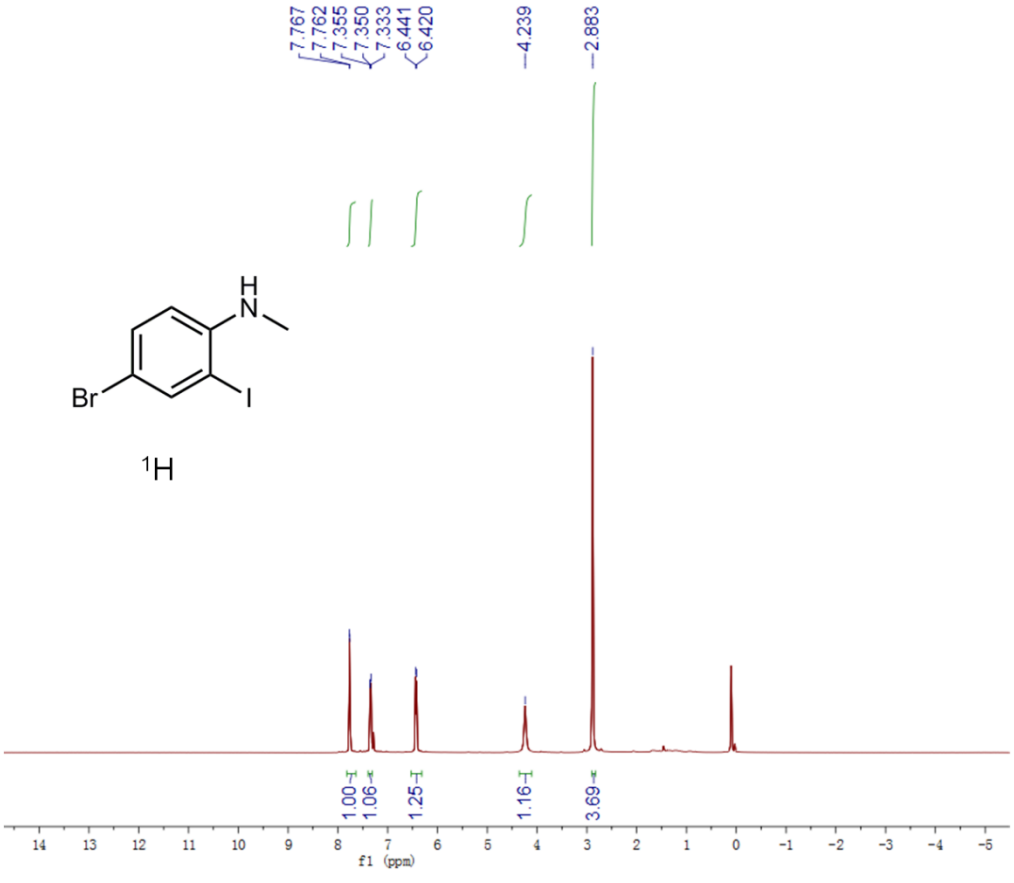
^{13}C


7.276
7.271
7.255
7.249
7.186
7.181
6.500
6.478
2.893
2.125
H
N
Br
1H
1.14
1.00
1.17
3.45
3.61
f1 (ppm)

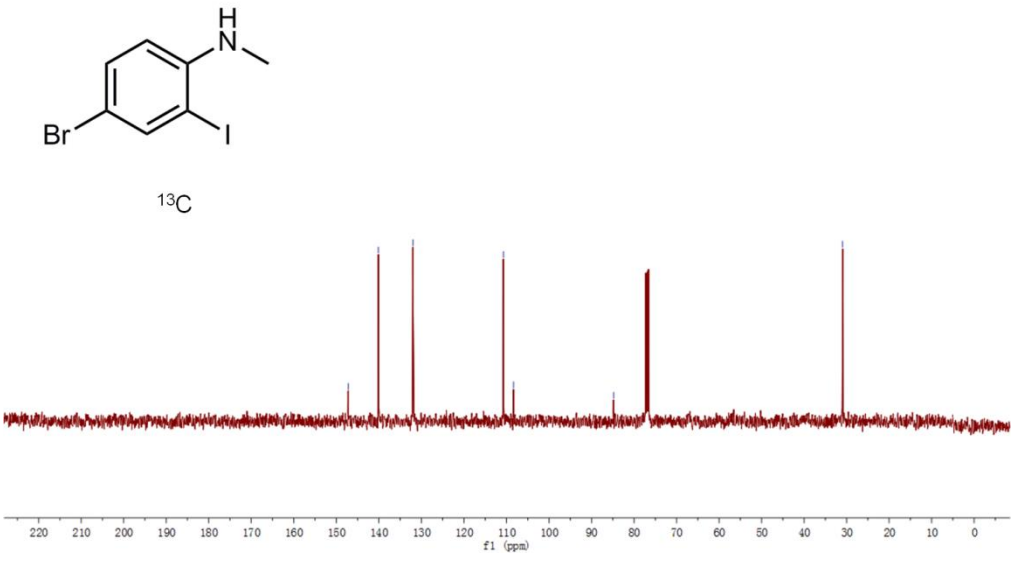

146.137
132.151
129.556
123.874
110.461
108.313
30.645
17.043
H
N
Br
13C
f1 (ppm)


7.305
7.064
7.044
6.594
6.573
2.908
2.275
H
N
Br
1H
1.06
1.12
1.17
1.17
3.54
3.27
f1 (ppm)

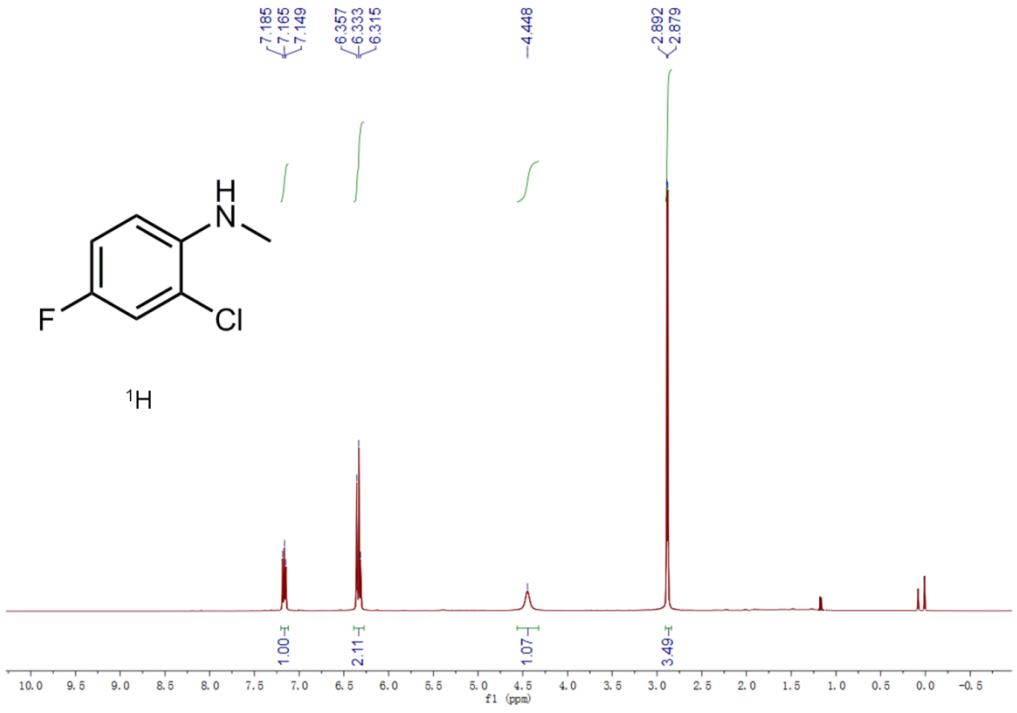

143.673
132.525
128.929
127.024
110.655
109.407
30.727
19.893
H
N
Br
13C
f1 (ppm)


7.767
7.762
7.355
7.350
7.333
6.441
6.420
4.239
2.883
H
N
Br
I
1.00
1.06
1.25
1.16
3.69
f1 (ppm)

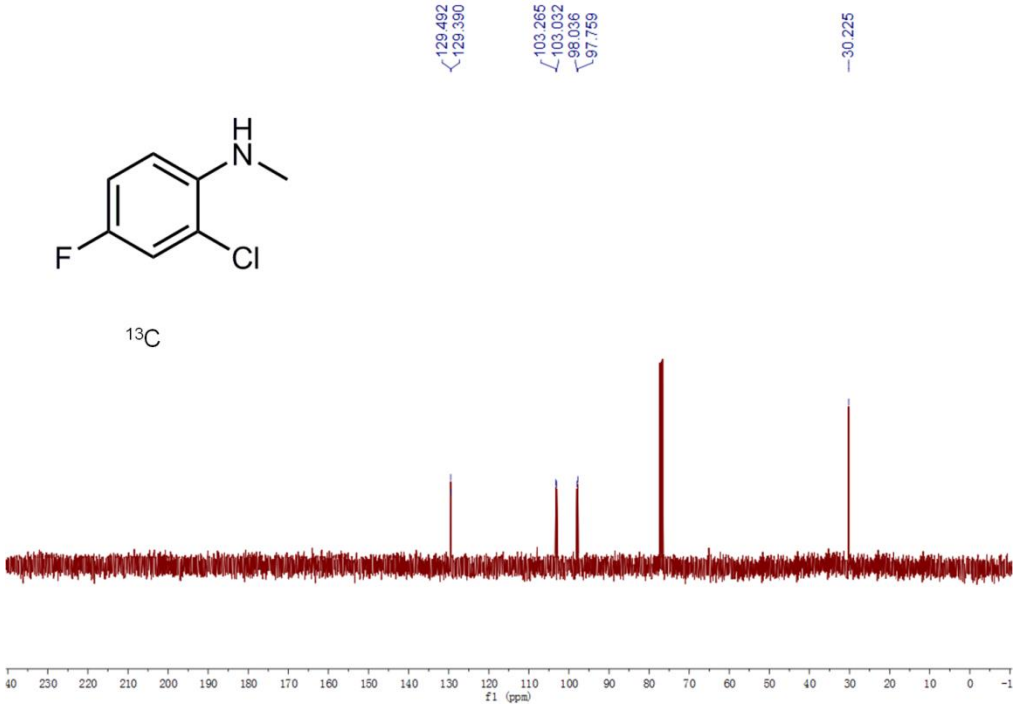
^{1}H


147.228
140.117
131.999
110.710
108.336
84.795
30.930
H
N
Br
I
f1 (ppm)

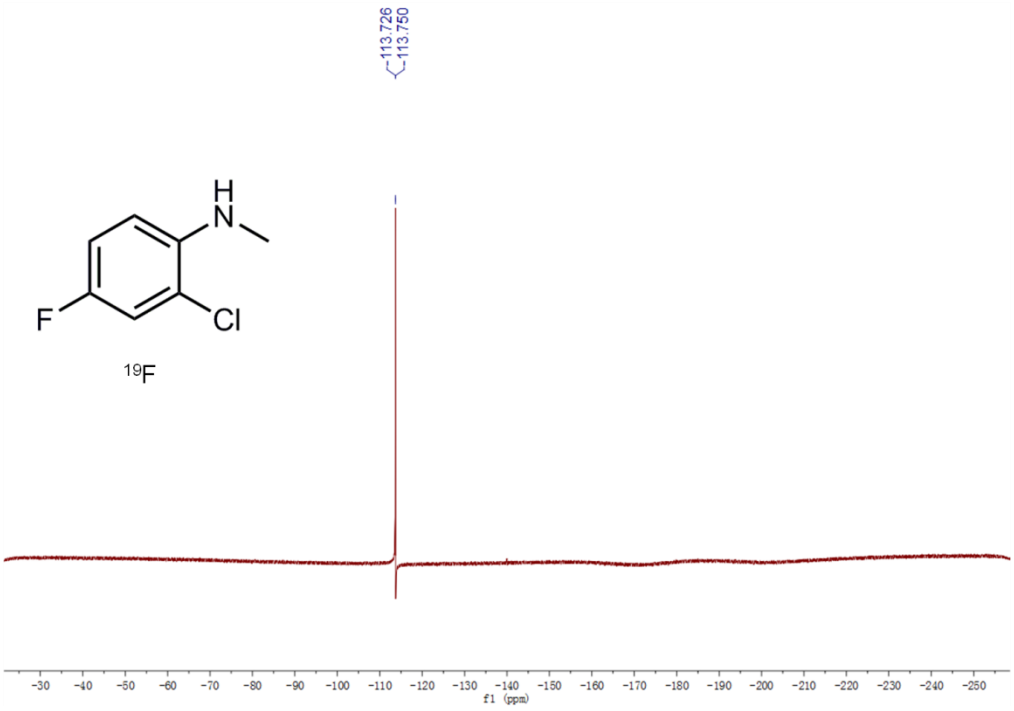
^{13}C

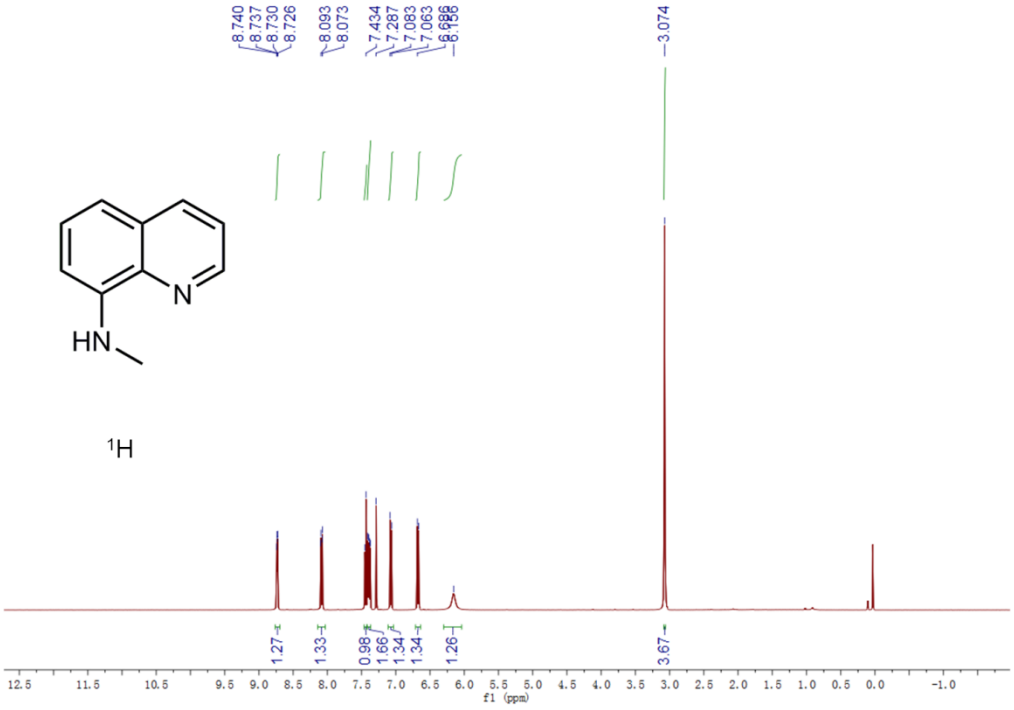

7.185
7.165
7.149
6.357
6.333
6.315
4.448
2.892
2.879
H
N
F
Cl
1.00
2.11
1.07
3.49
f1 (ppm)

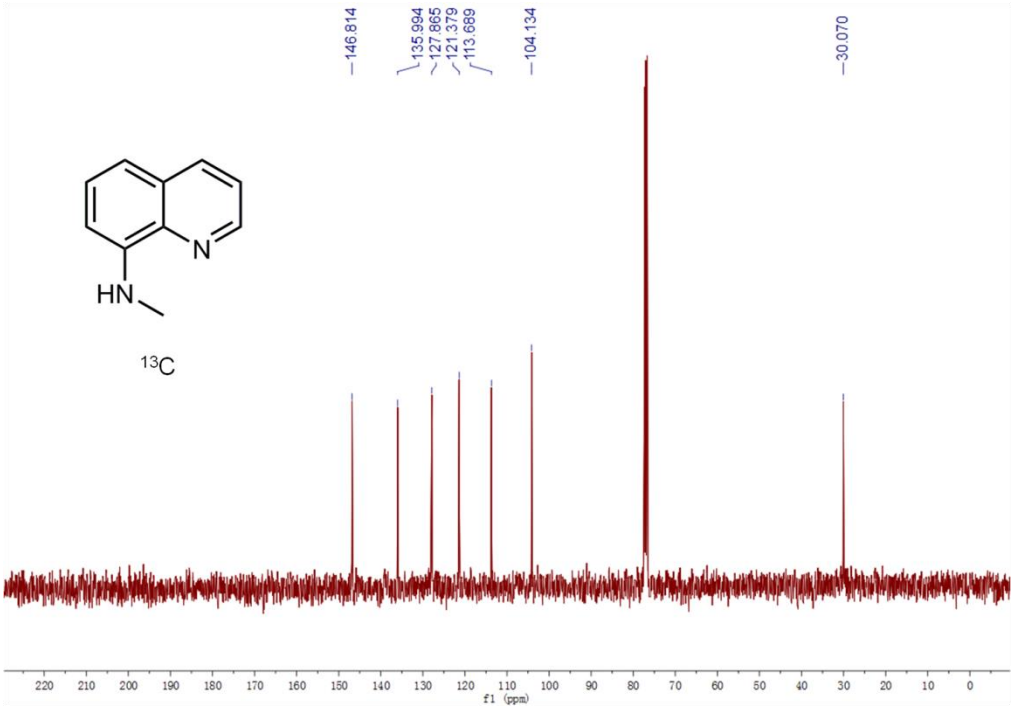
^{1}H

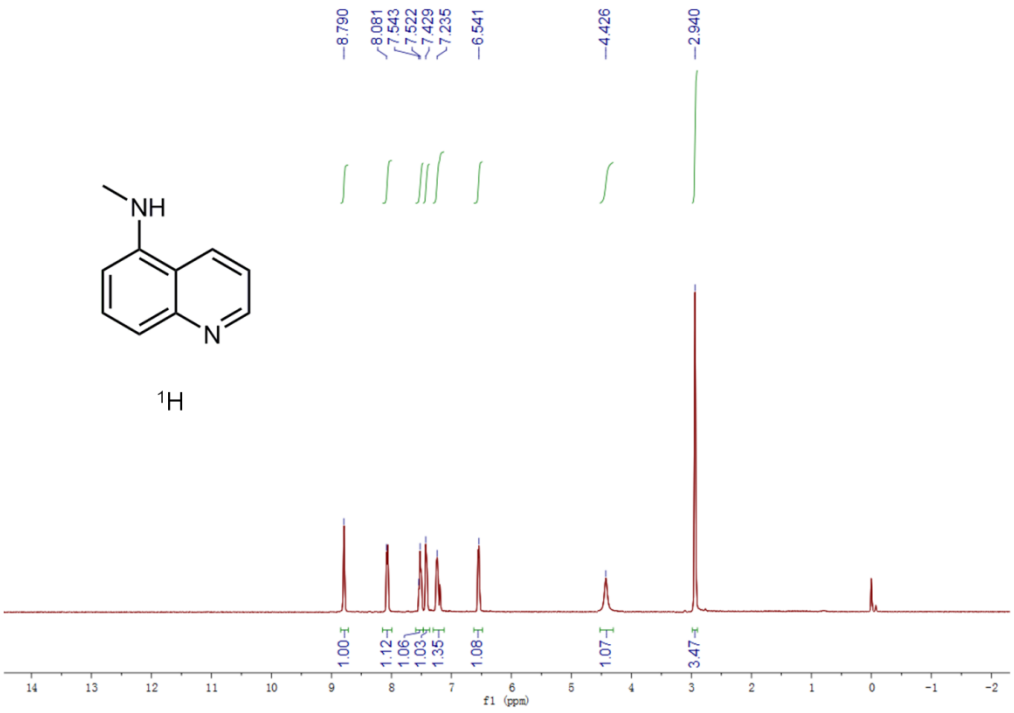

129.492
129.390
103.265
103.032
98.036
97.759
30.225
H
N
F
Cl
f1 (ppm)

^{13}C


113.726
113.750
H
N
F
Cl
19F
-30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240 -250
f1 (ppm)


8.740
8.737
8.730
8.726
8.093
8.073
7.434
7.287
7.083
7.063
3.074
N
HN
1H
1.27
1.33
0.98
1.66
1.34
1.34
1.26
3.67
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -1.0
f1 (ppm)


146.814
135.994
127.865
121.379
113.689
104.134
30.070
HN
N
13C
f1 (ppm)


8.790
8.081
7.543
7.522
7.429
7.235
6.541
4.426
2.940
NH
N
1H
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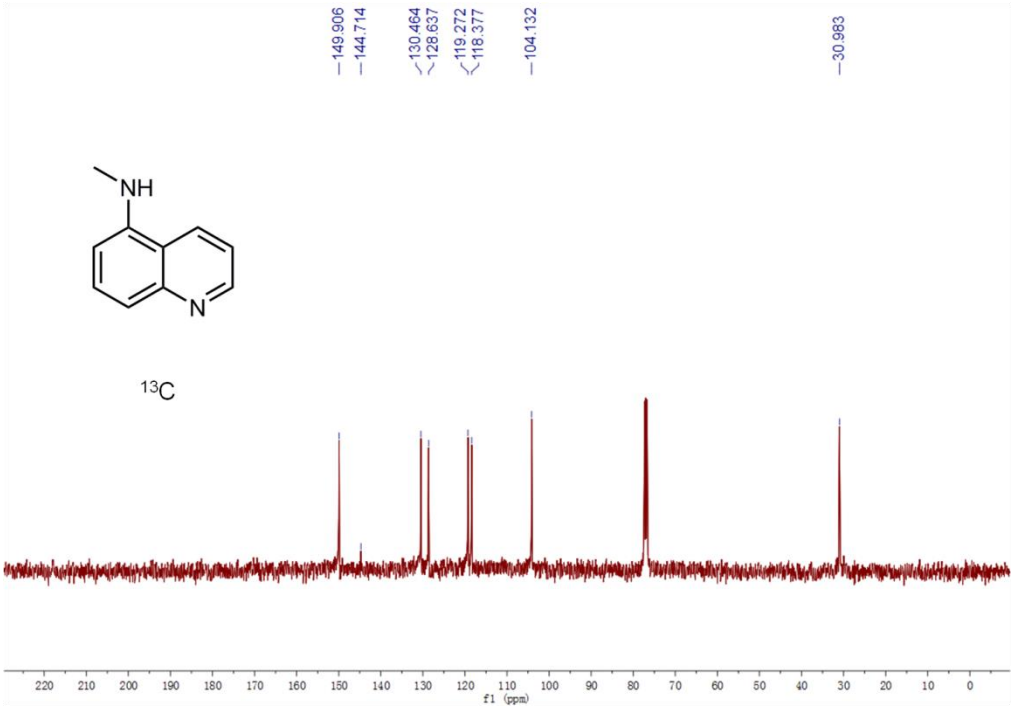
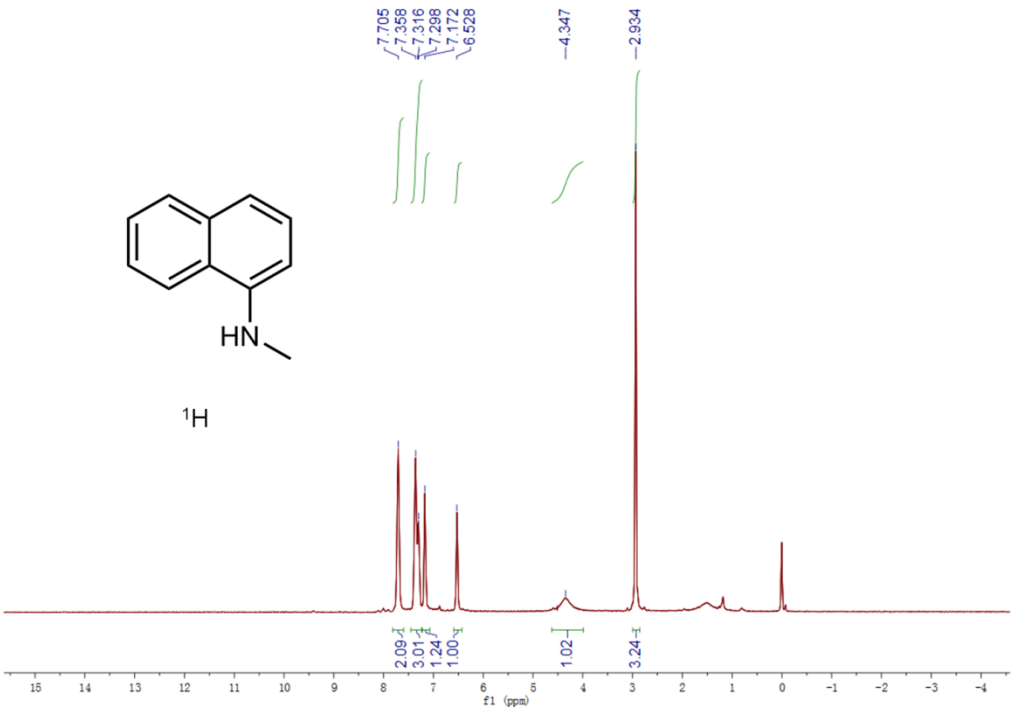
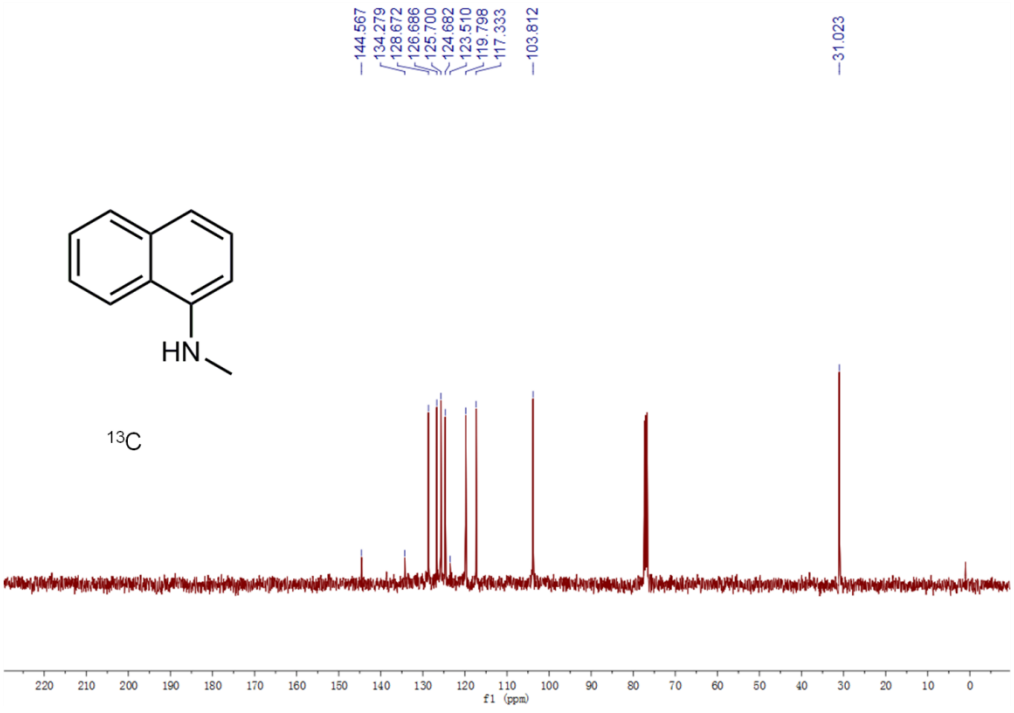
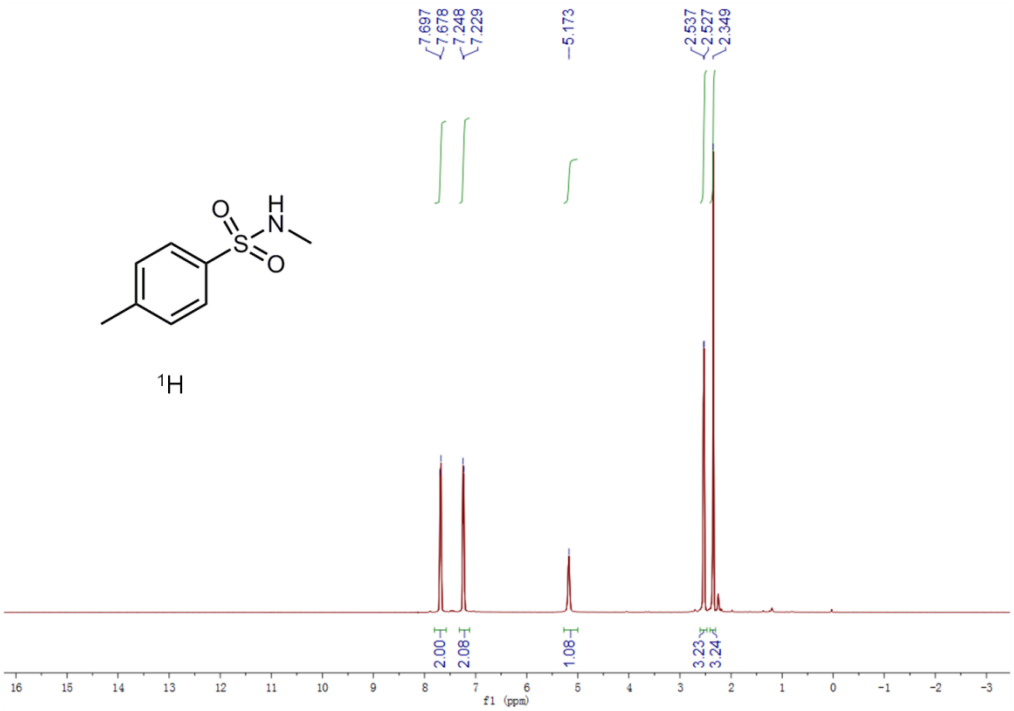
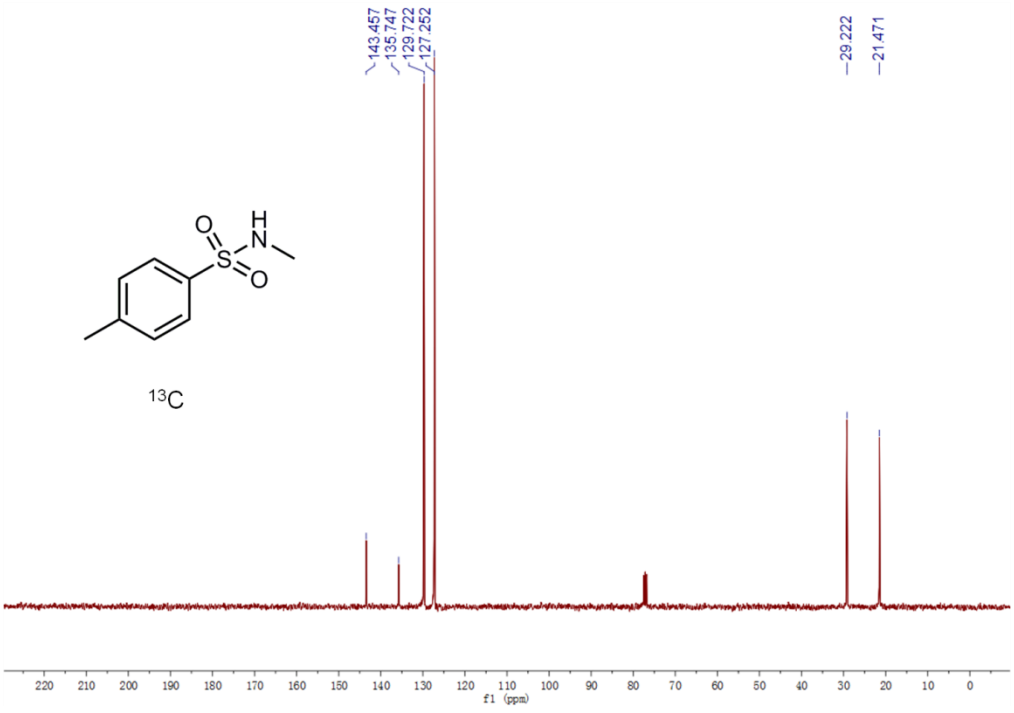
1.12
1.06
1.03
1.35
1.08
1.07
3.47
f1 (ppm)


149.906
144.714
130.464
128.637
119.272
118.377
104.132
30.983
NH
N
13C
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.705
7.358
7.316
7.298
7.172
6.528
4.347
2.934
HN
1H
2.09
3.01
1.24
1.00
1.02
3.24
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)


144.567
134.279
128.672
126.686
125.700
124.682
123.510
119.798
117.333
103.812
31.023
HN
13C
f1 (ppm)


7.697
7.678
7.248
7.229
5.173
2.537
2.527
2.349
O
S
O
H
N
1H
2.00
2.08
1.08
3.23
3.24
f1 (ppm)


143.457
135.747
129.722
127.252
29.222
21.471
O
H
N
S
O
^{13}C
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)