Support Information

$FeCl_3$-Catalyzed Oxidative Amidation of Benzylic C−H bonds Enabled by Photogenerated Chlorine-Radical

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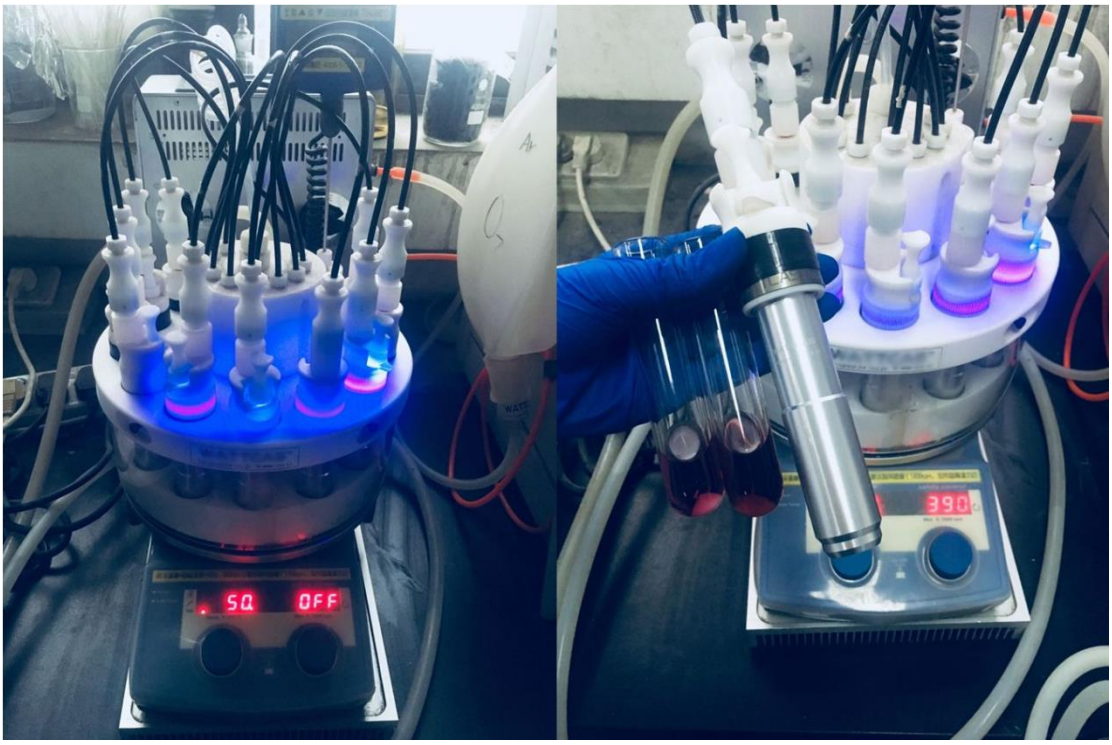


Figure S1. Details for the photochemical reaction setup.

The light Source and the Material of the Irradiation Vessel

Manufacturer: Xi'an WATTECS experimental equipment Co. Ltd

Model: WP-TEC-1020SL

Broadband source: X = 390 nm (light power: 16 W).

Material of the irradiation vessel: borosilicate reaction tube (20 ml)

Distance from the light source to the irradiation vessel: 2.0 cm

Not use any filters

1 General information

All chemicals and reagents were used of commercial grade and were used without further purification. The reactions were monitored by thin-layer chromatography (TLC) using silica gel GF254. Column chromatography was performed with 200–300 mesh silica gel. All yields refer to isolated products after purification. The intermediates and the products synthesized were fully characterized by spectroscopic data. The NMR spectra were recorded on Bruker DRX-400 (^{1}H: 400 MHz, ^{13}C: 101MHz) using $CDCl_3$ and DMSO-d6 as solvents. The following abbreviation were used to explain the multiplicities: (s) = singlet, (d) = doublet, (t) = triplet, (q) = quartet, (sept) = septuplet, (dd) = double doublet, (dt) = double triplet, (dq) = double quartet, (ddd) = double-double doublet, (m) = multiplet; Chemical shifts (δ) are expressed in parts per million (ppm) and J values are given in hertz (Hz). IR spectra were recorded on an FT-IR Thermo Nicolet Avatar 360 using a KBr pellet. HRMS was performed on an Agilent LC/MSD TOF instrument. The melting points were measured by the XT-4A melting point apparatus without correction.

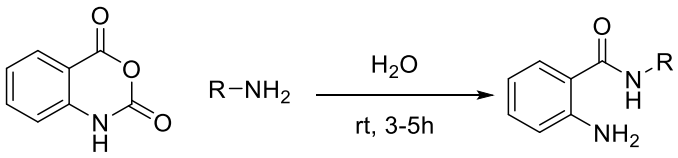
Table 1S. Optimization Study for benzylic C-H amidation [a,b]

entry	deviation from standard conditions	yield (%)
1	none	71
2	CuCl as cataylst	40
3	$Fe_2(SO_4)_3$, or $Cu(OAc)_2$ as catalyst	trace
4	$Fe_2(SO_4)_3$ + LiCl (10 mol %)	42
5	under O_2	73
6	$K_2S_2O_8$ as oxidant	12
7	$NaIO_4$ as oxidant	trace
8	DCM, or 1,2-dichloroethane as solvent	< 5
9	THF as solvent	40
10	5.0 equiv of methylarene **1a**	41
11	440 nm LED	36
12	50 ºC	65
13	no 4A molecular sieve	67
14	no $FeCl_3$	N.D.
15	under N_2	trace
16	in the dark	N.D.

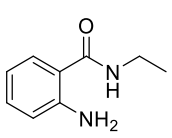
[a] Reaction conditions: **1a** (3.0 mmol, 10.0 equiv), **2a** (0.3 mmol, 1.0 equiv), $FeCl_3$ (0.03 mmol, 10 mol %) in CH_3CN (3.0 mL, 0.1 M) and in the presence of 4A molecular sieves under air atmosphere, room temperature, 390 nm light-emitting diodes (LEDs, 16W). [b] Yields are of isolated products after chromatographic purification based on **2a**.

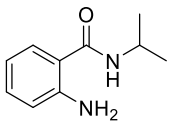
2 Synthesis of Substrates **4**

2.1 General Procedures for the Synthesis of Substrates **4a-4l**[1]



Under air atmosphere, Isatoic anhydride (5.0 mmol, 1.0 equiv) and alkyl amines (5.0 mmol, 1.0 equiv) were added to H_2O (20.0 mL) and the mixture was stirred reaction tube. The mixture was stirred at room temperature and monitored by TLC. After stirring for 3-5 h. After the reaction was quenched with saturated NaCl solution and extracted with 20 mL EtOAc for three times. The organic layers were combined, dried over Na_2SO_4, filtered and evaporated under reduced pressure. The residues were purified by flash column chromatography on silica gel to provide the Substrates **4a-4l**.


4a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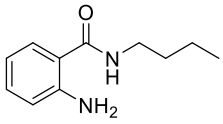
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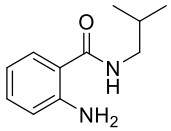
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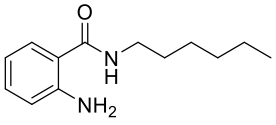
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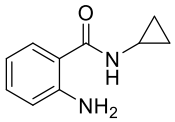
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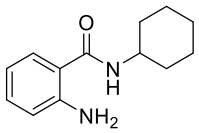
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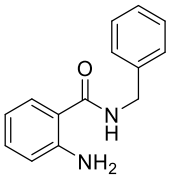
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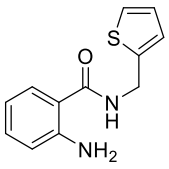
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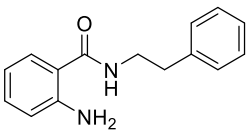
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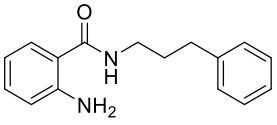
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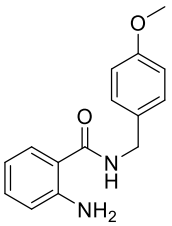
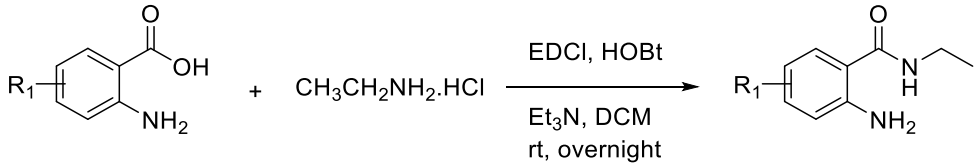
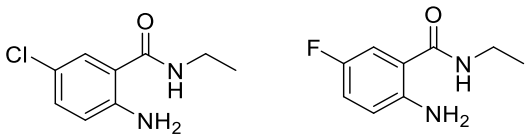

4l

2.2 Synthesis of substrates **4m-4n**[1]



Under air atmosphere, A mixture of substituted acid (2.5 mmol, 1.0 equiv), EDCl (3.0 mmol, 1.2 equiv), HOBt (3.0 mmol, 1.2 equiv), NH_4Cl (3.0 mmol, 1.2 equiv) and Et_3N (7.6 mmol, 3.0 equiv) in DMSO (12.6 ml) was stirred at room temperature 12h and monitored by TLC. After the reaction was quenched with saturated NaCl solution and extracted with 20.0 mL EtOAc for three times. The organic layers were combined, dried over Na_2SO_4, filtered and evaporated under reduced pressure. The residues were purified by flash column chromatography on silica gel to provide the Substrates **4m-4n**.

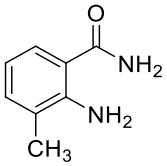


4n 4m

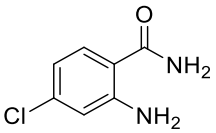
2.3 Synthesis of substrates **4o-4p**[3]

Under air atmosphere, A mixture of substituted acid (2.0 mmol, 1.0 equiv), EDC•HCl (3.0 mmol, 1.5 equiv), HOBt (3.3 mmol, 1.7 equiv), NH_4Cl (6.5 mmol, 3.3 equiv) and DIPEA (13.0 mmol, 6.5 equiv) in DMSO (7.0 ml) was stirred at room temperature for 15 h and monitored by TLC. After the reaction was quenched with saturated NaCl solution and extracted with 20.0 mL EtOAc for three times. The organic layers were combined, dried over Na_2SO_4, filtered and evaporated under reduced pressure. The

residues were purified by flash column chromatography on silica gel to provide the Substrates **4o-4p**.

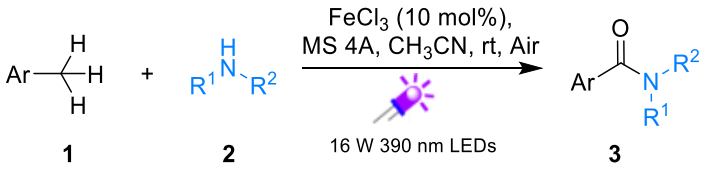


4o

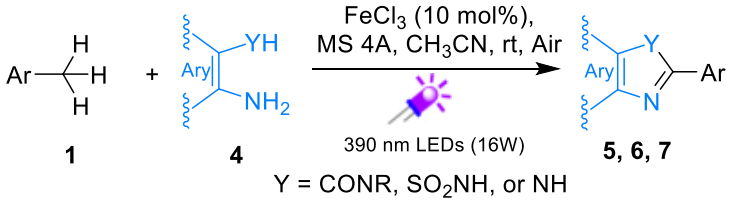


4p

3 Procedure for preparing compounds **3a-3y**, **5a-5t**, **6a-6c** and **7a-7n**.



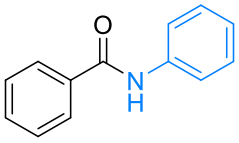
Under air atmosphere, methyl arenes **1** (3.0 mmol, 10.0 equiv), amine **2** (0.3 mmol, 1.0 equiv), $FeCl_3$ (10 mol%, 0.01mmol) in MeCN (3.0 mL, 0.1 M) and in the presence of 4A molecular sieves were added to 20.0 mL reaction tube. The mixture was stirred at 390 nm light-emitting diodes (LEDs, 16W) and monitored by TLC. After stirring for 10-24h. Than, the reaction was quenched with saturated NaCl solution and extracted with 20.0 mL EtOAc for three times. The organic layers were combined, dried over Na_2SO_4, filtered and evaporated under reduced pressure. The residues were purified by flash column chromatography on silica gel to provide the products **3**. The products were further identified by NMR spectroscop.



Under air atmosphere, methyl arenes **1** (3.0 mmol, 10.0 equiv), 2-aminobenzamide **4** (0.3 mmol, 1.0 equiv), $FeCl_3$ (10 mol%, 0.01mmol) in MeCN (3.0 mL, 0.1 M) and in the presence of 4A molecular sieves added to 20.0 mL reaction tube. The mixture was stirred at 390 nm light-emitting diodes (LEDs, 16W) and monitored by TLC. After stirring for 15-30 h. Than, the reaction was quenched with saturated NaCl solution and extracted with 20.0 mL EtOAc for three times. The organic layers were combined, dried over Na_2SO_4, filtered and evaporated under reduced pressure. The residues were purified by flash column chromatography on silica gel to provide the products **5, 6, 7**. The products were further identified by FTIR spectroscopy, NMR spectroscopy, and HRMS.

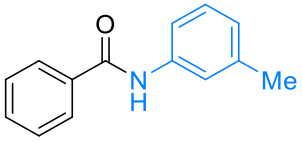
4 Spectroscopic Data of **3a-3y**, **5a-5t**, **6a-6c**,**7a-7n and 9**.

N-Phenylbenzamide(**3a**)



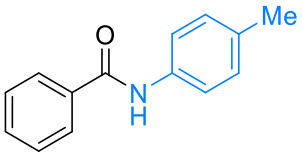
White solid; Mp: 163-165 °C; yield: 71% (41mg); **IR** (KBr): 3354, 3020, 1655, 1611, 1529, 1438, 1370, 1242, 746, 717, 686; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.31 (s, 1H), 8.03 – 7.97 (m, 2H), 7.83 (d, J = 8.0 Hz, 2H), 7.68 – 7.53 (m, 3H), 7.40 (t, J = 7.7 Hz, 2H), 7.14 (t, J = 7.4 Hz, 1H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 166.0, 139.6, 135.5, 132.0, 129.1, 128.9, 128.1, 124.1, 120.8; Data consistent with those previously reported.[4]

N-(m-tolyl)benzamide(**3b**)



White solid; Mp: 117-119 °C; yield: 71% yield (45 mg); **IR** (KBr): 3308, 2931, 1652, 1545, 1496, 1377, 1247, 1028, 832, 779; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.18 (s, 1H), 7.95 (d, J = 6.9 Hz, 2H), 7.63 (d, J = 2.0 Hz, 1H), 7.60 – 7.50 (m, 4H), 7.24 (t, J = 7.8 Hz, 1H), 6.93 (d, J = 7.5 Hz, 1H), 2.32 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 166.0, 139.6, 138.2, 135.5, 132.0, 128.9, 128.8, 128.1, 124.8, 121.4, 118.0, 21.7; Data consistent with those previously reported.[5]

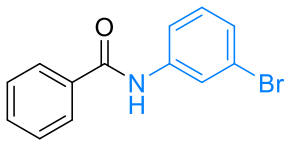
N-(p-tolyl)benzamide(**3c**)



White solid; Mp: 157-159 °C; yield: 76%(48 mg); **IR** (KBr): 3347, 2935, 1660, 1527, 1378, 1321, 1248, 1030, 832, 162; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.19 (s, 1H), 7.96 (d, J = 7.2 Hz, 2H), 7.68 (d, J = 8.0 Hz, 2H), 7.58 (d, J = 7.0 Hz, 1H), 7.53 (t, J =

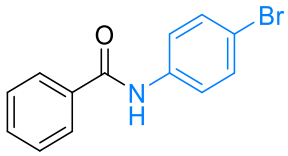
7.4 Hz, 2H), 7.16 (d, J = 8.1 Hz, 2H), 2.29 (s, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 165.8, 137.1, 135.5, 133.06, 131.9, 129.5, 128.8, 128.1, 120.9, 21.0; Data consistent with those previously reported.[6]

N-(4-bromophenyl)benzamide(**3d**)



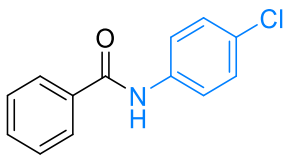
White solid; Mp: 130-132 °C; yield: 60% (50 mg); **IR** (KBr): 3380, 3092, 1658, 1589, 1533, 1492, 1318, 1245, 1026, 763, 701; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.42 (s, 1H), 8.13 (s, 1H), 7.96 (d, J = 7.5 Hz, 2H), 7.78 (d, J = 7.6 Hz, 1H), 7.65 – 7.58 (m, 1H), 7.55 (t, J = 7.7 Hz, 2H), 7.37 – 7.26 (m, 2H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 166.3, 141.3, 135.0, 132.3, 131.1, 128.9, 128.2, 126.7, 123.0, 121.9, 119.5; Data consistent with those previously reported.[7]

N-(4-bromophenyl)benzamide(**3e**)



White solid; Mp: 168-170 °C; yield: 66% (54 mg); **IR** (KBr): 3350, 3060, 1665, 1604, 1587, 1565, 1489, 1396, 1285, 1107, 796, 717; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.39 (s, 1H), 7.99 – 7.92 (m, 2H), 7.86 – 7.75 (m, 2H), 7.63 – 7.52 (m, 5H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 166.2, 139.2, 135.2, 132.2, 131.91, 128.9, 128.2, 122.7, 115.8; Data consistent with those previously reported.[8]

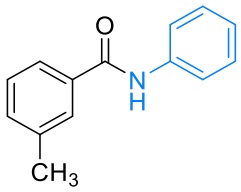
N-(4-chlorophenyl)benzamide(**3f**)



White solid; Mp: 183-185 °C; yield: 42% (30 mg); **IR** (KBr): 3326, 3052, 1662, 1531, 1495, 1378, 1248, 1037, 832, 765, 716; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.38 (s, 1H), 7.95 (d, J = 7.4 Hz, 2H), 7.83 (d, J = 8.8 Hz, 2H), 7.65 – 7.50 (m, 3H), 7.42 (d, J

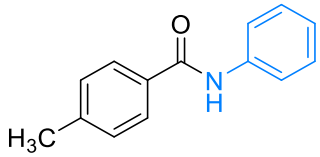
= 8.8 Hz, 2H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 166.1, 138.6, 135.2, 132.2, 129.0, 128.9, 128.2, 127.7, 122.3; Data consistent with those previously reported.[6]

3-methyl-*N*-phenylbenzamide(**3g**)



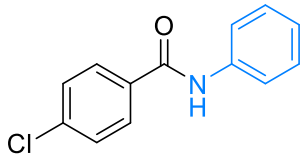
White solid; Mp: 131-133 °C; yield: 61% (38 mg); **IR** (KBr): 3301, 3064, 2986, 1652, 1596, 1584, 1533, 1489, 1326, 1246, 732, 706; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.22 (s, 1H), 7.82-7.72 (m, 4H), 7.41 (d, J = 4.2 Hz, 2H), 7.39–7.32 (m, 2H), 7.14–7.07 (m, 1H), 2.41 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 166.1, 139.7, 138.2, 135.5, 132.6, 129.1, 128.8, 128.6, 125.3, 124.1, 120.8, 21.4; Data consistent with those previously reported.[5]

4-methyl-*N*-phenylbenzamide(**3h**)



White solid; Mp: 115-117 °C; yield: 68% (43 mg); **IR** (KBr): 3263, 3036, 1639, 1494, 1424, 1365, 1255, 1150, 1077, 742, 702; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.14 (s, 1H), 7.87 (d, J = 7.9 Hz, 2H), 7.77 (d, J = 8.0 Hz, 2H), 7.34 (t, J = 7.5 Hz, 4H), 7.09 (t, J = 7.4 Hz, 1H), 2.39 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 165.8, 142.0, 139.7, 132.6, 129.4, 129.0, 128.2, 124.0, 120.8, 21.5; Data consistent with those previously reported.[4]

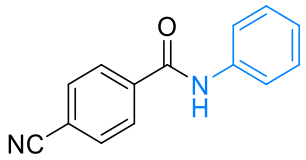
4-chloro-*N*-phenylbenzamide(**3i**)



White solid; Mp: 228-230 °C; yield: 42% (29 mg); **IR** (KBr): 3350, 1659, 1605, 1523, 1495, 1407, 1386, 1286, 1109, 869, 753; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.32 (s,

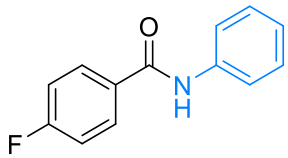
1H), 8.02 – 7.95 (m, 2H), 7.77 (dd, *J* = 8.7, 1.2 Hz, 2H), 7.65 – 7.58 (m, 2H), 7.36 (dd, *J* = 8.5, 7.3 Hz, 2H), 7.12 (t, *J* = 7.4 Hz, 1H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 164.9, 139.4, 136.9, 134.1, 130.1, 129.1, 128.9, 124.3, 120.9; Data consistent with those previously reported.[9]

4-cyano-*N*-phenylbenzamide (**3j**)



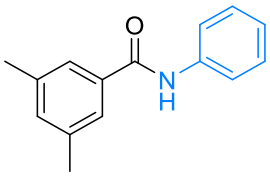
White solid; Mp: 174-176 °C; yield: 50% (33 mg); **IR** (KBr): 3360, 3079, 2920, 2855, 2240, 1670, 1558, 1489, 1330, 1260, 1060, 716; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.49 (s, 1H), 8.11 (d, *J* = 8.4 Hz, 2H), 8.03 (d, *J* = 8.4 Hz, 2H), 7.77 (d, *J* = 7.3 Hz, 2H), 7.42 – 7.33 (m, 2H), 7.14 (t, *J* = 7.4 Hz, 1H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 164.6, 139.5, 139.2, 132.9, 129.2, 129.0, 124.6, 121.0, 118.9, 114.3; Data consistent with those previously reported.[10]

4-fluoro-*N*-phenylbenzamide (**3k**)



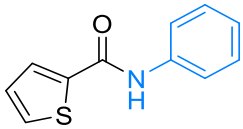
White solid; Mp: 180-182 °C; yield: 53% (34 mg); **IR** (KBr): 3406, 3093, 1654, 1542, 1491, 1440, 1245, 1032, 765; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.27 (s, 1H), 8.04 (dd, *J* = 8.9, 5.5 Hz, 2H), 7.76 (dd, *J* = 8.6, 1.2 Hz, 2H), 7.42 – 7.31 (m, 4H), 7.11 (t, *J* = 7.4 Hz, 1H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 164.9, 164.5 (d, $J_{C\text{-}F}$ =247.45 Hz), 139.5, 131.9 (d, $J_{C\text{-}F}$ =2.84 Hz), 130.9 (d, $J_{C\text{-}F}$ =9.06 Hz), 129.1, 124.29, 120.9, 115.8 (d, $J_{C\text{-}F}$ =21.64 Hz); **^{19}F NMR** (376 MHz, DMSO-d_6) δ -108.84. Data consistent with those previously reported.[10]

3,5-dimethyl-*N*-phenylbenzamide(**3l**)



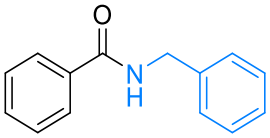
White solid; Mp: 120-122 °C; yield: 49% (33 mg); **IR** (KBr): 3331, 3008, 2964, 2873, 1750, 1651, 1607, 1537, 1442, 1328, 1245, 754, 702; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.71 (s, 1H), 7.57 (dd, *J* = 8.6, 1.2 Hz, 2H), 7.40 (s, 2H), 7.30 (dd, *J* = 8.5, 7.4 Hz, 2H), 7.13 – 7.04 (m, 2H), 2.32 (s, 6H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 165.0, 137.5, 137.0, 134.0, 132.4, 128.1, 123.7, 123.4, 119.1, 20.3; Data consistent with those previously reported.[12]

N-phenylthiophene-2-carboxamide(**3m**)



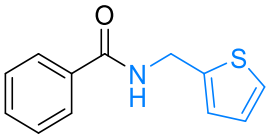
White solid; Mp: 150-152 °C; yield: 40% (24 mg); **IR** (KBr): 3338, 3097, 1643, 1606, 1541, 1443, 1364, 1322, 1262, 751, 722, 654; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.65 (s, 1H), 7.59 – 7.51 (m, 3H), 7.48 (d, *J* = 3.9 Hz, 1H), 7.30 (t, *J* = 7.9 Hz, 2H), 7.13 – 7.03 (m, 2H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 158.9, 138.2, 136.6, 129.7, 128.1, 127.4, 126.8, 123.6, 119.2; Data consistent with those previously reported.[13]

N-benzylbenzamide(**3n**)



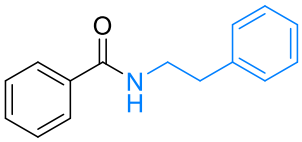
White solid; Mp: 103-105 °C; yield: 80% (51 mg); **IR** (KBr): 3310, 3054, 2926, 1661, 1554, 1441, 1399, 1254, 1086, 880, 702; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 9.09 (t, *J* = 6.1 Hz, 1H), 7.93 (d, *J* = 7.5 Hz, 2H), 7.55 (t, *J* = 7.2 Hz, 1H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.34 (d, *J* = 4.4 Hz, 4H), 7.25 (m, 1H), 4.52 (d, *J* = 6.0 Hz, 2H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 166.7, 140.2, 134.8, 131.7, 128.8, 128.8, 127.7, 127.7, 127.2, 43.1; Data consistent with those previously reported.[5]

N-(thiophen-2-ylmethyl)benzamide(**3o**)



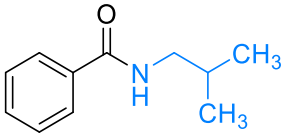
White solid; Mp: 120-122 °C; yield: 63% (41 mg); **IR** (KBr): 3348, 3020, 2925, 2863, 1656, 1540, 1487, 1376, 1249, 1031, 833, 794; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 9.16 (t, J = 6.0 Hz, 1H), 7.88 (d, J = 7.0 Hz, 2H), 7.53 (d, J = 7.2 Hz, 1H), 7.48 (t, J = 7.3 Hz, 2H), 7.40 – 7.36 (m, 1H), 7.03 (d, J = 2.3 Hz, 1H), 6.97 (dd, J = 5.1, 3.4 Hz, 1H), 4.64 (d, J = 5.0 Hz, 2H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 166.5, 143.2, 134.6, 131.8, 128.8, 127.7, 127.1, 125.8, 125.4, 38.2; Data consistent with those previously reported.[14]

N-phenethylbenzamide(**3p**)



White solid; Mp: 113-115 °C; yield: 72% (49 mg); **IR** (KBr): 3340, 3058, 2935, 2883, 1654, 1540, 1463, 1249, 1058, 741, 701, 662; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.59 (t, J = 5.6 Hz, 1H), 7.83 (d, J = 7.2 Hz, 2H), 7.56 – 7.42 (m, 3H), 7.31 (t, J = 7.4 Hz, 2H), 7.28 – 7.17 (m, 3H), 3.50 (q, J = 7.7, 7.2 Hz, 2H), 2.86 (t, J = 7.5 Hz, 2H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 166.6, 140.0, 135.1, 131.5, 129.1, 128.8, 128.7, 127.6, 126.6, 41.4, 35.6; Data consistent with those previously reported.[15]

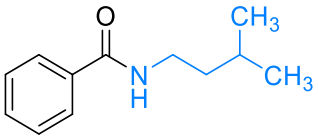
N-isobutylbenzamide(**3q**)



White solid; Mp: 56-58 °C; yield: 86% (46 mg); **IR** (KBr): 3343, 3071, 2965, 2880, 1642, 1546, 1488, 1462, 1299, 1159, 706; **^{1}H NMR** (400 MHz, Chloroform-d) δ 7.72 – 7.67 (m, 2H), 7.44 – 7.37 (m, 1H), 7.37 – 7.31 (m, 2H), 6.31 (s, 1H), 3.20 (dd, J = 6.9, 6.0 Hz, 2H), 1.82 (dp, J = 13.5, 6.8 Hz, 1H), 0.89 (d, J = 6.7 Hz, 6H); **^{13}C NMR**

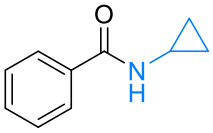
(100 MHz, Chloroform-*d*) δ 166.7, 133.9, 130.3, 127.5, 125.8, 46.4, 27.6, 19.2; Data consistent with those previously reported.[15]

N-Isopentylbenzamide(**3r**)



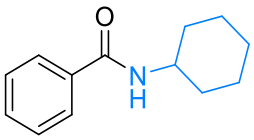
White solid; Mp: 40-42 °C; yield: 77% (44 mg); **IR** (KBr): 3317, 3072, 2962, 2877, 1643, 1545, 1463, 1308, 1164, 799, 707; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.72 – 7.67 (m, 2H), 7.41 – 7.34 (m, 1H), 7.34 – 7.27 (m, 2H), 6.43 (d, 1H), 3.36 (m, *J* = 10.6, 5.2 Hz, 2H), 1.62 – 1.52 (m, 1H), 1.45 – 1.37 (m, 2H), 0.90 – 0.80 (m, 6H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 166.7, 133.8, 130.2, 127.4, 125.9, 37.4, 37.4, 24.9, 21.5; Data consistent with those previously reported.[15]

N-cyclopropylbenzamide(**3s**)



White solid; Mp: 92-94 °C; yield: 72% (35 mg); **IR** (KBr): 3248, 3073, 2930, 1632, 1548, 1492, 1443, 1318, 1027, 804, 701; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.70 – 7.66 (m, 2H), 7.42 – 7.36 (m, 1H), 7.31 (t, *J* = 7.4 Hz, 2H), 6.57 (s, 1H), 2.80 (m, *J* = 7.2, 3.7 Hz, 1H), 0.75 (m, *J* = 7.1, 5.2 Hz, 2H), 0.58 – 0.52 (m, 2H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 168.0, 133.4, 130.39, 127.4, 125.9, 22.1, 5.7; Data consistent with those previously reported.[15]

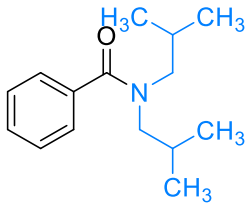
N-cyclohexylbenzamide(**3t**)



White solid; Mp: 148-150 °C; yield: 70% (42 mg); **IR** (KBr): 3336, 3028, 2930, 2676, 1691, 1533, 1426, 1245, 931, 707, 668; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.80 – 7.71 (m, 2H), 7.50 – 7.45 (m, 1H), 7.41 (dd, *J* = 8.1, 6.5 Hz, 2H), 6.07 – 6.01 (d, 1H),

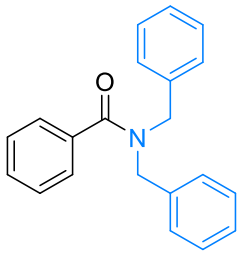
4.04 – 3.90 (m, 1H), 2.02 (dd, *J* = 12.6, 4.0 Hz, 2H), 1.79 – 1.71 (m, 2H), 1.64 (dt, *J* = 13.0, 3.9 Hz, 1H), 1.48 – 1.35 (m, 2H), 1.29 – 1.16 (m, 3H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 166.7, 135.1, 131.2, 128.5, 126.9, 48.7, 33.3, 25.6, 24.9; Data consistent with those previously reported.[15]

N,*N*-diisobutylbenzamide(**3u**)



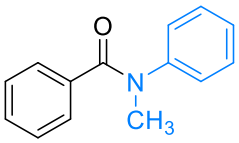
White solid; Mp: 48-50 °C; yield: 72% (51 mg); **IR** (KBr): 3065, 2966, 2879, 2526, 1636, 1463, 1426, 1381, 1270, 1106, 789, 718; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.29 (td, *J* = 6.4, 5.9, 3.9 Hz, 5H), 3.29 (d, *J* = 7.6 Hz, 2H), 3.02 (d, *J* = 7.5 Hz, 2H), 2.06 (m, *J* = 6.9 Hz, 1H), 1.77 (m, *J* = 13.5, 6.9 Hz, 1H), 0.92 (d, *J* = 6.7 Hz, 6H), 0.66 (d, *J* = 6.7 Hz, 6H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 171.5, 136.5, 128.0, 127.3, 126.0, 55.5, 50.12, 25.8, 25.2, 19.2, 18.8; Data consistent with those previously reported.[16]

N,*N*-dibenzylbenzamide(**3v**)



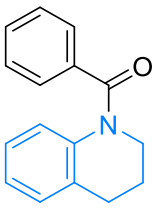
White solid; Mp: 207-209 °C; yield: 67% (60 mg); **IR** (KBr): 3039, 2973, 2934, 1717, 1610, 1498, 1447, 1249, 1075, 996, 716, 707; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.54 – 7.50 (m, 2H), 7.43 – 7.28 (m, 11H), 7.16 (d, *J* = 7.4 Hz, 2H), 4.73 (s, 2H), 4.42 (s, 2H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 172.3, 137.0, 136.5, 136.2, 129.7, 128.9, 128.8, 128.6, 128.5, 127.7, 127.6, 127.1, 126.8, 51.6, 46.9; Data consistent with those previously reported.[17]

N-methyl-*N*-phenylbenzamide(**3w**)



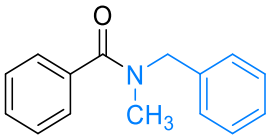
White solid; Mp: 55-57 °C; yield: 74% (47 mg); **IR** (KBr): 3068, 2962, 2871, 1647, 1590, 1496, 1370, 1297, 1105, 798, 703; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.24 – 7.20 (m, 2H), 7.19 – 7.11 (m, 3H), 7.11 – 7.04 (m, 3H), 6.96 (dd, *J* = 7.2, 1.5 Hz, 2H), 3.43 (s, 3H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 169.7, 143.9, 134.9, 128.6, 128.1, 127.7, 126.7, 125.9, 125.5, 37.4; Data consistent with those previously reported.[18]

(3,4-dihydroquinolin-1(2*H*)-yl)(phenyl)methanone(**3x**)



White solid; Mp: 113-115 °C; yield: 74% (47 mg); **IR** (KBr): 3065, 2957, 1644, 1493, 1377, 1265, 1153, 1101, 794, 756, 715; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.31 – 7.25 (m, 3H), 7.22 – 7.18 (m, 2H), 7.08 (d, *J* = 7.5 Hz, 1H), 6.92 (t, *J* = 7.5 Hz, 1H), 6.84 – 6.75 (m, 1H), 6.64 (d, *J* = 8.2 Hz, 1H), 3.84 (t, *J* = 6.5 Hz, 2H), 2.77 (t, *J* = 6.6 Hz, 2H), 1.98 (p, *J* = 6.6 Hz, 2H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 169.3, 138.3, 135.3, 130.6, 129.1, 127.6, 127.3, 127.1, 124.7, 124.4, 123.5, 43.4, 25.9, 23.1; Data consistent with those previously reported.[19]

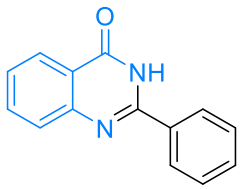
N-benzyl-*N*-methylbenzamide(**3y**)



White solid; Mp: 47-49 °C; yield: 75% (51 mg); **IR** (KBr): 3063, 3036, 2928, 1635, 1493, 1447, 1402, 1264, 1072, 1028, 789, 728; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.42 – 7.28 (m, 7H), 7.24 – 7.05 (m, 3H), 4.68 (s, 1H), 4.42 (s, 1H), 2.94 (s, 1.5H), 2.77 (s, 1.5H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 172.4, 171.7, 137.1, 136.6, 136.3,

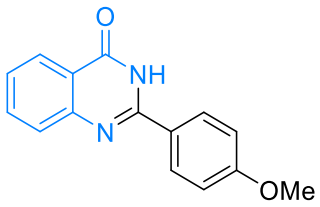
129.7, 128.9, 128.8, 128.5, 128.2, 127.6, 127.0, 126.8, 55.2, 50.8, 37.0, 33.2; Data consistent with those previously reported.[20]

2-phenylquinazolin-4(3*H*)-one (**5a**)



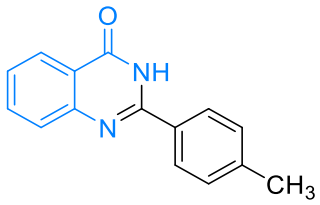
White solid; Mp: 237-238 ºC; yield: 83% (55 mg); IR (KBr): 3441, 3042, 1670, 1607, 1570, 1514, 1479, 1296, 1056, 768, 690; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.58 (s, 1H), 8.23 – 8.13 (m, 3H), 7.84 (dd, J = 8.4, 6.9 Hz, 1H), 7.75 (d, J = 7.1 Hz, 1H), 7.64 – 7.48 (m, 4H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.7, 152.8, 149.2, 135.1, 133.2, 131.9, 129.1, 128.2, 127.9, 127.1, 126.3, 121.4; **HRMS** (TOF-ESI$^+$): *m/z* calcd for $C_{14}H_{10}N_2O$ $[M+H]^+$, 223.0866; found, 223.0863; Data consistent with those previously reported.[1]

2-(4-methoxyphenyl)quinazolin-4(3*H*)-one (**5b**)



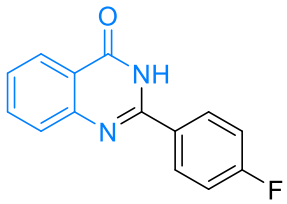
White solid; Mp: 246-247 °C; yield: 77% (58 mg); IR (KBr): 3436, 2920, 2850, 1676, 1634, 1484, 1248, 764, 686; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.37 (s, 1H), 8.13 (d, J = 8.5 Hz, 2H), 8.07 (d, J = 7.9 Hz, 1H), 7.76 (t, J = 7.6 Hz, 1H), 7.64 (d, J = 8.2 Hz, 1H), 7.42 (t, J = 7.5 Hz, 1H), 7.03 (d, J = 8.4 Hz, 2H), 3.79 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.8, 162.3, 152.3, 149.4, 135.0, 129.9, 127.8, 126.6, 126.3, 125.3, 121.2, 114.5, 55.9; **HRMS** (TOF-ESI$^+$): *m/z* calcd for $C_{15}H_{12}N_2O_2$ $[M+H]^+$, 253.0972; found, 253.0972; Data consistent with those previously reported.[21]

2-(*p*-tolyl)quinazolin-4(3*H*)-one (**5c**)



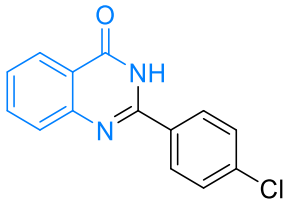
White solid; Mp: 243-244 °C; yield: 79% (56 mg); **IR** (KBr): 3240, 3199, 3140, 3071, 2944, 2892, 1763, 1691, 1648, 1601, 1545, 1502, 1446, 1326, 1253, 1207, 1170, 1065, 1007, 913, 756, 695; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.15 (d, J = 7.9 Hz, 1H), 8.10 (d, J = 8.1 Hz, 2H), 7.87 – 7.79 (m, 1H), 7.73 (d, J = 8.5 Hz, 1H), 7.54 – 7.49 (m, 1H), 7.36 (dd, J = 8.4, 3.3 Hz, 2H), 2.39 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.8, 152.7, 149.3, 141.9, 135.0, 130.4, 129.7, 128.2, 127.9, 126.9, 126.3, 121.4, 21.5; **HRMS** (TOF-ESI$^+$): *m/z* calcd for $C_{15}H_{12}N_2O$ $[M+H]^+$, 237.1022; found, 237.1018; Data consistent with those previously reported.[21]

2-(4-fluorophenyl)quinazolin-4(3*H*)-one (**5d**)



White solid; Mp: 258-259 °C; yield: 76% (55 mg); **IR** (KBr): 3440, 3043, 1667, 1607, 1444, 1285, 1050, 835, 762; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.59 (s, 1H), 8.26 (dd, J = 8.8, 5.5 Hz, 2H), 8.16 (d, J = 7.9 Hz, 1H), 7.88 – 7.80 (m, 1H), 7.74 (d, J = 8.1 Hz, 1H), 7.56 – 7.50 (m, 1H), 7.40 (t, J = 8.8 Hz, 2H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 164.5(d, $J_{C\text{-}F}$ = 248.16 Hz), 162.7, 151.9, 149.1, 135.1, 130.8(d, $J_{C\text{-}F}$ = 8.62 Hz), 129.7(d, $J_{C\text{-}F}$ = 2.49 Hz), 127.9, 127.1, 126.3, 121.3, 116.1(d, $J_{C\text{-}F}$ = 21.83 Hz); **^{19}F NMR** (376 MHz, DMSO-d_6) δ -109.02; **HRMS** (TOF-ESI$^+$): *m/z* calcd for $C_{14}H_9FN_2O$ $[M+H]^+$, 241.0772; found, 241.0773; Data consistent with those previously reported.[21]

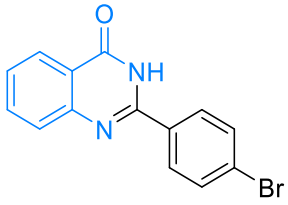
2-(4-chlorophenyl)quinazolin-4(3*H*)-one (**5e**)



White solid; Mp: 297-299 °C; yield: 74% (57 mg); **IR** (KBr): 3314, 3087, 1676, 1611,

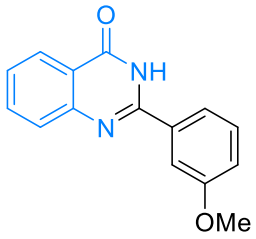
1567, 1482, 1444, 1006, 831; **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.61 (s, 1H), 8.20 (d, J = 8.5 Hz, 2H), 8.16 (d, J = 7.8 Hz, 1H), 7.85 (dd, J = 8.4, 7.0 Hz, 1H), 7.75 (d, J = 8.1 Hz, 1H), 7.63 (d, J = 8.5 Hz, 2H), 7.57 – 7.48 (m, 1H); **^{13}C NMR** (150 MHz, DMSO-d_6) δ 162.7, 151.9, 149.0, 136.8, 135.2, 132.1, 130.1, 129.2, 127.9, 127.3, 126.4, 121.4; **HRMS** (TOF-ESI$^+$): *m/z* calcd for $C_{14}H_9ClN_2O$ $[M+H]^+$, 257.0476; found, 257.0479; Data consistent with those previously reported.[21]

2-(4-bromophenyl)quinazolin-4(3*H*)-one (**5f**)



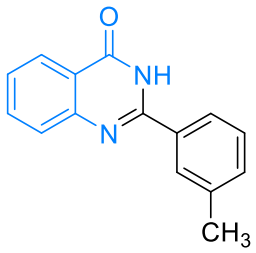
White solid; Mp: 296-297 °C; yield: 79% (70 mg); **IR** (KBr): 3456, 3047, 1673, 1600, 1569, 1447, 1049, 828, 772; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.64 (s, 1H), 8.18 – 8.12 (m, 3H), 7.88 – 7.83 (m, 1H), 7.76 (t, J = 8.0 Hz, 3H), 7.57 – 7.53 (m, 1H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.6, 151.9, 149.0, 135.2, 132.4, 132.1, 130.3, 128.0, 127.3, 126.4, 125.7, 121.5; **HRMS** (TOF-ESI+): m/z calcd for $C_{14}H_9BrN_2O$ $[M+H]^+$, 300.9971; found, 300.9971; Data consistent with those previously reported.[21]

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



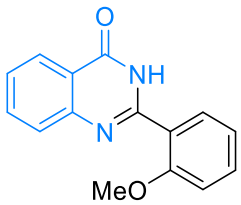
White solid; Mp: 210-212 °C; yield: 77% (58 mg); **IR** (KBr): 3415, 3046, 2963, 2874, 1670, 1610, 1499, 1220, 1028, 767, 685; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.56 (s, 1H), 8.17 (dd, J = 7.9, 1.6 Hz, 1H), 7.87 – 7.74 (m, 4H), 7.56 – 7.43 (m, 2H), 7.16 (d, J = 5.8 Hz, 1H), 3.87 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.7, 159.8, 152.5, 149.1, 135.1, 134.5, 130.2, 128.0, 127.1, 126.3, 121.5, 120.6, 118.1, 113.0, 55.9; **HRMS** (TOF-ESI$^+$): *m/z* calcd for $C_{15}H_{12}N_2O$ $[M+H]^+$, 253.0972; found, 253.0972. Data consistent with those previously reported.[22]

2-(*m*-tolyl)quinazolin-4(3*H*)-one (**5h**)



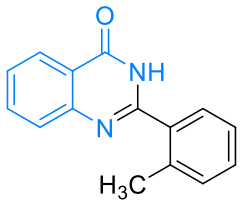
White solid; Mp: 209-211 °C; yield: 81% (57 mg); **IR** (KBr): 3411, 3055, 2978, 2878, 1680, 1610, 1495, 1026, 764, 714; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.49 (s, 1H), 8.16 (dd, J = 8.0, 1.5 Hz, 1H), 8.03 (s, 1H), 7.97 (d, J = 7.4 Hz, 1H), 7.87 – 7.79 (m, 1H), 7.75 (d, J = 7.2 Hz, 1H), 7.52 (t, J = 7.5 Hz, 1H), 7.46 – 7.36 (m, 2H), 2.41 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.7, 152.9, 149.2, 138.4, 135.1, 133.1, 132.5, 129.0, 128.8, 128.0, 127.0, 126.3, 125.4, 121.4, 21.4; **HRMS** (TOF-ESI$^+$): *m/z* calcd for $C_{15}H_{12}N_2O$ $[M+H]^+$, 237.1022; found, 237.1018; Data consistent with those previously reported.[22]

2-(2-methoxyphenyl)quinazolin-4(3*H*)-one (**5i**)



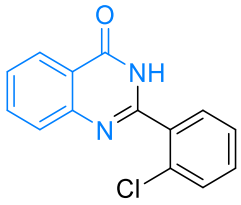
White solid; Mp: 202-203 °C; yield: 66% (50 mg); **IR** (KBr): 3329, 3053, 2980, 2897, 1681, 1604, 1462, 1382, 1050, 764, 690; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.12 (s, 1H), 8.16 (dd, J = 7.9, 1.6 Hz, 1H), 7.87 – 7.81 (m, 1H), 7.73 – 7.69 (m, 2H), 7.57 – 7.51 (m, 2H), 7.20 (d, J = 7.9 Hz, 1H), 7.10 (t, J = 7.0 Hz, 1H), 3.87 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 161.7, 157.6, 152.8, 149.5, 134.9, 132.7, 130.9, 127.9, 127.0, 126.3, 123.1, 121.5, 120.9, 112.3, 56.3; **HRMS** (TOF-ESI$^+$): *m/z* calcd for $C_{15}H_{12}N_2O_2$ $[M+H]^+$, 253.0972; found, 253.0972; Data consistent with those previously reported.[23]

2-(*o*-tolyl)quinazolin-4(3*H*)-one (**5j**)



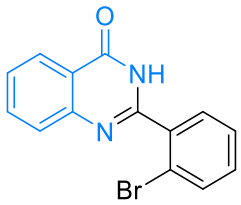
White solid; Mp: 222-224 °C; yield: 70% (50 mg); **IR** (KBr): 3437, 2919, 2850, 1726, 1684, 1611, 1594, 1242, 759, 721; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.47 (s, 1H), 8.17 (d, J = 7.9 Hz, 1H), 7.85 (t, J = 7.6 Hz, 1H), 7.70 (d, J = 8.2 Hz, 1H), 7.59 – 7.49 (m, 2H), 7.44 (t, J = 7.5 Hz, 1H), 7.34 (dd, J = 13.5, 7.1 Hz, 2H), 2.39 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.3, 154.8, 149.2, 136.6, 135.0, 134.7, 131.0, 130.4, 129.6, 127.8, 127.1, 126.3, 126.2, 121.4, 20.0; **HRMS** (TOF-ESI$^+$): *m/z* calcd for $C_{15}H_{12}N_2O$ $[M+H]^+$, 237.1022; found, 237.1018; Data consistent with those previously reported.[22]

2-(2-chlorophenyl)quinazolin-4(3*H*)-one (**5k**)



White solid; Mp: 185-186 °C; yield: 62% (48 mg); **IR** (KBr): 3445, 3057, 1667, 1514, 1435, 1295, 1142, 1050, 736; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.66 (s, 1H), 8.19 (d, J = 6.5 Hz, 1H), 7.87 (t, J = 7.7 Hz, 1H), 7.70 (dd, J = 16.7, 7.8 Hz, 2H), 7.60 (dt, J = 15.2, 7.9 Hz, 3H), 7.51 (t, J = 6.7 Hz, 1H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 161.9, 152.7, 149.1, 135.1, 134.3, 132.1, 131.9, 131.3, 130.1, 128.0, 127.7, 127.5, 126.3, 121.7. **HRMS** (TOF-ESI$^+$): *m/z* calcd for $C_{14}H_9ClN_2O$ $[M+H]^+$, 257.0476; found, 257.0479; Data consistent with those previously reported.[22]

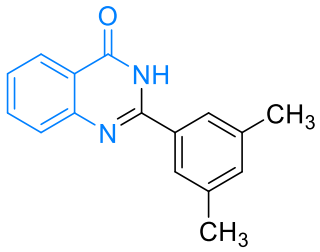
2-(2-bromophenyl)quinazolin-4(3*H*)-one (**5l**)



White solid; Mp: 185-187 °C; yield: 66% (59 mg); **IR** (KBr): 3407, 3087, 1688, 1609,

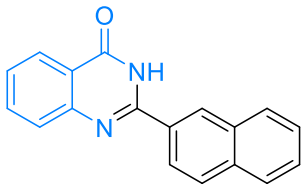
1566, 1472, 1307, 1050, 772; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.64 (s, 1H), 8.19 (dd, J = 7.9, 1.5 Hz, 1H), 7.87 (m, J = 8.6, 7.2, 1.6 Hz, 1H), 7.78 (dd, J = 7.9, 1.3 Hz, 1H), 7.72 (dd, J = 8.3, 1.2 Hz, 1H), 7.65 (dd, J = 7.5, 1.9 Hz, 1H), 7.62 – 7.51 (m, 2H), 7.51 – 7.45 (m, 1H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 161.9, 153.8, 149.0, 136.3, 135.1, 133.1, 132.1, 131.3, 128.2, 127.9, 127.5, 126.3, 121.7, 121.4. **HRMS** (TOF-ESI$^+$): *m/z* calcd for $C_{14}H_9N_2O$ $[M+H]^+$, 300.9971; found, 300.9971; Data consistent with those previously reported.[22]

2-(3,5-dimethylphenyl)quinazolin-4(3*H*)-one (**5m**)



White solid; Mp: 273-275 °C; yield: 80% (60 mg); **IR** (KBr): 3326, 3135, 3063, 2924, 1677, 1600, 1543, 1496, 1442, 1389, 1324, 1265, 1160, 1085, 897, 831, 756, 691; **^{1}H NMR** (400 MHz, DMSO-d6) δ 12.41 (s, 1H), 8.15 (d, J = 8.0 Hz, 1H), 7.87 – 7.78 (m, 3H), 7.75 (d, J = 8.5 Hz, 1H), 7.58 – 7.47 (m, 1H), 7.22 (s, 1H, 2.37 (s, 6H); **^{13}C NMR** (100 MHz, DMSO-d6) δ 162.6, 152.9, 149.3, 138.2, 135.1, 133.2, 133.0, 127.9, 127.0, 126.3, 125.9, 121.4, 21.3. **HRMS** (TOF-ESI$^+$): *m/z* calcd for $C_{16}H_{14}N_2O$ $[M+H]^+$, 251.1179; found, 251.1183; Data consistent with those previously reported.[24]

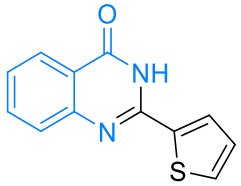
2-(naphthalen-2-yl)quinazolin-4(3*H*)-one (**5n**)



White solid; Mp: 278-288°C; yield: 50% (40 mg); **IR** (KBr): 3436, 2922, 2856, 1638, 1305, 817, 769, 743; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.70 (s, 1H), 8.83 (s, 1H), 8.31 (d, J = 6.8 Hz, 1H), 8.19 (d, J = 6.5 Hz, 1H), 8.11 – 8.05 (m, 2H), 8.03 (d, J = 9.3 Hz, 1H), 7.90 – 7.85 (m, 1H), 7.81 (d, J = 7.6 Hz, 1H), 7.69 – 7.61 (m, 2H), 7.59 – 7.53

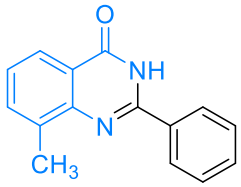
(m, 1H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.7, 152.6, 149.3, 135.2, 134.6, 132.8, 130.4, 129.4, 128.7, 128.6, 128.4, 128.2, 128.0, 127.4, 127.2, 126.4, 125.0, 121.5; **HRMS** (TOF-ESI$^+$): *m/z* calcd for $C_{18}H_{12}N_2O$ $[M+H]^+$, 273.1022; found, 273.1028; Data consistent with those previously reported.[25]

2-(thiophen-2-yl)quinazolin-4(3*H*)-one (**5o**)



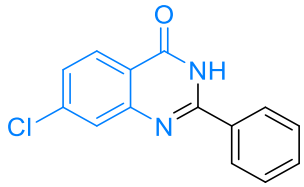
White solid; Mp: 271-272 °C; yield: 77% (53 mg); **IR** (KBr): 340, 3068, 1675, 1600, 1564, 1535, 1472, 750; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.69 (s, 1H), 8.24 (d, J = 3.9 Hz, 1H), 8.13 (d, J = 6.5 Hz, 1H), 7.88 (d, J = 5.0 Hz, 1H), 7.85 – 7.78 (m, 1H), 7.66 (d, J = 7.7 Hz, 1H), 7.53 – 7.46 (m, 1H), 7.27 – 7.22 (m, 1H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.3, 149.1, 148.3, 137.8, 135.2, 132.7, 129.9, 129.0, 127.4, 126.8, 126.5, 121.4. **HRMS** (TOF-ESI$^+$): *m/z* calcd for $C_{12}H_8N_2OS$ $[M+H]^+$, 229.0430; found, 229.0434; Data consistent with those previously reported.[22]

8-methyl-2-phenylquinazolin-4(3*H*)-one (**5p**)



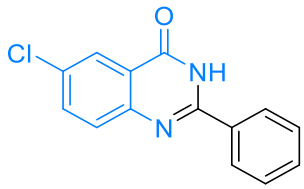
White solid; Mp: 246-248 °C; yield: 69% (49 mg); **IR** (KBr): 3450, 3071, 2961, 2875, 1675, 1599, 1544, 1493, 1328, 1280, 1056, 760, 698; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.55 (s, 1H), 8.24 (dd, J = 8.0, 1.7 Hz, 2H), 8.00 (dd, J = 8.1, 1.6 Hz, 1H), 7.71 (d, J = 7.3 Hz, 1H), 7.63 – 7.52 (m, 3H), 7.41 (t, J = 7.6 Hz, 1H), 2.63 (s, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 163.0, 151.5, 147.6, 136.1, 135.4, 133.4, 131.8, 129.1, 128.2, 126.5, 124.0, 121.4, 17.6; **HRMS** (TOF-ESI$^+$): *m/z* calcd for $C_{15}H_{12}N_2O$ $[M+H]^+$, 237.1022; found, 237.1022; Data consistent with those previously reported.[22]

7-chloro-2-phenylquinazolin-4(3*H*)-one (**5q**).



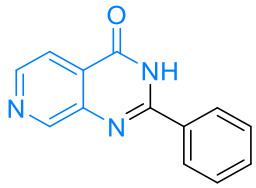
White solid; Mp: 287-288 °C; yield: 70% (54 mg); **IR** (KBr): 3458, 3041, 1669, 1604, 1555, 1447, 1294, 1050, 830, 764, 688; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.69 (s, 1H), 8.26 – 8.11 (m, 3H), 7.79 (d, J = 2.1 Hz, 1H), 7.67 – 7.46 (m, 4H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.1, 154.2, 150.3, 139.6, 132.8, 132.2, 129.1, 128.4, 128.4, 127.3, 127.0, 120.3; **HRMS** (TOF-ESI$^+$): *m/z* calcd for $C_{14}H_9ClN_2O$ $[M+H]^+$, 257.0476; found, 257.0479; Data consistent with those previously reported.[23]

6-chloro-2-phenylquinazolin-4(3*H*)-one (**5r**)



White solid; Mp: 296-297 °C; yield: 51% (39 mg); **IR** (KBr): 3407, 3086, 1678, 1608, 1476, 1096, 886, 842, 770, 685; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.18 (d, J = 7.7 Hz, 2H), 8.10 (d, J = 2.4 Hz, 1H), 7.88 (d, J = 8.5 Hz, 1H), 7.78 (d, J = 8.6 Hz, 1H), 7.64 – 7.53 (m, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 161.8, 153.3, 148.0, 135.2, 132.9, 132.1, 131.3, 130.2, 129.1, 128.3, 125.4, 122.7; **HRMS** (TOF-ESI$^+$): *m/z* calcd for $C_{14}H_9ClN_2O$ $[M+H]^+$, 257.0476; found, 257.0479; Data consistent with those previously reported.[26]

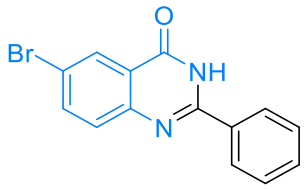
2-phenylpyrido[3,4-*d*]pyrimidin-4(3*H*)-one (**5s**)



White solid; Mp: 263-265 °C; yield: 60% (40 mg); **IR** (KBr): 3310, 3264, 3067, 1766, 1616, 1493, 1377, 1251, 926, 751, 698; yield: 60% (40 mg); **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.89 (s, 1H), 9.12 (s, 1H), 8.66 (d, J = 5.1 Hz, 1H), 8.19 (d, J = 8.1 Hz,

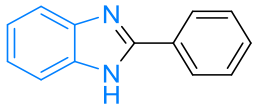
2H), 7.99 (d, *J* = 5.1 Hz, 1H), 7.59 (dt, *J* = 14.5, 7.2 Hz, 3H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.0, 154.9, 151.2, 146.3, 144.0, 132.8, 132.3, 129.2, 128.4, 126.4, 118.6. Data consistent with those previously reported.[1]

6-bromo-2-phenylquinazolin-4(3*H*)-one (**5t**).



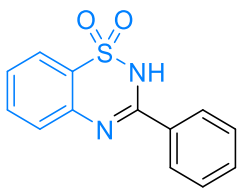
White solid; Mp: 285-286 °C; yield: 57% (51 mg); **IR** (KBr):3426, 3064, 1672, 1605, 1507, 1472, 1290, 1043, 832, 773, 690; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.75 (s, 1H), 8.23 (d, *J* = 2.3 Hz, 1H), 8.17 (d, *J* = 6.9 Hz, 2H), 7.99 (dd, *J* = 8.7, 2.4 Hz, 1H), 7.70 (d, *J* = 8.7 Hz, 1H), 7.61 (d, *J* = 7.1 Hz, 1H), 7.59 – 7.55 (m, 2H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 161.7, 153.4, 148.2, 137.9, 132.9, 132.1, 130.4, 129.1, 128.5, 128.3, 123.1, 119.4; **HRMS** (TOF-ESI$^+$): *m/z* calcd for $C_{14}H_9BrN_2O$ $[M+H]^+$, 300.9971; found, 300.9971; Data consistent with those previously reported.[23]

2-phenyl-1*H*-benzo[*d*]imidazole (**6a**)



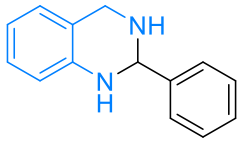
White solid; Mp: 289-292 °C; yield: 63% (37 mg); **IR** (KBr):3415, 3053, 1541, 1414, 1381, 1260, 1051, 743, 712, 690; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.95 (s, 1H), 8.19 (d, *J* = 7.0 Hz, 2H), 7.68 (d, *J* = 7.6 Hz, 1H), 7.60 – 7.47 (m, 4H), 7.22 (t, *J* = 8.2 Hz, 2H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 151.7, 144.2, 135.5, 130.6, 130.3, 129.4, 126.9, 123.0, 122.2, 119.3, 111.8; **HRMS** (TOF-ESI$^+$): *m/z* calcd for $C_{13}H_{10}N_2$ $[M+H]^+$, 195.0917; found, 195.0922; Data consistent with those previously reported.[21]

3-phenyl-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide (**6b**)



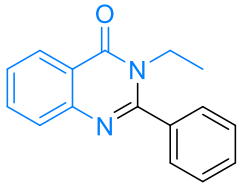
White solid; Mp: 293-295 °C; yield: 71% (55 mg); **IR** (KBr): 3315, 3037, 1658, 1558, 1529, 1483, 1381, 1299, 1030, 832, 696; yield: 71% (55 mg); **^{1}H NMR** (400 MHz, DMSO-d_6) δ 12.23 (s, 1H), 8.05 (d, J = 7.3 Hz, 2H), 7.88 (d, J = 8.0 Hz, 1H), 7.73 (dt, J = 13.9, 7.1 Hz, 2H), 7.68 – 7.60 (m, 3H), 7.52 (t, J = 7.6 Hz, 1H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 155.3, 135.9, 133.7, 133.4, 132.3, 129.4, 128.7, 127.2, 123.8, 121.9, 118.9; Data consistent with those previously reported.[1]

2-phenyl-1,2,3,4-tetrahydroquinazoline (**6c**)



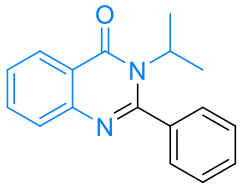
Yellow solid; Mp: 101-103 °C; yield: 70% (44 mg); **IR** (KBr): 3306, 3026, 2856, 1676, 1607, 1476, 1354, 1306, 1249, 1026, 854, 738, 692; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.52 (d, J = 7.8 Hz, 2H), 7.41 – 7.35 (m, 3H), 7.06 (d, J = 6.9 Hz, 1H), 6.95 (d, J = 8.1 Hz, 1H), 6.73 (t, J = 6.9 Hz, 1H), 6.59 (dd, J = 8.0, 1.1 Hz, 1H), 5.25 (s, 1H), 4.29 (d, J = 16.7 Hz, 1H), 4.00 (d, J = 16.7 Hz, 1H), 3.63 (s, 2H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 143.6, 141.3, 128.8, 128.7, 127.4, 126.7, 126.3, 121.1, 118.3, 115.1, 69.6, 46.4; Data consistent with those previously reported.[27]

3-ethyl-2-phenylquinazolin-4(3*H*)-one (**7a**)



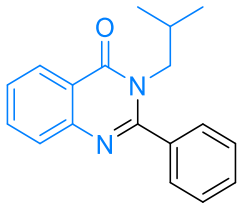
White solid; Mp: 155-156 °C; yield: 80% (60 mg); **IR** (KBr): 3192, 2974, 2930, 2867, 1676, 1587, 1571, 1472, 1381, 1052, 770, 701; **^{1}H NMR** (400 MHz, DMSO-*d*6) δ 8.20 (d, J = 8.1 Hz, 1H), 7.85 (td, J = 7.8, 7.1, 1.6 Hz, 1H), 7.69 – 7.63 (m, 3H), 7.60 – 7.55 (m, 4H), 3.90 (q, J = 7.0 Hz, 2H), 1.10 (t, J = 7.0 Hz, 3H); **^{13}C NMR** (100 MHz, DMSO-*d*6) δ 161.5, 156.5, 147.4, 135.9, 134.9, 130.1, 128.9, 128.3, 127.6, 127.4, 126.6, 121.0, 41.1, 14.1; **HRMS** (TOF-ESI$^+$): *m/z* calcd for $C_{16}H_{14}N_2O$ $[M+H]^+$, 251.1179; found, 251.1183; Data consistent with those previously reported.[28]

3-isopropyl-2-phenylquinazolin-4(3*H*)-one (**7b**)



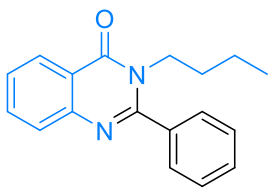
White solid; Mp: 131-133 °C; yield: 73% (58 mg); **IR** (KBr): 3071, 2973, 2878, 1677, 1568, 1471, 1338, 1052, 774, 705; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.31 (d, *J* = 7.6 Hz, 1H), 7.77 – 7.68 (m, 2H), 7.52 (m, 6H), 4.35 (h, *J* = 6.8 Hz, 1H), 1.59 (d, *J* = 6.8 Hz, 6H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 162.6, 156.7, 146.8, 136.5, 134.2, 129.7, 129.0, 127.3, 127.2, 126.9, 126.4, 122.2, 54.1, 19.7; **HRMS** (TOF-ESI$^+$): *m/z* calcd for $C_{17}H_{16}N_2O$ $[M+H]^+$, 265.1335; found, 265.1339; Data consistent with those previously reported.[1]

3-isobutyl-2-phenylquinazolin-4(3*H*)-one (**7c**)



White solid; Mp: 90-91 °C; yield: 78% (65 mg); **IR** (KBr): 3056, 2975, 2930 , 2876, 2860, 1680, 1605, 1588, 1496, 1379, 1057, 774, 705; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.34 (d, *J* = 7.7 Hz, 1H), 7.79 – 7.73 (m, 2H), 7.54 – 7.49 (m, 6H), 3.98 (d, *J* = 7.4 Hz, 2H), 1.94 (m, *J* = 6.9 Hz, 1H), 0.72 (d, J = 6.7 Hz, 6H); **^{13}C NMR** (100 MHz, Chloroform-d) δ 162.6, 156.5, 147.2, 135.7, 134.3, 129.8, 128.7, 128.3, 127.5, 127.0, 126.9, 120.9, 52.2, 27.7, 19.9; **HRMS** (TOF-ESI$^+$): *m/z* calcd for $C_{18}H_{18}N_2O$ $[M+H]^+$, 279.1492; found, 279.1495.

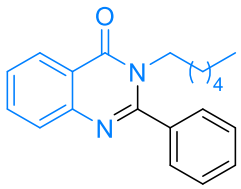
3-butyl-2-phenylquinazolin-4(3*H*)-one (**7d**)



White solid; Mp: 169-170 °C; yield: 66% (55 mg); **IR** (KBr): 3050, 2978, 2933, 2900,

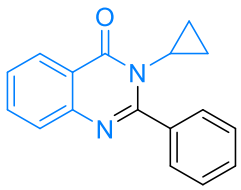
1677, 1588, 1470, 1379, 1052, 770, 690; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.34 (d, *J* = 7.4 Hz, 1H), 7.84 – 7.66 (m, 2H), 7.53 (m, 6H), 4.05 – 3.92 (m, 2H), 1.59 (p, *J* = 7.6 Hz, 2H), 1.19 (dt, *J* = 14.9, 7.4 Hz, 2H), 0.76 (t, *J* = 7.3 Hz, 3H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 162.2, 156.3, 147.2, 135.5, 134.3, 129.8, 128.8, 127.8, 127.4, 127.0, 126.8, 120.9, 45.7, 30.7, 19.9, 13.4; **HRMS** (TOF-ESI^{+}): *m/z* calcd for $C_{18}H_{18}N_2O$ $[M+H]^+$, 279.1492; found, 279.1495; Data consistent with those previously reported.[25]

3-hexyl-2-phenylquinazolin-4(3*H*)-one (**7e**)



White solid; Mp: 103.6-104.4 °C; yield: 60% (55 mg); **IR** (KBr): 3068, 2979, 2937, 2885, 2861, 1680, 1588, 1569, 1505, 1470, 1373, 1068, 768, 727, 689; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.26 (d, *J* = 8.8 Hz, 1H), 7.67 (dd, *J* = 6.4, 1.5 Hz, 2H), 7.45 (m, 6H), 3.96 – 3.85 (m, 2H), 1.58 – 1.48 (m, 2H), 1.08 (dq, *J* = 22.4, 8.7, 7.6 Hz, 6H), 0.72 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 161.1, 155.2, 146.2, 134.6, 133.3, 128.8, 127.7, 126.8, 126.4, 125.9, 125.7, 119.9, 44.9, 30.0, 27.5, 25.3, 21.3, 12.9; **HRMS** (TOF-ESI^{+}): *m/z* calcd for $C_{20}H_{22}N_2O$ $[M+H]^+$, 307.1805; found, 307.1807; Data consistent with those previously reported.[29]

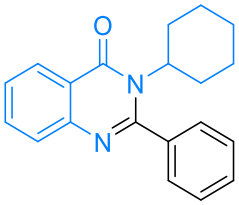
3-cyclopropyl-2-phenylquinazolin-4(3*H*)-one (**7f**)



White solid; Mp: 112-114 °C; yield: 71% (56 mg); **IR** (KBr): 3060, 3025, 2953, 2911, 2843, 1670, 1600, 1565, 1504, 1341, 1050, 772, 720, 689; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.31 (d, *J* = 8.0 Hz, 1H), 7.78 – 7.68 (m, 4H), 7.54 – 7.46 (m, 4H), 3.14 (dt, *J* = 7.2, 3.4 Hz, 1H), 0.93 (q, *J* = 7.0 Hz, 2H), 0.54 – 0.46 (m, 2H); **^{13}C NMR**

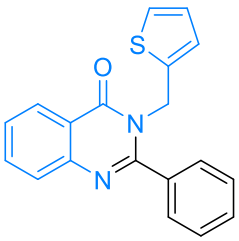
(100 MHz, Chloroform-*d*) δ 164.0, 156.9, 147.1, 136.2, 134.3, 129.9, 128.5, 128.3, 127.4, 126.9, 126.6, 120.9, 30.3, 11.3; **HRMS** (TOF-ESI$^+$): *m/z* calcd for $C_{17}H_{14}N_2O$ $[M+H]^+$, 263.1179; found, 263.1181; Data consistent with those previously reported.[28]

3-cyclohexyl-2-phenylquinazolin-4(3*H*)-one (**7g**)



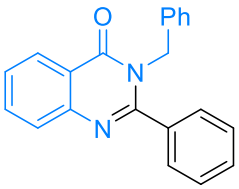
White solid; Mp: 135-137 °C; yield: 64% (58 mg); **IR** (KBr): 3043, 2977, 2928, 1681, 1595, 1569, 1269, 1089, 1049, 766, 758, 721, 689; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.30 (d, *J* = 9.1 Hz, 1H), 7.75 – 7.69 (m, 2H), 7.54 – 7.48 (m, 6H), 3.92 – 3.82 (m, 1H), 2.73 (qd, *J* = 12.6, 3.7 Hz, 2H), 1.74 (dd, *J* = 30.3, 13.1 Hz, 4H), 1.28 – 1.24 (m, 2H), 1.03 – 0.94 (m, 2H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 162.7, 157.0, 146.6, 136.3, 134.3, 134.2, 129.8, 128.9, 127.1, 127.1, 126.9, 126.5, 123.6, 122.2, 62.7, 28.9, 26.2, 25.0; **HRMS** (TOF-ESI$^+$): *m/z* calcd for $C_{20}H_{20}N_2O$ $[M+H]^+$, 305.1648; found, 305.1649; Data consistent with those previously reported.[30]

2-phenyl-3-(thiophen-2-ylmethyl)quinazolin-4(3*H*)-one (**7h**)



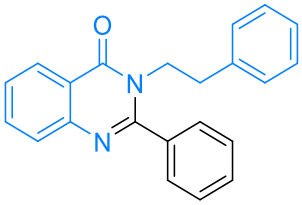
White solid; Mp: 128-129 °C; yield: 70% (66 mg); **IR** (KBr): 3084, 3056, 2912, 2883, 1677, 1589, 1570, 1472, 1431, 1215, 1027, 774, 713, 691; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.38 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.78 – 7.73 (m, 2H), 7.56 – 7.47 (m, 6H), 7.16 (dd, *J* = 5.1, 1.2 Hz, 1H), 6.83 (dd, *J* = 5.1, 3.5 Hz, 1H), 6.61 (d, *J* = 4.7 Hz, 1H), 5.38 (s, 2H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 162.2, 155.8, 147.2, 138.2, 135.0, 134.6, 130.1, 128.8, 128.3, 127.6, 127.3, 127.2, 127.0, 126.3, 126.0, 120.9, 44.1; **HRMS** (TOF-ESI$^+$): *m/z* calcd for $C_{19}H_{14}N_2OS$ $[M+H]^+$, 319.0900; found, 319.0897; Data consistent with those previously reported.[1]

3-benzyl-2-phenylquinazolin-4(3*H*)-one (**7i**)



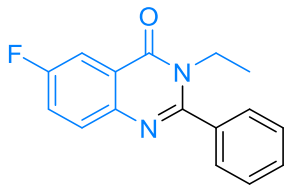
White solid; Mp: 125-128 °C; yield: 65% (61 mg); **IR** (KBr): 3060, 2928, 2890, 2677, 1609, 1580, 1452, 1382, 1050, 717, 688; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.23 (d, J = 8.0 Hz, 1H), 7.97 – 7.83 (m, 1H), 7.73 (d, J = 8.2 Hz, 1H), 7.61 (t, J = 7.5 Hz, 1H), 7.54 – 7.40 (m, 5H), 7.22 (d, J = 7.3 Hz, 3H), 6.98 – 6.85 (m, 2H), 5.19 (s, 2H); **^{13}C NMR** (100 MHz, DMSO-d_6) δ 161.9, 156.6, 147.4, 137.2, 135.6, 135.2, 130.2, 128.9, 128.7, 128.7, 127.8, 127.7, 127.6, 126.9, 126.7, 120.9, 48.7; **HRMS** (TOF-ESI$^+$): *m/z* calcd for $C_{21}H_{16}N_2O$ $[M+H]^+$, 313.1335; found, 313.1340; Data consistent with those previously reported.[1]

3-phenethyl-2-phenylquinazolin-4(3*H*)-one (**7j**)



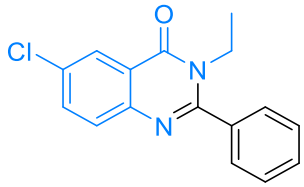
White solid; Mp: 176-179 °C; yield: 62% (60 mg); **IR** (KBr): 3411, 3065, 2979, 2893, 1677, 1585, 1446, 1380, 1051, 755, 690; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.30 (dd, J = 8.0, 1.4 Hz, 1H), 7.73 – 7.65 (m, 2H), 7.48 – 7.39 (m, 4H), 7.31 (dd, J = 7.9, 1.7 Hz, 2H), 7.10 (dd, J = 5.0, 1.9 Hz, 3H), 6.84 – 6.76 (m, 2H), 4.16 – 4.07 (t, 2H), 2.87 – 2.79 (t, 2H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 161.1, 155.1, 146.1, 136.7, 134.3, 133.4, 128.8, 127.7, 127.5, 126.7, 126.5, 126.1, 125.7, 125.6, 119.9, 46.5, 33.6; **HRMS** (TOF-ESI$^+$): *m/z* calcd for $C_{22}H_{18}N_2O$ $[M+H]^+$, 327.1492; found, 327.1496; Data consistent with those previously reported.[1]

3-ethyl-6-fluoro-2-phenylquinazolin-4(3*H*)-one (**7k**)



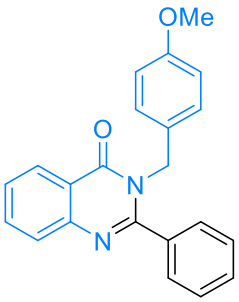
White solid; Mp: 89-90 °C; yield: 59% (47 mg); **IR** (KBr): 3049, 2964, 2919, 2883, 2853, 1680, 1570, 1483, 1446, 1376, 1346, 1225, 1104, 884, 846, 766, 699; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.96 (dd, *J* = 8.5, 2.9 Hz, 1H), 7.74 (dd, *J* = 8.9, 4.9 Hz, 1H), 7.53 (m, 6H), 4.04 (q, *J* = 7.1 Hz, 2H), 1.22 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 162.24, 161.4(d, J_{C-F} = 3.52 Hz), 159.8, 155.5(d, J_{C-F} = 2.4 Hz), 143.91, 135.35, 129.93(d, J_{C-F} = 8.13 Hz), 128.88, 127.68, 123.0(d, J_{C-F} = 24.29 Hz), 122.23(d, J_{C-F} = 8.5 Hz), 111.52(d, J_{C-F} = 23.47 Hz), 41.37, 14.05; **^{19}F NMR** (376 MHz, Chloroform-*d*) δ -112.41; **HRMS** (TOF-ESI^{+}): *m/z* calcd for $C_{16}H_{13}FN_2O$ $[M+H]^{+}$, 269.1085; found, 269.1087.

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



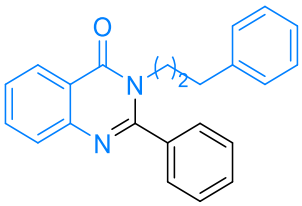
White solid; Mp: 93-94 °C; yield: 52% (44 mg); **IR** (KBr): 3468, 3066, 2985, 2924, 2882, 1679, 1583, 1464, 1382, 1263, 1169, 1059, 922, 878, 782, 702; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.26 (dd, *J* = 8.6, 1.4 Hz, 1H), 7.72 (d, *J* = 1.9 Hz, 1H), 7.53 (d, *J* = 1.7 Hz, 5H), 7.46 (d, *J* = 8.6 Hz, 1H), 4.03 (q, *J* = 6.8 Hz, 2H), 1.23 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 161.5, 157.5, 148.1, 140.5, 135.3, 130.0, 128.9, 128.3, 127.6, 127.57, 127.0, 119.4, 41.4, 14.1; **HRMS** (TOF-ESI^{+}): *m/z* calcd for $C_{16}H_{13}ClN_2O$ $[M+H]^{+}$, 285.0789; found, 285.0792.

4-(4-methoxybenzyl)-2-phenylquinazolin-4(3*H*)-one (**7m**)



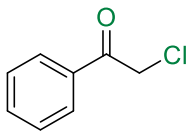
White solid; Mp: 187-189 °C; yield: 61% (63 mg); **IR** (KBr): 33066, 2966, 2877, 1670, 1607, 1586, 1570, 1471, 1381, 1254, 1084, 828, 774, 701; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.37 (d, *J* = 9.1 Hz, 1H), 7.80 – 7.73 (m, 2H), 7.56 – 7.40 (m, 4H), 7.36 (d, *J* = 6.7 Hz, 2H), 6.85 (d, *J* = 8.7 Hz, 2H), 6.72 (d, *J* = 8.7 Hz, 2H), 5.22 (s, 2H), 3.75 (s, 3H); **^{13}C NMR** (100 MHz, Chloroform-*d*)δ 162.5, 158.9, 156.4, 147.3, 135.4, 134.5, 129.9, 128.7, 128.6, 128.1, 127.6, 127.1, 127.1, 121.0, 113.8, 55.2, 48.2; **HRMS** (TOF-ESI$^+$): *m/z* calcd for $C_{22}H_{18}N_2O_2$ $[M+H]^+$, 343.1441; found 343.1441; Data consistent with those previously reported.[31]

2-phenyl-3-(3-phenylpropyl)quinazolin-4(3*H*)-one (**7n**)



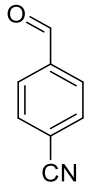
White solid; Mp: 135-136 °C; yield: 59% (60 mg); **IR** (KBr): 3078, 2922, 2856, 1674, 1587, 1570, 1503, 1469, 1051, 775, 698, 690; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.25 (d, *J* = 7.8 Hz, 1H), 7.67 (dd, *J* = 8.6, 1.9 Hz, 2H), 7.49 – 7.35 (m, 6H), 7.13 – 7.02 (m, 3H), 6.90 (d, *J* = 6.8 Hz, 2H), 4.02 – 3.81 (t, 2H), 2.43 (t, *J* = 7.6 Hz, 2H), 1.87 (p, *J* = 7.6 Hz, 2H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 162.2, 156.1, 147.2, 140.5, 135.4, 134.4, 129.8, 128.8, 128.4, 128.1, 127.7, 127.5, 127.0, 126.8, 126.0, 120.9, 45.6, 32.9, 29.8; **HRMS** (TOF-ESI$^+$): *m/z* calcd for $C_{23}H_{20}N_2O$ $[M+H]^+$, 341.1648; found, 341.1652; Data consistent with those previously reported.[25]

2-chloro-1-phenylethan-1-one (**9**)



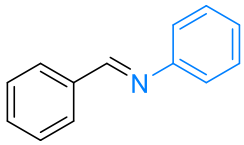
Yellow solid; yield: 15% (7 mg); **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.96 (dd, *J* = 8.4, 1.3 Hz, 2H), 7.65 – 7.60 (m, 1H), 7.53 – 7.48 (m, 2H), 4.73 (s, 2H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 191.10, 134.24, 134.05, 128.93, 128.54, 46.09; Data consistent with those previously reported.[33]

4-formylbenzonitrile



White solid; yield: 61% (80 mg); **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.10 (s, 1H), 8.08 (s, 4H).

(*E*)-N,1-diphenylmethanimine(11)



Yellow oil; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.46 (s, 1H), 7.95 – 7.88 (m, 2H), 7.48 (dd, *J* = 5.1, 1.9 Hz, 3H), 7.44 – 7.36 (m, 2H), 7.28 – 7.18 (m, 4H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 160.45, 152.10, 136.22, 131.40, 129.16, 128.82, 128.79, 125.95, 120.88; Data consistent with those previously reported. [33]

5 Control experiments

1. Benzaldehyde observation

In reaction of the synthesis of 2-aryl quinazolinones, benzaldehyde was detected in TLC. The mixture were purified by flash column chromatography on silica gel(Petroleum ether/EtOAc 20:1). Even though we couldn't provide purified product of benzaldehyde because of its volatility and instability, the product(mixture) were further identified by ^{1}H NMR spectroscopy. Fortunately, we separated 4-formylbenzonitrile.

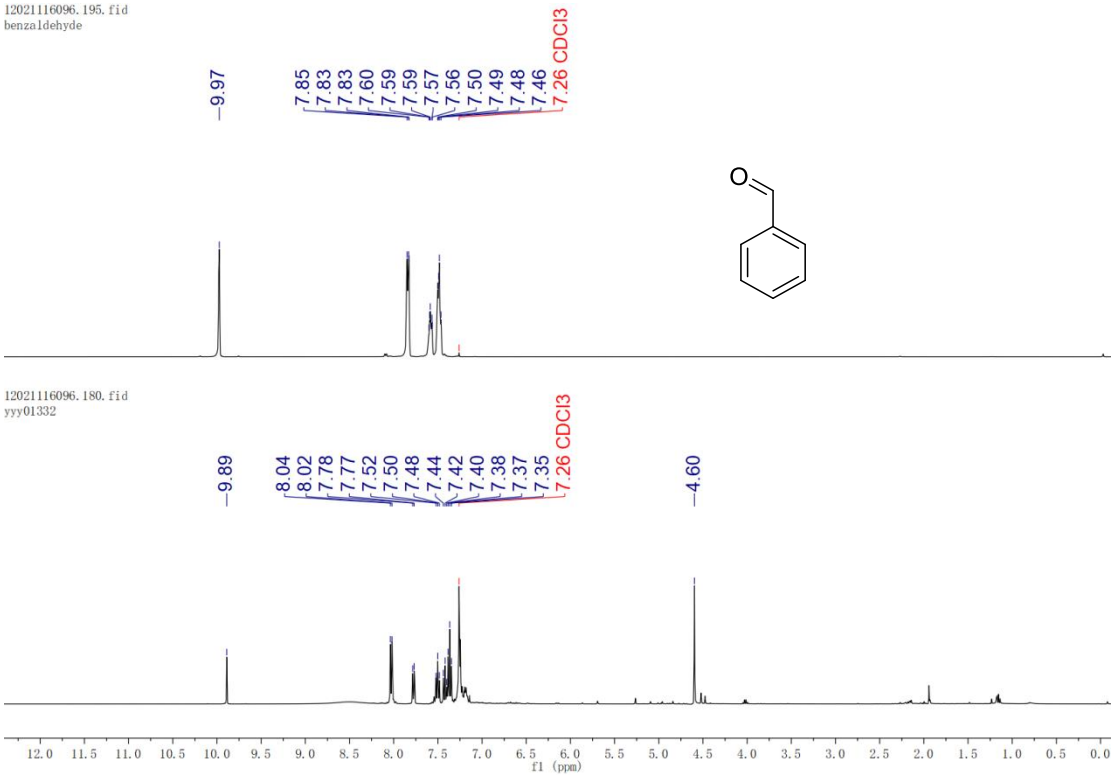
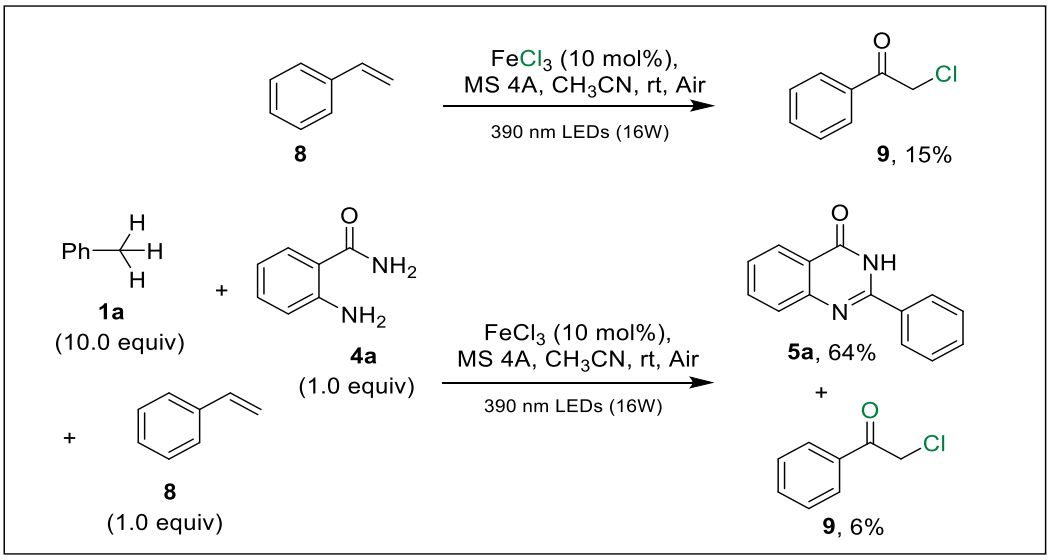


Figure S2 **^{1}H-NMR** spectrum of the mixture fraction and benzaldehyde

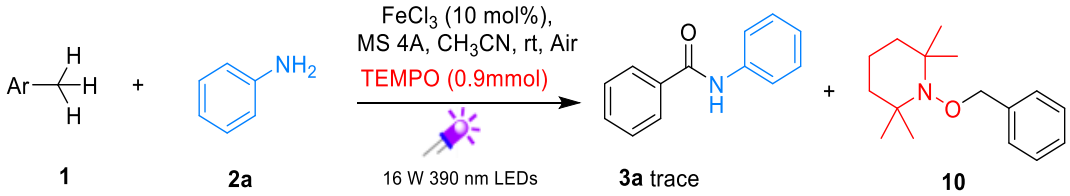
2. Capture of “Cl” radical



Scheme S1. Chlorine radical capture

Inspired by some literature,[32] we tried to capture chlorine free radicals in the reaction system (Scheme S1). We added 1.0 equiv of Styrene in the reaction, and the results showed that the yield of 2-arylquinazolinone product **5a** was reduced. and the presence of the chlorination product **9** suggested the generation of chlorine radical species during the reaction process.

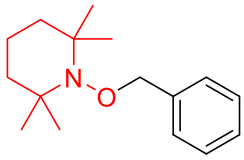
3. Capture of benzyl radical



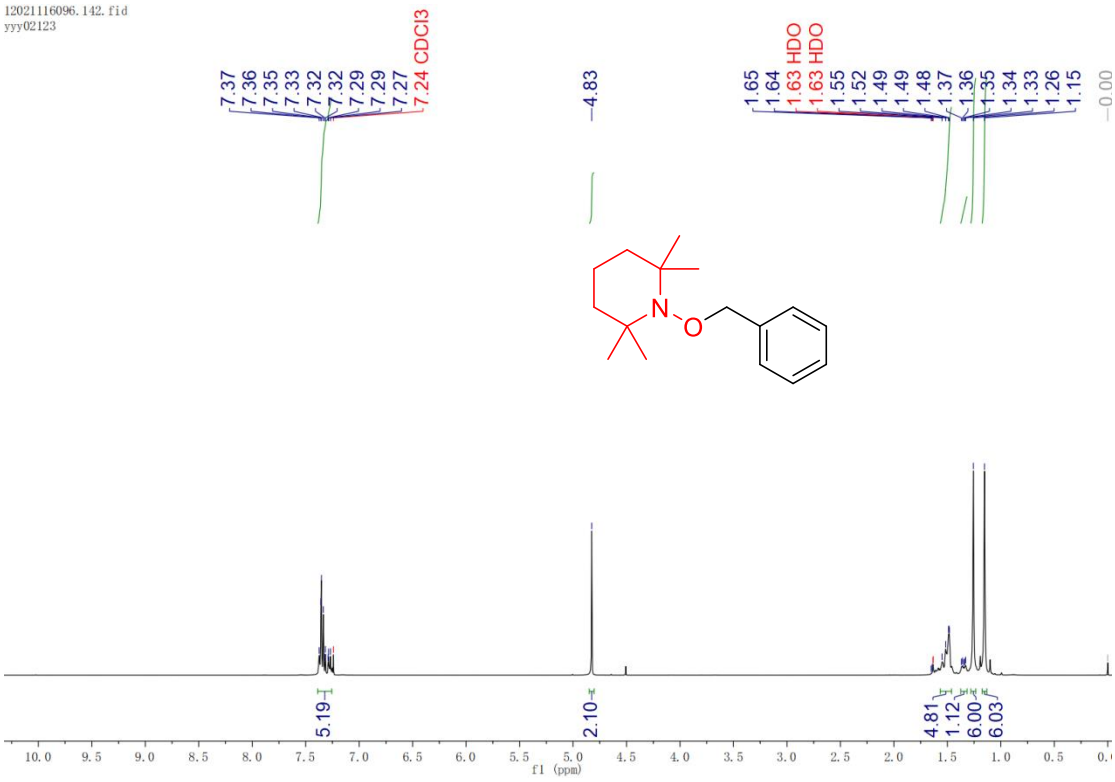
Under air atmosphere, toluene **1** (3.0 mmol, 10.0 equiv), amine **2a** (0.3 mmol, 1.0 equiv), $FeCl_3$ (10 mol%, 0.01mmol) and TEMPO (0.9 mmol, 3.0 equiv) in MeCN (3.0 mL, 0.1 M) and in the presence of 4A molecular sieves were added to 20.0 mL reaction tube. The mixture was stirred at 390 nm light-emitting diodes (LEDs, 16W) and monitored by TLC. After stirring for 12h. Than, the reaction was quenched with saturated NaCl solution and extracted with 20.0 mL EtOAc for three times. The organic layers were combined, dried over Na_2SO_4, filtered and evaporated under reduced

pressure. The residues were purified by flash column chromatography on silica gel. Benzylated-TEMPO was obtained and trace amount of 3a was obtained. This product was further identified by NMR spectroscop.

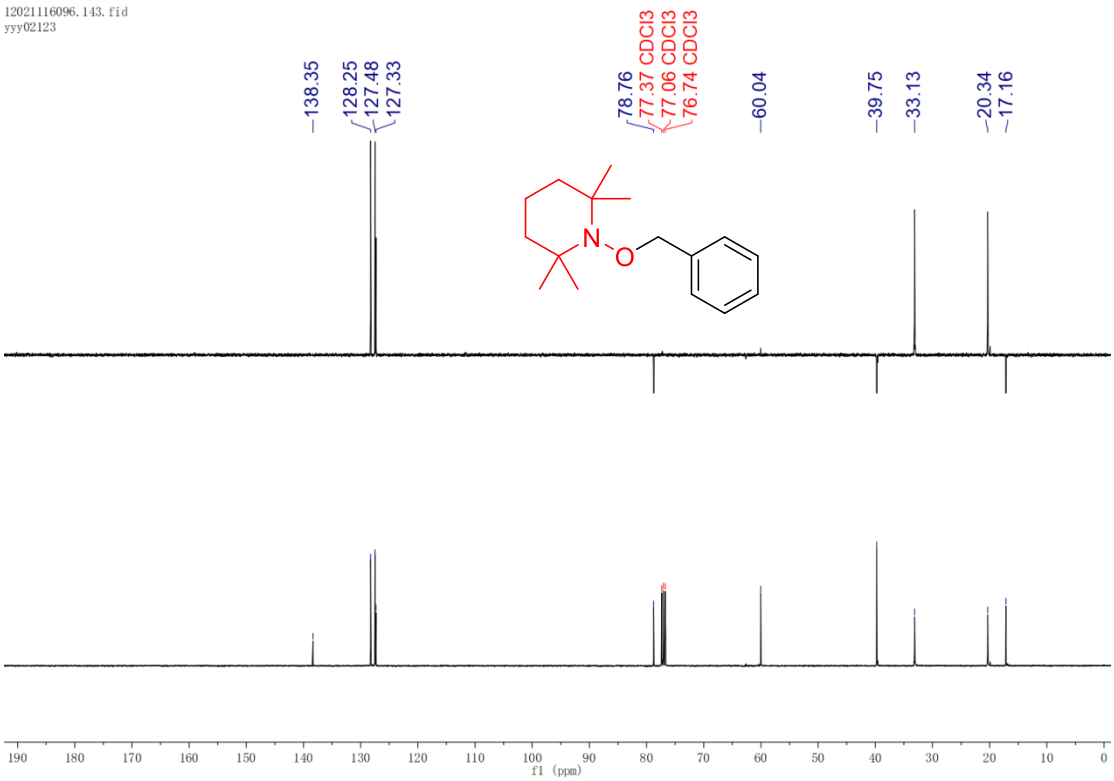
1-(benzyloxy)-2,2,6,6-tetramethylpiperidine(**10**)



White oil; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.39 – 7.26 (m, 5H), 4.83 (s, 2H), 1.57 – 1.46 (m, 5H), 1.37 – 1.32 (m, 1H), 1.26 (s, 6H), 1.15 (s, 6H); **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 138.35, 128.25, 127.48, 127.33, 78.76, 60.04, 39.75, 33.13, 20.34, 17.16; Data consistent with those previously reported.[1]

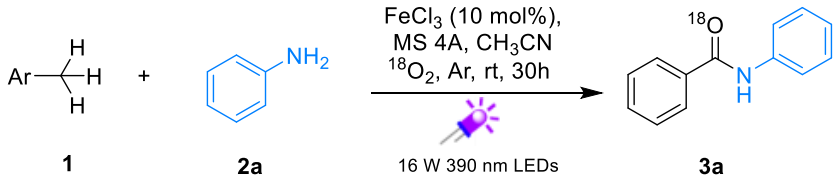


^{1}H-NMR (400 MHz, Chloroform-*d*) **Spectra of 10**



^{13}C-NMR (100 MHz, Chloroform-*d*) **Spectra of 10**

4. Isotope labeling experiments



1 2a 3a

In the glove box, the standard reaction was performed according to general procedure, with toluene **1** (3.0 mmol, 10.0 equiv), amine **2a** (0.3 mmol, 1.0 equiv) and $FeCl_3$ (10 mol%, 0.01mmol) in MeCN (3.0 mL, 0.1 M) and in the presence of 4A molecular sieves were added to 20.0 mL reaction tube and the reaction tube was backfilled with $^{18}O_2$, After thirty hours the reaction was filtered over a short plug of silica and analyzed by GC-MS.

MS Formula Results: + Scan (0.266 min) Sub (yyy02133.d)

m/z	Ion	Formula	Abundance
200.0952	(M+H)+	C13 H12 N [18O]	2493.6

Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
☑	C13 H11 N [18O]	C13 H12 N [18O]	46.84		200.0956	2.02	98.35	0	0

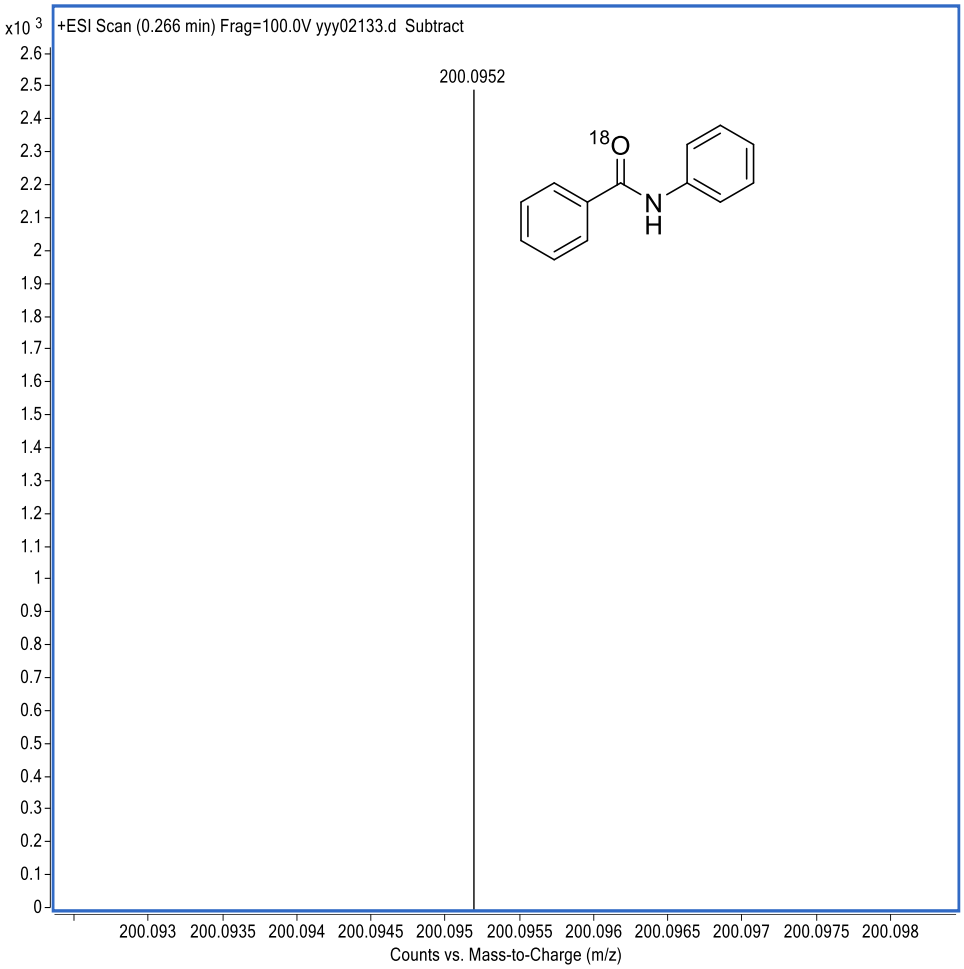
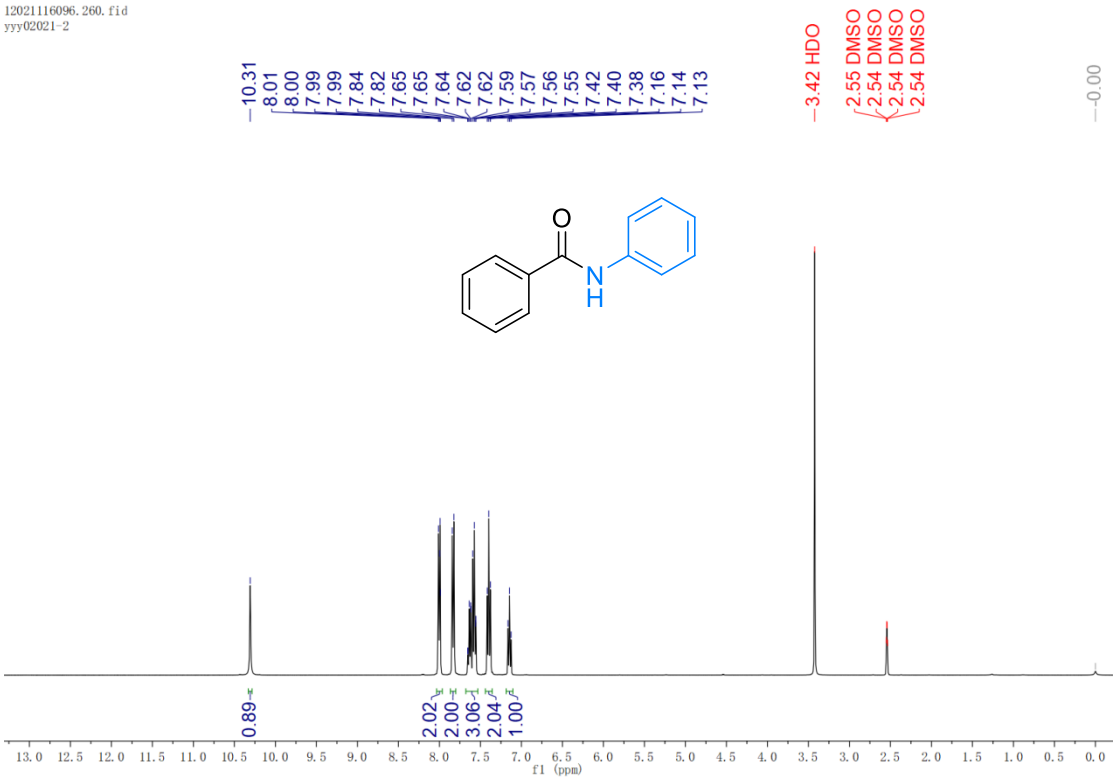
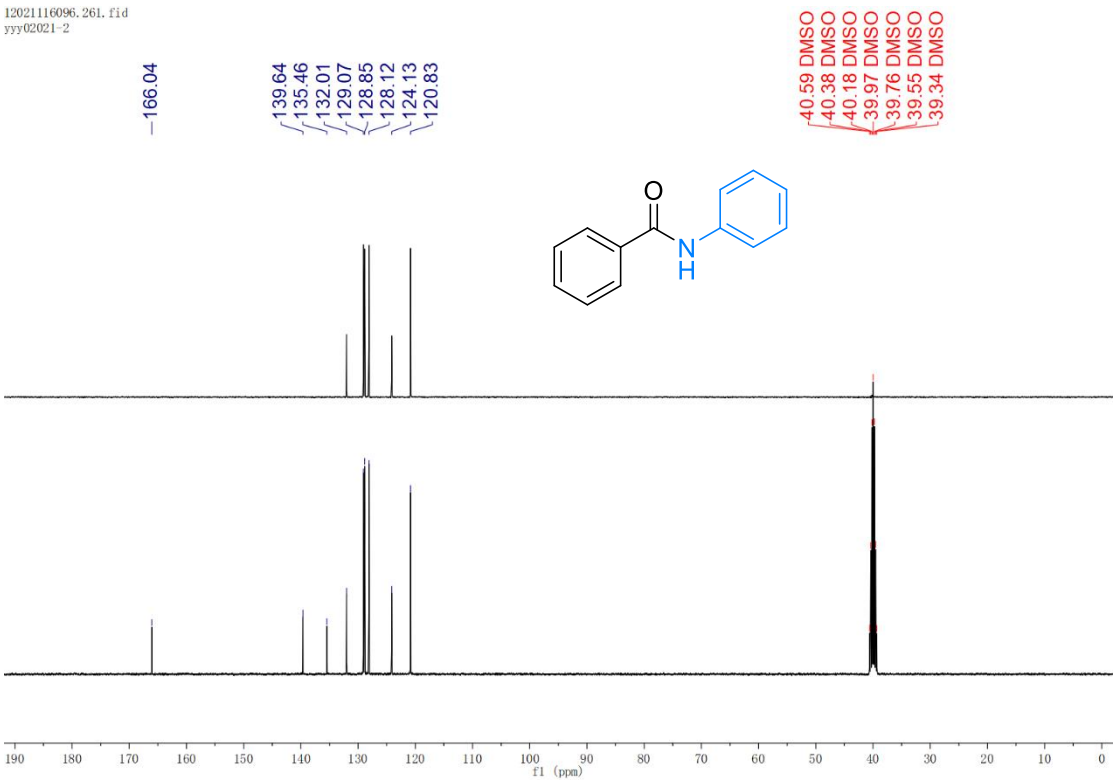


Figure S3 HRMS of *N*-phenylbenzamide-^{18}O

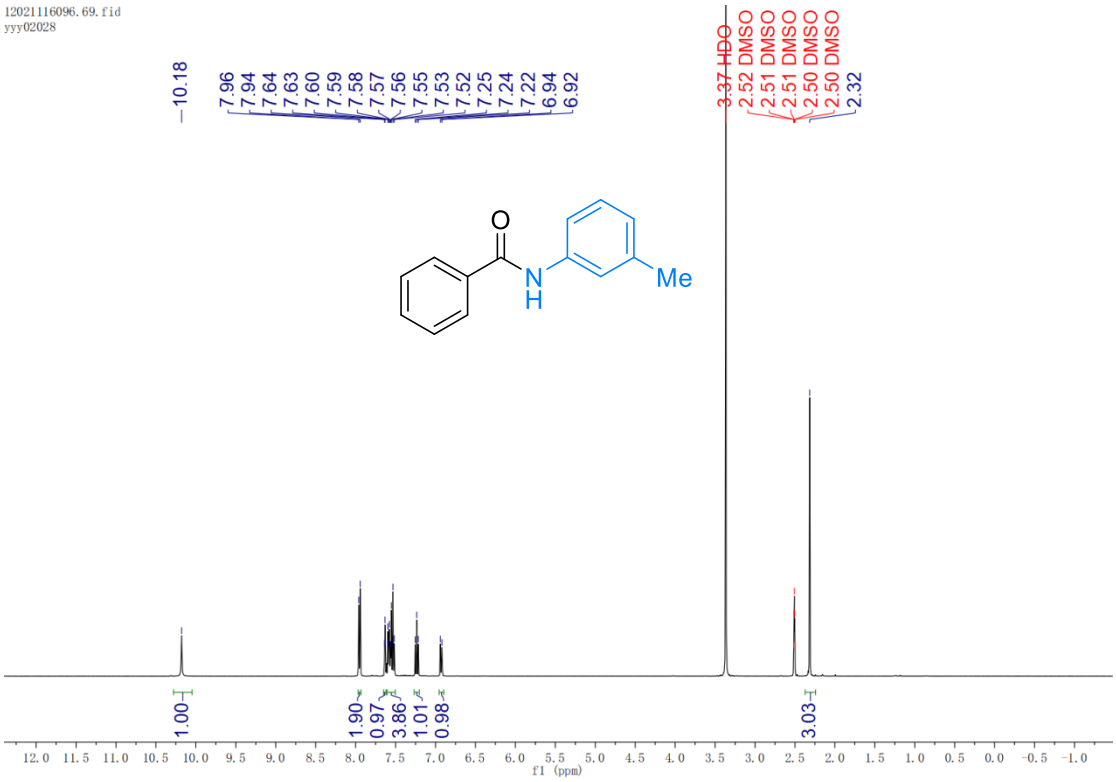
6 ^{1}H NMR and ^{13}C NMR Spectra of **3a-3y**, **5a-5t**, **6a-6c**,**7a-7n and 9**.



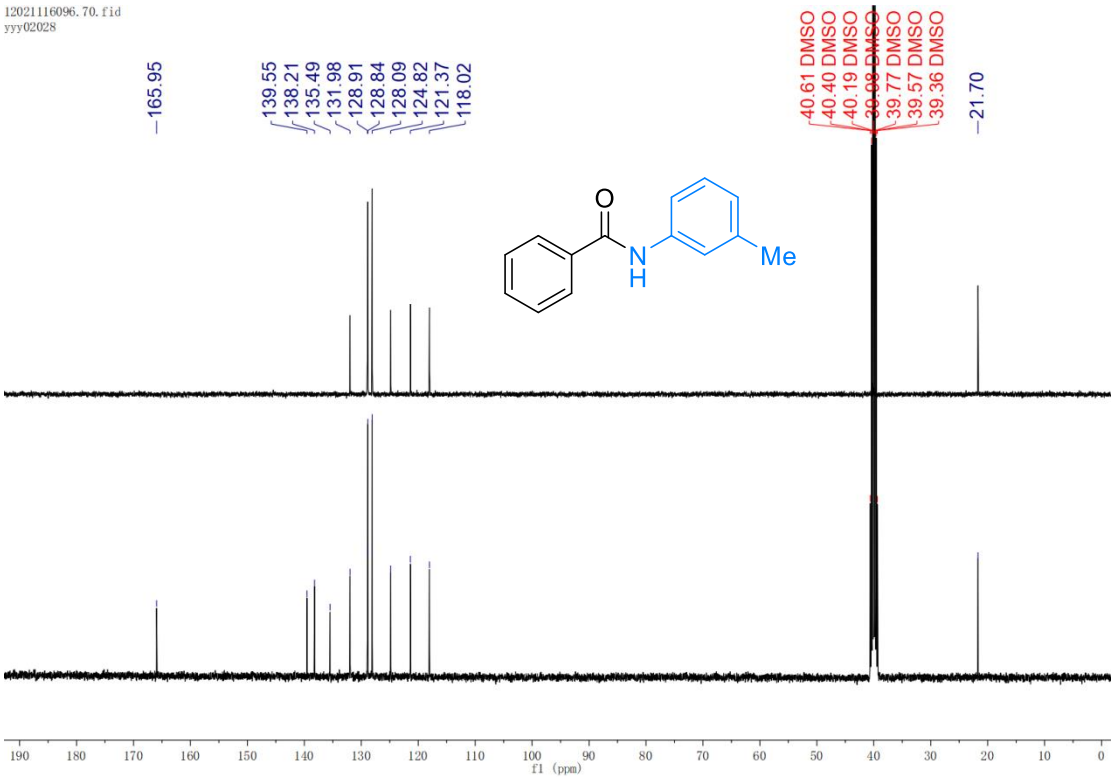
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 3a**



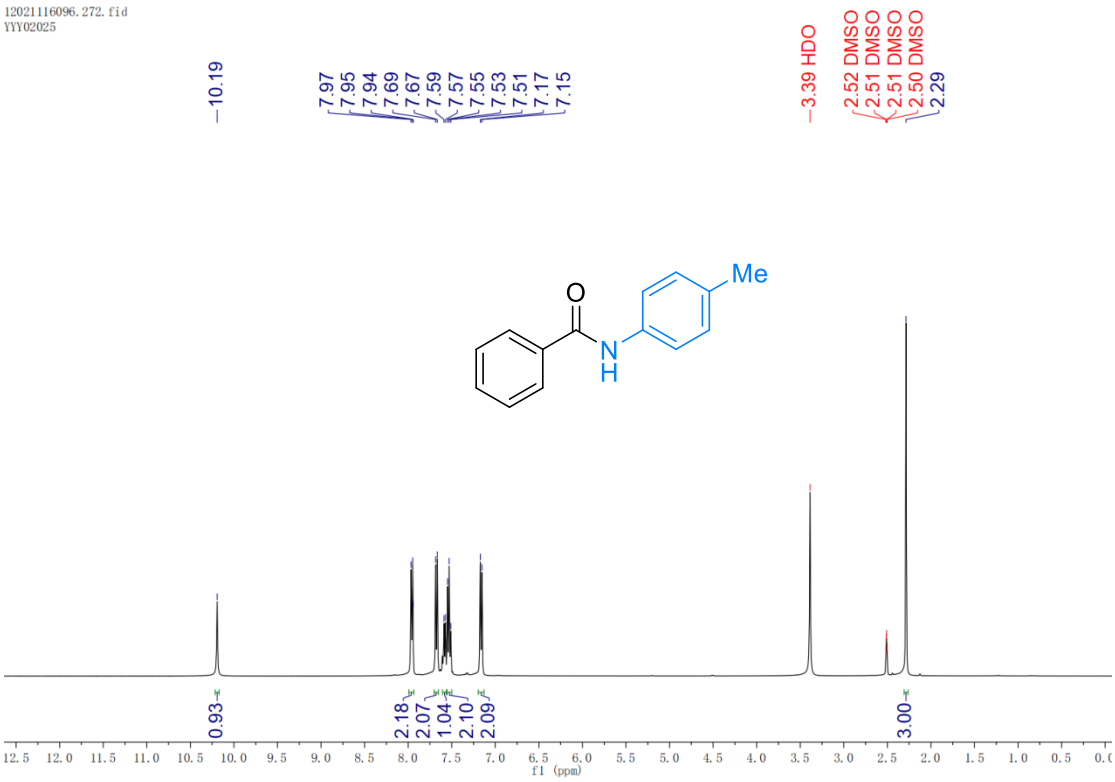
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 3a**



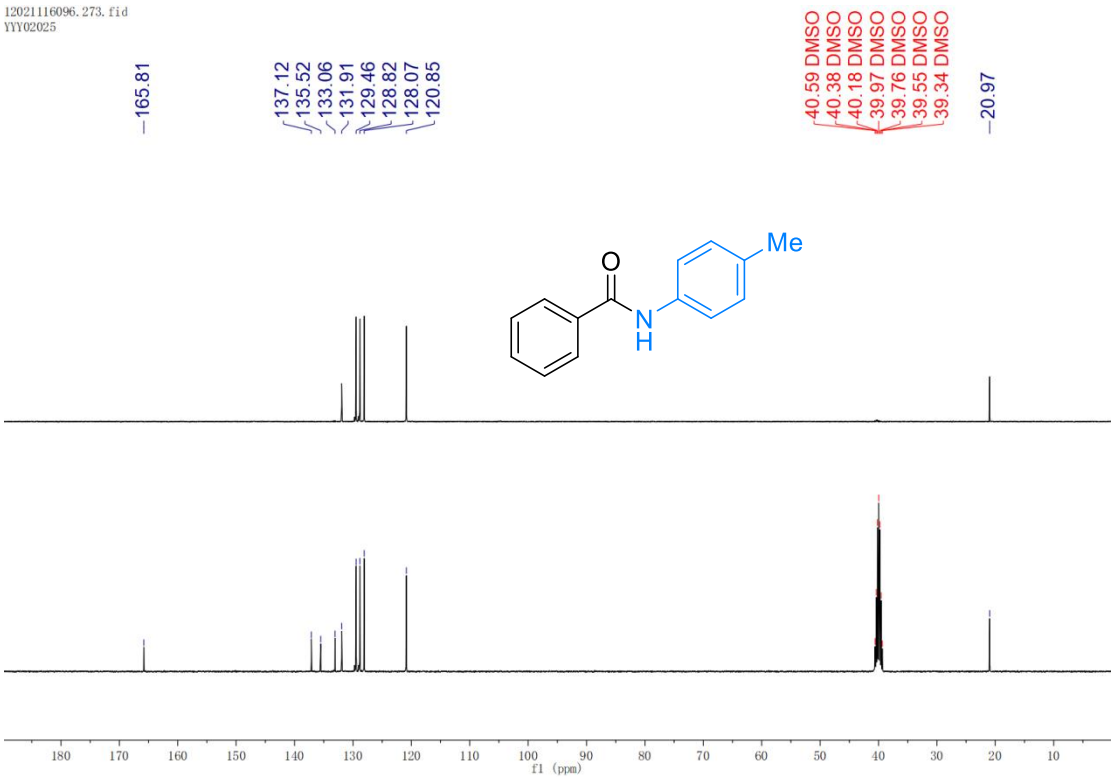
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 3b**



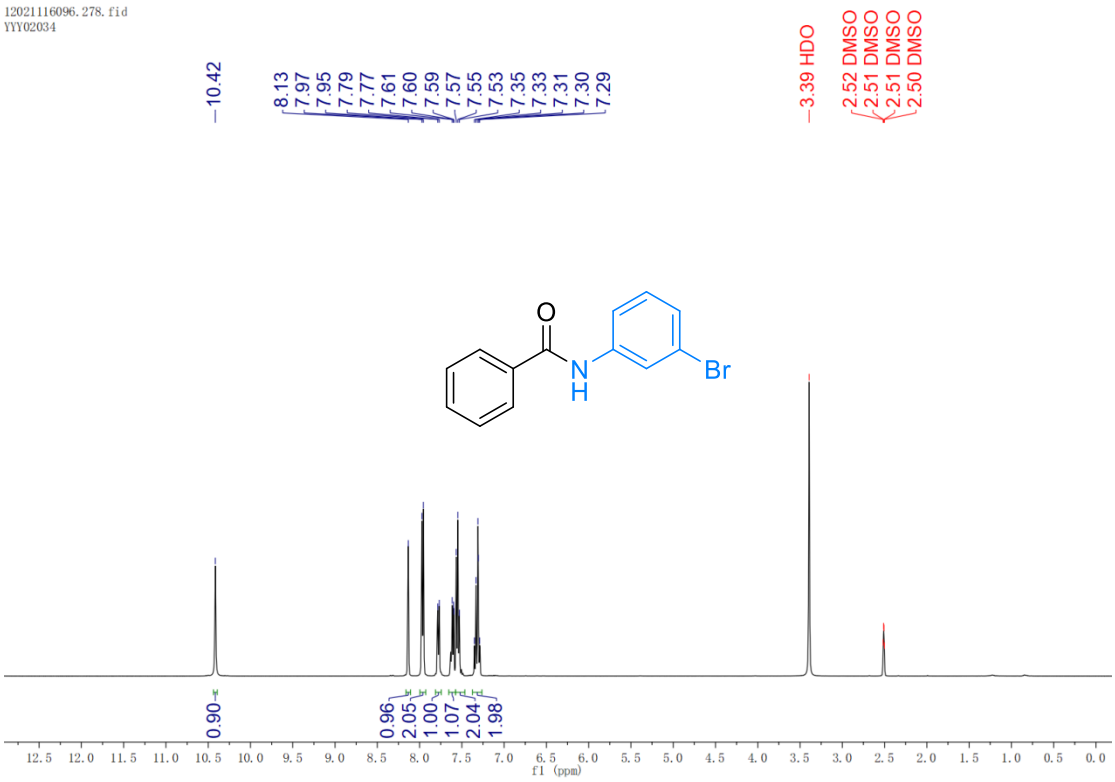
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 3b**



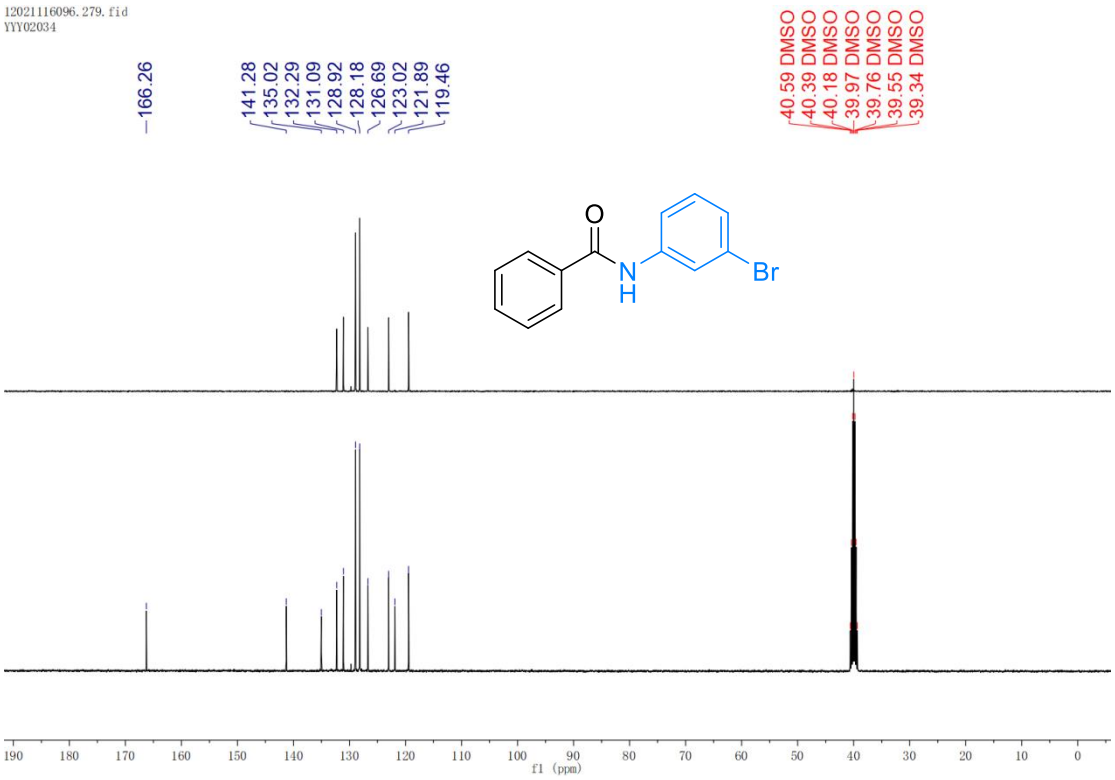
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 3c**



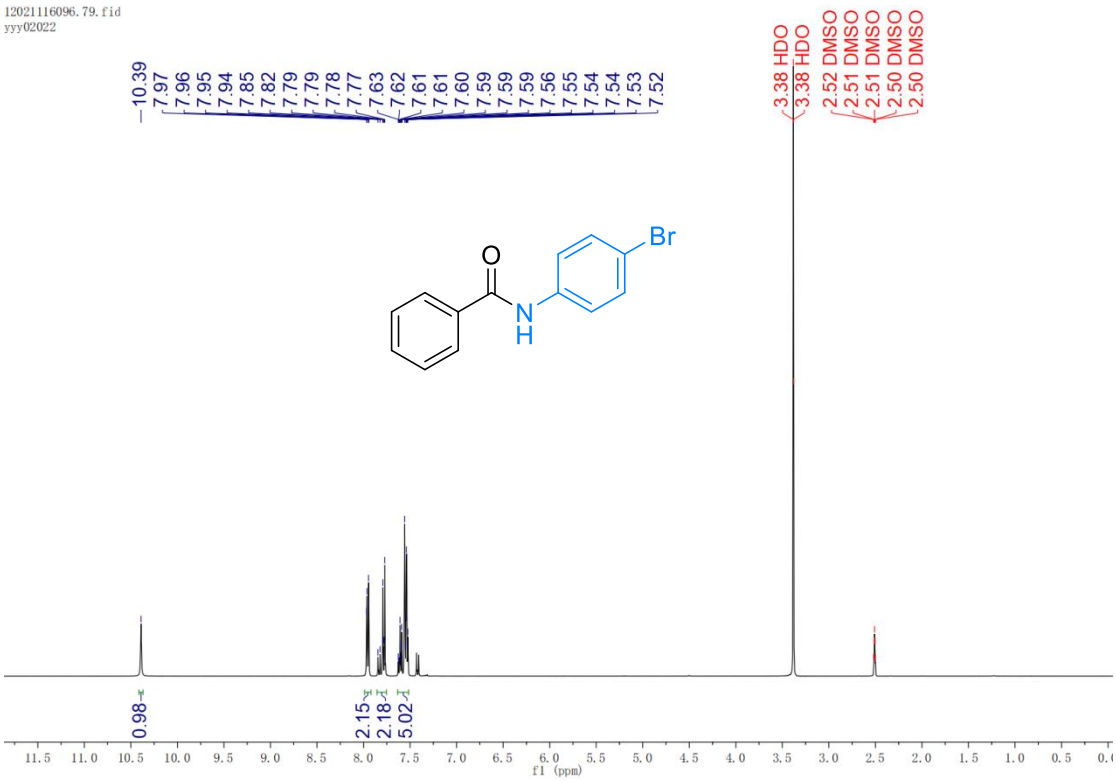
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 3c**



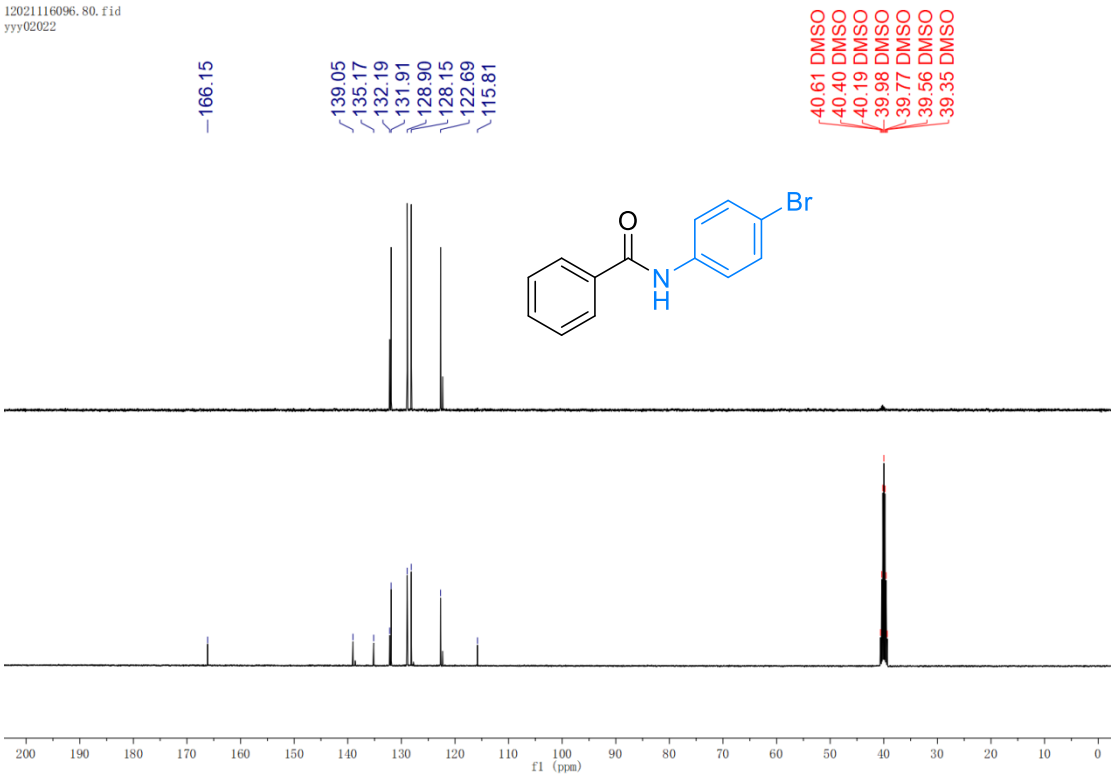
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 3d**



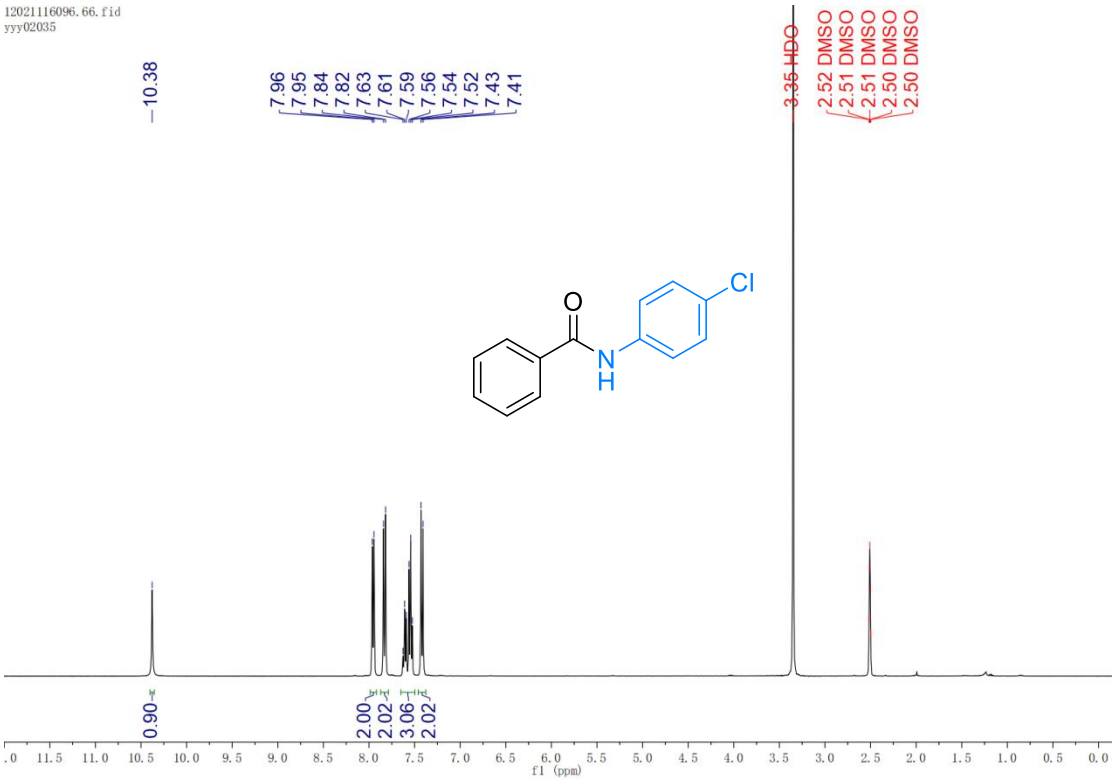
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 3d**



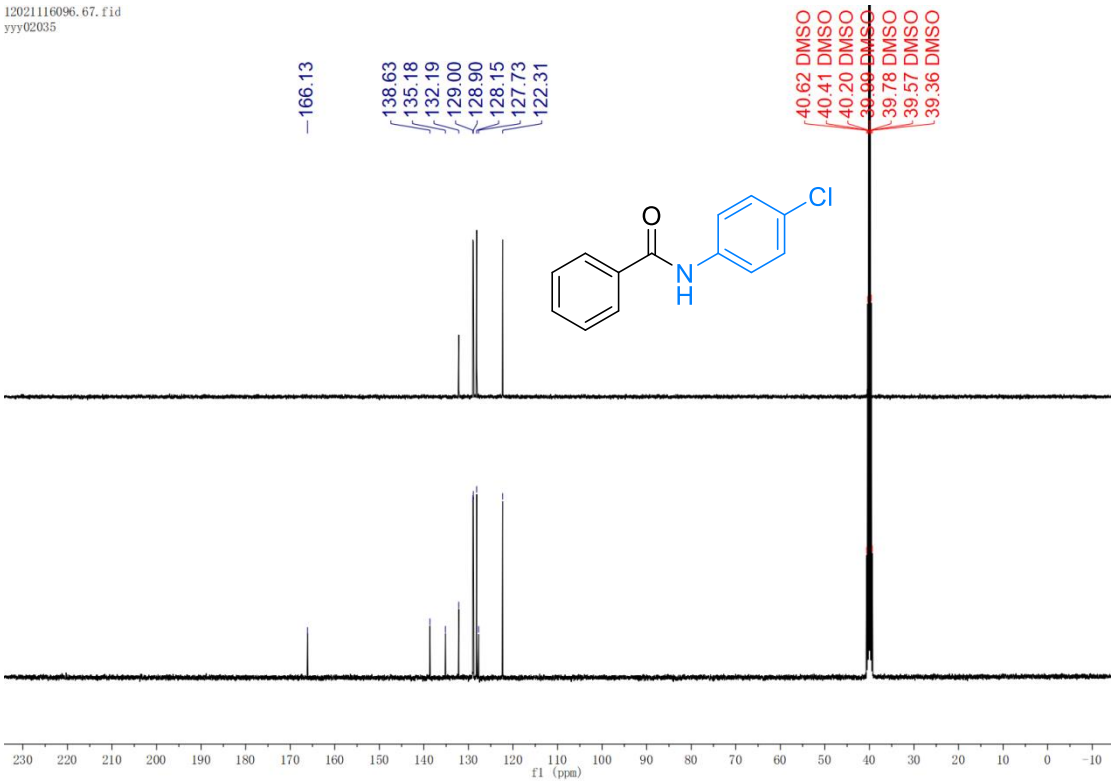
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 3e**



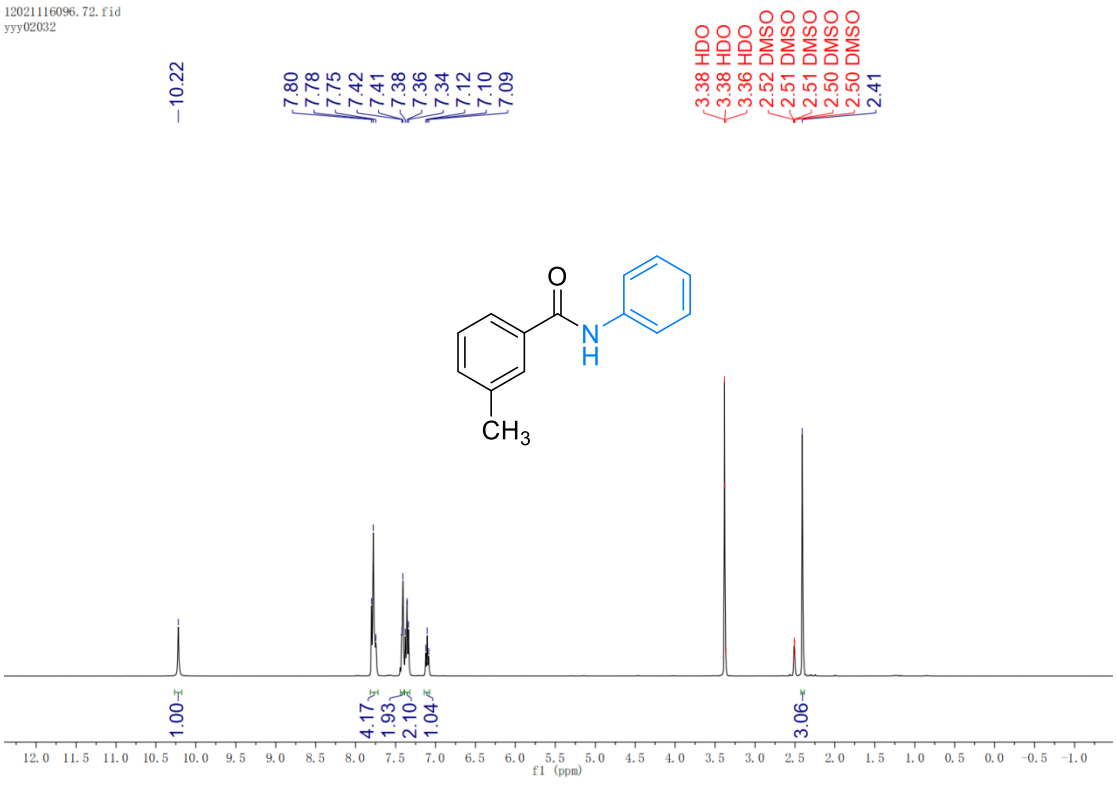
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 3e**



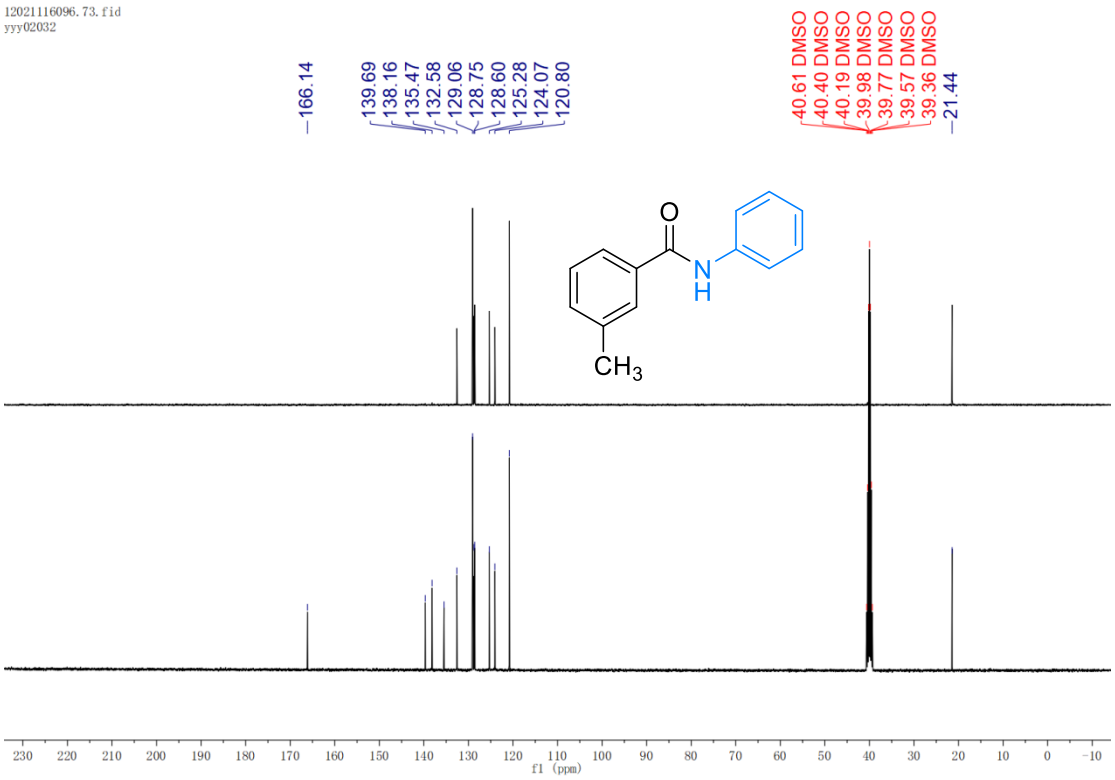
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 3f**



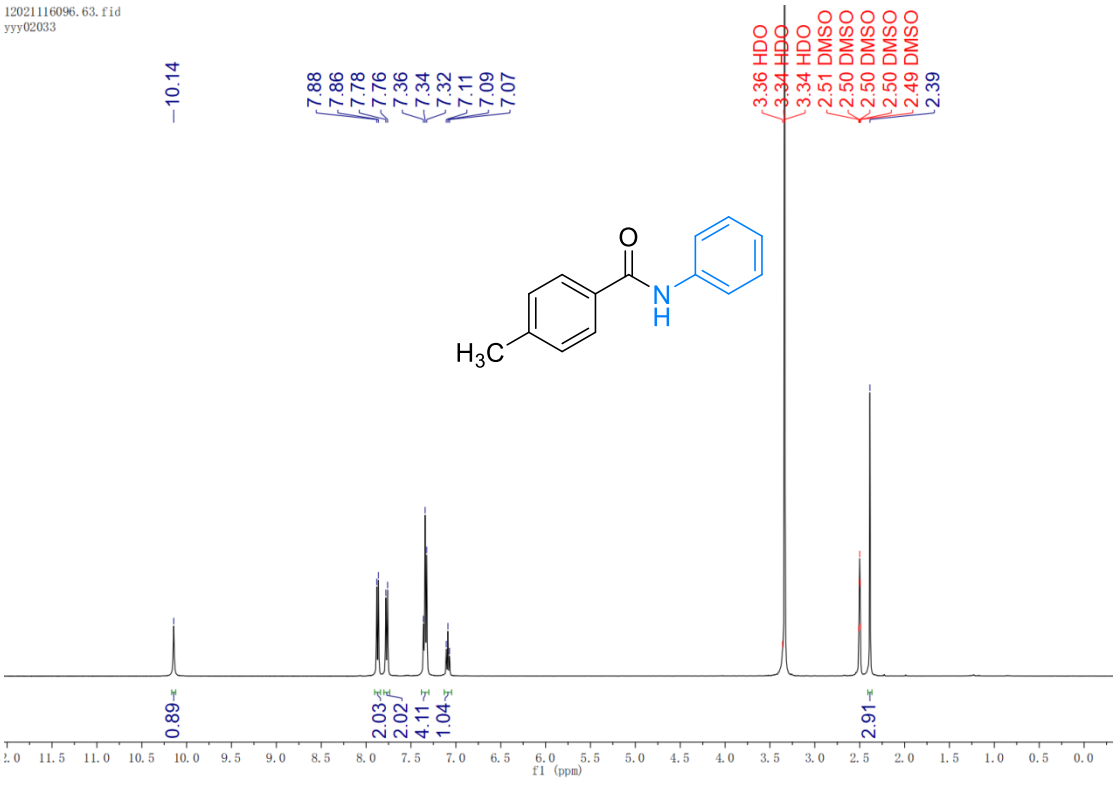
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 3f**



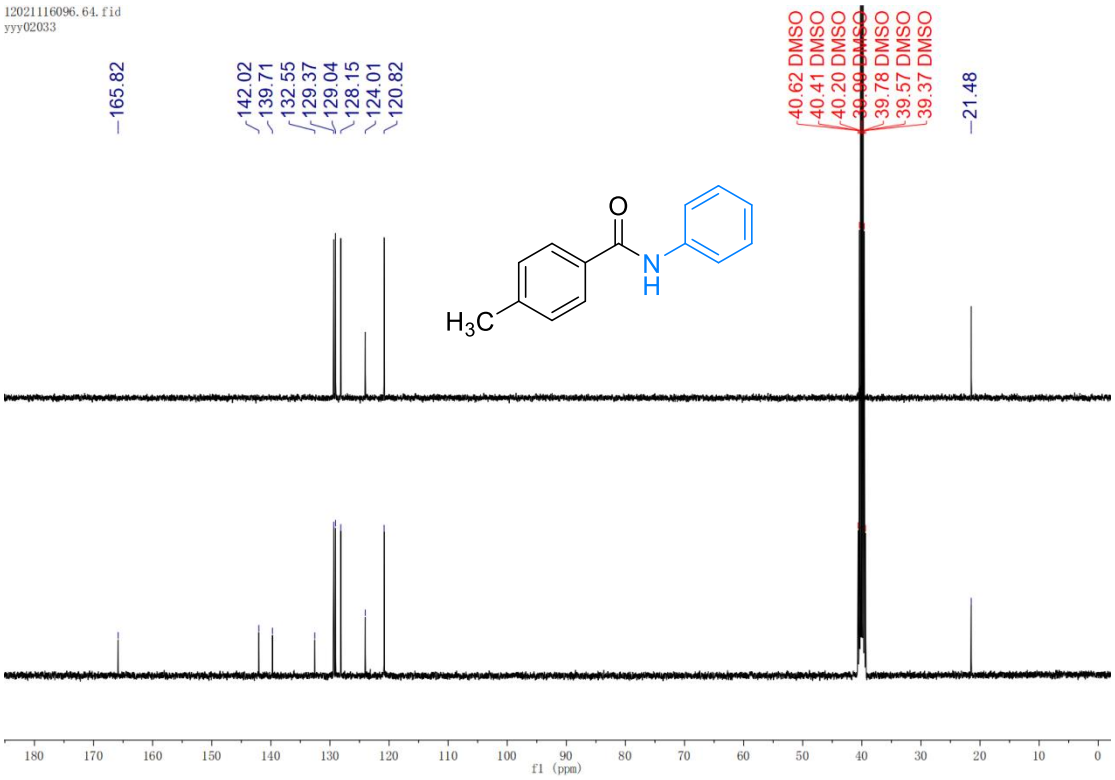
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 3g**



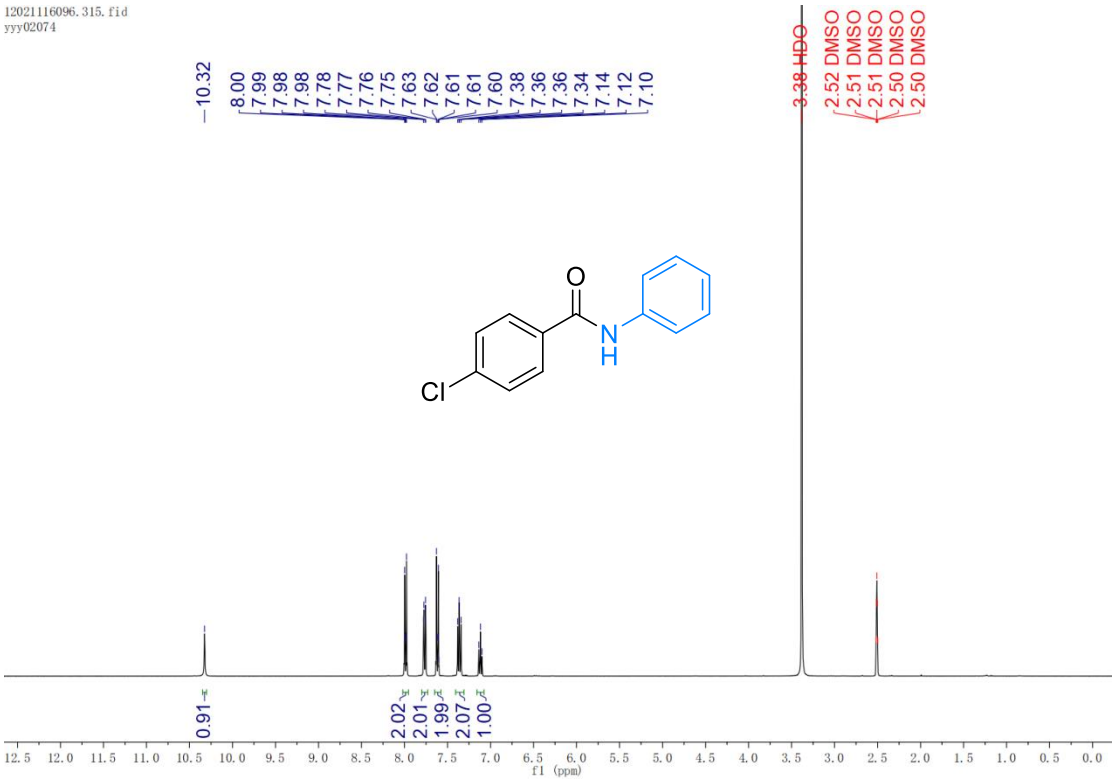
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 3g**



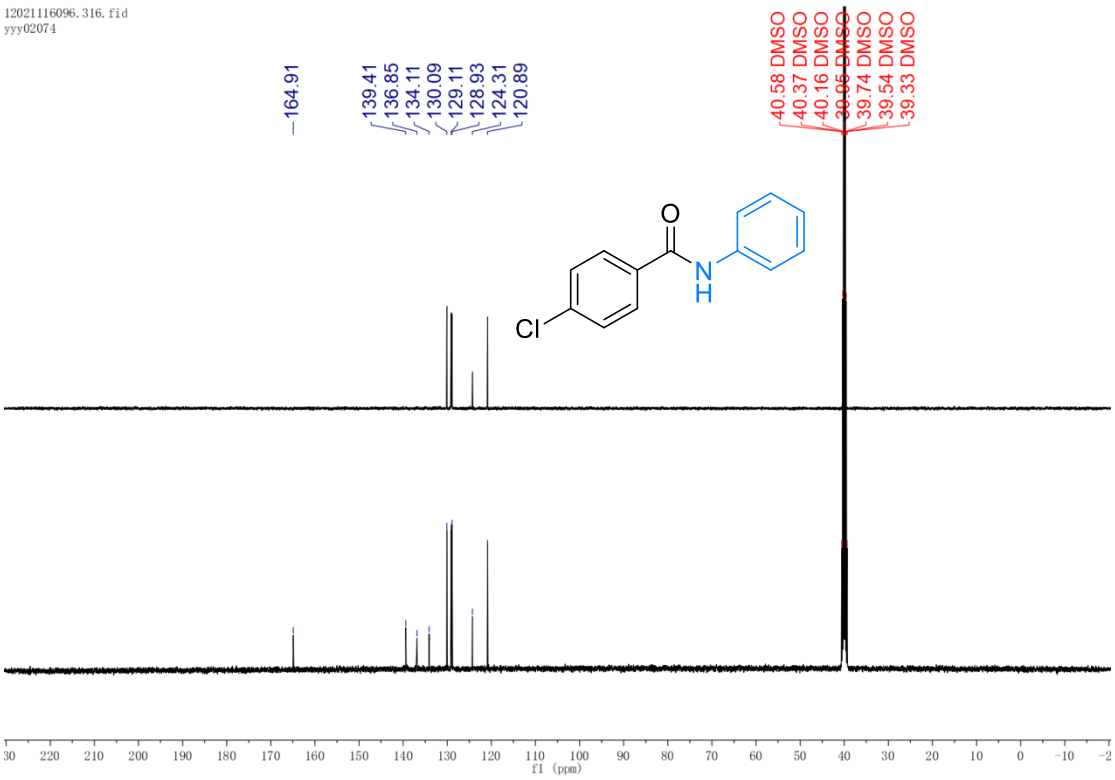
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 3h**



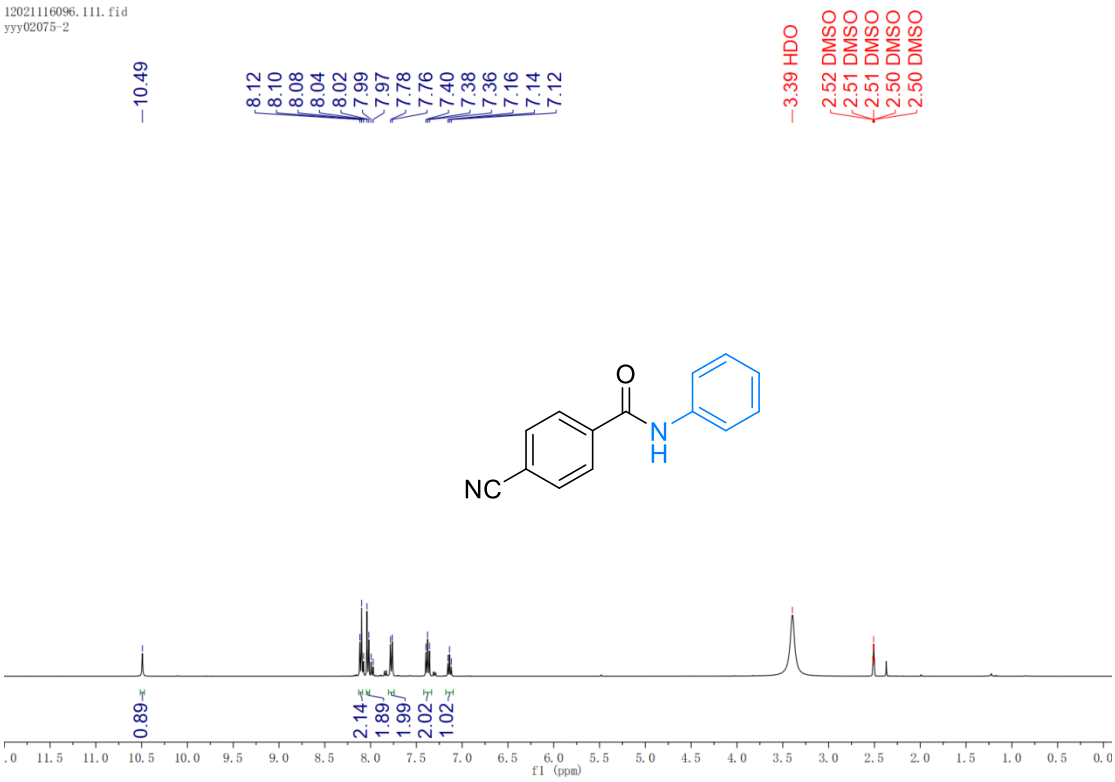
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 3h**



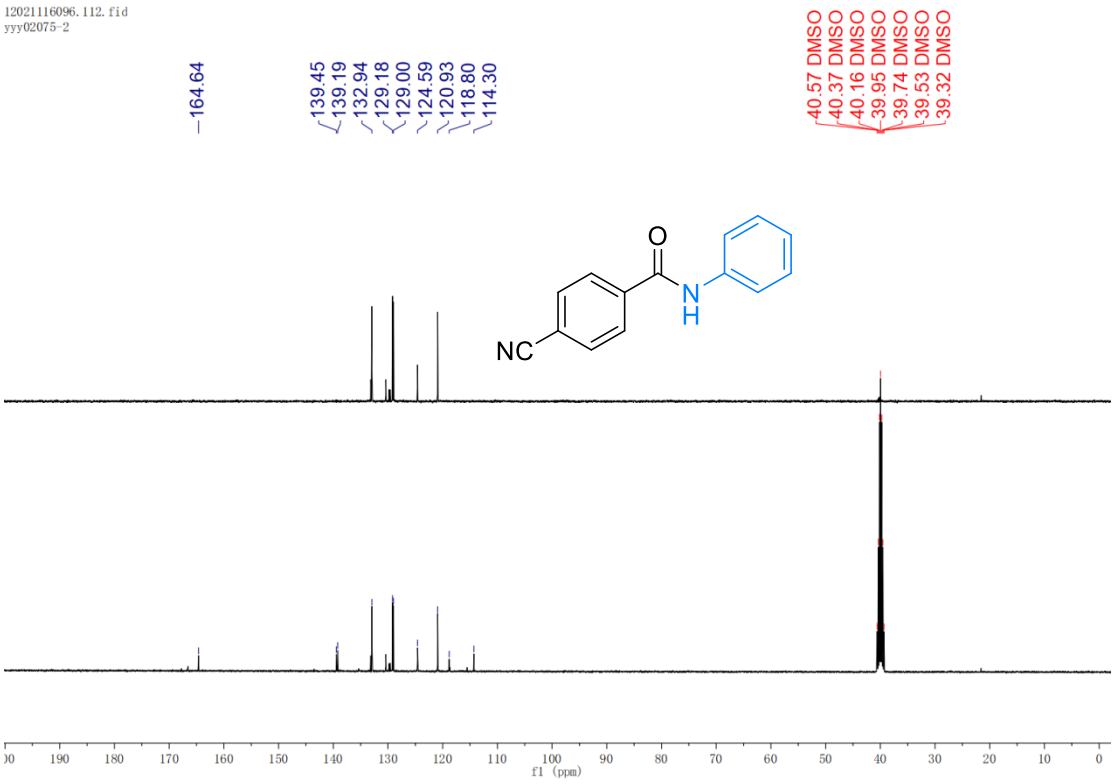
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 3i**



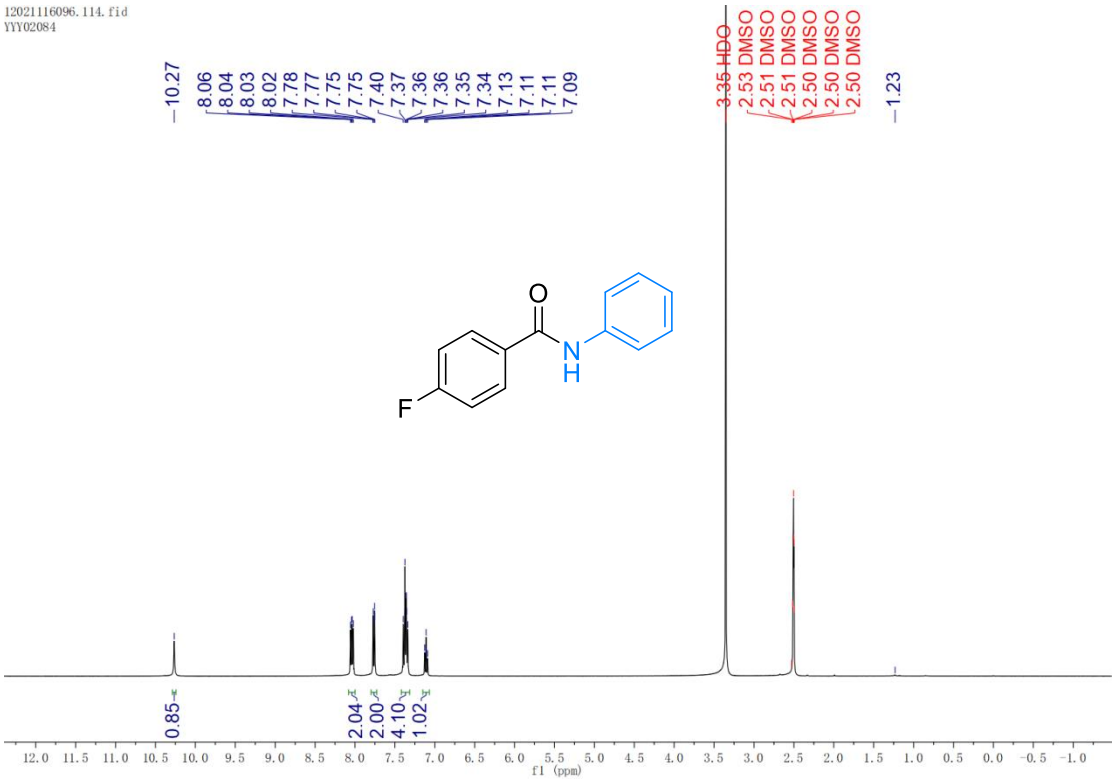
^{13}C-NMR ((100 MHz, DMSO-d_6) **Spectra of compound 3i**



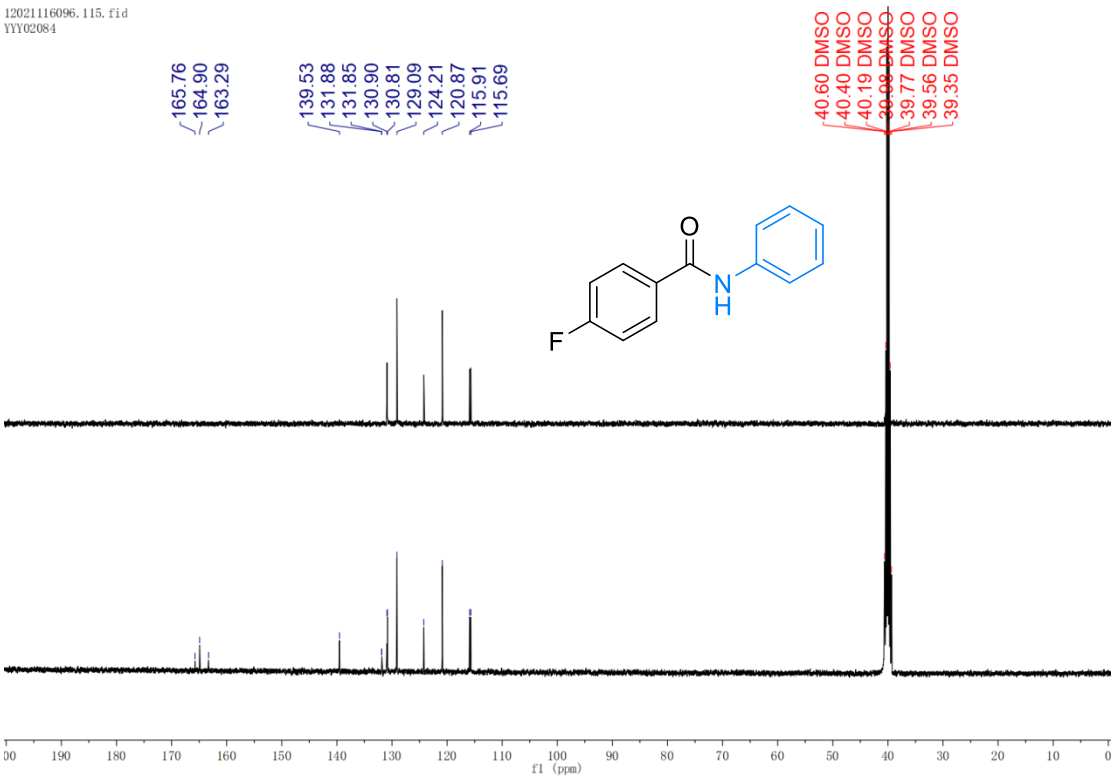
[1]H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 3j**



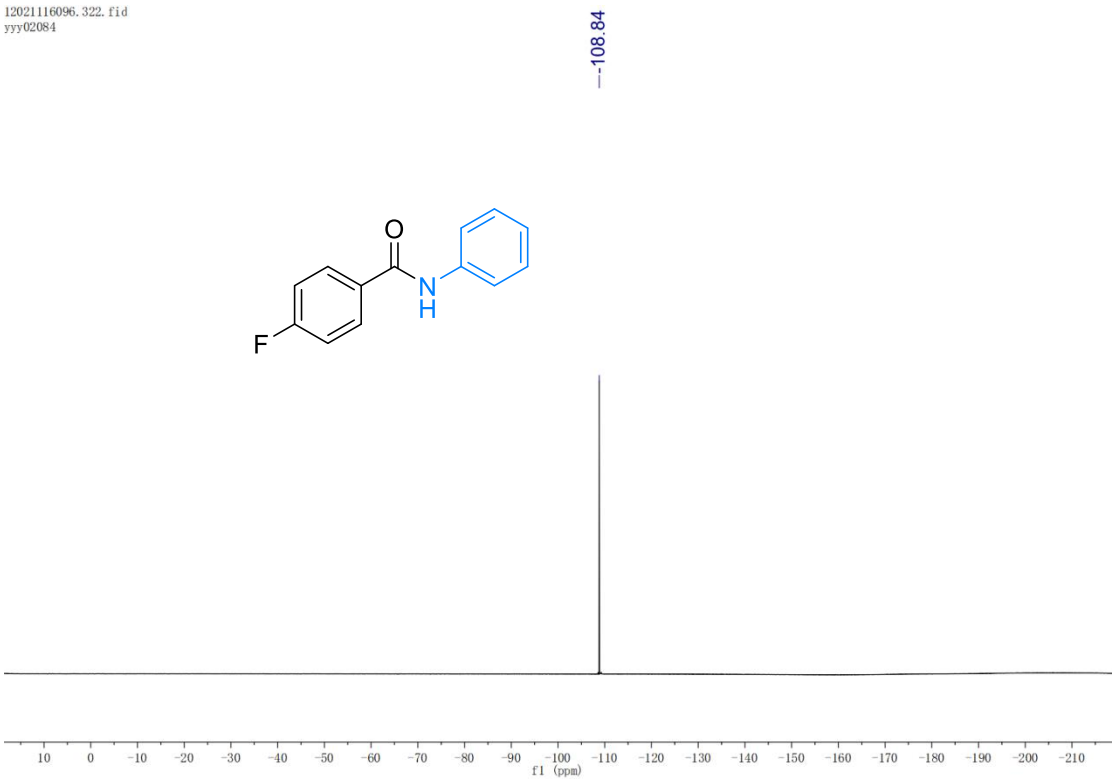
[13]C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 3j**



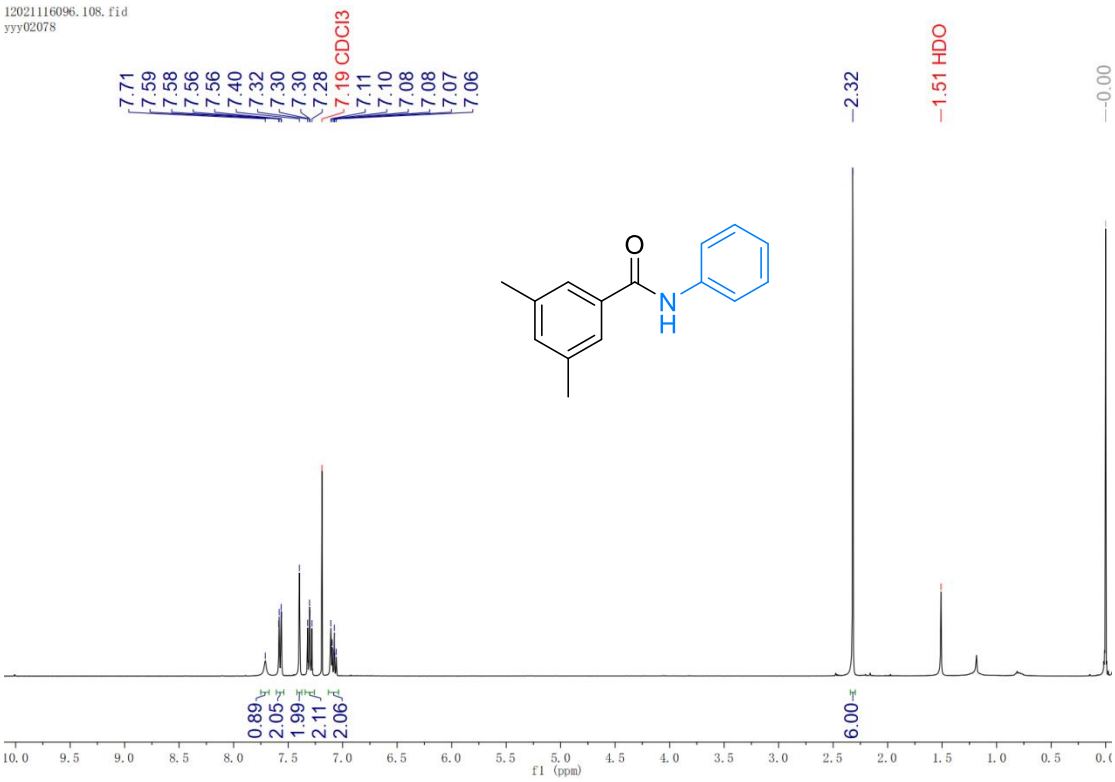
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 3k**



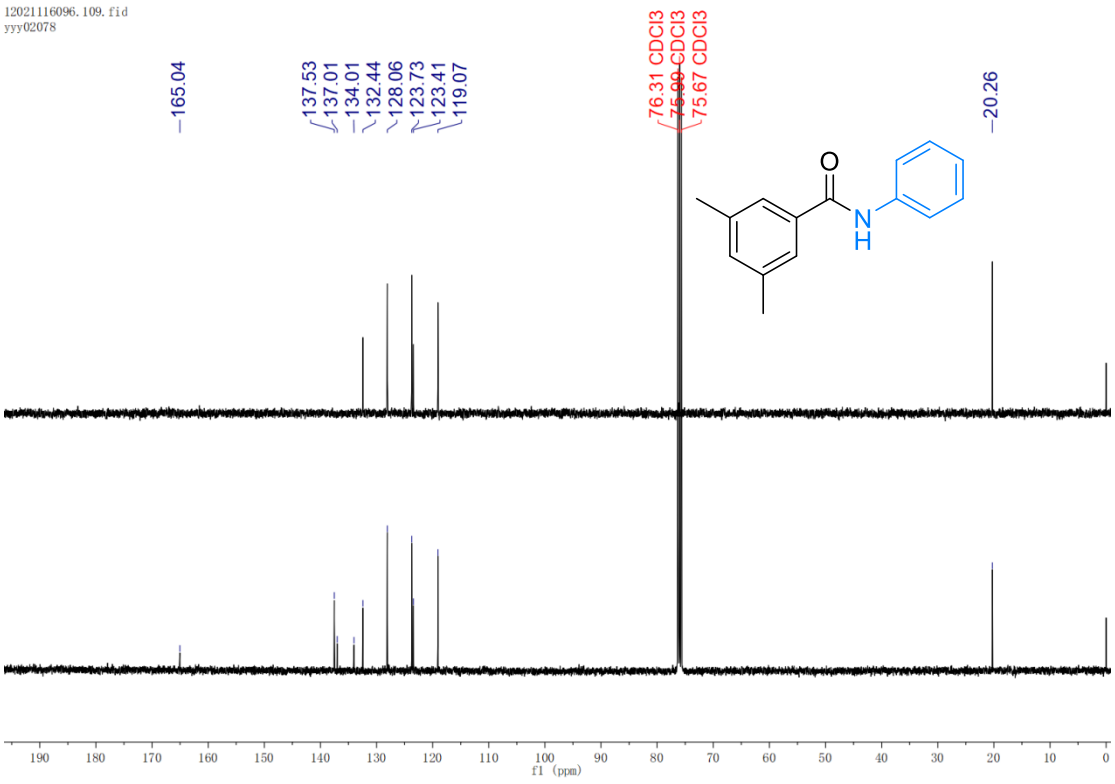
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 3k**



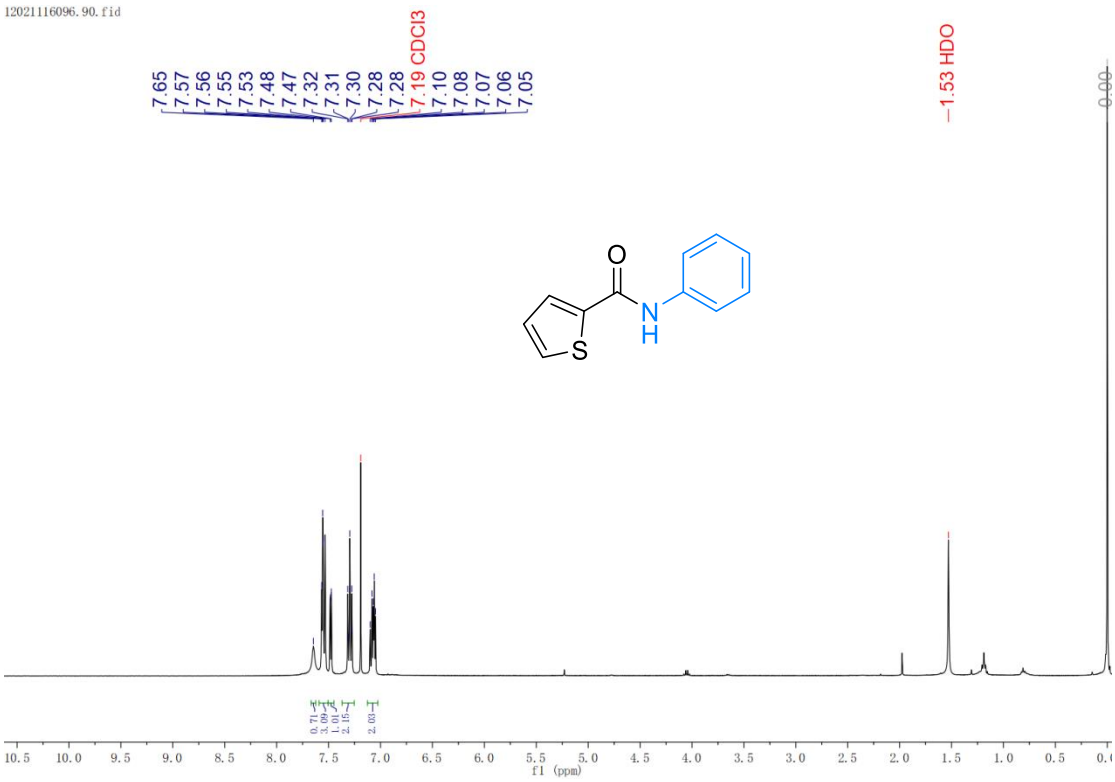
^{19}F NMR (376 MHz, DMSO-d_6) **Spectra of compound 3k**



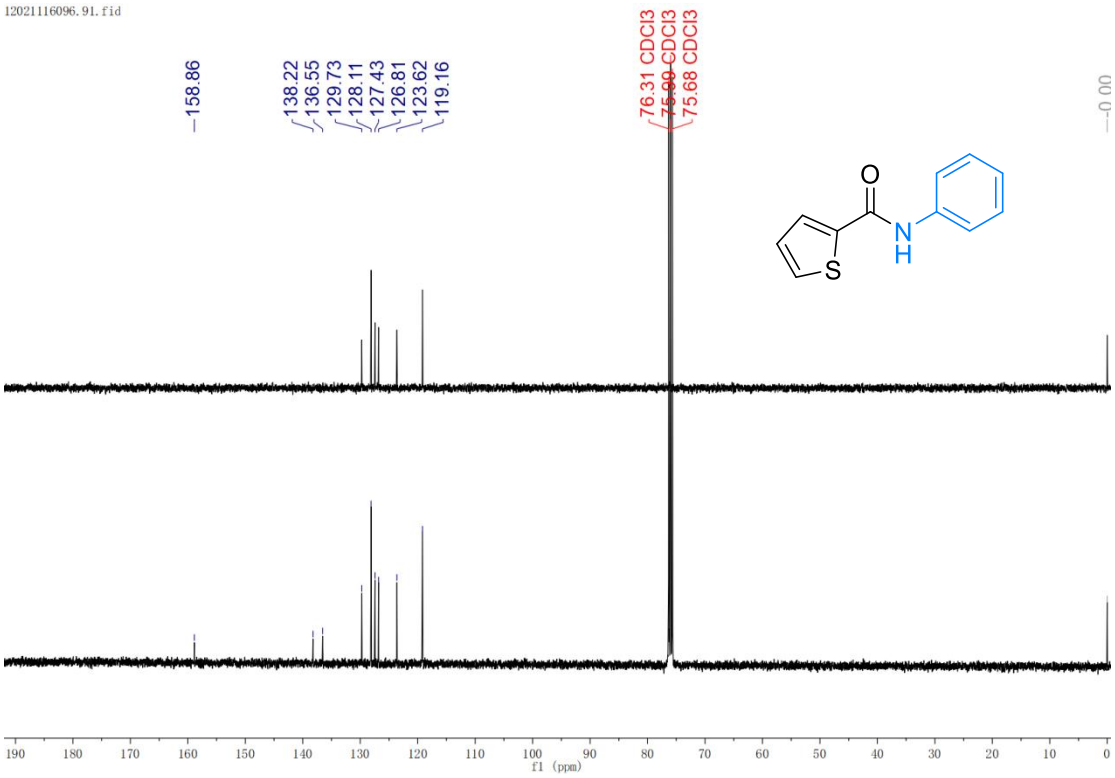
[1]H-NMR (400 MHz, Chloroform-*d*) **Spectra of compound 3l**



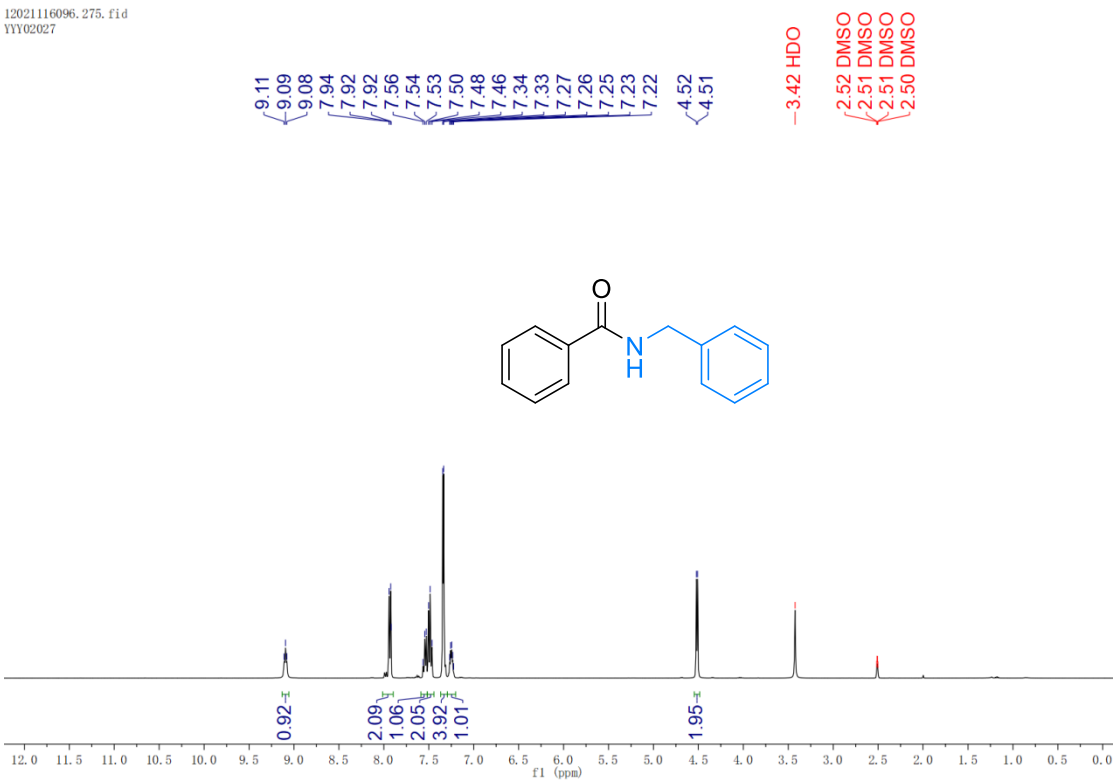
[13]C-NMR (100 MHz, Chloroform-*d*) **Spectra of compound 3l**



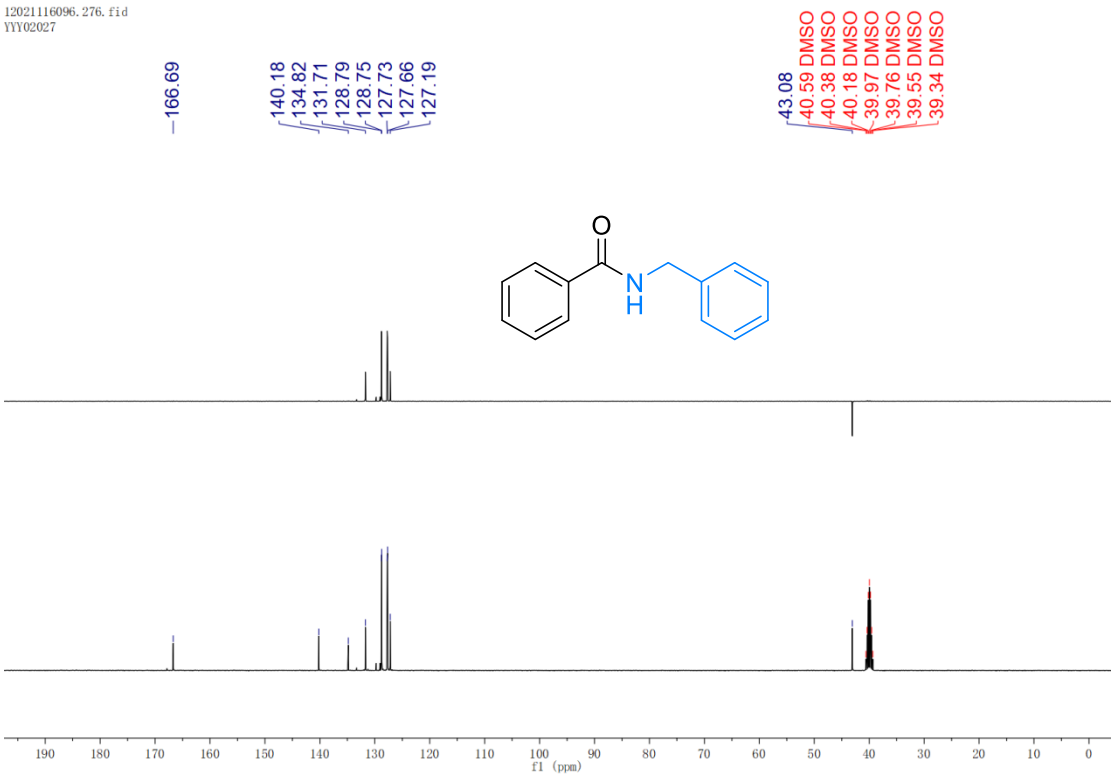
[1]H-NMR (400 MHz, Chloroform-*d*) **Spectra of compound 3m**



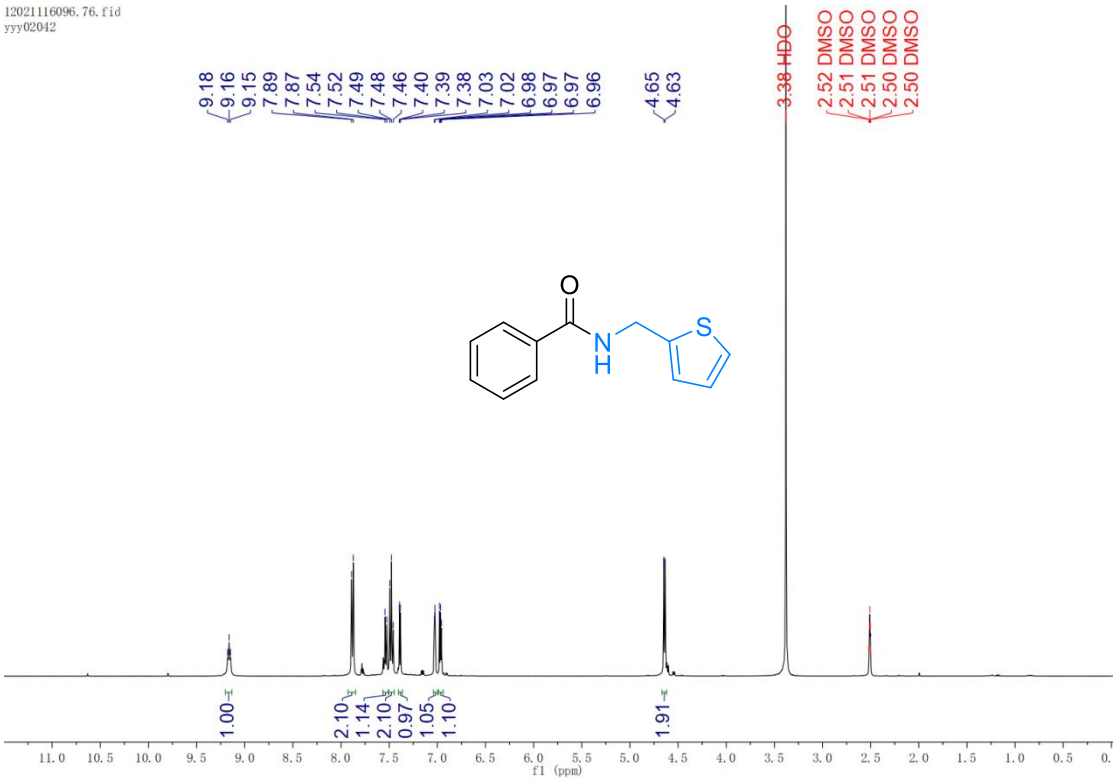
[13]C-NMR (100 MHz, Chloroform-*d*) **Spectra of compound 3m**



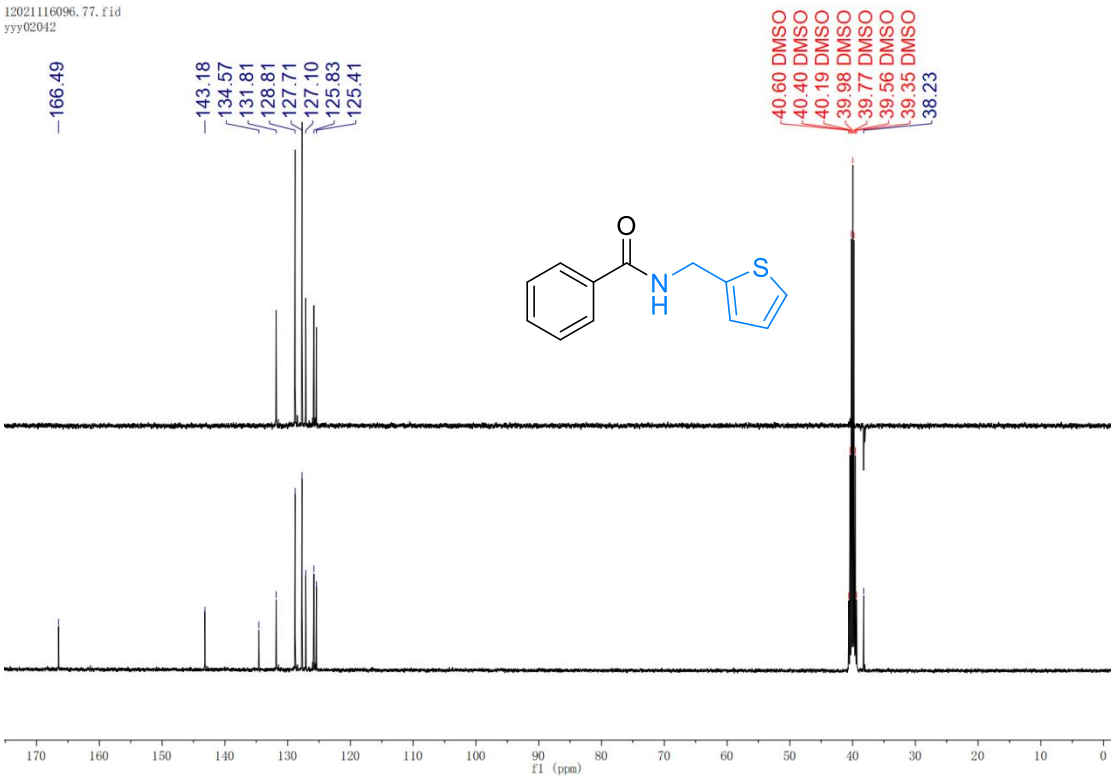
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 3n**



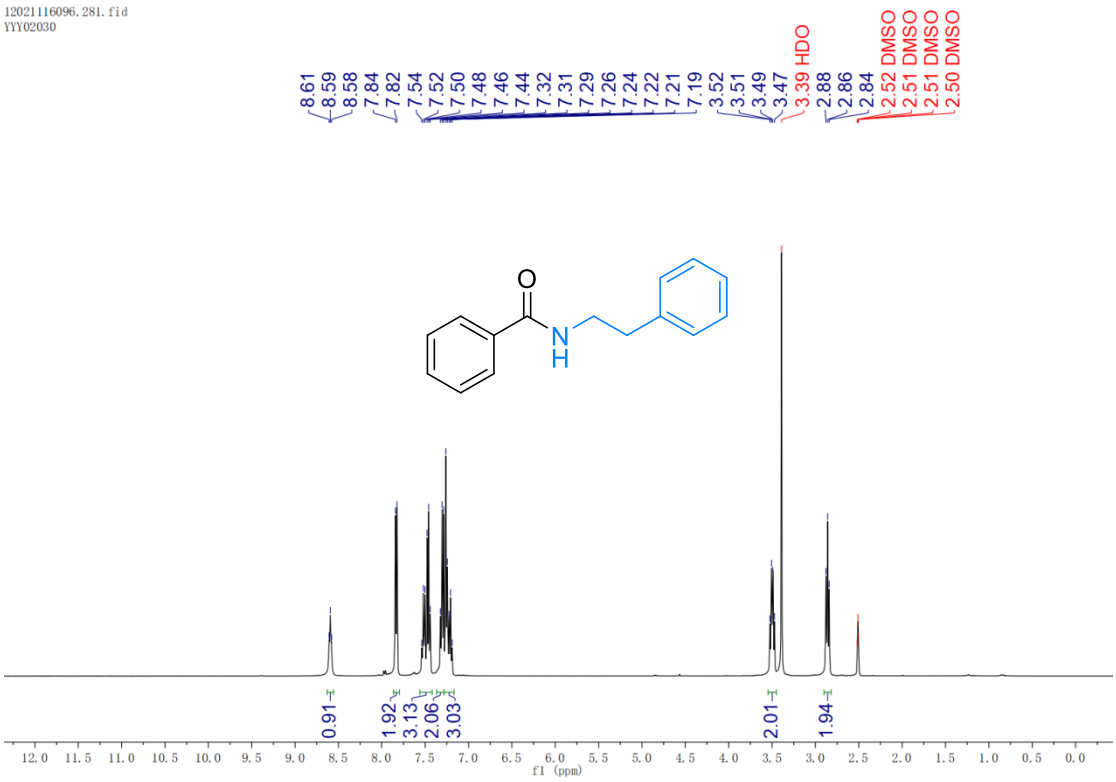
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 3n**



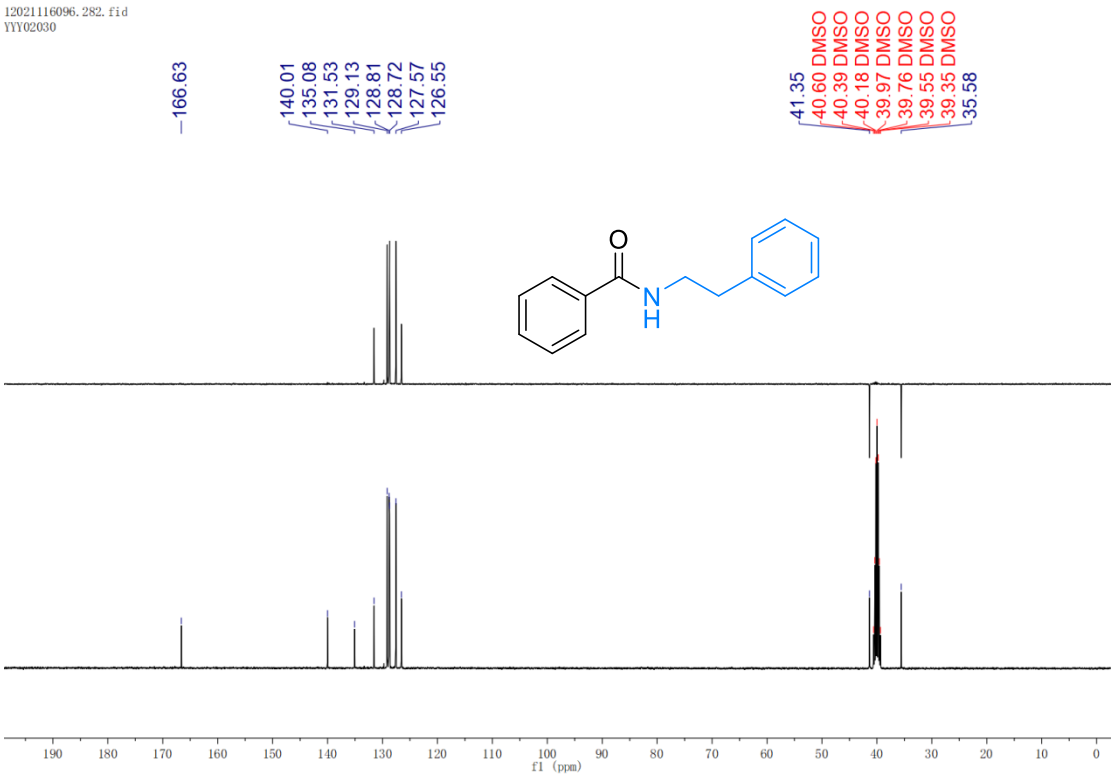
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 3o**



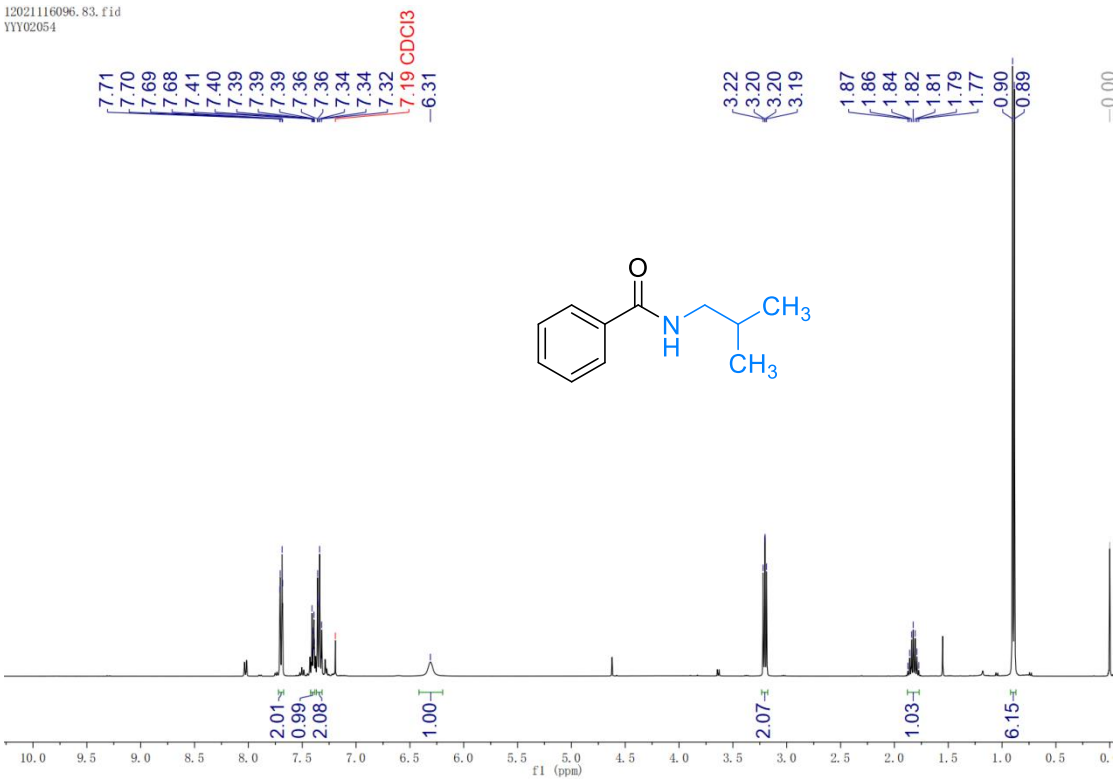
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 3o**



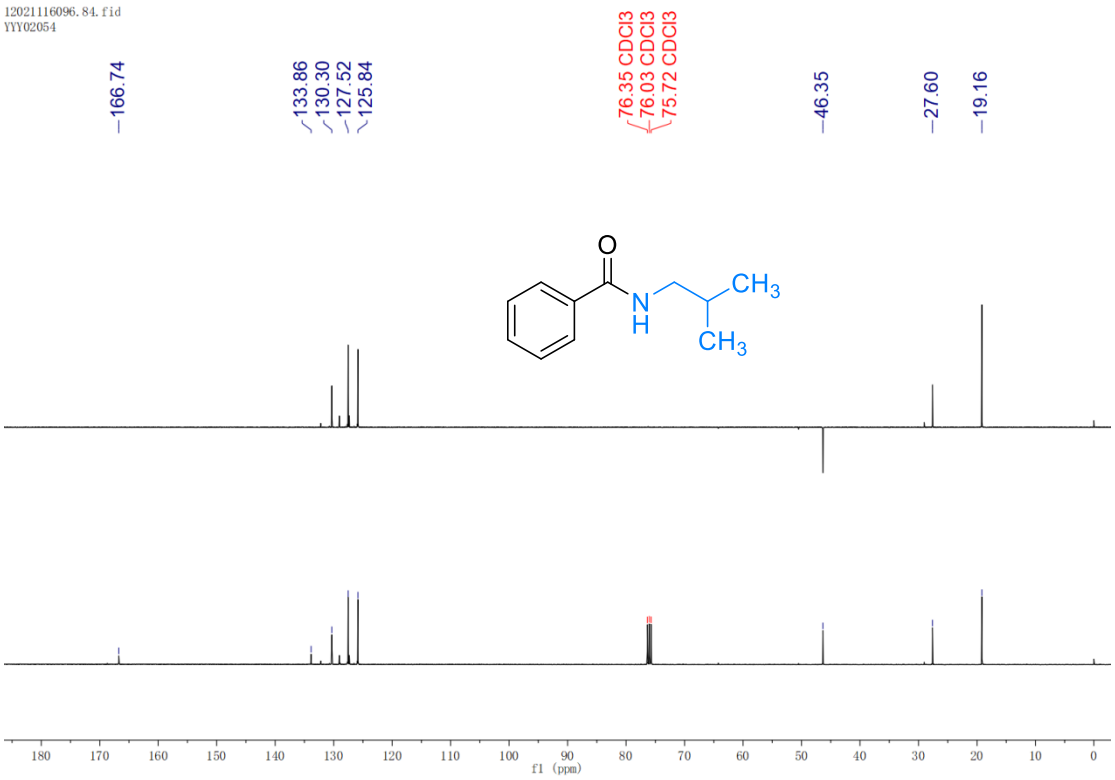
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 3p**



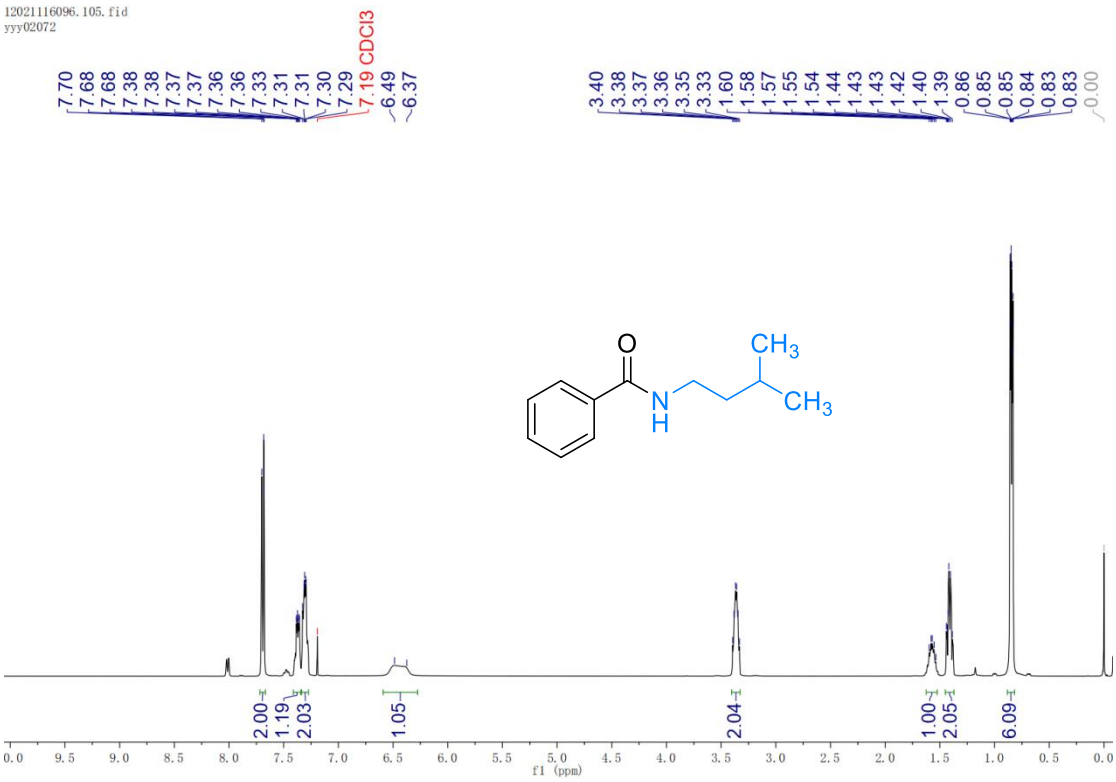
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 3p**



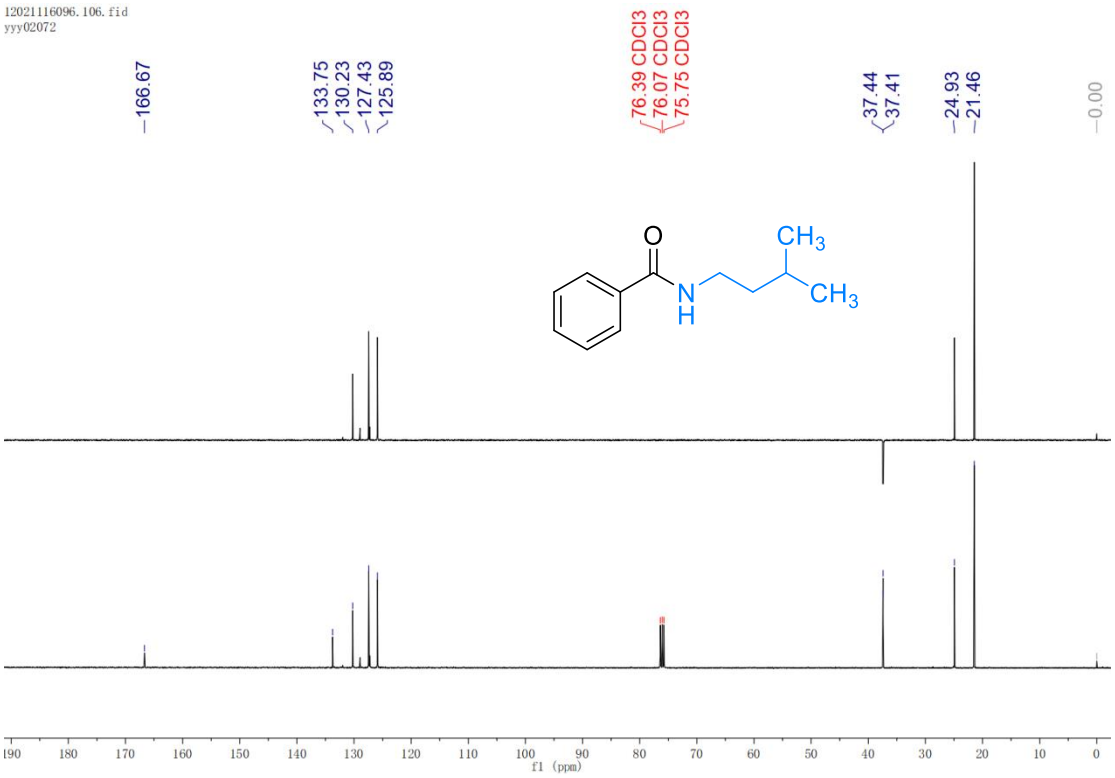
[1]H-NMR (400 MHz, Chloroform-*d*) **Spectra of compound 3q**



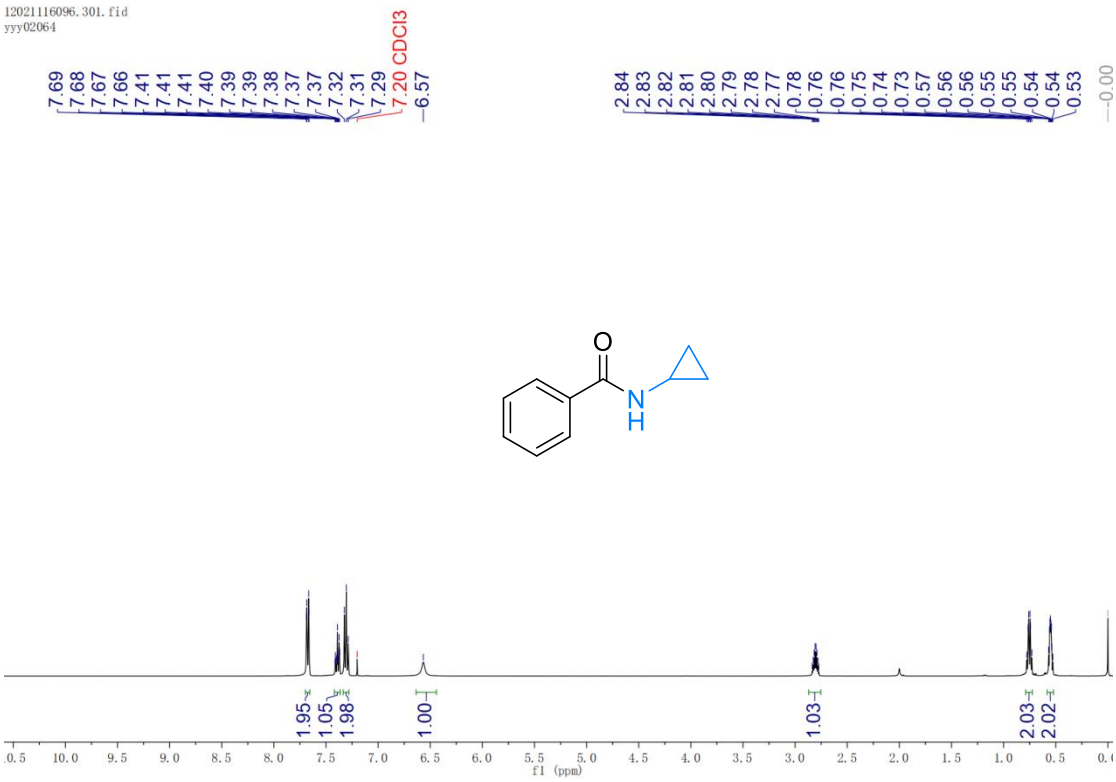
[13]C-NMR (100 MHz, Chloroform-*d*) **Spectra of compound 3q**



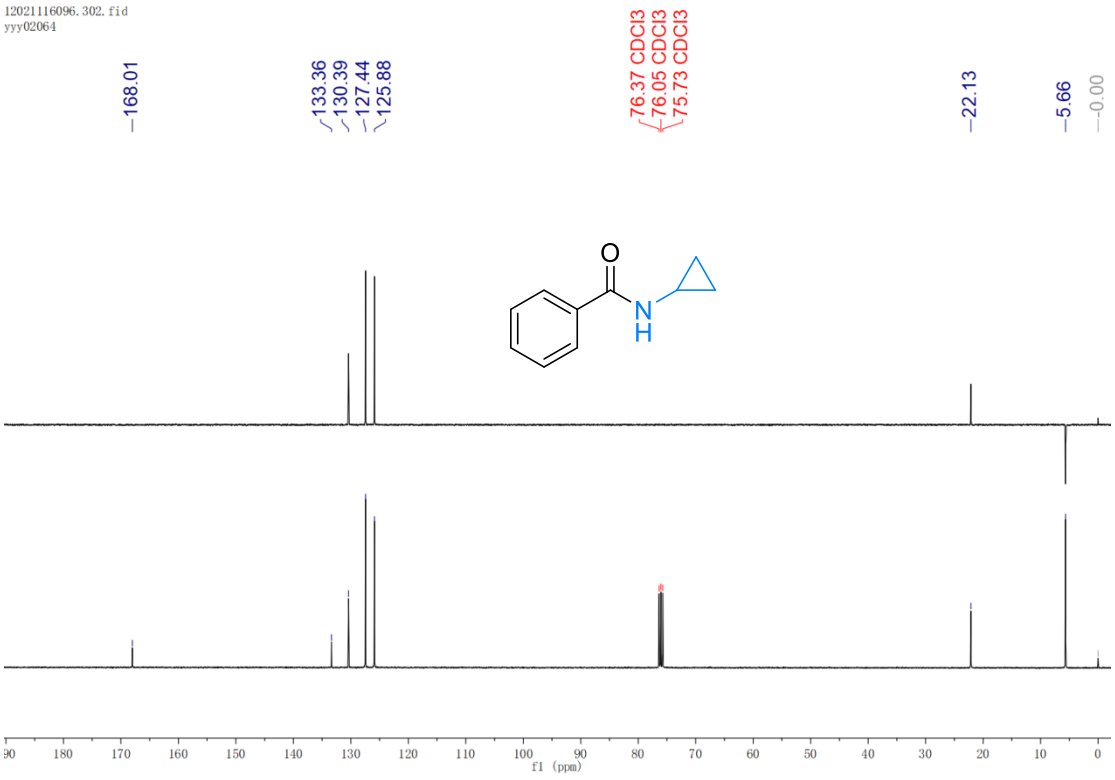
^{1}H-NMR (400 MHz, Chloroform-*d*) **Spectra of compound 3r**



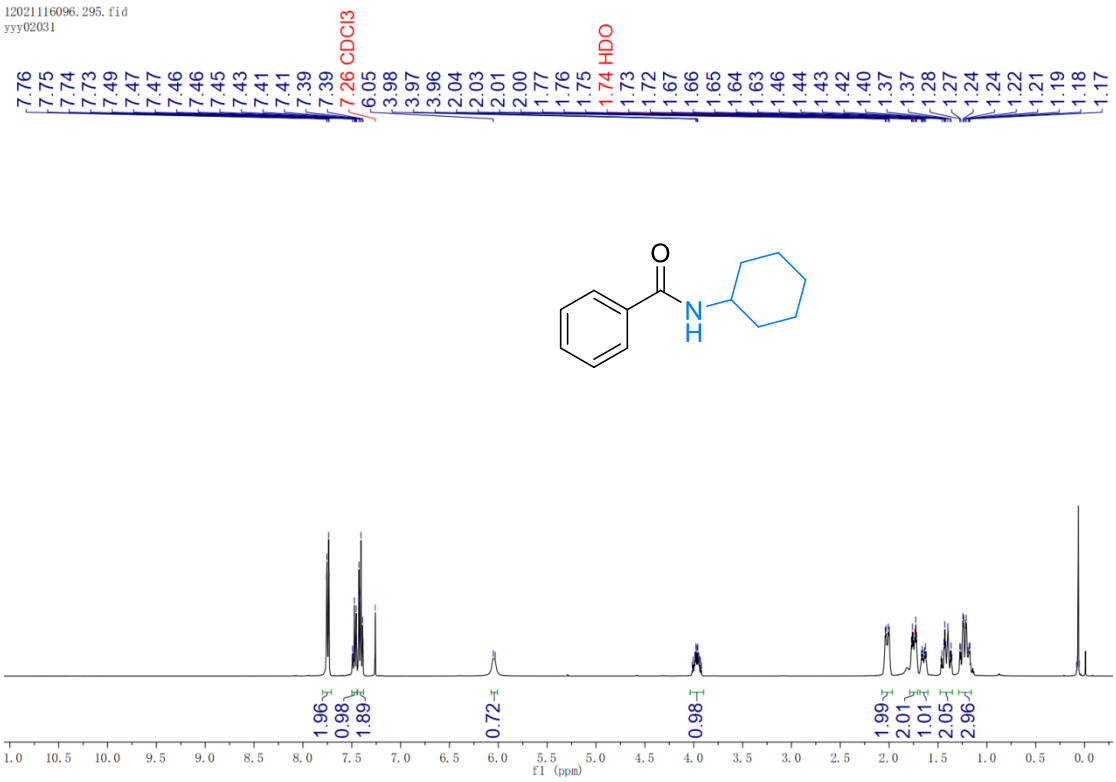
^{13}C-NMR (100 MHz, Chloroform-*d*) **Spectra of compound 3r**



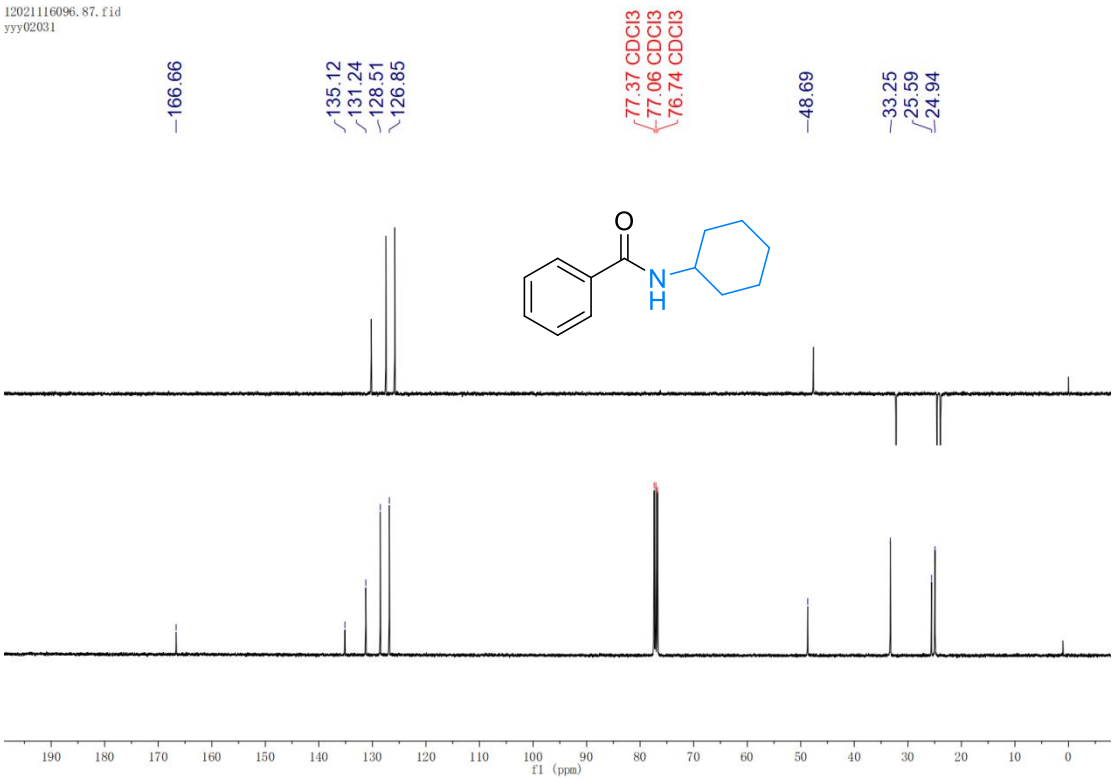
[1]H-NMR (400 MHz, Chloroform-*d*) **Spectra of compound 3s**



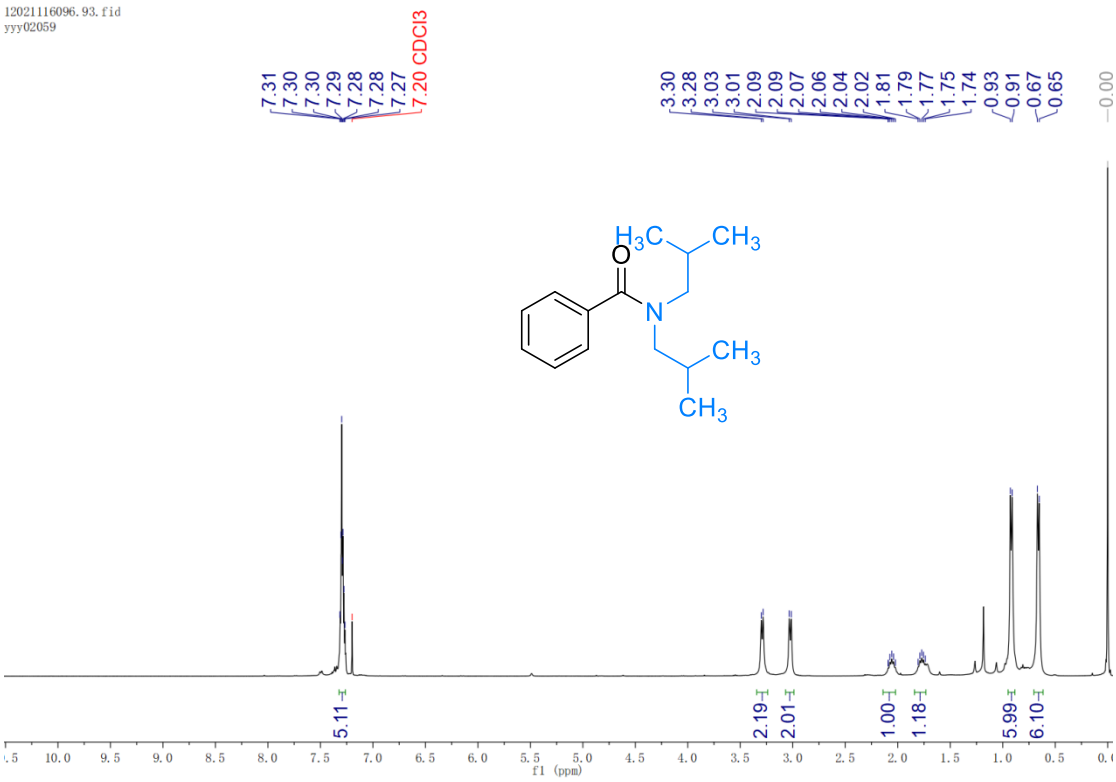
[13]C-NMR (100 MHz, Chloroform-*d*) **Spectra of compound 3s**



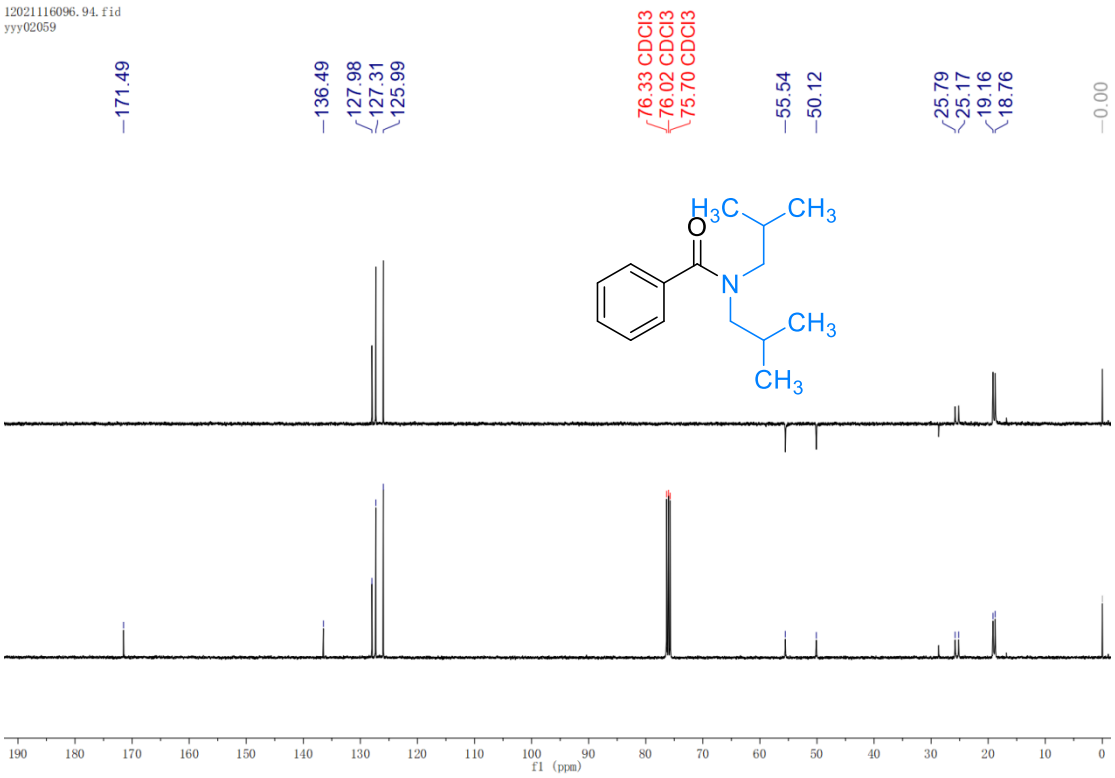
[1]H-NMR (400 MHz, Chloroform-*d*) **Spectra of compound 3t**



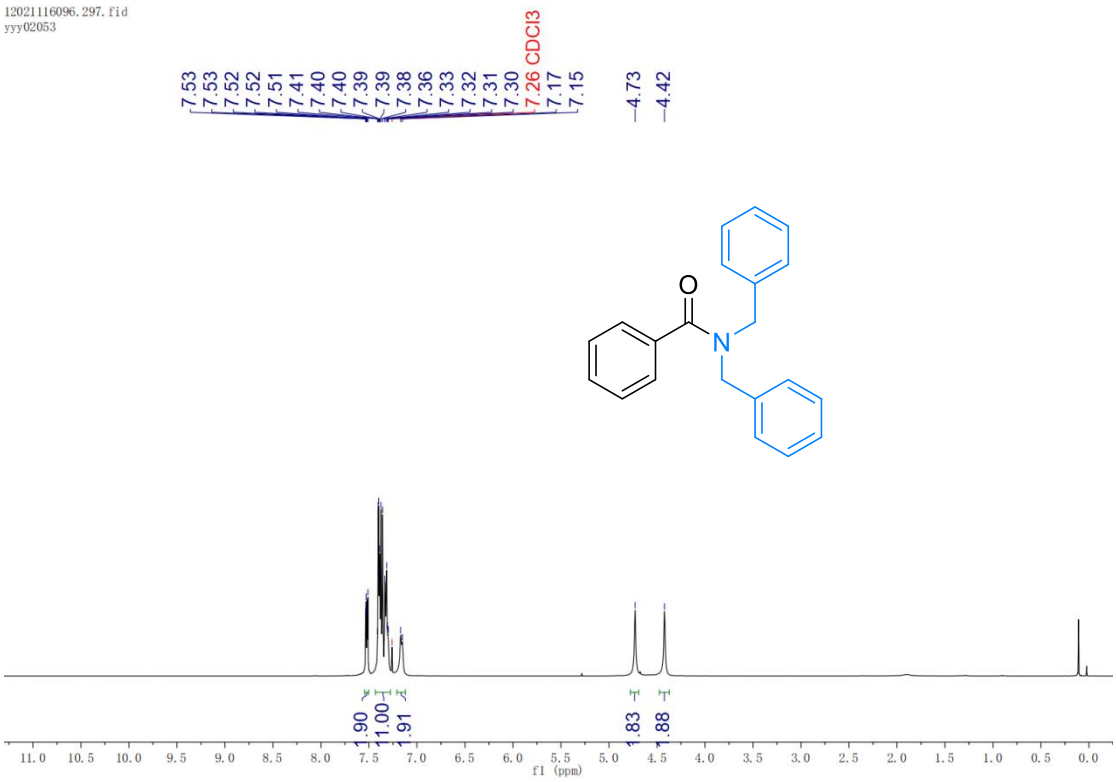
[13]C-NMR (100 MHz, Chloroform-*d*) **Spectra of compound 3t**



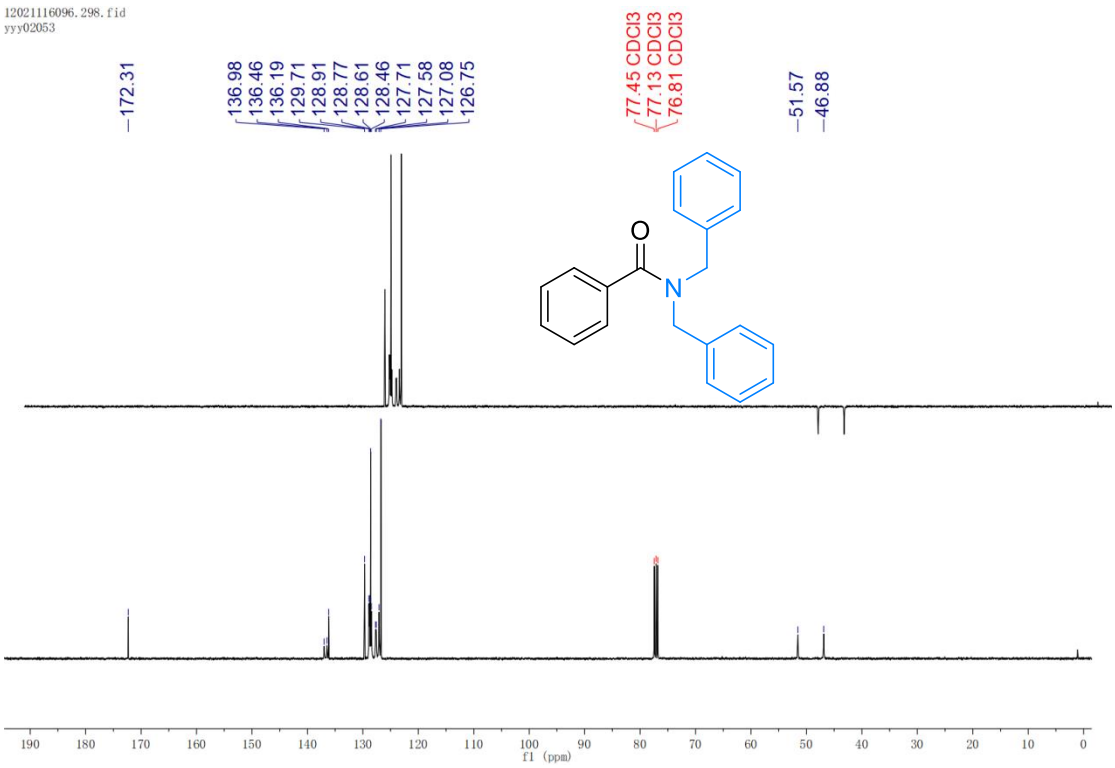
[1]H-NMR (400 MHz, Chloroform-*d*) **Spectra of compound 3u**



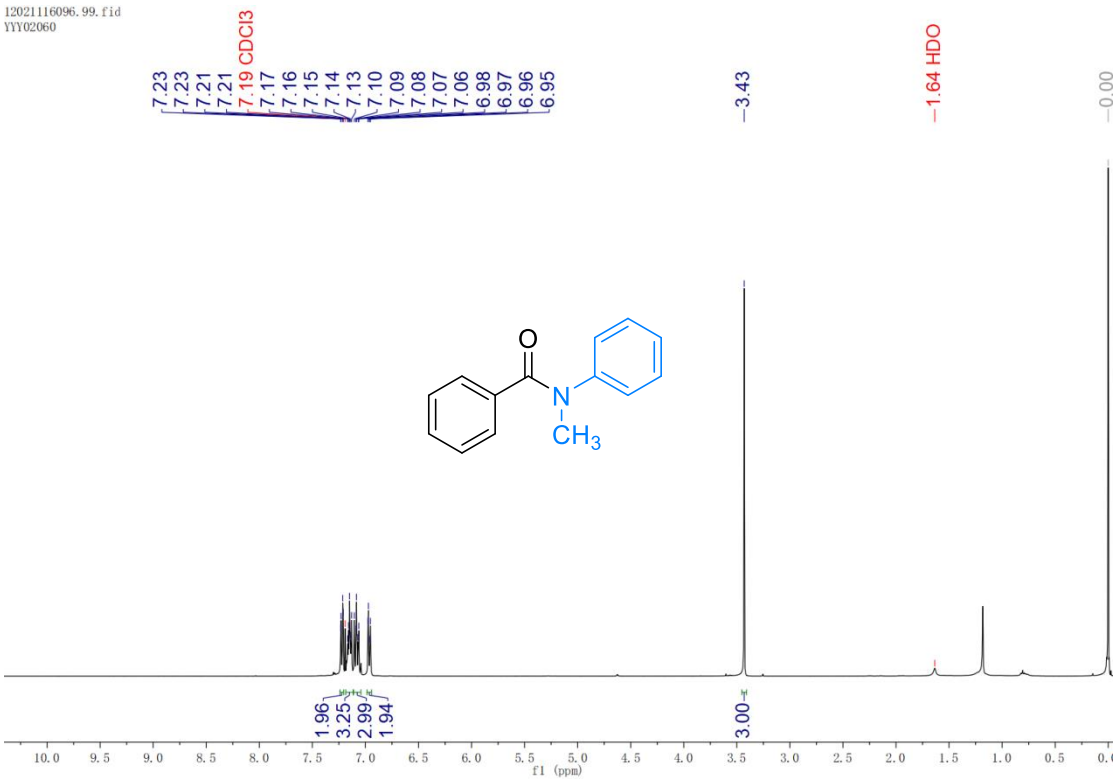
[13]C-NMR (100 MHz, Chloroform-*d*) **Spectra of compound 3u**



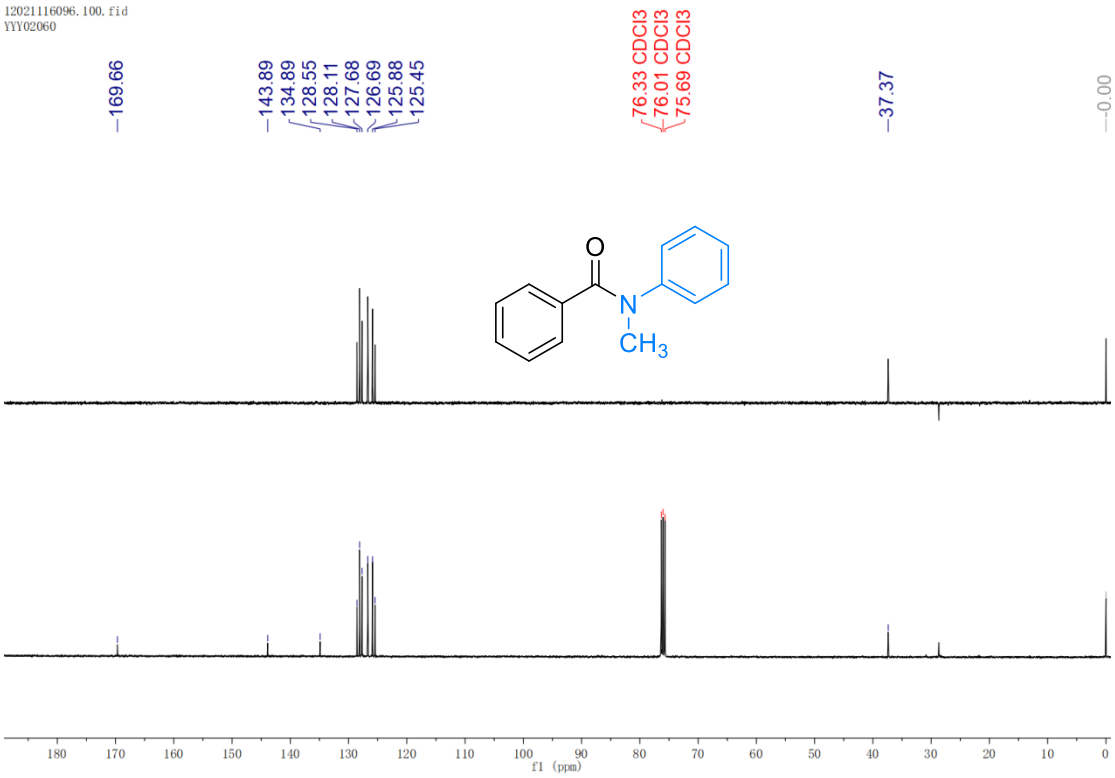
^{1}H-NMR (400 MHz, Chloroform-*d*) **Spectra of compound 3v**



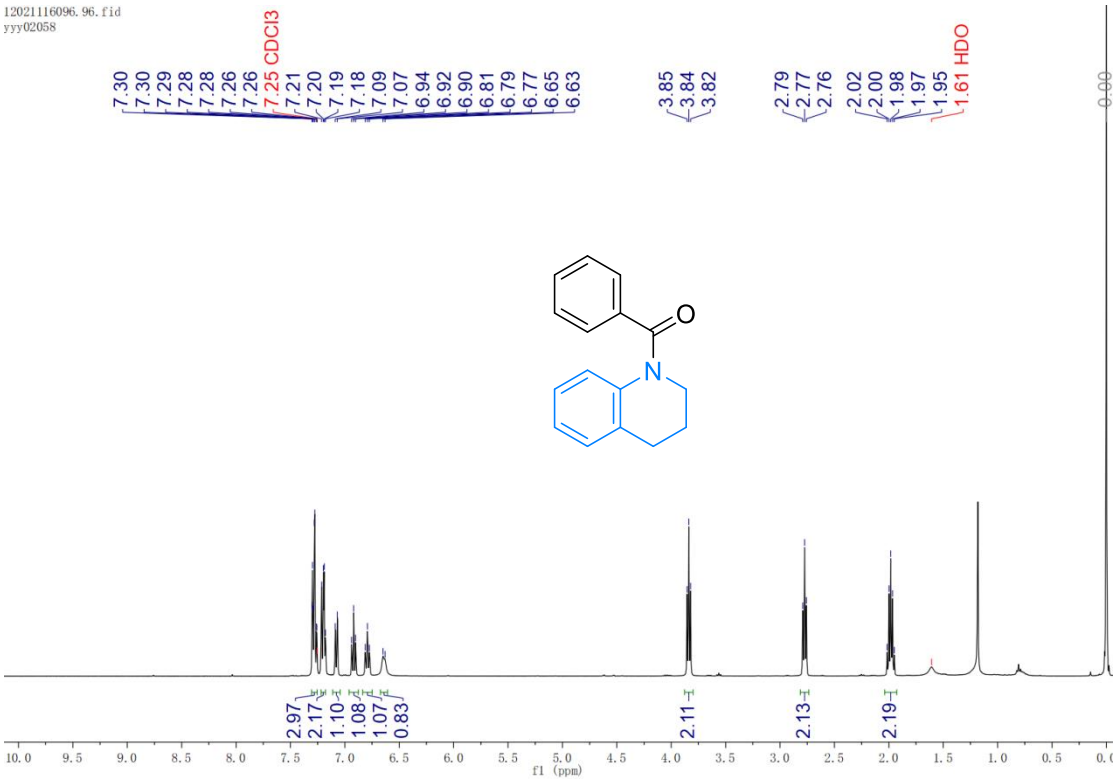
^{13}C-NMR (100 MHz, Chloroform-*d*) **Spectra of compound 3v**



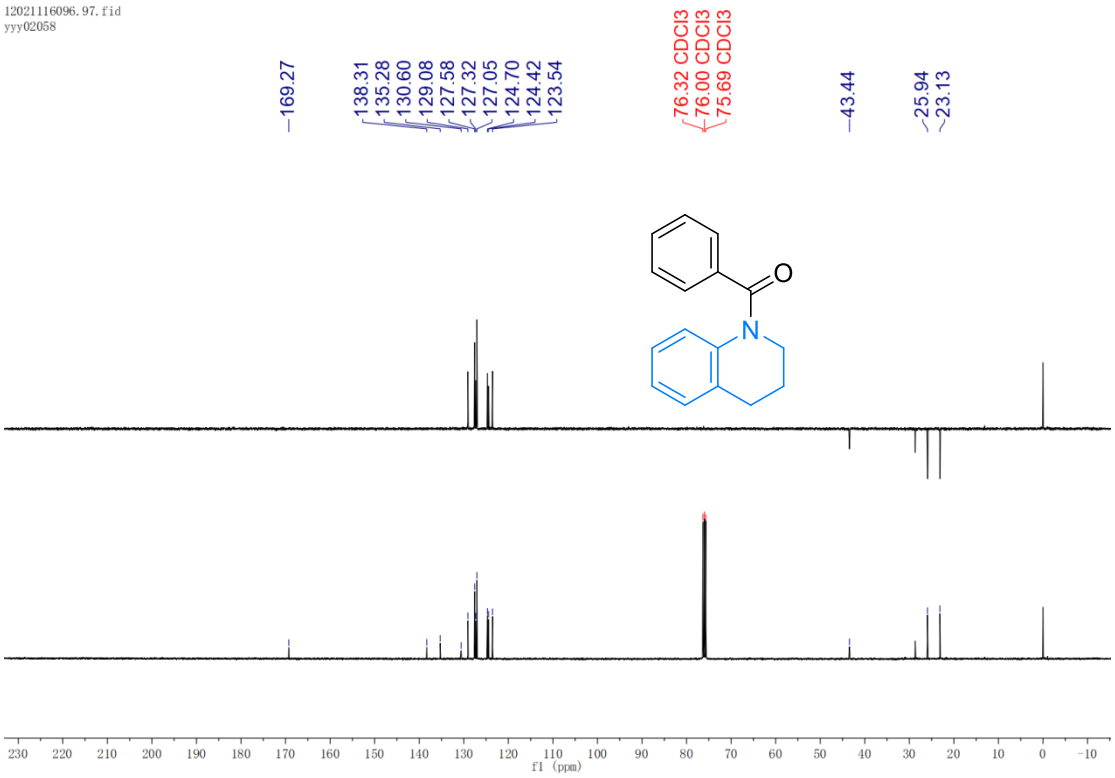
^{1}H-NMR (400 MHz, Chloroform-*d*) **Spectra of compound 3w**



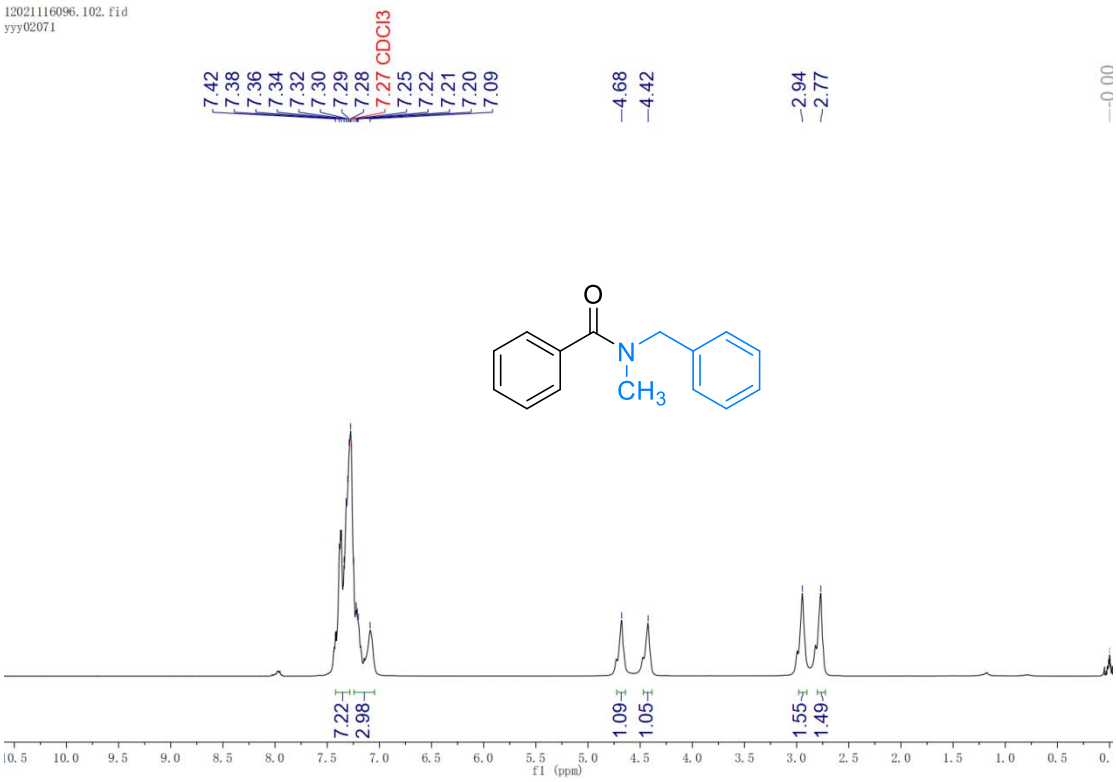
^{13}C-NMR (100 MHz, Chloroform-*d*) **Spectra of compound 3w**



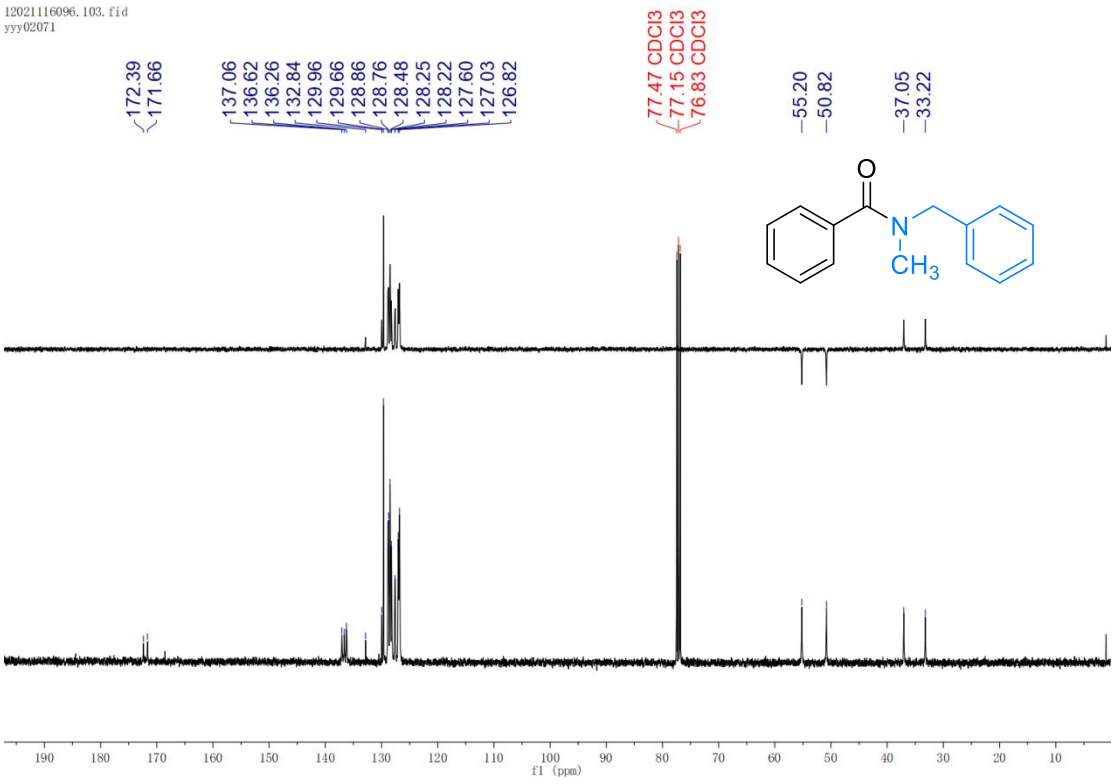
^{1}H-NMR (400 MHz, Chloroform-*d*) **Spectra of compound 3x**



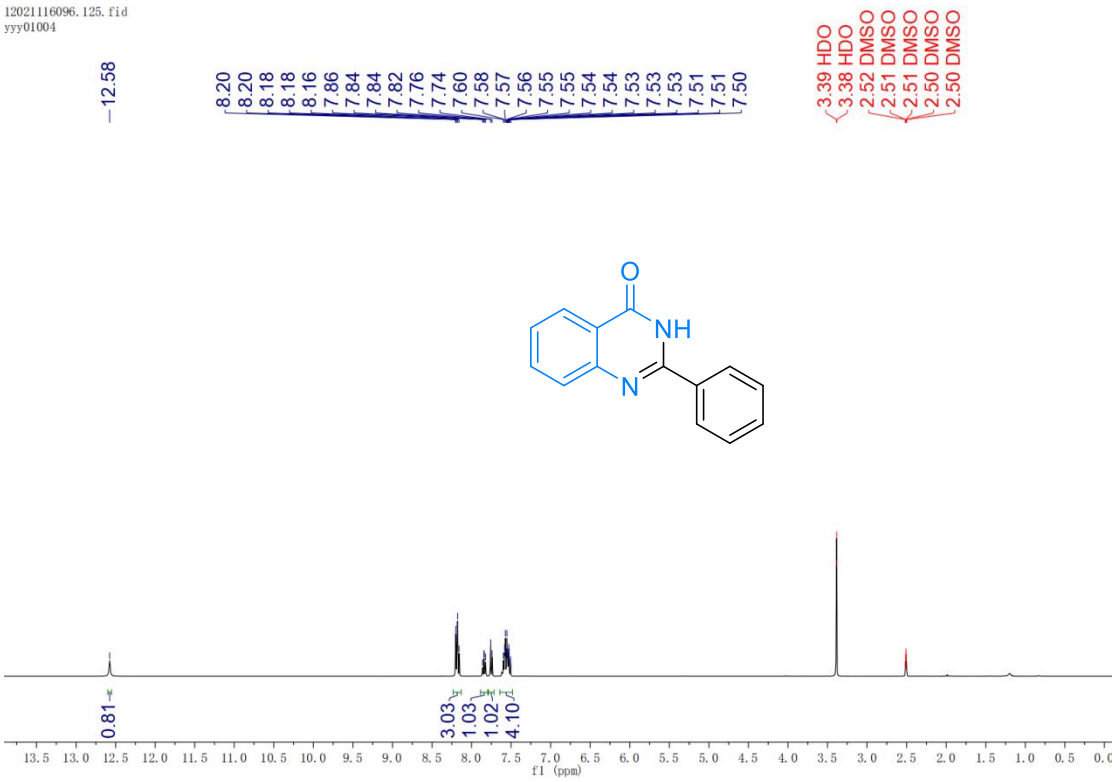
^{13}C-NMR (100 MHz, Chloroform-*d*) **Spectra of compound 3x**



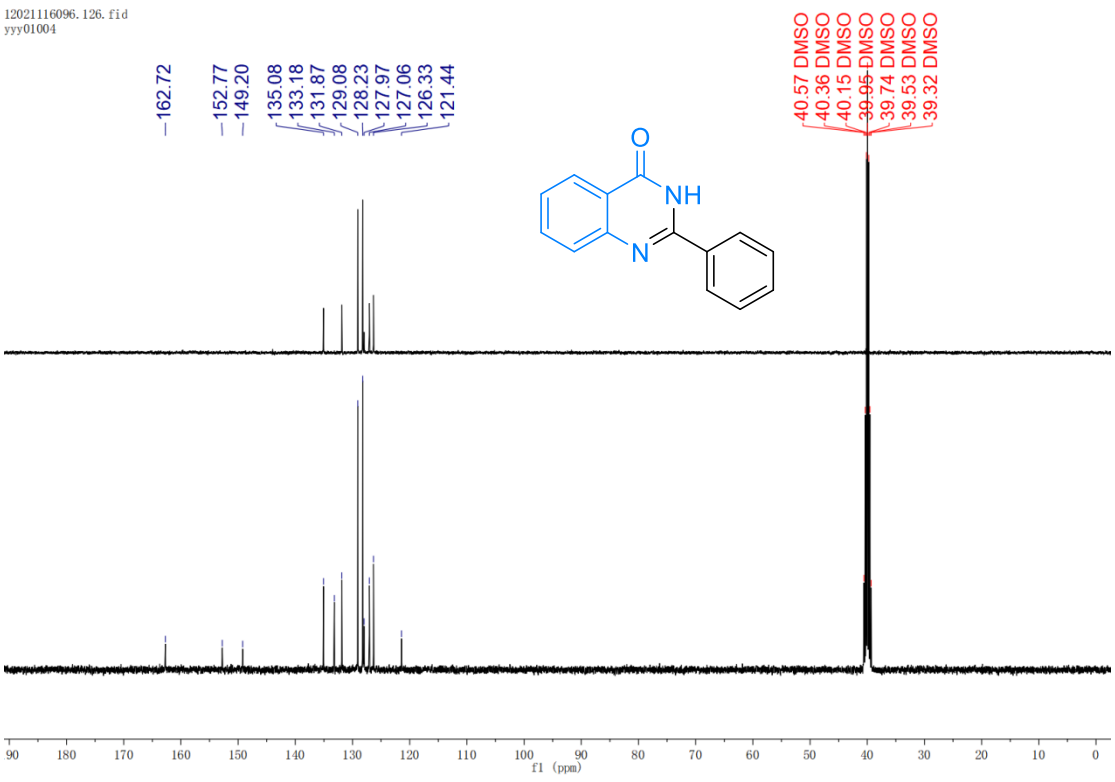
^{1}H-NMR (400 MHz, Chloroform-*d*) **Spectra of compound 3y**



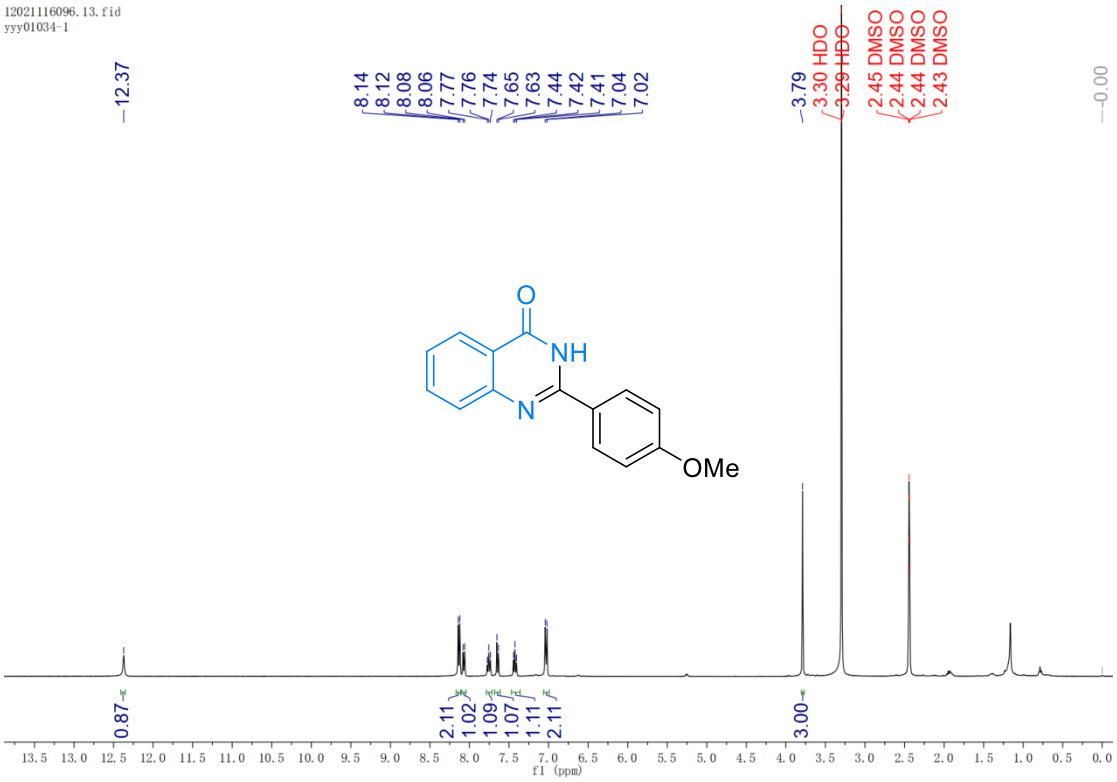
^{13}C-NMR (100 MHz, Chloroform-*d*) **Spectra of compound 3y**



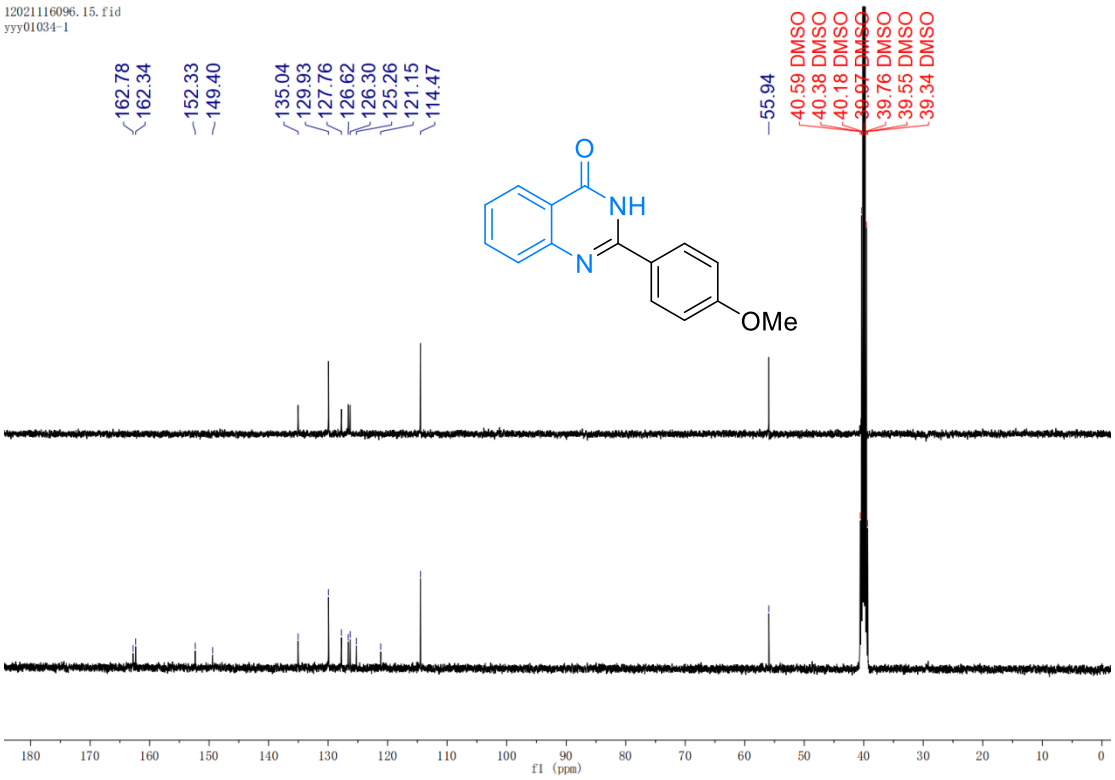
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 5a**



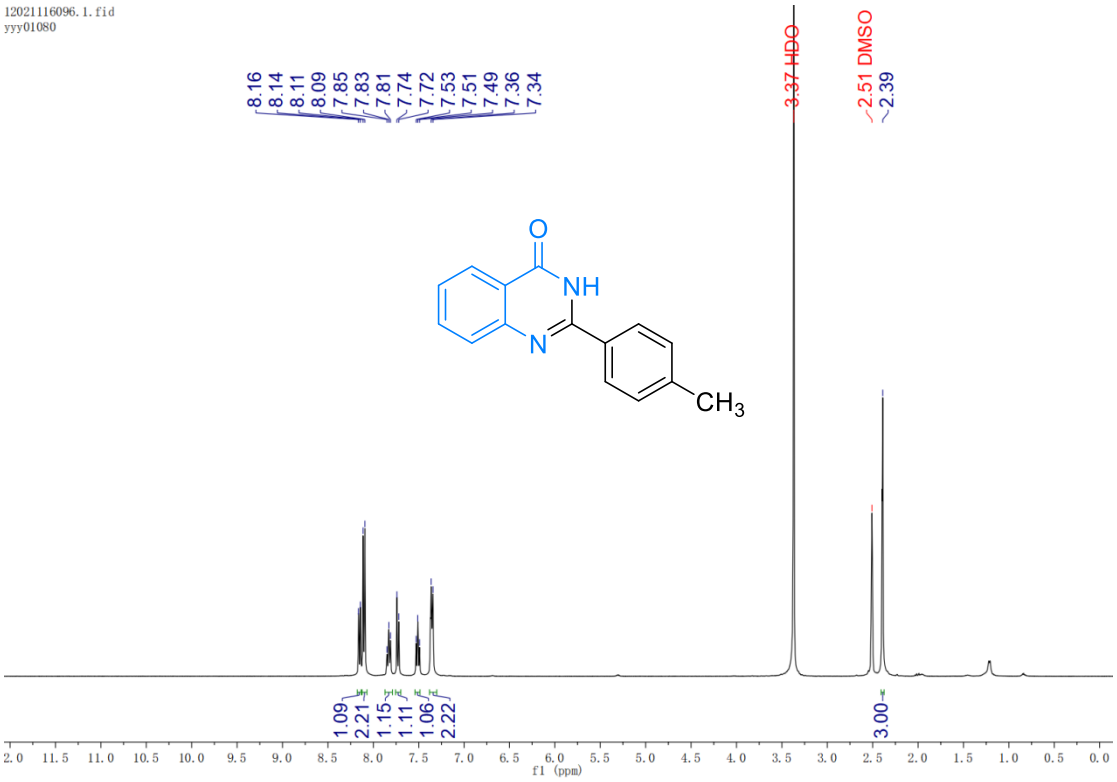
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 5a**



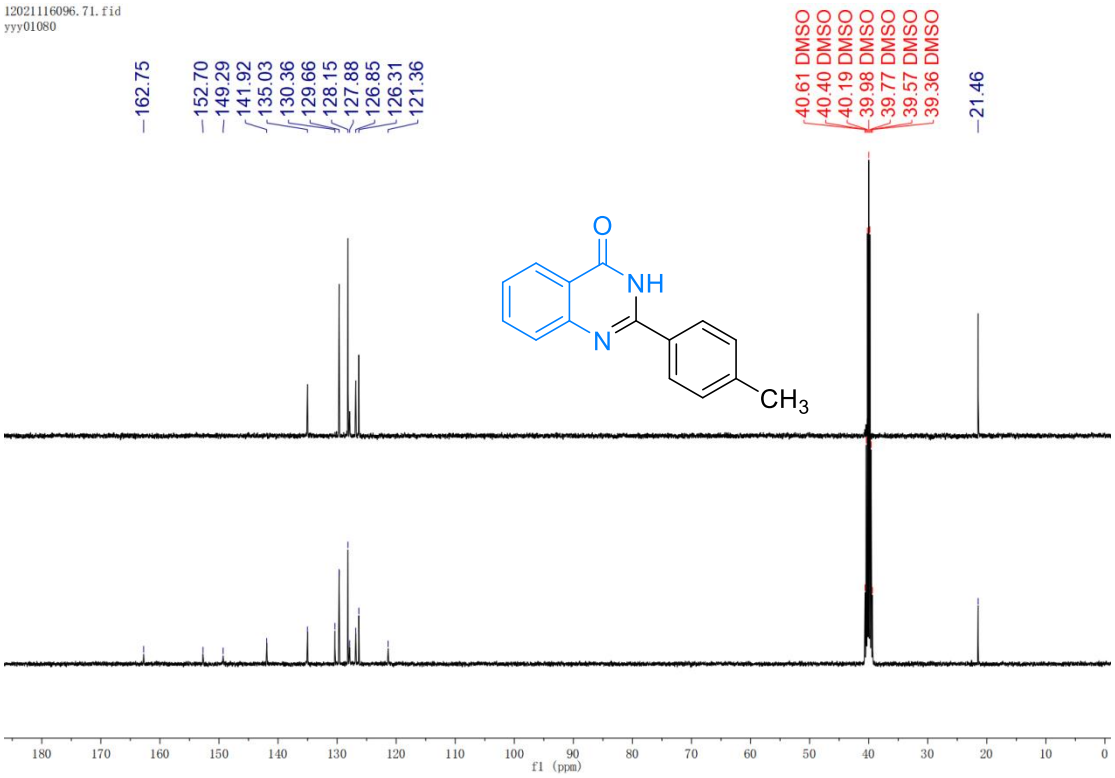
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 5b**



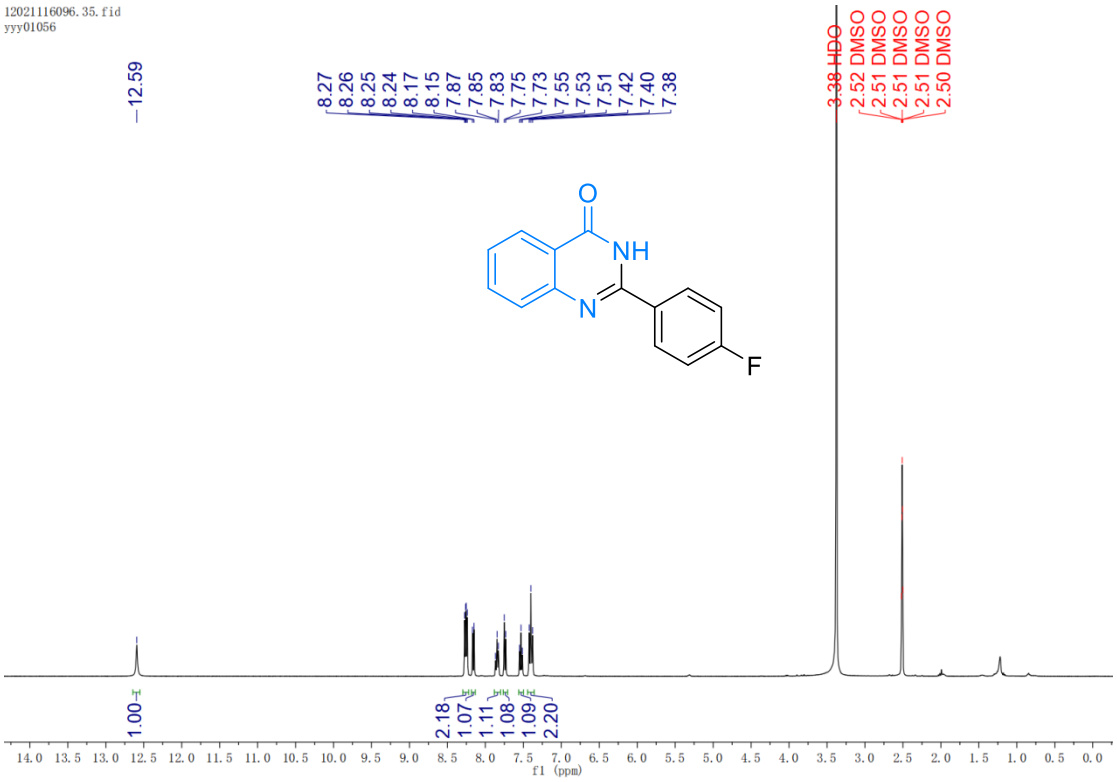
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 5b**



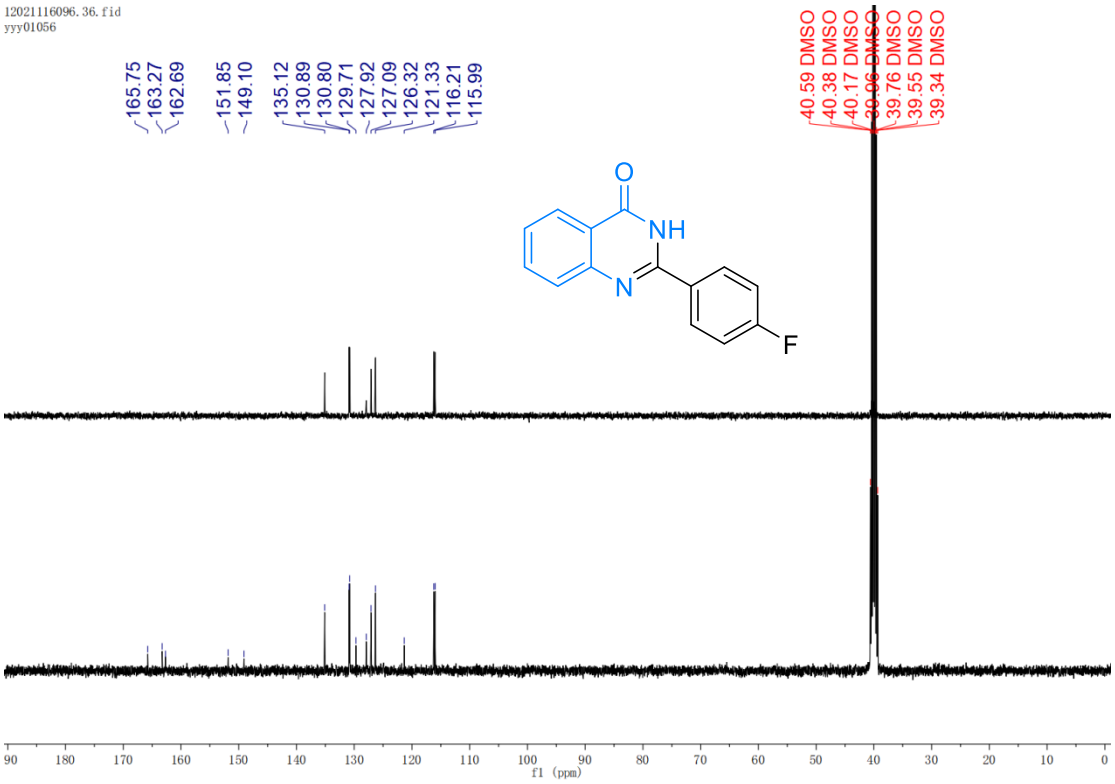
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 5c**



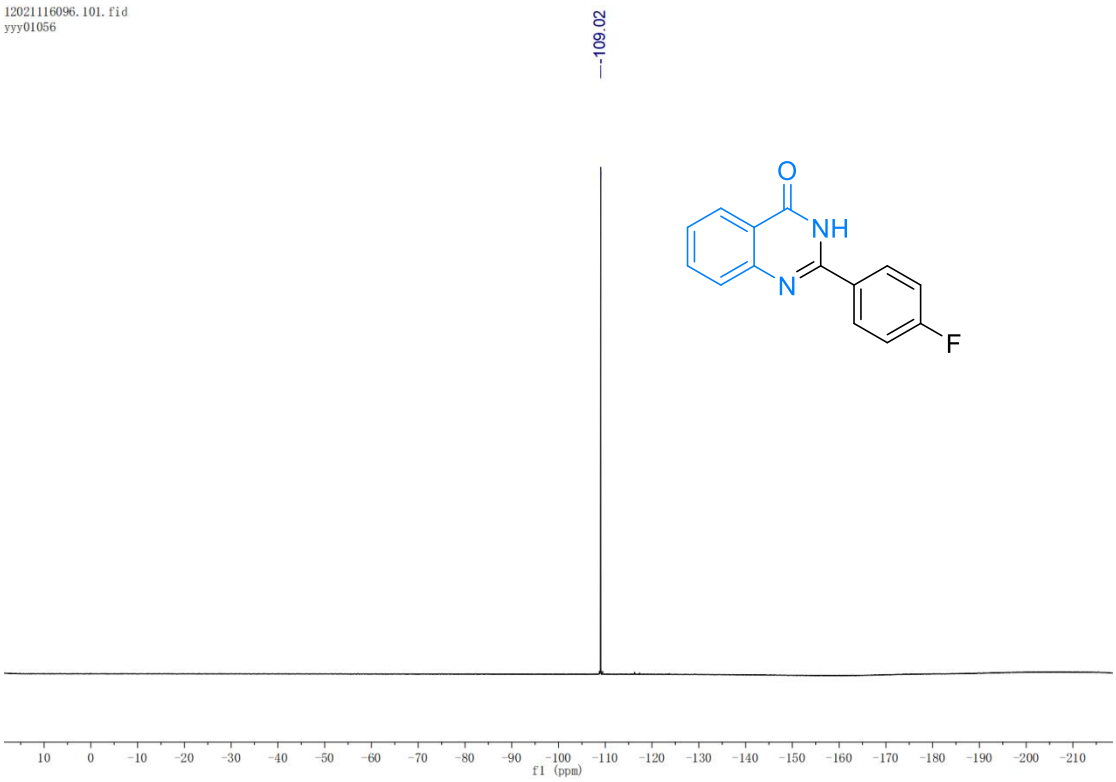
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 5c**



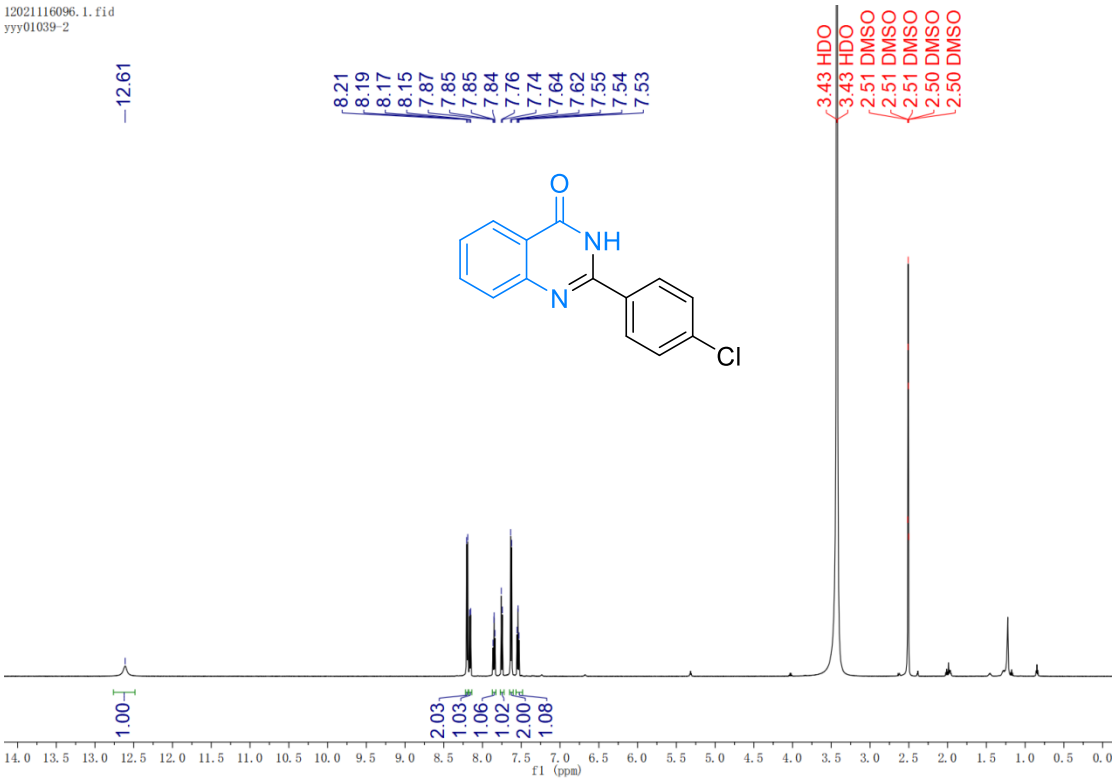
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 5d**



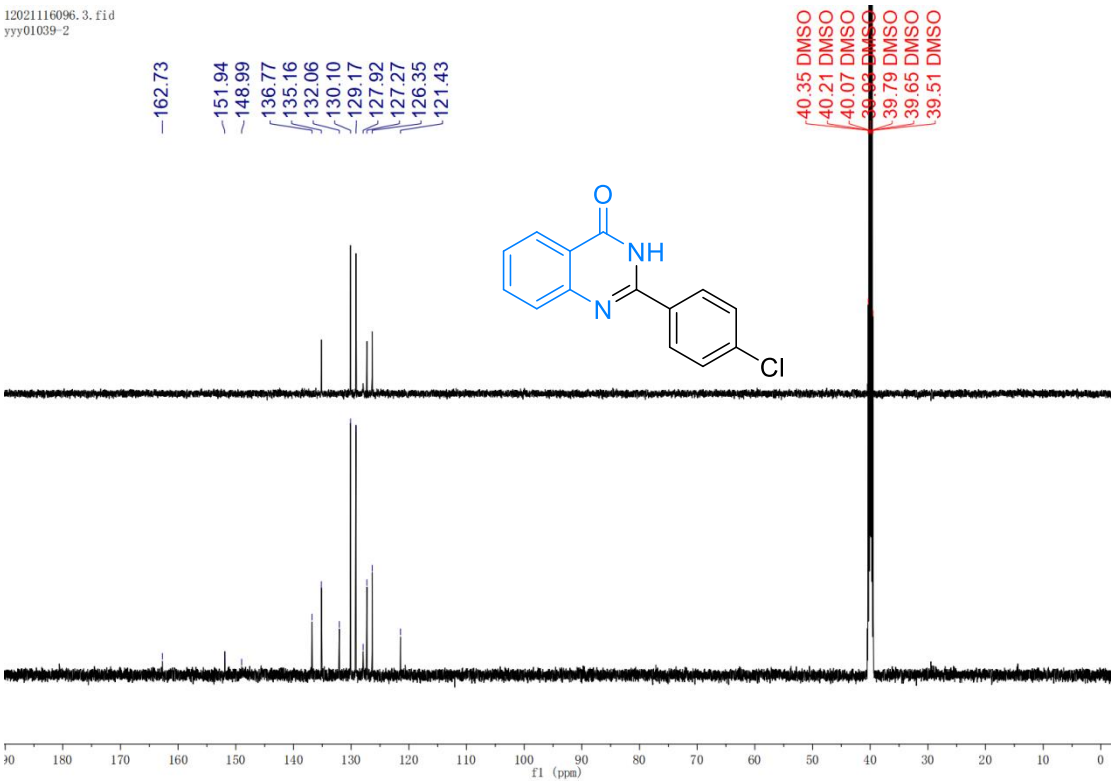
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 5d**



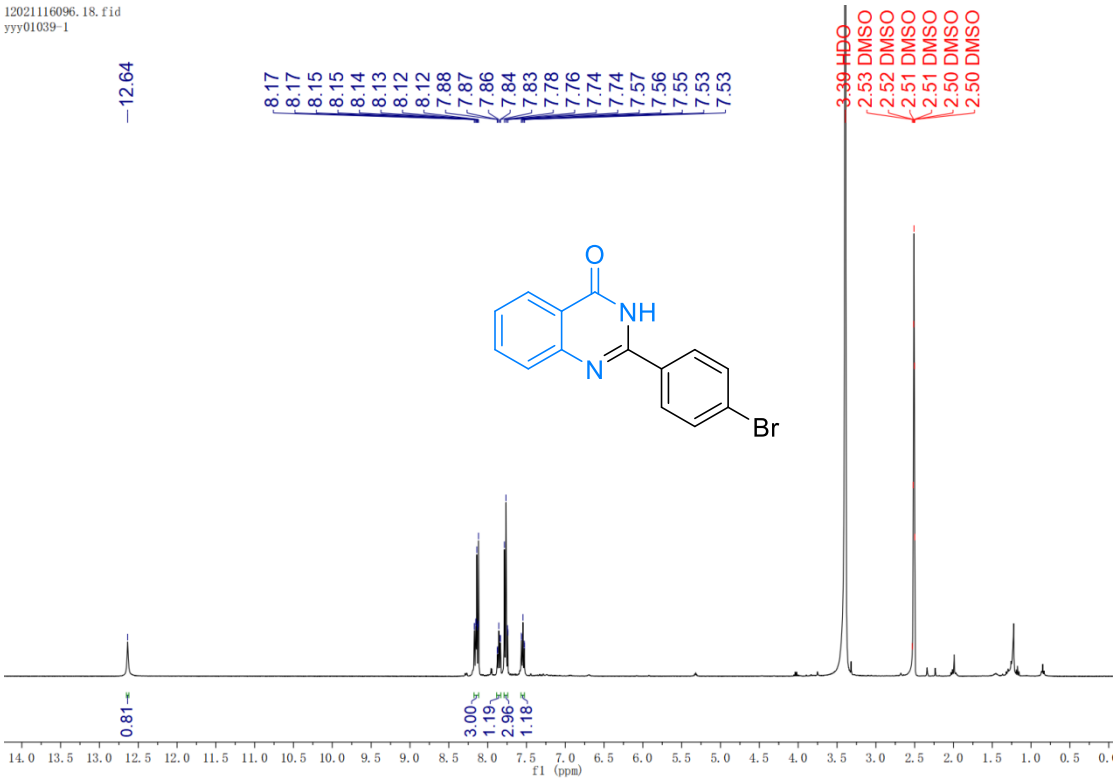
^{19}F NMR (376 MHz, DMSO-d_6) S**pectrum of compound 5d**



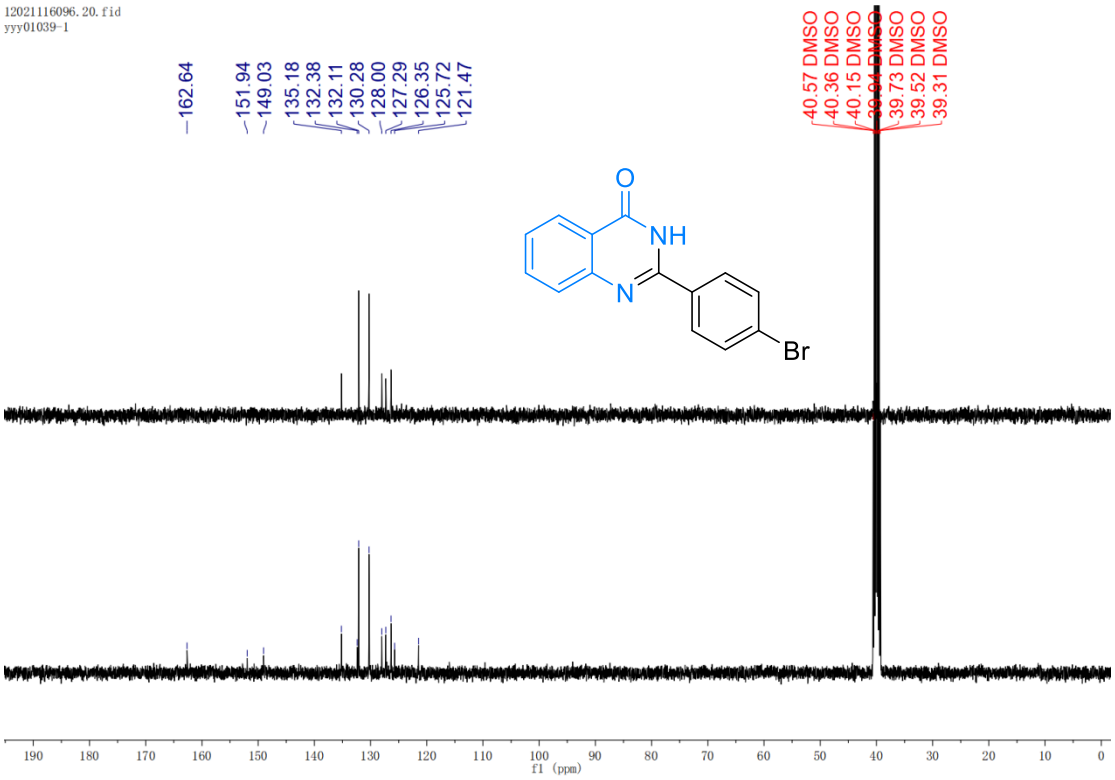
^{1}H-NMR (600 MHz, DMSO-d_6) **Spectra of compound 5e**



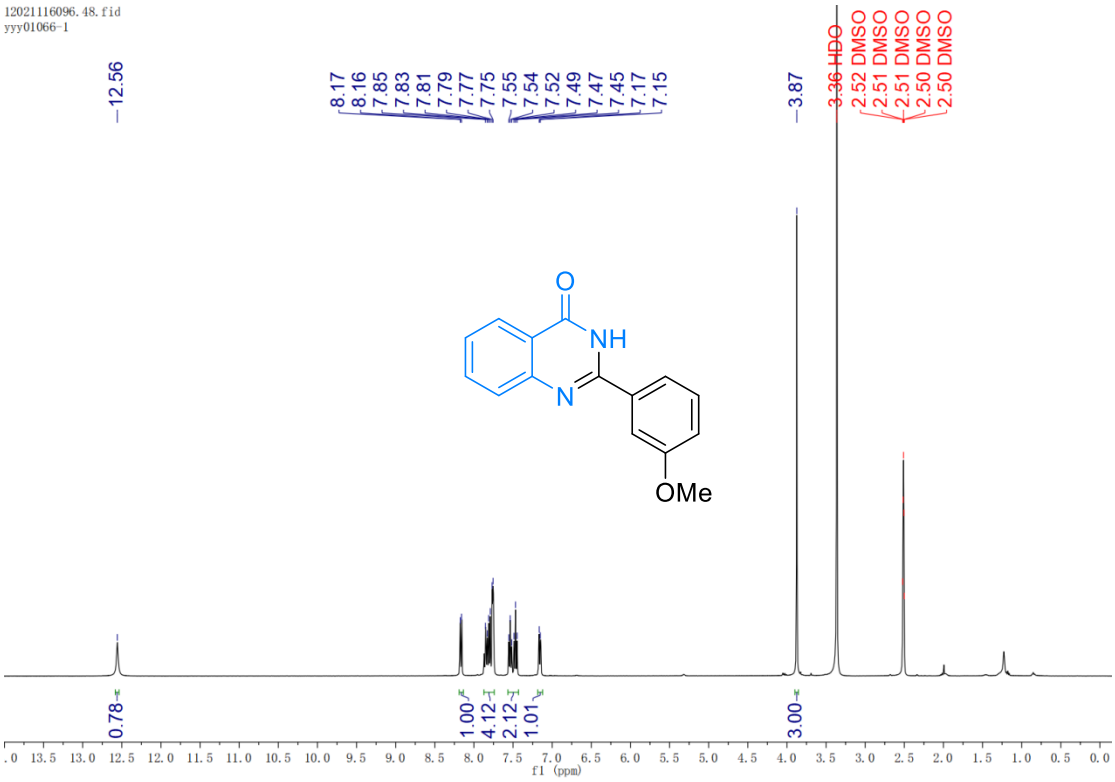
^{13}C-NMR (150 MHz, DMSO-d_6) **Spectra of compound 5e**



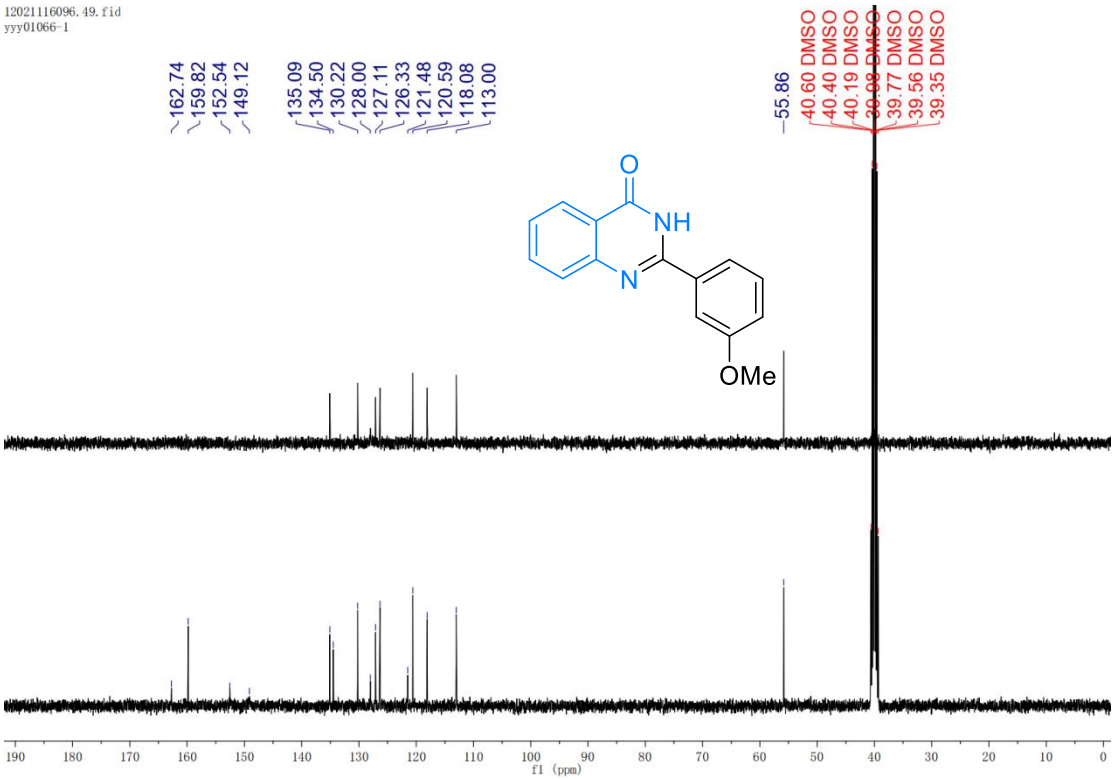
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 5f**



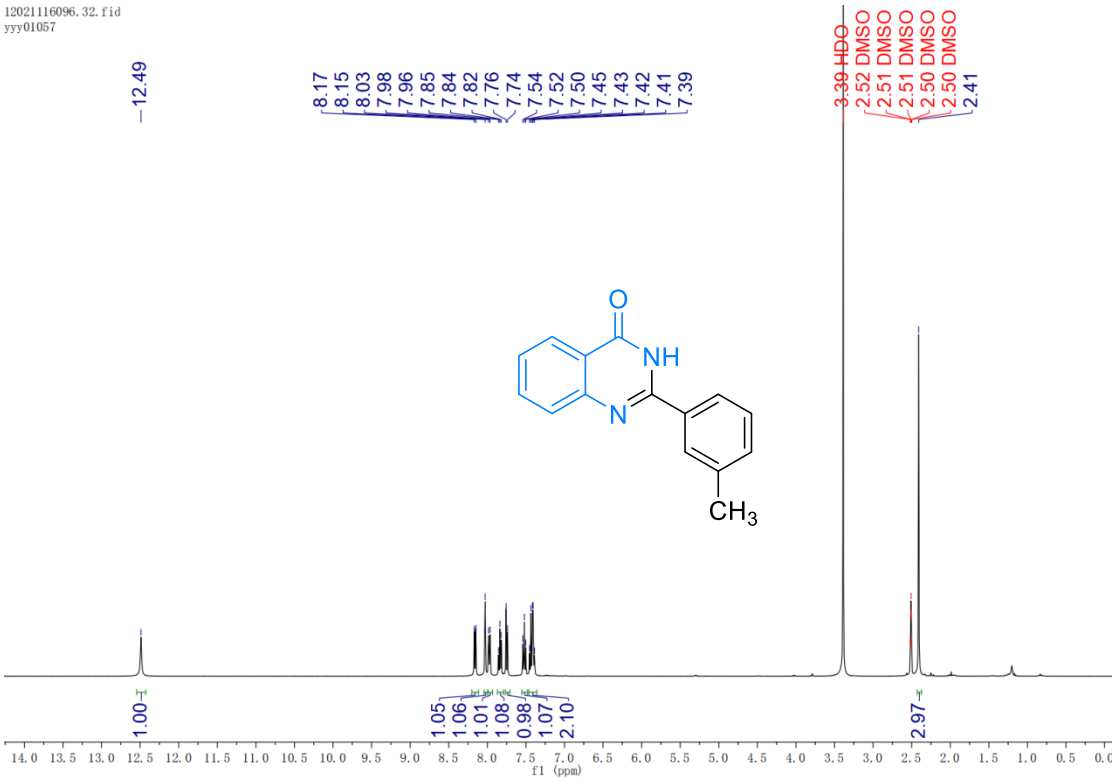
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 5f**



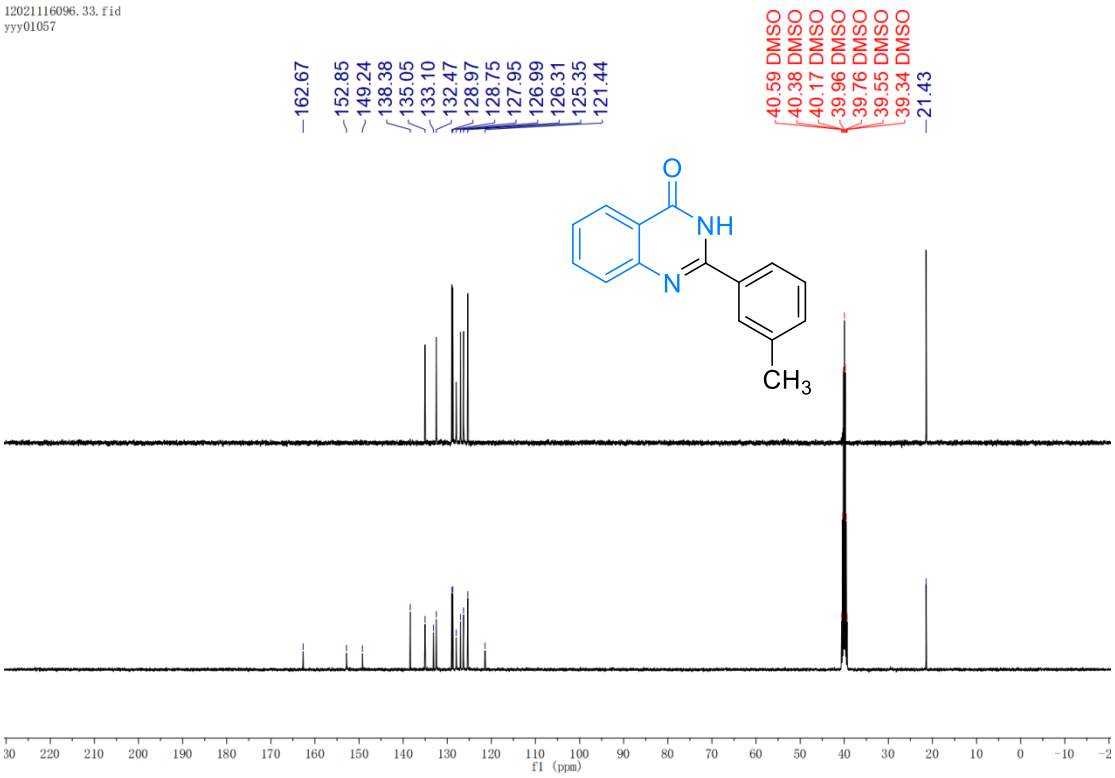
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 5g**



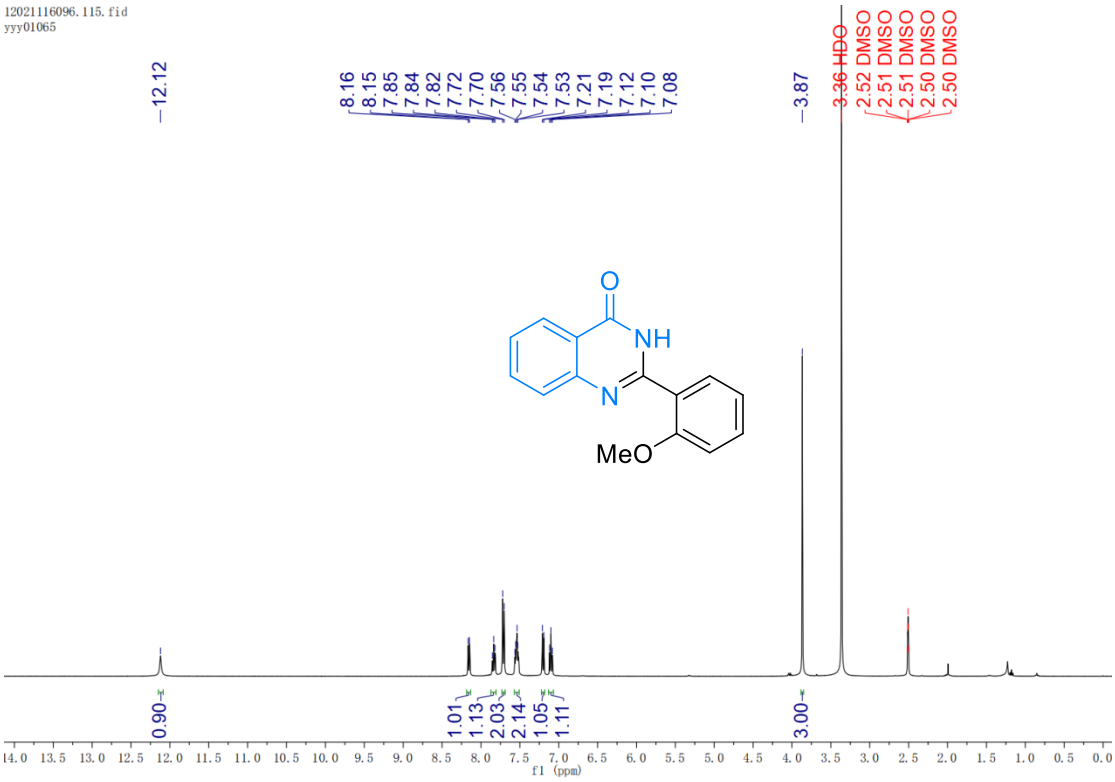
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 5g**



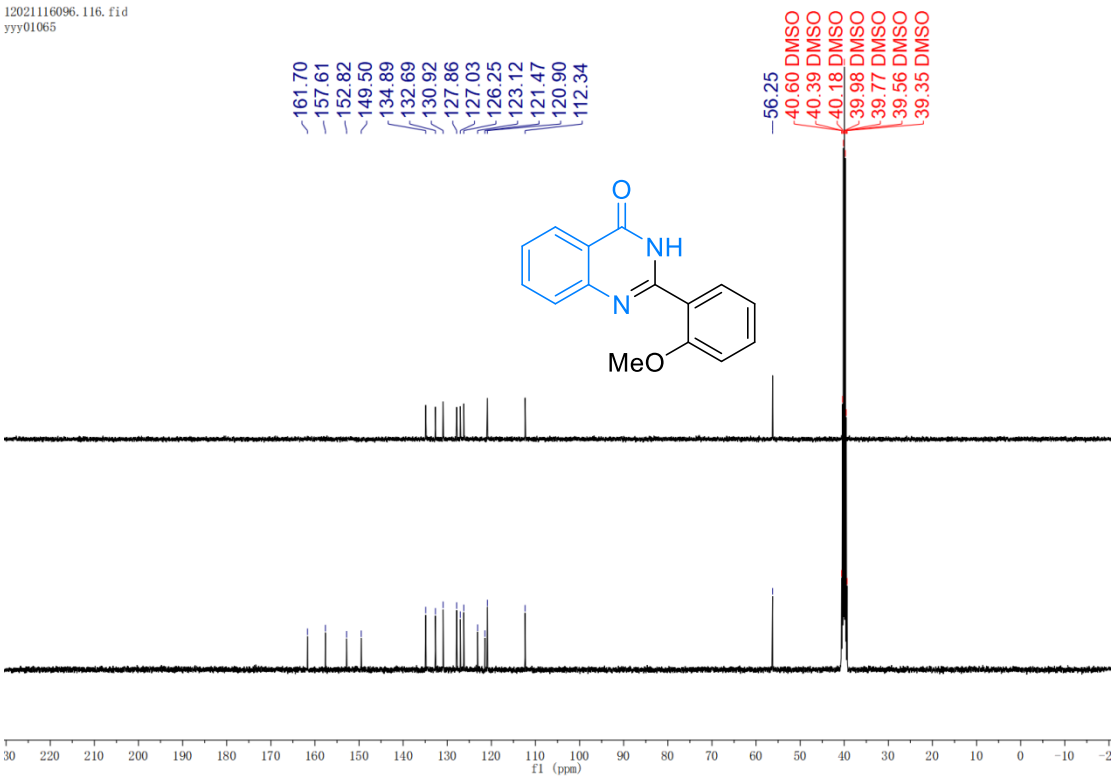
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 5h**



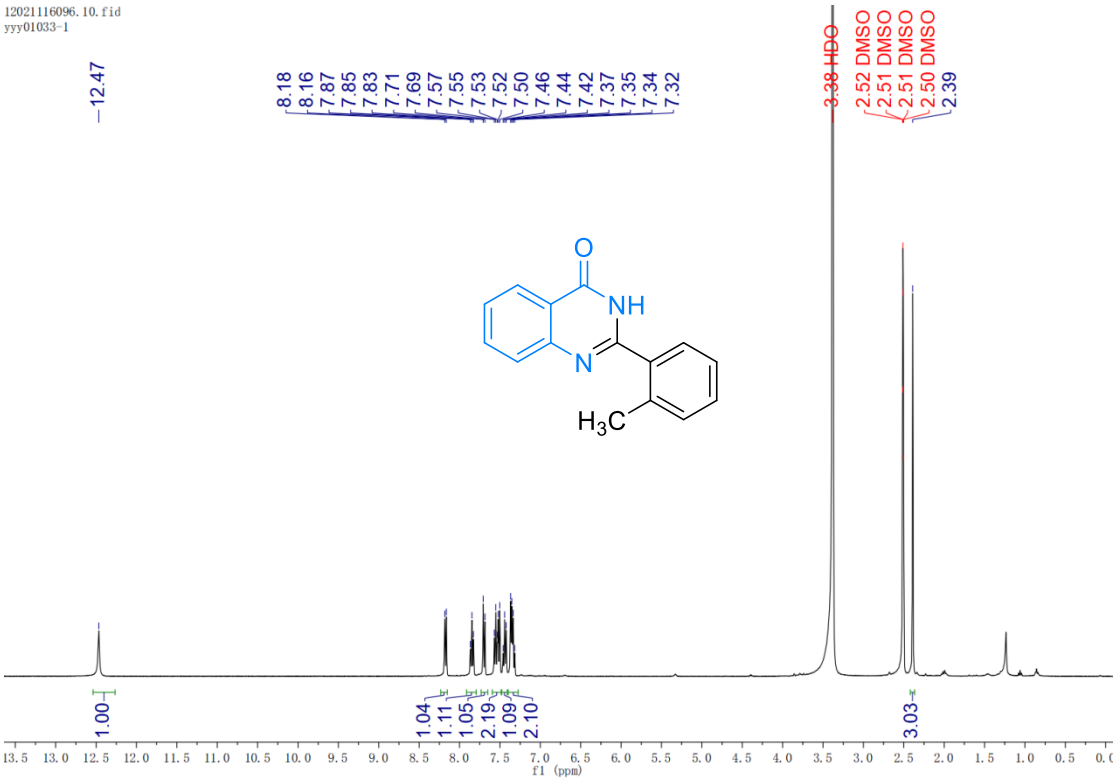
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 5h**



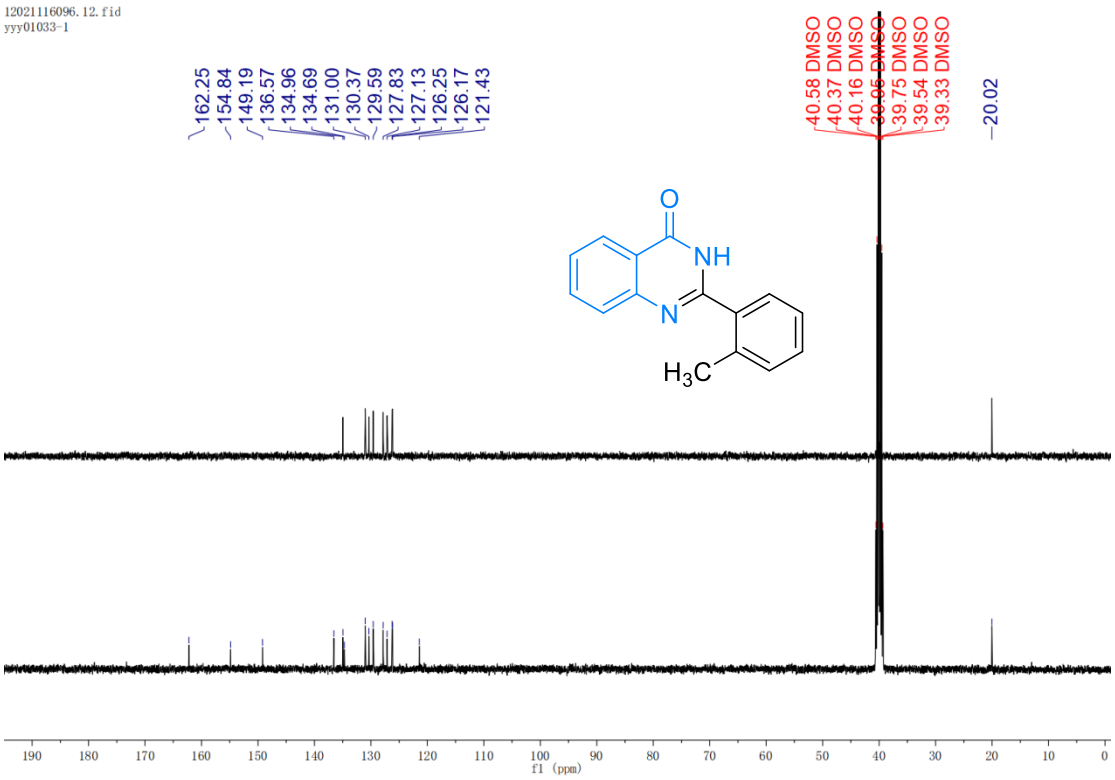
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 5i**



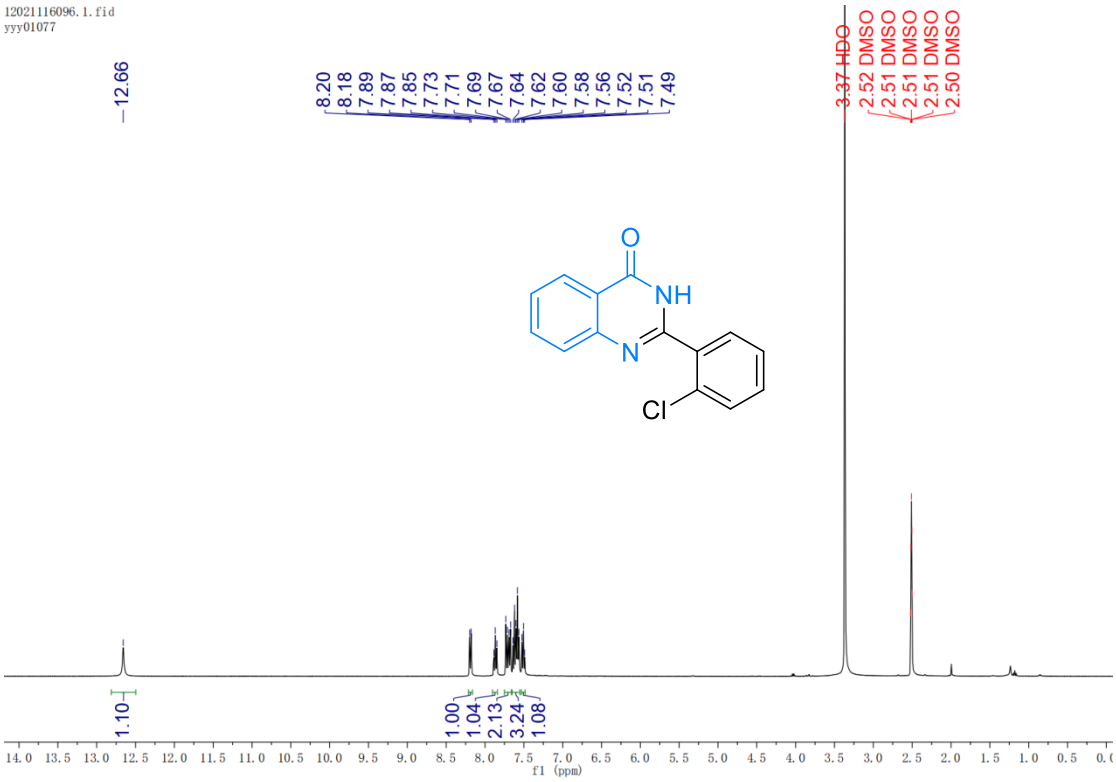
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 5i**



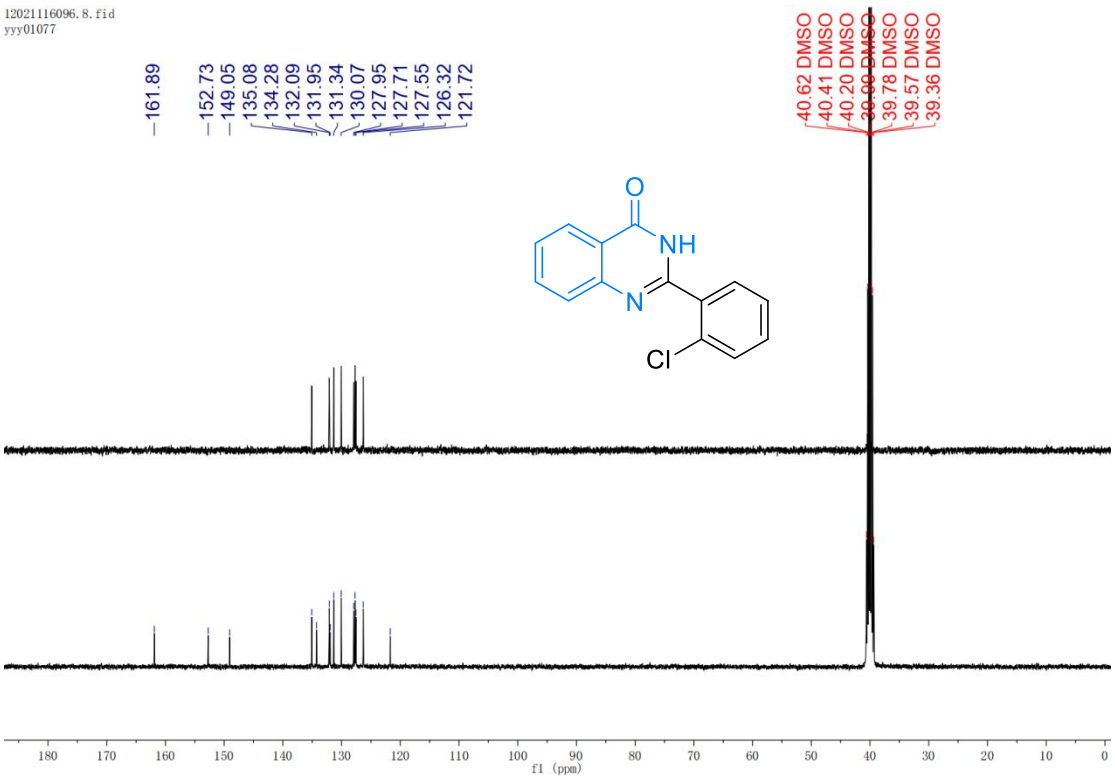
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 5j**



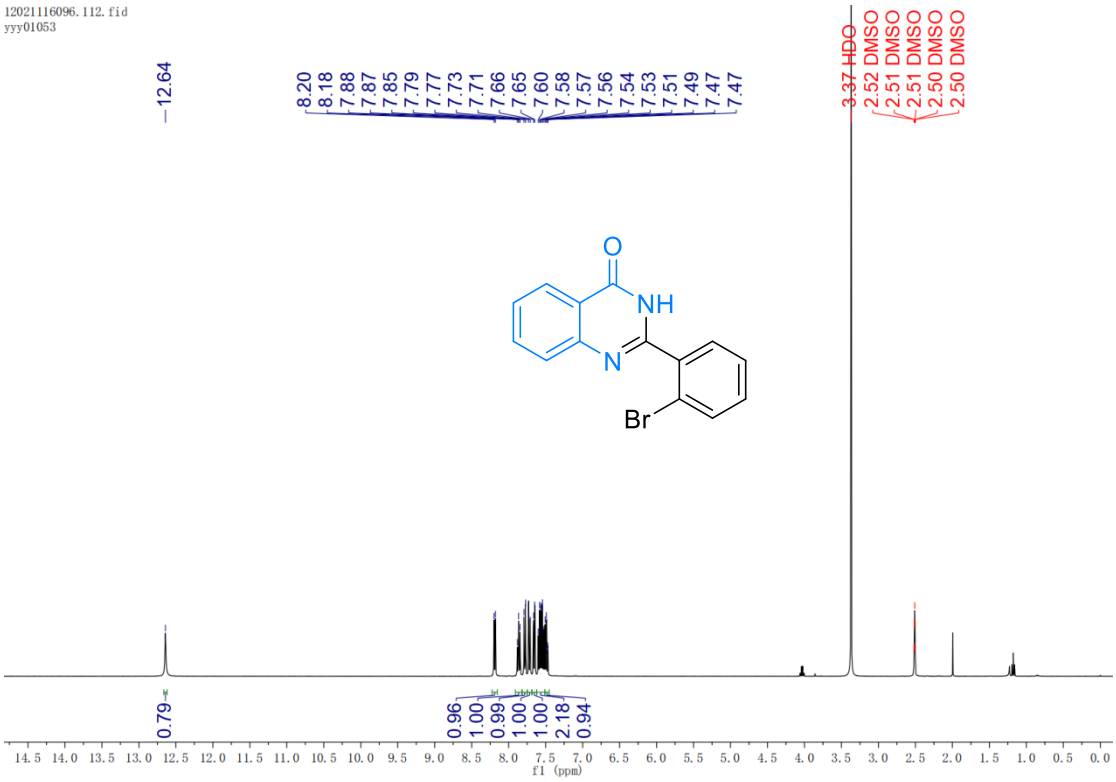
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 5j**



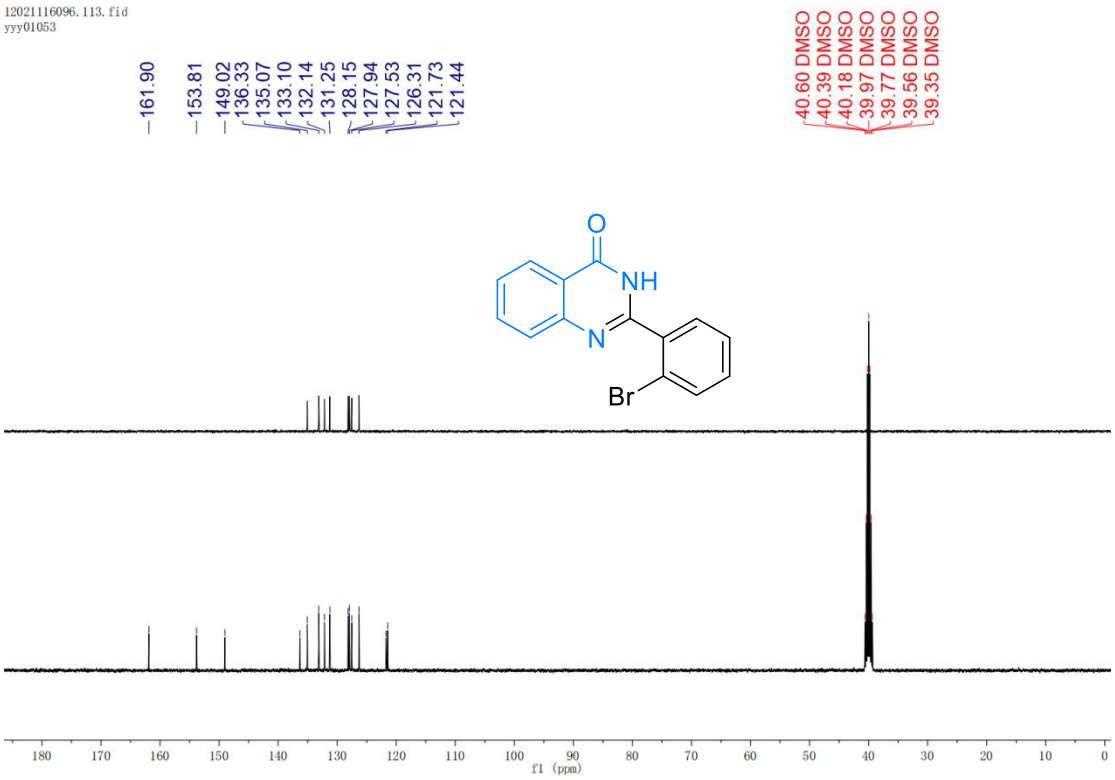
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 5k**



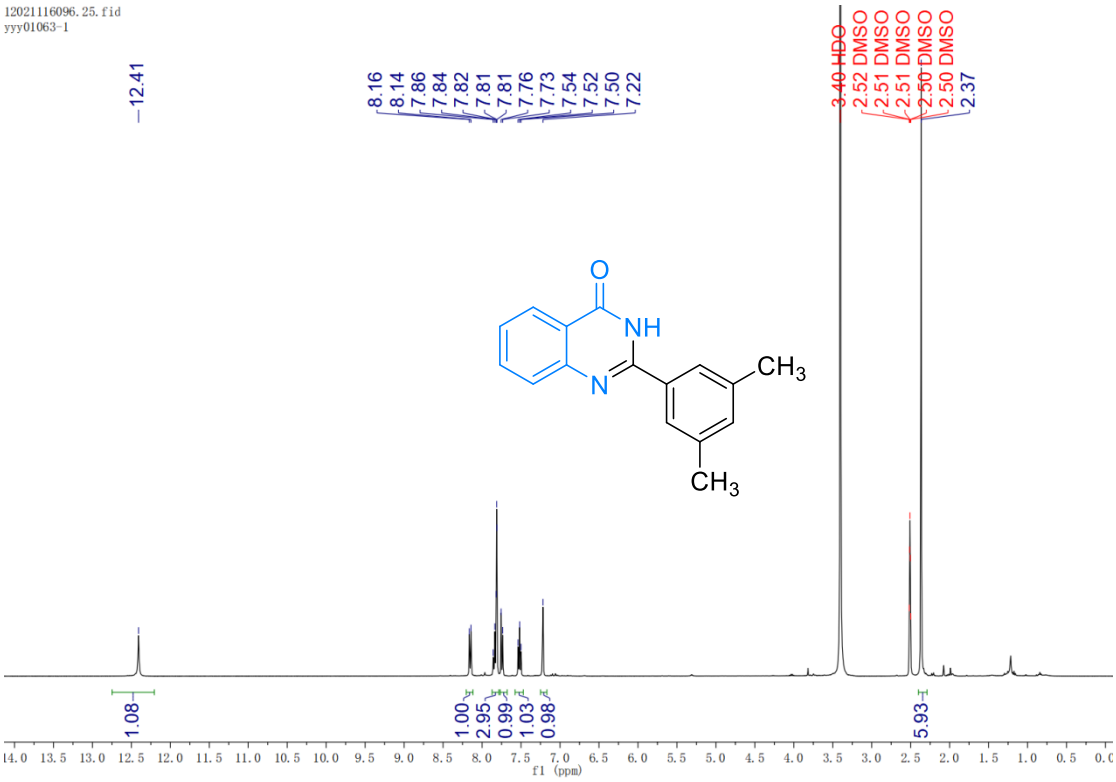
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 5k**



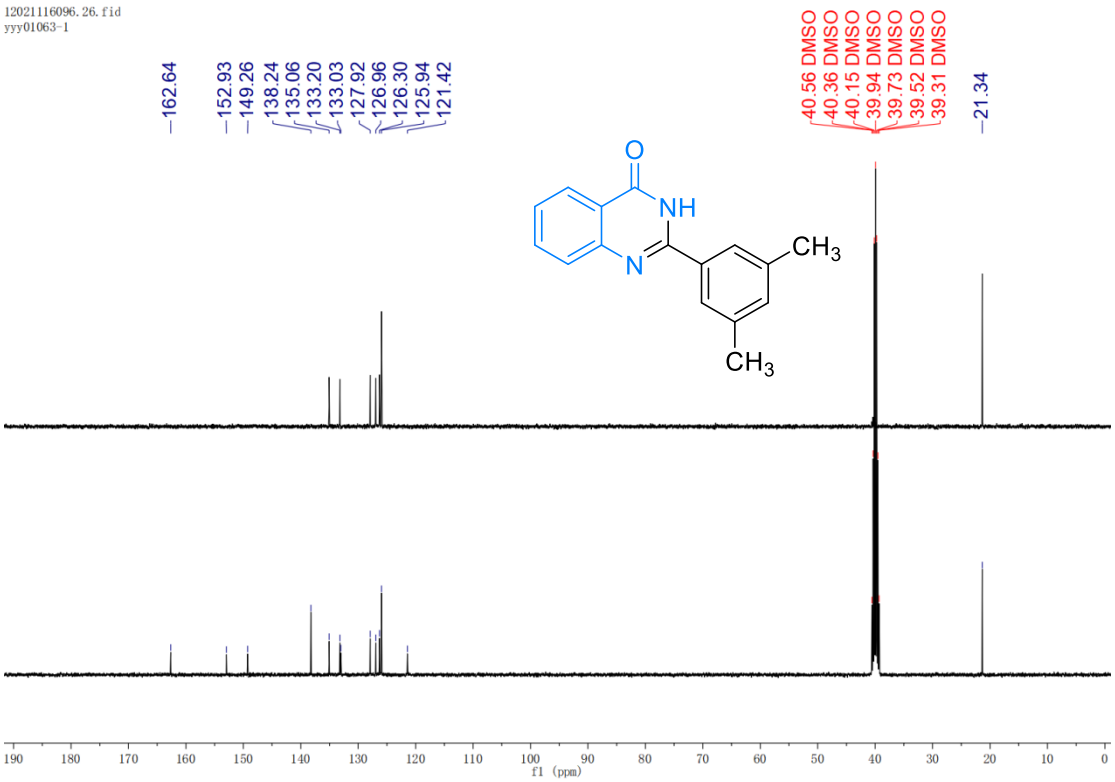
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 5l**



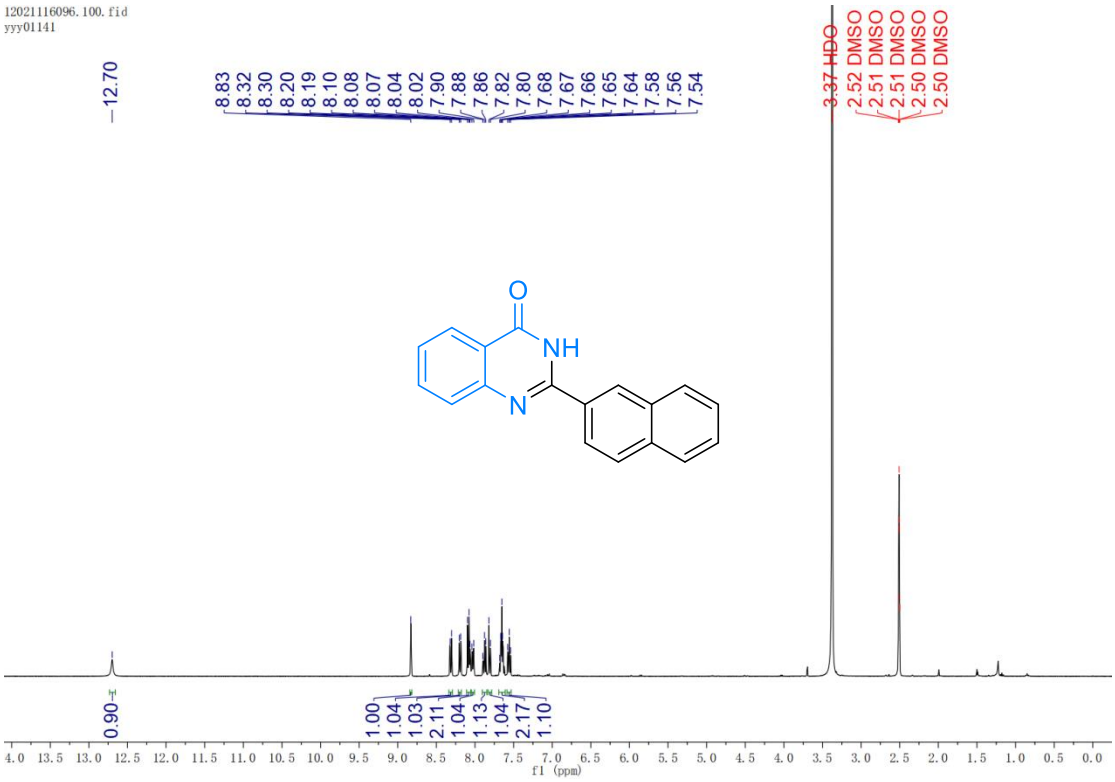
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 5l**



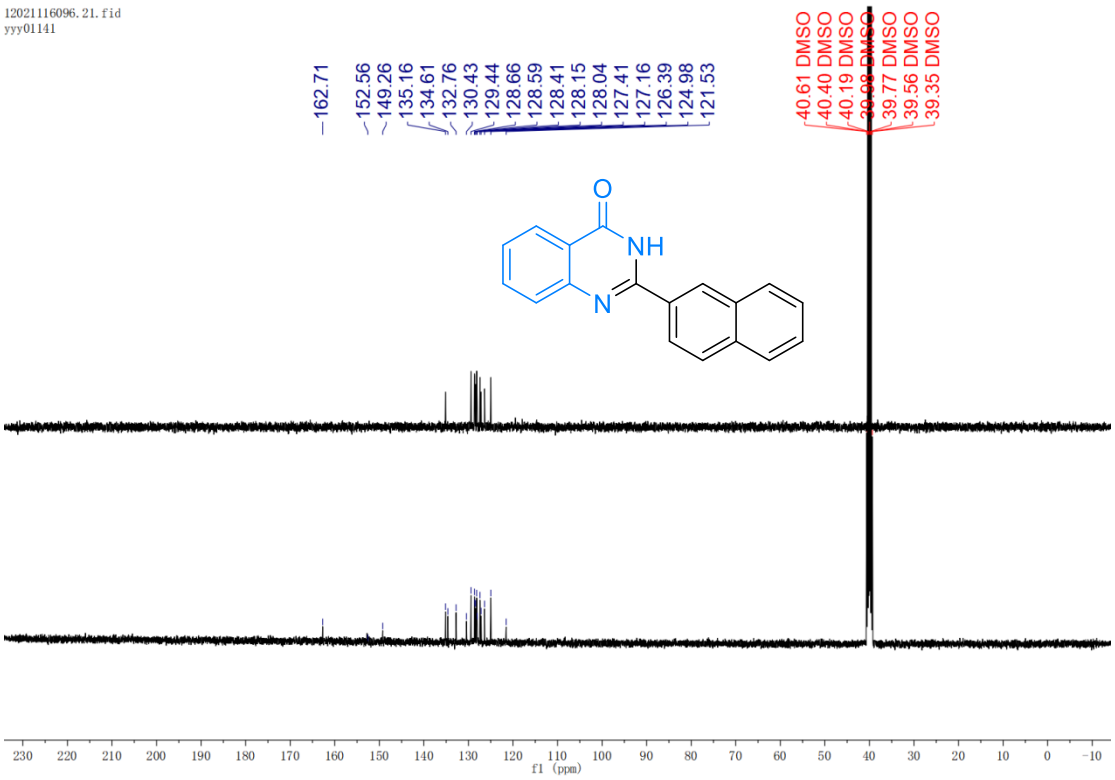
[1]H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 5m**



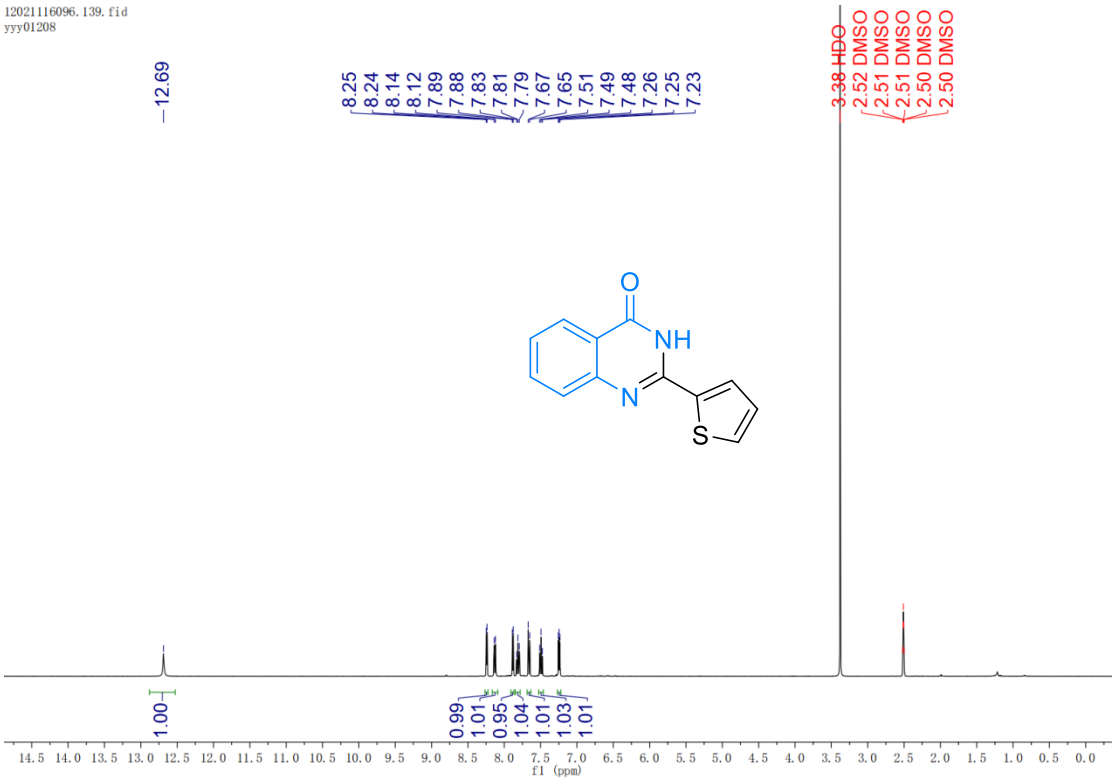
[13]C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 5m**



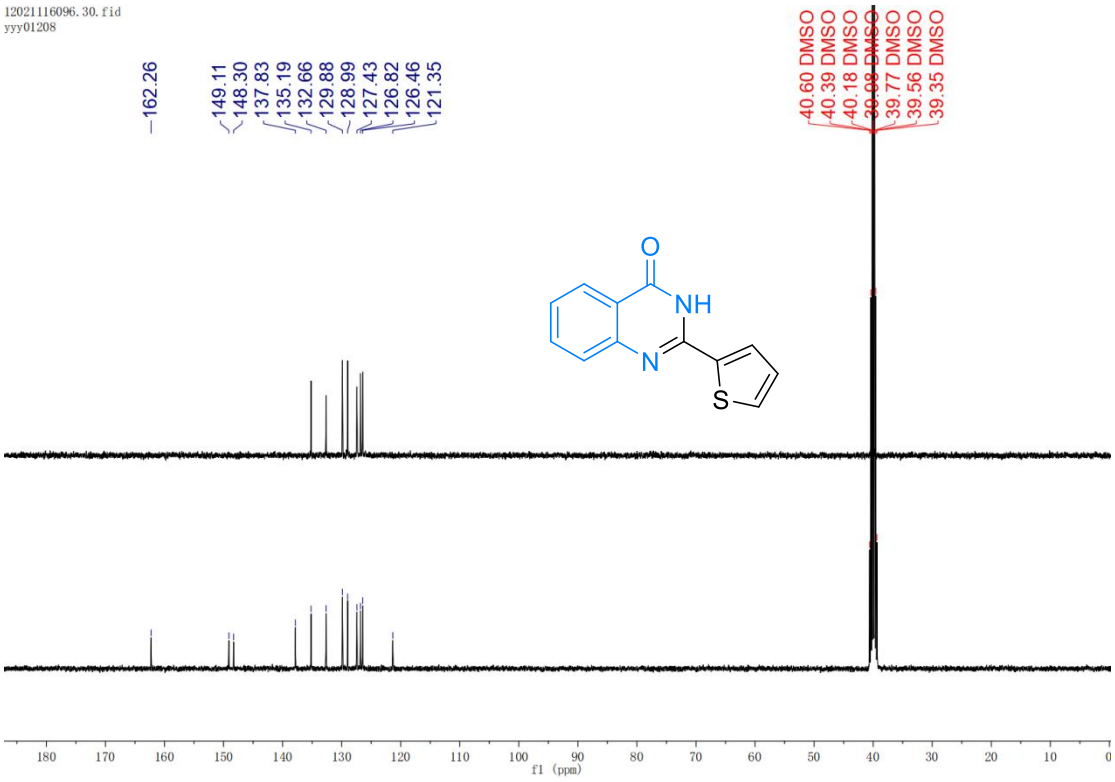
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 5n**



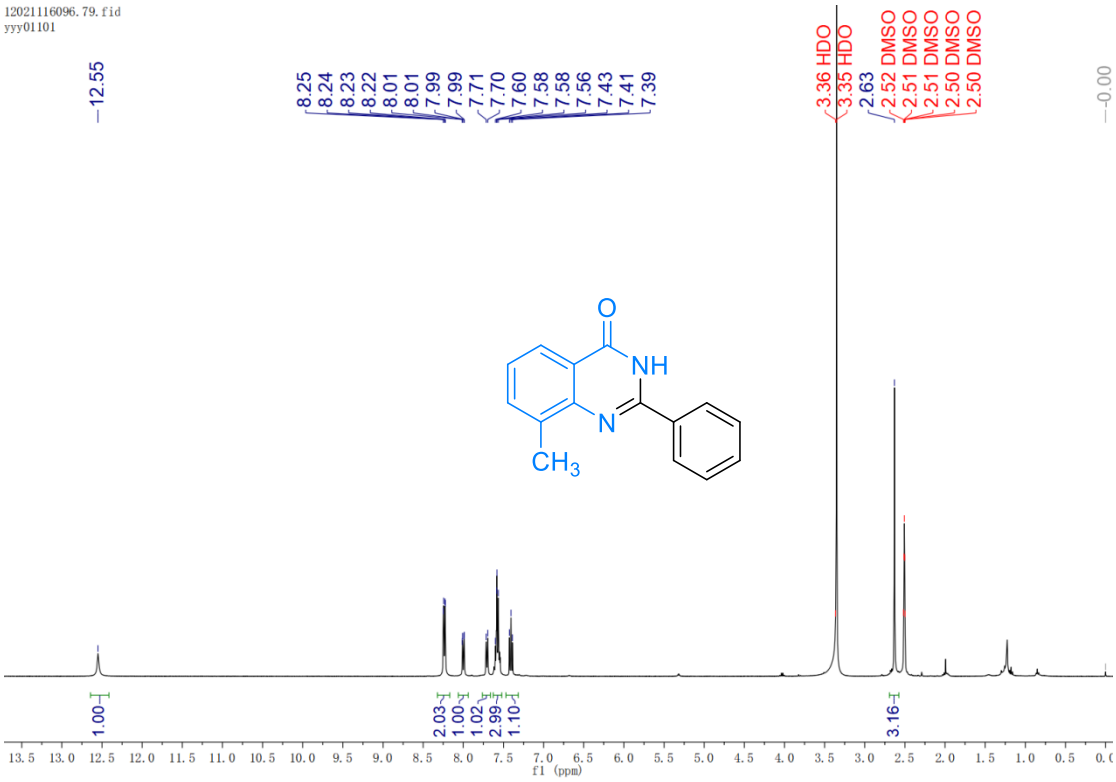
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 5n**



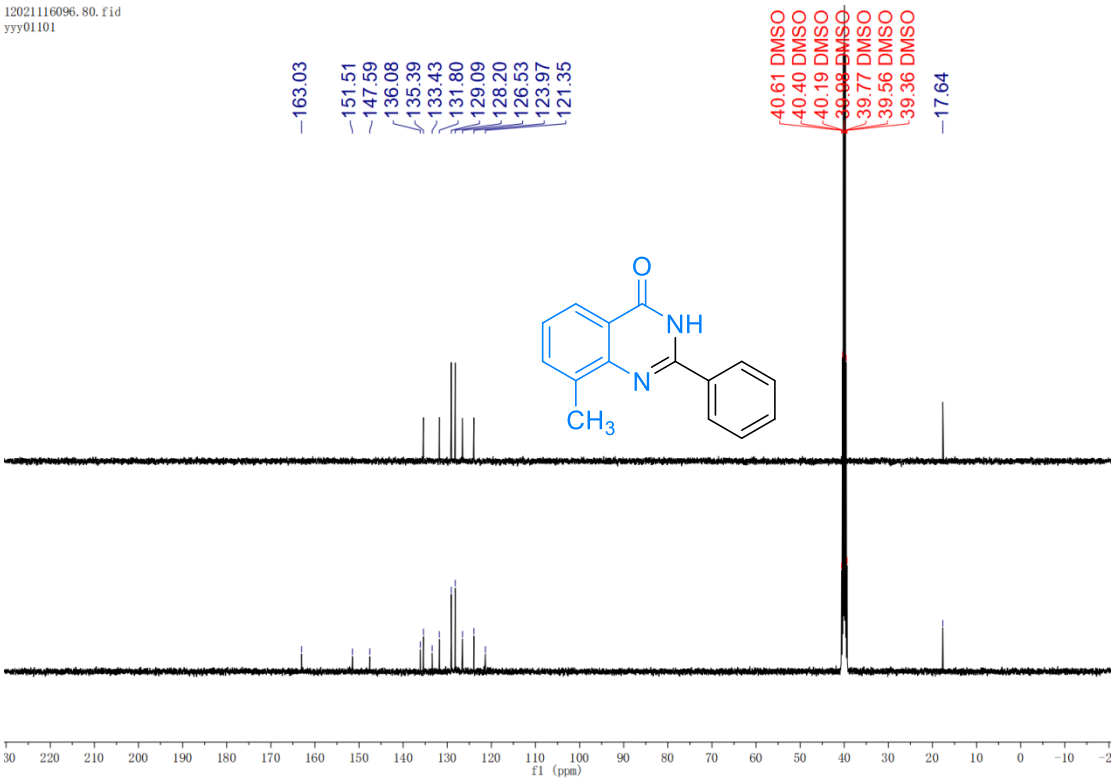
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 5o**



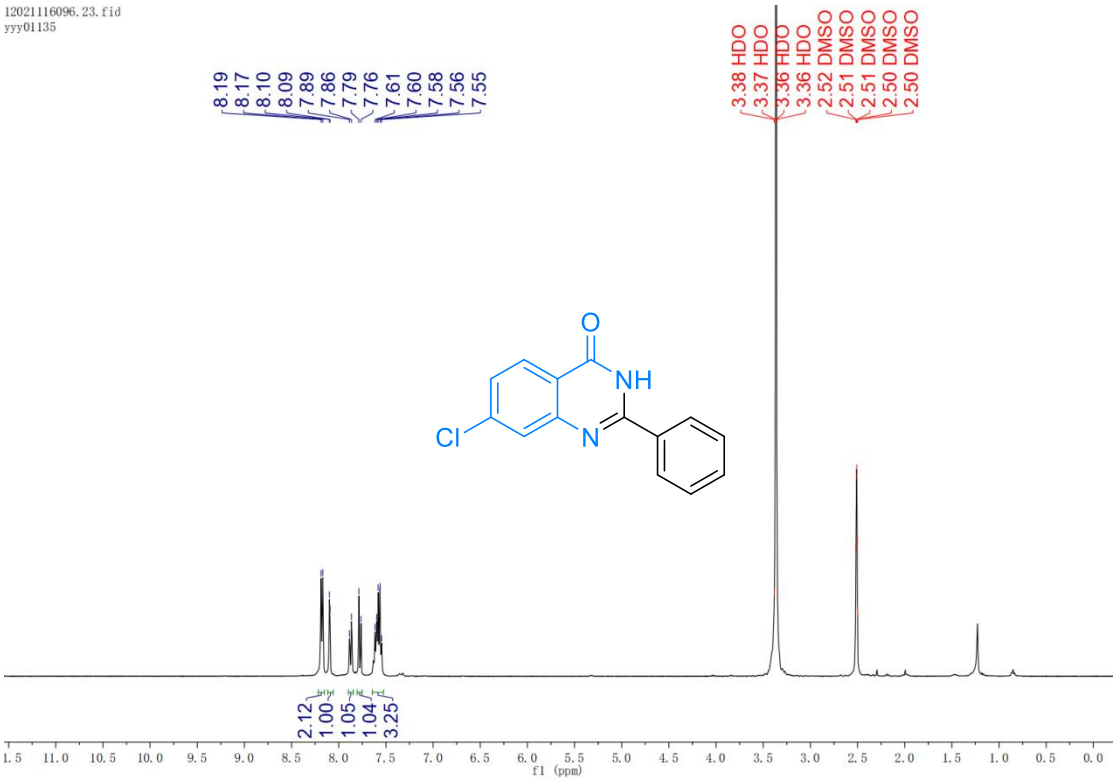
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 5o**



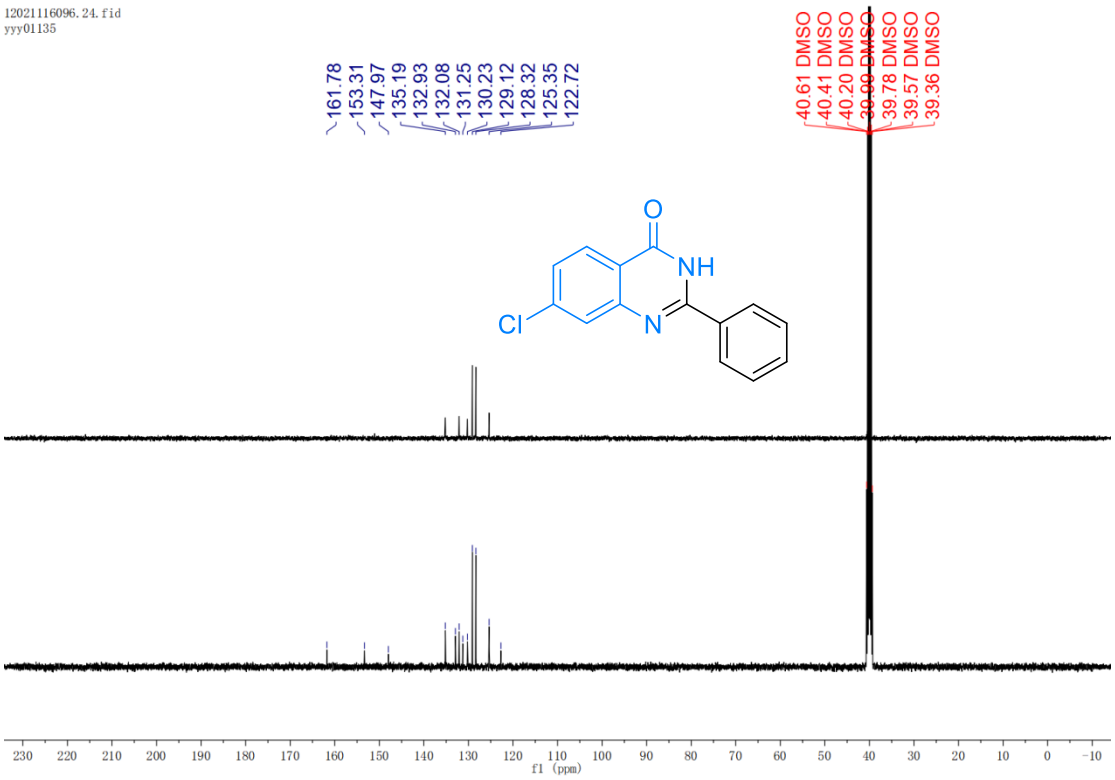
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 5p**



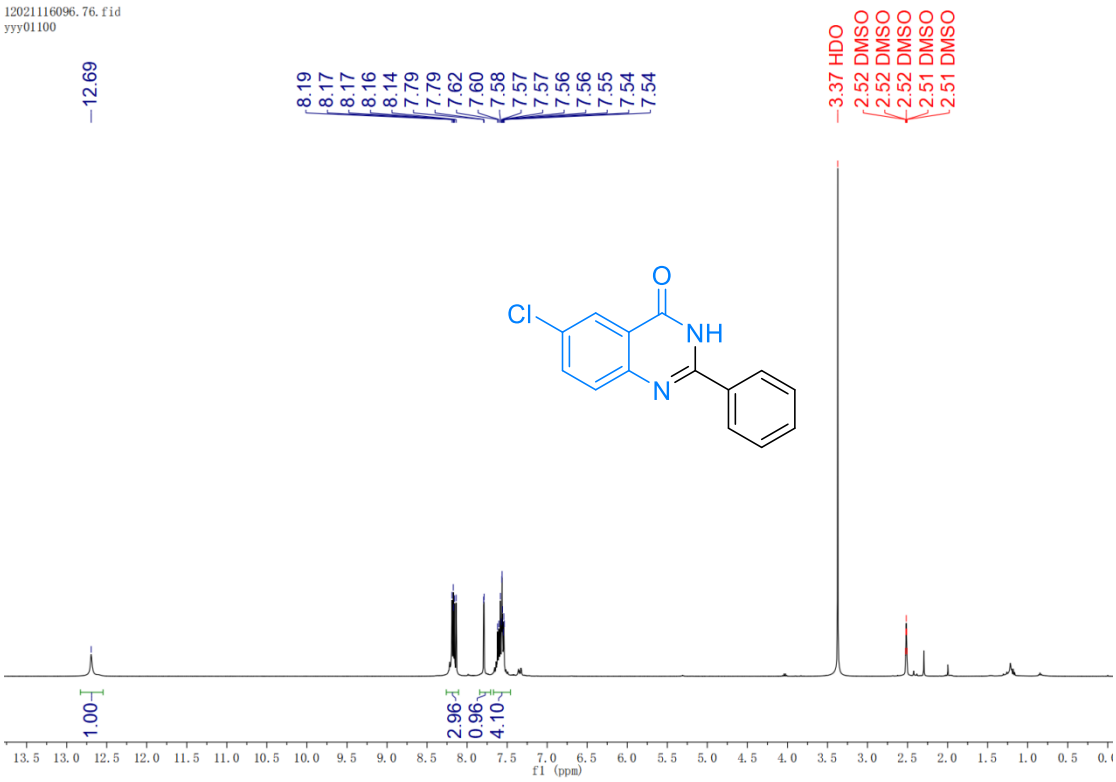
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 5p**



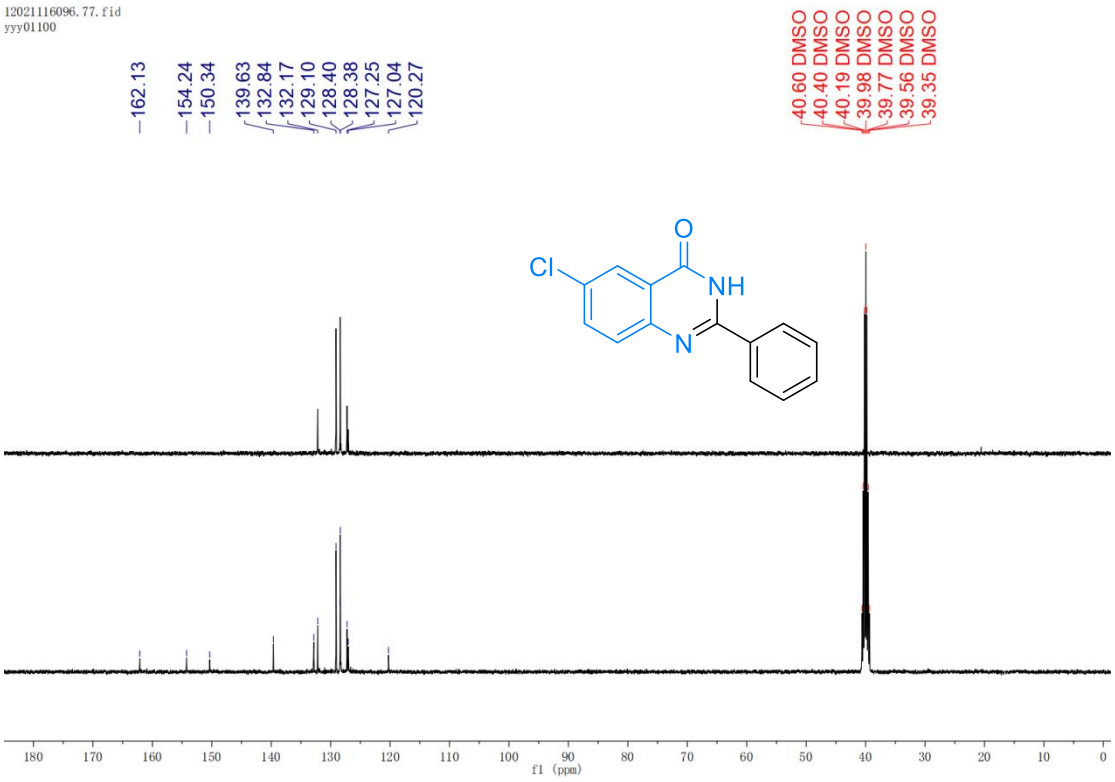
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 5q**



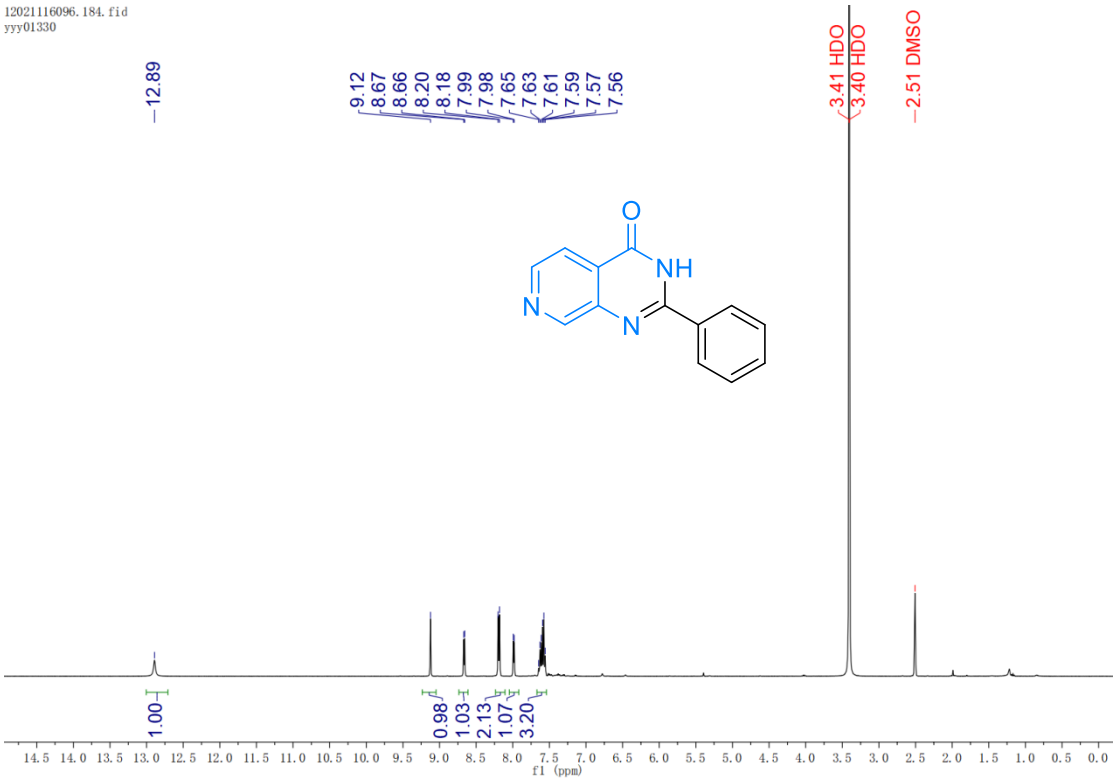
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 5q**



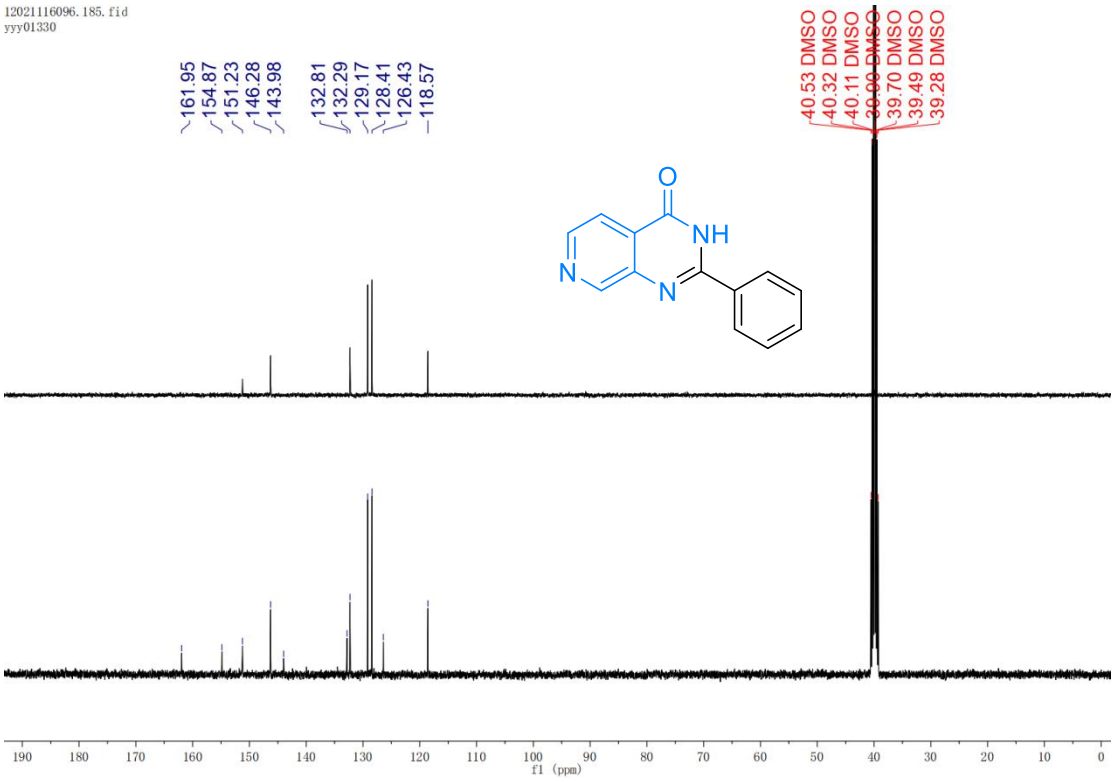
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 5r**



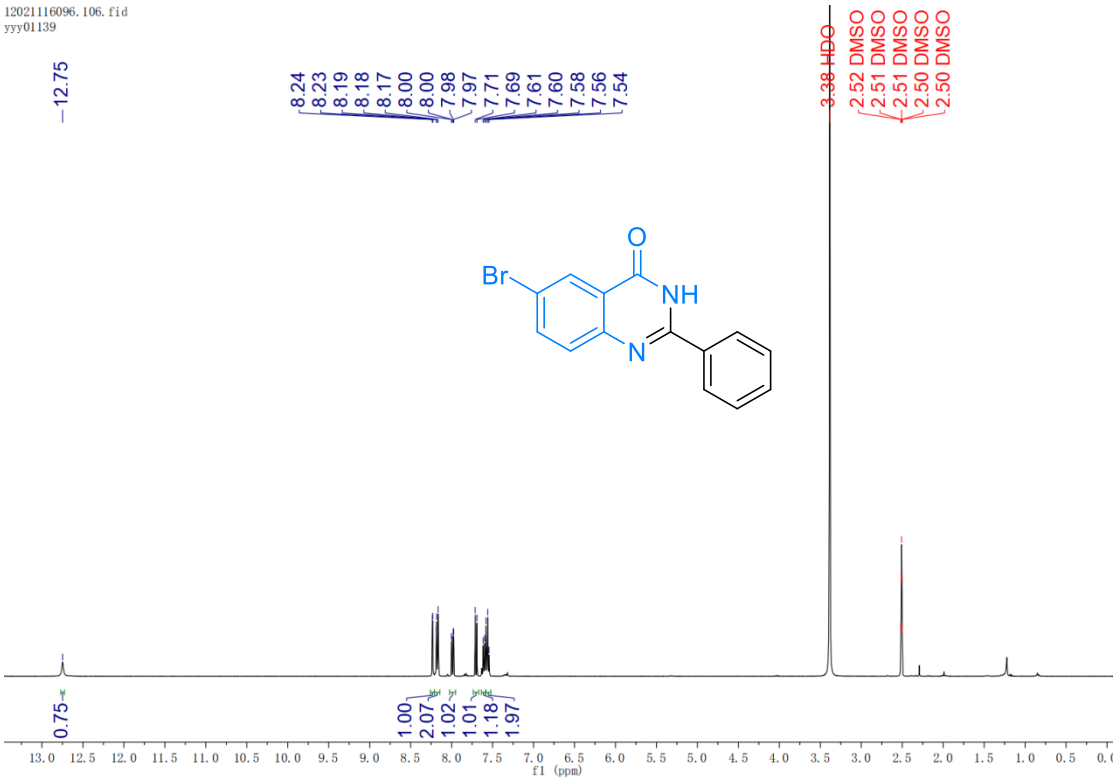
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 5r**



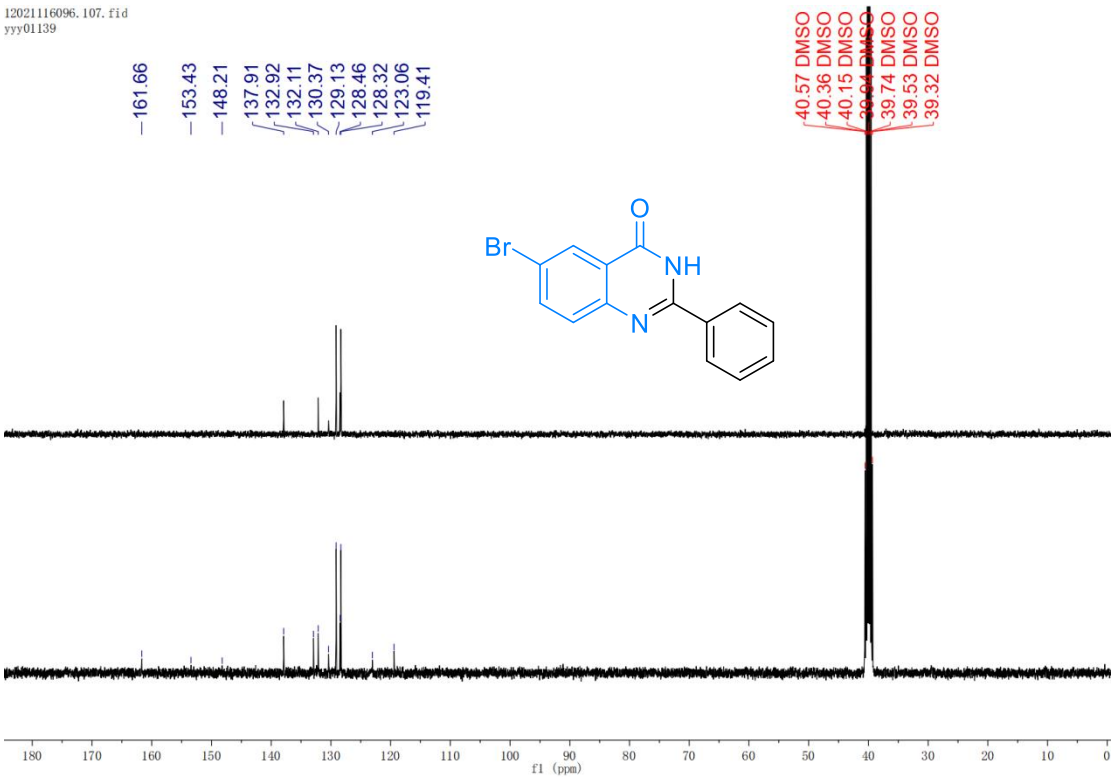
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 5s**



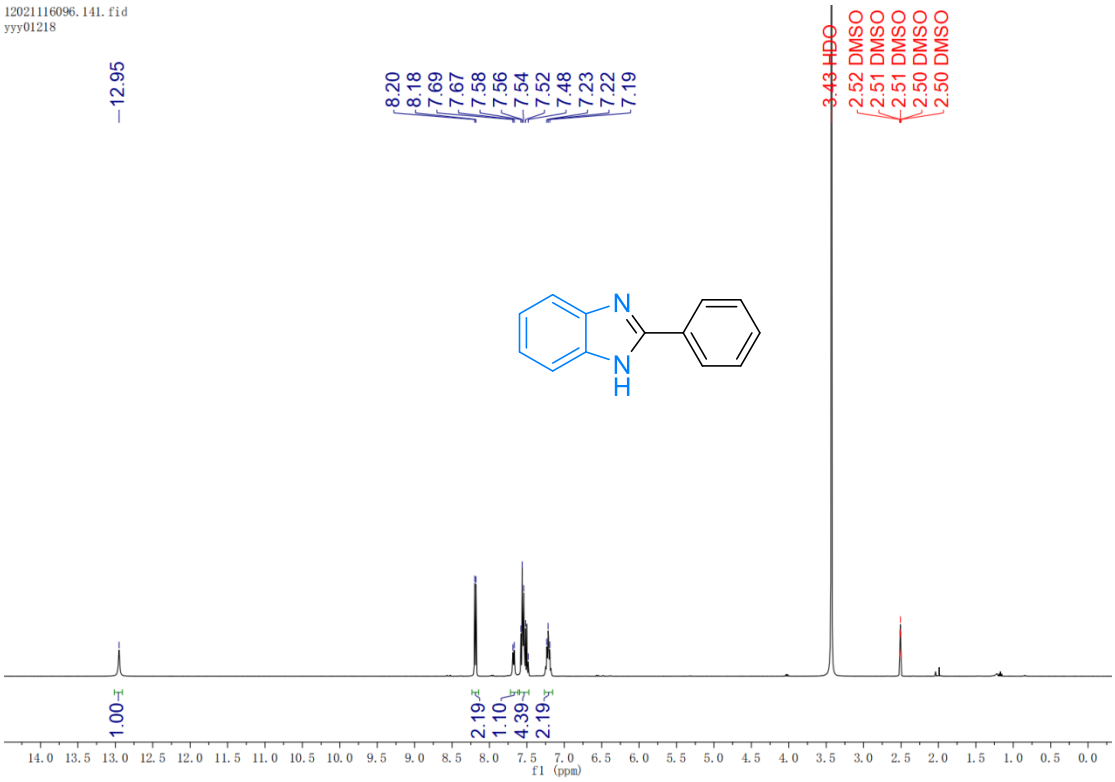
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 5s**



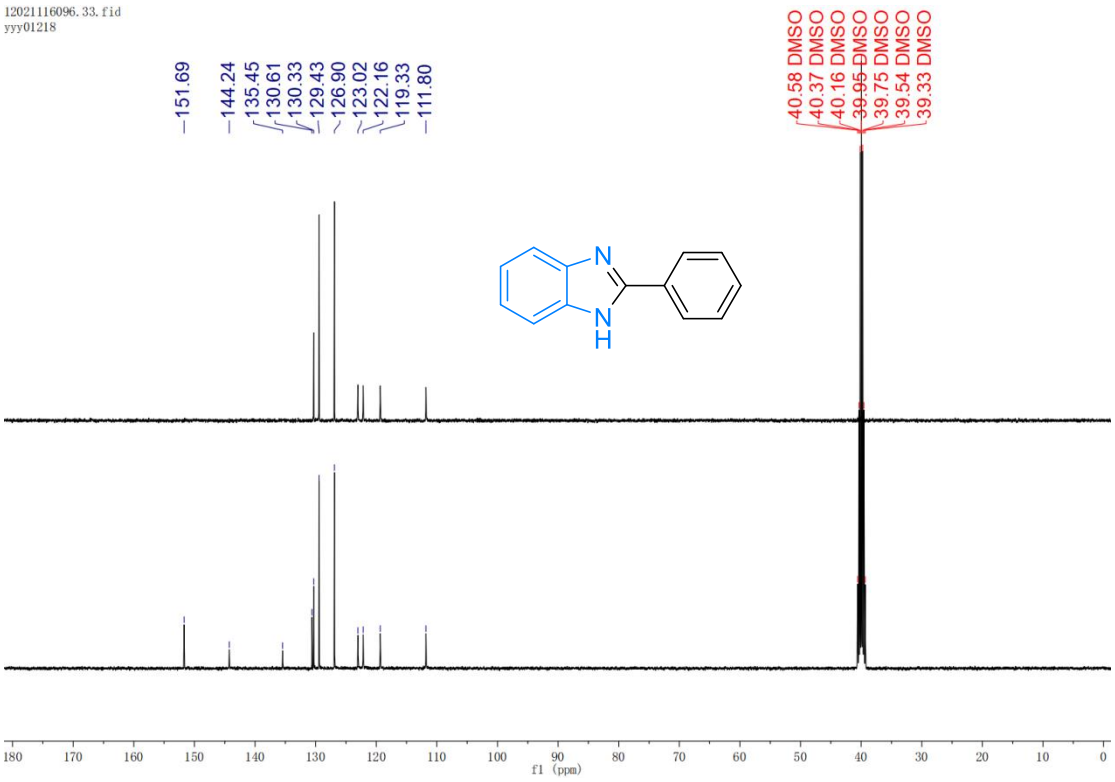
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 5t**



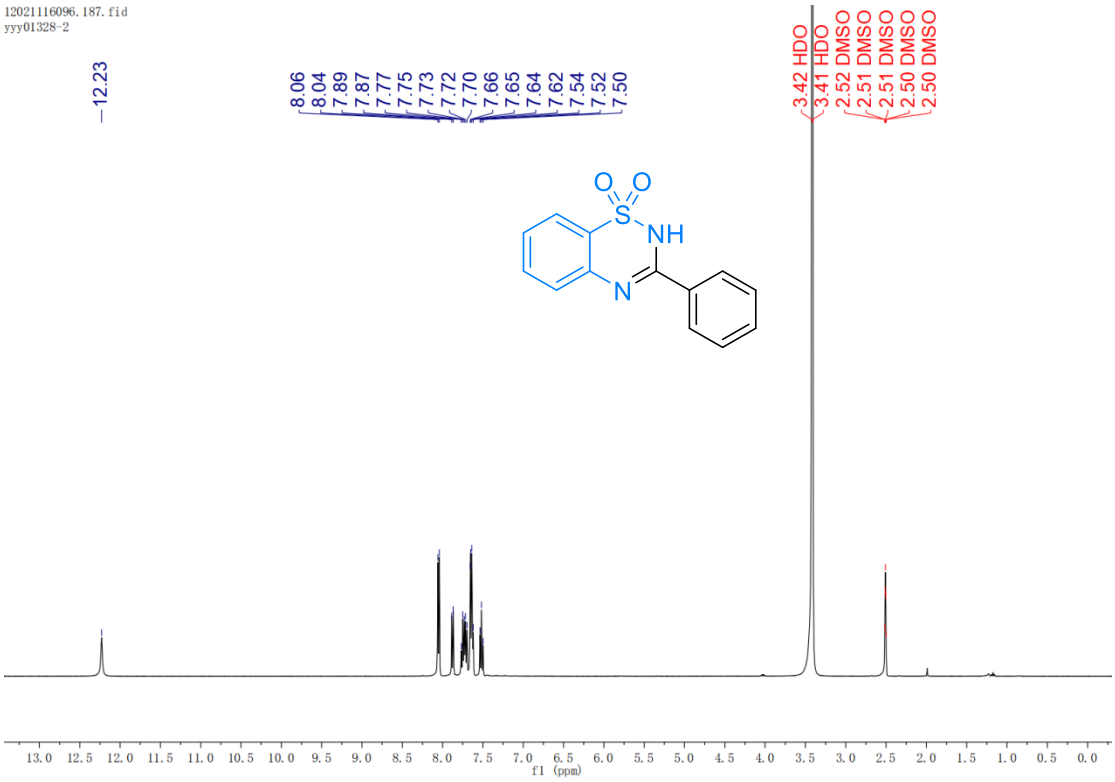
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 5t**



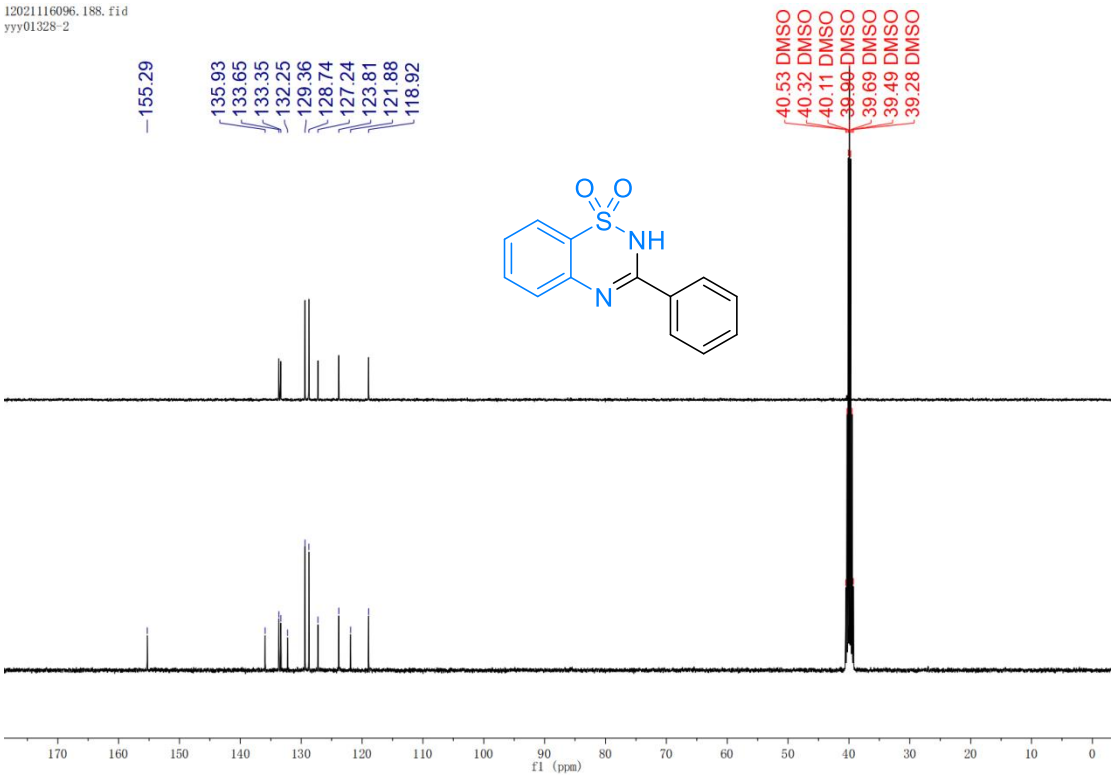
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 6a**



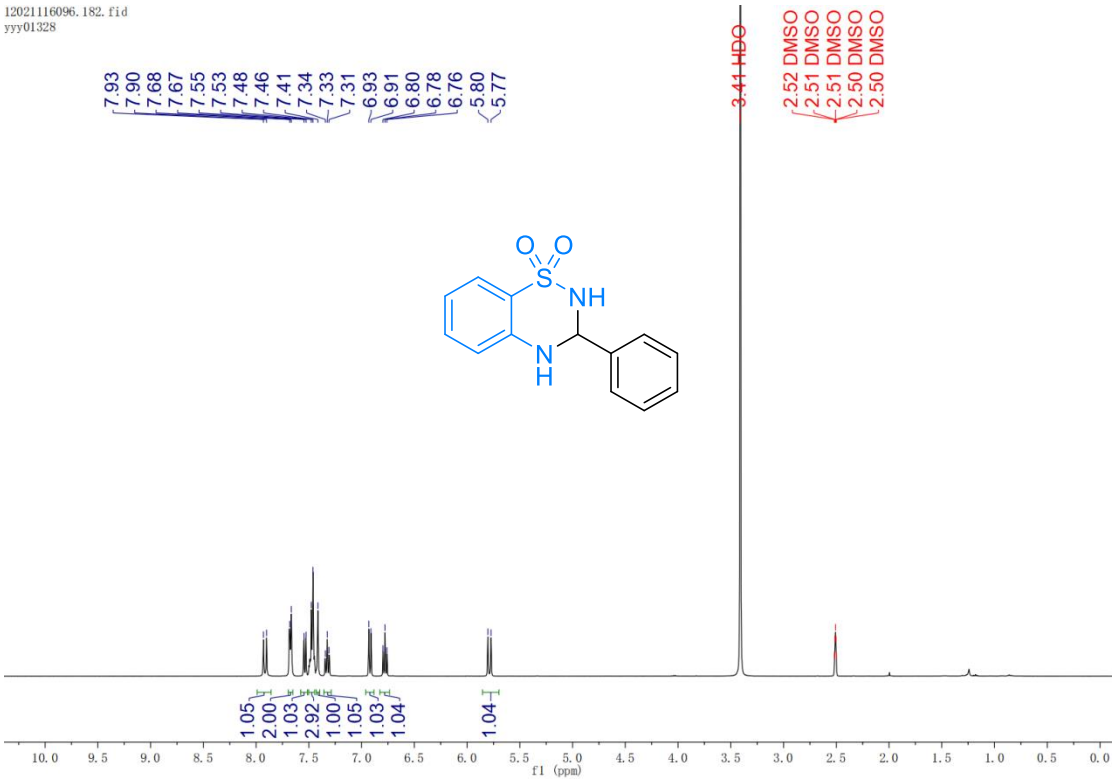
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 6a**



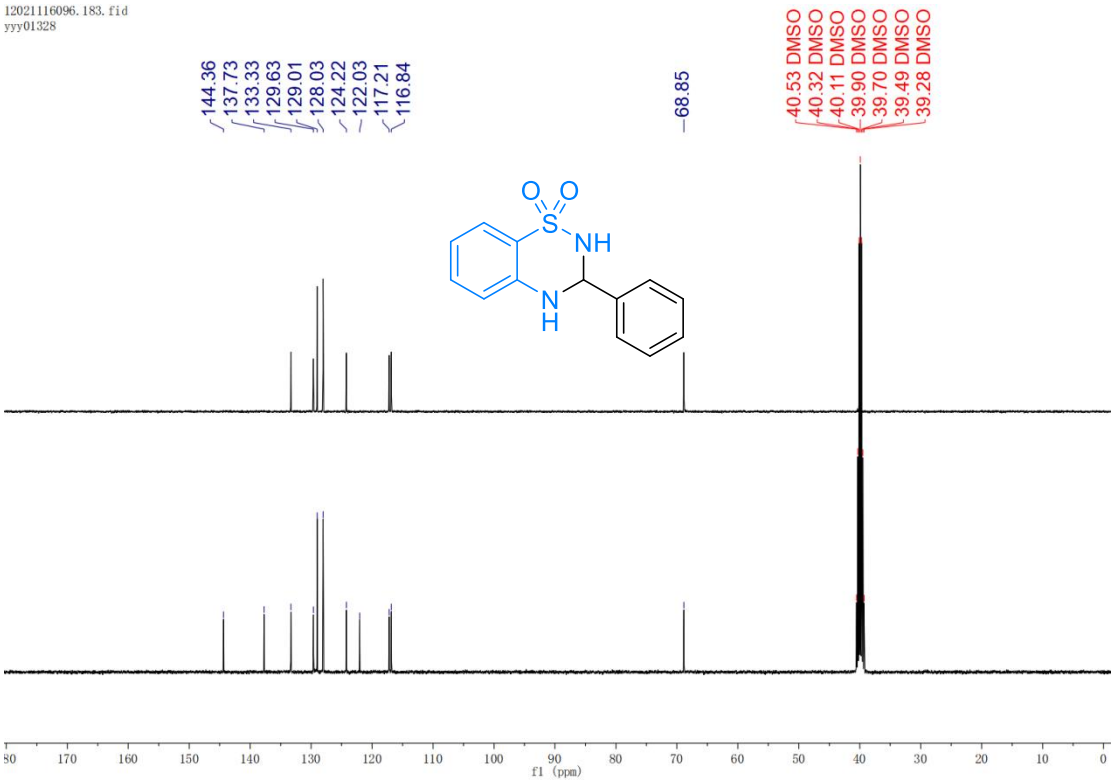
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 6b**



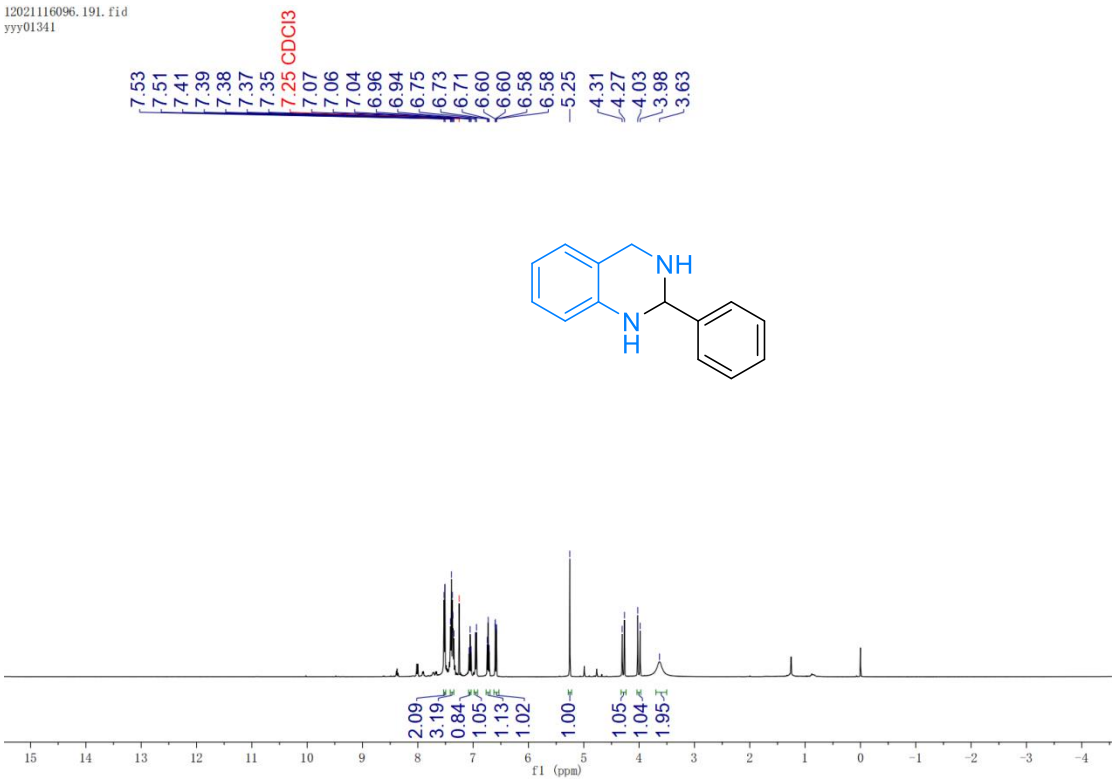
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 6b**



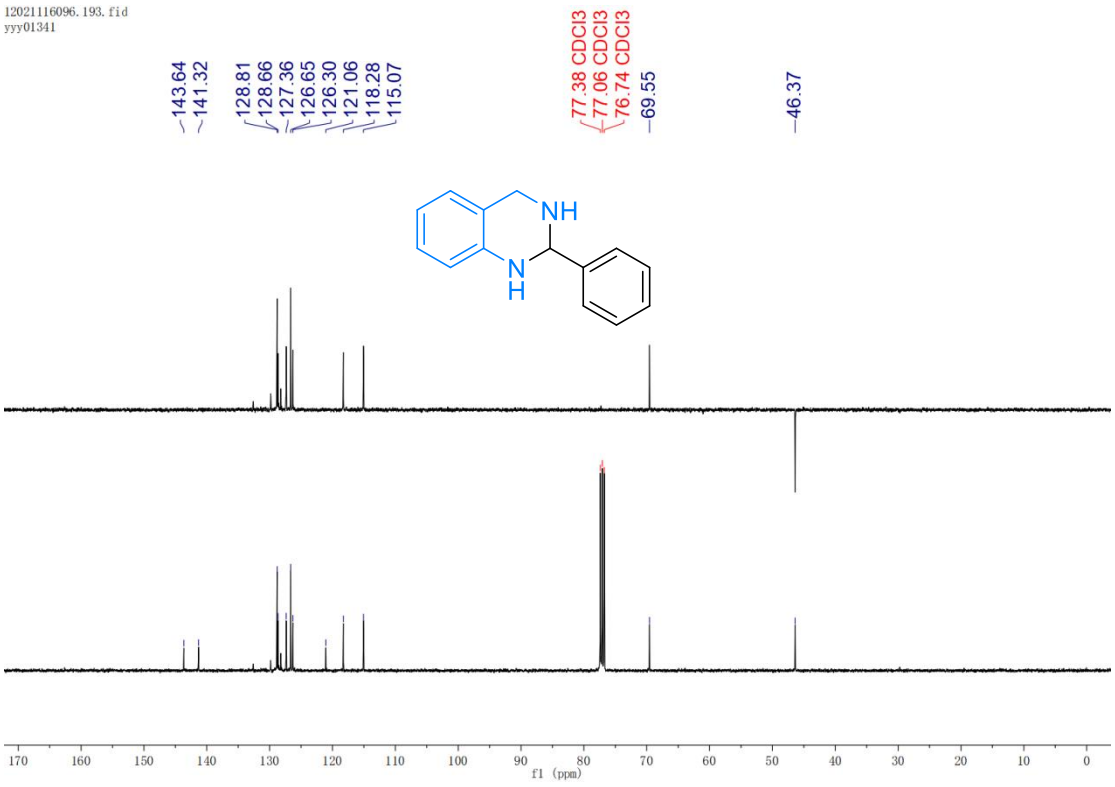
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 6b'**



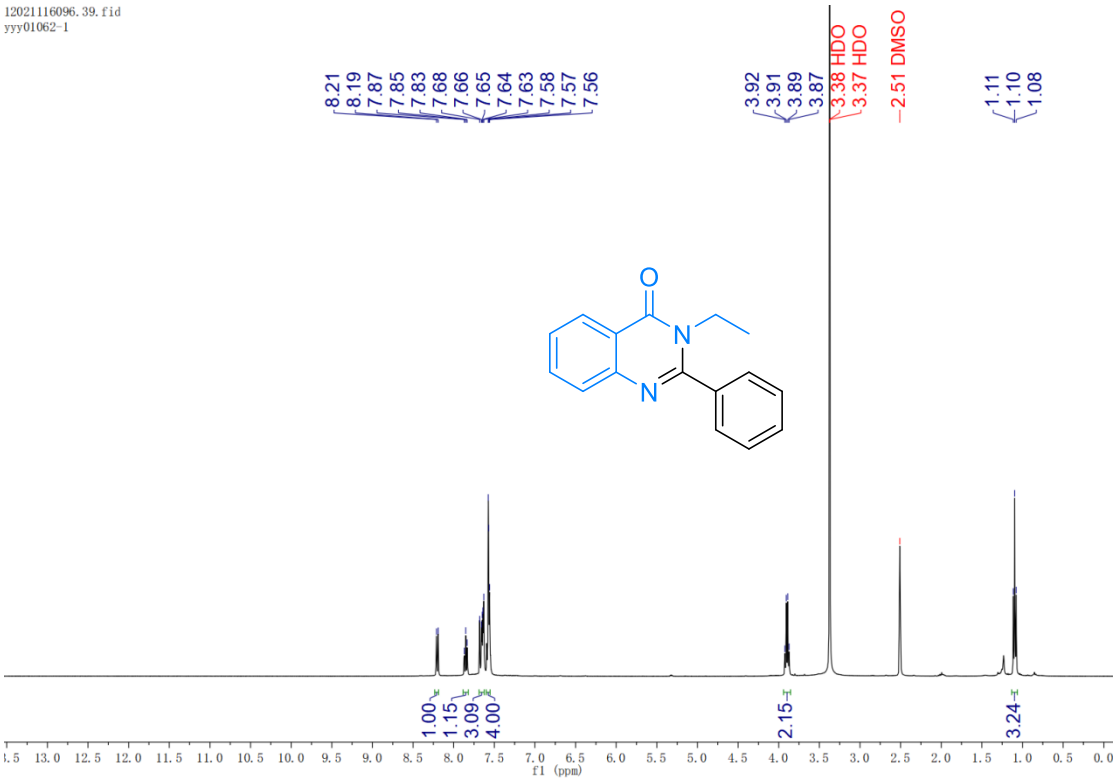
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 6b'**



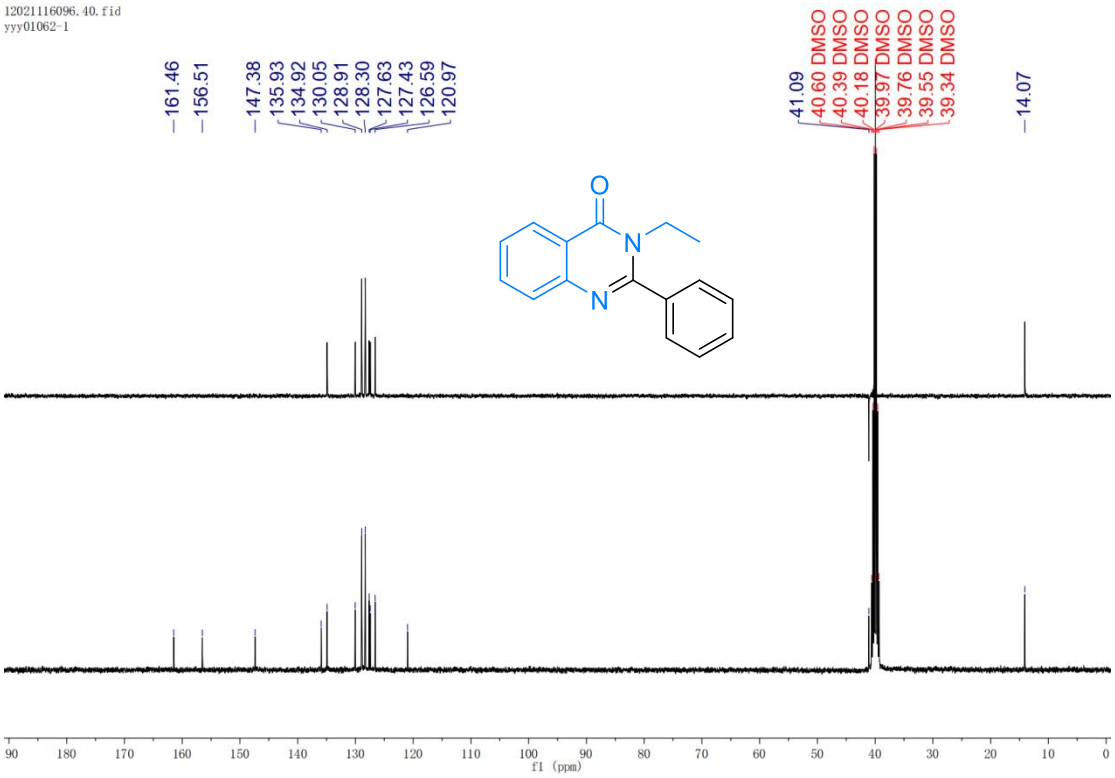
[1]H-NMR (400 MHz, Chloroform-*d*) **Spectra of compound 6c**



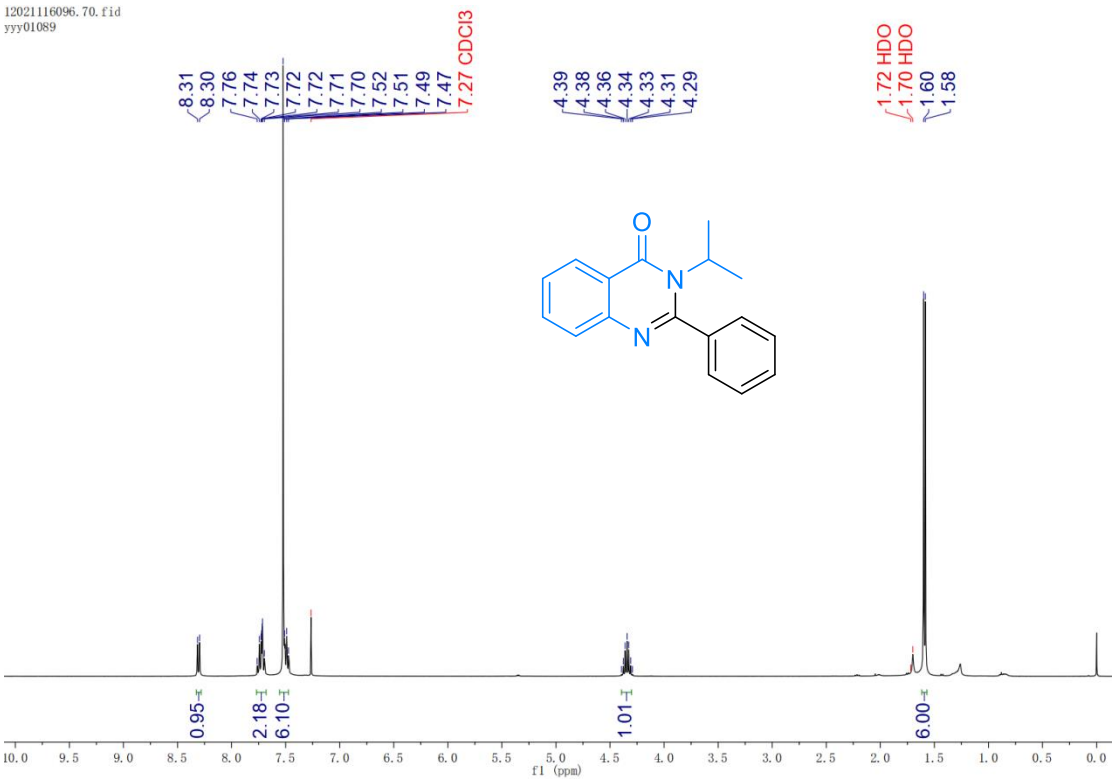
[13]C-NMR (100 MHz, Chloroform-*d*) **Spectra of compound 6c**



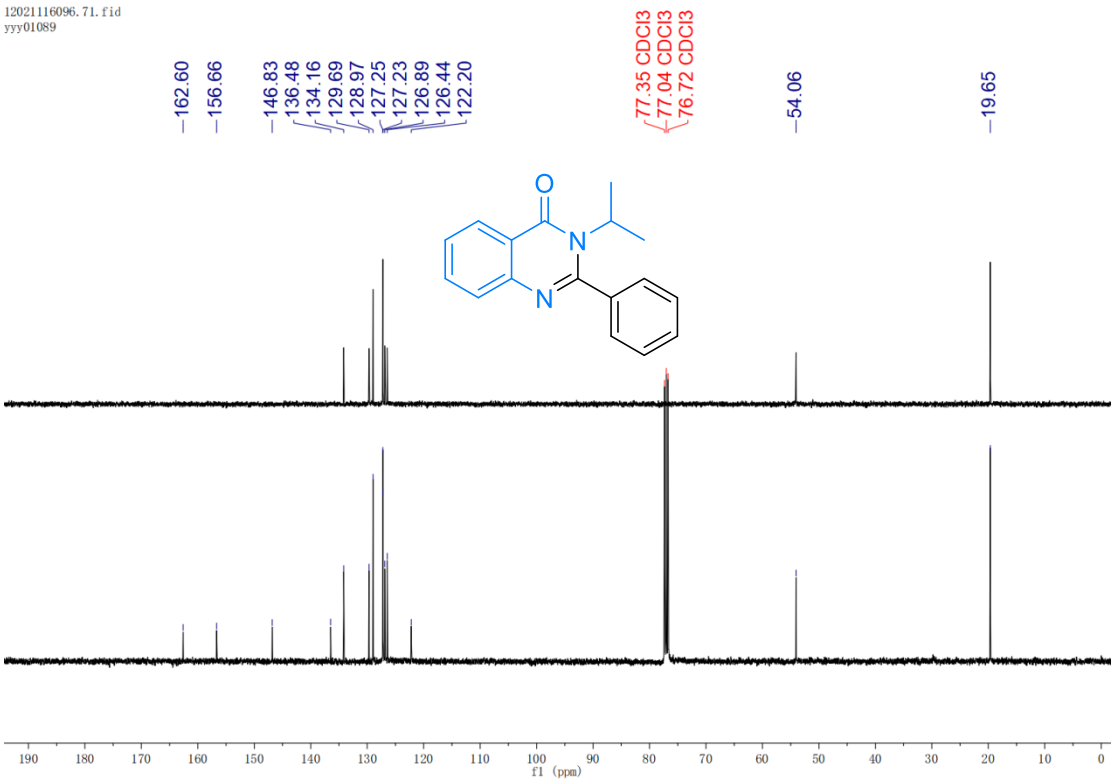
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 7a**



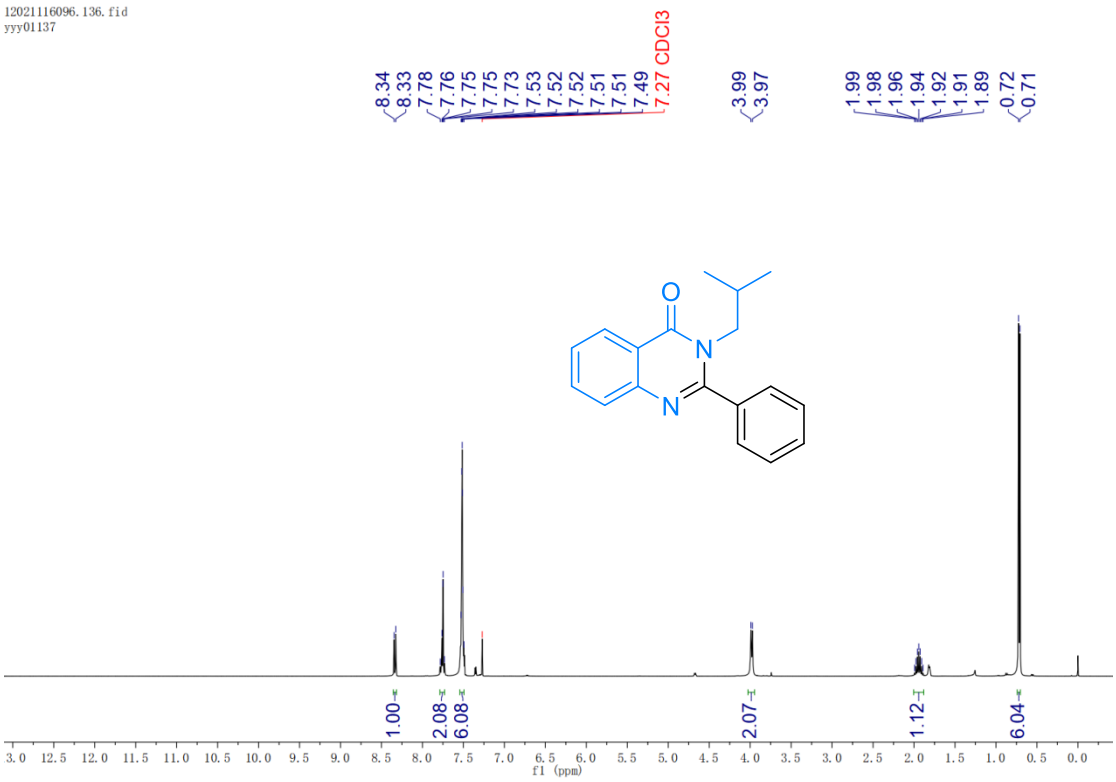
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 7a**



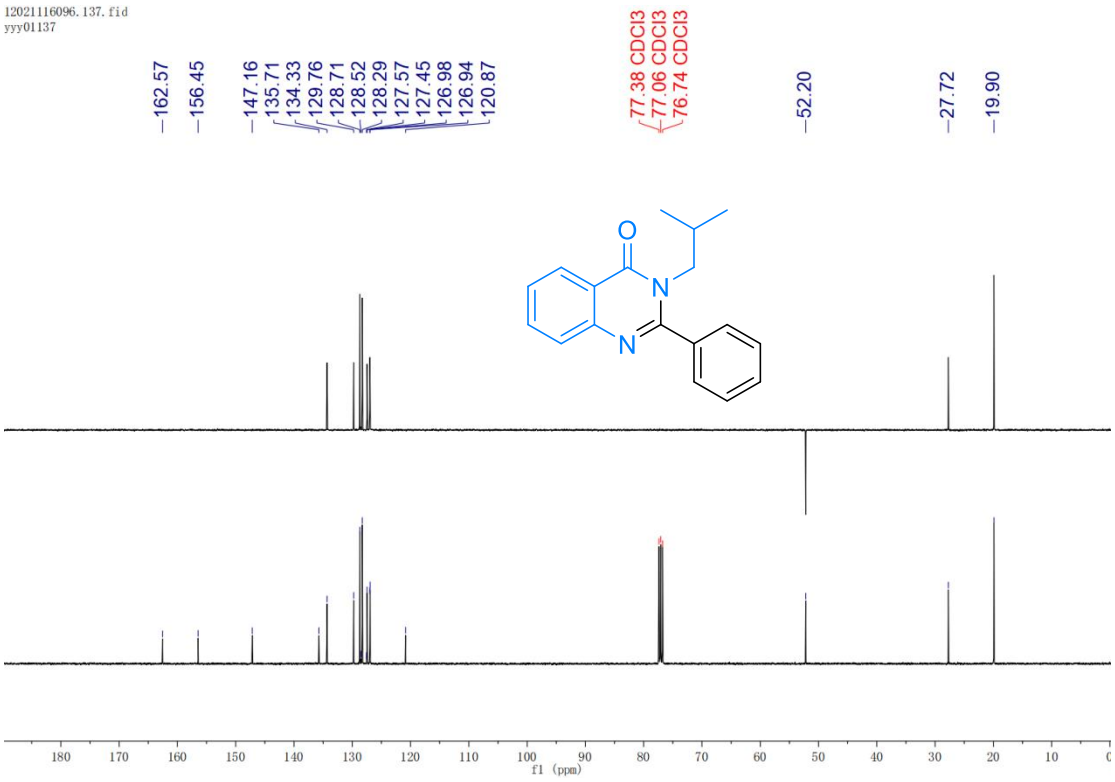
^{1}H-NMR (400 MHz, Chloroform-*d*) **Spectra of compound 7b**



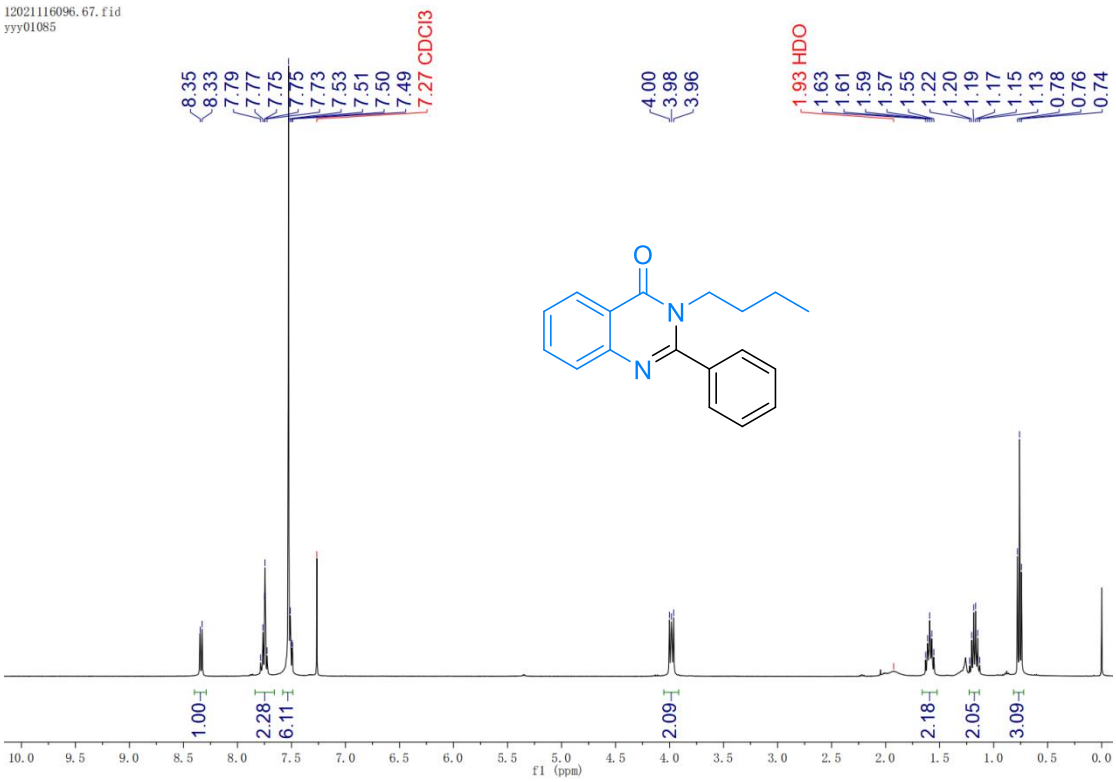
^{13}C-NMR (100 MHz, Chloroform-*d*) **Spectra of compound 7b**



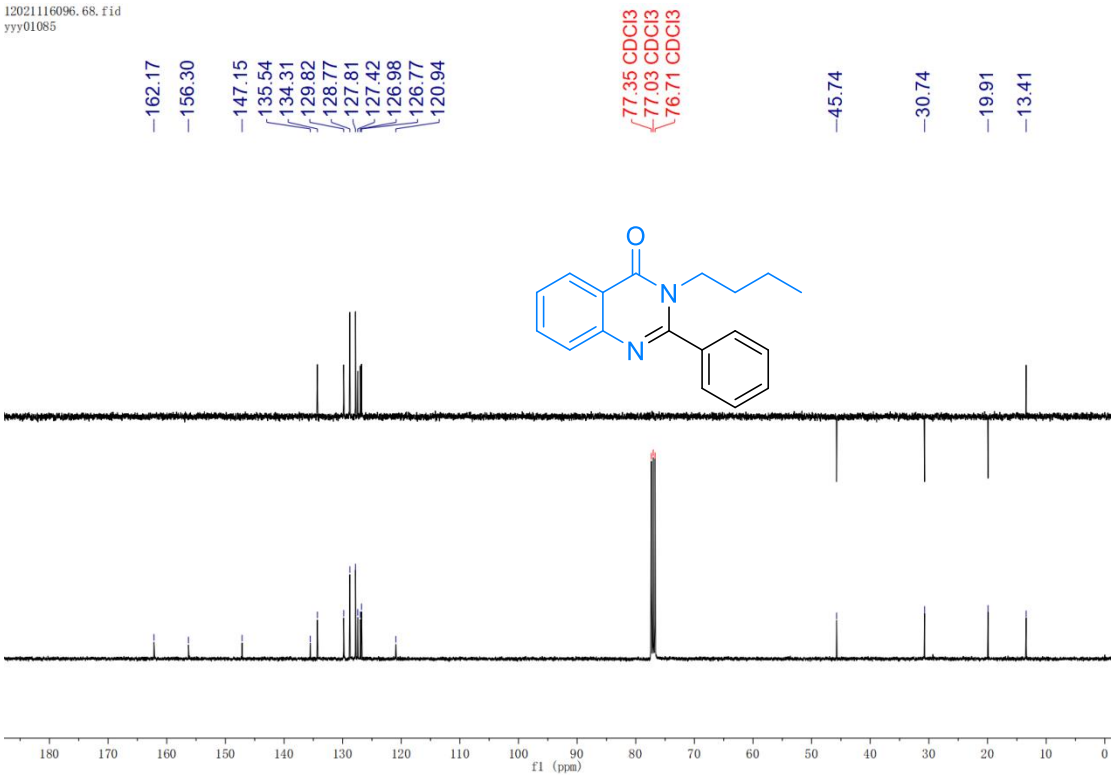
[1]H-NMR (400 MHz, Chloroform-*d*) **Spectra of compound 7c**



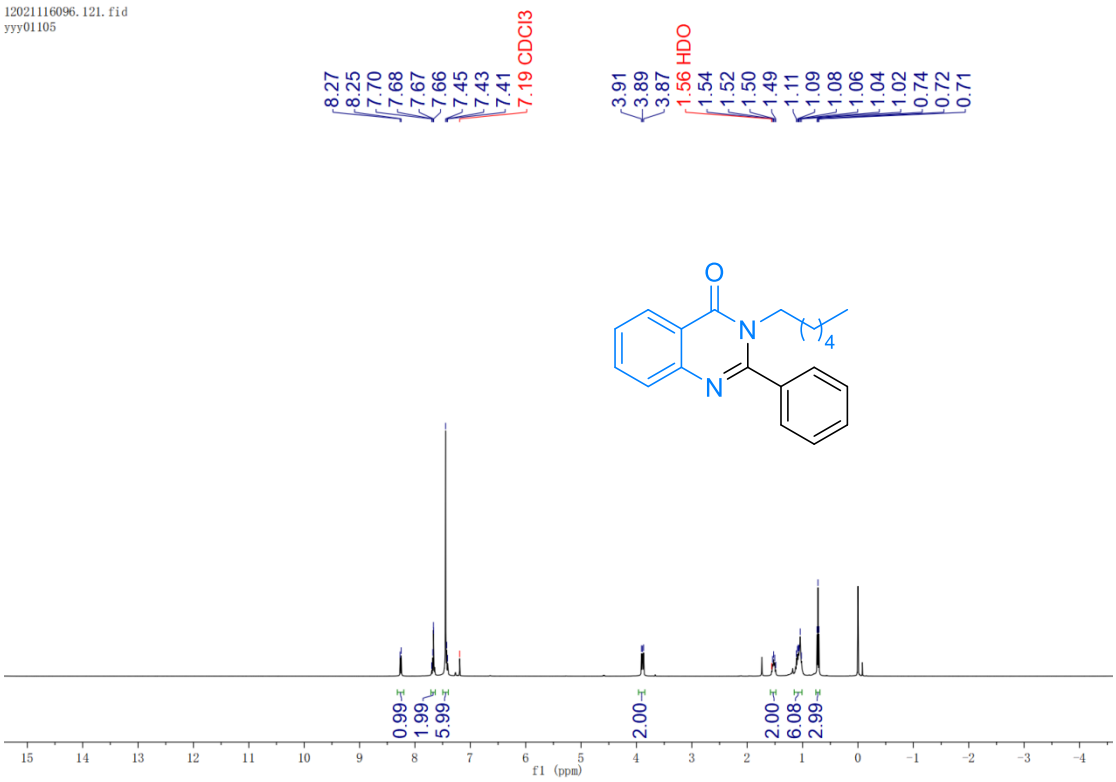
[13]C-NMR (100 MHz, Chloroform-*d*) **Spectra of compound 7c**



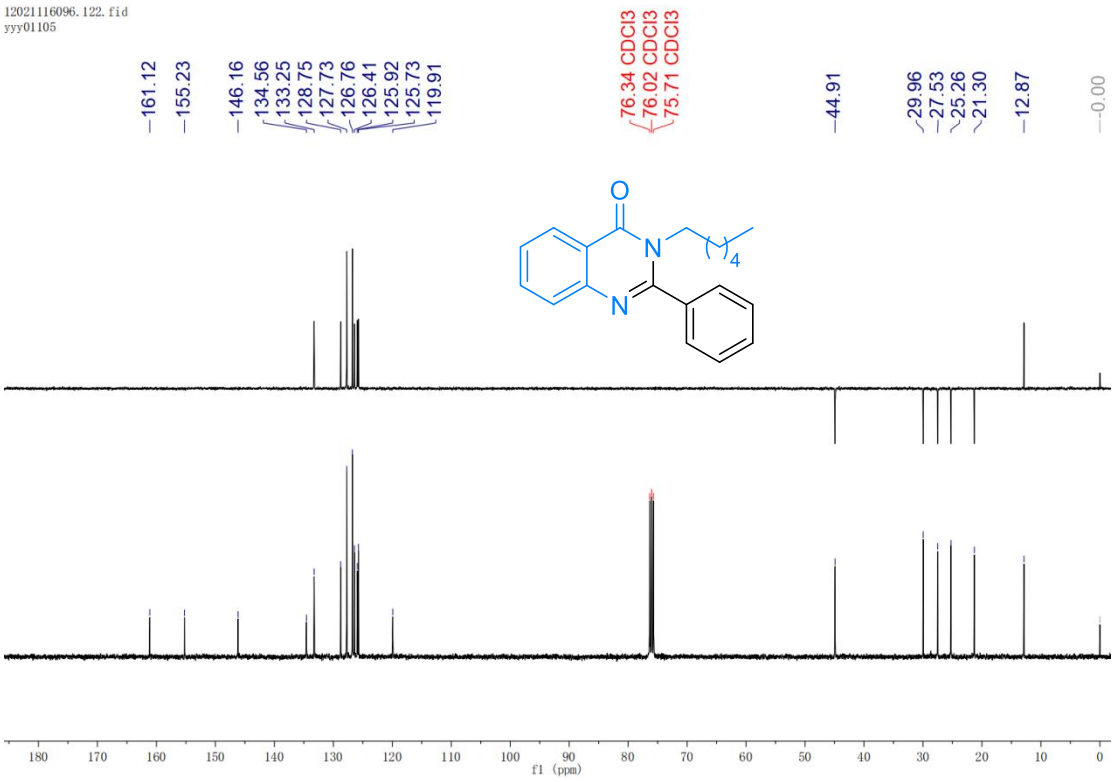
^{1}H-NMR (400 MHz, Chloroform-*d*) **Spectra of compound 7d**



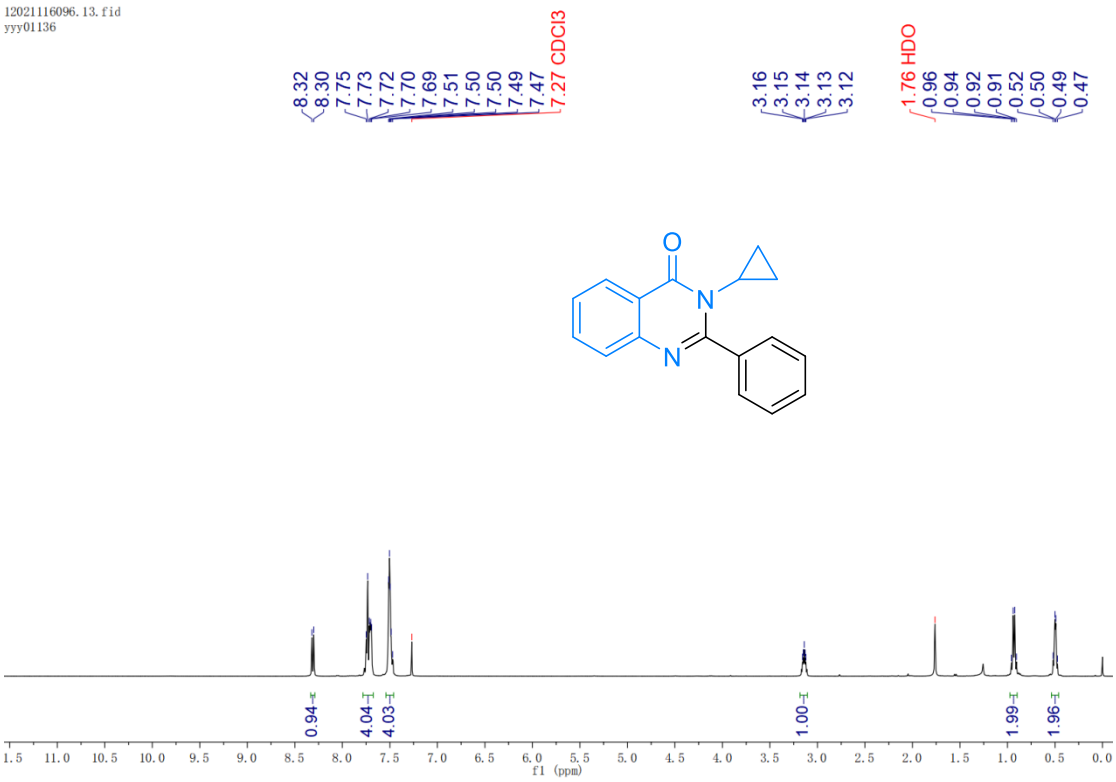
^{13}C-NMR (100 MHz, Chloroform-*d*) **Spectra of compound 7d**



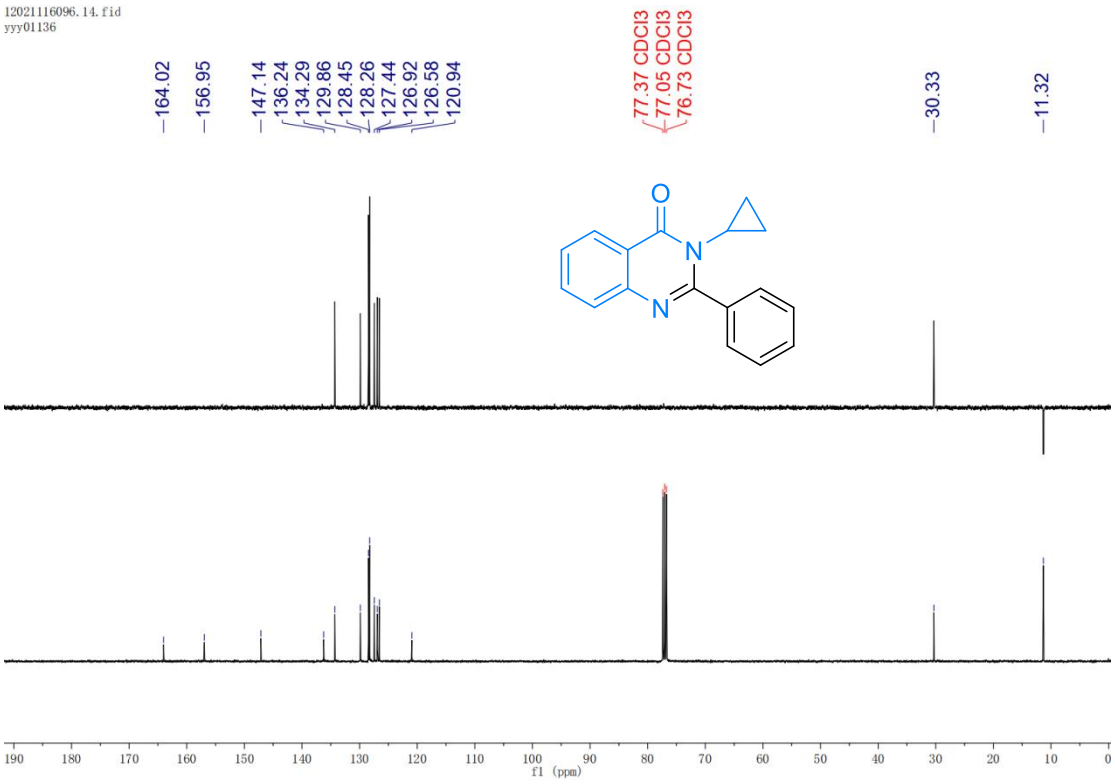
[1]H-NMR (400 MHz, Chloroform-*d*) **Spectra of compound 7e**



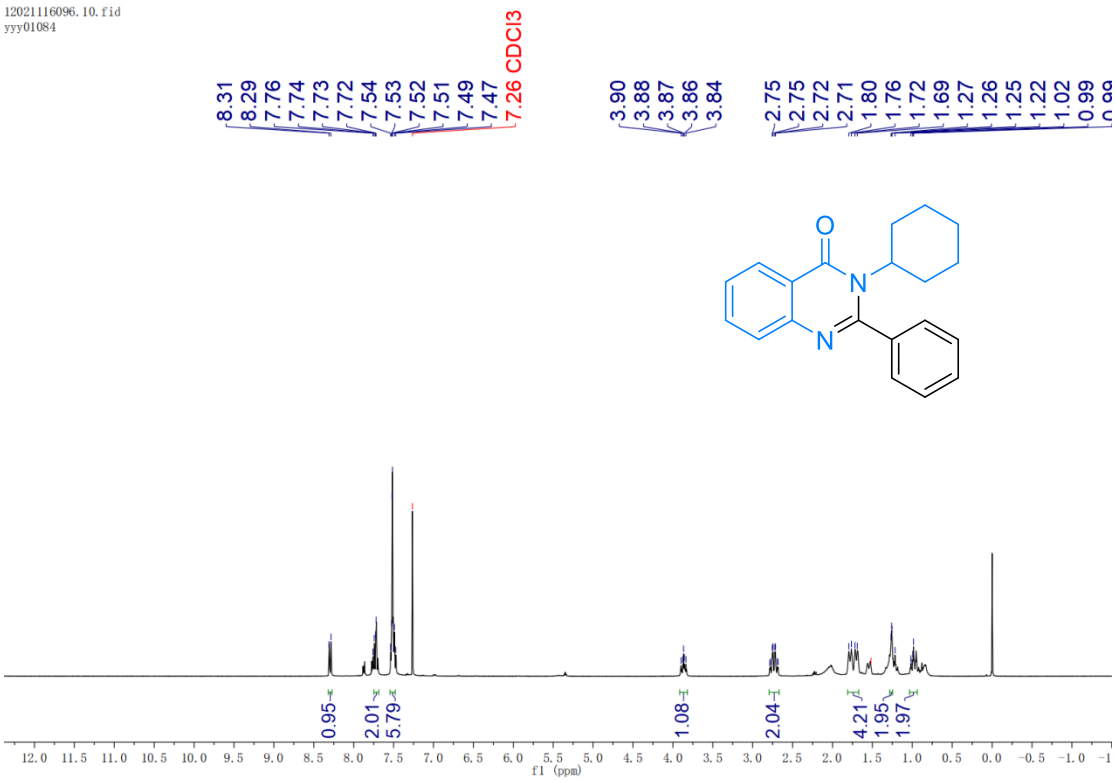
[13]C-NMR (100 MHz, Chloroform-*d*) **Spectra of compound 7e**



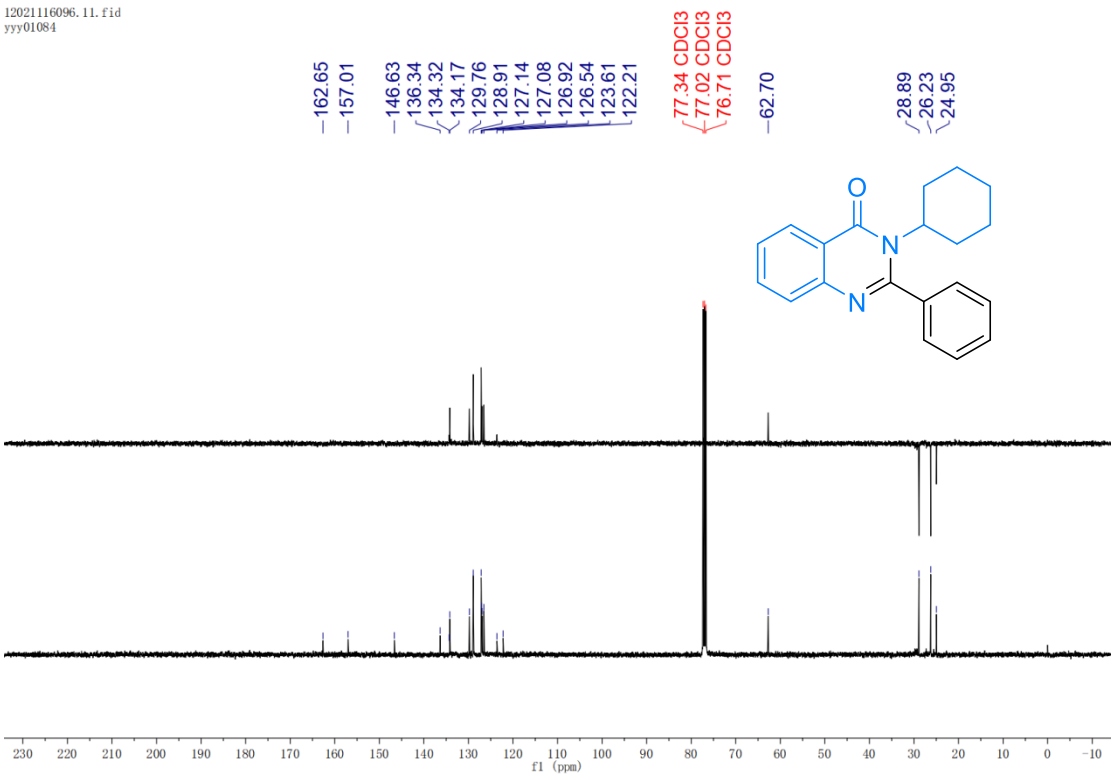
[1]H-NMR (400 MHz, Chloroform-*d*) **Spectra of compound 7f**



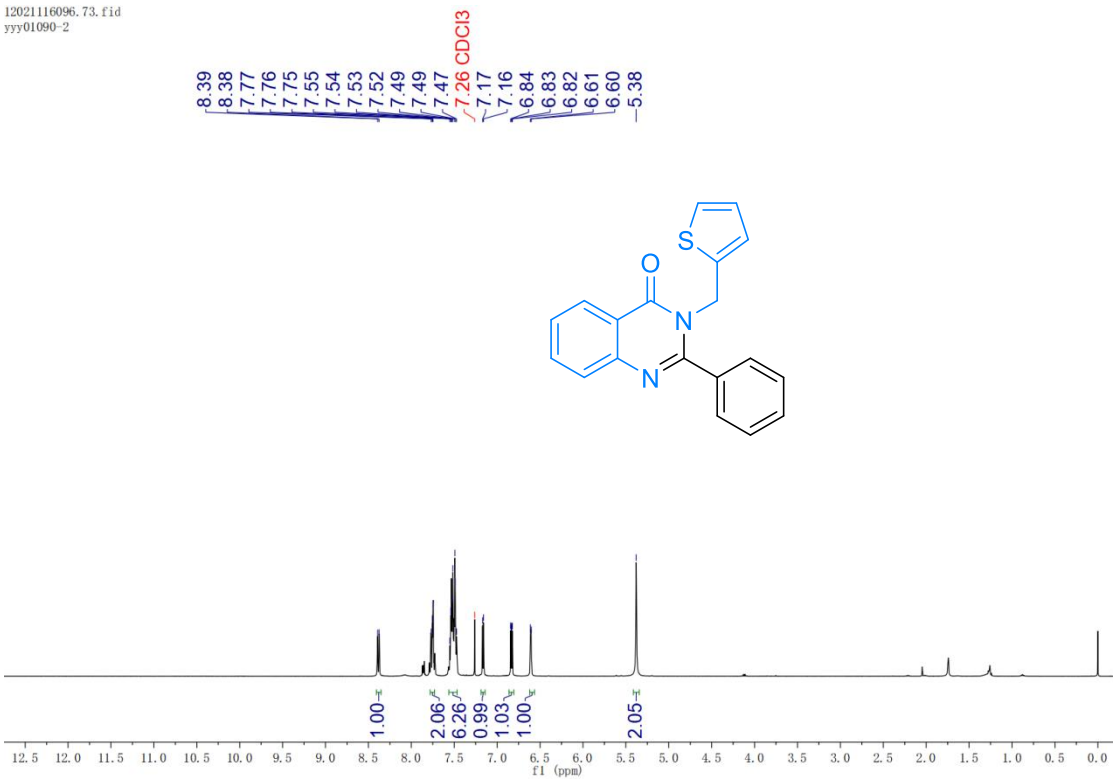
[13]C-NMR (100 MHz, Chloroform-*d*) **Spectra of compound 7f**



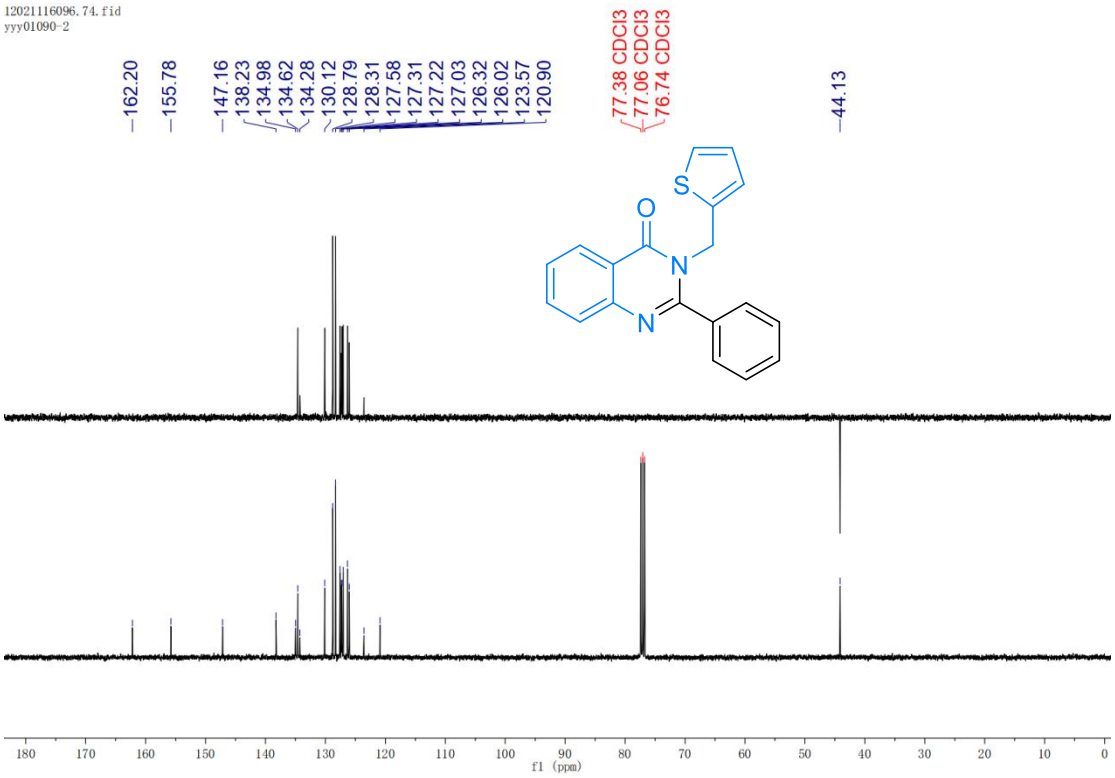
^{1}H-NMR (400 MHz, Chloroform-*d*) **Spectra of compound 7g**



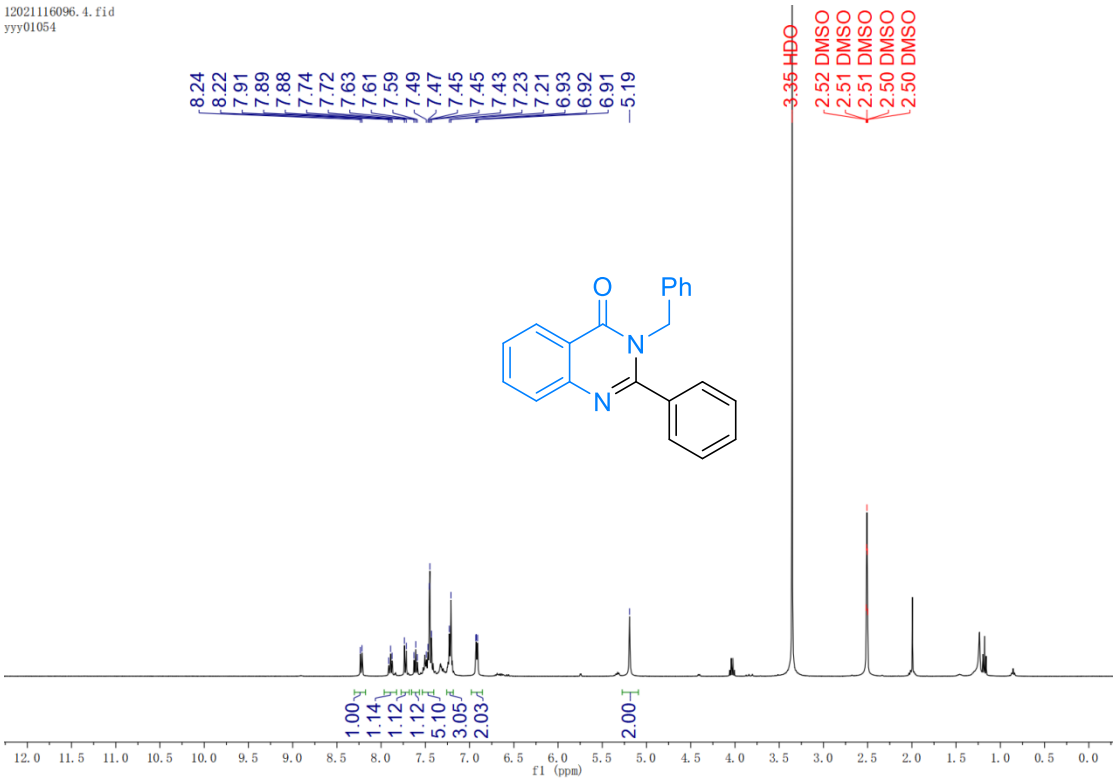
^{13}C-NMR (100 MHz, Chloroform-*d*) **Spectra of compound 7g**



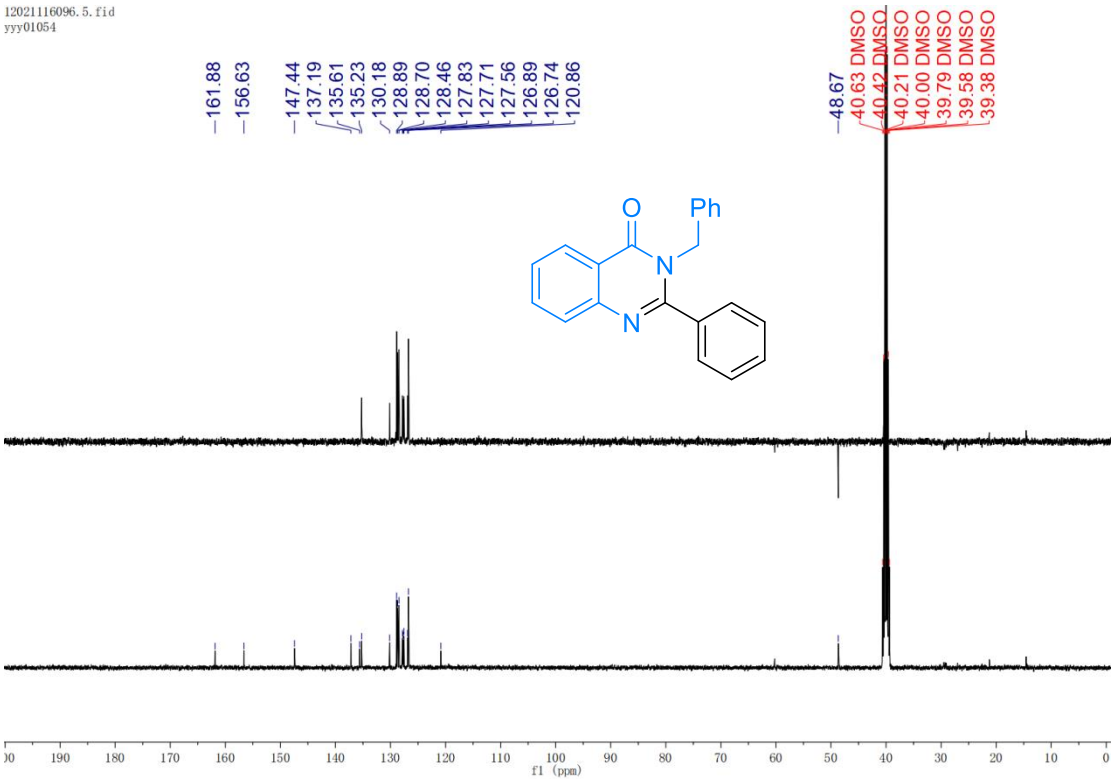
^{1}H-NMR (400 MHz, Chloroform-*d*) **Spectra of compound 7h**



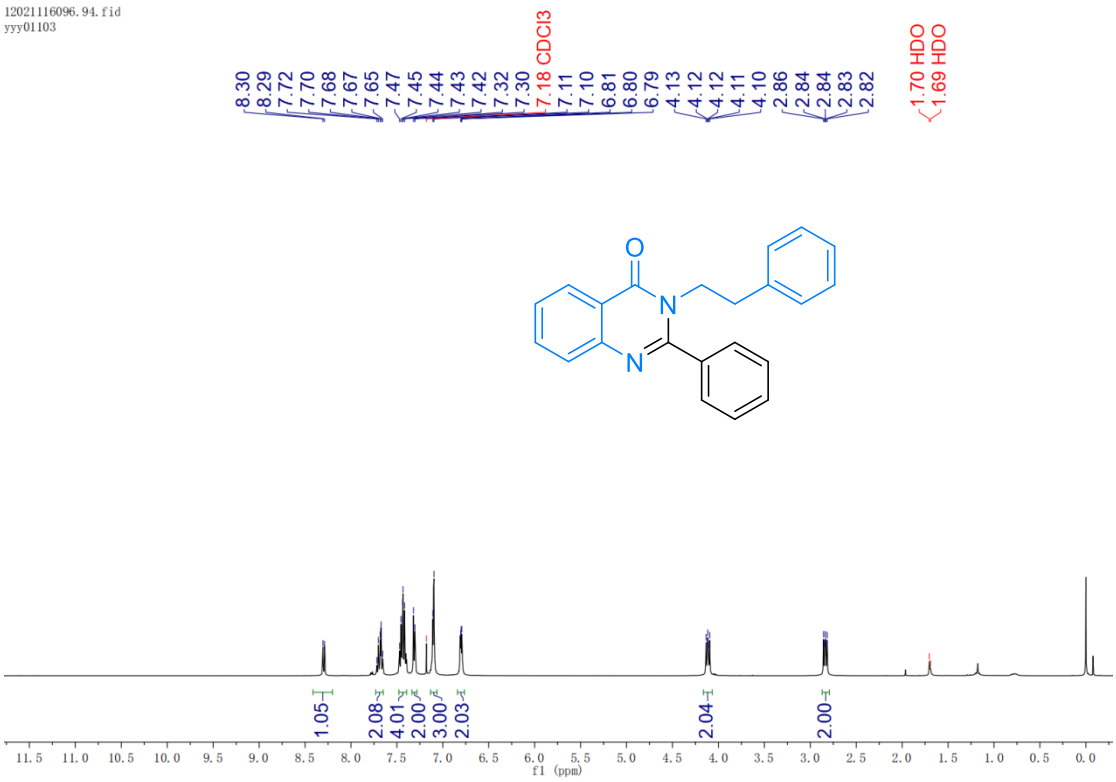
^{13}C-NMR (100 MHz, Chloroform-*d*) **Spectra of compound 7h**



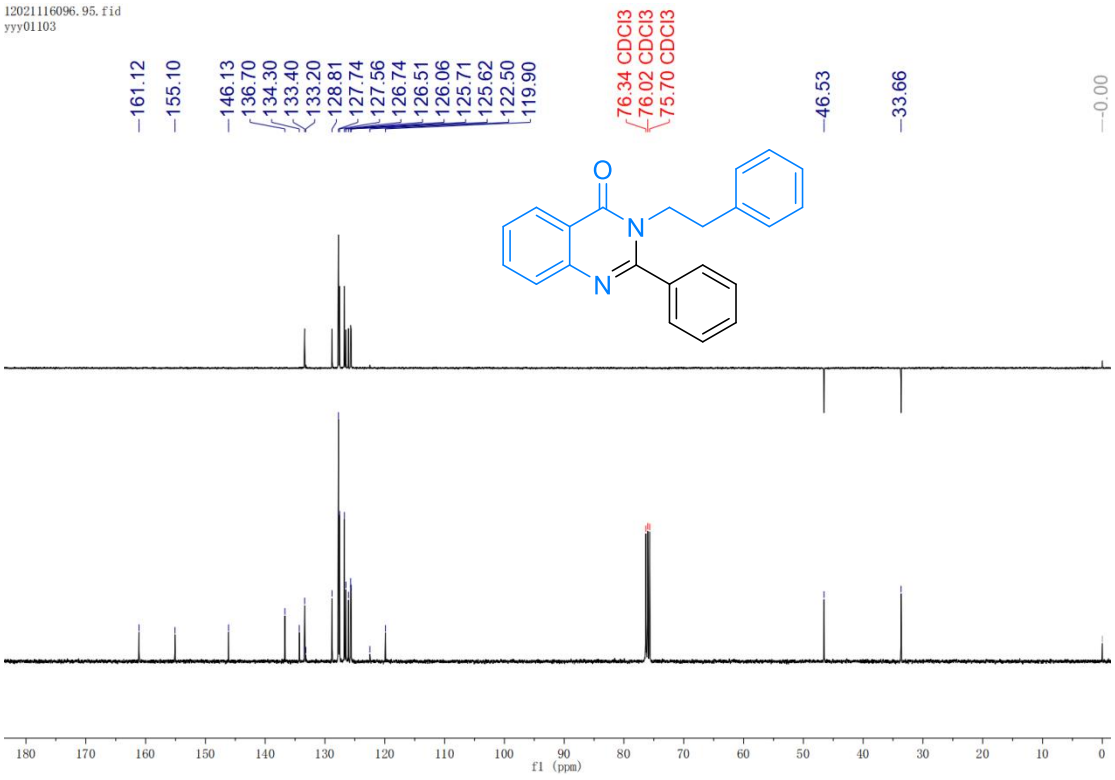
^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of compound 7i**



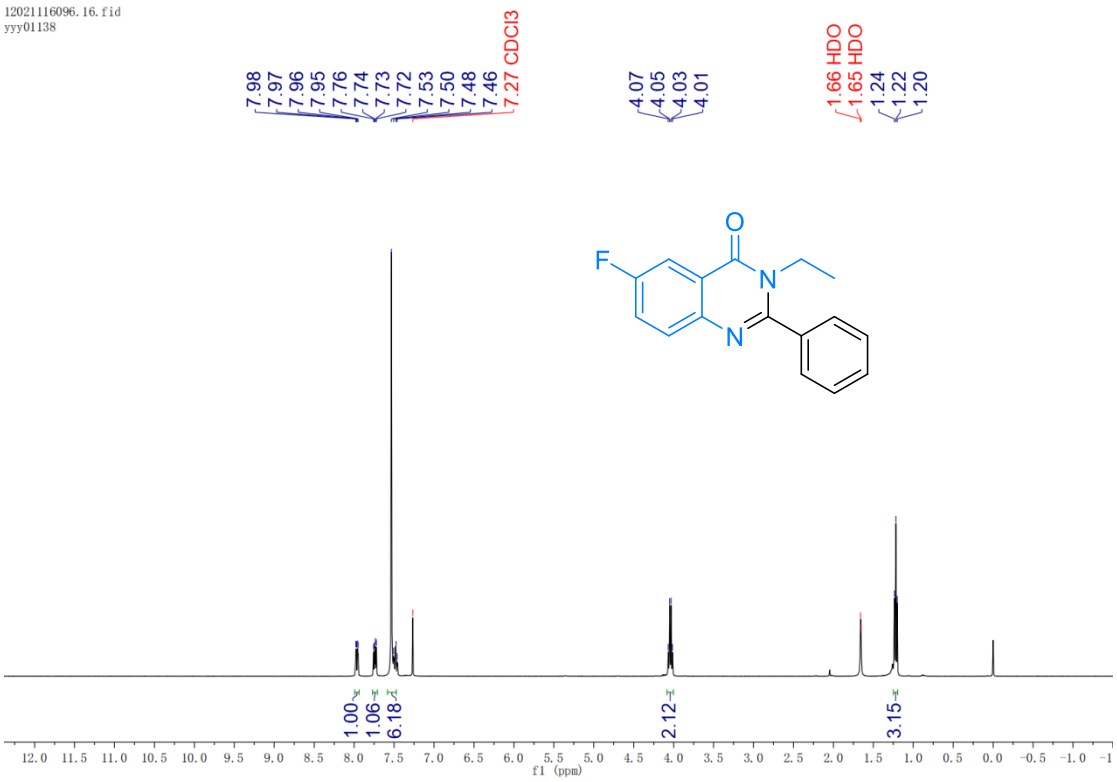
^{13}C-NMR (100 MHz, DMSO-d_6) **Spectra of compound 7i**



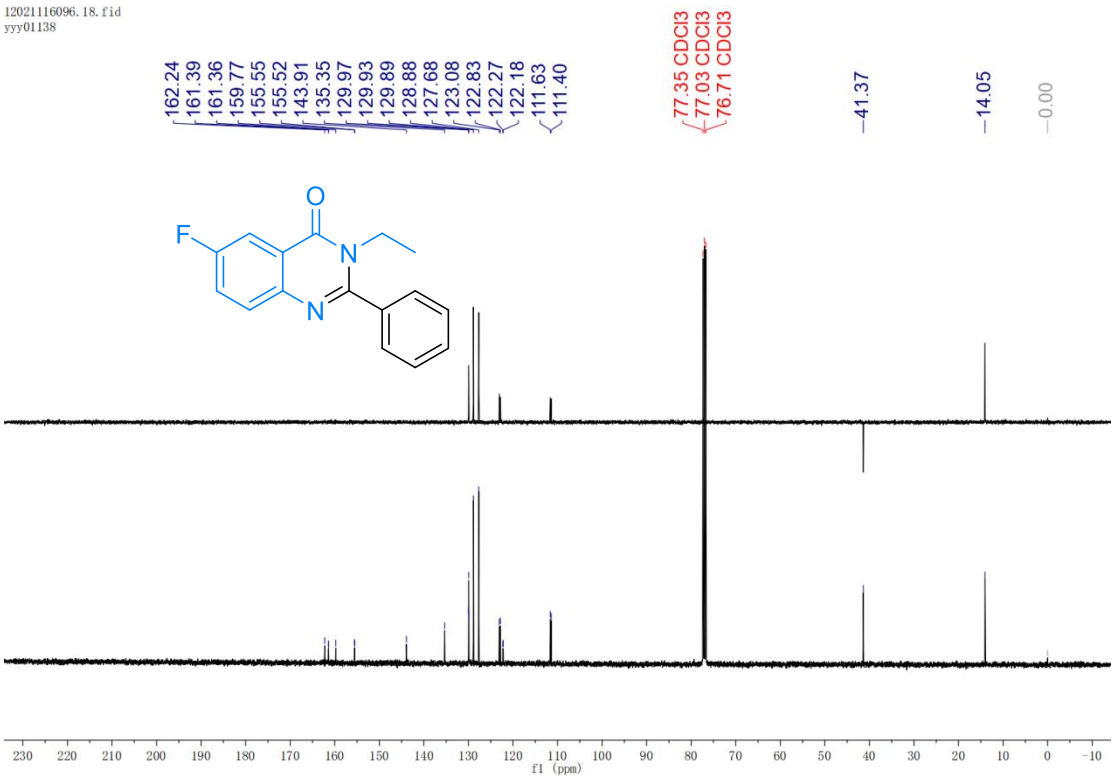
[1]H-NMR (400 MHz, Chloroform-*d*) **Spectra of compound 7j**



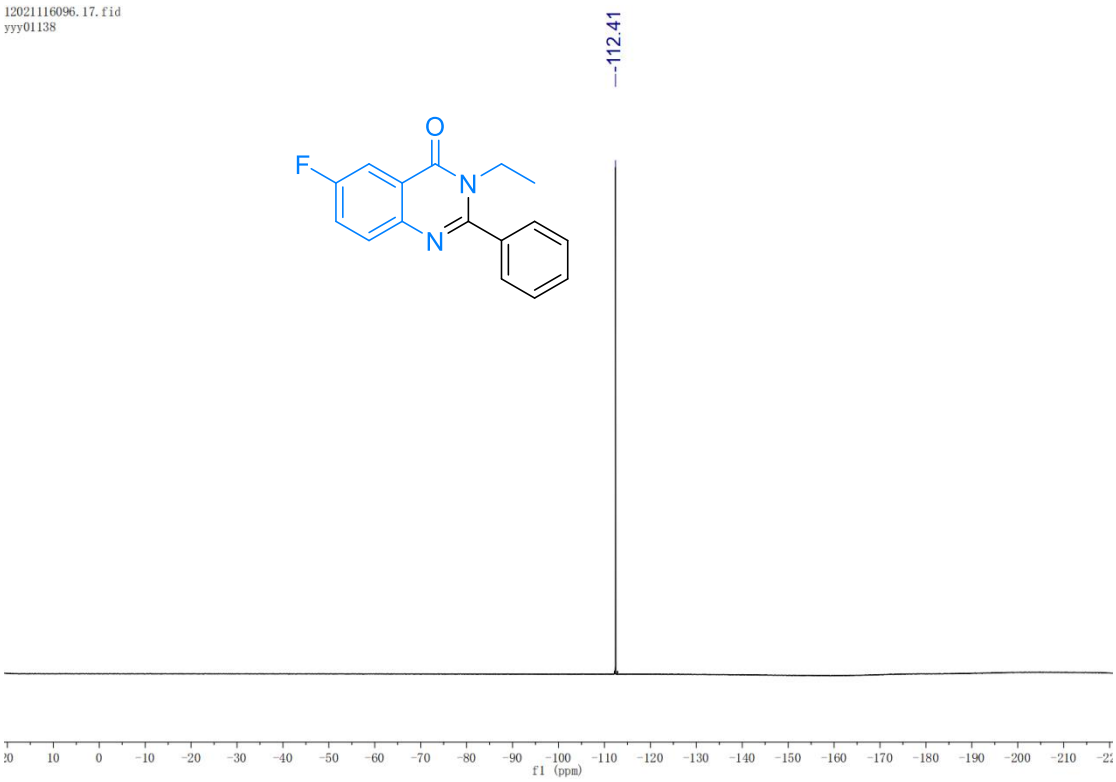
[13]C-NMR (100 MHz, Chloroform-*d*) **Spectra of compound 7j**



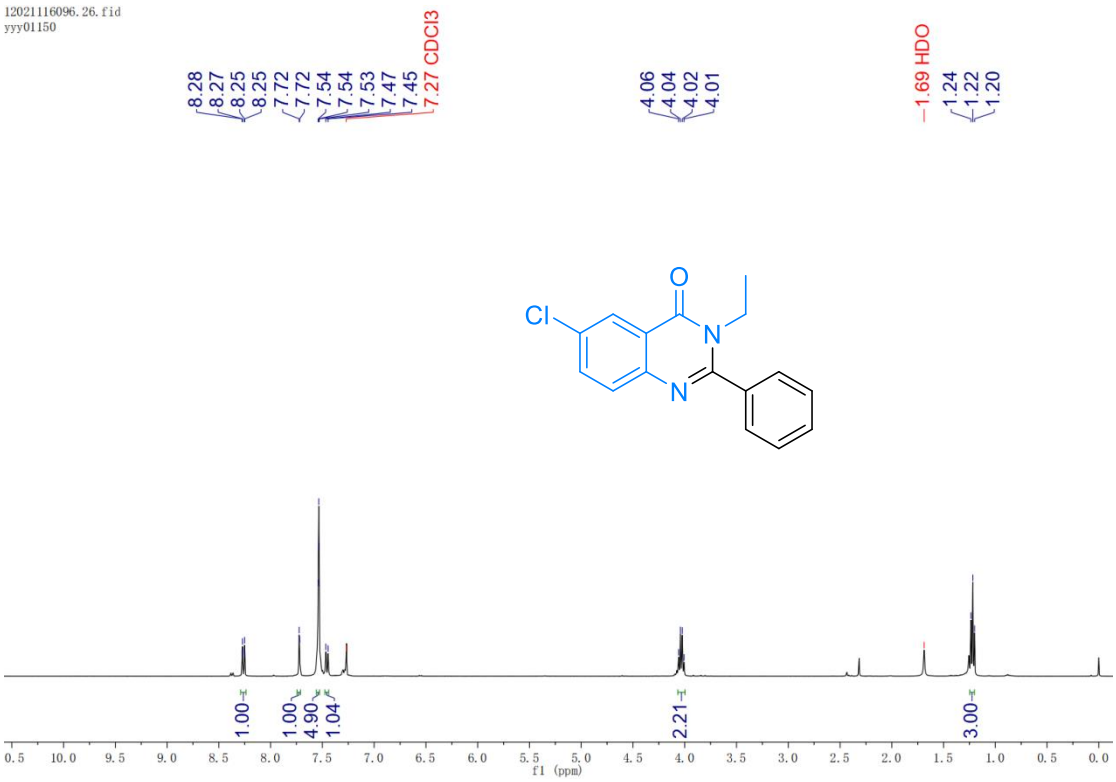
^{1}H-NMR (400 MHz, Chloroform-*d*) **Spectra of compound 7k**



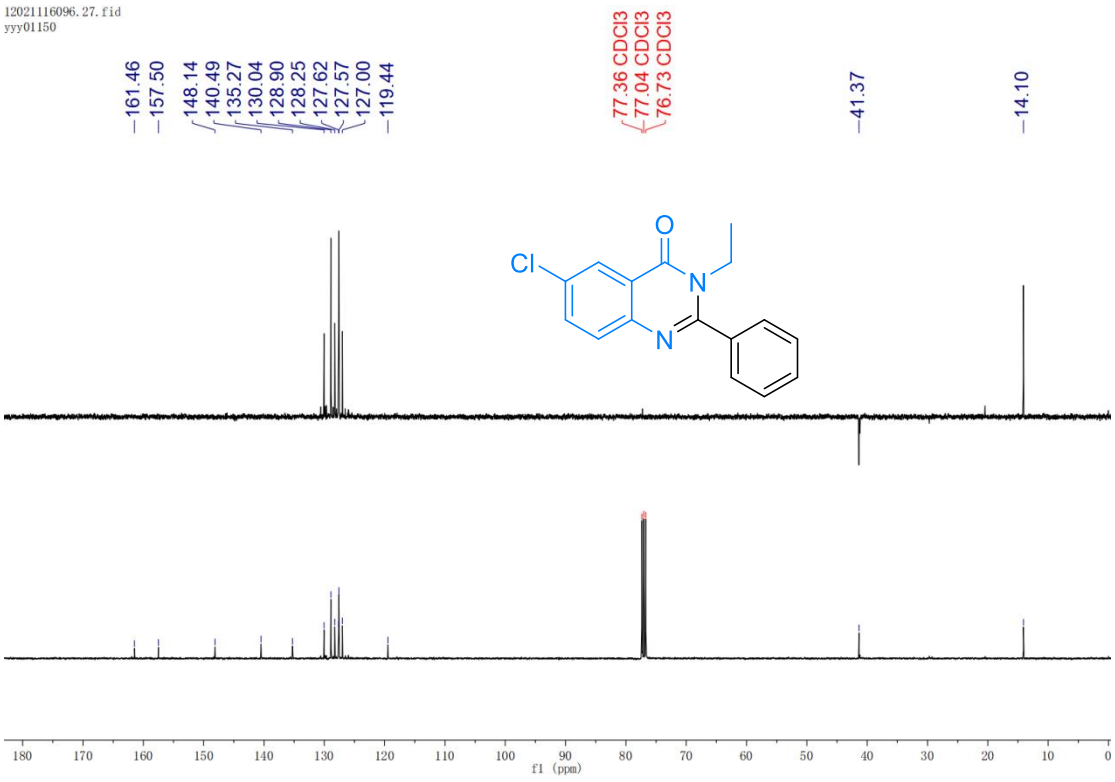
^{13}C-NMR (100 MHz, Chloroform-*d*) **Spectra of compound 7k**



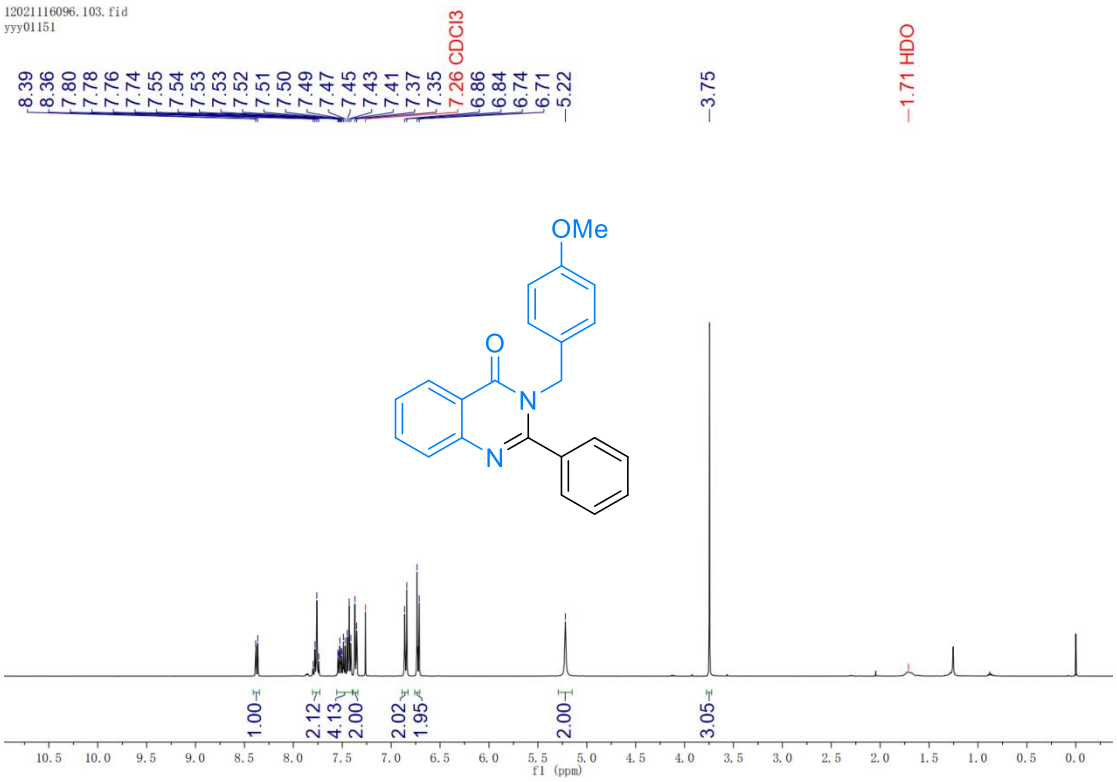
^{19}F NMR (376 MHz, Chloroform-*d*) **Spectra of compound 7k**



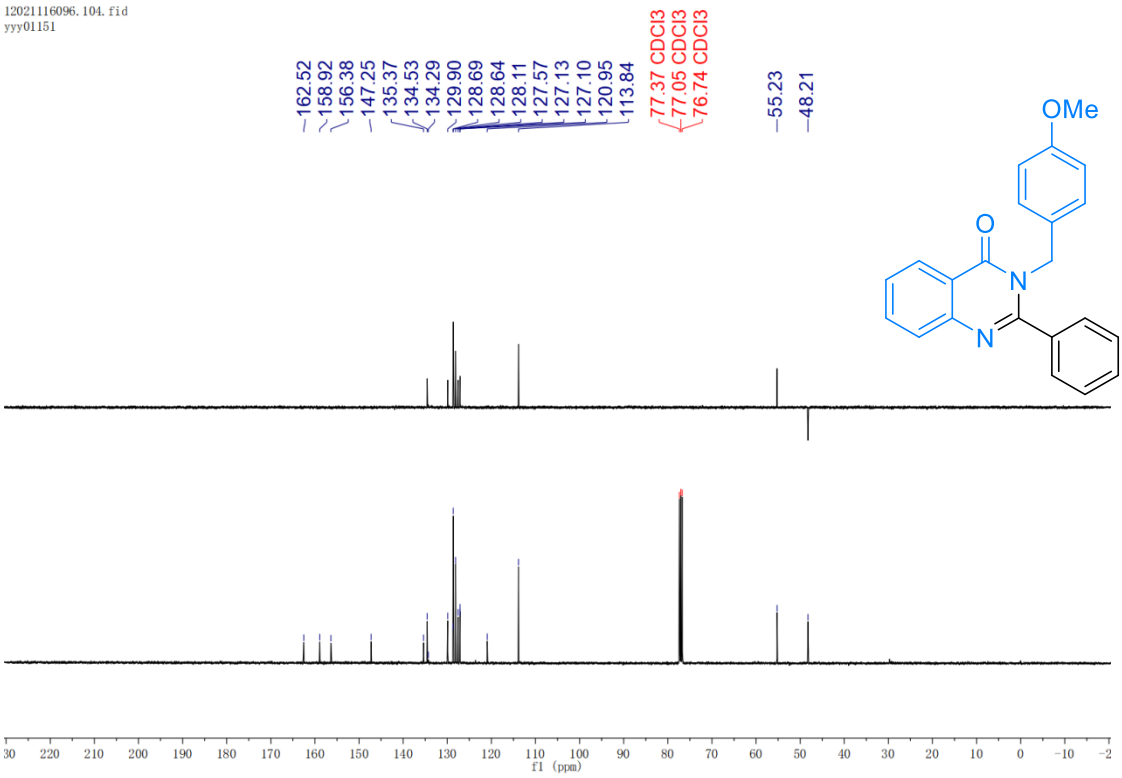
[1]H-NMR (400 MHz, Chloroform-*d*) **Spectra of compound 7l**



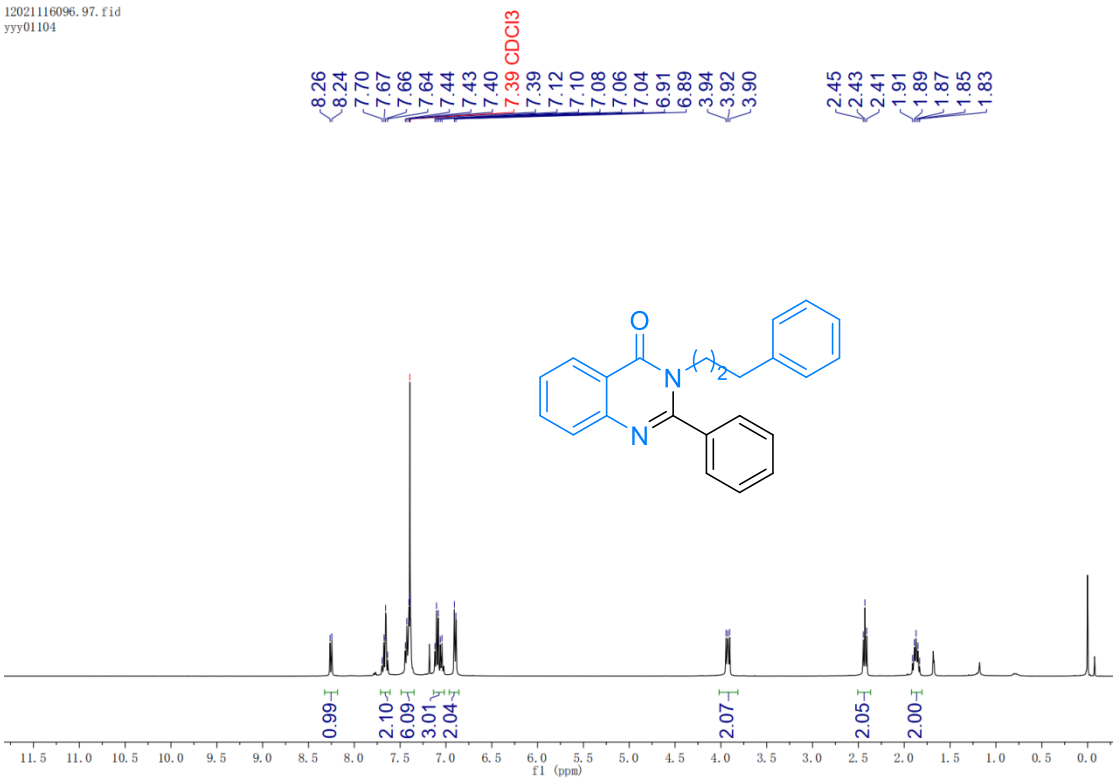
[13]C-NMR (100 MHz, Chloroform-*d*) **Spectra of compound 7l**



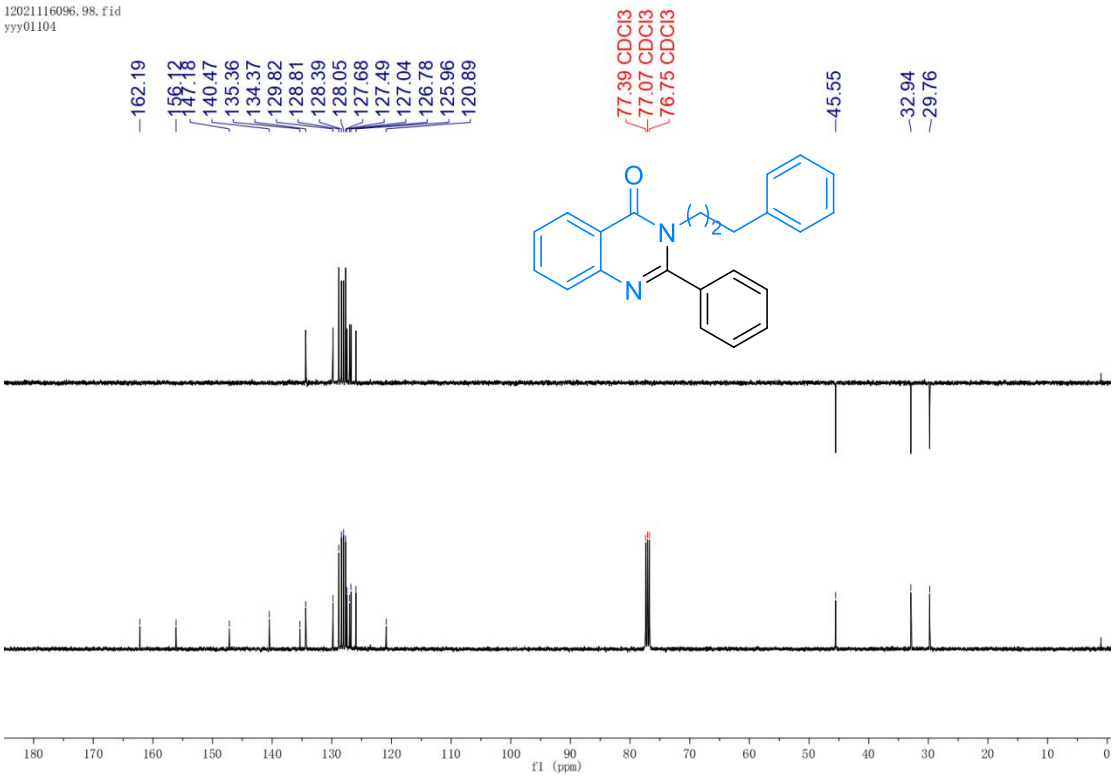
^{1}H-NMR (400 MHz, Chloroform-*d*) **Spectra of compound 7m**



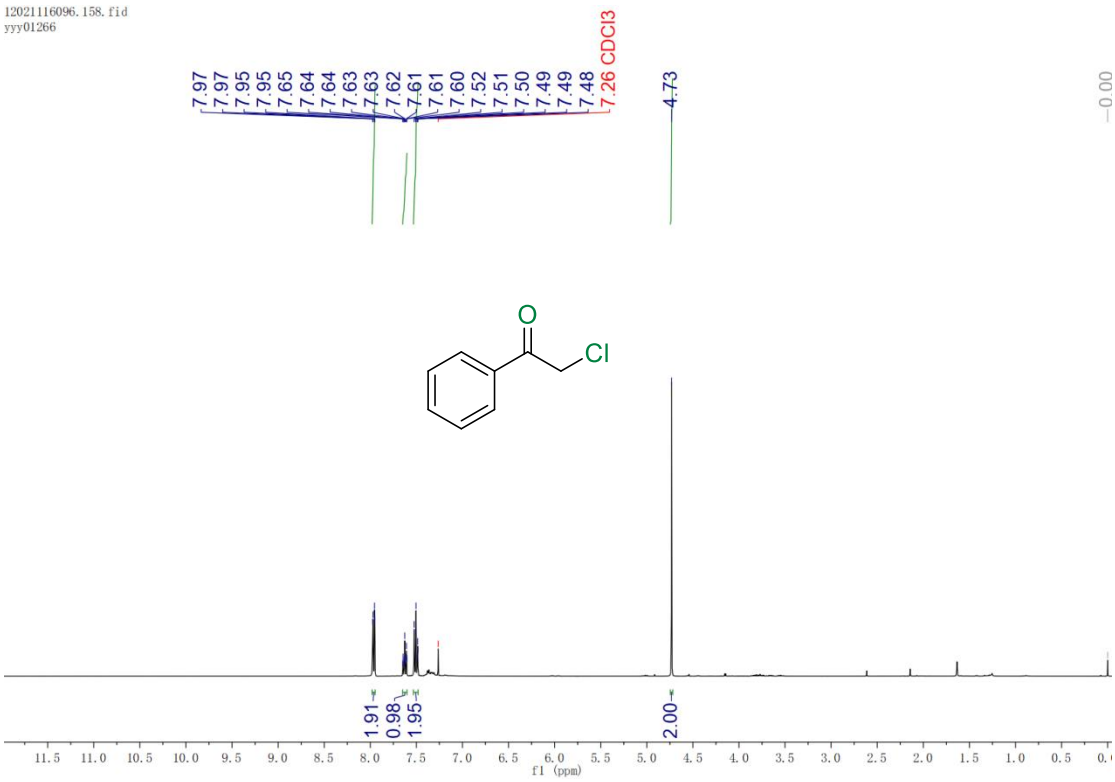
^{13}C-NMR (100 MHz, Chloroform-*d*) **Spectra of compound 7m**



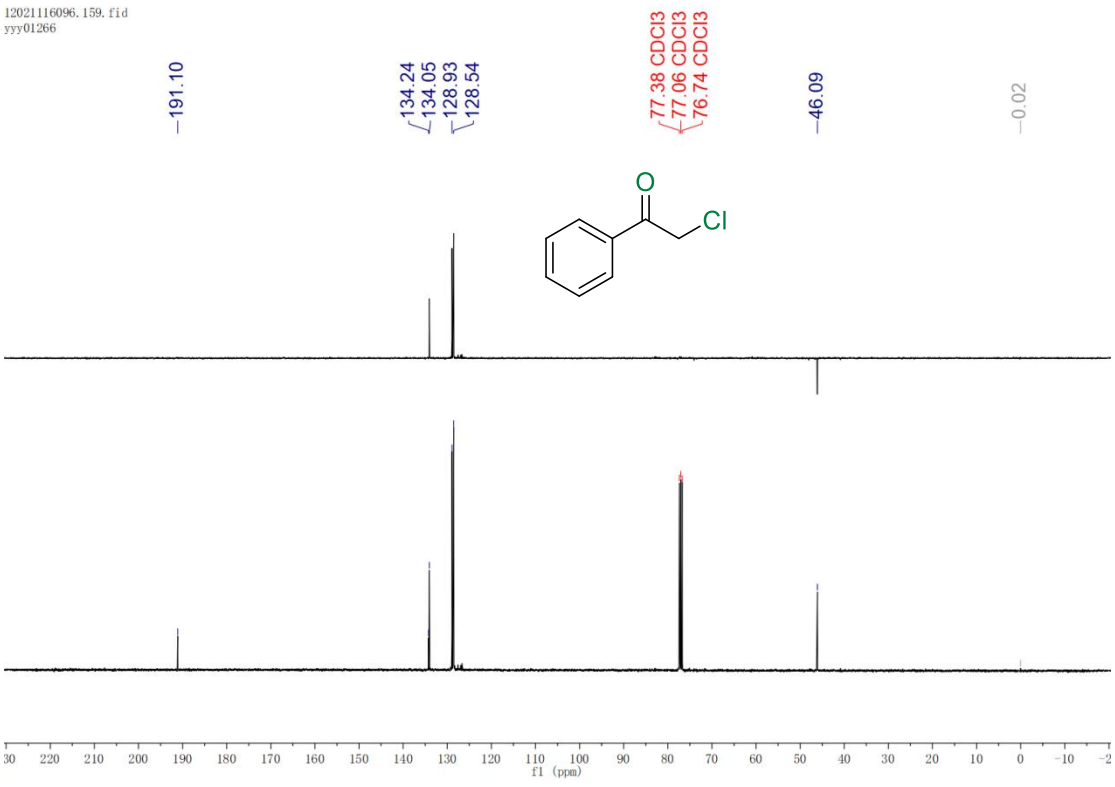
[1]H-NMR (400 MHz, Chloroform-*d*) **Spectra of compound 7n**



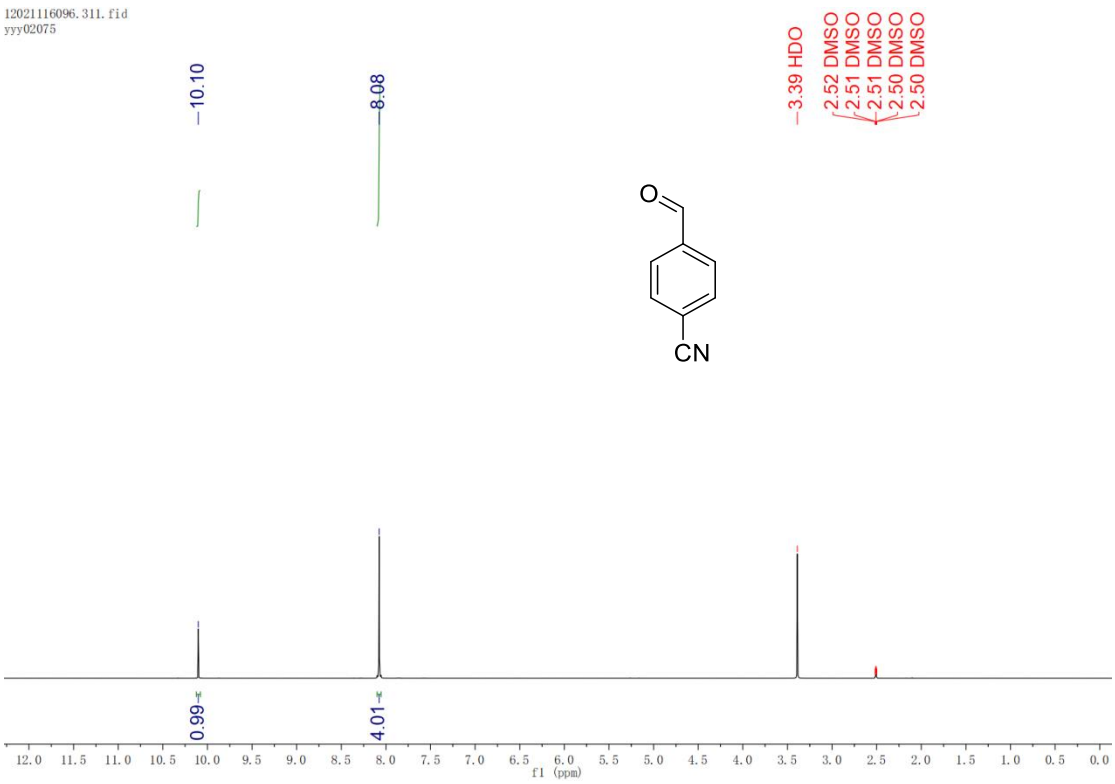
[13]C-NMR (100 MHz, Chloroform-*d*) **Spectra of compound 7n**



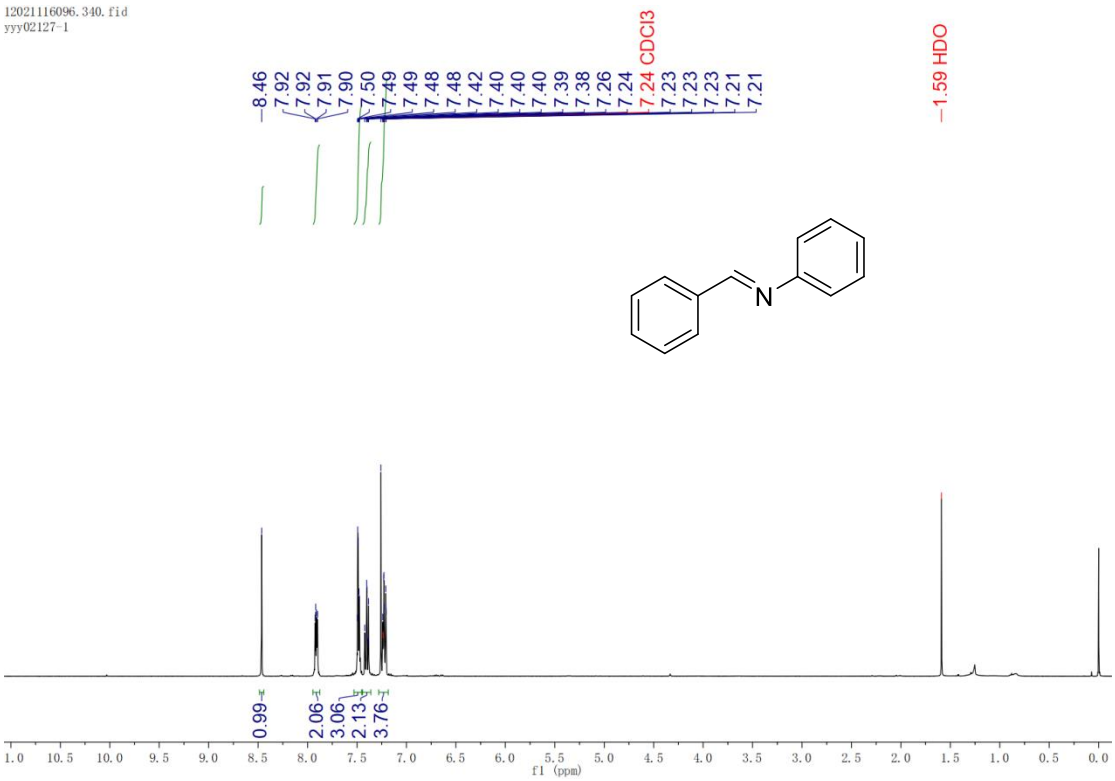
[1]H-NMR (400 MHz, Chloroform-*d*) **Spectra of 9**



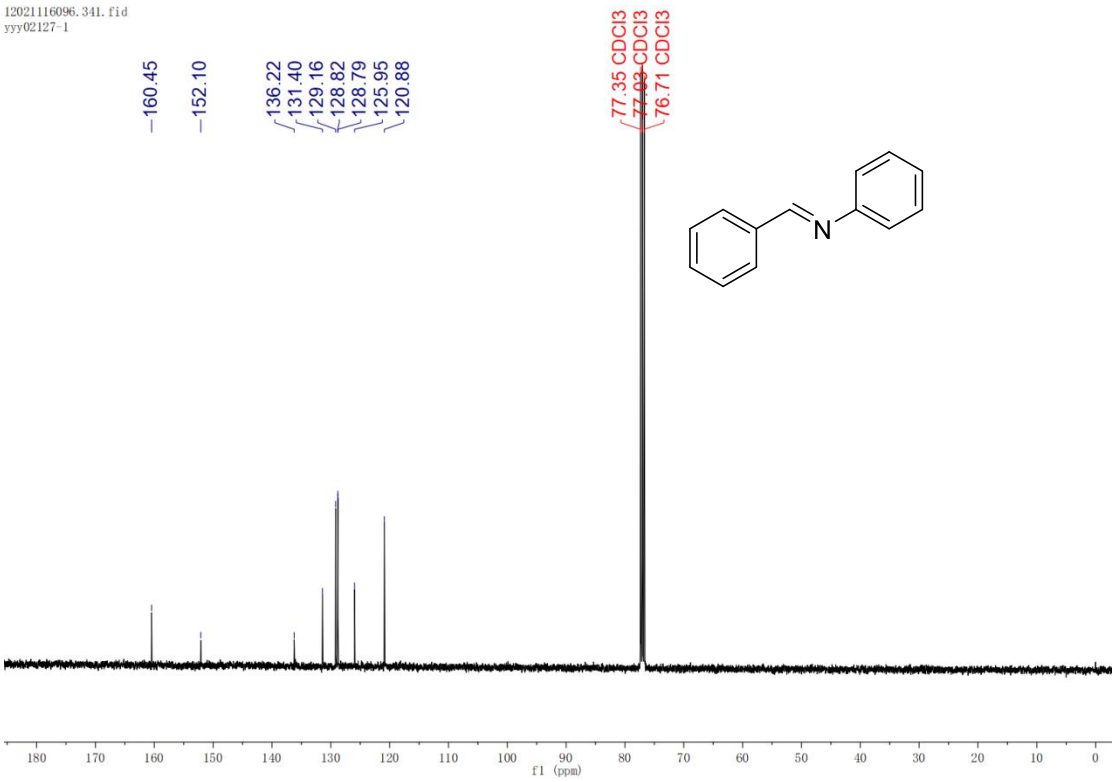
[13]C-NMR (100 MHz, Chloroform-*d*) **Spectra of 9**



^{1}H-NMR (400 MHz, DMSO-d_6) **Spectra of 4-formylbenzonitrile**



^{1}H-NMR (400 MHz, Chloroform-*d*) **Spectra of 11**



^{13}C-NMR (100 MHz, Chloroform-*d*) **Spectra of 11**

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