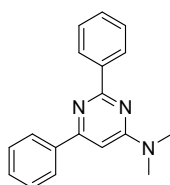


Procedure for model system: Under air, in a 25 mL reaction tube equipped with a stirring bar, benzonitrile (3 mmol), ^tBuOK (2 mmol) and DMAc (2 mL) were added. Then close the tube and heat it up to 110 °C for 16 h., cool the reaction mixture to room temperature when the reaction completed. The reaction solution was quenched with distilled water and extracted with ethyl acetate three times. The combined organic phases were washed with saturated NaCl solution and dried over Na₂SO₄. The crude product was purified by column chromatography to give the pure product.

N, N-Dimethyl-2, 6-diphenylpyrimidin-4-amine



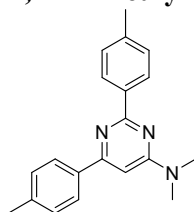
¹H NMR (300 MHz, Chloroform-*d*) δ 8.71 – 8.53 (m, 2H), 8.25 – 8.07 (m, 2H), 7.61 – 7.41 (m, 6H), 6.75 (s, 1H), 3.26 (s, 6H).

¹³C NMR (75 MHz, Chloroform-*d*) δ 163.48, 163.44, 163.14, 139.11, 138.96, 130.20, 130.00, 128.79, 128.44, 128.33, 127.26, 125.13, 96.18, 37.42.

GC-MS (EI, 70ev): *m/z*(%) = 246 (M+, 100), 276 (16), 275 (78), 261 (14), 260 (72), 247 (20), 232 (19), 231 (10).

HRMS(ESI): calcd. for [C₁₈H₁₇N₃ + H]⁺: 276.14952 ; found: 276.15003.

N, N-Dimethyl-2, 6-di-*p*-tolylpyrimidin-4-amine



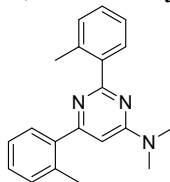
¹H NMR (300 MHz, Chloroform-*d*) δ 8.42 (d, *J* = 8.2 Hz, 2H), 8.00 (d, *J* = 8.1 Hz, 2H), 7.33 – 6.99 (m, 4H), 6.65 (s, 1H), 3.20 (s, 6H), 2.38 (s, 6H).

¹³C NMR (75 MHz, Chloroform-*d*) δ 163.49, 163.44, 163.05, 140.18, 140.07, 136.47, 136.20, 129.48, 25.46 – 16.39 (m), 129.07, 128.41, 127.16, 95.54, 37.40, 21.70, 21.60.

GC-MS (EI, 70ev): *m/z*(%) = 274 (M+, 100), 304 (15), 303 (67), 289 (15), 288 (66), 275 (21), 260 (16), 142 (19), 118 (27), 117 (11), 116 (35), 115 (38), 91 (11), 89 (12).

HRMS(ESI): calcd. for [C₂₀H₂₁N₃ + H]⁺: 304.18082; found: 304.18121.

N, N-Dimethyl-2,6-di-*o*-tolylpyrimidin-4-amine



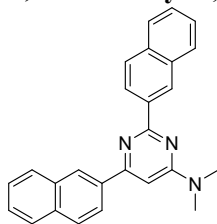
¹H NMR (300 MHz, Chloroform-*d*) δ 7.96 – 7.80 (m, 1H), 7.45 (dt, *J* = 6.6, 1.7 Hz, 1H), 7.36 – 7.15 (m, 6H), 6.44 (s, 1H), 3.20 (s, 5H), 2.64 (s, 3H), 2.49 (s, 3H).

¹³C NMR (75 MHz, Chloroform-*d*) δ 166.20, 162.59, 140.16, 139.65, 137.19, 136.13, 131.16, 130.89, 130.57, 129.47, 128.87, 128.75, 125.95, 125.80, 99.69, 37.41, 21.73, 20.70.

GC-MS (EI, 70ev): *m/z*(%) = 302 (M+, 100), 304 (18), 303 (93), 288 (47), 116 (16), 115 (24), 89 (10).

HRMS(ESI): calcd. for [C₂₀H₂₁N₃ + H]⁺: 304.18082; found: 304.18128.

N,N-Dimethyl-2, 6-di(naphthalen-2-yl)pyrimidin-4-amine



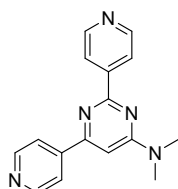
¹H NMR (300 MHz, Chloroform-*d*) δ 9.35 – 9.10 (m, 1H), 8.86 – 8.60 (m, 2H), 8.30 (dd, *J* = 8.6, 1.8 Hz, 1H), 8.14 – 7.77 (m, 6H), 7.67 – 7.39 (m, 4H), 6.89 (s, 1H), 3.32 (s, 6H).

¹³C NMR (75 MHz, Chloroform-*d*) δ 163.47, 163.06, 136.56, 136.26, 134.75, 134.43, 133.55 (d, *J* = 3.3 Hz), 129.40, 128.49, 128.44, 127.89 (d, *J* = 2.1 Hz), 127.04, 126.95, 126.79, 126.49, 126.08, 125.91, 124.75, 96.58, 37.53.

GC-MS (EI, 70ev): *m/z*(%) = 346 (M⁺, 100), 376 (19), 375 (73), 361 (15), 360 (55), 347 (26), 332 (17), 178 (29), 177 (12), 154 (16), 153 (24), 152 (41), 151 (20), 127 (13).

HRMS(ESI): calcd. for [C₂₆H₂₁N₃ + H]⁺: 376.18082; found: 376.18111.

N,N-Dimethyl-2, 6-di(pyridin-4-yl)pyrimidin-4-amine



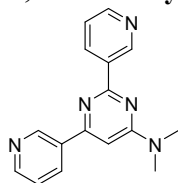
¹H NMR (300 MHz, Chloroform-*d*) δ 8.74 (td, *J* = 4.4, 1.7 Hz, 4H), 8.42 – 8.28 (m, 2H), 8.01 – 7.90 (m, 2H), 6.81 (s, 1H), 3.25 (s, 6H).

¹³C NMR (75 MHz, Chloroform-*d*) δ 163.34, 161.83, 160.68, 150.61, 150.25, 146.04, 145.62, 122.34, 121.24, 97.99, 37.53.

GC-MS (EI, 70ev): *m/z*(%) = 277 (M⁺, 100), 278 (20), 263 (14), 262 (77), 249 (15), 248 (90), 234 (18), 130 (33), 129 (36), 105 (67), 104 (15), 103 (61), 102 (15), 78 (35), 76 (23), 75 (10), 51 (21), 44 (44).

HRMS(ESI): calcd. for [C₁₆H₁₅N₃ + H]⁺: 278.14002; found: 278.14047.

N,N-Dimethyl-2, 6-di(pyridin-3-yl)pyrimidin-4-amine



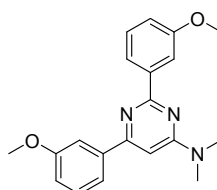
¹H NMR (300 MHz, Chloroform-*d*) δ 9.68 (dd, *J* = 2.2, 0.9 Hz, 1H), 9.25 (dd, *J* = 2.3, 0.9 Hz, 1H), 8.73 (dt, *J* = 7.9, 1.9 Hz, 1H), 8.66 (ddd, *J* = 5.0, 3.5, 1.7 Hz, 2H), 8.39 (ddd, *J* = 8.0, 2.3, 1.7 Hz, 1H), 7.37 (dddd, *J* = 9.6, 7.9, 4.8, 0.9 Hz, 2H), 6.70 (s, 1H), 3.21 (s, 6H).

¹³C NMR (75 MHz, Chloroform-*d*) δ 163.03, 161.85, 160.51, 150.95, 150.12, 148.43, 135.65, 134.36 – 133.05 (m), 134.65, 134.07, 133.99, 123.65, 123.24, 96.69, 37.41.

GC-MS (EI, 70ev): *m/z*(%) = 277 (M⁺, 100), 278 (19), 263 (14), 262 (73), 249 (16), 248 (90), 234 (24), 130 (41), 129 (55), 105 (65), 104 (15), 103 (61), 102 (19), 78 (22), 76 (23), 75 (10), 51 (13), 44 (22).

HRMS(ESI): calcd. for [C₁₆H₁₅N₃ + H]⁺: 278.14002; found: 278.1404.

2, 6-Bis (3-methoxyphenyl)-*N,N*-dimethylpyrimidin-4-amine



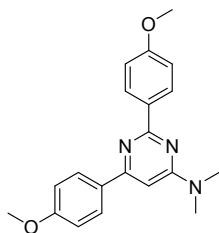
¹H NMR (300 MHz, Chloroform-*d*) δ 8.27 – 8.09 (m, 1H), 7.76 (dd, *J* = 2.6, 1.6 Hz, 1H), 7.69 (ddd, *J* = 7.7, 1.6, 0.9 Hz, 1H), 7.40 (td, *J* = 7.8, 0.7 Hz, 1H), 7.07 – 6.97 (m, 1H), 6.72 (s, 0H), 3.92 (d, *J* = 1.6 Hz, 3H), 3.23 (s, 3H).

¹³C NMR (75 MHz, Chloroform-*d*) δ 163.34, 163.14, 162.79, 160.07, 159.78, 140.60, 140.39, 129.73, 129.28, 121.03, 119.59, 116.04, 115.51, 113.59, 112.87, 96.41, 55.54 (d, *J* = 5.6 Hz), 37.37.

GC-MS (EI, 70ev): *m/z*(%) = 306 (M⁺, 100), 336 (20), 335 (97), 334 (69), 321 (12), 320 (59), 307 (21), 305 (26), 292 (13), 291 (10), 168 (30), 158 (25), 143 (12), 134 (30), 132 (42), 115 (13), 103 (14), 102 (16), 89 (12), 44 (13).

HRMS(ESI): calcd. for [C₂₀H₂₁N₃O₂ + H]⁺: 336.17065; found: 336.17106.

2, 6-Bis (4-methoxyphenyl)-*N, N*-dimethylpyrimidin-4-amine



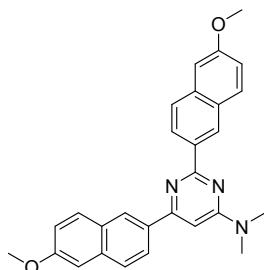
¹H NMR (300 MHz, Chloroform-*d*) δ 8.66 – 8.41 (m, 2H), 8.23 – 7.95 (m, 2H), 7.11 – 6.88 (m, 4H), 6.62 (s, 1H), 3.87 (d, *J* = 1.9 Hz, 6H), 3.22 (s, 6H).

¹³C NMR (75 MHz, Chloroform-*d*) δ 163.34, 163.05, 162.49, 161.44, 161.24, 131.95, 131.49, 129.93, 58.77 – 53.84 (m), 128.57, 114.04, 113.57, 94.54, 55.54, 55.50, 37.33.

GC-MS (EI, 70ev): *m/z*(%) = 306 (M⁺, 100), 336 (14), 335 (65), 321 (12), 320 (58), 307 (19), 292 (10), 158 (22), 134 (16), 133 (10), 132 (18).

HRMS(ESI): calcd. for [C₂₀H₂₁N₃O₂ + H]⁺: 336.17065; found: 336.17105.

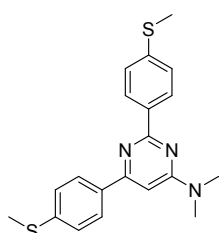
2, 6-Bis (6-methoxynaphthalen-2-yl)-*N, N*-dimethylpyrimidin-4-amine



¹H NMR (300 MHz, Chloroform-*d*) δ 9.06 (dd, *J* = 1.6, 0.8 Hz, 1H), 8.70 (dd, *J* = 8.6, 1.7 Hz, 1H), 8.66 – 8.59 (m, 1H), 8.26 (dd, *J* = 8.6, 1.8 Hz, 1H), 8.00 – 7.89 (m, 2H), 7.85 (dd, *J* = 8.7, 5.9 Hz, 2H), 7.25 – 7.12 (m, 4H), 6.86 (s, 1H), 3.96 (d, *J* = 1.0 Hz, 6H), 3.32 (s, 6H).

¹³C NMR (75 MHz, Chloroform-*d*) δ 163.37, 163.28, 162.86, 158.42, 158.34, 135.87, 135.58, 134.27, 133.87, 130.73, 130.43, 128.84, 128.79, 106.48 – 102.10 (m), 128.11, 126.69, 126.51, 126.30, 125.10, 119.16, 118.72, 105.71, 105.69, 95.74, 55.34 (d, *J* = 2.1 Hz), 37.34.

N, N-Dimethyl-2, 6-bis(4-(methylthio)phenyl)pyrimidin-4-amine



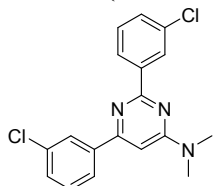
¹H NMR (300 MHz, Chloroform-*d*) δ 8.60 – 8.37 (m, 1H), 8.15 – 7.93 (m, 1H), 7.41 – 7.27 (m, 2H), 6.65 (s, 1H), 3.21 (s, 3H), 2.54 (d, *J* = 1.2 Hz, 3H).

¹³C NMR (75 MHz, Chloroform-*d*) δ 163.31, 162.96, 162.29, 141.02, 135.87, 135.42, 128.77, 127.50, 126.23, 125.81, 95.34, 37.37, 15.67.

GC-MS (EI, 70ev): *m/z*(%) = 338 (M+, 100), 369 (10), 368 (21), 367 (88), 353 (13), 352 (55), 340 (11), 339 (24), 324 (10), 277 (14), 184 (14), 175 (12), 174 (55), 159 (20), 150 (31), 149 (17), 148 (54), 134 (11), 133 (15), 127 (11), 44 (22).

HRMS(ESI): calcd. for [C₂₀H₂₁N₃S₂ + H]⁺: 368.12497; found: 368.12515.

2, 6-Bis (3-chlorophenyl)-*N,N*-dimethylpyrimidin-4-amine



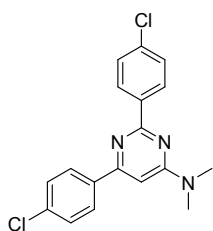
¹H NMR (300 MHz, Chloroform-*d*) δ 8.52 (td, *J* = 1.7, 0.8 Hz, 1H), 8.45 (ddd, *J* = 6.3, 2.4, 1.6 Hz, 1H), 8.10 (dt, *J* = 1.8, 1.1 Hz, 1H), 8.01 (ddd, *J* = 5.5, 3.1, 1.7 Hz, 1H), 7.50 – 7.36 (m, 4H), 6.71 (s, 1H), 3.26 (s, 7H).

¹³C NMR (75 MHz, Chloroform-*d*) δ 163.17, 162.16, 161.57, 140.56, 140.34, 134.74, 134.28, 130.13, 129.92, 129.46, 128.31, 127.20, 126.44, 125.22, 96.54, 37.37.

GC-MS (EI, 70ev): *m/z*(%) = 314 (M+, 100), 345 (40), 344 (12), 343 (59), 330 (39), 329 (11), 328 (57), 318 (11), 317 (12), 316 (66), 315 (20), 265 (12), 172 (13), 164 (23), 163 (18), 162 (61), 140 (18), 139 (13), 138 (84), 137 (24), 136 (95), 128 (10), 127 (46), 126 (30), 111 (20), 103 (12), 102 (21), 101 (22), 100 (14), 76 (13), 75 (31), 68 (12), 55 (15), 44 (96), 42 (15).

HRMS(ESI): calcd. for [C₁₈H₁₅Cl₂N₃ + H]⁺: 344.07158; found: 344.07205.

2, 6-Bis (4-chlorophenyl)-*N,N*-dimethylpyrimidin-4-amine



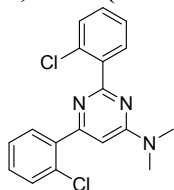
¹H NMR (300 MHz, Chloroform-*d*) δ 8.49 (d, *J* = 8.6 Hz, 1H), 8.13 – 8.01 (m, 1H), 7.55 – 7.29 (m, 3H), 6.69 (s, 1H), 3.25 (s, 4H).

¹³C NMR (75 MHz, Chloroform-*d*) δ 163.37, 162.59, 161.90, 137.39, 137.13, 136.41, 136.18, 129.81, 129.01, 128.55, 96.09, 37.51.

GC-MS (EI, 70ev): *m/z*(%) = 314 (M+, 100), 345 (36), 344 (12), 343 (54), 330 (36), 328 (53), 318 (11), 317 (12), 316 (64), 315 (18), 265 (10), 164 (25), 163 (18), 162 (71), 140 (17), 139 (13), 138 (80), 137 (26), 136 (99), 127 (37), 126 (31), 111 (17), 103 (17), 102 (21), 101 (18), 100 (12), 76 (10), 75 (26), 68 (11), 55 (14), 44 (70), 42 (12).

HRMS(ESI): calcd. for [C₁₈H₁₅Cl₂N₃ + H]⁺: 344.07158; found: 344.07169.

2, 6-Bis (2-chlorophenyl)-*N,N*-dimethylpyrimidin-4-amine



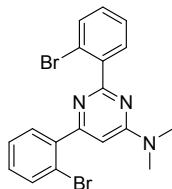
¹H NMR (300 MHz, Chloroform-*d*) δ 7.98 – 7.71 (m, 1H), 7.73 – 7.58 (m, 1H), 7.55 – 7.35 (m, 2H), 7.35 – 7.16 (m, 4H), 6.68 (s, 1H), 3.13 (s, 7H).

¹³C NMR (75 MHz, Chloroform-*d*) δ 164.29, 162.36, 162.18, 138.84, 138.39, 132.81, 132.13, 131.79, 131.49, 130.47, 130.19, 129.99, 129.79, 127.06, 126.62, 101.04, 37.24.

GC-MS (EI, 70ev): $m/z(\%) = 314 (M^+, 100), 345 (44), 344 (16), 343 (66), 330 (41), 329 (14), 328 (63), 318 (12), 317 (10), 316 (66), 315 (19), 205 (12), 164 (11), 163 (10), 162 (25), 140 (11), 138 (40), 137 (15), 136 (37), 127 (13), 126 (20), 102 (24), 101 (12), 100 (12), 75 (20), 44 (11), 42 (10).$

HRMS(ESI): calcd. for $[C_{18}H_{15}Cl_2N_3 + H]^+$: 344.07158; found: 344.07207.

2, 6-Bis (2-bromophenyl)-*N,N*-dimethylpyrimidin-4-amine



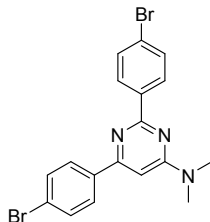
1H NMR (300 MHz, Chloroform-*d*) δ 7.86 (dd, $J = 7.7, 1.8$ Hz, 1H), 7.74 – 7.66 (m, 3H), 7.42 (tdd, $J = 7.5, 6.3, 1.3$ Hz, 2H), 7.33 – 7.19 (m, 2H), 6.72 (s, 1H), 3.25 (s, 6H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 165.16, 163.94, 162.19, 140.78, 140.55, 133.74, 133.50, 131.87, 130.20, 130.00, 127.69, 127.32, 121.92, 121.68, 101.04, 37.43.

GC-MS (EI, 70ev): $m/z(\%) = 404 (M^+, 100), 433 (64), 431 (33), 420 (26), 419 (10), 418 (52), 416 (27), 406 (50), 405 (19), 403 (11), 402 (53), 311 (12), 309 (12), 283 (13), 209 (14), 208 (29), 207 (15), 206 (28), 184 (30), 183 (11), 182 (69), 180 (39), 155 (10), 129 (19), 128 (20), 127 (60), 126 (20), 115 (12), 114 (11), 103 (14), 102(51), 101 (30), 100 (12), 76 (15), 75 (22), 44 (15).$

HRMS(ESI): calcd. for $[C_{18}H_{15}Br_2N_3 + H]^+$: 431.97055; found: 431.97089.

2, 6-Bis(4-bromophenyl)-*N,N*-dimethylpyrimidin-4-amine



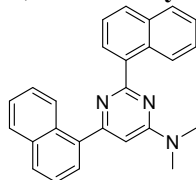
1H NMR (300 MHz, Chloroform-*d*) δ 8.41 (d, $J = 8.6$ Hz, 2H), 8.11 – 7.89 (m, 2H), 7.80 – 7.47 (m, 4H), 6.67 (s, 1H), 3.22 (s, 6H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 163.31, 162.61, 161.88, 137.85, 137.56, 131.94, 131.47, 130.06, 128.76, 124.92, 124.52, 96.05, 37.46.

GC-MS (EI, 70ev): $m/z(\%) = 404 (M^+, 100), 433 (59), 431 (31), 420 (24), 418 (47), 416 (25), 406 (49), 405 (19), 403 (10), 402 (51), 309 (10), 216 (14), 209 (10), 208 (41), 207 (13), 206 (42), 184 (26), 183 (14), 182 (77), 181 (13), 180 (50), 155 (11), 128 (17), 127 (84), 126 (16), 103 (13), 102(32), 101 (39), 100 (13), 76 (18), 75 (23), 44 (46).$

HRMS(ESI): calcd. for $[C_{18}H_{15}Br_2N_3 + H]^+$: 431.97055; found: 431.97054.

N,N-Dimethyl-2, 6-di (naphthalen-1-yl) pyrimidin-4-amine



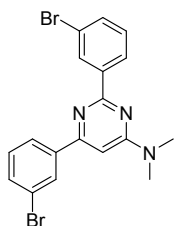
1H NMR (300 MHz, Chloroform-*d*) δ 9.02 – 8.84 (m, 1H), 8.38 – 8.28 (m, 1H), 8.17 (dd, $J = 7.2, 1.3$ Hz, 1H), 7.91 (ddd, $J = 9.2, 8.0, 2.5$ Hz, 4H), 7.73 (dd, $J = 7.1, 1.3$ Hz, 1H), 7.65 – 7.40 (m, 7H), 6.71 (s, 1H), 3.26 (s, 6H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 166.06, 165.63, 162.75, 138.31, 137.48, 134.29, 134.07, 131.55, 131.28, 129.90, 129.40, 129.04, 128.54, 128.47, 127.26, 126.74, 126.61, 126.30, 126.11, 125.98, 125.67, 125.45, 125.43, 101.07, 37.48.

GC-MS (EI, 70ev): $m/z(\%) = 374 (M^+, 100), 376 (15), 375 (71), 360 (10), 152 (12), 151 (20).$

HRMS(ESI): calcd. for $[C_{26}H_{21}N_3 + H]^+$: 376.18082; found: 376.18102.

2, 6-Bis (3-bromophenyl)-*N, N*-dimethylpyrimidin-4-amine



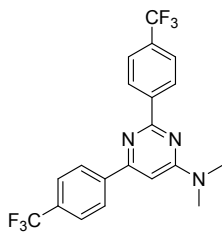
1H NMR (300 MHz, Chloroform-*d*) δ 8.67 (t, $J = 1.8$ Hz, 1H), 8.49 (dt, $J = 7.8, 1.3$ Hz, 1H), 8.25 (t, $J = 1.8$ Hz, 1H), 8.05 (ddd, $J = 7.8, 1.7, 1.0$ Hz, 1H), 7.59 (dddd, $J = 7.9, 4.0, 2.0, 1.1$ Hz, 2H), 7.36 (td, $J = 7.9, 6.6$ Hz, 2H), 6.70 (s, 1H), 3.26 (s, 7H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 163.32, 162.23, 161.69, 141.00, 140.81, 133.22, 133.02, 131.41, 130.39, 130.25, 129.94, 127.08, 125.88, 123.09, 122.69, 96.72, 37.55.

GC-MS (EI, 70ev): $m/z(\%) = 404$ (M+, 100), 435 (34), 434 (14), 433 (68), 431 (34), 420 (24), 419 (10), 418 (50), 416 (24), 406 (48), 405 (17), 402 (49), 208 (11), 206 (11), 184 (10), 182 (23), 180 (14), 127 (35), 102 (16), 101 (15), 76 (10), 75 (13), 44 (14).

HRMS(ESI): calcd. for $[C_{18}H_{15}Br_2N_3 + H]^+$: 431.97055; found: 431.9707.

N, N-Dimethyl-2,6-bis(4-(trifluoromethyl)phenyl)pyrimidin-4-amine



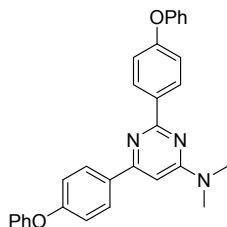
1H NMR (300 MHz, Chloroform-*d*) δ 8.64 (dp, $J = 7.7, 0.9$ Hz, 1H), 8.20 (dq, $J = 8.7, 0.9$ Hz, 1H), 7.87 – 7.62 (m, 2H), 6.72 (s, 0H), 3.22 (s, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 163.10, 162.09, 161.40, 141.99, 141.80, 131.70 (qd, $J = 32.3, 3.6$ Hz), 129.66 (d, $J = 16.4$ Hz), 128.50, 127.33, 126.05 (d, $J = 16.6$ Hz), 125.56 (q, $J = 3.8$ Hz), 125.06 (p, $J = 3.4, 2.9$ Hz), 122.44 (d, $J = 16.4$ Hz), 118.84 (d, $J = 16.4$ Hz), 96.97, 37.25.

GC-MS (EI, 70ev): $m/z(\%) = 382$ (M+, 100), 412 (16), 411 (69), 397 (14), 396 (67), 392 (14), 383 (20), 196 (17), 176 (15), 172 (18), 170 (27), 44 (13).

HRMS(ESI): calcd. for $[C_{20}H_{15}F_6N_3 + H]^+$: 412.12429; found: 412.12452.

N, N-Dimethyl-2, 6-bis(4-phenoxyphenyl)pyrimidin-4-amine



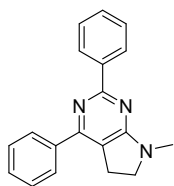
1H NMR (300 MHz, Chloroform-*d*) δ 8.63 – 8.49 (m, 2H), 8.22 – 8.07 (m, 2H), 7.47 – 7.33 (m, 4H), 7.20 – 7.01 (m, 5H), 6.68 (s, 1H), 3.24 (s, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 163.35, 162.92, 162.36, 159.22, 159.10, 157.17, 156.97, 134.23, 133.80, 130.14, 130.01, 129.94, 128.82, 123.80, 123.59, 119.39, 119.30, 118.75, 118.41, 95.24, 37.36.

GC-MS (EI, 70ev): $m/z(\%) = 430$ (M+, 100), 460 (21), 459 (67), 445 (16), 444 (43), 431 (31), 220 (16), 196 (11), 194 (12), 77 (21).

HRMS(ESI): calcd. for $[C_{30}H_{25}N_3O_2 + H]^+$: 460.20195; found: 460.20216.

7-Methyl-2, 4-diphenyl-6, 7-dihydro-5H-pyrrolo[2,3-*d*]pyrimidine



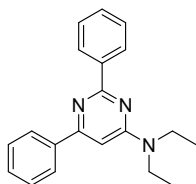
¹H NMR (300 MHz, Chloroform-*d*) δ 8.65 – 8.36 (m, 1H), 8.17 – 7.94 (m, 1H), 7.59 – 7.38 (m, 3H), 3.78 – 3.56 (m, 1H), 3.43 – 3.23 (m, 1H), 3.12 (s, 2H).

¹³C NMR (75 MHz, Chloroform-*d*) δ 169.04 , 163.45 , 154.48 , 138.97 , 138.45 , 130.01 , 129.34 , 128.61 , 128.31 , 114.12 , 51.45 , 31.64 , 26.31 .

GC-MS (EI, 70ev): m/z(%) = 286 (M⁺, 100), 287 (55).

HRMS(ESI): calcd. for [C₁₉H₁₇N₃ + H]⁺: 288.14952; found: 288.14962.

N, N-Diethyl-2,6-diphenylpyrimidin-4-amine



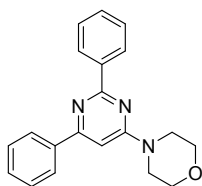
¹H NMR (300 MHz, Chloroform-*d*) δ 8.72 – 8.60 (m, 1H), 8.29 – 8.05 (m, 1H), 7.67 – 7.41 (m, 3H), 6.75 (s, 0H), 3.70 (q, *J* = 7.3 Hz, 4H), 1.32 (t, *J* = 7.1 Hz, 6H).

¹³C NMR (75 MHz, Chloroform-*d*) δ 163.62 , 163.04 , 161.84 , 139.26 , 139.14 , 130.05 , 129.82 , 128.71 , 128.35 , 128.24 , 127.18 , 96.12 , 42.56 , 13.10 .

GC-MS (EI, 70ev): m/z(%) = 274 (M⁺, 100), 304 (16), 302 (12), 288 (16), 275 (42), 261 (12), 260 (71), 129 (10), 128 (56), 104 (31), 103 (11), 102 (31), 101 (11), 77 (24), 29 (15).

HRMS(ESI): calcd. for [C₂₀H₂₁N₃ + H]⁺: 304.18082; found: 304.1812.

4-(2,6-Diphenylpyrimidin-4-yl)morpholine



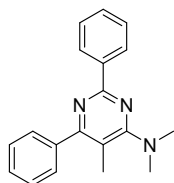
¹H NMR (300 MHz, Chloroform-*d*) δ 8.82 – 8.39 (m, 2H), 8.23 – 7.98 (m, 2H), 7.64 – 7.37 (m, 6H), 3.94 – 3.67 (m, 4H), 6.81 (s, 0H), 3.89 – 3.82 (m, 2H), 3.79 (dd, *J* = 5.7, 3.4 Hz, 2H).

¹³C NMR (75 MHz, Chloroform-*d*) δ 163.88 , 163.72 , 163.46 , 138.71 , 138.59 , 130.41 , 130.22 , 128.82 , 128.42 , 128.37 , 127.24 , 96.52 , 66.79 , 44.50 .

GC-MS (EI, 70ev): m/z(%) = 286 (M⁺, 100), 318 (14), 317 (66), 316 (21), 287 (37), 272 (23), 261 (14), 260 (68), 259 (25), 232 (17), 231 (11), 129 (14), 128 (41), 104 (33), 103 (22), 102 (53), 101 (14), 77 (29), 76 (13).

HRMS(ESI): calcd. for [C₂₀H₁₉N₃O + H]⁺: 318.16009; found: 318.16032.

N, N, 5-Trimethyl-2,6-diphenylpyrimidin-4-amine



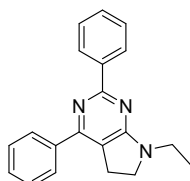
¹H NMR (300 MHz, Chloroform-*d*) δ 8.64 – 8.31 (m, 2H), 7.77 – 7.64 (m, 2H), 7.57 – 7.35 (m, 6H), 3.17 (s, 6H), 2.26 (s, 3H).

¹³C NMR (75 MHz, Chloroform-*d*) δ 167.45, 165.73, 160.07, 139.91, 138.62, 130.03, 129.99, 129.02, 128.36, 128.30, 128.22, 130.53 – 129.76 (m), 111.90, 41.06, 18.21.

GC-MS (EI, 70ev): $m/z(\%)$ = 288 (M+, 100), 289 (53), 274 (20), 260 (13), 245 (12), 116 (24), 104 (12), 103 (14), 77 (12).

HRMS(ESI): calcd. for [C₁₉H₁₉N₃ + H]⁺: 290.16517; found: 290.16539.

7-Ethyl-2,4-diphenyl-6,7-dihydro-5H-pyrrolo[2,3-*d*]pyrimidine

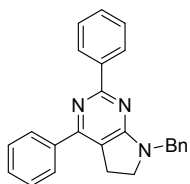


¹H NMR (300 MHz, Chloroform-*d*) δ 8.67 – 8.31 (m, 1H), 8.23 – 7.91 (m, 1H), 7.67 – 7.35 (m, 3H), 3.82 – 3.47 (m, 2H), 3.32 (dd, J = 8.8, 7.7 Hz, 1H), 1.27 (t, J = 7.2 Hz, 2H).

¹³C NMR (75 MHz, Chloroform-*d*) δ 168.51, 163.37, 154.41, 138.95, 138.42, 129.99, 129.31, 128.60, 128.30, 114.38, 48.39, 39.18, 26.16, 12.55.

GC-MS (EI, 70ev): $m/z(\%)$ = 301 (M+, 100), 302 (21), 300 (72), 299 (18), 287 (19), 286 (83), 104 (12), 273 (42), 272 (60), 271 (20), 140 (24), 128 (15), 127 (13), 116 (13), 115 (21), 104 (19), 103 (12), 77 (20).

7-Benzyl-2,4-diphenyl-6,7-dihydro-5H-pyrrolo[2,3-*d*]pyrimidine

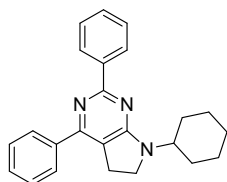


¹H NMR (300 MHz, Chloroform-*d*) δ 8.69 – 8.55 (m, 2H), 8.04 (d, J = 7.4 Hz, 2H), 7.60 – 7.28 (m, 12H), 4.79 (s, 2H), 3.56 (t, J = 8.1 Hz, 2H), 3.30 (t, J = 8.2 Hz, 2H).

¹³C NMR (75 MHz, Chloroform-*d*) δ 168.67, 163.33, 155.01, 138.96, 138.46, 137.45, 130.04, 129.36, 128.85, 128.61, 128.54, 128.47 – 128.20 (m), 128.29, 127.69, 114.00, 48.56, 48.44, 26.18.

GC-MS (EI, 70ev): $m/z(\%)$ = 91 (M+, 100), 364 (24), 363 (98), 362 (93), 361 (14), 360 (13), 286 (23), 284 (14), 272 (27), 259 (22), 182 (23), 140 (23), 128 (11), 115 (26), 104 (11), 77 (15), 65 (20).

8-Methyl-2,4-diphenyl-5,6,7,8-tetrahydropyrido[2,3-*d*]pyrimidine

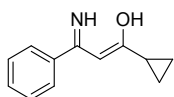


¹H NMR (300 MHz, Chloroform-*d*) δ 8.88 – 8.24 (m, 2H), 8.16 – 7.81 (m, 2H), 7.60 – 7.30 (m, 6H), 4.41 – 4.04 (m, 1H), 3.65 (dd, J = 8.9, 7.7 Hz, 2H), 3.27 (dd, J = 8.9, 7.7 Hz, 2H), 1.95 – 1.81 (m, 4H), 1.81 – 1.68 (m, 1H), 1.51 (td, J = 9.2, 3.9 Hz, 4H), 1.29 – 1.06 (m, 1H).

¹³C NMR (75 MHz, Chloroform-*d*) δ 167.97, 163.24, 154.21, 139.22, 138.66, 129.84, 129.14, 128.53, 128.27, 128.24, 128.20, 114.62, 52.36, 44.45, 29.93, 25.92.

GC-MS (EI, 70ev): $m/z(\%)$ = 273 (M+, 100), 355 (35), 298 (11), 274 (22).

(Z)-1-Cyclopropyl-3-imino-3-phenylprop-1-en-1-ol

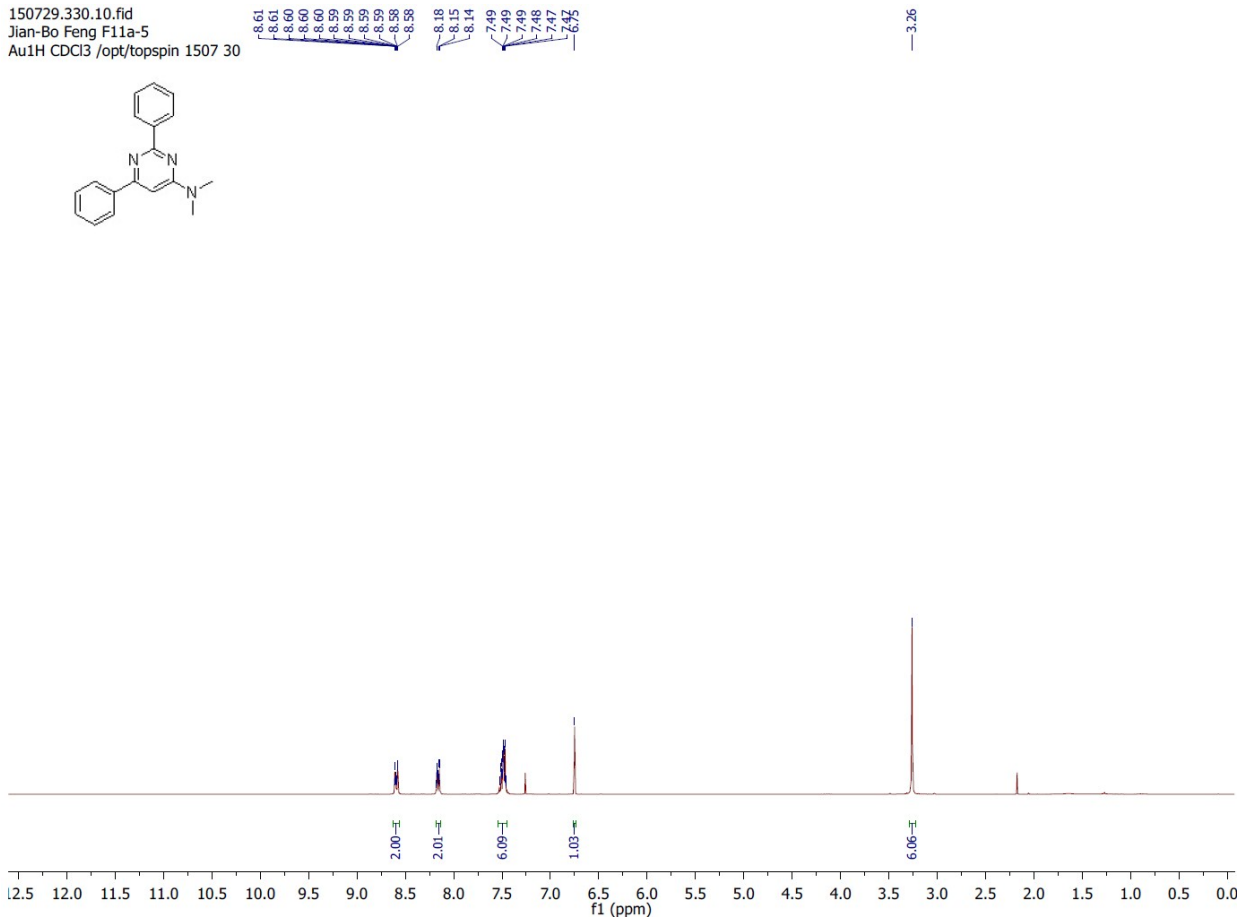
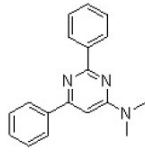


¹H NMR (300 MHz, Chloroform-*d*) δ 9.84 (s, 1H), 7.72 – 7.51 (m, 2H), 7.50 – 7.33 (m, 3H), 5.58 (s, 1H), 5.23 (s, 1H), 1.81 (tt, $J = 7.9, 4.6$ Hz, 1H), 1.12 – 0.95 (m, 2H), 0.92 – 0.54 (m, 2H).

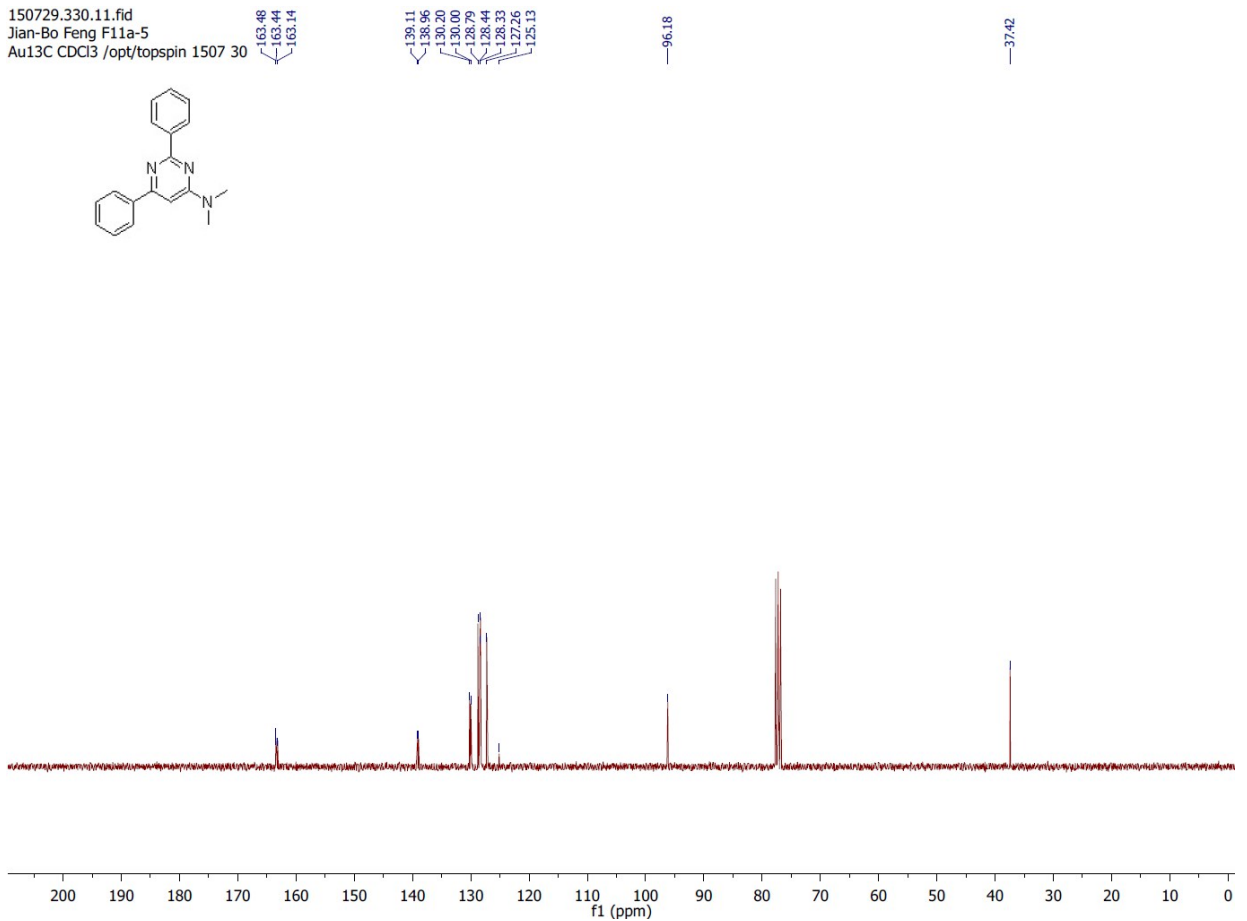
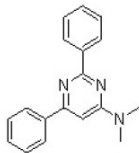
¹³C NMR (75 MHz, Chloroform-*d*) δ 199.39 , 160.24 , 137.60 , 130.59 , 129.05 , 126.44 , 95.12 , 21.01 , 9.61 .

GC-MS (EI, 70ev): $m/z(\%) = 146 (M^+, 100), 187 (52), 186 (40), 152 (14), 147 (12), 137 (20), 117 (16), 104 (30), 103 (36), 91(36), 77(30), 69(24), 51(20), 41(40), 39(46).$

150729.330.10.fid
Jian-Bo Feng F11a-5
Au1H CDCl3 /opt/topspin 1507 30



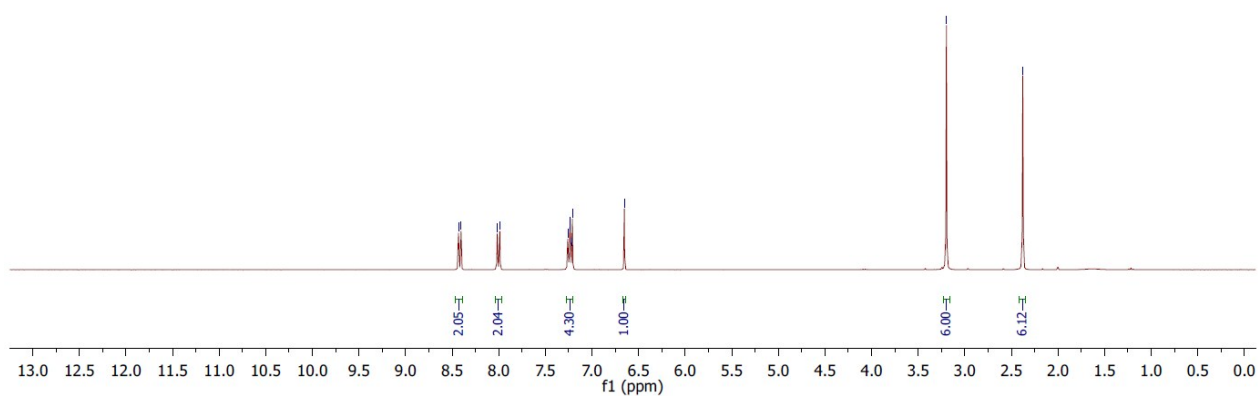
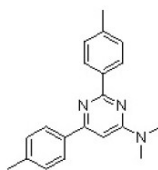
150729.330.11.fid
Jian-Bo Feng F11a-5
Au13C CDCl3 /opt/topspin 1507 30



150911.f311.10.fid
Jian-Bo Feng 39a171-1
PROTON CDCl3 {C:\Bruker\TopSpin3.2PL6} 1509 11

8.43
8.40
8.02
7.99
7.26
7.24
7.23
7.23
6.65

3.20
2.38



150911.f311.11.fid
Jian-Bo Feng 39a171-1
C13CPD CDCl3 {C:\Bruker\TopSpin3.2PL6} 1509 11

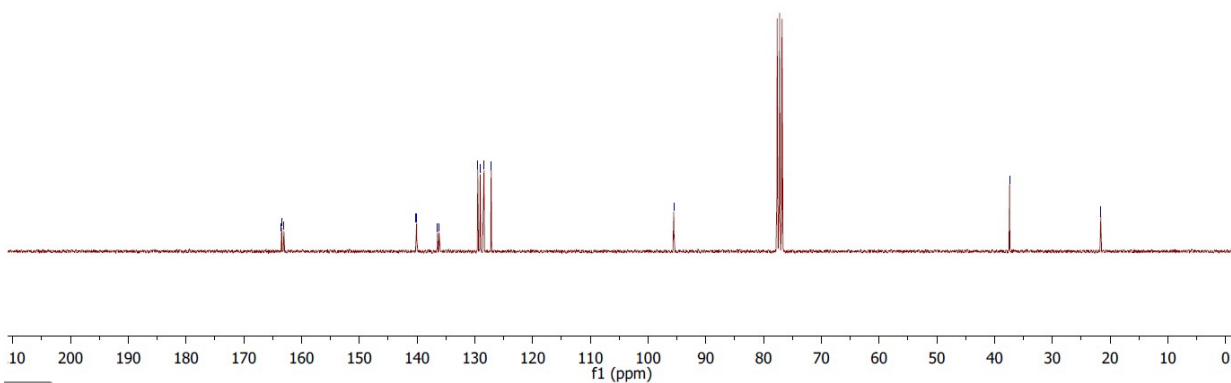
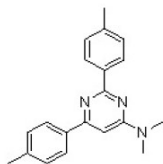
163.49
163.44
163.05

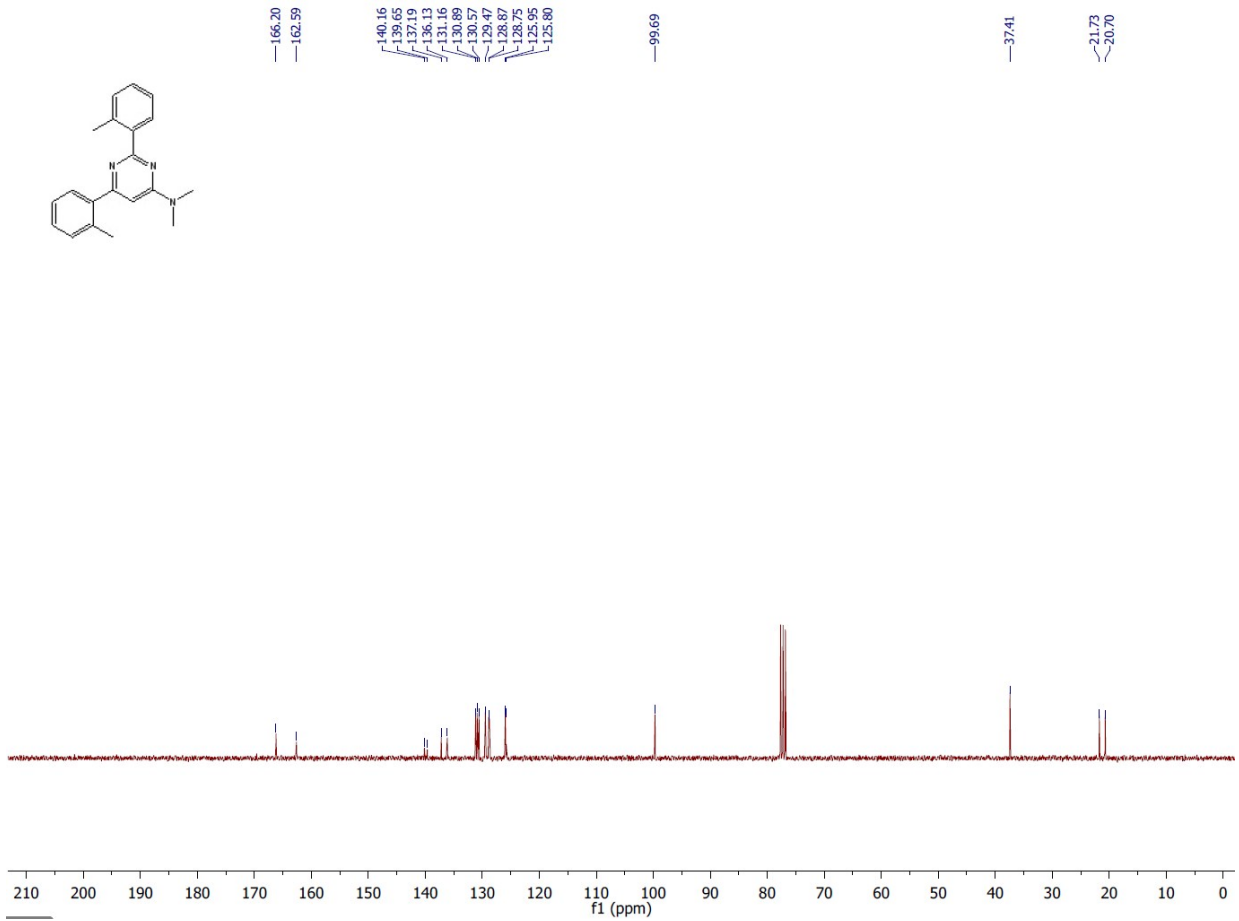
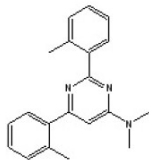
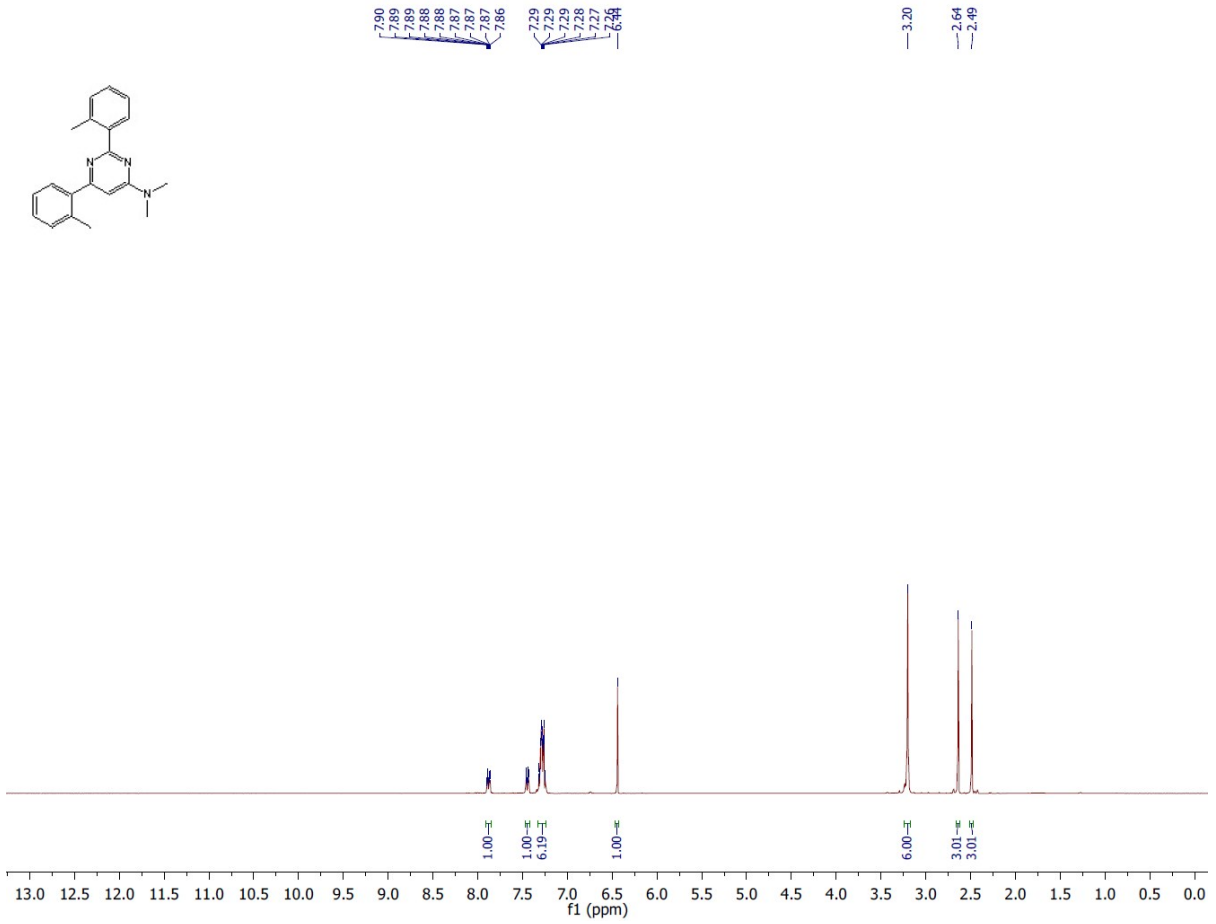
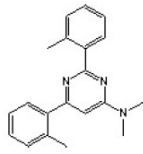
140.18
140.07
136.47
136.20
129.48
129.07
128.41
127.16

95.54

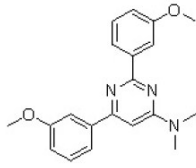
37.40

21.70
21.60



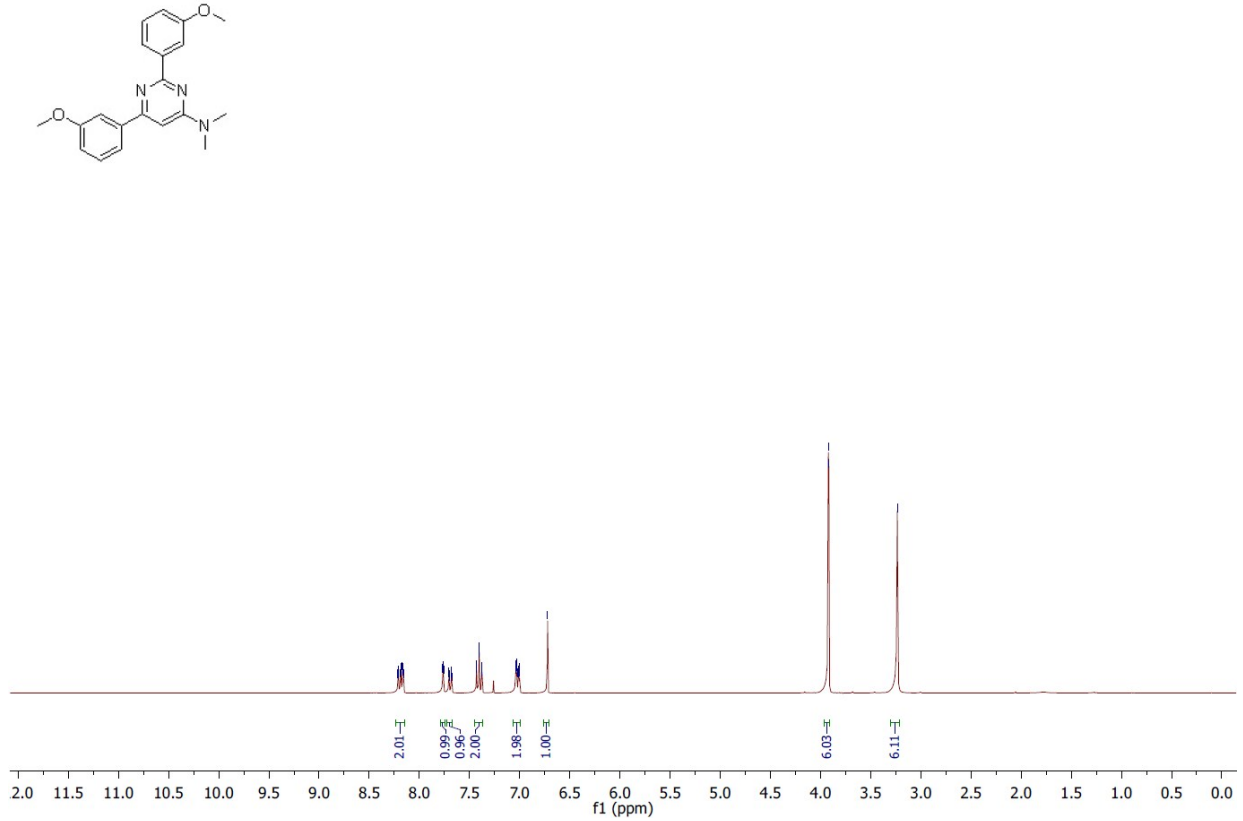


150914.301.10.fid
Jian-Bo Feng 39a173-7
Au1H CDCl3 /opt/topspin 1509 1

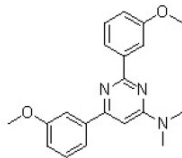


8.21
8.21
8.19
8.18
8.18
8.17
8.16
8.16
7.76
7.43
7.40
7.40
7.38
7.04
7.03
7.02
7.01
7.01
7.00
6.72

3.92
3.92
3.23



150914.301.11.fid
Jian-Bo Feng 39a173-7
Au13C CDCl3 /opt/topspin 1509 1

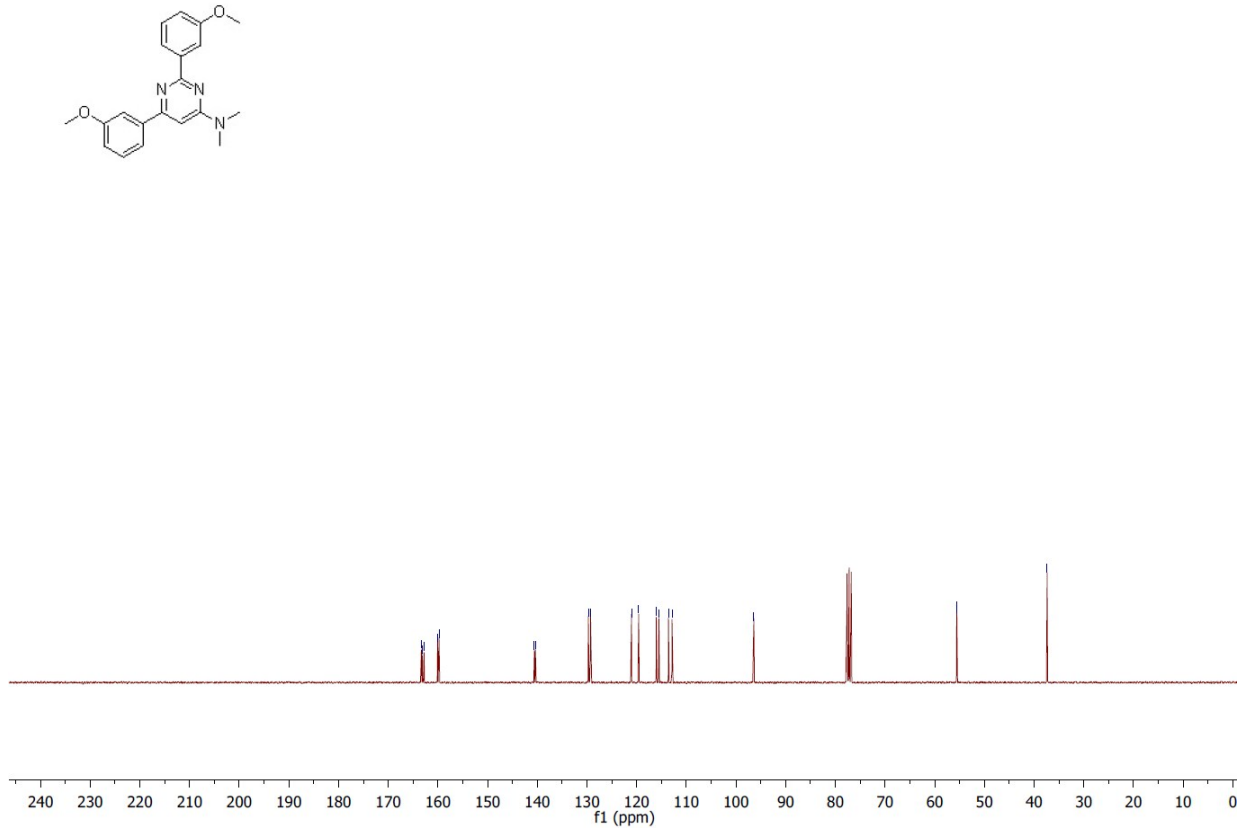


163.34
163.14
162.79
160.07
159.78
140.60
140.39
129.73
129.28
121.03
119.59
116.04
115.51
113.59
112.87

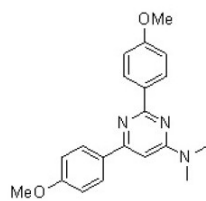
96.41

55.57
55.50

37.37

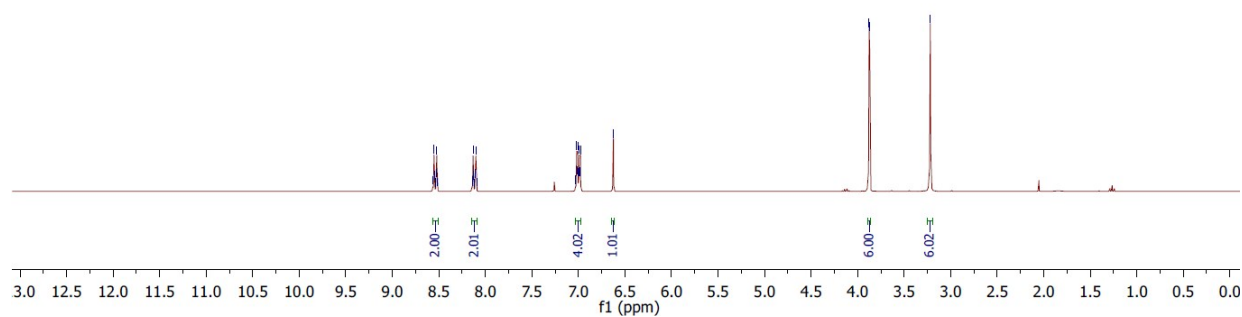


150925.318.10.fid
Jian-Bo Feng 39a193-1
Au1H CDCl3 /opt/topspin 1509 18

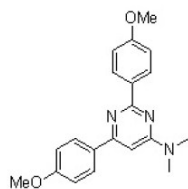


8.56
8.55
8.54
8.54
8.54
8.53
8.52
8.51
8.13
8.12
8.11
8.10
7.02
7.01
7.01
6.99
6.98

3.88
3.87
3.22



150925.318.11.fid
Jian-Bo Feng 39a193-1
Au13C CDCl3 /opt/topspin 1509 18



163.34
163.05
162.49
161.44
161.24

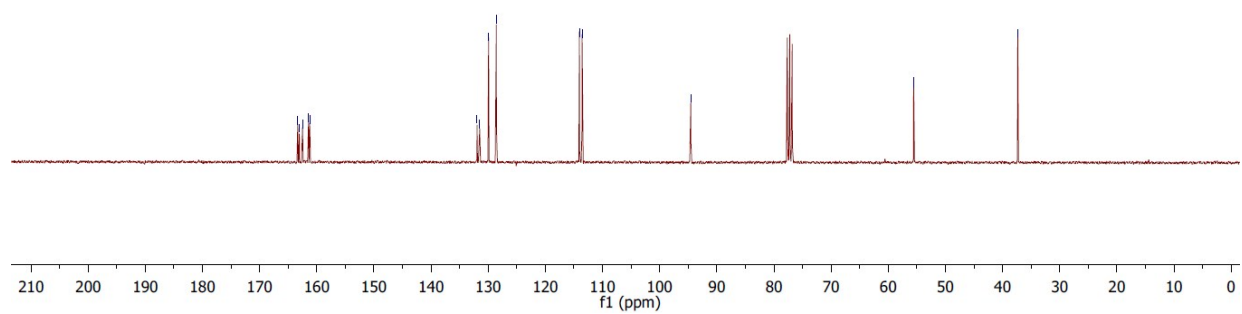
131.95
131.49
129.93
128.57

114.04
113.57

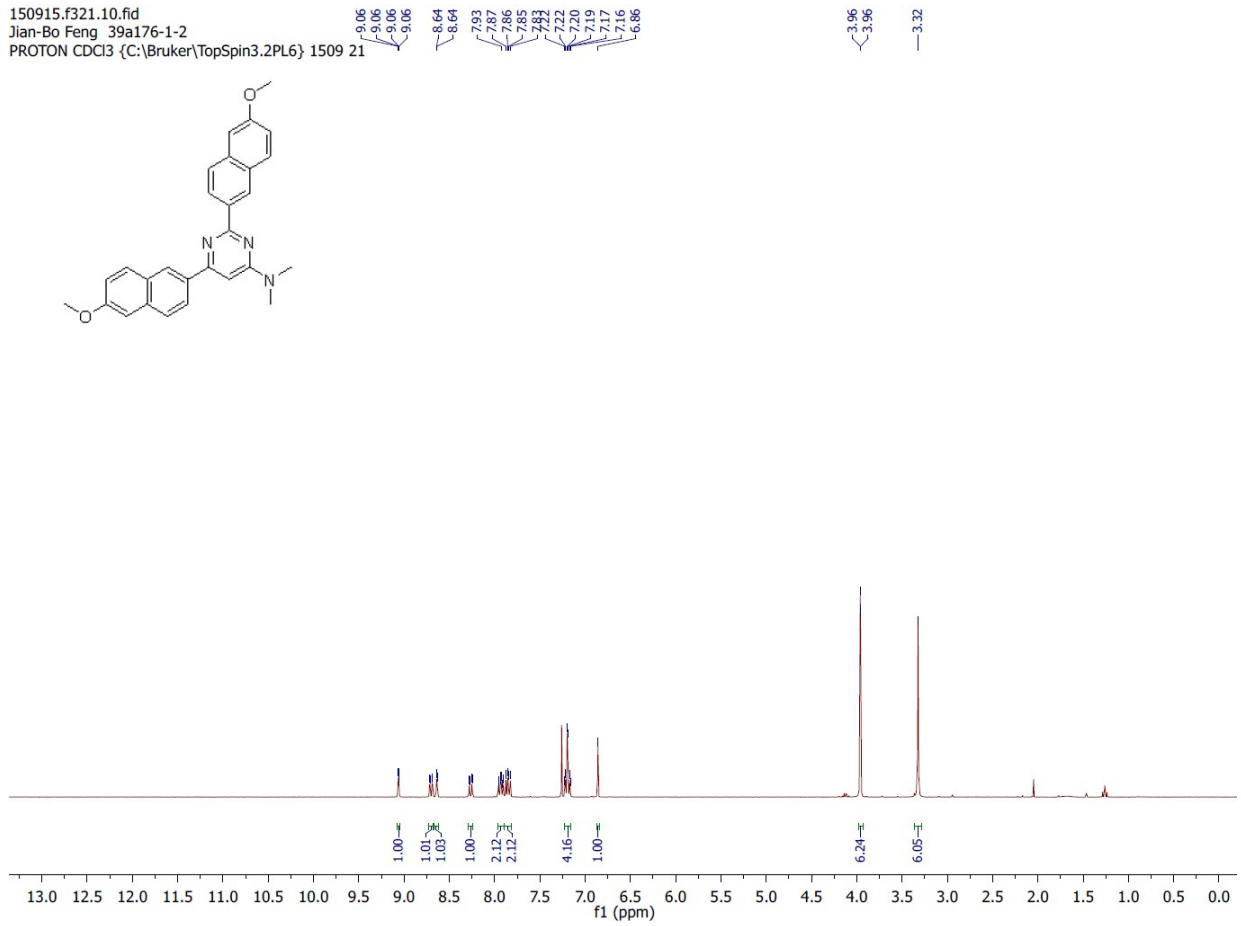
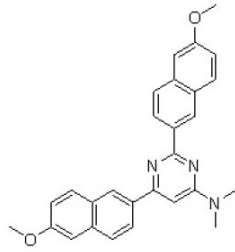
94.54

55.54
55.50

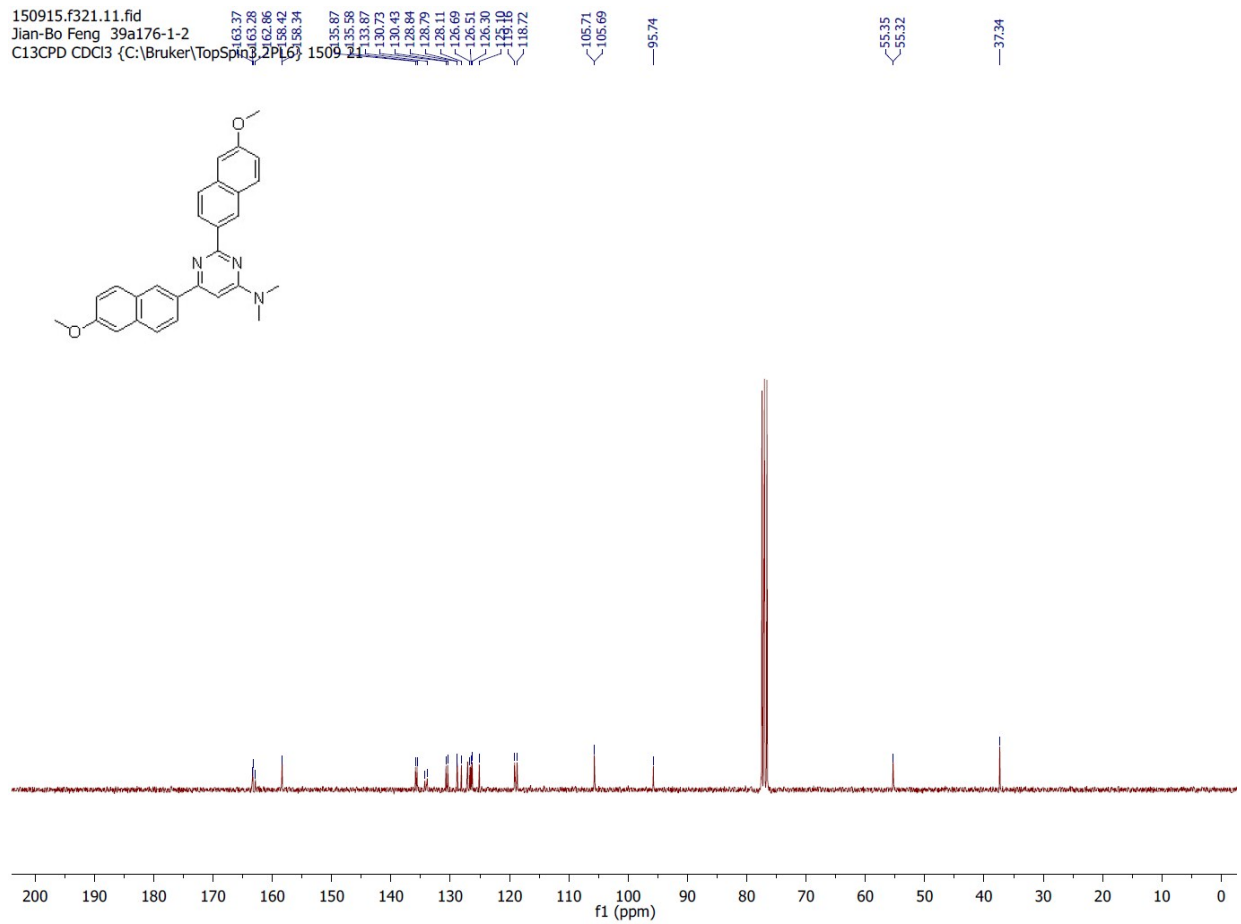
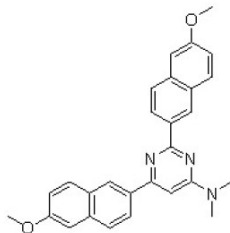
37.23



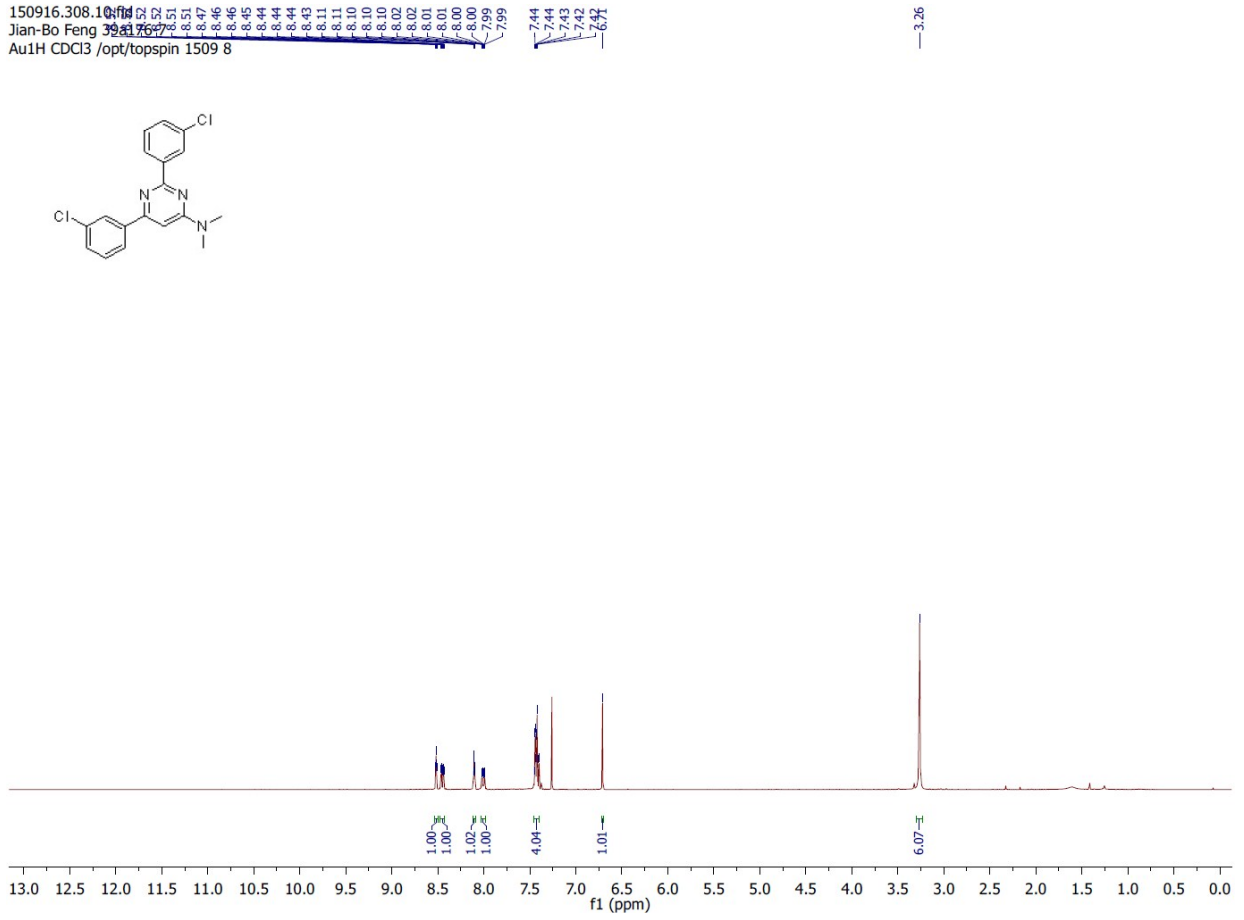
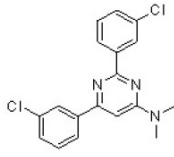
150915.f321.10.fid
Jian-Bo Feng 39a176-1-2
PROTON CDCl3 {C:\Bruker\TopSpin3.2PL6} 1509 21



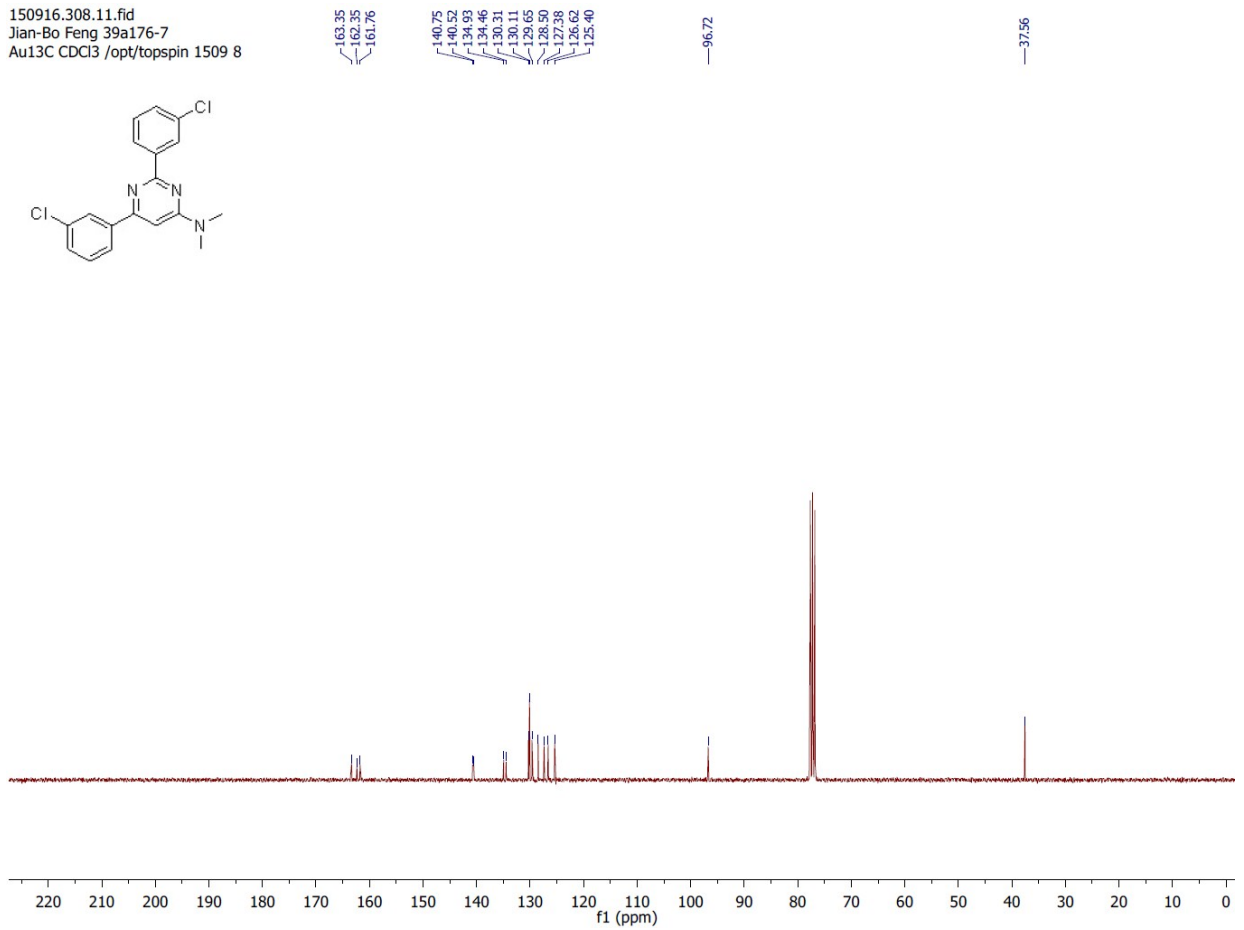
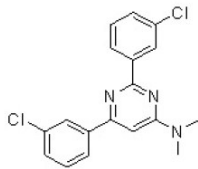
150915.f321.11.fid
Jian-Bo Feng 39a176-1-2
C13CPD CDCl3 {C:\Bruker\TopSpin3.2PL6} 1509 21



150916.308.10.fid
Jian-Bo Feng 39a176-7
Au1H CDCl3 /opt/topspin 1509 8



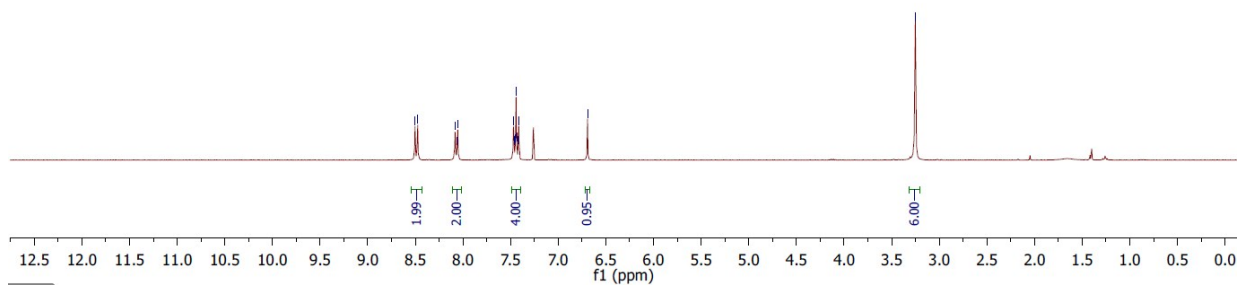
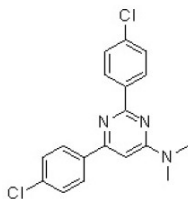
150916.308.11.fid
Jian-Bo Feng 39a176-7
Au13C CDCl3 /opt/topspin 1509 8



150916.309.10.fid
Jian-Bo Feng 39a176-8
Au1H CDCl3 /opt/topspin 1509 9

8.50
8.47
8.08
8.06
7.47
7.45
7.44
7.42
7.41
6.89

3.25



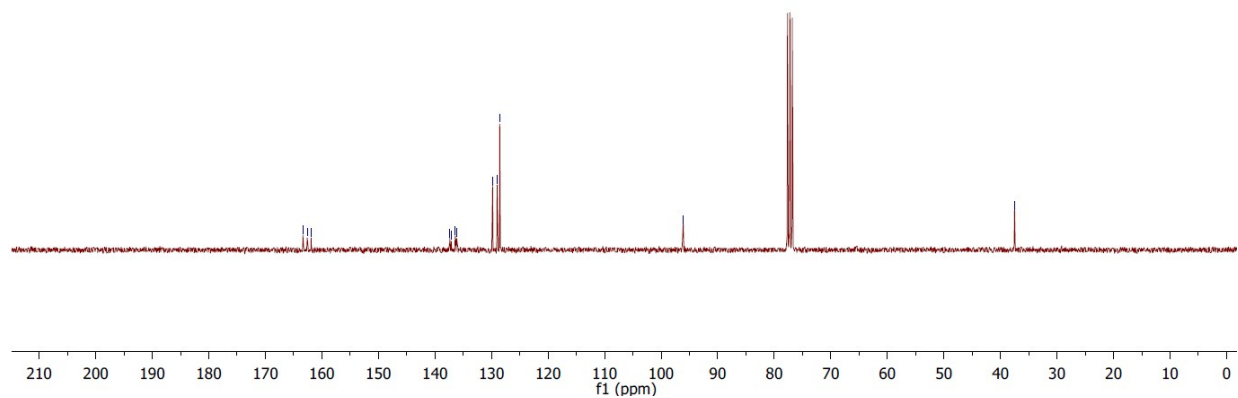
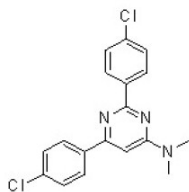
150916.309.11.fid
Jian-Bo Feng 39a176-8
Au13C CDCl3 /opt/topspin 1509 9

163.37
162.59
161.90

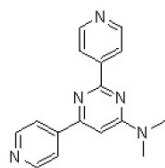
137.39
137.13
136.41
136.18
129.81
129.01
128.55

96.09

37.51



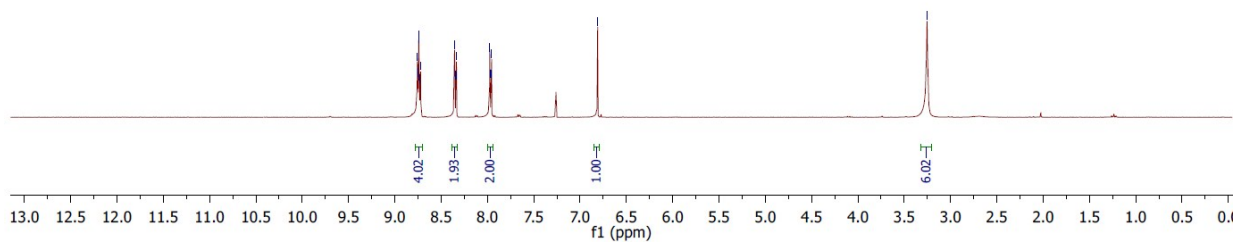
150916.307.10.fid
Jian-Bo Feng 39a179-3
Au1H CDCl3 /opt/topspin 1509 7



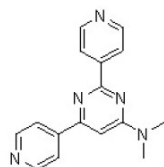
8.76
8.75
8.74
8.74
8.73
8.72
8.35
8.33
7.97
7.96
7.95

6.81

3.25



150916.307.11.fid
Jian-Bo Feng 39a179-3
Au13C CDCl3 /opt/topspin 1509 7



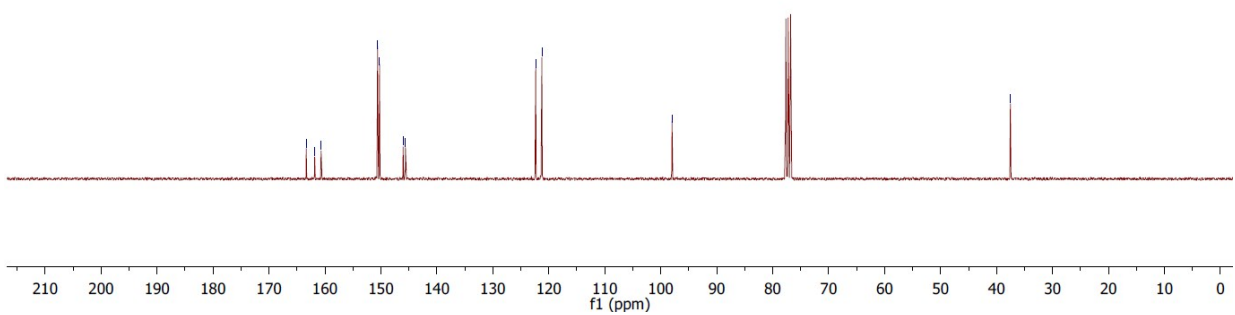
163.34
161.83
160.68

150.61
150.25
146.04
145.62

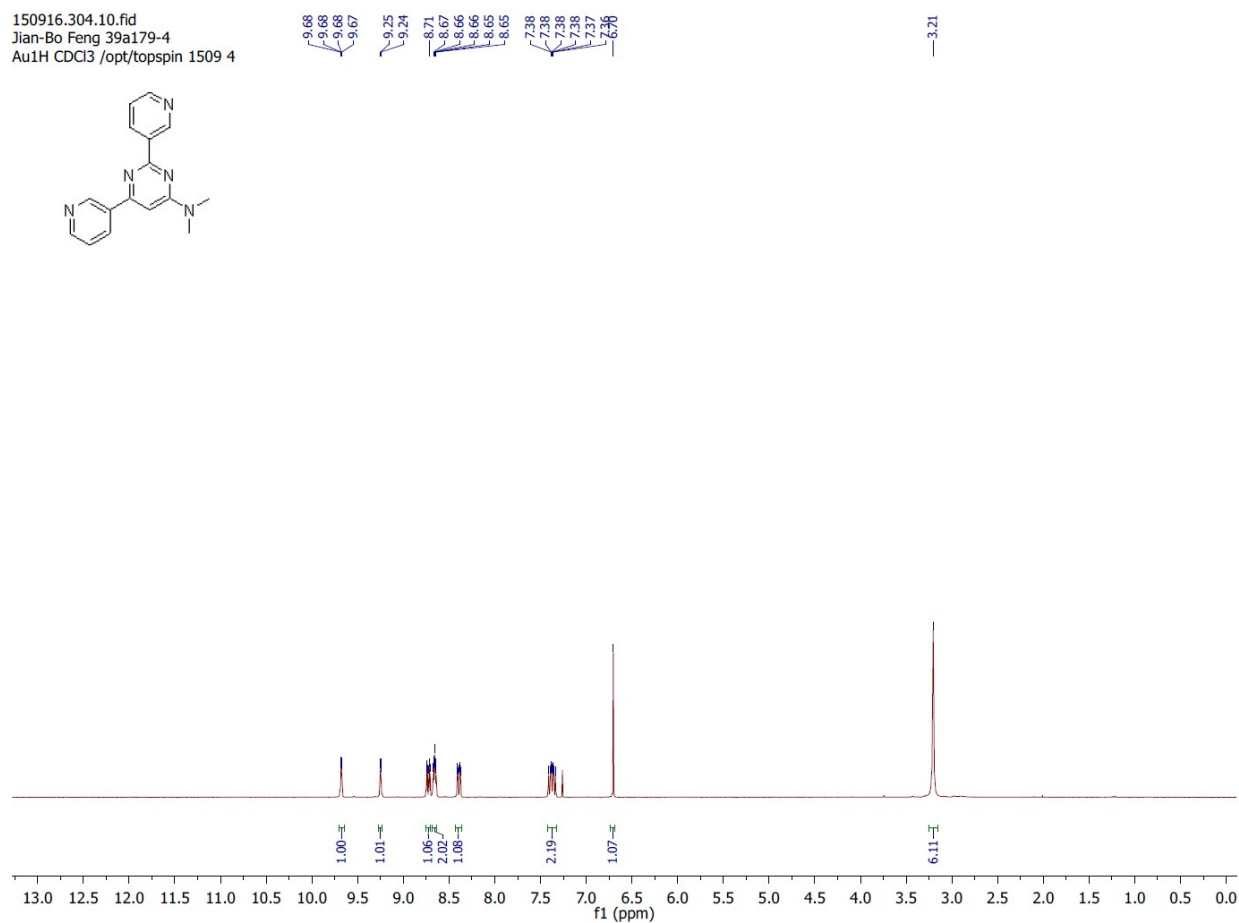
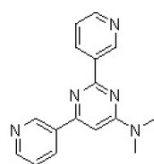
122.34
121.24

97.99

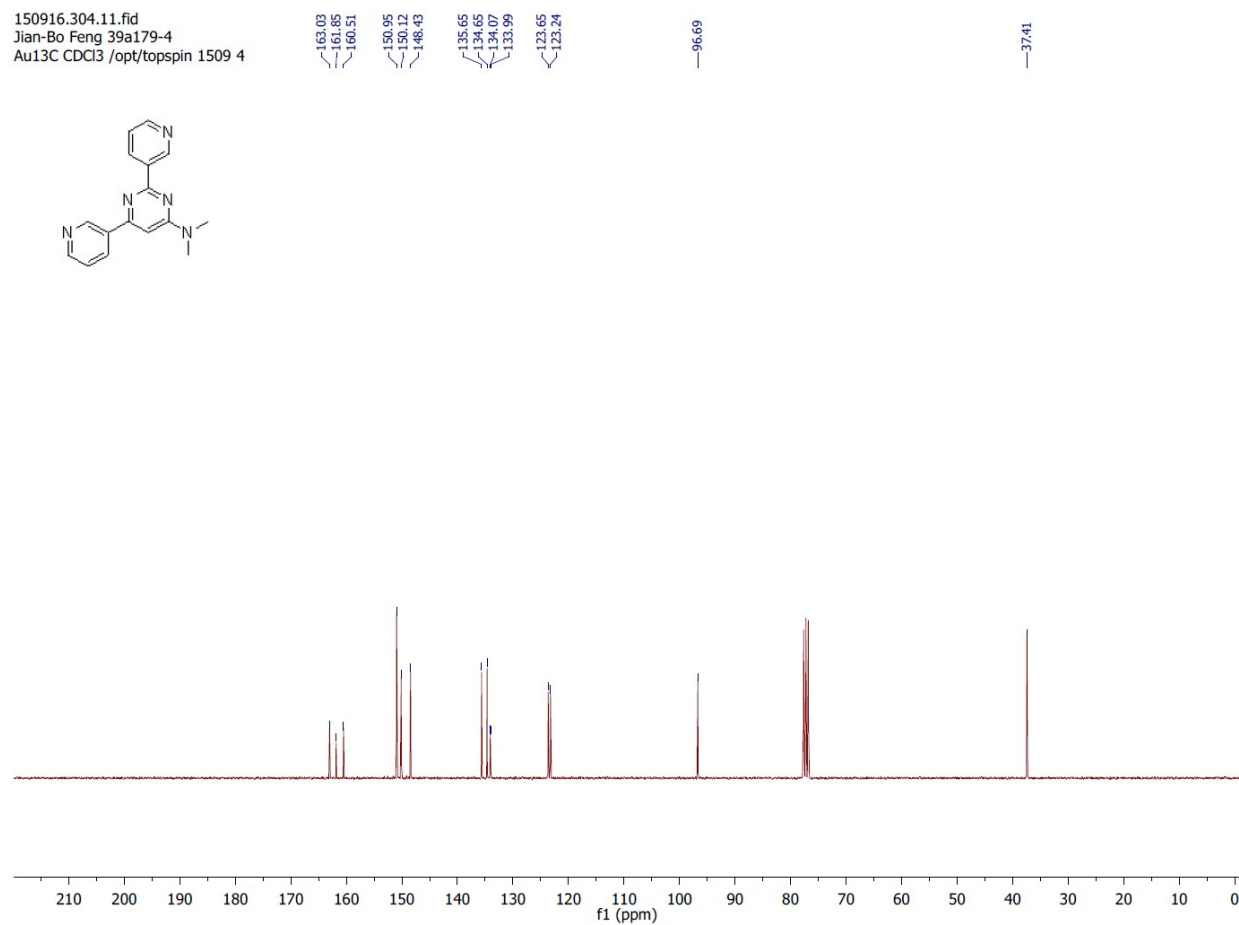
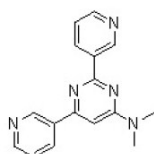
37.53



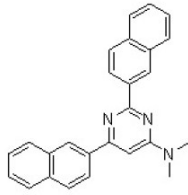
150916.304.10.fid
Jian-Bo Feng 39a179-4
Au1H CDCl3 /opt/topspin 1509 4



150916.304.11.fid
Jian-Bo Feng 39a179-4
Au13C CDCl3 /opt/topspin 1509 4

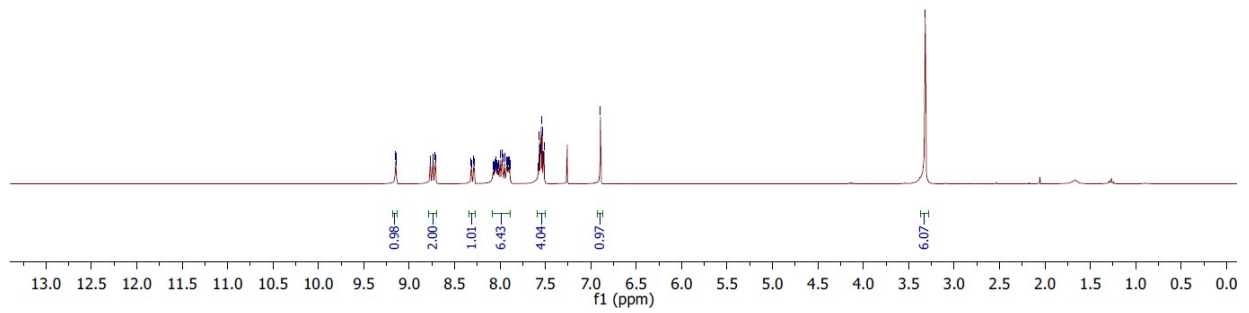


150917.314.10.fid
Jian-Bo Feng 39a183-1
Au1H CDCl3 /opt/topspin 1509 14

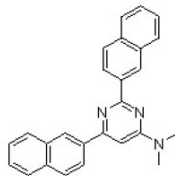


9.15
9.15
9.15
9.14
8.74
8.71
8.00
7.98
7.67
7.56
7.55
7.54
7.53
7.51

3.32



150917.314.11.fid
Jian-Bo Feng 39a183-1
Au13C CDCl3 /opt/topspin 1509 14

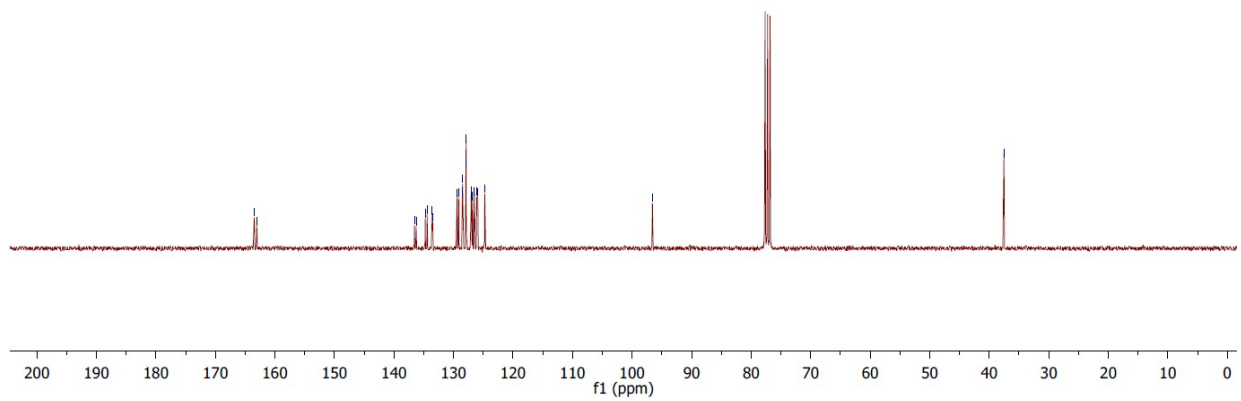


163.47
163.06

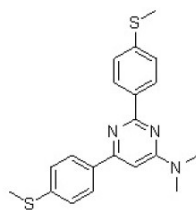
136.56
136.36
134.75
134.43
133.57
133.53
129.40
128.49
128.44
127.91
127.88
127.04
126.95
126.79
126.49
126.08
125.91
124.75

96.58

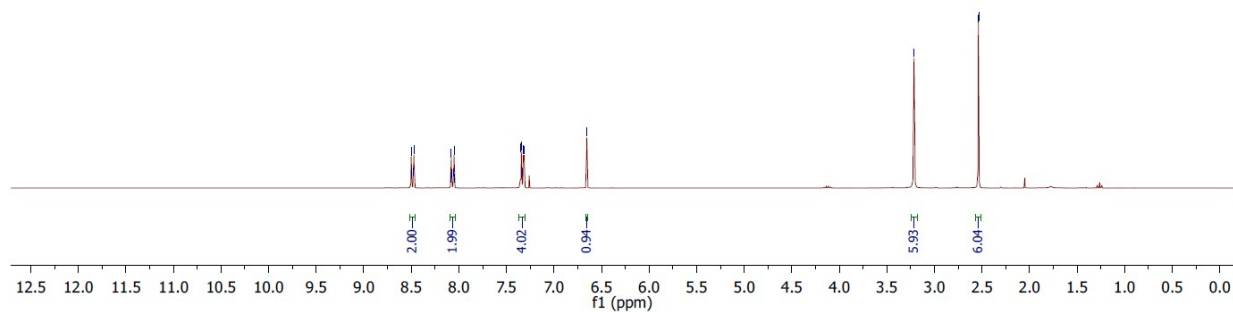
37.53



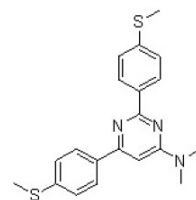
150917.312.10.fid
Jian-Bo Feng 39a183-12
Au1H CDCl3 /opt/topspin 1509 12



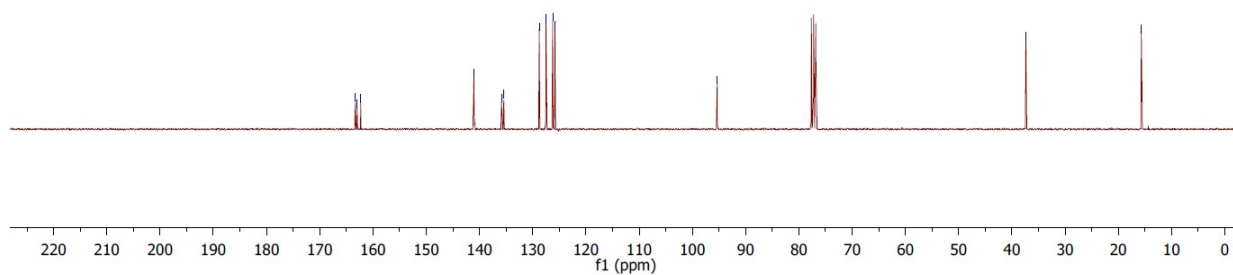
8.50
8.49
8.46
8.47
8.08
8.06
7.95
7.34
7.34
7.33
7.32
7.31
6.65
3.21
2.54
2.53



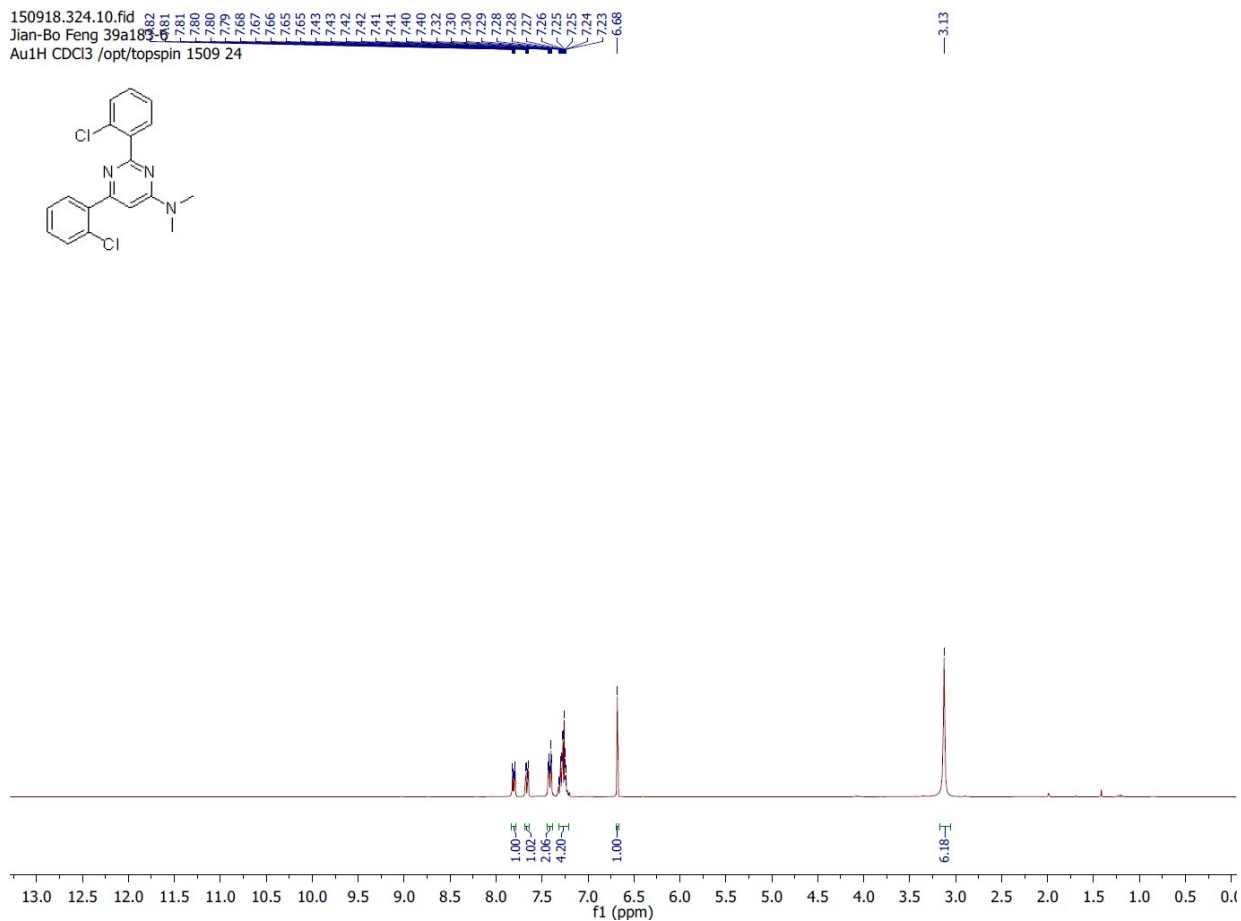
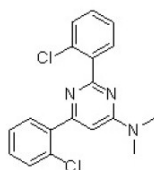
150917.312.11.fid
Jian-Bo Feng 39a183-12
Au13C CDCl3 /opt/topspin 1509 12



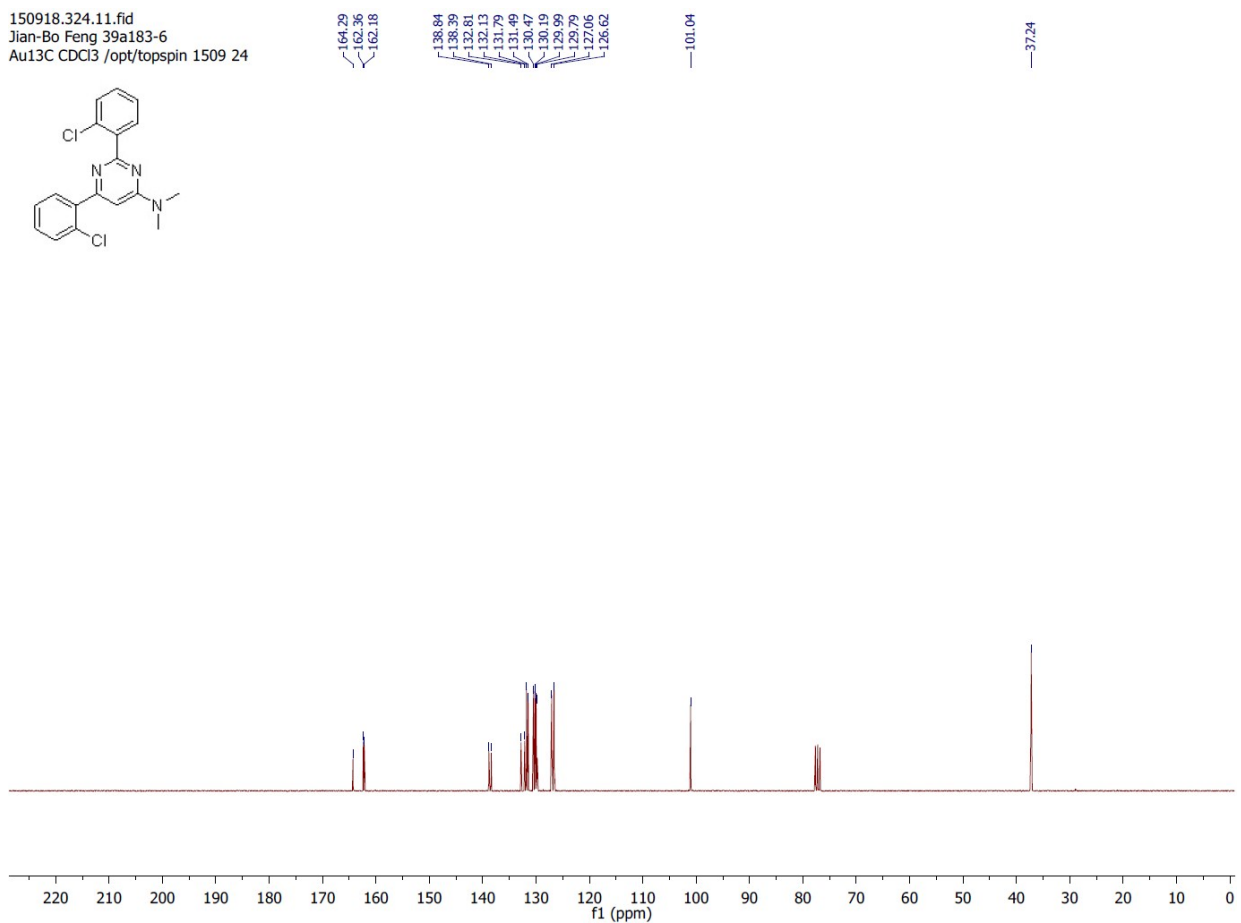
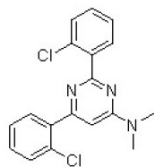
163.31
162.96
162.29
141.02
135.87
135.42
128.77
127.50
126.23
125.81
95.34
37.37
15.67



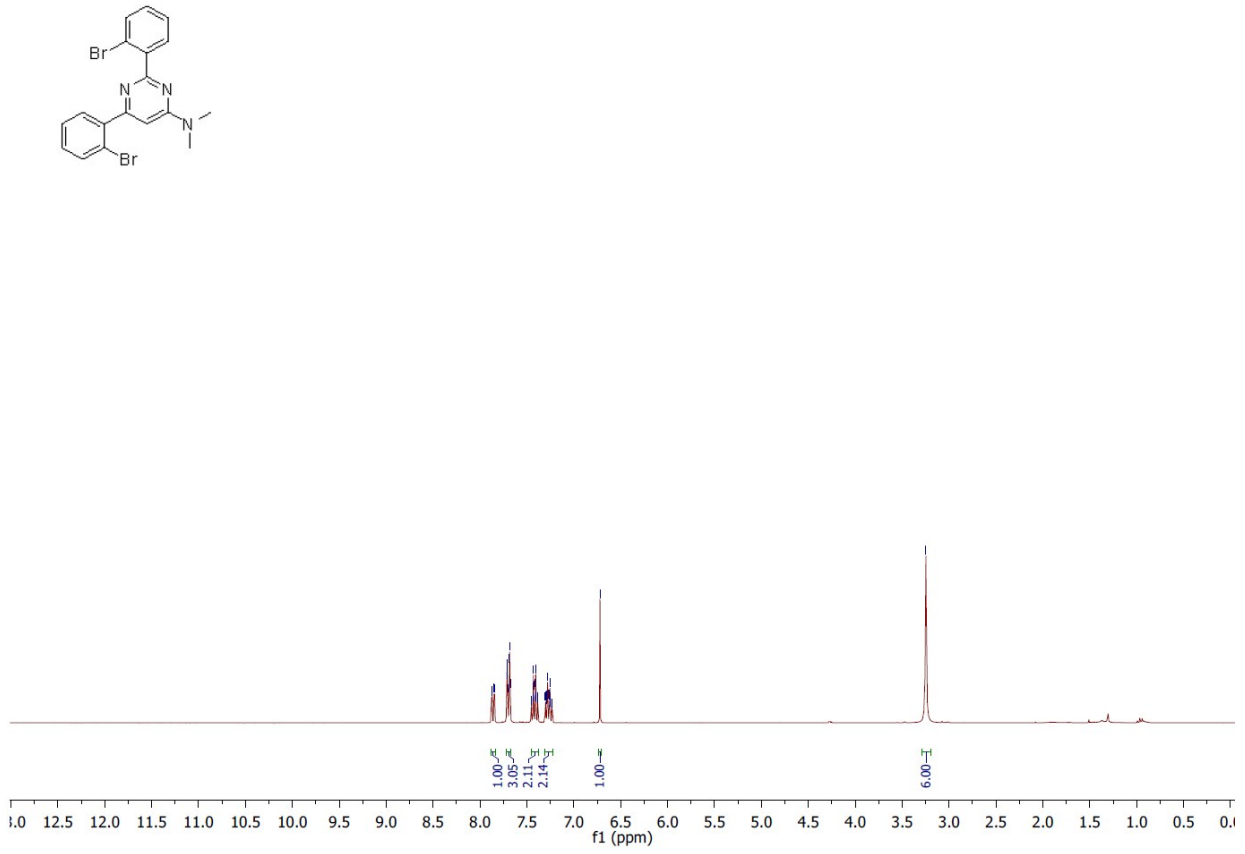
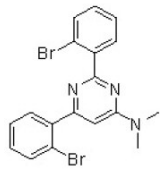
150918.324.10.fid
Jian-Bo Feng 39a183-6
Au1H CDCl3 /opt/topspin 1509 24



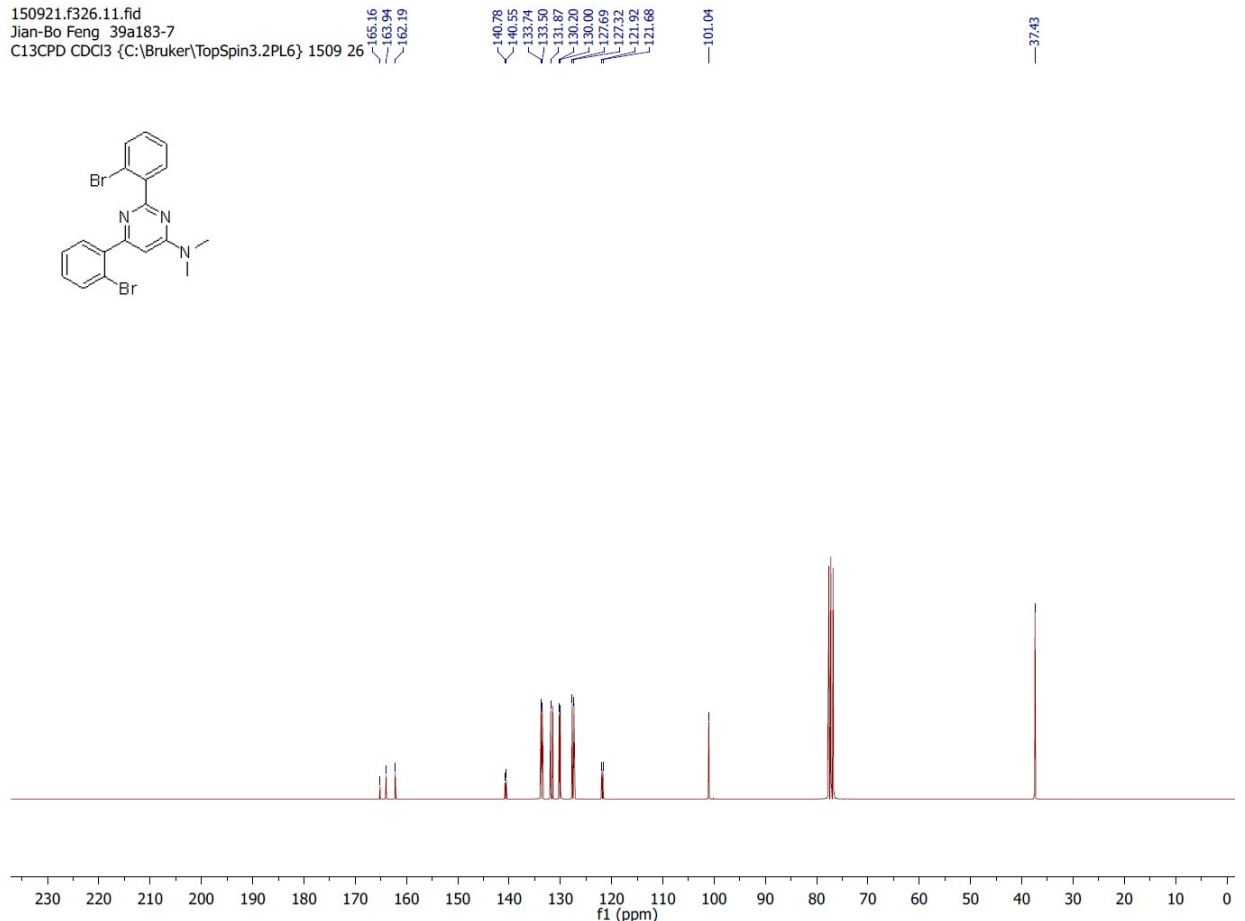
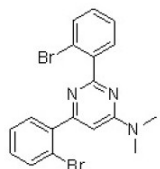
150918.324.11.fid
Jian-Bo Feng 39a183-6
Au13C CDCl3 /opt/topspin 1509 24



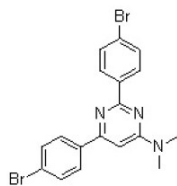
150921.f326.11.fid
 Jian-Bo Feng 39a183-7
 PROTON CDCl3 {C:\Bruker\TopSpin3.2PL6} 1509 26



150921.f326.11.fid
 Jian-Bo Feng 39a183-7
 C13CPD CDCl3 {C:\Bruker\TopSpin3.2PL6} 1509 26

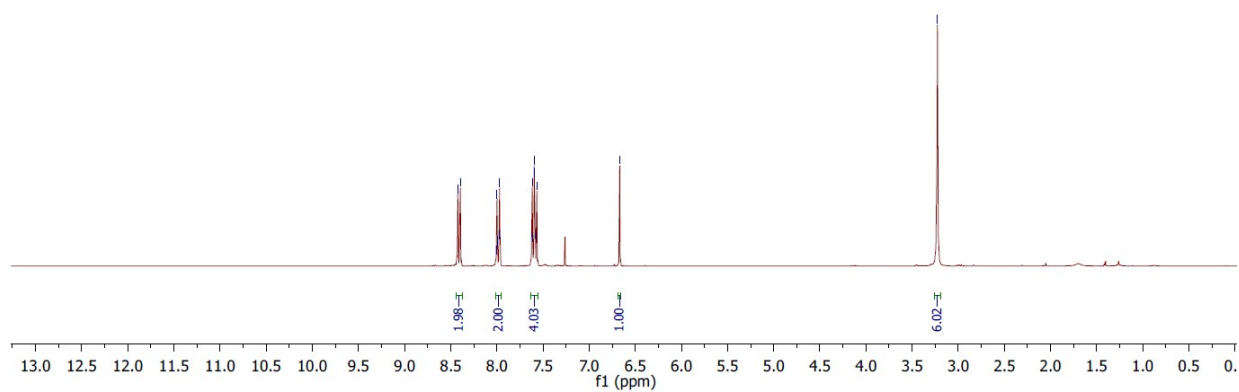


150921.320.10.fid
Jian-Bo Feng 39a185-6
Au1H CDCl3 /opt/topspin 1509 20

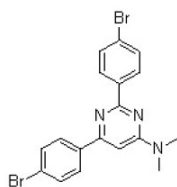


8.42
8.40
8.00
7.97
7.62
7.61
7.60
7.59
7.57
6.67

3.22



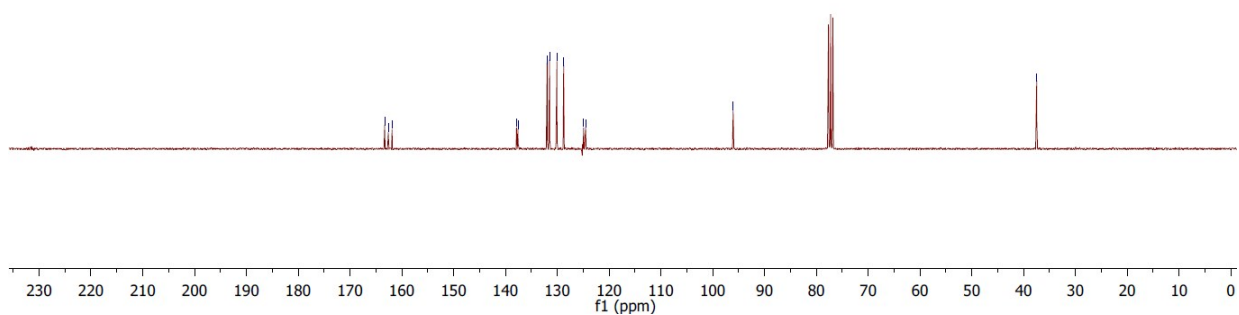
150921.320.11.fid
Jian-Bo Feng 39a185-6
Au13C CDCl3 /opt/topspin 1509 20



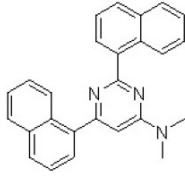
163.31
162.61
161.88
137.85
137.56
131.94
131.47
130.06
128.76
124.92
124.52

96.05

37.46

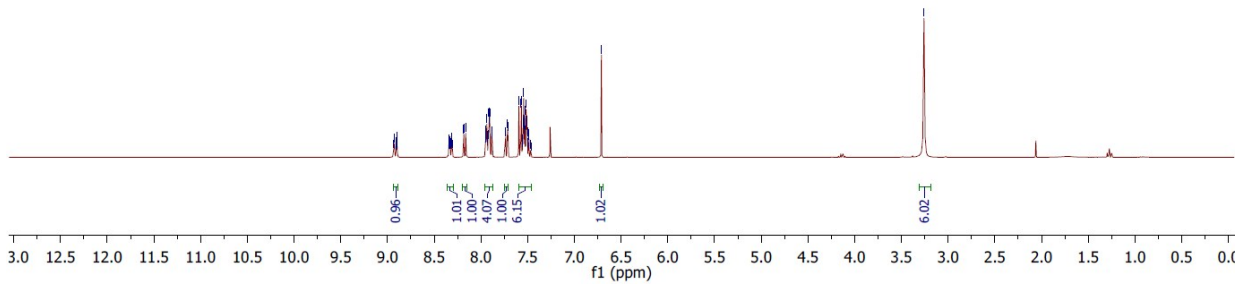


150923.322.10.fid
Jian-Bo Feng 39a183-2
Au1H CDCl3 /opt/topspin 1509 22

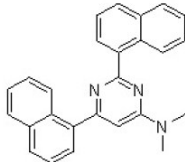


8.93
8.93
8.93
8.92
8.91
8.90
8.89
7.94
7.92
7.91
7.91
7.91
7.89
7.87
7.84
7.83
7.71

3.26

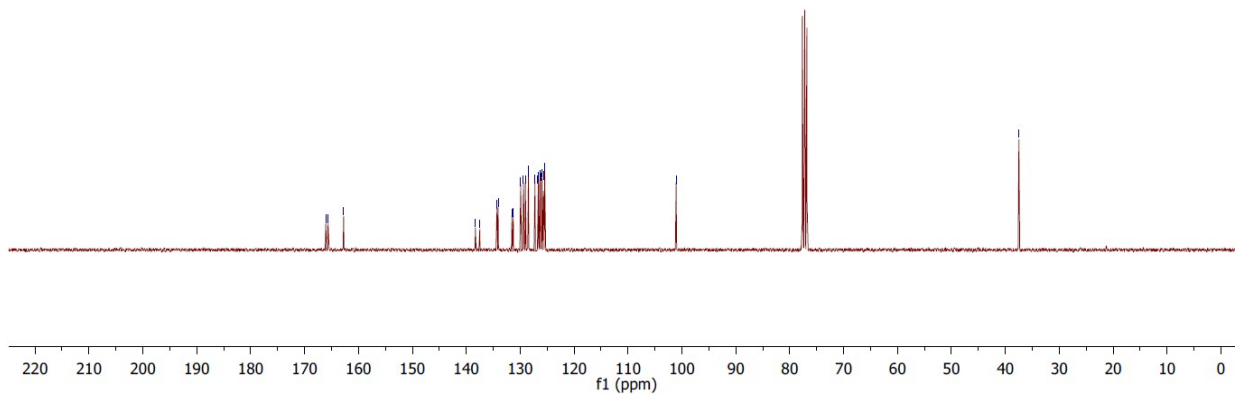


150923.322.11.fid
Jian-Bo Feng 39a183-2
Au13C CDCl3 /opt/topspin 1509 22

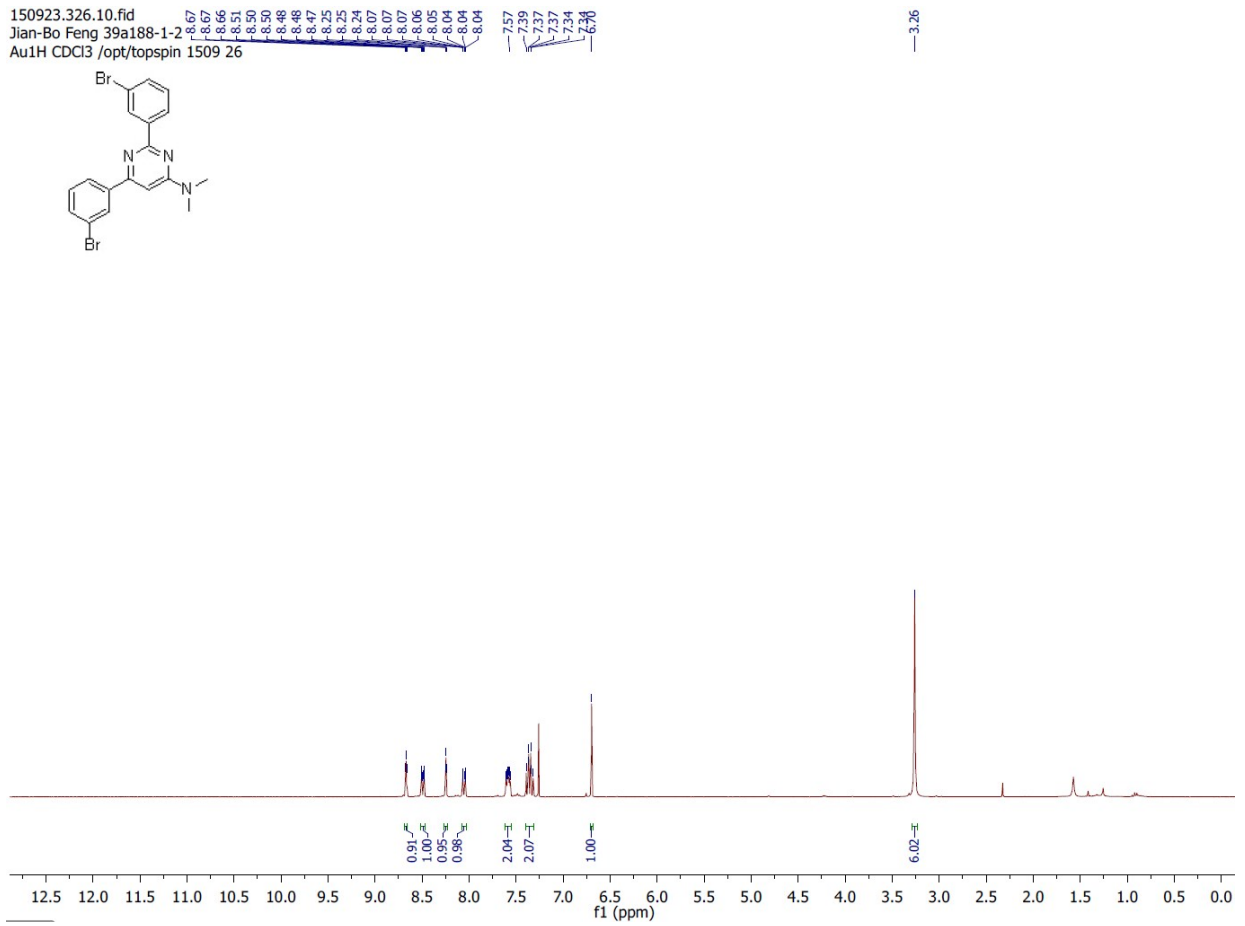
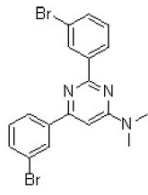


166.06
165.63
162.75
138.31
137.48
134.29
134.07
131.55
131.28
129.90
129.40
128.04
128.34
127.77
127.26
126.74
126.61
126.30
126.11
125.98
125.67
125.45
125.43
101.07

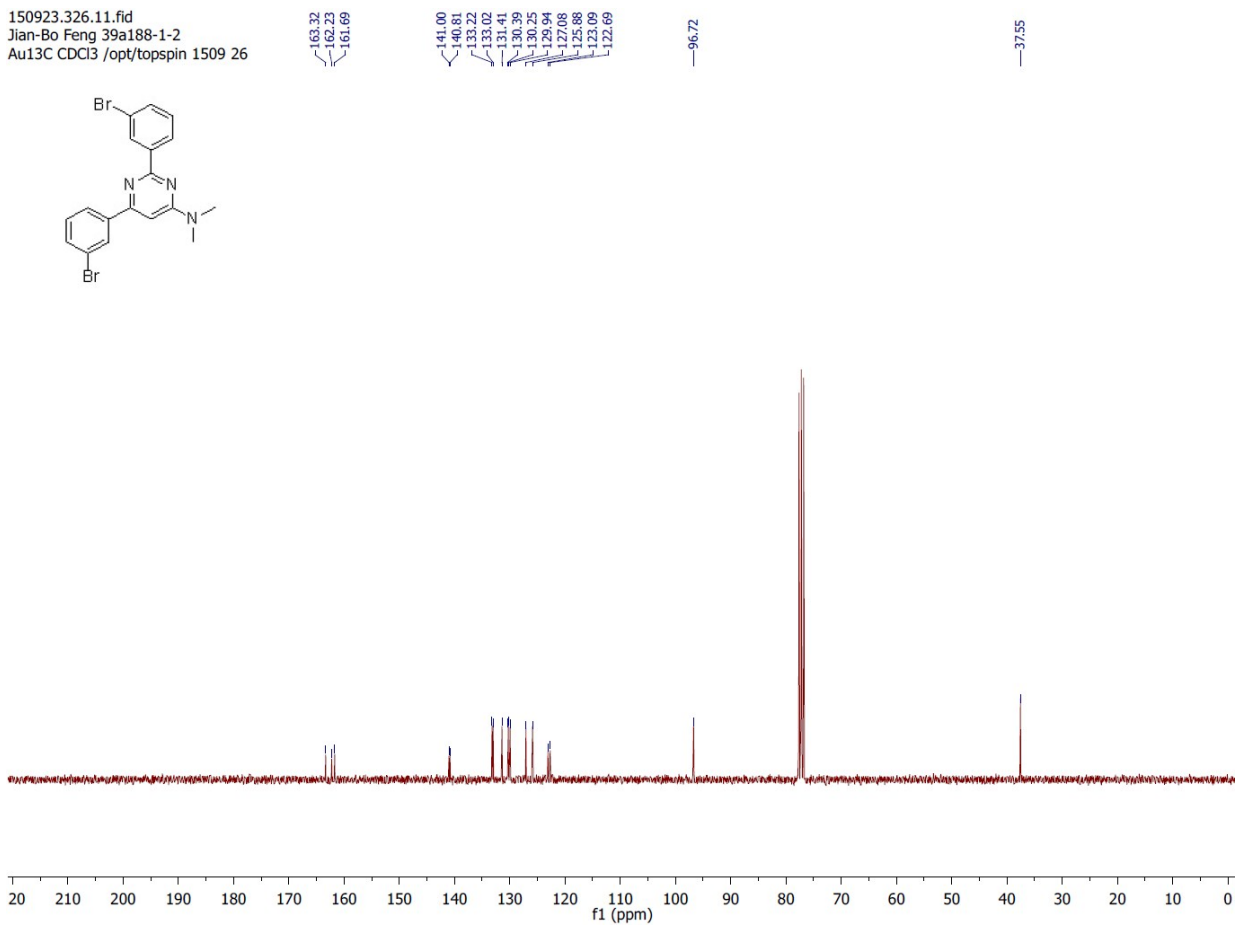
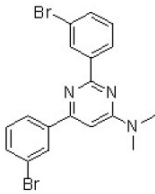
37.48



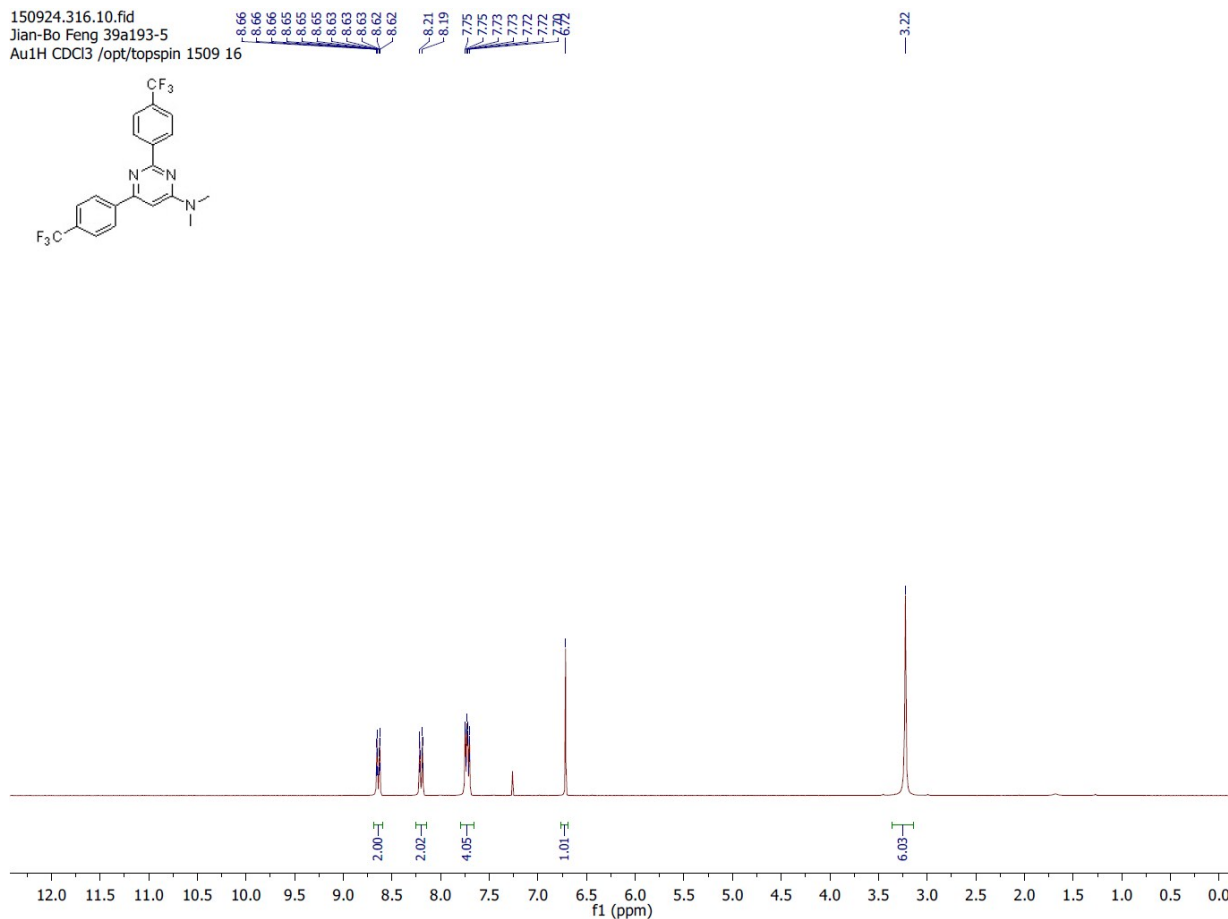
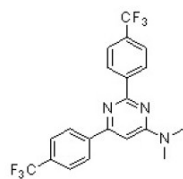
150923.326.10.fid
Jian-Bo Feng 39a188-1-2
Au1H CDCl3 /opt/topspin 1509 26



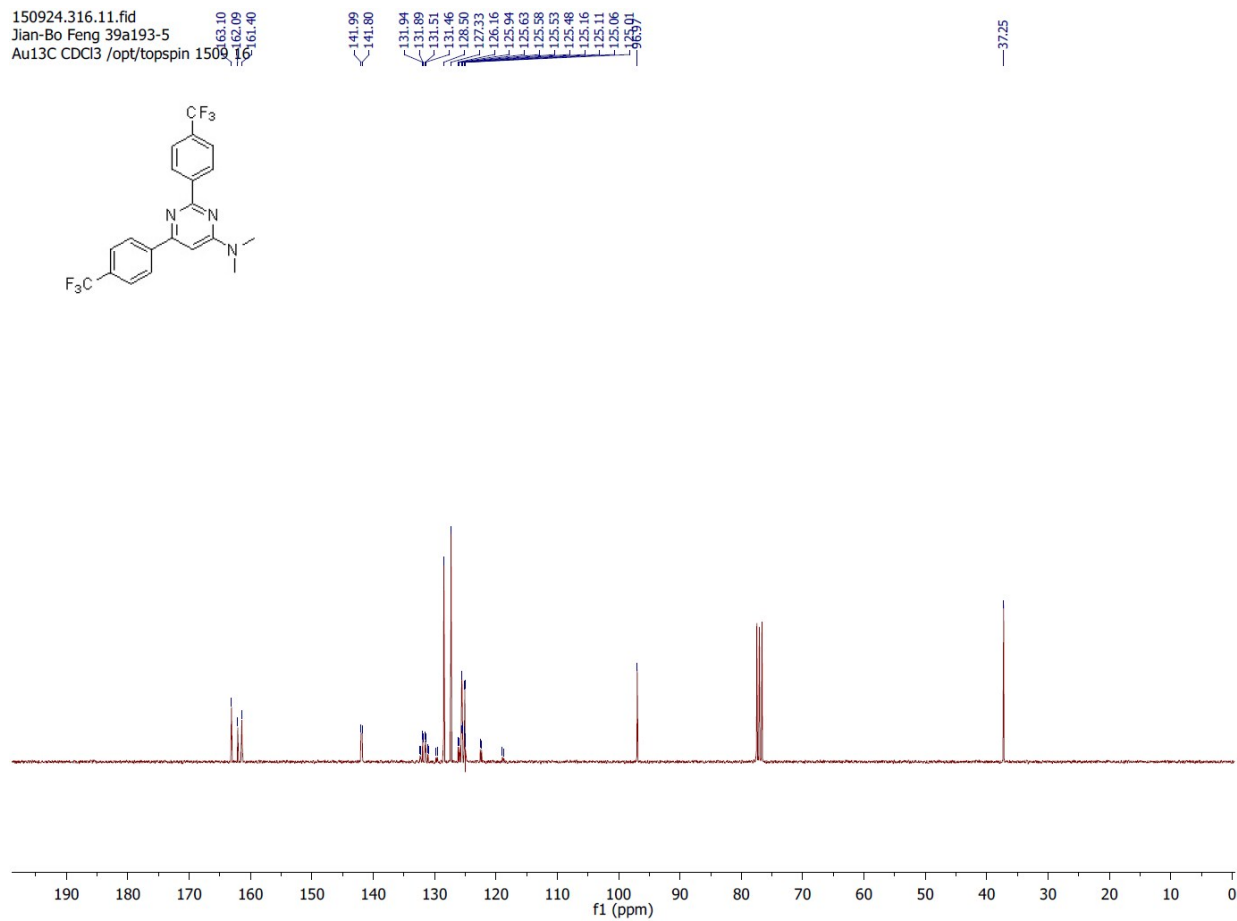
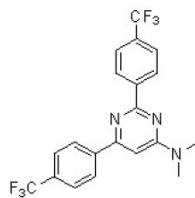
150923.326.11.fid
Jian-Bo Feng 39a188-1-2
Au13C CDCl3 /opt/topspin 1509 26



150924.316.10.fid
Jian-Bo Feng 39a193-5
Au1H CDCl3 /opt/topspin 1509 16



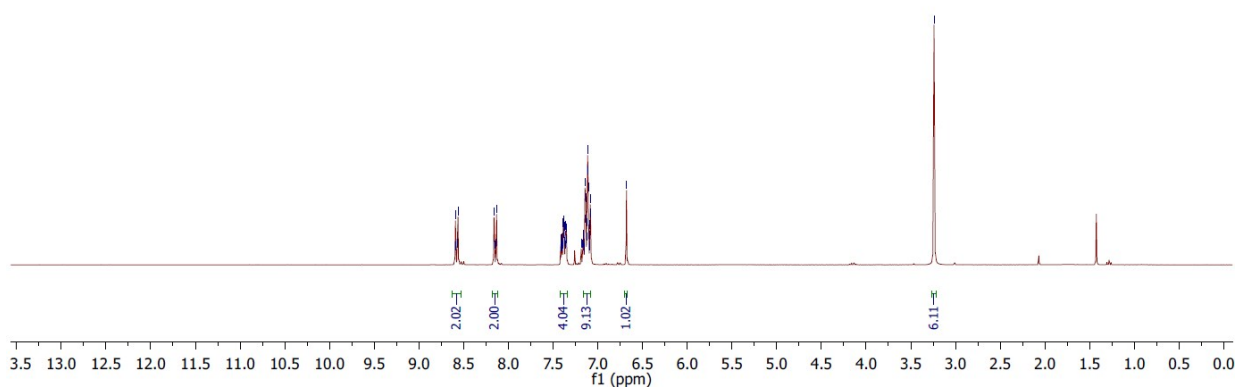
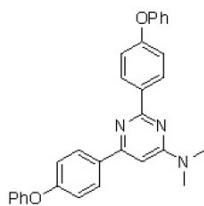
150924.316.11.fid
Jian-Bo Feng 39a193-5
Au13C CDCl3 /opt/topspin 1509 16



150924.f322.10.fid
Jian-Bo Feng 39a193-2
PROTON CDCl3 {C:\Bruker\TopSpin3.2PL6} 1509 22

8.69
8.68
8.57
8.56
8.16
8.14
8.13
7.14
7.13
7.11
7.10
7.08

3.24

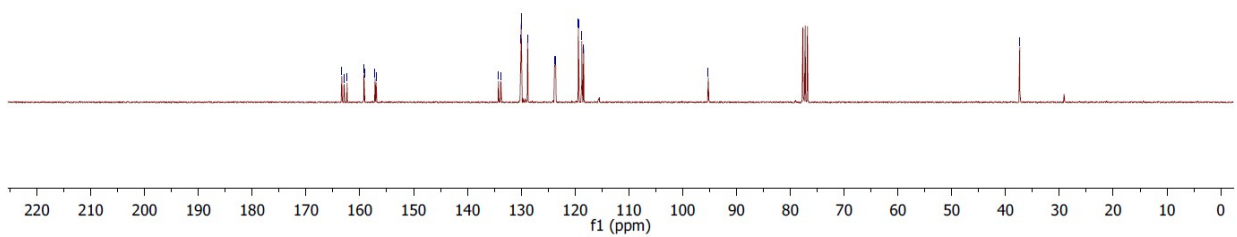
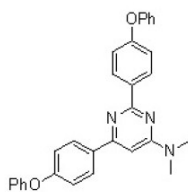


150924.f322.11.fid
Jian-Bo Feng 39a193-2
C13CPD CDCl3 {C:\Bruker\TopSpin3.2PL6} 1509 22

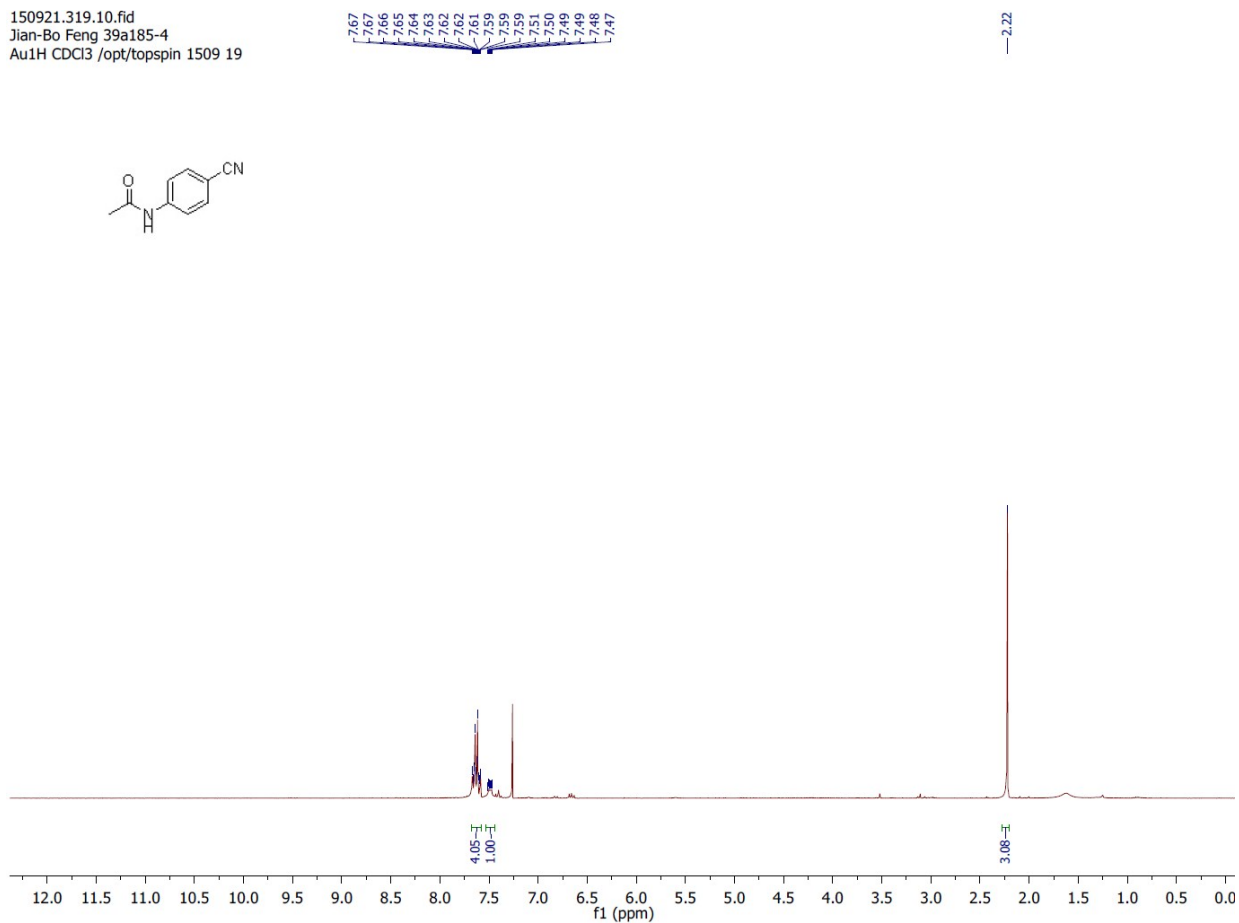
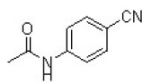
163.35
162.92
160.36
159.72
157.17
156.97
134.23
133.80
130.14
130.01
129.94
129.82
127.59
127.59
119.30
118.75
118.41

95.24

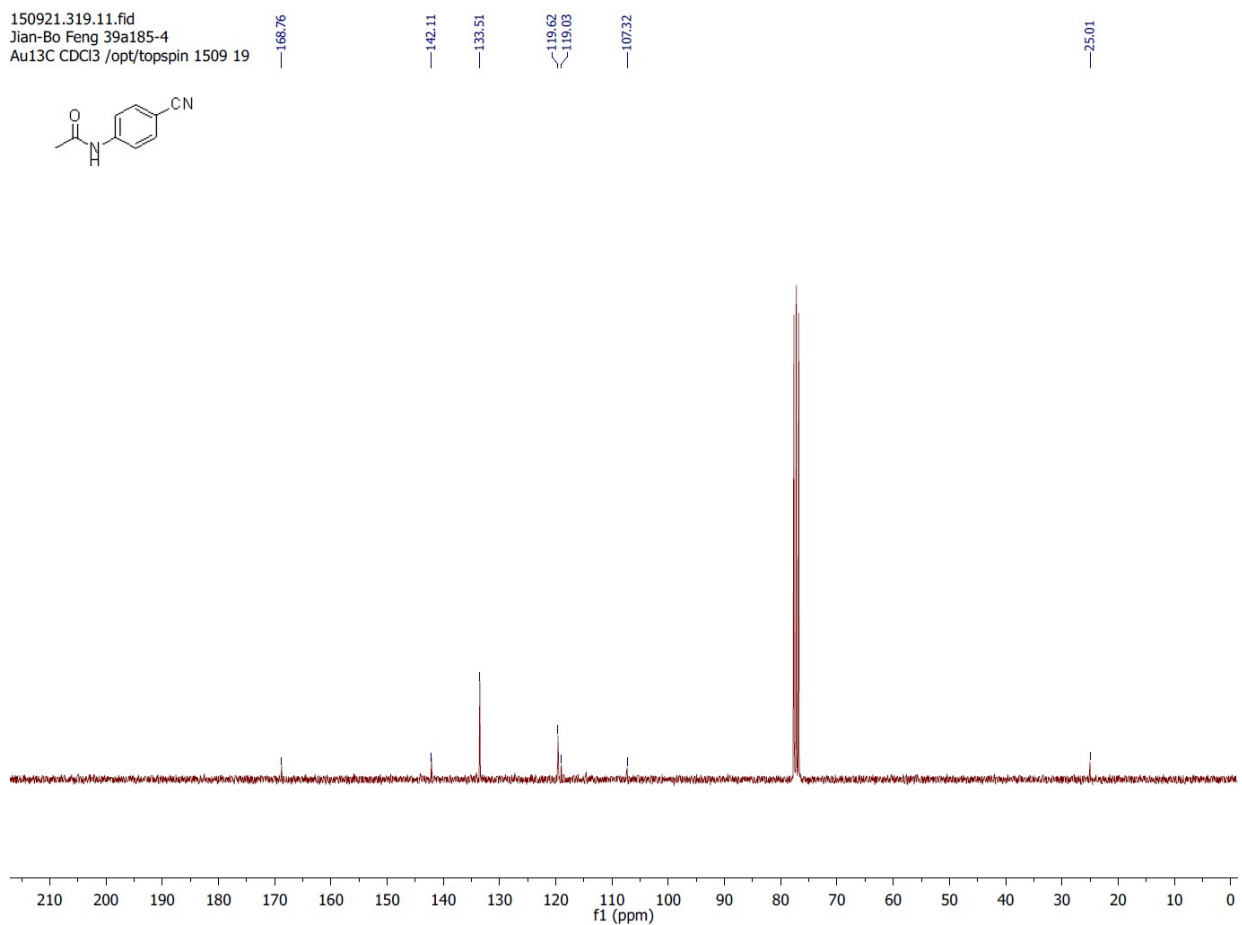
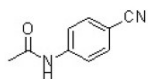
37.36



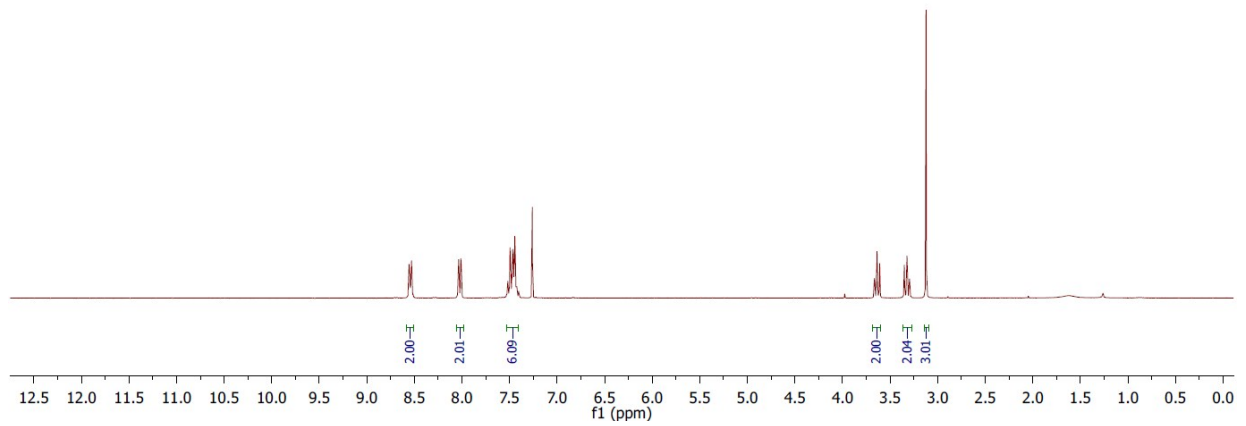
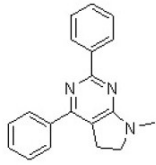
150921.319.10.fid
Jian-Bo Feng 39a185-4
Au1H CDCl3 /opt/topspin 1509 19



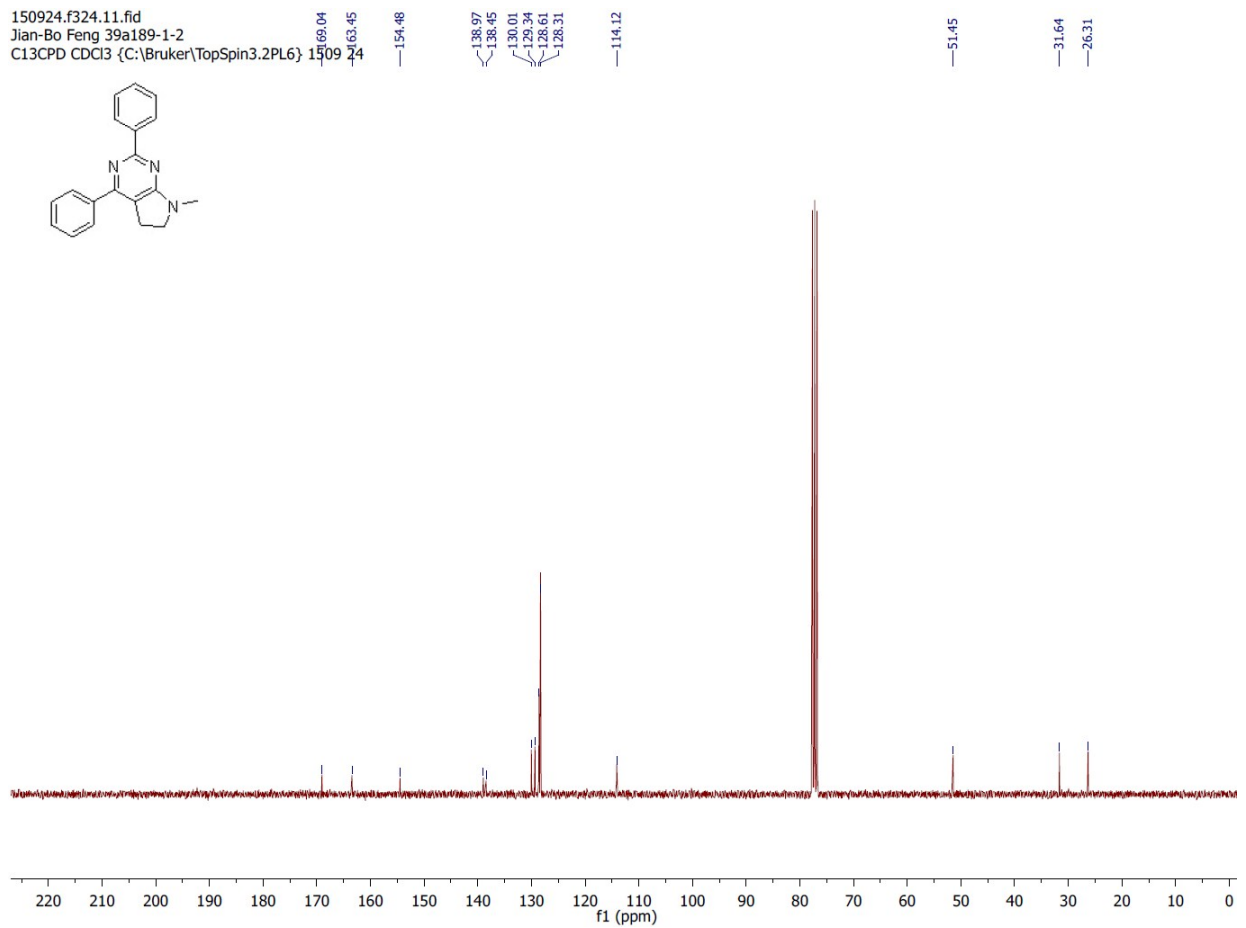
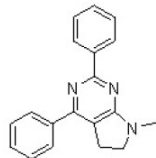
150921.319.11.fid
Jian-Bo Feng 39a185-4
Au13C CDCl3 /opt/topspin 1509 19



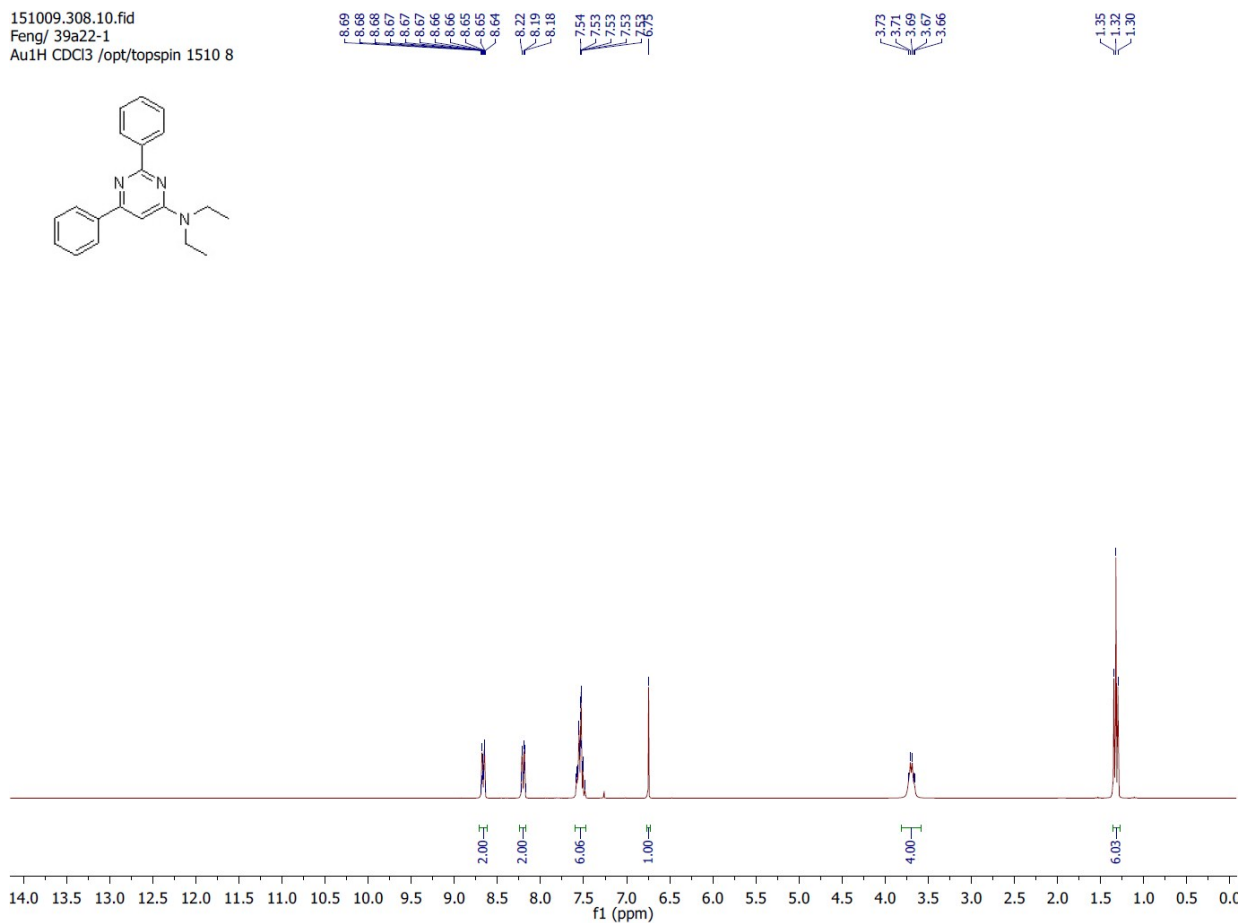
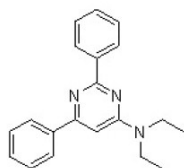
150924.f324.10.fid
Jian-Bo Feng 39a189-1-2
PROTON CDCl3 {C:\Bruker\TopSpin3.2PL6} 1509 24



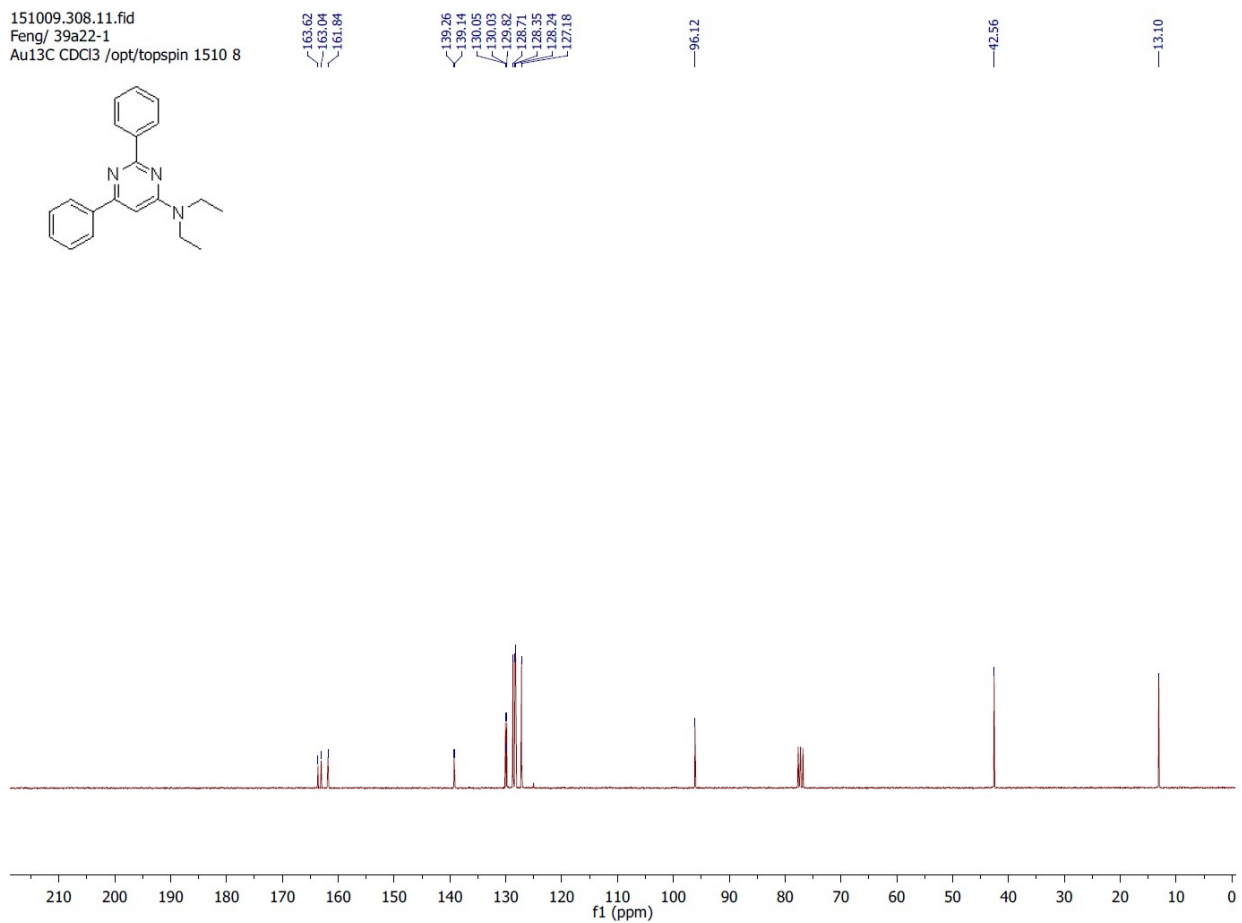
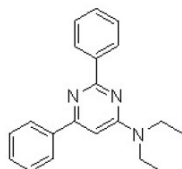
150924.f324.11.fid
Jian-Bo Feng 39a189-1-2
C13CPD CDCl3 {C:\Bruker\TopSpin3.2PL6} 1509 24



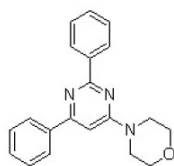
151009.308.10.fid
Feng/ 39a22-1
Au1H CDCl3 /opt/topspin 1510 8



151009.308.11.fid
Feng/ 39a22-1
Au13C CDCl3 /opt/topspin 1510 8

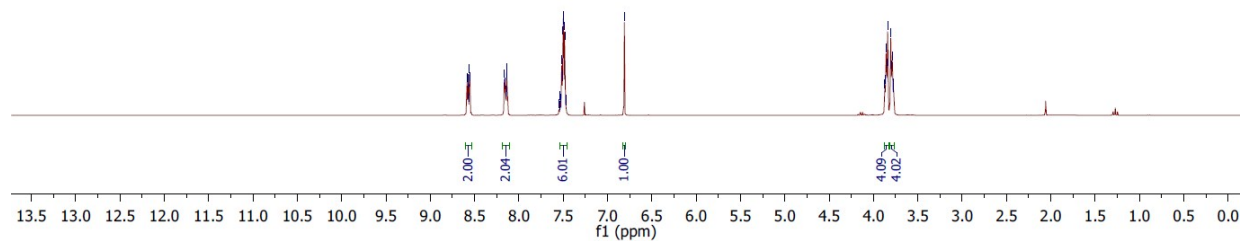


151009.309.11.fid
Feng/ 39a22-2
Au1H CDCl3 /opt/topspin 1510 9

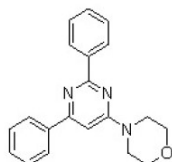


8.98
8.57
8.56
8.55
8.16
8.14
8.13
7.50
7.49
7.48
7.881

3.87
3.87
3.86
3.85
3.84
3.81
3.79
3.78
3.77



151009.309.10.fid
Feng/ 39a22-2
Au13C CDCl3 /opt/topspin 1510 9

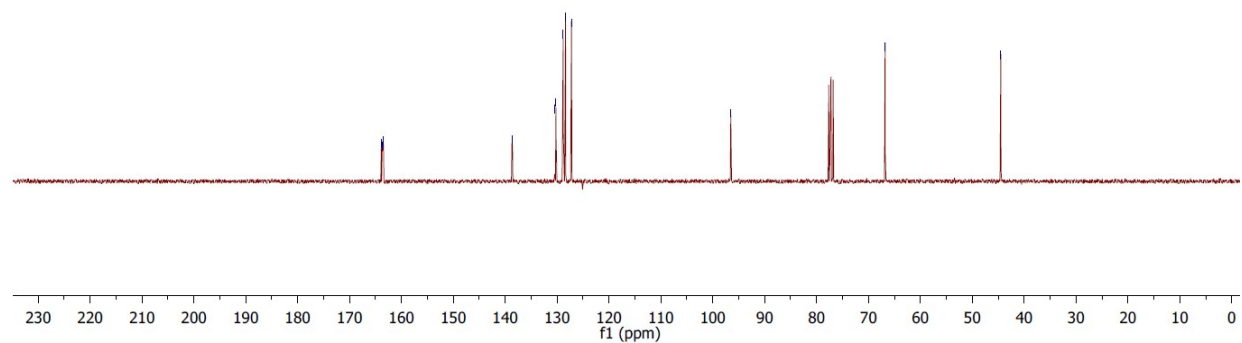


163.88
163.72
163.46
138.71
138.59
130.41
130.22
128.82
128.42
128.37
127.24

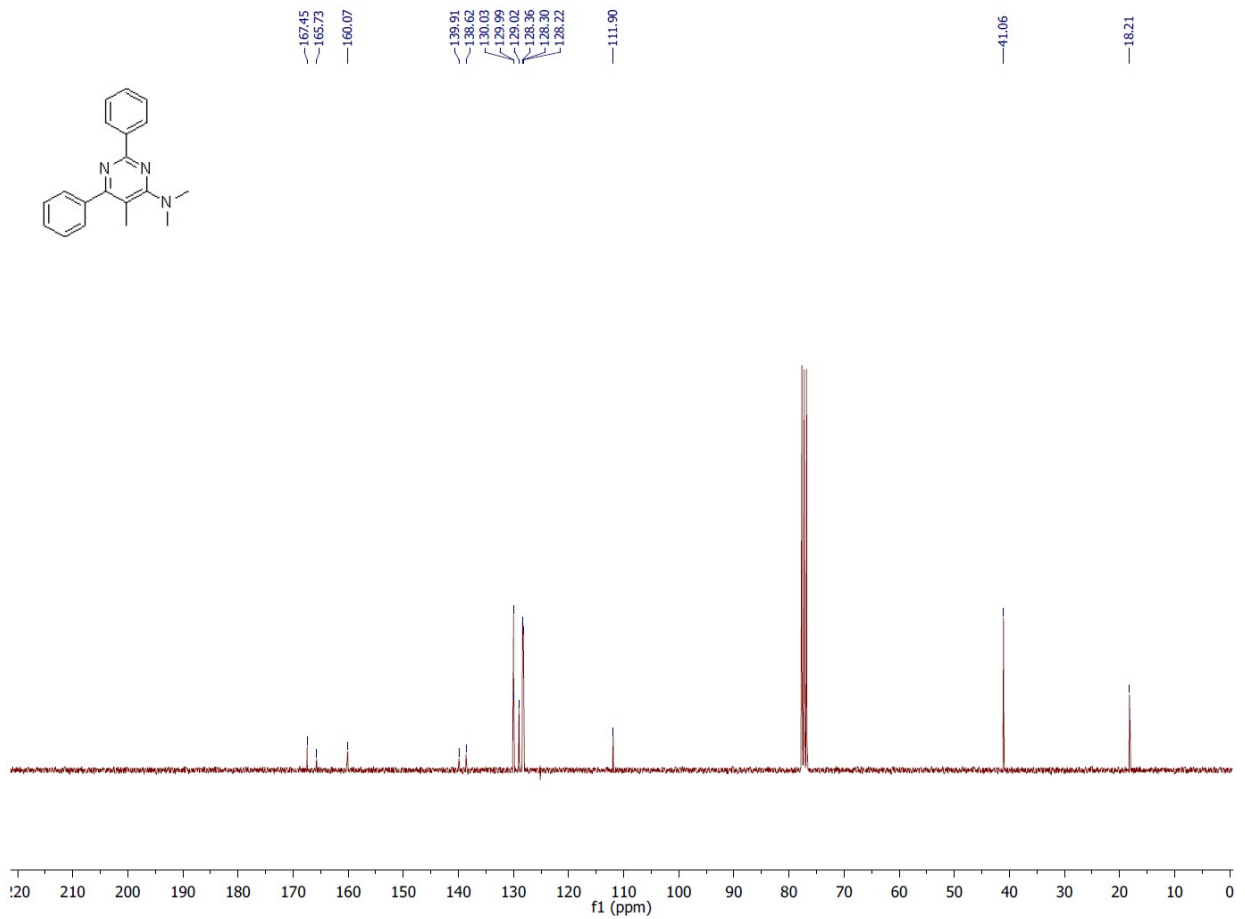
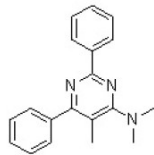
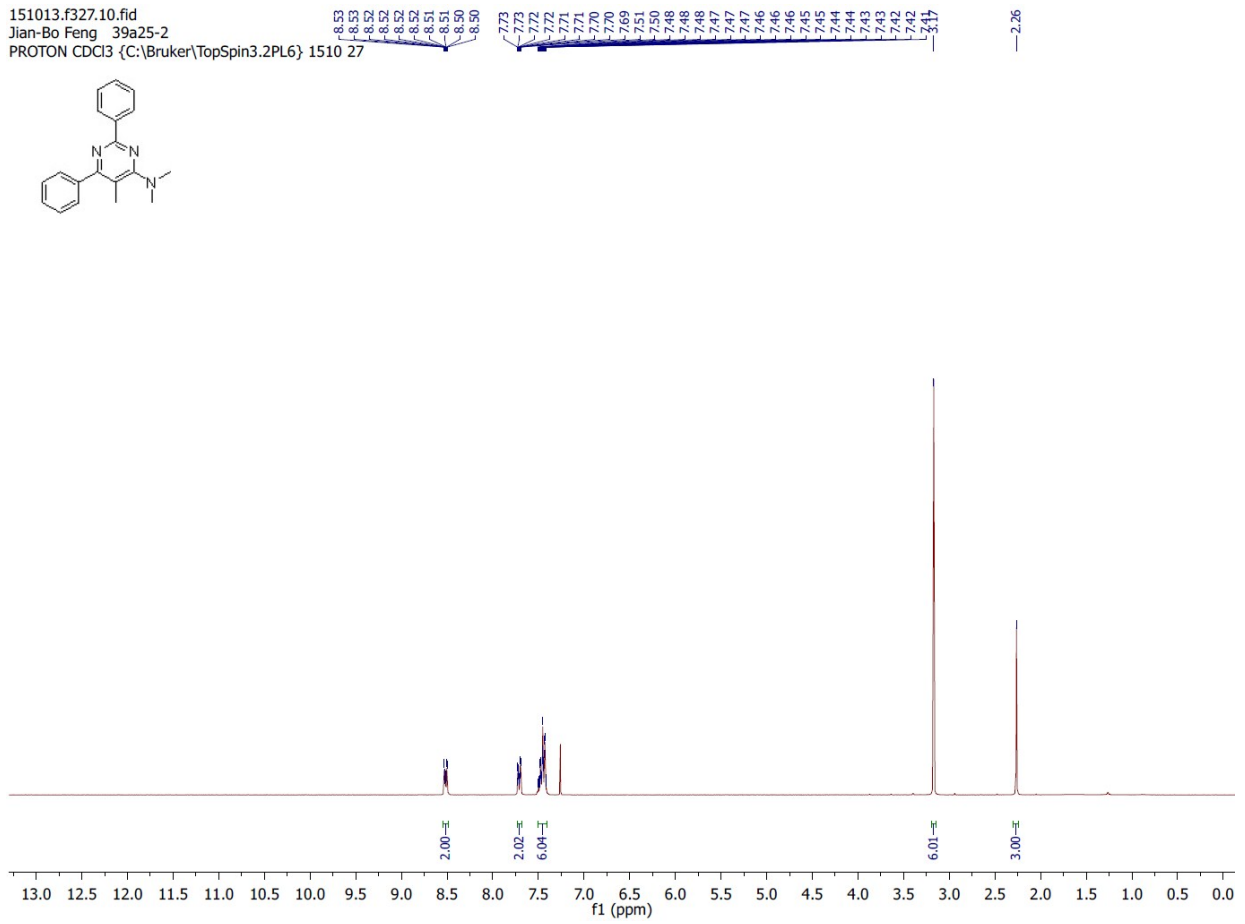
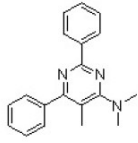
96.52

66.79

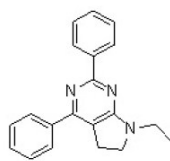
44.50



151013.f327.10.fid
Jian-Bo Feng 39a25-2
PROTON CDCl3 {C:\Bruker\TopSpin3.2PL6} 1510 27

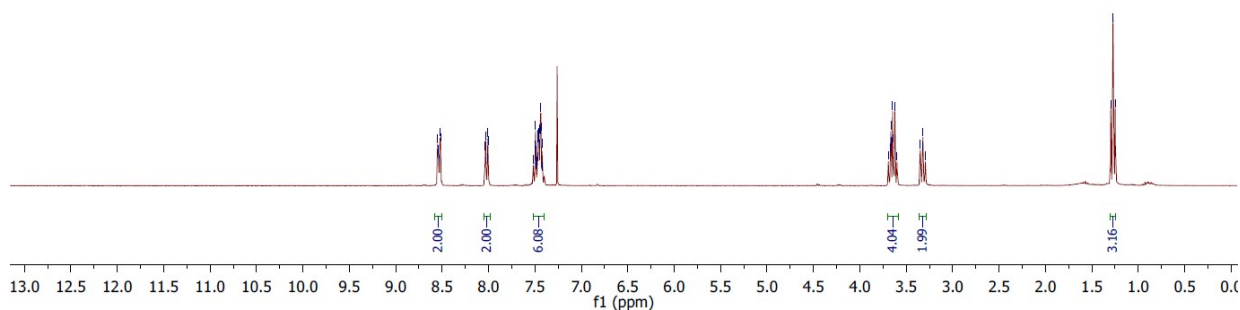


151021.f340.10.fid
 Jian-Bo Feng 39a49-1
 PROTON CDCl3 {C:\Bruker\TopSpin3.2PL6} 1510 40

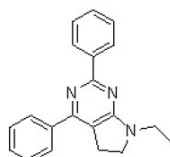


7.855
7.854
7.853
7.852
7.851
8.03
8.01
8.00
7.50
7.49
7.49
7.48
7.48
7.47
7.47
7.46
7.46
7.45
7.45
7.44
7.44
7.43
7.43
7.42
7.42
3.69
3.67
3.66
3.66
3.64
3.62
3.60
3.35
3.32
3.32
3.29

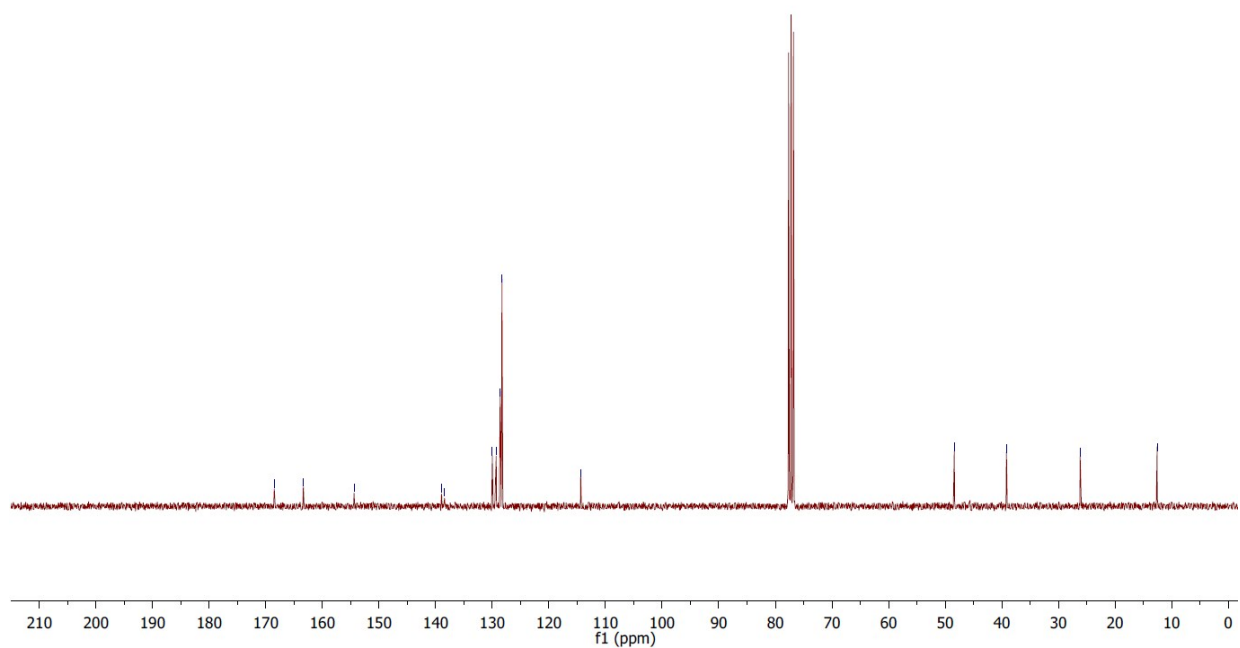
1.30
1.27
1.25



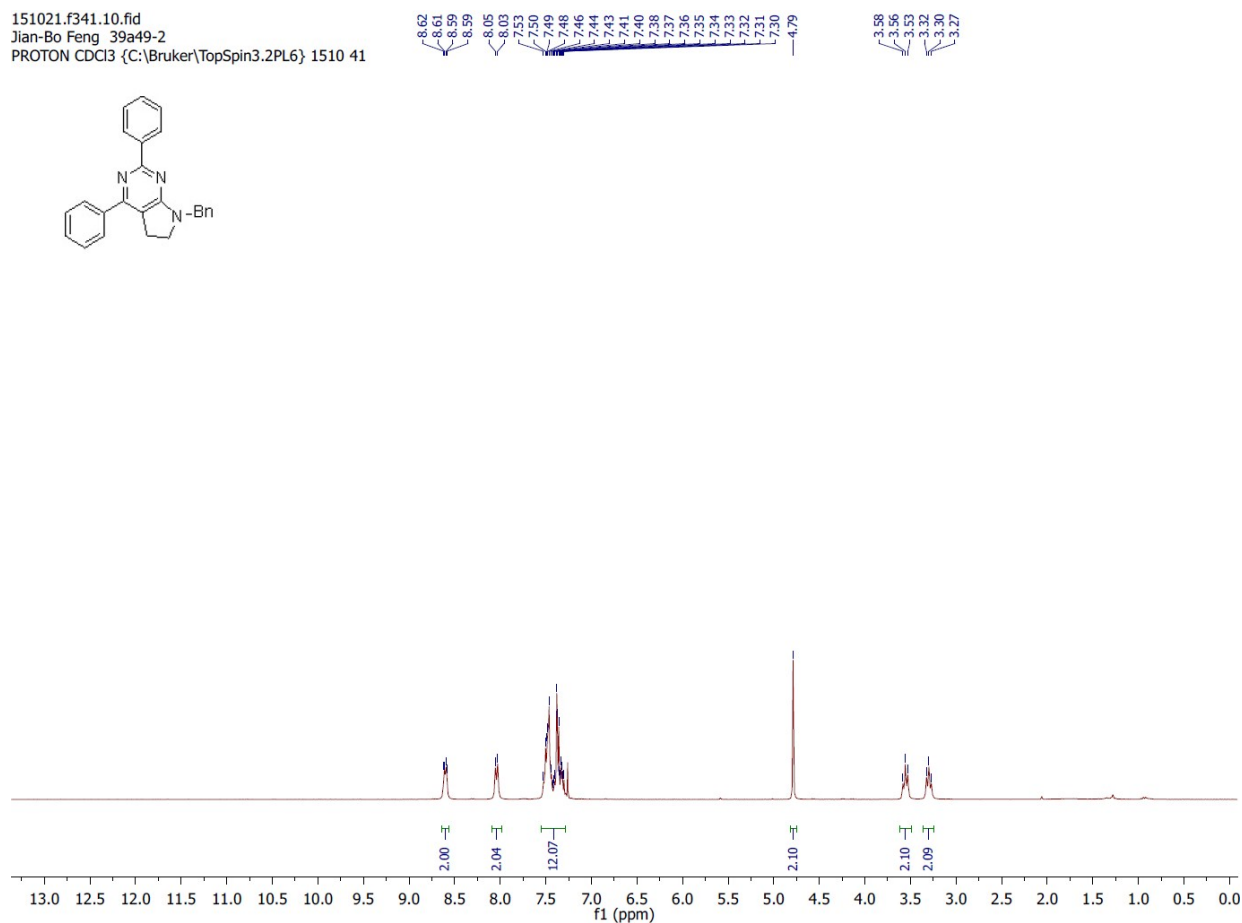
151022.324.10.fid
 Jian-Bo Feng 39a49-1
 Au13C CDCl3 /opt/topspin 1510 24



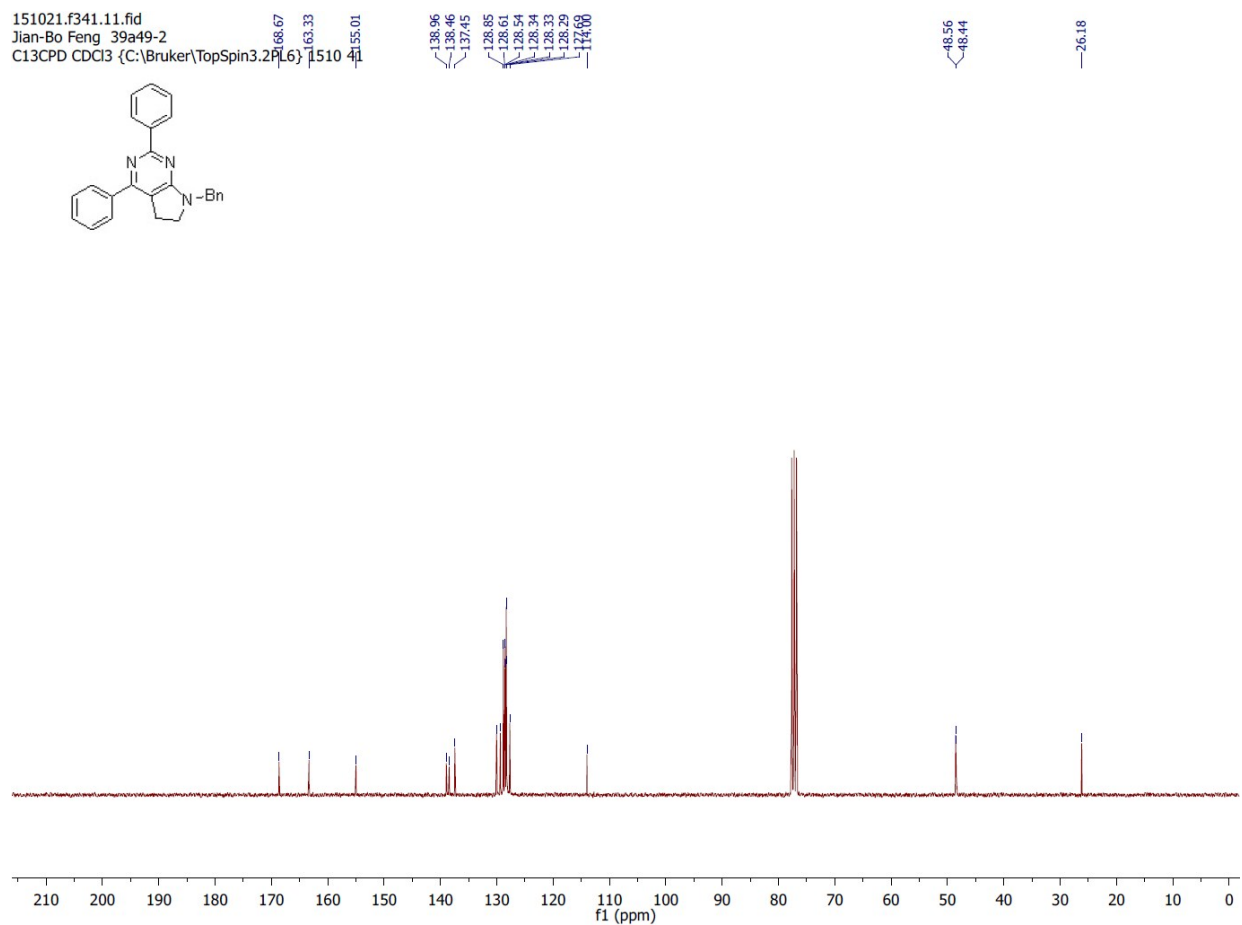
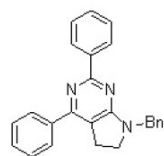
168.51
163.37
154.41
138.95
138.42
129.99
128.31
128.10
128.30
114.38
48.39
39.18
26.16
12.55



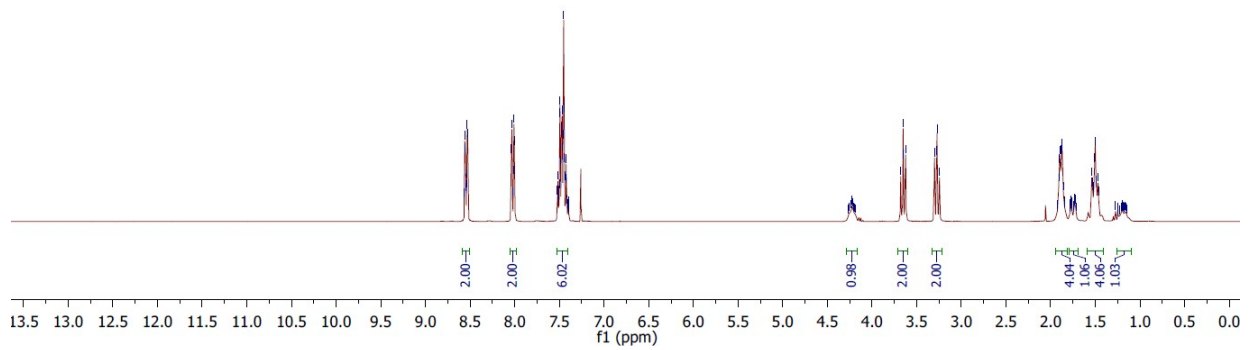
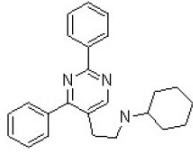
151021.f341.10.fid
 Jian-Bo Feng 39a49-2
 PROTON CDCl3 {C:\Bruker\TopSpin3.2PL6} 1510 41



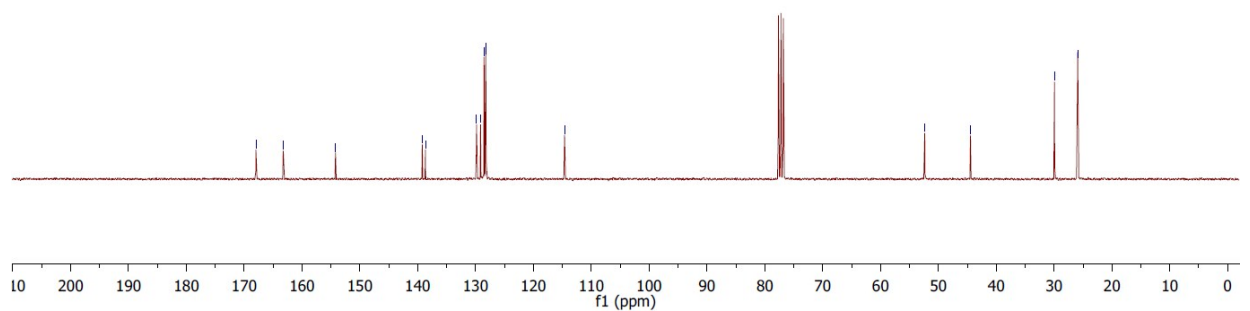
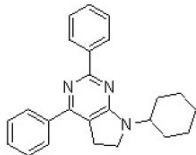
151021.f341.11.fid
 Jian-Bo Feng 39a49-2
 C13CPD CDCl3 {C:\Bruker\TopSpin3.2PL6} 1510 41



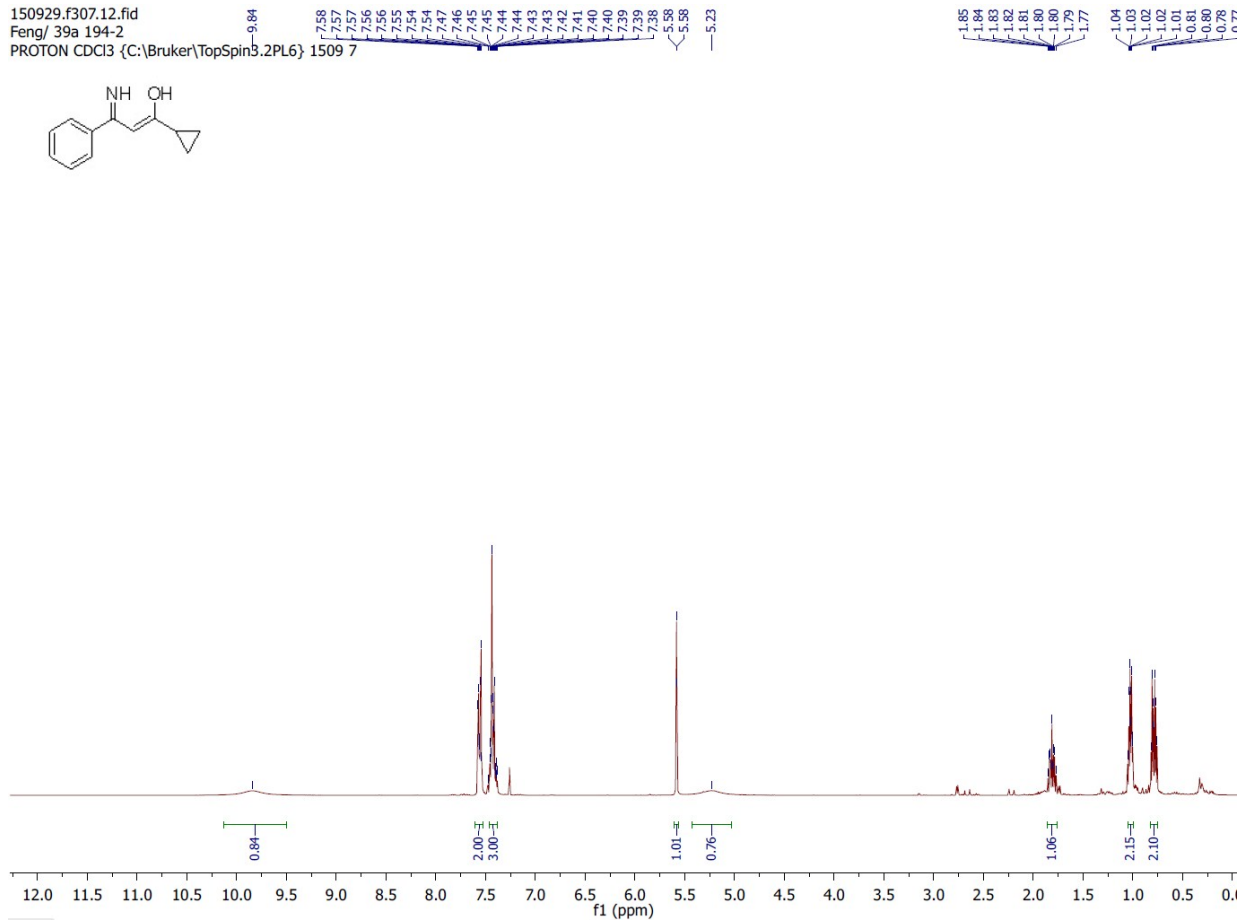
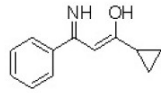
151028.f310.11.fid
 Feng/ 39a63
 PROTON CDCI3 {C:\Bruker\TopSpin3.2PL6} 1510 10



151028.f310.11.fid
 Feng/ 39a63
 C13CPD CDCI3 {C:\Bruker\TopSpin3.2PL6} 1510 10



150929.f307.12.fid
Feng/ 39a 194-2
PROTON CDCl3 {C:\Bruker\TopSpin3.2PL6} 1509 7



150929.f307.10.fid
Feng/ 39a 194-2
C13CPD CDCl3 {C:\Bruker\TopSpin3.2PL6} 1509 7

