Supporting Information

Selective synthesis of (1H-benzo[d]imidazol-2-yl)(phenyl)-methanone and quinoxaline from aromatic aldehyde and o-phenylenediamine

Experimental section

General experimental details

^{1}H-NMR spectra were recorded at 400 MHz. Chemical shifts (in ppm) were referenced to $CDCl_3$ (δ = 7.26 ppm) or DMSO-d_6 (δ = 2.50 ppm) in as an internal standard. ^{13}C-NMR spectra were obtained at 100 MHz and were calibrated with $CDCl_3$ (δ = 77.0 ppm) or DMSO-d_6 (δ = 39.5 ppm). Products were purified by flash chromatography on 200–300 mesh silica gels. Unless otherwise noted, commercially available reagents and solvents were used without further purification.

Typical procedure for the preparation of (1H-benzo[d]imidazol-2-yl)(phenyl)methanone (3aa) and 2-phenylquinoxaline(4aa)

1. (1H-benzo[d]imidazol-2-yl)(phenyl)methanone (3aa)

A mixture of and o-phenylenediamine (1a, 0.2 mmol), phenylacetaldehyde (2a, 0.24 mmol), S_8 (300 mol %), in DMF (2.0 mL) under the air. The reaction mixture was stirred at 100 ^{o}C (oil bath temperature) for 10 h. After cooling to room temperature, the solvent was extracted with ethyl acetate and washed with brine, dried with Na_2SO_4. The solvent was evaporated in vacuo, the residues were purified by column chromatography, eluting with petroleum ether / ethyl acetate(15:1) to afford pure **3aa**.

The crystal data for 3aa

Formula sum	C14 H10 N2 O
Formula weight	222.24 g/mol
Crystal system	orthorhombic
Space-group	P b c a (61)
Cell parameters	a=14.761(3) Å b=9.9736(8) Å c=15.8257(19) Å
Cell ratio	a/b=1.4800 b/c=0.6302 c/a=1.0721
Cell volume	2329.86(50) Å^3
Z	8
Calc. density	1.26708 g/cm^3
RAll	0.1334
Pearson code	oP216
Formula type	NO2P10Q14
Wyckoff sequence	c27

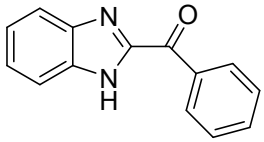
CCDC 1910163

2. 2-phenylquinoxaline(4aa)

Mix $NaHCO_3$ (0.4 mmol), o-phenylenediamine (1a, 0.2 mmol), phenylacetaldehyde (2a, 0.24 mmol), in 1,4-dioxane (2.0 mL) under the O_2 atmosphere(1 atm).The reaction mixture was stirred at 80 ^{o}C for 4

h. After cooling down to room temperature and concentrating in vacuum, the residues were purified by column chromatography, eluting with petroleum ether / ethyl acetate(40:1) to afford pure **4aa**.

Analytical data for products



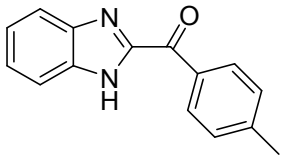
(1H-benzo[d]imidazol-2-yl)(phenyl)methanone (3aa)

mp = 222-223 ^{o}C; yield 85%

^{1}H NMR (300 MHz, $CDCl_3$) δ 10.92 (s, 1H), 8.75 – 8.64 (m, 2H), 7.98 (s, 1H), 7.72 – 7.51 (m, 4H), 7.42 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 184.16, 147.73, 143.96, 135.37, 133.97, 133.22, 131.35, 128.58, 126.51, 123.81, 122.29, 112.06.

HRMS calcd for $C_{14}H_{11}N_2O$ $[M+H]^+$223.0863, found 223.0866.



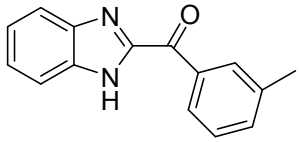
(1H-benzo[d]imidazol-2-yl)(p-tolyl)methanone (3ab)

mp = 263-264 ^{o}C; yield 71%

^{1}H NMR (300 MHz, DMSO) δ 13.50 (s, 1H), 8.51 (d, *J* = 8.2 Hz, 2H), 7.86 (s, 1H), 7.62 (s, 1H), 7.40 (d, *J* = 8.1 Hz, 4H), 2.40 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 183.51, 147.95, 145.05, 143.97, 133.05, 132.81, 131.45, 129.33, 126.34, 123.70, 122.26, 111.93, 21.93.

HRMS calcd for $C_{15}H_{13}N_2O$ $[M+H]^+$ 237.1019, found 237.1023.



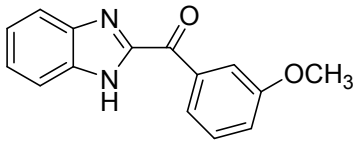
(1H-benzo[d]imidazol-2-yl)(m-tolyl)methanone (3ac)

mp = 162-163 ^oC; yield 60%

^1H NMR (400 MHz, $CDCl_3$) δ 11.01 (s, 1H), 8.55 – 8.35 (m, 2H), 7.98 (s, 1H), 7.60 (s, 1H), 7.51 – 7.34 (m, 4H), 2.46 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 184.39, 147.85, 138.30, 135.43, 134.77, 133.28, 131.53, 128.73, 128.45, 126.39, 124.07, 123.74, 122.25, 112.05, 21.47.

HRMS calcd for $C_{15}H_{13}N_2O$ $[M+H]^+$ 237.1020, found 237.1023.



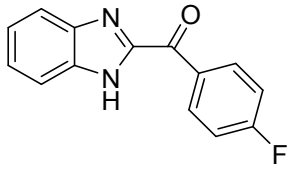
(1H-benzo[d]imidazol-2-yl)(3-methoxyphenyl)methanone (3ad)

mp = 205-208 ^oC; yield 65%

^1H NMR (300 MHz, DMSO) δ 13.44 (s, 1H), 8.17 (d, *J* = 7.7 Hz, 1H), 8.02 (s, 1H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.47 (t, *J* = 8.0 Hz, 1H), 7.28 (ddd, *J* = 11.1, 10.1, 4.3 Hz, 3H), 3.79 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 183.74, 159.57, 147.70, 136.52, 129.63, 126.38, 124.36, 123.80, 122.36, 120.66, 117.03, 115.08, 111.96, 99.98, 55.53.

HRMS calcd for $C_{15}H_{13}N_2O_2$ $[M+H]^+$ 253.0970, found 253.0972.



(1H-benzo[d]imidazol-2-yl)(4-fluorophenyl)methanone (3ae)

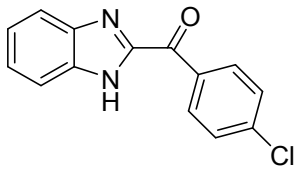
mp = 189-191 ^oC; yield 44%

^1H NMR (400 MHz, $CDCl_3$) δ 10.77 (s, 1H), 8.87 – 8.79 (m, 2H), 7.97 (d, *J* = 8.0 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.43 (dt, *J* = 15.0, 6.9 Hz, 2H), 7.27 – 7.22 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 182.28, 166.43 (d, *J* = 256.7 Hz), 147.56, 143.91, 134.27 (d, *J* = 9.5 Hz), 133.13, 131.68 (d, *J* = 2.9 Hz), 126.62, 123.92, 122.25, 115.82 (d, *J* = 21.8 Hz), 112.05.

^{19}F NMR (376 MHz, $CDCl_3$) δ -103.39 (tt, *J* = 8.4, 5.5 Hz).

HRMS calcd for $C_{14}H_{10}FN_2O$ $[M+H]^+$ 241.0769, found 241.0772.



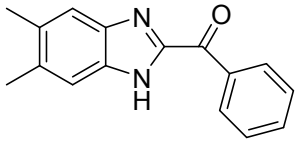
(1H-benzo[d]imidazol-2-yl)(4-chlorophenyl)methanone (3af)

mp = 148-150 ^oC; Yield 52%

^1H NMR (400 MHz, $CDCl_3$) δ 10.65 (s, 1H), 8.74 – 8.67 (m, 2H), 7.99 – 7.94 (m, 1H), 7.60 (d, *J* = 8.1 Hz, 1H), 7.57 – 7.52 (m, 2H), 7.49 – 7.44 (m, 1H), 7.43 – 7.37 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 182.60, 147.46, 143.90, 140.65, 133.62, 133.13, 132.79, 128.92, 126.71, 123.97, 122.32, 112.02.

HRMS calcd for $C_{14}H_{10}ClN_2O$ $[M+H]^+$ 257.0475, found 257.0476.



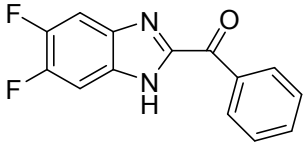
(5,6-dimethyl-1H-benzo[d]imidazol-2-yl)(phenyl)methanone (3ag)

mp = 199-200 ^{o}C; Yield 74%

^{1}H NMR (400 MHz, $CDCl_3$) δ 11.00 (s, 1H), 8.71 – 8.61 (m, 2H), 7.70 (s, 1H), 7.63 (t, *J* = 7.4 Hz, 1H), 7.54 (t, *J* = 7.6 Hz, 2H), 7.32 (s, 1H), 2.38 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 184.19, 147.17, 142.83, 136.57, 135.66, 133.70, 133.30, 132.07, 131.30, 128.48, 121.66, 111.87, 20.84, 20.62.

HRMS calcd for $C_{16}H_{15}N_2O$ $[M+H]^+$ 251.1179, found 251.1179.



(5,6-difluoro-1H-benzo[d]imidazol-2-yl)(phenyl)methanone (3ah)

mp = 232-233 ^{o}C; Yield 63%

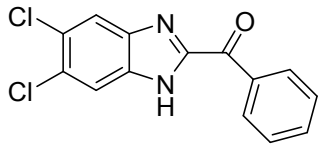
^{1}H NMR (400 MHz, DMSO) δ 13.79 (s, 1H), 8.58 – 8.51 (m, 2H), 8.00 (s, 1H), 7.79 – 7.72 (m, 1H), 7.63 (m, 3H).

^{13}C NMR (101 MHz, DMSO) δ 183.24, 150.07, 138.92 (d, *J* =

10.2 Hz), 135.69, 134.22, 131.30, 130.33 (d, *J* = 11.9 Hz), 128.89, 108.79 (d, *J* = 18.0 Hz), 100.74 (d, *J* = 21.6 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -135.01 (ddd, *J* = 20.3, 9.3, 7.4 Hz), -139.89 (ddd, *J* = 20.3, 10.2, 6.9 Hz).

HRMS calcd for $C_{14}H_9F_2N_2O$ $[M+H]^+$ 259.0674, found 259.0678.



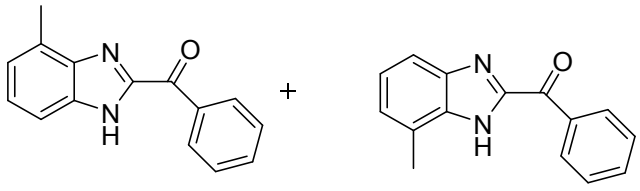
(5,6-dichloro-1H-benzo[d]imidazol-2-yl)(phenyl)methanone (3ai)

mp = 266-268 °C; Yield 40%

^{1}H NMR (300 MHz, DMSO) δ 12.97 (s, 1H), 7.72 (d, *J* = 6.2 Hz, 2H), 7.38 (s, 1H), 6.97 (d, *J* = 3.8 Hz, 1H), 6.93 (d, *J* = 7.0 Hz, 1H), 6.81 (m, 2H).

^{13}C NMR (101 MHz, DMSO) δ 183.59, 150.28, 138.53, 135.61, 134.37, 131.98, 131.32, 129.18, 128.92, 127.39, 118.92.

HRMS calcd for $C_{14}H_9Cl_2N_2O$ $[M+H]^+$ 291.0081, found 291.0087.



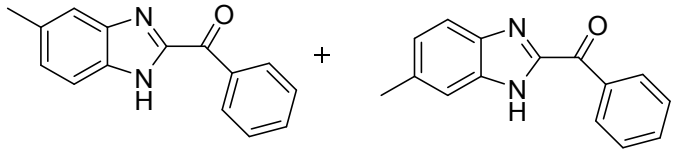
Mixture of (4-methyl-1H-benzo[d]imidazol-2-yl)(phenyl)methanone and (7-methyl-1H-benzo[d]imidazol-2-yl)(phenyl)methanone (3aj)

mp = 163-164 °C; Yield 80%

^{1}H NMR (300 MHz, $CDCl_3$) δ 11.09 (s, 0.5H), 11.05 (s, 0.5H), 8.79 (d, *J* = 7.5 Hz, 1H), 8.69 (d, *J* = 7.5 Hz, 1H), 7.81 (d, *J* = 8.1 Hz, 0.5H), 7.66 (dd, *J* = 8.5, 6.1 Hz, 1H), 7.56 (t, *J* = 7.5 Hz, 2H), 7.41 (d, *J* = 8.1 Hz, 0.5H), 7.32 (dd, *J* = 11.6, 7.4 Hz, 1H), 7.19 (dd, *J* = 16.8, 7.2 Hz, 1H), 2.76 (s, 1.5H), 2.60 (s, 1.5H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 184.73, 184.04, 147.52, 147.13, 143.73, 143.71, 135.62, 133.93, 133.41, 133.12, 132.59, 131.61, 131.45, 130.98, 128.87, 128.53, 126.74, 126.41, 123.99, 123.65, 122.19, 119.65, 109.46, 109.43, 17.15, 16.87.

HRMS calcd for $C_{15}H_{13}N_2O$ $[M+H]^+$ 237.1018, found 237.1023.



Mixture of (5-methyl-1H-benzo[d]imidazol-2-yl)(phenyl)methanone and (6-methyl-1H-benzo[d]imidazol-2-yl)(phenyl)methanone (3ak)

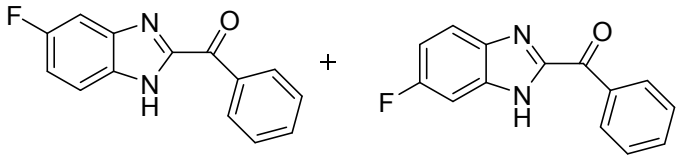
mp = 144-145 ^{o}C; Yield 78%

^{1}H NMR (300 MHz, CDCl3) δ 10.84 (s, 0.5H), 10.76 (s, 0.5H), 8.71 – 8.63 (m, 2H), 7.88 – 7.73 (m, 1H), 7.70 – 7.62 (m, 1H), 7.60 – 7.53 (m, 2H), 7.51 – 7.35 (m, 1H), 7.24 (m, 8.4 Hz, 1H), 2.52 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 184.15, 184.10, 147.71, 147.41, 144.37, 144.37, 142.21, 142.21, 137.04, 137.04, 135.49, 135.49, 133.82, 133.55, 131.32, 131.28, 128.54, 128.44, 125.89, 125.89,

121.74, 121.57, 111.56, 111.56, 22.14, 21.78.

HRMS calcd for $C_{15}H_{13}N_2O$ $[M+H]^+$ 237.1017, found 237.1023.



Mixture of (5-fluoro-1H-benzo[d]imidazol-2-yl)(phenyl)methanone and (6-fluoro-1H-benzo[d]imidazol-2-yl)(phenyl)methanone (3al)

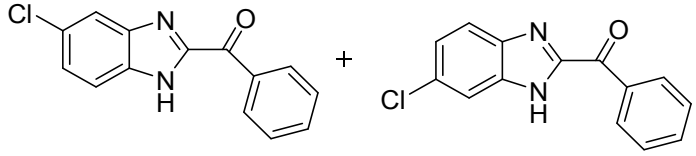
mp = 177-179 ^oC; Yield 80%

^1H NMR (400 MHz, $CDCl_3$) δ 11.30 (s, 1H), 8.68 (m, 2H), 7.91 (m, 1H), 7.69 – 7.62 (m, 1H), 7.56 (m, 2H), 7.30 – 7.10 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 184.17, 184.08, 161.75 (d, *J* = 245.6 Hz), 148.48, 140.50, 135.18, 134.16, 133.72 (d, *J* = 14.1 Hz), 131.36, 128.62, 123.42 (d, *J* = 10.1 Hz), 115.73 (d, *J* = 21.5 Hz), 113.24 (d, *J* = 25.2 Hz), 112.87 (d, *J* = 6.7 Hz), 107.16 (d, *J* = 27.3 Hz), 98.28 (d, *J* = 27.6 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -113.11 (td, *J* = 9.0, 4.9 Hz), -117.98 (td, *J* = 9.1, 4.5 Hz).

HRMS calcd for $C_{14}H_{10}FN_2O$ $[M+H]^+$ 241.0068, found 241.0072.



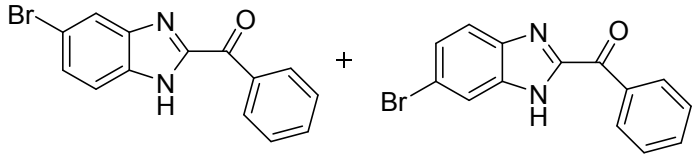
Mixture of (5-chloro-1H-benzo[d]imidazol-2-yl)(phenyl)methanone and (6-chloro-1H-benzo[d]imidazol-2-yl)(phenyl)methanone (3am)

mp = 191-192 ^{o}C; Yield 70%

^{1}H NMR (300 MHz, DMSO) δ 12.54 (s, 0.5H), 12.48 (s, 0.5H), 7.38 (m, 2H), 6.88 – 6.68 (m, 0.5H), 6.57 (m, 1H), 6.44 (m, 3H), 6.20 (s, 1H), 6.18 (s, 0.5H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 183.78, 183.74, 148.68, 148.37, 144.63, 142.52, 135.10, 135.06, 134.23, 134.17, 133.63, 132.33, 131.67, 131.36, 131.31, 129.35, 128.64, 128.63, 127.14, 124.89, 123.22, 121.78, 112.88, 111.90.

HRMS calcd for $C_{14}H_{10}ClN_2O$ $[M+H]^+$ 257.0472, found 257.0476



Mixture of (5-bromo-1H-benzo[d]imidazol-2-yl)(phenyl)methanone and (6-bromo-1H-benzo[d]imidazol-2-yl)(phenyl)methanone (3an)

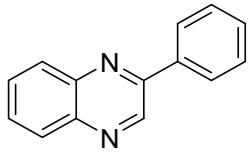
mp = 201-202^{o}C; Yield 86%

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.87 (s, 0.5H), 10.80 (s, 0.5H), 8.68 (d, J = 8.2 Hz, 2H), 8.13 (s, 0.5H), 7.84 (m, 0.5H), 7.76 (m, 0.5H), 7.71 – 7.65 (m, 1H), 7.57 (m, 2H), 7.54 (m, 0.5H), 7.51 – 7.46 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 183.80, 183.79, 148.46, 148.18, 145.11, 142.81, 135.10, 135.05, 134.26, 134.07, 132.01, 132.00, 131.37, 131.32, 131.25, 129.64, 128.64, 127.48, 124.92, 123.53,

120.06, 116.71, 114.99, 113.29.

HRMS calcd for $C_{14}H_{10}BrN_2O$ $[M+H]^+$ 300.9968, found 300.9971

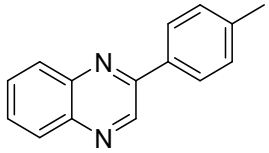


2-phenylquinoxaline(4aa)[1]

Yield: 83%

^1H NMR (400 MHz, $CDCl_3$) δ 9.33 (s, 1H), 8.22 – 8.10 (m, 4H), 7.82 – 7.71 (m, 2H), 7.60 – 7.51 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.86, 143.40, 142.30, 141.59, 136.78, 130.31, 130.21, 129.64, 129.57, 129.18, 129.14, 127.57.

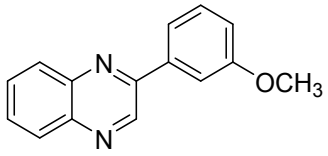


2-(p-tolyl)quinoxaline(4ab)[2]

Yield: 90%

^1H NMR (400 MHz, $CDCl_3$) δ 9.31 (s, 1H), 8.16 – 8.12 (m, 1H), 8.12 – 8.08 (m, 3H), 7.75 (m, 2H), 7.37 (d, J = 7.9 Hz, 2H), 2.45 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.84, 143.32, 142.33, 141.45, 140.51, 133.98, 130.20, 129.91, 129.54, 129.30, 129.10, 127.44, 21.45.

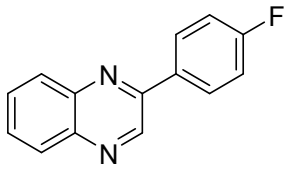


2-(3-methoxyphenyl)quinoxaline(4ac)[1]

Yield: 76%

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.32 (s, 1H), 8.15 (m, 2H), 7.82 – 7.73 (m, 4H), 7.49 (t, *J* = 7.9 Hz, 1H), 7.08 (dd, *J* = 8.2, 1.9 Hz, 1H), 3.95 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.32, 151.66, 143.47, 142.25, 141.67, 138.19, 130.32, 130.19, 129.65, 129.62, 129.14, 119.93, 116.24, 112.65, 55.49.



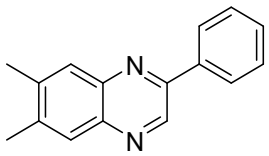
2-(4-fluorophenyl)quinoxaline(4ad)[2]

Yield: 25%

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.30 (s, 1H), 8.21 (m, 2H), 8.16 – 8.10 (m, 2H), 7.77 (ddd, *J* = 9.6, 7.8, 1.4 Hz, 2H), 7.28 – 7.24 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.26 (d, *J* = 250.8 Hz), 150.78, 142.96, 142.21, 141.51, 132.94, 130.43, 129.62, 129.55 (d, *J* = 2.3 Hz), 129.48, 129.15, 116.25 (d, *J* = 21.8 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -110.58 (dq, *J* = 8.5, 5.4 Hz).

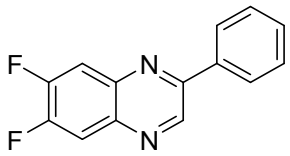


6,7-dimethyl-2-phenylquinoxaline(4ae)[1]

Yield: 60%

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.21 (s, 1H), 8.16 (dd, *J* = 5.2, 3.3 Hz, 2H), 7.87 (d, *J* = 20.2 Hz, 2H), 7.58 – 7.46 (m, 3H), 2.50 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.00, 142.41, 141.24, 140.79, 140.58, 140.11, 137.15, 129.82, 129.06, 128.66, 128.15, 127.38, 20.38, 20.35.



6,7-difluoro-2-phenylquinoxaline(4af)[3]

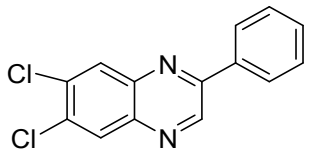
Yield: 95%

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.27 (s, 1H), 8.15 (dd, *J* = 7.6, 1.6 Hz, 2H), 7.85 (td, *J* = 10.6, 8.2 Hz, 2H), 7.59 – 7.50 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 153.64 (dd, *J* = 58.7, 15.8 Hz), 151.97 (d, *J* = 3.2 Hz), 151.09 (dd, *J* = 58.5, 15.8 Hz), 143.35 (d, *J* = 3.2 Hz), 139.23 (dd, *J* = 91.9, 10.4 Hz), 136.11, 130.53, 129.22, 129.17(d, *J* = 60 Hz),128.44 (d, *J* = 7.2 Hz), 127.45, 115.42 – 113.93 (m).

^{19}F NMR (376 MHz, $CDCl_3$) δ -129.42 (ddd, *J* = 20.9, 10.4, 8.3

Hz), -130.24 (ddd, J = 20.9, 10.3, 8.3 Hz).

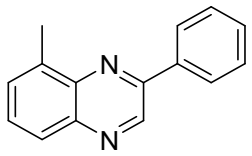


6,7-dichloro-2-phenylquinoxaline(4ag)[4]

Yield: 67%

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.28 (s, 1H), 8.21 (d, J = 15.1 Hz, 2H), 8.18 – 8.12 (m, 2H), 7.61 – 7.50 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 152.56, 144.22, 141.05, 140.24, 135.94, 134.89, 133.97, 130.75, 130.16, 129.76, 129.25, 127.55.

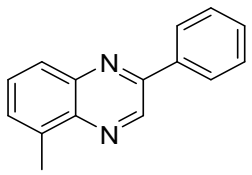


8-methyl-2-phenylquinoxaline(4ah)[3]

Yield: 15%, Less polar regioisomer

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.34 (s, 1H), 8.23 – 8.16 (m, 2H), 8.01 (d, J = 8.4 Hz, 1H), 7.72 – 7.65 (m, 1H), 7.61 – 7.51 (m, 4H), 2.84 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.42, 142.45, 142.03, 140.79, 137.33, 136.96, 130.11, 130.07, 129.64, 129.25, 129.16, 127.54, 17.36.

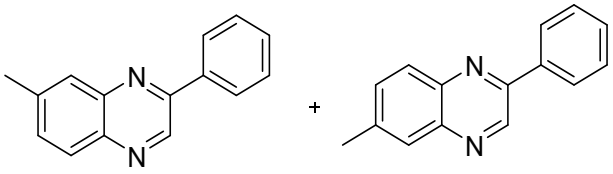


5-methyl-2-phenylquinoxaline(4ah')[3]

Yield: 60%, More polar regioisomer

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.32 (s, 1H), 8.29 – 8.21 (m, 2H), 7.94 (dd, *J* = 7.2, 2.5 Hz, 1H), 7.64 – 7.58 (m, 2H), 7.58 – 7.48 (m, 3H), 2.87 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 150.18, 142.60, 141.67, 141.33, 137.99, 137.07, 130.16, 130.03, 129.28, 129.08, 127.46, 126.90, 17.10.

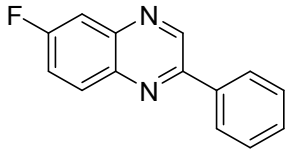


Mixture of 6-methyl-2-phenylquinoxaline and 7-methyl-2-phenylquinoxaline (4ai)[2]

Yield: 70%

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.27 (s, 0.5H), 9.24 (s, 0.5H), 8.18 (dd, *J* = 5.7, 3.5 Hz, 2H), 8.01 (dd, *J* = 15.8, 8.5 Hz, 1H), 7.89 (d, *J* = 18.3 Hz, 1H), 7.61 – 7.46 (m, 4H), 2.59 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.74, 151.04, 143.24, 142.45, 142.37, 141.65, 140.79, 140.76, 140.09, 136.96, 132.58, 131.85, 130.04, 129.94, 129.14, 129.10, 128.62, 128.48, 127.98, 127.50, 127.41, 21.87, 21.84.



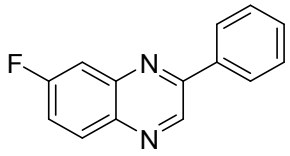
6-fluoro-2-phenylquinoxaline (4aj)[3]

Yield: 20%, Less polar regioisomer

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.33 (s, 1H), 8.17 (m, 3H), 7.75 (dd, *J* = 9.1, 2.8 Hz, 1H), 7.61 – 7.52 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.50 (d, *J* = 251.6 Hz), 151.34, 144.11, 142.17, 139.52, 136.49, 131.67 (d, *J* = 10.0 Hz), 130.28, 129.23, 127.44, 120.72 (d, *J* = 25.9 Hz), 112.72 (d, *J* = 21.5 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -108.52 (td, *J* = 8.5, 5.7 Hz).



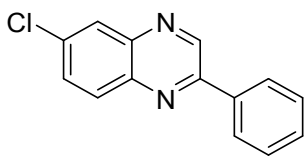
7-fluoro-2-phenylquinoxaline (4aj')[3]

Yield: 65%, More polar regioisomer

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.28 (s, 1H), 8.18 (d, *J* = 7.3 Hz, 2H), 8.10 (dd, *J* = 9.1, 5.8 Hz, 1H), 7.76 (dd, *J* = 9.3, 2.6 Hz, 1H), 7.59 – 7.48 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.04 (d, *J* = 252.1 Hz), 152.47, 143.19 (d, *J* = 13.3 Hz), 142.61 (d, *J* = 3.1 Hz), 138.80, 136.39, 131.17 (d, *J* = 10.2 Hz), 130.48, 129.19, 127.61, 119.84 (d, *J* = 26.0 Hz), 113.05 (d, *J* = 21.4 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -107.82 (td, *J* = 8.7, 5.9 Hz).

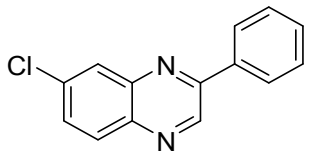


6-chloro-2-phenylquinoxaline(4ak)[4]

Yield: 33%, Less polar regioisomer

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.33 (s, 1H), 8.21 – 8.16 (m, 2H), 8.10 (dd, *J* = 9.8, 5.6 Hz, 2H), 7.73 (dd, *J* = 9.0, 2.3 Hz, 1H), 7.60 – 7.51 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.95, 144.16, 141.82, 140.85, 136.37, 135.25, 131.34, 130.84, 130.45, 129.23, 128.08, 127.52.

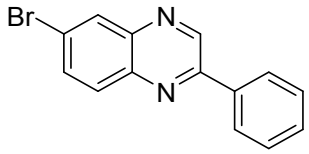


7-chloro-2-phenylquinoxaline(4ak')[4]

Yield: 63%, More polar regioisomer

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.29 (s, 1H), 8.17 (dt, *J* = 3.9, 2.2 Hz, 2H), 8.13 (d, *J* = 2.3 Hz, 1H), 8.03 (d, *J* = 8.9 Hz, 1H), 7.66 (dd, *J* = 8.9, 2.3 Hz, 1H), 7.59 – 7.51 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 152.50, 143.40, 142.62, 140.07, 136.27, 136.07, 130.55, 130.49, 130.34, 129.21, 128.48, 127.59.

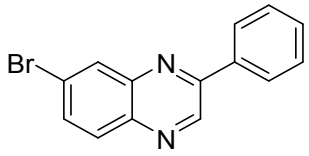


6-bromo-2-phenylquinoxaline(4al)[2]

Yield: 28%, Less polar regioisomer

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.32 (s, 1H), 8.30 (d, *J* = 2.1 Hz, 1H), 8.21 – 8.16 (m, 2H), 8.02 (d, *J* = 8.9 Hz, 1H), 7.86 (dd, *J* = 8.9, 2.2 Hz, 1H), 7.61 – 7.52 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 152.06, 144.12, 142.10, 141.08, 136.35, 133.89, 131.46, 130.93, 130.49, 129.25, 127.54, 123.40.



6-bromo-2-phenylquinoxaline(4al')[2]

Yield: 40%, More polar regioisomer

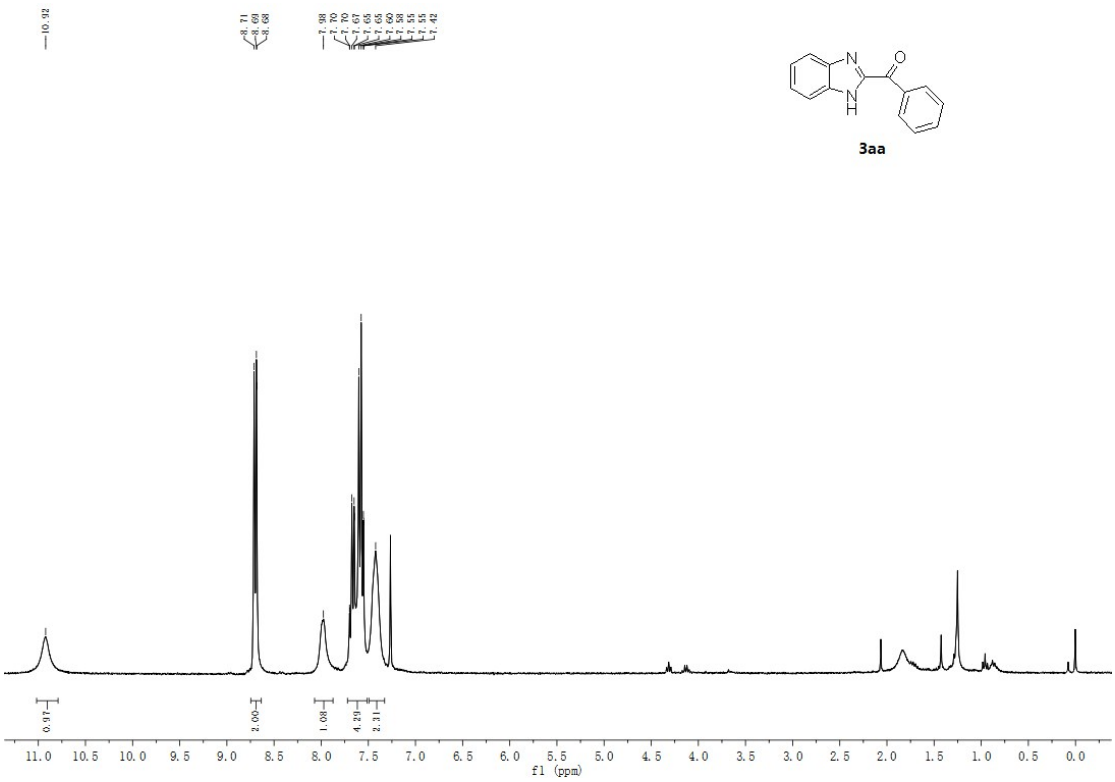
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.31 (s, 1H), 8.32 (d, *J* = 2.1 Hz, 1H), 8.17 (dt, *J* = 4.1, 2.3 Hz, 2H), 7.96 (d, *J* = 8.9 Hz, 1H), 7.80 (dd, *J* = 8.9, 2.2 Hz, 1H), 7.60 – 7.53 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 152.44, 143.54, 142.90, 140.32, 136.26, 133.04, 131.89, 130.57, 130.43, 129.22, 127.60, 124.29.

Reference

1. Harsha, K. B.; Rangappa, K. S., *RSC Adv.*, **2016,** *6*, 57154-57162.
2. Zhang, R.; Qin, Y.; Zhang, L.; Luo, S., *Org. Lett.*, **2017,** *19*, 5629-5632.
3. Zhang, C.; Xu, Z.; Zhang, L.; Jiao, N., *Tetrahedron*, **2012,** *68*, 5258-5262.
4. Gopalaiah, K.; Saini, A.; Chandrudu, S. N.; Rao, D. C.; Yadav, H.; Kumar, B., *Organic & Biomolecular Chemistry*, **2017,** *15*.

NMR spectra of all compounds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8.68
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7.70
7.70
7.67
7.66
7.65
7.60
7.58
7.55
7.55
7.43
7.42
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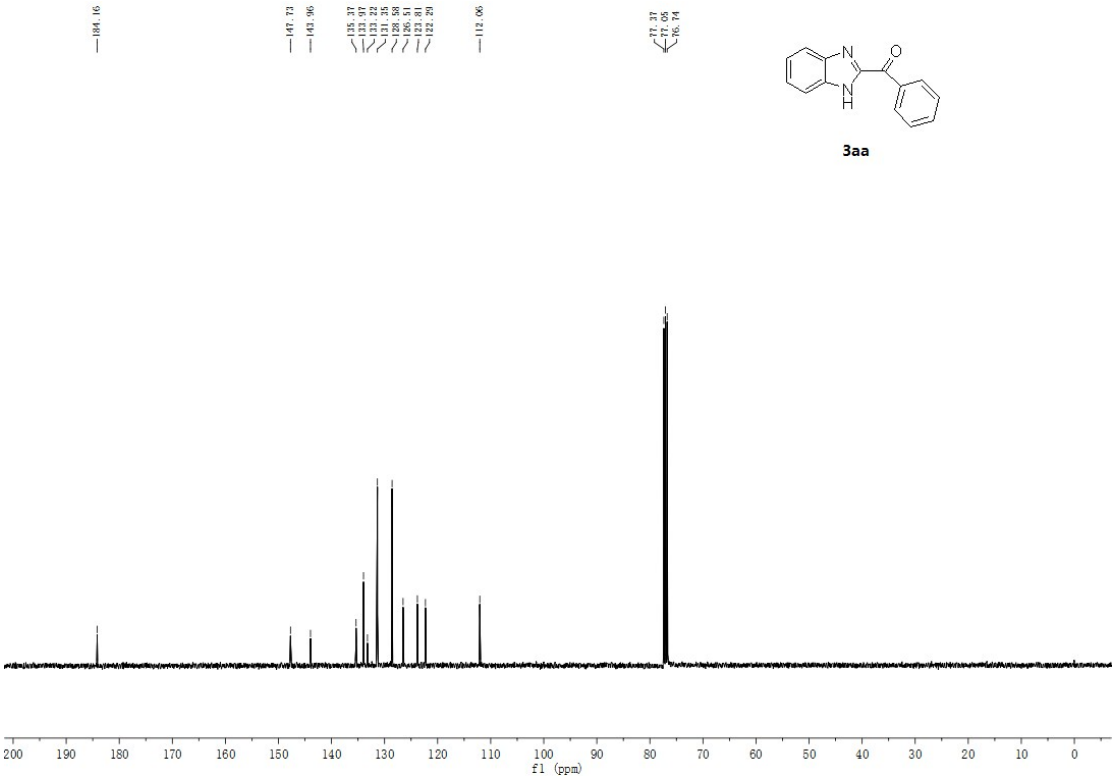
2.00
1.08
4.29
2.31
f1 (ppm)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77.05
76.74
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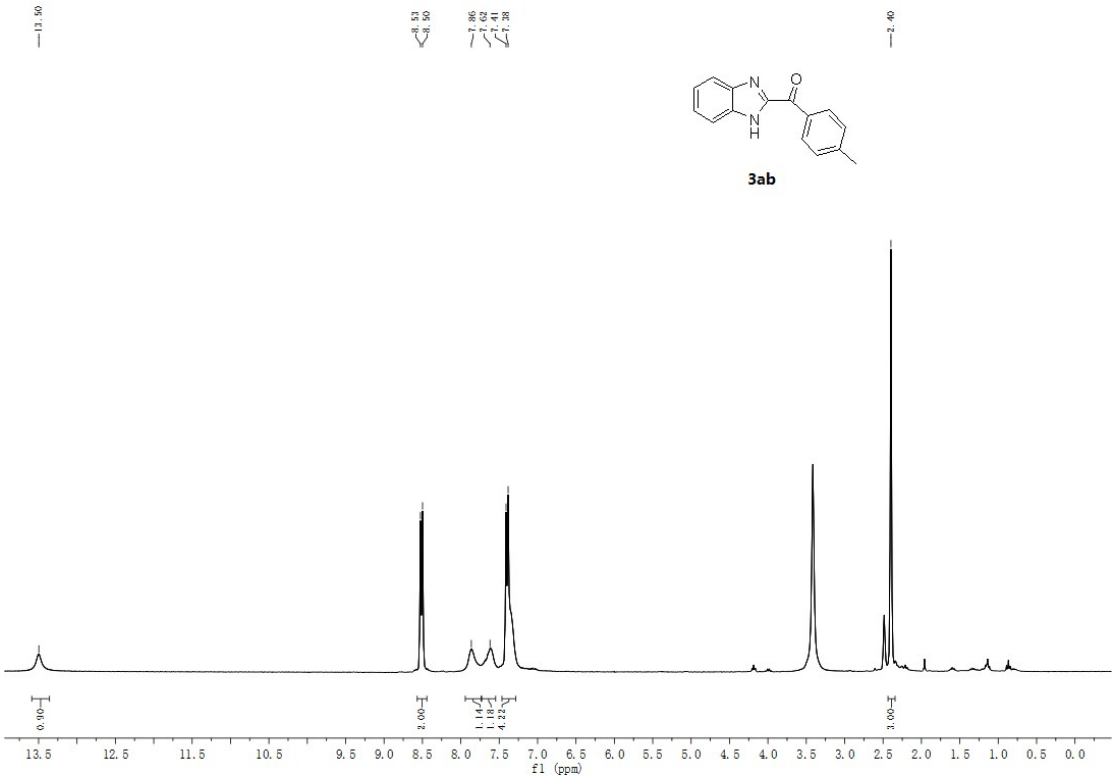
f1 (ppm)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8.50
7.86
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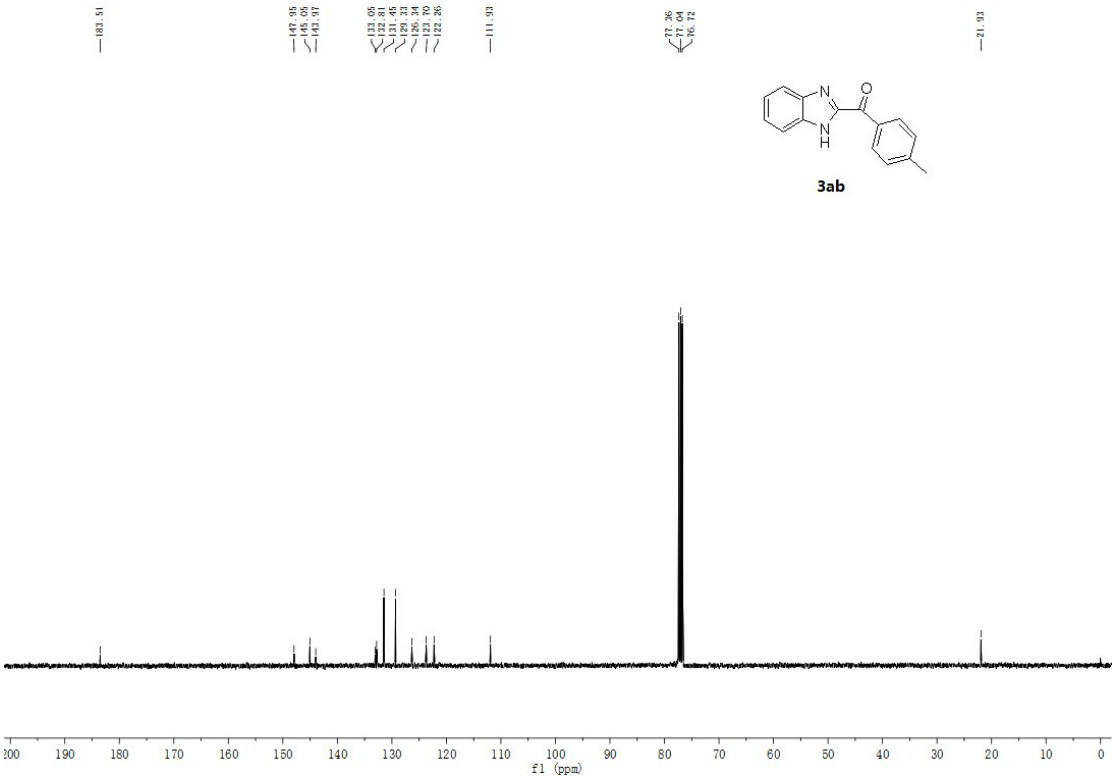
1.18
4.23
3.00
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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122.26
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77.04
76.72
21.93
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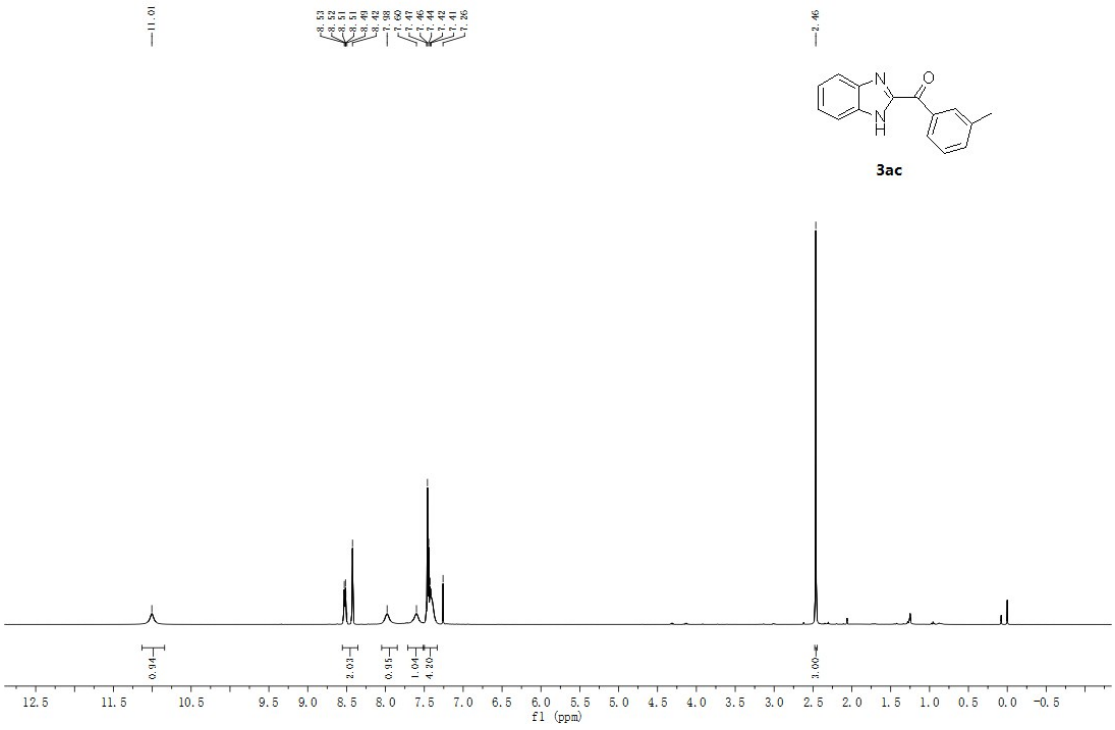
f1 (ppm)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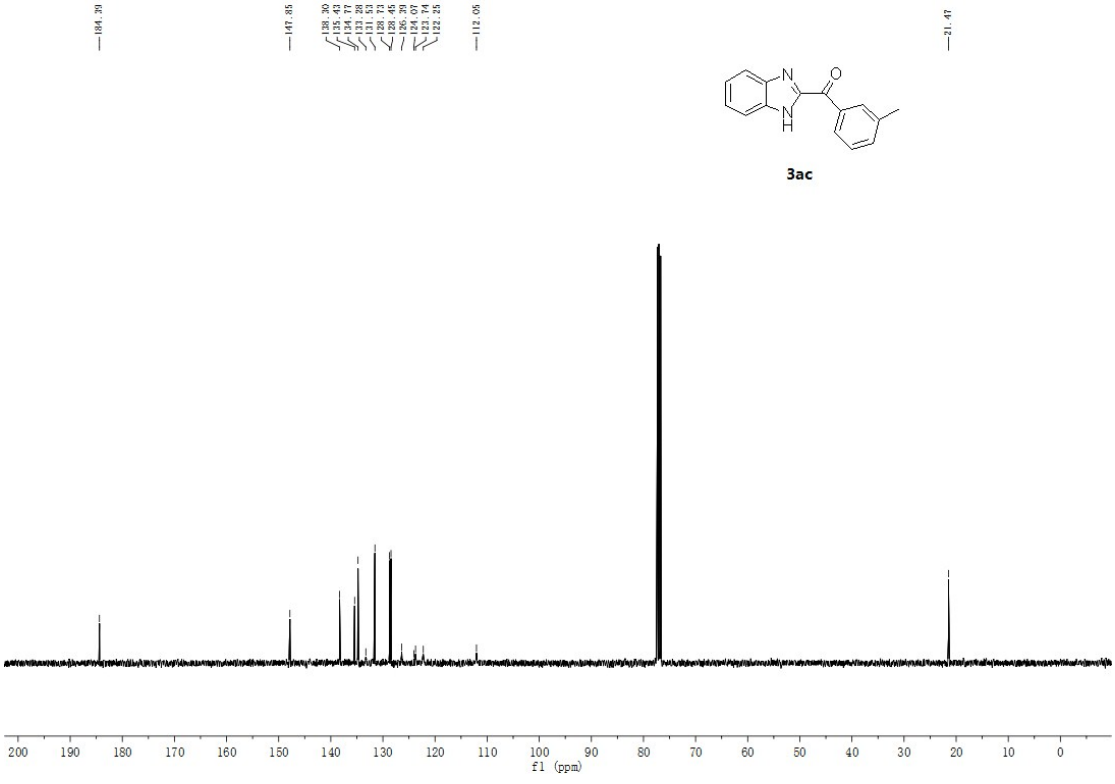
8.51
8.51
8.49
8.42
7.98
7.69
7.47
7.46
7.44
7.42
7.41
7.26
2.46
0.94
2.03
0.95
1.04
4.20
1.00
f1 (ppm)

3ac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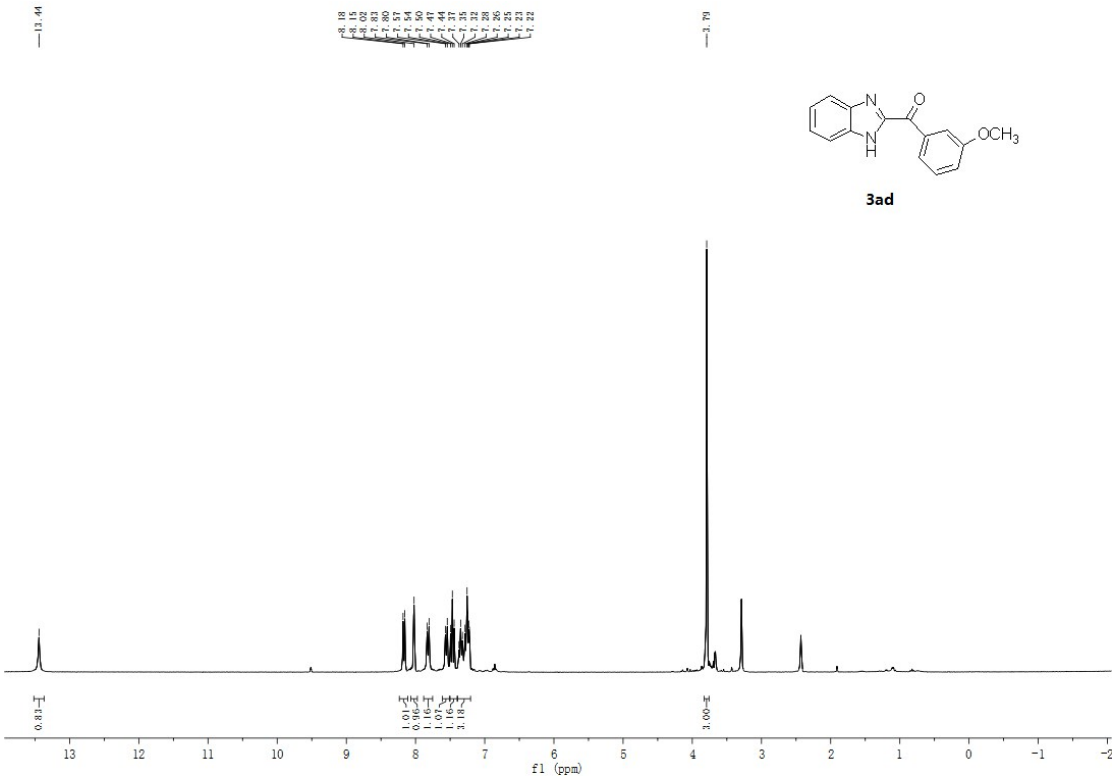
112.05
21.47
f1 (ppm)

3ac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7.47
7.44
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7.32
7.28
7.25
7.23
7.22
3.79
N
O
N
H
OCH3
0.83
1.01
0.96
1.16
1.07
1.65
3.18
3.00
13
12
11
10
9
8
7
6
5
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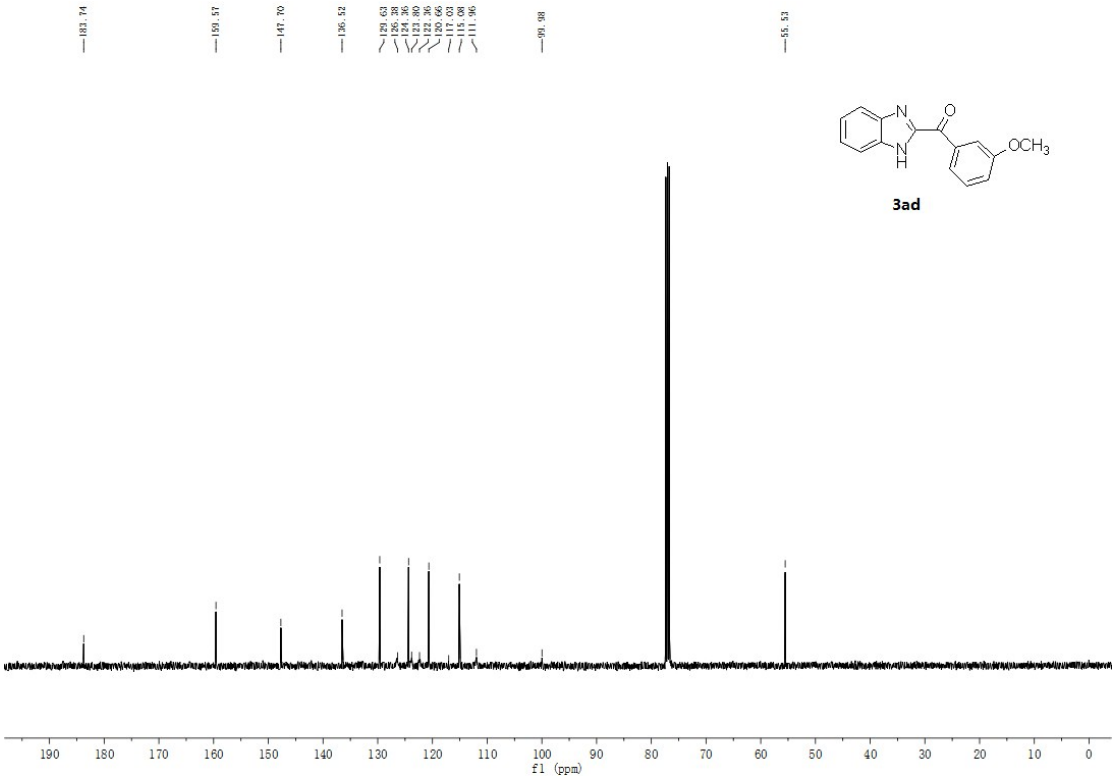
3
2
1
0
−1
−2
f1 (ppm)

3ad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120.66
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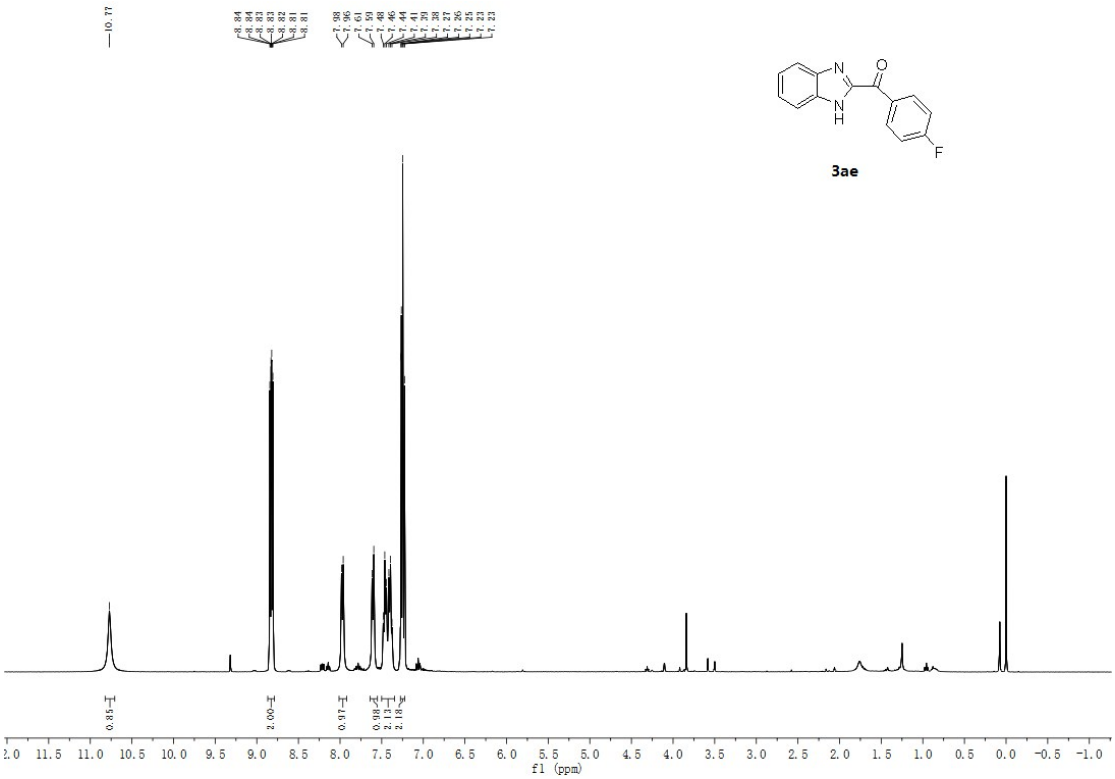
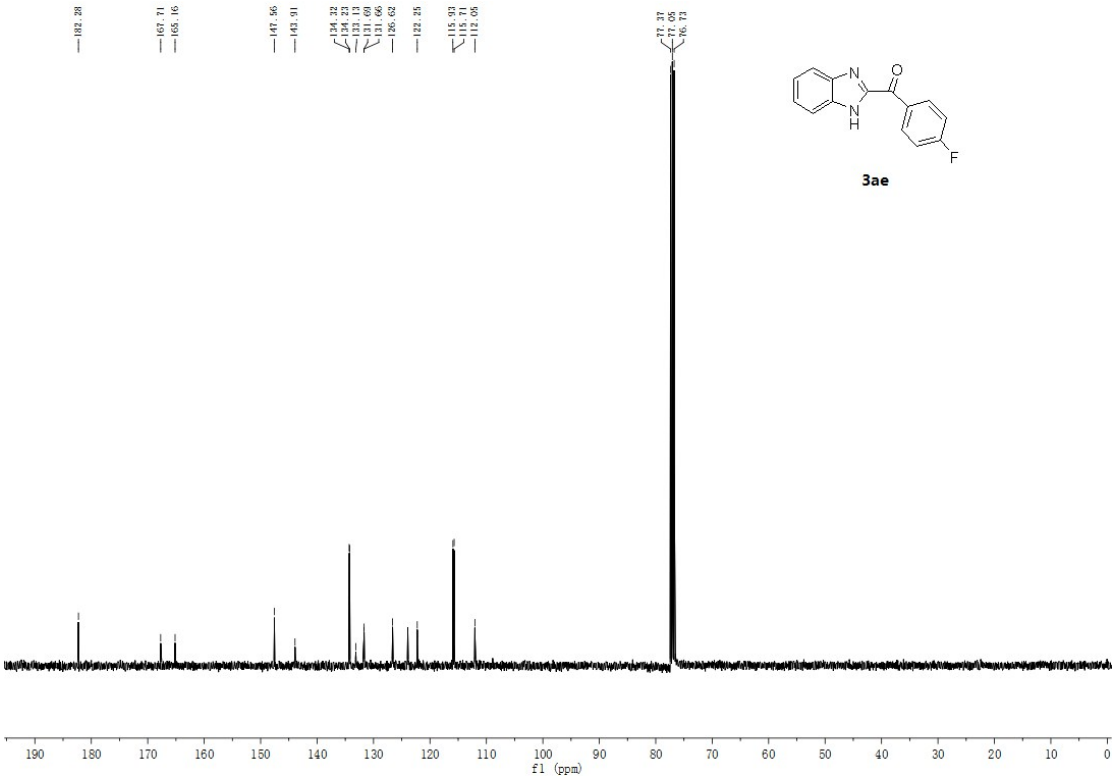
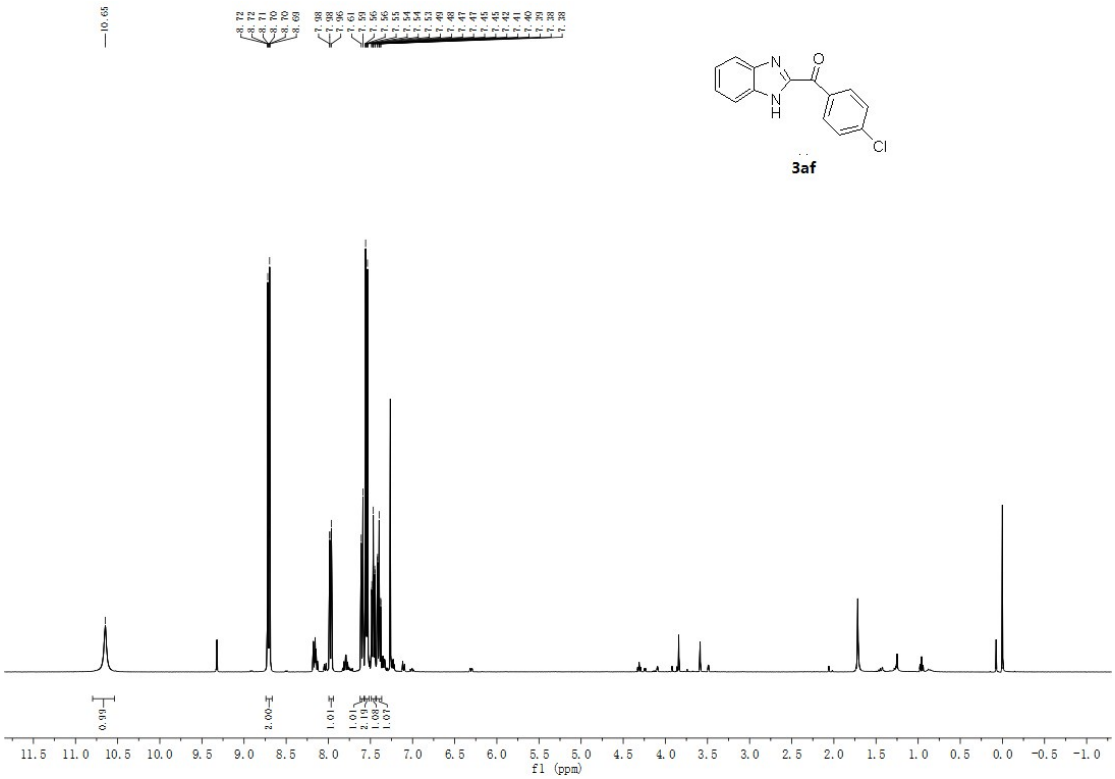
111.96
99.98
55.53
N
O
N
H
OCH3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

3ad


3ae
f1 (ppm)


3ae
f1 (ppm)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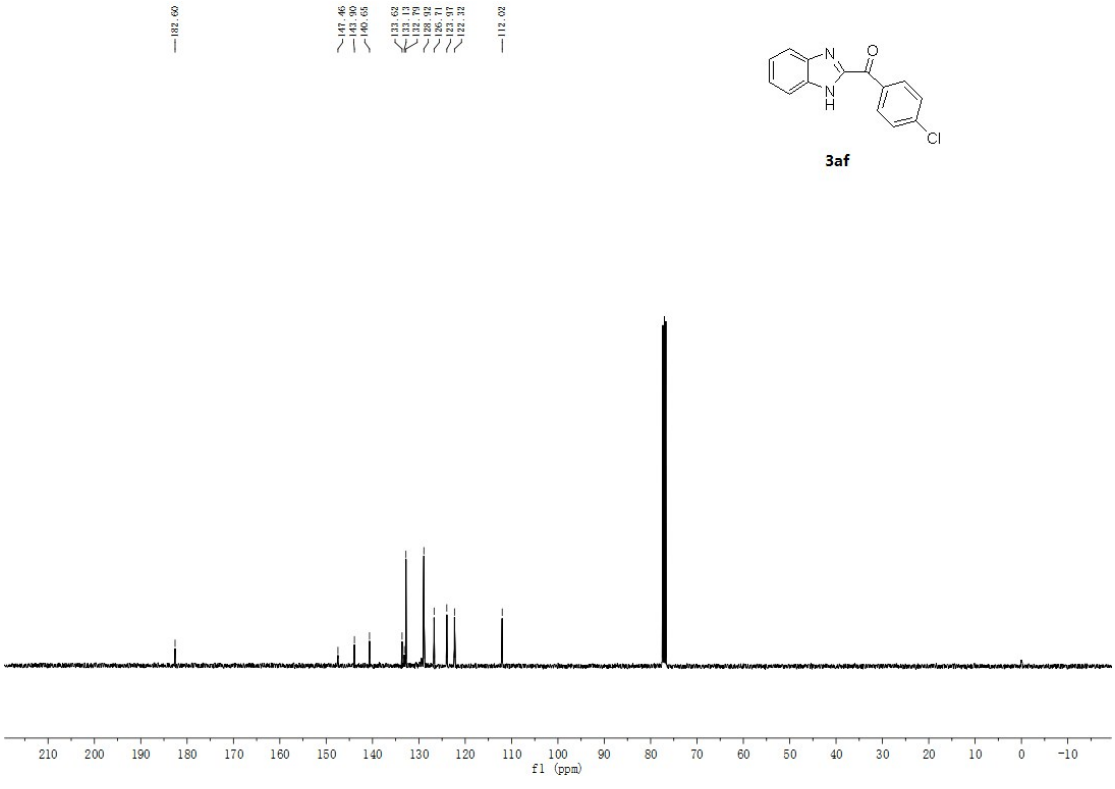
7.49
7.48
7.47
7.45
7.42
7.41
7.40
7.39
7.38
7.36
0.93
2.00
1.01
1.01
2.19
1.08
1.07
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)
N
H
O
Cl

3af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123.97
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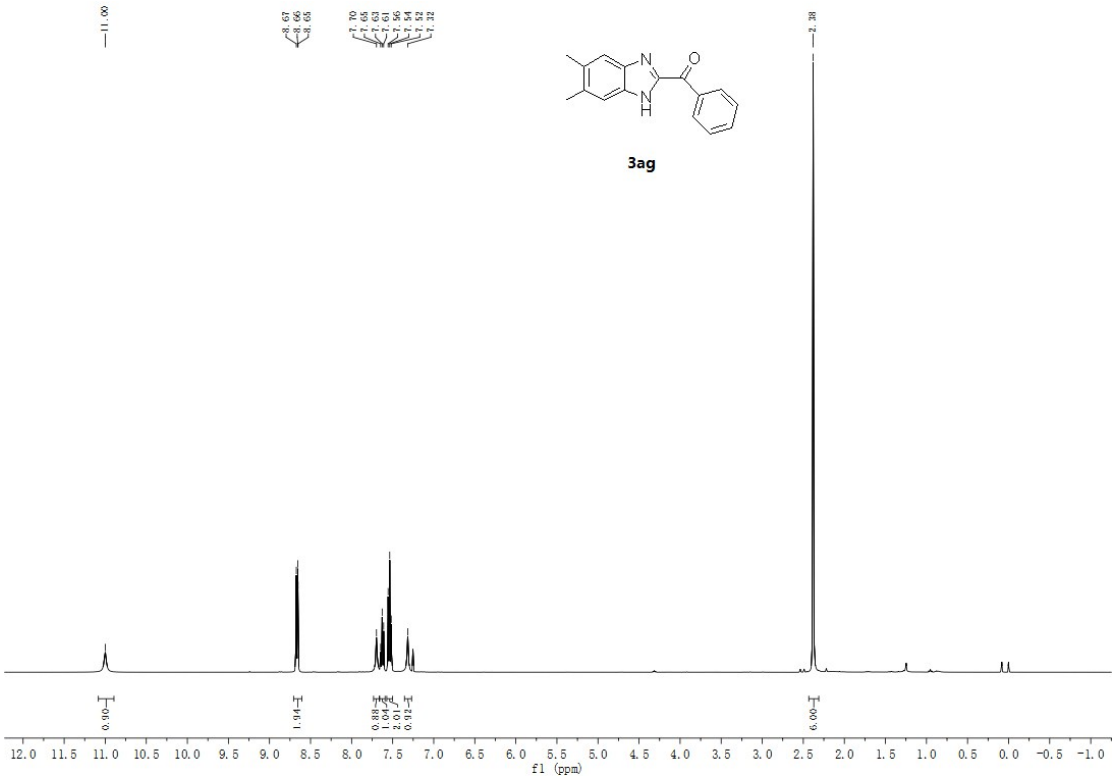
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
N
H
O
Cl

3af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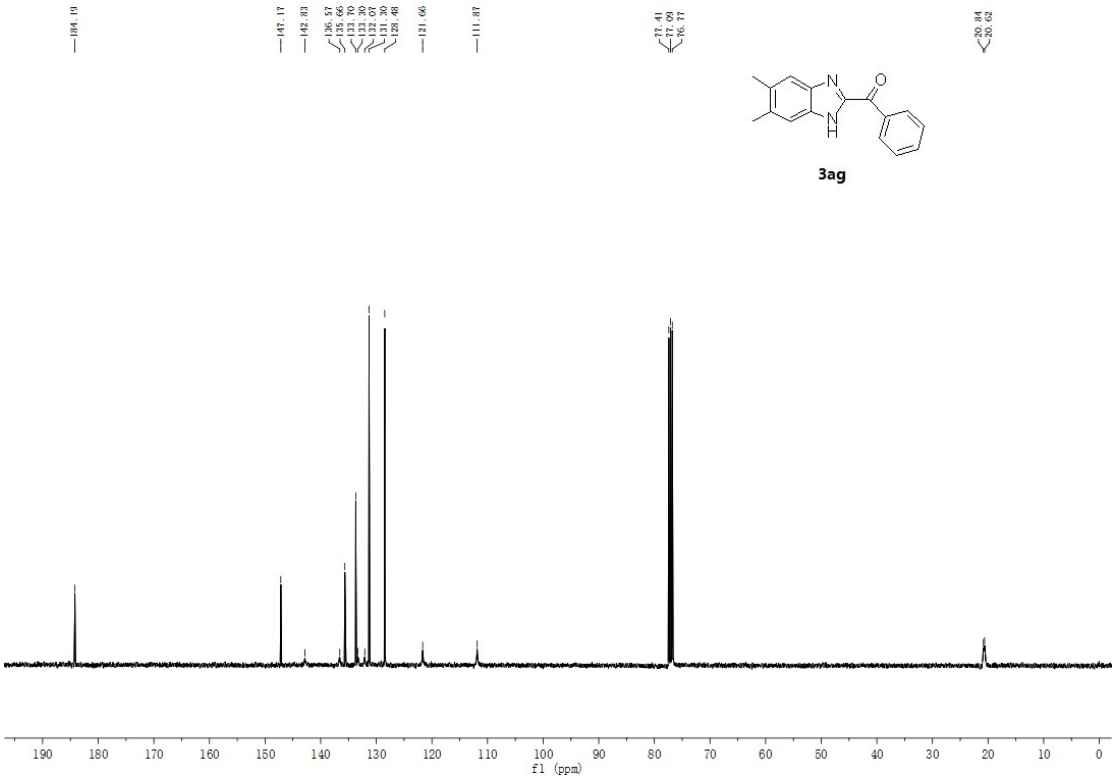
7.63
7.61
7.56
7.54
7.52
7.32
2.38
0.90
1.94
0.83
1.04
2.01
0.91
6.06
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

3ag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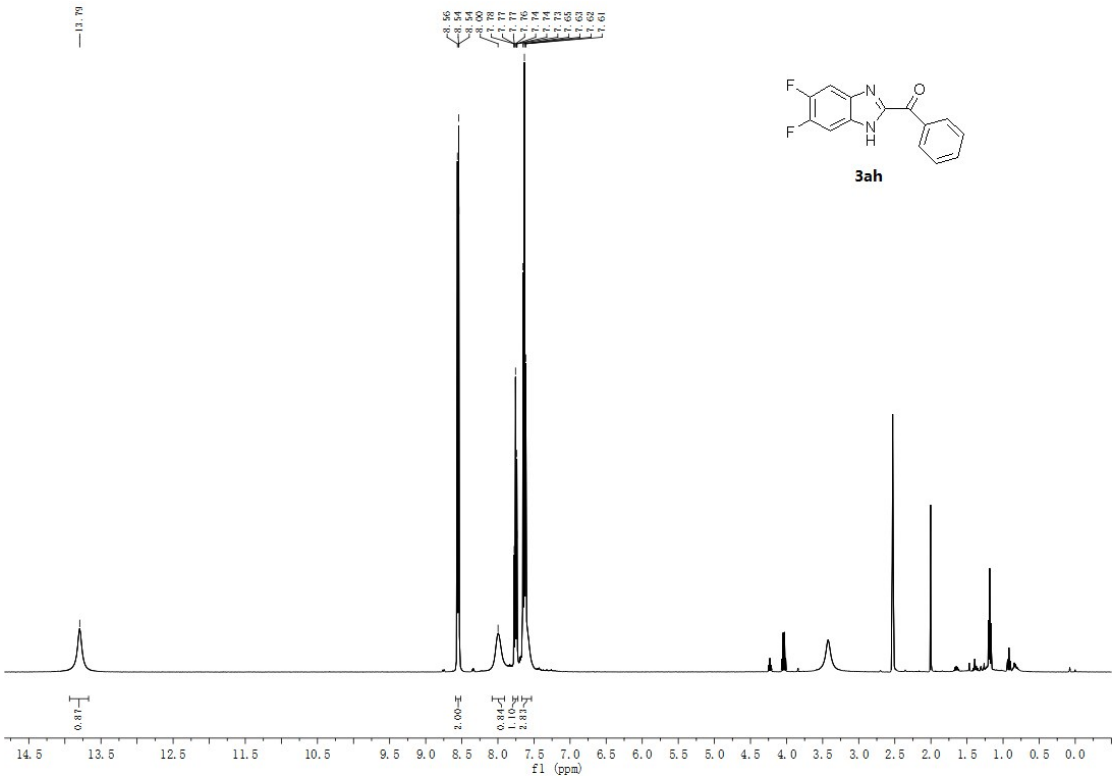
131.30
128.48
121.66
111.87
77.41
77.09
76.77
20.84
20.62
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3ag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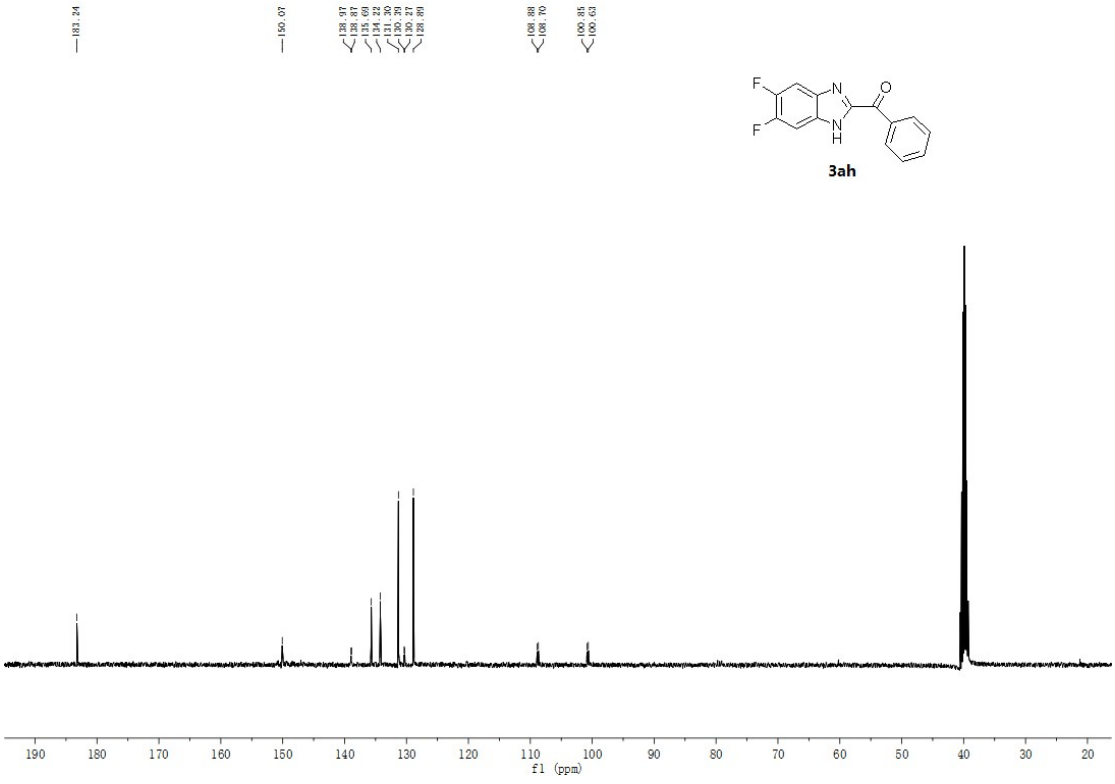
8.56
8.54
8.54
8.00
7.78
7.77
7.77
7.76
7.74
7.74
7.73
7.65
7.63
7.62
7.61
F
F
N
H
O
0.87
2.06
0.84
1.10
2.83
14.5 13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3ah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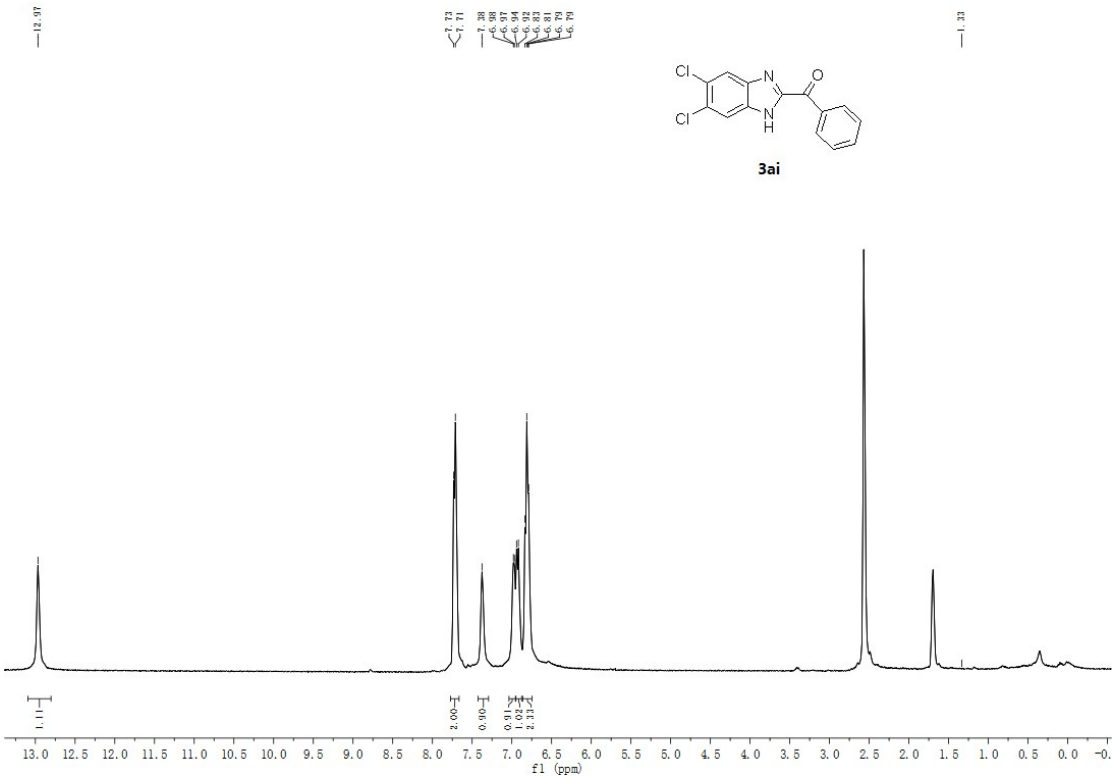
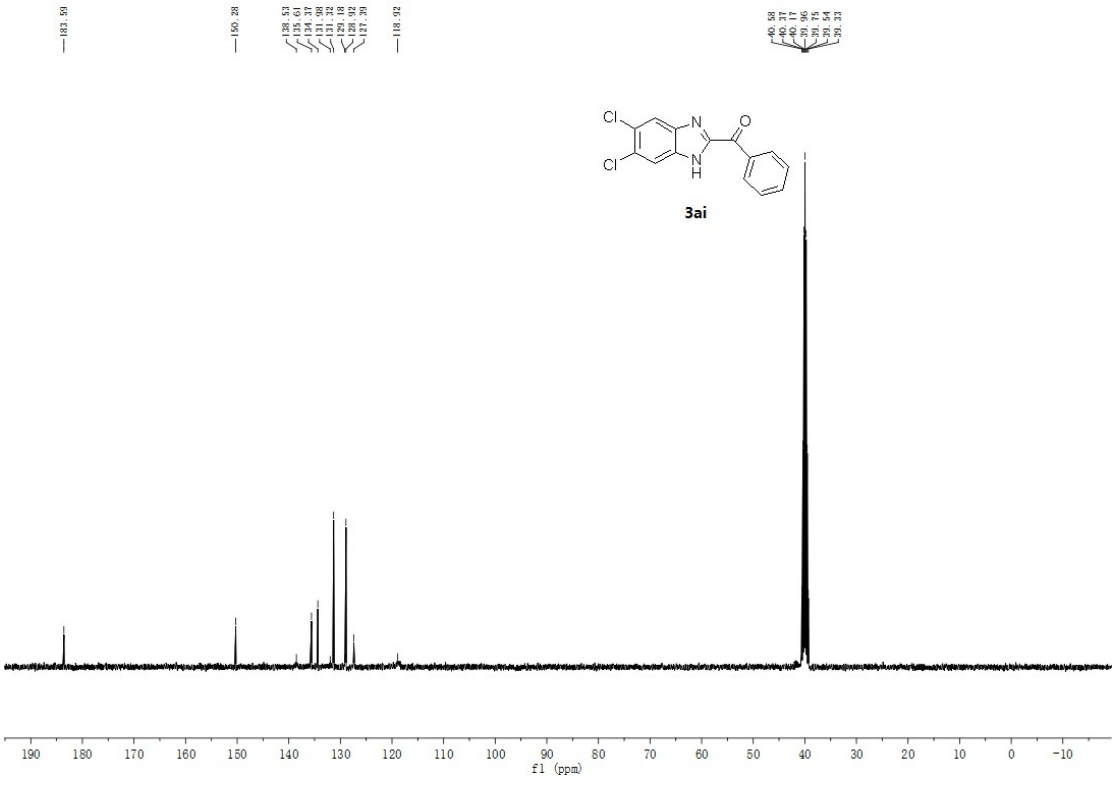
138.97
138.87
135.60
134.22
131.30
130.39
130.27
128.88
108.88
108.70
100.85
100.63
F
F
N
H
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20
f1 (ppm)

3ah


12.97
7.73
7.71
7.38
6.98
6.97
6.94
6.92
6.83
6.81
6.81
6.79
6.79
1.33
Cl
Cl
N
H
O
3ai
1.11
2.00
0.90
0.91
1.00
2.33
13.0 12.5 12.0 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 -0.
f1 (ppm)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134.37
131.98
131.32
129.18
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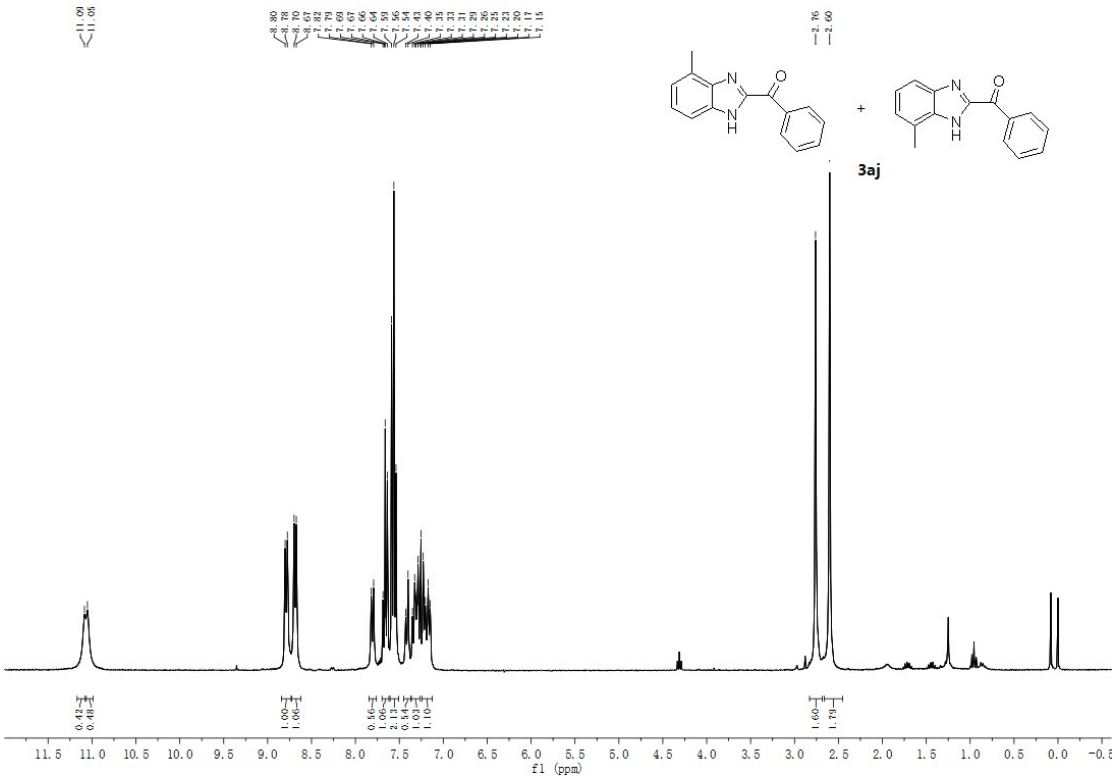
127.39
118.92
40.58
40.37
40.17
39.96
39.75
39.54
39.33
Cl
Cl
N
H
O
3ai
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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11.05
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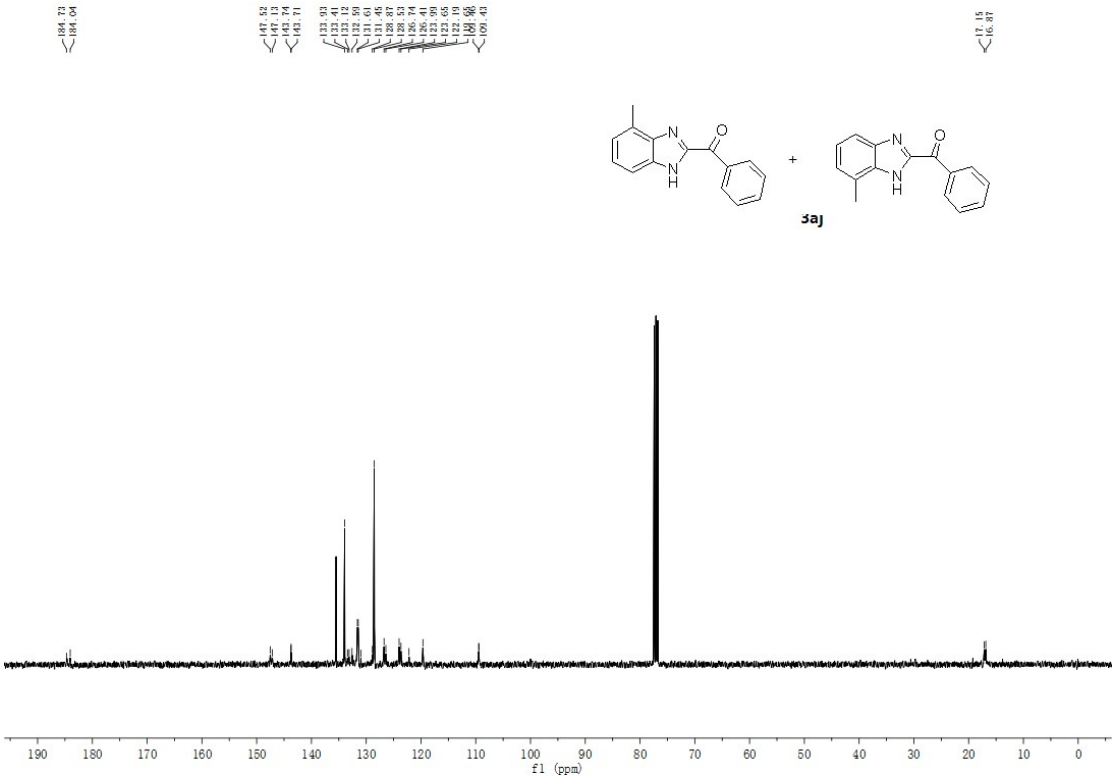
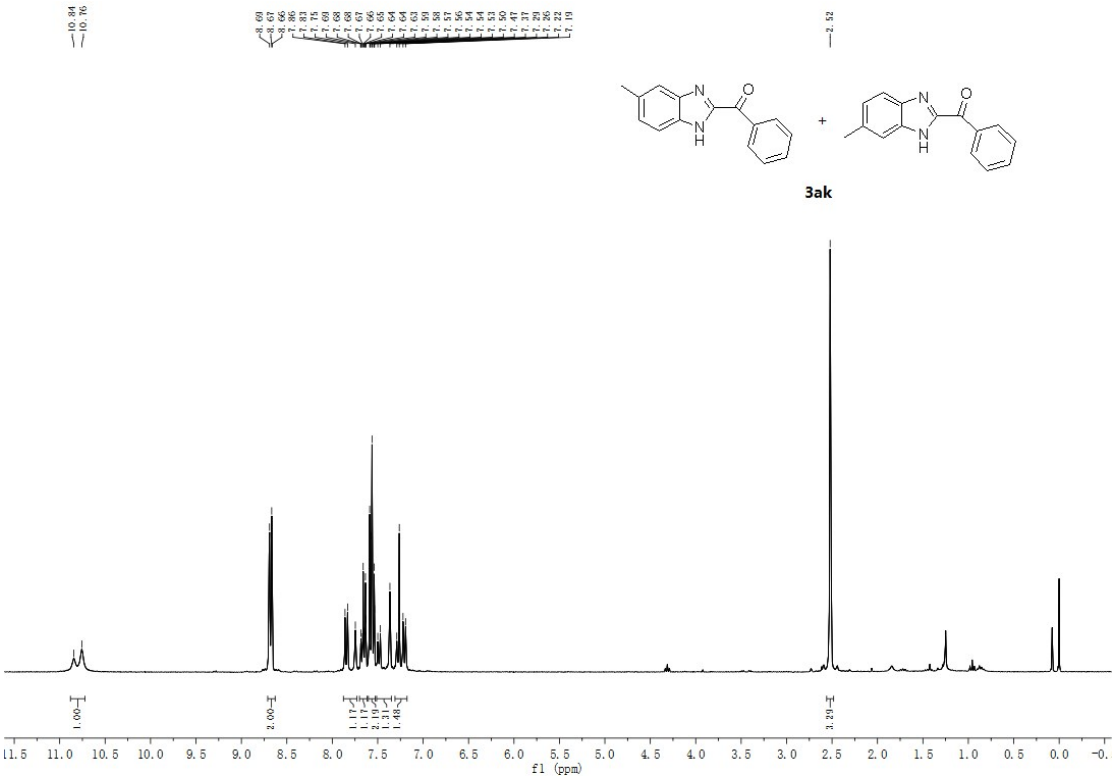
8.67
7.82
7.79
7.69
7.67
7.66
7.64
7.59
7.56
7.54
7.43
7.40
7.35
7.33
7.31
7.29
7.26
7.25
7.23
7.20
7.17
7.15
2.76
2.60
0.42
0.48
1.00
1.06
0.56
1.06
1.13
0.54
1.03
1.10
1.60
1.79
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3aj


184.73
184.04
147.52
147.13
143.74
143.71
132.93
133.41
133.12
132.59
131.64
131.46
128.87
128.53
126.74
126.44
125.95
123.65
122.19
109.43
17.15
16.87
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3aj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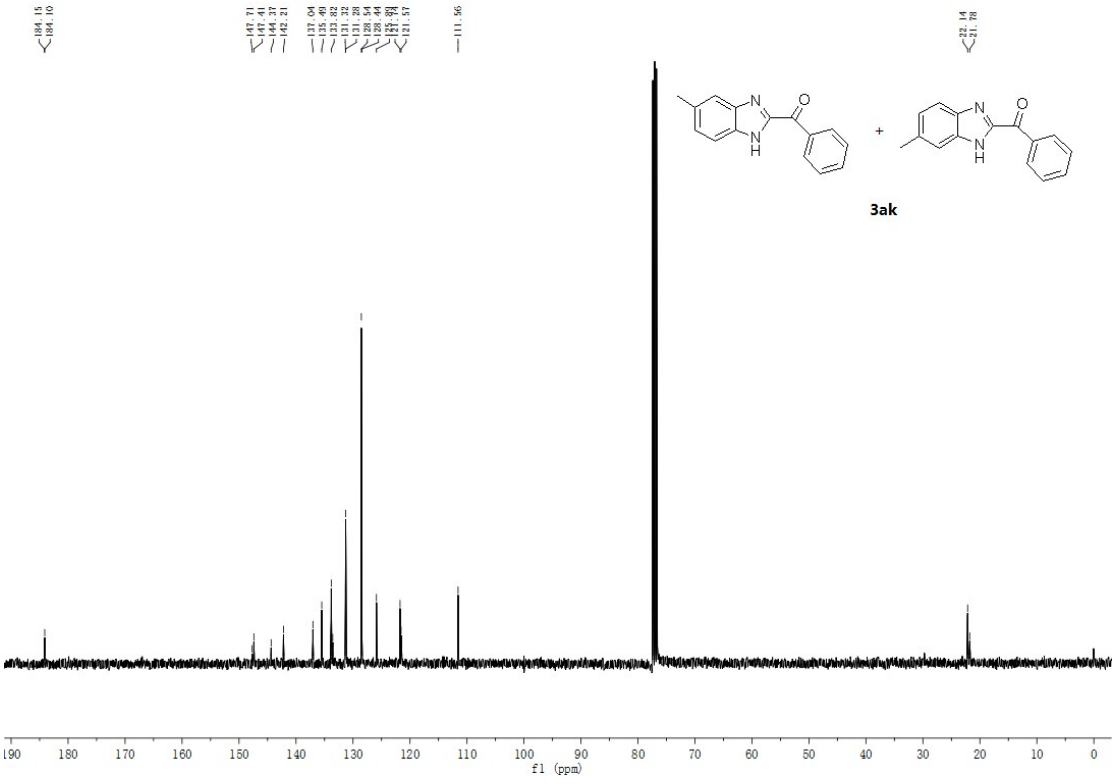
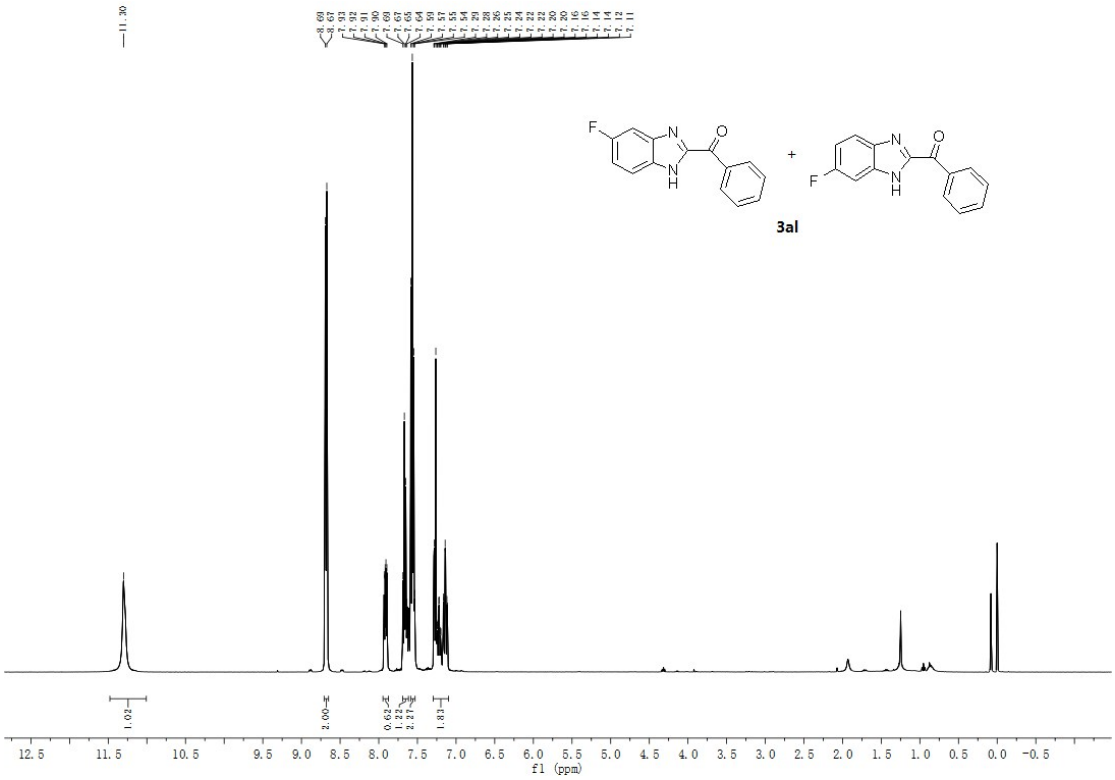
7.75
7.69
7.68
7.68
7.67
7.66
7.65
7.64
7.64
7.63
7.59
7.58
7.57
7.56
7.54
7.54
7.53
7.50
7.47
7.37
7.29
7.26
7.22
7.19
2.52
1.00
2.00
1.17
1.17
2.19
1.31
1.48
3.29
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


184.15
184.10
147.71
147.41
144.37
142.21
137.04
135.49
133.32
131.32
131.28
128.54
128.44
125.83
121.57
111.56
22.14
21.78
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3ak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8.67
7.93
7.92
7.91
7.90
7.69
7.67
7.65
7.64
7.59
7.57
7.55
7.54
7.29
7.28
7.25
7.24
7.22
7.22
7.20
7.20
7.16
7.16
7.14
7.14
7.12
7.11
F
N
H
O
+
3al
1.03
2.00
0.62
1.23
2.27
1.83
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
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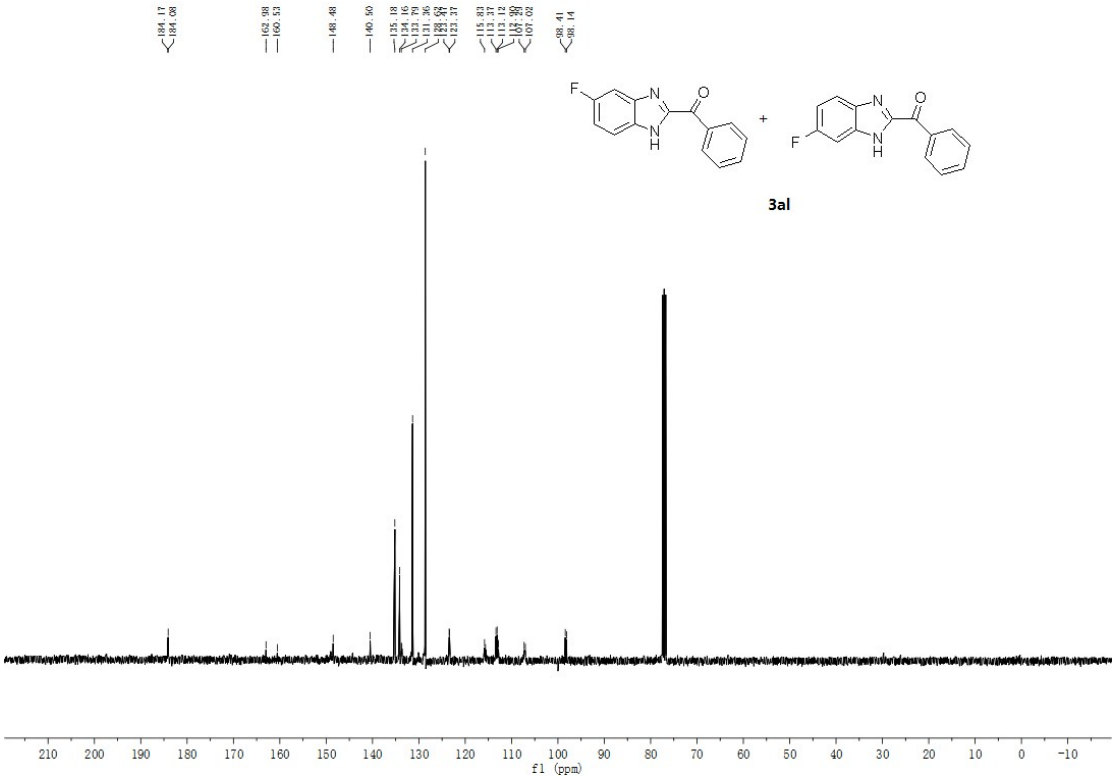
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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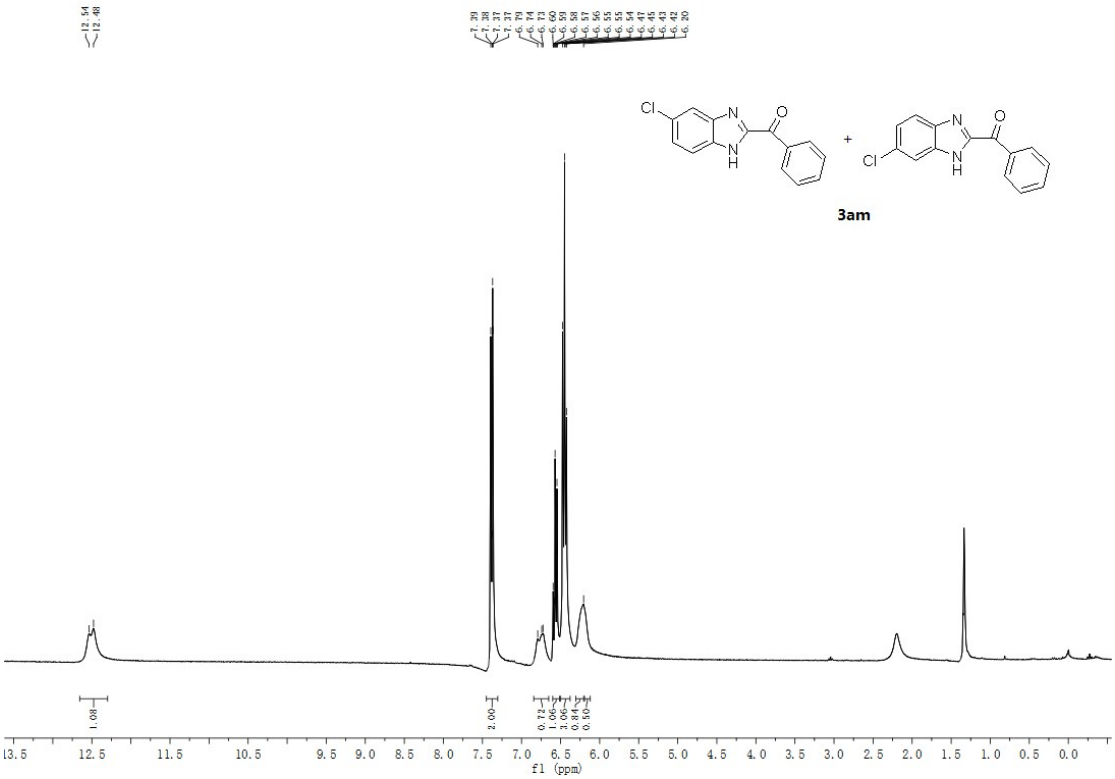
184.08
162.98
160.53
148.48
140.90
135.18
134.16
133.79
131.36
123.37
115.83
115.37
113.12
107.02
98.41
98.14
F
N
H
O
+
3al
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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12.48
7.39
7.38
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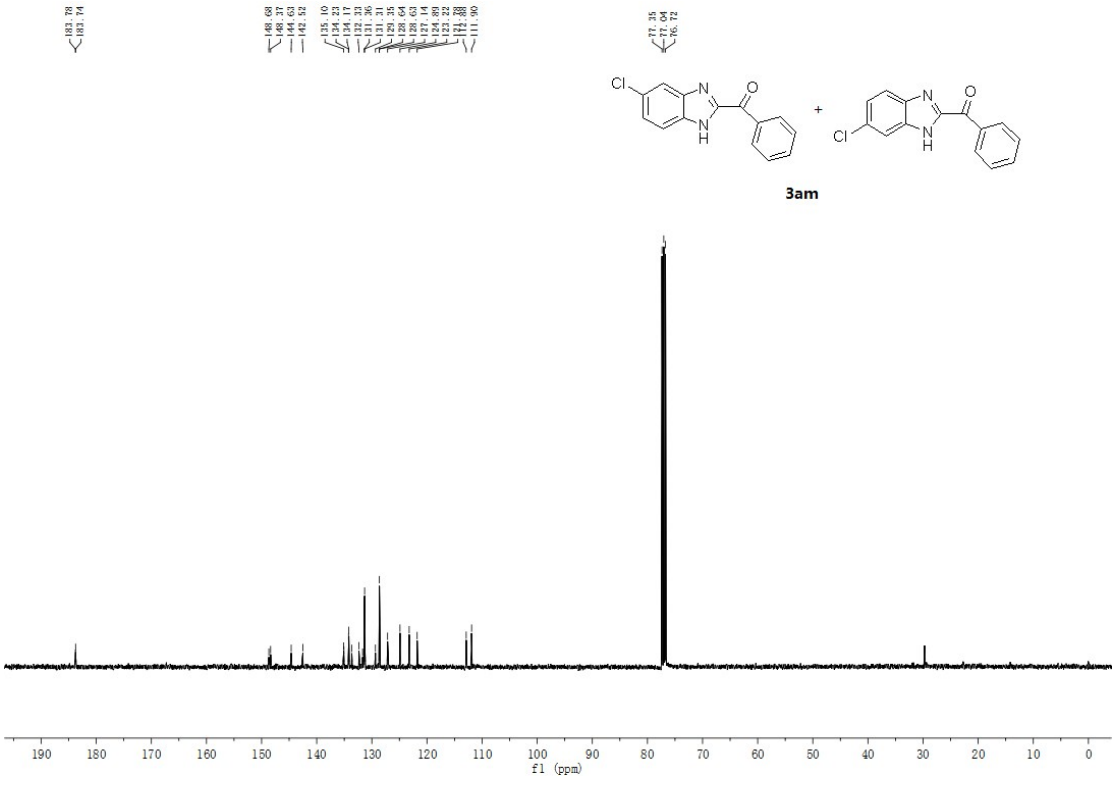
7.37
7.36
6.74
6.73
6.60
6.59
6.58
6.57
6.56
6.55
6.55
6.54
6.47
6.45
6.43
6.42
6.30
Cl
N
H
O
+
Cl
N
H
O
3am
1.08
2.00
0.72
1.06
3.06
0.84
0.93
f1 (ppm)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183.74
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144.63
142.52
135.10
134.23
134.17
132.33
131.36
131.31
129.35
128.64
128.63
127.14
124.89
123.22
111.88
111.90
77.35
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76.72
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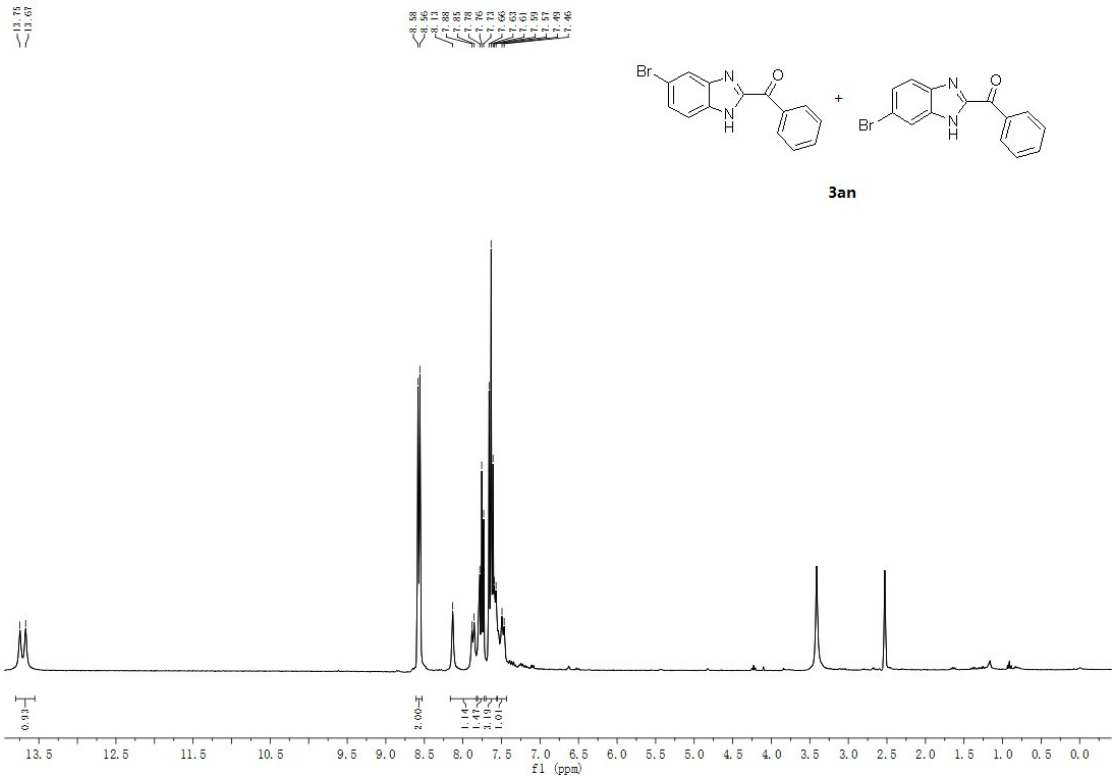
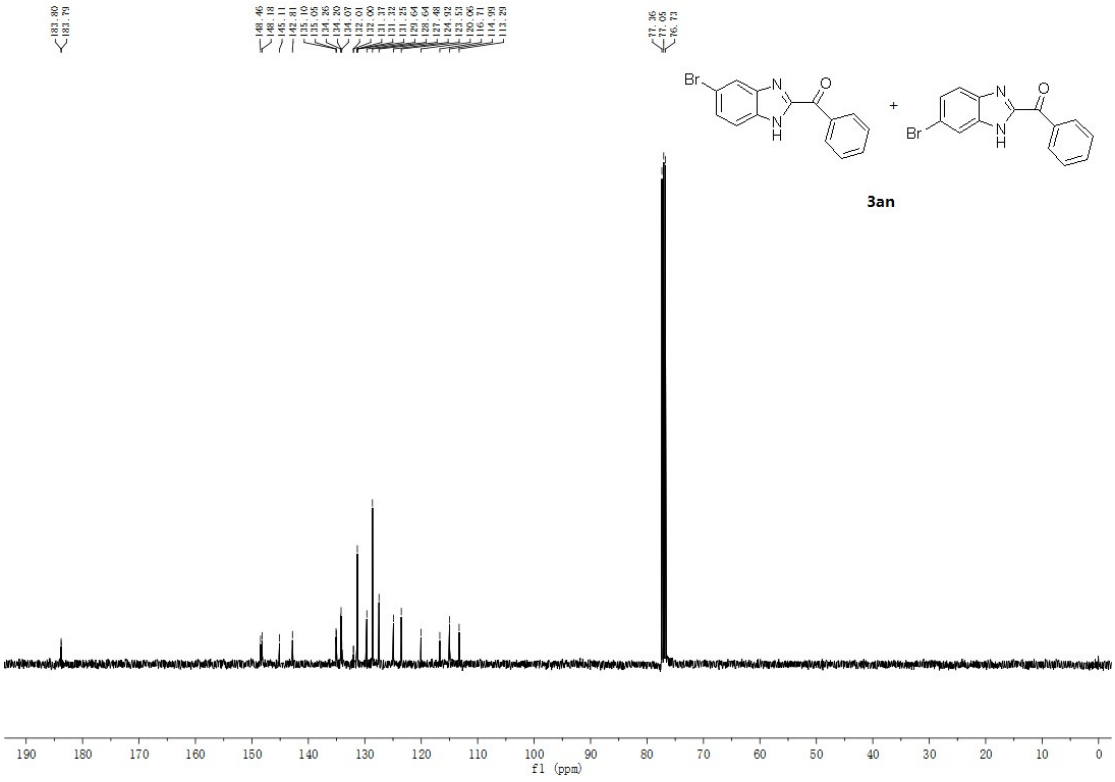
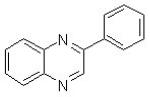
O
+
Cl
N
H
O
3am
f1 (ppm)


Br
N
H
O
+
Br
N
H
O
3an
f1 (ppm)


Br
N
H
O
+
Br
N
H
O
3an
f1 (ppm)



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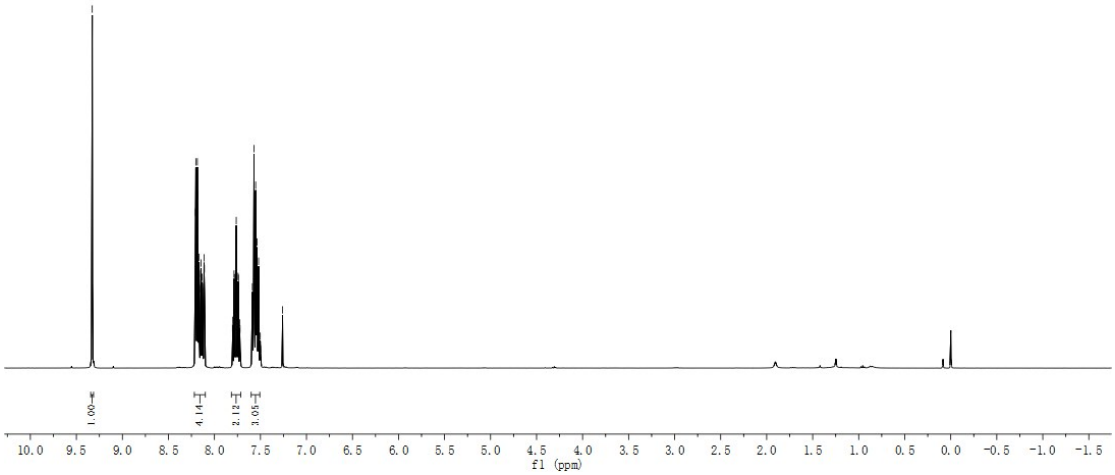

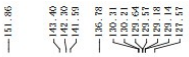

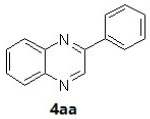

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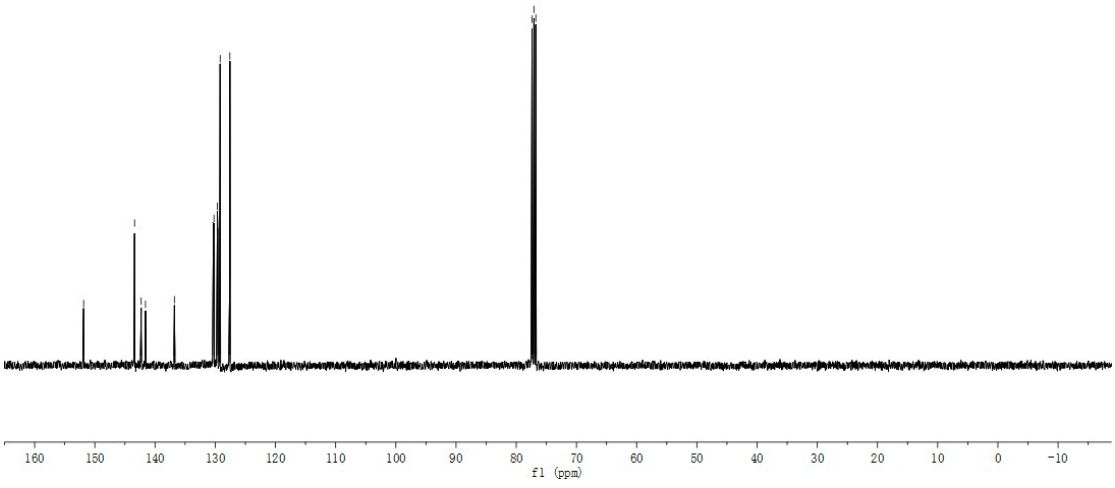

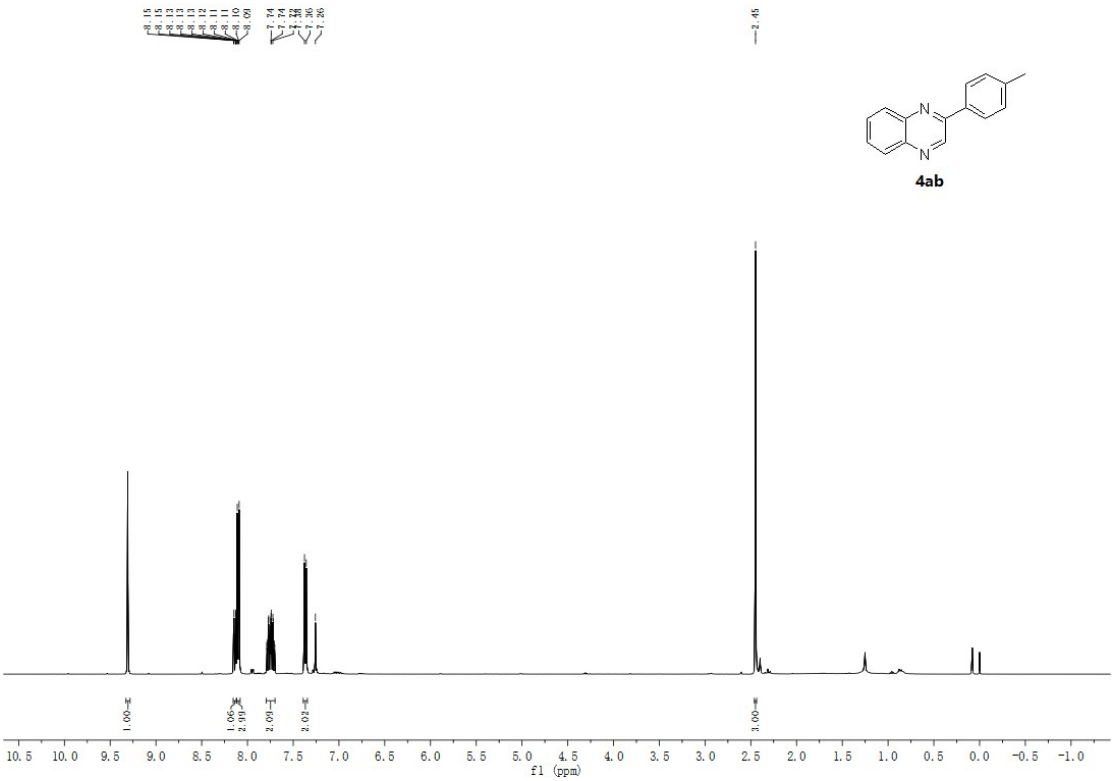
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8.13
8.13
8.13
8.12
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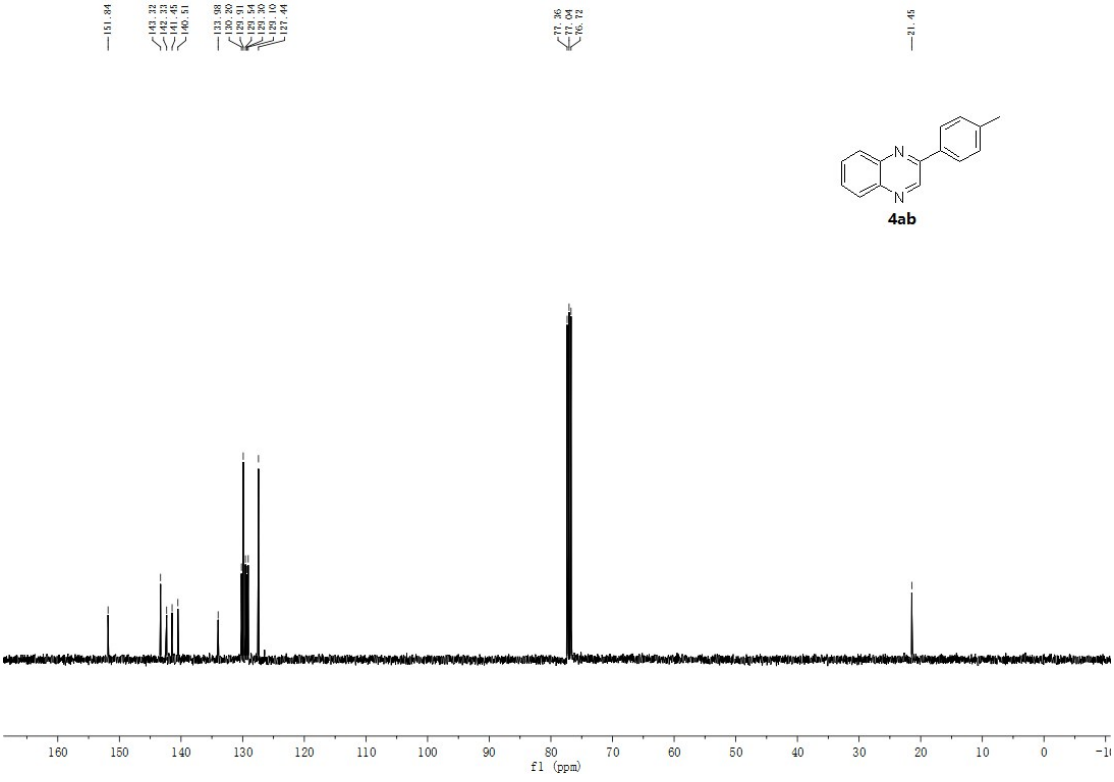
8.11
8.10
8.09
7.74
7.74
7.38
7.36
7.26
2.46
1.00
1.06
2.91
2.01
2.03
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

4ab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143.32
142.33
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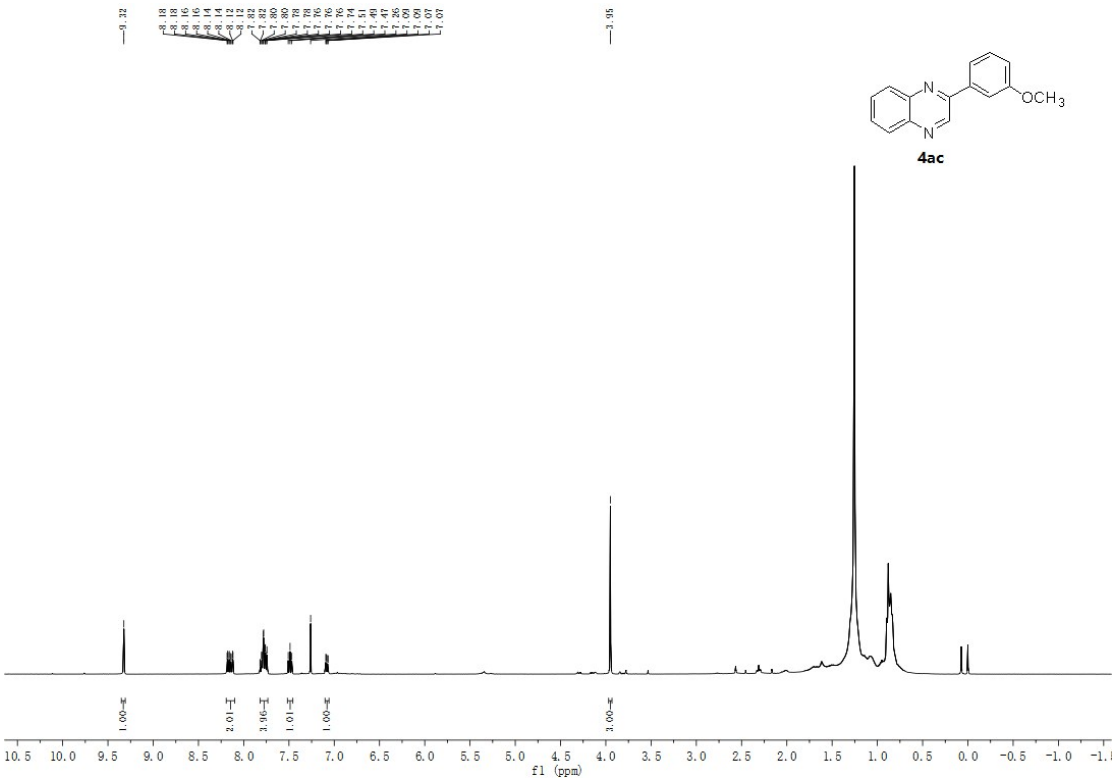
140.51
133.98
130.20
129.91
129.54
129.30
129.10
127.44
77.36
77.04
76.72
21.45
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

4ab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9.18
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8.16
8.14
8.14
8.12
8.12
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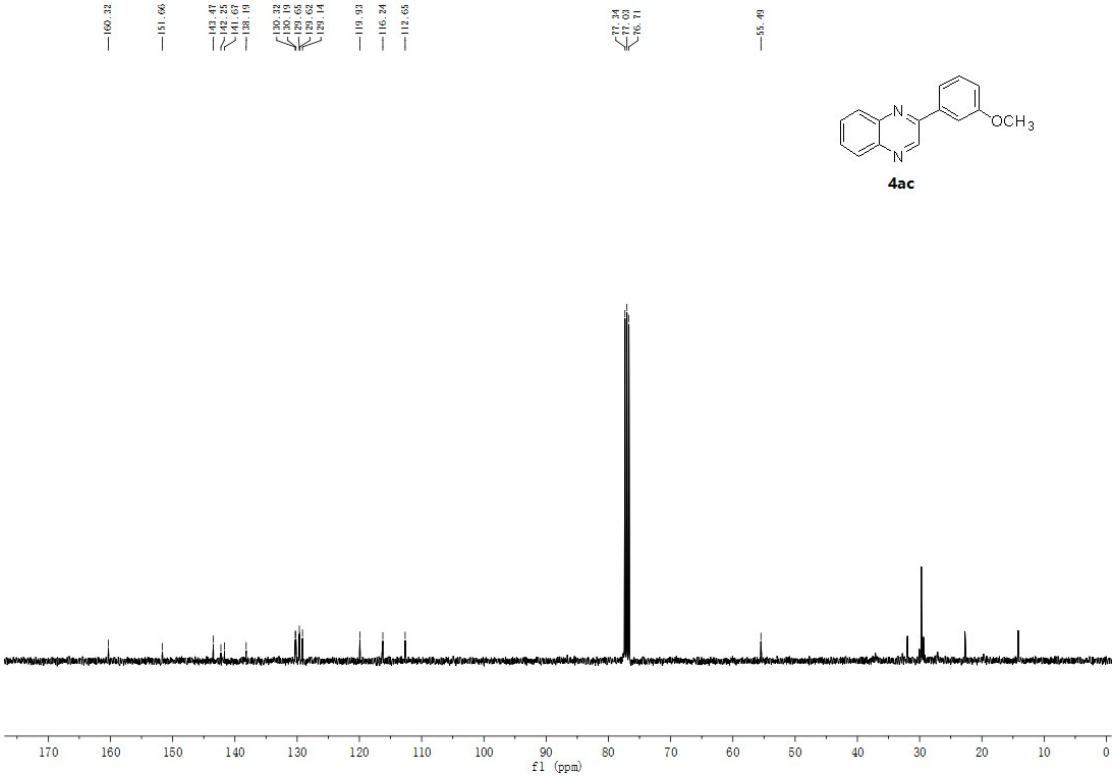
7.82
7.80
7.80
7.78
7.78
7.76
7.76
7.75
7.75
7.74
7.51
7.49
7.47
7.25
7.09
7.07
7.07
3.95
N
N
OCH3
4ac
1.00
2.01
3.96
1.01
1.00
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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138.19
130.32
130.19
129.65
129.64
129.14
119.93
116.24
112.65
77.34
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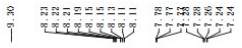
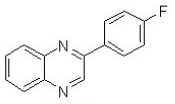
55.49
N
N
OCH3
4ac
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)





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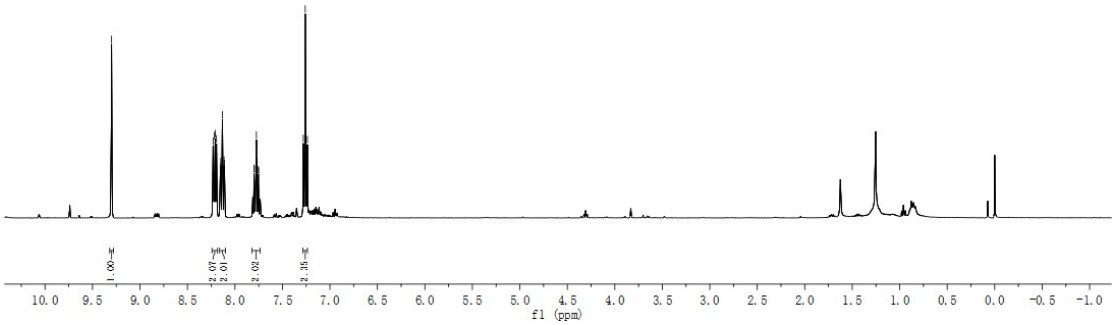
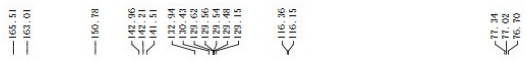
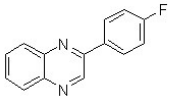
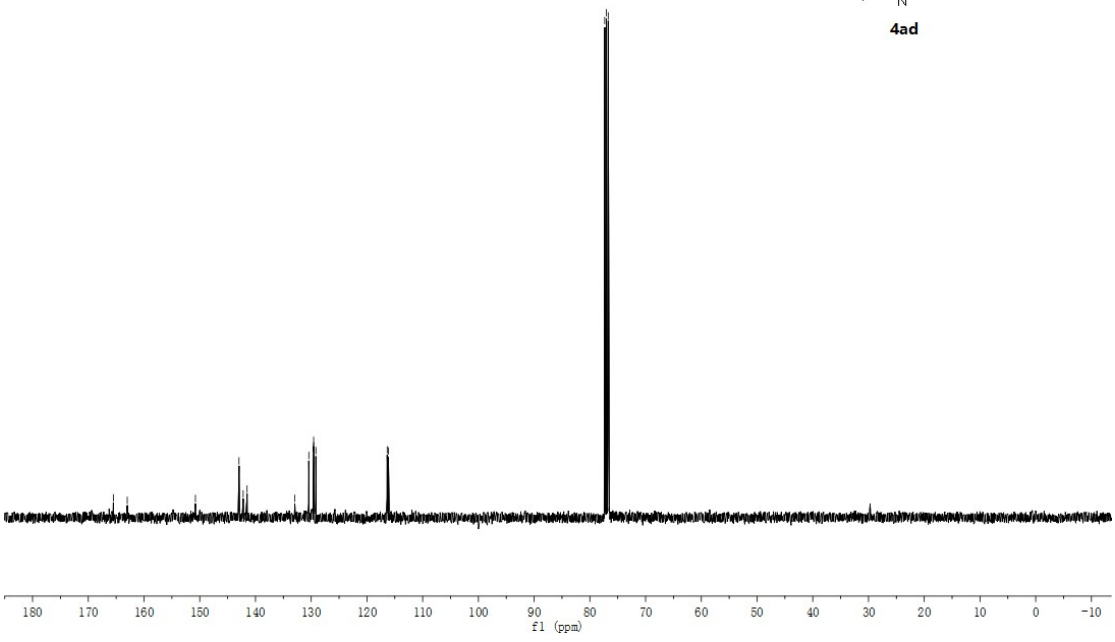
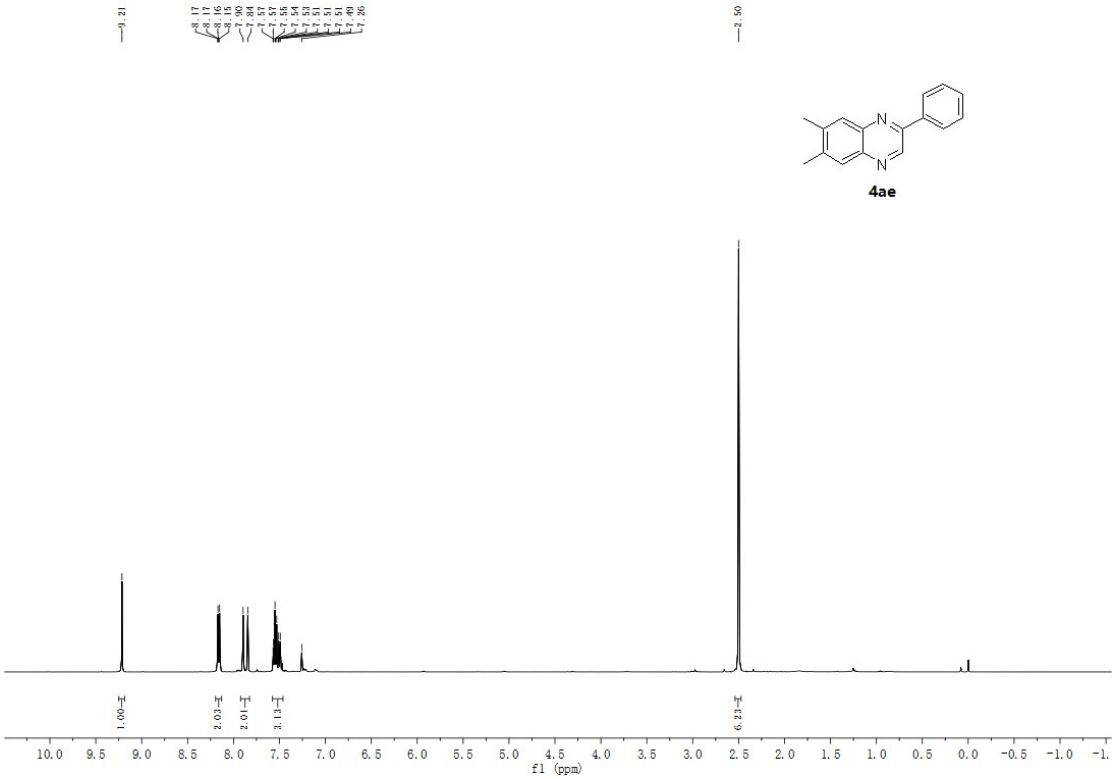






4ad

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7.55
7.54
7.53
7.51
7.51
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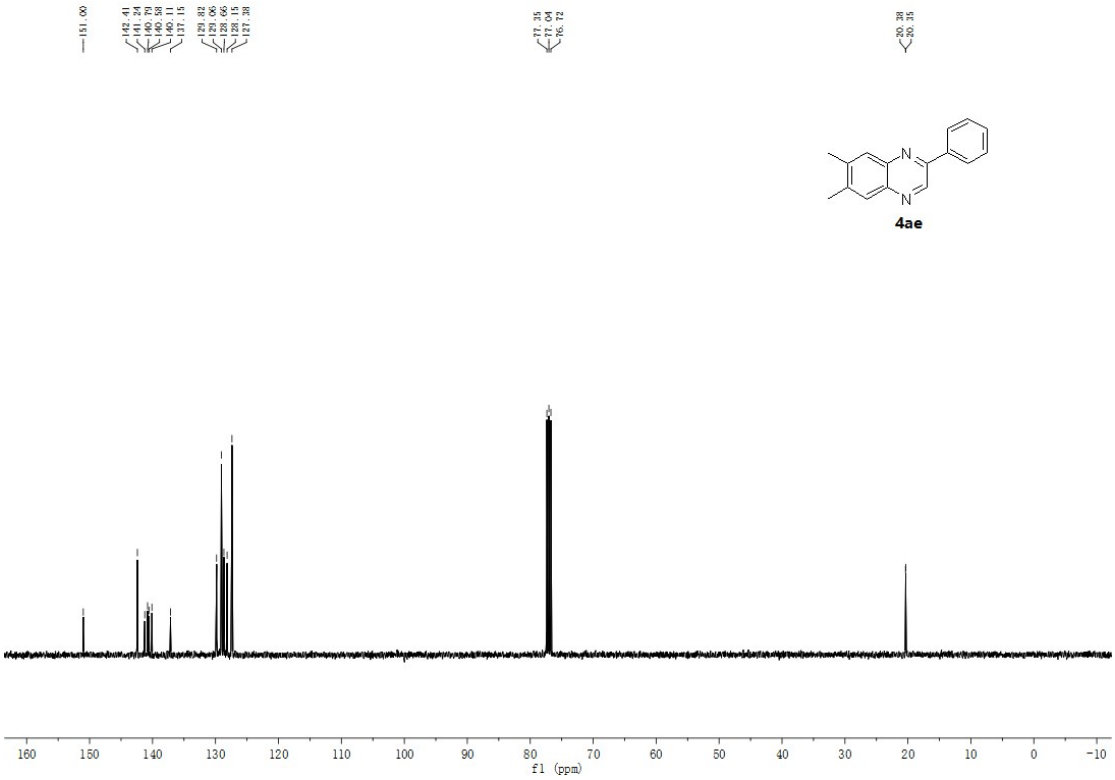
7.51
7.50
7.26
2.50
4ae
1.00
2.03
2.01
3.13
6.23
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.
f1 (ppm)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142.41
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140.79
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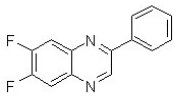
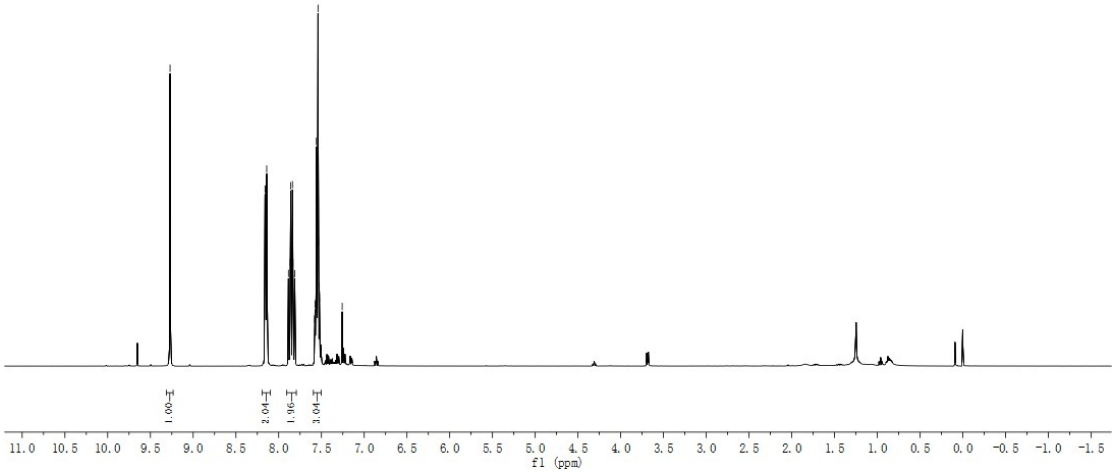
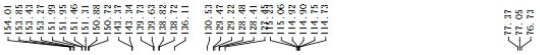
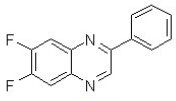
140.11
137.15
129.82
129.66
128.65
128.15
127.38
77.35
77.04
76.72
20.38
20.35
4ae
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



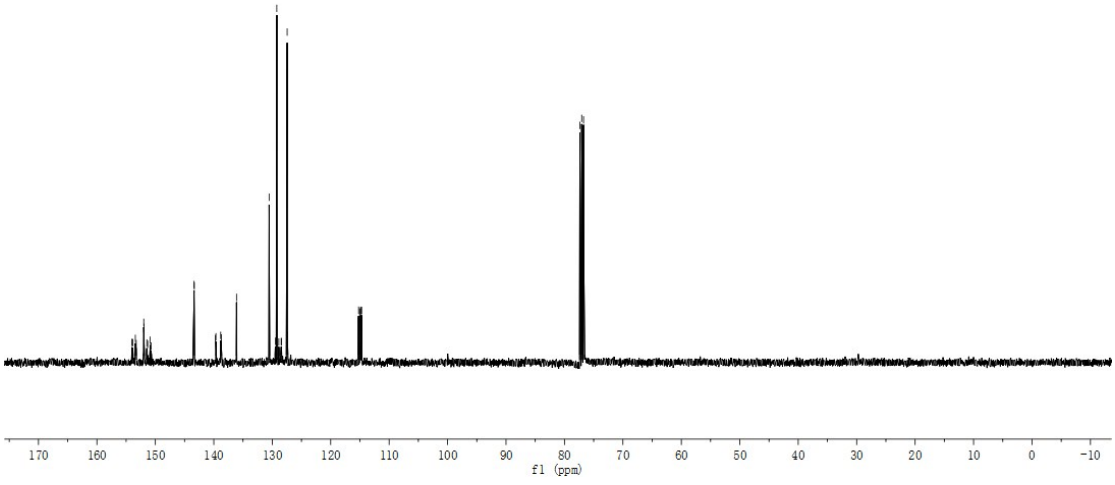
4af

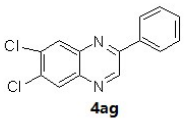






4af





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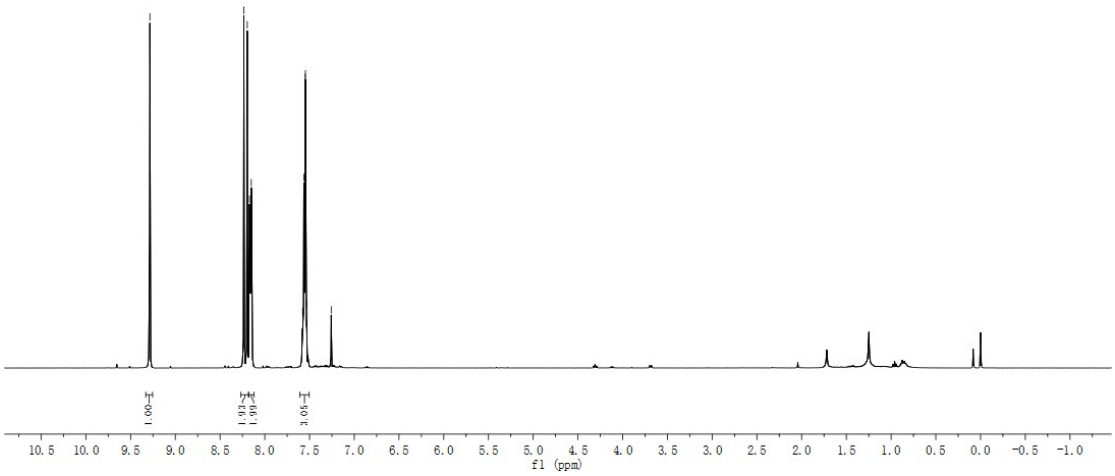

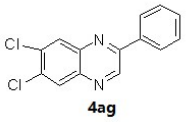

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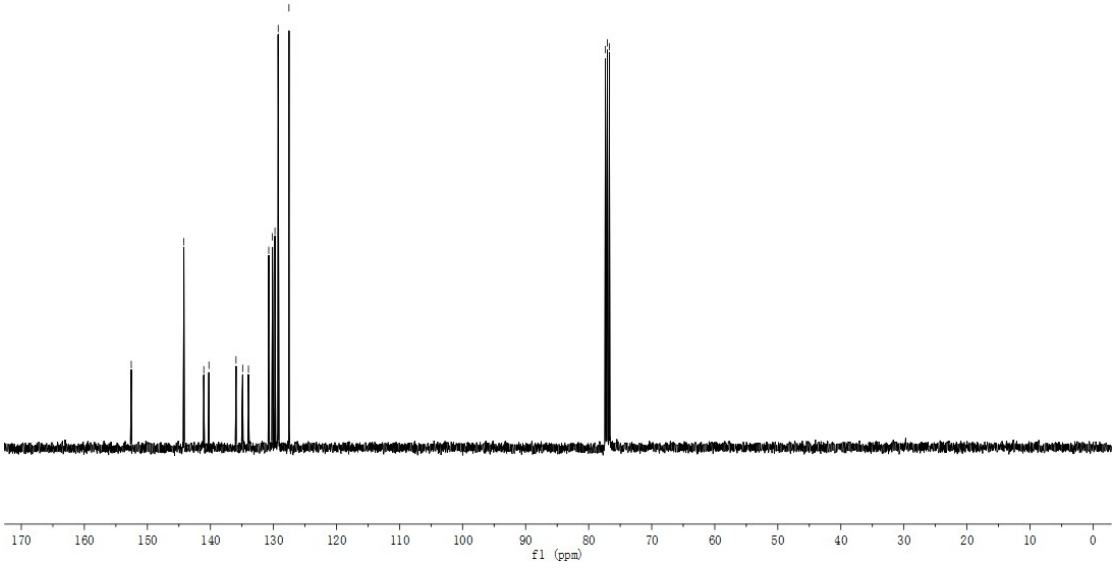
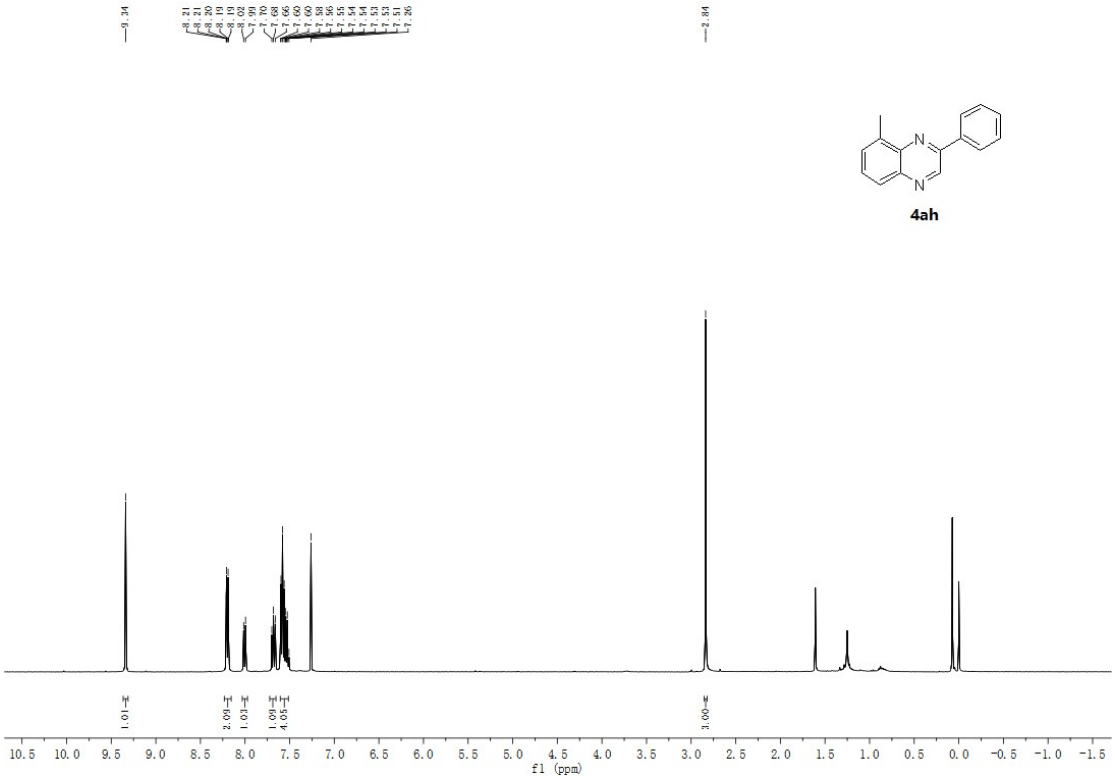
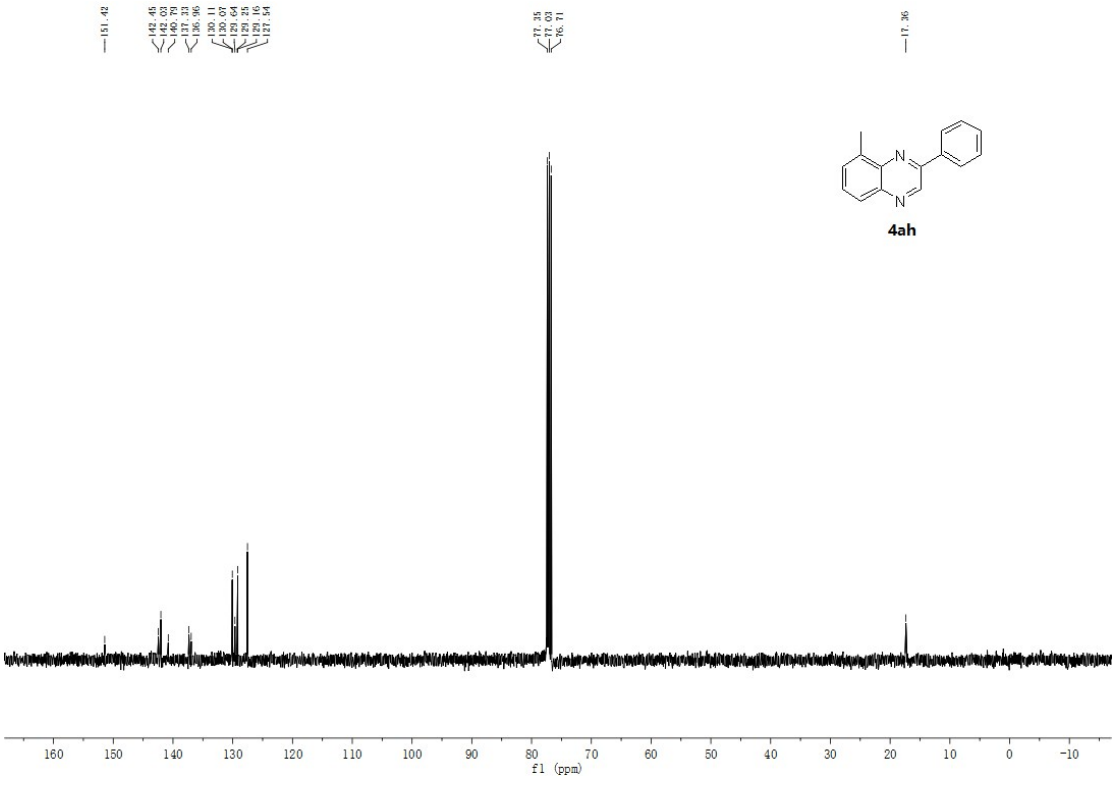
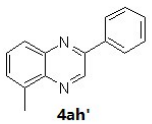
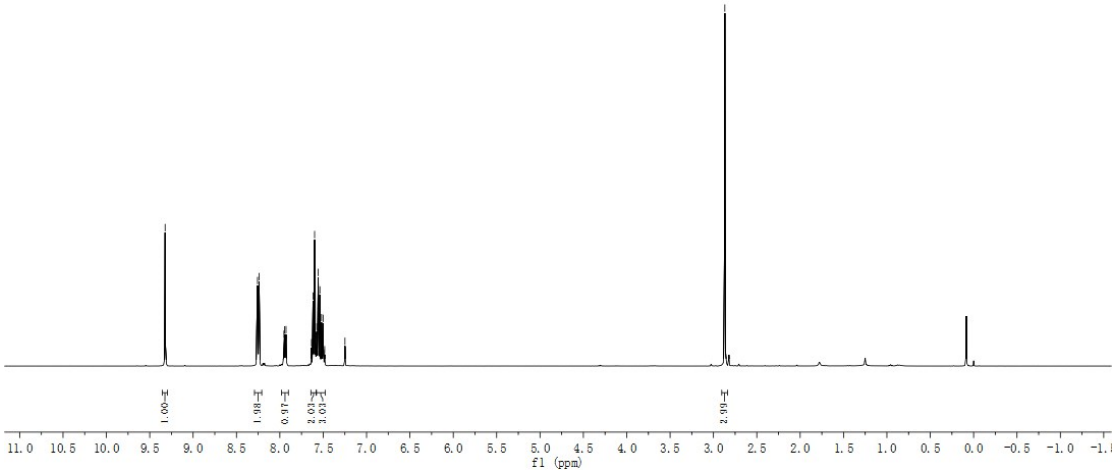


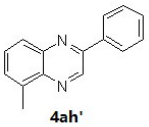

9.34
8.21
8.21
8.20
8.19
8.02
8.01
7.70
7.68
7.66
7.60
7.59
7.58
7.56
7.55
7.54
7.54
7.53
7.53
7.51
7.26
2.84
1.01
2.09
1.03
1.09
4.05
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)
N
N
4ah


151.42
142.45
142.03
140.79
137.33
136.96
130.11
130.07
129.64
129.25
129.16
127.54
77.35
77.03
76.71
17.36
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
N
N
4ah

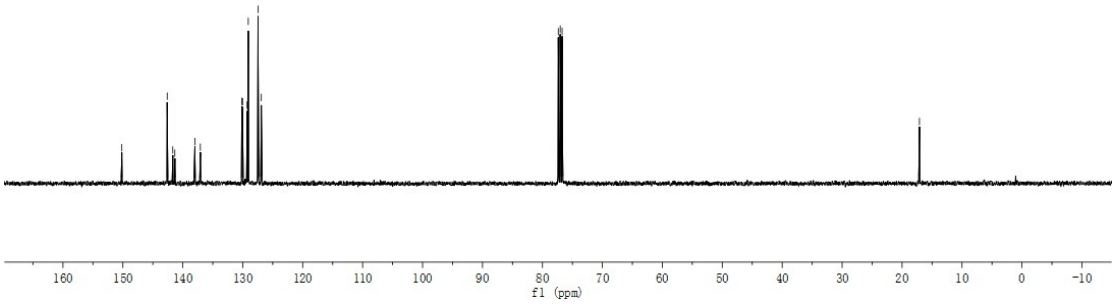


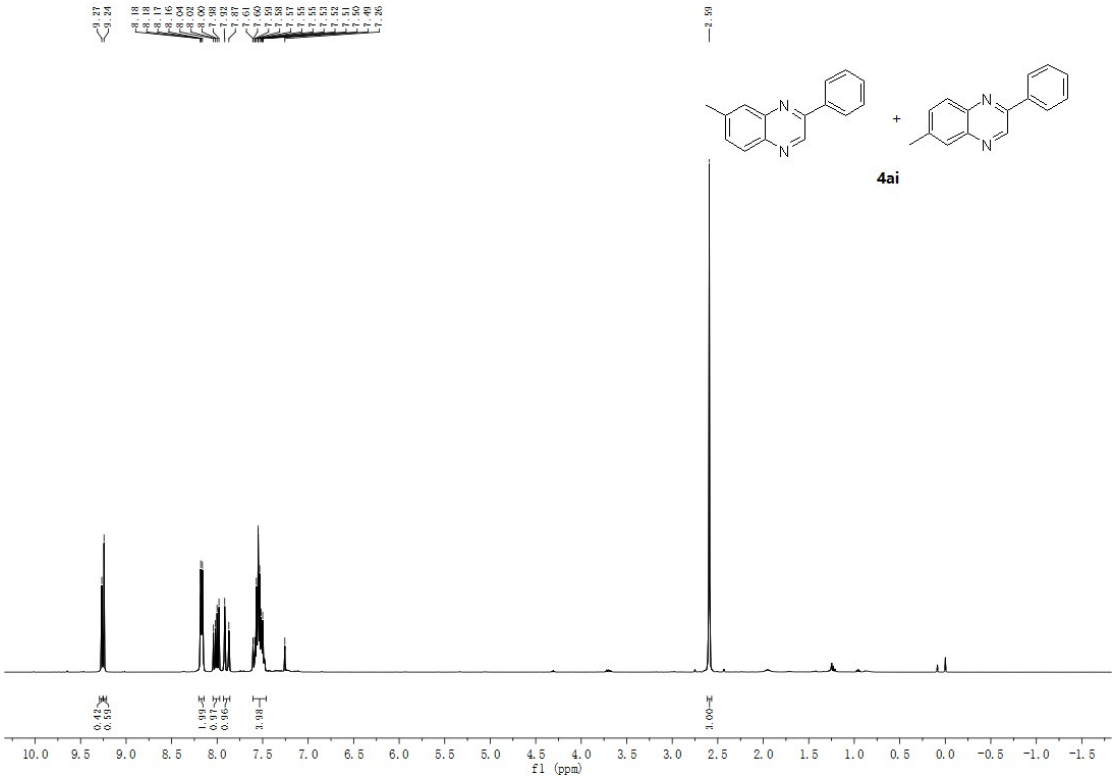
4ah'





4ah'

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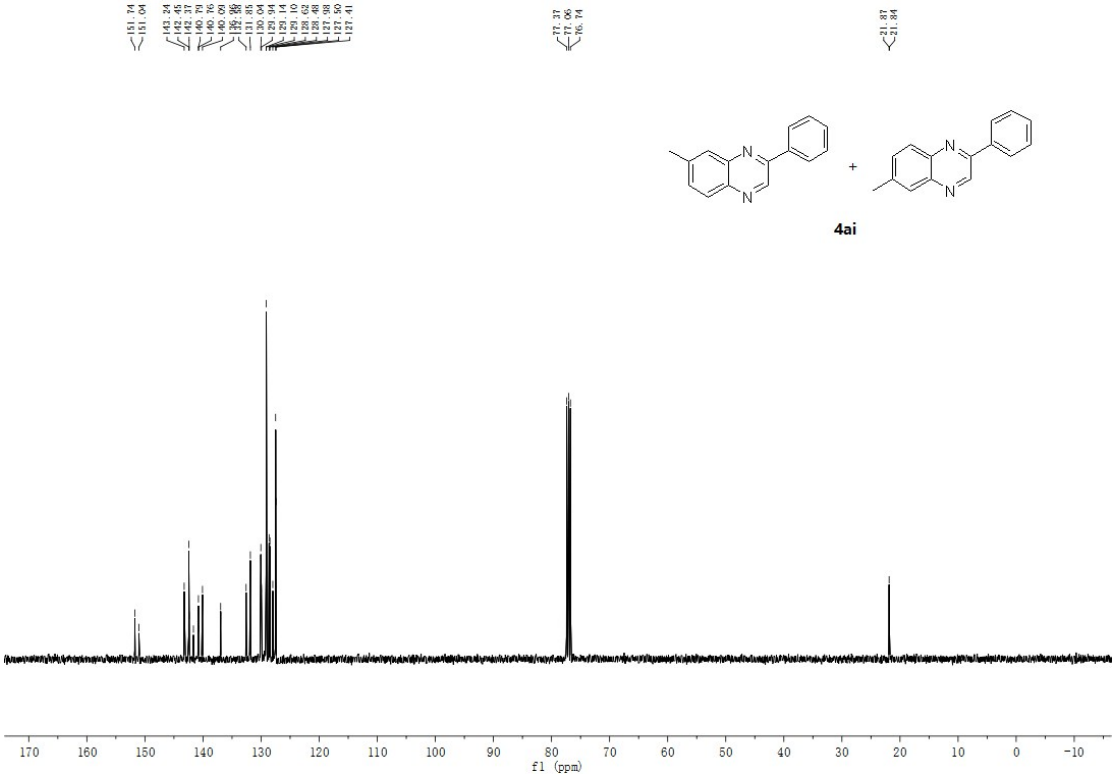
9.24
9.18
9.18
9.17
9.15
8.04
8.04
8.02
8.00
7.98
7.92
7.87
7.61
7.60
7.58
7.58
7.57
7.57
7.55
7.55
7.53
7.52
7.51
7.50
7.49
7.26
2.59
0.42
0.59
1.91
0.91
0.96
3.98
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)

4ai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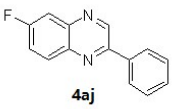
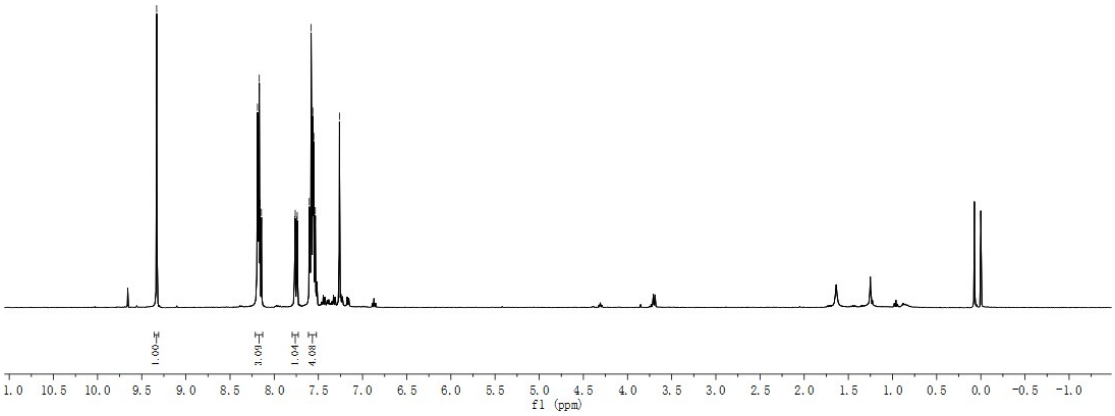
151.04
143.24
142.45
142.37
140.79
140.36
140.09
131.85
130.04
129.94
129.14
128.62
128.48
127.98
127.50
127.41
77.37
77.06
76.74
21.87
21.84
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

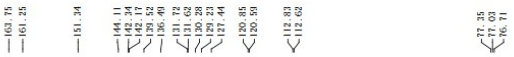
4ai


9.33
8.19
8.19
8.18
8.17
8.17
8.16
8.14
7.58
7.58
7.56
7.56
7.55
7.55


F
N
N

4aj


1.00
3.09
1.04
4.09
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


163.75
161.25
151.34
144.11
142.34
142.17
139.52
136.49
131.72
131.62
130.38
129.23
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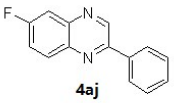
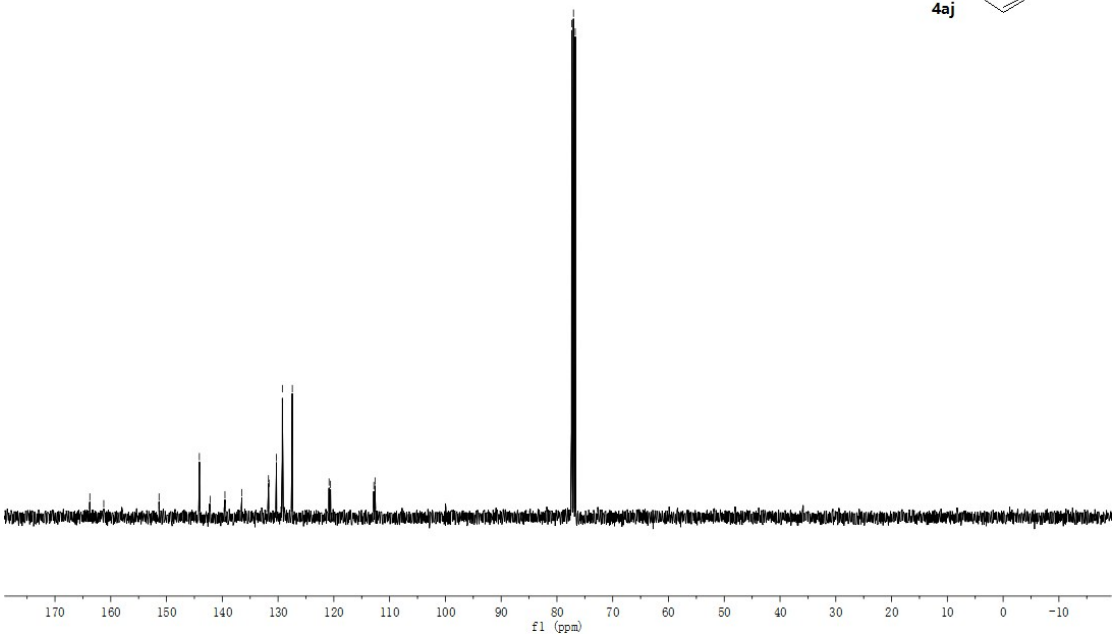
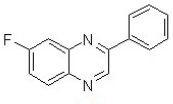
120.85
120.59
112.83
112.62
77.35
77.03
76.71

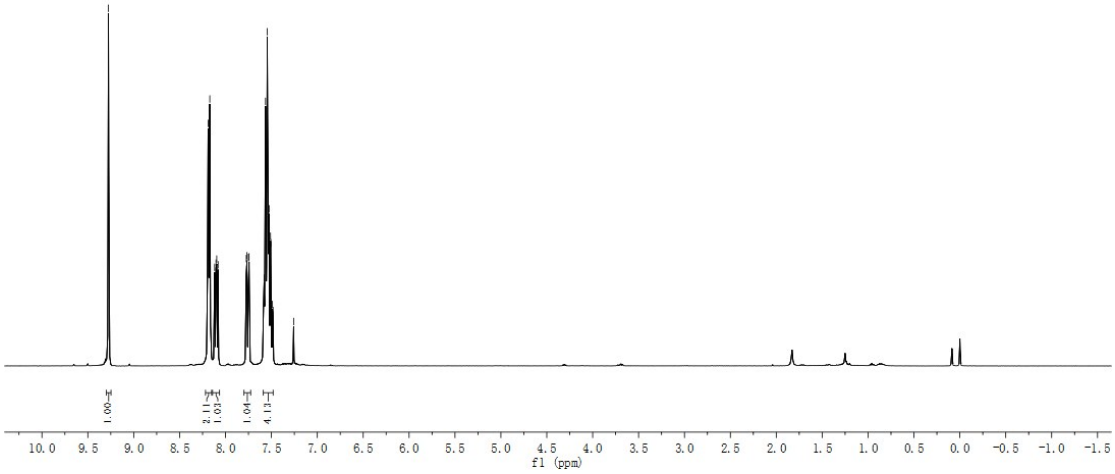

F
N
N

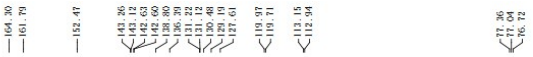
4aj

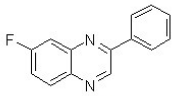

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



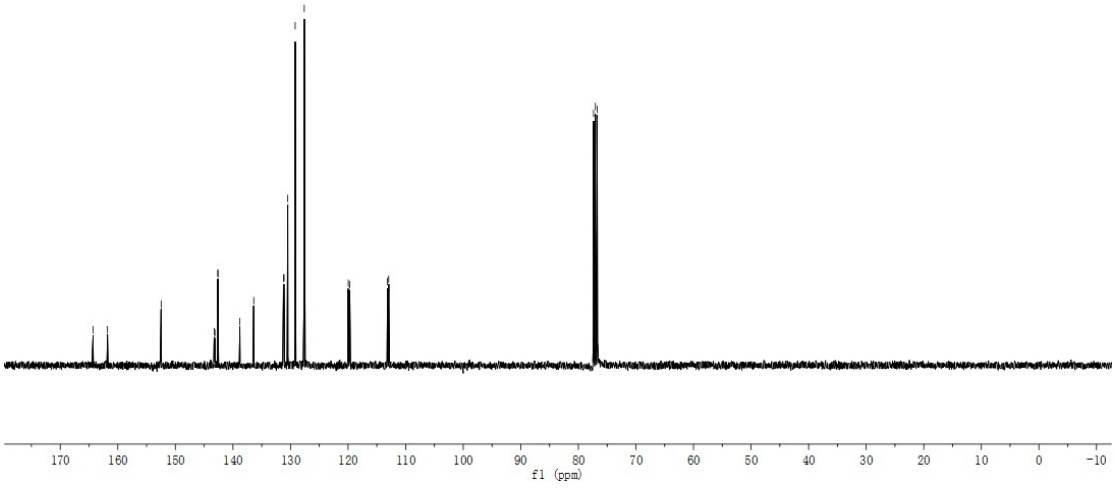
4aj'

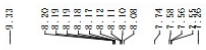


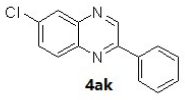




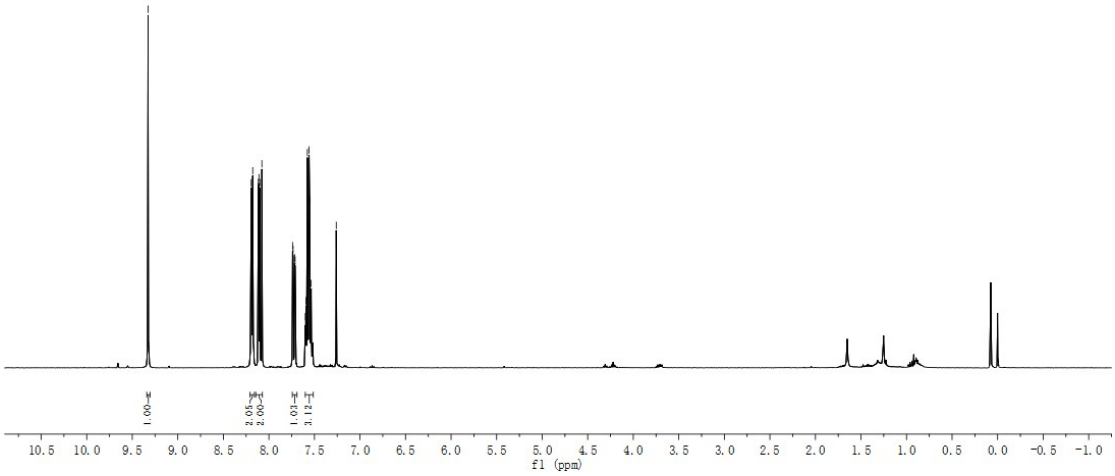
4aj'

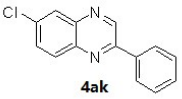




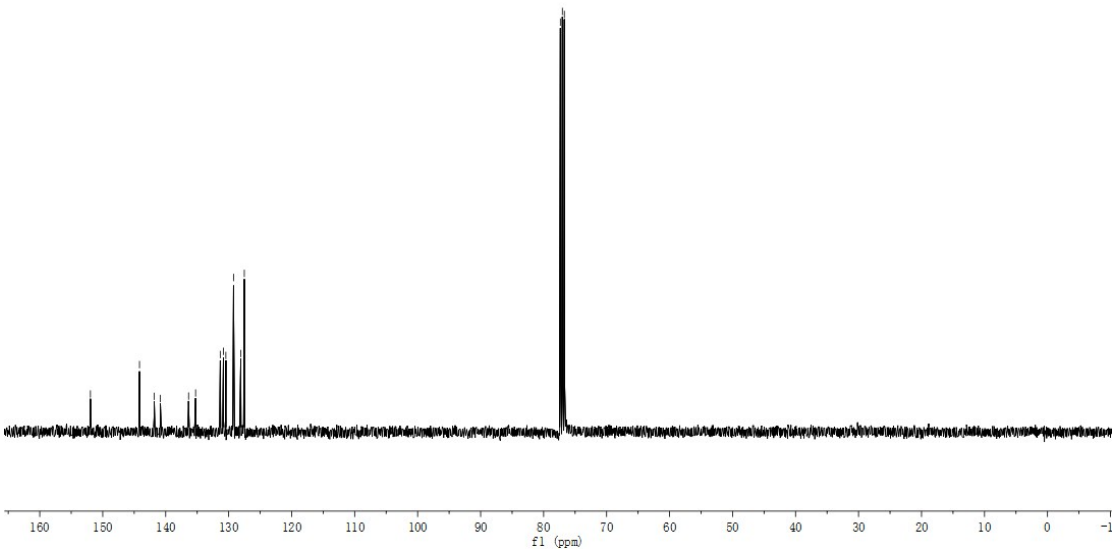

Cl
N
N

4ak


1.00
2.05
2.00
1.03
3.12
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)


Cl
N
N

4ak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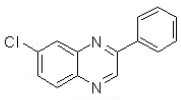
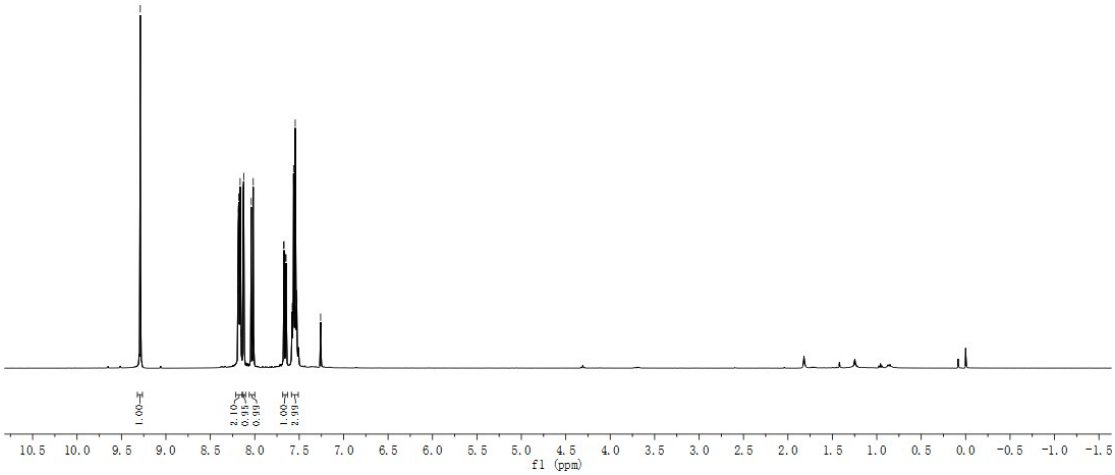
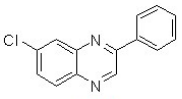
f1 (ppm)

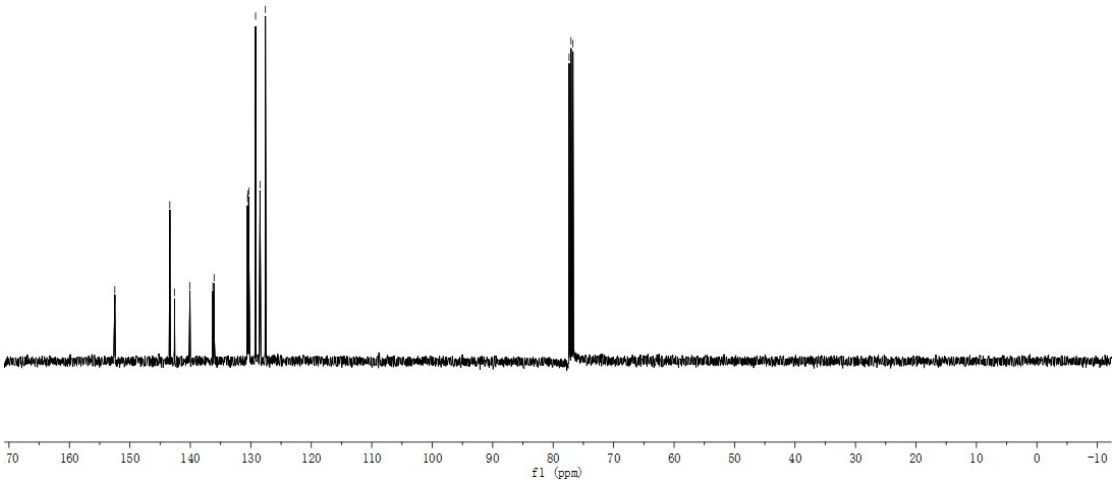


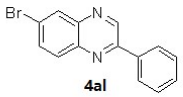
4ak'



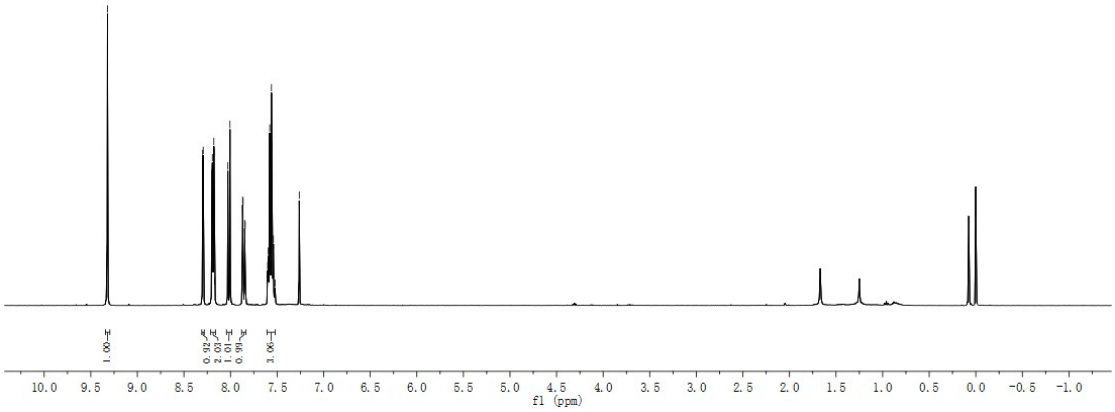


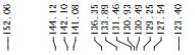
4ak'

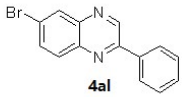



Br
N
N

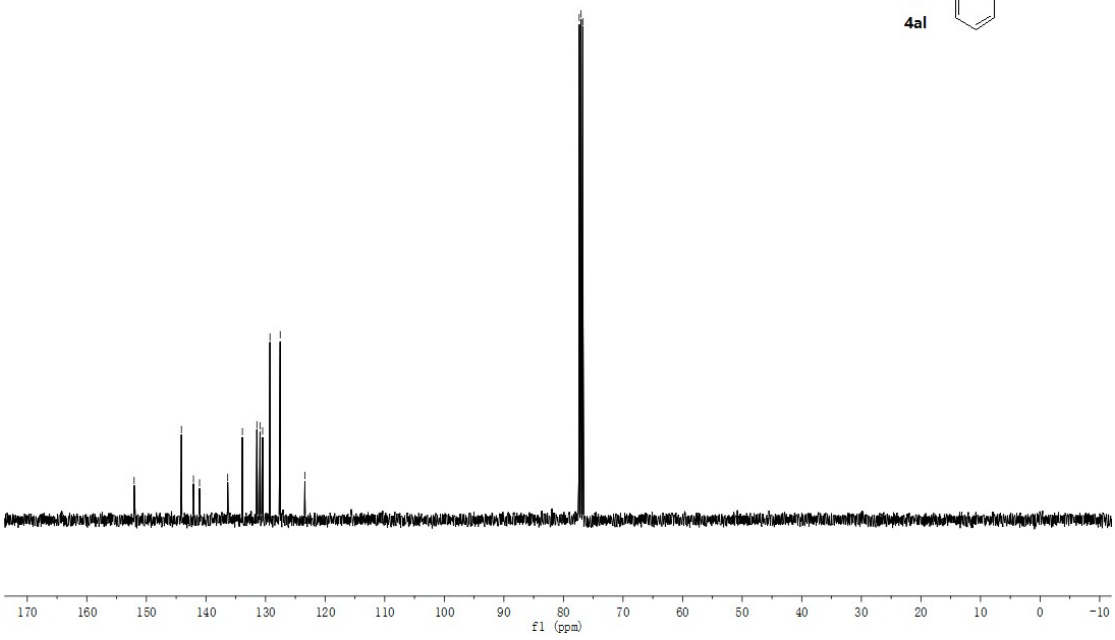
4al


1.00
0.92
2.03
1.01
0.99
3.06
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)




Br
N
N

4al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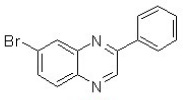
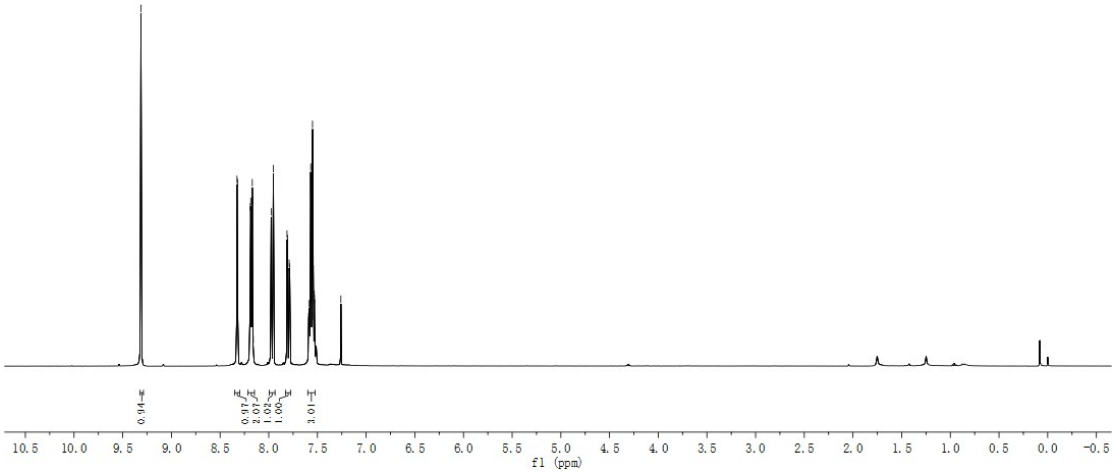
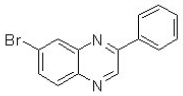
f1 (ppm)


Br
N
N

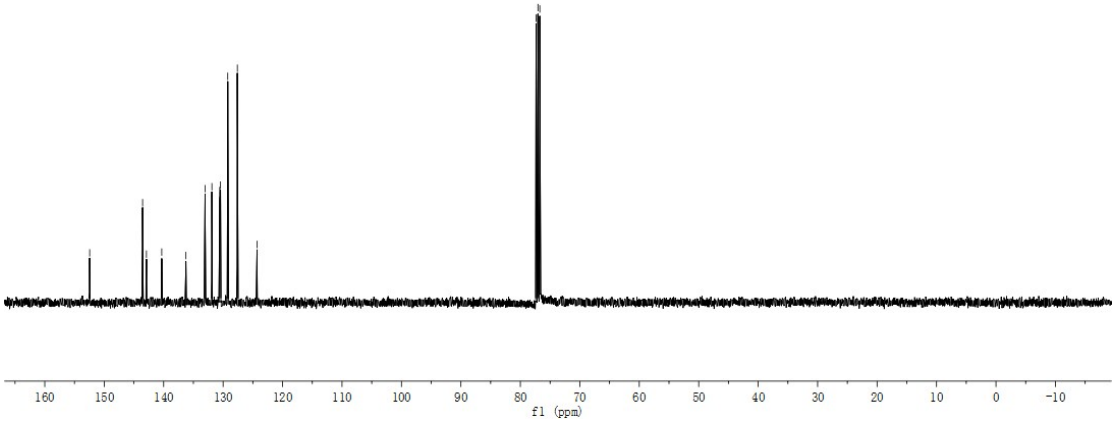
4al'

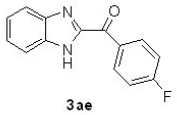

0.94
0.97
2.07
1.00
1.06
3.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


152.44
143.54
142.90
140.32
136.26
133.04
131.89
130.57
130.43
129.22
127.60
124.29
77.36
77.04
76.73

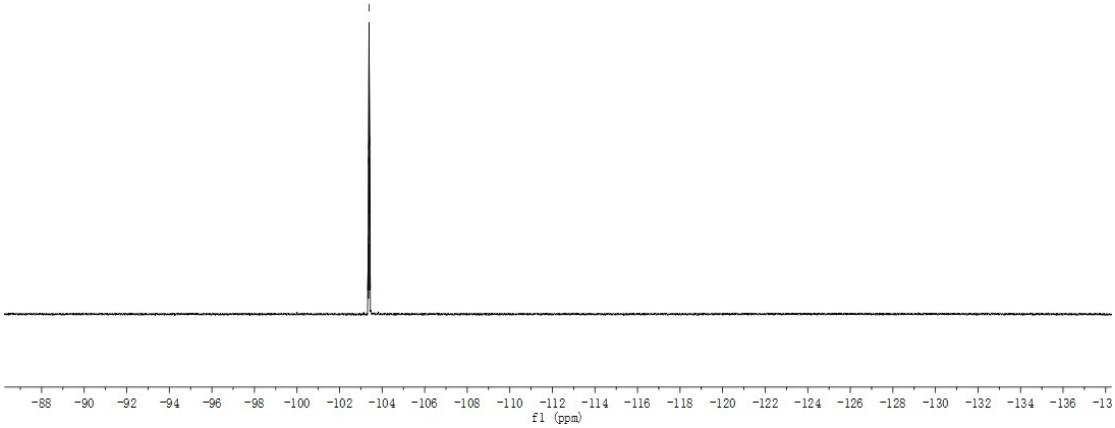

Br
N
N

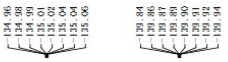
4al'

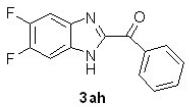

160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



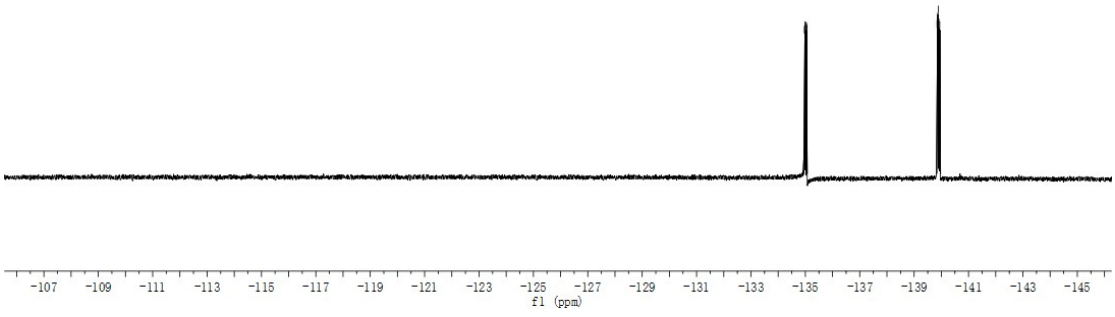
3ae

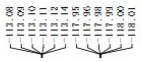






3ah




-113.08
-113.09
-113.10
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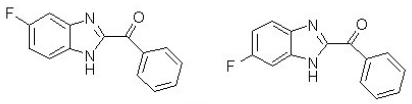
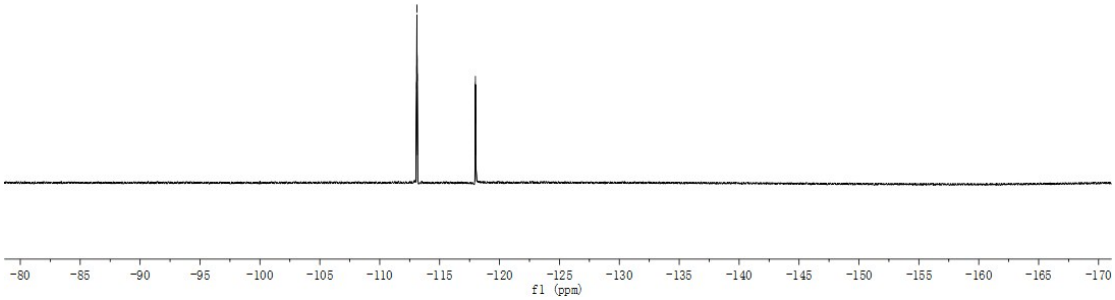
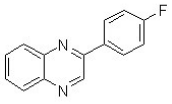
-113.13
-113.14
-113.15
-117.96
-117.98
-117.99
-118.00
-118.01



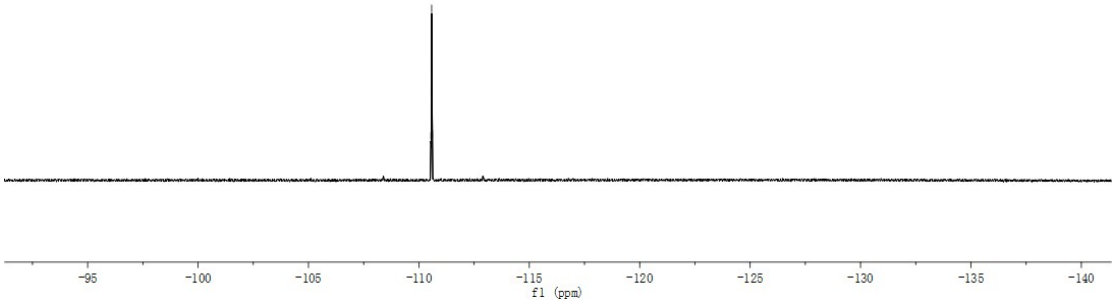
3al

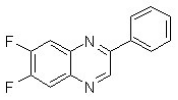

-80
-85
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
-155
-160
-165
-170
f1 (ppm)


-110.54
-110.56
-110.56
-110.58
-110.58
-110.59
-110.59
-110.60
-110.62



4ad


-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
f1 (ppm)



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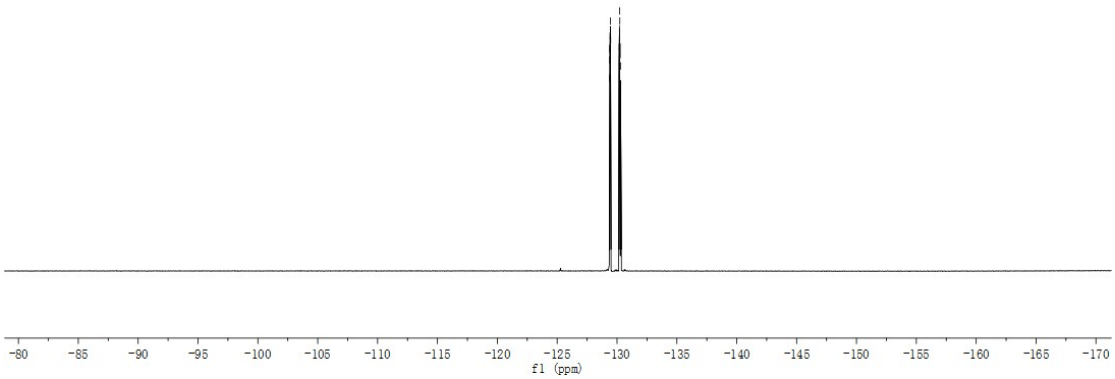
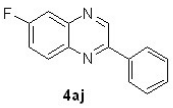
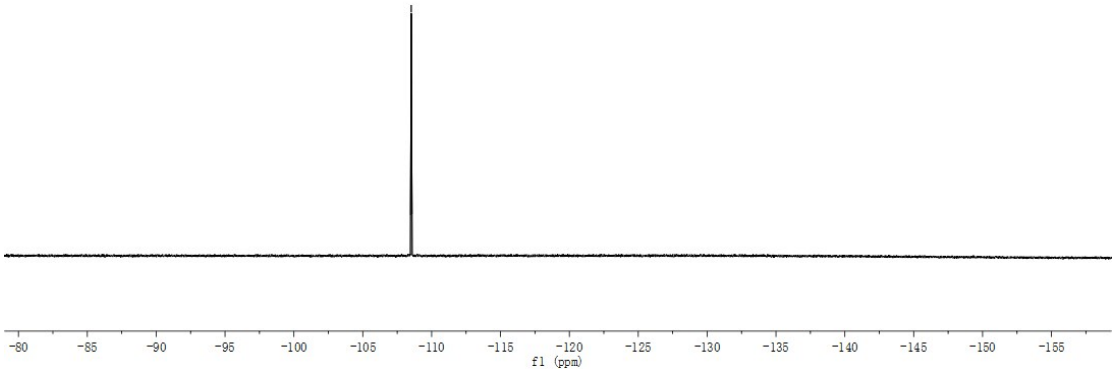
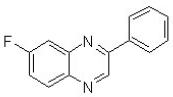

-80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150 -155 -160 -165 -170
f1 (ppm)



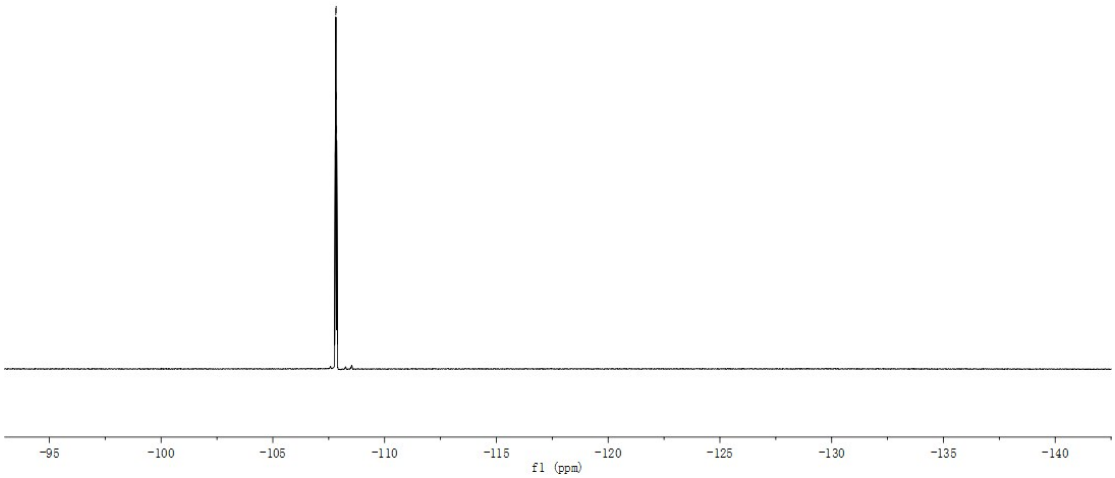
4aj


-80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150 -155
f1 (ppm)


-107.79
-107.81
-107.82
-107.83
-107.84
-107.85


F
N
N

4aj'


-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
f1 (ppm)