Supporting Information

for

The mechanochemical synthesis of quinazolin-4(3*H*)-ones by controlling the reactivity of IBX

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Characterization data, NMR spectra and crystallographic information

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Compounds characterization data

2-(4-Ethylphenyl)quinazolin-4(3*H*)-one (3a) [1]. R_f = 0.5 (hexane/ethyl acetate 4:1); white solid; Yield: 91% (100 mg); ^{1}H NMR (700 MHz, $CDCl_3$) δ 11.38 (s, 1H), 8.33 (dd, J_1 = 7.7, J_2 =0.7 Hz, 1H), 8.16 (d, *J* = 8.4 Hz, 2H), 7.85 (d, *J* = 8.4 Hz, 1H), 7.82 – 7.78 (m, 1H), 7.50 (t, *J* = 7.7 Hz, 1H), 7.41 (d, *J* = 8.4 Hz, 2H), 2.76 (q, *J* = 7.7 Hz, 2H), 1.31 (t, *J* = 7.7 Hz, 3H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 163.7, 152.1, 149.2, 148.9, 135.2, 129.8, 128.8, 127.8, 127.6, 126.9, 126.6, 120.8, 29.0, 15.4; HR-MS (ESI-TOF): m/z calculated for $C_{16}H_{14}NO_2$ $[M+H]^+$: 251.1179, found: 251.1200.

2-(2-Ethylphenyl)quinazolin-4(3*H*)-one (3b). R_f = 0.5 (hexane/ethyl acetate 7:3); white solid; Yield: 95% (105 mg); mp 145-147 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.11 (s, 1H), 8.20 (d, *J* = 8 Hz, 1H), 7.79 (m, 2H), 7.55 (d, *J* = 7.6 Hz, 1H), 7.51 – 7.42 (m, 2H), 7.39 (d, *J* = 7.6 Hz, 1H), 7.34 (t, *J* = 7.6 Hz, 1H), 2.89 (q, *J* = 7.2 Hz, 2H), 1.22 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.4, 153.8, 149.3, 143.2, 134.5, 133.4, 130.8, 129.8, 128.9, 127.9, 127.1, 126.5, 126.3, 120.8, 26.9, 15.7; IR (KBr): $\bar{\upsilon}$ = 1962, 2862, 2096, 1651, 1302, 1267, 1148 cm^{-1}; HR-MS (ESI-TOF): m/z calculated for $C_{16}H_{14}NO_2$ $[M+ H]^+$: 251.1179, found: 251.1191.

2-Phenylquinazolin-4(3*H*)-one (3c) [2]. R_f = 0.5 (hexane/ethyl acetate 4:1); white solid; Yield:79% (76mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.69 (s, 1H), 8.34 (d, *J* = 8 Hz, 1H), 8.27 (m, 2H), 7.86-7.79 (m, 2H), 7.60 (m, 3H), 7.51 (t, *J* = 7.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.9, 151.9, 149.7, 135.1, 132.9, 131.8, 129.2, 128.2, 127.5, 126.9, 126.5, 121.0

2-(*o*-Tolyl)quinazolin-4(3*H*)-one (3d) [2]. R_f = 0.4 (hexane: ethyl acetate 4:1); white solid; Yield: 92% (96 mg) ; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.79 (s, 1H), 8.24 (d, *J* = 8 Hz, 1H),

7.80 (d, *J* = 4 Hz, 2H), 7.57 (d, *J* = 7.2 Hz, 1H), 7.50 (dt, J_1 = 8, J_2 = 4 Hz, 1H), 7.43 (t, *J* = 7.2 Hz, 1H), 7.35 (d, *J* = 7.2 Hz, 2H), 2.53 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.14, 153.6, 149.2, 137.0, 134.9, 133.7, 131.6, 130.7, 128.9, 127.9, 127.1, 126.5, 126.4, 120.9, 20.2.

2-(*p*-Tolyl)quinazolin-4(3*H*)-one (3e) [2]. R_f = 0.5 (hexane/ethyl acetate 4:1); white solid; Yield: 82% (86 mg); ^{1}H NMR (700 MHz, DMSO-d_6) δ 12.46 (s, 1H), 8.14 (d, *J* = 7.7 Hz, 1H), 8.10 (d, *J* = 8.4 Hz, 2H), 7.83 (t, *J* = 7.7 Hz, 1H), 7.73 (d, *J* = 7.7 Hz, 1H), 7.51 (t, *J* = 7.7 Hz, 1H), 7.36 (d, *J* = 7.7 Hz, 2H), 2.39 (s, 3H); ^{13}C NMR (175 MHz, DMSO-d_6) δ 162.3, 152.3, 148.8, 141.5, 134.6, 129.9, 129.2, 127.7, 127.4, 126.4, 125.9, 21.0; HR-MS (ESI-TOF): m/z calculated for $C_{15}H_{12}NO_2$ $[M+H]^+$: 237.1022, found: 237.1026.

2-(4-Isopropylphenyl)quinazolin-4(3*H*)-one (3f) [2]. R_f = 0.5 (hexane/ethyl acetate 4:1); white solid; Yield: 84% (97 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.73 (s, 1H), 8.34 (d, *J* = 7.6 Hz, 1H), 8.21 (d, *J* = 8 Hz, 2H), 7.89 – 7.74 (m, 2H), 7.57 – 7.47 (m, 1H), 7.44 (d, *J* = 8.4 Hz, 2H), 3.15 – 2.91 (m, 1H), 1.32 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.1, 153.2, 151.9, 149.8, 134.9, 130.4, 128.1, 127.6, 127.3, 126.7, 126.5, 120.9, 34.3, 23.9.

2-Mesitylquinazolin-4(3*H*)-one (3g) [3]. R_f = 0.5 (hexane/ethyl acetate 4:1); white solid; Yield: 35% (40 mg), 50% (based on recovered aldehyde); ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.42 (s, 1H), 8.17 (d, *J* = 7.6 Hz, 1H), 7.83 (t, *J* = 7.6 Hz, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.54 (t, *J* = 7.6 Hz, 1H), 6.97 (s, 2H), 2.29 (s, 3H), 2.12 (s, 6H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.8, 154.3, 148.9, 138.4, 135.4, 134.5, 132.0, 128.0, 127.4, 126.7, 125.9, 121.1, 20.8, 19.1.

2-(2-Bromophenyl)quinazolin-4(3*H*)-one (3h) [4]. R_f = 0.4 (hexane/ethyl acetate 4:1); white solid; Yield: 94% (126 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.60 (s, 1H), 8.26 (d, *J* = 8 Hz, 1H), 7.82 (d, *J* = 4 Hz, 2H), 7.71 (t, *J* = 7.2 Hz, 2H), 7.57 – 7.49 (m, 1H), 7.47 (d, *J* = 7.2 Hz, 1H), 7.40 (t, *J* = 8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.6, 152.2, 149.1, 135.3, 135.0, 133.9, 132.1, 131.4, 128.1, 128.1, 127.5, 126.6, 121.2, 121.1.

2-(2-Fluorophenyl)quinazolin-4(3*H*)-one (3i) [5]. R_f = 0.4 (hexane/ethyl acetate 4:1); white solid; Yield: 68% (72 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.37 (s, 1H), 8.30 (m, 2H), 7.81 (m, 2H), 7.52 (m, 1H), 7.52 (d, *J* = 8 Hz, 1H), 7.35 (t, *J* = 8 Hz, 1H),7.23 (t, *J* = 8 Hz,1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.2, 160.9 (d, $^1J_{C,F}$ = 249.9 Hz), 149.1, 148.6 (d, $^4J_{C,F}$ = 1.6 Hz), 134.9, 133.6 (d, $^3J_{C,F}$ = 9.2 Hz), 131.5 (d, $^4J_{C,F}$ = 2.0 Hz), 128.13, 127.3, 126.7, 125.3 (d, $^4J_{C,F}$ = 3.3 Hz), 121.3, 120.4 (d, $^3J_{C,F}$ = 9.3 Hz), 116.8 (d, $^2J_{C,F}$ = 23 Hz).

2-(4-Methoxyphenyl)quinazolin-4(3*H*)-one (3j) [2]. R_f = 0.5 (hexane/ethyl acetate 4:1); white solid; Yield: 89% (99 mg); ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.41 (s, 1H), 8.19 (d, *J* = 7.6 Hz, 2H), 8.13 (d, *J* = 7.6 Hz, 1H), 7.79 (t, *J* = 7.2 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.47 (t, *J* = 7.2 Hz, 1H), 7.08 (d, *J* = 7.6 Hz, 2H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.4, 162.1, 151.9, 148.9, 134.5, 129.5, 127.3, 126.1, 125.9, 124.8, 120.7, 114.0, 55.5.

2-(Pyridin-4-yl)quinazolin-4(3*H*)-one (3k) [6]. R_f = 0.3 (hexane/ethyl acetate 1:1); white solid; Yield: 71 % (70 mg); ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.79 (s, 1H), 8.79 (d, *J* = 5.2 Hz, 1H), 8.18 (d, *J* = 7.6 Hz, 1H), 8.12 (d, *J* = 6 Hz, 2H), 7.88 (t, *J* = 8 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 1H), 7.59 (t, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.2, 150.7, 150.4, 148.4, 139.9, 134.9, 127.8, 127.5, 125.9, 121.7. 121.5.

2-(Naphthalen-1-yl)quinazolin-4(3*H*)-one (3l) [7]. R_f = 0.4 (hexane/ethyl acetate 7:3); white solid; Yield: 52% (62 mg); ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.66 (s, 1H), 8.23 (d, *J* = 8 Hz, 1H), 8.47 (d, *J* = 8.8, 1H), 8.13 (d, *J* = 8 Hz, 1H), 8.07 – 8.03 (m, 1H), 7.90 – 7.84 (m, 1H), 7.80 (d, *J* = 6.8 Hz, 1H), 7.74 (d, *J* = 8 Hz, 1H), 7.68 – 7.63 (m, 1H), 7.62 – 7.56 (m, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.9, 153.7, 148.7, 134.5, 133.1, 131.7, 130.3, 130.3, 128.3, 127.7, 127.5, 127.0, 126.8, 126.3, 125.8, 125.2, 125.0, 121.2; HR-MS (ESI-TOF): m/z calculated for $C_{18}H_{12}NO_2$ [M+ H] $^+$: 273.1022, found: 273.1039.

2-([1,1'-biphenyl]-2-yl)quinazolin-4(3*H*)-one (3m) [8]. R_f = 0.4 (hexane/ethyl acetate 4:1); white solid; Yield: 70% (92 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.43 (s, 1H), 8.17 (d, *J* = 7.6 Hz, 1H), 7.87 (d, *J* =7.6, 1H), 7.78 (m, 2H), 7.58 (t, *J* = 7.6 Hz, 1H), 7.49 (d, *J* =7.6 Hz, 3H), 7.32-7.26 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.9, 153.7, 149.2, 140.7, 139.3, 134.8, 132.8, 131.1, 131.0, 130.5, 129.1, 128.9, 128.2, 128.1, 127.9, 127.1, 126.5, 120.8.

2-Cyclohexylquinazolin-4(3*H*)-one (3n) [9]. R_f = 0.5 (hexane/ethyl acetate 3:2); white solid; Yield: 65% (65 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.86 (s, 1H), 8.27 (d, *J* = 7.6 Hz, 1H), 7.76 (t, *J* = 8, 1H), 7.70 (d, *J* = 8, 1H) 7.46 (t, *J* = 7.6 Hz, 1H), 2.70 (t, *J* = 12 Hz, 1H), 2.06 (d, *J* = 11.6 Hz, 2H), 1.92 (d, *J* = 12.8 Hz, 2H), 1.87 – 1.65 (m, 3H), 1.54 – 1.35 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.5, 160.4, 149.7, 134.9, 127.5, 126.4, 126.3, 120.9, 44.9, 30.6, 26.1, 25.8.

2-(2-Phenylpropyl)quinazolin-4(3*H*)-one (3o). R_f = 0.5 (hexane/ethyl acetate 7:3); white solid; Yield: 84% (102 mg); mp 165-166 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.05 (s, 1H), 8.33 (d, *J* = 7.6 Hz, 1H), 7.79 (m, 2H), 7.52 (t, *J* = 7.2 Hz, 1H), 7.37 (d, *J* = 6.8 Hz, 2H), 7.28 (d, *J* = 6.4 Hz, 2H), 7.20 (d, *J* = 6.8 Hz, 1H), 3.55 (m, 1H), 3.19 – 2.94 (m, 2H), 1.42 (d, *J* =

6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.4, 155.7, 149.6, 145.5, 134.9, 128.7, 127.5, 127.1, 126.7, 126.6, 126.4, 120.6, 44.7, 38.8, 21.1; IR (KBr): $\bar{\upsilon}$ = 2973, 2923, 2103, 1653, 1467, 1335, 1251 cm^{-1}; HR-MS (ESI-TOF): m/z calculated for $C_{17}H_{16}NO_2$ [M+ H] $^+$: 265.1335, found: 265.1361.

2-Propylquinazolin-4(3*H*)-one (3p) [10]. R_f = 0.3 (hexane/ethyl acetate 7:3); white solid; Yield: 68% (57 mg); ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.18 (s, 1H), 8.07 (d, *J* = 7.6 Hz, 1H), 7.77 (t, *J* = 6.8 Hz, 1H), 7.59 (d, *J* = 7.6 Hz, 1H), 7.45 (t, *J* = 7.1 Hz, 1H), 2.57 (t, *J* = 6.4 Hz, 2H), 1.74 (m, 2H), 0.93 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.9, 157.3, 148.9, 134.3, 126.8, 125.9, 125.7, 120.8, 36.4, 20.2, 13.5.

2-(4-Chlorophenyl)quinazolin-4(3*H*)-one (3q) [4]. R_f = 0.5 (hexane/ethyl acetate 4:1); white solid; Yield: 60% (67 mg); ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.62 (s, 1H), 8.20 (d, *J* = 8.4 Hz, 2H), 8.14 (d, *J* = 8, 1H), 7.85 (t, *J* = 7.6 Hz, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.63 (d, *J* = 8.0 Hz, 2H), 7.53 (t, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.7, 151.4, 148.6, 136.3, 134.7, 131.6, 129.6, 128.7, 127.5, 126.8, 125.9, 120.9; HR-MS (ESI-TOF): m/z calculated for $C_{14}H_9NO_2Cl$ [M+ H] $^+$: 257.0476, found: 257.0479.

2-(4-Bromophenyl)quinazolin-4(3*H*)-one (3r) [4]. R_f = 0.6 (hexane/ethyl acetate 4:1); white solid; Yield: 78% (104 mg); ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.60 (s, 1H), 8.13 (d, *J* = 8.4 Hz, 3H), 7.84 (t, *J* = 6.4, 1H), 7.76 (d, *J* = 6.4 Hz, 3H), 7.53 (t, *J* = 6.4, 1H); ^{13}C NMR (175 MHz, DMSO-d_6) δ 162.2, 151.5, 148.6, 134.7, 131.9, 131.7, 129.8, 127.5, 126.8, 125.9, 125.2, 121.0.

2-(2-Bromo-5-fluorophenyl)quinazolin-4(3*H*)-one (3s). R_f = 0.5 (hexane/ethyl acetate 7:3); white solid; Yield: 50% (69 mg); mp 229-230 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.56 (s, 1H), 8.28 (d, *J* = 8 Hz, 1H), 7.82 (m, 2H), 7.68 (dd, J_1 = 8.8, J_2 = 4 Hz, 1H), 7.61 – 7.49 (m, 2H), 7.16 (dd, J_1 = 8.4, J_2 = 5.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.4, 162.0 (d, $^{1}J_{C,\ F}$ = 250.3), 150.9, 148.9, 136.5 (d, $^{3}J_{C,\ F}$ = 7.9 Hz), 135.5 (d, $^{3}J_{C,\ F}$ = 7.9 Hz), 135.2, 128.2, 127.8, 126.7, 121.3, 119.6 (d, $^{2}J_{C,\ F}$ = 22.3 Hz), 118.9 (d, $^{2}J_{C,\ F}$ =24.6 Hz), 115.3 (d, $^{4}J_{C,\ F}$ = 3.5 Hz); IR (KBr): $\bar{\upsilon}$ = 3427, 2096, 1651, 1338, 1251, 1203 cm^{-1}; HR-MS (ESI-TOF): m/z calculated for $C_{14}H_8NO_2{}^{79}BrF$ $[M + H]^+$: 318.9877, found: 318.9904, $C_{14}H_8NO_2{}^{81}Br$ $[M + H]^+$: 320.9857, found: 320.9885.

2-(3-Bromo-4-methoxyphenyl)quinazolin-4(3*H*)-one (3t). R_f = 0.5 (hexane/ethyl acetate 7:3); white solid; Yield: 76% (110 mg); mp charred at 250 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.50 (s, 1H), 8.47 (s, 1H), 8.25 (d, *J* = 8 Hz, 1H), 8.13 (d, *J* = 8 Hz, 1H), 7.83 (t, *J* = 8.4 Hz, 1H), 7.73 (d, *J* = 8 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 1H), 7.28 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.3, 158.0, 150.8, 148.7, 134.7, 132.4, 128.8, 127.5, 126.5, 126.2, 125.9, 120.7, 112.7, 110.73, 56.7; IR (KBr): $\bar{\upsilon}$ = 3193, 2089, 1643, 1224, 1141, 1055 cm^{-1}; HR-MS (ESI-TOF): m/z calculated for $C_{15}H_{11}NO_2{}^{79}Br$ $[M + H]^+$: 331.0077, found: 331.0081, $C_{15}H_{11}NO_2{}^{81}Br$ $[M + H]^+$: 333.0057, found: 333.0059.

2-(2-Iodo-4,5-dimethylphenyl)quinazolin-4(3*H*)-one (3u). R_f = 0.4 (hexane/ethyl acetate 4:1); white solid; Yield: 40% (66 mg), 78% (based on recovered aldehyde) ; mp 215-216 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.49 (s, 1H), 8.17 (d, *J* = 7.6 Hz, 1H), 7.85 (t, *J* = 7.2 Hz, 1H), 7.76 (s, 1H), 7.69 (d, *J* = 8 Hz, 1H), 7.56 (t, *J* = 7.2 Hz, 1H), 7.35 (s, 1H), 2.26 (s, 3H), 2.23 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.6, 155.2, 148.6, 140.5, 139.3, 137.1, 136.6, 134.6, 130.8, 127.5, 126.9, 125.9, 121.2, 92.5, 18.8, 18.7; IR (KBr): $\bar{\upsilon}$ = 2873, 2090,

1644, 1463, 1288, 1138, 1020 cm^{-1}; HR-MS (ESI-TOF): m/z calculated for $C_{16}H_{13}NO_2I$ $[M+H]^+$: 377.0145, found: 377.0174.

2-(4-Fluorophenyl)quinazolin-4(3*H*)-one (3v) [2]. R_f = 0.5 (hexane/ethyl acetate 7:3); white solid; Yield: 59% (62 mg); ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.59 (s, 1H), 8.25 (t, *J* = 8.0, Hz, 2H), 8.15 (d, *J* = 7.6 Hz, 1H), 7.84 (t, *J* = 7.6 Hz, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.52 (t, *J* = 7.2 Hz, 1H), 7.40 (t, *J* = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 164.0 (d, $^1J_{C,\ F}$ = 247.0 Hz), 161.9, 150.7, 148.3, 134.7, 130.4 (d, $^3J_{C,\ F\ =}$ 9.1 Hz), 129.3 (d, $^4J_{C,\ F\ =}$ 2.5 Hz), 127.5, 126.7, 125.9, 120.7, 115.7 (d, $^2J_{C,\ F}$ =22.0 Hz).

4-(4-Oxo-3,4-dihydroquinazolin-2-yl)benzonitrile (3w) [7]. R_f = 0.4 (hexane/ethyl acetate 4:1); white solid; Yield: 60% (65 mg); ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.76 (s, 1H), 8.34 (d, *J* = 8.4 Hz, 2H), 8.18 (d, *J* = 8 Hz, 1H), 8.04 (d, *J* = 8 Hz, 2H), 7.87 (t, *J* = 7.2 Hz, 1H), 7.78 (d, *J* = 8.0 Hz, 1H), 7.57 (t, *J* = 7.2 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.2, 151.1, 148.2,137.0, 134.8, 132.6, 128.7, 127.7, 127.2,125.9, 121.3, 118.4, 113.6.

2-(Pyren-1-yl)quinazolin-4(3*H*)-one (3x): R_f = 0.4 (hexane/ethyl acetate 7:3); yellow solid; Yield: 65% (99 mg); mp charred at 250 ^oC ; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.84 (s, 1H), 8.48 (d, *J* = 9.2 Hz, 1H), 8.43 (d, *J* = 8.0 Hz, 1H), 8.42 – 8.36 (m, 2H), 8.34 – 8.32 (m, 2H), 8.30 – 8.25 (m, 3H), 8.15 (t, *J* = 7.6 Hz, 1H), 7.90 (t, *J* = 8.4, 1H), 7.81 (d, *J* = 8.0 Hz, 1H), 7.62 (t, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.1, 154.1, 148.9, 134.6, 131.9, 130.8, 130.2, 128.9, 128.8, 128.6, 128.5, 127.6, 127.3 (2C), 126.9, 126.8, 126.1, 125.9, 125.8, 124.5 (2C), 123.8, 123.6, 121.3; IR (KBr): ῡ = 3308, 2862, 2089, 1636, 1278, 1148 cm^{-1}; HR-MS (ESI-TOF): m/z calculated for $C_{24}H_{14}NO_2$ $[M+ H]^+$: 347.1179, found: 347.1199.

2-(Anthracen-9-yl)quinazolin-4(3*H*)-one (3y) [11]. R_f = 0.4 (hexane/ethyl acetate 7:3); white solid; Yield: 27% (34 mg), 64% (based on recovered aldehyde); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.27 (s, 1H), 8.63 (s, 1H), 8.41 (d, *J* = 7.6 Hz, 1H), 8.12 – 8.04 (m, 2H), 7.92 – 7.84 (m, 4H), 7.63 (m, Hz, 1H), 7.51 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.1, 152.2, 149.1, 135.2, 131.2, 130.1, 129.7, 128.9, 128.3, 127.7, 127.6, 127.2, 126.8, 125.8, 124.6, 121.4.

Crystallographic data collection

Good quality crystals of the compounds were obtained after slow evaporation of chloroform and hexane (1:1) mixture. The crystal data were collected with a Bruker SMART D8 goniometer equipped with an APEX CCD detector and with an INCOATEC micro source (MoKα radiation, λ = 0.71073 Å). SAINT+ [12] and SADABS [13] were used to integrate the intensities and to correct the absorption respectively. The structure was resolved by direct methods and refined on F^2 with SHELXL-97 [14].

Crystallographic Data

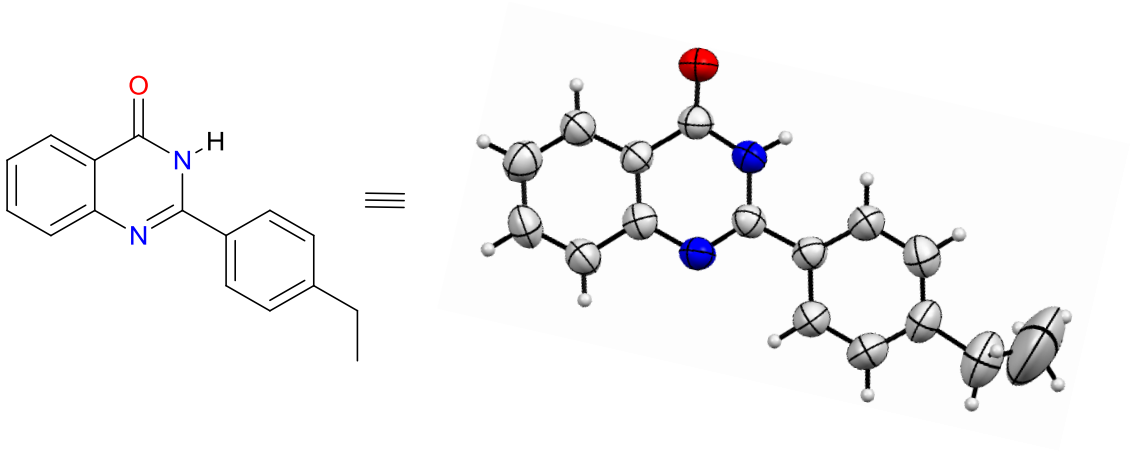

Figure S1: Crystal structure of **3a**

Table S1: Crystal data and structure refinement for 3a.

CCDC No.	**1823611**
Empirical formula	$C_{32}H_{28}N_4O_2$
Formula weight	500.58
Temperature	296.15 K
Crystal system	triclinic
Space group	P-1
Unit cell dimensions	a = 5.0503(3) Å α = 92.215(6)°
	b = 15.3328(10) β = 91.359(4)°
	c = 17.0240(10) γ = 99.349(4)°
Volume	1299.17(14) $Å^3$
Z	2
Density (calculated)	1.280 g/cm^3
Absorption coefficient	0.081 mm^{-1}
F(000)	528.0
Crystal size	0.31 × 0.26 × 0.21 mm^3
Radiation	MoKα (λ = 0.71073)
Theta range for data collection	2.396 to 50.922°
Index ranges	-6 ≤ h ≤ 6, -18 ≤ k ≤ 18, -20 ≤ l ≤ 20
Reflections collected	14947
Independent reflections	4773 [R_{int} = 0.0653, R_{sigma} = 0.1250]
Data/restraints/parameters	4773/3/345
Goodness-of-fit on F^2	0.971
Final R indexes [I>=2σ (I)]	R_1 = 0.0857, wR_2 = 0.2434
Final R indexes [all data]	R_1 = 0.2356, wR_2 = 0.3599
Largest diff. peak/hole	0.61/-0.35 e $Å^{-3}$

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NMR spectra

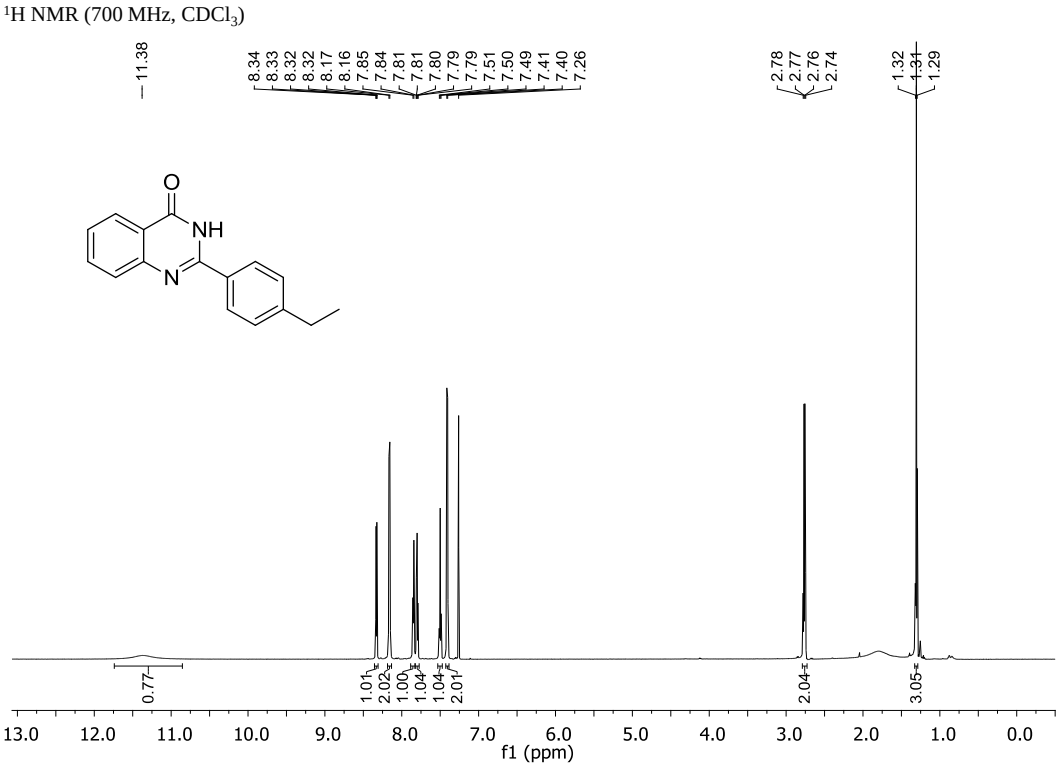

Figure S2. ^{1}H NMR spectra of 2-(4-ethylphenyl)quinazolin-4(3*H*)-one (**3a**).

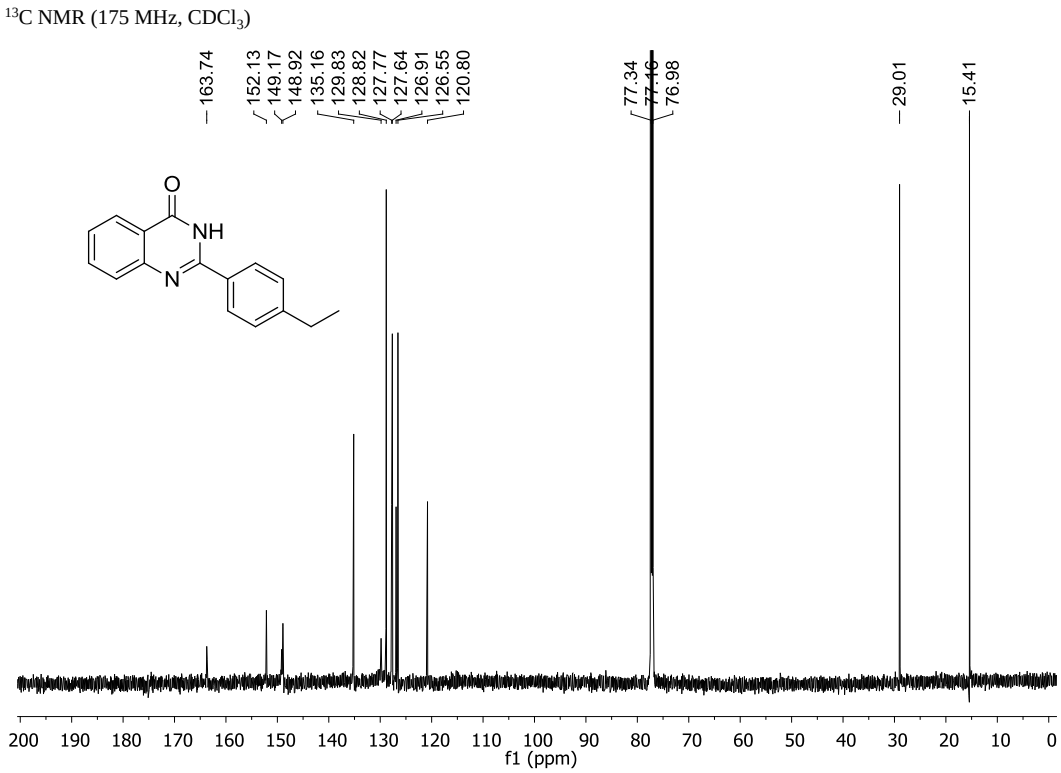

Figure S3. ^{13}C NMR spectra of 2-(4-ethylphenyl)quinazolin-4(3*H*)-one (**3a**).

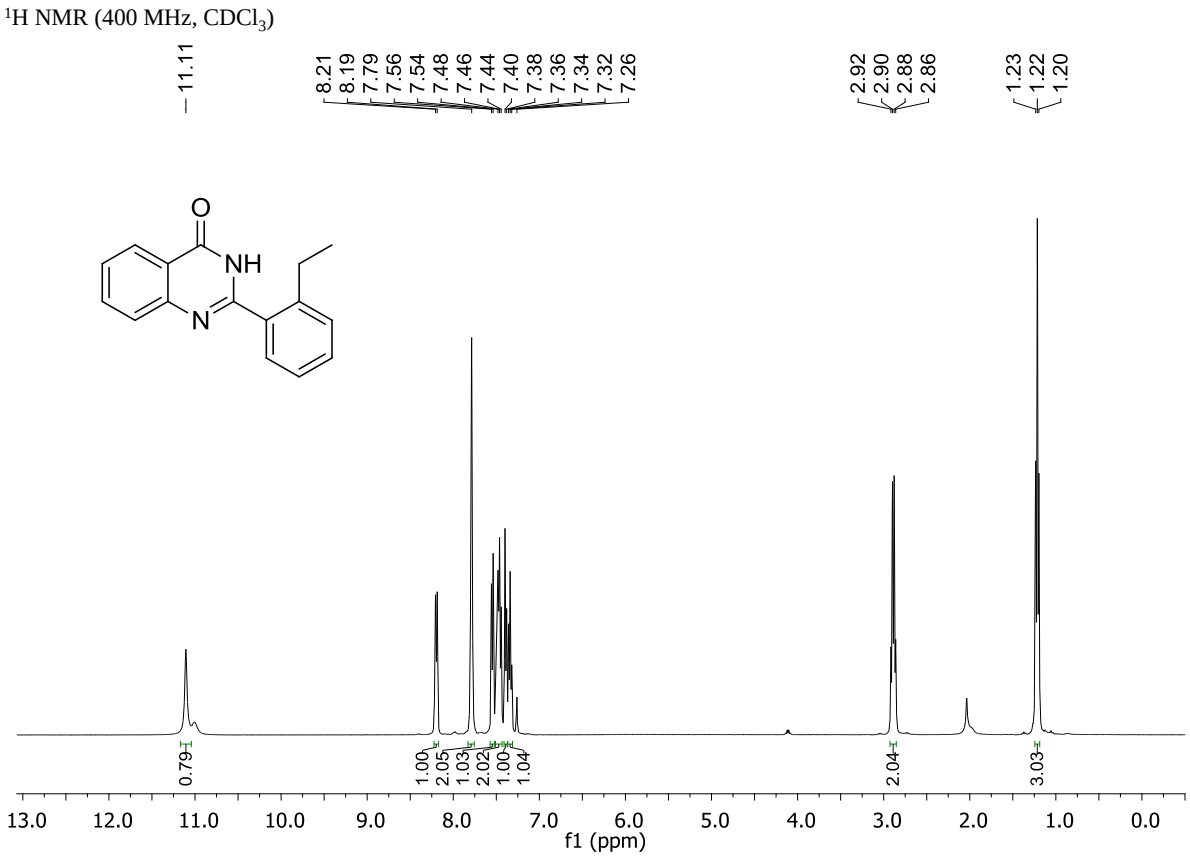

Figure S4. ^{1}H NMR spectra of 2-(2-ethylphenyl)quinazolin-4(3*H*)-one (**3b**).

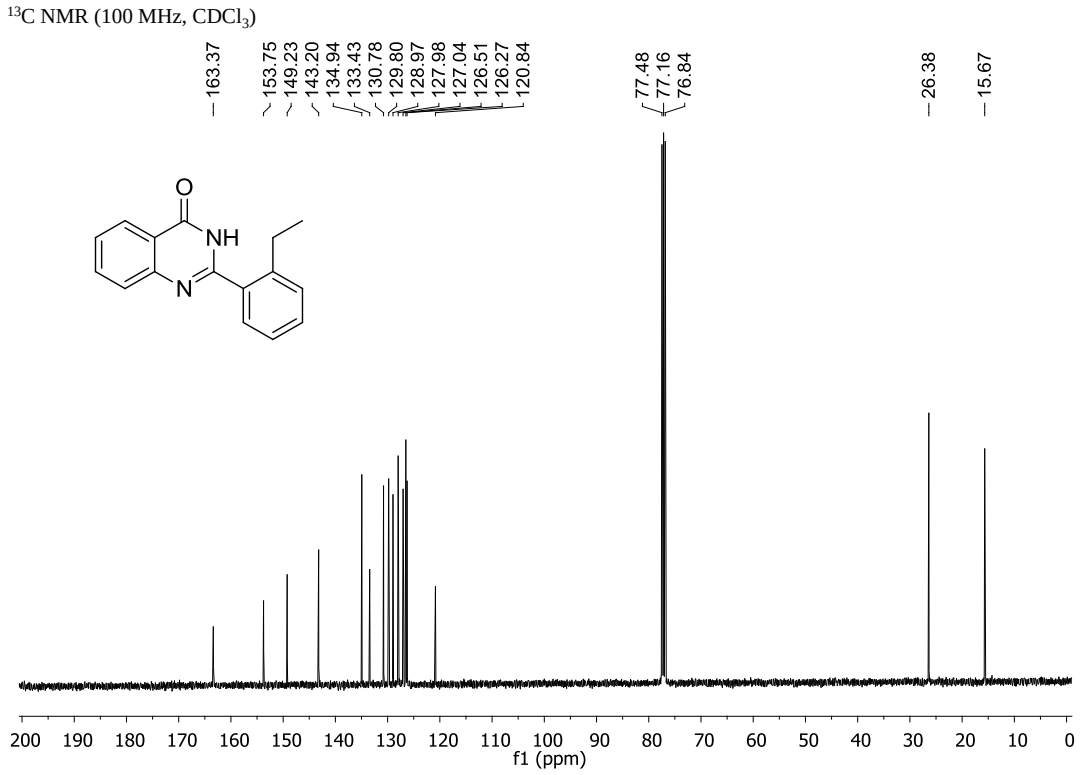

Figure S5. ^{13}C NMR spectra of 2-(2-ethylphenyl)quinazolin-4(3*H*)-one (**3b**)

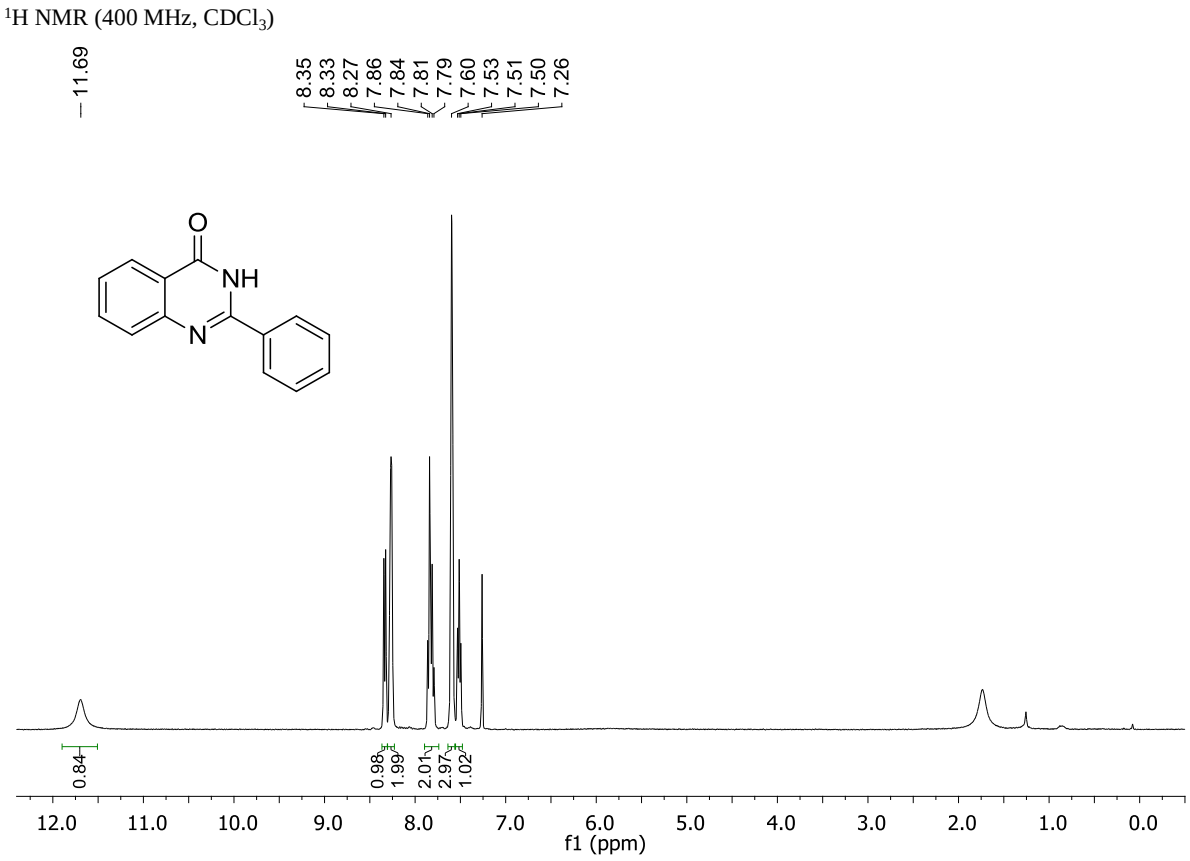

Figure S6. ^{1}H NMR spectra of 2-phenylquinazolin-4(3*H*)-one (**3c**).

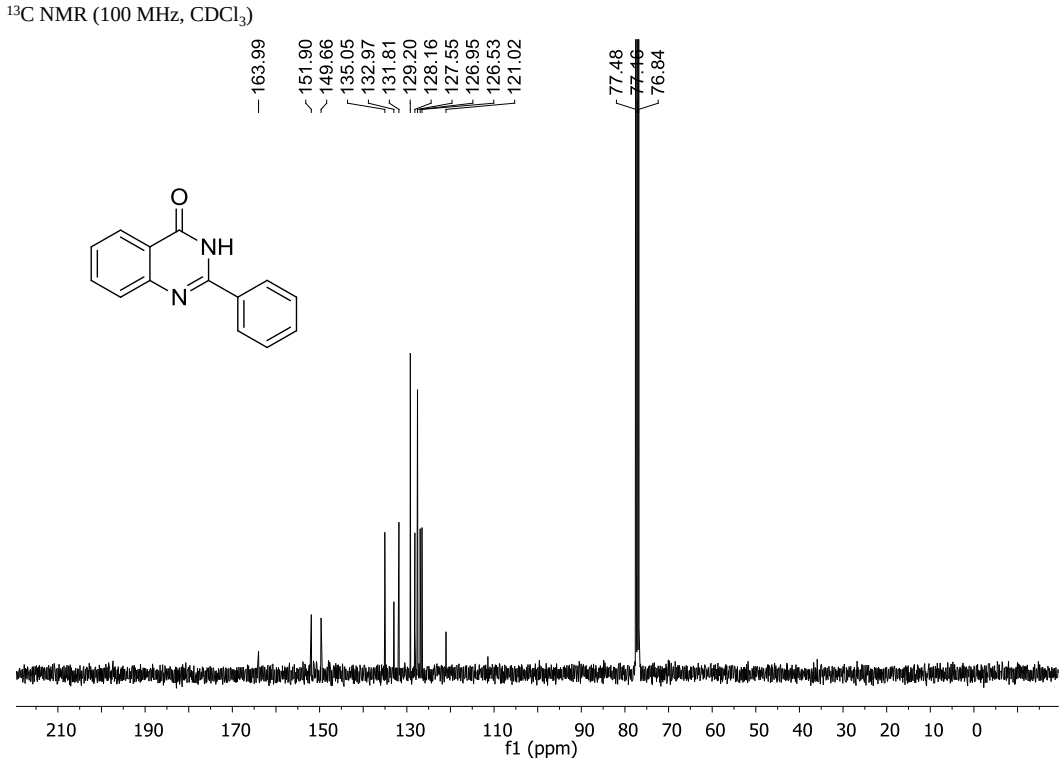

Figure S7. ^{13}C NMR spectra of 2-phenylquinazolin-4(3*H*)-one (**3c**).

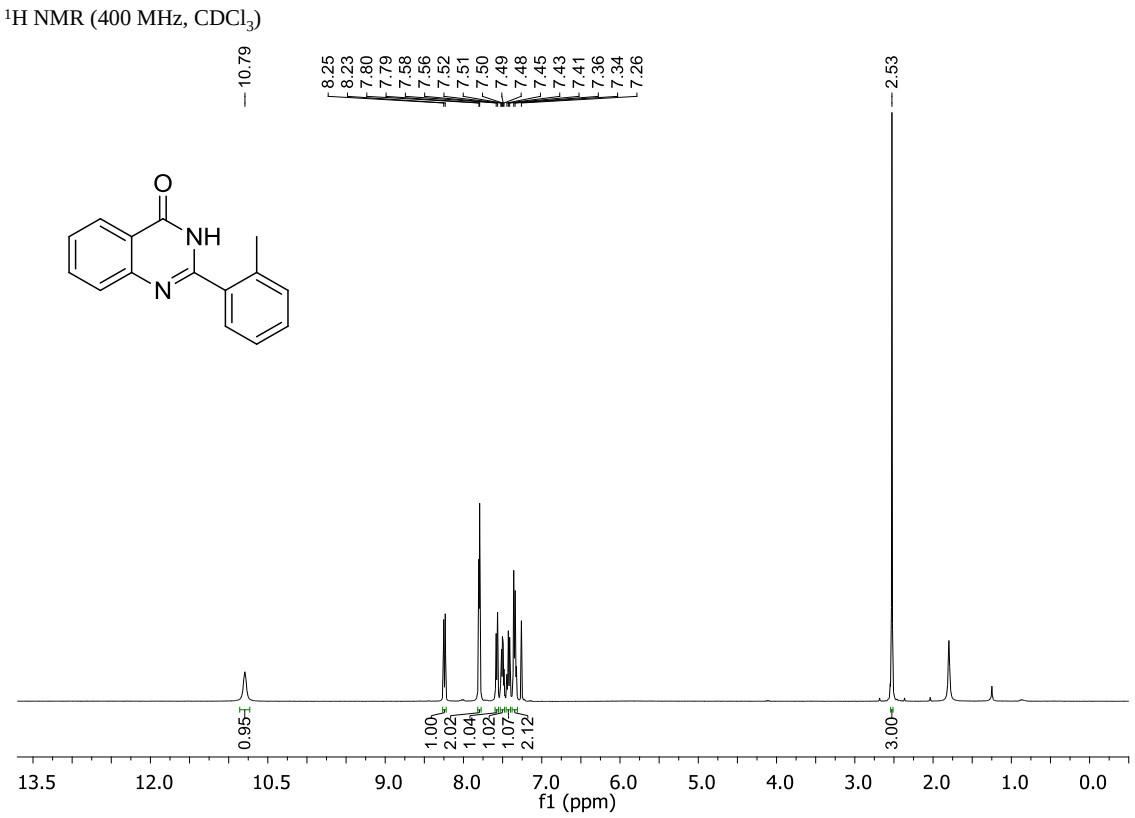

Figure S8. ^{1}H NMR spectra of 2-(*o*-tolyl)quinazolin-4(3*H*)-one (**3d**).

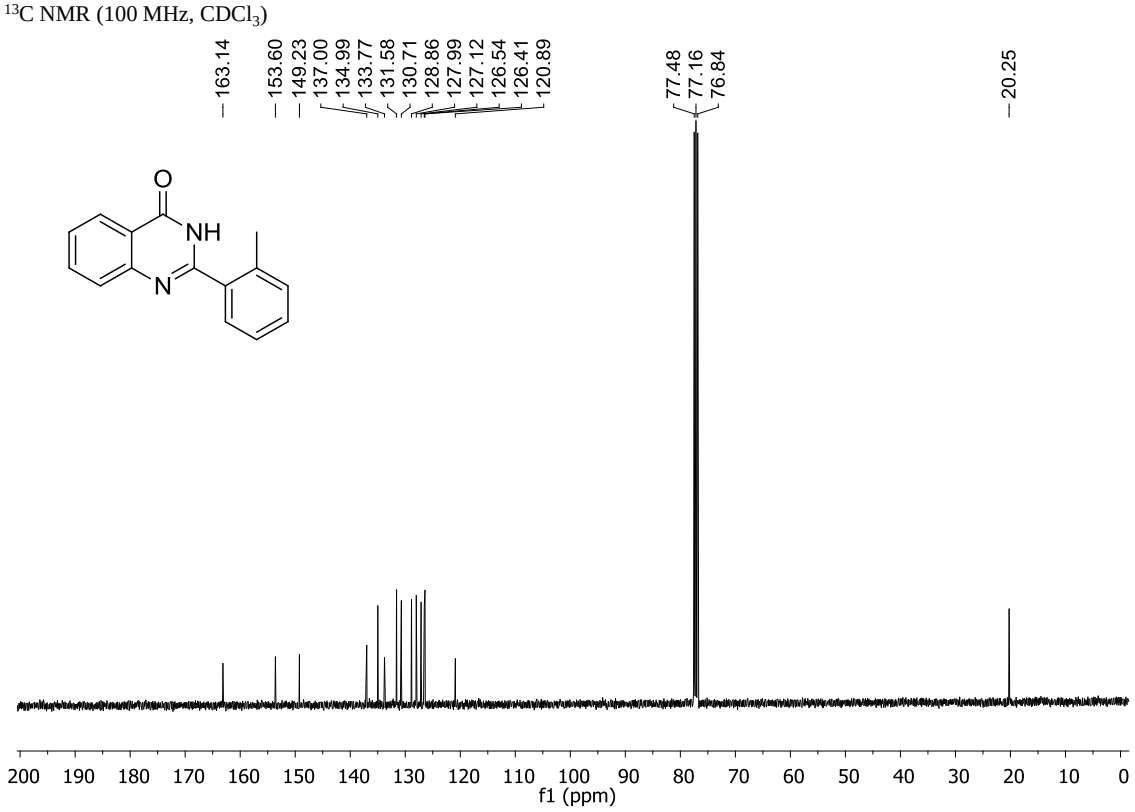

Figure S9. ^{13}C NMR spectra of 2-(*o*-tolyl)quinazolin-4(3*H*)-one (**3d**).

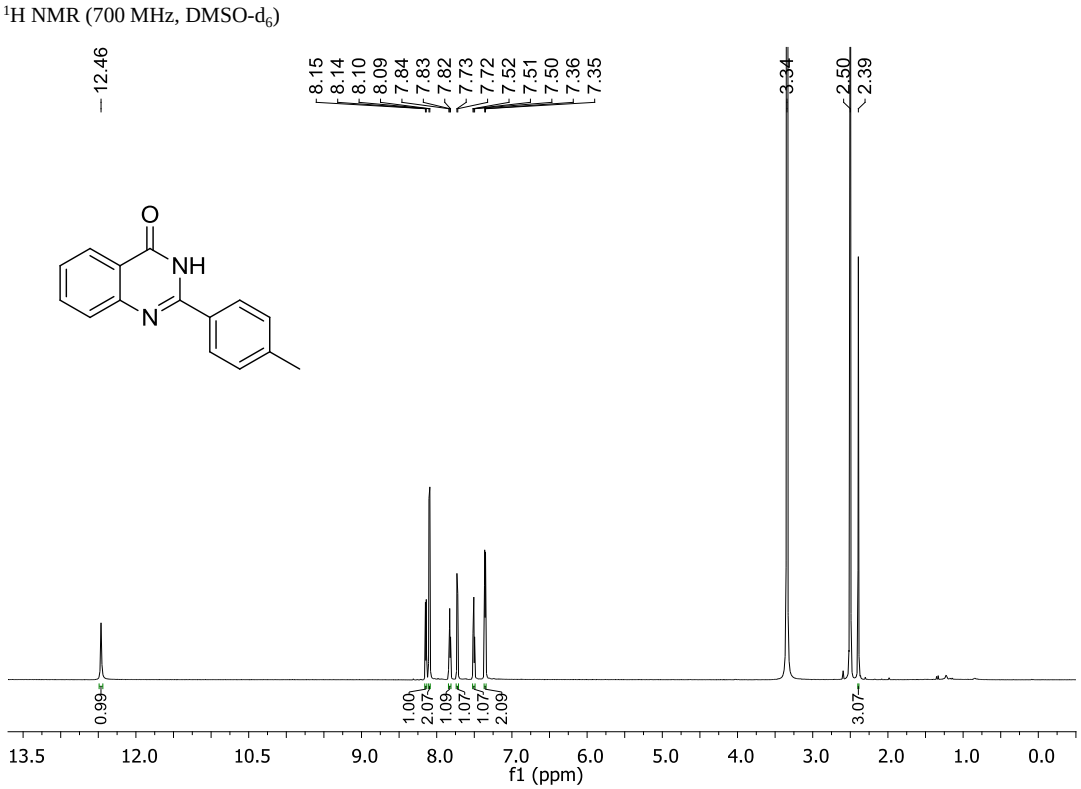

Figure S10. ^{1}H NMR spectra of 2-(*p*-tolyl)quinazolin-4(3*H*)-one (**3e**).

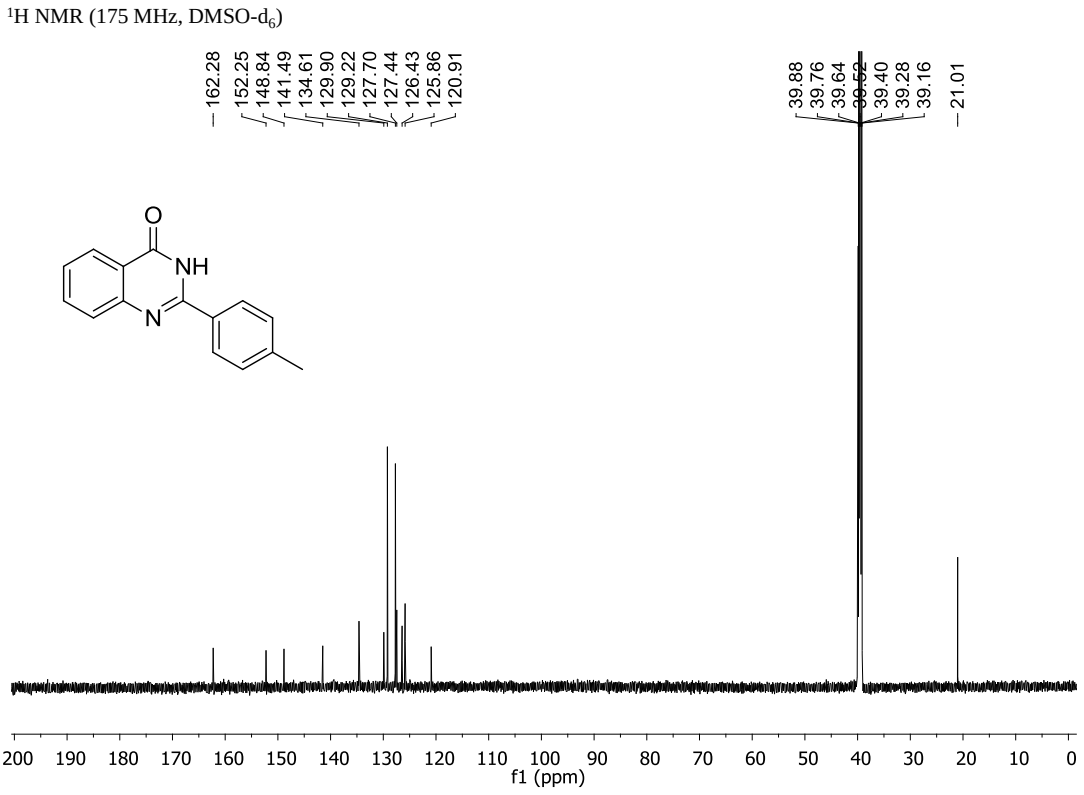

Figure S11. ^{13}C NMR spectra of 2-(*p*-tolyl)quinazolin-4(3*H*)-one (**3e**).

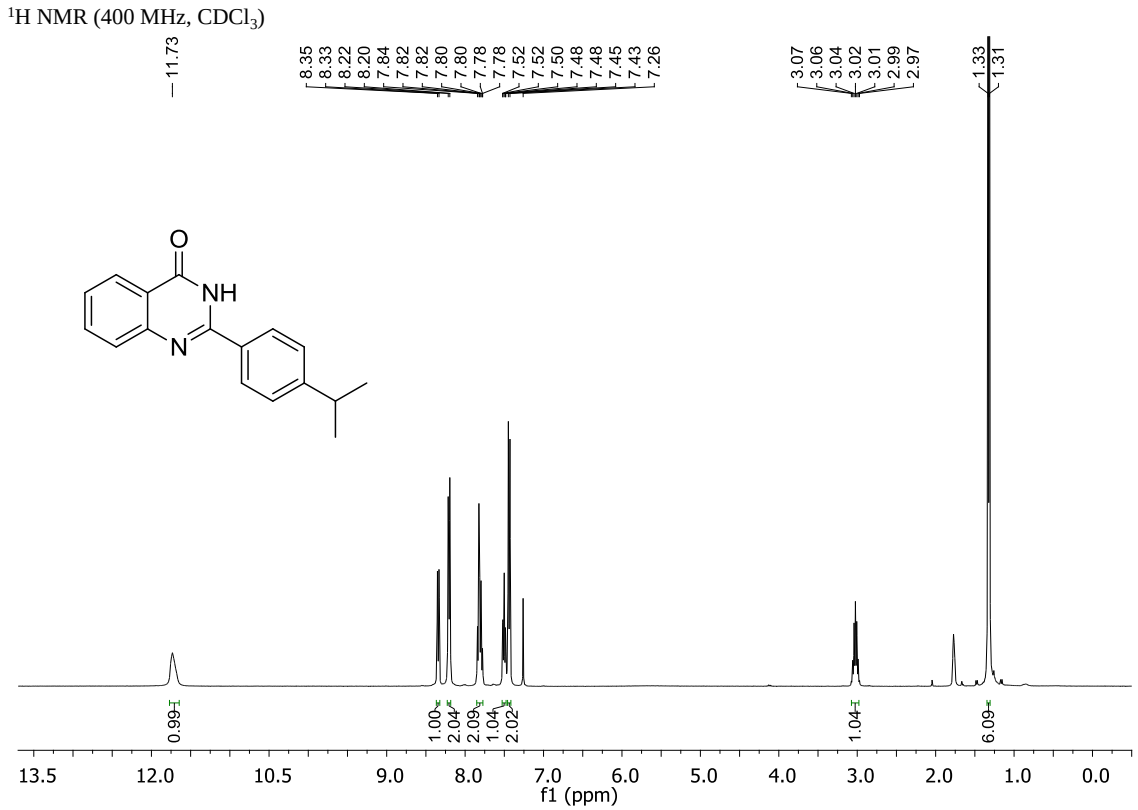

Figure S12. ^{1}H NMR spectra of 2-(4-isopropylphenyl)quinazolin-4(3*H*)-one (**3f**).

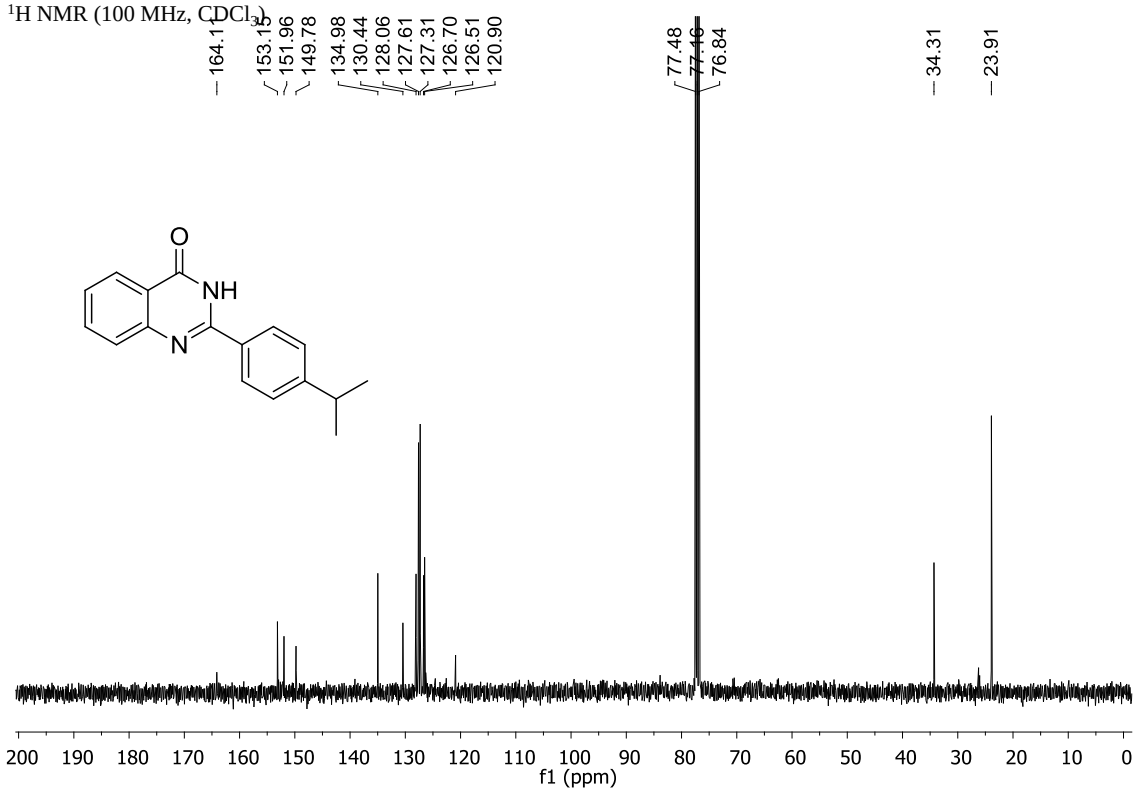

Figure S13. ^{13}C NMR spectra of 2-(4-isopropylphenyl)quinazolin-4(3*H*)-one (**3f**).

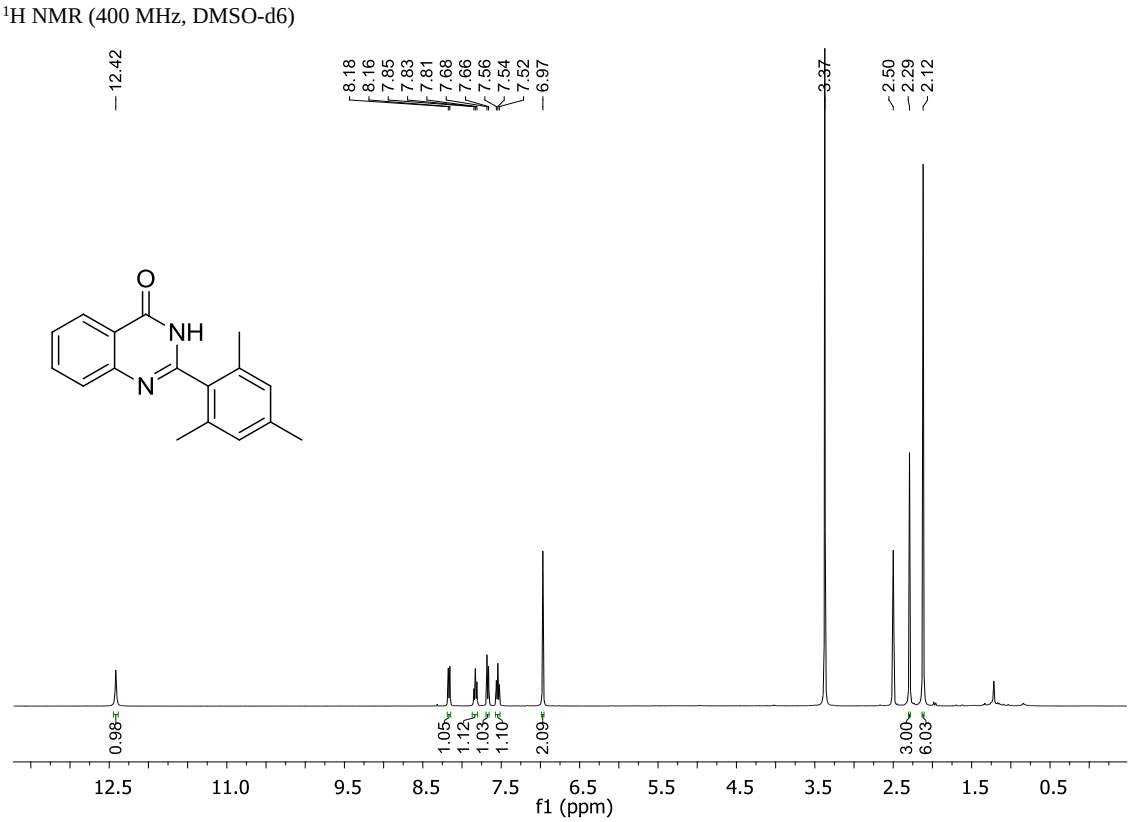

Figure S14. ^{1}H NMR spectra of 2-mesitylquinazolin-4(3*H*)-one (**3g**).

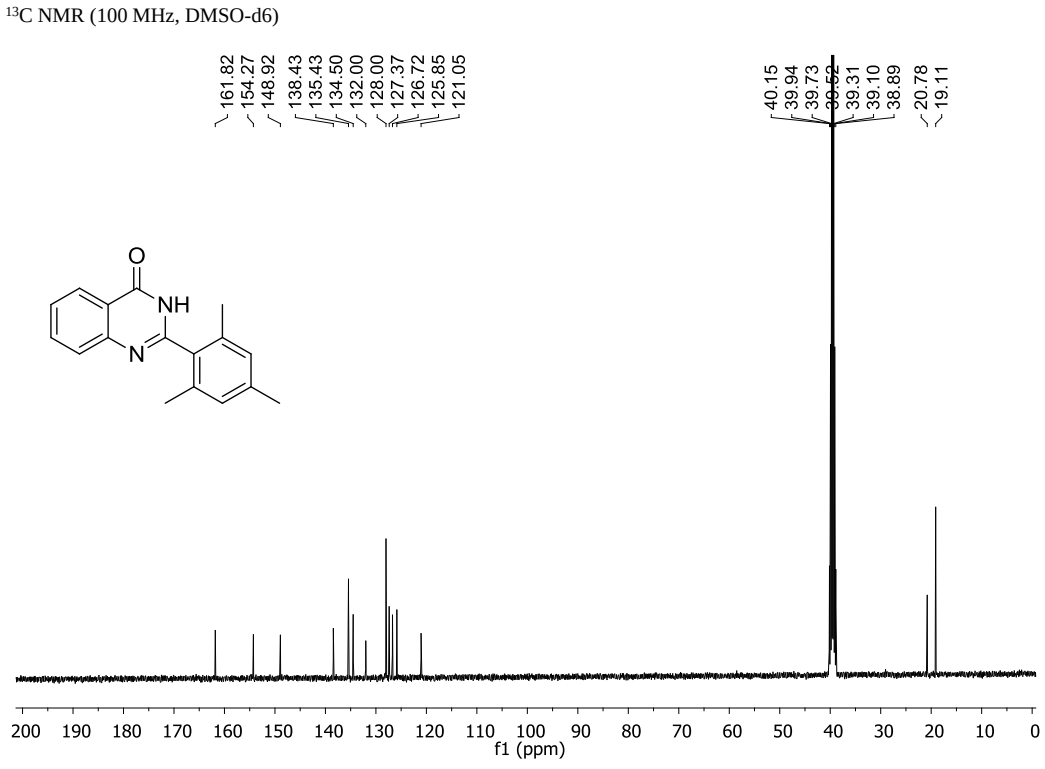

Figure S15. ^{13}C NMR spectra of 2-mesitylquinazolin-4(3*H*)-one (**3g**).

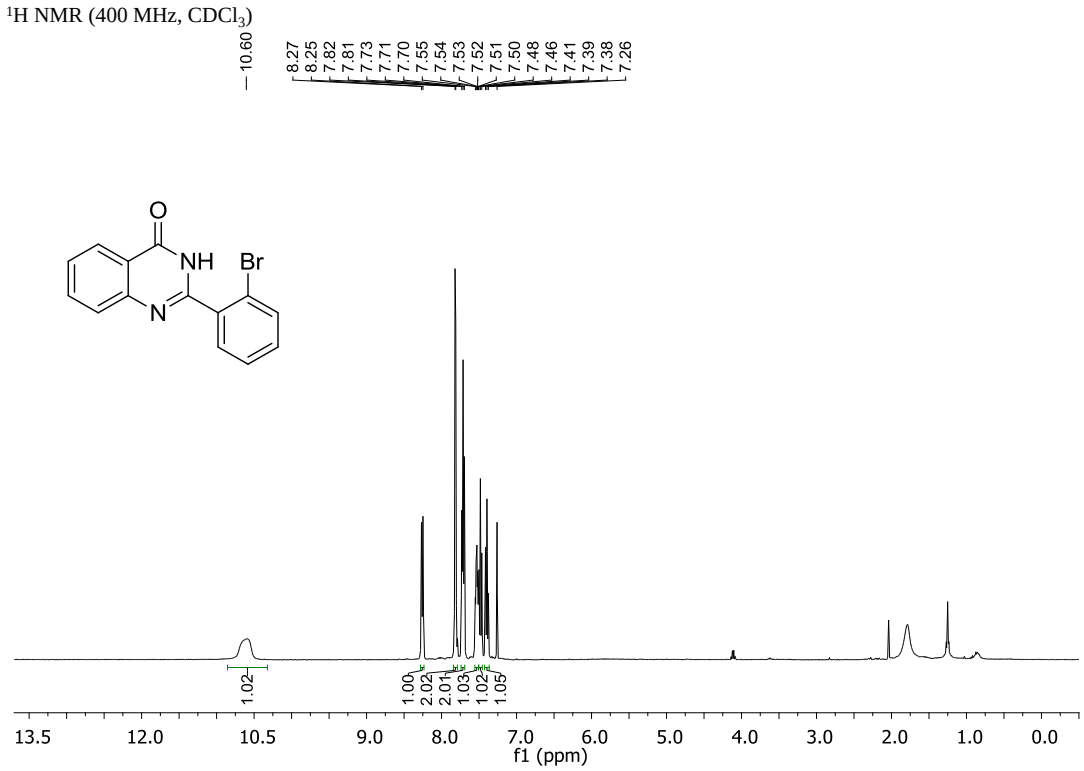

Figure S16. ^{1}H NMR spectra of 2-(2-bromophenyl)quinazolin-4(3*H*)-one (**3h**).

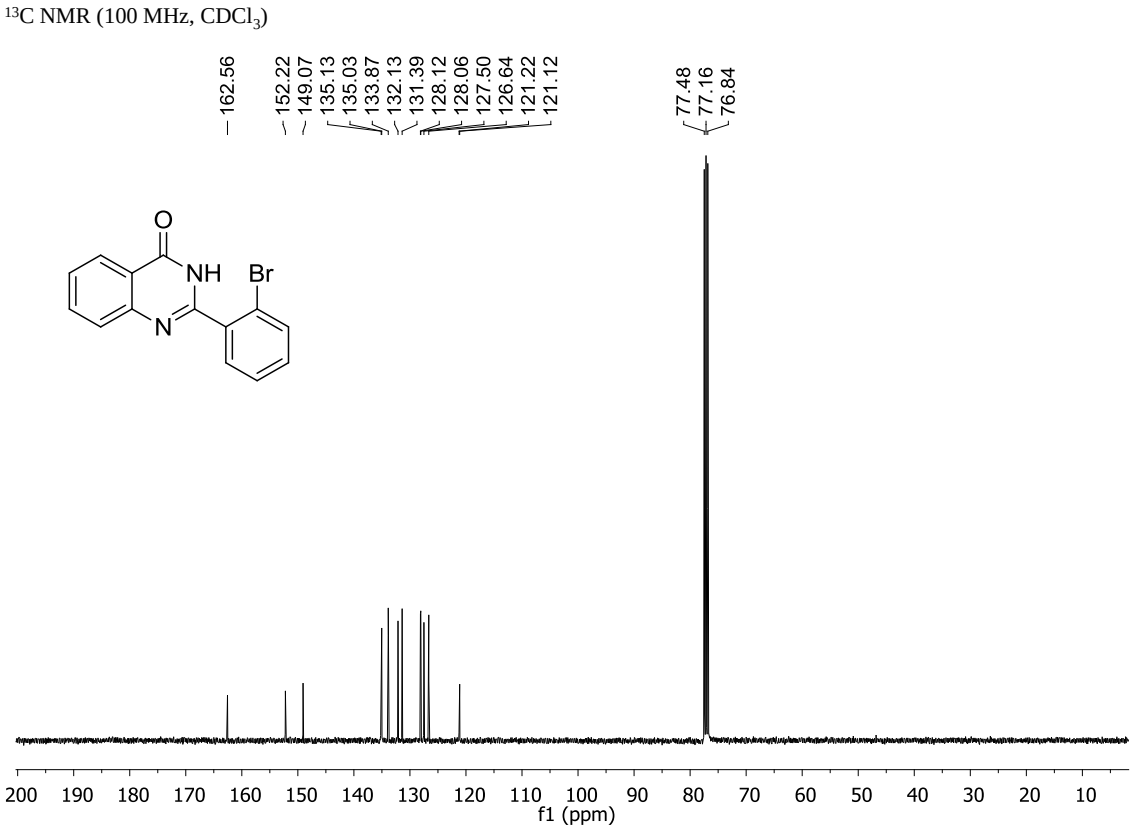

Figure S17. ^{13}C NMR spectra of 2-(2-bromophenyl)quinazolin-4(3*H*)-one (**3h**).

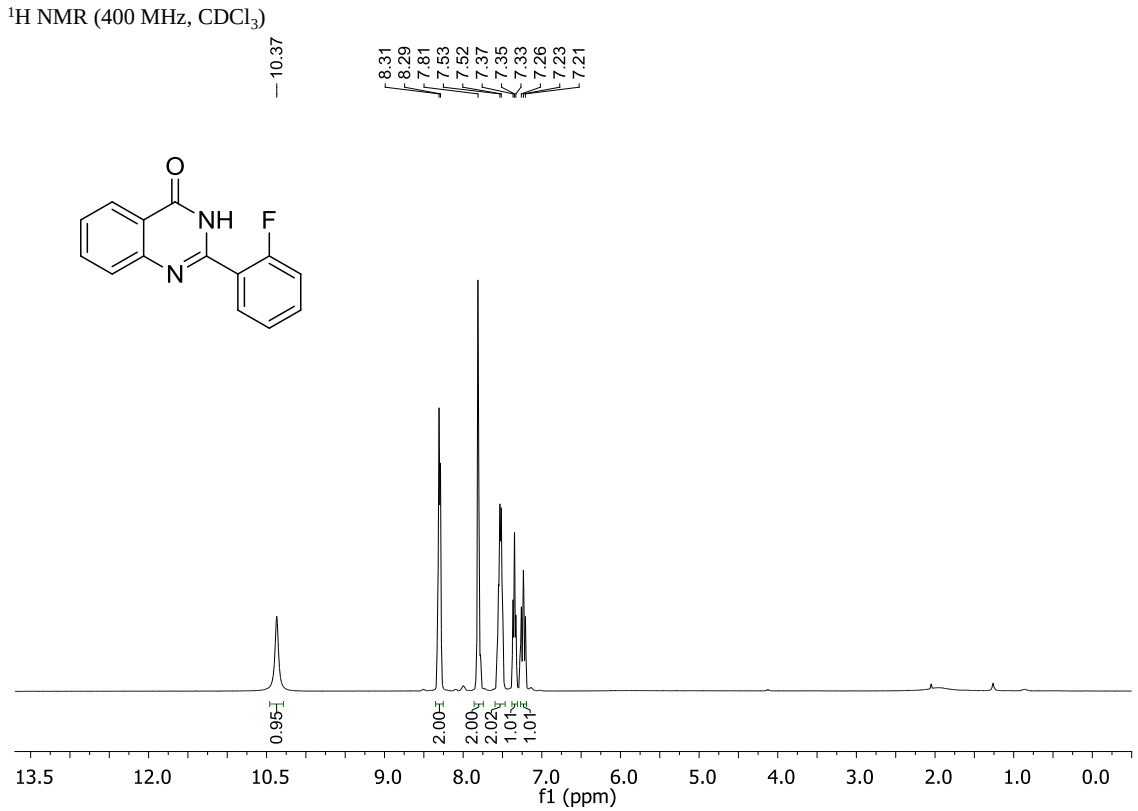

Figure S18. ^{1}H NMR spectra of 2-(2-fluorophenyl)quinazolin-4(3*H*)-one (**3i**).

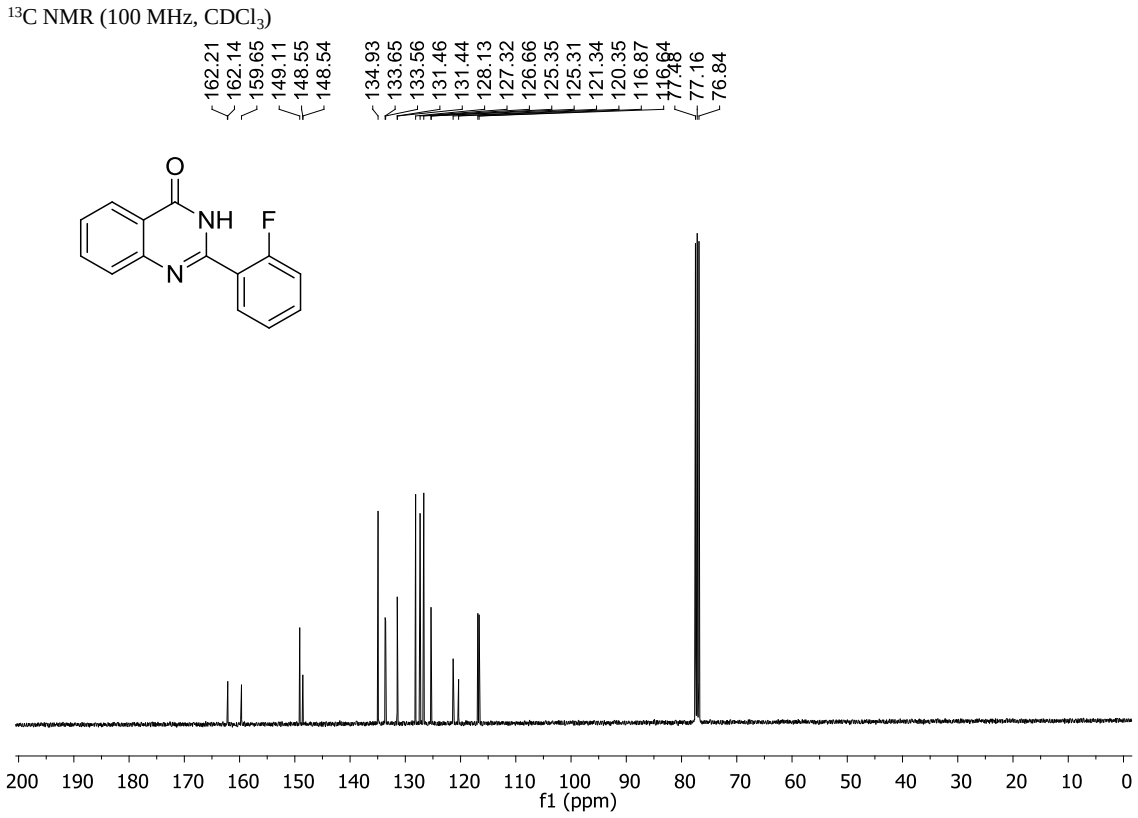

Figure S19. ^{13}C NMR spectra of 2-(2-fluorophenyl)quinazolin-4(3*H*)-one (**3i**).

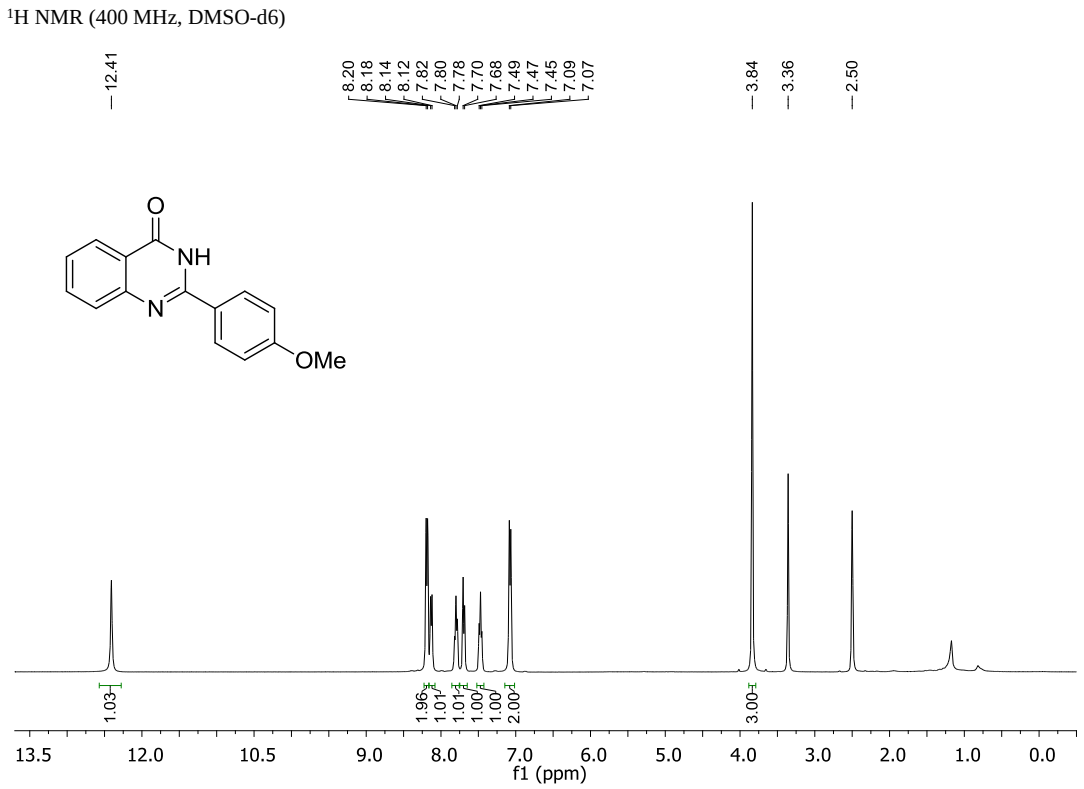

Figure S20. ^{1}H NMR spectra of 2-(4-methoxyphenyl)quinazolin-4(3*H*)-one (**3j**).

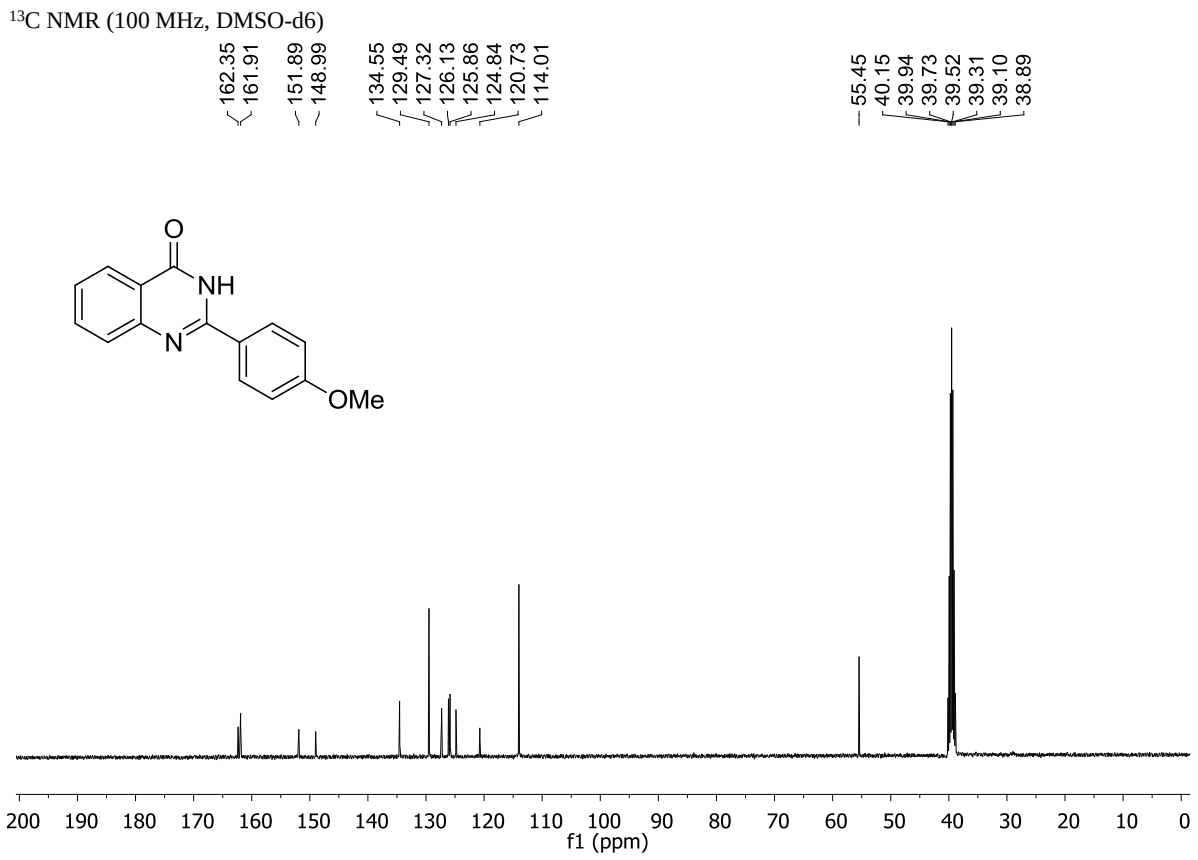

Figure S21. ^{13}C NMR spectra of 2-(4-methoxyphenyl)quinazolin-4(3*H*)-one (**3j**).

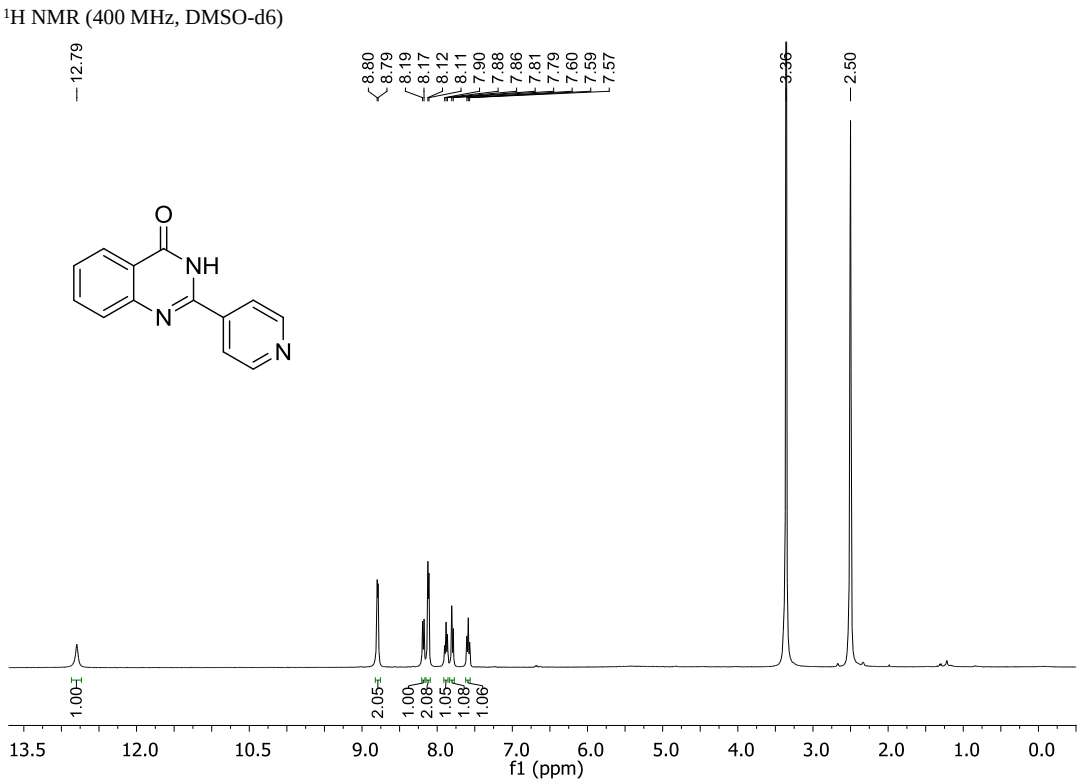

Figure S22. ^{1}H NMR spectra of 2-(pyridin-4-yl)quinazolin-4(3*H*)-one (**3k**).

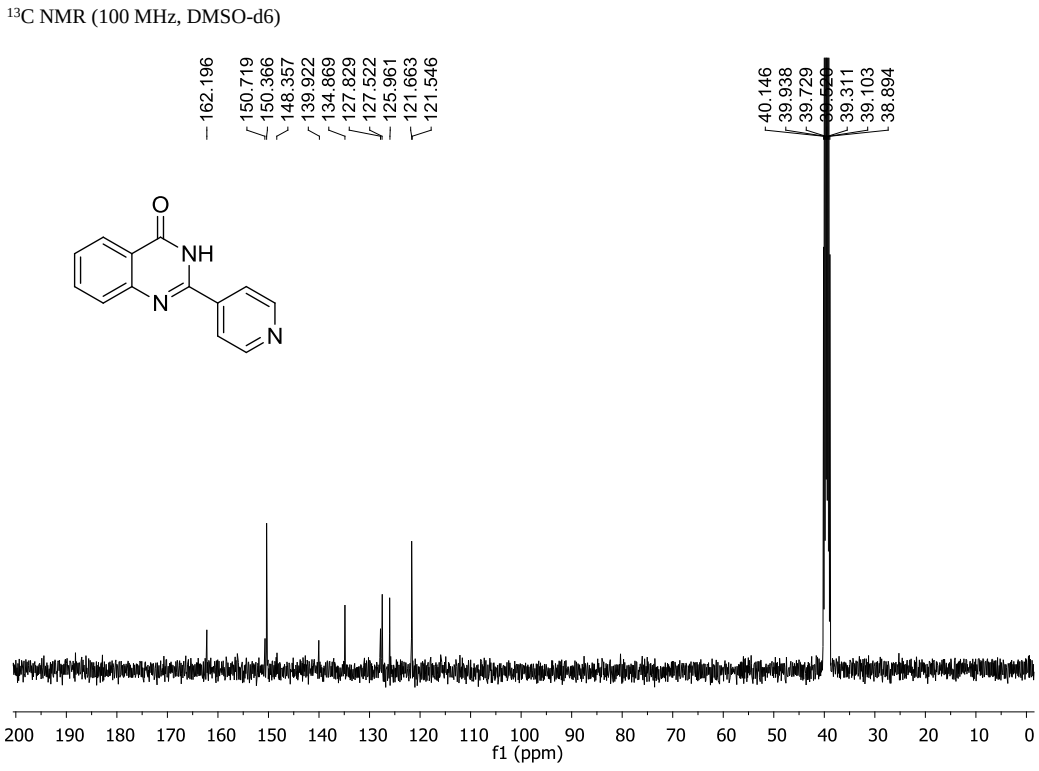

Figure S23. ^{13}C NMR spectra of 2-(pyridin-4-yl)quinazolin-4(3*H*)-one (**3k**).

[1]H NMR (400 MHz, DMSO-d6)

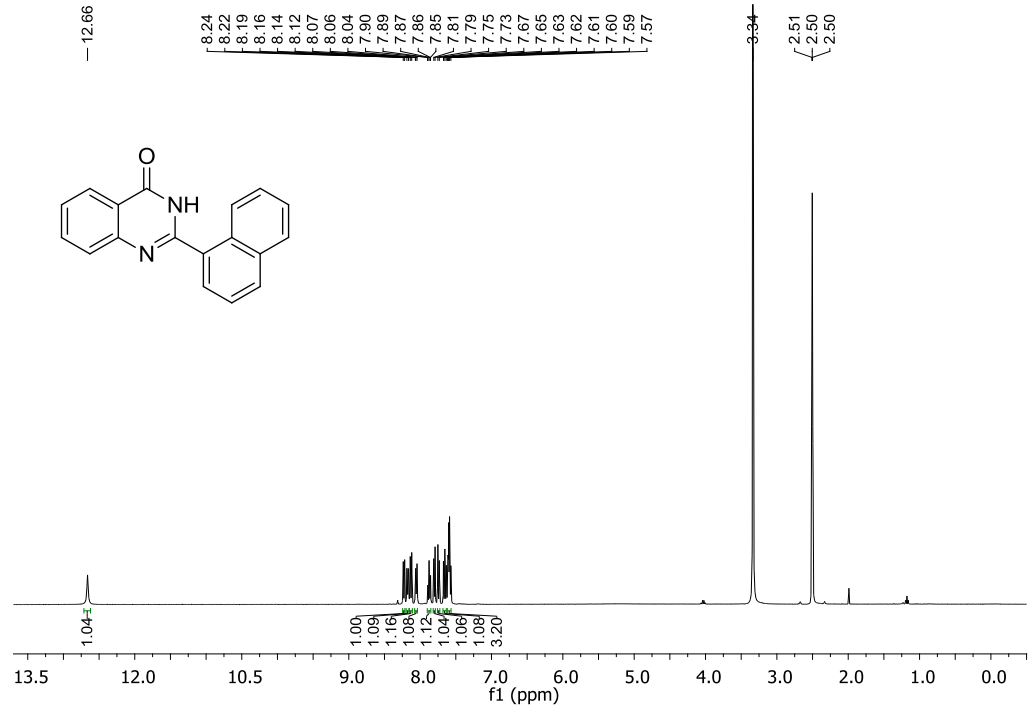

Figure S24. [1]H NMR spectra of 2-(naphthalen-1-yl)quinazolin-4(3*H*)-one (**3l**).

[13]C NMR (100 MHz, DMSO-d6)

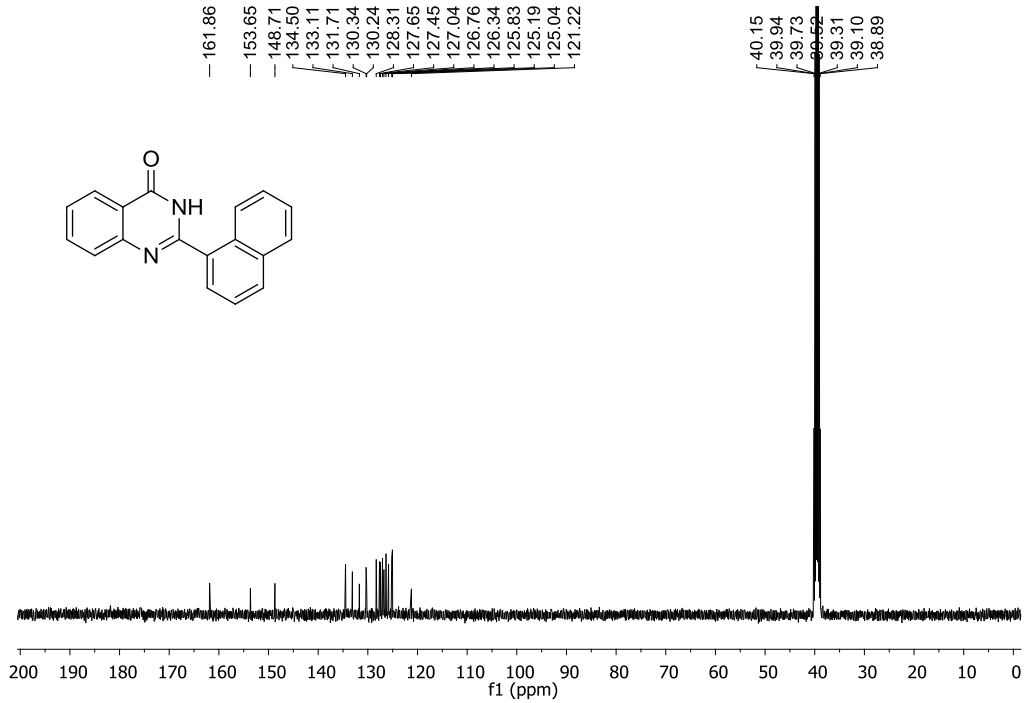

Figure S25. [13]C NMR spectra of 2-(naphthalen-1-yl)quinazolin-4(3*H*)-one (**3l**).

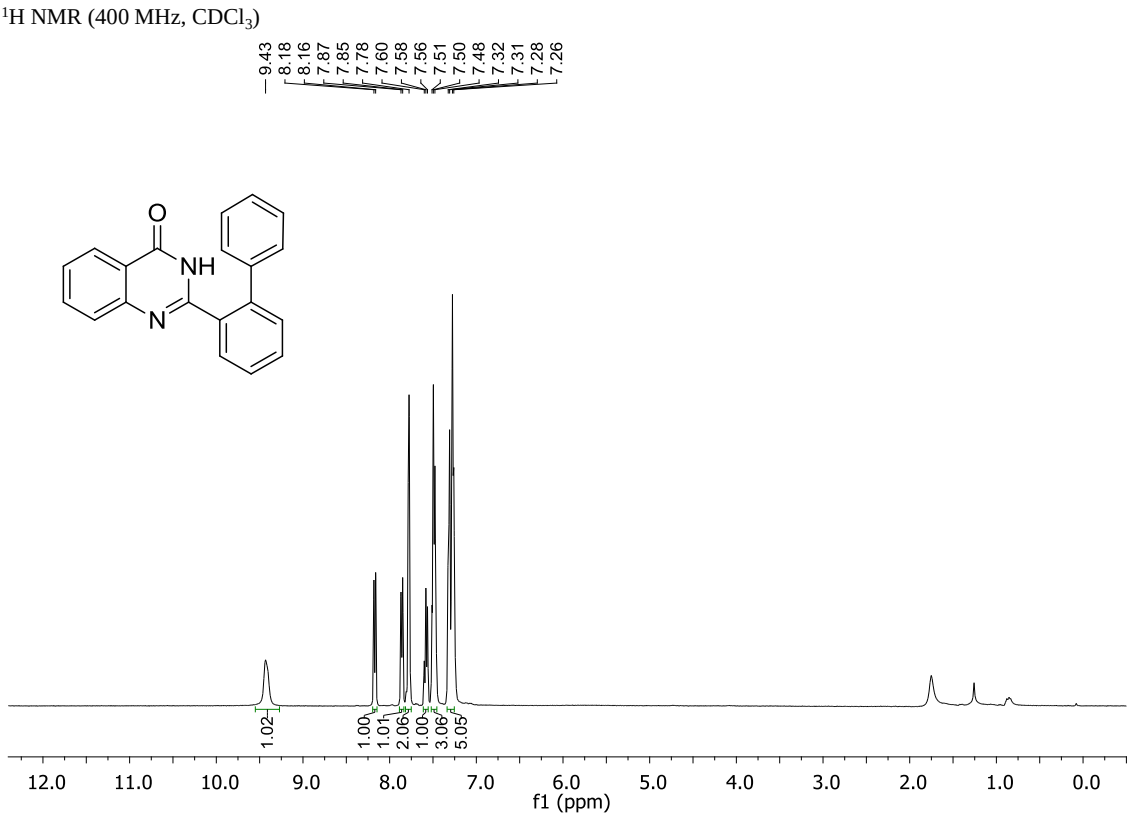

Figure S26. ^{1}H NMR spectra of 2-([1,1'-biphenyl]-2-yl)quinazolin-4(3*H*)-one (**3m**).

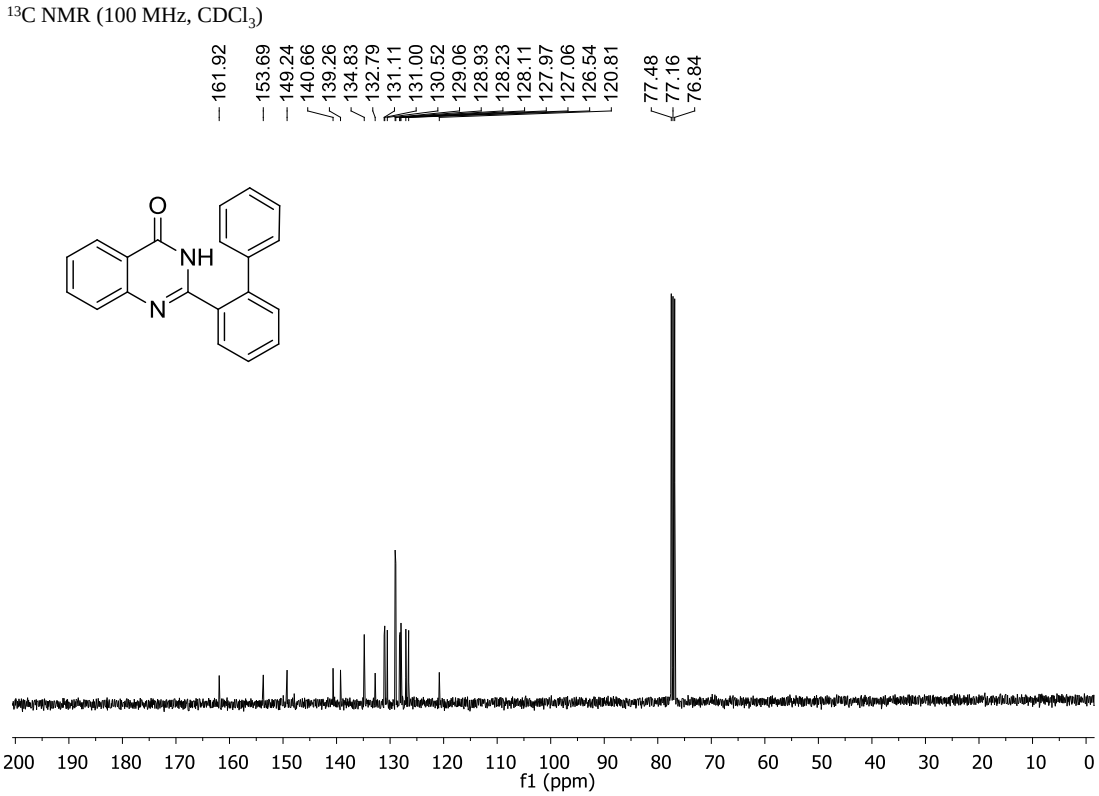

Figure S27. ^{13}C NMR spectra of 2-([1,1'-biphenyl]-2-yl)quinazolin-4(3*H*)-one (**3m**).

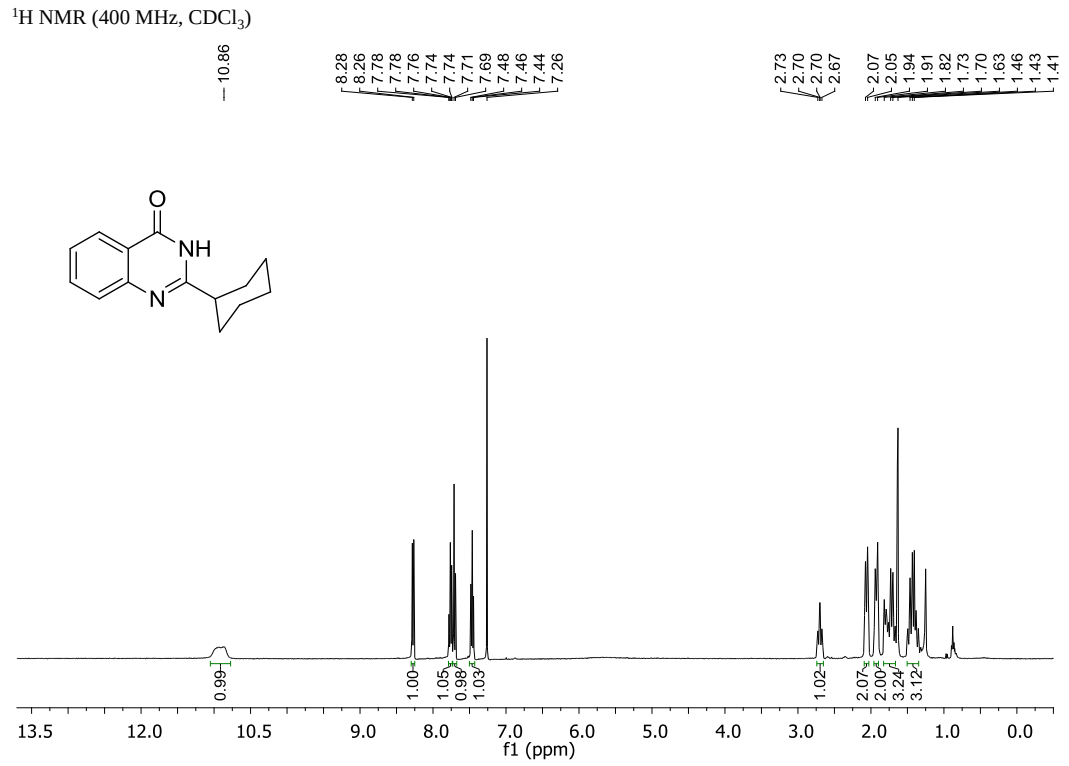

Figure S28. ^{1}H NMR spectra of 2-cyclohexylquinazolin-4(3*H*)-one (**3n**).

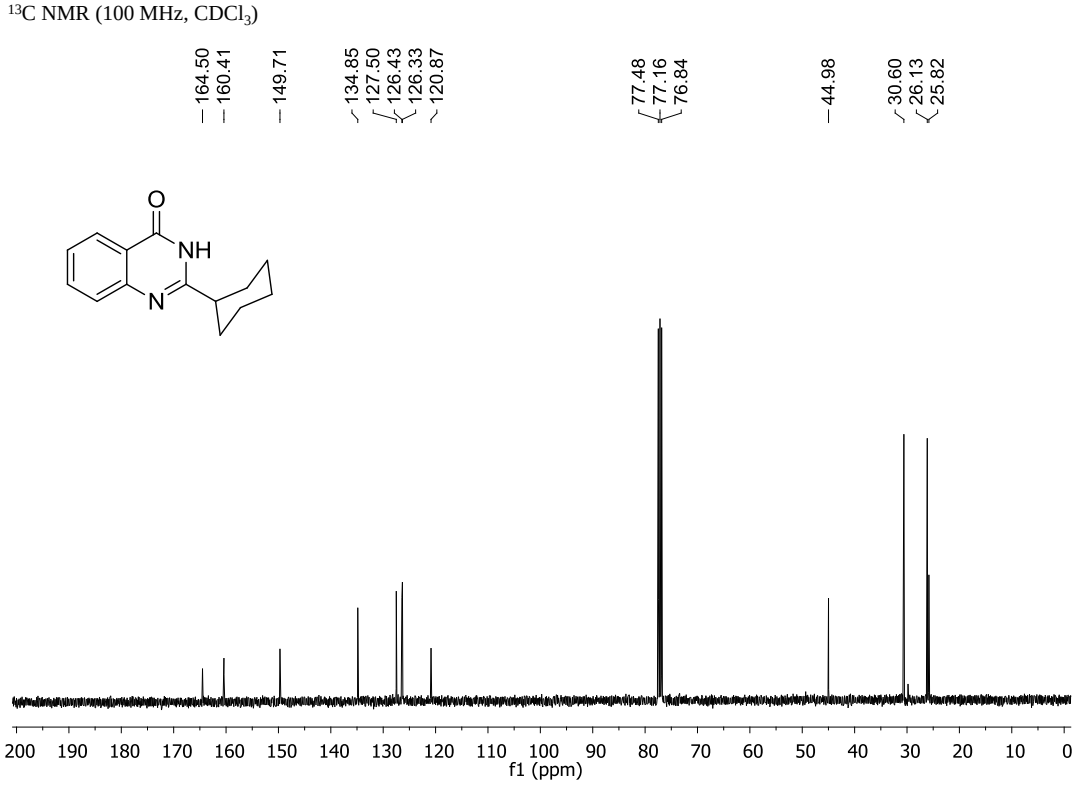

Figure S29. ^{13}C NMR spectra of 2-cyclohexylquinazolin-4(3*H*)-one (**3n**).

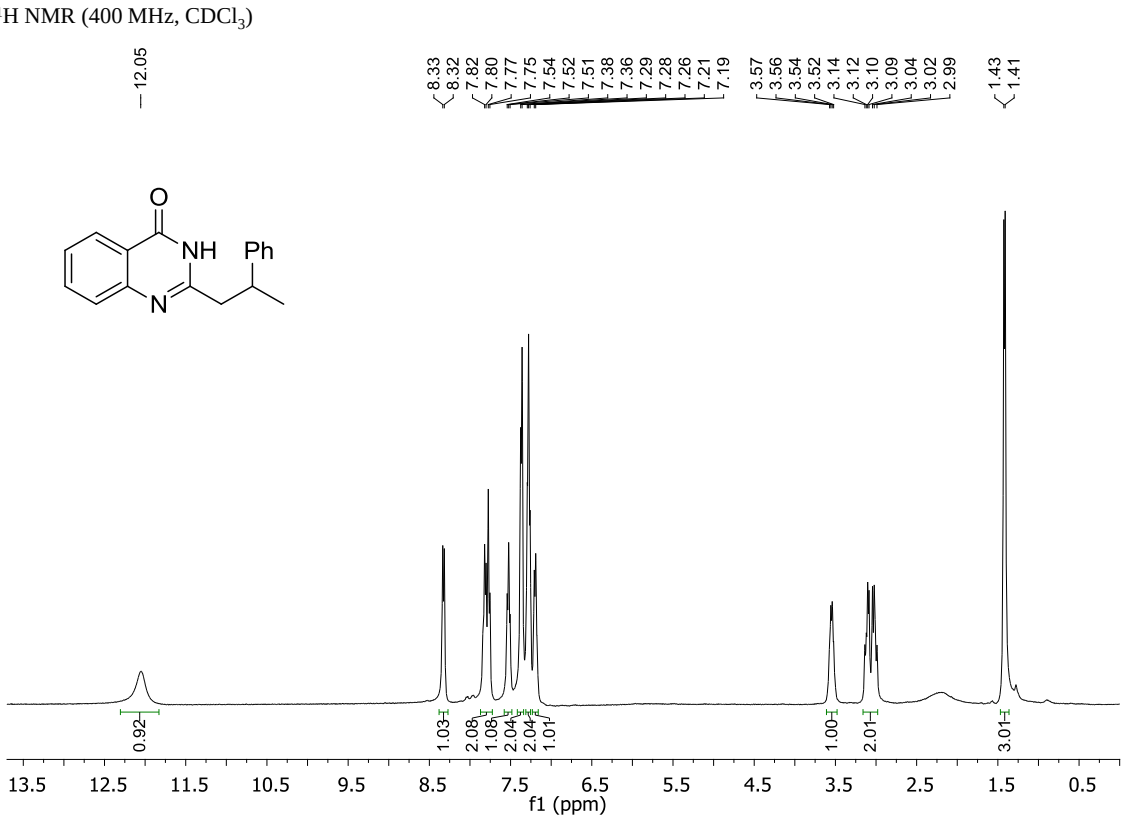

Figure S30. ^{1}H NMR spectra of 2-(2-phenylpropyl)quinazolin-4(3*H*)-one (**3o**).

.

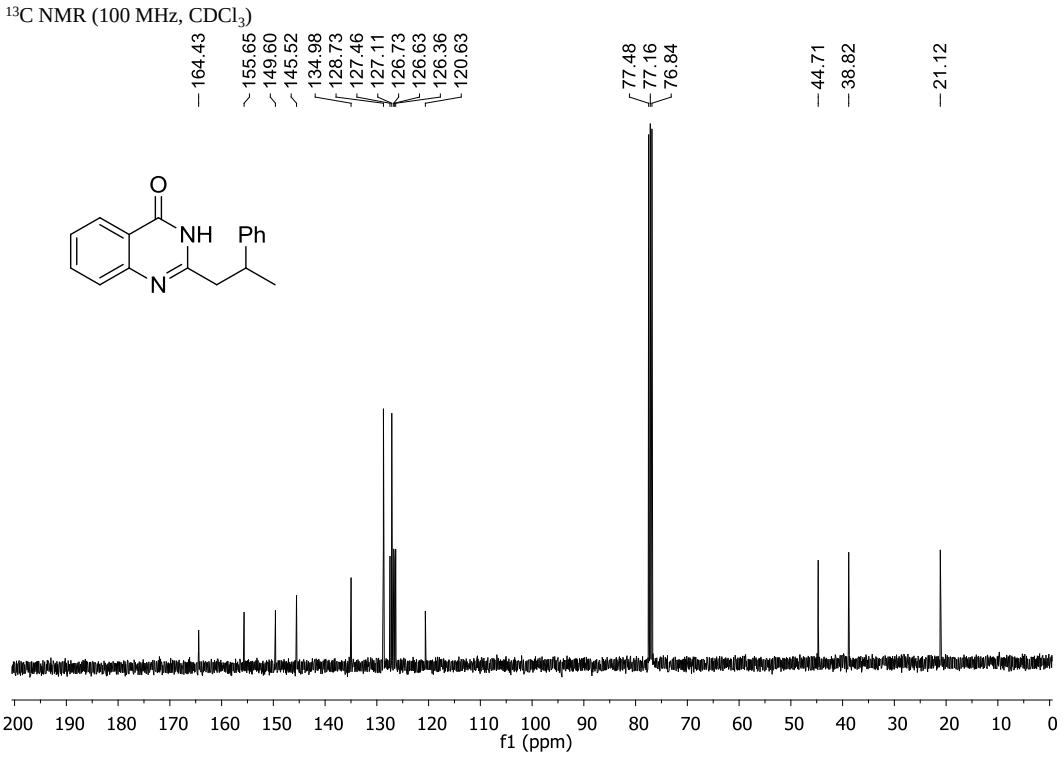

Figure S31. ^{13}C NMR spectra of 2-(2-phenylpropyl)quinazolin-4(3*H*)-one (**3o**).

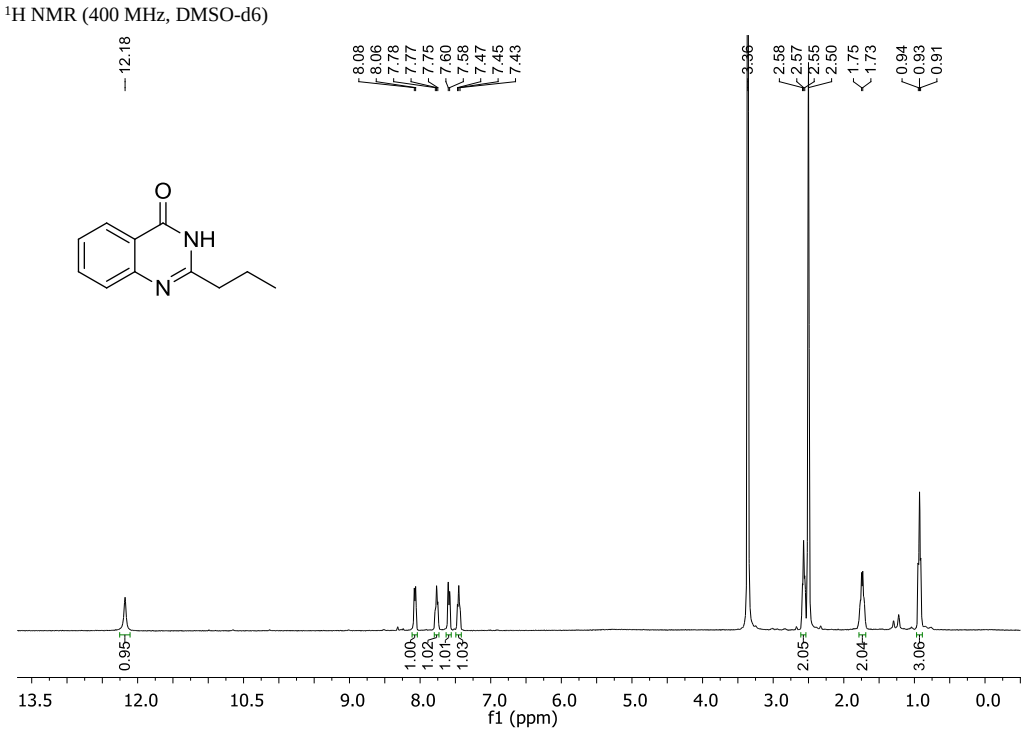

Figure S32. ^{1}H NMR spectra of 2-propylquinazolin-4(3*H*)-one (**3p**).

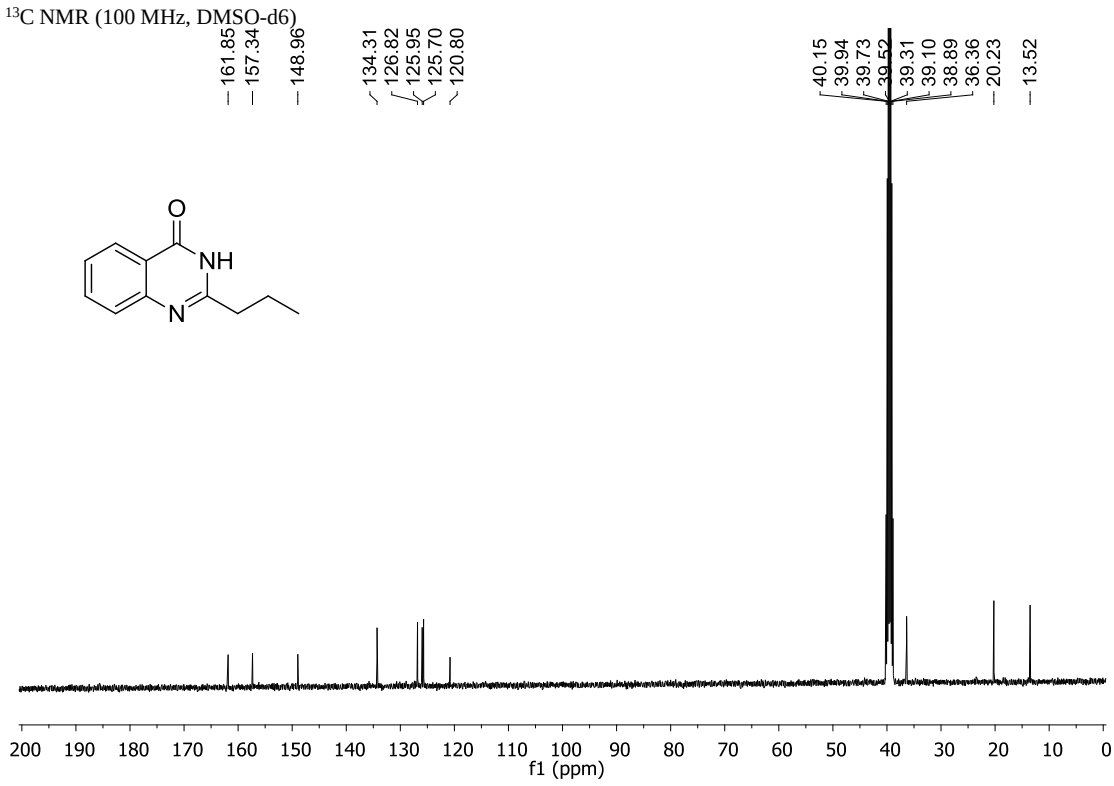

Figure S33. ^{13}C NMR spectra of 2-propylquinazolin-4(3*H*)-one (**3p**).

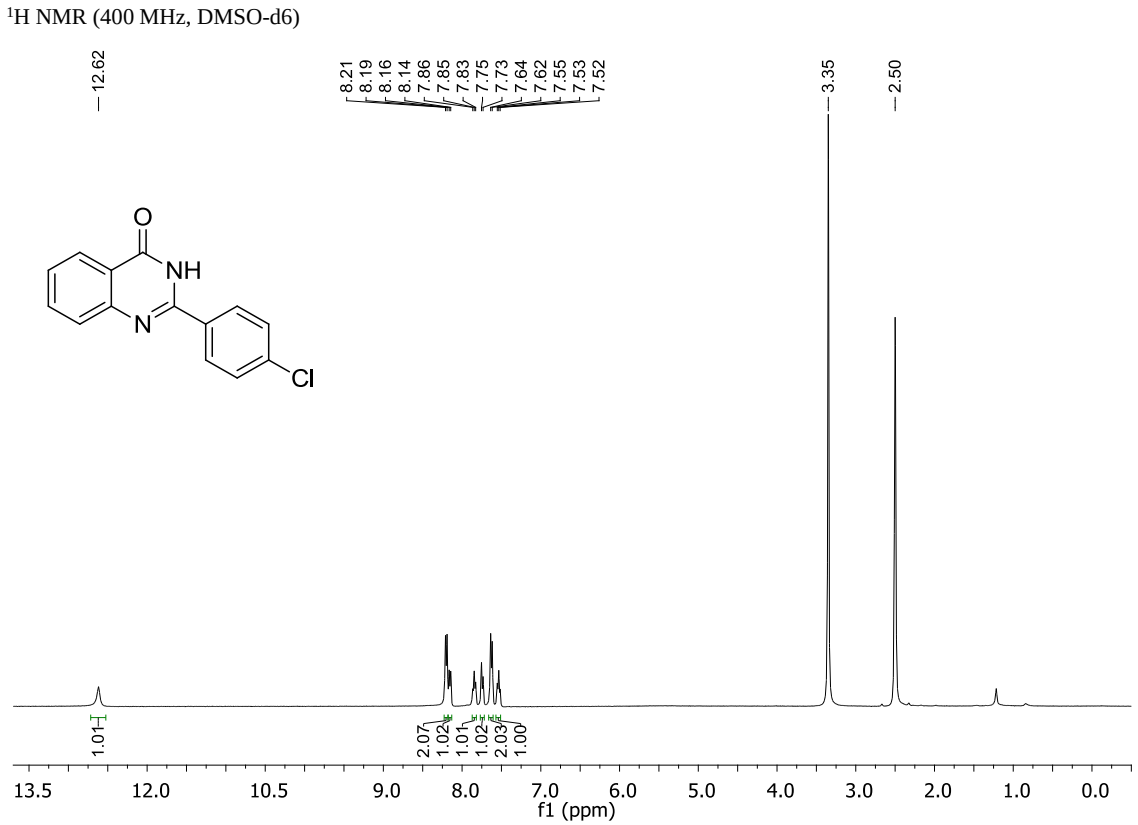

Figure S34. ^{1}H NMR spectra of 2-(4-chlorophenyl)quinazolin-4(3*H*)-one (**3q**).

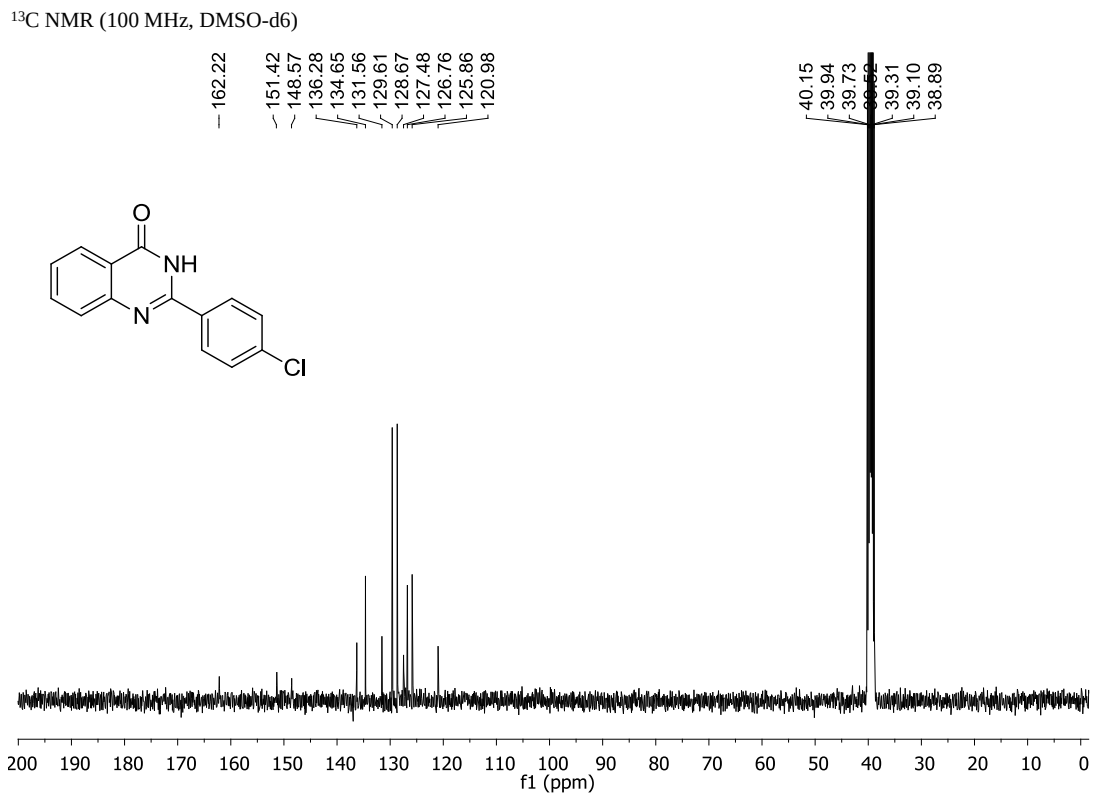

Figure S35. ^{13}C NMR spectra of 2-(4-chlorophenyl)quinazolin-4(3*H*)-one (**3q**).

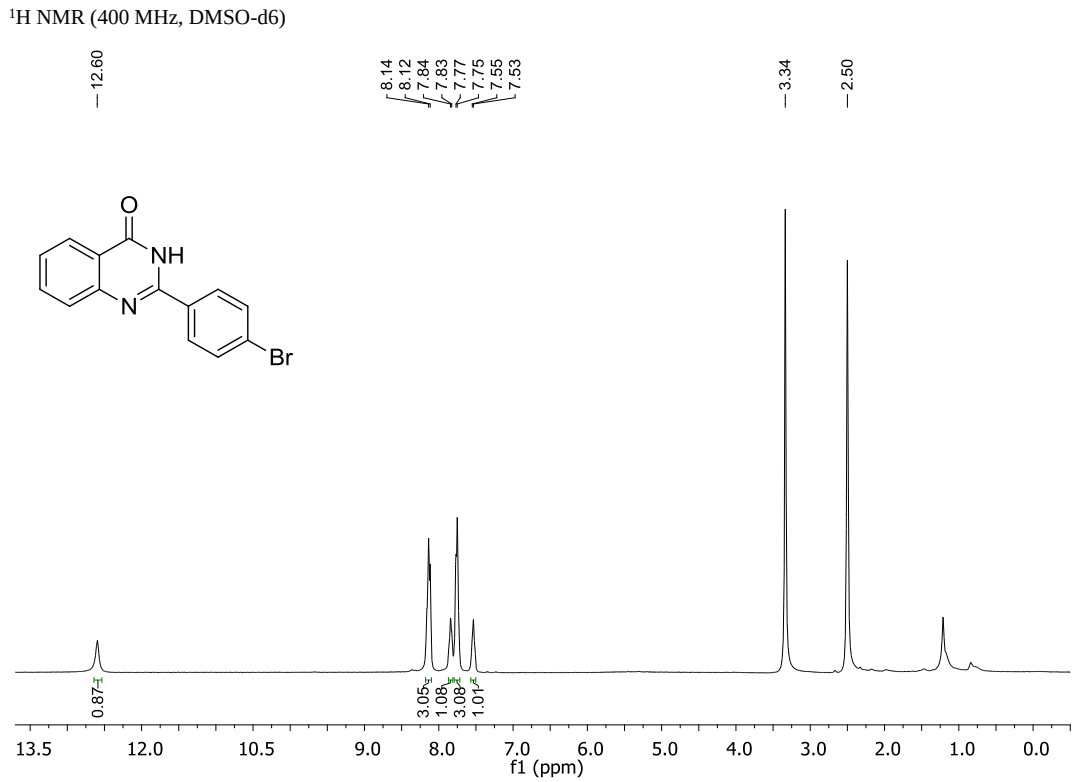

Figure S36. ^{1}H NMR spectra of 2-(4-bromophenyl)quinazolin-4(3*H*)-one (**3r**).

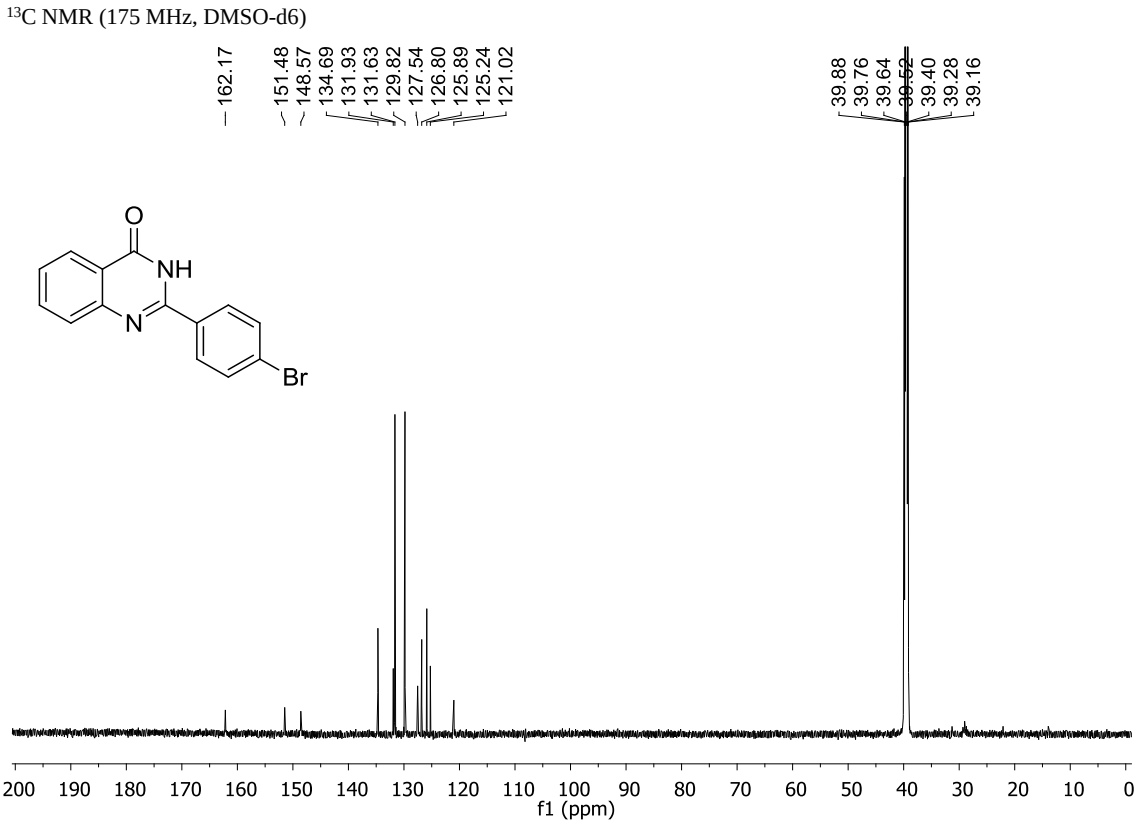

Figure S37. ^{13}C NMR spectra of 2-(4-bromophenyl)quinazolin-4(3*H*)-one (**3r**).

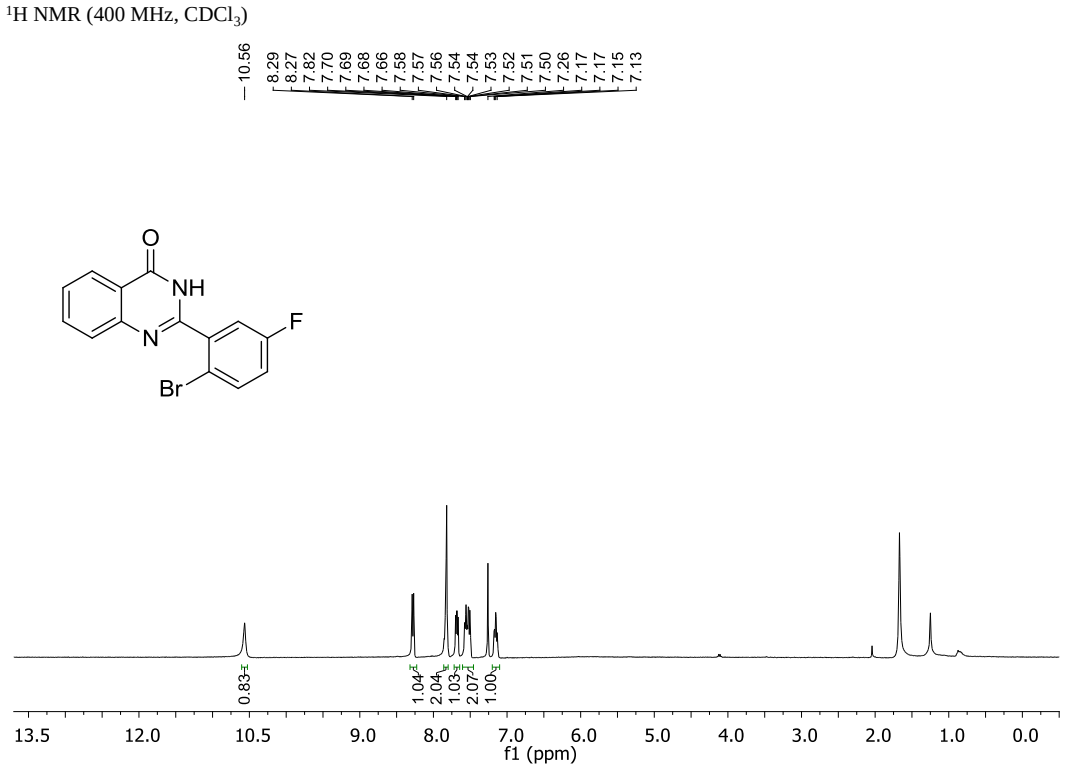

Figure S38. ^{1}H NMR spectra of 2-(2-bromo-5-fluorophenyl)quinazolin-4(3*H*)-one (**3s**).

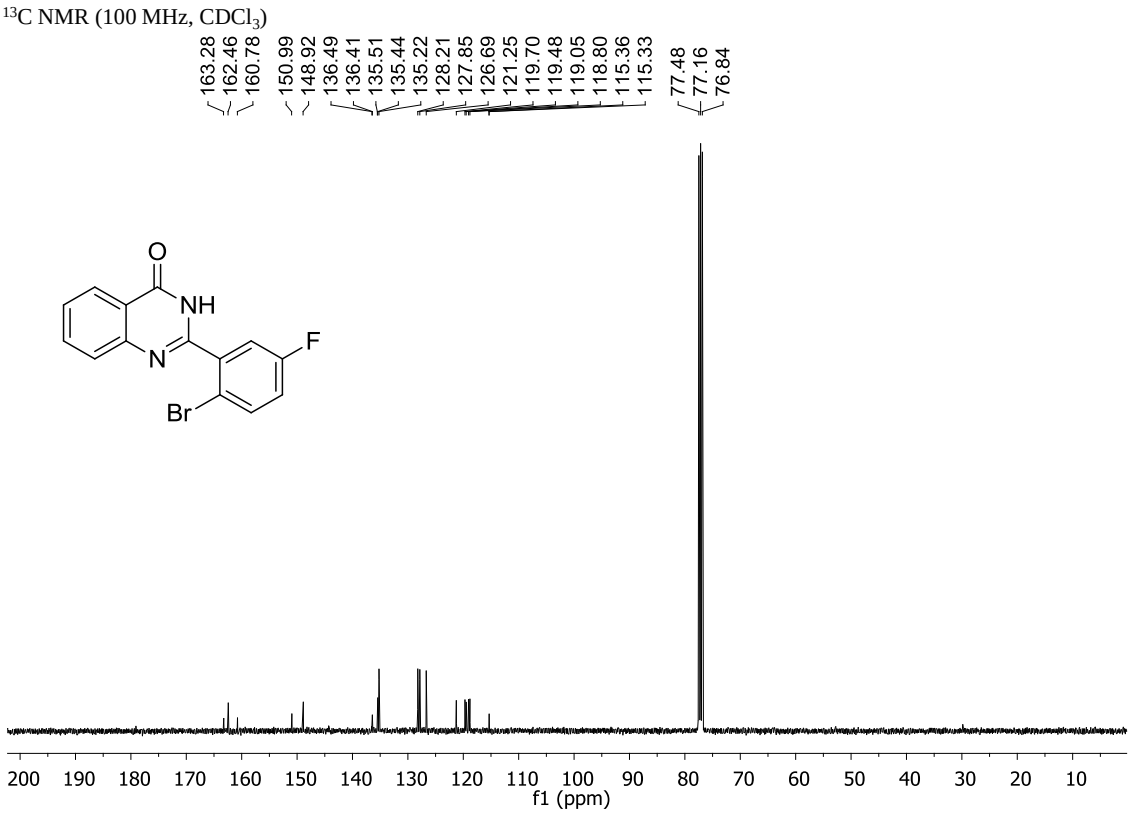

Figure S39. ^{13}C NMR spectra of 2-(2-bromo-5-fluorophenyl)quinazolin-4(3*H*)-one (**3s**).

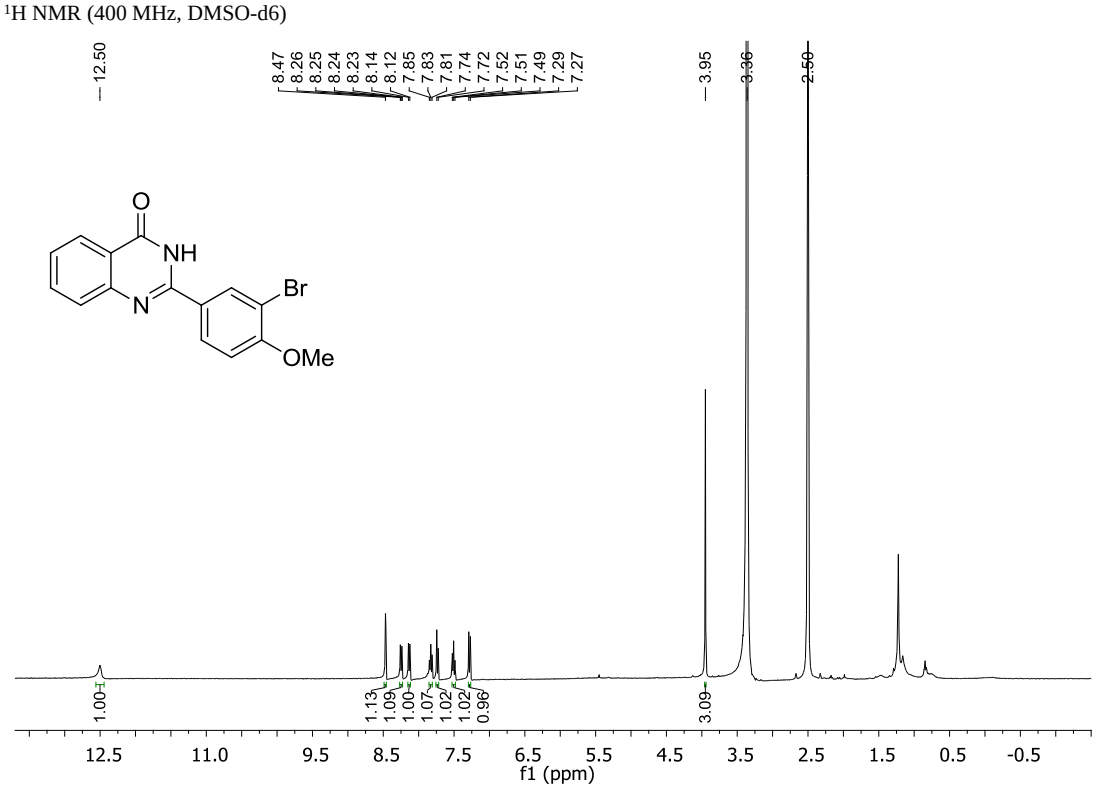

Figure S40. [1]H NMR spectra of 2-(3-bromo-4-methoxyphenyl)quinazolin-4(3*H*)-one (**3t**).

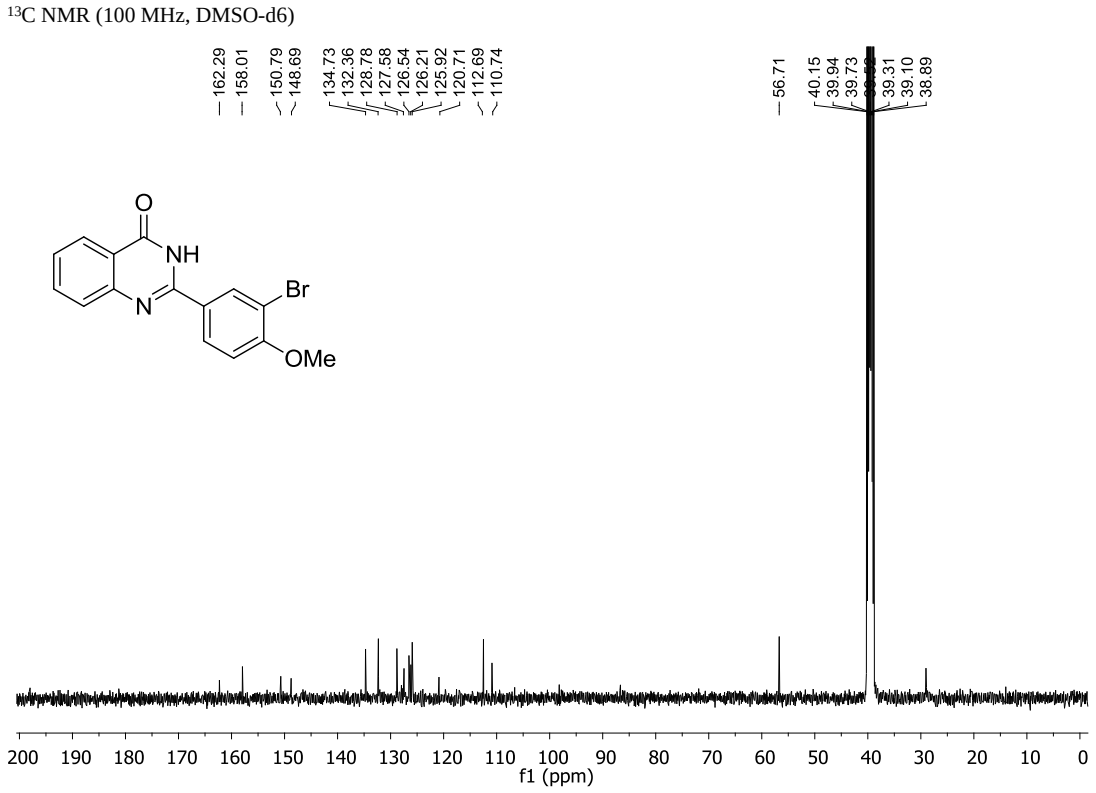

Figure S41. [13]C NMR spectra of 2-(3-bromo-4-methoxyphenyl)quinazolin-4(3*H*)-one (**3t**).

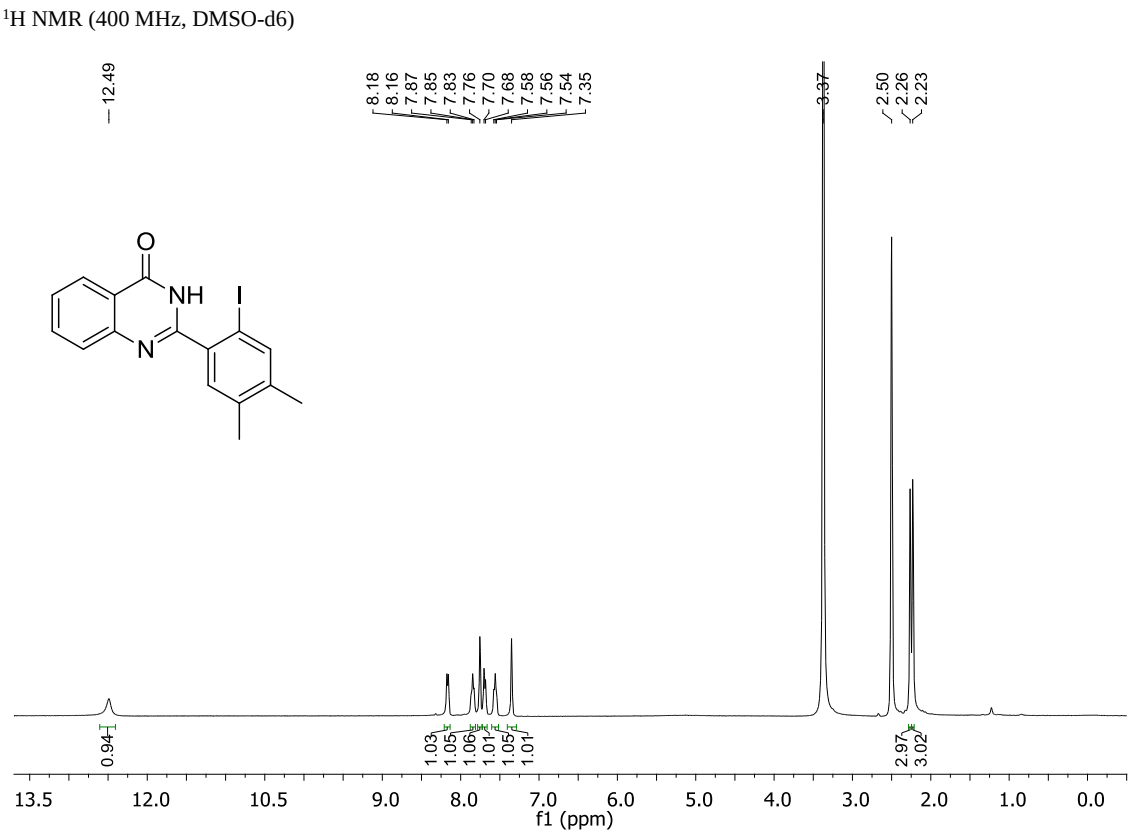

Figure S42. [1]H NMR spectra of 2-(2-iodo-4,5-dimethylphenyl)quinazolin-4(3*H*)-one (**3u**).

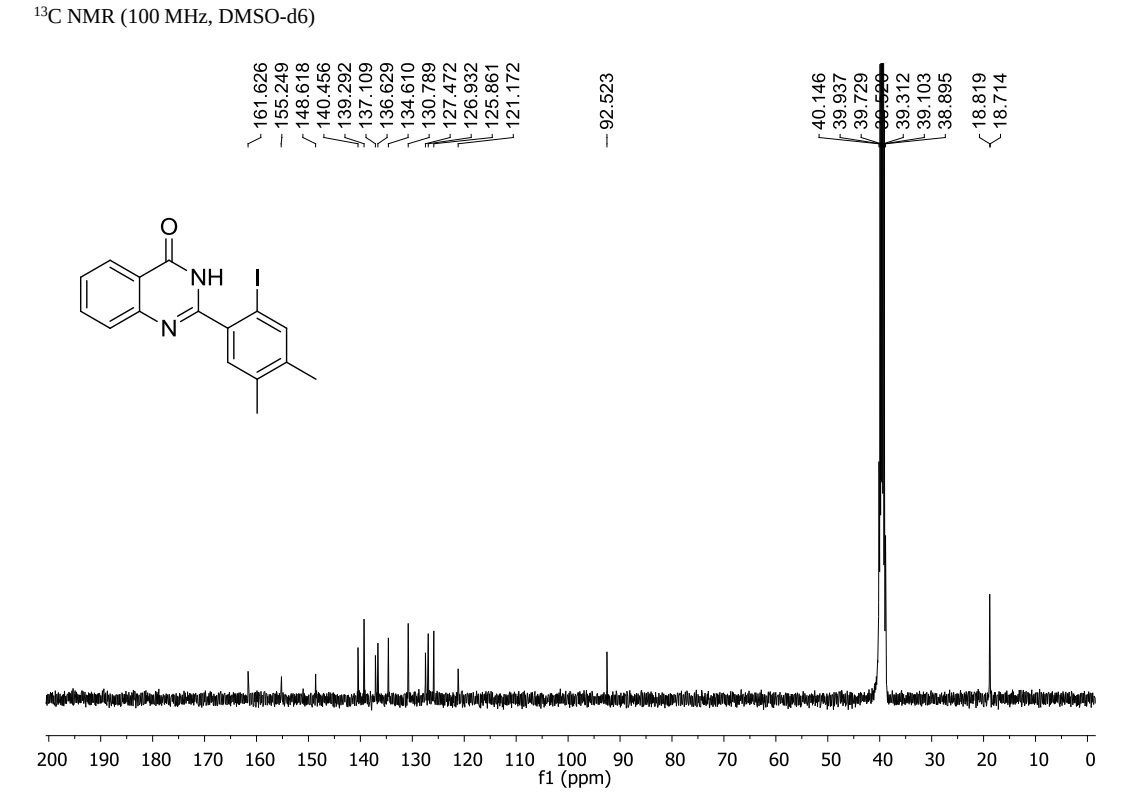

Figure S43. [13]C NMR spectra of 2-(2-iodo-4,5-dimethylphenyl)quinazolin-4(3*H*)-one (**3u**).

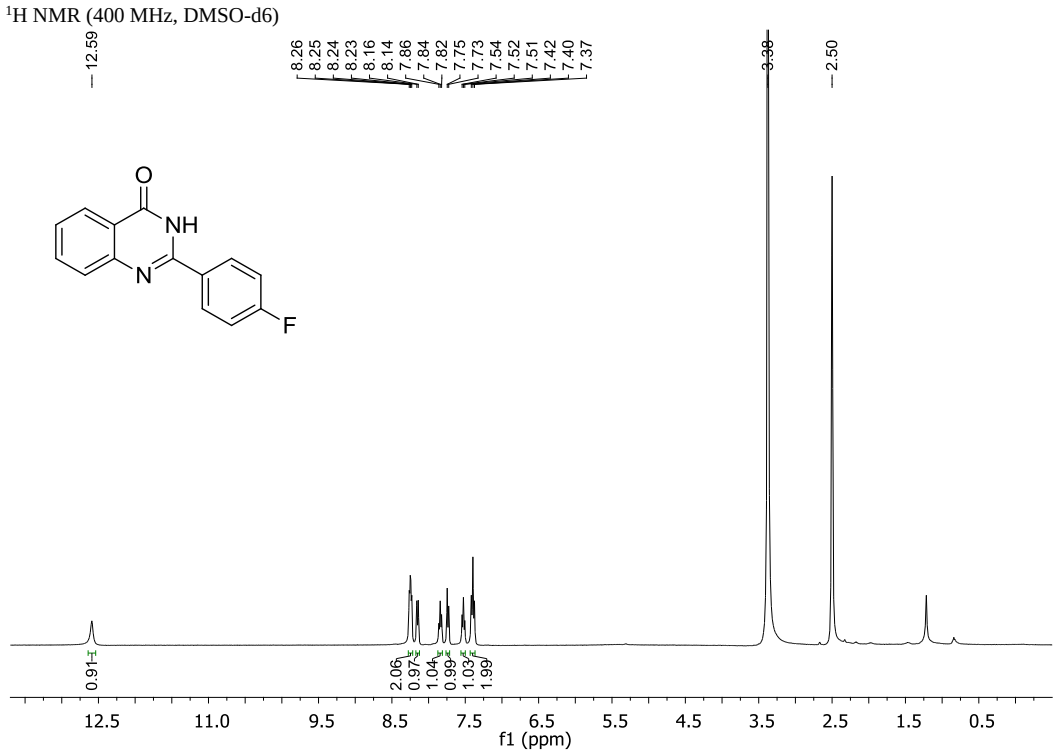

Figure S44. ^{1}H NMR spectra of 2-(4-fluorophenyl)quinazolin-4(3*H*)-one (**3v**).

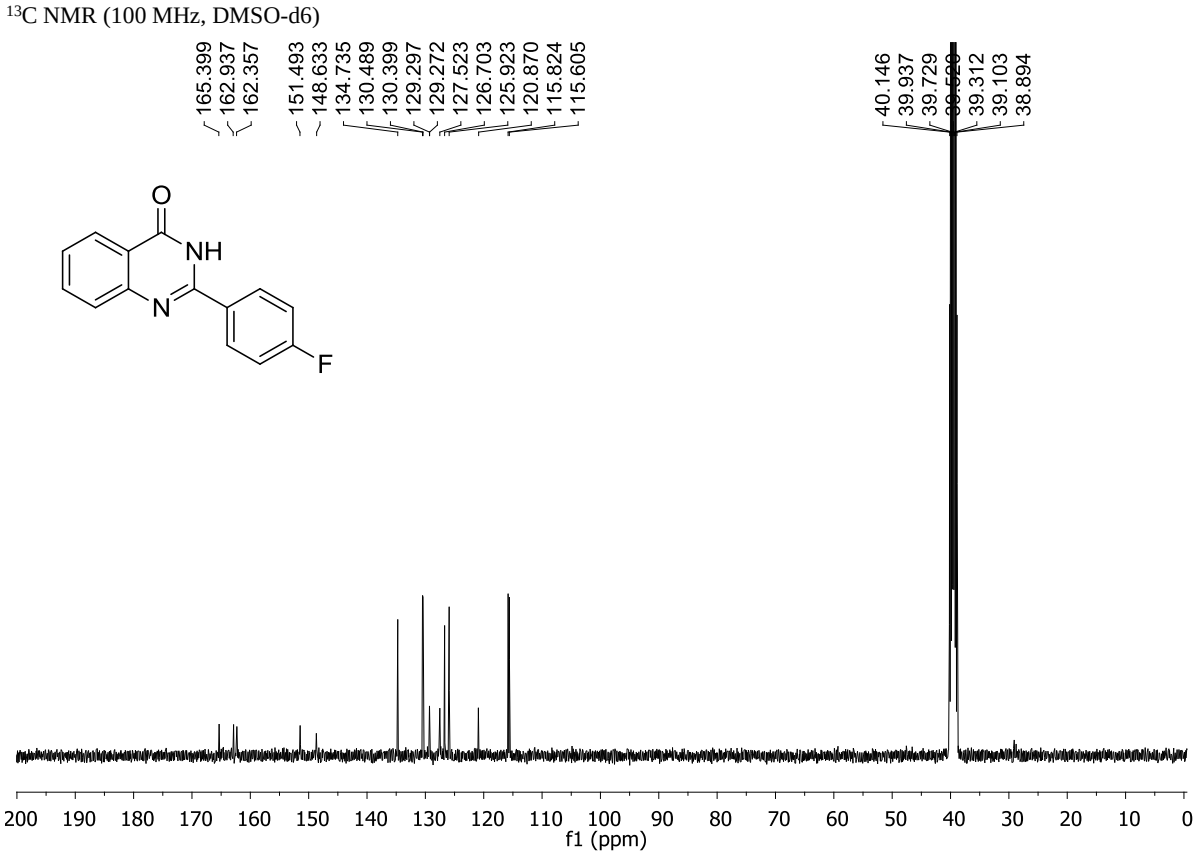

Figure S45. ^{13}C NMR spectra of 2-(4-fluorophenyl)quinazolin-4(3*H*)-one (**3v**).

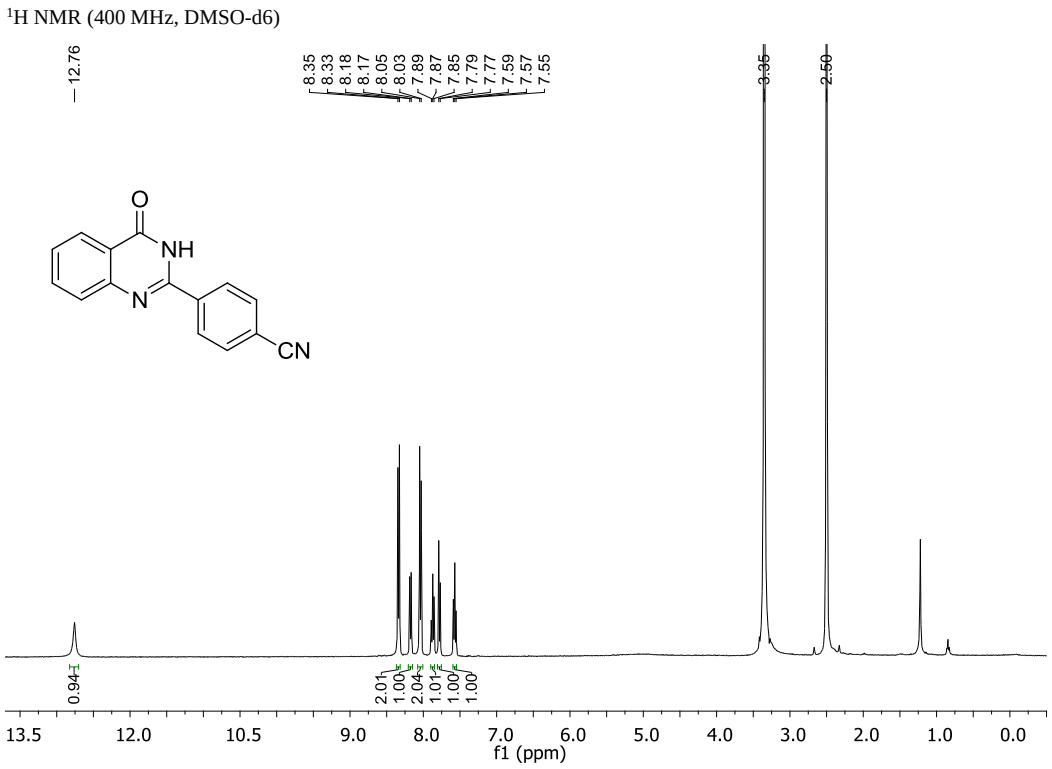

Figure S46. ^{1}H NMR spectra of 4-(4-oxo-3,4-dihydroquinazolin-2-yl)benzonitrile (**3w**).

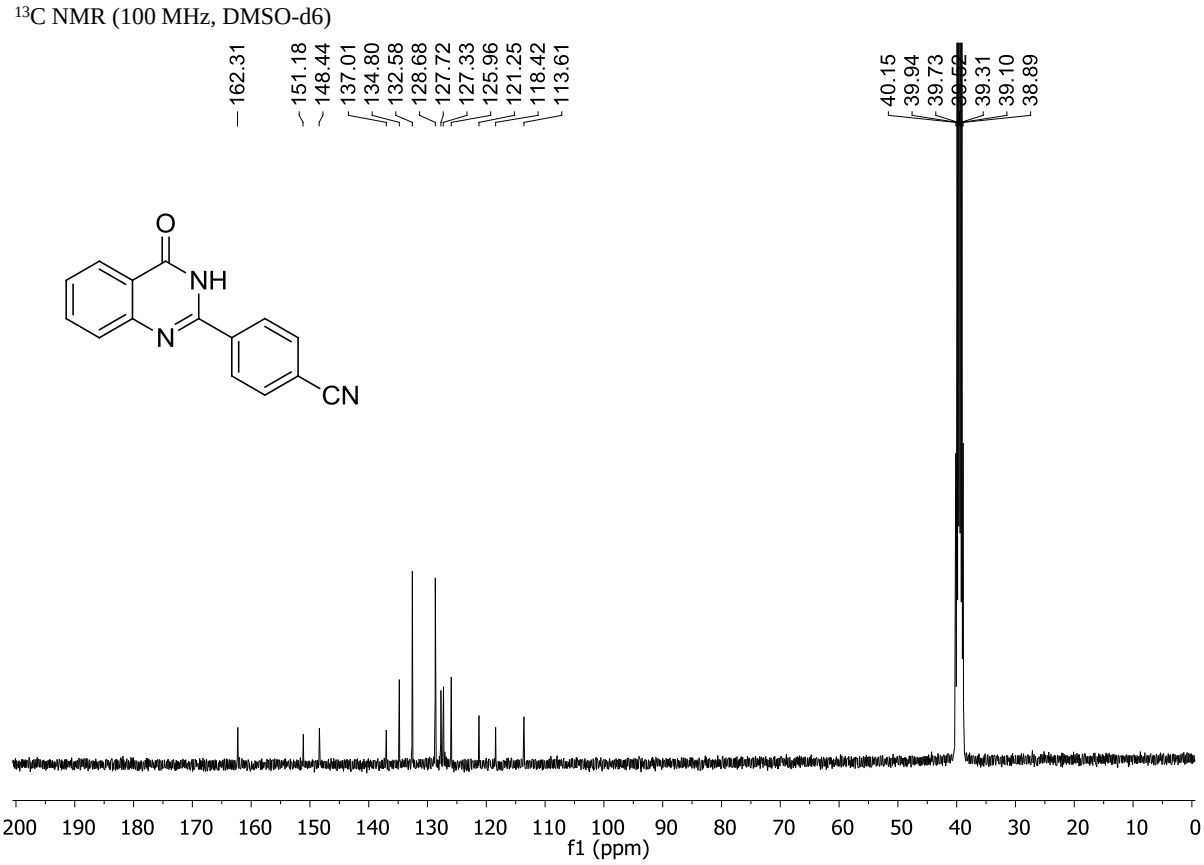

Figure S47. ^{13}C NMR spectra of 4-(4-oxo-3,4-dihydroquinazolin-2-yl)benzonitrile (**3w**).

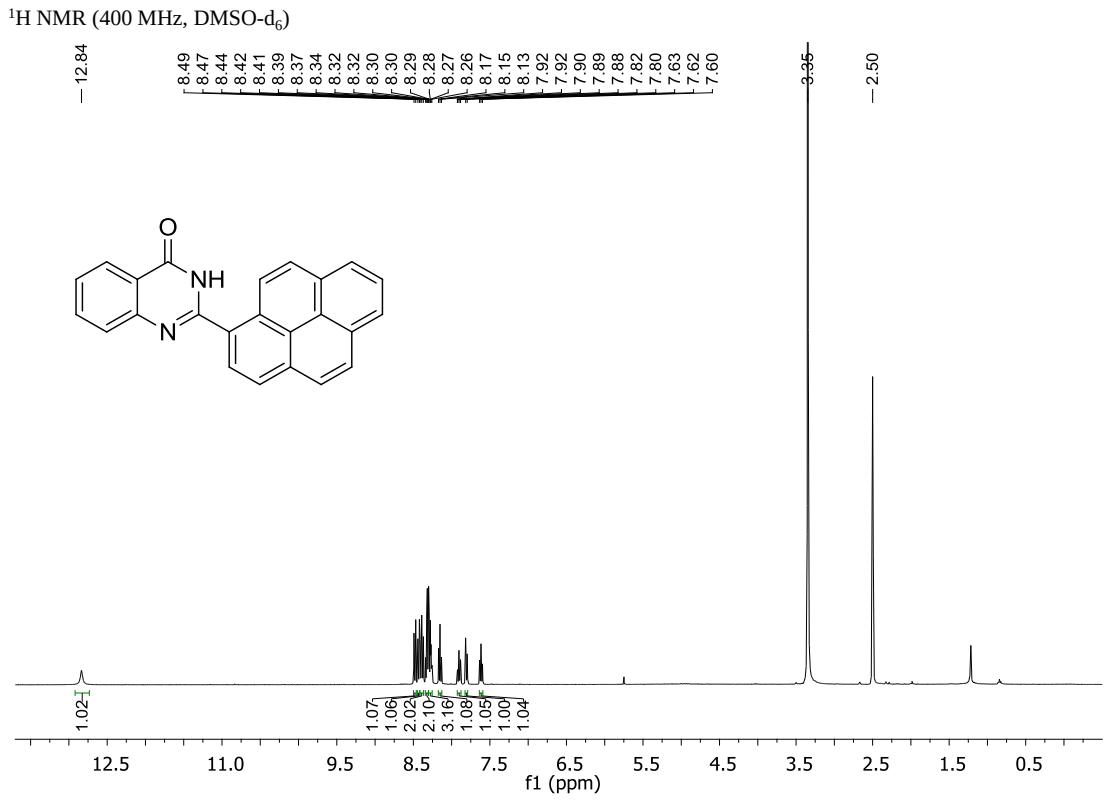

Figure S48. ^{1}H NMR spectra of 2-(pyren-1-yl)quinazolin-4(3*H*)-one (**3x**).

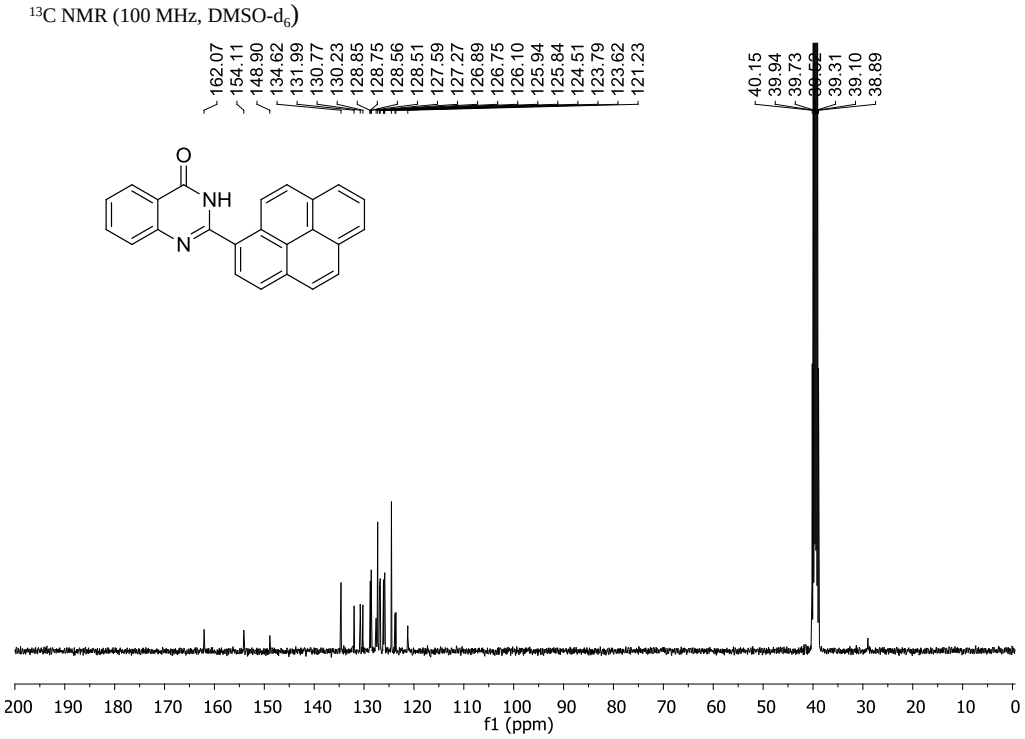

Figure S49. ^{13}C NMR spectra of 2-(pyren-1-yl)quinazolin-4(3*H*)-one (**3x**).

^{1}H NMR (400 MHz, $CDCl_3$)

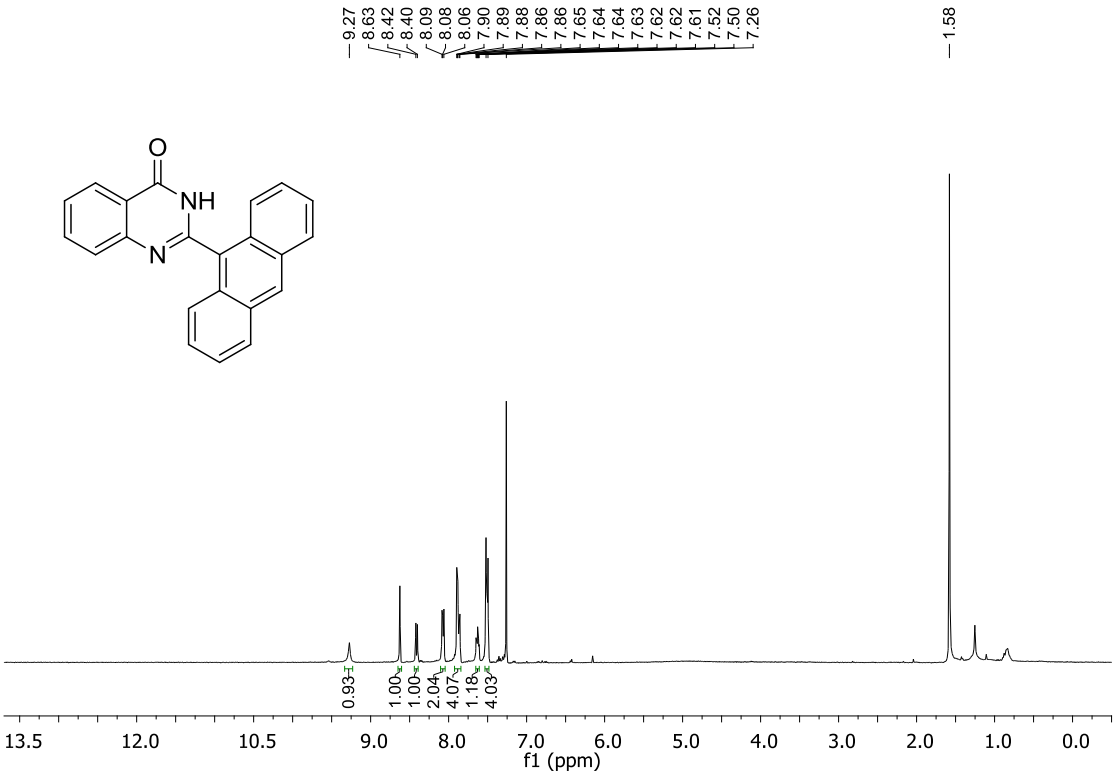

Figure S50. ^{1}H NMR spectra of 2-(anthracen-9-yl)quinazolin-4(3*H*)-one (**3y**).

^{13}C NMR (100 MHz, $CDCl_3$)

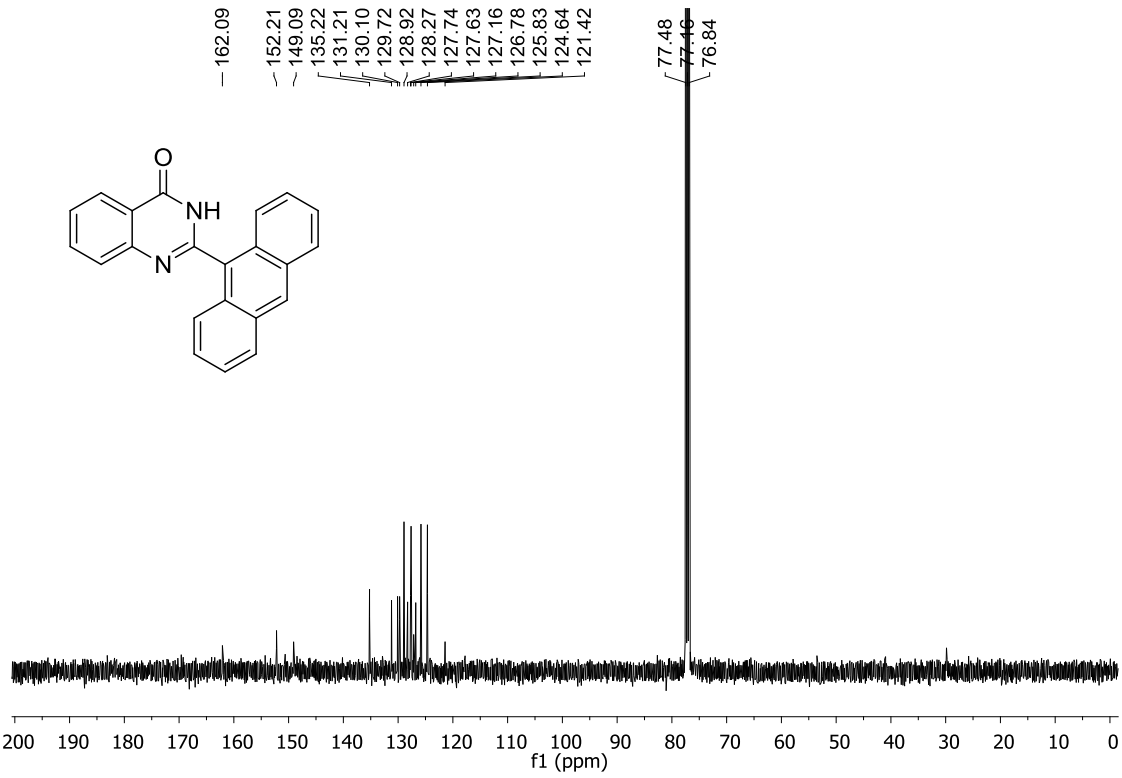

Figure S51. ^{13}C NMR spectra of 2-(anthracen-9-yl)quinazolin-4(3*H*)-one (**3y**).