Supporting Information

Divergent oxidative annulation of primary aliphatic amines to access semi-saturated fused pyrimidines or quinazolines

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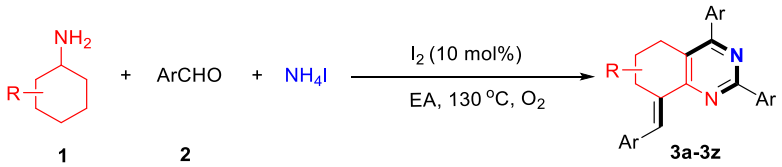
1. General Information

All reagents were obtained commercially and used without further purification. All solvents were dried and distilled according to standard procedures. Column chromatography was performed on silica gel (200-300 mesh). ^{1}H NMR and ^{13}C NMR spectrawere recorded on Bruker-AV (500 and 125 MHz, respectively) instrument internally referenced to tetramethylsilane (TMS) or chloroform. The chemical shifts (δ) were expressed in ppm and coupling constants (J) were in Hz. The following abbreviations are used for the multiplicities: s: singlet, d: doublet, t: triplet, q: quartet, m: multiplet. High-resolution mass spectra (HRMS) were recorded on a Thermo Scientific Exactive Orbitrap Mass Spectrometer using electrospray ionization. Analytical thin layer chromatography was performed on Polygram SIL G/UV254 plates. Visualization was accomplished with short wave UV light. The reaction temperature was detected by the magnetic stirrer of probe.

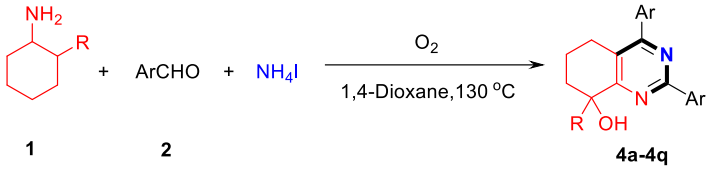
2.General procedure

2.1 General procedure for the synthesis of fused pyrimidines 3a-3z.



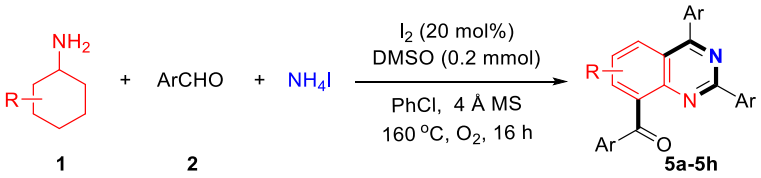
A 15 mL Pressure-resistant tube was charged with cyclohexylamines (0.2 mmol), aromatic aldehydes (1.0 mmol), ammonium iodide (0.4 mmol), iodine (0.02 mmol), freshly activated 4 Å molecular sieves (100 mg) and EA (1 mL). The reaction vessel was purged with oxygen for three times and stirred at 130 ℃ for 15 h. After cooling to room temperature, the reaction mixture was diluted with EA and filtered. The filtrate was then concentrated in vacuo, and the resulting residue was purified by column chromatography to afford the corresponding product.

2.2 General procedure for the synthesis of fused pyrimidines 4a-4q.



A 15 mL Pressure-resistant tube was charged with 2-methylcyclohexylamines (0.2 mmol), aromatic aldehydes (0.8 mmol), ammonium iodide (0.4 mmol), and 1,4-dioxane (1 mL). The reaction vessel was purged with oxygen for three times and stirred at 130 ℃ for 15 h. After cooling to room temperature, the reaction mixture was diluted with EA and filtered. The filtrate was then concentrated in vacuo, and the resulting residue was purified by column chromatography to afford the corresponding product.

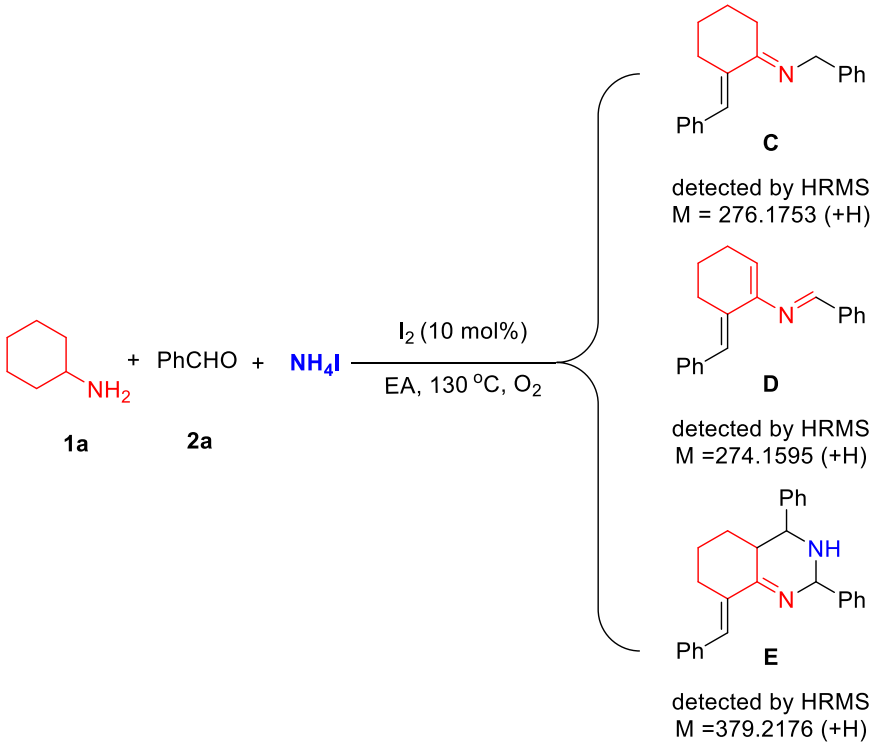
2.3 General procedure for the synthesis of 8-benzoylquinazolines 5a-5h.



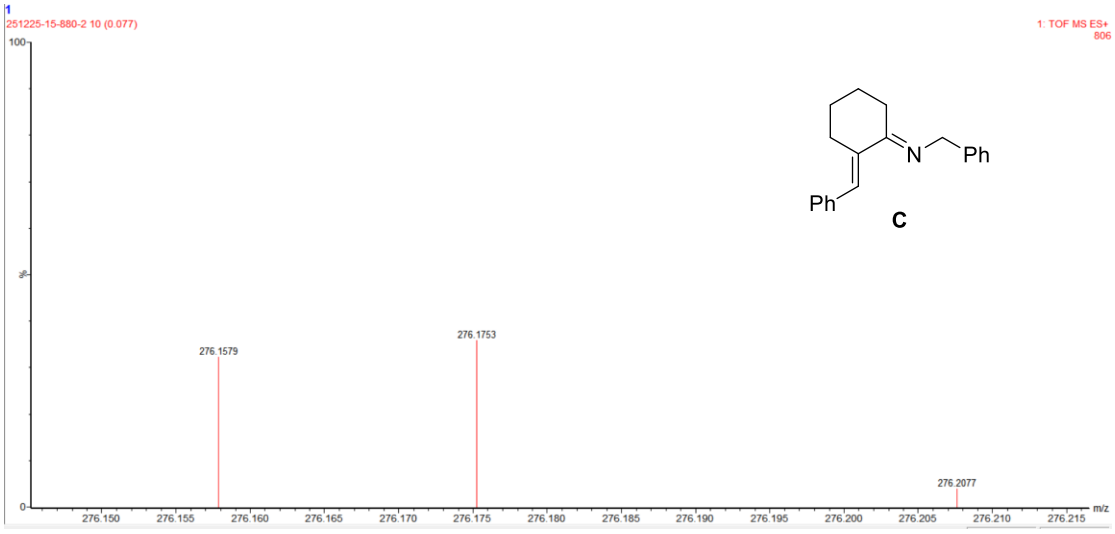
A 15 mL Pressure-resistant tube was charged with cyclohexylamines (0.2 mmol), aromatic aldehydes (1.2 mmol), ammonium iodide (0.4 mmol), iodine (0.04 mmol), DMSO (0.2 mmol), freshly activated 4 Å molecular sieves (100 mg) and PhCl (1 mL). The reaction vessel was purged with oxygen for three times and stirred at 160 ℃ for 16 h. After cooling to room temperature, the reaction mixture was diluted with EA and filtered. The filtrate was then concentrated in vacuo, and the resulting residue was purified by column chromatography to afford the corresponding product.

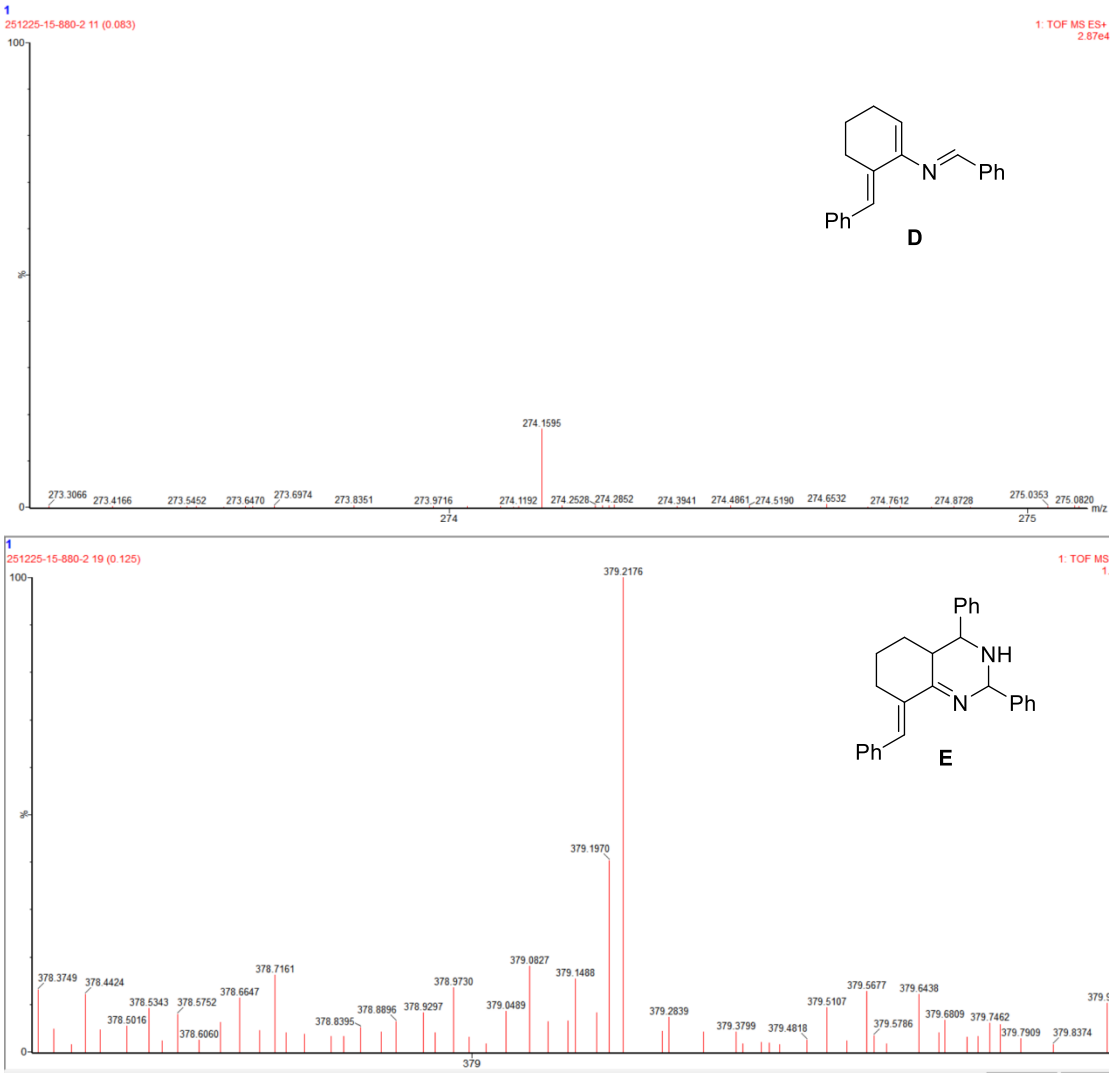
3. The control experiments

A 15 mL Pressure-resistant tube was charged with cyclohexylamines (0.2 mmol), aromatic aldehydes (1.0 mmol), ammonium iodide (0.4 mmol), iodine (0.02 mmol), freshly activated 4 Å molecular sieves (100 mg) and EA (1 mL). The reaction vessel was purged with oxygen for three times and stirred at 130 ℃ for 2 h. The mixture was tested by high-resolution mass spectrometry (HRMS) and the molecular mass of intermediate **C**, intermediate **D** and intermediate **E** were detected successfully.

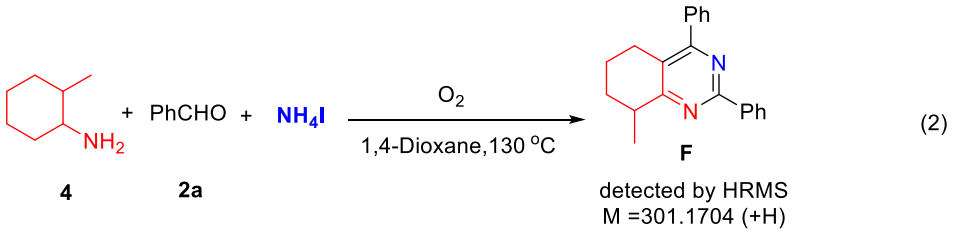


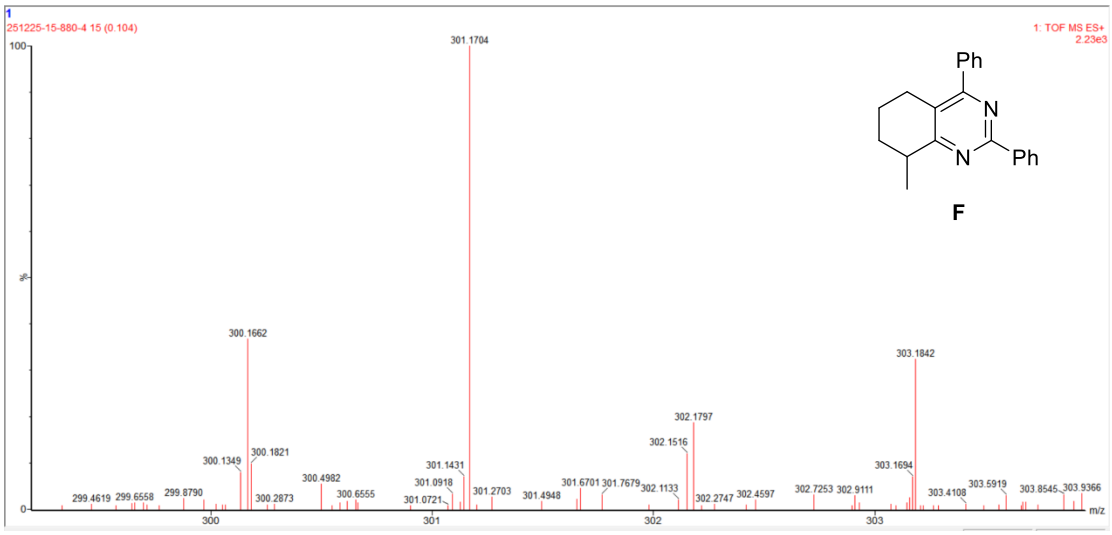
(1)





A 15 mL Pressure-resistant tube was charged with 2-methylcyclohexylamines (0.2 mmol), aromatic aldehydes (0.8 mmol), ammonium iodide (0.4 mmol), and 1,4-dioxane (1 mL). The reaction vessel was purged with oxygen for three times and stirred at 130 °C for 2 h. The mixture was tested by high-resolution mass spectrometry (HRMS) and the molecular mass of intermediate **C** were detected successfully.

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303.1694
300.4982
301.0918
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300.2873
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301.4948
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302
303
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Ph
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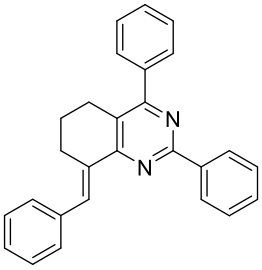
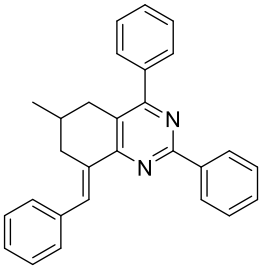
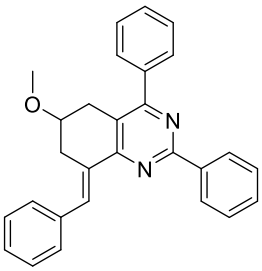
4. Characterization data of products



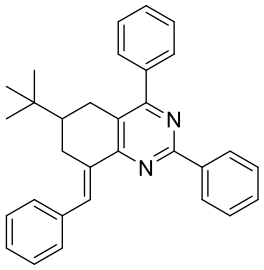
8-Benzylidene-2,4-diphenyl-5,6,7,8-tetrahydroquinazoline (3a): White solid (53.4 mg, 71% yield); R_f = 0.5 (PE:EA = 50:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.62 (d, *J* = 6.3 Hz, 2H), 8.51 (s, 1H), 7.72 (d, *J* = 6.3 Hz, 2H), 7.55 – 7.48 (m, 8H), 7.44 (t, *J* = 7.7 Hz, 2H), 7.33 (t, *J* = 7.4 Hz, 1H), 2.98 (t, *J* = 5.2 Hz, 2H), 2.91 (t, *J* = 6.0 Hz, 2H), 1.84 – 1.77 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 165.9, 161.7, 160.3, 138.7, 138.3, 137.3, 134.4, 130.6, 130.1, 129.9, 129.2, 129.1, 128.3, 128.24, 128.18, 128.1, 127.5, 124.7, 27.9, 27.5, 22.7. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{27}H_{23}N_2^+$: 375.1856, found: 375.1864.



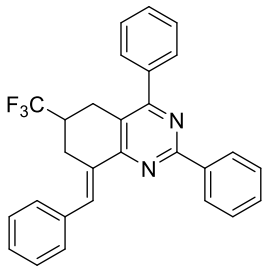
8-Benzylidene-6-methyl-2,4-diphenyl-5,6,7,8-tetrahydroquinazoline (3b): White solid (49.2 mg, 63% yield); R_f = 0.5 (PE:EA = 50:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.62 (d, *J* = 6.5 Hz, 2H), 8.52 (s, 1H), 7.72 (d, *J* = 6.4 Hz, 2H), 7.56 – 7.48 (m, 8H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.34 (t, *J* = 7.4 Hz, 1H), 3.16 (d, *J* = 15.4 Hz, 1H), 2.92 – 2.85 (m, 1H), 2.68 – 2.59 (m, 1H), 2.55 – 2.44 (m, 1H), 1.89 – 1.78 (m, 1H), 1.06 (d, *J* = 6.5 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 165.9, 161.0, 160.1, 138.7, 138.3, 137.2, 134.2, 130.7, 130.1, 129.9, 129.2, 129.1, 128.34, 128.25, 128.2, 128.1, 127.5, 124.2, 35.9, 35.6, 29.1, 21.5. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{28}H_{25}N_2^+$: 389.2012, found: 389.2017.



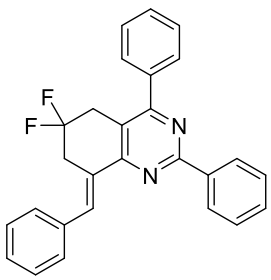
8-Benzylidene-6-methoxy-2,4-diphenyl-5,6,7,8-tetrahydroquinazoline (3c): White solid (50.1 mg, 62% yield); R_f = 0.5 (PE:EA = 50:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.64 – 8.57 (m, 3H), 7.71 (d, *J* = 6.0 Hz, 2H), 7.55 – 7.47 (m, 8H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.34 (t, *J* = 7.4 Hz, 1H), 3.65 – 3.59 (m, 1H), 3.29 – 3.23 (m, 4H), 3.19 – 3.13 (m, 1H), 3.05 – 2.96 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 166.6, 161.3, 159.7, 138.3, 138.1, 136.8, 132.6, 131.6, 130.2, 129.8, 129.2, 129.1, 128.32, 128.30, 128.2, 128.1, 127.7, 121.4, 74.1, 56.1, 32.6, 26.9. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{28}H_{25}N_2O^+$: 405.1961, found: 405.1968.



8-Benzylidene-6-(*tert*-butyl)-2,4-diphenyl-5,6,7,8-tetrahydro quinazoline (3d): White solid (51.6 mg, 60% yield); R_f = 0.3 (PE:EA = 50:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.61 (dd, *J* = 8.1, 1.7 Hz, 2H), 8.47 (s, 1H), 7.73 (d, *J* = 6.5 Hz, 2H), 7.53 (t, *J* = 8.0 Hz, 5H), 7.51 – 7.48 (m, 3H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.33 (t, *J* = 7.4 Hz, 1H), 3.32 (d, *J* = 15.3 Hz, 1H), 2.92 (d, *J* = 16.0 Hz, 1H), 2.71 – 2.63 (m, 1H), 2.38 (t, *J* = 15.4 Hz, 1H), 1.47 (t, *J* = 12.5 Hz, 1H), 0.92 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$, ppm) δ 166.1, 161.0, 160.3, 138.7, 138.3, 137.3, 135.2, 130.5, 130.1, 129.8, 129.2, 129.1, 128.34, 128.31, 128.2, 128.1, 127.4, 124.9, 44.4, 32.5, 29.0, 28.8, 27.3. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{31}H_{31}N_2^+$: 431.2482, found: 431.2482.

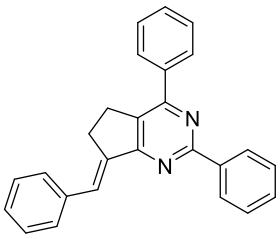


8-Benzylidene-2,4-diphenyl-6-(trifluoromethyl)-5,6,7,8-tetra hydroquinazoline (3e): White solid (58.0 mg, 66% yield); R_f = 0.5 (PE:EA = 50:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.68 – 8.59 (m, 3H), 7.74 – 7.69 (m, 2H), 7.58 – 7.46 (m, 10H), 7.38 (t, *J* = 7.2 Hz, 1H), 3.45 (d, *J* = 15.3 Hz, 1H), 3.12 – 2.99 (m, 2H), 2.82 – 2.73 (m, 1H), 2.47 – 2.35 (m, 1H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 166.4, 161.6, 159.1, 137.9, 137.8, 136.3, 132.8, 130.53, 130.46, 129.8, 129.5, 129.0, 128.51, 128.46, 128.4, 128.2, 128.1, 127.1 (q, *J* = 278.7 Hz), 121.0, 38.7(q, *J* = 27.6 Hz), 26.4 (d, *J* = 1.7 Hz), 26.2 (d, *J* = 2.8 Hz). ^{19}F NMR (471 MHz, $CDCl_3$, ppm) δ -73.1. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{28}H_{22}F_3N_2^+$: 443.1730, found: 443.1734.

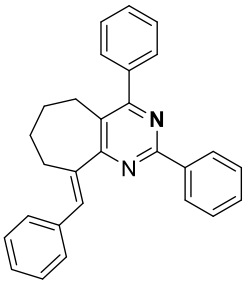


Benzylidene-6,6-difluoro-2,4-diphenyl-5,6,7,8-tetrahydroqu inazoline (3f): White solid (30.3 mg, 37% yield); R_f = 0.5 (PE:EA = 50:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.69 (s, 1H), 8.61 (d, *J* = 7.8 Hz, 2H), 7.65 (dd, *J* = 7.7, 1.8 Hz, 2H), 7.56 – 7.51 (m, 4H), 7.51 – 7.45 (m, 5H), 7.41 – 7.35 (m, 1H), 3.46 – 3.35 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 167.0, 162.1, 158.1, 137.8, 137.7, 136.0, 135.0, 130.6, 129.7, 129.6, 129.0 (d, *J* = 5.0 Hz), 128.9, 128.56, 128.55,

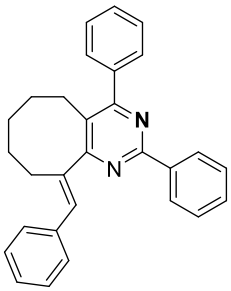
128.5, 128.33, 128.30, 120.7 (t, J = 240.7 Hz), 118.9 (t, J = 6.0 Hz), 35.9 (t, J = 26.6 Hz), 35.7 (t, J = 27.6 Hz). ^{19}F NMR (471 MHz, $CDCl_3$) δ -96.13. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{27}H_{21}F_2N_2^+$: 411.1667, found: 411.1674.



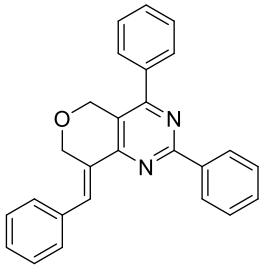
7-**Benzylidene-2,4-diphenyl-6,7-dihydro-5*H*-cyclopenta[d] pyrimidine (3g):** Yellow solid (35.3 mg, 49% yield); R_f = 0.6 (PE:EA = 50:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.68 (d, J = 6.7 Hz, 2H), 8.13 (d, J = 6.9 Hz, 2H), 7.91 (s, 1H), 7.64 (d, J = 7.7 Hz, 2H), 7.58 – 7.49 (m, 7H), 7.45 (t, J = 7.6 Hz, 2H), 7.33 (t, J = 7.4 Hz, 1H), 3.44 – 3.39 (m, 2H), 3.29 – 3.24 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 170.0, 163.6, 160.8, 139.9, 138.3, 138.1, 137.0, 130.24, 130.21, 130.0, 129.6, 128.65, 128.61, 128.6, 128.4, 128.3, 127.8, 126.2, 28.91, 28.90. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{26}H_{21}N_2^+$: 361.1699, found: 361.1707.



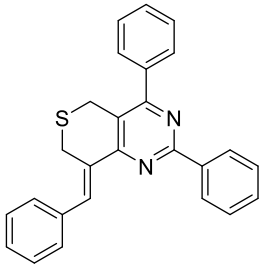
8-**benzylidene-2,4-diphenyl-6,7,8,9-tetrahydro-5H-cyclohepta [d]pyrimidine(3h)**: White solid (23.4mg, 32% yield); R_f = 0.5 (PE:EA = 50:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.60 (d, J = 7.2 Hz, 2H), 7.67 (d, J = 6.9 Hz, 2H), 7.56 (d, J = 7.7 Hz, 2H), 7.54 – 7.46 (m, 7H), 7.43 (t, J = 7.6 Hz, 2H), 7.32 (t, J = 7.3 Hz, 1H), 2.91 – 2.82 (m, 4H), 2.01 – 1.86 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 168.9, 165.6, 161.5, 141.5, 139.2, 138.1, 137.2, 133.8, 130.1, 129.4, 129.2, 128.9, 128.4, 128.3, 128.2, 128.1, 127.4, 126.9, 29.0, 28.0, 26.8, 26.5.



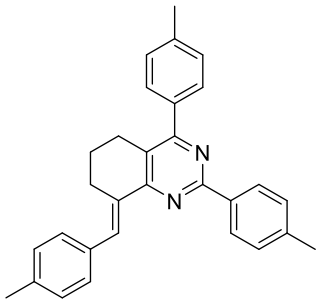
10-benzylidene-2,4-diphenyl-5,6,7,8,9,10-hexahydrocycloocta[d]pyrimidine (3i): White solid (24.1 mg, 30% yield); R_f = 0.5 (PE:EA = 50:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.56 (d, J = 7.7 Hz, 2H), 7.56 – 7.51 (m, 2H), 7.47 – 7.40 (m, 6H), 7.13 – 7.06 (m, 3H), 6.98 – 6.93 (m, 2H), 6.63 (s, 1H), 2.77 – 2.69 (m, 2H), 2.66 – 2.57 (m, 2H), 1.64 – 1.52 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 169.6, 165.9, 162.3, 140.9, 139.0, 137.9, 136.4, 130.3, 128.7, 128.4, 128.3, 128.18, 128.16, 127.8, 126.9, 41.5, 31.5, 26.8, 26.73, 26.70.



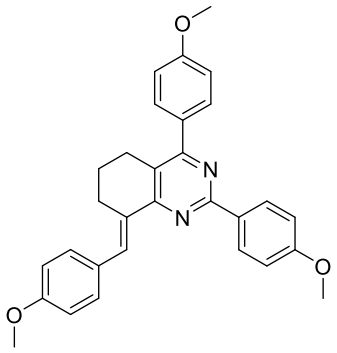
8-Benzylidene-2,4-diphenyl-7,8-dihydro-5*H*-pyrano[4,3-*d*]pyrimidine (3j): White solid (34.1 mg, 45% yield); R_f = 0.4 (PE:EA = 50:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.65 (d, *J* = 9.7 Hz, 2H), 8.46 (s, 1H), 7.69 – 7.66 (m, 2H), 7.55 – 7.51 (m, 6H), 7.45 (t, *J* = 7.5 Hz, 2H), 7.41 – 7.35 (m, 3H), 4.99 (d, *J* = 1.9 Hz, 2H), 4.92 (s, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 163.1, 162.3, 157.6, 138.0, 137.3, 135.8, 130.6, 130.5, 129.9, 129.83, 129.79, 128.9, 128.5, 128.4, 128.24, 128.21, 122.1, 67.7, 66.5. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{26}H_{21}N_2O^+$: 377.1648, found: 377.1656.



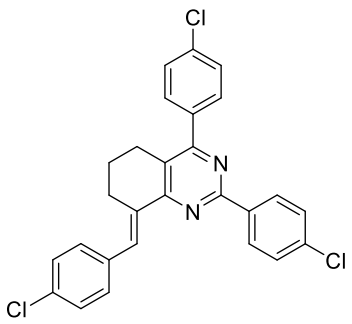
8-Benzylidene-2,4-diphenyl-7,8-dihydro-5H-thiopyrano[4,3-*d*]pyrimidine (3k): Brown solid (22.0 mg, 28% yield); R_f= 0.5 (PE:EA = 50:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.64 – 8.54 (m, 3H), 7.65 (dd, *J* = 7.8, 1.8 Hz, 2H), 7.55 – 7.44 (m, 10H), 7.39 – 7.33 (m, 1H), 3.98 (s, 2H), 3.94 (s, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 165.5, 161.3, 159.7, 138.1, 137.8, 136.4, 132.0, 131.2, 130.4, 129.8, 129.4, 129.1, 128.51, 128.47, 128.4, 128.2, 128.0, 122.6, 29.32, 29.30. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{26}H_{21}N_2S^+$: 393.1420, found: 393.1428.



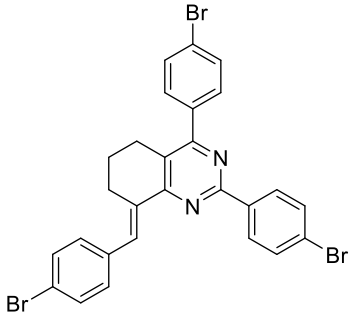
8-(4-Methylbenzylidene)-2,4-di-p-tolyl-5,6,7,8-tetrahydroquinazoline (3l): White solid (49.9 mg, 60% yield); R_f = 0.5 (PE:EA = 50:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.5 (d, *J* = 8.2 Hz, 2H), 8.4 (s, 1H), 7.6 (d, *J* = 8.1 Hz, 2H), 7.4 (d, *J* = 7.9 Hz, 2H), 7.3 – 7.3 (m, 4H), 7.2 (d, *J* = 7.9 Hz, 2H), 2.9 (t, *J* = 5.2 Hz, 2H), 2.9 (t, *J* = 6.0 Hz, 2H), 2.4 (s, 3H), 2.4 (s, 3H), 2.4 (s, 3H), 1.8 – 1.7 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 165.6, 161.0, 160.1, 140.0, 139.0, 137.3, 135.9, 135.7, 134.4, 133.8, 130.3, 129.9, 129.2, 129.0, 128.9, 128.8, 128.0, 124.2, 27.9, 27.6, 22.7, 21.5, 21.4, 21.3. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{30}H_{29}N_2^+$: 417.2325, found: 417.2329.



8-(4-Methoxybenzylidene)-2,4-bis(4-methoxyphenyl)-5,6,7,8-tetrahydroquinazoline (3m): White solid (50.7 mg, 55% yield); R_f= 0.4 (PE:EA = 50:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.56 (d, *J* = 8.9 Hz, 2H), 8.40 (s, 1H), 7.70 (d, *J* = 8.7 Hz, 2H), 7.50 (d, *J* = 8.7 Hz, 2H), 7.01 (t, *J* = 8.8 Hz, 4H), 6.96 (d, *J* = 8.7 Hz, 2H), 3.89 (s, 3H), 3.88 (s, 3H), 3.86 (s, 3H), 2.96 (t, *J* = 5.2 Hz, 2H), 2.90 (t, *J* = 5.9 Hz, 2H), 1.83 – 1.75 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 165.0, 161.3, 160.7, 160.31, 160.26, 158.9, 132.8, 131.4, 131.25, 131.24, 130.8, 129.9, 129.6, 123.6, 113.7, 113.6, 113.5, 55.4, 55.32, 55.29, 28.0, 27.7, 22.9. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{30}H_{29}N_2O_3^+$: 465.2173, found: 465.2176.

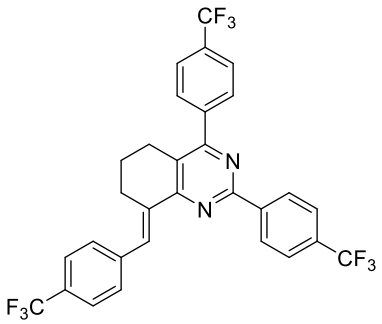


8-(4-Chlorobenzylidene)-2,4-bis(4-chlorophenyl)-5,6,7,8-tetrahydroquinazoline (3n): White solid (50.2 mg, 53% yield); R_f = 0.5 (PE:EA = 50:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.52 (d, *J* = 8.6 Hz, 2H), 8.38 (s, 1H), 7.65 (d, *J* = 8.5 Hz, 2H), 7.52 – 7.43 (m, 6H), 7.43 – 7.38 (m, 2H), 2.92 (t, 2H), 2.88 (t, *J* = 6.0 Hz, 2H), 1.85 – 1.76 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 164.9, 160.3, 160.2, 136.8, 136.5, 136.4, 135.5, 135.4, 134.6, 133.4, 131.2, 130.6, 129.7, 129.4, 128.6, 128.5, 124.9, 27.8, 27.5, 22.5. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{27}H_{20}N_2Cl_3^+$: 477.0687, found: 477.0692.

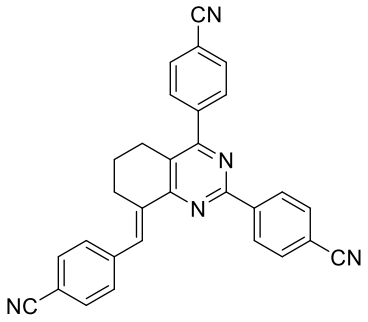


8-(4-Bromobenzylidene)-2,4-bis(4-bromophenyl)-5,6,7,8-tetrahydroquinazoline (3o): White solid (71.4 mg, 58% yield); R_f = 0.5 (PE:EA = 50:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.44 (d, *J* = 8.5 Hz, 2H), 8.35 (s, 1H), 7.66 – 7.59 (m, 4H), 7.56 (t, 4H), 7.38 (d, *J* = 8.5 Hz, 2H), 2.91 (t, *J* = 5.7 Hz, 2H), 2.86 (t, *J* = 6.0 Hz, 2H), 1.83 – 1.76 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 164.9, 160.3, 137.2, 136.9, 135.9, 134.7, 131.6, 131.48, 131.47, 131.4, 130.8, 129.8, 129.7, 124.99, 124.95,

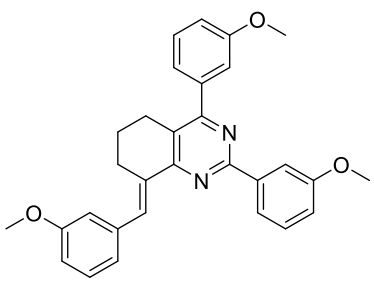
123.8, 121.7, 27.8, 27.5, 22.5. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{27}H_{20}N_2Br_3^+$: 608.9171, found: 608.9169.



8-(4-(Trifluoromethyl)benzylidene)-2,4-bis(4-(trifluoromethyl)phenyl)-5,6,7,8-tetrahydroquinazoline (3p): White solid (77.7 mg, 67% yield); R_f = 0.6 (PE:EA = 50:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.70 (d, *J* = 8.1 Hz, 2H), 8.50 (s, 1H), 7.84 – 7.79 (m, 4H), 7.76 (d, *J* = 8.2 Hz, 2H), 7.70 (d, *J* = 8.1 Hz, 2H), 7.62 (d, *J* = 8.1 Hz, 2H), 2.96 (t, *J* = 5.3 Hz, 2H), 2.91 (t, *J* = 6.0 Hz, 2H), 1.88 – 1.81 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 165.1, 160.4, 160.0, 141.7, 141.2, 140.5, 135.9, 132.0 (q, *J* = 32.2 Hz), 131.4(q, *J* = 32.7 Hz), 130.1, 129.8, 129.6, 129.2 (d, *J* = 32.6 Hz), 128.4, 125.9, 125.4 (q, *J* = 3.7 Hz), 125.3(q, *J* = 3.8 Hz), 122.1(q, *J* = 271.8 Hz), 124.2(q, *J* = 272.54 Hz), 124.0 (q, *J* = 272.3 Hz), 27.7, 27.4, 22.4. ^{19}F NMR (471 MHz, $CDCl_3$, ppm) δ -62.53, -62.62, -62.71. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{30}H_{20}F_9N_2^+$:579.1477, found: 579.1483.

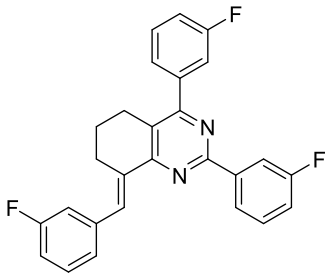


4,4'-(8-(4-Cyanobenzylidene)-5,6,7,8-tetrahydroquinazoline-2,4-diyl)dibenzonitrile (3q): Yellow solid (35.2 mg, 49% yield); R_f = 0.3 (PE:EA = 4:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.67 (d, *J* = 8.5 Hz, 2H), 8.45 (s, 1H), 7.87 – 7.77 (m, 6H), 7.73 (d, *J* = 8.2 Hz, 2H), 7.60 (d, *J* = 8.1 Hz, 2H), 2.96 (t, *J* = 5.3 Hz, 2H), 2.91 (t, *J* = 6.0 Hz, 2H), 1.91 – 1.80 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 164.7, 160.5, 159.7, 142.3, 141.7, 141.4, 136.5, 132.3, 132.2, 132.1, 130.4, 129.9, 129.8, 128.6, 126.3, 118.8, 118.8, 118.4, 113.9, 113.4, 111.2, 27.7, 27.4, 22.3. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{30}H_{20}N_5^+$: 450.1713, found: 450.1718.

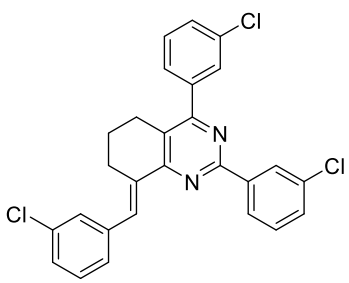


8-(3-Methoxybenzylidene)-2,4-bis(3-methoxyphenyl)-5,6,7,8-tetrahydroquinazoline (3r): White solid (58.9 mg, 63% yield); R_f = 0.5 (PE:EA = 10:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.44 (s, 1H), 8.20 (d,

J = 9.1 Hz, 1H), 8.16 (s, 1H), 7.41 (t, *J* = 7.5 Hz, 2H), 7.34 (t, *J* = 7.9 Hz, 1H), 7.27 – 7.23 (m, 2H), 7.11 (d, *J* = 7.6 Hz, 1H), 7.06 – 6.99 (m, 3H), 6.88 (dd, *J* = 8.1, 2.6 Hz, 1H), 3.91 (s, 3H), 3.88 (s, 3H), 3.86 (s, 3H), 2.96 (t, *J* = 5.3 Hz, 2H), 2.89 (t, *J* = 6.0 Hz, 2H), 1.82 – 1.76 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 165.8, 160.8, 160.2, 159.8, 159.41, 159.38, 139.9, 139.8, 138.6, 134.7, 130.5, 129.4, 129.21, 129.19, 124.9, 122.4, 121.6, 120.7, 116.0, 115.3, 114.8, 114.7, 113.2, 113.0, 55.39, 55.37, 55.3, 27.9, 27.5, 22.6. HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{30}H_{29}N_2O_3^+$: 465.2173, found: 465.2176.

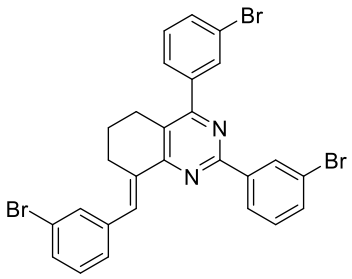


8-(3-Fluorobenzylidene)-2,4-bis(3-fluorophenyl)-5,6,7,8-tetrahydroquinazoline (3s): White solid (44.3 mg, 52% yield); R_f = 0.1 (pure PE); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.42 (s, 1H), 8.38 (d, *J* = 7.9 Hz, 1H), 8.28 (d, *J* = 10.3 Hz, 1H), 7.51 – 7.37 (m, 5H), 7.32 – 7.27 (m, 1H), 7.25 – 7.15 (m, 3H), 7.07 – 7.00 (m, 1H), 2.95 (t, *J* = 5.2 Hz, 2H), 2.89 (t, *J* = 6.0 Hz, 2H), 1.85 – 1.78 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 164.7 (d, *J* = 2.4 Hz), 163.2(d, *J* = 244.6 Hz), 162.6 (d, *J* = 245.5 Hz), 162.6(d, *J* = 246.7 Hz), 160.3, 160.0 (d, *J* = 3.2 Hz), 140.4 (d, *J* = 2.5 Hz), 140.4(d, *J* = 2.2 Hz), 139.1 (d, *J* = 7.8 Hz), 135.1, 129.90, 129.86, 129.83, 129.80, 129.78, 129.77, 129.7, 125.8(d, *J* = 2.9 Hz), 125.3, 124.9 (d, *J* = 2.9 Hz), 123.7 (d, *J* = 2.8 Hz), 117.1 (d, *J* = 21.3 Hz), 116.4(d, *J* = 20.3 Hz), 116.2 (d, *J* = 19.7 Hz),116.3 (d, *J* = 22.5 Hz), 114.9(d, *J* = 23.2 Hz), 114.5(d, *J* = 21.2 Hz). 27.1, 27.4, 22.4. ^{19}F NMR (471 MHz, $CDCl_3$, ppm) δ -112.55, -113.15, -113.37. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{27}H_{20}N_2F_3$: 429.1573, found: 429.1582.

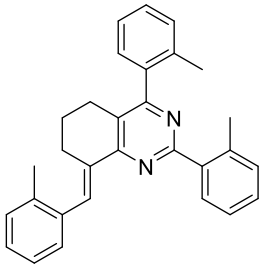


8-(3-Chlorobenzylidene)-2,4-bis(3-chlorophenyl)-5,6,7,8-tetrahydroquinazoline (3t): White solid (57.2 mg, 60% yield); R_f = 0.1 (pure PE); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.55 (s, 1H), 8.47 (d, *J* = 6.9 Hz, 1H), 8.38 (s, 1H), 7.68 (s, 1H), 7.56 (d, *J* = 7.0 Hz, 1H), 7.50 (s, 1H), 7.48 – 7.42 (m, 3H), 7.40 – 7.34 (m, 2H), 7.32 – 7.28 (m, 1H), 2.93 (t, *J* = 5.2 Hz, 2H),

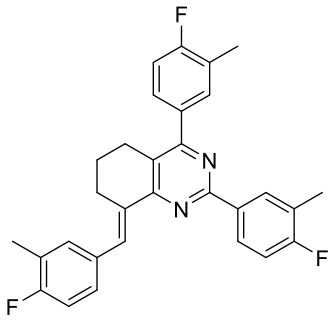
2.87 (t, J = 6.0 Hz, 2H), 1.85 – 1.76 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 164.8, 160.3, 159.9, 140.0, 139.8, 138.8, 135.2, 134.5, 134.3, 134.2, 130.3, 129.7, 129.63, 129.56, 129.5, 129.4, 129.2, 128.08, 128.06, 127.6, 127.3, 126.2, 125.4, 27.7, 27.4, 22.4. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{27}H_{20}N_2Cl_3^+$: 477.0687, found: 477.0692.



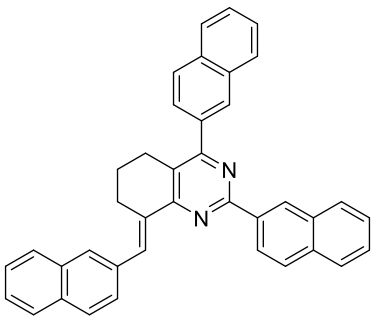
8-(3-Bromobenzylidene)-2,4-bis(3-bromophenyl)-5,6,7,8-tetrahydroquinazoline (3u): White solid (72.9 mg, 60% yield); R_f = 0.1 (pure PE); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.70 (s, 1H), 8.51 (d, J = 7.9 Hz, 1H), 8.36 (s, 1H), 7.83 (s, 1H), 7.67 – 7.57 (m, 4H), 7.47 – 7.41 (m, 2H), 7.41 – 7.34 (m, 2H), 7.30 (t, J = 7.8 Hz, 1H), 2.91 (t, J = 5.2 Hz, 2H), 2.86 (t, J = 6.0 Hz, 2H), 1.85 – 1.75 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 164.6, 160.2, 159.8, 140.2, 140.0, 139.1, 135.2, 133.2, 132.5, 132.3, 132.1, 131.0, 130.5, 130.0, 129.80, 129.78, 129.6, 128.5, 127.7, 126.7, 125.4, 122.7, 122.41, 122.38, 27.6, 27.3, 22.4. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{27}H_{20}N_2Br_3^+$: 608.9171, found: 608.9169.



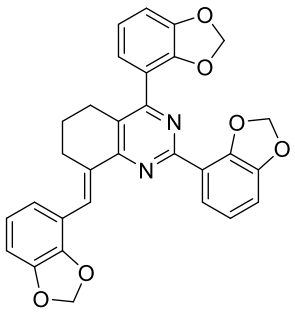
9-(2-Methylbenzylidene)-2,4-di-o-tolyl-5,6,7,8-tetrahydroquinazoline (3v): yellow solid (57.5 mg, 69% yield); R_f = 0.5 (PE:EA = 50:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.41 (s, 1H), 7.94 (d, J = 7.5 Hz, 1H), 7.33 – 7.26 (m, 7H), 7.24 – 7.20 (m, 4H), 2.77 (s, 2H), 2.69 (s, 3H), 2.56 (s, 2H), 2.37 (s, 3H), 2.23 (s, 3H), 1.78 (s, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 167.6, 163.9, 159.6, 138.6, 138.2, 137.4, 137.3, 136.3, 135.2, 134.4, 131.2, 130.7, 130.4, 130.0, 129.8, 129.1, 128.9, 128.5, 128.0, 127.5, 125.78, 125.76, 125.3, 124.6, 27.4, 26.3, 22.4, 21.6, 20.2, 19.6. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{30}H_{29}N_2^+$: 417.2325, found: 417.2329.



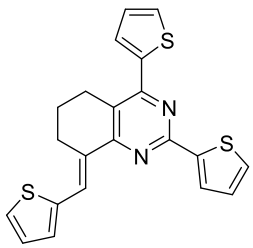
8-(4-Fluoro-3-methylbenzylidene)-2,4-bis(4-fluoro-3-methylphenyl)-5,6,7,8-tetrahydroquinazoline (3w): White solid (54.8 mg, 58% yield); R_f = 0.5 (PE:EA = 50:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.43 – 8.38 (m, 2H), 8.37 (s, 1H), 7.54 (d, *J* = 7.4 Hz, 1H), 7.50 – 7.45 (m, 1H), 7.37 – 7.29 (m, 2H), 7.12 (q, *J* = 9.5 Hz, 2H), 7.06 (t, *J* = 8.9 Hz, 1H), 2.92 (t, *J* = 5.3 Hz, 2H), 2.86 (t, *J* = 6.0 Hz, 2H), 2.39 (s, 6H), 2.34 (s, 3H), 1.83 – 1.75 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 165.1, 163.0 (d, *J* = 248.2 Hz), 161.9(d, *J* = 247.8 Hz), 160.6 (d, *J* = 247.2 Hz), 160.4, 160.2, 134.3(d, *J* = 3.7 Hz), 134.0 (d, *J* = 3.2 Hz), 133.8, 133.1 (d, *J* = 5.3 Hz), 132.9(d, *J* = 3.7 Hz), 132.5(d, *J* = 5.5 Hz), 131.3 (d, *J* = 5.6 Hz), 129.8, 128.9(d, *J* = 8.1 Hz), 128.3 (d, *J* = 8.4 Hz), 127.5(d, *J* = 8.5 Hz), 124.9 (d, *J* = 17.5 Hz), 124.7 (d, *J* = 17.5 Hz).124.6 (d, *J* = 17.5 Hz), 124.3, 114.9 (d, *J* = 22.7 Hz), 114.9(d, *J* = 22.5 Hz), 114.8(d, *J* = 22.8 Hz), 27.8, 27.5, 22.6, 14.7, 14.7, 14.6. ^{19}F NMR (471 MHz, $CDCl_3$, ppm) δ -115.55, -116.21, -117.77. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{30}H_{26}F_3N_2^+$: 471.2043, found: 471.2046.



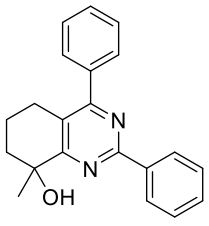
2,4-Di(naphthalen-2-yl)-8-(naphthalen-2-ylmethylene)-5,6,7,8-tetrahydroquinazoline(3x): White solid (32.6 mg, 31% yield); R_f = 0.4 (PE:EA = 30:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 9.20 (s, 1H), 8.82 (d, *J* = 8.6 Hz, 1H), 8.75 (s, 1H), 8.22 (s, 1H), 8.08 – 7.98 (m, 5H), 7.96 – 7.87 (m, 6H), 7.72 (d, *J* = 8.5 Hz, 1H), 7.62 – 7.50 (m, 6H), 3.10 (t, *J* = 5.3 Hz, 2H), 3.00 (t, *J* = 6.0 Hz, 2H), 1.89 – 1.78 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 166.0, 161.1, 160.4, 136.0, 135.7, 134.83, 134.78, 134.5, 133.5, 133.4, 133.2, 132.8, 132.6, 130.8, 129.18, 129.17, 128.9, 128.5, 128.2, 128.1, 128.0, 127.9, 127.74, 127.73, 127.69, 127.65, 126.9, 126.71, 126.67, 126.4, 126.29, 126.26, 126.0, 125.4, 125.1, 28.0, 27.7, 22.7. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{39}H_{29}N_2^+$: 525.2325, found: 525.2331.



2,4-Bis(benzo[d][1,3]dioxol-4-yl)-8-(benzo[d][1,3]dioxol-4-ylmethylene)-5,6,7,8-tetrahydroquinazoline (3y): White solid (34.4 mg, 34% yield); R_f = 0.3 (PE:EA = 10:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.37 (s, 1H), 7.89 (dd, *J* = 7.6, 1.9 Hz, 1H), 7.13 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.00 – 6.96 (m, 2H), 6.95 – 6.90 (m, 3H), 6.87 (t, *J* = 7.8 Hz, 1H), 6.80 (d, *J* = 6.7 Hz, 1H), 6.13 (s, 2H), 6.02 (s, 2H), 6.01 (s, 2H), 2.88 (t, *J* = 5.3 Hz, 2H), 2.82 (t, *J* = 6.1 Hz, 2H), 1.85 – 1.78 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 162.1, 159.9, 159.8, 148.6, 147.5, 147.4, 147.0, 145.8, 145.3, 136.0, 125.9, 124.1, 123.2, 122.6, 122.5, 121.9, 121.7, 121.20, 121.19, 120.7, 119.8, 109.7, 109.3, 107.9, 101.2, 101.0, 100.8, 27.9, 25.9, 22.2. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{30}H_{23}N_2O_6^+$: 507.1551, found: 507.1559.

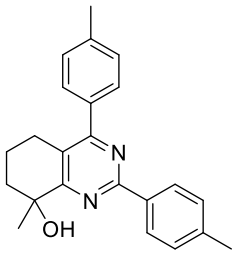


2,4-Di(thiophen-2-yl)-8-(thiophen-2-ylmethylene)-5,6,7,8-tetrahydroquinazoline (3z): White solid (23.0 mg, 30% yield); R_f = 0.5 (PE:EA = 25:1);^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.50 (s, 1H), 8.09 (dd, *J* = 3.6, 1.2 Hz, 1H), 7.63 (d, *J* = 2.8 Hz, 1H), 7.54 (d, *J* = 5.1 Hz, 1H), 7.46 (d, *J* = 5.0 Hz, 2H), 7.36 (d, *J* = 3.6 Hz, 1H), 7.20 – 7.13 (m, 3H), 3.07 (t, *J* = 6.1 Hz, 2H), 2.98 (t, *J* = 5.4 Hz, 2H), 2.00 – 1.92 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 160.8, 157.7, 144.1, 143.0, 140.5, 131.2, 130.8, 129.8, 129.6, 128.9, 128.2, 128.0, 127.9, 127.8, 127.3, 123.9, 122.5, 27.5, 27.2, 22.0. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{21}H_{17}N_2S_3^+$: 393.0548, found: 393.0556.

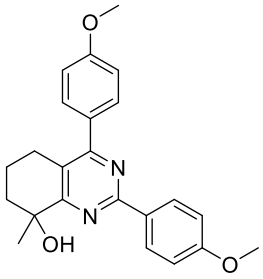


8-Methyl-2,4-diphenyl-5,6,7,8-tetrahydroquinazolin-8-ol (4a): White solid (43.0 mg, 68% yield); R_f = 0.5 (PE: EA = 10:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.54 – 8.49 (m, 2H), 7.68 – 7.65 (m, 2H), 7.53 – 7.46 (m, 6H), 3.68 (s, 1H), 2.90 – 2.78 (m, 2H), 2.16 – 2.06 (m, 2H), 1.98 – 1.89 (m, 1H), 1.82 – 1.73 (m, 1H), 1.66 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 169.5, 165.9, 161.7, 138.4, 137.5, 130.4, 129.2, 129.0, 128.4, 128.3, 128.0, 123.4, 70.8, 36.0, 30.5, 27.0, 20.0. HRMS (ESI-TOF): m/z

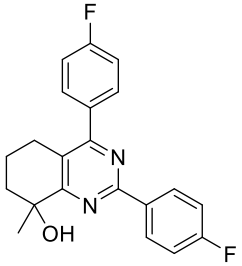
$[M+H]^+$ calcd for $C_{21}H_{21}N_2O^+$: 317.1648, found: 317.1656.



8-Methyl-2,4-di-p-tolyl-5,6,7,8-tetrahydroquinazolin-8-ol (4b): White solid (33.8 mg, 49% yield); R_f = 0.4 (PE: EA =10:1); ^1H NMR (500 MHz, $CDCl_3$, ppm) δ 8.40 (d, *J* = 8.2 Hz, 2H), 7.57 (d, *J* = 8.1 Hz, 2H), 7.32 – 7.27 (m, 4H), 3.70 (s, 1H), 2.86 – 2.80 (m, 2H), 2.44 (s, 3H), 2.42 (s, 3H), 2.13 – 2.08 (m, 2H), 1.95 – 1.88 (m, 1H), 1.81 – 1.73 (m, 1H), 1.64 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 169.1, 166.0, 161.6, 140.7, 139.4, 135.6, 134.7, 129.1, 129.0, 128.9, 128.1, 123.1, 70.7, 36.1, 30.5, 27.0, 21.5, 21.4, 19.8. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{23}H_{25}N_2O^+$: 345.1961, found: 345.1967.

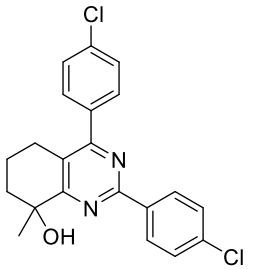


2,4-Bis(4-methoxyphenyl)-8-methyl-5,6,7,8-tetrahydroquinazolin-8-ol (4c): White solid (37.6 mg, 50% yield); R_f = 0.3 (PE: EA = 10:1); ^1H NMR (500 MHz, $CDCl_3$, ppm) δ 8.47 (d, *J* = 8.9 Hz, 2H), 7.66 (d, *J* = 8.7 Hz, 2H), 7.03 – 6.97 (m, 4H), 3.88 (d, *J* = 1.8 Hz, 6H), 3.68 (s, 1H), 2.88 – 2.77 (m, 2H), 2.13 – 2.05 (m, 2H), 1.95 – 1.88 (m, 1H), 1.81 – 1.73 (m, 1H), 1.63 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 169.2, 165.1, 161.5, 161.4, 160.4, 131.0, 130.7, 130.4, 129.5, 122.3, 113.7, 113.6, 70.7, 55.4, 55.3, 36.1, 30.5, 27.1, 19.9. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{23}H_{25}N_2O_3^+$: 377.1860, found: 377.1865.

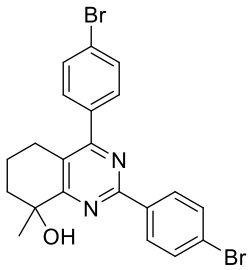


2,4-Bis(4-fluorophenyl)-8-methyl-5,6,7,8-tetrahydroquinazolin-8-ol (4d): Yellow solid (32.4 mg, 46% yield); R_f = 0.5 (PE: EA = 10:1); ^1H NMR (500 MHz, $CDCl_3$, ppm) *δ* 8.51 (dd, *J* = 8.7, 5.7 Hz, 2H), 7.67 (dd, *J* = 8.6, 5.5 Hz, 2H), 7.17 (dt, *J* = 19.7, 8.6 Hz, 4H), 3.55 (s, 1H), 2.89 – 2.74 (m, 2H), 2.14 – 2.06 (m, 2H), 1.99 – 1.89 (m, 1H), 1.84 – 1.73 (m, 1H), 1.65 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 169.8, 164.9, 164.6(d, *J* = 250.0 Hz), 163.4(d, *J* = 249.5 Hz), 160.9, 134.4(d, *J* = 3.6 Hz), 133.6(d, *J* = 3.0 Hz), 131.0(d, *J* = 8.6 Hz), 130.1(d, *J* = 8.7 Hz), 123.3, 115.5 (d, *J* = 1.4 Hz), 115.3(d, *J* = 1.3 Hz), 70.8, 36.1, 30.5, 27.8, 19.8. ^{19}F NMR (471

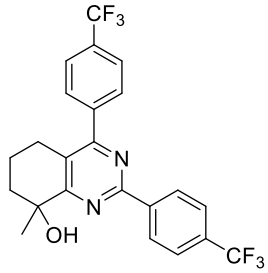
MHz, $CDCl_3$, ppm) δ -110.7, -111.5. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{21}H_{19}F_2N_2O^+$: 353.1460, found: 353.1467.



2,4-Bis(4-chlorophenyl)-8-methyl-5,6,7,8-tetrahydroquinazolin-8-ol (4e): White solid (40.8 mg, 53% yield); R_f = 0.5 (PE:EA = 10:1); ^1H NMR (500 MHz, $CDCl_3$, ppm) δ 8.44 (d, *J* = 8.6 Hz, 2H), 7.61 (d, *J* = 8.5 Hz, 2H), 7.48 (d, *J* = 8.5 Hz, 2H), 7.44 (d, *J* = 8.6 Hz, 2H), 3.53 (s, 1H), 2.88 – 2.75 (m, 2H), 2.16 – 2.06 (m, 2H), 1.99 – 1.90 (m, 1H), 1.84 – 1.73 (m, 1H), 1.65 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 169.9, 164.8, 160.9, 136.7, 136.6, 135.8, 135.6, 130.4, 129.3, 128.7, 128.6, 123.7, 70.8, 36.0, 30.4, 27.1, 19.7. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{21}H_{19}Cl_2N_2O^+$: 385.0869, found: 385.0876.

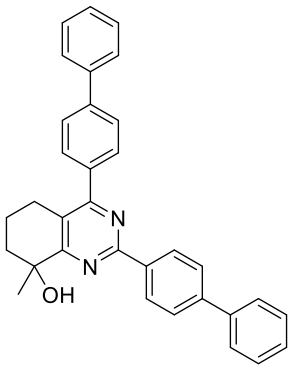


2,4-Bis(4-bromophenyl)-8-methyl-5,6,7,8-tetrahydroquinazolin-8-ol (4f): White solid (47.4mg, 50% yield); R_f = 0.5 (PE:EA =10:1); ^1H NMR (500 MHz, $CDCl_3$, ppm) δ 8.37 (d, *J* = 8.6 Hz, 2H), 7.64 (d, *J* = 8.4 Hz, 2H), 7.60 (d, *J* = 8.6 Hz, 2H), 7.53 (d, *J* = 8.5 Hz, 2H), 3.51 (s, 1H), 2.86 – 2.74 (m, 2H), 2.14 – 2.07 (m, 2H), 1.97 – 1.86 (m, 1H), 1.86 – 1.72 (m, 1H), 1.64 (s, 3H). ^{13}C NMR (125MHz, $CDCl_3$, ppm) δ 169.9, 164.9, 161.0, 137.1, 136.3, 131.4, 131.5, 130.6, 129.6, 125.3, 123.9, 123.8, 70.7, 36.0, 30.4, 27.0, 19.7. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{21}H_{19}Br_2N_2O^+$: 472.9859, found: 472.9865.

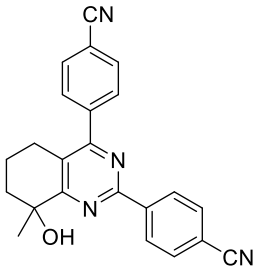


8-Methyl-2,4-bis(4-(trifluoromethyl)phenyl)-5,6,7,8-tetrahydroquinazolin-8-ol (4g): White solid (41.6 mg, 46% yield); R_f = 0.4 (PE:EA = 10:1); ^1H NMR (500 MHz, $CDCl_3$, ppm) δ 8.61 (d, *J* = 8.2 Hz, 2H), 7.78 (s, 4H), 7.74 (d, *J* = 8.2 Hz, 2H), 3.48 (s, 1H), 2.90 – 2.74 (m, 2H), 2.18 – 2.08 (m, 2H), 2.01 – 1.92 (m, 1H), 1.86 – 1.75 (m, 1H), 1.68 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.3, 164.8, 160.7, 141.6, 140.5, 132.2 (q, *J* = 32.3 Hz), 131.4 (q, *J* = 32.7 Hz), 129.4, 128.3, 125.4 (d, *J* = 4.0 Hz), 125.4 (d, *J* = 3.6 Hz), 124.6, 124.1 (q, *J* = 272.4 Hz), 123.9 (q, *J* = 272.3 Hz), 70.8, 36.0, 30.4, 27.0, 19.6. ^{19}F NMR (471 MHz, $CDCl_3$,

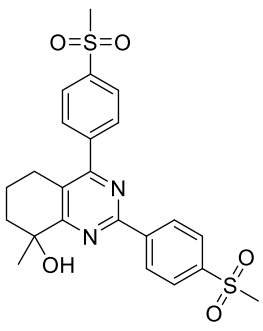
ppm) δ -62.69, -62.75. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{23}H_{19}N_2OF_6^+$: 453.1396, found: 453.1402.



2,4-Di([1,1'-biphenyl]-4-yl)-8-methyl-5,6,7,8-tetrahydroquinazolin-8-ol (4h): White solid (37.5 mg, 40% yield); R_f = 0.3 (PE: EA =10:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.62 (d, *J* = 8.1 Hz, 2H), 7.82 – 7.77 (m, 2H), 7.77 – 7.71 (m, 4H), 7.68 (t, *J* = 6.0 Hz, 4H), 7.49 (q, *J* = 7.9 Hz, 4H), 7.43 – 7.36 (m, 2H), 3.87 (s, 1H), 3.00 – 2.85 (m, 2H), 2.20 – 2.10 (m, 2H), 2.03 – 1.93 (m, 1H), 1.88 – 1.75 (m, 1H), 1.71 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 169.4, 165.8, 161.4, 143.2, 142.3, 140.6, 140.4, 137.2, 136.1, 129.6, 128.9, 128.8, 128.6, 127.74, 127.65, 127.20, 127.16, 127.0, 123.6, 70.8, 36.2, 30.5, 27.2, 19.8. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{33}H_{29}N_2O^+$: 469.2274, found: 469.2276.

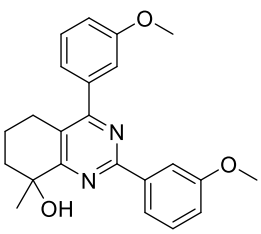


4,4'-(8-Hydroxy-8-methyl-5,6,7,8-tetrahydroquinazoline-2,4-diyl)dibenzonitrile (4i): White solid (31.5 mg, 43% yield); R_f = 0.2 (PE: EA =2:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.60 (d, *J* = 8.4 Hz, 2H), 7.84 – 7.80 (m, 2H), 7.79 – 7.74 (m, 4H), 3.39 (s, 1H), 2.88 – 2.75 (m, 2H), 2.18 – 2.08 (m, 2H), 2.02 – 1.93 (m, 1H), 1.86 – 1.76 (m, 1H), 1.68 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 170.7, 164.3, 160.3, 142.3, 141.1, 132.4, 132.2, 129.7, 128.5, 125.0, 118.8, 118.3, 114.0, 113.3, 70.8, 36.0, 30.4, 27.1, 19.6. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{23}H_{19}N_4O^+$: 367.1553, found: 367.1555

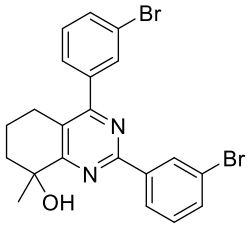


8-Methyl-2,4-bis(4-(methylsulfonyl)phenyl)-5,6,7,8-tetrahydroquinazolin-8-ol (4j): White solid (44.4 mg, 47% yield); R_f = 0.2 (PE: EA =1:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.68 (d, *J* = 7.9 Hz, 2H), 8.11 (d, *J* = 7.8 Hz, 2H), 8.05 (d, *J* = 8.0 Hz, 2H), 7.85 (d, *J* = 7.7 Hz, 2H), 3.13 (s, 3H), 3.10 (s, 3H), 2.92 – 2.74 (m, 2H), 2.20 – 2.07 (m, 2H), 2.03 – 1.93 (m, 1H), 1.85 – 1.78 (m, 1H), 1.69 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 170.7, 164.4, 160.3,

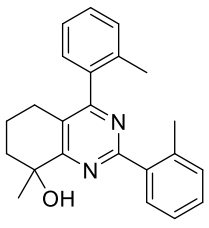
143.3, 142.10, 141.96, 141.3, 130.0, 128.9, 127.59, 127.57, 125.2, 70.8, 44.5, 36.0, 30.4, 27.0, 19.5. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{23}H_{25}N_2O_5S_2^+$: 473.1199, found: 473.1197.



2,4-Bis(3-methoxyphenyl)-8-methyl-5,6,7,8-tetrahydroquinazolin-8-ol (4k): White solid (36.9 mg, 49% yield); R_f = 0.4 (PE: EA =4:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.12 (d, *J* = 7.8 Hz, 1H), 8.06 (s, 1H), 7.44 – 7.37 (m, 2H), 7.23 – 7.18 (m, 2H), 7.02 (d, *J* = 7.3 Hz, 2H), 3.90 (s, 3H), 3.88 (s, 3H), 3.64 (s, 1H), 2.87 – 2.78 (m, 2H), 2.15 – 2.06 (m, 2H), 1.97 – 1.90 (m, 1H), 1.83 – 1.73 (m, 1H), 1.65 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 169.5, 165.7, 161.5, 159.8, 159.5, 139.7, 139.0, 129.4, 129.3, 123.6, 121.3, 120.6, 116.1, 114.8, 114.7, 113.3, 70.8, 55.4, 55.4, 36.0, 30.5, 27.0, 19.8. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{23}H_{25}N_2O_3^+$: 377.1860, found: 377.1865.

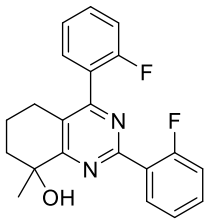


2,4-Bis(3-bromophenyl)-8-methyl-5,6,7,8-tetrahydroquinazolin-8-ol (4l): White solid (42.7 mg, 45% yield); R_f = 0.4 (PE: EA =10:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.63 (s, 1H), 8.44 (d, *J* = 7.9 Hz, 1H), 7.79 (s, 1H), 7.61 (t, *J* = 9.7 Hz, 2H), 7.56 (d, *J* = 7.7 Hz, 1H), 7.41 – 7.33 (m, 2H), 3.51 (s, 1H), 2.88 – 2.74 (m, 2H), 2.16 – 2.06 (m, 2H), 2.00 – 1.90 (m, 1H), 1.84 – 1.73 (m, 1H), 1.66 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 170.1, 164.6, 160.5, 140.1, 139.4, 133.5, 132.4, 131.9, 130.9, 130.0, 129.9, 127.5, 126.6, 124.2, 122.8, 122.5, 70.8, 36.0, 30.4, 26.9, 19.6. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{21}H_{19}Br_2N_2O^+$: 472.9859, found: 472.9865.

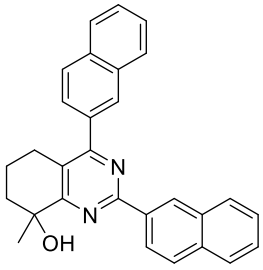


9-Methyl-2,4-di-o-tolyl-5,6,7,8-tetrahydroquinazolin-8-ol (4m): White solid (26.9 mg, 39% yield); R_f = 0.4 (PE: EA =10:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.84 (d, *J* = 7.0 Hz, 1H), 7.36 – 7.26 (m, 6H), 7.19 (d, *J* = 7.5 Hz, 1H), 3.67 (s, 1H), 2.58 (s, 3H), 2.50 (s, 2H), 2.18 (s, 3H), 2.12 – 2.04 (m, 2H), 1.98 – 1.90 (m, 1H), 1.82 – 1.75 (m, 1H), 1.65 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 168.9, 167.6, 164.5, 138.0, 137.8, 137.1, 135.0, 131.2, 130.50, 130.48, 129.2, 128.7, 127.8, 125.9, 125.8, 123.6, 70.7, 35.9,

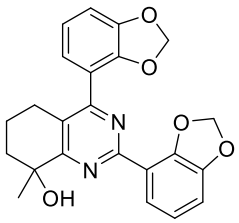
30.2, 25.7, 21.5, 19.6, 19.4. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{23}H_{25}N_2O^+$: 345.1961, found: 345.1967.



2,4-Bis(2-fluorophenyl)-8-methyl-5,6,7,8-tetrahydroquinazolin-8-ol (4n): White solid (35.2 mg, 50% yield); R_f = 0.5 (PE:EA = 10:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.07 (t, *J* = 7.7 Hz, 1H), 7.51 – 7.40 (m, 3H), 7.29 (t, *J* = 7.5 Hz, 1H), 7.26 – 7.22 (m, 1H), 7.21 – 7.15 (m, 2H), 3.61 (s, 1H), 2.74 – 2.62 (m, 2H), 2.14 – 2.07 (m, 2H), 1.98 – 1.91 (m, 1H), 1.85 – 1.77 (m, 1H), 1.65 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 169.4, 162.4, 162.2, 161.2 (d, *J* = 255.5 Hz), 160.6(d, *J* = 4.8 Hz), 159.5 (d, *J* = 248.5 Hz), 131.7 (d, *J* = 1.7 Hz), 131.5(d, *J* = 8.5 Hz), 131.2(d, *J* = 8.2 Hz), 131.0 (d, *J* = 3.4 Hz), 126.4 (d, *J* = 9.7 Hz), 126.1(d, *J* = 15.9 Hz), 125.4, 124.6(d, *J* = 3.4 Hz), 124.0 (d, *J* = 3.9 Hz), 116.8(d, *J* = 22.3 Hz), 115.8 (d, *J* = 21.8 Hz), 35.9, 30.2, 25.2 (d, *J* = 4.9 Hz), 19.3. ^{19}F NMR (471 MHz, $CDCl_3$, ppm) δ -113.8, -114.3. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{21}H_{19}F_2N_2O^+$: 353.1460, found: 353.1467.

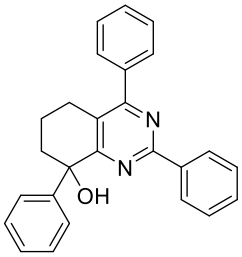


8-Methyl-2,4-di(naphthalen-2-yl)-5,6,7,8-tetrahydroquinazolin-8-ol (4o): White solid (41.6 mg, 50% yield); R_f = 0.5 (PE:EA = 10:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 9.08 (s, 1H), 8.66 (dd, *J* = 8.6, 1.7 Hz, 1H), 8.17 (s, 1H), 8.04 – 7.99 (m, 2H), 7.99 – 7.92 (m, 3H), 7.91 – 7.87 (m, 1H), 7.84 (dd, *J* = 8.5, 1.7 Hz, 1H), 7.61 – 7.56 (m, 2H), 7.55 – 7.49 (m, 2H), 3.78 (s, 1H), 2.99 – 2.87 (m, 2H), 2.22 – 2.12 (m, 2H), 2.01 – 1.92 (m, 1H), 1.88 – 1.79 (m, 1H), 1.74 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 169.6, 166.0, 161.8, 135.8, 134.9, 134.6, 133.5, 133.3, 132.9, 129.1, 128.8, 128.5, 128.14, 128.08, 128.0, 127.8, 127.7, 127.0, 126.9, 126.5, 126.4, 126.2, 125.1, 123.8, 70.9, 36.1, 30.5, 27.1, 19.1. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{29}H_{25}N_2O^+$: 417.1961, found: 417.1971.

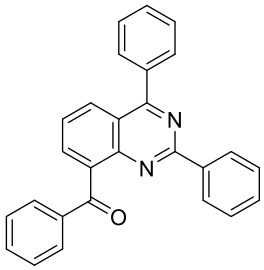


2,4-Bis(benzo[d][1,3]dioxol-4-yl)-8-methyl-5,6,7,8-tetrahydroquinazolin-8-ol (4p): White solid (38.8 mg, 48% yield); R_f = 0.3 (PE:EA = 5:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.79 (dd, *J* = 6.5, 3.0 Hz, 1H), 7.06 (dd, *J* = 7.7, 1.5 Hz, 1H), 6.97 (t, *J* = 7.8

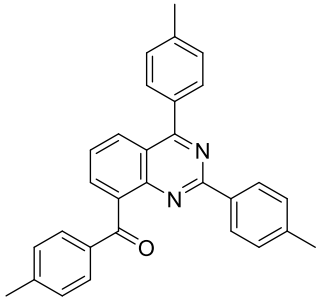
Hz, 1H), 6.95 – 6.93 (m, 1H), 6.93 – 6.90 (m, 2H), 6.10 (dd, *J* = 12.9, 1.5 Hz, 2H), 6.02 – 5.99 (m, 2H), 3.85 (s, 1H), 2.80 – 2.74 (m, 2H), 2.14 – 2.04 (m, 2H), 1.98 – 1.91 (m, 1H), 1.86 – 1.77 (m, 1H), 1.62 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 169.4, 162.1, 160.2, 148.6, 147.6, 147.0, 145.0, 124.5, 123.0, 122.3, 122.0, 121.3, 121.0, 120.4, 109.9, 109.4, 101.2, 101.0, 70.6, 35.8, 30.3, 25.0, 19.3. HRMS (ESI-TOF): m/z $[M + H]^+$ calcd for $C_{23}H_{21}N_2O_5^+$: 405.1445, found: 405.1452.



2,4,8-Triphenyl-5,6,7,8-tetrahydroquinazolin-8-ol (4q): White solid (28.0 mg, 37% yield); R_f = 0.3 (PE:EA = 10:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.41 (d, *J* = 8.0 Hz, 2H), 7.74 (d, *J* = 6.3 Hz, 2H), 7.56 – 7.48 (m, 3H), 7.44 – 7.38 (m, 3H), 7.30 (t, *J* = 7.3 Hz, 2H), 7.26 – 7.22 (m, 3H), 4.41 (s, 1H), 2.97 – 2.89 (m, 2H), 2.40 – 2.26 (m, 2H), 1.90 – 1.80 (m, 1H), 1.68 – 1.59 (m, 1H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 168.3, 166.1, 161.9, 147.8, 138.4, 137.3, 130.5, 129.3, 129.0, 128.3, 128.1, 127.9, 127.1, 126.6, 125.2, 75.4, 37.9, 26.6, 18.7. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{26}H_{23}N_2O^+$: 379.1805, found: 379.1812.

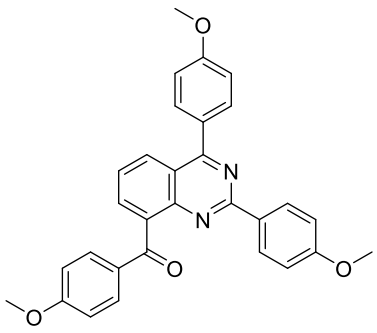


(2,4-Diphenylquinazolin-8-yl)(phenyl)methanone (5a): White solid (42.5 mg, 55% yield); R_f = 0.4 (PE:EA = 20:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.28 (d, *J* = 8.4 Hz, 1H), 8.22 (d, *J* = 7.0 Hz, 2H), 8.05 (d, *J* = 7.1 Hz, 1H), 7.94 – 7.85 (m, 4H), 7.68 – 7.56 (m, 5H), 7.46 (t, *J* = 7.7 Hz, 2H), 7.39 (t, *J* = 7.2 Hz, 1H), 7.33 (t, *J* = 7.4 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 197.4, 168.5, 159.7, 149.9, 138.91, 138.88, 137.6, 137.5, 133.3, 132.9, 130.7, 130.21, 130.15, 129.9, 129.5, 128.7, 128.6, 128.29, 128.28, 126.4, 121.4. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{27}H_{19}N_2O^+$: 387.1492, found: 387.1492.

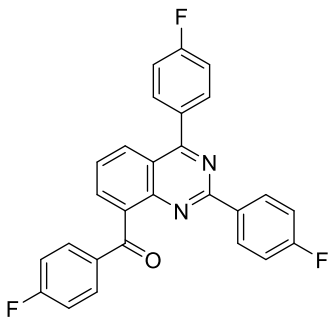


(2,4-Di-*p*-tolylquinazolin-8-yl)(*p*-tolyl)methanone (5b): White solid (39.4 mg, 46% yield); R_f = 0.4 (PE:EA = 20:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.27 (d, *J* = 8.4 Hz, 1H), 8.15 (d, *J* = 8.3 Hz, 2H), 7.98 (d, *J* = 7.0 Hz, 1H), 7.81 (d, *J* = 8.1 Hz, 2H), 7.77 (d, *J* = 8.3 Hz, 2H), 7.60 (dd,

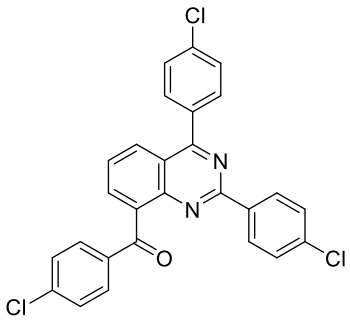
J = 8.4, 7.0 Hz, 1H), 7.43 (d, *J* = 7.8 Hz, 2H), 7.25 (d, *J* = 7.9 Hz, 2H), 7.14 (d, *J* = 8.0 Hz, 2H), 2.51 (s, 3H), 2.43 (s, 3H), 2.36 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 197.2, 168.3, 159.7, 149.8, 143.7, 140.8, 140.4, 139.0, 136.3, 135.0, 134.7, 132.9, 130.2, 130.1, 129.31, 129.25, 129.0, 128.9, 128.7, 126.0, 121.3, 21.7, 21.5. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{30}H_{25}N_2O^+$: 429.1961, found: 429.1966.



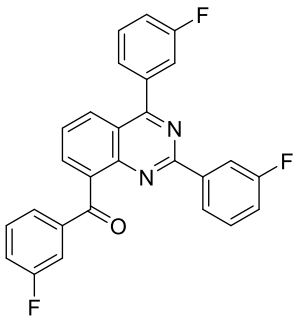
(2,4-Bis(4-methoxyphenyl)quinazolin-8-yl)(4-methoxyphenyl)methanone (5c): White solid (39.1 mg, 41% yield); R_f = 0.2 (PE:EA = 10:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.26 (d, *J* = 8.7 Hz, 3H), 7.95 – 7.83 (m, 5H), 7.58 (t, *J* = 7.6 Hz, 1H), 7.13 (d, *J* = 7.7 Hz, 2H), 6.92 (d, *J* = 7.8 Hz, 2H), 6.86 (d, *J* = 8.8 Hz, 2H), 3.94 (s, 3H), 3.87 (s, 3H), 3.83 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 196.1, 167.7, 163.5, 161.8, 161.4, 159.5, 150.0, 139.1, 132.6, 132.4, 131.9, 131.7, 130.5, 130.4, 130.1, 129.1, 125.8, 121.1, 114.1, 113.6, 113.5, 55.5, 55.3. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{30}H_{25}N_2O_4^+$: 477.1809, found: 477.1817



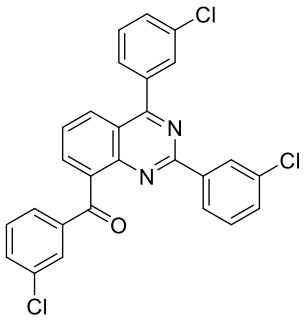
(2,4-Bis(4-fluorophenyl)quinazolin-8-yl)(4-fluorophenyl)methanone (5d): White solid (43.2 mg, 49% yield); R_f= 0.4 (PE:EA = 20:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.28 – 8.20 (m, 3H), 8.04 (d, *J* = 7.0 Hz, 1H), 7.93 – 7.86 (m, 4H), 7.67 (t, *J* = 7.8 Hz, 1H), 7.32 (t, *J* = 8.6 Hz, 2H), 7.13 (t, *J* = 8.6 Hz, 2H), 7.03 (t, *J* = 8.7 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 195.6, 167.5, 165.7 (d, *J* = 255.1 Hz), 164.8(d, *J* = 251.1 Hz), 164.2(d, *J* = 251.2 Hz). 158.8, 149.7, 138.5, 135.0 (d, *J* = 3.1 Hz), 133.5, 133.3 (d, *J* = 3.2 Hz), 132.5 (d, *J* = 9.5 Hz), 132.2 (d, *J* = 8.6 Hz), 130.7 (d, *J* = 8.8 Hz), 129.3, 126.6, 121.1, 115.9(d, *J* = 21.9 Hz), 115.5(d, *J* = 22.0 Hz), 115.4(d, *J* = 21.7 Hz). ^{19}F NMR (471 MHz, $CDCl_3$, ppm) δ -104.98, -109.79, -109.92. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{27}H_{16}F_3N_2O^+$: 441.1209, found: 441.1205.



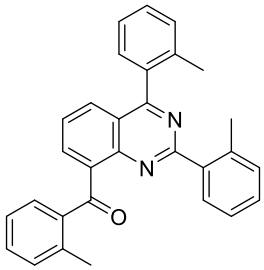
(2,4-Bis(4-chlorophenyl)quinazolin-8-yl)(4-chlorophenyl)methanone (5e): White solid (48.9 mg, 50% yield); R_f = 0.4 (PE:EA = 20:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.25 (d, *J* = 8.4 Hz, 1H), 8.13 (d, *J* = 8.6 Hz, 2H), 8.07 (d, *J* = 6.1 Hz, 1H), 7.84 (d, *J* = 8.5 Hz, 2H), 7.79 (d, *J* = 8.5 Hz, 2H), 7.69 (t, *J* = 7.8 Hz, 1H), 7.61 (d, *J* = 8.4 Hz, 2H), 7.43 (d, *J* = 8.5 Hz, 2H), 7.33 (d, *J* = 8.6 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 195.9, 167.6, 158.8, 149.7, 139.5, 138.3, 137.2, 137.1, 136.8, 135.7, 135.5, 133.8, 131.5, 131.2, 129.9, 129.4, 129.0, 128.7, 126.9, 121.2. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{27}H_{16}Cl_3N_2O^+$: 489.0323, found: 489.0319.



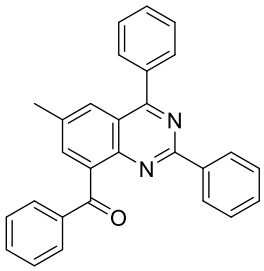
(2,4-Bis(3-fluorophenyl)quinazolin-8-yl)(3-fluorophenyl)methanone (5f): White solid (41.4 mg, 47% yield); R_f = 0.4 (PE:EA = 20:1);^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.29 (d, *J* = 8.4 Hz, 1H), 8.10 (d, *J* = 7.0 Hz, 1H), 8.02 (d, *J* = 7.8 Hz, 1H), 7.84 (d, *J* = 10.4 Hz, 1H), 7.72 (t, *J* = 7.8 Hz, 1H), 7.66 (d, *J* = 7.6 Hz, 1H), 7.61 (t, *J* = 6.8 Hz, 3H), 7.56 (d, *J* = 9.2 Hz, 1H), 7.47 – 7.41 (m, 1H), 7.37 – 7.27 (m, 3H), 7.10 (t, *J* = 8.3 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 195.9 (d, *J* = 2.3 Hz), 167.3 (d, *J* = 2.3 Hz), 163.0 (d, *J* = 245.0 Hz). 162.8 (d, *J* = 247.7 Hz). 162.7 (d, *J* = 247.8 Hz). 158.6 (d, *J* = 3.2 Hz), 149.6, 140.9 (d, *J* = 6.4 Hz), 139.6 (d, *J* = 7.9 Hz), 139.1 (d, *J* = 7.4 Hz), 138.2, 133.9, 130.4 (d, *J* = 8.2 Hz), 130.0 (d, *J* = 7.6 Hz), 129.9 (d, *J* = 7.9 Hz), 129.5, 127.1, 126.0 (d, *J* = 3.1 Hz), 125.6 (d, *J* = 2.9 Hz), 124.2 (d, *J* = 2.8 Hz), 121.3, 120.0 (d, *J* = 21.5 Hz), 117.8 (d, *J* = 21.4 Hz), 117.7, 117.4 (d, *J* = 20.2 Hz), 117.2 (d, *J* = 22.4 Hz), 116.2(d, *J* = 22.5 Hz), 115.3 (d, *J* = 23.2 Hz). ^{19}F NMR (471 MHz, $CDCl_3$, ppm) δ -111.78, -112.31, -113.22. HRMS (ESI-TOF): m/z $[M+H]^+$calcd for $C_{27}H_{16}F_3N_2O^+$: 441.1209, found: 441.1205.



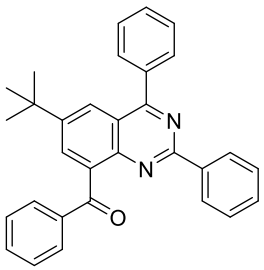
(2,4-Bis(3-chlorophenyl)quinazolin-8-yl)(3-chlorophenyl)methanone (5g): White solid (37.2 mg, 38% yield); R_f = 0.4 (PE:EA = 20:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.28 (d, *J* = 8.4 Hz, 1H), 8.16 – 8.09 (m, 2H), 8.03 (s, 1H), 7.88 (s, 1H), 7.84 (s, 1H), 7.78 – 7.71 (m, 2H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.63 – 7.56 (m, 3H), 7.43 – 7.37 (m, 2H), 7.30 (t, *J* = 7.9 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 195.9, 167.4, 158.5, 149.6, 140.7, 139.0 138.7, 138.0, 134.9, 134.7, 134.6, 134.3, 132.9, 130.9, 130.4, 130.1, 130.0, 129.70, 129.65, 129.3, 128.6, 128.3, 127.8, 127.2, 126.7, 121.4. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{27}H_{16}Cl_3N_2O^+$: 489.0323, found: 489.0319.



(2,4-Di-*o*-tolylquinazolin-8-yl)(*o*-tolyl)methanone (5h): White solid (35.1 mg, 41% yield); R_f = 0.4 (PE:EA = 50:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.00 (d, *J* = 6.5 Hz, 1H), 7.81 (t, *J* = 7.4 Hz, 2H), 7.59 (t, *J* = 7.8 Hz, 1H), 7.47 – 7.42 (m, 1H), 7.41 – 7.34 (m, 6H), 7.26 – 7.24 (m, 1H), 7.21 – 7.12 (m, 3H), 2.68 (s, 3H), 2.32 (s, 3H), 2.24 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 199.4, 169.6, 162.6, 148.9, 140.2, 139.5, 138.5, 138.2, 137.5, 136.7, 136.3, 133.2, 132.0, 131.9, 131.7, 131.6, 131.3, 130.7, 129.6, 129.5, 129.33, 129.27, 126.5, 125.7, 125.6, 125.4, 121.6, 21.60, 21.58, 20.1. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{30}H_{25}N_2O^+$: 429.1961, found: 429.1966.



(6-Methyl-2,4-diphenylquinazolin-8-yl)(phenyl)methanne (5i): White solid (32.8 mg, 41% yield); R_f = 0.4 (PE:EA = 20:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.18 (d, *J* = 8.3 Hz, 2H), 8.03 (s, 1H), 7.92 – 7.85 (m, 5H), 7.66 – 7.61 (m, 3H), 7.59 (t, *J* = 7.3 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.39 – 7.35 (m, 1H), 7.35 – 7.29 (m, 2H), 2.58 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 197.6, 167.8, 159.0, 148.4, 138.9, 138.5, 137.6, 136.7, 135.4, 132.8, 130.4, 130.1, 130.0, 129.9, 128.6, 128.5, 128.3, 128.23, 128.18, 121.4, 21.8. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{28}H_{21}N_2O^+$: 401.1648, found: 401.1640.

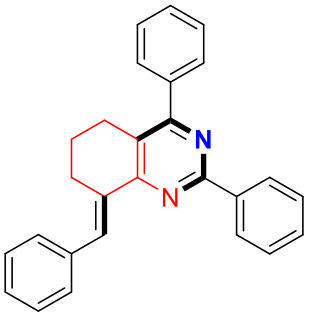


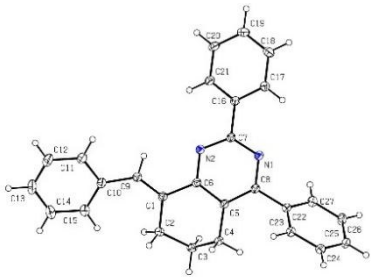
(6-(*Tert*-butyl)-2,4-diphenylquinazolin-8-yl)(phenyl)methanone (5j) : White solid (35.4 mg, 40% yield); R_f = 0.4 (PE:EA = 20:1); ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 8.22 (d, *J* = 15.8 Hz, 2H), 8.17 (d, *J* = 16.5 Hz, 2H), 7.92 (d, *J* = 5.2 Hz, 2H), 7.88 (d, *J* = 7.7 Hz, 2H), 7.64 (d, *J* = 5.8 Hz, 3H), 7.59 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.38 (t, *J* = 7.2 Hz, 1H), 7.32 (t, *J* = 7.4 Hz, 2H), 1.42 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$, ppm) δ 197.8, 168.1, 159.2, 149.7, 148.4, 138.9, 138.3, 137.69, 137.67, 132.8, 132.3, 130.5, 130.2, 130.1, 129.9, 128.6, 128.5, 128.2, 124.5, 121.0, 35.4, 31.1. HRMS (ESI-TOF): m/z $[M+H]^+$ calcd for $C_{31}H_{27}N_2O^+$: 443.2118, found: 443.2126.

5. Crystal data and structure refinement for 3a and 4f

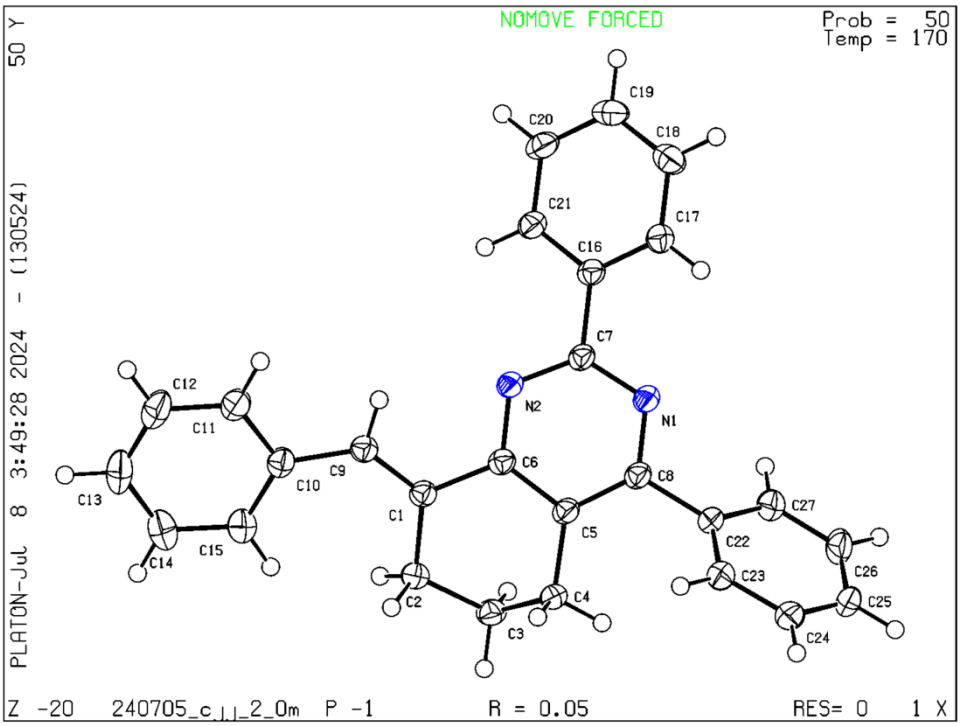
The single crystal of compound **3a** and **4f** were obtained by slowly evaporating a mixture of dichloromethane and petroleum ether solution at ambient temperature.

The single crystal X-ray diffraction data were collected at 150 K by a diffractometer Rigaku Oxford Diffraction Supernova Dual Source, Cu at Zero equipped with an AtlasS2 CCD using Cu Kα radiation (1.54178 Å) by using a w scan mode. The data were collected and processed using CrysAlisPro. The structures were solved by direct methods using Olex2 software with the SHELXT structure solution program via intrinsic phasing algorithm, and the non-hydrogen atoms were located from the trial structure and then refined anisotropically with SHELXL-2018 using a full-matrix least squares procedure based on F^2. The weighted *R* factor, *wR* and goodness-of-fit *S* values were obtained based on F^2. Crystallographic data for the structure reported in this paper have been deposited at the Cambridge Crystallographic Data Center.





3a **CCDC**: 2447285



The ellipsoids are shown at 50% probability levels.

Table 1 Crystal data and structure refinement for 3a.

Identification code	**3a**
Empirical formula	$C_{27}H_{22}N_2$
Formula weight	374.46
Temperature/K	170.00
Crystal system	triclinic
Space group	P-1

a/Å	9.1534(9)
b/Å	10.4460(11)
c/Å	10.8289(11)
α/°	82.743(4)
β/°	85.912(4)
γ/°	71.848(4)
Volume/$Å^3$	975.45(17)
Z	2
$\rho_{calc}g/cm^3$	1.275
μ/mm^{-1}	0.364
F(000)	396.0
Crystal size/mm^3	0.1 × 0.05 × 0.03
Radiation	GaKα (λ = 1.34139)
2Θ range for data collection/°	7.164 to 122.322
Index ranges	$-11 \leq h \leq 11$, $-13 \leq k \leq 13$, $-14 \leq l \leq 14$
Reflections collected	17660
Independent reflections	4444 [R_{int} = 0.0569, R_{sigma} = 0.0694]
Data/restraints/parameters	4444/0/262
Goodness-of-fit on F^2	1.090
Final R indexes [I>=2σ (I)]	R_1 = 0.0509, wR_2 = 0.1265
Final R indexes [all data]	R_1 = 0.0598, wR_2 = 0.1311
Largest diff. peak/hole / e $Å^{-3}$	0.33/-0.23

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

Atom	*x*	*y*	*z*	U(eq)
N1	5101.4(12)	4835.3(10)	2742.2(9)	24.1(2)
C1	1948.7(13)	4228.4(11)	5628.8(11)	22.6(3)
N2	3084.8(11)	5688.6(10)	4226.0(9)	23.0(2)
C2	1554.9(14)	2909.9(12)	5754.1(12)	25.8(3)
C3	2344.6(15)	1981.8(12)	4764.8(12)	27.2(3)
C4	4037.4(15)	1887.9(12)	4586.7(12)	26.1(3)
C5	4141.7(14)	3285.6(11)	4140.0(11)	22.8(3)
C6	3090.5(13)	4412.9(11)	4637.0(11)	21.9(3)
C7	4078.8(13)	5834.4(11)	3298.3(11)	22.2(3)
C8	5140.9(14)	3567.0(12)	3183.8(11)	23.3(3)
C9	1376.7(14)	5219.9(12)	6377.5(11)	23.7(3)
C10	256.6(14)	5356.9(12)	7429.1(11)	25.6(3)
C11	17.5(15)	6492.1(13)	8078.8(12)	30.8(3)
C12	-1064.5(17)	6760.2(15)	9047.7(13)	38.6(3)
C13	-1944.8(17)	5907.6(17)	9397.8(13)	40.6(4)
C14	-1715.8(16)	4774.4(16)	8782.9(13)	38.6(3)
C15	-630.0(15)	4491.9(14)	7819.6(12)	31.4(3)
C16	4041.7(14)	7240.3(12)	2807.9(11)	23.3(3)
C17	5297.9(15)	7474.6(13)	2115.4(12)	27.2(3)
C18	5271.5(16)	8786.5(14)	1657.7(13)	32.7(3)
C19	3989.5(17)	9874.2(13)	1877.2(13)	33.3(3)
C20	2733.2(16)	9651.6(13)	2554.0(12)	31.3(3)
C21	2757.8(15)	8342.9(12)	3028.0(12)	26.8(3)

C22	6315.6(14)	2476.6(12)	2568.0(12)	24.9(3)
C23	7347.9(15)	1410.8(13)	3267.5(13)	30.8(3)
C24	8453.8(16)	416.4(13)	2677.9(15)	37.0(3)
C25	8519.2(17)	468.6(13)	1394.5(15)	38.1(4)
C26	7496.0(17)	1524.1(14)	690.0(14)	36.5(3)
C27	6408.8(15)	2535.8(13)	1271.9(12)	30.3(3)

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

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N1	27.2(5)	21.4(5)	22.7(5)	-4.8(4)	1.1(4)	-5.4(4)
C1	24.1(6)	20.9(5)	21.3(6)	-1.1(4)	-1.8(5)	-4.8(4)
N2	26.6(5)	20.0(5)	21.5(5)	-3.6(4)	0.7(4)	-5.7(4)
C2	29.9(6)	22.7(6)	24.9(6)	-2.4(5)	1.5(5)	-9.1(5)
C3	34.8(7)	21.6(6)	26.5(7)	-4.3(5)	0.2(5)	-10.3(5)
C4	32.7(6)	18.9(6)	24.5(6)	-3.0(4)	3.0(5)	-5.4(5)
C5	26.8(6)	19.4(5)	21.1(6)	-4.3(4)	-0.6(5)	-4.6(5)
C6	25.4(6)	20.3(5)	19.8(6)	-2.9(4)	-2.3(5)	-5.9(4)
C7	25.6(6)	20.6(6)	19.9(6)	-4.6(4)	-1.0(5)	-5.3(4)
C8	27.2(6)	20.8(5)	20.6(6)	-4.4(4)	-0.6(5)	-4.7(5)
C9	25.1(6)	22.2(6)	23.0(6)	-1.7(4)	-0.8(5)	-6.5(5)
C10	24.7(6)	26.5(6)	22.0(6)	-2.1(5)	-1.5(5)	-2.5(5)
C11	31.9(7)	28.7(6)	28.4(7)	-5.2(5)	-0.1(5)	-4.0(5)
C12	39.7(8)	39.6(8)	29.0(7)	-11.5(6)	1.4(6)	1.1(6)
C13	30.8(7)	56.2(9)	26.1(7)	-7.6(6)	4.8(6)	-0.8(6)
C14	30.5(7)	52.7(9)	31.6(8)	-2.0(6)	4.4(6)	-13.5(6)
C15	30.2(6)	36.1(7)	27.5(7)	-5.3(5)	1.4(5)	-9.2(5)

C16	30.2(6)	20.9(6)	18.8(6)	-3.5(4)	-1.6(5)	-6.9(5)
C17	30.8(6)	25.9(6)	23.6(6)	-3.2(5)	1.6(5)	-7.2(5)
C18	39.8(7)	32.6(7)	28.4(7)	0.4(5)	0.7(6)	-16.9(6)
C19	48.7(8)	22.6(6)	30.4(7)	0.8(5)	-5.7(6)	-14.3(6)
C20	40.8(7)	20.6(6)	30.5(7)	-6.0(5)	-2.2(6)	-5.1(5)
C21	31.6(6)	22.1(6)	25.8(6)	-5.1(5)	1.1(5)	-6.3(5)
C22	27.7(6)	20.4(6)	26.6(6)	-6.2(5)	4.9(5)	-7.4(5)
C23	32.5(7)	25.0(6)	30.4(7)	-1.5(5)	6.1(5)	-4.4(5)
C24	32.5(7)	23.7(6)	47.6(9)	0.1(6)	12.1(6)	-3.0(5)
C25	38.2(7)	26.2(7)	49.4(9)	-14.7(6)	21.5(7)	-10.0(6)
C26	41.8(8)	39.9(8)	31.4(7)	-16.2(6)	12.9(6)	-16.2(6)
C27	33.6(7)	30.4(7)	27.3(7)	-6.5(5)	3.7(5)	-10.4(5)

Table 4 Bond Lengths for 3a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	C7	1.3408(15)	C11	C12	1.3833(19)
N1	C8	1.3408(15)	C12	C13	1.380(2)
C1	C2	1.5168(16)	C13	C14	1.383(2)
C1	C6	1.4819(16)	C14	C15	1.3822(19)
C1	C9	1.3483(16)	C16	C17	1.3966(17)
N2	C6	1.3491(15)	C16	C21	1.3966(17)
N2	C7	1.3333(15)	C17	C18	1.3906(18)
C2	C3	1.5250(17)	C18	C19	1.386(2)
C3	C4	1.5216(18)	C19	C20	1.385(2)
C4	C5	1.5089(16)	C20	C21	1.3922(17)
C5	C6	1.4080(16)	C22	C23	1.3927(18)
C5	C8	1.3967(17)	C22	C27	1.3948(18)

C7	C16	1.4881(16)	C23	C24	1.3898(18)
C8	C22	1.4915(16)	C24	C25	1.382(2)
C9	C10	1.4669(17)	C25	C26	1.386(2)
C10	C11	1.4058(18)	C26	C27	1.3885(18)
C10	C15	1.4019(18)			

Table 5 Bond Angles for 3a.

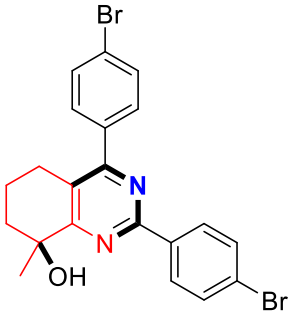
Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C7	N1	C8	116.38(10)	C15	C10	C11	117.14(12)
C6	C1	C2	117.28(10)	C12	C11	C10	121.57(13)
C9	C1	C2	124.85(11)	C13	C12	C11	120.17(13)
C9	C1	C6	117.83(10)	C12	C13	C14	119.29(13)
C7	N2	C6	117.00(10)	C15	C14	C13	121.00(14)
C1	C2	C3	113.77(10)	C14	C15	C10	120.81(13)
C4	C3	C2	111.23(10)	C17	C16	C7	120.18(11)
C5	C4	C3	108.16(10)	C17	C16	C21	118.97(11)
C6	C5	C4	118.96(10)	C21	C16	C7	120.85(11)
C8	C5	C4	124.54(10)	C18	C17	C16	120.44(12)
C8	C5	C6	116.31(10)	C19	C18	C17	120.18(12)
N2	C6	C1	118.00(10)	C20	C19	C18	119.83(12)
N2	C6	C5	121.34(11)	C19	C20	C21	120.34(12)
C5	C6	C1	120.66(10)	C20	C21	C16	120.24(12)
N1	C7	C16	116.21(10)	C23	C22	C8	120.96(11)
N2	C7	N1	126.40(10)	C23	C22	C27	119.26(11)
N2	C7	C16	117.38(10)	C27	C22	C8	119.76(11)
N1	C8	C5	122.50(11)	C24	C23	C22	120.23(13)
N1	C8	C22	115.16(10)	C25	C24	C23	120.14(13)

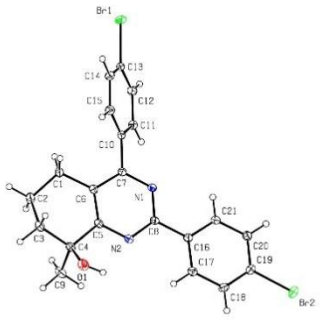
C5	C8	C22	122.34(10)	C24	C25	C26	120.08(12)
C1	C9	C10	131.71(11)	C25	C26	C27	120.07(13)
C11	C10	C9	116.52(11)	C26	C27	C22	120.20(13)
C15	C10	C9	126.30(11)				

Table 6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 3a.

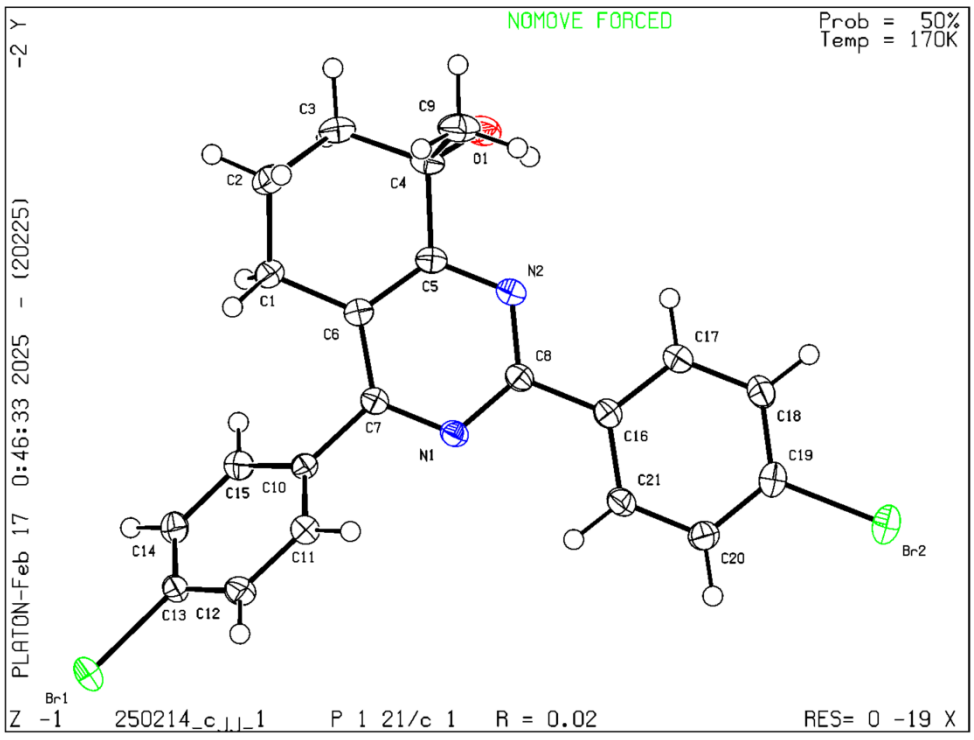
Atom	*x*	*y*	*z*	U(eq)
H2A	427.3	3120.76	5703.52	31
H2B	1851.07	2420.2	6586.79	31
H3A	2250.67	1065.4	5016.42	33
H3B	1825.7	2334.88	3965.17	33
H4A	4565.07	1546.67	5383.96	31
H4B	4539.51	1253.8	3966.26	31
H9	1770.67	5965.48	6189.75	28
H11	613.22	7089.36	7846.86	37
H12	-1201.9	7533.15	9473.16	46
H13	-2700.08	6097.03	10054.16	49
H14	-2313.86	4181.32	9026.4	46
H15	-482.63	3701.76	7417.11	38
H17	6176.3	6732.76	1955.91	33
H18	6134.19	8937.81	1193.27	39
H19	3973.21	10769.89	1564.1	40
H20	1849.76	10395.87	2695.59	38
H21	1898.13	8199.25	3502.92	32
H23	7295.95	1363.36	4150.7	37
H24	9166.11	-300.68	3158.33	44

H25	9266.52	-219.75	994.57	46
H26	7538.48	1555.37	-192.03	44
H27	5726.38	3270.63	785.76	36





4f **CCDC**: 2447284



The ellipsoids are shown at 50% probability levels.

Table 1 Crystal data and structure refinement for 4f.

Identification code	**4f**
Empirical formula	$C_{21}H_{18}Br_2N_2O$

Formula weight	474.19
Temperature/K	170.00
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	15.4730(9)
b/Å	8.6296(5)
c/Å	14.0649(8)
α/°	90
β/°	98.097(2)
γ/°	90
Volume/Å^3	1859.30(19)
Z	4
ρ_{calc}g/cm^3	1.694
μ/mm^{-1}	3.723
F(000)	944.0
Crystal size/mm^3	0.19 × 0.16 × 0.1
Radiation	GaKα (λ = 1.34139)
2Θ range for data collection/°	10.048 to 121.124
Index ranges	$-20 \leq h \leq 11$, $-10 \leq k \leq 11$, $-18 \leq l \leq 18$
Reflections collected	15839
Independent reflections	4211 [R_{int} = 0.0372, R_{sigma} = 0.0373]
Data/restraints/parameters	4211/0/237
Goodness-of-fit on F^2	1.050
Final R indexes [I>=2σ (I)]	R_1 = 0.0235, wR_2 = 0.0609
Final R indexes [all data]	R_1 = 0.0352, wR_2 = 0.0626
Largest diff. peak/hole / e Å^{-3}	0.33/-0.81

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

Atom	*x*	*y*	*z*	U(eq)
Br1	-111.0(2)	1219.8(2)	7107.7(2)	35.55(7)
Br2	7908.3(2)	3573.5(2)	6779.5(2)	28.15(7)
O1	3653.7(8)	9924.2(14)	4434.4(9)	31.1(3)
N1	3521.4(7)	5219.6(15)	6321.6(9)	19.3(3)
N2	4050.4(8)	7565.8(15)	5732.7(9)	20.6(3)
C1	1604.3(9)	7929.8(18)	5596.8(12)	22.5(3)
C2	1603.7(10)	9692(2)	5534.6(13)	27.5(4)
C3	2230.1(10)	10230(2)	4854.4(13)	26.3(3)
C4	3172.7(10)	9801.1(18)	5235.0(12)	23.5(3)
C5	3237.1(9)	8129.2(18)	5595.5(11)	19.4(3)
C6	2517.7(9)	7266.6(18)	5781.1(11)	18.4(3)
C7	2704.3(9)	5769.9(18)	6138.6(11)	18.0(3)
C8	4161.7(9)	6137.0(18)	6097.8(11)	18.6(3)
C9	3563.4(12)	10883(2)	6031.0(14)	32.4(4)
C10	2013.1(9)	4681.1(17)	6364.6(11)	19.1(3)
C11	2097.5(10)	3969.7(19)	7259.0(12)	22.6(3)
C12	1458.0(10)	2955.4(19)	7486.7(12)	24.5(3)
C13	744.7(9)	2642.7(18)	6800.9(12)	23.4(3)
C14	658.2(10)	3304(2)	5902.4(13)	25.9(3)
C15	1291.9(10)	4340.7(19)	5685.7(12)	24.0(3)
C16	5065.0(9)	5513.4(18)	6268.0(11)	19.8(3)
C17	5755.4(10)	6393.8(19)	6024.6(13)	25.4(3)
C18	6600.4(10)	5807(2)	6164.8(13)	26.8(3)

C19	6747.8(9)	4348(2)	6552.5(11)	22.7(3)
C20	6071.1(10)	3445.3(19)	6802.6(12)	23.2(3)
C21	5231.9(9)	4042.3(19)	6662.0(12)	22.4(3)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 4f. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Br1	22.31(10)	31.05(12)	55.00(15)	8.52(9)	11.33(8)	-6.72(7)
Br2	19.95(9)	38.78(12)	25.54(11)	-1.43(8)	2.54(7)	5.58(6)
O1	37.7(6)	26.9(6)	31.2(7)	9.1(5)	13.8(5)	1.2(5)
N1	19.9(6)	16.7(6)	21.6(7)	0.0(5)	3.9(5)	-1.9(5)
N2	22.3(6)	17.5(6)	21.9(7)	0.6(6)	3.5(5)	-2.2(5)
C1	22.0(7)	20.2(8)	25.7(8)	1.8(7)	4.1(6)	3.3(6)
C2	29.3(8)	22.9(8)	30.4(9)	2.4(7)	5.1(7)	6.8(6)
C3	33.1(8)	19.6(8)	25.8(9)	5.6(7)	2.4(6)	2.6(6)
C4	30.1(7)	17.7(8)	23.4(8)	4.0(7)	5.7(6)	-1.8(6)
C5	25.1(7)	16.7(7)	16.2(7)	-1.3(6)	2.1(5)	-1.1(6)
C6	21.7(6)	17.6(7)	15.9(7)	-1.2(6)	2.3(5)	0.7(6)
C7	19.6(6)	17.7(7)	16.5(7)	-1.5(6)	1.9(5)	-1.4(6)
C8	20.1(7)	17.5(7)	18.0(7)	-2.5(6)	2.4(5)	-2.7(5)
C9	43.8(10)	19.0(8)	32.2(10)	1.5(8)	-1.9(8)	-3.7(7)
C10	18.4(6)	15.5(7)	24.2(8)	0.3(6)	5.3(5)	1.3(5)
C11	21.1(7)	21.5(8)	25.4(8)	1.5(7)	4.0(6)	-0.8(6)
C12	25.6(7)	23.3(8)	25.6(8)	4.5(7)	6.9(6)	-1.0(6)
C13	18.0(6)	16.7(7)	37.2(9)	0.4(7)	9.6(6)	-0.5(6)
C14	18.3(7)	24.2(8)	33.6(9)	0.6(7)	-1.8(6)	-1.8(6)
C15	22.4(7)	22.4(8)	26.6(9)	2.6(7)	1.7(6)	-0.7(6)

C16	20.2(6)	21.0(8)	18.3(8)	-1.2(6)	2.6(5)	-2.2(6)
C17	22.9(7)	22.8(8)	30.6(9)	5.5(7)	4.1(6)	-2.4(6)
C18	19.8(7)	29.9(9)	31.1(9)	4.7(8)	5.0(6)	-3.6(6)
C19	19.1(6)	29.4(9)	19.3(8)	-3.8(7)	1.9(5)	1.5(6)
C20	24.0(7)	20.7(8)	24.2(8)	0.4(7)	1.3(6)	0.7(6)
C21	21.4(7)	19.5(7)	26.6(9)	-0.4(7)	4.4(6)	-3.6(6)

Table 4 Bond Lengths for 4f.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br1	C13	1.8995(15)	C7	C10	1.4911(19)
Br2	C19	1.9004(15)	C8	C16	1.485(2)
O1	C4	1.4385(18)	C10	C11	1.389(2)
N1	C7	1.3411(18)	C10	C15	1.394(2)
N1	C8	1.3399(19)	C11	C12	1.392(2)
N2	C5	1.3374(19)	C12	C13	1.386(2)
N2	C8	1.337(2)	C13	C14	1.376(2)
C1	C2	1.523(2)	C14	C15	1.392(2)
C1	C6	1.513(2)	C16	C17	1.392(2)
C2	C3	1.527(2)	C16	C21	1.395(2)
C3	C4	1.527(2)	C17	C18	1.390(2)
C4	C5	1.528(2)	C18	C19	1.378(2)
C4	C9	1.516(2)	C19	C20	1.389(2)
C5	C6	1.394(2)	C20	C21	1.385(2)
C6	C7	1.401(2)			

Table 5 Bond Angles for 4f.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C8	N1	C7	117.01(13)	N2	C8	C16	117.60(13)
C5	N2	C8	117.28(12)	C11	C10	C7	119.51(13)
C6	C1	C2	112.37(13)	C11	C10	C15	119.43(14)
C1	C2	C3	110.11(13)	C15	C10	C7	121.05(14)
C4	C3	C2	111.48(13)	C10	C11	C12	120.46(15)
O1	C4	C3	106.36(13)	C13	C12	C11	118.98(15)
O1	C4	C5	108.23(12)	C12	C13	Br1	118.68(12)
O1	C4	C9	109.64(13)	C14	C13	Br1	119.74(12)
C3	C4	C5	111.07(12)	C14	C13	C12	121.56(14)
C9	C4	C3	111.81(14)	C13	C14	C15	119.15(15)
C9	C4	C5	109.62(14)	C14	C15	C10	120.39(16)
N2	C5	C4	114.03(13)	C17	C16	C8	119.99(14)
N2	C5	C6	122.60(14)	C17	C16	C21	119.27(14)
C6	C5	C4	123.36(13)	C21	C16	C8	120.74(13)
C5	C6	C1	121.15(14)	C18	C17	C16	120.34(15)
C5	C6	C7	115.45(13)	C19	C18	C17	119.27(14)
C7	C6	C1	123.40(13)	C18	C19	Br2	119.18(11)
N1	C7	C6	122.43(13)	C18	C19	C20	121.58(14)
N1	C7	C10	114.90(13)	C20	C19	Br2	119.23(13)
C6	C7	C10	122.65(12)	C21	C20	C19	118.69(15)
N1	C8	C16	117.28(14)	C20	C21	C16	120.84(14)
N2	C8	N1	125.12(13)				

Table 6 Torsion Angles for 4f.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Br1	C13	C14	C15	-179.76(12)	C6	C7	C10	C11	-128.37(16)
Br2	C19	C20	C21	177.97(12)	C6	C7	C10	C15	53.0(2)
O1	C4	C5	N2	49.14(18)	C7	N1	C8	N2	1.9(2)
O1	C4	C5	C6	-131.81(15)	C7	N1	C8	C16	-177.98(13)
N1	C7	C10	C11	50.35(19)	C7	C10	C11	C12	179.68(14)
N1	C7	C10	C15	-128.31(15)	C7	C10	C15	C14	179.04(14)
N1	C8	C16	C17	178.18(15)	C8	N1	C7	C6	-3.6(2)
N1	C8	C16	C21	-1.2(2)	C8	N1	C7	C10	177.70(13)
N2	C5	C6	C1	-178.65(14)	C8	N2	C5	C4	176.45(13)
N2	C5	C6	C7	1.0(2)	C8	N2	C5	C6	-2.6(2)
N2	C8	C16	C17	-1.7(2)	C8	C16	C17	C18	-178.78(16)
N2	C8	C16	C21	178.93(14)	C8	C16	C21	C20	178.63(15)
C1	C2	C3	C4	-64.17(18)	C9	C4	C5	N2	-70.40(17)
C1	C6	C7	N1	-178.13(14)	C9	C4	C5	C6	108.65(17)
C1	C6	C7	C10	0.5(2)	C10	C11	C12	C13	1.3(2)
C2	C1	C6	C5	-19.4(2)	C11	C10	C15	C14	0.4(2)
C2	C1	C6	C7	160.95(15)	C11	C12	C13	Br1	178.55(12)
C2	C3	C4	O1	163.01(13)	C11	C12	C13	C14	0.4(2)
C2	C3	C4	C5	45.47(18)	C12	C13	C14	C15	-1.6(2)
C2	C3	C4	C9	-77.33(17)	C13	C14	C15	C10	1.2(2)
C3	C4	C5	N2	165.54(13)	C15	C10	C11	C12	-1.6(2)
C3	C4	C5	C6	-15.4(2)	C16	C17	C18	C19	-0.4(3)
C4	C5	C6	C1	2.4(2)	C17	C16	C21	C20	-0.7(2)
C4	C5	C6	C7	-177.93(14)	C17	C18	C19	Br2	-178.11(13)
C5	N2	C8	N1	1.1(2)	C17	C18	C19	C20	0.3(3)

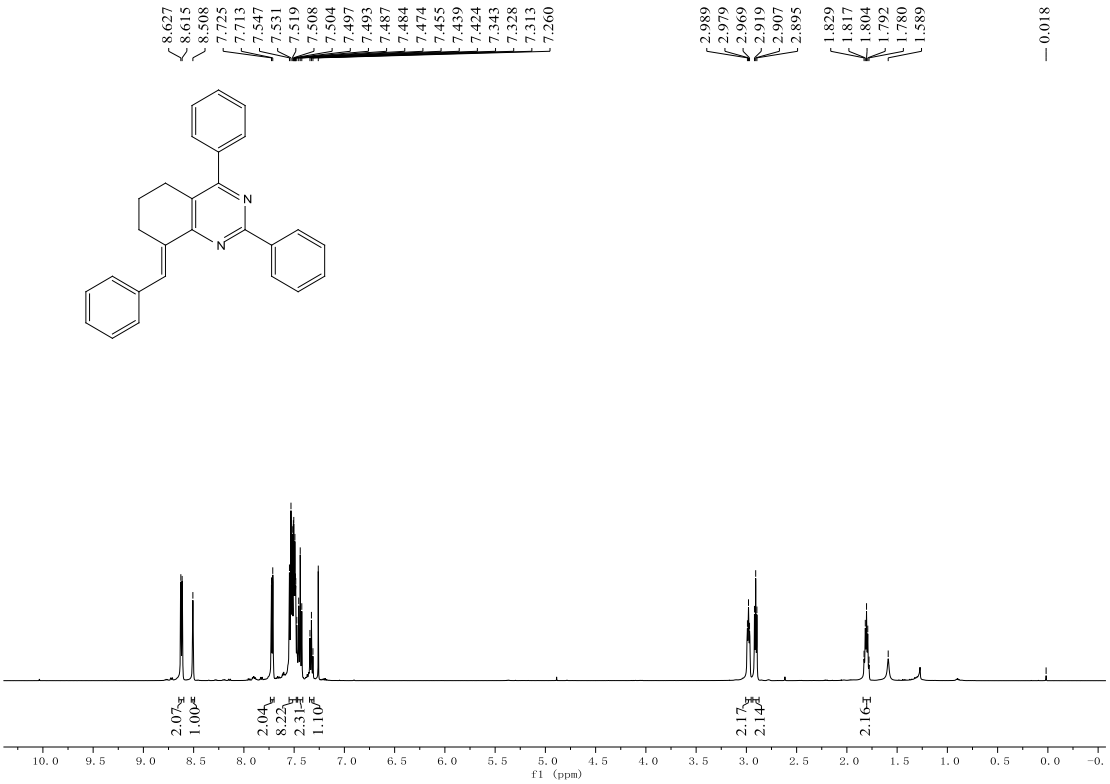
C5	N2	C8	C16	-178.97(13)	C18	C19	C20	C21	-0.5(2)
C5	C6	C7	N1	2.2(2)	C19	C20	C21	C16	0.7(2)
C5	C6	C7	C10	-179.19(14)	C21	C16	C17	C18	0.6(3)
C6	C1	C2	C3	49.09(18)					

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

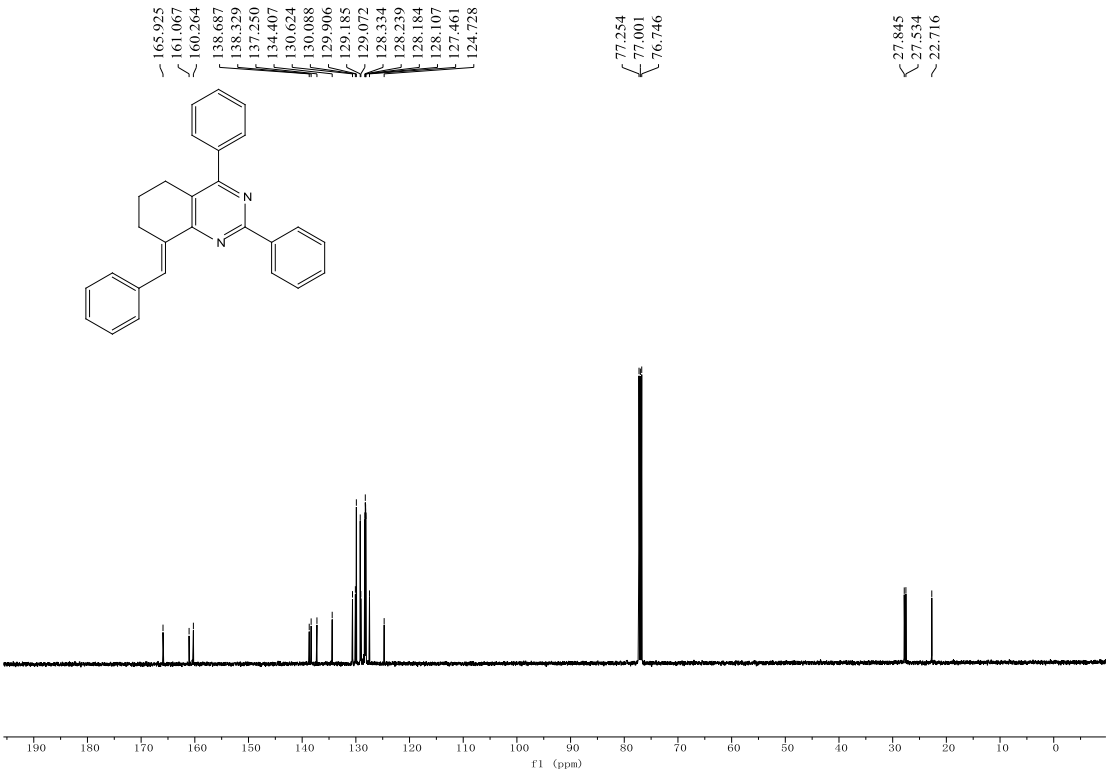
Atom	*x*	*y*	*z*	U(eq)
H1	4139.72	9484.63	4570.6	47
H1A	1278.18	7606.53	6120.6	27
H1B	1298.62	7500.37	4987.98	27
H2A	1784.11	10136.33	6181.07	33
H2B	1006.68	10064.13	5298.6	33
H3A	2062.44	9745.77	4216.84	32
H3B	2183.53	11367.44	4773.43	32
H9A	4173.08	10595.39	6241.07	49
H9B	3232.44	10801.37	6573.93	49
H9C	3537	11951.31	5792.39	49
H11	2595.31	4176.96	7718.41	27
H12	1509.51	2484.58	8102.63	29
H14	172.41	3056.19	5435.77	31
H15	1232.38	4818.86	5071.54	29
H17	5648.37	7400.84	5761.36	30
H18	7071.14	6404.74	5995.22	32
H20	6181.86	2438.53	7064.92	28
H21	4763.97	3441.97	6836.12	27

6. ^{1}H NMR and ^{13}C NMR spectra of all products

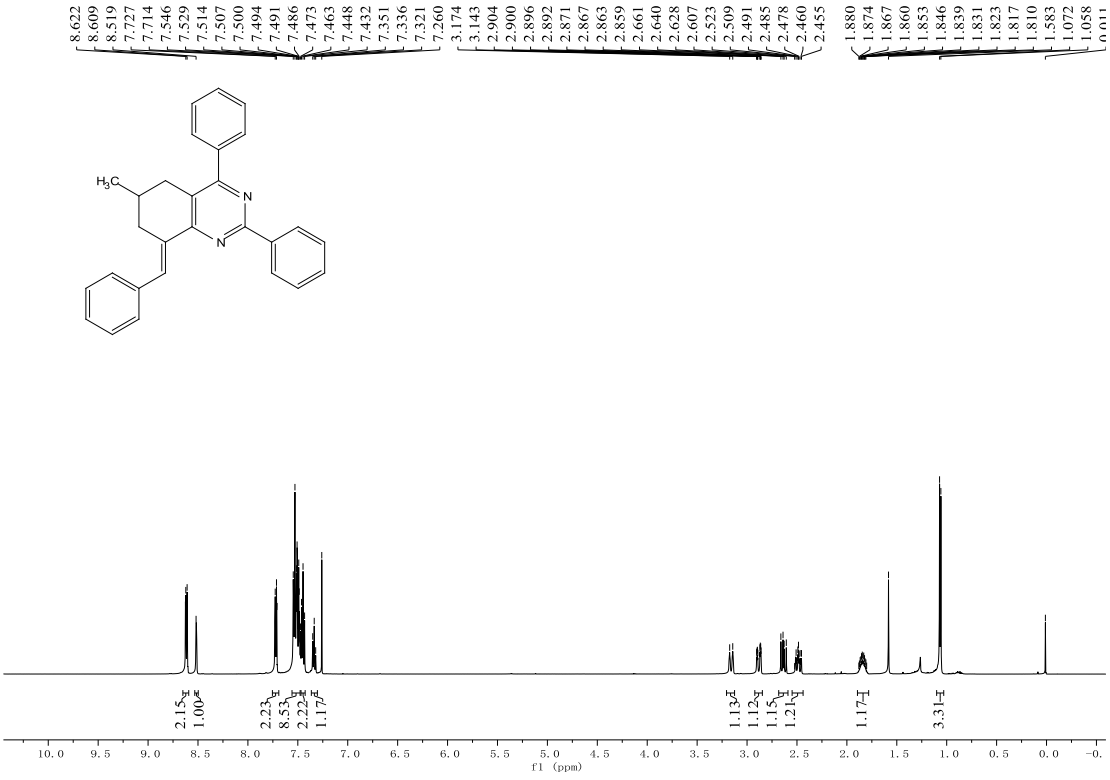
^{1}H NMR of **3a** (500 MHz, $CDCl_3$)



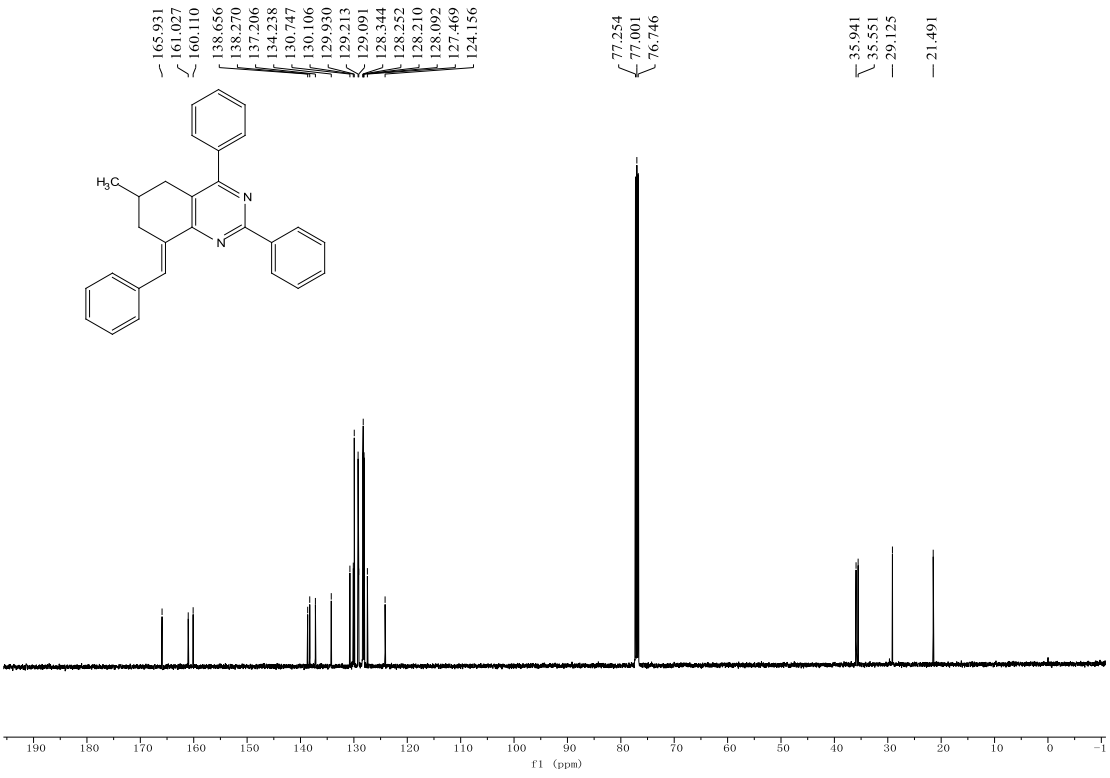
^{13}C NMR of **3a** (125 MHz, $CDCl_3$)



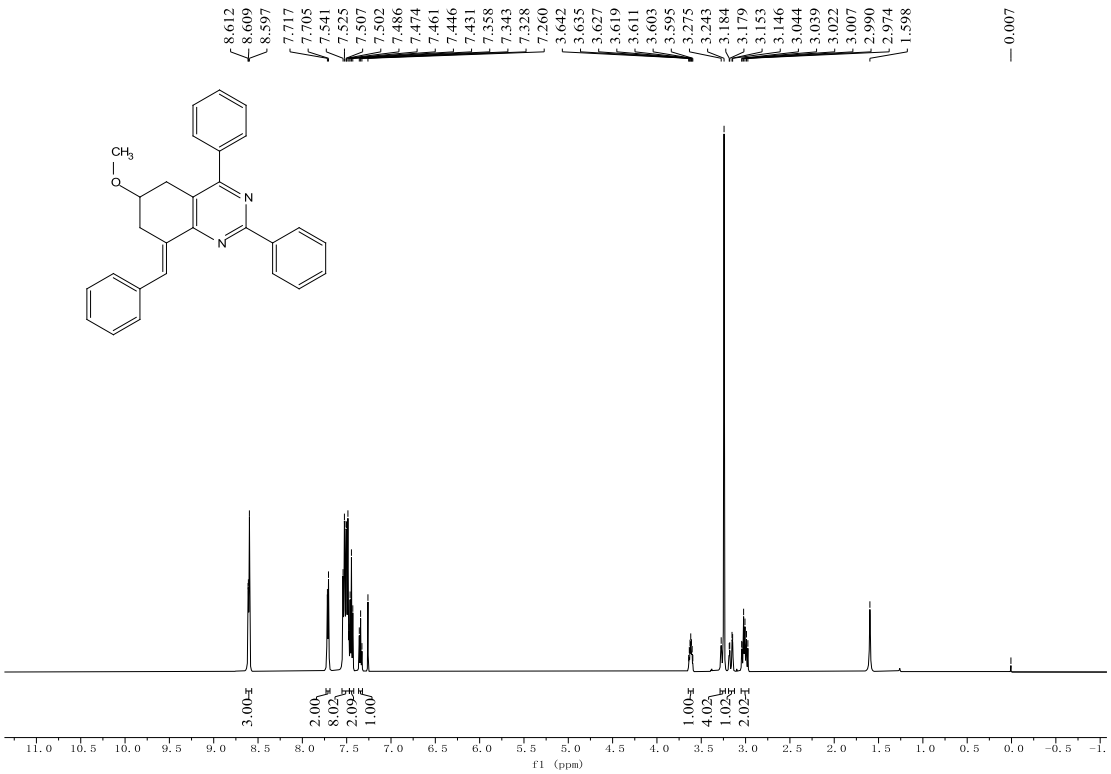
^{1}H NMR of **3b** (500 MHz, $CDCl_3$)



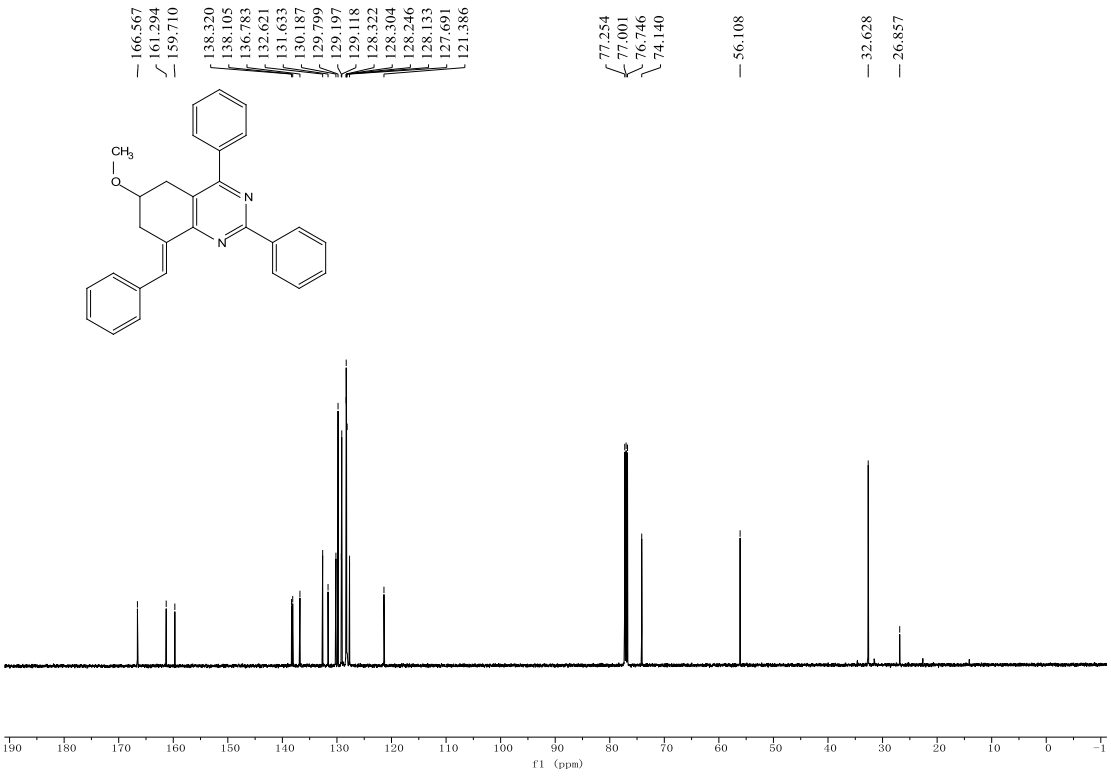
^{13}C NMR of **3b** (125 MHz, $CDCl_3$)



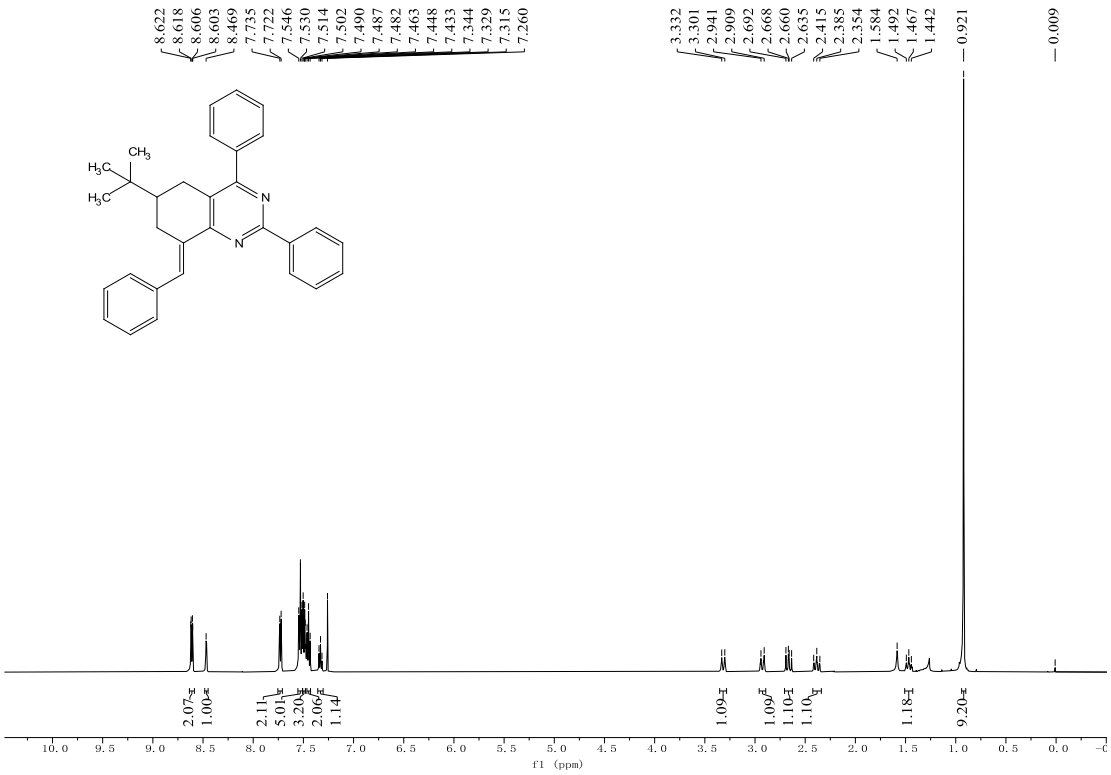
^{1}H NMR of **3c** (500 MHz, $CDCl_3$)



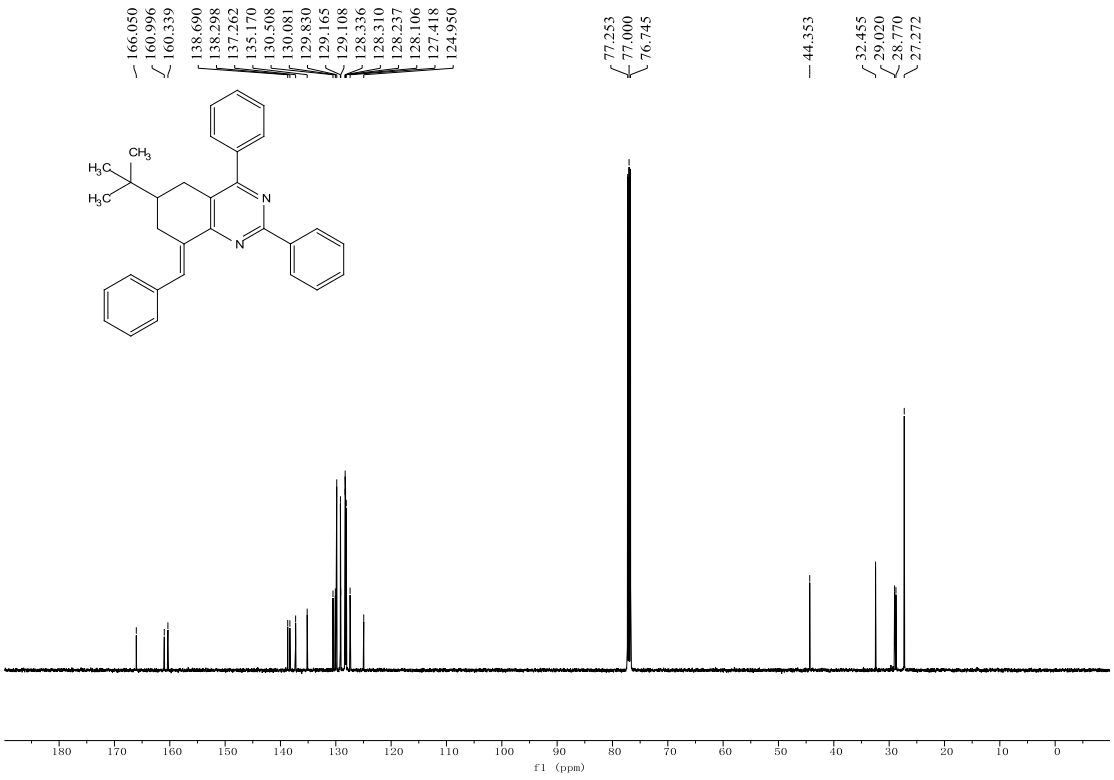
^{13}C NMR of **3c** (125 MHz, $CDCl_3$)



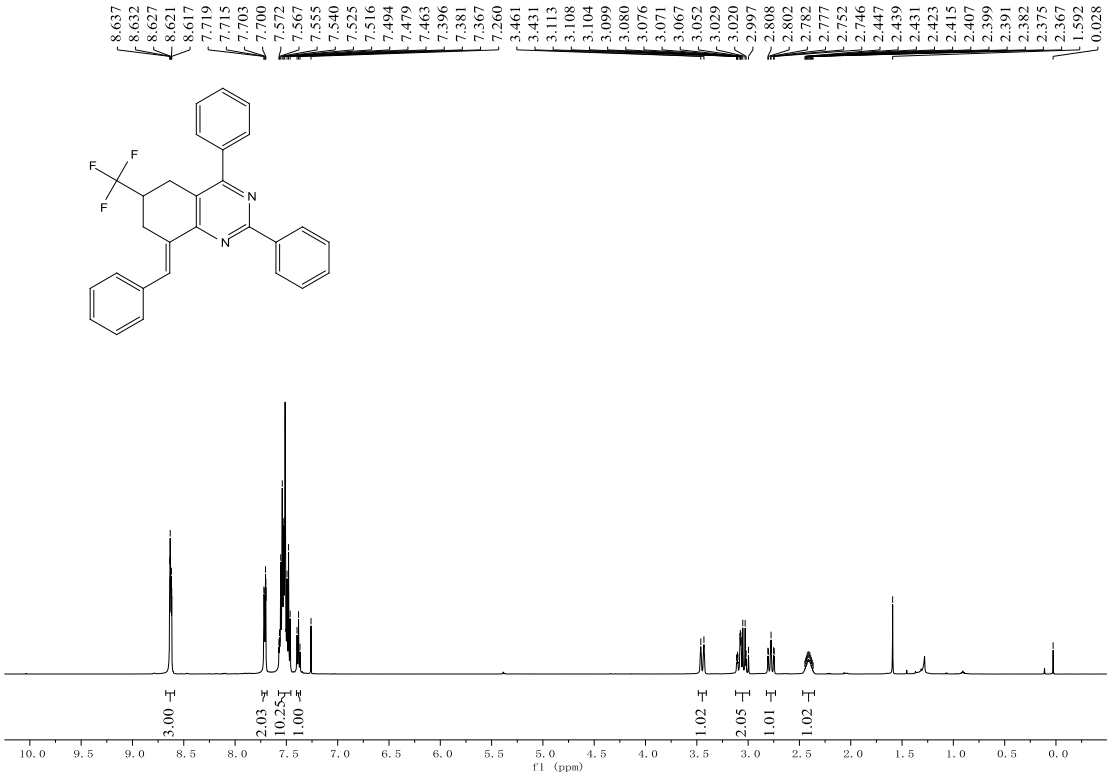
^{1}H NMR of **3d** (500 MHz, $CDCl_3$)



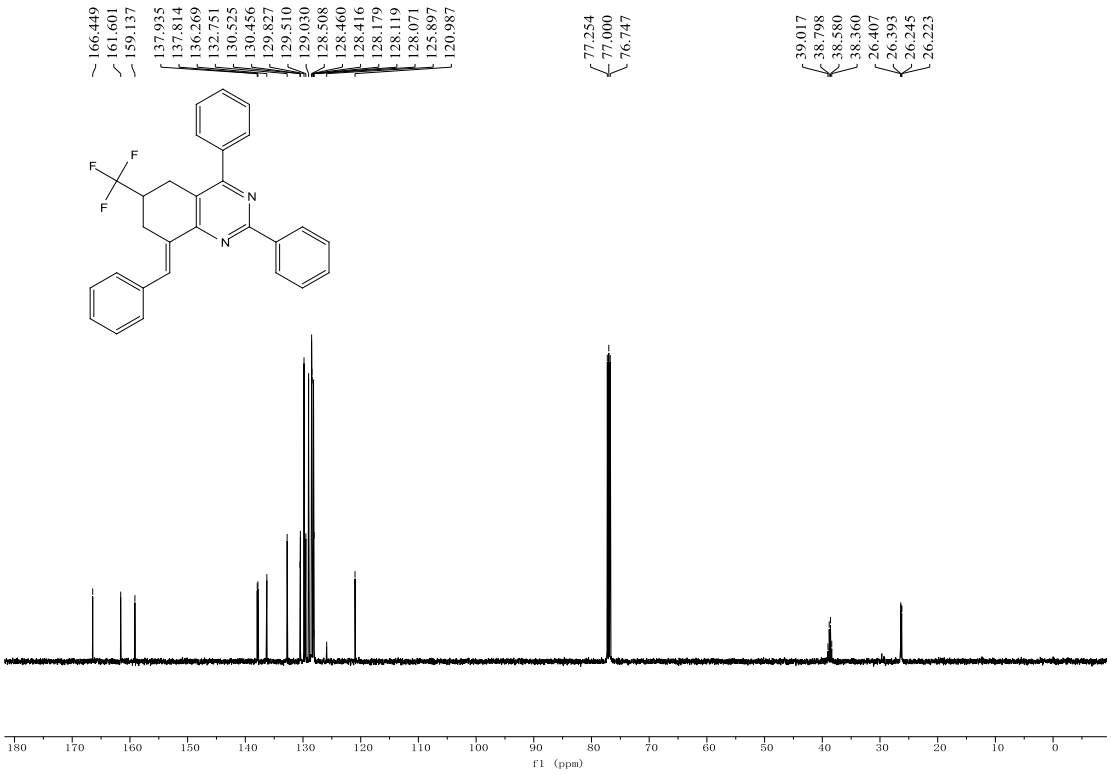
^{13}C NMR of **3d** (125 MHz, $CDCl_3$)



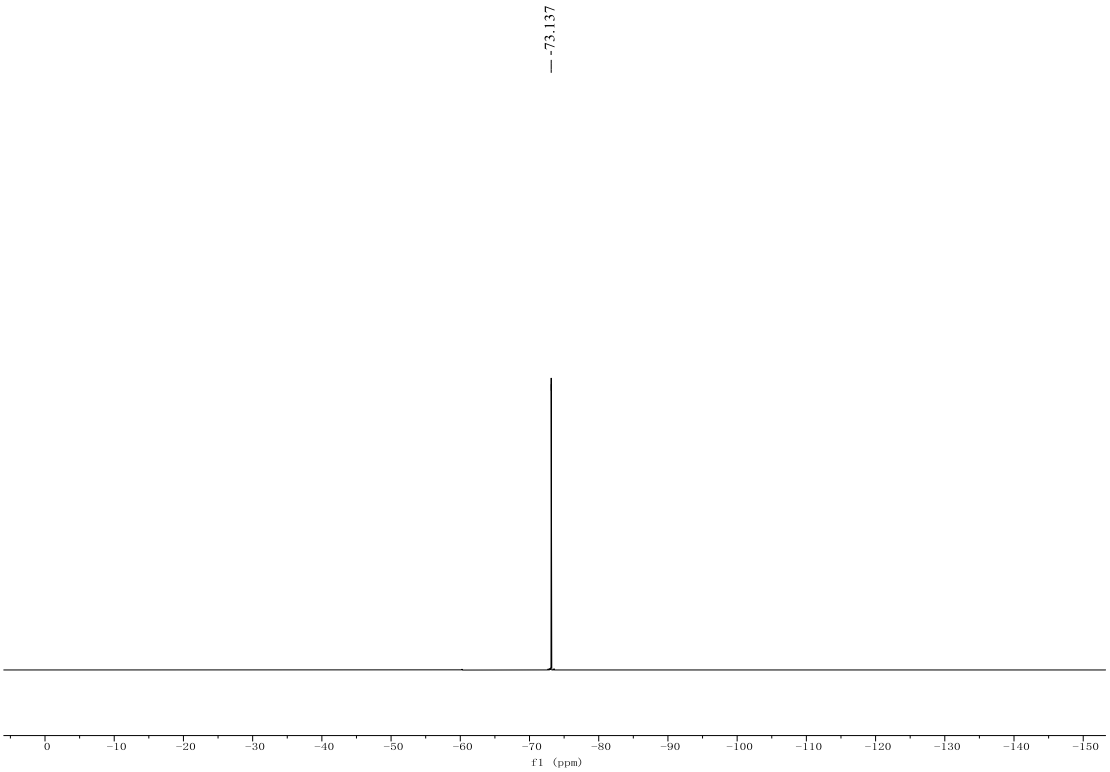
^{1}H NMR of **3e** (500 MHz, $CDCl_3$)



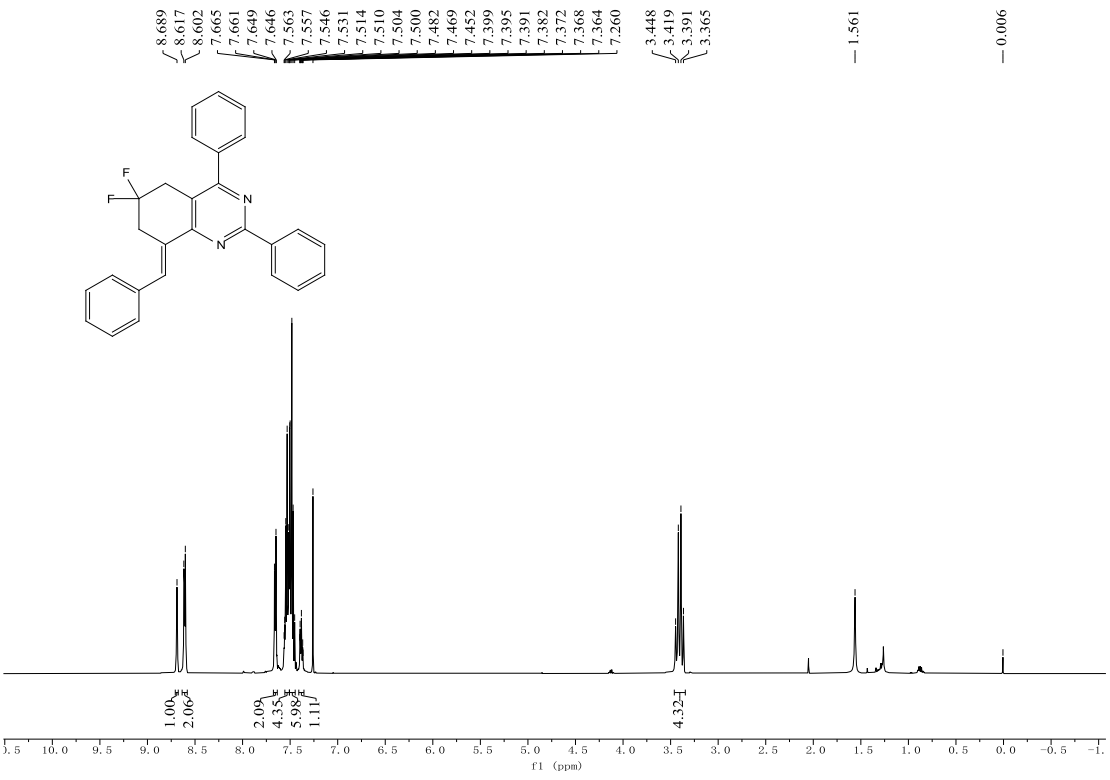
^{13}C NMR of **3e** (125 MHz, $CDCl_3$)



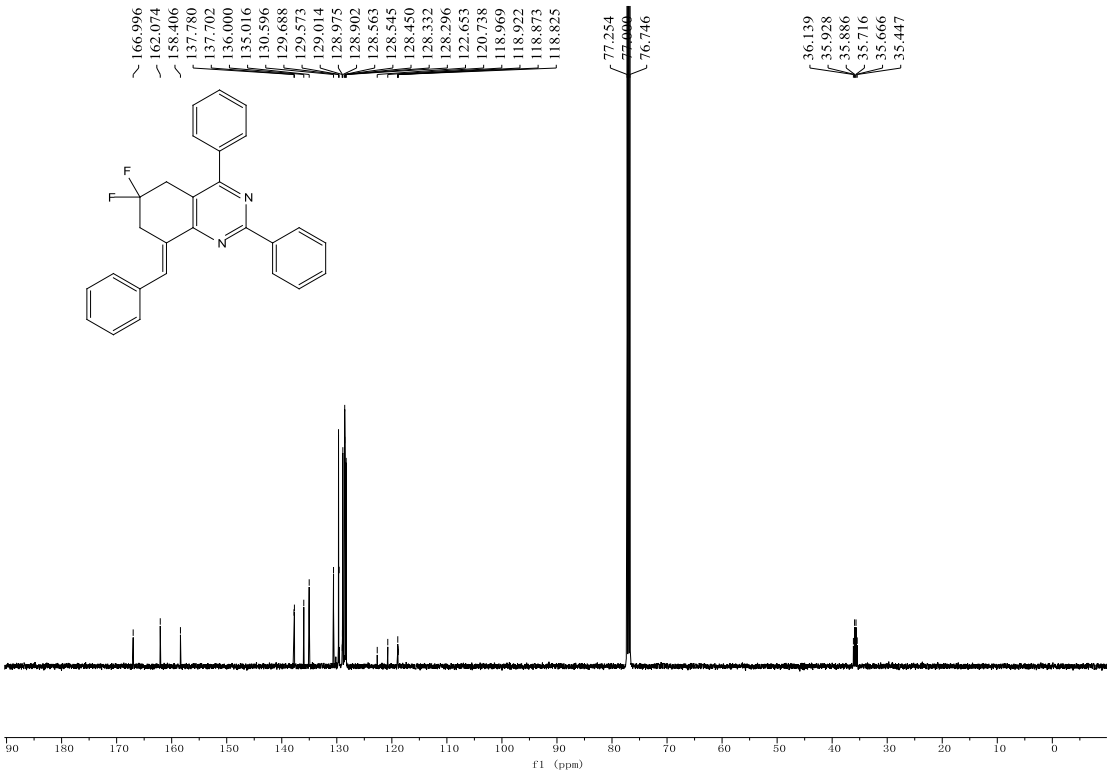
^{19}F NMR of **3e** (471 MHz, $CDCl_3$)



^{1}H NMR of **3f** (500 MHz, $CDCl_3$)

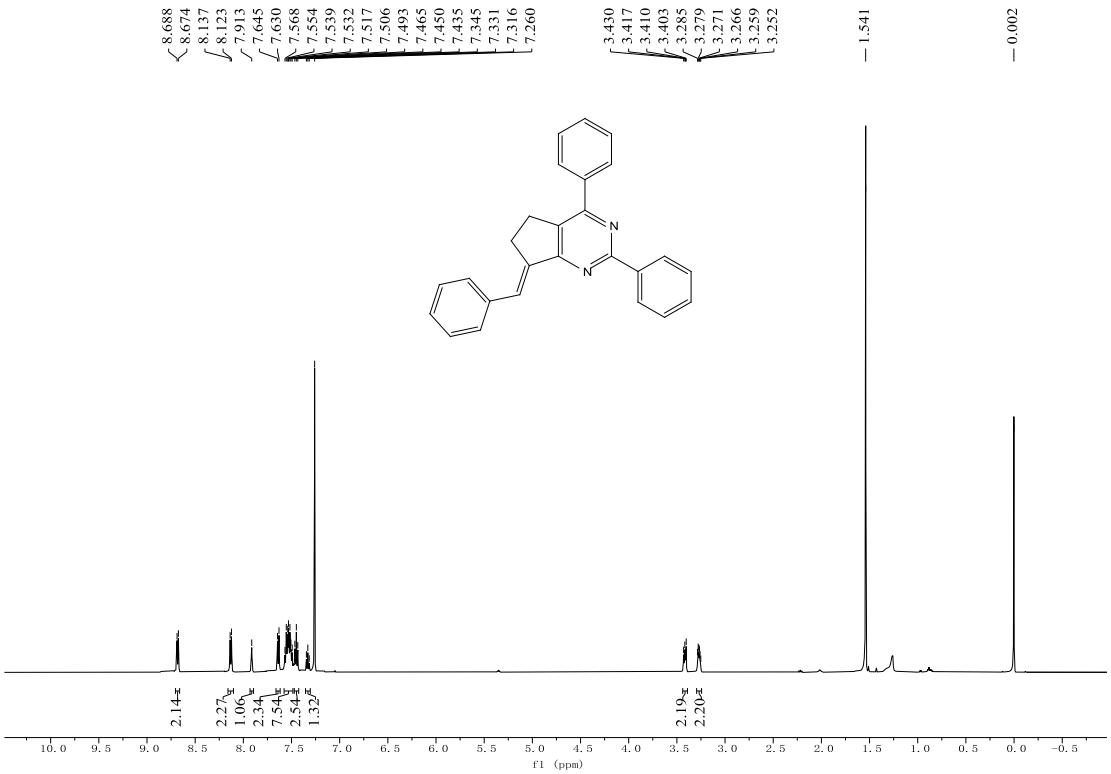


^{13}C NMR of **3f** (125 MHz, $CDCl_3$)

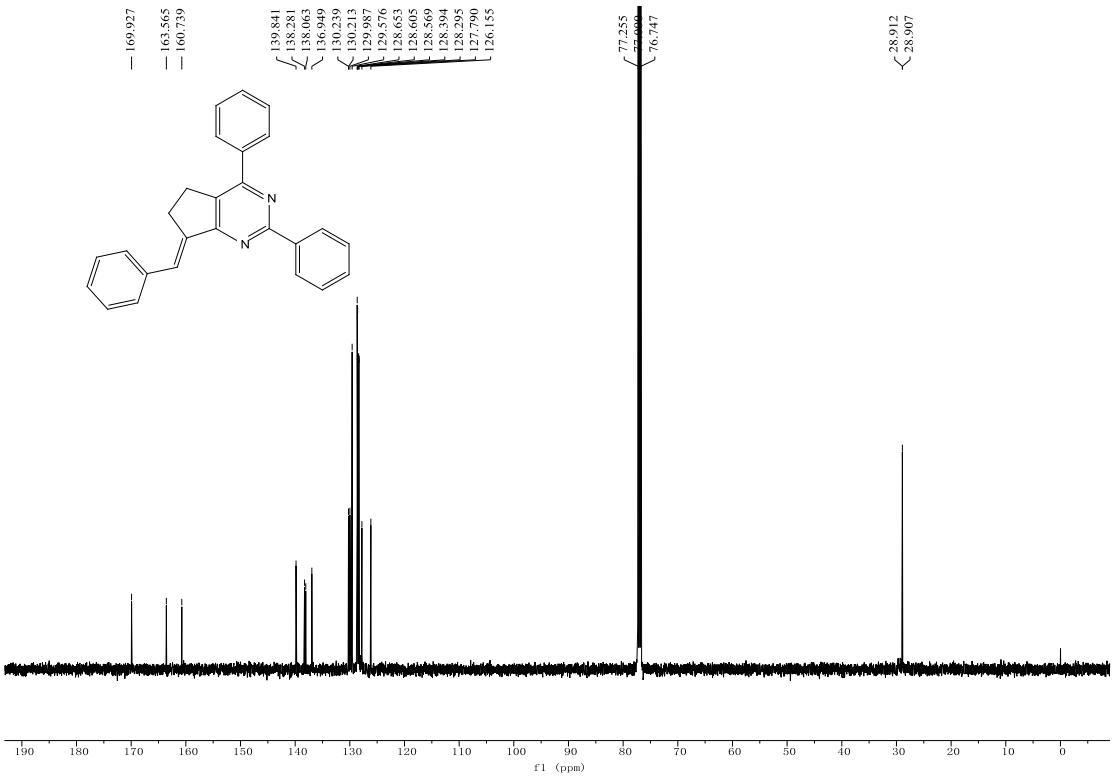


^{19}F NMR of **3f** (471 MHz, $CDCl_3$)

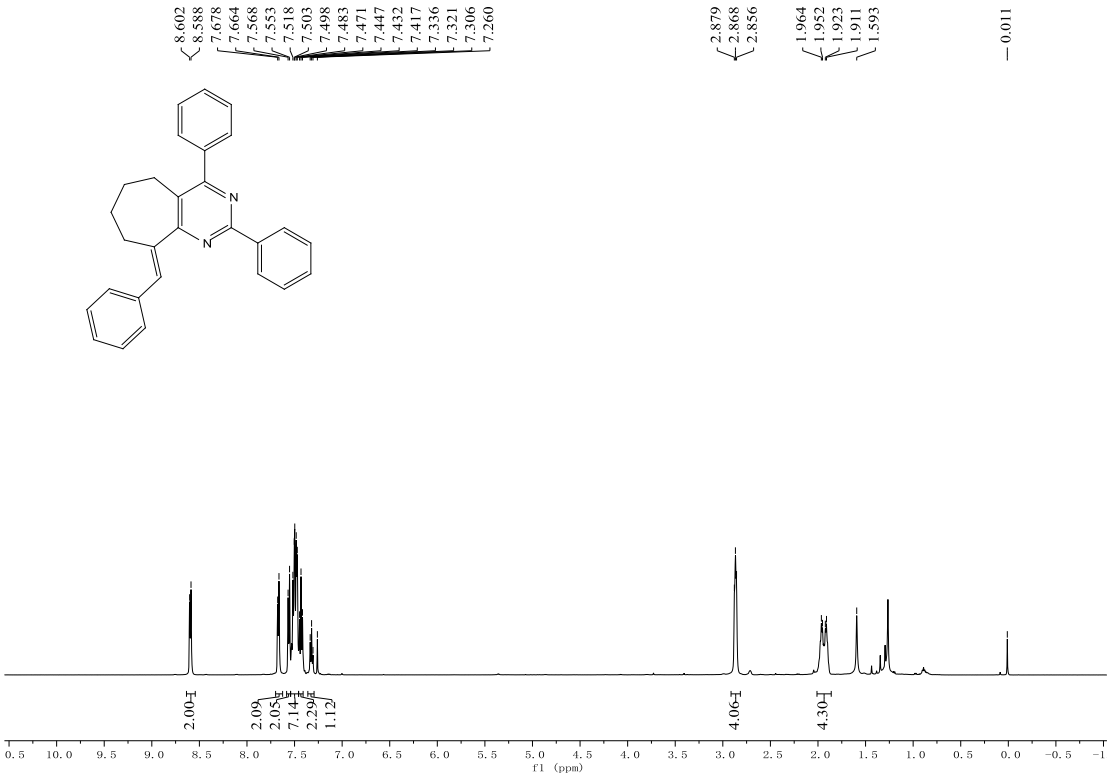
^{1}H NMR of **3g** (500 MHz, $CDCl_3$)



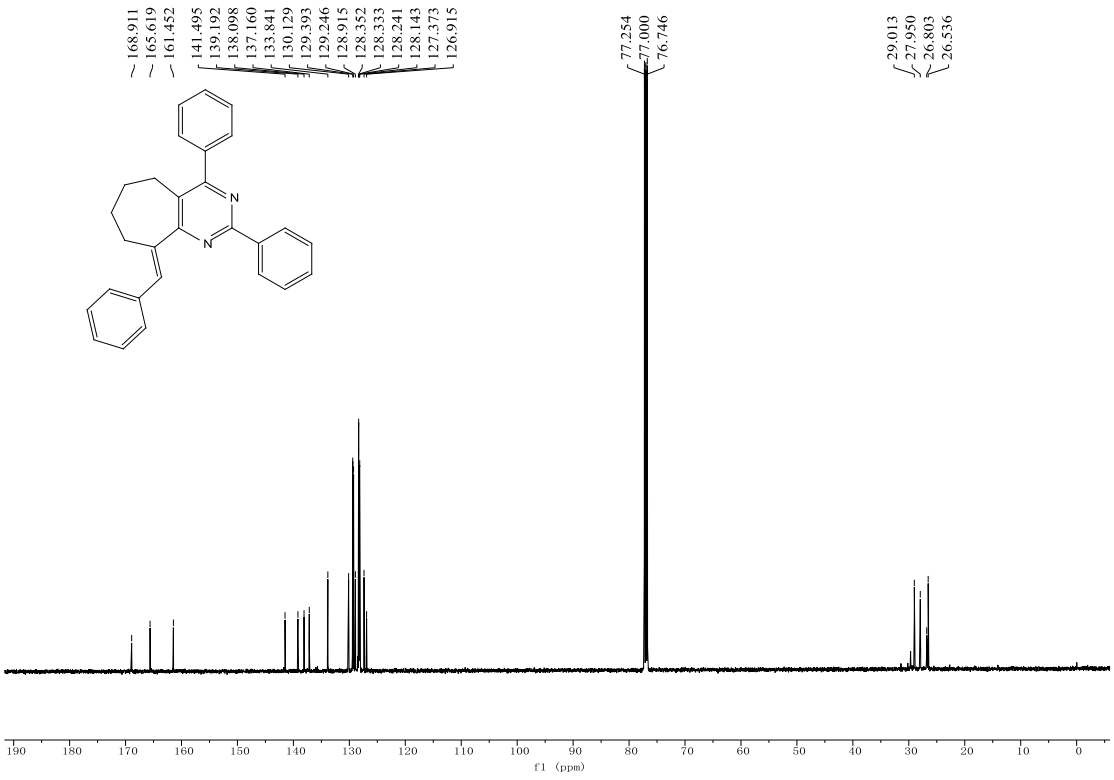
^{13}C NMR of **3g** (125 MHz, $CDCl_3$)



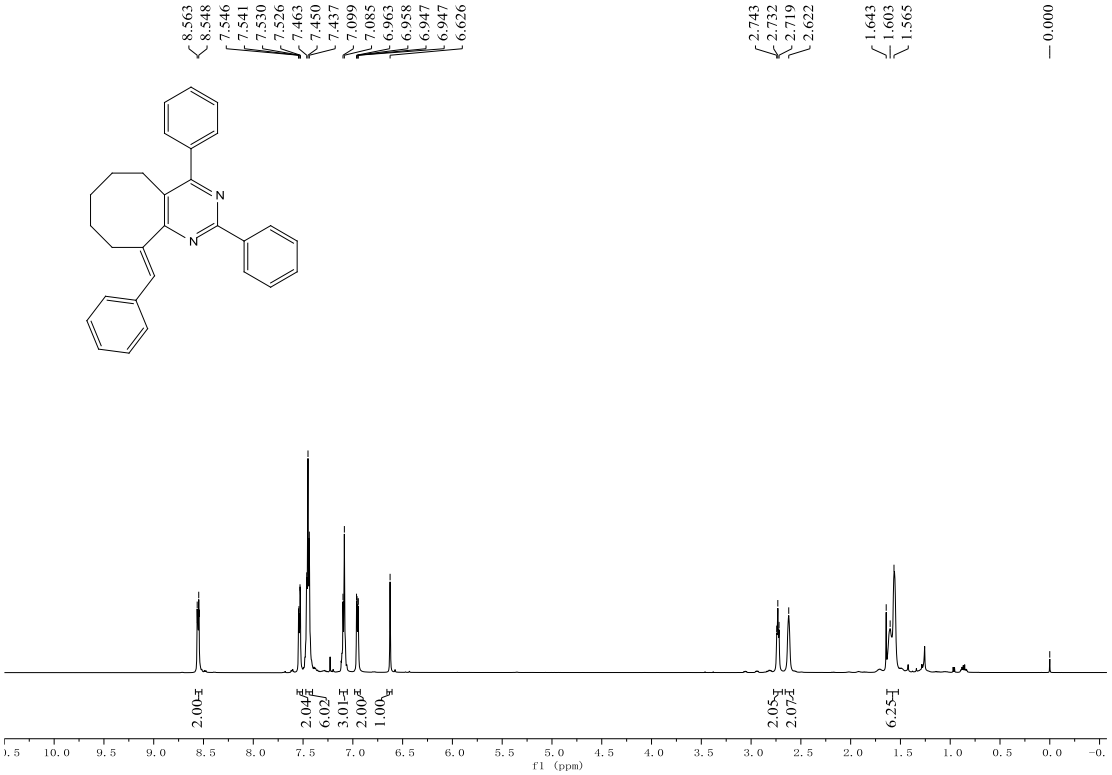
^{1}H NMR of **3h** (500 MHz, $CDCl_3$)



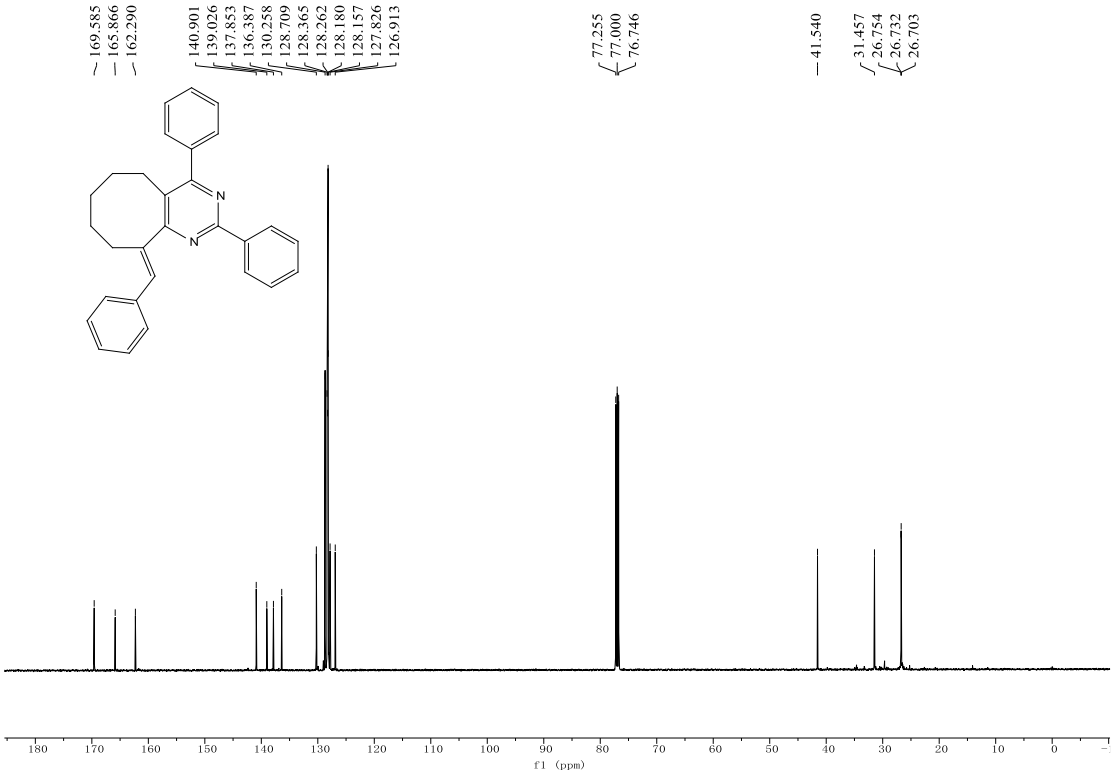
^{13}C NMR of **3h** (125 MHz, $CDCl_3$)



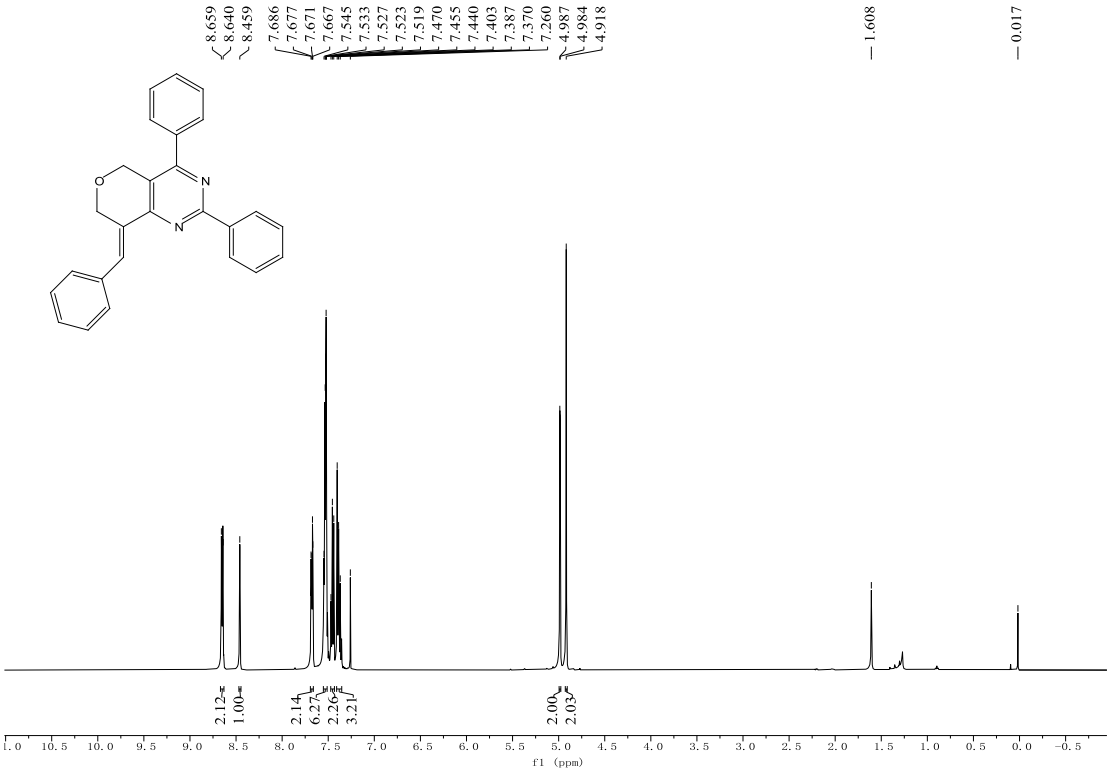
^{1}H NMR of **3i** (500 MHz, $CDCl_3$)



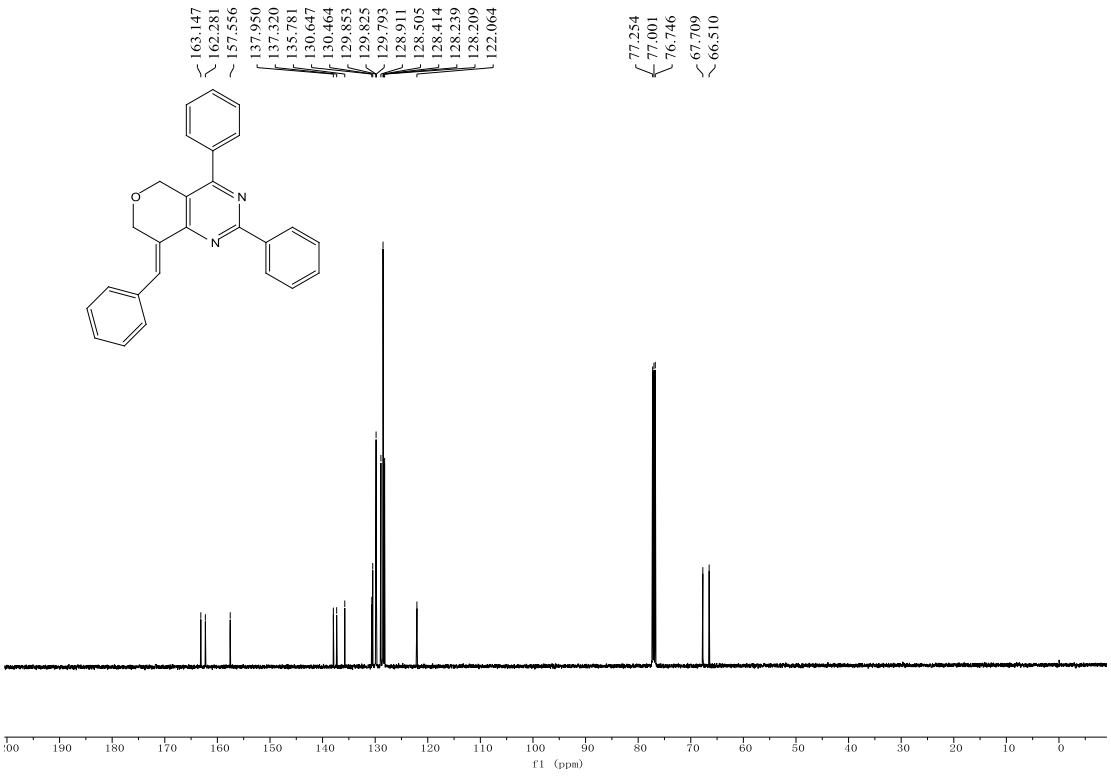
^{13}C NMR of **3i** (125 MHz, $CDCl_3$)



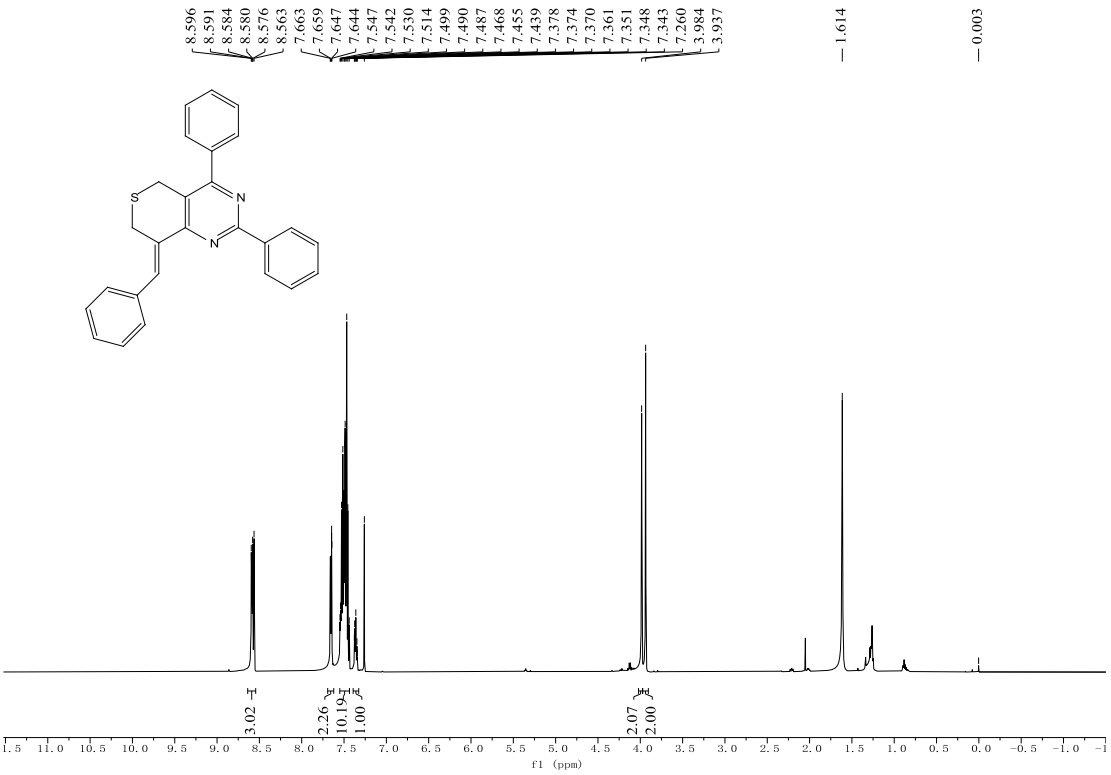
^{1}H NMR of **3j** (500 MHz, $CDCl_3$)



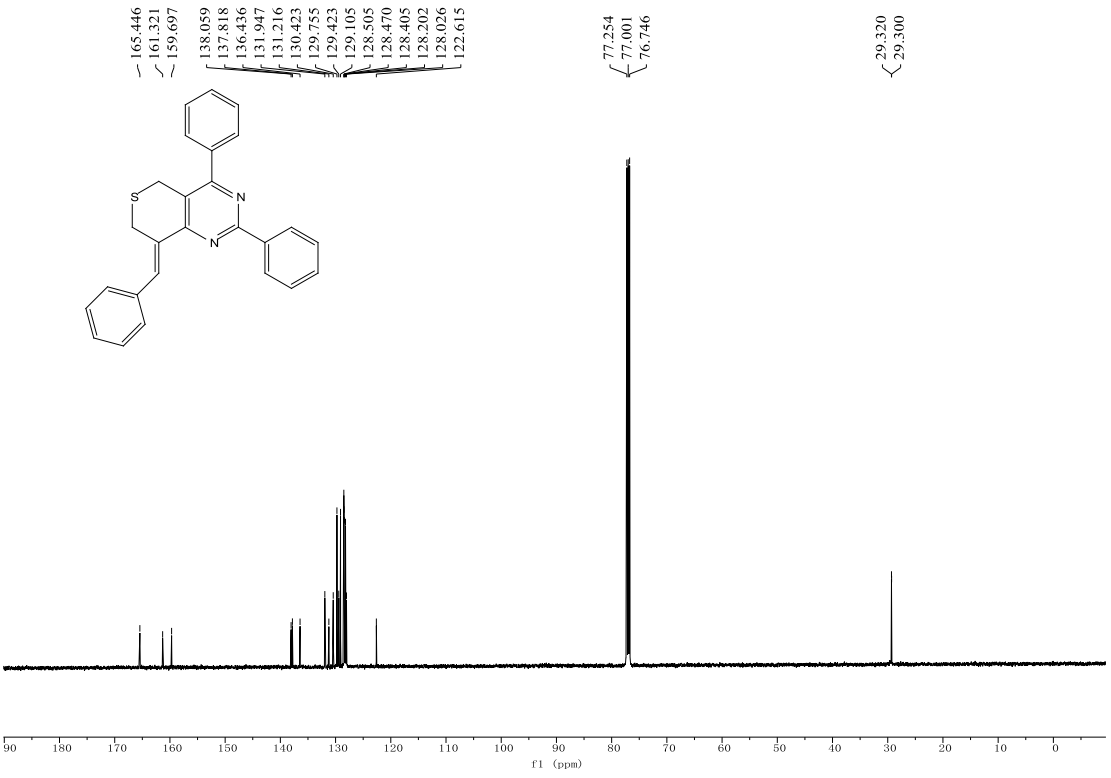
^{13}C NMR of **3j** (125 MHz, $CDCl_3$)



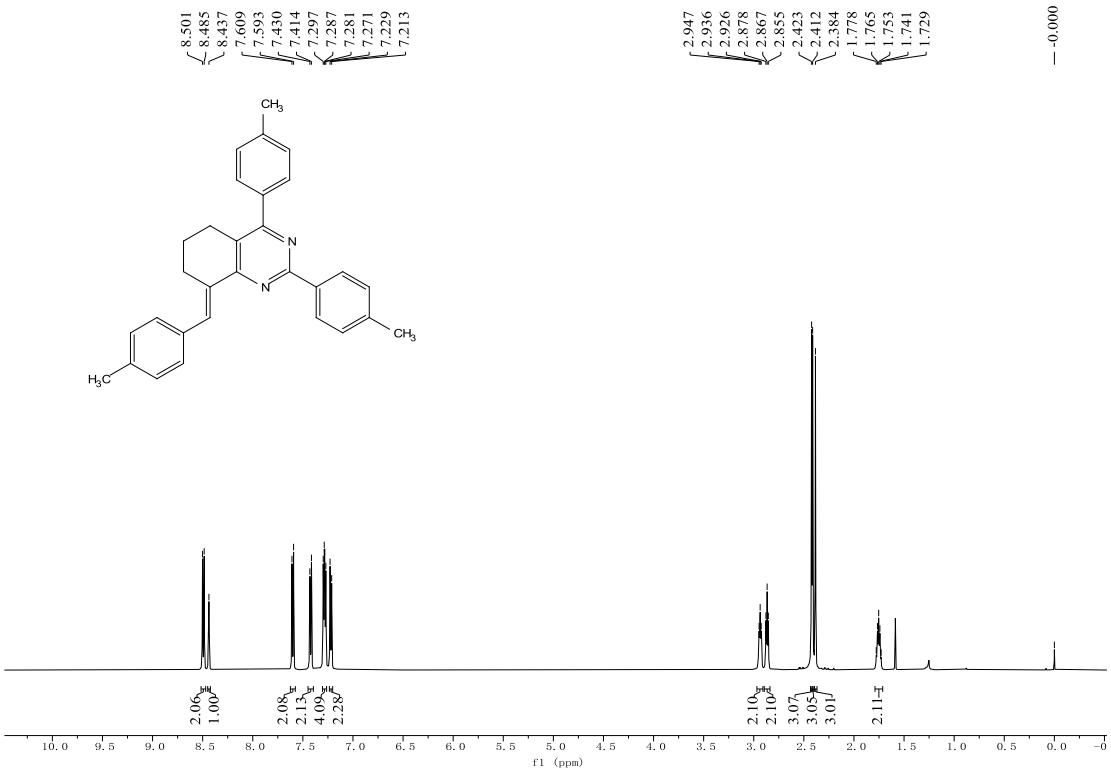
^{1}H NMR of **3k** (500 MHz, $CDCl_3$)



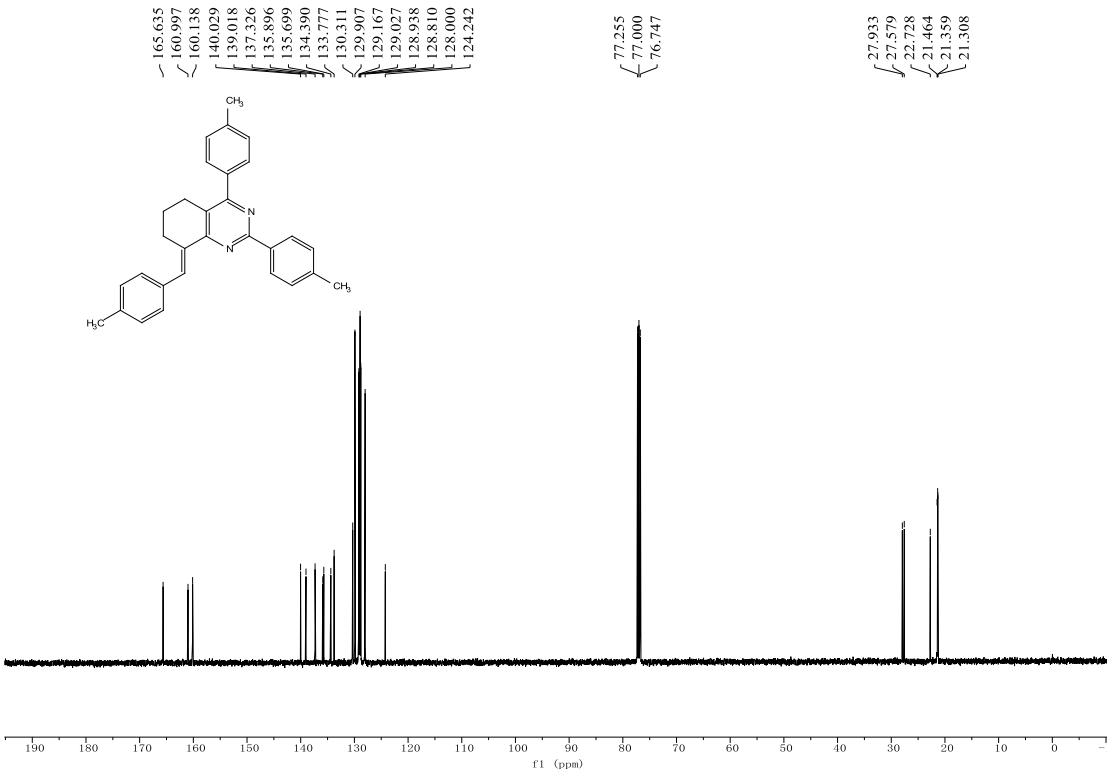
^{13}C NMR of **3k** (125 MHz, $CDCl_3$)



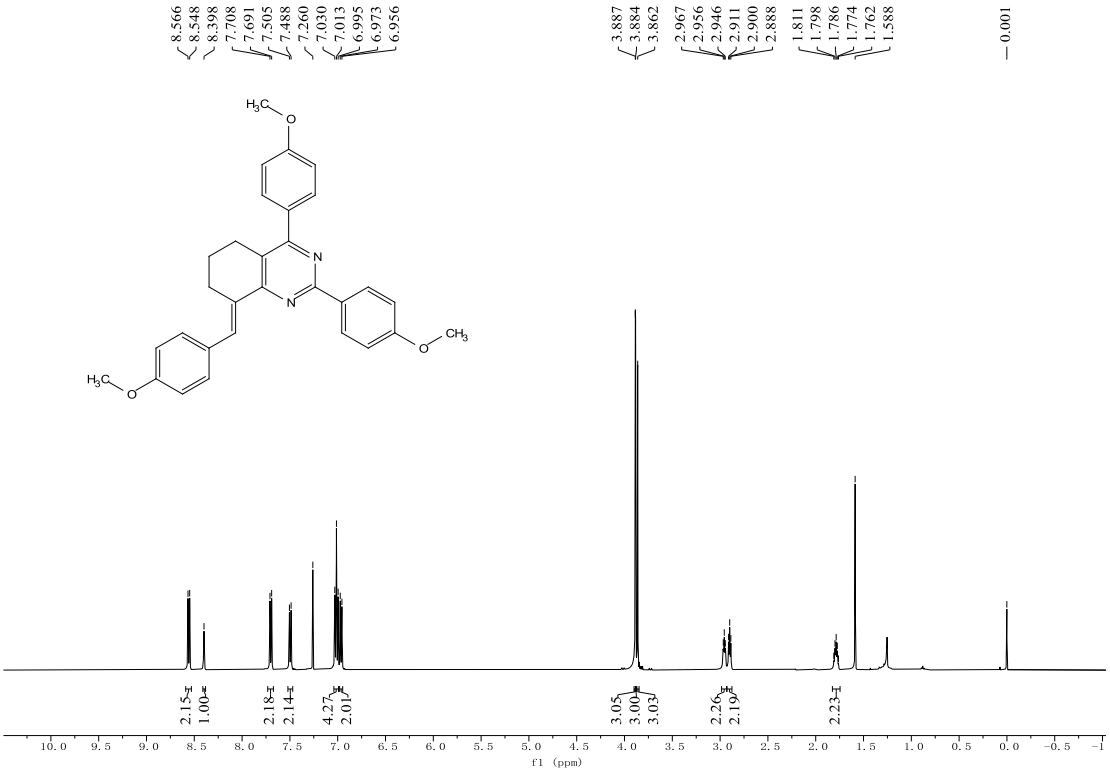
^{1}H NMR of **3l** (500 MHz, $CDCl_3$)



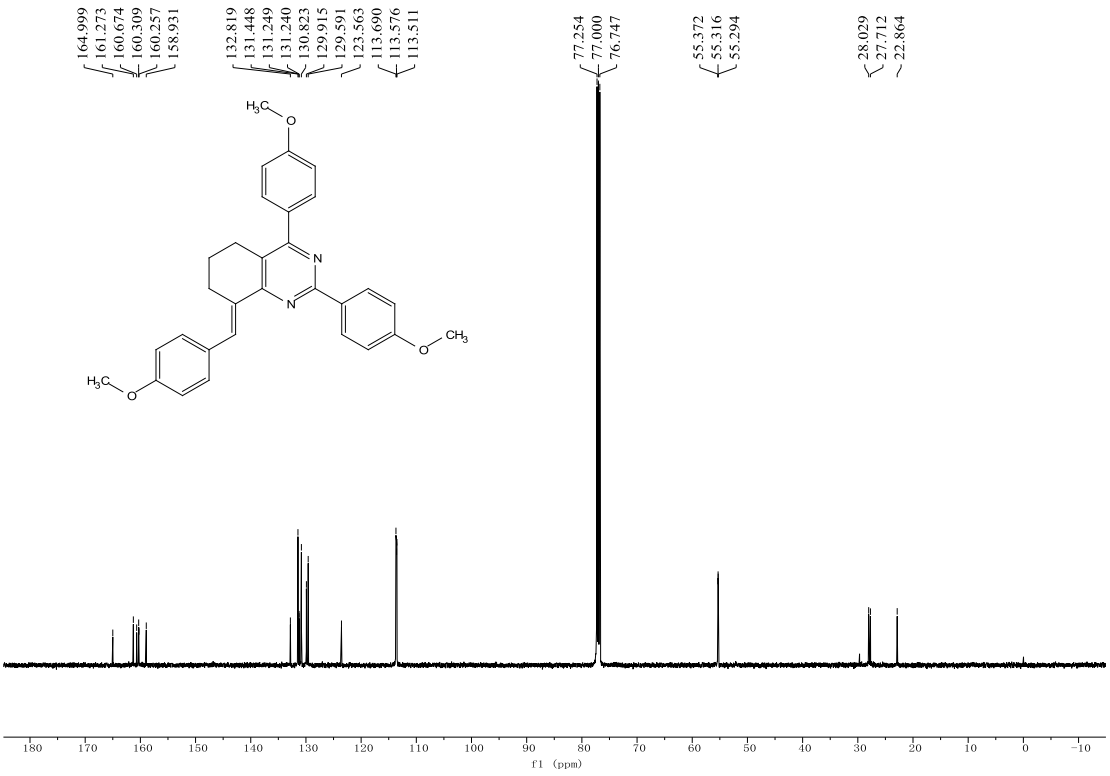
^{13}C NMR of **3l** (125 MHz, $CDCl_3$)



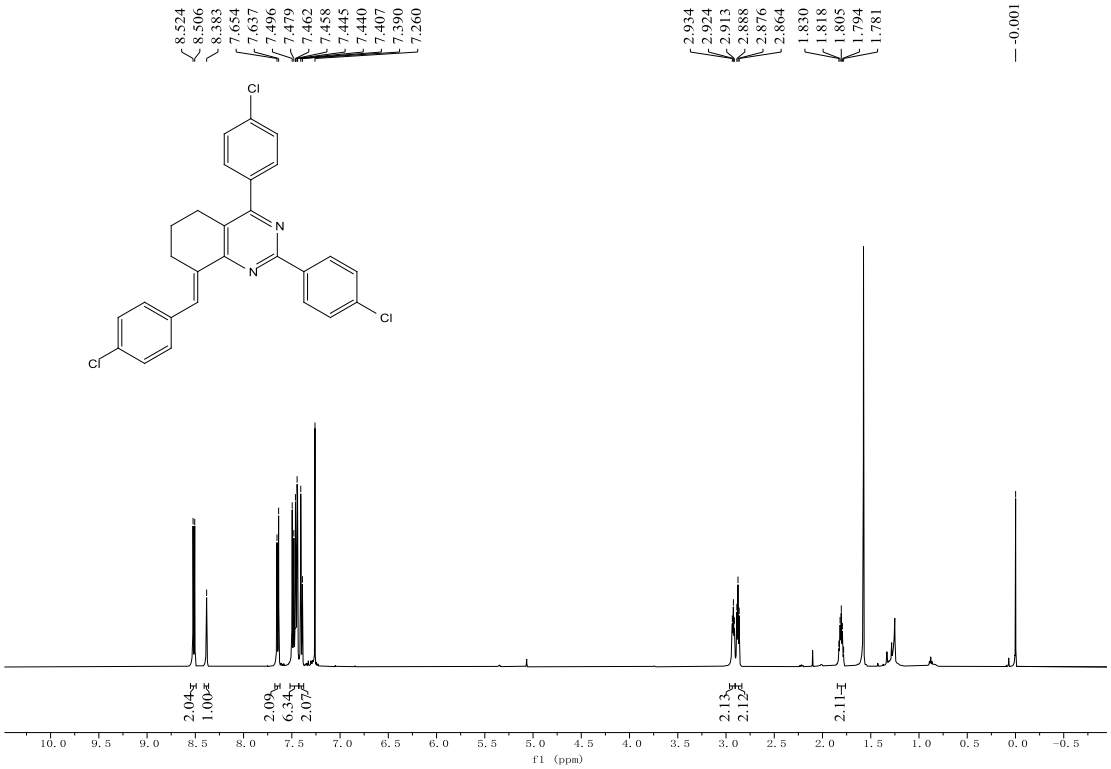
^{1}H NMR of **3m** (500 MHz, $CDCl_3$)



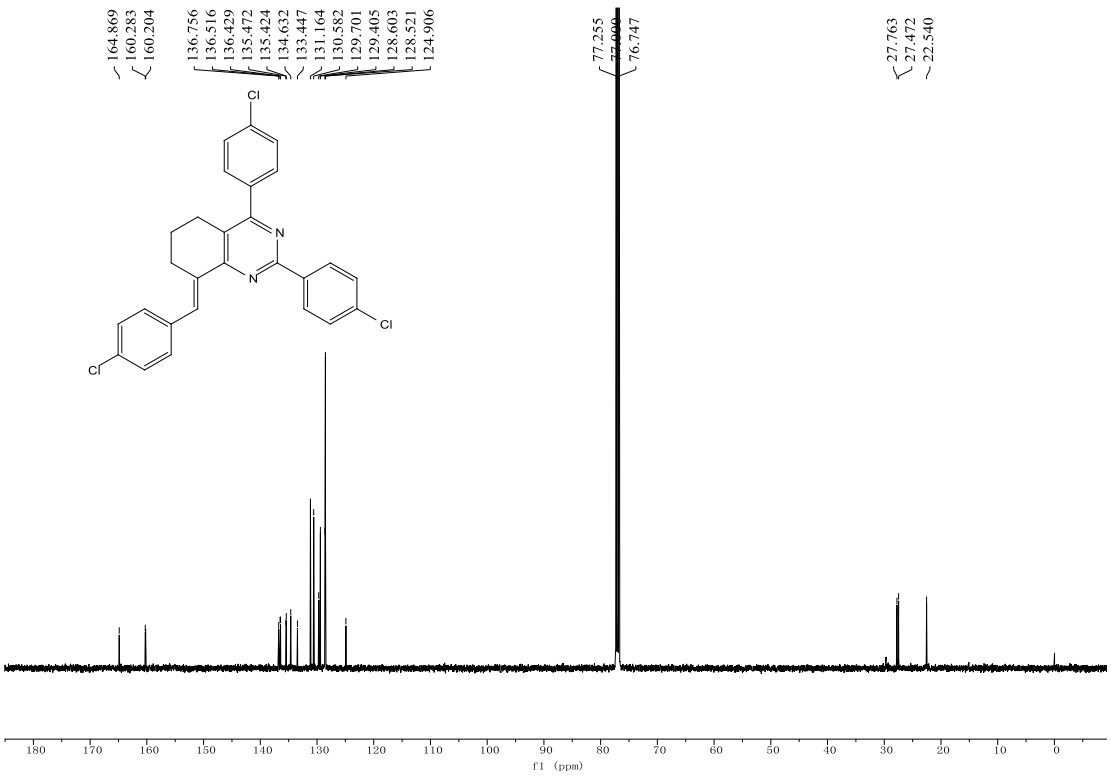
^{13}C NMR of **3m** (125 MHz, $CDCl_3$)



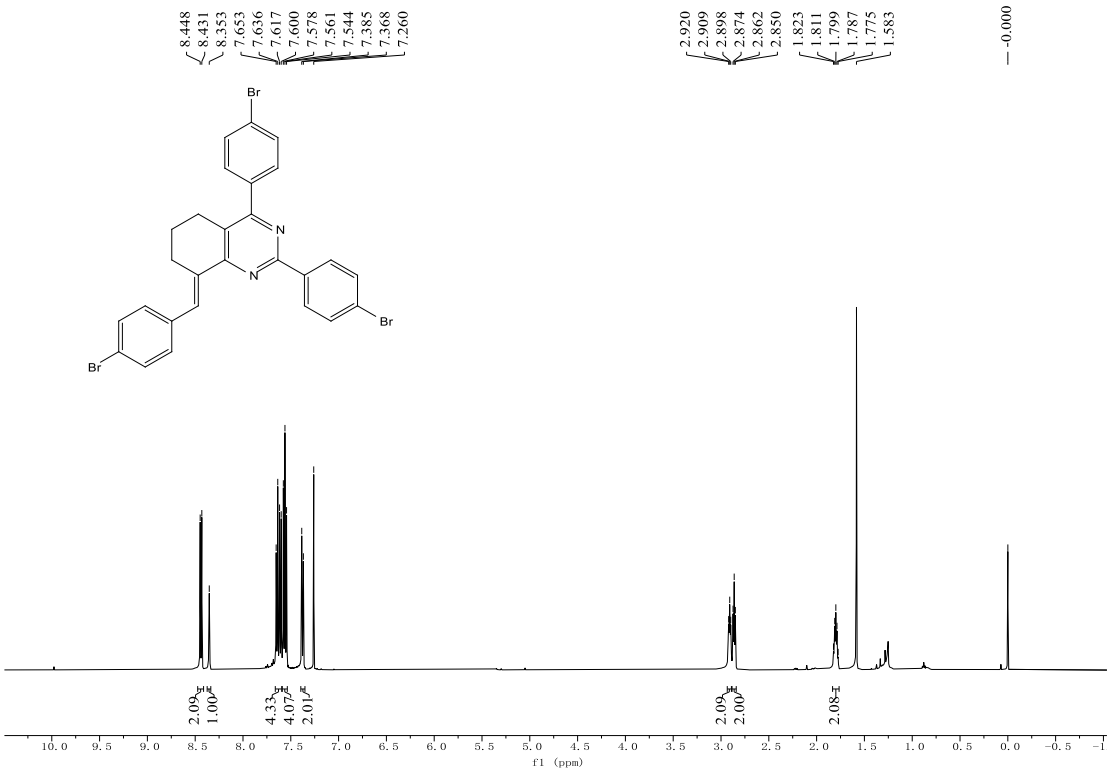
^{1}H NMR of **3n** (500 MHz, $CDCl_3$)



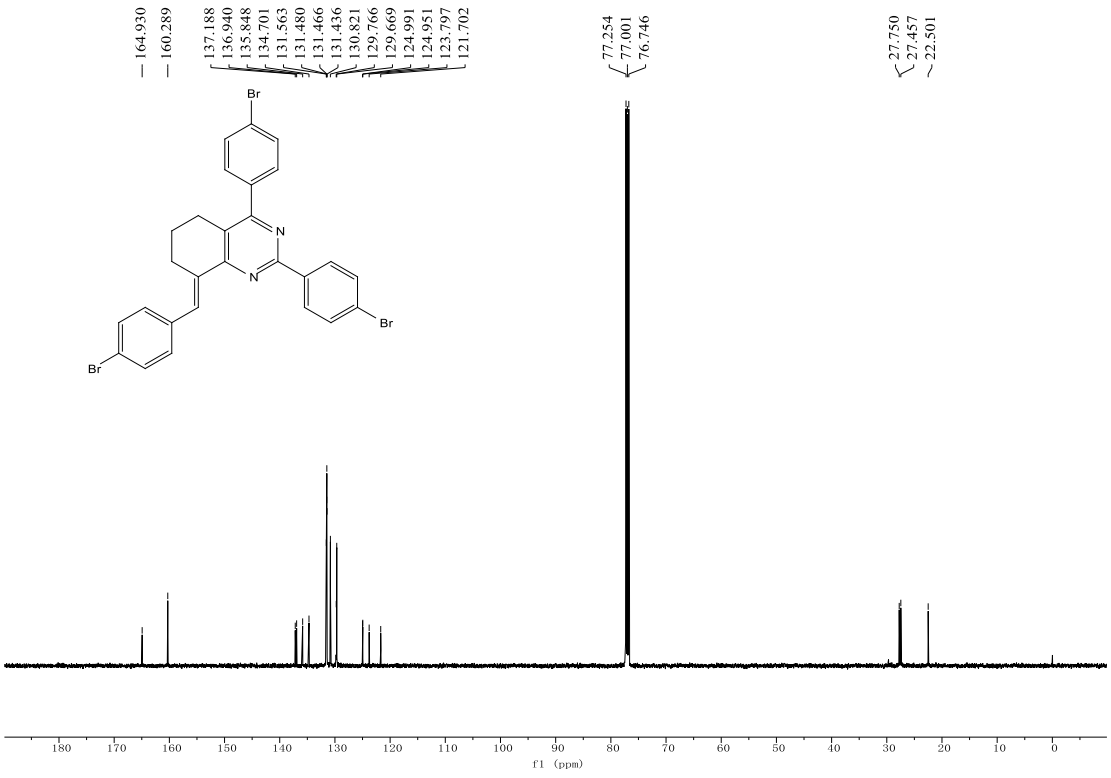
^{13}C NMR of **3n** (125 MHz, $CDCl_3$)



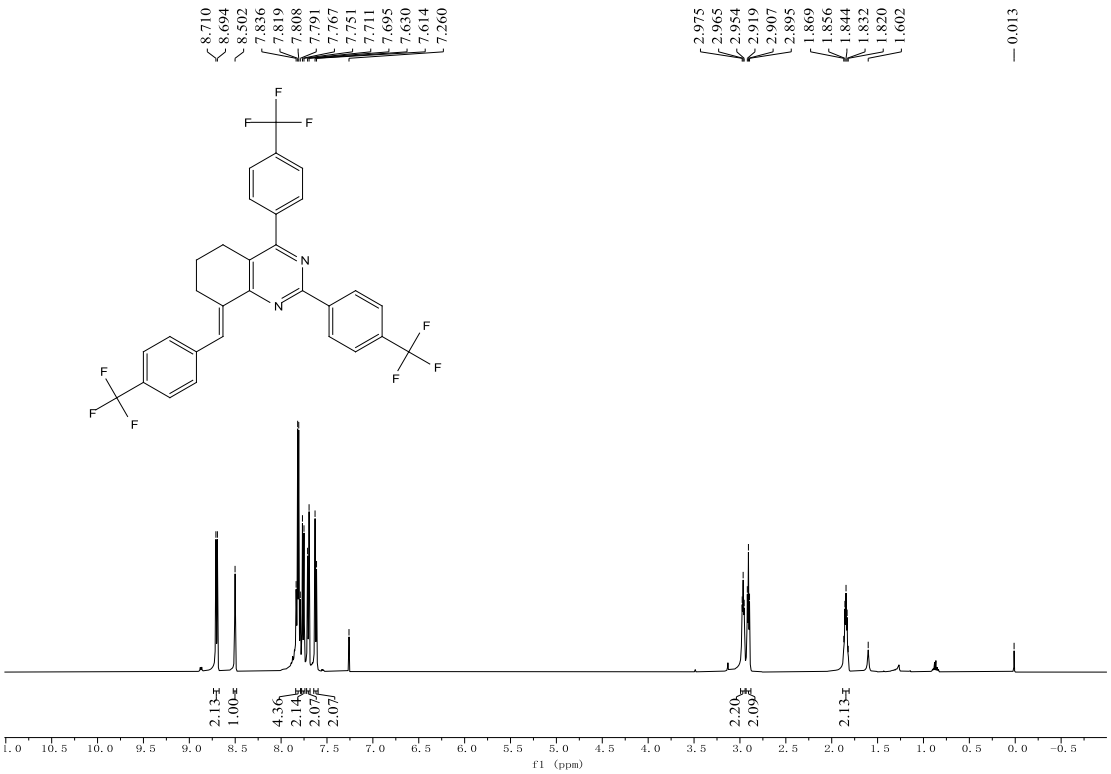
^{1}H NMR of **3o** (500 MHz, $CDCl_3$)



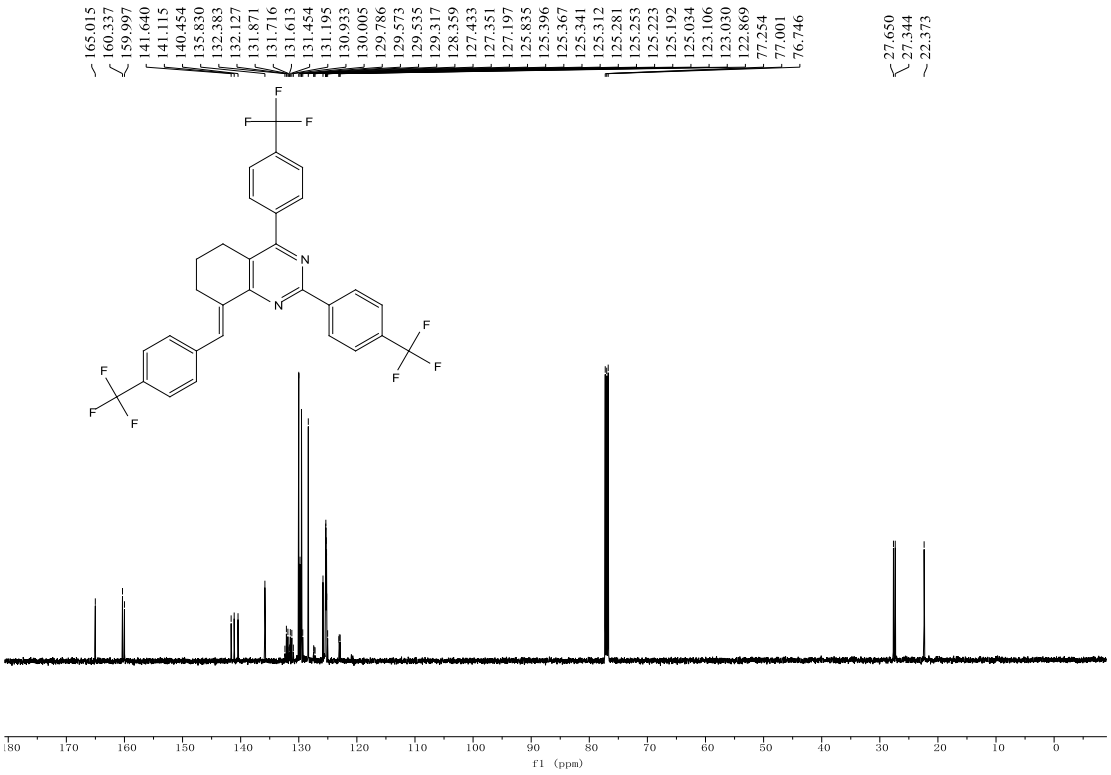
^{13}C NMR of **3o** (125 MHz, $CDCl_3$)



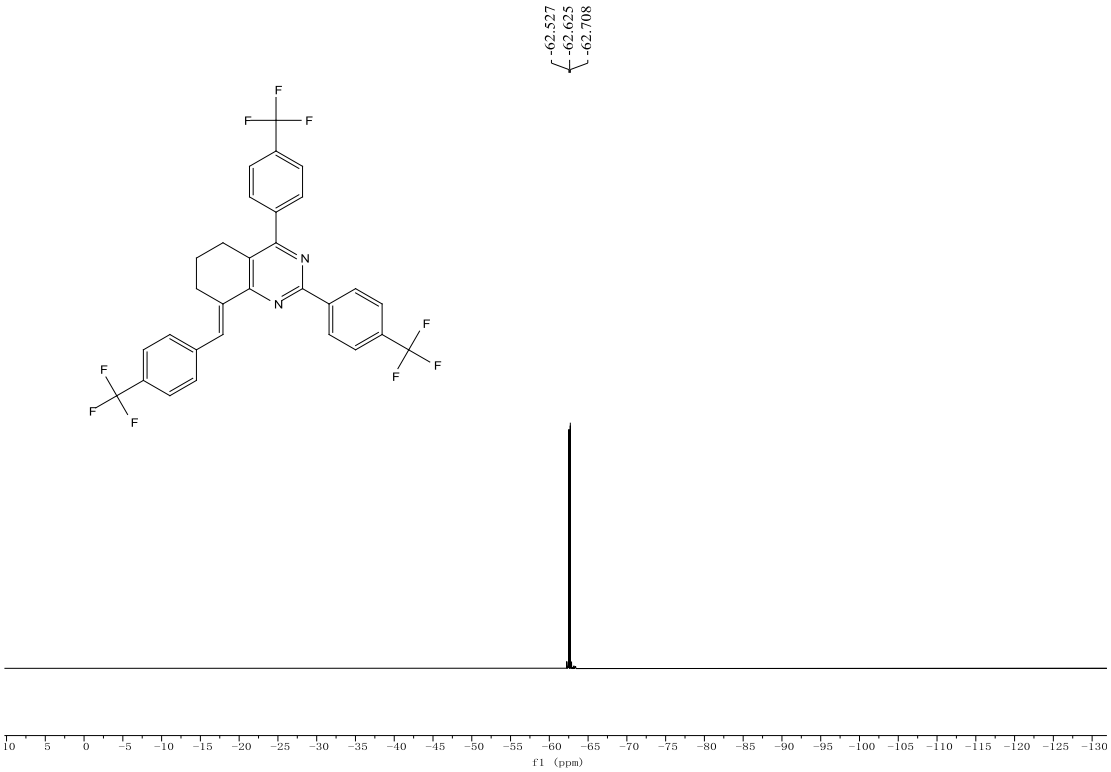
^{1}H NMR of **3p** (500 MHz, $CDCl_3$)



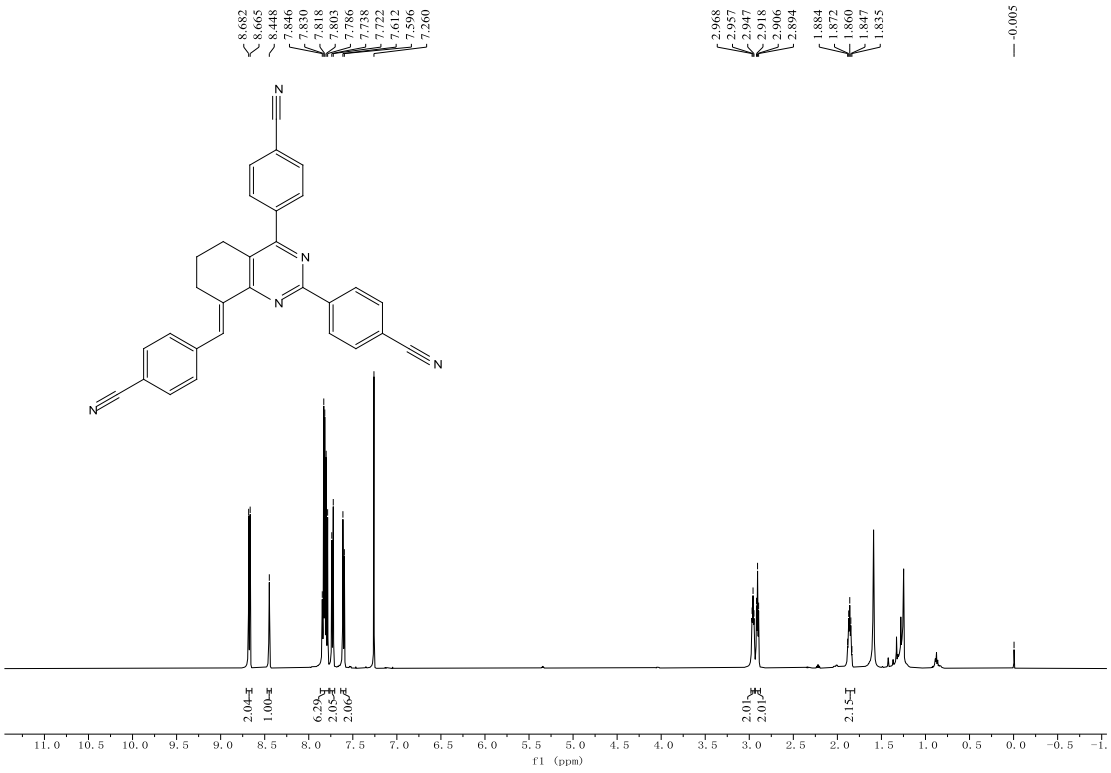
^{13}C NMR of **3p** (125 MHz, $CDCl_3$)



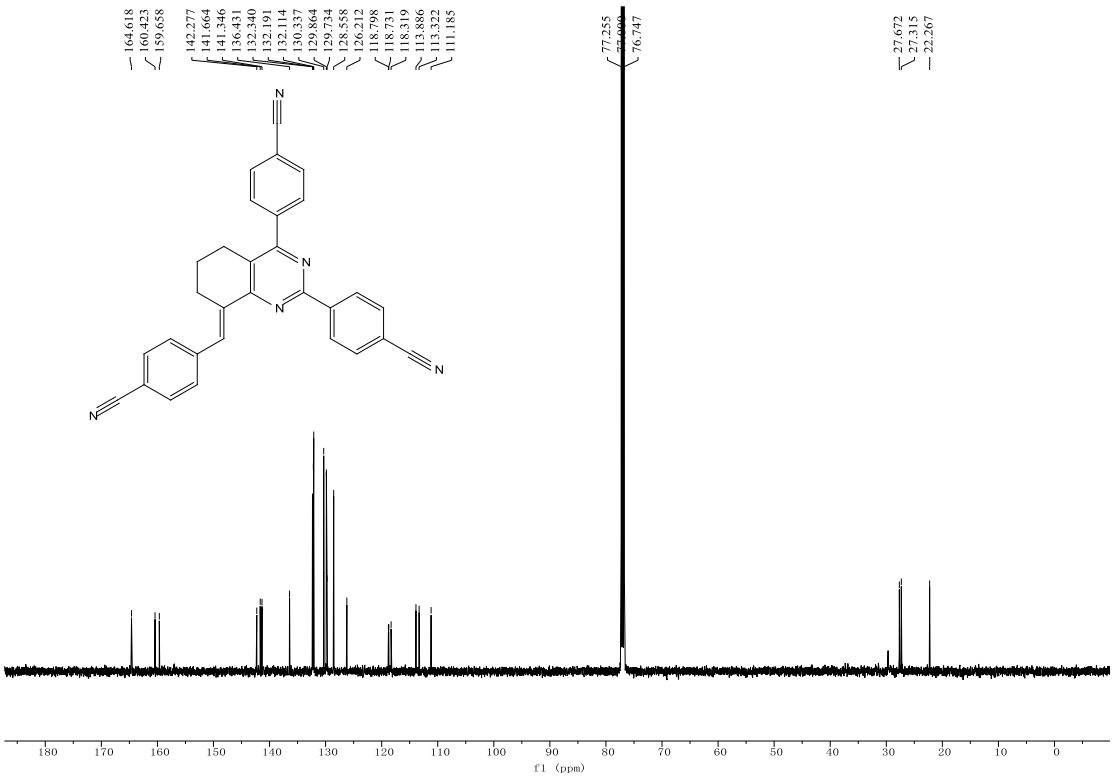
^{19}F NMR of **3p** (471 MHz, $CDCl_3$)



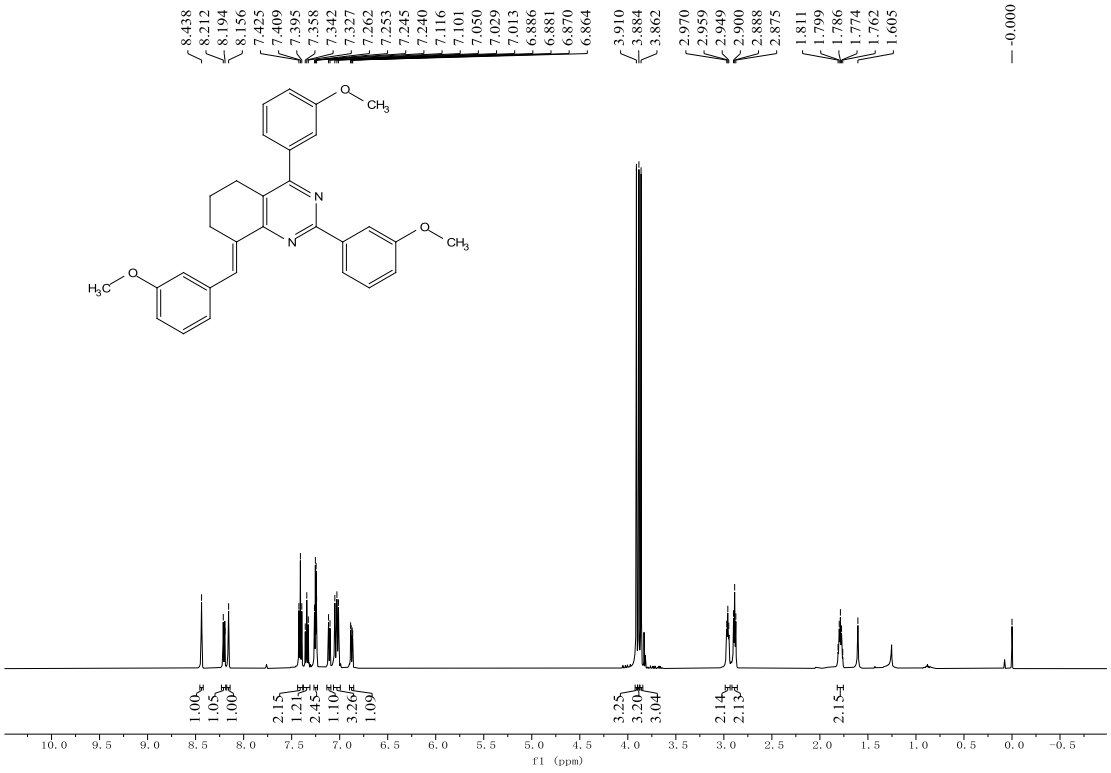
^{1}H NMR of **3q** (500 MHz, $CDCl_3$)



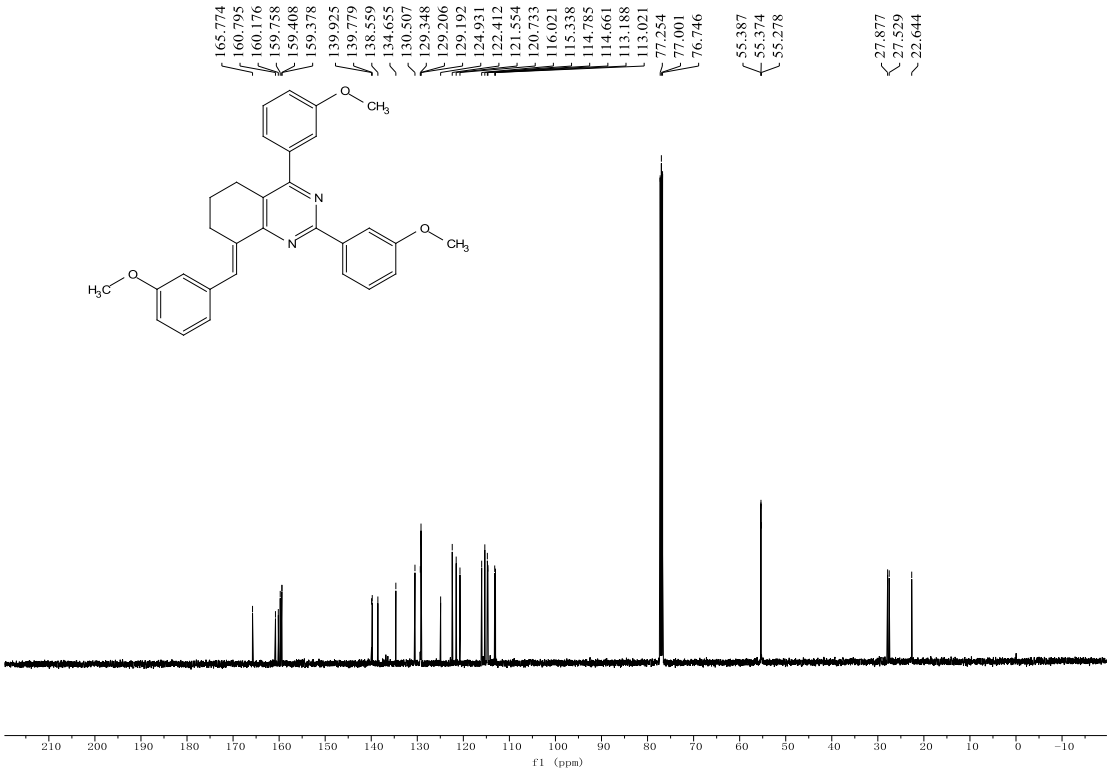
^{13}C NMR of **3q** (125 MHz, $CDCl_3$)



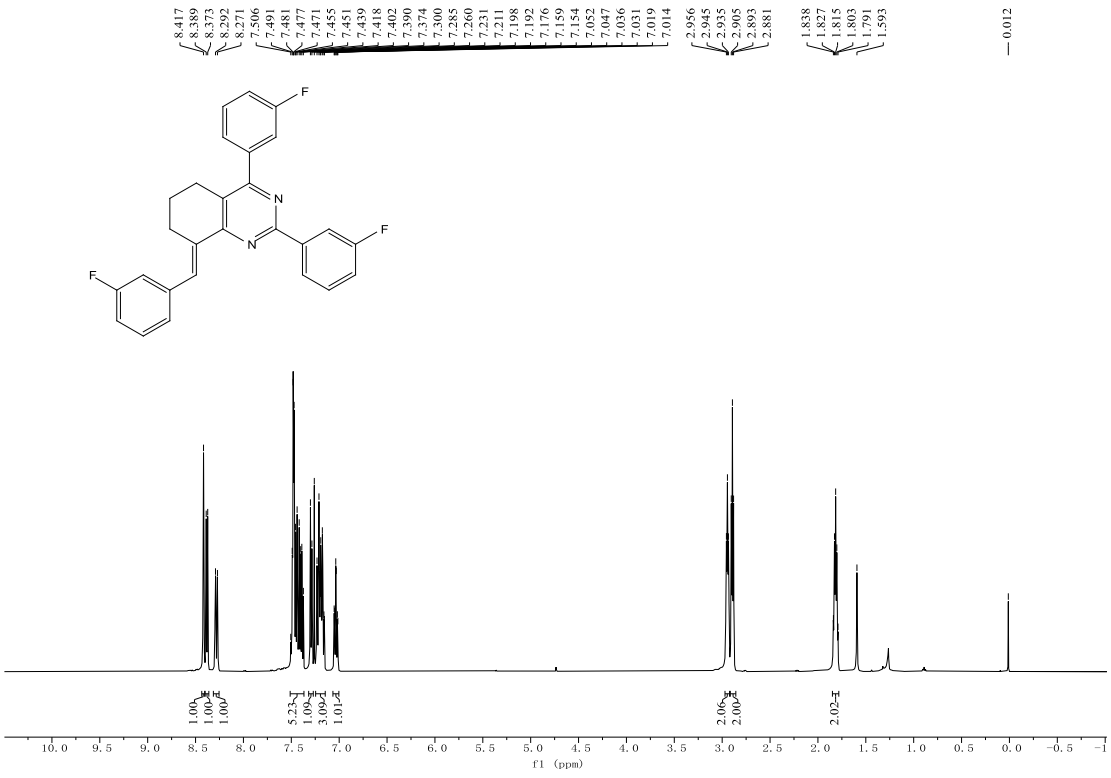
^{1}H NMR of **3r** (500 MHz, $CDCl_3$)



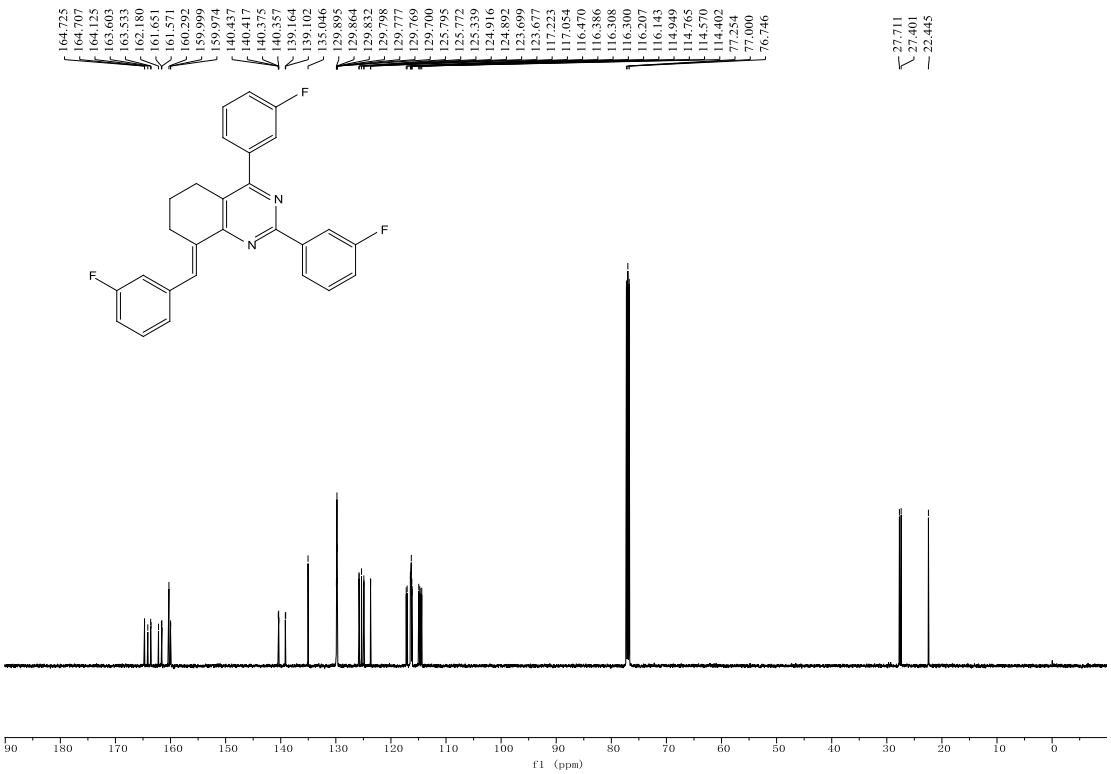
^{13}C NMR of **3r** (125 MHz, $CDCl_3$)



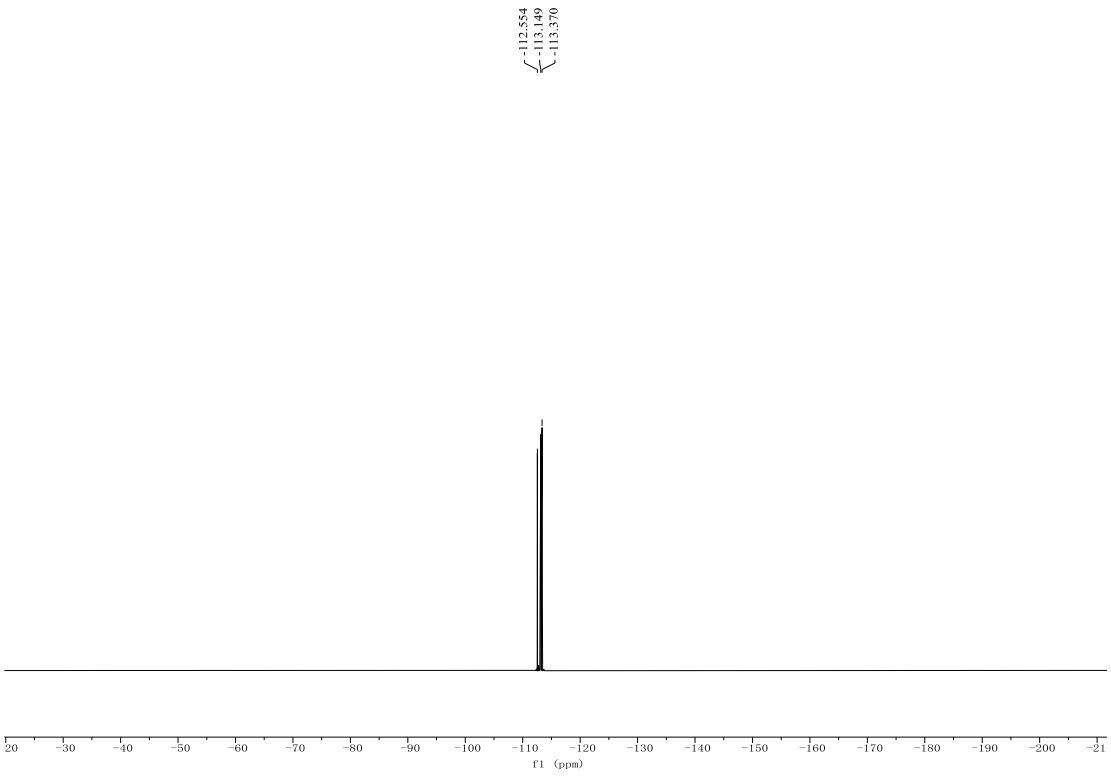
^{1}H NMR of **3s** (500 MHz, $CDCl_3$)



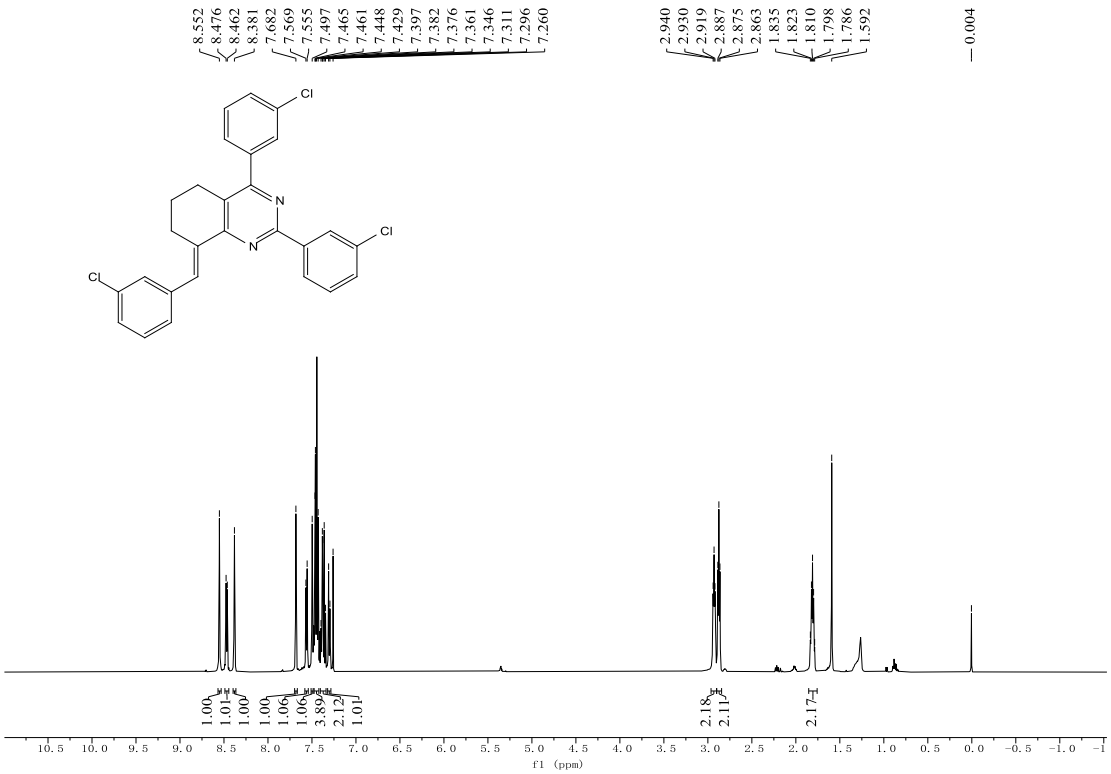
^{13}C NMR of **3s** (125 MHz, $CDCl_3$)



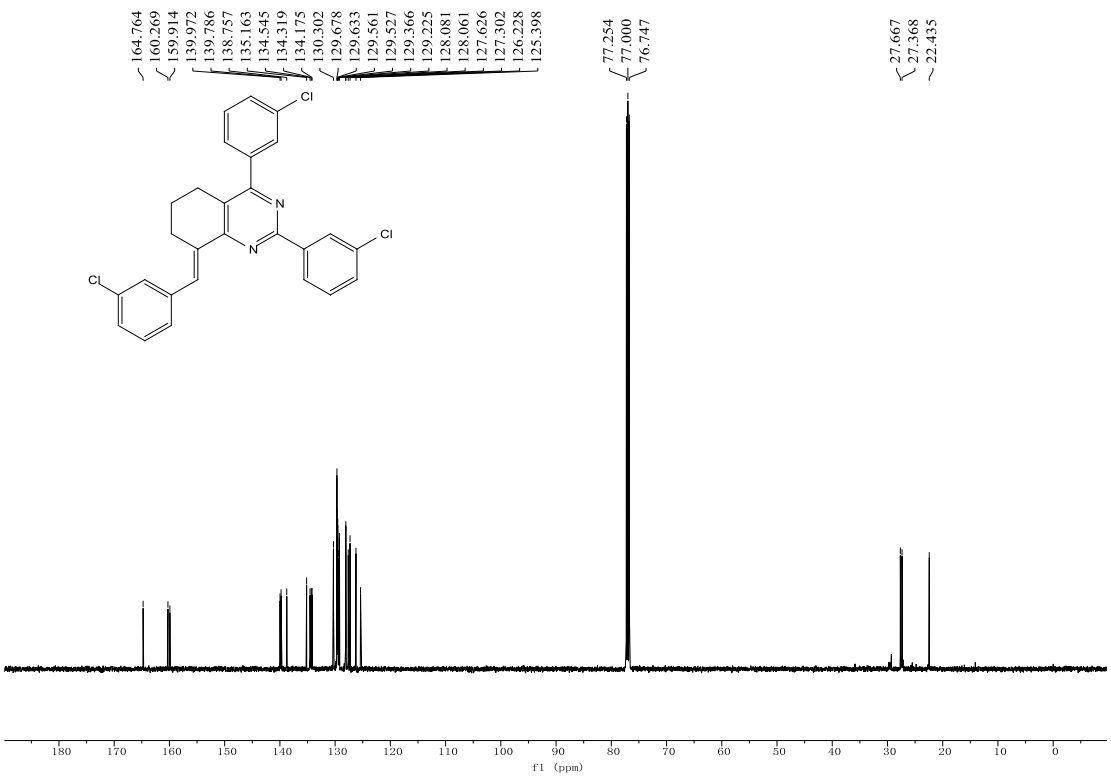
^{19}F NMR of **3s** (471 MHz, $CDCl_3$)



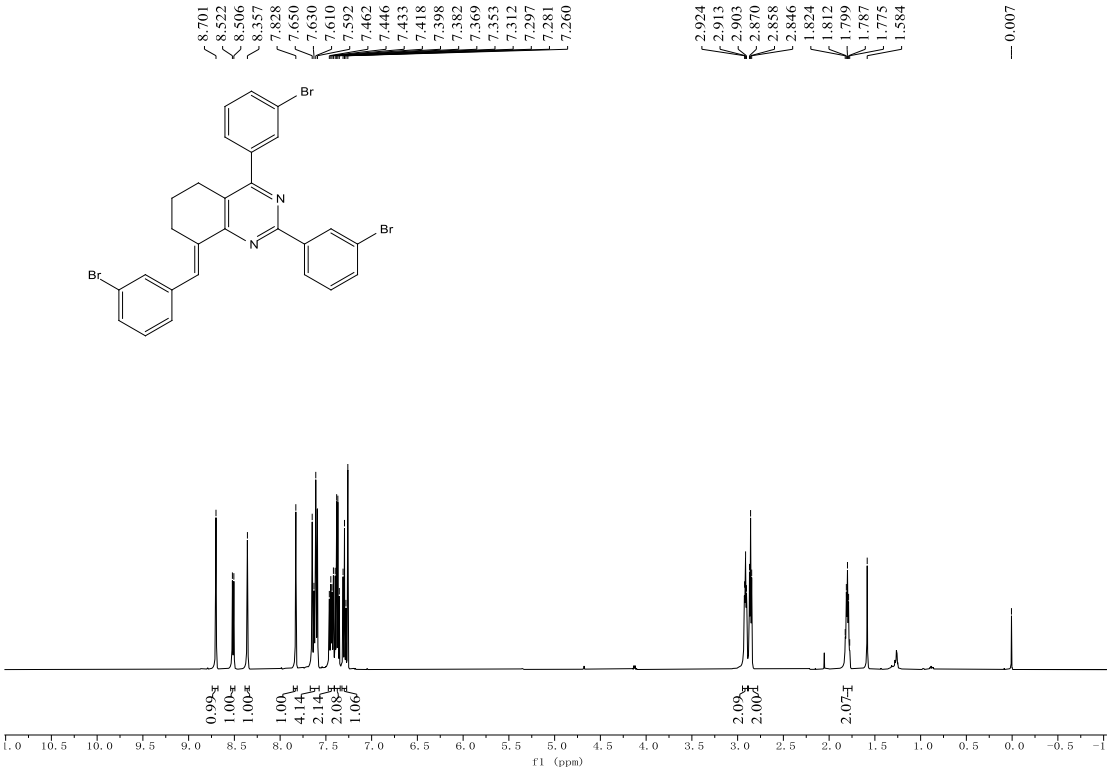
^{1}H NMR of **3t** (500 MHz, $CDCl_3$)



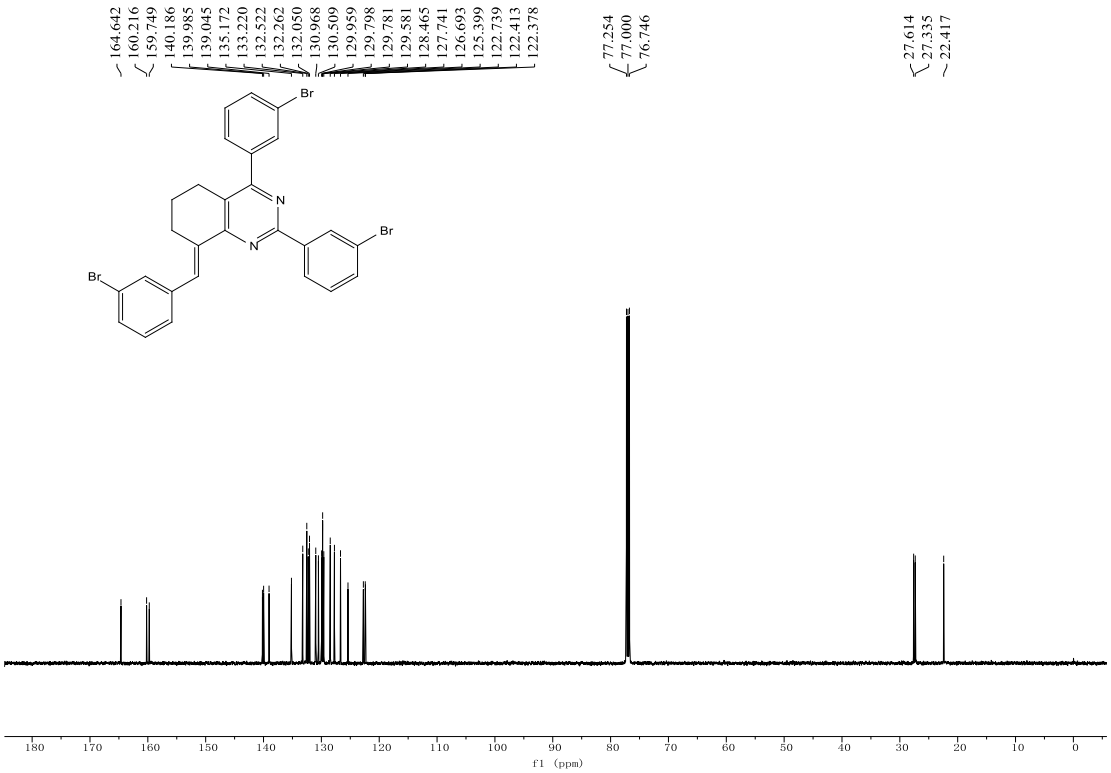
^{13}C NMR of **3t** (125 MHz, $CDCl_3$)



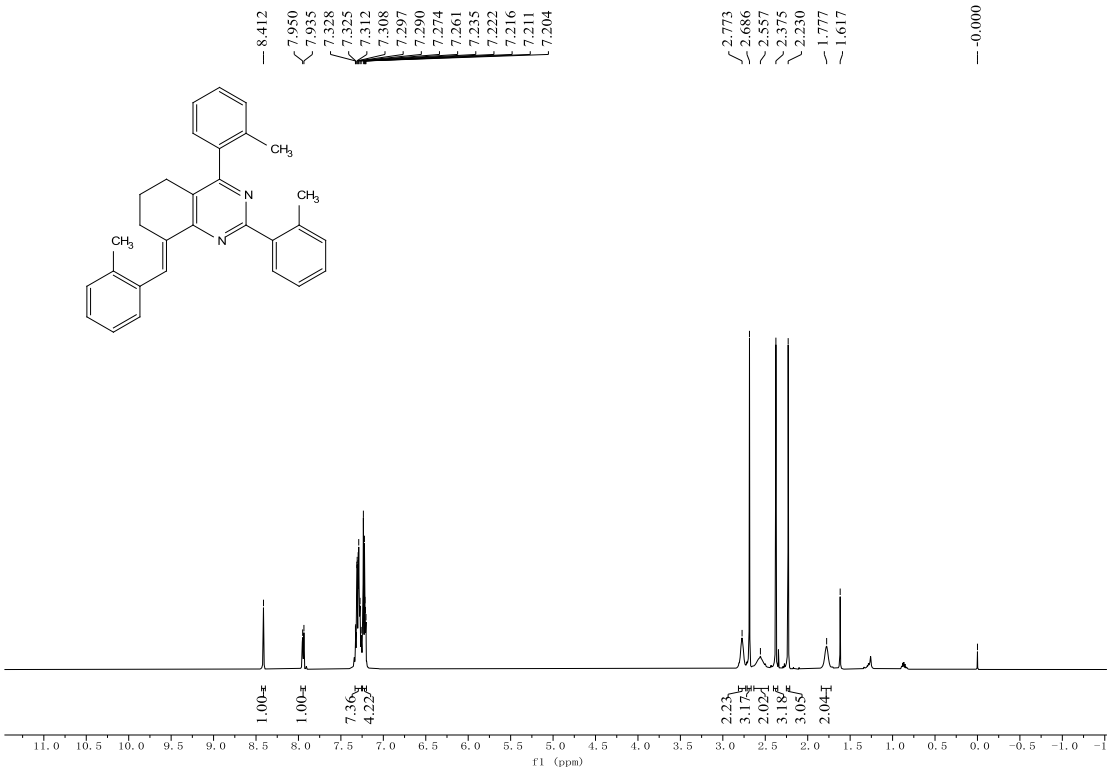
^{1}H NMR of **3u** (500 MHz, $CDCl_3$)



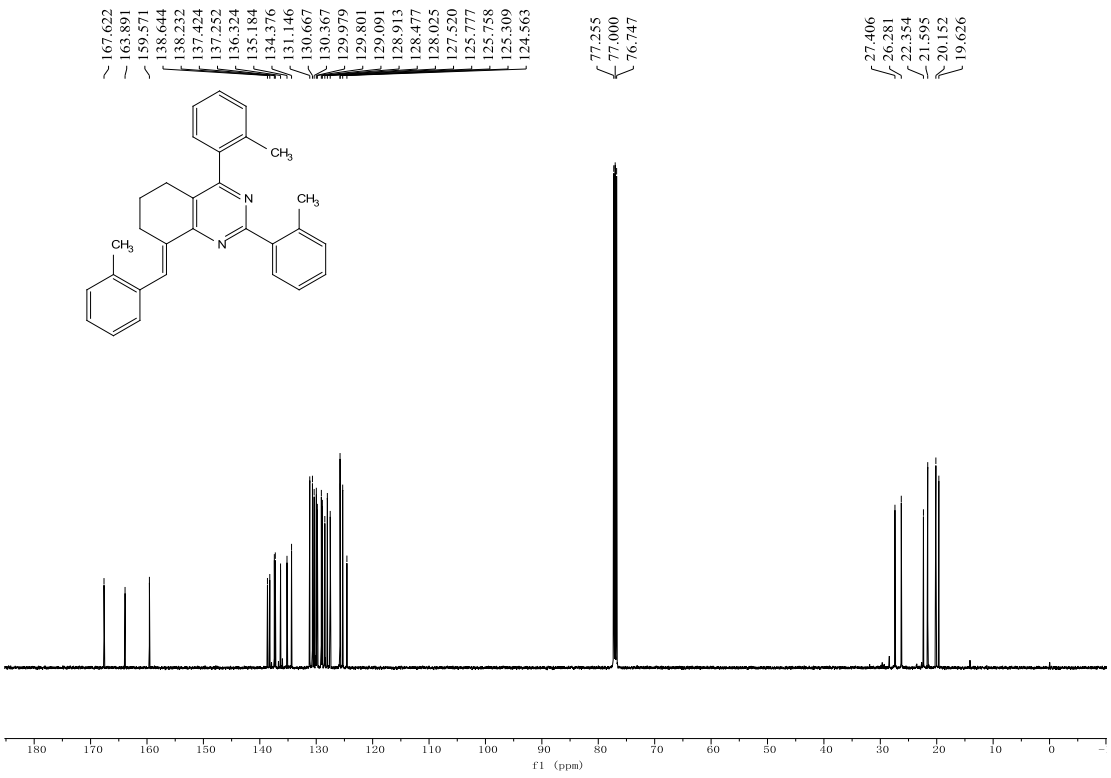
^{13}C NMR of **3u** (125 MHz, $CDCl_3$)



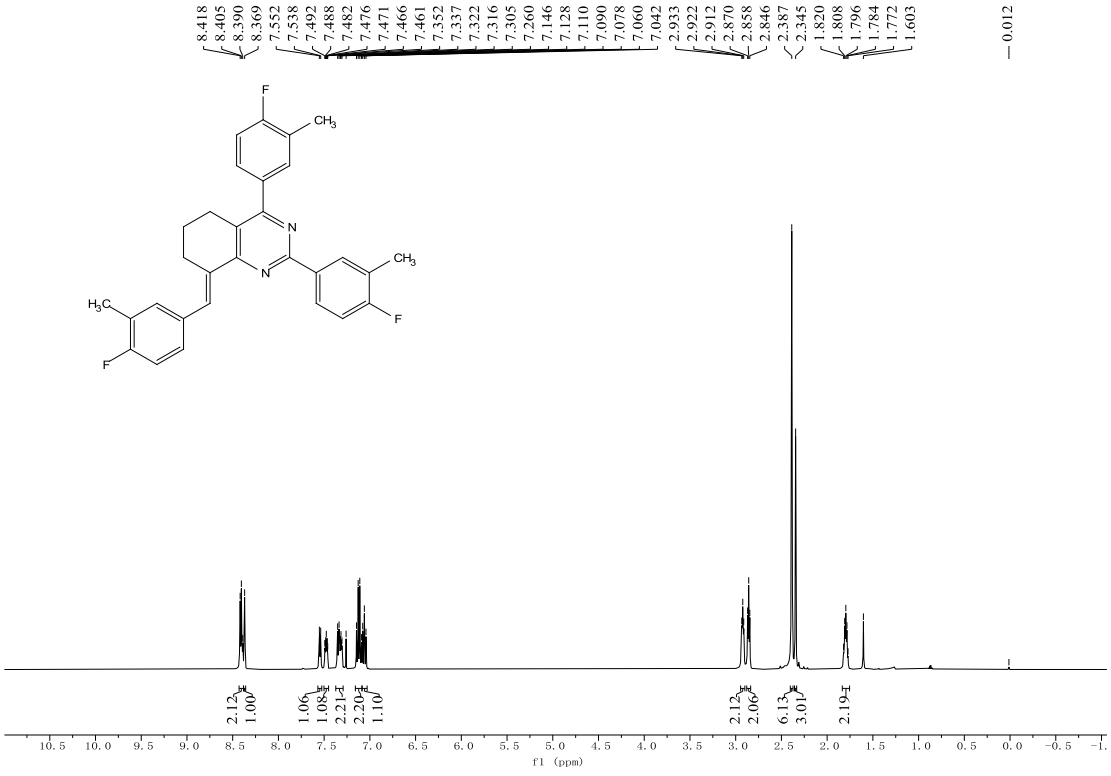
^{1}H NMR of **3v** (500 MHz, $CDCl_3$)



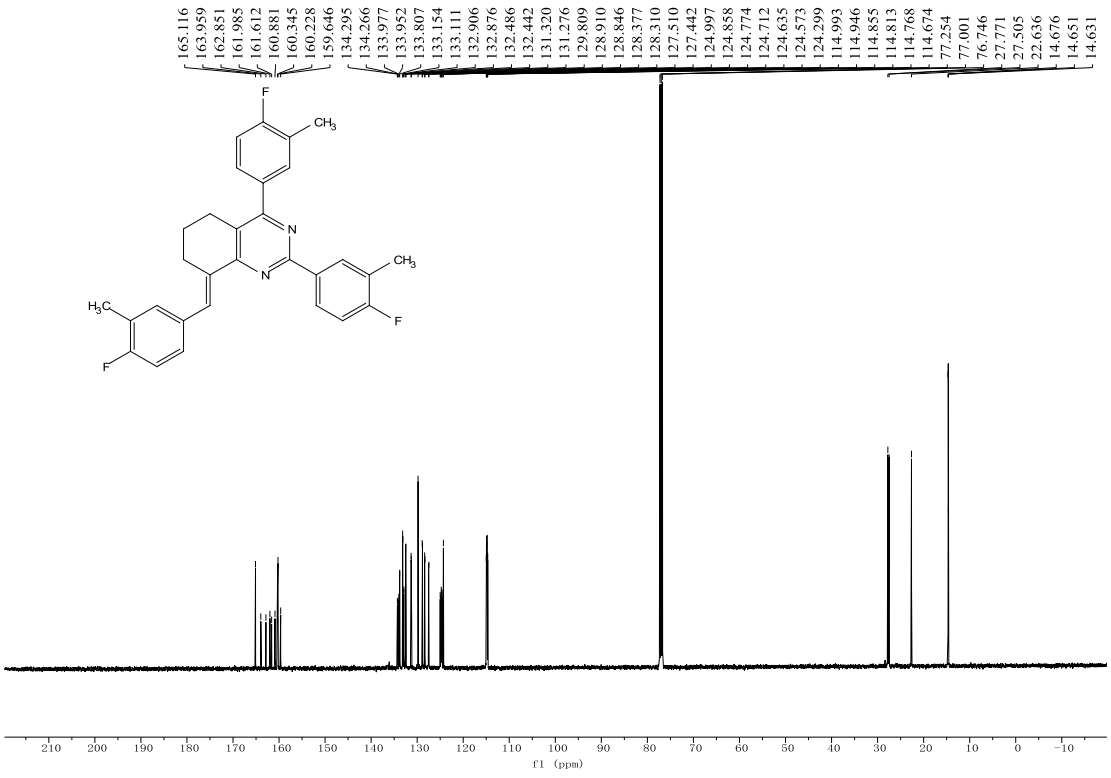
^{13}C NMR of **3v**(125 MHz, $CDCl_3$)



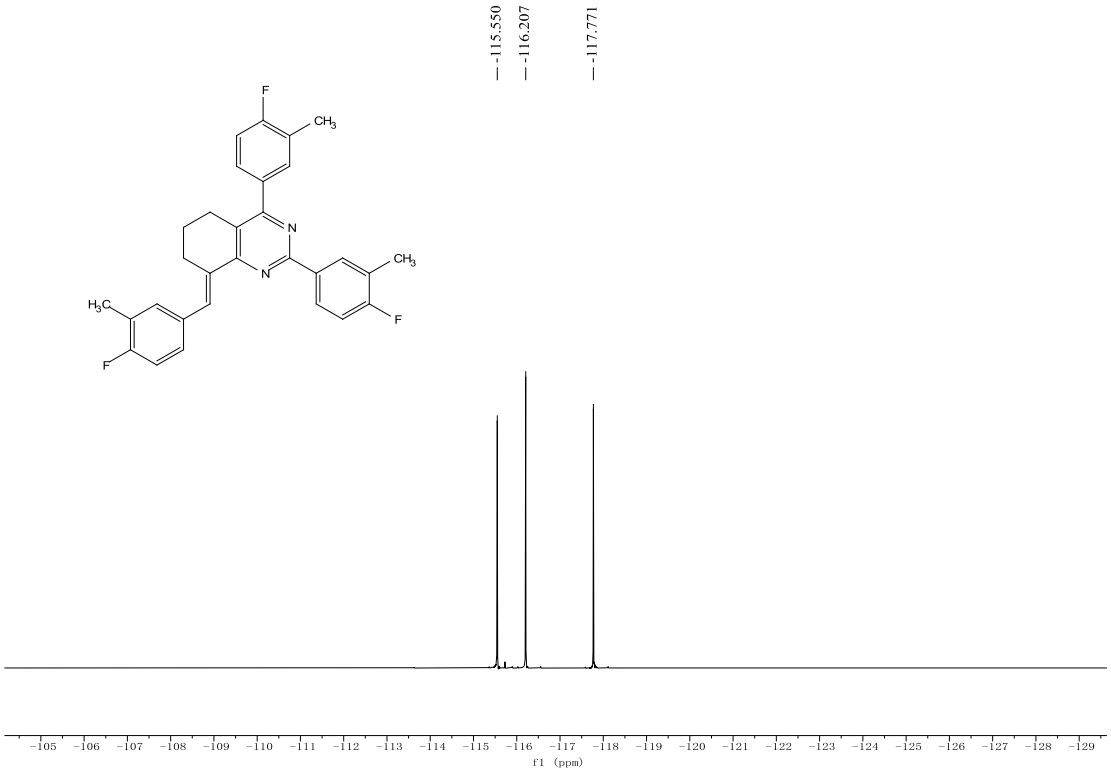
^{1}H NMR of **3w** (500 MHz, $CDCl_3$)



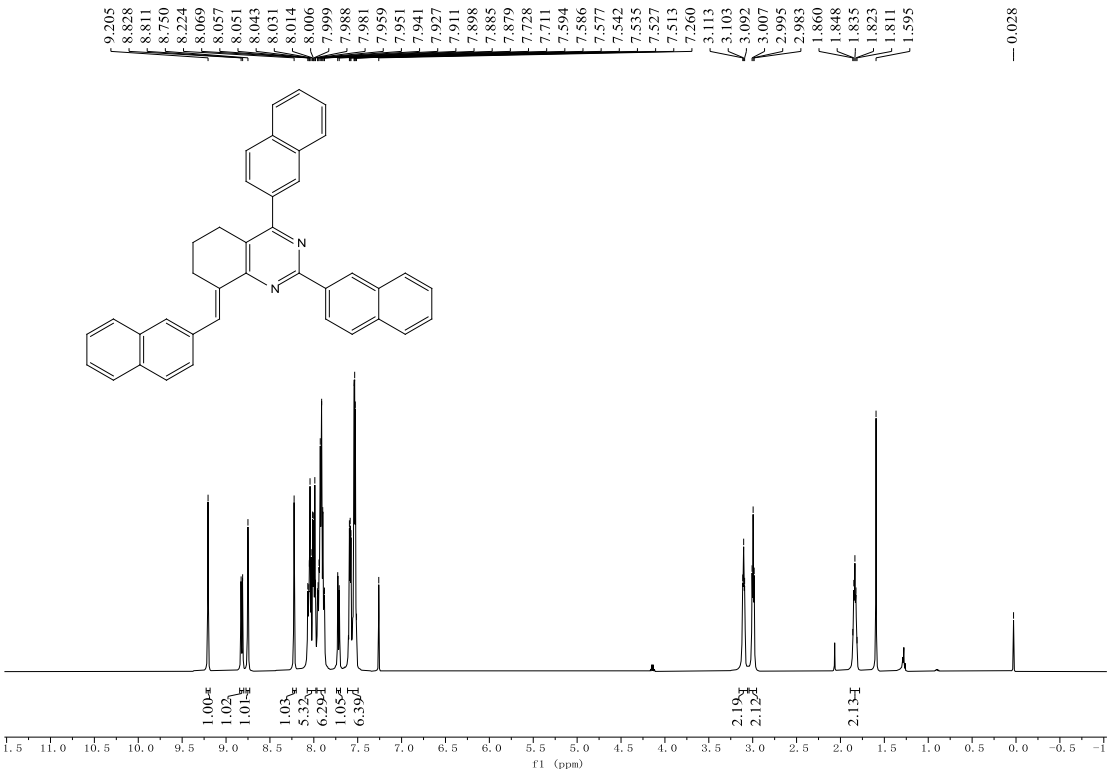
^{13}C NMR of **3w** (125 MHz, $CDCl_3$)



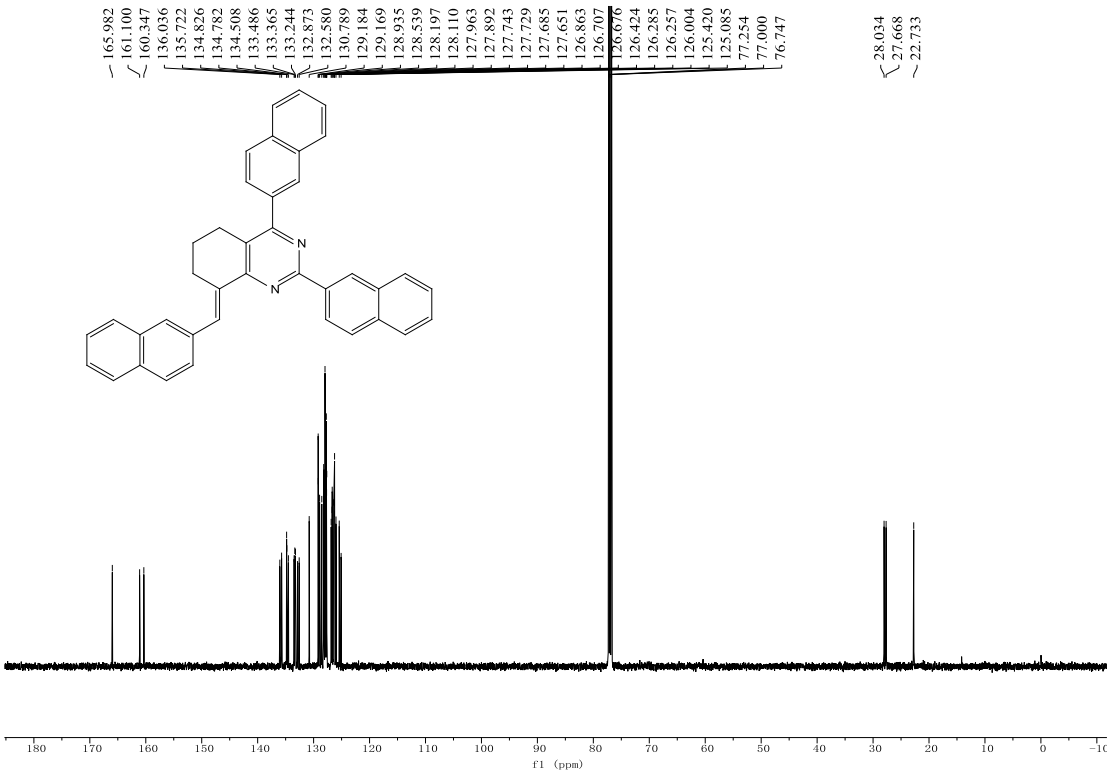
^{19}F NMR of **3w** (471 MHz, $CDCl_3$)



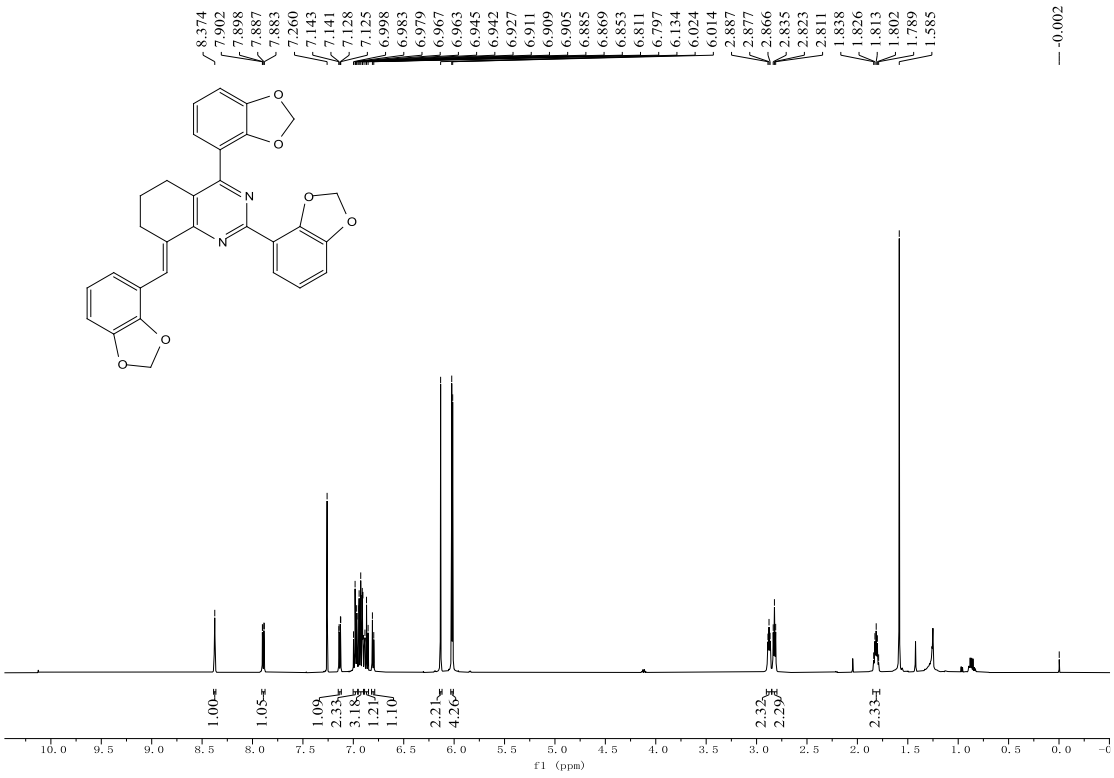
^{1}H NMR of **3x** (500 MHz, $CDCl_3$)



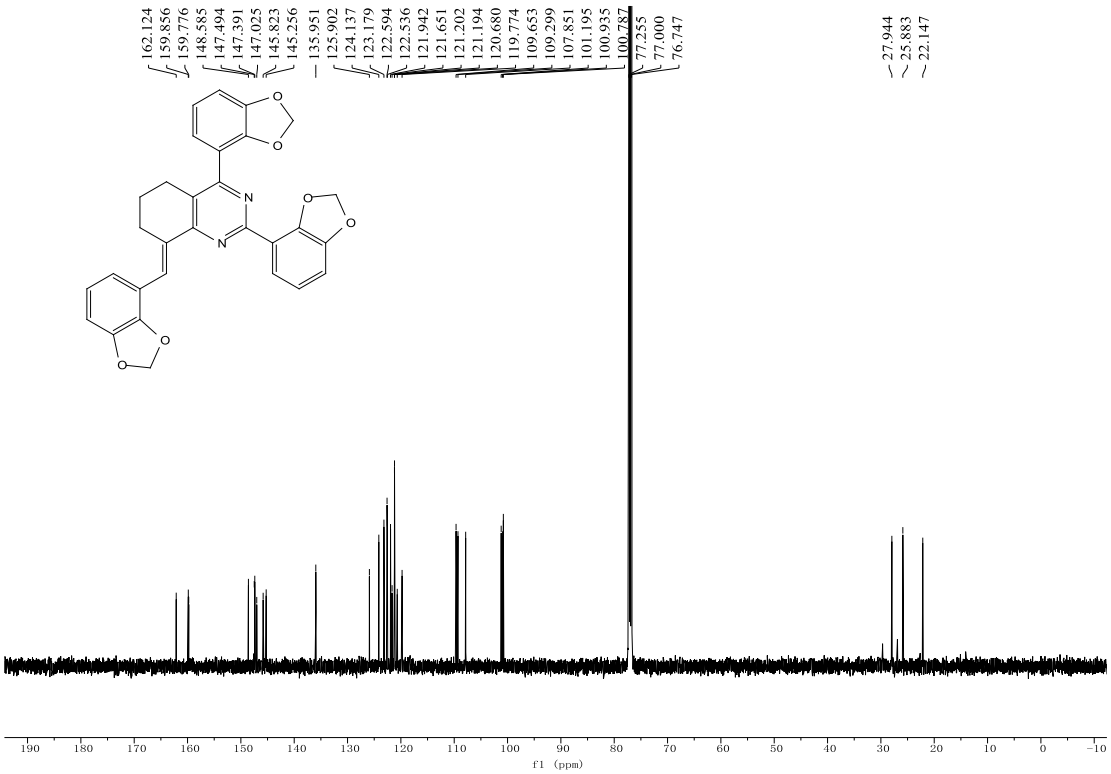
^{13}C NMR of **3x** (125 MHz, $CDCl_3$)



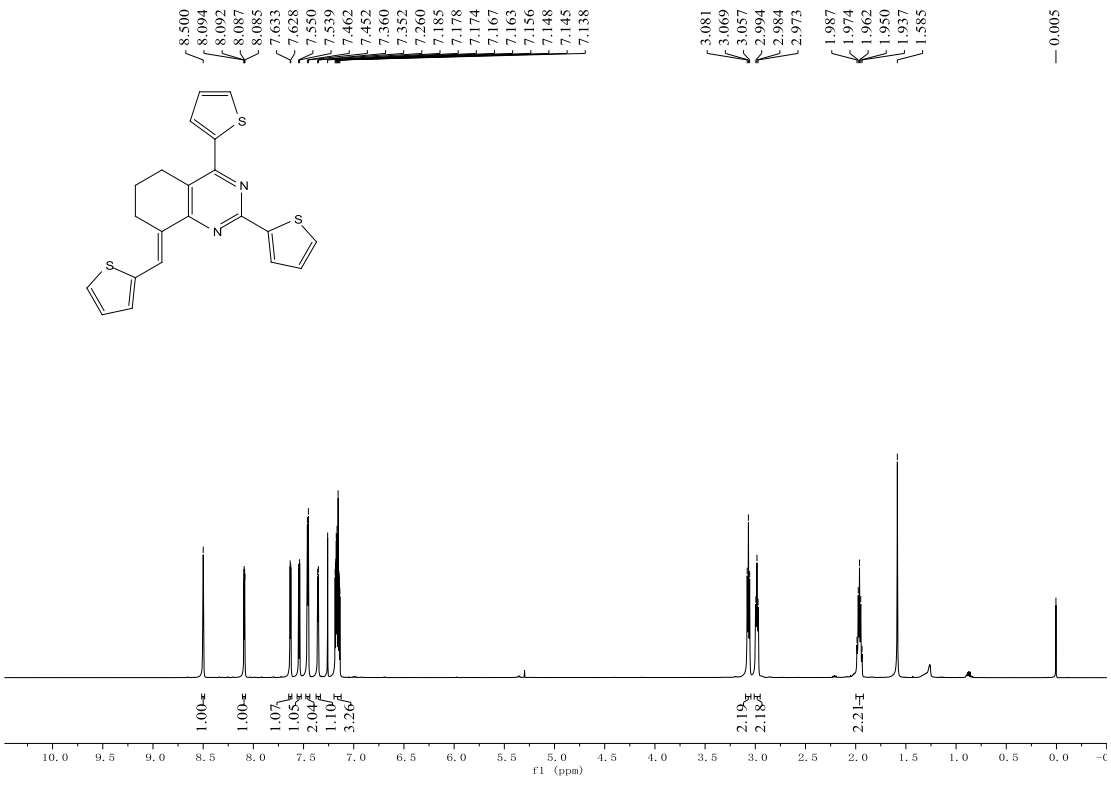
^{1}H NMR of **3y** (500 MHz, $CDCl_3$)



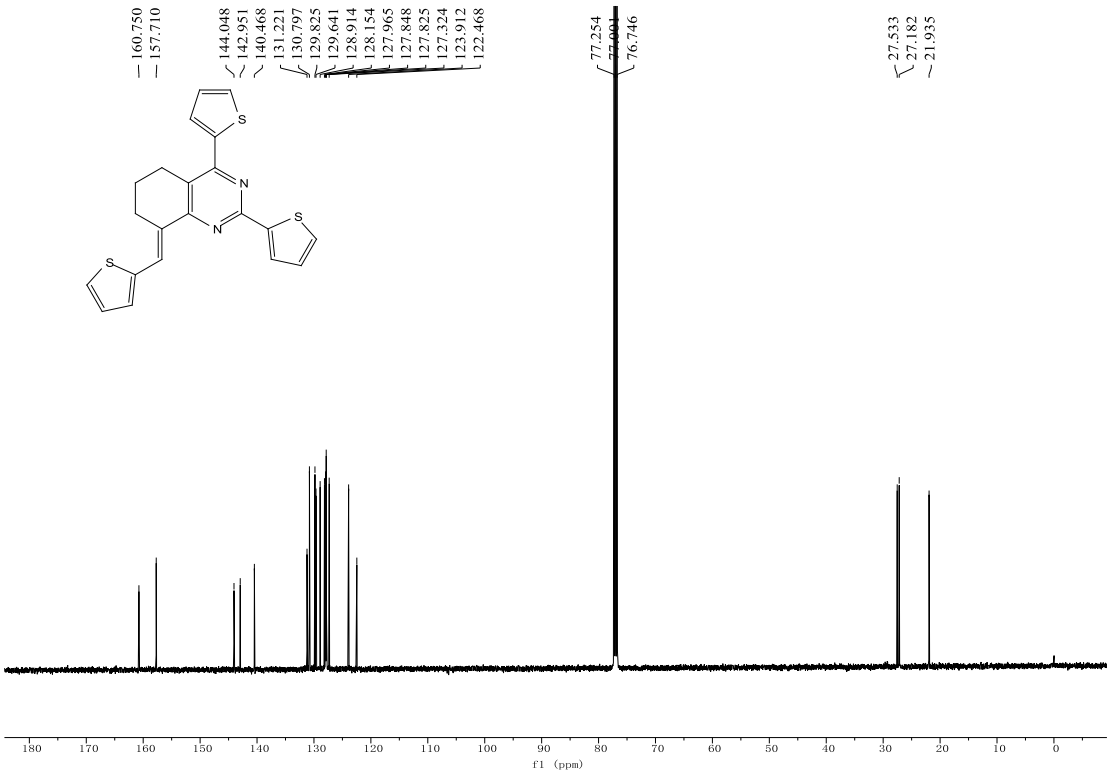
^{13}C NMR of **3y** (125 MHz, $CDCl_3$)



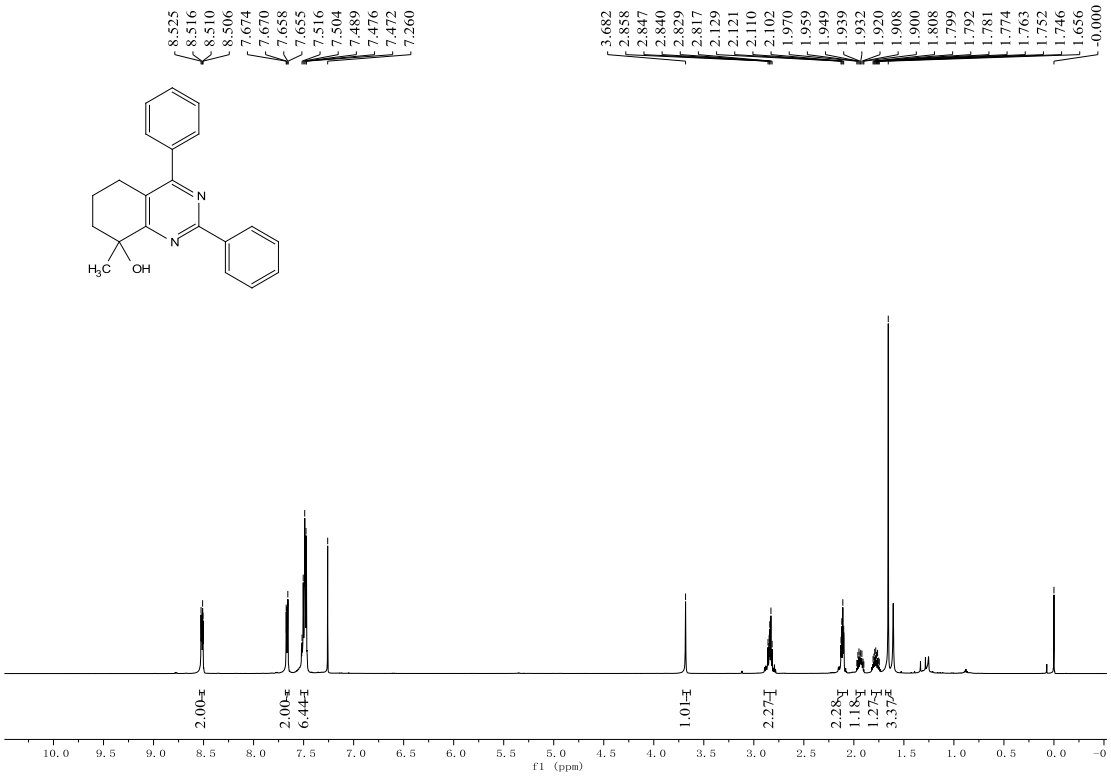
^{1}H NMR of **3z** (500 MHz, $CDCl_3$)



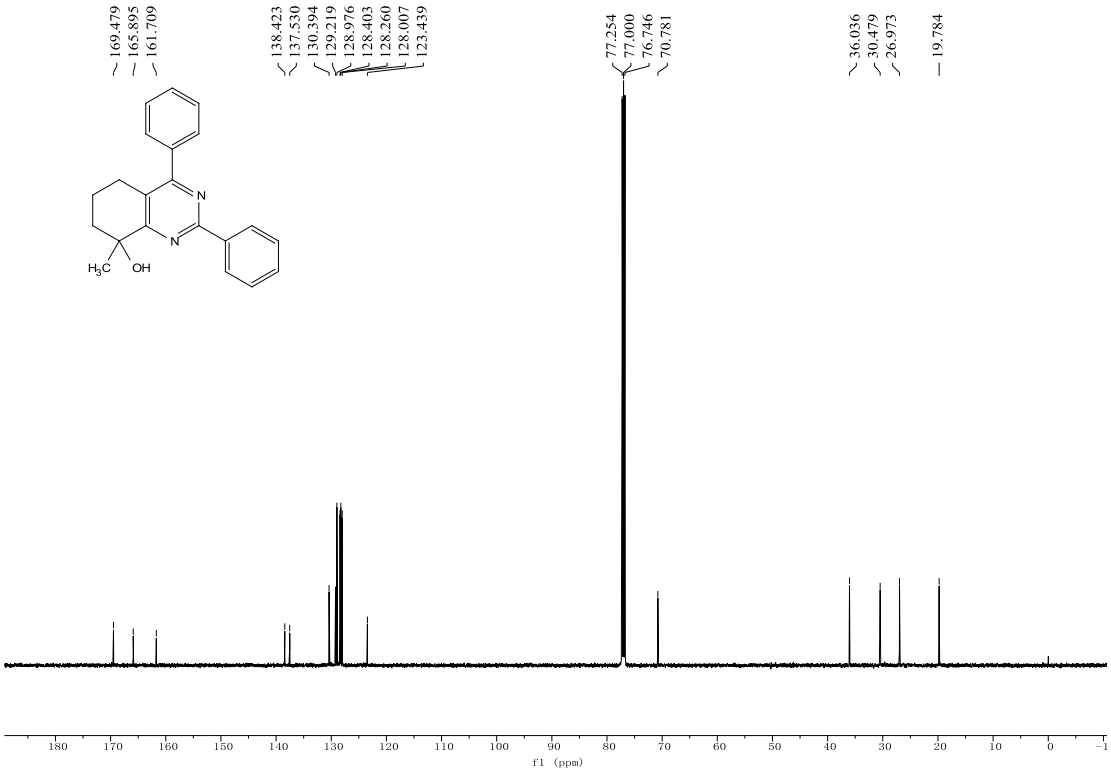
^{13}C NMR of **3z** (125 MHz, $CDCl_3$)



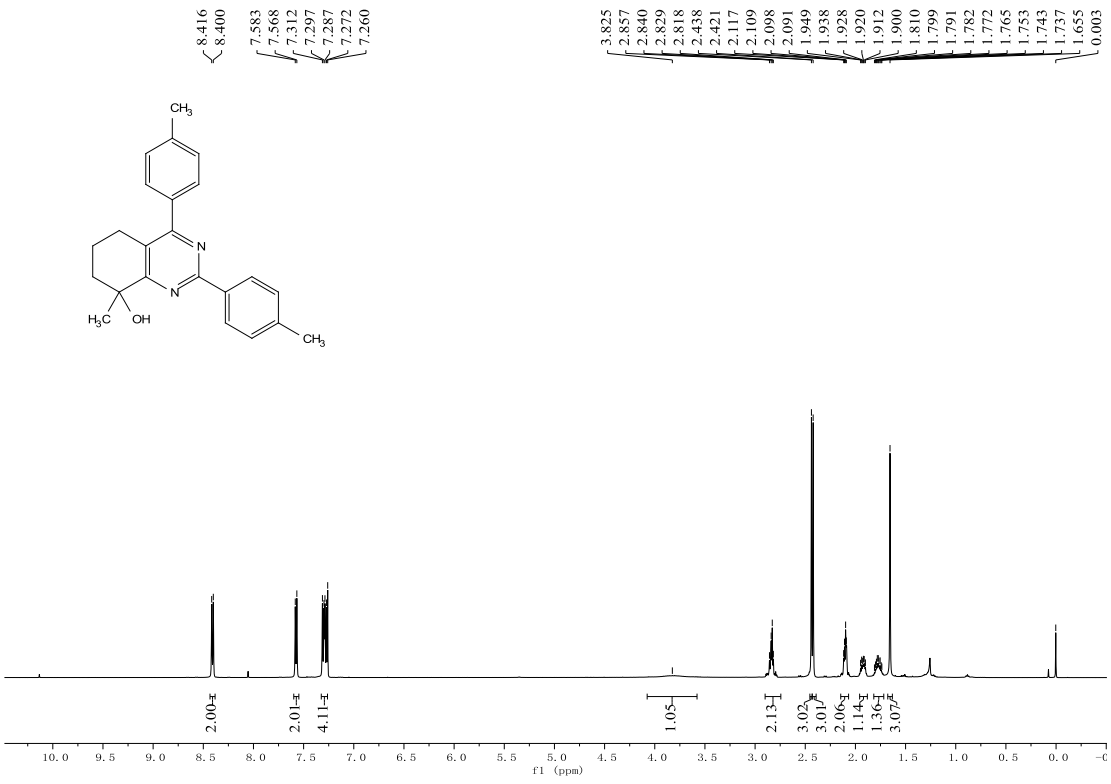
^{1}H NMR of **4a** (500 MHz, $CDCl_3$)



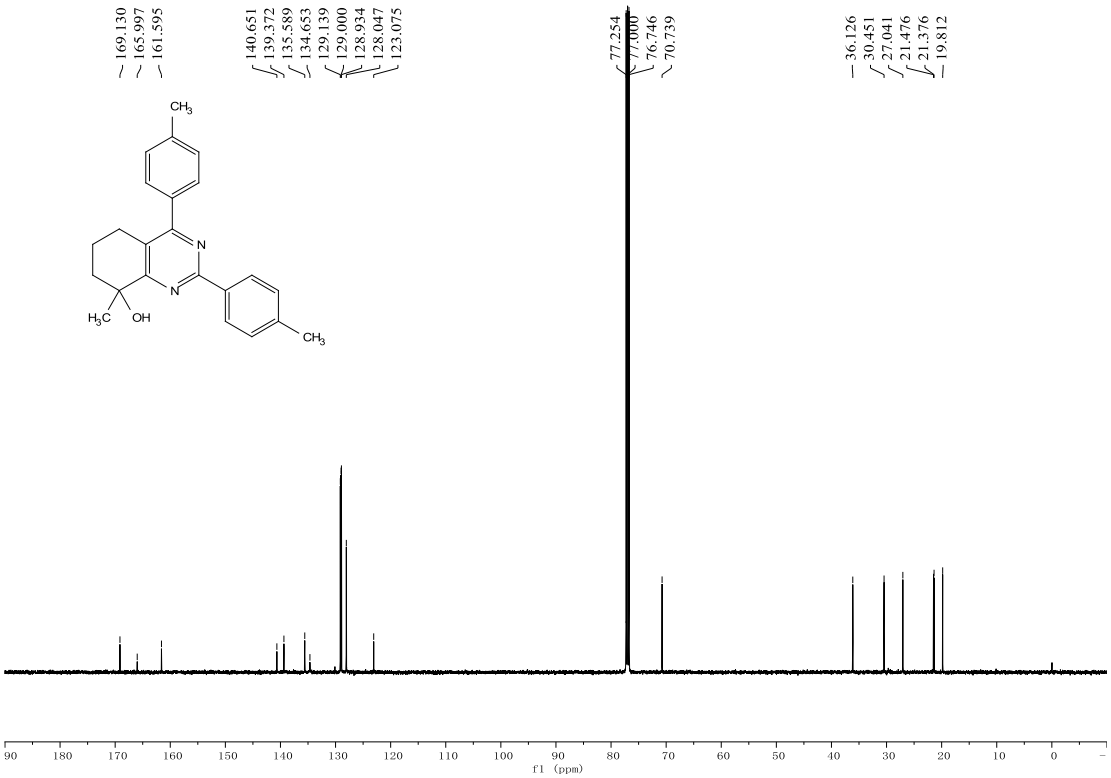
^{13}C NMR of **4a** (125 MHz, $CDCl_3$)



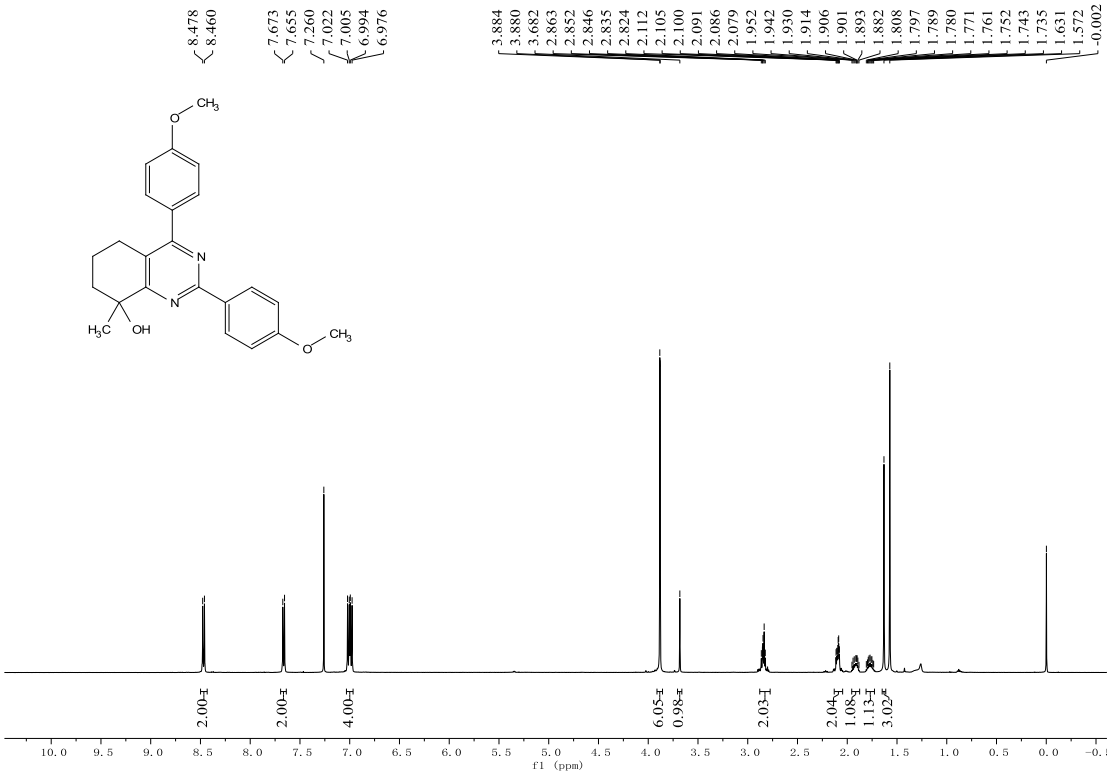
^{1}H NMR of **4b** (500 MHz, $CDCl_3$)



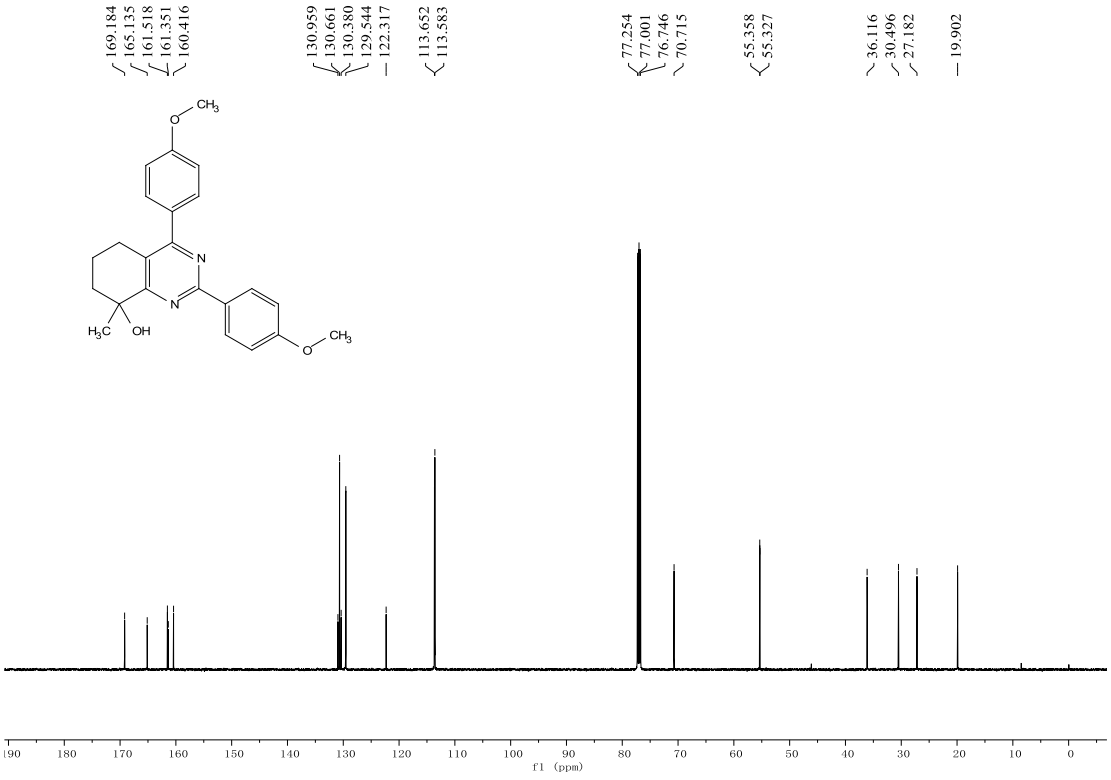
^{13}C NMR of **4b** (125 MHz, $CDCl_3$)



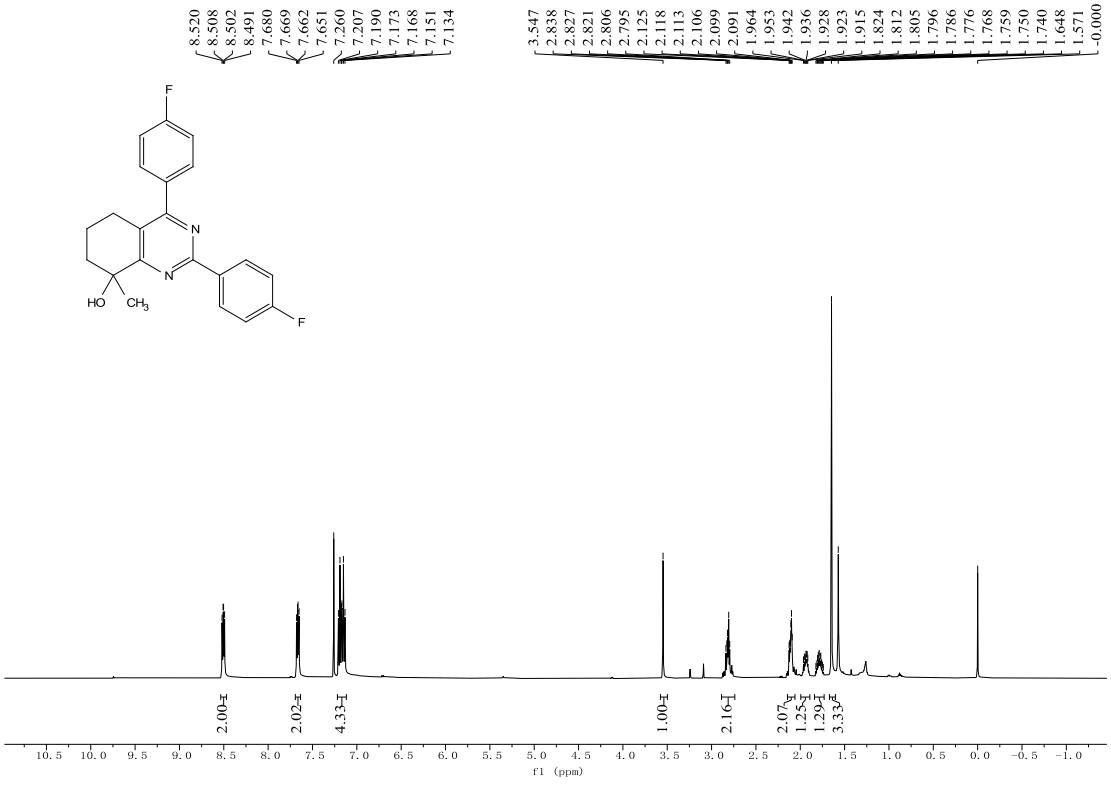
^{1}H NMR of **4c** (500 MHz, $CDCl_3$)



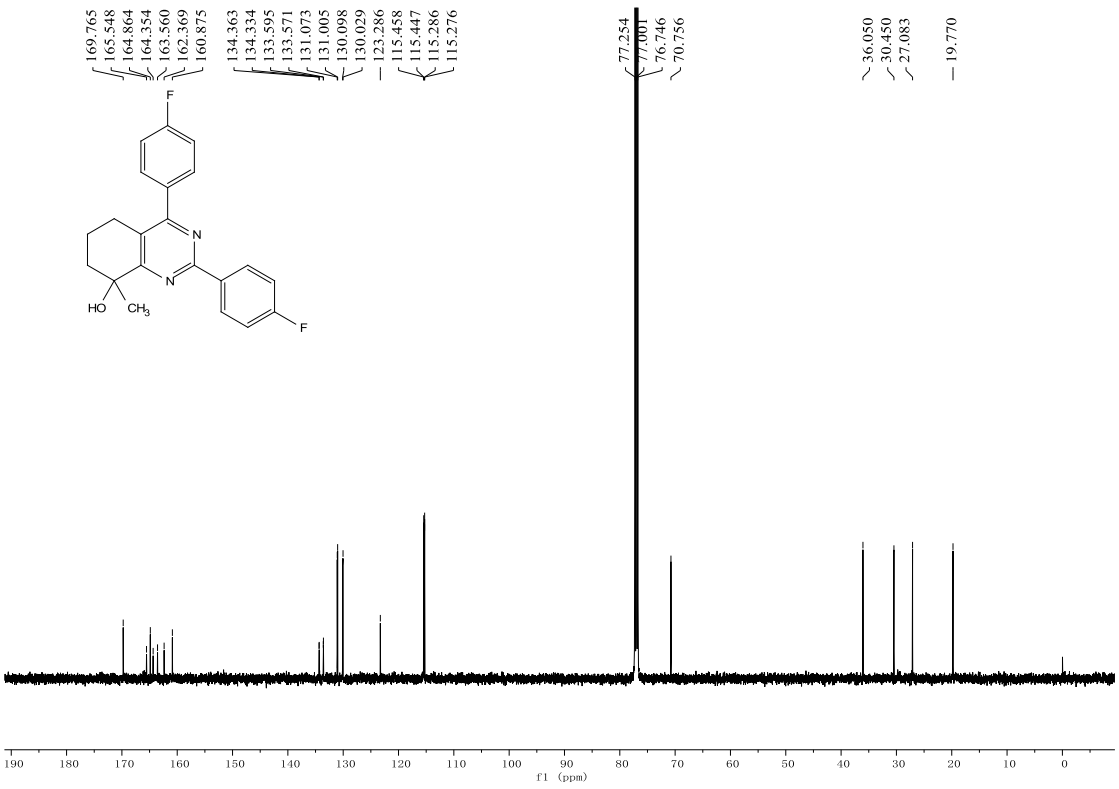
^{13}C NMR of **4c** (125 MHz, $CDCl_3$)



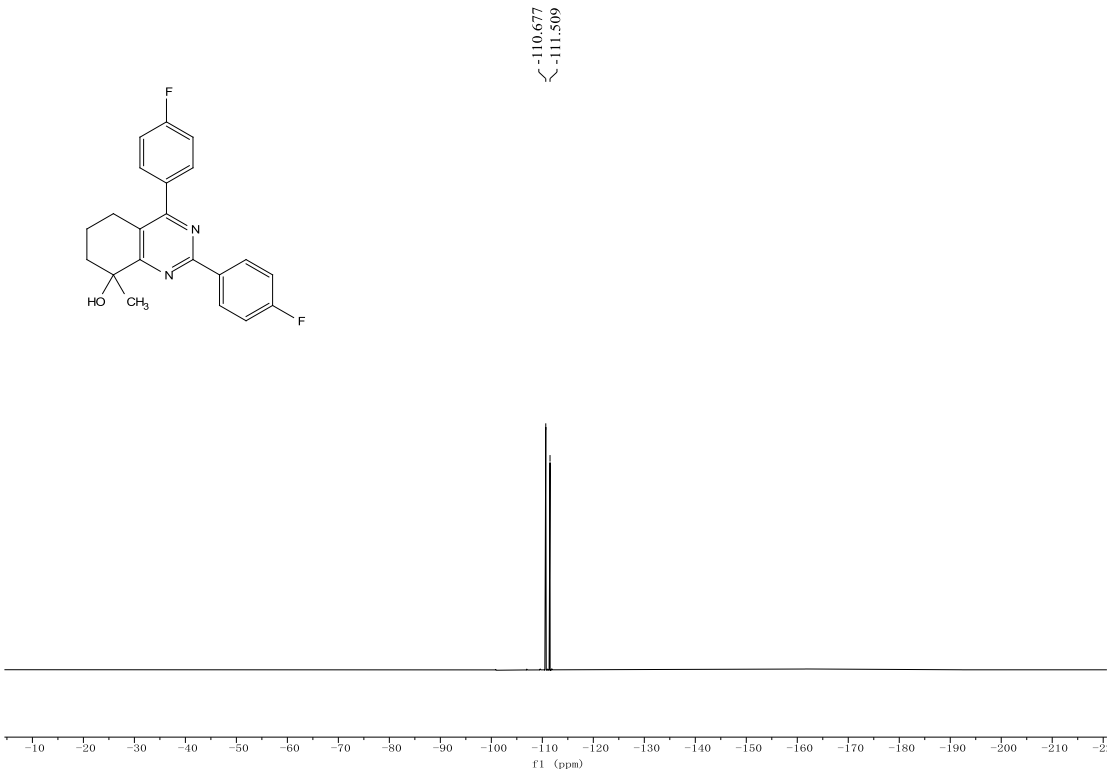
^{1}H NMR of **4d** (500 MHz, $CDCl_3$)



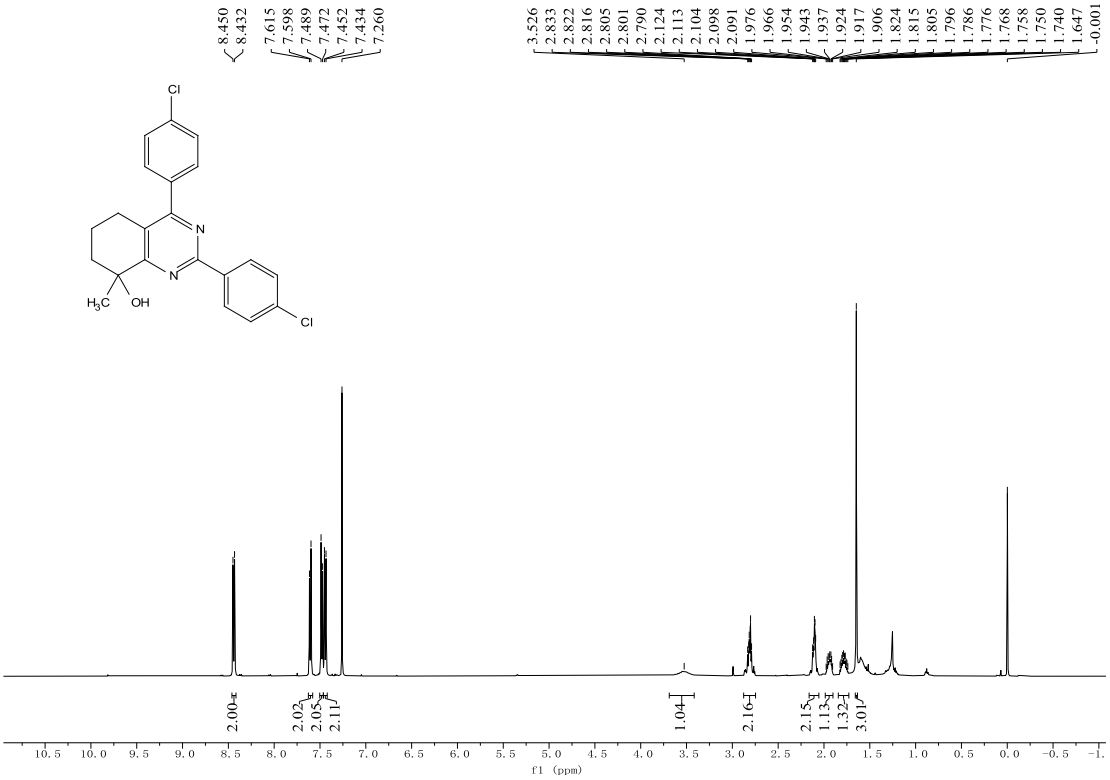
^{13}C NMR of **4d** (125 MHz, $CDCl_3$)



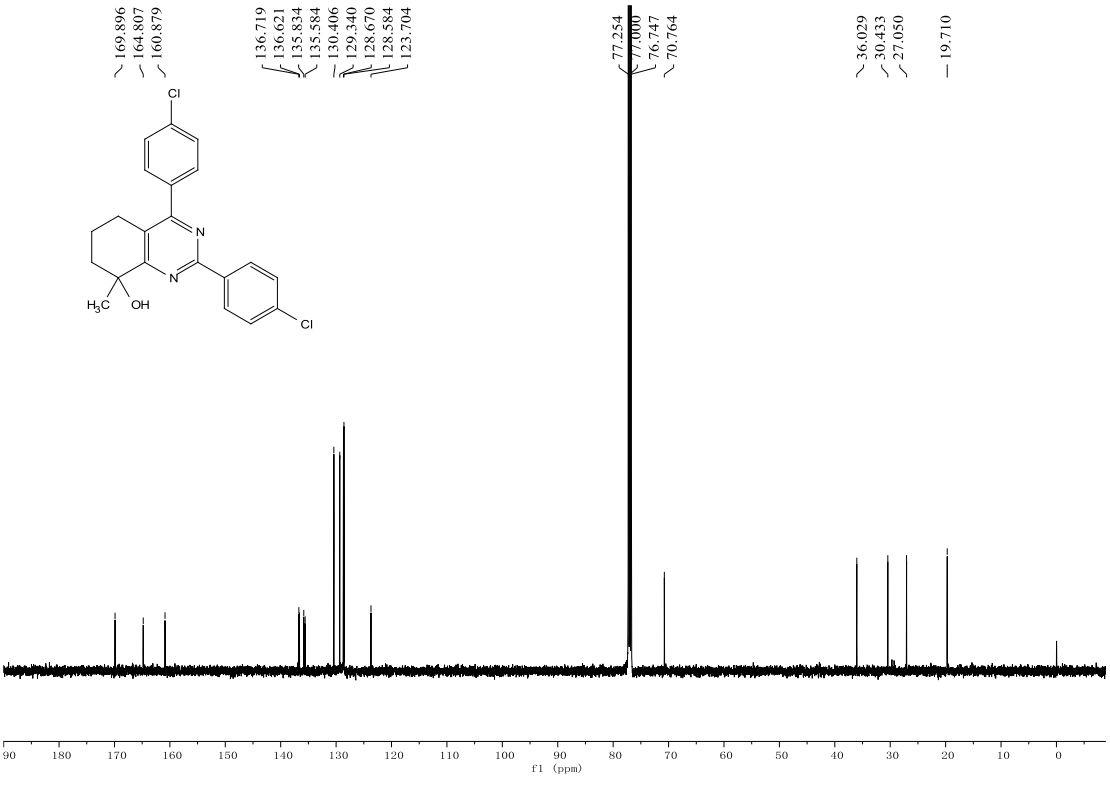
^{19}F NMR of **4d** (471 MHz, $CDCl_3$)



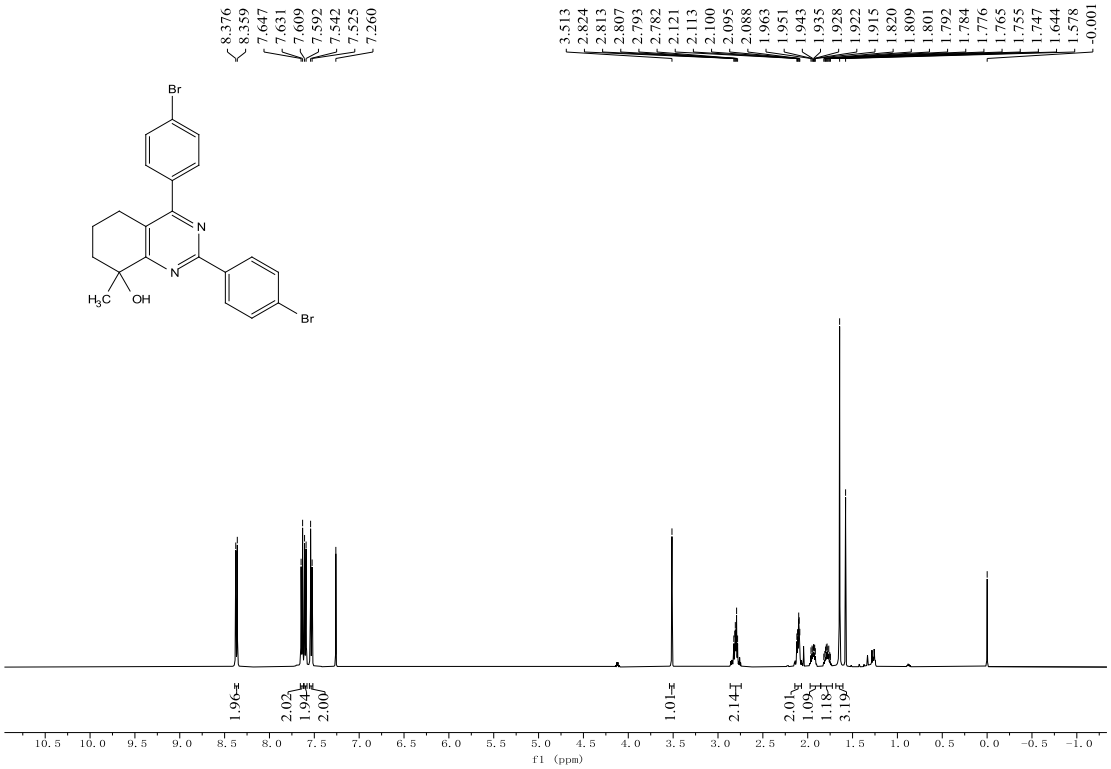
^{1}H NMR of **4e** (500 MHz, $CDCl_3$)



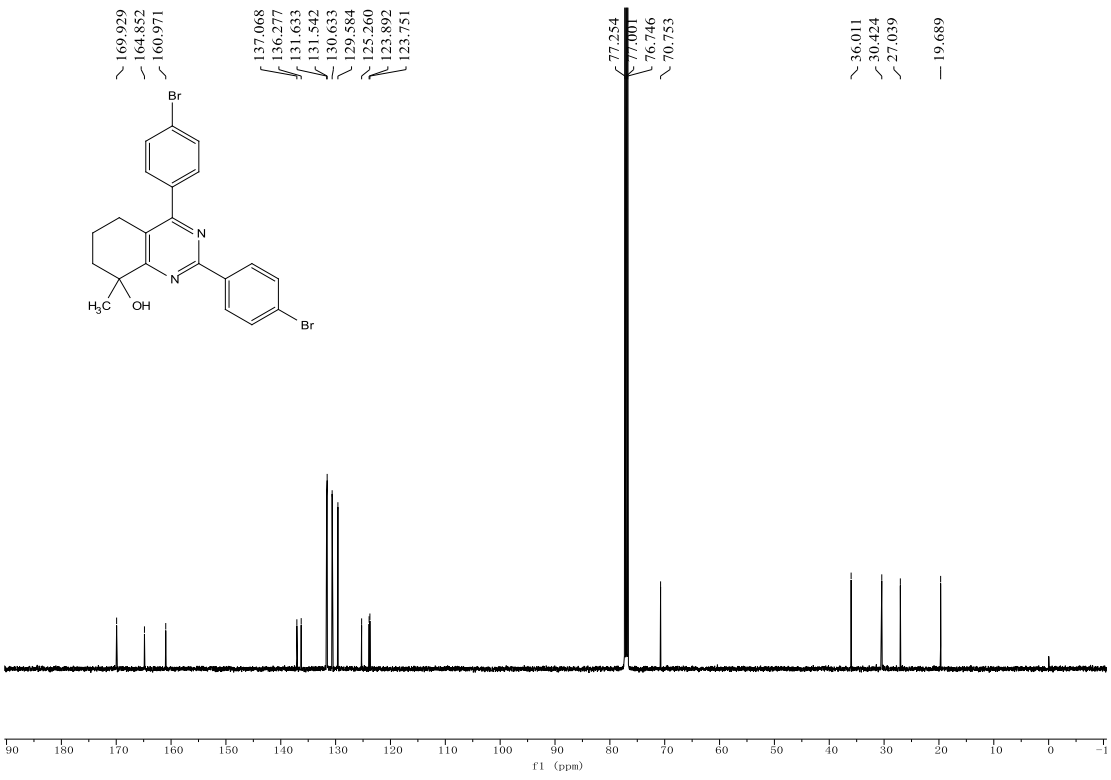
^{13}C NMR of **4e** (125 MHz, $CDCl_3$)



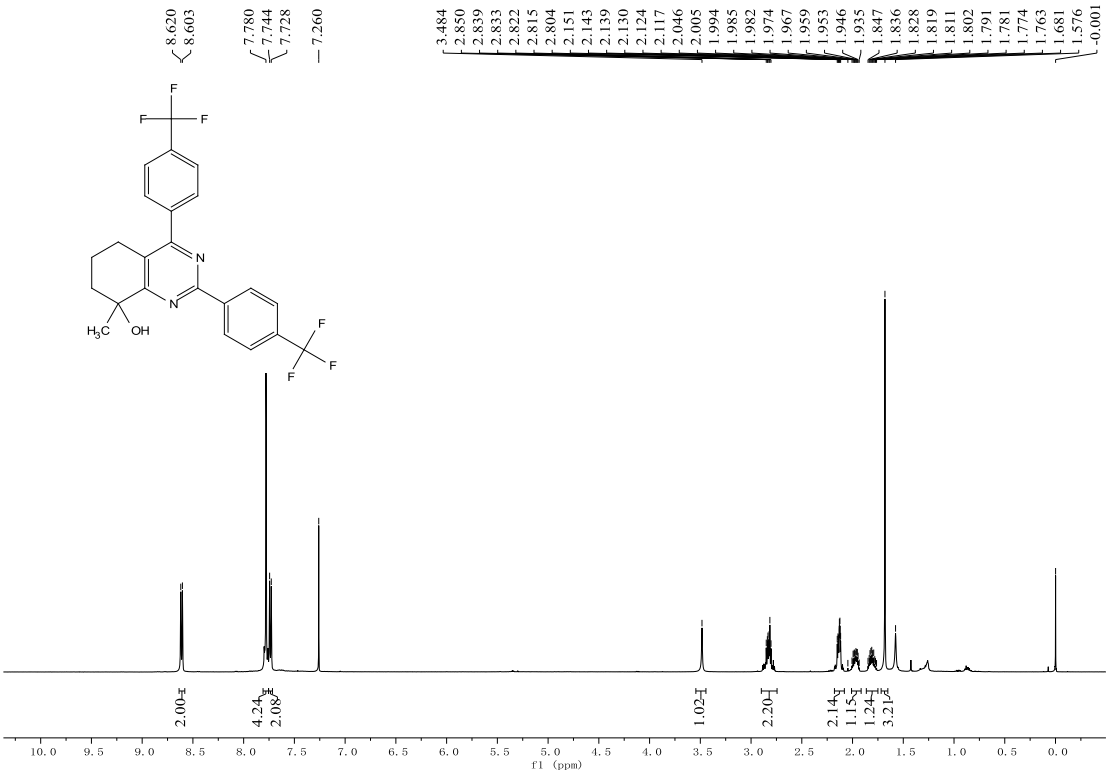
^{1}H NMR of **4f** (500 MHz, $CDCl_3$)



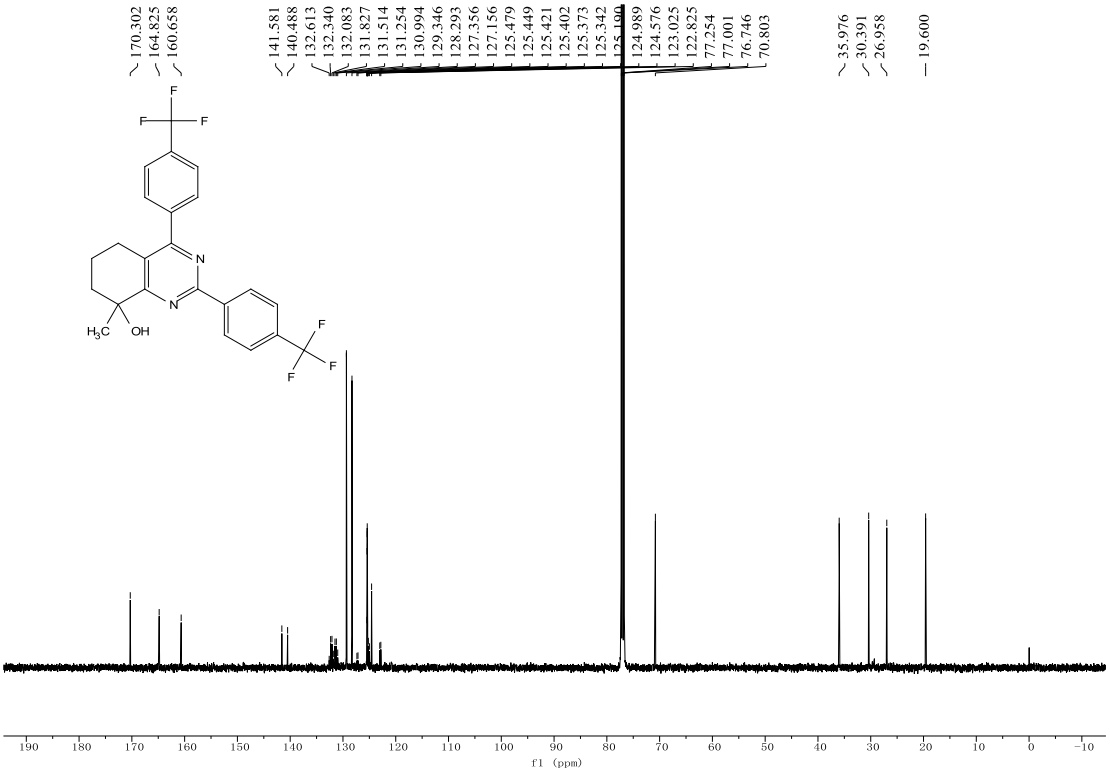
^{13}C NMR of **4f** (125 MHz, $CDCl_3$)



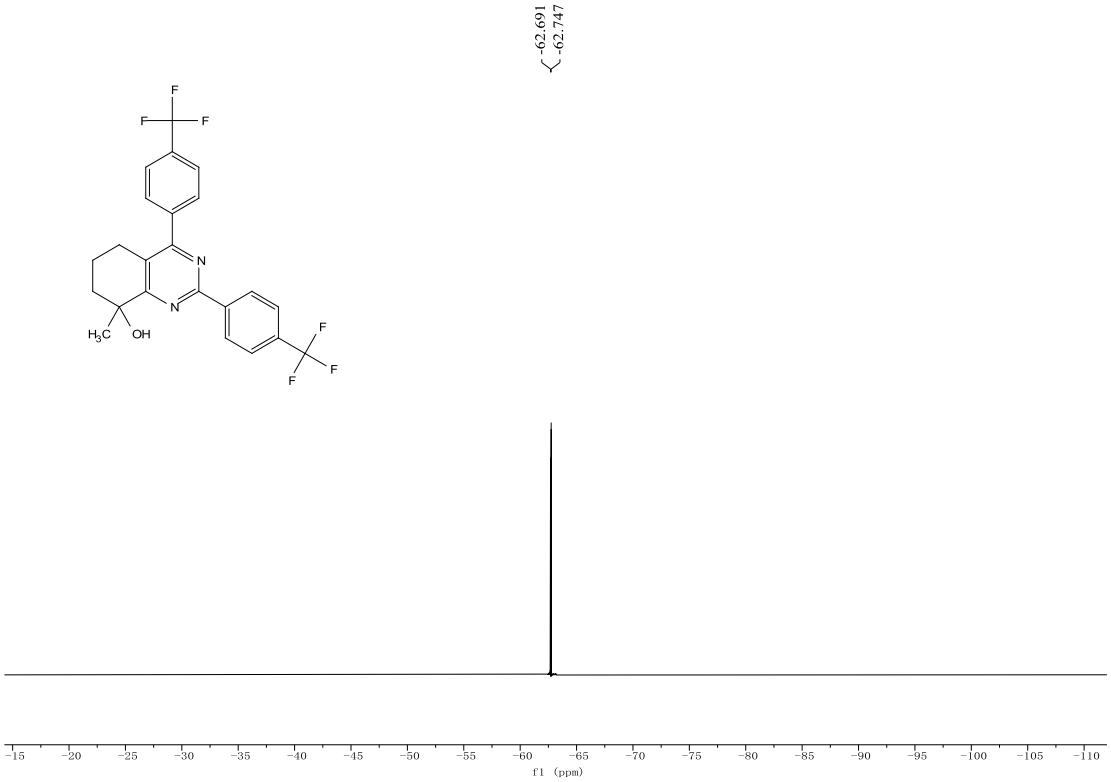
^{1}H NMR of **4g** (500 MHz, $CDCl_3$)



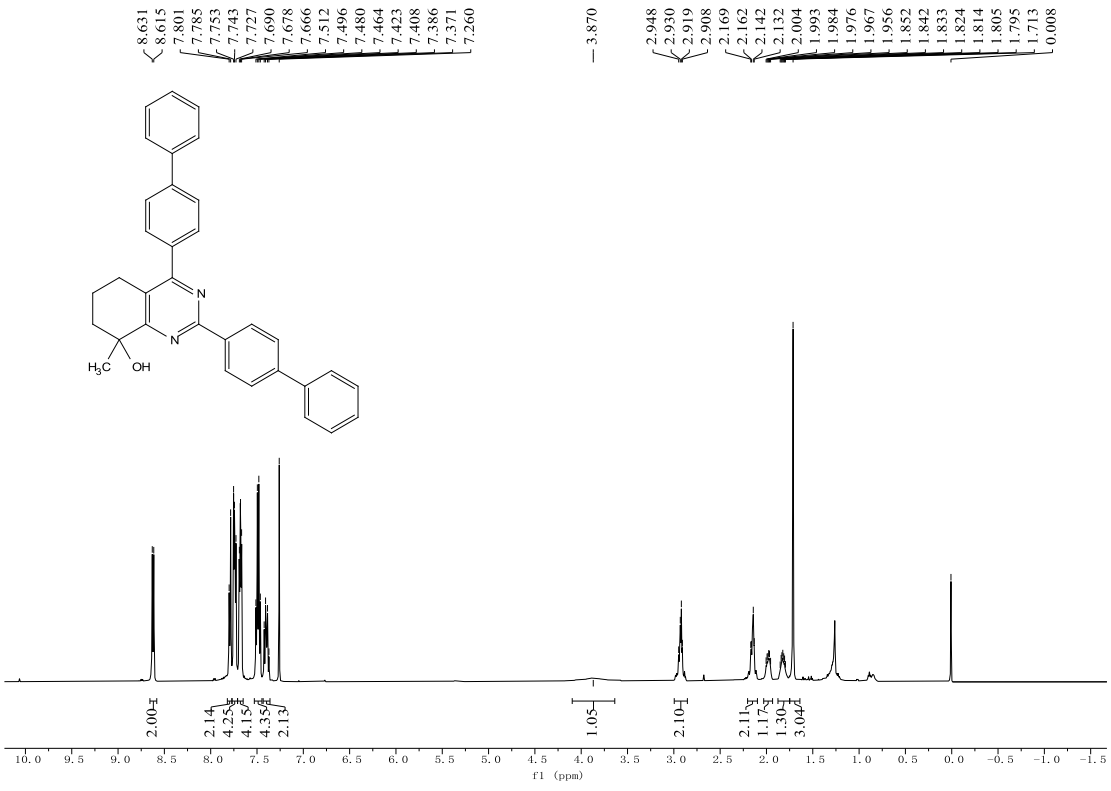
^{13}C NMR of **4g** (125 MHz, $CDCl_3$)



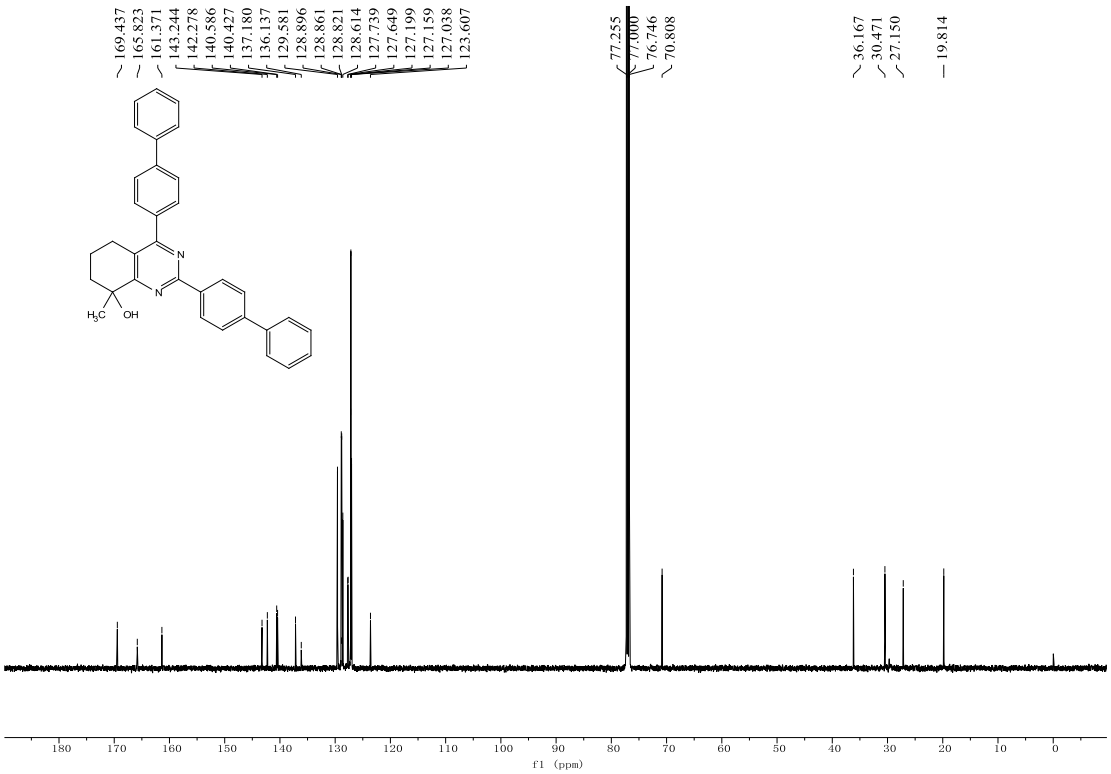
^{19}F NMR of **4g** (471MHz, $CDCl_3$)



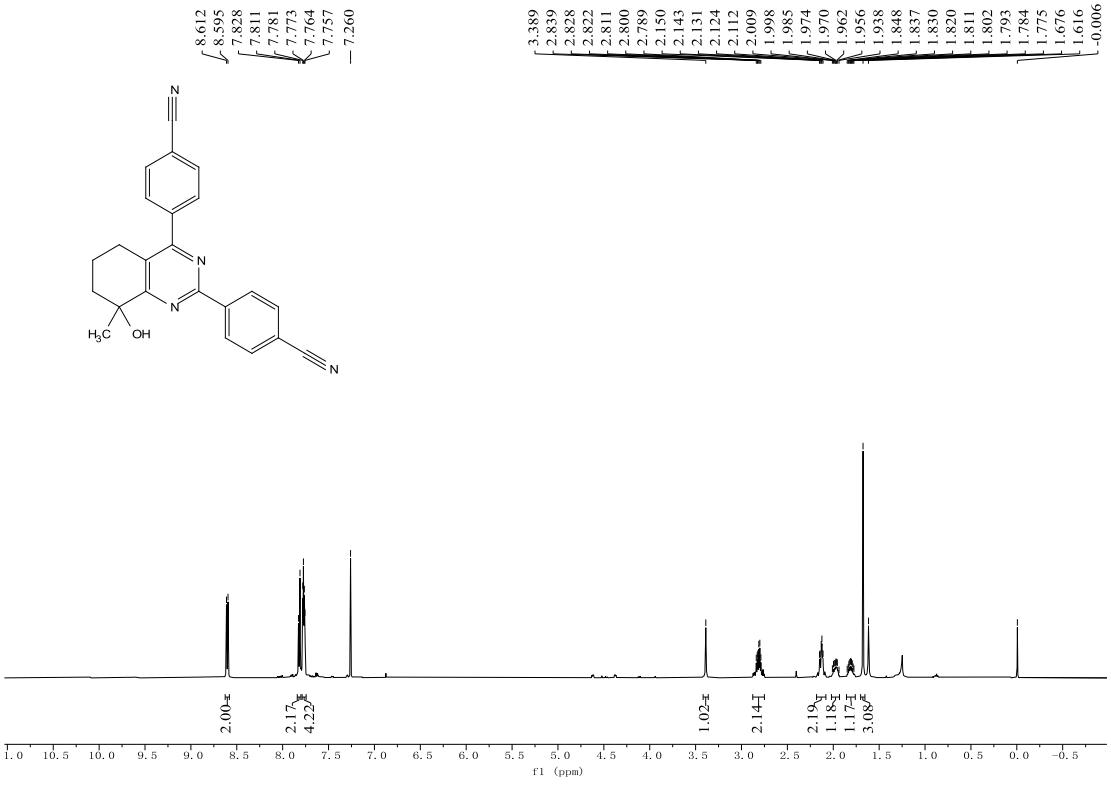
^{1}H NMR of **4h** (500 MHz, $CDCl_3$)



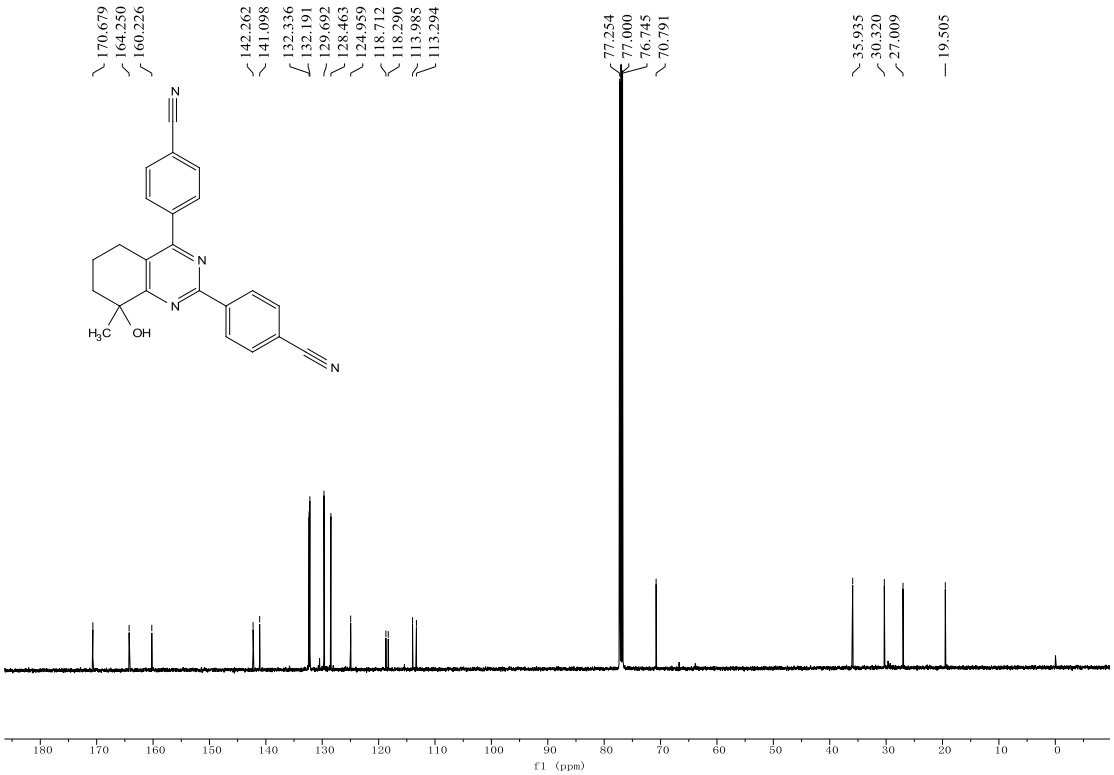
^{13}C NMR of **4h** (125 MHz, $CDCl_3$)



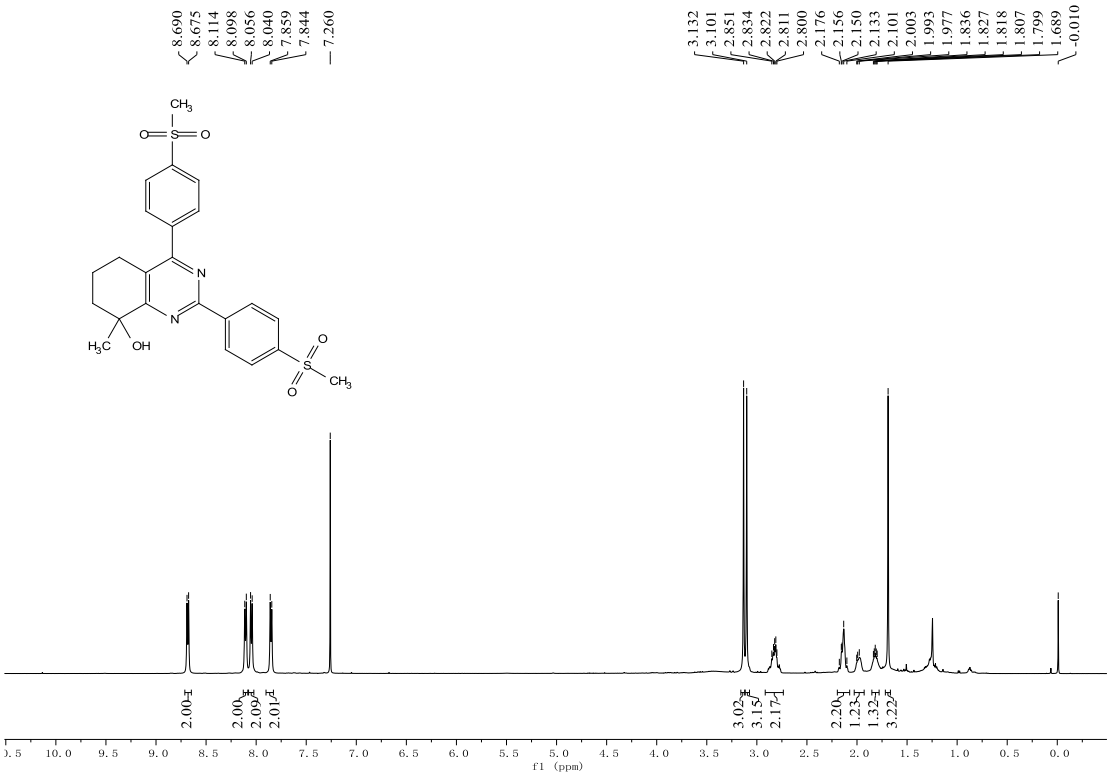
^{1}H NMR of **4i** (500 MHz, $CDCl_3$)



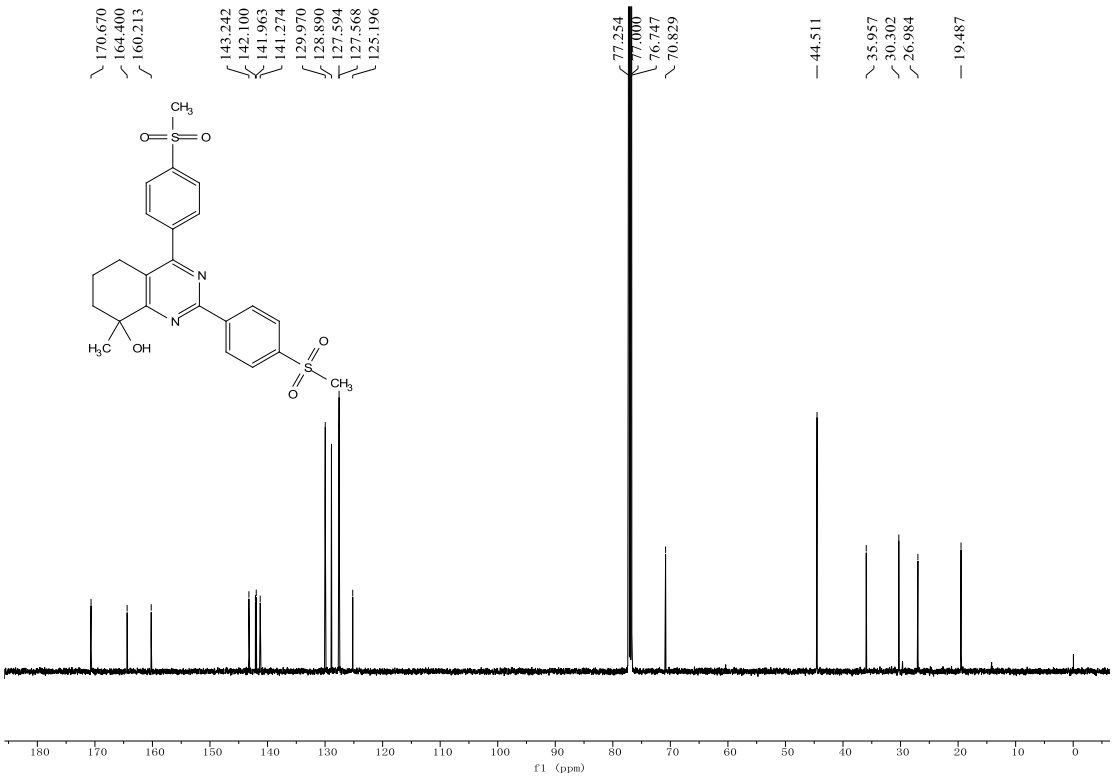
^{13}C NMR of **4i** (125 MHz, $CDCl_3$)



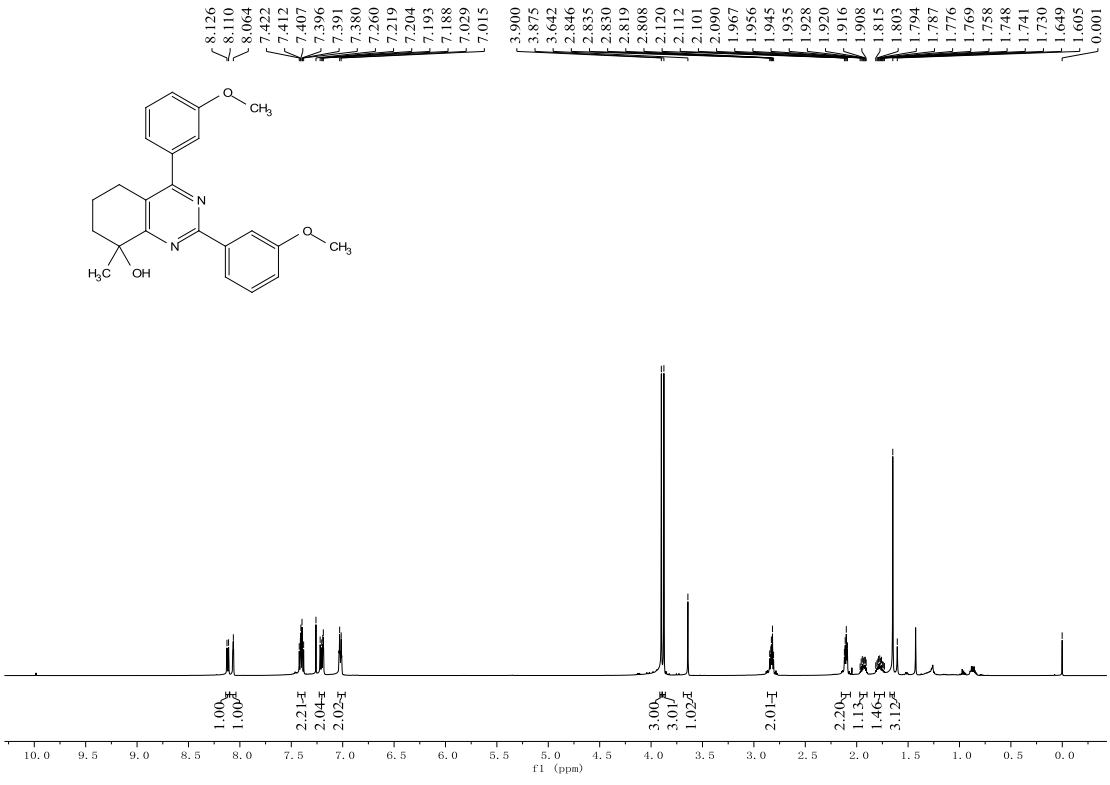
^{1}H NMR of **4j** (500 MHz, $CDCl_3$)



^{13}C NMR of **4j** (125 MHz, $CDCl_3$)

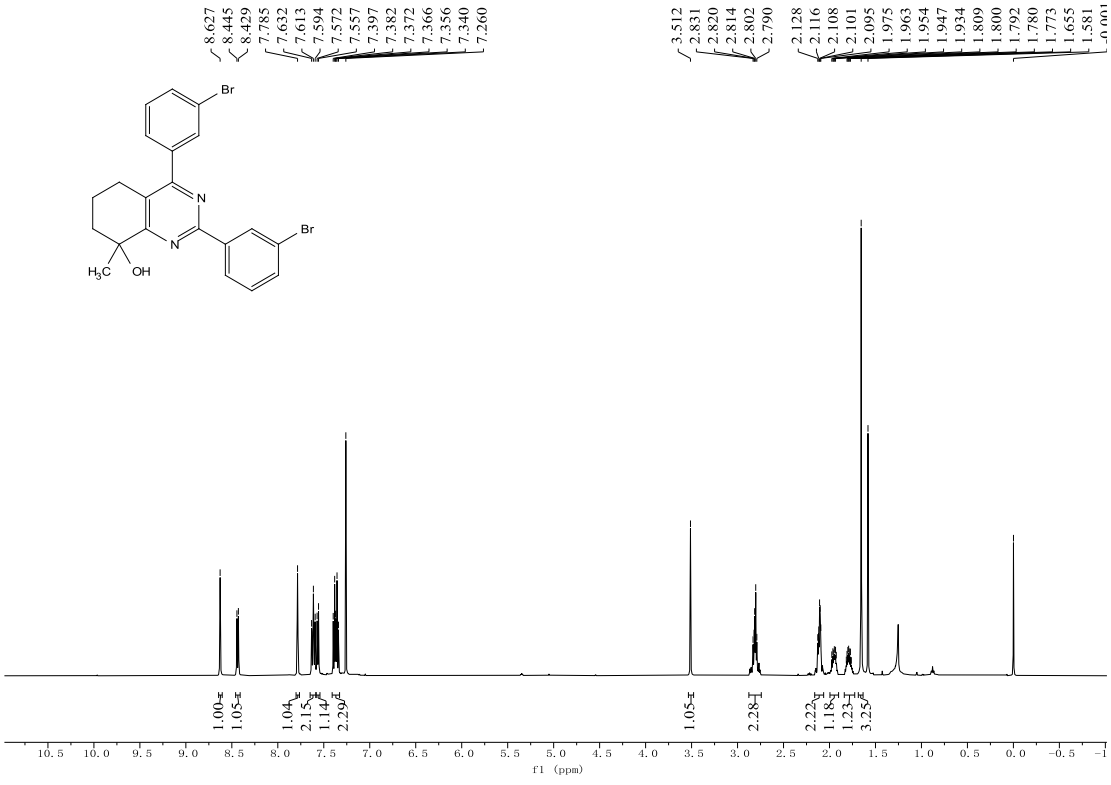


^{1}H NMR of **4k** (500 MHz, $CDCl_3$)

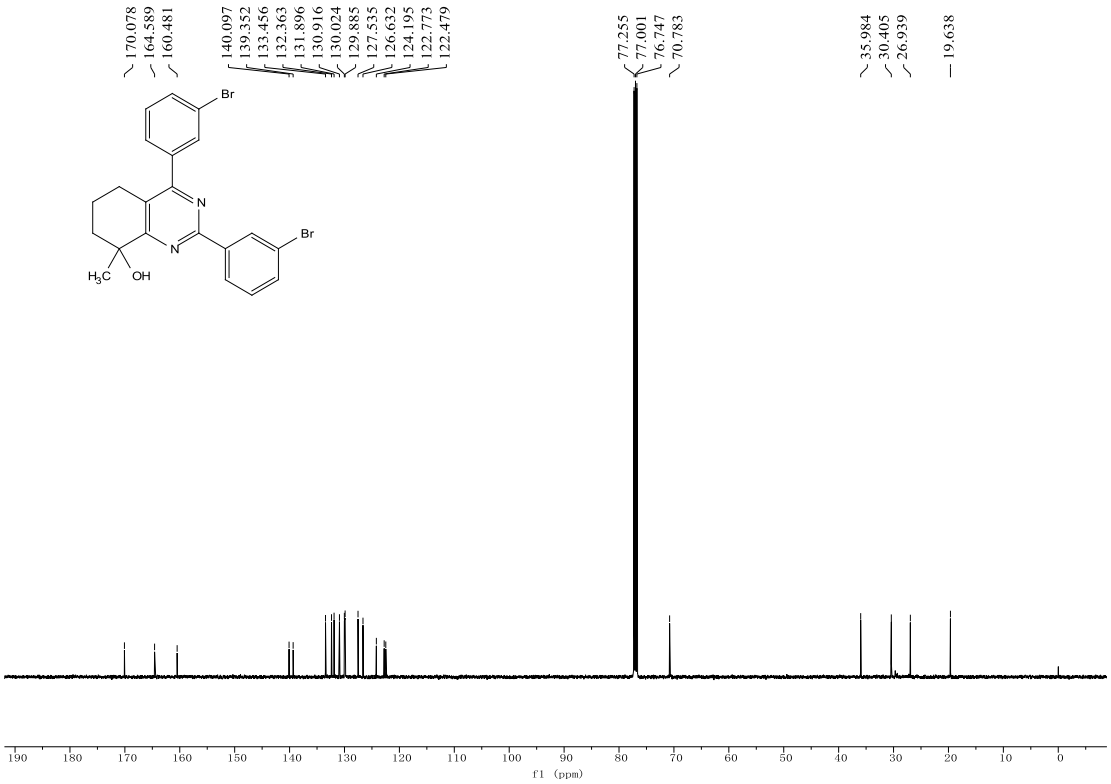


^{13}C NMR of **4k** (125 MHz, $CDCl_3$)

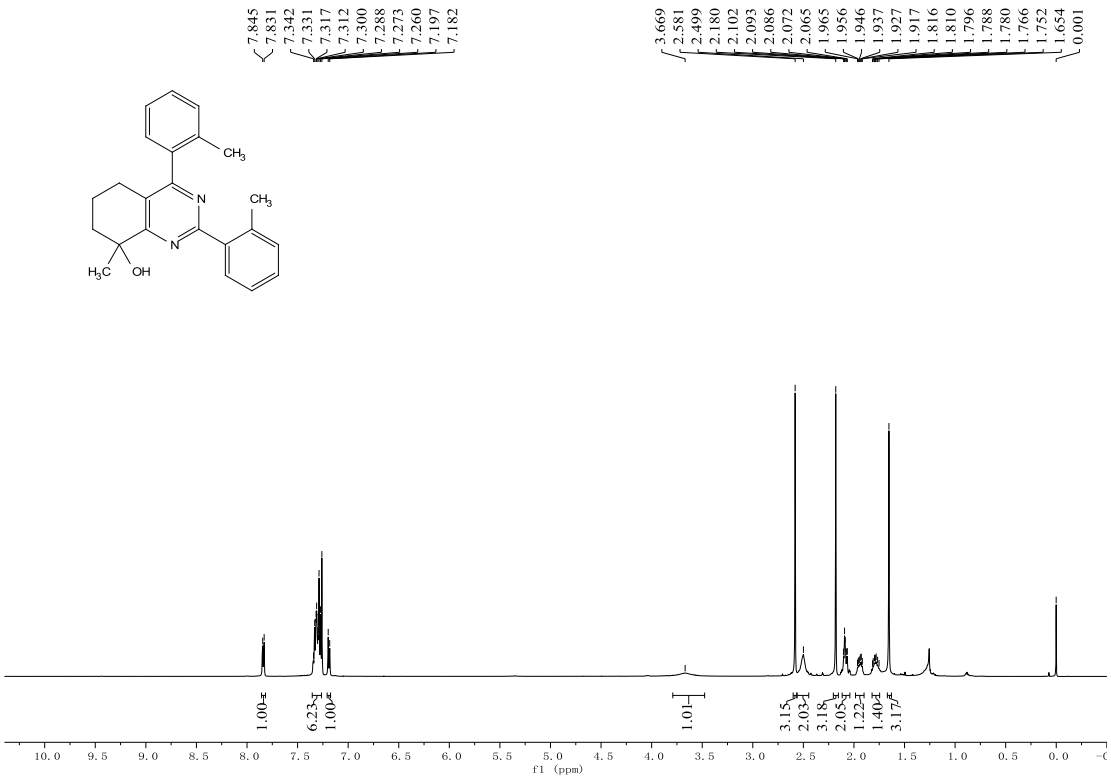
^{1}H NMR of **4l** (500 MHz, $CDCl_3$)



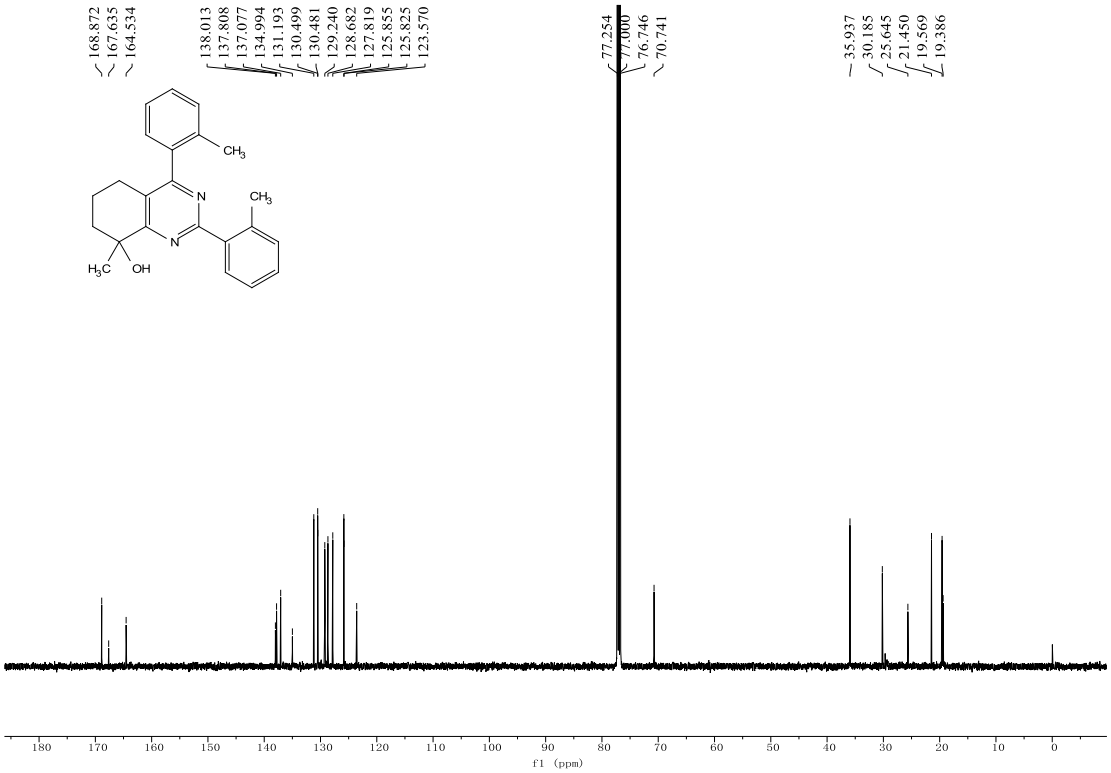
^{13}C NMR of **4l** (125 MHz, $CDCl_3$)



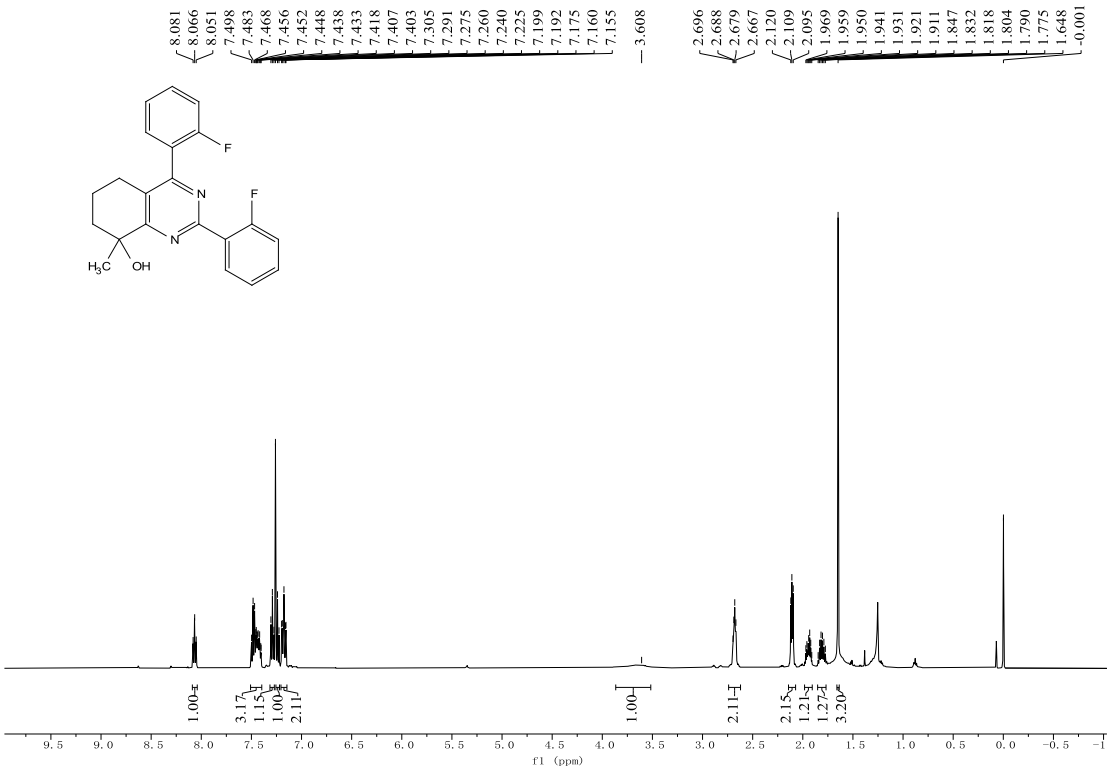
^{1}H NMR of **4m** (500 MHz, $CDCl_3$)



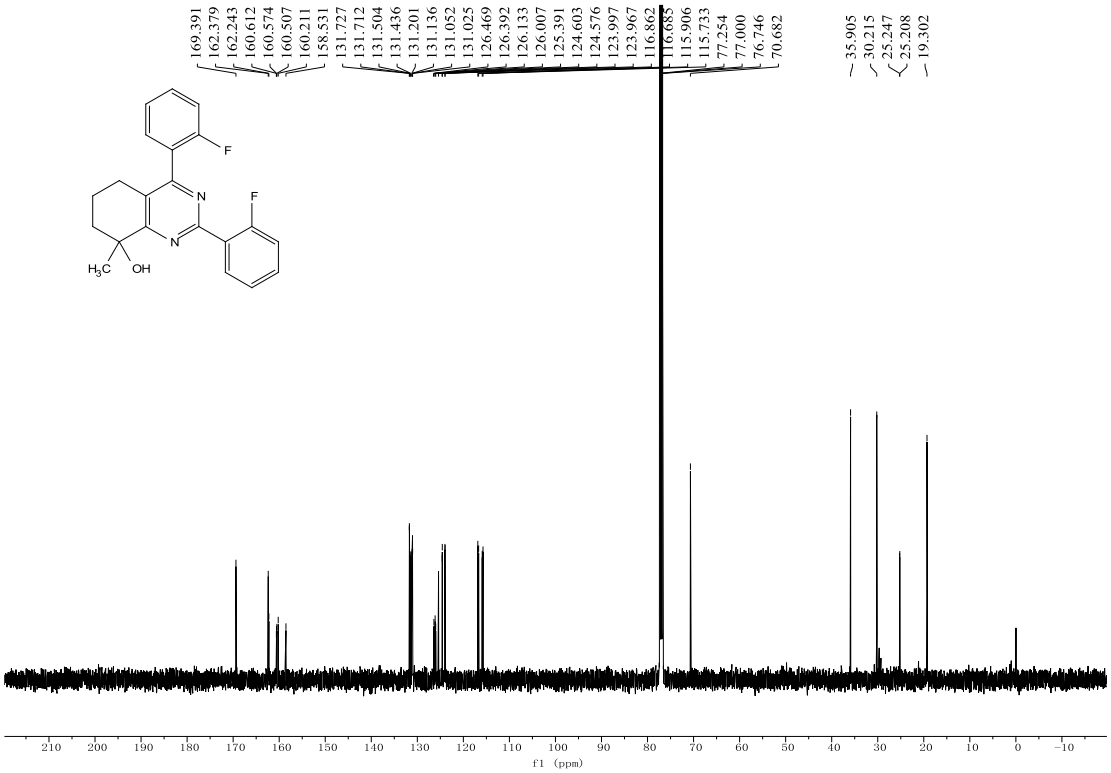
^{13}C NMR of **4m** (125 MHz, $CDCl_3$)



^{1}H NMR of **4n** (500 MHz, $CDCl_3$)

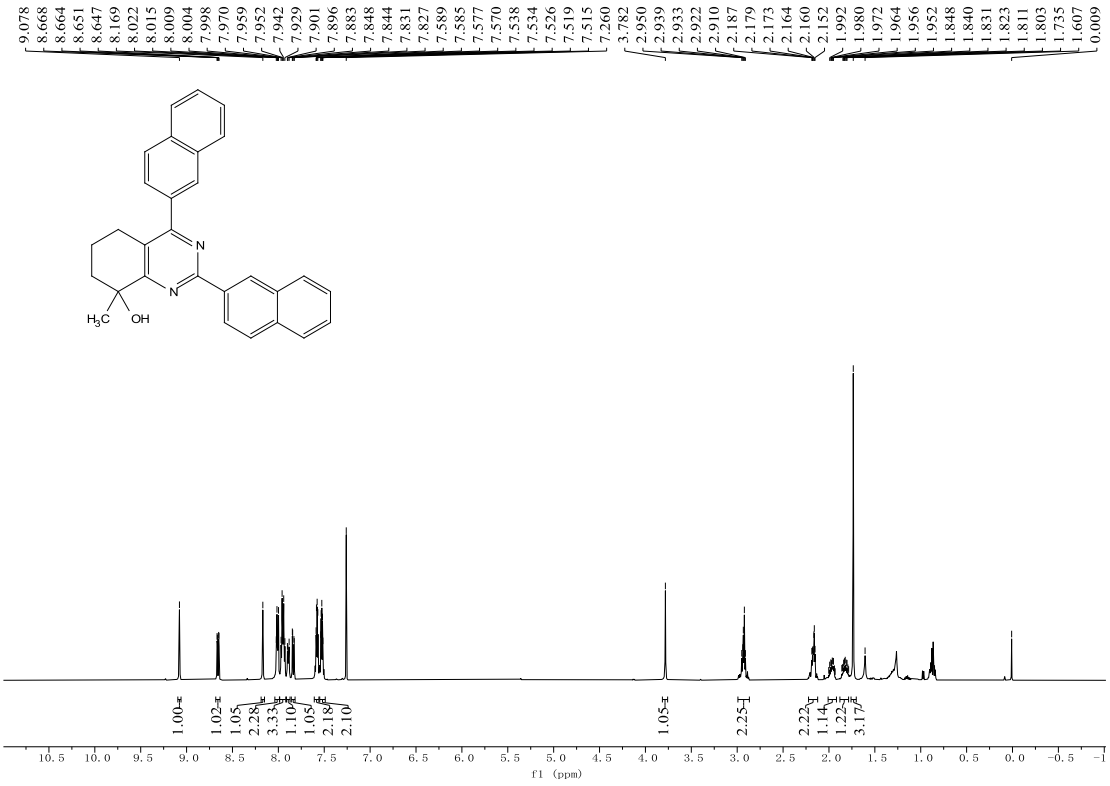


^{13}C NMR of **4n** (125 MHz, $CDCl_3$)

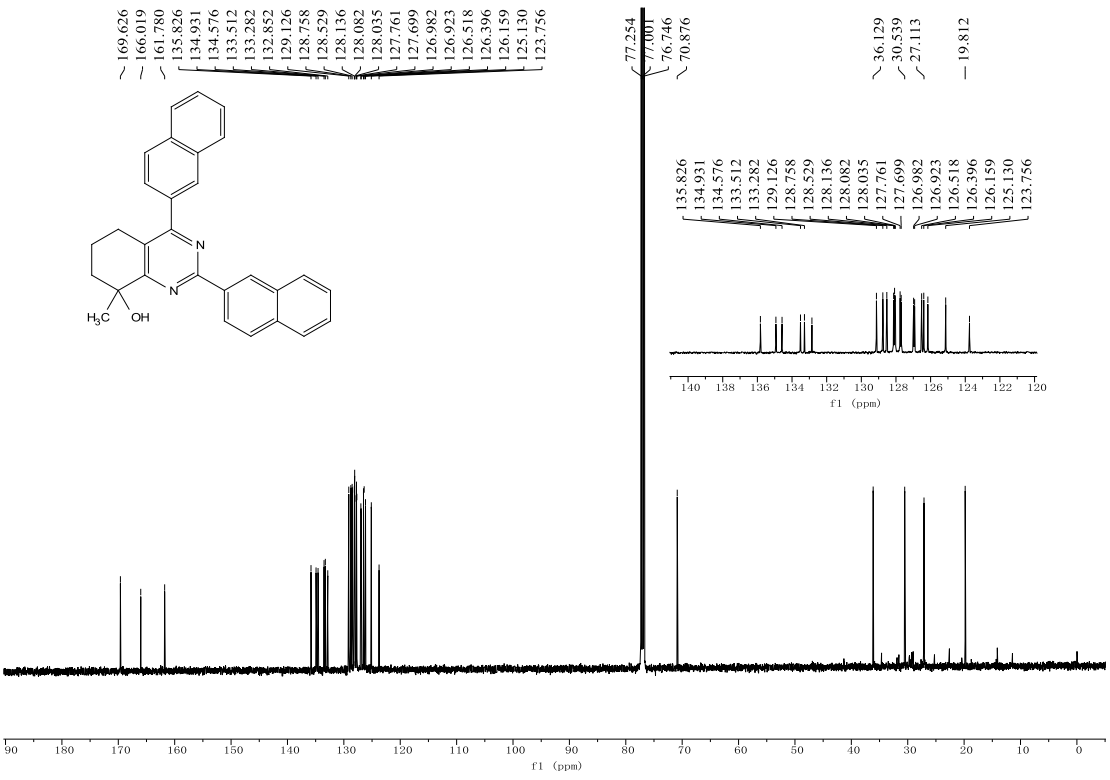


^{19}F NMR of **4n** (471 MHz, $CDCl_3$)

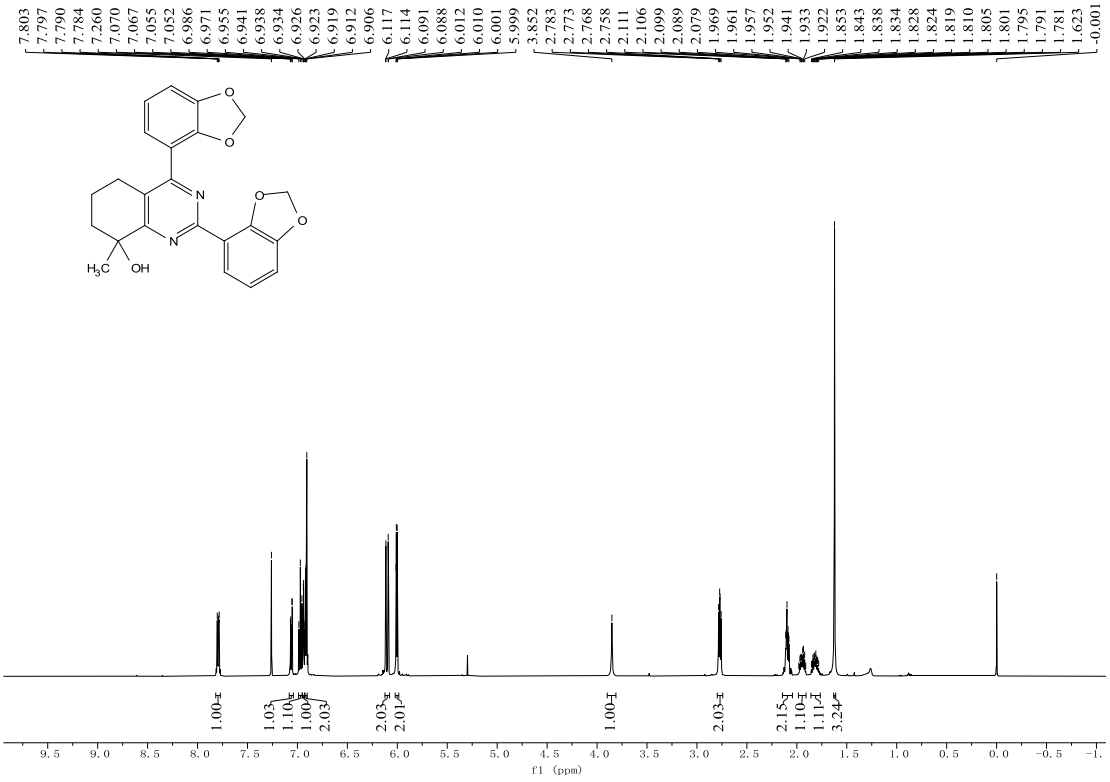
^{1}H NMR of **4o** (500 MHz, $CDCl_3$)



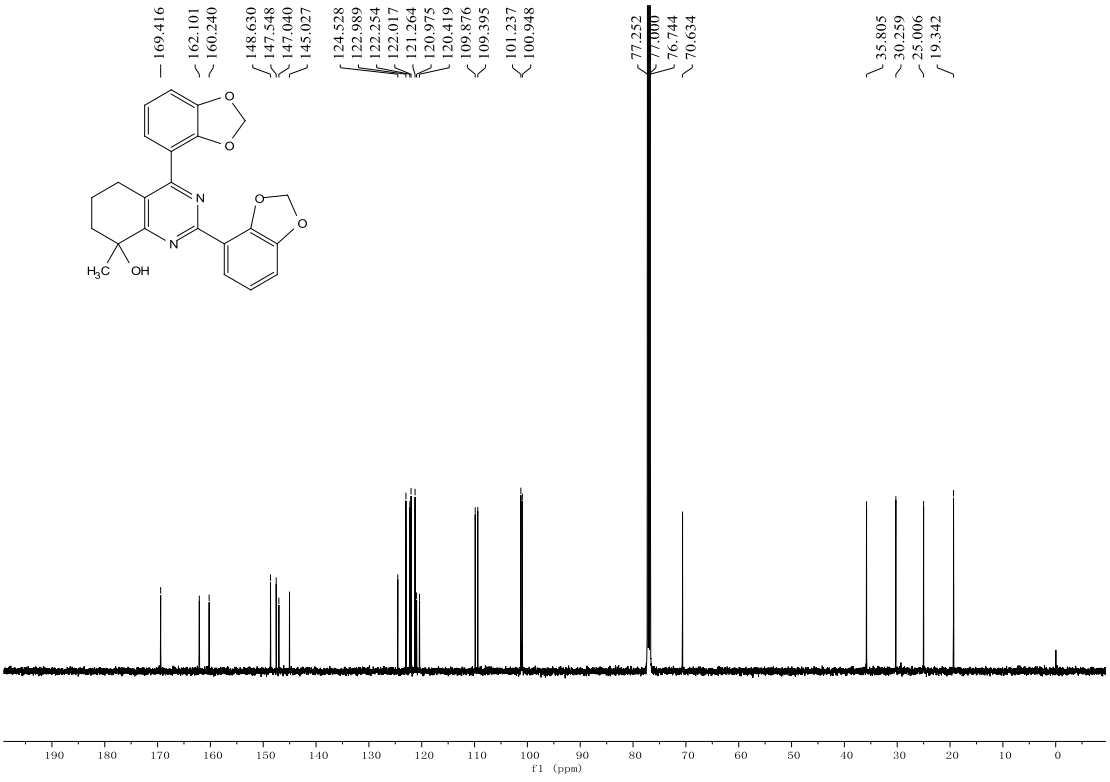
^{13}C NMR of **4o** (125 MHz, $CDCl_3$)



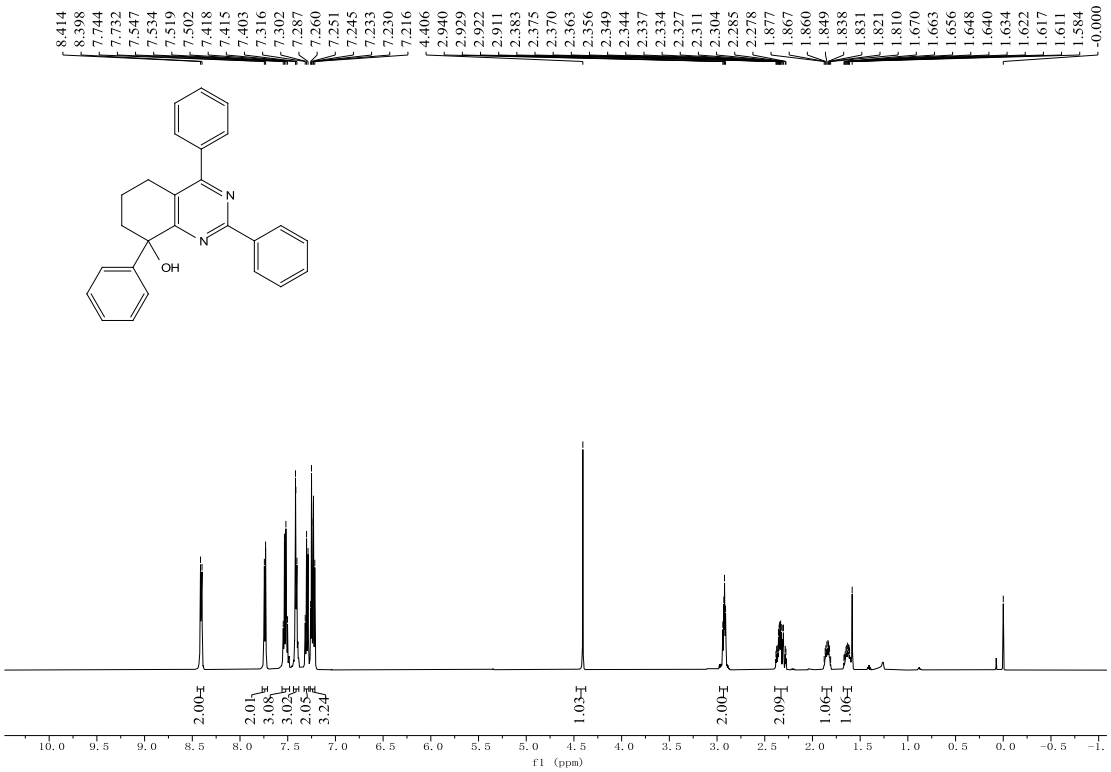
^{1}H NMR of **4p** (500 MHz, $CDCl_3$)



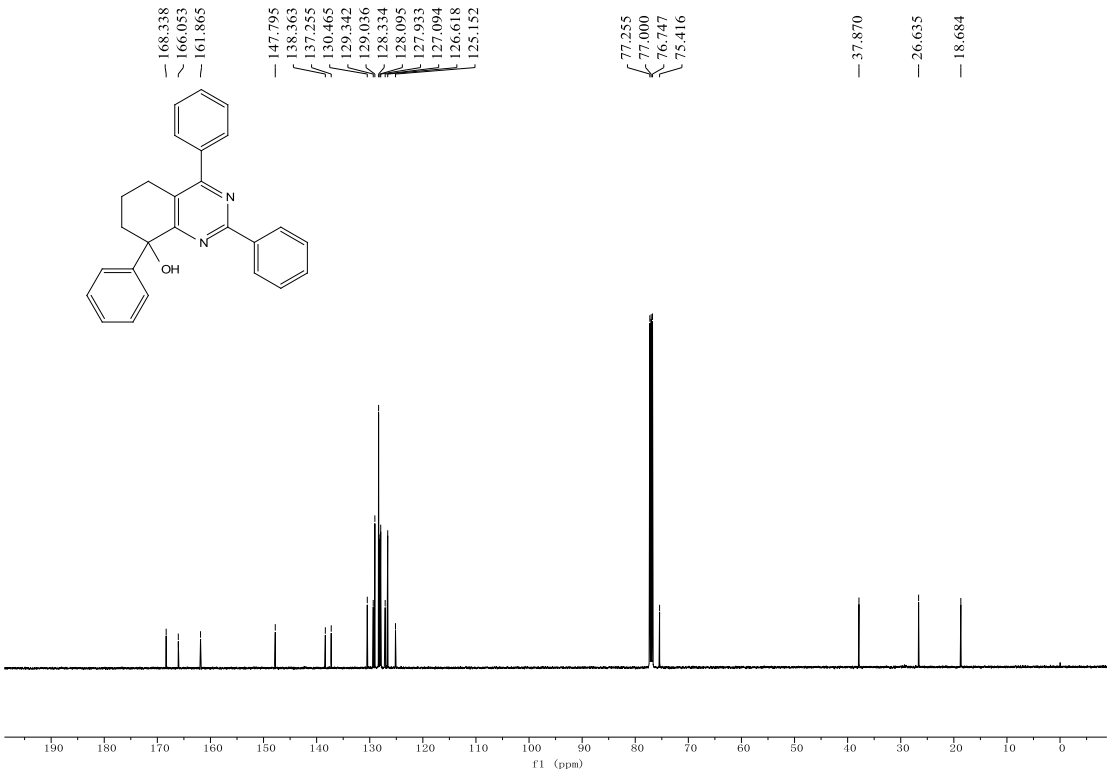
^{13}C NMR of **4p** (125 MHz, $CDCl_3$)



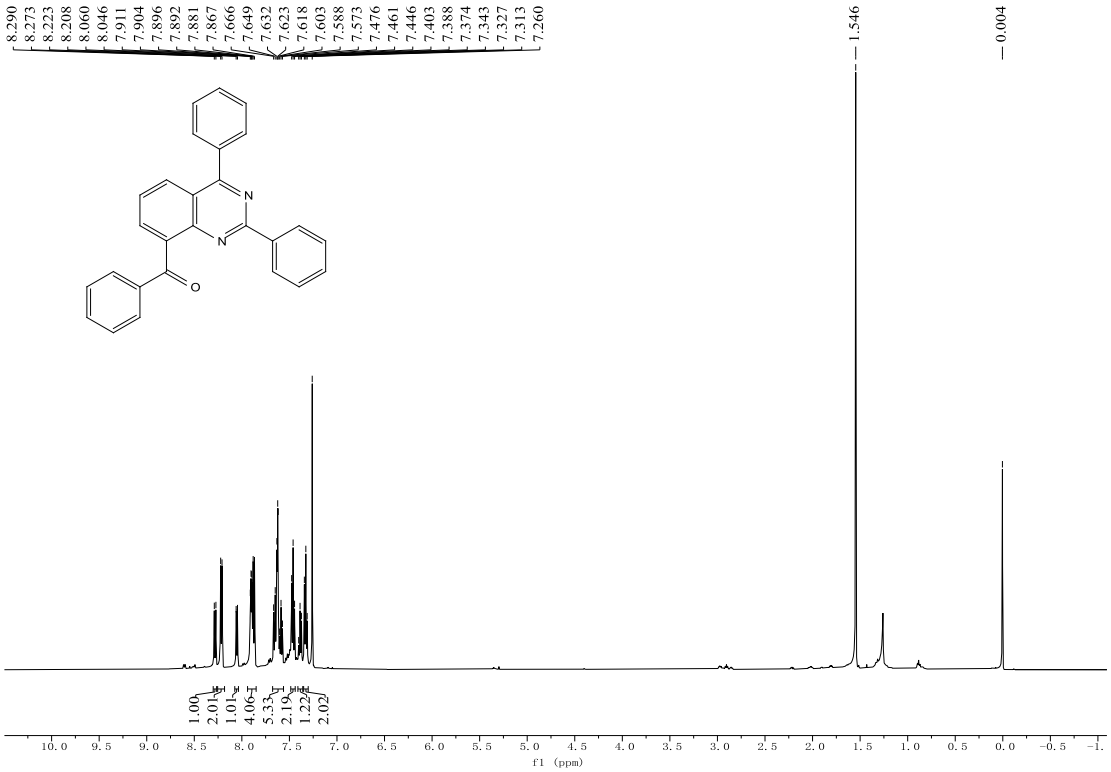
^{1}H NMR of **4q** (500 MHz, $CDCl_3$)



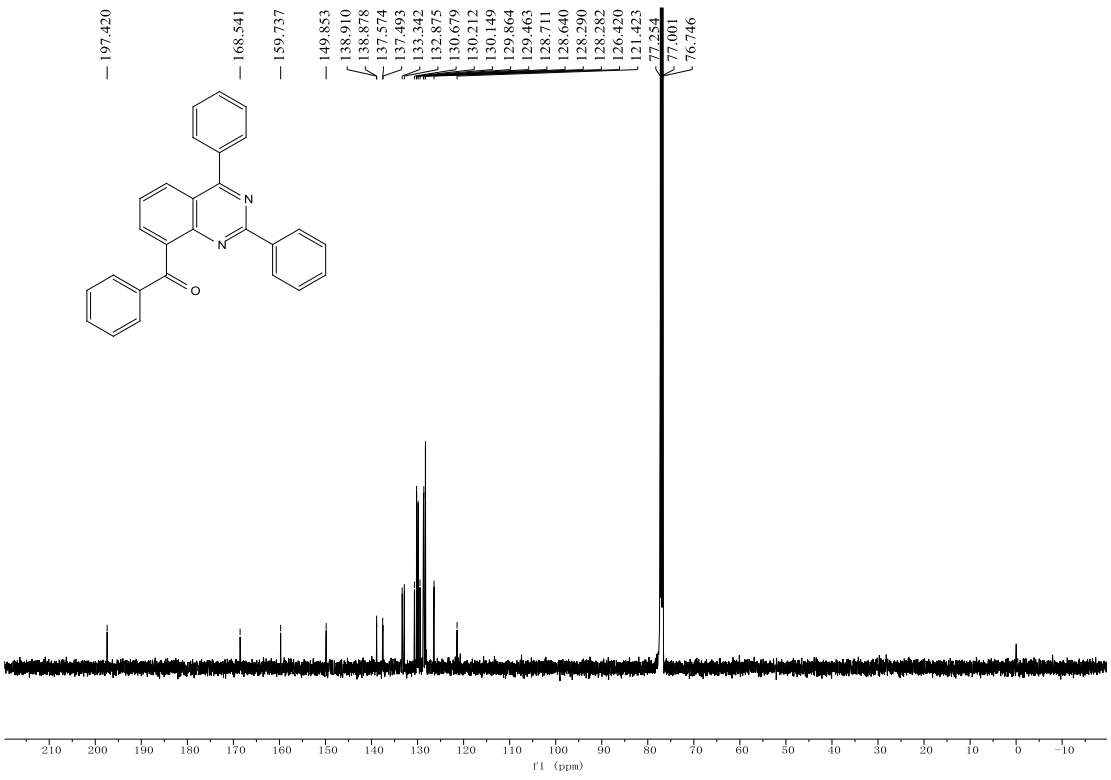
^{13}C NMR of **4q** (125 MHz, $CDCl_3$)



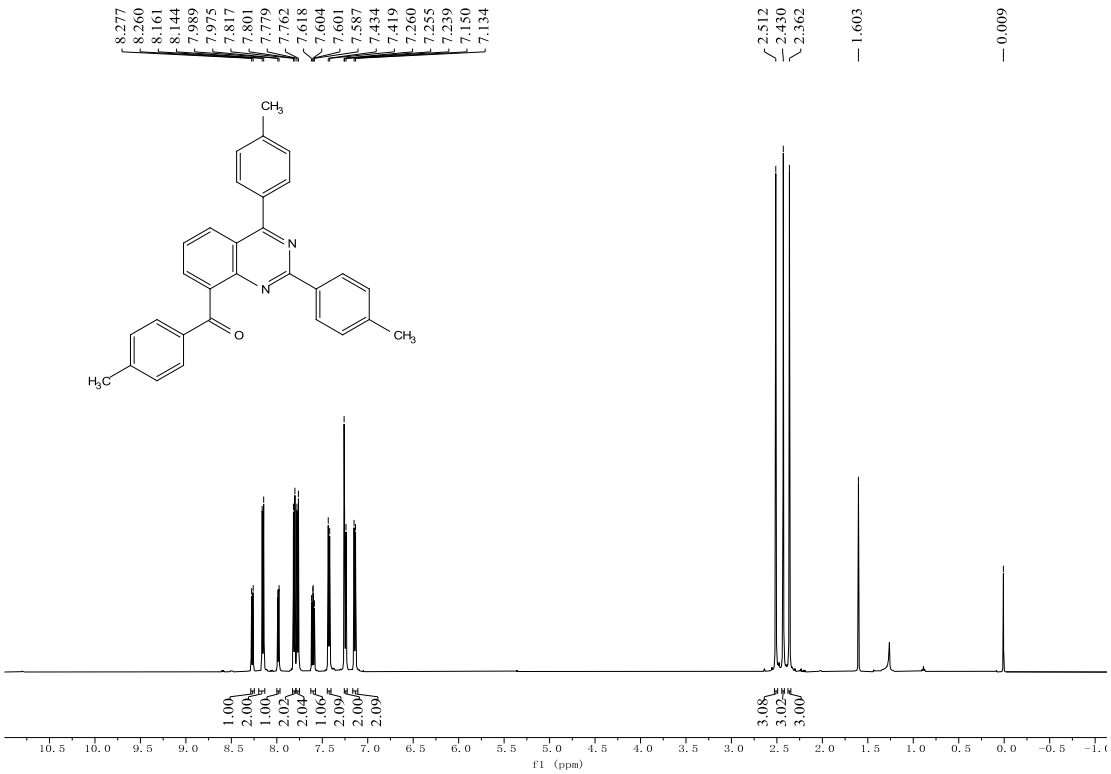
^{1}H NMR of **5a** (500 MHz, $CDCl_3$)



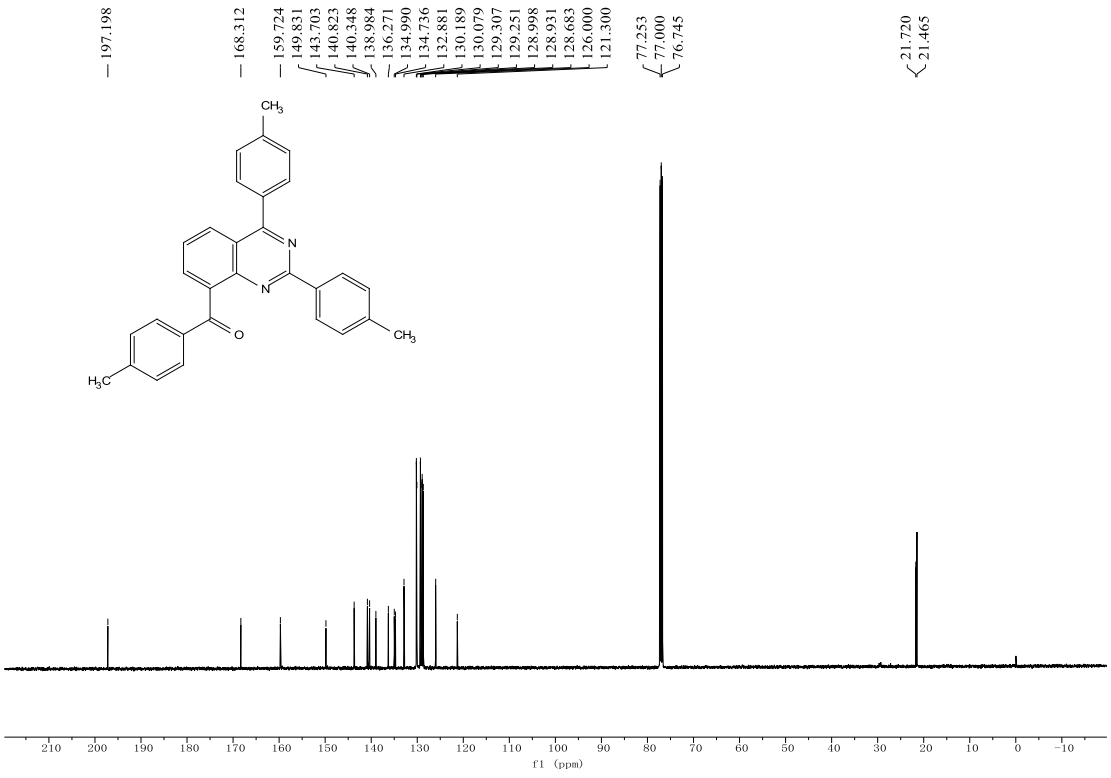
^{13}C NMR of **5a** (125 MHz, $CDCl_3$)



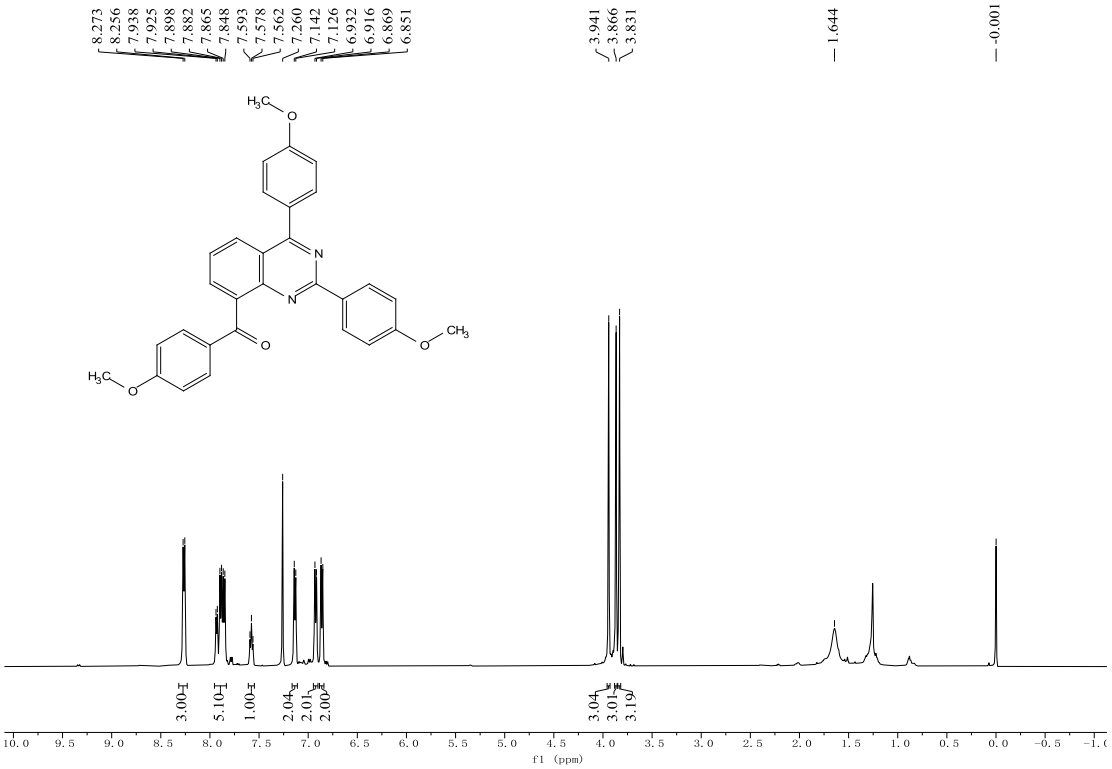
^{1}H NMR of **5b** (500 MHz, $CDCl_3$)



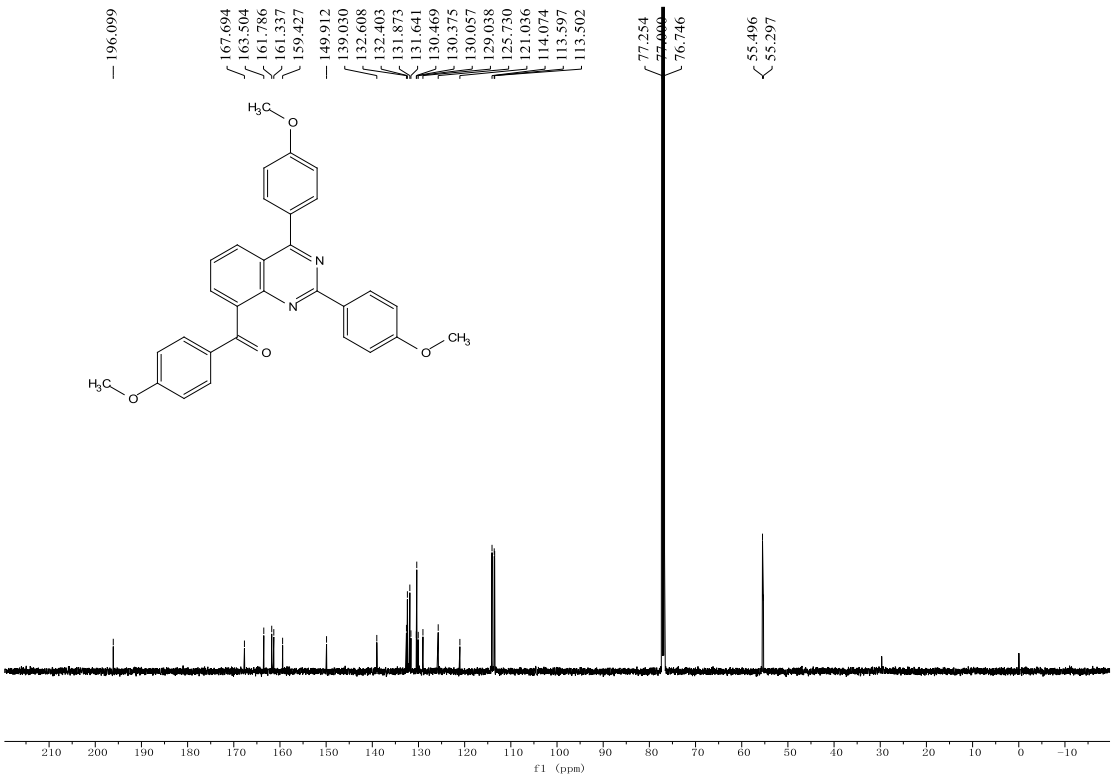
^{13}C NMR of **5b** (125 MHz, $CDCl_3$)



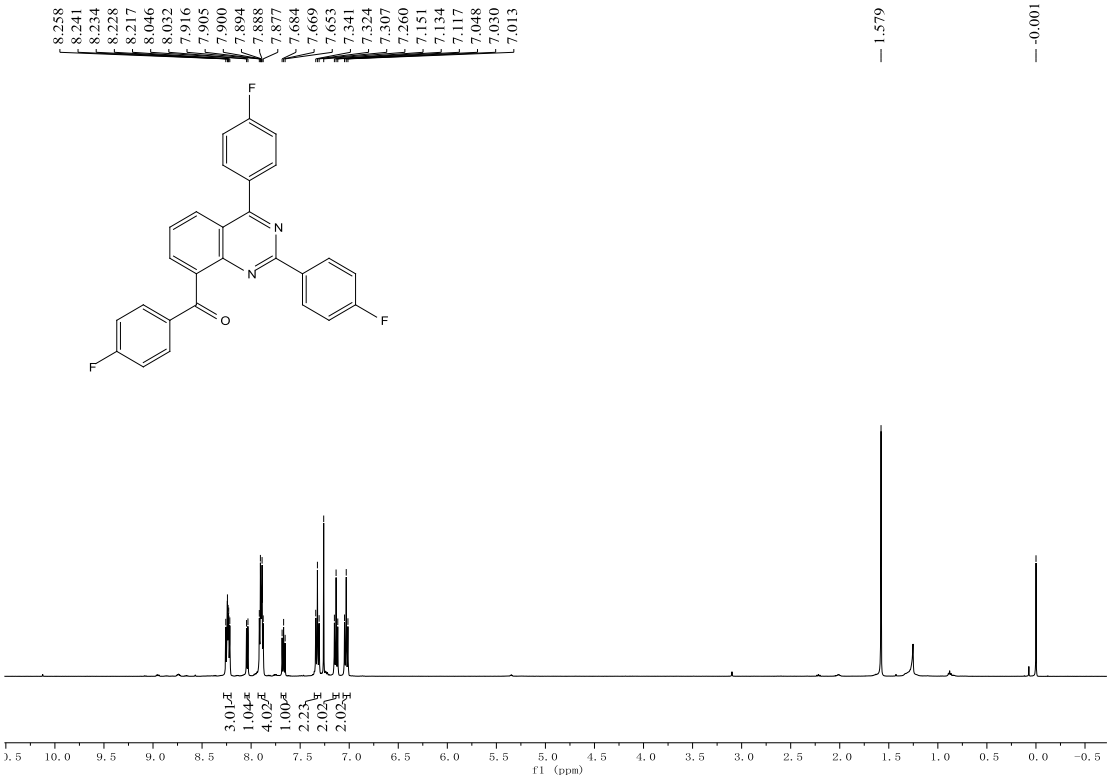
^{1}H NMR of **5c** (500 MHz, $CDCl_3$)



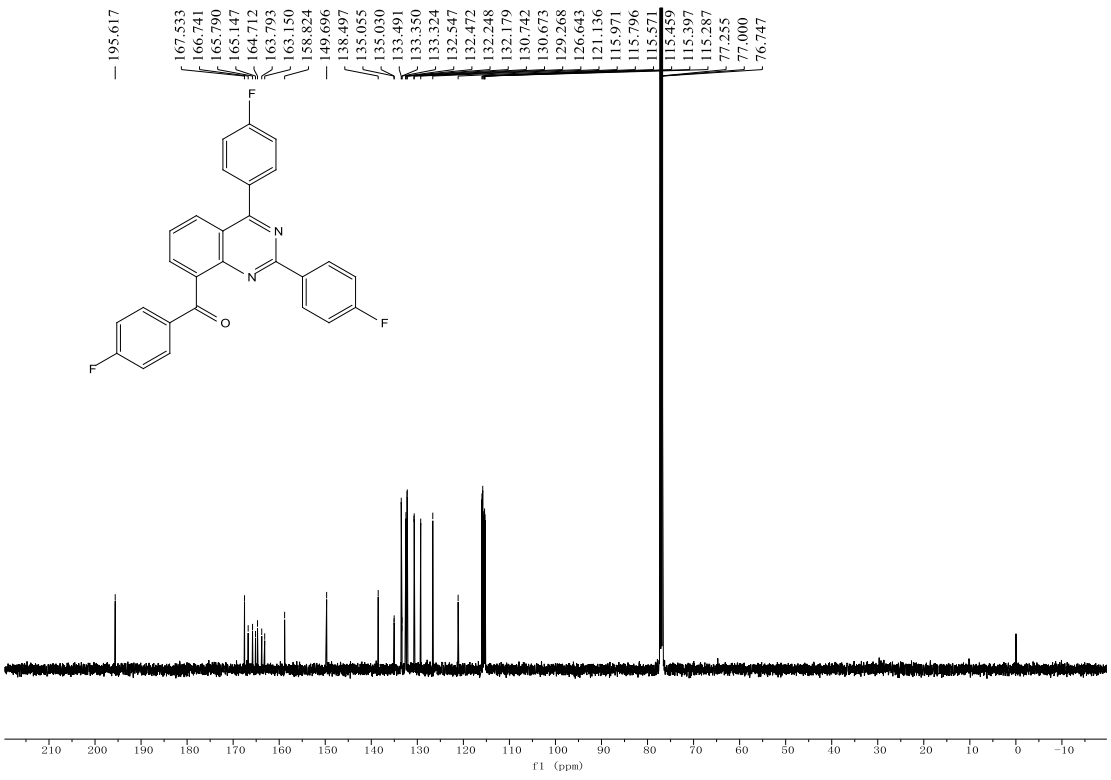
^{13}C NMR of **5c** (125 MHz, $CDCl_3$)



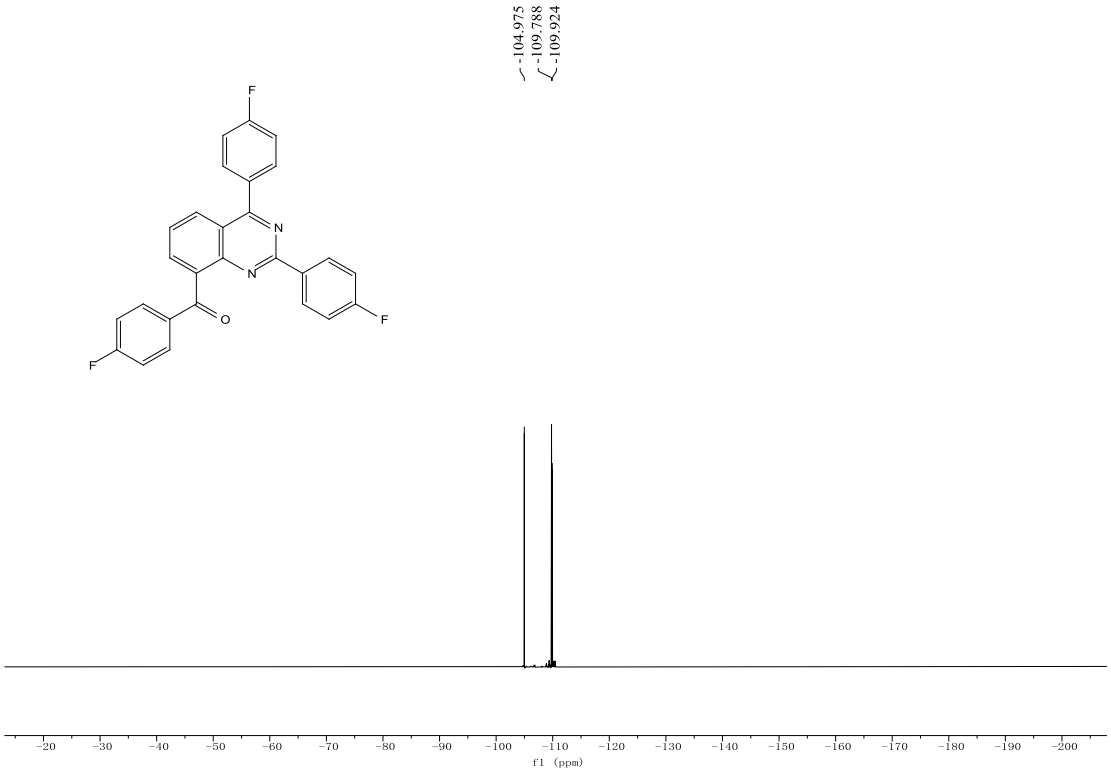
^{1}H NMR of **5d** (500 MHz, $CDCl_3$)



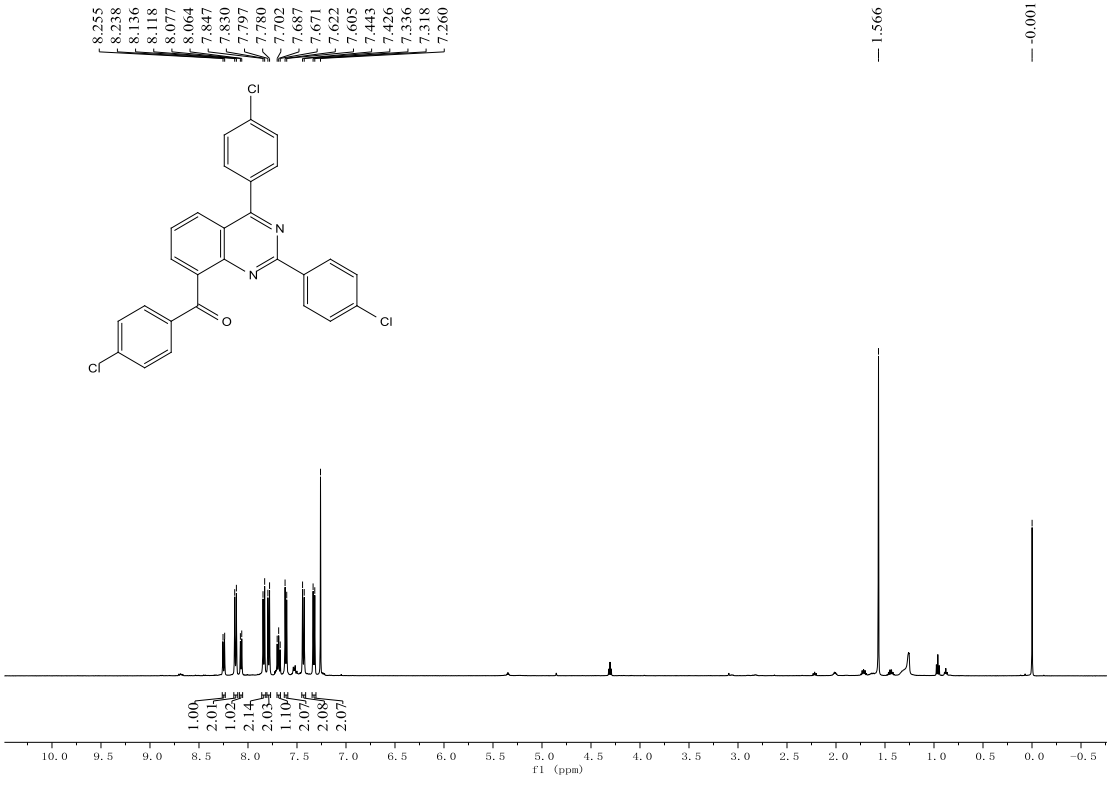
^{13}C NMR of **5d** (125 MHz, $CDCl_3$)



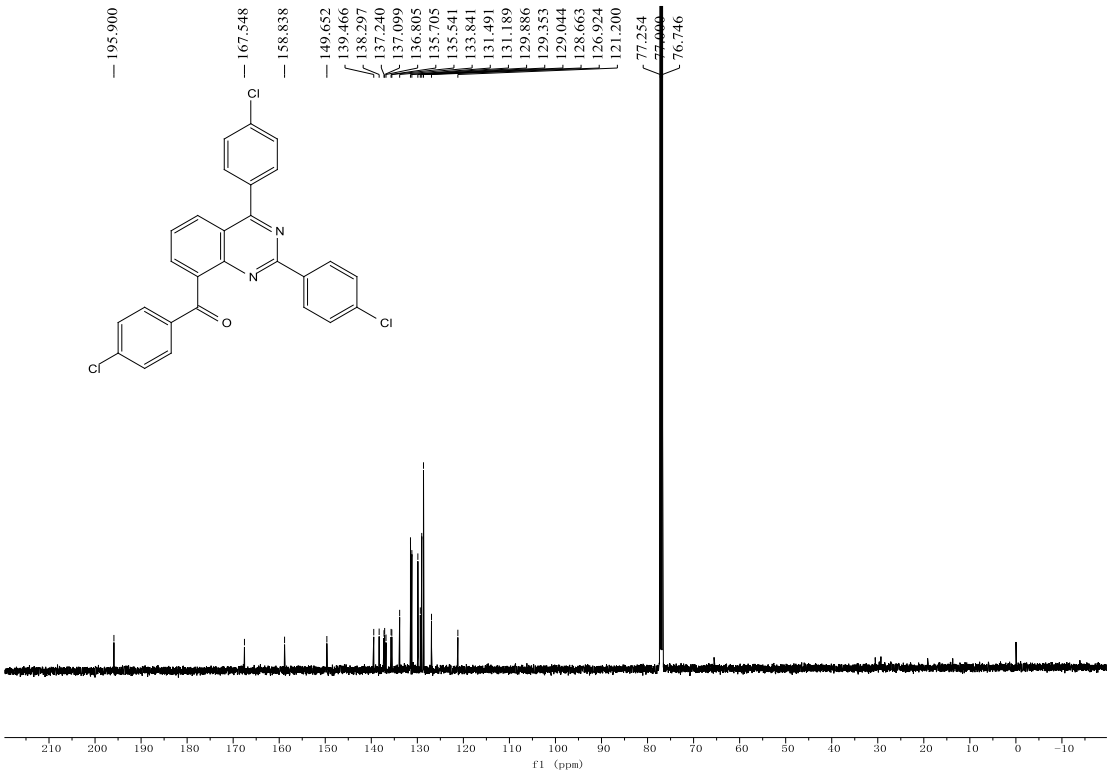
^{19}F NMR of **5d** (471 MHz, $CDCl_3$)



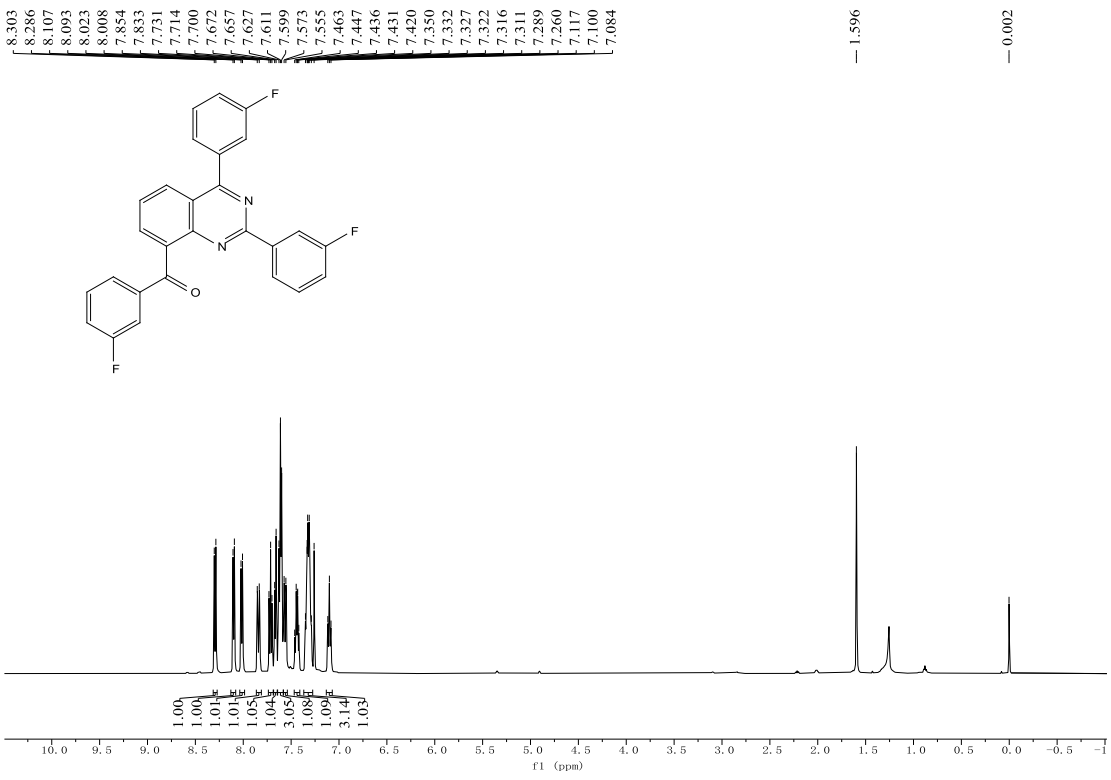
^{1}H NMR of **5e** (500 MHz, $CDCl_3$)



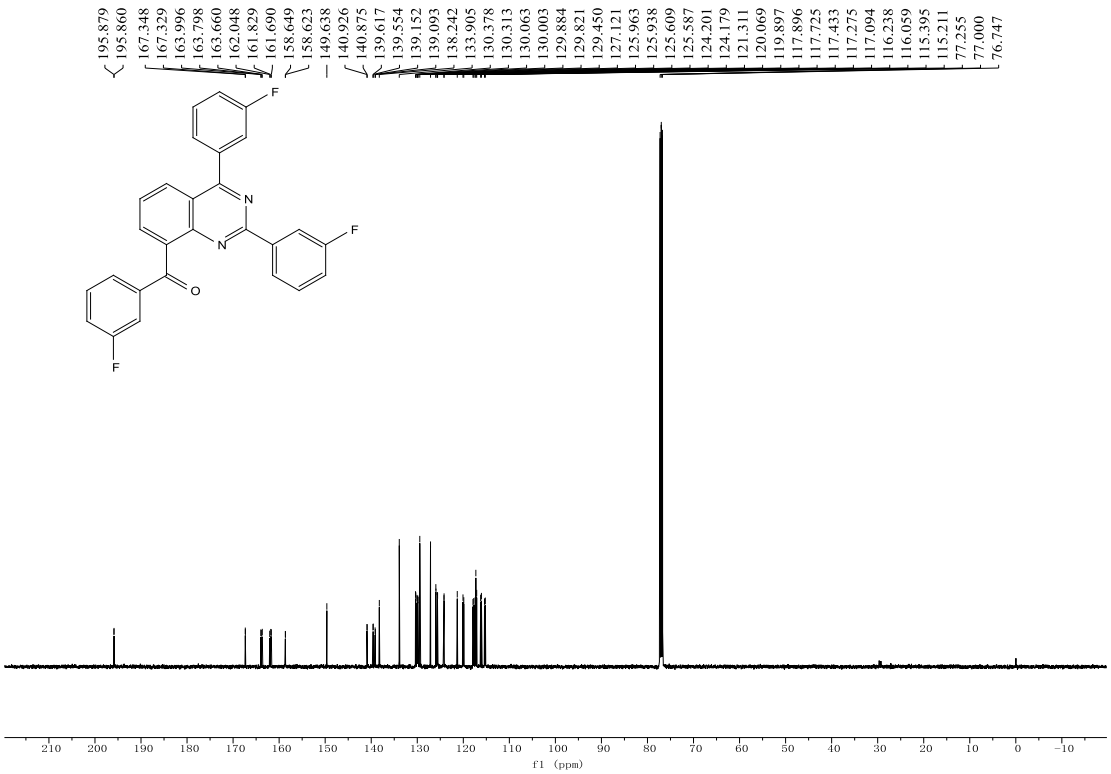
^{13}C NMR of **5e** (125 MHz, $CDCl_3$)



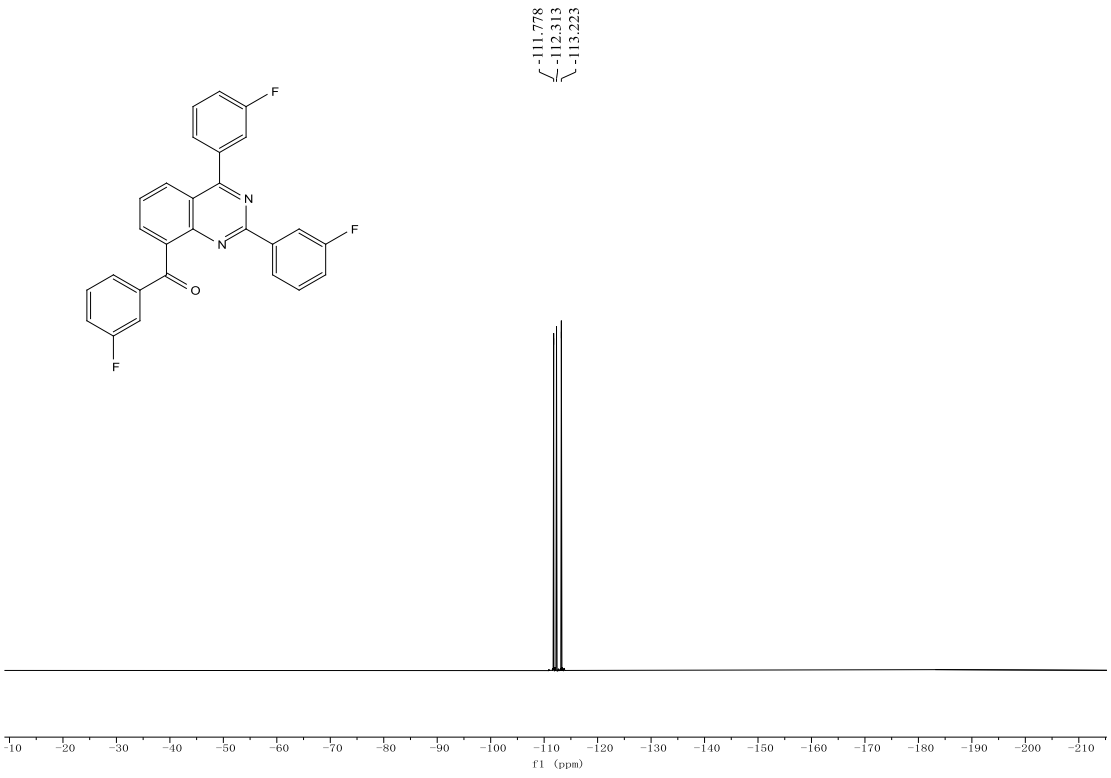
^{1}H NMR of **5f** (500 MHz, $CDCl_3$)



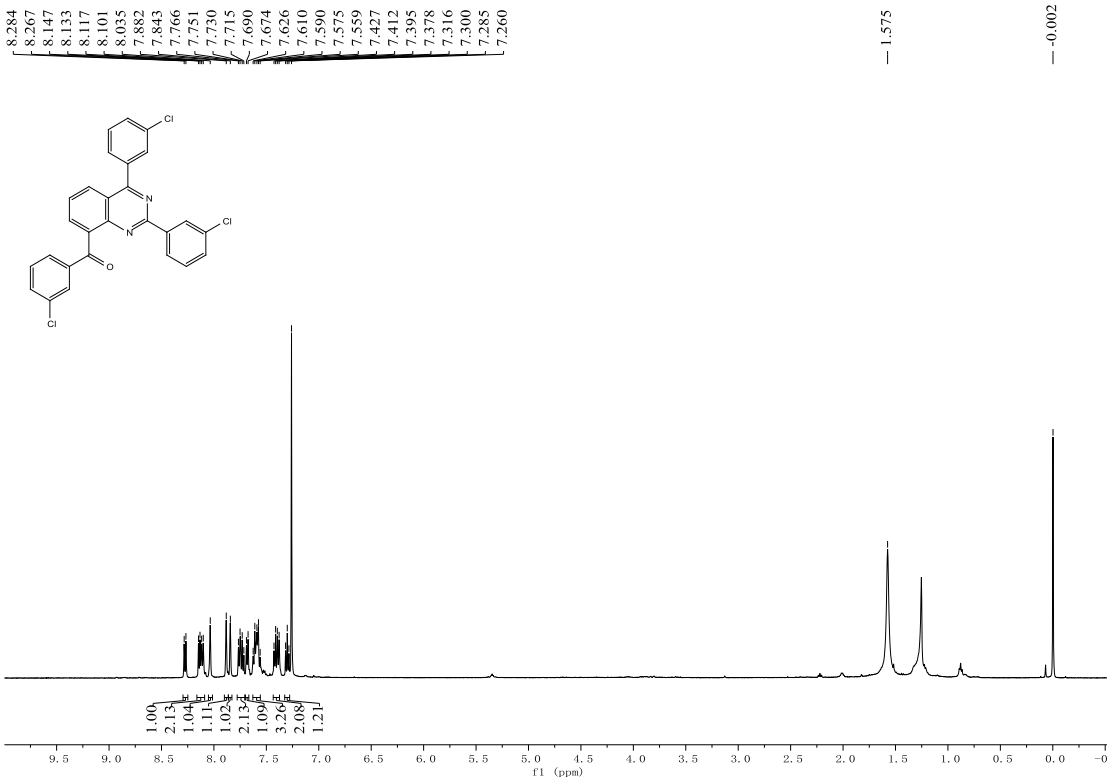
^{13}C NMR of **5f** (125 MHz, $CDCl_3$)



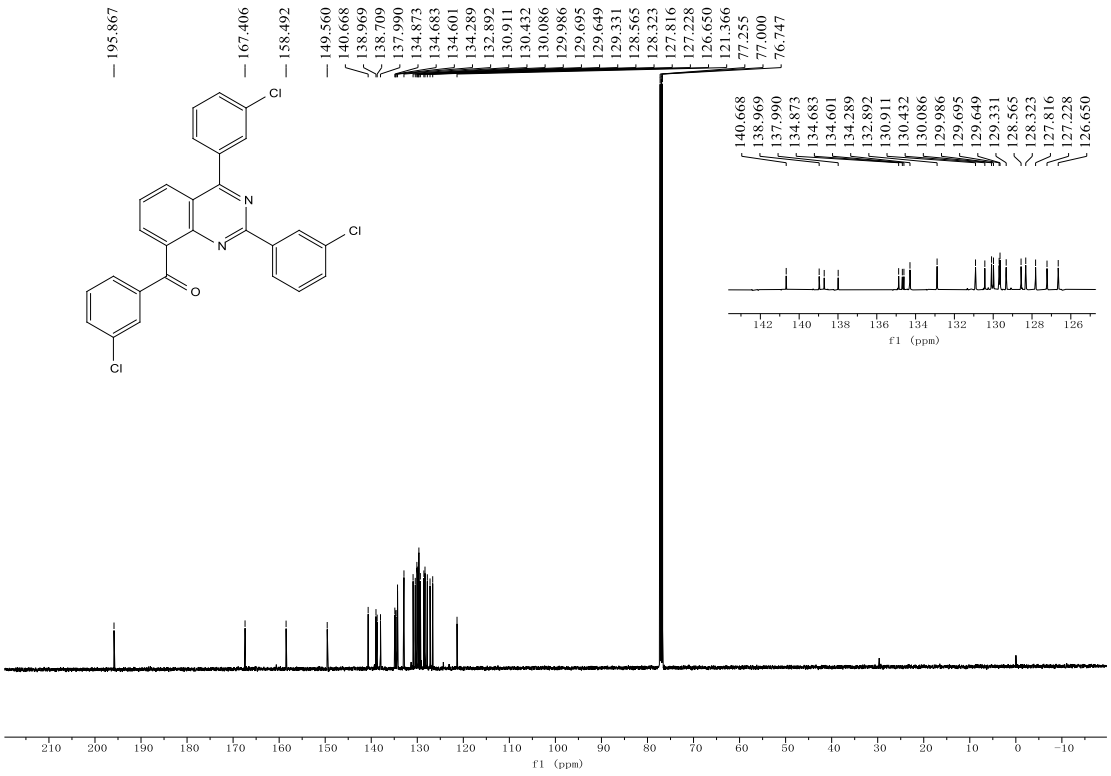
^{19}F NMR of **5f** (471 MHz, $CDCl_3$)



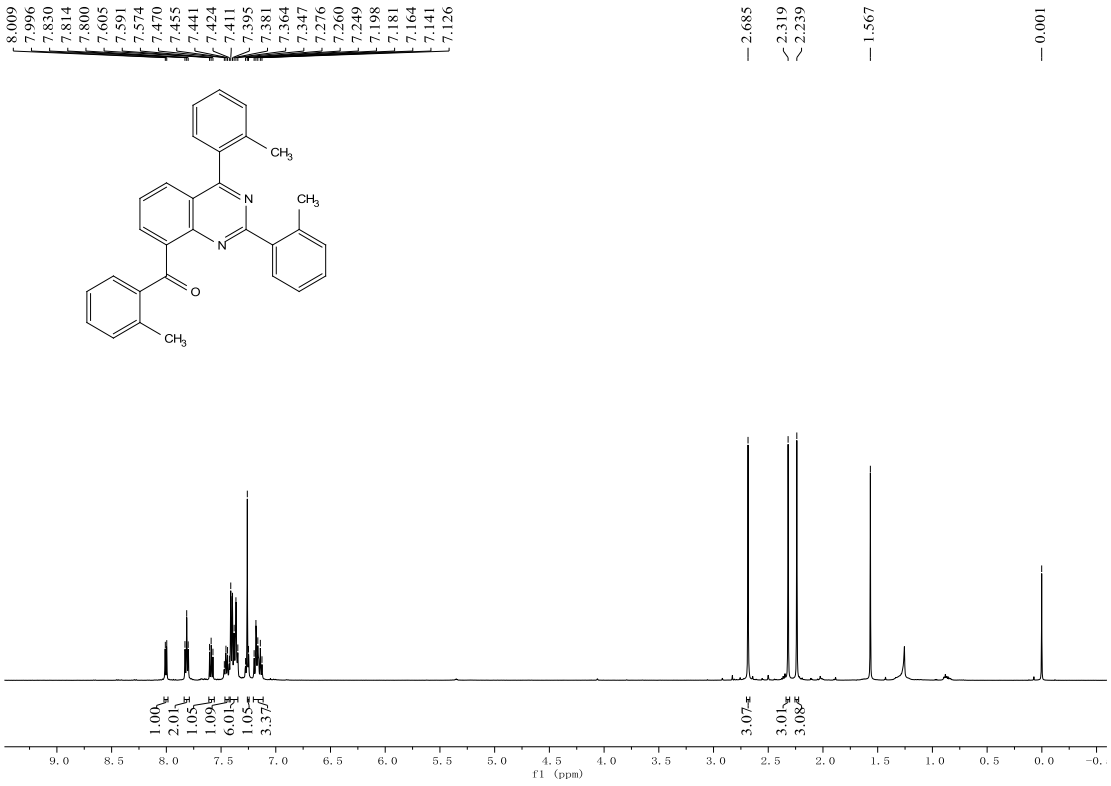
^{1}H NMR of **5g** (500 MHz, $CDCl_3$)



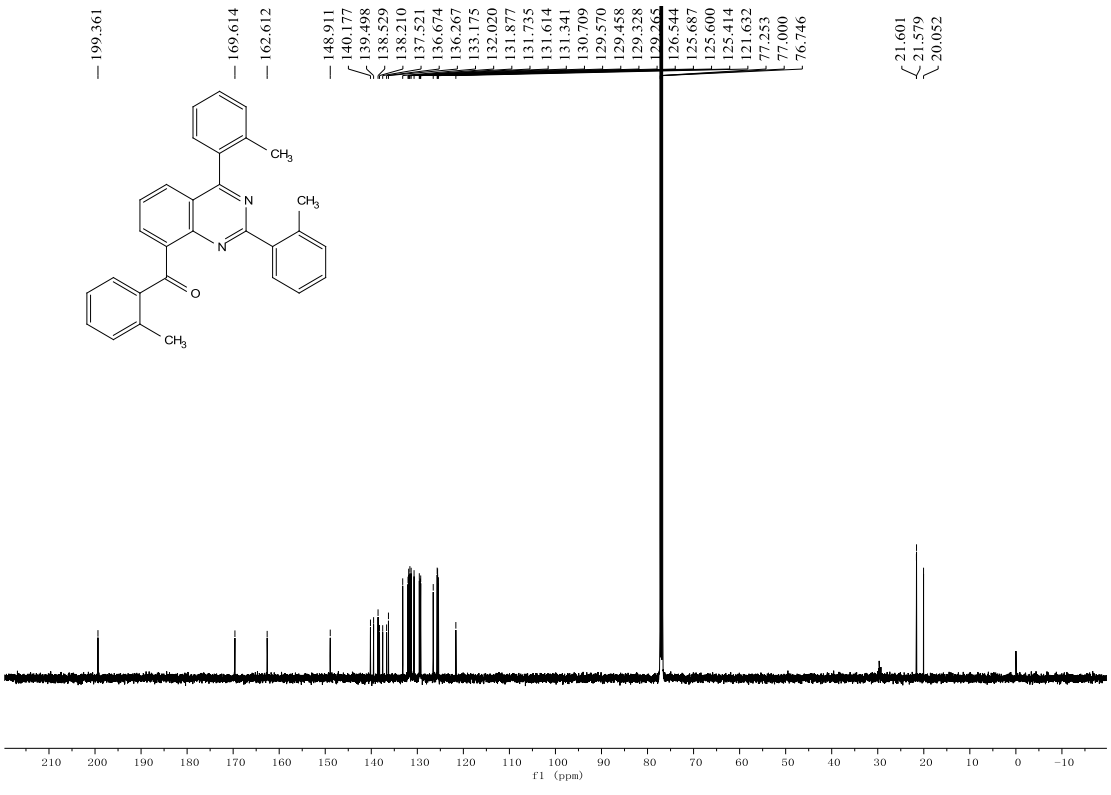
^{13}C NMR of **5g** (125 MHz, $CDCl_3$)



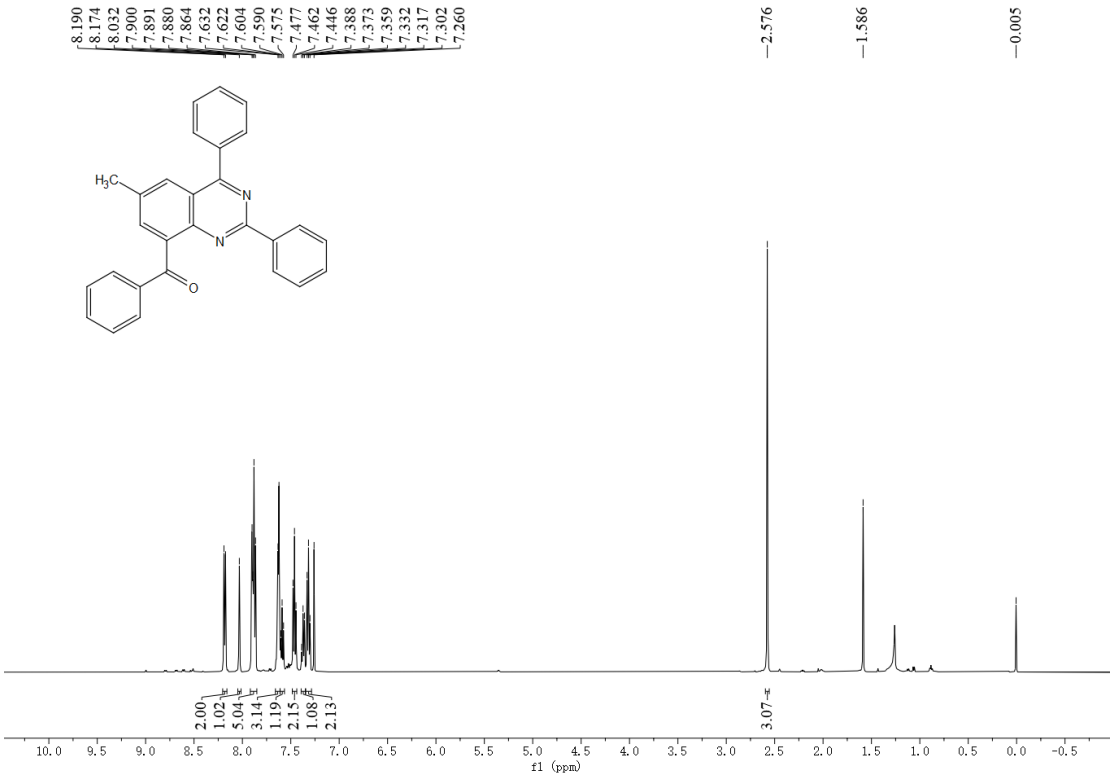
^{1}H NMR of **5h** (500 MHz, $CDCl_3$)



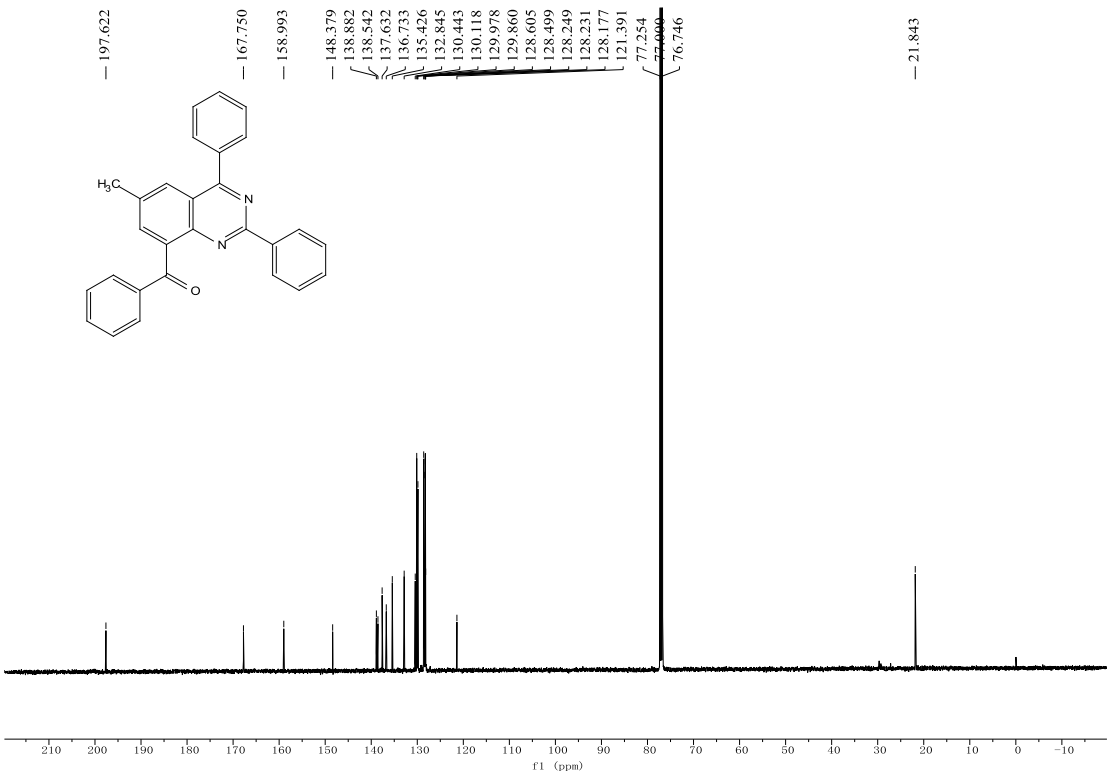
^{13}C NMR of **5h** (125 MHz, $CDCl_3$)



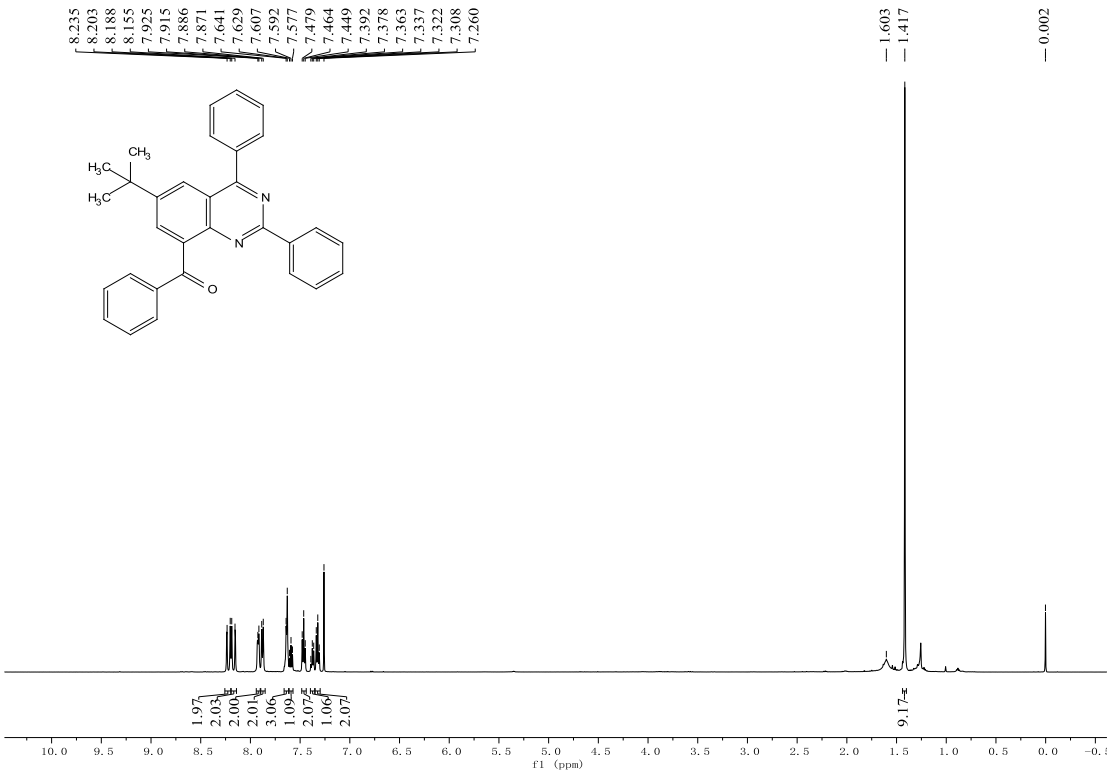
^{1}H NMR of **5i** (500 MHz, $CDCl_3$)



^{13}C NMR of **5i** (125 MHz, $CDCl_3$)



^{1}H NMR of **5j** (500 MHz, $CDCl_3$)



^{13}C NMR of **5j** (125 MHz, $CDCl_3$)