

Supporting Information

Room Temperature ligand free Cu₂O-H₂O₂ Catalyzed tandem oxidative synthesis of quinazoline-4(3H)-one and quinazoline derivatives

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1) General information

All reactions were carried out in oven dried glassware under atmospheric conditions otherwise noted. Starting materials and solvents were obtained from common commercial sources and used without further purification. All reported yields are isolated yields. TLC was carried out using aluminium sheets pre-coated with silica gel 60F₂₅₄ (Merck) and was visualized under 254 nm UV light. Melting points were obtained by an open capillary method and are uncorrected. ¹H NMR (500 MHz) and ¹³C NMR (125 MHz) were recorded on a Bruker Advance 500 MHz spectrometer using TMS as an internal standard. Chemical shifts are reported in parts per million (ppm), downfield from residual solvents peaks and coupling constants are reported as Hertz (Hz). Splitting patterns are designated as s (singlet), d (doublet), t (triplet), q (quartet), dd (doublet of doublet), br (broad) and m (multiplet, for unresolved lines). The mass spectra were recorded on a Q-TOF micromass (YA-105) spectrometer in ESI (electrospray ionization) mode. Single crystal X-ray diffractions were collected on a Bruker SMART APEX-II CCD diffractometer.

2) General procedure for synthesis of 2-arylquinazolin-4(3H)-one and 2-phenylquinazoline derivatives

2-aminobenzonitrile (0.5 mmol), benzyl alcohol derivatives (0.6 mmol), Cu₂O (10 mol %), H₂O₂ (1.5 mmol), KOH (0.75 mmol), DMSO (2 ml) were subjected under vigorous stirring in a round bottom flask which was maintained at room temperature for 10 hours. For the extension work 2-aminobenzylamine (0.6 mmol), benzaldehyde derivatives (0.5 mmol), Cu₂O (20 mol %), KOH (0.75 mmol), DMSO (2 ml) were subjected to round bottom flask fitted with a condenser under 60 °C and stirred for 3 hours. The progress of the reaction was monitored by TLC under UV light. After completion of the reaction the mixture was extracted with ethyl acetate (3 x 10 mL) and washed with water (3 x 10 mL). The combined extract was dried over anhydrous Na₂SO₄. The

filtrate was concentrated under reduced pressure. The product was purified by column chromatography over silica gel using n-hexane/ethyl acetate (3:1 v/v) as eluent to get the purified product. The products were then characterized by ESI-MS, ¹H NMR, ¹³C NMR spectra.

3) Single crystal X-ray diffraction

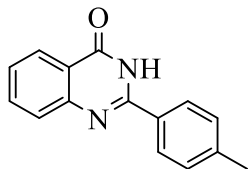
Single crystal X-ray diffractions were collected on a Bruker SMART APEX-II CCD diffractometer using Mo K α ($\lambda = 0.71073$ Å) radiation.¹ Bruker SAINT software has been employed for reducing the data and SADABS for correcting the intensities of absorption.² Structure was solved and refined using SHELXL with anisotropic displacement parameters for non-H atoms. In the crystal structure H-atoms are located experimentally, whereas C–H atoms were fixed geometrically using the HFIX command in SHELX-TL.³ No missed symmetry observed in the final check of CIF file using PLATON.^{4,5} Information of crystallographic parameters for all structures is furnished in **Table S1**.

Table S1: Crystallographic parameters of structures of multicomponent systems 3a

Crystal data	Compound 3a
Formula unit	C ₁₅ H ₁₂ N ₂ O
Formula weight (gmol ⁻¹)	236.27
Crystal system	Triclinic
T [K]	100
<i>a</i> [Å]	4.803(3)
<i>b</i> [Å]	15.071(11)
<i>c</i> [Å]	17.003(12)
α [°]	94.37(2)
β [°]	93.80(2)
γ [°]	97.93(2)
Volume [Å ³]	1211.7(15)
Space group	<i>P</i> -1
Z	4
D _{cal} [g/cm ³]	1.295
Absorption correction	SADABS/Multi-scan
R ₁ , wR ₂	0.0635, 0.1195
Instrument	Bruker CCD Apex II
CCDC No	2213373

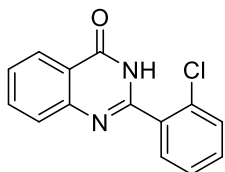
4) Spectral data of products

2-(p-tolyl)quinazolin-4(3H)-one (Table 2;6a1)



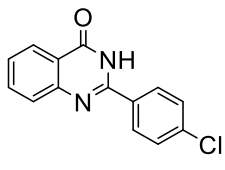
^1H NMR (500 MHz, DMSO- d_6) δ 12.42 (s, 1H), 8.11 (d, J = 6.9 Hz, 1H), 8.06 (d, J = 8.2 Hz, 2H), 7.78 (t, J = 7.6 Hz, 1H), 7.68 (d, J = 8.0 Hz, 1H), 7.46 (t, J = 7.5 Hz, 1H), 7.30 (d, J = 8.1 Hz, 2H), 2.34 (s, 3H). $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, DMSO- d_6) δ 162.55, 152.50, 149.00, 141.69, 134.79, 130.12, 129.42, 127.92, 126.62, 126.08, 121.12, 21.22. MS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{15}\text{H}_{12}\text{N}_2\text{O}$ 237.09; Found 237.11

2-(2-chlorophenyl)quinazolin-4(3H)-one (Table 2;6a2)



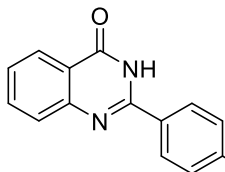
^1H NMR (500 MHz, CDCl_3) δ 11.80 (s, 1H), 8.30 (d, J = 8.0 Hz, 1H), 7.80 (d, J = 8.2 Hz, 1H), 7.75 (d, J = 8.0 Hz, 1H), 7.50 (t, J = 7.5 Hz, 1H), 7.41 (d, J = 9.1 Hz, 2H), 7.38 – 7.34 (m, 1H), 7.27 – 7.23 (m, 1H). $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) δ 163.80, 156.49, 148.99, 135.06, 134.56, 133.16, 128.26, 127.30, 126.17, 125.86, 124.59, 120.01. MS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{14}\text{H}_9\text{ClN}_2\text{O}$ 257.06; Found 257.08.

2-(4-chlorophenyl)quinazolin-4(3H)-one (Table 2; 6a3)



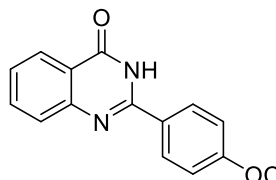
^1H NMR (500 MHz, DMSO- d_6) δ 12.66 (s, 1H), 8.25 (d, J = 8.5 Hz, 1H), 8.21 (d, J = 7.7 Hz, 1H), 7.90 (t, J = 7.6 Hz, 1H), 7.80 (d, J = 8.1 Hz, 2H), 7.68 (d, J = 8.5 Hz, 2H), 7.59 (t, J = 7.4 Hz, 1H). $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, DMSO- d_6) δ 162.99, 152.15, 149.20, 136.93, 135.33, 132.29, 130.29, 129.35, 126.54, 121.64. MS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{14}\text{H}_9\text{ClN}_2\text{O}$ 257.06; Found 257.09.

2-(4-fluorophenyl)quinazolin-4(3H)-one (Table 2; 6a4)



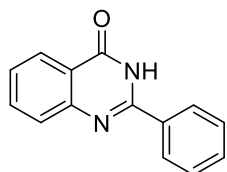
^1H NMR (500 MHz, DMSO- d_6) δ 12.70 (s, 1H), 8.38 (d, J = 14.2 Hz, 2H), 8.28 (d, J = 7.7 Hz, 1H), 7.96 (t, J = 7.0 Hz, 1H), 7.86 (d, J = 8.1 Hz, 1H), 7.65 (t, J = 7.4 Hz, 1H), 7.52 (t, J = 8.8 Hz, 2H). $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, DMSO- d_6) δ 162.25, 151.40, 148.70, 134.66, 130.44, 127.50, 126.64, 125.89, 120.93, 115.75, 115.57. MS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{14}\text{H}_9\text{FN}_2\text{O}$ 241.06; Found 241.08.

2-(4-methoxyphenyl)quinazolin-4(3H)-one (Table 2; 6a5)



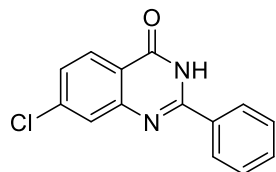
¹H NMR (500 MHz, DMSO-d₆) δ 12.34 (s, 1H), 8.13 (d, *J* = 8.9 Hz, 2H), 8.07 (d, *J* = 7.9 Hz, 1H), 7.74 (t, *J* = 6.9 Hz, 1H), 7.64 (d, *J* = 8.0 Hz, 1H), 7.41 (t, *J* = 7.9 Hz, 1H), 7.02 (d, *J* = 8.9 Hz, 2H), 3.78 (s, 3H). ¹³C{¹H} NMR (125 MHz, DMSO-d₆) δ 162.73, 162.29, 152.27, 149.35, 134.93, 131.75, 129.87, 127.69, 126.52, 126.24, 125.22, 121.10, 114.40, 55.87. MS (ESI) *m/z*: [M+H]⁺ calcd for C₁₅H₁₂N₂O₂H 253.08; Found 253.10.

2-phenylquinazolin-4(3H)-one (Table 2; 6a6)



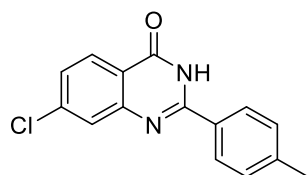
¹H NMR (500 MHz, DMSO-d₆) δ 12.66 (s, 1H), 8.30 (d, *J* = 7.0 Hz, 2H), 8.28 (d, *J* = 8.9 Hz, 1H), 7.94 (d, *J* = 6.9 Hz, 1H), 7.86 (d, *J* = 7.9 Hz, 1H), 7.67 (m, 4H). ¹³C{¹H} NMR (125 MHz, DMSO-d₆) δ 162.68, 152.74, 149.19, 135.02, 133.17, 131.82, 129.04, 128.22, 128.08, 127.01, 126.30, 121.44. MS (ESI) *m/z*: [M+H]⁺ calcd for C₁₄H₁₀N₂O 223.07; Found 223.08.

7-chloro-2-phenylquinazolin-4(3H)-one (Table 2; 6a7)



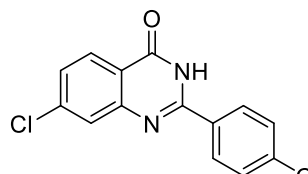
¹H NMR (500 MHz, DMSO-d₆) δ 12.55 (s, 1H), 8.08 (m, 3H), 7.70 (s, 1H), 7.66 (d, *J* = 8.1 Hz, 1H), 7.53 – 7.43 (m, 3H). ¹³C{¹H} NMR (125 MHz, DMSO-d₆) δ 162.35, 154.48, 139.84, 133.07, 132.38, 129.30, 128.59, 127.46, 126.52. MS (ESI) *m/z*: [M+H]⁺ calcd for C₁₄H₉ClN₂O 257.04; Found 257.07.

7-chloro-2-(p-tolyl)quinazolin-4(3H)-one (Table 2; 6a9)



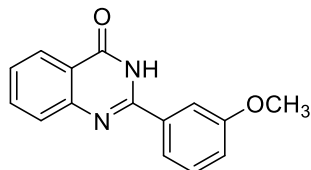
¹H NMR (500 MHz, DMSO-d₆) δ 12.69 (s, 1H), 7.93 (d, *J* = 8.1 Hz, 1H), 7.85 (s, 1H), 7.61 (d, *J* = 8.5 Hz, 2H), 7.45 (d, *J* = 8.0 Hz, 1H), 7.38 (d, *J* = 8.0 Hz, 2H), 2.48 (s, 3H). ¹³C{¹H} NMR (125 MHz, DMSO-d₆) δ 162.16, 154.15, 143.47, 142.33, 129.93, 128.31, 126.94, 123.62, 123.18, 21.59. MS (ESI) *m/z*: [M+H]⁺ calcd for C₁₅H₁₁ClN₂O 271.05; Found 271.08.

7-chloro-2-(4-chlorophenyl)quinazolin-4(3H)-one (Table 2; 6a10)



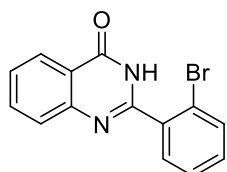
¹H NMR (500 MHz, DMSO) δ 10.88 (s, 1H), 9.09 (d, *J* = 20.9 Hz, 1H), 8.34 (s, 1H), 8.20 (d, *J* = 8.5 Hz, 1H), 7.35 (m, 4H). ¹³C{¹H} NMR (125 MHz, DMSO-d₆) δ 141.76, 131.27, 128.98, 128.64, 128.36, 128.17, 115.78, 114.77. MS (ESI) *m/z*: [M+H]⁺ calcd for C₁₄H₈Cl₂N₂O 291.00; Found 291.03.

2-(3-methoxyphenyl)quinazolin-4(3H)-one (Table 2; 6a11)



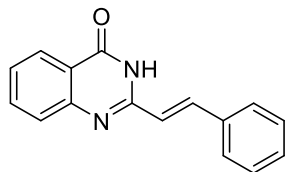
^1H NMR (500 MHz, DMSO- d_6) δ 12.48 (s, 1H), 8.10 (d, J = 7.6 Hz, 2H), 7.82 – 7.75 (m, 1H), 7.74 (d, J = 7.5 Hz, 1H), 7.69 (s, 1H), 7.46 (t, J = 7.3 Hz, 1H), 7.40 (t, J = 7.8 Hz, 1H), 7.09 (d, J = 7.5 Hz, 1H), 3.81 (s, 3H). $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, DMSO- d_6) δ 172.18, 169.30, 161.99, 158.60, 144.53, 143.97, 139.67, 137.48, 136.55, 135.79, 130.97, 130.07, 127.53, 122.49, 65.33. MS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{15}\text{H}_{12}\text{N}_2\text{O}_2\text{H}$ 253.08; Found 253.10.

2-(2-bromophenyl)quinazolin-4(3H)-one (Table 2; 6a12)



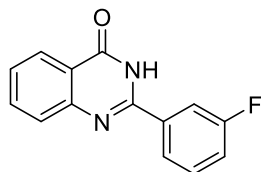
^1H NMR (500 MHz, DMSO- d_6) δ 12.62 (s, 1H), 8.28 (d, J = 7.2 Hz, 1H), 7.93 (t, J = 7.5 Hz, 1H), 7.84 (d, J = 8.1 Hz, 2H), 7.69 (d, J = 7.1 Hz, 1H), 7.67 – 7.63 (m, 2H), 7.63 – 7.59 (m, 1H). $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, DMSO- d_6) δ 162.77, 152.85, 149.30, 135.15, 133.27, 131.93, 129.14, 128.31, 128.06, 127.13, 126.40, 121.54. MS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{14}\text{H}_9\text{BrN}_2\text{O}_2\text{H}$ 299.98; Found 300.00.

(E)-2-styrylquinazolin-4(3H)-one (Table 2; 6a13)



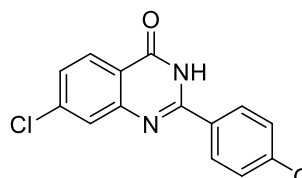
^1H NMR (500 MHz, CDCl_3) δ 8.14 (d, J = 7.1 Hz, 1H), 7.83 (d, J = 16.0 Hz, 1H), 7.61 – 7.57 (m, 2H), 7.51 (d, J = 7.9 Hz, 2H), 7.45 – 7.42 (m, 1H), 7.35 – 7.31 (m, 2H), 7.27 – 7.22 (m, 1H), 6.49 (d, J = 16.0 Hz, 1H). MS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{16}\text{H}_{12}\text{N}_2\text{O}_2\text{H}$ 248.09; Found 248.10.

2-(3-fluorophenyl)quinazolin-4(3H)-one (Table 2; 6a15)



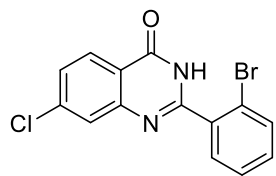
^1H NMR (500 MHz, DMSO- d_6) δ 12.65 (s, 1H), 8.06 (d, J = 10.3 Hz, 1H), 7.90 (t, J = 7.0 Hz, 1H), 7.80 (s, 1H), 7.66 (dd, J = 14.1, 8.0 Hz, 2H), 7.60 (t, J = 7.5 Hz, 1H), 7.50 (td, J = 8.4, 2.2 Hz, 2H). $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, DMSO- d_6) δ 162.43, 161.43, 151.30, 148.78, 135.00, 131.05, 127.93, 127.22, 126.19, 124.23, 118.65. MS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{14}\text{H}_9\text{FN}_2\text{O}_2\text{H}$ 241.06; Found 241.09.

7-chloro-2-(4-methoxyphenyl)quinazolin-4(3H)-one (Table 2; 6a16)



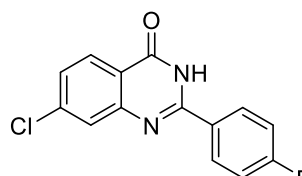
$^1\text{H NMR}$ (500 MHz, DMSO- d_6) δ 12.70 (s, 1H), 8.23 (d, $J = 8.5$ Hz, 1H), 7.55 (s, 1H), 7.25 (d, $J = 7.8$ Hz, 1H), 6.97 (d, $J = 9.0$ Hz, 2H), 6.87 (d, $J = 7.7$ Hz, 2H), 3.96 (s, 3H). $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, DMSO- d_6) δ 159.36, 153.57, 139.24, 129.82, 129.13, 127.99, 126.87, 126.68, 120.33, 118.55, 112.78, 55.46. MS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{15}\text{H}_{11}\text{ClN}_2\text{O}_2\text{H}$ 287.05; Found 287.07.

2-(2-bromophenyl)-7-chloroquinazolin-4(3H)-one (Table 2; 6a17)



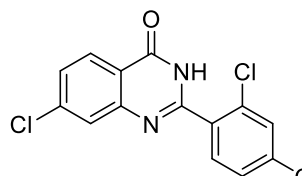
$^1\text{H NMR}$ (500 MHz, DMSO- d_6) δ 12.62 (s, 1H), 8.12 (d, $J = 7.3$ Hz, 1H), 8.09 (d, $J = 8.4$ Hz, 1H), 7.85 (s, 1H), 7.73 (d, $J = 1.5$ Hz, 1H), 7.55 (d, $J = 7.1$ Hz, 1H), 7.53 – 7.49 (m, 1H), 7.41 (t, $J = 7.7$ Hz, 1H). $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, DMSO- d_6) δ 162.13, 154.24, 150.36, 139.65, 132.85, 132.18, 129.11, 128.39, 127.26, 127.06, 120.30, 119.42, 118.38. MS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{14}\text{H}_8\text{BrClN}_2\text{O}_2\text{H}$ 333.95; Found 334.02

7-chloro-2-(4-fluorophenyl)quinazolin-4(3H)-one (Table 2; 6a18)



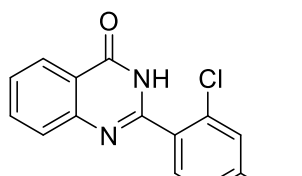
$^1\text{H NMR}$ (500 MHz, DMSO) δ 12.73 (s, 1H), 9.07 (d, $J = 21.6$ Hz, 2H), 8.53 (s, 1H), 8.22 (d, $J = 8.1$ Hz, 1H), 7.78 (d, $J = 17.0$ Hz, 1H), 7.25 (d, $J = 16.0$ Hz, 2H). $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, DMSO- d_6) δ 162.41, 162.01, 139.02, 130.97, 130.21, 128.69, 128.26, 127.65, 115.08. MS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{14}\text{H}_8\text{ClFN}_2\text{O}_2\text{H}$ 275.03; Found 275.05.

7-chloro-2-(2,4-dichlorophenyl)quinazolin-4(3H)-one (Table 2; 6a19)



$^1\text{H NMR}$ (500 MHz, DMSO- d_6) δ 12.85 (s, 1H), 8.34 (s, 1H), 8.20 (d, $J = 8.6$ Hz, 1H), 8.16 (s, 1H), 7.86 (d, $J = 1.8$ Hz, 1H), 7.83 (d, $J = 1.9$ Hz, 1H), 7.74 (d, $J = 8.3$ Hz, 1H). $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, DMSO- d_6) δ 173.34, 161.10, 153.13, 139.56, 132.95, 132.49, 129.48, 128.24, 127.81, 126.95, 120.41. MS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{14}\text{H}_7\text{Cl}_3\text{N}_2\text{O}_2\text{H}$ 323.96; Found 324.00.

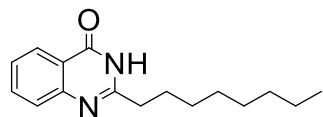
2-(2,4-dichlorophenyl)quinazolin-4(3H)-one (Table 2; 6a20)



$^1\text{H NMR}$ (500 MHz, DMSO- d_6) δ 12.82 (s, 1H), 8.34 (d, $J = 7.7$ Hz, 1H), 8.02 (t, $J = 7.2$ Hz, 1H), 7.98 (s, 1H), 7.87 (d, $J = 8.3$ Hz, 2H), 7.77 (d, $J = 1.8$ Hz, 1H), 7.76 – 7.72 (m, 1H). $^{13}\text{C}\{^1\text{H}\}$ NMR (125

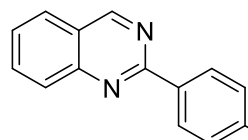
MHz, DMSO-d₆) δ 161.65, 151.64, 148.75, 135.71, 134.93, 132.99, 132.52, 129.44, 127.77, 127.50, 126.13, 121.56. MS (ESI) m/z: [M+H]⁺ calcd for C₁₄H₈Cl₂N₂OH 290.00; Found 290.10.

2-octylquinazolin-4(3H)-one (Table 2; 6a22)



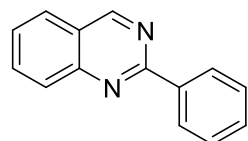
¹H NMR (500 MHz, CDCl₃) δ 11.87 (s, 1H), 8.21 (d, *J* = 7.7 Hz, 1H), 7.78 – 7.58 (m, 2H), 7.39 (t, *J* = 7.2 Hz, 1H), 2.81 – 2.65 (m, 2H), 1.88 – 1.72 (m, 2H), 1.52 – 1.03 (m, 10H), 0.80 (t, *J* = 3.8 Hz, 3H). ¹³C{¹H} NMR (125 MHz, CDCl₃) δ 163.99, 156.74, 149.05, 134.48, 126.81, 125.96, 120.18, 35.60, 31.32, 29.36, 28.60, 27.25, 22.27, 13.71. MS (ESI) m/z: [M+H]⁺ calcd for C₁₆H₂₂N₂O 258.17; Found 258.16.

2-(p-tolyl)quinazoline (12a1)



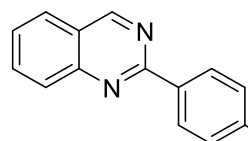
¹H NMR (400 MHz, CDCl₃) δ 9.44 (s, 1H), 8.49 (d, *J* = 8.3 Hz, 2H), 8.06 (d, *J* = 7.6 Hz, 1H), 7.94 – 7.84 (m, 2H), 7.59 (ddd, *J* = 8.1, 7.0, 1.1 Hz, 1H), 7.33 (d, *J* = 8.0 Hz, 2H), 2.44 (s, 3H). ¹³C{¹H} NMR (100 MHz, CDCl₃) δ 160.92, 141.00, 134.19, 129.54, 128.64, 127.21, 123.62, 21.63. MS (ESI) m/z: [M+H]⁺ calcd for C₁₅H₁₂N₂ 220.10; Found 220.09.

2-phenylquinazoline (Table 6; 12a2)



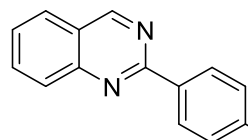
¹H NMR (400 MHz, CDCl₃) δ 9.47 (s, 1H), 8.60 (d, *J* = 6.3 Hz, 2H), 8.09 (d, *J* = 9.1 Hz, 1H), 7.96 – 7.90 (m, 1H), 7.89 (d, *J* = 1.4 Hz, 1H), 7.61 (t, *J* = 7.0 Hz, 1H), 7.52 (t, *J* = 7.1 Hz, 3H). ¹³C{¹H} NMR (100 MHz, CHLOROFORM-D) δ 161.16, 160.64, 134.27, 130.72, 128.70, 127.33, 125.10, 123.69. MS (ESI) m/z: [M+H]⁺ calcd for C₁₄H₁₀N₂ 206.08; Found 206.10.

4-(quinazolin-2-yl)benzotrile (Table 6; 12a3)



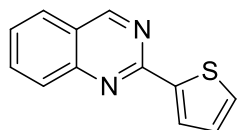
¹H NMR (500 MHz, CDCl₃) δ 9.48 (s, 1H), 8.65 (d, *J* = 3.3 Hz, 1H), 8.52 (d, *J* = 9.3 Hz, 2H), 8.10 (d, *J* = 9.0 Hz, 1H), 7.97 – 7.95 (m, 1H), 7.93 (d, *J* = 7.1 Hz, 2H), 7.65 (t, *J* = 6.9 Hz, 1H). MS (ESI) m/z: [M+H]⁺ calcd for C₁₅H₉N₃ 231.08; Found 231.09.

2-(4-fluorophenyl)quinazoline (Table 6; 12a4)



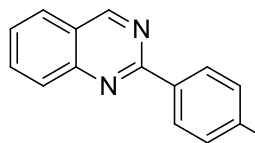
¹H NMR (500 MHz, CDCl₃) δ 7.72 (s, 1H), 7.55 (d, *J* = 3.3 Hz, 1H), 7.42 (d, *J* = 3.7 Hz, 1H), 7.40 (d, *J* = 3.6 Hz, 2H), 7.37 – 7.32 (m, 1H), 6.78 – 6.76 (m, 1H), 6.75 (d, *J* = 3.7 Hz, 2H). ¹³C{¹H} NMR (125 MHz, CDCl₃) δ 149.58, 135.22, 134.02, 132.39, 130.91, 128.81, 125.04, 118.03, 117.61, 115.14, 96.08. MS (ESI) m/z: [M+H]⁺ calcd for C₁₄H₉FN₂ 224.07; Found 224.08.

2-(thiophen-2-yl)quinazoline (Table 6; 12a7)



^1H NMR (500 MHz, CDCl_3) δ 9.37 (s, 1H), 8.19 (d, $J = 3.1$ Hz, 1H), 8.04 (d, $J = 8.7$ Hz, 1H), 7.93 – 7.86 (m, 2H), 7.59 (t, $J = 7.3$ Hz, 1H), 7.55 (d, $J = 4.4$ Hz, 1H), 7.25 – 7.19 (m, 1H). $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, CDCl_3) δ 160.54, 157.83, 150.59, 143.81, 134.37, 129.97, 129.26, 128.39, 128.16, 127.27, 127.00, 123.35. MS (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{12}\text{H}_8\text{N}_2\text{S}$ 212.04; Found 212.09.

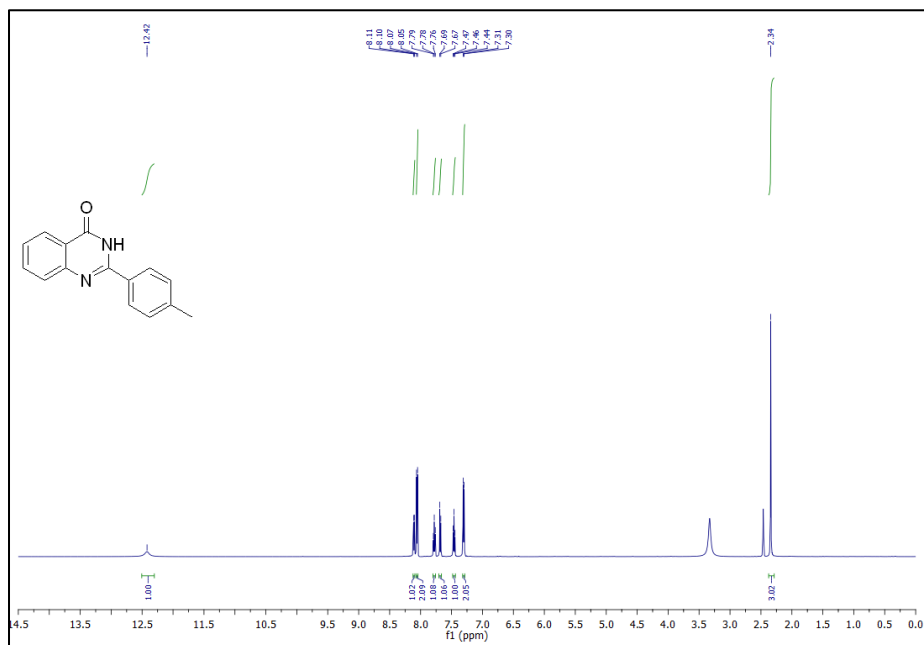
2-(4-Bromophenyl)quinazoline (Table 6; 12a8)



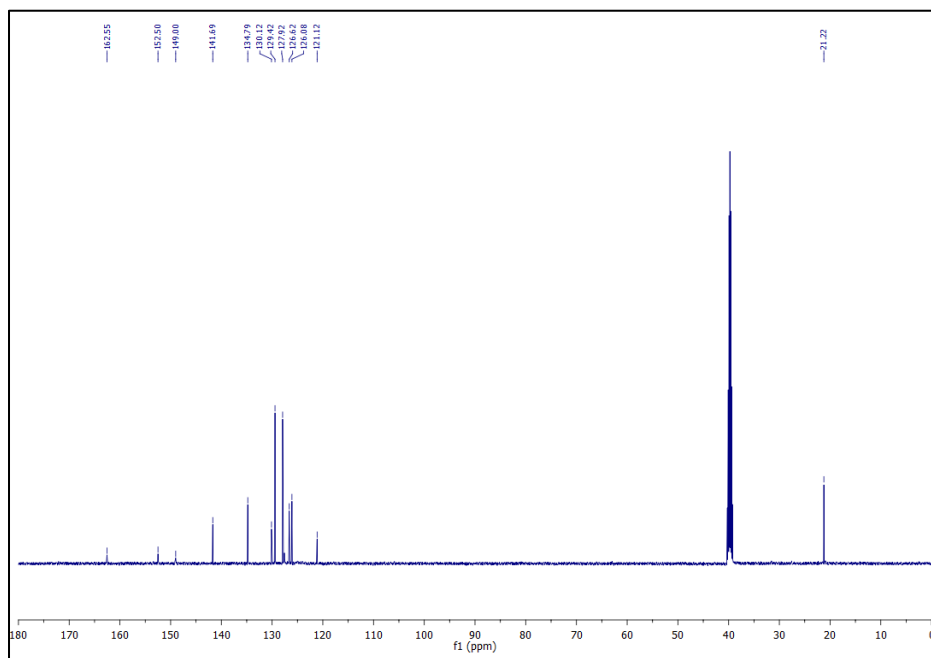
^1H NMR (500 MHz, CDCl_3) δ 9.48 (s, 1H), 8.54 (d, $J = 8.3$ Hz, 1H), 8.11 (d, $J = 8.4$ Hz, 1H), 7.95 (t, $J = 8.9$ Hz, 2H), 7.67 (dd, $J = 18.7, 7.9$ Hz, 4H). $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, CDCl_3) δ 160.51, 160.10, 150.68, 136.93, 134.27, 131.78, 130.16, 128.59, 127.48, 127.14, 125.42, 123.65. (ESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{14}\text{H}_9\text{BrN}_2$ 283.99; Found 283.89.

5) Copies of ^1H NMR and $^{13}\text{C}\{^1\text{H}\}$ NMR of the products

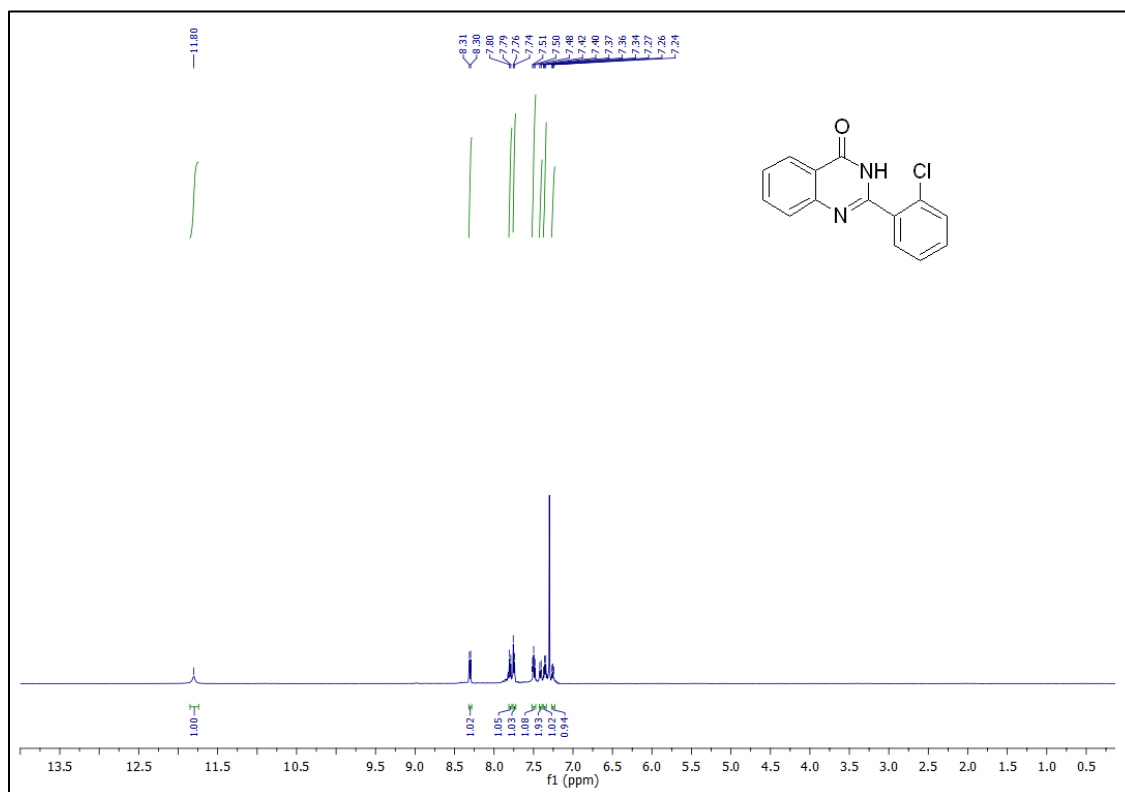
^1H spectrum of 2-(p-tolyl)quinazolin-4(3H)-one (6a1) (DMSO- d_6 , 500 MHz)



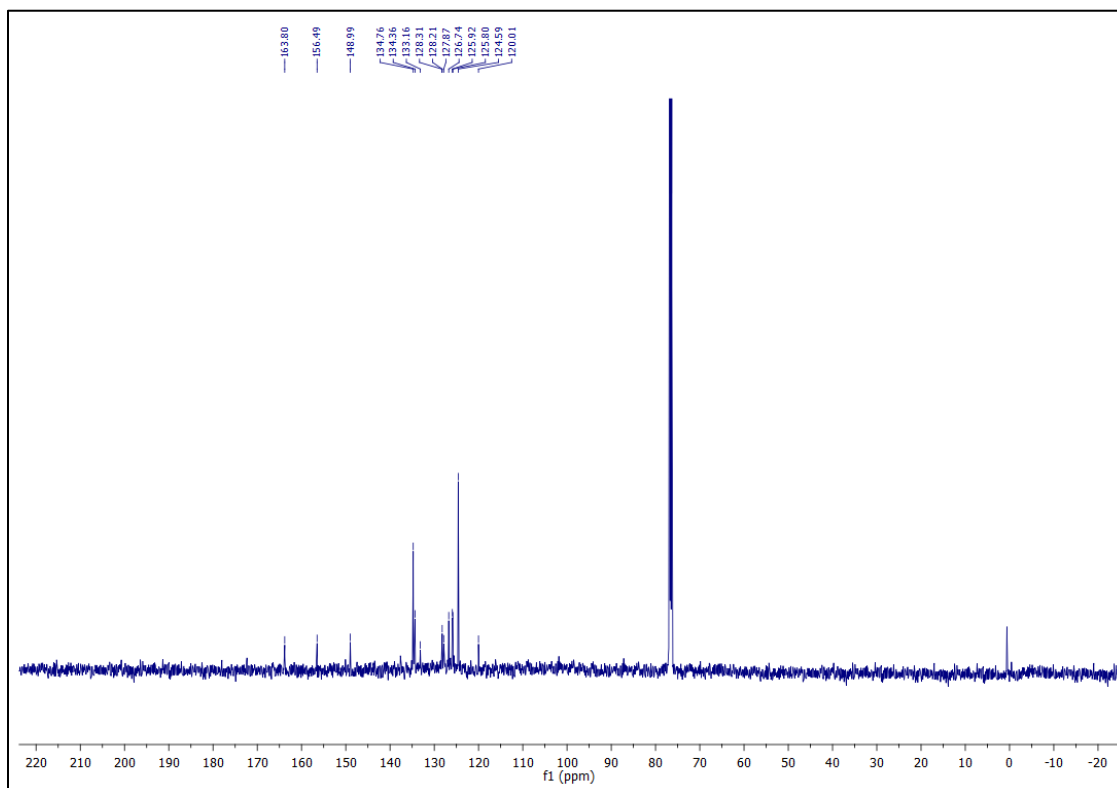
$^{13}\text{C}\{^1\text{H}\}$ spectrum of 2-(p-tolyl)quinazolin-4(3H)-one (6a1) (DMSO-d6, 125 MHz)



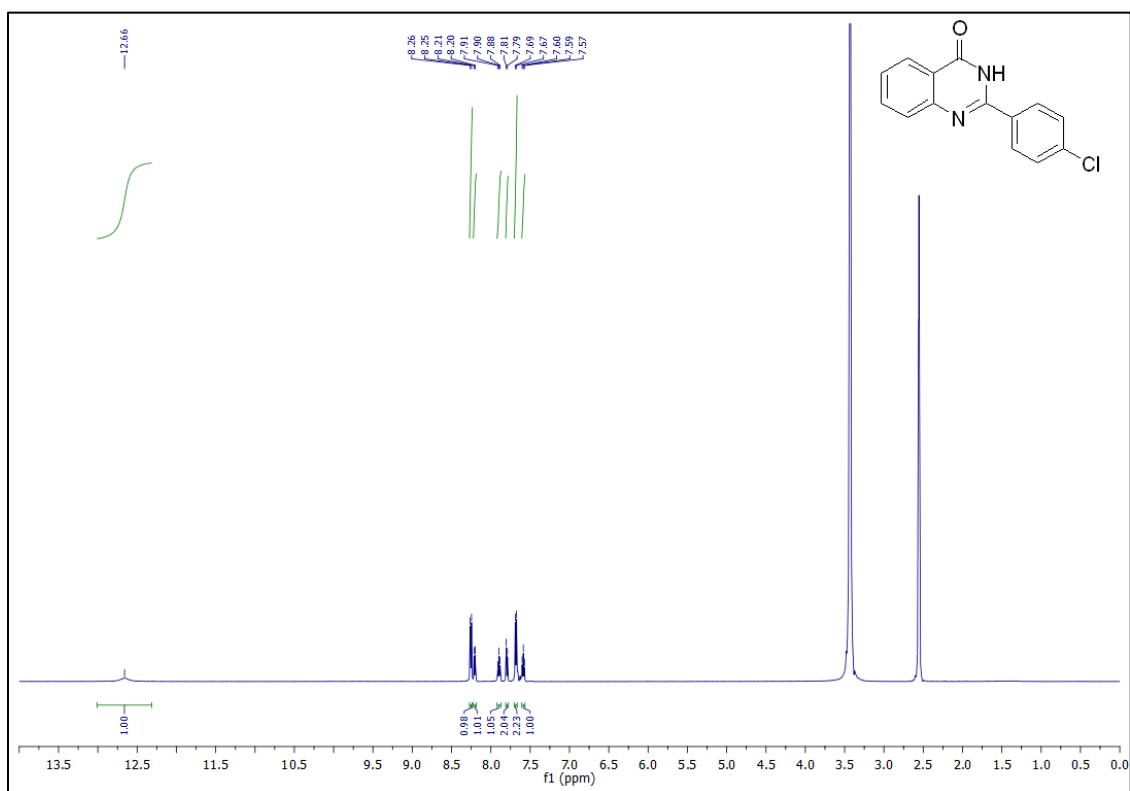
^1H spectrum of 2-(2-chlorophenyl)quinazolin-4(3H)-one (6a2) (CDCl_3 , 500 MHz)



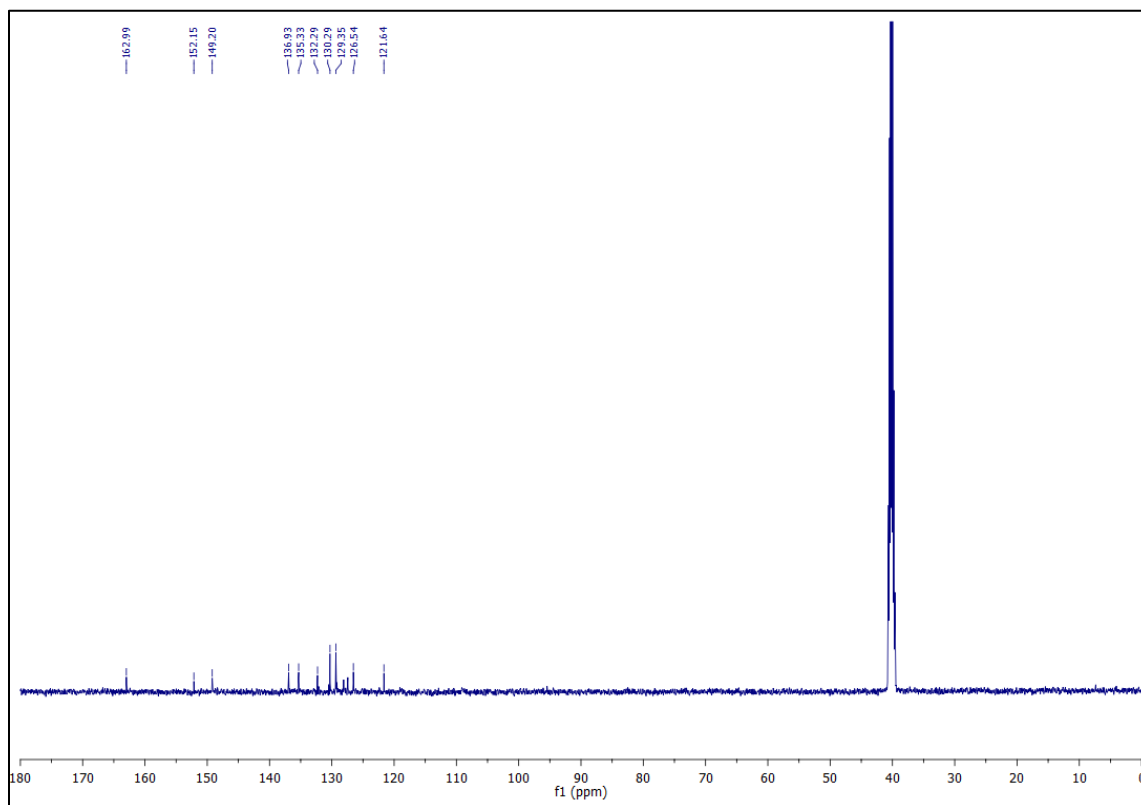
$^{13}\text{C}\{^1\text{H}\}$ spectrum of 2-(2-chlorophenyl)quinazolin-4(3H)-one (6a2) (CDCl_3 , 125 MHz)



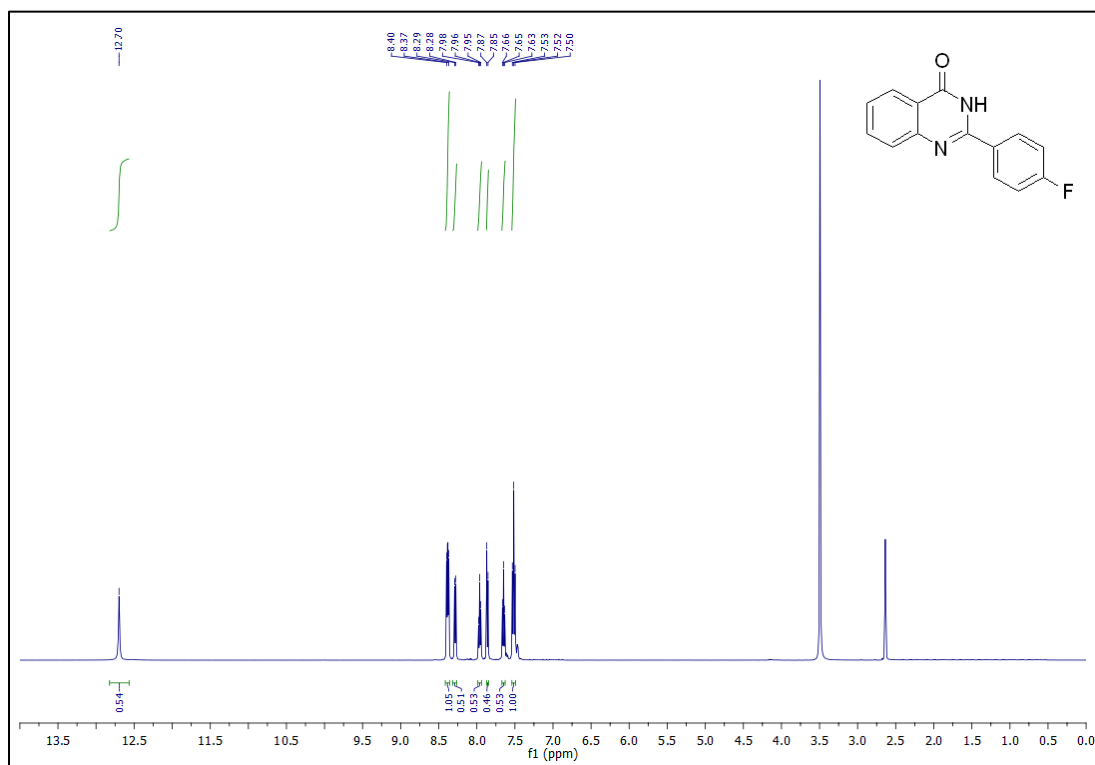
^1H spectrum 2-(4-chlorophenyl)quinazolin-4(3H)-one (6a3) (DMSO-d_6 , 500 MHz)



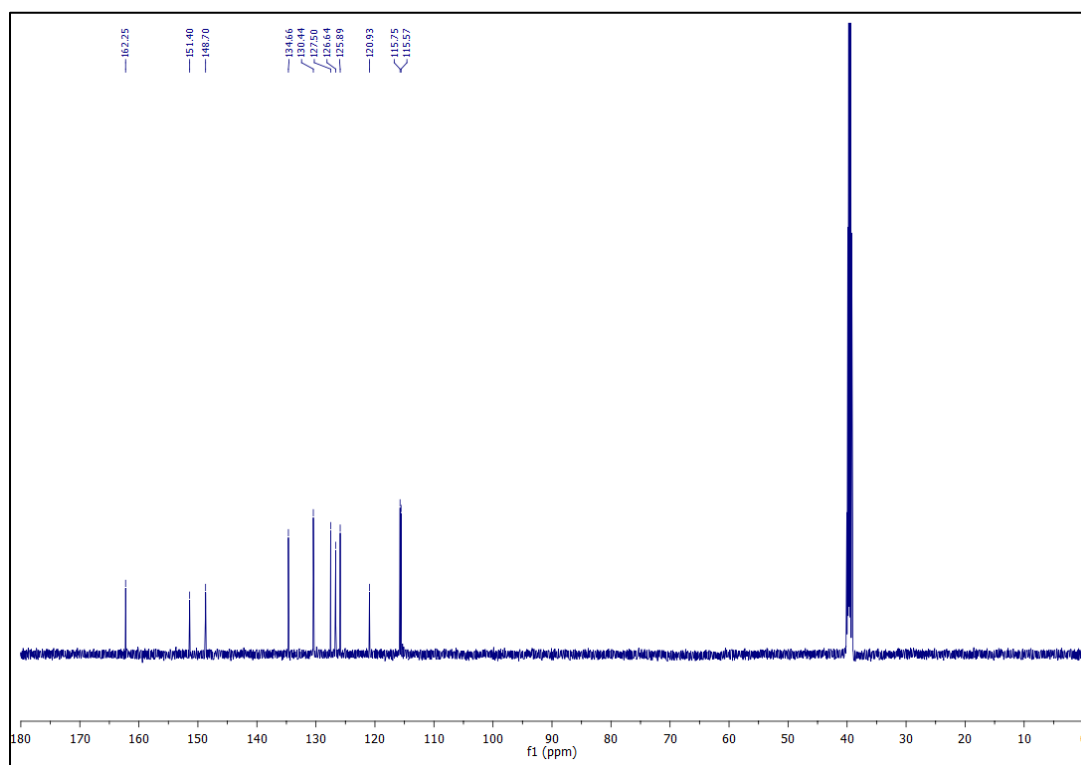
$^{13}\text{C}\{^1\text{H}\}$ spectrum 2-(4-chlorophenyl) quinazolin-4(3H)-one (6a3) (DMSO-d₆, 125 MHz)



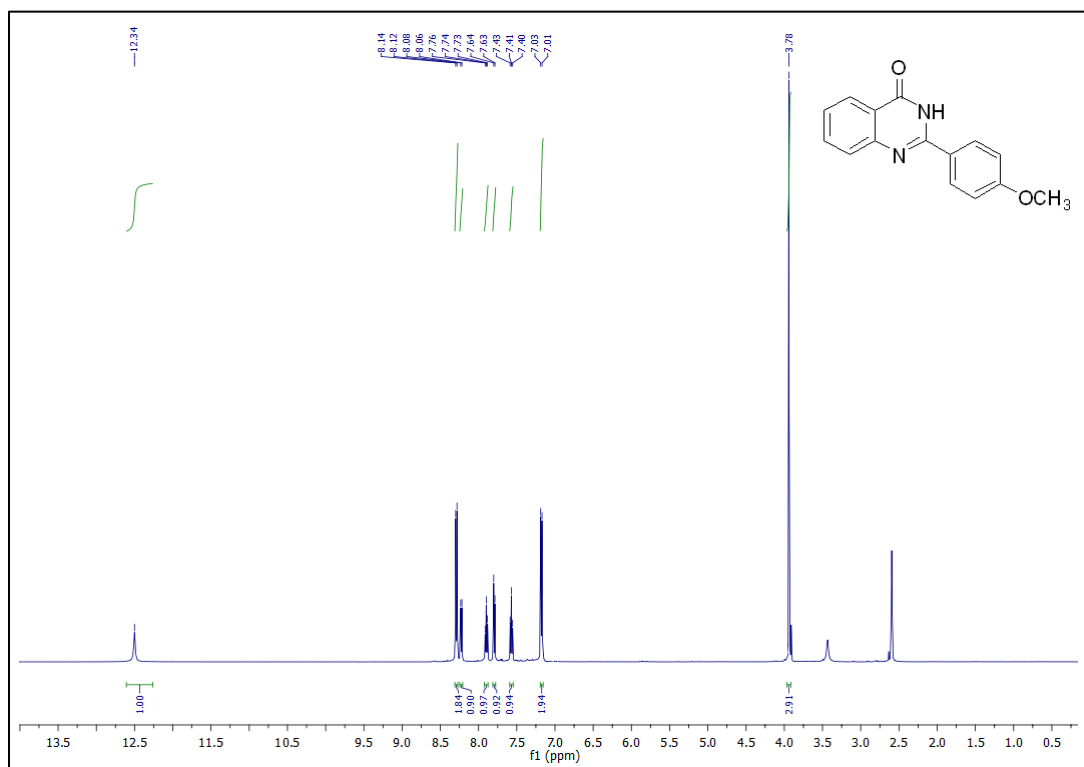
^1H spectrum 2-(4-fluorophenyl)quinazolin-4(3H)-one (6a4) (DMSO-d₆, 500 MHz)



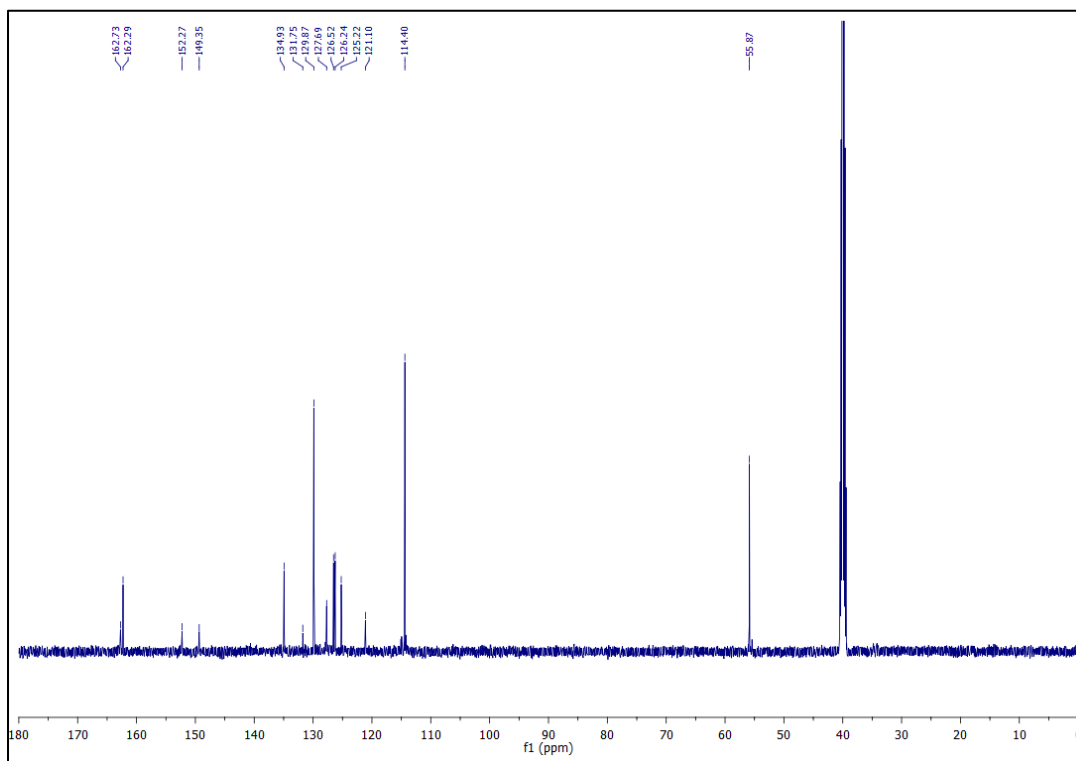
$^{13}\text{C}\{^1\text{H}\}$ spectrum 2-(4-fluorophenyl)quinazolin-4(3H)-one (6a4) (DMSO- d_6 , 125 MHz)



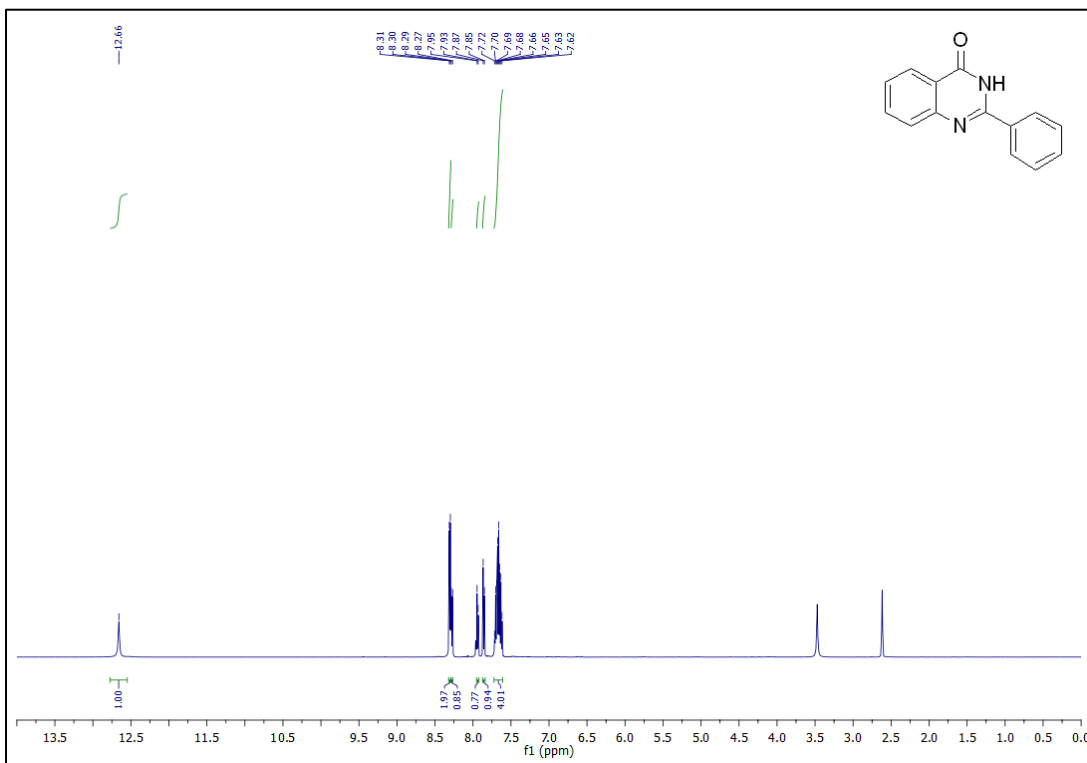
^1H spectrum 2-(4-methoxyphenyl)quinazolin-4(3H)-one(6a5) (DMSO- d_6 , 500 MHz)



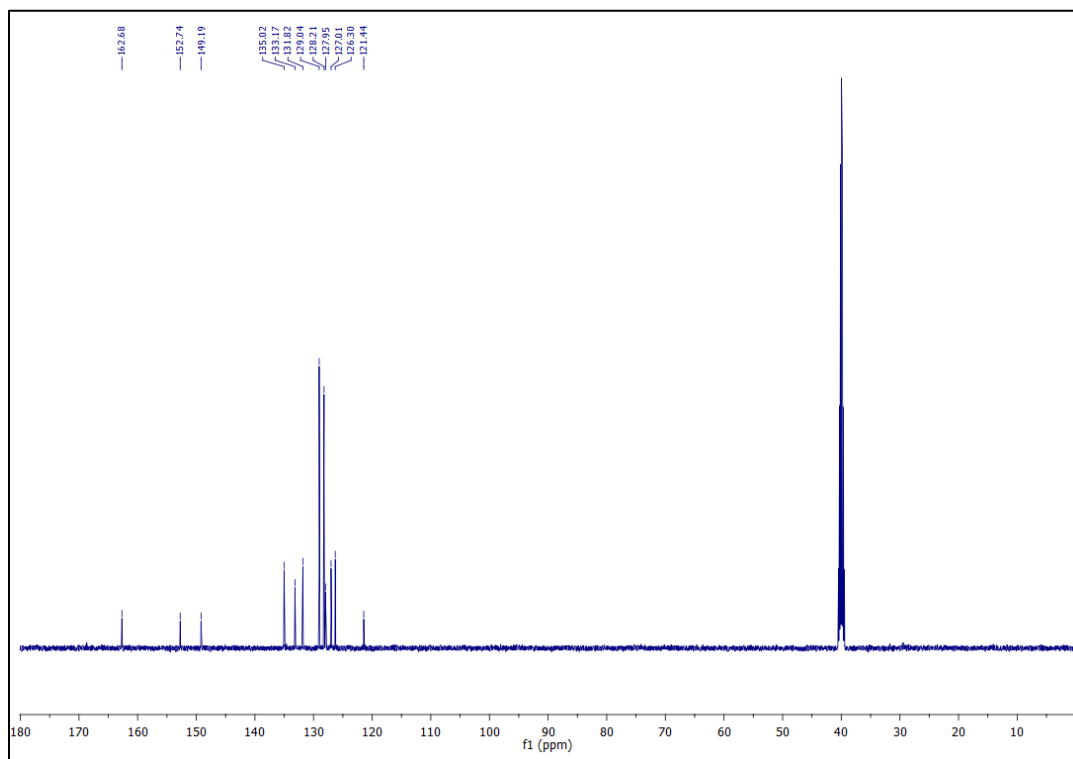
$^{13}\text{C}\{^1\text{H}\}$ spectrum 2-(4-methoxyphenyl)quinazolin-4(3H)-one(6a5) (DMSO-d6, 125 MHz)



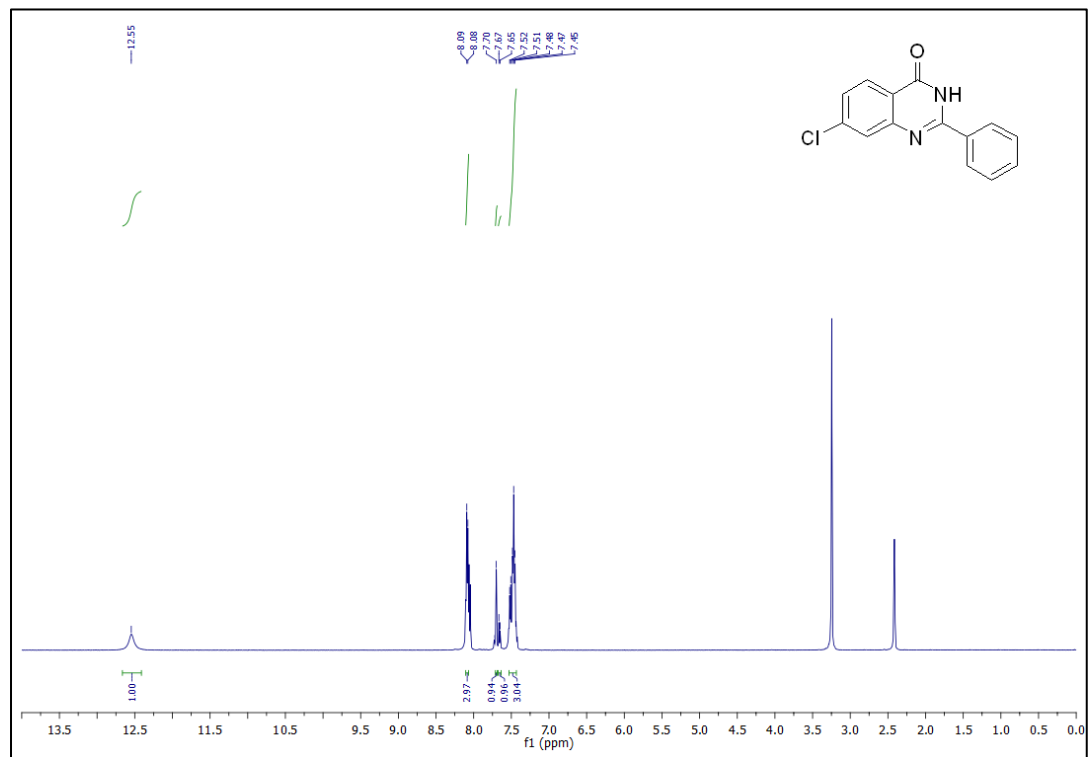
^1H spectrum 2-phenylquinazolin-4(3H)-one (6a6) (DMSO-d6, 500 MHz)



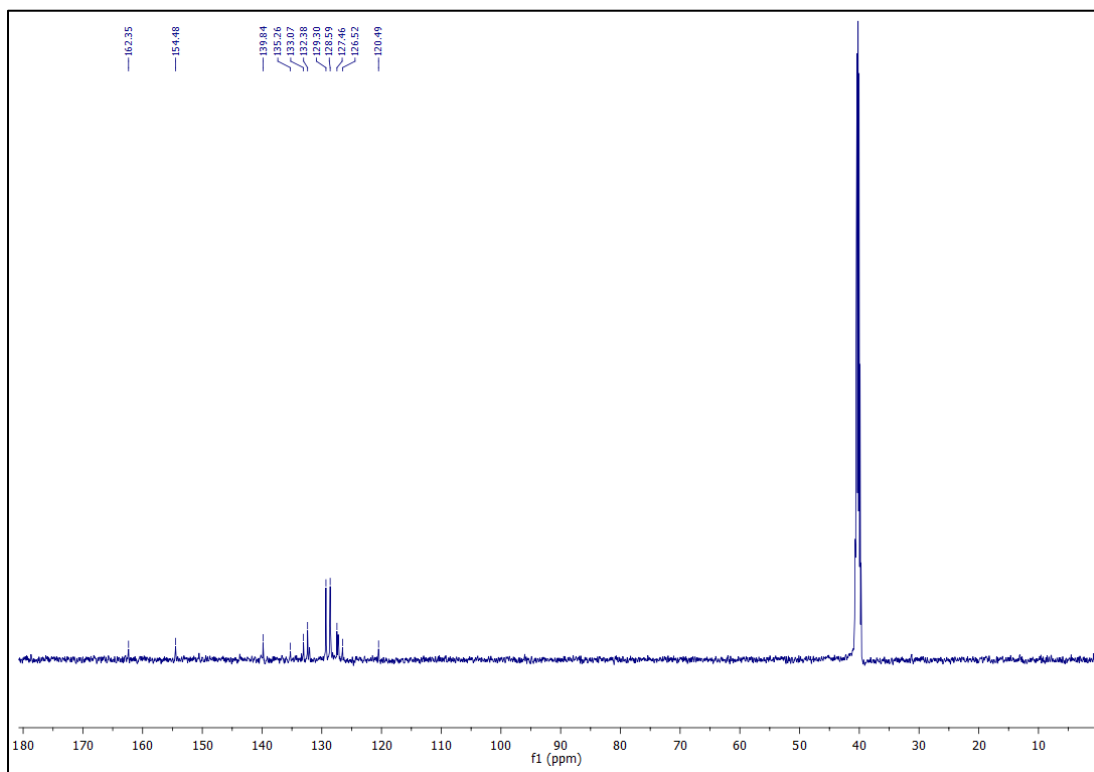
$^{13}\text{C}\{^1\text{H}\}$ spectrum 2-phenylquinazolin-4(3H)-one (6a6) (DMSO-d₆, 125 MHz)



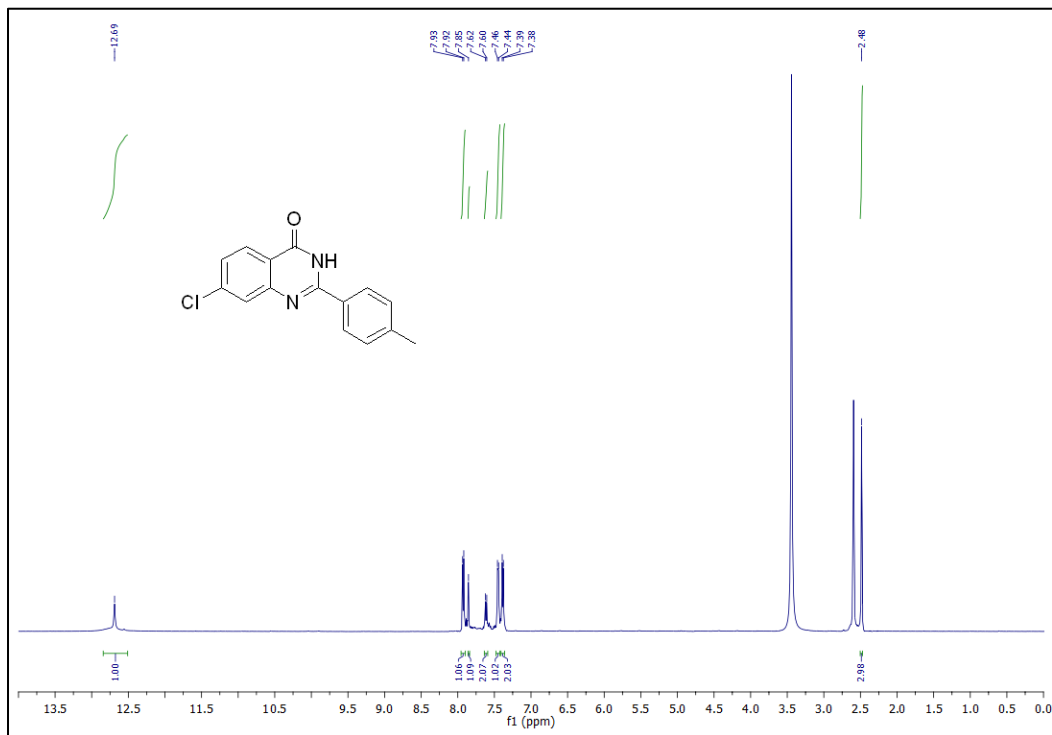
^1H spectrum 7-chloro-2-phenylquinazolin-4(3H)-one (6a7) (DMSO-d₆, 500 MHz)



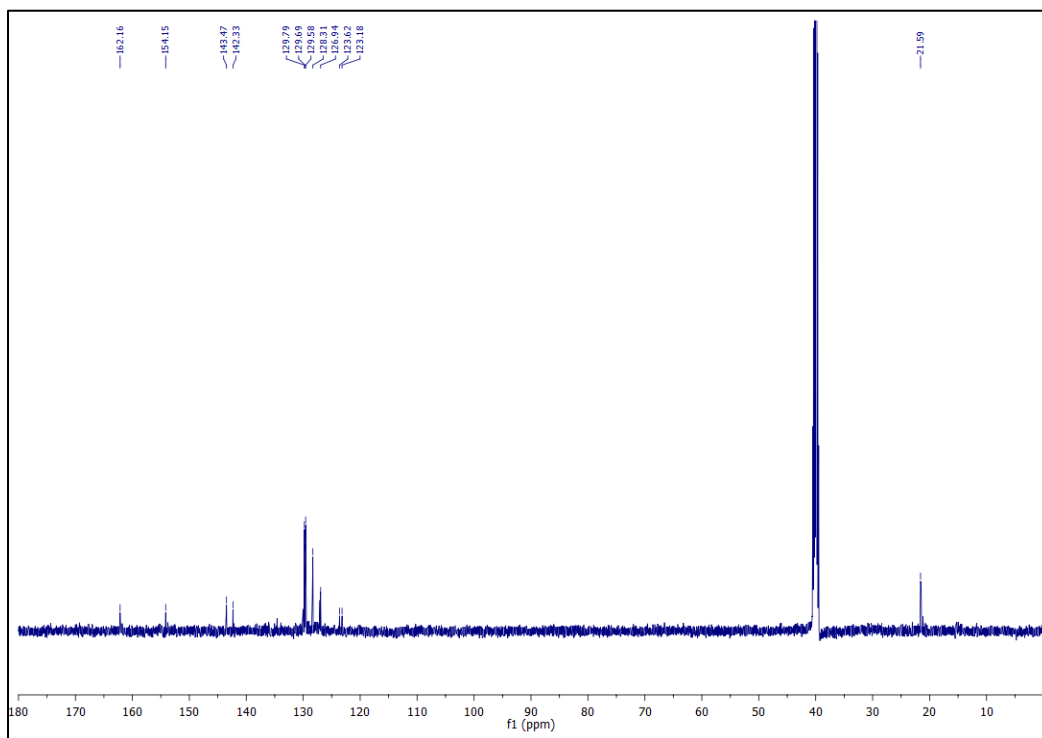
$^{13}\text{C}\{^1\text{H}\}$ spectrum 7-chloro-2-phenylquinazolin-4(3H)-one (6a7) (DMSO-d₆, 125 MHz)



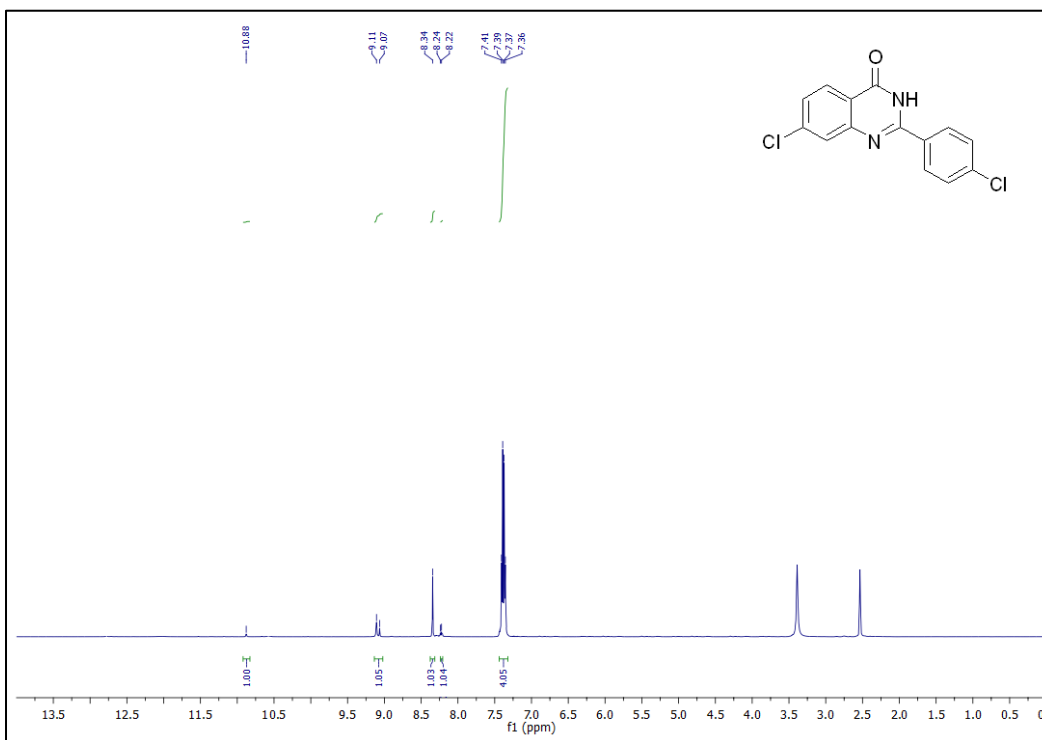
^1H spectrum 7-chloro-2-(p-tolyl)quinazolin-4(3H)-one(6a9) (DMSO-d₆, 500 MHz)



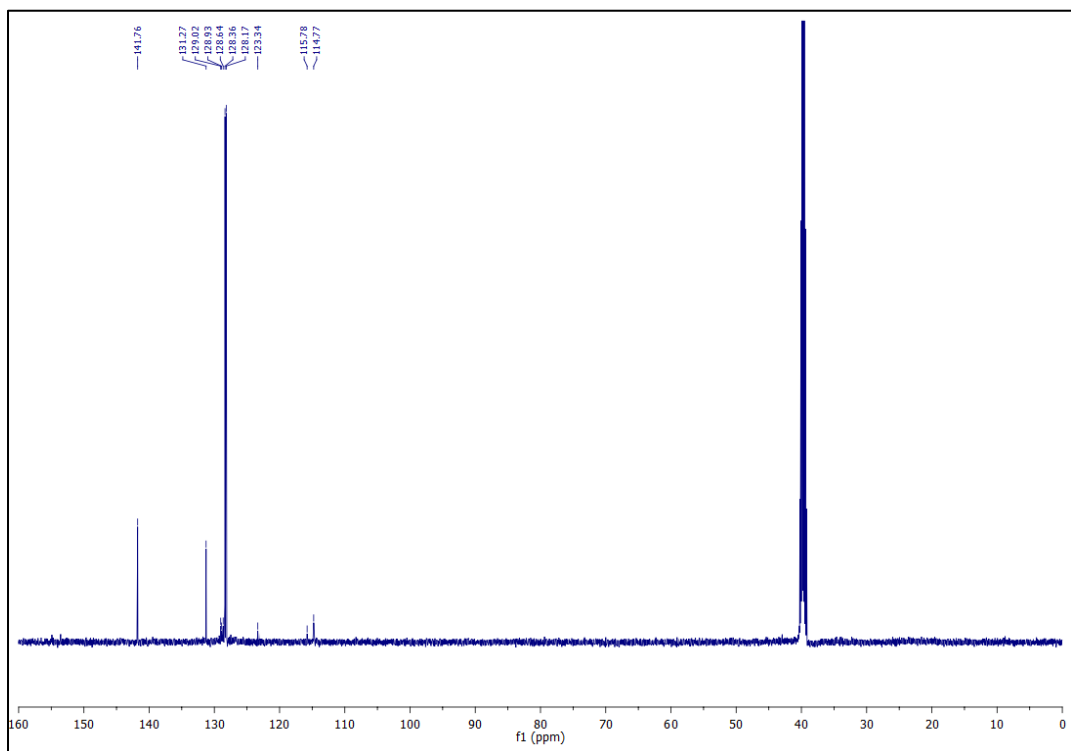
$^{13}\text{C}\{^1\text{H}\}$ spectrum 7-chloro-2-(p-tolyl)quinazolin-4(3H)-one(6a9) (DMSO-d6, 125 MHz)



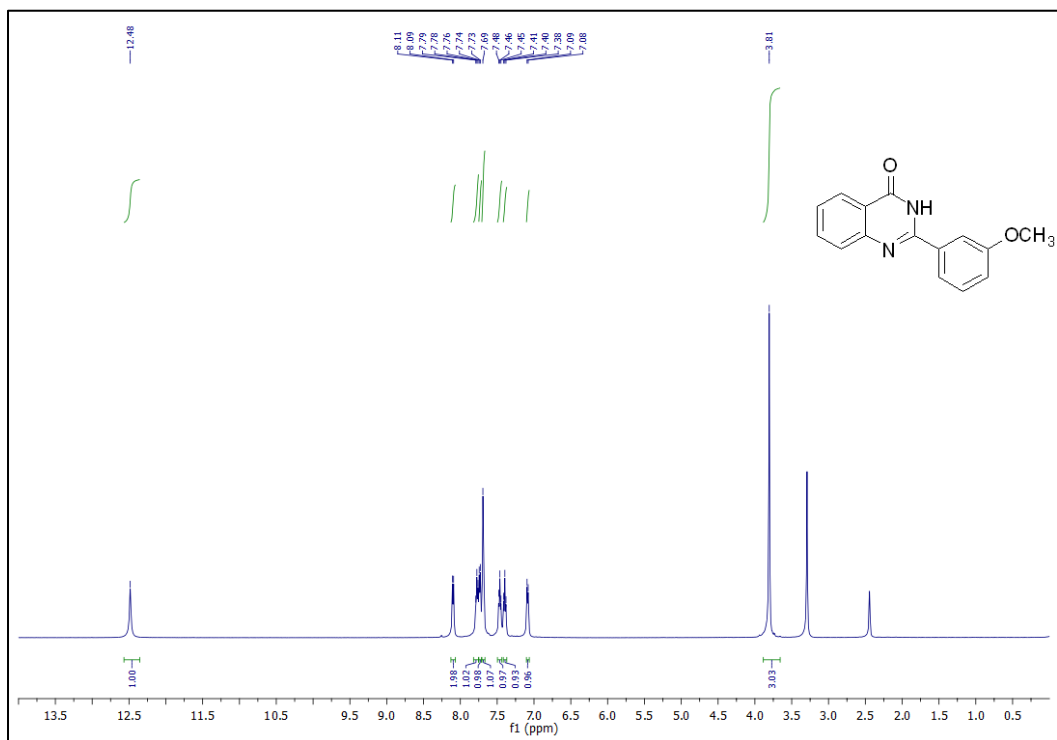
^1H spectrum 7-chloro-2-(4-chlorophenyl)quinazolin-4(3H)-one (6a10) (DMSO-d6, 500 MHz)



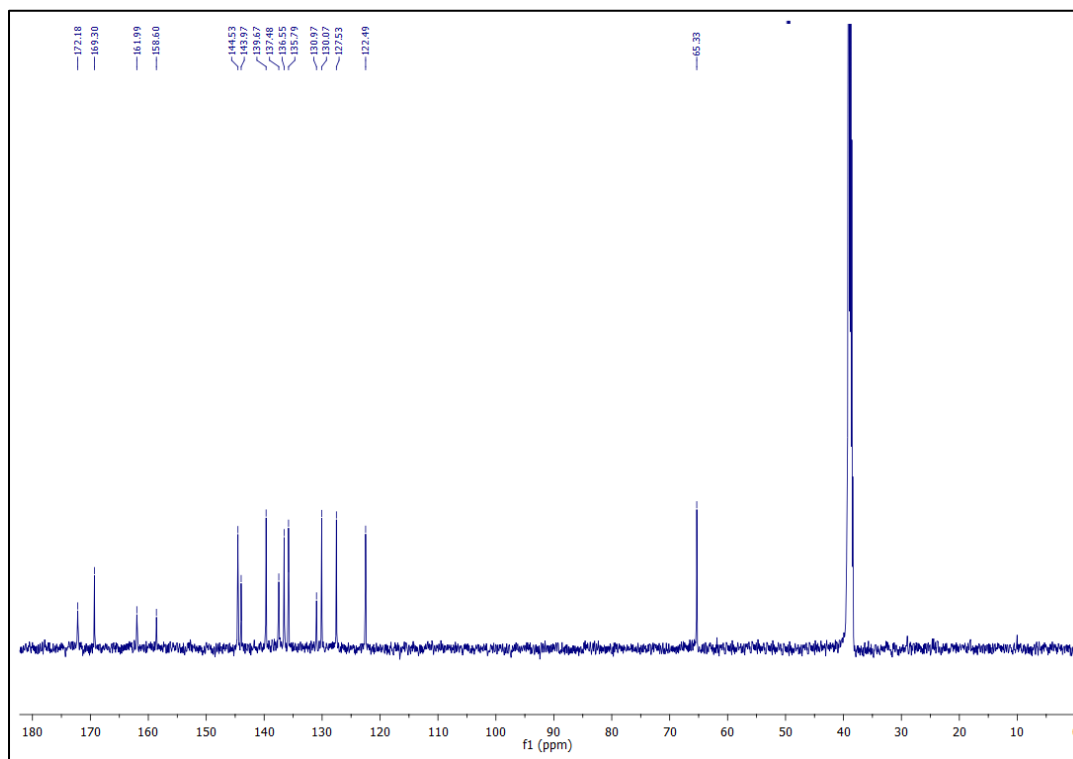
$^{13}\text{C}\{^1\text{H}\}$ spectrum 7-chloro-2-(4-chlorophenyl)quinazolin-4(3H)-one (6a10) (DMSO-d₆, 125 MHz)



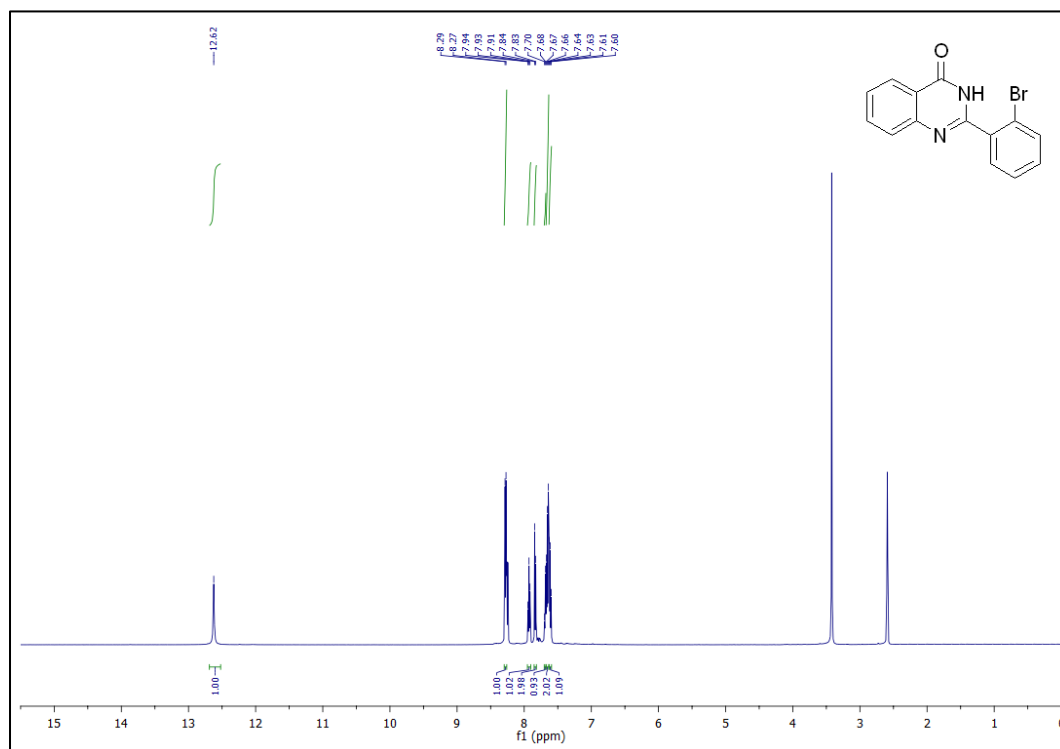
^1H spectrum 2-(3-methoxyphenyl)quinazolin-4(3H)-one (6a11) (DMSO-d₆, 500 MHz)



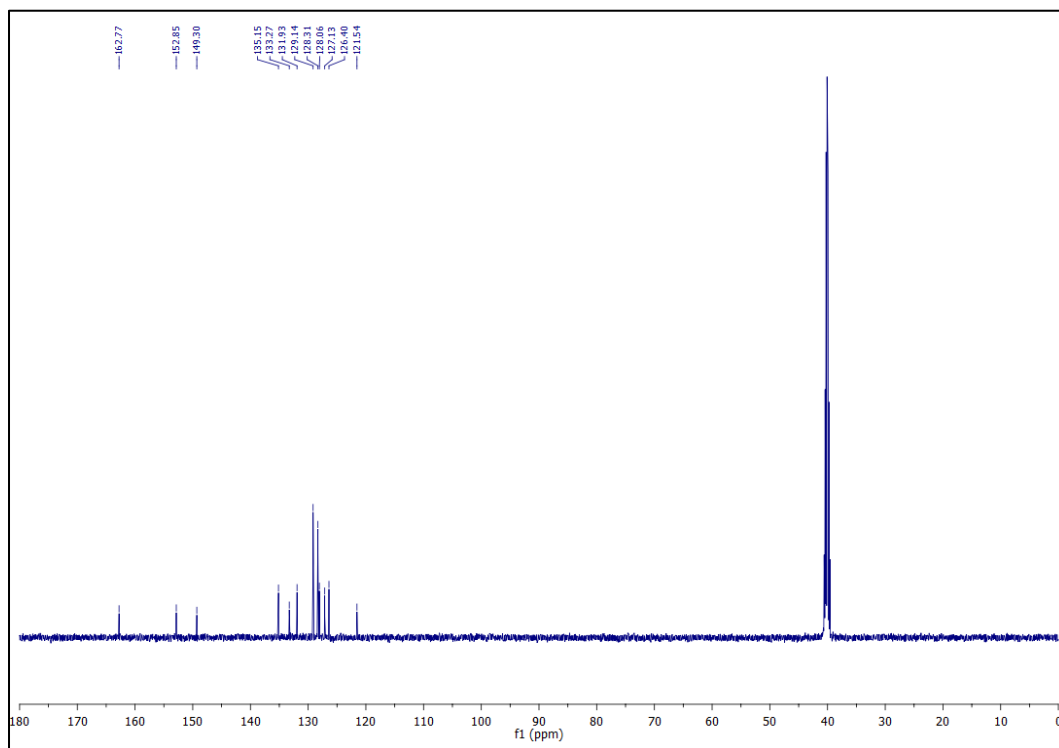
$^{13}\text{C}\{^1\text{H}\}$ spectrum 2-(3-methoxyphenyl)quinazolin-4(3H)-one (6a11) (DMSO-d₆, 125 MHz)



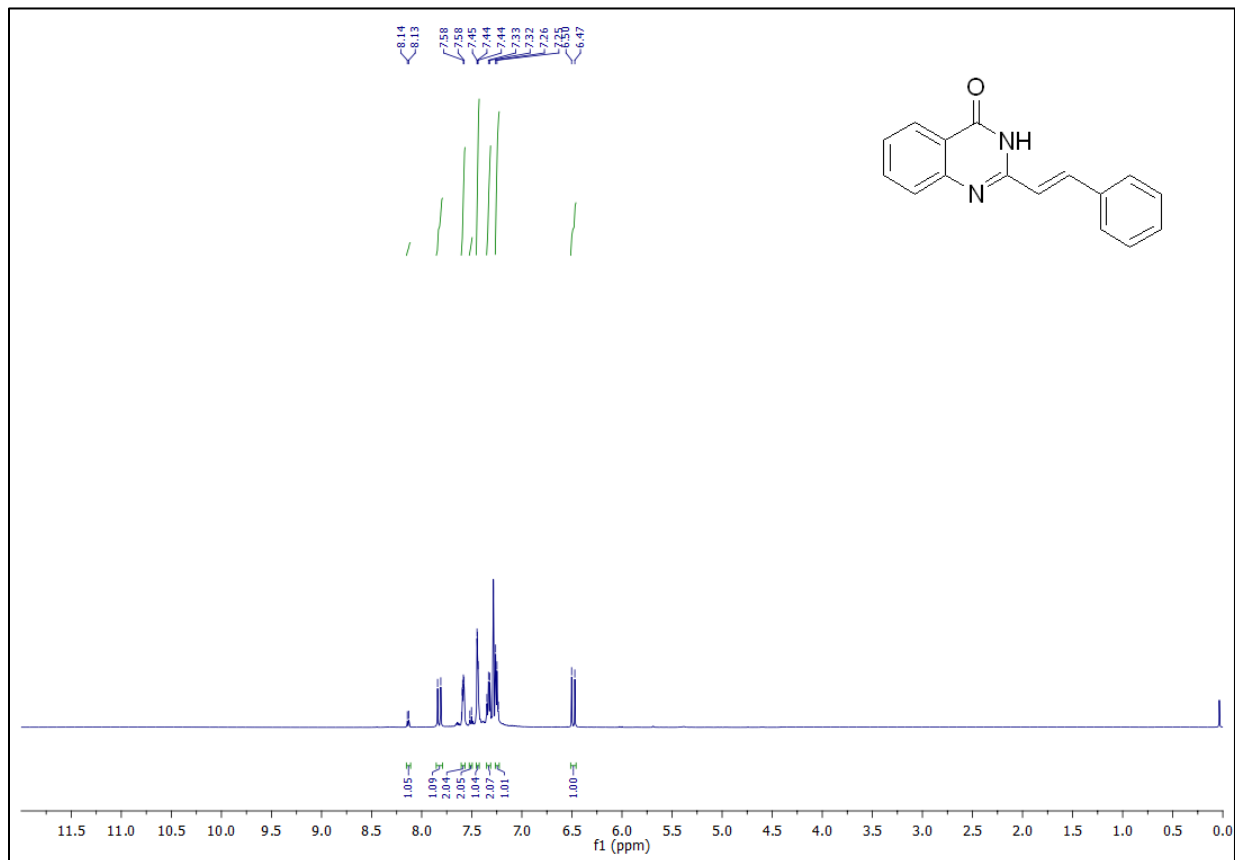
^1H spectrum 2-(2-bromophenyl)quinazolin-4(3H)-one (6a12) (DMSO-d₆, 500 MHz)



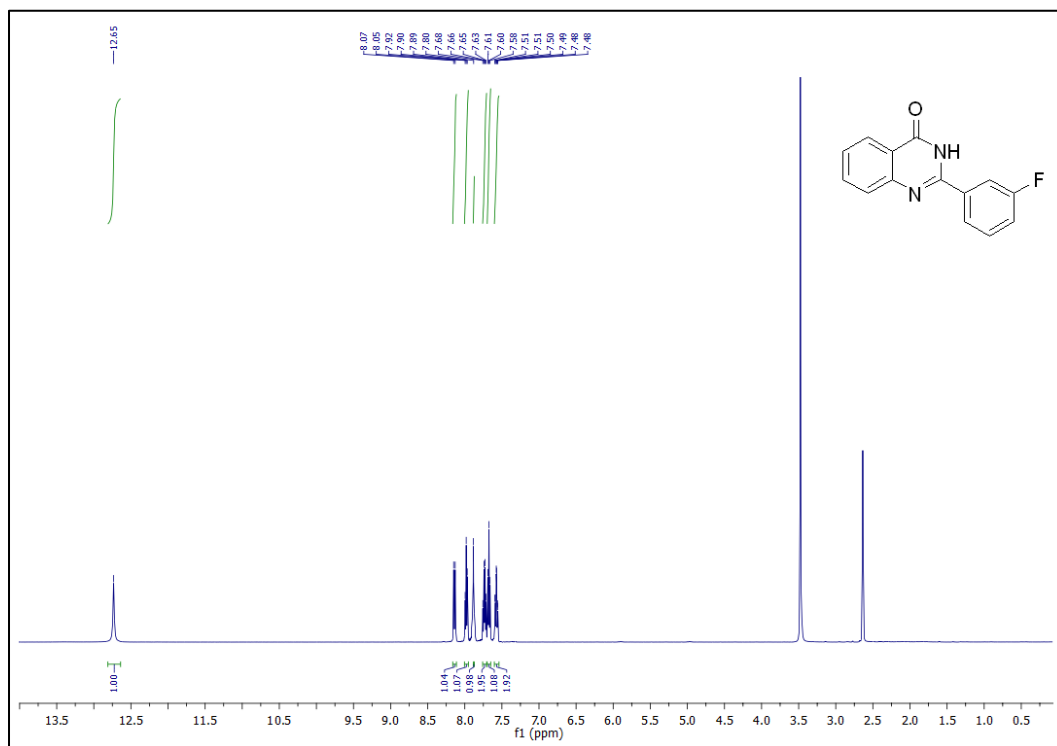
$^{13}\text{C}\{^1\text{H}\}$ spectrum 2-(2-bromophenyl)quinazolin-4(3H)-one (6a12) (DMSO-d₆, 125 MHz)



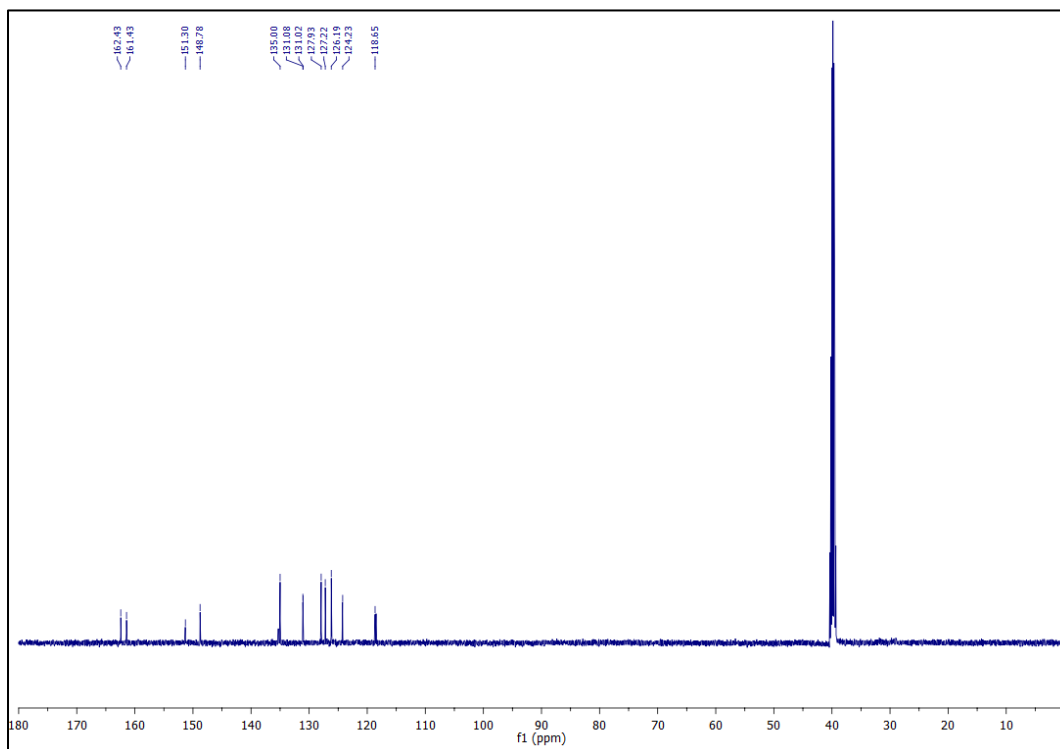
^1H spectrum (E)-2-styrylquinazolin-4(3H)-one (6a13) (CDCl₃, 500 MHz)



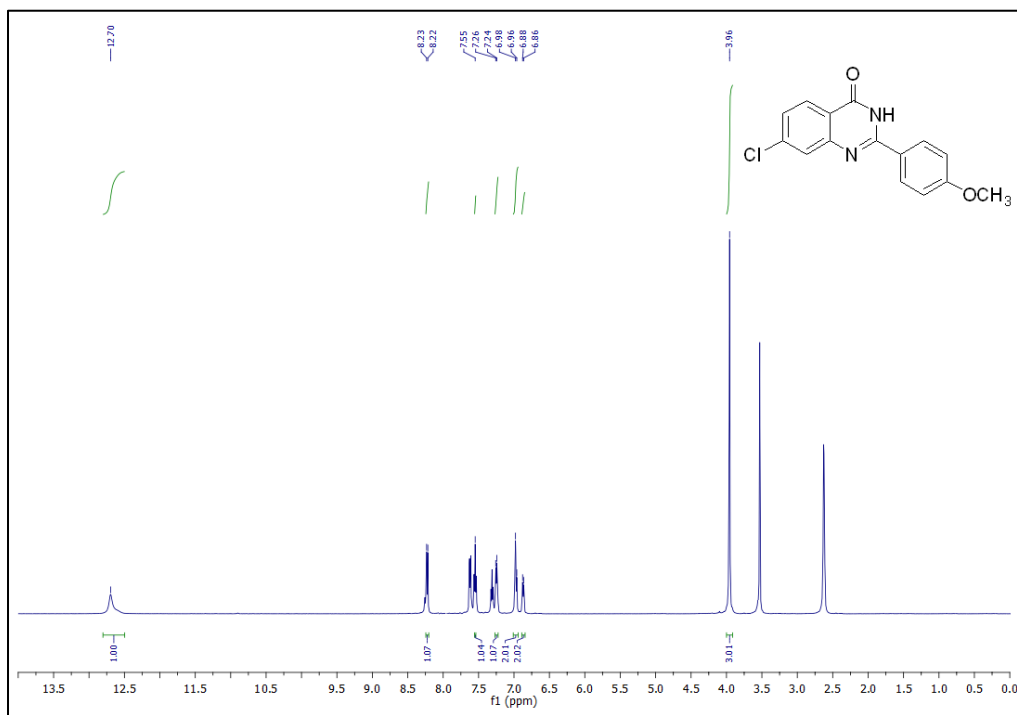
¹H spectrum 2-(3-fluorophenyl)quinazolin-4(3H)-one (6a15) (DMSO-d6, 500 MHz)



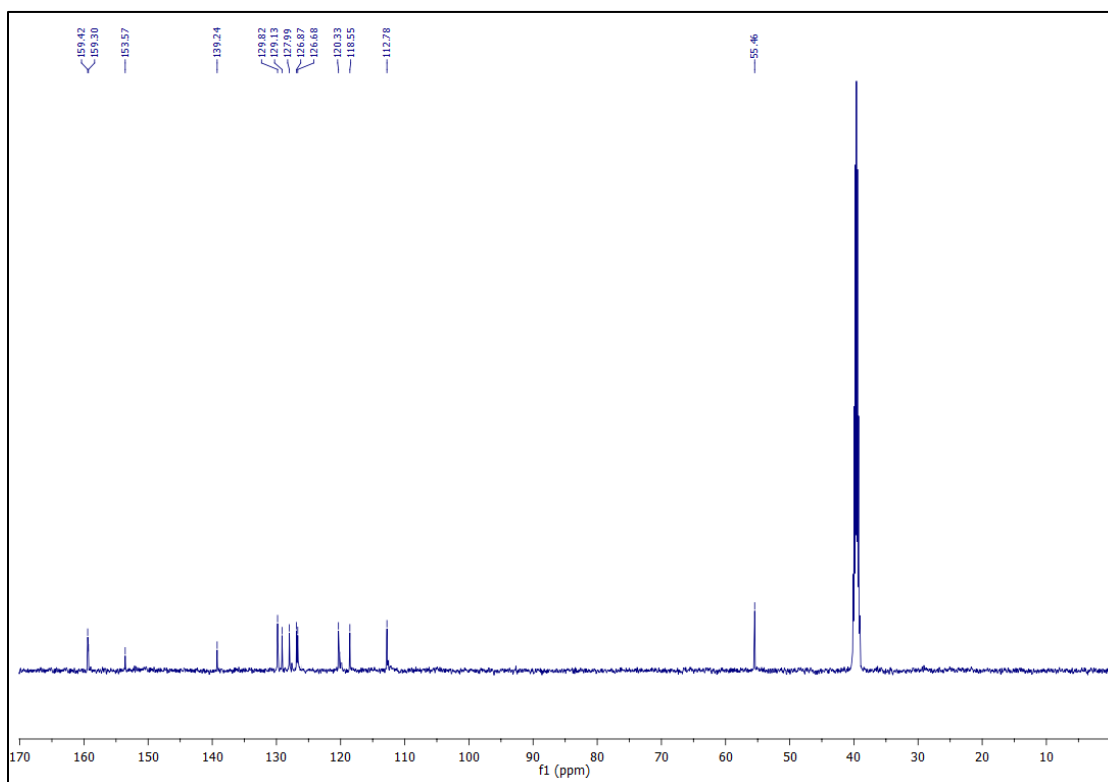
¹³C{¹H} spectrum 2-(3-fluorophenyl)quinazolin-4(3H)-one (6a15) (DMSO-d6, 125 MHz)



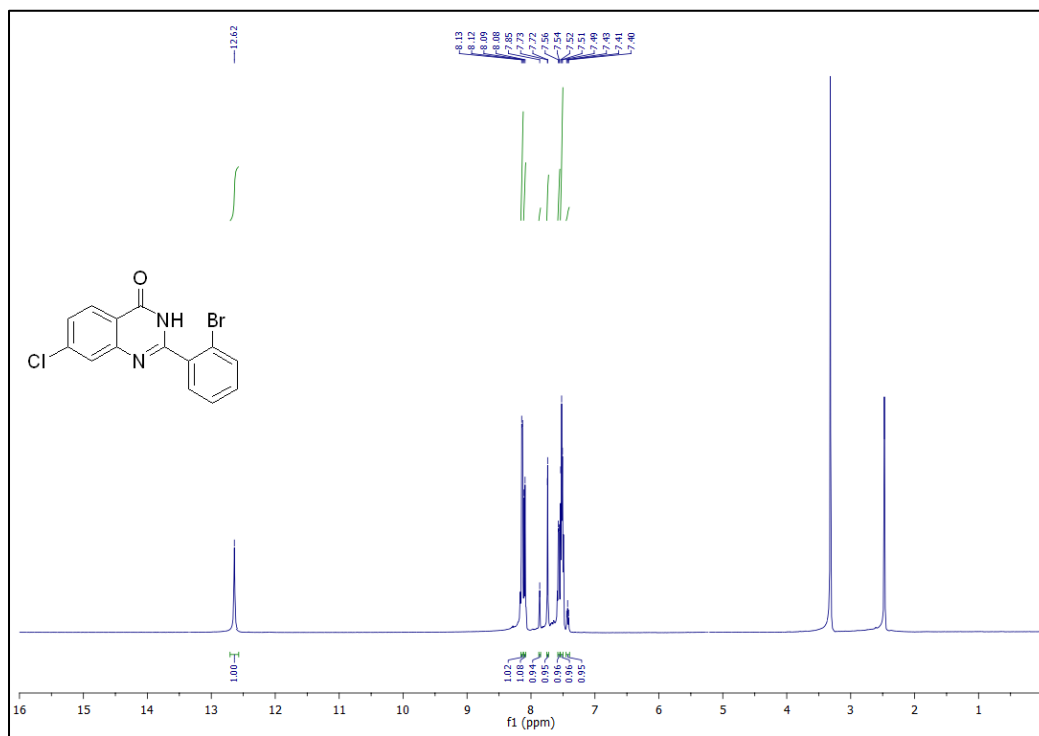
^1H spectrum 7-chloro-2-(4-methoxyphenyl)quinazolin-4(3H)-one (6a16) (DMSO- d_6 , 500 MHz)



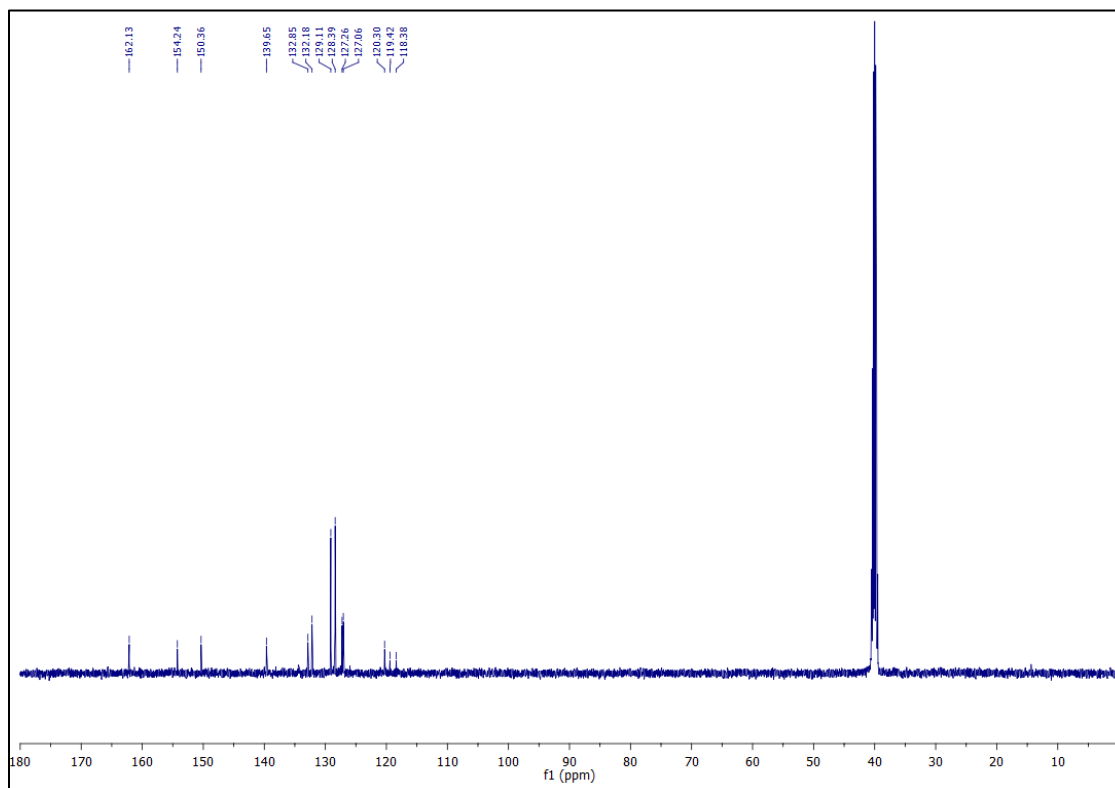
$^{13}\text{C}\{^1\text{H}\}$ spectrum 7-chloro-2-(4-methoxyphenyl)quinazolin-4(3H)-one (6a16) (DMSO- d_6 , 125 MHz)



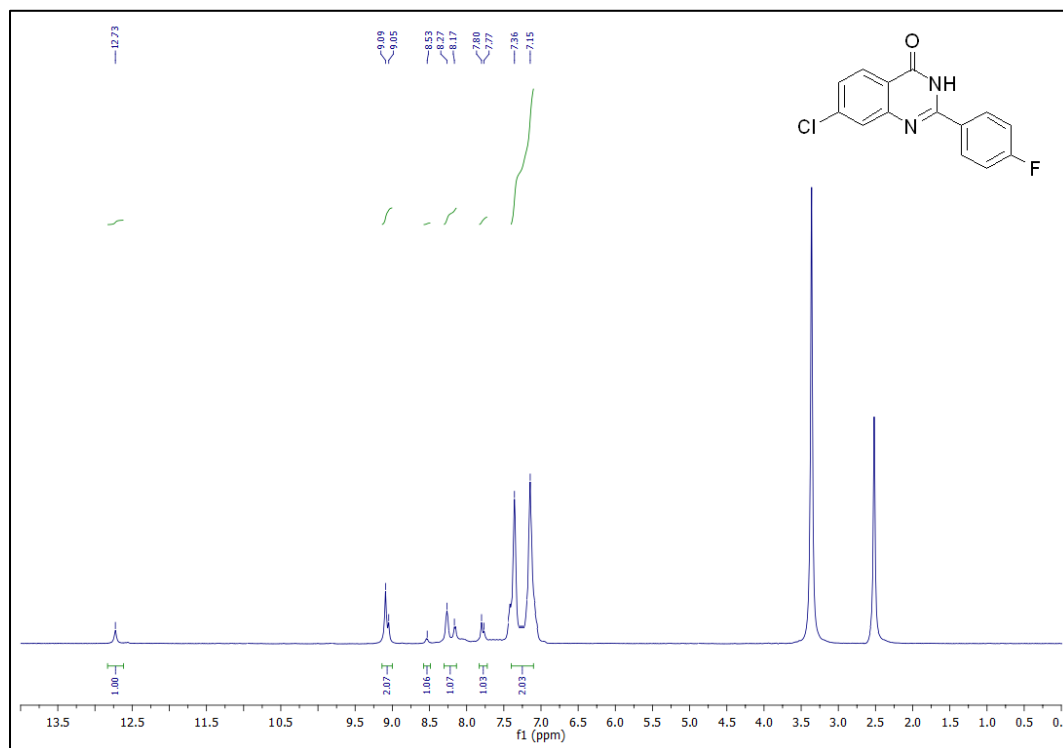
^1H spectrum 2-(2-bromophenyl)-7-chloroquinazolin-4(3H)-one (6a17) (DMSO-d₆, 500 MHz)



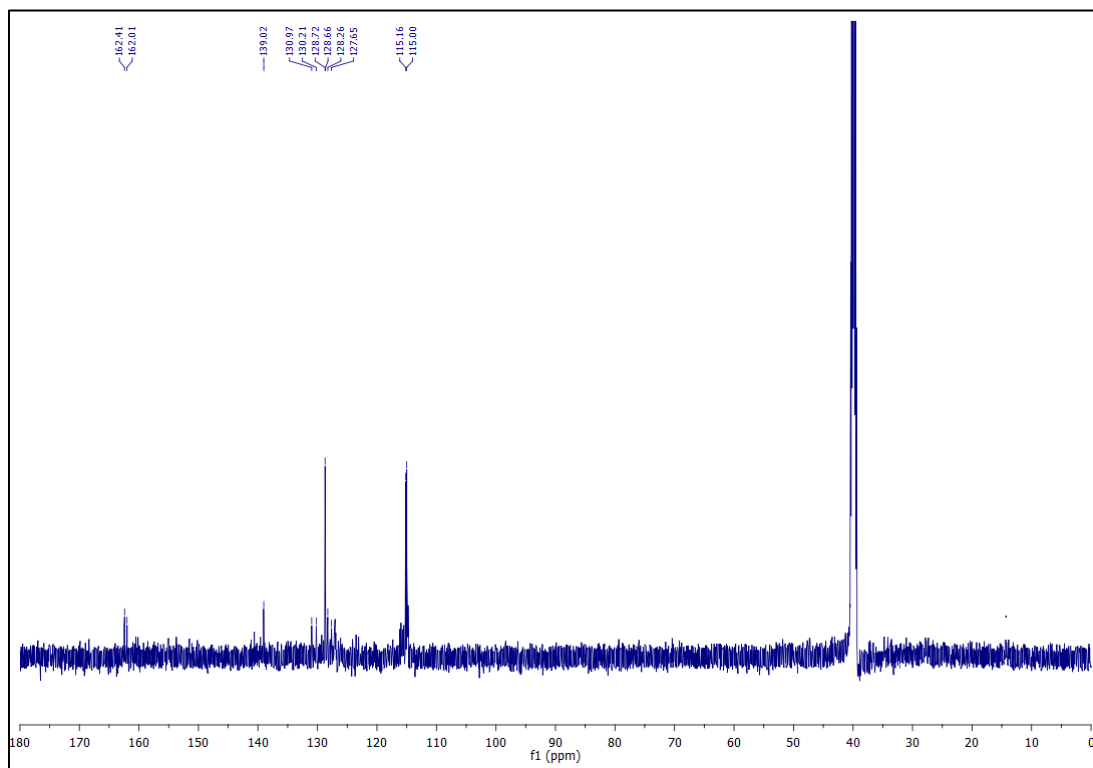
$^{13}\text{C}\{^1\text{H}\}$ spectrum 2-(2-bromophenyl)-7-chloroquinazolin-4(3H)-one (6a17) (DMSO-d₆, 125 MHz)



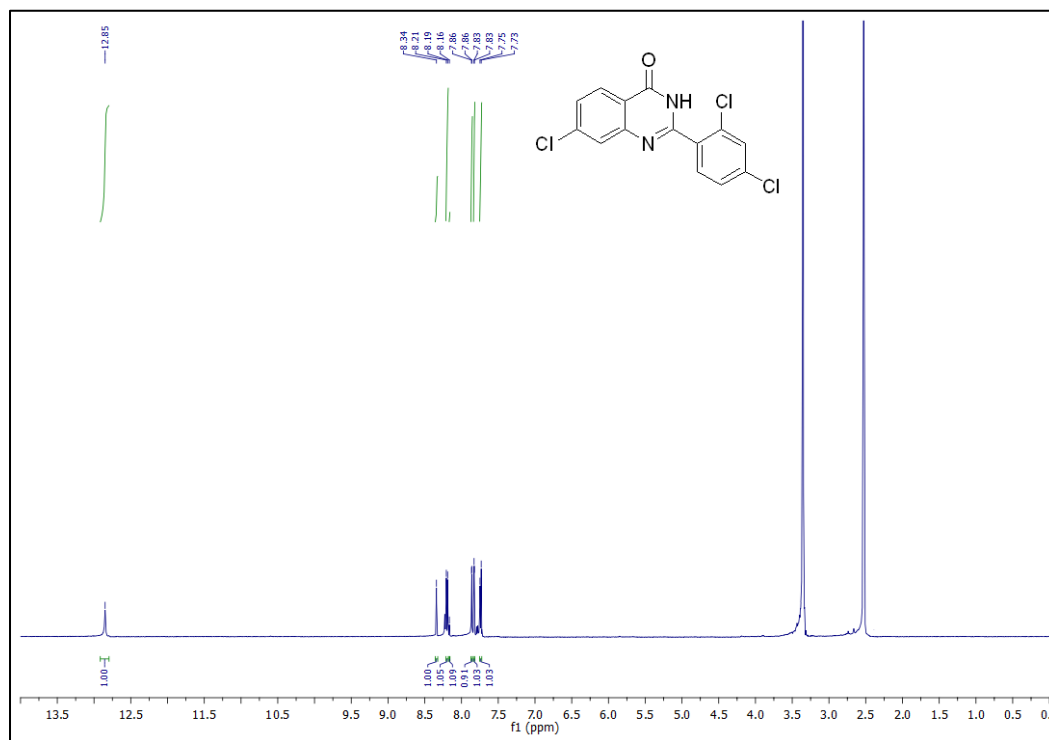
¹H spectrum 7-chloro-2-(4-fluorophenyl)quinazolin-4(3H)-one (6a18) (DMSO-d₆, 500 MHz)



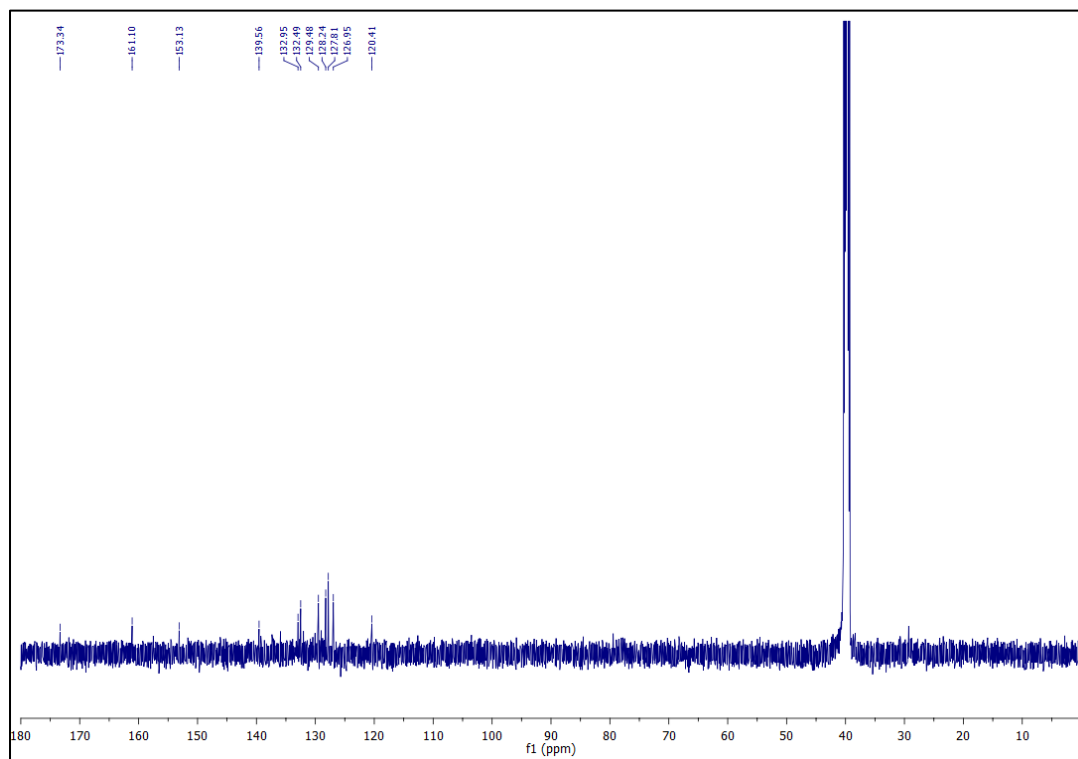
¹³C{¹H} spectrum 7-chloro-2-(4-fluorophenyl)quinazolin-4(3H)-one (6a18) (DMSO-d₆, 125 MHz)



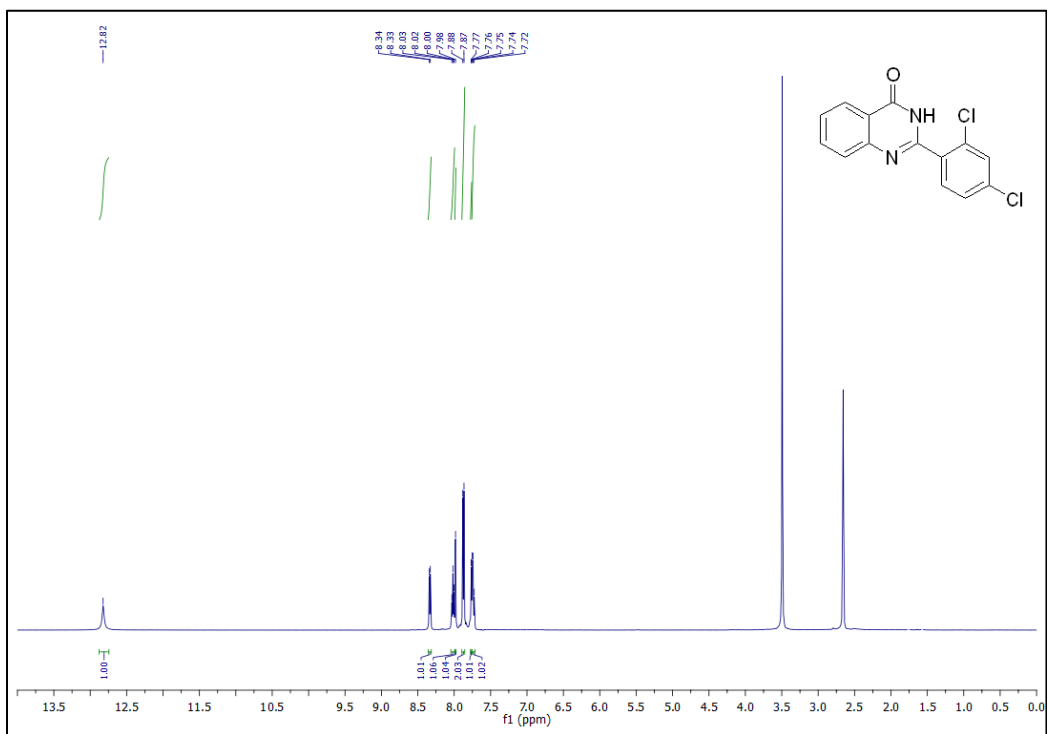
^1H spectrum 7-chloro-2-(2,4-dichlorophenyl)quinazolin-4(3H)-one (6a19) (DMSO-d₆, 500 MHz)



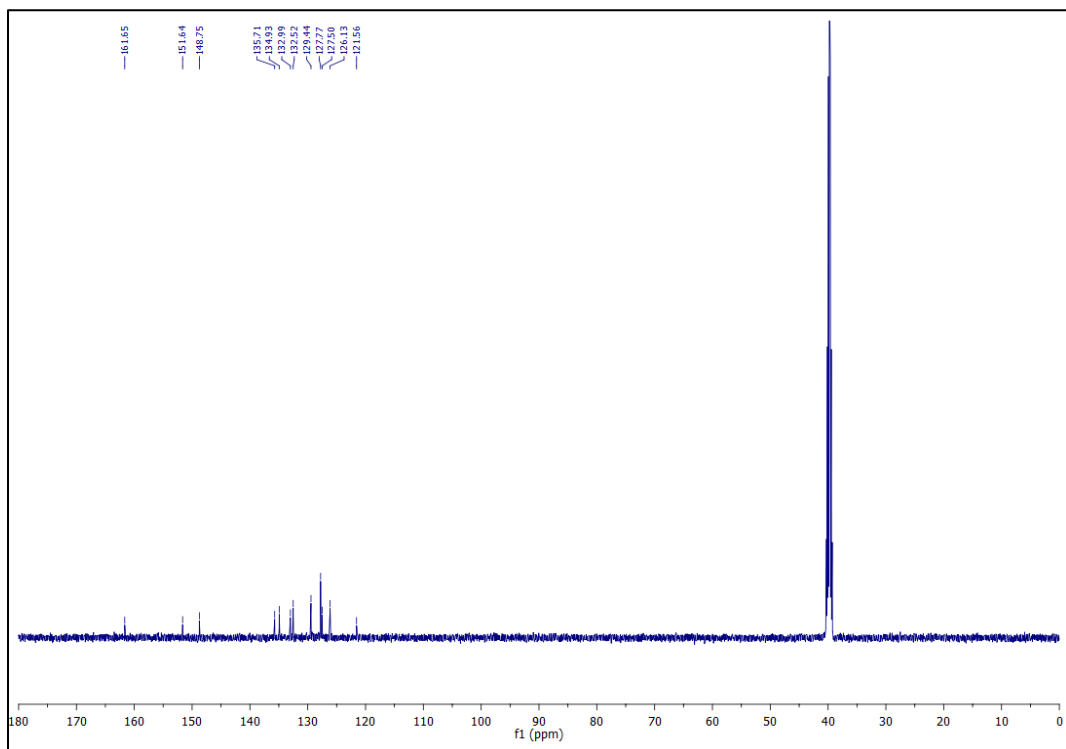
$^{13}\text{C}\{^1\text{H}\}$ spectrum 7-chloro-2-(2,4-dichlorophenyl)quinazolin-4(3H)-one (6a19) (DMSO-d₆, 125 MHz)



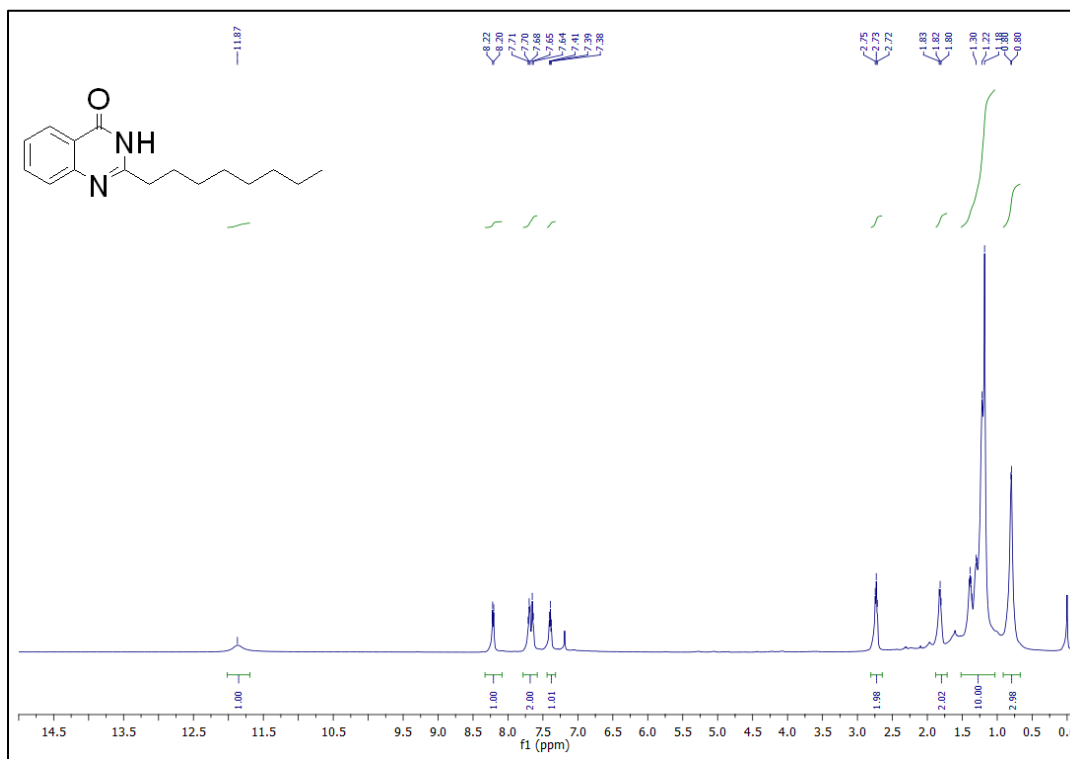
¹H spectrum 2-(2,4-dichlorophenyl)quinazolin-4(3H)-one (6a20) (DMSO-d6, 500 MHz)



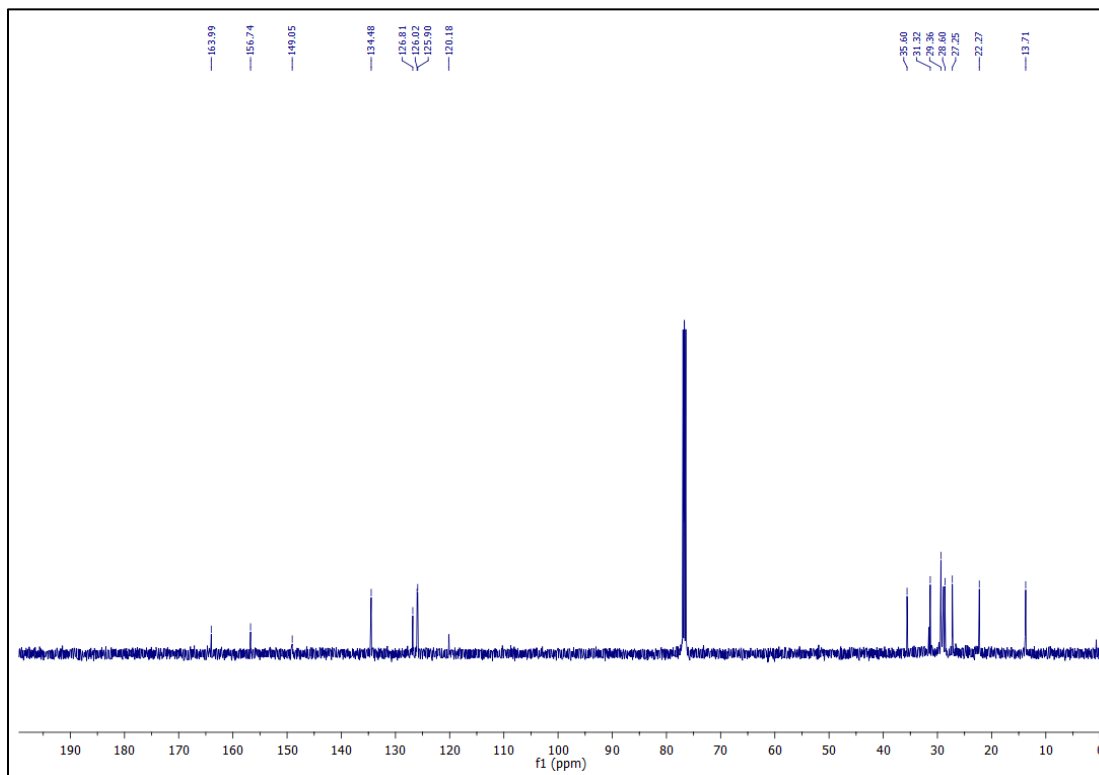
¹³C{¹H} spectrum 2-(2,4-dichlorophenyl)quinazolin-4(3H)-one (6a20) (DMSO-d6, 125 MHz)



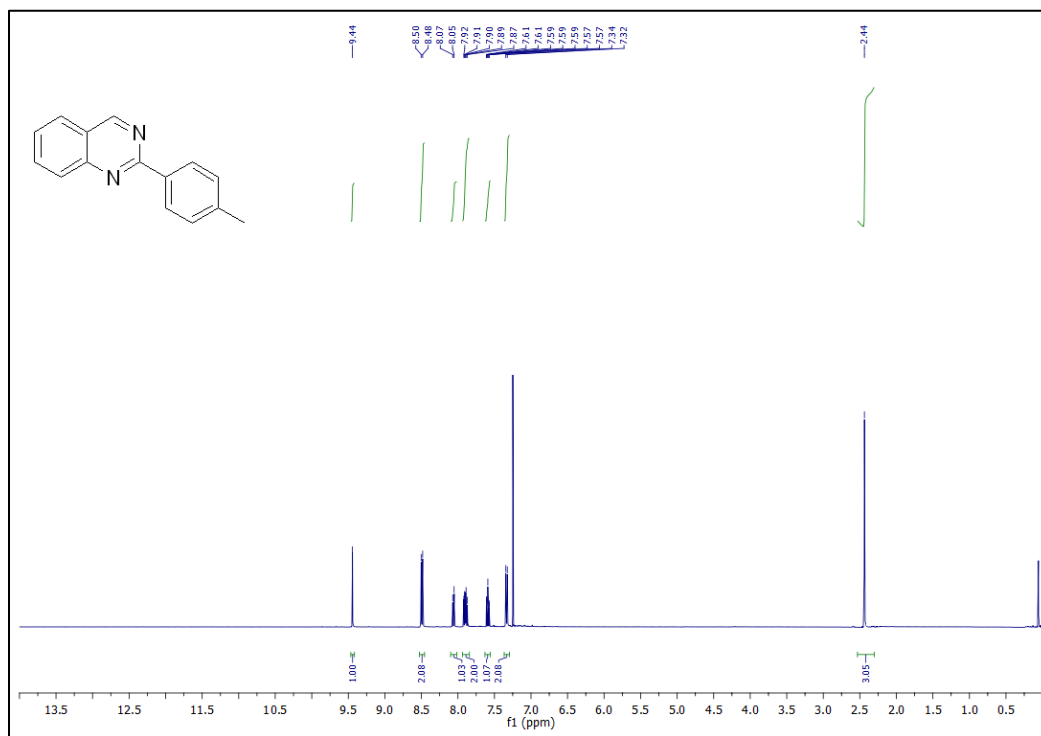
¹H spectrum 2-octylquinazolin-4(3H)-one (6a22) (DMSO-d₆, 500 MHz)



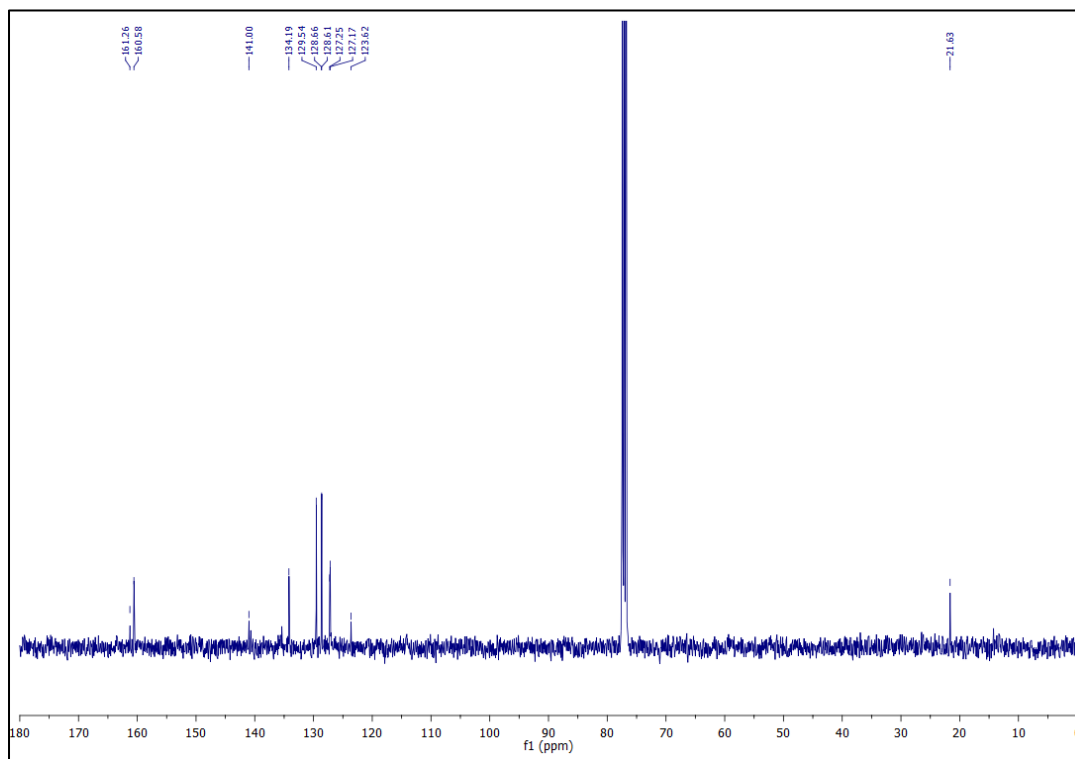
¹³C{¹H} spectrum 2-octylquinazolin-4(3H)-one (6a22) (DMSO-d₆, 125 MHz)



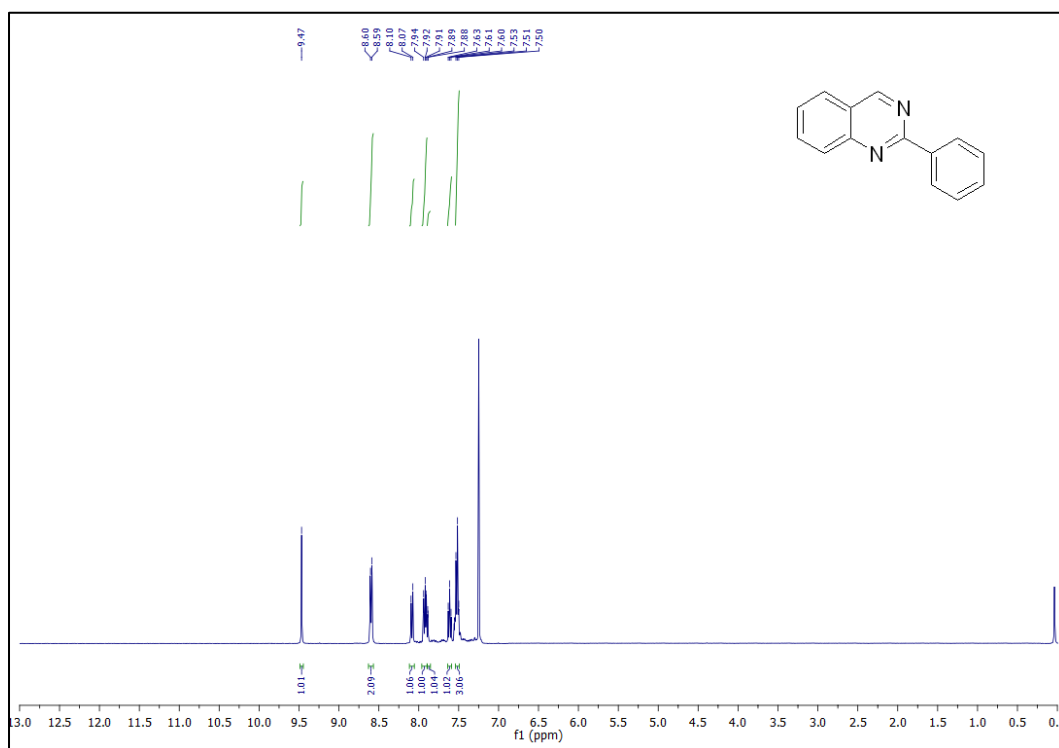
^1H spectrum 2-(p-tolyl)quinazoline (12a1) (CDCl_3 , 400 MHz)



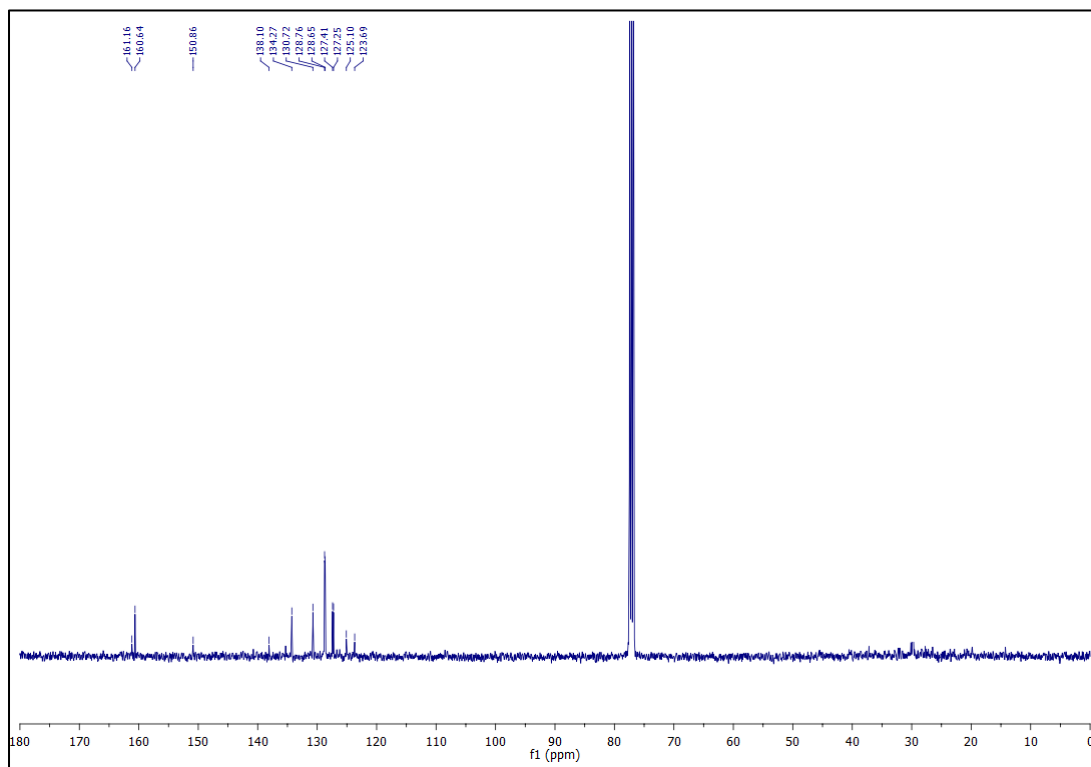
$^{13}\text{C}\{^1\text{H}\}$ spectrum 2-(p-tolyl)quinazoline (12a1) (CDCl_3 , 100 MHz)



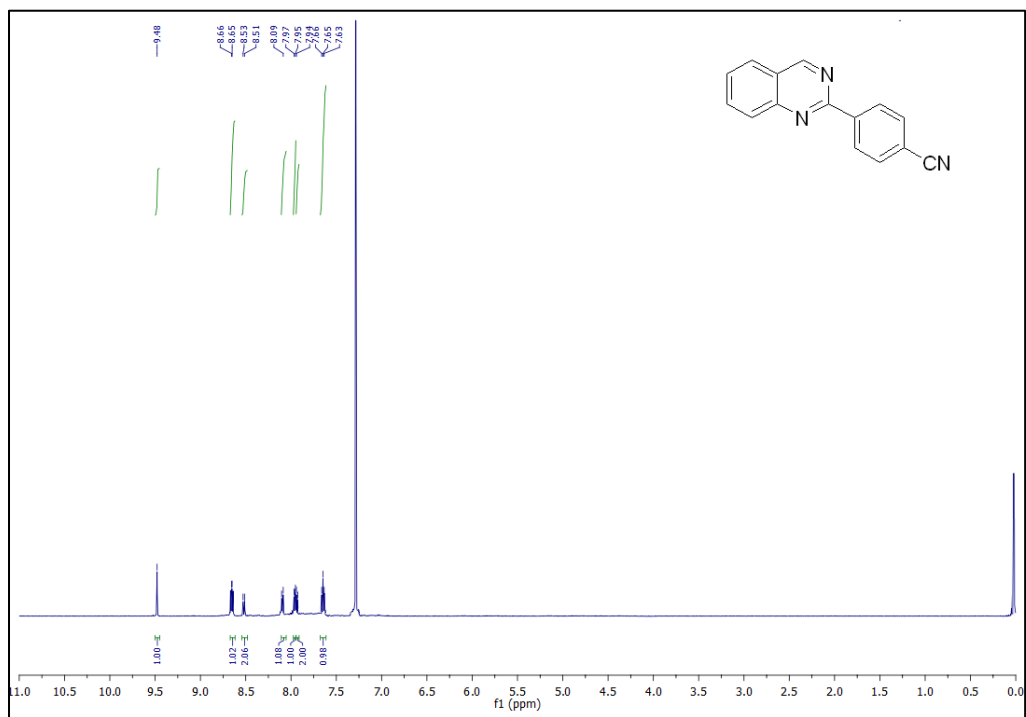
^1H spectrum 2-phenylquinazoline (12a2) (CDCl_3 , 400 MHz)



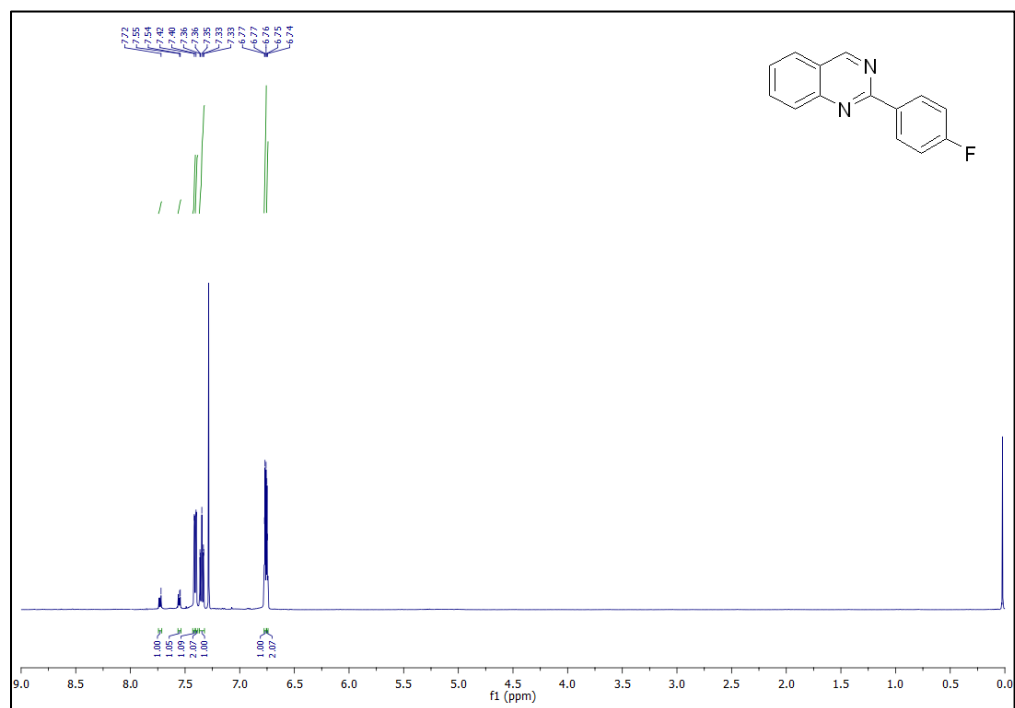
$^{13}\text{C}\{^1\text{H}\}$ spectrum 2-phenylquinazoline (12a2) (CDCl_3 , 100 MHz)



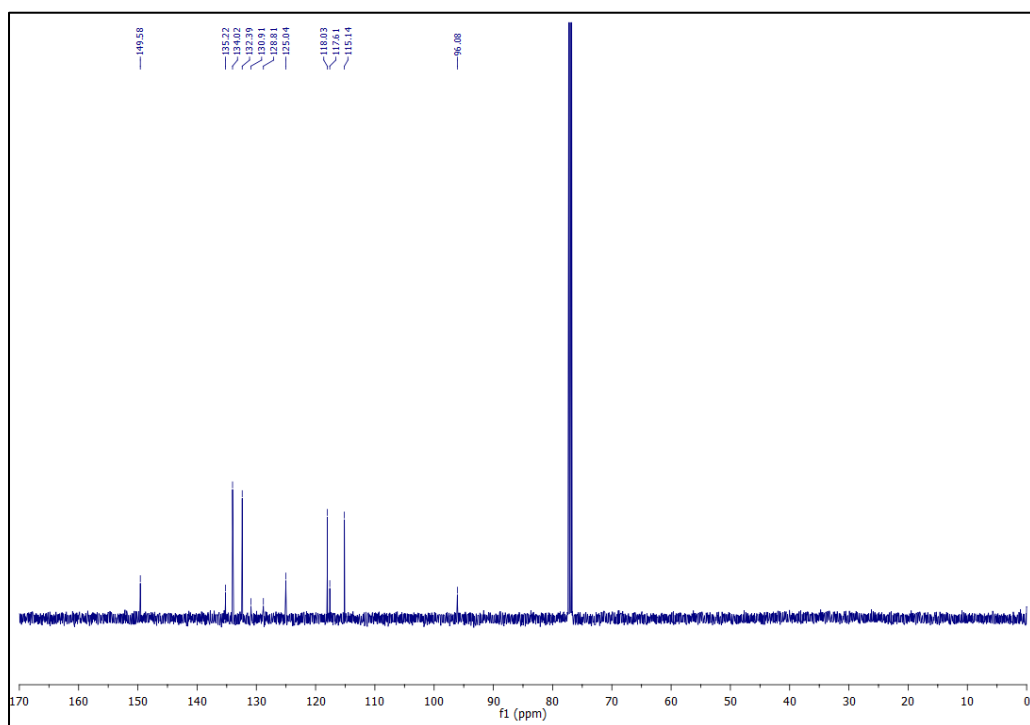
¹H spectrum 4-(quinazolin-2-yl)benzonitrile(12a3) (CDCl₃, 500 MHz)



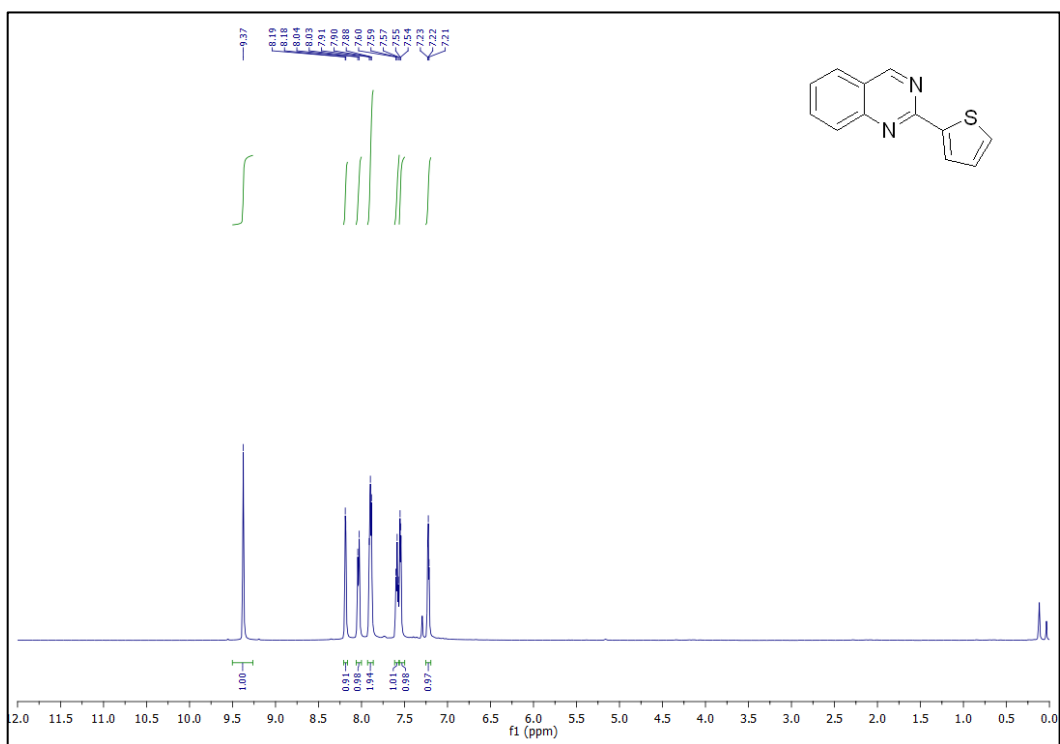
¹H spectrum 2-(4-fluorophenyl)quinazoline (12a4) (CDCl₃, 500 MHz)



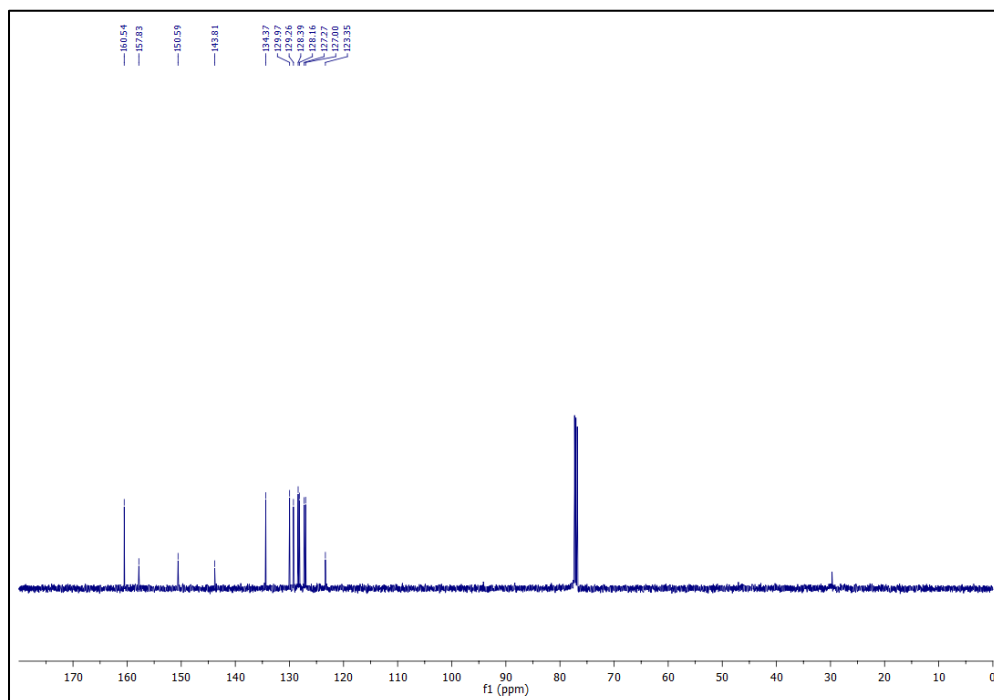
$^{13}\text{C}\{^1\text{H}\}$ spectrum 2-(4-fluorophenyl)quinazoline (12a4) (CDCl_3 , 125 MHz)



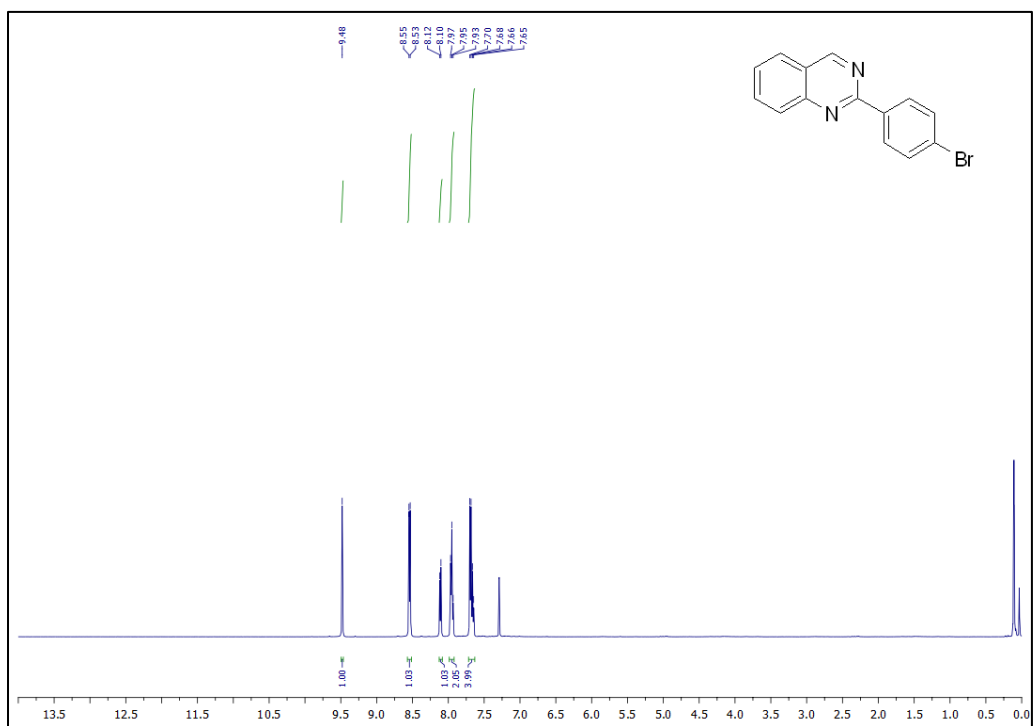
^1H spectrum 2-(thiophen-2-yl)quinazoline (12a7) (CDCl_3 , 500 MHz)



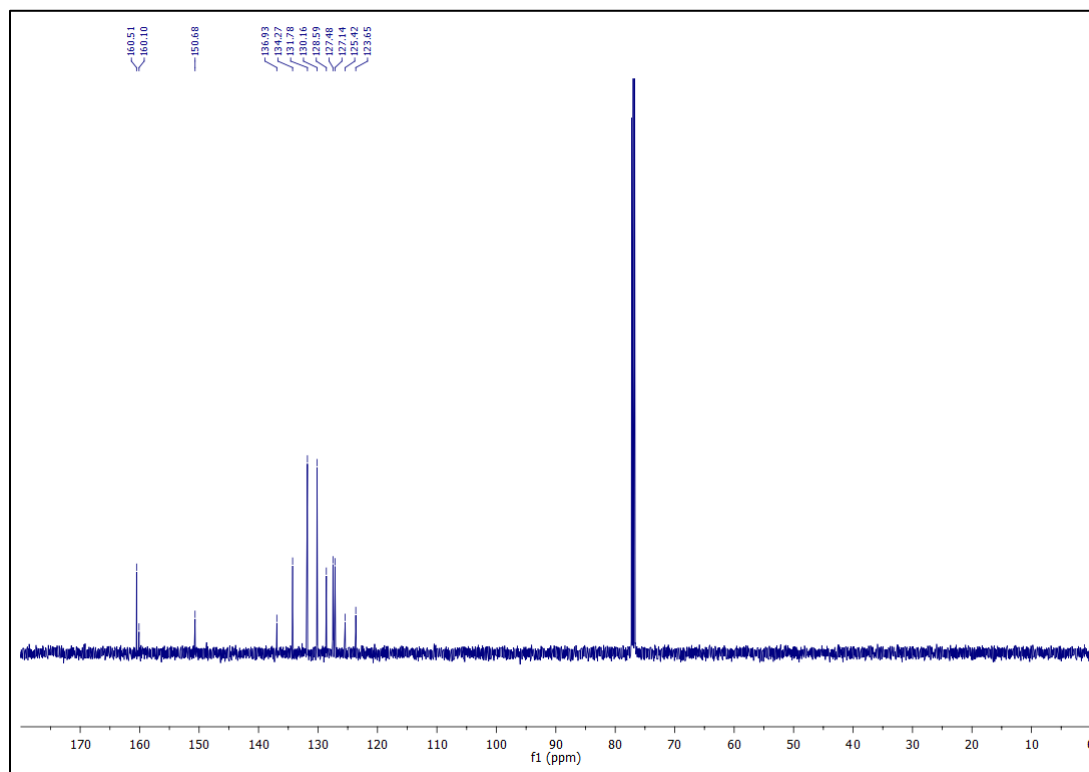
¹³C spectrum 2-(thiophen-2-yl)quinazoline (12a7) (CDCl₃, 125 MHz)



¹H spectrum 2-(4-Bromophenyl)quinazoline (12a8) (CDCl₃, 500 MHz)



^{13}C spectrum 2-(4-Bromophenyl)quinazoline (12a8) (CDCl_3 , 125 MHz)



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