Supporting Information

Synthesis of Indoles and Quinazolines via additive-controlled selective C-H activation/annulation of *N*-arylamidines and sulfoxonium ylides

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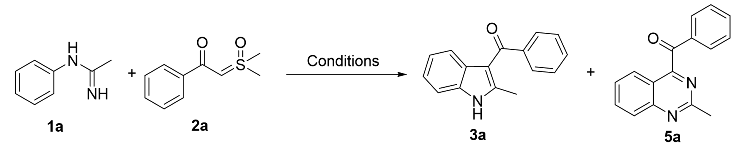
I. General details

Unless otherwise noted, materials were purchased from commercial suppliers and used without further purification. Except for the specially mentioned dry solvent, all the solvents were treated according to general methods. All the reactions were monitored by thin-layer chromatography (TLC) and were visualized using UV light. The product purification was done using silica gel column chromatography. Thin-layer chromatography (TLC) characterization was performed with precoated silica gel GF254 (0.2 mm), while column chromatography characterization was performed with silica gel (100-200 mesh). ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded with tetramethylsilane (TMS, δ = 0.00 ppm) as the internal standard. ^{1}H NMR spectra were recorded at 400 or 600 MHz (Varian), ^{13}C NMR spectra were recorded at 100 or 150 MHz (Varian) and ^{19}F NMR spectra were recorded at 376 MHz (Varian). Chemical shifts are reported in ppm downfield from $CDCl_3$ (δ = 7.26 ppm) or DMSO-d_6 (δ = 2.50 ppm; H_2O signal was found at δ = 3.34 ppm) for ^{1}H NMR and chemical shifts for ^{13}C NMR spectra are reported in ppm relative to the central $CDCl_3$ (δ = 77.0 ppm) or DMSO-d_6 (δ = 39.6 ppm). Coupling constants were given in Hz. Melting points were measured with YRT-3 melting point apparatus (Shantou Keyi Instrument & Equipment Co., Ltd., Shantou, China).

II. Experimental Section

(a). Optimization of the reaction conditions (Table S1)

Table S1. Reaction optimization[a]



Entry	Catalyst	Additive	Solvent	Yield[b] (%) 3a	5a
1	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	/	DCE	33	29
2	[Cp*RhCl$_2$]$_2$ / AgOTf or AgOAc or AgCO$_3$	/	DCE	N.R.	
3	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	HOAc	DCE	28	31
4	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	NaOAc	DCE	62	10
5	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	AgOAc	DCE	58	10
6	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	CsOAc	DCE	21	43
7	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	Cs_2CO_3	DCE	27	35
8	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	$Zn(OAc)_2$	DCE	14	24
9	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	$Cu(OAc)_2$	DCE	<5	51
10	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	$Cu(TFA)_2$	DCE	<5	42
11	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	$Cu(OTf)_2$	DCE	<5	45
12	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	$CuCl_2$	DCE	<5	31
13	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	CuF_2	DCE	<5	54
14	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	NaOAc	MeOH	N.R.	
15	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	NaOAc	THF	N.R.	
16	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	NaOAc	DMF	N.R.	
17	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	NaOAc	1,4-Dioxane	51	9
18	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	NaOAc	Tol	55	10
19	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	CuF_2	1,4-Dioxane	<5	43
20	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	CuF_2	MeOH	N.R.	
21	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	CuF_2	Tol	<5	48
22	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	CuF_2	THF	N.R.	
23	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	CuF_2	DMF	N.R.	
24[c]	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	NaOAc	DCE	57	8
25[d]	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	NaOAc	DCE	78	<5
26[c]	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	CuF_2	DCE	<5	47
27[d]	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	CuF_2	DCE	<5	58
28[e]	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	CuF_2/CsOAc	DCE	<5	68
29[d][e]	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	CuF_2/CsOAc	DCE	<5	74
30[f]	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	CuF_2/NaOAc	DCE	<5	40
31[g]	[Cp*RhCl$_2$]$_2$ / AgSbF$_6$	NaOAc/CsOAc	DCE	54	12

[a] Unless otherwise noted, all the reactions were carried out using *N*-phenylacetimidamide **1a** (0.20 mmol) and dimethyloxosulfonium benzoylmethylide **2a** (0.40 mmol) in the presence of [Cp*RhCl$_2$]$_2$ (0.01 mmol) AgSbF$_6$ (0.04 mmol), additive (0.40 mmol) and DCE (1.0 mL) in a Schlenk tube, and stirred at 80 °C for 24 h under Ar. [b] Isolated yield by chromatography on silica gel. [c] Dimethyloxosulfonium benzoylmethylide **2a** = 0.60 mmol. [d] O_2 atmosphere. [e] CsOAc = 0.20 mmol. [f] CuF_2 = 0.20 mmol, NaOAc = 0.20 mmol. [g] NaOAc = 0.20 mmol, CsOAc = 0.20 mmol.

We initially selected *N*-phenylacetimidamide **1a** as a substrate for the coupling with dimethyloxosulfonium benzoylmethylide **2a** using $[Cp^*RhCl_2]_2$ (5 mol%)/$AgSbF_6$ (20 mol%) as a catalyst system.[1] To our delight, (2-methyl-*1H*-indol-3-yl)(phenyl)methanone **3a** and 2-methyl-4-benzoylquinazoline **5a** were obtained in 1:1 rate with a 62% yield totally (Table S1, entry 1). The experiments replacing $AgSbF_6$ by AgOTf, AgOAc or $AgCO_3$ were also carried out, but there were no reaction (entry 2). Then, the relationship between additive and reaction results were observed (entries 3-13). It showed that NaOAc was obviously favored as a base to generate indole products (entry 4), and only quinazoline product was found in the presence of Cu salt expetially CuF_2 (entry 13). Effects of the solvent were also examined, and 1,4-Dioxane and toluene also showed reactivity but not better than DCE (entries 14-23). Increasing the amount of **2a** will be helpful to form **3a** (entry 24) but unfavorable to form **5a** (entry 26) and the oxygen environment (entries 25 and 27) promoted the formation of **5a**. In addition, as we found CsOAc had a mild preference on **5a** (entry 6), we combined it with CuF_2 to see if it can further boost the yield (entries 28 and 29). Fortunately, the 74% yield of **5a** was obtained. Finally, the experiments using NaOAc/CuF_2 and NaOAc/CsOAc were also carried out. Using NaOAc/CuF_2 tended to produce quinazoline product in a low yield, and using NaOAc/CsOAc mainly produced indole product in a moderate yield. In some extent, the results above can indicate the different catalytic capability of the NaOAc, CsOAc and CuF_2 in this reaction.

(b) General procedure for the synthesis of imidamides **1** (**1a** as an example)[2]

A mixture of aniline (1.0 equiv.), $AlCl_3$ (1.2 equiv.) and carbonitrile (2 equiv.) was stirred at 130 °C in a sealed reaction tube overnight. After completion of the reaction, a concentrated NaOH solution in a mixture of water and ice was added into the residual crude product and stirred for about 15 minutes. Then the mixture was extracted with EtOAc (25 mL × 3). The combined organic layers were washed with brine (30 mL × 3), dried over anhydrous Na_2SO_4, and evaporated under vacuum. The residue was purified by column chromatography on silica gel.

(c) General procedure for the synthesis of sulfoxonium ylides **2** (**2a** as an example)[3]

To a stirred solution of potassium tert-butoxide (1.0 g, 9.1 mmol) in THF (10 mL) was added trimethylsulfoxonium iodide (1.5 g, 6.9 mmol) at room temperature. The resulting mixture was refluxed for 2h. Then the reaction mixture was cooled to 0 °C, followed by addition of acylchlorides (2.3 mmol) in THF (2 mL). The reaction was allowed to room temperature and stirred for 3h. After the solvent was evaporated, water (20 mL) and ethyl acetate (20 mL) were added to the residual crude product. The aqueous layer was separated and washed with ethylacetate (3 × 20 mL) and the organic layers were combined. The organic solution was dried over anhydrous Na_2SO_4, and evaporated under vacuum. The residue was purified by column chromatography on silica gel.

(d) General procedure for the synthesis of **3a-u**, **4a-i** and **11a-d** (**3a** as an example)

Add *N*-phenylethanimidamide **1a** (26.8 mg, 0.20 mmol), dimethyloxosulfonium benzoylmethylide **2a** (117.6 mg, 0.60 mmol), $[Cp^*RhCl_2]_2$ (6.2 mg, 0.01 mmol), $AgSbF_6$ (13.7 mg, 0.04 mmol), NaOAc (32.8 mg, 0.40 mmol) and DCE (1.0 ml) to a Schlenk tube. The mixture was stirred at 80 °C for 24h under Ar. Then, without any post processing, the reaction mixture was purified by column chromatography on silica gel (eluent: PE/ DCM = 1/ 1) to afford desired product **3a**, 36.5 mg, yield 78%.

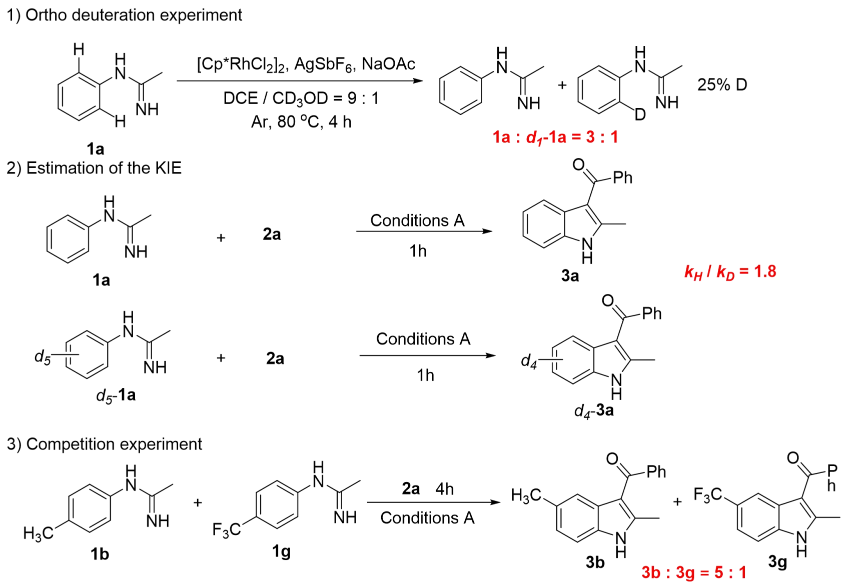
(e) General procedure for the synthesis of **5a-r** and **6a-g** (**5a** as an example)

Add *N*-phenylethanimidamide **1a** (26.8 mg, 0.20 mmol), dimethyloxosulfonium benzoylmethylide **2a** (78.4 mg, 0.40 mmol), $[Cp^*RhCl_2]_2$ (6.2 mg, 0.01 mmol), $AgSbF_6$ (13.7 mg, 0.04 mmol), CuF_2 (40.3 mg, 0.40 mmol), CsOAc (38.3 mg, 0.20 mmol) and DCE (1.0 ml) to a Schlenk tube. The mixture was stirred at 80 °C for 24h under O_2. Then, without any post processing, the reaction mixture was purified by column chromatography on silica gel (eluent: PE/ acetone = 50/ 1) to afford desired product **5a**, 36.7 mg, yield 74%.

III. Mechanism study[4]

(a) Mechanism study of condition A: the synthesis of indoles

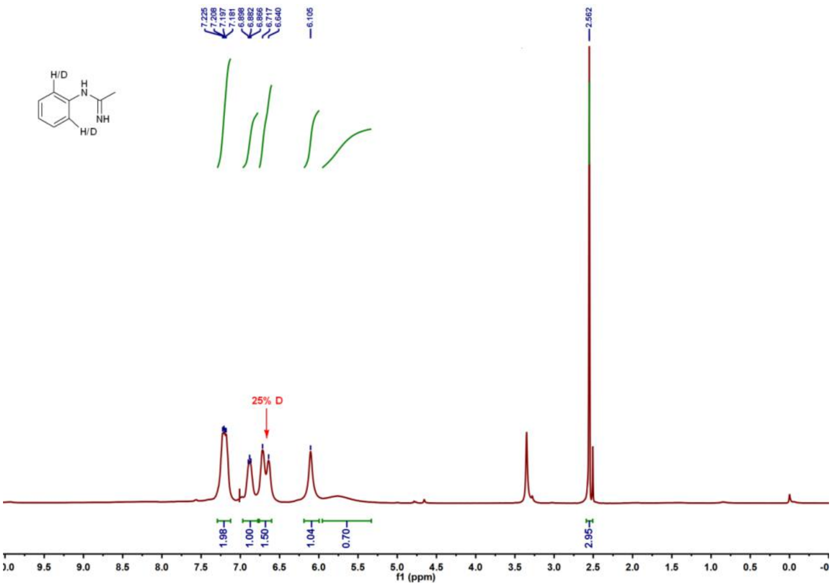
Scheme S1. Mechanism study of the synthesis of indoles.



1). Ortho deuteration experiments

N-phenylethanimidamide **1a** (0.10 mmol) was dissolved in DCE (0.9 ml)/ CD_3OD(0.1 mL) in the presence of $[Cp^*RhCl_2]_2$ (5 mol%), $AgSbF_6$ (0.02 mmol) and NaOAc (0.20 mmol). The reaction was stopped after 4h, and the mixture of **1a** and d_1-**1a** were analyzed by ^1H NMR spectroscopy.

Figure S1. The ^1H NMR (400 MHz, DMSO-d_6) of the mixture of **1a** and d_1-**1a**



2) KIE experiments (parallel experiments)

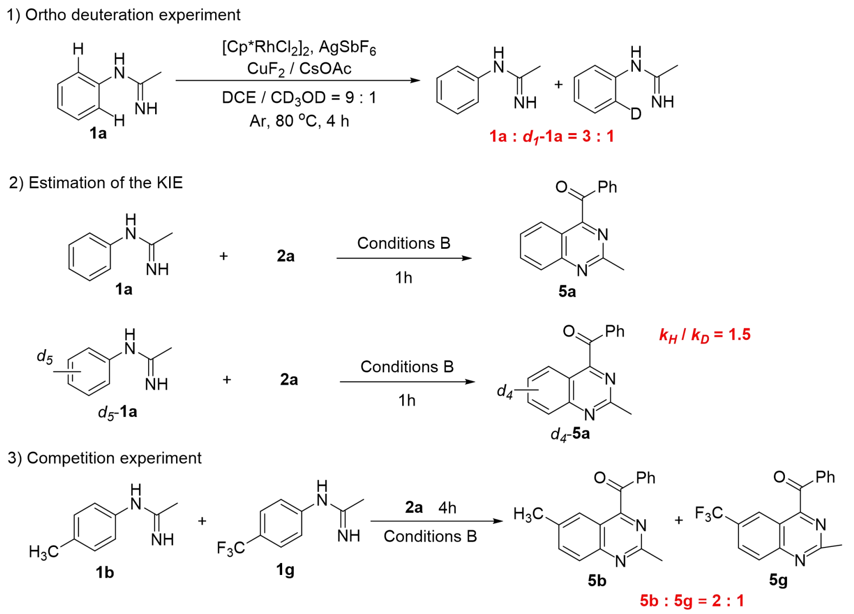
Two Schlenk tubes each was charged with *N*-phenylethanimidamide **1a** (0.20 mmol) or d_5-**1a** (0.20 mmol) and a stir bar. Sulfoxonium ylide **2a** (0.60 mmol), $[Cp^*RhCl_2]_2$ (5 mmol%), $AgSbF_6$ (0.04 mmol), NaOAc (0.40 mmol) and DCE (1.0 mL) were added to each tube, and the two reactions were stirred side-by-side at 80 °C for 1h. After rapidly evaporating the two mixtures solely, the product **3a** and d_4-**3a** were purified by flash column chromatography on silica gel (eluent: PE/DCM = 1:1). The KIE value was determined to be k_H/k_D = 1.8 on the yield ratio of **3a** and d_4-**3a**, which indicated that the cleavage of the C−H bond is likely not involved in the turnover-limiting step.

3) Competitive experiment

An equimolar mixture of *N*-(4-methylphenyl)ethanimidamide **1b** (0.20 mmol) and *N*-(4-trifluromethylphenyl)ethanimidamide **1g** (0.20 mmol) were allowed to react with sulfoxonium ylide **2a** (0.60 mmol) in DCE (1.0 mL) in the presence of $[Cp^*RhCl_2]_2$ (5 mmol%), $AgSbF_6$ (0.04 mmol) and NaOAc (0.40 mmol). The reaction was stopped after 4h, and the product **3b** and **3g** were isolated by chromatography on silica gel with the rate **3b**:**3g** = 5:1.

(b) Mechanism study of condition B: the synthesis of quinazolines

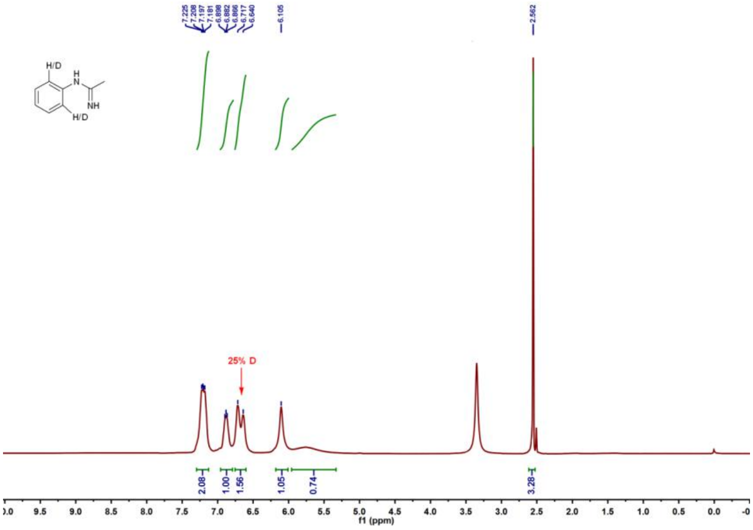
Scheme S2. Mechanism study of the synthesis of quinazolines.



1). Ortho deuteration experiments

N-phenylethanimidamide **1a** (0.10 mmol) was dissolved in DCE (0.9 ml)/ CD_3OD(0.1 mL) in the presence of $[Cp^*RhCl_2]_2$ (5 mol%), $AgSbF_6$ (0.02 mmol), CuF_2 (0.20 mmol) and CsOAc (0.10 mmol). The reaction was stopped after 4h, and the mixture of **1a** and d_1-**1a** were analyzed by ^{1}H NMR spectroscopy.

Figure S2. The ^{1}H NMR (400 MHz, DMSO-d_6) of the mixture of **1a** and d_1-**1a**.



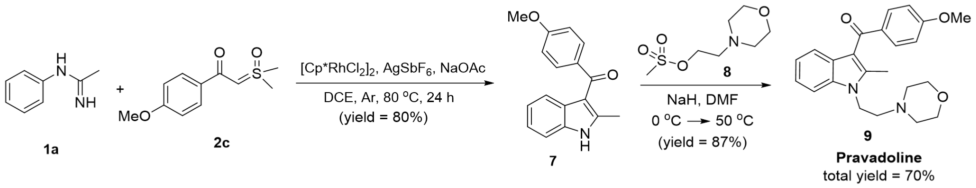
2) KIE experiments (parallel experiments)

Two Schlenk tubes each was charged with *N*-phenylethanimidamide **1a** (0.20 mmol) or d_5-**1a** (0.20 mmol) and a stir bar. Sulfoxonium ylide **2a** (0.40 mmol), $[Cp^*RhCl_2]_2$ (5 mmol%), $AgSbF_6$ (0.04 mmol), CuF_2 (0.40 mmol), CsOAc (0.20 mmol) and DCE (1.0 mL) were added to each tube, and the two reactions were stirred side-by-side at 80 ^{o}C for 1h. After rapidly evaporating the two mixtures solely, the product **5a** and d_4-**5a** were purified by flash column chromatography on silica gel (eluent: PE/acetone = 50/1). The KIE value was determined to be k_H /k_D = 1.5 on the yield ratio of **5a** and d_4-**5a**, which indicated that the cleavage of the C−H bond is likely not involved in the turnover-limiting step.

3) Competitive experiment

An equimolar mixture of *N*-(4-methylphenyl)ethanimidamide **1b** (0.20 mmol) and *N*-(4-trifluromethylphenyl)ethanimidamide **1g** (0.20 mmol) were allowed to react with sulfoxonium ylide **2a** (0.60 mmol) in DCE (1.0 mL) in the presence of $[Cp^*RhCl_2]_2$ (5 mmol%), $AgSbF_6$ (0.04 mmol), CuF_2 (0.20 mmol) and CsOAc (0.10 mmol). The reaction was stopped after 4h, and the product **5b** and **5g** were isolated by chromatography on silica gel with the rate **5b**:**5g** = 2:1.

IV. The synthesis of Pravadoline 9[5]



Scheme S3. The synthesis of Pravadoline.

Add *N*-phenylethanimidamide **1a** (26.8 mg, 0.20 mmol), dimethyloxosulfonium 4-methoxybenzoylmethylide **2c** (135.6 mg, 0.60 mmol), [Cp*RhCl$_2$]$_2$ (6.2 mg, 0.01 mmol), AgSbF$_6$ (13.7 mg, 0.04 mmol), NaOAc (32.8 mg, 0.40 mmol) and DCE (1.0 ml) to a Schlenk tube. The mixture was stirred at 80 °C for 24h under Ar. Then, without any post processing, the reaction mixture was purified by column chromatography on silica gel (eluent: PE/ DCM = 1:1) to afford desired product **3ac**, 42.2 mg, yield 80%. To **3ac** (42.2 mg, 0.16 mmol) in 4 ml of DMF at 0 °C was added NaH (60% dispersion in mineral oil, 31.7 mg, 0.48 mmol). The mixture was stirred for 15 min at 0 °C and then was allowed to warm to room temperature. The mixture was stirred for 1 h at room temperature and then was cooled to 0 °C. The 2-morpholin-4-ylethyl methanesulfonate **6** in 1 ml of DMF was added rapidly via cannula. After the addition was completed, the mixture was stirred for 4h at 50 °C. The mixture was then cooled to 0 °C, quenched with 10 ml of NH$_4$Cl saturated aqueous, and diluted with 10 ml of EtOAc. The layers were separated, and the aqueous layer was extracted with EtOAc (3 × 10 ml). The combined organics were washed with water and brine, dried over anhydrous Na$_2$SO$_4$, filtered, concentrated under reduced pressure, and purified by column chromatography on silica gel (eluent: DCM/ MeOH/ Et$_3$N = 50:1:0.1) to give the title compound (52.2 mg, 87% yield). The total yield of pravadoline **7** was 70%.

V. Cell growth inhibitory assay[6]

(a) Experimental details

Carcinoma cells were maintained in DMEM medium supplemented with 10% fetal bovine serum. For in vitro treatment, the carcinoma cells were seeded in 96 well plates and incubated in a CO$_2$ incubator at 37 °C for 24 h. The seeding numbers were 2000 per well for A549, Hela, MCF-7 and HepG2, respectively. The cells were treated with at least five different concentrations of test compounds in a CO$_2$ incubator for 72 h. The number of viable cells was estimated using MTT assay, and the experiment was performed as the manufacturer recommended (Abcam ab211091). The absorbance was measured at 570 nm on a iMark Microplate Absorbance Reader (Bio-Rad). The results of these assays were used to obtain the dose-response curves from which IC$_{50}$ (nM) values were determined. An IC$_{50}$ value represents the concentration (nM) of the tested compound at which a 50% cell growth inhibition after 3 days of incubation is produced. The values represent averages of three or more independent experiments, each with duplicate samples.

(b) Cytotoxic activities data (Table S2)

Table S2. IC$_{50}$ Values (nM ±SD[a]) of 3-aroylindoles and 4-aroylquinazolines.

Compound	Lung carcinoma A549	Breast carcinoma MCF-7	Cervical carcinoma Hela	Liver carcinoma HepG2
11a	575 ± 86	122 ± 12	1909 ± 347	102 ± 46
11b	6 ±2	1 ± 0.1	5 ±1	3 ±1
11c	111 ± 59	0.8 ± 0.1	111 ± 47	0.9 ± 0.6
11d	0.5 ± 0.2	0.4 ± 0.1	9 ± 6	1 ± 0
5n	>50000	101 ± 47	>50000	35673 ± 2411
5o	>50000	3255 ± 772	>50000	42607 ± 157
5q	>50000	>50000	>50000	>50000
5r	26793 ±6923	1391 ±271	33113 ±4823	25963 ±1969

VI. References

[1] (a) T. Satoh, M. Miura, *Chem. Eur. J.,* 2010, **16**, 11212; (b) G. Song, F. Wang, X. Li, *Chem. Soc. Rev.*, 2012, **41**, 3651; (c) Y. Yang, M.-B. Zhou, X.-H. Ouyang, R. Pi, R.-J. Song, J.-H. Li, *Angew. Chem., Int. Ed.,* 2015, **54**, 6595.

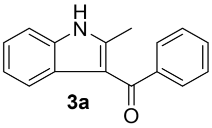
[2] Z. Qi, S. Yu, X. Li, *Org. Lett.,* 2016, **18**, 700.

[3] M. Barday, C. Janot, N. R. Halcovitch, J. Muir, C. Aïssa, *Angew. Chem., Int. Ed.,* 2017, **56**, 13117.

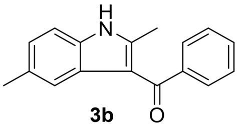
[4] (a) J. Zhou, J. Li, Y. Li, C. Wu, G. He, Q. Yang, Y. Zhou, H. Liu, *Org. Lett.,* 2018, **20**, 7645; (b) E. M. Simmons, J. F. Hartwig, *Angew. Chem., Int. Ed.,* 2012, **51**, 3066; (c) M. Tian, B. Liu, J. Sun, X. Li, *Org. Lett.,* 2018, **20**, 4946.

[5] J. M. Frost, M. J. Dart, K. R. Tietje, T. R. Garrison, G. K. Grayson, A. V. Daza, O. F. El-Kouhen, B. B. Yao, G. C. Hsieh, M. Pai, C. Z. Zhu, P. Chandran, M. D. Meyer, *J. Med. Chem.,* 2010, **53**, 295.
[6] J.-P. Liou, Y.-L. Chang, F.-M. Kuo, C.-W. Chang, H.-Y. Tseng, C.-C. Wang, Y.-N. Yang, J.-Y. Chang, S.-J. Lee, H.-P. Hsieh, *J. Med. Chem.,* 2004, **47**, 4247.

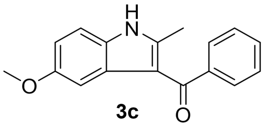
VII. Characterization data of products


3a

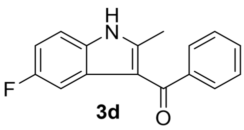
(2-methyl-*1H*-indol-3-yl)(phenyl)methanone (3a): Yield 78%, 36.5 mg; white solid; m.p. 172 - 173 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.97 (s, 1H), 7.64 – 7.57 (m, 3H), 7.51 (t, *J* = 7.2 Hz, 2H), 7.40 (d, *J* = 8.0 Hz, 1H), 7.34 (d, *J* = 8.0 Hz, 1H), 7.13 (dt, *J* = 8.0, 0.8 Hz, 1H), 7.02 (dt, *J* = 8.0 Hz, 0.8 Hz, 1H), 2.39 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 192.1, 144.9, 142.1, 135.4, 131.4, 128.8, 128.4, 127.7, 122.2, 121.4, 120.4, 112.9, 111.7, 14.6. HRMS (ESI) Calcd. For $C_{16}H_{13}NO$: $[M+H]^+$, 236.1075; Found: m/z 236.1075.


3b

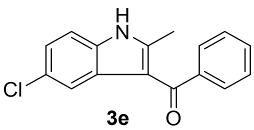
(2,5-dimethyl-*1H*-indol-3-yl)(phenyl)methanone (3b): Yield 79%, 39.3 mg; white solid; m.p. 198 - 199 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.05 (s, 1H), 7.74 (d, *J* = 7.8 Hz, 2H), 7.54 (t, *J* = 6.8 Hz, 1H), 7.45 (t, *J* = 7.4 Hz, 2H), 7.30 (s, 1H), 7.16 (d, *J* = 8.2 Hz, 1H), 6.97 (d, *J* = 8.2 Hz, 1H), 2.42 (s, 3H), 2.33 (s, 3H). ^{13}C NMR (150 MHz, Chloroform-*d*) δ 193.4, 143.9, 141.4, 133.1, 131.4, 131.0, 128.8, 128.2, 127.9, 123.8, 120.7, 113.6, 110.3, 21.6, 14.6. HRMS (ESI) Calcd. For $C_{17}H_{15}NO$: $[M+H]^+$, 250.1232; Found: m/z 250.1232.


3c

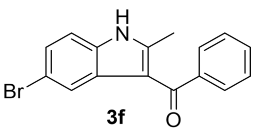
(2-methyl-5-methoxyl-*1H*-indol-3-yl)(phenyl)methanone (3c): Yield 85%, 45.0 mg; white solid; m.p. 224 - 225 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.61 (m, 3H), 7.53 (m, 3H), 7.38 (d, *J* = 8.4 Hz, 1H), 7.27 (dd, *J* = 8.4, 2.0 Hz, 1H), 3.38 (s, 3H), 2.35 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 192.0, 146.2, 141.7, 134.2, 131.7, 129.6, 128.9, 128.4, 124.9, 122.7, 114.2, 113.7, 112.6, 55.7, 14.7. HRMS (ESI) Calcd. For $C_{17}H_{15}NO_2$: $[M+H]^+$, 266.1181; Found: m/z 266.1182.


3d

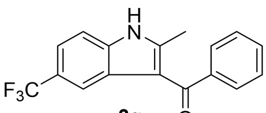
(2-methyl-5-fluoro-*1H*-indol-3-yl)(phenyl)methanone (3d): Yield 81%, 41.0 mg; white solid; m.p. 229 - 230 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.11 (s, 1H), 7.64 – 7.59 (m, 3H), 7.55 – 7.51 (m, 2H), 7.41 (dd, *J* = 8.8, 4.8 Hz, 1H), 7.06 (dd, *J* = 10.4, 2.4 Hz, 1H), 6.99 (td, *J* = 9.2, 2.4 Hz, 1H), 2.37 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 192.0, 159.3, 158.0 (d, *J* = 232.1 Hz, 1C), 146.6, 141.8, 132.0, 131.5, 128.8, 128.4 (d, *J* = 10.7 Hz, 1C), 128.3, 113.1 (d, *J* = 3.9 Hz, 1C), 112.8 (d, *J* = 9.6 Hz, 1C), 110.2 (d, *J* = 25.7 Hz, 1C), 105.6 (d, *J* = 24.8 Hz, 1C), 14.8. ^{19}F NMR (376 MHz, DMSO-d_6) δ -122.3. HRMS (ESI) Calcd. For $C_{16}H_{12}FNO$: $[M+H]^+$, 254.0981; Found: m/z 254.0982.


3e

(2-methyl-5-chloro-*1H*-indol-3-yl)(phenyl)methanone (3e): Yield 80%, 42.8 mg; white solid; m.p. 231 - 232 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.16 (s, 1H), 7.65 – 7.58 (m, 3H), 7.56 – 7.51 (m, 2H), 7.42 (d, *J* = 8.4 Hz, 1H), 7.37 (d, *J* = 2.0 Hz, 1H), 7.15 (dd, *J* = 8.4, 2.0 Hz, 1H), 2.35 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 191.9, 146.4, 141.7, 133.9, 131.7, 129.0, 128.9, 128.4, 126.1, 122.3, 119.7, 113.3, 112.6, 14.7. HRMS (ESI) Calcd. For $C_{16}H_{12}ClNO$: $[M+H]^+$, 270.0686; Found: m/z 270.0686.

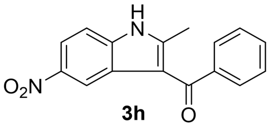

3f

(2-methyl-5-bromo-*1H*-indol-3-yl)(phenyl)methanone (3f): Yield 81%, 50.2 mg; white solid; m.p. 238 - 239 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.17 (s, 1H), 7.64 – 7.59 (m, 3H), 7.56 – 7.50 (m, 3H), 7.38 (d, *J* = 8.4 Hz, 1H), 7.27 (dd, *J* = 8.4, 2.0 Hz, 1H), 2.35 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 191.9, 146.2, 141.7, 134.2, 131.7, 129.6, 128.9, 128.4, 124.8, 122.7, 114.2, 113.7, 112.5, 14.7. HRMS (ESI) Calcd. For $C_{16}H_{12}BrNO$: $[M+H]^+$, 314.0181; Found: m/z 314.0181.



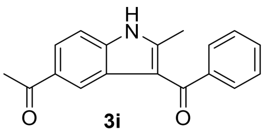
3g

(2-methyl-5-trifluoromethyl-*1H*-indol-3-yl)(phenyl)methanone (3g): Yield 70%, 41.7 mg; white solid; m.p. 232 - 233 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.37 (s, 1H), 7.75 (s, 1H), 7.66 – 7.56 (m, 4H), 7.55 – 7.50 (m, 2H), 7.44 (d, J = 8.4 Hz, 1H), 2.36 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 192.1, 147.0, 141.6, 137.2, 131.8, 128.9, 128.5, 127.3, 125.7 (q, J = 269.8 Hz, 1C), 122.2 (q, J = 30.8 Hz, 1C), 118.9 (q, J = 3.3 Hz, 1C), 117.7 (q, J = 4.3 Hz, 1C), 113.5, 112.6, 14.8. ^{19}F NMR (376 MHz, DMSO-d_6) δ -59.1. HRMS (ESI) Calcd. For $C_{17}H_{12}F_3NO$: [M+H]$^+$, 303.0871; Found: m/z 303.0870.



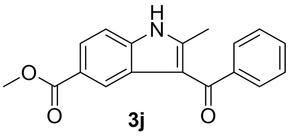
3h

(2-methyl-5-bromo-*1H*-indol-3-yl)(phenyl)methanone (3h): Yield 69%, 39.8 mg; white solid; m.p. 258 - 259 °C. H NMR (400 MHz, DMSO-d_6) δ 12.56 (s, 1H), 8.38 (d, J = 2.4 Hz, 1H), 8.04 (dd, J = 8.8, 2.4 Hz, 1H), 7.68 – 7.65 (m, 2H), 7.64 (dd, J = 8.0, 1.8 Hz, 1H), 7.59 – 7.52 (m, 3H), 2.39 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 191.8, 148.2, 142.6, 141.2, 138.8, 132.0, 128.9, 128.6, 127.3, 117.8, 116.9, 114.4, 112.1, 14.6. HRMS (ESI) Calcd. For $C_{16}H_{12}N_2O_3$: [M+H]$^+$, 280.0848; Found: m/z 280.0848.



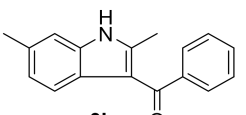
3i

1-(3-benzoyl-2-methyl-*1H*-indol-5-yl)ethan-1-one (3i): Yield 66%, 36.2 mg; yellow solid; m.p. 241 - 242 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.32 (s, 1H), 8.10 (d, J = 1.4 Hz, 1H), 7.82 (dd, J = 8.6, 1.8 Hz, 1H), 7.71 – 7.67 (m, 3H), 7.59 (dd, J = 7.4, 1.4 Hz, 2H), 7.52 (d, J = 8.6 Hz, 1H), 2.51 (s, 3H), 2.43 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 197.7, 192.1, 146.6, 141.6, 138.1, 131.8, 130.9, 128.9, 128.6, 127.3, 122.6, 122.2, 113.9, 111.6, 26.9, 14.7. HRMS (ESI) Calcd. For $C_{18}H_{15}NO_2$: [M+H]$^+$, 278.1181; Found: m/z 278.1181.



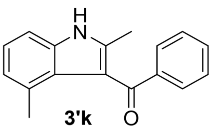
3j

Methyl 3-benzoyl-2-methyl-*1H*-indole-5-carboxylate (3j): Yield 60%, 35.2 mg; yellow solid; m.p. 257 - 258 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.30 (s, 1H), 8.21 (s, 1H), 7.78 (dd, J = 8.6, 1.6 Hz, 1H), 7.67 – 7.59 (m, 3H), 7.53 (t, J = 7.4 Hz, 2H), 7.49 (d, J = 8.6 Hz, 1H), 3.80 (s, 3H), 2.34 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 192.1, 167.4, 146.5, 141.6, 138.2, 131.9, 128.9, 128.6, 127.5, 123.5, 122.9, 113.7, 111.7, 52.3, 14.8. HRMS (ESI) Calcd. For $C_{18}H_{15}NO_3$: [M+H]$^+$, 294.1130; Found: m/z 294.1130.



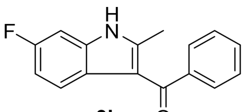
3k

(2,6-dimethyl-*1H*-indol-3-yl)(phenyl)methanone (3k): Yield 65%, 32.4 mg; white solid; m.p. 197 - 198 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.82 (s, 1H), 7.60 – 7.56 (m, 3H), 7.50 (t, J = 7.4 Hz, 2H), 7.18 (d, J = 8.2 Hz, 1H), 7.17 (s, 1H), 6.84 (d, J = 8.2 Hz, 1H), 2.37 (s, 3H), 2.36 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 192.3, 148.8, 142.2, 133.9, 131.5, 129.9, 128.8, 128.5, 128.0, 123.7, 120.5, 112.4, 111.5, 21.9, 14.2. HRMS (ESI) Calcd. For $C_{17}H_{15}NO$: [M+H]$^+$, 250.1232; Found: m/z 250.1232.



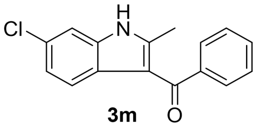
3'k

(2,4-trimethyl-*1H*-indol-3-yl)(phenyl)methanone (3'k): Yield 13%, 6.4 mg; white solid; m.p. 193 - 194 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.74 (s, 1H), 7.55 – 7.50 (m, 3H), 7.44 (t, J = 7.4 Hz, 2H), 7.10 – 7.04 (m, 1H), 6.88 – 6.81 (m, 2H), 2.42 (s, 3H), 2.34 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 192.3, 144.7, 142.2, 134.9, 131.5, 128.8, 128.5, 127.5, 122.9, 121.5, 121.0, 118.1, 113.3, 17.2, 14.6. HRMS (ESI) Calcd. For $C_{17}H_{15}NO$: [M+H]$^+$, 250.1232; Found: m/z 250.1232.



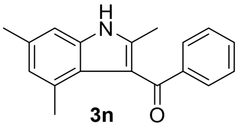
3l

(2-methyl-6-fluoro-*1H*-indol-3-yl)(phenyl)methanone (3l): Yield 78%, 50.5 mg; white solid; m.p. 200 - 201 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.13 (s, 1H), 7.68 (d, J = 7.2 Hz, 2H), 7.58 (t, J = 7.2 Hz, 1H), 7.47 (t, J = 7.6 Hz, 2H), 7.26 (d, J = 8.0 Hz, 1H), 7.11 (td, J = 7.8, 5.0 Hz, 1H), 6.76 (dd, J = 11.2, 8.0 Hz, 1H), 2.43 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 191.8, 155.2 (d, J = 254.4 Hz), 143.3, 141.0, 138.0 (d, *J* = 10.8 Hz), 132.4, 129.2 (d, *J* = 0.6 Hz), 128.6, 122.9 (d, *J* = 7.8 Hz), 115.6 (d, *J* = 18.9 Hz), 111.3 (d, *J* = 3.7 Hz), 108.2 (d, *J* = 3.4 Hz), 106.8 (d, *J* = 20.1 Hz), 13.7. ^{19}F NMR (376 MHz, DMSO-d_6) δ -113.6. HRMS (ESI) Calcd. For $C_{16}H_{12}FNO$: $[M+H]^+$, 254.0981; Found: m/z 254.0981.



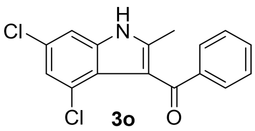
3m

(2-methyl-6-chloro-*1H*-indol-3-yl)(phenyl)methanone (3m): Yield 78%, 53.6 mg; white solid; m.p. 208 - 209 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.09 (s, 1H), 7.60 (m, 3H), 7.52 (t, *J* = 7.6 Hz, 2H), 7.44 (d, *J* = 1.6 Hz, 1H), 7.34 (d, *J* = 8.4 Hz, 1H), 7.06 (dd, *J* = 8.4, 1.8 Hz, 1H), 2.36 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 192.0, 145.8, 141.7, 135.9, 131.8, 128.9, 128.5, 126.8, 126.5, 121.8, 121.7, 112.9, 111.4, 14.7. HRMS (ESI) Calcd. For $C_{16}H_{12}ClNO$: $[M+H]^+$, 270.0686; Found: m/z 270.0686.



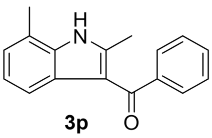
3n

(2,4,6-trimethyl-*1H*-indol-3-yl)(phenyl)methanone (3n): Yield 72%, 37.4 mg; white solid; m.p. 217 - 218 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.68 (s, 1H), 7.59 (m, 3H), 7.50 (t, *J* = 7.4 Hz, 2H), 7.02 (s, 1H), 6.75 (s, 1H), 2.44 (s, 3H), 2.35 (s, 3H), 2.24 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 192.3, 144.6, 142.2, 133.2, 131.3, 130.1, 128.7, 127.7, 124.5, 120.5, 118.0, 113.0, 17.1, 14.6. HRMS (ESI) Calcd. For $C_{18}H_{17}NO$: $[M+H]^+$, 264.1388; Found: m/z 264.1388.



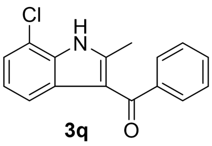
3o

(2-methyl-4,6-dichloro-*1H*-indol-3-yl)(phenyl)methanone (3o): Yield 67%, 40.1 mg; yellow solid; m.p. 287 - 288 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.17 (s, 1H), 7.70 – 7.65 (m, 2H), 7.61 (tt, *J* = 7.4, 1.6 Hz, 1H), 7.51 – 7.45 (m, 3H), 7.13 (d, *J* = 1.6 Hz, 1H), 2.32 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 192.4, 142.3, 140.6, 136.7, 133.1, 129.4, 129.0, 126.5, 124.8, 123.8, 121.3, 112.9, 110.6, 13.1. HRMS (ESI) Calcd. For $C_{16}H_{11}Cl_2NO$: $[M+H]^+$, 304.0296; Found: m/z 304.0295.



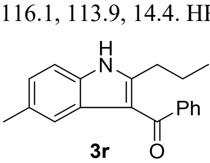
3p

(2,7-dimethyl-*1H*-indol-3-yl)(phenyl)methanone (3p): Yield 73%, 36.0 mg; white solid; m.p. 190 - 192 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.81 (s, 1H), 7.59 (m, 3H), 7.50 (t, *J* = 7.3 Hz, 2H), 7.20 – 7.08 (m, 1H), 6.95 – 6.88 (m, 2H), 2.41 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 192.3, 144.7, 142.1, 134.8, 131.4, 128.7, 128.5, 127.4, 122.8, 121.5, 120.9, 118.0, 113.3, 17.1, 14.5. HRMS (ESI) Calcd. For $C_{17}H_{15}NO$: $[M+H]^+$, 250.1232; Found: m/z 250.1232.



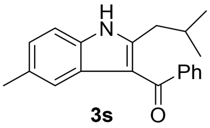
3q

(2-methyl-7-chloro-*1H*-indol-3-yl)(phenyl)methanone (3q): Yield 76%, 40.4 mg; white solid; m.p. 240 - 242 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.23 (s, 1H), 7.66 – 7.59 (m, 3H), 7.52 (t, *J* = 7.4 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 1H), 7.22 (dd, *J* = 7.6, 0.4 Hz, 1H), 7.04 (t, *J* = 8.0 Hz, 1H), 2.43 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 192.1, 146.0, 141.5, 132.4, 131.8, 129.5, 128.8, 128.6, 122.4, 121.8, 119.3, 116.1, 113.9, 14.4. HRMS (ESI) Calcd. For $C_{16}H_{12}ClNO$: $[M+H]^+$, 270.0686; Found: m/z 270.0686.



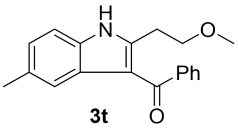
3r

(2-propyl-5-methyl-*1H*-indol-3-yl)(phenyl)methanone (3r): Yield 77%, 42.0 mg; white solid; m.p. 207 - 208 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.84 (s, 1H), 7.66 – 7.58 (m, 3H), 7.53 (t, *J* = 7.4 Hz, 2H), 7.32 (d, *J* = 8.2 Hz, 1H), 7.12 (s, 1H), 6.97 (d, *J* = 8.2 Hz, 1H), 2.73 (t, *J* = 7.4 Hz, 2H), 2.28 (s, 3H), 1.65 (h, *J* = 7.2 Hz, 2H), 0.81 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 192.3, 148.7, 142.2, 133.8, 131.4, 129.9, 128.7, 128.4, 127.9, 123.6, 120.4, 112.3, 111.4, 29.6, 23.0, 21.8, 14.1. HRMS (ESI) Calcd. For $C_{19}H_{19}NO$: $[M+H]^+$, 278.1545; Found: m/z 278.1545.



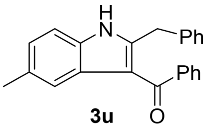
3s

(2-isobutyl-5-methyl-*1H*-indol-3-yl)(phenyl)methanone (3s): Yield 76%, 43.8 mg; white solid; m.p. 205 - 206 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.79 (s, 1H), 7.65 – 7.55 (m, 3H), 7.49 (t, J = 7.4 Hz, 2H), 7.28 (d, J = 8.2 Hz, 1H), 7.02 (s, 1H), 6.93 (d, J = 8.2 Hz, 1H), 2.66 (d, J = 7.2 Hz, 2H), 2.23 (s, 3H), 1.93 (h, J = 7.2 Hz, 1H), 0.77 (d, J = 6.6 Hz, 6H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 192.4, 147.8, 142.0, 133.7, 131.5, 129.8, 128.7, 128.6, 128.0, 123.6, 120.3, 112.7, 111.5, 36.5, 29.4, 22.6, 21.8. HRMS (ESI) Calcd. For $C_{20}H_{21}NO$: [M+H]$^+$, 292.1701; Found: m/z 292.1701.



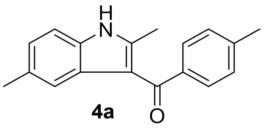
3t

(2-(2-methoxyethyl)-5-methyl-*1H*-indol-3-yl)(phenyl)methanone (3t): Yield 76%, 44.2 mg; white solid; m.p. 219 - 220 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.85 (s, 1H), 7.61 (t, J = 7.2 Hz, 3H), 7.51 (t, J = 7.6 Hz, 2H), 7.31 (d, J = 8.0 Hz, 1H), 7.00 (s, 1H), 6.95 (d, J = 8.0 Hz, 1H), 3.59 (t, J = 6.8 Hz, 2H), 3.36 (s, 3H), 3.03 (t, J = 6.8 Hz, 2H), 2.24 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 192.2, 145.5, 142.0, 133.9, 131.7, 129.9, 128.8, 128.6, 127.8, 123.8, 120.3, 112.7, 111.7, 71.2, 58.2, 28.4, 21.8. HRMS (ESI) Calcd. For $C_{19}H_{19}NO_2$: [M+H]$^+$, 294.1494; Found: m/z 294.1494.



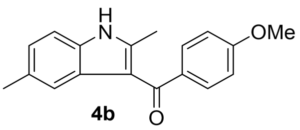
3u

(2-benzyl-5-methyl-*1H*-indol-3-yl)(phenyl)methanone (3u): Yield 71%, 45.7 mg; white solid; m.p. 247 - 248 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.91 (s, 1H), 7.62 (d, J = 7.4 Hz, 2H), 7.59 (d, J = 7.4 Hz, 1H), 7.49 (t, J = 7.4 Hz, 2H), 7.29 (d, J = 8.4 Hz, 1H), 7.28 – 7.21 (m, 2H), 7.21 – 7.15 (m, 3H), 6.95 (d, J = 7.0 Hz, 2H), 4.21 (s, 2H), 2.22 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 192.2, 146.3, 141.7, 139.2, 134.0, 131.8, 129.9, 128.8, 128.8, 128.7, 127.7, 126.7, 123.9, 120.4, 112.6, 111.7, 33.3, 21.8. HRMS (ESI) Calcd. For $C_{23}H_{19}NO$: [M+H]$^+$, 326.1545; Found: m/z 326.1546.



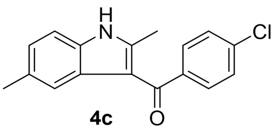
4a

(2,5-dimethyl-*1H*-indol-3-yl)(*p*-tolyl)methanone (4a): Yield 78%, 40.5 mg; white solid; m.p. 206 - 207 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.78 (s, 1H), 7.53 (d, J = 8.0 Hz, 2H), 7.33 – 7.25 (m, 4H), 6.94 (dd, J = 8.0, 1.2 Hz, 1H), 2.40 (s, 3H), 2.33 (s, 3H), 2.29 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 191.9, 144.3, 141.5, 139.3, 133.7, 129.9, 129.3, 128.9, 128.1, 123.6, 120.4, 112.8, 111.3, 21.9, 21.6, 14.7. HRMS (ESI) Calcd. For $C_{18}H_{17}NO$: [M+H]$^+$, 264.1388; Found: m/z 264.1388.



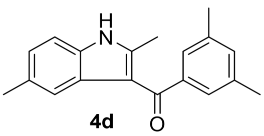
4b

(2,5-dimethyl-*1H*-indol-3-yl)(4-methoxylphenyl)methanone (4b): Yield 82%, 45.1 mg; white solid; m.p. 181 - 182 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.99 (s, 1H), 7.79 (d, J = 8.4 Hz, 2H), 7.31 (s, 1H), 7.16 (d, J = 8.2 Hz, 1H), 6.99 – 6.91 (m, 3H), 3.88 (s, 3H), 2.43 (s, 3H), 2.34 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 192.1, 162.6, 142.6, 133.6, 133.0, 131.5, 130.8, 129.6, 127.9, 123.8, 120.7, 113.9, 113.4, 55.4, 21.6, 14.4. HRMS (ESI) Calcd. For $C_{18}H_{17}NO_2$: [M+H]$^+$, 280.1338; Found: m/z 280.1338.



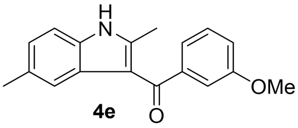
4c

(4-chlorophenyl)(2,5-dimethyl-*1H*-indol-3-yl)methanone (4c): Yield 79%, 44.4 mg; white solid; m.p. 216 - 217 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.90 (s, 1H), 7.63 (d J = 8.2 Hz, 2H), 7.57 (d J = 8.2 Hz, 2H), 7.29 (d, J = 8.2 Hz, 1H), 7.25 (s, 1H), 6.96 (dd, J = 8.2, 1.2 Hz, 1H), 2.34 (s, 3H), 2.30 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 190.7, 145.0, 140.7, 136.1, 133.7, 130.5, 130.2, 128.9, 127.9, 123.8, 120.3, 112.4, 111.4, 21.8, 14.8. HRMS (ESI) Calcd. For $C_{17}H_{14}ClNO$: [M+H]$^+$, 284.0842; Found: m/z 284.0842.



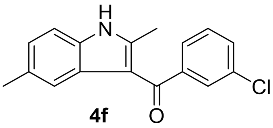
4d

(2,5-dimethyl-*1H*-indol-3-yl)(3,5-dimethylphenyl)methanone (4d): Yield 79%, 43.2 mg; white solid; m.p. 220 - 221 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.79 (s, 1H), 7.29 (s, 1H), 7.26 (d, J = 8.2 Hz, 1H), 7.20 (s, 3H), 6.95 (dd, J = 8.2, 1.2 Hz, 1H), 2.32 (s, 6H), 2.30 (s, 3H), 2.30 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 192.3, 144.5, 142.2, 137.8, 133.7, 132.6, 129.9, 128.1, 126.2, 123.6, 120.5, 112.8, 111.2, 21.8, 21.2, 14.8. HRMS (ESI) Calcd. For $C_{19}H_{19}NO$: [M+H]$^+$, 278.1545; Found: m/z 278.1545.



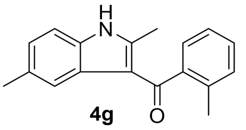
4e

(2,5-dimethyl-*1H*-indol-3-yl)(3-methoxylphenyl)methanone (4e): Yield 80%, 44.7 mg; white solid; m.p. 172 - 173 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.83 (s, 1H), 7.41 (t, *J* = 7.8 Hz, 1H), 7.27 (t, *J* = 4.0 Hz, 2H), 7.14 (dd, *J* = 8.2, 1.6 Hz, 2H), 7.11 (t, *J* = 1.2 Hz, 1H), 6.95 (d, *J* = 8.2 Hz, 1H), 3.79 (s, 3H), 2.32 (s, 3H), 2.29 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 191.8, 159.6, 144.9, 143.7, 133.7, 130.1, 130.0, 128.0, 123.8, 120.8, 120.5, 117.3, 113.1, 112.6, 111.3, 55.7, 21.9, 14.8. HRMS (ESI) Calcd. For $C_{18}H_{17}NO_2$: $[M+H]^+$, 280.1338; Found: m/z 280.1338.



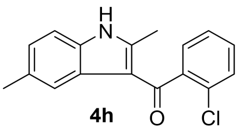
4f

(3-chlorophenyl)(2,5-dimethyl-*1H*-indol-3-yl)methanone (4f): Yield 78%, 43.7 mg; white solid; m.p. 220 - 221 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.95 (s, 1H), 7.66 (m, 1H), 7.60 (s, 1H), 7.54 (d, *J* = 4.9 Hz, 2H), 7.29 (d, *J* = 8.2 Hz, 1H), 7.23 (s, 1H), 6.97 (d, *J* = 8.1 Hz, 1H), 2.33 (s, 3H), 2.29 (s, 3H).^{13}C NMR (100 MHz, DMSO-d_6) δ 192.1, 167.4, 146.5, 141.6, 138.2, 131.9, 128.9, 128.6, 127.5, 123.5, 122.9, 113.7, 111.7, 52.3, 14.8. HRMS (ESI) Calcd. For $C_{17}H_{14}ClNO$: $[M+H]^+$, 284.0842; Found: m/z 284.0842.



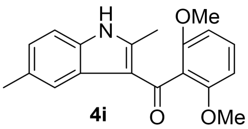
4g

(2,5-dimethyl-*1H*-indol-3-yl)(*o*-tolyl)methanone (4g): Yield 80%, 41.6 mg; white solid; m.p. 202 - 203 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.87 (s, 1H), 7.39 (t, *J* = 7.4 Hz, 1H), 7.36 – 7.22 (m, 4H), 7.19 (d, *J* = 7.4 Hz, 1H), 6.95 (d, *J* = 8.2 Hz, 1H), 2.28 (s, 3H), 2.19 (s, 3H), 2.16 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 193.2, 146.0, 143.5, 134.0, 133.7, 130.8, 130.5, 129.3, 127.8, 126.5, 126.4, 123.9, 120.6, 113.2, 111.3, 21.9, 19.1, 14.4. HRMS (ESI) Calcd. For $C_{18}H_{17}NO$: $[M+H]^+$, 264.1388; Found: m/z 264.1388.



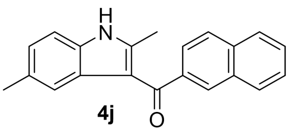
4h

(2-chlorophenyl)(2,5-dimethyl-*1H*-indol-3-yl)methanone (4h): Yield 75%, 42.0 mg; white solid; m.p. 233 - 234 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.98 (s, 1H), 7.59 (d, *J* = 7.6 Hz, 1H), 7.53 (dt, *J* = 7.6, 1.6 Hz 1H), 7.48 (dt, *J* = 7.6, 0.8 Hz 1H), 7.38 (dd, *J* = 7.6, 1.6 Hz 1H), 7.29 (s, 1H), 7.27 (d, *J* = 8.2 Hz, 1H), 6.98 (d, *J* = 8.2 Hz, 1H), 2.29 (s, 3H), 2.17 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 189.0, 146.6, 142.5, 133.8, 131.0, 130.9, 130.1, 129.4, 128.3, 128.2, 127.7, 124.1, 120.5, 112.7, 111.5, 21.9, 14.3. HRMS (ESI) Calcd. For $C_{17}H_{14}ClNO$: $[M+H]^+$, 284.0842; Found: m/z 284.0842.



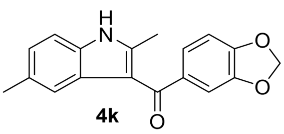
4i

(2,6-dimethoxyphenyl)(2,5-dimethyl-*1H*-indol-3-yl)methanone (4i): Yield 66%, 40.5 mg; white solid; m.p. 192 - 193 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.68 (s, 1H), 7.38 (t, *J* = 8.4 Hz, 1H), 7.21 (d, *J* = 8.0 Hz, 1H), 6.94 (d, *J* = 8.0 Hz, 1H), 6.76 (d, *J* = 8.4 Hz, 3H), 3.65 (s, 6H), 2.31 (s, 3H), 2.10 (d, *J* = 13.0 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 188.2, 156.8, 145.3, 133.5, 130.5, 127.9, 123.7, 121.7, 120.8, 114.1, 111.1, 105.0, 56.1, 21.9, 13.8. HRMS (ESI) Calcd. For $C_{19}H_{19}NO_3$: $[M+H]^+$, 310.1443; Found: m/z 310.1444.



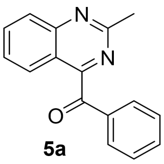
4j

(2,5-dimethyl-*1H*-indol-3-yl)(naphthalen-2-yl)methanone (4j): Yield 80%, 47.2 mg; white solid; m.p. 292 - 293 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.91 (s, 1H), 8.08 (d, *J* = 8.2 Hz, 1H), 8.03 (d, *J* = 8.2 Hz, 1H), 7.83 (d, *J* = 8.2 Hz, 1H), 7.61 (dt, *J* = 7.6, 1.2 Hz, 1H), 7.56 (tt, *J* = 7.6, 1.2 Hz, 1H), 7.52 – 7.46 (m, 2H), 7.30 (s, 1H), 7.27 (d, *J* = 8.2 Hz, 1H), 6.96 (dd, *J* = 8.2, 1.2 Hz, 1H), 2.25 (s, 3H), 2.03 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 192.4, 146.1, 141.1, 133.7, 133.6, 130.6, 129.9, 129.6, 128.7, 127.8, 127.2, 126.7, 125.9, 125.2, 124.7, 123.9, 120.8, 114.0, 111.3, 21.8, 14.5. HRMS (ESI) Calcd. For $C_{21}H_{17}NO$: $[M+H]^+$, 300.1388; Found: m/z 300.1388.



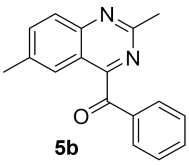
4k

Benzo[*d*][1,3]dioxol-5-yl(2,5-dimethyl-*1H*-indol-3-yl)methanone (4k): Yield 70%, 41.2 mg; white solid; m.p. 252 - 253 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.76 (s, 1H), 7.26 (d, *J* = 8.8 **Hz**, 2H), 7.22 – 7.15 (m, 2H), 7.00 (d, *J* = 8.0 Hz, 1H), 6.94 (d, *J* = 8.0 Hz, 1H), 6.14 (s, 2H), 2.37 (s, 3H), 2.30 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 190.5, 150.4, 147.8, 143.9, 135.9, 133.7, 129.8, 128.1, 124.7, 123.6, 120.3, 112.7, 111.3, 108.7, 108.2, 102.1, 21.8, 14.6. HRMS (ESI) Calcd. For $C_{18}H_{15}NO_3$: [M+H]$^+$, 294.1130; Found: m/z 294.1130.



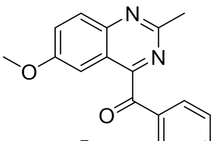
5a

(2-methylquinazolin-4-yl)(phenyl)methanone (5a): Yield 74%, 36.9 mg; yellow solid; m.p. 133 - 134 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.09 (qd, *J* = 24.4, 7.6 Hz, 1H), 8.07 (d, *J* = 8.4 Hz, 1H), 7.95 – 7.90 (m, 3H), 7.64 (t, *J* = 7.4 Hz, 1H), 7.56 (t, *J* = 7.6 Hz, 1H), 7.49 (t, *J* = 7.8 Hz, 2H), 2.95 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 192.1, 163.7, 162.3, 150.3, 134.1, 133.6, 133.5, 129.6, 127.7, 127.2, 126.7, 124.6, 118.8, 25.3. HRMS (ESI) Calcd. For $C_{16}H_{12}N_2O$: [M+H]$^+$, 249.1028; Found: m/z 249.1028.



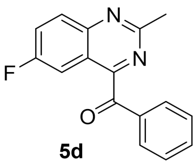
5b

(2,6-dimethylquinazolin-4-yl)(phenyl)methanone (5b): Yield 74%, 38.8 mg; yellow solid; m.p. 140 - 141 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.98 (d, *J* = 8.7 Hz 1H), 7.90 (ddd, *J* = 8.4, 3.5, 1.6 Hz, 3H), 7.77 (t, *J* = 7.4 Hz, 1H), 7.67 (s, 1H), 7.59 (t, *J* = 7.8 Hz, 2H), 2.80 (s, 3H), 2.47 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 193.6, 164.0, 162.4, 150.0, 138.5, 137.7, 135.3, 135.2, 130.8, 129.5, 128.2, 124.1, 119.5, 26.2, 21.6. HRMS (ESI) Calcd. For $C_{17}H_{14}N_2O$: [M+H]$^+$, 263.1184; Found: m/z 263.1184.



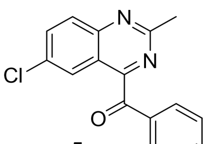
5c

(6-methoxy-2-methylquinazolin-4-yl)(phenyl)methanone (5c): Yield 78%, 43.3 mg; yellow solid; m.p. 144 - 145 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.15 (d, *J* = 1.6 Hz 1H), 8.00 – 7.90 (m, 4H), 7.68 (t, *J* = 7.4 Hz, 1H), 7.52 (t, *J* = 7.6 Hz, 2H), 2.96 (s, 3H), 2.93 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 192.5, 163.7, 163.3, 150.2, 138.1, 134.9, 134.7, 130.8, 130.1, 128.8, 127.9, 121.6, 120.8, 29.7, 26.4. HRMS (ESI) Calcd. For $C_{17}H_{14}N_2O_2$: [M+H]$^+$, 279.1134; Found: m/z 279.1134.



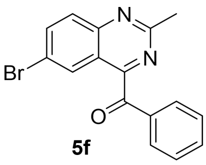
5d

(6-fluoro-2-methylquinazolin-4-yl)(phenyl)methanone (5d): Yield 80%, 42.5 mg; yellow solid; m.p. 99 - 100 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.07 (dd, *J* = 9.2, 5.2 Hz, 1H), 7.96 (dd, *J* = 8.0, 1.2 Hz, 2H), 7.73 – 7.61 (m, 3H), 7.50 (t, *J* = 7.8 Hz, 2H), 2.94 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 192.7, 163.5 (d, *J* = 5.9 Hz), 162.8 (d, *J* = 2.7 Hz), 160.5 (d, *J* = 250.0 Hz), 148.8, 135.0, 134.6, 131.0 (d, *J* = 8.6 Hz), 130.8, 128.8, 125.1 (d, *J* = 25.8 Hz), 120.3 (d, *J* = 9.7 Hz), 109.2 (d, *J* = 23.2 Hz), 26.2. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -109.3. HRMS (ESI) Calcd. For $C_{16}H_{11}FN_2O$: [M+H]$^+$, 267.0934; Found: m/z 267.0934.



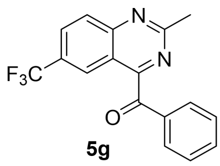
5e

(6-chloro-2-methylquinazolin-4-yl)(phenyl)methanone (5e): Yield 78%, 44.0 mg; yellow solid; m.p. 104 - 105 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.12 (d, *J* = 0.4 Hz 1H), 8.11 (d, *J* = 2.0 Hz, 1H), 8.05 (dd, *J* = 2.0, 0.8 Hz, 1H), 7.98 (dt, *J* = 8.4, 1.2 Hz, 2H), 7.81 (t, *J* = 7.4 Hz, 1H), 7.62 (t, *J* = 7.8 Hz, 2H), 2.86 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 192.9, 163.7, 163.5, 150.1, 136.0, 135.3, 135.1, 131.0, 130.8, 129.4, 129.0, 124.7, 120.2, 26.3. HRMS (ESI) Calcd. For $C_{16}H_{11}ClN_2O$: [M+H]$^+$, 283.0638; Found: m/z 283.0638.



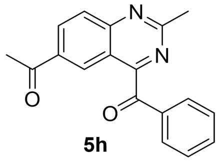
5f

(6-bromo-2-methylquinazolin-4-yl)(phenyl)methanone (5f): Yield 77%, 49.8 mg; yellow solid; m.p. 137 - 138 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.23 (d, *J* = 2.4 Hz, 1H), 8.20 (q, *J* = 2.0 Hz, 1H), 8.06 (d, *J* = 8.8 Hz, 1H), 7.98 (dd, *J* = 8.4, 1.2 Hz, 2H), 7.81 (t, *J* = 7.4 Hz, 1H), 7.63 (t, *J* = 7.8 Hz, 2H), 2.85 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 192.9, 163.7, 163.4, 150.2, 138.6, 135.3, 135.1, 131.1, 130.8, 129.4, 127.9, 121.3, 120.7, 26.4. HRMS (ESI) Calcd. For $C_{16}H_{11}BrN_2O$: [M+H]$^+$, 327.0133; Found: m/z 327.0134.



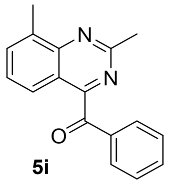
5g

(2-methyl-6-(trifluoromethyl)quinazolin-4-yl)(phenyl)methanone (5g): Yield 62%, 39.2 mg; yellow solid; m.p. 139 - 140 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.31 (s, 1H), 8.18 (d, *J* = 8.8 Hz, 1H), 8.08 (dd, *J* = 8.8, 1.6 Hz, 1H), 7.97 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.69 (t, *J* = 7.4 Hz, 1H), 7.53 (t, *J* = 7.8 Hz, 2H), 2.98 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 192.3, 165.5, 165.0, 152.7, 134.8, 134.8, 130.8, 130.1 (q, *J* = 2.9 Hz), 129.8, 129.6 (q, *J* = 33.0 Hz), 128.9, 123.9 (q, *J* = 4.5 Hz), 123.3 (q, *J* = 271.1 Hz), 119.0, 26.6. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.7. HRMS (ESI) Calcd. For $C_{17}H_{11}F_3N_2O$: [M+H]$^+$, 317.0902; Found: m/z 317.0902.



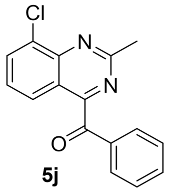
5h

1-(4-benzoyl-2-methylquinazolin-6-yl)ethan-1-one (5h): Yield 54%, 31.4 mg; yellow solid; m.p. 183 - 184 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.57 (d, *J* = 1.2 Hz, 1H), 8.48 (dd, *J* = 8.8, 1.2 Hz, 1H), 8.11 (d, *J* = 8.8 Hz, 1H), 7.98 (d, *J* = 7.6 Hz, 2H), 7.68 (t, *J* = 7.4 Hz, 1H), 7.52 (t, *J* = 7.6 Hz, 2H), 2.97 (s, 3H), 2.65 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 195.5, 191.5, 164.5, 164.4, 152.4, 134.7, 133.9, 133.7, 131.6, 129.8, 128.0, 127.8, 126.5, 118.2, 28.7, 25.6. HRMS (ESI) Calcd. For $C_{18}H_{14}N_2O_2$: [M+H]$^+$, 291.1134; Found: m/z 291.1134.



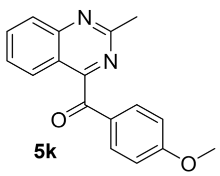
5i

(2,8-dimethylquinazolin-4-yl)(phenyl)methanone (5i): Yield 70%, 36.4 mg; yellow solid; m.p. 139 - 140 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92 (d, *J* = 7.6 Hz, 2H), 7.74 (d, *J* = 7.6 Hz, 2H), 7.64 (dd, *J* = 7.4, 1.2 Hz,, 1H), 7.52 – 7.40 (m, 3H), 2.96 (d, *J* = 1.2 Hz, 3H), 2.81 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 193.6, 164.8, 162.4, 150.6, 136.8, 135.3, 134.4, 134.3, 130.6, 128.7, 127.1, 123.3, 119.6, 26.7, 17.4. HRMS (ESI) Calcd. For $C_{17}H_{14}N_2O$: [M+H]$^+$, 263.1184; Found: m/z 263.1184.



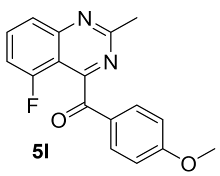
5j

(8-chloro-2-methylquinazolin-4-yl)(phenyl)methanone (5j): Yield 76%, 42.8 mg; yellow solid; m.p. 104 - 105 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.02 (dd, *J* = 7.6, 1.0 Hz, 1H), 7.92 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.88 (dd, *J* = 8.2, 1.0 Hz, 1H), 7.67 (t, *J* = 7.4 Hz, 1H), 7.53 – 7.45 (m, 3H), 3.02 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 192.8, 165.1, 164.4, 148.0, 134.9, 134.7, 134.3, 132.9, 130.7, 128.9, 127.5, 124.6, 121.1, 26.8. HRMS (ESI) Calcd. For $C_{16}H_{11}ClN_2O$: [M+H]$^+$, 283.0638; Found: m/z 283.0638.



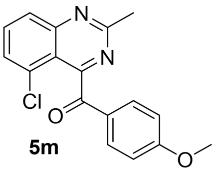
5k

(4-methoxyphenyl)(2-methylquinazolin-4-yl)methanone (5k): Yield 80%, 44.2 mg; yellow solid; m.p. 140 - 141 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.12 (d, *J* = 1.2 Hz, 1H), 7.89 (dd, *J* = 8.4, 6.0 Hz, 4H), 7.68 (dd, *J* = 8.8, 1.6 Hz, 1H), 7.08 (d, *J* = 8.8 Hz, 2H), 3.87 (s, 3H), 2.82 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 186.9, 160.5, 160.0, 158.6, 146.6, 129.7, 128.4, 124.5, 123.5, 122.8, 121.1, 116.0, 109.4, 50.9, 21.7. HRMS (ESI) Calcd. For $C_{17}H_{14}N_2O_2$: [M+H]$^+$, 279.1134; Found: m/z 279.1134.



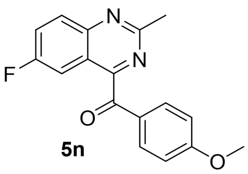
5l

(5-fluoro-2-methylquinazolin-4-yl)(4-methoxyphenyl)methanone (5l): Yield 75%, 44.2 mg; yellow solid; m.p. 132 - 133 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.00 (dd, *J* = 9.2, 6.0 Hz, 1H), 7.92 (d, *J* = 8.8 Hz, 2H), 7.67 (dd, *J* = 9.6, 2.4 Hz, 1H), 7.33 (td, *J* = 8.8, 2.4 Hz, 1H), 6.97 (d, *J* = 8.8 Hz, 2H), 3.90 (s, 3H), 2.94 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 191.2, 167.3, 164.9, 164.7 (d, *J* = 2.7 Hz), 164.5, 153.2 (d, J = 13.9 Hz), 133.2, 128.7 (d, J = 10.6 Hz), 128.0, 118.4, 118.2, 114.2, 112.1 (d, J = 20.6 Hz), 55.7, 26.4. ^{19}F NMR (376 MHz, Chloroform-d) δ -100.4. HRMS (ESI) Calcd. For $C_{17}H_{13}FN_2O_2$: [M+H]$^+$, 297.1039; Found: m/z 297.1039.



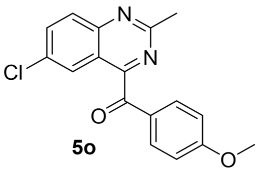
5m

(5-chloro-2-methylquinazolin-4-yl)(4-methoxyphenyl)methanone (5m): Yield 73%, 45.1 mg; yellow solid; m.p. 152 - 153 ^{o}C. ^{1}H NMR (400 MHz, Chloroform-d) δ 8.04 (d, J = 8.0 Hz, 1H), 7.91 (d, J = 8.4 Hz, 3H), 7.55 (t, J = 7.4 Hz, 1H), 6.96 (d, J = 8.8 Hz, 2H), 3.88 (s, 3H), 2.94 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-d) δ 191.0, 164.9, 164.0, 163.6, 149.9, 135.5, 133.2, 132.2, 131.8, 130.0, 127.9, 124.7, 114.2, 55.7, 26.4. HRMS (ESI) Calcd. For $C_{17}H_{13}ClN_2O_2$: [M+H]$^+$, 313.0744; Found: m/z 313.0744.



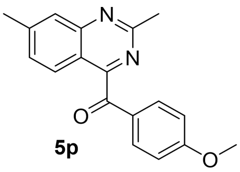
5n

(6-fluoro-2-methylquinazolin-4-yl)(4-methoxyphenyl)methanone (5n): Yield 85%, 49.9 mg; yellow solid; m.p. 144 - 145 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.14 (dd, J = 9.2, 5.2 Hz, 1H), 7.98 (td, J = 9.0, 2.6 Hz, 1H), 7.90 (d, J = 8.2 Hz, 2H), 7.64 (dd, J = 8.8, 2.4 Hz, 1H), 7.09 (d, J = 8.4 Hz, 2H), 3.87 (s, 3H), 2.81 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 191.3, 165.0, 164.4 (d, J = 5.8 Hz), 162.8 (d, J = 2.6 Hz), 160.3 (d, J = 247.2 Hz), 148.8, 133.5, 131.8, 131.7 (d, J = 9.0 Hz), 125.7 (d, J = 25.8 Hz), 120.0 (d, J = 9.9 Hz), 114.8, 109.3 (d, J = 23.1 Hz), 56.3, 26.2. ^{19}F NMR (376 MHz, DMSO-d_6) δ -110.1. HRMS (ESI) Calcd. For $C_{17}H_{13}FN_2O_2$: [M+H]$^+$, 297.1039; Found: m/z 297.1039.



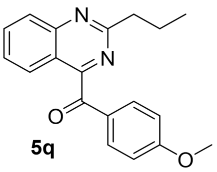
5o

(6-chloro-2-methylquinazolin-4-yl)(4-methoxyphenyl)methanone (5o): Yield 82%, 50.8 mg; yellow solid; m.p. 176 - 177 ^{o}C. ^{1}H NMR (400 MHz, Chloroform-d) δ 8.04 – 7.95 (m, 2H), 7.93 (d, J = 8.8 Hz, 2H), 7.83 (d, J = 8.8 Hz, 1H), 6.97 (d, J = 8.8 Hz, 2H), 3.89 (s, 3H), 2.93 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-d) δ 191.0, 164.9, 164.0, 163.6, 149.9, 135.5, 133.4, 133.2, 130.0, 127.9, 126.9, 124.7, 114.2, 55.7, 26.4. HRMS (ESI) Calcd. For $C_{17}H_{13}ClN_2O_2$: [M+H]$^+$, 313.0744; Found: m/z 313.0745.



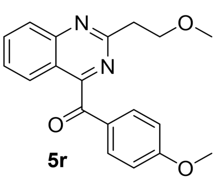
5p

(2,7-dimethylquinazolin-4-yl)(4-methoxyphenyl)methanone (5p): Yield 71%, 41.0 mg; yellow solid; m.p. 157 - 158 ^{o}C. ^{1}H NMR (400 MHz, Chloroform-d) δ 7.90 (d, J = 9.2 Hz, 2H), 7.82 – 7.78 (m, 2H), 7.37 (d, J = 8.4 Hz, 1H), 6.95 (d, J = 8.8 Hz, 2H), 3.88 (s, 3H), 2.92 (s, 3H), 2.58 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-d) δ 190.8, 163.7, 162.4, 163.6, 150.6, 144.7, 132.1, 133.4, 128.8, 127.3, 126.1, 124.4, 117.0, 113.1, 54.6, 25.4, 21.3. HRMS (ESI) Calcd. For $C_{18}H_{16}N_2O_2$: [M+H]$^+$, 293.1290; Found: m/z 293.1290.



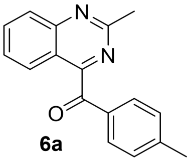
5q

(4-methoxyphenyl)(2-propylquinazolin-4-yl)methanone (5q): Yield 74%, 44.8 mg; yellow oil. ^{1}H NMR (400 MHz, Chloroform-d) δ 8.05 (d, J = 8.4 Hz, 1H), 8.00 – 7.90 (m, 3H), 7.88 (dd, J = 6.8, 1.6 Hz, 2H), 7.54 (t, J = 7.8 Hz, 1H), 6.95 (d, J = 9.0 Hz, 2H), 3.87 (s, 3H), 3.13 (t, J = 7.8 Hz, 2H), 1.95 (h, J = 7.4 Hz, 2H), 1.04 (t, J = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-d) δ 191.7, 166.6, 165.0, 164.7, 151.4, 134.3, 133.1, 128.4, 128.3, 127.5, 125.8, 120.0, 114.1, 55.6, 41.8, 22.3, 14.0. HRMS (ESI) Calcd. For $C_{19}H_{18}N_2O_2$: [M+H]$^+$, 307.1447; Found: m/z 307.1447.



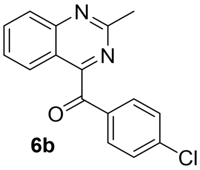
5r

(2-(2-methoxyethyl)quinazolin-4-yl)(4-methoxyphenyl)methanone (5r): Yield 72%, 45.9 mg; yellow oil. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.08 (d, *J* = 8.4 Hz, 1H), 7.99 – 7.93 (m, 3H), 7.90 (t, *J* = 7.6 Hz, 1H), 7.56 (t, *J* = 7.6 Hz, 1H), 6.95 (d, *J* = 8.8 Hz, 2H), 4.00 (t, *J* = 6.6 Hz, 2H), 3.88 (s, 3H), 3.44 (t, *J* = 6.6 Hz, 2H), 3.38 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 191.6, 164.9, 164.7, 163.8, 151.4, 134.4, 133.2, 132.2, 128.5, 128.3, 127.7, 125.8, 114.0, 70.9, 58.7, 55.6, 39.8. HRMS (ESI) Calcd. For $C_{19}H_{18}N_2O_3$: $[M+H]^+$, 323.1396; Found: m/z 323.1396.



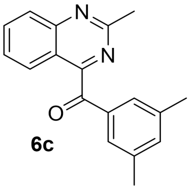
6a

(2-methylquinazolin-4-yl)(*p*-tolyl)methanone (6a): Yield 75%, 38.8 mg; yellow solid; m.p. 137 - 138 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.05 (d, *J* = 8.4 Hz, 1H), 7.95 – 7.86 (m, 2H), 7.83 (d, *J* = 8.2 Hz, 2H), 7.55 (t, *J* = 7.6 Hz, 1H), 7.29 (d, *J* = 8.0 Hz, 2H), 2.95 (s, 3H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 192.8, 165.0, 163.4, 151.3, 145.8, 134.5, 132.8, 130.8, 129.5, 128.2, 127.6, 125.7, 119.8, 26.4, 21.9. HRMS (ESI) Calcd. For $C_{17}H_{14}N_2O$: $[M+H]^+$, 263.1184; Found: m/z 263.1184.



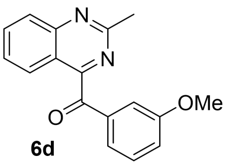
6b

(4-chlorophenyl)(2-methylquinazolin-4-yl)methanone (6b): Yield 78%, 43.7 mg; yellow solid; m.p. 142 - 143 °C. ^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 8.06 (d, *J* = 3.6 Hz, 2H), 7.97 – 7.92 (m, 3H), 7.72 – 7.67 (m, 1H), 7.65 (d, *J* = 8.6 Hz, 2H), 2.82 (s, 3H). ^{13}C NMR (100 MHz, DMSO-*d*$_6$) δ 192.4, 163.9, 163.2, 151.4, 140.4, 135.6, 133.9, 132.7, 129.7, 129.2, 128.7, 125.8, 119.5, 26.4. HRMS (ESI) Calcd. For $C_{16}H_{11}ClN_2O$: $[M+H]^+$, 283.0638; Found: m/z 283.0638.



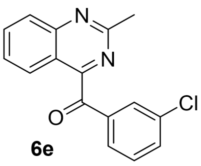
6c

(3,5-dimethylphenyl)(2-methylquinazolin-4-yl)methanone (6c): Yield 71%, 38.7 mg; yellow solid; m.p. 145 - 146 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.06 (d, *J* = 8.6 Hz, 1H), 7.89 (dd, *J* = 13.4, 8.0 Hz, 2H), 7.72 (s, 1H), 7.54 (t, *J* = 8.0 Hz, 1H), 7.49 (s, 2H), 2.94 (s, 3H), 2.32 (s, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 193.6, 165.4, 163.5, 151.2, 138.6, 138.1, 135.3, 135.2, 134.6, 128.3, 127.8, 125.7, 119.8, 26.4, 21.2. HRMS (ESI) Calcd. For $C_{18}H_{16}N_2O$: $[M+H]^+$, 277.1341; Found: m/z 277.1341.



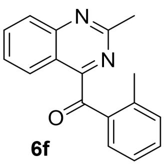
6d

(3-methoxyphenyl)(2-methylquinazolin-4-yl)methanone (6d): Yield 77%, 42.4 mg; yellow solid; m.p. 138 - 139 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.04 (d, *J* = 8.4 Hz, 1H), 7.91 (t, *J* = 7.6 Hz, 2H), 7.60 – 7.53 (m, 2H), 7.39 – 7.32 (m, 2H), 7.19 (dt, *J* = 6.4, 2.8 Hz, 1H), 3.86 (s, 3H), 2.94 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 193.0, 164.7, 163.4, 159.9, 151.4, 136.5, 134.5, 129.7, 128.3, 127.7, 125.6, 124.0, 121.3, 119.8, 114.0, 55.5, 26.4. HRMS (ESI) Calcd. For $C_{17}H_{14}N_2O_2$: $[M+H]^+$, 279.1134; Found: m/z 279.1134.



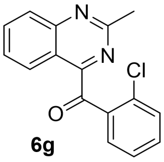
6e

(3-chlorophenyl)(2-methylquinazolin-4-yl)methanone (6e): Yield 74%, 41.3 mg; yellow solid; m.p. 124 - 125 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.06 (d, *J* = 8.4 Hz, 1H), 7.99 – 7.90 (m, 3H), 7.81 (d, *J* = 8.0 Hz, 1H), 7.60 (q, *J* = 7.4 Hz, 2H), 7.43 (t, *J* = 8.0 Hz, 1H), 2.95 (s, 3H). ^{13}C NMR (150 MHz, Chloroform-*d*) δ 191.8, 163.4, 163.3, 151.6, 136.7, 135.1, 134.7, 134.3, 130.4, 130.0, 128.8, 128.4, 127.9, 125.4, 119.7, 26.4. HRMS (ESI) Calcd. For $C_{16}H_{11}ClN_2O$: $[M+H]^+$, 283.0638; Found: m/z 283.0638.



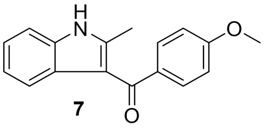
6f

(2-methylquinazolin-4-yl)(*o*-tolyl)methanone (6f): Yield 67%, 35.0 mg; yellow solid; m.p. 111 - 112 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.98 (d, *J* = 8.4 Hz, 1H), 7.70 (p, *J* = 4.0 Hz, 1H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.49 – 7.35 (m, 3H), 7.27 (t, *J* = 7.6 Hz, 2H), 2.77 (s, 3H), 2.56 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 195.9, 165.6, 163.4, 151.4, 140.3, 139.4, 132.2, 131.9, 130.6, 128.7, 128.4, 126.6, 126.3, 125.9, 119.4, 26.3, 21.7. HRMS (ESI) Calcd. For $C_{17}H_{14}N_2O$: $[M+H]^+$, 263.1184; Found: m/z 263.1184.



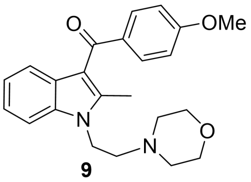
6g

(2-chlorophenyl)(2-methylquinazolin-4-yl)methanone (6g): Yield 68%, 37.9 mg; yellow solid; m.p. 114 - 115 ºC. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.32 (d, *J* = 8.4 Hz, 1H), 8.04 (d, *J* = 8.4 Hz, 1H), 7.93 (s, 1H), 7.80 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.65 (t, *J* = 7.6 Hz, 1H), 7.51 (td, *J* = 7.6, 1.6 Hz, 1H), 7.46 – 7.39 (m, 2H), 2.85 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 194.5, 163.5, 162.8, 151.9, 136.9, 134.3, 133.3, 133.3, 131.9, 130.5, 128.3, 128.0, 127.0, 125.8, 119.5, 26.3. HRMS (ESI) Calcd. For $C_{16}H_{11}ClN_2O$: $[M+H]^+$, 283.0638; Found: m/z 283.0638.



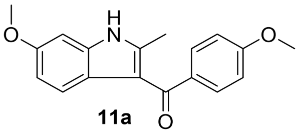
7

(4-methoxyphenyl)(2-methyl-*1H*-indol-3-yl)methanone (7): Yield 80%, 42.2 mg; white solid; m.p. 179 - 180 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.86 (s, 1H), 7.64 (d, *J* = 8.8 Hz, 2H), 7.38 (d, *J* = 8.0 Hz, 1H), 7.33 (d, *J* = 8.0 Hz, 1H), 7.11 (t, *J* = 7.2 Hz, 1H), 7.06 – 6.97 (m, 3H), 3.85 (s, 3H), 2.42 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 191.0, 162.3, 143.8, 135.4, 134.1, 131.2, 127.8, 122.1, 121.1, 120.4, 114.0, 113.1, 111.6, 55.8, 14.5. HRMS (ESI) Calcd. For $C_{17}H_{15}NO_2$: $[M+H]^+$, 266.1181; Found: m/z 266.1181.



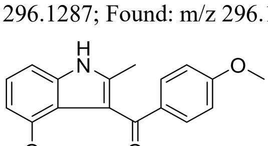
9

Pravadoline (9): Total yield 70%, 52.2 mg; yellow oil. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.78 (d, *J* = 8.8 Hz, 2H), 7.34 (d, *J* = 9.2 Hz, 2H), 7.19 (t, *J* = 7.4 Hz, 1H), 7.07 (t, *J* = 7.4 Hz, 1H), 6.93 (d, *J* = 8.8 Hz, 2H), 4.27 (t, *J* = 7.2 Hz, 2H), 3.88 (s, 3H), 3.74 – 3.69 (t, *J* = 4.4 Hz, 4H), 2.70 (t, *J* = 7.2 Hz, 2H), 2.61 (s, 3H), 2.53 (t, *J* = 4.0 Hz, 4H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 191.7, 162.6, 143.4, 135.7, 133.7, 131.6, 127.3, 121.9, 121.2, 121.1, 114.1, 113.4, 109.1, 66.9, 57.5, 55.4, 54.1, 41.1, 12.4. HRMS (ESI) Calcd. For $C_{23}H_{26}N_2O_3$: $[M+H]^+$, 379.2022; Found: m/z 379.2022.



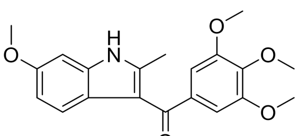
11a

(6-methoxy-2-methyl-*1H*-indol-3-yl)(4-methoxyphenyl)methanone (11a): Yield 57%, 33.4 mg; white solid; m.p. 224 - 225 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.67 (s, 1H), 7.62 (d, *J* = 8.6 Hz, 2H), 7.23 (d, *J* = 8.6 Hz, 1H), 7.03 (d, *J* = 8.6 Hz, 2H), 6.87 (d, *J* = 2.2 Hz, 1H), 6.68 (dd, *J* = 8.6, 2.2 Hz, 1H), 3.84 (s, 3H), 3.77 (s, 3H), 2.37 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 190.9, 162.2, 156.1, 142.7, 136.2, 134.2, 131.1, 121.8, 121.1, 114.0, 113.0, 110.6, 95.1, 55.8, 55.7, 14.5. HRMS (ESI) Calcd. For $C_{18}H_{17}NO_3$: $[M+H]^+$, 296.1287; Found: m/z 296.1287.



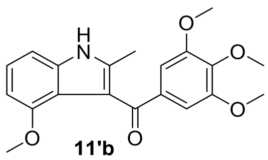
11'a

(4-methoxy-2-methyl-*1H*-indol-3-yl)(4-methoxyphenyl)methanone (11'a): Yield 18%, 10.5 mg; white solid; m.p. 242 - 243 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.63 (s, 1H), 7.60 (d, *J* = 8.8 Hz, 2H), 7.05 – 6.97 (m, 2H), 6.94 (d, *J* = 8.8 Hz, 2H), 6.48 (d, *J* = 7.4 Hz, 1H), 3.80 (s, 3H), 3.33 (s, 3H), 2.36 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 191.8, 162.5, 152.7, 139.1, 136.6, 131.4, 122.9, 117.2, 113.4, 112.9, 104.8, 101.8, 55.8, 55.1, 13.0. HRMS (ESI) Calcd. For $C_{18}H_{17}NO_3$: $[M+H]^+$, 296.1287; Found: m/z 296.1287.



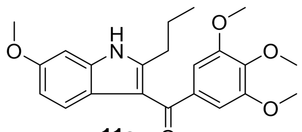
11b

(6-methoxy-2-methyl-*1H*-indol-3-yl)(3,4,5-trimethoxyphenyl)methanone (11b): Yield 54%, 38.0 mg; white solid; m.p. 257 - 258 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.74 (s, 1H), 7.34 (d, *J* = 8.6 Hz, 1H), 6.93 (s, 2H), 6.87 (s, 1H), 6.71 (d, *J* = 8.6 Hz, 1H), 3.76 (s, 6H), 3.75 (s, 3H), 3.36 (s, 3H), 2.37 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 190.9, 156.2, 153.1, 143.6, 140.4, 137.2, 136.3, 121.7, 121.4, 112.8, 110.7, 106.3, 95.1, 60.7, 56.4, 55.7, 14.7. HRMS (ESI) Calcd. For $C_{20}H_{21}NO_5$: $[M+H]^+$, 356.1498; Found: m/z 356.1498.



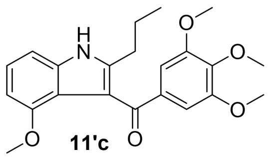
11'b

(4-methoxy-2-methyl-*1H*-indol-3-yl)(3,4,5-trimethoxyphenyl)methanone (11'b): Yield 11%, 7.8 mg mg; white solid; m.p. 270 - 271 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.71 (s, 1H), 7.06 (t, J = 7.8 Hz, 1H), 7.00 (d, J = 8.0 Hz, 1H), 6.97 (s, 2H), 6.52 (d, J = 7.6 Hz, 1H), 3.73 (s, 3H), 3.67 (s, 6H), 3.38 (s, 3H), 2.40 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 191.5, 152.7, 152.6, 141.2, 140.1, 136.7, 136.6, 123.1, 117.1, 112.6, 107.2, 104.9, 101.9, 60.6, 56.3, 55.1, 13.3. HRMS (ESI) Calcd. For $C_{20}H_{21}NO_5$: $[M+H]^+$, 356.1498; Found: m/z 356.1498.



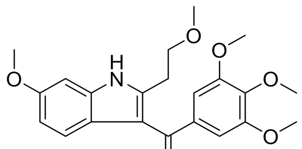
11c

(6-methoxy-2-propyl-*1H*-indol-3-yl)(3,4,5-trimethoxyphenyl)methanone (11c): Yield 52%, 39.5 mg; white solid; m.p. 227 - 228 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.72 (s, 1H), 7.25 (d, J = 8.8 Hz, 1H), 6.94 (s, 2H), 6.88 (d, J = 2.2 Hz, 1H), 6.69 (dd, J = 8.8, 2.2 Hz, 1H), 3.76 (s, 3H), 3.75 (s, 3H), 3.74 (s, 6H), 2.72 (d, J = 7.6 Hz, 2H), 1.66 (h, J = 7.4 Hz, 2H), 0.82 (t, J = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 191.0, 156.1, 153.0, 147.7, 140.4, 137.2, 136.3, 121.5, 121.4, 112.4, 110.7, 106.2, 95.1, 60.7, 56.4, 55.6, 29.7, 23.2, 14.2. HRMS (ESI) Calcd. For $C_{22}H_{25}NO_5$: $[M+H]^+$, 384.1811; Found: m/z 384.1811.



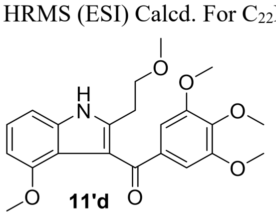
11'c

(4-methoxy-2-propyl-*1H*-indol-3-yl)(3,4,5-trimethoxyphenyl)methanone (11'c): Yield 10%, 7.3 mg; white solid; m.p. 241 - 242 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.66 (s, 1H), 7.03 (dt, J = 15.2, 7.8 Hz, 2H), 6.95 (s, 2H), 6.50 (d, J = 7.4 Hz, 1H), 3.72 (s, 3H), 3.65 (s, 6H), 3.36 (s, 3H), 2.73 (t, J = 7.4 Hz, 2H), 1.67 (h, J = 7.4 Hz, 2H), 0.84 (t, J = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 191.8, 152.7, 152.5, 143.9, 141.2, 136.8, 136.6, 123.1, 117.0, 112.4, 107.0, 105.0, 101.7, 60.6, 56.3, 55.1, 28.8, 23.2, 14.1. HRMS (ESI) Calcd. For $C_{22}H_{25}NO_5$: $[M+H]^+$, 384.1811; Found: m/z 384.1811.



11d

(6-methoxy-2-(2-methoxyethyl)-*1H*-indol-3-yl)(3,4,5-trimethoxyphenyl)methanone (11d): Yield 52%, 41.1 mg; white solid; m.p. 229 - 230 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.73 (s, 1H), 7.18 (d, J = 8.8 Hz, 1H), 6.95 (s, 2H), 6.91 (d, J = 2.2 Hz, 1H), 6.69 (dd, J = 8.8, 2.2 Hz, 1H), 3.76 (s, 3H), 3.75 (s, 3H), 3.74 (s, 6H), 3.61 (t, J = 6.8 Hz, 2H), 3.21 (s, 3H), 3.04 (t, J = 6.8 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 190.8, 156.2, 153.0, 144.4, 140.5, 136.9, 136.3, 121.4, 121.3, 112.9, 110.9, 106.3, 95.2, 71.3, 60.7, 58.3, 56.4, 55.6, 28.4. HRMS (ESI) Calcd. For $C_{22}H_{25}NO_6$: $[M+H]^+$, 400.1760; Found: m/z 400.1760.



11'd

(4-methoxy-2-(2-methoxyethyl)-1H-indol-3-yl)(3,4,5-trimethoxyphenyl)methanone (11'd): Yield 11%, 8.4 mg; white solid; m.p. 243 - 244 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.68 (s, 1H), 7.08 – 7.01 (m, 2H), 6.95 (s, 2H), 6.51 (d, J = 7.4 Hz, 1H), 3.73 (s, 3H), 3.66 (s, 6H), 3.61 (t, J = 6.7 Hz, 2H), 3.36 (s, 3H), 3.20 (s, 3H), 2.99 (t, J = 6.7 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 191.8, 152.8, 152.5, 141.2, 141.0, 136.7, 123.3, 117.0, 113.0, 107.0, 105.1, 101.7, 71.6, 60.6, 58.3, 56.3, 55.4, 55.1, 27.6. HRMS (ESI) Calcd. For $C_{22}H_{25}NO_6$: $[M+H]^+$, 400.1760; Found: m/z 400.1760.

VIII. ^{1}H NMR, ^{13}C NMR and ^{19}F NMR Spectra of Products

Figure S3. The ^{1}H NMR (400 MHz, DMSO-d_6) of **3a**

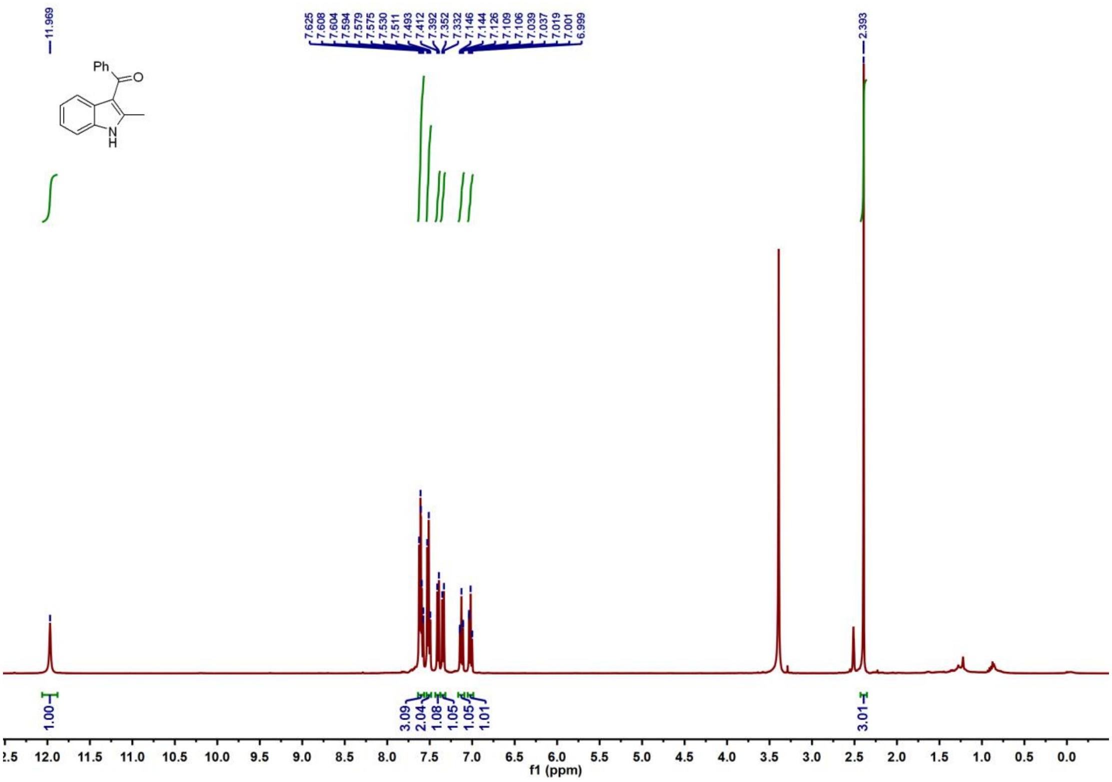


Figure S4. The ^{13}C NMR (150 MHz, DMSO-d_6) of **3a**

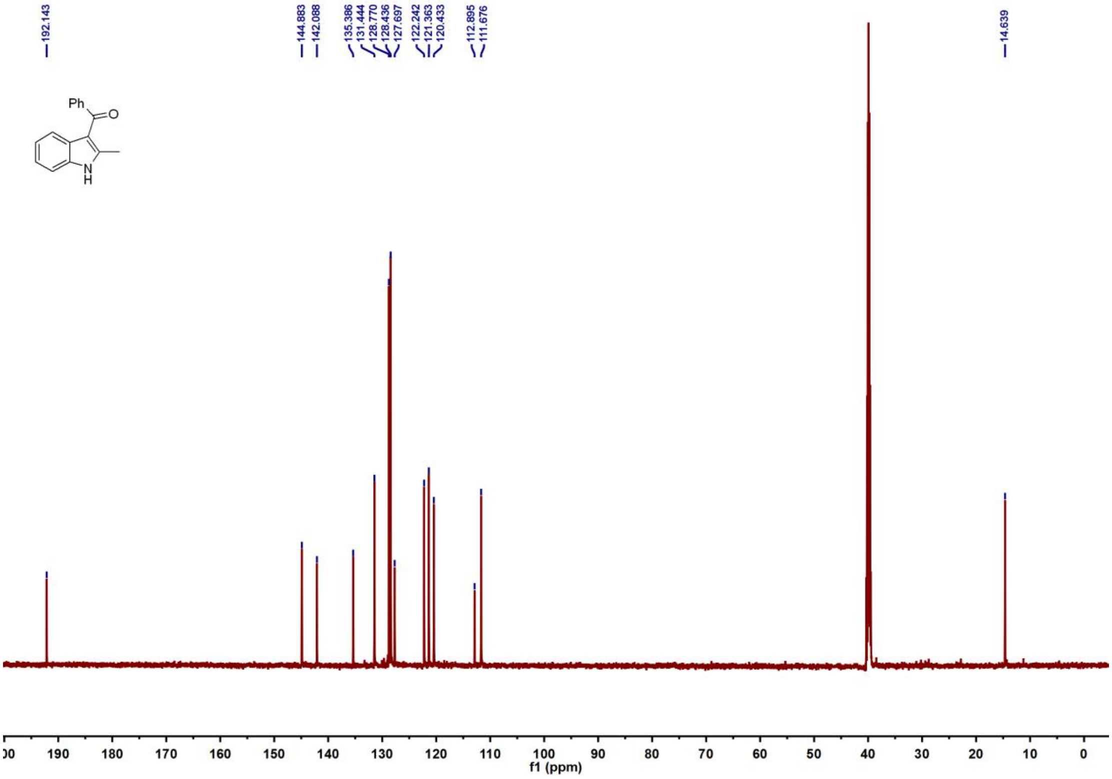


Figure S5. The ^{1}H NMR (400 MHz, DMSO-d_6) of **3b**

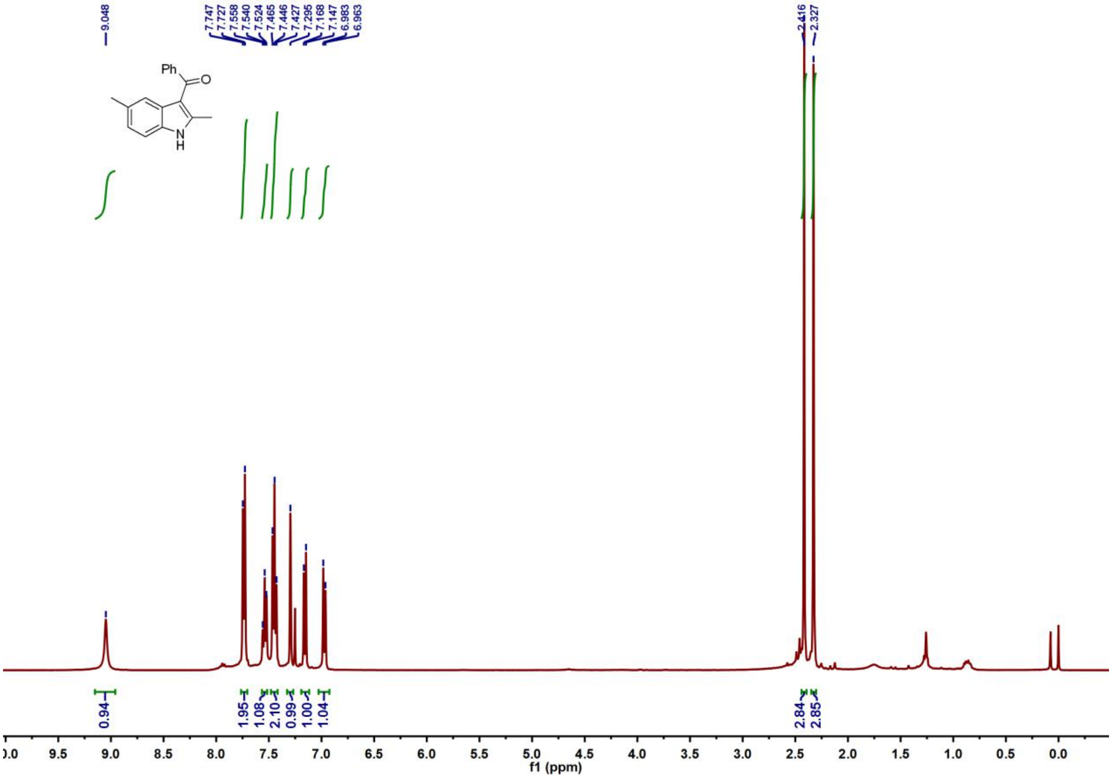


Figure S6. The ^{13}C NMR (150 MHz, DMSO-d_6) of **3b**

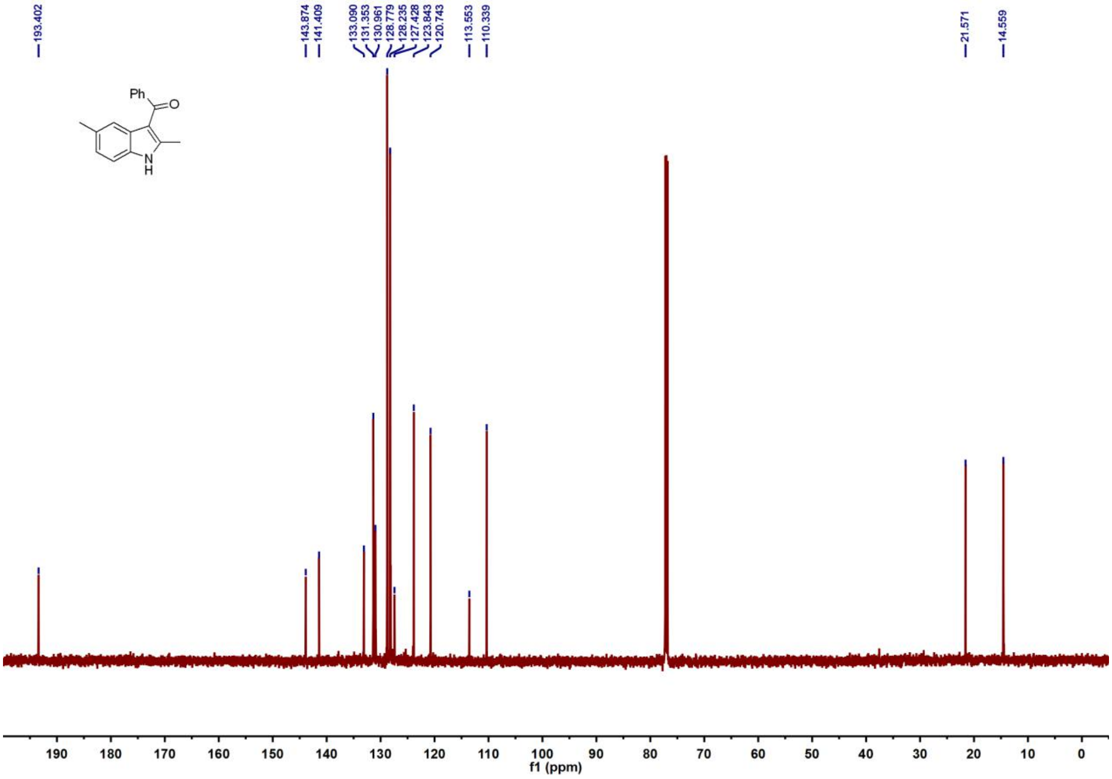


Figure S7. The ^{1}H NMR (400 MHz, DMSO-d_6) of **3c**

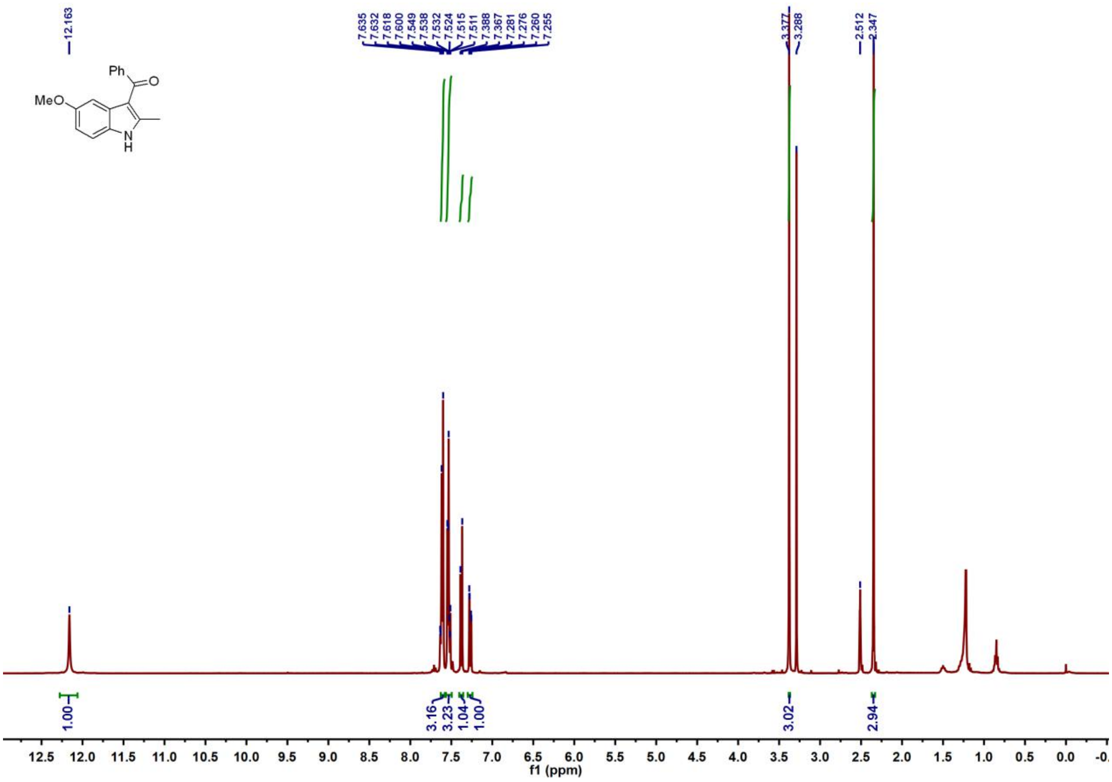


Figure S8. The ^{13}C NMR (100 MHz, DMSO-d_6) of **3c**

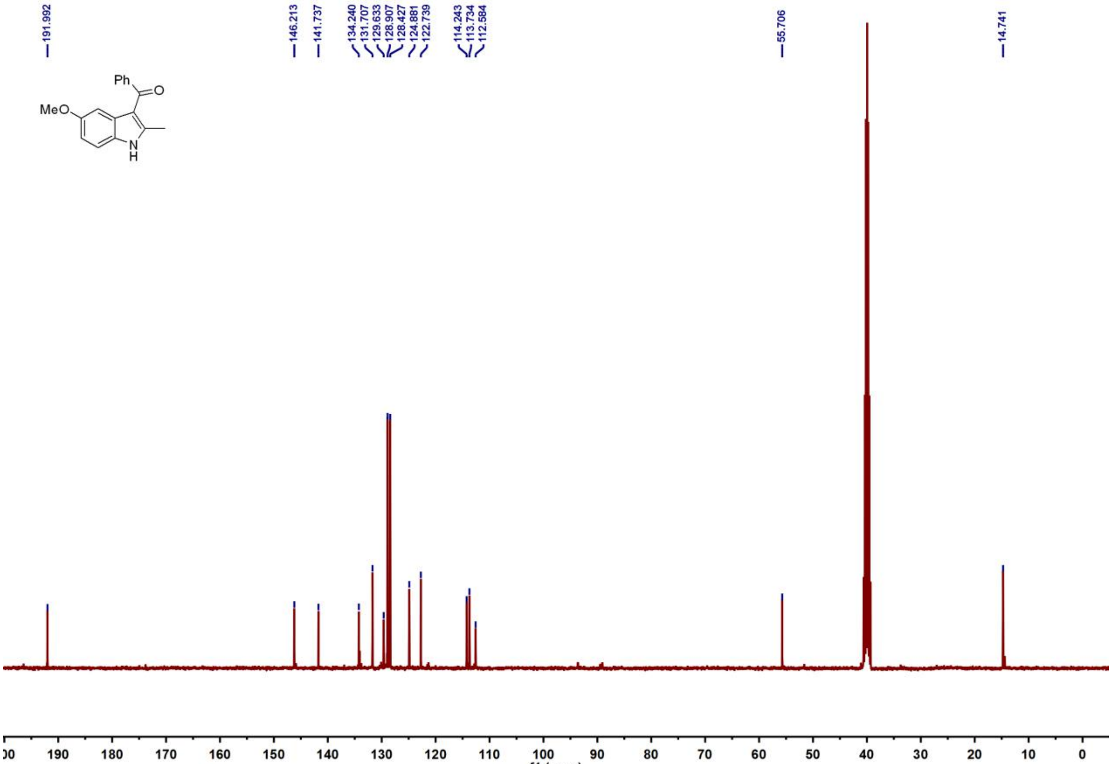


Figure S9. The ^{1}H NMR (400 MHz, DMSO-d_6) of **3d**

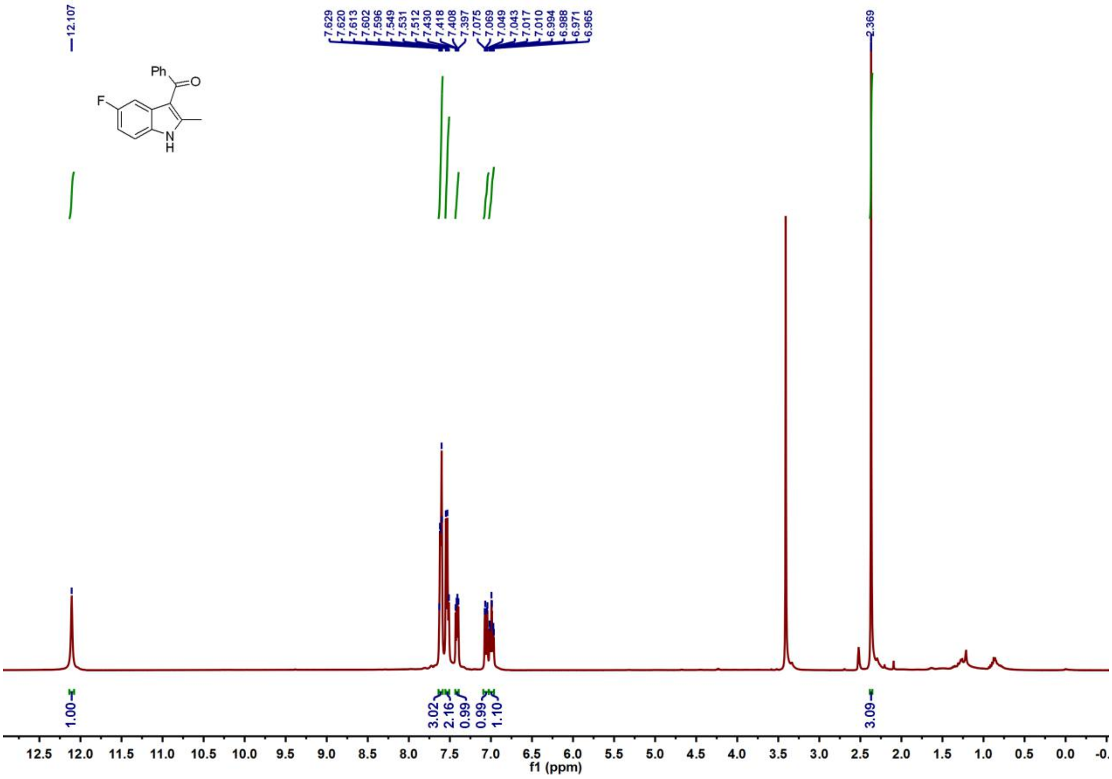


Figure S10. The ^{13}C NMR (150 MHz, DMSO-d_6) of **3d**

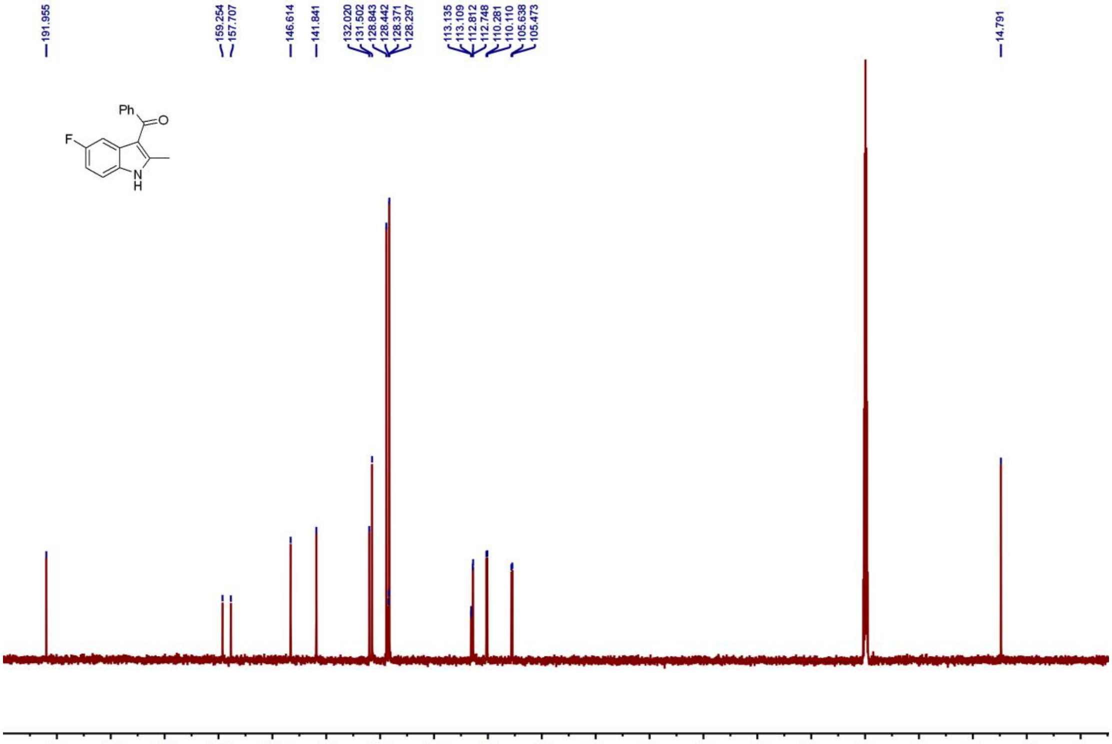


Figure S11. The ^{19}F NMR (376 MHz, DMSO-d_6) of **3d**

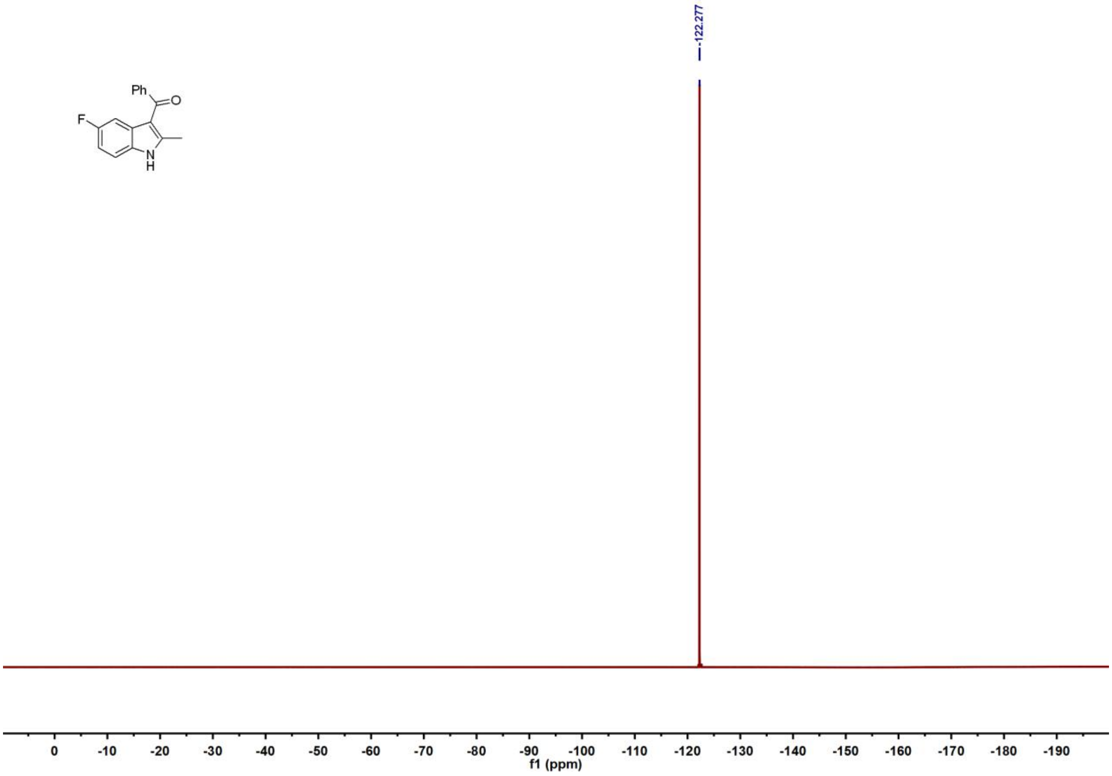


Figure S12. The ^{1}H NMR (400 MHz, DMSO-d_6) of **3e**

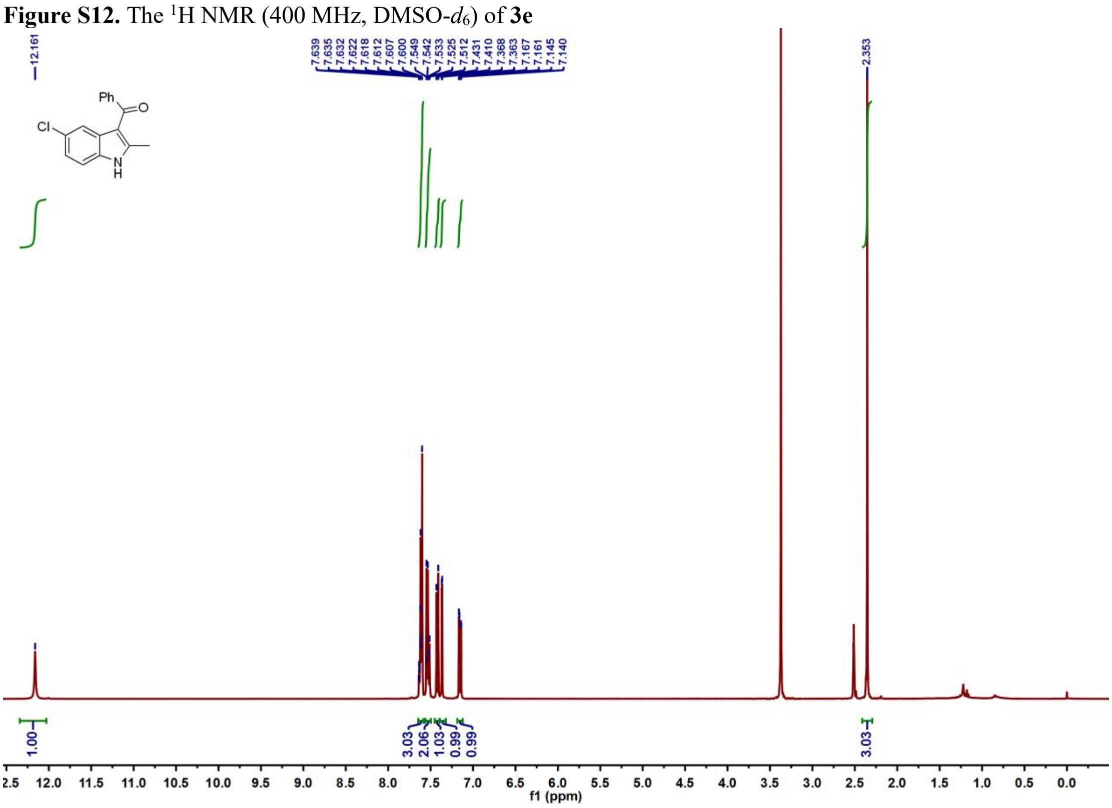


Figure S13. The ^{13}C NMR (150 MHz, DMSO-d_6) of **3e**

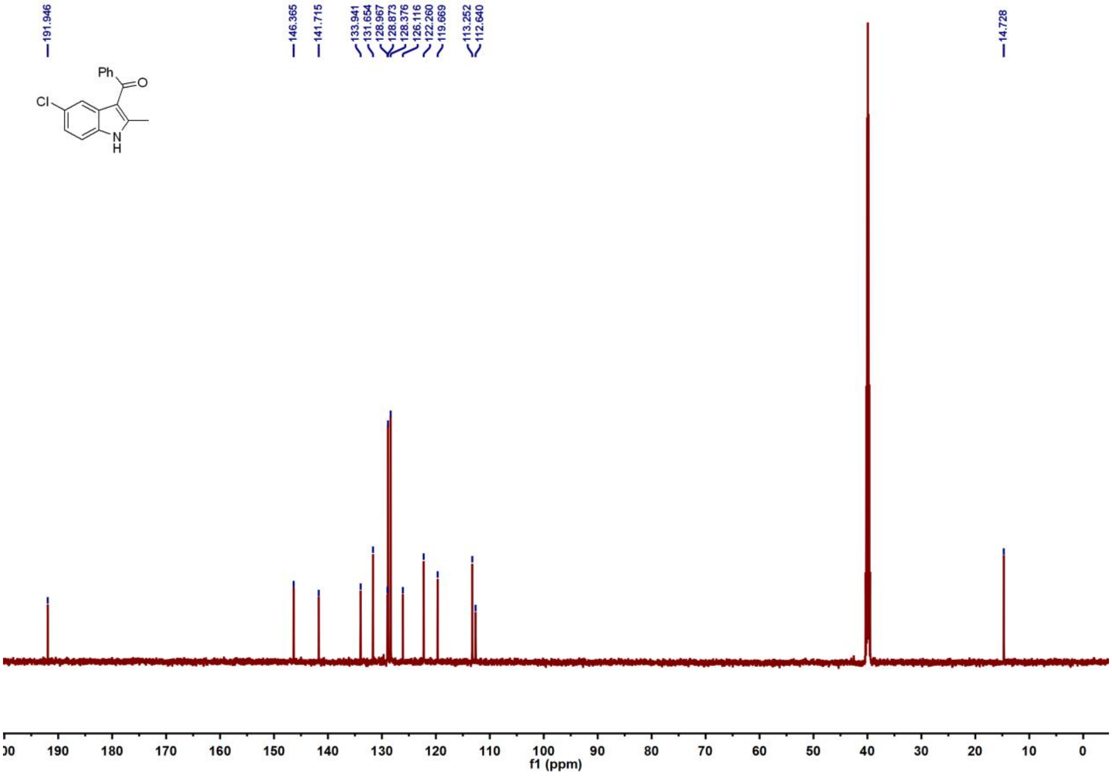


Figure S14. The ^{1}H NMR (400 MHz, DMSO-d_6) of **3f**

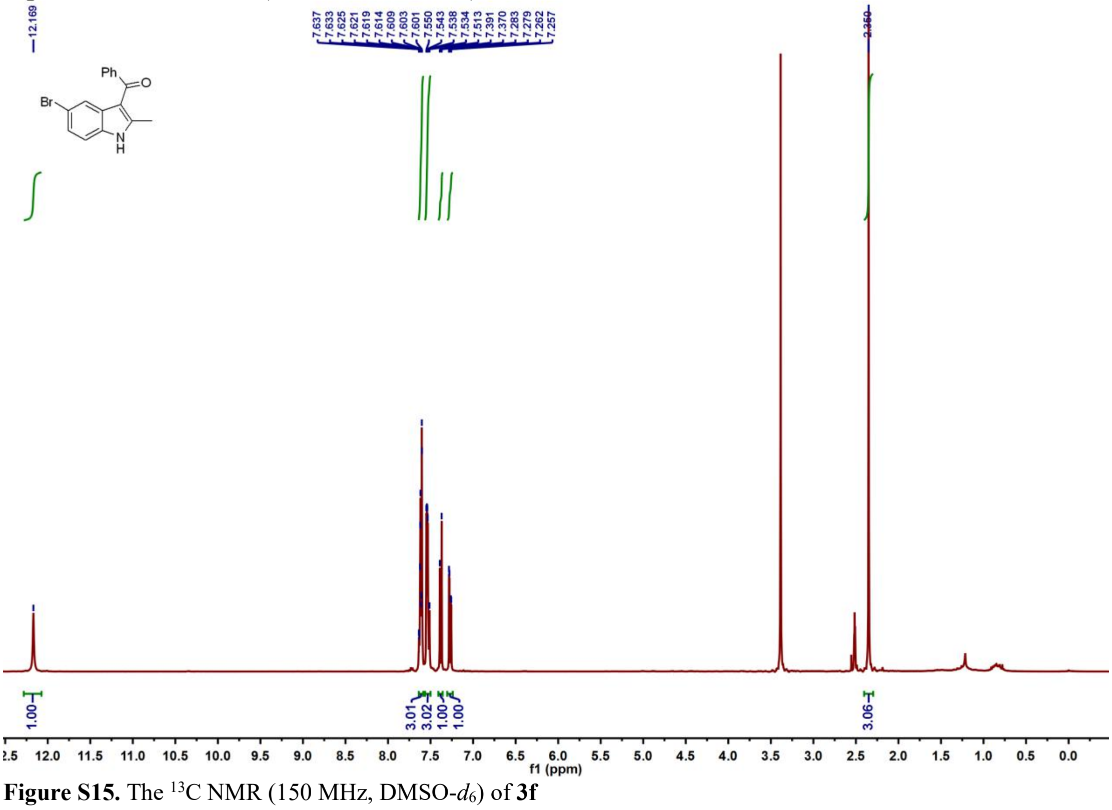


Figure S15. The ^{13}C NMR (150 MHz, DMSO-d_6) of **3f**

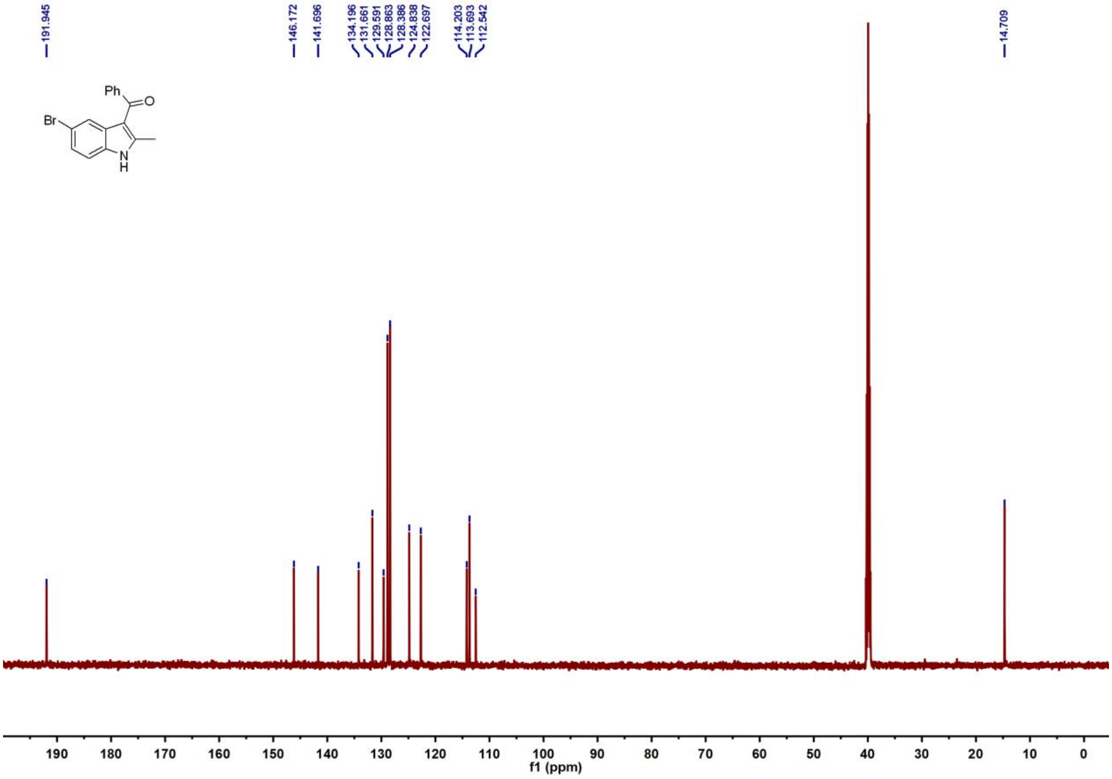


Figure S16. The ^{1}H NMR (400 MHz, DMSO-d_6) of **3g**

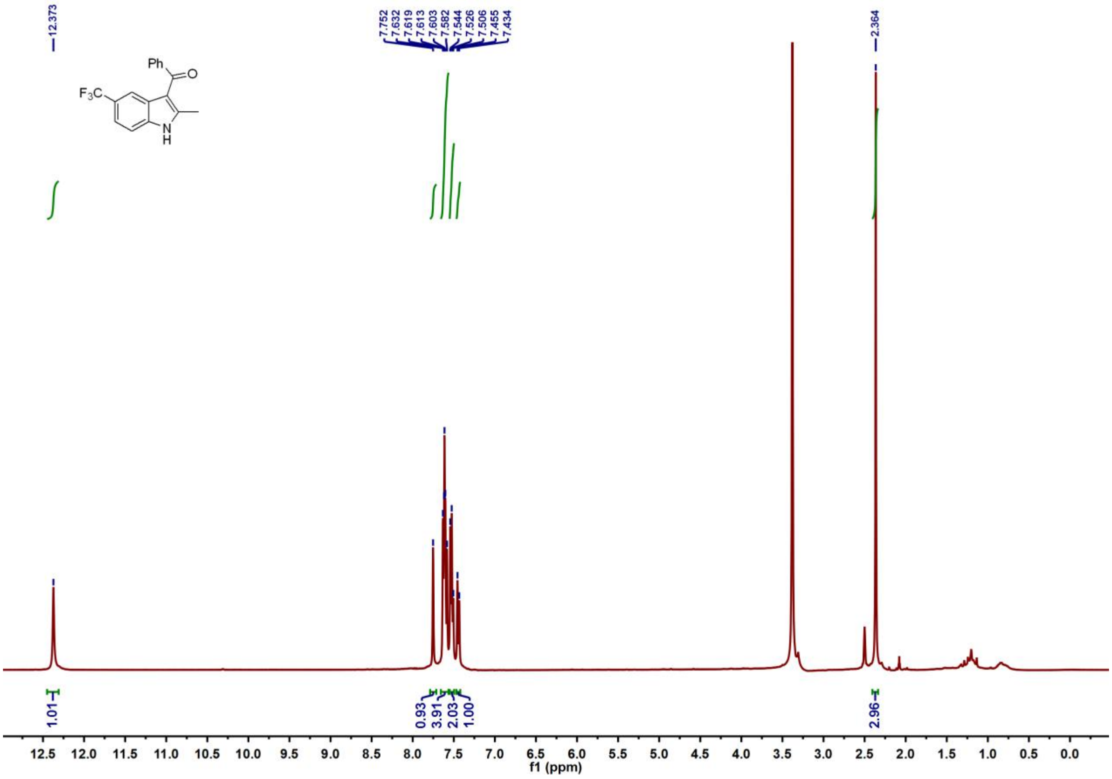


Figure S17. The ^{13}C NMR (100 MHz, DMSO-d_6) of **3g**

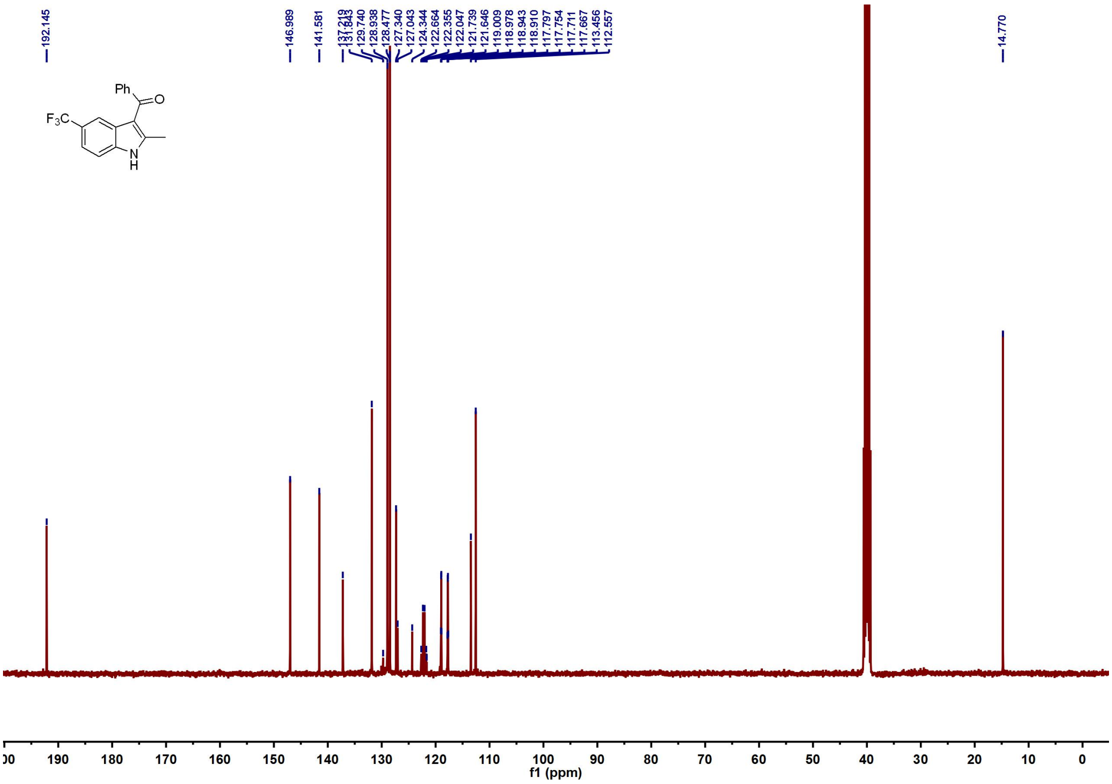


Figure S18. The ^{19}F NMR (376 MHz, DMSO-d_6) of **3g**

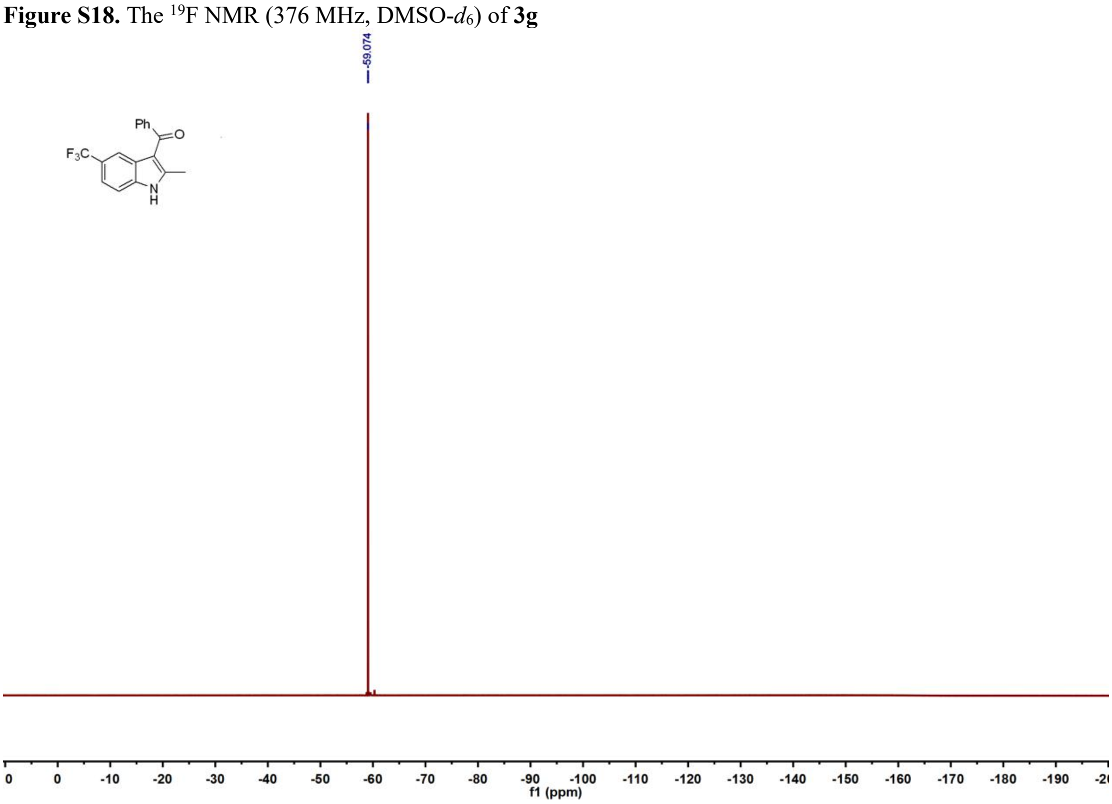


Figure S19. The ^{1}H NMR (400 MHz, DMSO-d_6) of **3h**

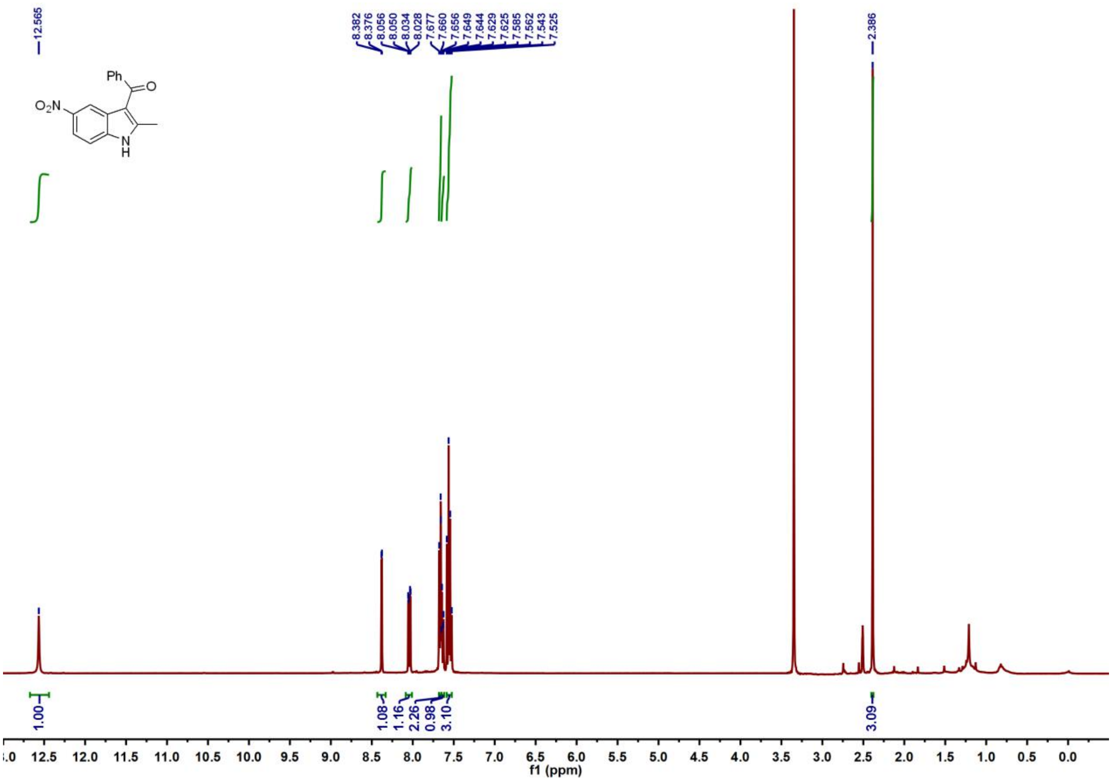


Figure S20. The ^{13}C NMR (100 MHz, DMSO-d_6) of **3h**

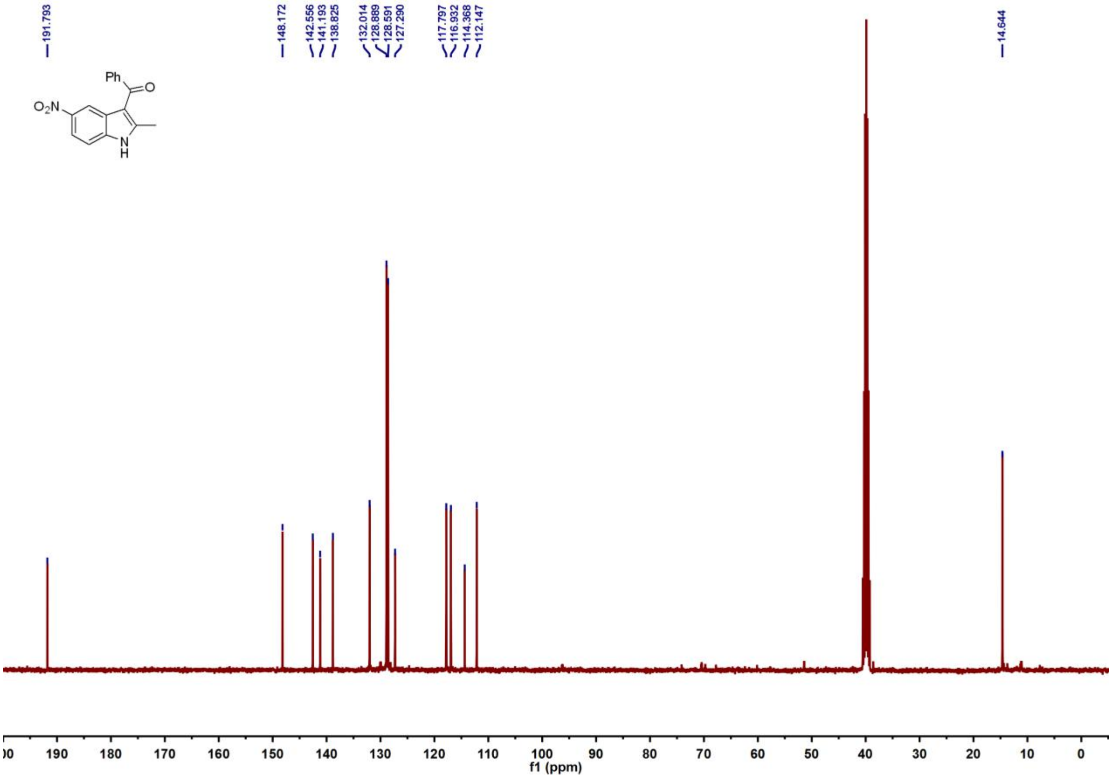


Figure S21. The ^{1}H NMR (400 MHz, DMSO-d_6) of **3i**

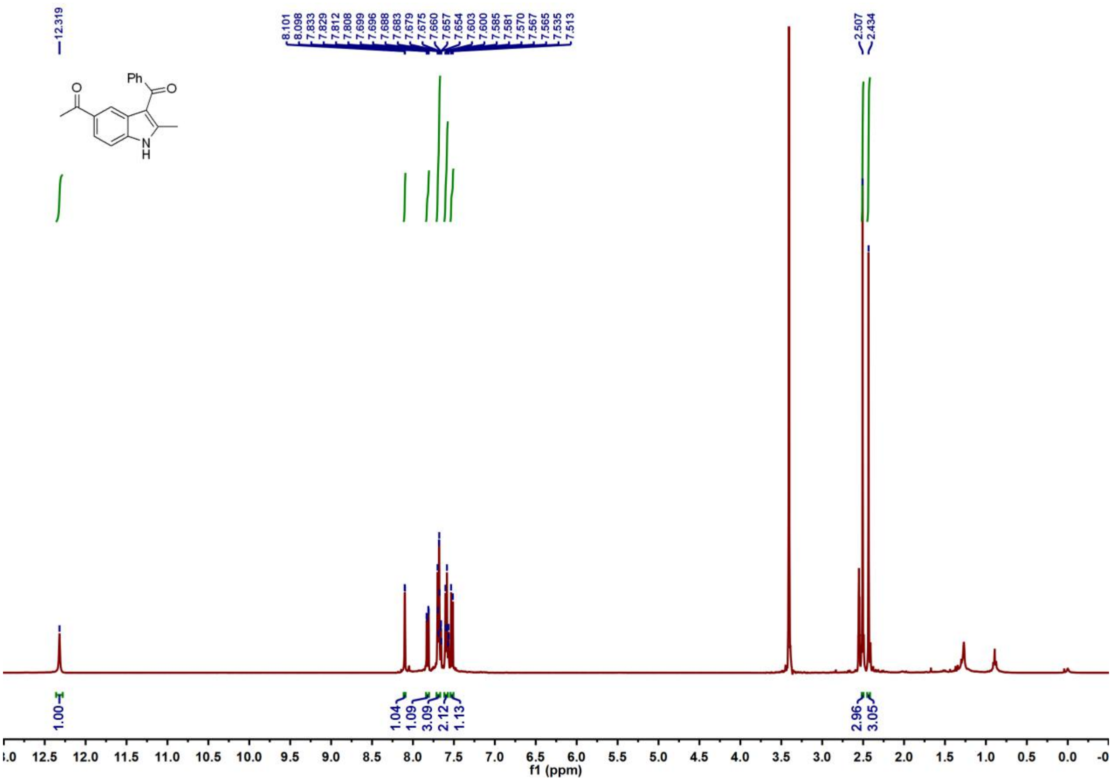


Figure S22. The ^{13}C NMR (150 MHz, DMSO-d_6) of **3i**

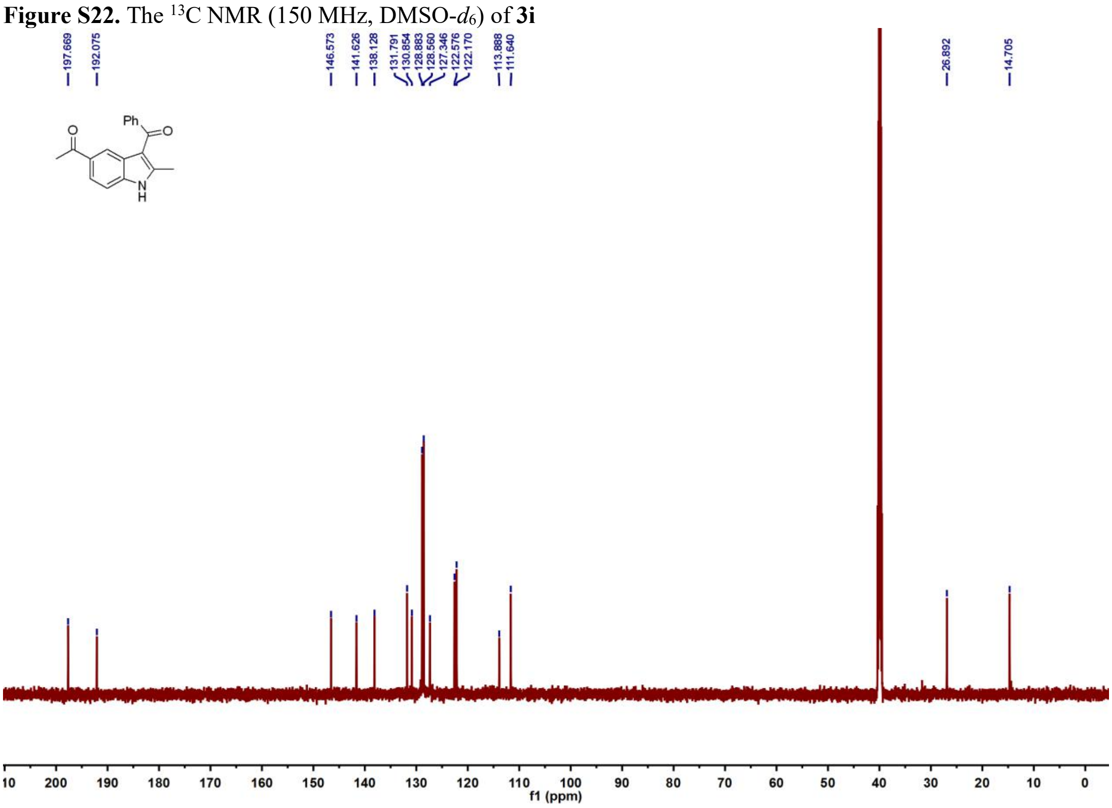


Figure S23. The ^{1}H NMR (400 MHz, DMSO-d_6) of **3j**

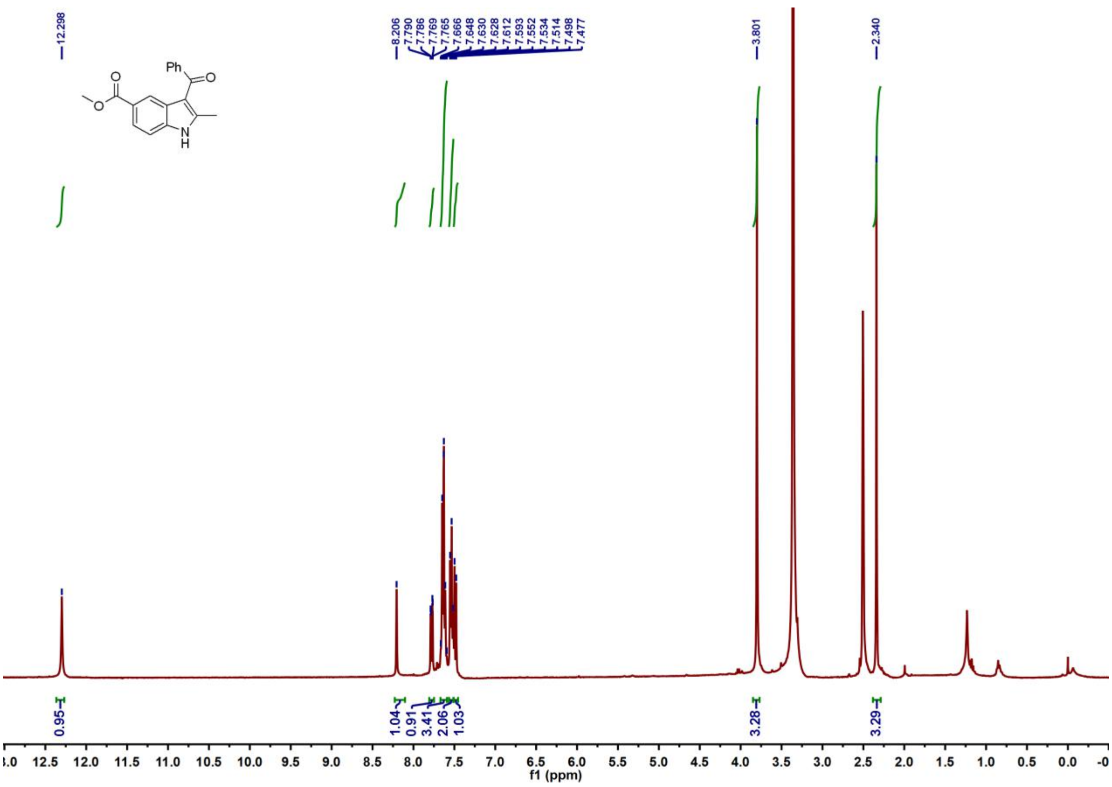


Figure S24. The ^{13}C NMR (100 MHz, DMSO-d_6) of **3j**

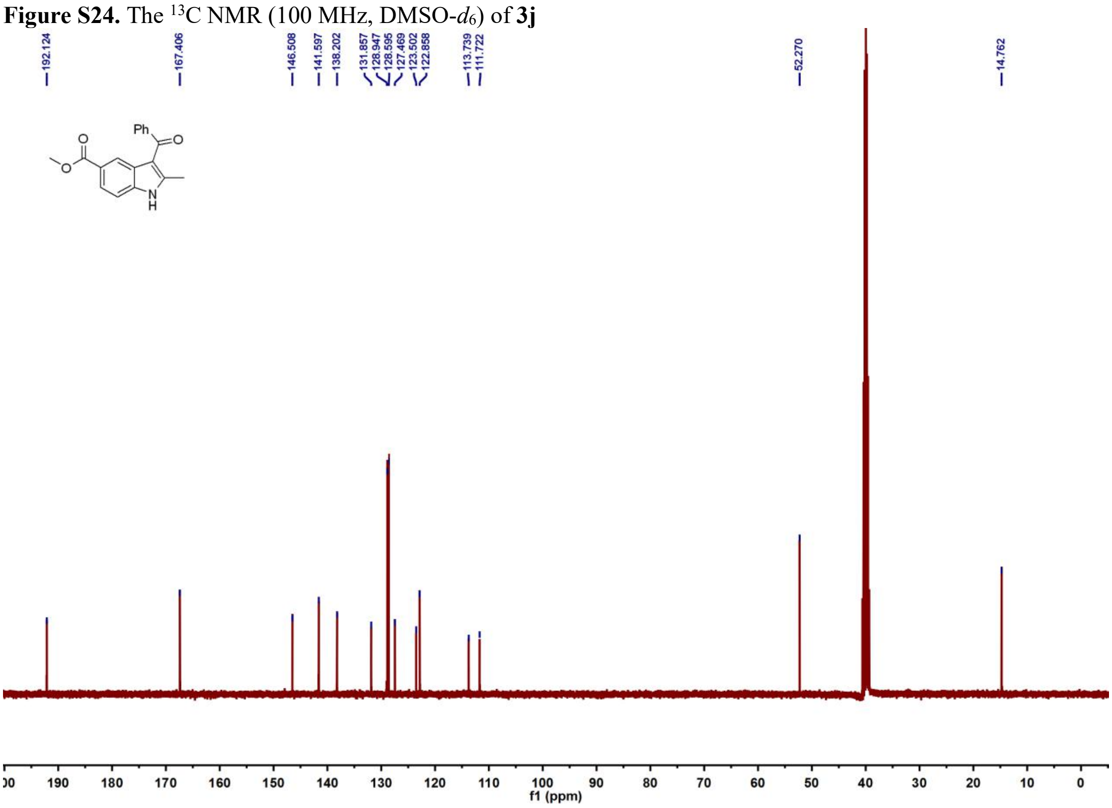


Figure S25. The ^{1}H NMR (400 MHz, DMSO-d_6) of **3k**

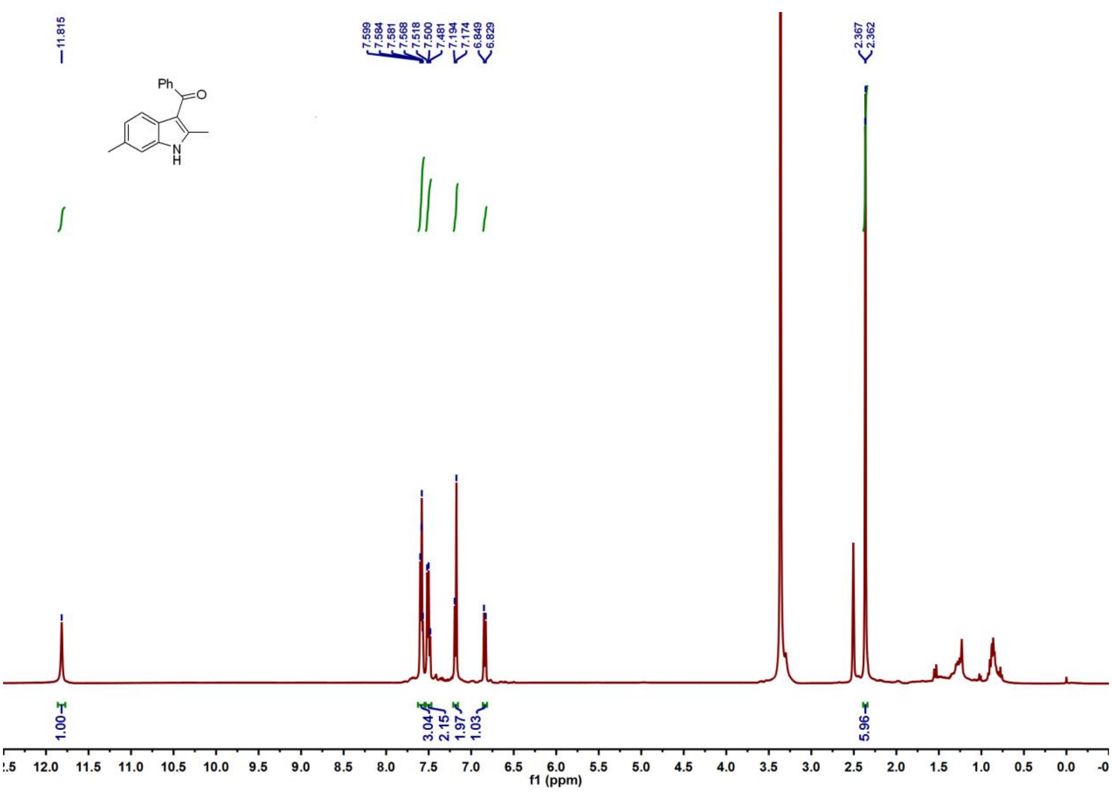


Figure S26. The ^{13}C NMR (150 MHz, DMSO-d_6) of **3k**

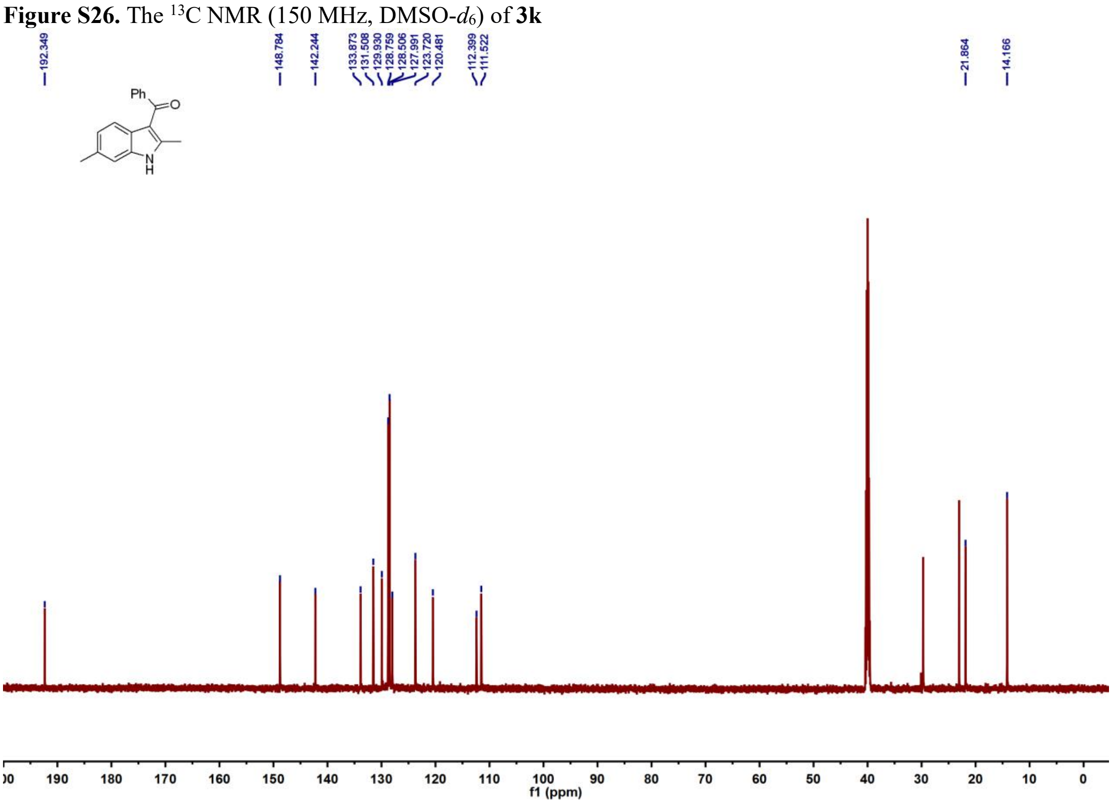


Figure S27. The ^{1}H NMR (400 MHz, DMSO-d_6) of **3k'**

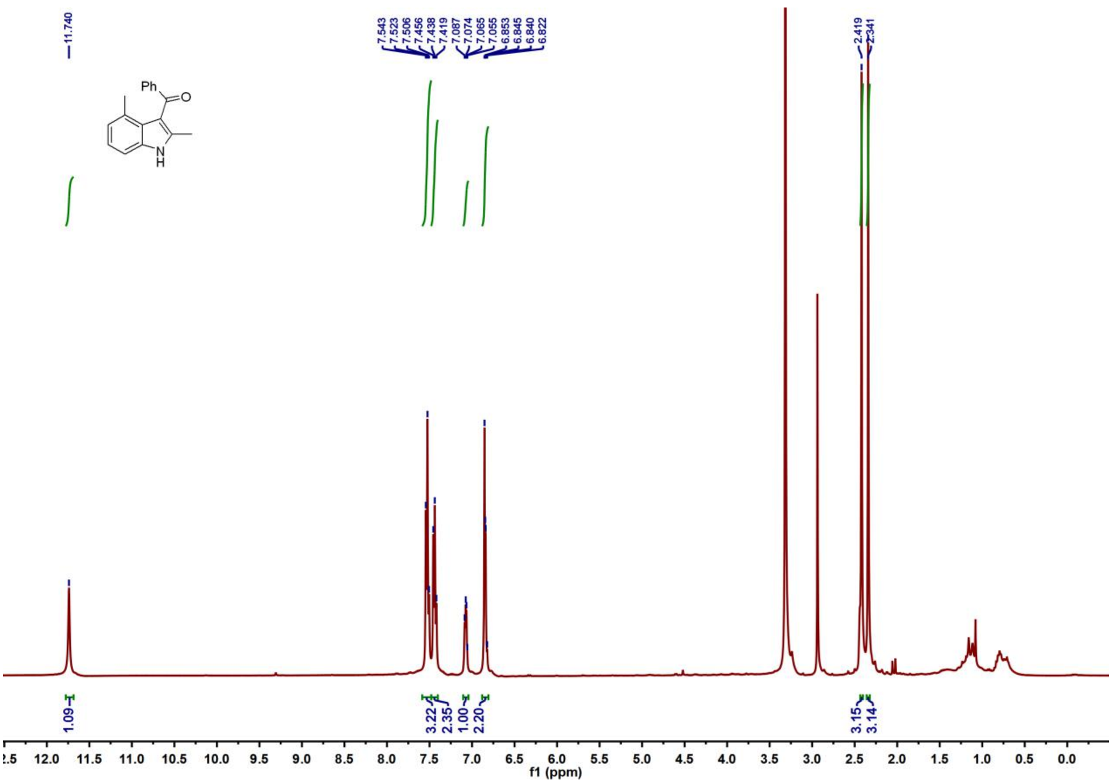


Figure S28. The [13]C NMR (150 MHz, DMSO-d_6) of **3k'**

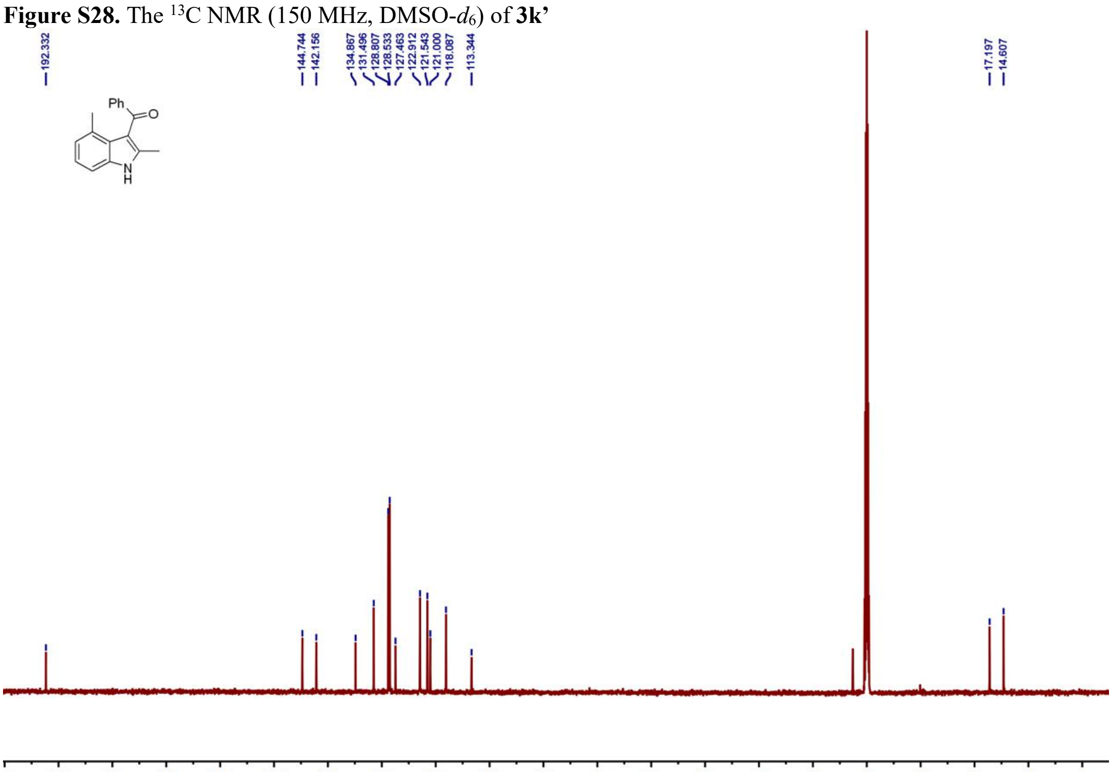


Figure S29. The [1]H NMR (400 MHz, DMSO-d_6) of **3l**

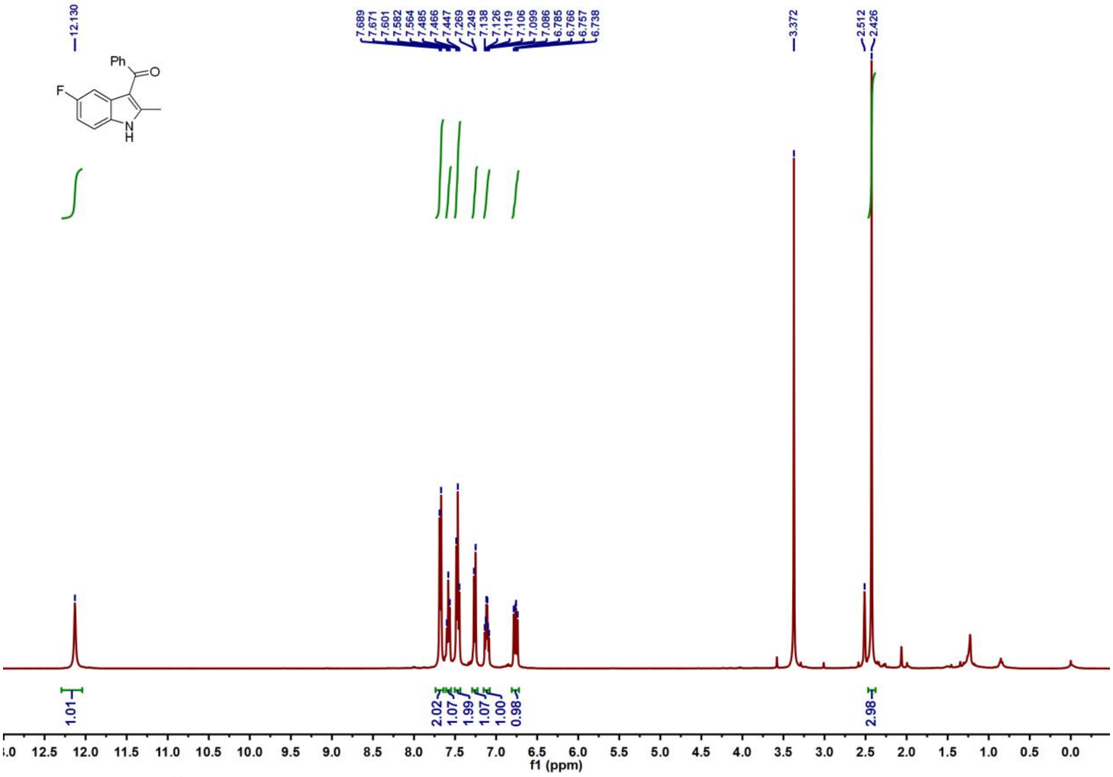


Figure S30. The [13]C NMR (100 MHz, DMSO-d_6) of **3l**

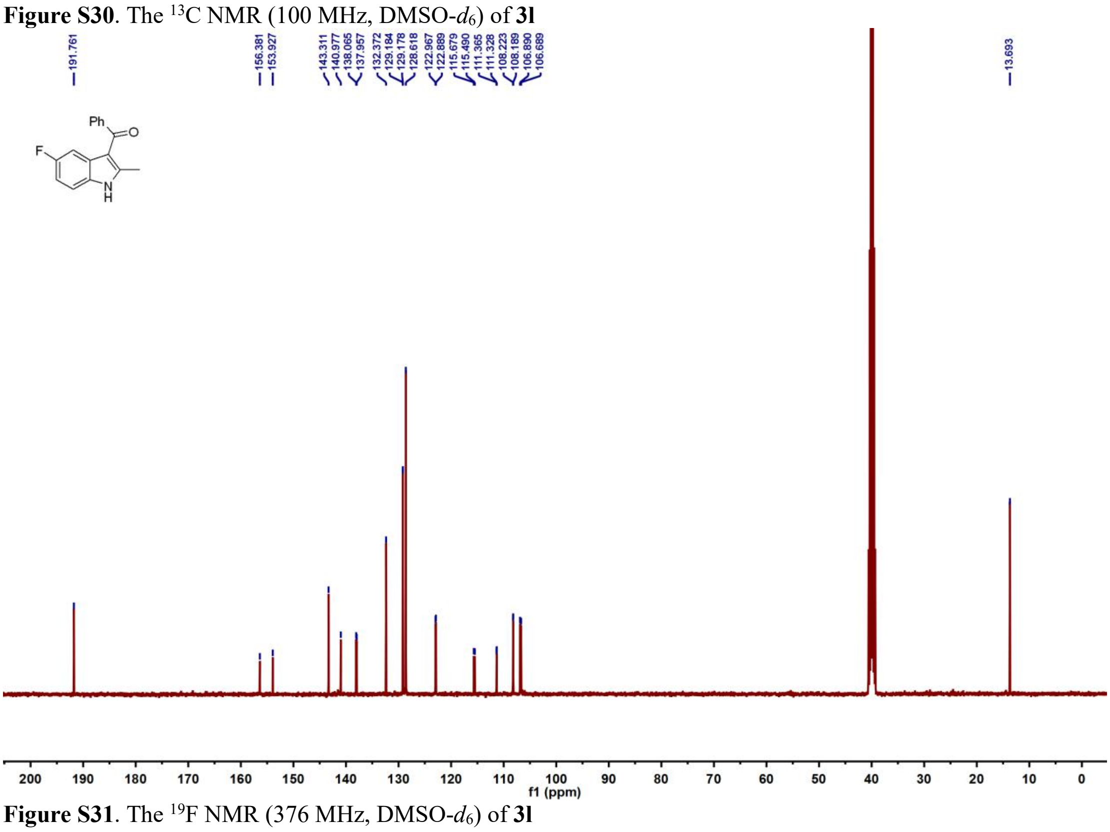


Figure S31. The [19]F NMR (376 MHz, DMSO-d_6) of **3l**

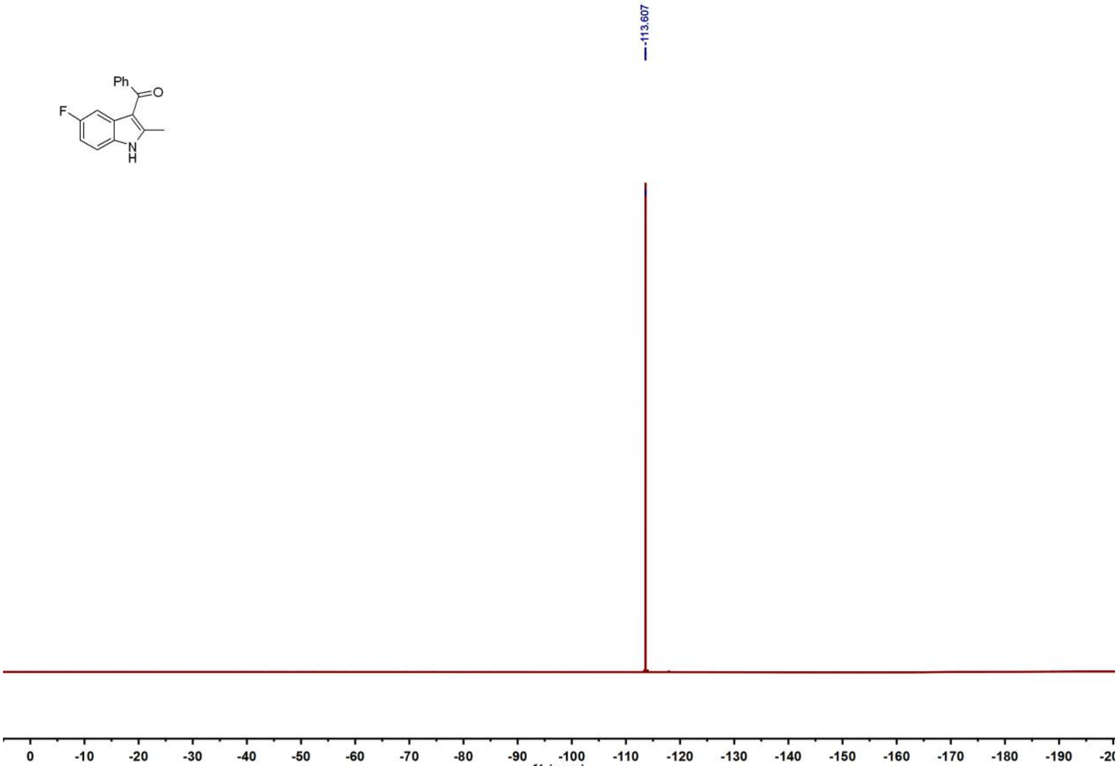


Figure S32. The [1]H NMR (400 MHz, DMSO-d_6) of **3m**

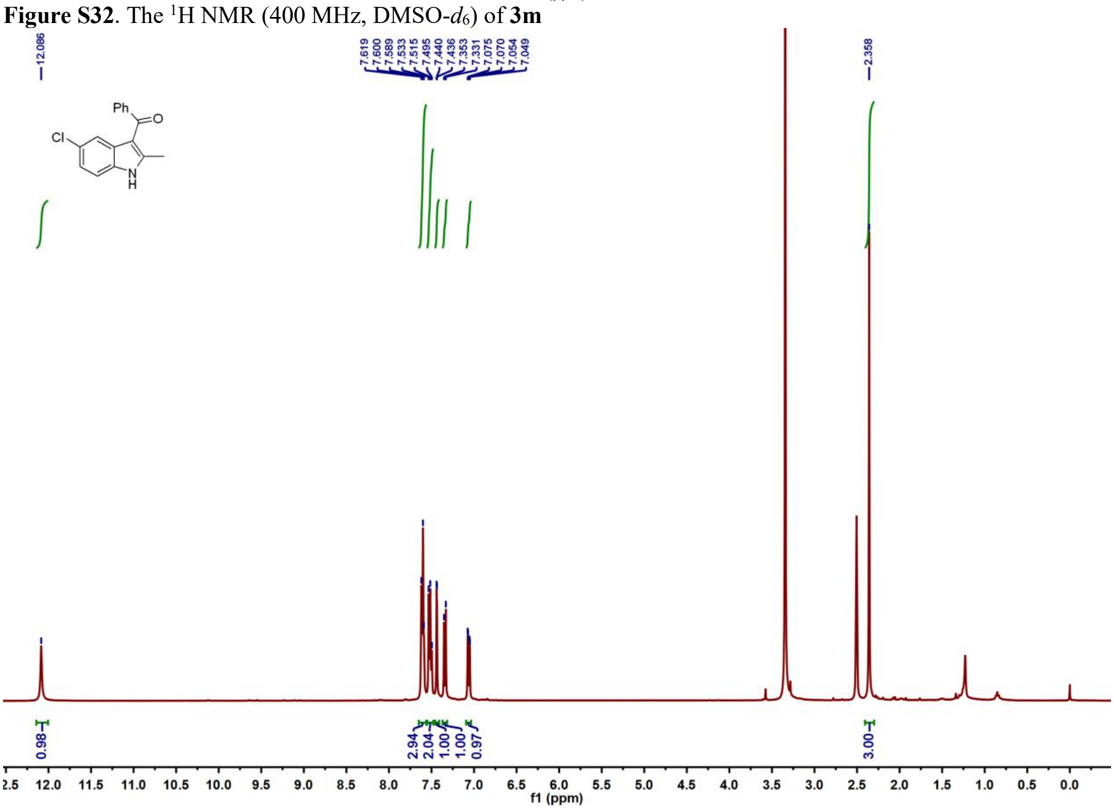


Figure S33. The [13]C NMR (100 MHz, DMSO-d_6) of **3m**

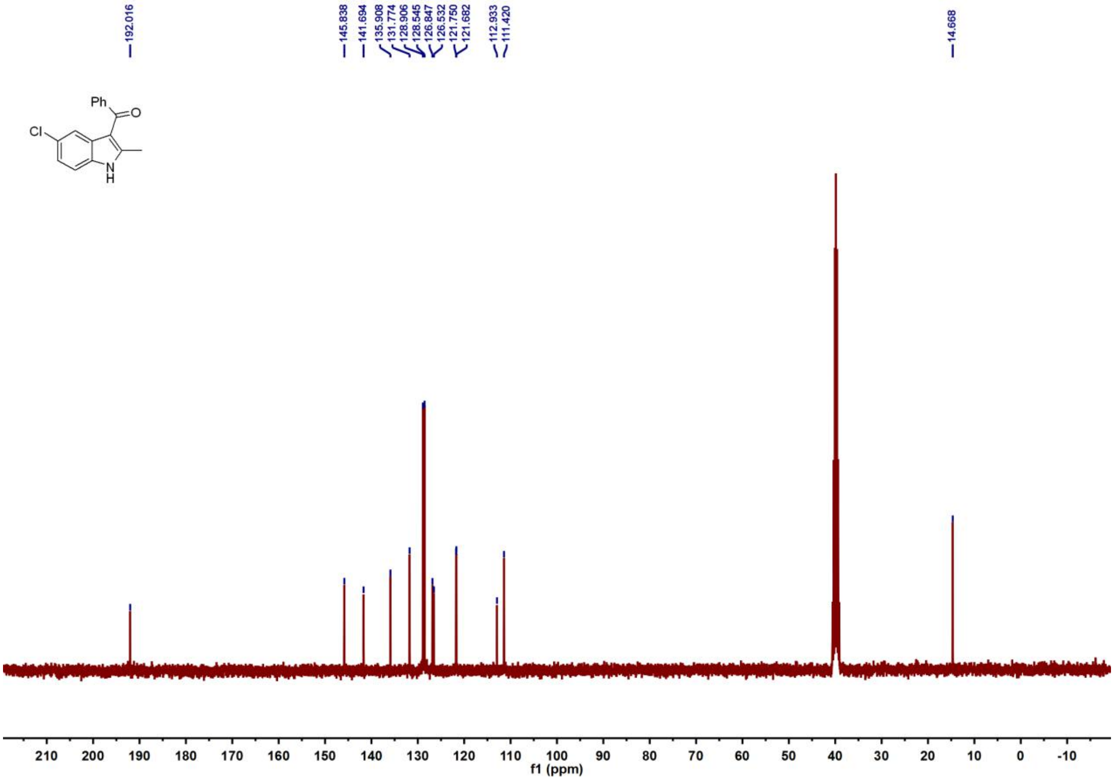


Figure S34. The ^{1}H NMR (400 MHz, DMSO-d_6) of **3n**

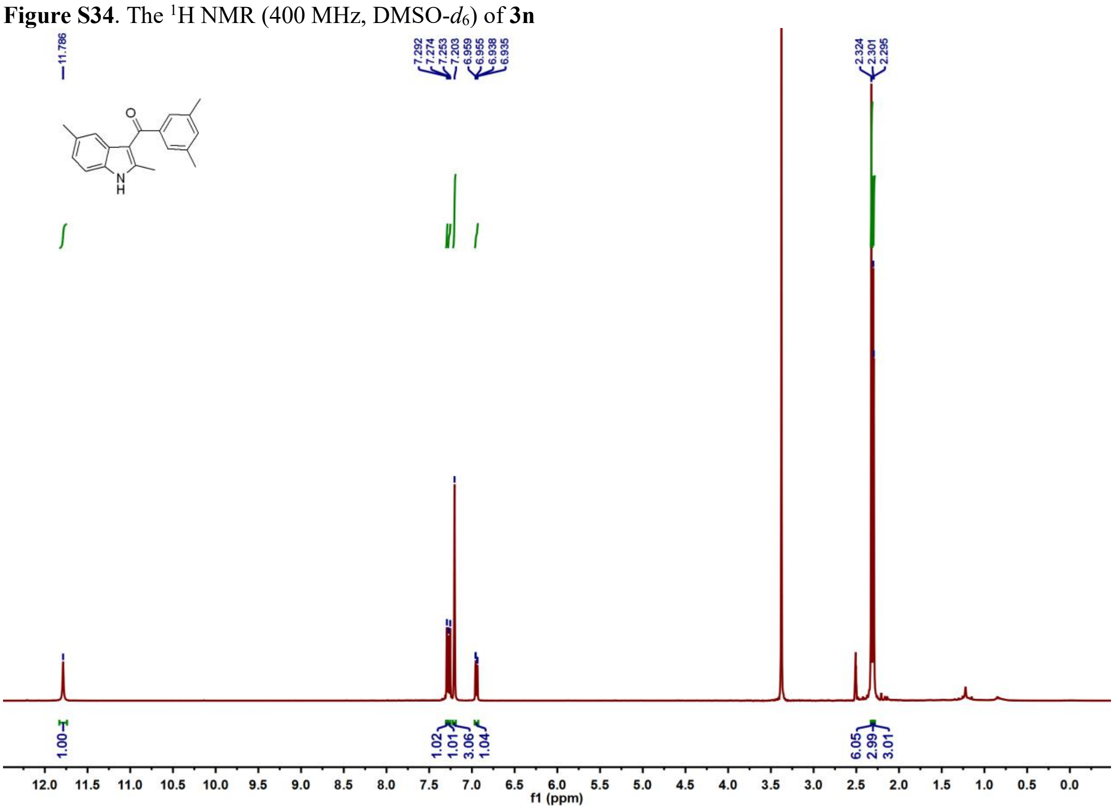


Figure S35. The ^{13}C NMR (150 MHz, DMSO-d_6) of **3n**

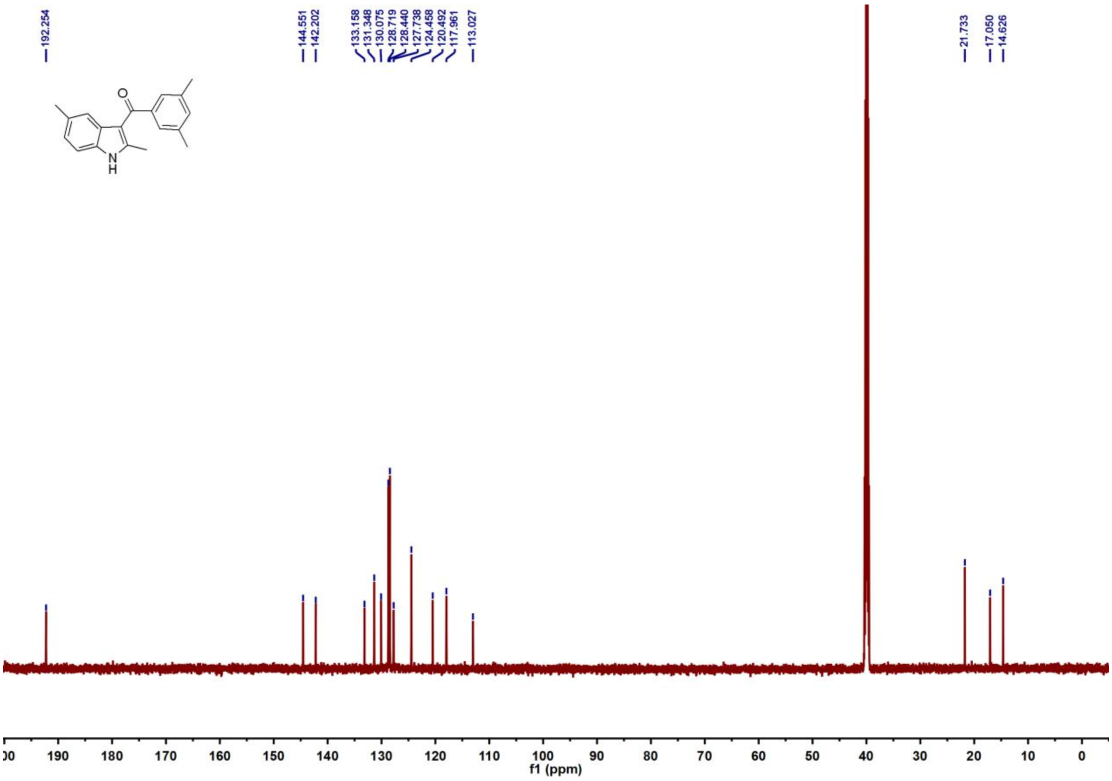


Figure S36. The ^{1}H NMR (400 MHz, DMSO-d_6) of **3o**

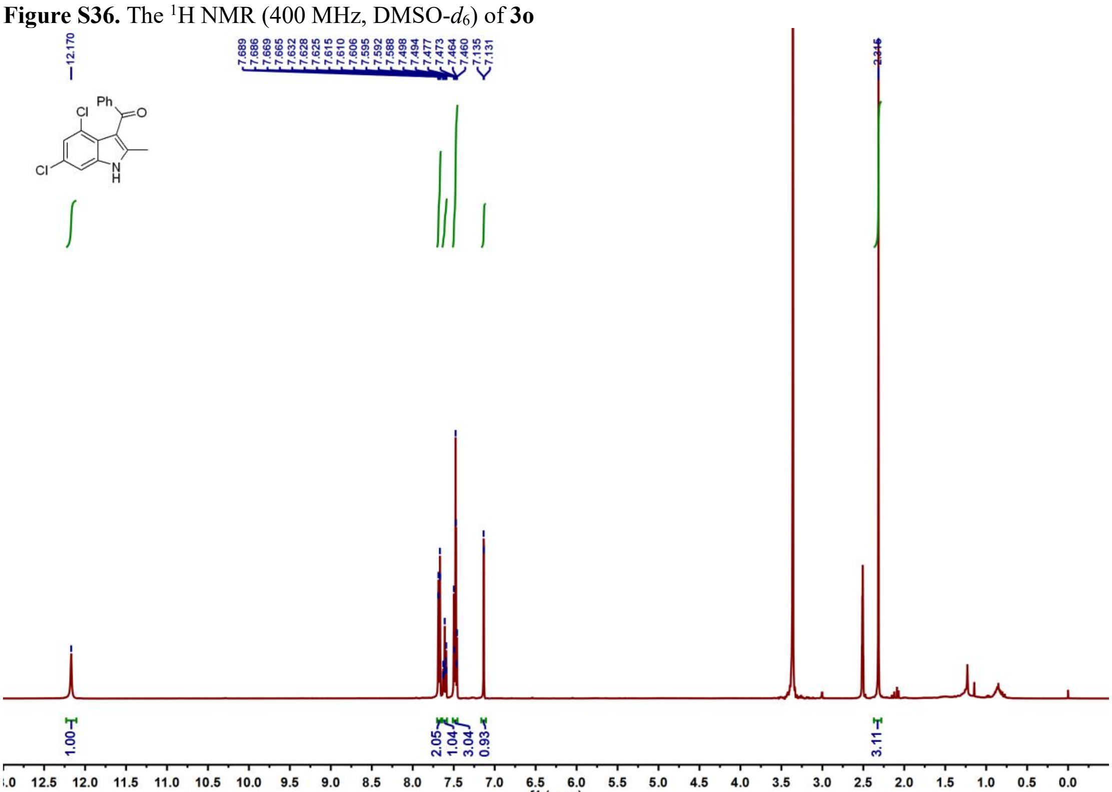


Figure S37. The ^{13}C NMR (150 MHz, DMSO-d_6) of **3o**

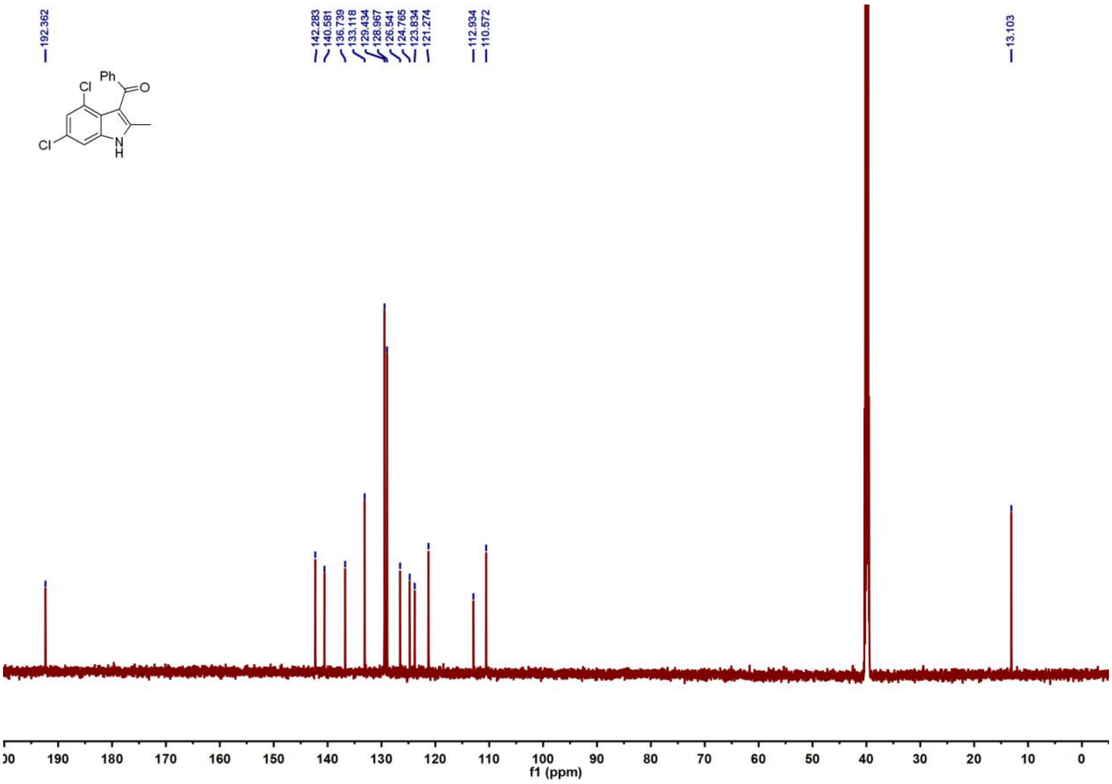


Figure S38. The ^{1}H NMR (400 MHz, DMSO-d_6) of **3p**

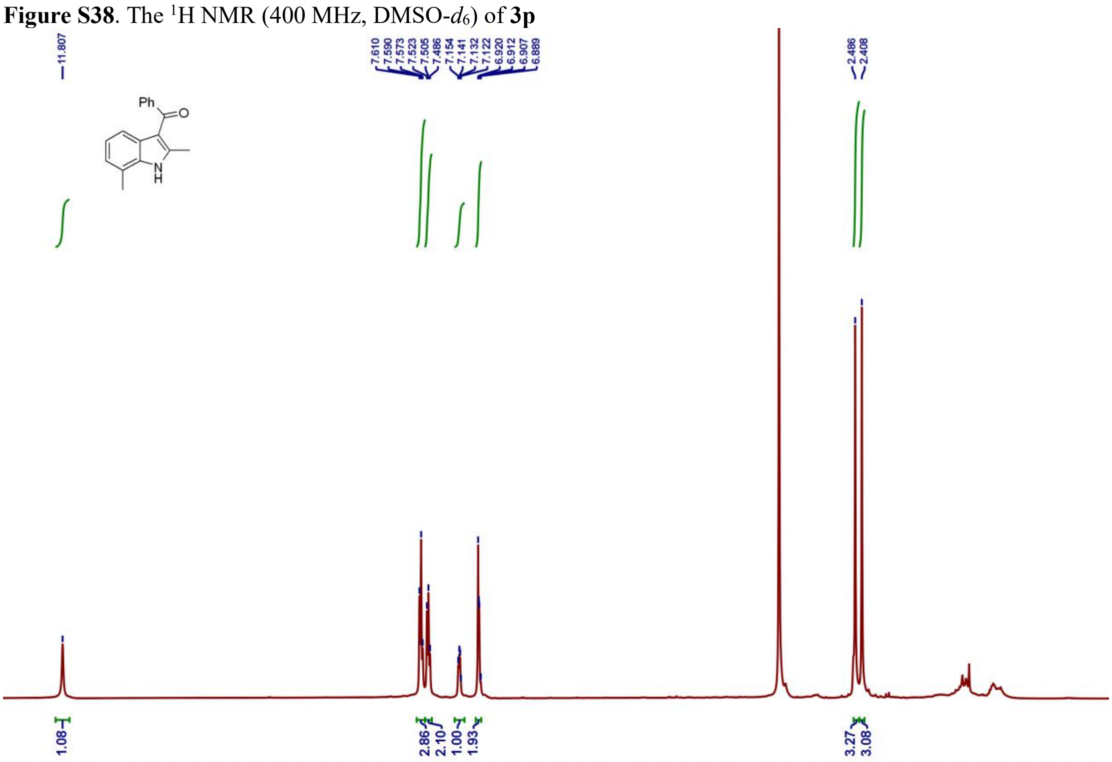


Figure S39. The ^{13}C NMR (150 MHz, DMSO-d_6) of **3p**

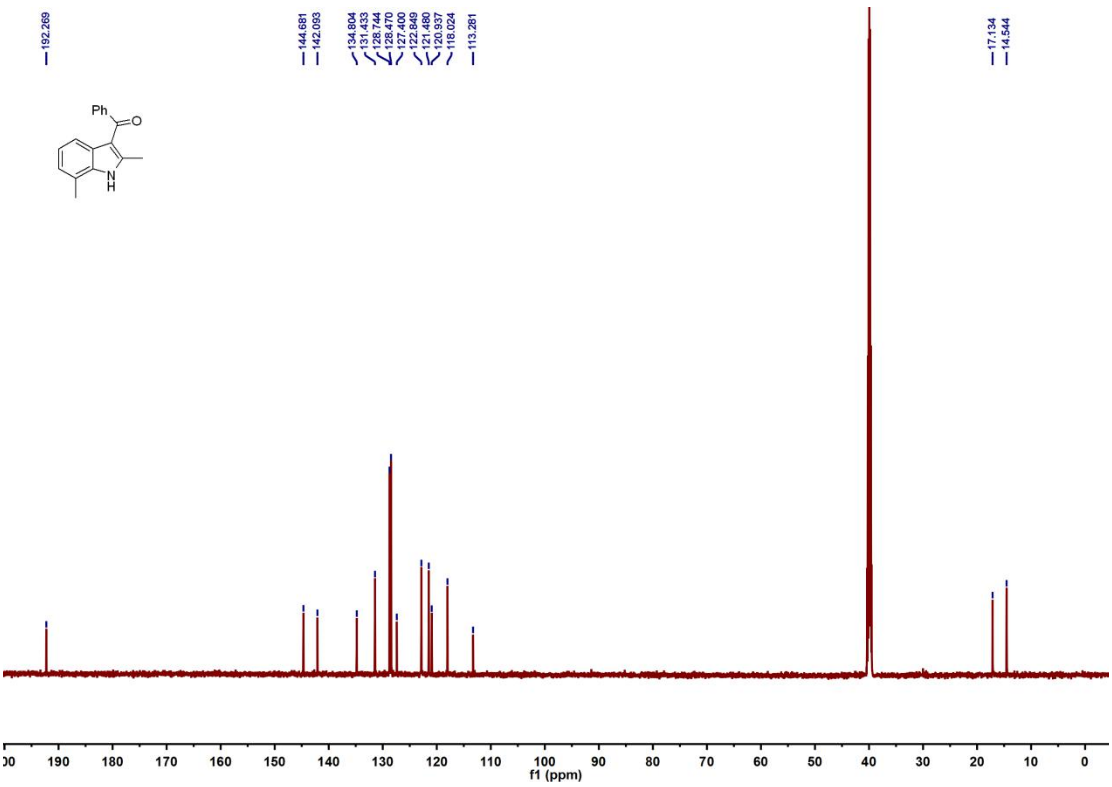


Figure S40. The [1]H NMR (400 MHz, DMSO-d_6) of **3q**

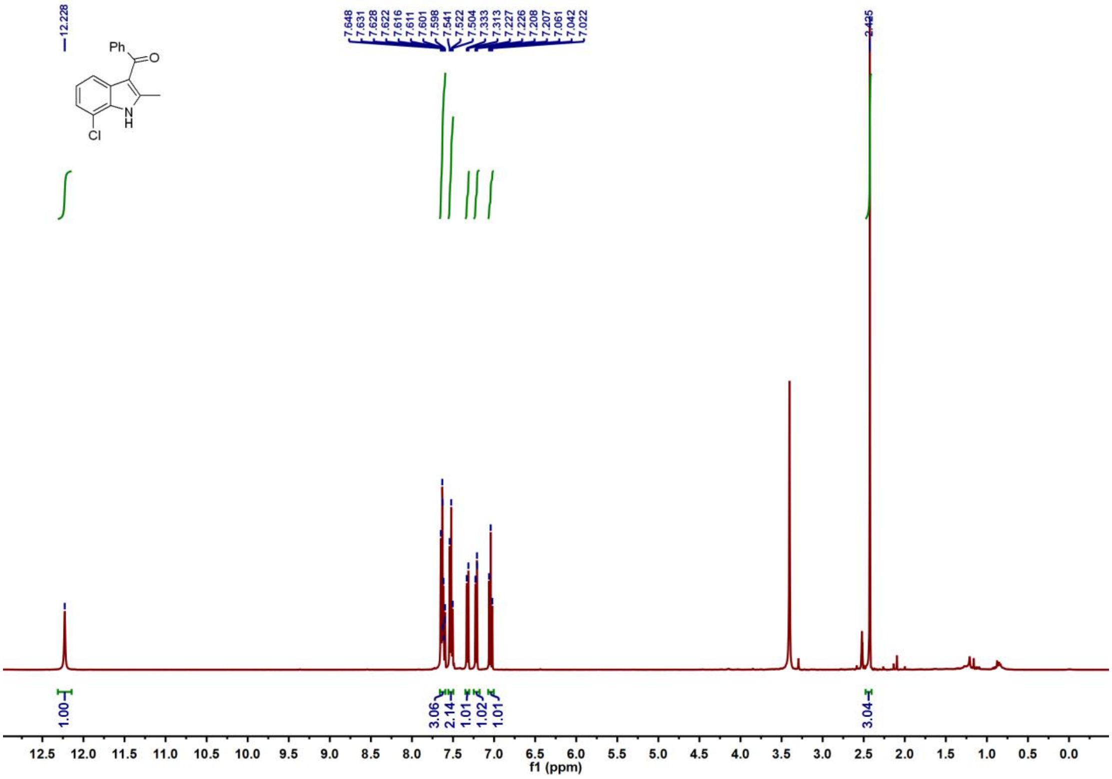


Figure S41. The [13]C NMR (150 MHz, DMSO-d_6) of **3q**

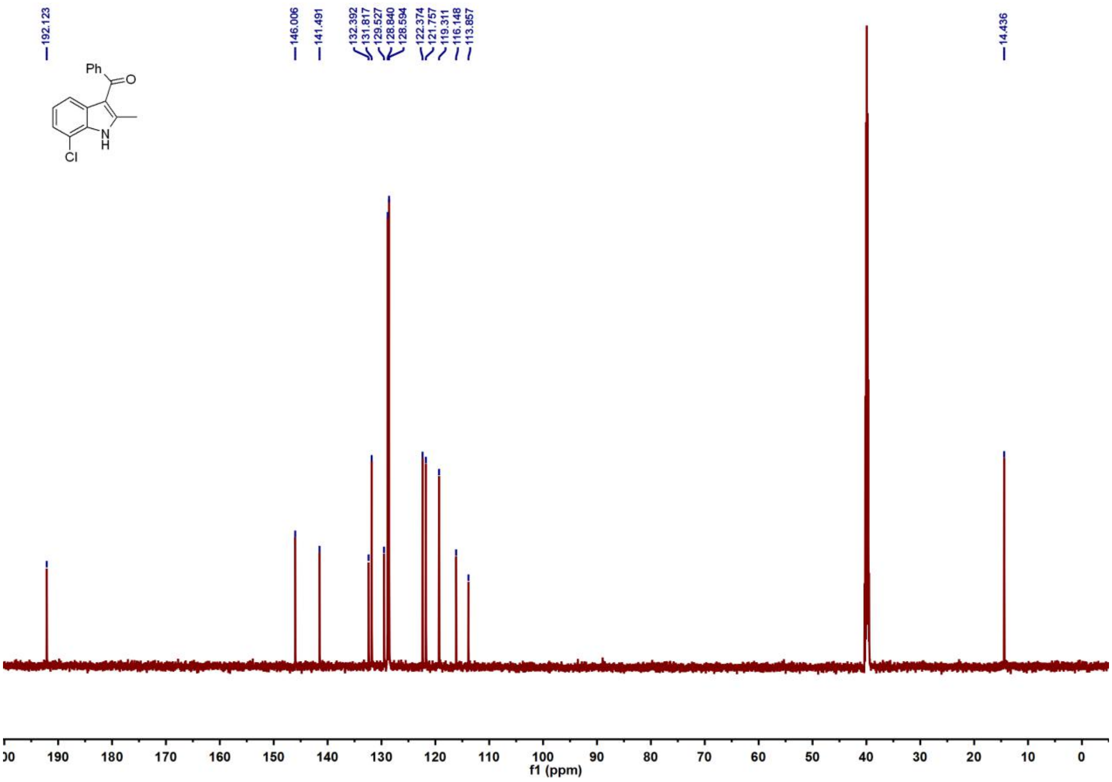


Figure S42. The ^{1}H NMR (400 MHz, DMSO-d_6) of **3r**

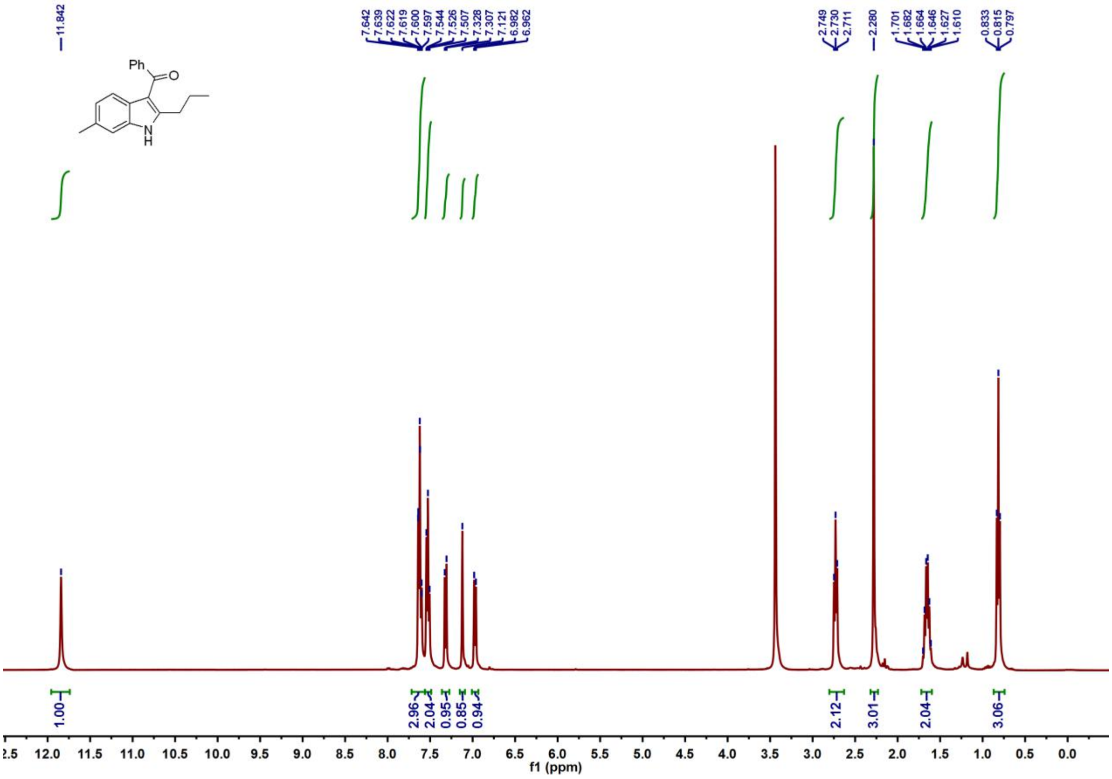


Figure S43. The ^{13}C NMR (150 MHz, DMSO-d_6) of **3r**

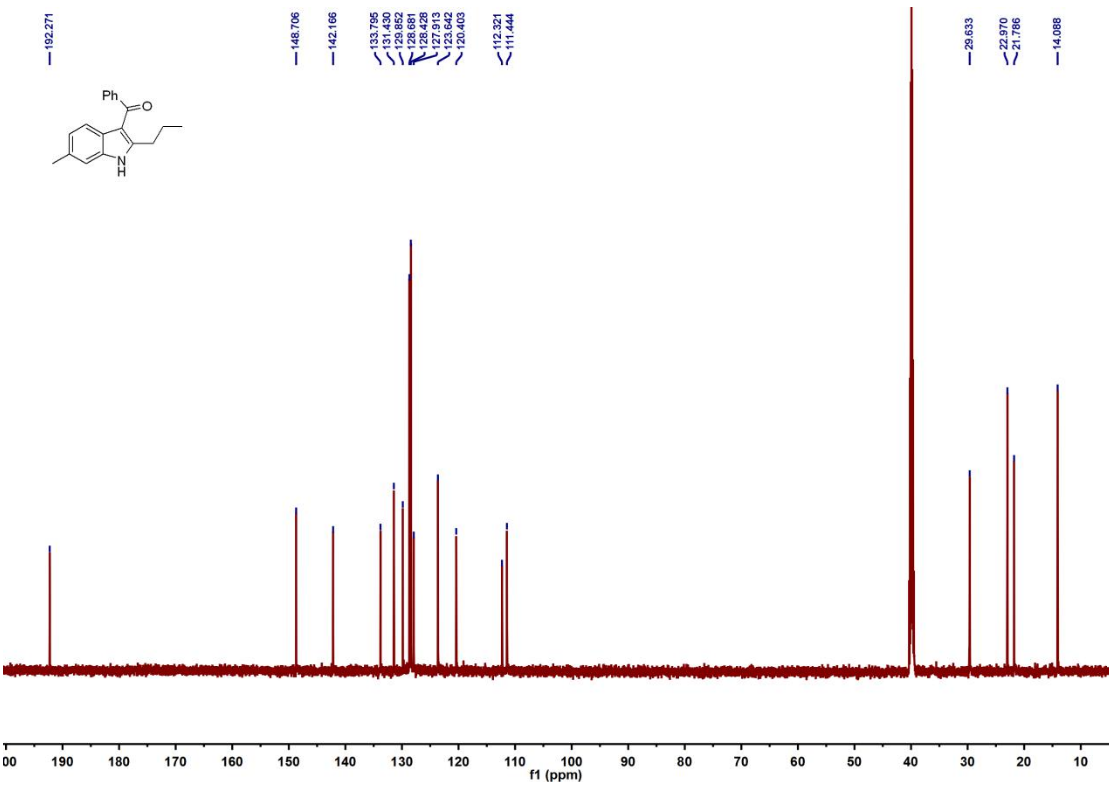


Figure S44. The ^{1}H NMR (400 MHz, DMSO-d_6) of **3s**

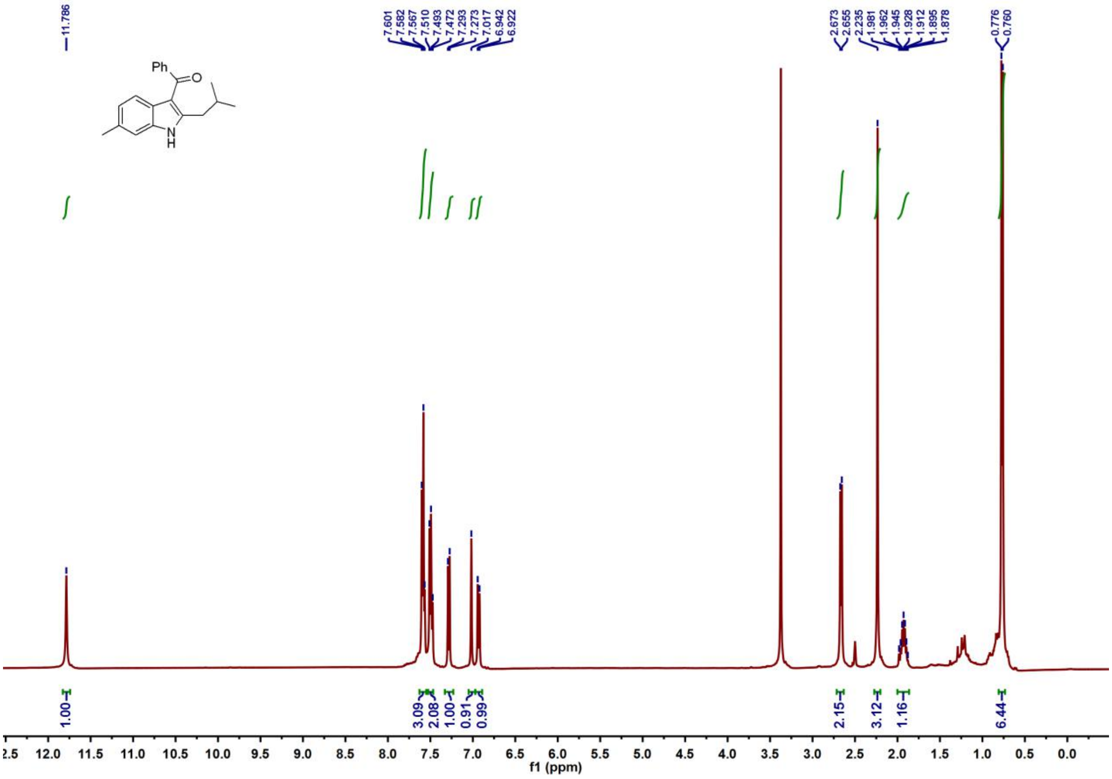


Figure S45. The ^{13}C NMR (150 MHz, DMSO-d_6) of **3s**

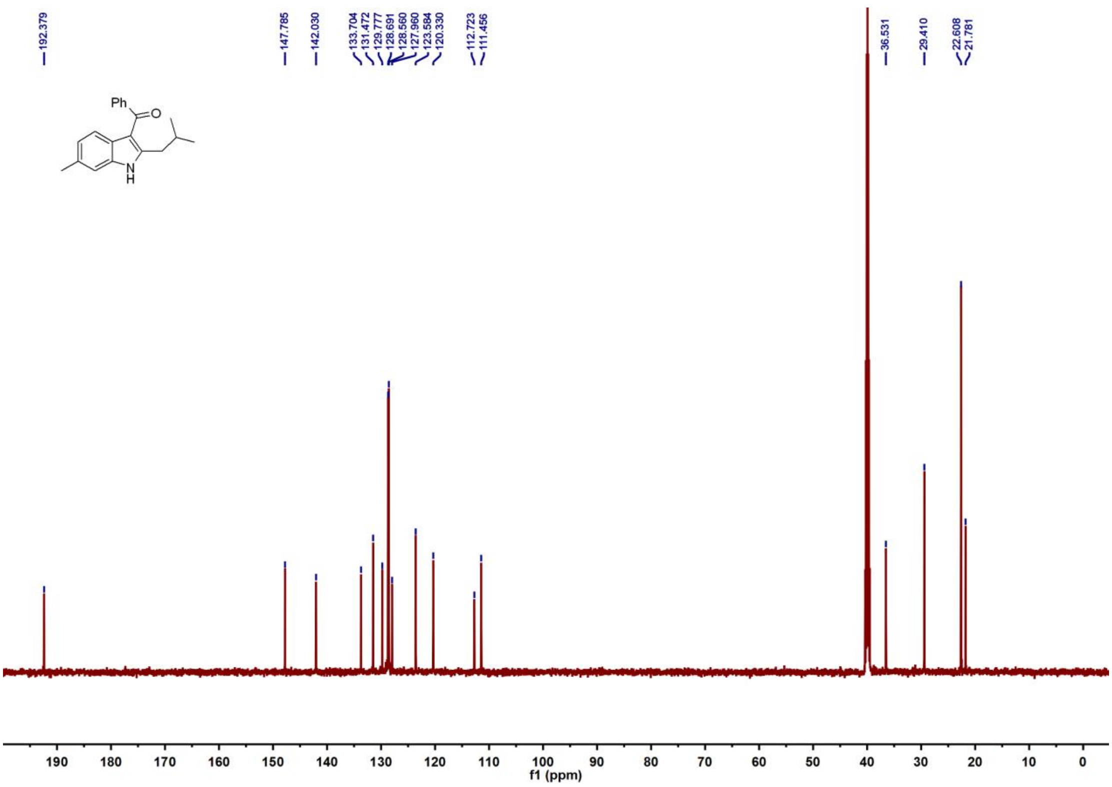


Figure S46. The ^{1}H NMR (400 MHz, DMSO-d_6) of **3t**

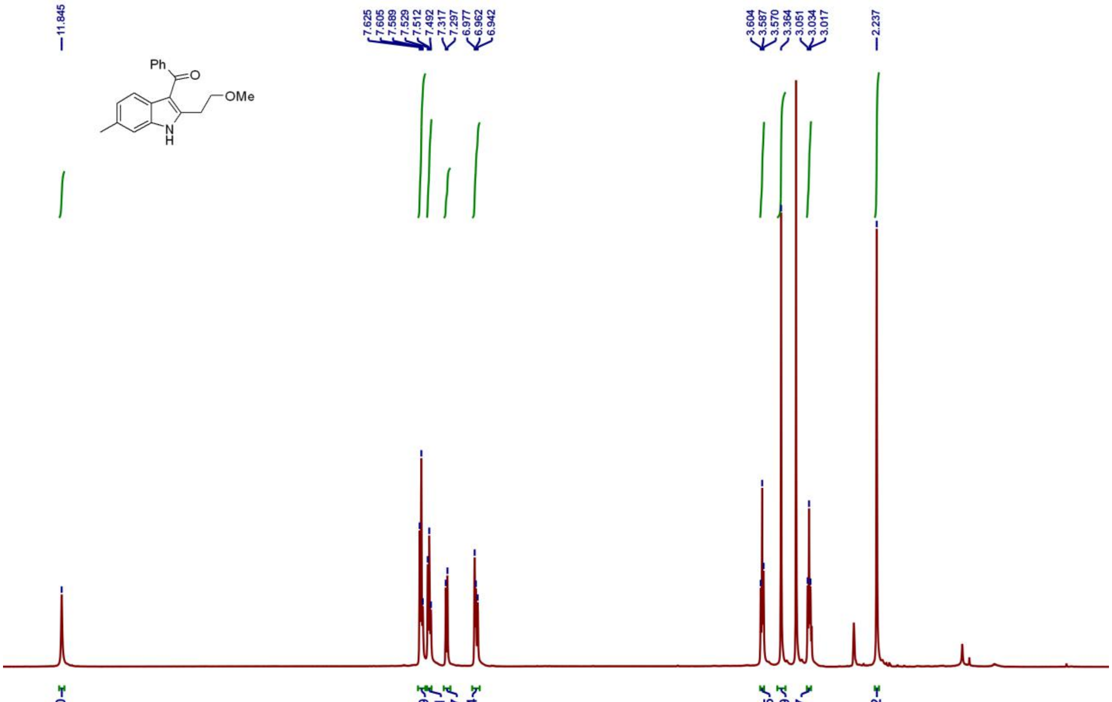


Figure S47. The ^{13}C NMR (100 MHz, DMSO-d_6) of **3t**

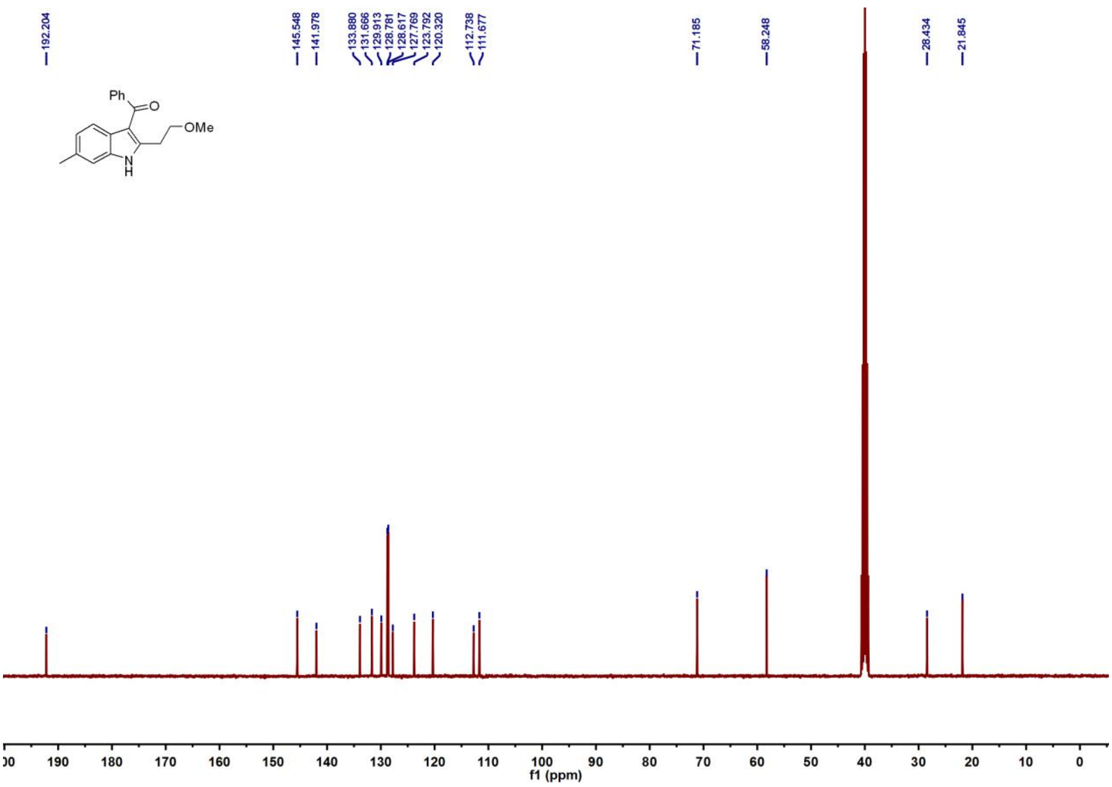


Figure S48. The ^{1}H NMR (400 MHz, DMSO-d_6) of **3u**

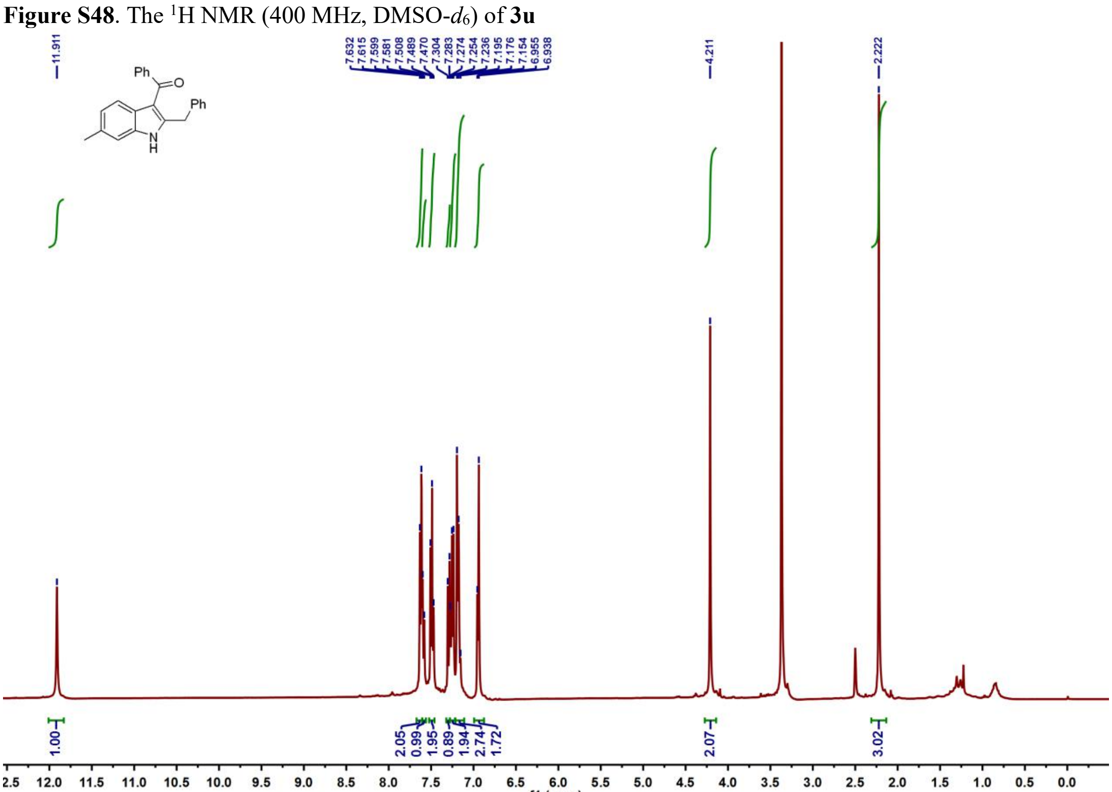


Figure S49. The ^{13}C NMR (150 MHz, DMSO-d_6) of **3u**

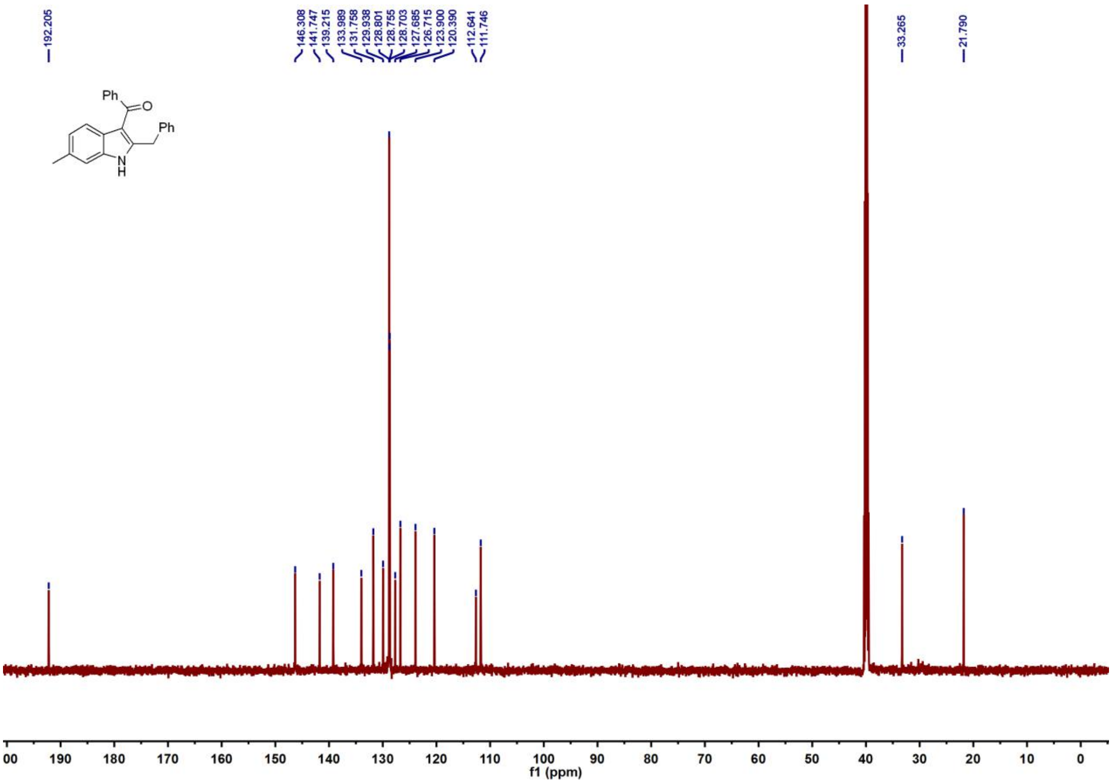


Figure S50. The ^{1}H NMR (400 MHz, DMSO-d_6) of **4a**

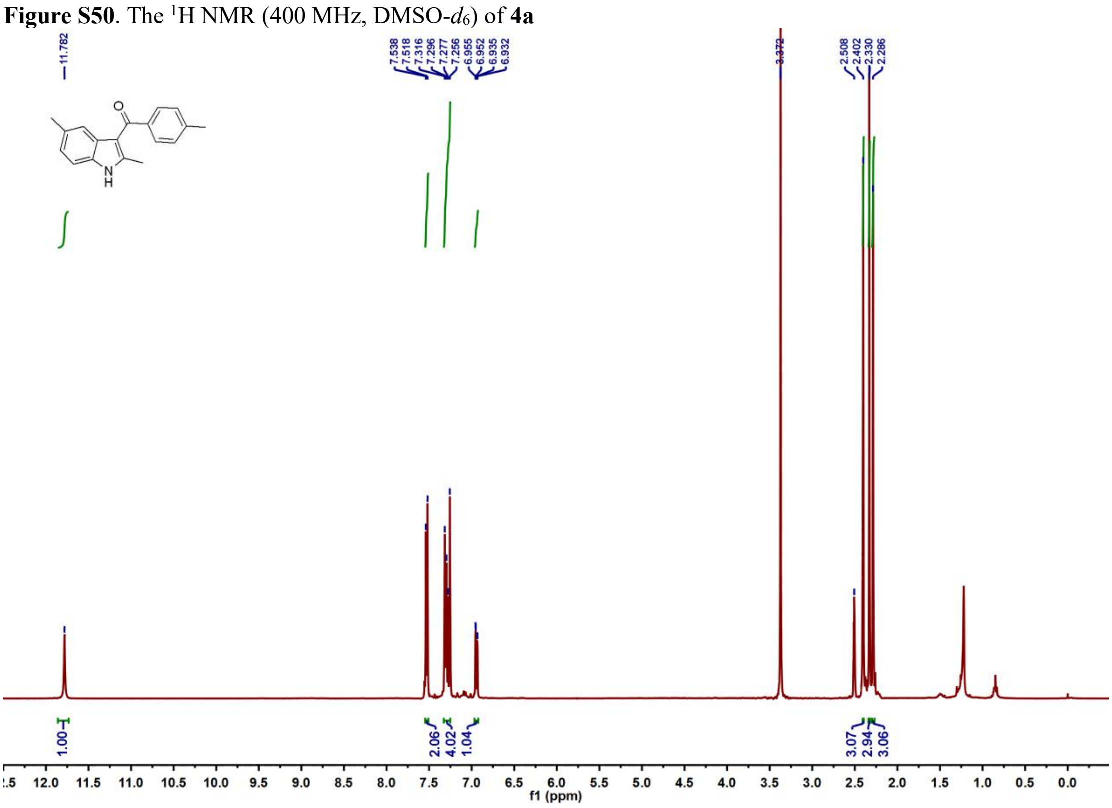


Figure S51. The ^{13}C NMR (100 MHz, DMSO-d_6) of **4a**

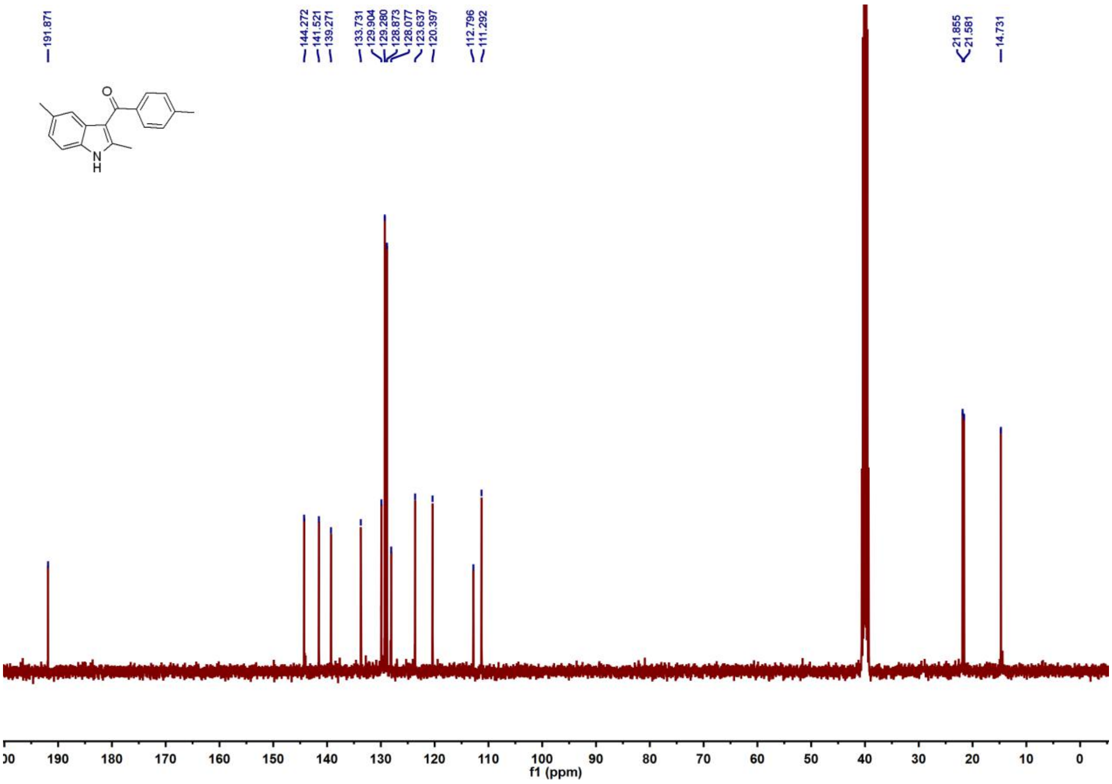


Figure S52. The ^{1}H NMR (400 MHz, DMSO-d_6) of **4b**

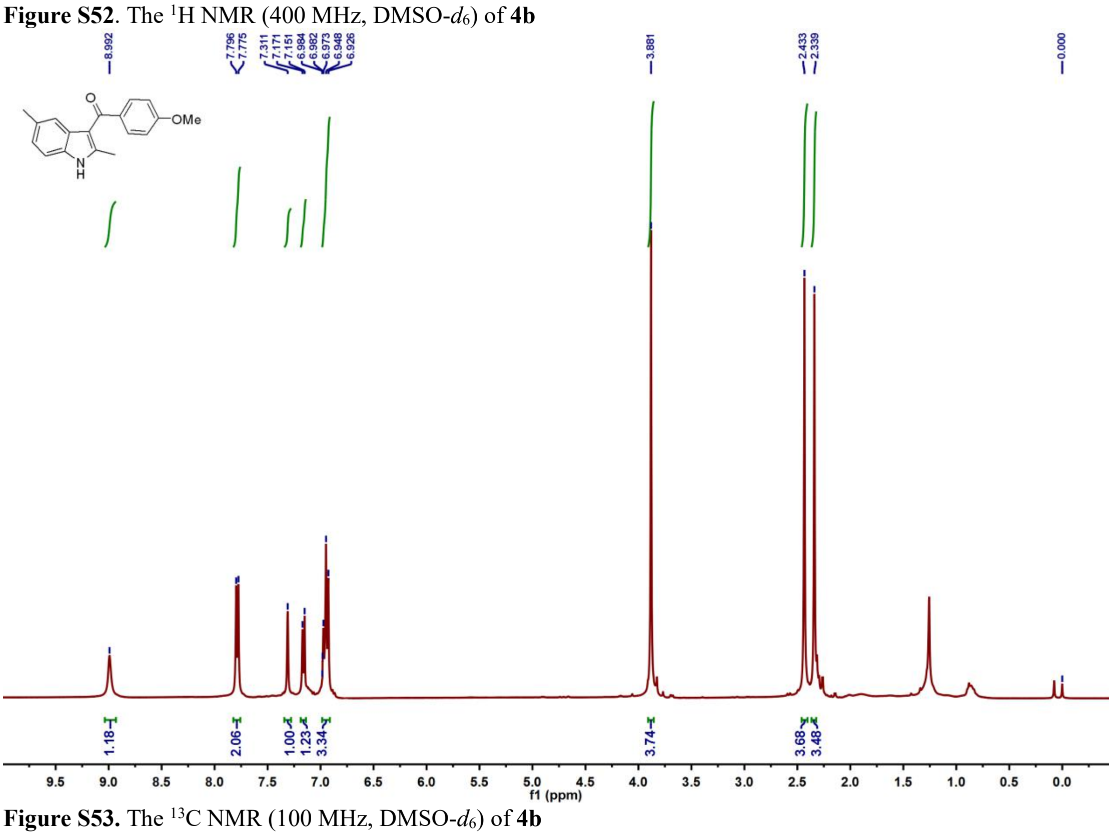


Figure S53. The ^{13}C NMR (100 MHz, DMSO-d_6) of **4b**

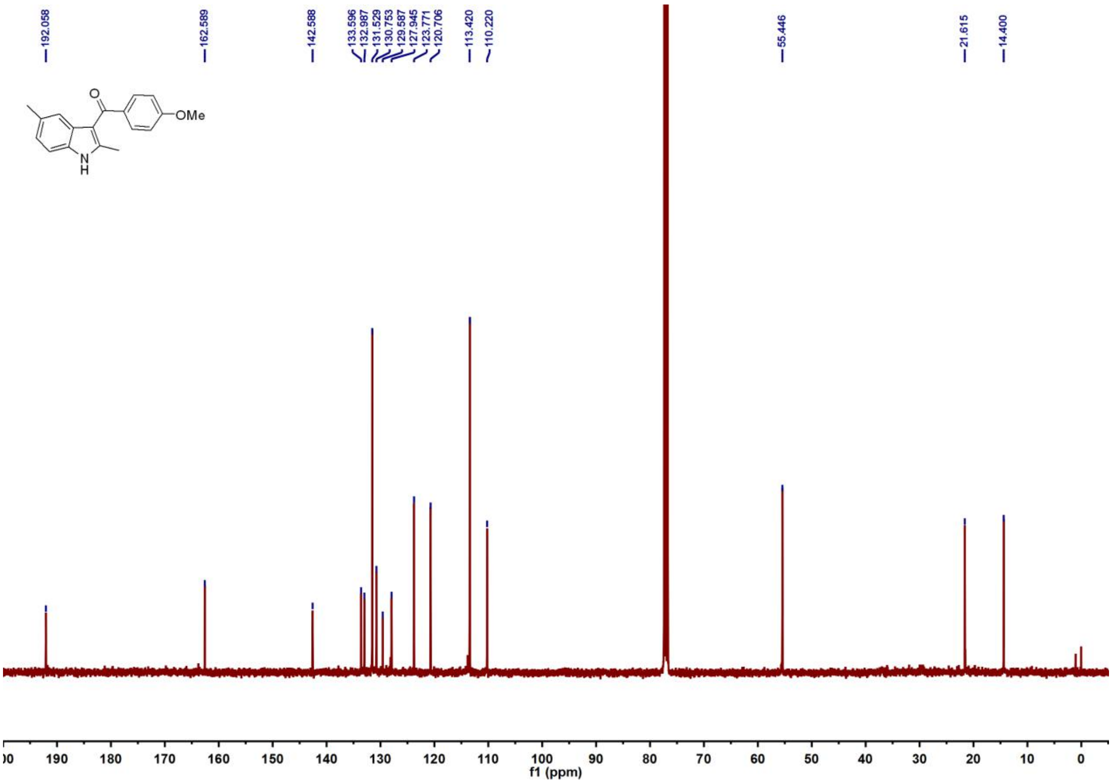


Figure S54. The ^{1}H NMR (400 MHz, DMSO-d_6) of **4c**

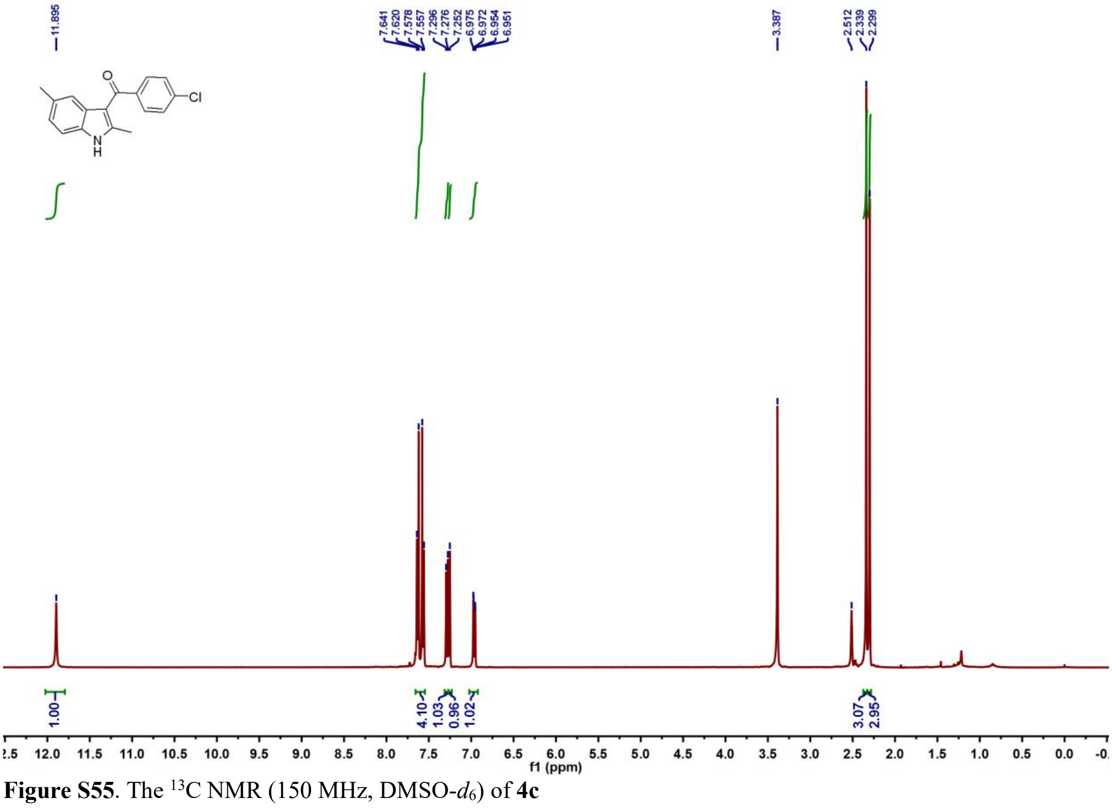


Figure S55. The ^{13}C NMR (150 MHz, DMSO-d_6) of **4c**

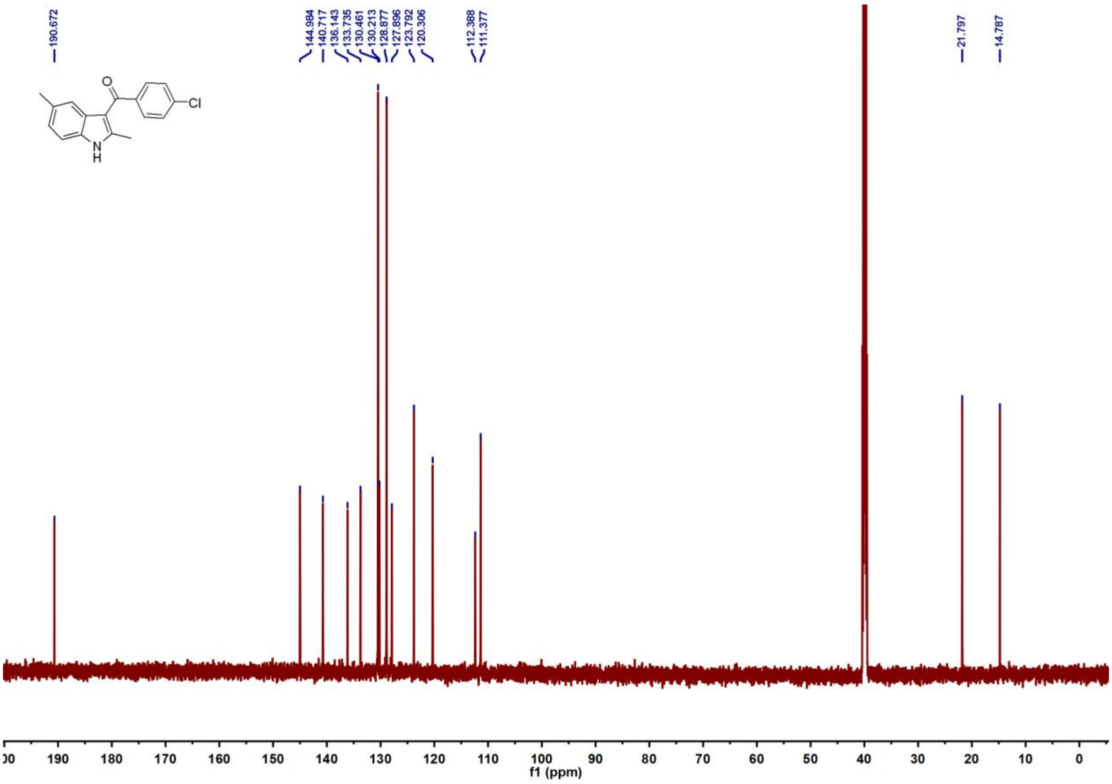


Figure S56. The ^{1}H NMR (400 MHz, DMSO-d_6) of **4d**

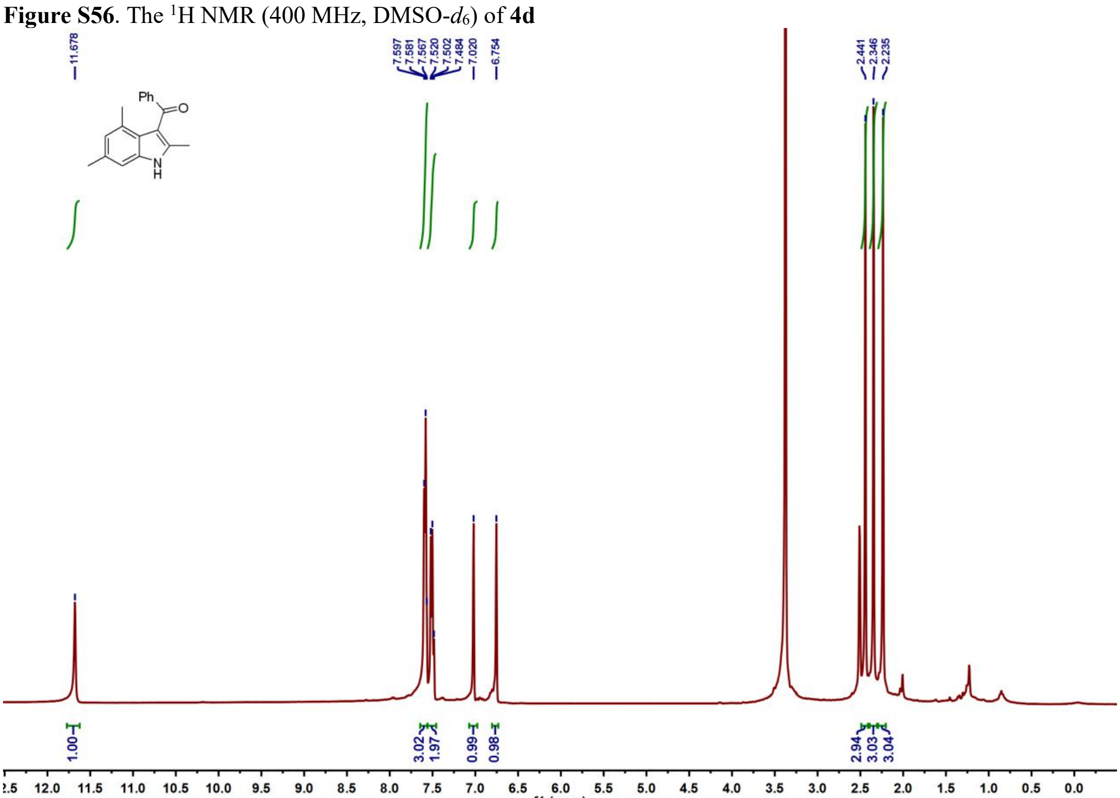


Figure S57. The ^{13}C NMR (150 MHz, DMSO-d_6) of **4d**

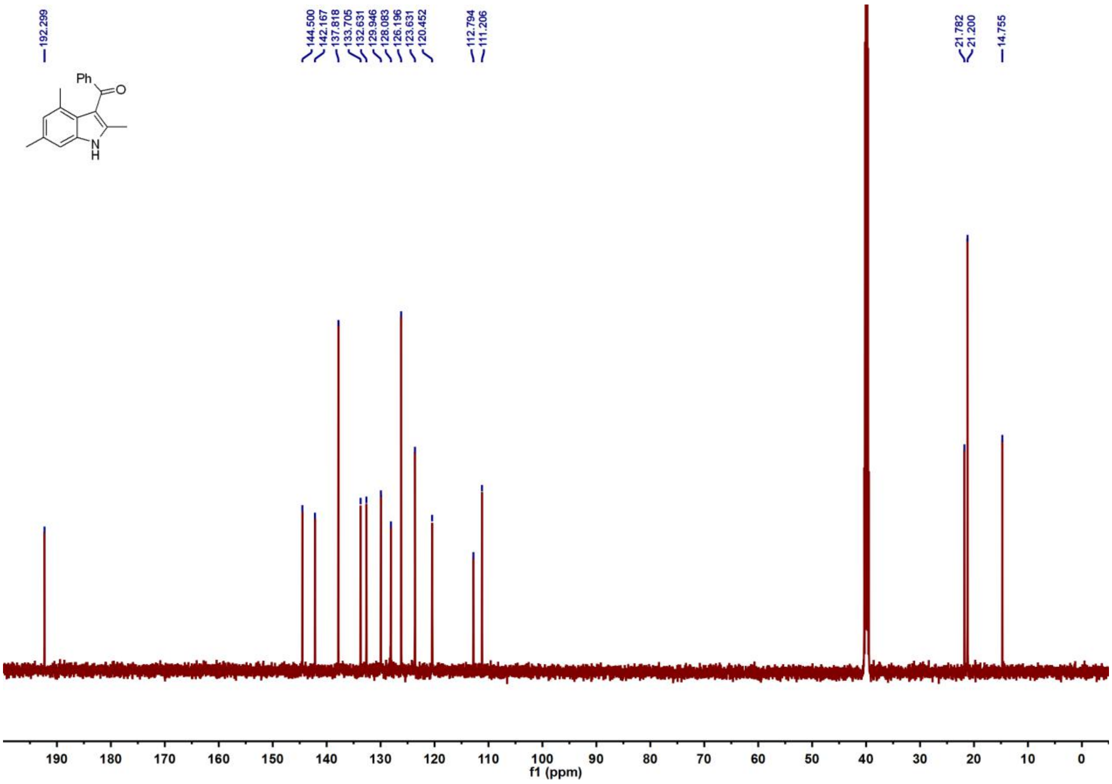


Figure S58. The ^{1}H NMR (400 MHz, DMSO-d_6) of **4e**

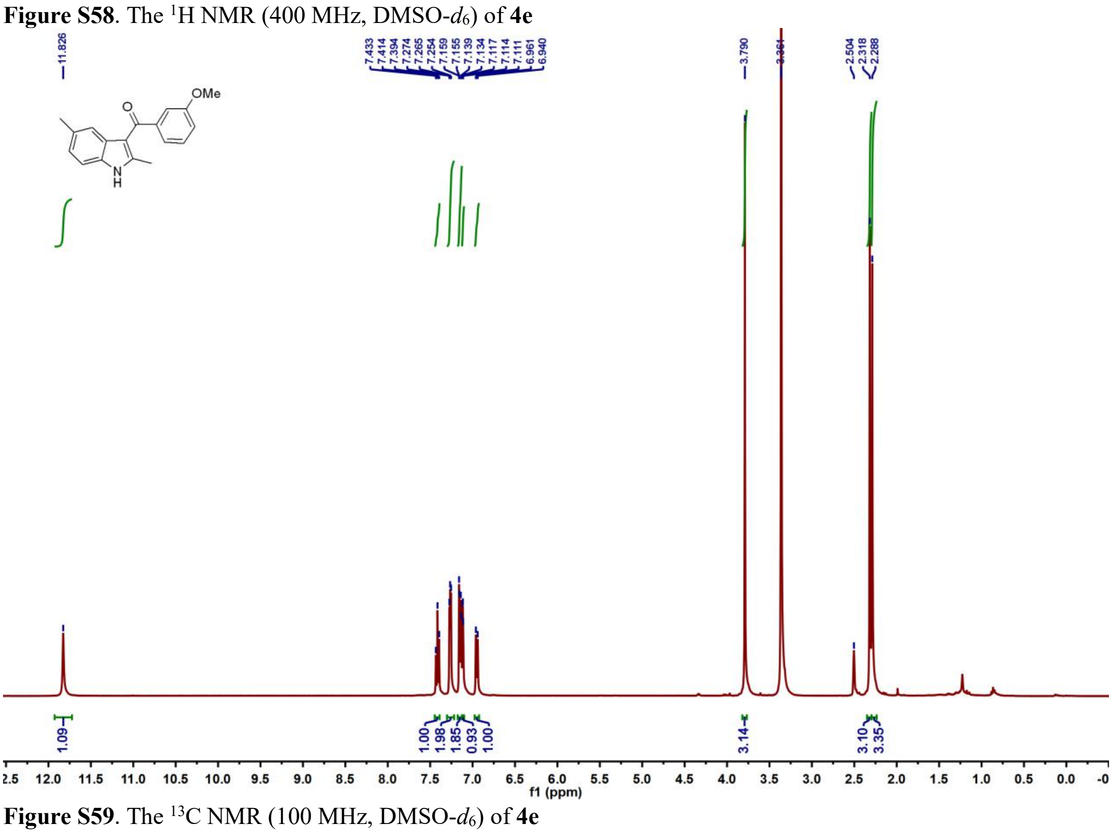


Figure S59. The ^{13}C NMR (100 MHz, DMSO-d_6) of **4e**

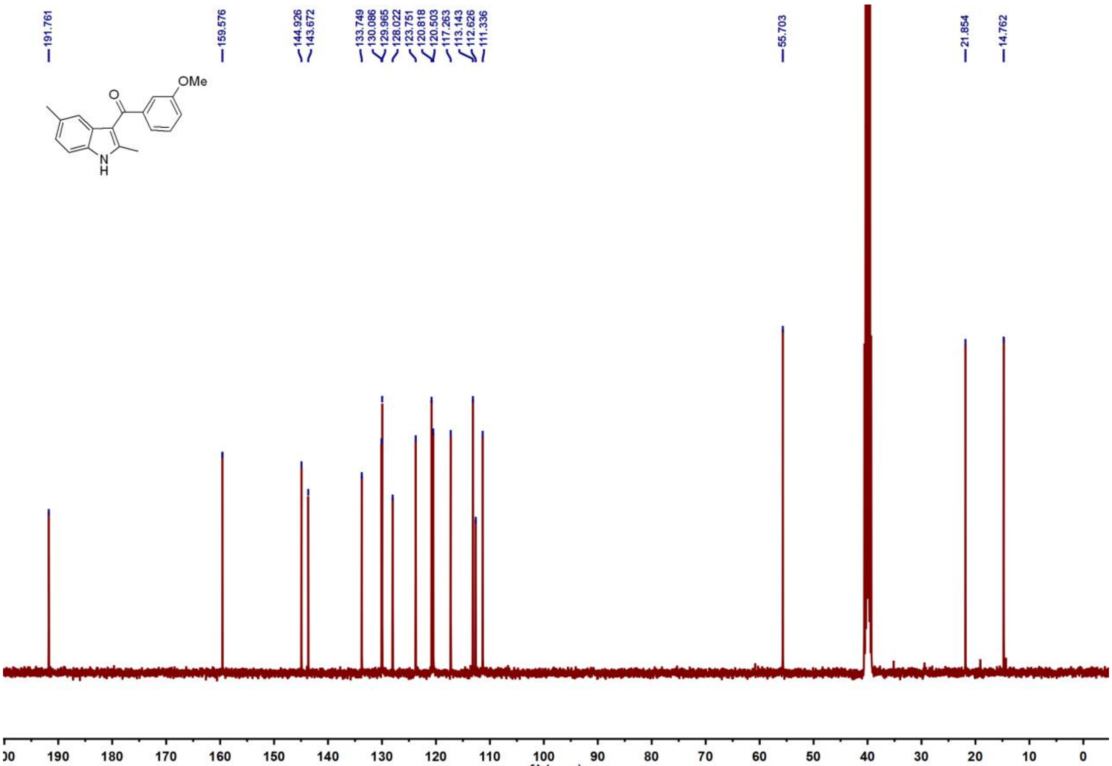


Figure S60. The ^{1}H NMR (400 MHz, DMSO-d_6) of **4f**

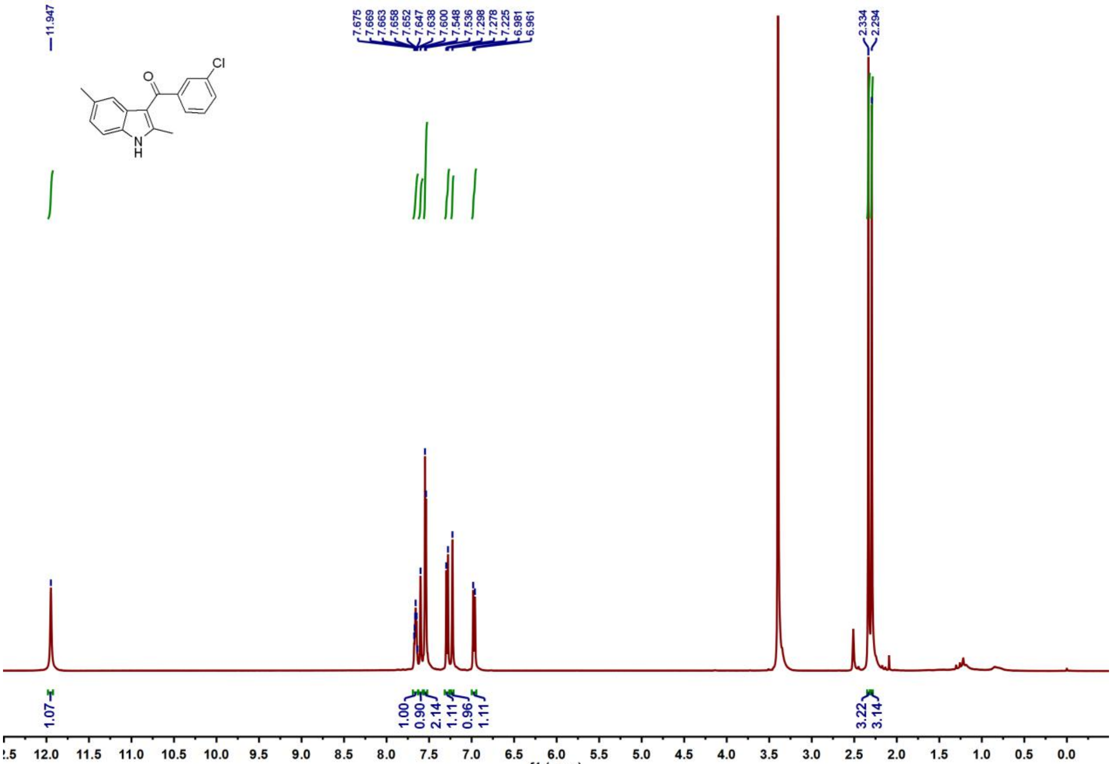


Figure S61. The ^{13}C NMR (100 MHz, DMSO-d_6) of **4f**

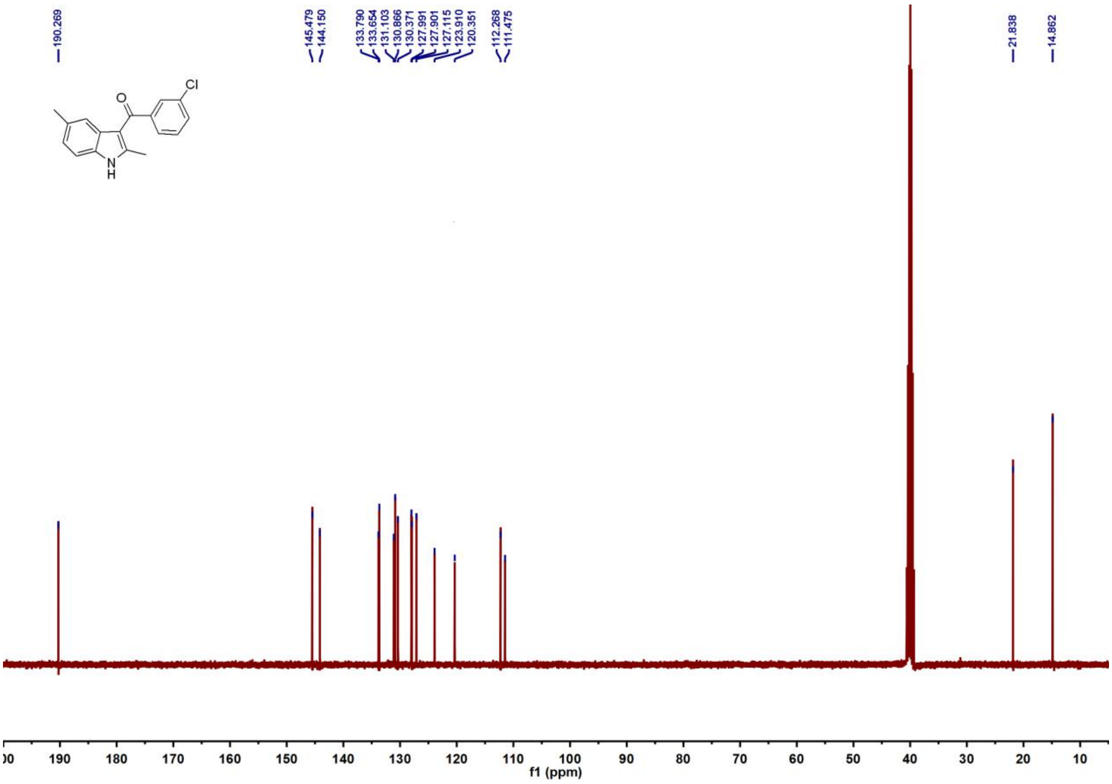


Figure S62. The [1]H NMR (400 MHz, DMSO-d_6) of **4g**

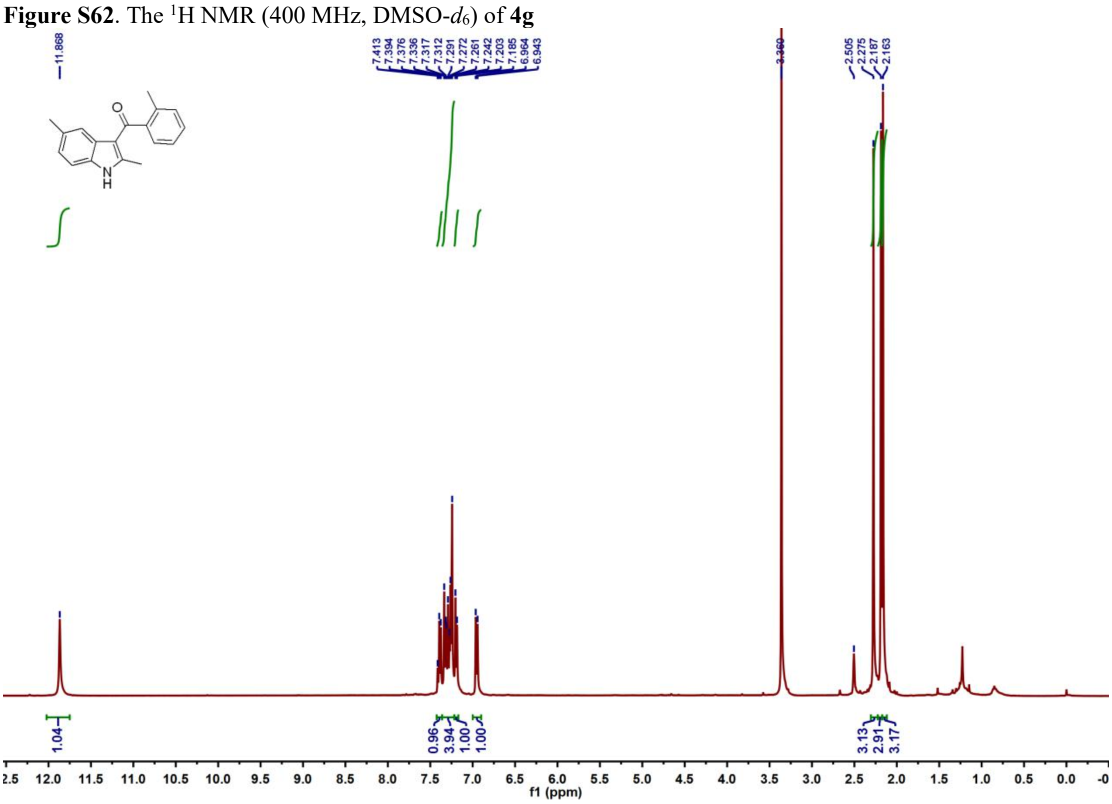


Figure S63. The [13]C NMR (100 MHz, DMSO-d_6) of **4g**

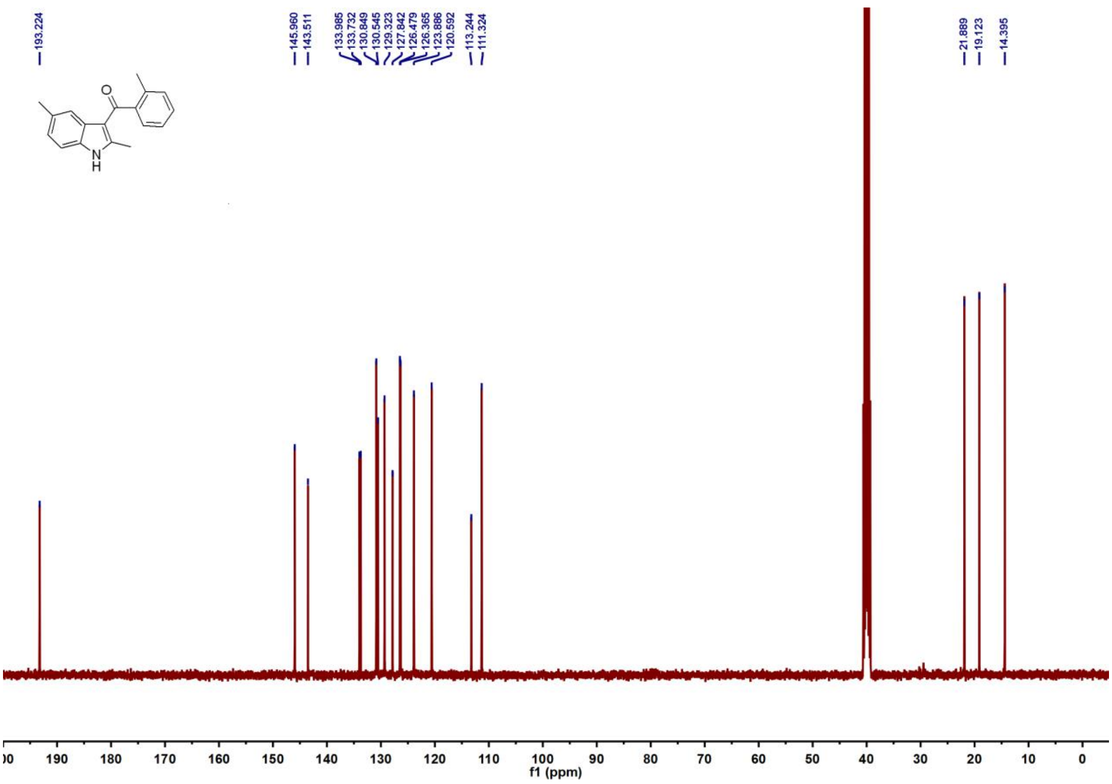


Figure S64. The ^{1}H NMR (400 MHz, DMSO-d_6) of **4h**

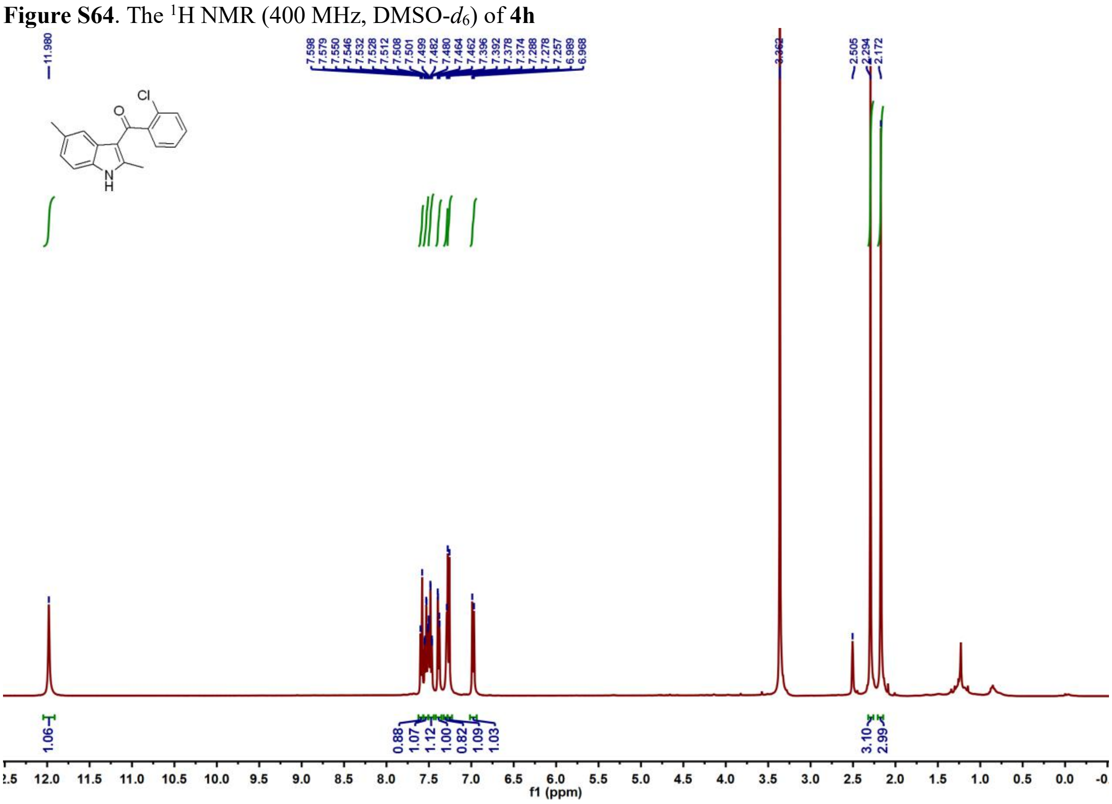


Figure S65. The ^{13}C NMR (100 MHz, DMSO-d_6) of **4h**

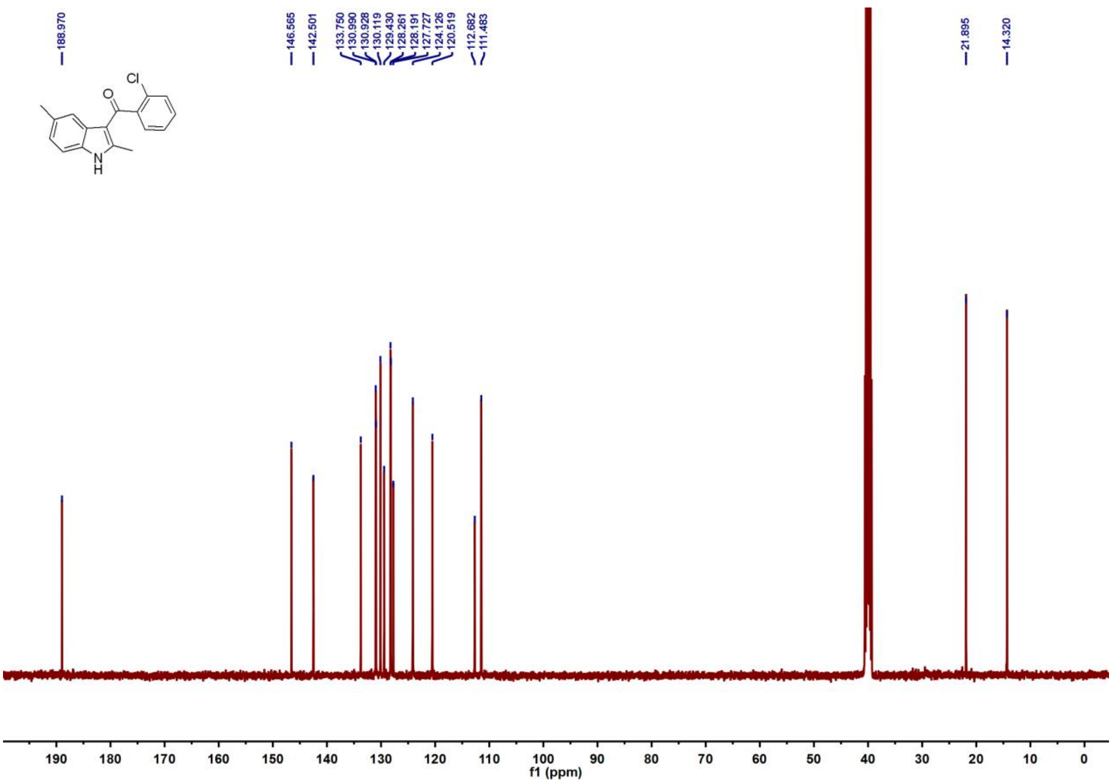


Figure S66. The ^{1}H NMR (400 MHz, DMSO-d_6) of **4i**

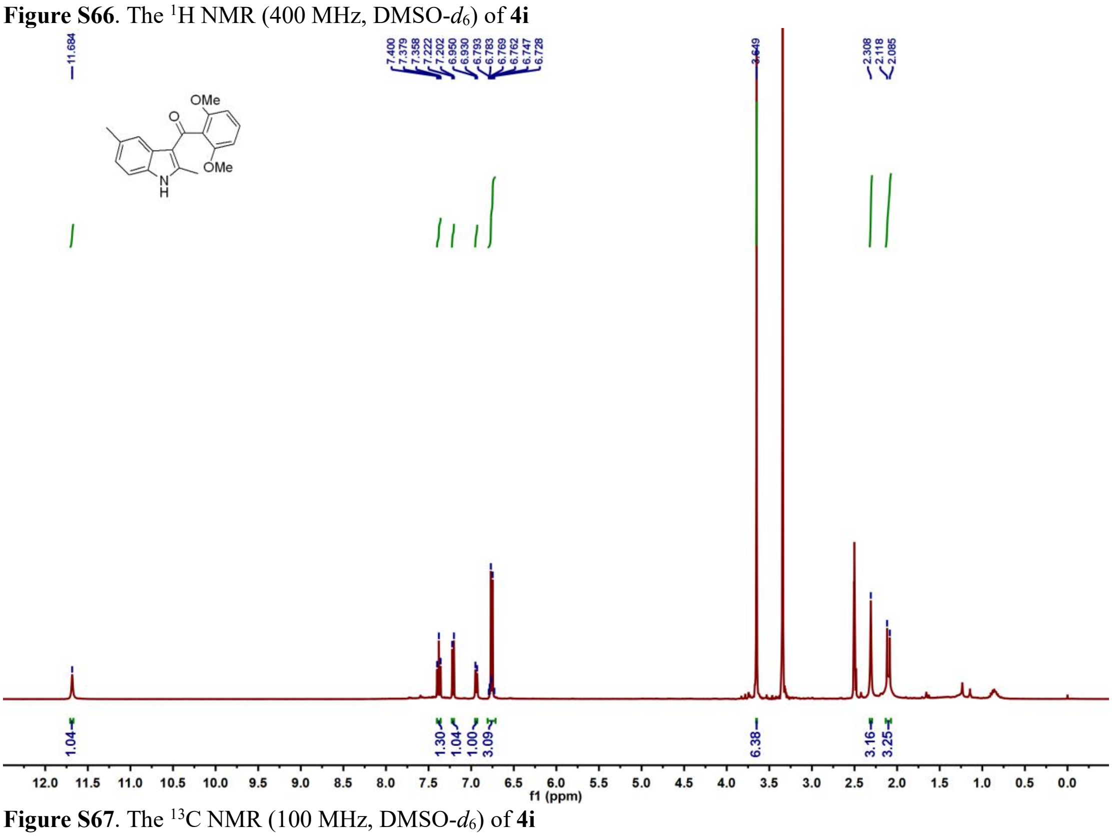


Figure S67. The ^{13}C NMR (100 MHz, DMSO-d_6) of **4i**

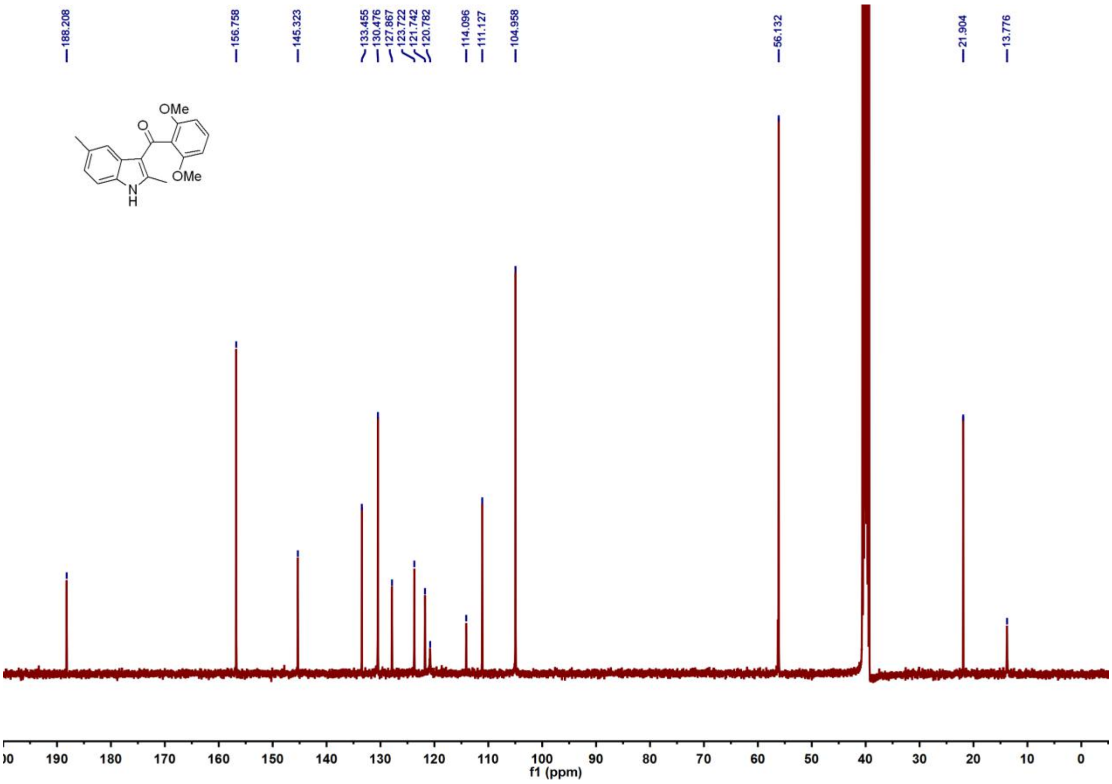


Figure S68. The ^{1}H NMR (400 MHz, DMSO-d_6) of **4j**

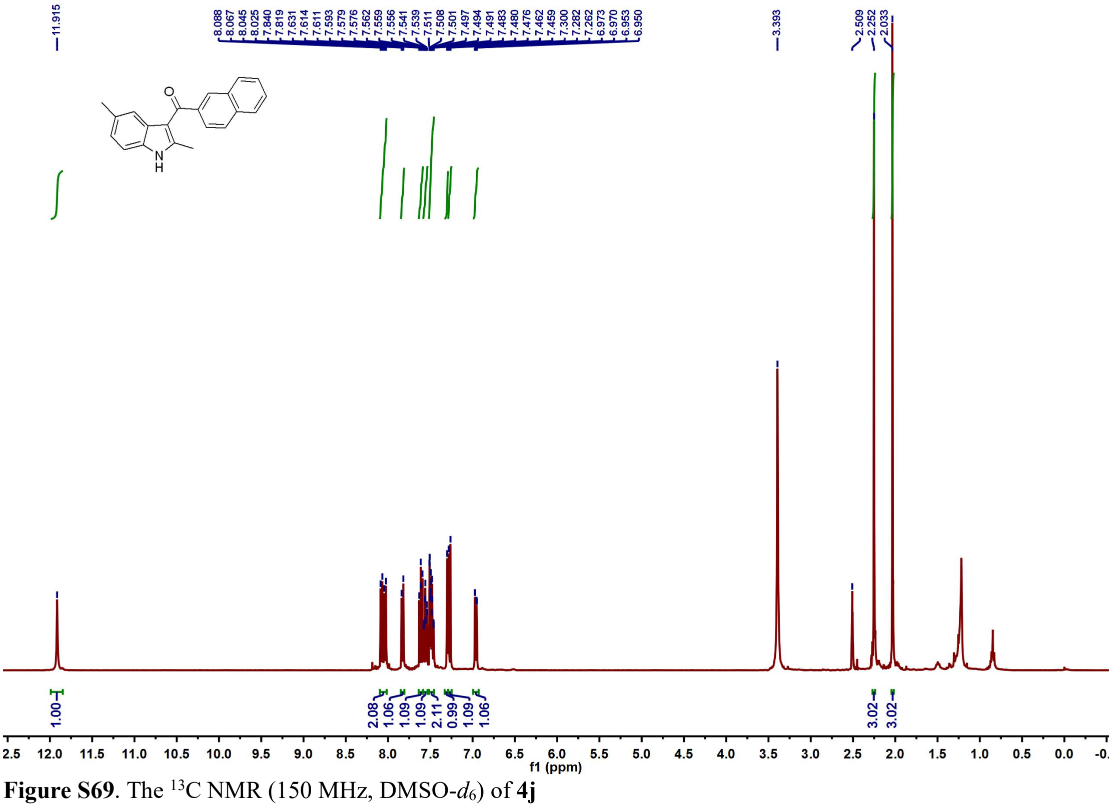


Figure S69. The ^{13}C NMR (150 MHz, DMSO-d_6) of **4j**

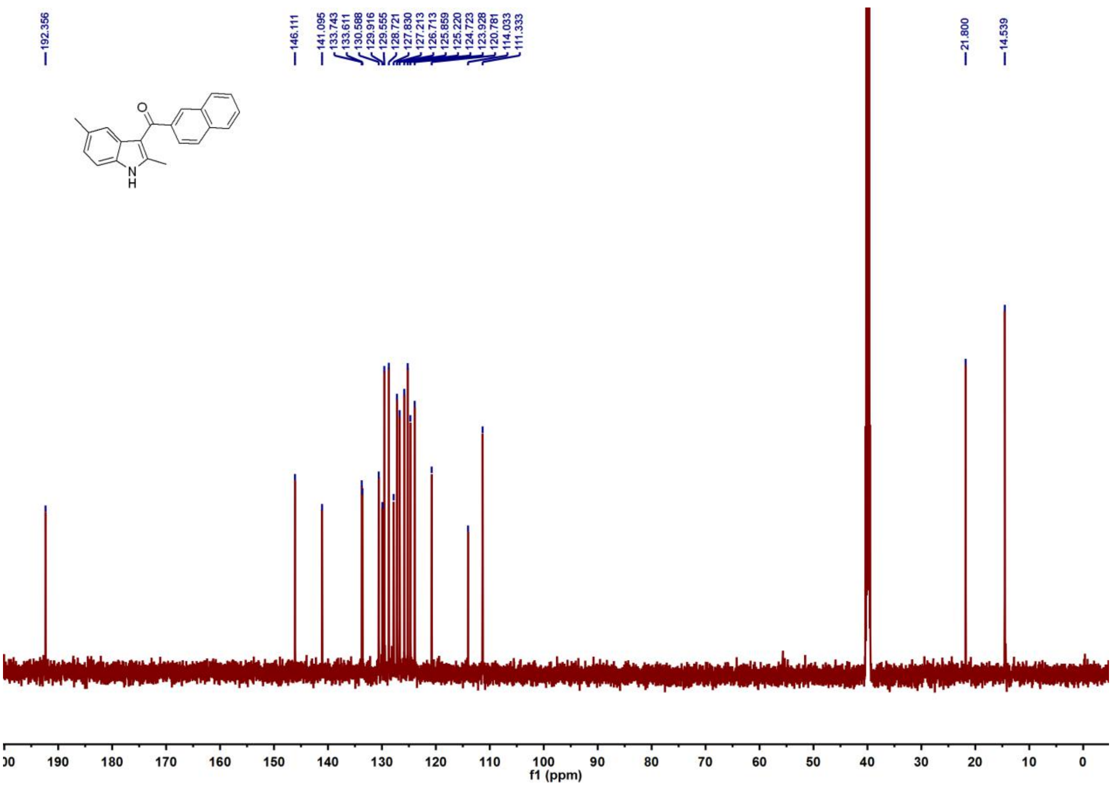


Figure S70. The ^{1}H NMR (400 MHz, DMSO-d_6) of **4k**

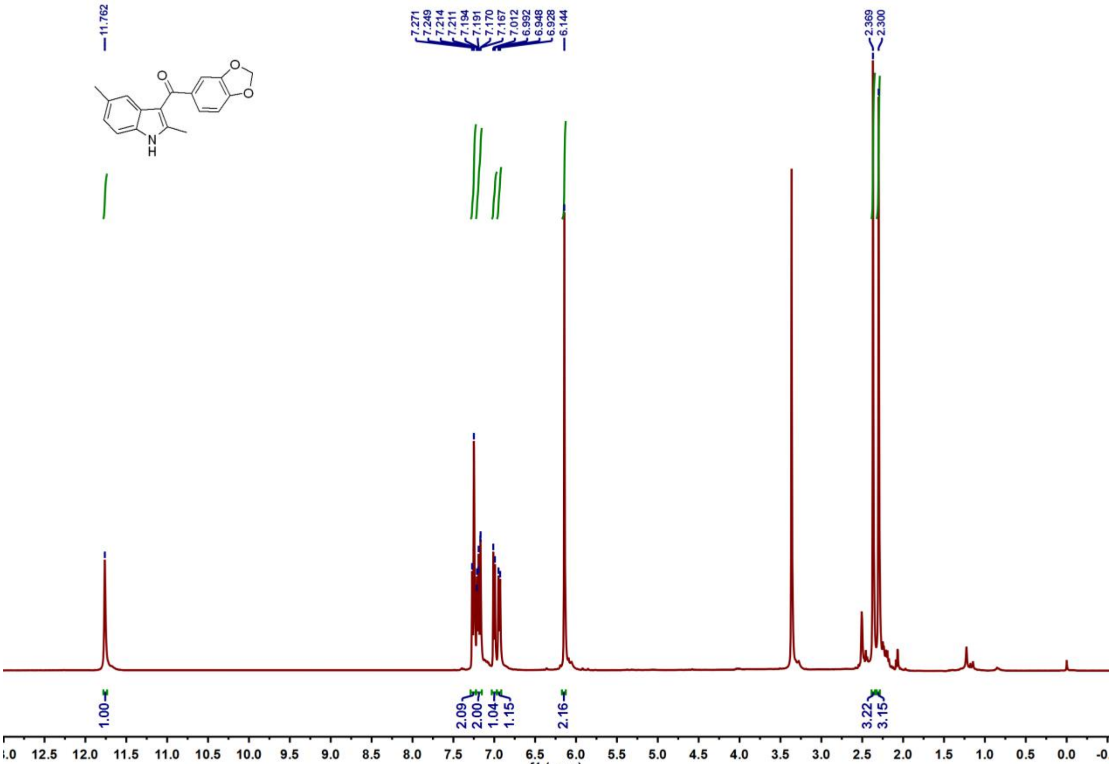


Figure S71. The ^{13}C NMR (100 MHz, DMSO-d_6) of **4k**

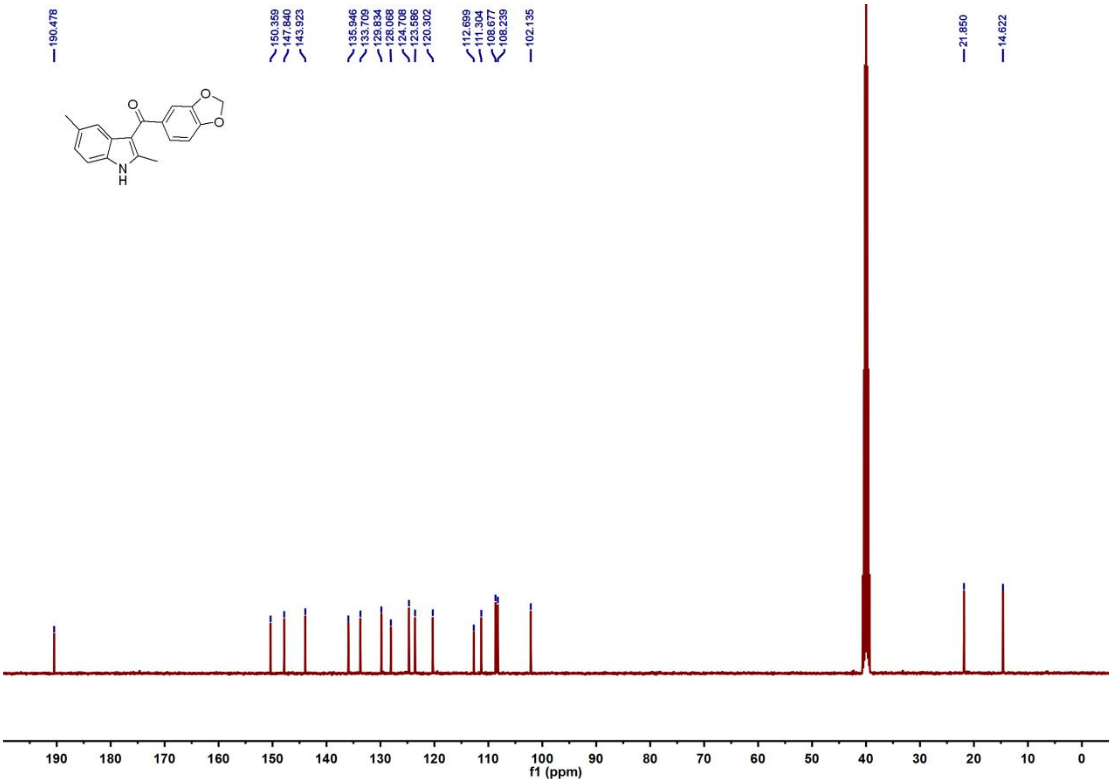


Figure S72. The ^{1}H NMR (400 MHz, Chloroform-*d*) of **5a**

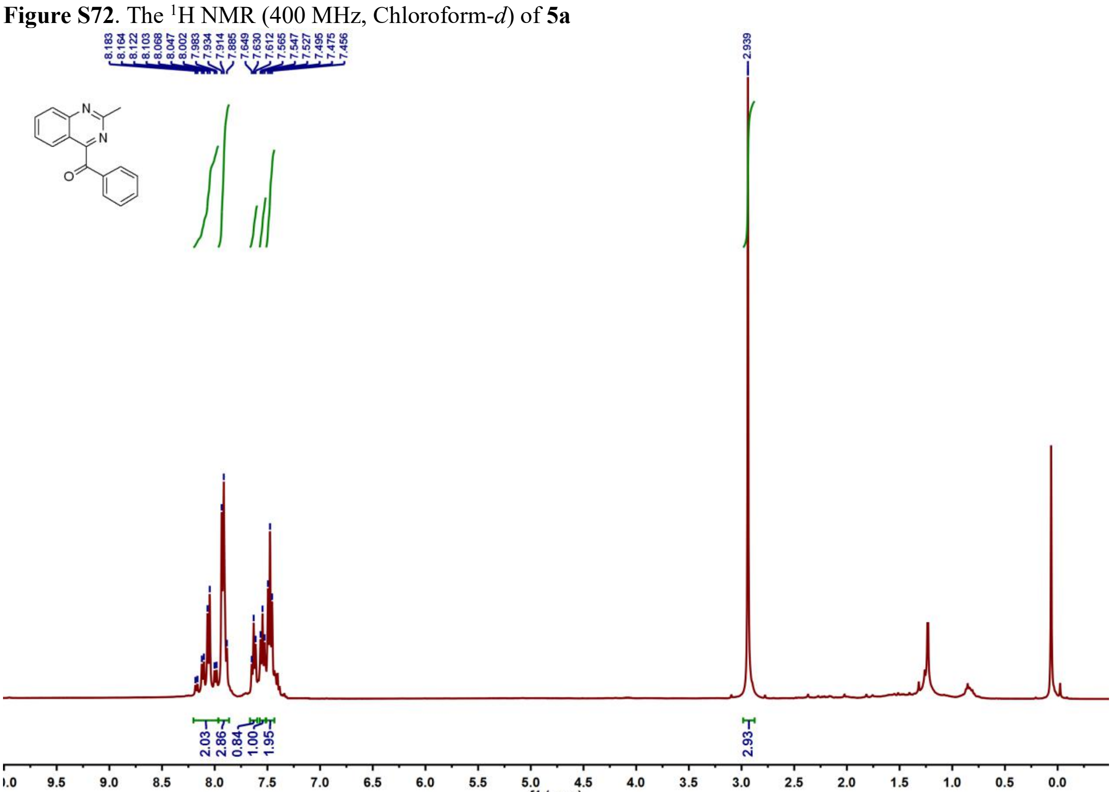


Figure S73. The ^{13}C NMR (100 MHz, Chloroform-*d*) of **5a**

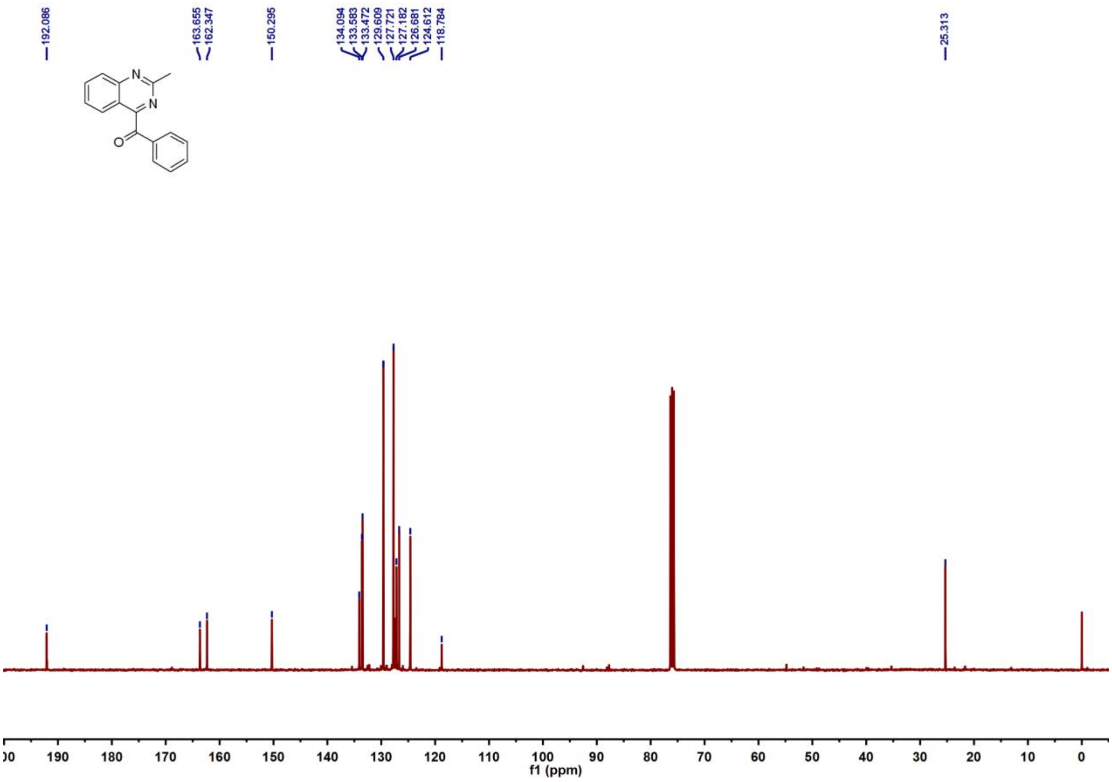


Figure S74. The [1]H NMR (400 MHz, Chloroform-*d*) of **5b**

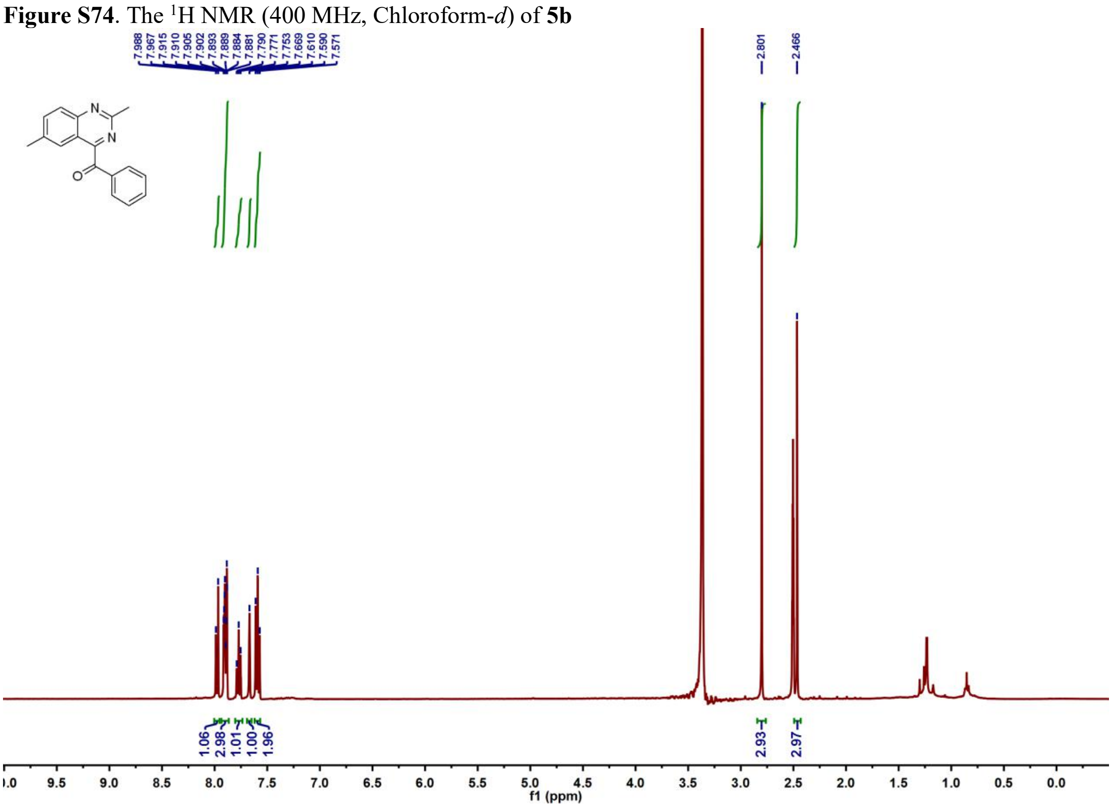


Figure S75. The [13]C NMR (100 MHz, Chloroform-*d*) of **5b**

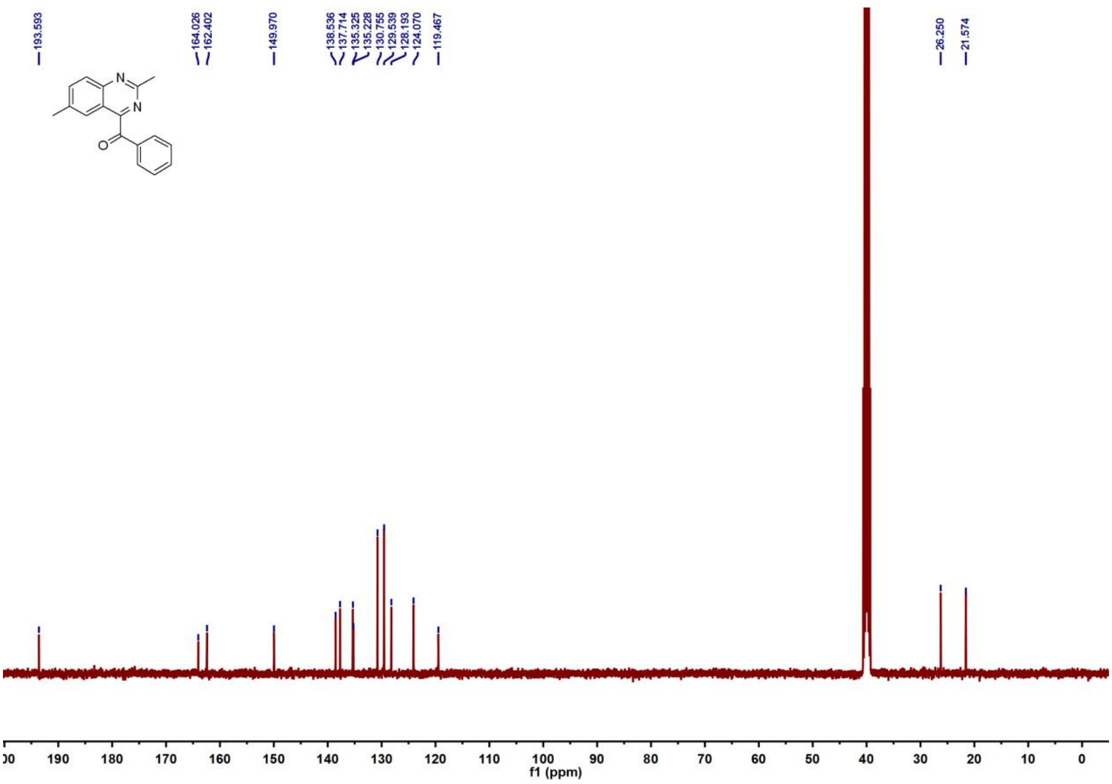


Figure S76. The [1]H NMR (400 MHz, Chloroform-*d*) of **5c**

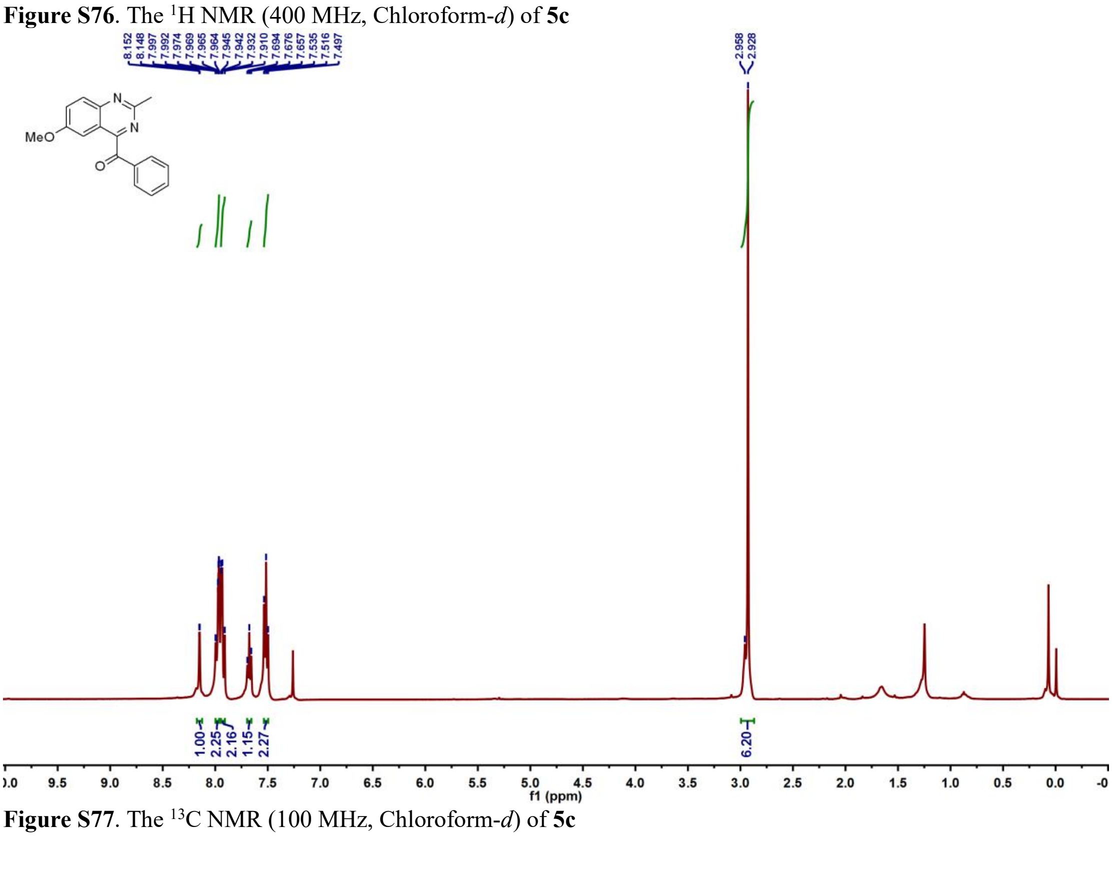


Figure S77. The [13]C NMR (100 MHz, Chloroform-*d*) of **5c**

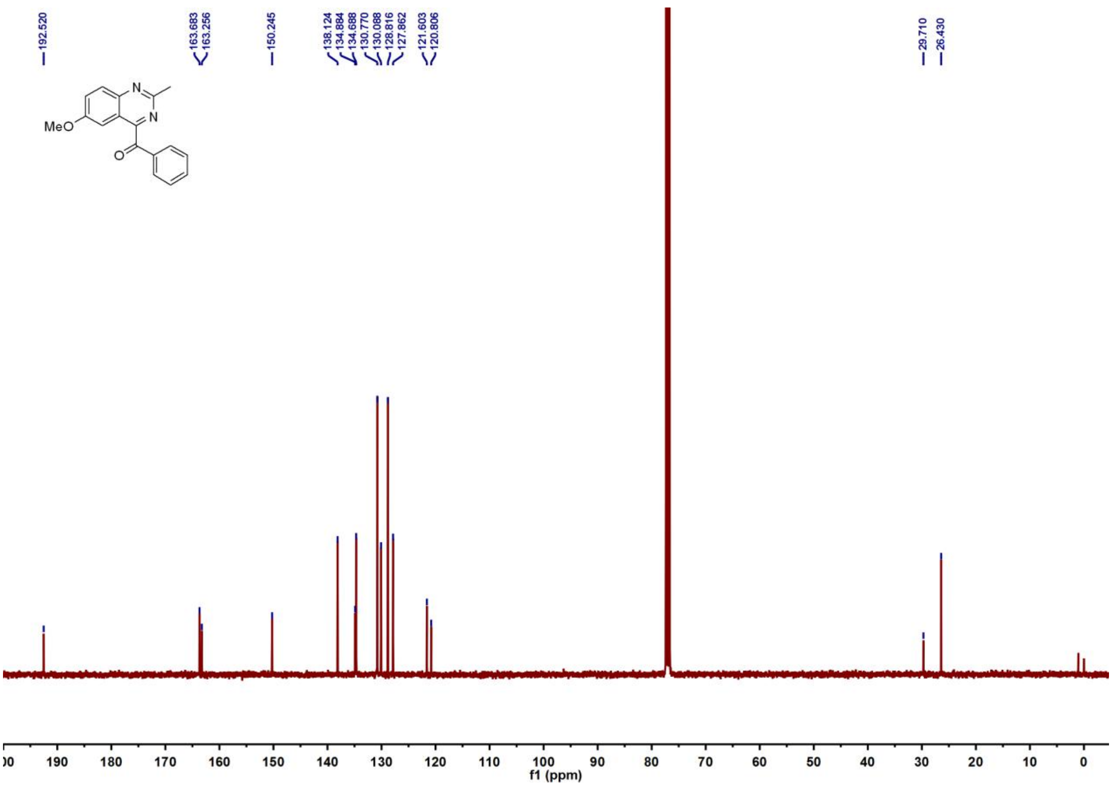


Figure S78. The [1]H NMR (400 MHz, Chloroform-*d*) of **5d**

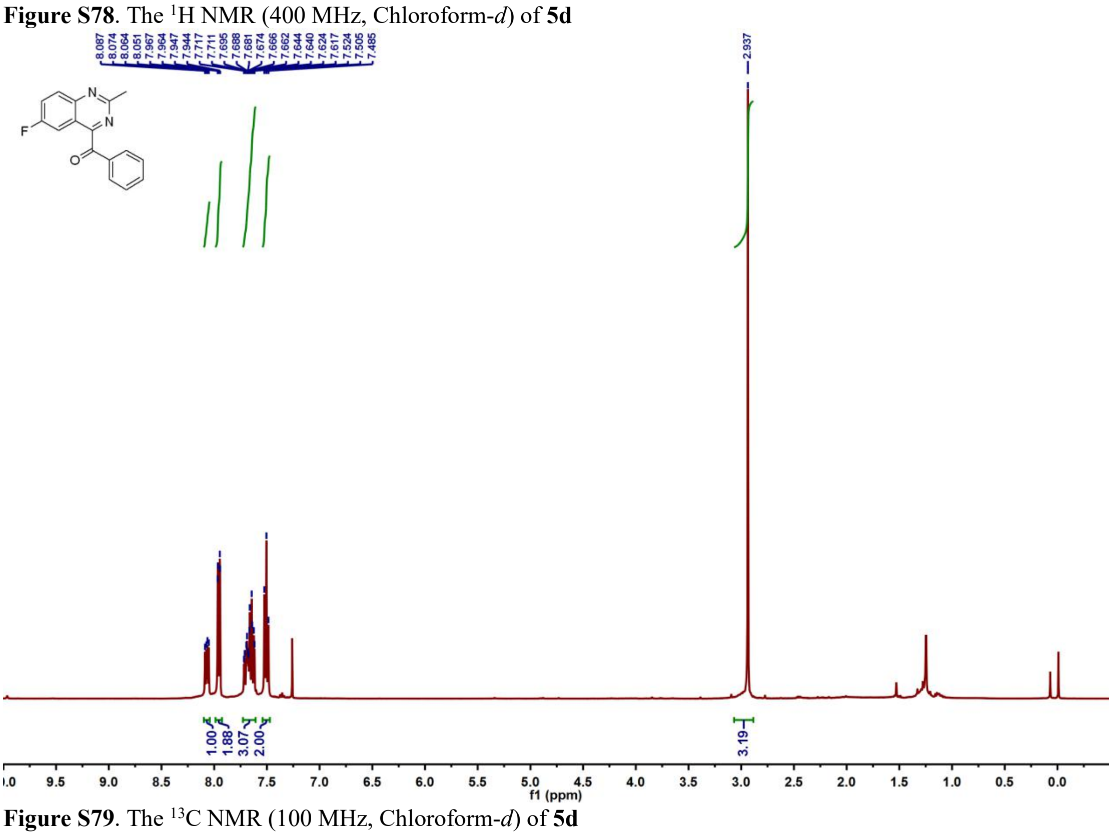


Figure S79. The [13]C NMR (100 MHz, Chloroform-*d*) of **5d**

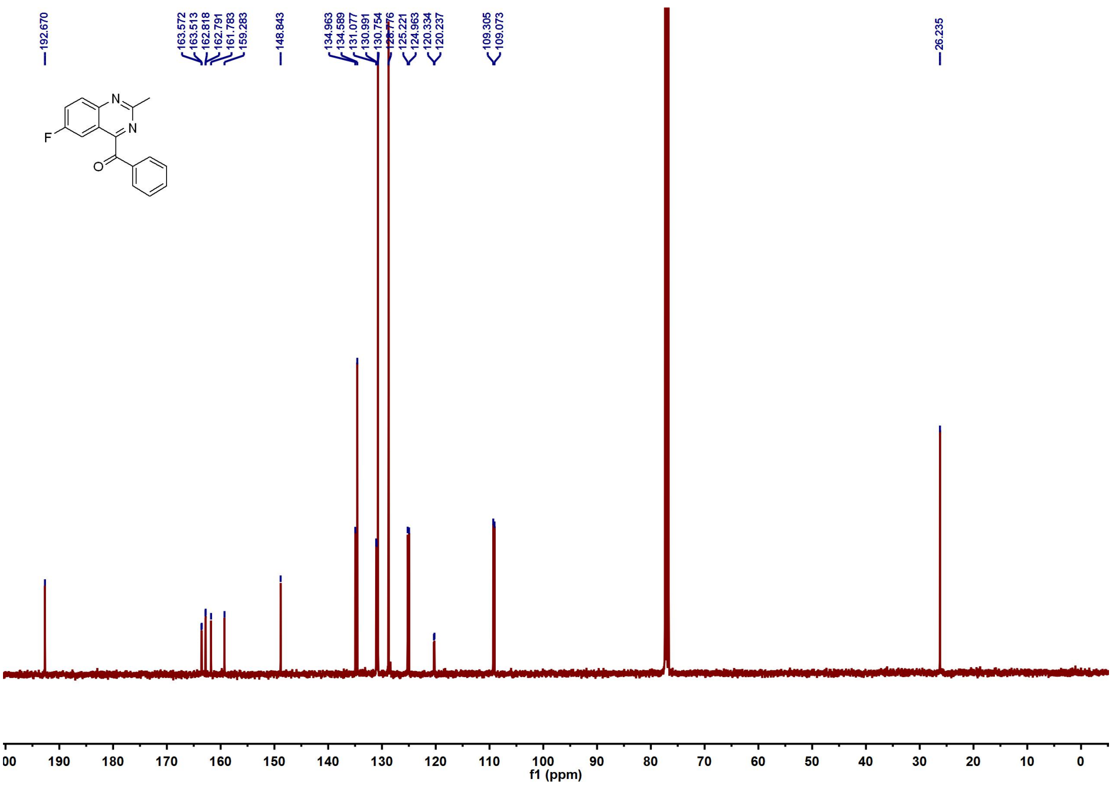


Figure S80. The [19]F NMR (376 MHz, Chloroform-*d*) of **5d**

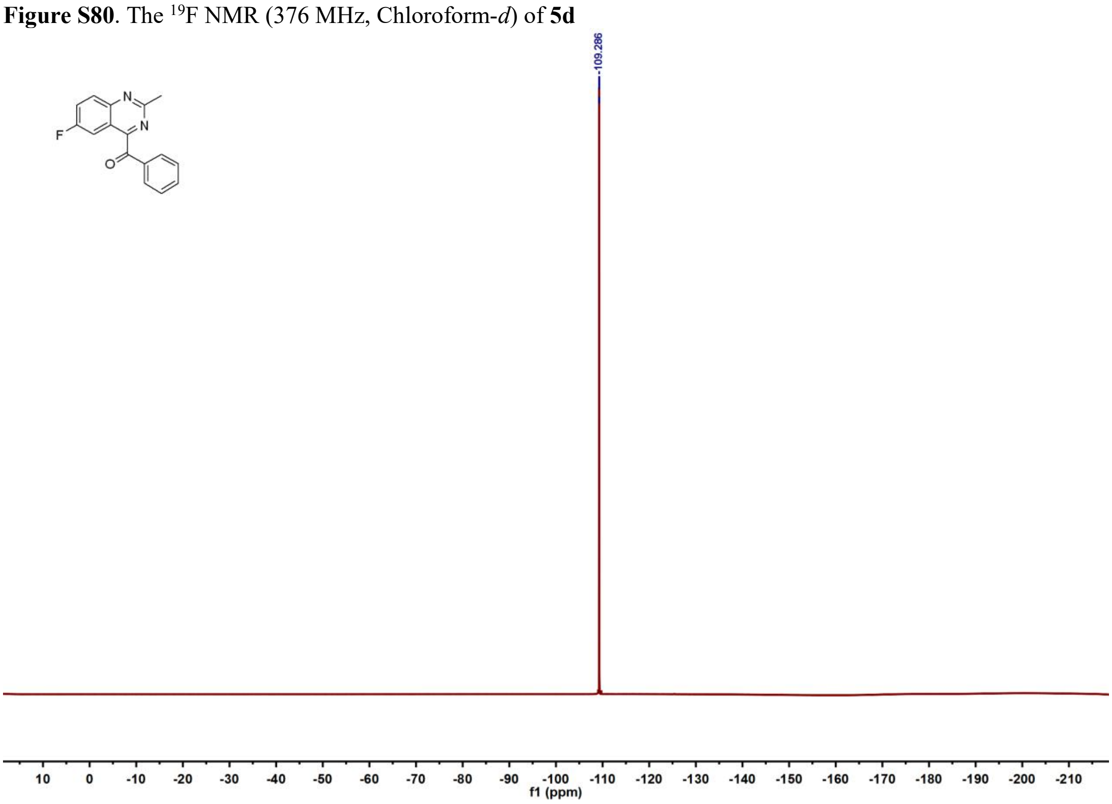


Figure S81. The [1]H NMR (400 MHz, Chloroform-*d*) of **5e**

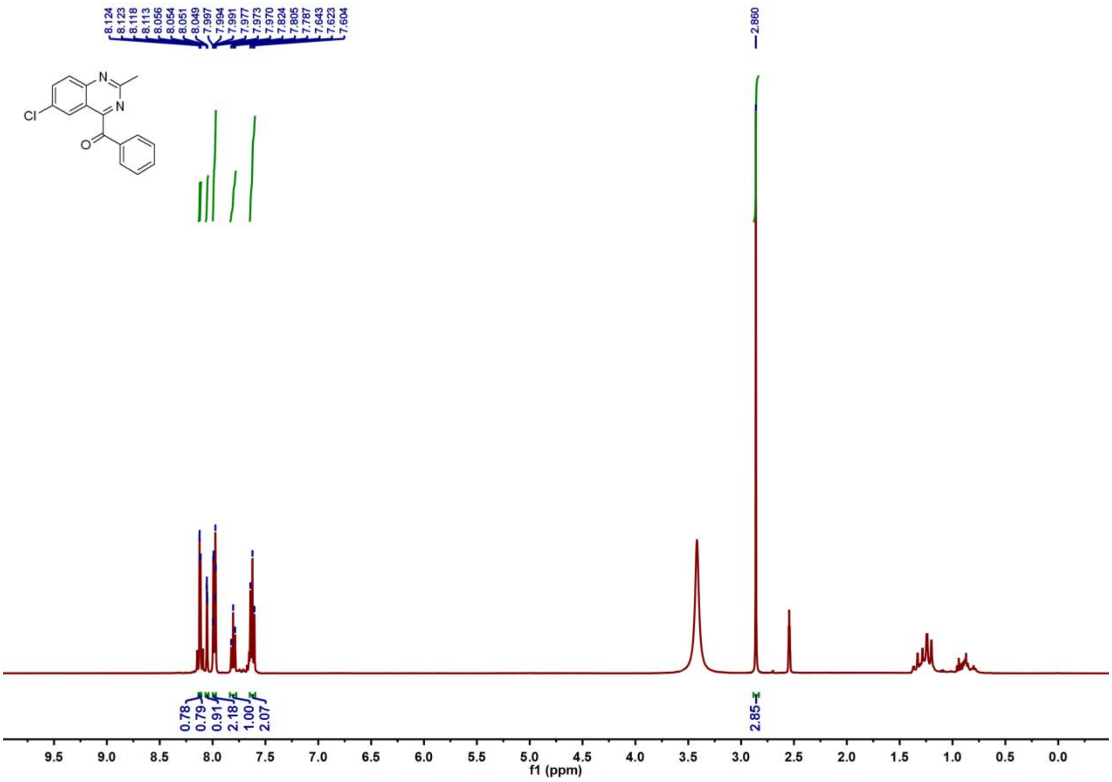


Figure S82. The ^{13}C NMR (100 MHz, Chloroform-*d*) of **5e**

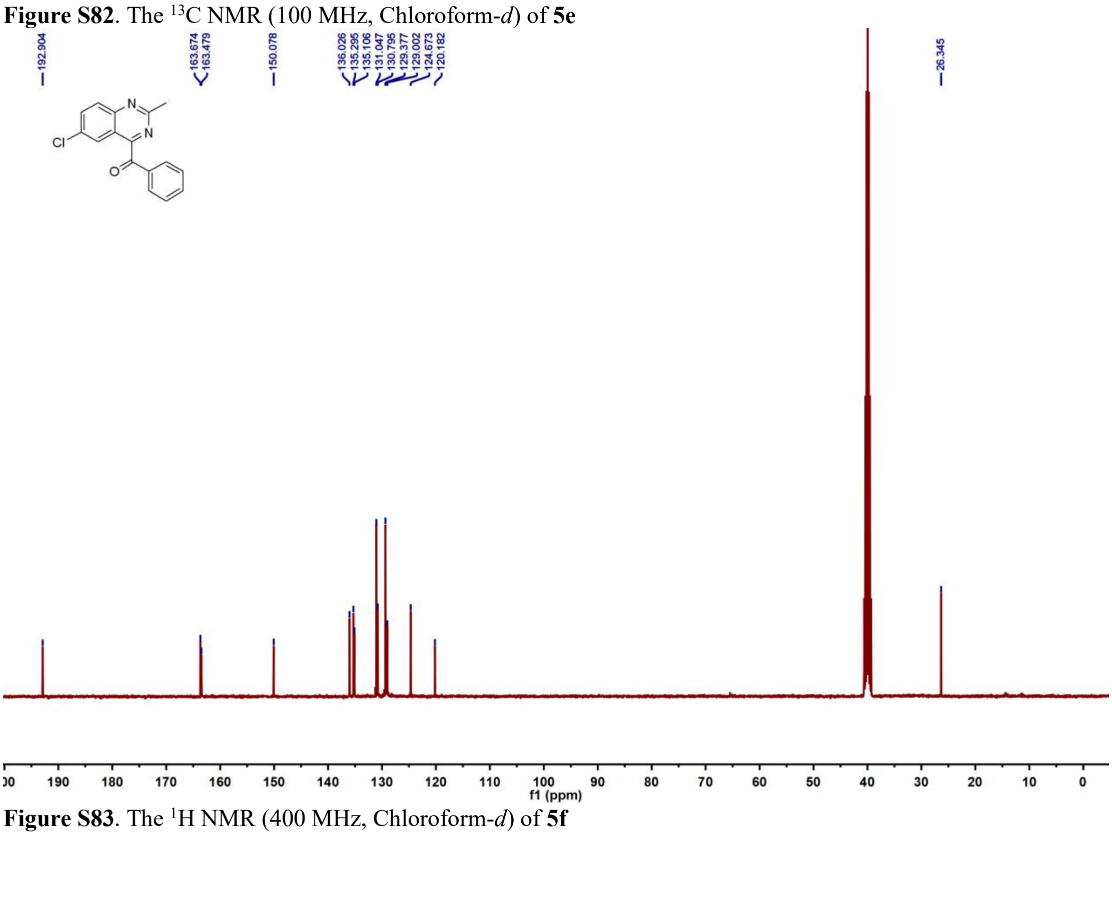


Figure S83. The ^{1}H NMR (400 MHz, Chloroform-*d*) of **5f**

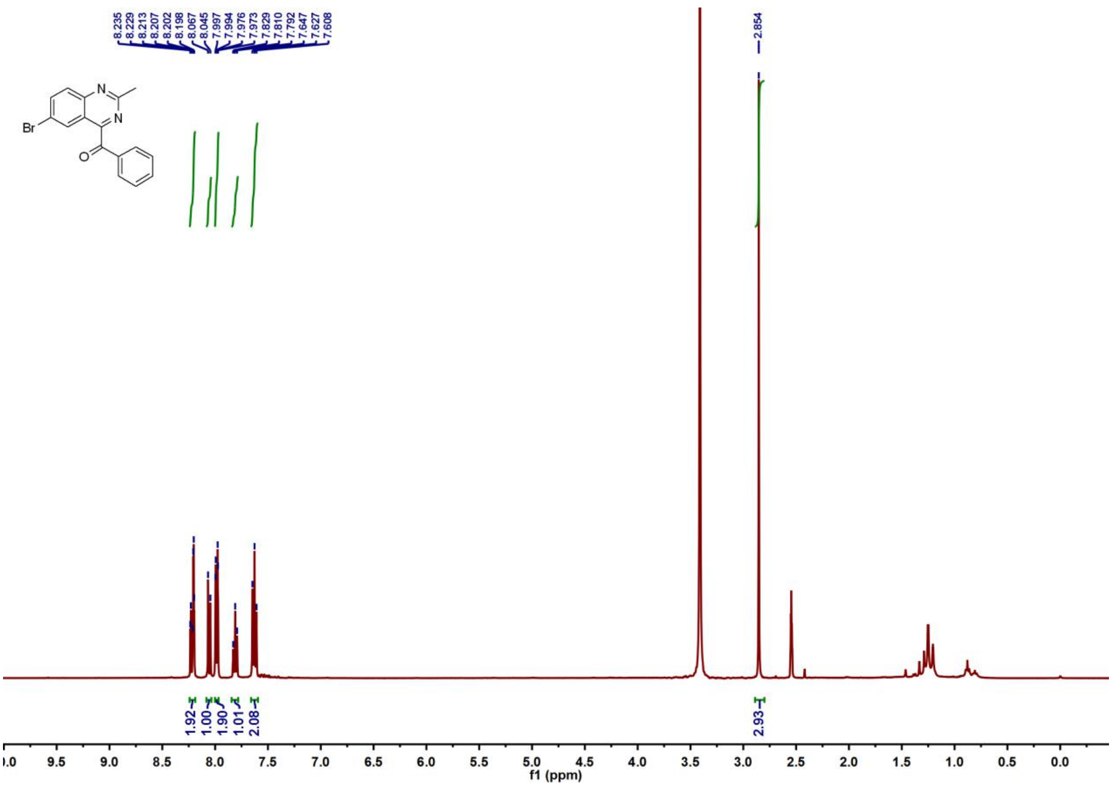


Figure S84. The ^{13}C NMR (100 MHz, Chloroform-*d*) of **5f**

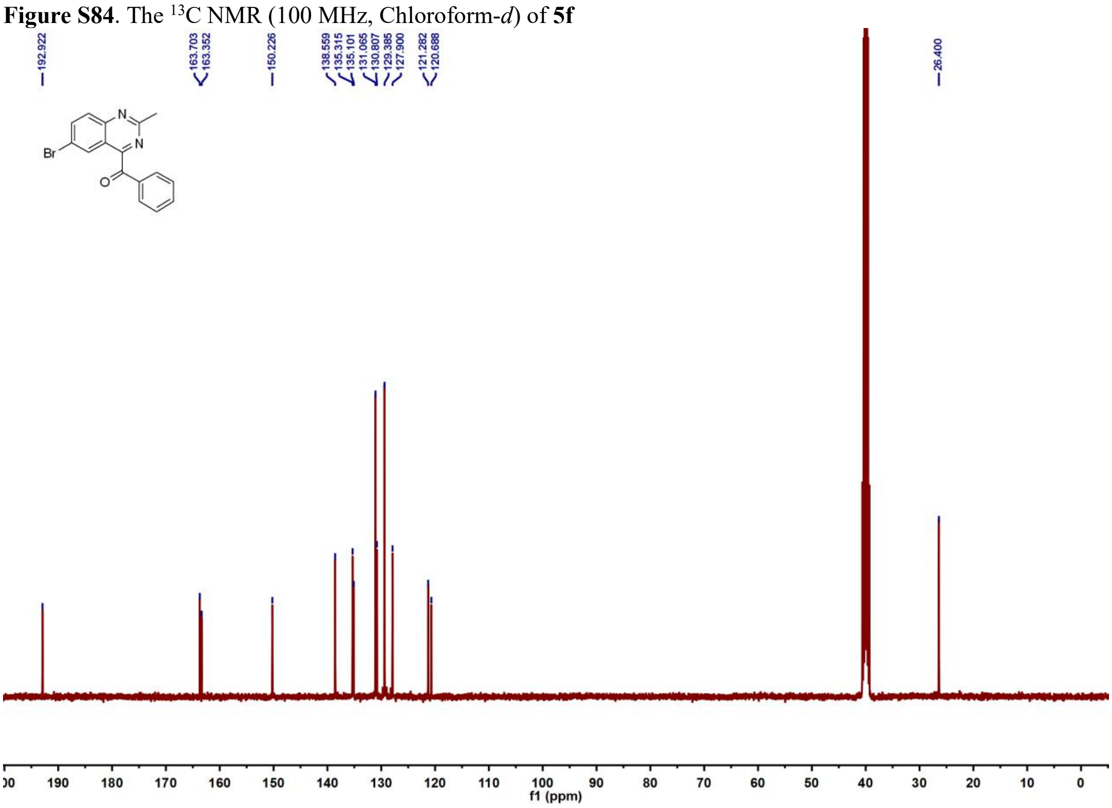


Figure S85. The ^{1}H NMR (400 MHz, Chloroform-*d*) of **5g**

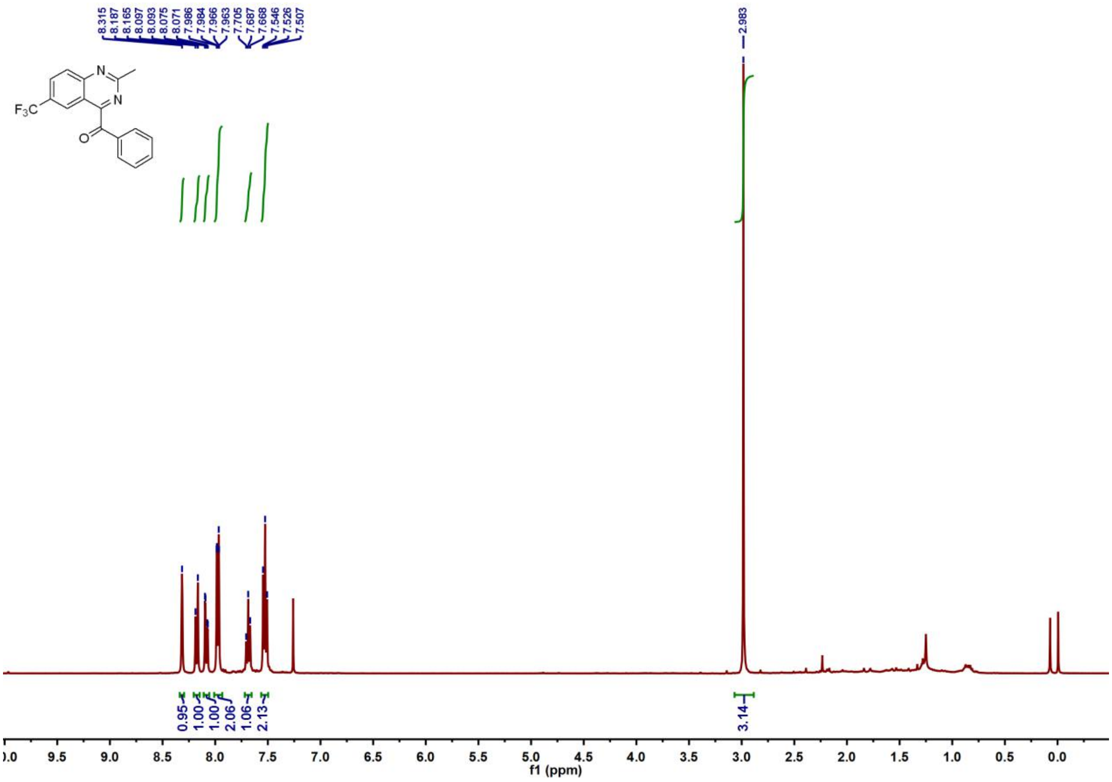


Figure S86. The ^{13}C NMR (100 MHz, Chloroform-*d*) of **5g**

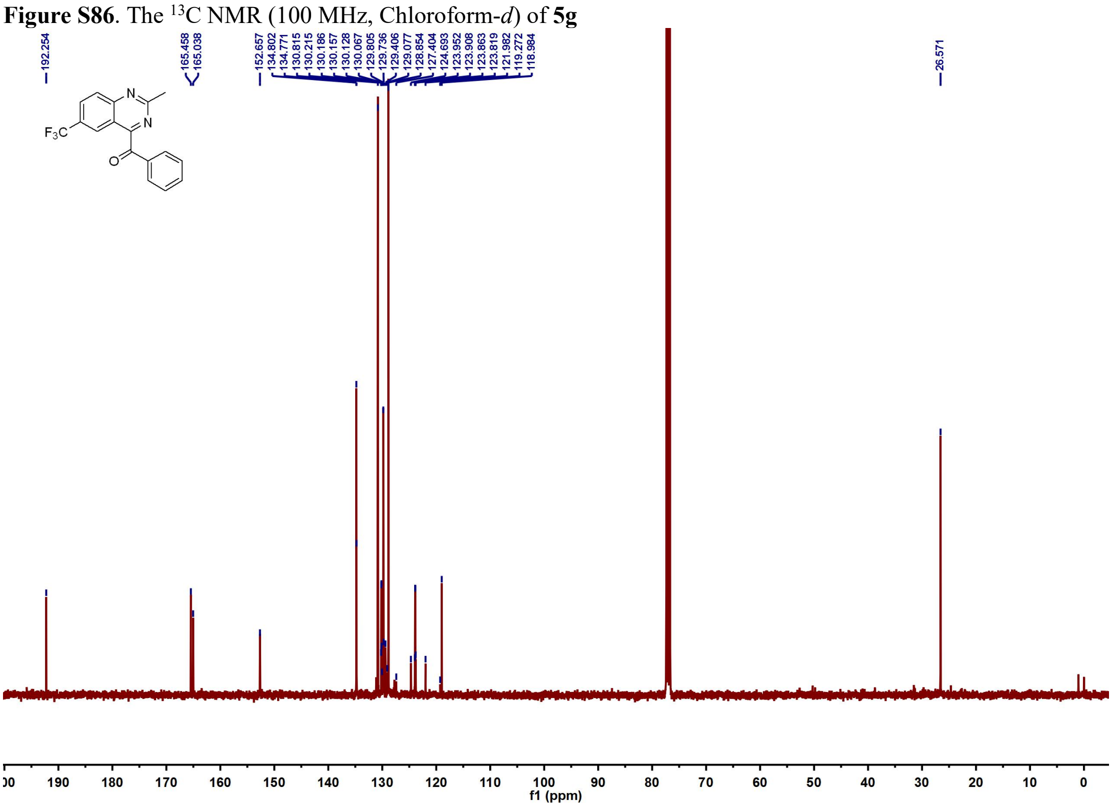


Figure S87. The ^{19}F NMR (376 MHz, Chloroform-*d*) of **5g**

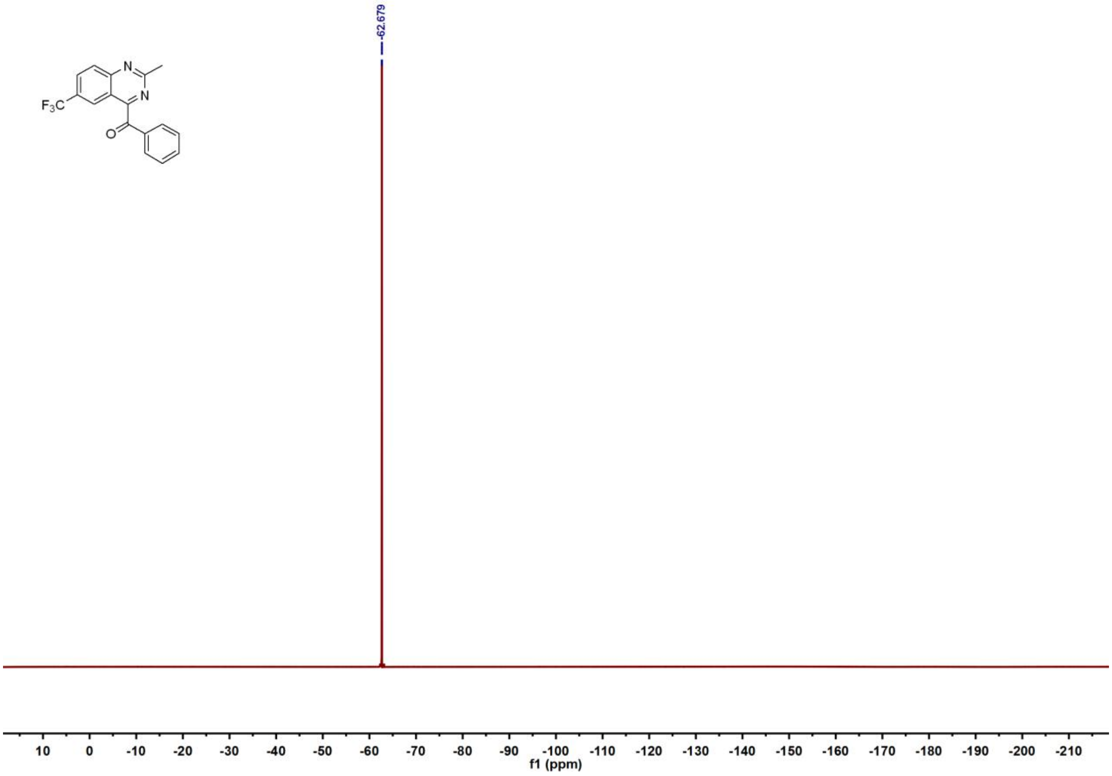


Figure S88. The [1]H NMR (400 MHz, Chloroform-*d*) of **5h**

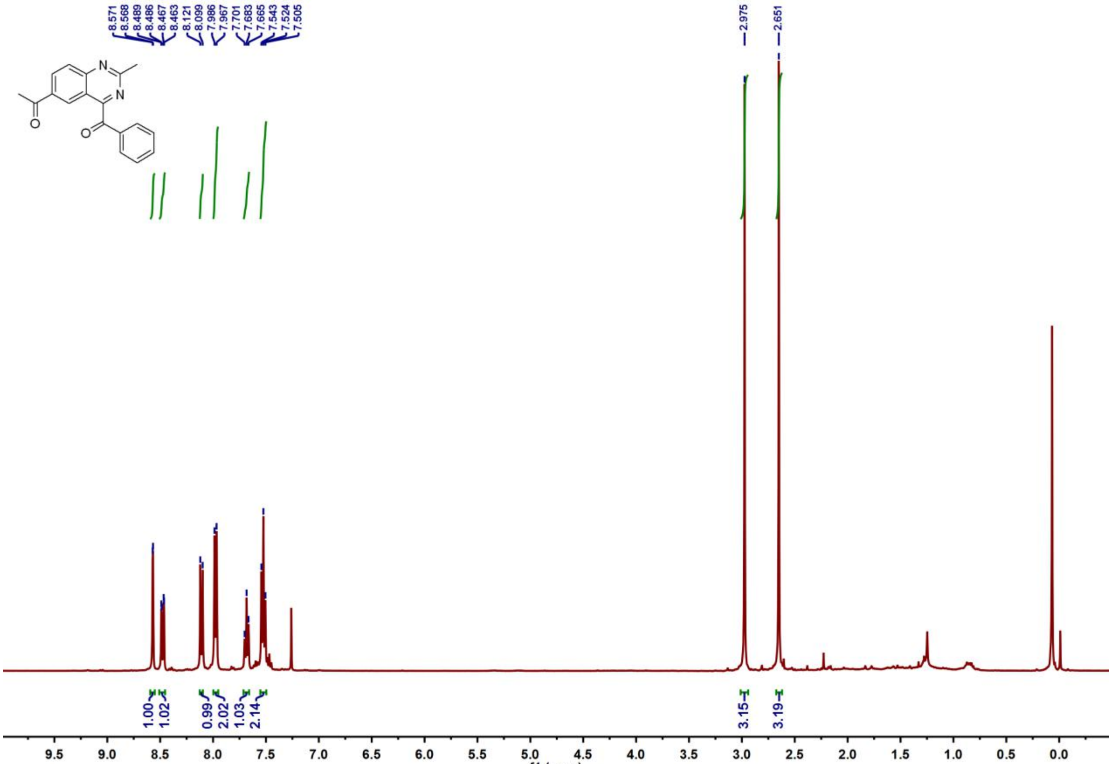


Figure S89. The [13]C NMR (100 MHz, Chloroform-*d*) of **5h**

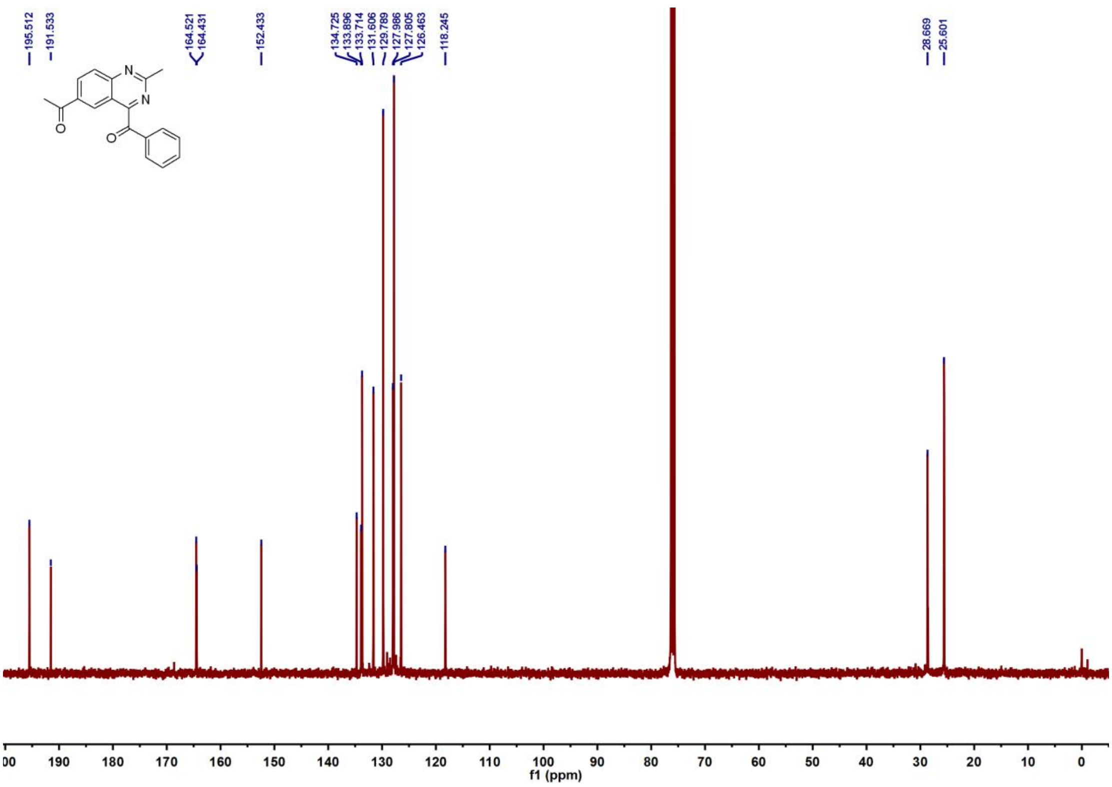


Figure S90. The ^{1}H NMR (400 MHz, Chloroform-*d*) of **5i**

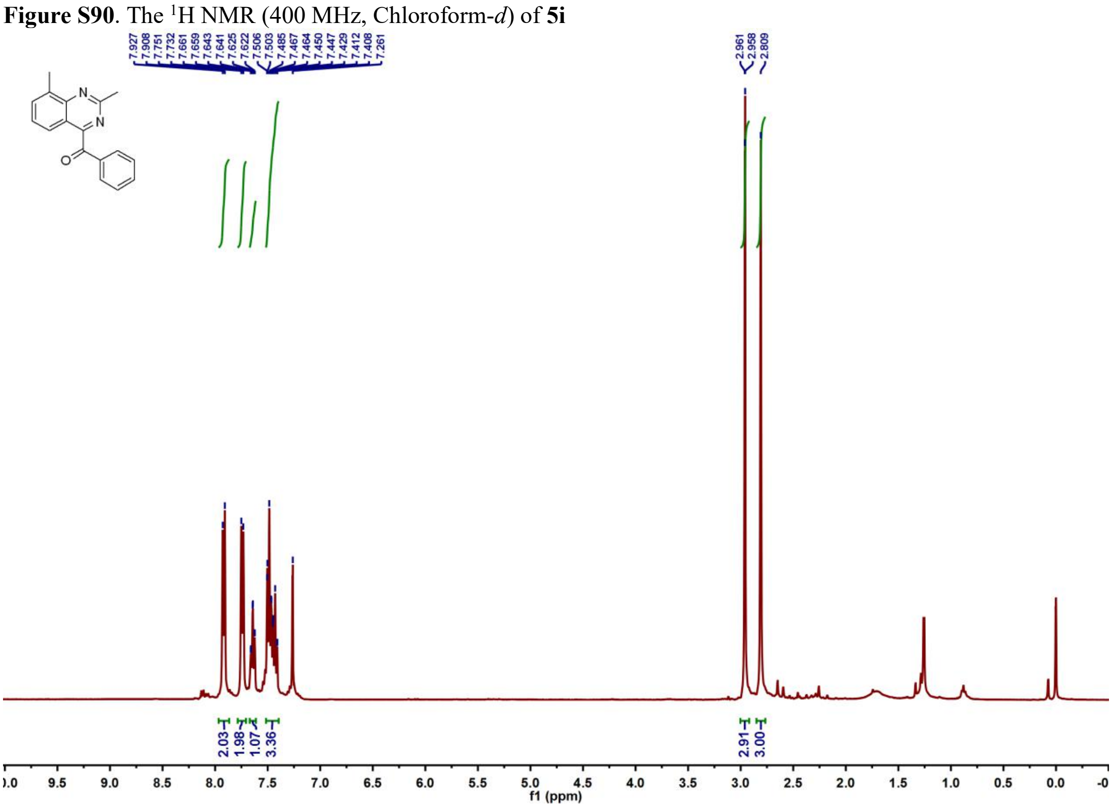


Figure S91. The ^{13}C NMR (100 MHz, Chloroform-*d*) of **5i**

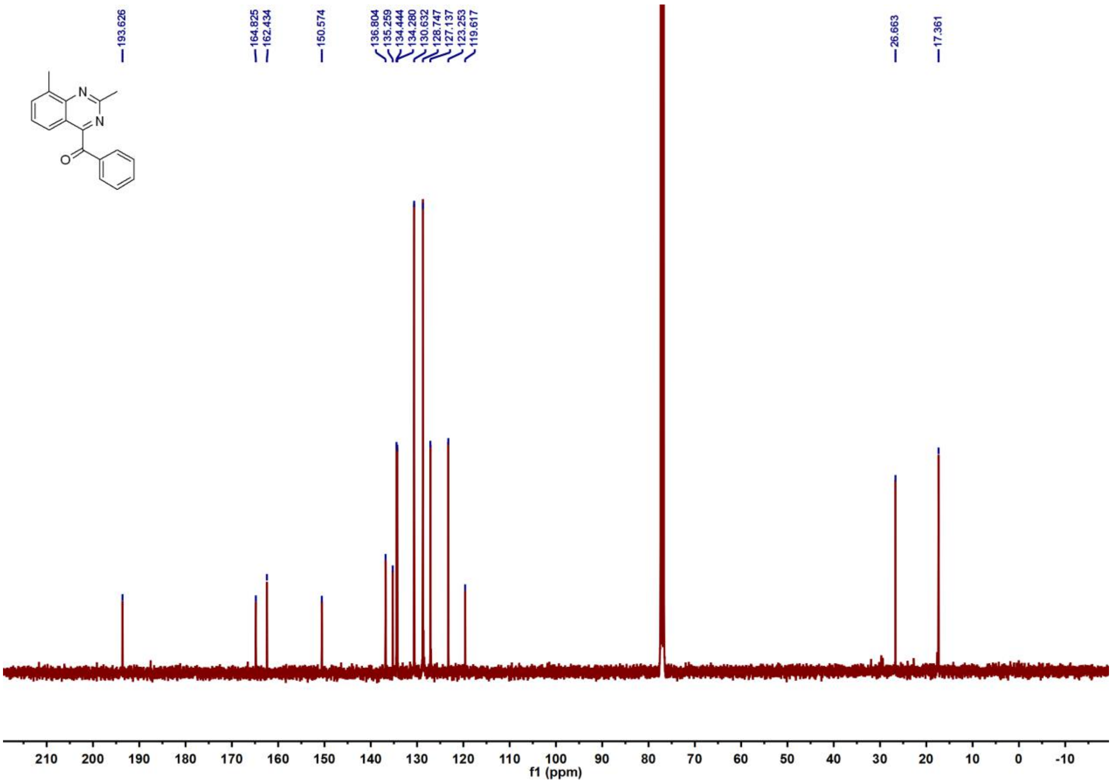


Figure S92. The ^{1}H NMR (400 MHz, Chloroform-*d*) of **5j**

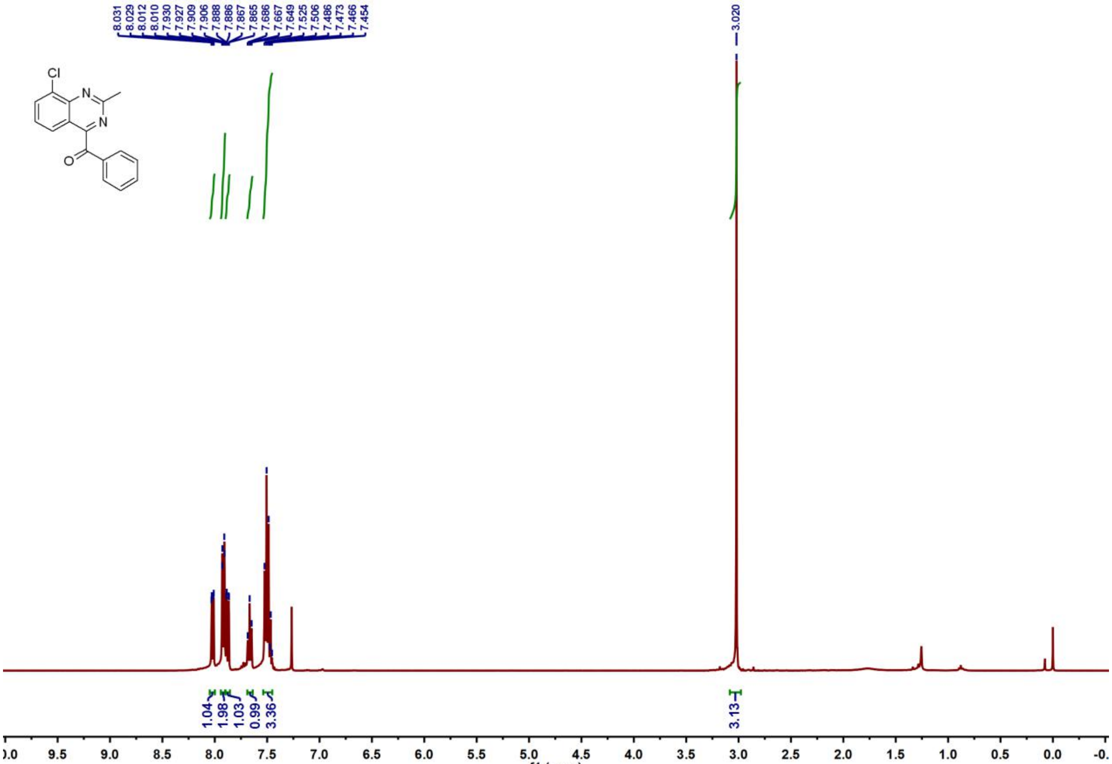


Figure S93. The ^{13}C NMR (100 MHz, Chloroform-*d*) of **5j**

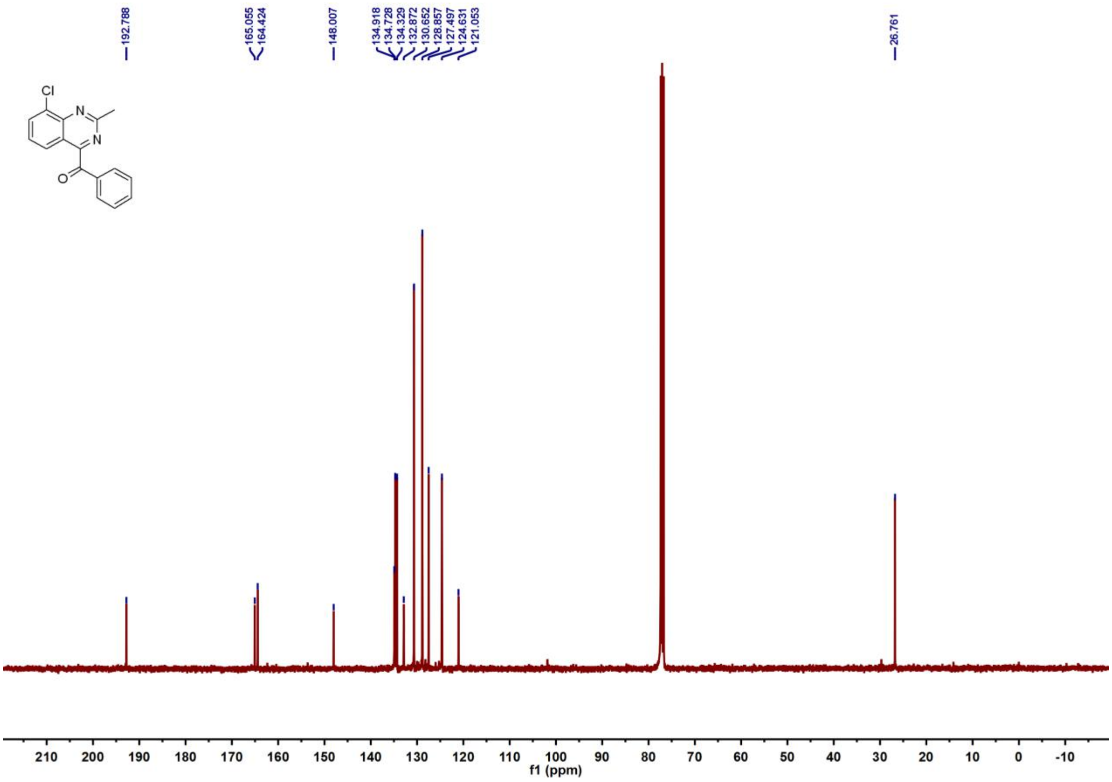


Figure S94. The [1]H NMR (400 MHz, Chloroform-*d*) of **5k**

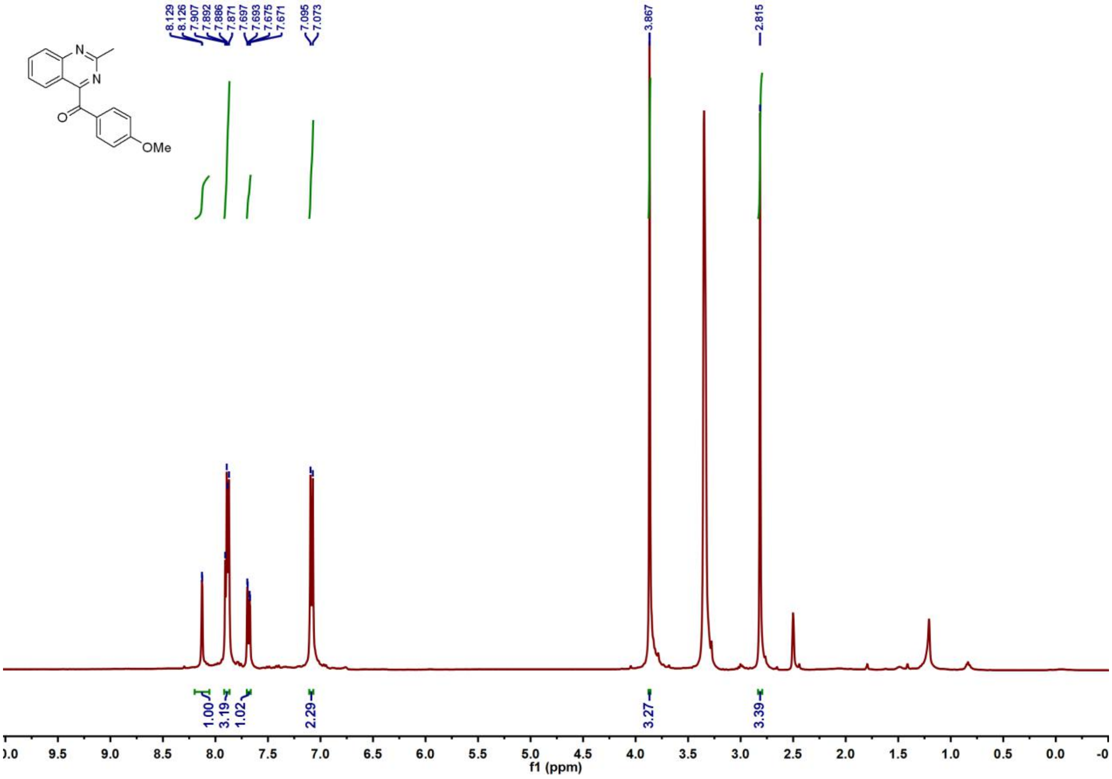


Figure S95. The [13]C NMR (100 MHz, Chloroform-*d*) of **5k**

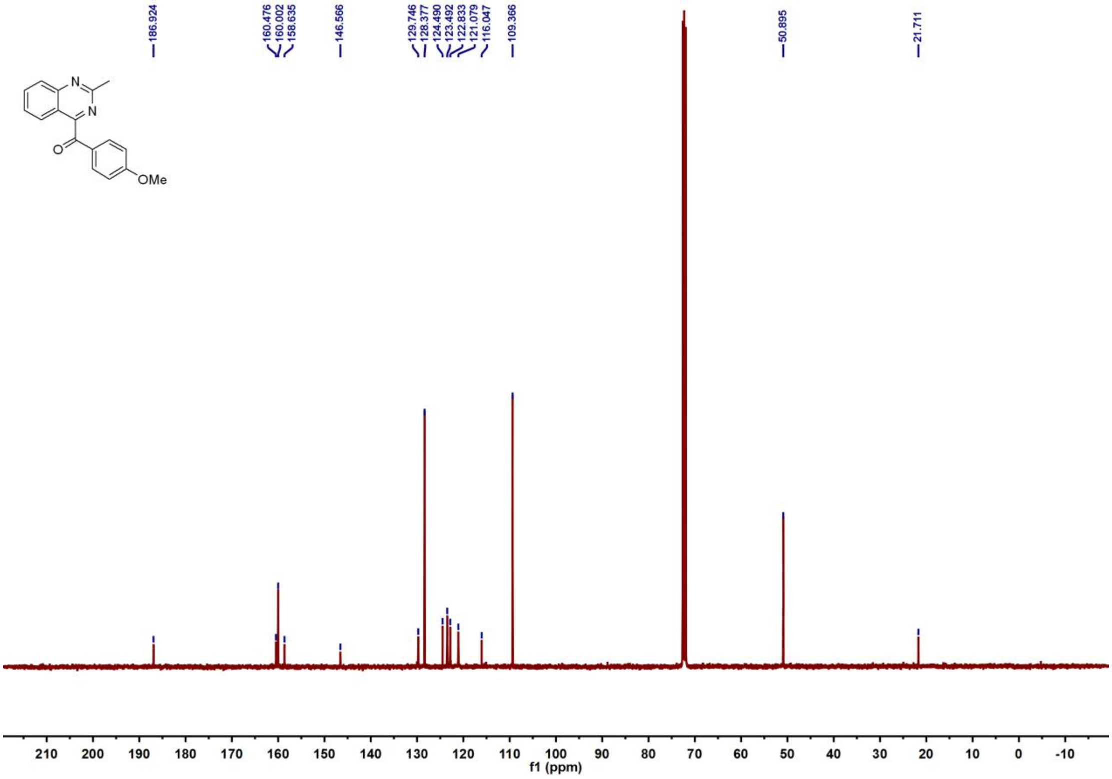


Figure S96. The [1]H NMR (400 MHz, Chloroform-*d*) of **5l**

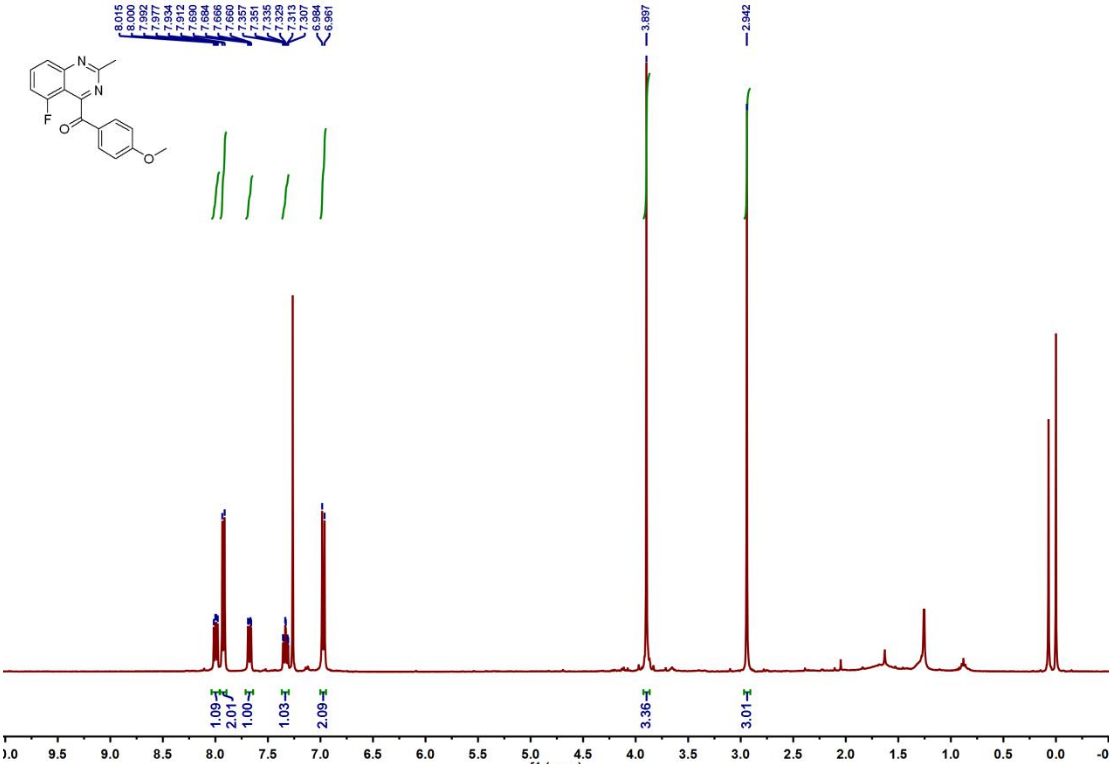


Figure S97. The [13]C NMR (100 MHz, Chloroform-*d*) of **5l**

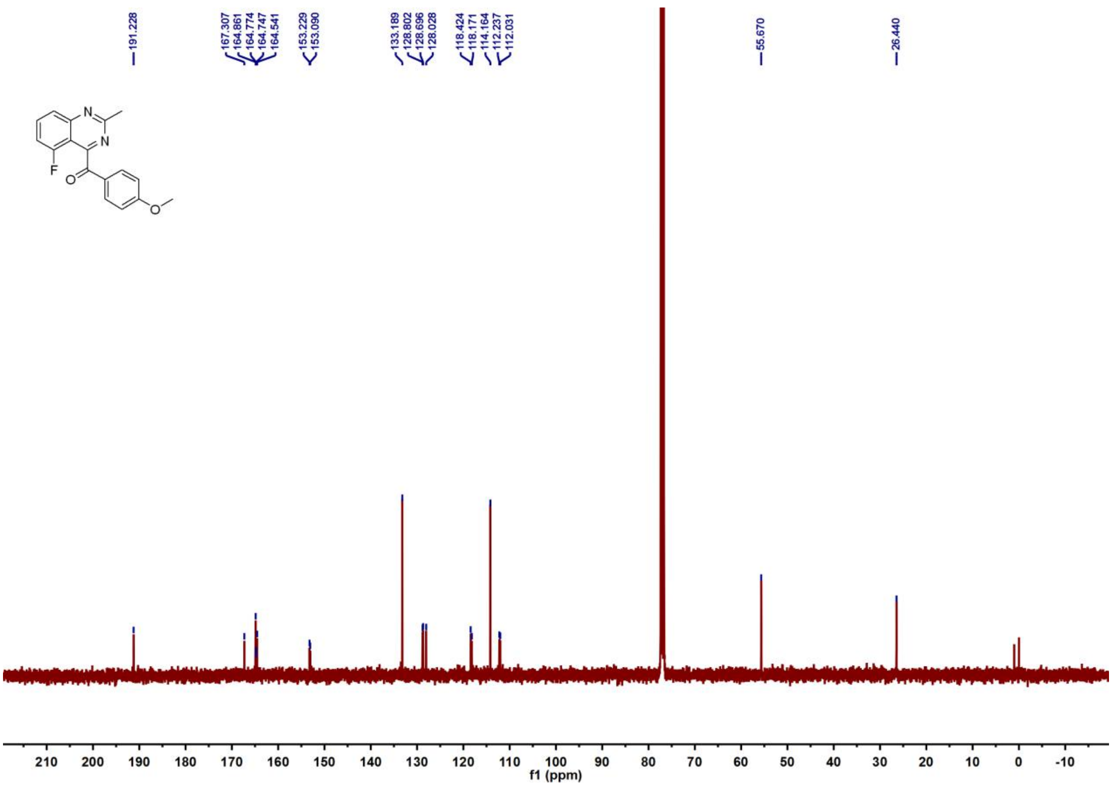


Figure S98. The ^{19}F NMR (376 MHz, Chloroform-*d*) of **5l**

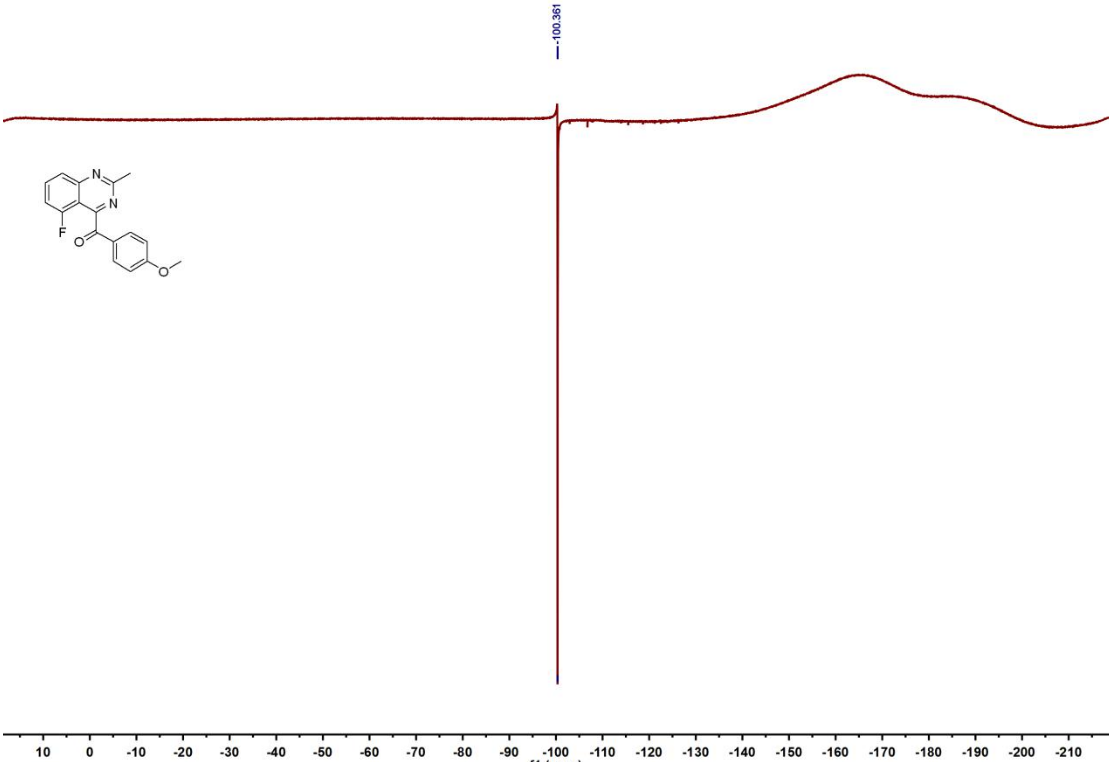


Figure S99. The ^{1}H NMR (400 MHz, Chloroform-*d*) of **5m**

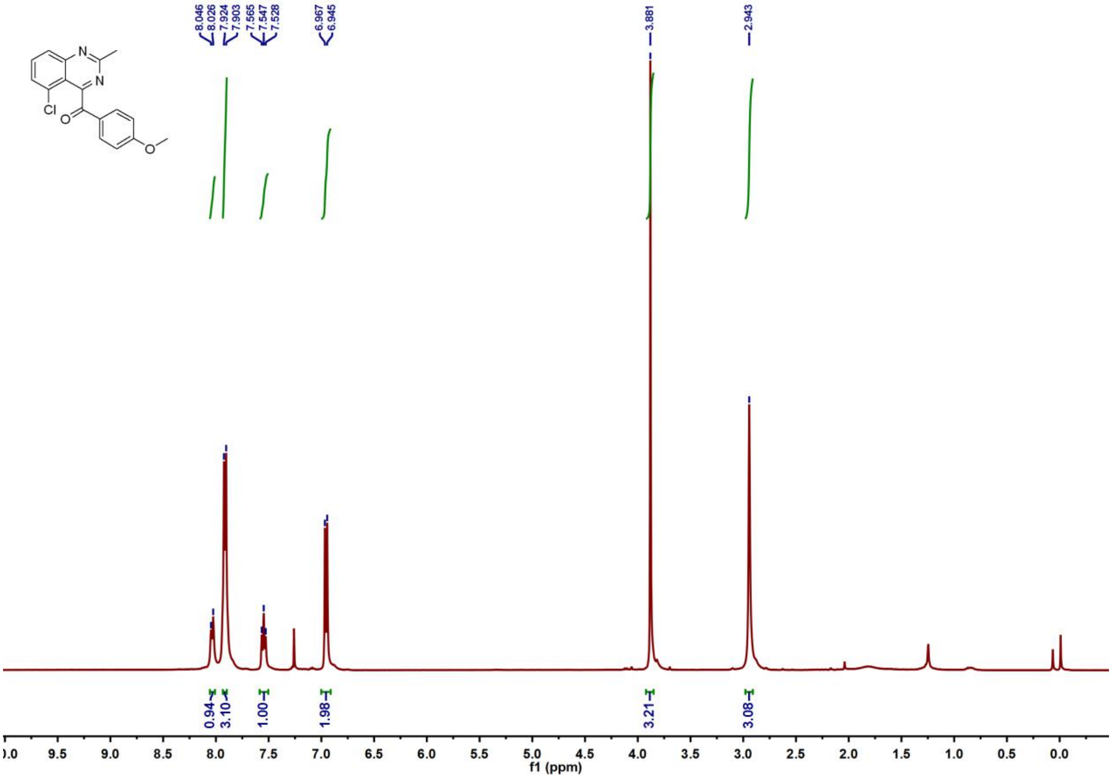


Figure S100. The [13]C NMR (100 MHz, Chloroform-*d*) of **5m**

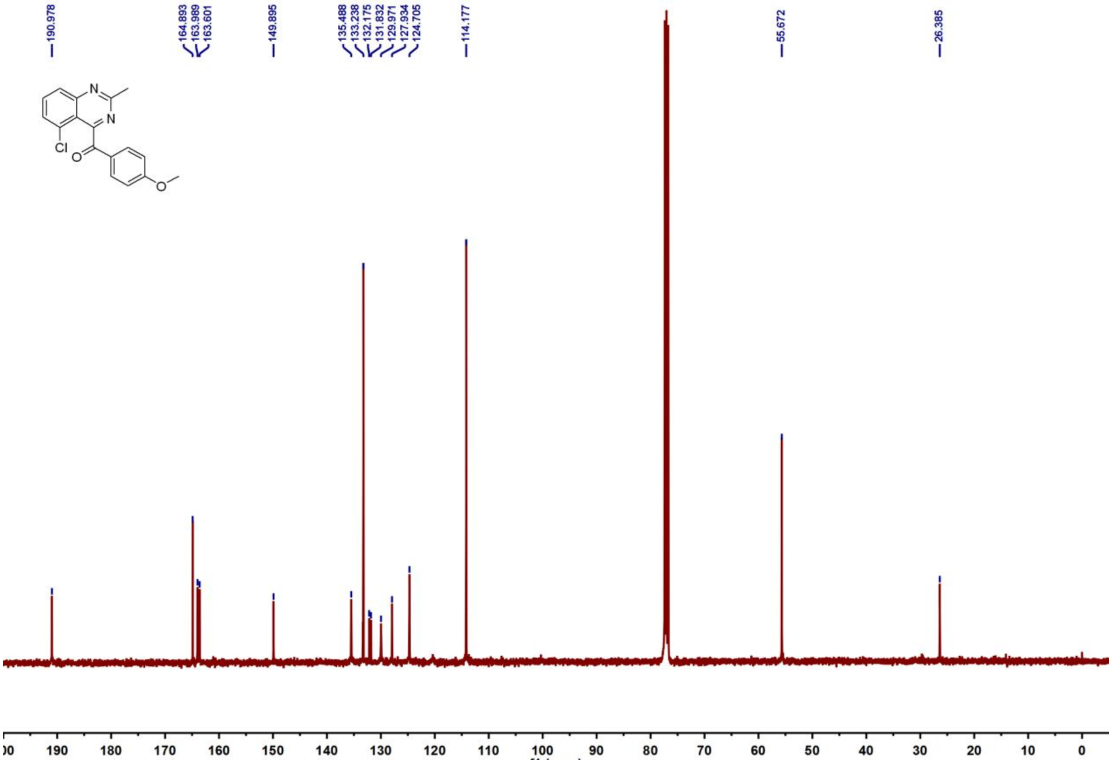


Figure S101. The [1]H NMR (400 MHz, Chloroform-*d*) of **5n**

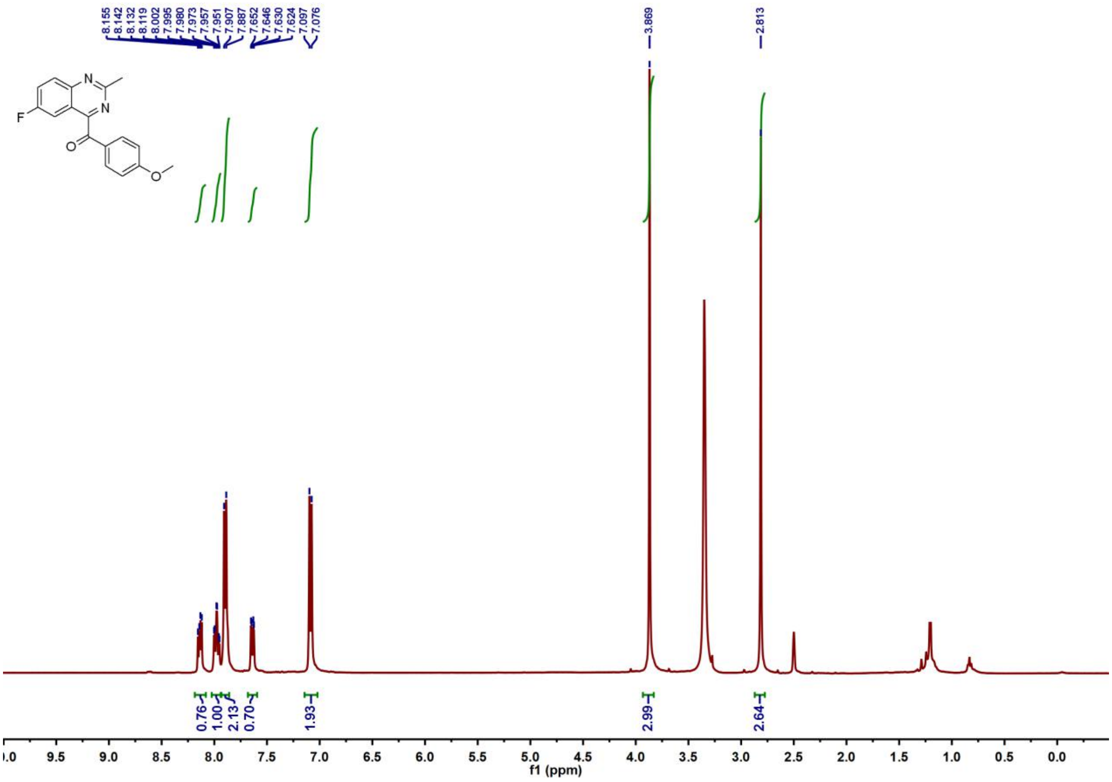


Figure S102. The [13]C NMR (100 MHz, Chloroform-*d*) of **5n**

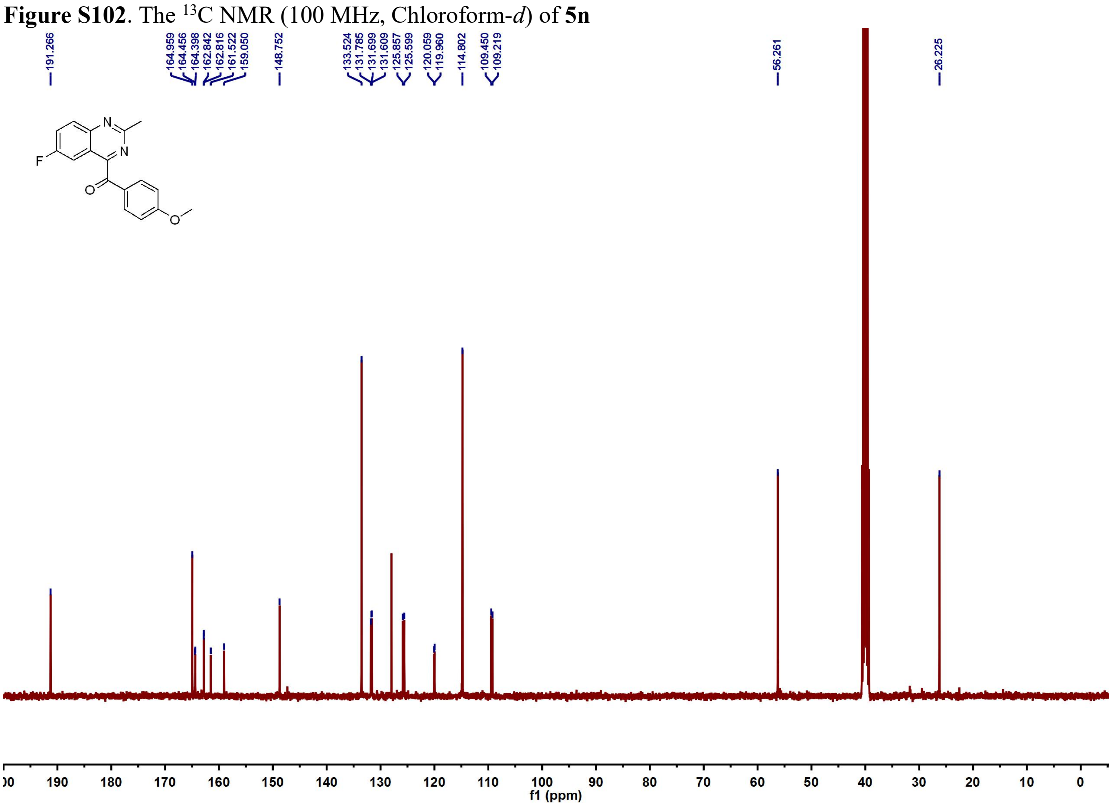


Figure S103. The [19]F NMR (376 MHz, Chloroform-*d*) of **5n**

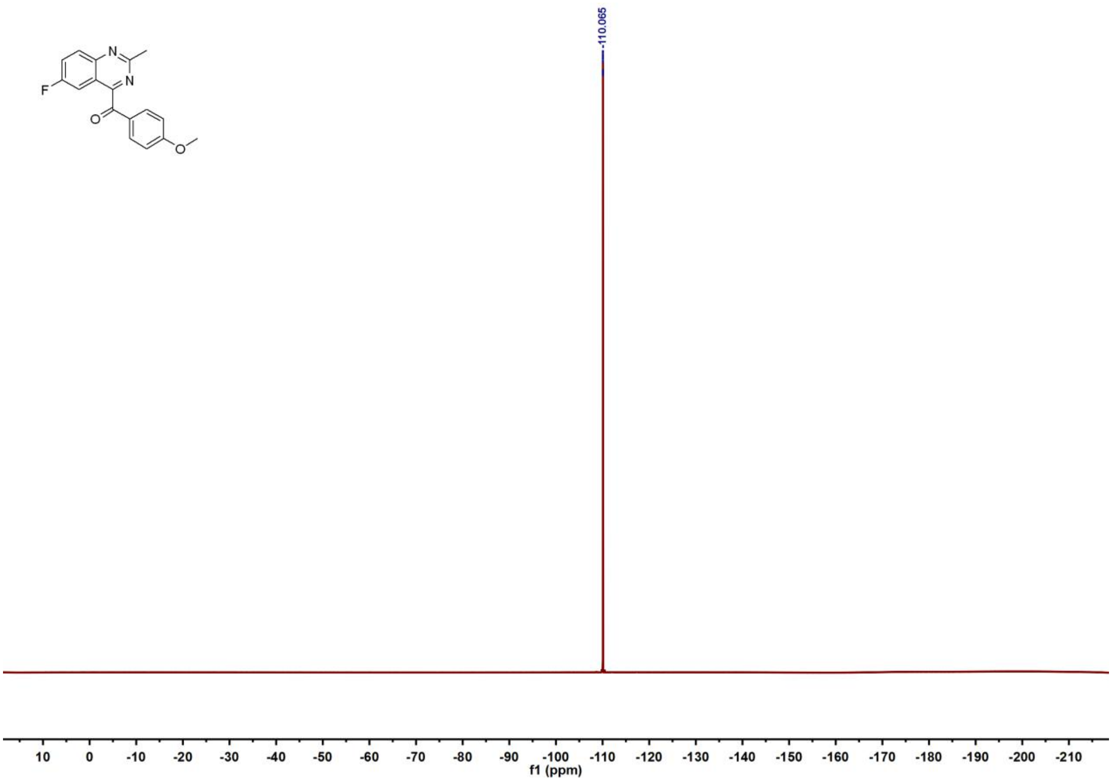


Figure S104. The [1]H NMR (400 MHz, Chloroform-*d*) of **5o**

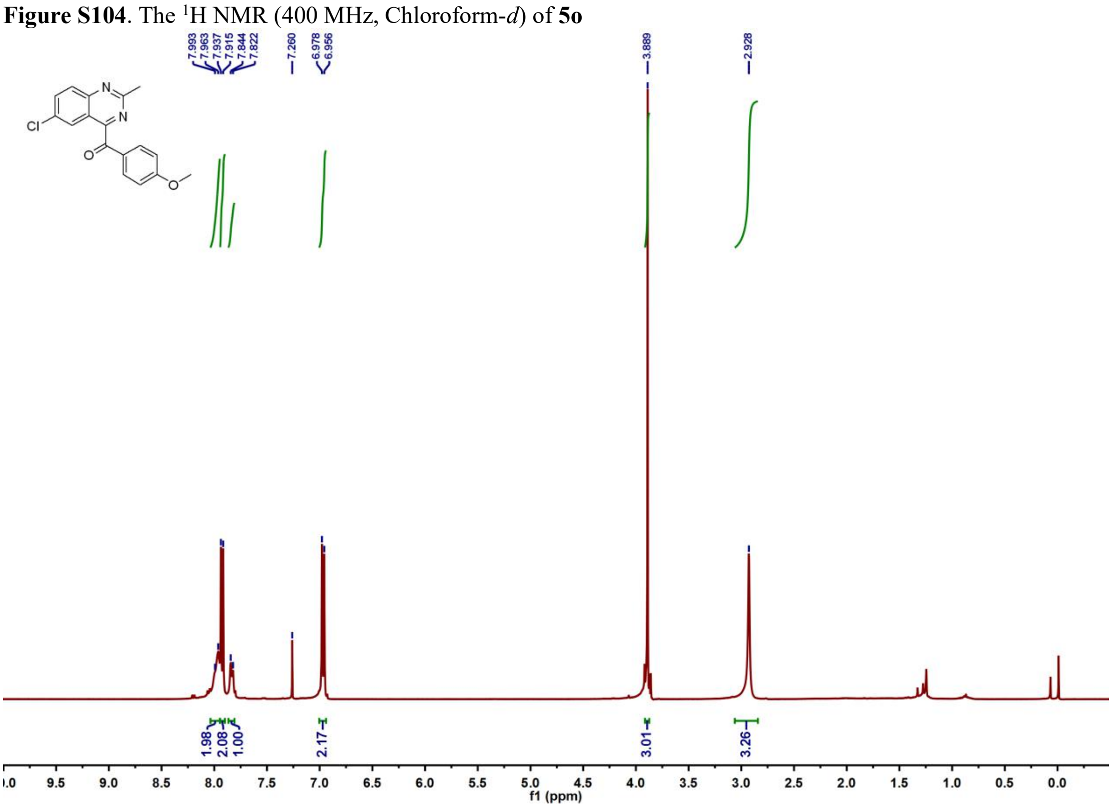


Figure S105. The [13]C NMR (100 MHz, Chloroform-*d*) of **5o**

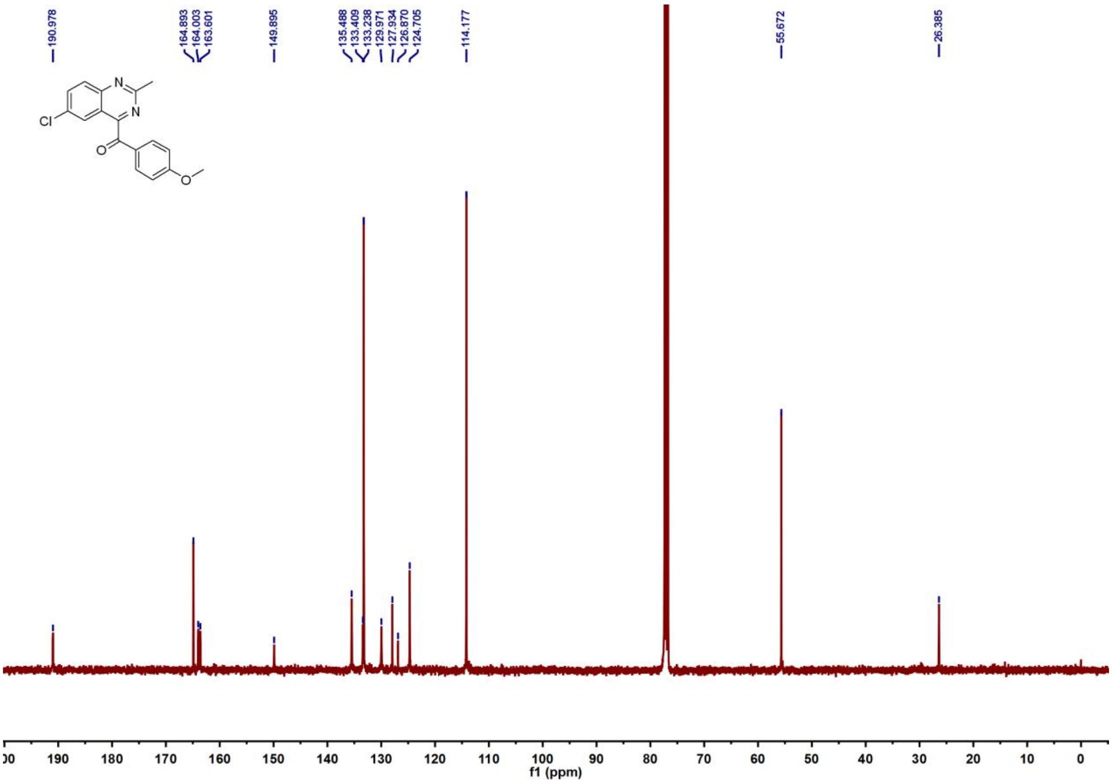


Figure S106. The [1]H NMR (400 MHz, Chloroform-*d*) of **5p**

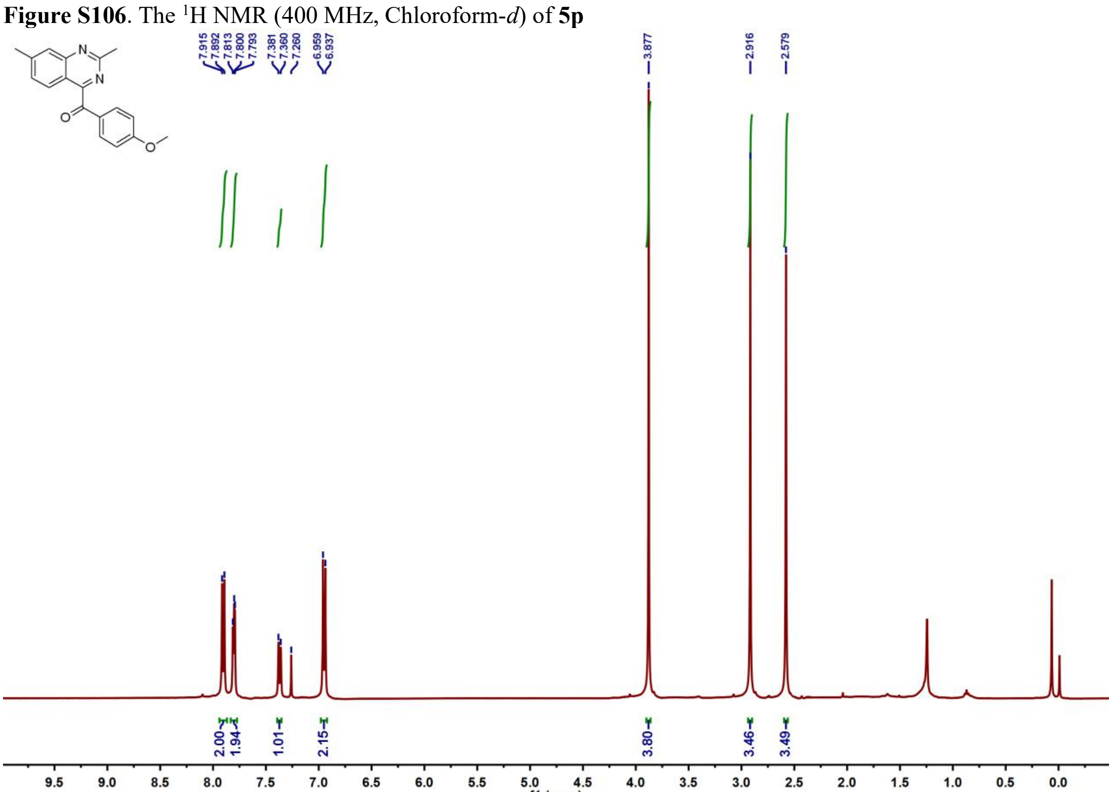


Figure S107. The [13]C NMR (100 MHz, Chloroform-*d*) of **5p**

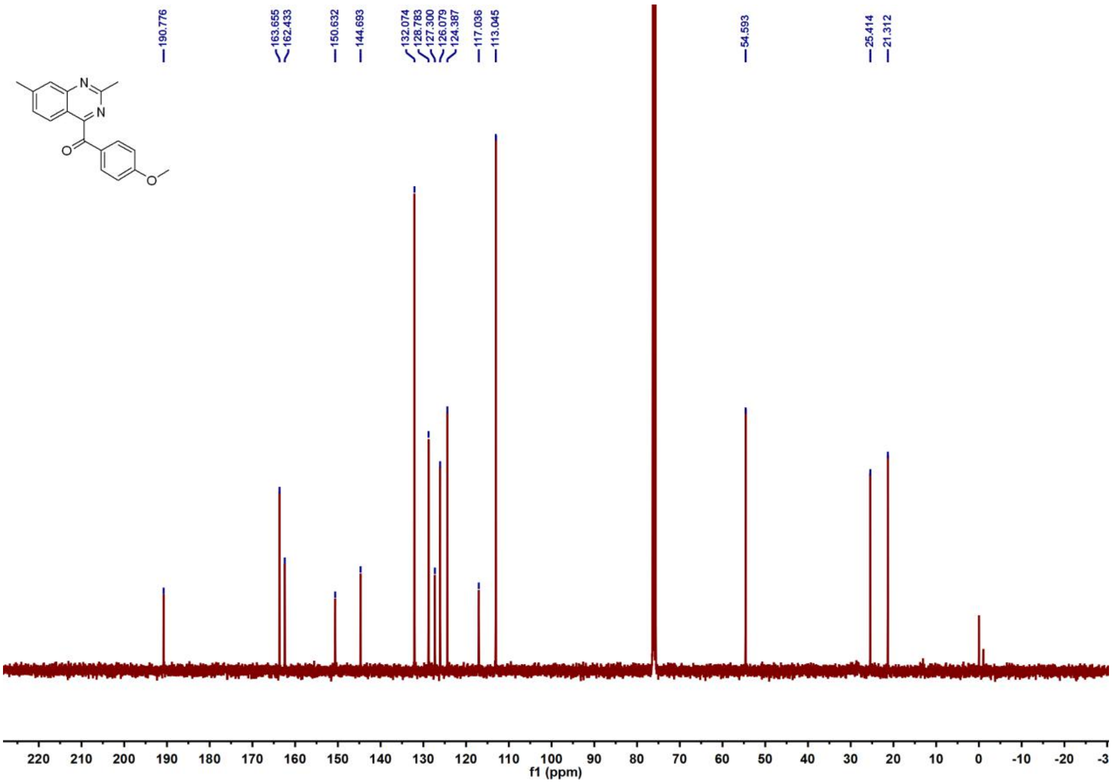


Figure S108. The [1]H NMR (400 MHz, Chloroform-*d*) of **5q**

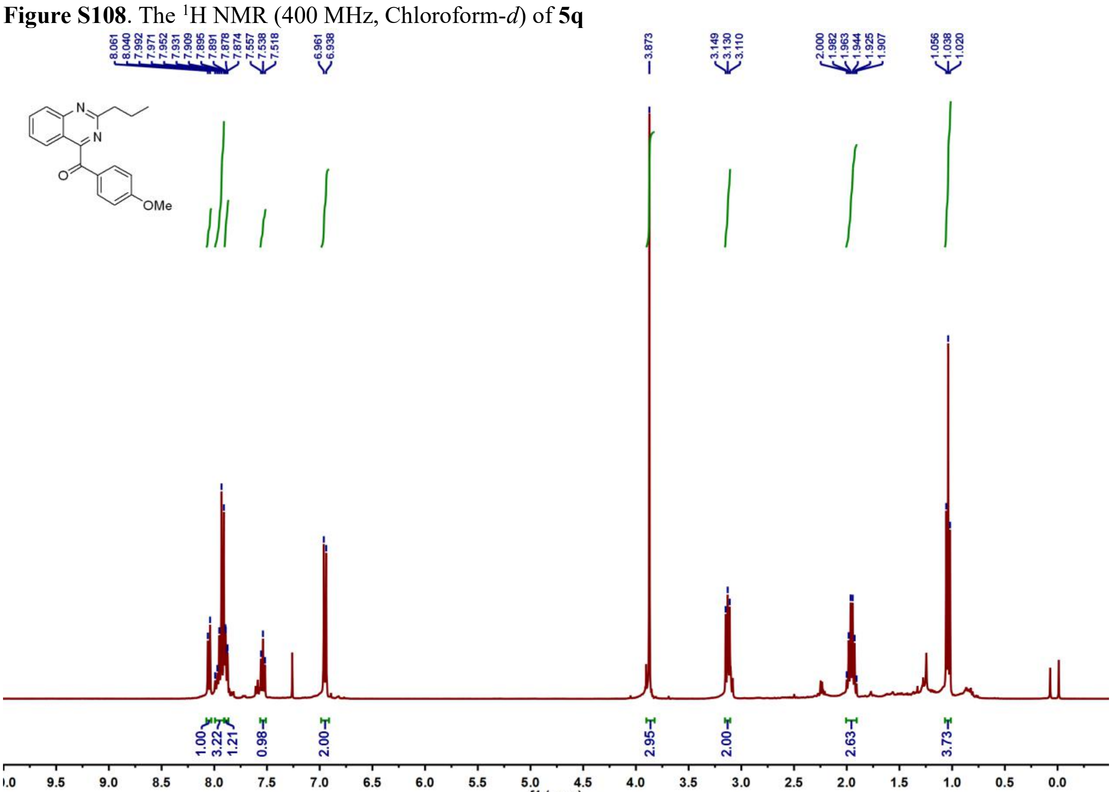


Figure S109. The [13]C NMR (100 MHz, Chloroform-*d*) of **5q**

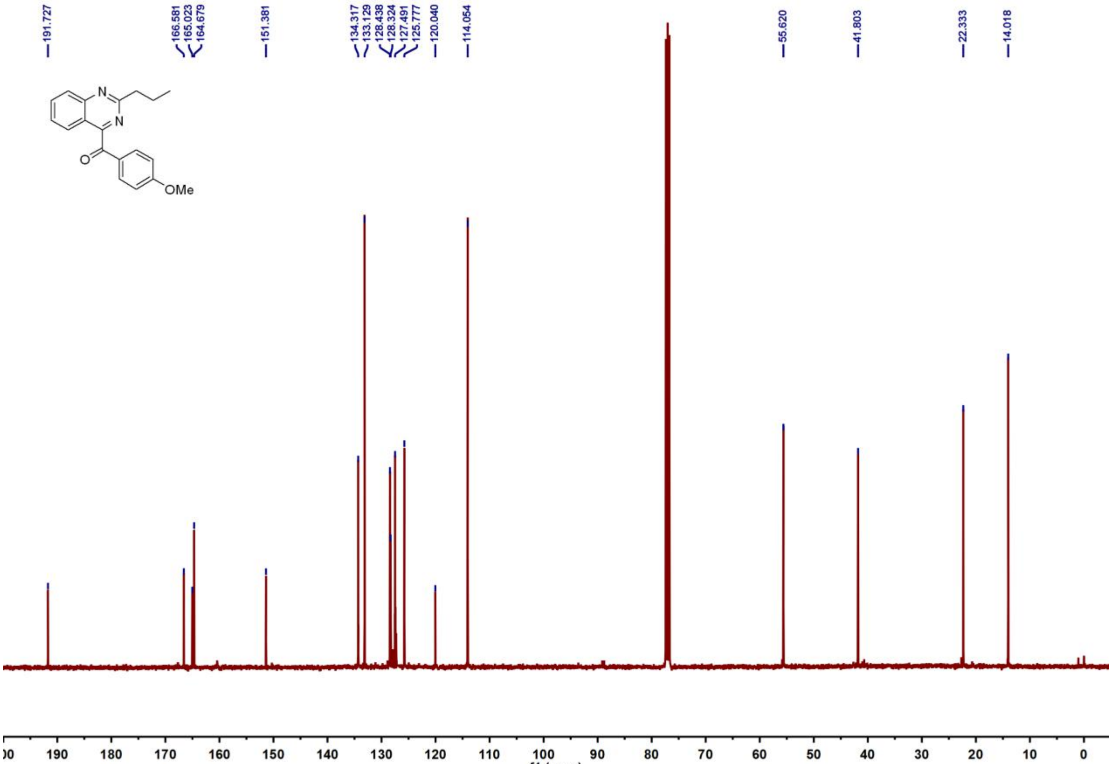


Figure S110. The [1]H NMR (400 MHz, Chloroform-*d*) of **5r**

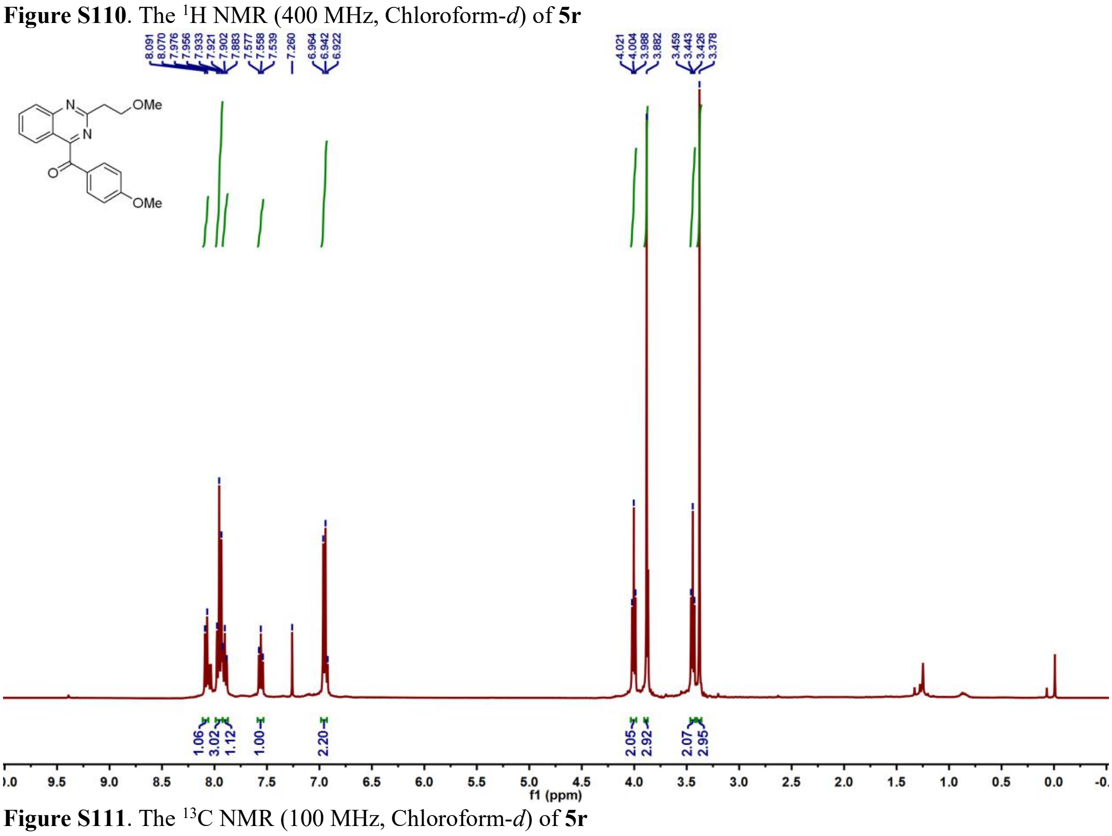


Figure S111. The [13]C NMR (100 MHz, Chloroform-*d*) of **5r**

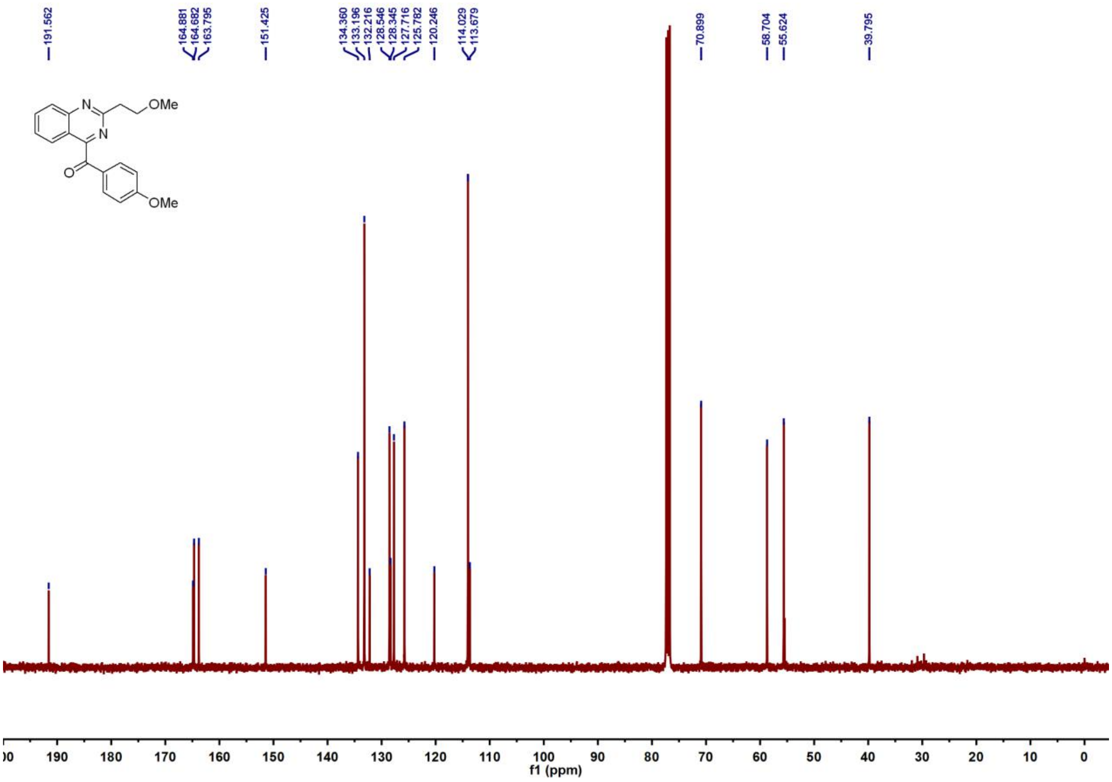


Figure S112. The [1]H NMR (400 MHz, Chloroform-*d*) of **6a**

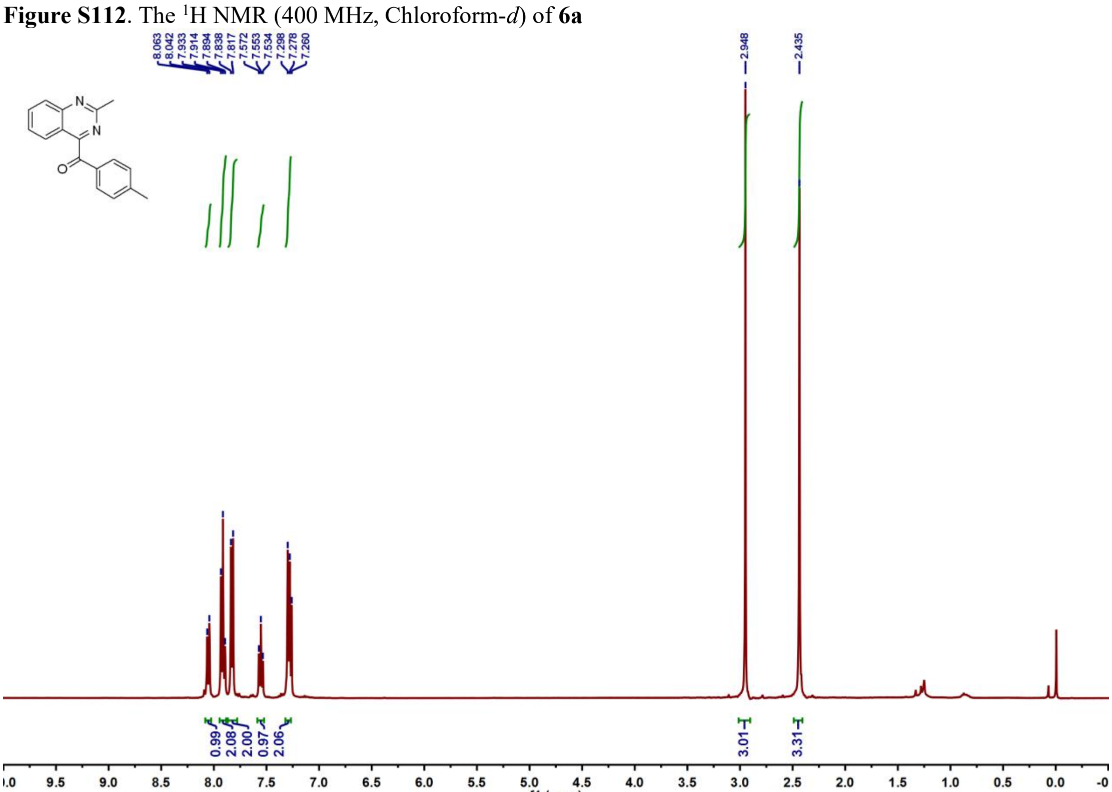


Figure S113. The [13]C NMR (100 MHz, Chloroform-*d*) of **6a**

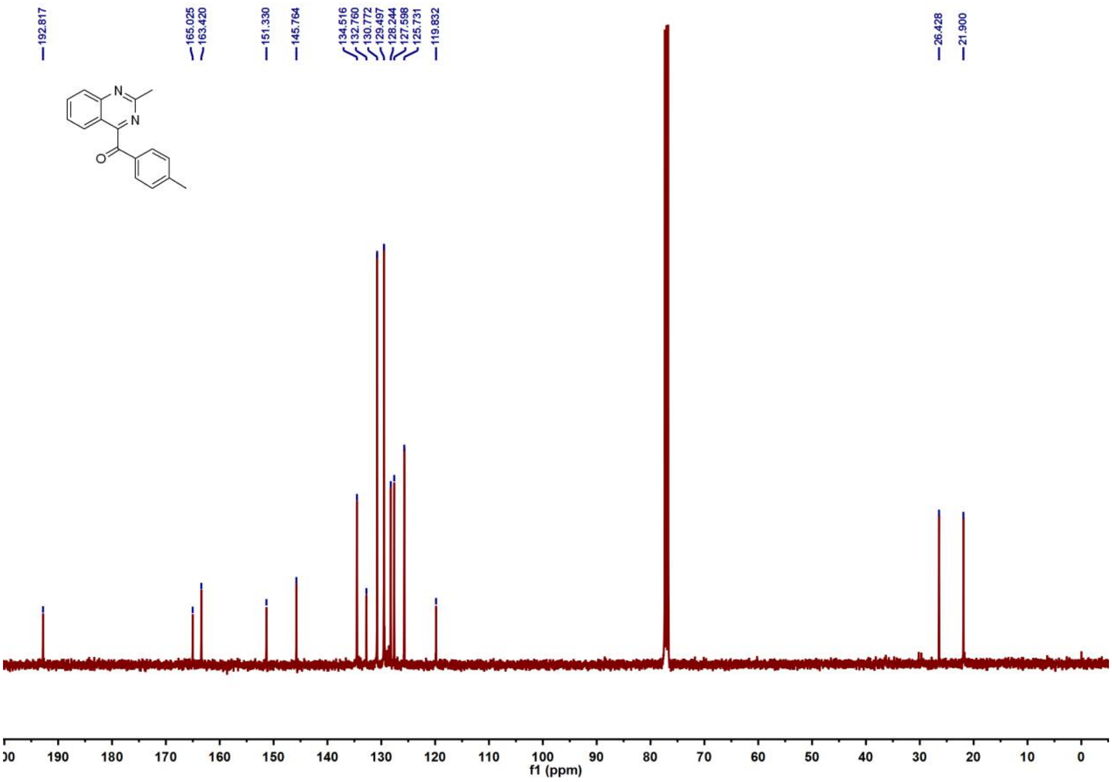


Figure S114. The [1]H NMR (400 MHz, Chloroform-*d*) of **6b**

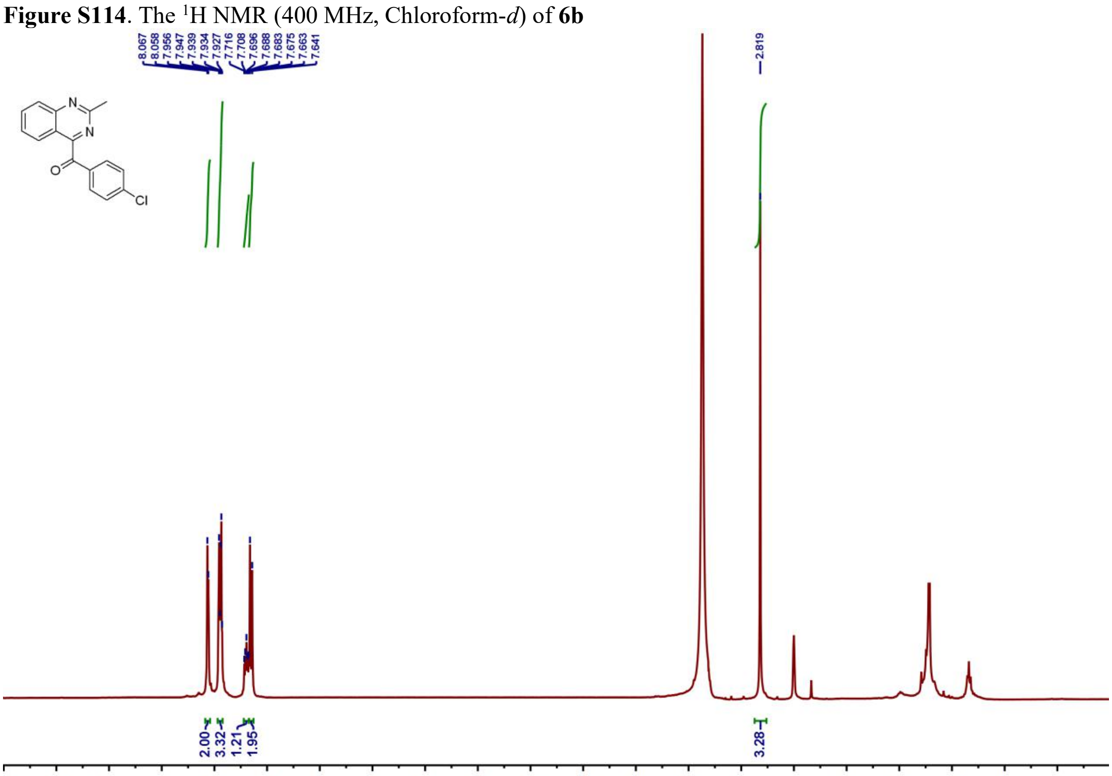


Figure S115. The [13]C NMR (100 MHz, Chloroform-*d*) of **6b**

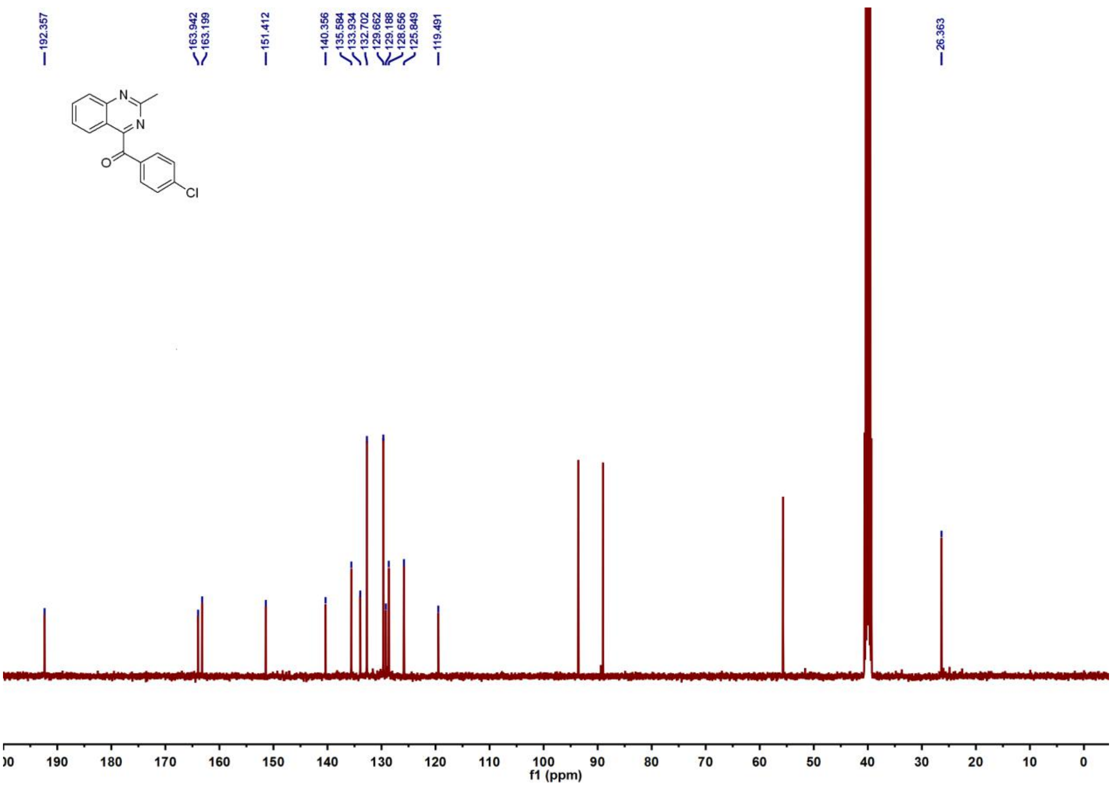


Figure S117. The ^{1}H NMR (400 MHz, Chloroform-*d*) of **6c**

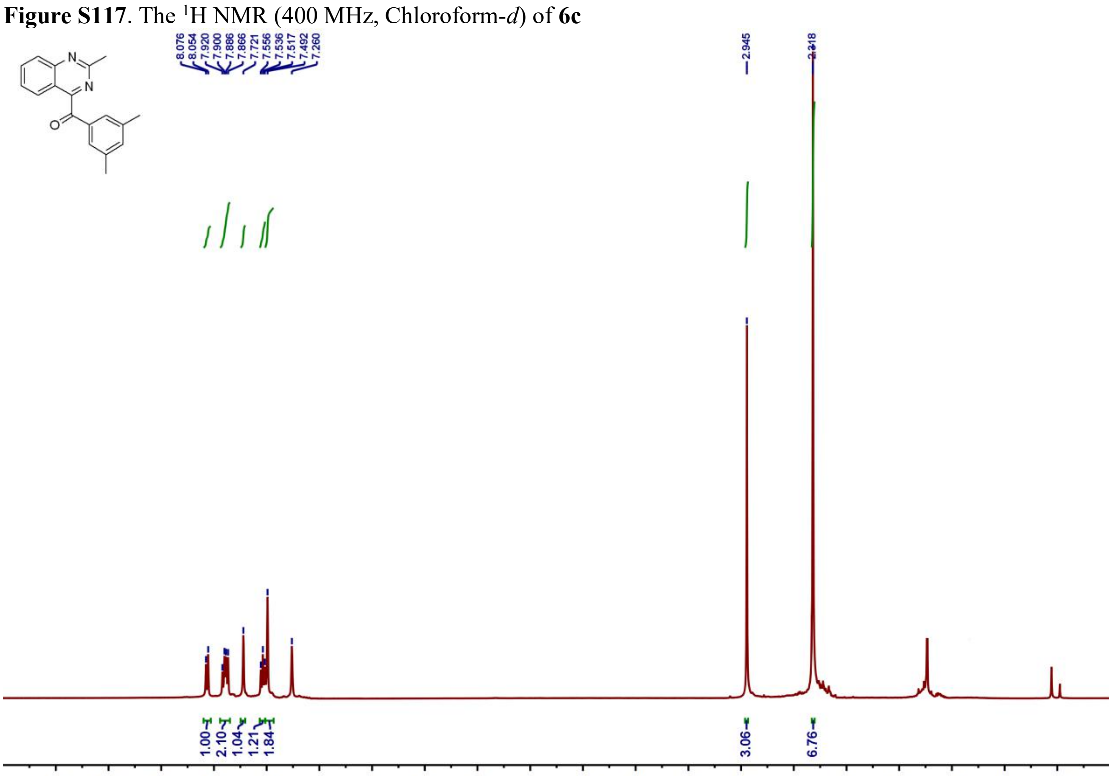


Figure S117. The ^{13}C NMR (100 MHz, Chloroform-*d*) of **6c**

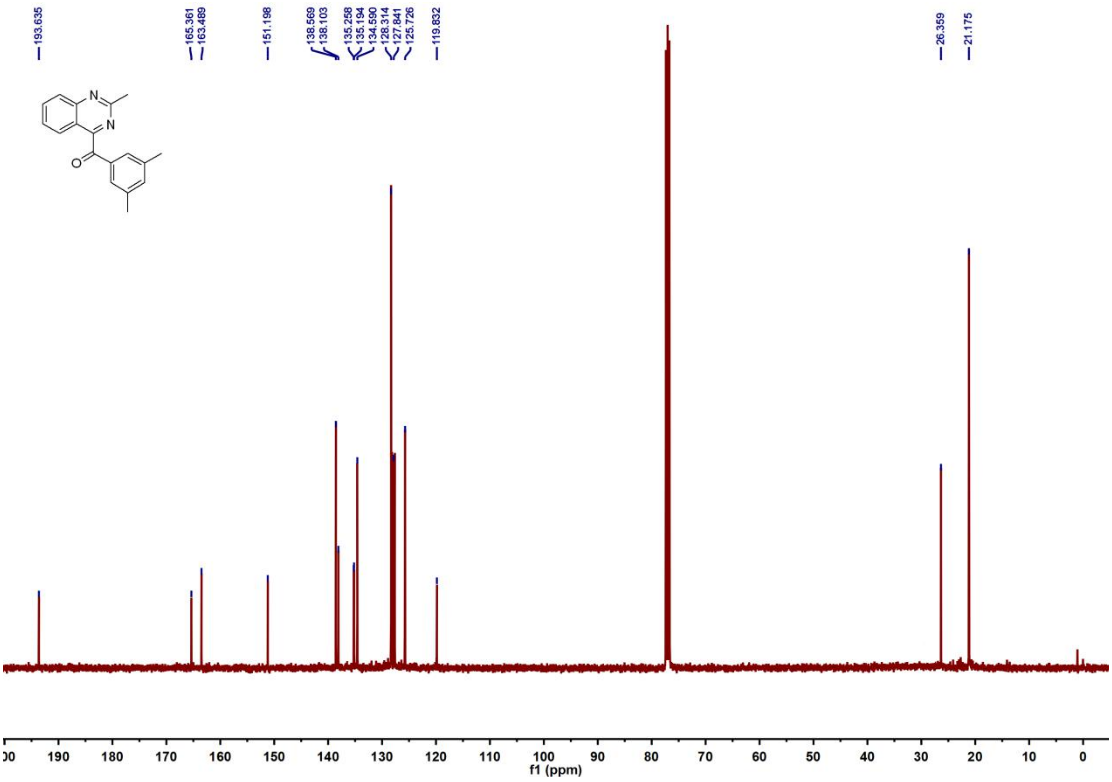


Figure S118. The ^{1}H NMR (400 MHz, Chloroform-*d*) of **6d**

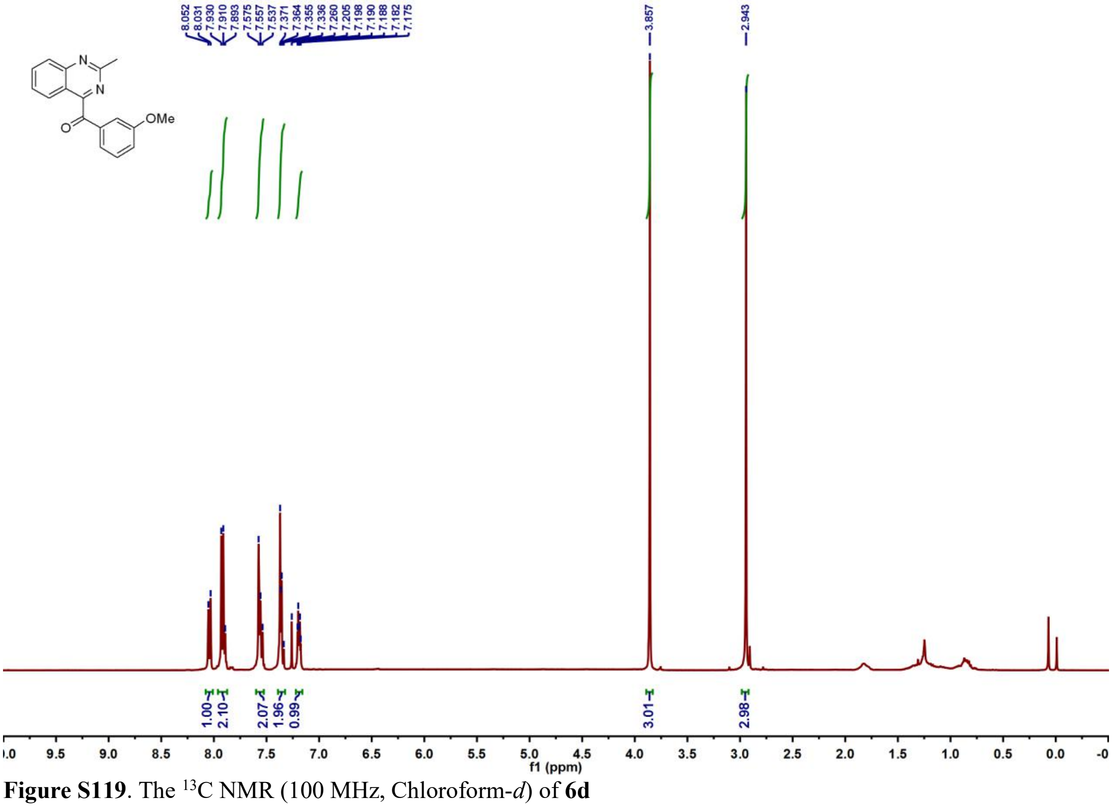


Figure S119. The ^{13}C NMR (100 MHz, Chloroform-*d*) of **6d**

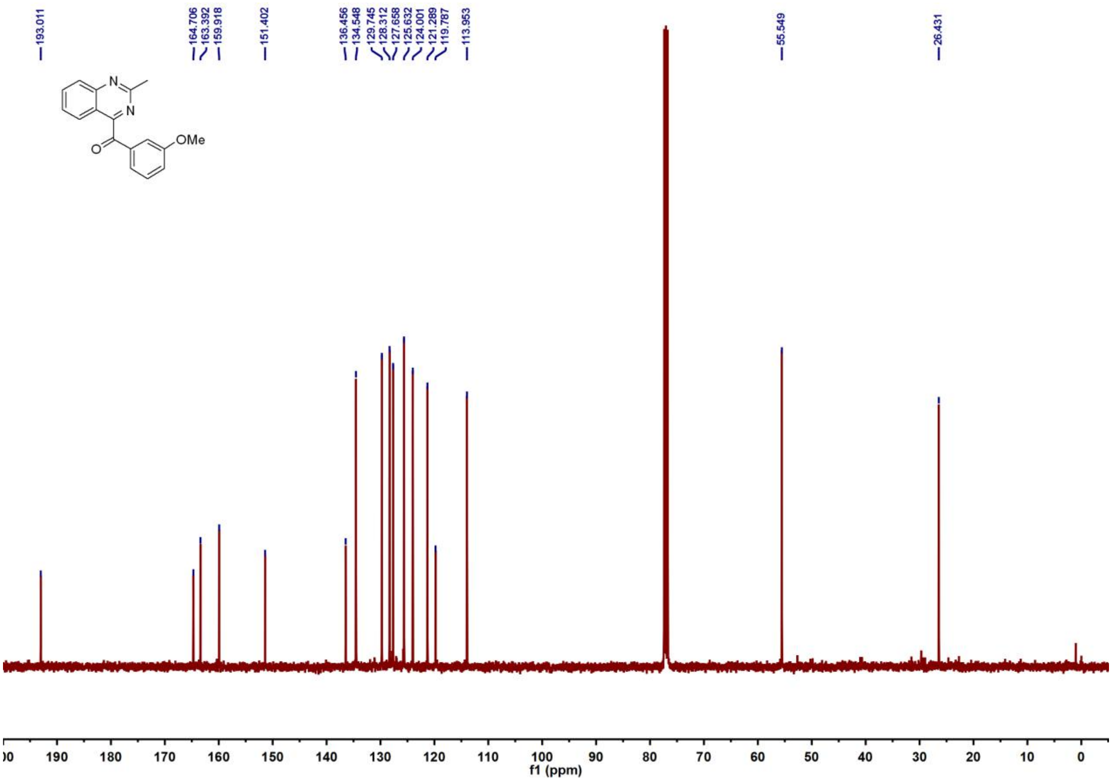


Figure S120. The ¹H NMR (400 MHz, Chloroform-*d*) of **6e**

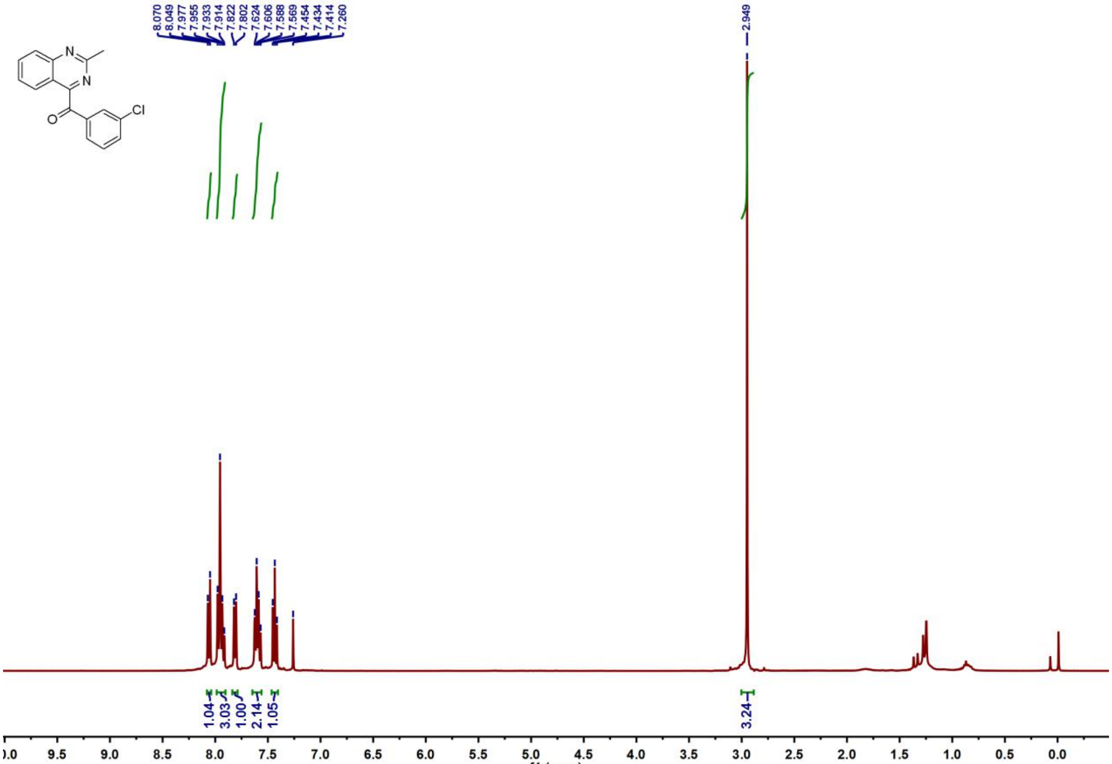


Figure S121. The ¹³C NMR (150 MHz, Chloroform-*d*) of **6e**

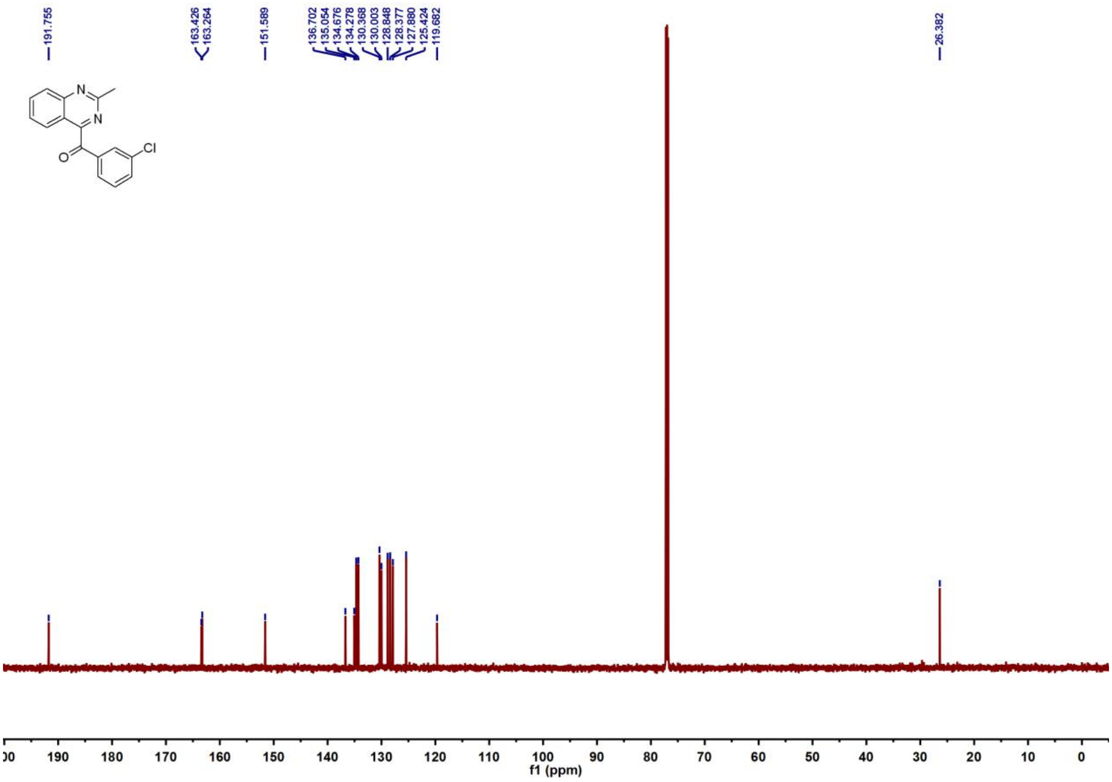


Figure S122. The [1]H NMR (400 MHz, Chloroform-*d*) of **6f**

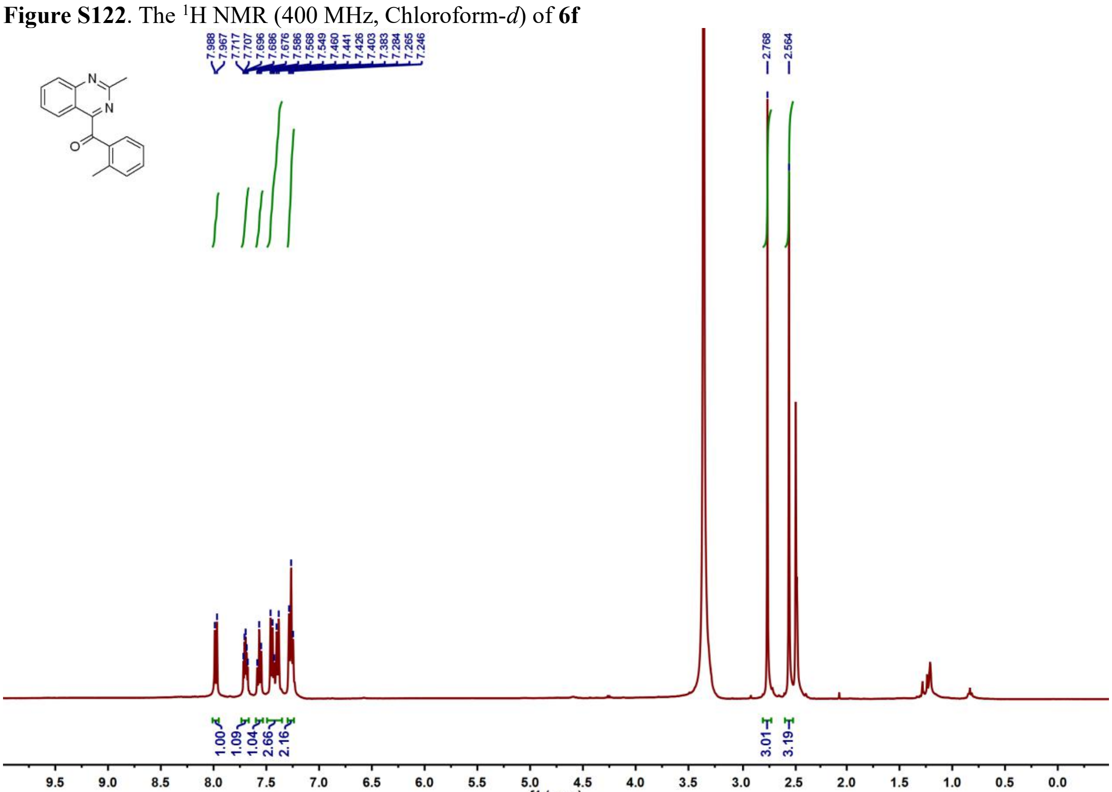


Figure S123. The [13]C NMR (150 MHz, Chloroform-*d*) of **6f**

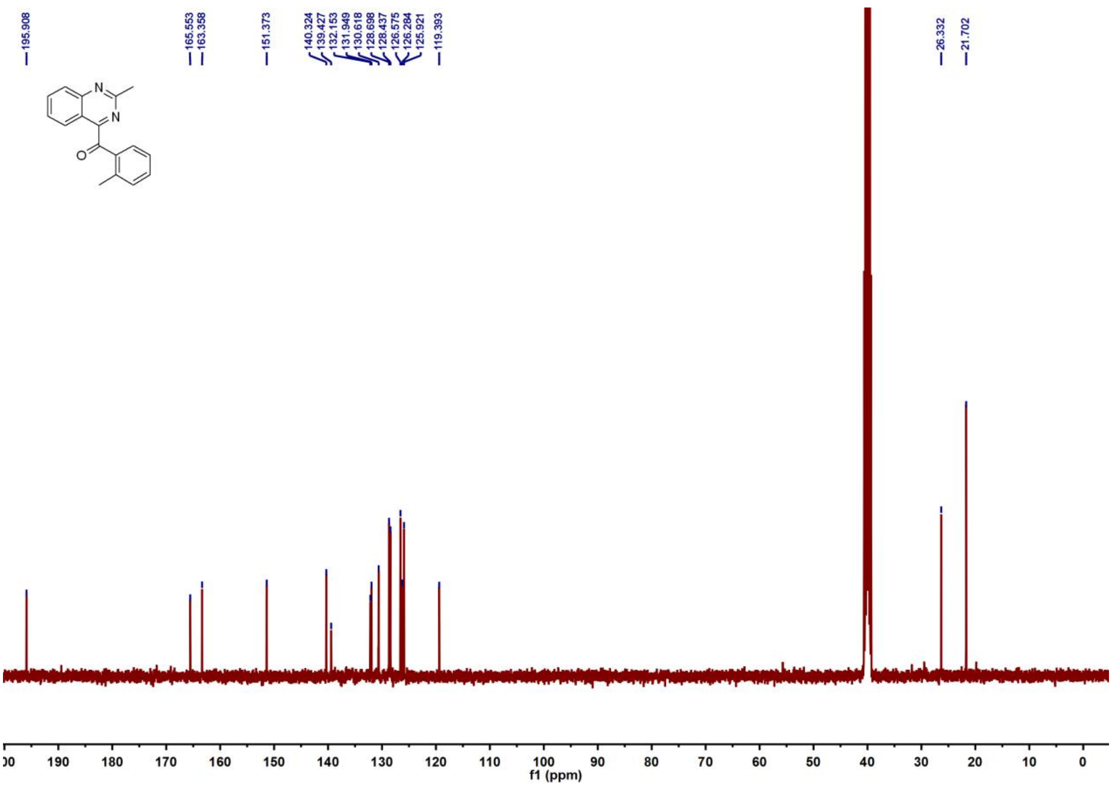


Figure S124. The ^{1}H NMR (400 MHz, Chloroform-*d*) of **6g**

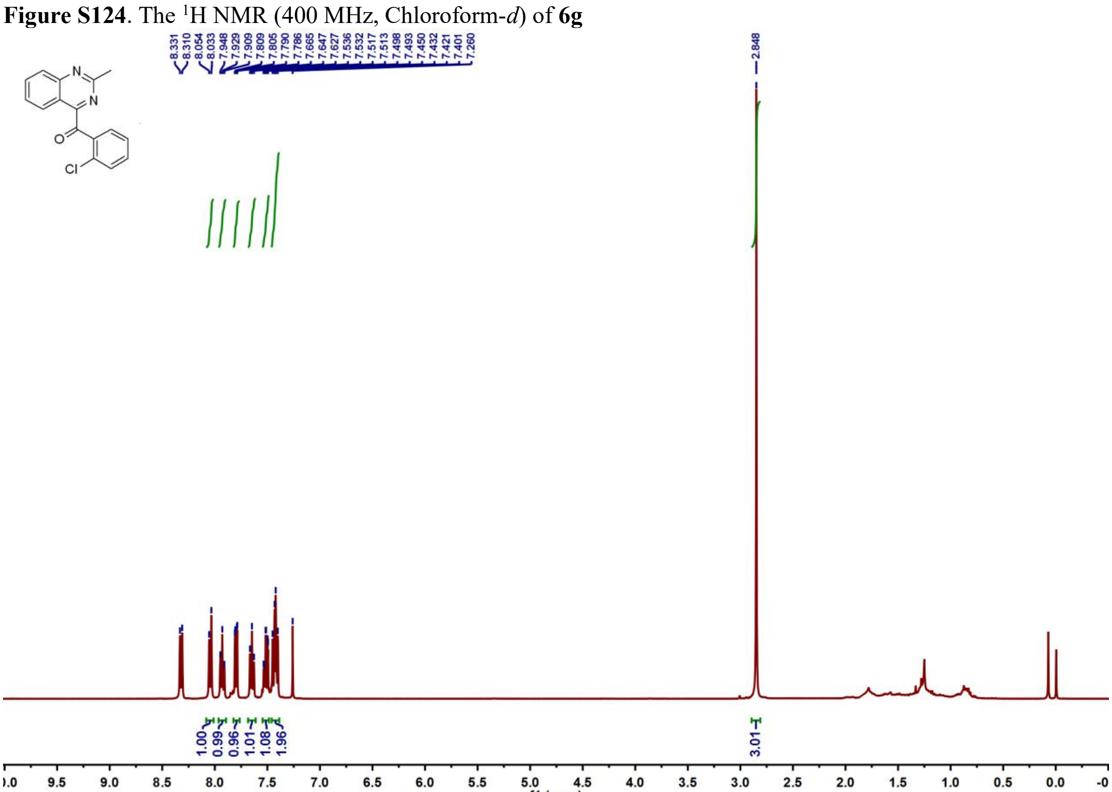


Figure S125. The ^{13}C NMR (100 MHz, Chloroform-*d*) of **6g**

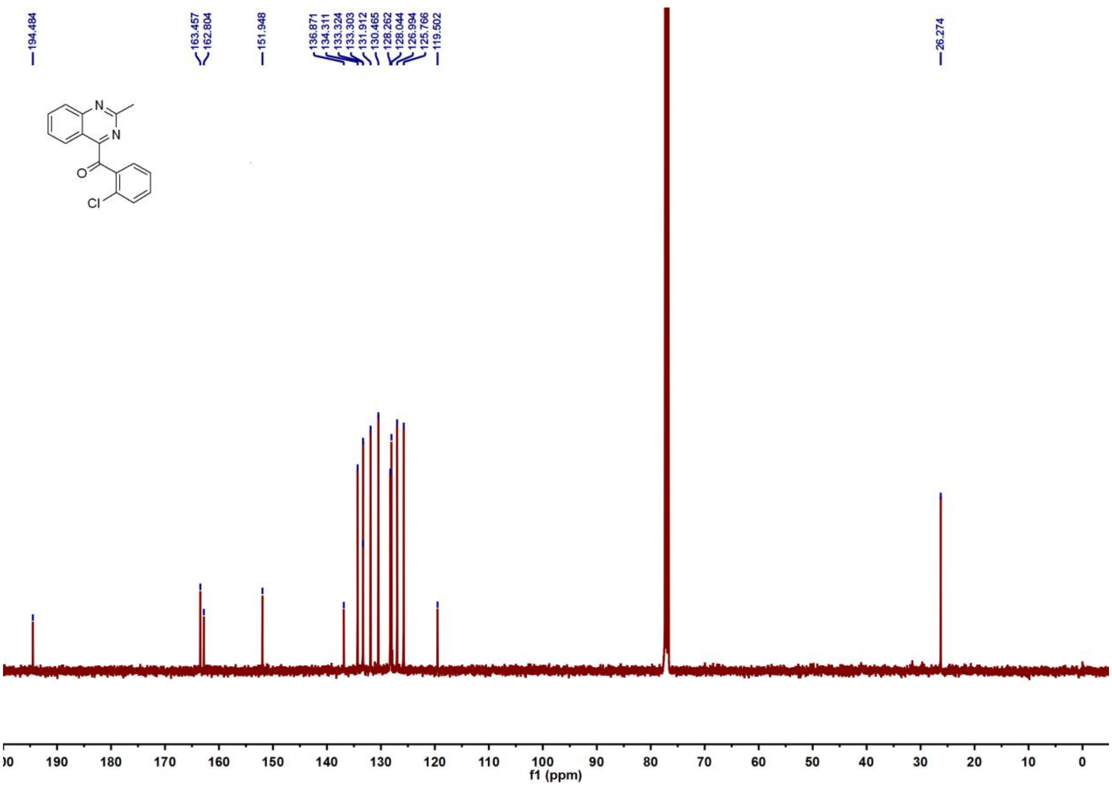


Figure S126. The [1]H NMR (400 MHz, DMSO-d_6) of **7**

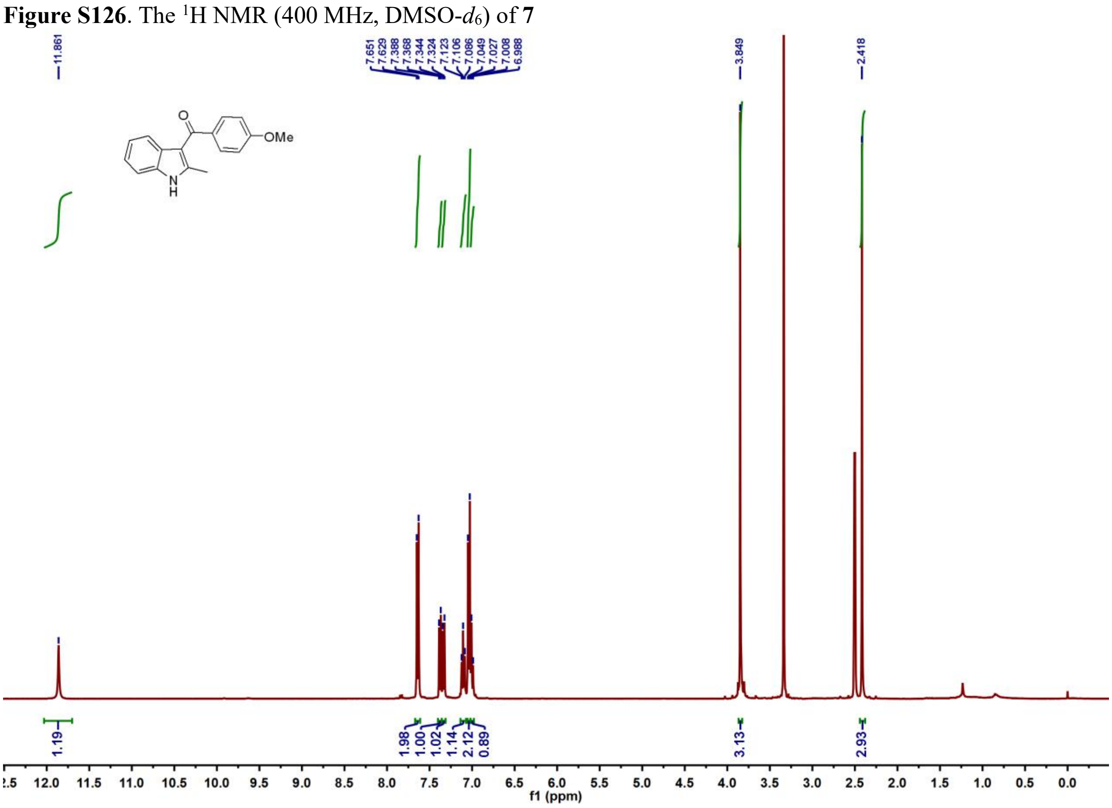


Figure S127. The [13]C NMR (100 MHz, DMSO-d_6) of **7**

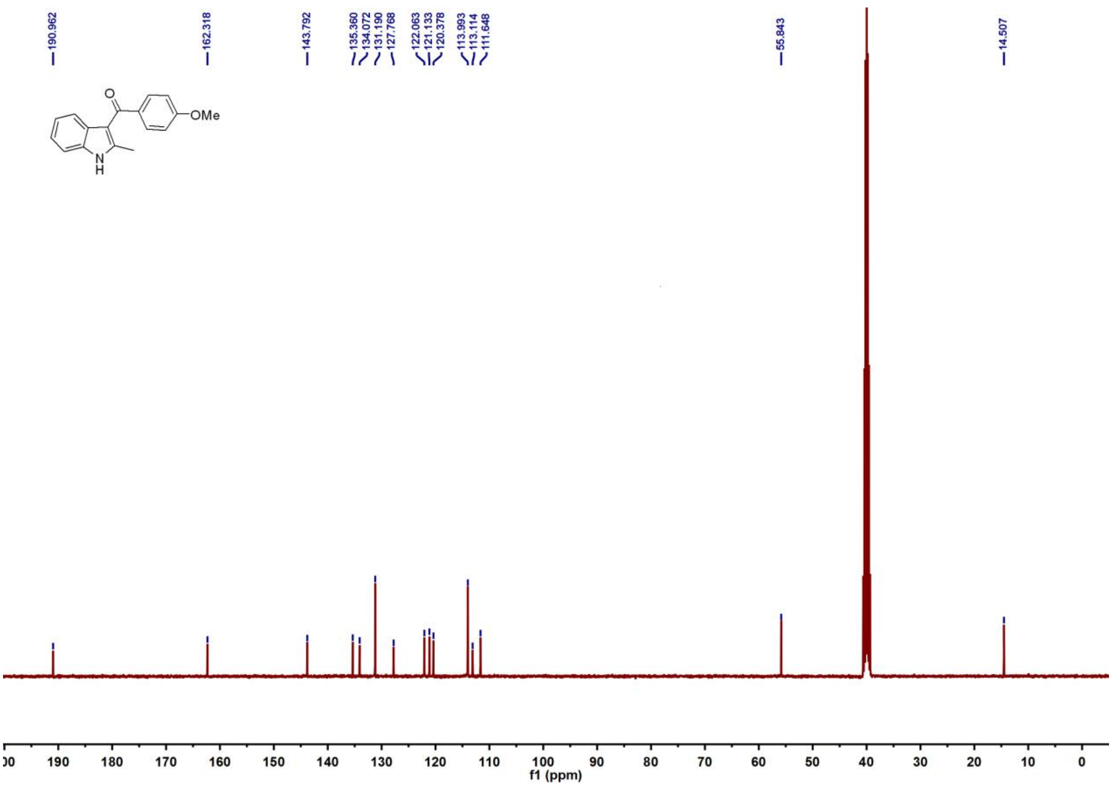


Figure S128. The ^{1}H NMR (400 MHz, Chloroform-*d*) of **9**

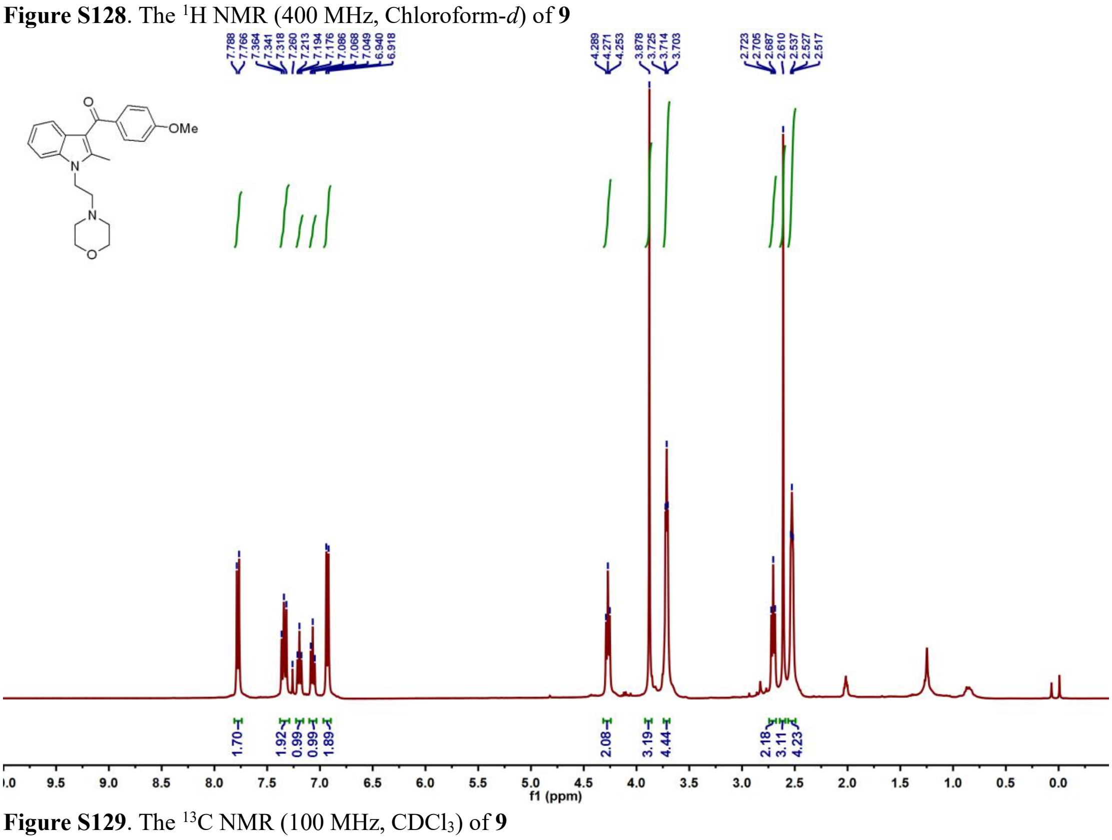


Figure S129. The ^{13}C NMR (100 MHz, $CDCl_3$) of **9**

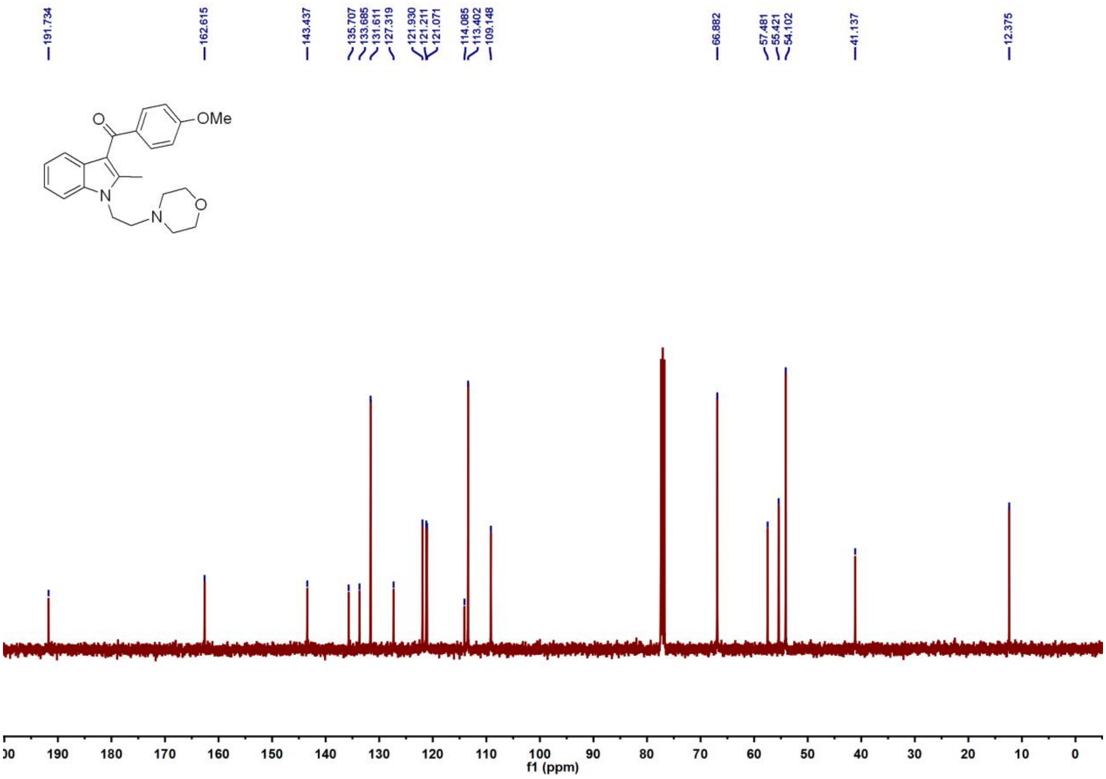


Figure S130. The [1]H NMR (400 MHz, Chloroform-*d*) of **11a**

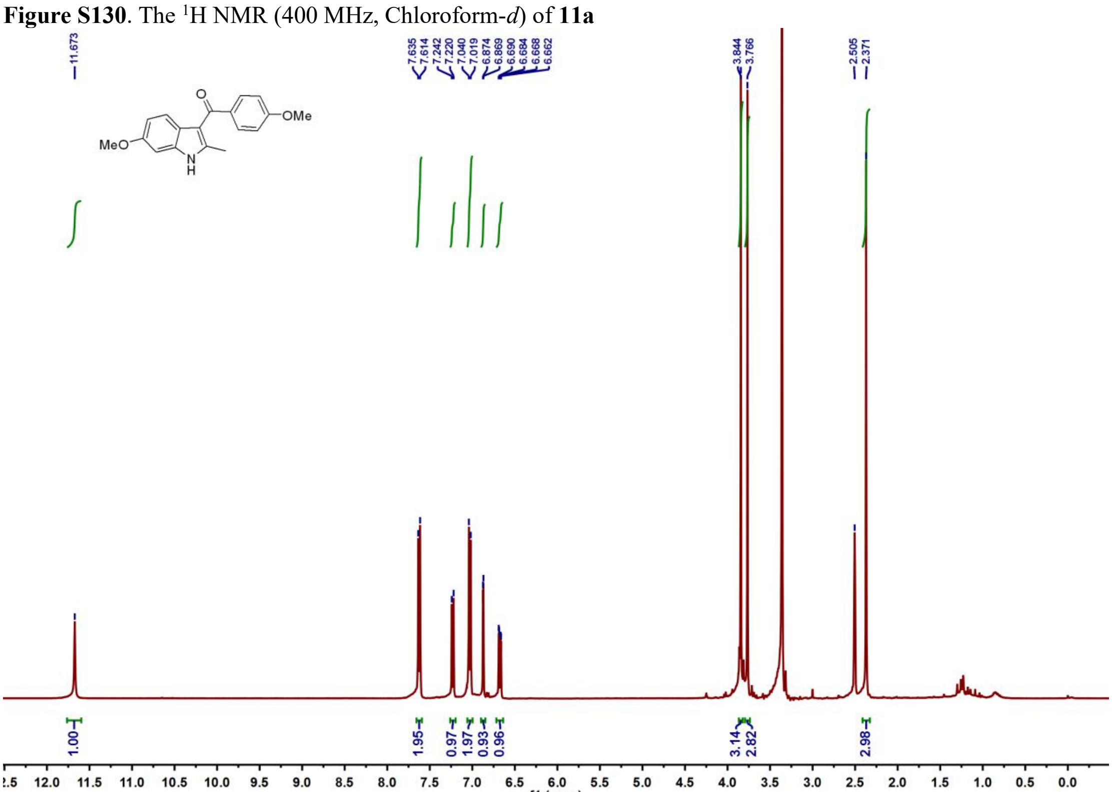


Figure S131. The [13]C NMR (100 MHz, Chloroform-*d*) of **11a**

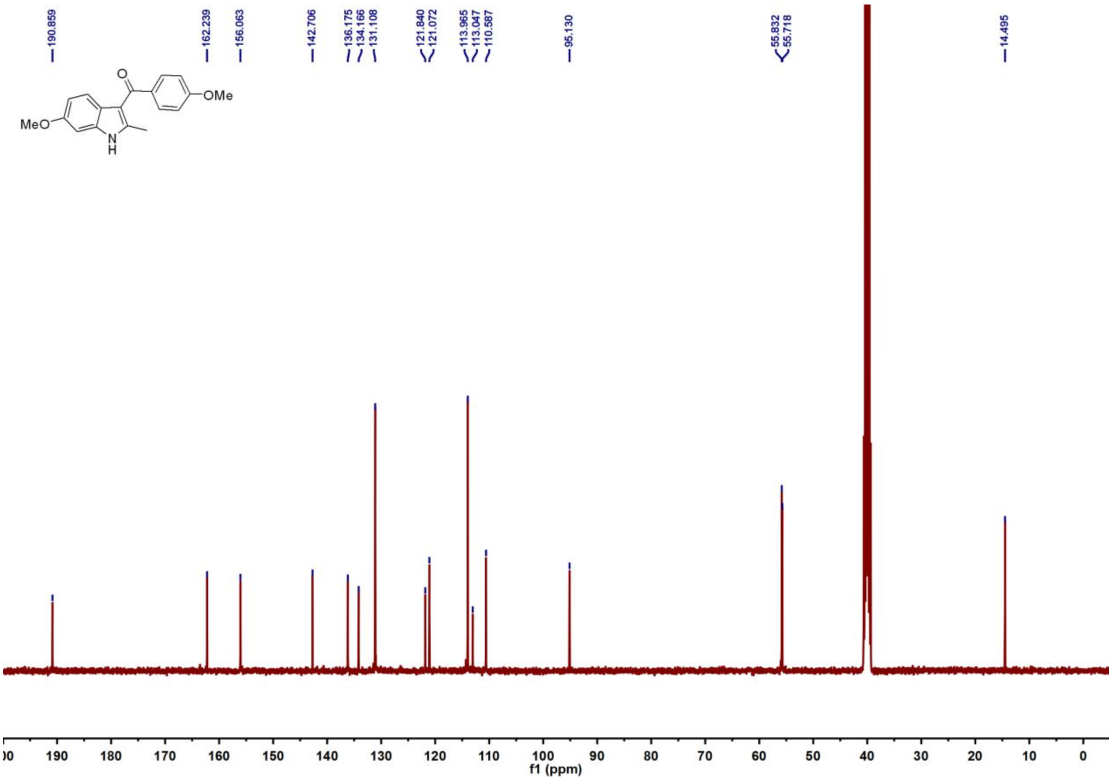


Figure S132. The [1]H NMR (400 MHz, Chloroform-*d*) of **11'a**

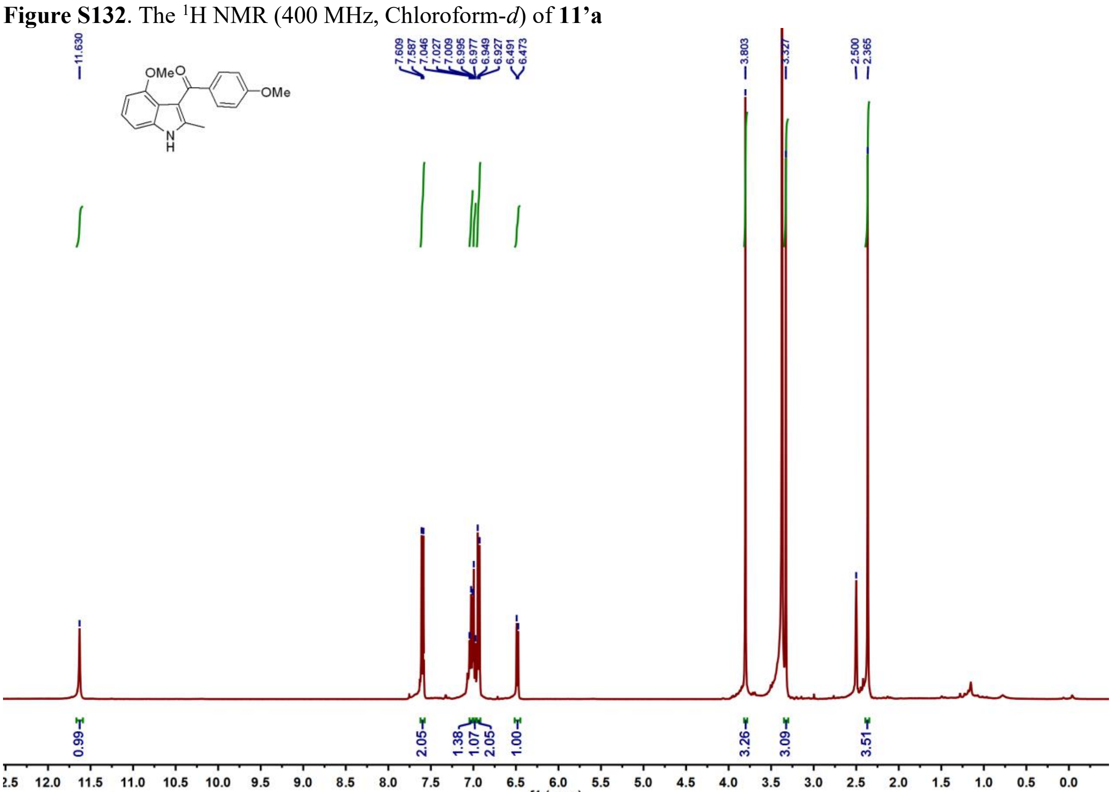


Figure S133. The [13]C NMR (100 MHz, Chloroform-*d*) of **11'a**

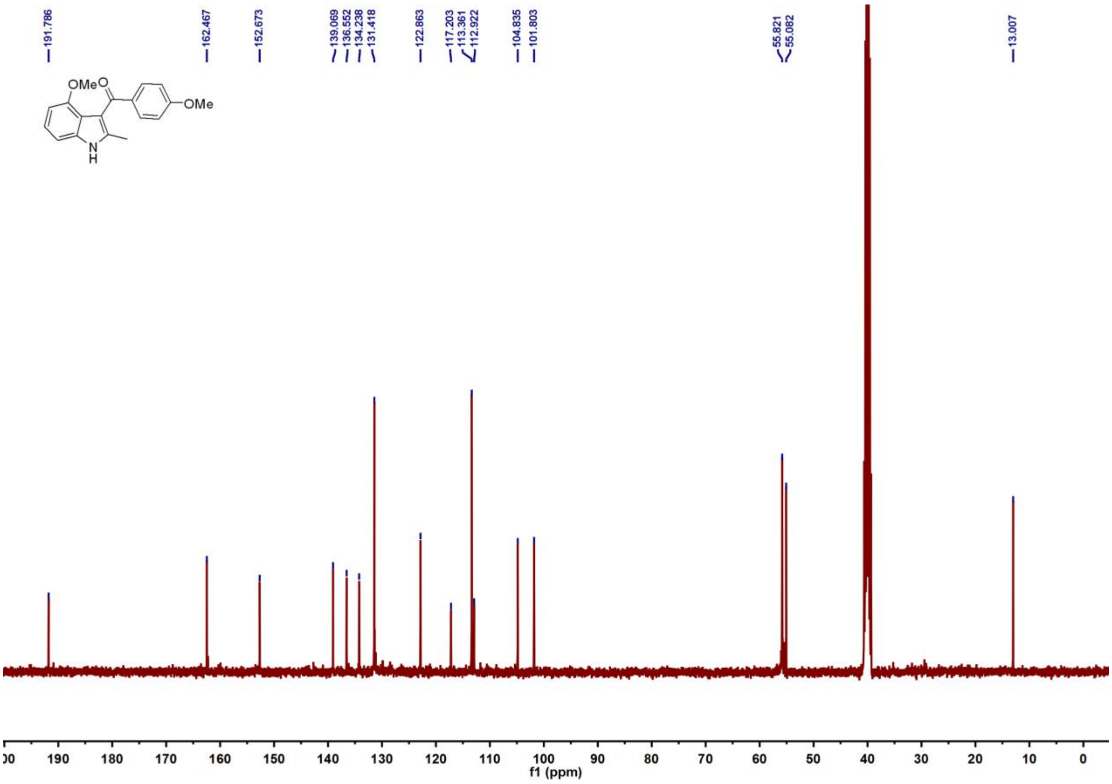


Figure S134. The ^{1}H NMR (400 MHz, Chloroform-*d*) of **11b**

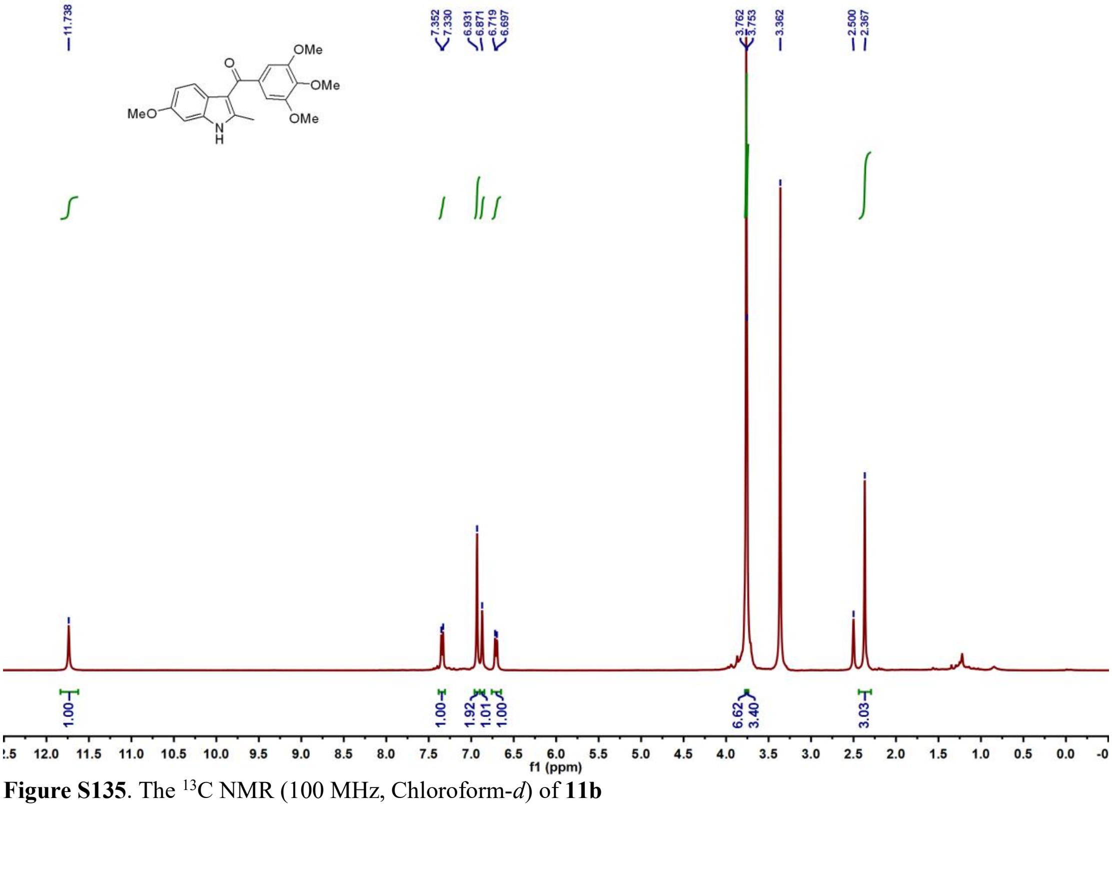


Figure S135. The ^{13}C NMR (100 MHz, Chloroform-*d*) of **11b**

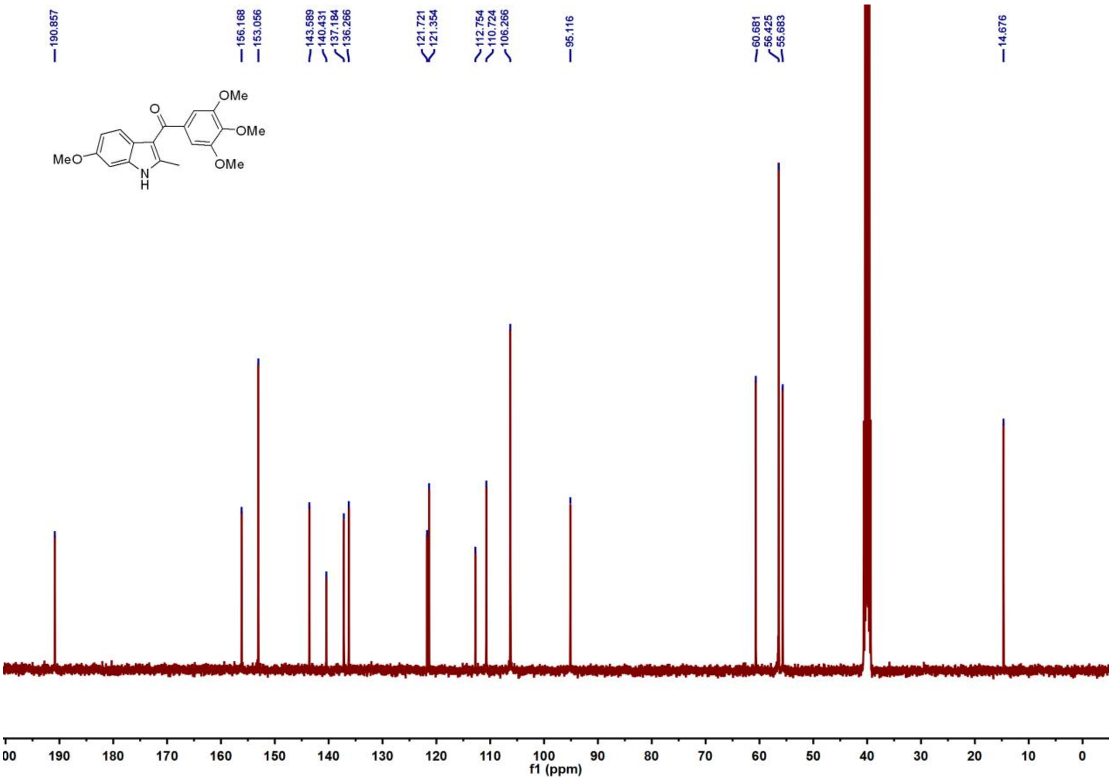


Figure S136. The [1]H NMR (400 MHz, Chloroform-*d*) of **11'b**

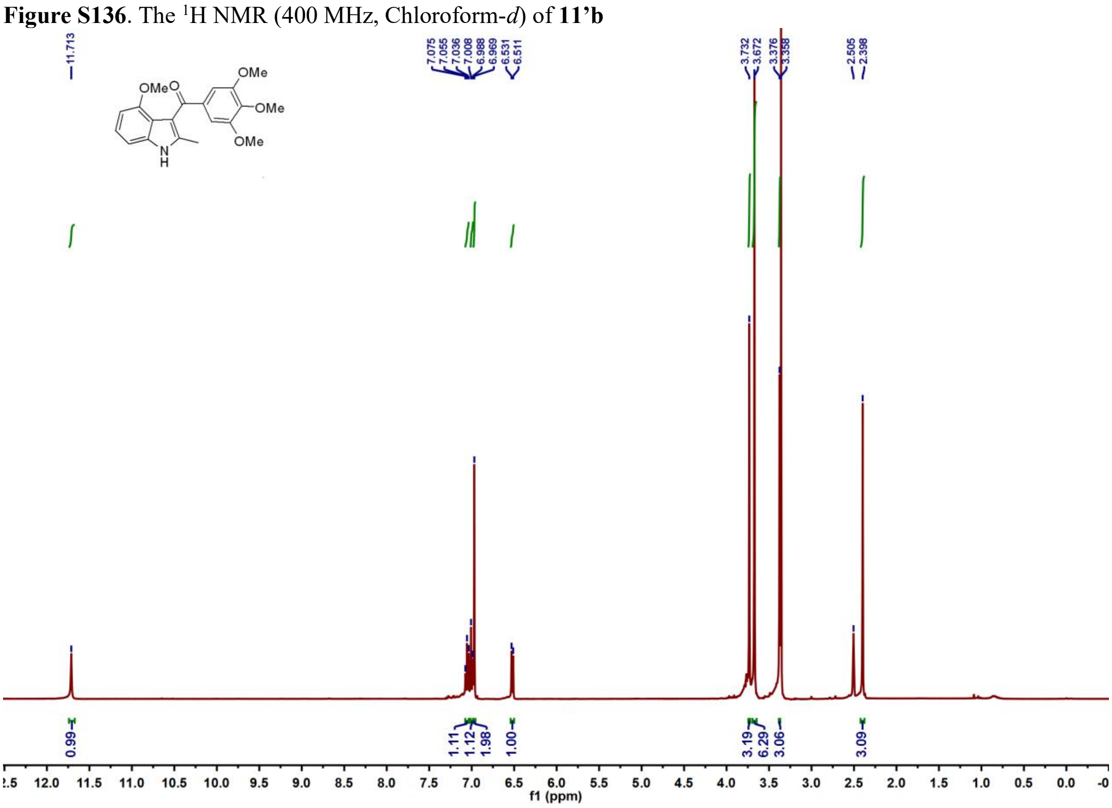


Figure S137. The [13]C NMR (100 MHz, Chloroform-*d*) of **11'b**

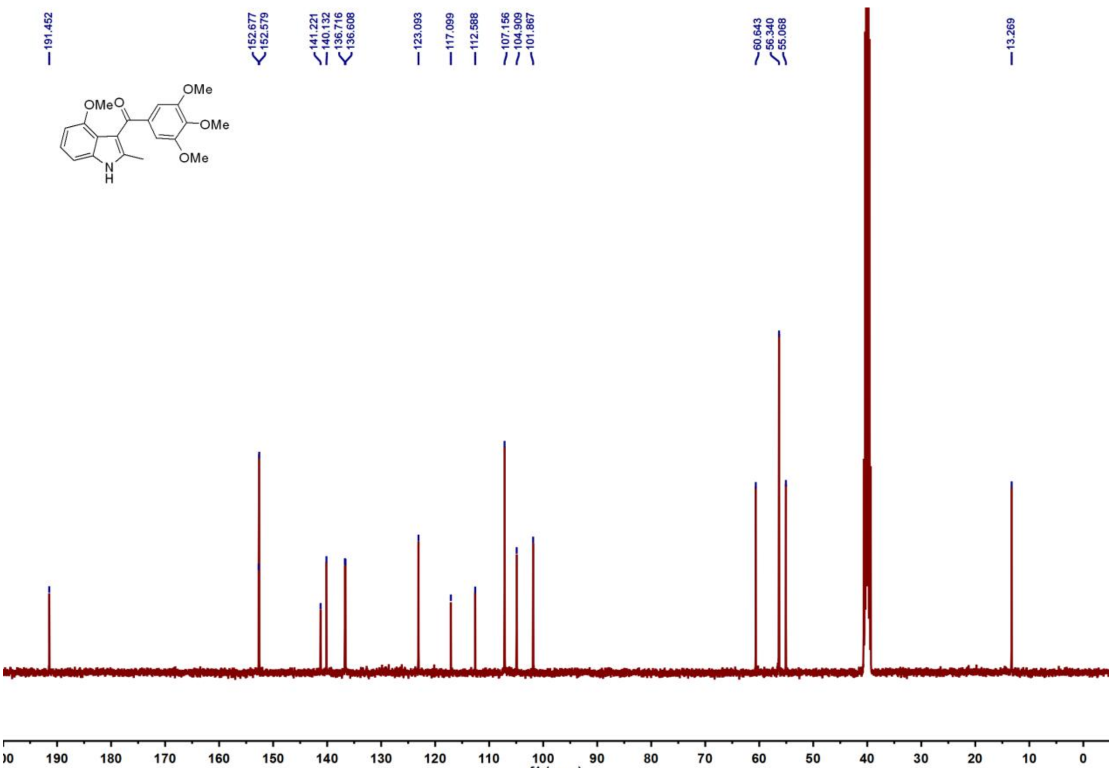


Figure S138. The [1]H NMR (400 MHz, Chloroform-*d*) of **11c**

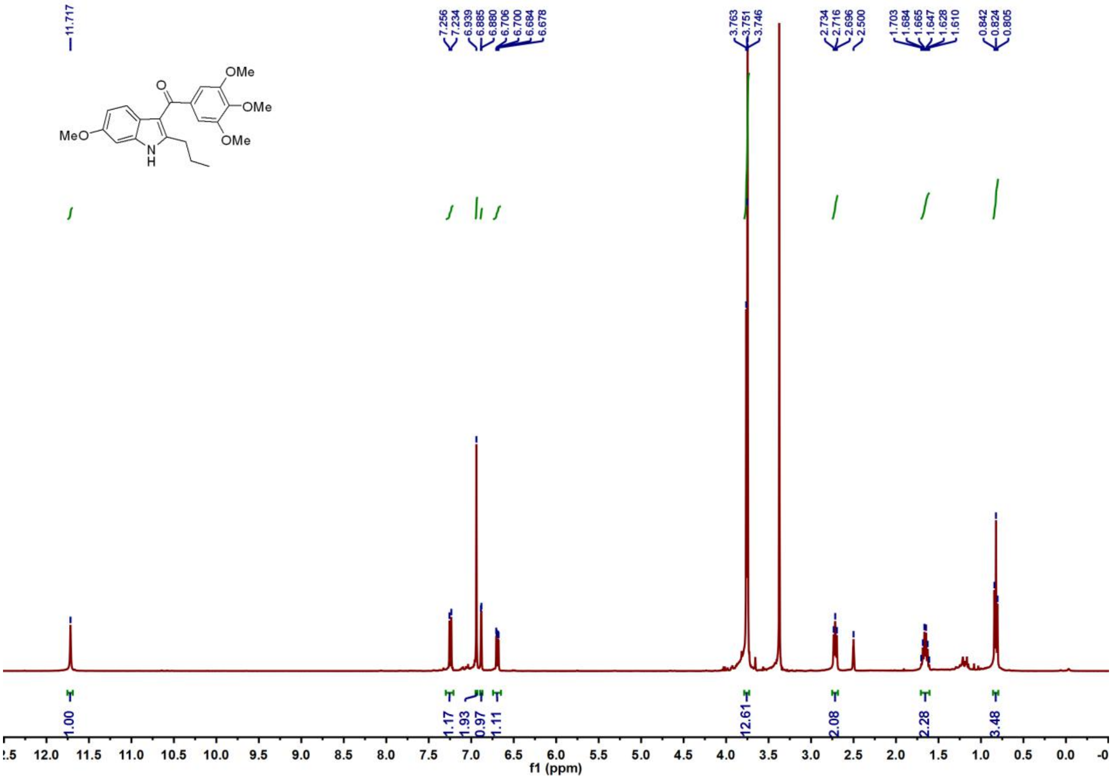


Figure S139. The [13]C NMR (100 MHz, Chloroform-*d*) of **11c**

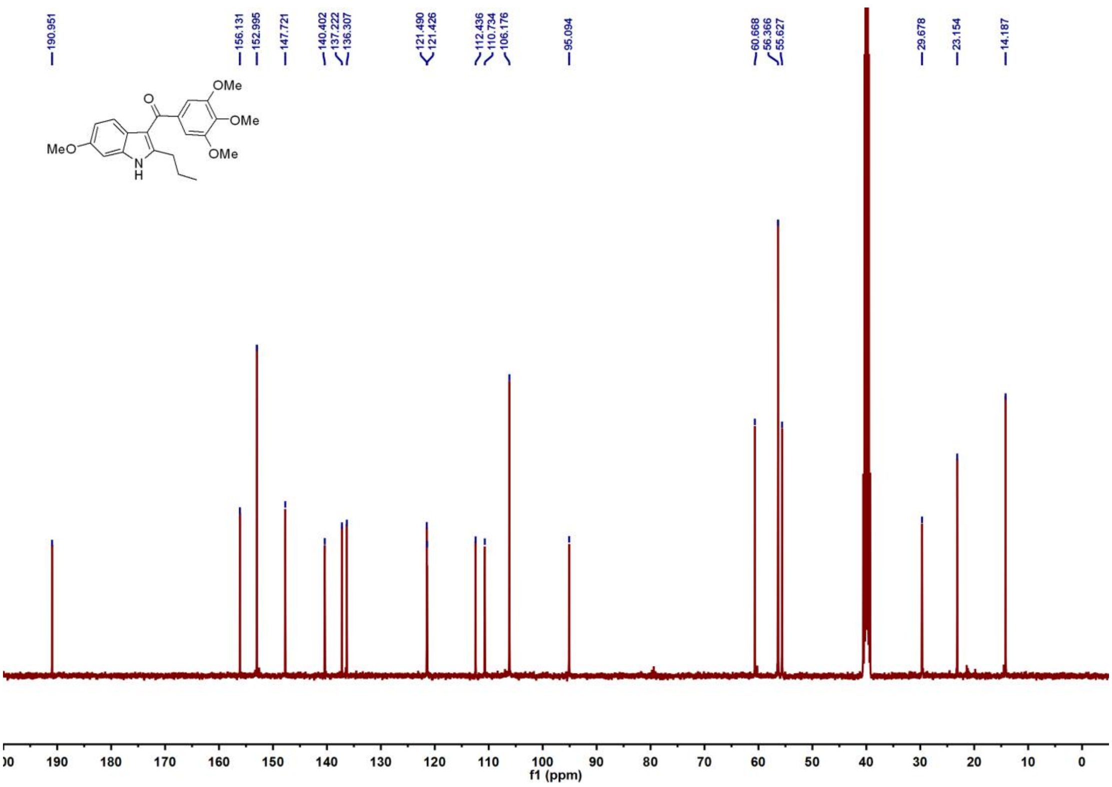


Figure S140. The [1]H NMR (400 MHz, Chloroform-*d*) of **11'c**

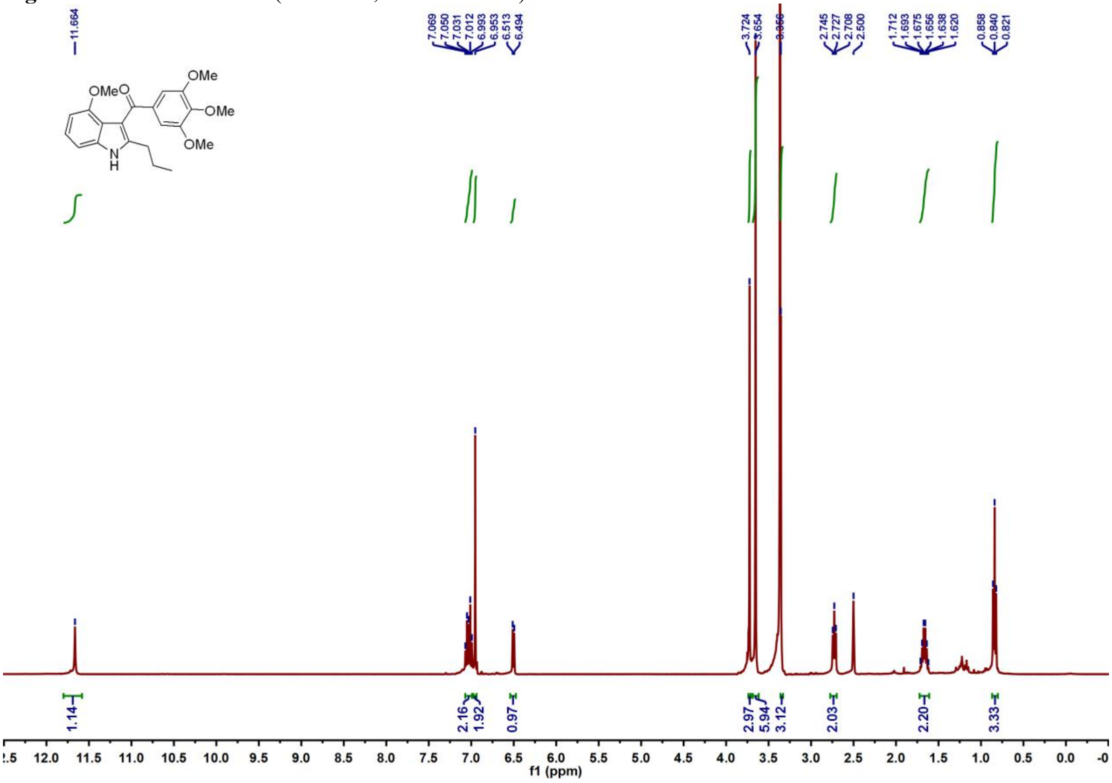


Figure S141. The [13]C NMR (100 MHz, Chloroform-*d*) of **11'c**

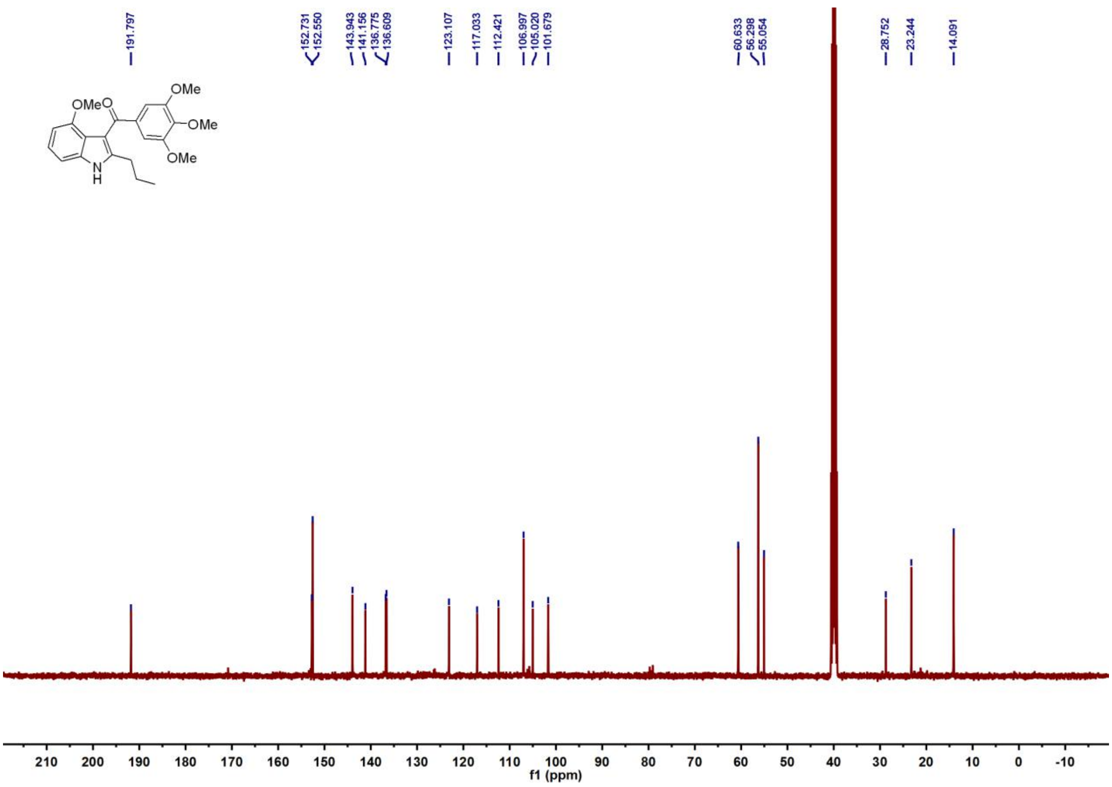


Figure S142. The ^{1}H NMR (400 MHz, Chloroform-*d*) of **11d**

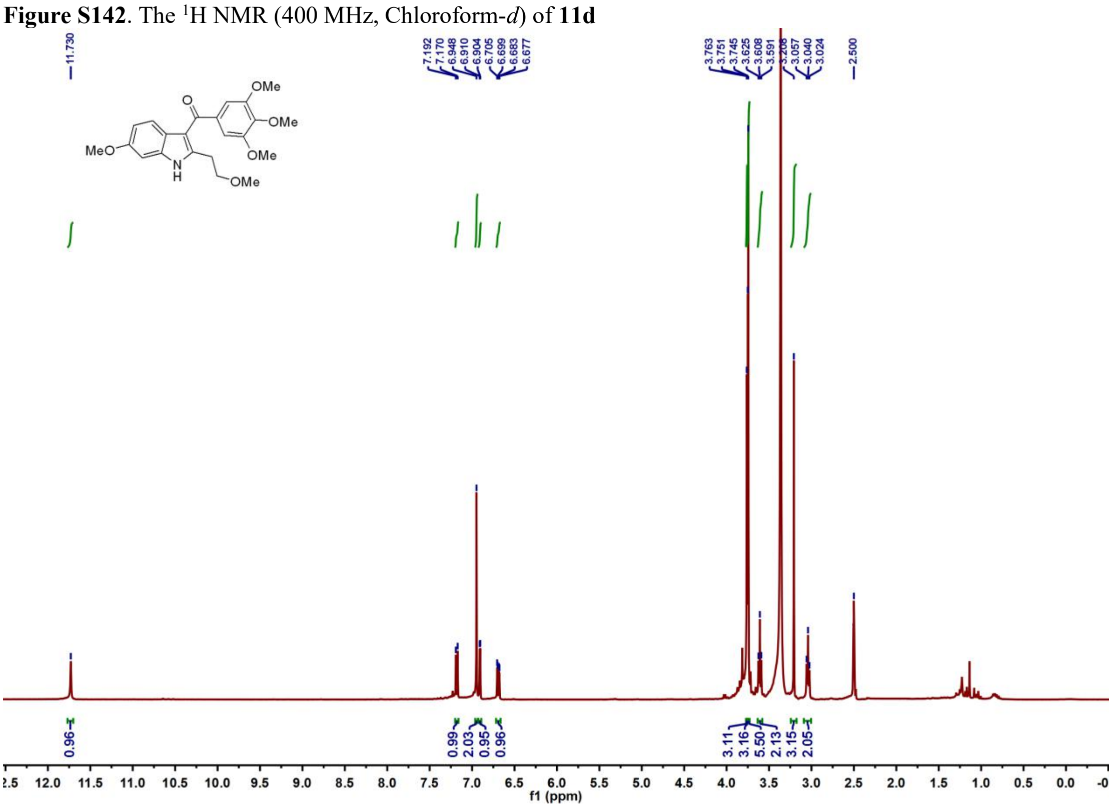


Figure S143. The ^{13}C NMR (100 MHz, Chloroform-*d*) of **11d**

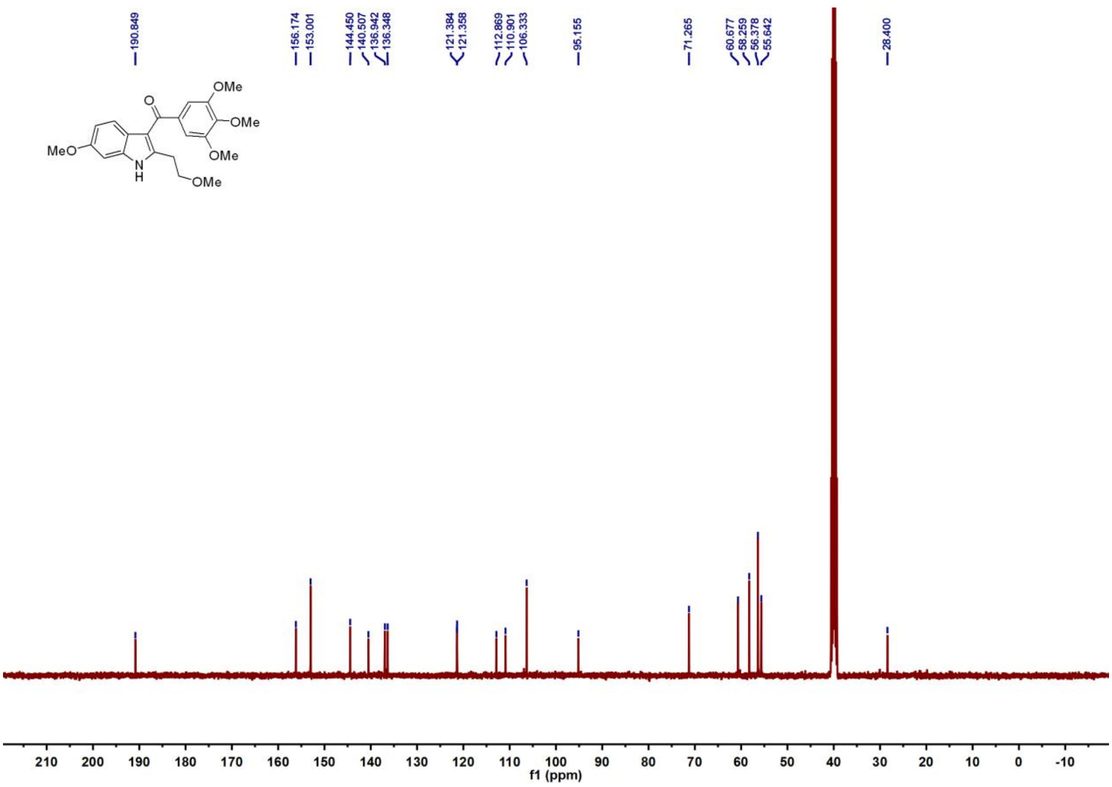


Figure S144. The ^{1}H NMR (400 MHz, Chloroform-*d*) of **11'd**

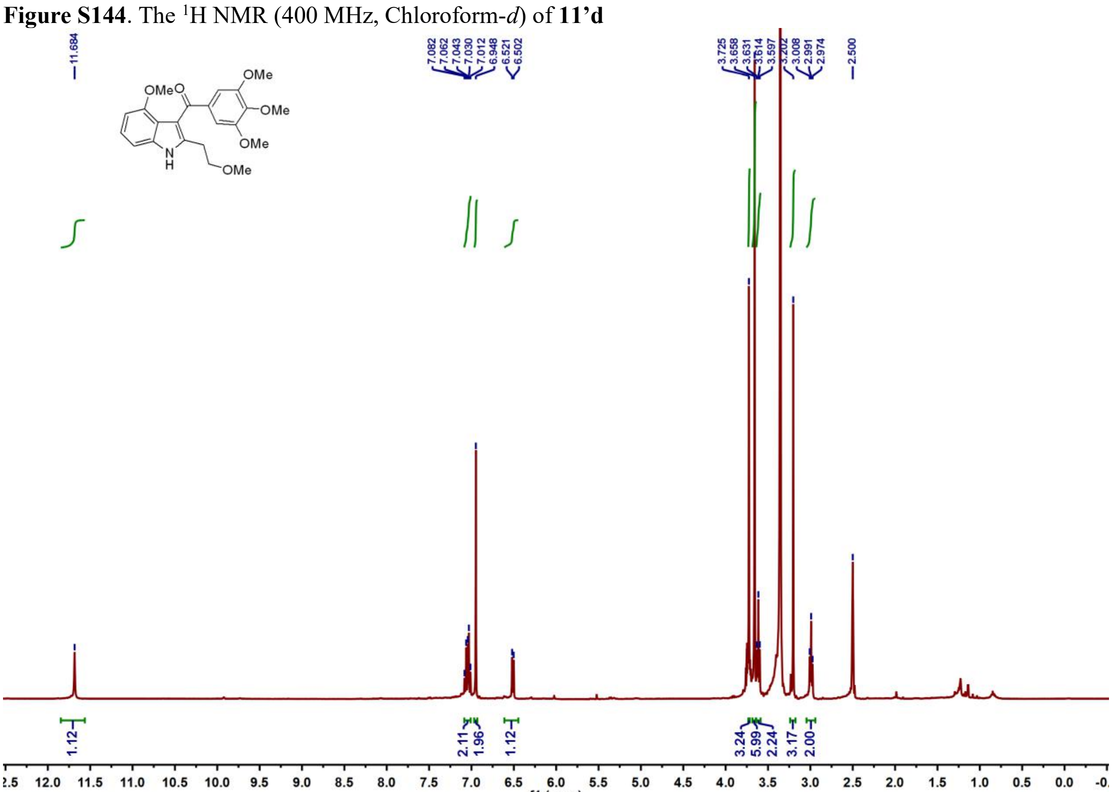
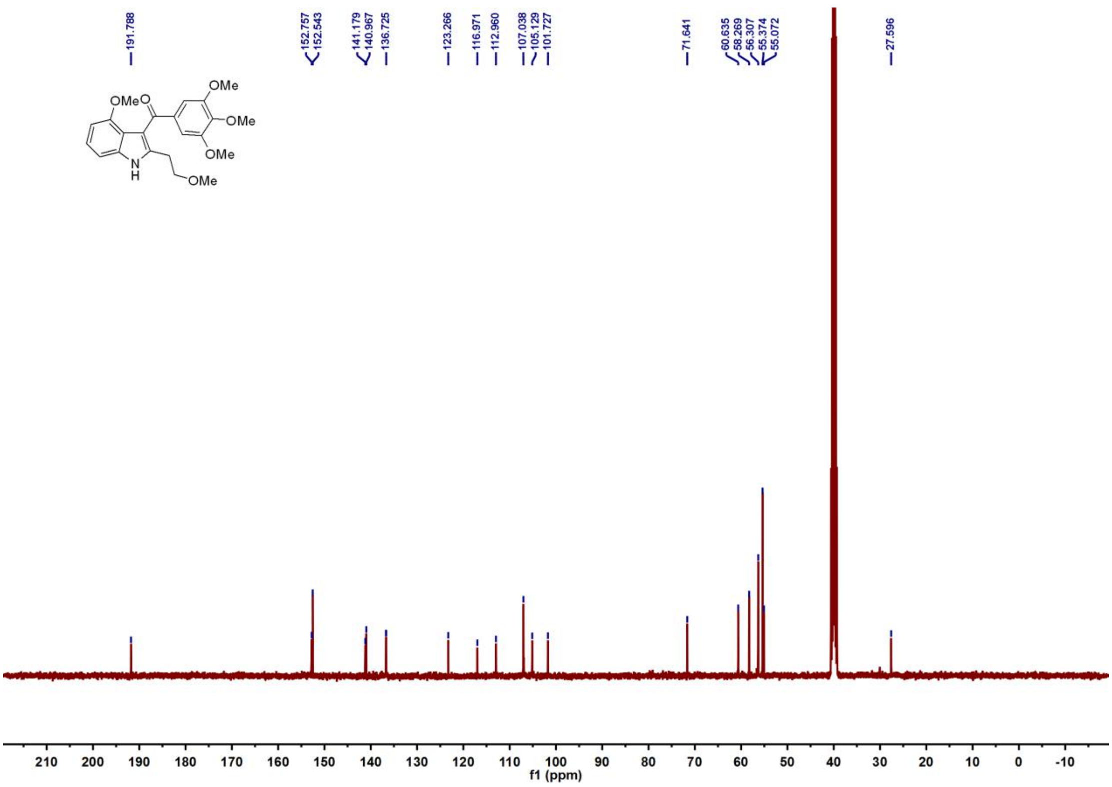


Figure S145. The ^{13}C NMR (100 MHz, Chloroform-*d*) of **11'd**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60.635
58.269
56.307
55.374
55.072
27.596
OMe
OMe
OMe
OMe
O
N
H
OMe
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)