Supporting Information

Facile Ru-catalysed synthesis of quinazolin-4(3H)-ones by tandem cyclization of 2-nitrobenzonitrile and alcohol derivatives under air

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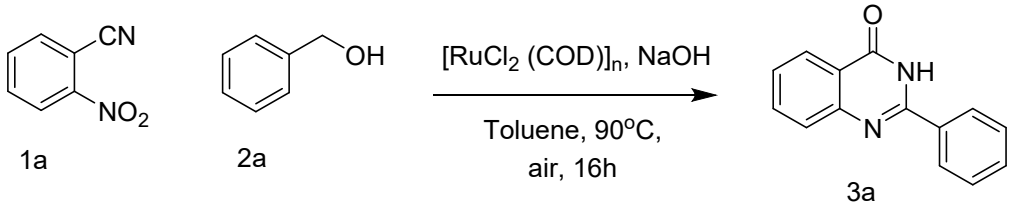
CONTENT

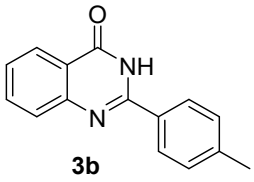
Experimental Section

General procedure for preparing of 2-phenylquinazolin-4(3*H*)-one 3a[1]



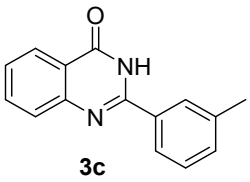
1a 2a 3a

A pressure tube with a magnetic stirring bar was charged with 2-nitrobenzonitrile (50 mg, 0.338 mmol, 1 equiv.), benzyl alcohol (146 mg, 1.352 mmol, 4 equiv.), NaOH (27 mg, 0.675 mg, 2 equiv.). Then, add the catalyst with $[RuCl_2COD)]_n$ (3.79 mg, 4 mol%). Toluene solvent (0.5 ml) was then introduced at the end. The reaction was carried out under air at a temperature of 90°C for 16 hours. After that, the reaction mixture was purified by column chromatography (eluent: hexane/ ethyl acetate (5/1)). Product **3a** was obtained as white solids, with yield of 92%. ^{1}H NMR (600 MHz, DMSO) δ 12.53 (s, 1H), 8.26 – 8.18 (m, 2H), 8.17 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.88 – 7.82 (m, 1H), 7.76 (dd, *J* = 8.2, 1.1 Hz, 1H), 7.63 – 7.58 (m, 1H), 7.58 – 7.55 (m, 2H), 7.55 – 7.51 (m, 1H). ^{13}C NMR (151 MHz, DMSO) δ 199.8, 190.0, 186.4, 172.2, 170.4, 169.0, 166.2, 165.4, 165.1, 164.2, 163.5, 158.6, 77.6, 77.4, 77.3, 77.2, 77.0, 76.9, 76.7.



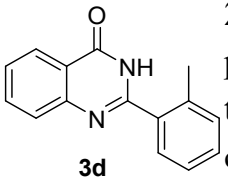
3b

2-(p-tolyl)quinazolin-4(3*H*)-one 3b[1] prepared following general procedure A using compound **1a** (50 mg, 0.338 mmol) and p-tolylmethanol (122 mg, 1.352 mmol). The product was purified by column chromatography (silica gel, hexane/ethylacetate (5:1)) to yield **3b** (89%) as a white solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 11.73 (s, 1H), 8.35 – 8.30 (m, 1H), 8.19 – 8.14 (m, 2H), 7.83 – 7.80 (m, 1H), 7.78 (ddd, *J* = 8.2, 6.8, 1.5 Hz, 1H), 7.48 (ddd, *J* = 8.1, 6.8, 1.5 Hz, 1H), 7.39 – 7.35 (m, 2H), 2.45 (s, 3H).^{13}C NMR (126 MHz, $CDCl_3$) δ 164.1, 152.0, 149.8, 142.3, 134.9, 130.2, 129.9, 128.1, 127.5, 126.6, 126.5, 120.9, 77.4, 77.1, 76.9, 21.6.



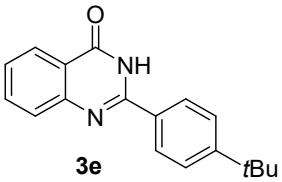
3c

2-(m-tolyl)quinazolin-4(3*H*)-one 3c[1] prepared following general procedure A using compound **1a** (50 mg, 0.338 mmol) and m-tolylmethanol (122 mg, 1.352 mmol). The product was purified by column chromatography (silica gel, hexane/ethylacetate (5:1)) to yield **3c** (90%) as a white solid. ^{1}H NMR (600 MHz, DMSO) δ 12.5 (s, 1H), 8.2 (dd, *J* = 7.9, 1.5 Hz, 1H), 8.0 (tt, *J* = 1.8, 0.8 Hz, 1H), 8.0 – 8.0 (m, 1H), 7.8 (ddd, *J* = 8.5, 7.1, 1.6 Hz, 1H), 7.8 – 7.7 (m, 1H), 7.5 (ddd, *J* = 8.1, 7.1, 1.2 Hz, 1H), 7.4 (t, *J* = 7.5 Hz, 1H), 7.4 – 7.4 (m, 1H), 2.4 (s, 3H).^{13}C NMR (126 MHz, DMSO) δ 152.4, 148.7, 137.9, 134.5, 132.6, 131.94, 128.4, 128.2, 127.4, 126.5, 125.8, 124.8, 120.9, 40.0, 39.9, 39.7, 39.5, 39.4, 39.2, 39.0, 20.9.



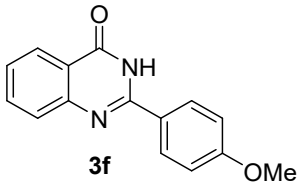
3d

2-(o-tolyl)quinazolin-4(3*H*)-one 3d[1] prepared following general procedure A using compound **1a** (50 mg, 0.338 mmol) and o-tolylmethanol (165 mg, 1,352 mmol). The product was purified by column chromatography (silica gel, hexane/ethylacetate (5:1)) to yield **3d** (85%) as a white solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.8 (s, 1H), 8.3 (dt, *J* = 7.9, 1.2 Hz, 1H), 7.8 – 7.8 (m, 2H), 7.6 – 7.5 (m, 2H), 7.4 (td, *J* = 7.4, 1.4 Hz, 1H), 7.4 (dq, *J* = 7.7, 0.7 Hz, 2H), 2.5 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.7, 153.4, 149.2, 136.9, 135.0, 133.8, 131.7, 130.8, 128.7, 128.1, 127.2, 126.6, 126.5, 121.0, 77.4, 77.2, 76.9, 20.2.



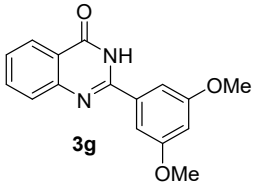
3e

2-(4-(tert-butyl)phenyl)quinazolin-4(3*H*)-one 3e[5] prepared following general procedure A using compound **1a** (50 mg, 0.338 mmol) and (4-(tert-butyl)phenyl)methanol (165 mg, 1,352 mmol). The product was purified by column chromatography (silica gel, hexane/ethylacetate (5:1)) to yield **3e** (93%) as a white solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 11.59 (s, 1H), 8.34 (ddd, *J* = 7.9, 1.6, 0.6 Hz, 1H), 8.22 – 8.15 (m, 2H), 7.83 (ddd, *J* = 8.2, 1.3, 0.6 Hz, 1H), 7.79 (ddd, *J* = 8.3, 6.9, 1.5 Hz, 1H), 7.62 – 7.56 (m, 2H), 7.50 (ddd, *J* = 8.1, 6.9, 1.3 Hz, 1H), 1.39 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.0, 155.4, 151.9, 149.8, 134.9, 130.1, 128.1, 127.3, 126.7, 126.5, 126.2, 121.0, 77.4, 77.2, 76.9, 35.2, 31.3.



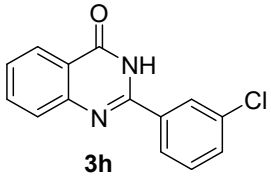
3f

2-(4-methoxyphenyl)quinazolin-4(3*H*)-one 3f[1] prepared following general procedure A using compound **1a** (50 mg, 0.338 mmol) and (4-methoxyphenyl)methanol (138 mg, 1,352 mmol). The product was purified by column chromatography (silica gel, hexane/ethylacetate (5:1)) to yield **3f** (83%) as a white solid.[1]H NMR (600 MHz, DMSO) δ 12.40 (s, 1H), 8.24 – 8.18 (m, 2H), 8.15 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.82 (ddd, *J* = 8.5, 7.1, 1.6 Hz, 1H), 7.74 – 7.69 (m, 1H), 7.49 (ddd, *J* = 8.1, 7.1, 1.2 Hz, 1H), 7.12 – 7.07 (m, 2H), 3.86 (s, 3H). [13]C NMR (151 MHz, DMSO) δ 162.3, 161.9, 151.9, 148.9, 134.5, 129.4, 127.2, 126.1, 125.8, 124.8, 120.65, 114.0, 55.4, 40.1, 39.9, 39.8, 39.7, 39.5, 39.4, 39.2, 39.1.



3g

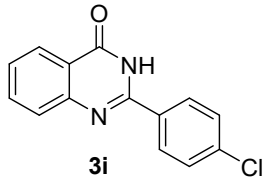
2-(3,5-dimethoxyphenyl)quinazolin-4(3*H*)-one 3g[4] prepared following general procedure A using compound **1a** (50 mg, 0.338 mmol) and (3,5-dimethoxyphenyl)methanol (168 mg, 1,352 mmol). The product was purified by column chromatography (silica gel, hexane/ethylacetate (5:1)) to yield **3g** (76%) as a white solid. [1]H NMR (600 MHz, DMSO) δ 12.47 (s, 1H), 8.17 – 8.13 (m, 1H), 7.85 – 7.79 (m, 1H), 7.76 – 7.71 (m, 1H), 7.51 (ddd, *J* = 8.0, 7.0, 1.0 Hz, 1H), 7.38 (d, *J* = 2.3 Hz, 2H), 6.68 (t, *J* = 2.3 Hz, 1H), 3.84 (s, 6H). [13]C NMR (151 MHz, DMSO) δ 162.2, 160.5, 151.9, 148.5, 134.6, 134.5, 127.5, 126.6, 125.8, 121.1, 105.5, 103.8, 55.5, 40.1, 39.9, 39.8, 39.7, 39.5, 39.4, 39.2, 39.1.



3h

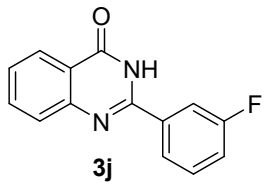
2-(3-chlorophenyl)quinazolin-4(3*H*)-one 3h[2] prepared following general procedure A using compound **1a** (50 mg, 0.338 mmol) and (3-chlorophenyl)methanol (142 mg, 1,352 mmol). The product was purified by column chromatography (silica gel, hexane/ethylacetate (5:1)) to yield **3h** (61%) as a white solid. [1]H NMR (600 MHz, DMSO) δ 12.60 (s, 1H), 8.25 (d, *J* = 2.1 Hz, 1H), 8.17 (td, *J* = 5.4, 2.5 Hz, 2H), 7.88 – 7.83 (m, 1H), 7.77 (d, *J* = 8.1 Hz, 1H), 7.66 (dd, *J* = 7.9, 2.1 Hz, 1H), 7.57 (dt, *J* = 23.7, 7.7 Hz, 2H). [13]C NMR

(151 MHz, DMSO) δ 162.1, 151.0, 148.4, 134.7, 134.6, 133.4, 131.1, 130.5, 127.5, 126.9, 126.4, 125.8, 121.1, 39.9, 39.8, 39.7, 39.5, 39.4, 39.2, 39.1.



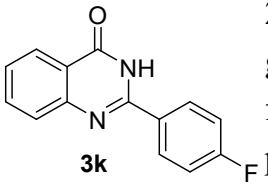
3i

2-(4-chlorophenyl)quinazolin-4(3H)-one 3i[3] prepared following general procedure A using compound **1a** (50 mg, 0.338 mmol) and (4-chlorophenyl)methanol (142 mg, 1,352 mmol). The product was purified by column chromatography (silica gel, hexane/ethylacetate (5:1)) to yield **3i** (68%) as a white solid. ^{1}H NMR (600 MHz, DMSO) δ 12.59 (s, 1H), 8.31 – 8.19 (m, 2H), 8.16 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.85 (tt, *J* = 8.2, 1.2 Hz, 1H), 7.75 (d, *J* = 8.1 Hz, 1H), 7.63 (d, *J* = 8.2 Hz, 2H), 7.54 (td, *J* = 7.5, 1.2 Hz, 1H). ^{13}C NMR (126 MHz, DMSO) δ 162.1, 151.3, 148.5, 136.2, 134.6, 131.5, 129.5, 128.6, 127.5, 126.7, 125.8, 121.0, 40.1, 40.0, 40.0, 39.8, 39.8, 39.7, 39.6, 39.5, 39.4, 39.3, 39.2, 39.0.



3j

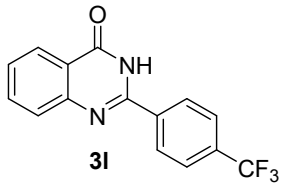
2-(3-fluorophenyl)quinazolin-4(3*H*)-one 3j[5] prepared following general procedure A using compound **1a** (50 mg, 0.338 mmol) and (3-fluorophenyl)methanol (126 mg, 1,352 mmol). The product was purified by column chromatography (silica gel,hexane/ethylacetate (5:1)) to yield **3j** (90%) as a white solid. ^{1}H NMR (600 MHz, DMSO) δ 12.59 (s, 1H), 8.17 (dd, *J* = 7.9, 1.5 Hz, 1H), 8.07 (dt, *J* = 7.8, 1.2 Hz, 1H), 8.01 (dt, *J* = 10.5, 2.1 Hz, 1H), 7.86 (ddd, *J* = 8.4, 7.1, 1.6 Hz, 1H), 7.77 (dd, *J* = 8.3, 1.1 Hz, 1H), 7.61 (td, *J* = 8.0, 5.9 Hz, 1H), 7.58 – 7.51 (m, 1H), 7.45 (td, *J* = 8.7, 3.1 Hz, 1H). ^{13}C NMR (126 MHz, DMSO) δ 162.0 (d, *J* = 243.8 Hz), 162.0, 151.0, 148.4, 135.0 (d, *J* = 7.8 Hz), 134.6, 130.7 (d, *J* = 8.4 Hz), 127.5, 126.8, 125.8, 123.9 (d, *J* = 2.8 Hz), 121.1, 118.2 (d, *J* = 21.1 Hz), 114.5 (d, *J* = 24.0 Hz).



3k

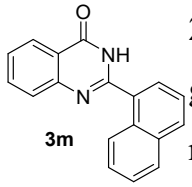
2-(4-fluorophenyl)quinazolin-4(3*H*)-one 3k[1] prepared following general procedure A using compound **1a** (50 mg, 0.338 mmol) and (4-fluorophenyl)methanol (126 mg, 1,352 mmol). The product was purified by column chromatography (silica gel, hexane/ethylacetate (5:1)) to yield **3k** (92%) as a white solid. ^{1}H NMR (600 MHz, DMSO) δ 12.54 (s, 1H), 8.33 – 8.19 (m, 2H), 8.16 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.84 (ddd, *J* = 8.5, 7.1, 1.6 Hz, 1H), 7.74 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.53 (ddd, *J* = 8.1, 7.1, 1.2 Hz, 1H), 7.39 (td, *J* = 8.7, 1.7 Hz, 2H). ^{13}C NMR (126 MHz, DMSO) δ 164.0 (d, *J* = 249.5 Hz), 162.2, 151.4,

134.6, 130.4 (d, *J* = 9.0 Hz), 129.2 (d, *J* = 3.1 Hz), 127.4, 126.6, 125.8, 120.8, 115.6 (d, *J* = 21.9 Hz).



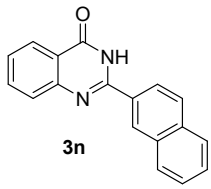
3l

2-(4-(trifluoromethyl)phenyl)quinazolin-4(3*H*)-one 3l[2] prepared following general procedure A using compound **1a** (50 mg, 0.338 mmol) and (4-(trifluoromethyl)phenyl)methanol (176 mg, 1,352 mmol). The product was purified by column chromatography (silica gel, hexane/ethylacetate (5:1)) to yield **3l** (75%) as a white solid. ^{1}H NMR (600 MHz, DMSO) δ 12.73 (s, 1H), 8.38 (d, *J* = 8.1 Hz, 2H), 8.19 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.93 (d, *J* = 8.1 Hz, 2H), 7.87 (ddd, *J* = 8.7, 7.1, 1.6 Hz, 1H), 7.78 (d, *J* = 8.1 Hz, 1H), 7.59 – 7.55 (m, 1H). ^{13}C NMR (151 MHz, DMSO) δ 162.1, 151.1, 148.4, 136.6, 134.6, 131.1 (d, *J* = 31.9 Hz), 128.7, 127.6, 127.0, 125.8, 125.4 (q, *J* = 3.8 Hz), 124.8, 123.0, 121.2.



3m

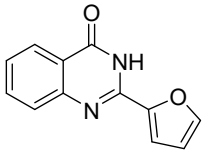
2-(naphthalen-1-yl)quinazolin-4(3*H*)-one 3m[2] prepared following general procedure A using compound **1a** (50 mg, 0.338 mmol) and naphthalen-1-ylmethanol (158 mg, 1,352 mmol). The product was purified by column chromatography (silica gel, hexane/ethylacetate (5:1)) to yield **3m** (80%) as a white solid.^{1}H NMR (600 MHz, DMSO) δ 12.65 (s, 1H), 8.25 – 8.20 (m, 1H), 8.20 – 8.15 (m, 1H), 8.12 (dt, *J* = 8.3, 1.1 Hz, 1H), 8.07 – 8.03 (m, 1H), 7.87 (ddd, *J* = 8.1, 7.1, 1.6 Hz, 1H), 7.80 (dd, *J* = 7.1, 1.2 Hz, 1H), 7.76 – 7.72 (m, 1H), 7.65 (dd, *J* = 8.3, 7.1 Hz, 1H), 7.62 – 7.56 (m, 3H). ^{13}C NMR (151 MHz, DMSO) δ 161.8, 153.6, 148.7, 134.5, 133.1, 131.7, 130.3, 130.2, 128.3, 127.6, 127.4, 127.0, 126.7, 126.3, 125.8, 125.2, 125.0, 121.2.



3n

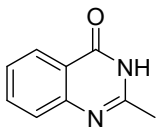
2-(naphthalen-2-yl)quinazolin-4(3*H*)-one 3n[4] prepared following general procedure A using compound **1a** (50 mg, 0.338 mmol) and naphthalen-2-ylmethanol (158 mg, 1,352 mmol). The product was purified by column chromatography (silica gel, hexane/ethylacetate (5:1)) to yield **3n** (85%) as a white solid. ^{1}H NMR (600 MHz, DMSO) δ 12.66 (s, 1H),

8.83 (d, *J* = 1.9 Hz, 1H), 8.32 (dd, *J* = 8.6, 1.9 Hz, 1H), 8.20 (dd, *J* = 7.9, 1.5 Hz, 1H), 8.10 – 8.04 (m, 2H), 8.05 – 7.99 (m, 1H), 7.87 (ddd, *J* = 8.4, 7.0, 1.6 Hz, 1H), 7.81 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.69 – 7.61 (m, 2H), 7.55 (ddd, *J* = 8.1, 7.0, 1.2 Hz, 1H). ^{13}C NMR (151 MHz, DMSO) δ 162.2, 152.2, 148.8, 134.6, 134.1, 132.3, 129.4, 128.9, 128.1, 128.1, 127.9, 127.6, 127.5, 126.9, 126.6, 125.9, 124.5, 121.0, 40.1, 39.9, 39.9, 39.8, 39.7, 39.5, 39.4, 39.2, 39.1.



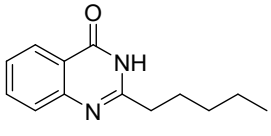
3o

2-(furan-2-yl)quinazolin-4(3*H*)-one 3o[5] prepared following general procedure A using compound **1a** (50 mg, 0.338 mmol) and furan-2-ylmethanol (98 mg, 1,352 mmol). The product was purified by column chromatography (silica gel, hexane/ethylacetate (5:1)) to yield **3o** (84%) as a white solid.^{1}H NMR (600 MHz, $CDCl_3$) δ 10.87 (s, 1H), 8.36 – 8.29 (m, 1H), 7.81 – 7.75 (m, 2H), 7.67 (dd, *J* = 1.7, 0.7 Hz, 1H), 7.56 (dd, *J* = 3.5, 0.8 Hz, 1H), 7.48 (ddd, *J* = 8.1, 5.4, 2.8 Hz, 1H), 6.67 (dd, *J* = 3.5, 1.7 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 162.6, 149.5, 146.5, 145.6, 143.6, 135.1, 127.9, 126.9, 126.7, 121.2, 114.1, 113.1, 77.4, 77.2, 76.9.



3p

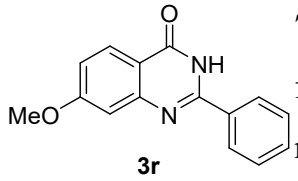
2-methylquinazolin-4(3*H*)-one 3p[6] prepared following general procedure A using compound **1a** (50 mg, 0.338 mmol) and Ethanol (0.5 mml). The product was purified by column chromatography (silica gel, hexane/ethylacetate (2:1)) to yield **3p** (66%) as a white solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 12.1 (s, 1H), 8.3 (d, *J* = 8.0 Hz, 1H), 7.8 (t, *J* = 7.6 Hz, 1H), 7.7 (d, *J* = 8.2 Hz, 1H), 7.5 (t, *J* = 7.6 Hz, 1H), 2.6 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.4, 153.4, 149.5, 134.9, 127.0, 126.4, 126.2, 120.3, 22.0.



3q

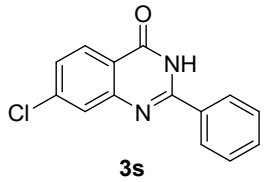
2-hexylquinazolin-4(3*H*)-one 3q[6] prepared following general procedure A using compound **1a** (50 mg, 0.338 mmol) and hexan-1-ol (80 mg, 1,352 mmol). The product was purified by column chromatography (silica gel, hexane/ethylacetate (3:1)) to yield **3q**

(40%) as a white solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 12.5 (s, 1H), 8.3 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.7 (ddd, *J* = 8.4, 6.9, 1.6 Hz, 1H), 7.7 (dd, *J* = 8.2, 1.3 Hz, 1H), 7.4 (ddd, *J* = 8.1, 6.9, 1.3 Hz, 1H), 2.8 – 2.8 (m, 2H), 1.9 – 1.8 (m, 2H), 1.5 – 1.3 (m, 5H), 0.9 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.6, 157.3, 149.6, 134.6, 127.2, 126.2, 126.1, 120.5, 35.8, 31.4, 27.3, 22.3, 13.9.



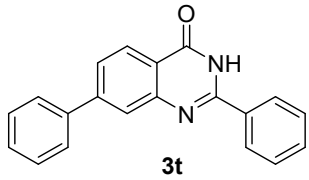
3r

7-methoxy-2-phenylquinazolin-4(3*H*)-one 3r[2] prepared following general procedure A using compound 4-methoxy-2-nitrobenzonitrile (50 mg, 0.281 mmol) and benzyl alcohol (121 mg, 1.124 mmol). The product was purified by column chromatography (silica gel, hexane/ethylacetate (5:1)) to yield **3r** (89%) as a white solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 11.06 (s, 1H), 8.25 – 8.16 (m, 3H), 7.26 (s, 1H), 7.23 (d, *J* = 2.5 Hz, 1H), 7.08 (dd, *J* = 8.8, 2.5 Hz, 1H), 3.96 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.2, 163.1, 152.6, 151.9, 133.1, 131.8, 129.2, 128.1, 127.4, 117.2, 114.5, 108.7, 77.4, 77.2, 76.9, 55.9.



3s

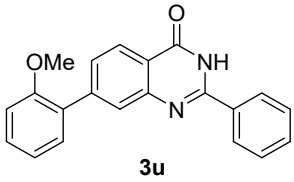
7-chloro-2-phenylquinazolin-4(3H)-one 3s[1] prepared following general procedure A using compound 4-chloro-2-nitrobenzonitrile (50 mg, 0.274 mmol) and benzyl alcohol (120 mg,1.096 mmol). The product was purified by column chromatography (silica gel, hexane/ethylacetate (5:1)) to yield **3s** (70%) as a white solid. ^{1}H NMR (600 MHz, DMSO) δ 12.67 – 12.64 (m, 1H), 8.24 – 8.17 (m, 2H), 8.15 (d, *J* = 8.5 Hz, 1H), 7.79 (dd, *J* = 2.1, 1.0 Hz, 1H), 7.65 – 7.59 (m, 1H), 7.59 – 7.51 (m, 3H). ^{13}C NMR (126 MHz, DMSO) δ 161.7, 153.8, 149.8, 139.1, 132.4, 131.7, 128.6, 127.9, 127.9, 126.7, 126.5, 119.8, 40.0, 39.95, 39.9, 39.8, 39.7, 39.6, 39.5, 39.4, 39.2, 39.0.



3t

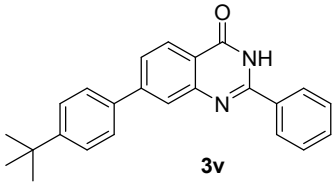
2,7-diphenylquinazolin-4(3H)-one 3t prepared following general procedure A using compound 3-nitro-[1,1'-biphenyl]-4-carbonitrile (50 mg, 0.223 mmol) and benzyl alcohol (96.336 mg, 0.892 mmol). The product was purified by column

chromatography (silica gel, hexane/ethylacetate (5:1)) to yield **3t** (90%) as a white solid.^{1}H NMR (600 MHz, DMSO) δ 12.54 (s, 1H), 8.25 – 8.19 (m, 3H), 8.00 (d, *J* = 1.8 Hz, 1H), 7.84 (dt, *J* = 8.3, 2.6 Hz, 3H), 7.64 – 7.58 (m, 1H), 7.60 – 7.51 (m, 4H), 7.47 (dd, *J* = 8.4, 6.6 Hz, 1H). ^{13}C NMR (151 MHz, DMSO) δ 162.0, 152.8, 149.3, 146.2, 138.8, 132.7, 131.4, 129.2, 128.6, 128.6, 127.8, 127.2, 126.6, 125.3, 124.9, 119.9, 39.9, 39.8, 39.7, 39.5, 39.4, 39.2, 39.1.



3u

7-(2-methoxyphenyl)-2-phenylquinazolin-4(3H)-one 3u prepared following general procedure A using compound 2'-methoxy-3-nitro-[1,1'-biphenyl]-4-carbonitrile (50 mg, 0.197 mmol) and benzyl alcohol (85 mg, 0.788 mmol). The product was purified by column chromatography (silica gel, hexane/ethylacetate (5:1)) to yield **3u** (72%) as a white solid. ^{1}H NMR (600 MHz, DMSO) δ 12.51 (s, 1H), 8.23 – 8.19 (m, 2H), 8.17 (d, *J* = 8.2 Hz, 1H), 7.82 (d, *J* = 1.6 Hz, 1H), 7.64 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.62 – 7.53 (m, 3H), 7.43 (td, *J* = 7.3, 1.7 Hz, 2H), 7.21 – 7.16 (m, 1H), 7.10 (td, *J* = 7.4, 1.1 Hz, 1H), 3.82 (s, 3H). ^{13}C NMR (151 MHz, DMSO) δ 162.1, 156.2, 152.5, 148.6, 144.5, 132.8, 131.4, 130.5, 129.9, 128.6, 128.4, 127.9, 127.8, 127.7, 127.2, 125.5, 120.9, 119.5, 111.9, 55.6, 40.1, 39.9, 39.8, 39.7, 39.5, 39.4, 39.2, 39.1. HRMS (ESI) m/z: $[M]^+$ Calcd for $C_{21}H_{16}N_2O_2$ 329.1245; found: 329.1283.



3v

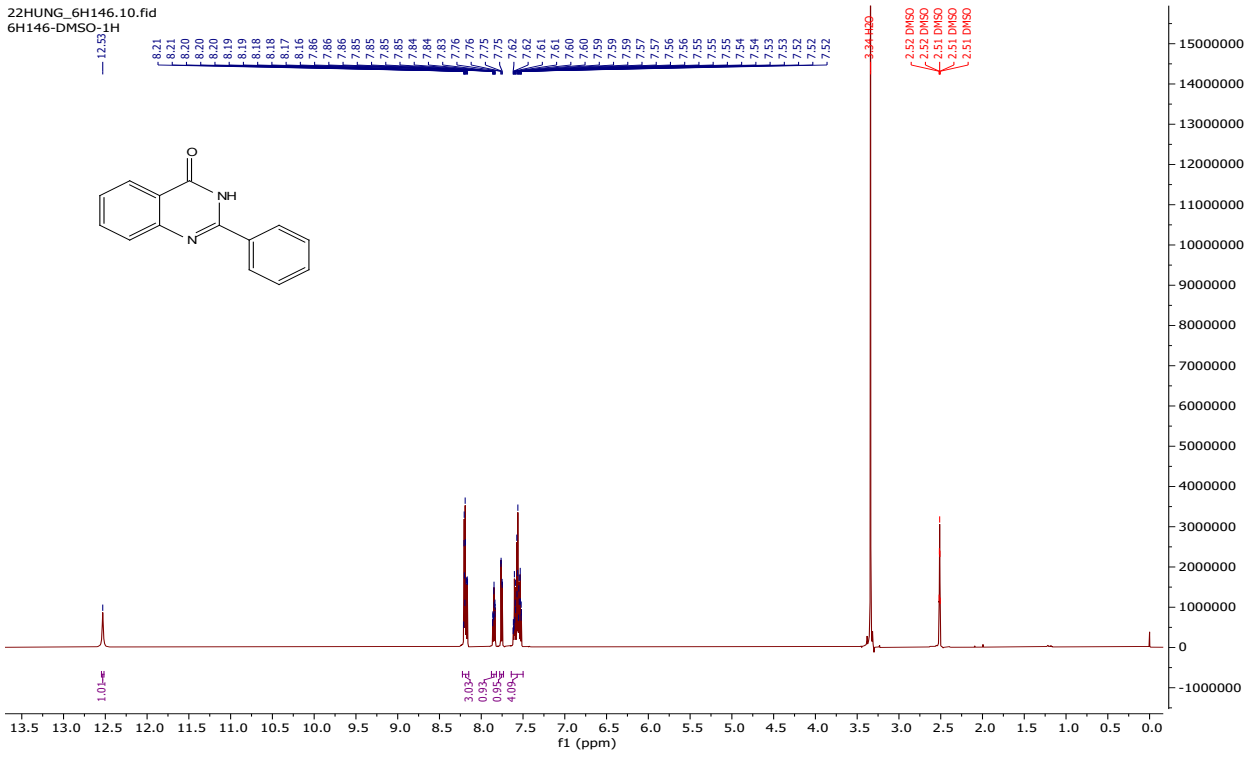
7-(4-(tert-butyl)phenyl)-2-phenylquinazolin-4(3H)-one 3v prepared following general procedure A using compound 4'-(tert-butyl)-3-nitro-[1,1'-biphenyl]-4-carbonitrile (50 mg, 0.179 mmol) and benzyl alcohol (77 mg, 0.716 mmol). The product was purified by column chromatography (silica gel, hexane/ethylacetate (5:1)) to yield **3v** (76%) as a white solid. ^{1}H NMR (600 MHz, DMSO) δ 12.52 (s, 1H), 8.25 – 8.18 (m, 3H), 7.97 (d, *J* = 1.8 Hz, 1H), 7.81 – 7.72 (m, 3H), 7.63 – 7.48 (m, 5H), 1.31 (s, 9H). ^{13}C NMR (151 MHz, DMSO) δ 161.7, 152.5, 150.9, 145.7, 135.7, 132.6, 130.9, 128.2, 127.5, 126.5, 126.2, 125.6, 124.7, 124.3, 119.5, 39.9, 39.8, 39.7, 39.5, 39.4, 39.2, 39.1, 34.0, 30.7. HRMS (ESI) m/z: $[M]^+$ Calcd for $C_{24}H_{22}N_2O$ 355.1766; found: 355.1799.

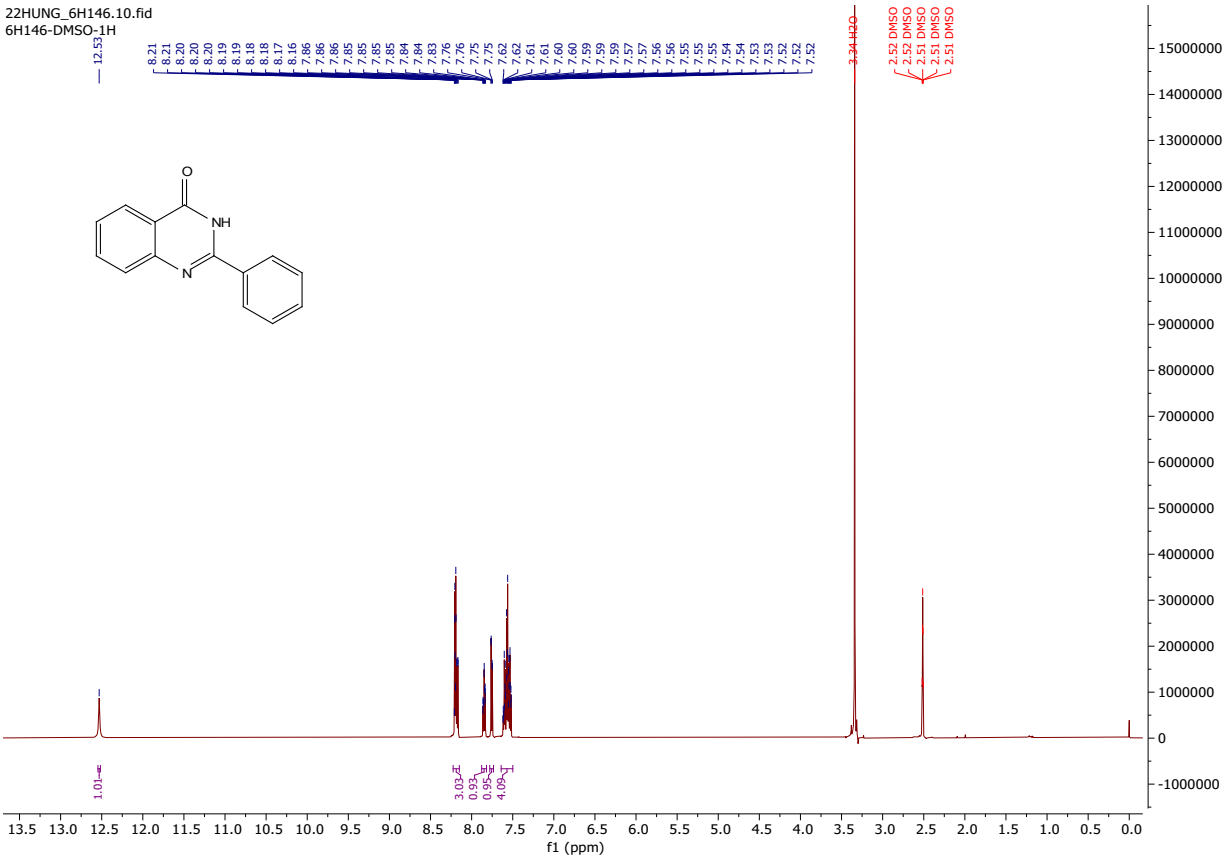
References

1. T. Su, K. Sun, G. Lu and C. Cai, *ACS Sustain. Chem. Eng*., 2022, **10**, 3872.
2. T. T. Nguyen, D. T. M. Chung, K. X. Nguyen, V. P. T. Nguyen, N. T. S. Phan and T. T. Nguyen, *ChemistrySelect*, 2024, **9**, e202303762.
3. L. Tang, X. Zhao, G. Zou, Y. Zhou and X. Yang, *Asian J. Org. Chem*., 2016, **5**, 335.
4. Y. Hu, S. Li, H. Li, Y. Li, J. Li, C. Duanmu and B. Li, *Org. Chem. Front*., 2019, **6**, 2744.
5. S. Mondal, S. Chakraborty, S. Khanra, S. Chakraborty, S. Pal, P. Brandao, and N. D. Paul, *J. Org. Chem*., 2024, **89**, 5250.
6. Zhang, Z., et al., *Chem. Commun.,* 2015, **51**, 9205.

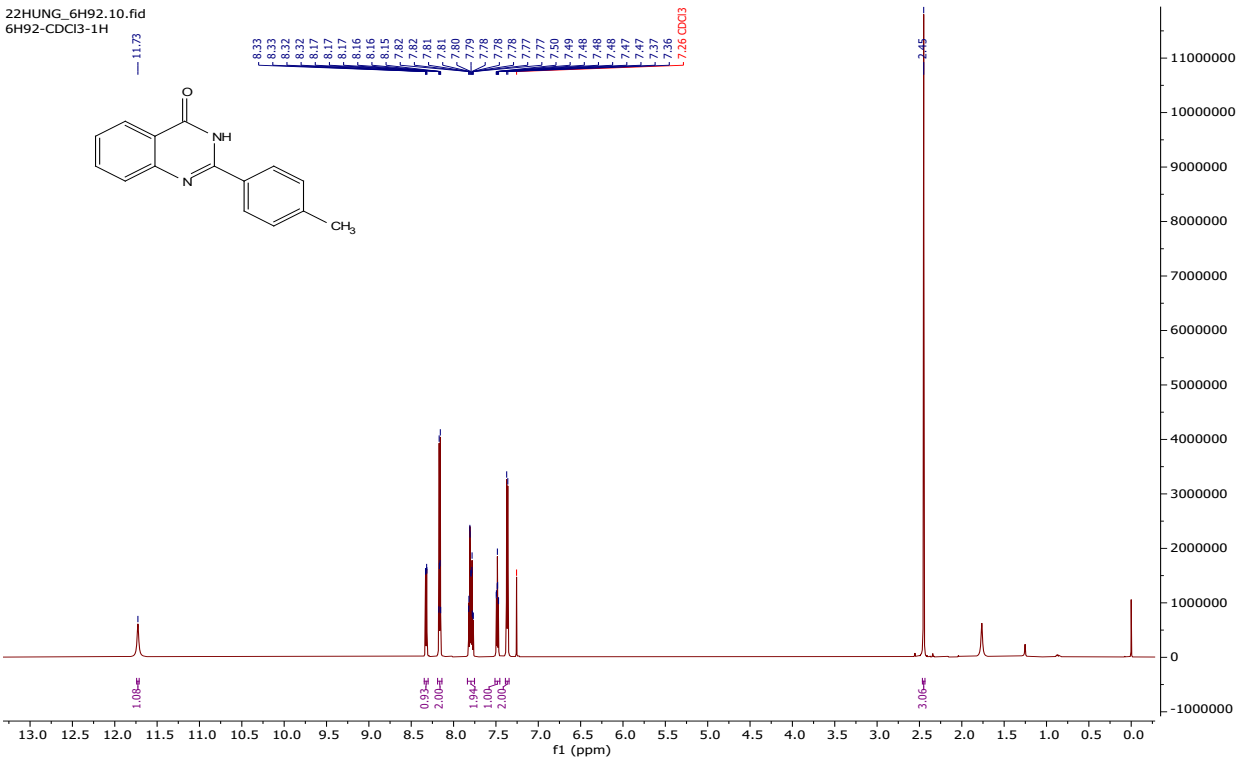
Copies of NMR spectra

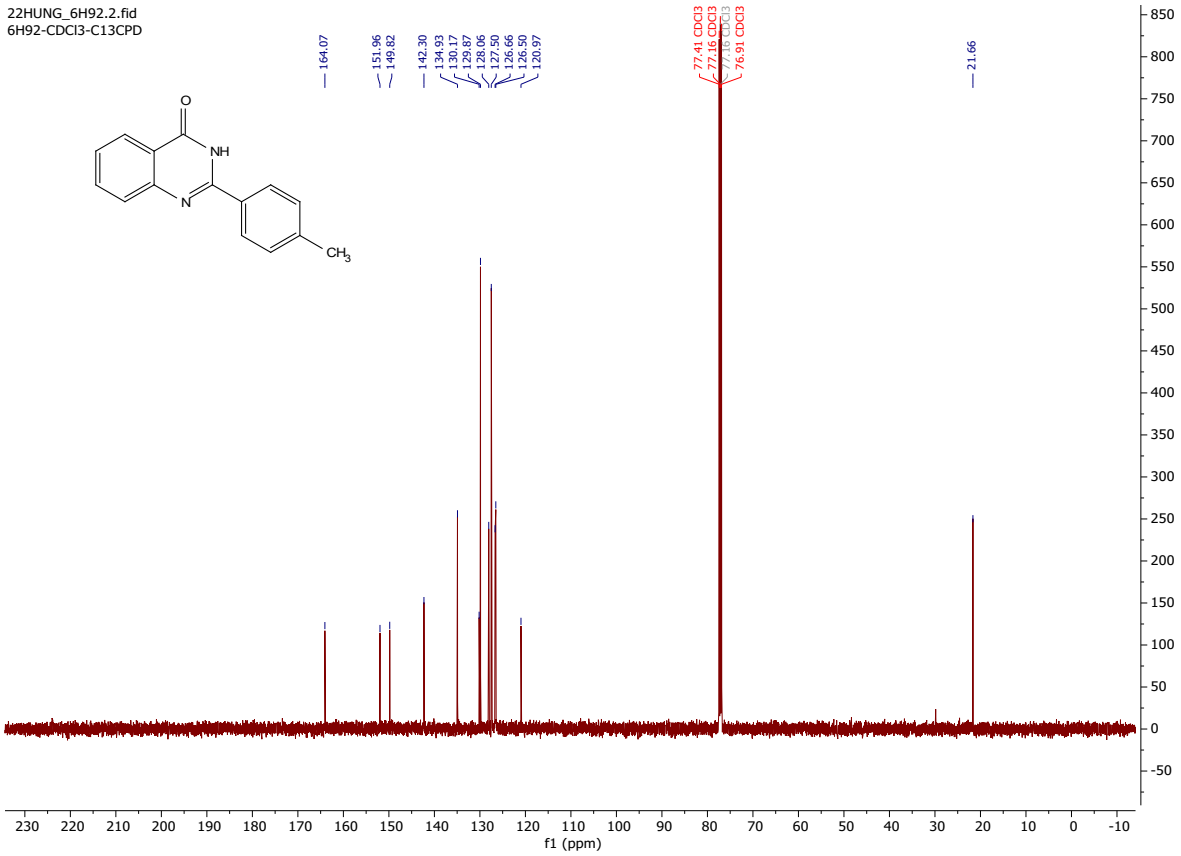
2-phenylquinazolin-4(3*H*)-one 3a



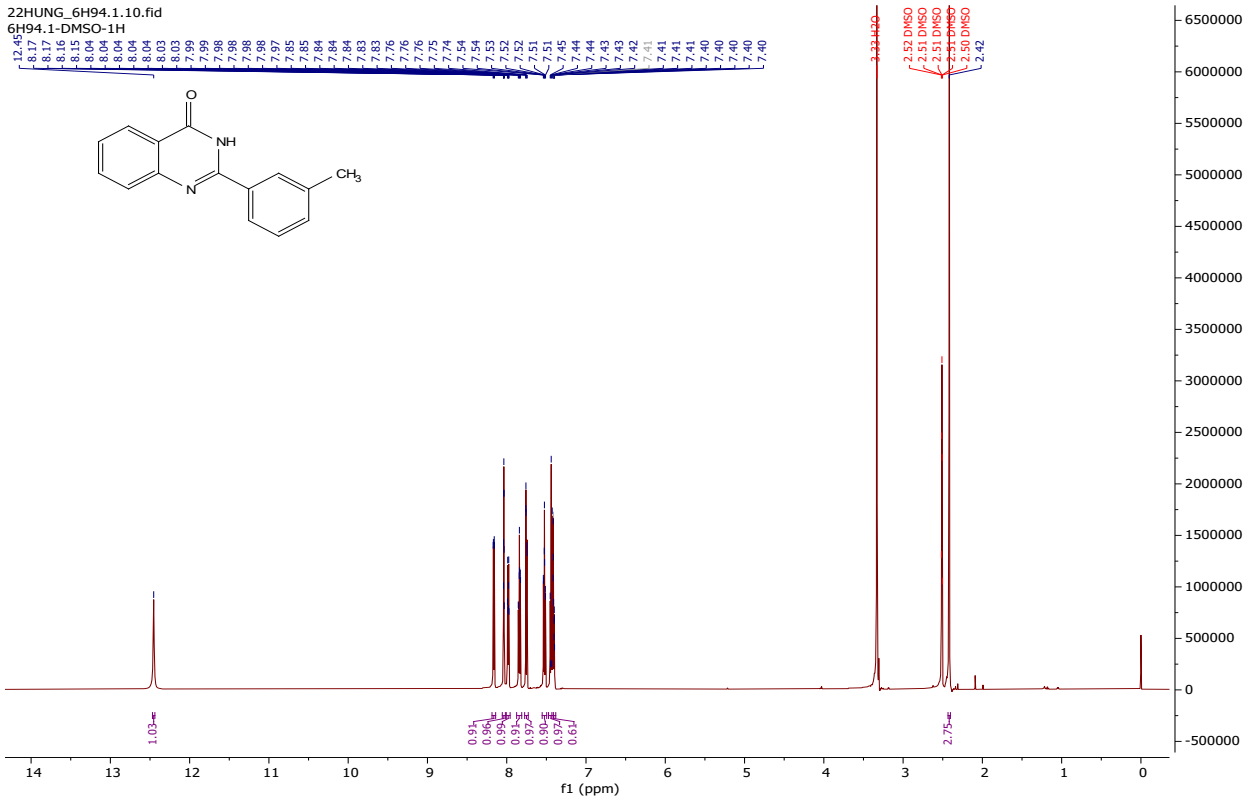


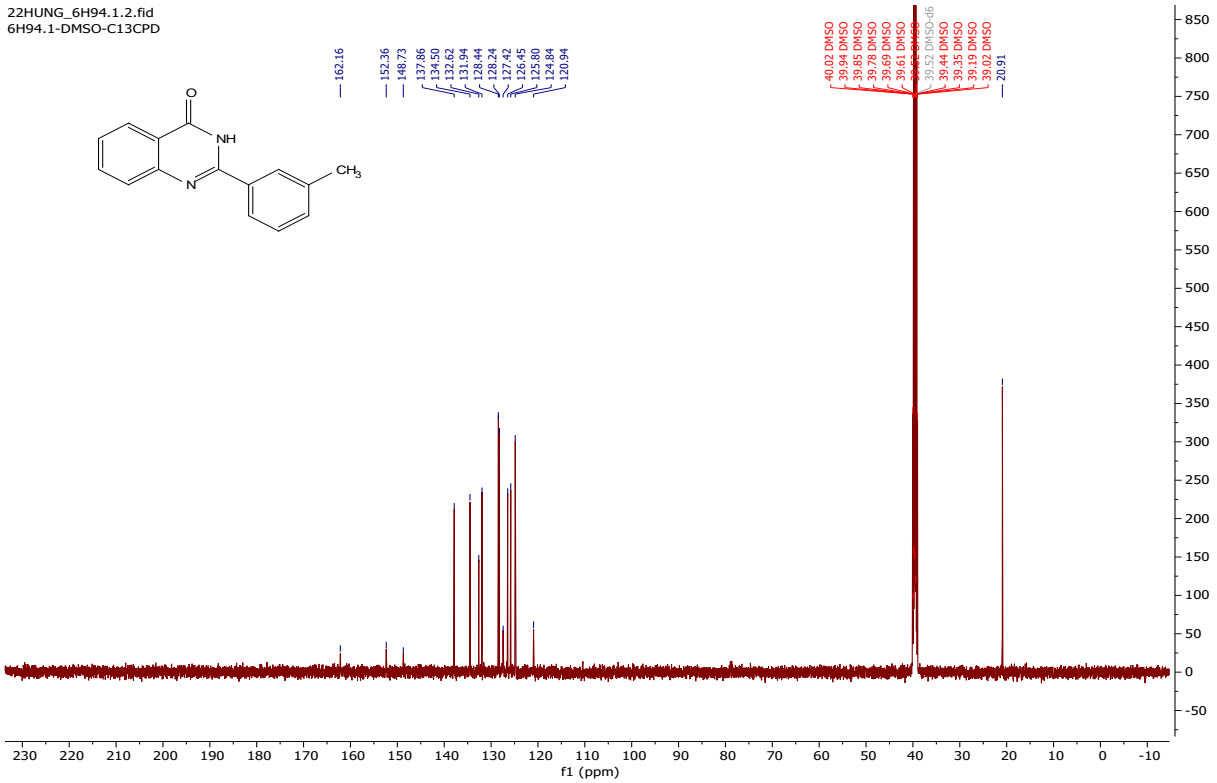
2-(p-tolyl)quinazolin-4(3*H*)-one 3b



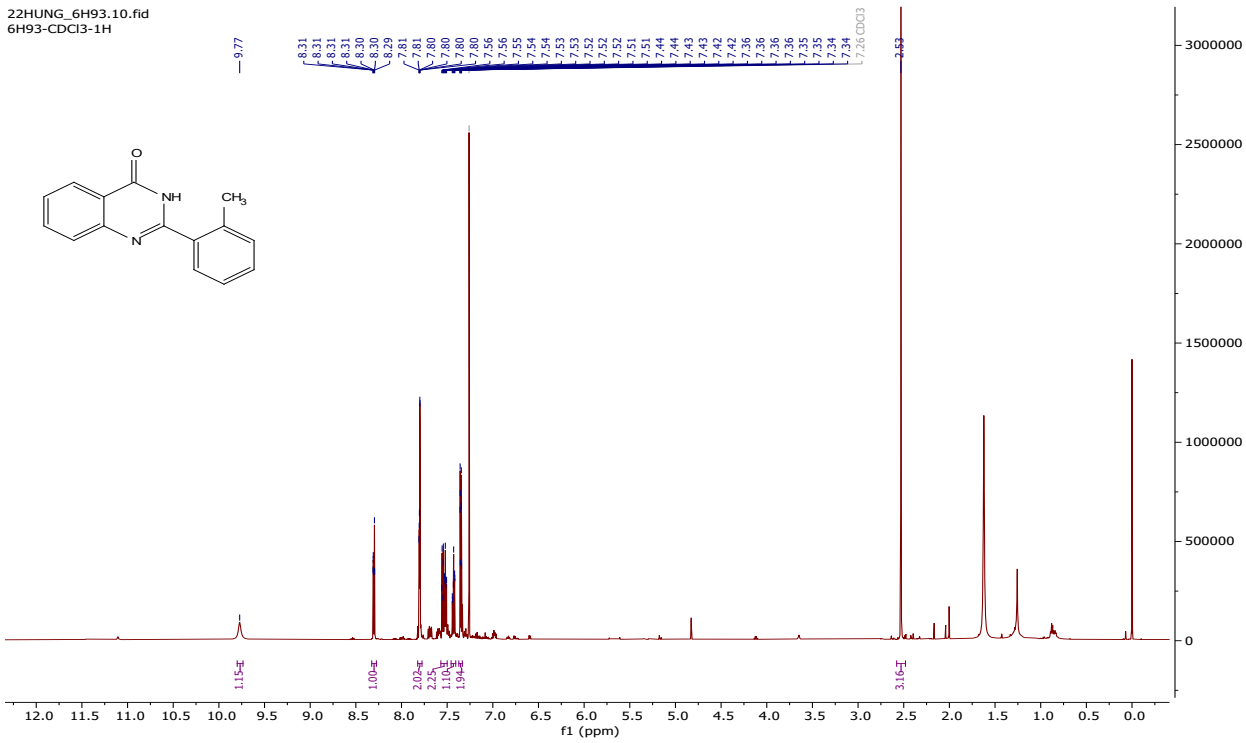


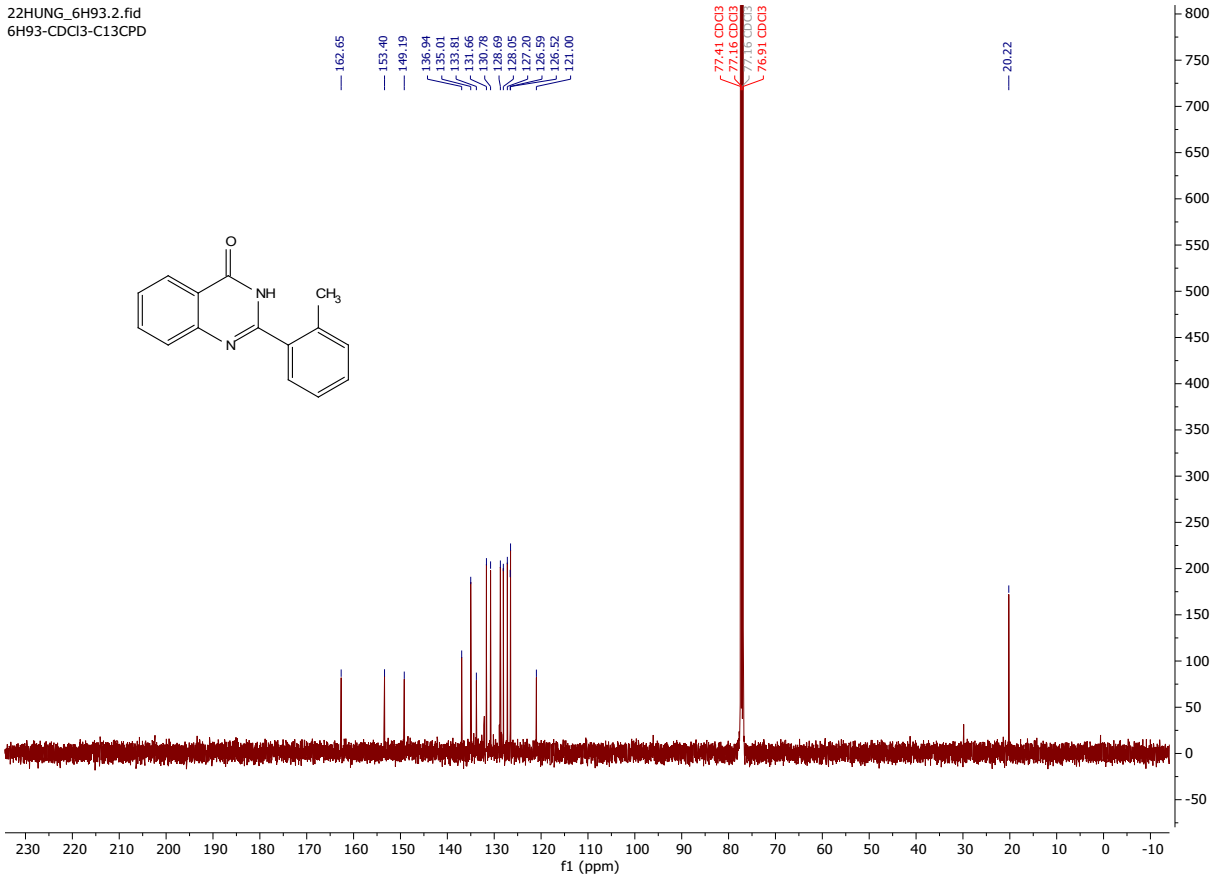
2-(m-tolyl)quinazolin-4(3*H*)-one 3c



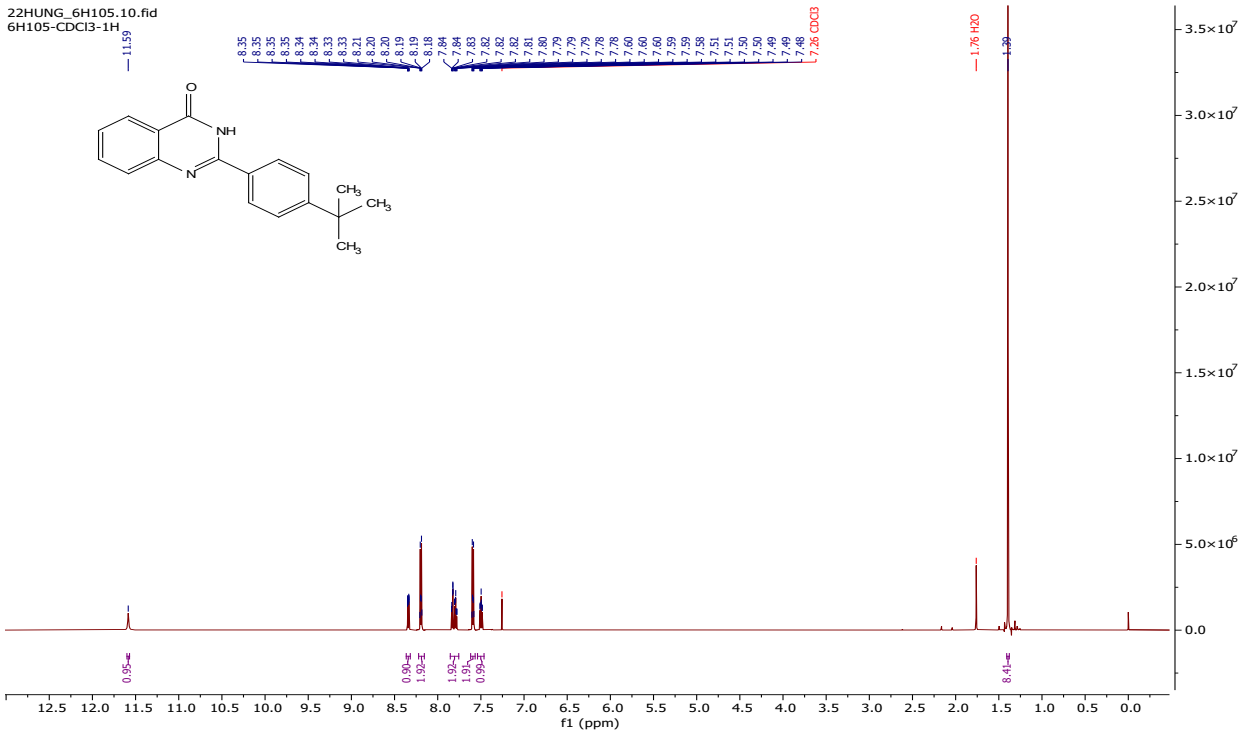


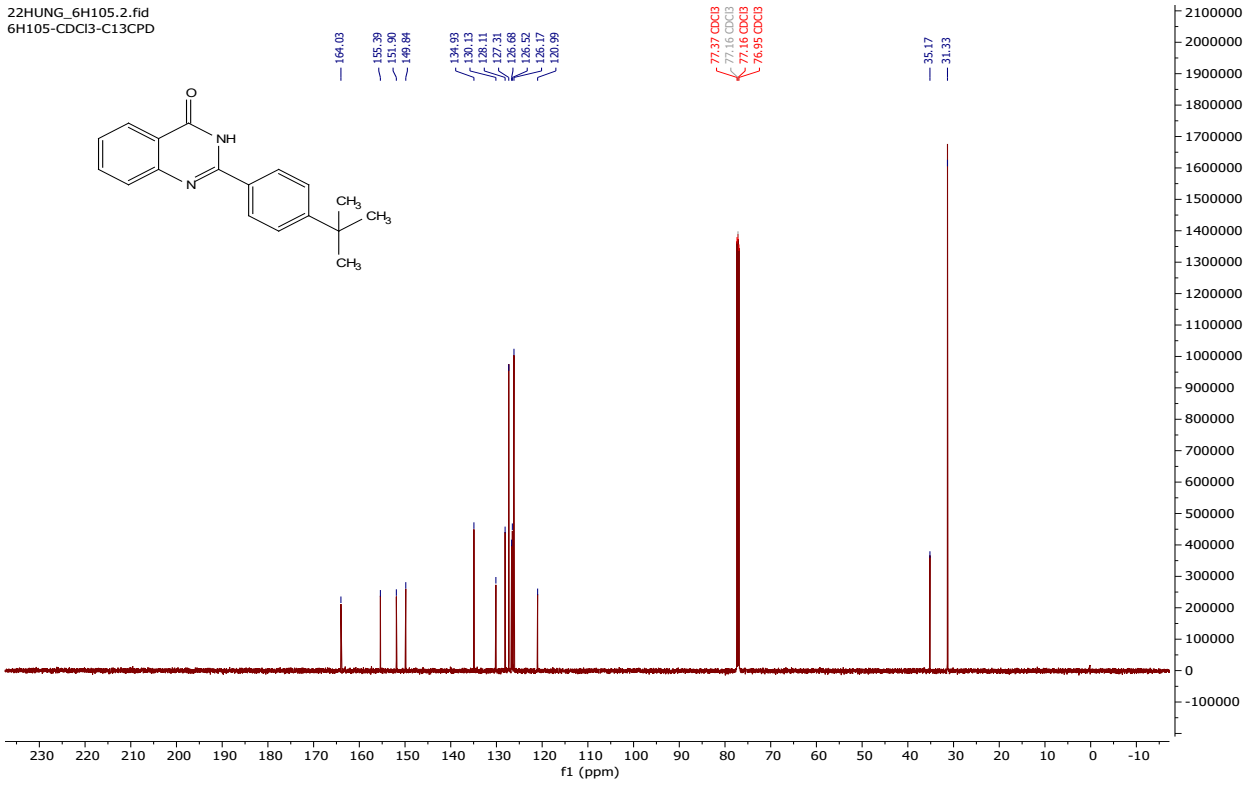
2-(o-tolyl)quinazolin-4(3*H*)-one 3d



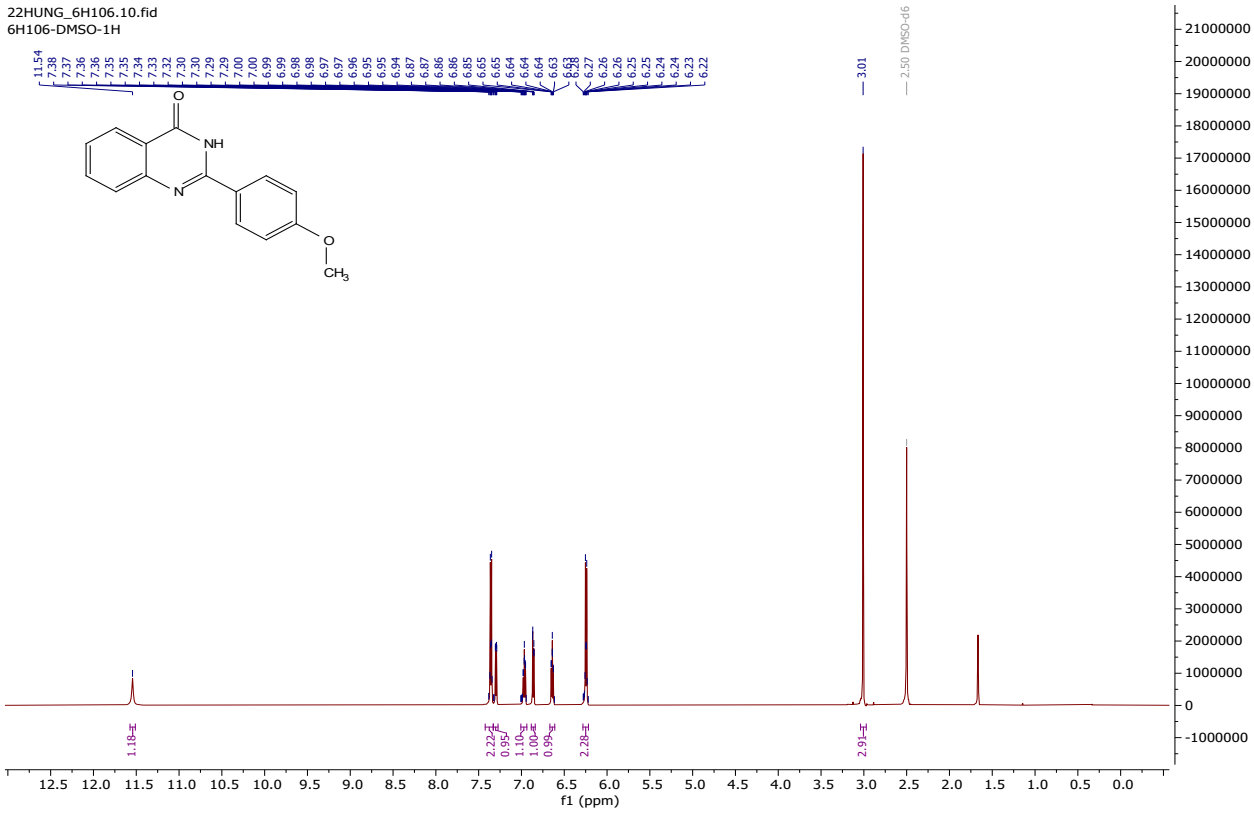


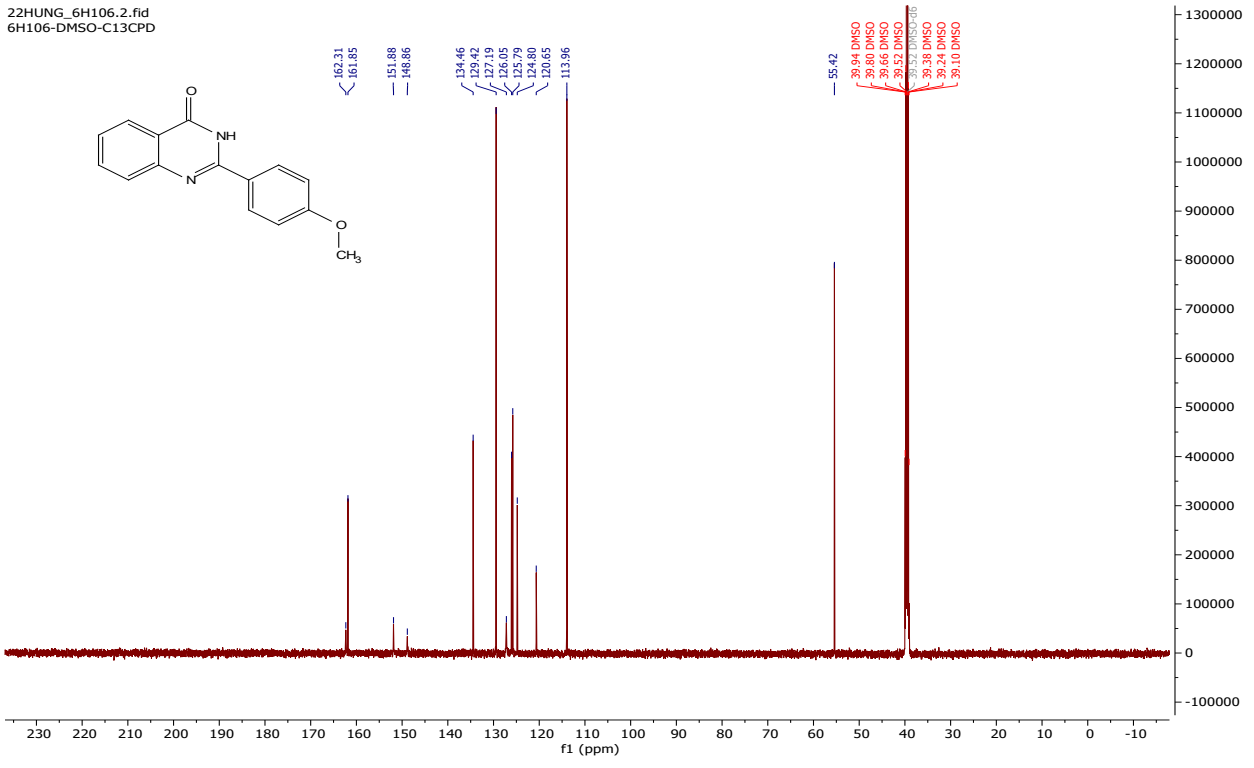
2-(4-(tert-butyl)phenyl)quinazolin-4(3*H*)-one 3e



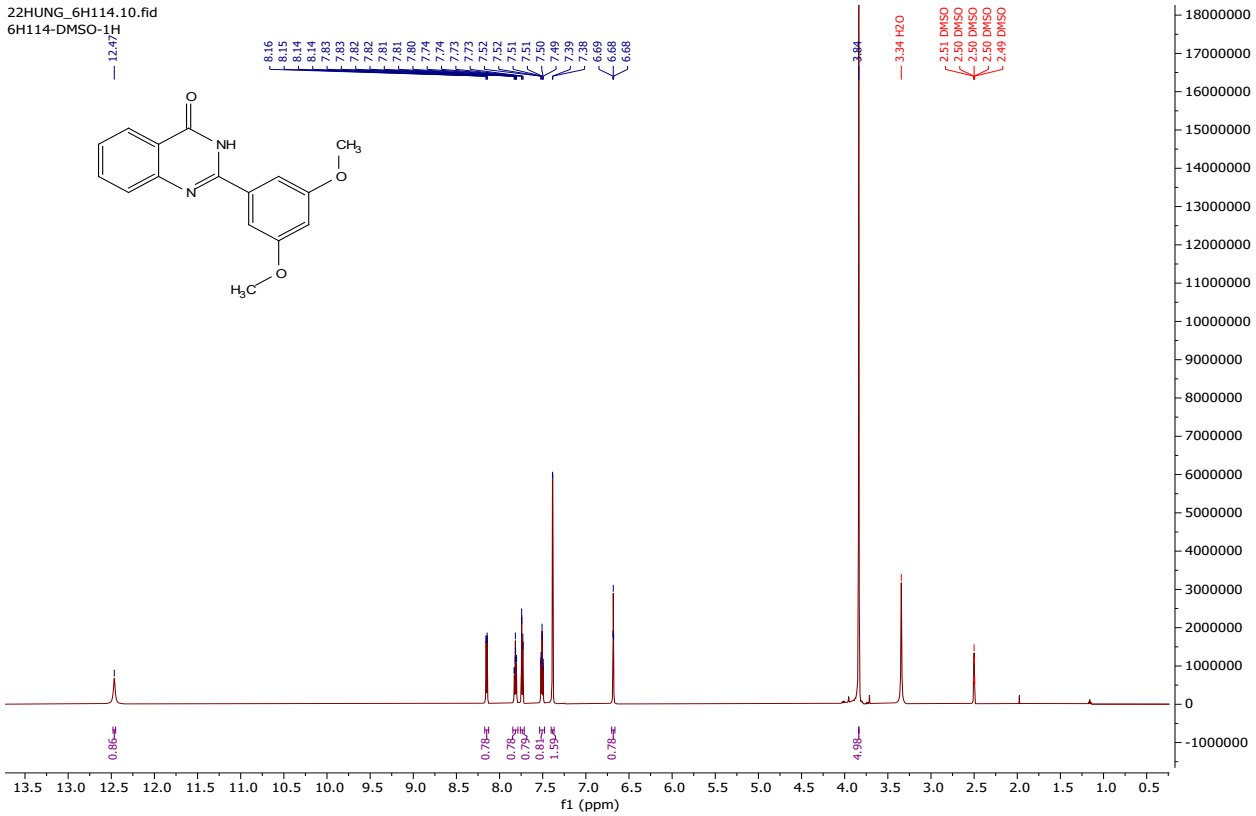


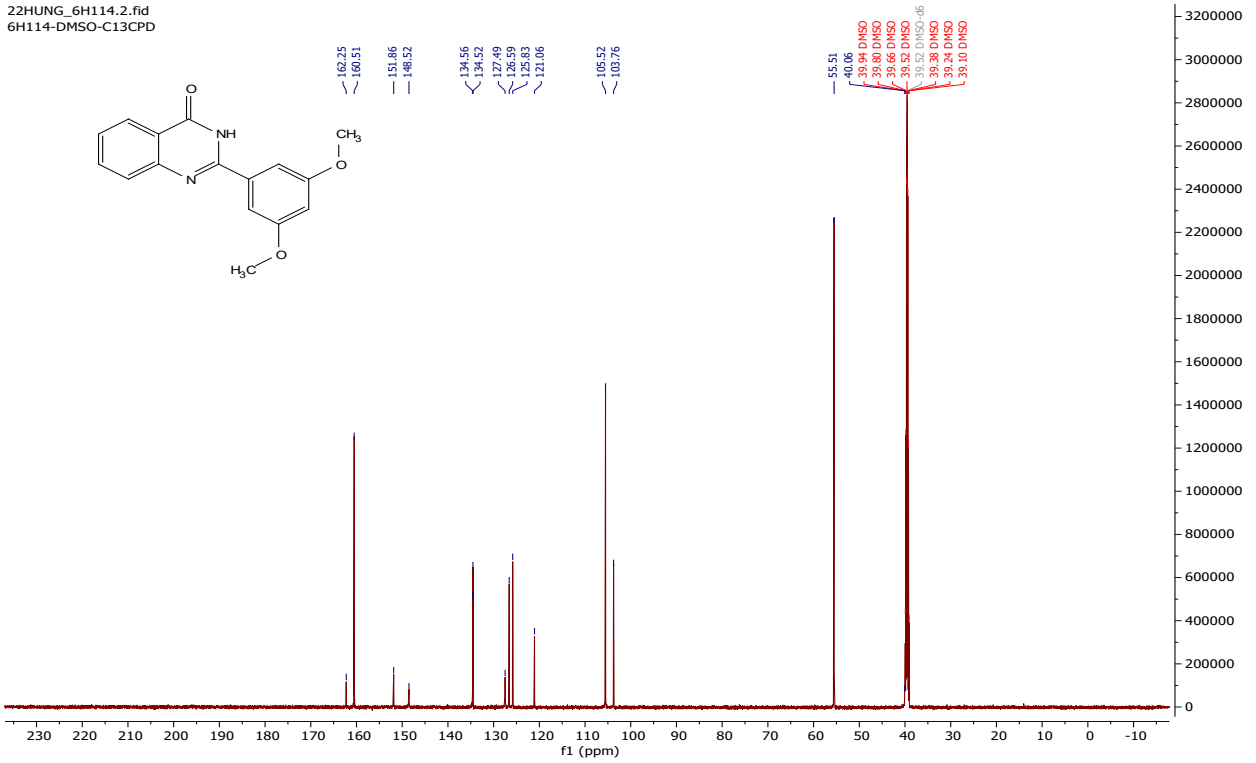
2-(4-methoxyphenyl)quinazolin-4(3*H*)-one 3f



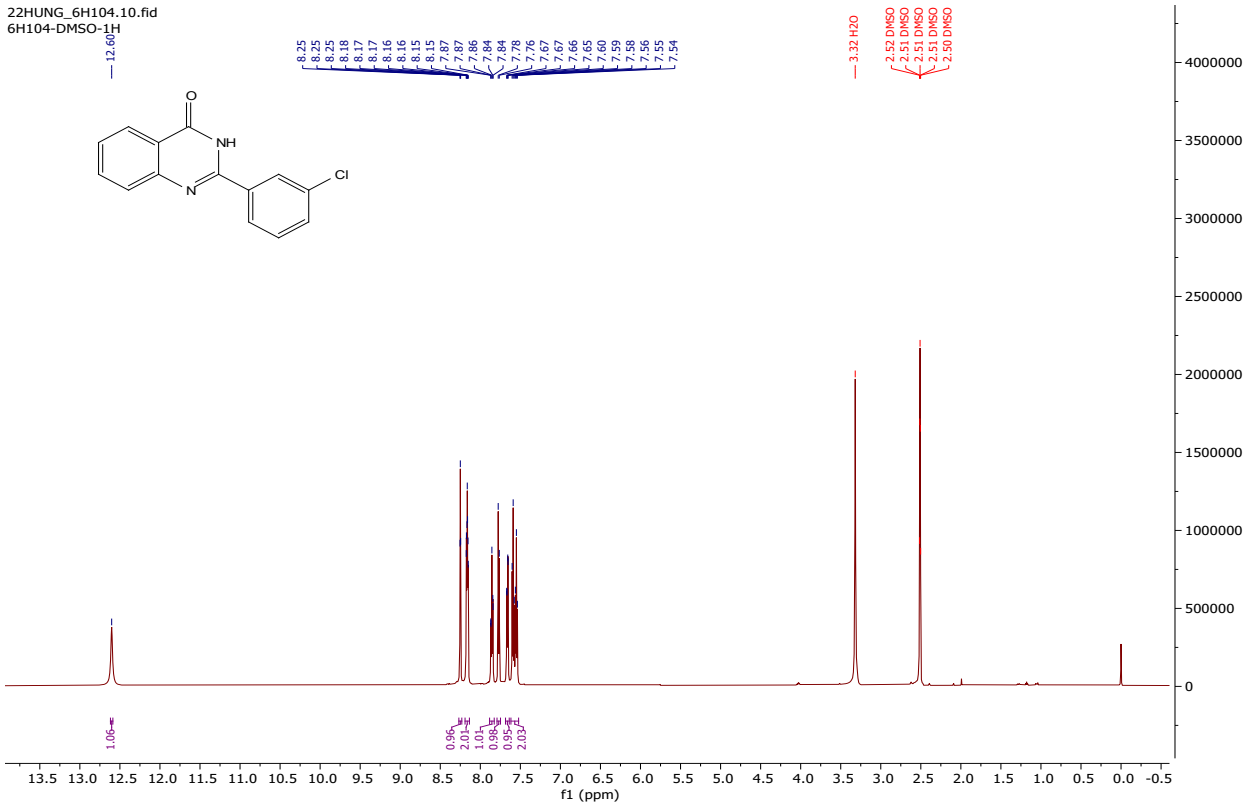


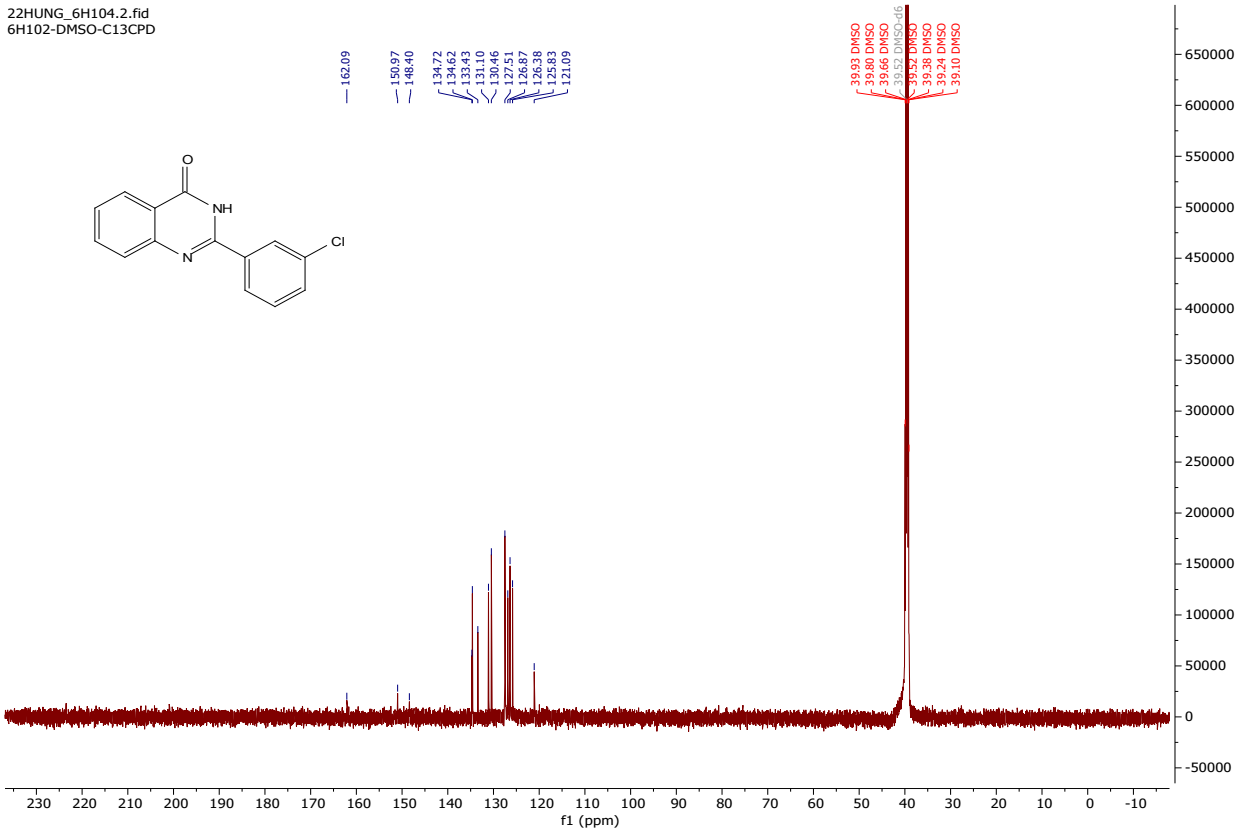
2-(3,5-dimethoxyphenyl)quinazolin-4(3*H*)-one 3g



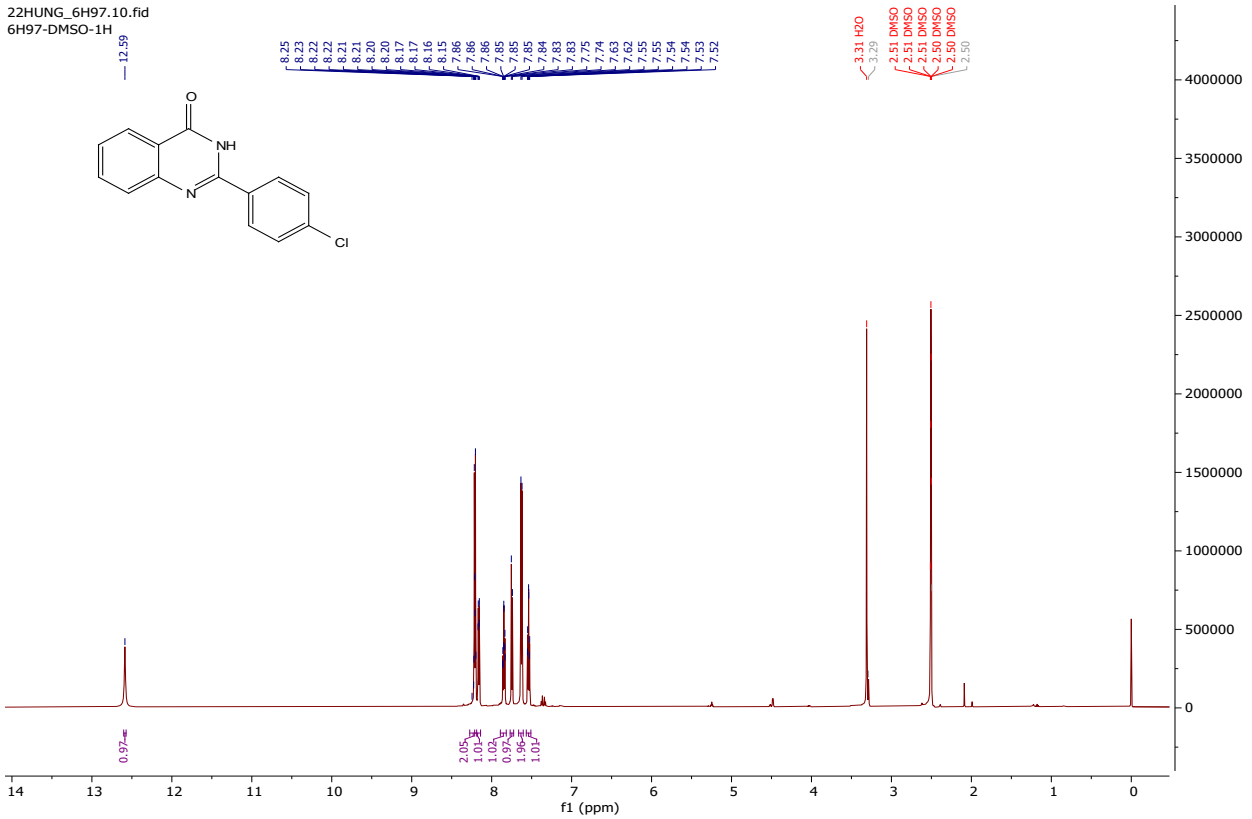


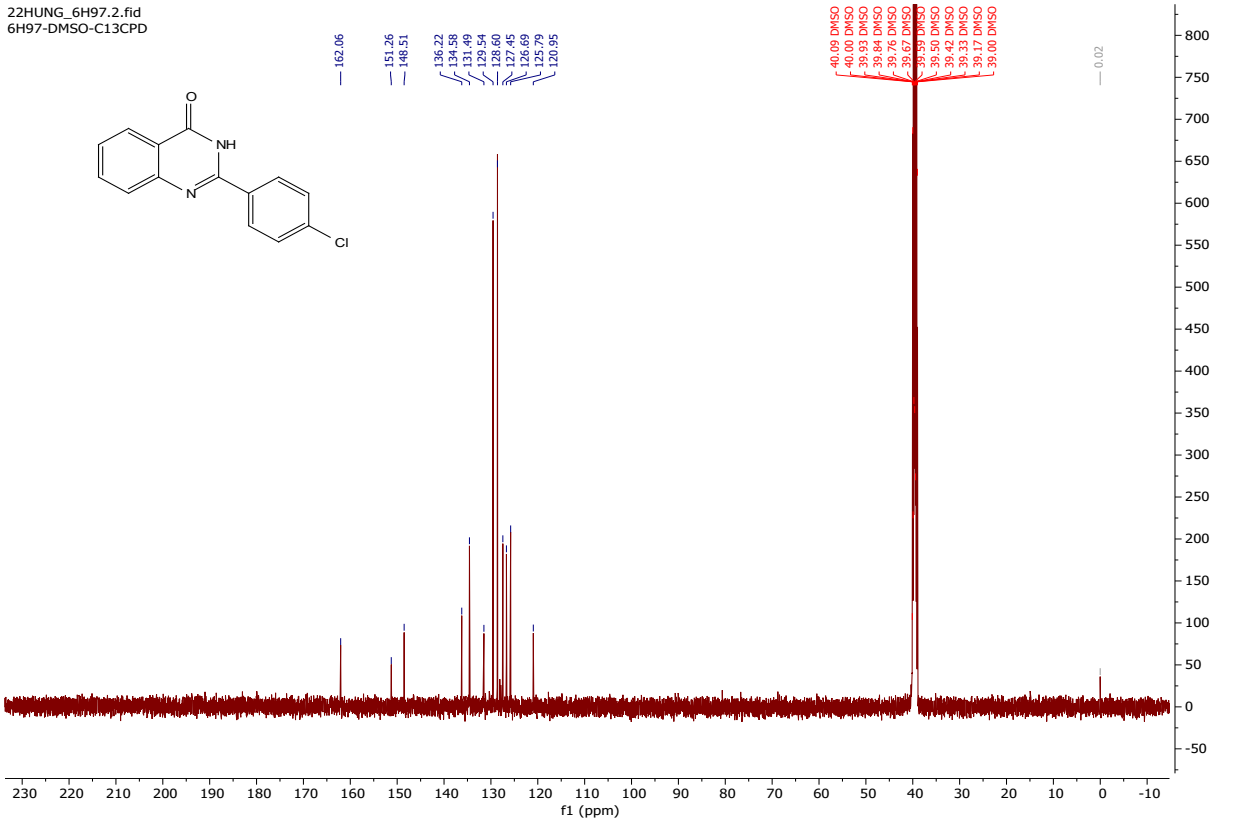
2-(3-chlorophenyl)quinazolin-4(3*H*)-one 3h



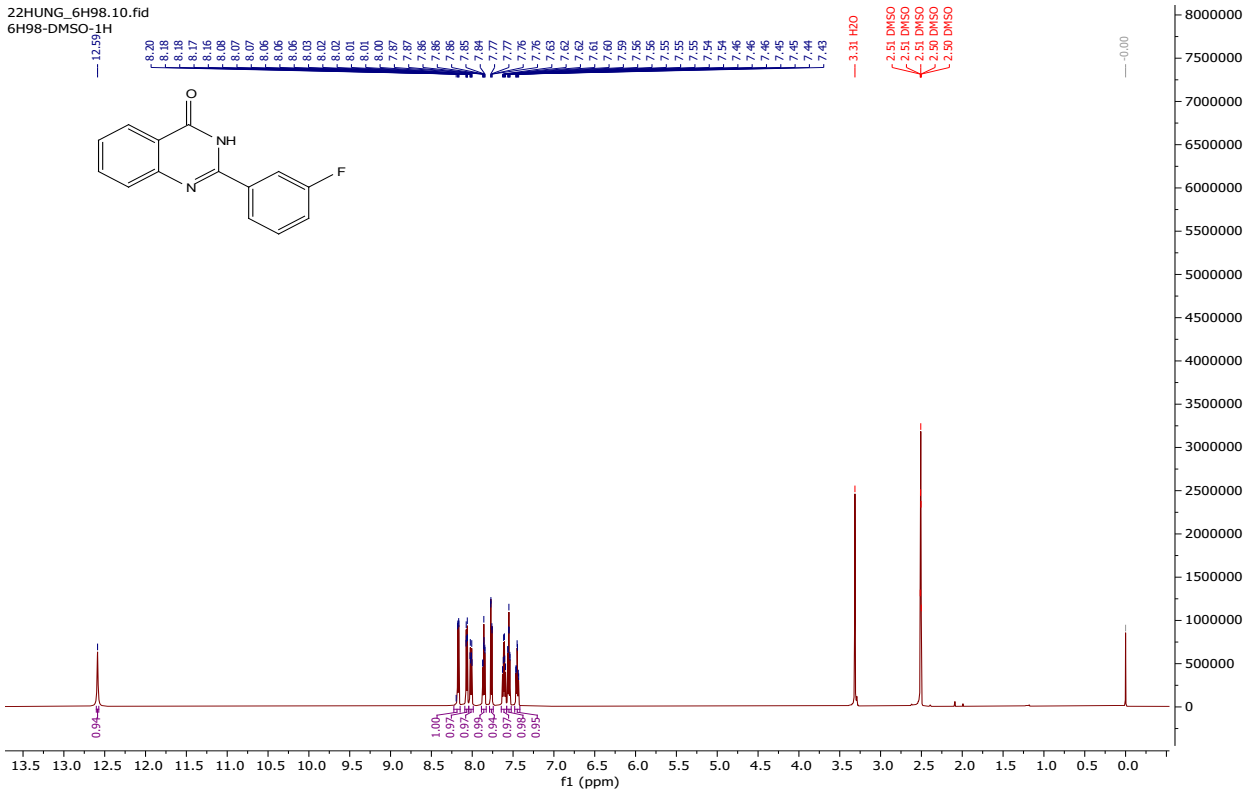


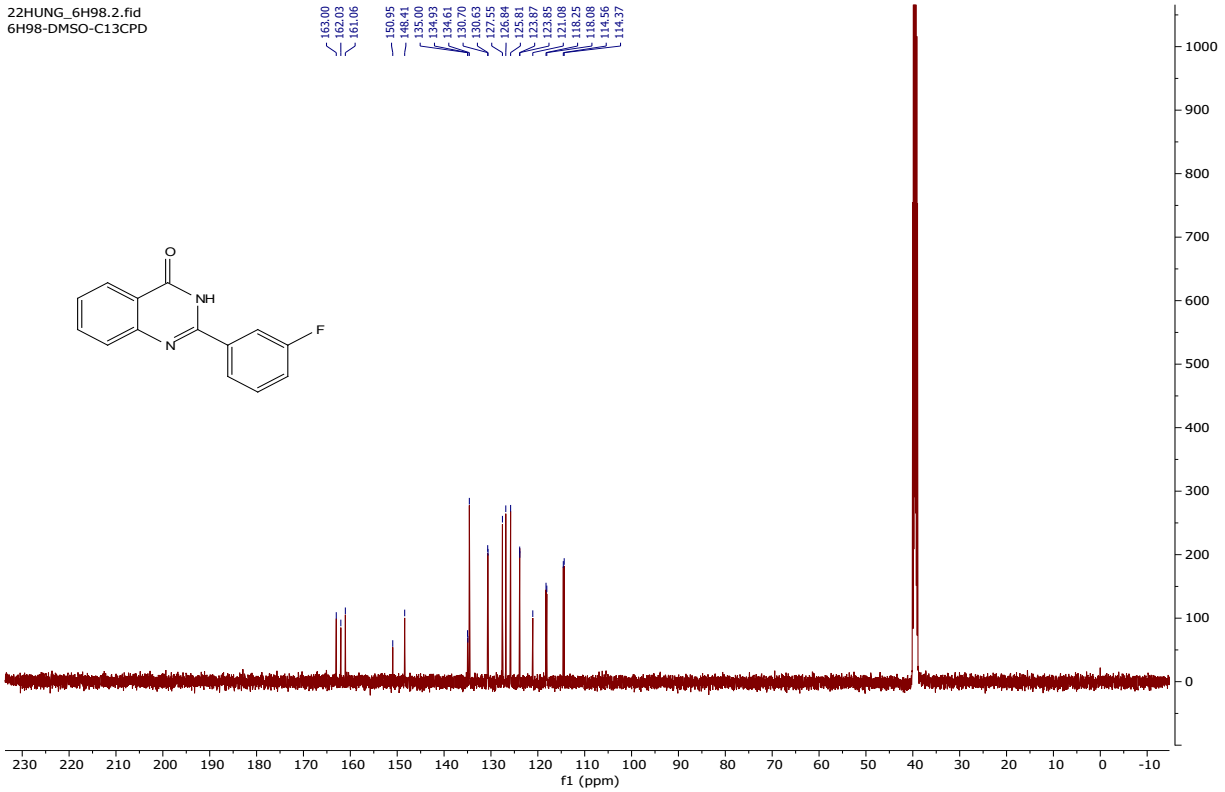
2-(4-chlorophenyl)quinazolin-4(3*H*)-one 3i



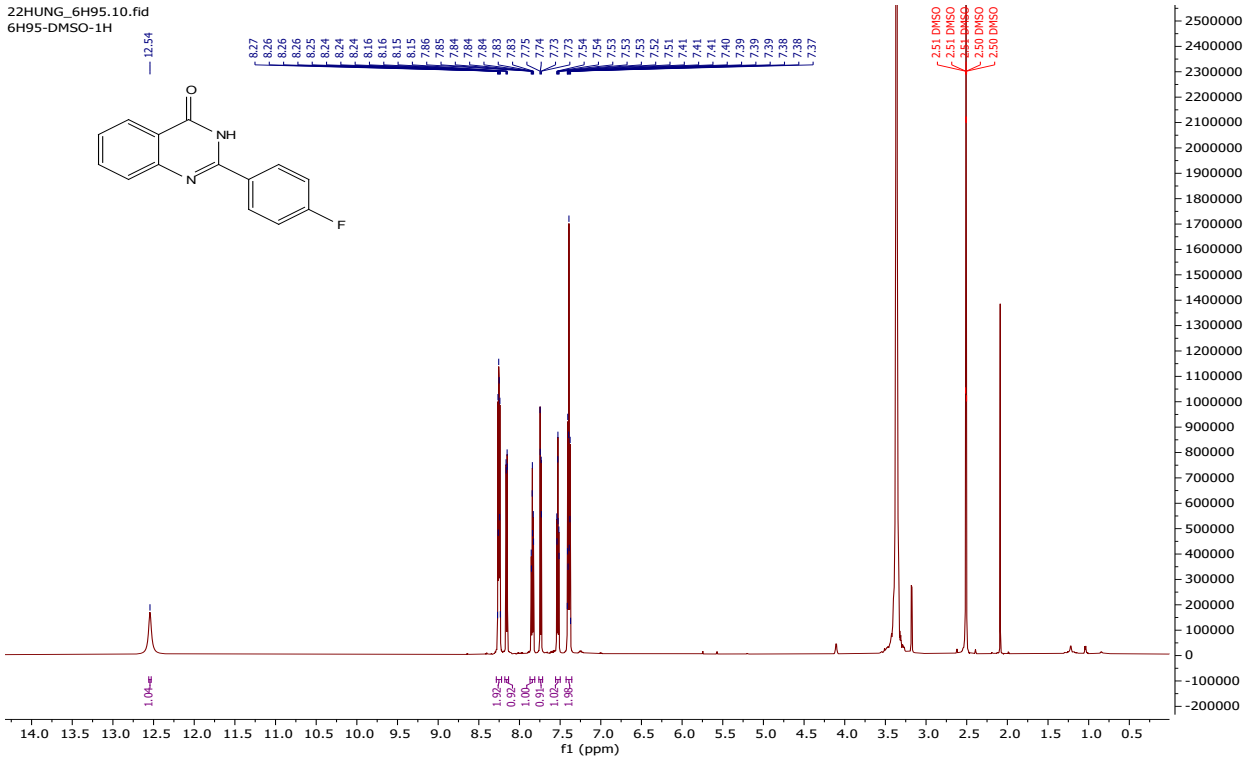


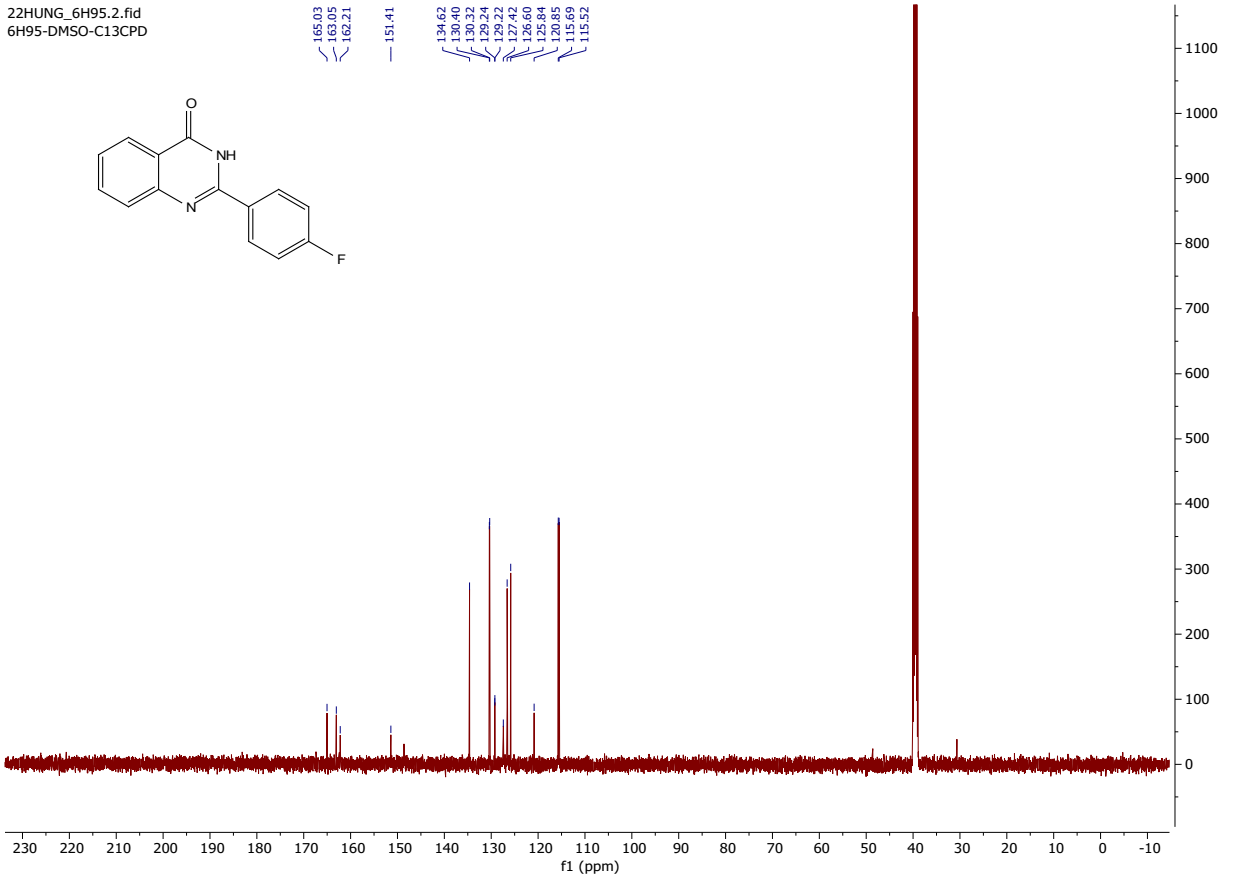
2-(3-fluorophenyl)quinazolin-4(3*H*)-one 3j



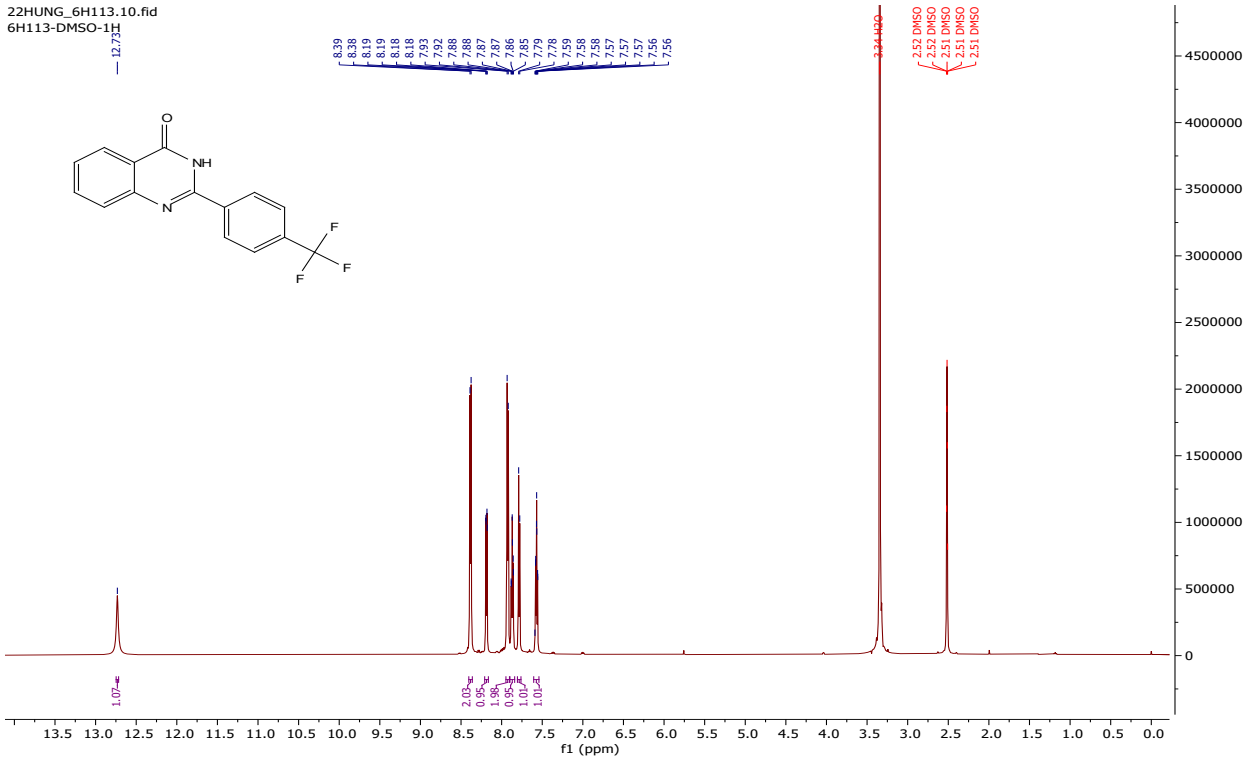


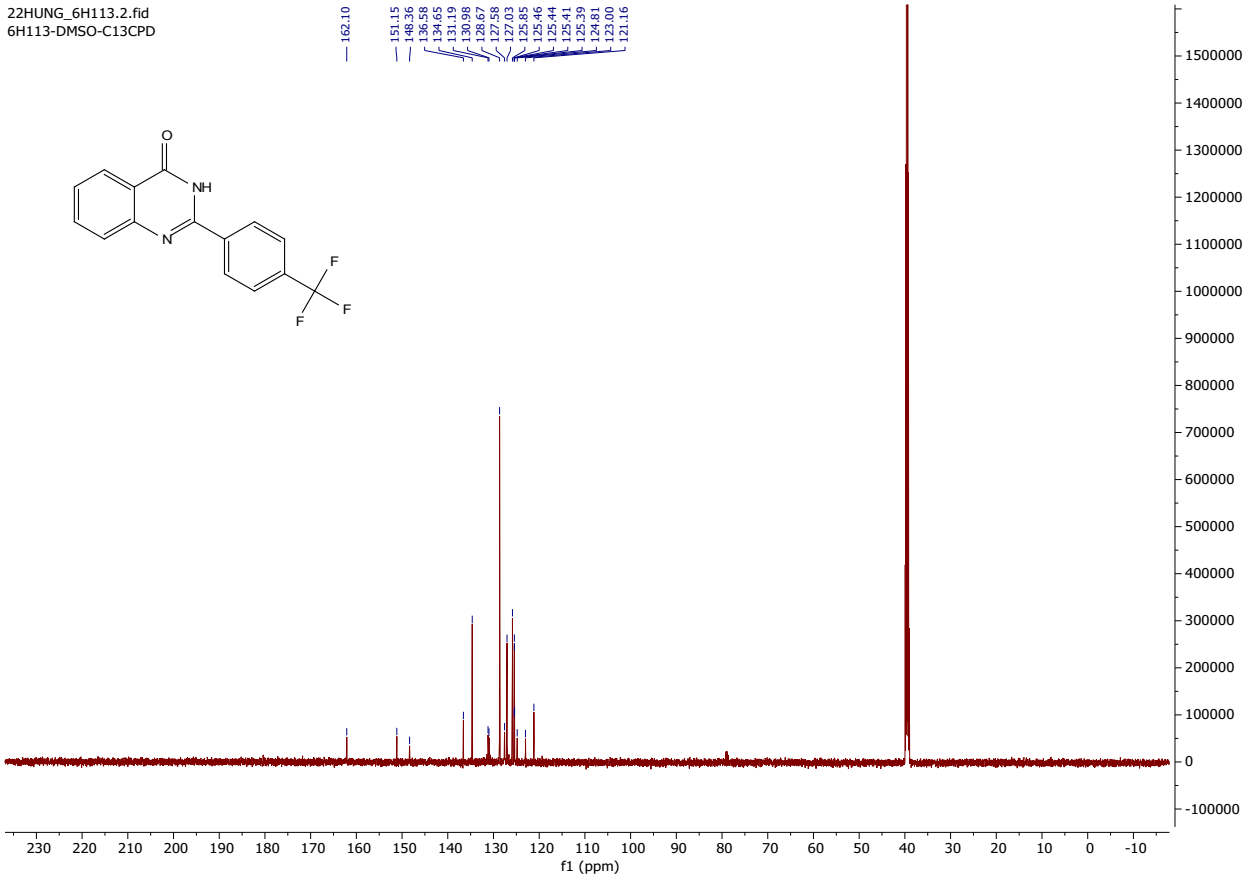
2-(4-fluorophenyl)quinazolin-4(3*H*)-one 3k



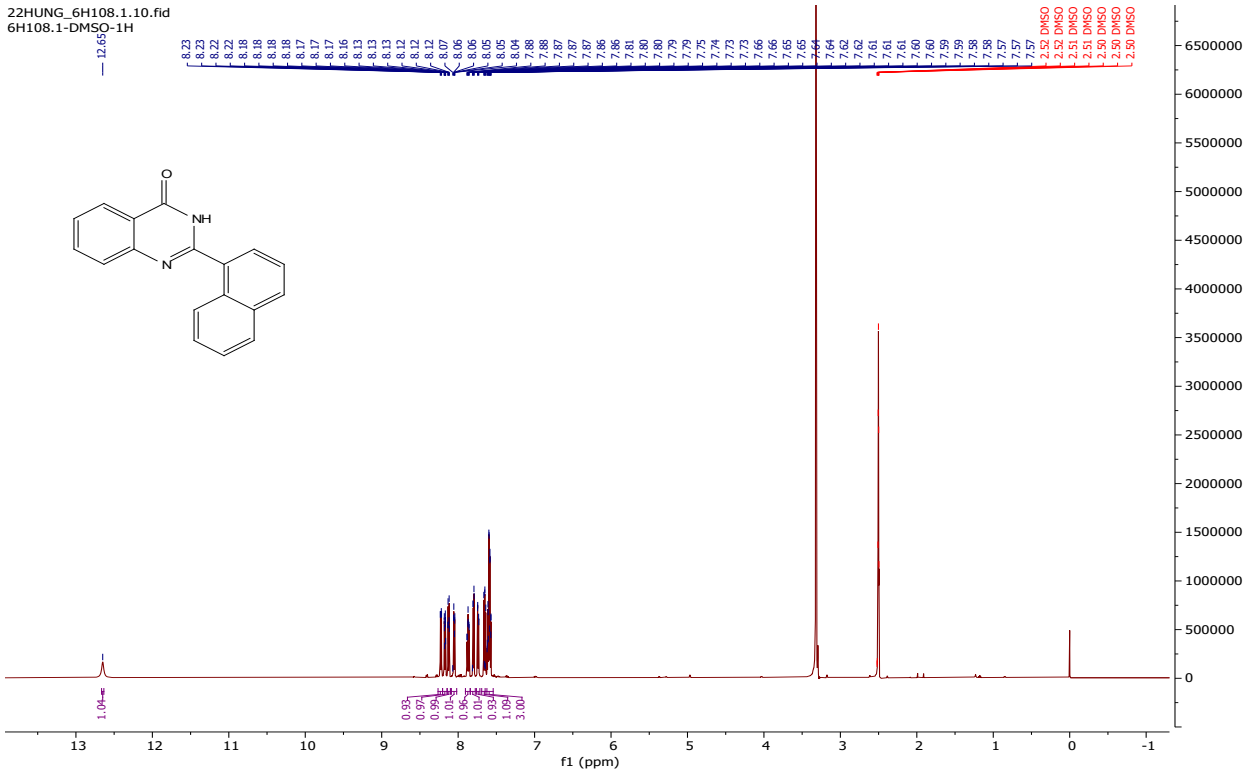


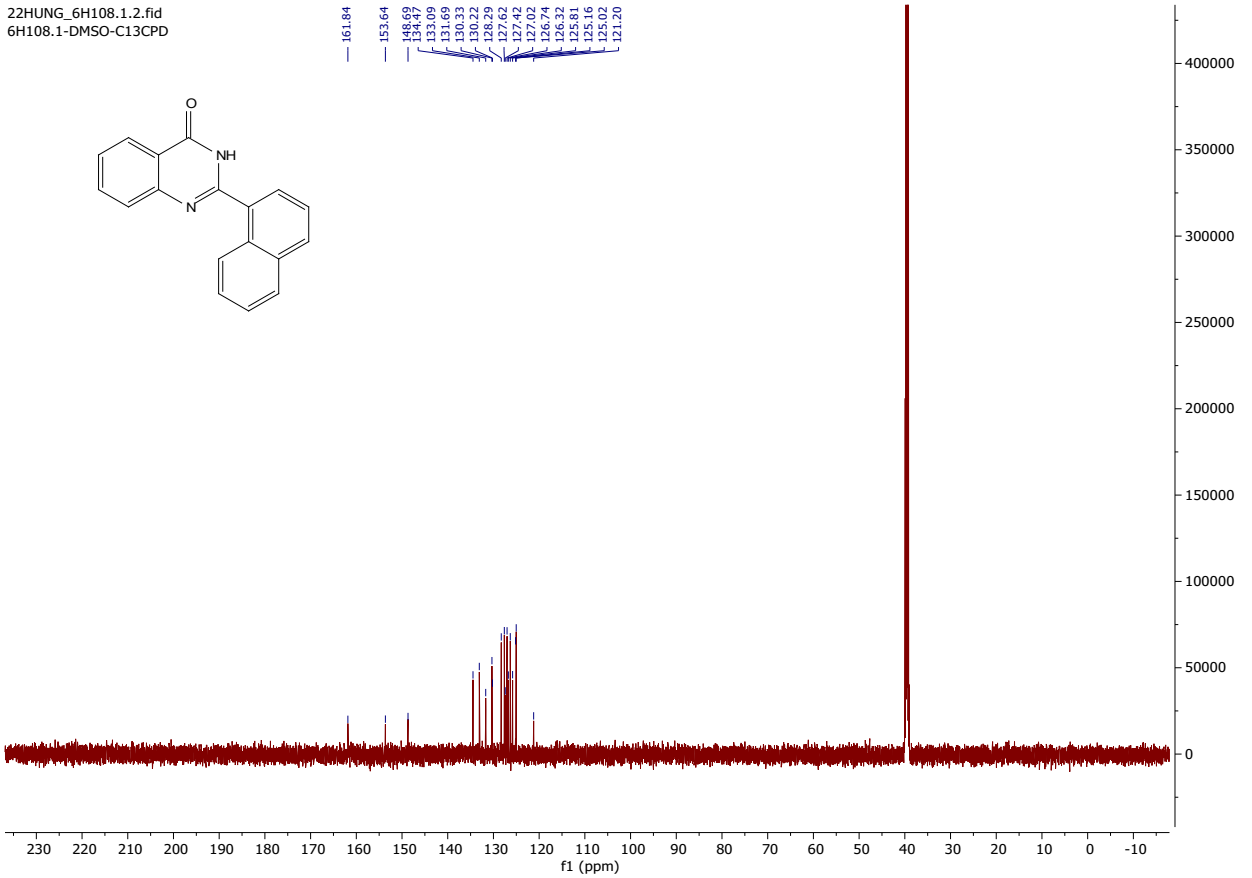
2-(4-(trifluoromethyl)phenyl)quinazolin-4(3*H*)-one 3l



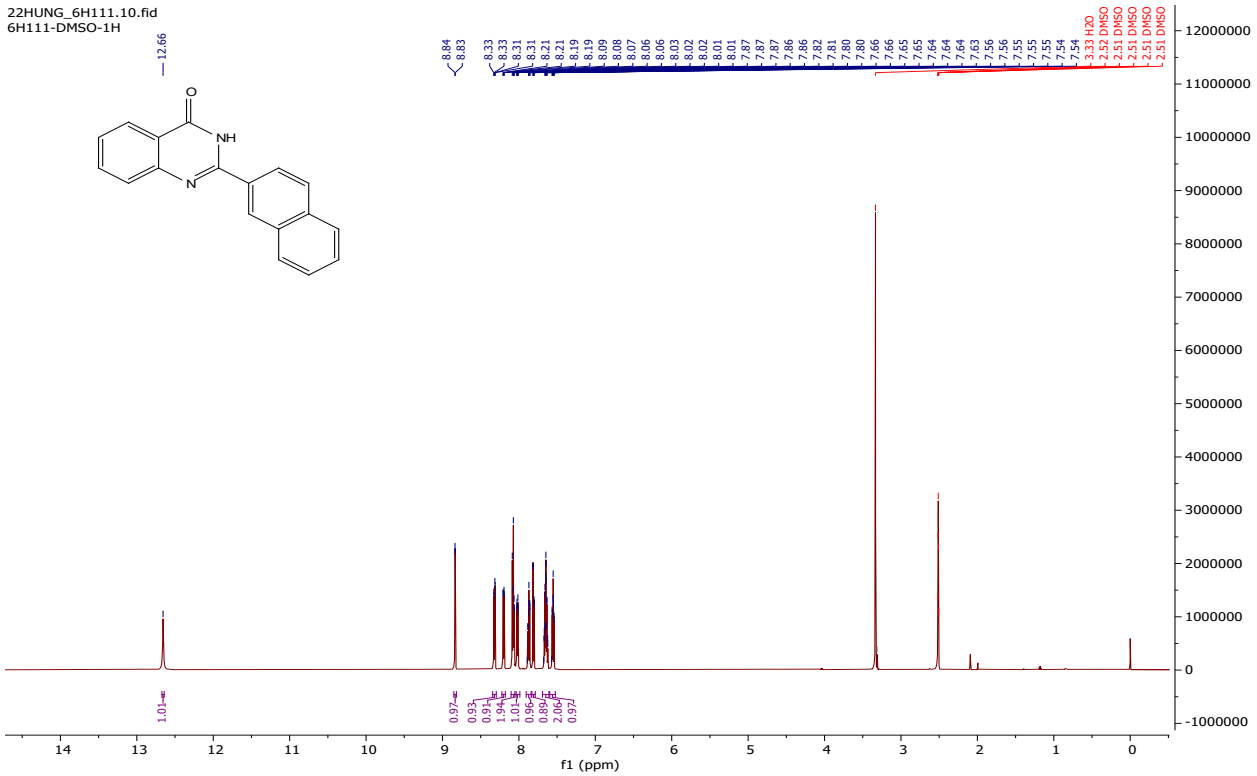


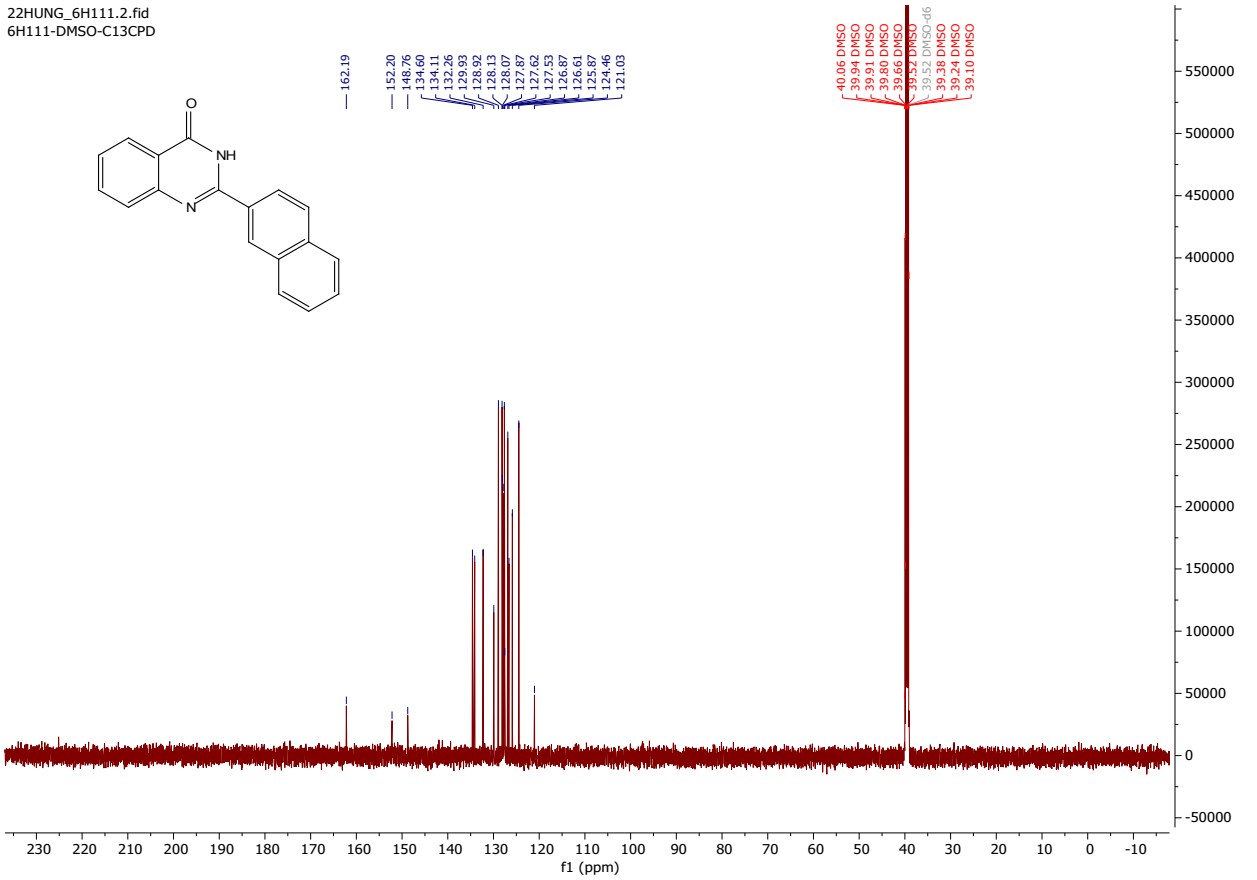
2-(naphthalen-1-yl)quinazolin-4(3*H*)-one 3m



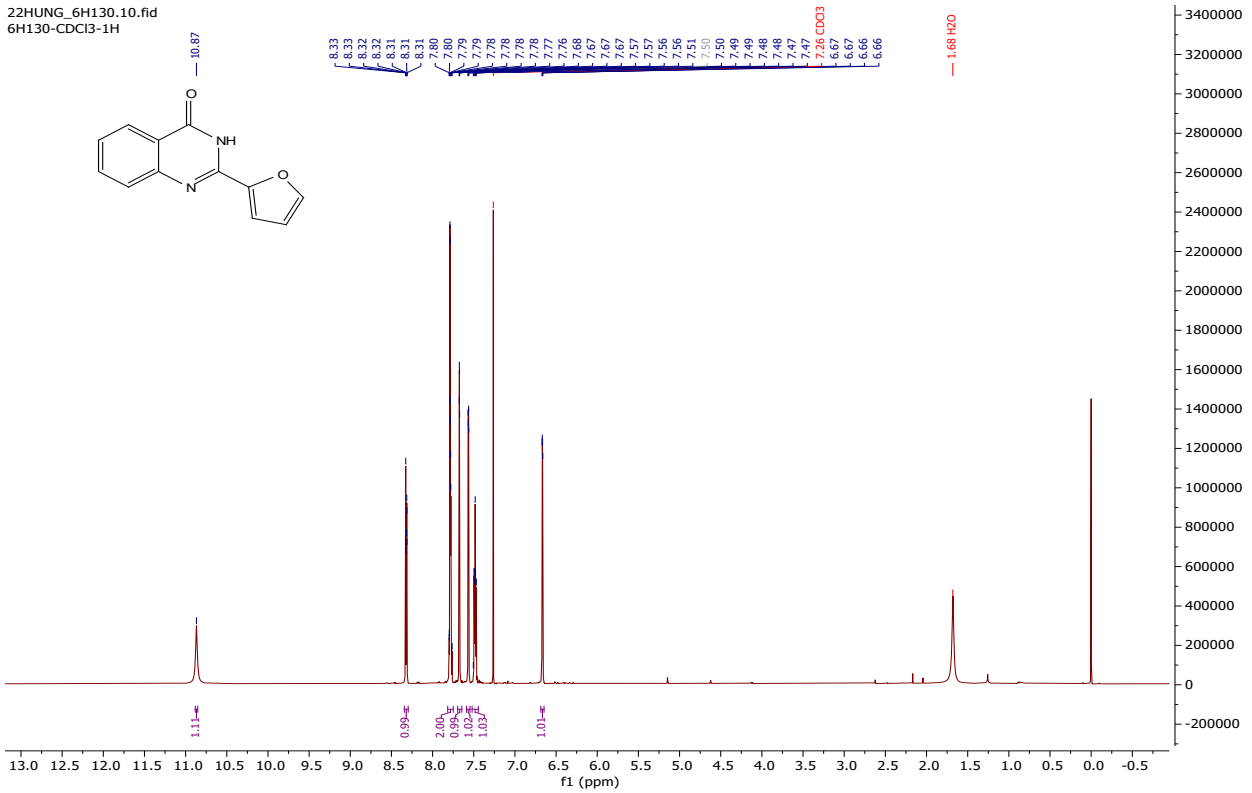


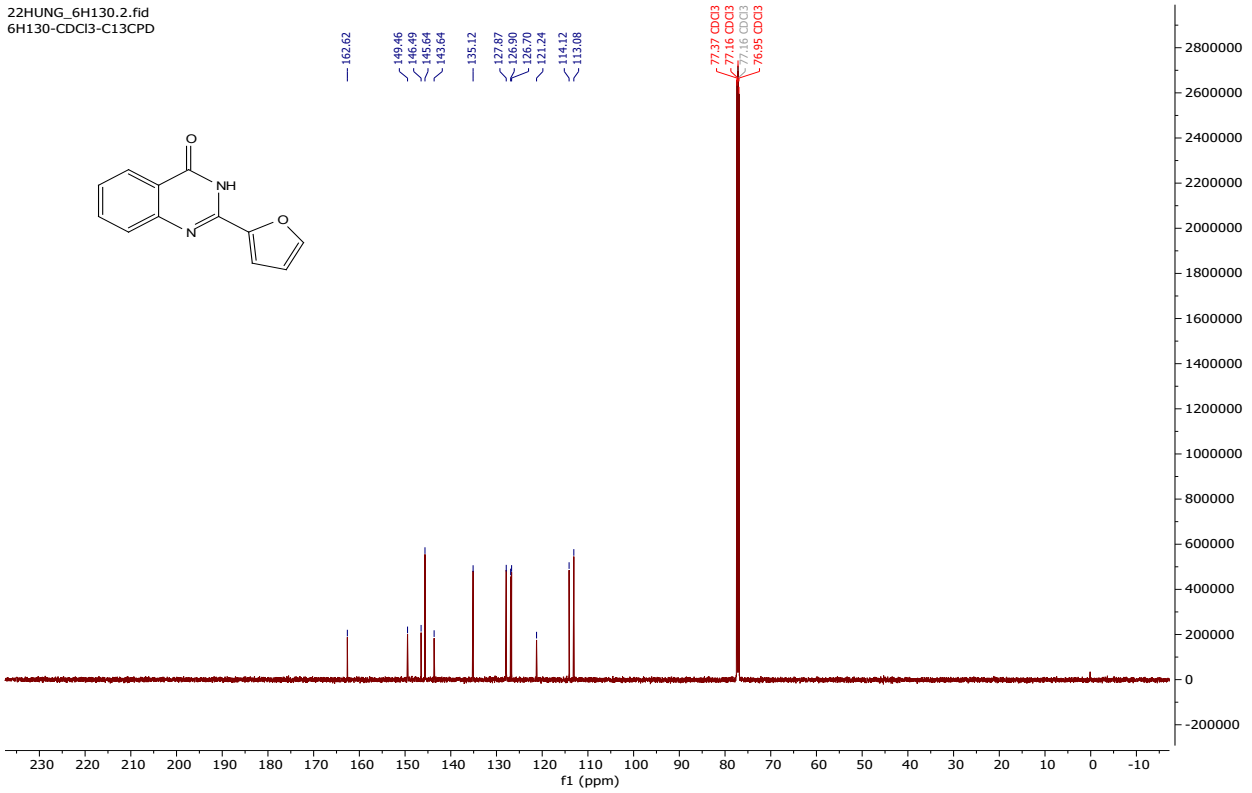
2-(naphthalen-2-yl)quinazolin-4(3*H*)-one 3n



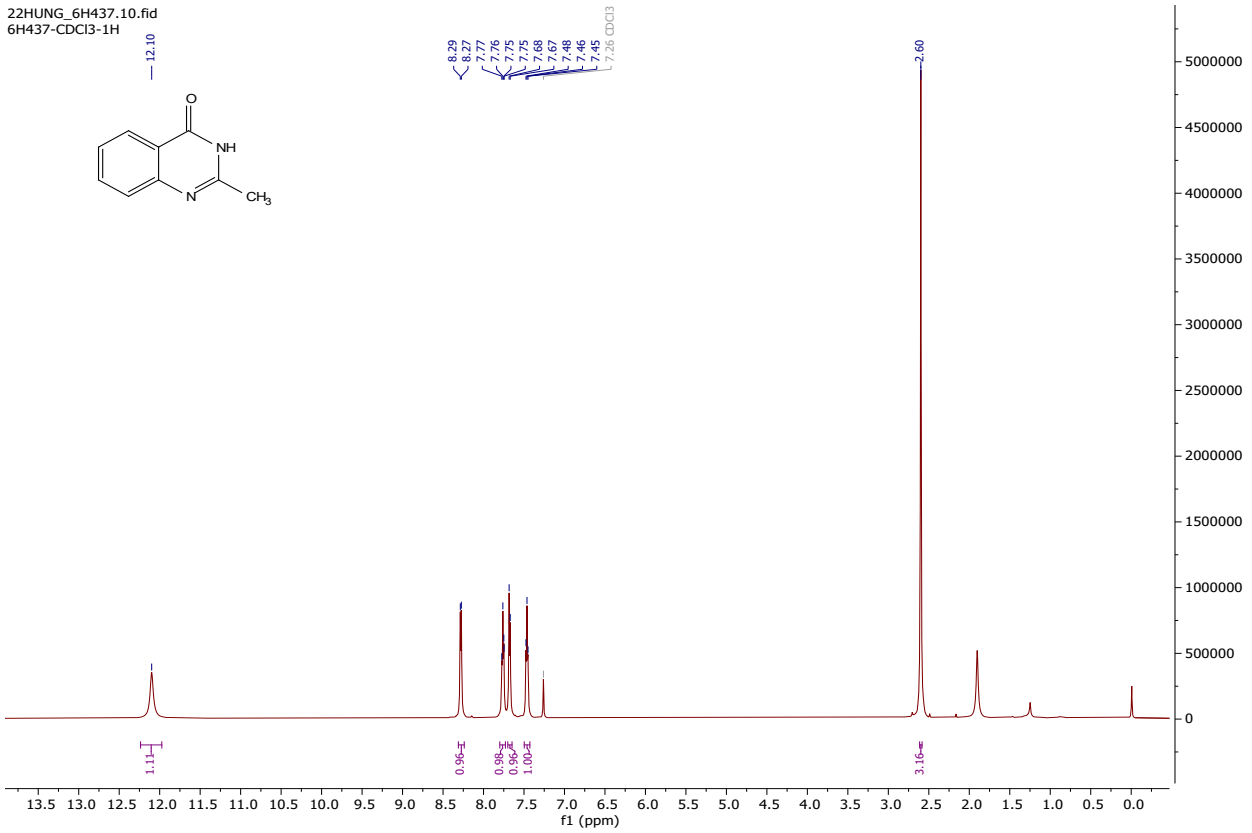


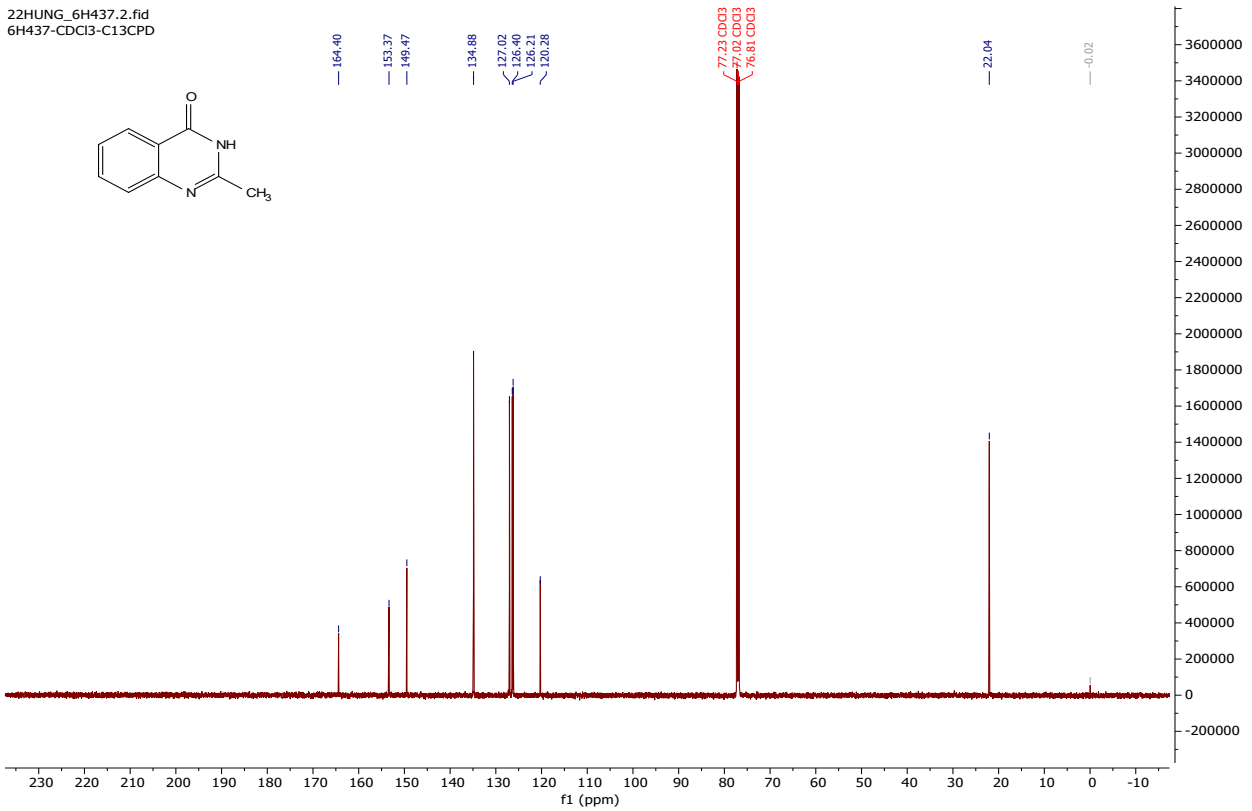
2-(furan-2-yl)quinazolin-4(3*H*)-one 3o



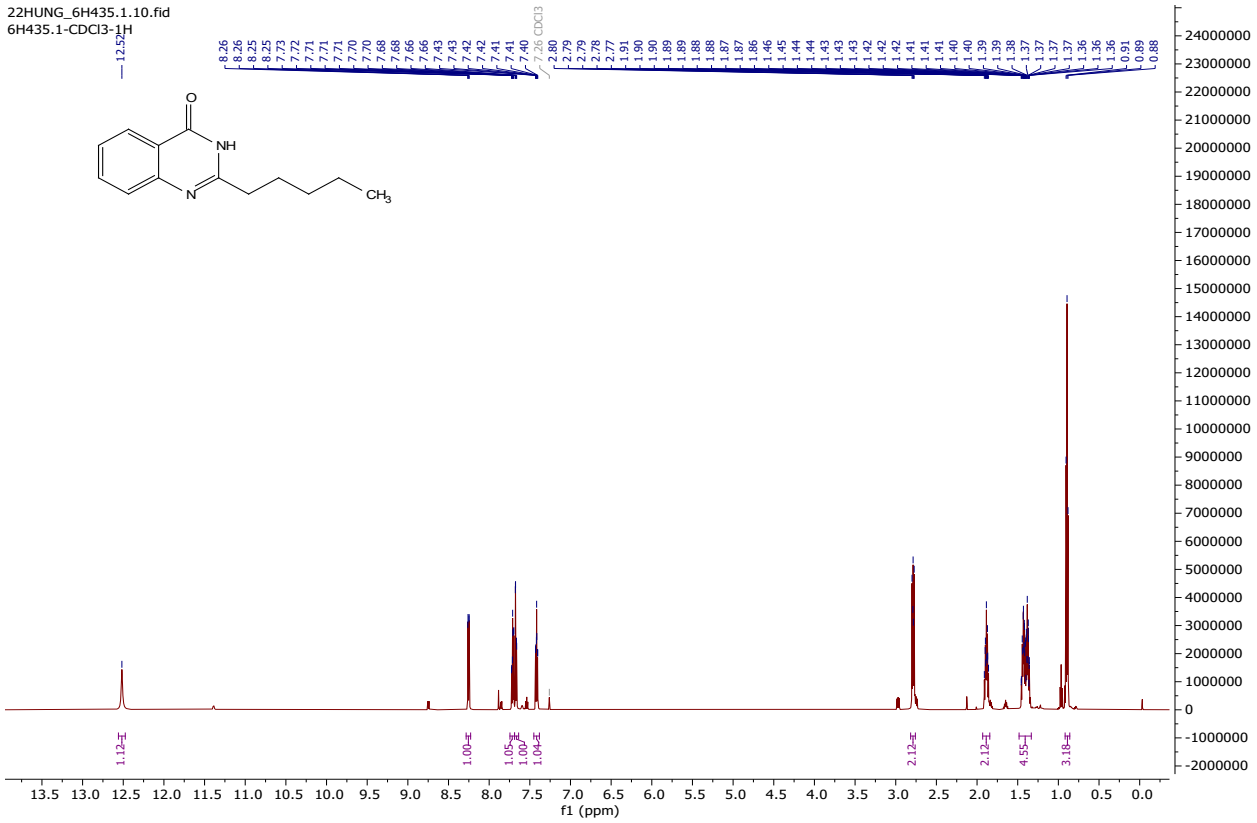


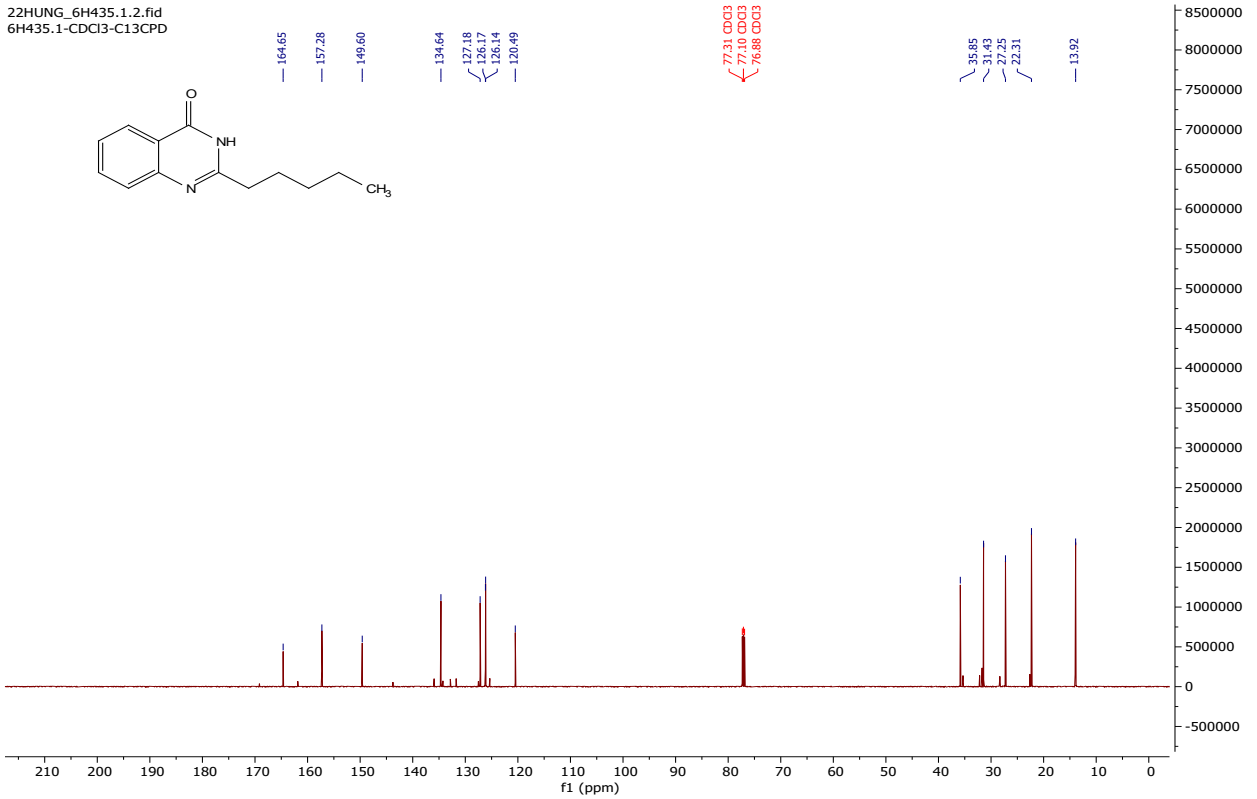
2-methylquinazolin-4(3*H*)-one 3p



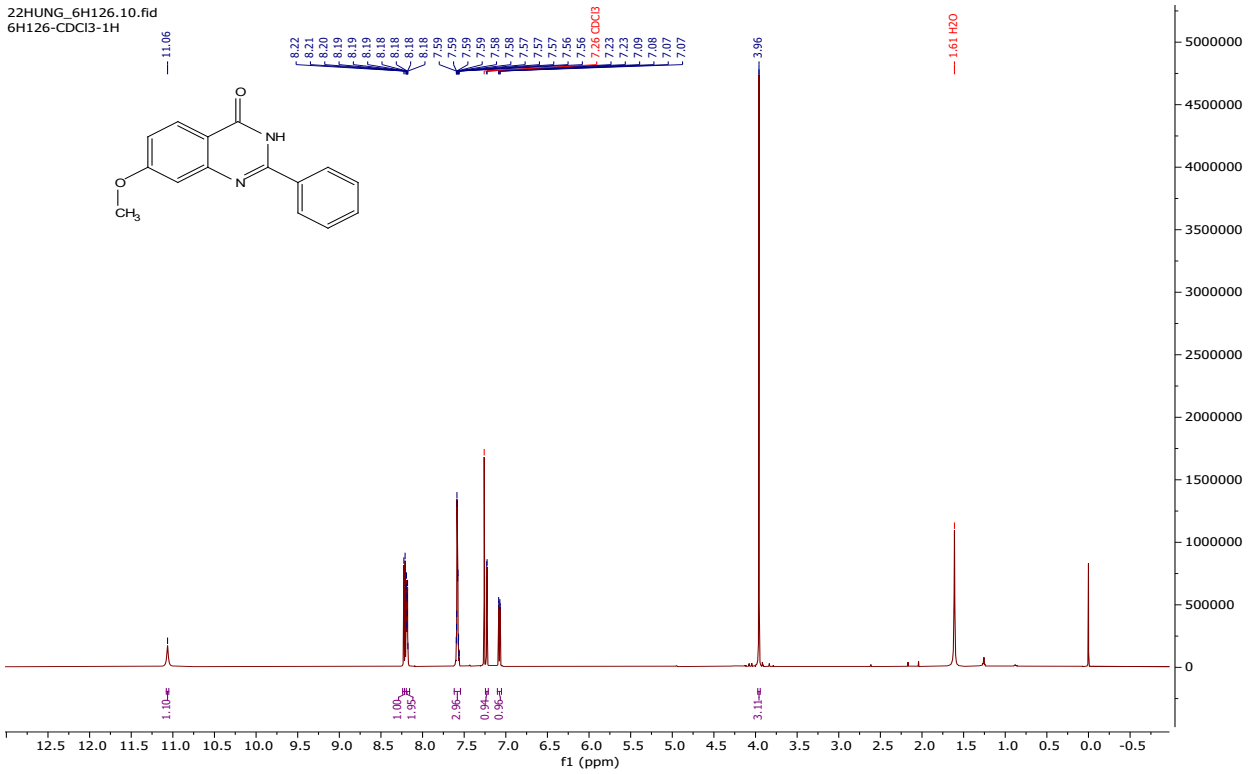


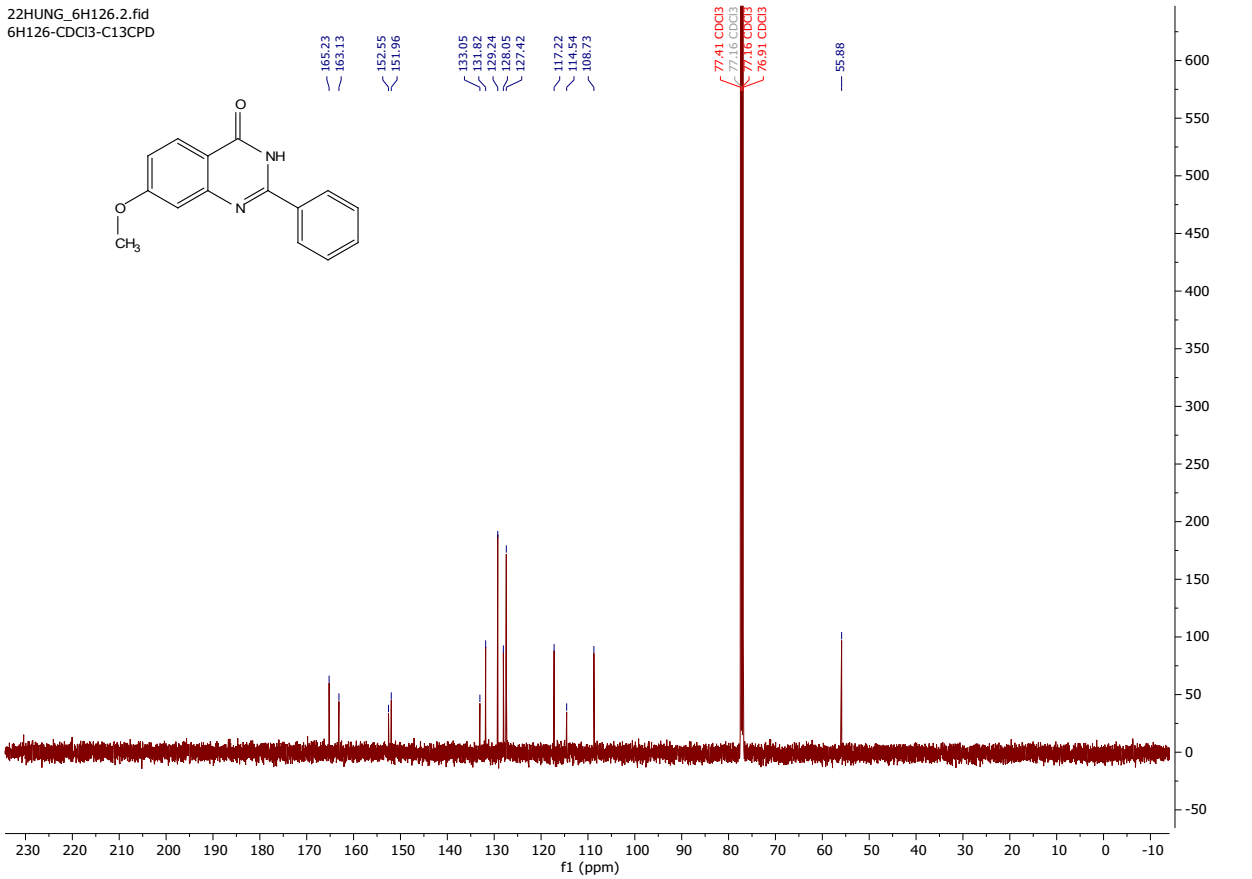
2-hexylquinazolin-4(3*H*)-one 3q



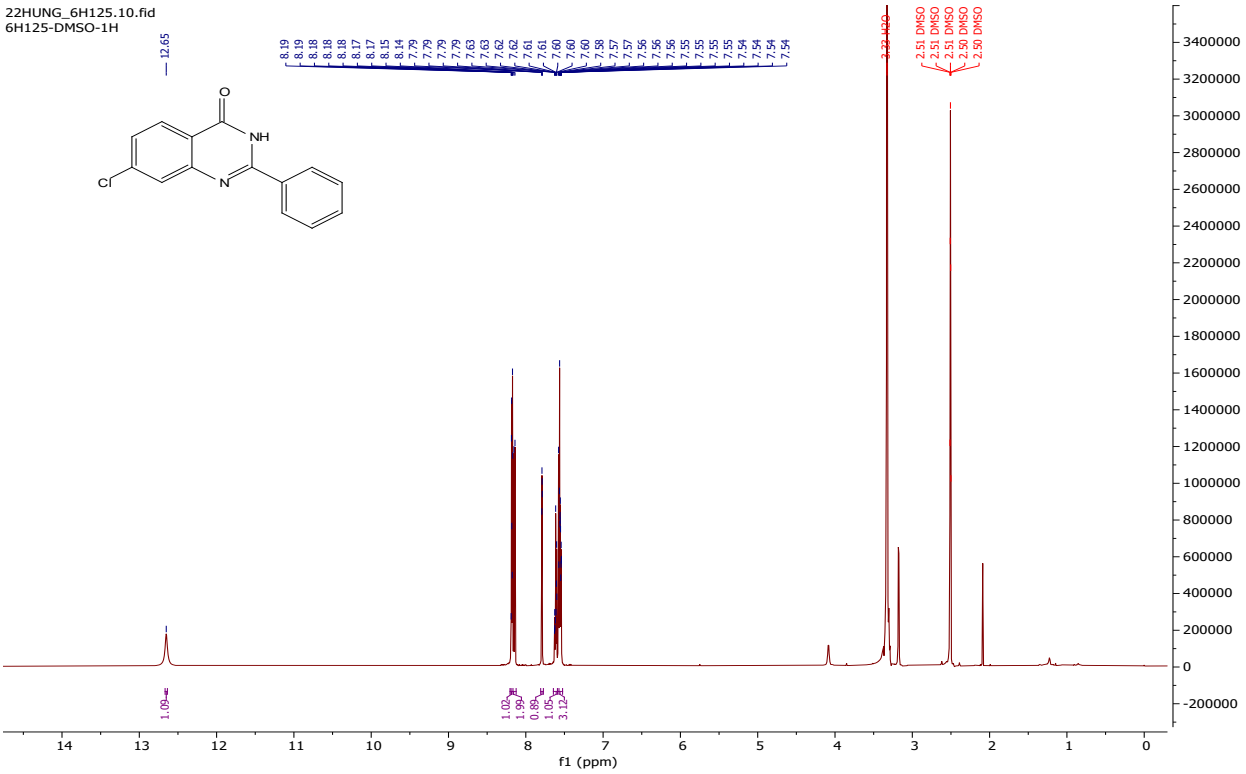


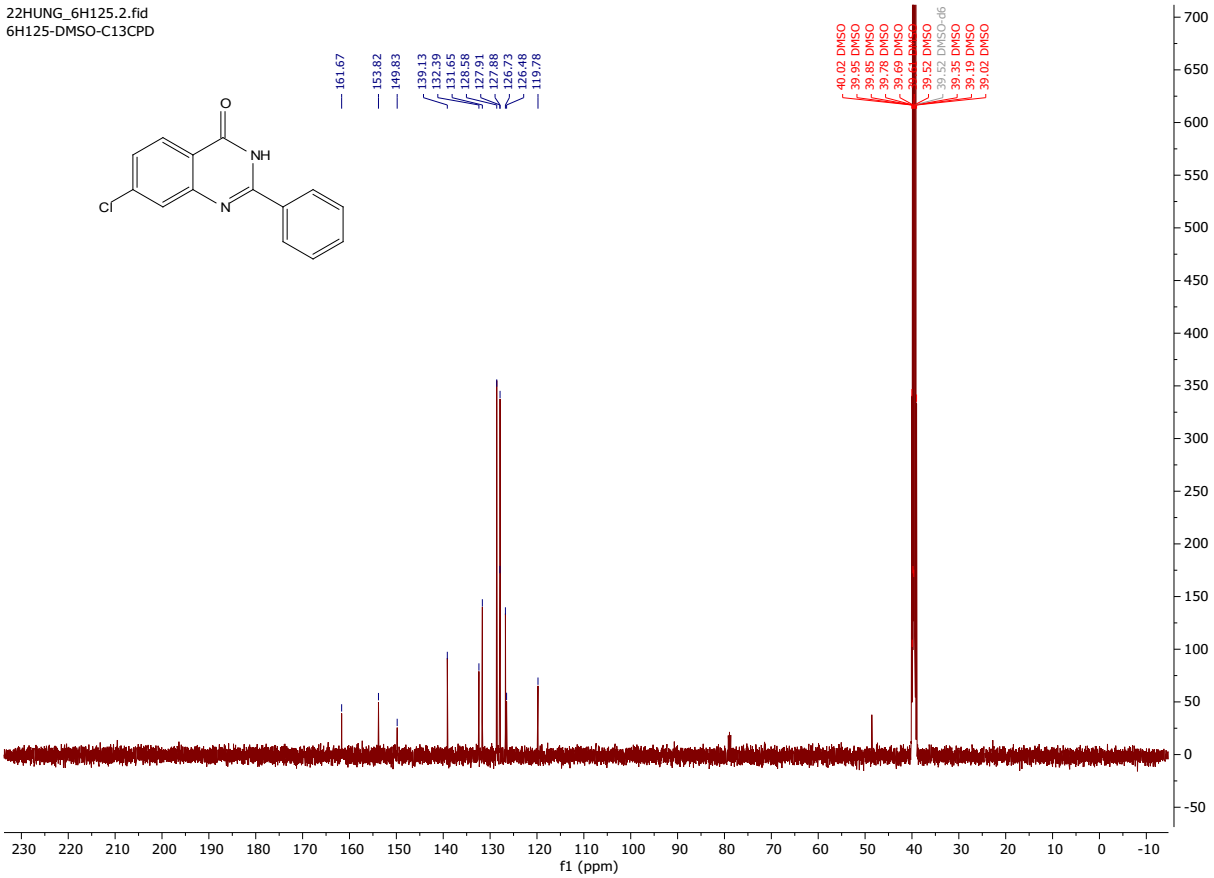
7-methoxy-2-phenylquinazolin-4(3*H*)-one 3r



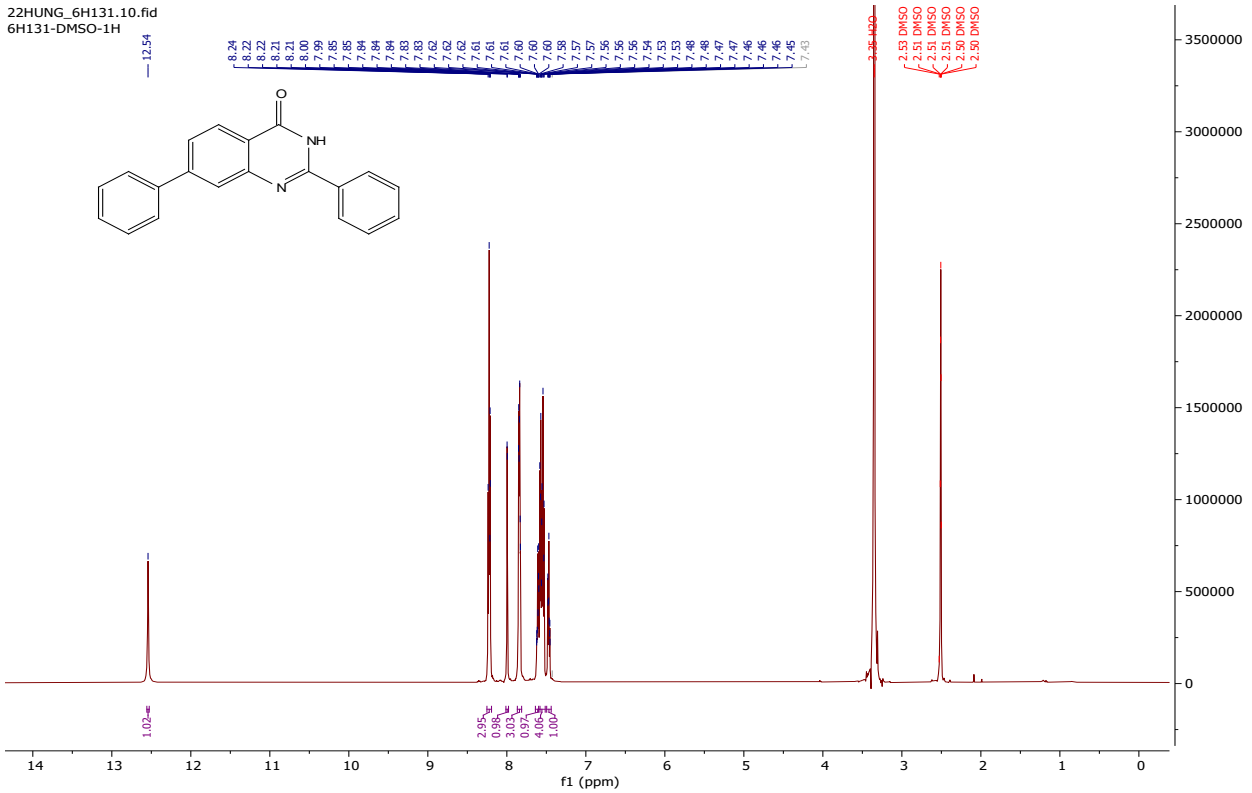


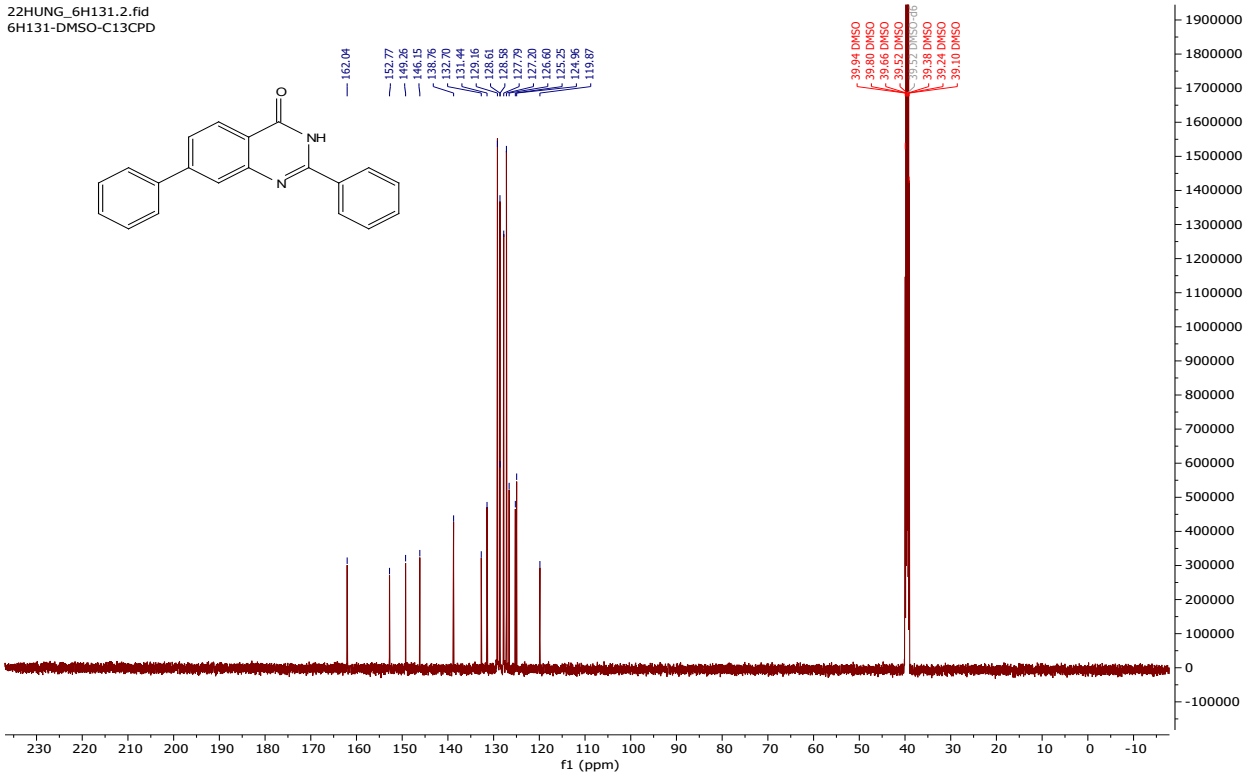
7-chloro-2-phenylquinazolin-4(3*H*)-one 3s



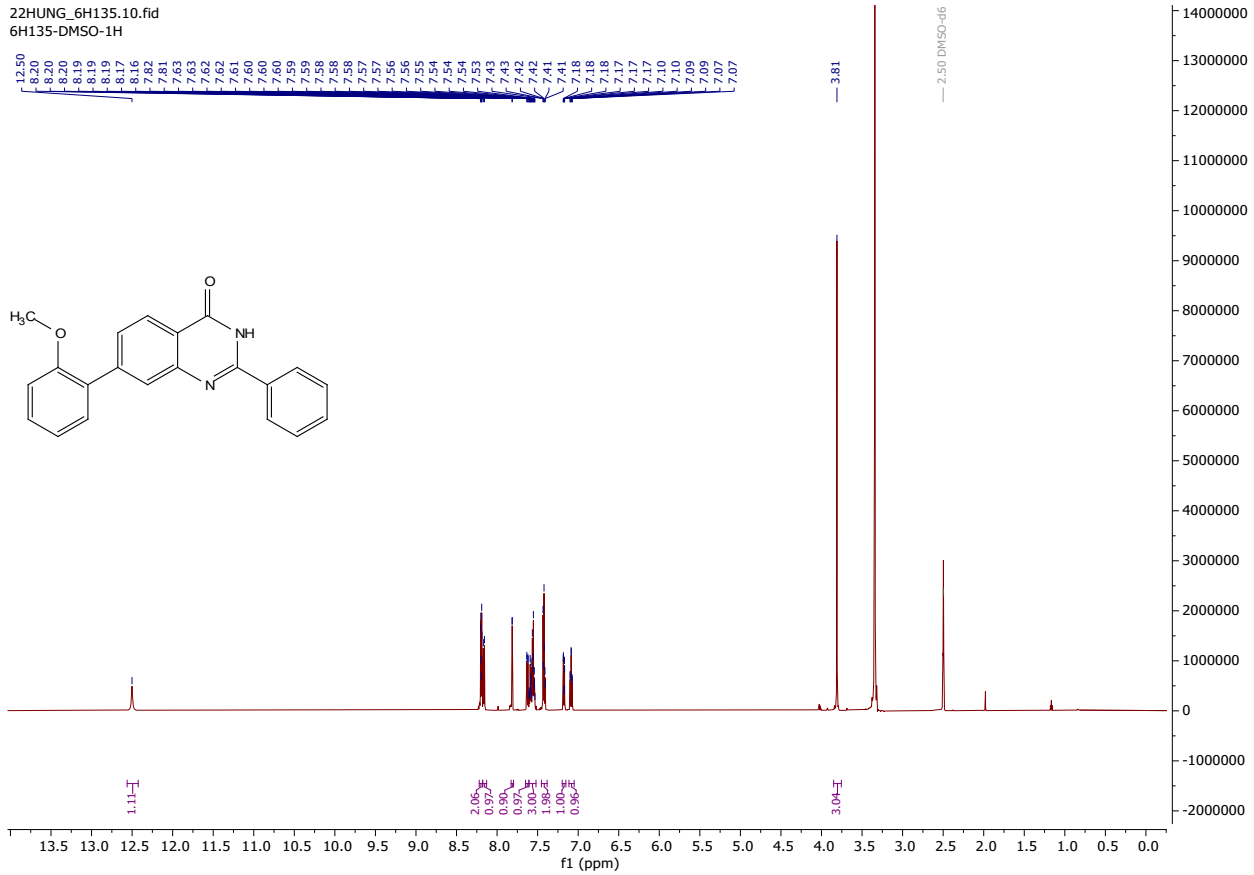


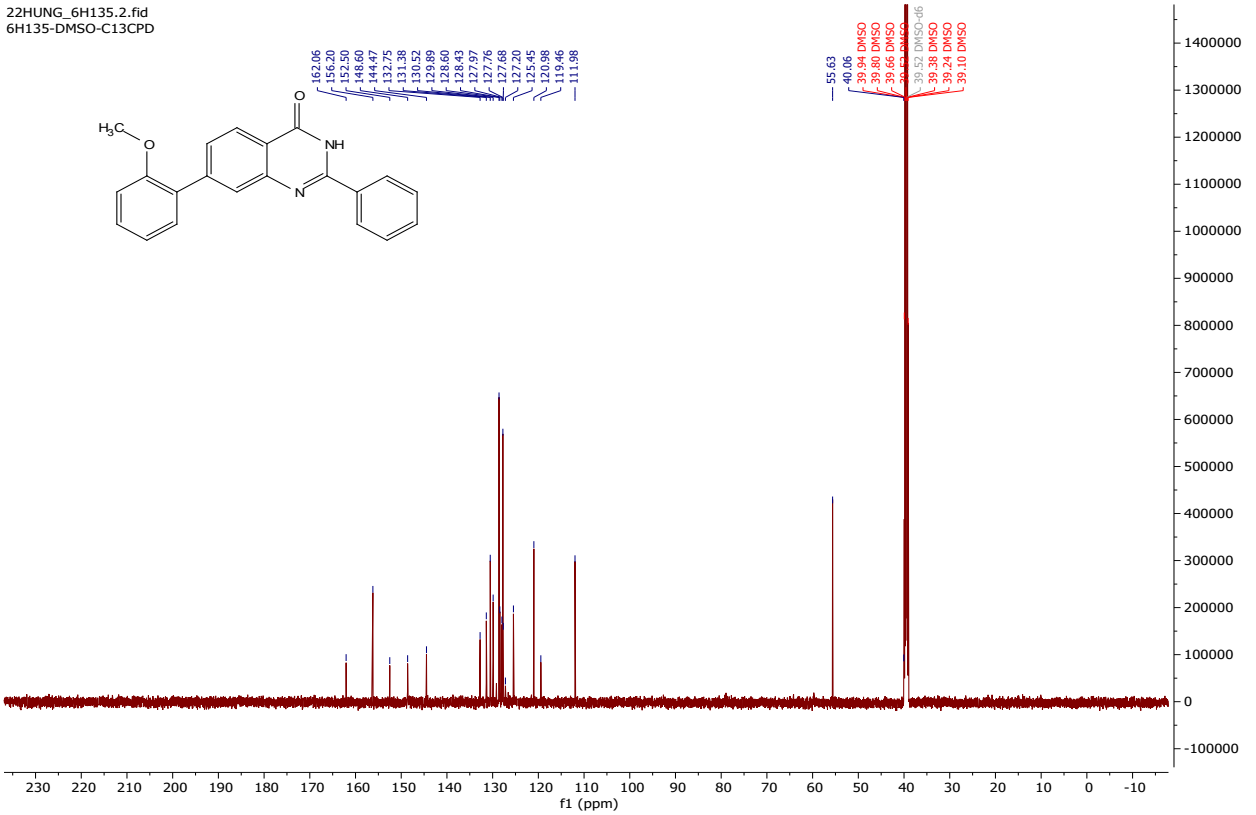
2,7-diphenylquinazolin-4(3*H*)-one 3t

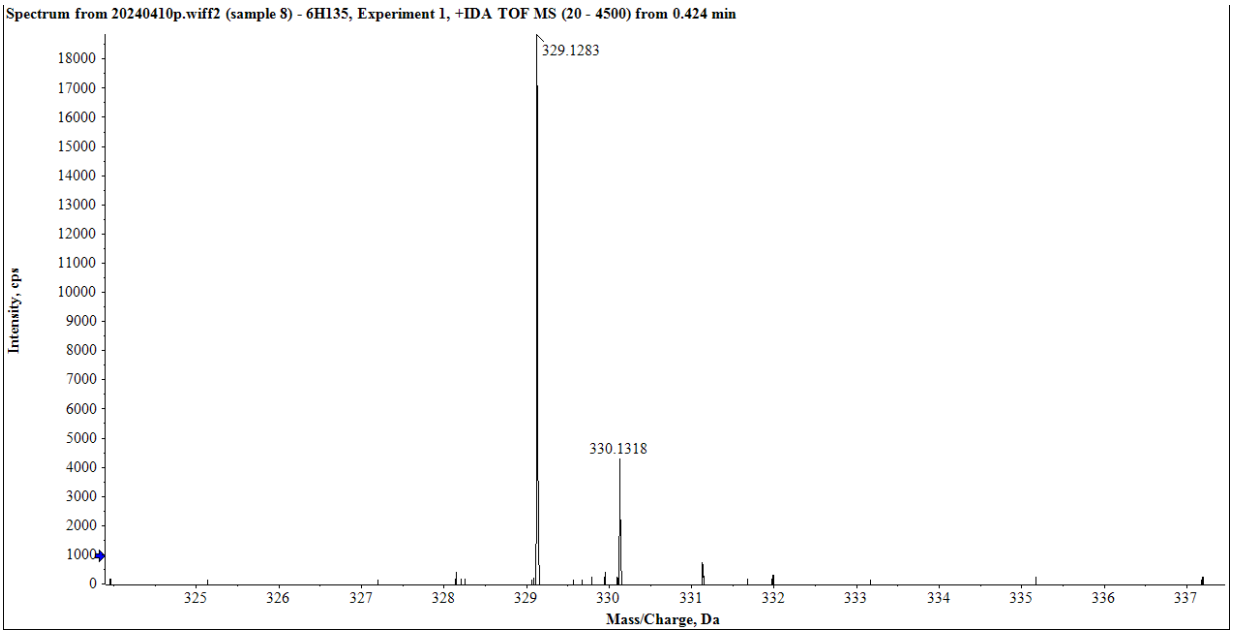




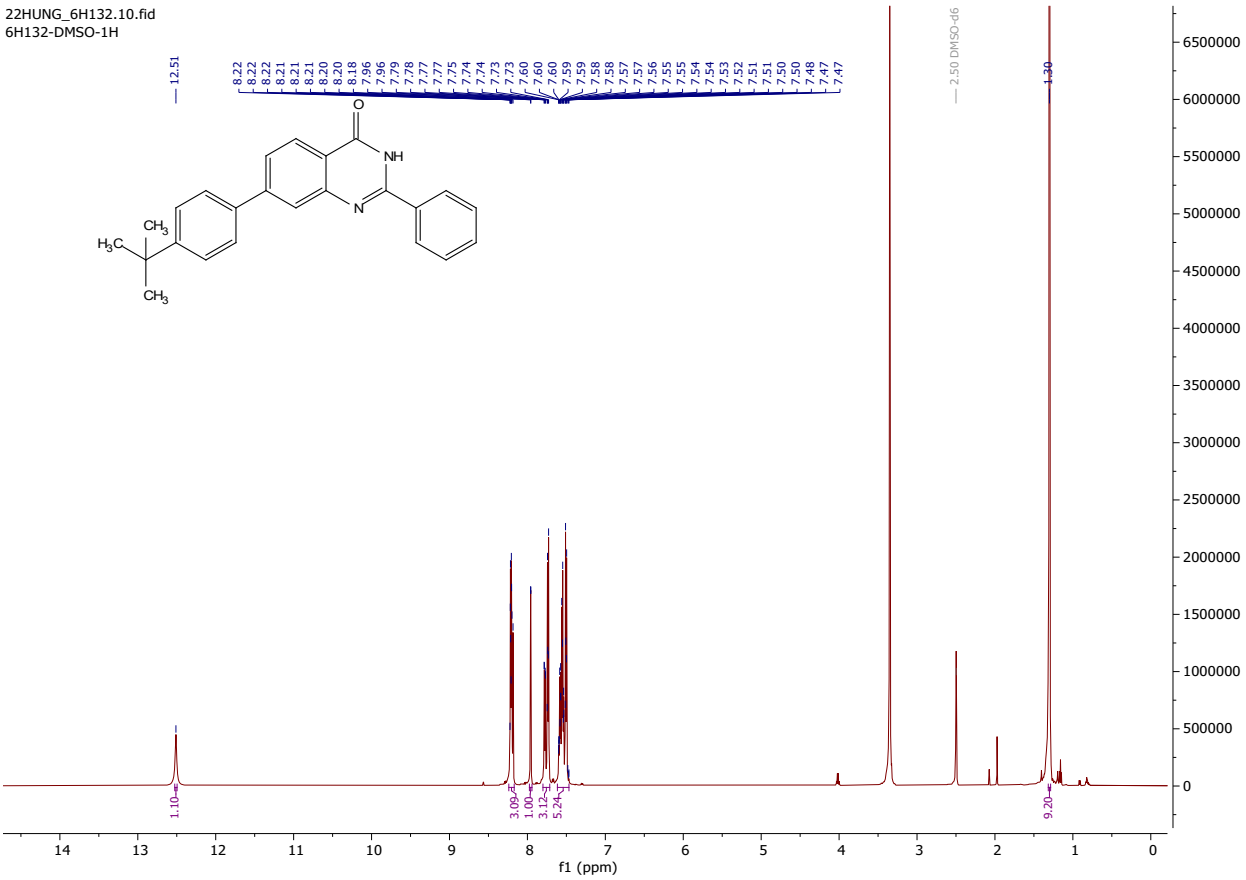
7-(2-methoxyphenyl)-2-phenylquinazolin-4(3*H*)-one 3u

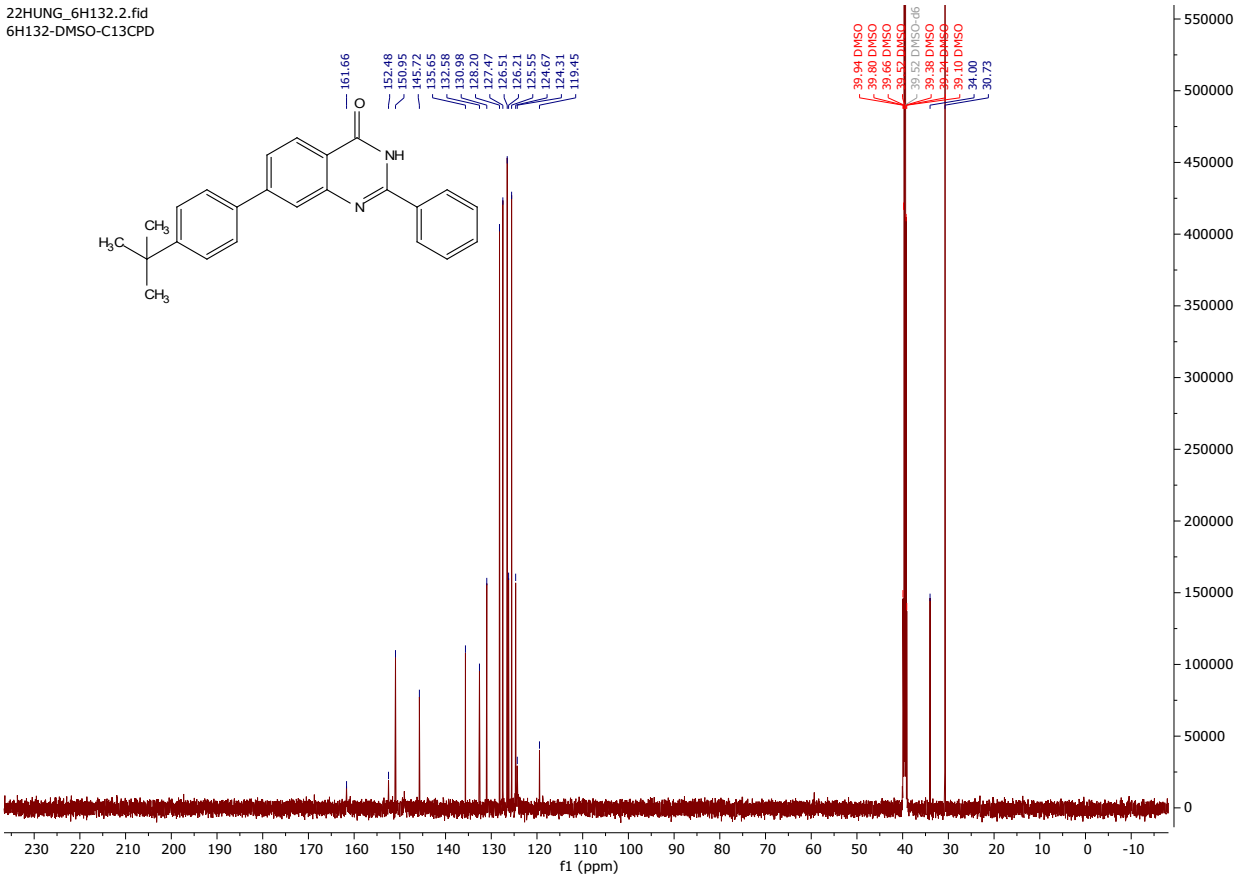

22HUNG_6H135.10.fid
6H135-DMSO-1H
12.50
8.20
8.20
8.19
8.19
8.19
8.17
8.16
7.82
7.81
7.63
7.63
7.62
7.62
7.61
7.60
7.60
7.60
7.59
7.59
7.58
7.58
7.58
7.57
7.57
7.56
7.56
7.55
7.54
7.54
7.54
7.53
7.43
7.43
7.42
7.42
7.41
7.41
7.18
7.18
7.17
7.17
7.17
7.10
7.10
7.09
7.09
7.07
7.07
3.81
2.50 DMSO-d6
O
NH
N
H3C
O
1.11
2.06
0.97
0.90
0.97
3.00
1.98
1.00
0.96
3.04
f1 (ppm)

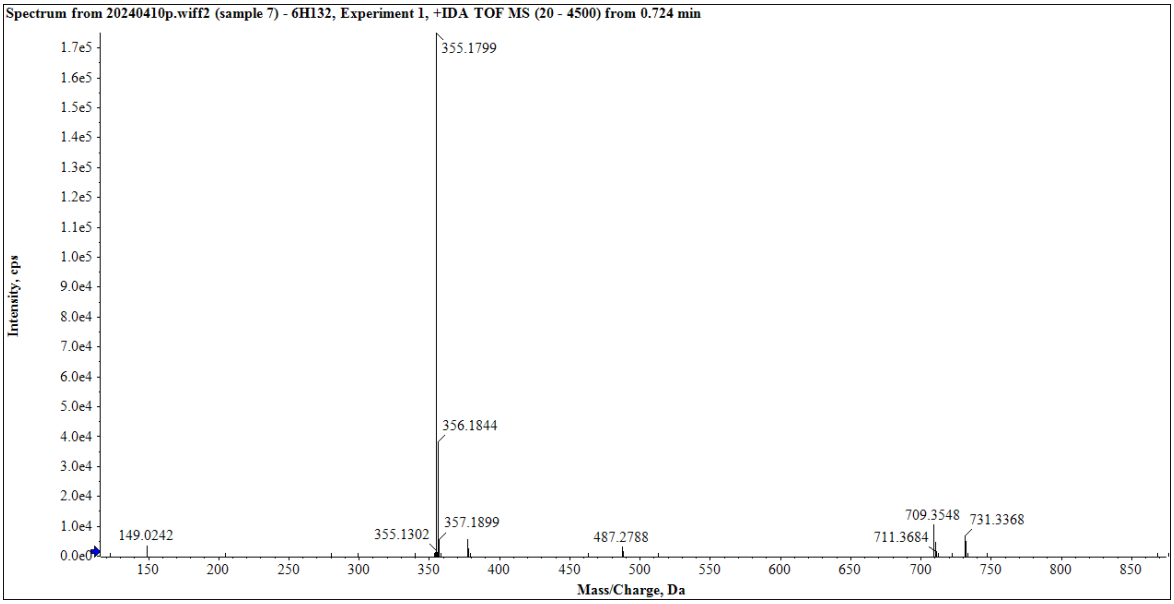

22HUNG_6H135.2.fid
6H135-DMSO-C13CPD
162.06
155.20
152.50
146.60
144.47
132.75
131.38
130.52
129.89
128.60
128.43
127.97
127.76
127.68
127.20
125.45
120.98
119.46
111.98
55.63
40.06
39.94 DMSO
39.80 DMSO
39.66 DMSO
39.52 DMSO
39.38 DMSO
39.24 DMSO
39.10 DMSO
O
NH
N
H3C
O
f1 (ppm)



7-(4-(tert-butyl)phenyl)-2-phenylquinazolin-4(3*H*)-one 3v




22HUNG_6H132.2.fid
6H132-DMSO-C13CPD
161.66
152.48
150.95
145.72
135.65
132.58
130.98
128.20
127.47
126.51
126.21
125.55
124.67
124.31
119.45
39.94 DMSO
39.80 DMSO
39.66 DMSO
39.52 DMSO
39.52 DMSO-d6
39.38 DMSO
39.24 DMSO
39.10 DMSO
34.00
30.73
O
NH
N
CH3
H3C
CH3
f1 (ppm)


Spectrum from 20240410p.wiff2 (sample 7) - 6H132, Experiment 1, +IDA TOF MS (20 - 4500) from 0.724 min
Intensity, cps
355.1799
356.1844
357.1899
149.0242
355.1302
487.2788
709.3548
711.3684
731.3368
Mass/Charge, Da