Supporting Information

Visible-light-mediated photocatalytic sequential *N*-arylation: An eco-friendly synthetic route to unsymmetrical di-arylamines and imatinib drug

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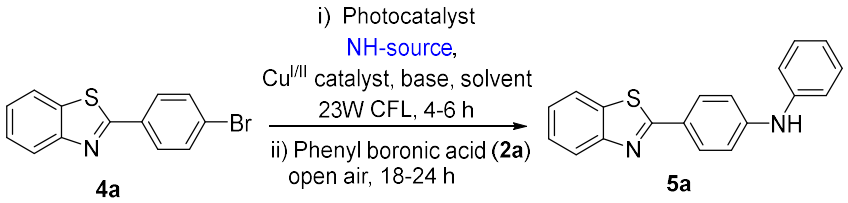
Content

I. Detailed Optimization:

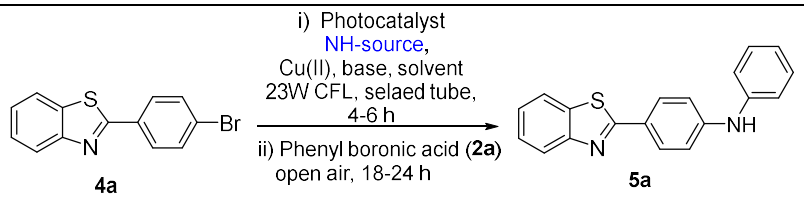
Table S1. Detailed optimization conditions for Cu-catalyzed sequential *N*-arylation of ammonia with aryl bromides under visible-light mediated ruthenium photoredox catalysis



Entry	Catalyst (mol%)	Co-catalyst (mol%)	NH-Source	Light source °(CFL)/temp.	Solvent	Yield (%)[b]
1	Eosin Y (5)	$Cu(OAc)_2$ (5)	NH_3 (aq.)	5W	toluene	N.R
2	Eosin Y (10)	Cu_2O (10)	NH_3 (aq.)	5W	toluene	N.R
3	Eosin Y (10)	$Cu(OAc)_2$ (10)	NH_3 (aq.)	8W	toluene	N.R
4	Eosin Y (10)	$Cu(OAc)_2$ (10)	NH_3 (aq.)	23W	toluene	N.R
5	Rose Bengal (5)	$Cu(OAc)_2$ (5)	NH_3 (aq.)	23W	toluene	trace
6	Rose Bengal (10)	$Cu(OAc)_2$ (10)	NH_3 (aq.)	23W	toluene	20
7	$Ru(bpy)_3Cl_2.6H_2O$ (5)	Cu_2O (5)	NH_3 (aq.)	23W	CH_3CN: H_2O	20
8	$Ru(bpy)_3Cl_2.6H_2O$ (5)	CuI (5)	NH_3 (aq.)	23W	CH_3CN: H_2O	-
9	$Ru(bpy)_3Cl_2.6H_2O$ (5)	$Cu(OAc)_2$ (5)	NH_4HCO_3	23W	CH_3CN: H_2O	-
10	$Ru(bpy)_3Cl_2.6H_2O$ (5)	$Cu(OAc)_2$ (5)	NH_4Cl	23W	CH_3CN: H_2O	-
11	$Ru(bpy)_3Cl_2.6H_2O$ (5)	$Cu(OAc)_2$ (5)	NH_3 (aq.) +NH_4OAc	23W	CH_3CN: H_2O	50
12	$Ru(bpy)_3Cl_2.6H_2O$ (5)	$Cu(OAc)_2$ (5)	NH_3 (aq.)	23W	H_2O	35
13	$Ru(bpy)_3Cl_2.6H_2O$ (5)	$(nBu_4N)_2Cu_2I_4$	NH_3 (aq.)	23W	CH_3CN: H_2O	-
14	Ru(*p*-cymene)$_2Cl_2$ (5)	$Cu(OAc)_2$ (5)	NH_3 (aq.)	80–100 °C	CH_3CN: H_2O	-
15	-	$Cu(OAc)_2$ (5)	NH_3 (aq.)	23W	CH_3CN: H_2O	25
16	$Ru(bpy)_3Cl_2.6H_2O$ (5)	$Cu(OAc)_2$ (5)	NH_3 (aq.)	-	CH_3CN: H_2O	-

[a]Reaction conditions: i) **4a**/**1a** (1 mmol), photocatalyst (5 mol%), co-catalyst (5 mol%), N-H source (10 mmol), Base (1.5 mmol), 23W CFL, reaction carried out under 23W CFL, rt, 4-6 h in a seal-tube; ii) **2a** (1.1 mmol) reaction carried out under 23W CFL, rt, 18-24 h, open air. Solvent 5 mL. [b]Isolated yields.

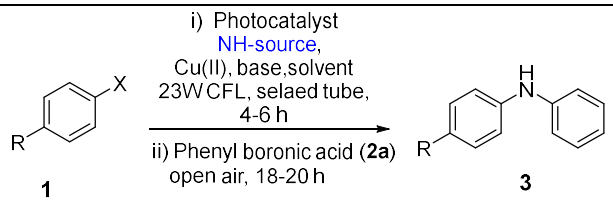
Table S2. Detailed optimization conditions for Cu^{II}-catalyzed sequential *N*-arylation of ammonia with aryl bromides under visible-light mediated ruthenium photoredox catalysis



entry	base	yield (%)[b]
1	DIPEA	68
2	Et_3N	25
3	K_2CO_3	NR
4	CS_2CO_3	55
5	$NaHCO_3$	NR
6	K_3PO_4	NR
7	DBU	NR
8	NaO*t*Bu	35
9	DMAP	NR
10	-	NR

[a]Reaction conditions: i) **4a** (1 mmol), photocatalyst (2 mol%), co-catalyst (2 mol%), N-H source (10 mmol), Base (1.5 mmol), 23W CFL, reaction carried out under 23W CFL, rt, 4-6 h in a seal-tube; ii) **2a** (1.1 mmol) reaction carried out under 23W CFL, rt, 18-24 h, open air. Solvent 5 mL. [b]Isolated yields.

Table S3. Additional substrate scope with complex functional groups

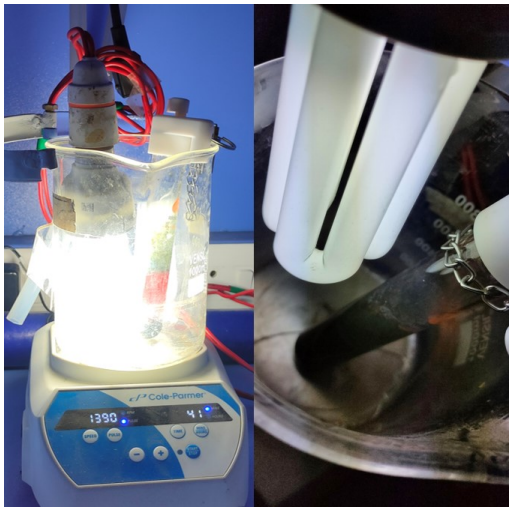


entry	R	X	yield (%)[b]
1	CO_2Et	Br	12
2	CHO	Br	ND
3	CN	Br	trace
4	Ac	Br	20
5	1-bromo butane	Br	NR
6	-	Cl	NR
7	-	I	25
8	-	OTf	ND
9	-	F	NR

II. Experimental Data

General information: Commercially available reagents and solvents were used without further purification. ^{1}H NMR spectra were recorded on a 500 MHz Bruker NMR spectrometer. Chemical shifts are reported in ppm with the solvent resonance as the internal standard (DMSO-d_6: δ = 2.50 ppm and $CDCl_3$: δ = 7.26 ppm). ^{13}C NMR spectra were recorded on the same spectrometer operating at 125 MHz with proton decoupling. Chemical shifts are reported in ppm with the solvent resonance as the internal standard (DMSO-d_6: δ = 39.52 ppm and $CDCl_3$: δ = 77.16 ppm). The following abbreviations were used for ^{1}H NMR spectra to indicate the signal multiplicity: s (singlet), d (doublet), t (triplet), q (quartet) and m (multiplet). HRMS was measured in ESI-QTOF mass spectrophotometer. Thin-layer chromatography was performed on MERCK precoated silica gel 60F-254 (0.5 mm) aluminum plates and visualized under UV light at 254 nm. Column chromatography was performed using silica gel 60-120 and 100-200 mesh. Spectro-fluorescence experiments were performed on the Perkin Elmer EnVision® Multimode Plate Reader using fluorescence intensity experiment.

Reaction Apparatus: 23W CFL bulb; Reaction vessel is approximately 4 cm away from light source.



II-1 General procedure for the synthesis of diarylamines: Aryl halide (**1**, 1 mmol), aq. ammonia (10 mmol), $Ru(bpy)_3Cl_2$ (5 mol%), $Cu(OAc)_2$ (5 mol%), DIPEA (1.5 mol%) in CH_3CN:H_2O (1:1, 5.0 mL) were added to an oven-dried reaction vessel equipped with a magnetic stir bar, and the reaction vessel was irradiated in a seal tube under 23W CFL bulb at room temperature for 4-6 h. Then the reaction mixture was stirred for 30 minutes under open air

until the reaction mixture becomes clear solution and then substituted aryl boronic acids (**2**, 1.1 mmol) were added to the reaction mixture. TLC was used to monitor the progress of the reaction. After completion of the reaction, the reaction mixture was extracted with ethyl acetate. The organic phase was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to get the crude residue, which was purified by column chromatography on silica gel (60−120 mesh) using petroleum ether/ethyl acetate (100% to 80:30) as an eluent to afford the *N*-arylated products (**3a**–**k** and **5a**–**v**).

II-2 General experimental procedure for the synthesis of compound 8: Compound **6** (1 mmol), aq. ammonia (10 mmol), $Ru(bpy)_3Cl_2$ (10 mol%), $Cu(OAc)_2$ (10 mol%), DIPEA (1.5 mol%) were added to CH_3CN: H_2O (1:1, 5.0 mL) in an oven-dried reaction vessel equipped with a magnetic stir bar, and the reaction vessel was irradiated in a sealed tube under 23W CFL bulb at room temperature for 4-8 h. Then compound **7** (1.1 mmol) was added to the reaction mixture. The progress of the reaction was monitored by TLC. After completion of the reaction in 24 h, the reaction mixture was extracted with ethyl acetate. The organic phase was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to get the crude residue, which was purified by column chromatography on silica gel (60−120 mesh) using petroleum ether/ethyl acetate (20:80) as an eluent to afford the imatinib drug in 84% yield.

Diphenylamine (3a). White solid; yield 84%; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.08 (d, J = 7.5 Hz, 2H), 7.49 (t, J = 6.5 Hz, 1H), 7.36 (t, J = 6.8 Hz, 2H), 7.28 (t, J = 7.3 Hz, 2H), 7.11 (t, J = 7.2 Hz, 1H), 7.06 (d, J = 7.1 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.2, 150.9, 133.6, 130.2, 129.6, 129.5, 128.5, 125.9, 121.7; HRMS (ESI-QTOF): *m/z* $[M + H]^+$ calcd. for $C_{12}H_{11}N$ 170.0970 found 170.0977.

2-Methyl-N-phenylaniline (3b). White solid; yield 52%; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.29–7.23 (m, 3H), 7.19 (d, J = 7.3 Hz, 1H), 7.13 (t, J = 7.7 Hz, 1H), 7.02–6.83 (m, 4H), 2.25 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 144.0, 141.2, 131.0, 129.3, 129.2, 128.4, 126.8, 122.0, 120.5, 118.9, 117.5, 17.9; HRMS (ESI-QTOF): *m/z* $[M + H]^+$ calcd. for $C_{13}H_{13}N$ 184.1126 found 184.1131.

3,5-Dimethoxy-N-phenylaniline (3c). White solid; yield 83%; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.32–7.26 (m, 2H), 7.15-7.06 (m, 2H), 6.99–6.93 (m, 1H), 6.24 (d, J = 2.1 Hz, 2H), 6.07 (t, J =

2.1 Hz, 1H), 3.76 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 161.6, 145.2, 142.5, 129.3, 121.5, 118.8, 95.8, 93.0, 55.3; HRMS (ESI-QTOF): *m/z* $[M + H]^+$ calcd. for $C_{14}H_{16}NO_2$ 230.1181 found 230.1183.

4-Chloro-N-phenylaniline (3d). Brown solid; yield 78%; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.27-7.37 (m, 2H), 7.14 - 7.19 (m, 1H), 7.08 - 7.12 (m, 2H), 7.03-7- 05(m, 1H), 6.98 – 7.01 (m, 1H); 6.89- 6.92 (m, 1H) 6.85 - 6.88 (m, 1H)^{13}C NMR (125 MHz, $CDCl_3$): δ 144.9, 141.9, 130.6, 129.5, 123.4, 123.1, 122.1, 119.5, 119.0, 115.5; HRMS (ESI-QTOF): *m/z* $[M + H]^+$ calcd. for $C_{12}H_9ClN$ 204.0580 found 204.0586.

4-Fluoro-N-phenylaniline (3e). Brown oil; yield 75%; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.28–7.24 - 7.27 (m, 2H), 7.02 – 7.06 (m, 2H), 7.00–6.95 (m, 4H), 6.89 (t, J = 7.7 Hz, 1H); ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$): δ 159.0, 157.14, 143.9, 138.9, 129.4, 120.6, 120.5, 116.8, 116.0, 115.8; HRMS (ESI-QTOF): *m/z* $[M + H]^+$ calcd. for $C_{12}H_{10}FN$ 188.0876 found 188.0879.

3-Bromo-N-phenylaniline (3f). Brown solid; yield 79%; ^{1}H NMR (500 MHz, $CDCl_3$): δ 77.33–7.28 (m, 2H), 7.20 (t, J = 2.1 Hz, 1H), 7.12–7.07 (m, 3H), 7.03–6.97 (m, 2H), 6.94 (dd, J = 10.2 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 144.9, 141.9, 130.6, 129.5, 123.4, 123.1, 122.1, 119.5, 119.0, 115.5; HRMS (ESI-QTOF): *m/z* $[M + H]^+$ calcd. for $C_{12}H_{10}BrN$ 248.0075 found 249.0005.

4-Iodo-N-phenylaniline (3g). Brown solid; yield 82%; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.32–7.27 (m, 2H), 7.15 (t, J = 8.0 Hz, 1H), 7.12–7.07 (m, 2H), 7.04 (t, J = 2.1 Hz, 1H), 6.99 (t, J = 7.3 Hz, 1H), 6.89 (dd, J = 8.2 Hz, 1H), 6.86 (dd, J = 7.9 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 144.8, 141.9, 135.0, 130.3, 129.5, 122.1, 120.4, 119.0, 116.6, 115.1; HRMS (ESI-QTOF): *m/z* $[M + H]^+$ calcd. for $C_{12}H_{10}IN$ 295.9936 found 295.9941.

3-Chloro-4-fluoro-N-phenylaniline (3h). White solid; yield 62%; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.31–7.26 (m, 2H), 7.10 (dd, J = 6.3, 2.8 Hz, 1H), 7.05–6.99 (m, 3H), 6.99–6.94 (m, 1H), 6.93–6.86 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.9, 152.0, 142.7, 140.1, 129.5, 121.6, 119.6, 117.9, 117.6, 117.6, 117.0, 116.9; HRMS (ESI-QTOF): *m/z* $[M + H]^+$ calcd. for $C_{12}H_9ClFN$ 222.0486 found 222.0496.

4-Nitro-N-phenylaniline (3i). Lime-yellow solid; yield 68%; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.55–7.48 (m, 2H), 7.31–7.26 (m, 2H), 7.06 (dd, J = 4.2, 3.2, Hz, 2H), 6.97 (td, J = 8.4, 2.1 Hz, 1H), 6.86–6.80 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 143.1, 142.2, 138.0, 129.4, 121.8, 119.2, 118.5; HRMS (ESI-QTOF): *m/z* $[M + H]^+$ calcd. for $C_{12}H_{10}N_2O_2$ 215.0821 found 215.0825.

4-(Phenylamino)benzonitrile (3j). White solid; yield 69%; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.51–7.45 (m, 2H), 7.40–7.33 (m, 2H), 7.17 (dd, J = 3.1, 1.7 Hz, 2H), 7.15–7.09 (m, 1H), 7.00–6.94 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 148.16, 140.08, 133.78, 129.65, 123.95, 121.24, 120.04, 114.94, 101.30; HRMS (ESI-QTOF): *m/z* $[M + H]^+$ calcd. for $C_{13}H_{10}N_2$ 195.0922 found 195.0928.

N-Phenylpyridin-2-amine (3k). Off-white solid; yield 71%; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.21–8.09 (m, 2H), 7.60–7.54 (m, 1H), 7.44 (t, J = 10.7, 4.8 Hz, 2H), 7.40–7.33 (m, 2H), 7.22–7.19 (m, 1H), 7.18–7.09 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 164.1, 149.9, 132.5, 129.1, 128.7, 128.5, 128.4, 127.5, 124.8, 122.1, 120.7, 117.8; HRMS (ESI-QTOF): *m/z* $[M + H]^+$ calcd. for $C_{11}H_{10}N_2$ 171.0922 found 171.0932.

4-(Benzo[d]thiazol-2-yl)-N-phenylaniline (5a). Off-white solid; yield 82%; mp: 140–142 °C; FT-IR (cm^{-1}): 3337, 3162, 2982, 1648, 1485, 1296; ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.31 (d, J = 8.0 Hz, 1H), 8.24 (d, J = 8.1 Hz, 1H), 8.12 (d, J = 3.7 Hz, 1H), 7.98 (d, J = 8.5 Hz, 1H), 7.86 (d, J = 8.3, 1H), 7.63 (t, J = 8.1 Hz, 1H), 7.45 (d, J = 7.2 Hz, 1H), 7.39 (t, J = 6.7 Hz, 1H), 7.36 (t, 1H), 7.36–7.33 (m, 1H), 7.29 (d, J = 7.0 Hz, 2H), 7.04 (d, J = 8.2, 1H), 6.95–6.91 (m, 1H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 147.5, 140.8, 137.1, 131.9, 130.7, 129.5, 129.1, 129.0, 128.4, 127.0, 126.1, 124.5, 121.7, 117.6, 111.4; HRMS (ESI-QTOF): *m/z* $[M + H]^+$ calcd. for $C_{19}H_{14}N_2S$ 303.0956 found 303.0963.

4-(Benzo[d]thiazol-2-yl)-N-(p-tolyl)aniline (5b). Off-white solid; yield 90%; mp: 137–139 °C; FT-IR (cm^{-1}): 3325, 3154, 2955, 1626, 1365, 1272; ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.30 (d, J = 1.7 Hz, 1H), 8.21 (d, J = 7.9 Hz, 1H), 8.05 (s, 1H), 7.99–7.94 (m, 1H), 7.84 (d, J = 7.9 Hz, 1H), 7.62 (t, J = 7.5 Hz, 1H), 7.45–7.40 (m, 1H), 7.31 (s, 1H), 7.15 (s, 3H), 7.01 (d, J = 7.9 Hz, 1H), 6.91 (t, J = 7.6 Hz, 1H), 2.28 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 160.1, 148.2,

147.8, 145.7, 138.0, 136.9, 135.4, 134.1, 129.5, 127.7, 127.1, 126.1, 120.4, 119.2, 116.3, 20.9; HRMS (ESI-QTOF): *m/z* $[M + H]^+$ calcd. for $C_{20}H_{16}N_2S$ 317.1112 found 317.1114.

N-(4-(Benzo[d]thiazol-2-yl)phenyl)-3,5-dimethoxyaniline (5c). White solid; yield 82%; mp: 166–168 °C; FT-IR (cm^{-1}): 3321, 3127, 2942, 1655, 1373, 1165; ^1H NMR (500 MHz, DMSO-d_6): δ 8.77 (d, J = 9.0 Hz, 1H), 7.99 - 8.04 (m, 2H), 7.72 (s, 3H), 7.65 (s, 1H), 7.52 (d, J = 9.3 Hz, 1H), 7.34 (d, J = 11.4 Hz, 3H), 7.03 (t, J = 6.9 Hz, 1H), 4.08 (s, 3H), 4.00 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 160.1, 153.2, 148.1, 147.6, 145.8, 137.9, 135.5, 134.2, 127.7, 126.8, 120.3, 119.3, 116.2, 116.1, 103.9, 56.2; HRMS (ESI-QTOF): *m/z* $[M + H]^+$ calcd. for $C_{21}H_{18}N_2O_2S$ 363.1167 found 363.1169.

4-(Benzo[d]thiazol-2-yl)-N-(4-isopropylphenyl)aniline (5d). Off-white solid; yield 75%; mp: 145–147 °C; FT-IR (cm^{-1}): 3321, 3027, 2872, 1637, 1382, 1165; ^1H NMR (500 MHz, DMSO-d_6): δ 8.35 (d, J = 8.2 Hz, 1H), 8.30 (d, J = 7.9 Hz, 1H), 8.14 (s, 1H), 8.02 – 8.09 (m,1H), 7.91 (d, J = 8.1 Hz, 1H), 7.68 – 7.80 (m, 1H), 7.50 (t, J = 7.3 Hz, 1H), 7.38 (s, 1H), 7.28- 7.31 (m, 3H), 7.08 (d, J = 8.1 Hz, 1H), 6.98 (t, J = 7.6 Hz, 1H), 2.99–2.84 (m, 1H), 1.25 (d, J = 7.0 Hz, 6H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 160.1, 148.8, 148.2, 147.7, 145.6, 137.4, 135.4, 134.1, 129.0, 127.7, 126.9, 126.1, 120.4, 119.1, 116.3, 33.4, 24.1; HRMS (ESI-QTOF): *m/z* $[M + H]^+$ calcd. for $C_{22}H_{20}N_2S$ 345.1425 found 345.1428.

4-(Benzo[d]thiazol-2-yl)-N-(4-chlorophenyl)aniline (5e). White solid; yield 81%; mp: 120–122 °C; FT-IR (cm^{-1}): 3336, 3137, 2956, 1662, 1242, 824; ^1H NMR (500 MHz, DMSO-d_6): δ 8.56 (s, 1H), 8.08 (d, J = 8.1 Hz, 1H), 7.99–7.96 (m, 1H), 7.95 (d, J = 1.8 Hz, 1H), 7.93 (s, 1H), 7.75 – 7.80 (m, 1H), 7.52–7.48 (m, 2H), 7.27 - 7.32 (m, 1H), 7.22 – 7.28 (m,1H), 7.09 – 7.15 (m,1H), 7.06 (d, J = 2.9 Hz, 2H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 167.9, 156.2, 154.2, 154.2, 147.6, 134.4, 129.5, 129.0, 126.8, 125.4, 125.2, 124.3, 123.3, 122.6, 116.8, 116.6, 115.6; HRMS (ESI-QTOF): *m/z* $[M + H]^+$ calcd. for $C_{19}H_{13}ClN_2S$ 337.0566 found 337.0574. (m, 3

N-(4-(Benzo[d]thiazol-2-yl)phenyl)-3-bromoaniline (5f). Off-white solid; yield 81%; mp: 170–172 °C; FT-IR (cm^{-1}): 3327, 3147, 2892, 1626, 1212, 678; ^1H NMR (500 MHz, DMSO-d_6): δ 8.43-8.48 (m, 1H), 8.35 - 8.41(m, 1H), 8.2 - 8.32 (m, 1H), 8.03 - 8.12 (m, 1H), 7.98 – 8.02 (m, 1H), 7.85 (s, 1H), 7.68 – 7.82 (m, 2H), 7. 50 (s, 1H)7.38 (s, 1H), 7.20 – 7.25 (m, 1H), 6.93 (s, 2H) ; ^{13}C NMR (125 MHz, DMSO-d_6): δ 162.7, 152.7, 149.2, 135.1,

133.1, 131.8, 129.0, 128.2, 126.5, 126.3, 125.9, 121.4, 116.0, 115.8; HRMS (ESI-QTOF): *m/z* $[M + 2]^+$ calcd. for $C_{19}H_{13}BrN_2S$ 381.0061 found 381.0001(this is not $[M+2]^+$ value).

N-(4-(Benz[d]thiazol-2-yl)phenyl)-3-fluoro-4-methoxyaniline (5g). Off-white solid; yield 72%; mp: 160–162 °C; FT-IR (cm^{-1}): 3342, 3156, 2956, 1686, 1476, 1065; ^1H NMR (500 MHz, DMSO-d_6): δ 8.70 (d, J = 9.0 Hz, 1H), 7.98 (s, 1H), 7.94 (d, J = 10.1 Hz, 2H), 7.90 (d, J = 7.9 Hz, 1H), 7.75 (d, J = 6.1 Hz, 1H), 7.70–7.64 (m, 3H), 7.61–7.56 (m, 1H), 7.46 (d, J = 8.9 Hz, 1H), 6.97 (t, J = 7.4 Hz, 1H), 4.01 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 158.3, 147.8, 141.9, 140.4, 132.8, 132.2, 131.4, 128.8, 126.5, 124.4, 122.9, 120.8, 117.9, 111.6, 108.5, 55.7; HRMS (ESI-QTOF): *m/z* $[M + H]^+$ calcd. for $C_{20}H_{15}FN_2OS$ 351.0967 found 351.0971

N-(4-(Benzo[d]thiazol-2-yl)phenyl)pyridin-4-amine (5h). Off-white solid; yield 76%; mp: 157–159 °C; FT-IR (cm^{-1}): 3316, 3176, 2979, 1636, 1382, 1288; ^1H NMR (500 MHz, DMSO-d_6): δ 9.28 (s, 1H), 8.30 (s, 2H), 8.12 (d, J = 8.1, 1.3 Hz, 1H), 8.06 (d, J = 8.7 Hz, 2H), 8.01 (d, J = 8.2 Hz 1H), 7.56–7.51 (m, 1H), 7.44 (t, 1H), 7.38 (d, J = 4.9 Hz, 2H), 7.09 (s, 2H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 167.4, 154.2, 150.7, 149.2, 144.3, 134.6, 129.1, 127.0, 126.5, 125.5, 122.9, 122.6, 119.1, 111.0; HRMS (ESI-QTOF): *m/z* $[M + H]^+$ calcd. for $C_{18}H_{13}N_3S$ 304.0908 found 304.0912.

N-(4-(Benzo[d]thiazol-2-yl)phenyl)naphthalen-1-amine (5i). Light-yellow solid; yield 79%; mp: 180–182 °C; FT-IR (cm^{-1}): 3321, 3027, 2942, 1655, 1582, 1165; ^1H NMR (500 MHz, DMSO-d_6): δ 8.36 (d, J = 8.1 Hz, 1H), 8.30 (s, 1H), 8.20 (d, J = 7.9 Hz, 1H), 7.97 (s, 1H), 7.89 (s, 1H), 7.79 (s, 1H), 7.65 (d, J = 8.1 Hz, 2H), 7.61 (s, 1H), 7.53 (s, 1H), 7.42 (s, 2H), 7.24 (t, J = 7.6 Hz, 1H), 6.99 (d, J = 7.9 Hz, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 147.3, 141.7, 140.3, 132.2, 131.9, 131.5, 130.1, 128.8, 127.9, 126.4, 125.2, 124.0, 122.7, 121.4, 121.0, 118.1, 112.3; HRMS (ESI-QTOF): *m/z* $[M + H]^+$ calcd. for $C_{23}H_{16}N_2S$ 353.1112 found 353.1124.

N-(4-(6-Methoxybenzo[d]thiazol-2-yl)phenyl)naphthalen-1-amine (5j). Light-yellow solid; yield 84%; mp: 175–177 °C; FT-IR (cm^{-1}): 3338, 3092, 2852, 1635, 1223, 1096; ^1H NMR (500 MHz, DMSO-d_6): δ 9.40 (s, 1H), 8.77 (s, 1H), 8.36 (d, J = 9.5 Hz, 1H), 8.21 (d, J = 7.8 Hz, 1H), 7.96 (dd, J = 8.1 Hz, 2H), 7.80 (s, 1H), 7.70–7.60 (m, 3H), 7.58–7.54 (m, 1H), 7.35–7.28 (m, 2H), 7.25 (d, J = 8.4 Hz, 1H), 6.98 (t, J = 6.8 Hz, 1H), 3.89 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 160.0, 147.3, 141.6, 139.3, 131.8, 130.6, 130.2, 129.2, 128.5, 127.4, 126.4, 125.1,

123.5, 121.3, 118.0, 114.9, 112.1, 55.8; HRMS (ESI-QTOF): *m/z* $[M + H]^+$ calcd. for $C_{24}H_{19}N_2OS$ 383.1218 found 383.1214.

N-(4-(Benzo[d]thiazol-2-yl)-2-chlorophenyl)naphthalen-1-amine (5k). Light-yellow solid; yield 68%; mp: 178–180 °C; FT-IR (cm^{-1}): 3342, 3115, 2886, 1646, 1242, 878; ^1H NMR (500 MHz, DMSO-d_6): δ 9.48 (s, 1H), 8.88 (s, 1H), 8.45 (d, J = 7.8 Hz, 1H), 8.30 (d, J = 7.8 Hz, 1H), 8.11–8.05 (m, 2H), 7.99 (m, 2H), 7.91 (s, 1H), 7.86 (d, J = 7.6 Hz, 1H), 7.75 (t, J = 7.6 Hz, 3H), 7.68–7.64 (m, 1H), 7.09 (t, J = 6.9 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 137.9, 130.2, 129.6, 129.5, 129.0, 128.8, 128.5, 127.8, 127.4, 126.3, 126.1, 123.6, 121.3, 118.1, 112.1; HRMS (ESI-QTOF): *m/z* $[M + H]^+$ calcd. for $C_{23}H_{15}ClN_2S$ 387.0723 found 387.0727.

N-(4-(1H-Benzo[d]imidazol-2-yl)phenyl)-3-methylaniline (5l). Off-white solid; yield 85%; mp:166–168 °C; FT-IR (cm^{-1}): 3328, 3056, 2924, 1625, 1450; ^1H NMR (500 MHz, DMSO-d_6): δ 12.57 (s, 1H), 7.99 (d, J = 4.7 Hz, 1H), 7.97 (d, J = 2.0 Hz, 1H), 7.89 (s, 1H), 7.59 (s, 1H), 7.47 (s, 1H), 7.26 (s, 2H), 7.25 – 7.29 (m, 1H), 7.22 – 7.23 (m, 2H), 7.18- 7.19 (m, 1H), 7.02- 7.05 (m, 1H), 6.93 (d, J = 2.0 Hz, 1H), 2.23 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 152.5, 147.6, 140.5, 131.5, 131.5, 128.1, 127.1, 123.8, 122.5, 120.3, 115.0, 18.4; HRMS (ESI-QTOF): *m/z* $[M + H]^+$ calcd. for $C_{20}H_{17}N_3$ 300.1501 found 300.1510.

N-(4-(1H-Benzo[d]imidazol-2-yl)phenyl)-3,4,5-trimethoxyaniline (5m). Off-white solid; yield 57%; ^1H NMR (500 MHz, $CDCl_3$): 13.17 (s, 1H), 8.98 (d, J = 8.4 Hz, 1H), 7.93 (dt, J = 9.1, 4.7 Hz, 3H), 7.54 (dd, J = 11.5, 4.3 Hz, 1H), 7.50 (dd, J = 11.2, 4.1 Hz, 1H), 7.45–7.41 (m, 1H), 7.44 (s, 3H), 7.22–7.18 (m, 1H), 3.96 (d, J = 7.6 Hz, 9H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 152.4, 137.4, 131.2, 130.5, 129.0, 125.7, 124.9, 122.3, 121.3, 120.6, 119.8, 118.3, 105.0, 60.0, 55.8; HRMS (ESI-QTOF): *m/z* $[M + H]^+$ calcd. for $C_{22}H_{21}N_3O_3$ 376.1661 found 376.1659.

N-(4-(1H-Benzo[d]imidazol-2-yl)phenyl)-4-isopropylaniline (5n). Off-white solid; yield 62%; ^1H NMR (500 MHz, $CDCl_3$): 13.38 (s, 1H), 8.99 (d, J = 1.6 Hz, 1H), 8.26–8.22 (m, 2H), 7.98 (d, J = 8.1 Hz, 1H), 7.92 (d, J = 7.9 Hz, 1H), 7.83 (d, J = 8.1 Hz, 1H), 7.63–7.52 (m, 4H), 7.52 (t, J = 7.7 Hz, 1H), 7.42 (dd, J = 11.2, 4.0 Hz, 1H), 7.07 (s, 1H), 3.04 (m, 1H), 1.33 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.9, 138.4, 131.7, 129.9, 128.5, 127.7, 126.5, 125.5, 121.9, 121.4, 121.4, 118.8, 34.5, 23.5; HRMS (ESI-QTOF): *m/z* $[M + H]^+$ calcd. for $C_{22}H_{21}N_3$ 328.1814 found 328.1816.

4-(6-Nitro-1H-benzo[d]imidazol-2-yl)-N-phenylaniline (5o). Lime-yellow solid; yield 52%; ^{1}H NMR (500 MHz, $CDCl_3$): 13.36 (s, 1H), 8.90 (s, 1H), 8.25–8.22 (m, 2H), 7.97 (d, *J* = 8.1 Hz, 1H), 7.92–7.89 (d, *J* = 8.2, 1H), 7.78 (d, *J* = 8.0 Hz, 1H), 7.62–7.58 (m, 3H), 7.51 (dd, *J* = 11.2, 4.1 Hz, 1H), 7.42 (t, *J* = 7.6 Hz, 1H), 7.02–6.99 (m, 1H), 2.47 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): *δ* 152.7, 143.1, 138.3, 135.6, 133.1, 131.8, 129.8, 128.6, 127.8, 126.6, 125.6, 124.2, 122.0, 121.5, 121.1, 22.0; HRMS (ESI-QTOF): *m/z* $[M + H]^+$ calcd. for $C_{19}H_{14}N_4O_2$ 331.1195 found 331.1192.

N-(3-(9H-Pyrido[3,4-b]indol-1-yl)phenyl)-3-methylaniline (5p). White solid; yield 81%; mp: 200–202 °C; FT-IR (cm^{-1}): 3338, 3043, 2942, 1636, 1450, 1386; ^{1}H NMR (500 MHz, DMSO-*d*$_6$): *δ* 11.96 (s, 1H), 9.34 (s, 1H), 8.74 (s, 1H), 8.30 (d, *J* = 5.7 Hz 1H), 8.17 (d, *J* = 6.3 Hz 1H), 7.93–7.90 (m, 2H), 7.73 (d, *J* = 6.1 Hz, 5H), 7.61 (m, 2H), 7.54 – 7.62 (m, 1H), 6.96 (t, *J* = 6.3 Hz, 1H), 1.92 (s, 3H); ^{13}C NMR (125 MHz, DMSO-*d*$_6$): *δ* 172.4, 147.4, 141.7, 136.8, 133.8, 131.5, 130.1, 129.5, 128.8, 127.5, 126.5, 123.9, 121.4, 121.1, 118.0, 112.3, 21.5; HRMS (ESI-QTOF): *m/z* $[M + H]^+$ calcd. for $C_{24}H_{19}N_3$ 350.1657 found 350.1659.

N-(3-(9H-Pyrido[3,4-b]indol-1-yl)phenyl)pyridin-4-amine (5q). White solid; yield 78%; mp: 220–222 °C; FT-IR (cm^{-1}): 3325, 3065, 2894, 1645, 1323; ^{1}H NMR (500 MHz, DMSO-*d*$_6$): *δ* 12.56 (s, 1H), 8.26 (d, *J* = 8.1 Hz, 1H), 8.19 (s, 1H), 8.10 (d, *J* = 7.9 Hz, 1H), 7.88 (s, 1H), 7.79 (s, 1H), 7.70 (s, 1H), 7.56 (s, 2H), 7.51 (s, 1H), 7.43 (s, 1H), 7.31 (s, 2H), 7.13 (d, *J* = 7.5 Hz, 1H), 6.87 (d, *J* = 4.6 Hz, 2H); ^{13}C NMR (125 MHz, DMSO-*d*$_6$): *δ* 163.8, 147.9, 145.0, 133.9, 131.6, 131.0, 130.1, 127.8, 126.2, 122.0, 117.8, 115.3, 114.9; HRMS (ESI-QTOF): *m/z* $[M + H]^+$ calcd. for $C_{22}H_{16}N_4$ 337.1453 found 337.1456.

2-(4-(Phenylamino)phenyl)quinazolin-4(3H)-one (5r). White solid; yield 78%; mp: 190–192 °C; FT-IR (cm^{-1}): 3326, 3021, 2966, 1640, 1438, 1243; ^{1}H NMR (500 MHz, DMSO-*d*$_6$): *δ* 10.40 (s, 1H), 10.02 (s, 1H), 8.68–8.50 (m, 3H), 8.02–7.94 (m, 3H), 7.91 (s, 3H), 7.82 (d, *J* = 7.7 Hz, 2H), 7.69 (s, 1H), 7.30 (s, 1H); ^{13}C NMR (125 MHz, DMSO-*d*$_6$): *δ* 159.5, 158.3, 150.9, 139.8, 138.8, 135.8, 134.5, 134.2, 133.6, 130.7, 129.4, 128.8, 128.3, 126.3, 123.1, 121.0, 114.4; HRMS (ESI-QTOF): *m/z* $[M + H]^+$ calcd. for $C_{20}H_{15}N_3O$ 314.1293 found 314.1295.

2-(4-((3,5-Dimethoxyphenyl)amino)phenyl)quinazolin-4(3H)-one (5s). White solid; yield 72%; mp: 222–224 °C; FT-IR (cm^{-1}): 3332, 3056, 2985, 1639, 1473, 1195; ^{1}H NMR (500 MHz,

DMSO-d_6): δ 11.82 (s, 1H), 10.11 (d, J = 15.7 Hz, 1H), 8.13 (d, J = 5.9 Hz, 1H), 8.04–7.99 (m, 1H), 7.92–7.76 (m, 2Hs), 7.70 – 7.75 (m, 1H), 7.50 – 7.62 (m, 1H) 7.42–7.36 (m, 1H), 6.86–6.63 (m, 2H), 6.60–6.54 (m, 1H), 4.99 (d, J = 14.2 Hz, 1H), 4.05–3.70 (m, 6H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 163.4, 161.6, 152.3, 149.6, 146.0, 140.3, 134.8, 133.5, 132.3, 128.5, 127.7, 126.6, 122.8, 114.1, 56.5, 56.0; HRMS (ESI-QTOF): m/z [M + H]$^+$ calcd. for $C_{22}H_{19}N_3O_3$ 374.1505 found 374.1505.

2-(3-Nitro-4-(phenylamino)phenyl)quinazolin-4(3H)-one (5t). Lime-yellow solid; yield 50%; ^{1}H NMR (500 MHz, $CDCl_3$): 13.39 (s, 1H), 9.06 (dd, J = 8.5, 1.0 Hz, 1H), 8.27–8.21 (m, 2H), 8.01 (d, J = 8.1 Hz, 1H), 7.96–7.89 (m, 2H), 7.52 – 6.58 (m, 3H), 7.47- 7.49 (m, 2H), 7.45 (s, 1H), 7.21 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 169.0, 132.2, 131.8, 129.9, 128.6, 127.8, 126.7, 125.9, 123.3, 122.2, 121.6, 120.8; HRMS (ESI-QTOF): m/z [M + H]$^+$ calcd. for $C_{20}H_{14}N_4O_3$ 359.1144 found 359.1146.

2-(4-(Naphthalen-2-ylamino) phenyl) quinazolin-4(3H)-one (5u). White solid; yield 65%; mp: 232–234 °C; FT-IR (cm^{-1}): 3343, 3054, 2987, 1640, 1538, 1267; ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.56 (s, 1H), 9.92 (s, 1H), 8.97 (s, 1H), 8.59 (d, J = 8.2 Hz, 1H), 8.46 (d, J = 6.2 Hz, 2H), 8.32–8.27 (m, 1H), 7.97 (d, J = 8.7 Hz, 2H), 7.88 (d, J = 3.7 Hz, 4H), 7.63 (t, J = 7.8 Hz, 1H), 7.52 (d, J = 6.8 Hz, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 163.2, 159.5, 158.3, 150.9, 150.1, 144.6, 139.0, 138.8, 135.9, 134.9, 133.6, 130.7, 128.8, 128.6, 128.5, 128.4, 128.3, 126.3, 123.4, 123.1, 121.0, 114.4; HRMS (ESI-QTOF): m/z [M + H]$^+$ calcd. for $C_{24}H_{17}N_3O$ 364.1450 found.

2-(4-(Quinolin-6-ylamino)phenyl)quinazolin-4(3H)-one (5v). White solid; yield 58%; mp: 246–248 °C; FT-IR (cm^{-1}): 3335, 3081, 2973, 1635, 1472, 1234; ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.63 (s, 1H), 9.92 (s, 1H), 8.59 (d, J = 8.4 Hz, 1H), 8.46 (dd, J = 8.0, 1.5 Hz, 2H), 7.96 (d, J = 8.9 Hz, 2H), 7.89 (d, J = 2.6 Hz, 1H), 7.88 – 7.92 (m, 1H), 7.81 (d, J = 8.9 Hz, 2H), 7.74 (dd, J = 8.2, 2.0 Hz, 1H), 7.62 (dd, J = 7.8, 3.6 Hz, 1H), 7.57 (d, J = 8.2 Hz, 1H), 7.52 – 7.55 (m, 2H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 164.7, 161.0, 159.8, 152.4, 151.6, 146.1, 140.5, 137.4, 136.3, 135.1, 132.2, 130.3, 129.9, 127.8, 124.6, 122.5, 115.9; HRMS (ESI-QTOF): m/z [M + H]$^+$ calcd. for $C_{23}H_{16}N_4O$ 365.1402 found 365.1406.

N-(4-Methyl-3-((4-(pyridin-3-yl)pyrimidin-2-yl)amino)phenyl)-4-((4-methylpiperazin-1-yl)methyl)benzamide (8). White solid; yield 84%; mp: 207–210 °C; FT-IR (cm^{-1}): 3422, 3289,

2965, 2966, 2938, 2810, 2720, 1630, 1480, 1452, 1414, 666; ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.17 (s, 1H), 9.28 (s, 1H), 9.00 (s, 1H), 8.70 (d, J = 1.8 Hz, 1H), 8.52 (d, J = 5.2 Hz, 1H), 8.48 (s, 1H), 8.09 (s, 1H), 7.91 (d, J = 8.2 Hz, 2H), 7.53 (dd, J = 8.1, 4.7 Hz, 1H), 7.49 (d, J = 8.2 Hz, 1H), 7.45–7.42 (m, 3H), 7.21 (d, J = 8.4 Hz, 1H), 3.53 (s, 2H), 2.37 (s, 8H), 2.23 (s, 3H), 2.15 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 165.7, 162.0, 161.6, 159.9, 151.8, 148.6, 142.5, 138.2, 137.6, 134.8, 134.2, 132.6, 130.5, 129.1, 128.0, 128.0, 124.2, 117.6, 117.2, 107.9, 62.0, 55.1, 53.0, 46.2, 18.1; HRMS (ESI-QTOF): *m/z* $[M + H]^+$ calcd. for $C_{29}H_{32}N_7O$ 494.2668 found 494.2672.

4-(Benzo[d]thiazol-2-yl)aniline (5w). White solid; yield 26%; ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.03 (dd, J = 7.9, 0.6 Hz, 1H), 7.93–7.87 (m, 1H), 7.82–7.64 (m, 1H), 7.37–7.30 (m, 1H), 6.71–6.55 (m, 1H), 5.91 (s, 1H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 168.6, 154.3, 152.6, 134.1, 129.2, 126.6, 124.7, 122.3, 122.2, 120.5, 114.0; HRMS (ESI-QTOF): *m/z* $[M+H]^+$ calcd. for $C_{13}H_{11}N_2S$ 227.0637, found 227.0647.

2-(2-Aminophenyl) quinazolin-4(3H)-one (5x). White solid; yield 21%; ^{1}H NMR (500 MHz, DMSO-d_6): δ 12.36 (s, 1H), 8.15 (d, J = 7.2, 1H), 7.83 (t, 1H), 7.71 (d, J = 7.6, 1H), 7.52 (t, 1H), 7.4 (d, J = 7.8, 1H), 7.31 (d, J = 7.2, 1H), 7.1 (t, 1H), 5.32 (s, 1H). ^{13}C NMR (126 MHz, DMSO-d_6): δ 162.6, 153.5, 149.4, 149.3, 135.0, 133.9, 129.5, 127.8, 126.7, 126.3, 212.4, 117.3, 115.4, 113.3; HRMS (ESI-QTOF): *m/z* $[M+H]^+$ calcd. for $C_{14}H_{12}N_3O$ 238.0975, found 238.098.

III-1. Emission quenching experiments:

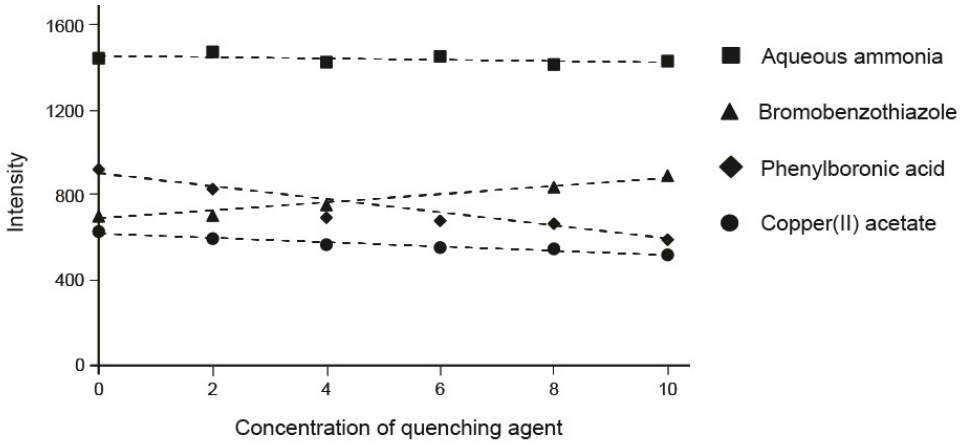


Figure S1. $[Ru(bpy)_3]^{2+}$ emission quenching by aqueous ammonia, bromobenzothiazole, phenylboronic acid, and copper (II) acetate. Note the increase in emission intensity of tris(bipyridine)ruthenium(II) chloride (100 μM) after addition of increasing volumes of aqueous

ammonia (0-10 μL) in $CH_3CN:H_2O$ (1:1) and the slight decrease in emission intensity $[Ru(bpy)_3]^{2+}$ (200 μM) after addition of increasing concentrations of bromobenzothiazole (0-10 mM) in *N,N* dimethylformamide. The emission intensity of $[Ru(bpy)_3]^{2+}$ (100 μM) is decreased significantly after addition of increasing concentrations of phenylboronic acid (0-20 mM) and copper (II) acetate (0-10 mM) in $CH_3CN:H_2O$ (1:1).

2. Determination of reaction quantum yield:

The quantum yield calculation of the reaction was determined in two stages:

Determination of the light intensity obtained from the CFL lamp:

The photon flux of the CFL lamp was obtained using the standard potassium ferrioxalate actinometer method described in literature.[1,2] The iron (III) actinometer complex potassium trisoxalatoferrate(III) trihydrate was synthesized according to literature reports.[3] For the evaluation of the light intensity an experiment was set by preparing a 0.15 M solution of ferrioxalate actinometer by dissolving 0.737 g of potassium tris oxalato ferrate trihydrate complex

in 10 mL of a 0.05 M H_2SO_4 solution. A 0.2% by weigh solution of 1,10-phenanthroline ligand was prepared in a buffer solution prepared by dissolving 5.63 g sodium acetate in 25 mL of a 0.5 M solution H_2SO_4 Both solutions were stored in the dark. The actinometer measurement was done as follows: 2.0 mL of actinometer solution was placed in a cuvette and irradiated for 90 seconds, after irradiation, of the actinometer solution, 0.35 mL of the phenanthroline solution was added to the cuvette and the mixture was allowed to stir in the dark for 1.0 h to allow the complexation of phenanthroline ligand with the produced ferrous forming $[Fe(phen)_3]^{2+}$ complex whose absorbance was measured after dilution (1:1) at λ 510 nm against reagent blank. Using the similar procedure, a non-irradiated sample (which contains actinometer solution, buffer, and phenanthroline ligand in the same proportion as mentioned except it is not irradiated) was also prepared and its absorbance at λ 510 nm was also measured. The moles of Fe^{2+} formed can be determined according to the Beer's Laws using equation:[4]

$$\text{moles of } Fe^{2+} = \frac{V(L)\times\Delta A(510)nm}{l(cm)\times\varepsilon(L\,mol^{-1}cm^{-1}} = 4.08 \times 10^{-7}$$

Where V is the total volume of the solution (0.00235 L) after addition of all reagents, ΔA is the difference in absorbance at λ 510 nm between the irradiated and non-irradiated actinometer solutions (2.05 - 0.12). l is the path length (1.00 cm), and ε is the molar absorptivity of the

ferrioxalate actinometer at λ 510 nm (11,100 L $mol^{-1}cm^{-1}$). The photon flux of the CFL lamp was calculated as under:[5]

$$\text{Photon flux} = \frac{moles\ of\ Fe^{2+}}{\emptyset \times t \times f} = 4.08 \times 10^{-9}$$

Where Φ is the quantum yield for the ferrioxalate actinometer (1.12), t is the irradiation time (90 s), and f is the fraction of light absorbed by the ferrioxalate actinometer. An absorption spectrum gave an absorbance value of >3, indicating that the fraction of absorbed light (f) is > 0.999. The photon flux was thus calculated (average of three experiments) to be 4.08 x 10^{-9} Einstein's s^{-1}.

2. Determination of Reaction quantum yield: 2-(4-Bromophenyl)benzothiazole (22.3 mg, 0.077 mmol, 1.0 equiv), aq. ammonia (0.0.3 ml, 0.77 mmol, 10 equiv), $Cu(OAc)_2$ (0.7 mg, 0.003 mmol, 0.05 equiv), $[Ru(bpy)_3]Cl_2$ (2.9 mg, 0.003 mmol, 0.05 equiv), DIPEA (0.2 mL, 0.116 mmol, 1.5 equiv), phenyl boronic acid (10.3 mg, 0.085 mmol, 1.1 equiv), and 0.5 ml each of MeCN and H_2O (HPLC grade) were placed in a quartz cuvette. The sample was stirred and irradiated for 90s. After irradiation, the yield of product **5a** formed was determined using GC technique. The yield of the product **5a** formed after 90s of irradiation with 27W CFL was found to be 1.25 % corresponding to (2.2 × 10^{-6} mol). The reaction quantum yield (Φ) was then arrived at using equation:[6]

$$\emptyset = \frac{moles\ of\ product\ formed}{photon\ flux \times t \times f}$$

Where the photon flux is 4.05 x 10^{-9} einsteins s^{-1} (determined by actinometry as described in step 1), t is the reaction time (90 s) and f is the fraction of incident light absorbed by the reaction mixture. An initial absorption spectrum of the aforementioned reaction mixture gave an absorbance value of > 3 at 410 nm, indicating that essentially all the incident light is absorbed by the photo catalyst in the reaction mixture and therefore (f ~ 0.999).

The reaction quantum yield (Φ) was thus determined to be 6.04. Quantum yields greater than 1 are normally the hallmark of photo-induced chain reactions, in which a single photon triggers a chain of transformations diagnostic of radical path of the reaction.[7]

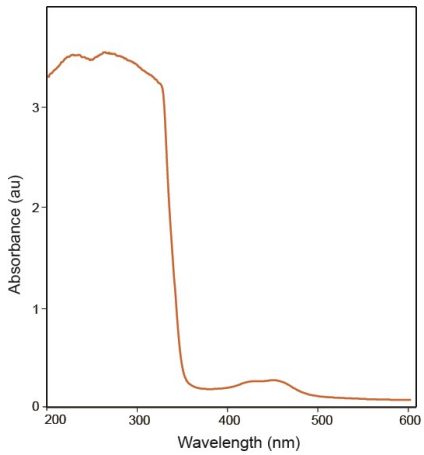


Figure S2: Initial absorption spectra of the reaction mixture showing the absorption > 3 indicating that essentially all the incident light is absorbed by the photo catalyst and therefore (f ~0.999).

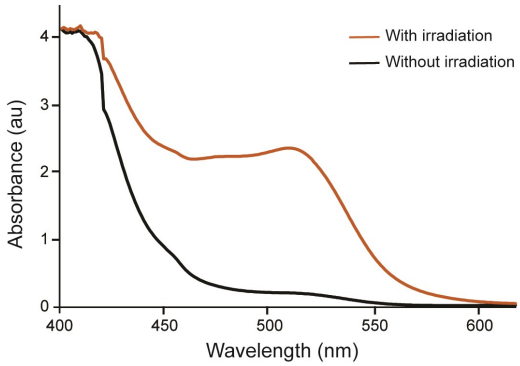


Figure S3. Absorption spectra's of actinometer solution without and after irradiation for 90s.

References:

1. T. Aillet, K. Loubière, O. Dechy-Cabaret, L. Prat, Accurate Measurement of the Photon Flux Received inside Two Continuous Flow Microphotoreactors by Actinometry, *International Journal of Chemical Reactor Engineering* 2014, **12** (1), 1–13.
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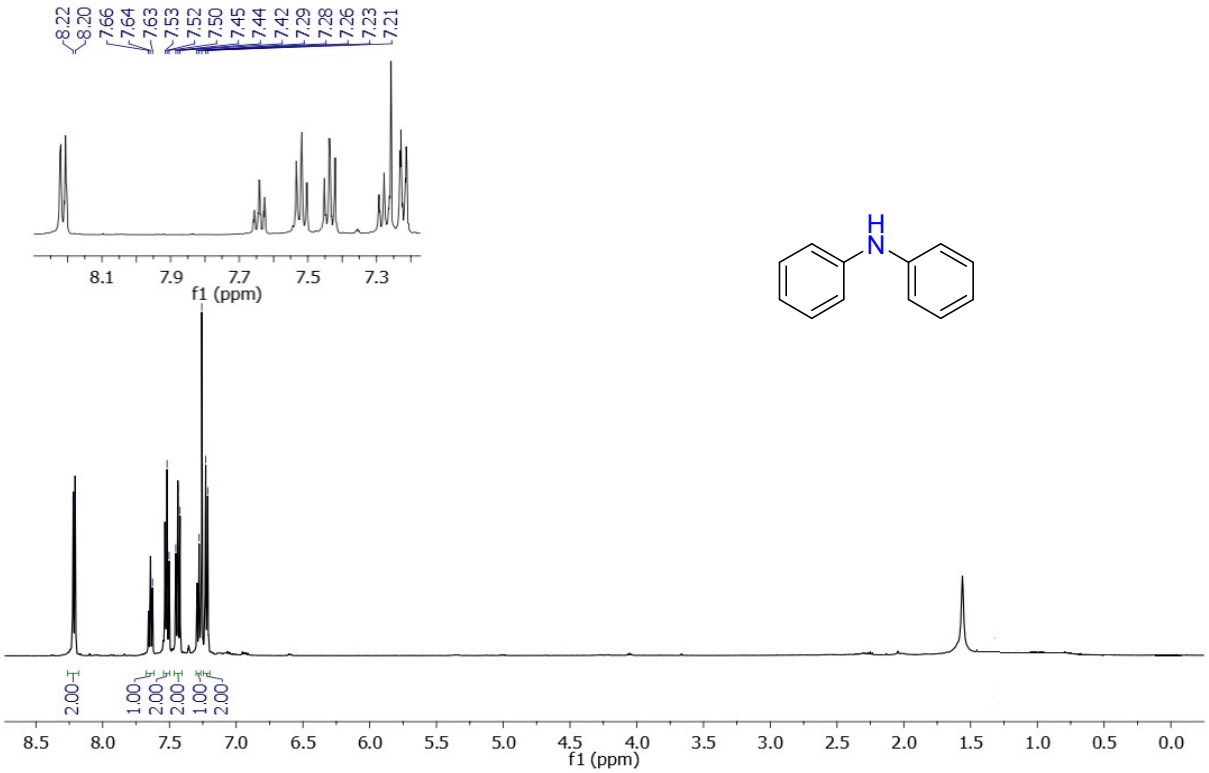
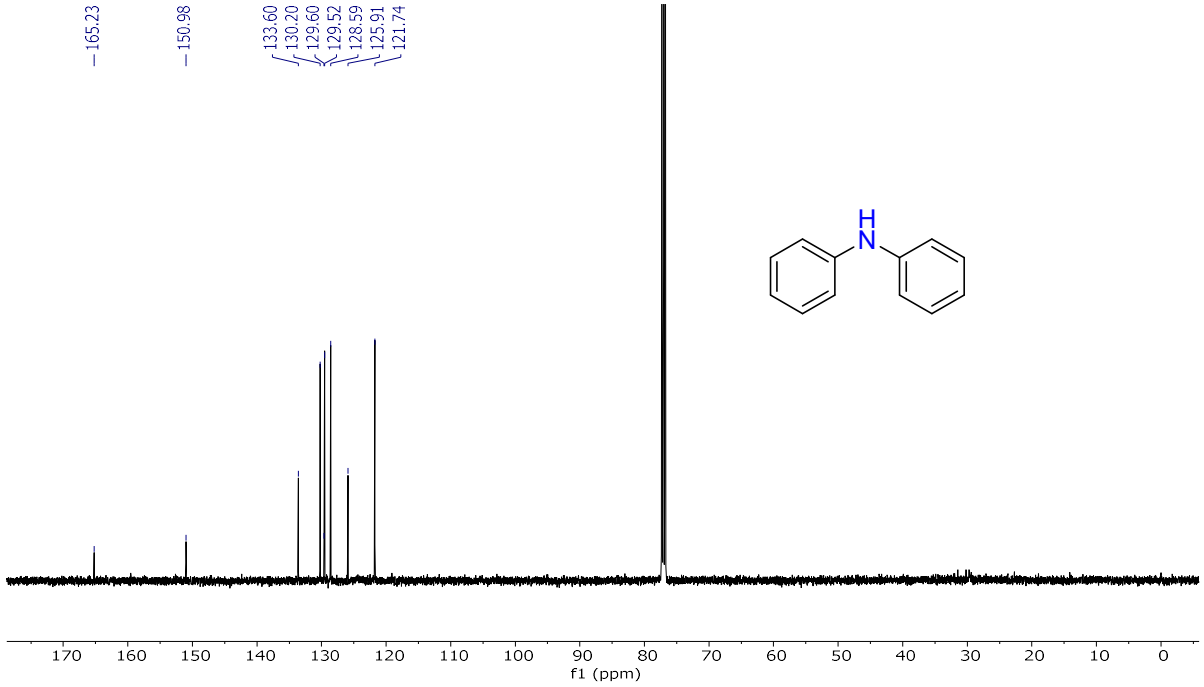
7. G. A. Crosby, J. N. Demas, Measurement of Photoluminescence Quantum Yields. Review, *The Journal of Physical Chemistry* 1971, **75** (8), 991–1024.

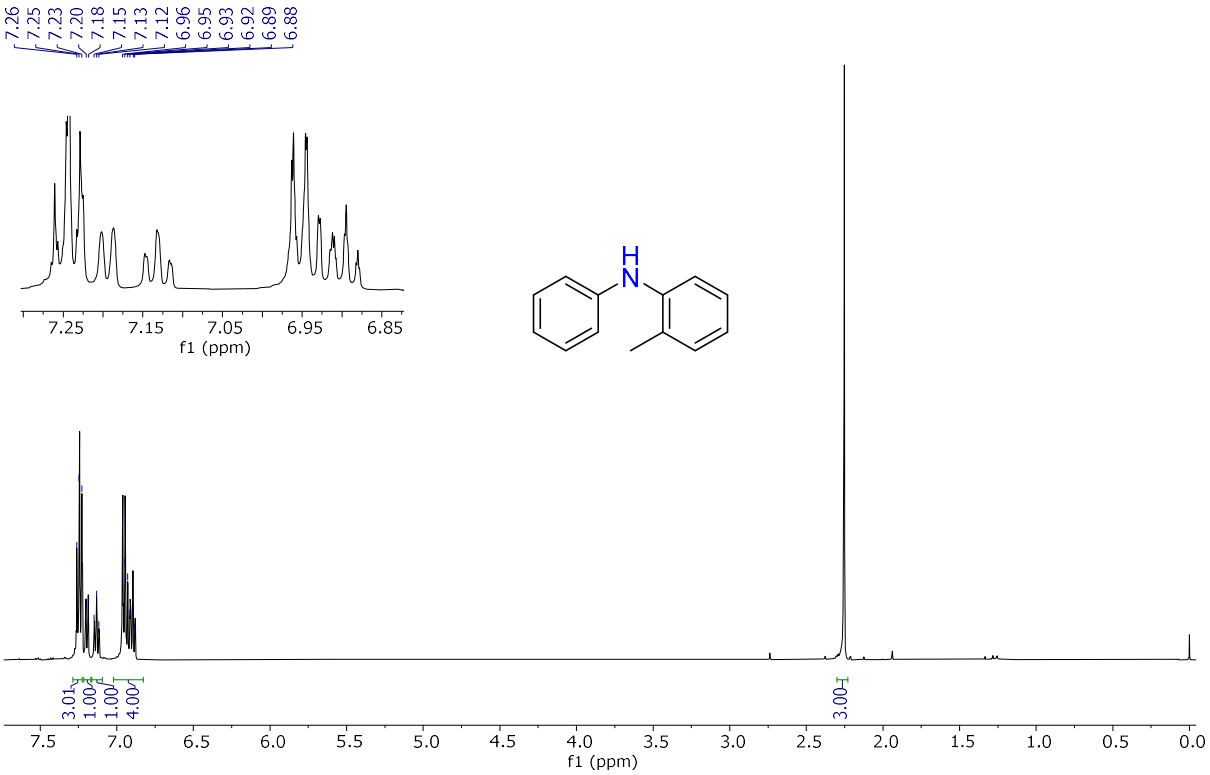
IV. Copies of NMR Spectra:



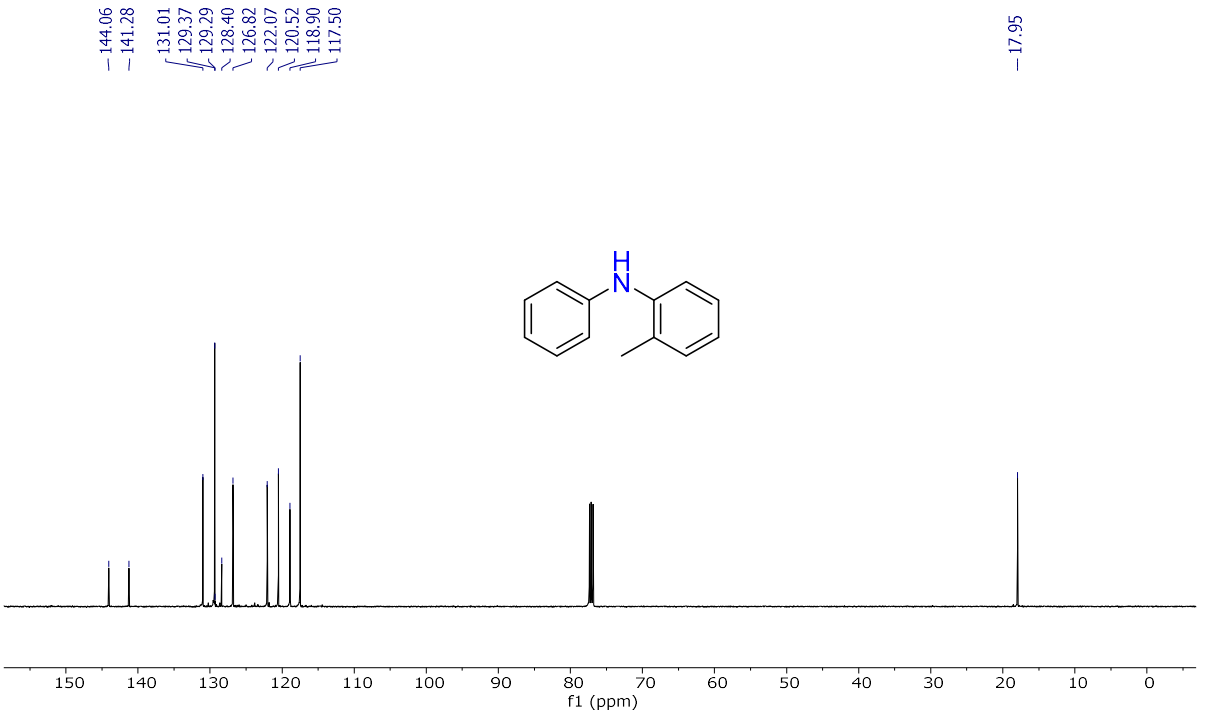
Compound **3a**: ^{1}H NMR (500 MHz, $CDCl_3$).



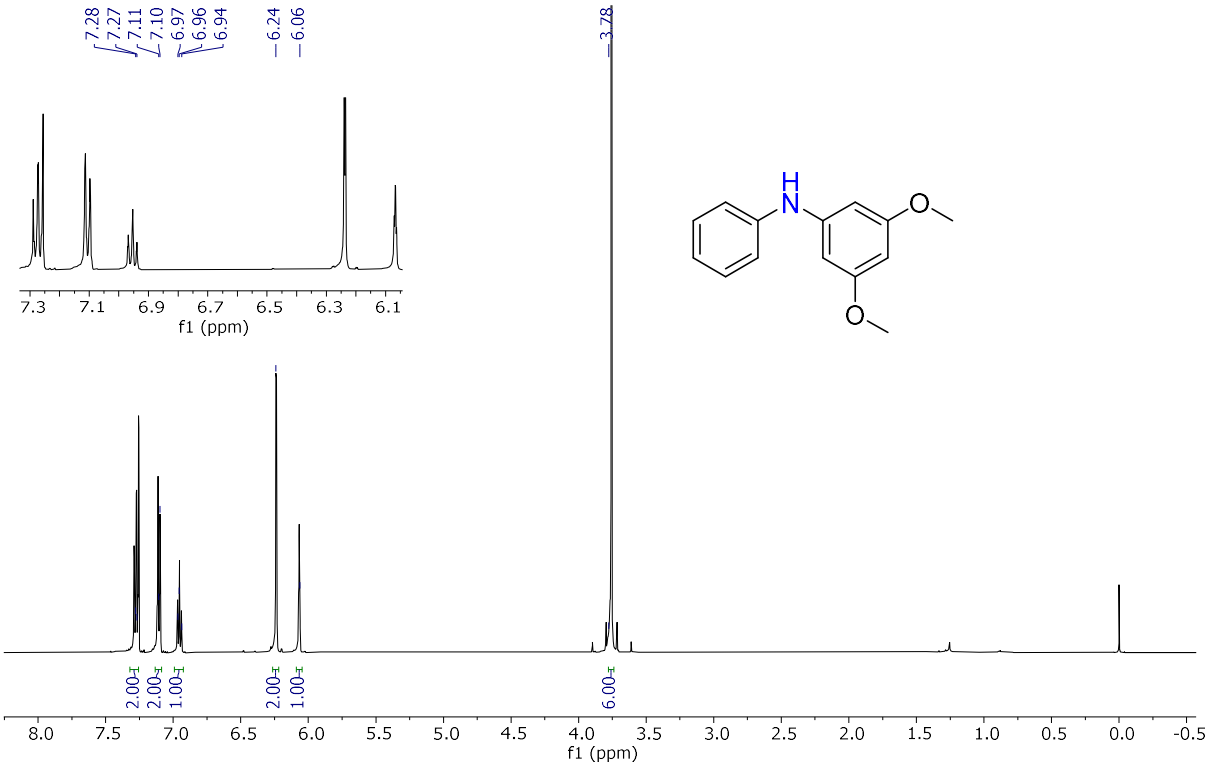
Compound **3a**: ^{13}C NMR (125 MHz, $CDCl_3$).



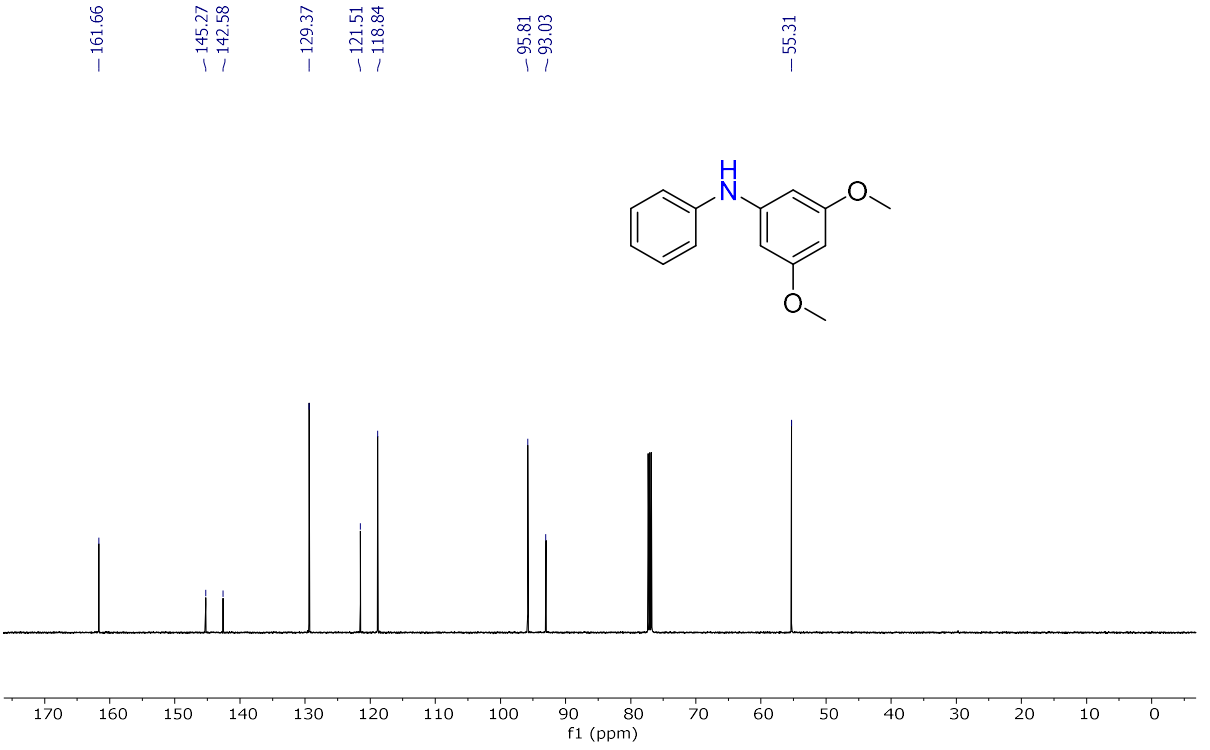
Compound **3b**: ^{1}H NMR (500 MHz, $CDCl_3$).



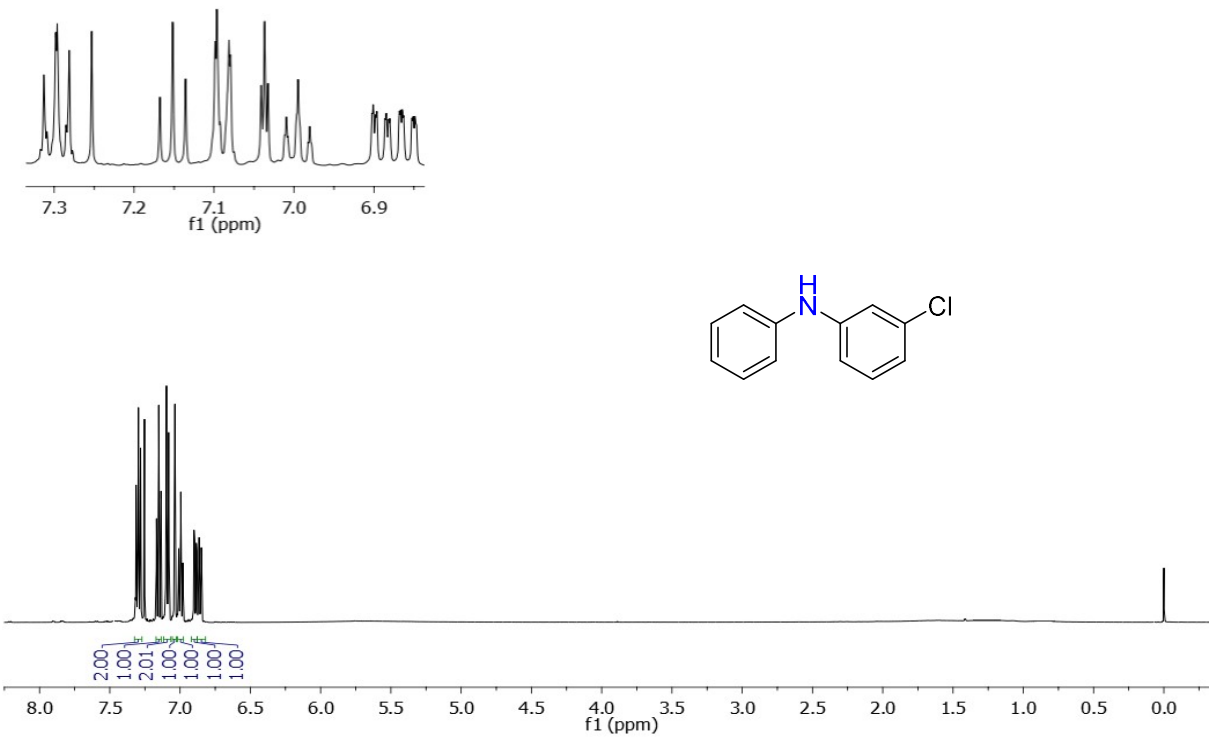
Compound **3b**: ^{13}C NMR (125 MHz, $CDCl_3$).



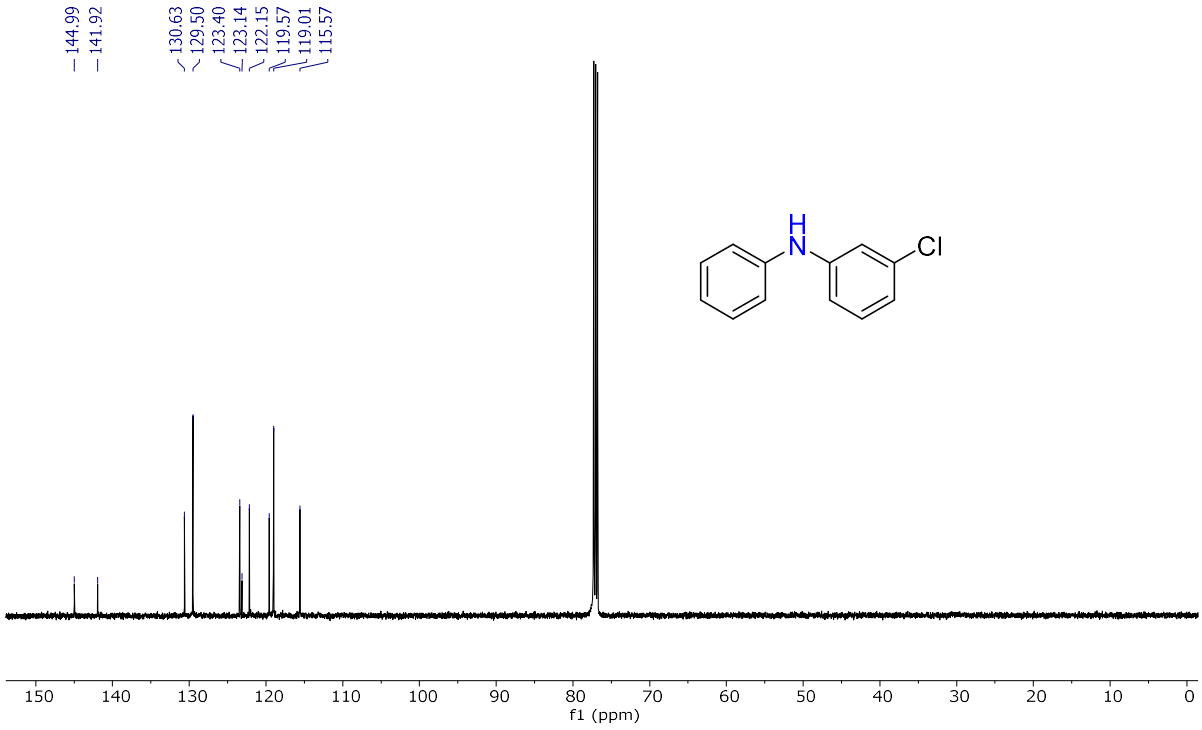
Compound **3c**: ^{1}H NMR (500 MHz, $CDCl_3$).



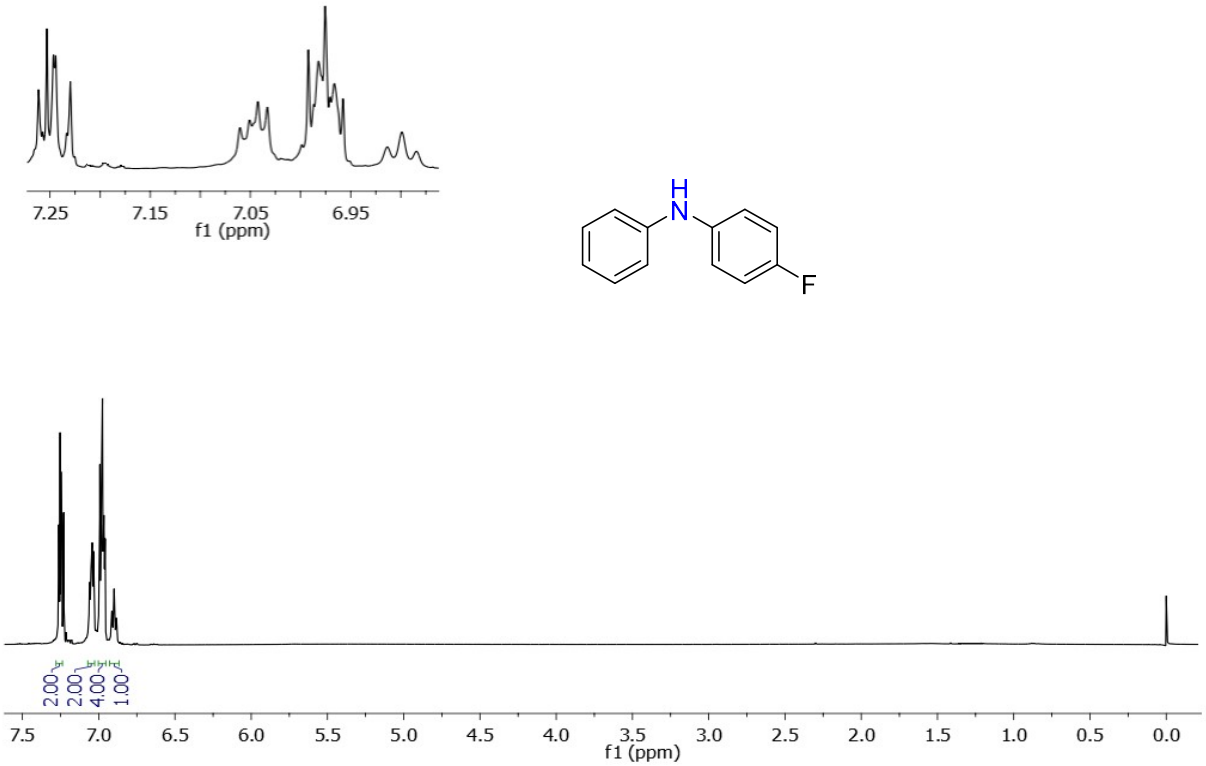
Compound **3c**: ^{13}C NMR (125 MHz, $CDCl_3$).



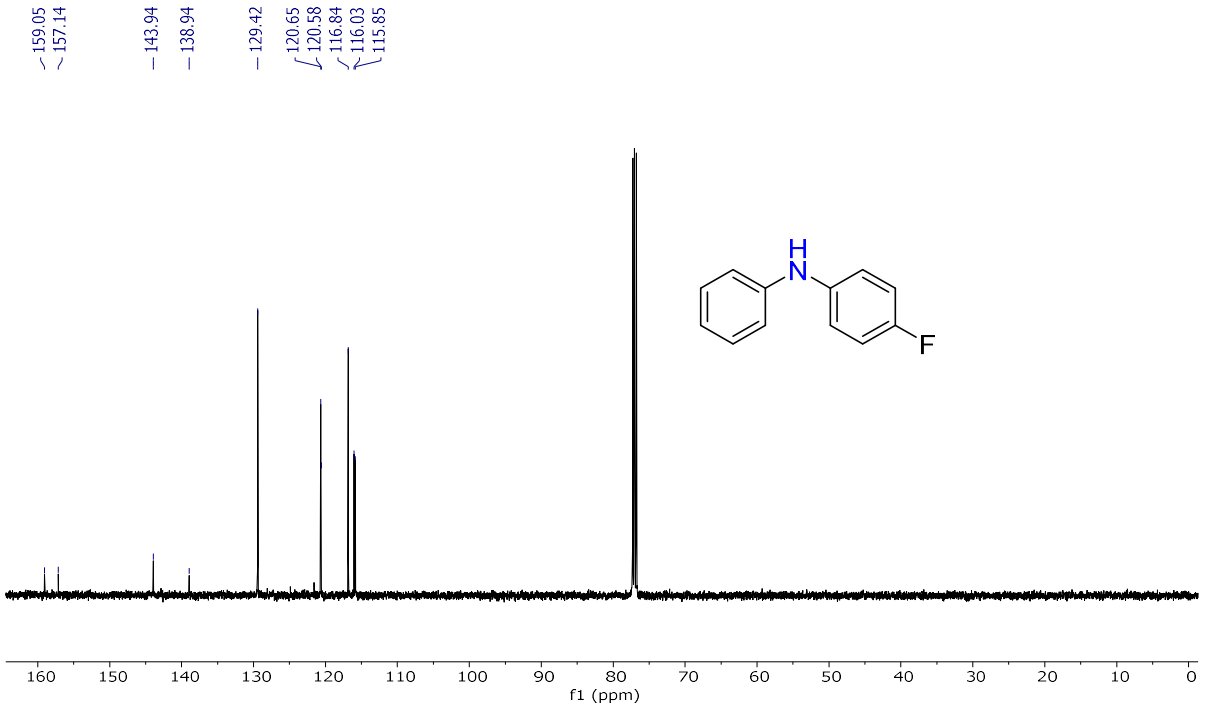
Compound **3d**: ^{1}H NMR (500 MHz, $CDCl_3$).



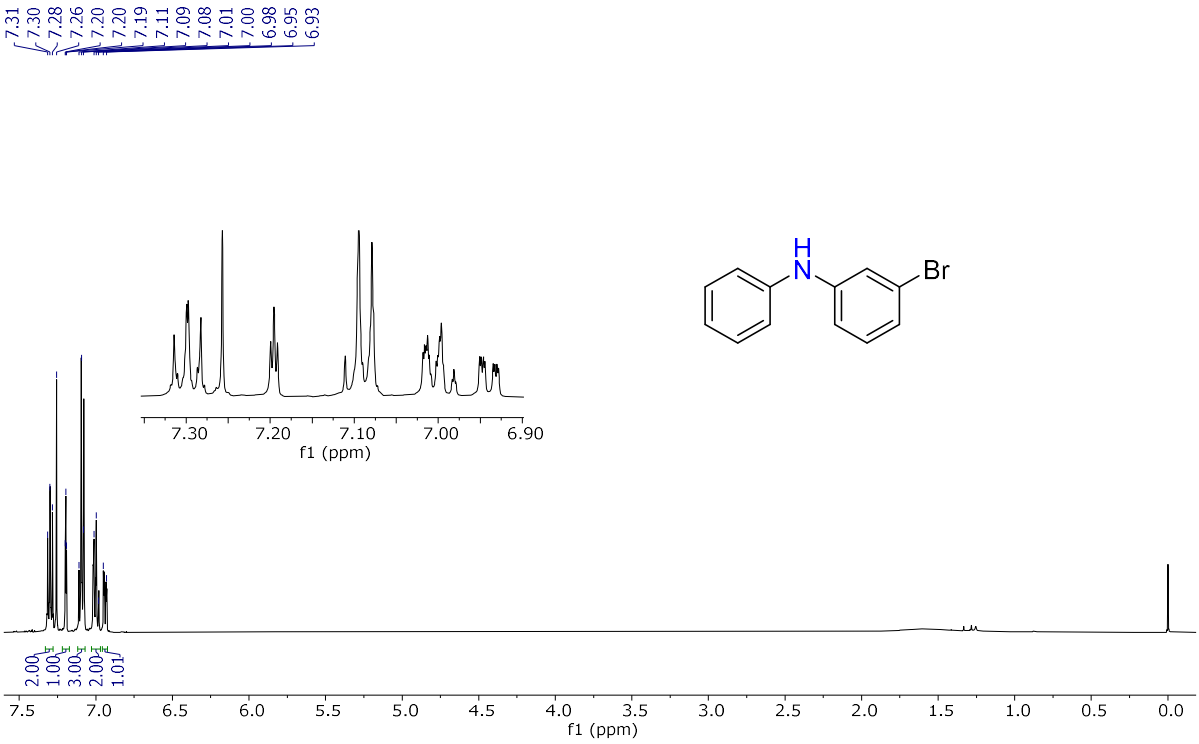
Compound **3d**: ^{13}C NMR (125 MHz, $CDCl_3$).



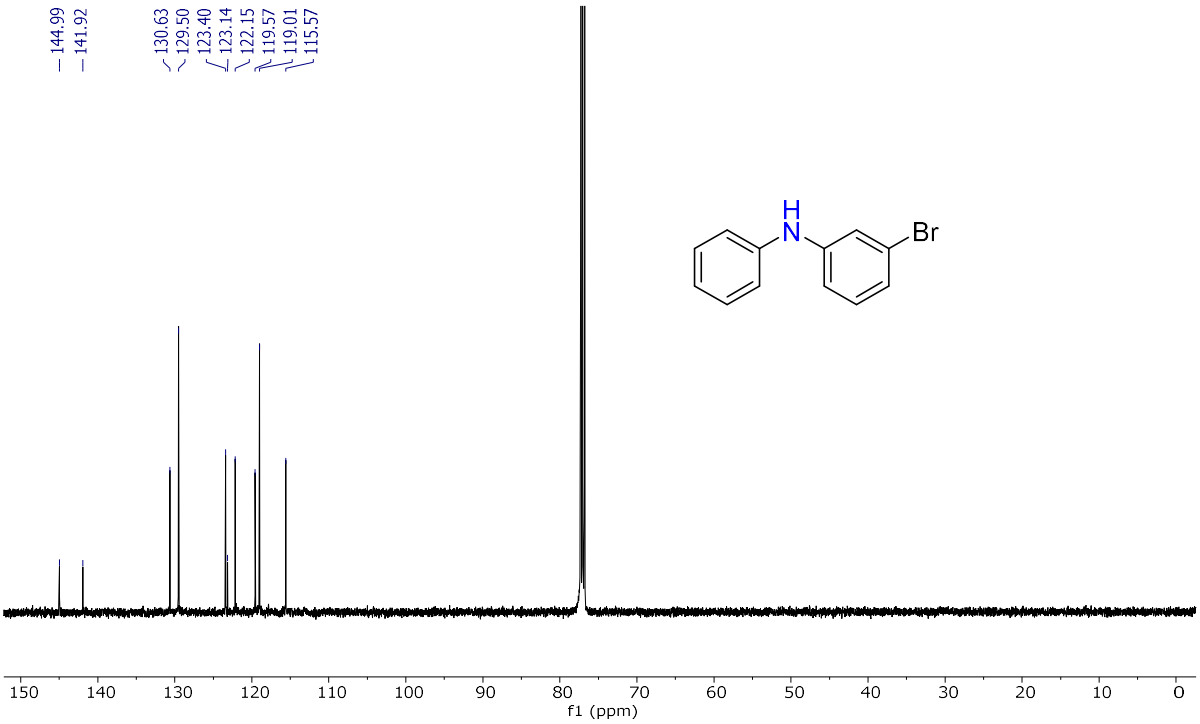
Compound **3e**: ^{1}H NMR (500 MHz, $CDCl_3$).



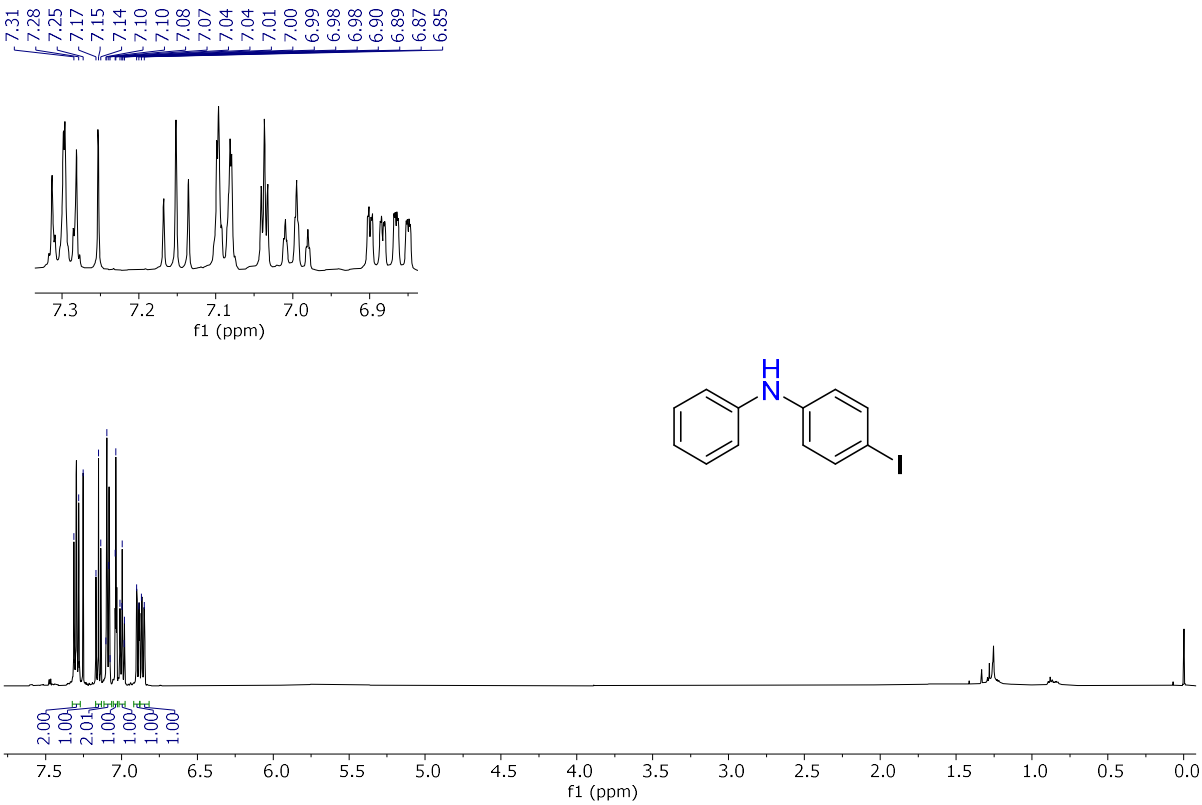
Compound **3e**: ^{13}C NMR (125 MHz, $CDCl_3$).



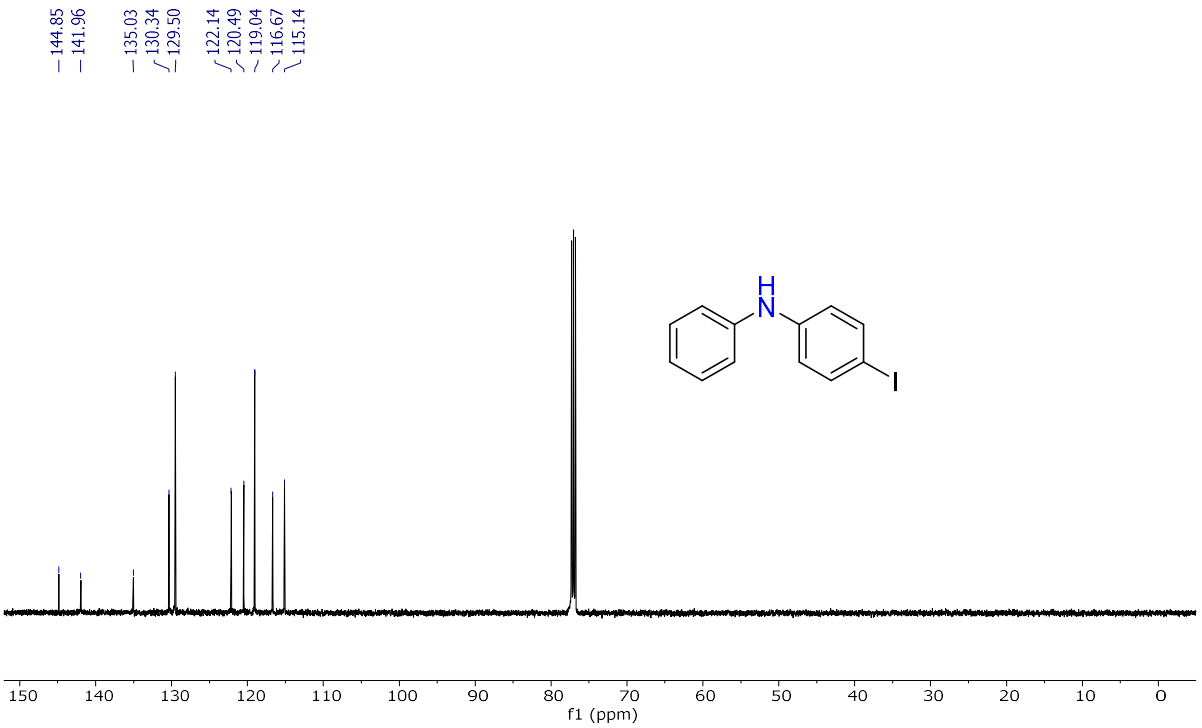
Compound **3f**: ^{1}H NMR (500 MHz, $CDCl_3$).



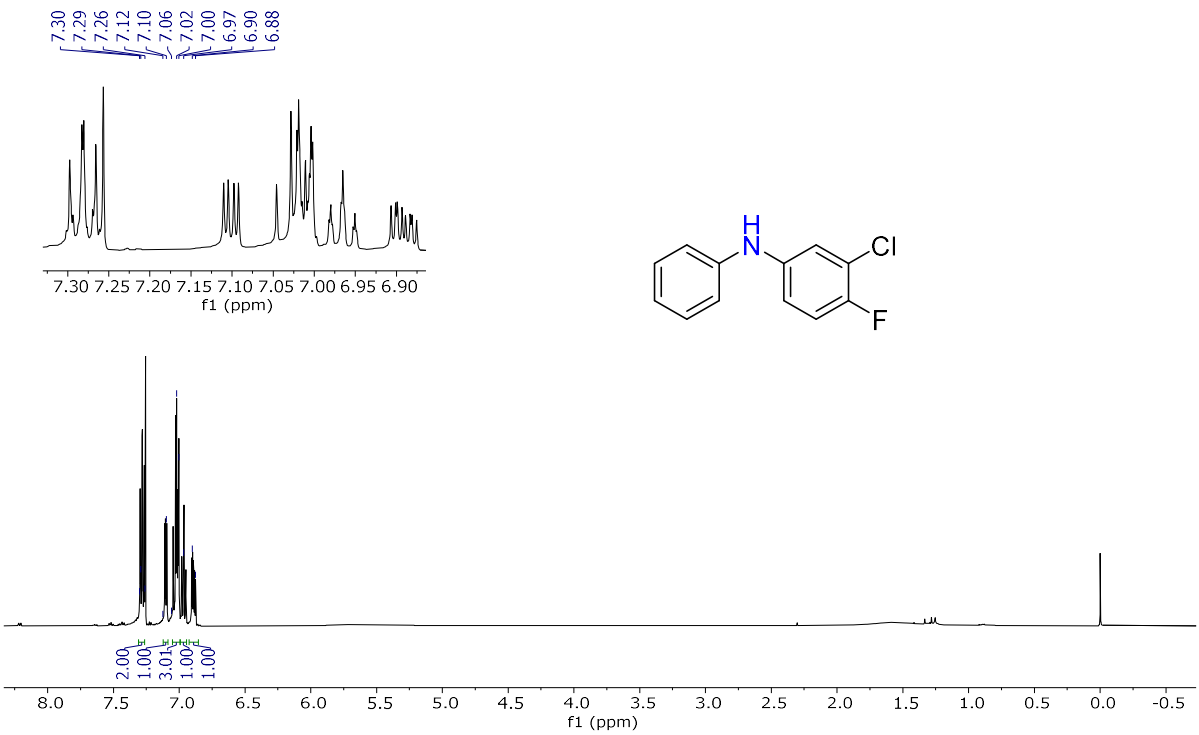
Compound **3f**: ^{13}C NMR (125 MHz, $CDCl_3$).



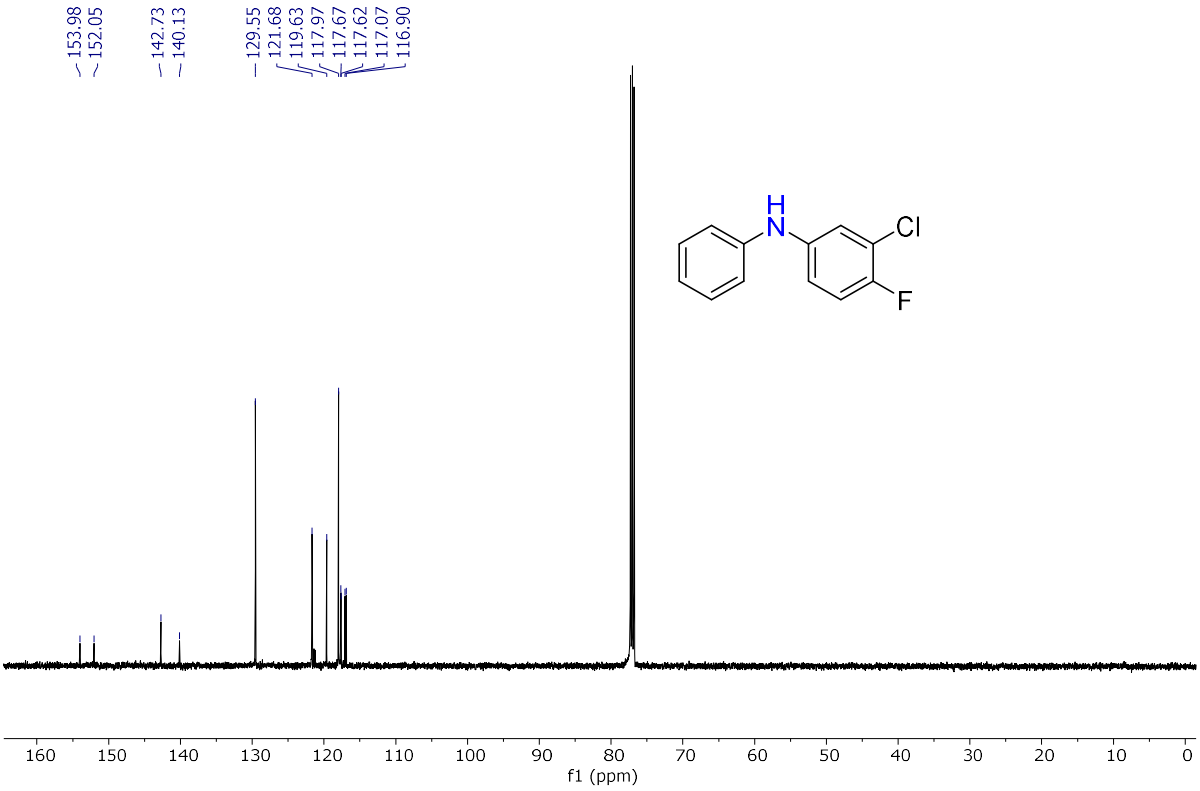
Compound **3g**: ^{1}H NMR (500 MHz, $CDCl_3$).



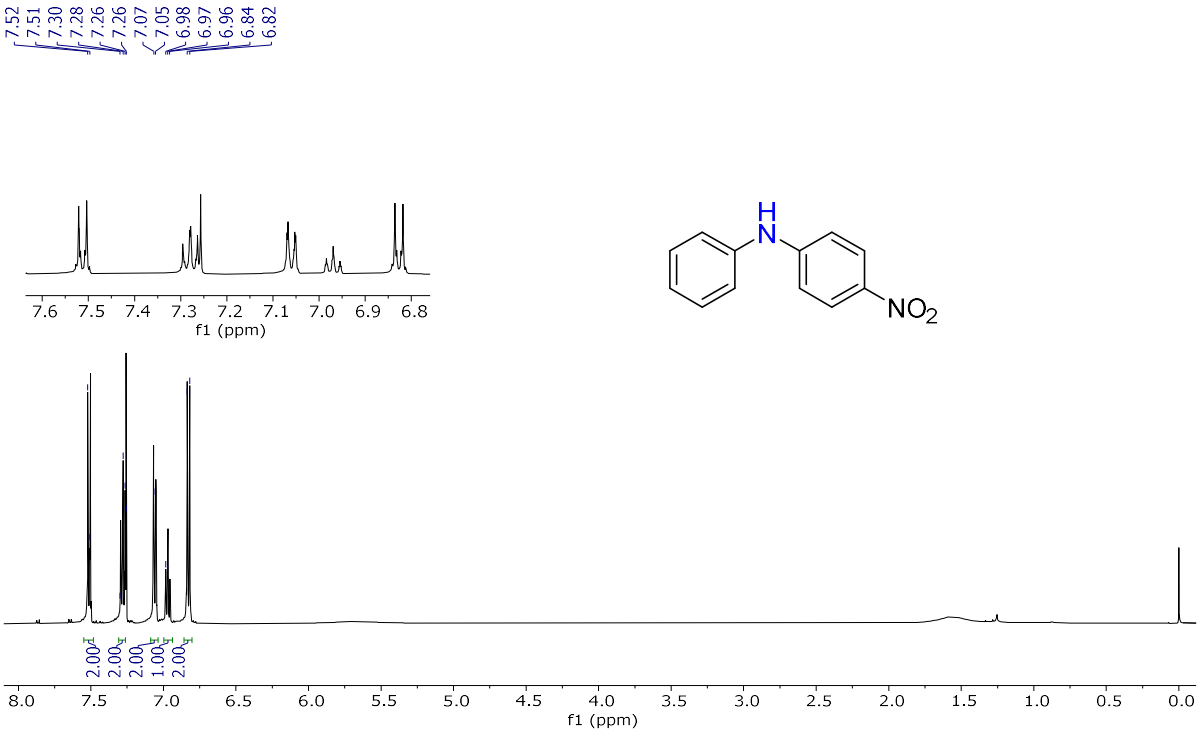
Compound **3g**: ^{13}C NMR (125 MHz, $CDCl_3$).



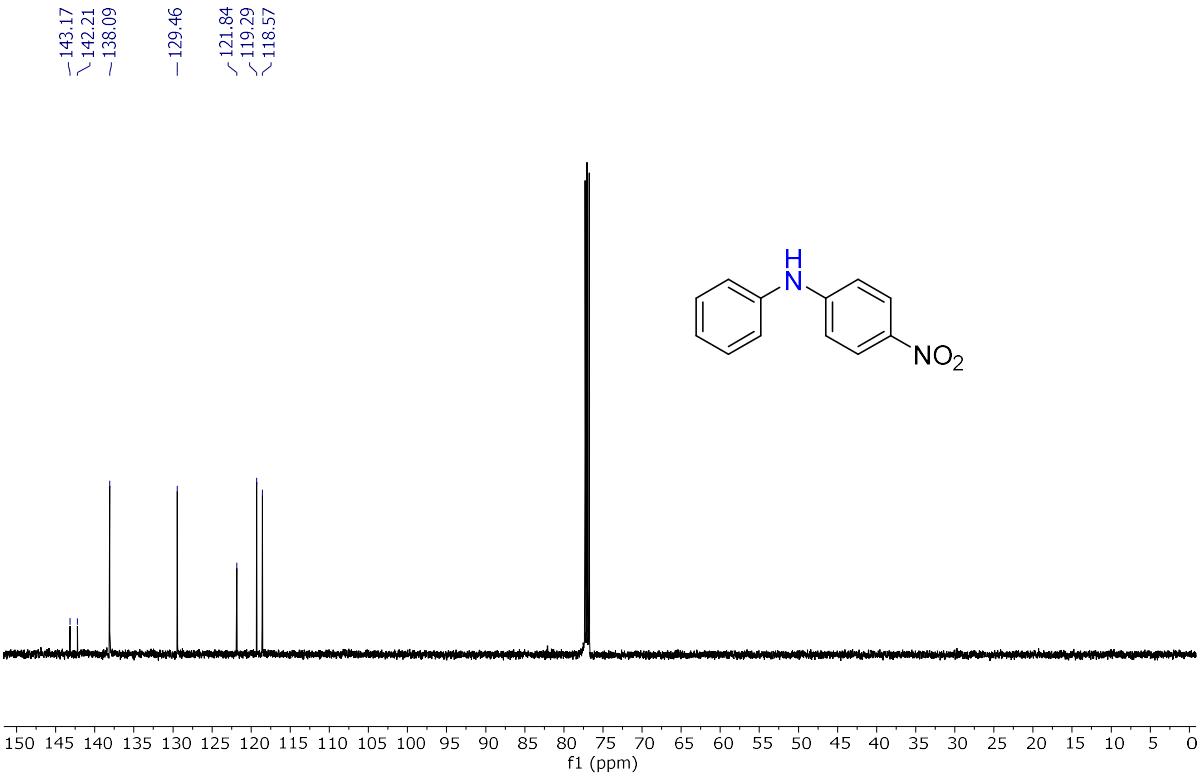
Compound **3h**: ^{1}H NMR (500 MHz, $CDCl_3$).



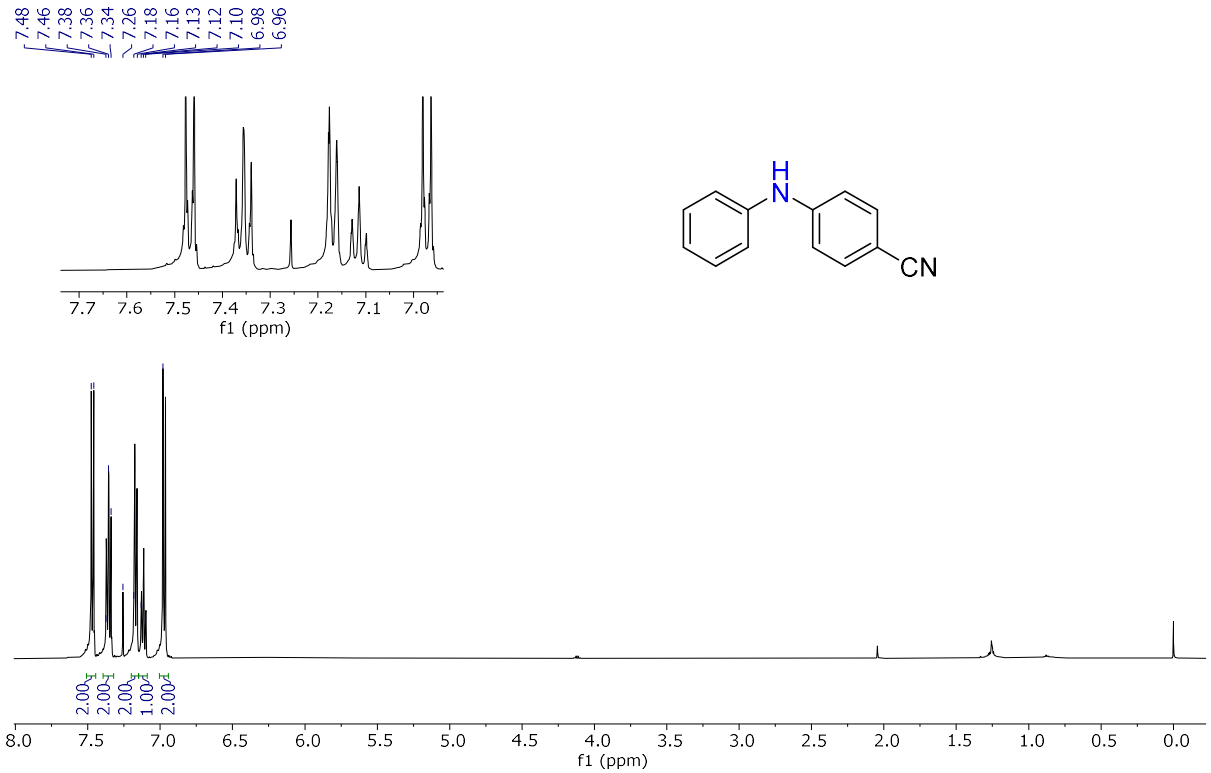
Compound **3h**: ^{13}C NMR (125 MHz, $CDCl_3$).



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



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



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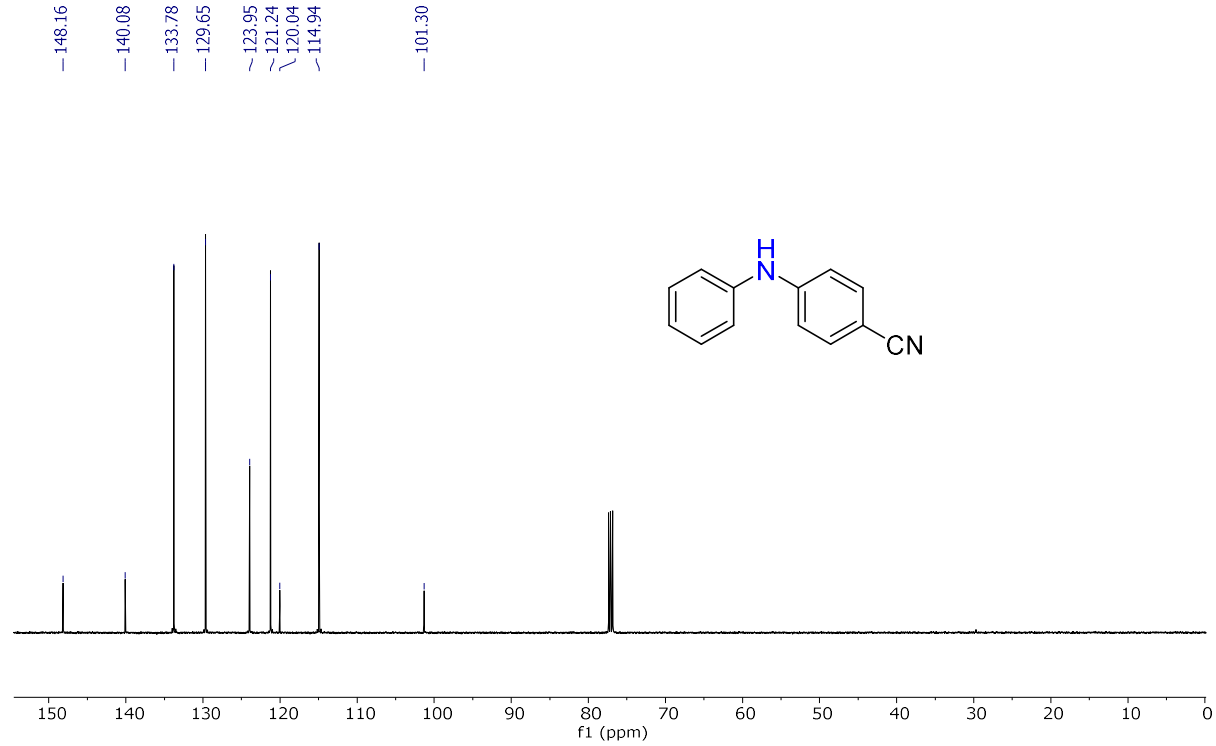
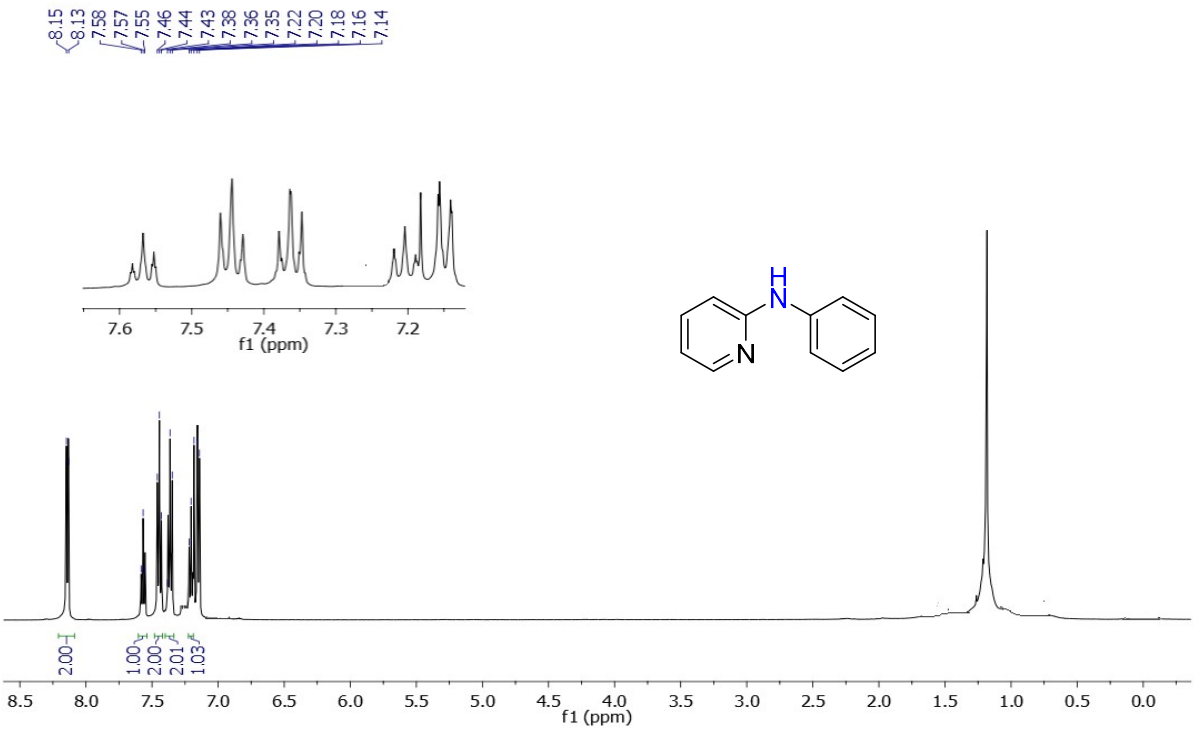


Compound **3j**: ^{13}C NMR (125 MHz, $CDCl_3$).



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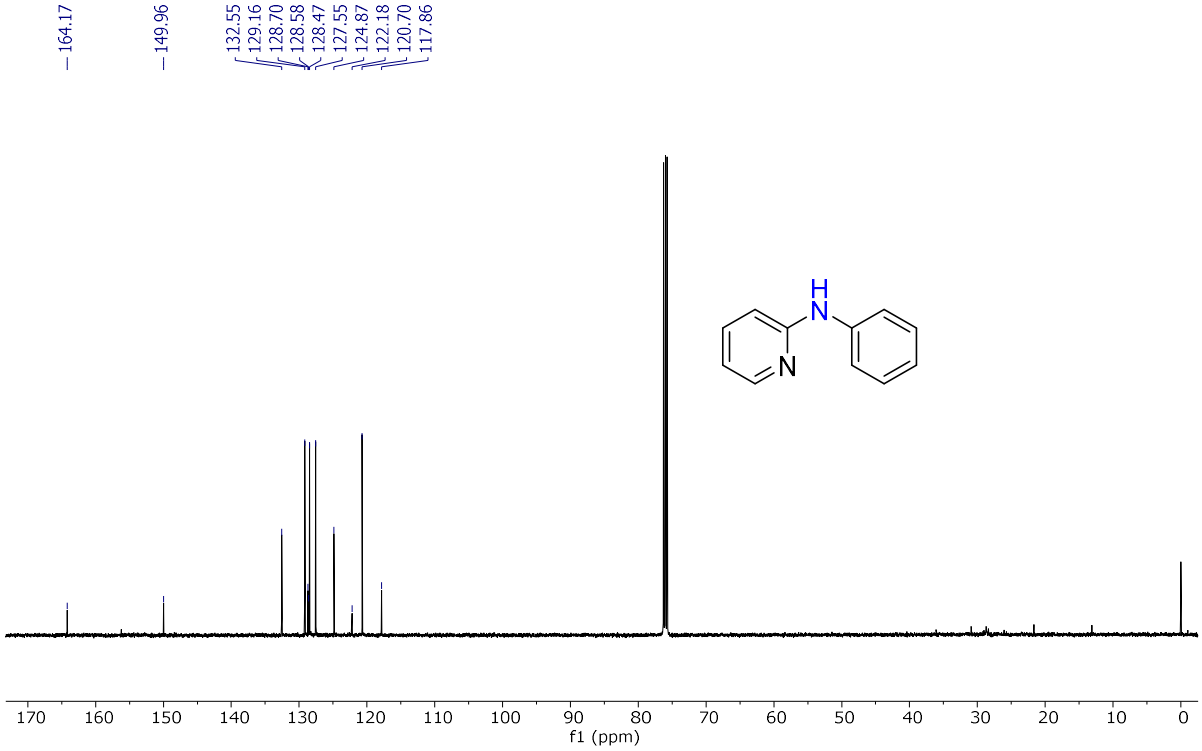
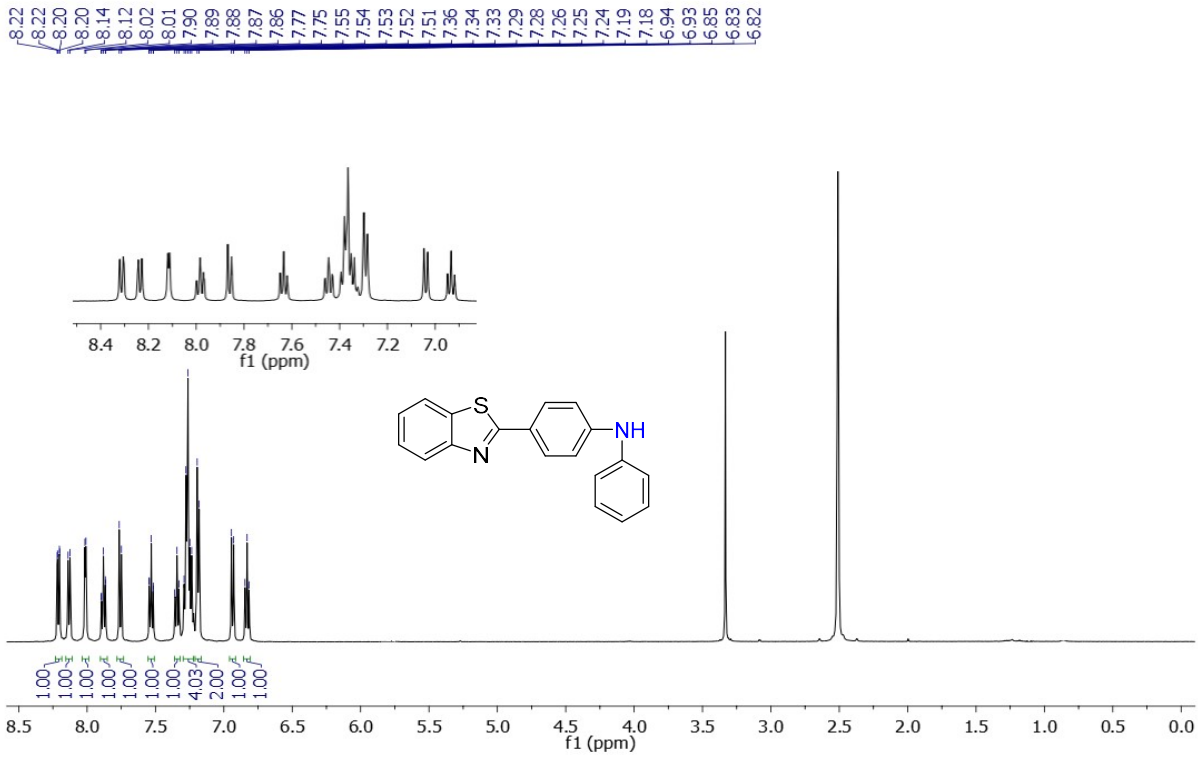
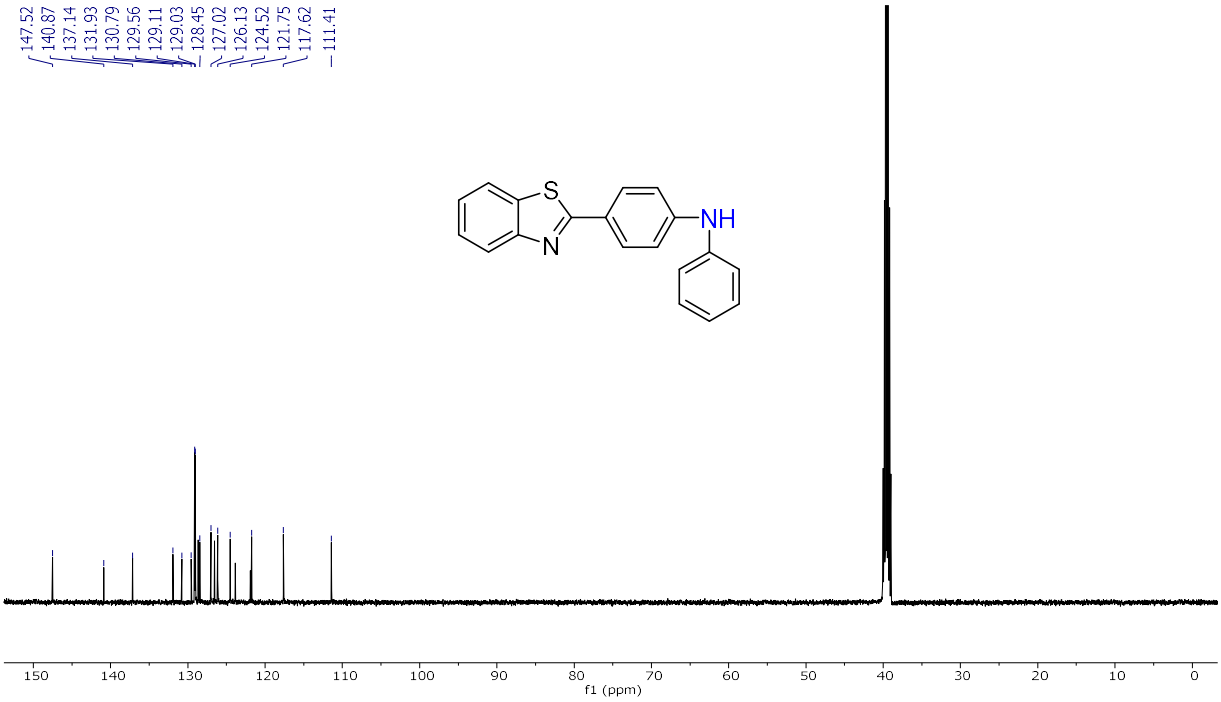


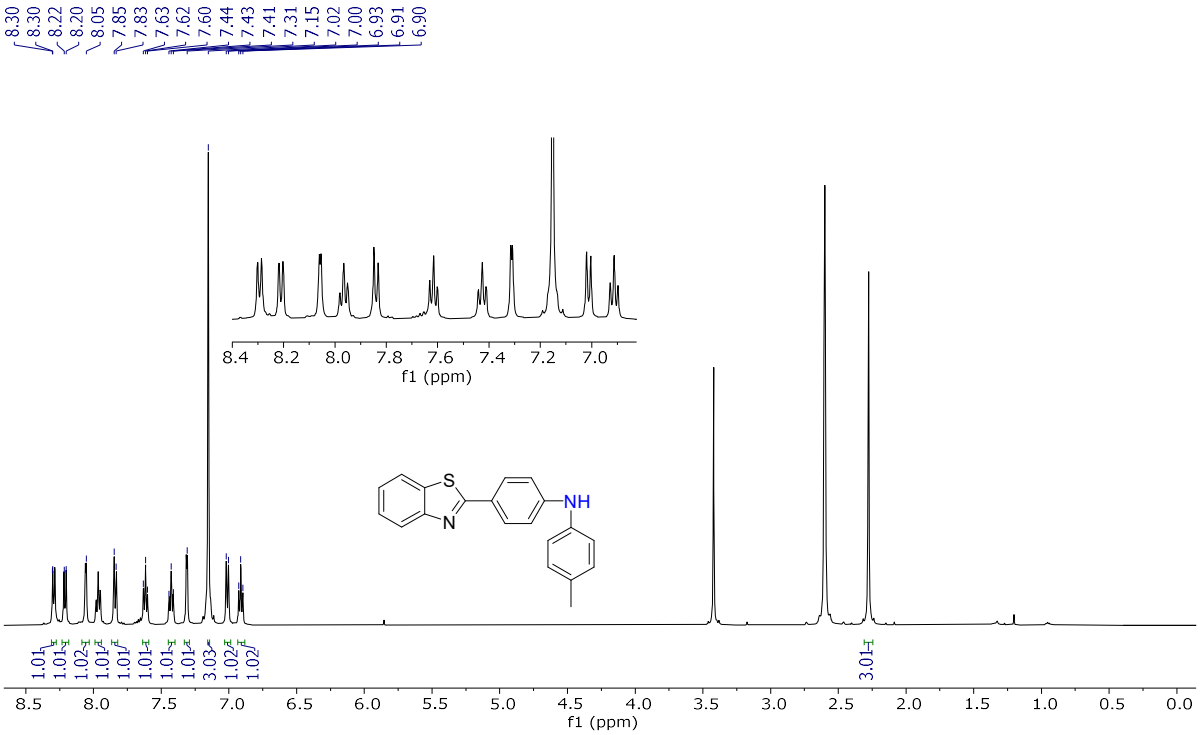
Compound **3k**: ^{13}C NMR (125 MHz, $CDCl_3$).



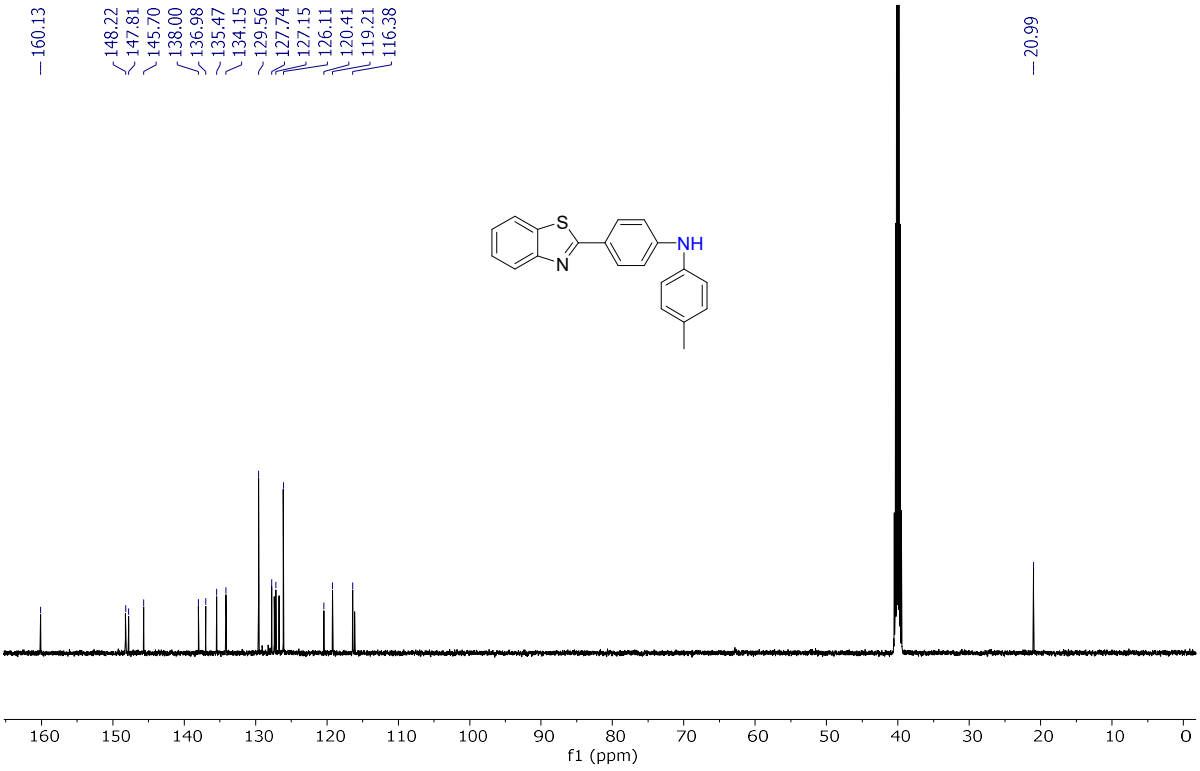
Compound **5a**: ^{1}H NMR (500 MHz, DMSO-d_6).



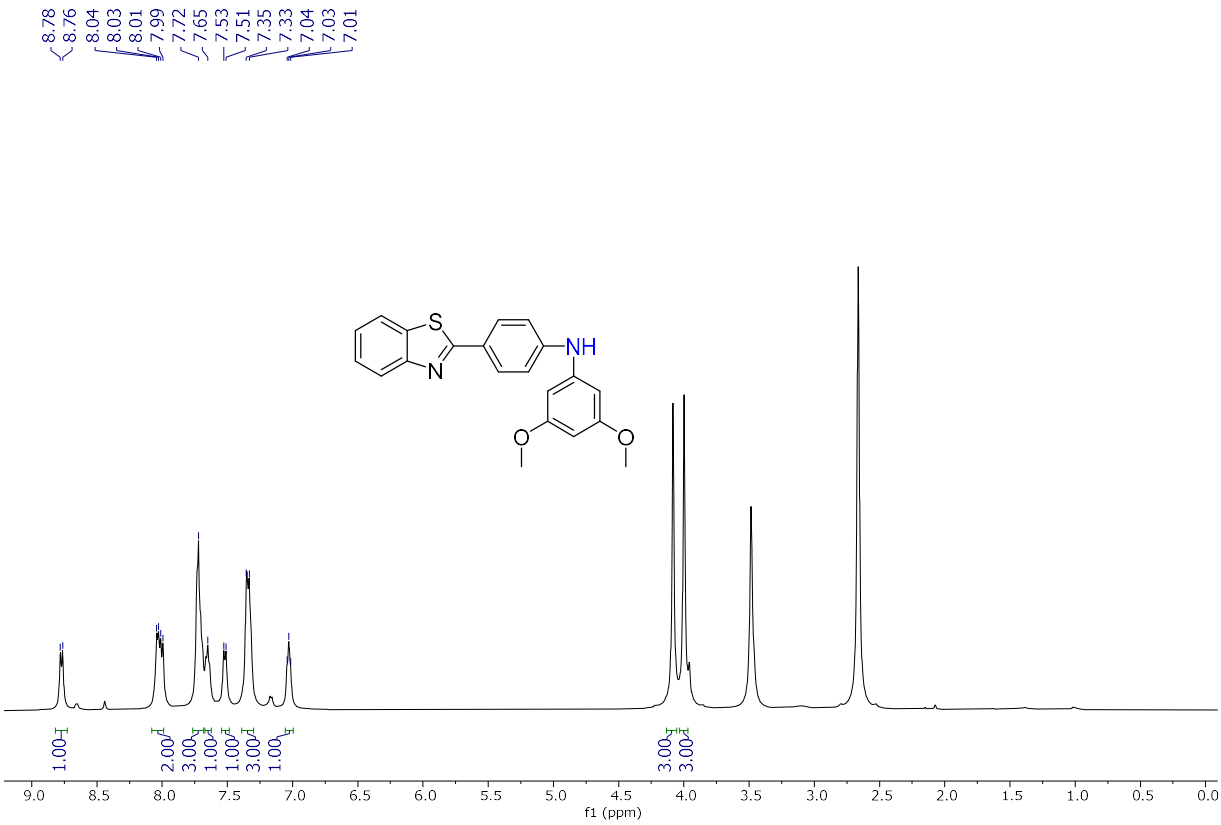
Compound **5a**: ^{13}C NMR (125 MHz, DMSO-d_6).



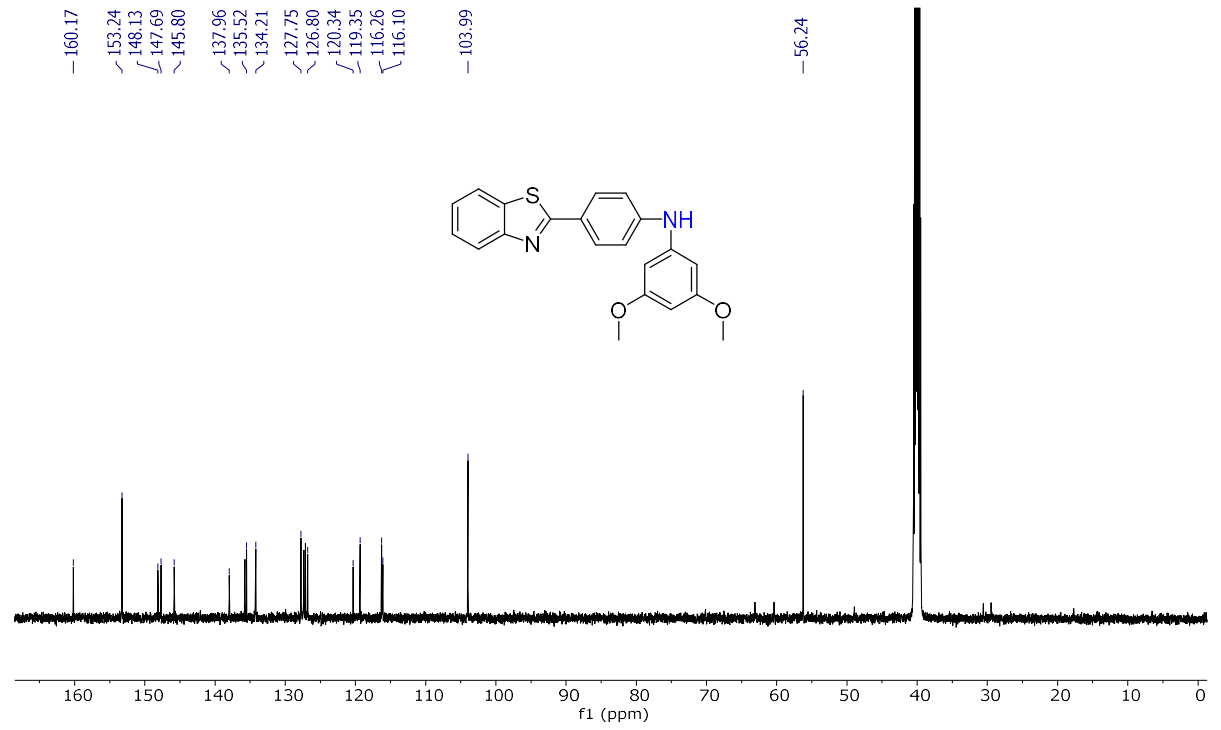
Compound **5b**: ^{1}H NMR (500 MHz, DMSO-d_6).



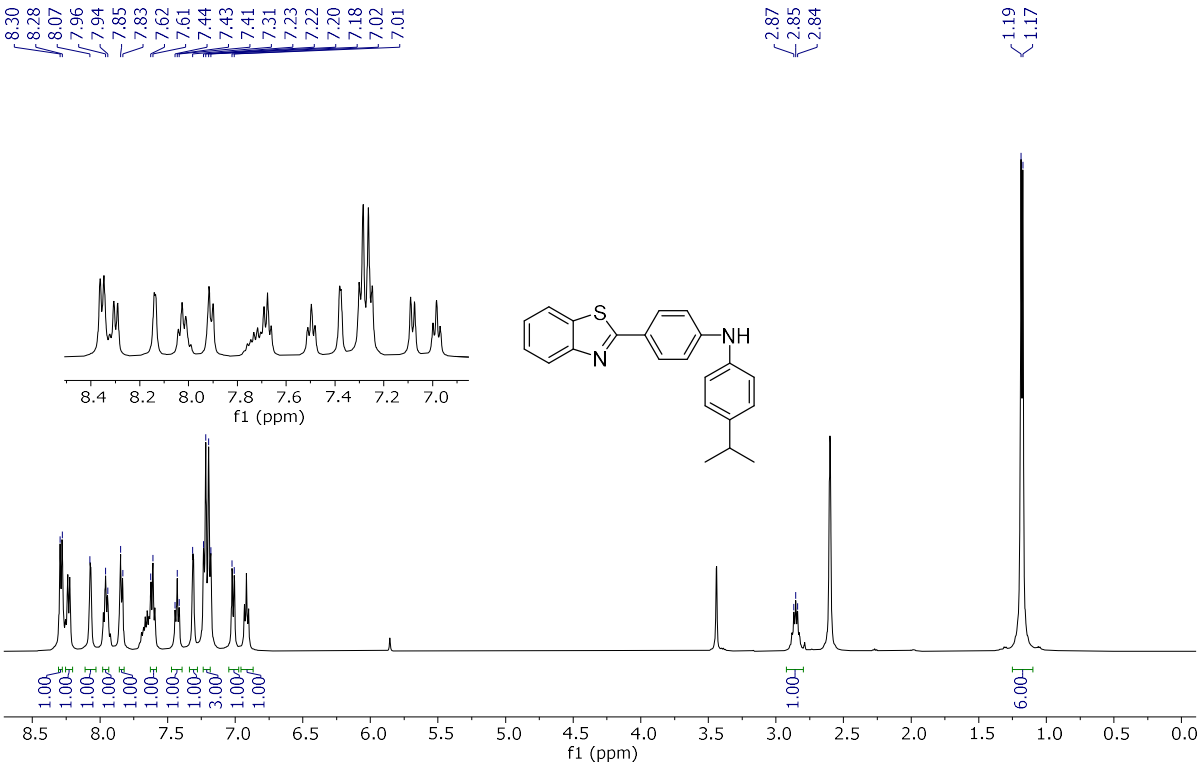
Compound **5b**: ^{13}C NMR (125 MHz, DMSO-d_6).



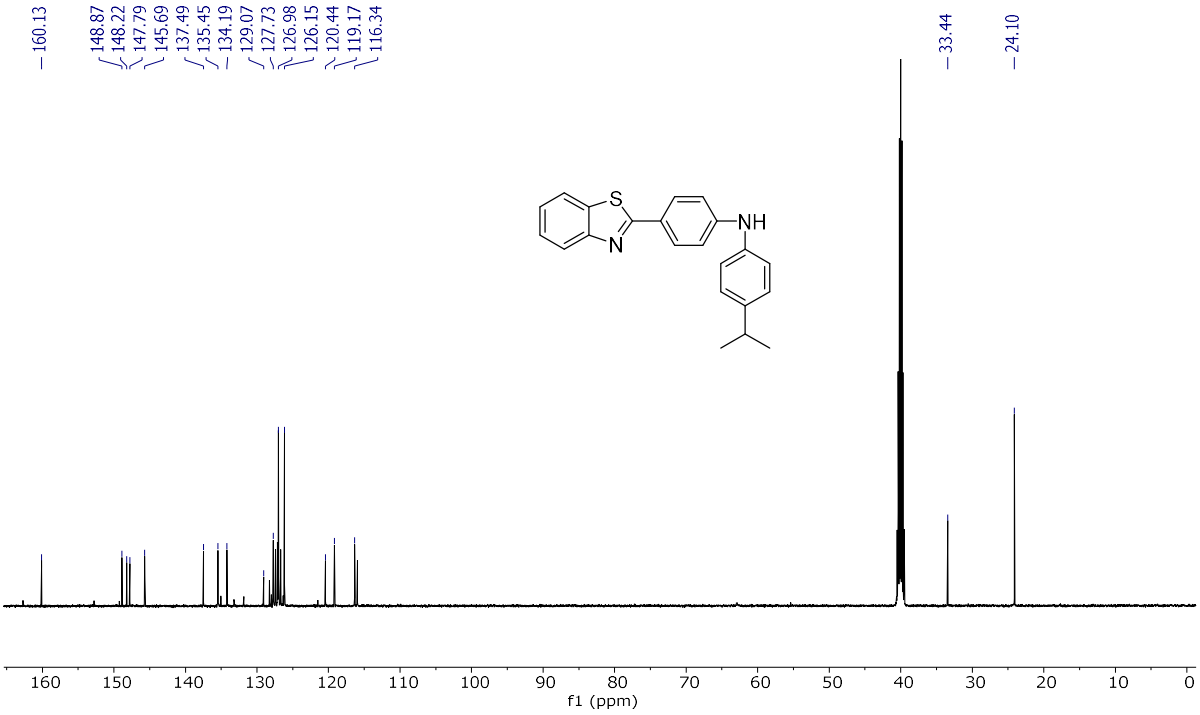
Compound **5c**: ^{1}H NMR (500 MHz, DMSO-d_6).



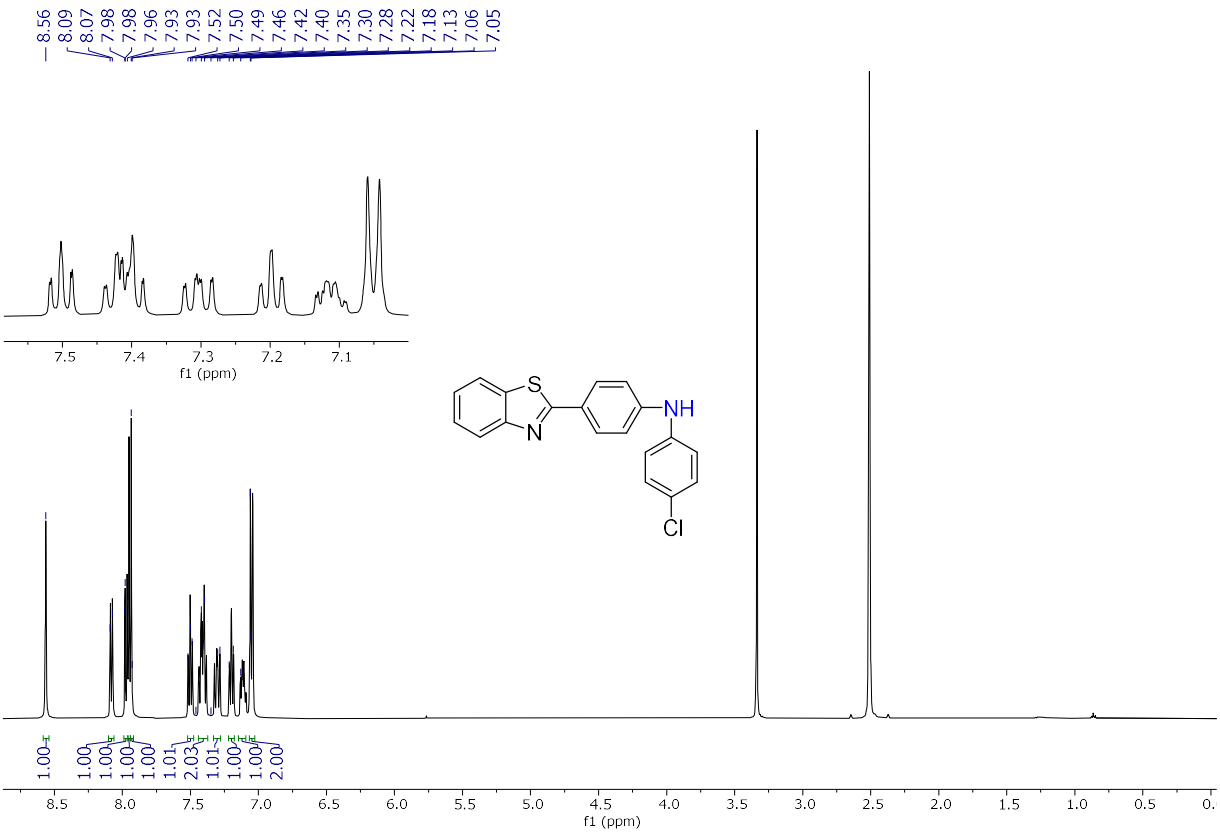
Compound **5c**: ^{13}C NMR (125 MHz, DMSO-d_6).



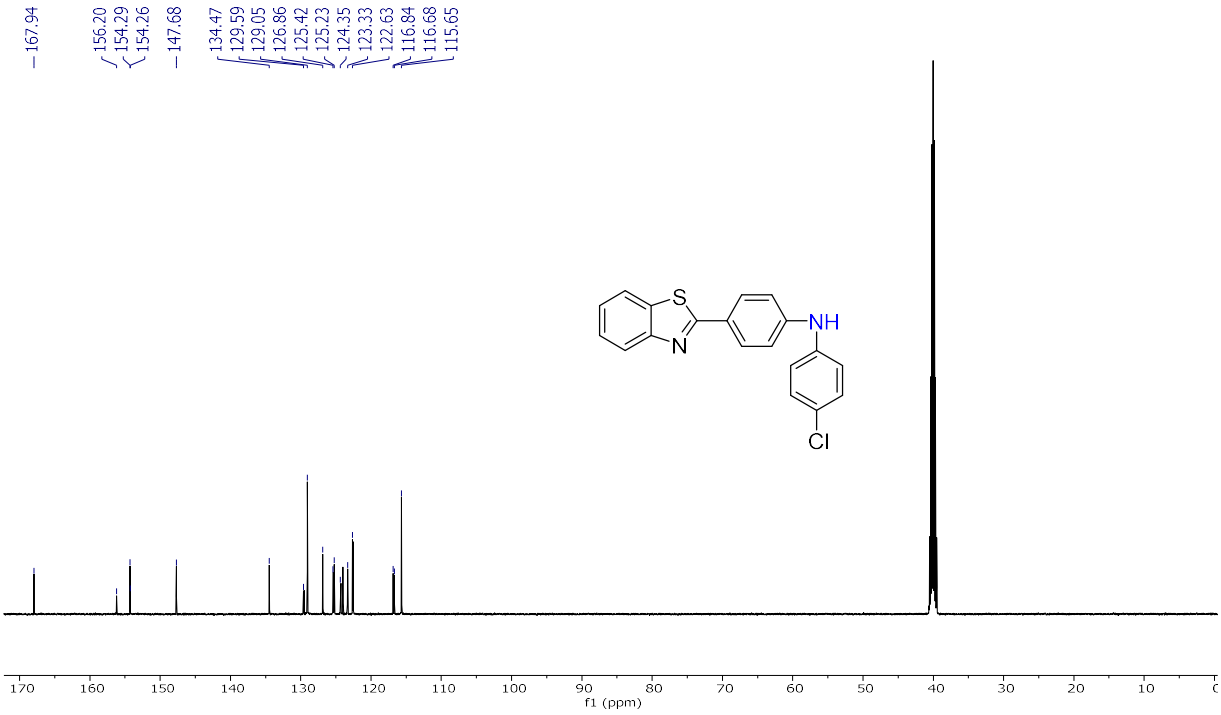
Compound **5d**: ^{1}H NMR (500 MHz, DMSO-d_6).



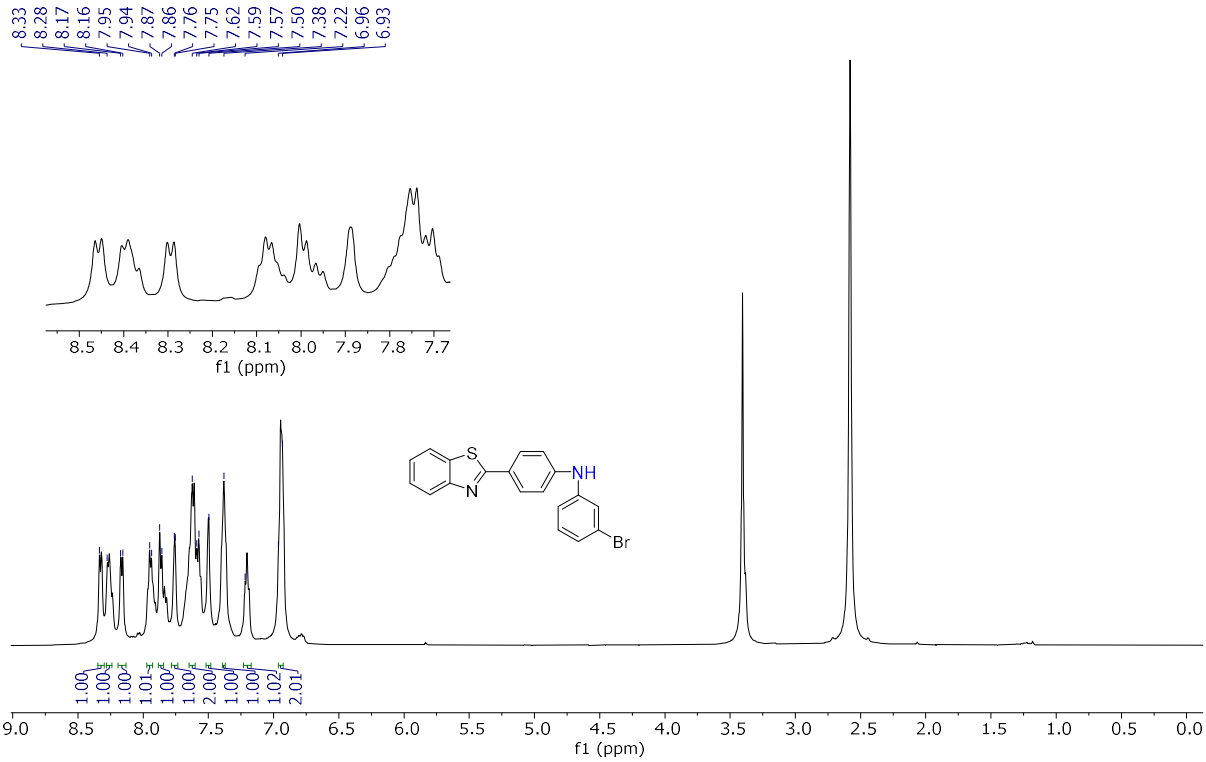
Compound **5d**: ^{13}C NMR (125 MHz, DMSO-d_6).



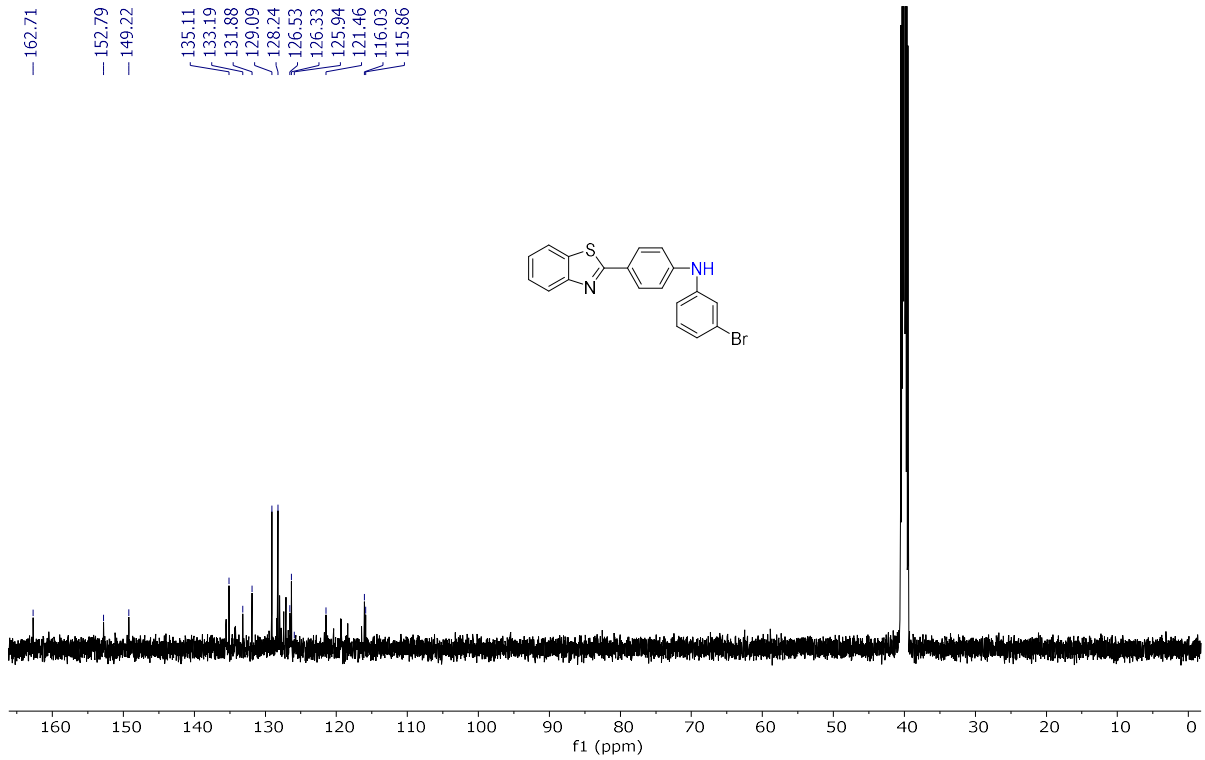
Compound **5e**: ^{1}H NMR (500 MHz, DMSO-d_6).



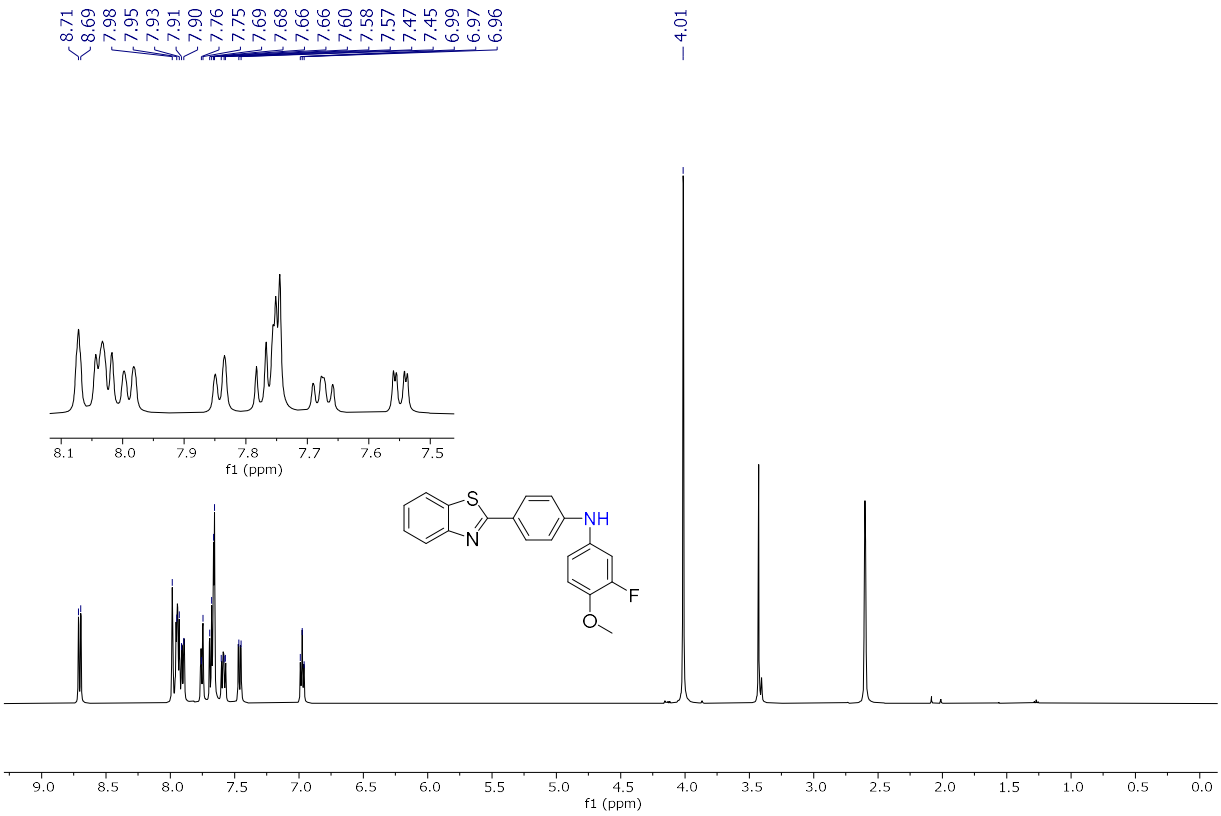
Compound **5e**: ^{13}C NMR (125 MHz, DMSO-d_6).



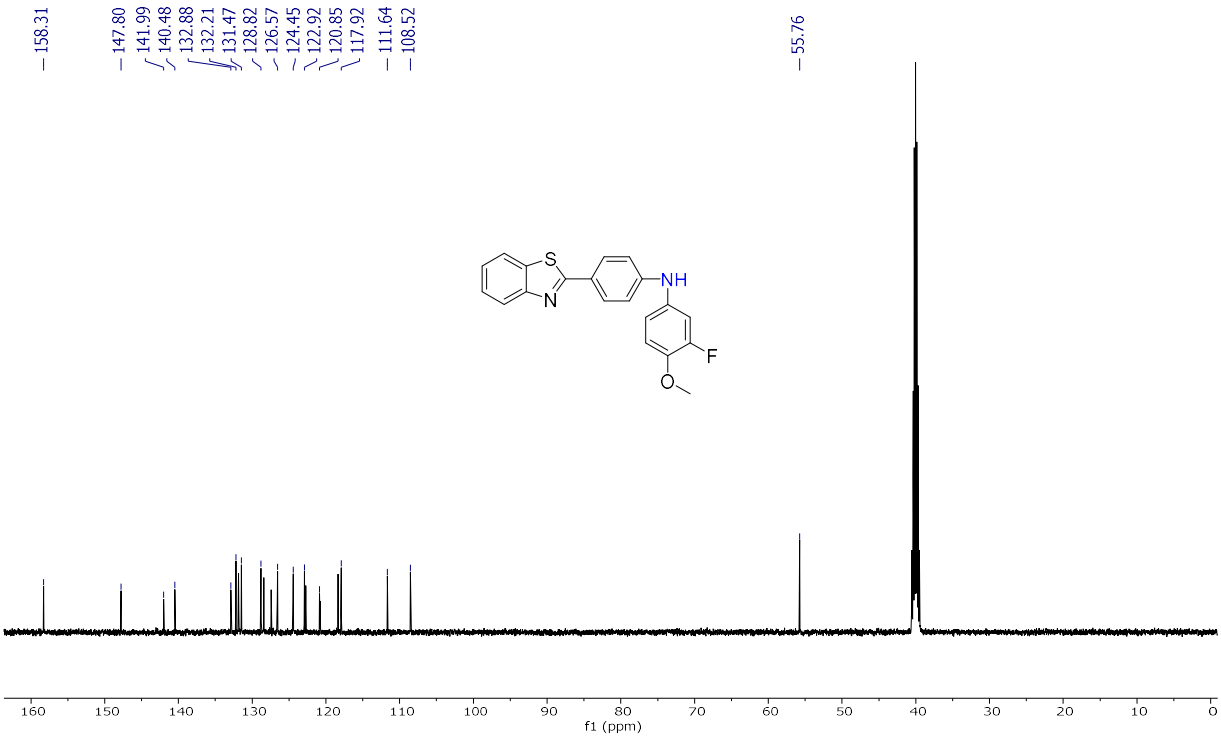
Compound **5f**: ^{1}H NMR (500 MHz, DMSO-d_6).



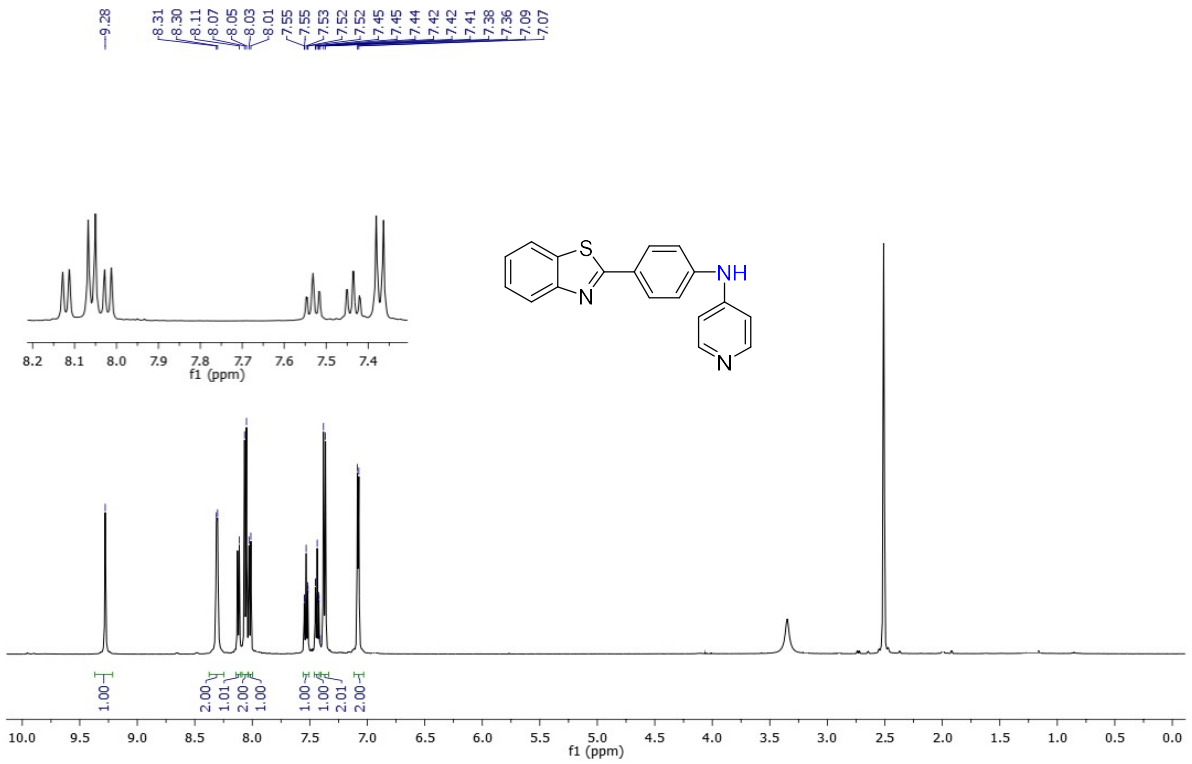
Compound **5f**: ^{13}C NMR (125 MHz, DMSO-d_6).



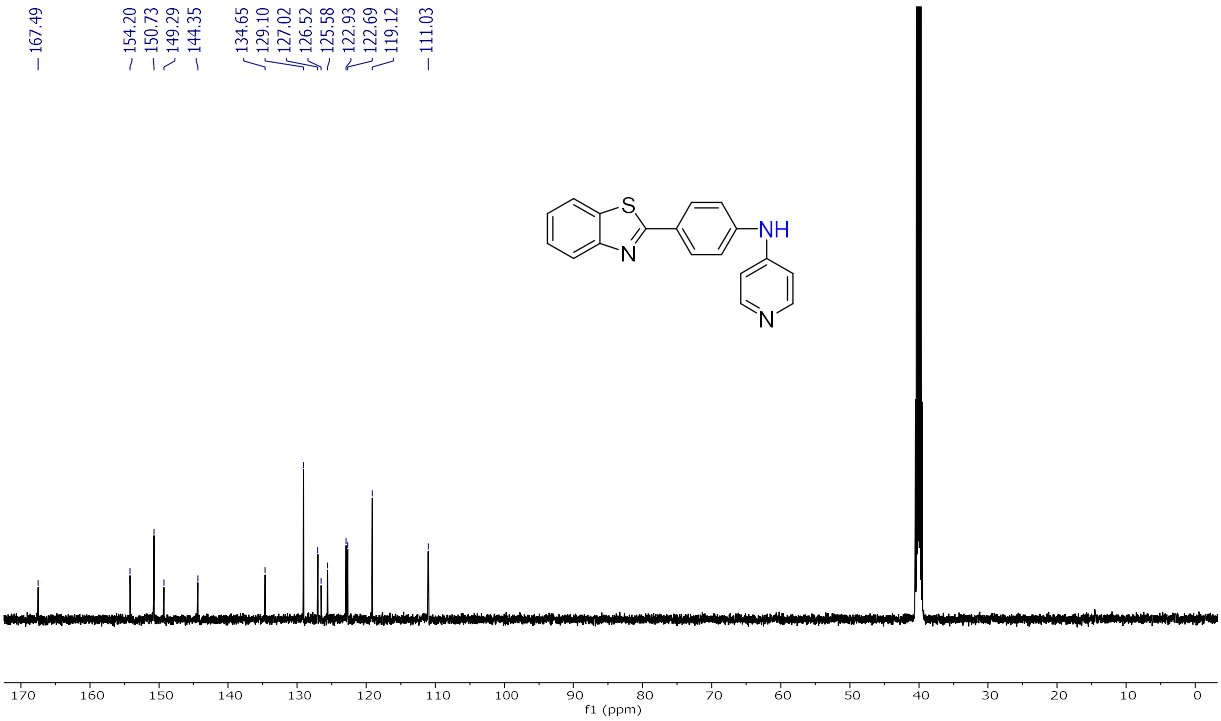
Compound **5g**: ^{1}H NMR (500 MHz, DMSO-d_6).



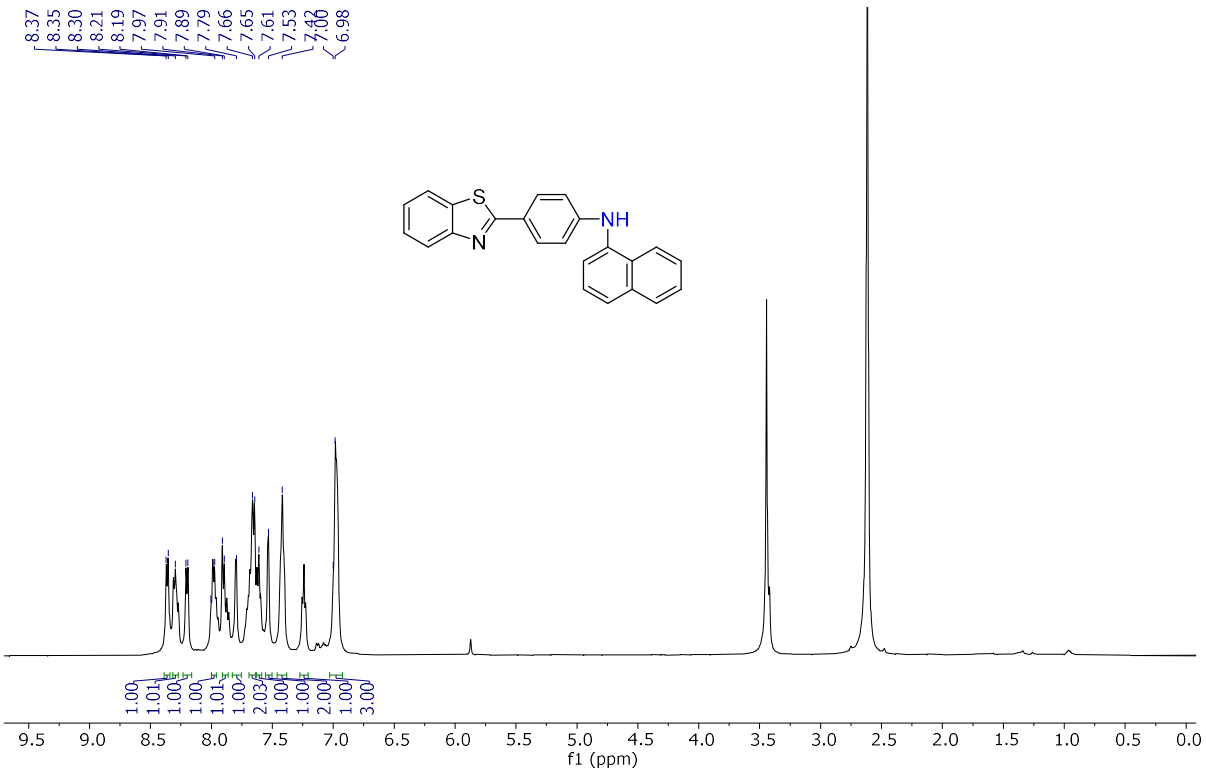
Compound **5g**: ^{13}C NMR (125 MHz, DMSO-d_6).



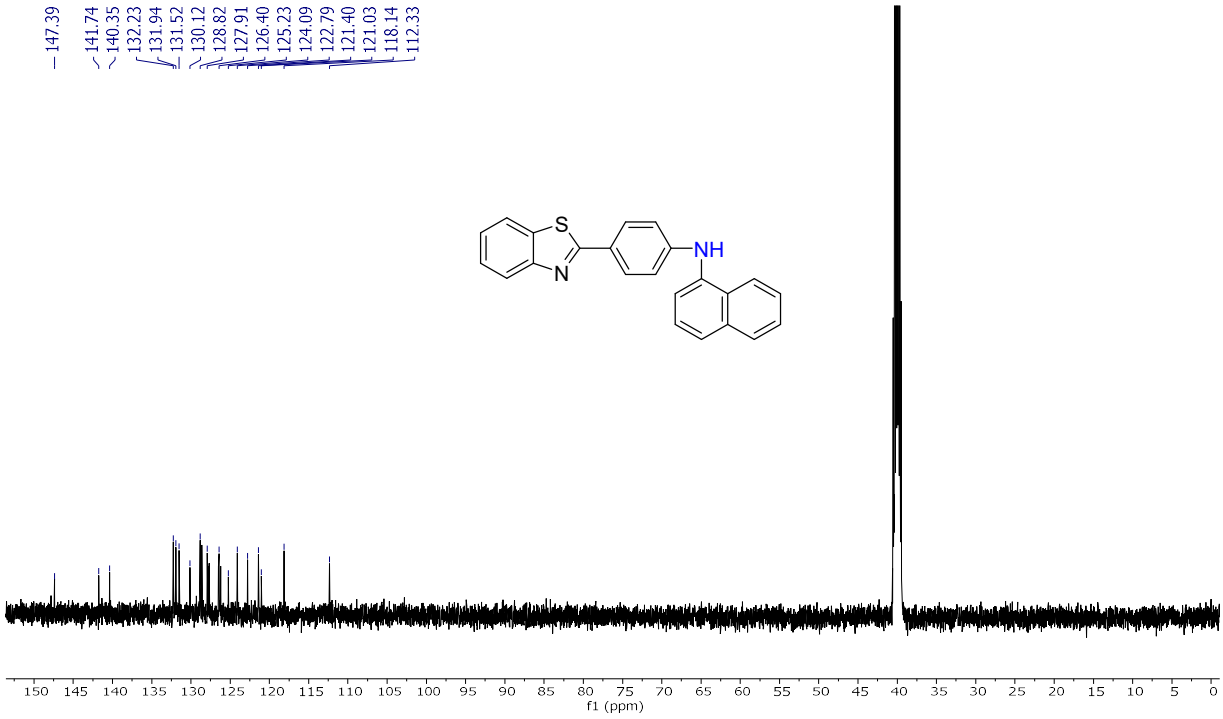
Compound **5h**: ^{1}H NMR (500 MHz, DMSO-d_6).



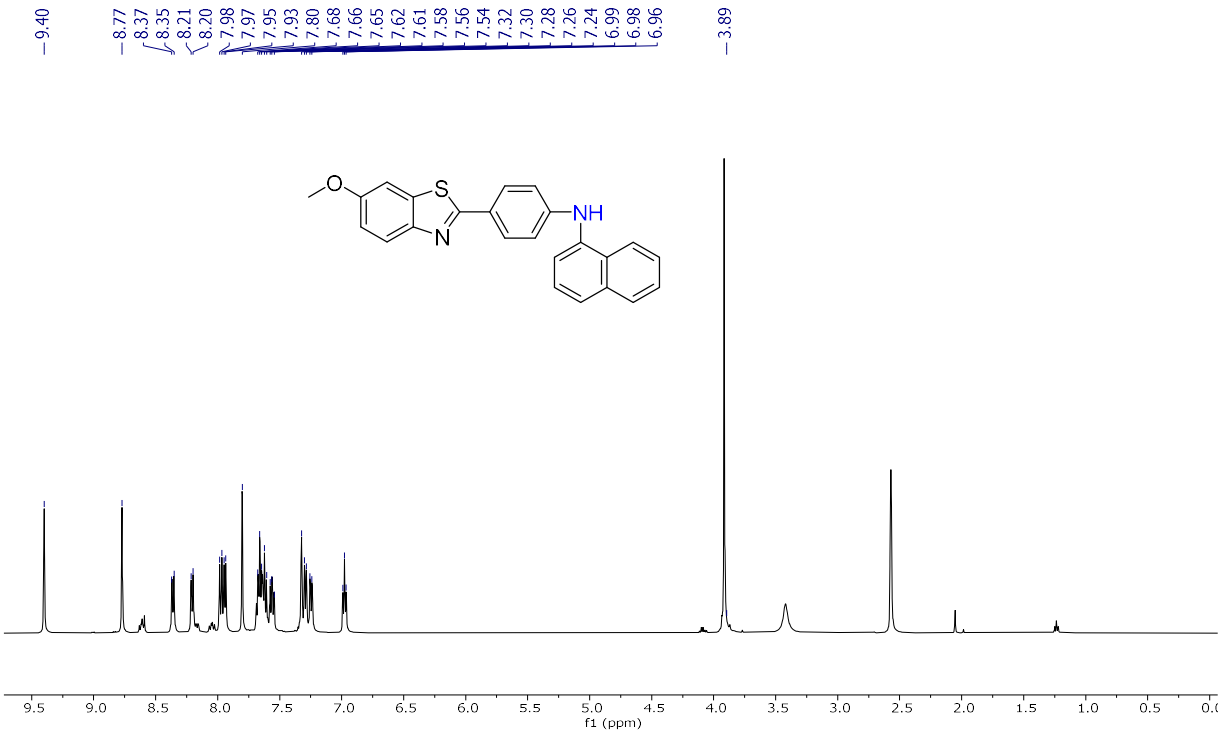
Compound **5h**: ^{13}C NMR (125 MHz, DMSO-d_6).



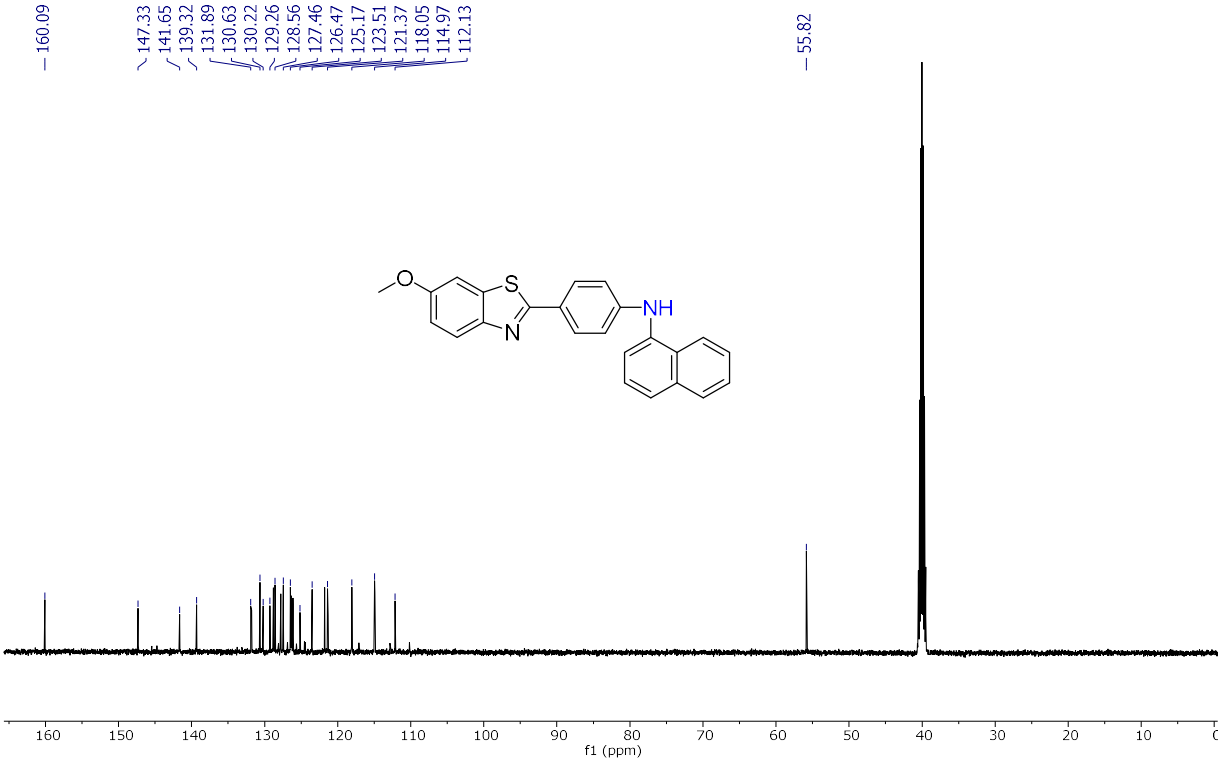
Compound **5i**: ^{1}H NMR (500 MHz, DMSO-d_6).



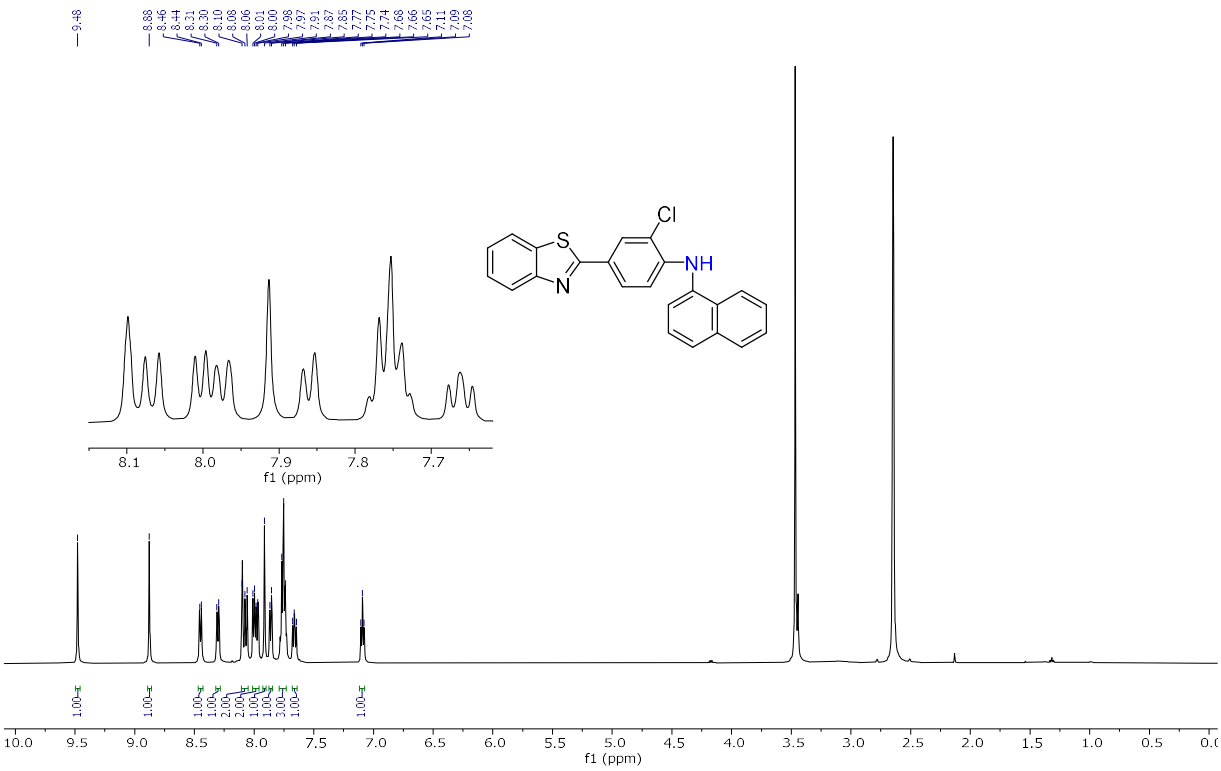
Compound **5i**: ^{13}C NMR (125 MHz, DMSO-d_6).



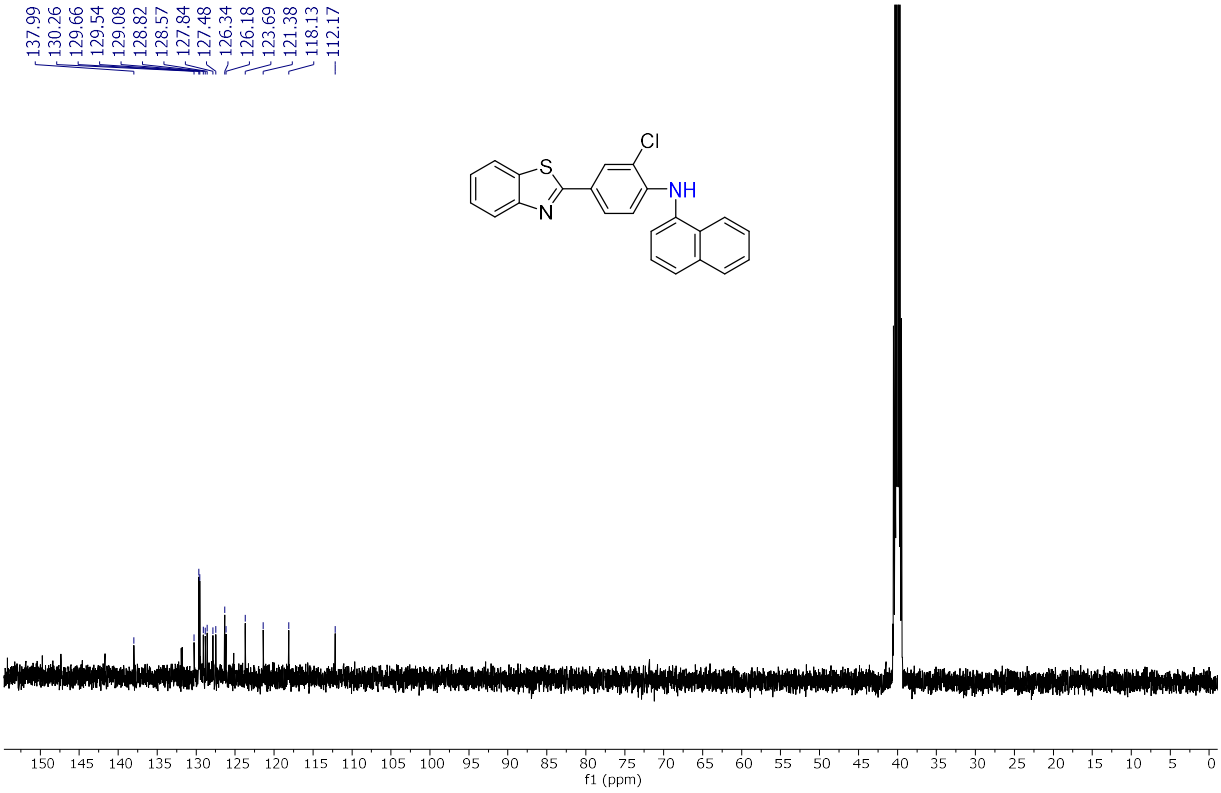
Compound **5j**: ^{1}H NMR (500 MHz, DMSO-d_6).



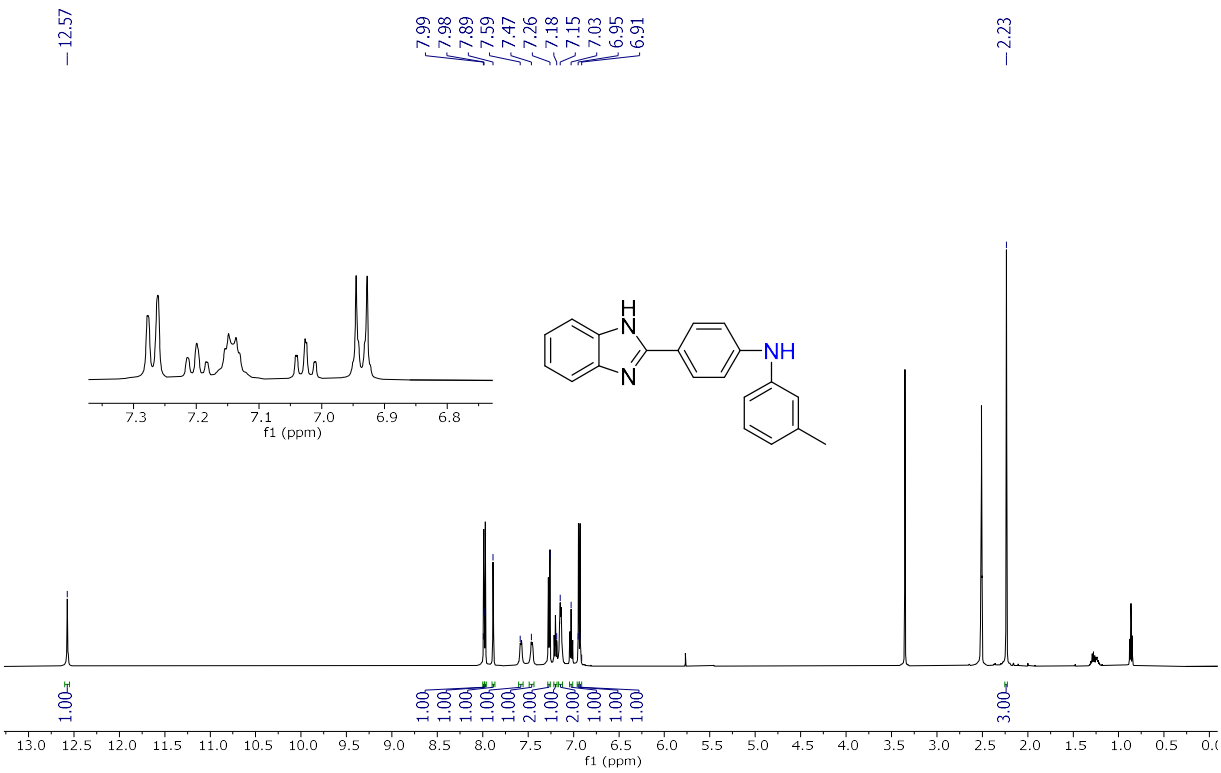
Compound **5j**: ^{13}C NMR (125 MHz, DMSO-d_6).



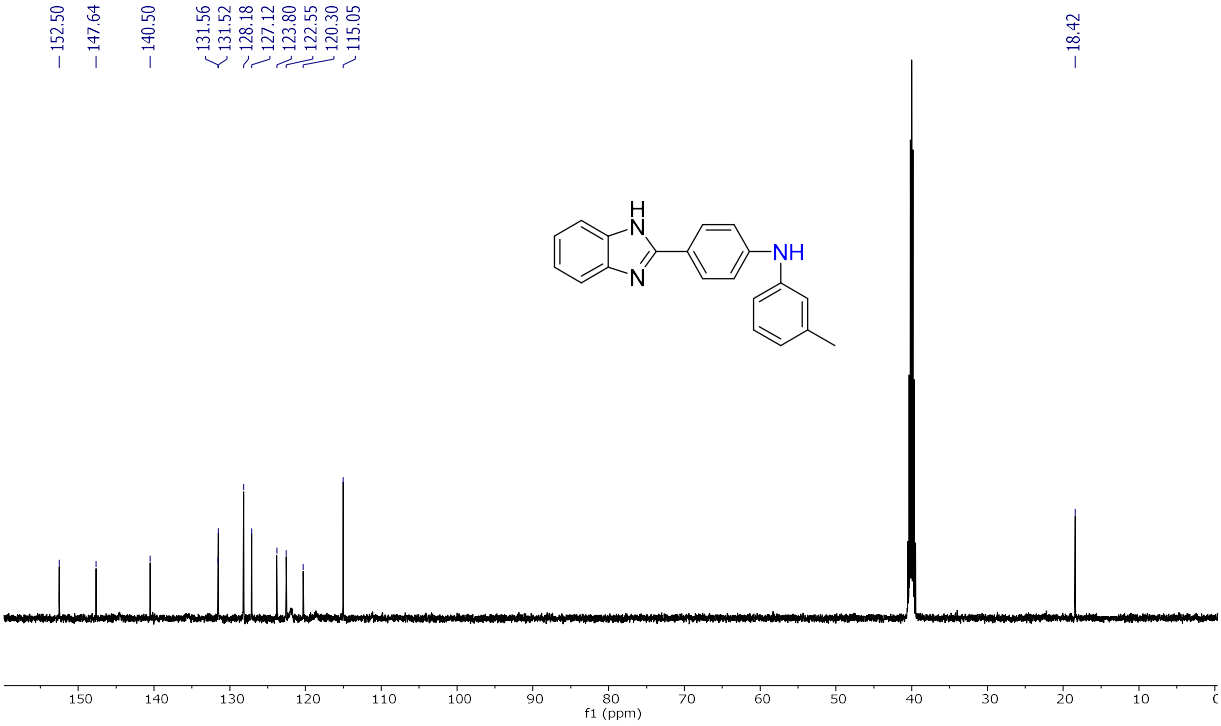
Compound **5k**: ^{1}H NMR (500 MHz, DMSO-d_6).



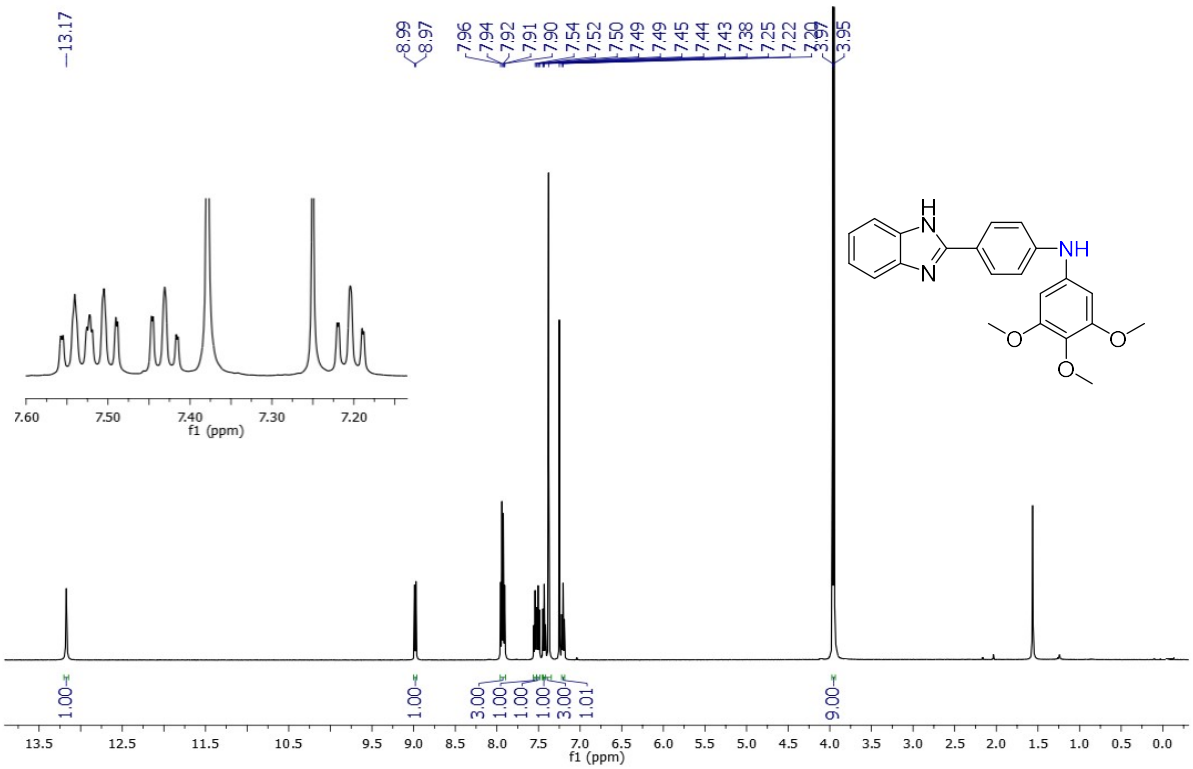
Compound **5k**: ^{13}C NMR (125 MHz, DMSO-d_6).



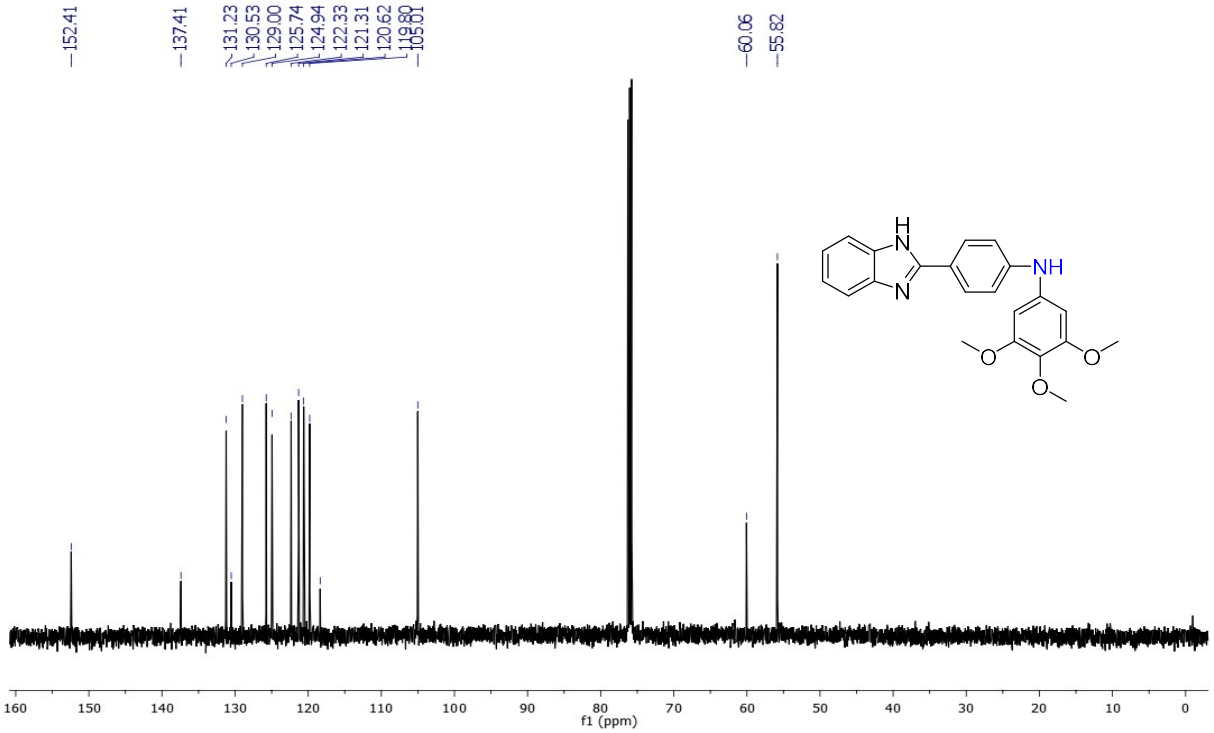
Compound **5l**: ^{1}H NMR (500 MHz, DMSO-d_6).



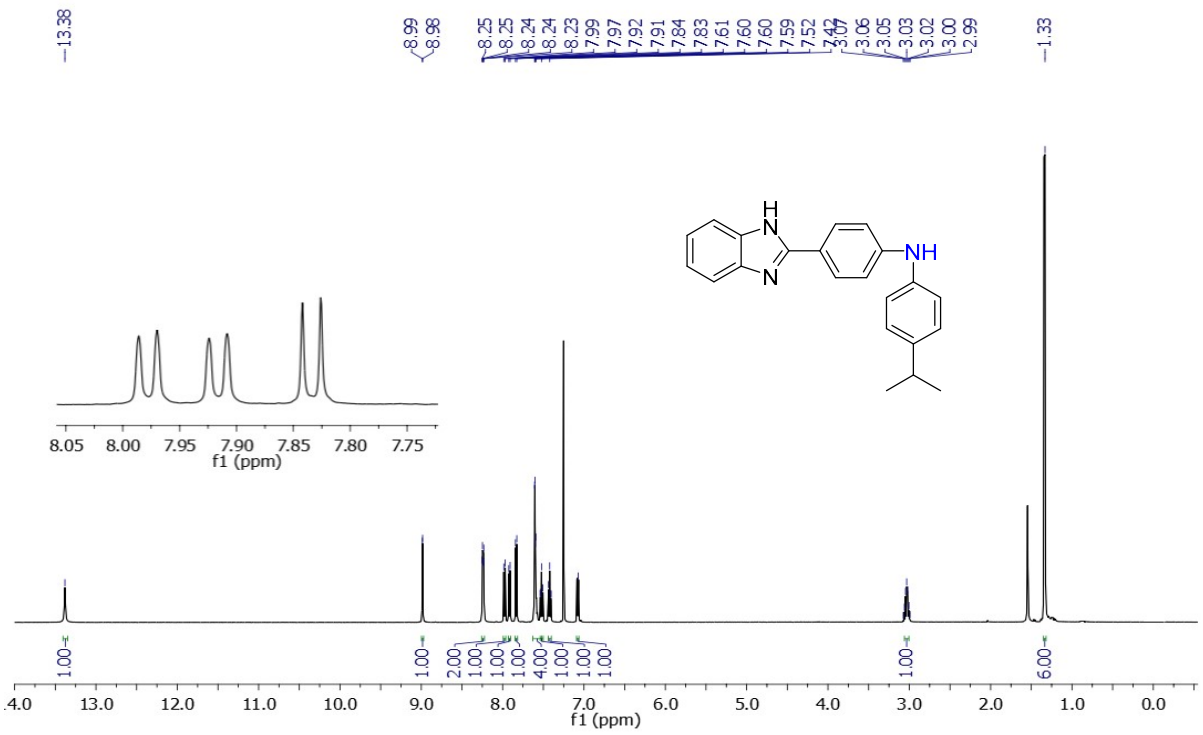
Compound **5l**: ^{13}C NMR (125 MHz, DMSO-d_6).



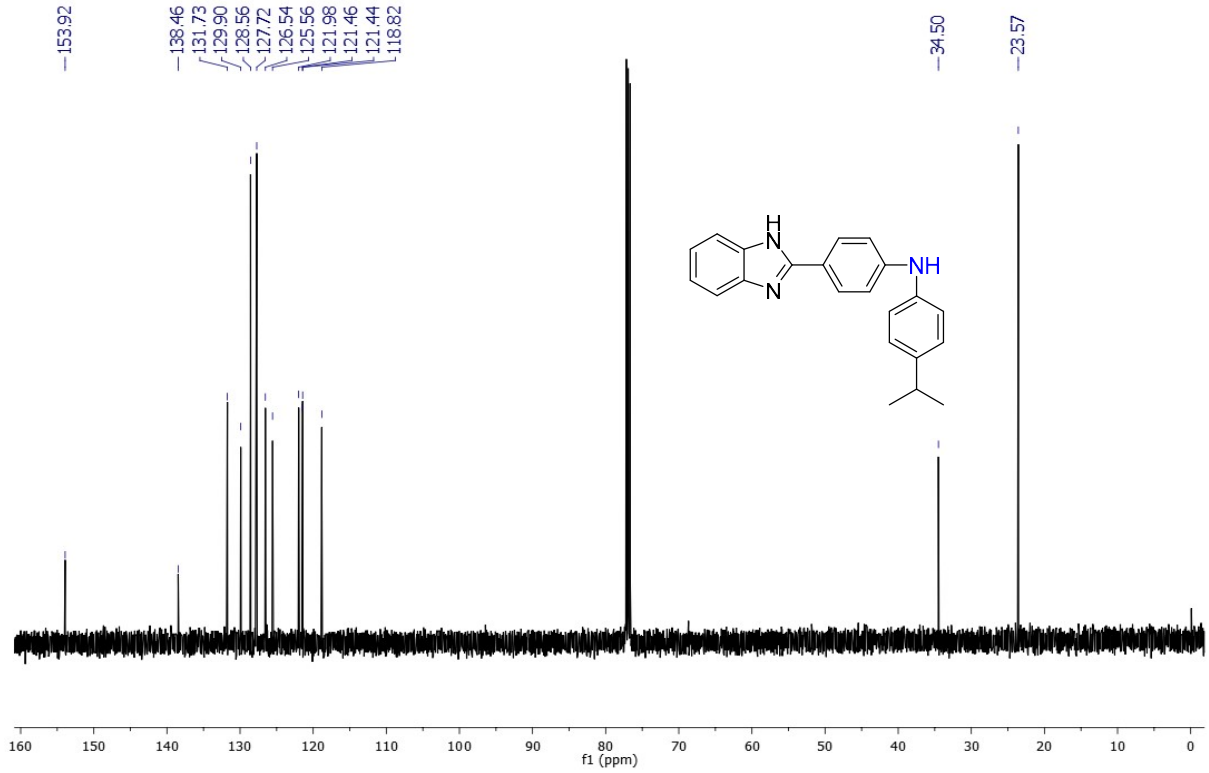
Compound **5m**: ^{1}H NMR (500 MHz, $CDCl_3$).



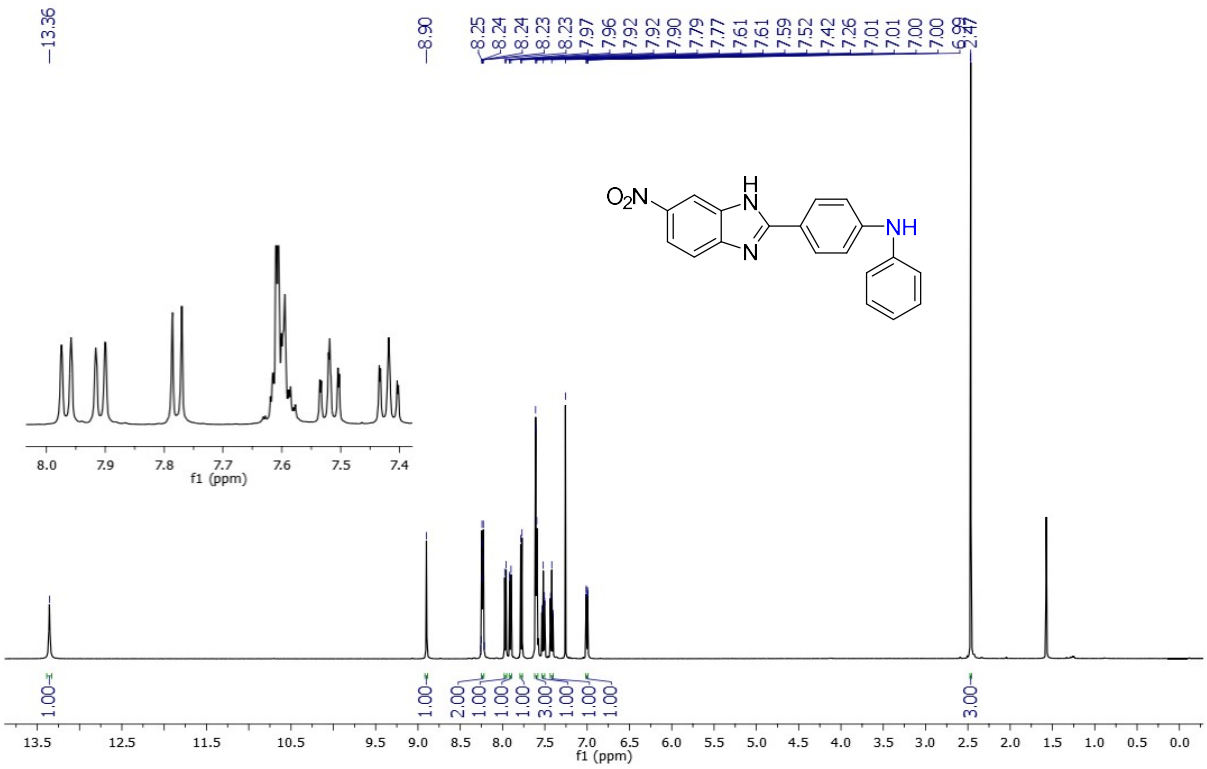
Compound **5m**: ^{13}C NMR (125 MHz, $CDCl_3$).



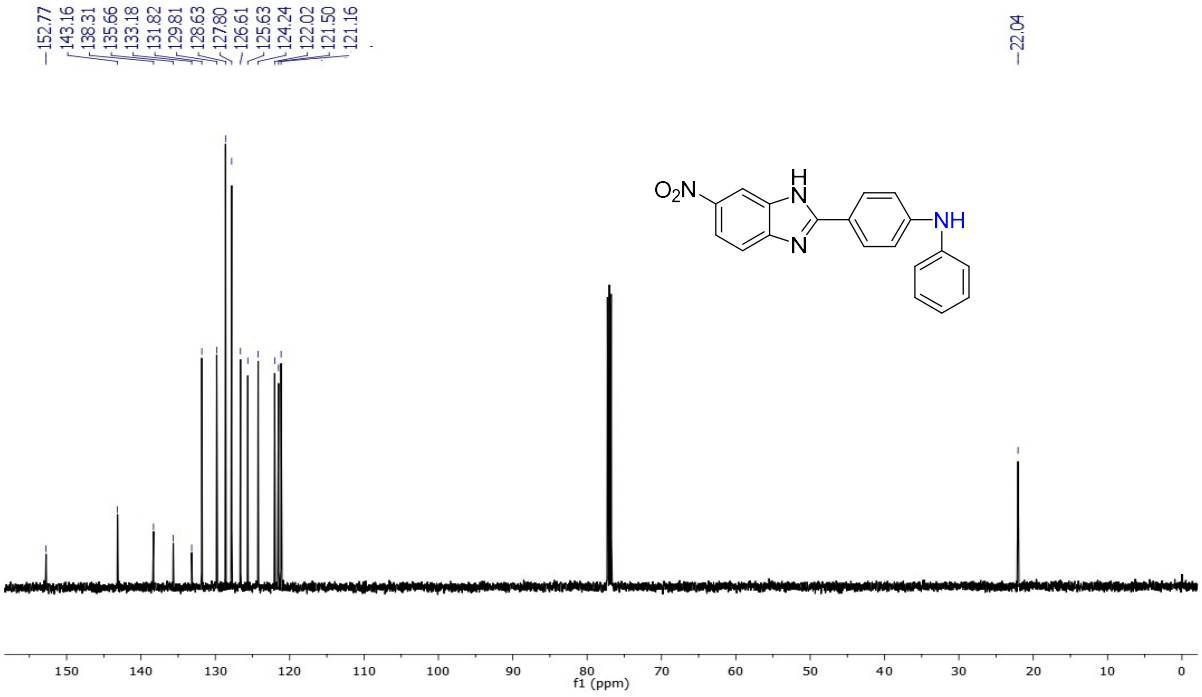
Compound **5n**: ^{1}H NMR (500 MHz, $CDCl_3$).



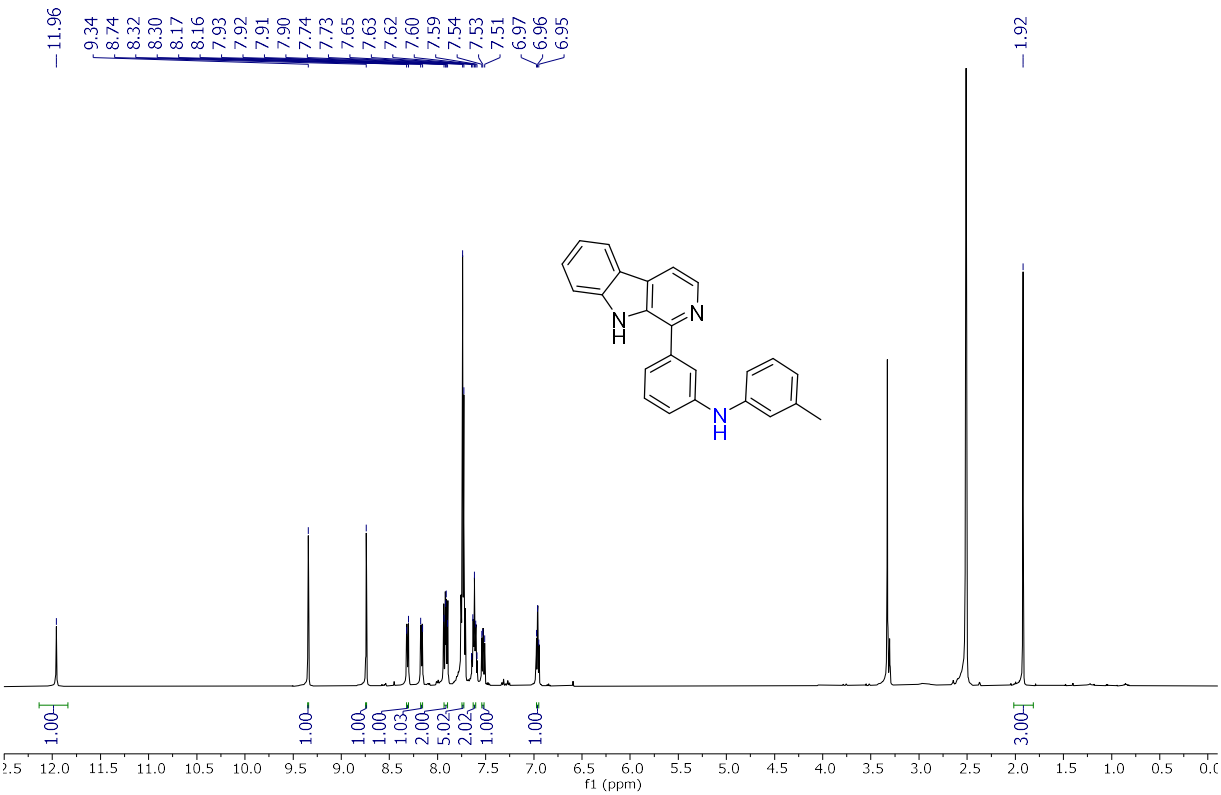
Compound **5n**: ^{13}C NMR (125 MHz, $CDCl_3$).



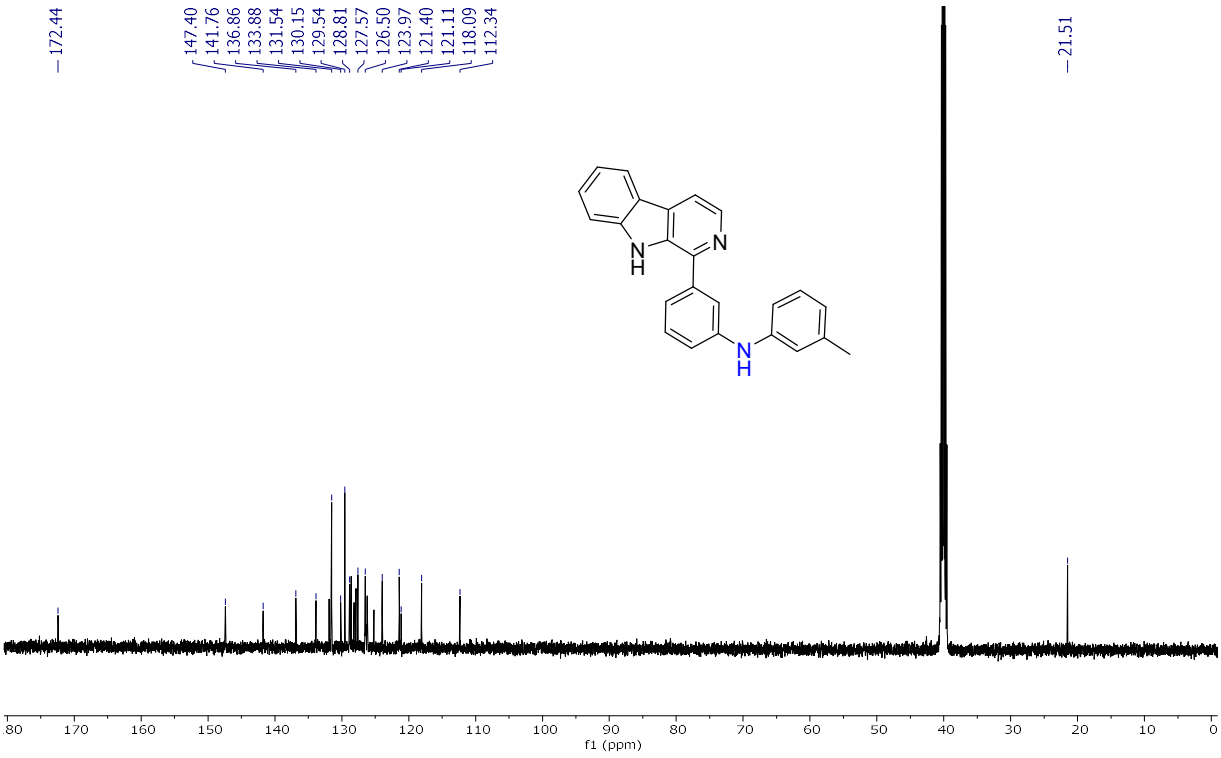
Compound **5o**: ^{1}H NMR (500 MHz, $CDCl_3$).



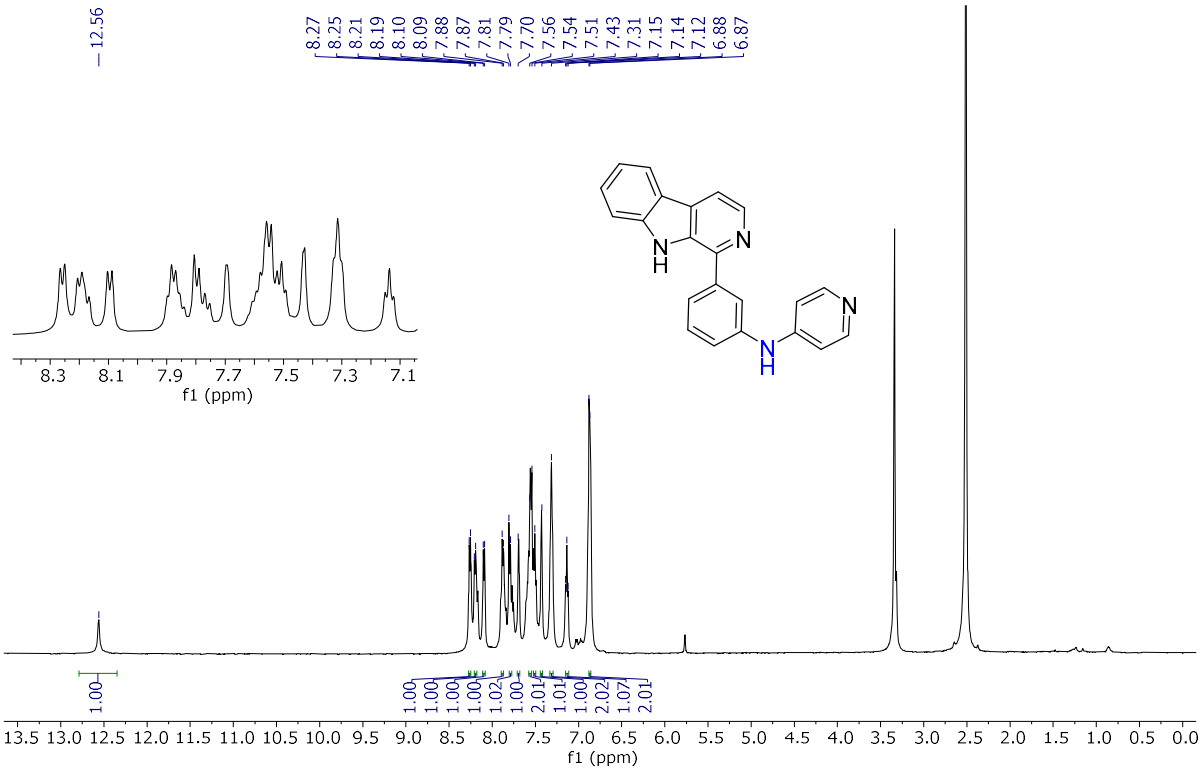
Compound **5o**: ^{13}C NMR (125 MHz, $CDCl_3$).



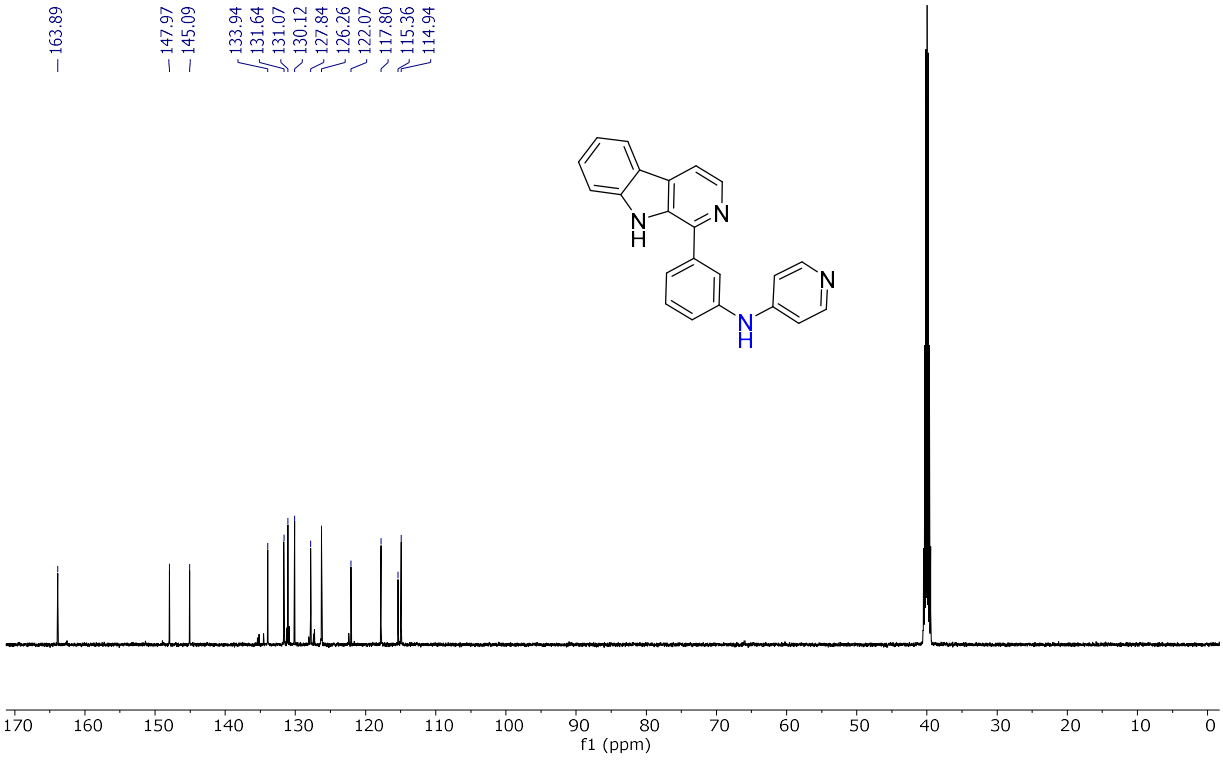
Compound **5p**: ^{1}H NMR (500 MHz, DMSO-d_6).



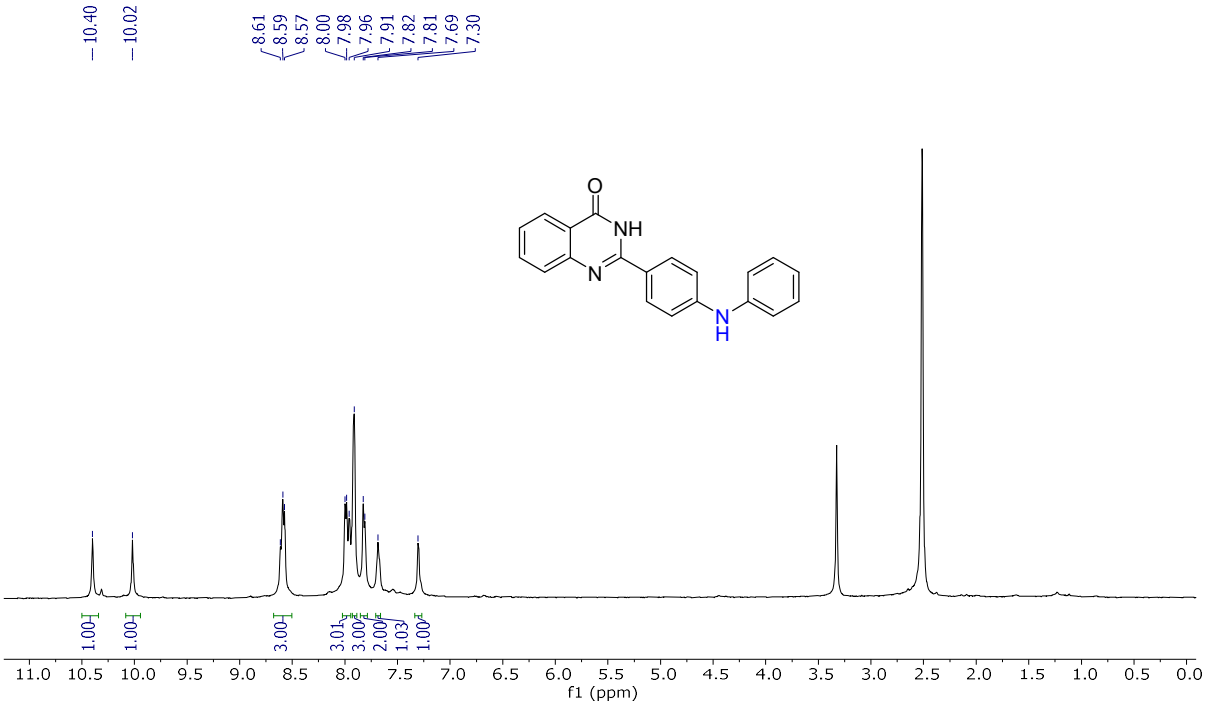
Compound **5p**: ^{13}C NMR (125 MHz, DMSO-d_6).



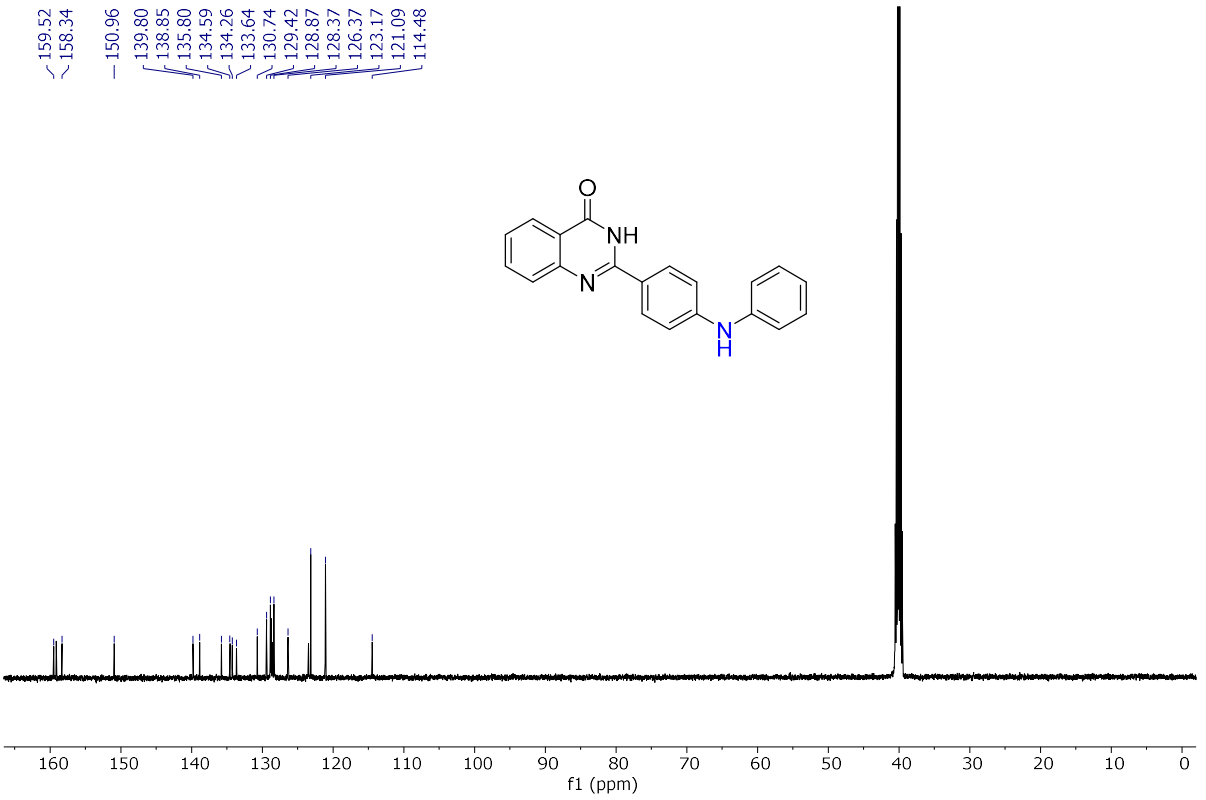
Compound **5q**: ^{1}H NMR (500 MHz, DMSO-d_6).



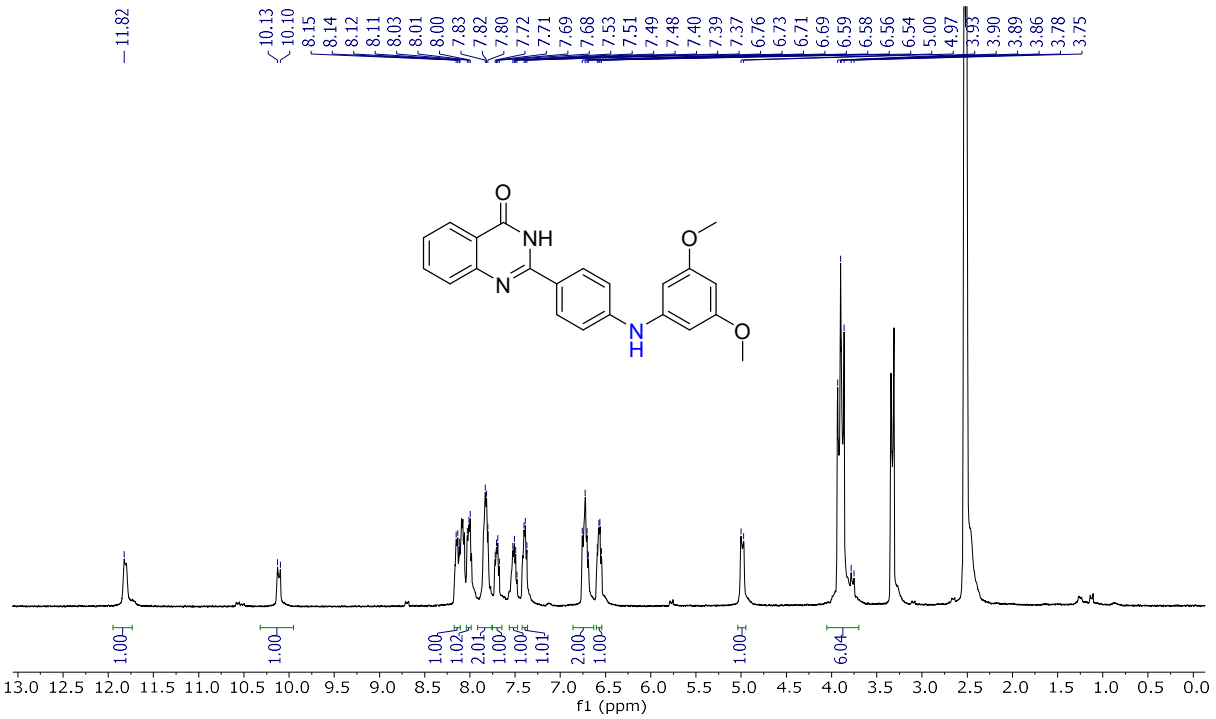
Compound **5q**: ^{13}C NMR (125 MHz, DMSO-d_6).



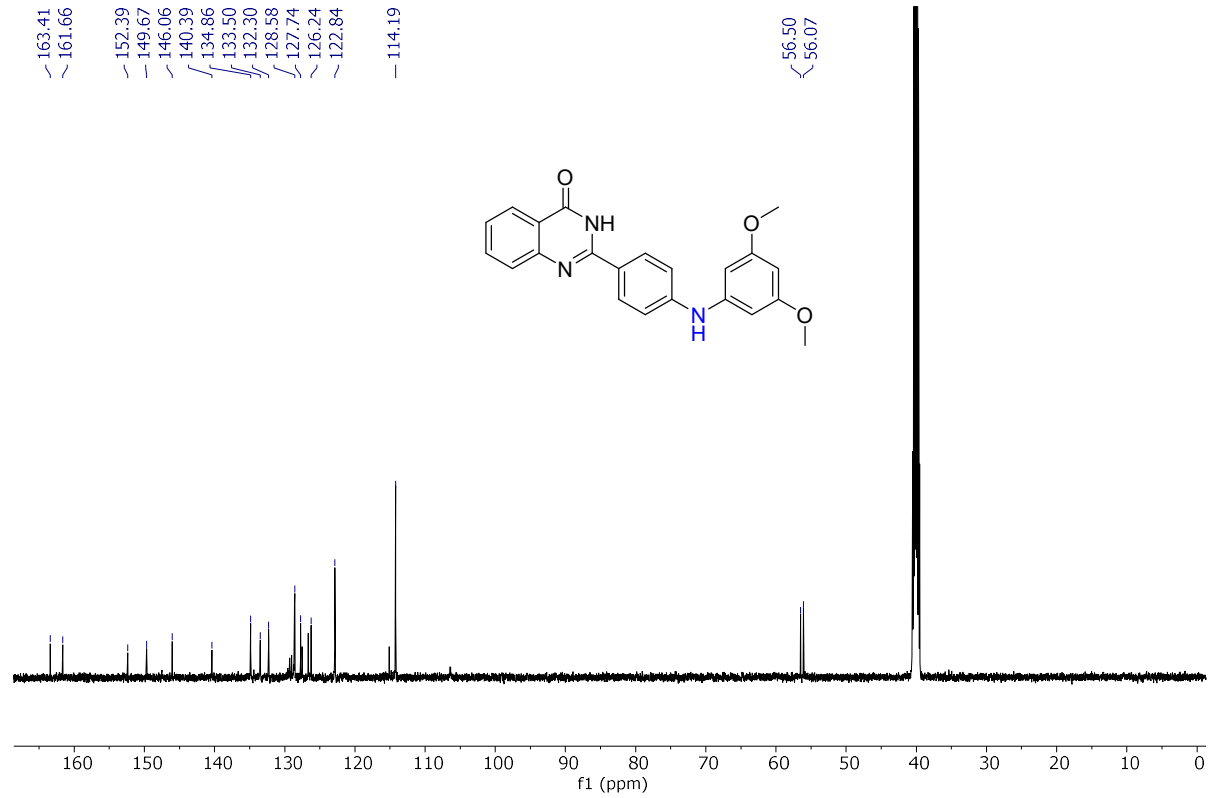
Compound **5r**: ^{1}H NMR (500 MHz, DMSO-d_6).



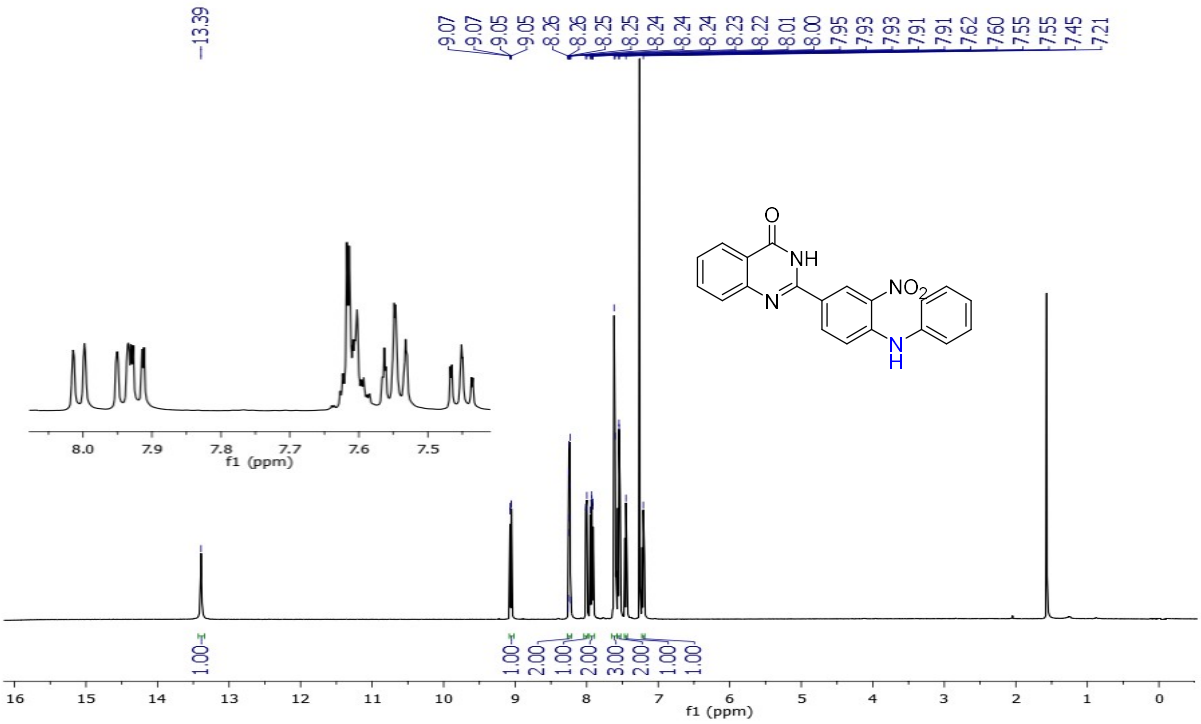
Compound **5r**: ^{13}C NMR (125 MHz, DMSO-d_6).



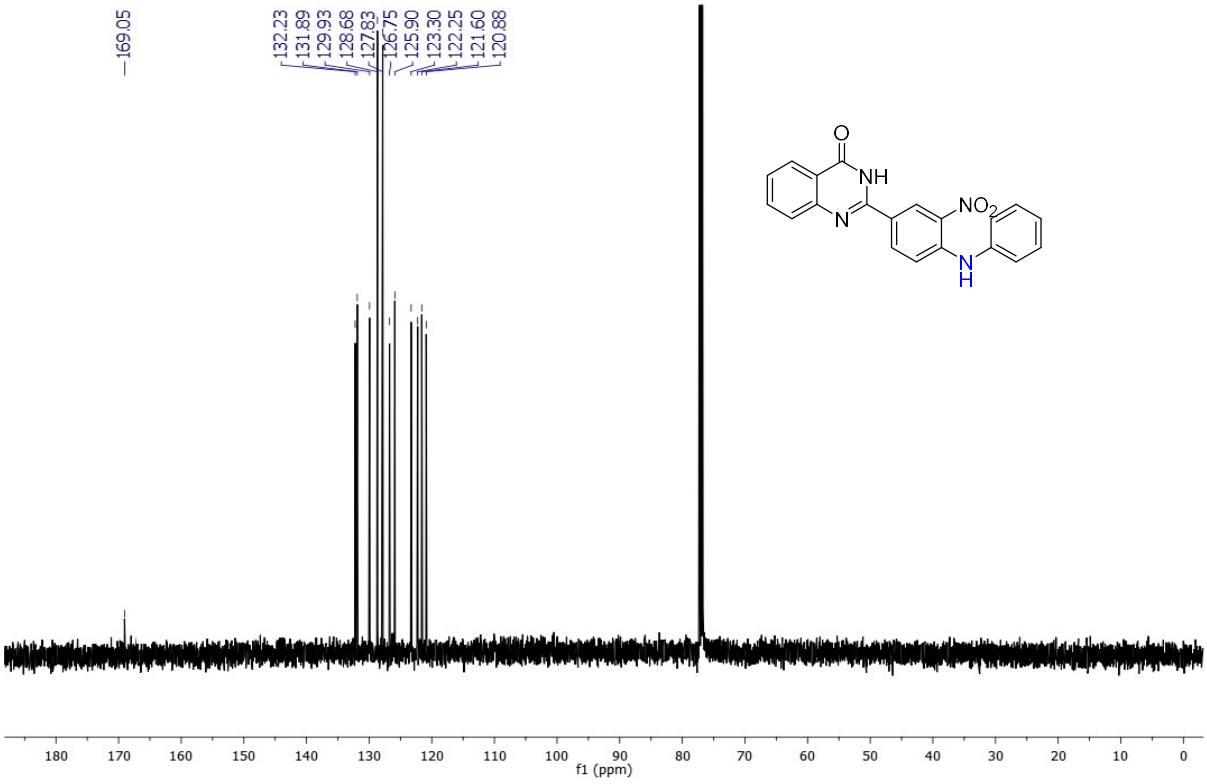
Compound **5s**: ^{1}H NMR (500 MHz, DMSO-d_6).



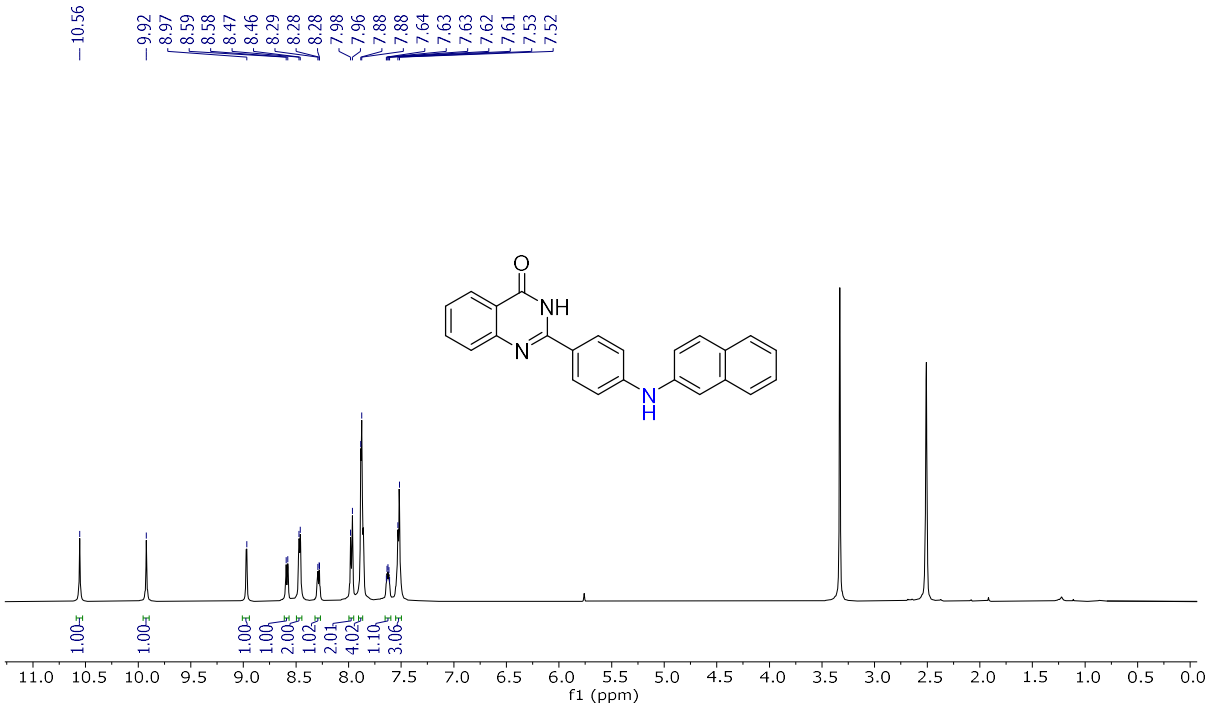
Compound **5s**: ^{13}C NMR (125 MHz, DMSO-d_6).



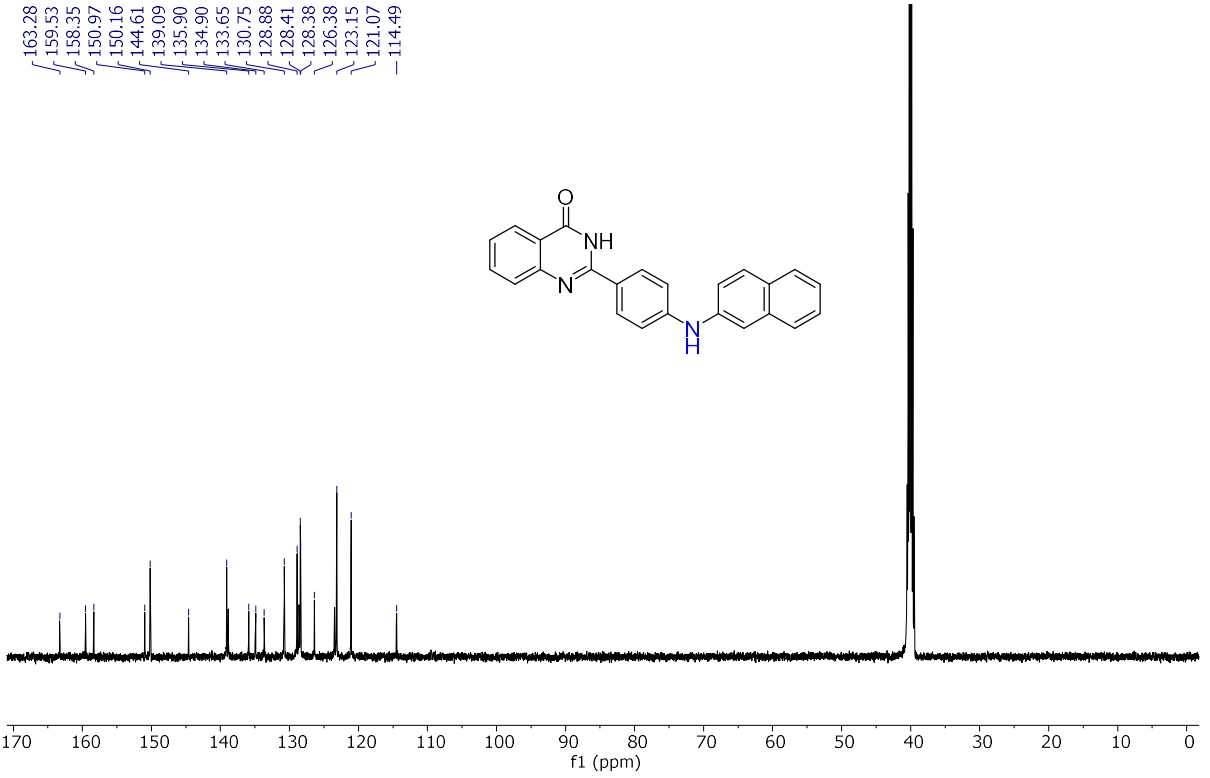
Compound **5t**: ^{1}H NMR (500 MHz, $CDCl_3$).



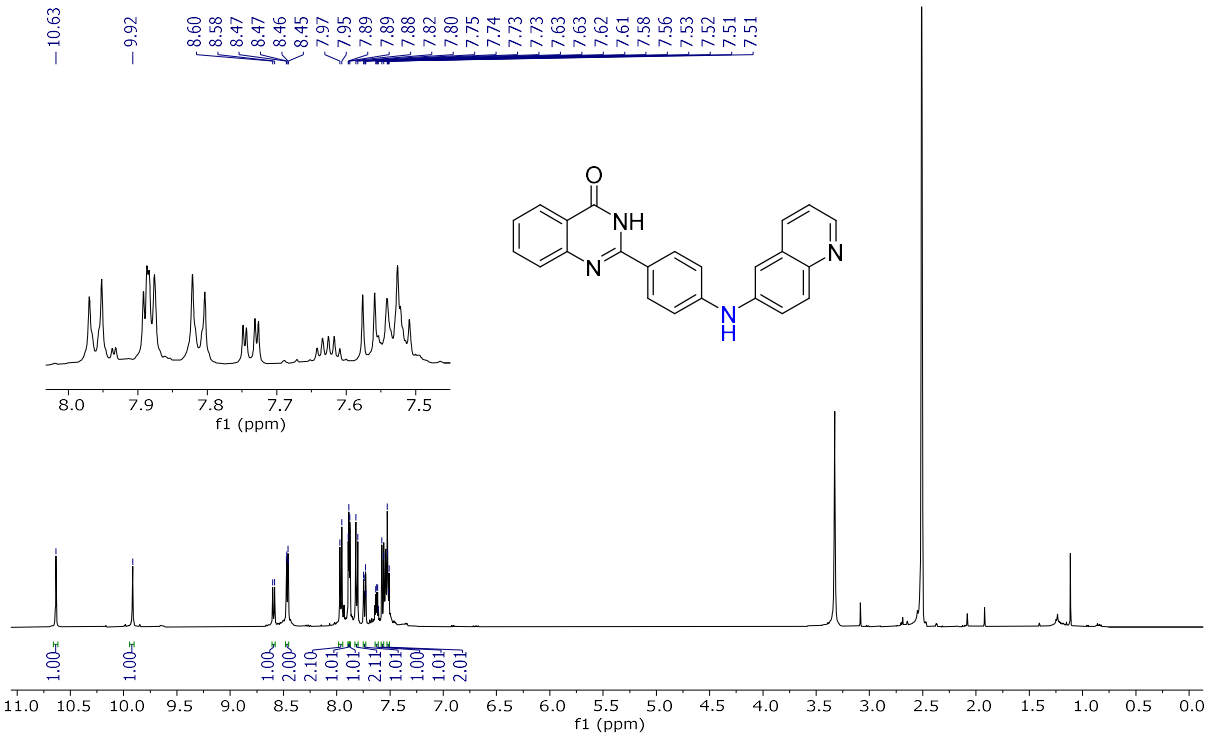
Compound **5t**: ^{13}C NMR (125 MHz, $CDCl_3$).



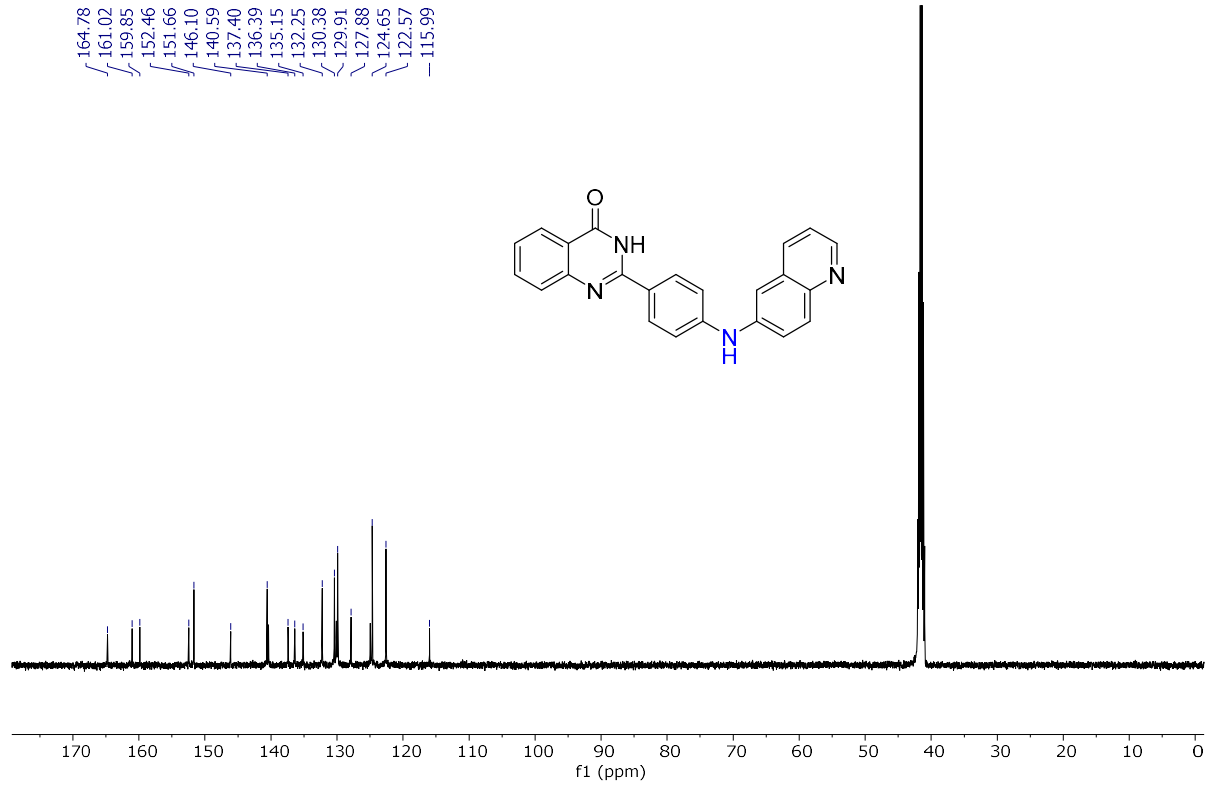
Compound **5u**: ^{1}H NMR (500 MHz, DMSO-d_6).



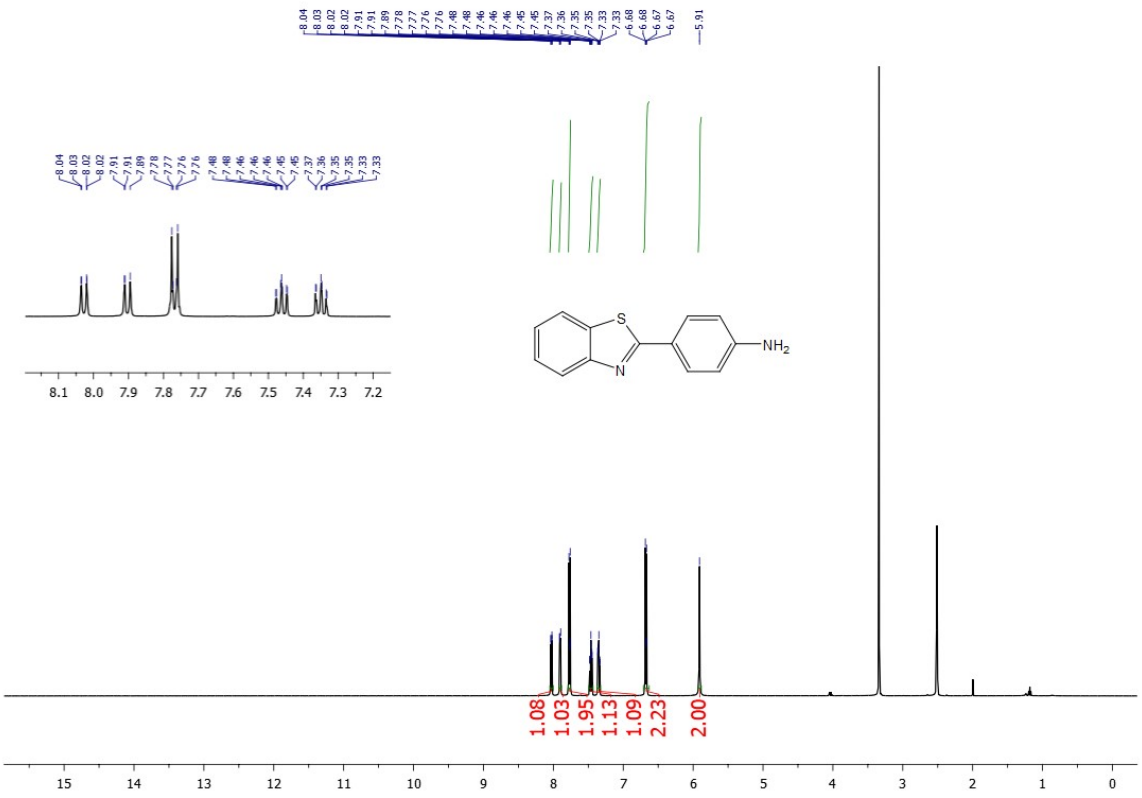
Compound **5u**: ^{13}C NMR (125 MHz, DMSO-d_6).



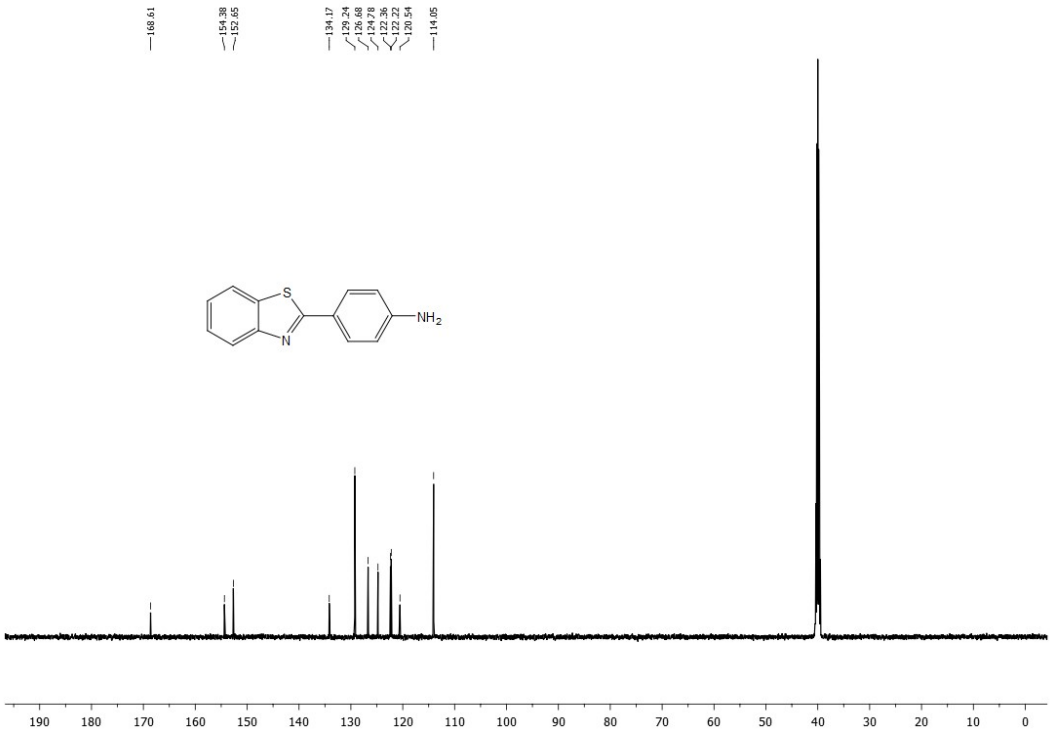
Compound **5v**: ^{1}H NMR (500 MHz, DMSO-d_6).



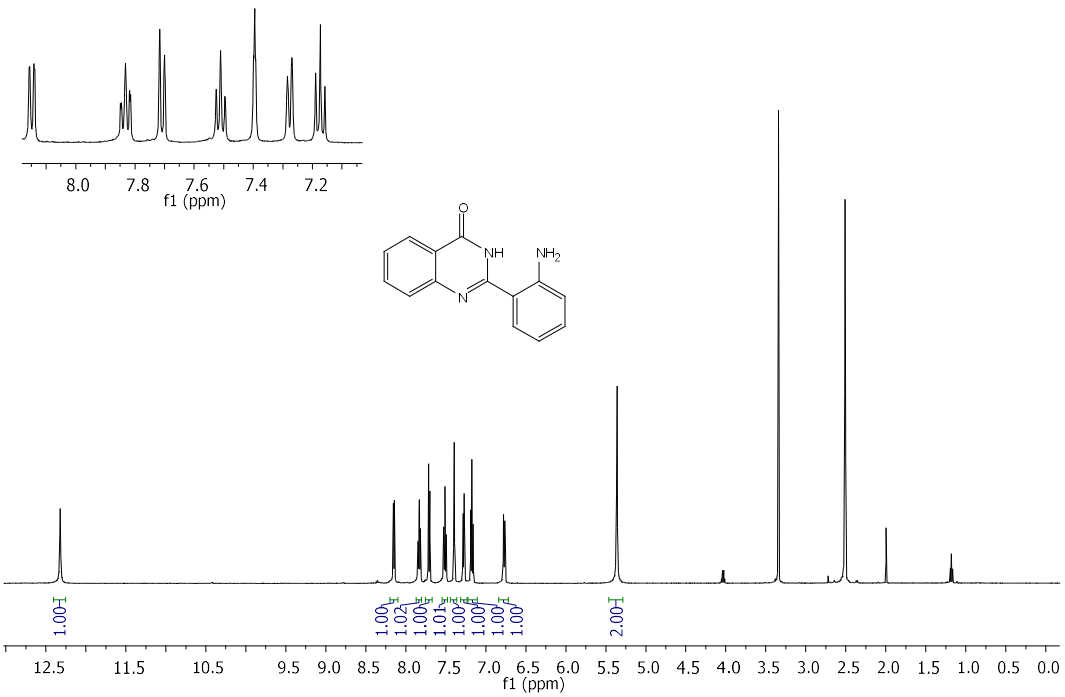
Compound **5v**: ^{13}C NMR (125 MHz, DMSO-d_6).



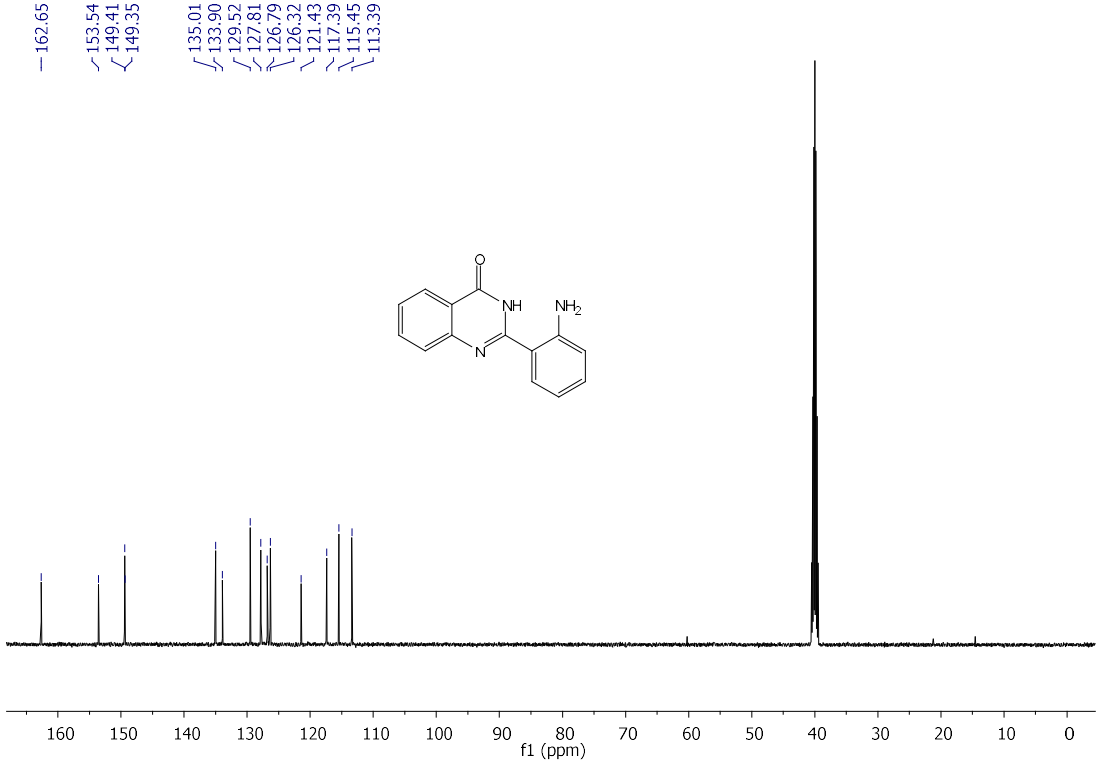
Compound **5w**: ^{1}H NMR (500 MHz, DMSO-d_6).



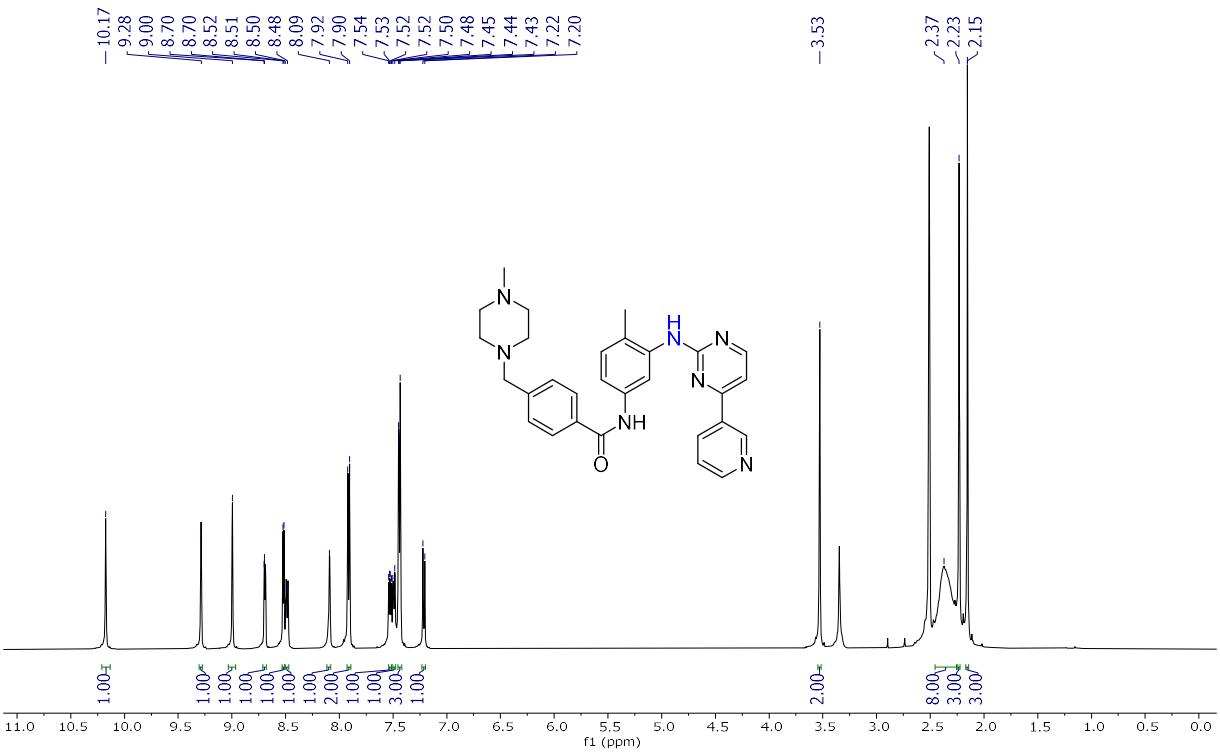
Compound **5w**: ^{13}C NMR (125 MHz, DMSO-d_6).



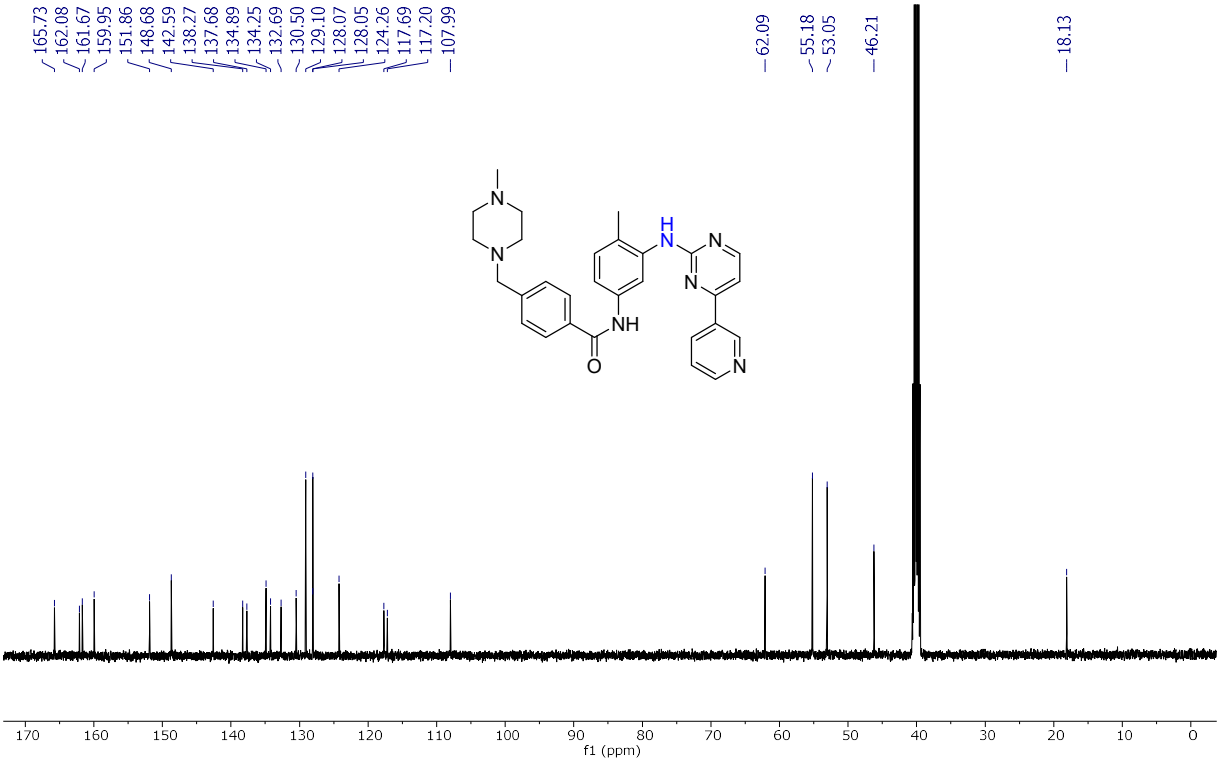
Compound **5x**: ^{1}H NMR (500 MHz, DMSO-d_6).



Compound **5x**: ^{13}C NMR (125 MHz, DMSO-d_6).



Compound **8**: ^{1}H NMR (500 MHz, DMSO-d_6).



Compound **8**: ^{13}C NMR (125 MHz, DMSO-d_6).