Supporting Information

Synthesis of 2-Amino-quinazolin-4(*3H*)-ones using 2-Bromo-*N*-phenylbenzamide and Cyanamide Ullmann Cross-Coupling

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1 General considerations

1.1 Materials

Unless otherwise noted, all materials were used as received from commercial sources without further purification.

Table S1. Source of starting material

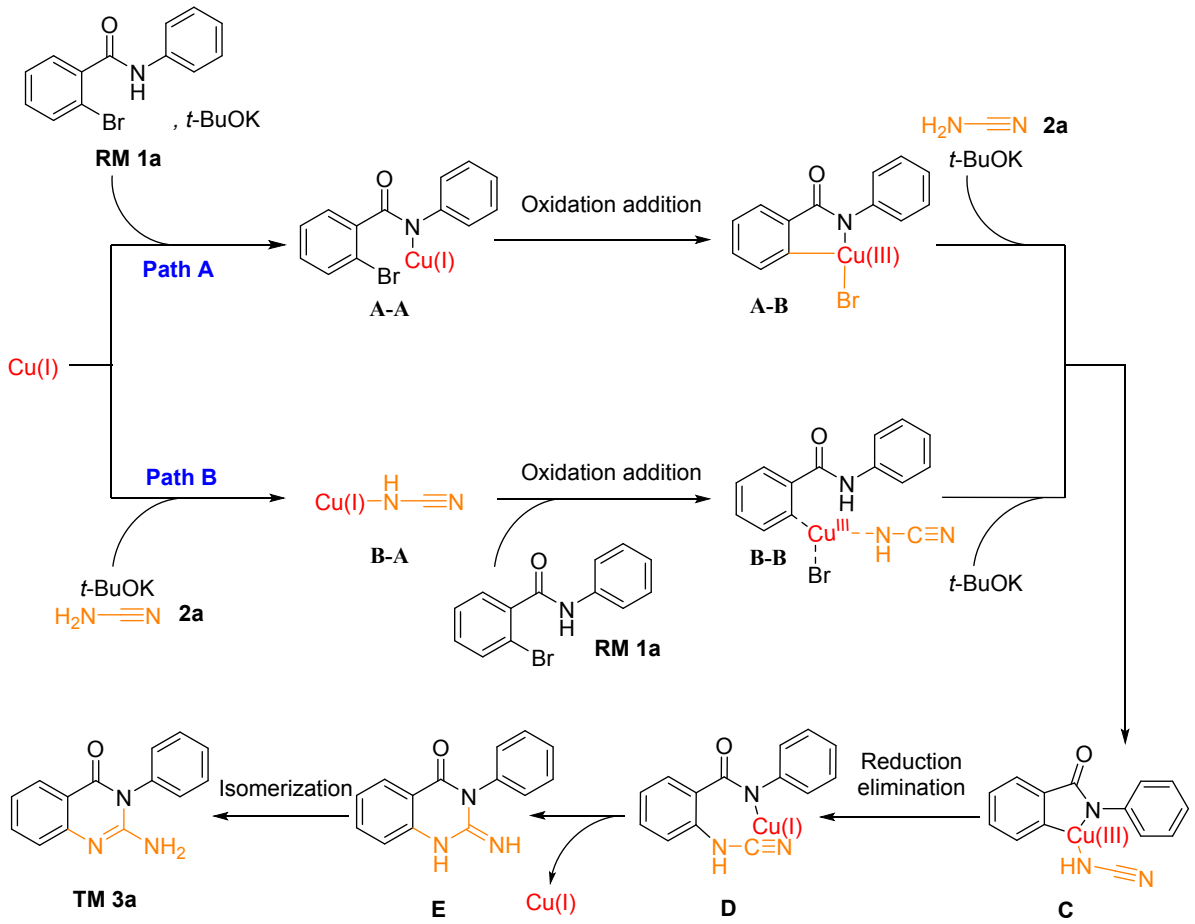
Entry	Material Name	Effective Content	Company
1	Cyanamide	≥95%	Aladdin ®
2	2-Bromobenzoyl chlorides	≥98%	Adamas-beta®
3	Anilines	≥98%	Adamas-beta®
4	Copper(I) Iodide	≥99%	Adamas-beta®
5	Potassium Tert-Butoxide Solution	≥99%	Adamas-beta®
6	Dimethyl Sulfoxide	≥99.9%	Adamas-beta®
7	Ethyl Acetate	≥99.9%	Adamas-beta®
8	Petroleum Ether	Boiling range 60-90˚C	Adamas-beta®
9	Acetonitrile	≥99.9%	Adamas-beta®
10	Other compounds	≥98%	Adamas-beta®

1.2 Instrumentations

^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded on Bruker AV-400/500 MHz NMR spectrometers instrument using $CDCl_3$ or DMSO-d_6 as solvent and Me_4Si as internal standard. High-resolution mass spectra (HRMS) (ESI) were obtained with a Bruker Daltonics APEX II 47e and quadrupole Orbitrap Elite (Q-Exactive) mass spectrometer. Cyanamide was purchased from Aladdin Company (China, purity: 95%) and other commercially available reagents purchased from Tansoole Chemicals, Macklin Biochemical Technology and used as received. Column chromatography was carried out on a flash chromatographic system using silica gel, petroleum ether (60-90 °C) and ethyl acetate as eluent. For thin layer chromatography (TLC), silica gel plates precoated with GF-254 were used. Various 2-bromo-*N*-phenylbenzamides were synthesized by the reaction of the corresponding 2-bromobenzoyl chloride and aniline according to literature procedures.[1-2]

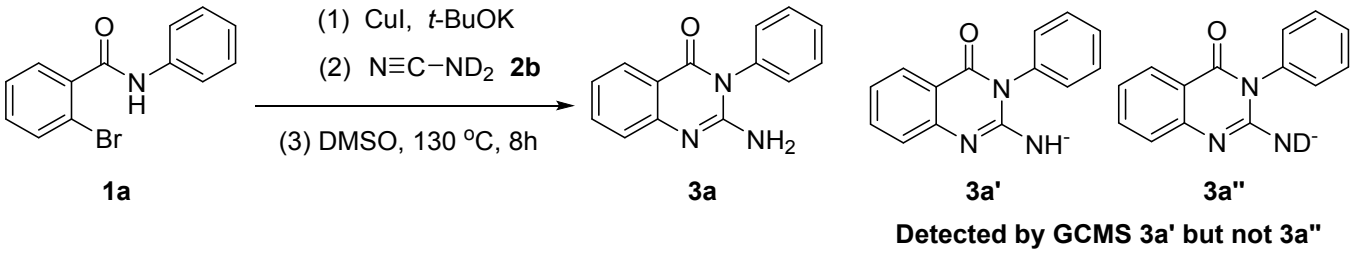
1.3 Possible Mechanistic

Based on control experiments (Supporting Information) and previous literature,[3-4] we propose that a rational mechanism may have two reaction pathways at the initial stage, which coexist and influence the reaction (**Scheme S1**). **Path A**: When a strong base is present, 2-bromobenzamide loses a hydrogen atom and then reacts with Cu(I) to form the Cu(I)-containing intermediate **A-A**. This intermediate undergoes an oxidation addition reaction, resulting in the generation of intermediate **A-**



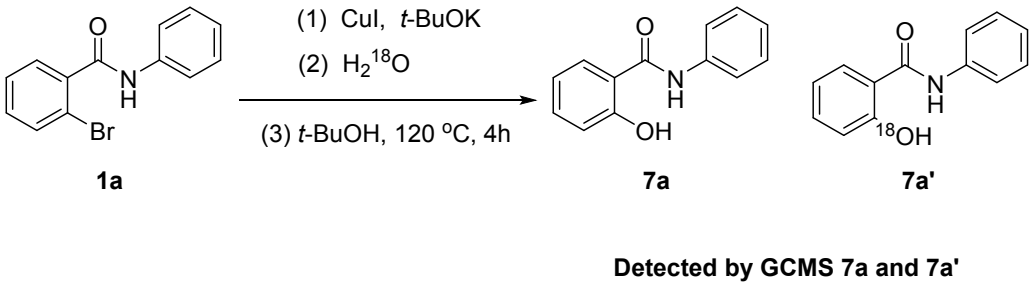
Scheme S1. Proposed mechanism

B. The interaction of cyanamide with potassium *tert*-butoxide, followed by the exchange of ligands with intermediate **A**-**B**, leads to the formation of intermediate **C**. **Path B**: Initially, cyanamide, in the presence of potassium *tert*-butoxide, undergoes deprotonation and coordinates with Cu(I), leading to the formation of the intermediate **B**-**A**. This is followed by an oxidation addition reaction between the intermediate **B**-**A** and 2-bromophenylbenzamide, which results in the formation of the intermediate **B**-**B**. Subsequently, the intermediate **B**-**B** undergoes intramolecular debromination and ligand exchange with the amide, resulting in the formation of intermediate **C**. Intermediate **C** undergoes a reduction elimination to form intermediate **D**, which is ring-closed to form intermediate **E**. Then, Cu(I) is then released and re-enters the catalytic cycle. Finally, the target product **3a** is formed by the intramolecular isomerization of intermediate **E**.



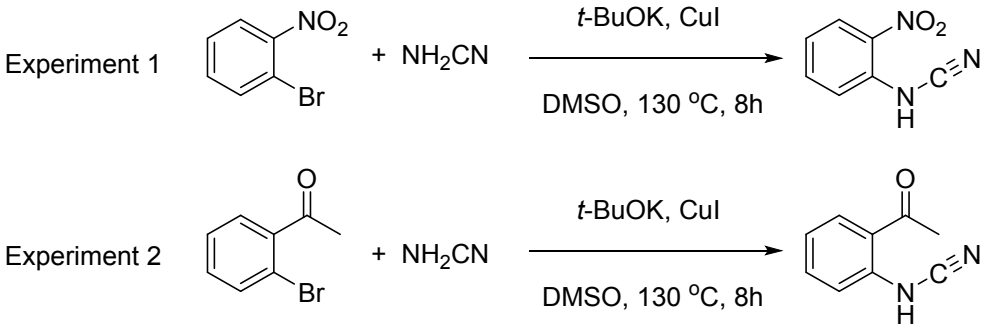
Scheme S2. Mechanism Experiment

We designed a mechanism experiment in which we added deuterated cyanamide instead of cyanamide under optimal conditions. The reacted solution detected by GCMS (**Scheme S2** and **Figure S187-S188**), and there was not obtained deuterated **3a′**but not **3a″**, unexpected. Indirectly, it was demonstrated that the hydrogen atom was not come from cyanamide during the aromatization.



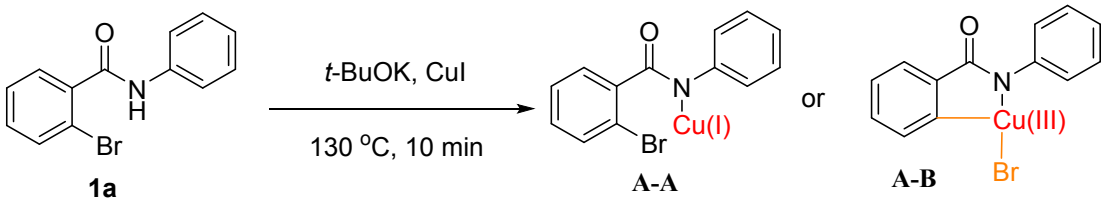
Scheme S3. Mechanism Experiment

Another mechanistic experiment was designed that under the optimal conditions, $H_2{}^{18}O$ instead of cyanamide reacted with 2-bromo-N-phenylbenzamide to obtain compounds **7a**, **7a′** and were confirmed by HRMS. The ratio of **7a** and **7a′** was determined to be 24.1:75.9 (**Scheme S3** and **Figure S189**). The absence of the heavy oxygen-substituted product **7a** was attributed to the presence of a little of water in the DMSO.



Scheme S4. Mechanism Experiment

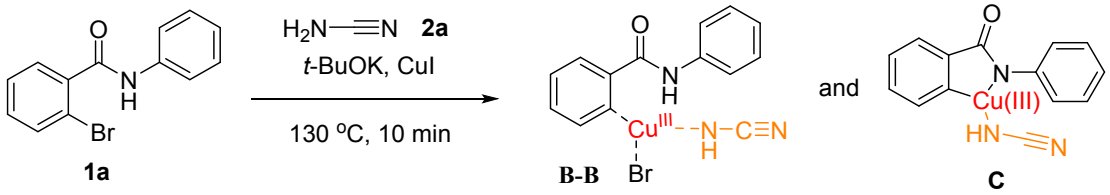
To demonstrate the effect of the presence of a strong electron-absorbing group in the adjacent position on the reaction, we designed two sets of experiments in which 2-bromonitrobenzene and 2-bromoacetophenone were used instead of 2-bromo-*N*-phenylbenzamide for the reaction with cyanamide under optimal conditions (**Scheme S4**). We monitored their production in small quantities by high-resolution mass spectrometry detection, but unfortunately, probably due to a bad reaction, we finally did not get a pure compound after many experiments and purification (**Figure S190-S191**).



Scheme S5. Mechanism Experiment

In the initial stage of the experiment, the addition of raw material cyanamine **2a** was omitted, and the reaction was allowed

to proceed for a period of 10 minutes (**Scheme S5**). Subsequently, the sample was subjected to high-resolution mass spectrometry, which found a mass spectrum with a molecular weight of 335.9092 (exact mass of intermediate **A-A** or intermediate **A-B**: 335.9091, **Figure S192**). This finding corroborated the presence of either intermediate **A-A** or intermediate **A-B**. Although it is not possible to distinguish with certainty between intermediate **A-A** or intermediate **A-B**, in combination with the incomplete reaction of 2-bromonitrobenzene, it is possible to determine that the reaction mechanism undergoes a **Path A** process.



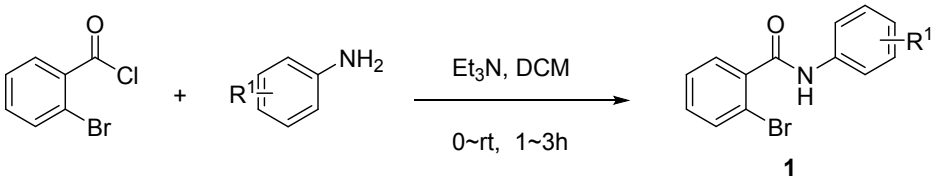
Scheme S6. Mechanism Experiment

The reaction duration was shortened to 10 minutes, and the reaction mixture was cooled in accordance with the parameters specified in the standard experimental protocol (**Scheme S6**). Subsequently, high-resolution mass spectrometry analysis was conducted, which identified intermediates **B-B** and **C** with molecular weights of 377.9297 and 298.0042, respectively (with exact masses of 377.9309 for intermediates **B-B** and 298.0047 for intermediates **C**, **Figure S193-S194**). The data presented herein supports the hypothesis that **2a**, copper, and cyanamide undergo oxidative addition and subsequent intramolecular ligand exchange to form intermediate **B-B** along **Path B**. The absence of intermediate **B-A** in the mass spectrometry data may be attributed to the insufficient stability of the cyanamide and copper complexes, which prevents their detection by high-resolution mass spectrometry.

2. General Procedure

2.1 Synthesis Procedure of Substrates.

Synthesis 1



R^1=Me, OMe, *t*-Bu, F, Cl, Br, I, CF_3, OCF_3, NO_2 et al.

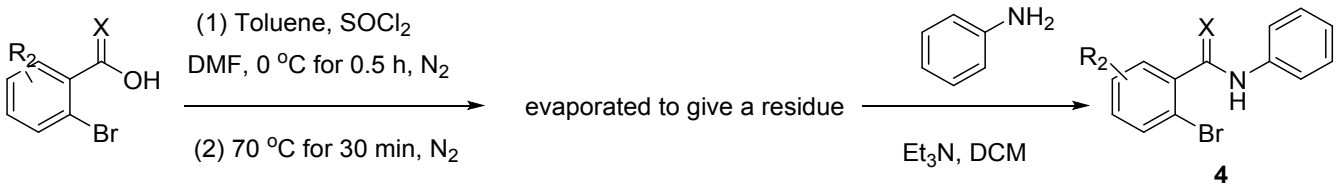
Scheme S7. Synthesis procedure of substrates **1**

The appropriate amine (5 mmol) was added dropwise to 2-bromobenzoyl chloride (1.10 g, 5.0 mmol), THF (20 mL, 0.25 M) and NEt_3 (1.7 mL) at 0 °C. After the addition of amine, the reaction mixture was stirred at room temperature for 1 h. The reaction mixture was then poured into 30 mL of ethyl acetate and washed with saturated aqueous $NaHCO_3$ solution (30 mL) and brine (20 mL). The organic layer was dried over anhydrous $MgSO_4$ and concentrated using a rotary evaporator under

reduced pressure (20 mmHg). This resulted in the formation of a solid, which was then dried under high-vacuum conditions to afford the desired 2-bromo-*N*-phenylbenzamide **1**(1.18 g 86%).

Under nitrogen atmosphere, add 2 g (10 mmol) 2-bromobenzoic acid, 25 mL of toluene (0.25 M), 2 mL of thionyl chloride and several drops of DMF to a 50 mL eggplant-shaped flask, and stop heating after refluxing for 2-3 h. The solvent was evaporated to obtain a yellow oily liquid. Add 20 mL of dichloromethane, and simultaneously add 3 mL of triethylamine and 1.5 mL of benzylamine with a syringe under ice bath conditions. The reaction is basically completed by TLC, washed with 20 mL of hydrochloric acid for 3 times, and washed with saturated saline once. Ethanol was recrystallized to obtain pure product **4** (1.53 g 76%).

Synthesis 4

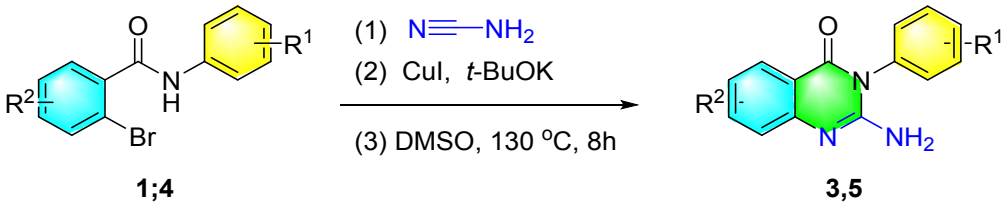


R^2=Me, OMe, Cl; X=O, S

Scheme S8. Synthesis procedure of substrates **4**

2.2 The General Procedure for the Synthesis of Aminoquinazolinone Derivatives 3,5

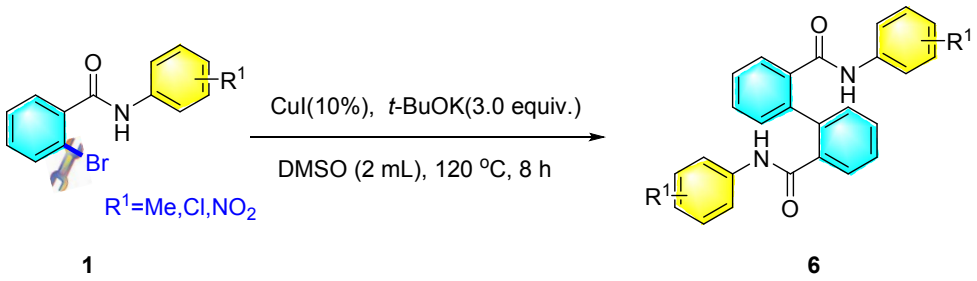
Synthesis 3,5



Scheme S9. Synthesis procedure of substrate **3, 5**

General procedure was followed with 2-bromo-*N*-phenylbenzamide **1a** (0.5 mmol, 138 mg), cyanamide **2a** (1.25 mmol, 53 mg, 2.5 eq.), CuI (0.05 mmol, 10 mg, 10 mol%) in 2 mL dimethyl sulfoxide (0.25 M) and added BuOK (1.5 mmol, 168 mg, 3.0 eq.). Note: The addition of potassium tert-butoxide needed to be added after the addition of the dimethyl sulfoxide solvent, which prevented to act cyanamide with potassium tert-butoxide. After that stirred at 130 ˚C by heating mantle for 8 h under the air atmosphere the reaction completion, the resulting mixture was filtered to remove the solid, the liquor was extracted with ethyl acetate (3×10 mL) and washed with saturated brine (3×10 mL). The resulting organic phase was dried with anhydrous sodium sulfate, and concentrated under reduced pressure. The residue was isolated by column chromatography using petroleum ether and ethyl acetate (v/v 10:1 to 2:1) as eluent to give the pure products and obtain **3a**.

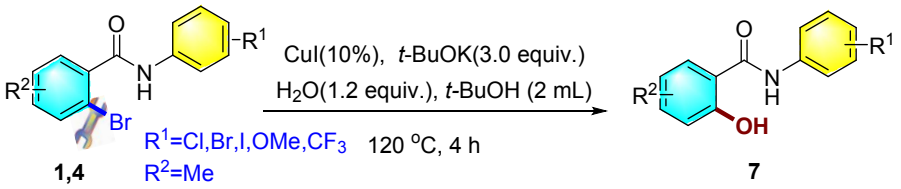
Synthesis 6



Scheme S10. Synthesis procedure of substrate **6**

General procedure was followed with 2-bromo-*N*-phenylbenzamide **1a** (0.5 mmol, 138 mg), CuI (0.05 mmol, 10 mg, 10 mol%), 2 mL DMSO (0.25 M) and added *t*-BuOK (1.5 mmol, 168 mg, 3.0 eq.) in Schlenk reactor. After that stirred at 120 ˚C by heating mantle for 8 h under the air atmosphere the reaction completion, the resulting mixture was filtered to remove the solid, and the liquor was extracted with ethyl acetate (3×10 mL), and washed with saturated brine (3×10 mL). The resulting organic phase was dried with anhydrous sodium sulfate, and concentrated under reduced pressure. The residue was isolated by column chromatography using petroleum ether and ethyl acetate (v/v 15:1) as eluent to give the pure products and obtain **6a**.

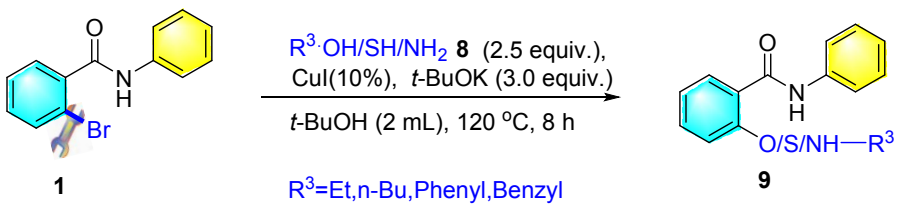
Synthesis 7



Scheme S11. Synthesis procedure of substrate **7**

General procedure was followed with 2-bromo-*N*-phenylbenzamide **1a** (0.5 mmol, 138 mg), H_2O (0.06 mmol, 11 mg, 1.2 eq.), CuI (0.05 mmol, 10 mg,10 mol%), 2 mL *t*-BuOH (0.25 M) and added *t*-BuOK (1.5 mmol, 168 mg, 3.0 eq.) in Schlenk reactor. After that stirred at 120 ˚C by heating mantle for 4 h under the air atmosphere the reaction completion, the resulting mixture was filtered to remove the solid, and the liquor was extracted with ethyl acetate (3×10 mL), and washed with saturated brine (3×10 mL). The resulting organic phase was dried with anhydrous sodium sulfate, and concentrated under reduced pressure. The residue was isolated by column chromatography using petroleum ether and ethyl acetate (v/v 10:1) as eluent to give the pure products and obtain **7a**.

Synthesis 9



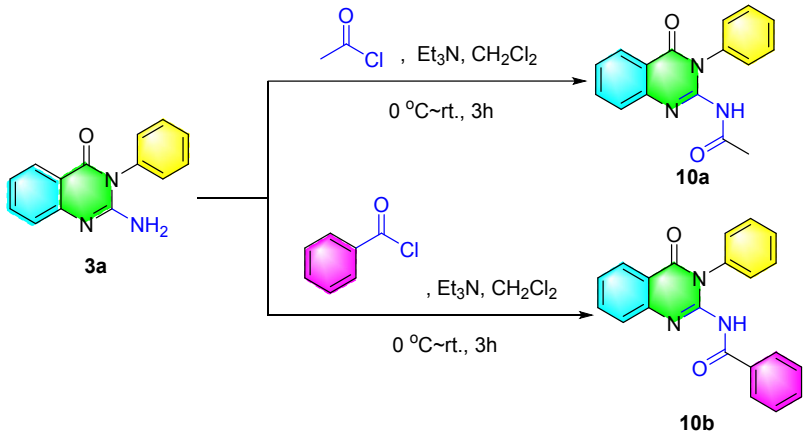
Scheme S12. Synthesis procedure of substrate **9**

General procedure was followed with 2-bromo-*N*-phenylbenzamide **1a** (0.5 mmol, 138 mg), **8a** EtOH (1.25 mmol, 58 mg, 2.5 eq.), CuI (0.05 mmol, 10 mg, 10 mol%), 2 mL *t*-BuOH (0.25 M) and added *t*-BuOK (1.5 mmol, 168 mg, 3.0 eq.) in Schlenk

reactor. After that stirred at 120 ˚C by heating mantle for 4 h under the air atmosphere the reaction completion, the resulting mixture was filtered to remove the solid, and the liquor was extracted with ethyl acetate (3×10 mL), and washed with saturated brine (3×10 mL). The resulting organic phase was dried with anhydrous sodium sulfate, and concentrated under reduced pressure. The residue was isolated by column chromatography using petroleum ether and ethyl acetate (v/v 20:1) as eluent to give the pure products and obtain **9a**.

2.3 The General Procedure for the Synthesis of 2-hydroxy-*N*-phenylbenzamide Derivatives 10

Synthesis 10

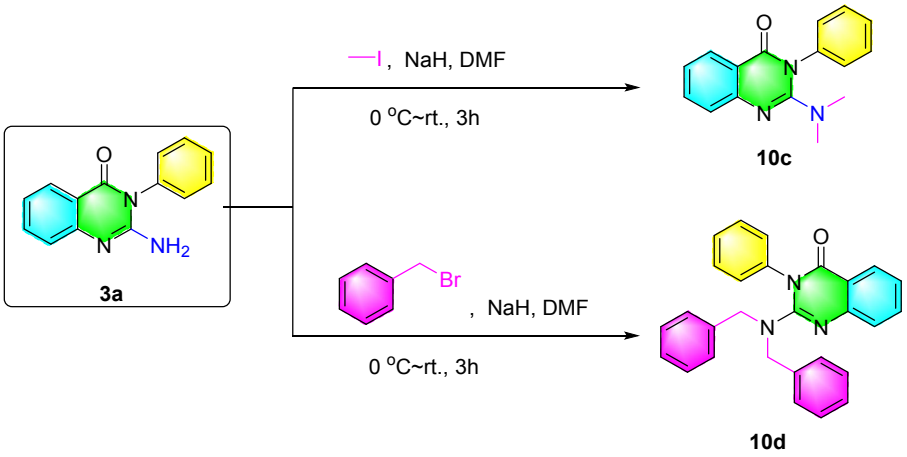


Scheme S13. Synthesis of Quinolinone Derivatives **10a, 10b**

Mixing **3a** (0.5 mmol, 118 mg) and Et_3N (1.5 mmol, 152 mg, 3 eq.) in 5 mL (0.1 M) dichloromethane were stirred at 0-10 °C by ice bath for 30 min, and added acetyl chloride (0.55 mmol, 43mg, 1.1 eq.). Three hours later, the reaction is basically completed by TLC, washed with 20 mL of hydrochloric acid for 3 times, and washed with saturated saline once. Ethanol was recrystallized to obtain pure product **10a** 112 mg (80%).

Mixing **3a** (0.5 mmol, 118 mg) and Et_3N (1.5 mmol, 152 mg, 3 eq.) in 5 mL (0.1 M) dichloromethane were stirred at 0-10 °C by ice bath for 30 min, and added benzoyl chloride (0.55 mmol, 77mg, 1.1 eq.). Three hours later, the reaction is basically completed by TLC, washed with 20 mL of hydrochloric acid for 3 times, and washed with saturated saline once. Ethanol was recrystallized to obtain pure product **10b** 127 mg (74%).

Mixing **3a** (0.5 mmol, 118 mg) and NaH (1.25 mmol, 61 mg, 2.5 eq.) in 5 mL DMF (0.1 M) were stirred at 0 °C by ice-salt bath for 30 min, and added iodomethane (1.0 mmol, 142 mg, 2.0 eq.). Three hours later, the reaction is basically completed by TLC. The reaction liquid was extracted with ethyl acetate (3×10 mL), and washed with saturated brine (3×10 mL). The resulting organic phase was dried with anhydrous sodium sulfate, and concentrated under reduced pressure. The residue was isolated by column chromatography using petroleum ether and ethyl acetate (v/v 20:1) as eluent to give the pure products and obtain **10c** 112 mg (84%).

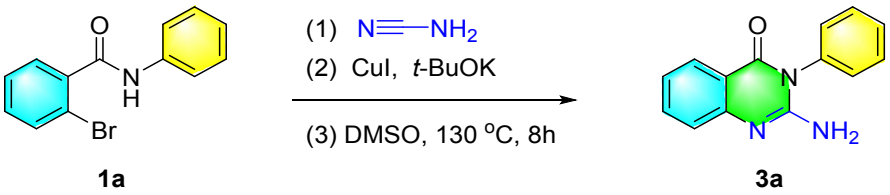


Scheme S14. Synthesis of Quinolinone Derivatives **10c, 10d**

Mixing **3a** (0.5 mmol, 118 mg) and NaH (1.25 mmol, 61 mg, 2.5 eq.) in 5 mL DMF (0.1 M) were stirred at 0 °C by ice-salt bath for 30 min, and added bromoacetonitrile (1.0 mmol, 171 mg, 2.0 eq.). Three hours later, the reaction is basically completed by TLC. The reaction liquid was extracted with ethyl acetate (3×10 mL), and washed with saturated brine (3×10 mL). The resulting organic phase was dried with anhydrous sodium sulfate, and concentrated under reduced pressure. The residue was isolated by column chromatography using petroleum ether and ethyl acetate (v/v 20:1) as eluent to give the pure products and obtain **10d** 162 mg (78%).

2.4 Gram-Scale Synthesis of 3a and Amidation Reaction for the Synthesis of Quinolinone Derivative

(a) Gram-Scale Synthesis of **3a**



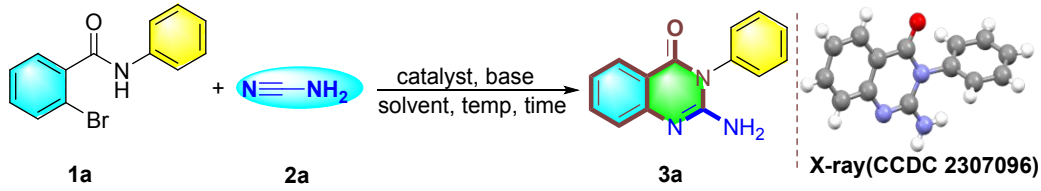
Scheme S15. Gram-Scale Synthesis of **3a**

2-Bromo-*N*-phenylbenzamide (6 mmol, 1.65 g), Cyanamide (15 mmol, 0.63 g, 2.5 eq.), CuI (0.6 mmol, 0.12 g, 10 %mmol) in 24 mL (0.25 M) dimethyl sulfoxide and added *t*-BuOK (18 mmol, 2.02 g, 3.0 eq.) were stirred at 130 ˚C by heating mantle for 12 h under the air atmosphere. After the completion of the reaction, the resulting mixture was filtered to remove the solid, and the liquor was extracted with ethyl acetate (3×50 mL), and washed with saturated brine (3×50 mL). The resulting organic phase was dried with anhydrous sodium sulfate, and concentrated under reduced pressure. The residue was isolated by column chromatography using petroleum ether and ethyl acetate (v/v 4:1) as eluent to give **3a** white solid the pure product (1.07 g, 75%).

3. Analytical Data for Compounds 3-10

3.1 Optimization of the reaction conditions

Table S2. Optimization of Reaction Conditions[a]

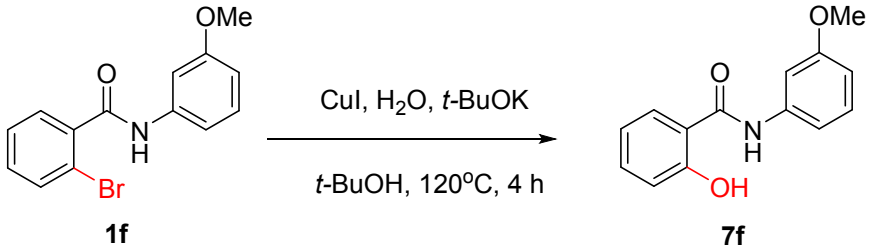


1a **2a** **3a**

Entry	Catalyst	Base	Solvent	Yield/%[b]
1	$CuCl_2$	*t*-BuOK	DMSO	Trace
2	CuCl	*t*-BuOK	DMSO	46
3	CuBr	*t*-BuOK	DMSO	52
4	CuI	*t*-BuOK	DMSO	78
5	CuI	*t*-BuOK	DMSO	77[c]
6	CuI	*t*-BuOK	DMSO	58[d]
7	CuI	*t*-BuOK	DMSO	76[e]
8	CuI	Na_2CO_3	DMSO	28
9	CuI	K_2CO_3	DMSO	35
10	CuI	Cs_2CO_3	DMSO	Trace
11	CuI	KOH	DMSO	40
12	CuI	NaAc	DMSO	62
13	CuI	*t*-BuOK	MeCN	Trace
14	CuI	*t*-BuOK	DMF	33
15	CuI	*t*-BuOK	THF	Trace
16	CuI	*t*-BuOK	MeOH	Trace
17	CuI	*t*-BuOK	DMSO	52[f]
18	CuI	*t*-BuOK	DMSO	78[g]
19	CuI	*t*-BuOK	DMSO	40[h]
20	CuI	*t*-BuOK	DMSO	62[i]
21	CuI	*t*-BuOK	DMSO	55[j]
22	CuI	*t*-BuOK	DMSO	Trace[k]
23	CuI	*t*-BuOK	DMSO	75[l]

[a]Reaction conditions: **1a** (0.5 mmol, 138 mg), cyanamide (1.25 mmol, 53mg, 2.5 equiv.), base (1.5 mmol, 168 mg, 3.0 equiv.) and copper catalyst (0.05 mmol, 10 mg, 10 mol%,) in 2 mL of solvent (0.25 M) stirred at 130 ˚C for 8 h. [b]Isolated yield. [c]Under argon atmosphere. [d]CuI (0.025 mmol, 5 mg, 5 mol%). [e]CuI (0.075 mmol, 15 mg,15 mol%). [f]Cyanamide (1 mmol, 42 mg, 2 equiv.). [g]Cyanamide (1.5 mmol, 63 mg, 3 equiv.). [h]*t*-BuOK (1 mmol, 140 mg, 2.0 equiv.). [i]*t*-BuOK (1.25 mmol, 140 mg, 2.5 equiv.). [j]120 ˚C. [k]2-chloro-N-phenylbenzamide as a reactant. [l]2-iodo-N-phenylbenzamide as a reactant.

Table S3. Optimization of Reaction Conditions[a]



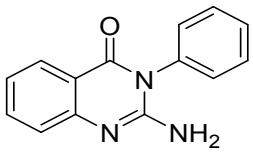
1f **7f**

Entry	Catalyst	Base	Solvent	Yield/%[b]
1	$CuCl_2$	*t*-BuOK	*t*-BuOH	Trace
2	CuCl	*t*-BuOK	*t*-BuOH	22
3	CuBr	*t*-BuOK	*t*-BuOH	34
4	***CuI***	*t-BuOK*	*t*-BuOH	***65***
5	CuI	*t*-BuOK	*t*-BuOH	65[c]
6	CuI	Na_2CO_3	*t*-BuOH	<10
7	CuI	K_2CO_3	*t*-BuOH	<10
8	CuI	KOH	*t*-BuOH	28
9	CuI	NaAc	*t*-BuOH	42
10	CuI	Cs_2CO_3	*t*-BuOH	50
11	CuI	*t*-BuOK	MeCN	Trace
12	CuI	*t*-BuOK	DMSO	52
13	CuI	*t*-BuOK	THF	<10
14	CuI	*t*-BuOK	MeOH	Trace
15	CuI	*t*-BuOK	*t*-BuOH	52[d]
16	CuI	*t*-BuOK	*t*-BuOH	64[e]
17	CuI	*t*-BuOK	*t*-BuOH	38[f]
18	CuI	*t*-BuOK	*t*-BuOH	60[g]
19	CuI	*t*-BuOK	*t*-BuOH	33[h]

[a]Reaction conditions: **1a** (0.5 mmol, 138 mg), H_2O (0.6 mmol, 11 mg, 1.2 equiv.), base (1.5 mmol, 168 mg, 3.0 equiv.) and copper catalyst (0.05 mmol, 10 mg, 10 mol%) in 2 mL of solvent stirred at 120 ˚C for 4 h, under the air atmosphere. [b]Isolated yield. [c]Under the argon atmosphere. [d]CuI (0.025 mmol, 5 mg, 5 mol%), [e]CuI (0.075 mmol, 15 mg,15 mol%). [f]Base 2 equiv. [g]Base 2.5 equiv. [h]110 ˚C.

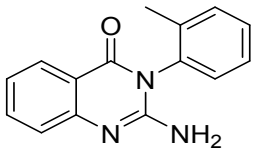
3.2 Analytical Data for Compounds 3-10

2-Amino-3-phenylquinazolin-4(*3H*)-one (**3a**)[5-8]



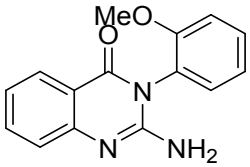
White solid. (93 mg, 78% yield); m. p. 249–251 ˚C. R_f = 0.2 (PE:EA = 1:1, v/v); ^{1}H NMR (400 MHz, DMSO - d_6) δ 7.93 (dd, J = 8.0, 1.6 Hz, 1H), 7.64 - 7.50 (m, 4H), 7.39 (d, J = 7.2 Hz, 2H), 7.30 (d, J = 8.0 Hz, 1H), 7.15 - 7.11 (m, 1H), 6.46 (s, 2H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 161.8, 151.7, 150.0, 135.4, 134.4, 130.0, 129.2, 128.8, 126.5, 123.9, 121.5, 116.8; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{14}H_{12}N_3O$ 238.0975, found 238.0973.

2-Amino-3-(o-tolyl)quinazolin-4(*3H*)-one (**3b**)[6,7]



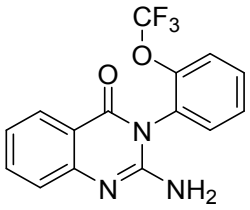
White solid. (103 mg, 82% yield); m. p. 199–200 ˚C. R_f = 0.21 (PE:EA = 1:1, v/v);^{1}H NMR (400 MHz, DMSO - d_6) δ 7.98 (d, J = 8.0 Hz, 1H), 7.65 - 7.61 (m, 1H), 7.47 - 7.39 (m, 3H), 7.36 - 7.31 (m, 2H), 7.15 (t, J = 7.6 Hz, 1H), 6.59 (s, 2H), 2.10 (s, 3H); ^{13}C{^{1}H} NMR (101 MHz, DMSO - d_6) δ 161.3, 151.5, 150.0, 135.8, 134.5, 134.4, 131.3, 129.5, 128.8, 127.7, 126.6, 123.9, 121.6, 116.6, 16.8; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{15}H_{14}N_3O$ 252.1131, found 252.1128.

2-Amino-3-(2-methoxyphenyl)quinazolin-4(*3H*)-one (**3c**)[7]



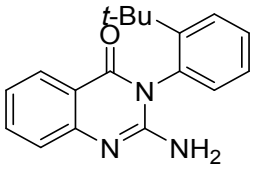
White solid. (111 mg, 83% yield); m. p. 229−231 ˚C. R_f = 0.25 (PE:EA = 1:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 7.91 (dd, J = 8.0, 1.0 Hz, 1H), 7.62-7.58 (m, 1H), 7.51 - 7.48 (m, 1H), 7.31 - 7.22 (m, 3H), 7.13 - 7.10 (m, 2H), 6.39 (s, 2H), 3.75 (s, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 161.4, 154.9, 151.9, 150.2, 134.3, 130.9, 130.1, 126.5, 123.9, 123.5, 121.4, 121.2, 116.7, 112.9, 55.7; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{15}H_{14}N_3O_2$ 268.1081, found 268.1080.

2-Amino-3-(2-(trifluoromethoxy)phenyl) quinazolin-4(*3H*)-one (**3d**)



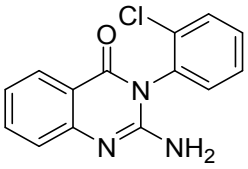
White solid. (128 mg, 80% yield); m. p. 242−246 ˚C. R_f = 0.21 (PE:EA = 1:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 7.80 (dd, J = 7.5, 1.0 Hz, 1H), 7.70-7.54 (m, 5H), 7.31 (d, J = 8.5 Hz, 1H), 7.18 - 7.14 (m, 1H), 6.78 (s, 2H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 161.2, 151.3, 149.8, 144.9 (d, J = 1.3 Hz), 134.8, 131.6, 131.5, 128.6, 127.3, 126.6, 123.7, 121.8, 121.4, 119.9 (q, J = 258.3 Hz), 116.1; ^{19}F NMR (376 MHz, DMSO-d_6) δ -56.1; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{15}H_{11}F_3N_3O_2$ 322.0798, found 322.0797.

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



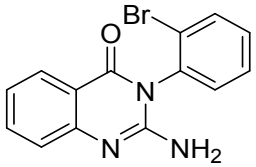
White solid. (68 mg, 46% yield); m. p. 256–258 ˚C. R_f = 0.25 (PE:EA = 1:1, v/v); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, J = 8.0 Hz, 1H), 7.73 (d, J = 8.0 Hz, 1H), 7.61 (t, J = 7.6 Hz, 1H), 7.51 (t, J = 7.6 Hz, 1H), 7.40 (t, J = 7.2 Hz, 1H), 7.28 (d, J = 8.0 Hz, 1H), 7.21 (t, J = 7.6 Hz, 1H), 7.11 (d, J = 8.0 Hz, 1H), 5.47 (s, 2H), 1.32 (s, 9H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 163.1, 152.1, 149.0, 147.9, 134.9, 132.4, 130.9, 130.6, 130.3, 128.4, 127.7, 123.8, 123.0, 117.7, 36.5, 31.7; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{18}H_{20}N_3O$ 294.1601, found 294.1599.

2-Amino-3-(2-chlorophenyl)quinazolin-4(*3H*)-one (**3f**)



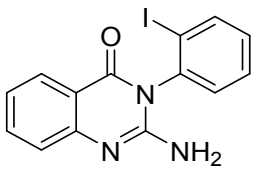
White solid. (106 mg, 78% yield); m. p. 232–234 ˚C. R_f = 0.2 (PE:EA = 1:1, v/v); ^{1}H NMR (400 MHz, DMSO - d_6) δ 7.95 (dd, J = 8.0, 1.6 Hz, 1H), 7.74 - 7.72 (m, 1H), 7.66 - 7.62 (m, 1H), 7.60 - 7.55 (m, 3H), 7.31 (d, J = 8.4 Hz, 1H), 7.15 (t, J = 7.6 Hz, 1H), 6.70 (s, 2H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 161.2, 151.1, 150.2, 134.7, 132.9, 132.1, 131.2, 131.2, 130.5, 128.9, 126.6, 123.9, 121.7, 116.4; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{14}H_{11}ClN_3O$ 272.0585, found 272.0584.

2-Amino-3-(2-bromophenyl)quinazolin-4(*3H*)-one (**3g**)[6]



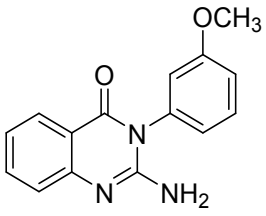
White solid. (115 mg, 73% yield); m. p. 238–240 ˚C. R_f = 0.2 (PE:EA = 1:1, v/v); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 7.6 Hz, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.58 (t, *J* = 7.2 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 1H), 7.38-7.35 (m, 2H), 7.27 (d, *J* = 8.4 Hz, 1H), 7.18 (d, *J* = 8.0 Hz, 1H), 4.74 (s, 2H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 161.5, 150.2, 148.6, 135.3, 134. 7, 134.4, 131.8, 130.6, 129.7, 127.7, 124.1, 123.5, 117.5; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{14}H_{11}BrN_3O$ 316.0080, found 316.0080.

2-Amino-3-(2-iodophenyl)quinazolin-4(*3H*)-one (**3h**)



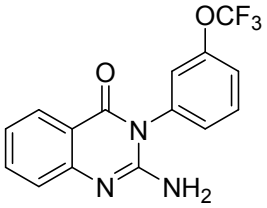
White solid. (11 mg, <10% yield); m. p. 244–246˚C. R_f = 0.2 (PE:EA = 1:1, v/v); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.0 Hz, 1H), 7.90 (d, *J* = 7.6 Hz, 1H), 7.64-7.56 (m, 2H), 7.48 (d, *J* = 7.2 Hz, 1H), 7.29 - 7.24 (m, 2H), 7.12 (t, *J* = 7.6 Hz, 1H), 6.37 (s, 2H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 161.2, 150.8, 150.4, 139.8, 138.3, 134.6, 131.0, 130.2, 130.1, 126.6, 124.0, 121.4, 116.7, 100.4; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{14}H_{11}IN_3O$ 363.9941, found 363.9945.

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



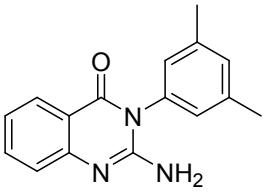
White solid. (107 mg, 80% yield); m. p. 231−233 ˚C. R_f = 0.24 (PE:EA = 1:1, v/v); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, *J* = 8.0 Hz, 1H), 7.63 (t, *J* = 7.6 Hz, 1H), 7.50 (t, *J* = 8.0 Hz, 1H), 7.32 (d, *J* = 8.4 Hz, 1H), 7.22 (t, *J* = 7.6 Hz, 1H), 7.08 (d, *J* = 8.8 Hz, 1H), 6.93 (d, *J* = 7.6 Hz, 1H), 6.87 (s, 1H), 5.22 (s, 2H), 3.84 (s, 3H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 162.2, 161.4, 151.0, 148.4, 135.9, 135.1, 131.5, 127.6, 123.8, 123.4, 120.4, 117.6, 116.2, 114.0, 55.7; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{15}H_{14}N_3O_2$ 268.1080, found 268.1079.

Amino-3-(3-(trifluoromethoxy)phenyl)quinazolin-4(*3H*)-one (**3j**)



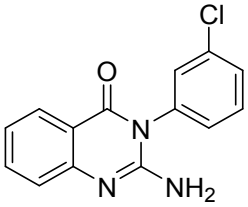
White solid. (119 mg, 74% yield); m. p. 243−246 ˚C. R_f = 0.21 (PE:EA = 1:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 7.91 (dd, J = 7.5, 1.0 Hz, 1H), 7.72 - 7.68 (m, 1H), 7.63 - 7.60 (m, 1H), 7.52 - 7.51 (m, 2H), 7.45-7.43 (d, J = 8.0 Hz, 1H), 7.27 (d, J = 8.5 Hz, 1H), 7.13 (t, J = 7.5 Hz, 1H), 6.51 (s, 2H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 161.8, 151.4, 150.2, 149.1 (d, J = 1.25 Hz), 137.0, 134.5, 131.5, 128.3, 126.5, 123.9, 122.1, 121.6, 121.5, 120.0 (q, J = 258.0), 116.7; ^{19}F NMR (376 MHz, DMSO-d_6) δ -56.8; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{15}H_{11}F_3N_3O_2$ 322.0798, found 322.0796.

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



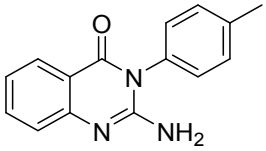
White solid. (103 mg, 78% yield); m. p. 235−237 ˚C. R_f = 0.23 (PE:EA = 1:1, v/v); ^{1}H NMR (400 MHz, DMSO - d_6) δ 7.02 (dd, J = 8.0, 1.6 Hz, 1H), 6.70 - 6.66 (m, 1H), 6.38 (d, J = 8.0 Hz, 1H), 6.22 - 6.18 (m, 2H), 6.06 (s, 2H), 5.57 (s, 2H), 1.42 (s, 6H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 161.8, 151.7, 150.0, 139.2, 135.2, 134.3, 130.6, 126.4, 126.1, 123.9, 121.5, 116.8, 20.8; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{16}H_{16}N_3O$ 266.1288, found 266.1287.

2-Amino-3-(3-chlorophenyl)quinazolin-4(*3H*)-one (**3l**)



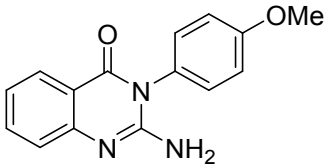
White solid. (102 mg, 75% yield); m. p. 241–243 ˚C. R_f = 0.2 (PE:EA = 1:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 7.91 (d, J = 8.0 Hz, 1H), 7.63 - 7.56 (m, 4H), 7.38 - 7.36 (m, 1H), 7.27 (d, J = 7.5 Hz, 1H), 7.12 (t, J = 7.5 Hz, 1H), 6.54 (s, 2H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 161.8, 151.4, 150.0, 136.8, 134.5, 133.9, 131.4, 129.3, 129.2, 127.9, 126.5, 123.8, 121.5, 116.6; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{14}H_{11}ClN_3O$ 272.0585, found 272.0583.

2-Amino-3-(p-tolyl)quinazolin-4(*3H*)-one (**3m**)[6,8]



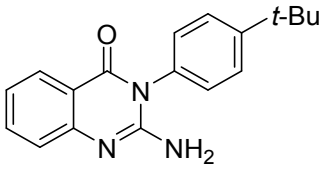
White solid. (108 mg, 86% yield); m. p. 265–267 ˚C. R_f = 0.21 (PE:EA = 1:1, v/v); ^{1}H NMR (400 MHz, DMSO - d_6) δ 7.90 (dd, J = 8.0, 1.6 Hz, 1H), 7.63 - 7.59 (m, 1H), 7.37 (d, J = 8.4 Hz, 2H), 7.27 - 7.22 (m, 3H), 7.14 - 7.10 (m, 1H), 6.37 (s, 2H), 2.40 (s, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 161.8, 151.8, 149.8, 138.5, 134.3, 132.7, 130.5, 128.5, 126.5, 123.8, 121.5, 116.8, 20.8; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{15}H_{14}N_3O$ 252.1131, found 252.1130.

2-Amino-3-(4-methoxyphenyl)quinazolin-4(*3H*)-one (**3n**)[6-8]



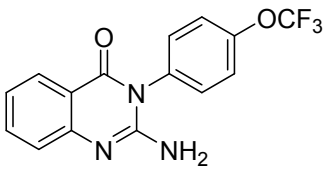
White solid. (111 mg, 83% yield); m. p. 216–218 ˚C. R_f = 0.21 (PE:EA = 1:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 7.90 (dd, J = 8.0, 1.5 Hz, 1H), 7.61 - 7.58 (m, 1H), 7.29 - 7.24 (m, 3H), 7.13 - 7.09 (m, 3H), 6.33 (s, 2H), 3.83 (s, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 162.0, 159.5, 152.1, 150.1, 134.3, 129.9, 127.8, 126.5, 123.9, 121.4, 116.8, 115.2, 55.4; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{15}H_{14}N_3O_2$ 268.1081, found 268.1079.

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



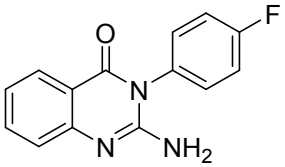
White solid. (123 mg, 84% yield); m. p. 272–274 ˚C. R_f = 0.24 (PE:EA = 1:1, v/v); ^{1}H NMR (400 MHz, DMSO - d_6) δ 7.89 (d, J = 8.0 Hz, 1H), 7.62 - 7.56 (m, 3H), 7.27 - 7.24 (m, 3H), 7.12 (t, J = 8.0 Hz, 1H), 6.24 (s, 2H), 1.35 (s, 9H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 161.9, 151.7, 151.4, 150.0, 134.3, 132.7, 128.2, 126.7, 126.5, 123.9, 121.4, 116.8, 34.5, 31.1; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{18}H_{20}N_3O$ 294.1601, found 294.1598.

2-Amino-3-(4-(trifluoromethoxy)phenyl)quinazolin-4(*3H*)-one (**3p**)



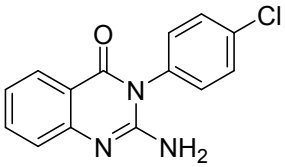
White solid. (122 mg, 76% yield); m. p. 253–255 ˚C. R_f = 0.21 (PE:EA = 1:1, v/v); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.0 Hz, 1H), 7.64 (t, *J* = 8.0 Hz, 1H), 7.46 -7.41 (m, 4H), 7.32 (d, *J* = 8.0 Hz, 1H), 7.23 (t, *J* = 7.6 Hz, 1H), 5.08 (s, 2H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 162.2, 150.5, 150.2(d, *J* = 2.0 Hz), 148.4, 135.3, 133.2, 130.5, 127.6, 124.0, 123.6, 123.0, 121.8, 119.2, 117.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.8; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{15}H_{11}F_3N_3O_2$ 322.0798, found 322.0797.

2-Amino-3-(4-fluorophenyl)quinazolin-4(*3H*)-one (**3q**)[8]



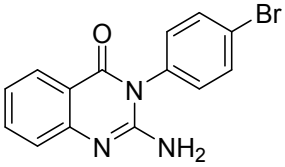
White solid. (97 mg, 76% yield); m. p. 247–249 ˚C. R_f = 0.2 (PE:EA = 1:1, v/v); ^{1}H NMR (400 MHz, DMSO - d_6) δ 7.91 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.63 - 7.59 (m, 1H), 7.47 - 7.38 (m, 4H), 7.27 (d, *J* = 8.4 Hz, 1H), 7.12 (t, *J* = 7.2 Hz, 1H), 6.54 (s, 2H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 163.2, 161.9, 161.3, 151.8, 150.1, 134.4, 131.7 (d, *J* = 2.5 Hz), 131.2 (d, *J* = 8.8 Hz), 126.5, 123.9, 121.5, 116.8 (d, *J* = 23.9 Hz), 116.7; ^{19}F NMR (376 MHz, DMSO-d_6) δ -112.9; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{14}H_{11}FN_3O$ 256.0881, found 256.0878.

2-Amino-3-(4-chlorophenyl)quinazolin-4(*3H*)-one (**3r**)[6]



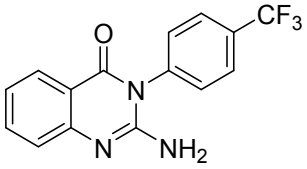
White solid. (109 mg, 80% yield); m. p. 255–258 ˚C. R_f = 0.2 (PE:EA = 1:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 7.89 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.63 - 7.59 (m, 3H), 7.43 - 7.40 (m, 2H), 7.25 (d, *J* = 8.0 Hz, 1H), 7.13 - 7.10 (m, 1H), 6.46 (s, 2H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 161.8, 151.5, 150.1, 134.4, 133.8, 130.9, 123.0, 126.5, 123.9, 121.4, 116.6; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{14}H_{11}ClN_3O$ 272.0585, found 272.0584.

2-Amino-3-(4-bromophenyl)quinazolin-4(*3H*)-one (**3s**)[8]



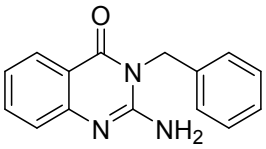
White solid. (111 mg, 70% yield); m. p. 231–233 ˚C. R_f = 0.2 (PE:EA = 1:1, v/v); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 7.6 Hz, 1H), 7.76 (d, *J* = 8.4 Hz, 2H), 7.65 (t, *J* = 7.2 Hz, 1H), 7.32 (d, *J* = 8.4 Hz, 1H), 7.28-7.23 (m, 3H), 4.94 (s, 2H); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 162.2, 150.6, 148.4, 135.3, 134.0, 134.0, 130.4, 127.6, 124.5, 124.0, 123.6, 117.5; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{14}H_{11}BrN_3O$ 316.0080, found 316.0080.

Amino-3-(4-(trifluoromethyl)phenyl)quinazolin-4(*3H*)-one (**3t**)



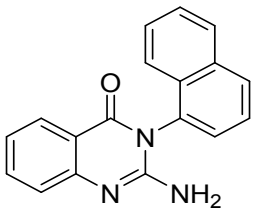
White solid. (119 mg, 78% yield); m. p. 268−2270 ˚C. R_f = 0.2 (PE:EA = 1:1, v/v); ^{1}H NMR (400 MHz, DMSO - d_6) δ 7.95 - 7.90 (m, 3H), 7.67-7.61 (m, 3H), 7.29 (d, *J* = 8.0 Hz, 1H), 7.15 - 7.11 (m, 1H), 6.60 (s, 2H); ^{13}C{^{1}H} NMR (101 MHz, DMSO - d_6) δ 161.8, 151.3, 150.1, 139.3, 134.5, 130.2, 130.1 (q, *J* = 3.2 Hz), 127.5(q, *J* = 2.8 Hz), 127.0, 124.6 (q, *J* = 219.2 Hz), 124.4, 122.0, 116.6; ^{19}F NMR (376 MHz, DMSO-d_6) δ -61.0; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{15}H_{11}F_3N_3O$ 306.0849, found 306.0845.

2-Amino-3-benzylquinazolin-4(*3H*)-one (**3w**)[5-7]



White solid. (82 mg, 65% yield); m. p. 198−200 ˚C. R_f = 0.22 (PE:EA = 1:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 7.94 (dd, *J* = 8.0, 1.5 Hz,1H), 7.61 - 7.58 (m, 1H), 7.34 - 7.31 (m, 2H), 7.27 - 7.21 (m, 4H), 7.14 - 7.11 (m, 1H), 7.01 (s, 2H), 5.31 (s, 2H), 3.37 (s, 2H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 162.0, 151.9, 149.8, 136.3, 134.3, 128.4, 127.1, 126.7, 126.6, 123.8, 121.5, 116.0, 43.9; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{15}H_{14}N_3O$ 250.0986, found 250.0972.

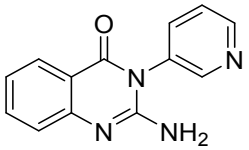
2-Amino-3-(naphthalen-1-yl)quinazolin-4(*3H*)-one (**3x**)[5]



White solid. (78 mg, 54% yield); m. p. 224−226 ˚C. R_f = 0.22 (PE:EA = 1:1, v/v); ^{1}H NMR (400 MHz, DMSO - d_6) δ 8.10 (d, *J* = 8.4 Hz, 1H), 8.05 - 7.99 (m, 3H), 7.93 (d, *J* = 7.6 Hz, 1H), 7.64 - 7.58 (m, 3H), 7.44 (d, *J* = 8.8 Hz, 1H), 7.29

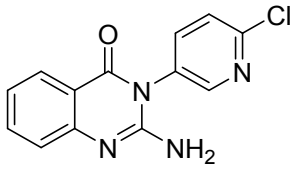
(d, J = 8.4 Hz, 1H), 7.13 (t, J = 7.6 Hz, 1H), 6.50 (s, 2H); $^{13}C\{^1H\}$ NMR (101 MHz, DMSO - d_6) δ 162.1, 151.8, 150.3, 134.4, 133.6, 133.0, 129.8, 128.2, 128.0, 127.8, 127.0, 126.5, 126.5, 126.4, 124.0, 121.5, 116.8; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{18}H_{14}N_3O$ 288.1131, found 288.1130.

2-Amino-3-(pyridin-3-yl)quinazolin-4(*3H*)-one (**3y**)



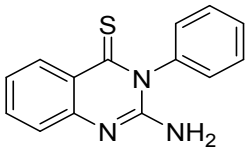
White solid. (83 mg, 70% yield); m. p. 242–245 ˚C. R_f = 0.22 (PE:EA = 1:1, v/v);^1H NMR (500 MHz, DMSO - d_6) δ 8.70 (dd, J = 5.0, 1.5 Hz, 1H), 8.59 (d, J = 2.0 Hz, 1H), 7.92-7.86 (m, 2H), 7.64-7.60 (m, 2H), 7.27 (d, J = 8.0 Hz, 1H), 7.15-7.12 (m, 1H), 6.57 (s, 2H); $^{13}C\{^1H\}$ NMR (126 MHz, DMSO - d_6) δ 162.0, 151.5, 150.2, 150.0, 149.7, 137.0, 134.6, 132.4, 126.5, 124.8, 124.0, 121.6, 116.5; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{13}H_{11}N_4O$ 239.0927, found 239.0926.

2-Amino-3-(6-chloropyridin-3-yl)quinazolin-4(*3H*)-one (**3z**)



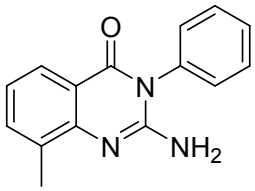
White solid. (93 mg, 68% yield); m. p. 263–265 ˚C. R_f = 0.21 (PE:EA = 1:1, v/v);^1H NMR (400 MHz, DMSO - d_6) δ 8.48 (s, 1H), 7.97 (d, J = 8.4 Hz, 1H), 7.90 (d, J = 8.0 Hz, 1H), 7.73 (d, J = 8.4 Hz, 1H), 7.62 (t, J = 7.6 Hz, 1H), 7.26 (d, J = 8.4 Hz, 1H), 7.13 (t, J = 7.2 Hz, 1H), 6.71 (s, 2H); $^{13}C\{^1H\}$ NMR (101 MHz, DMSO - d_6) δ 162.0, 151.4, 150.5, 150.3, 150.2, 140.7, 134.67 132.1, 126.5, 125.7, 124.0, 121.6, 116.4; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{13}H_{10}ClN_4O$ 273.0538, found 273.0535.

2-Amino-3-phenylquinazoline-4(*3H*)-thione (**5a**)



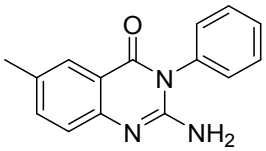
White solid. (71 mg, 56% yield); m. p. 263–265 ˚C. R_f = 0.2 (PE:EA = 1:1, v/v);^1H NMR (500 MHz, DMSO - d_6) δ 8.41 (dd, J = 8.0, 1.0 Hz, 1H), 7.68-7.65 (m, 1H), 7.61-7.58 (m, 2H), 7.51 (t, J = 7.5 Hz, 1H), 7.32-7.30 (m, 3H), 7.20-7.17 (m, 1H), 6.40 (s, 2H); $^{13}C\{^1H\}$ NMR (126 MHz, DMSO - d_6) δ 189.6, 150.8, 146.1, 139.6, 134.9, 130.8, 130.3, 129.2, 128.2, 124.8, 124.6, 122.8; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{14}H_{12}N_3S$ 254.0746, found 254.0742.

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



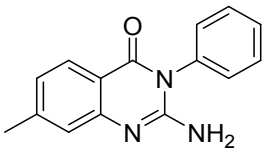
White solid. (90 mg, 72% yield); m. p. 237–239 ˚C. R_f = 0.22 (PE:EA = 1:1, v/v); ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.77 (d, J = 7.5 Hz, 1H), 7.59 - 7.56 (m, 2H), 7.53 - 7.48 (m, 2H), 7.37 - 7.35 (m, 2H), 7.02 (t, J = 7.5 Hz, 1H), 6.21 (s, 2H), 2.43 (s, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 162.0, 150.8, 135.5, 134.5, 131.6, 129.9, 129.1, 128.8, 124.2, 121.1, 116.5, 17.4; HRMS (ESI) m/z: [M+H]$^+$ calcd for $C_{15}H_{14}N_3O$ 252.1131, found 252.1132.

2-Amino-6-methyl-3-phenylquinazolin-4(*3H*)-one (**5c**)[6]



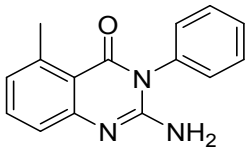
White solid. (93 mg, 74% yield); m. p. 251–253 ˚C. R_f = 0.22 (PE:EA = 1:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 7.70 (s, 1H), 7.57 (t, J = 8.0 Hz, 2H), 7.53 - 7.50 (m, 1H), 7.44 (d, J = 8.5 Hz, 1H), 7.34 (d, J = 7.5 Hz, 2H), 7.18 (d, J = 7.0 Hz, 1H), 6.14 (s, 2H), 2.34 (s, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 161.7, 151.0, 148.0, 135.7, 135.6, 130.6, 129.9, 129.1, 128.8, 128.5, 125.7, 123.9, 116.5, 20.4; HRMS (ESI) m/z: [M+H]$^+$ calcd for $C_{15}H_{14}N_3O$ 252.1131, found 252.1130.

2-Amino-7-methyl-3-phenylquinazolin-4(*3H*)-one (**5d**)



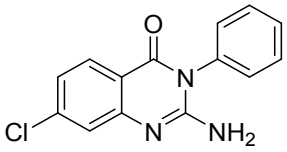
White solid. (94 mg, 75% yield); m. p. 253–255 ˚C. R_f = 0.22 (PE:EA = 1:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 7.78 (d, J = 8.0 Hz, 1H), 7.56 (t, J = 7.5 Hz, 2H), 7.51 (t, J = 7.5 Hz, 1H), 7.34 (d, J = 7.0 Hz, 2H), 7.06 (s, 1H), 6.95 (d, J = 8.0 Hz, 1H), 6.18 (s, 2H), 2.38 (s, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 161.7, 151.6, 150.2, 144.6, 135.5, 129.9, 129.1, 128.8, 126.4, 123.5, 123.1, 114.5, 21.4; HRMS (ESI) m/z: [M+H]$^+$ calcd for $C_{15}H_{14}N_3O$ 252.1131, found 252.1129.

2-Amino-5-methyl-3-phenylquinazolin-4(*3H*)-one (**5e**)



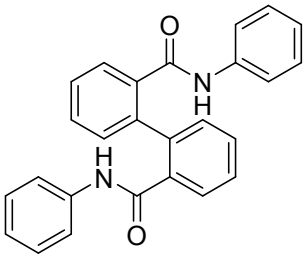
White solid. (82 mg, 65% yield); m. p. 244–246 ˚C R_f = 0.22 (PE:EA = 1:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 7.58-7.55 (m, 2H), 7.52 - 7.49 (m, 1H), 7.42 (t, J = 8.0 Hz, 1H), 7.34 - 7.32 (m, 2H), 7.08 (d, J = 8.0 Hz, 1H), 6.87 (d, J = 7.0 Hz, 1H), 6.12 (s, 2H), 2.62 (s, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 162.3, 151.6, 151.2, 140.1, 135.7, 133.4, 129.8, 128.9, 128.9, 128.6, 124.2, 122.3, 115.2, 22.6; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{15}H_{14}N_3O$ 252.1131, found 252.1131.

2-Amino-7-chloro-3-phenylquinazolin-4(*3H*)-one (**5f**)



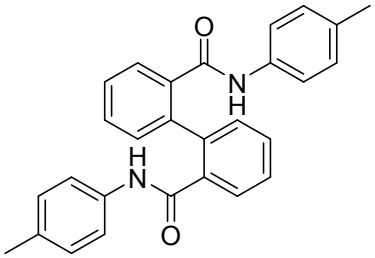
White solid. (92 mg, 68% yield); m. p. 263–265 ˚C. R_f = 0.2 (PE:EA = 1:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 7.88 (d, J = 8.5 Hz, 1H), 7.60-7.51 (m, 3H), 7.38 (d, J = 7.5 Hz, 2H), 7.27 (s, 1H), 7.12 (d, J = 8.5 Hz, 2H), 6.51 (s, 2H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 161.2, 152.7, 151.4, 139.0, 135.1, 130.0, 129.3, 128.8, 128.6, 122.8, 121.5, 115.6; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{14}H_{11}ClN_3O$ 272.0585, found 272.0585.

N^2,*N*$^{2'}$-diphenyl-[1,1'-biphenyl]-2,2'-dicarboxamide (**6a**)[9-11]



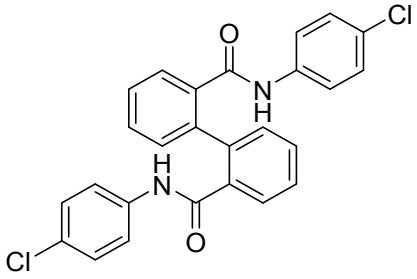
Yellow solid. (63 mg, 64% yield); m. p. 227–228 ˚C. R_f = 0.33 (PE:EA = 5:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 10.62 (s, 2H), 7.70 (s, 2H), 7.47 (d, J = 7.0 Hz, 8H), 7.28 – 7.26 (m, 4H), 7.19 (s, 2H), 7.05 (d, J = 7.0 Hz, 2H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 168.4, 139.1, 139.0, 136.7, 130.4, 129.8, 129.3, 128.4, 128.1, 124.4, 120.0; HRMS (ESI) m/z: $[M-H]^-$ calcd for $C_{26}H_{19}N_2O_2$ 391.1452 found 391.1450.

N^2,*N*$^{2'}$-di-*p*-tolyl-[1,1'-biphenyl]-2,2'-dicarboxamide (**6b**)[9-11]



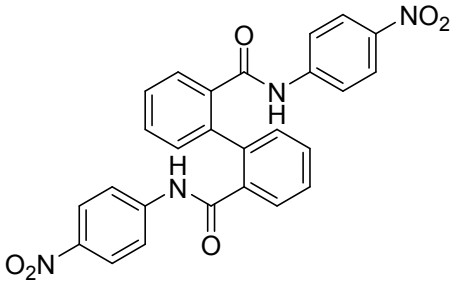
Yellow solid. (74mg, 70% yield); m. p. 177–179 ˚C. R_f = 0.32 (PE:EA = 5:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 10.54 (s, 2H), 7.68 (dd, J = 5.5, 2.0 Hz, 2H), 7.49 – 7.44 (m, 4H), 7.34 (d, J = 8.0 Hz, 4H), 7.18 – 7.16 (m, 2H), 7.06 (d, J = 8.0 Hz, 4H), 2.22 (s, 6H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 168.2, 139.1, 136.8, 136.5, 133.4, 130.2, 129.7, 129.6, 128.3, 128.0, 119.9, 20.9; HRMS (ESI) m/z: [M+H]$^+$ calcd for $C_{28}H_{25}N_2O_2$ 421.1911 found 421.1907.

N^2,*N*$^{2'}$-bis(4-chlorophenyl)-[1,1'-biphenyl]-2,2'-dicarboxamide (**6c**)[9-11]



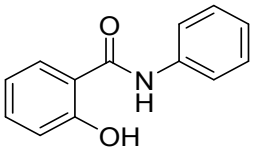
Yellow solid. (68 mg, 68% yield); m. p. 222–223 ˚C. R_f = 0.3 (PE:EA = 5:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 11.67 (s, 2H), 8.70 – 8.68 (m, 2H), 8.50 – 8.48 (m, 8H), 8.32 – 8.30 (m, 4H), 8.21 – 8.19 (m, 2H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 168.4, 139.1, 138.0, 136.3, 130.5, 130.0, 129.1, 128.4, 128.1, 127.9, 121.4; HRMS (ESI) m/z: [M-H]$^-$ calcd for $C_{26}H_{17}Cl_2N_2O_2$ 459.0672 found 459.0669.

N^2,*N*$^{2'}$-bis(4-nitrophenyl)-[1,1'-biphenyl]-2,2'-dicarboxamide (**6d**)



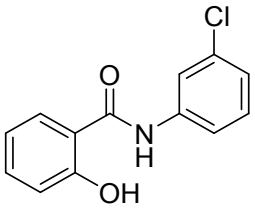
Yellow solid. (54 mg, 45% yield); m. p. 201–202 ˚C. R_f = 0.32 (PE:EA = 5:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 11.00 (s, 2H), 8.10 (d, J = 9.0 Hz, 2H), 7.74 – 7.70 (m, 6H), 7.57 – 7.50 (m, 4H), 7.30 (d, J = 7.5 Hz, 2H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 168.7, 145.3, 1430, 139.4, 135.8, 131.0, 130.64, 128.3, 125.2, 119.6; HRMS (ESI) m/z: [M-H]$^-$ calcd for $C_{26}H_{17}N_4O_6$ 483.1299 found 483.1294.

2-Hydroxy-*N*-phenylbenzamide (**7a**)[12]



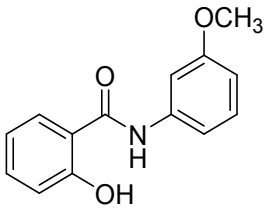
White solid. (69 mg, 65 % yield); m. p. 135–136 ˚C. R_f = 0.3 (PE:EA = 10:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 11.94 (s, 1H), 10.59 (s, 1H), 7.98 (d, J = 6.5 Hz, 1H), 7.20 (d, J = 6.5 Hz, 2H), 7.43 - 7.37 (m, 3H), 7.15 - 7.12 (m, 1H), 7.00 – 6.93 (m, 2H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 166.5, 158.9, 138.2, 133. 6, 129.1, 128.7, 124.1, 120.9, 118.7, 117.6, 117.4; HRMS (ESI) m/z: [M-H]$^-$ calcd for $C_{13}H_{10}NO_2$ 212.0717, found 212.0712.

N-(3-chlorophenyl)-2-hydroxybenzamide (**7e**)[13]



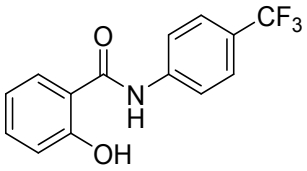
White solid. (84 mg, 68 % yield); m. p. 170–171 ˚C. R_f = 0.3 (PE:EA = 10:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 11.66 (s, 1H), 10.56 (s, 1H), 7.96 – 7.93 (m, 2H), 7.63 (d, J = 8.0 Hz, 1H), 7.44 (t, J = 8.0 Hz, 1H), 7.39 (t, J = 8.0 Hz, 1H), 7.19 - 7.18 (m, 1H), 7.01 (d, J = 8.0 Hz, 1H), 6.96 (t, J = 8.0 Hz, 1H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 166.6, 158.3, 139.8, 133.7, 133.1, 130.3, 129.2, 123.7, 120.2, 119.1, 119.0, 117.8, 117.3; HRMS (ESI) m/z: [M-H]$^-$ calcd for $C_{13}H_9ClNO_2$ 246.0327 found 246.0326.

2-Hydroxy-*N*-(3-methoxyphenyl)benzamide (**7f**)[14]



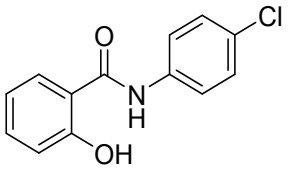
White solid. (79 mg, 65 % yield); m. p. 134–135 ˚C. R_f = 0.31 (PE:EA = 10:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 11.86 (s, 1H), 10.59 (s, 1H), 7.96 (dd, J = 8.0, 1.5 Hz, 1H), 7.44 – 7.40 (m, 2H), 7.29 – 7.26 (m, 2H), 6.99 (d, J = 8.0 Hz, 1H), 6.94 (d, J = 7.5 Hz, 1H), 6.73 – 6.71 (m, 1H), 3.77 (s, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 166.4, 159.5, 158.9, 139.5, 133.5, 129.5, 129.1, 118.6, 117.7, 117.4, 113.0, 109.5, 106.5, 55.0; HRMS (ESI) m/z: [M-H]$^-$ calcd for $C_{14}H_{12}NO_3$ 242.0817 found 242.0819.

2-Hydroxy-*N*-(4-(trifluoromethyl)phenyl)benzamide (**7g**)[13]



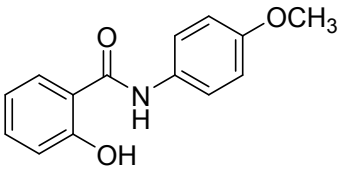
White solid. (85 mg, 60 % yield); m. p. 204–205 ˚C. R_f = 0.32 (PE:EA = 10:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 11.61 (s, 1H), 10.76 (s, 1H), 7.96 (d, J = 8.5 Hz, 2H), 7.93 (dd, J = 7.5, 1.5 Hz, 1H), 7.73 (d, J = 9.0 Hz, 2H), 7.46 – 7.43 (m, 1H), 7.02 (dd, J = 8.0, 1.0 Hz, 1H), 6.98 – 6.95 (m, 1H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 166.6, 158.1, 142.1, 133.7, 129.4, 126.0 (q, J = 3.8 Hz), 124.4 (q, J = 272.2 Hz), 123.9 (q, J = 31.5 Hz), 120.5, 119.0, 118.2, 117.2; ^{19}F NMR (376 MHz, DMSO - d_6) δ -60.4; HRMS (ESI) m/z: [M-H]$^-$ calcd for $C_{14}H_9F_3NO_2$ 280.0591 found 280.0593.

N-(4-chlorophenyl)-2-hydroxybenzamide (**7h**)[14]



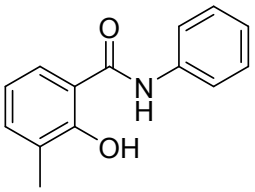
White solid. (77 mg, 62% yield); m. p. 168–169 ˚C. R_f = 0.3 (PE:EA = 10:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 11.67 (s, 1H), 10.56 (s, 1H), 7.95 (dd, J = 8.0, 2.0 Hz, 1H), 7.79 – 7.76 (m, 2H), 7.45 – 7.41 (m, 3H), 7.00 (d, J = 8.0 Hz, 1H), 6.96 (t, J = 7.5 Hz, 1H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 166.6, 158.5, 137.3, 133.7, 129.2, 128.6, 127.8, 122.4, 118.9, 117.7, 117.3; HRMS (ESI) m/z: [M-H]$^-$ calcd for $C_{13}H_9ClNO_2$ 246.0327 found 246.0324.

2-Hydroxy-*N*-(4-methoxyphenyl)benzamide (**7i**)[14]



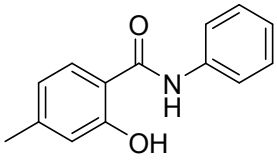
White solid. (73 mg, 60% yield); m. p. 125–126 ˚C. R_f = 0.31 (PE:EA = 10:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 10.75 (s, 2H), 7.97 (dd, J = 8.0, 1.5 Hz, 1H), 7.63 – 7.60 (m, 2H), 7.39 (t, J = 7.0 Hz, 1H), 6.96 – 6.93 (m, 3H), 6.89 (t, J = 7.5 Hz, 1H), 3.76 (s, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 166.5, 160.0, 155.8, 133.4, 131.3, 128.9, 122.5, 118.1, 117.6, 117.2, 113.9, 55.2; HRMS (ESI) m/z: [M-H]$^-$ calcd for $C_{14}H_{12}NO_3$ 242.0823 found 242.0819.

2-Hydroxy-3-methyl-*N*-phenylbenzamide (**7j**)



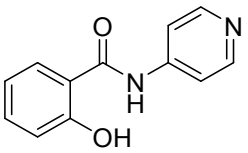
White solid. (43 mg, 38% yield); m. p. 135–136 ˚C. R_f = 0.31 (PE:EA = 10:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 12.56 (s, 1H), 10.59 (s, 1H), 7.93 (dd, J = 8.0, 1.5 Hz, 1H), 7.71 (d, J = 8.0 Hz, 2H), 7.41 – 7.36 (m, 3H), 7.17 (t, J = 7.5 Hz, 1H), 6.86 (t, J = 8.0 Hz, 1H), 2.20 (s, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 169.1, 159.6, 137. 8, 134.9, 128.6, 126.2, 125.4, 124.5, 121.9, 117.8, 114.3, 15.6; HRMS (ESI) m/z: [M-H]$^-$calcd for $C_{14}H_{12}NO_2$ 226.0873 found 226.0869.

2-Hydroxy-4-methyl-*N*-phenylbenzamide (**7k**)



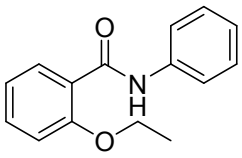
White solid. (45mg, 40% yield); m. p. 158–159 ˚C. R_f = 0.31 (PE:EA = 10:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 12.08 (s, 1H), 10.49 (s, 1H), 7.91 (d, J = 8.5 Hz, 1H), 7.70 (d, J = 8.0 Hz, 2H), 7.37 (t, J = 7.5 Hz, 2H), 7.14 (t J = 7.5 Hz, 1H), 6.08 (s, 1H), 6.78 (d, J = 8.0 Hz, 1H), 2.31 (s, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 166.8, 159.3, 144.2, 138.2, 128.8, 128.7, 124.05, 121.0, 119.8, 117.6, 114.2, 21.1; HRMS (ESI) m/z: [M-H]$^-$calcd for $C_{14}H_{12}NO_2$ 226.0874 found 226.0868.

2-Hydroxy-*N*-(pyridin-4-yl)benzamide (**7l**)



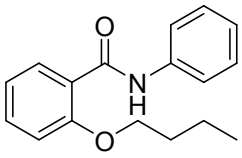
White solid. (34 mg, 32% yield); m. p. 202–203 ˚C. R_f = 0.3 (PE:EA = 10:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 11.67 (s, 1H), 10.67 (s, 1H), 8.89 (s, 1H), 8.35 (d, J = 4.5 Hz, 1H), 8.17 (d, J = 8.5 Hz, 1H), 7.97 (dd, J = 8.0, 1.5 Hz, 1H), 7.47 – 7.40 (m, 2H), 7.02 (d, J = 8.0 Hz, 1H), 6.97 (t, J = 7.5 Hz, 1H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 166.9, 158.5, 144.9, 142.4, 135.0, 133.8, 129.3, 127.9, 123.6, 118.9, 117.6, 117.3; HRMS (ESI) m/z: [M-H]$^-$ calcd for $C_{12}H_9N_2O_2$ 213.0670 found 213.0666.

2-Ethoxy-*N*-phenylbenzamide (**9a**)[15]



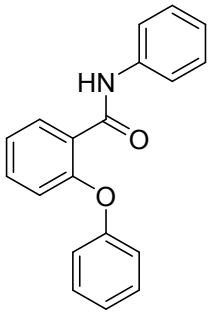
White solid. (87 mg, 72% yield); m. p. 195–196 ˚C. R_f = 0.35 (PE:EA = 10:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 10.15 (s, 1H), 7.73 (d, J = 7.5 Hz, 3H), 7.52 – 7.48 (m, 1H), 7.36 (t, J = 7.5 Hz, 2H), 7.18 (d, J = 8.0 Hz, 1H), 7.11 – 7.06 (m, 2H), 4.19 (q, J = 7.0 Hz, 2H), 1.42 (t, J = 7.0 Hz, 3H),; ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 164.6, 156.5, 139.5, 132.8, 130.6, 129.3, 124.8, 124.0, 121.1, 120.0, 113.5, 64.8, 15.1; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{15}H_{16}NO_2$ 242.1176 found 242.1170.

2-Butoxy-*N*-phenylbenzamide (**9b**)



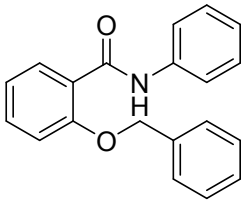
White solid. (89 mg, 66% yield); m. p. 202–204 ˚C. R_f = 0.37 (PE:EA = 10:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 10.11 (s, 1H), 7.73 – 7.70 (m, 3H), 7.51 – 7.48 (m, 1H), 7.35 (t, J = 8.0 Hz, 1H), 7.18 (d, J = 8.0 Hz, 1H), 7.11 – 7.06 (m, 2H), 4.13 (t, J = 6.5 Hz, 2H), 1.81 – 1.76 (m, 2H), 1.49 – 1.42 (m, 2H), 0.91 (t, J = 8.0 Hz, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 164.7, 156.6, 139.5, 132.7, 130.5, 129.3, 125.0, 123.9, 121.0, 119.9, 113.4, 68.7, 31.1, 19.2, 14.1; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{17}H_{20}NO_2$ 270.1489 found 270.1482.

2-Phenoxy-*N*-phenylbenzamide (**9c**)[16]



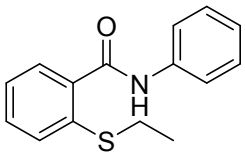
White solid. (107 mg, 74% yield); m. p. 97–98 ˚C. R_f = 0.4 (PE:EA = 10:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 10.30 (s, 1H), 7.67 (d, J = 8.0 Hz, 3H), 7.52 – 7.48 (m, 1H), 7.38 (t, J = 8.0 Hz, 2H), 7.33 – 7.26 (m, 3H), 7.14 (t, J = 7.0 Hz, 1H), 7.08 – 7.06 (m, 3H), 6.97 (d, J = 8.0 Hz, 1H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 164.9, 157.0, 154.0, 139.5, 132.2, 130.5, 130.1, 129.6, 129.2, 124.2, 124.1, 120.1, 119.5, 119.2; HRMS (ESI) m/z: $[M-H]^-$ calcd for $C_{19}H_{14}NO_2$ 290.1176 found 290.1172.

2-(Benzyloxy)-*N*-phenylbenzamide (**9d**)[17]



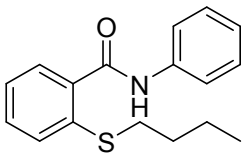
White solid. (103 mg, 68% yield); m. p. 167–168 ˚C. R_f = 0.4 (PE:EA = 10:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 11.19 (s, 1H), 7.74 (d, J = 7.5 Hz, 1H), 7.59 – 7.52 (m, 4H), 7.53 (t, J = 8.0 Hz, 1H), 7.41 – 7.48 (m, 3H), 7.32 – 7.29 (m, 3H), 7.47 – 7.40 (m, 2H), 7.12 (t, J = 7.5 Hz, 1H), 7.07 (t, J = 7.5 Hz, 1H), 5.27 (s, 2H),; ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 164.6, 156.2, 139.4, 137.0, 132.7, 130.6, 129.2, 129.0, 128.6, 128.5, 125.3, 123.9, 121.4, 119.8, 113.8, 70.7; HRMS (ESI) m/z: [M-H]$^-$ calcd for $C_{20}H_{16}NO_2$ 302.1187 found 302.1183.

2-(Ethylthio)-*N*-phenylbenzamide (**9e**)



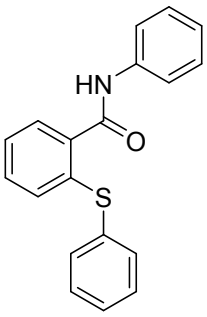
White solid. (87 mg, 68% yield); m. p. 212–214 ˚C. R_f = 0.35 (PE:EA = 10:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 11.31 (s, 1H), 7.73 (d, J = 8.0 Hz, 2H), 7.50 – 7.45 (m, 3H), 7.34 (t, J = 8.0 Hz, 2H), 7.31 – 7.28 (m, 1H), 7.10 (t, J = 7.5 Hz, 1H), 2.96 (q, J = 7.5 Hz, 2H), 1.22 (t, J = 8.0 Hz, 1H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 167.0, 139.7, 138.1, 135.6, 130.6, 129.2, 128.5, 128.2, 125.6, 124.0, 120.1, 26.8, 14.4; HRMS (ESI) m/z: [M+H]$^+$ calcd for $C_{15}H_{16}NOS$ 258.0947 found 258.0945.

2-(Butylthio)-*N*-phenylbenzamide (**9f**)



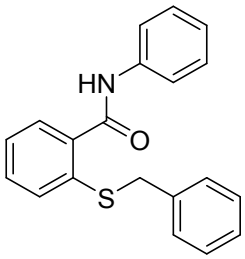
White solid. (100 mg, 70% yield); m. p. 237–238 ˚C. R_f = 0.36 (PE:EA = 10:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 10.33 (s, 1H), 7.76 (d, J = 8.0 Hz, 2H), 7.50 – 7.45 (m, 3H), 7.35 (t, J = 8.0 Hz, 2H), 7.31 – 7.28 (m, 1H), 7.10 (t, J = 8.0 Hz, 1H), 2.95 (t, J = 7.0 Hz, 2H), 1.58 - 1.52 (m, 2H), 1.43 - 1.35 (m, 2H), 0.87 (t, J = 7.5 Hz, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 167.0, 139.7, 138.3, 135.7, 130.6, 129.1, 128.7, 128.1, 125.6, 124.0, 120.1, 32.6, 30.9, 21.8, 14.0; HRMS (ESI) m/z: [M+H]$^+$ calcd for $C_{17}H_{20}NOS$ 286.1260 found 286.1257.

N-phenyl-2-(phenylthio)benzamide (**9g**)



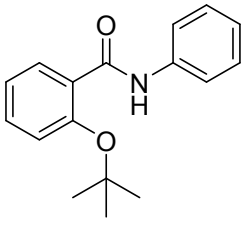
White solid. (55 mg, 36% yield); m. p. 146–148 ˚C. R_f = 0.4 (PE:EA = 10:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 10.45 (s, 1H), 7.74 (d, J = 8.0 Hz, 2H), 7.62 (d, J = 7.0 Hz, 1H), 7.42 – 7.34 (m, 9H), 7.13 – 7.10 (m, 2H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) 166.7, 139.6, 138.4, 135.4, 134.7, 132.9, 131.0, 131.0, 130.1, 129.2, 128.5, 128.5, 127.0, 124.2, 120.2; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{19}H_{16}NOS$ 306.0947 found 306.0944.

2-(Benzylthio)-*N*-phenylbenzamide (**9h**)



White solid. (110 mg, 69% yield); m. p. 151–152 ˚C. R_f = 0.4 (PE:EA = 10:1, v/v);^{1}H NMR (500 MHz, DMSO - d_6) δ 10.36 (s, 1H), 7.76 (d, J = 8.0 Hz, 2H), 7.544 – 7.51 (m, 2H), 7.44 (t, J = 7.5 Hz, 1H), 7.39 – 7.33 (m, 4H), 7.32 – 7.28 (m, 3H), 7.24 (t, J = 7.5 Hz, 1H), 7.10 (t, J = 7.5 Hz, 1H), 4.25 (s, 2H); ^{13}C NMR (126 MHz, DMSO - d_6) δ 166.9, 139.7, 137.6, 137.5, 135.9, 130.6, 129.5, 129.2, 128.9, 128.7, 128.3, 127.6, 125.8, 124.1, 120.2, 37.3; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{20}H_{18}NOS$ 320.1104 found 320.1097.

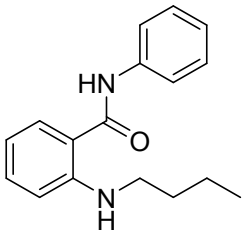
2-(tert-butoxy)-N-phenylbenzamide (**9i**)



White solid. (38 mg, 28% yield); m. p. 210-212 ˚C. R_f = 0.36 (PE:EA = 10:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 11.05 (s, 1H), 10.67 (d, J = 8.5 Hz, 2H), 8.89 (dd, J = 7.5, 1.5 Hz, 1H), 7.48 – 7.45 (m, 1H), 7.35 (t, J = 7.5 Hz, 2H), 7.23 – 7.19 (m, 2H), 7.09 (td, J = 7.0, 1.0 Hz, 1H), 1.34 (s, 9H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 165.3, 153.2,

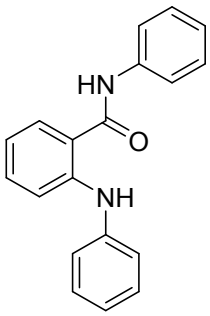
139.4, 131.8, 131.2, 130.3, 129.3, 124.0, 123.8, 123.6, 119.9, 81.2, 29.0; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{17}H_{20}NO_2$ 270.1489 found 270.1483.

2-(Butylamino)-*N*-phenylbenzamide (**9j**)



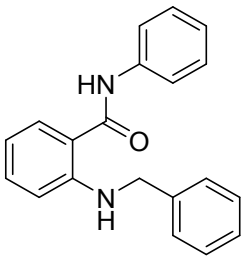
White solid. (83 mg, 62% yield); m. p. 166-167 ˚C. R_f = 0.33 (PE:EA = 10:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 10.06 (s, 1H), 7.70 (d, J = 8.0 Hz, 3H), 7.45 (t, J = 5.0 Hz, 1H), 7.34 (t, J = 8.0 Hz, 3H), 7.09 (t, J = 7.0 Hz, 1H), 6.73 (d, J = 8.0 Hz, 1H), 6.32 (t, J = 7.5 Hz, 1H), 3.13 (q, J = 7.0 Hz, 2H), 1.60 – 1.55 (m, 2H), 1.44 – 1.36 (m, 2H), 0.93 (t, J = 7.0 Hz, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 168.7, 150.0, 139.6, 133.3, 129.5, 129.0 124.0, 121.2, 115.7, 114.5, 111.6, 42.4, 31.2, 20.3, 14.2; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{17}H_{21}N_2O$ 269.1648 found 269.1645.

N-phenyl-2-(phenylamino)benzamide (**9k**)[18]



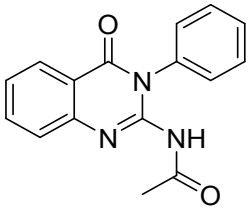
White solid. (83 mg, 58% yield); m. p. 142–143 ˚C. R_f = 0.4 (PE:EA = 10:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 11.34 (s, 1H), 9.12 (s, 1H), 7.77 (dd, J = 8.0, 2.0 Hz, 1H), 7.72 (d, J = 8.0 Hz, 2H), 7.41 – 7.29 (m, 6H), 7.17 (d, J = 7.5 Hz, 2H), 7.11 (t, J = 7.0 Hz, 1H), 6.98 – 6.92 (m, 2H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 168.1, 144.4, 142.2, 139.3, 132.6, 129.9, 129.9, 129.1, 124.3, 122.2, 121.2, 121.0, 119.7, 119.1, 116.2; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{19}H_{17}N_2O$ 289.1335 found 289.1332.

2-(Benzylamino)-N-phenylbenzamide (**9l**)[19]



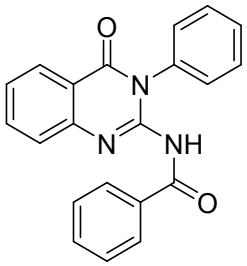
White solid. (97 mg, 64% yield); m. p. 150–151 ˚C. R_f = 0.3 (PE:EA = 10:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 10.13 (s, 1H), 7.87 (d, J = 5.5 Hz, 1H), 7.72 – 7.70 (m, 3H), 7.37 – 7.32 (m, 6H), 7.29 – 7.23 (m, 2H), 7.09 (t, J = 7.0 Hz, 1H), 6.69 – 6.63 (m, 2H), 4.41 (d, J = 6.0 Hz, 2H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 168.7, 149.5, 140.0, 139.6, 133.2, 129.6, 129.0, 129.0, 127.7, 127.4, 124.1, 121.2, 116.5, 115.1, 112.1, 46.6; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{20}H_{19}N_2O$ 306.0947 found 306.0944.

N-(4-oxo-3-phenyl-3,4-dihydroquinazolin-2-yl)acetamide (**10a**)



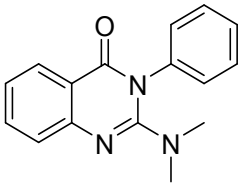
White solid. (112 mg, 80% yield); m. p. 216–218 ˚C. R_f = 0.33 (PE:EA = 5:1, v/v);^{1}H NMR (500 MHz, DMSO - d_6) δ 10.38 (s, 1H), 8.13 (d, J = 7.5 Hz, 1H), 7.89 - 7.86 (m, 1H), 7.68 (d, J = 8.5 Hz, 1H), 7.55 (t, J = 7.5 Hz, 1H), 7.52 – 7.45 (m, 3H), 7.33 (d, J = 7.0 Hz, 2H), 1.77 (s, 3H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 170.6, 161.8, 136.1, 135.0, 128.7, 128.6, 126.7, 126.6, 119.9, 22.8; HRMS (ESI) m/z: $[M-H]^-$ calcd for $C_{16}H_{12}N_3O_2$ 278.0935, found 278.0938.

N-(4-oxo-3-phenyl-3,4-dihydroquinazolin-2-yl)benzamide (**10b**)



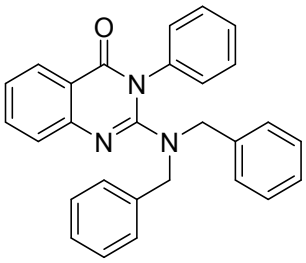
White solid. (127 mg, 74% yield); m. p. 201–203 ˚C. R_f = 0.35 (PE:EA = 5:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 13.17 (s, 1H), 8.06 (d, J = 7.5 Hz, 1H), 7.83 – 7.76 (m, 2H), 7.67 (d, J = 7.5 Hz, 2H), 7.53 (t, J = 7.5 Hz, 2H), 7.48 – 7.39 (m, 5H), 7.30 (t, J = 7.5 Hz, 2H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 176.6, 161.3, 154.2, 138.0, 137.4, 137.1, 136.0, 132.6, 129.4, 129.3, 129.2, 128.7, 128.6, 127.8, 125.4, 118.1, 117.2; HRMS (ESI) m/z: $[M-H]^-$ calcd for $C_{21}H_{14}N_3O_2$ 340.1091, found 340.1089.

2-(Dimethylamino)-3-phenylquinazolin-4(*3H*)-one (**10c**)



White solid. (112 mg, 84% yield); m. p. 165–167 ˚C. R_f = 0.35 (PE:EA = 10:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 7.98 (d, J = 7.5 Hz, 1H), 7.71 (t, J = 8.0 Hz, 1H), 7.52 (t, J = 7.5 Hz, 2H), 7.45 – 7.42 (m, 4H), 7.27 (t, J = 7.5 Hz, 1H), 2.60 (s, 6H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 162.5, 154.5, 148.0, 137.8, 134.6, 128.9, 128.7, 127.8, 126.6, 125.3, 123.5, 117.9, 40.5; HRMS (ESI) m/z: [M+H]$^+$ calcd for $C_{16}H_{16}N_3O$ 266.1288, found 266.1282.

2-(Dibenzylamino)-3-phenylquinazolin-4(*3H*)-one (**10d**)



White solid. (162 mg, 78% yield); m. p. 134–135 ˚C. R_f = 0.4 (PE:EA=10:1, v/v); ^{1}H NMR (500 MHz, DMSO - d_6) δ 8.05 (d, J = 7.5 Hz, 1H), 7.65 – 7.61 (m, 2H), 7.30 – 7.17 (m, 11H), 7.13 – 7.09 (m, 4H), 6.65 (d, J = 8.5 Hz, 1H), 5.26 (s, 2H), 5.13 (s, 2H); ^{13}C{^{1}H} NMR (126 MHz, DMSO - d_6) δ 160.9, 145.0, 141.2, 136.8, 135.8, 135.2, 133.7, 130.6, 128.3, 128.1, 127. 9, 127.1, 127.0, 126.9, 126.3, 123.2, 122.7, 116.1, 115.6, 115.3, 112.9, 49.8, 46.0; HRMS (ESI) m/z: [M+H]$^+$ calcd for $C_{28}H_{24}N_3O$ 418.1914, found 418.1907.

4. X-raySpectra of 3a.

4.1 Single crystal data for compound 3a

The crystal samples of **3a** were prepared via a slow volatilization process in ethanol. This was accomplished by adding 0.1 g of purified 3a to a round-bottomed flask containing 2 ml of ethanol, heating the solution in a metal sand bath to 70 ˚C, allowing for the complete dissolution of **3a**, leaving the flask open at room temperature, and then cooling the solution slowly. This process facilitated the formation of the target crystals, which were obtained by allowing the ethanol to evaporate slowly. The ellipsoid contour % probability level of **3a** is 50%.

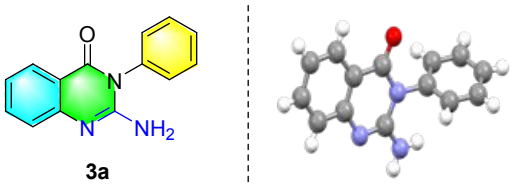


Figure S1. X-ray (CCDC 2307096) Spectra of **3a**

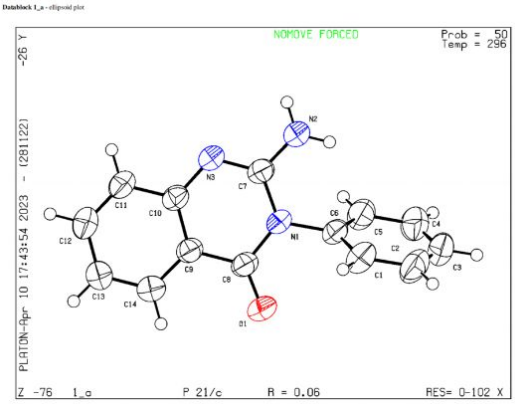


Figure S2. X-ray (CCDC 2307096) Spectra of **3a**.

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 1_a

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Bond precision:   C-C = 0.0032 A          Wavelength=0.71073

Cell:               a=5.83100      b=8.62100          c=22.69900
                    alpha=90       beta=96.7200       gamma=90
Temperature:        296 K

                 Calculated                Reported
Volume           1133.218                  1133
Space group      P 21/c                    P 21/c
Hall group       -P 2ybc                   -P 2ybc
Moiety formula   C14 H11 N3 O              ?
Sum formula      C14 H11 N3 O              C14 H11 N3 O
Mr               237.26                    237.26
Dx,g cm-3        1.391                     1.391
Z                4                         4
Mu (mm-1)        0.091                     0.091
F000             496.0                     496.0
F000'            496.19
h,k,lmax         6,10,27                   6,10,27
Nref             2027                      2002
Tmin,Tmax        0.982,0.982               0.864,0.864
Tmin'            0.982

Correction method= # Reported T Limits: Tmin=0.864 Tmax=0.864
AbsCorr = MULTI-SCAN

Data completeness= 0.988          Theta(max)= 25.149

R(reflections)= 0.0569( 1192)                    wR2(reflections)=
                                                 0.1590( 2002)
S = 0.975                 Npar= 163
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The following ALERTS were generated. Each ALERT has the format
      test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.
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Alert level C

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PLAT141_ALERT_4_C s.u. on a - Axis Small or Missing ..............    0.00000 Ang.
PLAT142_ALERT_4_C s.u. on b - Axis Small or Missing ..............    0.00000 Ang.
PLAT143_ALERT_4_C s.u. on c - Axis Small or Missing ..............    0.00000 Ang.
PLAT145_ALERT_4_C s.u. on beta     Small or Missing ..............     0.0000 Degree
PLAT151_ALERT_1_C No s.u. (esd) Given on Volume ..................     Please Do !
PLAT411_ALERT_2_C Short Inter H...H Contact  H14      ..H14      .       2.14 Ang.
                                                 -x,-y,1-z  =      3_556 Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N2       --H2B      .     Please Check
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4     Please Check
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Alert level G

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PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          2 Report
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        1.8 Low
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```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   3 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 ALERT type 2 Indicator that the structure model may be wrong or deficient
   1 ALERT type 3 Indicator that the structure quality may be low
   5 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Figure S3. Single crystal data of **3a** (X-ray (CCDC2219270))

5. ^{1}H, ^{13}C and ^{19}F NMR spectra

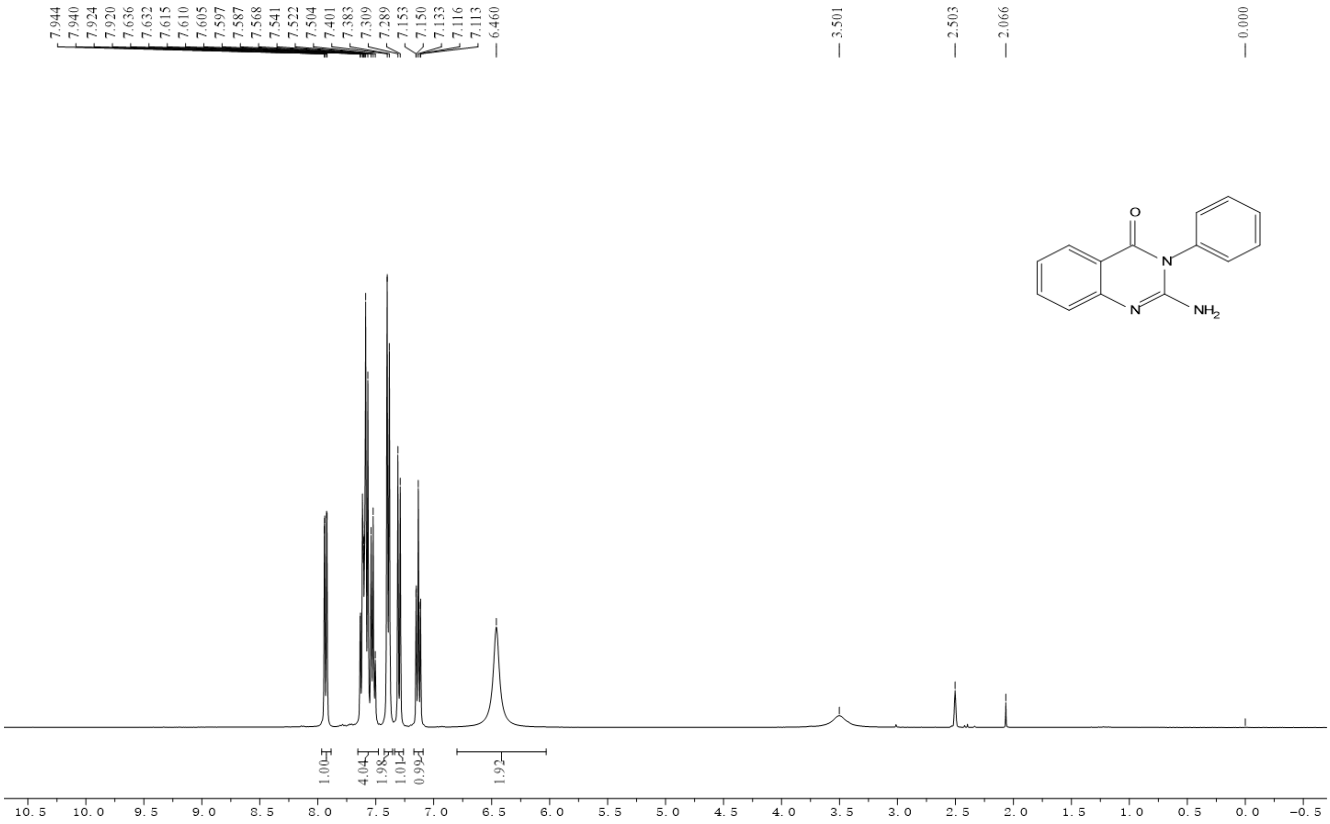

Figure S4. ^{1}H NMR (400 MHz) of **3a** in DMSO - d_6.

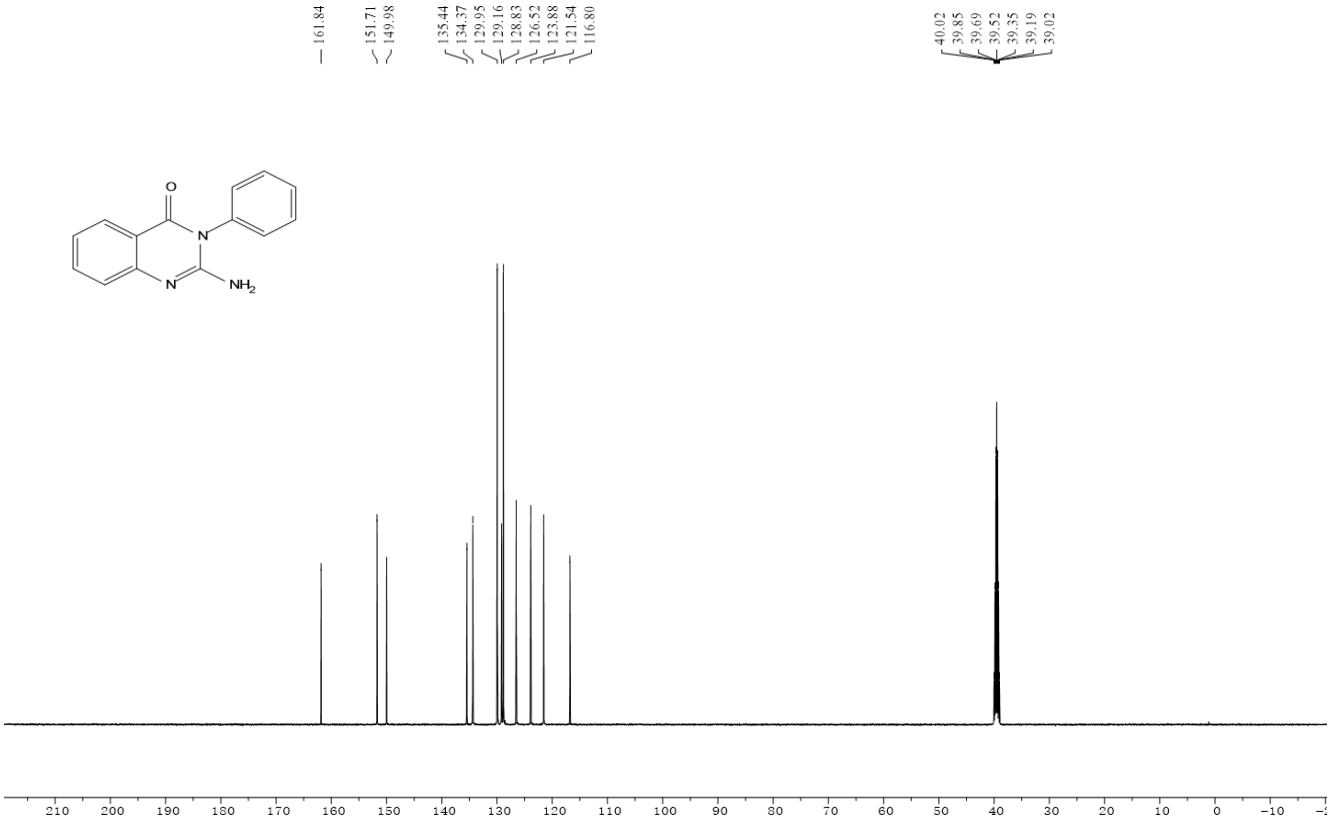

Figure S5. ^{13}C NMR (126 MHz) of **3a** in DMSO - d_6.

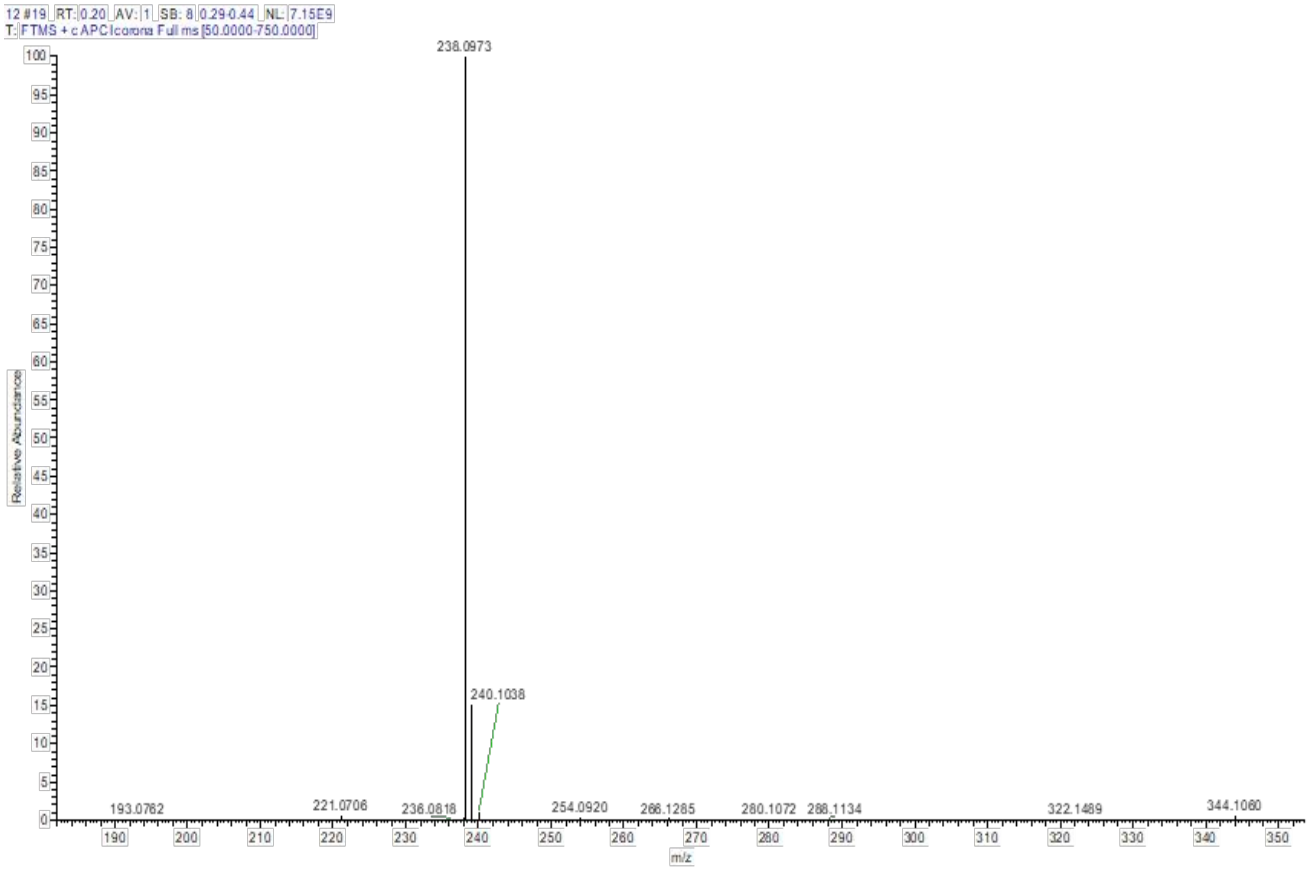

Figure S6. HRMS spectra for **3a**.

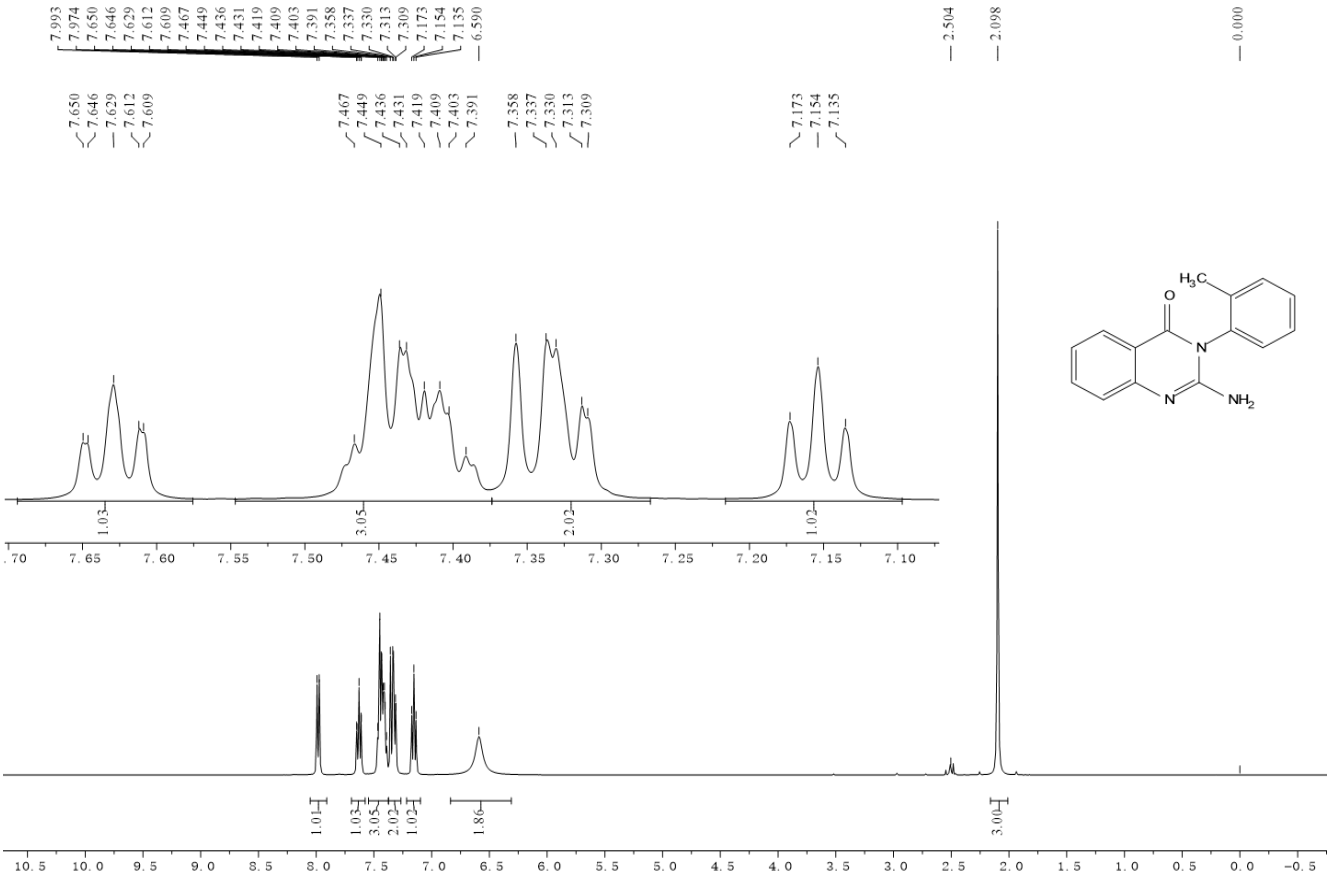

Figure S7. ^{1}H NMR (400 MHz) of **3b** in DMSO - d_6.

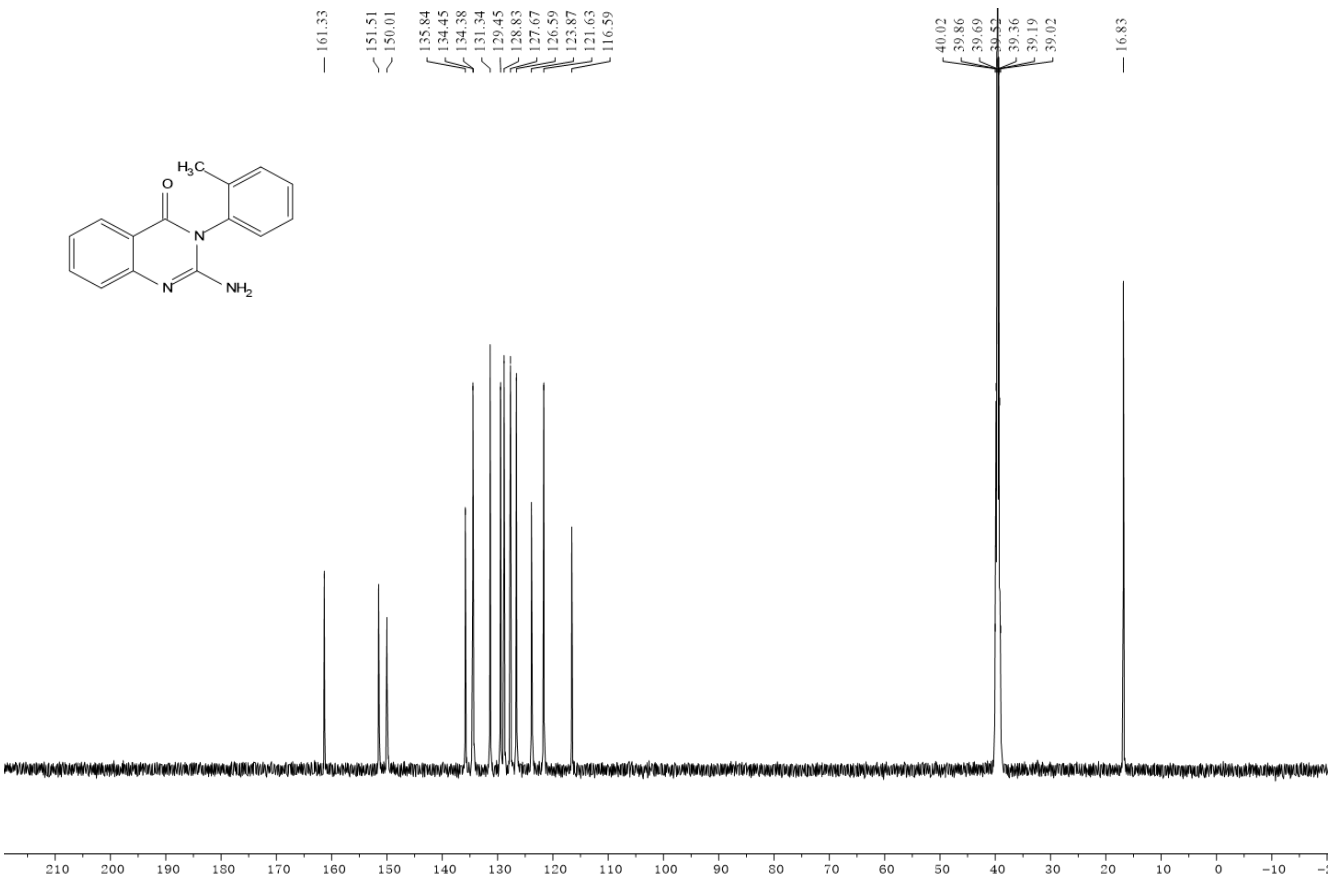

Figure S8. ^{13}C NMR (101 MHz) of **3b** in DMSO - d_6.

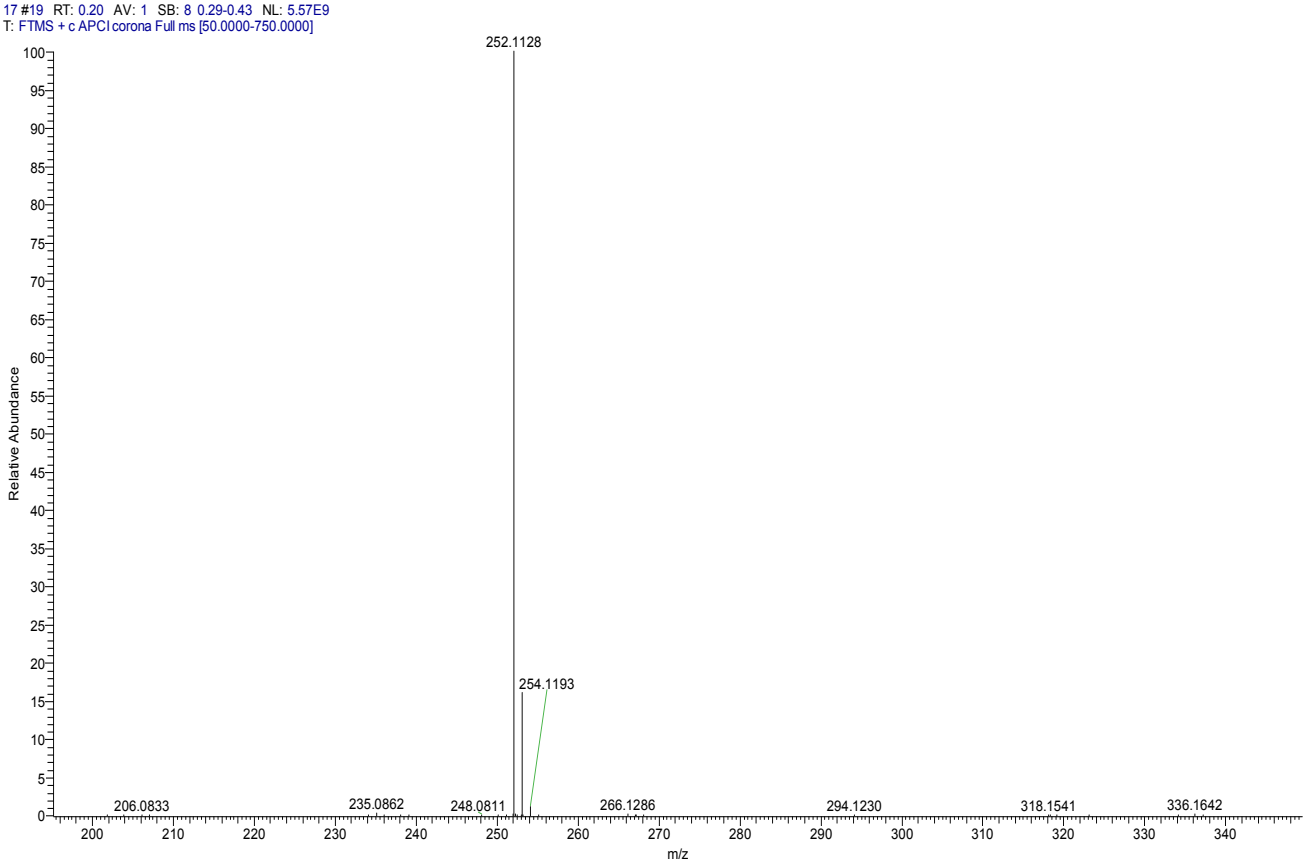

Figure S9. HRMS spectra for **3b**.

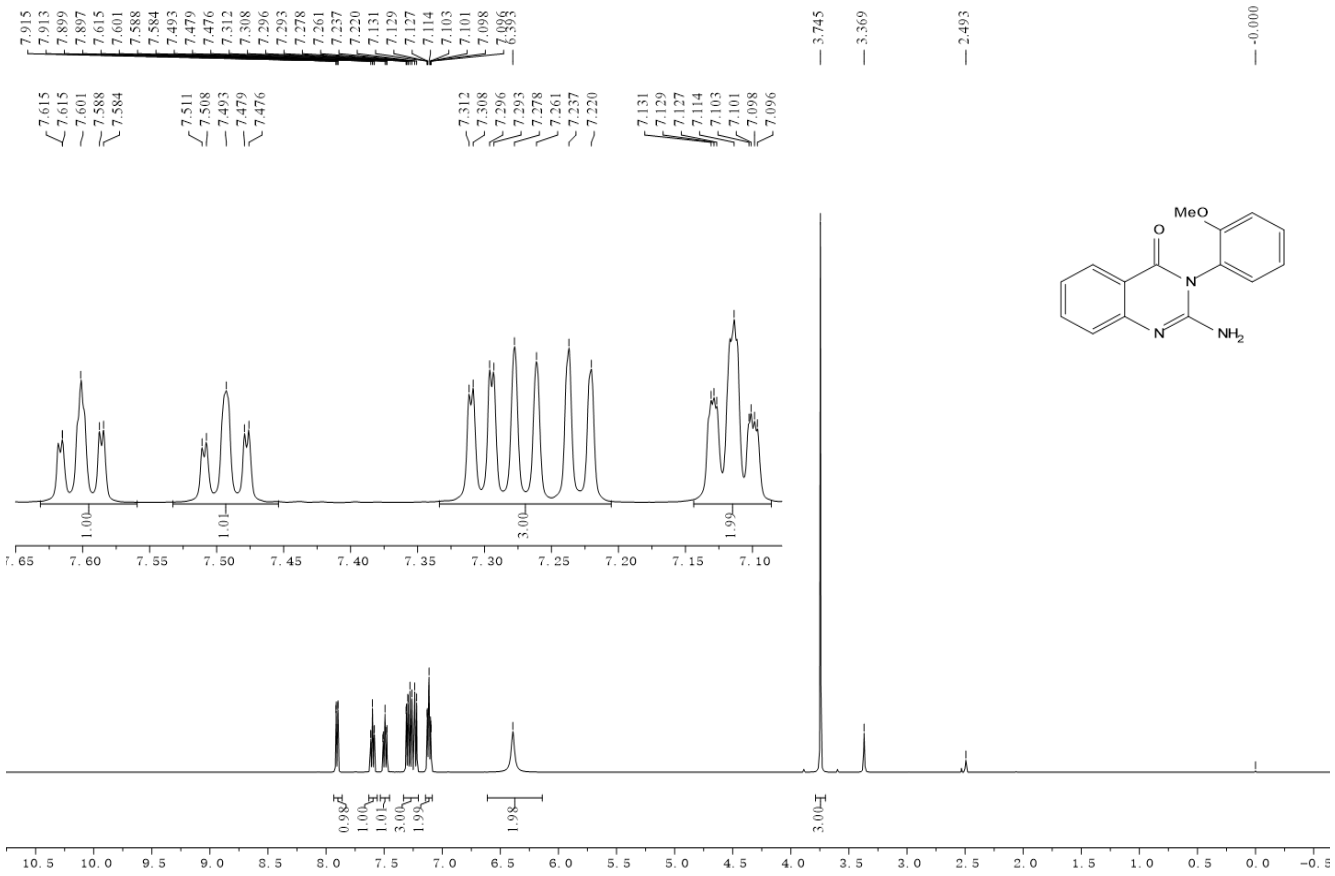

Figure S10. ^{1}H NMR (500 MHz) of **3c** in DMSO - d_6.

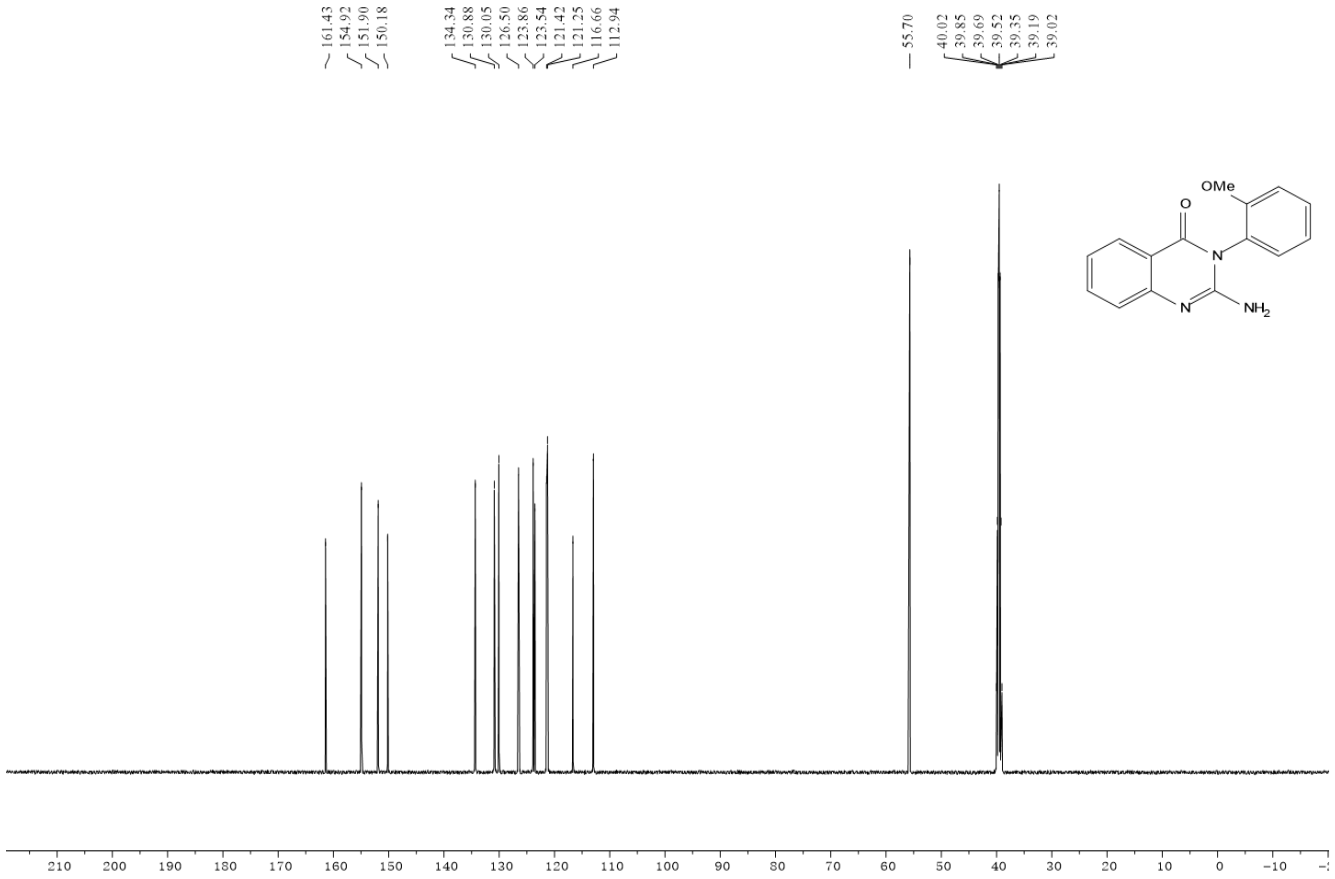

Figure S11. ^{13}C NMR (126 MHz) of **3c** in DMSO - d_6.

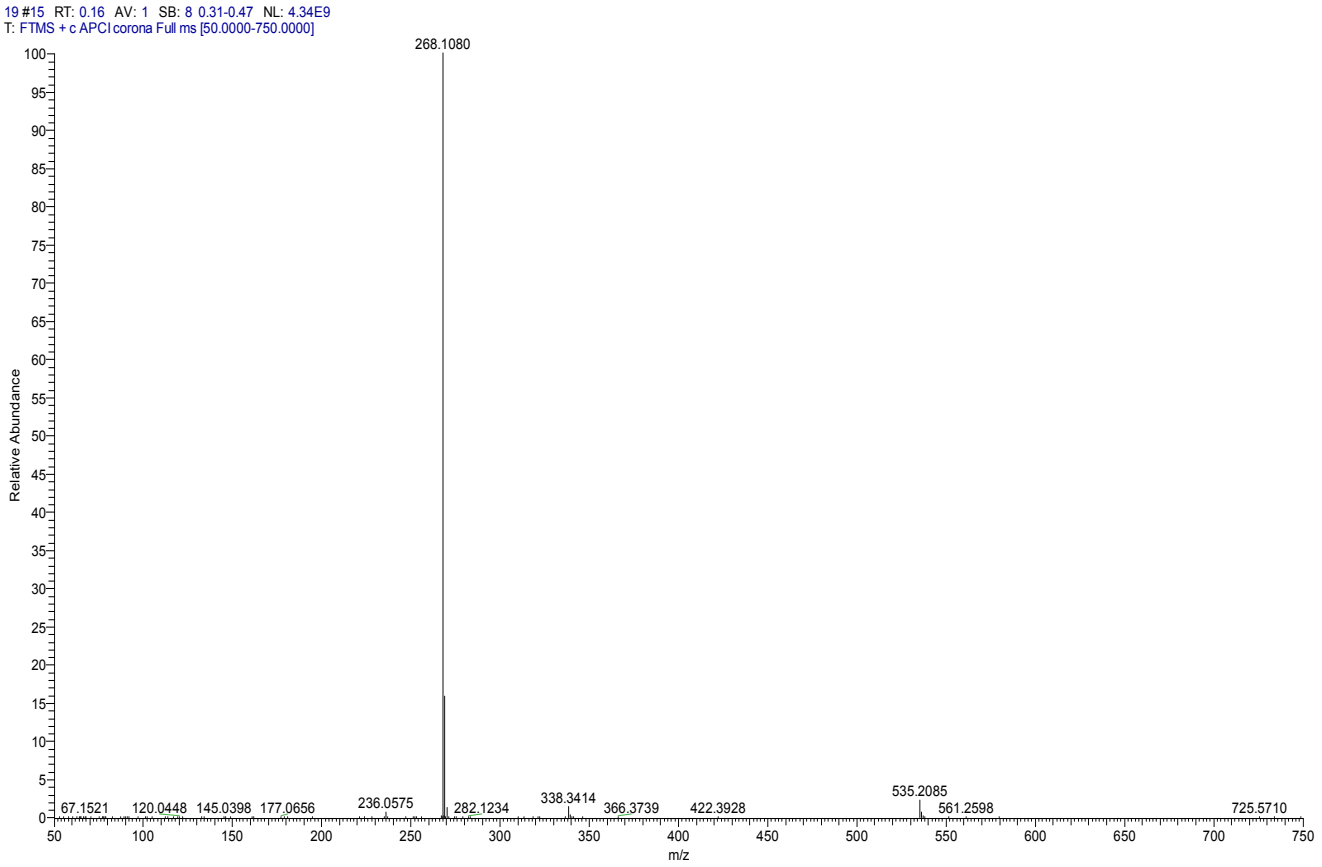

Figure S12. HRMS spectra for **3c**.

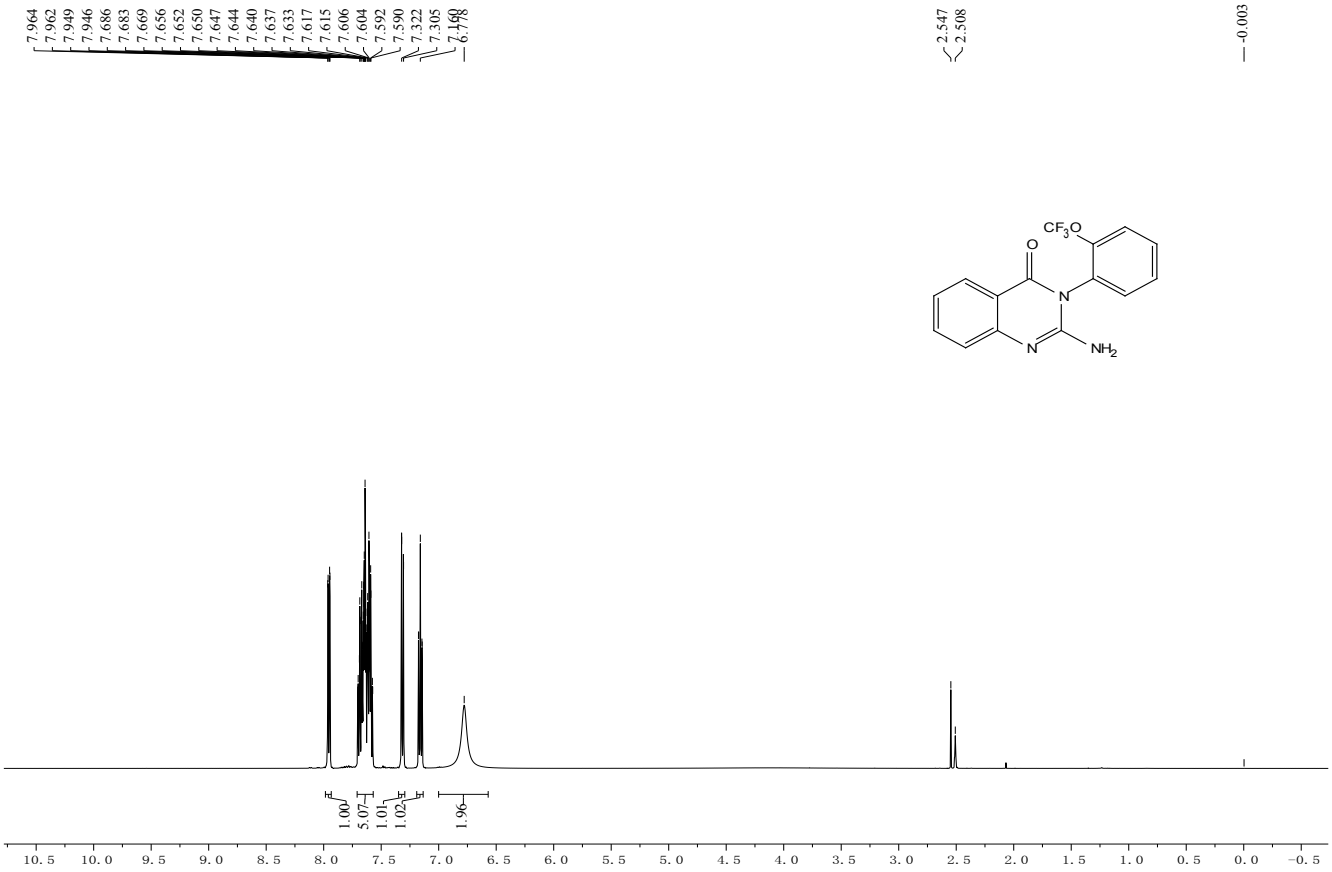

Figure S13. ^{1}H NMR (500 MHz) of **3d** in DMSO - d_6.

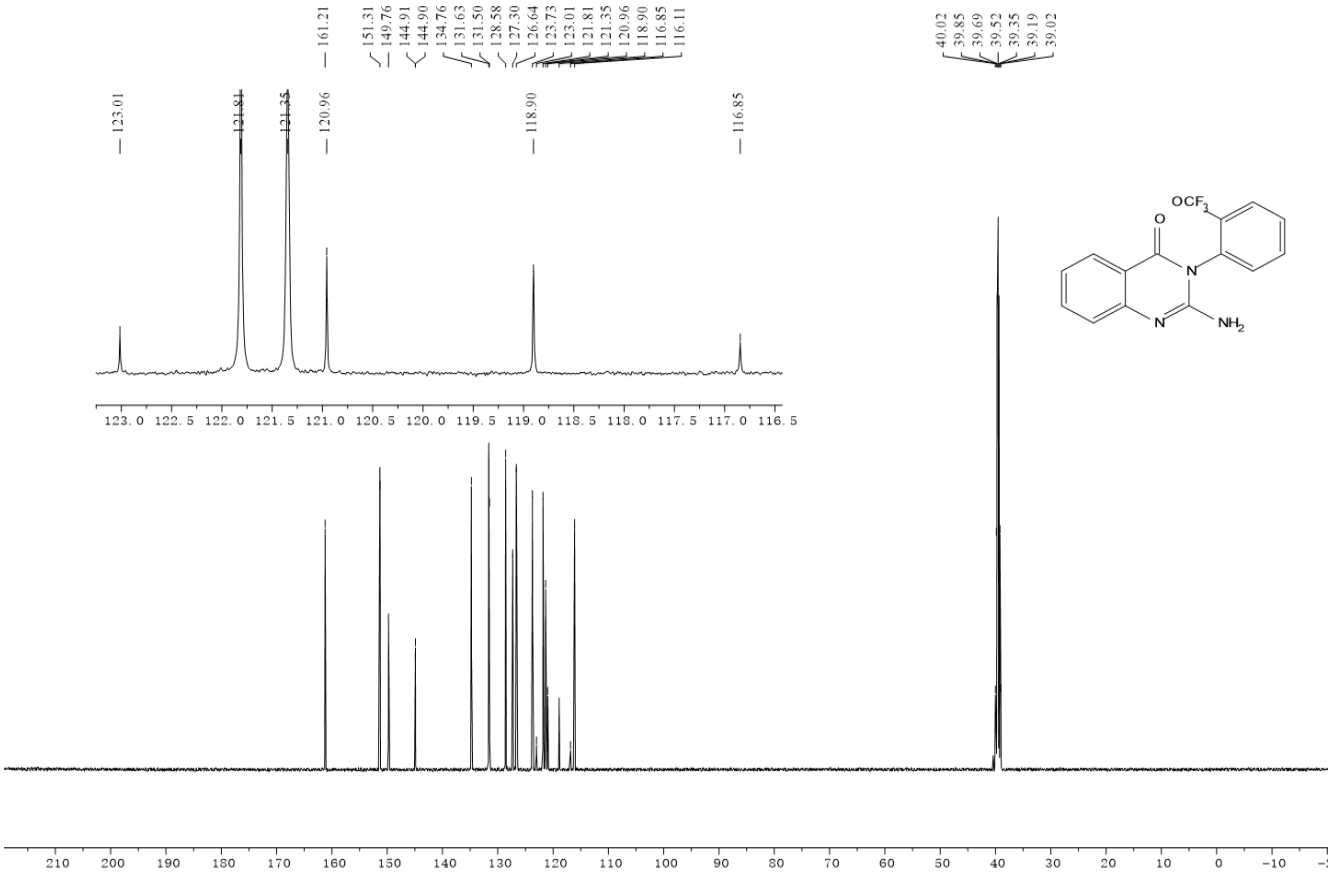

Figure S14. ^{13}C NMR (126 MHz) of **3d** in DMSO - d_6.

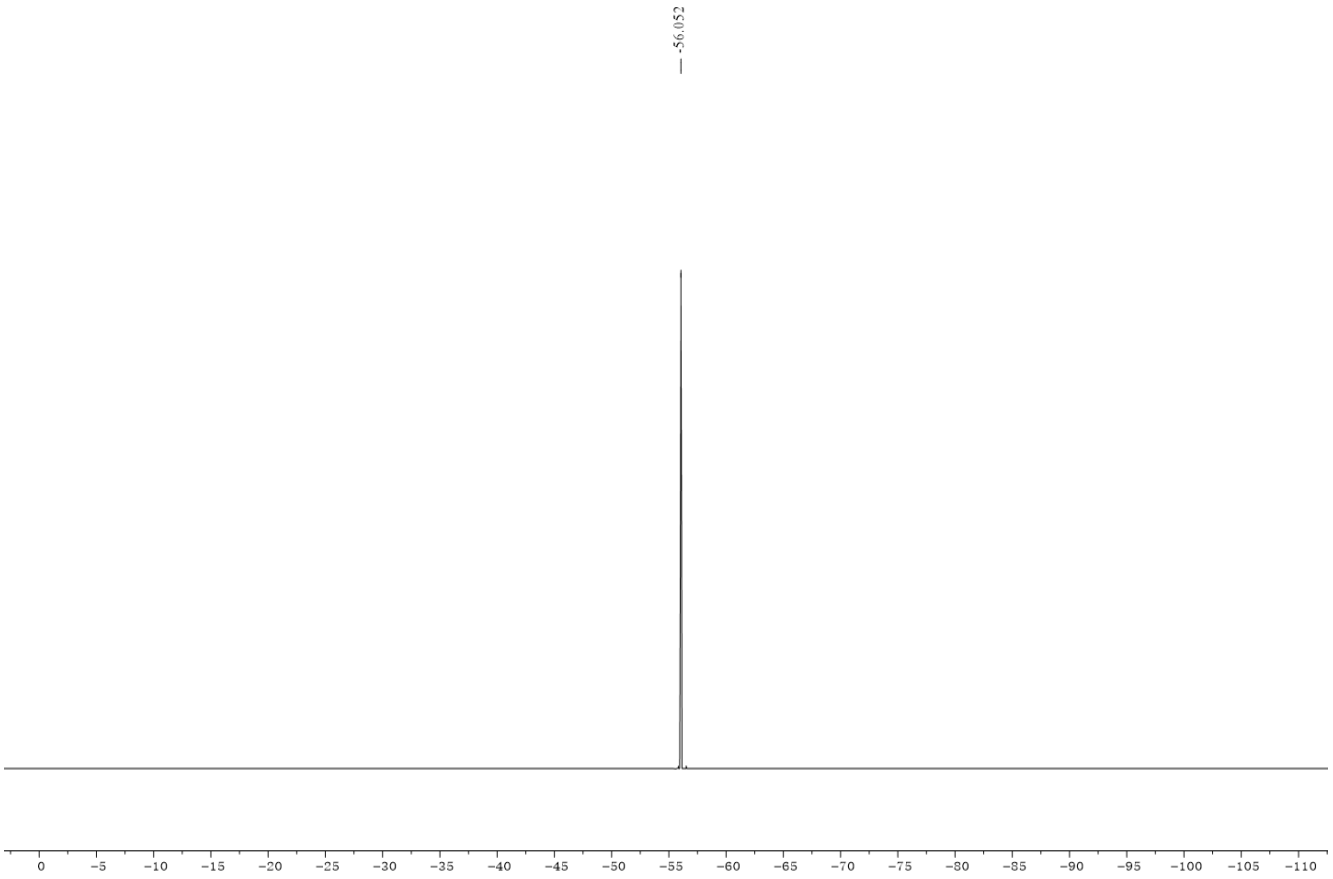

Figure S15. ^{19}F NMR (376 MHz) of **3d** in DMSO - d_6.

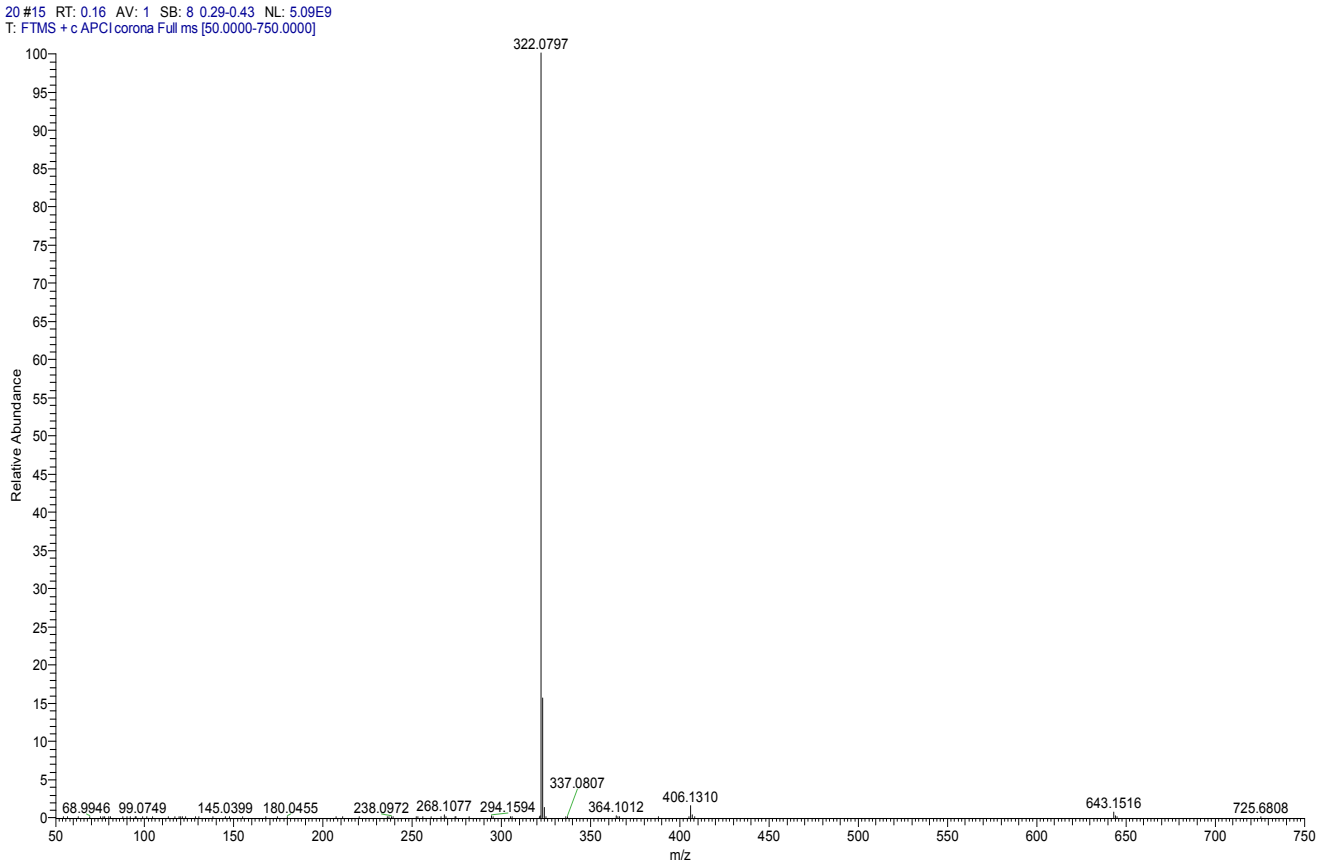

Figure S16. HRMS spectra for **3d**.

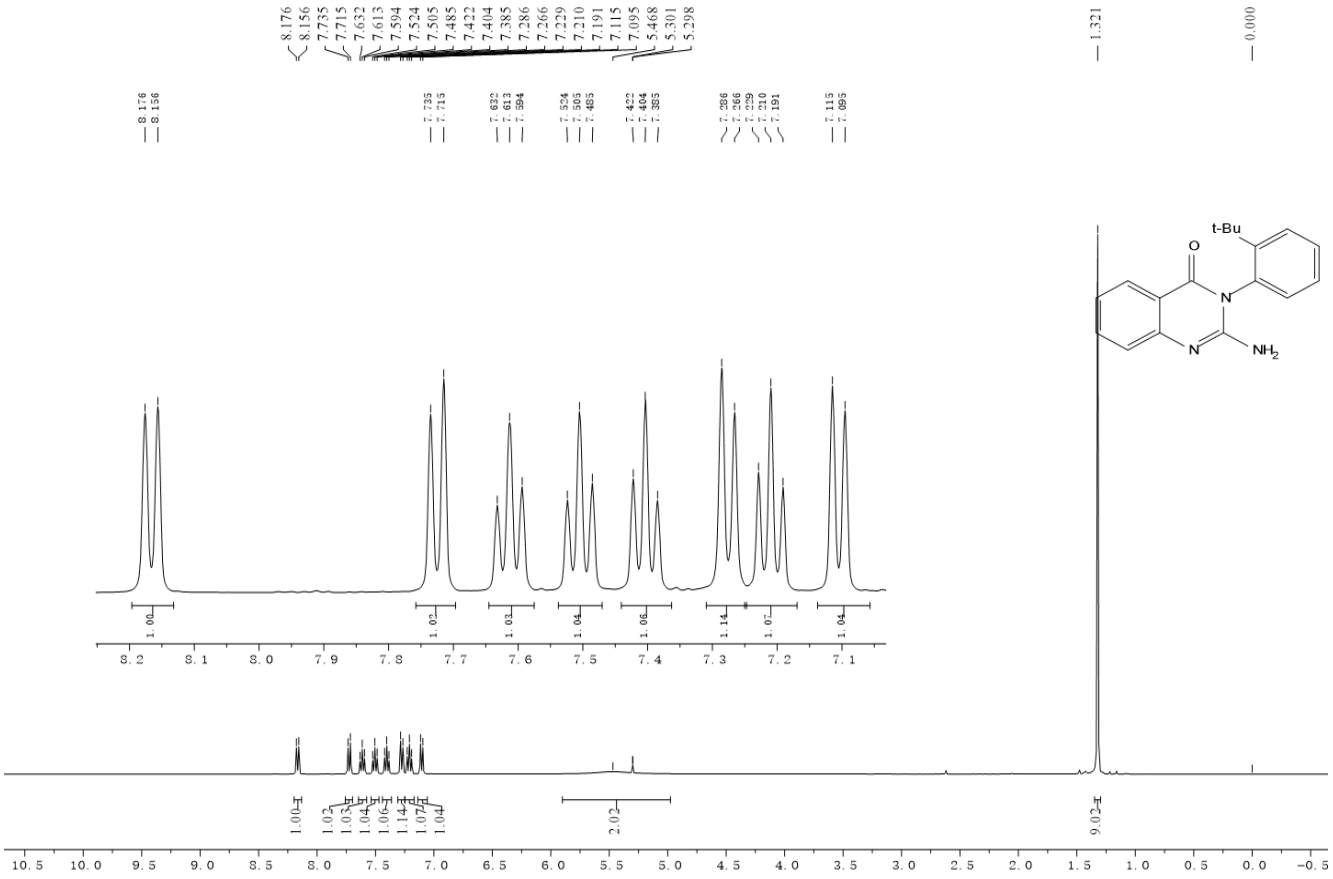

Figure S17. ^{1}H NMR (400 MHz) of **3e** in $CDCl_3$.

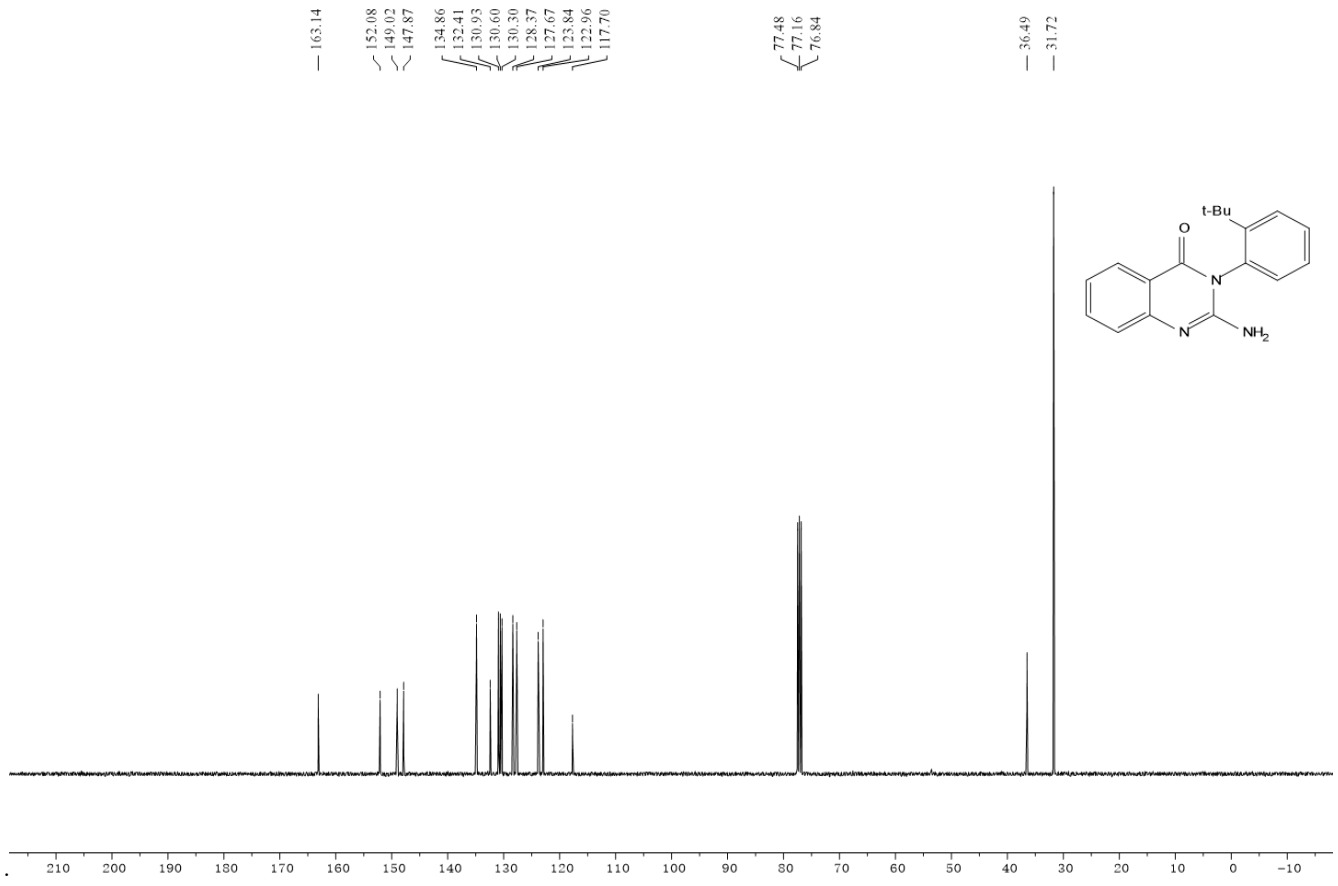

Figure S18. ^{13}C NMR (101 MHz) of **3e** in $CDCl_3$.

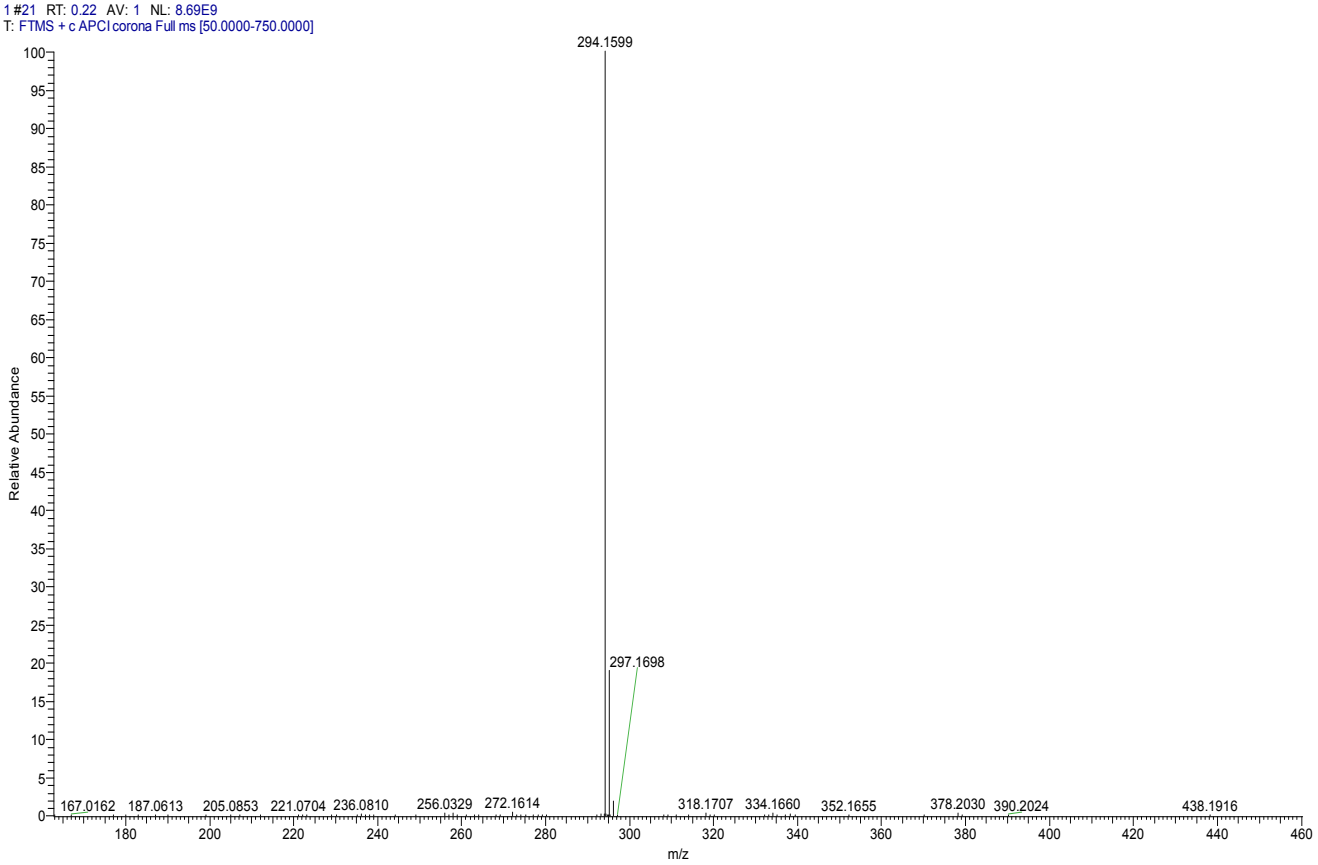

Figure S19. HRMS spectra for **3e**.

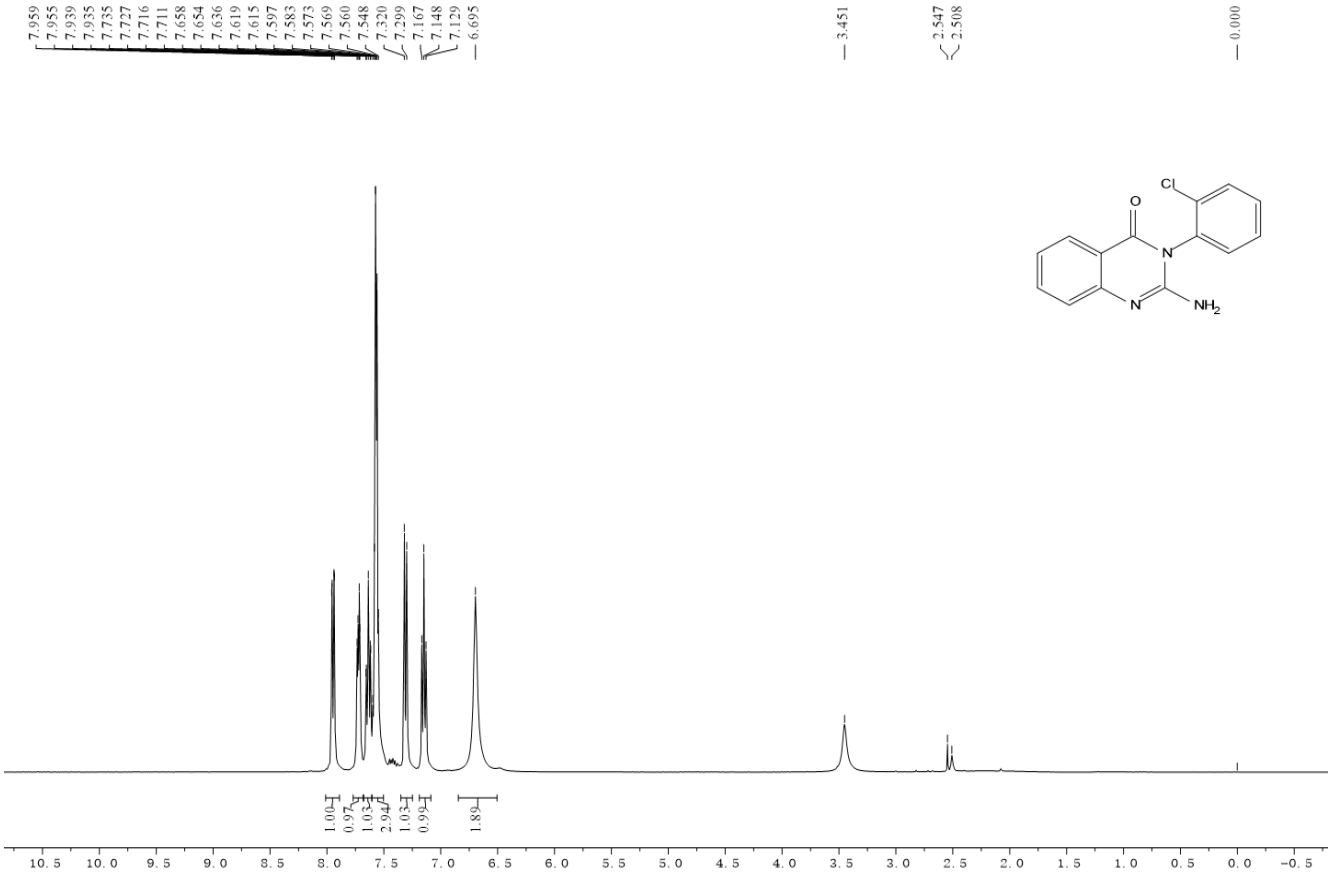

Figure S20. ^{1}H NMR (400 MHz) of **3f** in DMSO - d_6.

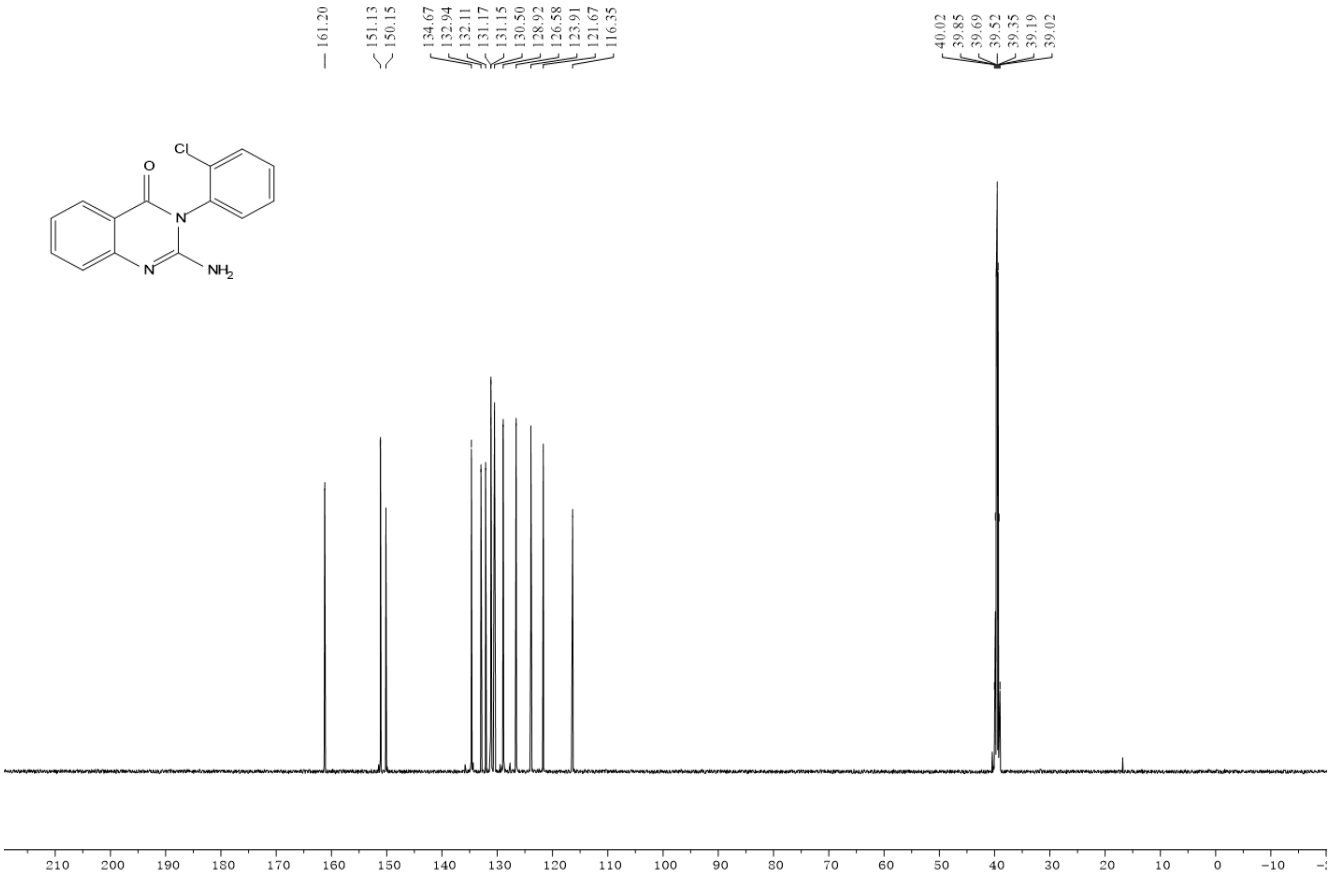

Figure S21. ^{13}C NMR (126 MHz) of **3f** in DMSO - d_6.

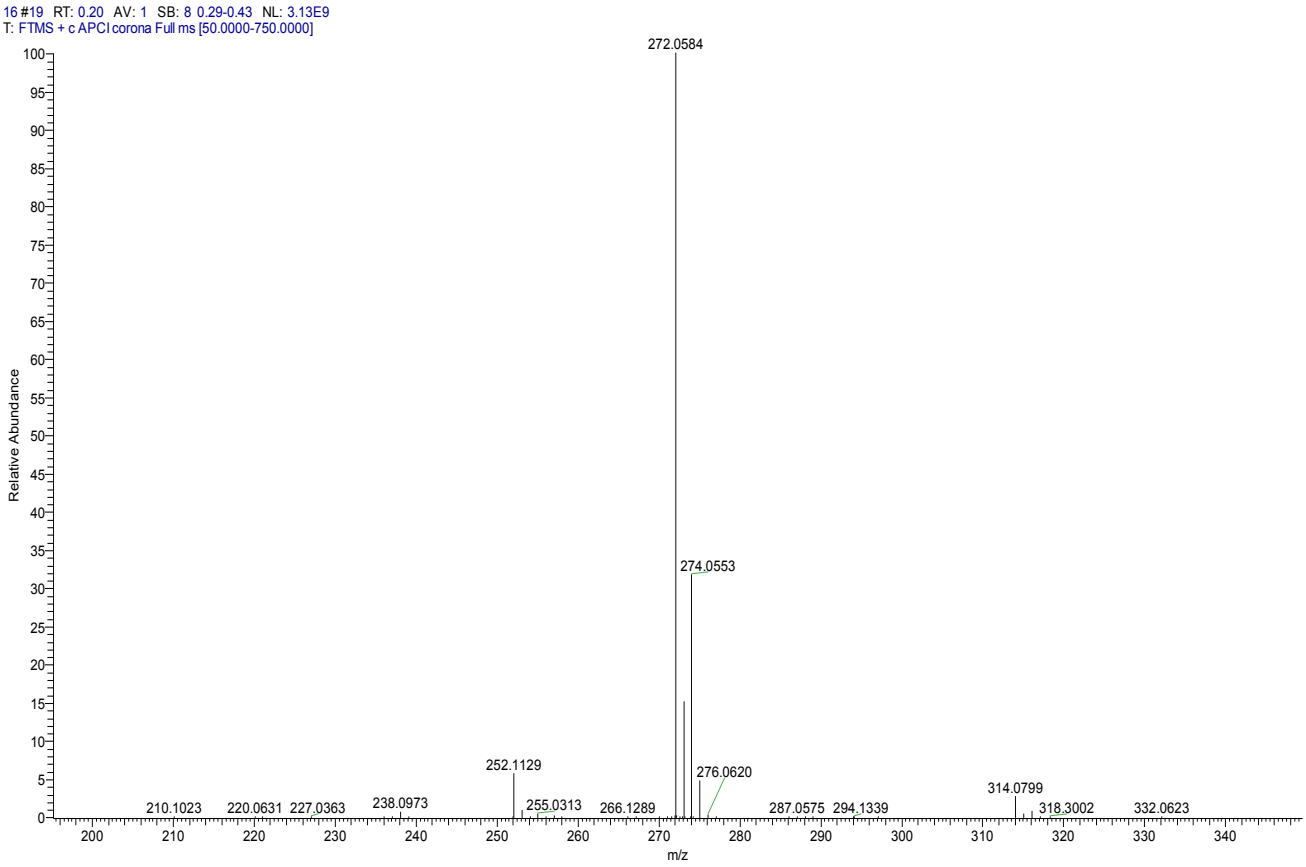

Figure S22. HRMS spectra for **3f**.

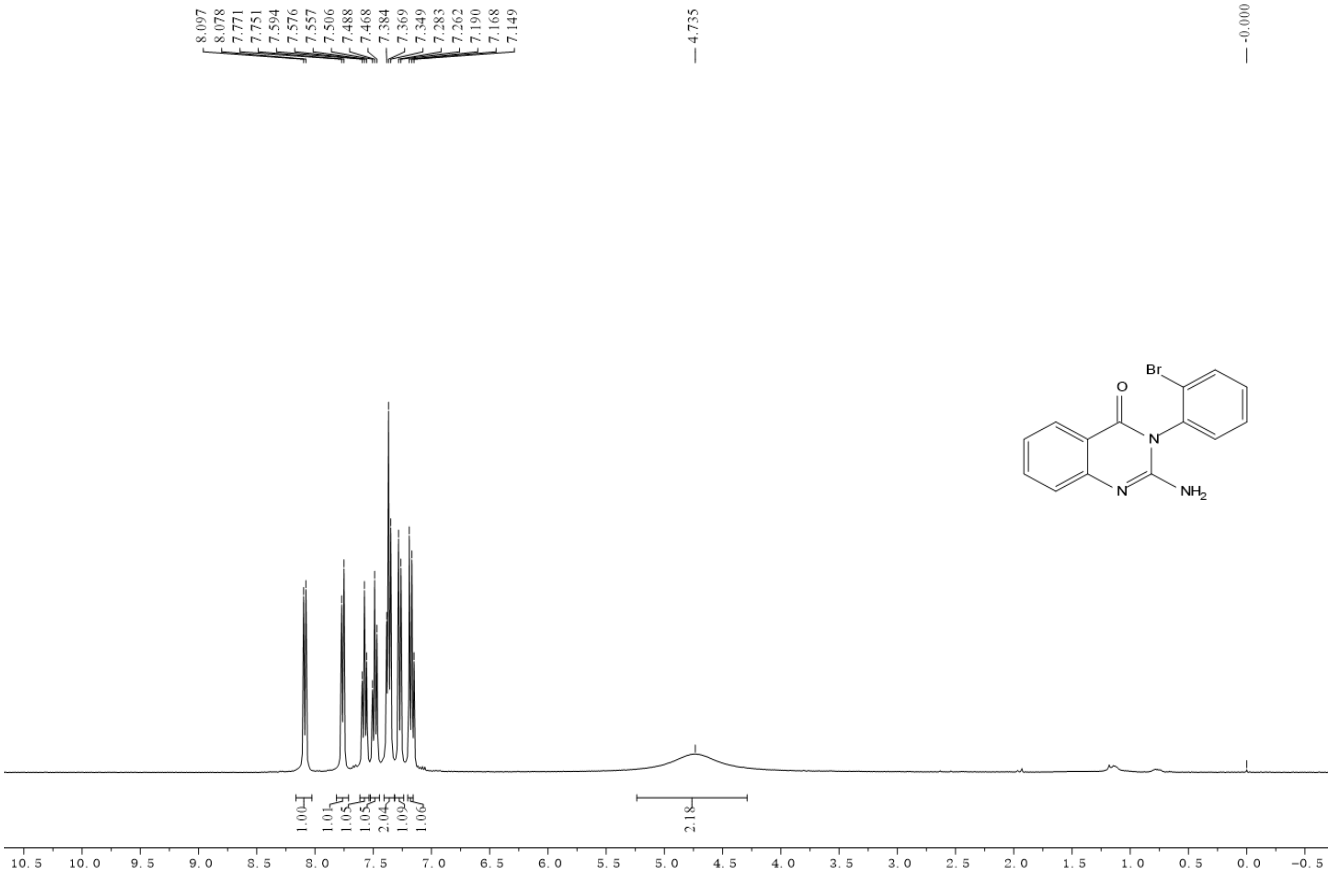

Figure S23. ^{1}H NMR (400 MHz) of **3g** in $CDCl_3$.

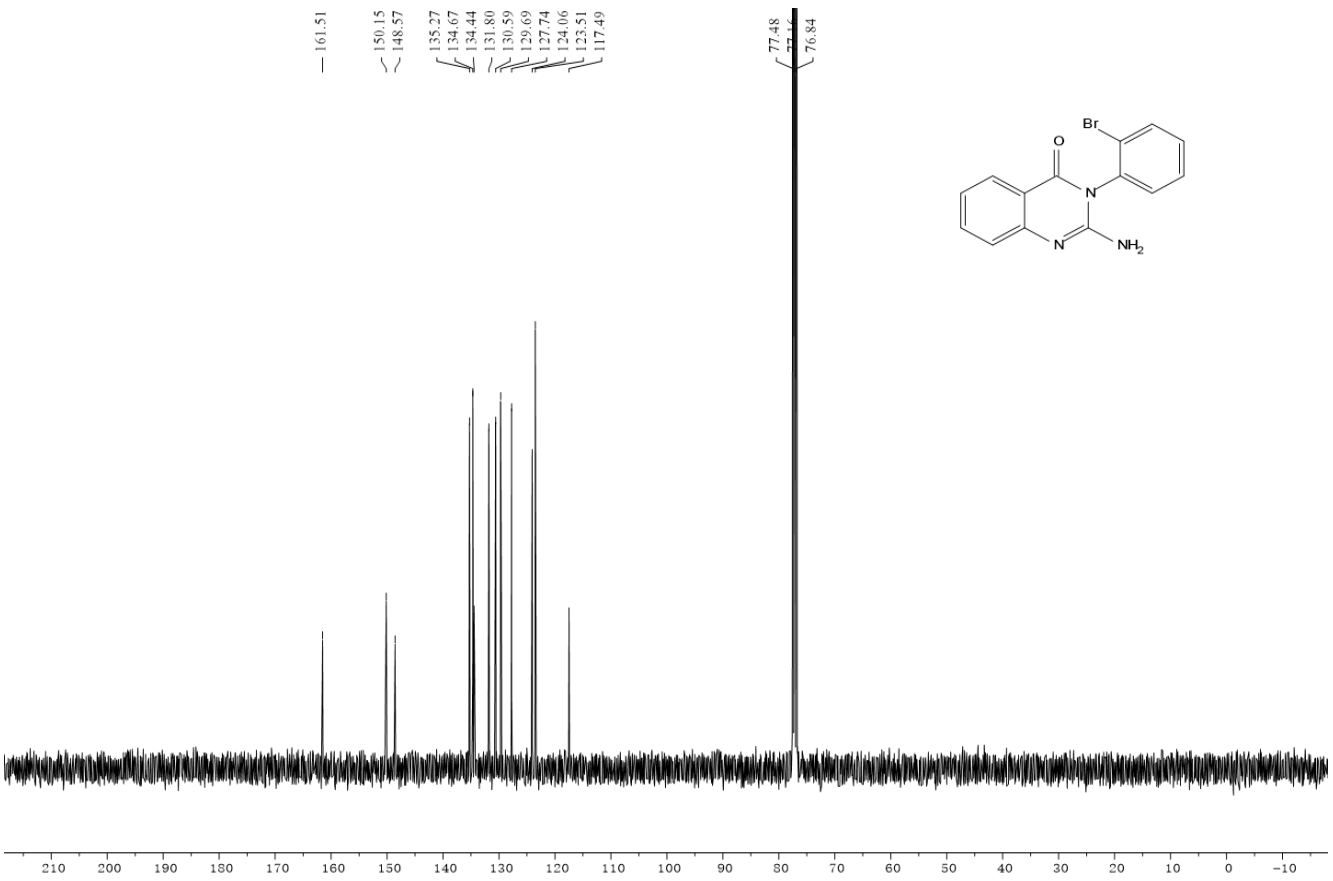

Figure S24. ^{13}C NMR (101 MHz) of **3g** in $CDCl_3$.

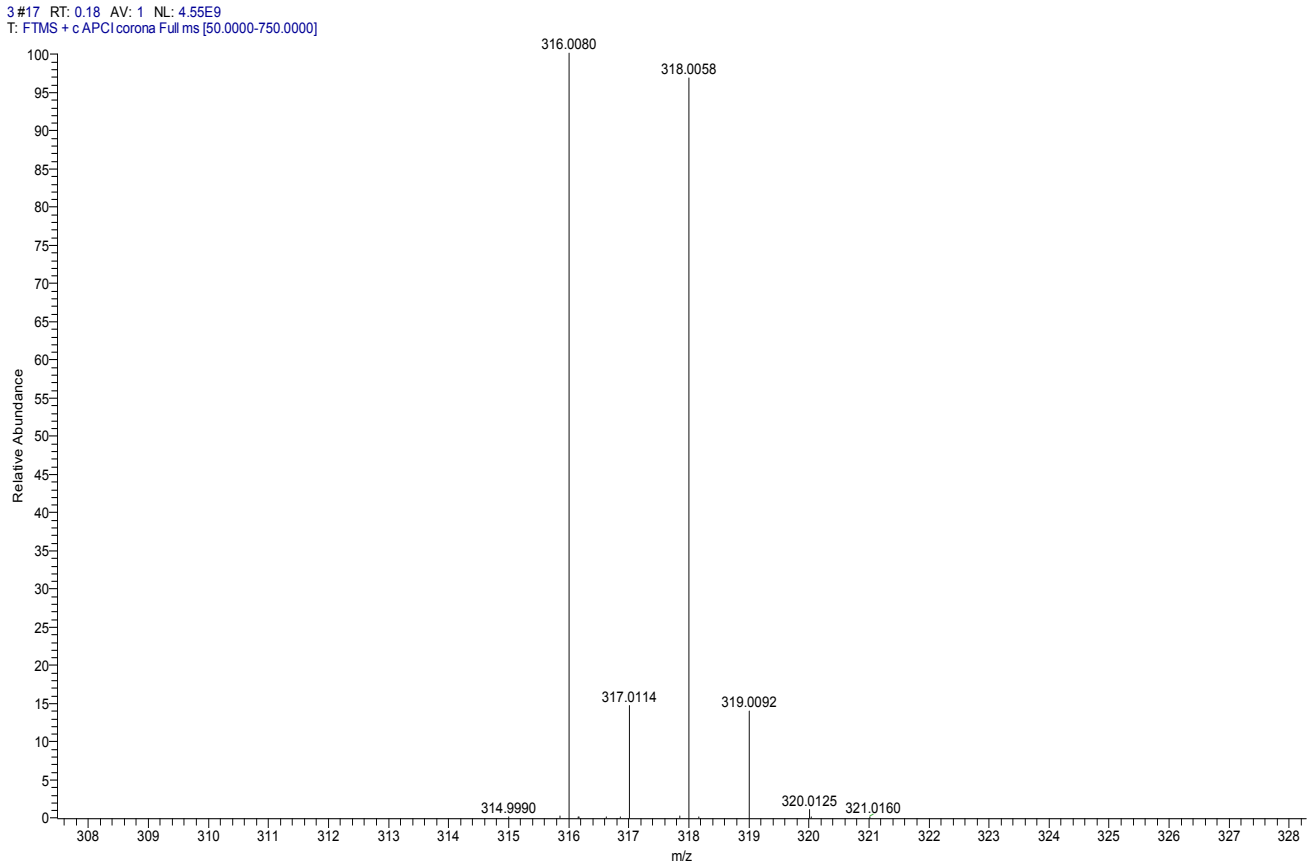

Figure S25. HRMS spectra for **3g**.

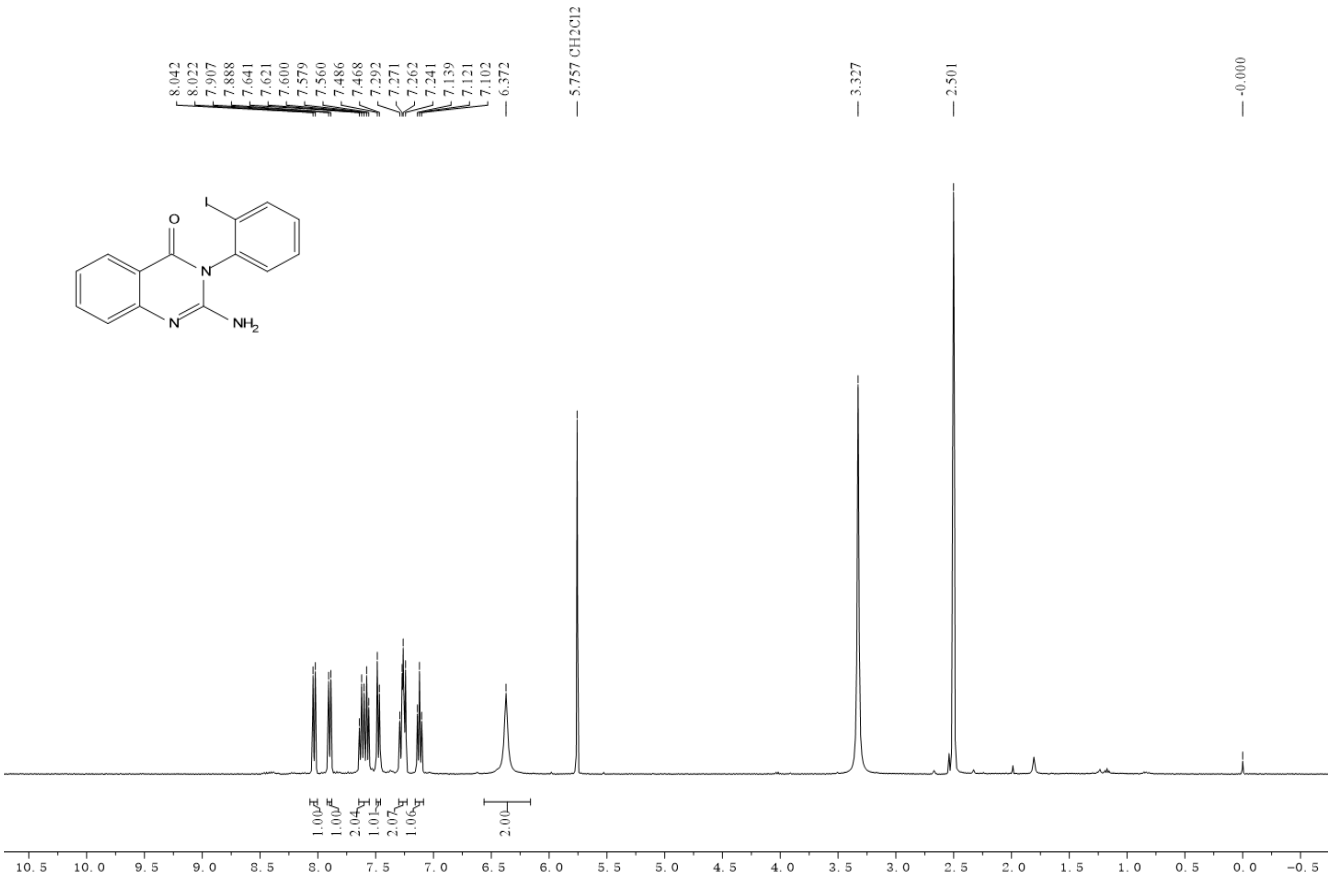

Figure S26. ^{1}H NMR (400 MHz) of **3h** in $CDCl_3$.

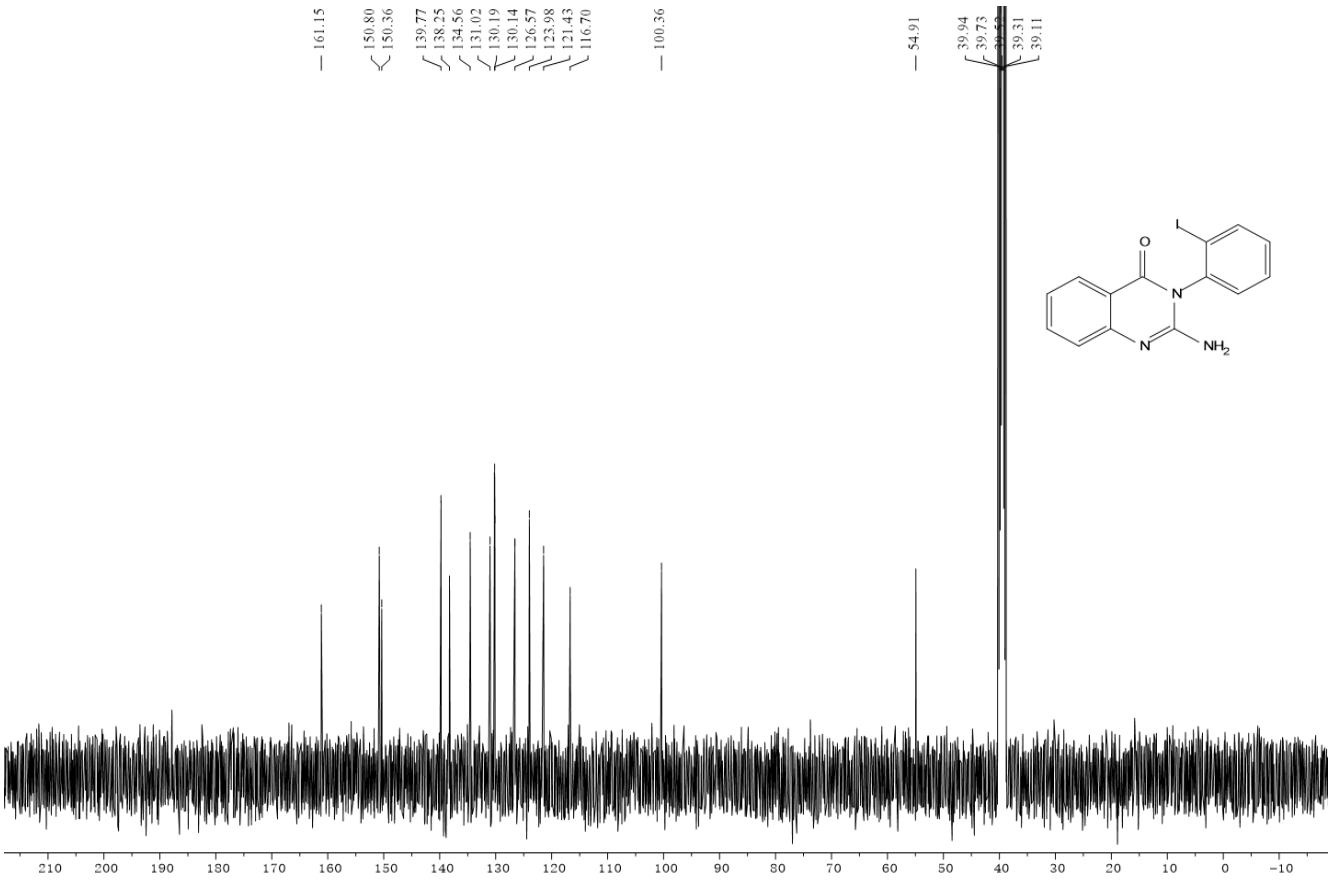

Figure S27. ^{13}C NMR (101 MHz) of **3h** in $CDCl_3$.

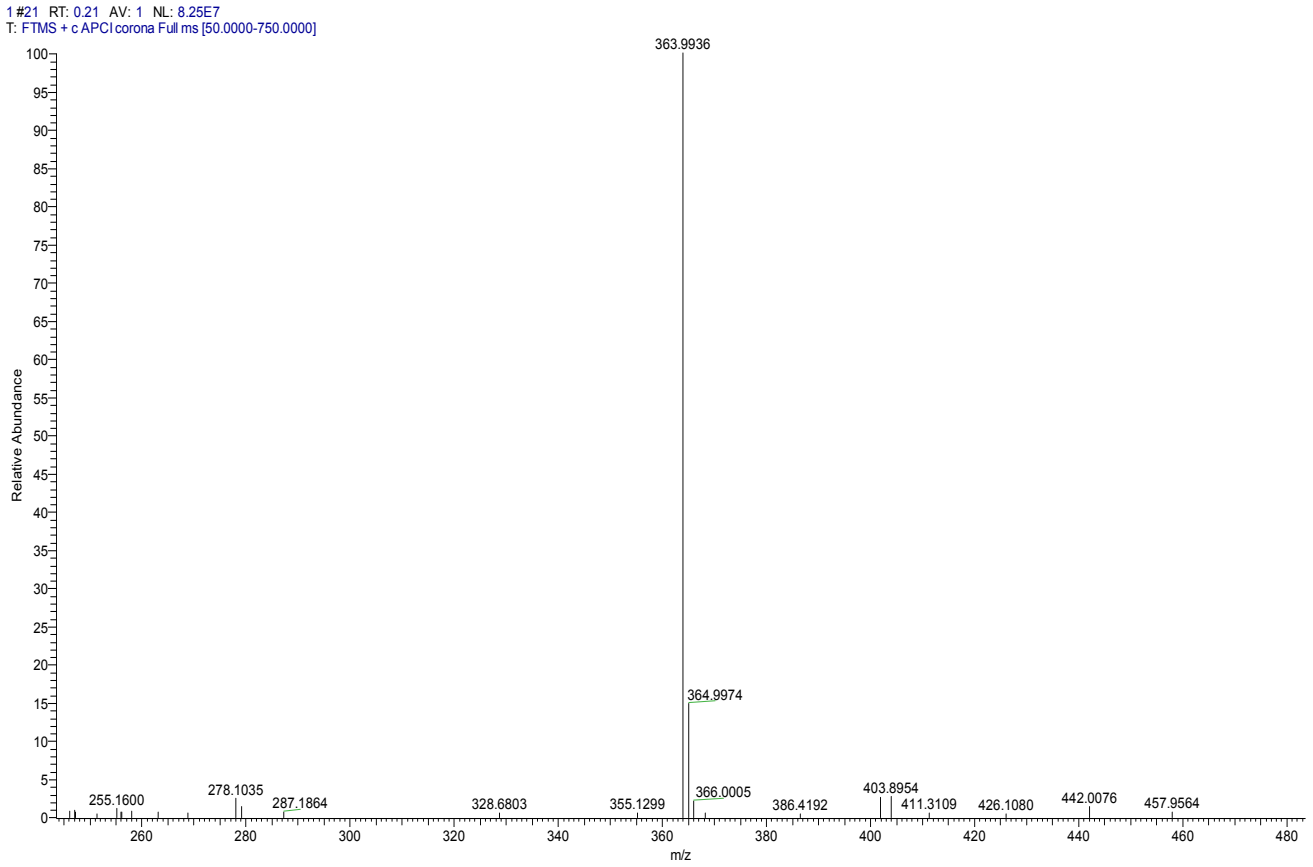

Figure S28. HRMS spectra for **3h**.

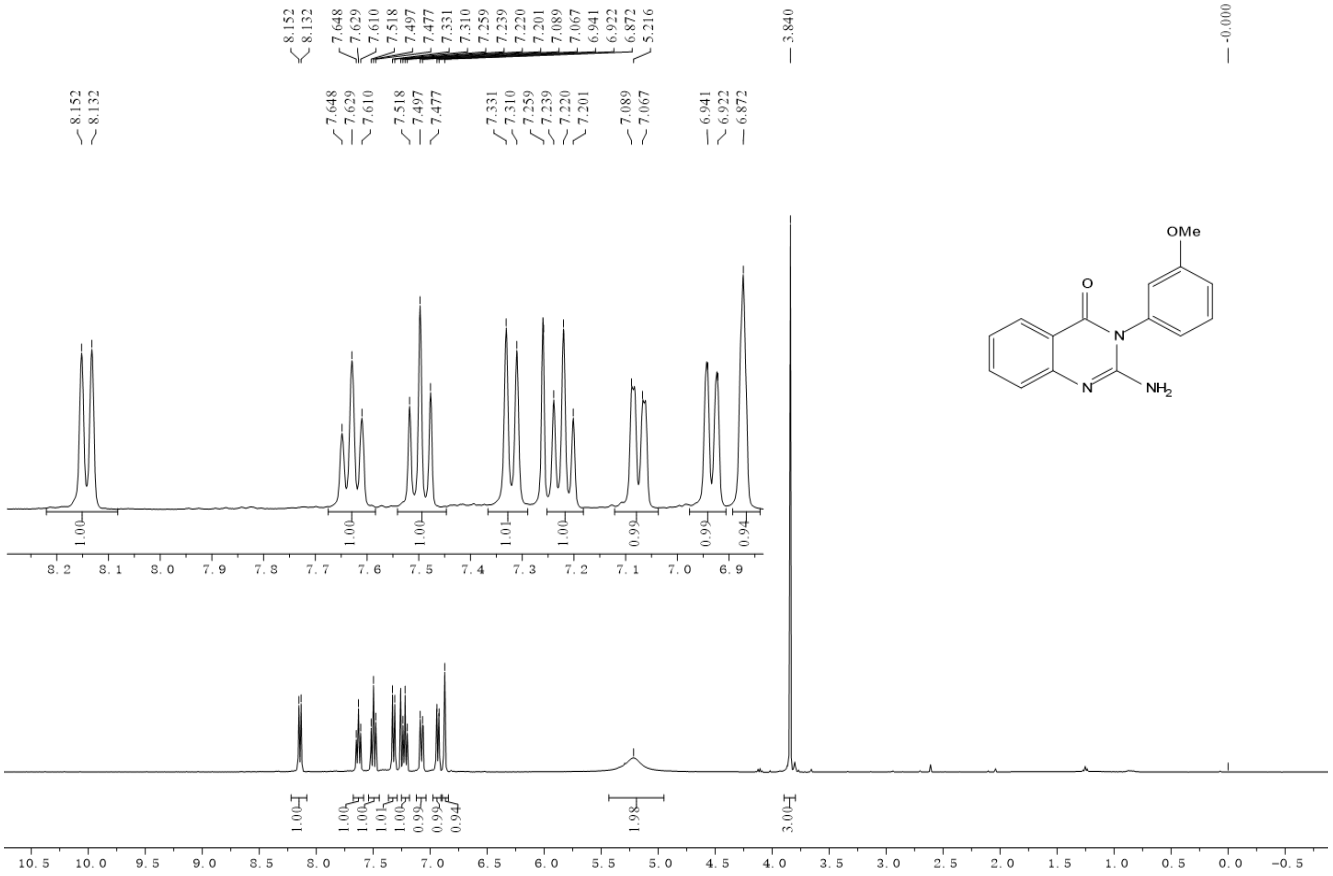

Figure S29. ^{1}H NMR (400 MHz) of **3i** in $CDCl_3$.

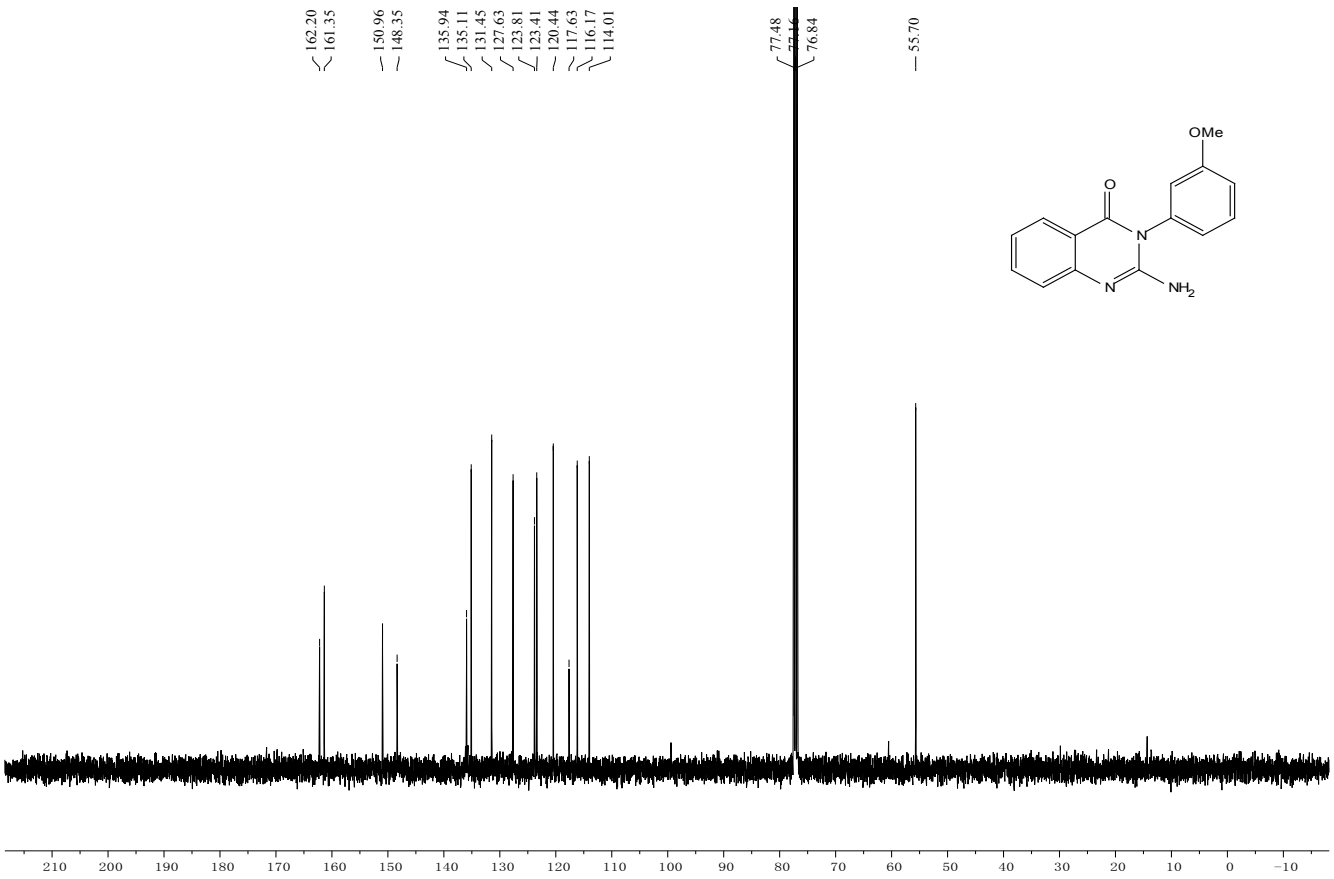

Figure S30. ^{13}C NMR (101 MHz) of **3i** in $CDCl_3$.

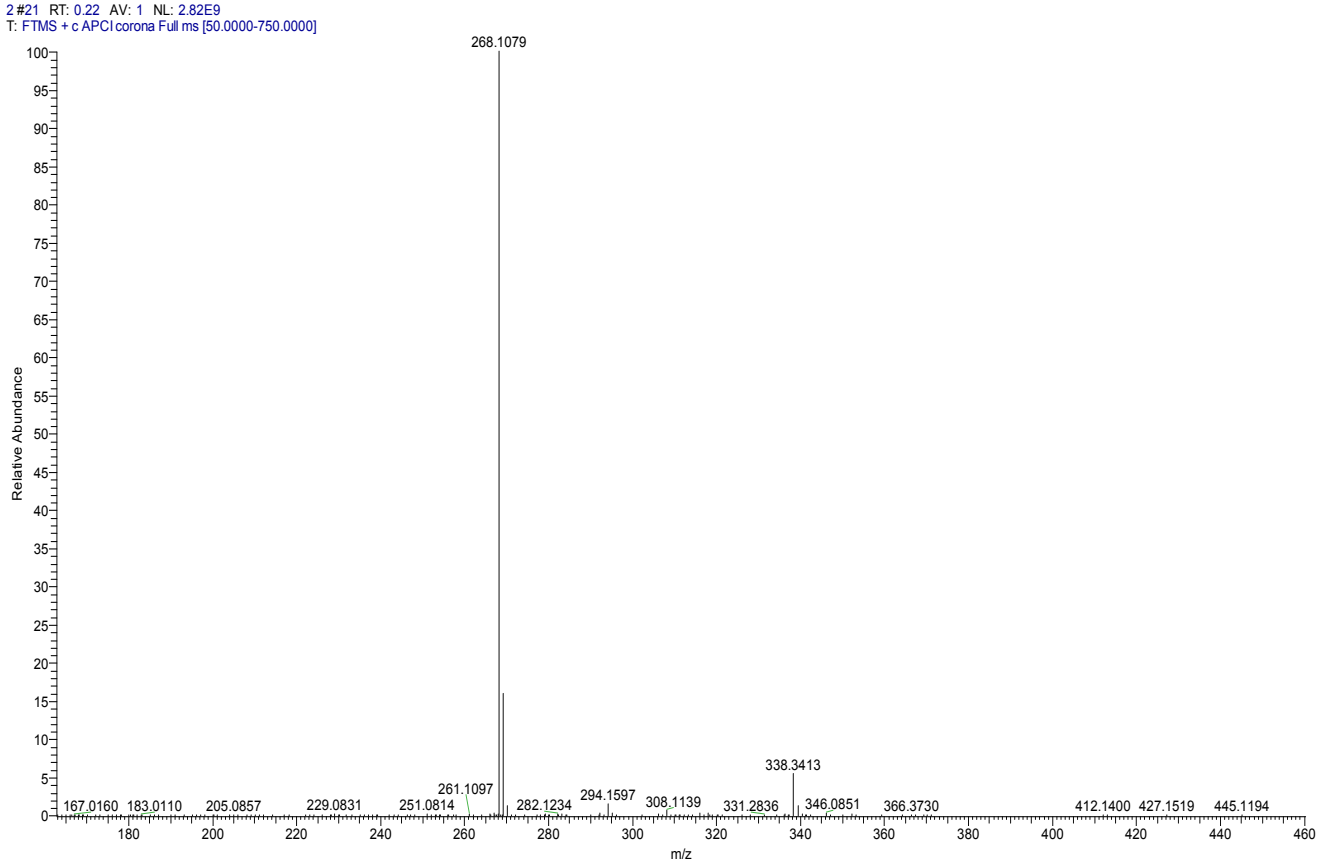

Figure S31. HRMS spectra for **3i**.

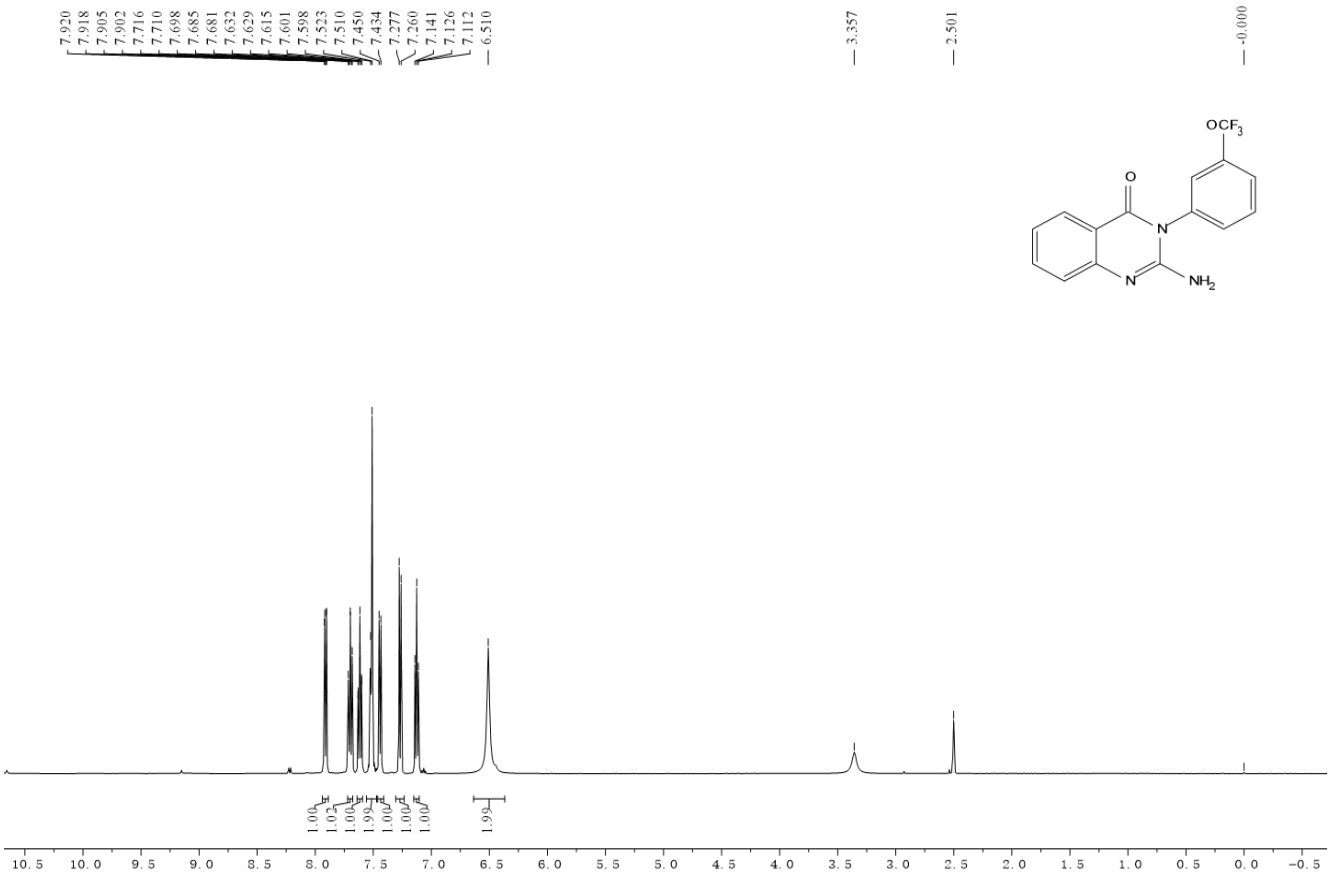

Figure S32. ^{1}H NMR (500 MHz) of **3j** in DMSO - d_6.

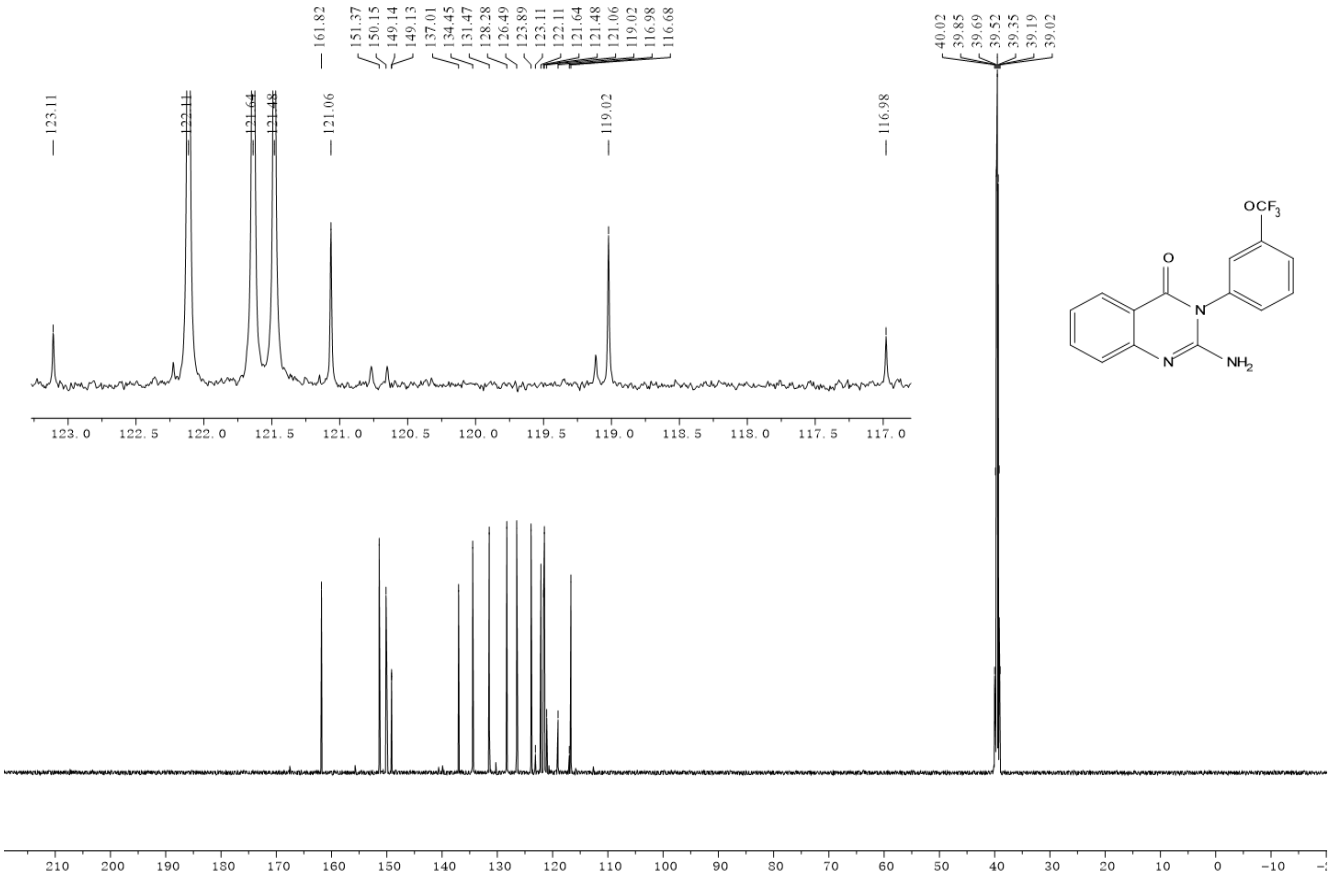

Figure S33. ^{13}C NMR (126 MHz) of **3j** in DMSO - d_6.

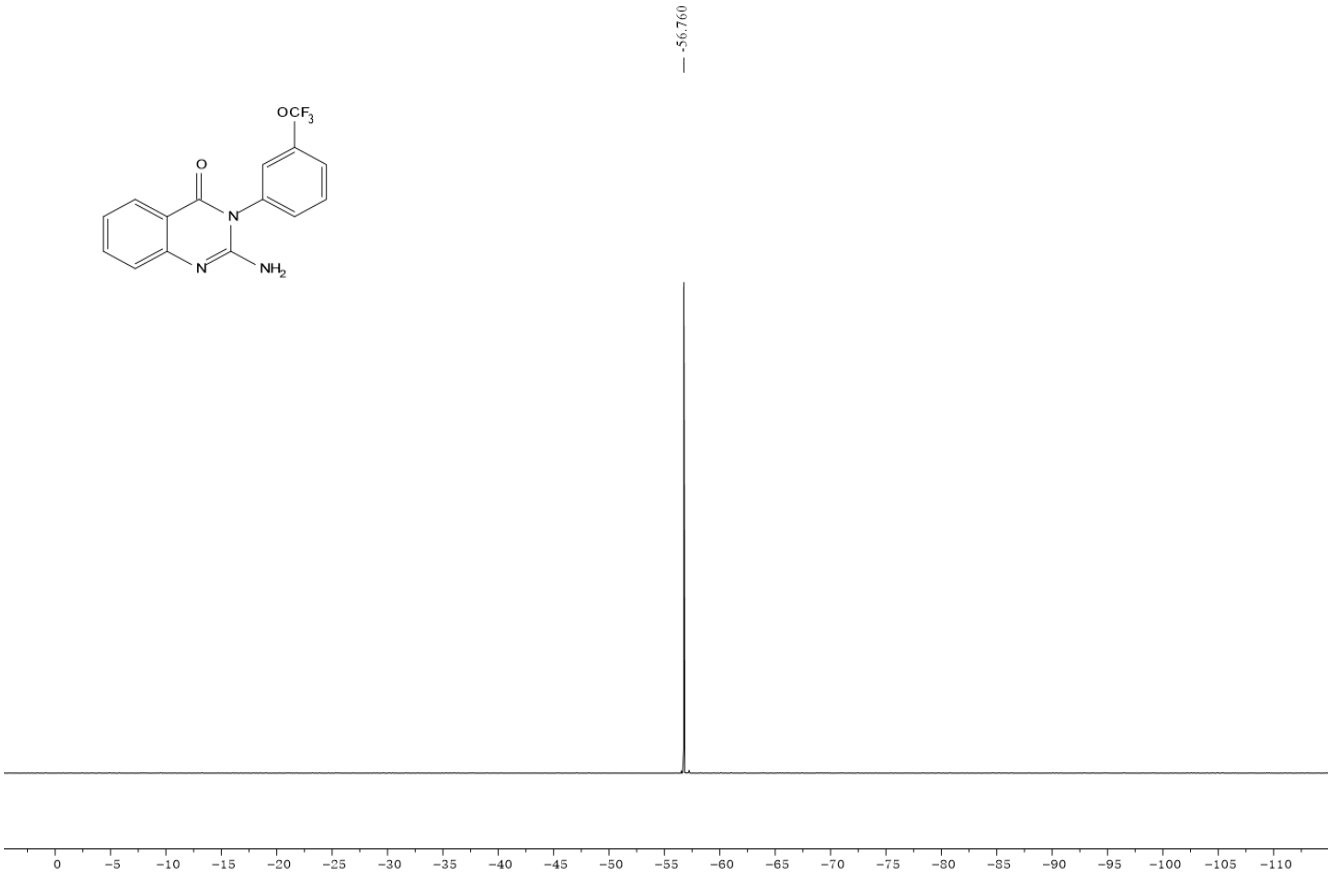

Figure S34. ^{19}F NMR (376 MHz) of **3j** in DMSO - d_6.

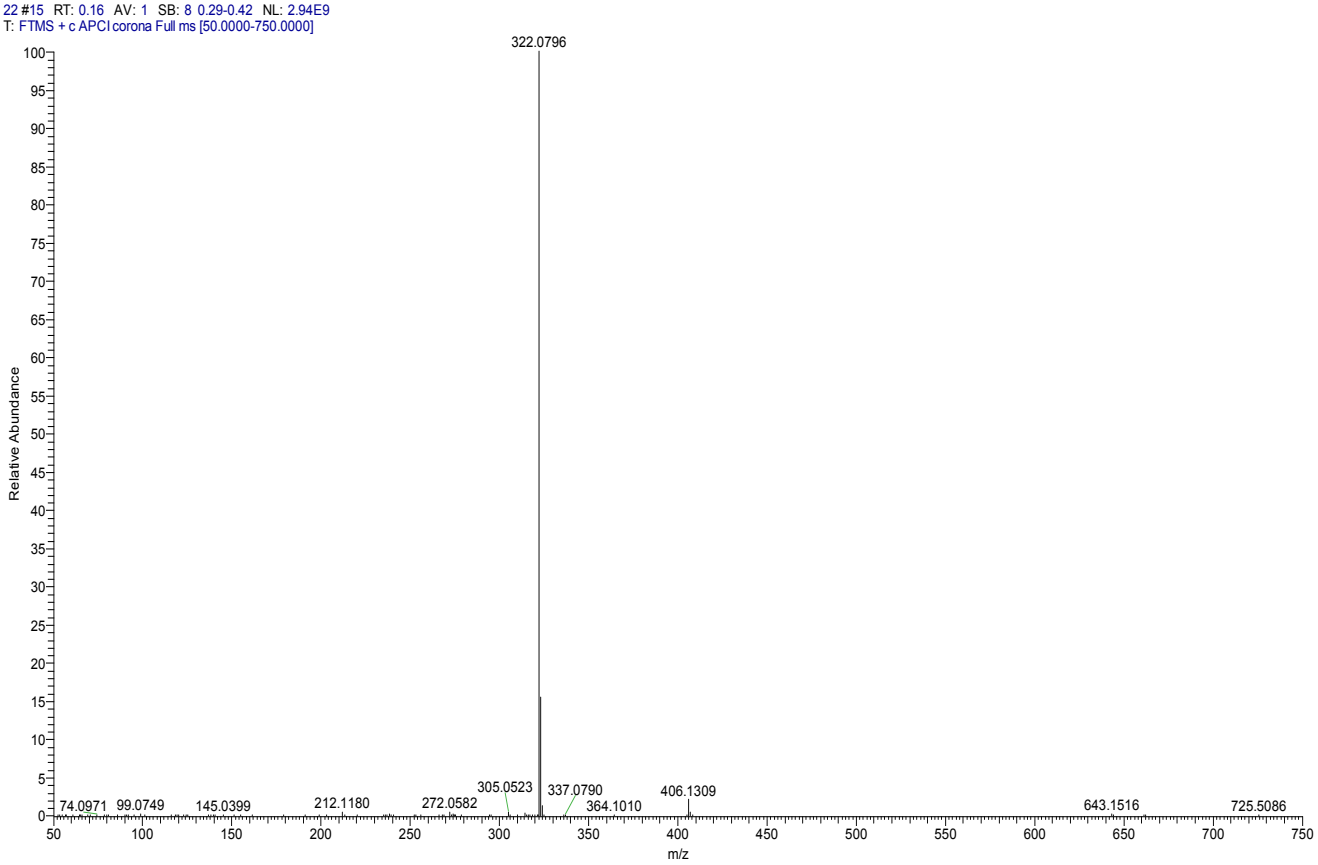

Figure S35. HRMS spectra for **3j**.

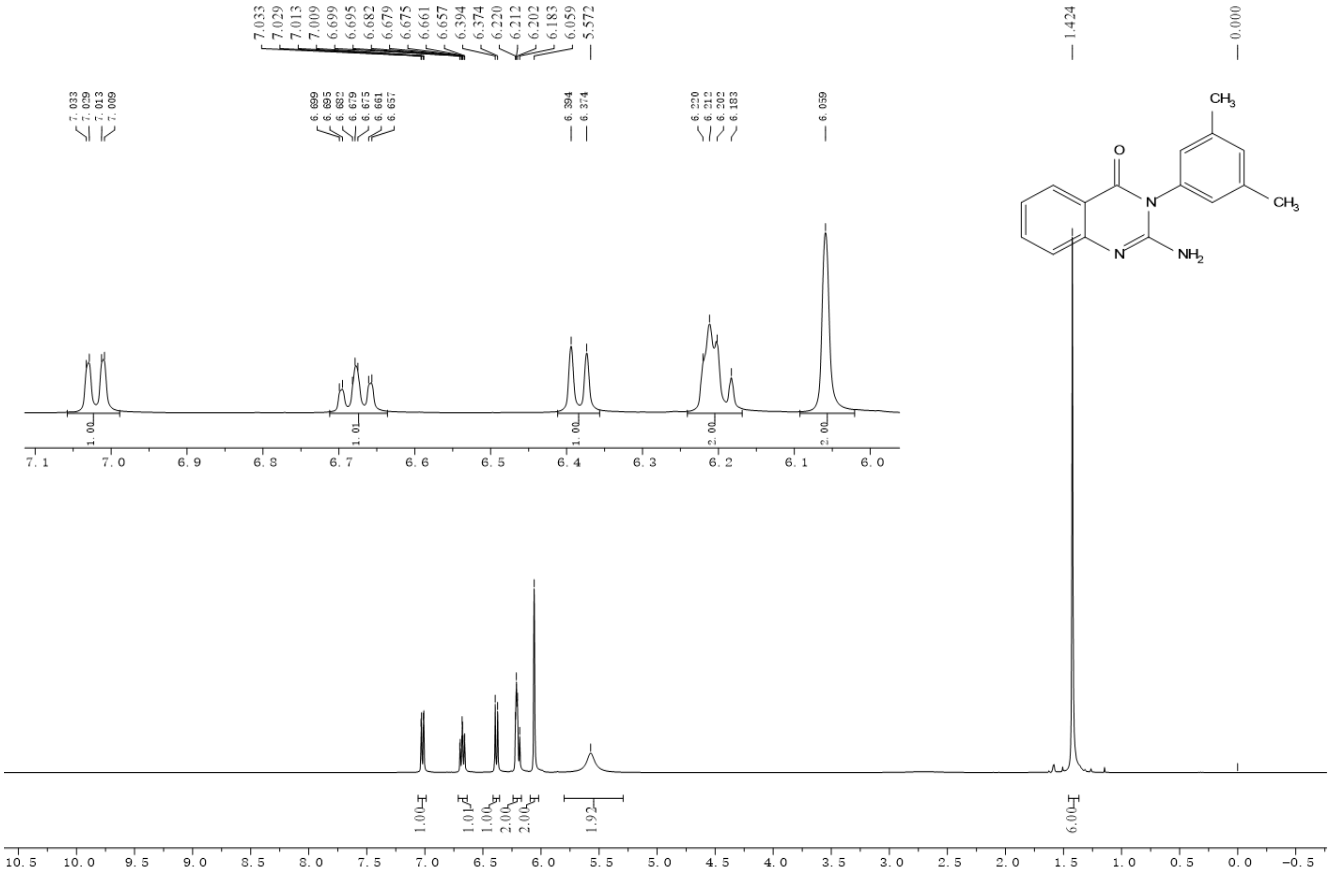

Figure S36. [1]H NMR (400 MHz) of **3k** in DMSO - d_6.

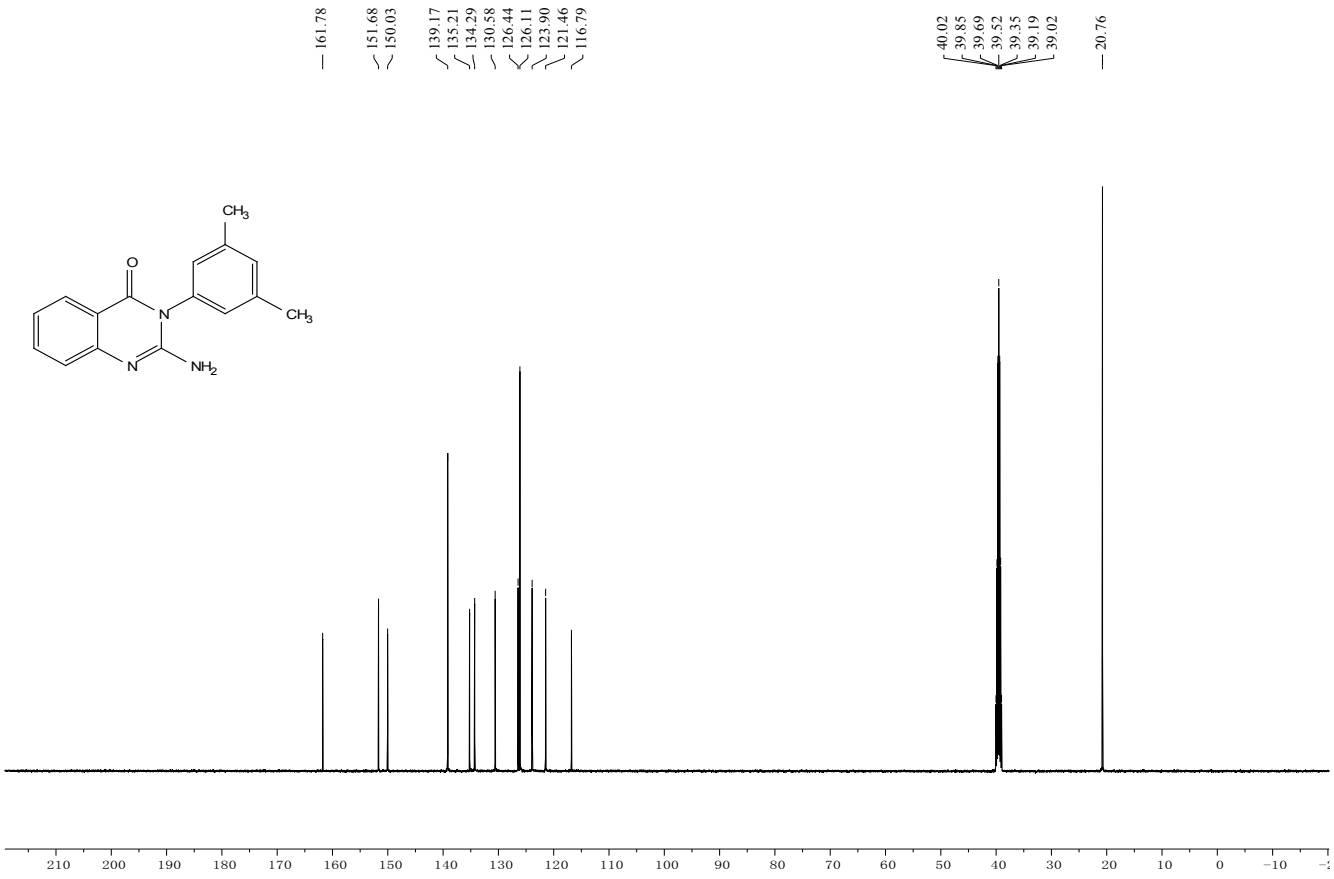

Figure S37. [13]C NMR (126 MHz) of **3k** in DMSO - d_6.

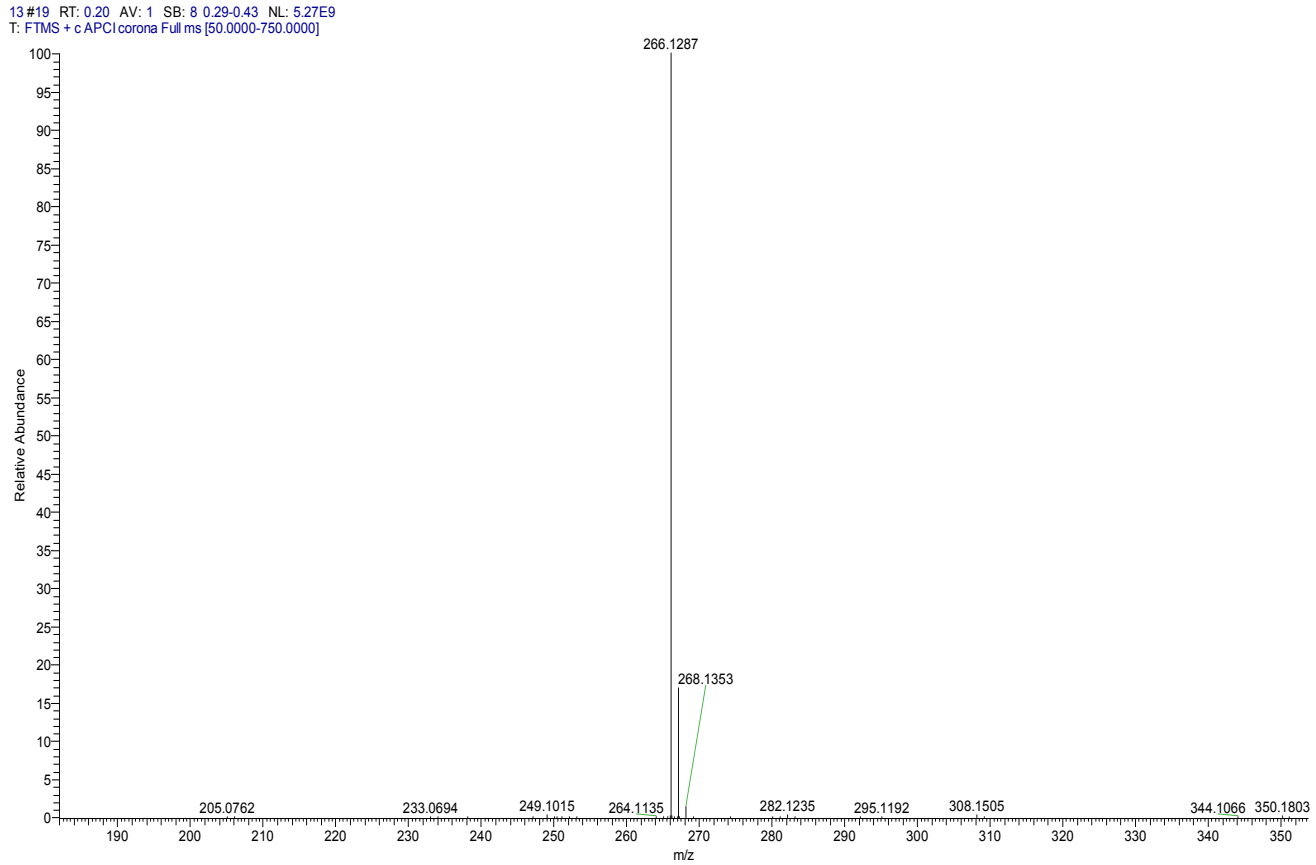

Figure S38. HRMS spectra for **3k**

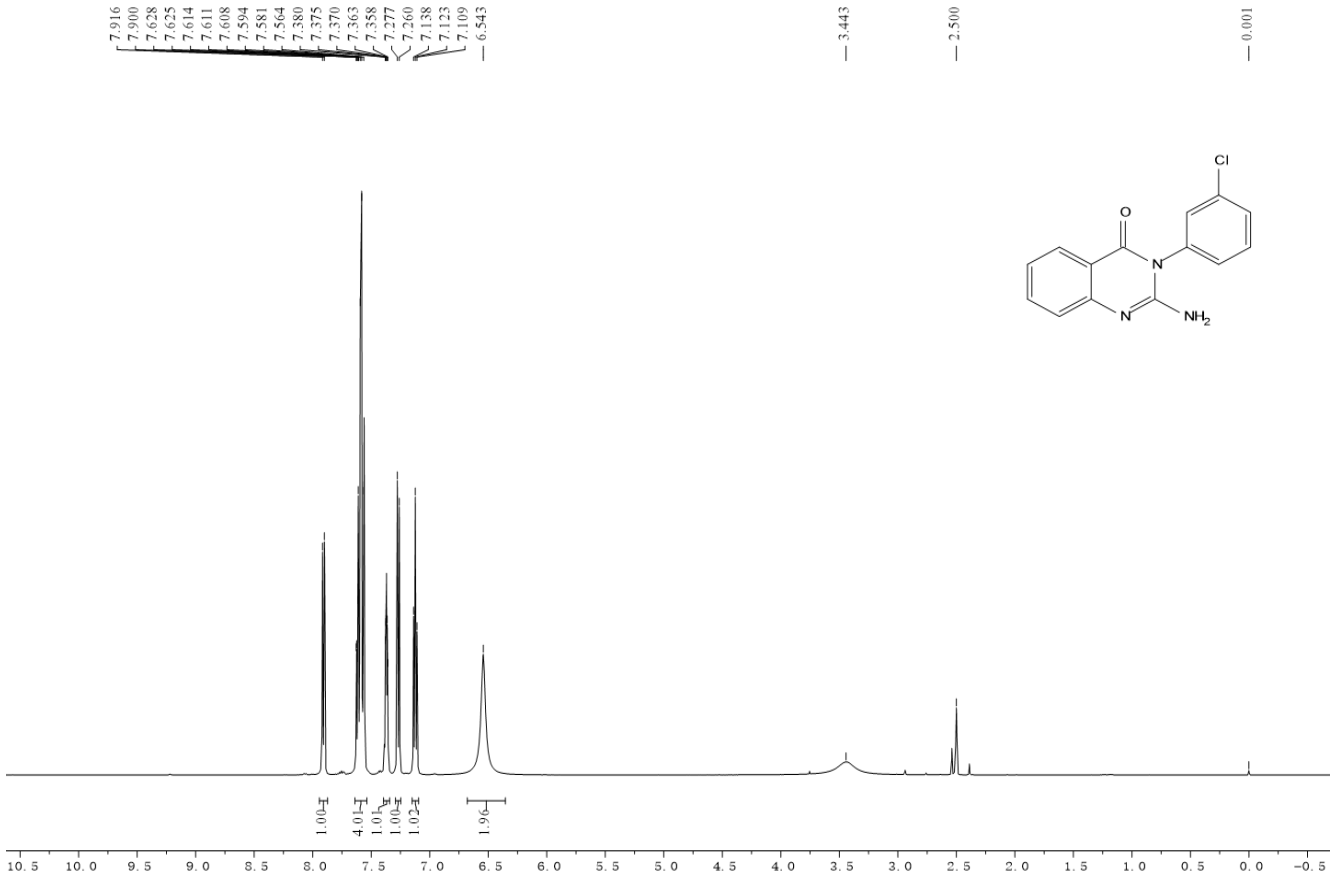

Figure S39. ^{1}H NMR (500 MHz) of **3l** in DMSO - d_6.

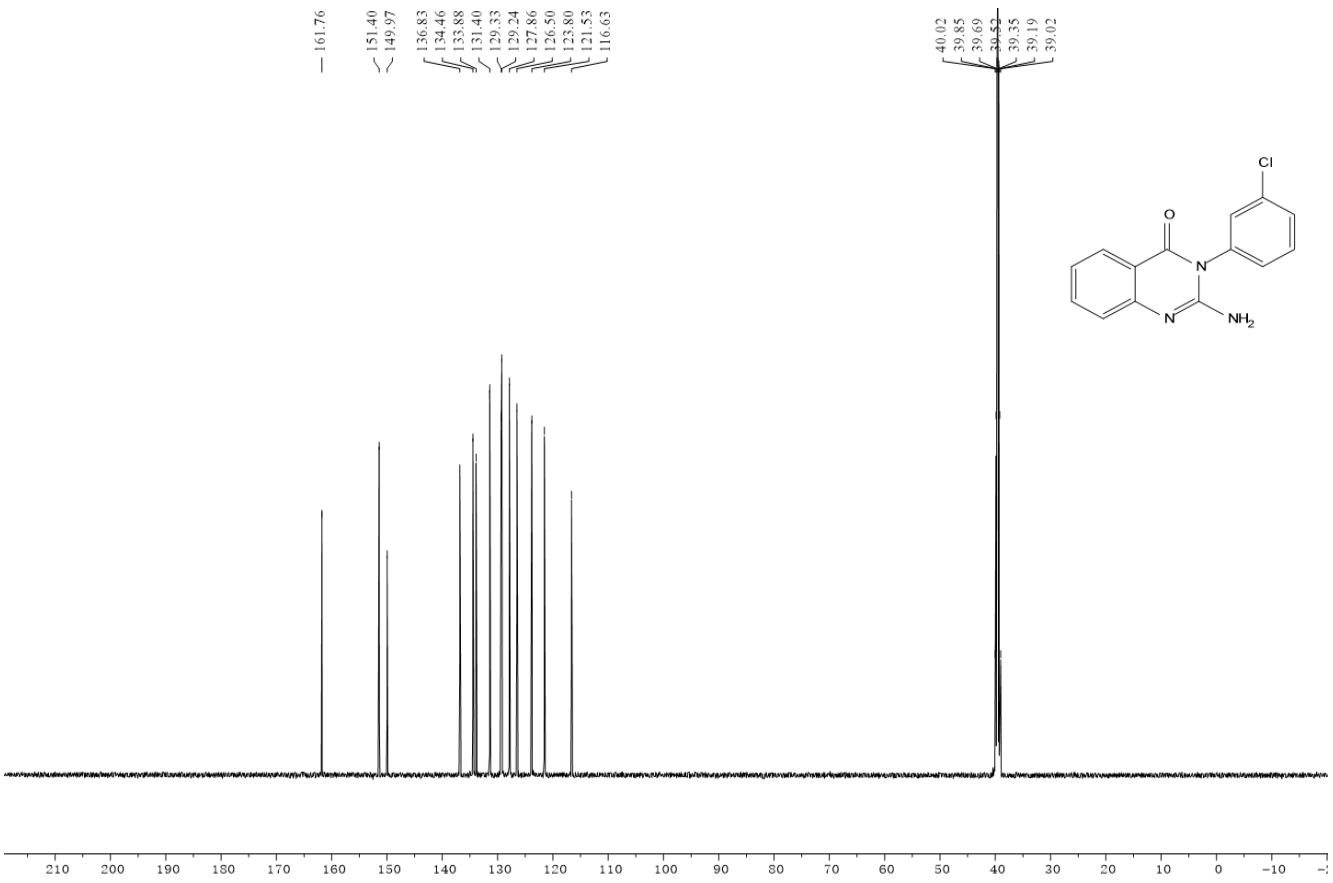

Figure S40. ^{13}C NMR (126 MHz) of **31** in DMSO - d_6.

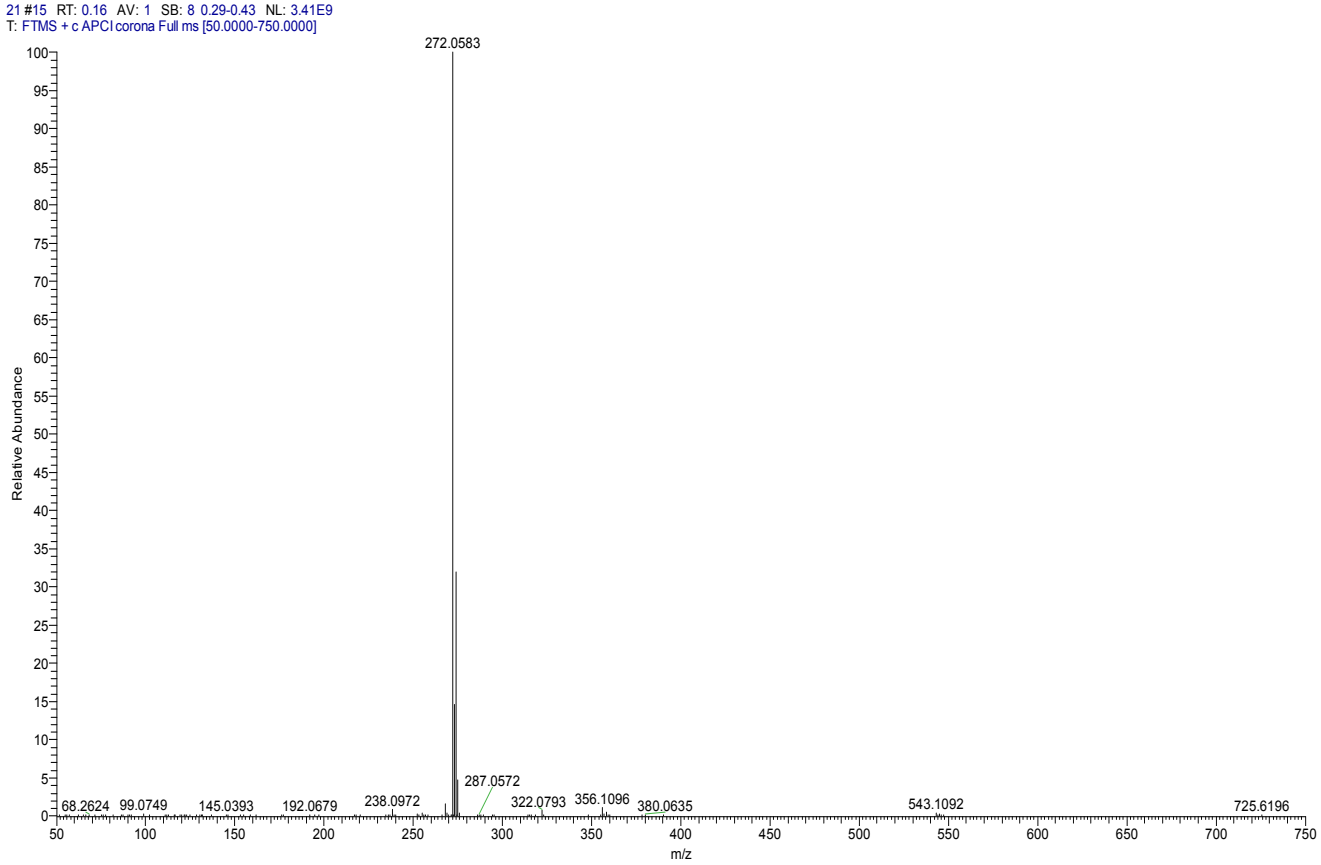

Figure S41. HRMS spectra for **31**.

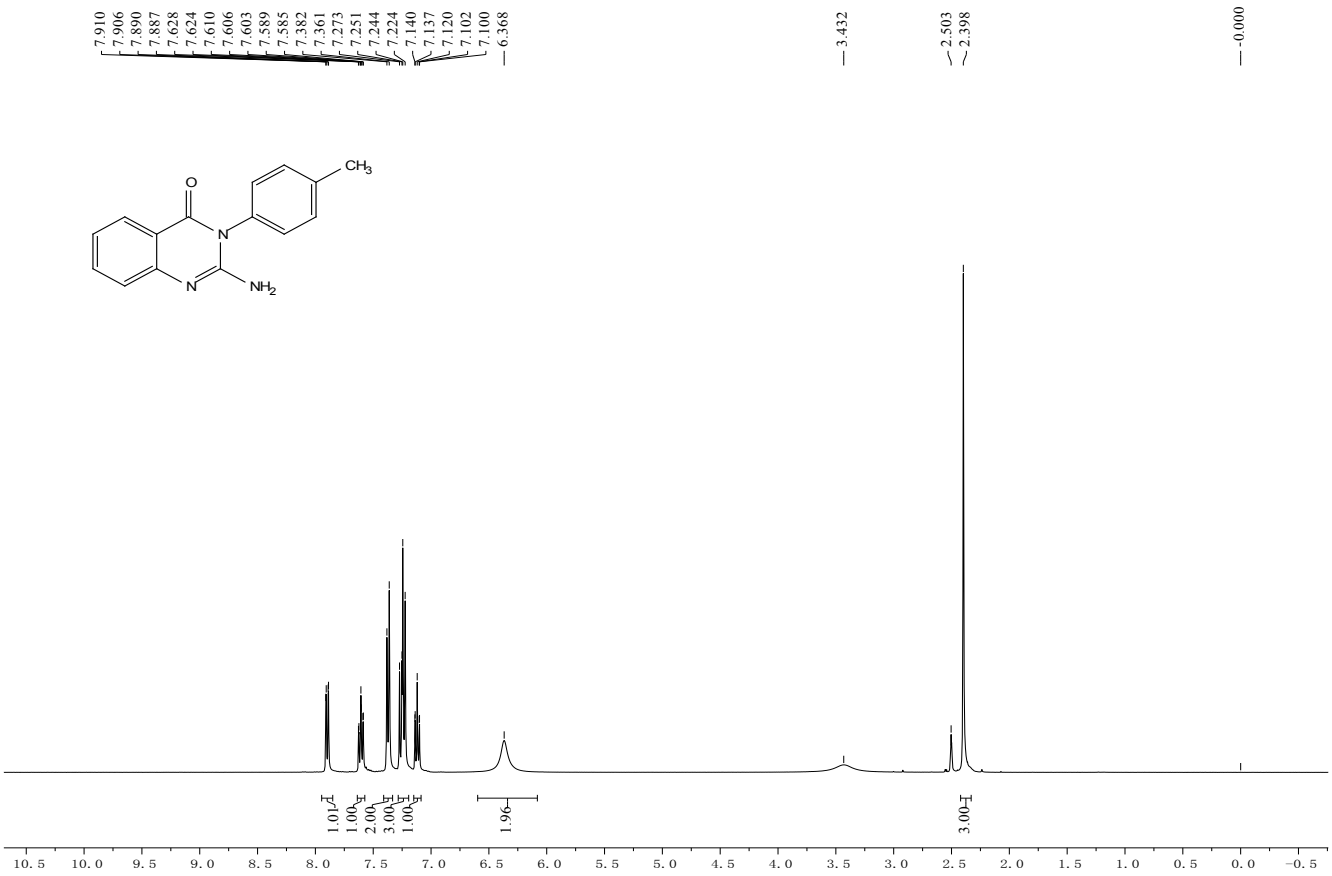

Figure S42. [1]H NMR (400 MHz) of **3m** in DMSO - d_6.

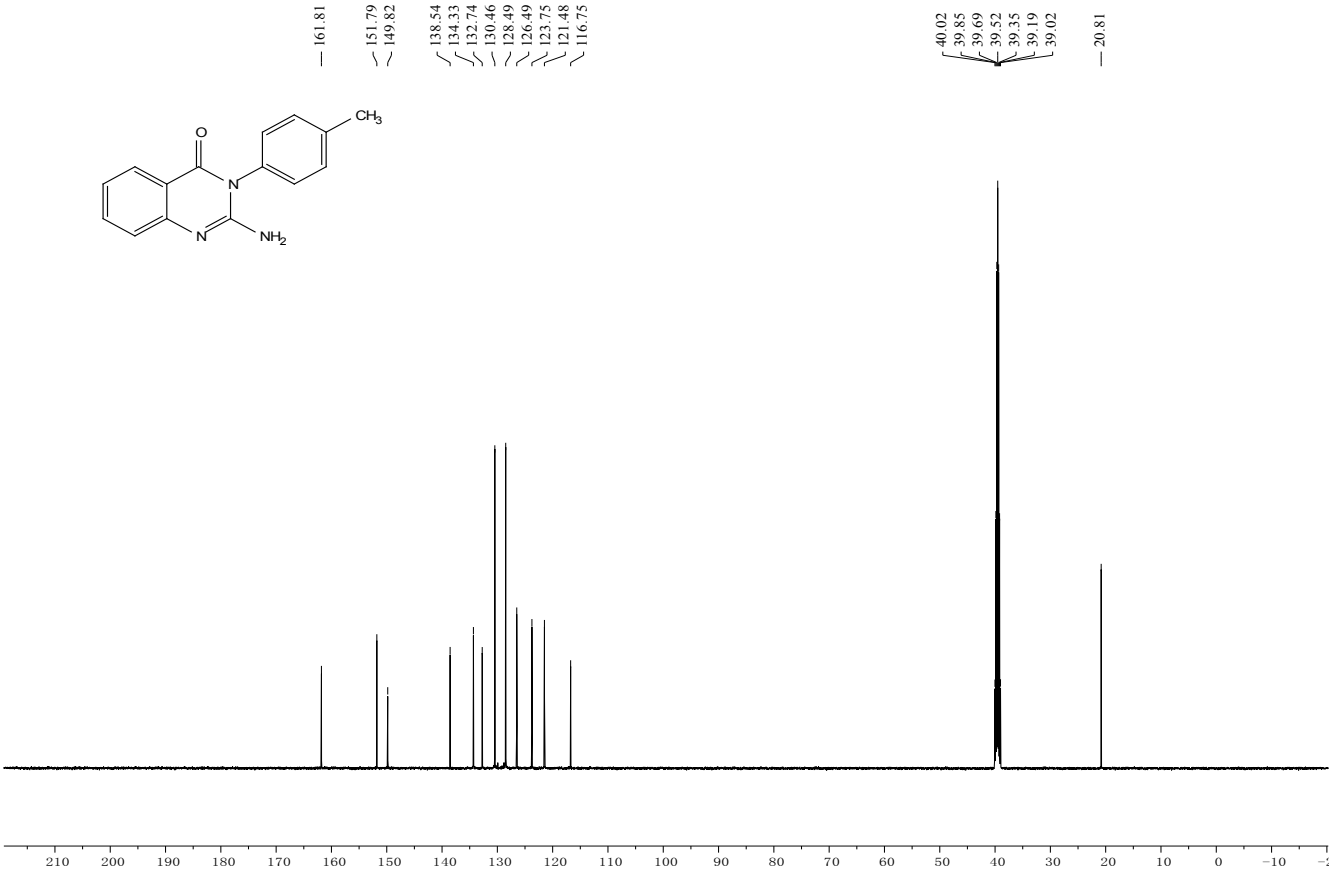

Figure S43. [13]C NMR (126 MHz) of **3m** in DMSO - d_6.

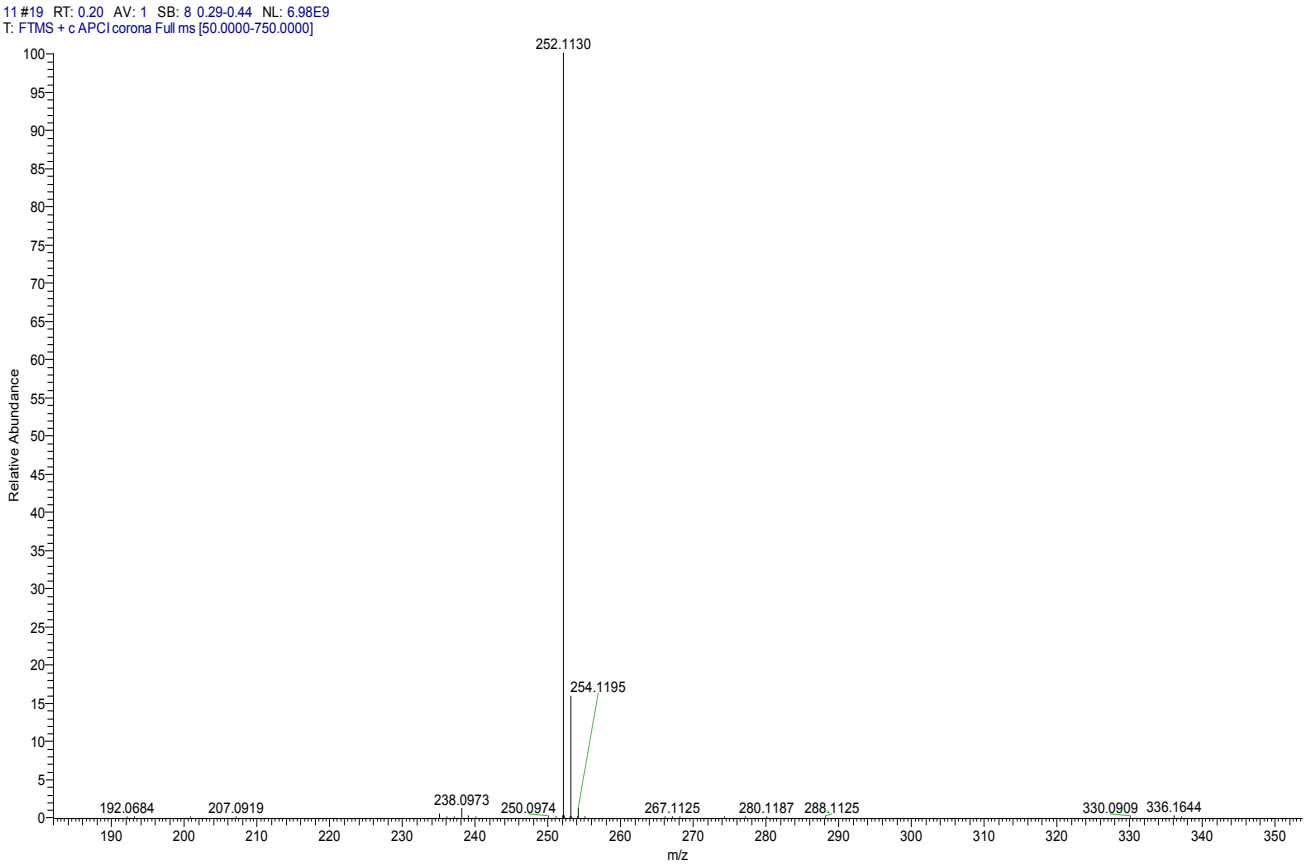

Figure S44. HRMS spectra for **3m**.

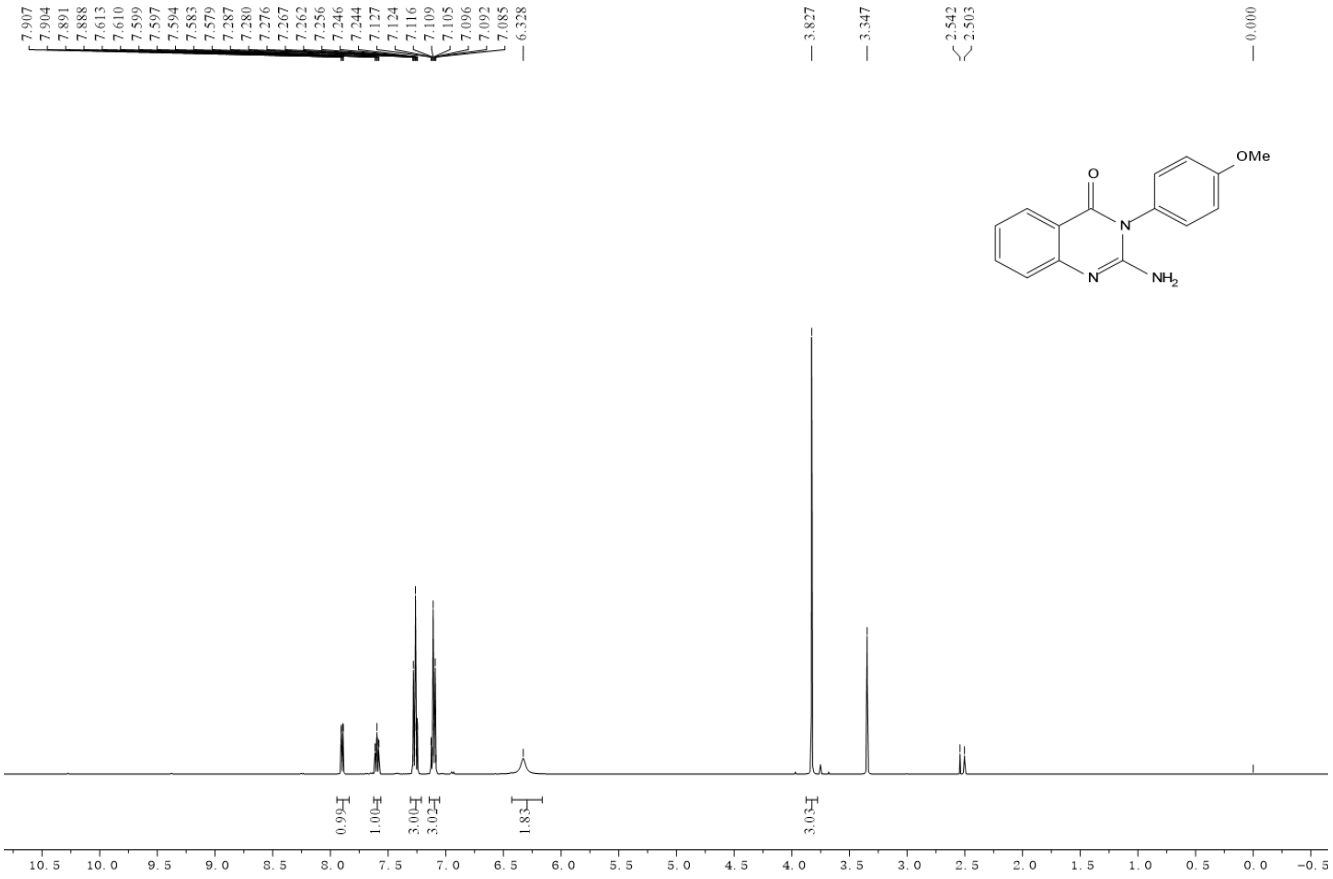

Figure S45. ^{1}H NMR (500 MHz) of **3n** in DMSO - d_6.

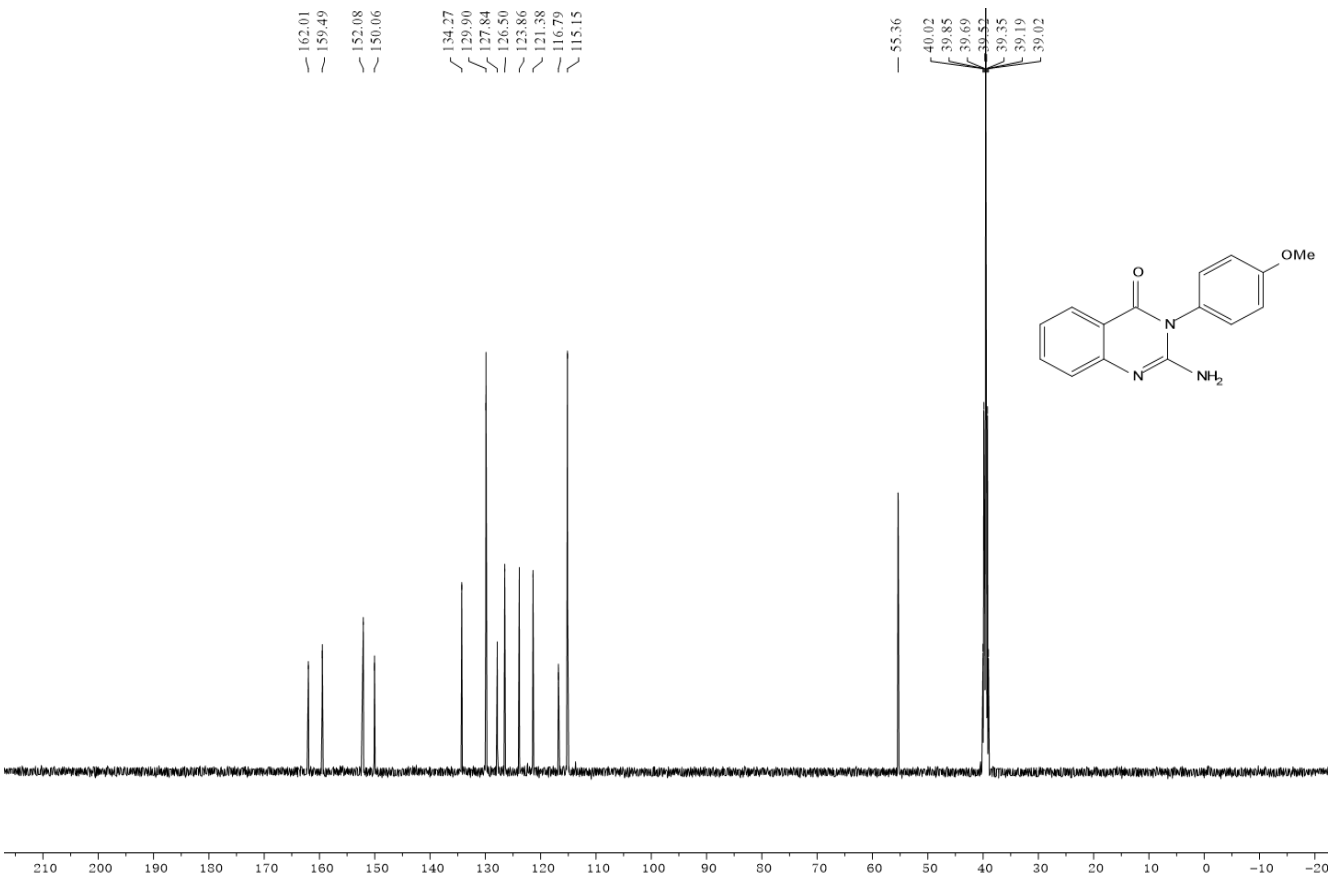

Figure S46. ^{13}C NMR (126 MHz) of **3n** in DMSO - d_6.

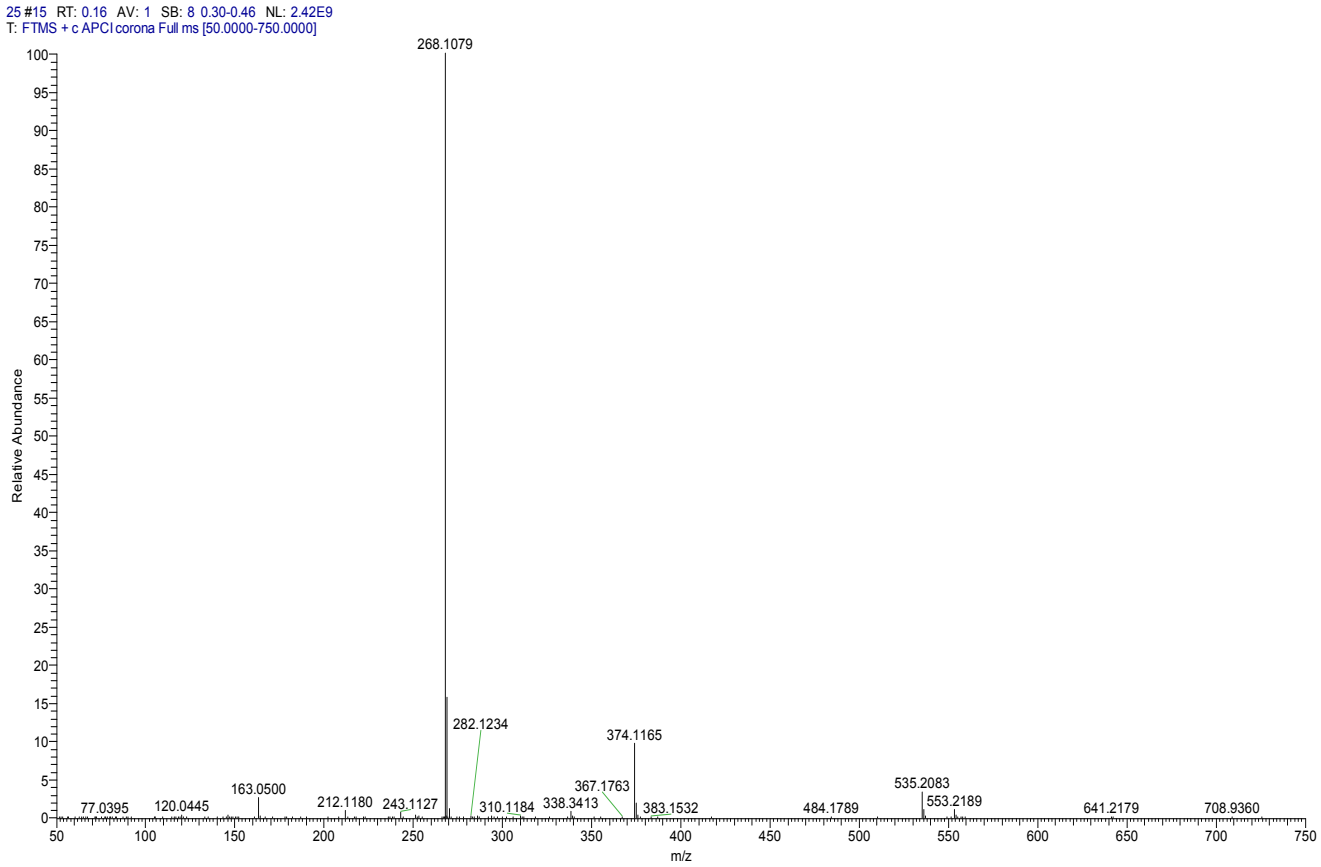

Figure S47. HRMS spectra for **3n**.

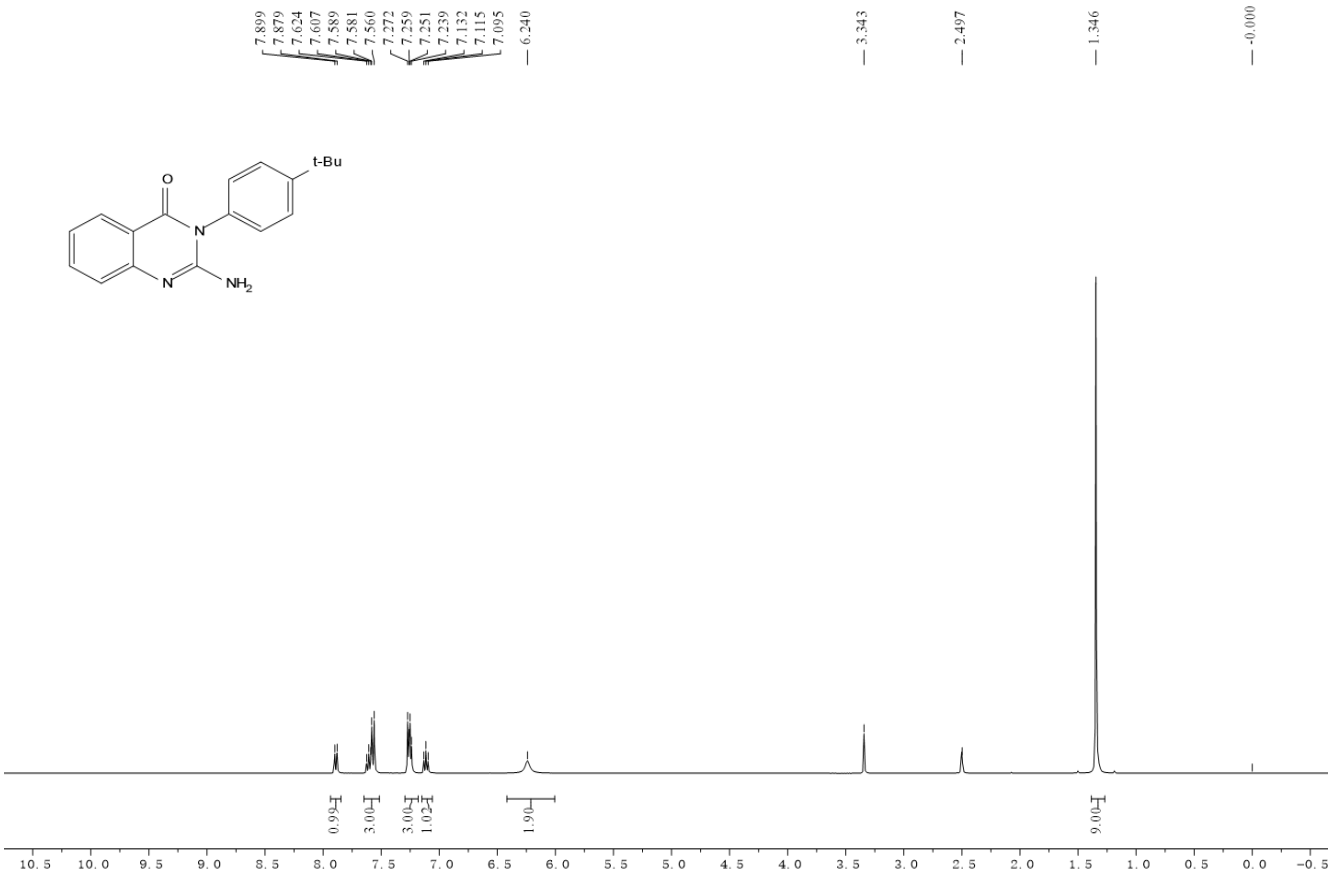

Figure S48. ^{1}H NMR (400 MHz) of **3o** in DMSO - d_6.

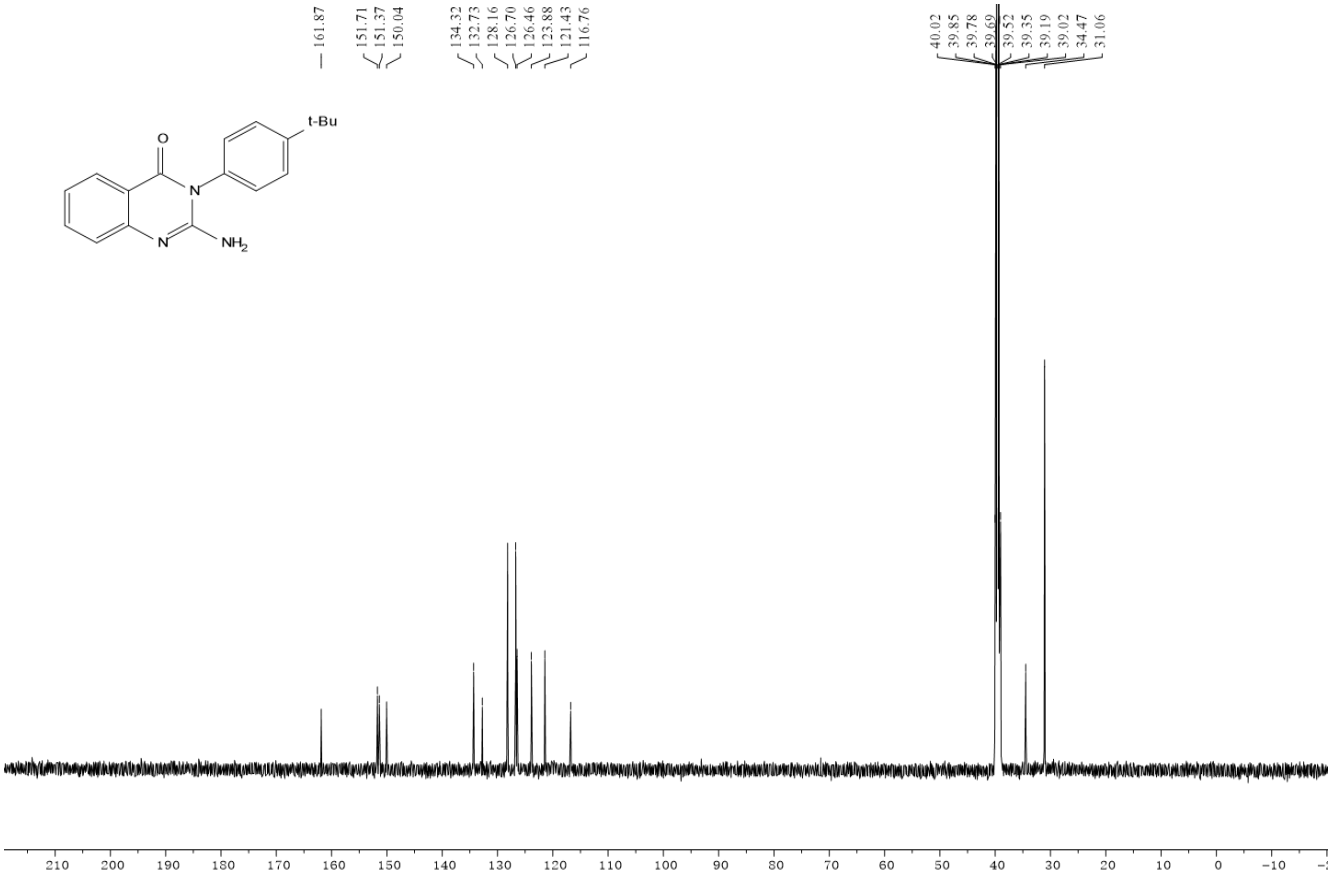

Figure S49. ^{13}C NMR (126 MHz) of **3o** in DMSO - d_6.

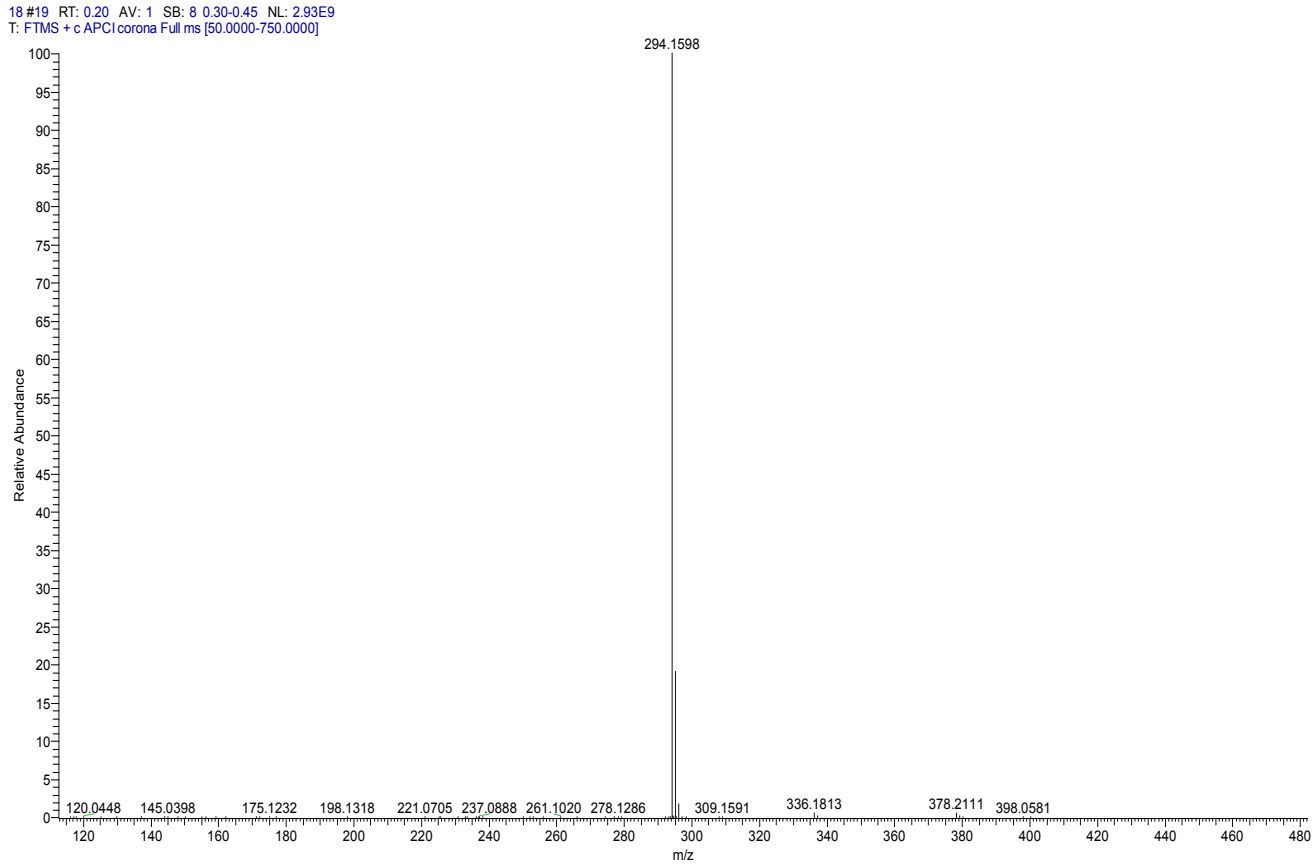

Figure S50. HRMS spectra for **3o**.

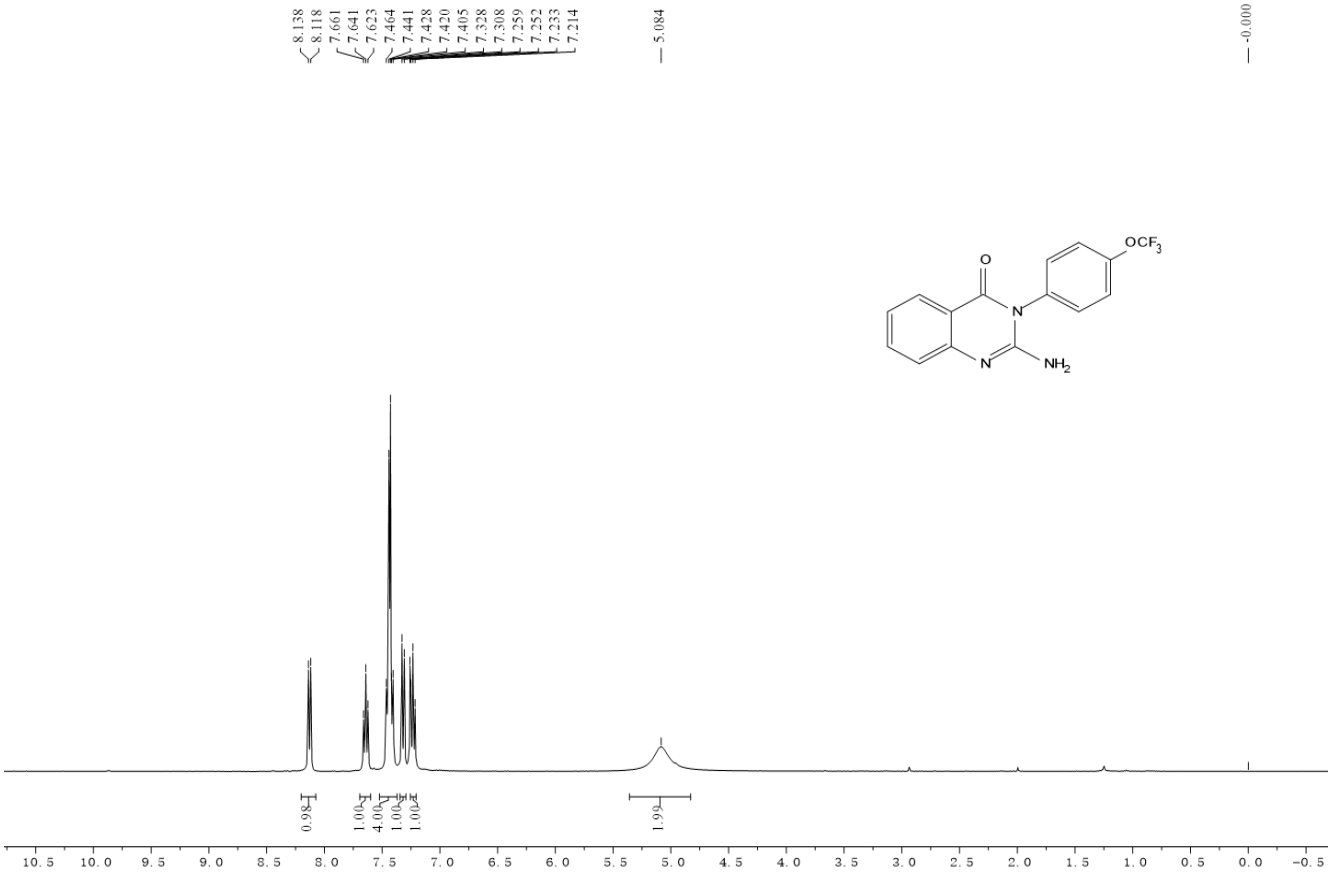

Figure S51. ^{1}H NMR (400 MHz) of **3p** in $CDCl_3$.

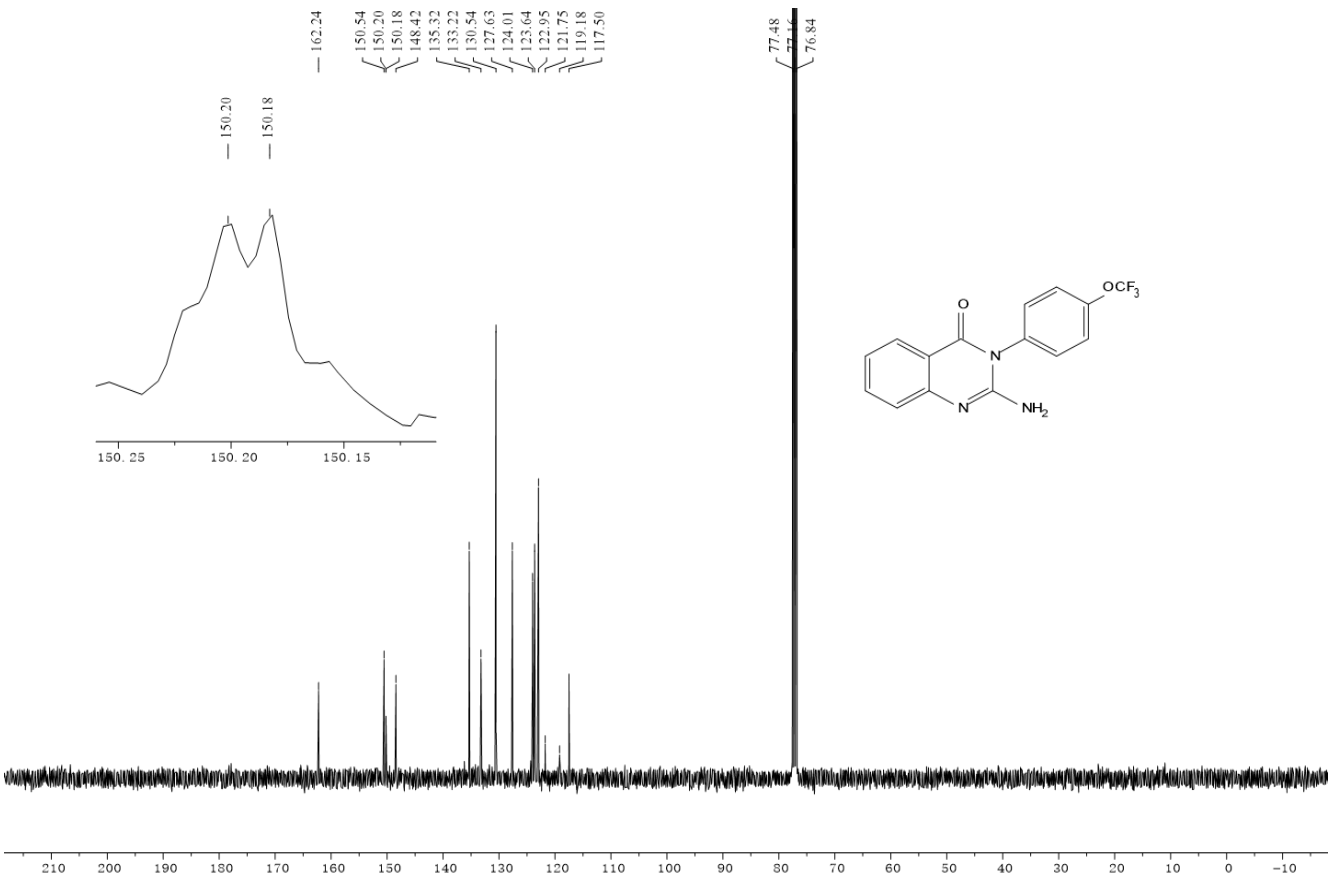

Figure S52. ^{13}C NMR (101 MHz) of **3p** in $CDCl_3$.

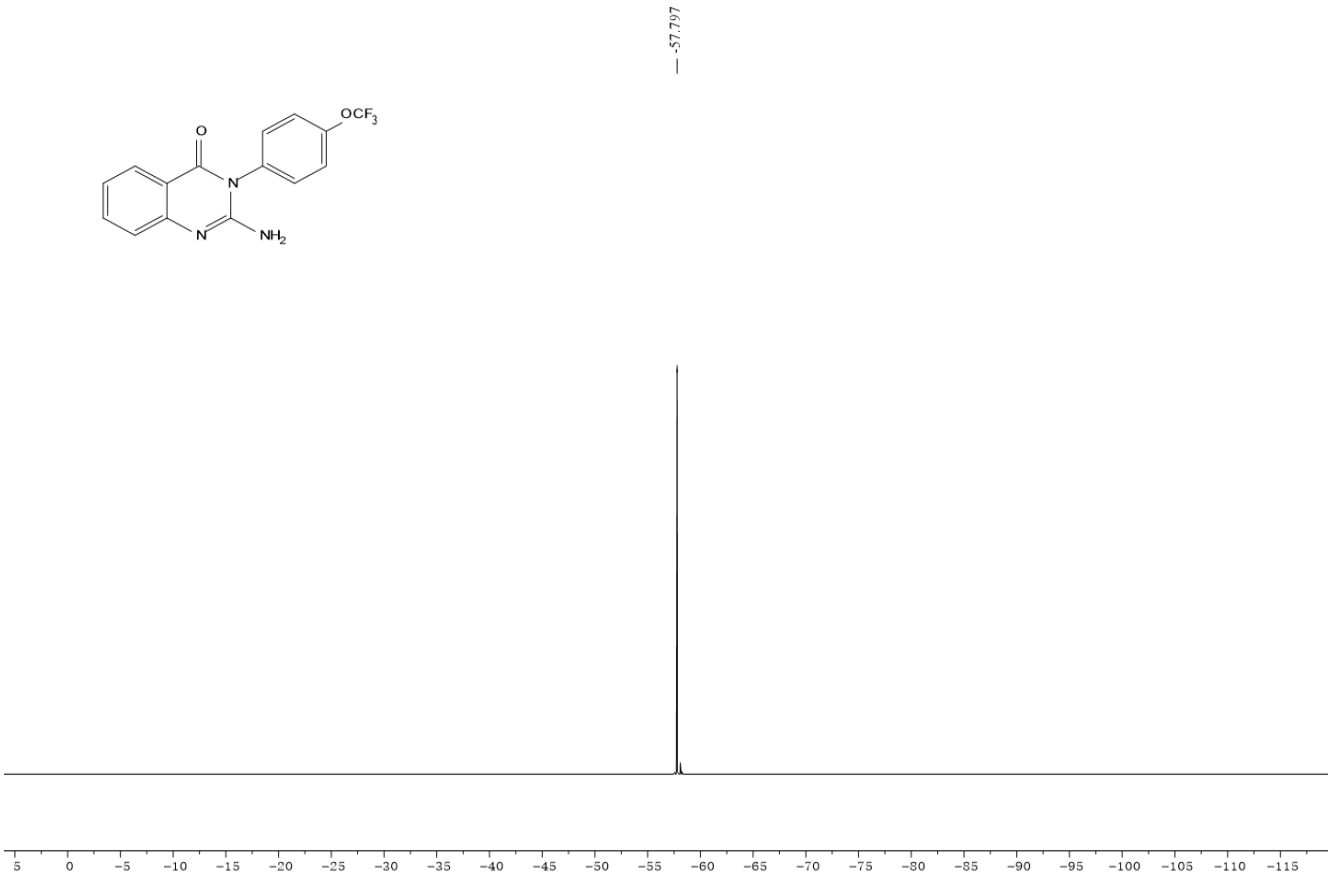

Figure S53. ^{19}F NMR (376 MHz) of **3p** in $CDCl_3$.

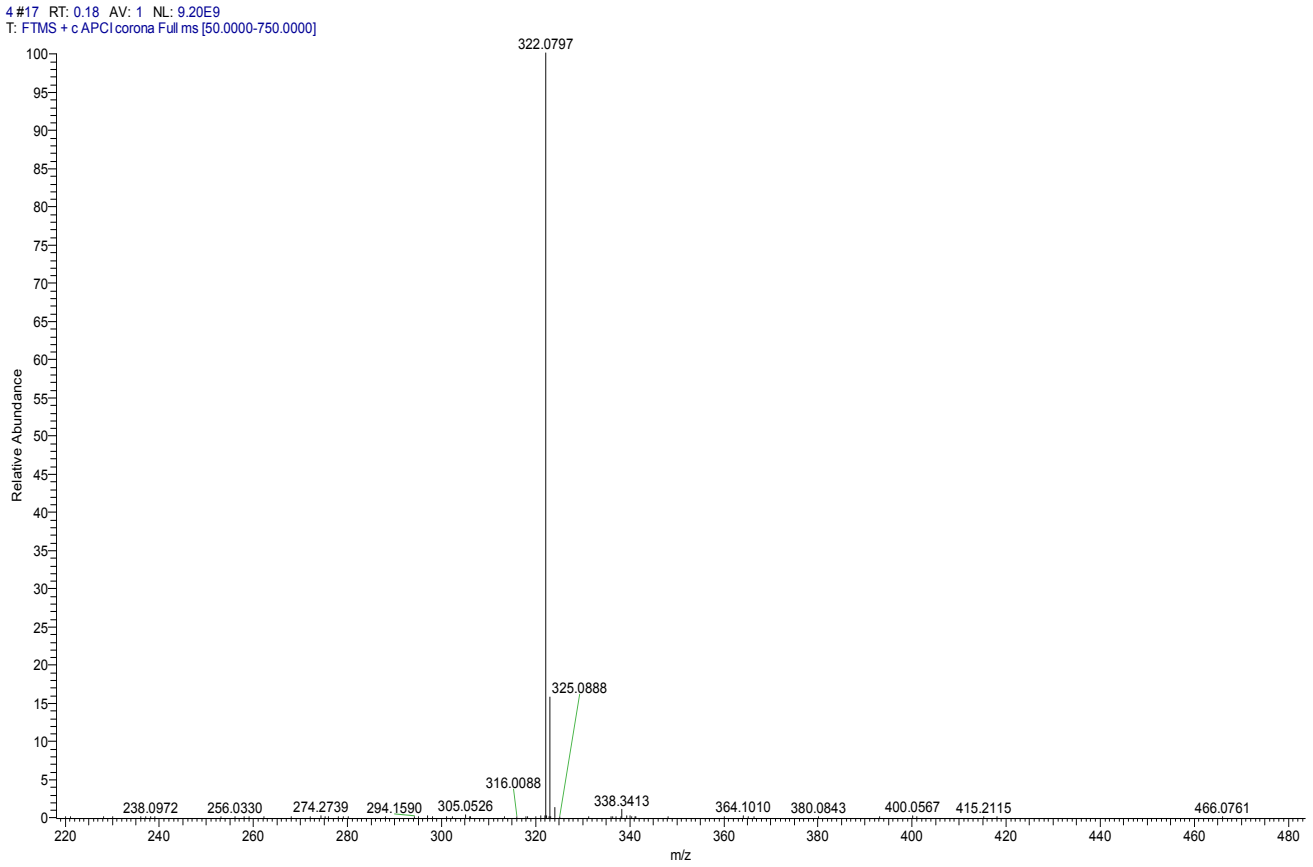

Figure S54. HRMS spectra for **3p**.

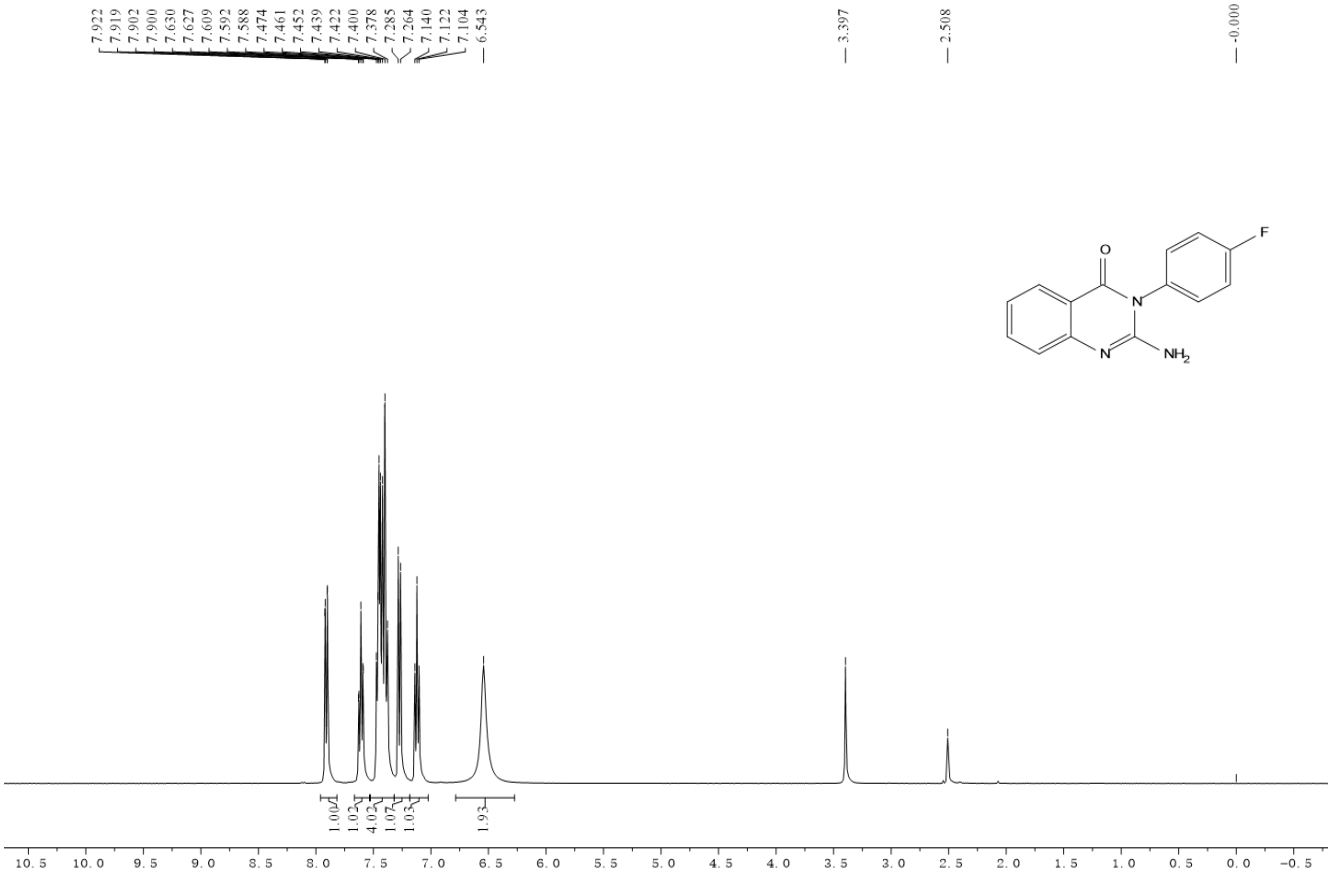

Figure S55. ^{1}H NMR (400 MHz) of **3q** in DMSO - d_6.

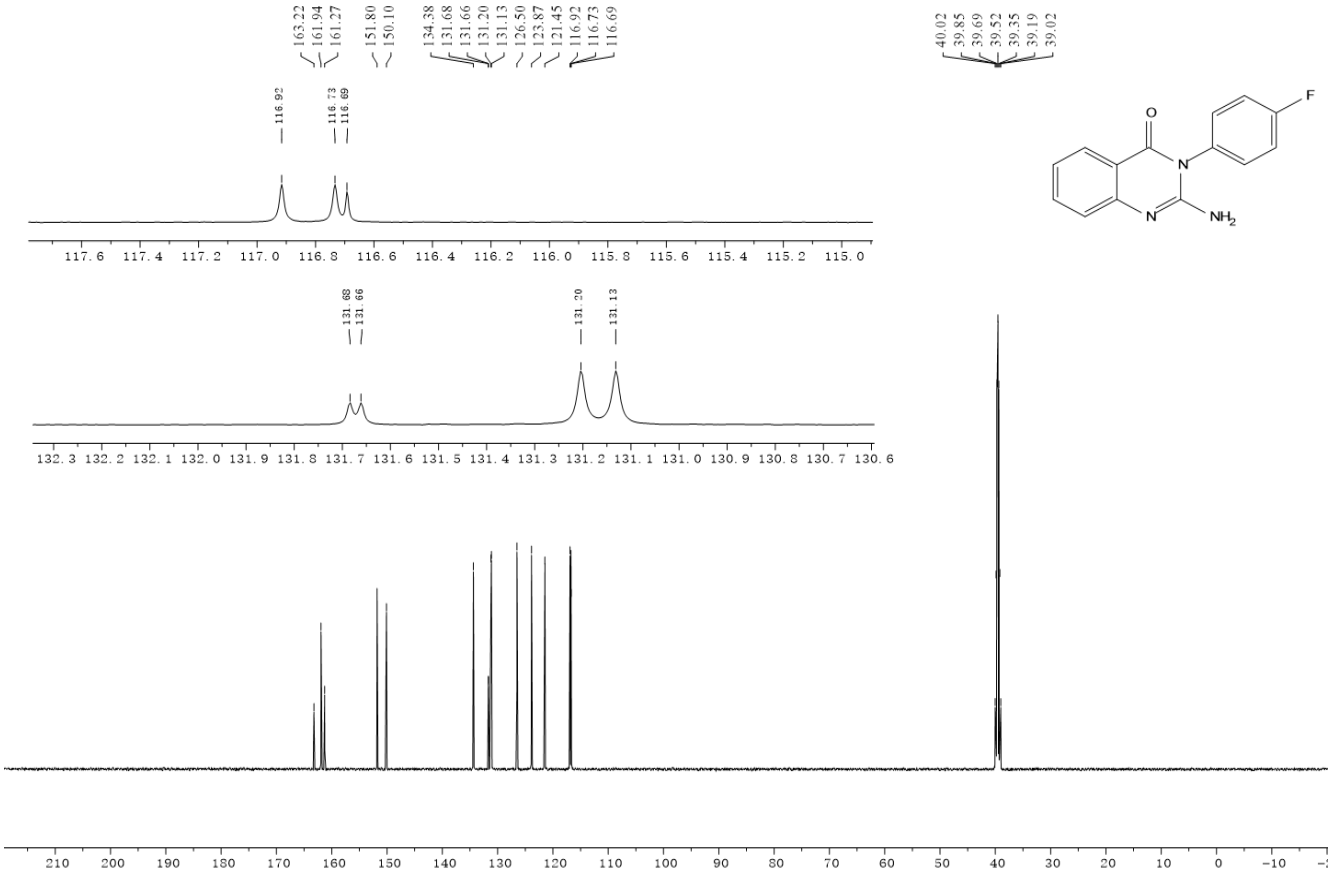

Figure S56. ^{13}C NMR (126 MHz) of **3q** in DMSO - d_6.

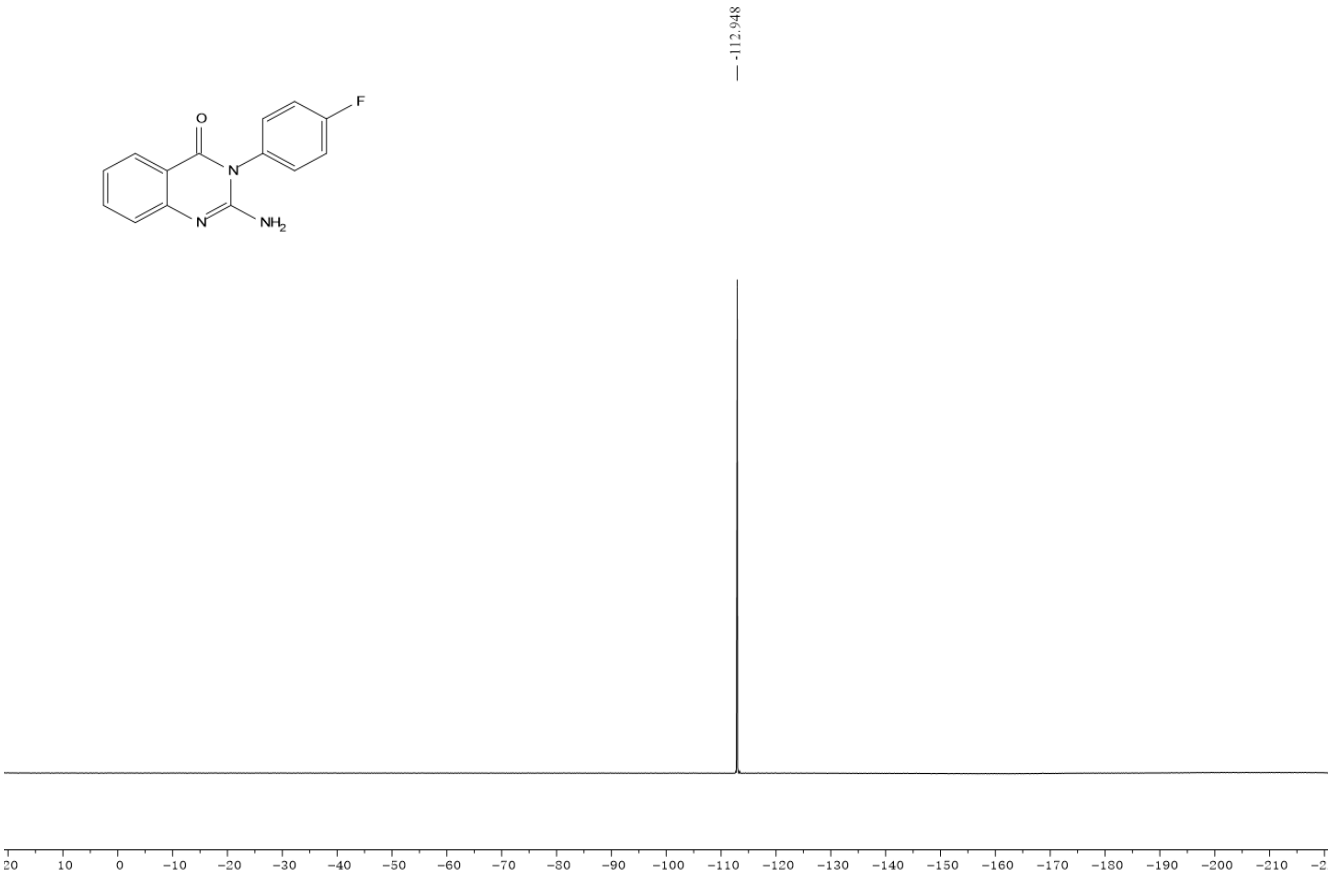

Figure S57. ^{19}F NMR (376 MHz) of **3q** in DMSO-d_6.

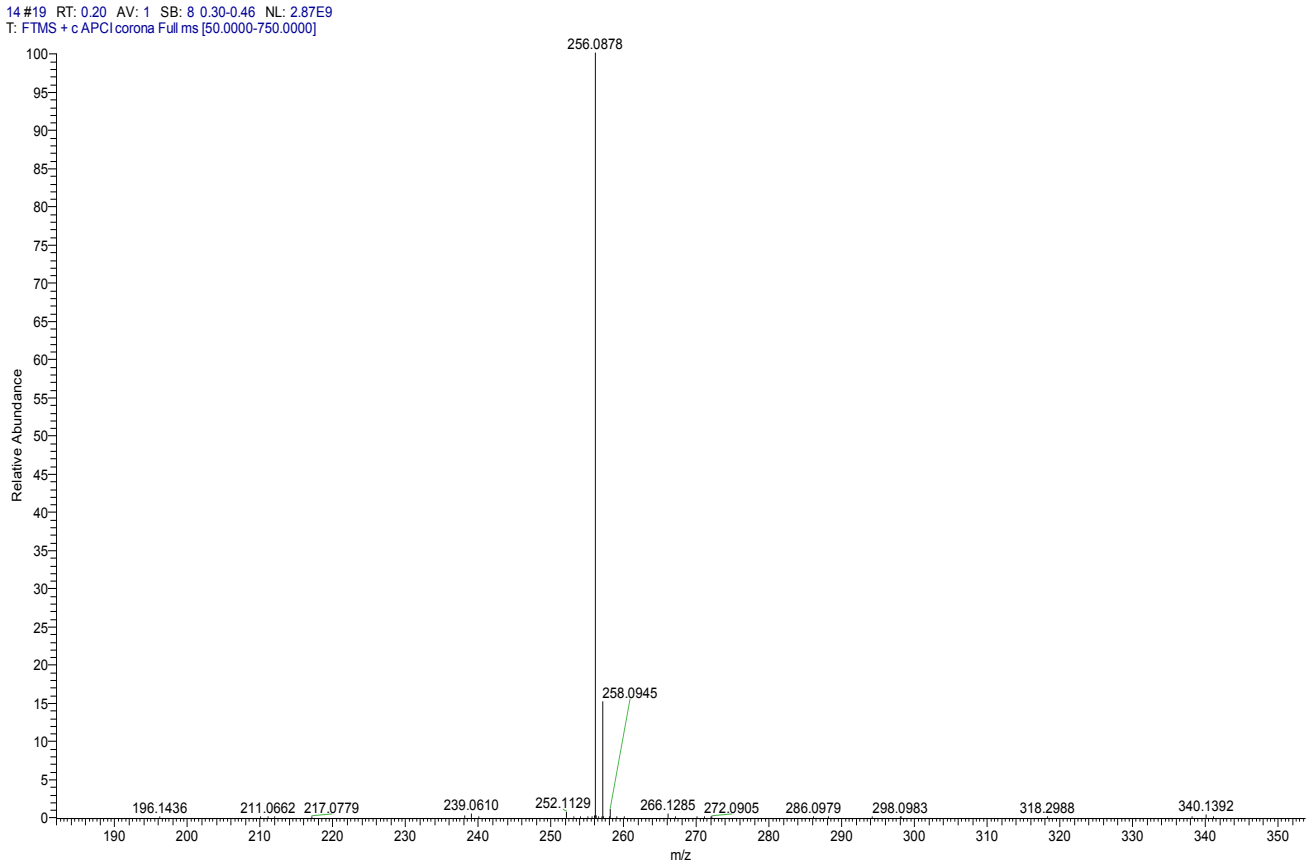

Figure S58. HRMS spectra for **3q**.

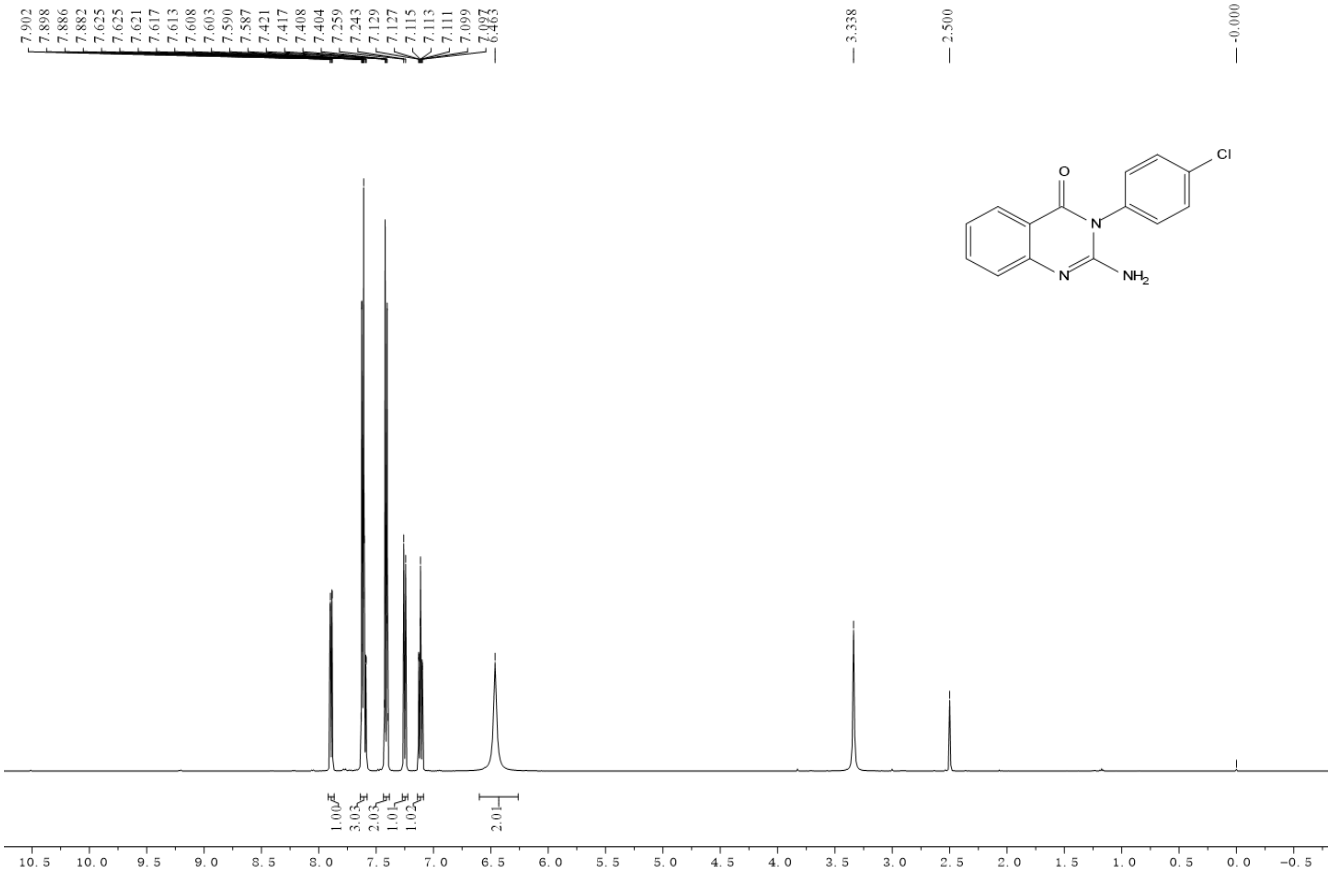

Figure S59. ^{1}H NMR (500 MHz) of **3r** in DMSO-d_6.

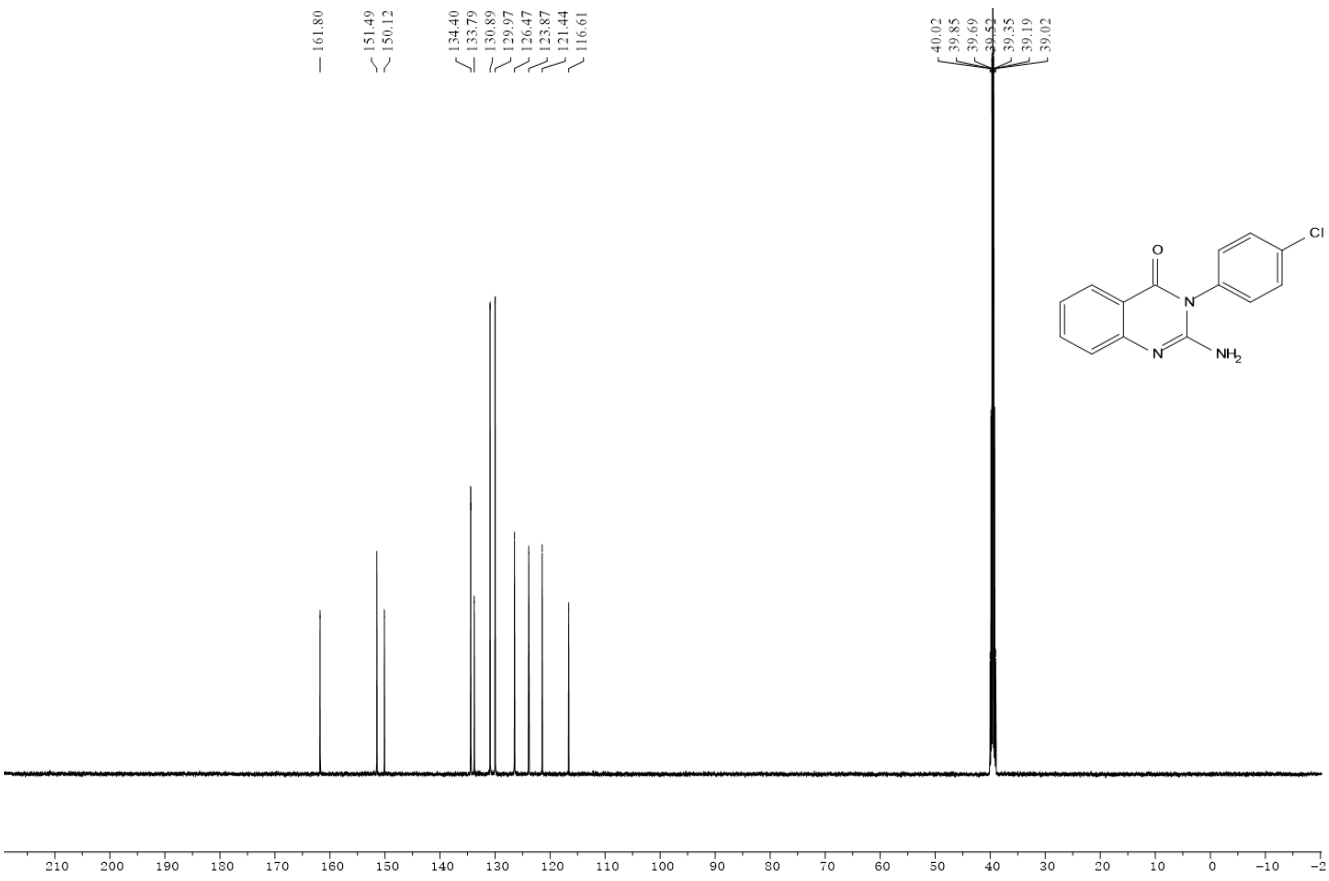

Figure S60. ^{13}C NMR (126 MHz) of **3r** in DMSO-d_6.

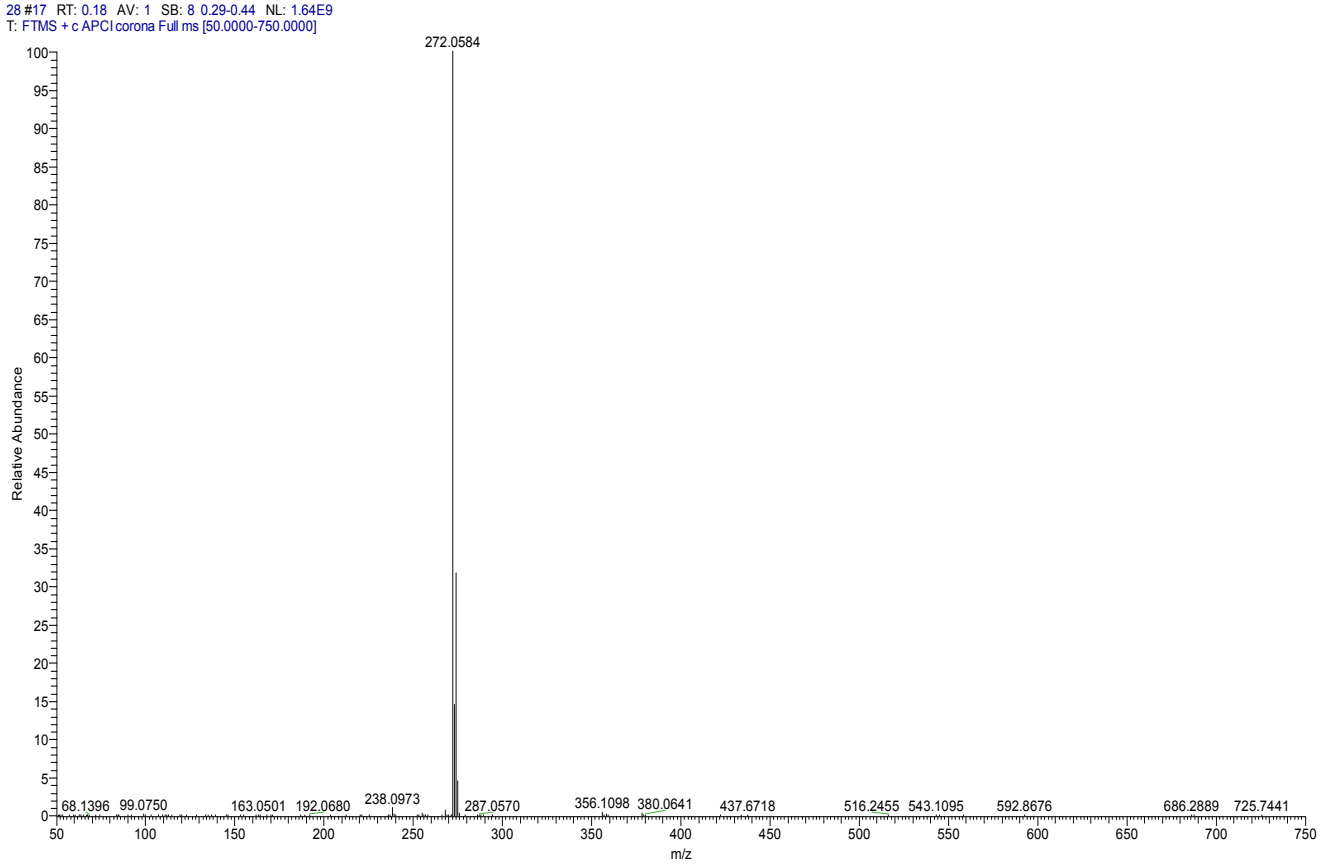

Figure S61. HRMS spectra for **3r**.

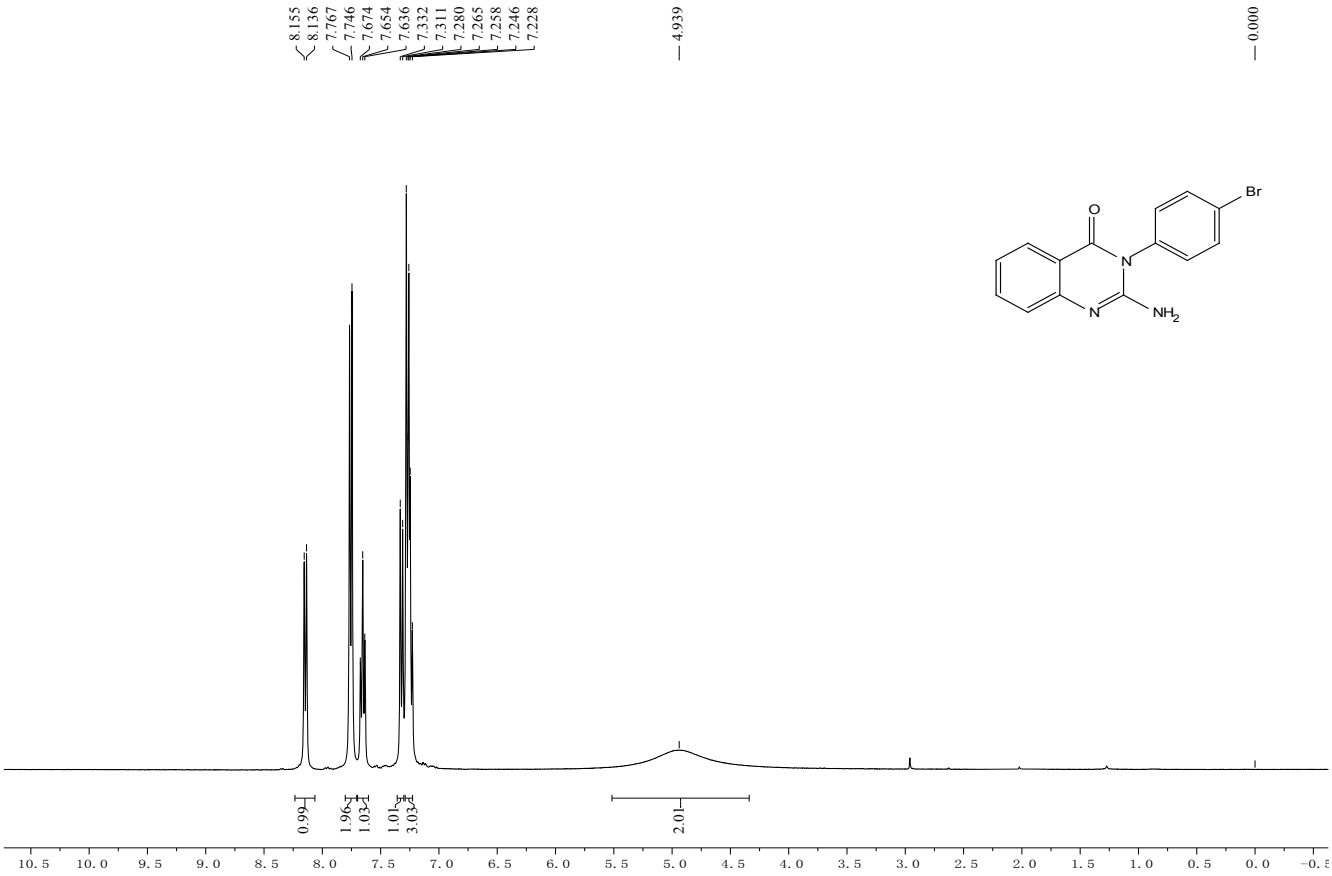

Figure S62. ^{1}H NMR (400 MHz) of **3s** in $CDCl_3$.

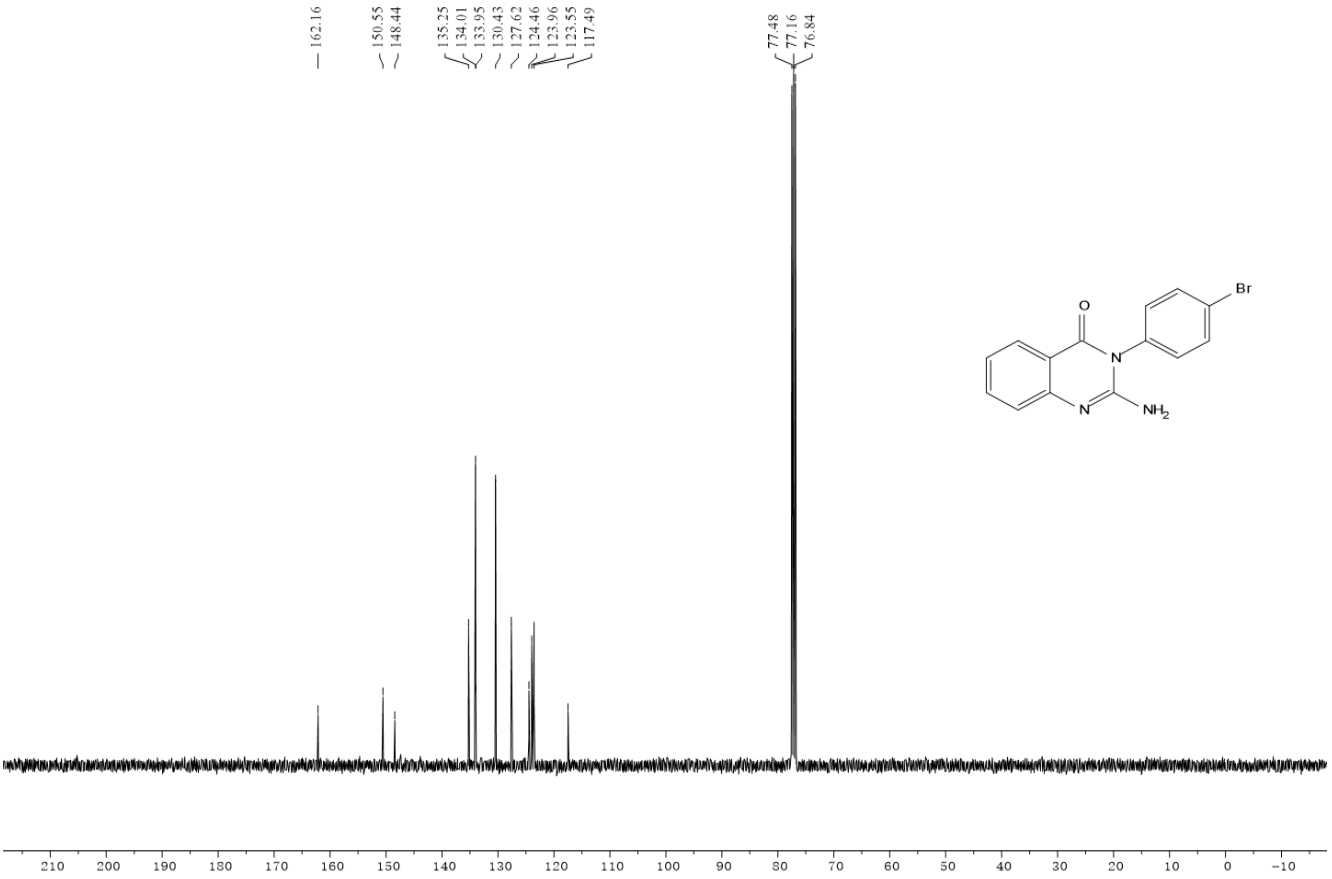

Figure S63. ^{13}C NMR (101 MHz) of **3s** in $CDCl_3$.

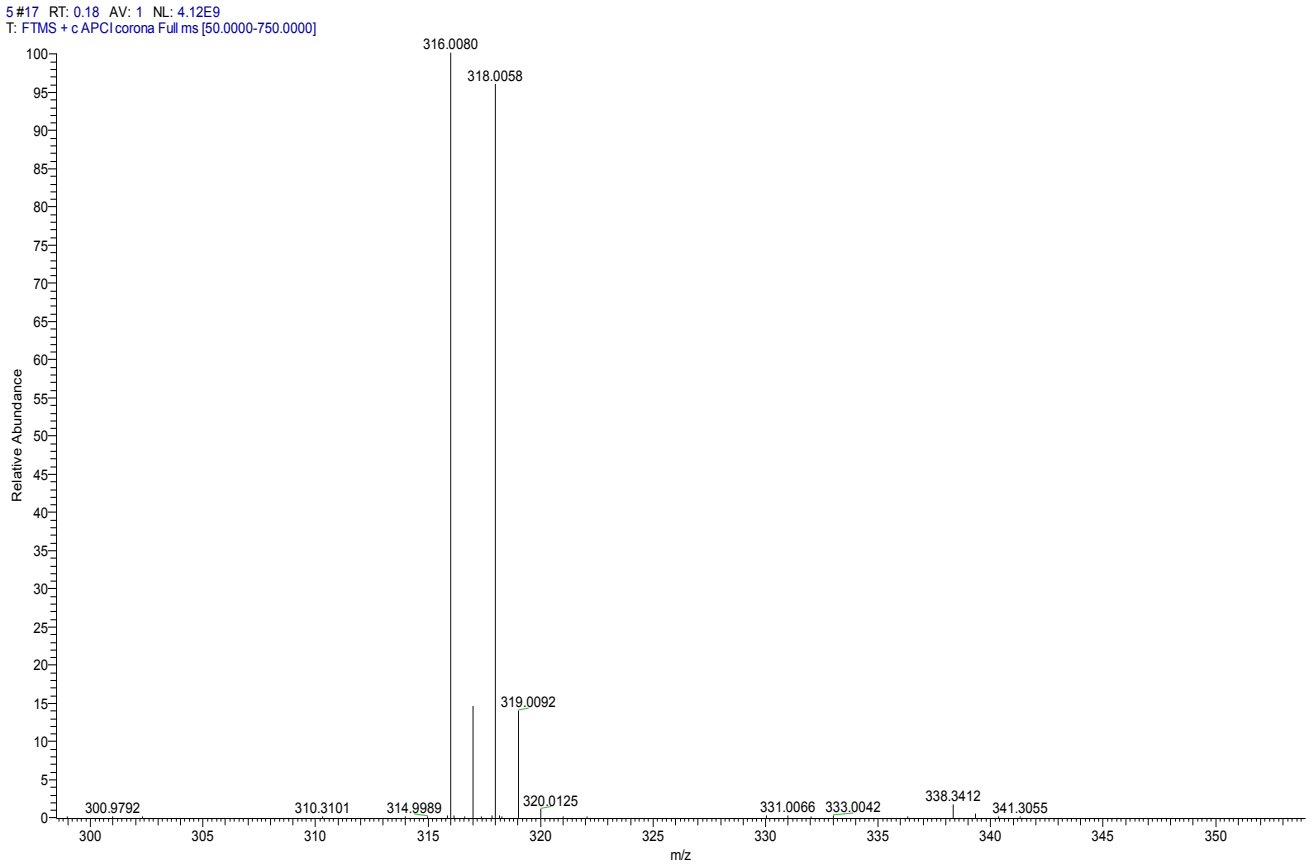

Figure S64. HRMS spectra for **3s**.

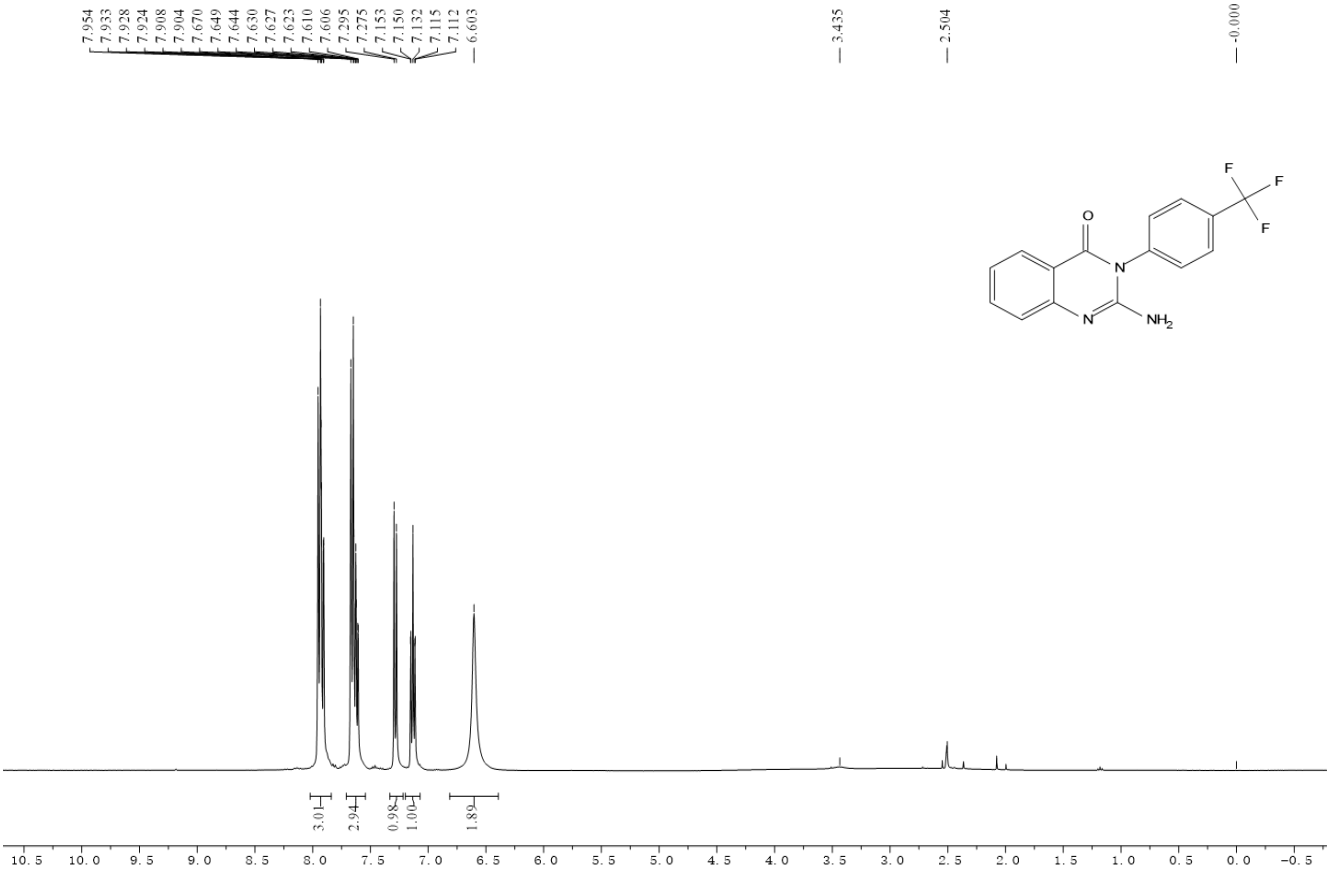

Figure S65. ^{1}H NMR (400 MHz) of **3t** in DMSO - d_6.

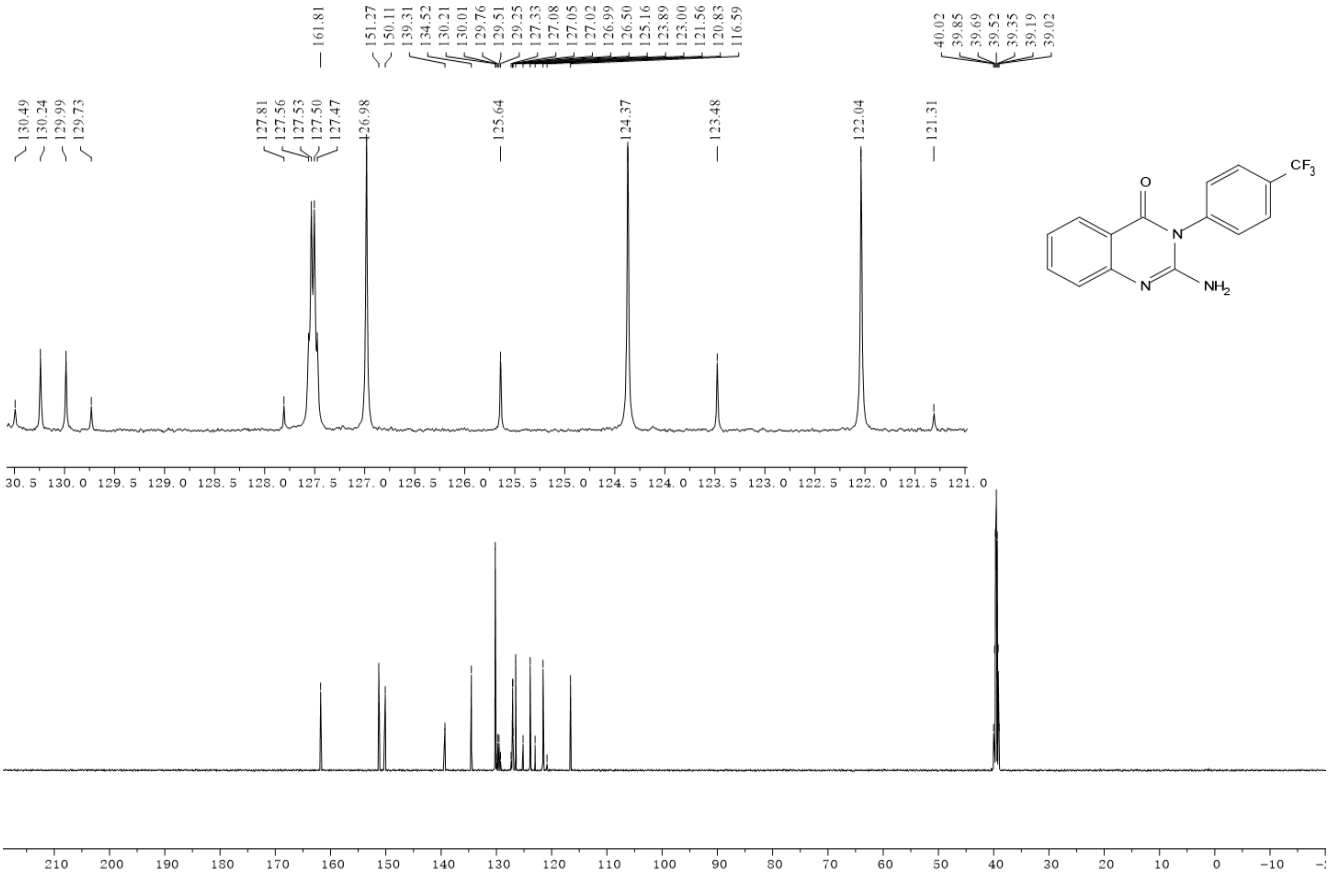

Figure S66. ^{13}C NMR (101 MHz) of **3t** in DMSO-d_6.

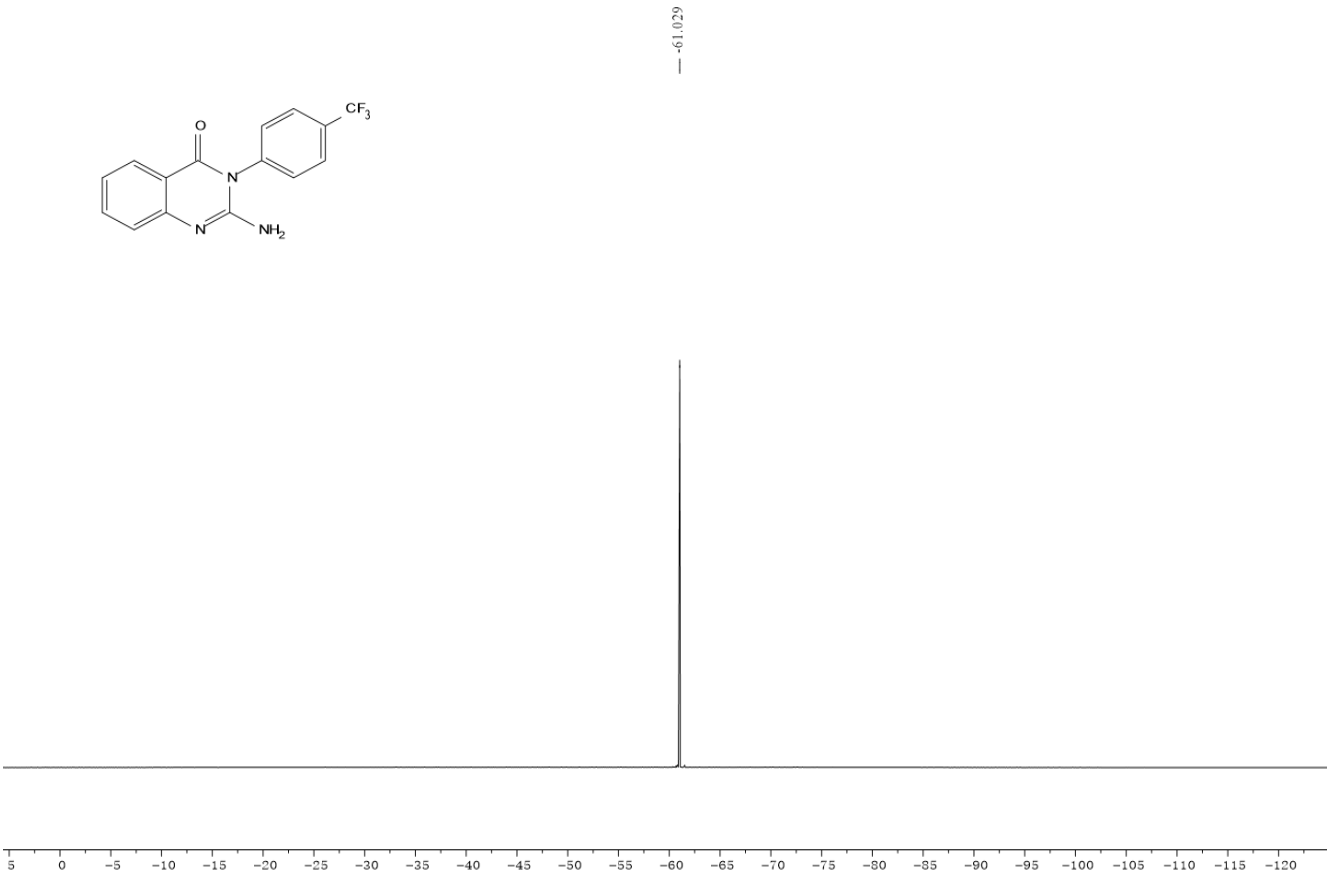

Figure S67. ^{19}F NMR (376 MHz) of **3t** in DMSO - d_6.

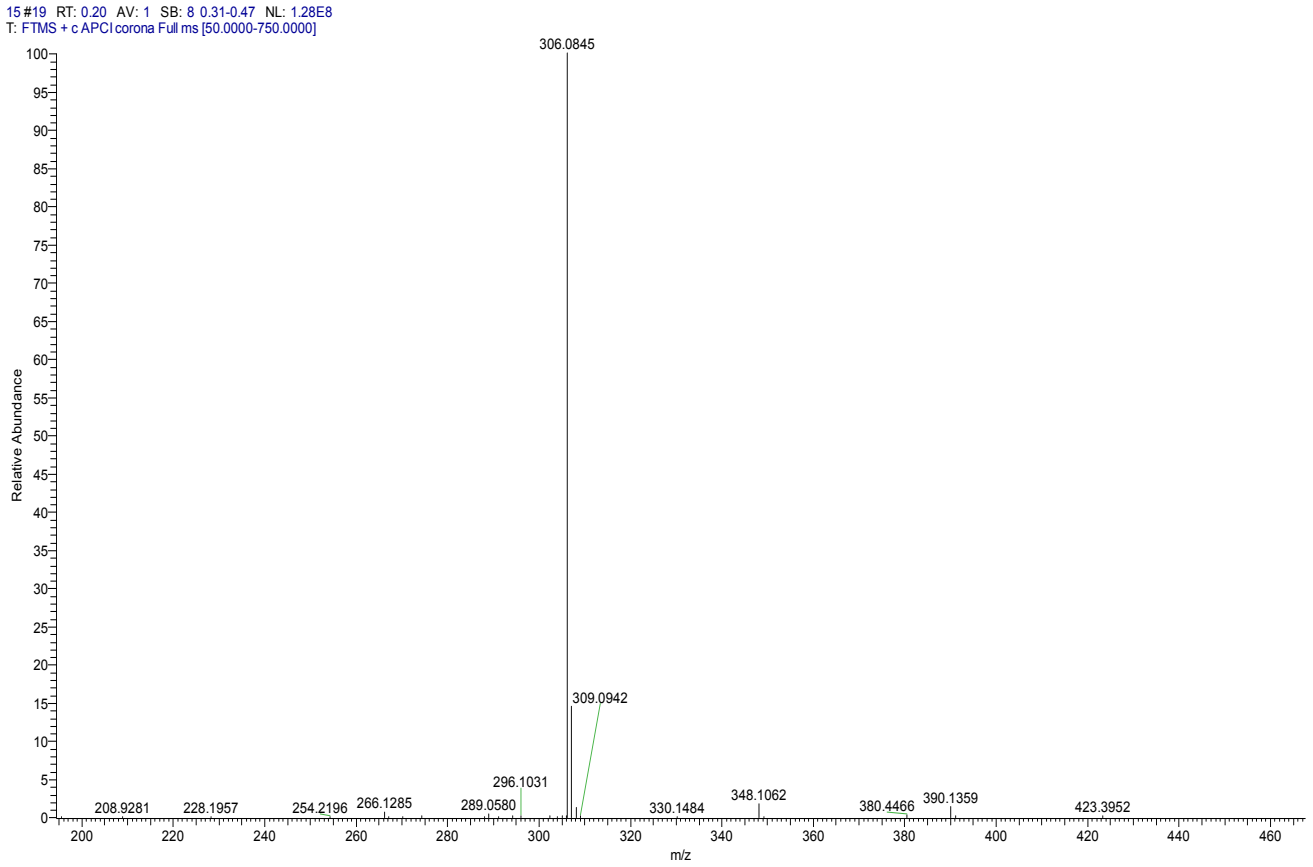

Figure S68. HRMS spectra for **3t**.

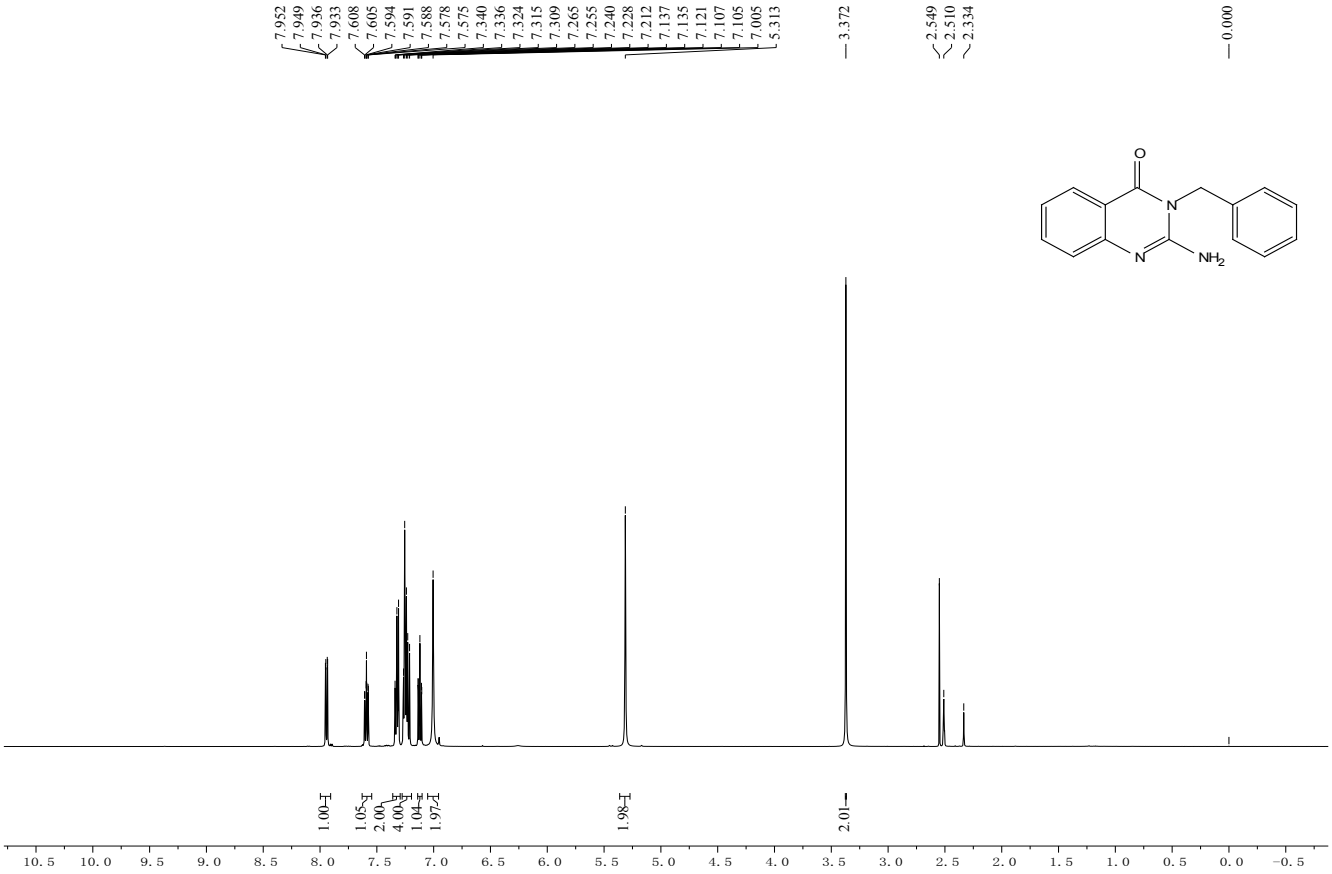

Figure S69. ^{1}H NMR (500 MHz) of **3w** in DMSO - d_6.

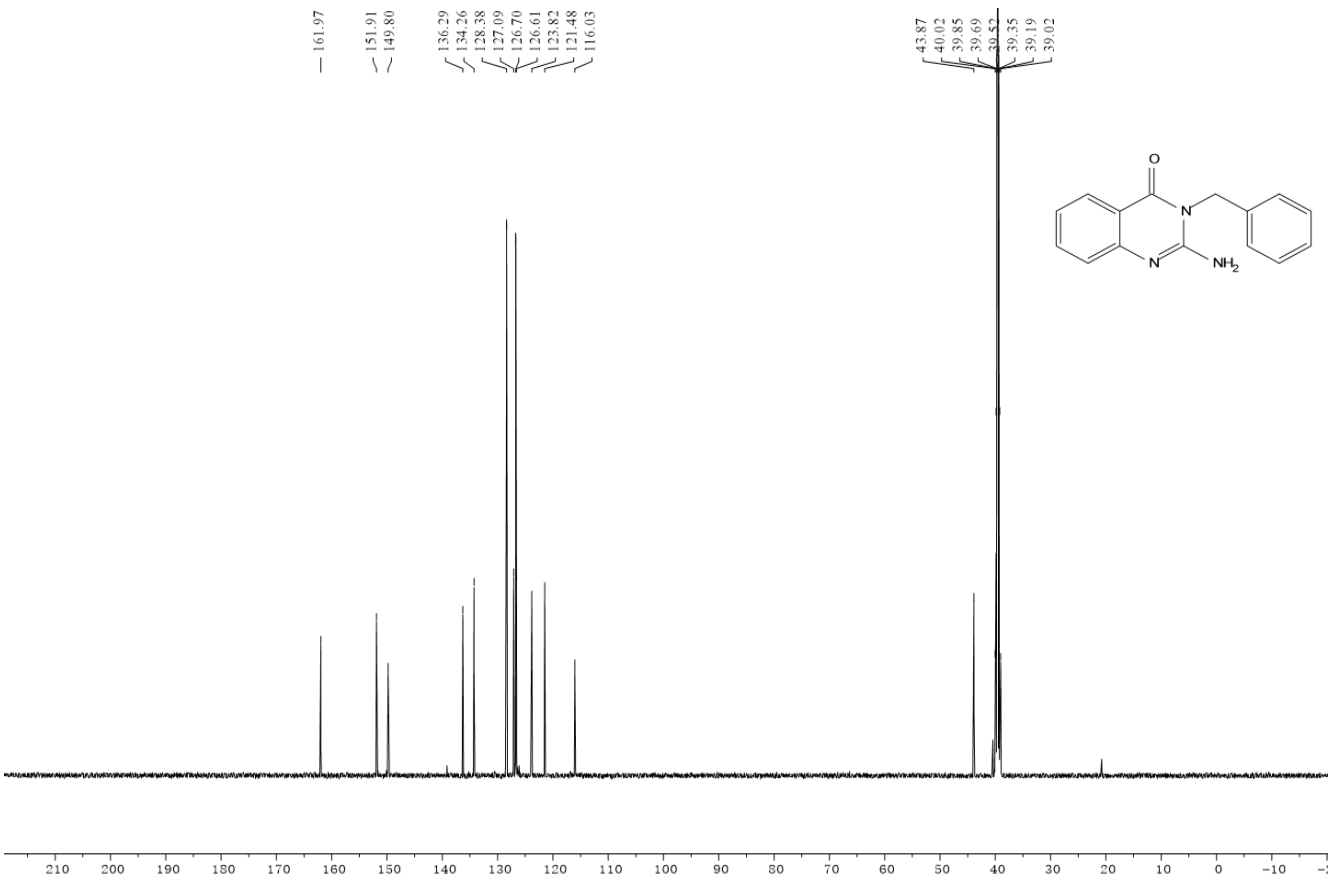

Figure S70. ^{13}C NMR (126 MHz) of **3w** in DMSO - d_6.

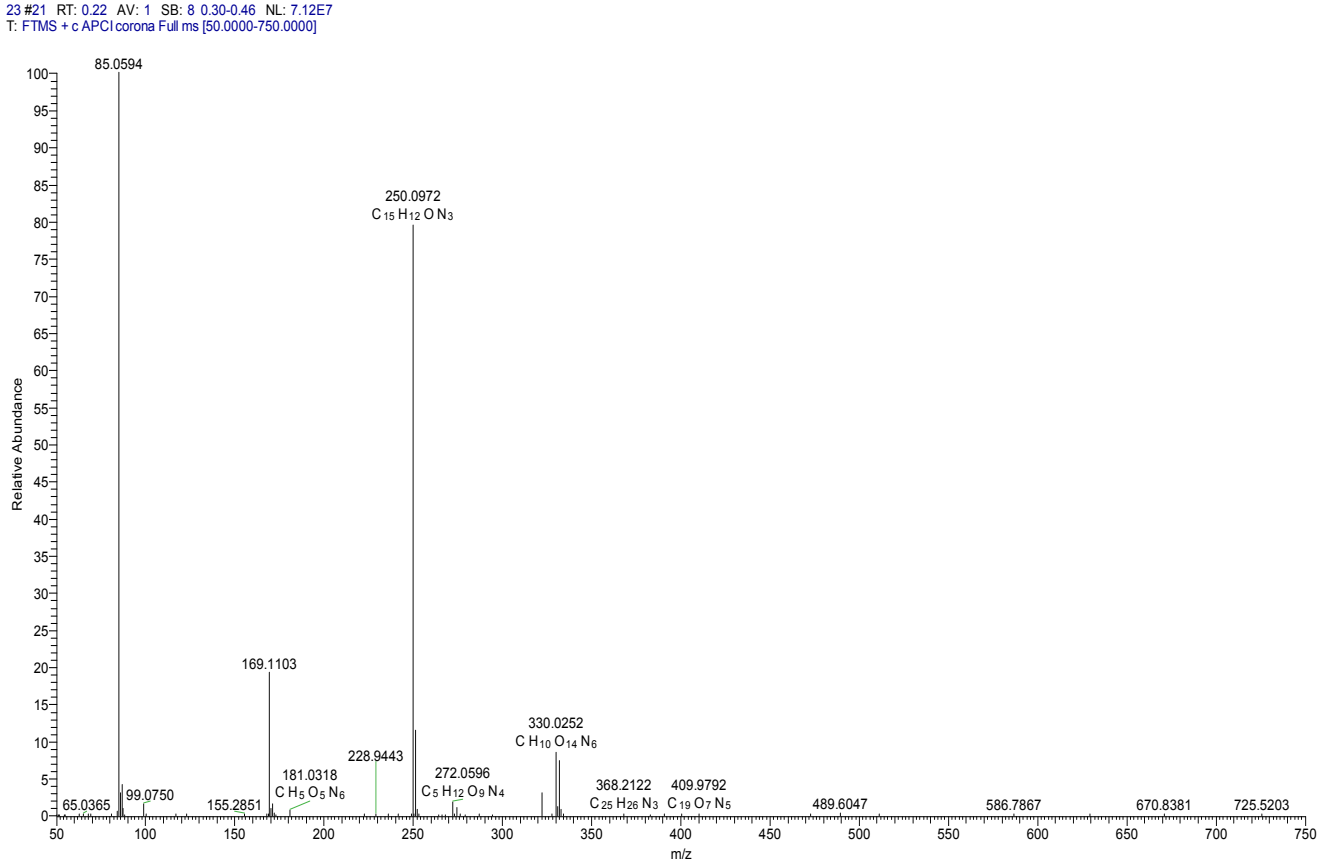

Figure S71. HRMS spectra for **3w**.

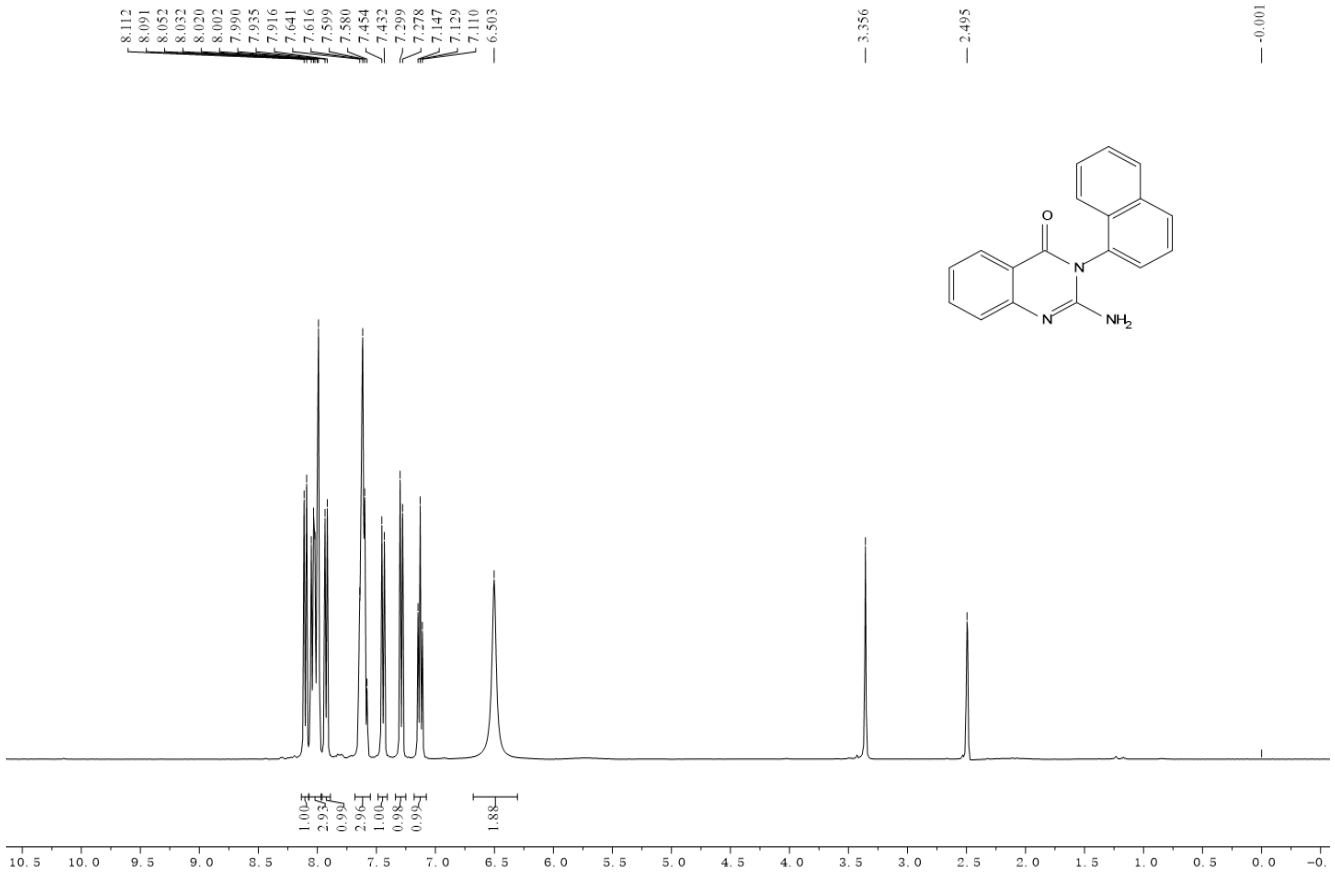

Figure S72. [1]H NMR (400 MHz) of **3x** in DMSO - d_6.

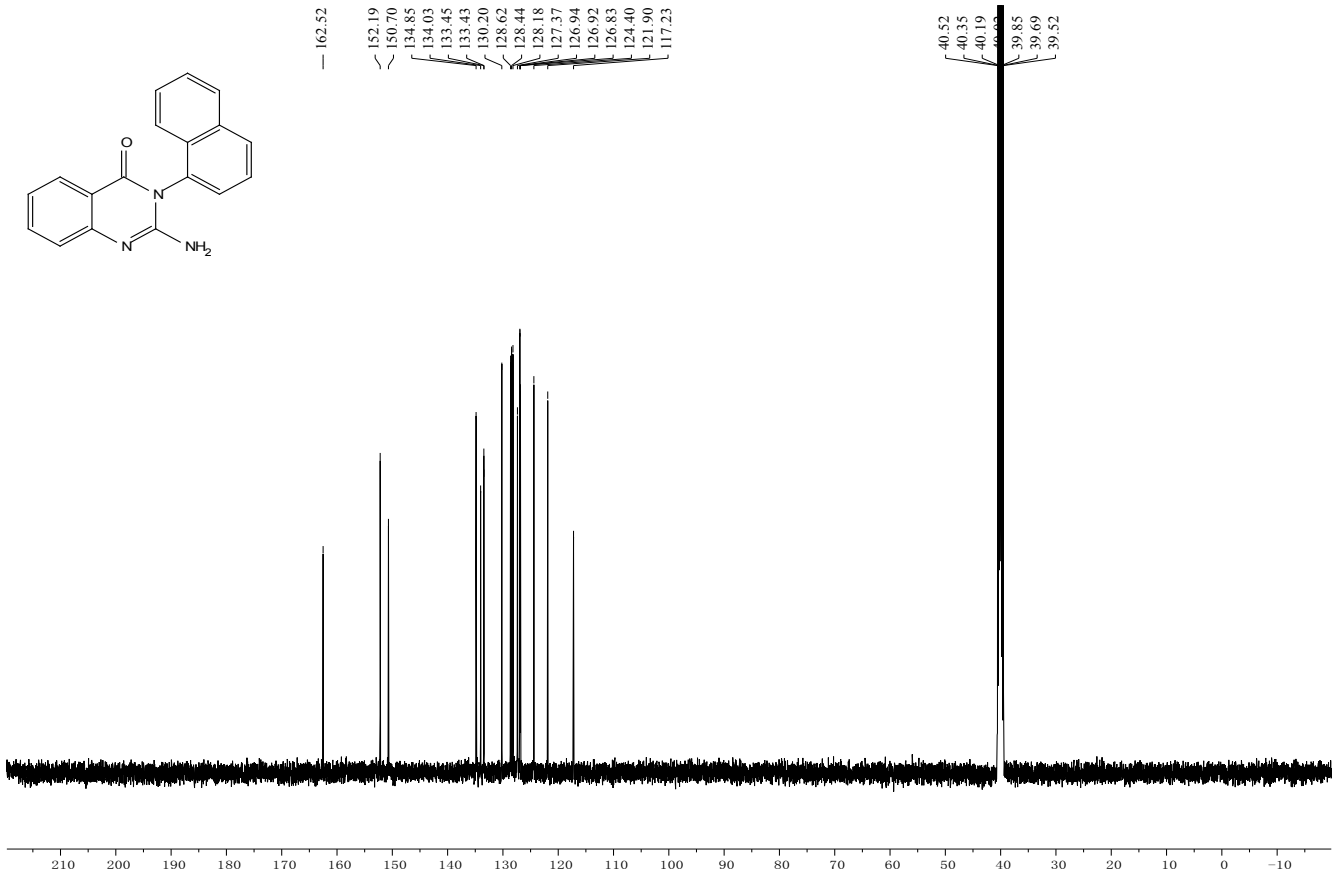

Figure S73. [13]C NMR (101 MHz) of **3x** in DMSO - d_6.

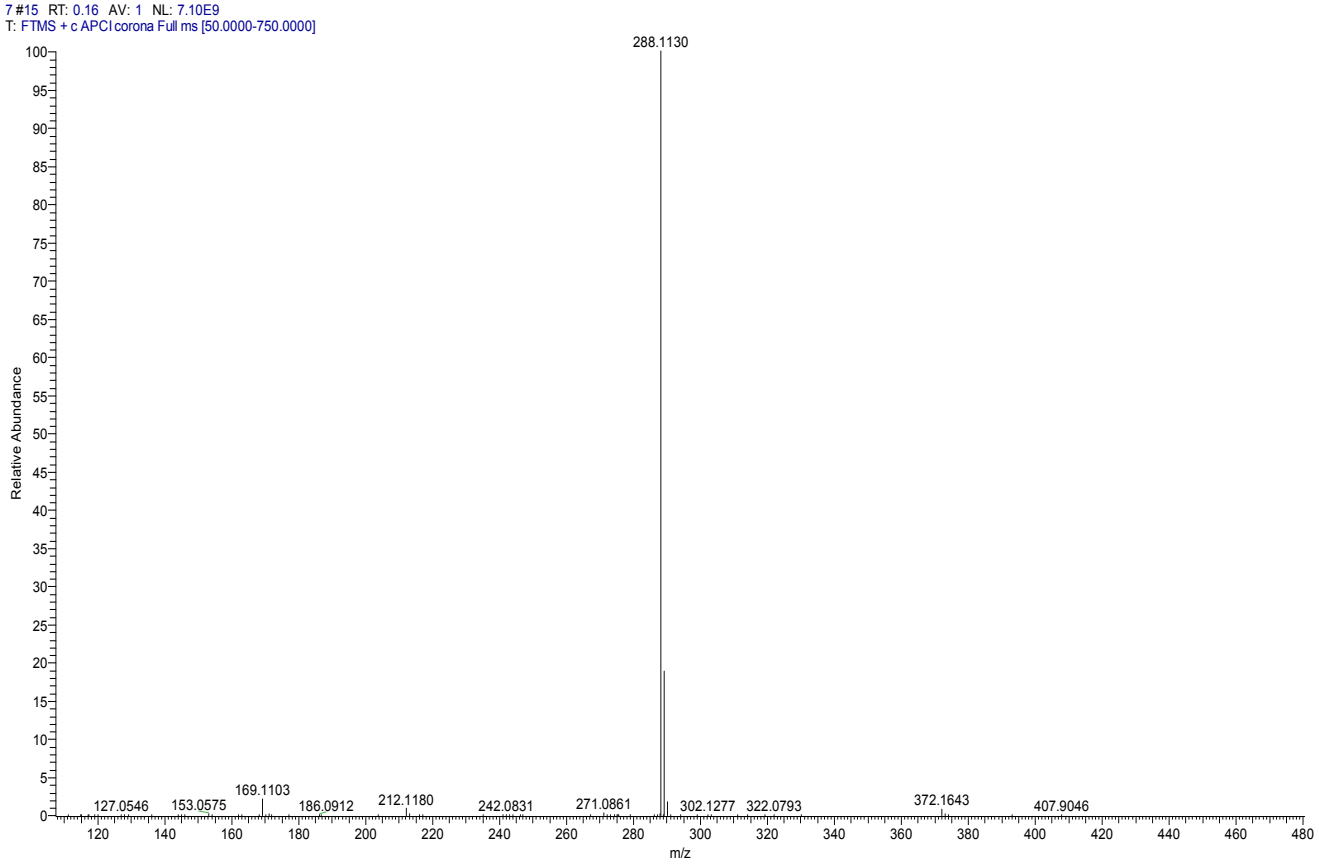

Figure S74. HRMS spectra for **3x**.

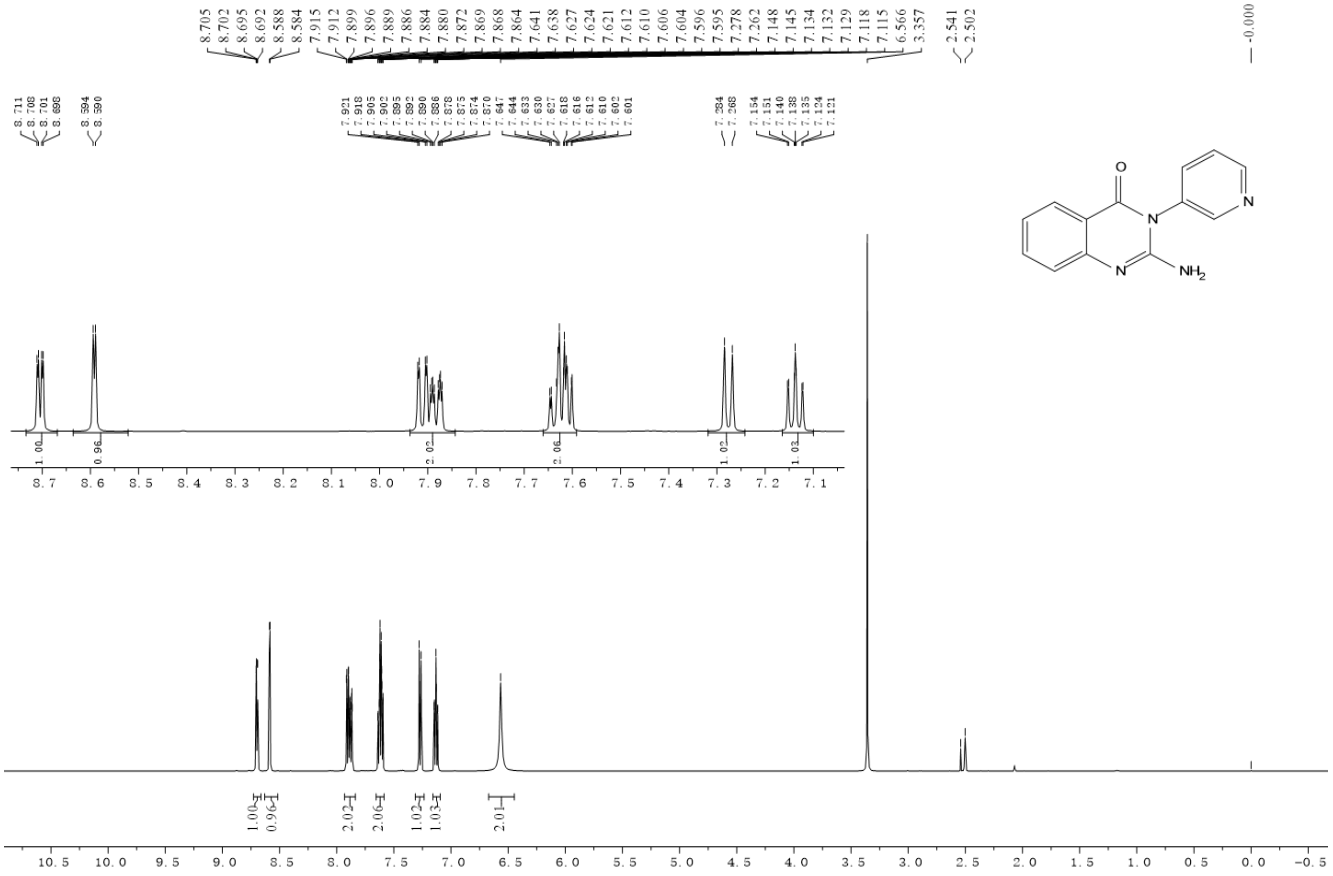

Figure S75. ^{1}H NMR (500 MHz) of **3y** in DMSO - d_6.

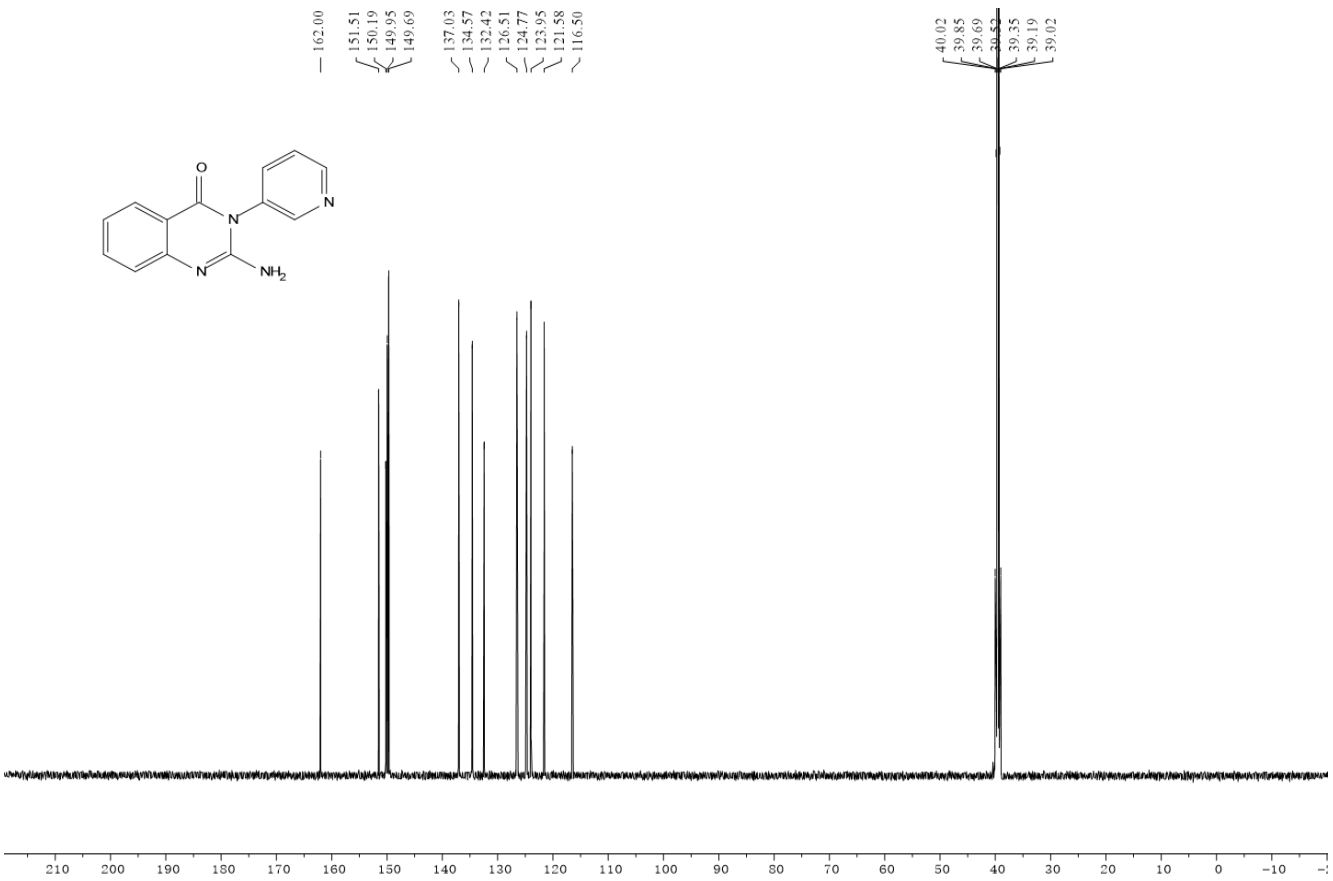

Figure S76. ^{13}C NMR (126 MHz) of **3y** in DMSO-d_6.

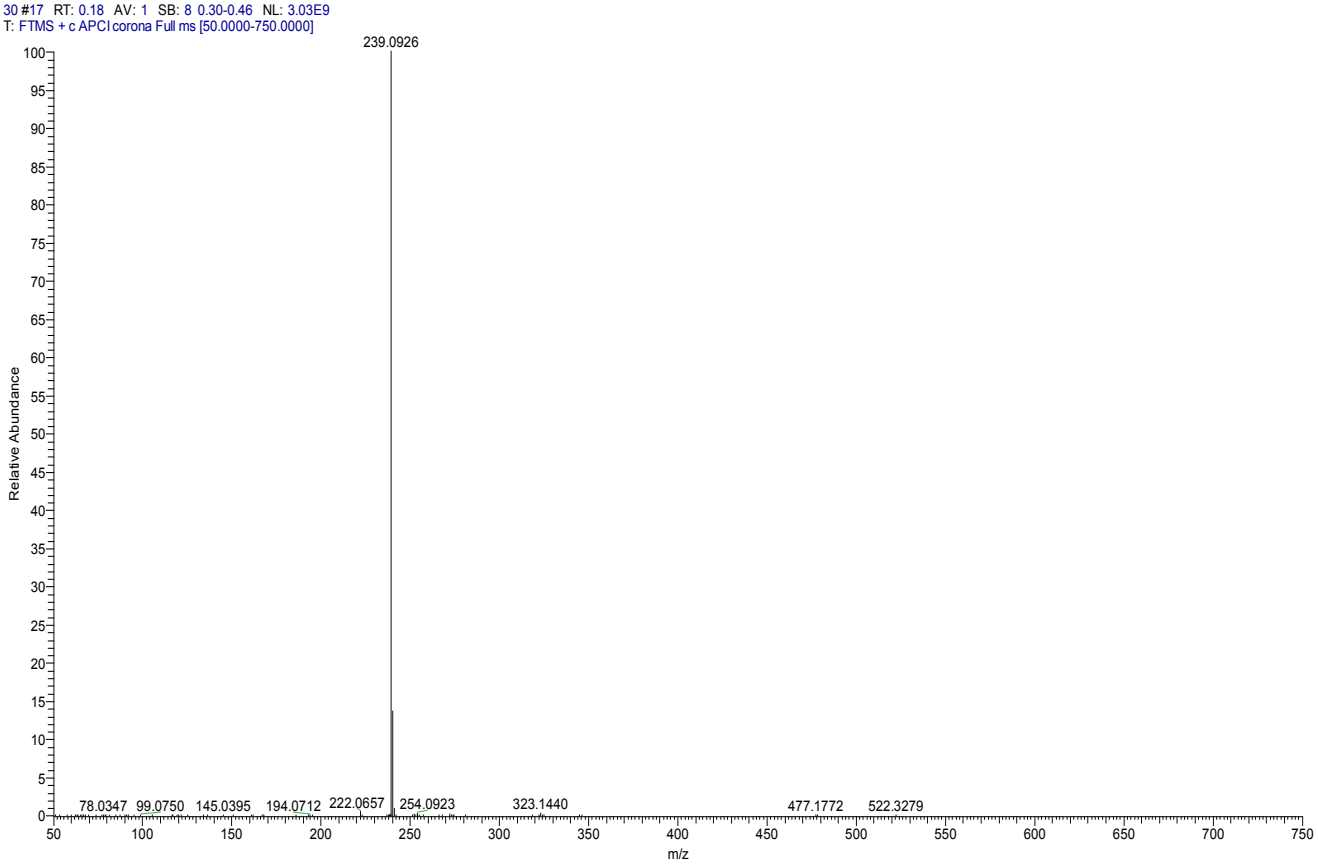

Figure S77. HRMS spectra for **3y**.

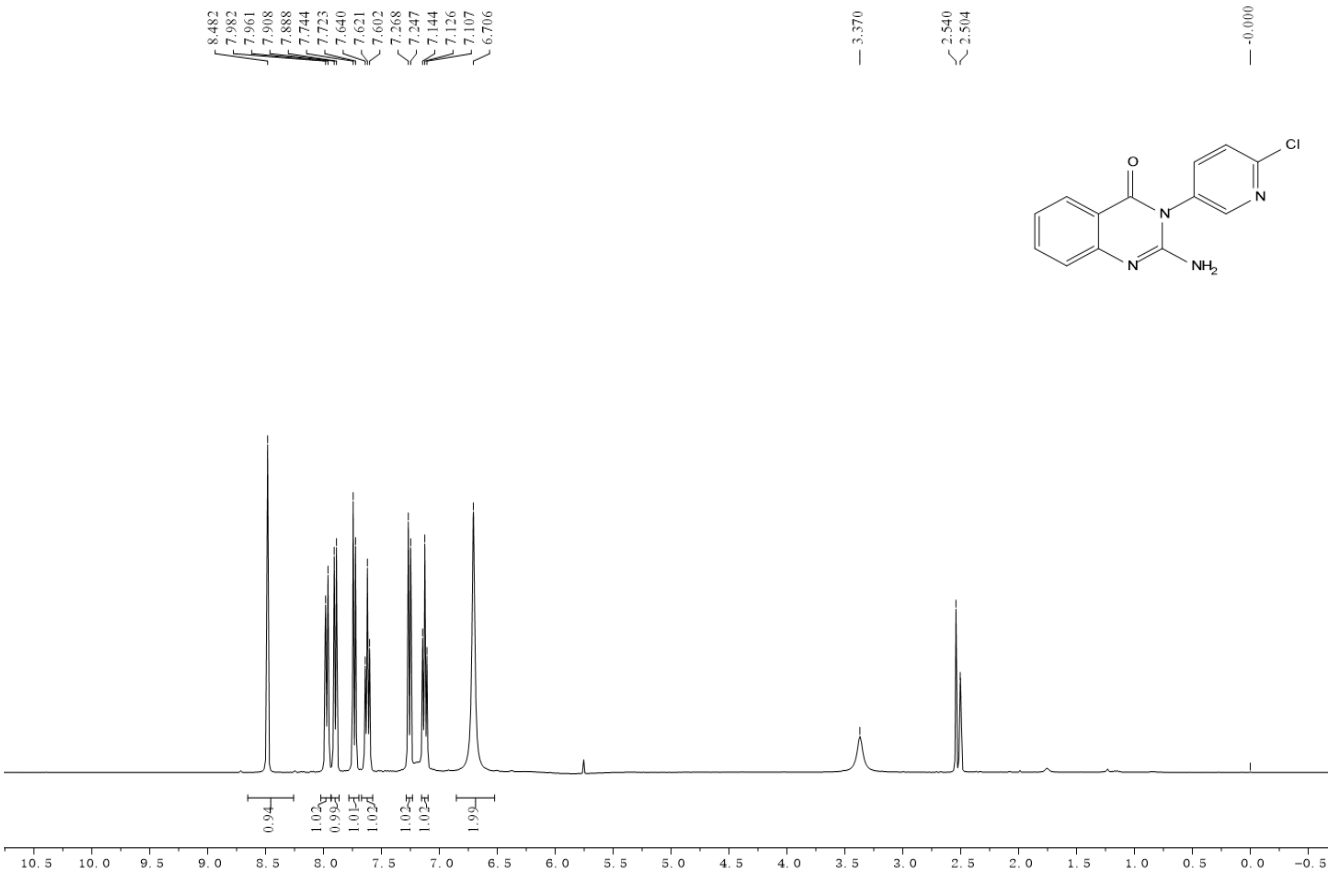

Figure S78. ^{1}H NMR (400 MHz) of **3z** in DMSO - d_6.

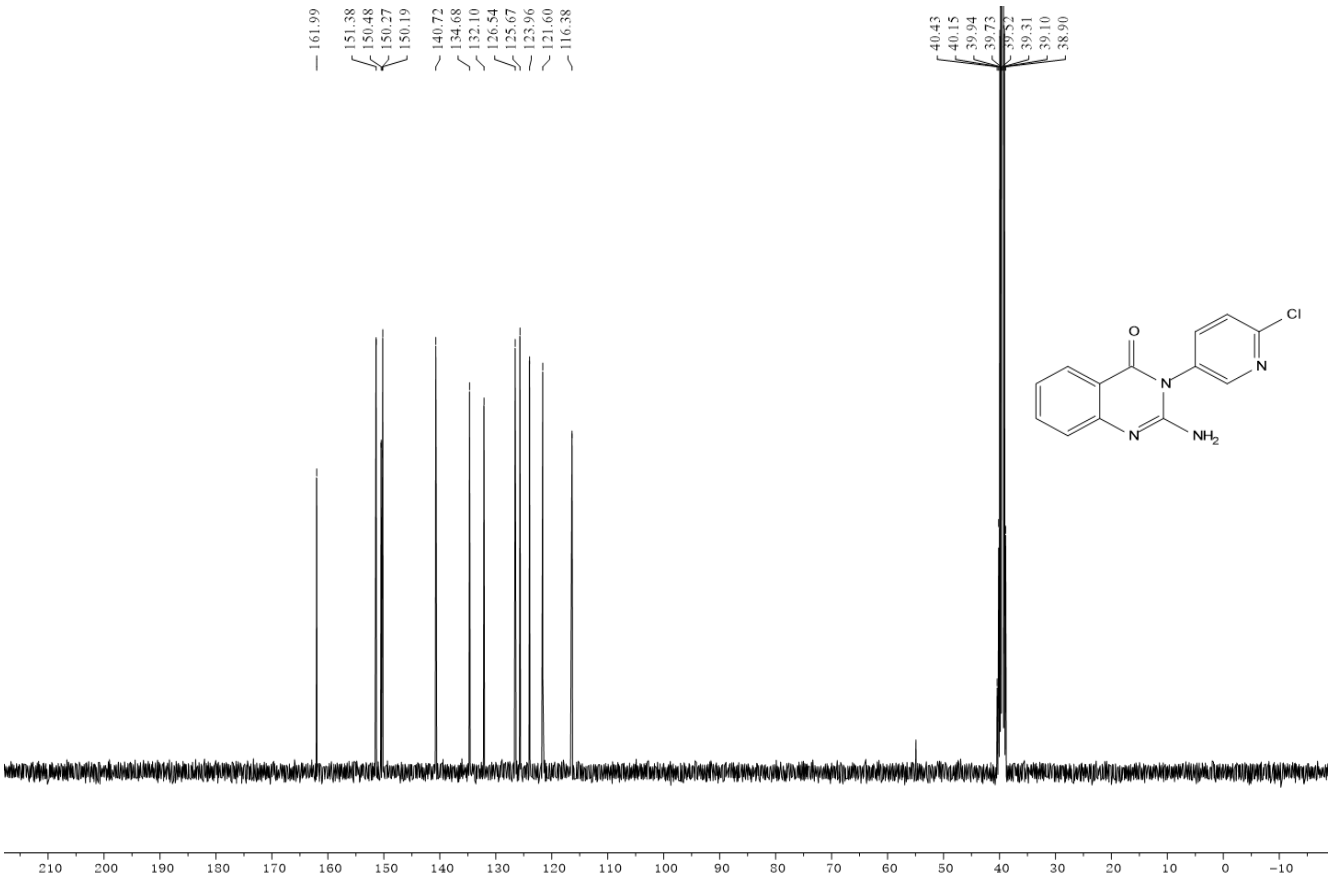

Figure S79. ^{13}C NMR (101 MHz) of **3z** in DMSO-d_6.

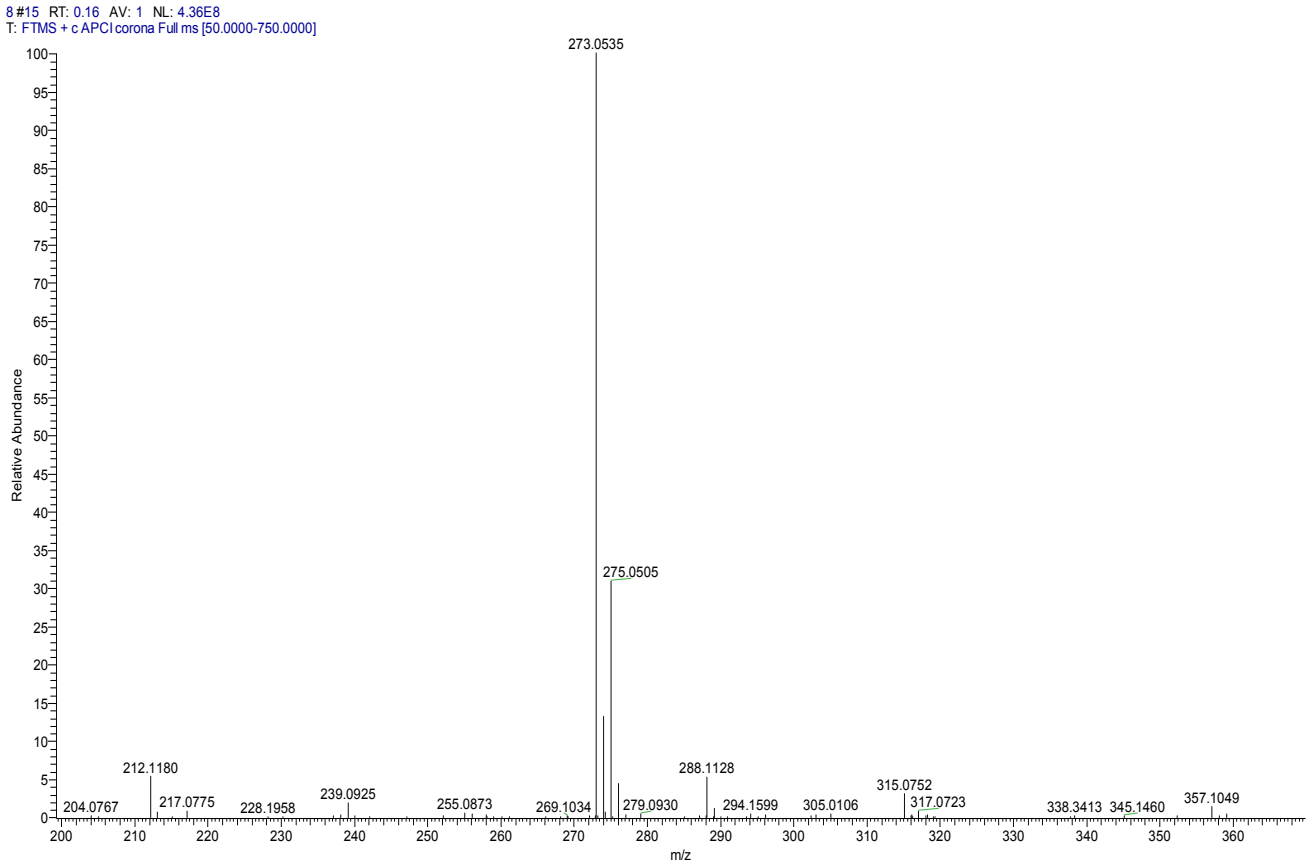

Figure S80. HRMS spectra for **3z**.

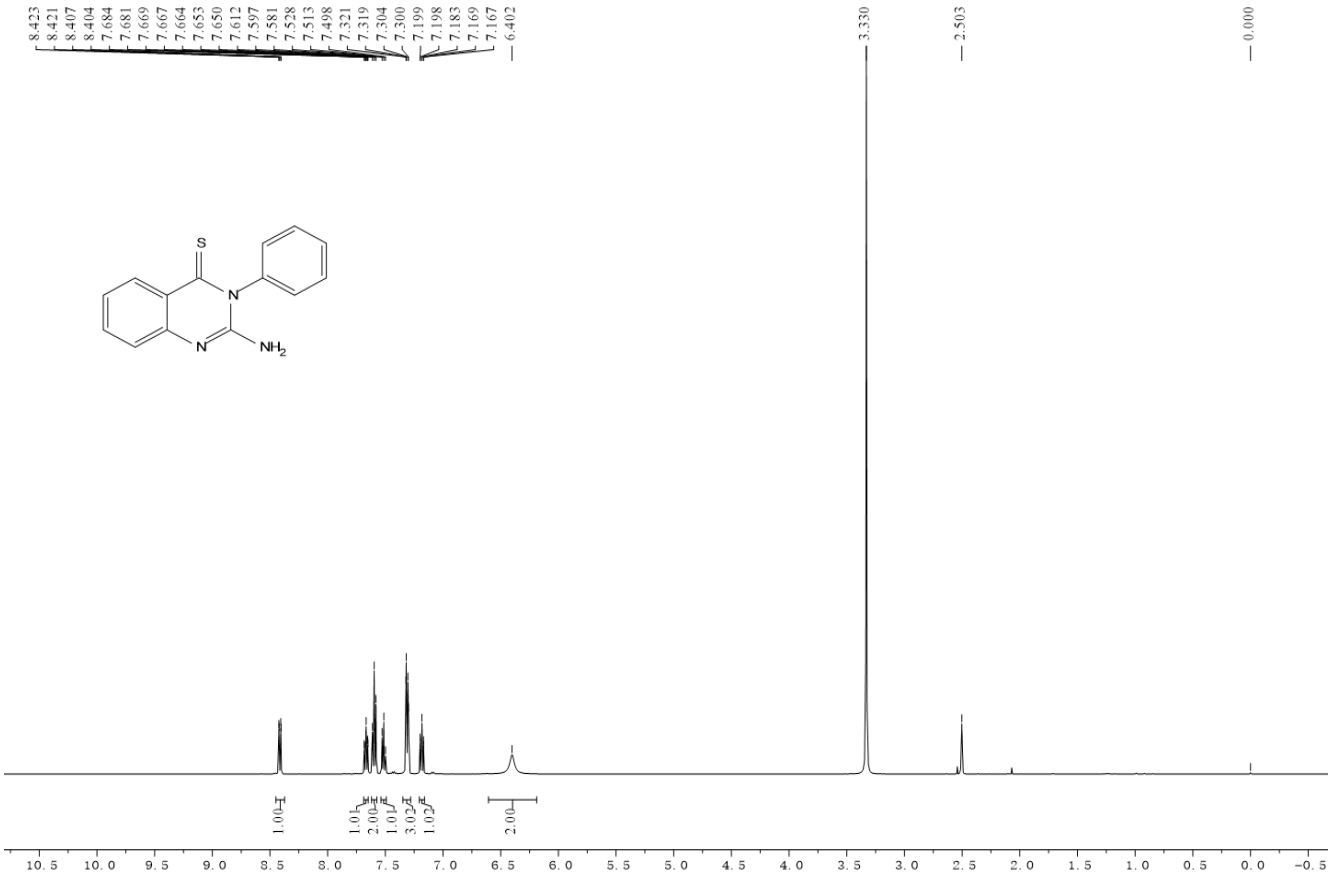

Figure S81. ^{1}H NMR (500 MHz) of **5a** in DMSO - d_6.

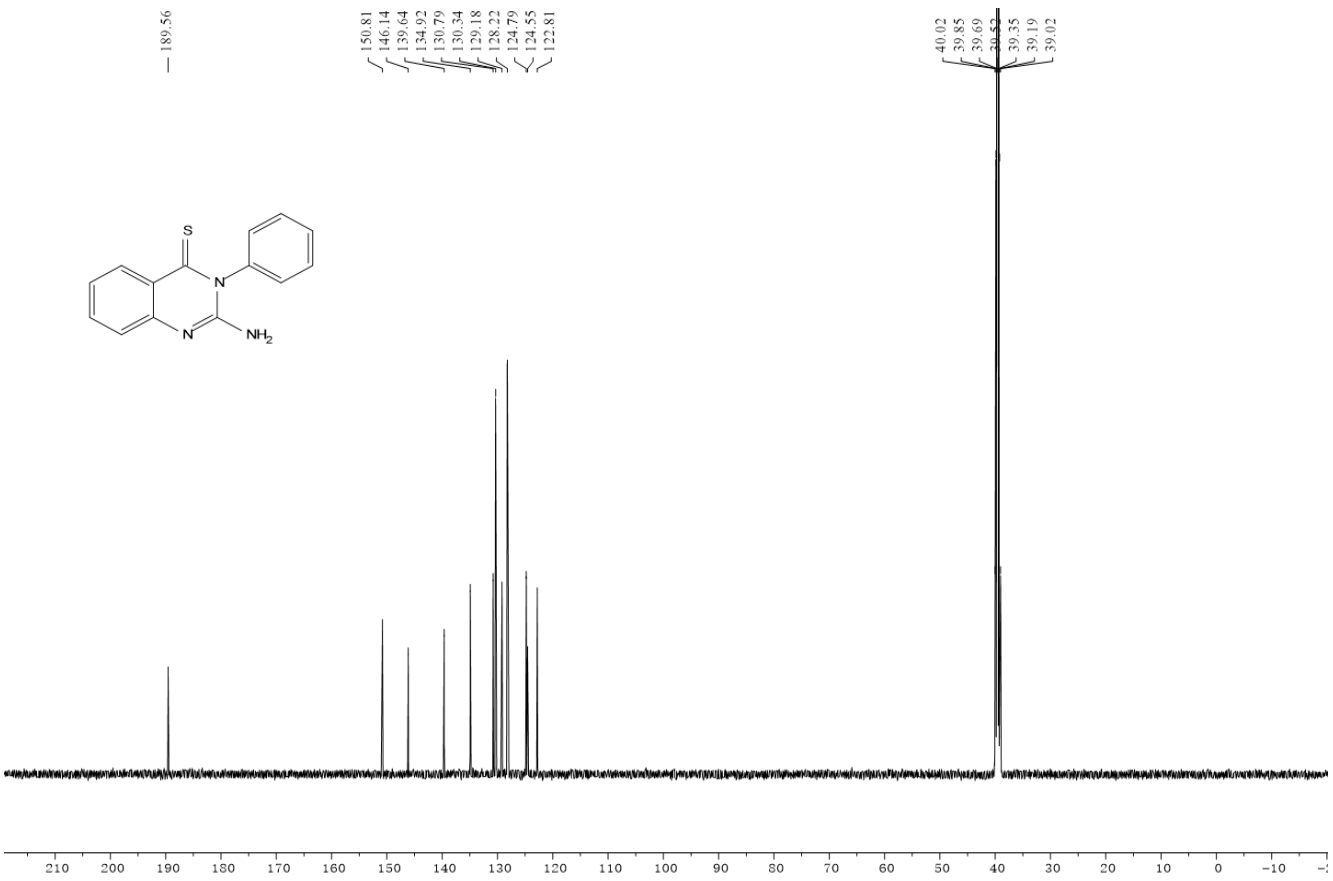

Figure S82. ^{13}C NMR (126 MHz) of **5a** in DMSO - d_6.

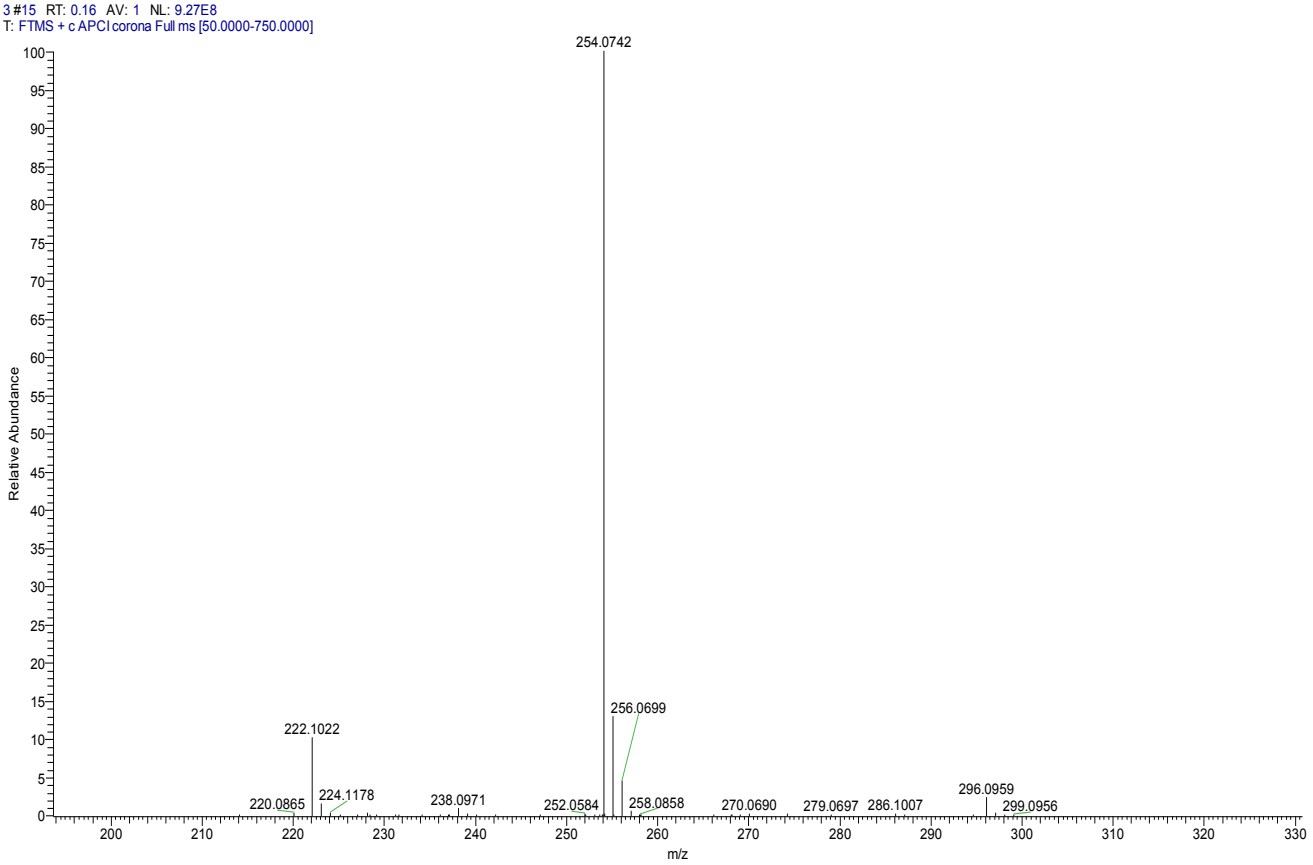

Figure S83. HRMS spectra for **5a**.

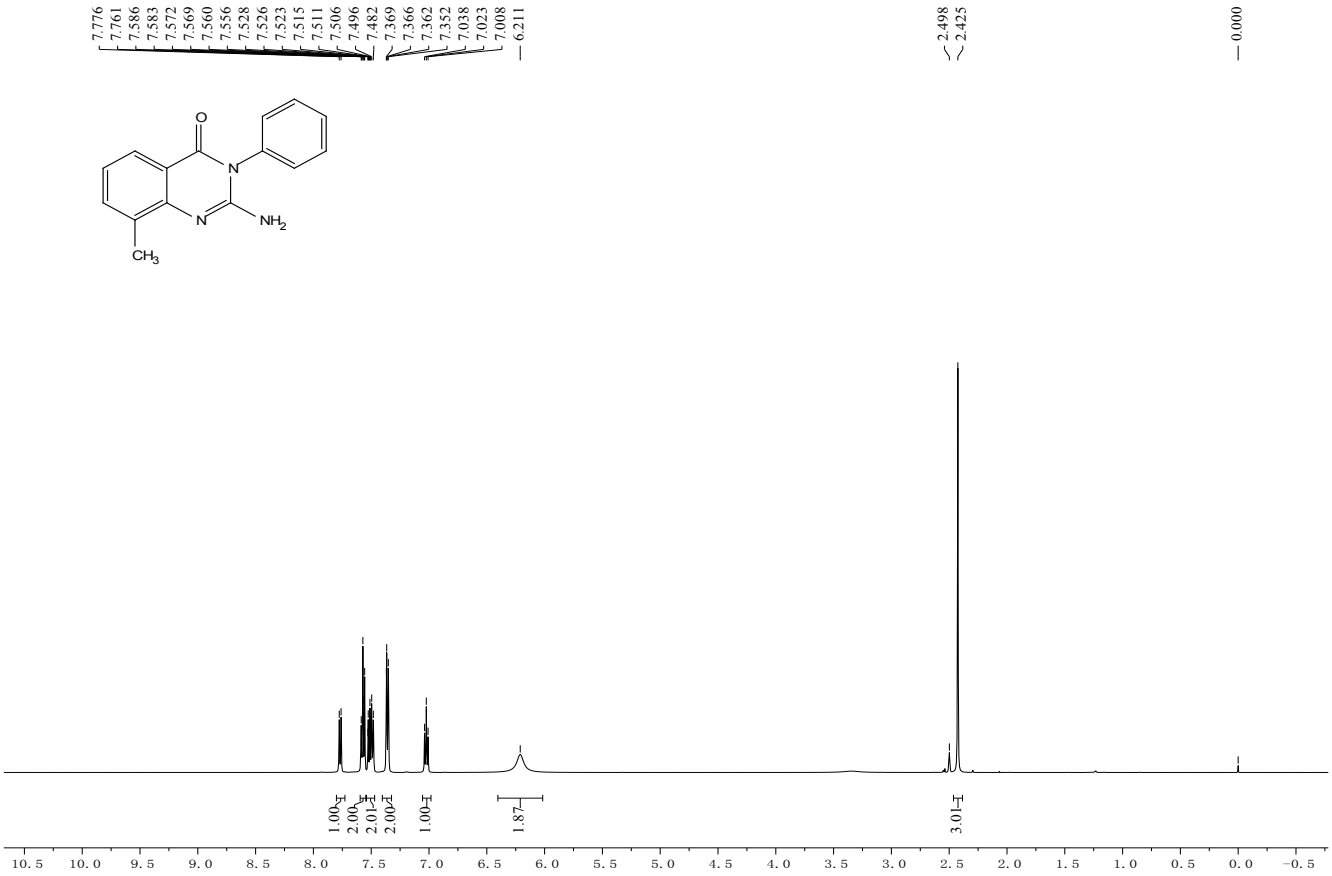

Figure S84. ^{1}H NMR (500 MHz) of **5b** in DMSO - d_6.

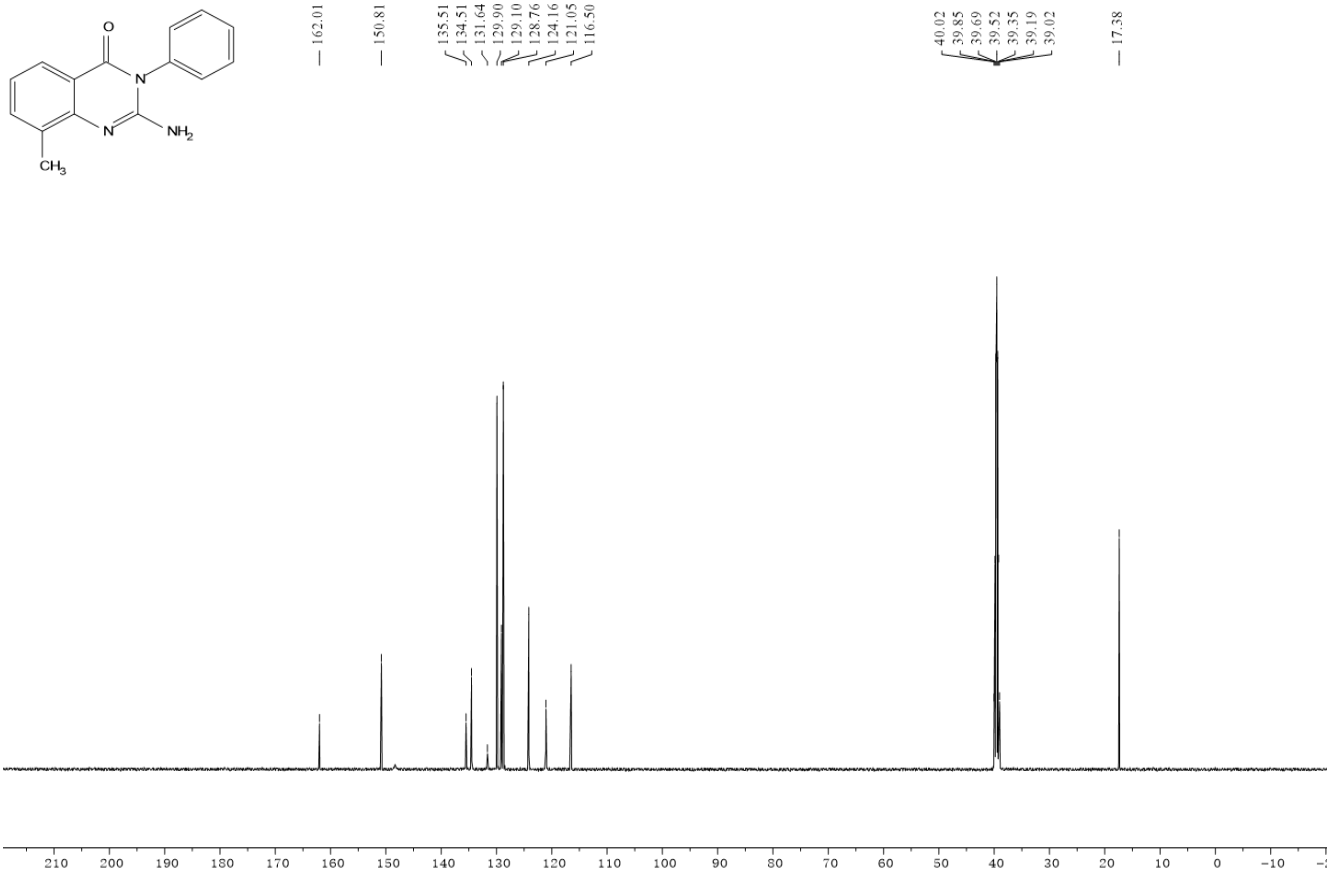

Figure S85. ^{13}C NMR (126 MHz) of **5b** in DMSO - d_6.

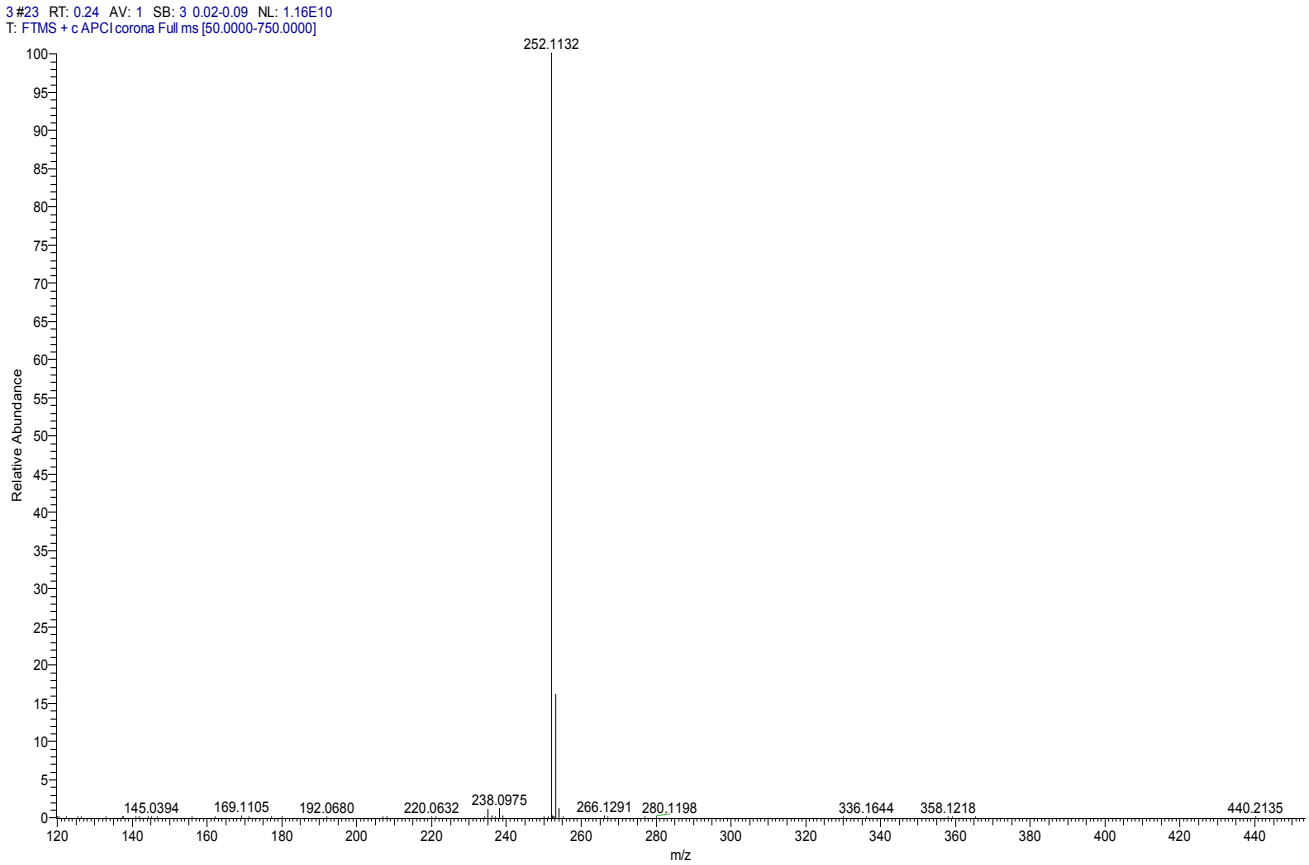

Figure S86. HRMS spectra for **5b**.

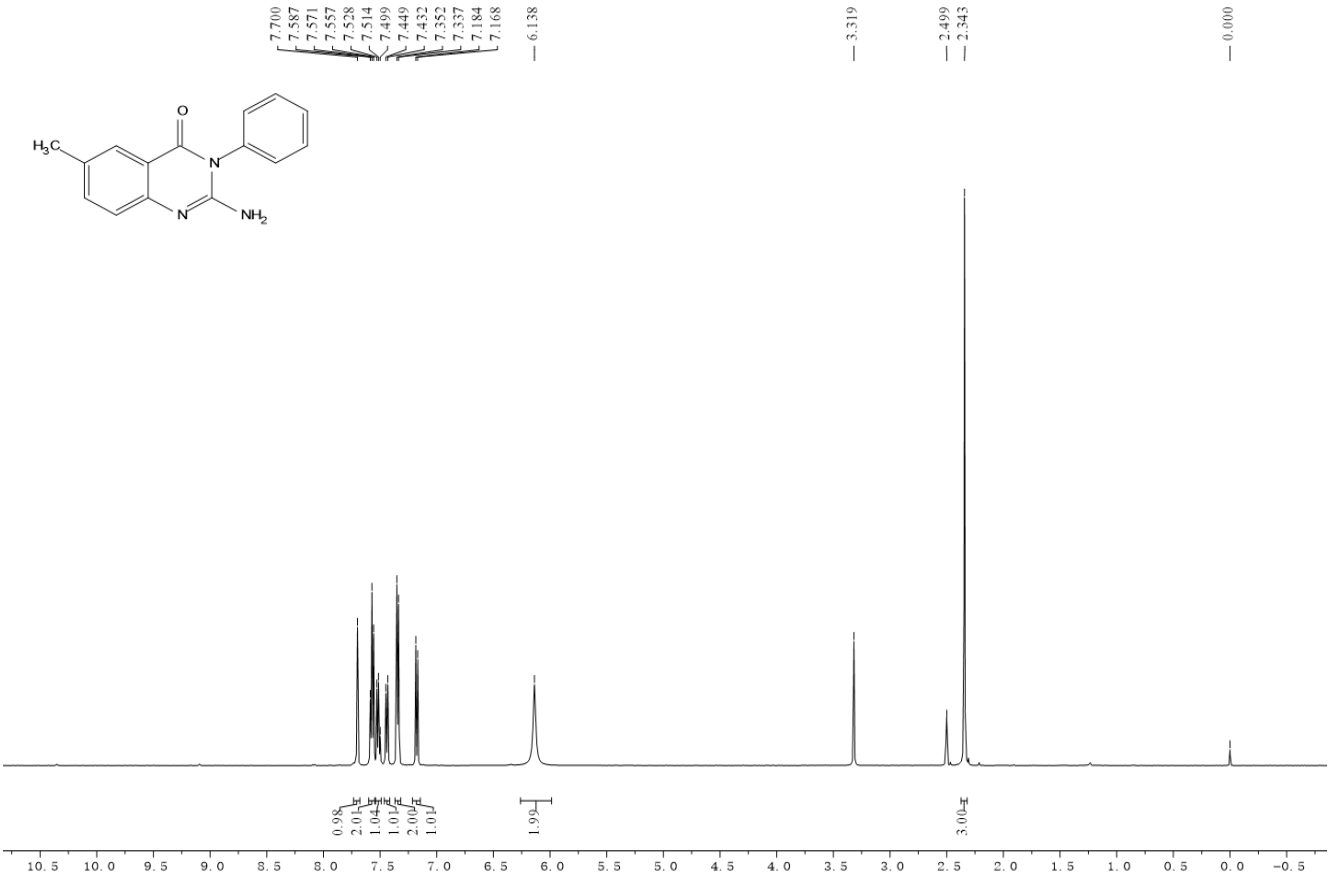

Figure S87. ^{1}H NMR (500 MHz) of **5c** in DMSO - d_6.

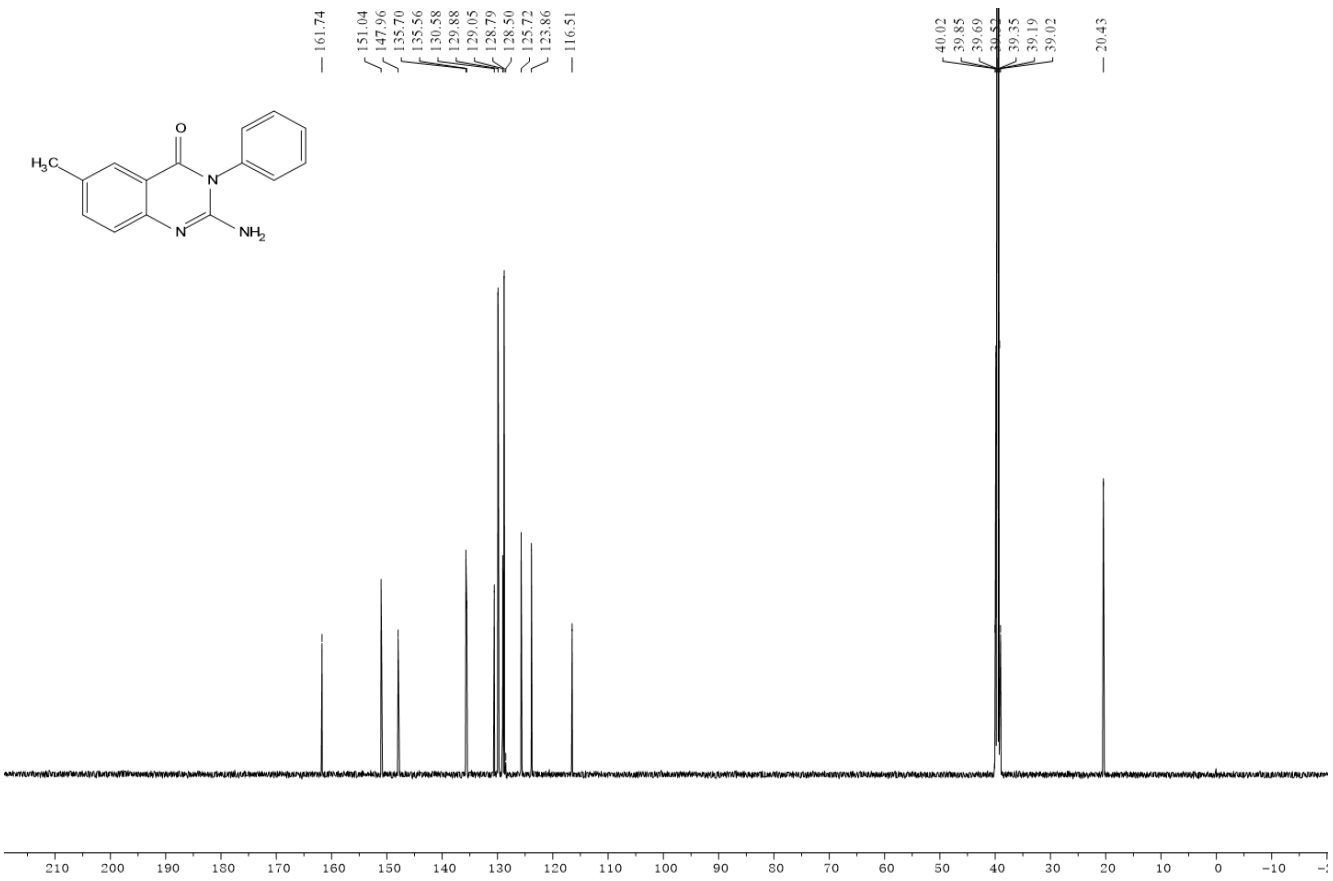

Figure S88. ^{13}C NMR (126 MHz) of **5c** in DMSO - d_6.

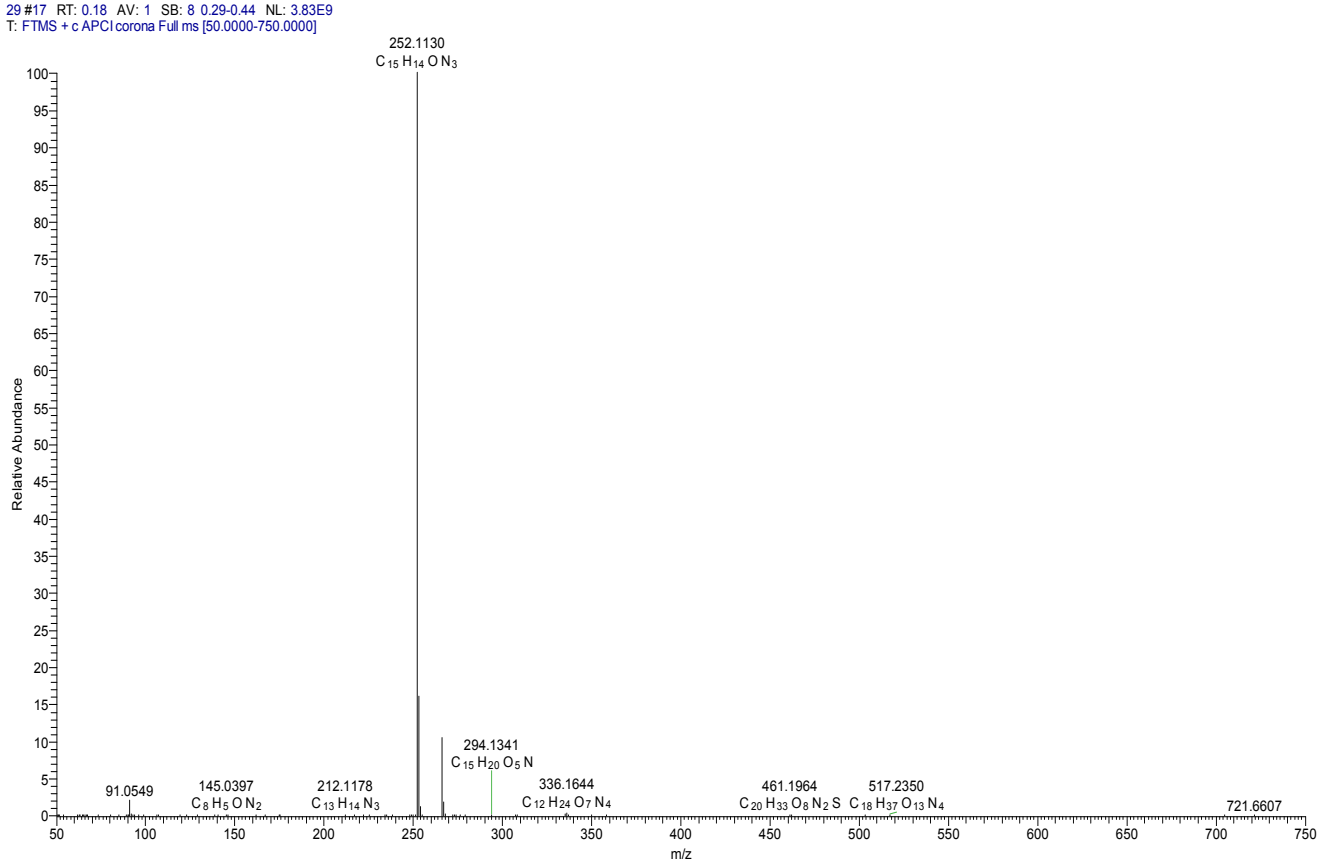

Figure S89. HRMS spectra for **5c**.

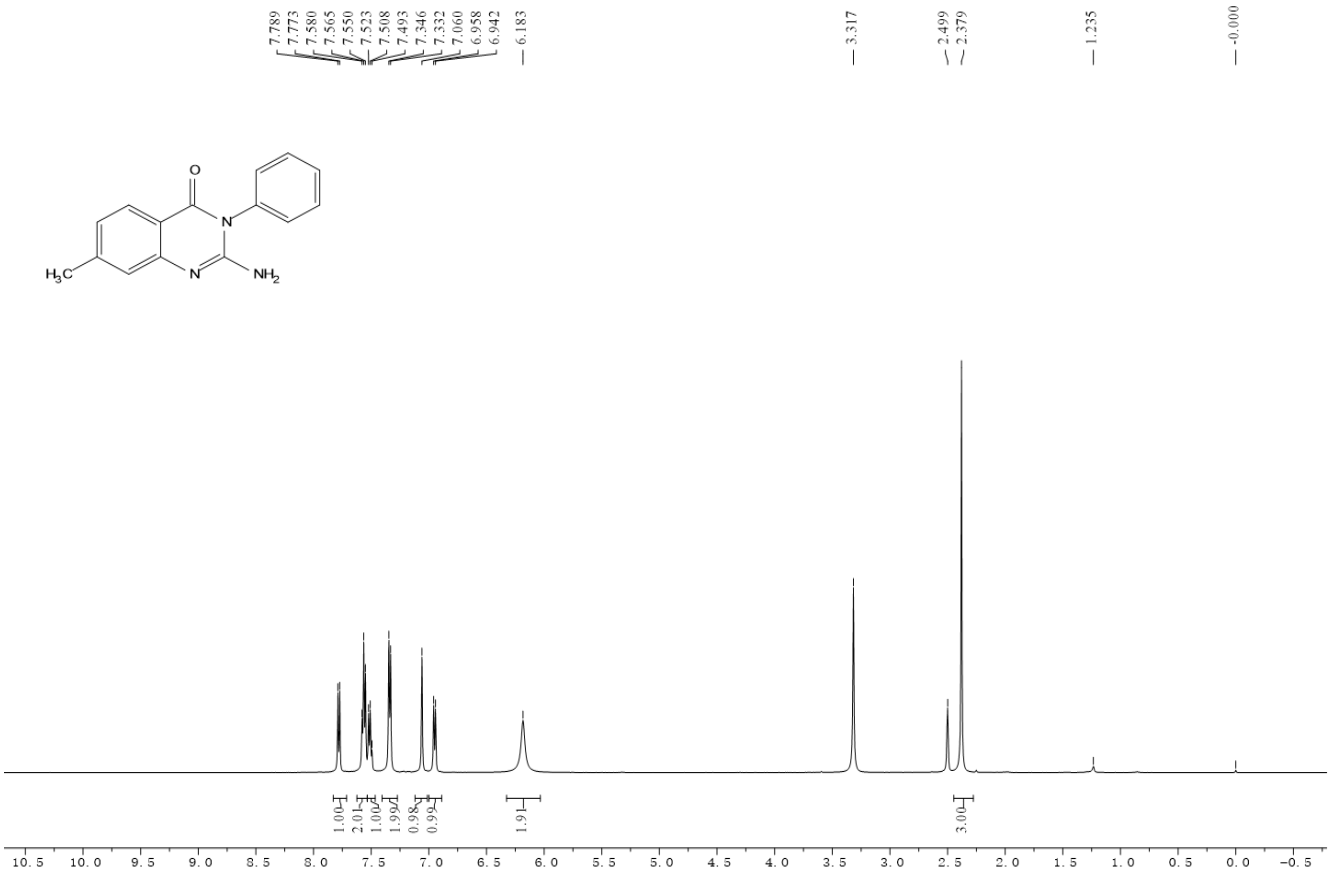

Figure S90. ^{1}H NMR (500 MHz) of **5d** in DMSO - d_6.

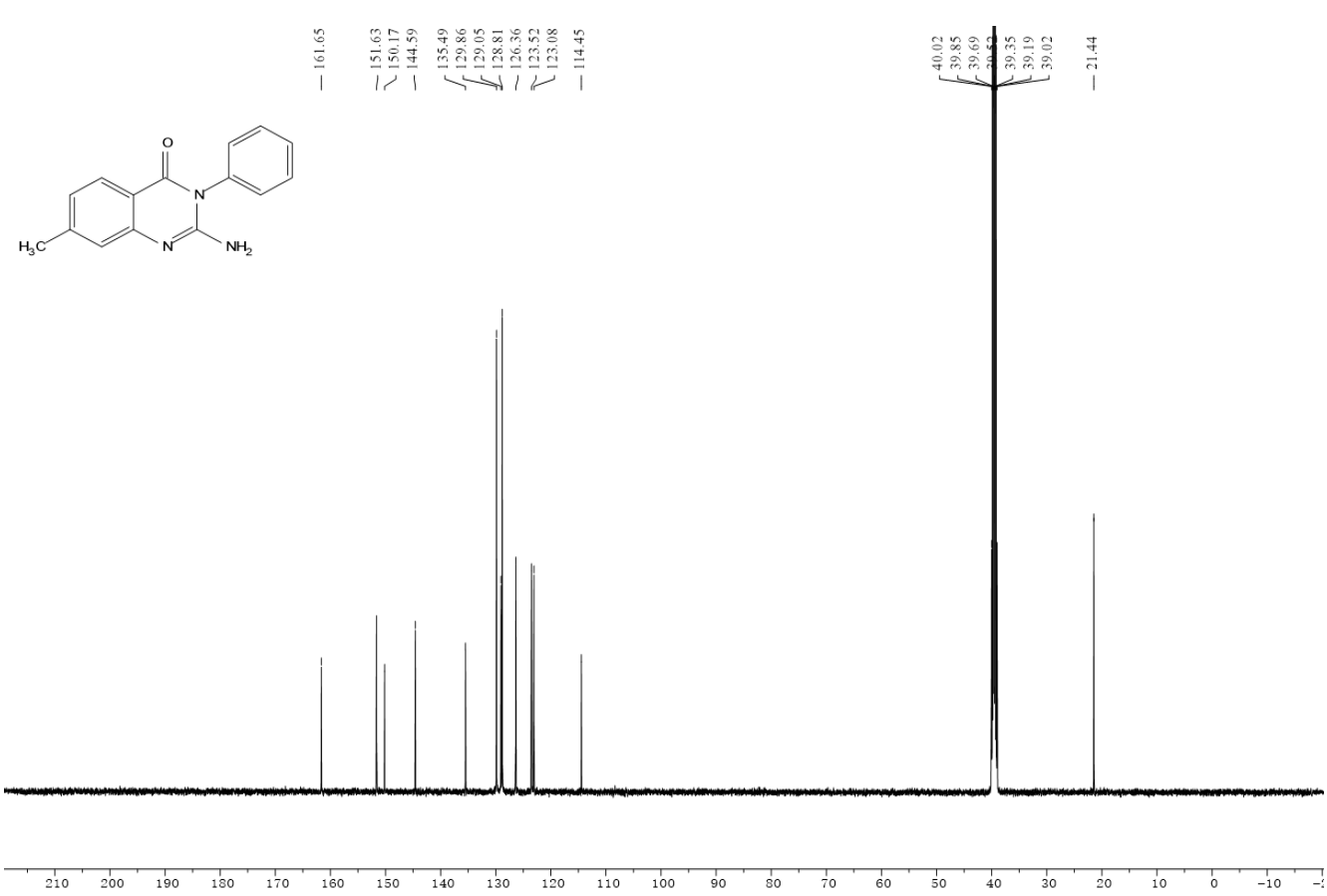

Figure S91. ^{13}C NMR (126 MHz) of **5d** in DMSO - d_6.

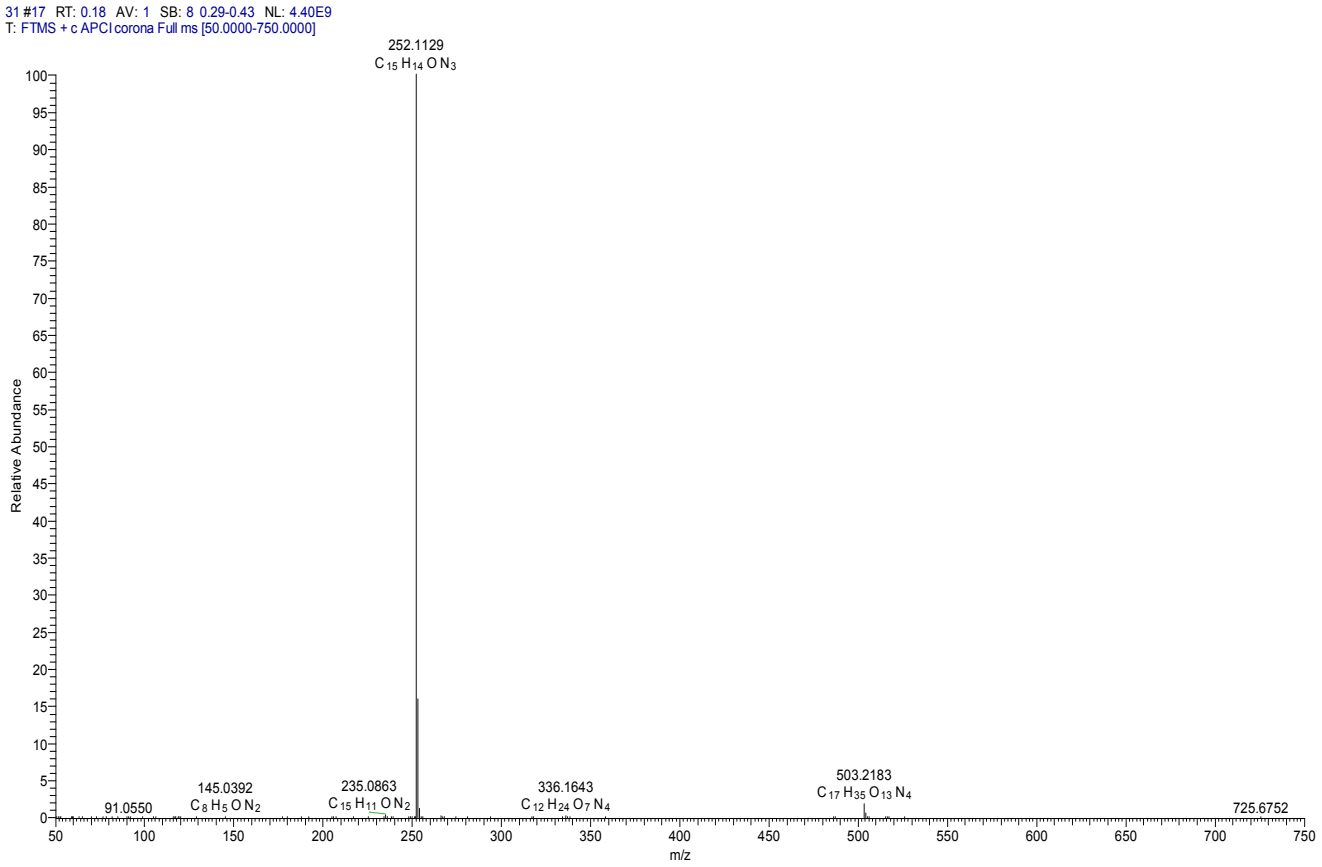

Figure S92. HRMS spectra for **5d**.

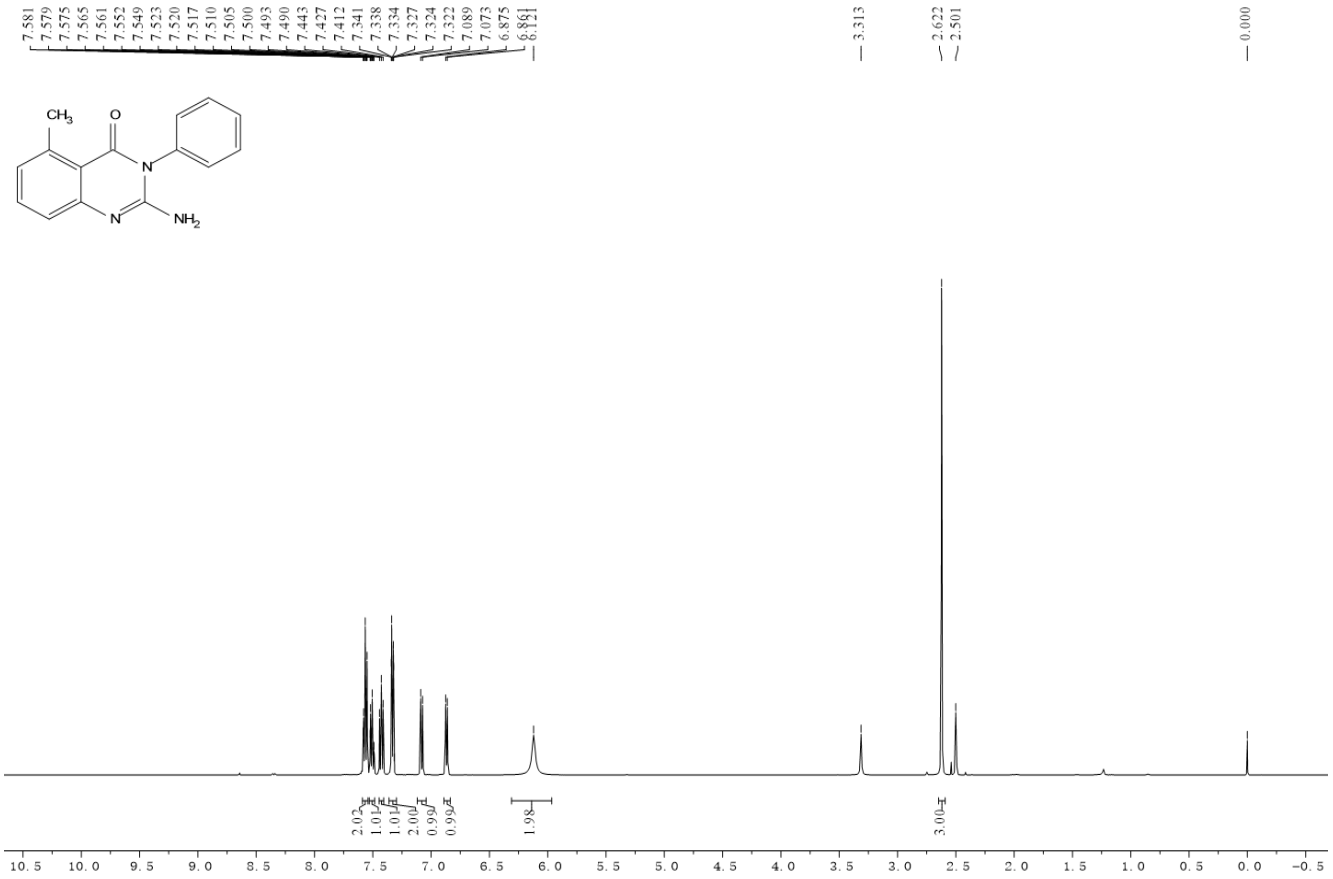

Figure S93. ^{1}H NMR (500 MHz) of **5e** in DMSO - d_6.

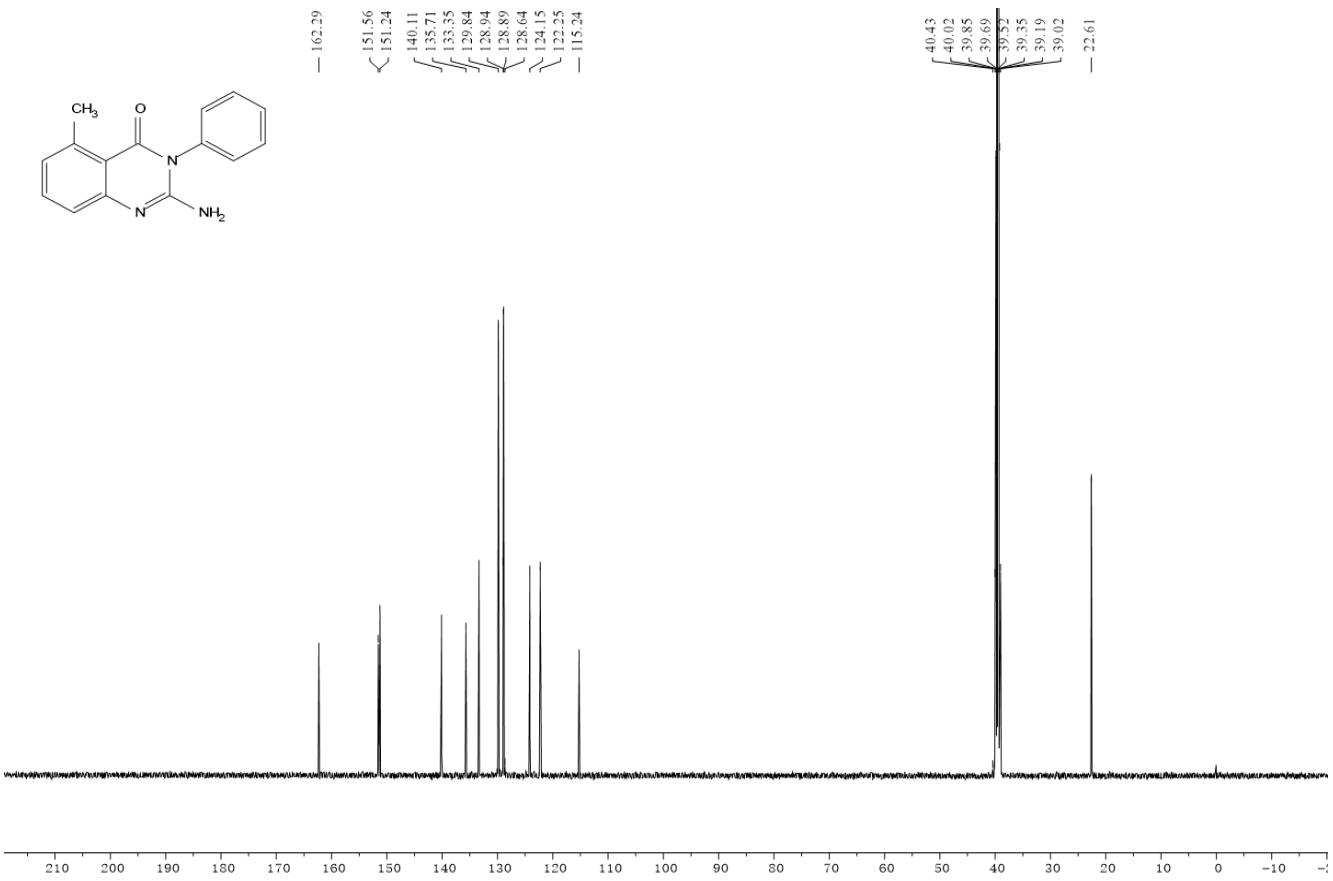

Figure S94. ^{13}C NMR (126 MHz) of **5e** in DMSO - d_6.

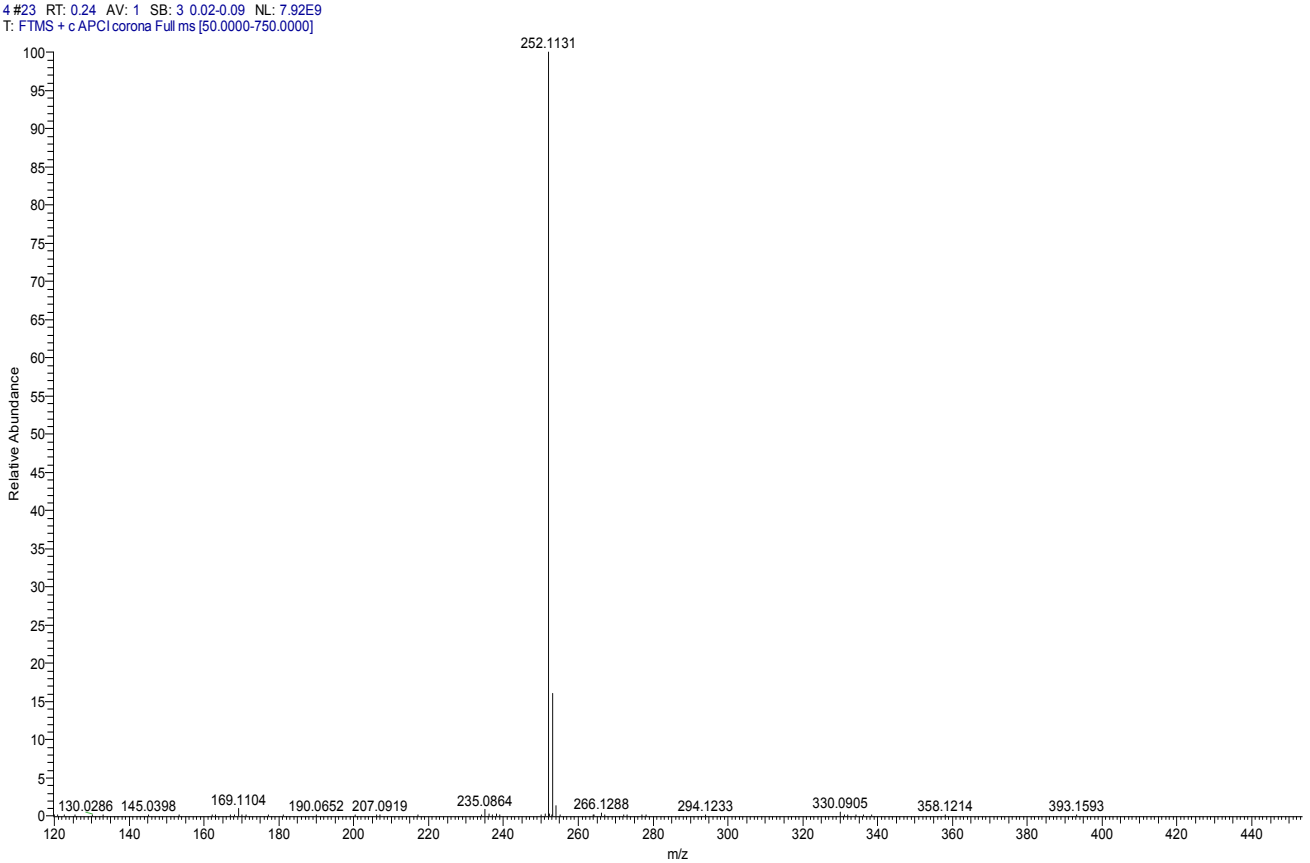

Figure S95. HRMS spectra for **5e**.

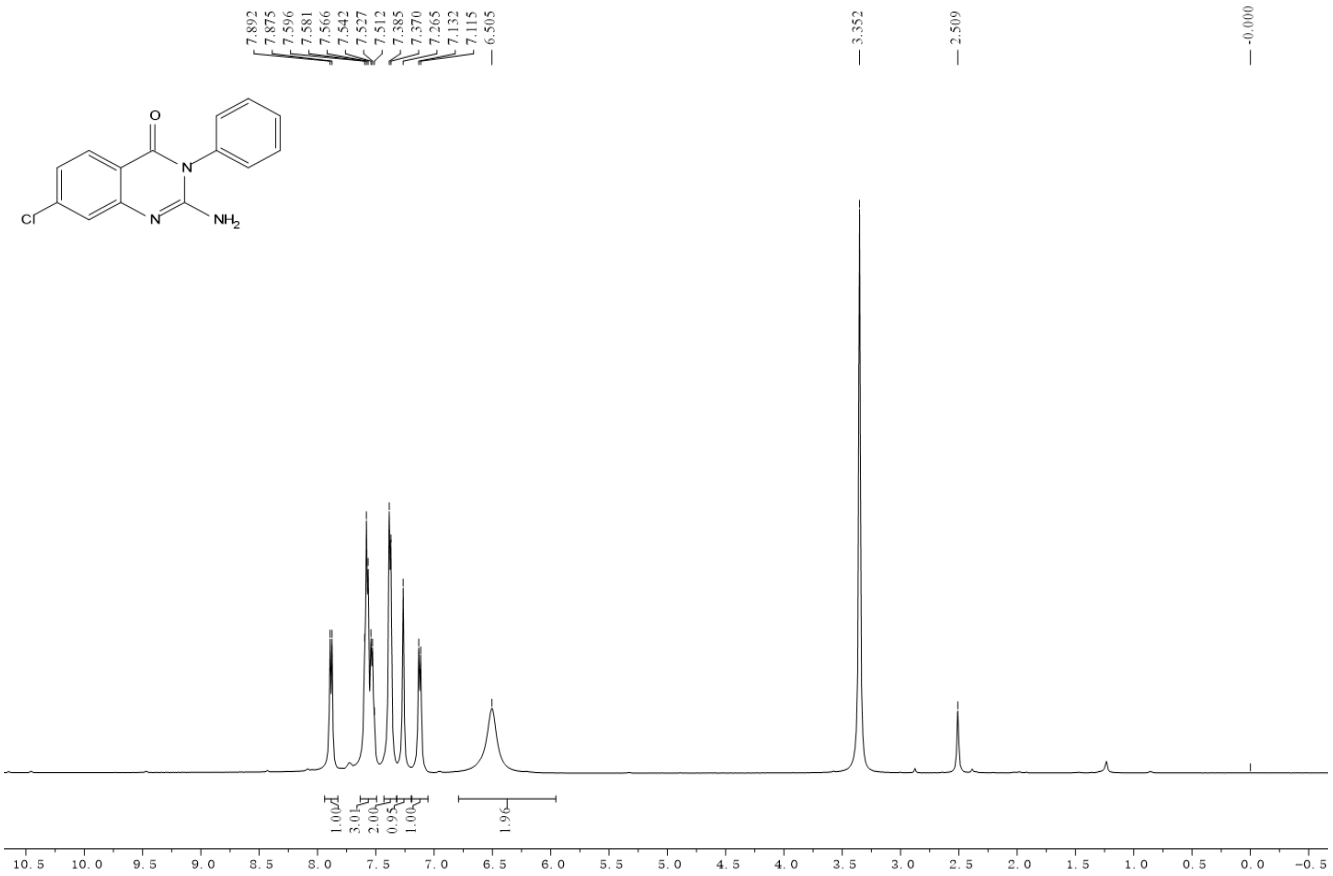

Figure S96. ^{1}H NMR (500 MHz) of **5f** in DMSO - d_6.

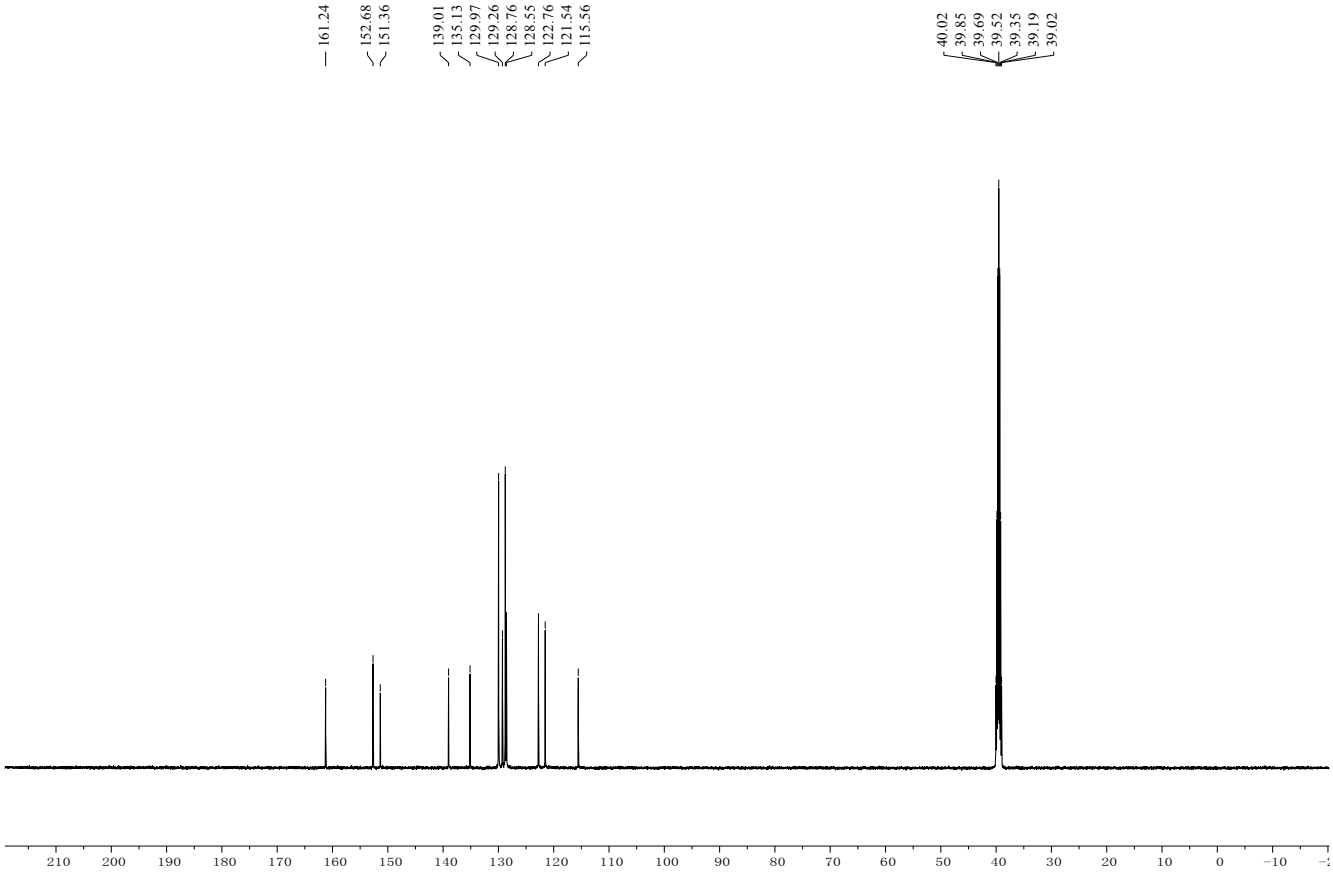

Figure S97. ^{13}C NMR (126 MHz) of **5f** in DMSO - d_6.

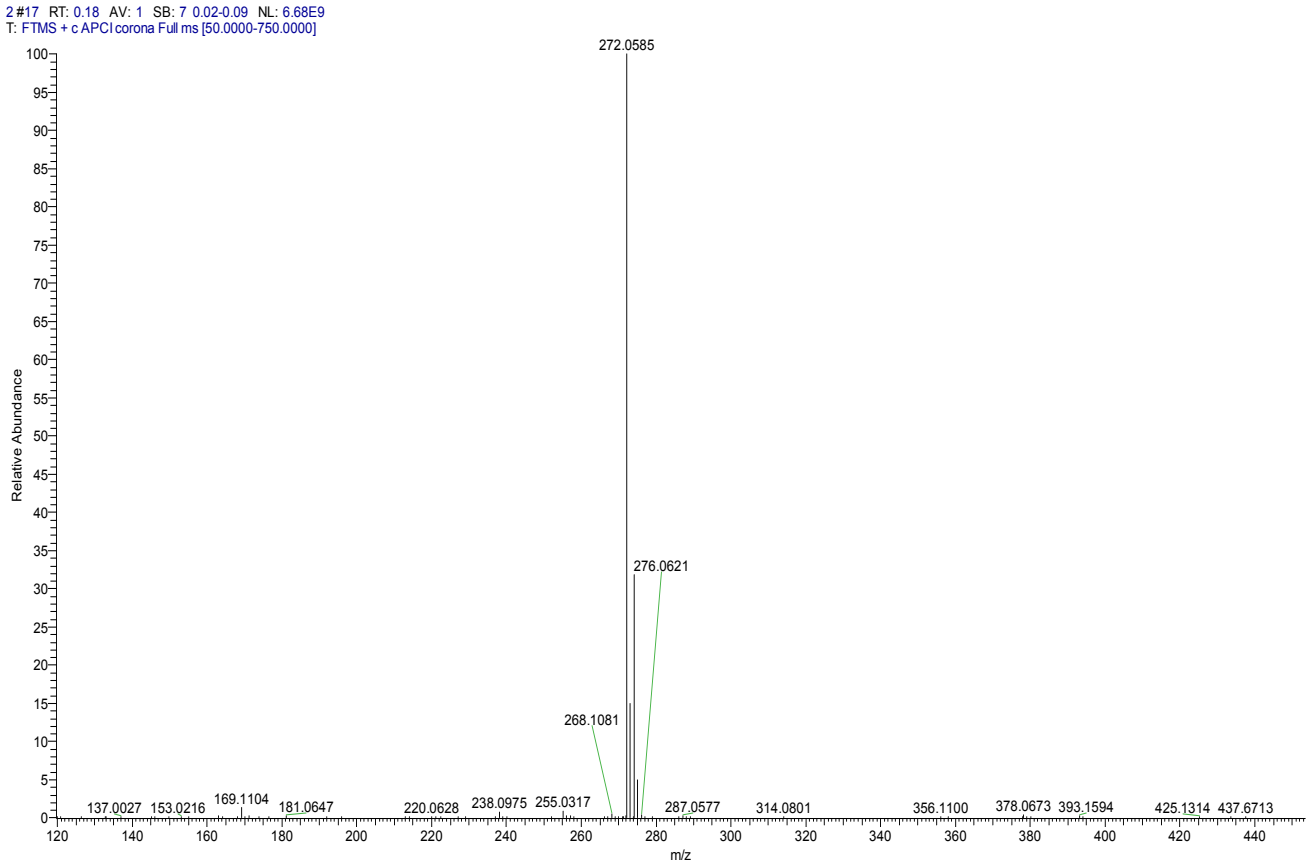

Figure S98. HRMS spectra for **5f**.

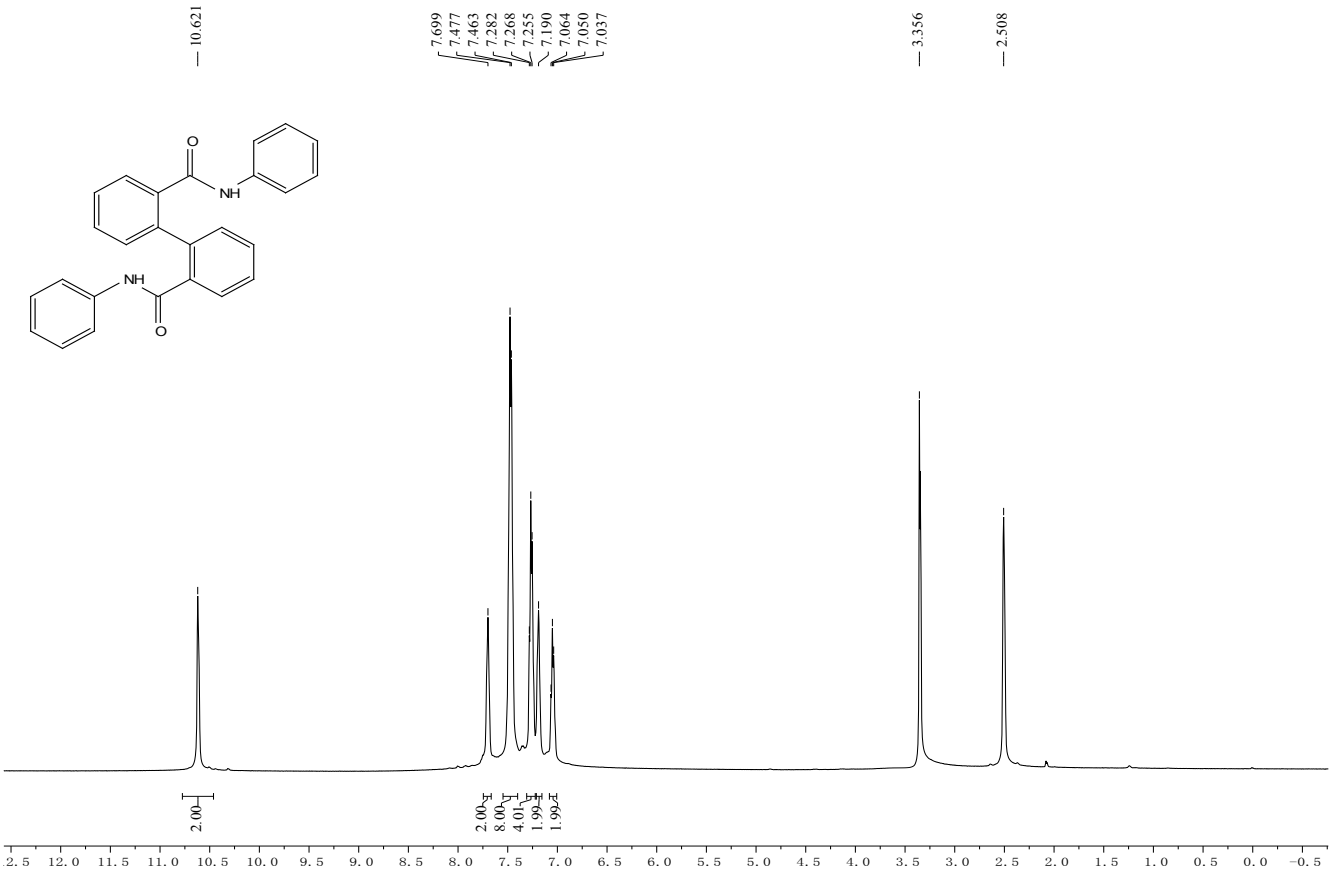

Figure S99. ^{1}H NMR (500 MHz) of **6a** in DMSO-d_6.

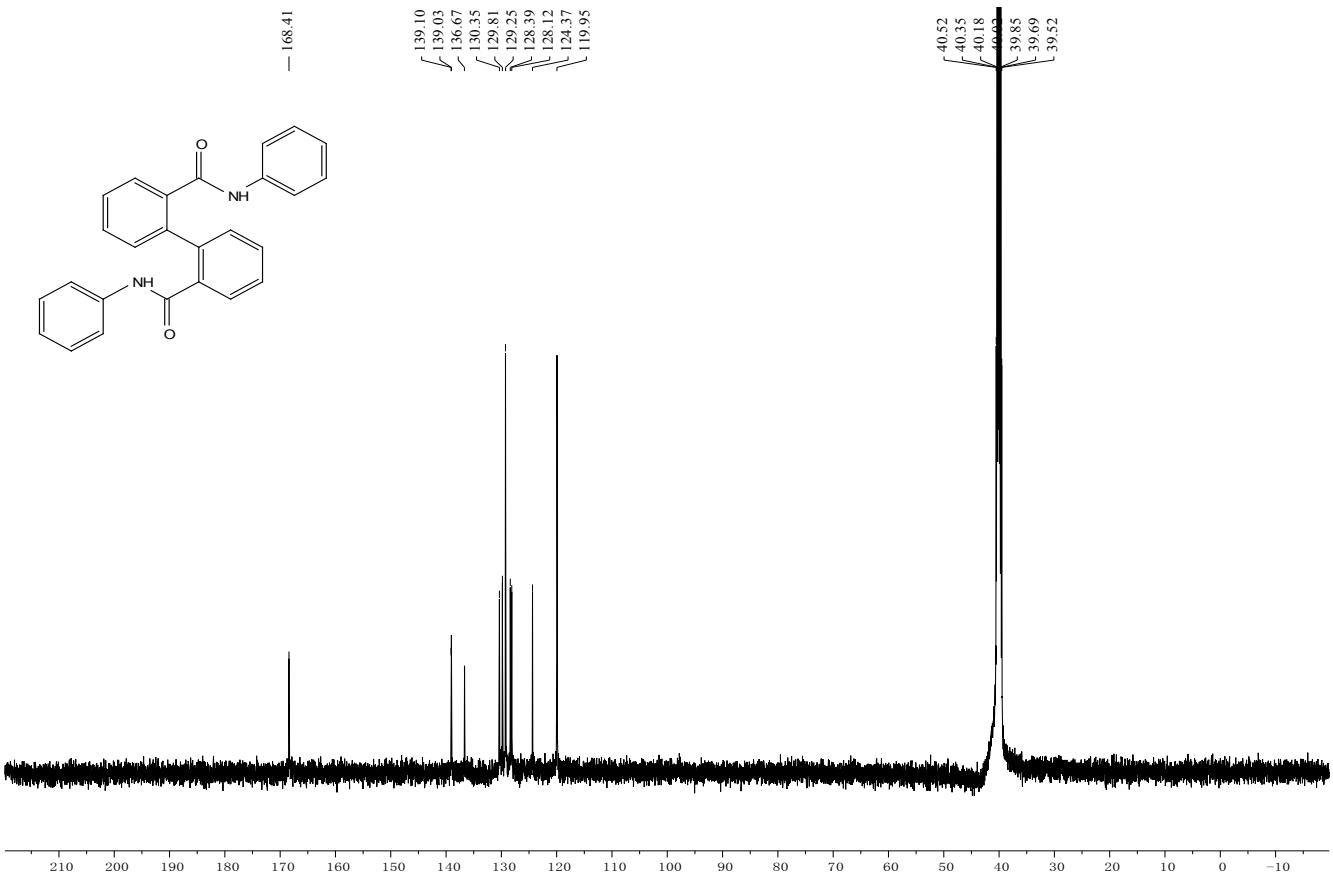

Figure S100. ^{13}C NMR (126 MHz) of **6a** in DMSO-d_6.

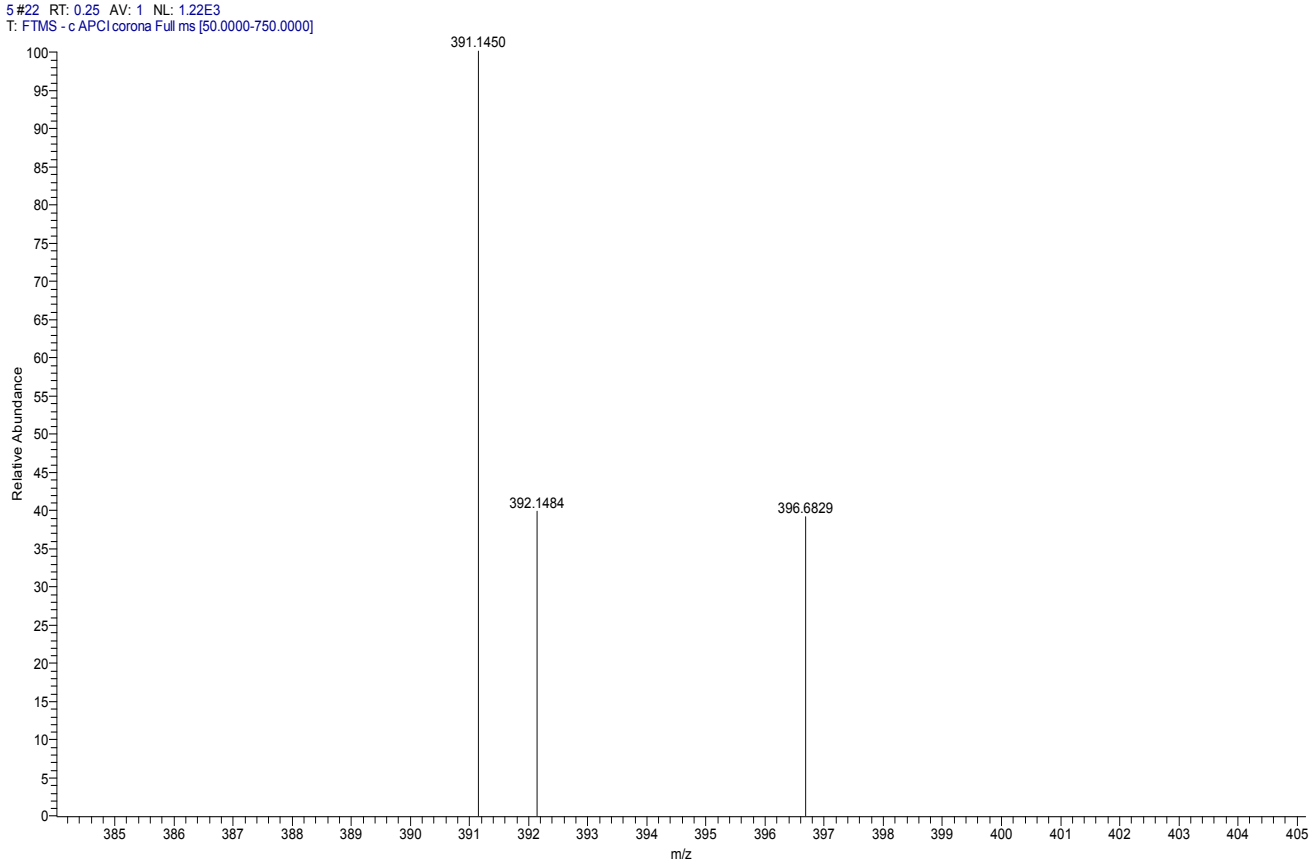

Figure S101. HRMS spectra for **6a**.

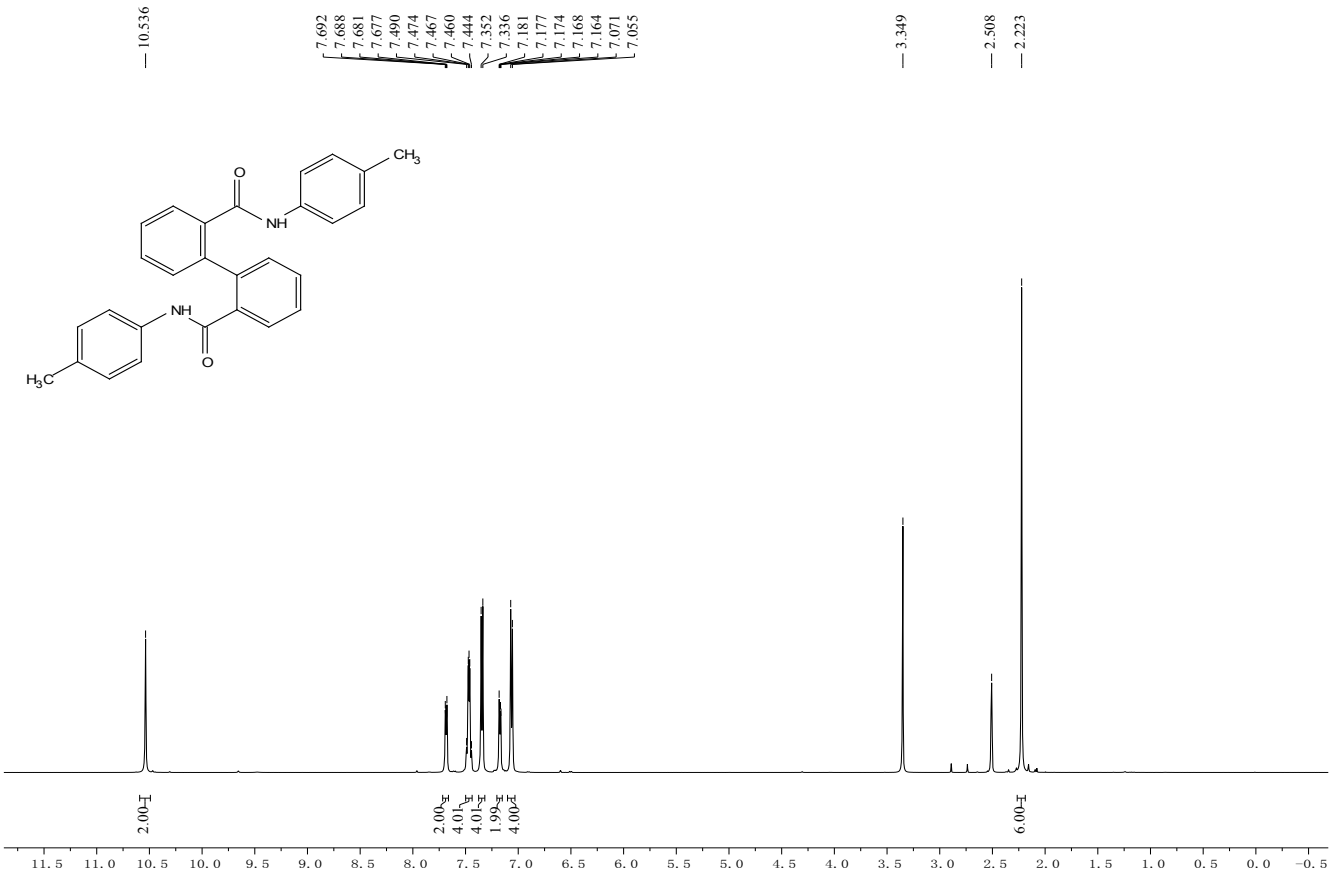

Figure S102. ^{1}H NMR (500 MHz) of **6b** in DMSO-d_6.

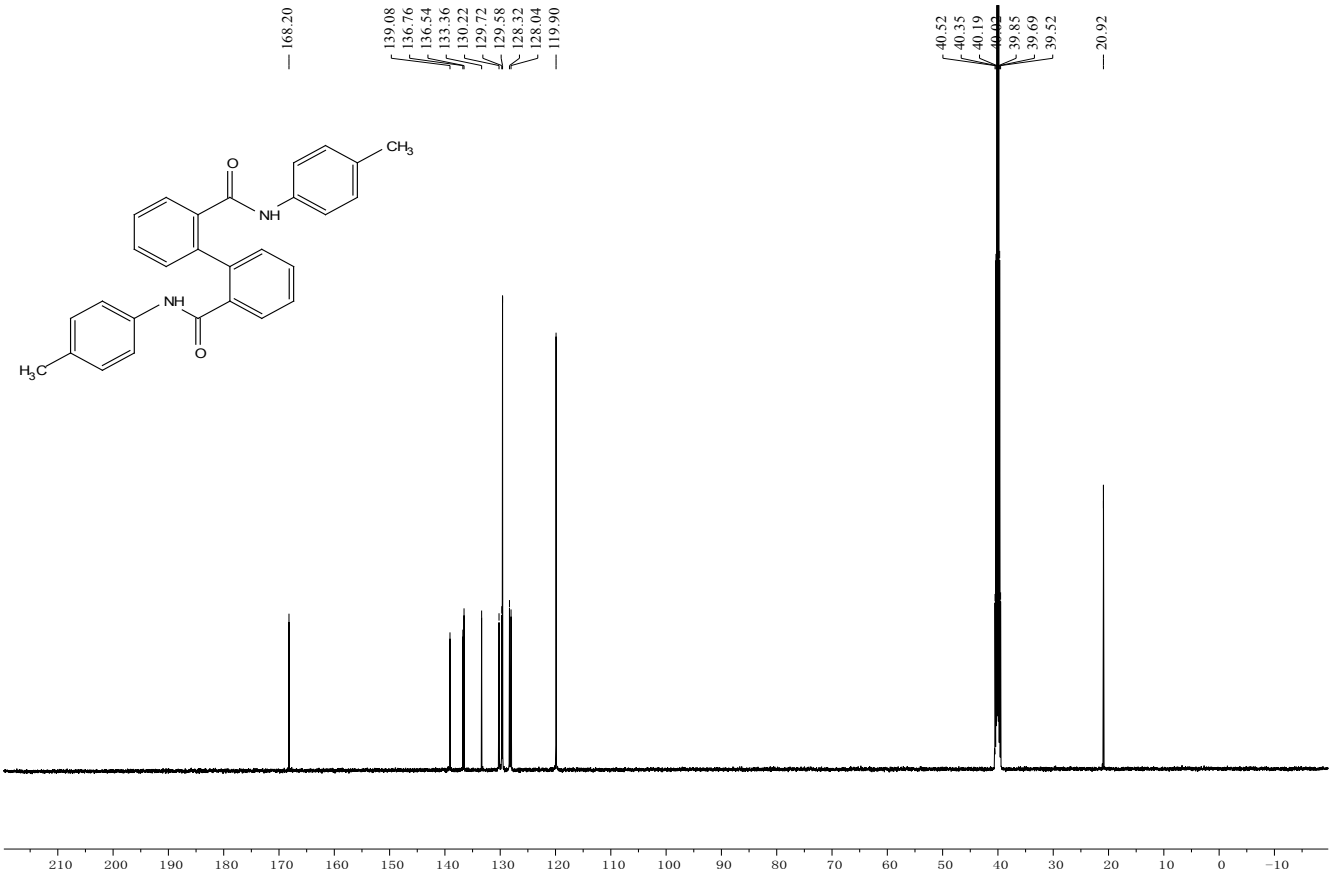

Figure S103. ^{13}C NMR (126 MHz) of **6b** in DMSO-d_6.

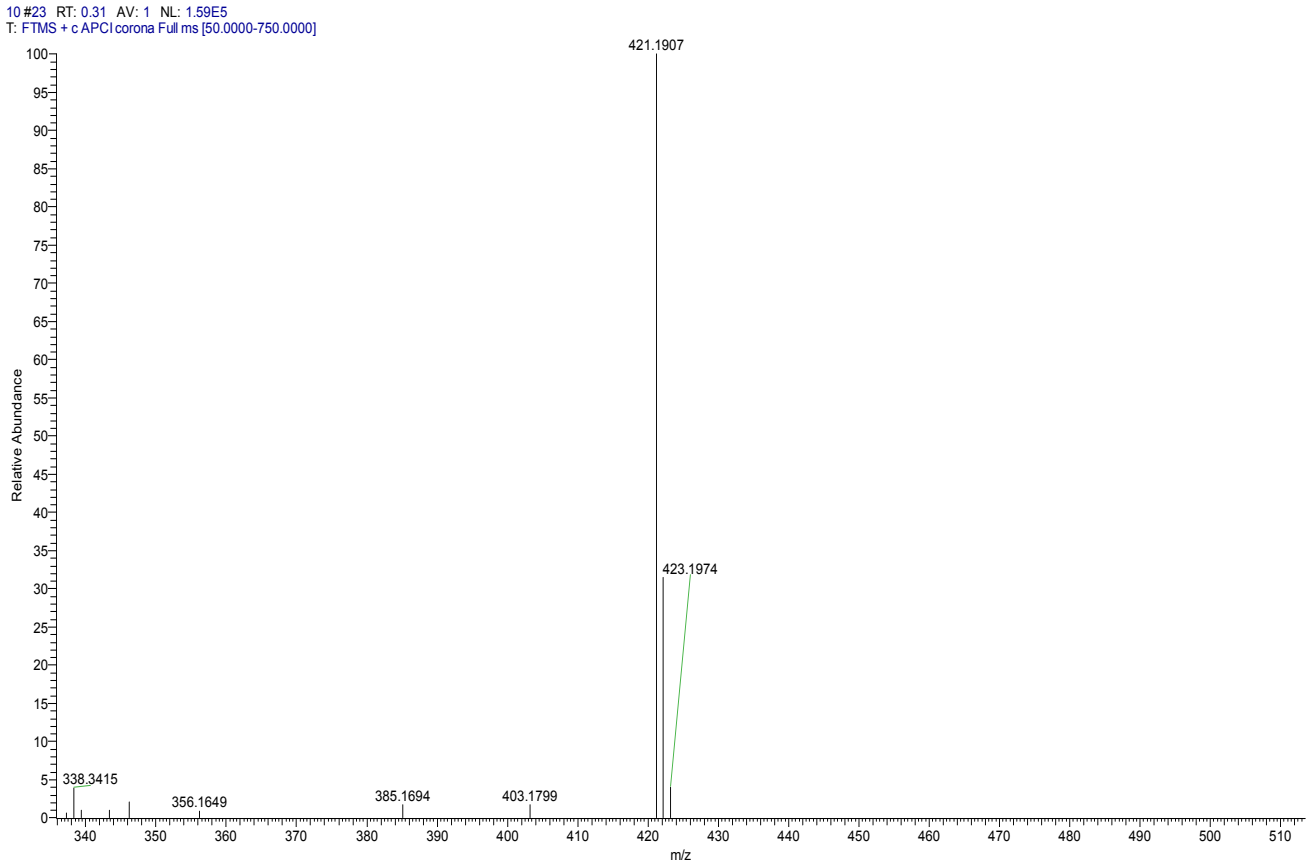

Figure S104. HRMS spectra for **6b**.

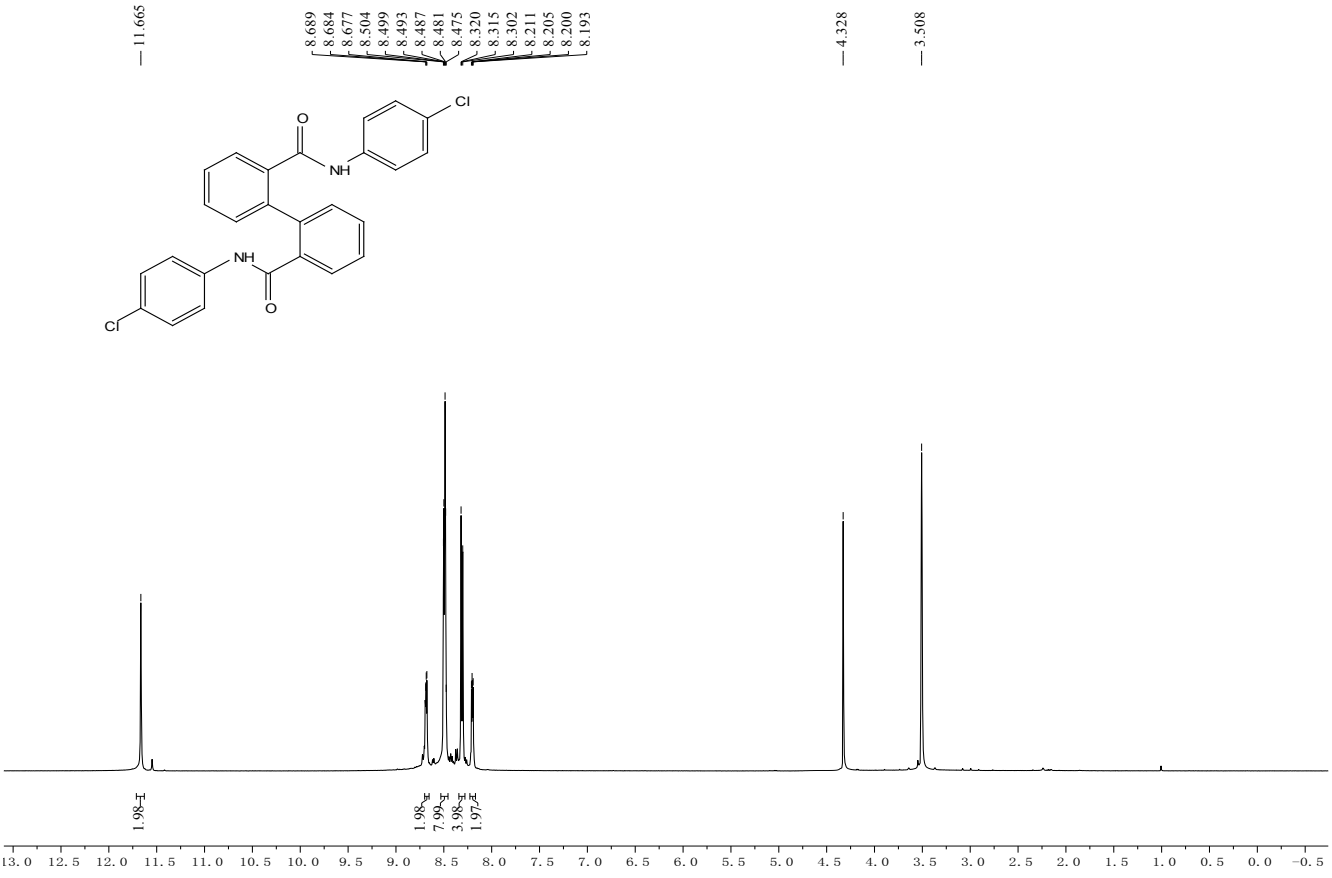

Figure S105. ^{1}H NMR (500 MHz) of **6c** in DMSO-d_6.

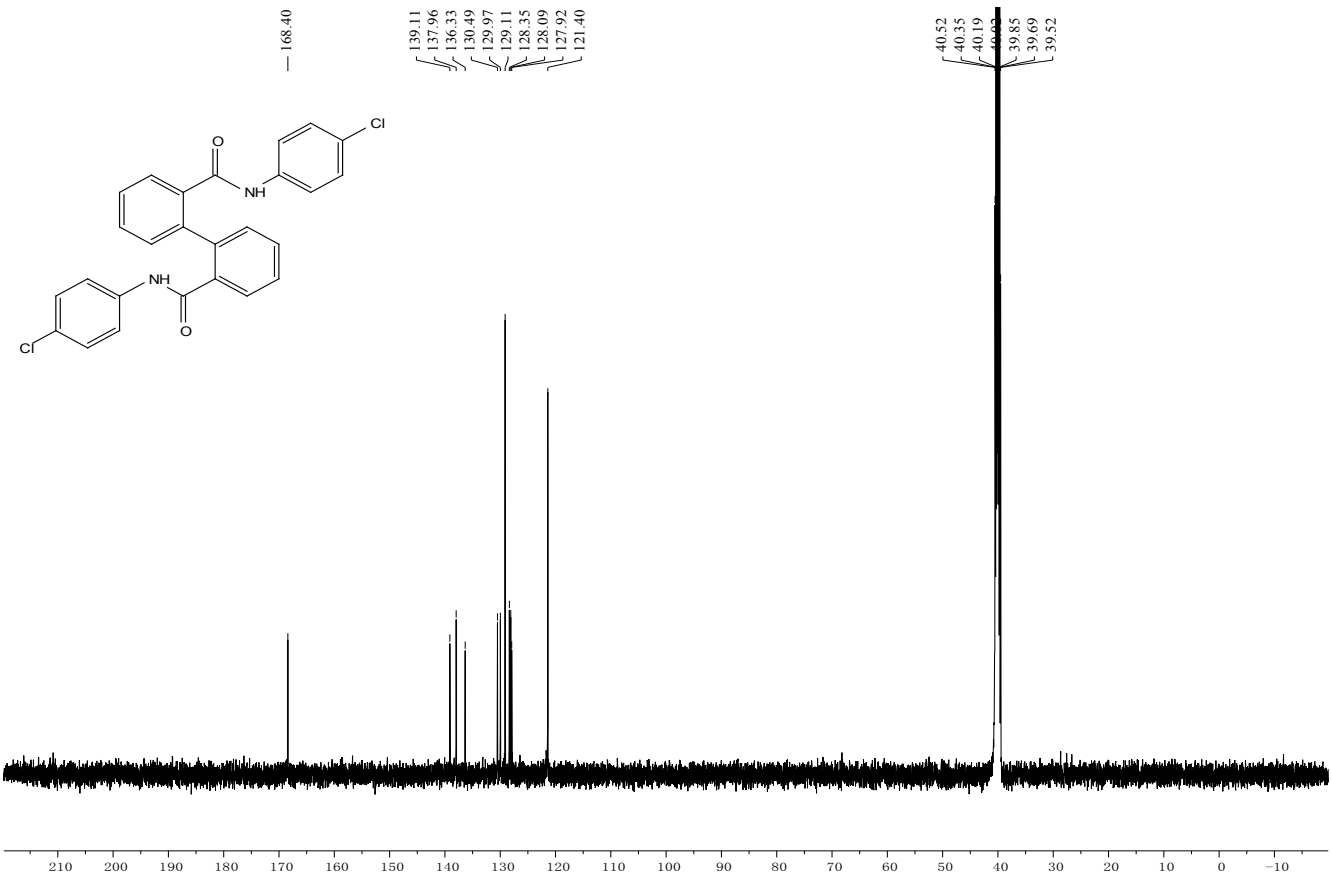

Figure S106. ^{13}C NMR (126 MHz) of **6c** in DMSO-d_6.

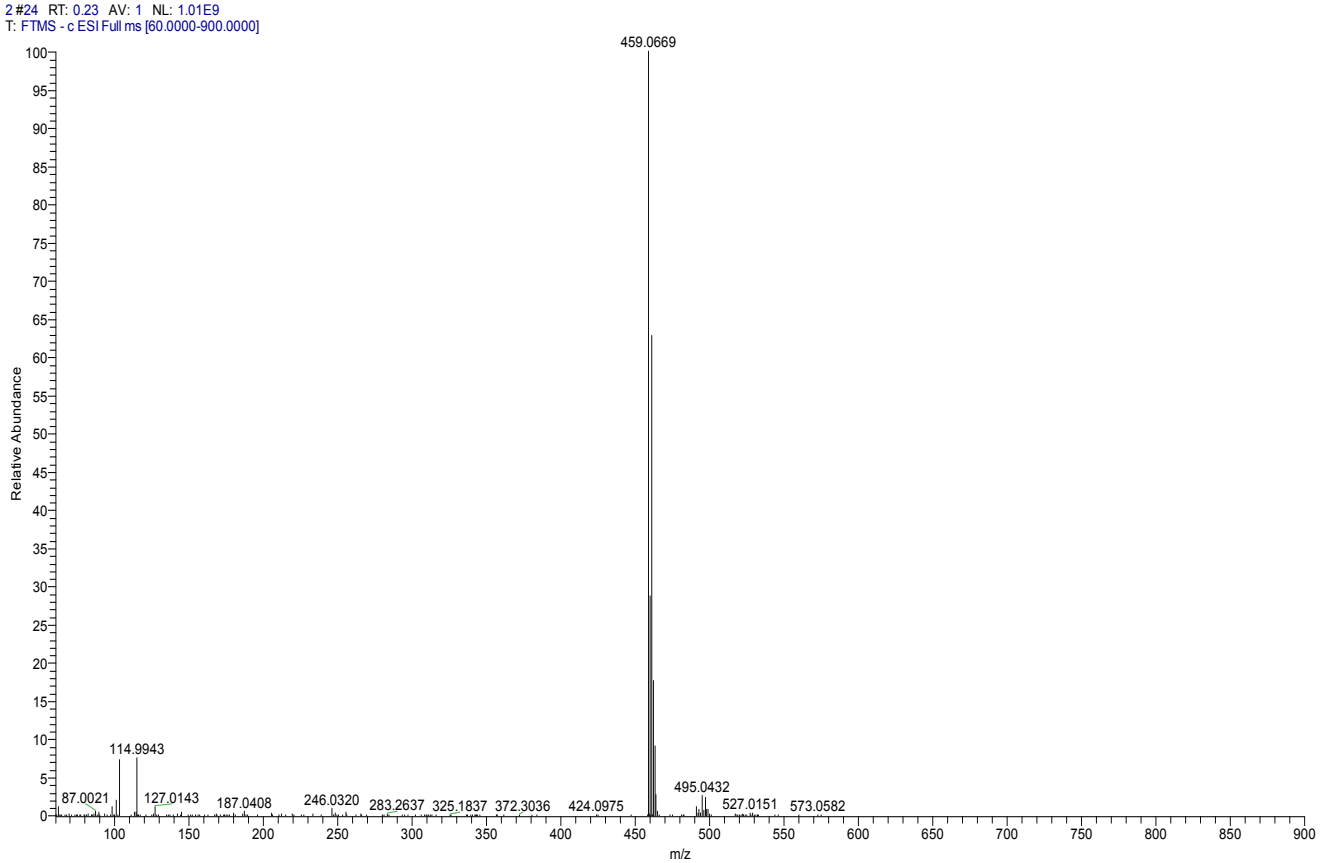

Figure S107. HRMS spectra for **6c**.

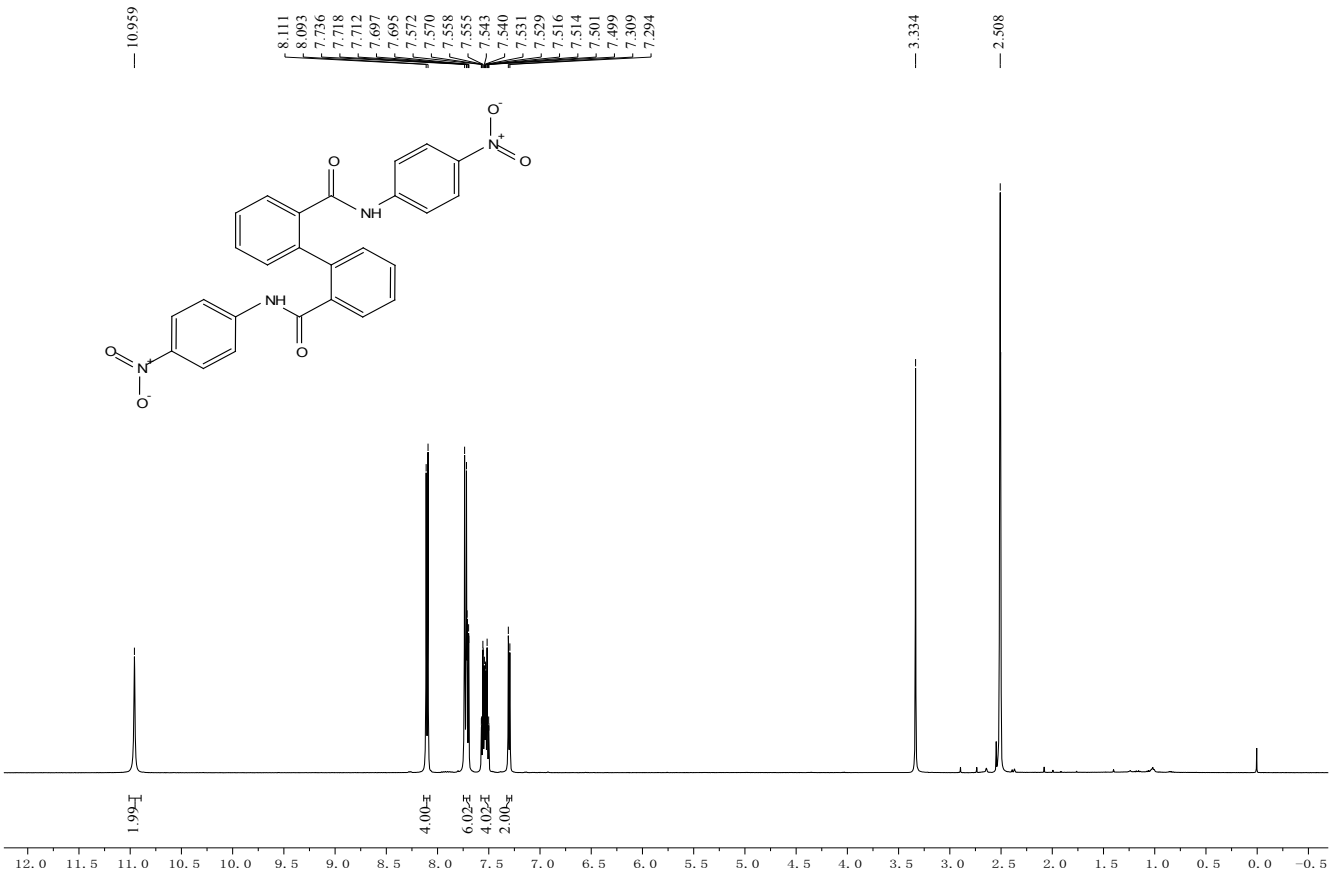

Figure S108. ^{1}H NMR (500 MHz) of **6d** in DMSO-d_6.

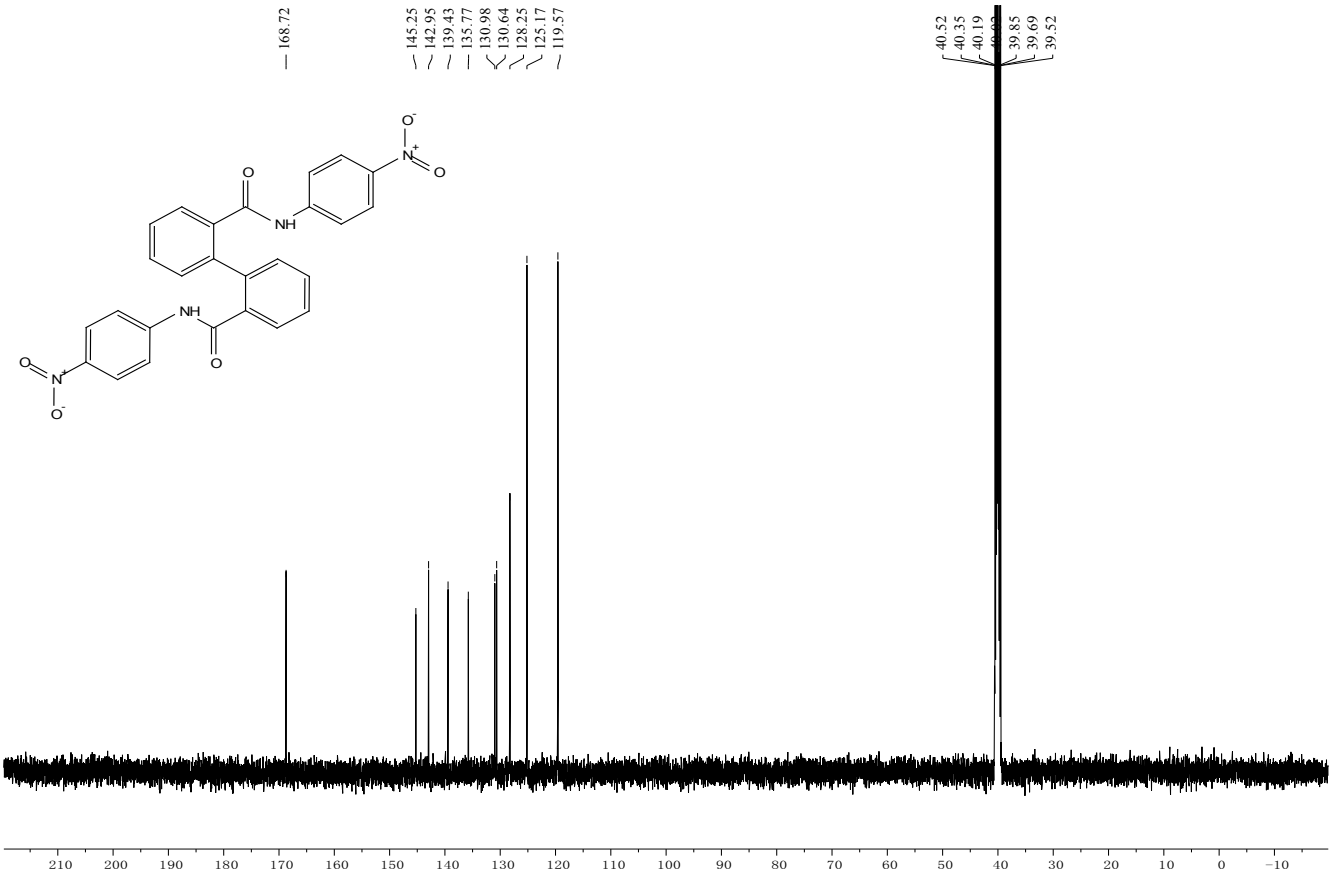

Figure S109. ^{13}C NMR (126 MHz) of **6d** in DMSO-d_6.

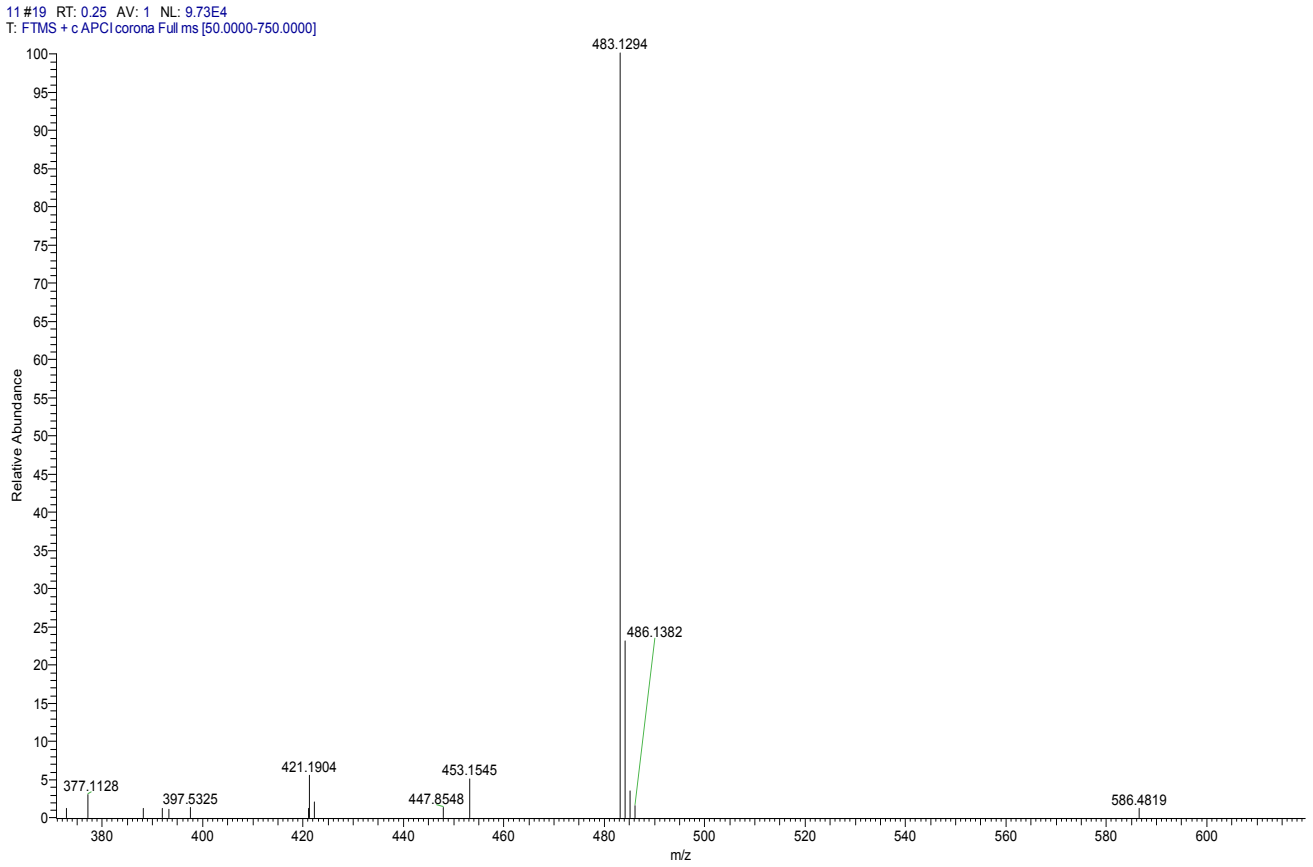

Figure S110. HRMS spectra for **6d**.

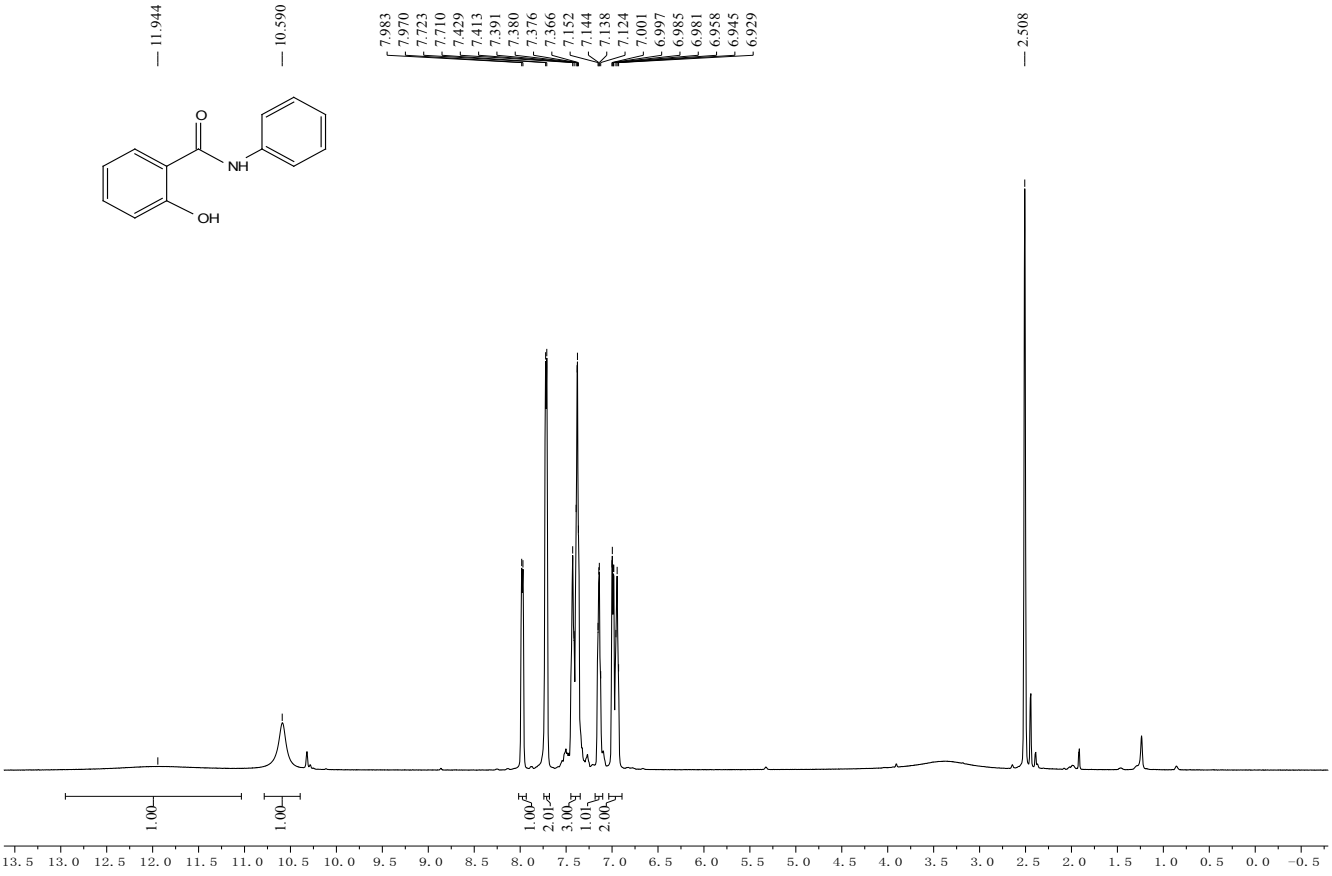

Figure S111. ^{1}H NMR (500 MHz) of **7a** in DMSO-d_6.

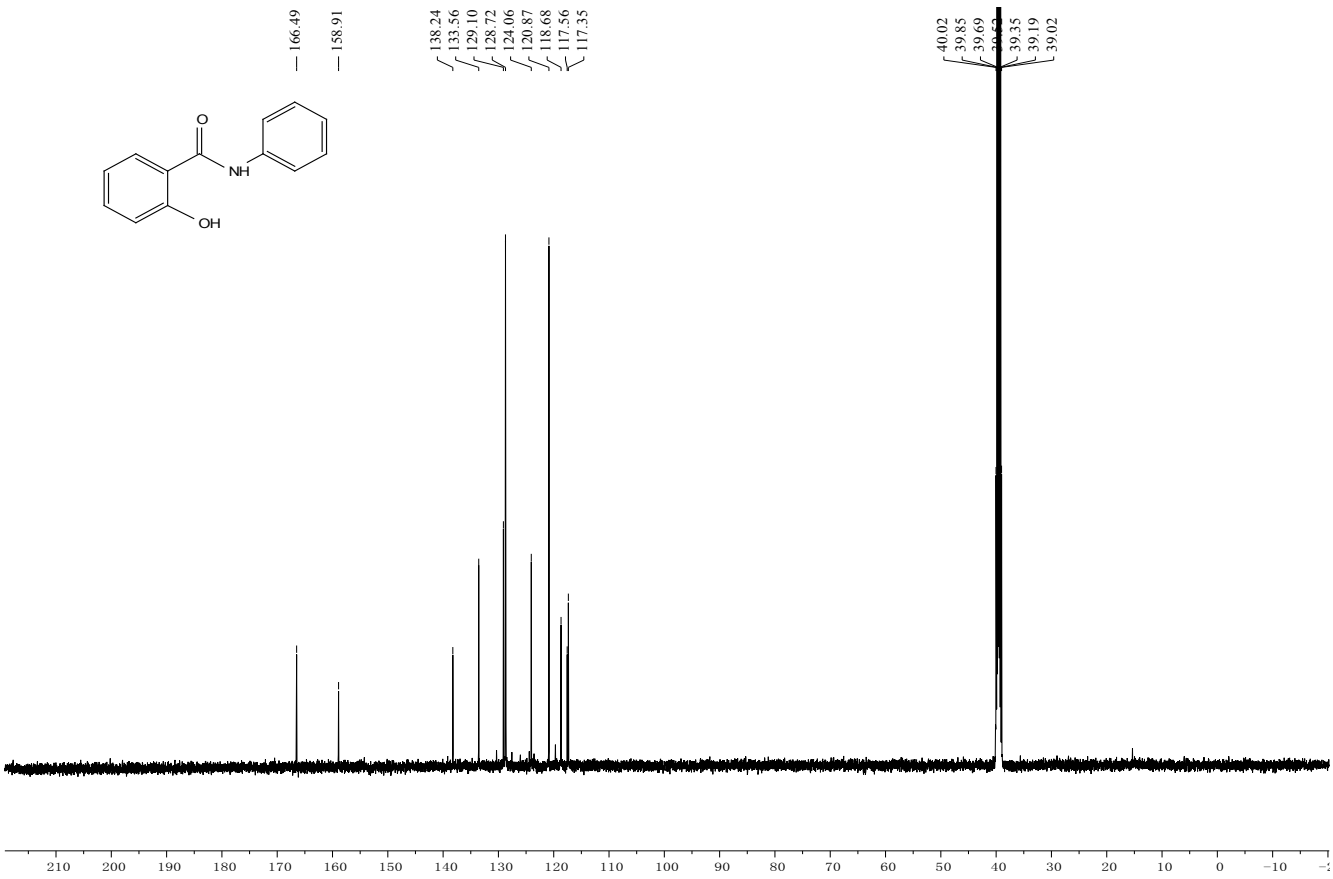

Figure S112. ^{13}C NMR (126 MHz) of **7a** in DMSO-d_6.

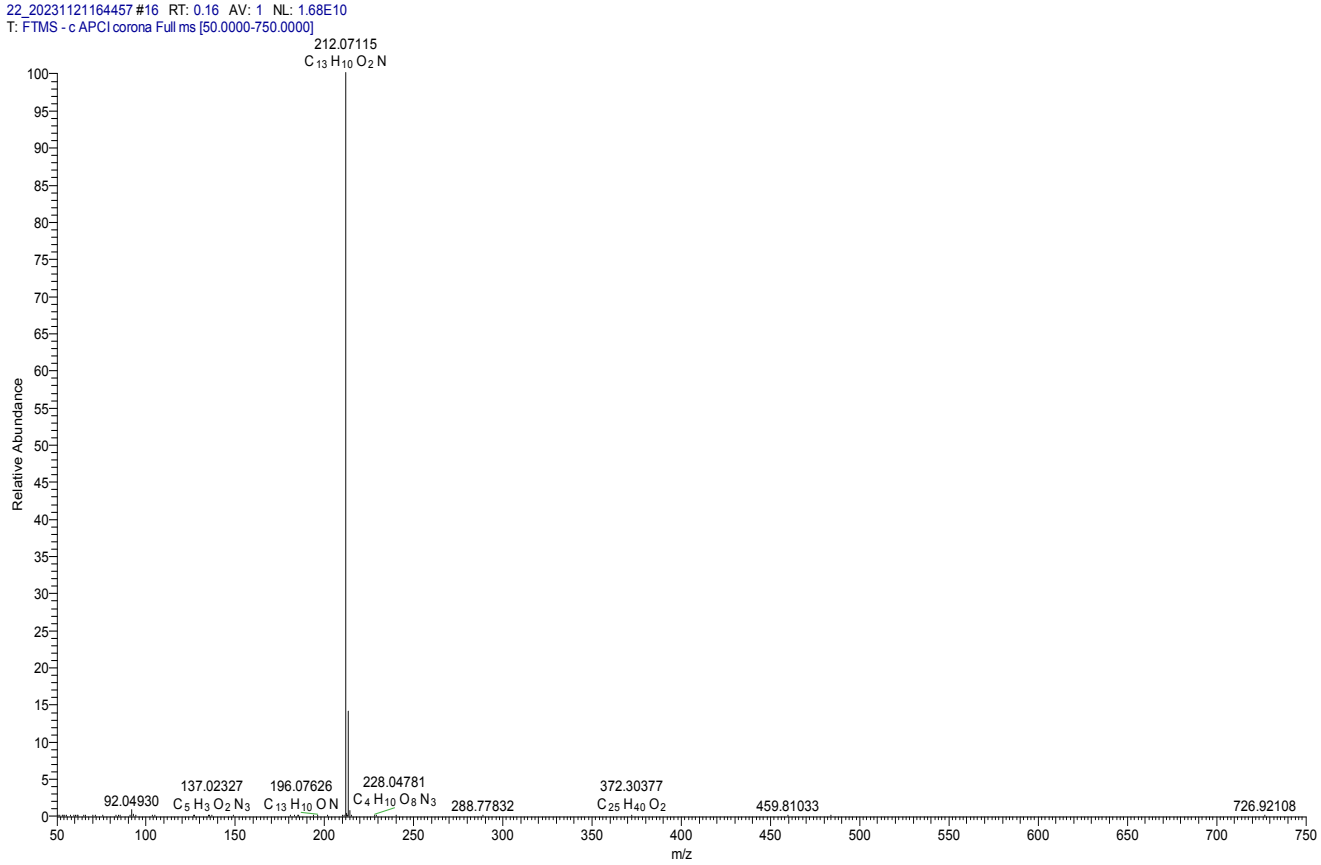

Figure S113. HRMS spectra for **7a'**.

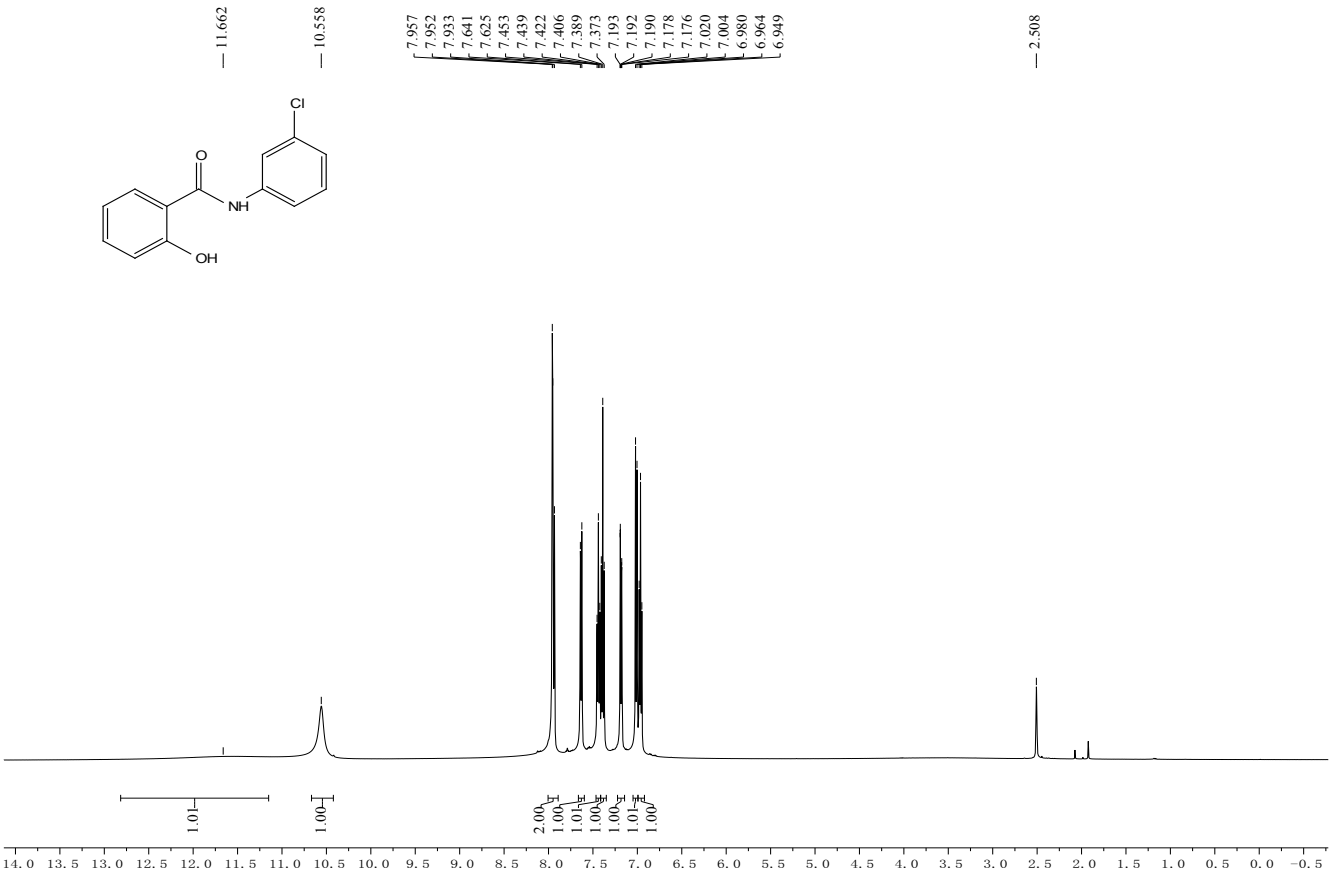

Figure S114. ^{1}H NMR (500 MHz) of **7e** in DMSO-d_6.

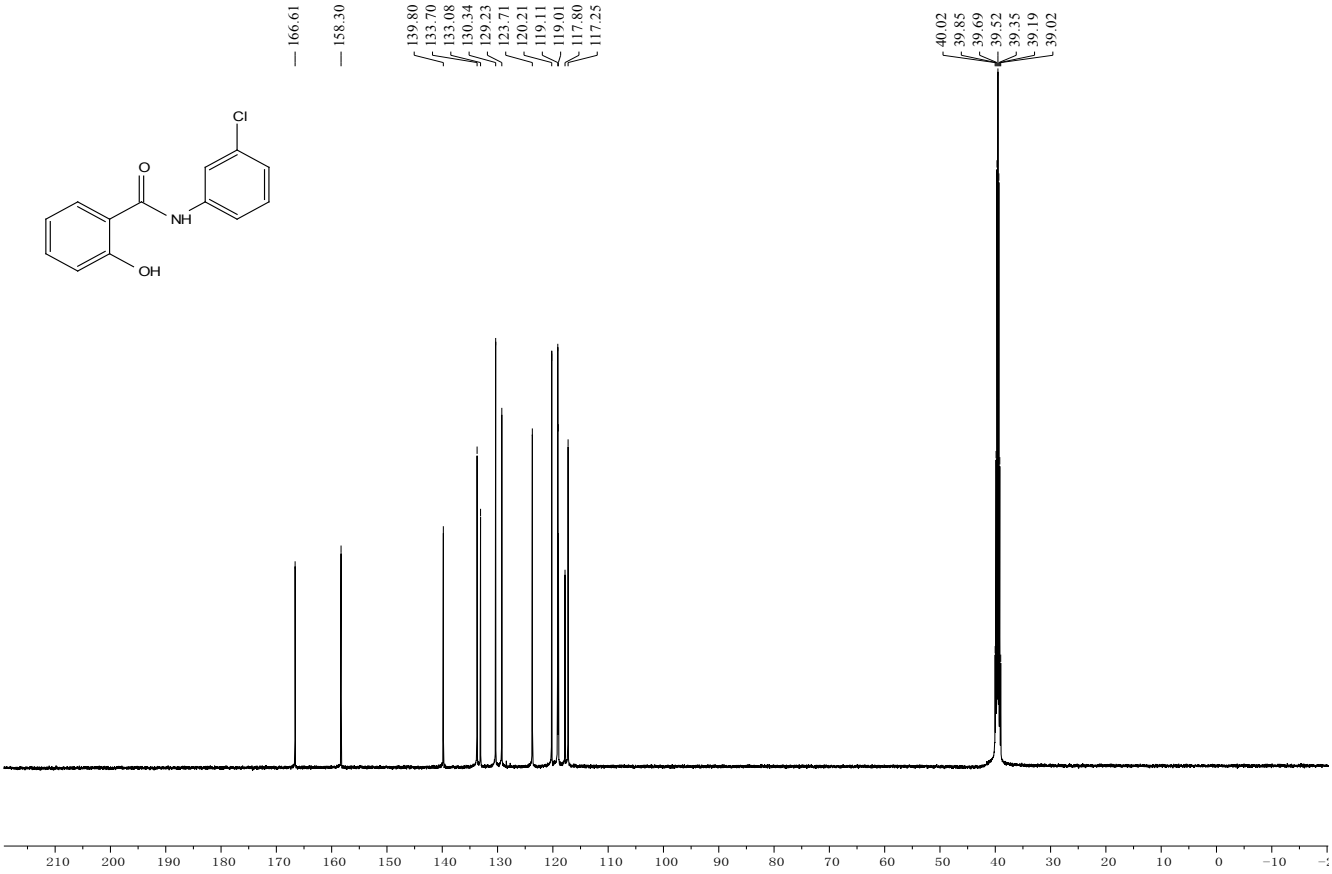

Figure S115. ^{13}C NMR (126 MHz) of **7e** in DMSO-d_6.

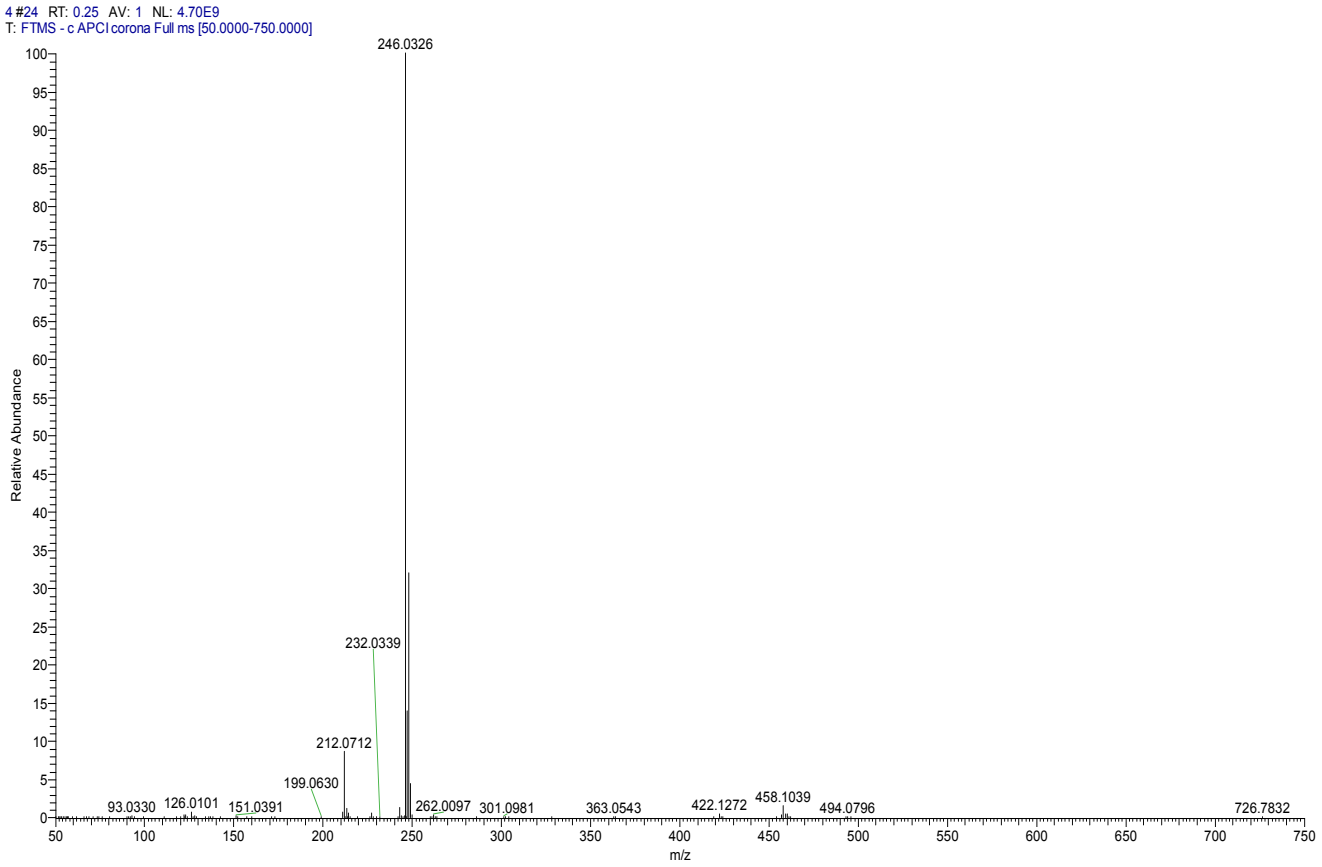

Figure S116. HRMS spectra for **7e**.

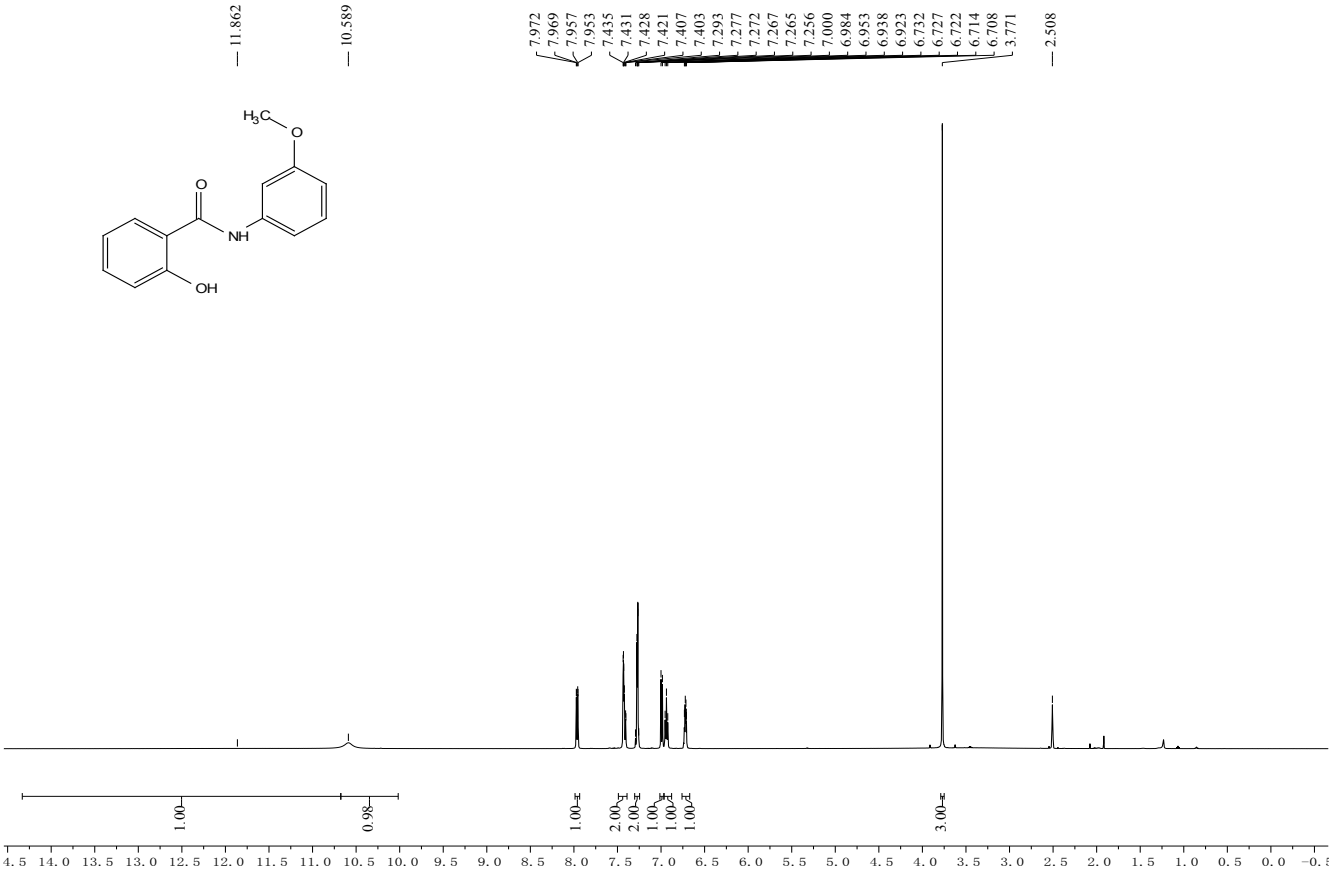

Figure S117. ^{1}H NMR (500 MHz) of **7f** in DMSO-d_6.

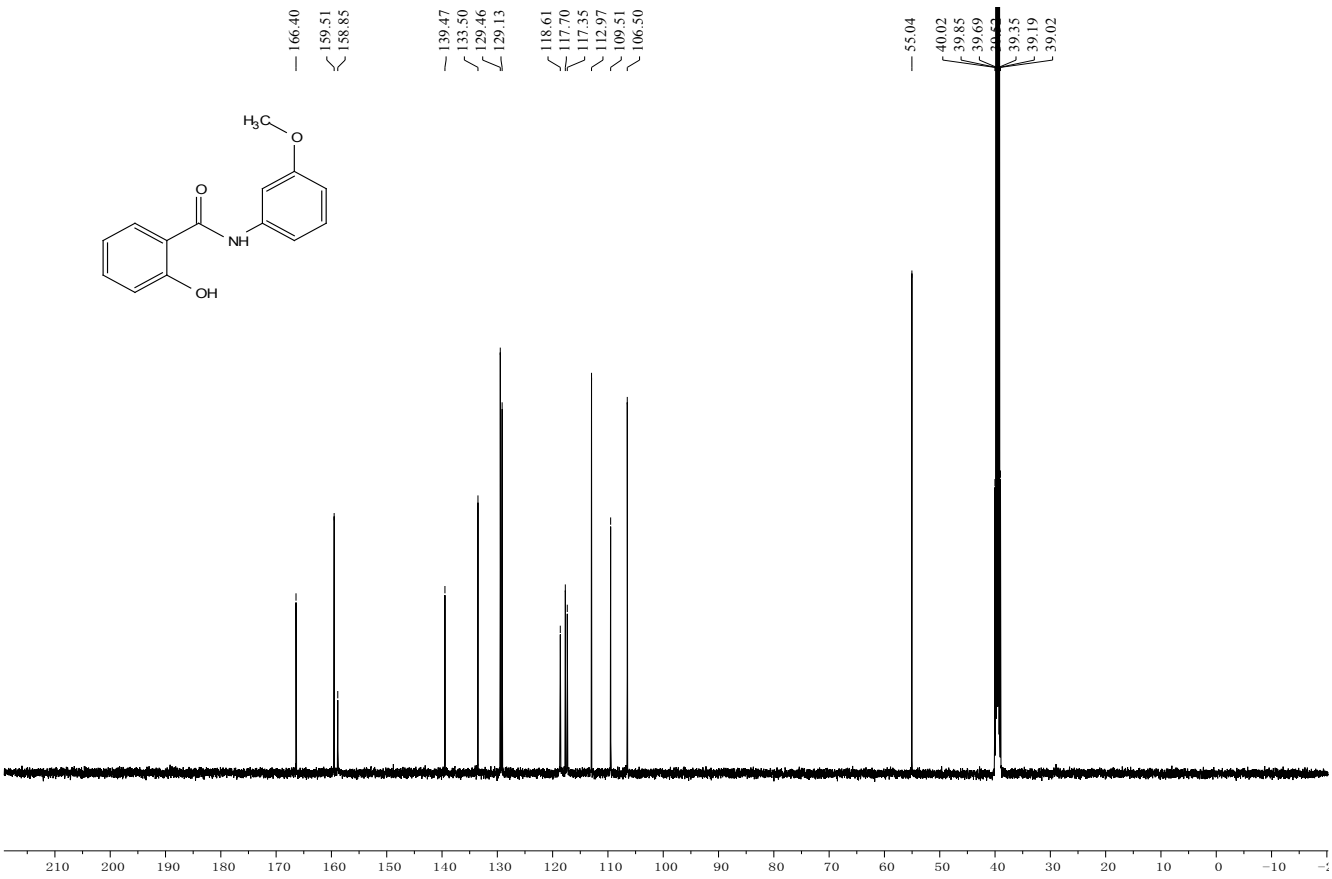

Figure S118. ^{13}C NMR (126 MHz) of **7f** in DMSO-d_6.

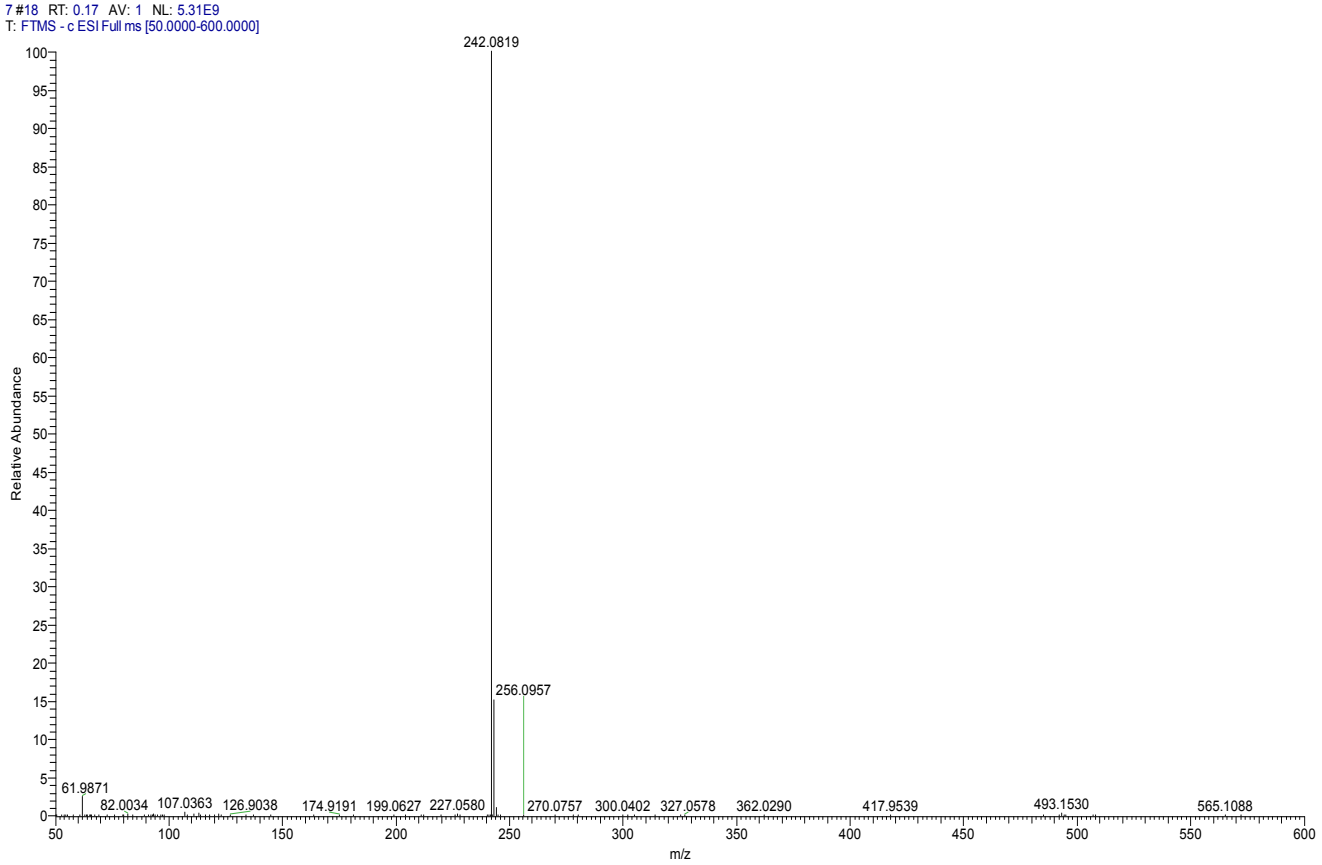

Figure S119. HRMS spectra for **7f**.

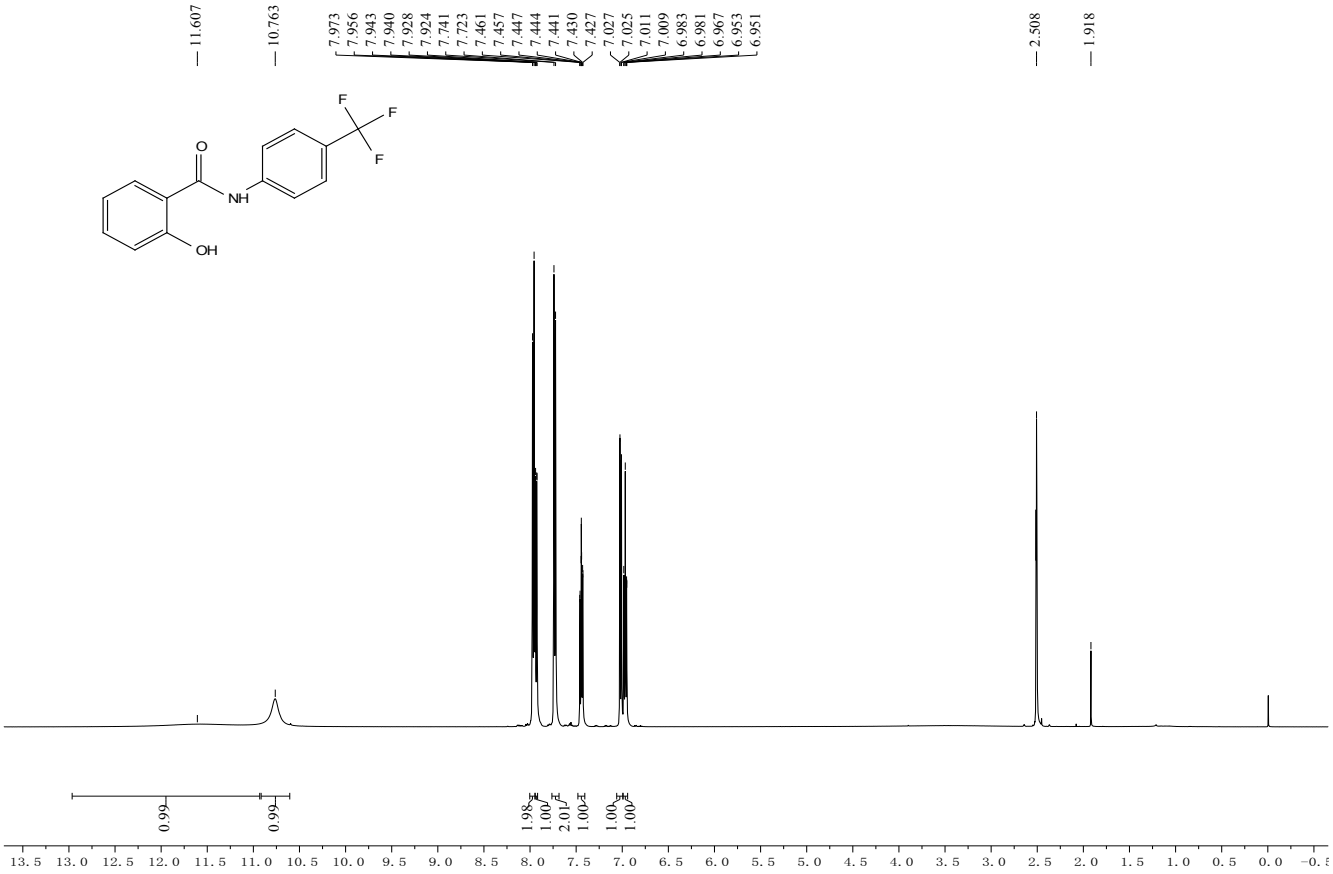

Figure S120. ^{1}H NMR (500 MHz) of **7g** in DMSO-d_6.

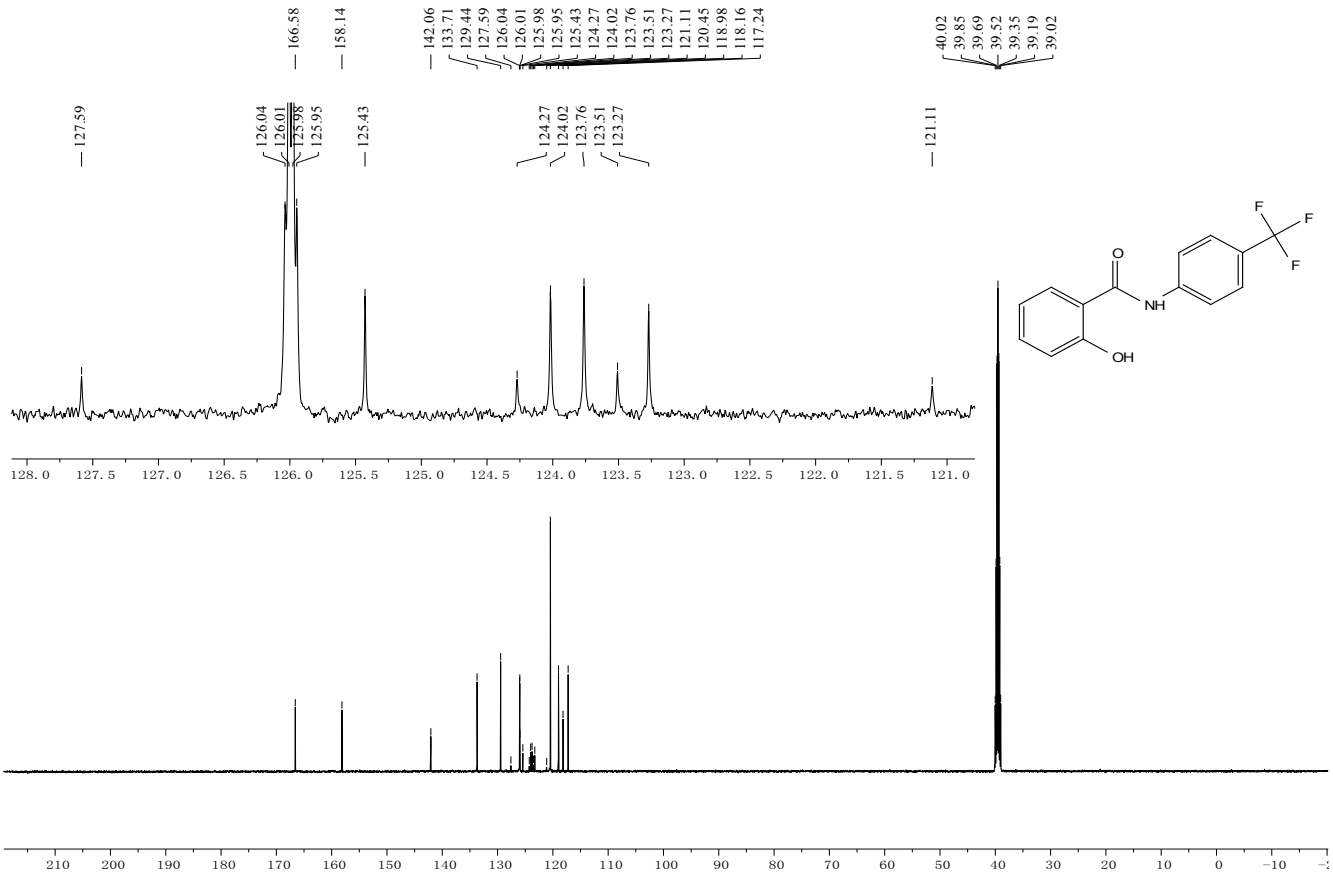

Figure S121. ^{13}C NMR (126 MHz) of **7g** in DMSO-d_6.

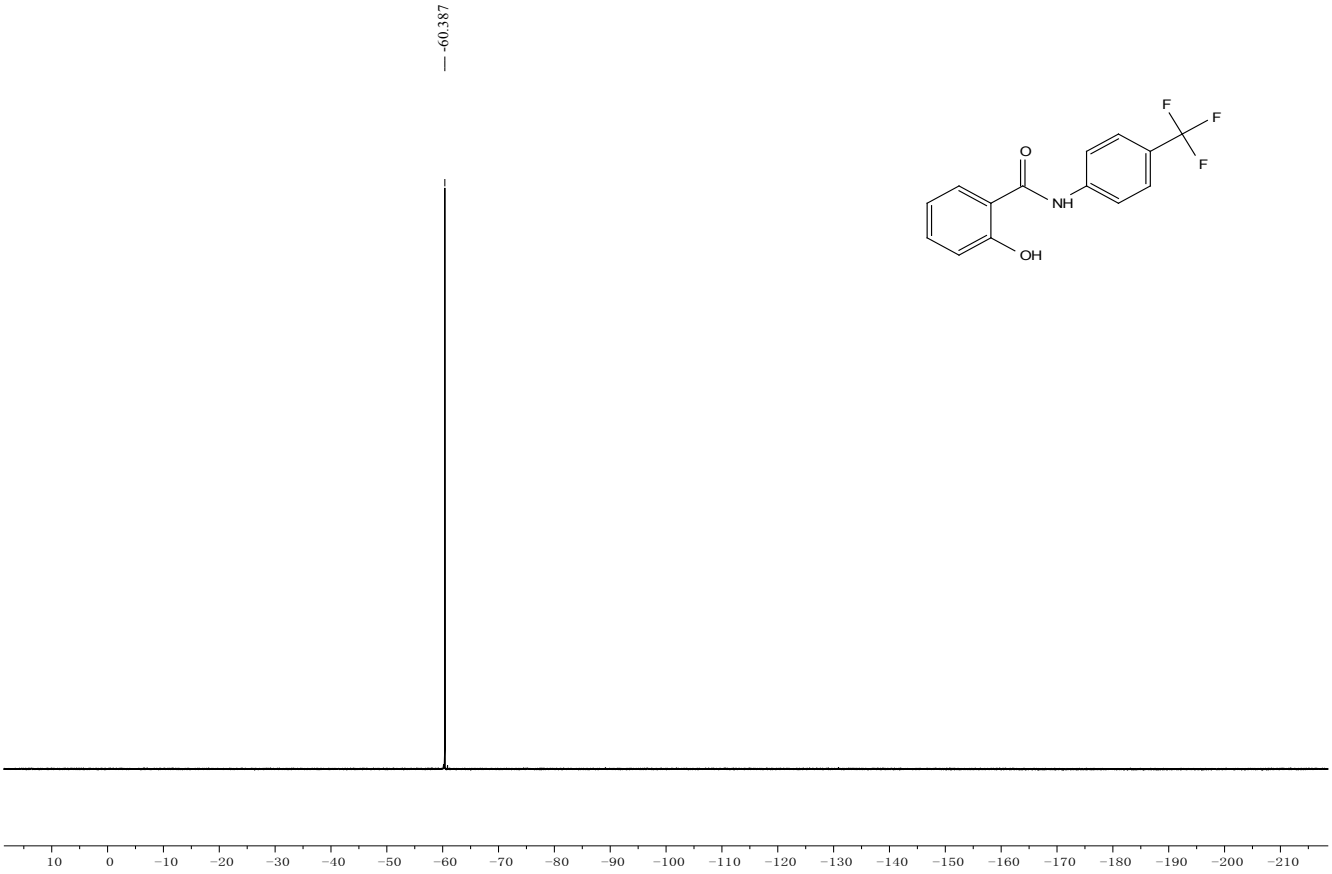

Figure S122. ^{19}F NMR (376 MHz) of **7g** in DMSO-d_6.

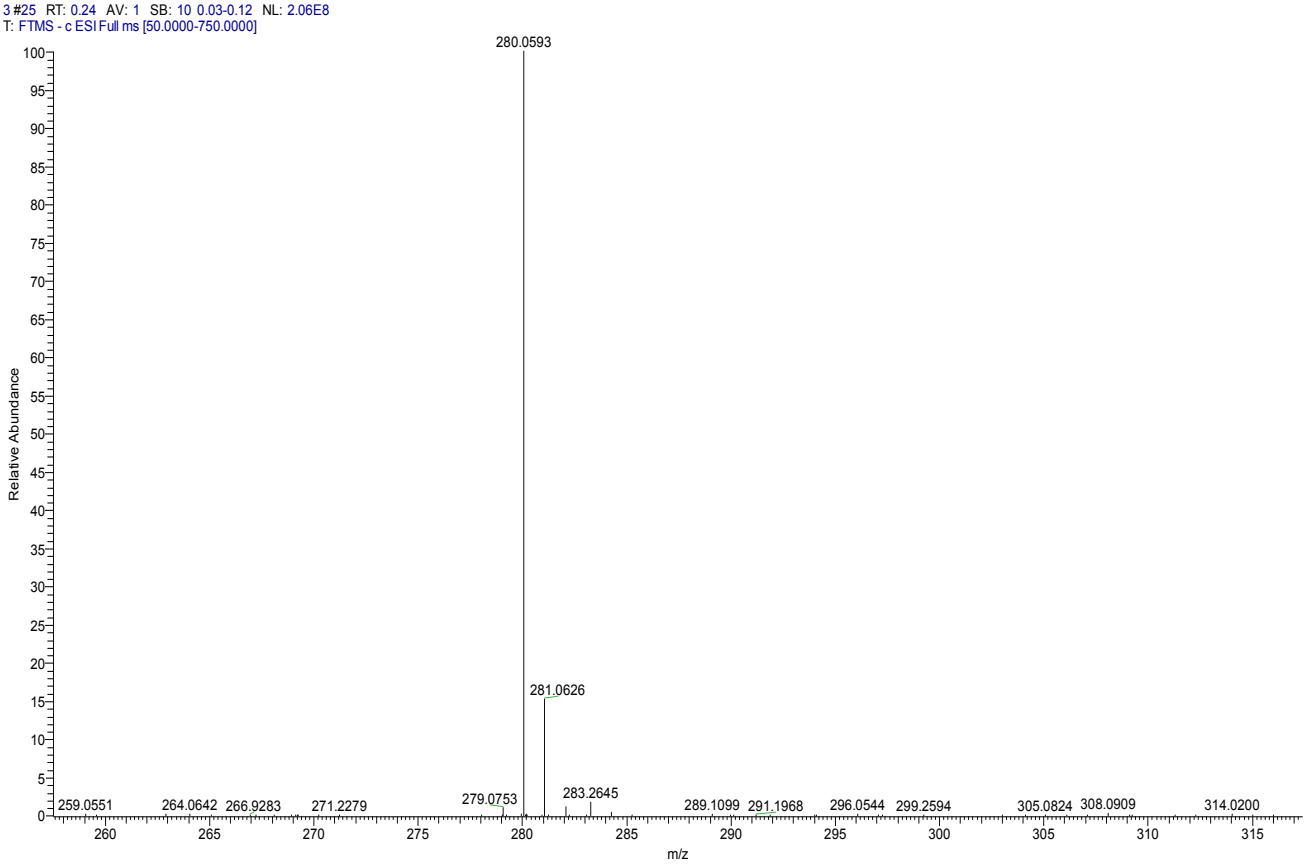

Figure S123. HRMS spectra for **7g**.

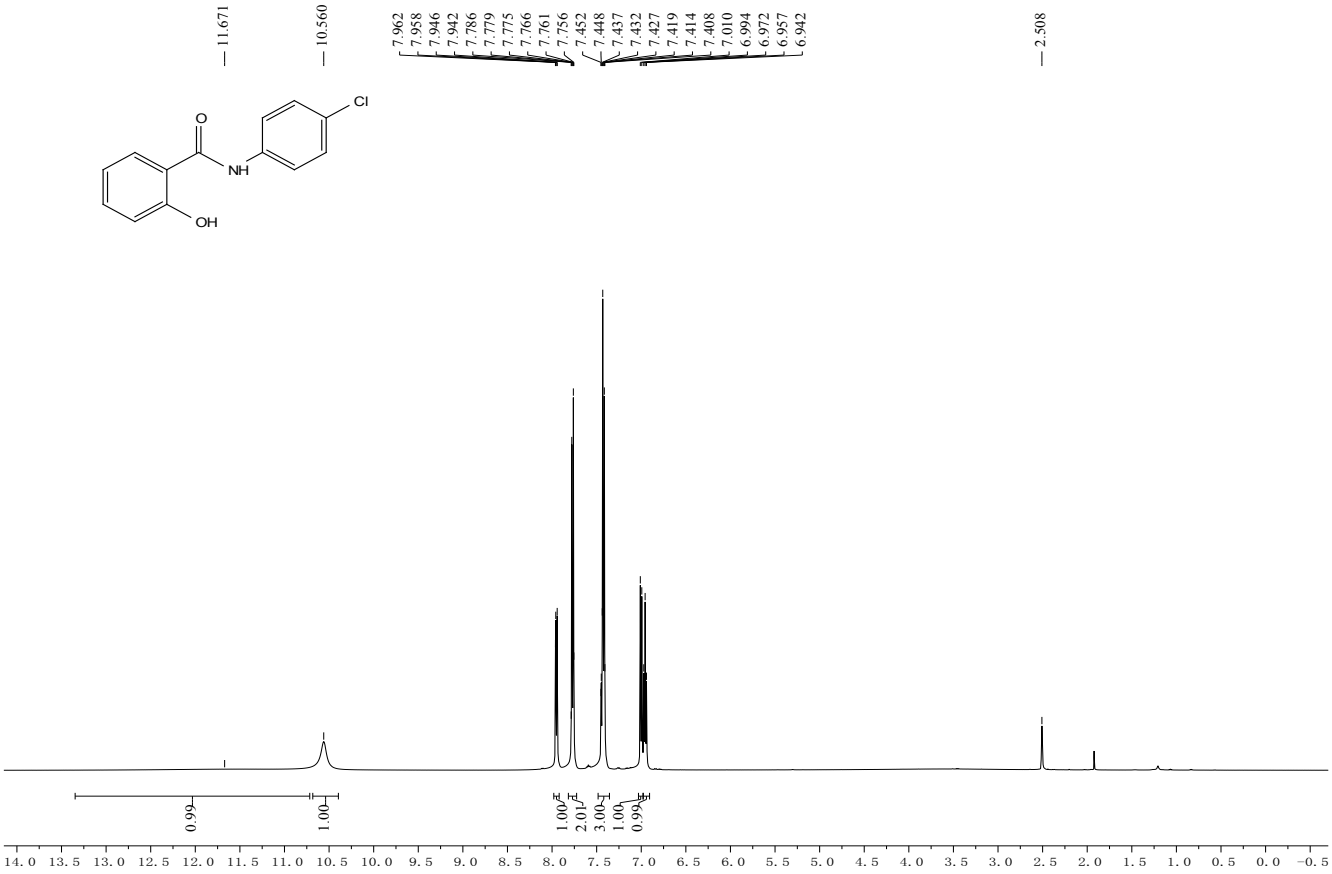

Figure S124. ^{1}H NMR (500 MHz) of **7h** in DMSO-d_6.

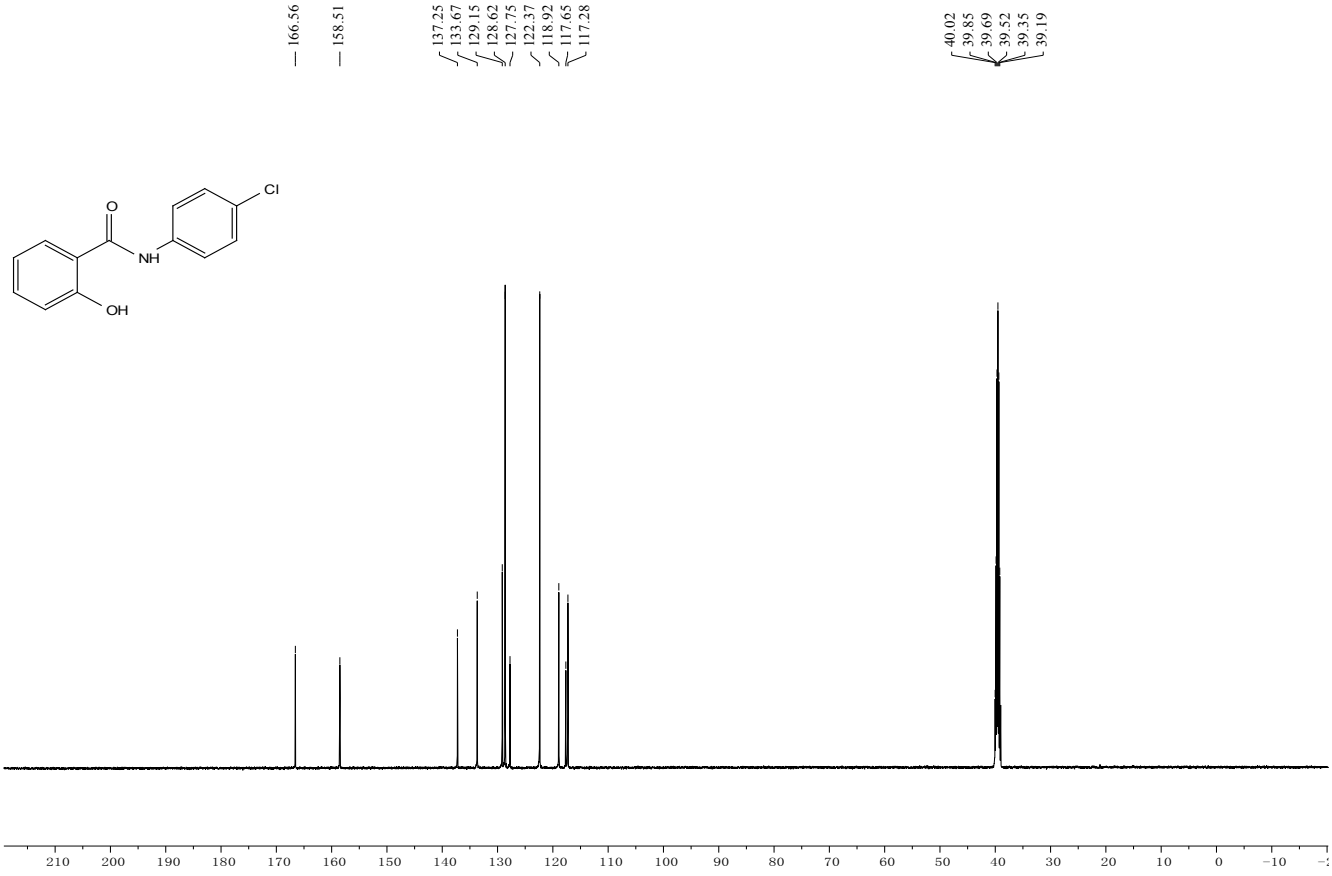

Figure S125. ^{13}C NMR (126 MHz) of **7h** in DMSO-d_6.

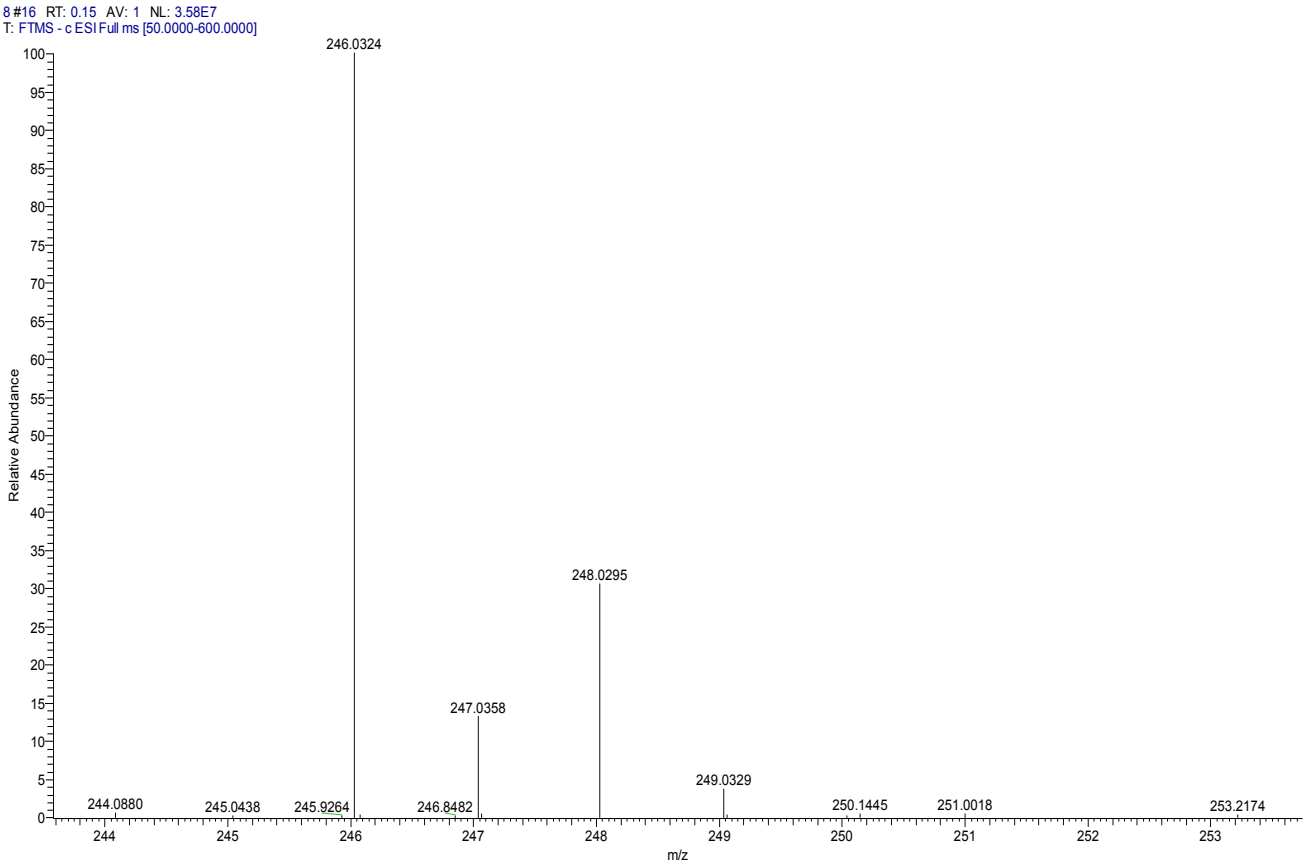

Figure S126. HRMS spectra for **7h**.

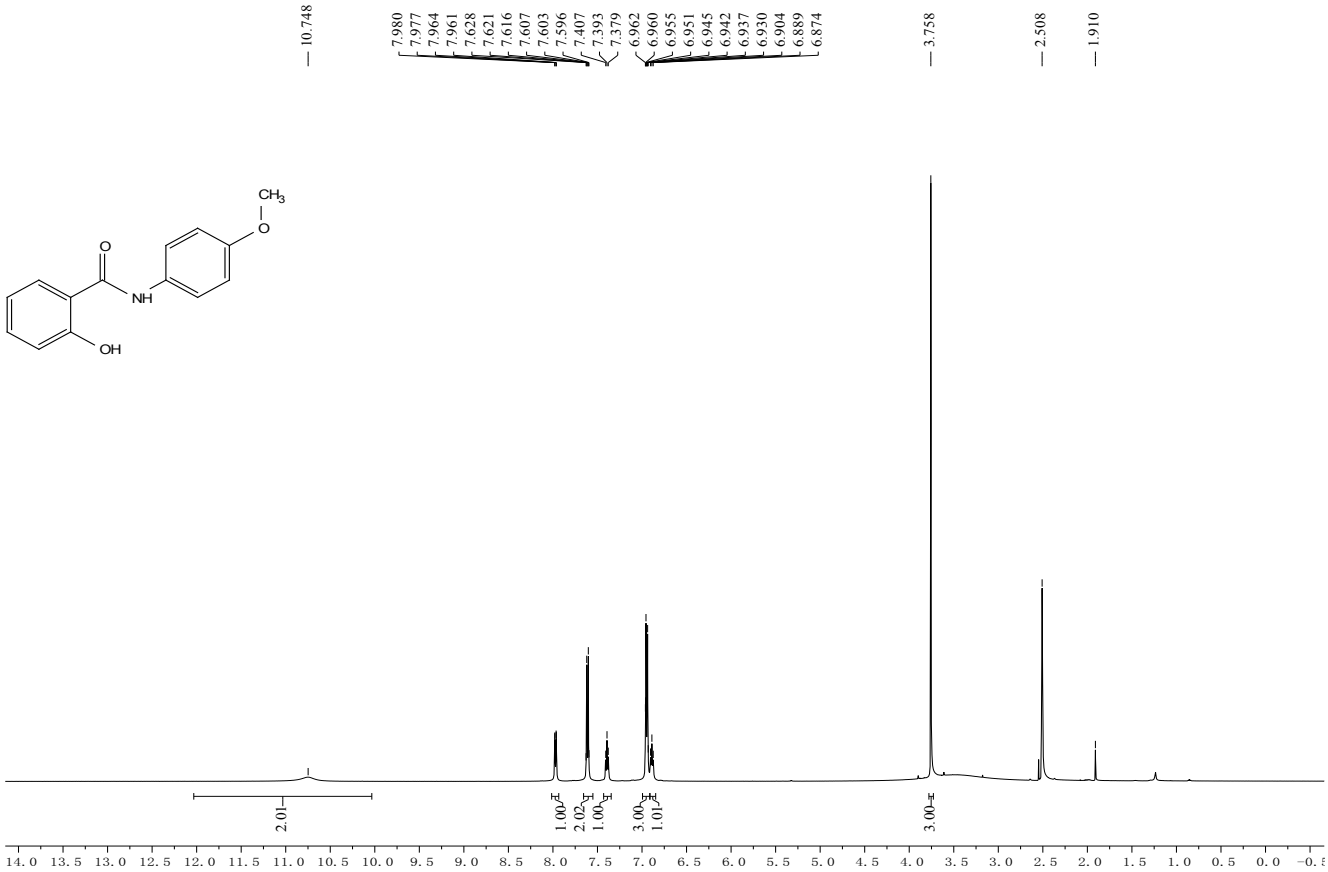

Figure S127. ^{1}H NMR (500 MHz) of **7i** in DMSO-d_6.

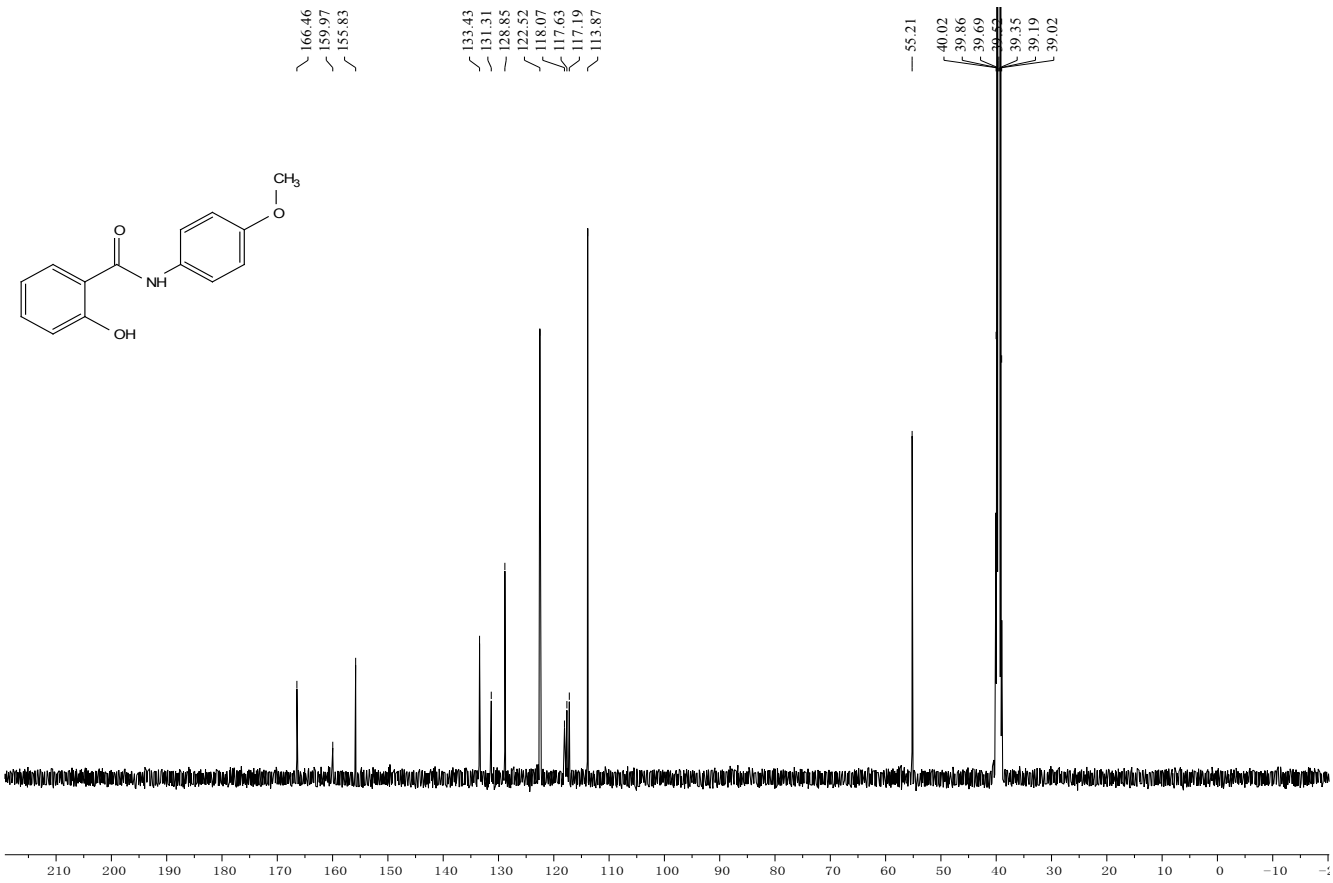

Figure S128. ^{13}C NMR (126 MHz) of **7i** in DMSO-d_6.

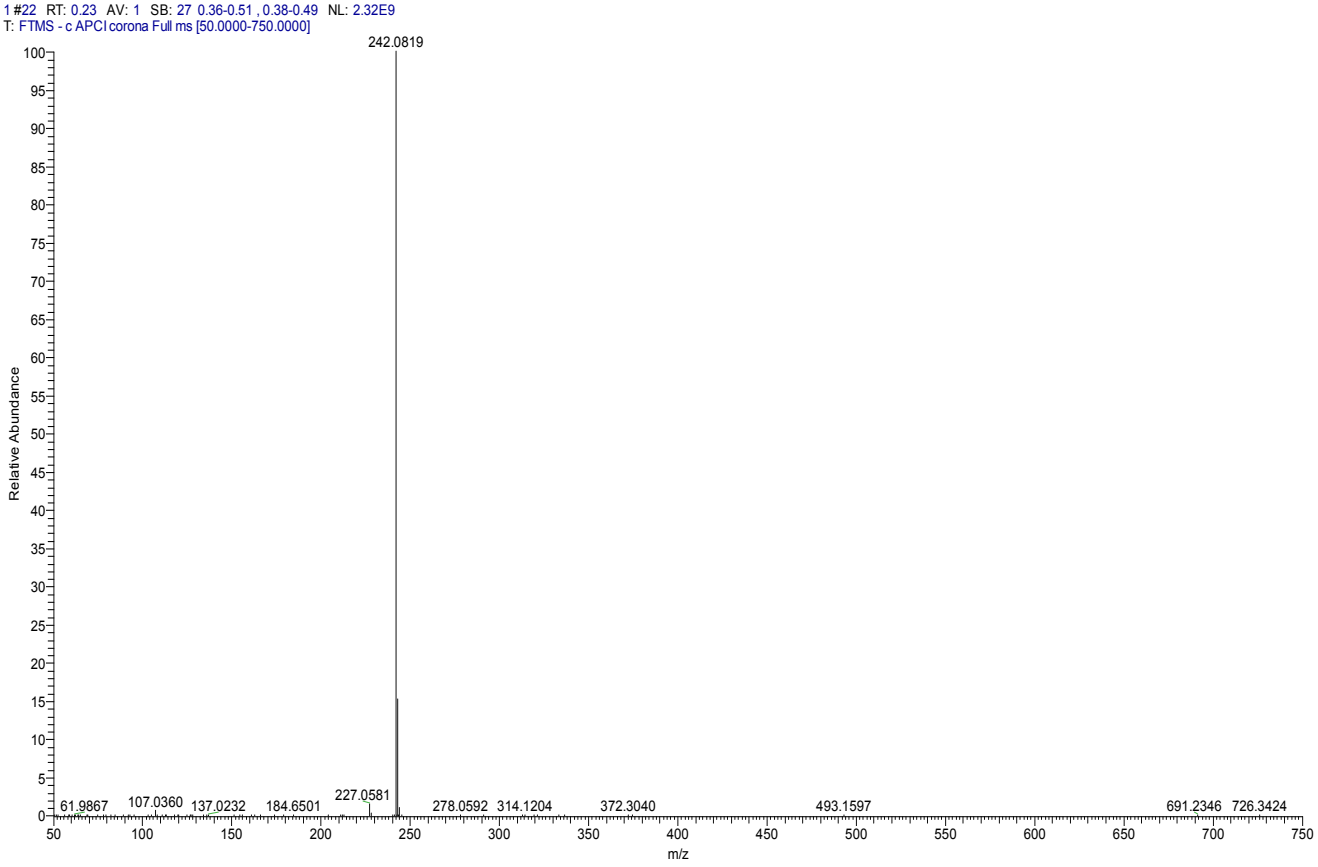

Figure S129. HRMS spectra for **7i**.

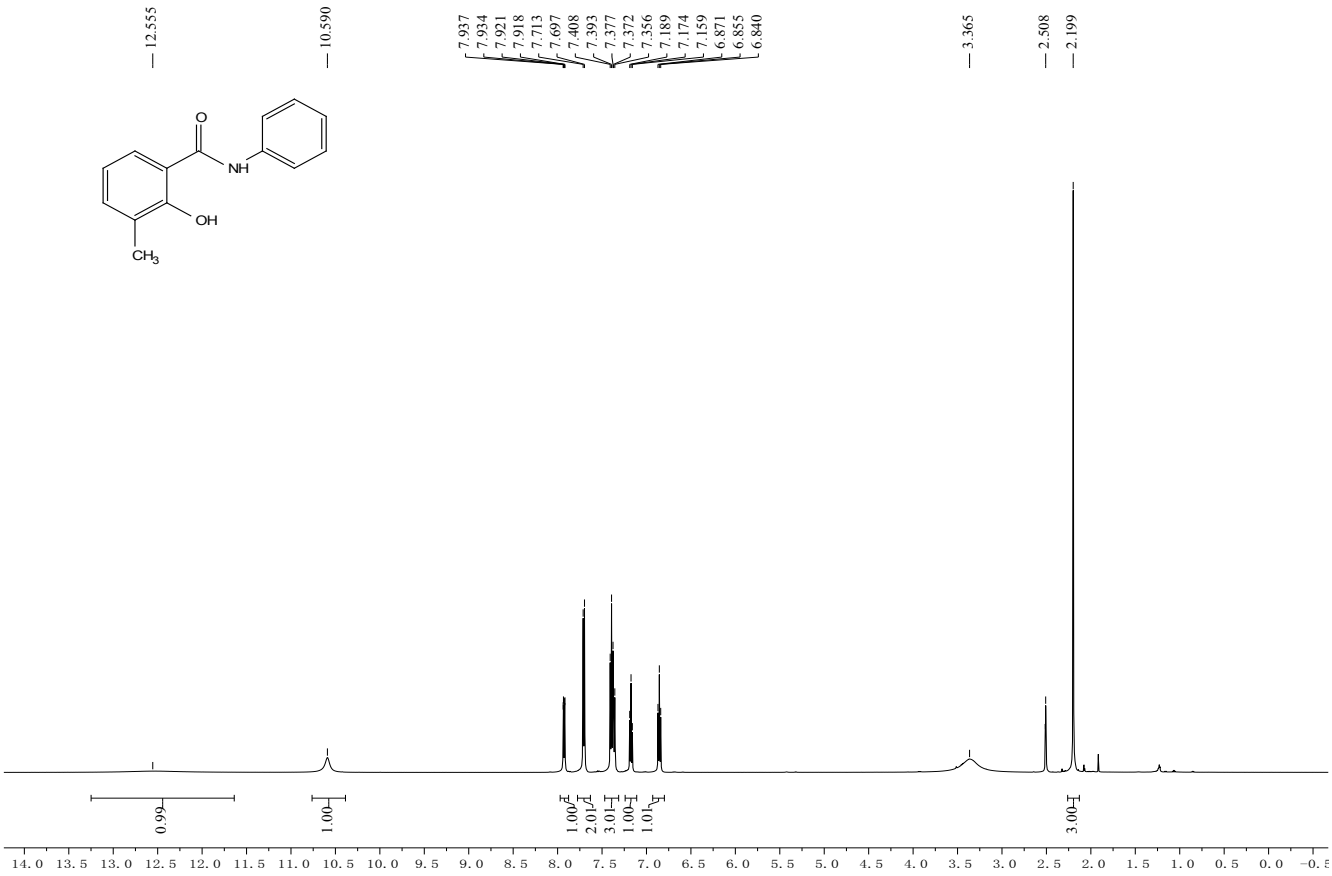

Figure S130. ^{1}H NMR (500 MHz) of **7j** in DMSO-d_6.

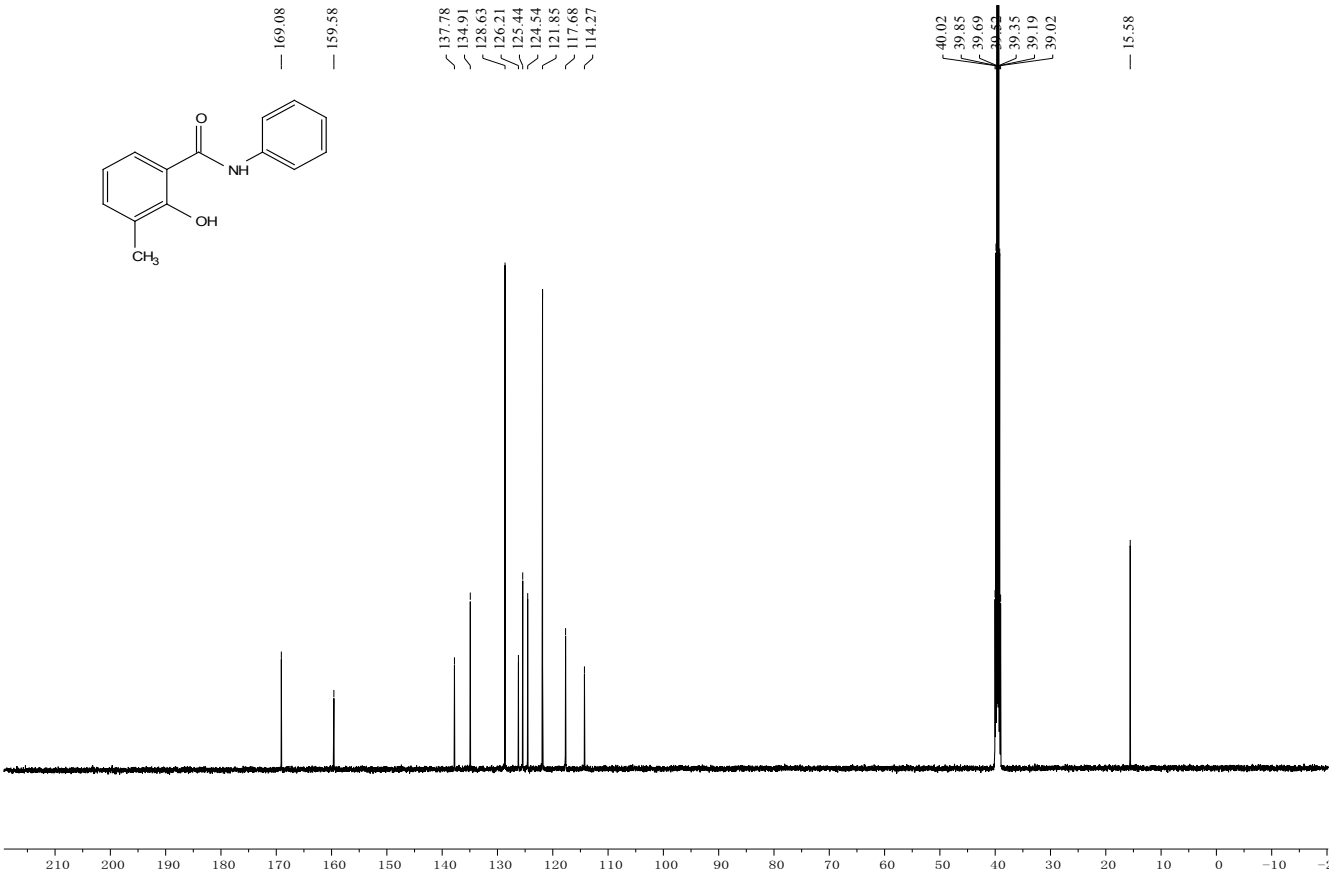

Figure S131. ^{13}C NMR (126 MHz) of **7j** in DMSO-d_6.

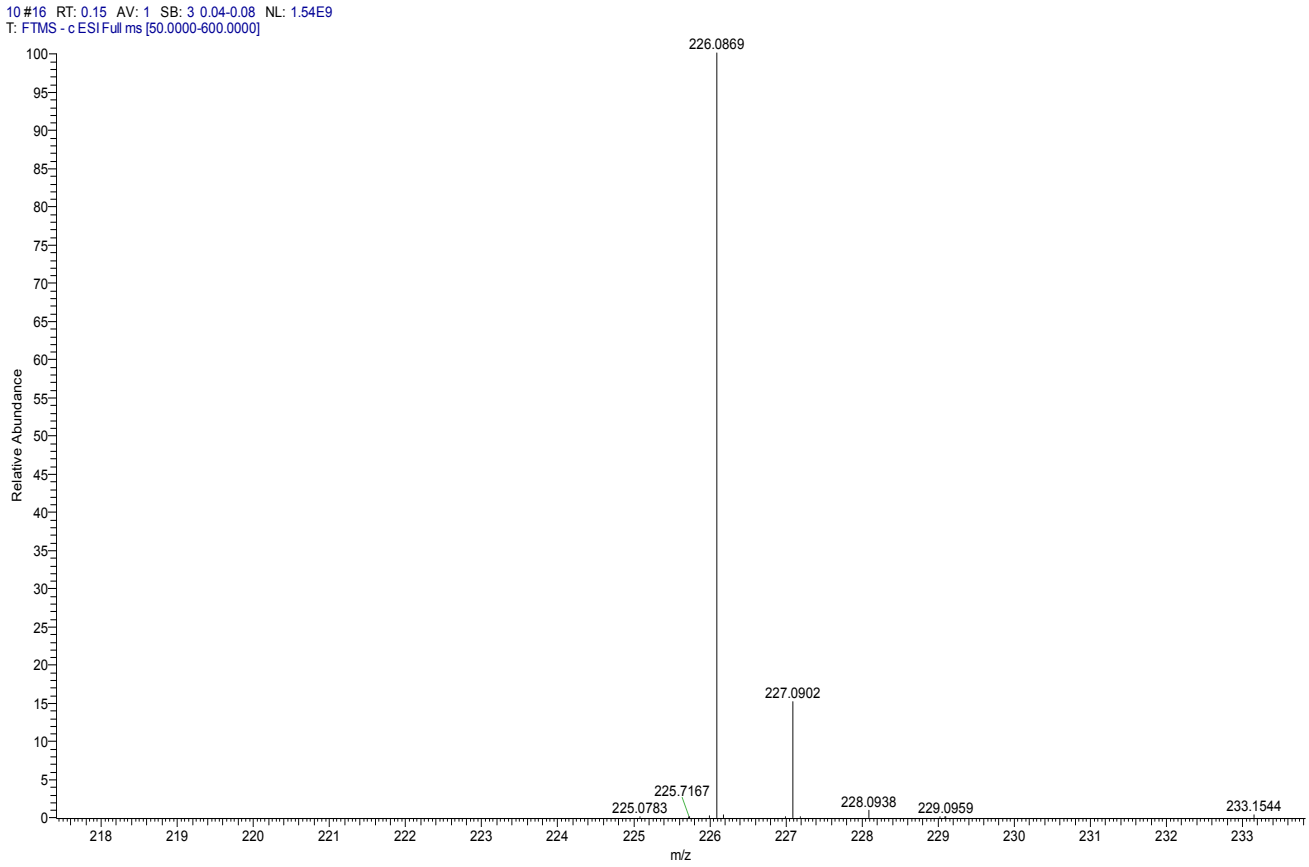

Figure S132. HRMS spectra for **7j**.

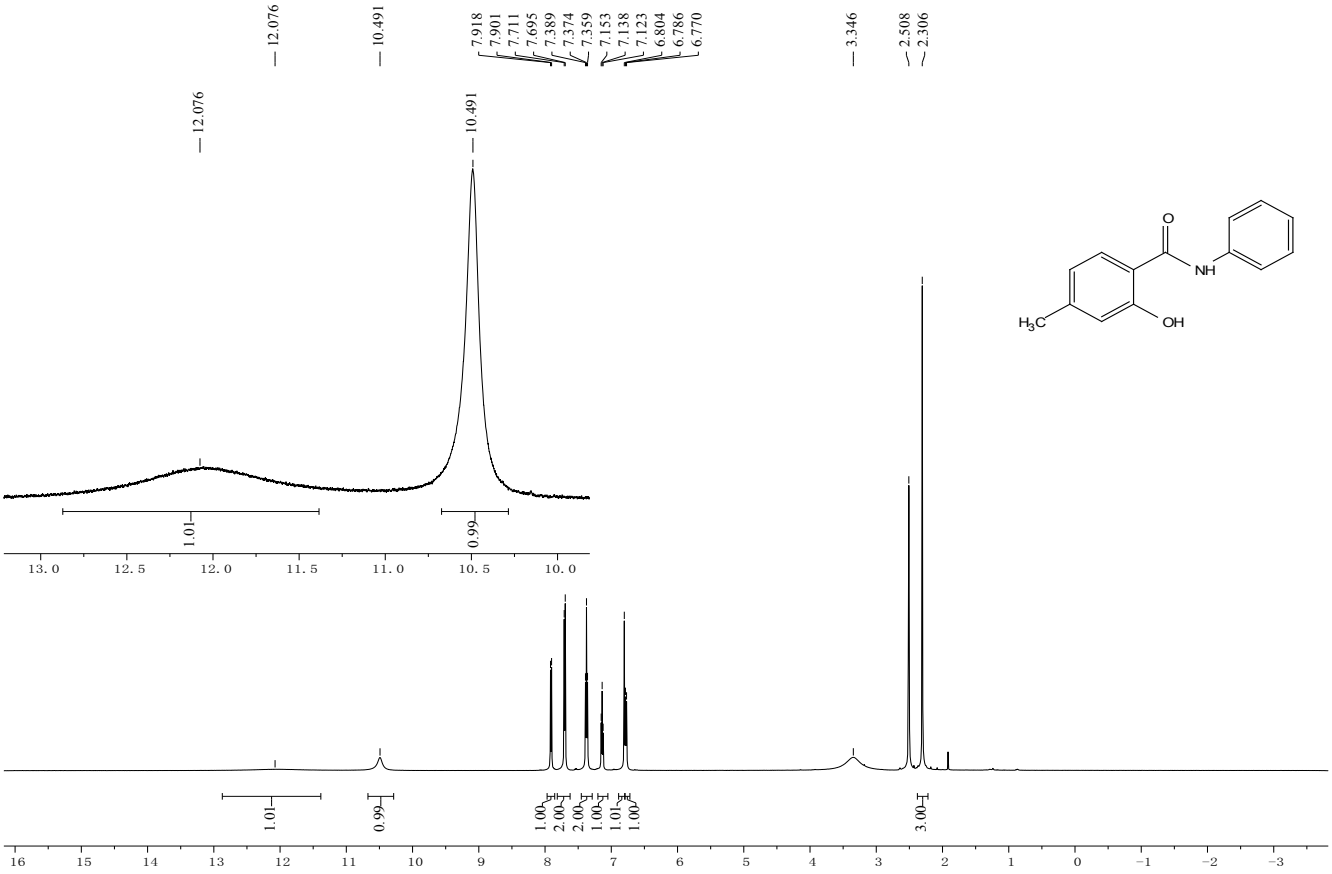

Figure S133. ^{1}H NMR (500 MHz) of **7k** in DMSO-d_6.

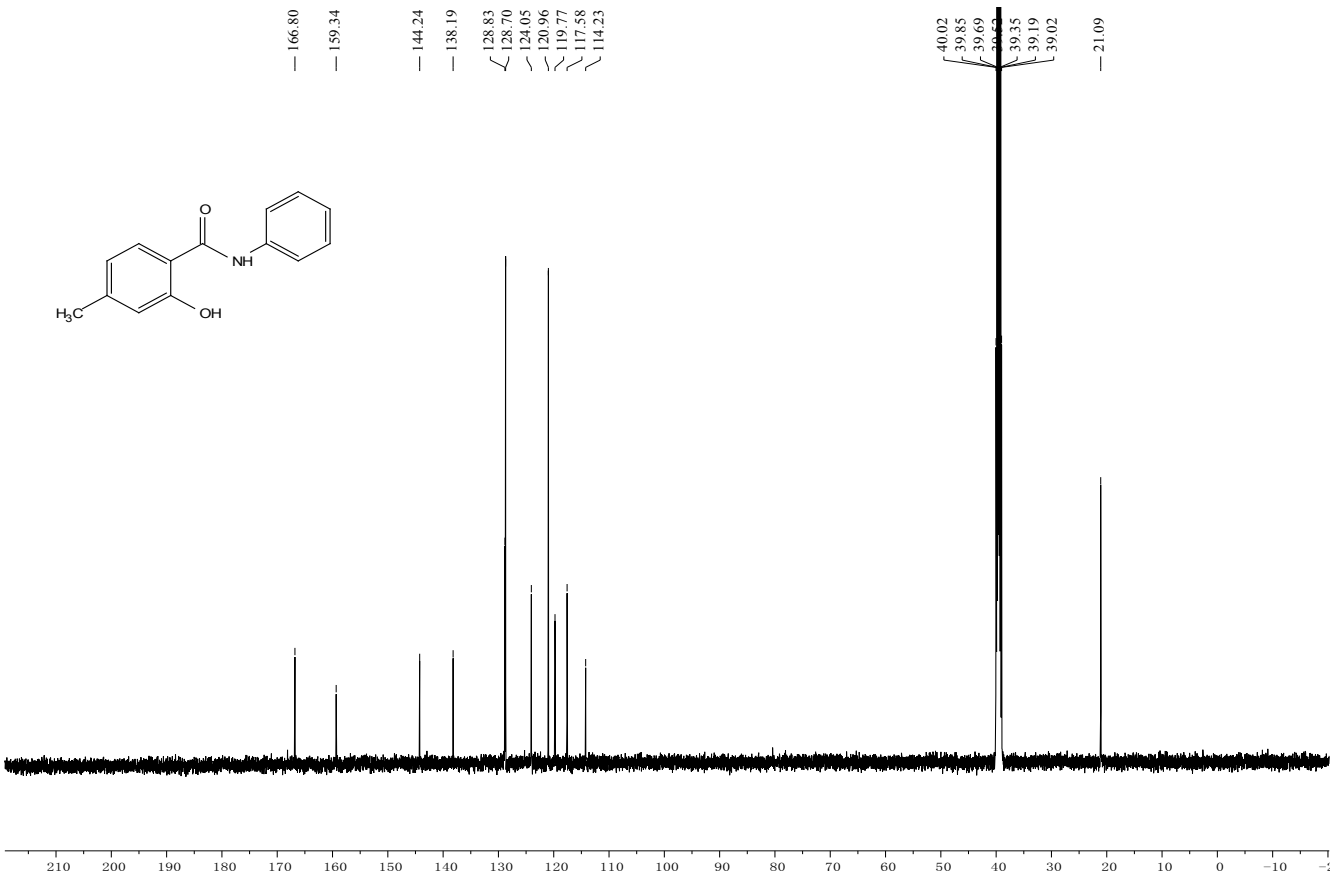

Figure S134. ^{13}C NMR (126 MHz) of **7k** in DMSO-d_6.

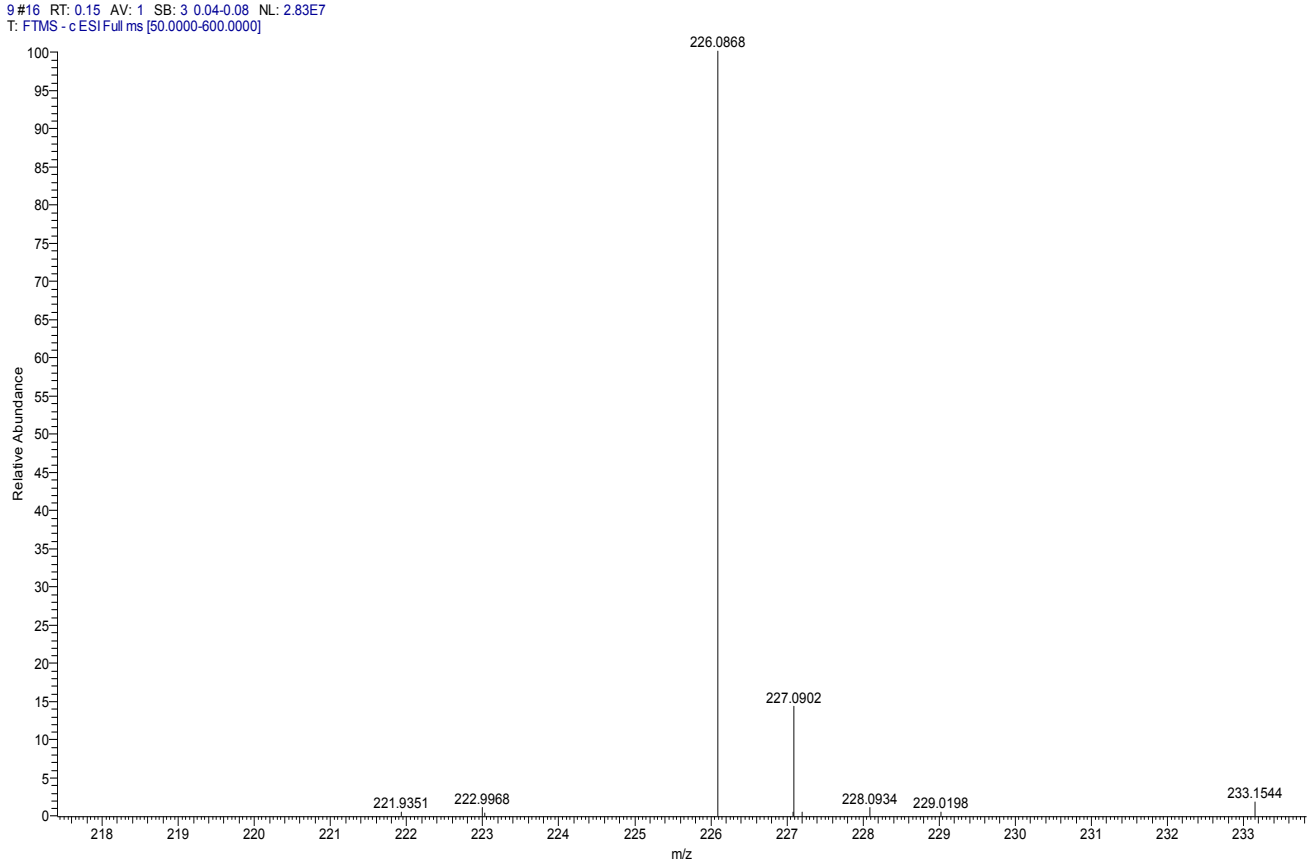

Figure S135. HRMS spectra for **7k**.

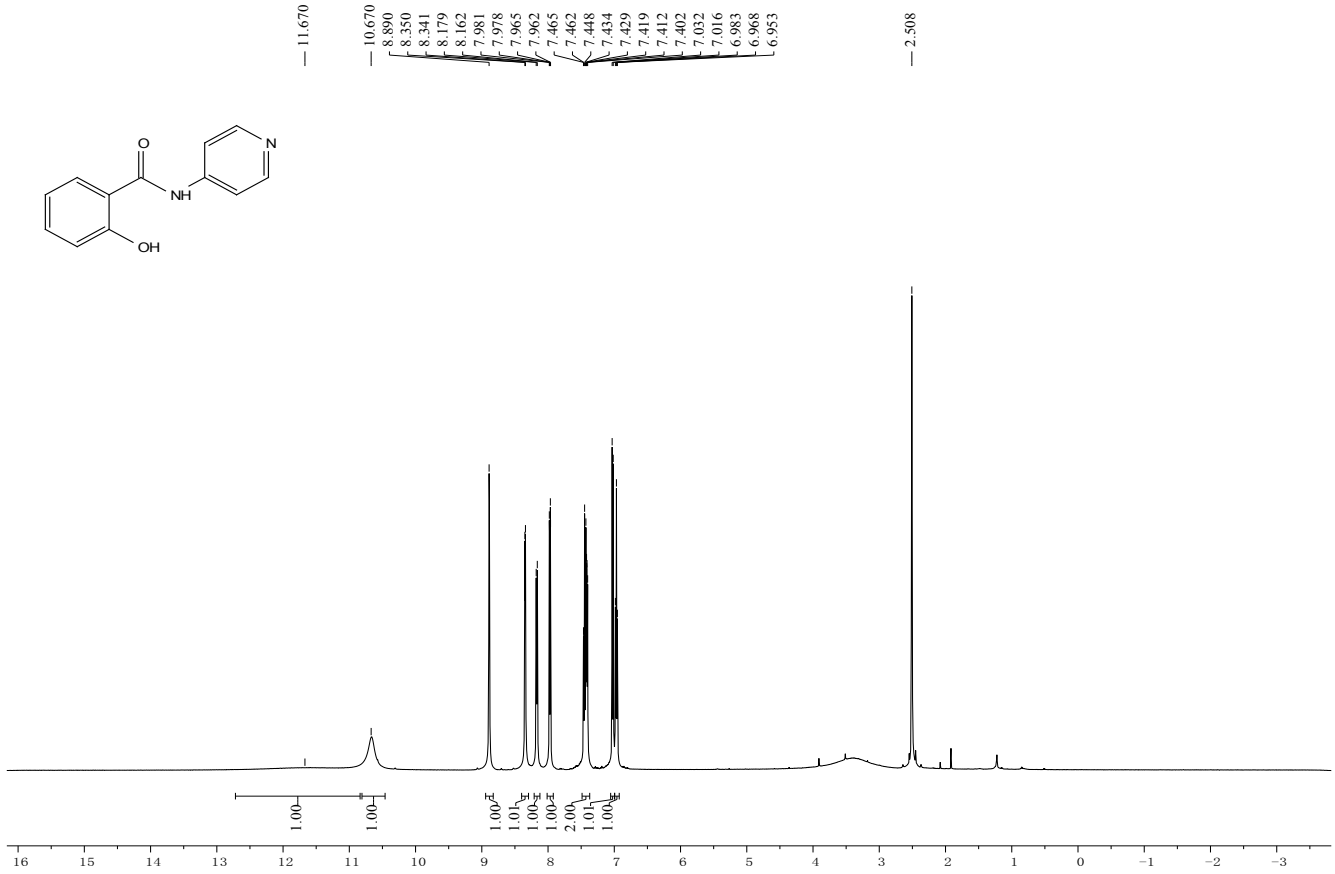

Figure S136. ^{1}H NMR (500 MHz) of **7l** in DMSO-d_6.

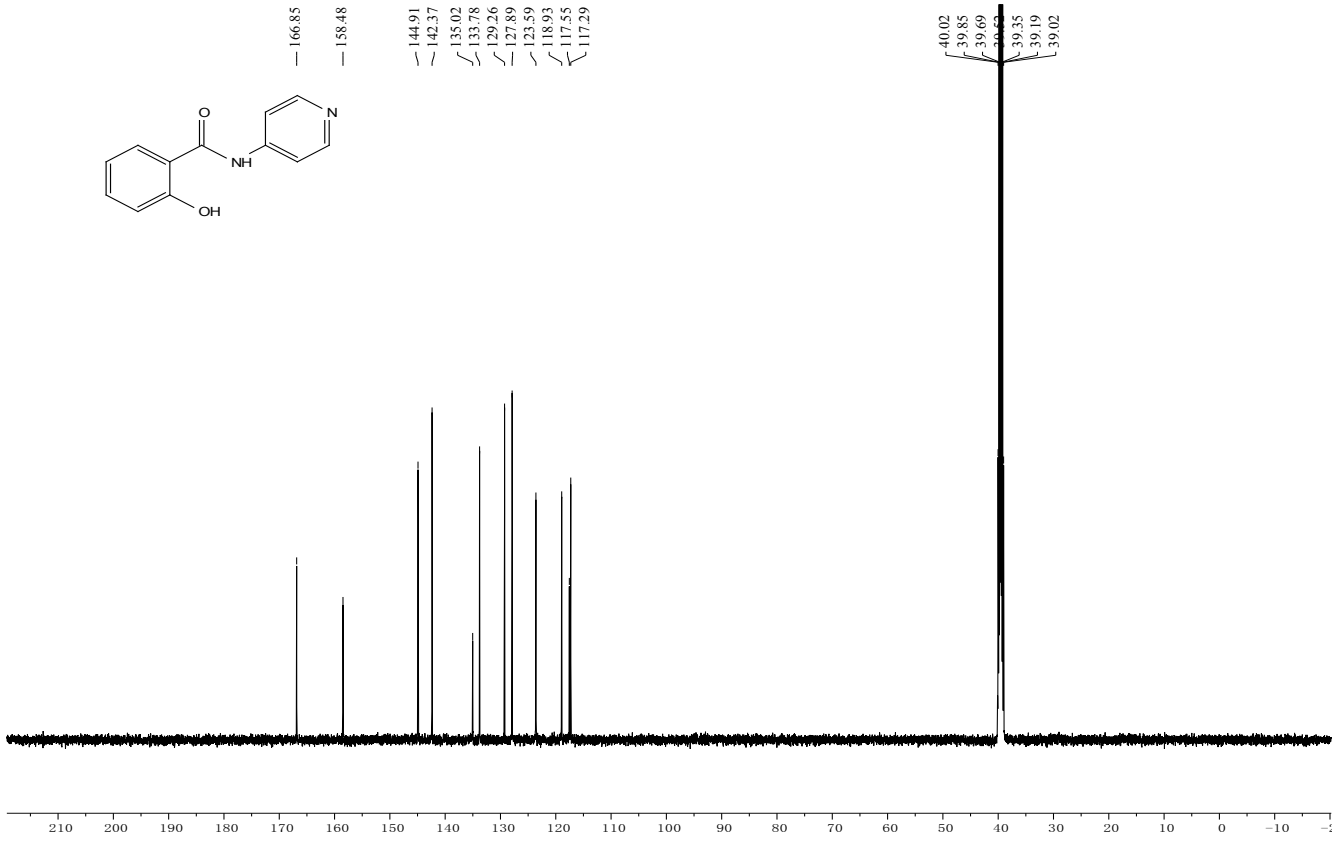

Figure S137. ^{13}C NMR (126 MHz) of **7l** in DMSO-d_6.

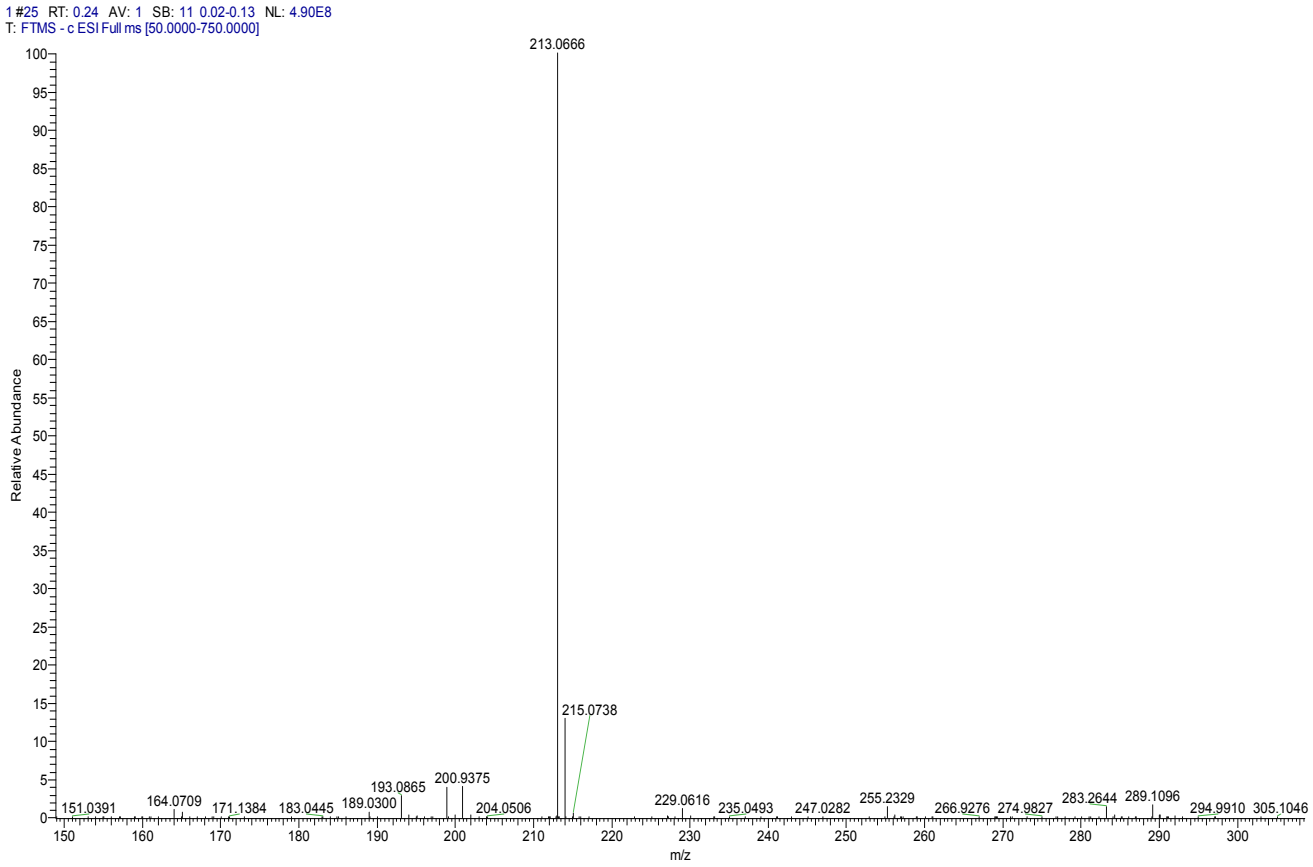

Figure S138. HRMS spectra for **7l**.

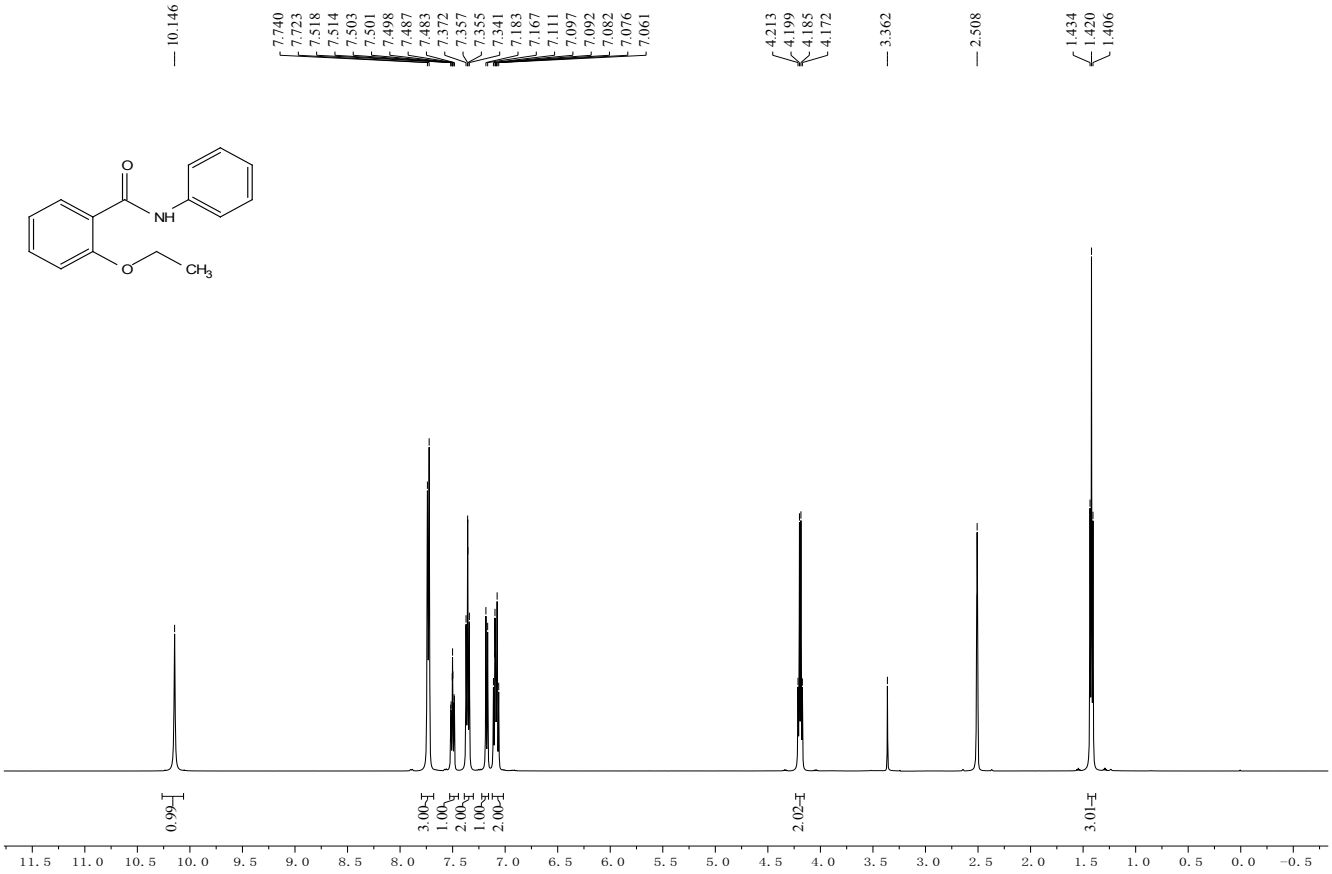

Figure S139. ^{1}H NMR (500 MHz) of **9a** in DMSO-d_6.

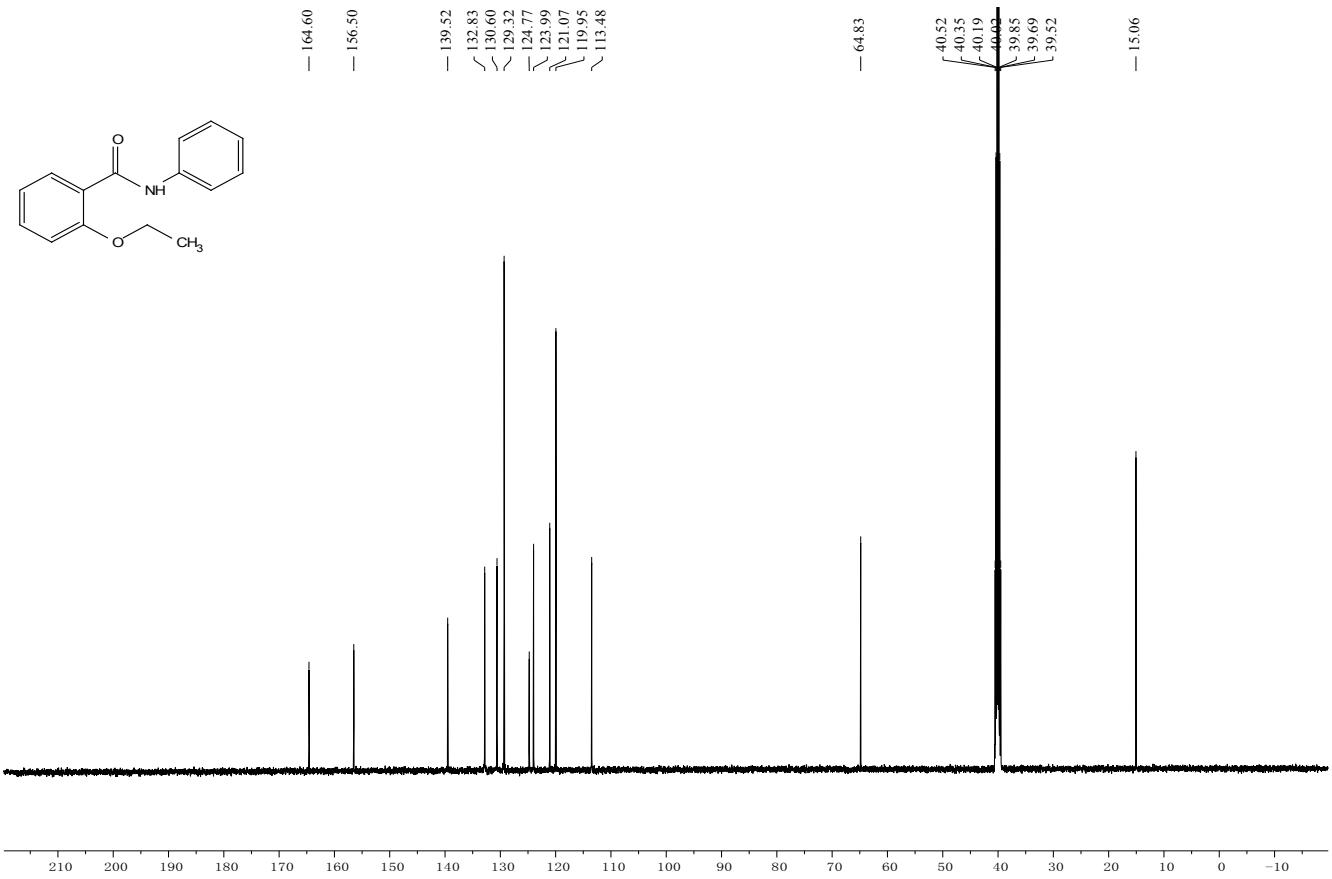

Figure S140. ^{13}C NMR (126 MHz) of **9a** in DMSO-d_6.

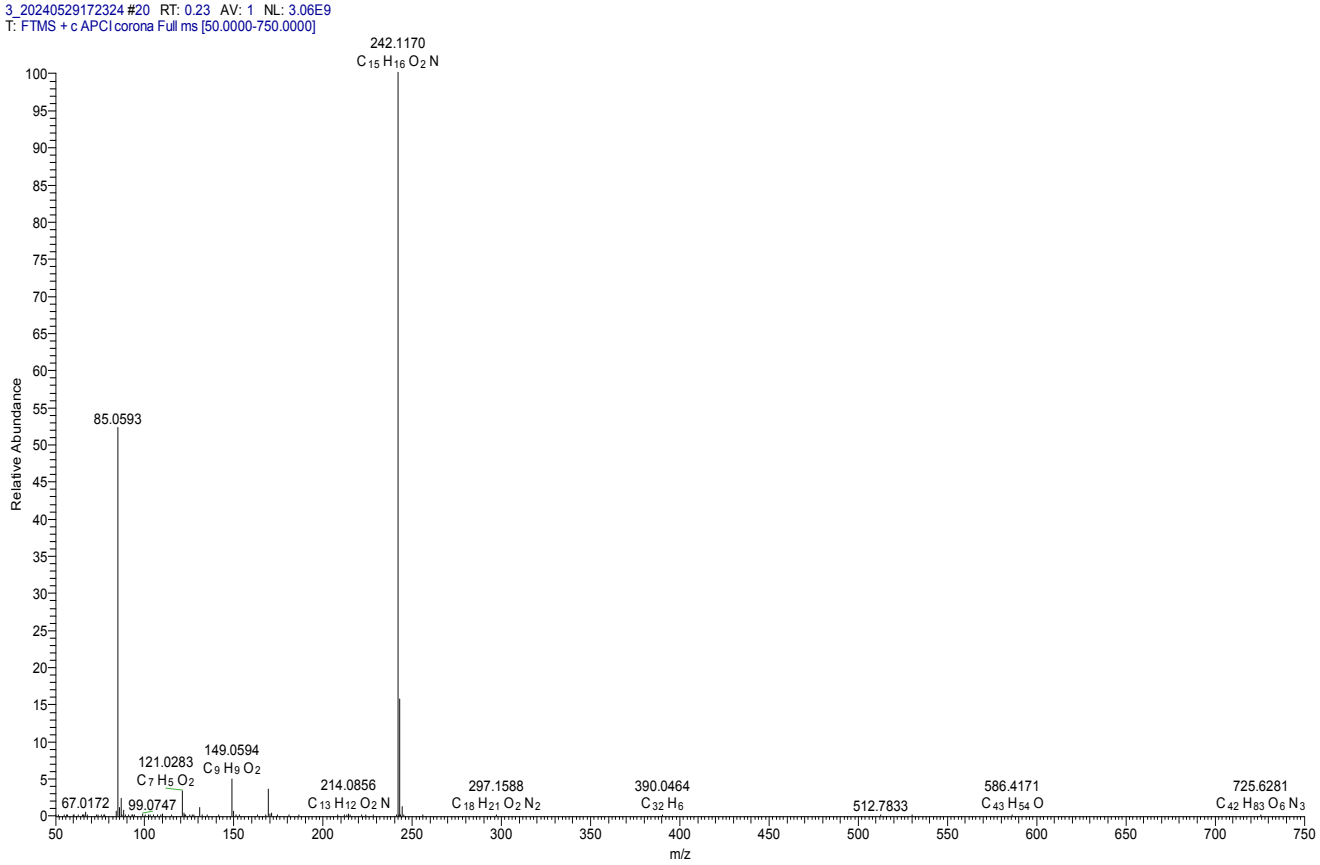

Figure S141. HRMS spectra for **9a**.

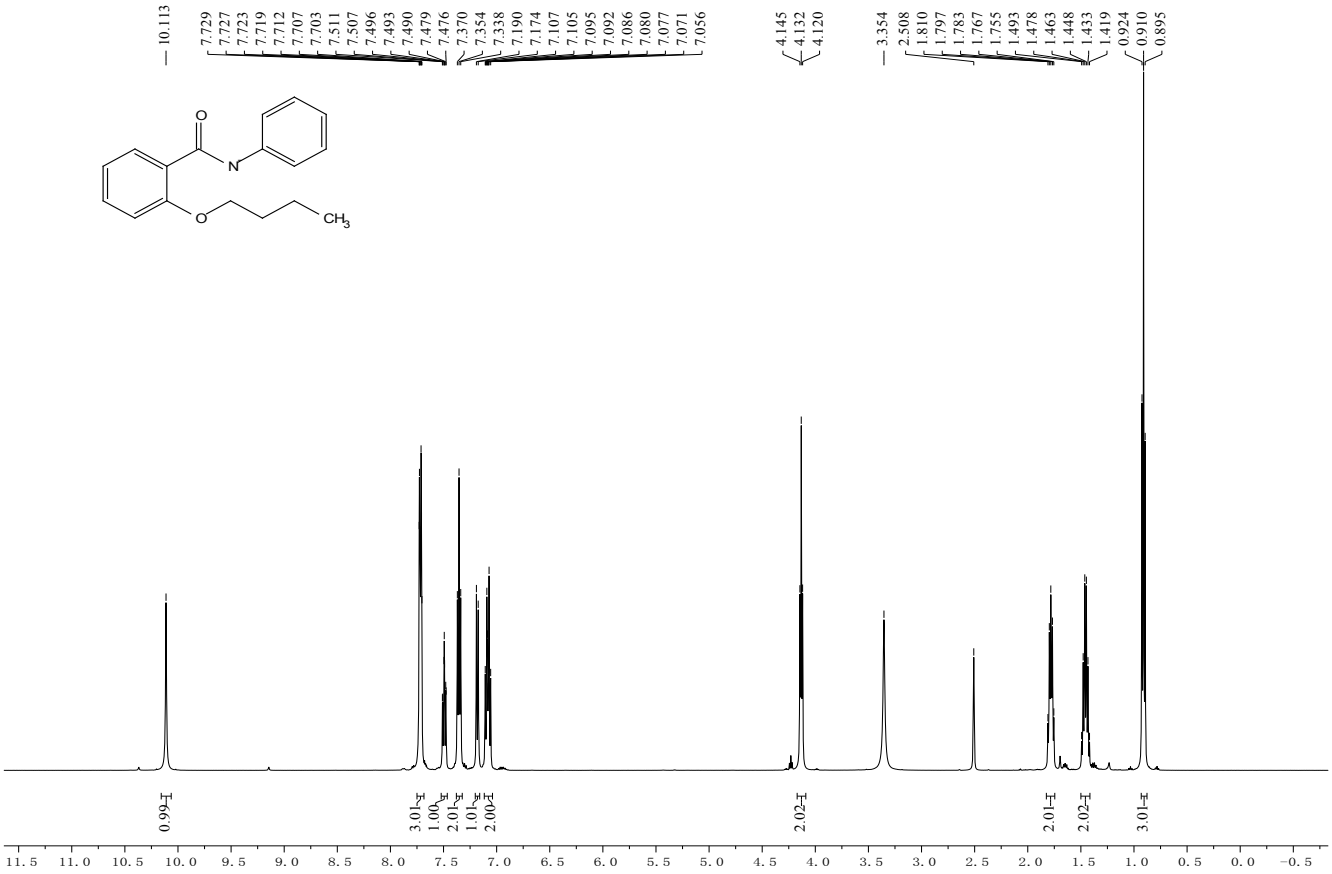

Figure S142. ^{1}H NMR (500 MHz) of **9b** in DMSO-d_6.

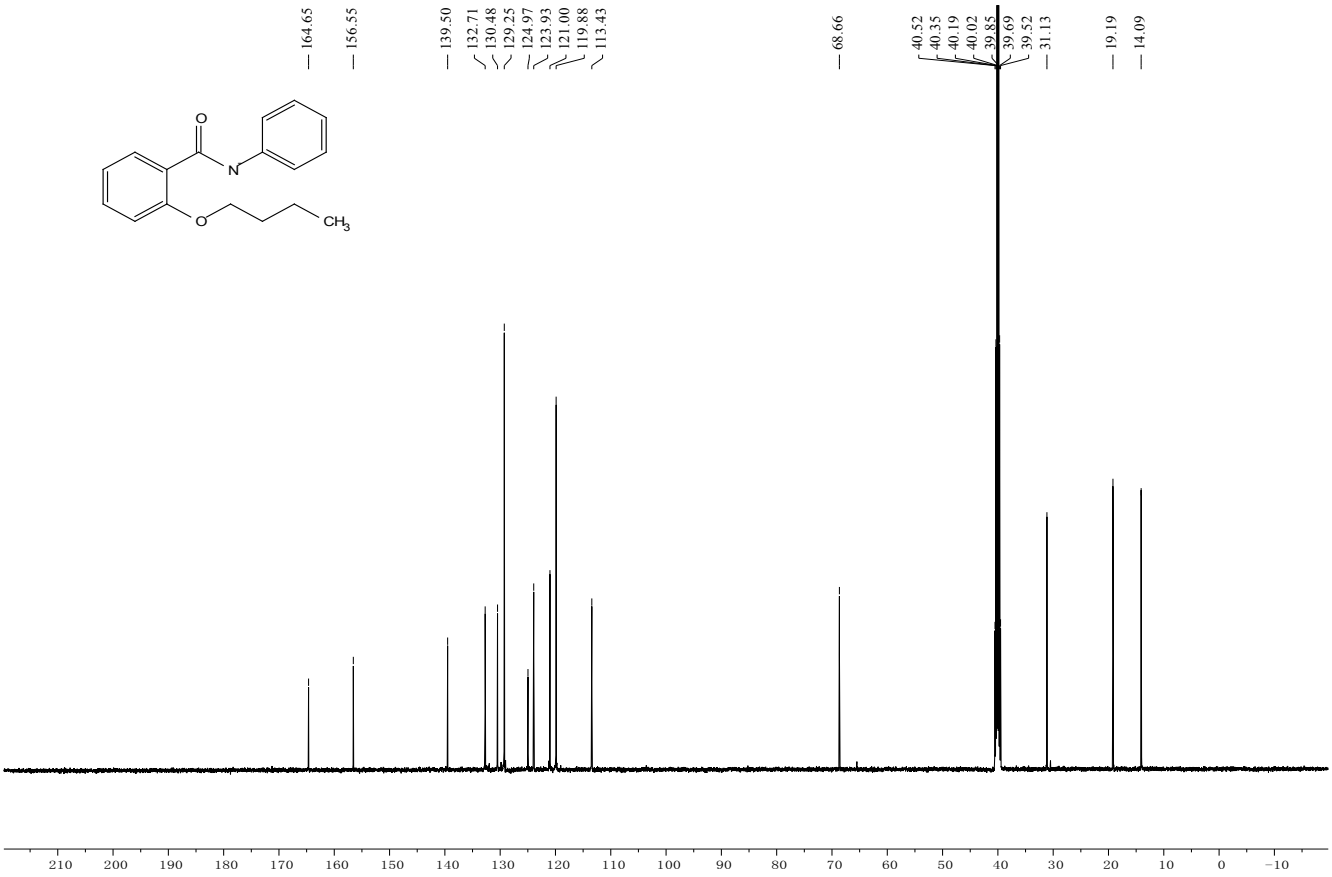

Figure S143. ^{13}C NMR (126 MHz) of **9b** in DMSO-d_6.

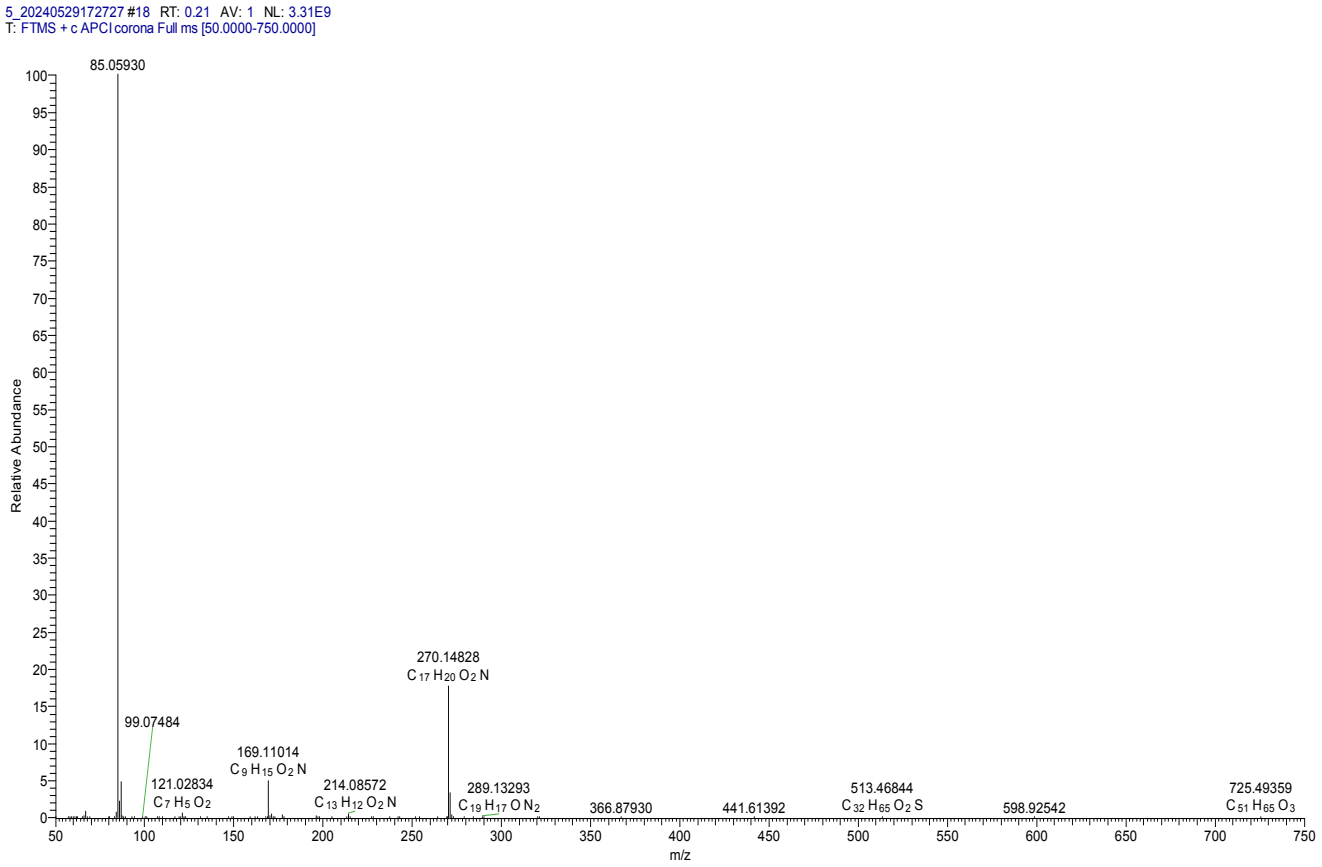

Figure S144. HRMS spectra for **9b**.

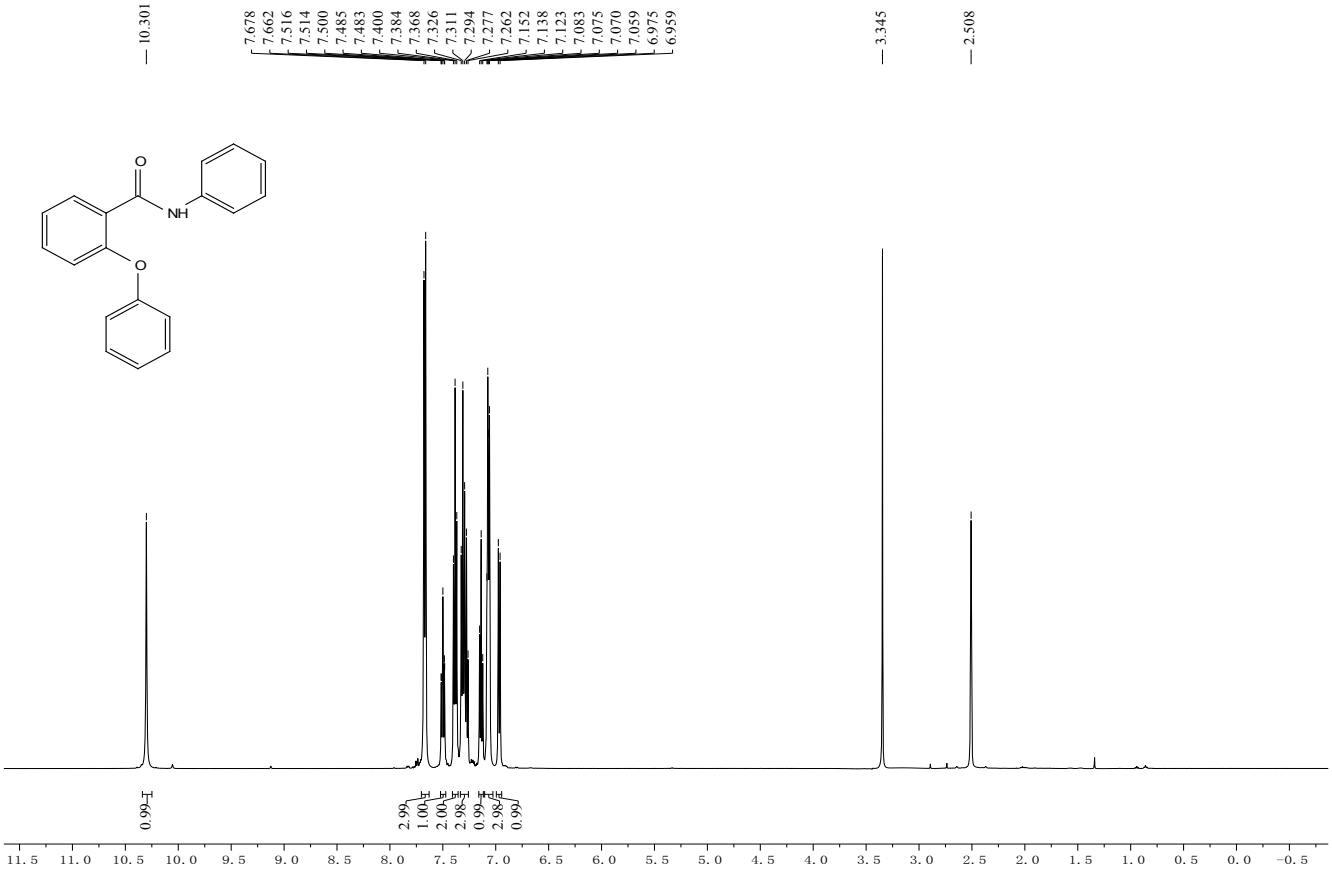

Figure S145. ^{1}H NMR (500 MHz) of **9c** in DMSO-d_6.

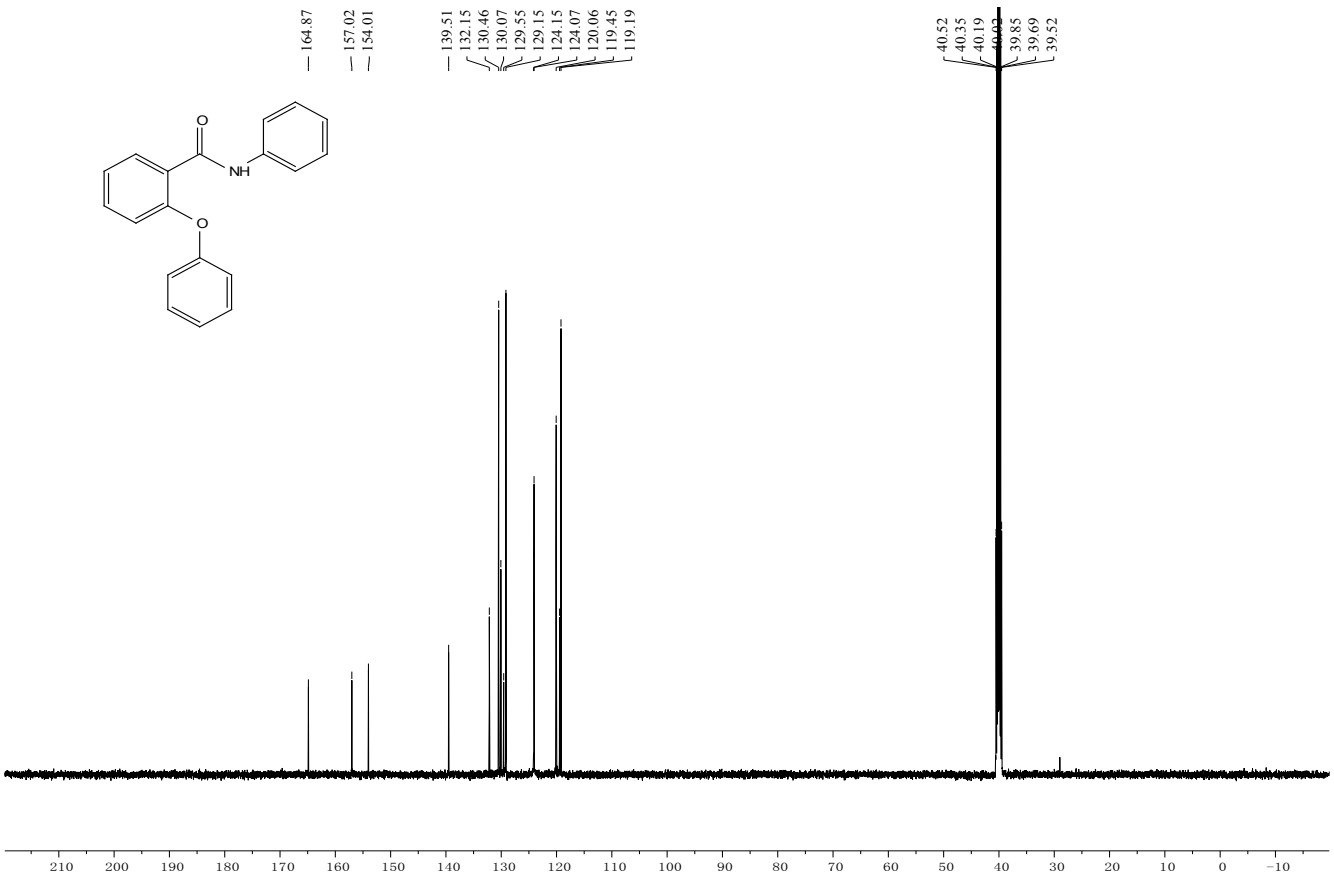

Figure S146. ^{13}C NMR (126 MHz) of **9c** in DMSO-d_6.

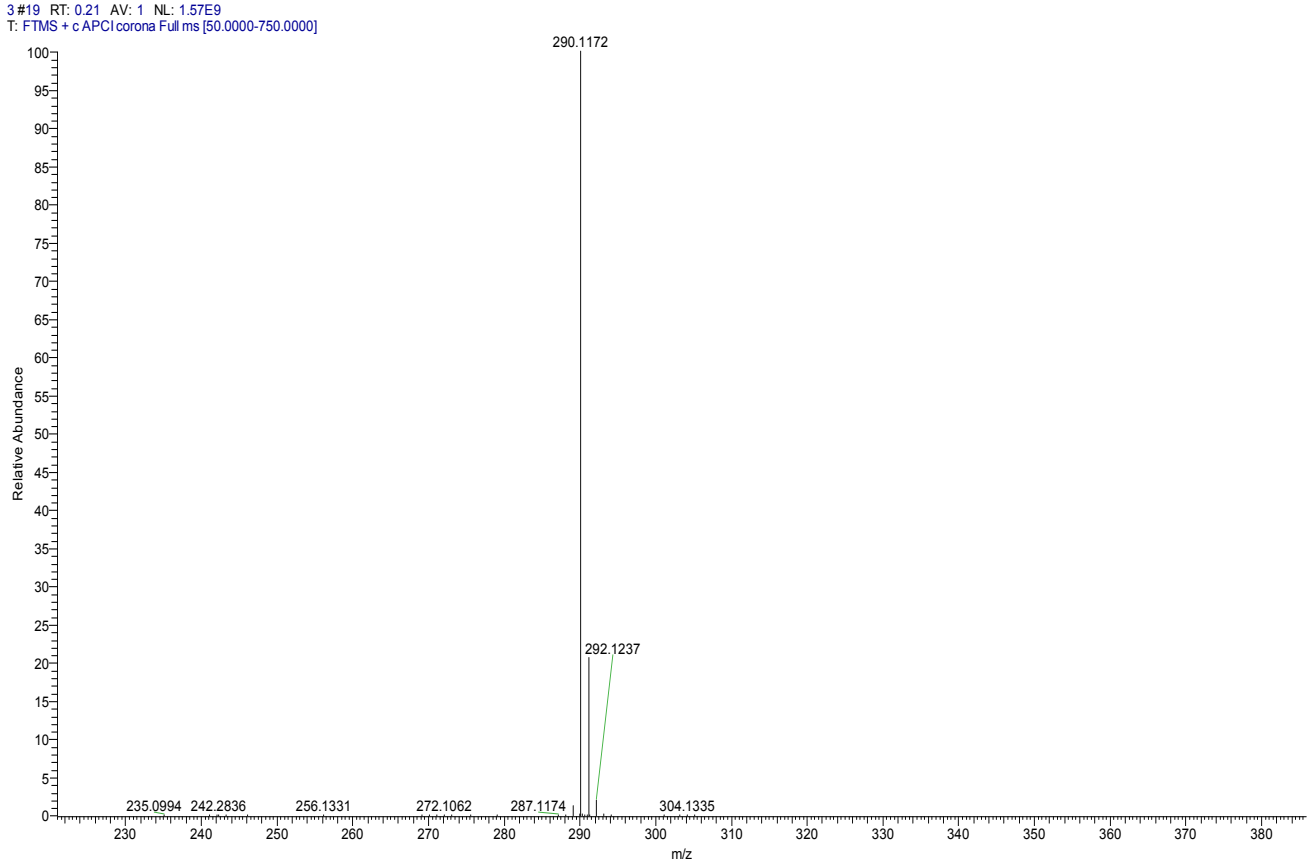

Figure S147. HRMS spectra for **9c**.

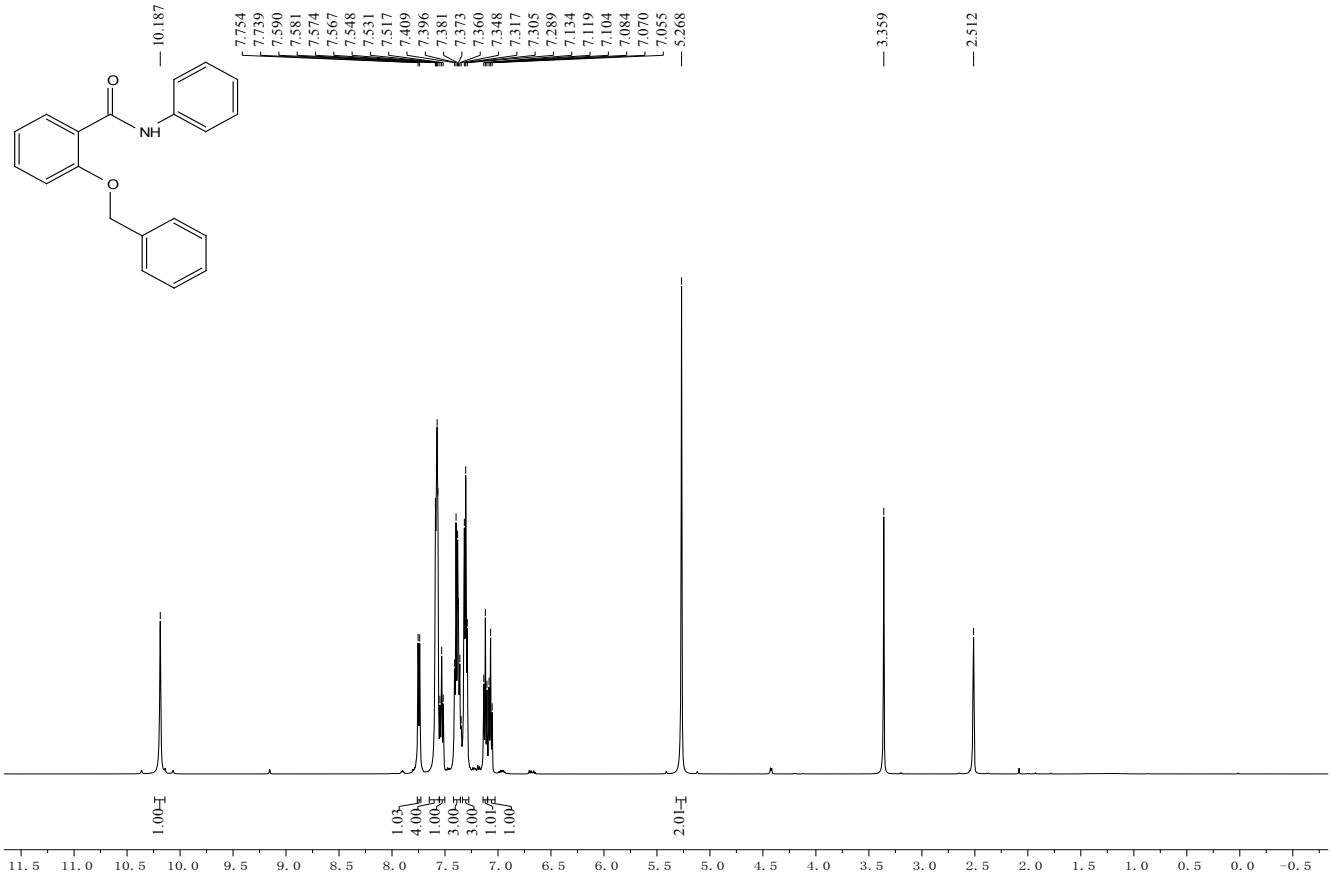

Figure S148. ^{1}H NMR (500 MHz) of **9d** in DMSO-d_6.

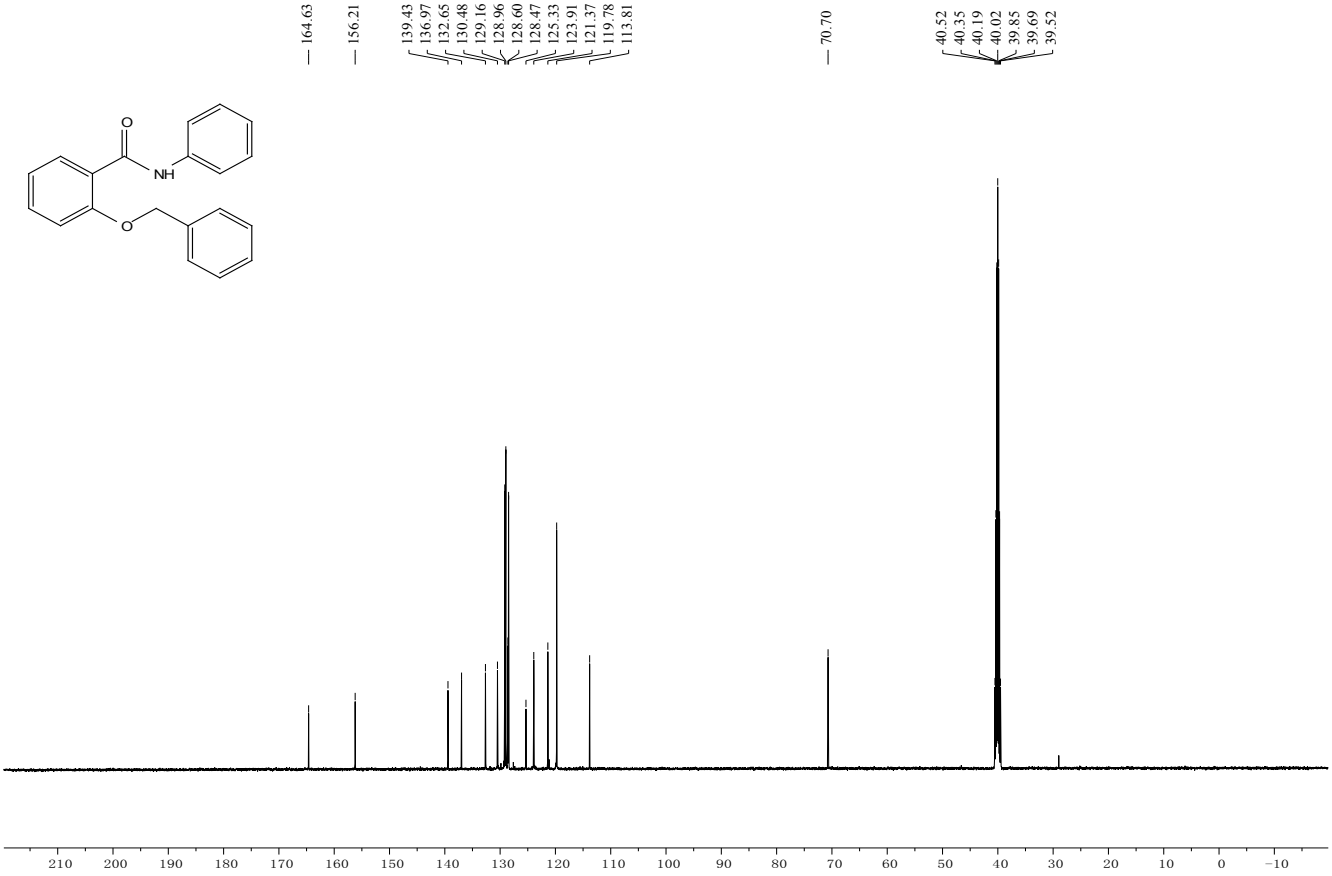

Figure S149. ^{13}C NMR (126 MHz) of **9d** in DMSO-d_6.

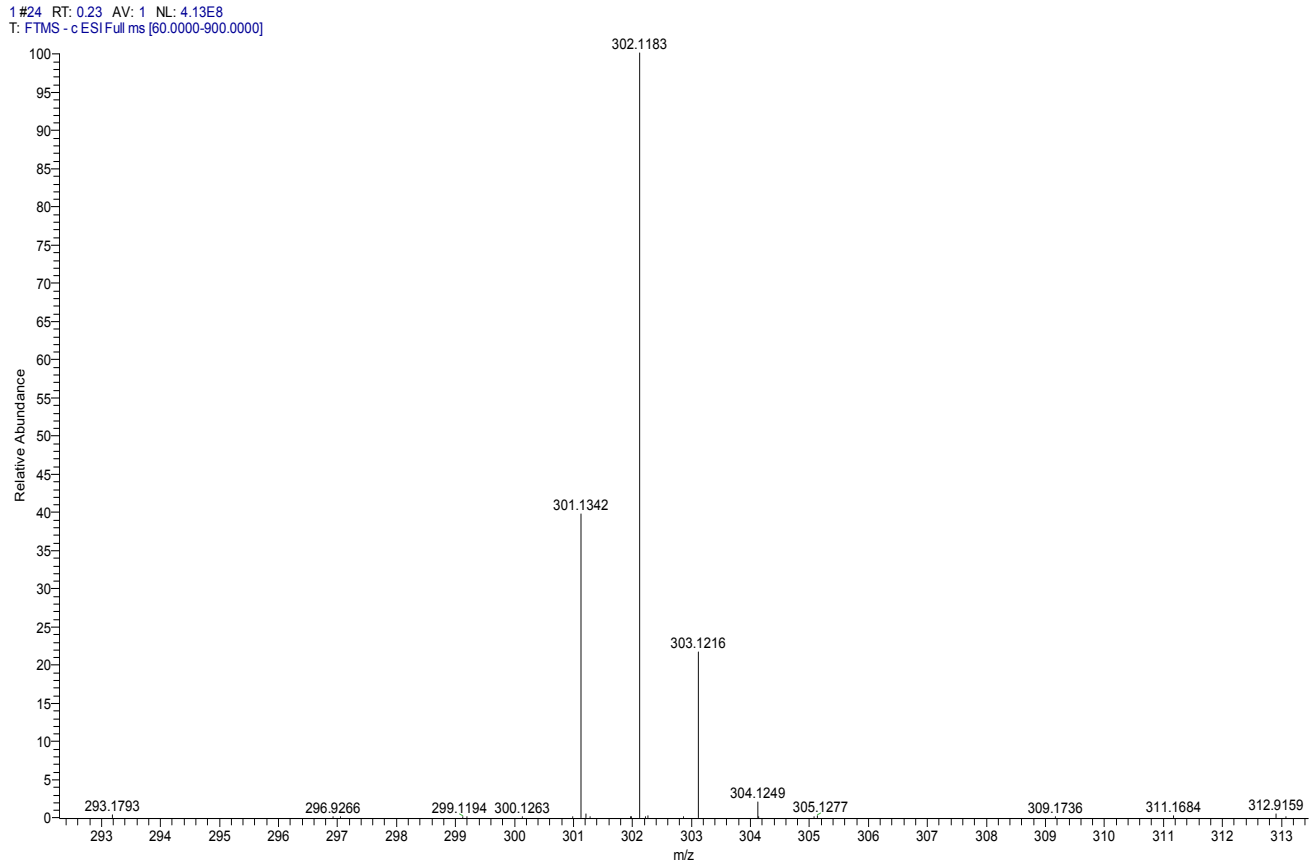

Figure S150. HRMS spectra for **9d**.

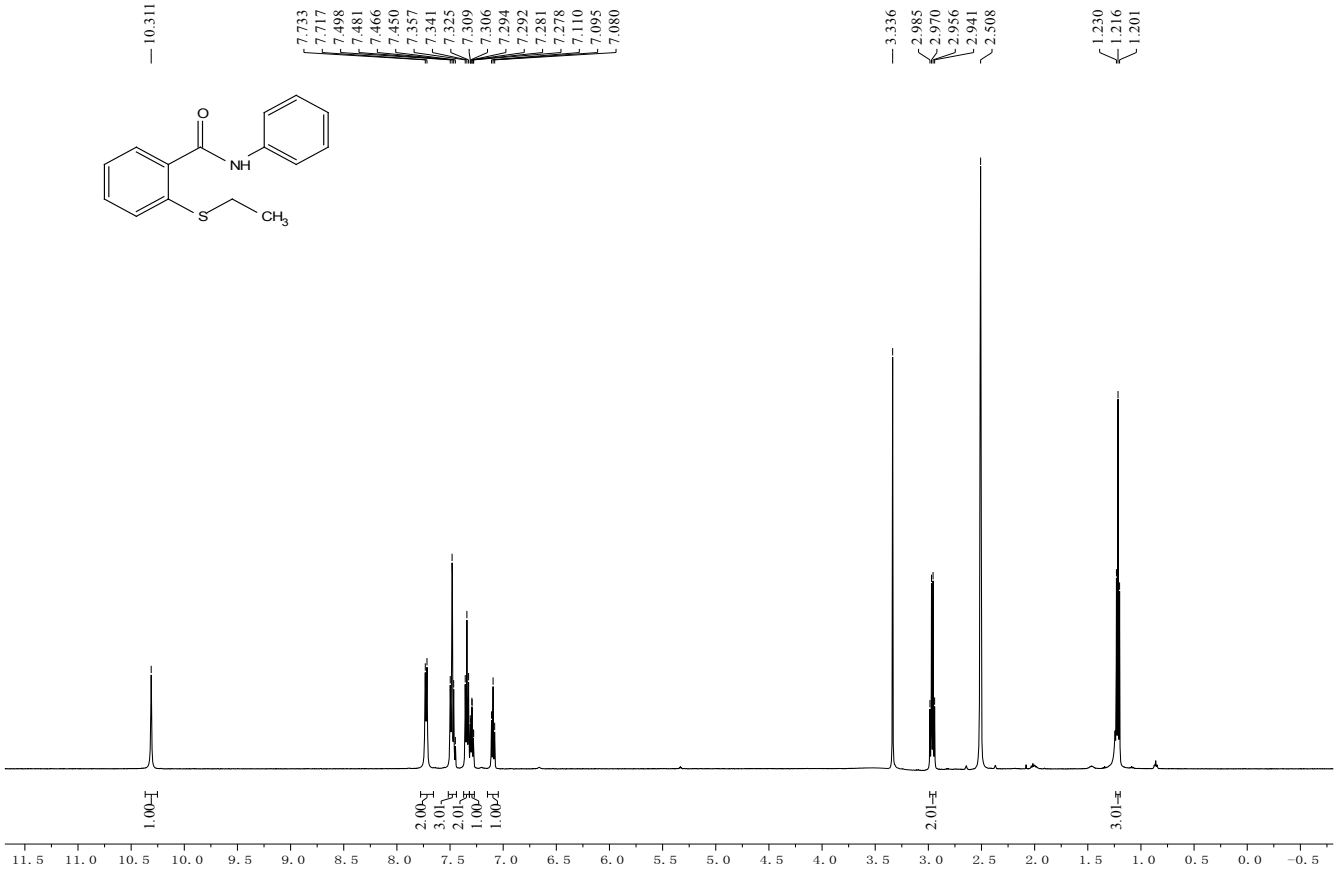

Figure S151. ^{1}H NMR (500 MHz) of **9e** in DMSO-d_6.

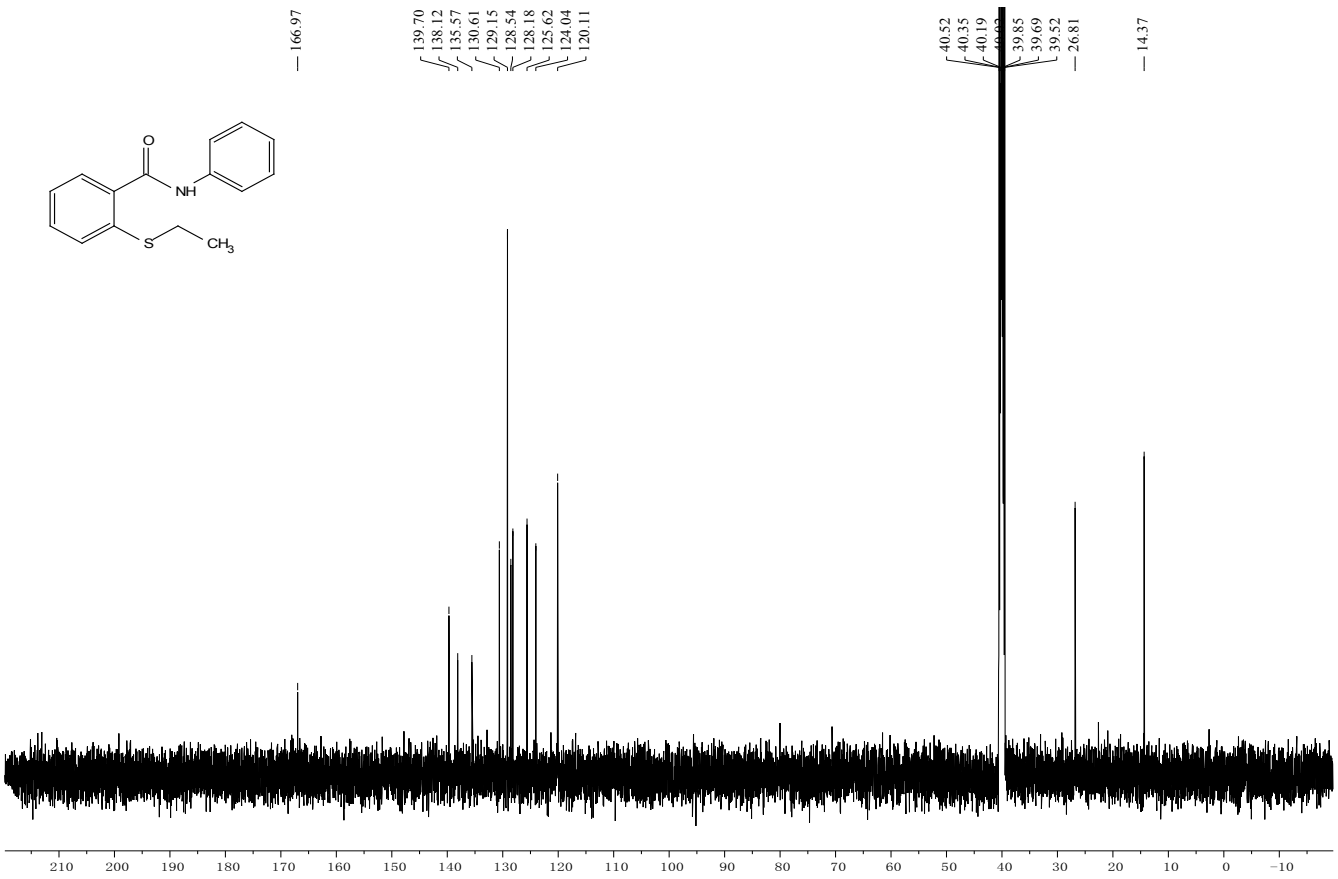

Figure S152. ^{13}C NMR (126 MHz) of **9e** in DMSO-d_6.

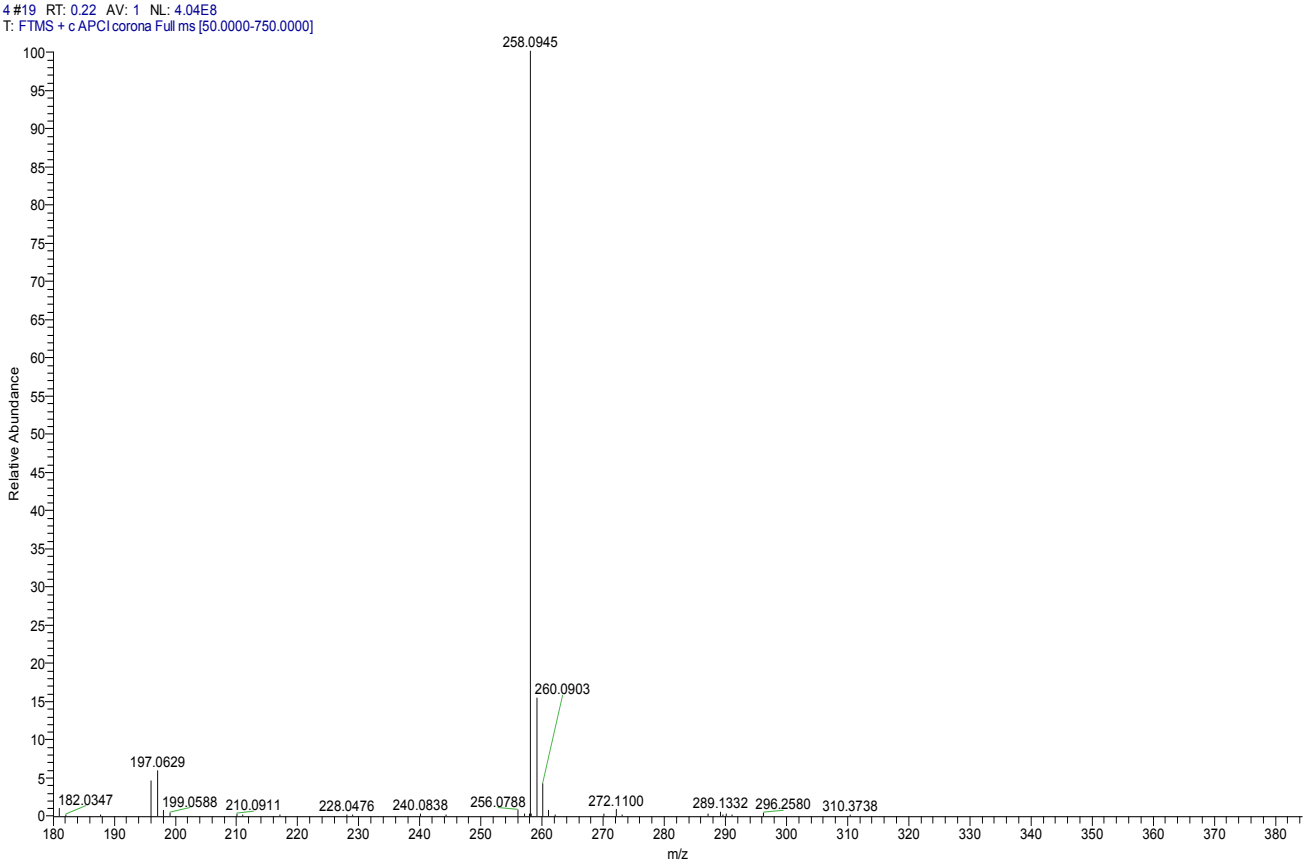

Figure S153. HRMS spectra for **9e**.

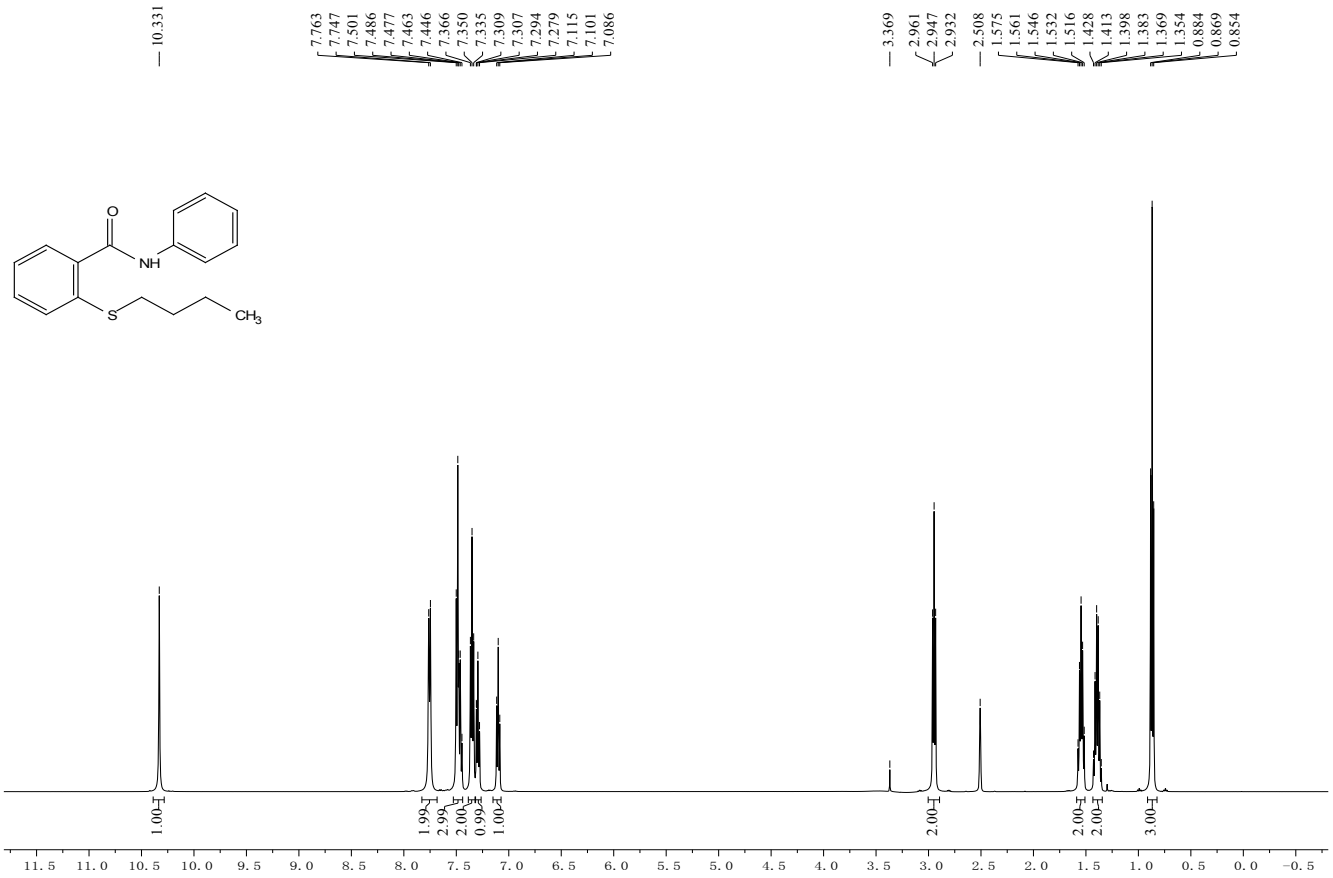

Figure S154. ^{1}H NMR (500 MHz) of **9f** in DMSO-d_6.

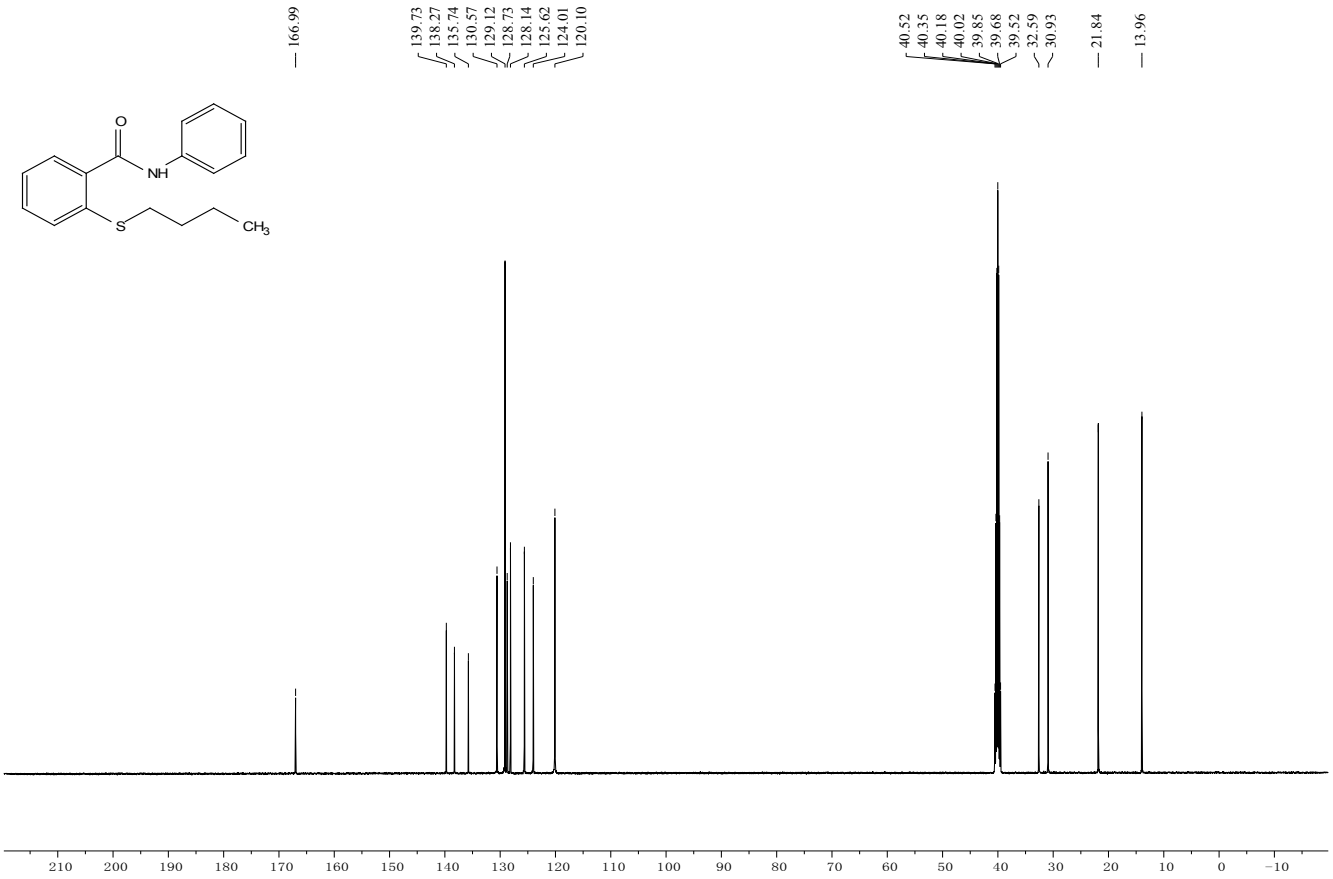

Figure S155. ^{13}C NMR (126 MHz) of **9f** in DMSO-d_6.

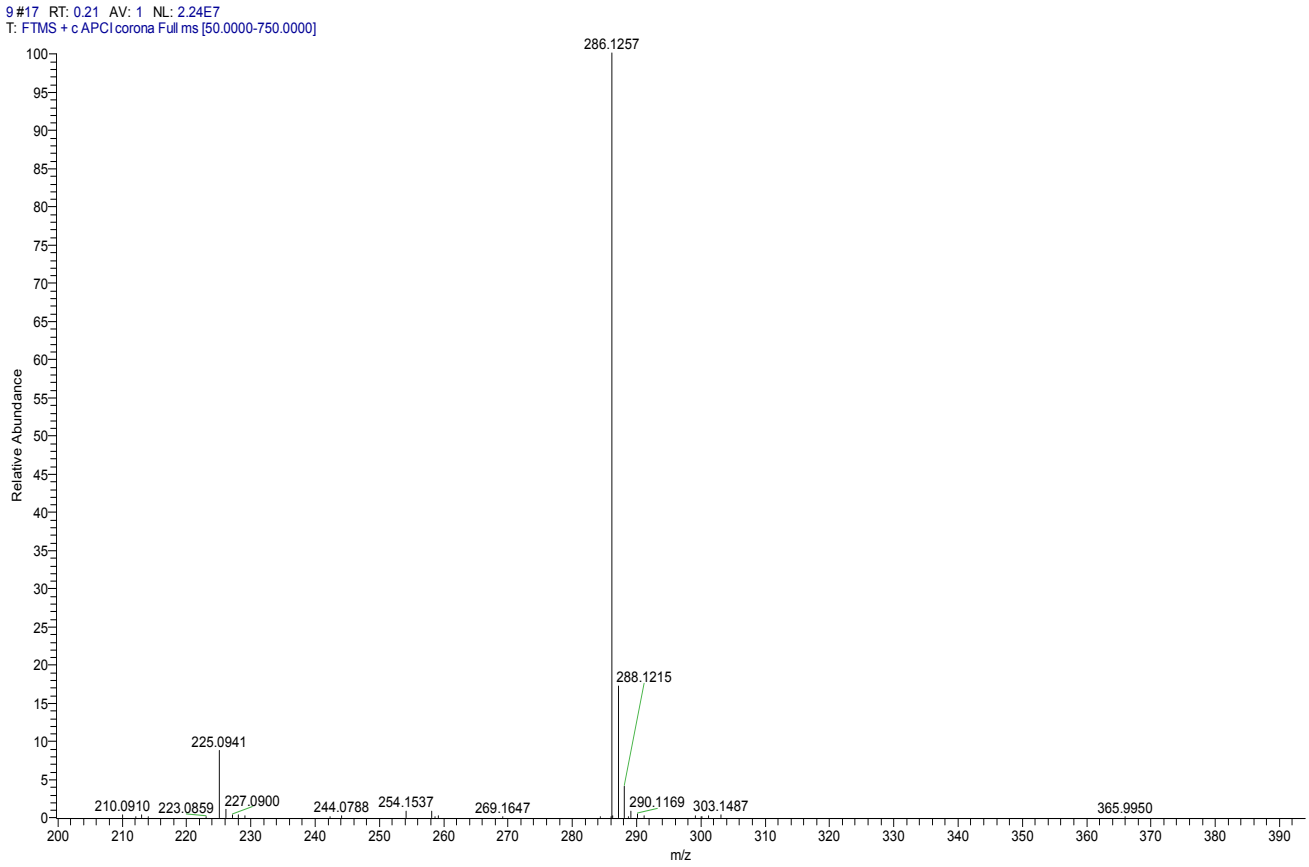

Figure S156. HRMS spectra for **9f**.

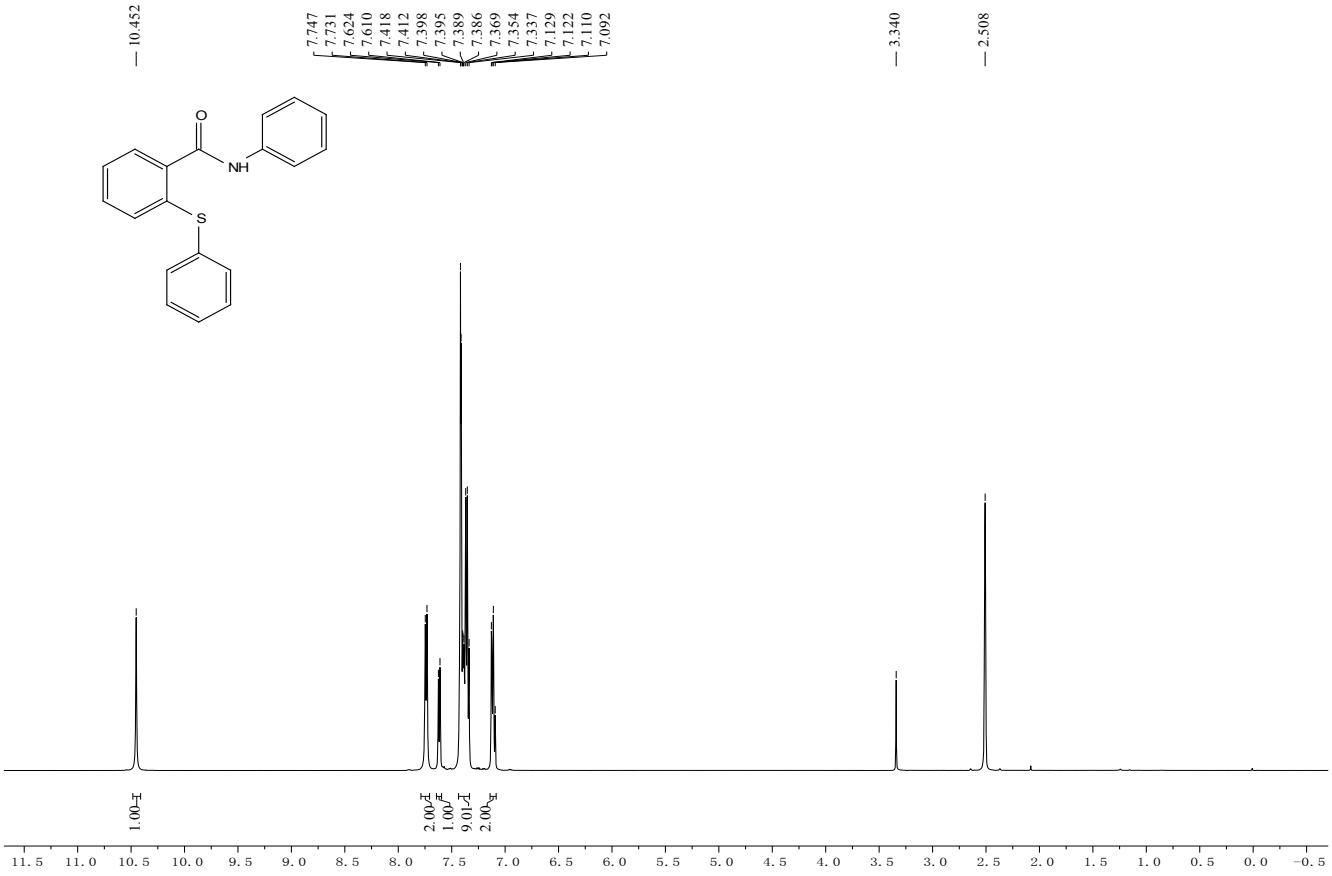

Figure S157. ^{1}H NMR (500 MHz) of **9g** in DMSO-d_6.

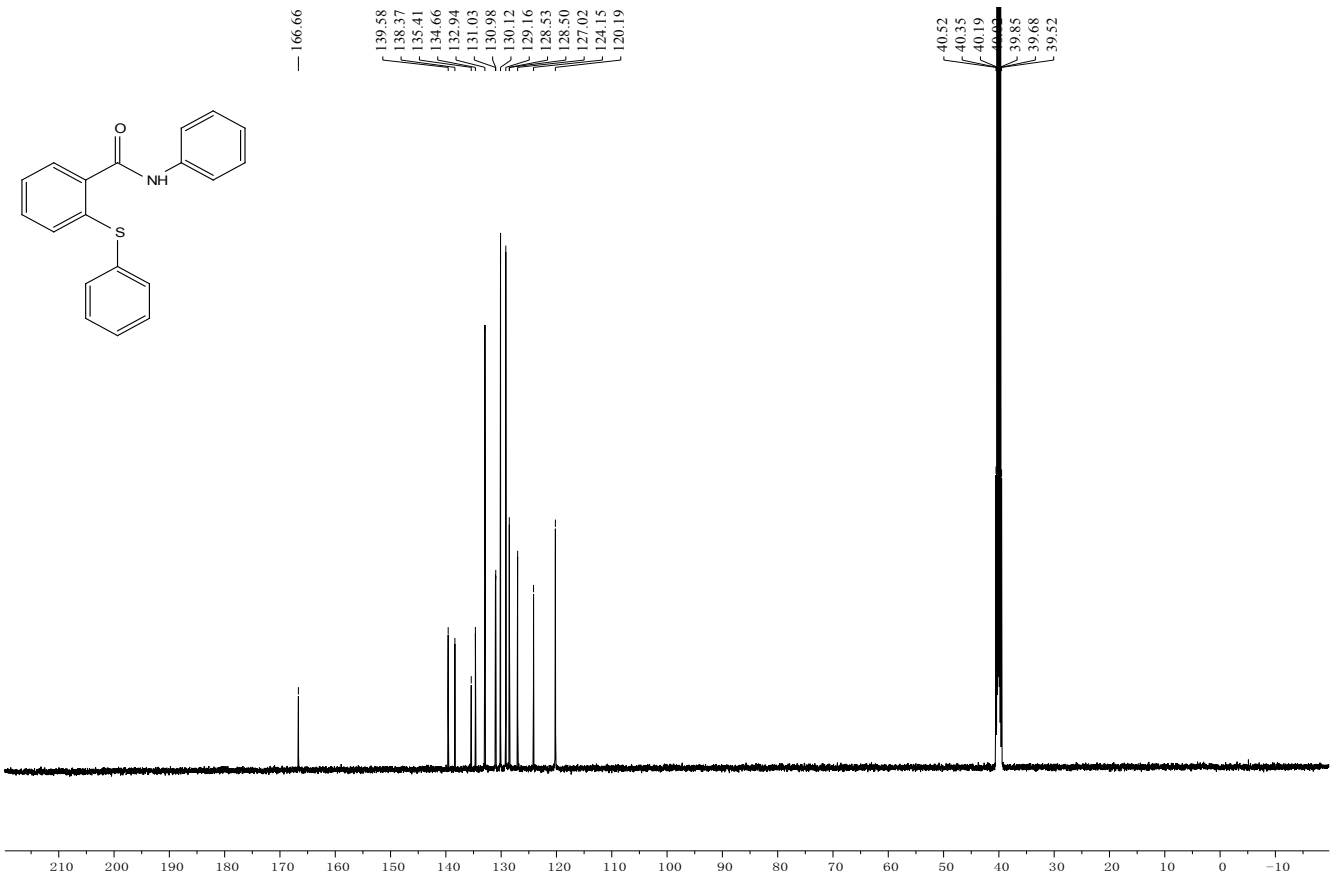

Figure S158. ^{13}C NMR (126 MHz) of **9g** in DMSO-d_6

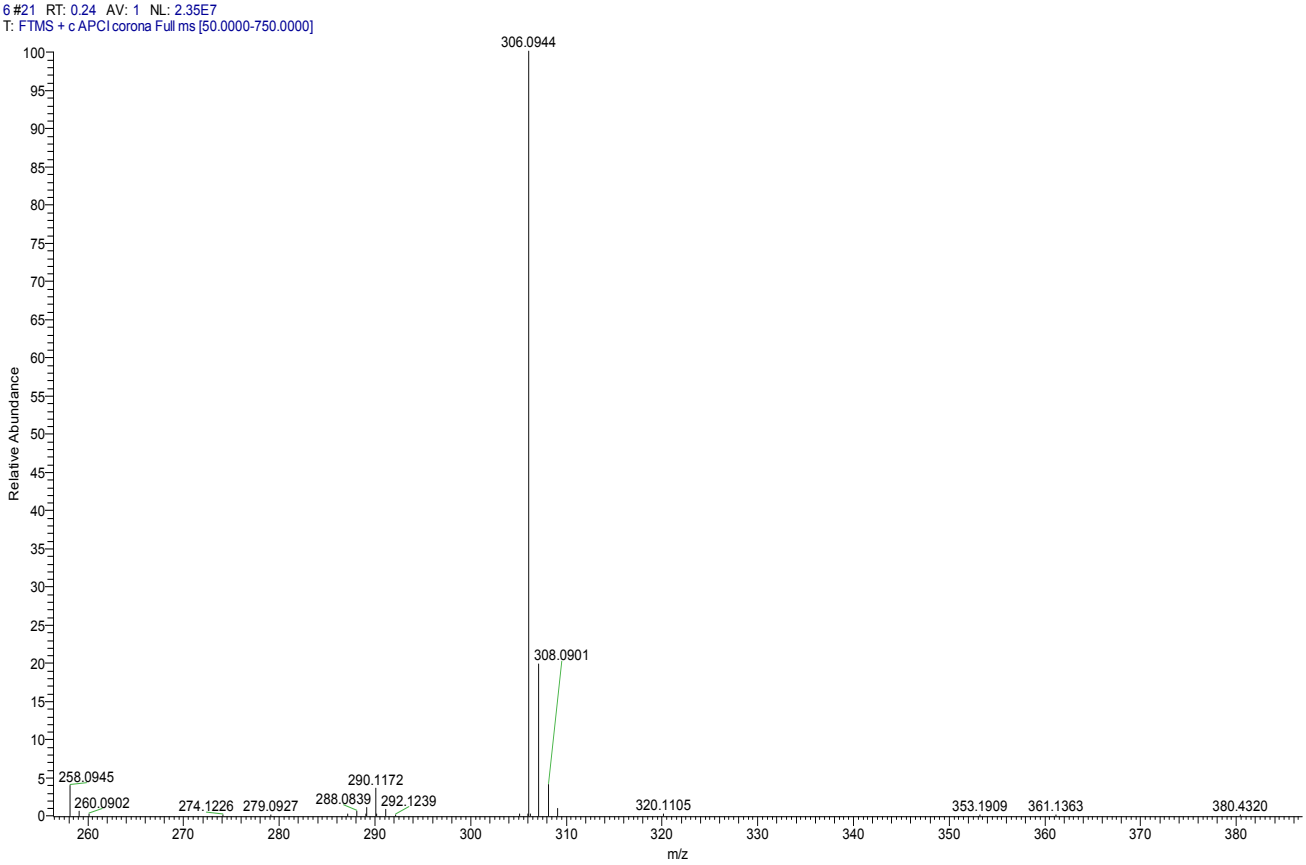

Figure S159. HRMS spectra for **9g**.

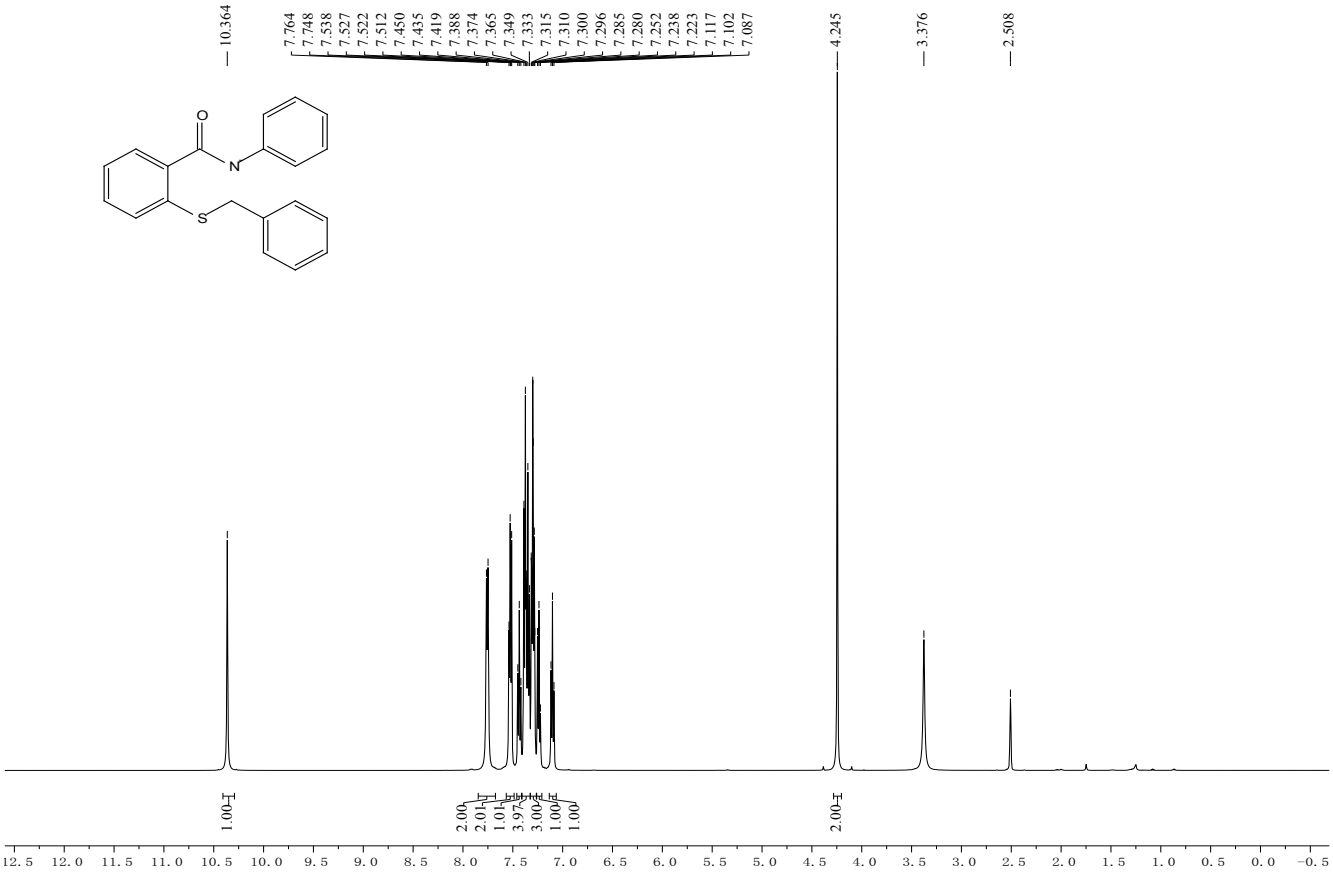

Figure S160. ^{1}H NMR (500 MHz) of **9h** in DMSO-d_6.

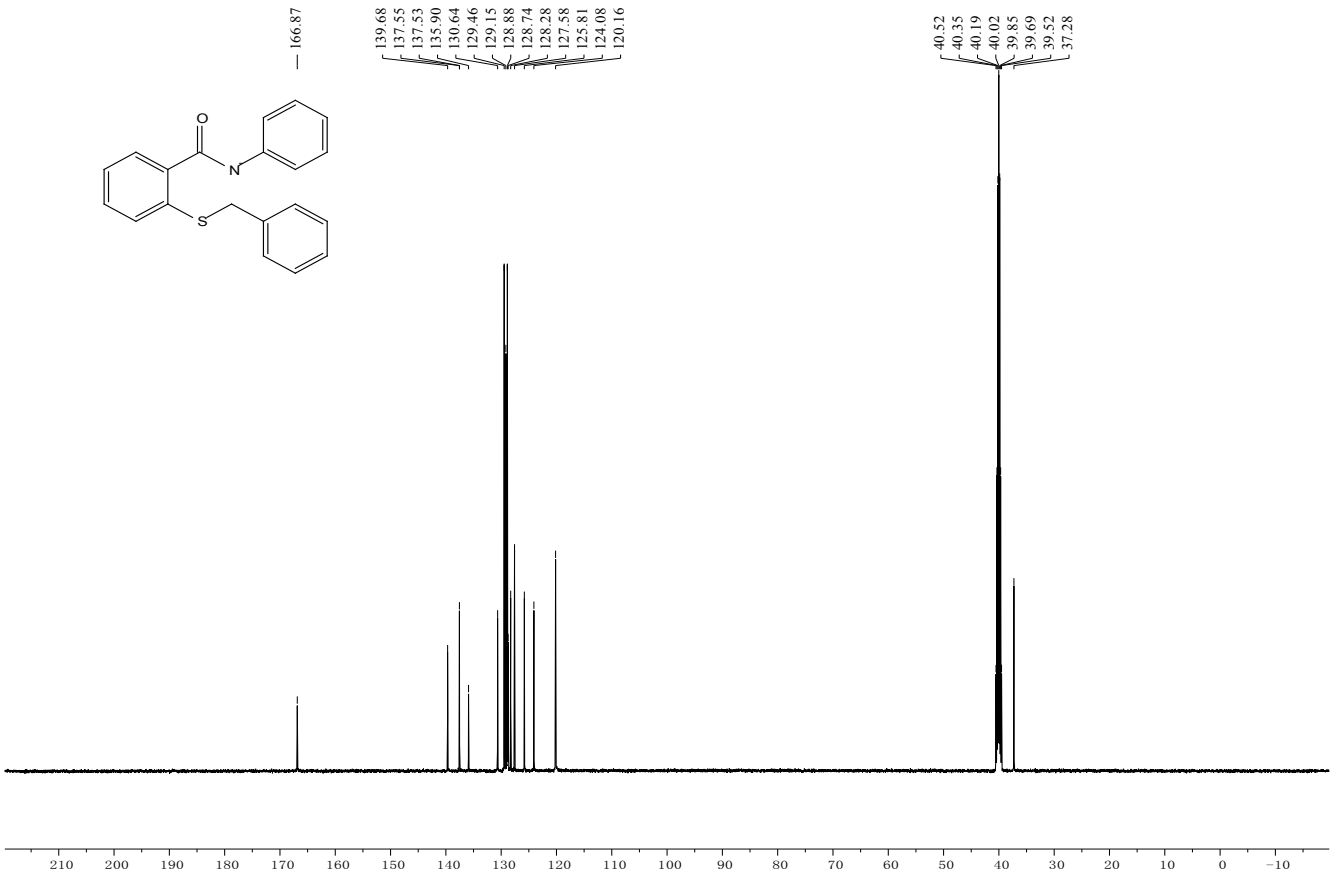

Figure S161. ^{13}C NMR (126 MHz) of **9h** in DMSO-d_6

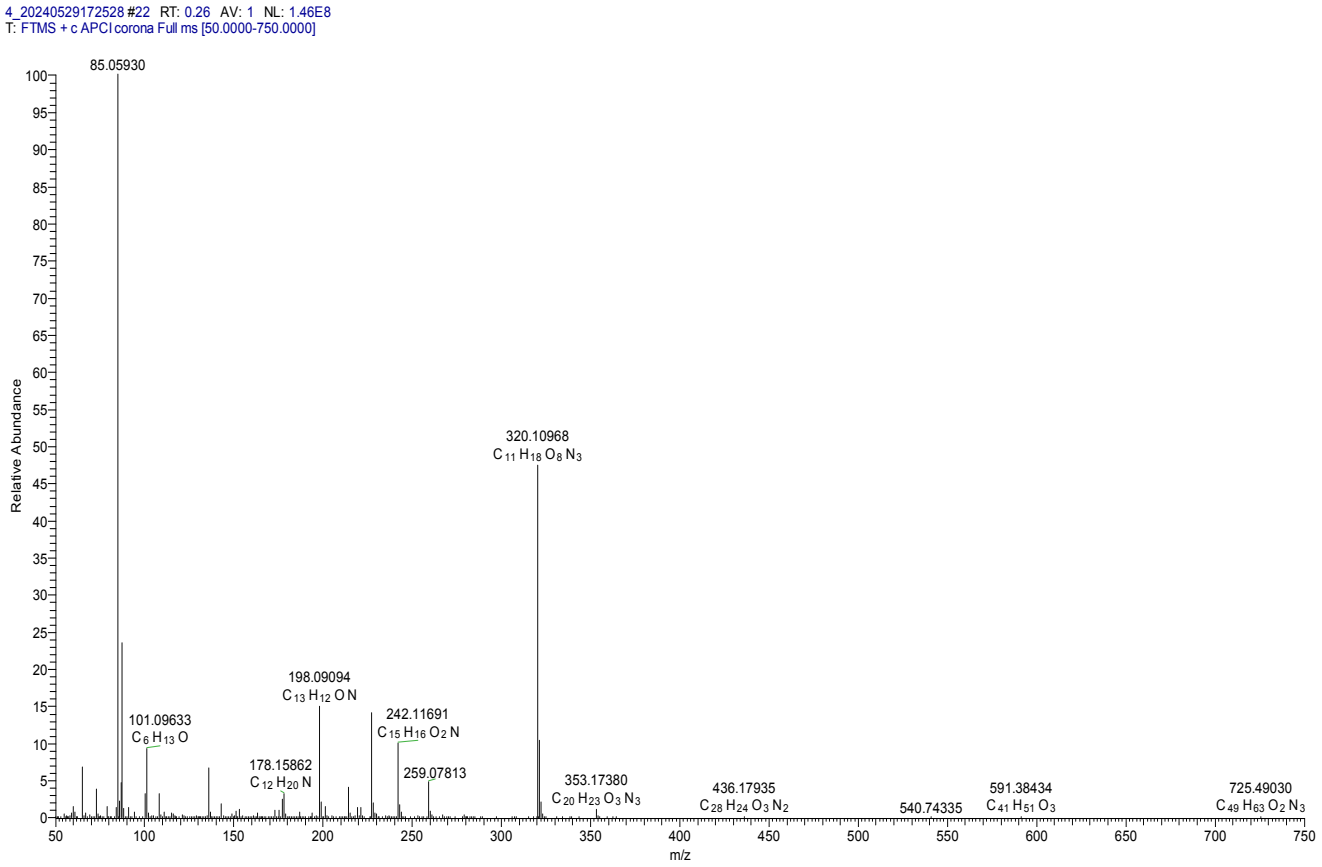

Figure S162. HRMS spectra for **9h**.

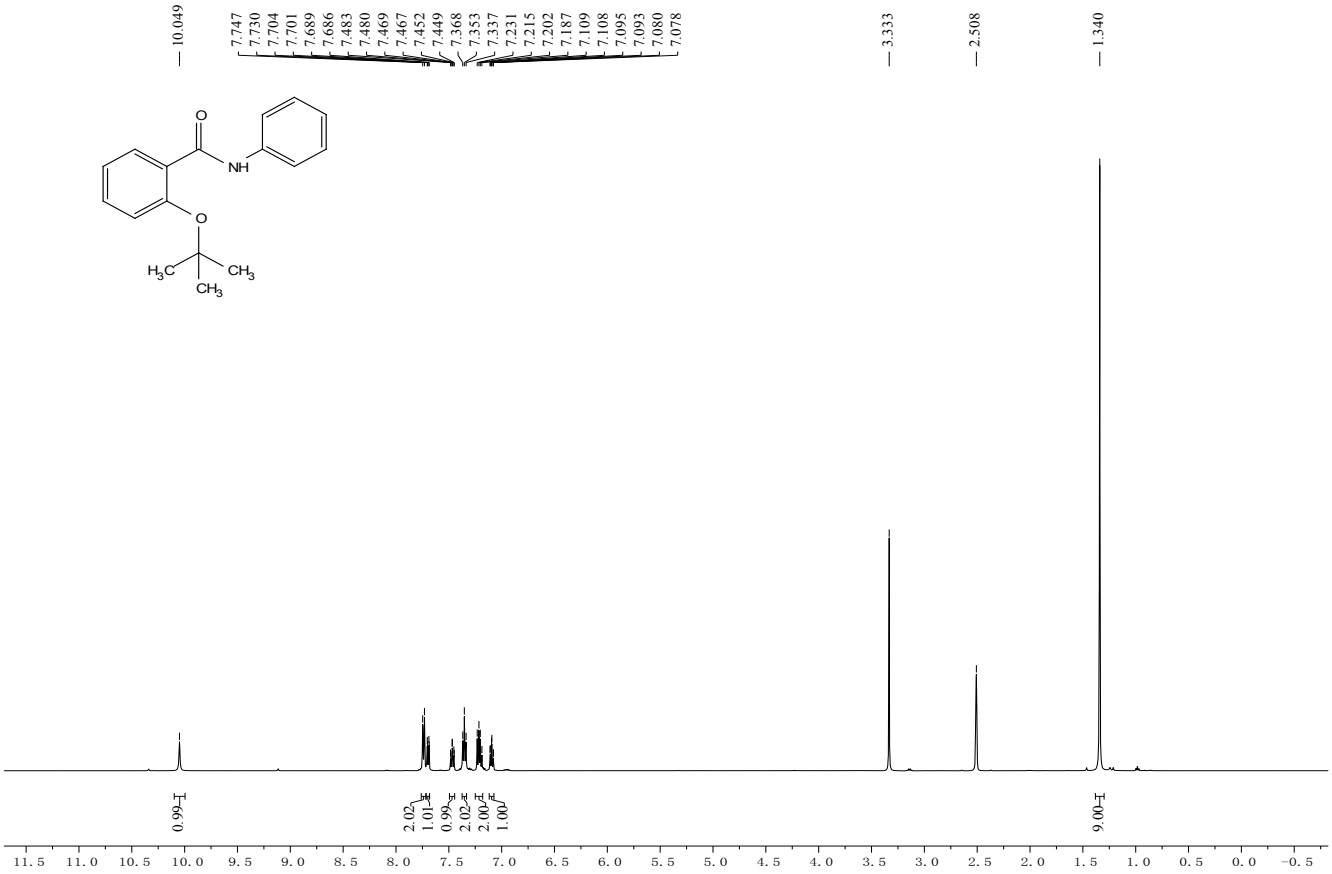

Figure S163. ^{1}H NMR (500 MHz) of **9i** in DMSO-d_6.

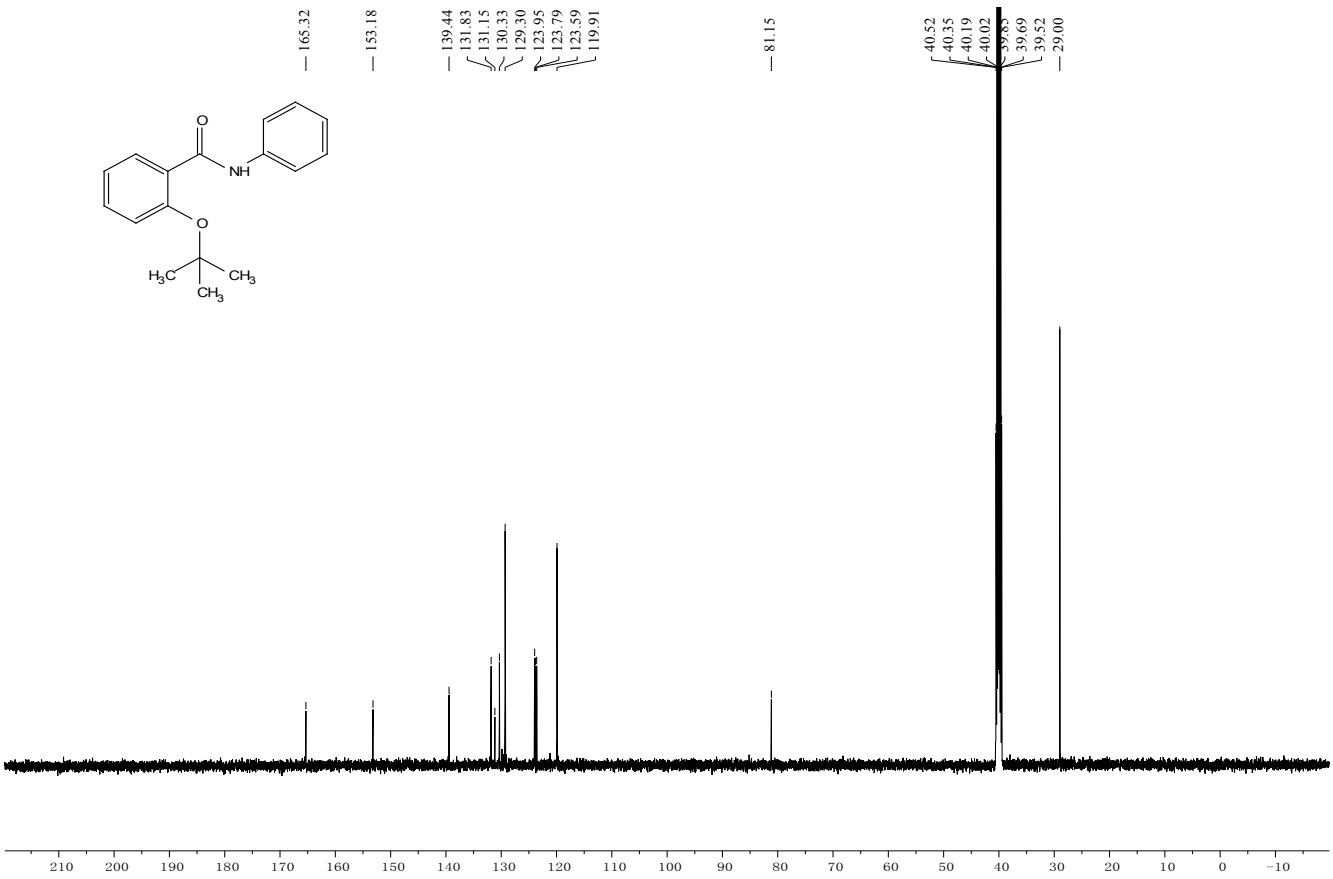

Figure S164. ^{13}C NMR (126 MHz) of **9i** in DMSO-d_6

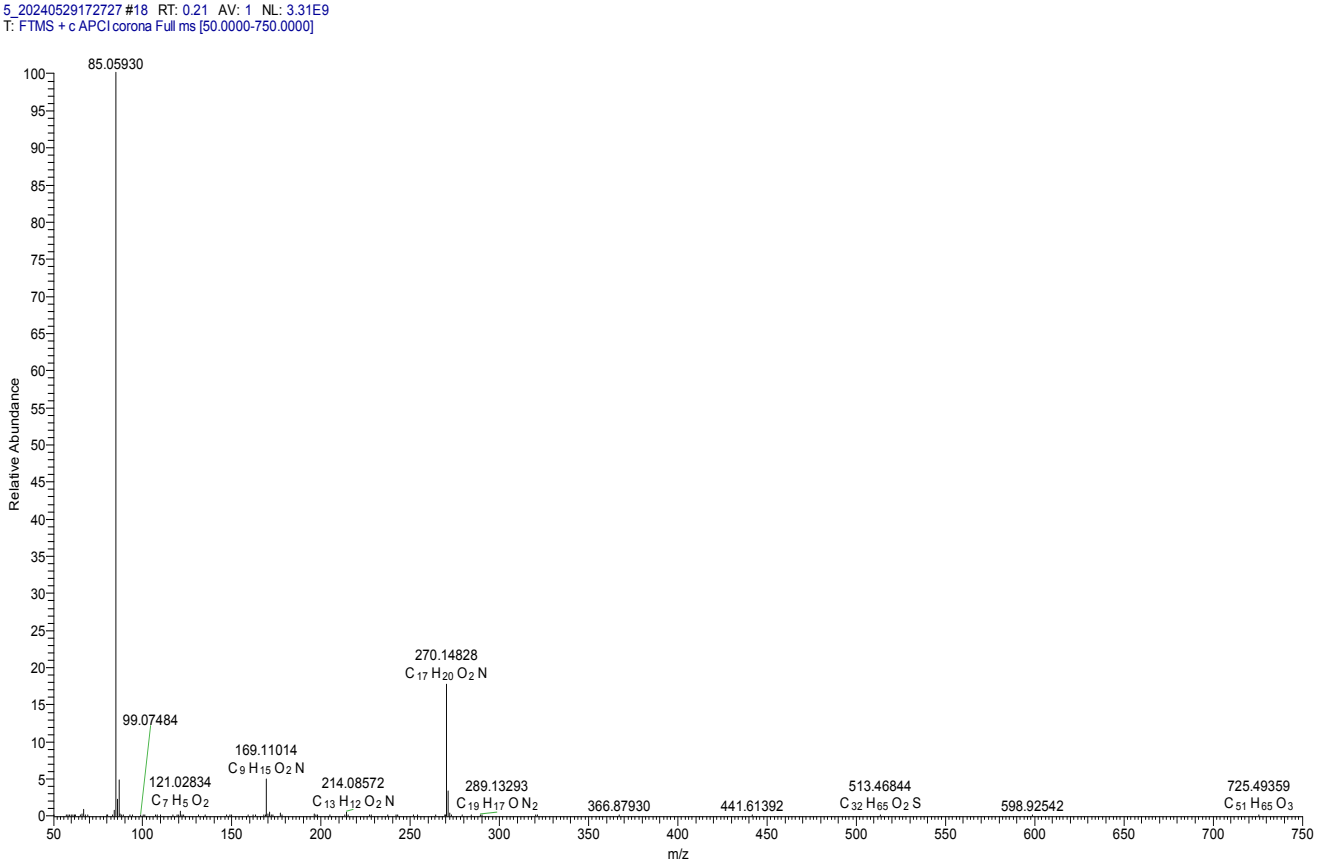

Figure S165. HRMS spectra for **9i.**

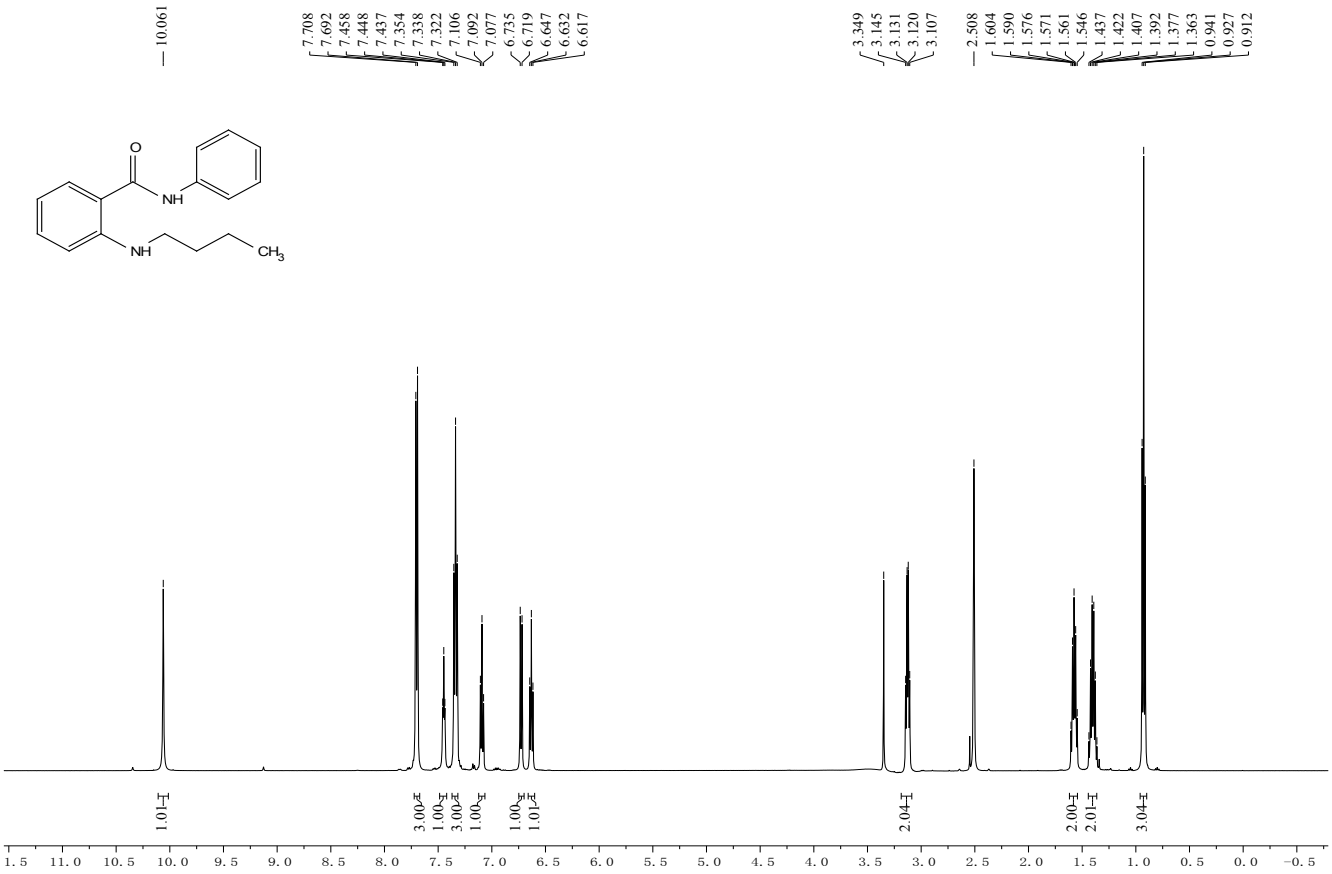

Figure S166. ^{1}H NMR (500 MHz) of **9j** in DMSO-d_6.

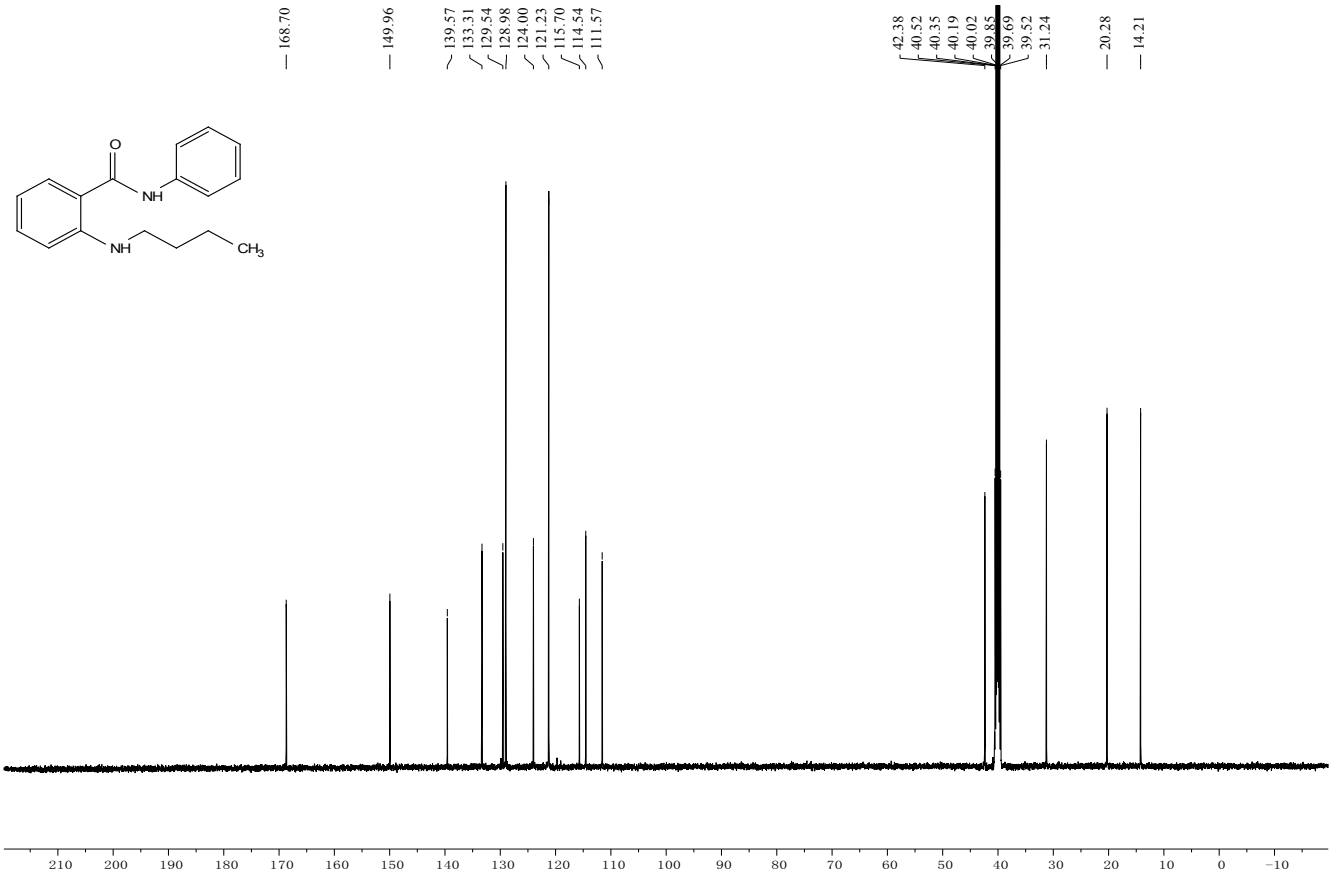

Figure S167. ^{13}C NMR (126 MHz) of **9j** in DMSO-d_6.

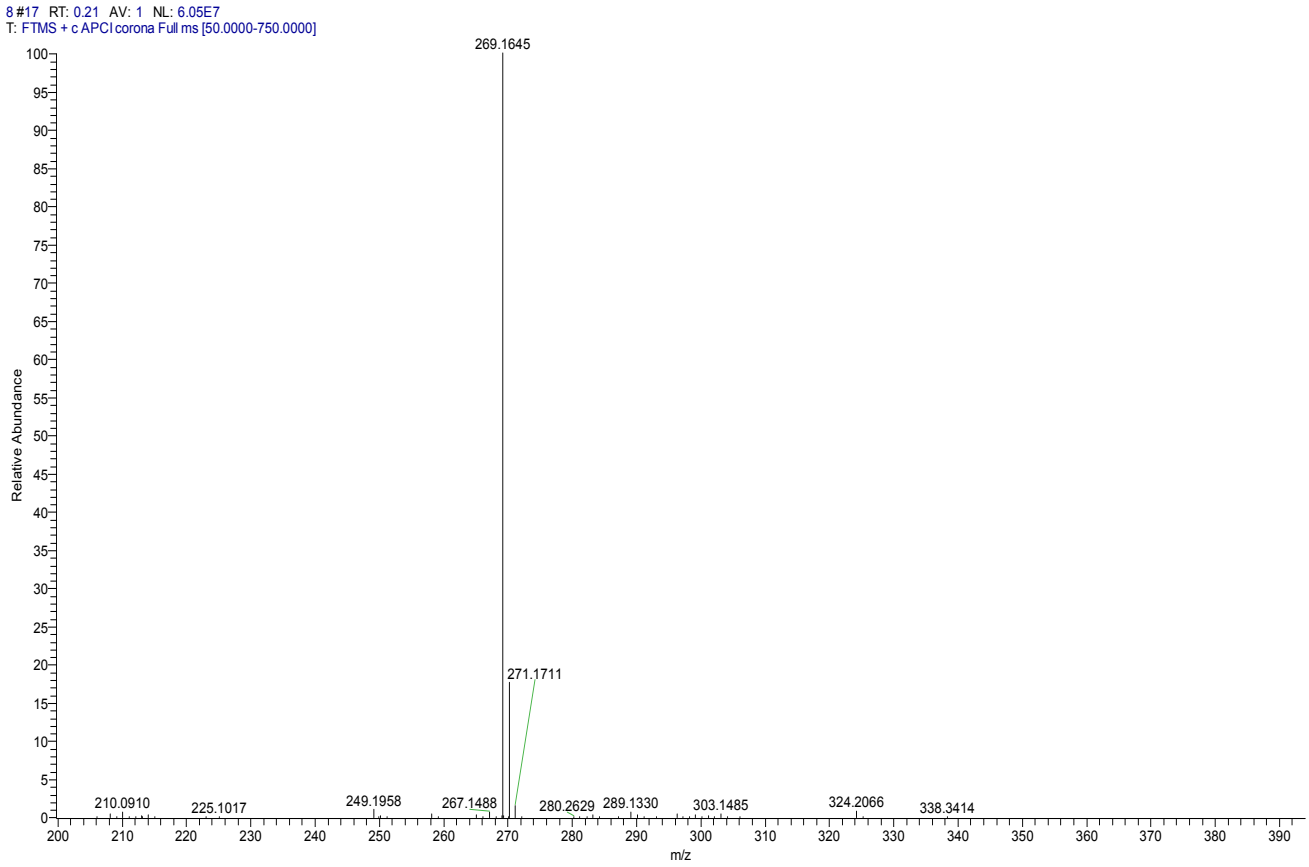

Figure S168. HRMS spectra for **9j**.

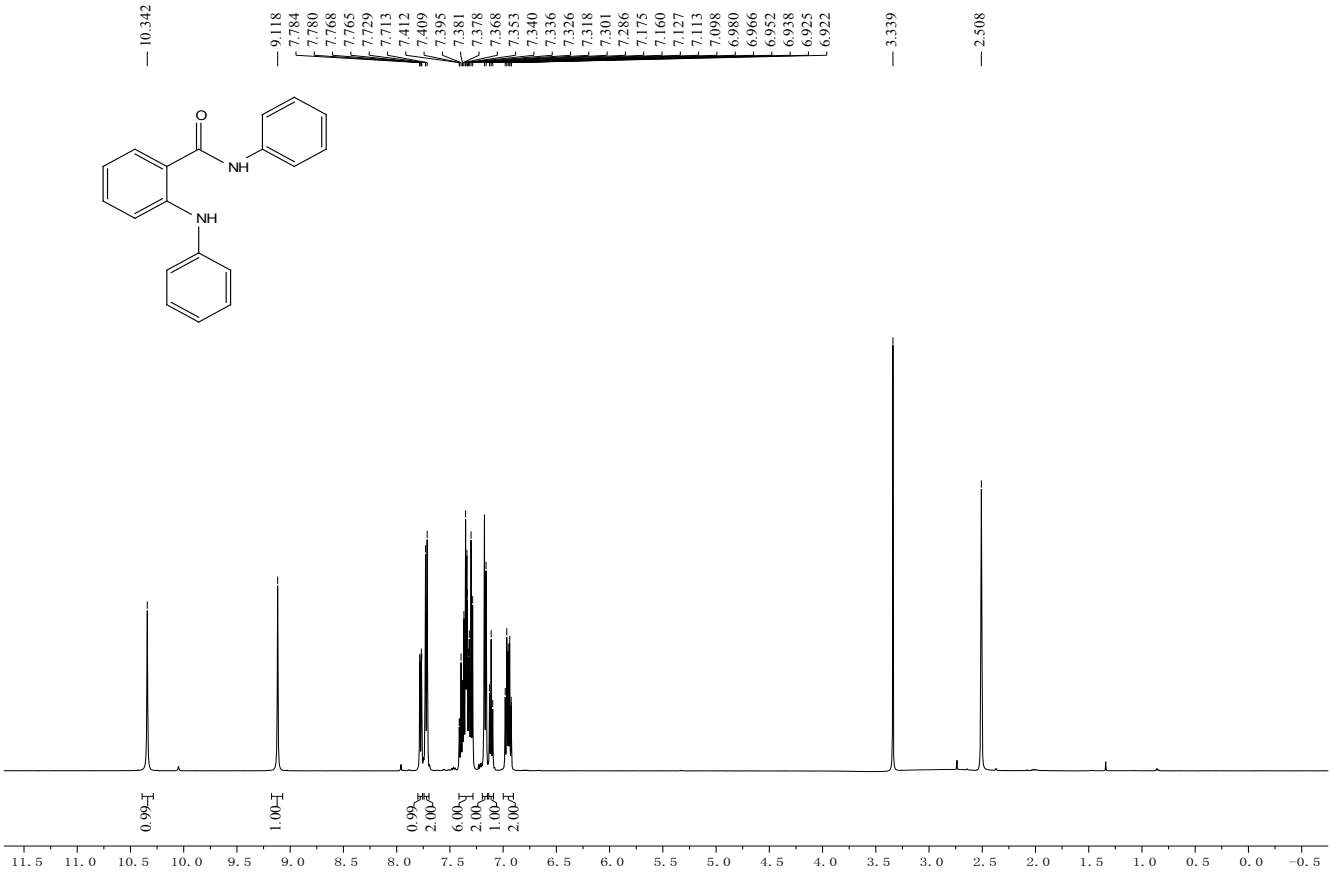

Figure S169. ^{1}H NMR (500 MHz) of **9k** in DMSO-d_6.

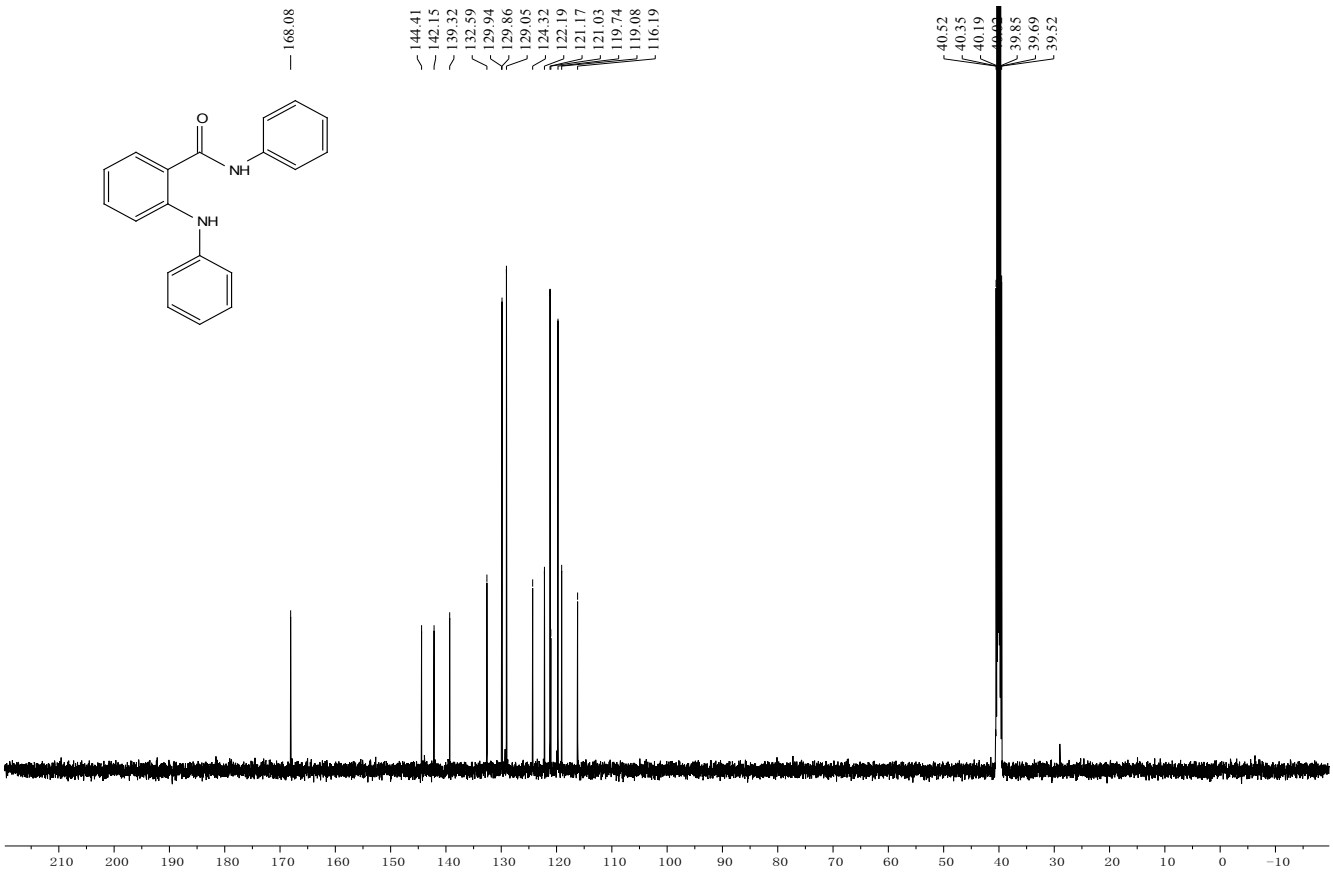

Figure S170. ^{13}C NMR (126 MHz) of **9k** in DMSO-d_6.

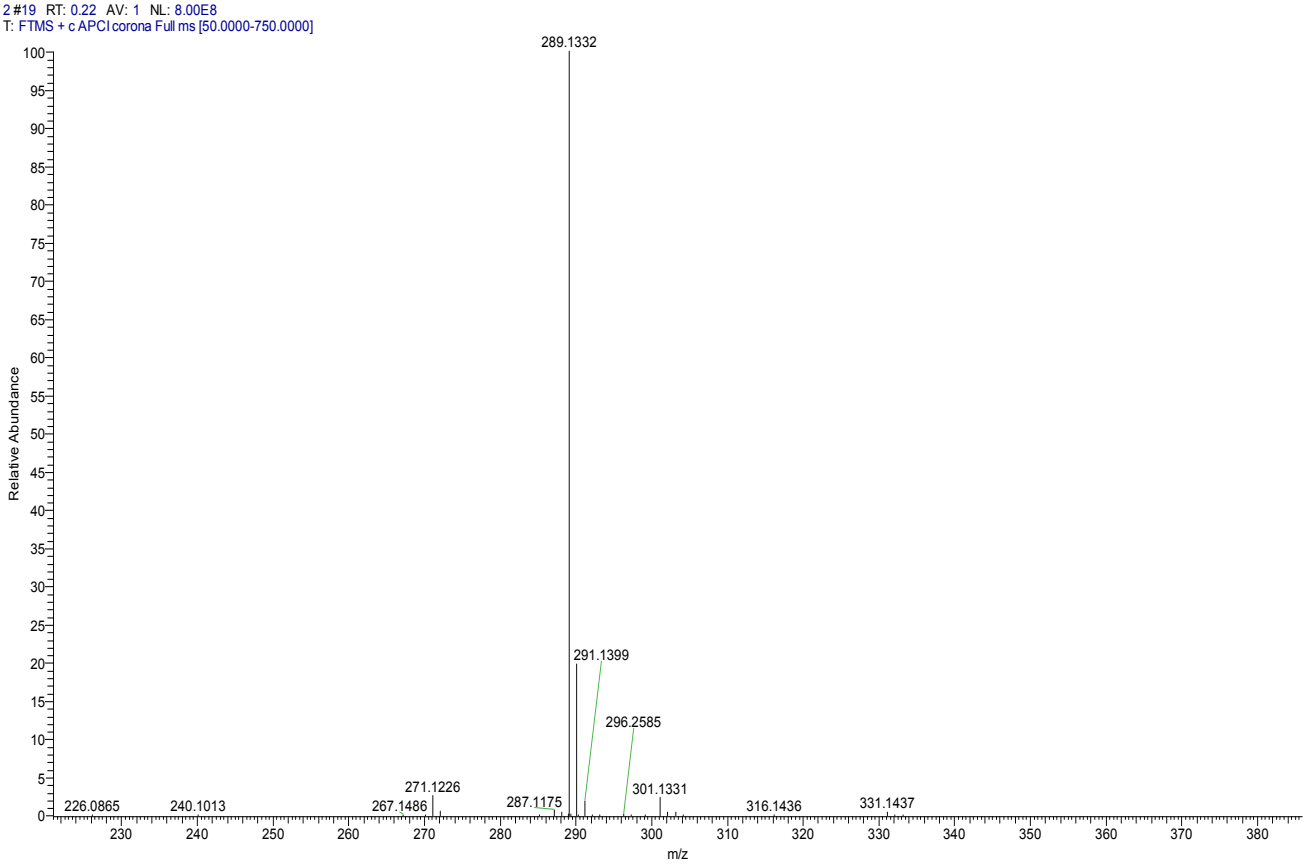

Figure S171. HRMS spectra for **9k**.

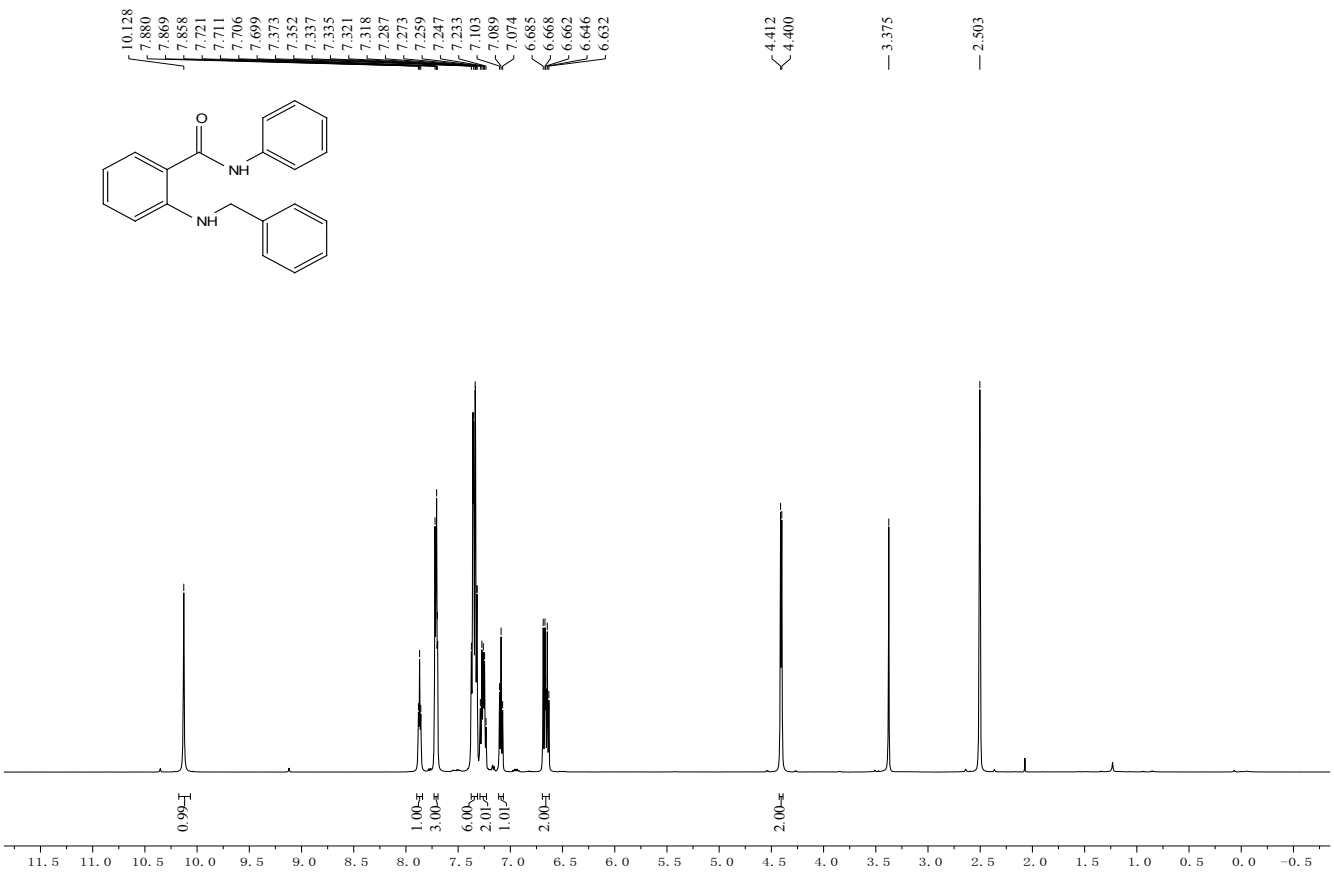

Figure S172. ^{1}H NMR (500 MHz) of **91** in DMSO-d_6.

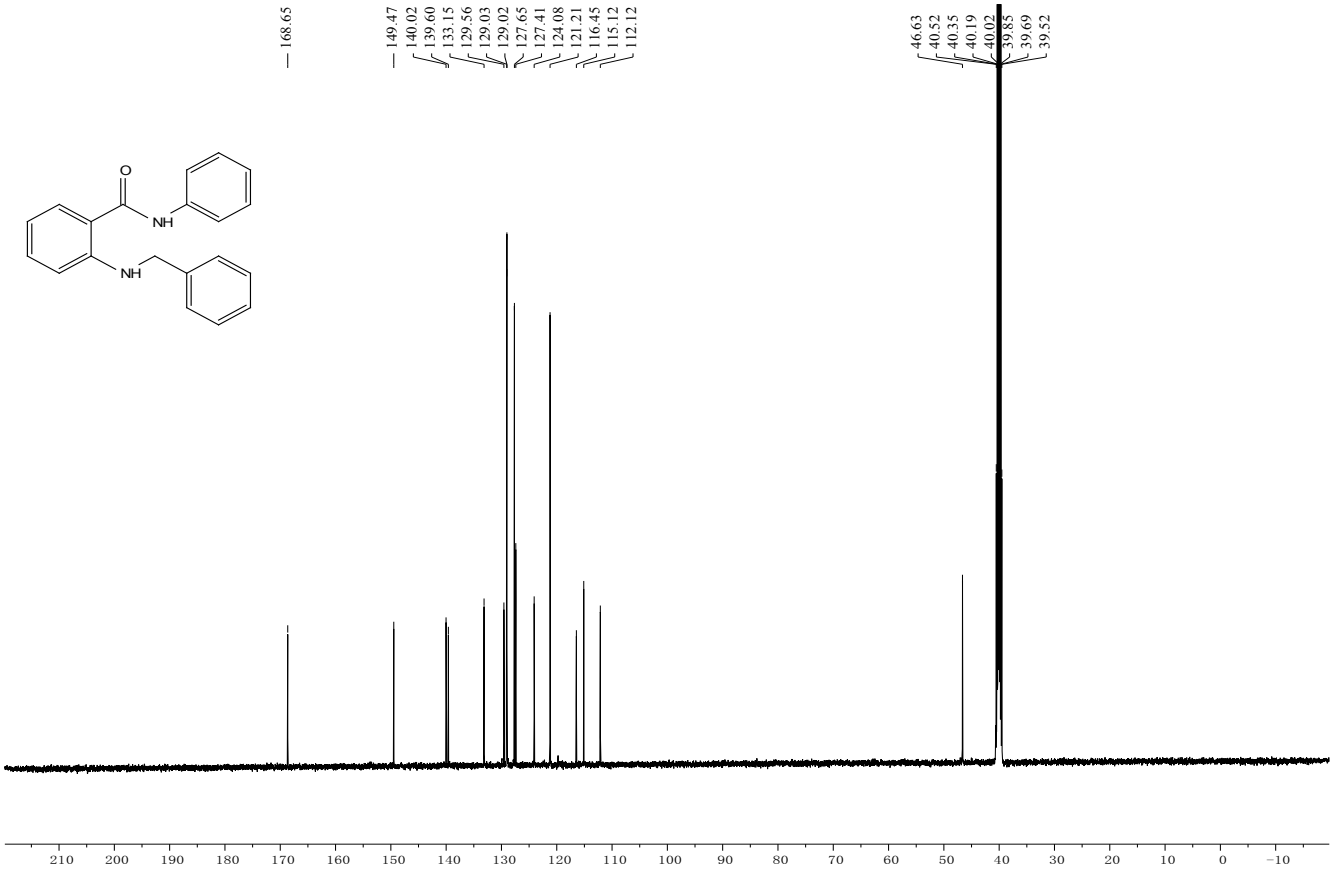

Figure S173. ^{13}C NMR (126 MHz) of **91** in DMSO-d_6.

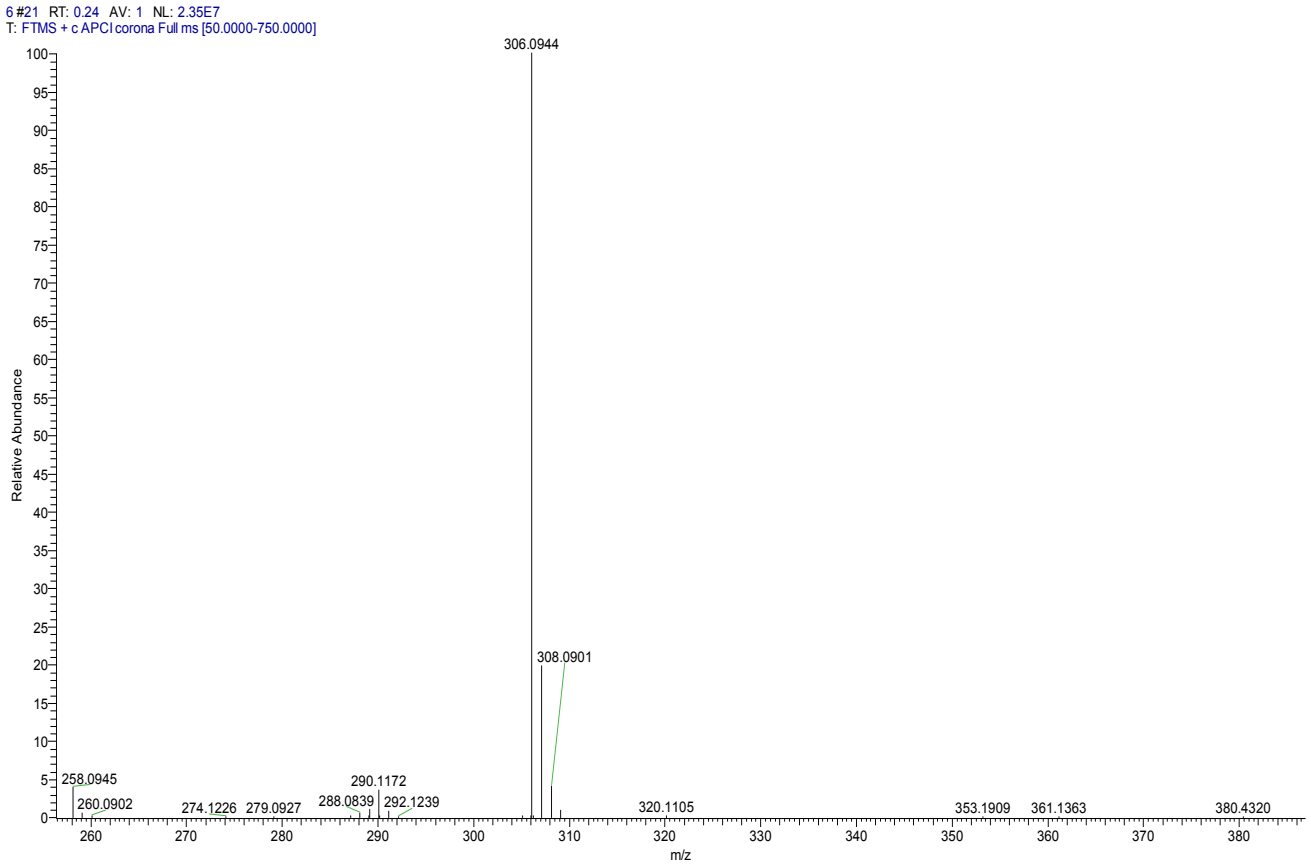

Figure S174. HRMS spectra for **9l**.

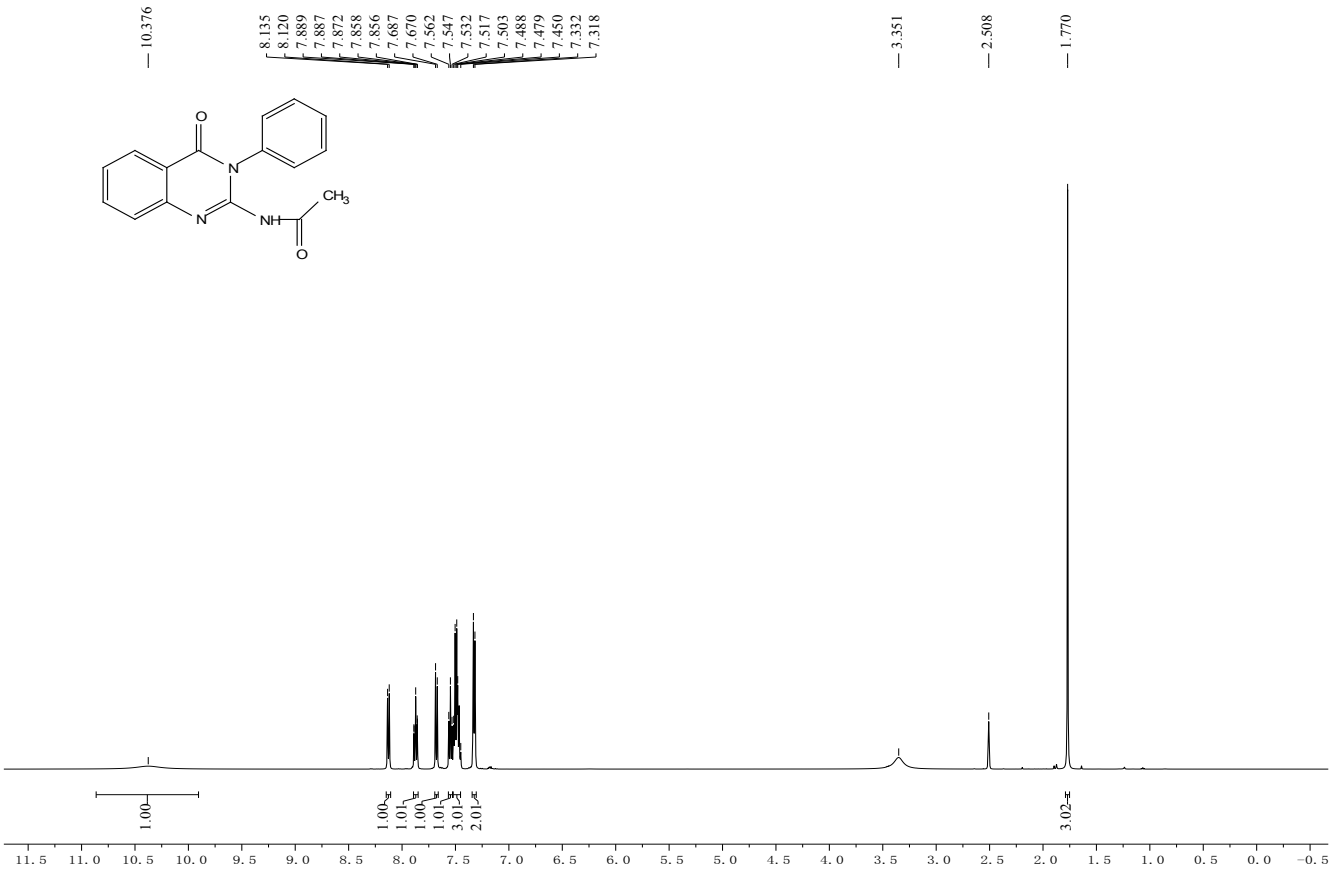

Figure S175. ^{1}H NMR (500 MHz) of **10a** in DMSO-d_6.

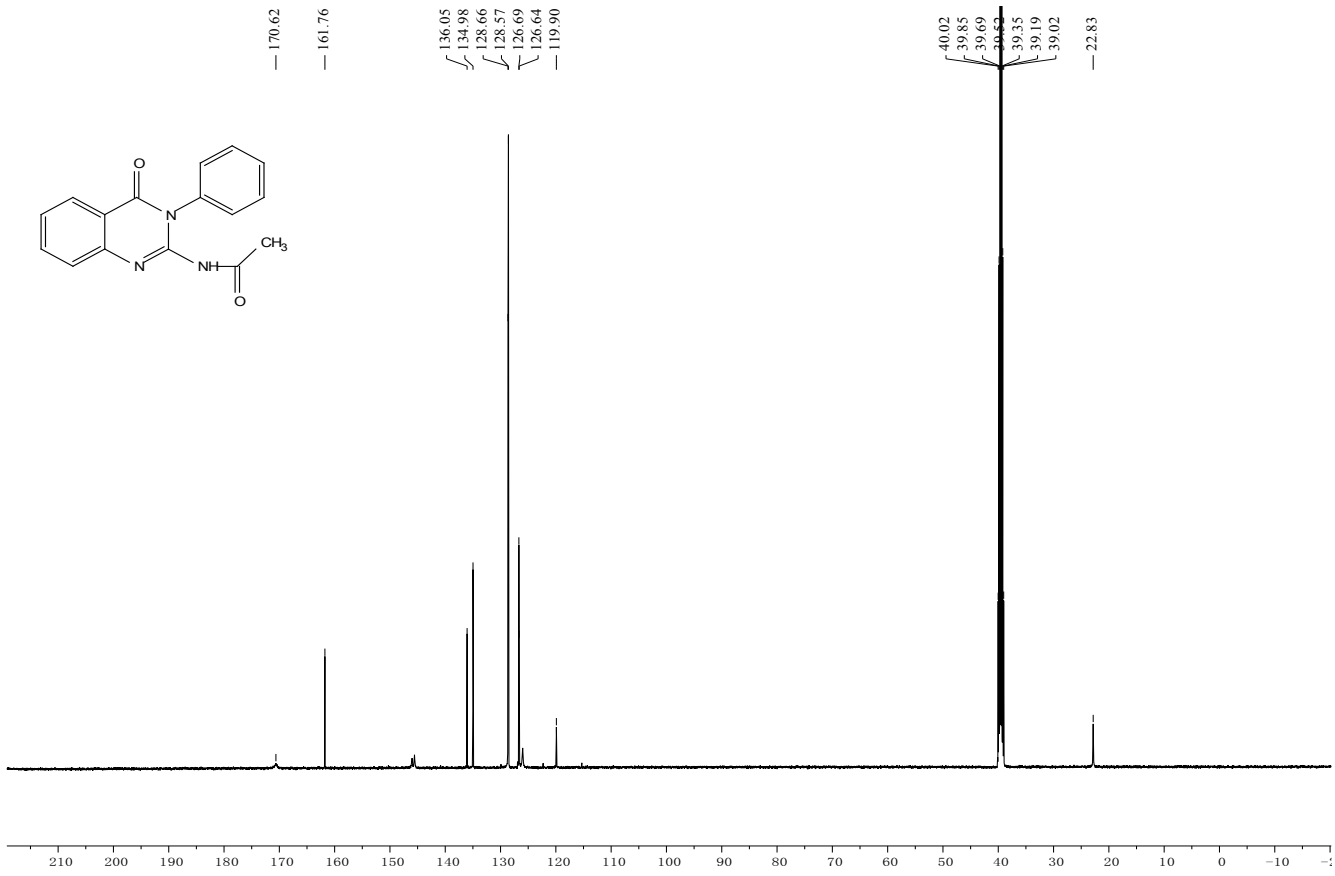

Figure S176. ^{13}C NMR (126 MHz) of **10a** in DMSO-d_6.

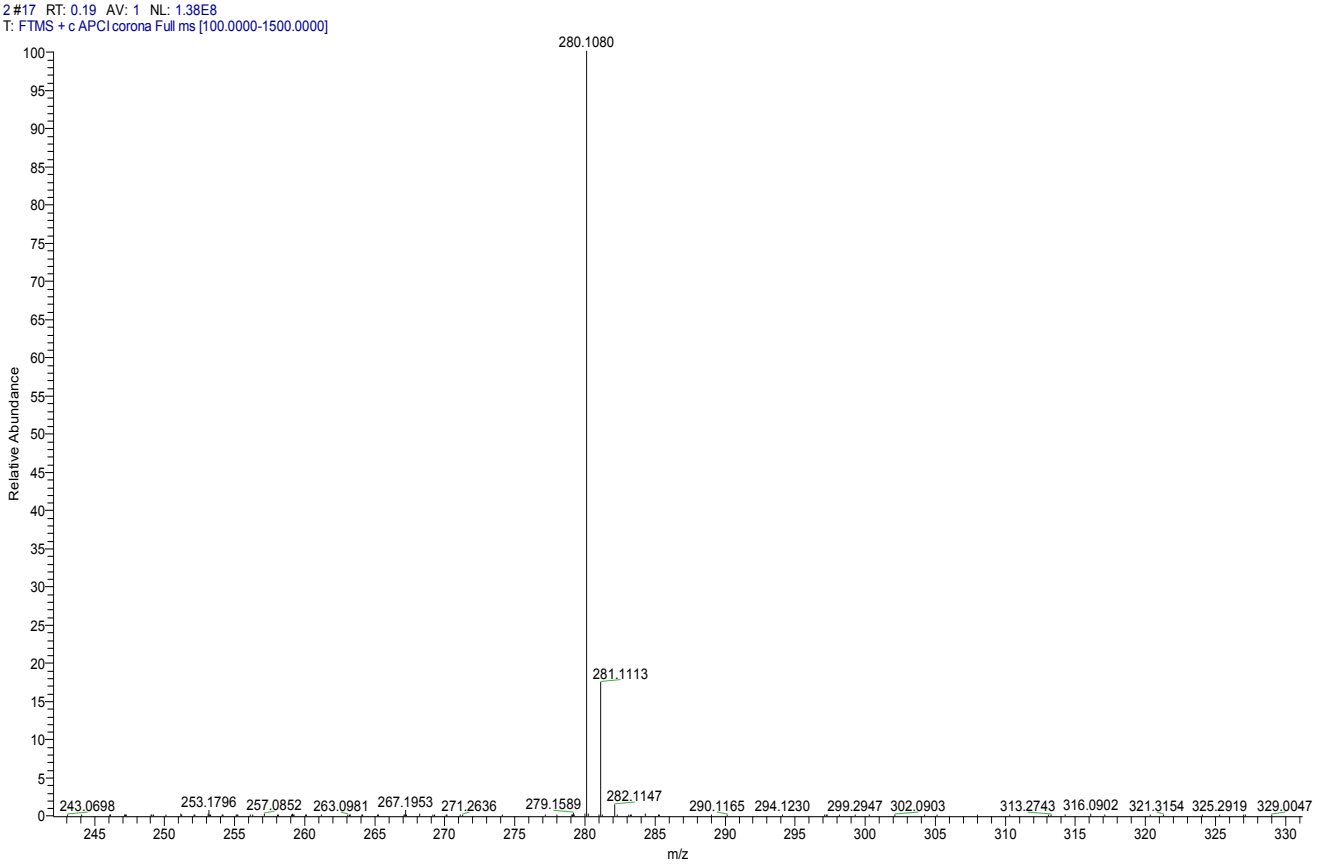

Figure S177. HRMS spectra for **10a**.

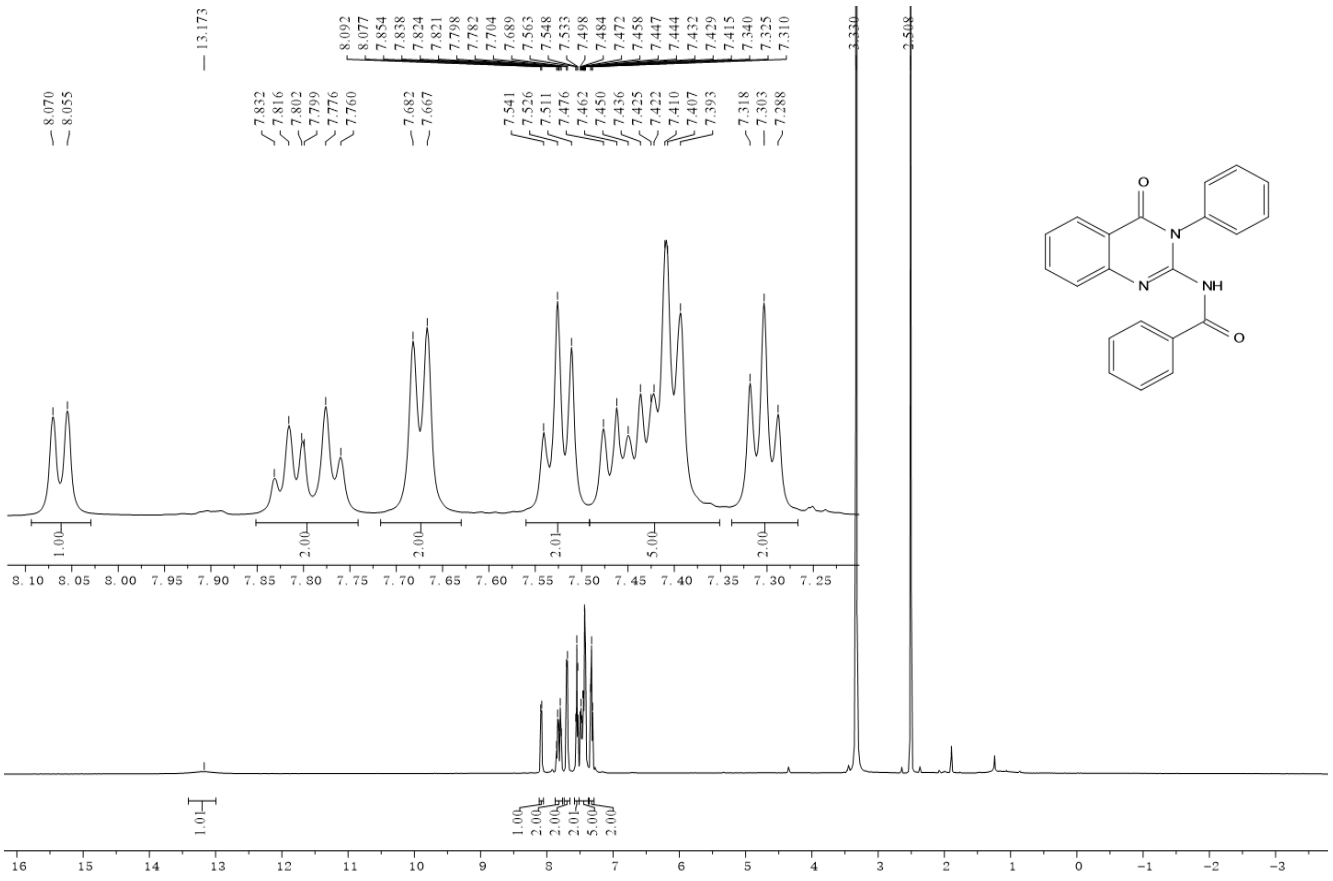

Figure S178. ^{1}H NMR (500 MHz) of **10b** in DMSO-d_6.

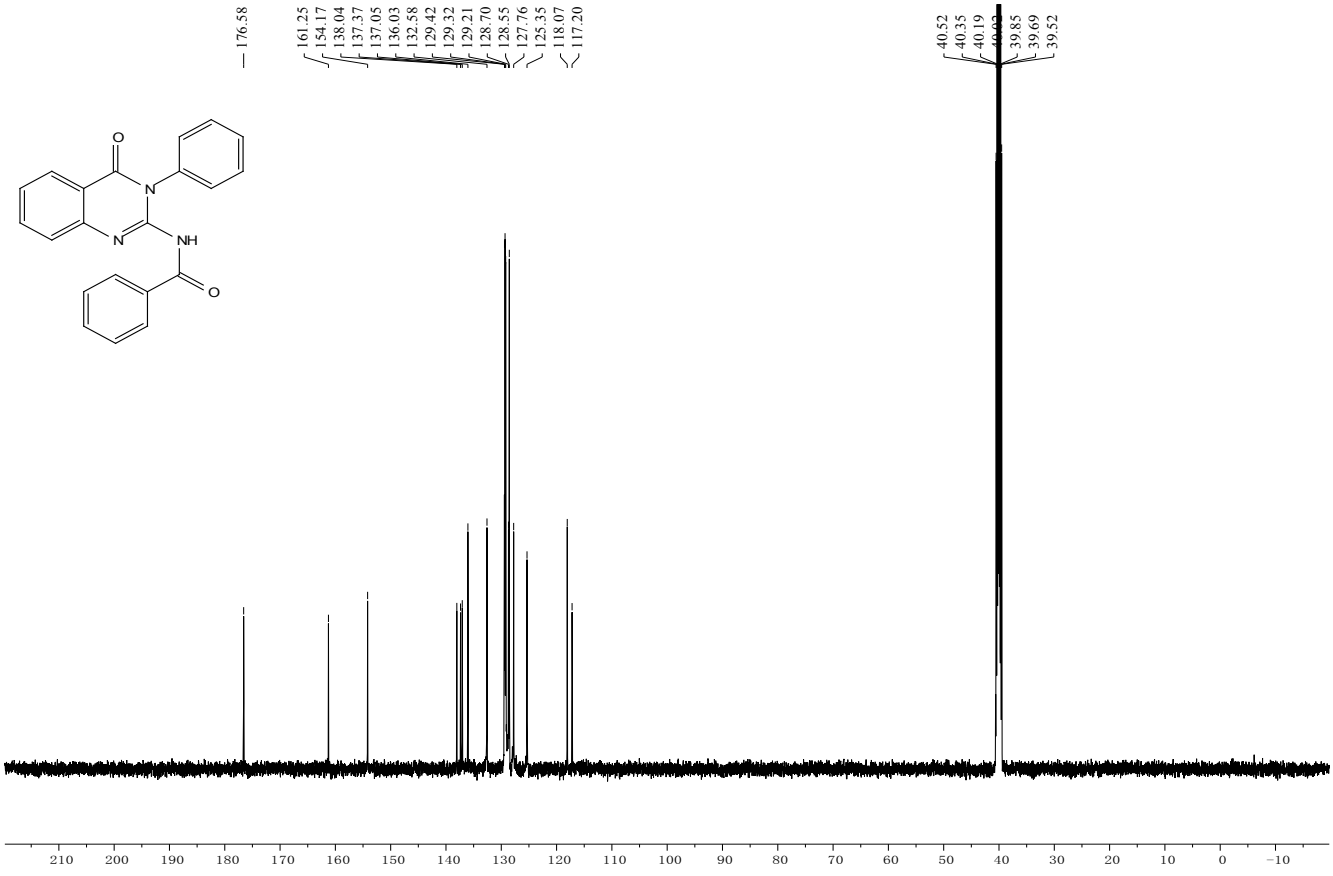

Figure S179. ^{13}C NMR (126 MHz) of **10b** in DMSO-d_6.

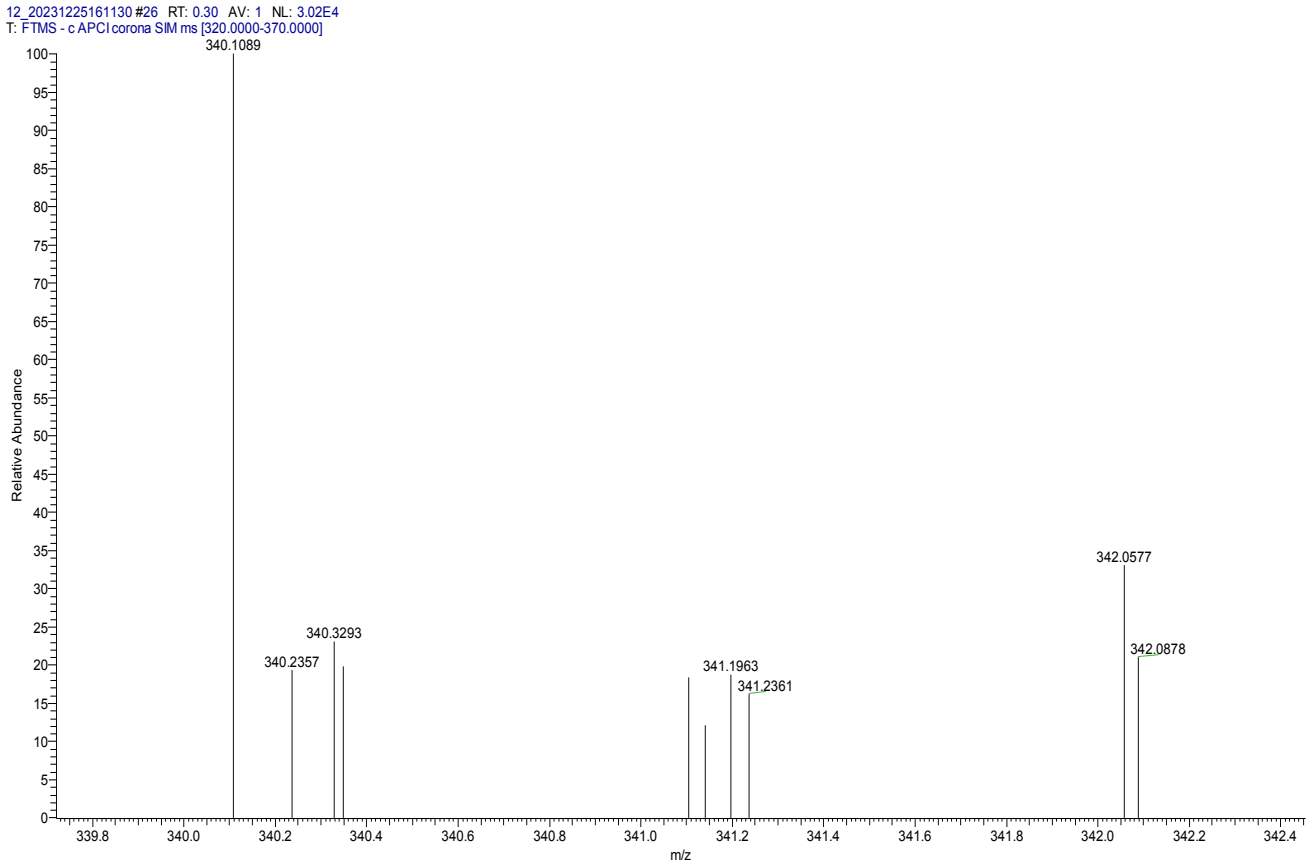

Figure S180. HRMS spectra for **10b**.

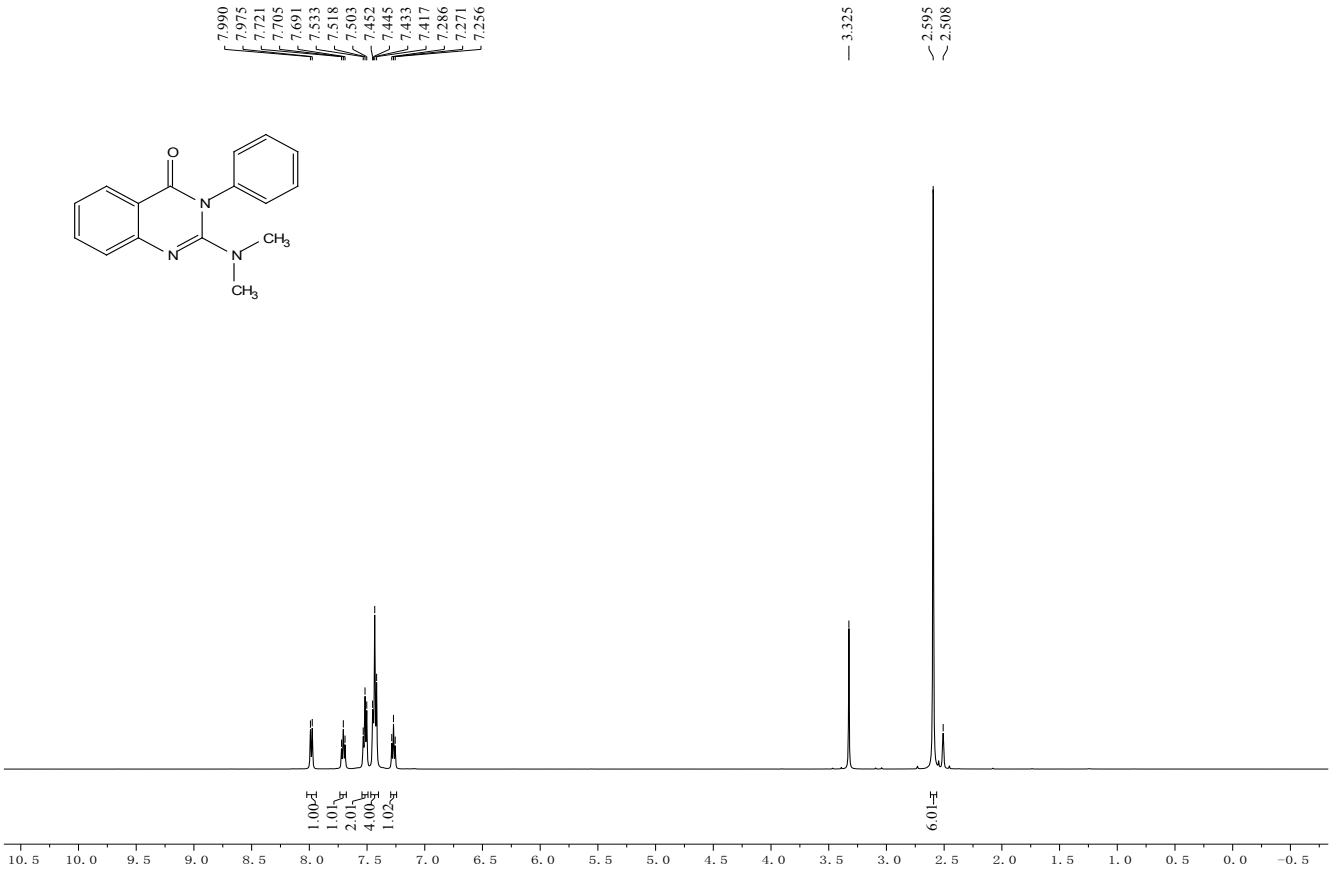

Figure S181. ^{1}H NMR (500 MHz) of **10c** in DMSO-d_6.

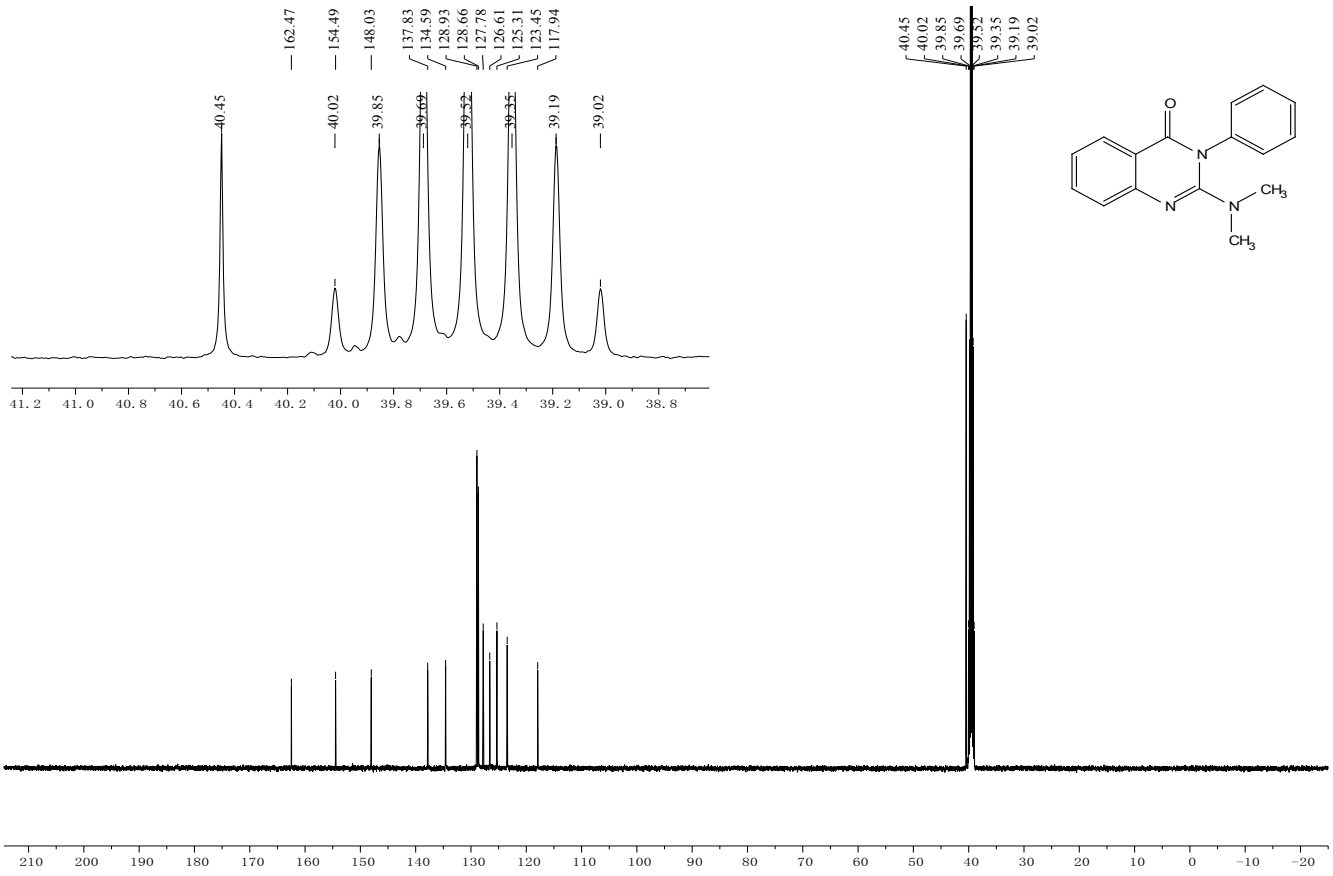

Figure S182. ^{13}C NMR (126 MHz) of **10c** in DMSO-d_6.

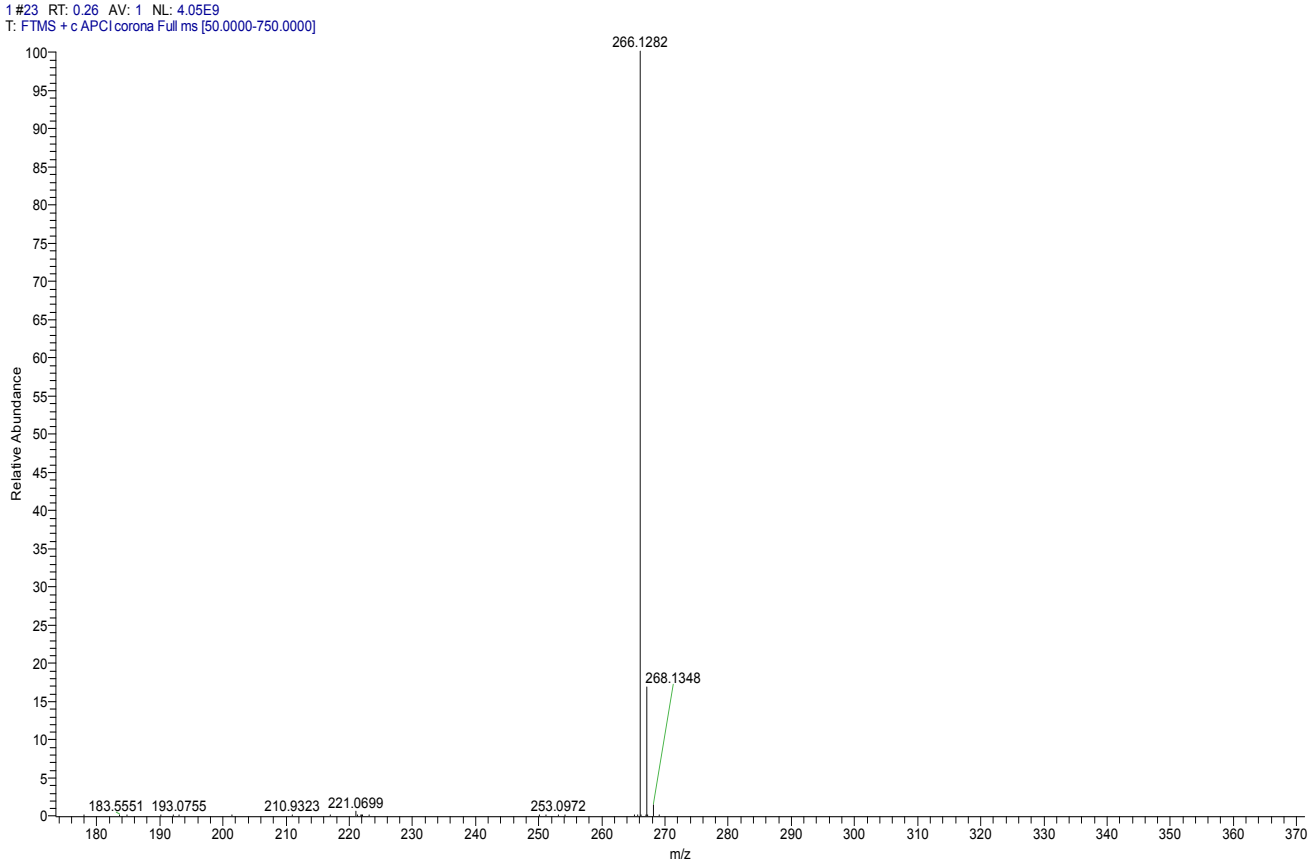

Figure S183. HRMS spectra for **10c**.

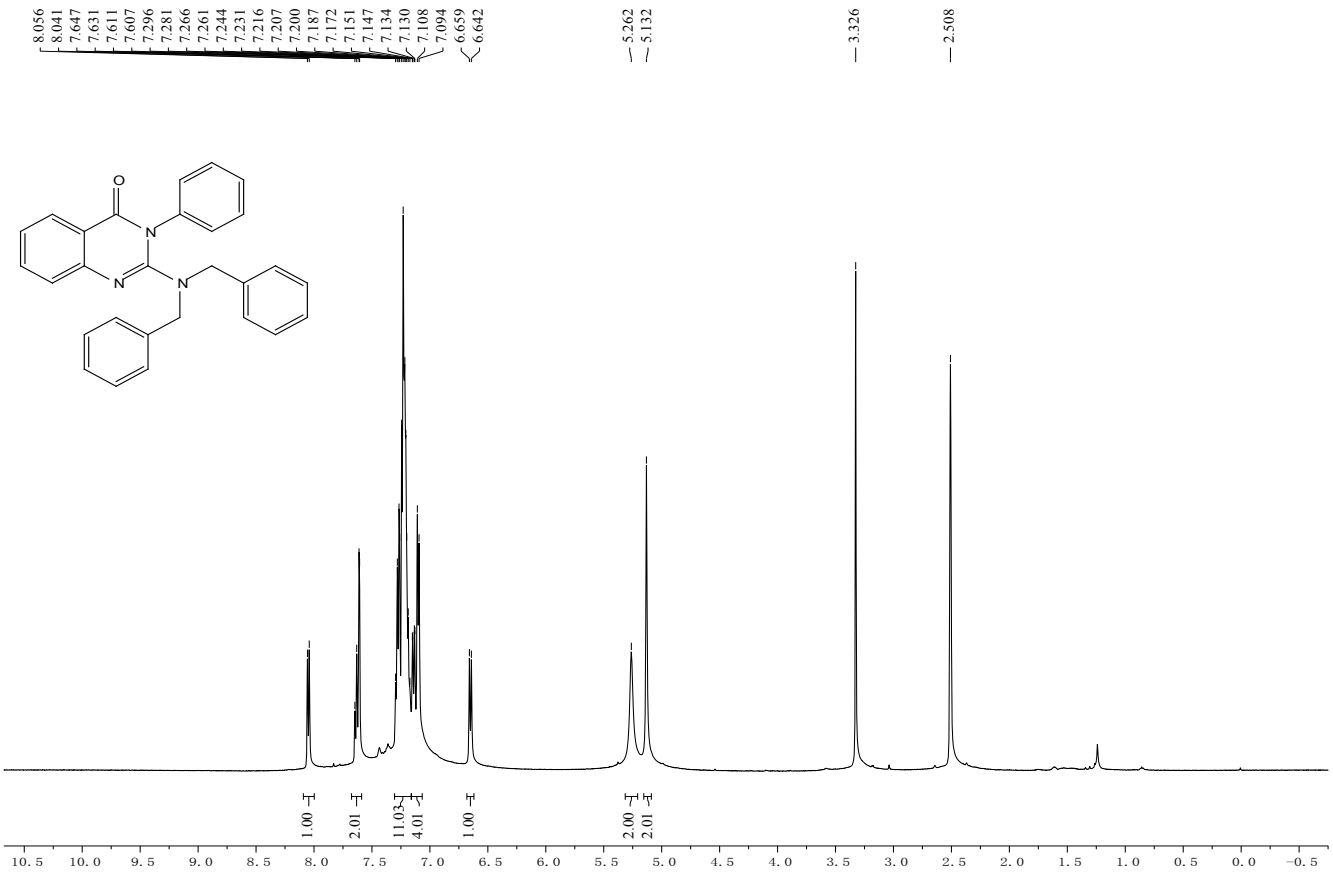

Figure S184. ^{1}H NMR (500 MHz) of **10d** in DMSO-d_6.

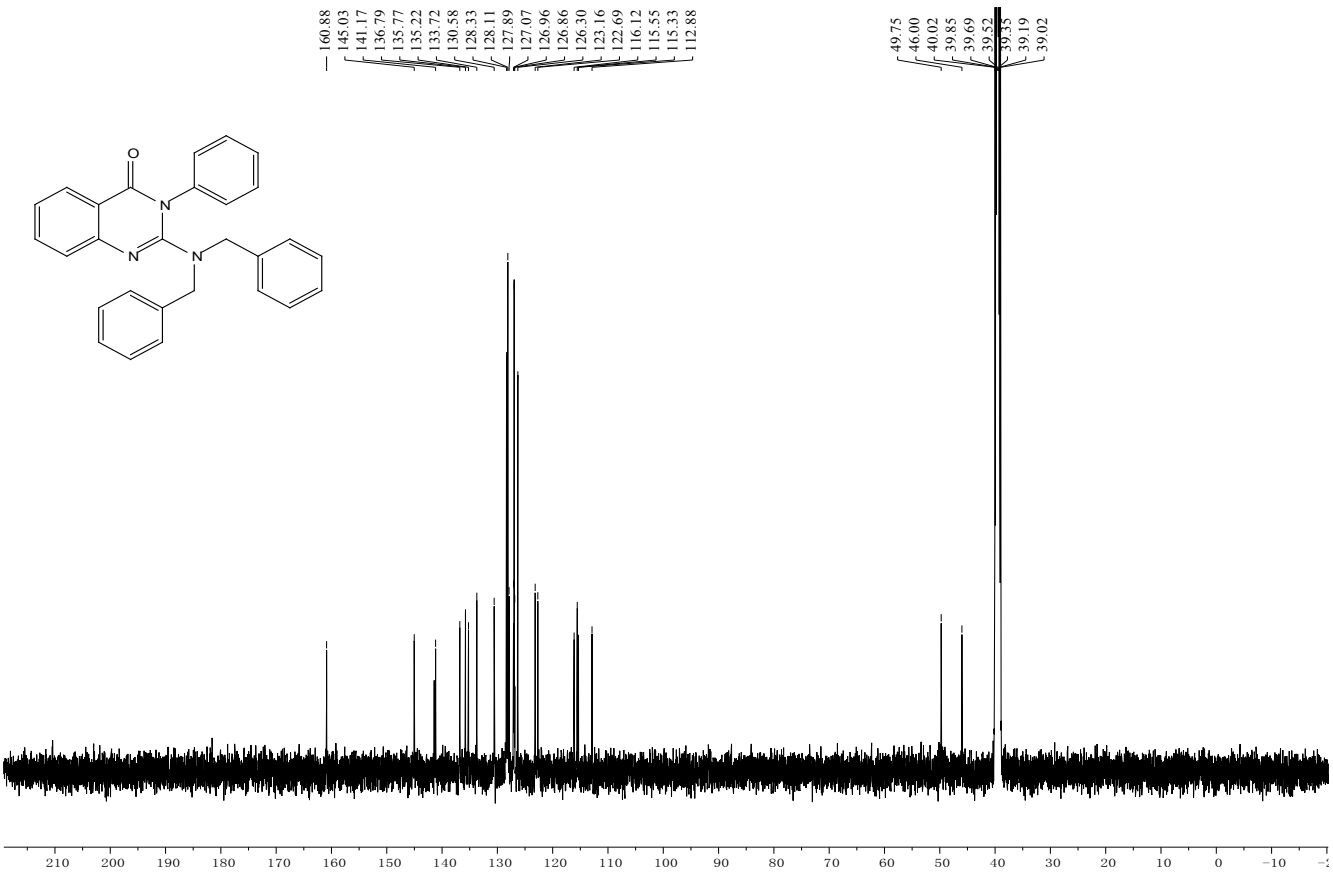

Figure S185. ^{13}C NMR (126 MHz) of **10d** in DMSO-d_6.

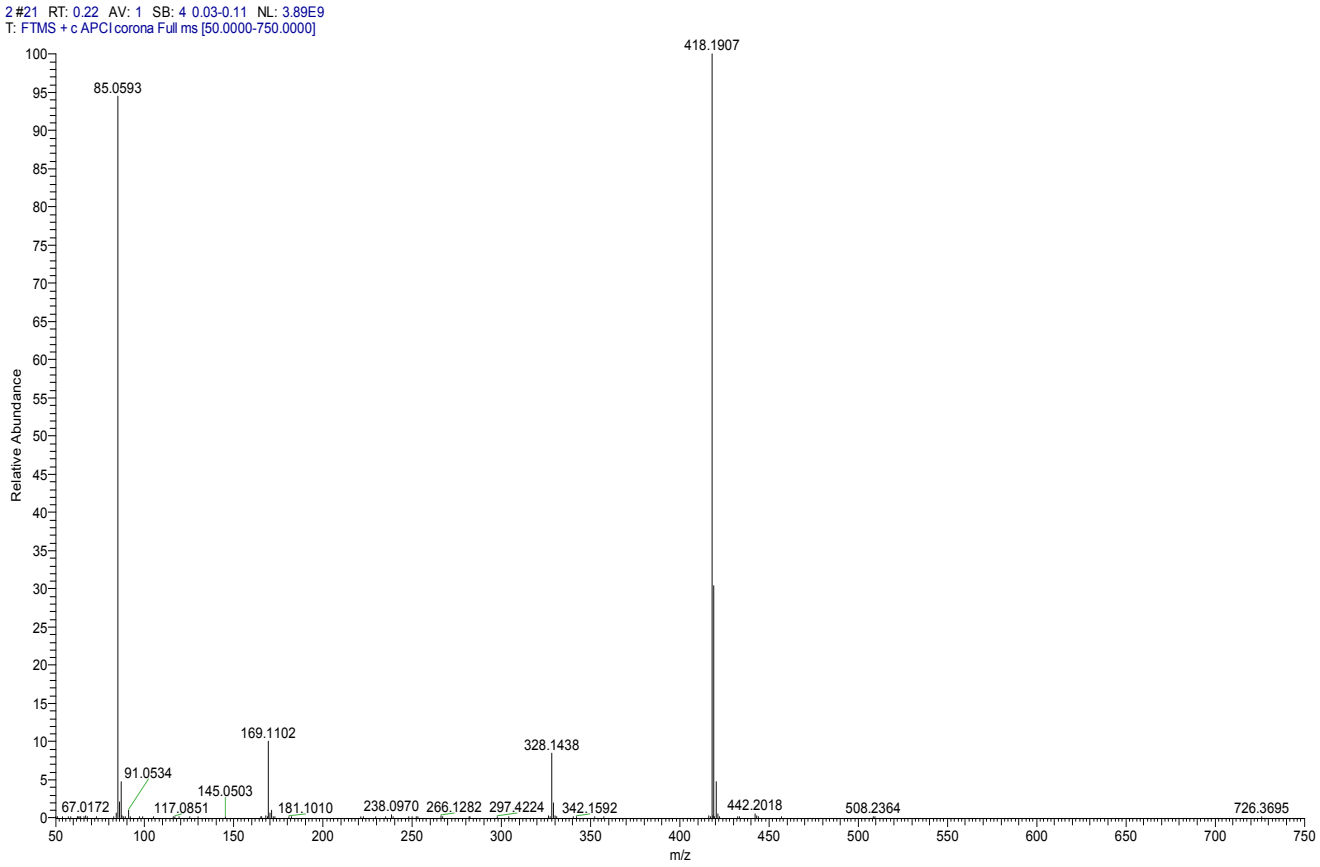

Figure S186. HRMS spectra for **10d**.

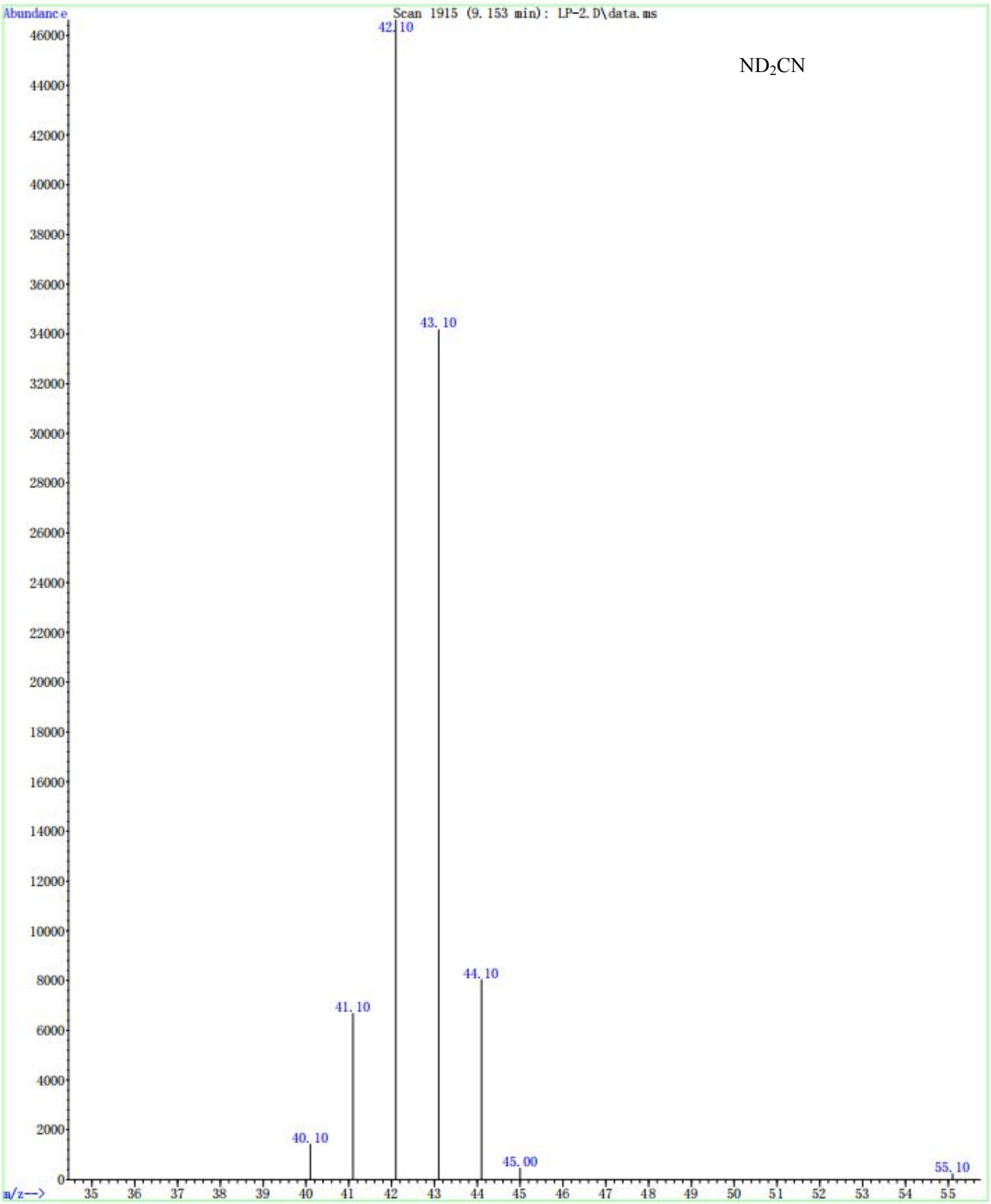

Figure S187. GCMS of **2b**

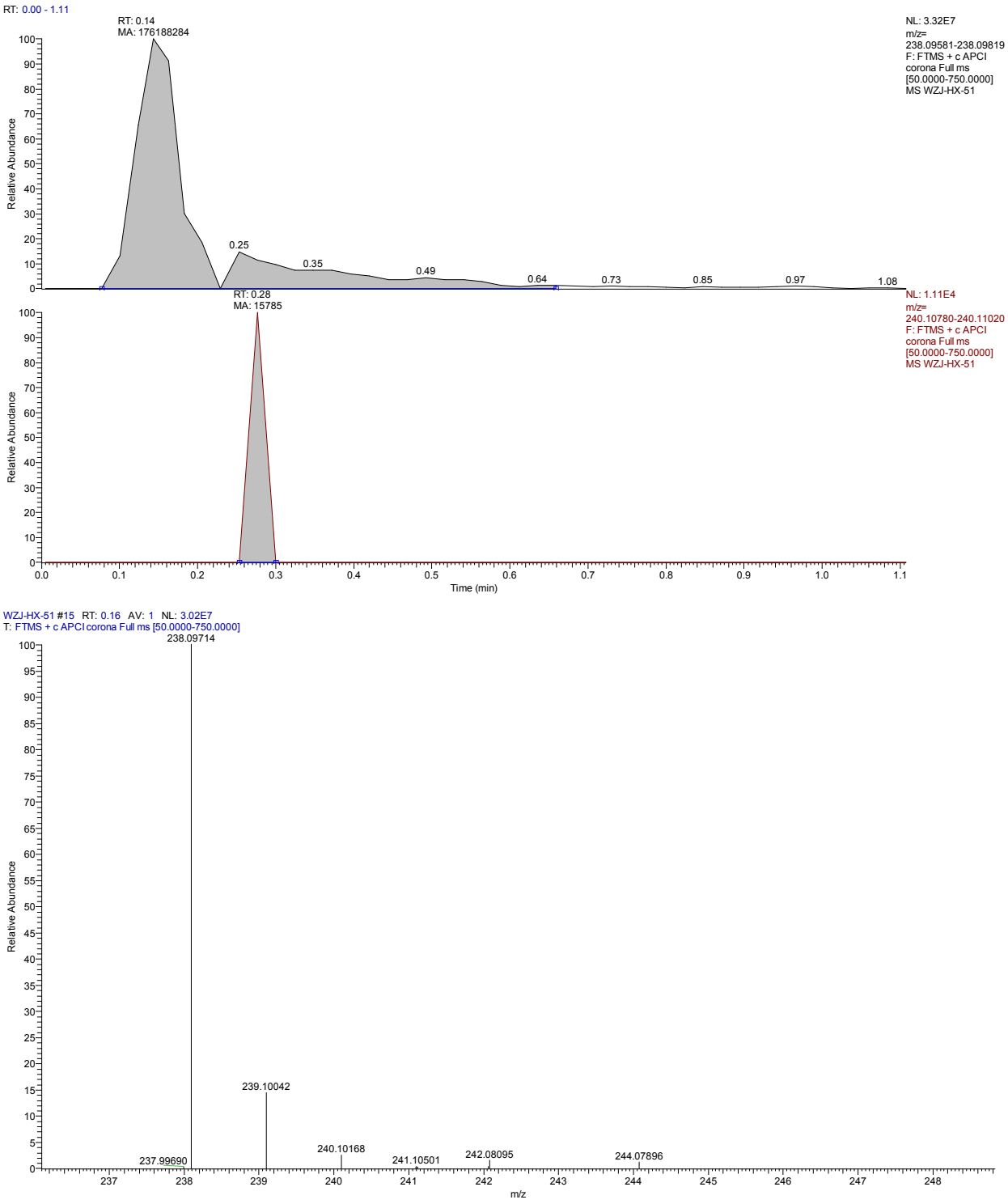

Figure S188. HRMS of 3a' but not 3a''

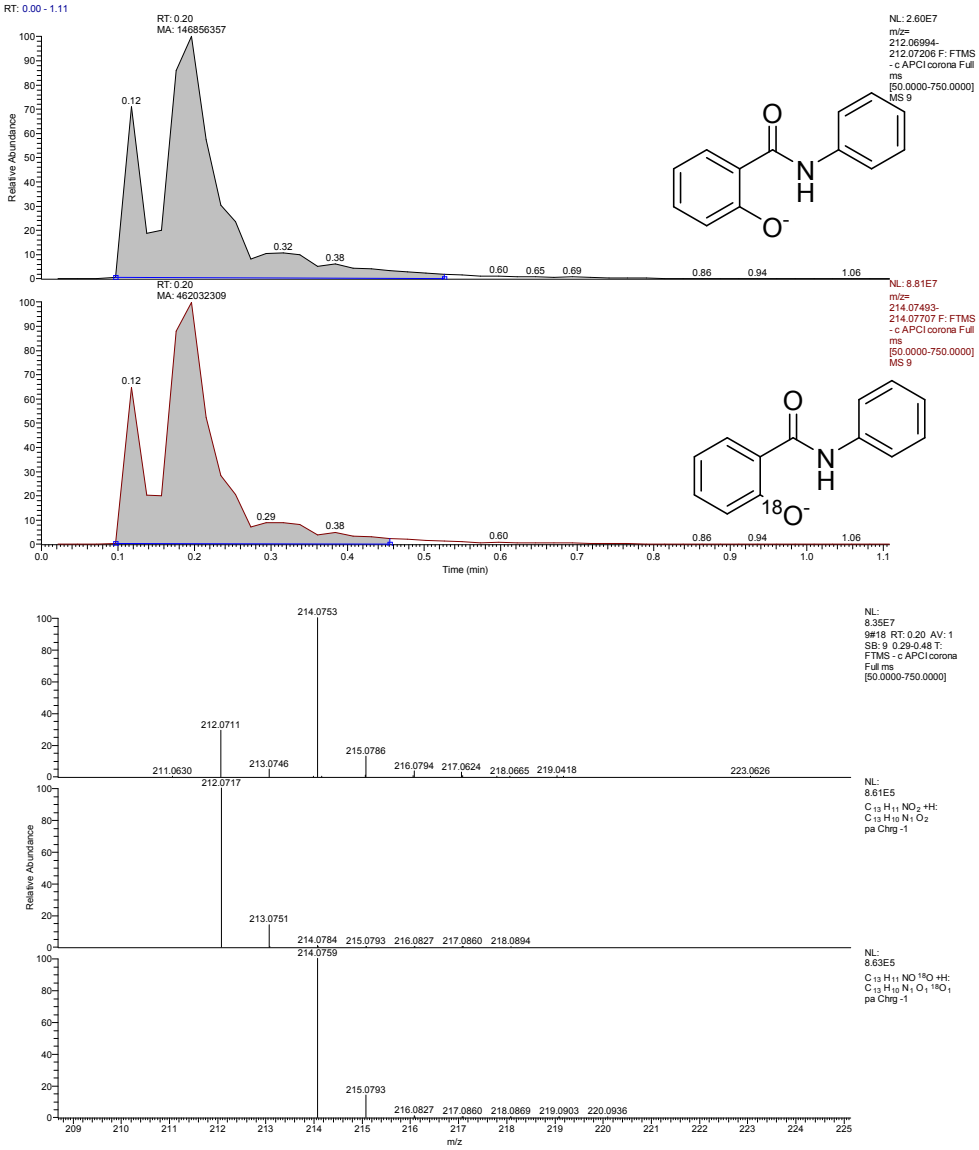

Figure S189. HRMS of **7a'**

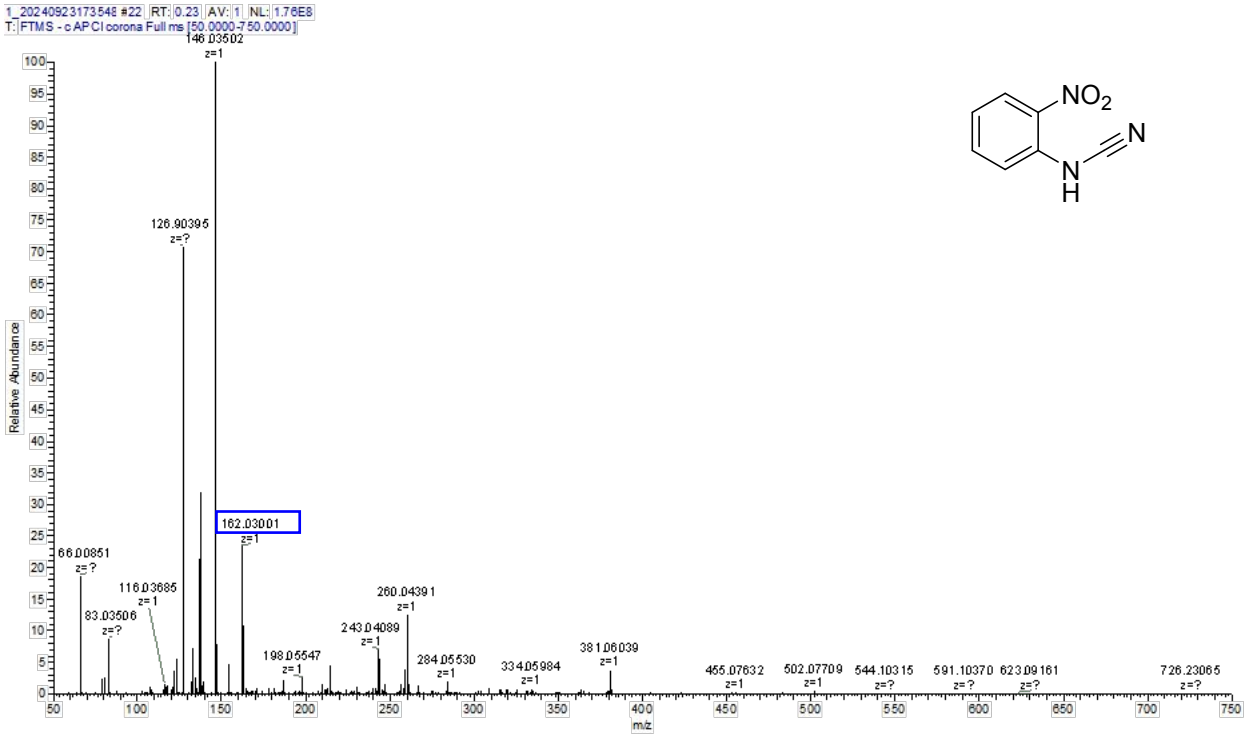

Figure S190. HRMS of *N*-(2-nitrophenyl)cyanamide

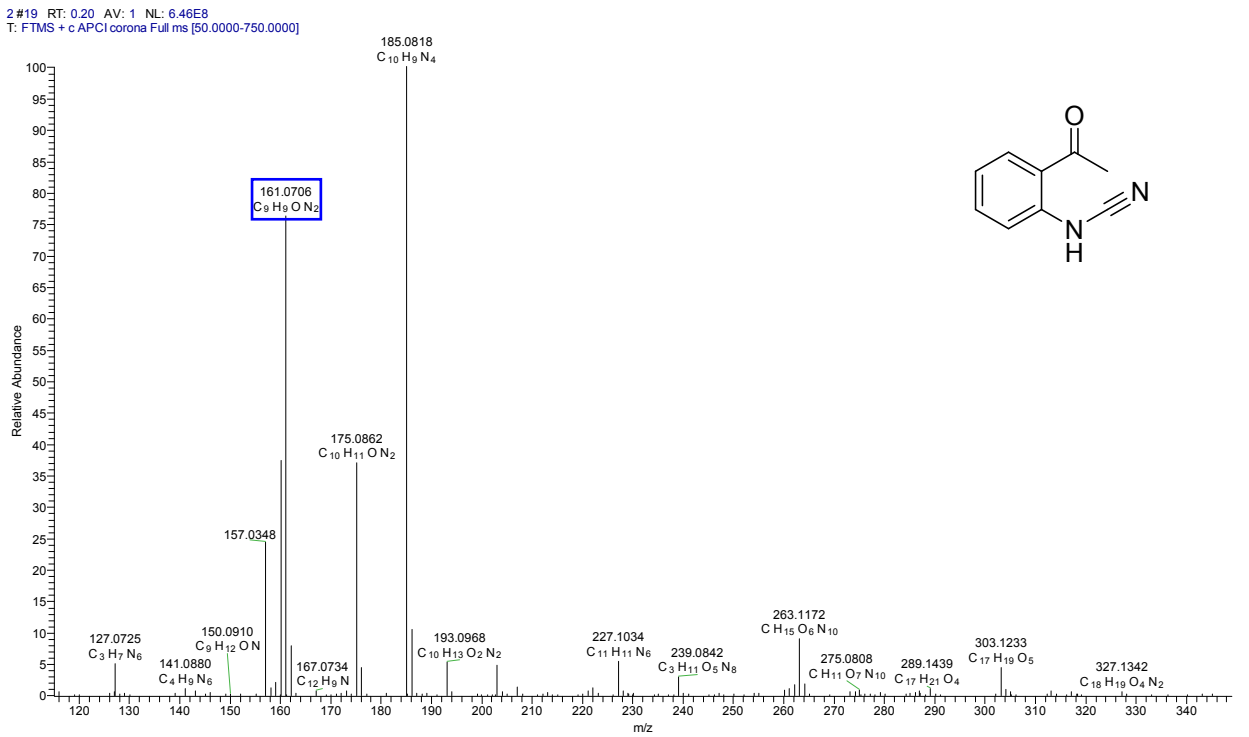

Figure S191. HRMS of *N*-(2-acetylphenyl)cyanamide

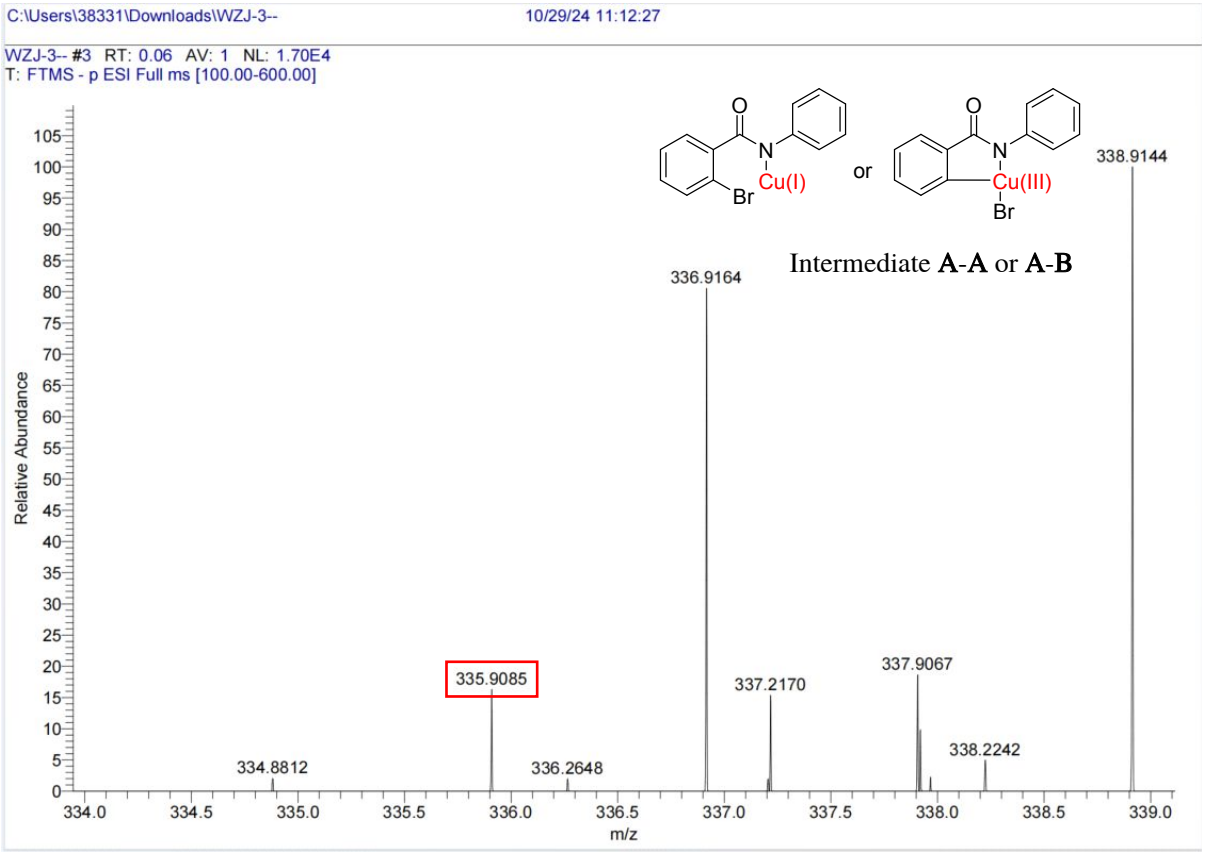

Figure S192. HRMS of Intermediate **A-A** or **A-B**

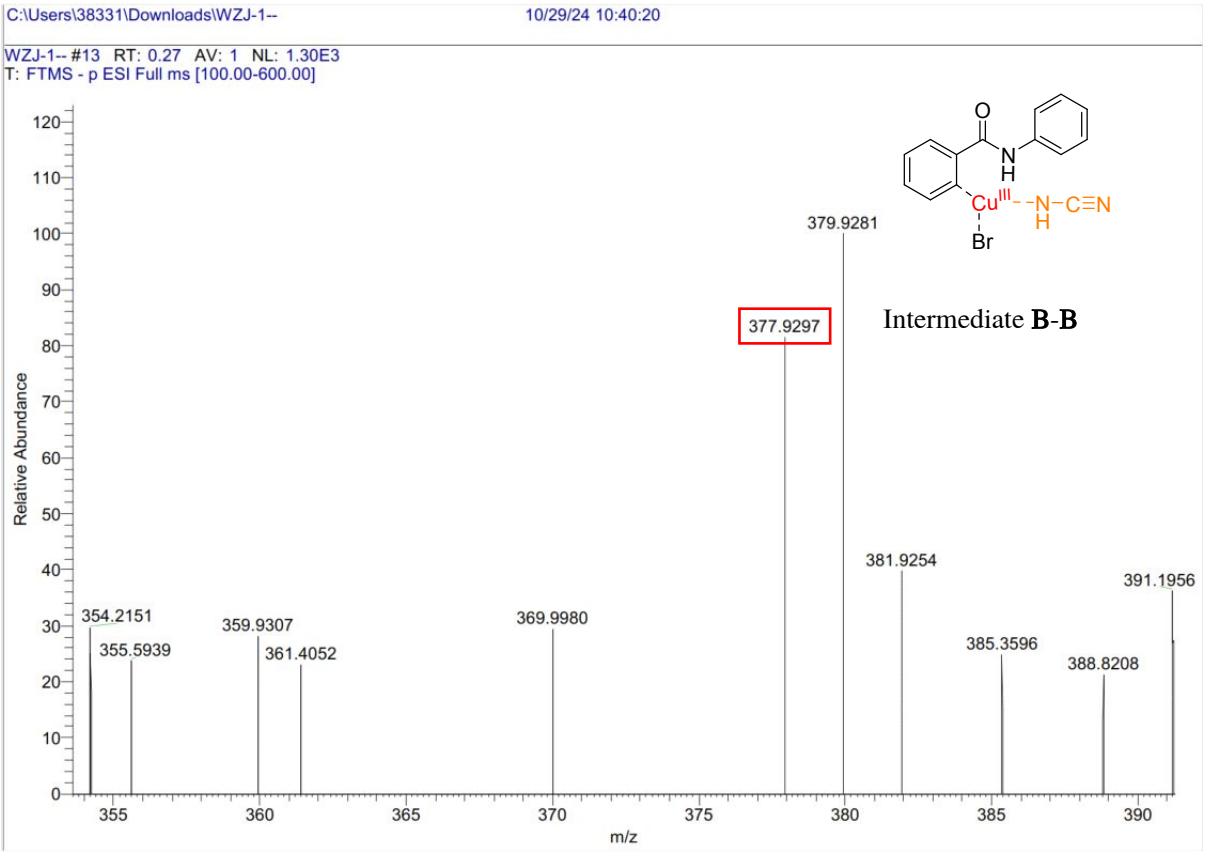

Figure S193. HRMS of Intermediate **B-B**

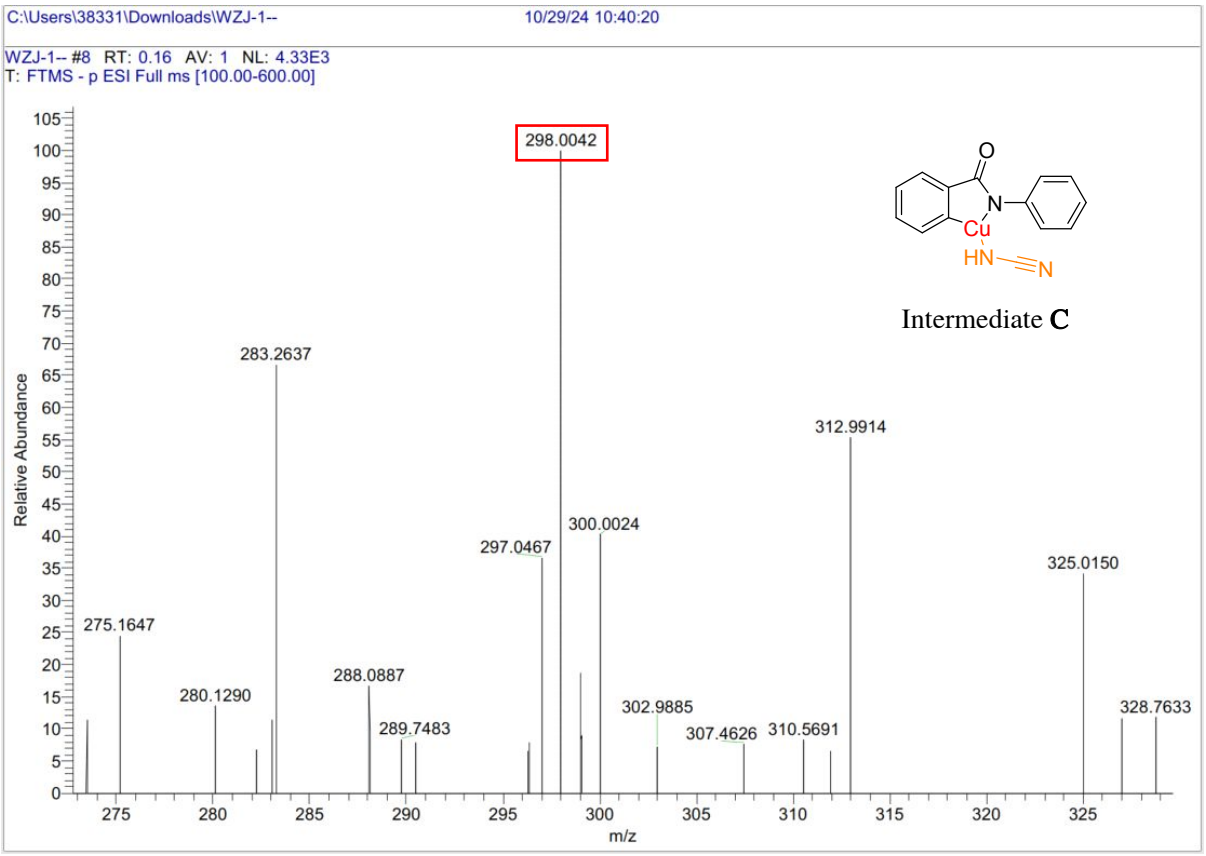

Figure S194. HRMS of Intermediate **C**

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