Metal-Catalyzed Divergent Synthesis from Ylides with 3-arylbenzo[d][1,2,3]triazin-4(3*H*)-ones

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Supporting Information

1. General information

Unless otherwise noted, all reactions were carried out at room temperature under an atmosphere of nitrogen with flame-dried glassware. If reaction was not conducted at room temperature, reaction temperatures are reported as the temperature of the bath surrounding the vessel unless otherwise stated. The dry solvents used were purified by distillation over the drying agents indicated in parentheses and were transferred under nitrogen: THF (Na-benzophenone), 1,2-dichloroethane (CaH_2), dichloromethane (CaH_2). Anhydrous CF_3CH_2OH, CH_3CN, DMF and MeOH were purchased from Acros Organics and stored under nitrogen atmosphere. Commercially available chemicals were obtained from commercial suppliers and used without further purification unless otherwise stated.

Proton NMR (^1H) were recorded at 400 MHz, and Carbon NMR (^{13}C) at 101 MHz NMR spectrometer unless otherwise stated. The following abbreviations are used for the multiplicities: s: singlet, d: doublet, t: triplet, q: quartet, m: multiplet, br s: broad singlet for proton spectra. Coupling constants (*J*) are reported in Hertz (Hz).

High-resolution mass spectra HRMS-ESI (Quadrupole) were recorded on a BRUKER VPEXII spectrometer with EI and ESI mode unless otherwise stated.

Analytical thin layer chromatography was performed on Polygram SIL G/UV_{254} plates. Visualization was accomplished with short wave UV light, or $KMnO_4$ staining solutions followed by heating. Flash column chromatography was performed using silica gel (200-300 mesh) with solvents distilled prior to use.

No attempts were made to optimize yields for substrate synthesis.

2. Synthesis of substrates 1, 2 and 3

The substrates of 1,2,3-benzotriazinone **1**, sulfoxonium ylide **2** and iodonium ylide **3** were prepared accroding to the previous procedure. [1-3] All the characteristic data are consistent with the data reported before.

3. General procedure and characterization of products

General procedure A

In an oven-dried Schlenk tube under air, a mixture of corresponding 3-phenylbenzo[*d*][1,2,3]triazin-4(3*H*)-one **1** (0.20 mmol, 1.0 equiv), 2-(dimethyl(oxo)- λ^6-sulfaneyli-dene)-1-phenylethan-1-one **2** (0.22 mmol, 1.1 equiv), $(Cp^*RhCl_2)_2$ (3.1 mg, 0.005 mmol, 2.5 mol%), $AgSbF_6$ (6.9 mg, 0.02 mmol, 10 mol%), 1-AdCOOH (36.0 mg, 0.20 mmol, 1.0 equiv), AgF (6.3 mg, 0.05 mmol, 25 mol%), and HFIP (1.0 mL) was stirred at 80-130 °C (oil bath) for 24.0 h. The reaction mixture was then diluted with DCM (10.0 mL) and washed with H_2O. The aqueous phase was extracted with DCM again. The organic layers were combined, washed with brine and dried over Na_2SO_4. The pure product was purified by flash column chromatography on silica with an appropriate solvent to afford the pure product **4**.

General procedure B

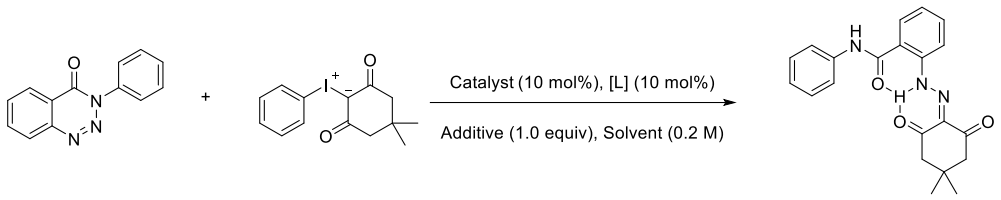
In an oven-dried Schlenk tube under air, a mixture of corresponding 3-phenylbenzo[*d*][1,2,3]triazin-4(3*H*)-one **1** (0.20 mmol, 1.0 equiv), 2-(phenyl- λ^3-iodaneylidene)cyclohexane-1,3-dione **3** (0.30 mmol, 1.5 equiv), $(Cp^*IrCl_2)_2$ (4.0 mg, 0.005 mmol, 2.5 mol%), $AgSbF_6$ (6.9 mg, 0.02 mmol, 10 mol%), PivOH (20.4 mg, 0.2 mmol, 1.0 equiv) and HFIP (1.0 mL) was stirred at 35 °C (oil bath) for 4.0 h. The reaction mixture was then diluted with DCM (10.0 mL) and washed with H_2O. The aqueous phase was extracted with DCM again. The organic layers were combined, washed with brine and dried over Na_2SO_4. The pure product was purified by flash column chromatography on silica with an appropriate solvent to afford the pure product **5**.

General procedure C

In an oven-dried Schlenk tube under air, a mixture of corresponding 3-phenylbenzo[*d*][1,2,3]triazin-4(3*H*)-one **1** (0.20 mmol, 1.0 equiv), 2-(phenyl- λ^3-iodaneylidene)cyclohexane-1,3-dione **3** (0.30 mmol, 1.5 equiv), $CuBr_2$ (4.5 mg, 0.02 mmol, 10 mol%), 4,4'-dimethyl-2,2'-bipyridine (3.7 mg, 0.02 mmol, 10 mol%), 1-AdCOOH

(36.0 mg, 0.20 mmol, 1.0 equiv) and HFIP (1.0 mL) was stirred at 80 ^{o}C (oil bath) for 4.0 h. The reaction mixture was then diluted with DCM (10.0 mL) and washed with H_2O. The aqueous phase was extracted with DCM again. The organic layers were combined, washed with brine and dried over Na_2SO_4. The pure product was purified by flash column chromatography on silica with an appropriate solvent to afford the pure product **6**.

4. Table 6 Optimization of the reaction conditions[a]

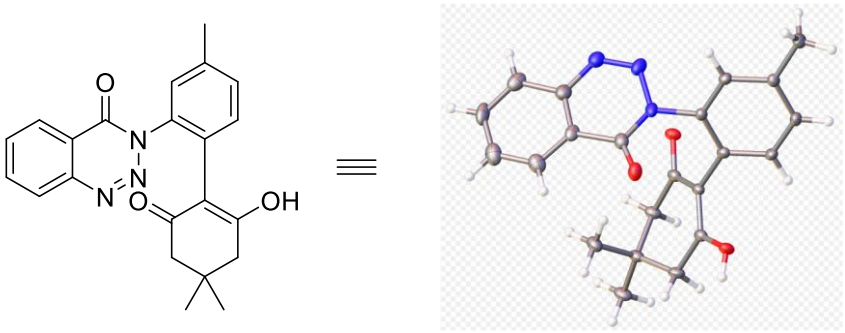


1a 3a 6aa

Entry	Catalyst	[L]	Additives	Solvent	Yields[b]
1	CuBr	Xantphos		HFIP	5%
2	CuBr	Xantphos	KF	HFIP	15%
3	CuBr	Xantphos	Na_2CO_3	HFIP	21%
4	CuBr	Xantphos	NaOAc	HFIP	32%
5	CuBr	Xantphos	CsOPiv	HFIP	36%
6	CuBr	Xantphos	AcOH	HFIP	31%
7	CuBr	Xantphos	$B(OH)_3$	HFIP	35%
8	CuBr	Xantphos	PivOH	HFIP	40%
9	CuBr	Xantphos	1-AdCOOH	HFIP	60%
10	CuBr	Xantphos	1-AdCOOH	TFE	50%
11	CuBr	Xantphos	1-AdCOOH	DCM	32%
12	CuBr	Xantphos	1-AdCOOH	MeOH	24%
13	CuBr	Xantphos	1-AdCOOH	MeCN	16%
14	CuBr	Xantphos	1-AdCOOH	PhCl	10%
15	CuOTf	Xantphos	1-AdCOOH	HFIP	40%
16	$Cu(OAc)_2$	Xantphos	1-AdCOOH	HFIP	36%
17	$CuCl_2$	Xantphos	1-AdCOOH	HFIP	31%
18	CuO	Xantphos	1-AdCOOH	HFIP	27%
19	NHC-Cu	Xantphos	1-AdCOOH	HFIP	15%
20	CuBr	5,5'-dimethyl-2,2'-bipyridine	1-AdCOOH	HFIP	72%
21	CuBr	$(o\text{-}MePh)_3P$	1-AdCOOH	HFIP	58%
22	CuBr	2,2'-bipyridine	1-AdCOOH	HFIP	57%
23	CuBr	2,2'-biquinoline	1-AdCOOH	HFIP	59%
24	CuBr	4,4'-dimethoxy-2,2'-bipyridine	1-AdCOOH	HFIP	55%
25	CuBr	1,10-phenanthroline	1-AdCOOH	HFIP	27%
26	CuBr	4,4'-dibromo-2,2'-bipyridine	1-AdCOOH	HFIP	38%
27[c]	**CuBr**	**5,5'-dimethyl-2,2'-bipyridine**	**1-AdCOOH**	**HFIP**	**83%**
28		5,5'-dimethyl-2,2'-bipyridine	1-AdCOOH	HFIP	-
29	CuBr	-	1-AdCOOH	HFIP	65%

[a]Reaction conditions: **1a** (0.10 mmol), **3a** (0.10 mmol), catalyst (10 mol%), [L] (10 mol%), additives (1.2 equiv.), Solvent (0.2 M), 80 °C, 4 h. [b]Isolated yield. [c]**3a** (0.15 mmol).

5. X-Ray crystal data for compound 5ba and 6ab



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The crystal structure of **5ba** by X-ray analysis.

X-ray-quality crystal was obtained by slow diffusion of Petroleum ether into a dilute dichloromethane solution of **5ba** at room temperature under air. Thermal ellipsoids drawn at the 50 % probability level. Crystal data were obtained on a SuperNova, Dual, Cu at zero, AtlasS2 diffractometer using Mo Kα radiation (λ = 0.71073 Å). The crystal was kept at 200.00(10) K during data collection.

Table 1 Crystal data and structure refinement for 5ba.

Identification code	**5ba**
Empirical formula	$C_{22}H_{21}N_3O_3$
Formula weight	375.42
Temperature/K	149.99(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	10.6241(2)
b/Å	20.0539(4)
c/Å	18.4446(4)
α/°	90
β/°	92.354(2)
γ/°	90
Volume/Å^3	3926.39(14)
Z	8
ρ_{calc}g/cm^3	1.270
μ/mm^{-1}	0.697
F(000)	1584.0
Crystal size/mm^3	0.14 × 0.12 × 0.1

Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.514 to 147.35
Index ranges	$-13 \leq h \leq 12$, $-24 \leq k \leq 21$, $-22 \leq l \leq 17$
Reflections collected	15823
Independent reflections	7720 [R_{int} = 0.0419, R_{sigma} = 0.0531]
Data/restraints/parameters	7720/419/580
Goodness-of-fit on F^2	1.047
Final R indexes [I>=2σ (I)]	R_1 = 0.0746, wR_2 = 0.1969
Final R indexes [all data]	R_1 = 0.0863, wR_2 = 0.2093
Largest diff. peak/hole / e Å^{-3}	0.57/-0.58

Crystal structure determination of [5ba]

Crystal Data for $C_{22}H_{21}N_3O_3$ (*M* =375.42 g/mol): monoclinic, space group $P2_1/n$ (no. 14), *a* = 10.6241(2) Å, *b* = 20.0539(4) Å, *c* = 18.4446(4) Å, *β* = 92.354(2)°, *V* = 3926.39(14) Å^3, *Z* = 8, *T* = 149.99(10) K, μ(Cu Kα) = 0.697 mm^{-1}, *Dcalc* = 1.270 g/cm^3, 15823 reflections measured (6.514° ≤ 2Θ ≤ 147.35°), 7720 unique (R_{int} = 0.0419, R_{sigma} = 0.0531) which were used in all calculations. The final R_1 was 0.0746 (I > 2σ(I)) and wR_2 was 0.2093 (all data).

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 5ba. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	8522(2)	7669.8(10)	8751.9(11)	39.0(5)
O2	9023.8(16)	8745.7(10)	10767.0(10)	30.8(4)
O3	10633.1(16)	6733.1(10)	9957.8(11)	32.6(4)
N1	6631(2)	9268.5(13)	9425.8(15)	41.8(5)
N2	6642(2)	8748.9(13)	9803.8(15)	41.2(6)
N3	7412.9(19)	8193.1(12)	9563.4(12)	31.0(5)
C1	8101(2)	8817.3(14)	8547.7(16)	33.9(5)
C2	8824(3)	8924.0(18)	7956.9(17)	45.2(7)
C3	8843(3)	9532.7(19)	7648.1(19)	52.5(7)
C4	8123(3)	10044.4(17)	7890(2)	50.1(7)
C5	7370(3)	9963.4(17)	8476(2)	47.4(7)
C6	7377(3)	9320.4(16)	8824.7(18)	40.8(5)
C7	8059(3)	8173.0(15)	8941.3(15)	34.0(6)
C8	7374(2)	7643.5(12)	10068.9(13)	24.0(5)
C9	6209(2)	7383.2(13)	10213.5(14)	25.9(5)
C10	6104(2)	6863.2(13)	10708.4(14)	26.1(5)
C11	7203(2)	6615.0(14)	11038.1(15)	30.2(6)
C12	8362(2)	6885.3(14)	10892.4(14)	29.0(5)
C13	8481(2)	7412.8(13)	10410.8(13)	24.2(5)
C14	9735(2)	7731.3(13)	10311.9(13)	24.7(5)

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 5ba. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C15	9906(2)	8417.1(14)	10529.2(13)	26.5(5)
C16	11197(2)	8726.5(15)	10508.5(14)	30.6(6)
C17	12023(2)	8442.5(14)	9921.1(14)	29.2(6)
C18	10748(2)	7378.3(14)	10086.8(13)	27.0(5)
C19	12022(2)	7686.3(15)	9998.0(15)	32.4(6)
C20	11504(3)	8645.4(17)	9170.0(15)	38.1(7)
C21	13366(2)	8706.4(17)	10030.1(16)	38.2(7)
C22	4825(3)	6596.9(15)	10875.5(18)	37.3(6)
O4	4372(5)	7430(3)	8745(3)	29.3(11)
O5	4372.6(16)	5892.1(10)	7118.2(10)	30.6(4)
O6	2539.1(16)	6170.5(10)	9346.0(10)	31.4(4)
OA	6942(9)	6722(4)	7358(5)	38.7(15)
N00F	4798(7)	7366(4)	8604(6)	36.7(15)
N4	6768(4)	7380(2)	7099(2)	26.5(9)
N5	6608(7)	6874(4)	7484(4)	36.5(14)
N6	5719(2)	6925.6(11)	8140.9(14)	36.4(5)
N7	4586(5)	7953(2)	8376(3)	30.6(11)
C0	5650(6)	9129.3(18)	7006(3)	37(3)
C47	5019(5)	8861(2)	7583(3)	37.5(15)
C46	5218(5)	8200(2)	7784(3)	28.3(15)
C00{	6048(6)	7807.4(17)	7407(3)	28.8(15)
C01L	6679(4)	8076(2)	6829(2)	32.8(13)
C48	6480(5)	8737(2)	6628(3)	37.0(16)
C24	6391(4)	8521(2)	6811.2(19)	31.2(12)
C25	5790(5)	9124.4(17)	6928(3)	38(2)
C26	4923(4)	9177.0(14)	7470(2)	36.2(12)
C27	4657(3)	8625.7(19)	7893.8(18)	28.0(10)
C28	5258(4)	8021.9(16)	7777(2)	22.7(12)
C23	6126(4)	7969.4(15)	7235(2)	21.4(10)
C29	5071(5)	7453(2)	8245(3)	25.7(9)
C30	5833(2)	6312.6(12)	8545.3(14)	25.3(5)
C31	6994(2)	6164.1(12)	8869.1(14)	26.5(5)
C32	7178(2)	5580.4(13)	9267.9(13)	26.0(5)
C33	6142(2)	5160.5(13)	9336.5(14)	27.8(5)
C34	4976(2)	5319.5(13)	9016.0(13)	26.7(5)
C35	4784(2)	5895.5(12)	8606.3(13)	23.0(5)

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 5ba. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C36	3536(2)	6038.5(13)	8242.9(14)	25.7(5)
C37	8436(3)	5415.7(14)	9625.1(16)	35.0(6)
C38	2457(2)	6152.0(14)	8676.0(15)	31.6(5)
C39	1171(3)	6192.5(18)	8289.2(17)	42.6(7)
C40	1184(2)	6526.2(16)	7546.1(15)	34.7(6)
C41	2178(2)	6200.0(17)	7099.5(16)	39.3(7)
C42	3388(2)	6047.2(13)	7505.6(14)	27.4(5)
C43	1538(3)	7269.5(18)	7663(2)	51.8(8)
C44	-92(3)	6506(3)	7161(2)	62.5(11)
C45	6281(8)	7123(4)	7617(4)	33.8(13)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 5ba. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	47.5(11)	31.6(11)	37.6(11)	5.0(9)	-2.4(9)	-6.6(9)
O2	23.1(8)	37.7(11)	32.0(9)	-5.8(8)	4.2(7)	1.2(7)
O3	25.2(9)	34.2(10)	39.0(10)	-1.7(8)	10.3(8)	2.4(7)
N1	32.5(9)	39.3(10)	53.1(12)	5.9(8)	-3.1(8)	-2.0(8)
N2	33.6(12)	31.4(11)	57.6(15)	9.4(10)	-10.1(11)	-4.6(9)
N3	22.8(10)	35.2(12)	34.3(11)	11.3(9)	-6.9(8)	-5.5(8)
C1	28.5(12)	29.6(12)	42.4(14)	3.7(10)	-12.2(10)	-9.4(9)
C2	45.4(16)	50.1(16)	39.6(15)	-4.4(12)	-4.2(12)	-15.0(13)
C3	58.1(19)	57.5(16)	40.7(16)	5.9(13)	-12.5(14)	-21.2(13)
C4	52.6(17)	38.1(15)	57.9(18)	18.5(13)	-20.3(12)	-22.7(12)
C5	40.2(15)	35.9(14)	64.4(18)	-1.4(13)	-18.3(12)	-5.2(12)
C6	30.6(9)	39.9(10)	51.6(12)	4.6(9)	-4.0(8)	-3.8(8)
C7	32.1(13)	37.9(15)	31.5(12)	2.9(11)	-5.0(10)	-6.2(11)
C8	25.1(11)	23.5(12)	23.6(11)	0.8(9)	1.7(9)	1.2(9)
C9	21.0(11)	27.8(13)	28.7(12)	1.0(10)	-2.4(9)	1.0(9)
C10	26.6(12)	23.1(12)	28.8(12)	0.2(10)	2.6(10)	-1.2(9)
C11	30.8(13)	27.7(14)	32.4(13)	7.7(10)	3.8(11)	1.6(10)
C12	22.5(11)	35.0(15)	29.4(13)	6.6(11)	0.8(10)	5.9(10)
C13	21.0(11)	30.2(13)	21.4(11)	-2.0(9)	1.6(9)	2.6(9)
C14	18.7(10)	33.1(14)	22.2(11)	2.6(10)	1.5(9)	1.0(9)
C15	21.8(11)	37.1(14)	20.7(11)	-0.5(10)	2.3(9)	0.1(10)
C16	21.6(11)	39.0(15)	31.4(13)	-7.1(11)	2.6(10)	-3.3(10)
C17	18.6(11)	41.9(15)	27.2(12)	-2.7(11)	1.4(9)	-2.1(10)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 5ba. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C18	21.5(11)	36.0(14)	23.7(12)	1.2(10)	2.1(9)	1.3(10)
C19	19.3(11)	42.1(16)	36.0(14)	-4.5(12)	4.0(10)	1.7(10)
C20	28.7(13)	52.4(19)	33.4(14)	2.0(13)	2.8(11)	-8.0(12)
C21	21.6(12)	53.9(19)	39.2(15)	-5.2(13)	2.0(11)	-6.1(12)
C22	28.9(13)	33.4(15)	49.9(17)	11.0(13)	3.1(12)	-6.9(11)
O4	28(3)	28(2)	31.3(19)	3.4(15)	-5.6(15)	0.4(16)
O5	24.6(8)	40.6(11)	27.1(9)	-0.6(8)	4.1(7)	5.9(7)
O6	28.0(9)	37.6(11)	29.0(8)	0.3(7)	5.7(7)	3.8(7)
OA	38(4)	30(3)	48(3)	9(2)	-2(2)	-4(2)
N00F	32(5)	21(2)	56(5)	4(2)	-15(3)	-2(2)
N4	27.3(18)	26.0(17)	26.5(19)	2.9(13)	5.0(14)	-0.4(13)
N5	32(5)	30(4)	46(4)	15(3)	-11.0(19)	-9(2)
N6	30.6(11)	23.3(10)	54.1(14)	8.8(9)	-11.6(10)	-3.9(8)
N7	37(2)	20(2)	35(2)	-0.9(16)	2.3(18)	4.9(17)
C0	46(5)	23(4)	42(4)	6(3)	-9(4)	-10(3)
C47	45(3)	24(3)	42(3)	5(2)	-5(3)	-2(2)
C46	31(3)	23(3)	30(3)	-0.5(19)	-7(2)	-6(2)
C00{	30(3)	26(2)	30(3)	1.5(19)	-5(2)	-6(2)
C01L	32(3)	31(3)	36(3)	6(2)	-4(2)	-7(2)
C48	37(3)	32(3)	41(4)	10(2)	-10(3)	-8(2)
C24	31(2)	31(3)	31(3)	10(2)	-7.8(19)	-8(2)
C25	38(4)	29(3)	47(4)	11(3)	-7(3)	-7(3)
C26	41(3)	23(2)	44(3)	3(2)	-8(2)	-5(2)
C27	29(2)	20(2)	35(2)	-1.7(16)	-3.4(18)	2.5(16)
C28	22(2)	18(2)	28(2)	1.0(15)	-1.7(18)	-1.0(16)
C23	19(2)	23.6(19)	21(2)	0.2(16)	-5.4(17)	-3.9(15)
C29	24.3(19)	22.0(17)	30(2)	5.2(14)	-9.7(17)	-5.3(13)
C30	25.5(10)	18.9(11)	31.4(12)	-0.7(9)	-0.1(9)	0.3(8)
C31	24.9(10)	21.9(11)	32.5(12)	-0.8(9)	0.8(9)	-1.8(9)
C32	28.2(10)	23.8(11)	26.0(11)	-2.8(9)	1.7(9)	3.5(8)
C33	32.8(10)	25.1(12)	25.8(12)	2.2(9)	3.5(9)	1.2(9)
C34	27.7(10)	26.0(12)	27.0(12)	-0.3(9)	5.6(9)	-2.9(9)
C35	23.1(10)	22.6(11)	23.7(11)	-4.6(8)	4.4(8)	0.6(8)
C36	22.8(10)	25.5(12)	29.0(10)	-2.4(9)	2.6(8)	-0.1(9)
C37	33.5(12)	31.0(14)	40.0(15)	-0.7(12)	-5.1(11)	5.1(11)
C38	27.6(11)	36.5(15)	30.9(10)	-2.4(10)	4.4(9)	1.4(10)
C39	28.9(12)	61(2)	37.9(14)	-0.6(13)	3.4(11)	-0.9(13)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 5ba. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C40	23.0(11)	47.5(15)	33.5(12)	-2.1(11)	1.3(9)	5.9(10)
C41	26.3(12)	60(2)	31.2(13)	-7.1(13)	-1.0(10)	6.3(12)
C42	22.3(10)	30.6(13)	29.6(10)	-3.7(10)	3.8(8)	0.4(9)
C43	47.5(18)	47.4(16)	60(2)	-1.5(16)	-5.4(16)	10.0(14)
C44	30.0(14)	110(3)	47.2(19)	-13(2)	-6.4(13)	13.1(17)
C45	30(3)	26(3)	44(3)	4(2)	-13.7(19)	-7(2)

Table 4 Bond Lengths for 5ba.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C7	1.181(4)	N4	N5	1.254(7)
O2	C15	1.240(3)	N4	C23	1.393(5)
O3	C18	1.320(3)	N5	N6	1.570(7)
N1	N2	1.253(4)	N6	C29	1.281(5)
N1	C6	1.393(4)	N6	C30	1.440(3)
N2	N3	1.463(4)	N6	C45	1.223(7)
N3	C7	1.362(4)	N7	C46	1.397(6)
N3	C8	1.445(3)	C0	C47	1.3900
C1	C2	1.375(4)	C0	C48	1.3900
C1	C6	1.379(4)	C47	C46	1.3900
C1	C7	1.484(4)	C46	C00{	1.3900
C2	C3	1.348(5)	C00{	C01L	1.3900
C3	C4	1.365(6)	C00{	C45	1.445(7)
C4	C5	1.380(5)	C01L	C48	1.3900
C5	C6	1.441(5)	C24	C25	1.3900
C8	C9	1.380(3)	C24	C23	1.3900
C8	C13	1.391(3)	C25	C26	1.3900
C9	C10	1.393(4)	C26	C27	1.3900
C10	C11	1.387(4)	C27	C28	1.3900
C10	C22	1.504(3)	C28	C23	1.3900
C11	C12	1.382(4)	C28	C29	1.450(6)
C12	C13	1.390(4)	C30	C31	1.381(4)
C13	C14	1.495(3)	C30	C35	1.401(3)
C14	C15	1.442(4)	C31	C32	1.392(4)
C14	C18	1.367(3)	C32	C33	1.396(4)
C15	C16	1.508(3)	C32	C37	1.502(4)
C16	C17	1.532(3)	C33	C34	1.388(4)
C17	C19	1.523(4)	C34	C35	1.391(4)

Table 4 Bond Lengths for 5ba.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C17	C20	1.525(4)	C35	C36	1.489(3)
C17	C21	1.527(3)	C36	C38	1.442(3)
C18	C19	1.503(3)	C36	C42	1.363(4)
O4	C29	1.209(7)	C38	C39	1.517(4)
O5	C42	1.327(3)	C39	C40	1.526(4)
O6	C38	1.236(3)	C40	C41	1.514(4)
OA	C45	1.180(9)	C40	C43	1.550(5)
N00F	N6	1.592(8)	C40	C44	1.505(4)
N00F	N7	1.267(10)	C41	C42	1.493(4)

Table 5 Bond Angles for 5ba.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N2	N1	C6	120.8(3)	N00F	N7	C46	120.3(6)
N1	N2	N3	117.2(3)	C47	C0	C48	120.0
C7	N3	N2	125.9(2)	C46	C47	C0	120.0
C7	N3	C8	123.3(2)	C47	C46	N7	118.3(4)
C8	N3	N2	110.8(2)	C47	C46	C00{	120.0
C2	C1	C6	121.2(3)	C00{	C46	N7	121.7(4)
C2	C1	C7	123.5(3)	C46	C00{	C01L	120.0
C6	C1	C7	115.3(3)	C46	C00{	C45	120.6(4)
C3	C2	C1	119.6(4)	C01L	C00{	C45	119.4(4)
C2	C3	C4	121.6(3)	C48	C01L	C00{	120.0
C3	C4	C5	121.2(3)	C01L	C48	C0	120.0
C4	C5	C6	117.6(3)	C25	C24	C23	120.0
N1	C6	C5	115.5(3)	C24	C25	C26	120.0
C1	C6	N1	125.8(3)	C25	C26	C27	120.0
C1	C6	C5	118.8(3)	C28	C27	C26	120.0
O1	C7	N3	120.3(3)	C27	C28	C23	120.0
O1	C7	C1	125.3(3)	C27	C28	C29	121.2(3)
N3	C7	C1	114.4(3)	C23	C28	C29	118.7(3)
C9	C8	N3	117.6(2)	C24	C23	N4	117.4(3)
C9	C8	C13	122.4(2)	C28	C23	N4	122.6(3)
C13	C8	N3	120.0(2)	C28	C23	C24	120.0
C8	C9	C10	120.4(2)	O4	C29	N6	115.7(5)
C9	C10	C22	119.8(2)	O4	C29	C28	126.1(4)
C11	C10	C9	117.9(2)	N6	C29	C28	118.2(5)
C11	C10	C22	122.3(2)	C31	C30	N6	117.5(2)
C12	C11	C10	121.0(2)	C31	C30	C35	122.4(2)

Table 5 Bond Angles for 5ba.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C11	C12	C13	121.8(2)	C35	C30	N6	120.0(2)
C8	C13	C14	122.9(2)	C30	C31	C32	120.9(2)
C12	C13	C8	116.5(2)	C31	C32	C33	117.5(2)
C12	C13	C14	120.5(2)	C31	C32	C37	121.3(2)
C15	C14	C13	118.4(2)	C33	C32	C37	121.2(2)
C18	C14	C13	122.2(2)	C34	C33	C32	121.1(2)
C18	C14	C15	119.1(2)	C33	C34	C35	122.0(2)
O2	C15	C14	121.1(2)	C30	C35	C36	123.0(2)
O2	C15	C16	119.4(2)	C34	C35	C30	116.1(2)
C14	C15	C16	119.3(2)	C34	C35	C36	120.8(2)
C15	C16	C17	114.4(2)	C38	C36	C35	119.7(2)
C19	C17	C16	107.6(2)	C42	C36	C35	121.0(2)
C19	C17	C20	110.4(2)	C42	C36	C38	119.3(2)
C19	C17	C21	109.7(2)	O6	C38	C36	122.2(2)
C20	C17	C16	110.3(2)	O6	C38	C39	119.6(2)
C20	C17	C21	109.1(2)	C36	C38	C39	118.0(2)
C21	C17	C16	109.7(2)	C38	C39	C40	113.9(2)
O3	C18	C14	119.6(2)	C39	C40	C43	107.9(3)
O3	C18	C19	117.4(2)	C41	C40	C39	109.3(2)
C14	C18	C19	123.0(2)	C41	C40	C43	108.7(3)
C18	C19	C17	115.0(2)	C44	C40	C39	111.8(3)
N7	N00F	N6	116.3(8)	C44	C40	C41	111.5(3)
N5	N4	C23	120.4(5)	C44	C40	C43	107.4(3)
N4	N5	N6	118.9(6)	C42	C41	C40	114.9(2)
C29	N6	N5	121.0(4)	O5	C42	C36	118.3(2)
C29	N6	C30	131.4(3)	O5	C42	C41	117.3(2)
C30	N6	N00F	103.6(4)	C36	C42	C41	124.4(2)
C30	N6	N5	107.6(3)	OA	C45	N6	114.7(7)
C45	N6	N00F	125.1(5)	OA	C45	C00{	129.5(7)
C45	N6	C30	130.7(4)	N6	C45	C00{	115.8(6)

Table 6 Torsion Angles for 5ba.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O2	C15	C16	C17	-153.2(2)	N5	N6	C30	C35	-117.1(4)
O3	C18	C19	C17	161.9(2)	N6	N00F	N7	C46	-4.8(10)
N1	N2	N3	C7	-4.4(4)	N6	C30	C31	C32	-179.9(2)
N1	N2	N3	C8	177.5(2)	N6	C30	C35	C34	-179.0(2)
N2	N1	C6	C1	5.5(5)	N6	C30	C35	C36	2.6(4)

Table 6 Torsion Angles for 5ba.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N2	N1	C6	C5	-174.4(3)	N7	N00F	N6	C30	177.0(6)
N2	N3	C7	O1	-170.3(2)	N7	N00F	N6	C45	4.4(10)
N2	N3	C7	C1	9.1(4)	N7	C46	C00{	C01L	-178.7(6)
N2	N3	C8	C9	56.9(3)	N7	C46	C00{	C45	0.2(6)
N2	N3	C8	C13	-120.6(2)	C0	C47	C46	N7	178.8(6)
N3	C8	C9	C10	-178.5(2)	C0	C47	C46	C00{	0.0
N3	C8	C13	C12	179.6(2)	C47	C0	C48	C01L	0.0
N3	C8	C13	C14	3.3(4)	C47	C46	C00{	C01L	0.0
C1	C2	C3	C4	-2.5(5)	C47	C46	C00{	C45	178.9(7)
C2	C1	C6	N1	-178.9(3)	C46	C00{	C01L	C48	0.0
C2	C1	C6	C5	1.1(4)	C46	C00{	C45	OA	179.5(12)
C2	C1	C7	O1	-8.4(4)	C46	C00{	C45	N6	-0.8(10)
C2	C1	C7	N3	172.2(3)	C00{	C01L	C48	C0	0.0
C2	C3	C4	C5	1.9(5)	C01L	C00{	C45	OA	-1.5(17)
C3	C4	C5	C6	0.3(5)	C01L	C00{	C45	N6	178.2(5)
C4	C5	C6	N1	178.3(3)	C48	C0	C47	C46	0.0
C4	C5	C6	C1	-1.7(4)	C24	C25	C26	C27	0.0
C6	N1	N2	N3	-3.3(4)	C25	C24	C23	N4	-179.3(4)
C6	C1	C2	C3	1.0(4)	C25	C24	C23	C28	0.0
C6	C1	C7	O1	173.0(3)	C25	C26	C27	C28	0.0
C6	C1	C7	N3	-6.4(3)	C26	C27	C28	C23	0.0
C7	N3	C8	C9	-121.3(3)	C26	C27	C28	C29	175.3(5)
C7	N3	C8	C13	61.2(3)	C27	C28	C23	N4	179.2(4)
C7	C1	C2	C3	-177.5(3)	C27	C28	C23	C24	0.0
C7	C1	C6	N1	-0.2(4)	C27	C28	C29	O4	3.1(8)
C7	C1	C6	C5	179.7(2)	C27	C28	C29	N6	-175.1(3)
C8	N3	C7	O1	7.6(4)	C23	N4	N5	N6	-2.6(9)
C8	N3	C7	C1	-172.9(2)	C23	C24	C25	C26	0.0
C8	C9	C10	C11	-0.8(4)	C23	C28	C29	O4	178.5(6)
C8	C9	C10	C22	178.4(2)	C23	C28	C29	N6	0.2(6)
C8	C13	C14	C15	61.2(3)	C29	N6	C30	C31	-115.2(4)
C8	C13	C14	C18	-124.9(3)	C29	N6	C30	C35	64.0(5)
C9	C8	C13	C12	2.2(4)	C29	C28	C23	N4	3.8(4)
C9	C8	C13	C14	-174.1(2)	C29	C28	C23	C24	-175.5(5)
C9	C10	C11	C12	1.4(4)	C30	N6	C29	O4	-4.8(8)
C10	C11	C12	C13	-0.2(4)	C30	N6	C29	C28	173.6(3)
C11	C12	C13	C8	-1.6(4)	C30	N6	C45	OA	7.9(15)
C11	C12	C13	C14	174.8(2)	C30	N6	C45	C00{	-171.8(4)

Table 6 Torsion Angles for 5ba.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C12	C13	C14	C15	-115.0(3)	C30	C31	C32	C33	-1.1(4)
C12	C13	C14	C18	58.9(3)	C30	C31	C32	C37	-179.7(2)
C13	C8	C9	C10	-1.0(4)	C30	C35	C36	C38	-117.2(3)
C13	C14	C15	O2	-2.7(4)	C30	C35	C36	C42	64.5(3)
C13	C14	C15	C16	173.6(2)	C31	C30	C35	C34	0.2(4)
C13	C14	C18	O3	-0.7(4)	C31	C30	C35	C36	-178.2(2)
C13	C14	C18	C19	-178.8(2)	C31	C32	C33	C34	0.2(4)
C14	C15	C16	C17	30.5(3)	C32	C33	C34	C35	0.8(4)
C14	C18	C19	C17	-20.0(4)	C33	C34	C35	C30	-1.0(4)
C15	C14	C18	O3	173.1(2)	C33	C34	C35	C36	177.4(2)
C15	C14	C18	C19	-5.0(4)	C34	C35	C36	C38	64.5(3)
C15	C16	C17	C19	-51.5(3)	C34	C35	C36	C42	-113.8(3)
C15	C16	C17	C20	69.0(3)	C35	C30	C31	C32	0.9(4)
C15	C16	C17	C21	-170.7(2)	C35	C36	C38	O6	4.0(4)
C16	C17	C19	C18	46.3(3)	C35	C36	C38	C39	-171.0(3)
C18	C14	C15	O2	-176.8(2)	C35	C36	C42	O5	3.3(4)
C18	C14	C15	C16	-0.5(4)	C35	C36	C42	C41	-178.7(3)
C20	C17	C19	C18	-74.1(3)	C36	C38	C39	C40	-35.8(4)
C21	C17	C19	C18	165.6(2)	C37	C32	C33	C34	178.9(2)
C22	C10	C11	C12	-177.7(3)	C38	C36	C42	O5	-175.0(2)
O6	C38	C39	C40	149.1(3)	C38	C36	C42	C41	3.0(4)
N00F	N6	C30	C31	-113.0(4)	C38	C39	C40	C41	51.6(4)
N00F	N6	C30	C35	66.3(4)	C38	C39	C40	C43	-66.5(3)
N00F	N6	C45	OA	178.3(10)	C38	C39	C40	C44	175.6(3)
N00F	N6	C45	C00{	-1.4(10)	C39	C40	C41	C42	-41.5(4)
N00F	N7	C46	C47	-175.7(6)	C40	C41	C42	O5	-166.4(3)
N00F	N7	C46	C00{	3.0(8)	C40	C41	C42	C36	15.6(4)
N4	N5	N6	C29	6.6(8)	C42	C36	C38	O6	-177.7(3)
N4	N5	N6	C30	-172.4(5)	C42	C36	C38	C39	7.3(4)
N5	N4	C23	C24	177.0(5)	C43	C40	C41	C42	76.1(3)
N5	N4	C23	C28	-2.3(7)	C44	C40	C41	C42	-165.6(3)
N5	N6	C29	O4	176.6(6)	C45	N6	C30	C31	58.9(7)
N5	N6	C29	C28	-5.0(7)	C45	N6	C30	C35	-121.8(6)
N5	N6	C30	C31	63.6(4)	C45	C00{	C01L	C48	-178.9(7)

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 5ba.

Atom	*x*	*y*	*z*	U(eq)

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 5ba.

Atom	*x*	*y*	*z*	U(eq)
H3	11288.75	6591.62	9770.03	49
H2	9306.62	8570.53	7767.55	54
H3A	9370.03	9607.71	7252.59	63
H4	8139.88	10463.4	7649.98	60
H5A	6866.42	10318.57	8642.74	57
H9	5473.13	7559.61	9974.16	31
H11	7158.64	6253.71	11369.17	36
H12	9098.77	6705.65	11127.86	35
H16A	11636.11	8662.29	10987.31	37
H16B	11100.61	9212.31	10428.97	37
H19A	12395.04	7490.61	9563.15	39
H19B	12572.96	7564.14	10423.35	39
H20A	10651	8466.49	9091.97	57
H20B	12048.84	8467.27	8800.05	57
H20C	11479.28	9132.92	9135.24	57
H21A	13358.56	9194.2	9998.88	57
H21B	13890.79	8524.37	9652.88	57
H21C	13709.51	8569.93	10508.51	57
H22A	4372.47	6928.73	11155.35	56
H22B	4920.54	6185.37	11158.98	56
H22C	4347.09	6502.94	10421.08	56
H5	4175.1	5928.87	6674.31	46
H0	5513.47	9581.05	6868.5	44
H47	4451.59	9129.6	7840.93	45
H01L	7245.99	7807.08	6571.35	39
H48	6910.69	8919.77	6233.7	44
H24	6984	8484.67	6441.19	37
H25	5971.93	9501.13	6638.35	46
H26	4512.3	9589.63	7549.64	43
H27	4064.73	8661.67	8263.77	34
H31	7677.04	6464.37	8818.92	32
H33	6236.76	4759.18	9606.99	33
H34	4286.75	5025.82	9078.52	32
H37A	9066.63	5375.31	9254.39	52
H37B	8377.14	4993	9888.13	52
H37C	8685.39	5771.46	9965.89	52
H39A	596.14	6443.79	8597.91	51

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 5ba.

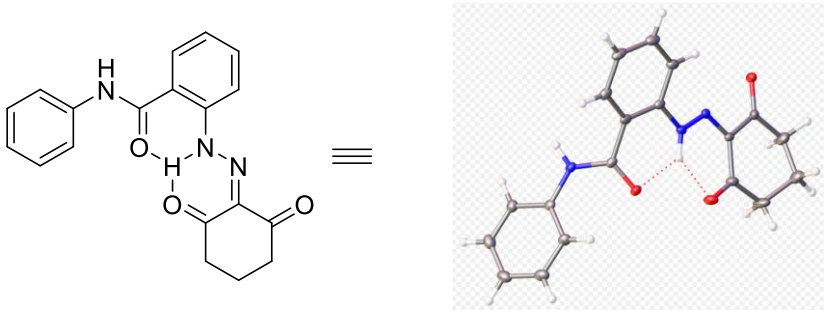
Atom	*x*	*y*	*z*	U(eq)
H39B	829.79	5735.68	8229.01	51
H41A	1829.34	5779.46	6894.14	47
H41B	2358.46	6497.4	6688.15	47
H43A	2372.02	7299.81	7907.95	78
H43B	913.06	7483.52	7962.28	78
H43C	1552.71	7494.98	7191.83	78
H44A	-58.77	6746.41	6699.36	94
H44B	-713.25	6717.75	7464.87	94
H44C	-334.34	6041.67	7067.72	94

Table 8 Atomic Occupancy for 5ba.

Atom	*Occupancy*	Atom	*Occupancy*	Atom	*Occupancy*
O4	0.544(4)	OA	0.456(4)	N00F	0.456(4)
N4	0.544(4)	N5	0.544(4)	N7	0.456(4)
C0	0.456(4)	H0	0.456(4)	C47	0.456(4)
H47	0.456(4)	C46	0.456(4)	C00{	0.456(4)
C01L	0.456(4)	H01L	0.456(4)	C48	0.456(4)
H48	0.456(4)	C24	0.544(4)	H24	0.544(4)
C25	0.544(4)	H25	0.544(4)	C26	0.544(4)
H26	0.544(4)	C27	0.544(4)	H27	0.544(4)
C28	0.544(4)	C23	0.544(4)	C29	0.544(4)
C45	0.456(4)				

Table 9 Solvent masks information for 5ba.

Number	X	Y	Z	Volume	Electron count	Content
1	-0.197	0.524	0.315	69.4	6.3	?
2	0.197	0.476	0.685	69.4	6.3	?
3	0.303	0.976	0.815	69.4	6.3	?
4	0.697	0.024	0.185	69.4	6.3	?



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The crystal structure of **6ab** by X-ray analysis.

X-ray-quality crystal was obtained by slow diffusion of Petroleum ether into a dilute dichloromethane solution of **6ab** at room temperature under air. Thermal ellipsoids drawn at the 50 % probability level. Crystal data were obtained on a SuperNova, Dual, Cu at zero, AtlasS2 diffractometer using Mo Kα radiation (λ = 0.71073 Å). The crystal was kept at 200.00(10) K during data collection.

Table 1 Crystal data and structure refinement for 6ab.

Identification code	**6ab**
Empirical formula	$C_{20}H_{18}Cl_3N_3O_3$
Formula weight	454.72
Temperature/K	150.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	10.2448(4)
b/Å	14.5349(5)
c/Å	14.7931(5)
α/°	70.151(3)
β/°	89.702(3)
γ/°	85.415(3)
Volume/Å^3	2064.74(13)
Z	4
ρ_{calc}g/cm^3	1.463
μ/mm^{-1}	4.254
F(000)	936.0
Crystal size/mm^3	0.15 × 0.13 × 0.12
Radiation	Cu Kα (λ = 1.54184)

2Θ range for data collection/°	6.354 to 147.526
Index ranges	$-12 \le h \le 11$, $-18 \le k \le 16$, $-18 \le l \le 17$
Reflections collected	14771
Independent reflections	8122 [R_{int} = 0.0411, R_{sigma} = 0.0491]
Data/restraints/parameters	8122/7/527
Goodness-of-fit on F^2	1.055
Final R indexes [I>=2σ (I)]	R_1 = 0.0590, wR_2 = 0.1578
Final R indexes [all data]	R_1 = 0.0673, wR_2 = 0.1692
Largest diff. peak/hole / e Å^{-3}	1.09/-0.69

Crystal structure determination of 6ab

Crystal Data for $C_{20}H_{18}Cl_3N_3O_3$ (*M* =454.72 g/mol): triclinic, space group P-1 (no. 2), *a* = 10.2448(4) Å, *b* = 14.5349(5) Å, *c* = 14.7931(5) Å, *α* = 70.151(3)°, *β* = 89.702(3)°, *γ* = 85.415(3)°, *V* = 2064.74(13) Å^3, *Z* = 4, *T* = 150.00(10) K, μ(Cu Kα) = 4.254 mm^{-1}, *Dcalc* = 1.463 g/cm^3, 14771 reflections measured (6.354° ≤ 2Θ ≤ 147.526°), 8122 unique (R_{int} = 0.0411, R_{sigma} = 0.0491) which were used in all calculations. The final R_1 was 0.0590 (I > 2σ(I)) and wR_2 was 0.1692 (all data).

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 6ab. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Cl1	1026.8(8)	840.0(6)	-224.7(7)	54.4(2)
Cl2	3216.3(11)	835.3(8)	-1453.9(7)	70.0(3)
Cl3	3642.0(9)	891.1(7)	452.7(7)	60.9(2)
C40	2557(3)	1259(2)	-549(2)	41.3(6)
Cl4	1798.9(7)	3310.2(5)	300.2(5)	44.62(19)
Cl5	4576.5(8)	3455.7(7)	446.1(6)	53.8(2)
Cl6	2742.7(9)	4562.0(6)	1254.4(6)	55.5(2)
C39	3068(3)	3463(2)	1018.3(19)	38.5(6)
O1	8010.8(18)	2952.5(15)	6249.0(14)	38.1(4)
O2	6008(2)	4205.4(16)	4599.8(16)	48.0(5)
O3	7902.4(19)	6643.5(16)	2091.4(14)	41.4(5)
N1	9550(2)	3053.0(16)	7307.0(16)	33.1(5)
N2	8517(2)	4319.0(16)	4468.3(16)	30.0(4)
N3	8285(2)	5050.8(16)	3673.1(15)	29.5(4)
C1	8833(2)	2768.6(18)	8161.7(19)	30.9(5)
C2	9069(3)	3196(2)	8846(2)	38.8(6)

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 6ab. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C3	8431(3)	2904(3)	9716(2)	49.7(8)
C4	7550(3)	2195(2)	9902(2)	49.5(8)
C5	7317(3)	1772(2)	9219(2)	47.7(7)
C6	7949(3)	2055(2)	8352(2)	39.4(6)
C7	9128(2)	3099.5(18)	6427(2)	30.8(5)
C8	10144(2)	3330.6(18)	5668(2)	31.4(5)
C9	11431(3)	2932(2)	5890(2)	38.3(6)
C10	12373(3)	3117(2)	5185(3)	46.8(8)
C11	12034(3)	3702(2)	4257(3)	46.9(7)
C12	10773(3)	4129(2)	4021(2)	38.7(6)
C13	9822(2)	3925.9(19)	4723(2)	30.8(5)
C14	7066(2)	5373.7(19)	3377.5(18)	30.3(5)
C15	6943(3)	6234(2)	2484.3(19)	36.4(6)
C16	5592(3)	6635(3)	2079(3)	57.0(7)
C17	4605(3)	5928(3)	2319(3)	59.0(7)
C18	4590(3)	5365(3)	3394(3)	70.2(12)
C19	5898(3)	4925(2)	3849(2)	42.0(7)
O4	4591.0(17)	2571.9(13)	3503.3(14)	35.0(4)
O5	2233(2)	1814.4(15)	2774.2(14)	42.4(5)
O6	916.0(19)	-1148.4(14)	4912.1(14)	40.2(5)
N4	6770.9(19)	2283.4(14)	3923.8(15)	26.7(4)
N5	3298.5(19)	975.1(14)	4480.6(14)	25.6(4)
N6	2456.5(19)	318.1(14)	4604.7(14)	24.0(4)
C20	7343(2)	2927.2(17)	3092.0(17)	26.3(5)
C21	6628(3)	3588(2)	2320.2(19)	34.3(6)
C22	7276(3)	4202(2)	1550(2)	39.5(6)
C23	8625(3)	4163(2)	1541.2(19)	36.5(6)
C24	9337(3)	3500(2)	2310(2)	33.5(6)
C25	8705(2)	2887.9(18)	3087.4(18)	29.0(5)
C26	5485(2)	2176.0(16)	4095.0(18)	26.0(5)
C27	5207(2)	1503.3(17)	5086.5(17)	25.2(5)
C28	5972(2)	1469.1(19)	5875.3(19)	30.2(5)
C29	5776(3)	810(2)	6783.9(19)	34.9(6)
C30	4813(3)	161(2)	6908.6(18)	32.5(5)
C31	3989(2)	213.0(18)	6154.5(17)	27.7(5)
C32	4158(2)	895.5(16)	5242.8(17)	24.1(5)

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 6ab. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C33	1615(2)	368.1(17)	3917.5(17)	25.4(5)
C34	1516(2)	1139.3(18)	2968.6(18)	30.3(5)
C35	534(3)	1070(2)	2245(2)	40.0(6)
C36	-660(3)	546(2)	2718(2)	45.6(7)
C37	-242(3)	-457(2)	3422(2)	36.7(6)
C38	771(2)	-464.1(18)	4157.1(18)	29.2(5)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 6ab. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl1	39.6(4)	57.2(5)	62.7(5)	-16.3(4)	1.7(3)	-0.8(3)
Cl2	84.6(7)	70.3(6)	63.0(6)	-35.4(5)	23.9(5)	2.3(5)
Cl3	57.2(5)	55.5(5)	66.1(5)	-16.7(4)	-19.6(4)	1.5(4)
C40	48.8(17)	36.8(14)	36.7(14)	-11.7(12)	3.8(12)	2.7(12)
Cl4	43.4(4)	44.1(4)	46.1(4)	-14.2(3)	-3.1(3)	-6.9(3)
Cl5	40.1(4)	74.0(5)	44.6(4)	-16.0(4)	3.7(3)	-6.6(4)
Cl6	74.3(6)	46.4(4)	51.2(4)	-22.3(3)	5.2(4)	-12.3(4)
C39	44.1(15)	38.0(14)	27.6(12)	-2.6(11)	2.4(11)	-8.0(12)
O1	30.0(9)	47.3(11)	38.5(10)	-14.2(9)	-0.7(8)	-12.9(8)
O2	37.4(11)	50.1(12)	49.4(12)	-5.5(10)	12.1(9)	-14.0(9)
O3	32.9(10)	55.5(12)	30.5(9)	-5.3(9)	-0.5(8)	-14.4(9)
N1	26.1(10)	35.1(11)	37.2(12)	-10.5(9)	-4.0(9)	-5.7(9)
N2	29.8(11)	33.0(11)	30.9(11)	-14.5(9)	5.9(9)	-7.9(9)
N3	32.2(11)	34.9(11)	26.6(10)	-15.6(9)	3.4(8)	-10.2(9)
C1	24.9(12)	28.1(12)	35.4(13)	-6.2(10)	-4.5(10)	3.2(9)
C2	37.0(14)	38.7(14)	40.4(15)	-14.2(12)	-4.1(11)	1.4(11)
C3	52.8(19)	54.4(19)	42.7(16)	-21.0(14)	-1.7(14)	10.8(15)
C4	42.3(17)	53.0(18)	43.0(16)	-5.8(14)	8.7(13)	6.6(14)
C5	39.1(16)	39.9(16)	52.5(18)	-1.1(13)	4.8(13)	-1.6(12)
C6	39.3(15)	31.0(13)	43.7(15)	-7.2(11)	-0.2(12)	-3.5(11)
C7	27.2(12)	24.9(12)	41.1(14)	-12.4(10)	-2.8(10)	-1.8(9)
C8	30.5(13)	26.0(12)	45.0(14)	-20.5(11)	4.5(11)	-7.1(10)
C9	31.6(13)	31.8(13)	59.3(18)	-26.2(13)	-2.1(12)	-0.5(10)
C10	26.8(13)	47.4(17)	81(2)	-41.2(17)	6.6(14)	-1.9(12)
C11	37.4(15)	49.3(17)	68(2)	-36.7(16)	17.1(14)	-11.0(13)
C12	35.4(14)	41.2(15)	46.6(16)	-22.7(13)	12.6(12)	-11.0(12)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 6ab. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C13	27.8(12)	30.4(12)	42.4(14)	-22.3(11)	4.9(10)	-5.7(10)
C14	27.1(12)	37.7(13)	31.3(12)	-16.9(11)	4.8(10)	-9.7(10)
C15	31.7(13)	52.2(16)	27.4(12)	-14.6(12)	0.7(10)	-11.3(12)
C16	35.9(12)	69.7(16)	57.1(15)	-10.0(13)	-8.7(11)	-8.1(11)
C17	36.8(12)	69.7(16)	61.3(15)	-9.7(13)	-8.7(11)	-7.8(11)
C18	30.0(16)	90(3)	68(2)	4(2)	8.6(16)	-13.3(17)
C19	33.2(14)	50.4(17)	43.9(16)	-16.1(13)	11.9(12)	-12.9(12)
O4	23.5(9)	31.4(9)	41.4(10)	-1.1(8)	-1.7(7)	-2.6(7)
O5	41.6(11)	39.6(11)	35.0(10)	4.6(8)	-4.3(8)	-16.3(9)
O6	35.5(10)	34.8(10)	38.6(10)	4.6(8)	-5.9(8)	-11.4(8)
N4	22.9(10)	26.1(10)	27.6(10)	-4.3(8)	1.3(8)	-4.0(8)
N5	22.9(9)	24.1(9)	26.5(10)	-4.2(8)	3.0(8)	-3.7(7)
N6	21.5(9)	23.7(9)	26.9(9)	-8.6(8)	3.6(7)	-1.9(7)
C20	29.1(12)	24.2(11)	27.7(11)	-10.1(9)	2.5(9)	-8.8(9)
C21	31.7(13)	35.0(13)	31.7(13)	-5.0(11)	-0.3(10)	-5.0(10)
C22	45.3(16)	36.9(14)	29.6(13)	-2.1(11)	-0.8(11)	-5.8(12)
C23	46.5(16)	35.9(14)	28.5(12)	-10.7(11)	9.1(11)	-13.3(12)
C24	33.0(13)	34.2(13)	36.1(13)	-13.8(11)	9.1(10)	-11.3(10)
C25	29.2(12)	26.8(11)	29.4(12)	-6.7(10)	2.2(9)	-5.3(9)
C26	23.6(11)	21.6(11)	33.3(12)	-9.6(9)	2.4(9)	-3.0(9)
C27	22.8(11)	23.5(11)	29.7(12)	-9.9(9)	5.0(9)	0.0(9)
C28	27.5(12)	33.3(13)	35.2(13)	-18.5(11)	5.0(10)	-4.5(10)
C29	32.9(13)	49.1(15)	28.4(12)	-20.1(11)	2.8(10)	-5.9(11)
C30	32.9(13)	40.8(14)	24.3(12)	-11.4(10)	5.2(10)	-3.8(11)
C31	26.6(12)	30.4(12)	27.0(12)	-10.5(10)	7.1(9)	-5.0(9)
C32	21.5(11)	22.8(11)	28.4(11)	-9.8(9)	2.7(9)	0.5(8)
C33	22.7(11)	24.8(11)	26.3(11)	-6.1(9)	2.3(9)	-0.7(9)
C34	29.8(12)	30.0(12)	26.7(12)	-3.7(10)	1.7(9)	-2.6(10)
C35	44.7(16)	40.9(15)	30.0(13)	-4.9(11)	-6.1(11)	-8.6(12)
C36	43.8(16)	45.0(16)	44.3(16)	-9.5(13)	-11.1(13)	-7.1(13)
C37	35.4(14)	34.4(13)	38.6(14)	-9.0(11)	-4.3(11)	-7.4(11)
C38	24.1(11)	28.5(12)	33.5(13)	-8.3(10)	2.9(9)	-2.8(9)

Table 4 Bond Lengths for 6ab .

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl1	C40	1.734(3)	C16	C17	1.456(5)
Cl2	C40	1.764(3)	C17	C18	1.522(5)

Table 4 Bond Lengths for 6ab .

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl3	C40	1.761(3)	C18	C19	1.496(5)
Cl4	C39	1.757(3)	O4	C26	1.232(3)
Cl5	C39	1.760(3)	O5	C34	1.227(3)
Cl6	C39	1.754(3)	O6	C38	1.218(3)
O1	C7	1.227(3)	N4	C20	1.425(3)
O2	C19	1.238(4)	N4	C26	1.351(3)
O3	C15	1.229(3)	N5	N6	1.304(3)
N1	C1	1.412(3)	N5	C32	1.402(3)
N1	C7	1.352(3)	N6	C33	1.316(3)
N2	N3	1.298(3)	C20	C21	1.383(4)
N2	C13	1.411(3)	C20	C25	1.392(3)
N3	C14	1.320(3)	C21	C22	1.389(4)
C1	C2	1.387(4)	C22	C23	1.379(4)
C1	C6	1.387(4)	C23	C24	1.381(4)
C2	C3	1.389(4)	C24	C25	1.386(3)
C3	C4	1.381(5)	C26	C27	1.502(3)
C4	C5	1.379(5)	C27	C28	1.394(3)
C5	C6	1.382(4)	C27	C32	1.414(3)
C7	C8	1.499(4)	C28	C29	1.385(4)
C8	C9	1.391(4)	C29	C30	1.388(4)
C8	C13	1.396(4)	C30	C31	1.380(4)
C9	C10	1.390(4)	C31	C32	1.396(3)
C10	C11	1.376(5)	C33	C34	1.467(3)
C11	C12	1.380(4)	C33	C38	1.486(3)
C12	C13	1.393(4)	C34	C35	1.506(4)
C14	C15	1.477(4)	C35	C36	1.531(4)
C14	C19	1.467(4)	C36	C37	1.506(4)
C15	C16	1.503(4)	C37	C38	1.504(4)

Table 5 Bond Angles for 6ab.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Cl1	C40	Cl2	110.89(17)	O2	C19	C14	120.3(3)
Cl1	C40	Cl3	111.02(16)	O2	C19	C18	121.9(3)
Cl3	C40	Cl2	109.88(17)	C14	C19	C18	117.8(3)
Cl4	C39	Cl5	110.22(16)	C26	N4	C20	127.8(2)
Cl6	C39	Cl4	110.04(17)	N6	N5	C32	118.72(19)
Cl6	C39	Cl5	110.61(15)	N5	N6	C33	121.1(2)
C7	N1	C1	126.4(2)	C21	C20	N4	124.0(2)

Table 5 Bond Angles for 6ab.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N3	N2	C13	119.0(2)	C21	C20	C25	119.4(2)
N2	N3	C14	120.1(2)	C25	C20	N4	116.5(2)
C2	C1	N1	118.2(2)	C20	C21	C22	119.8(3)
C2	C1	C6	119.4(3)	C23	C22	C21	121.0(3)
C6	C1	N1	122.4(3)	C22	C23	C24	119.2(2)
C1	C2	C3	120.1(3)	C23	C24	C25	120.5(2)
C4	C3	C2	120.3(3)	C24	C25	C20	120.1(2)
C5	C4	C3	119.4(3)	O4	C26	N4	124.7(2)
C4	C5	C6	120.7(3)	O4	C26	C27	121.1(2)
C5	C6	C1	120.0(3)	N4	C26	C27	114.3(2)
O1	C7	N1	123.7(3)	C28	C27	C26	120.7(2)
O1	C7	C8	121.5(2)	C28	C27	C32	118.5(2)
N1	C7	C8	114.8(2)	C32	C27	C26	120.8(2)
C9	C8	C7	120.2(3)	C29	C28	C27	121.2(2)
C9	C8	C13	118.6(3)	C28	C29	C30	119.4(2)
C13	C8	C7	121.2(2)	C31	C30	C29	120.8(2)
C10	C9	C8	120.7(3)	C30	C31	C32	119.9(2)
C11	C10	C9	119.9(3)	N5	C32	C27	119.9(2)
C10	C11	C12	120.7(3)	C31	C32	N5	120.3(2)
C11	C12	C13	119.4(3)	C31	C32	C27	119.8(2)
C8	C13	N2	120.0(2)	N6	C33	C34	124.9(2)
C12	C13	N2	119.3(3)	N6	C33	C38	114.3(2)
C12	C13	C8	120.7(3)	C34	C33	C38	120.8(2)
N3	C14	C15	114.4(2)	O5	C34	C33	120.2(2)
N3	C14	C19	124.9(3)	O5	C34	C35	121.4(2)
C19	C14	C15	120.6(2)	C33	C34	C35	118.4(2)
O3	C15	C14	121.9(2)	C34	C35	C36	112.6(2)
O3	C15	C16	119.9(3)	C37	C36	C35	110.6(3)
C14	C15	C16	118.1(2)	C38	C37	C36	114.5(2)
C17	C16	C15	115.3(3)	O6	C38	C33	121.4(2)
C16	C17	C18	111.9(3)	O6	C38	C37	120.6(2)
C19	C18	C17	115.1(3)	C33	C38	C37	118.0(2)

Table 6 Torsion Angles for 6ab.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	C7	C8	C9	-140.3(3)	O4	C26	C27	C28	-145.5(2)
O1	C7	C8	C13	38.1(4)	O4	C26	C27	C32	34.1(3)
O3	C15	C16	C17	155.9(3)	O5	C34	C35	C36	-151.4(3)

Table 6 Torsion Angles for 6ab.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N1	C1	C2	C3	-177.0(3)	N4	C20	C21	C22	178.5(2)
N1	C1	C6	C5	177.0(3)	N4	C20	C25	C24	-179.1(2)
N1	C7	C8	C9	38.7(3)	N4	C26	C27	C28	35.5(3)
N1	C7	C8	C13	-143.0(2)	N4	C26	C27	C32	-145.0(2)
N2	N3	C14	C15	177.6(2)	N5	N6	C33	C34	-0.4(4)
N2	N3	C14	C19	-4.4(4)	N5	N6	C33	C38	177.0(2)
N3	N2	C13	C8	163.0(2)	N6	N5	C32	C27	170.4(2)
N3	N2	C13	C12	-17.8(3)	N6	N5	C32	C31	-9.1(3)
N3	C14	C15	O3	-4.3(4)	N6	C33	C34	O5	-1.6(4)
N3	C14	C15	C16	178.3(3)	N6	C33	C34	C35	177.6(2)
N3	C14	C19	O2	2.4(5)	N6	C33	C38	O6	-3.5(4)
N3	C14	C19	C18	-177.7(3)	N6	C33	C38	C37	178.6(2)
C1	N1	C7	O1	4.7(4)	C20	N4	C26	O4	6.7(4)
C1	N1	C7	C8	-174.3(2)	C20	N4	C26	C27	-174.3(2)
C1	C2	C3	C4	-0.6(5)	C20	C21	C22	C23	0.2(4)
C2	C1	C6	C5	-0.4(4)	C21	C20	C25	C24	-0.6(4)
C2	C3	C4	C5	0.5(5)	C21	C22	C23	C24	0.1(4)
C3	C4	C5	C6	-0.4(5)	C22	C23	C24	C25	-0.6(4)
C4	C5	C6	C1	0.4(5)	C23	C24	C25	C20	0.9(4)
C6	C1	C2	C3	0.5(4)	C25	C20	C21	C22	0.1(4)
C7	N1	C1	C2	-148.2(3)	C26	N4	C20	C21	2.4(4)
C7	N1	C1	C6	34.3(4)	C26	N4	C20	C25	-179.2(2)
C7	C8	C9	C10	178.0(2)	C26	C27	C28	C29	-176.1(2)
C7	C8	C13	N2	-0.2(3)	C26	C27	C32	N5	-5.2(3)
C7	C8	C13	C12	-179.4(2)	C26	C27	C32	C31	174.3(2)
C8	C9	C10	C11	0.1(4)	C27	C28	C29	C30	1.0(4)
C9	C8	C13	N2	178.2(2)	C28	C27	C32	N5	174.3(2)
C9	C8	C13	C12	-1.0(4)	C28	C27	C32	C31	-6.2(3)
C9	C10	C11	C12	1.6(4)	C28	C29	C30	C31	-4.8(4)
C10	C11	C12	C13	-3.0(4)	C29	C30	C31	C32	2.9(4)
C11	C12	C13	N2	-176.5(2)	C30	C31	C32	N5	-177.9(2)
C11	C12	C13	C8	2.7(4)	C30	C31	C32	C27	2.6(4)
C13	N2	N3	C14	174.0(2)	C32	N5	N6	C33	178.9(2)
C13	C8	C9	C10	-0.4(4)	C32	C27	C28	C29	4.4(4)
C14	C15	C16	C17	-26.7(5)	C33	C34	C35	C36	29.5(4)
C15	C14	C19	O2	-179.7(3)	C34	C33	C38	O6	174.0(2)
C15	C14	C19	C18	0.2(4)	C34	C33	C38	C37	-3.8(4)
C15	C16	C17	C18	50.7(5)	C34	C35	C36	C37	-55.6(4)

Table 6 Torsion Angles for 6ab.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C16	C17	C18	C19	-50.1(5)	C35	C36	C37	C38	52.8(4)
C17	C18	C19	O2	-155.5(4)	C36	C37	C38	O6	158.7(3)
C17	C18	C19	C14	24.5(5)	C36	C37	C38	C33	-23.5(4)
C19	C14	C15	O3	177.6(3)	C38	C33	C34	O5	-178.8(3)
C19	C14	C15	C16	0.2(4)	C38	C33	C34	C35	0.3(4)

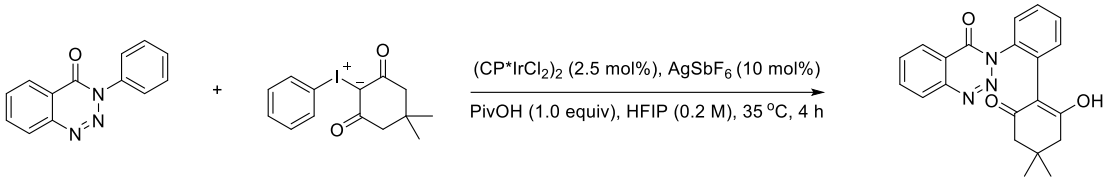
Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 6ab.

Atom	*x*	*y*	*z*	U(eq)
H40	2456.45	1993.15	-809.03	50
H39	3114.04	2904.18	1642.55	46
H1	10350.07	3216.03	7351.36	40
H2	7860(40)	4030(30)	4850(30)	78(14)
H2A	9667.53	3688.75	8719.92	47
H3	8601.33	3194.02	10185.76	60
H4	7108.12	1999.44	10495.44	59
H5	6716.17	1280.52	9346.77	57
H6	7776.84	1761.62	7885.34	47
H9	11668.31	2528.14	6529.91	46
H10	13248.52	2839.95	5343.03	56
H11	12674.31	3813.03	3772.96	56
H12	10555.21	4557.21	3386.5	46
H16A	5300.95	7179.57	2312.09	68
H16B	5640.59	6914.51	1370.16	68
H17A	4782.98	5458.67	1971.55	71
H17B	3731.64	6277.24	2102.91	71
H18A	4217.28	5815.7	3719.91	84
H18B	3999.36	4832.77	3506.03	84
H4A	7321.24	1911.13	4380.76	32
H5A	3326.48	1459.04	3929.15	31
H21	5698.36	3621.47	2316.46	41
H22	6781.65	4656.17	1022.45	47
H23	9058.99	4586.04	1012.1	44
H24	10266.74	3462.87	2307.11	40
H25	9202.39	2440.77	3617.72	35
H28	6641.43	1905.86	5788.24	36
H29	6295.07	802.23	7316.92	42
H30	4719.4	-324.94	7520.21	39

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 6ab.

Atom	*x*	*y*	*z*	U(eq)
H31	3307.41	-215.19	6255.56	33
H35A	963.82	712.32	1846.85	48
H35B	238.11	1740.31	1813.48	48
H36A	-1152.53	940.15	3056.3	55
H36B	-1247.26	481.54	2217.06	55
H37A	-1023.95	-749.47	3761.95	44
H37B	112	-879	3060.19	44

6. Scale-up experiment and mechanism studies



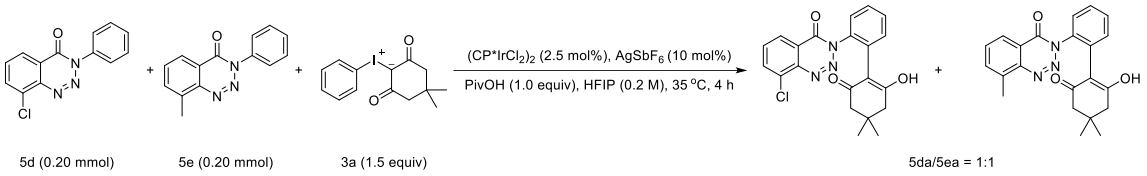
1a (2.0 mmol) **3a** (1.5 equiv) **5aa**, 679.0 mg, 94 %

In an oven-dried Schlenk tube under air, a mixture of 3-phenylbenzo[*d*][1,2,3]triazin-4(3*H*)-one **1a** (2.0 mmol, 1.0 equiv), 5,5-dimethyl-2-(phenyl-λ^3-iodaneylidene)cyclohexane-1,3-dione **3a** (3.0 mmol, 1.5 equiv), $(Cp^*IrCl_2)_2$ (39.8 mg, 0.05 mmol, 2.5 mol%), $AgSbF_6$ (68.6 mg, 0.2 mmol, 10 mol%), PivOH (204.0 mg, 2.0 mmol, 1.0 equiv) and HFIP (10.0 mL) was stirred at 35 °C (oil bath) for 4.0 h. Upon completion of reaction, the solvent was evaporated under reduced pressure and the crude product was directly purified by a silica gel column chromatography by using EA/PE = 1/1 as the eluent to afford the corresponding product **5aa** (679.0 mg, 94 %).

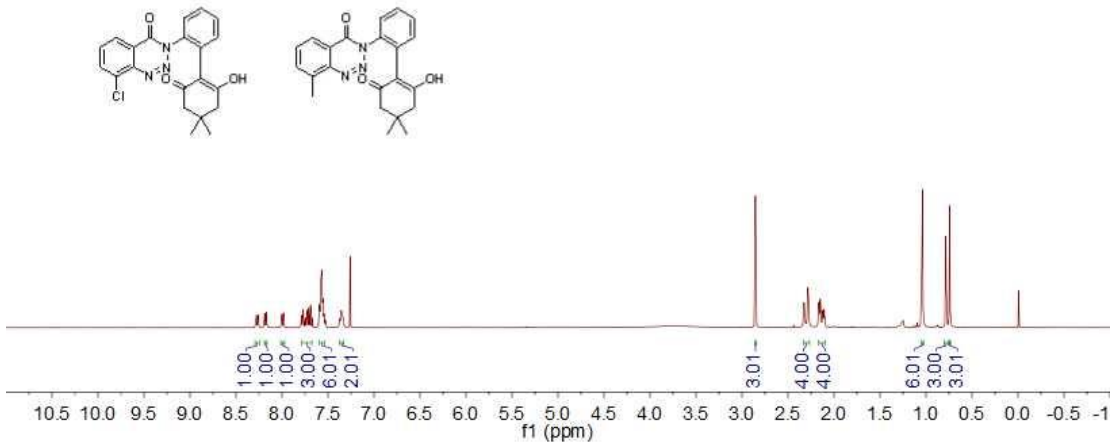
1a (2.0 mmol) **3a** (1.5 equiv) **6aa**, 592.3 mg, 81 %

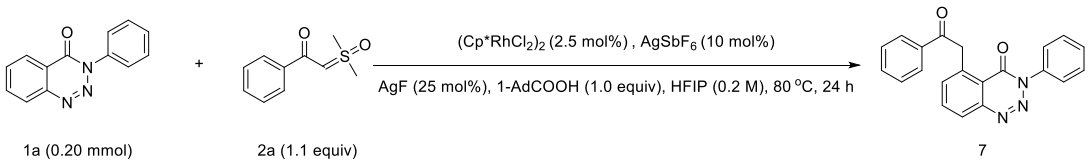
In an oven-dried Schlenk tube under air, a mixture of 3-phenylbenzo[*d*][1,2,3]triazin-4(3*H*)-one **1a** (2.0 mmol, 1.0 equiv), 5,5-dimethyl-2-(phenyl-λ^3-iodaneylidene)cyclohexane-1,3-dione **3a** (3.0 mmol, 1.5 equiv), $CuBr_2$ (44.6 mg, 0.2 mmol, 10 mol%), 4,4'-dimethyl-2,2'-bipyridine (36.8 mg, 0.2 mmol, 10 mol%), 1-AdCOOH (360.0 mg, 2.0 mmol, 1.0 equiv) and HFIP (10.0 mL) was stirred at 80 °C (oil bath) for 4.0 h. The reaction mixture was then diluted with DCM (10.0 mL) and washed with H_2O. The aqueous phase was extracted with DCM again. The organic layers were combined, washed with brine and dried over Na_2SO_4. The pure product was purified by flash column chromatography by using EA/PE = 1/2 as the eluent to afford the pure product **6aa** (592.3 mg, 81 %).

Competitive reaction between benzotriazinone substrates.

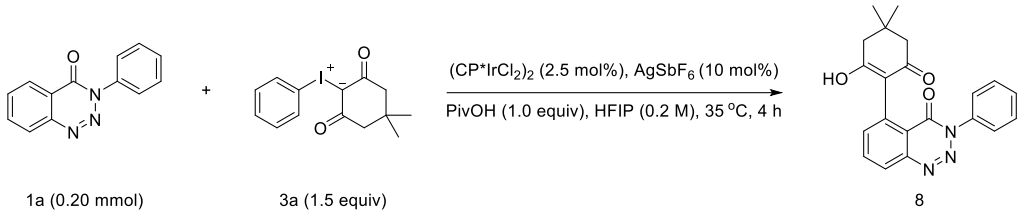


In a 10 mL oven dried reaction tube with a magnetic stir bar was charged with **5d** (51.5 mg, 0.2 mmol, 1.0 equiv), **5e** (47.5 mg, 0.2 mmol, 1.0 equiv), 5,5-dimethyl-2-(phenyl- λ^3-iodaneylidene)cyclohexane-1,3-dione **3a** (102.9 mg, 0.30 mmol, 1.5 equiv), $(Cp^*IrCl_2)_2$ (4.0 mg, 0.005 mmol, 2.5 mol%), PivOH (20.4 mg, 0.20 mmol, 1.0 equiv), $AgSbF_6$ (6.9 mg, 0.02 mmol, 10 mol%) and HFIP (1.0 mL) was added. Then, the tube was capped with septa and the resulting mixture was stirred at 35 ℃ for 4.0 h. The solvent was evaporated under reduced pressure, and **5da** and **5ea** were obtained directly by silica gel column chromatography. The mass of **5da** and **5ea** is 39.6 mg and 37.5 mg respectively.





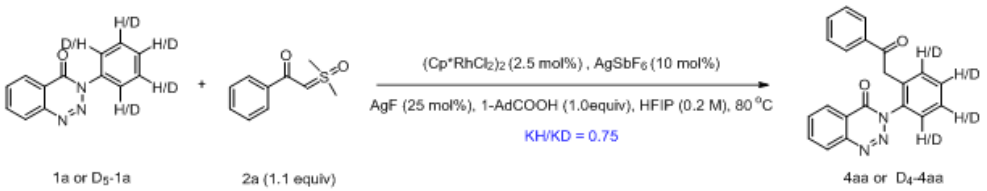
In an oven-dried Schlenk tube under air, a mixture of corresponding 3-phenylbenzo[*d*][1,2,3]triazin-4(3*H*)-one **1a** (0.20 mmol, 1.0 equiv), 2-(dimethyl(oxo)-l^6-sulfaneylidene)-1-phenylethan-1-one **2a** (0.22 mmol, 1.1 equiv), $(Cp^*RhCl_2)_2$ (3.1 mg, 0.005 mmol, 2.5 mol%), $AgSbF_6$ (6.9 mg, 0.02 mmol, 10 mol%), 1-AdCOOH (36.0 mg, 0.20 mmol, 1.0 equiv), AgF (6.3 mg, 0.05 mmol, 25 mol%), and HFIP (1.0 mL) was stirred at 80- ^{o}C (oil bath) for 24.0 h. The reaction mixture was then diluted with DCM (10.0 mL) and washed with H_2O. The aqueous phase was extracted with DCM again. The organic layers were combined, washed with brine and dried over Na_2SO_4. The pure product was purified by flash column chromatography on silica with an appropriate solvent to afford the pure product **7**, the product **7** was obtained in 0 % yield.



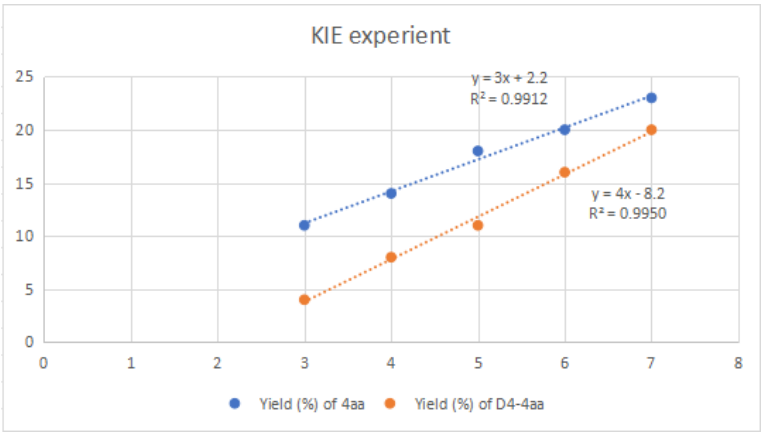
In an oven-dried Schlenk tube under air, a mixture of corresponding 3-phenylbenzo[*d*][1,2,3]triazin-4(3*H*)-one **1a** (0.20 mmol, 1.0 equiv), 5,5-dimethyl-2-(phenyl-l^3-iodaneylidene)cyclohexane-1,3-dione **3a** (0.30 mmol, 1.5 equiv), $(Cp^*IrCl_2)_2$ (4.0 mg, 0.005 mmol, 2.5 mol%), $AgSbF_6$ (6.9 mg, 0.02 mmol, 10 mol%), PivOH (20.4 mg, 0.2 mmol, 1.0 equiv) and HFIP (1.0 mL) was stirred at 35 ^{o}C (oil bath) for 4.0 h. The reaction mixture was then diluted with DCM (10.0 mL) and washed with H_2O. The aqueous phase was extracted with DCM again. The organic layers were combined, washed with brine and dried over Na_2SO_4. The pure product was purified by flash column chromatography on silica with an appropriate solvent to afford the pure product **8**, the product **8** was obtained in 0 % yield.

Conclusion: The results of competitive experiments show that the directing ability of nitrogen atoms is greater than that of carbonyl oxygen atoms, and the electrical properties of the 1,2,3-benzotriazinone have little effect on the product **5** yield.

Procedure for kinetic isotopic effect experiments



The kinetic isotope effect (KIE) was determined by measuring the initial rates of the reactions with hydrogenated and deuterated substrates. Five reactions with hydrogenated substrates and five reactions with deuterated substrates were stopped at 3.0, 4.0, 5.0, 6.0 and 7.0 h, using the following procedure: in an oven-dried Schlenk tube under air, a mixture of 3-phenylbenzo[*d*][1,2,3]triazin-4(3*H*)-one **1a** or **D_5-1a** (0.10 mmol, 1.0 equiv), 2-(dimethyl(oxo)- λ^6-sulfaneyli-dene)-1-phenylethan-1-one **2a** (21.6 mg, 0.11 mmol, 1.1 equiv), $(Cp^*RhCl_2)_2$ (1.5 mg, 0.0025 mmol, 2.5 mol%), $AgSbF_6$ (3.4 mg, 0.01 mmol, 10 mol%), 1-AdCOOH (18.0 mg, 0.10 mmol, 1.0 equiv), AgF (3.2 mg, 0.025 mmol, 25 mol%) and HFIP (0.5 mL) was stirred at 80 °C (oil bath) for the indicated time. Quickly cooled to room temperature under the ice water. the solvent was evaporated under reduced pressure and the crude product was directly purified by a silica gel column chromatography by using EA/PE = 1/4 as the eluent to afford the corresponding the yield. The K_H/K_D value was 3/4 = **0.75**.



For **4aa**: y = 3X+2.2; R^2 = 0.9912

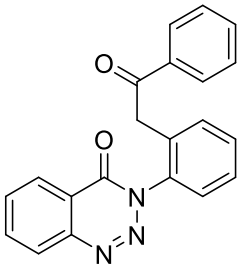
For **D_4-4aa**: y = 4X–8.2; R^2 = 0.9950

KIE = K_H/K_D = 0.75

Conclusion: KIE results indicate that the reaction rate may not undergo the first-order kinetic process.

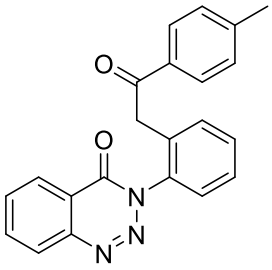
7. Product characterization

3-(2-(2-oxo-2-phenylethyl)phenyl)benzo[*d*][1,2,3]triazin-4(3*H*)-one (4aa)



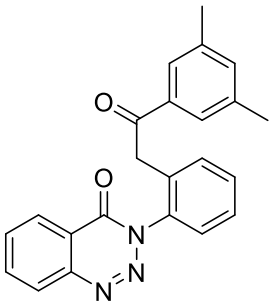
Following the above procedure 4, the product **4aa** was obtained in 78 % yield (53.2 mg, 0.156 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 4:1 v/v). Rf (Petroleum ether/EtOAc 4:1): 0.26. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 7.9 Hz, 1H), 8.12 (d, *J* = 8.1 Hz, 1H), 7.91 (t, *J* = 7.7 Hz, 1H), 7.78 (t, *J* = 8.0 Hz, 3H), 7.45 (d, 4H), 7.38 (t, *J* = 7.4 Hz, 1H), 7.26 (t, *J* = 7.3 Hz, 2H), 4.24 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.39, 155.14, 143.56, 137.76, 137.42, 136.15, 135.13, 133.07, 132.86, 132.78, 131.60, 129.96, 128.47, 128.40, 128.27, 128.24, 125.37, 120.04, 41.48. ESI-MS: calculated $C_{21}H_{16}N_3O_2$ $[M+H]^+$ 342.1237; Found 342.1230.

3-(2-(2-oxo-2-(p-tolyl)ethyl)phenyl)benzo[*d*][1,2,3]triazin-4(3*H*)-one (4ab)



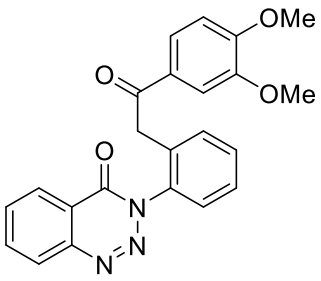
Following the above procedure 4, the product **4ab** was obtained in 52 % yield (37.3 mg, 0.104 mmol) as a yellow oil after column chromatography (eluent = Petroleum ether/EtOAc 4:1 v/v). Rf (Petroleum ether/EtOAc 4:1): 0.22. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (d, *J* = 7.9, 1.0 Hz, 1H), 8.16 (d, *J* = 7.8 Hz, 1H), 7.96 (t, *J* = 8.2, 7.8, 1.4 Hz, 1H), 7.86 – 7.77 (t, 1H), 7.68 (d, *J* = 8.2 Hz, 2H), 7.57 – 7.38 (m, 4H), 7.07 (d, *J* = 8.0 Hz, 2H), 4.21 (s, 2H), 2.29 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.26, 155.35, 144.06, 143.84, 137.88, 135.16, 133.94, 133.33, 132.83, 131.71, 130.19, 129.27, 128.70, 128.65, 128.56, 128.38, 125.67, 120.32, 41.56, 21.70. ESI-MS: calculated $C_{22}H_{18}N_3O_2$ $[M+H]^+$ 356.1394; Found 356.1389.

3-(2-(2-(3,5-dimethylphenyl)-2-oxoethyl)phenyl)benzo[*d*][1,2,3]triazin-4(3*H*)-one (4ac)



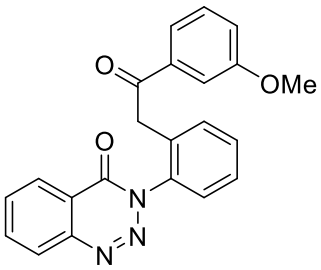
Following the above procedure 4, the product **4ac** was obtained in 55 % yield (40.6 mg, 0.110 mmol) as a yellow oil after column chromatography (eluent = Petroleum ether/EtOAc 4:1 v/v). Rf (Petroleum ether/EtOAc 4:1): 0.21. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (dd, J = 7.9, 1.2 Hz, 1H), 8.16 (d, J = 8.1 Hz, 1H), 8.00 – 7.90 (m, 1H), 7.84 – 7.76 (m, 1H), 7.55 – 7.41 (m, 4H), 7.37 (s, 2H), 7.01 (s, 1H), 4.21 (s, 2H), 2.22 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.98, 155.30, 143.76, 138.19, 137.83, 136.53, 135.17, 134.86, 133.30, 132.79, 131.74, 130.15, 128.63, 128.52, 128.35, 126.22, 125.60, 120.30, 41.53, 21.19. ESI-MS: calculated $C_{23}H_{19}N_3O_2Na$ $[M+Na]^+$ 392.1369; Found 392.1360.

3-(2-(2-(3,4-dimethoxyphenyl)-2-oxoethyl)phenyl)benzo[*d*][1,2,3]triazin-4(3*H*)-one (4ad)



Following the above procedure 4, the product **4ad** was obtained in 39 % yield (31.3 mg, 0.078 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 2:1 v/v). Rf (Petroleum ether/EtOAc 2:1): 0.25. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, *J* = 7.9 Hz, 1H), 8.14 (d, *J* = 8.1 Hz, 1H), 7.95 (t, *J* = 7.7 Hz, 1H), 7.80 (t, *J* = 7.6 Hz, 1H), 7.50 – 7.39 (m, 5H), 7.32 (d, *J* = 1.6 Hz, 1H), 6.65 (d, *J* = 8.4 Hz, 1H), 4.18 (s, 2H), 3.83 (d, *J* = 3.0 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.33, 155.23, 153.13, 148.75, 143.71, 137.63, 135.11, 133.66, 132.72, 131.44, 130.14, 129.47, 128.54, 128.47, 128.26, 125.50, 123.22, 120.19, 110.39, 109.75, 55.97, 55.92, 41.10. ESI-MS: calculated $C_{23}H_{20}N_3O_4$ $[M+H]^+$ 402.1448; Found 402.1449.

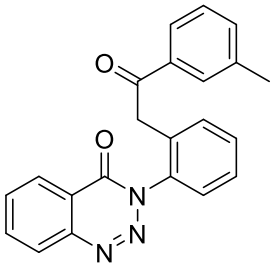
3-(2-(2-(3-methoxyphenyl)-2-oxoethyl)phenyl)benzo[*d*][1,2,3]triazin-4(3*H*)-one (4ae)



Following the above procedure 4, the product **4ae** was obtained in 42 % yield (31.2 mg, 0.084 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 4:1 v/v). Rf (Petroleum ether/EtOAc 4:1): 0.21. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (dd, 1H), 8.16 (d, *J* = 8.1 Hz, 1H), 8.00 – 7.93 (m, 1H), 7.85 – 7.77 (m, 1H), 7.55 – 7.42 (m, 4H), 7.37 (d, *J* = 7.7 Hz, 1H), 7.33 – 7.28 (m, 1H), 7.18 (t, *J* = 7.9

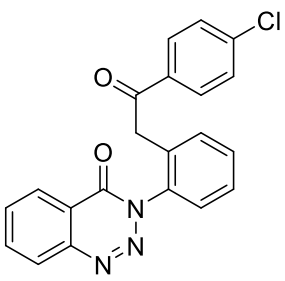
Hz, 1H), 6.98 – 6.90 (m, 1H), 4.23 (s, 2H), 3.75 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.46, 159.72, 155.32, 143.85, 137.82, 137.66, 135.24, 135.19, 133.11, 132.90, 131.66, 130.29, 129.49, 128.64, 128.51, 128.39, 125.65, 121.15, 120.01, 112.33, 55.48, 41.74. ESI-MS: calculated $C_{22}H_{18}N_3O_3$ $[M+H]^+$ 372.1343; Found 372.1336.

3-(2-(2-oxo-2-(m-tolyl)ethyl)phenyl)benzo[*d*][1,2,3]triazin-4(3*H*)-one (4af)



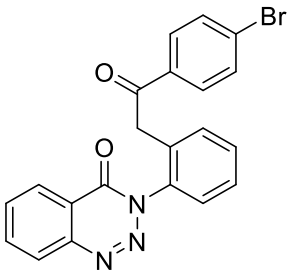
Following the above procedure 4, the product **4af** was obtained in 50 % yield (35.5 mg, 0.100 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 6:1 v/v). Rf (Petroleum ether/EtOAc 6:1): 0.25. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 – 8.34 (dd, 1H), 8.16 (d, *J* = 7.7 Hz, 1H), 7.96 (td, *J* = 8.2, 7.8, 1.4 Hz, 1H), 7.84 – 7.78 (m, 1H), 7.59 (d, *J* = 7.0 Hz, 2H), 7.54 – 7.39 (m, 4H), 7.19 (dt, *J* = 15.8, 7.5 Hz, 2H), 4.23 (s, 2H), 2.27 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.70, 155.25, 143.72, 138.31, 137.79, 136.34, 135.14, 133.93, 133.07, 132.78, 131.65, 130.09, 128.87, 128.61, 128.47, 128.38, 128.33, 125.63, 125.56, 120.22, 41.53, 21.25. ESI-MS: calculated $C_{22}H_{18}N_3O_2$ $[M+H]^+$ 356.1394; Found 356.1387.

3-(2-(2-(4-chlorophenyl)-2-oxoethyl)phenyl)benzo[*d*][1,2,3]triazin-4(3*H*)-one (4ag)



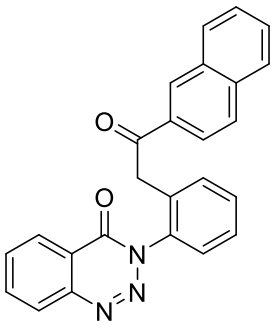
Following the above procedure 4, the product **4ag** was obtained in 33 % yield (24.6 mg, 0.066 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 8:1 v/v). Rf (Petroleum ether/EtOAc 8:1): 0.21. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (dd, *J* = 7.9, 1.1 Hz, 1H), 8.16 (d, *J* = 8.6 Hz, 1H), 7.98 (td, *J* = 8.2, 7.8, 1.4 Hz, 1H), 7.89 – 7.80 (m, 1H), 7.74 – 7.69 (m, 2H), 7.54 – 7.41 (m, 4H), 7.27 – 7.21 (m, 2H), 4.20 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.51, 155.33, 143.78, 139.70, 137.82, 135.36, 134.68, 133.01, 132.81, 131.69, 130.29, 129.93, 128.91, 128.73, 128.66, 128.61, 125.62, 120.21, 41.66. ESI-MS: calculated $C_{21}H_{15}N_3O_2Cl$ $[M+H]^+$ 376.0847; Found 376.0843.

3-(2-(2-(4-bromophenyl)-2-oxoethyl)phenyl)benzo[*d*][1,2,3]triazin-4(3*H*)-one (4ah)



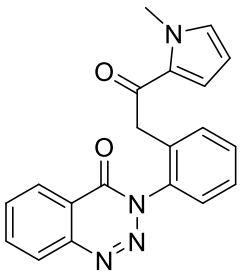
Following the above procedure 4, the product **4ah** was obtained in 40 % yield (33.3 mg, 0.080 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 8:1 v/v). Rf (Petroleum ether/EtOAc 8:1): 0.24. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (dd, *J* = 7.9, 1.2 Hz, 1H), 8.16 (d, *J* = 8.0 Hz, 1H), 7.98 (td, *J* = 8.3, 7.8, 1.4 Hz, 1H), 7.87 – 7.79 (m, 1H), 7.67 – 7.60 (m, 2H), 7.52 – 7.38 (m, 6H), 4.19 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.71, 155.32, 143.76, 137.80, 135.36, 135.07, 133.01, 132.79, 131.88, 131.69, 130.28, 130.00, 128.72, 128.66, 128.60, 128.49, 125.60, 120.19, 41.62. ESI-MS: calculated $C_{21}H_{15}N_3O_2Br$ $[M+H]^+$ 420.0342; Found 420.0338.

3-(2-(2-(naphthalen-2-yl)-2-oxoethyl)phenyl)benzo[*d*][1,2,3]triazin-4(3*H*)-one (4ai)



Following the above procedure 4, the product **4ai** was obtained in 57 % yield (44.6 mg, 0.114 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 6:1 v/v). Rf (Petroleum ether/EtOAc 6:1): 0.27. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (dd, *J* = 8.0, 1.1 Hz, 1H), 8.28 (s, 1H), 8.04 (d, *J* = 8.6 Hz, 1H), 7.91 – 7.78 (m, 3H), 7.78 – 7.65 (m, 3H), 7.60 – 7.42 (m, 6H), 4.36 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.59, 155.31, 143.60, 137.73, 135.44, 135.02, 133.64, 133.31, 132.68, 132.24, 131.65, 130.34, 130.19, 129.66, 128.54, 128.53, 128.43, 128.40, 128.40, 127.62, 126.67, 125.37, 123.97, 120.07, 41.45. ESI-MS: calculated $C_{25}H_{18}N_3O_2$ $[M+H]^+$ 392.1394; Found 392.1386.

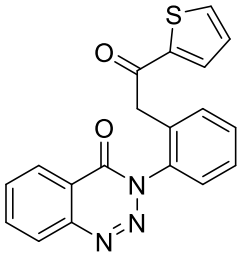
3-(2-(2-(1-methyl-1*H*-pyrrol-2-yl)-2-oxoethyl)phenyl)benzo[*d*][1,2,3]triazin-4(3*H*)-one (4aj)



Following the above procedure 4, the product **4aj** was obtained in 51 % yield (35.1 mg, 0.102 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 4:1 v/v). Rf (Petroleum ether/EtOAc 4:1): 0.22. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (dd, *J* = 7.9, 1.0 Hz, 1H), 8.15 (d, *J* = 7.6 Hz, 1H), 7.95 (td, *J* = 8.2, 7.8, 1.4 Hz, 1H), 7.84 – 7.76 (m, 1H), 7.56 – 7.38 (m, 4H), 6.70 (dd, *J* = 4.1, 1.7 Hz, 1H), 6.58 (t, *J* = 1.8 Hz, 1H),

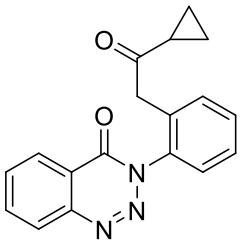
5.78 (dd, *J* = 4.1, 2.5 Hz, 1H), 4.02 (s, 2H), 3.76 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 186.88, 155.58, 143.96, 137.95, 135.19, 134.28, 132.84, 132.18, 131.59, 130.30, 128.68, 128.57, 128.39, 125.61, 120.52, 120.03, 119.78, 108.01, 42.27, 37.79. ESI-MS: calculated $C_{20}H_{17}N_4O_2$ $[M+H]^+$ 345.1346; Found 345.1346.

3-(2-(2-oxo-2-(thiophen-2-yl)ethyl)phenyl)benzo[*d*][1,2,3]triazin-4(3*H*)-one (4ak)



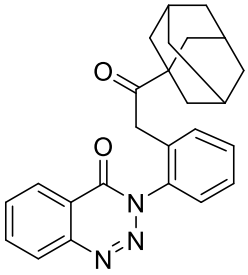
Following the above procedure 4, the product **4ak** was obtained in 37 % yield (25.6 mg, 0.074 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 4:1 v/v). Rf (Petroleum ether/EtOAc 4:1): 0.26. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (d, *J* = 7.8 Hz, 1H), 8.18 (d, *J* = 8.1 Hz, 1H), 7.97 (t, *J* = 7.7 Hz, 1H), 7.83 (t, *J* = 7.6 Hz, 1H), 7.62 – 7.38 (m, 6H), 6.91 (t, *J* = 3.9 Hz, 1H), 4.15 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 189.28, 155.39, 143.82, 143.59, 137.86, 135.29, 134.32, 132.95, 132.85, 131.58, 130.25, 128.74, 128.62, 128.59, 128.40, 128.15, 125.66, 120.29, 42.43. ESI-MS: calculated $C_{19}H_{14}N_3O_2S$ $[M+H]^+$ 348.0801; Found 348.0801.

3-(2-(2-cyclopropyl-2-oxoethyl)phenyl)benzo[*d*][1,2,3]triazin-4(3*H*)-one (4al)



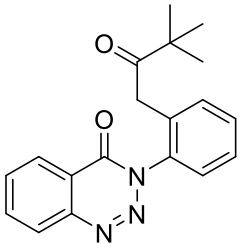
Following the above procedure 4, the product **4al** was obtained in 51 % yield (31.1 mg, 0.102 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 4:1 v/v). Rf (Petroleum ether/EtOAc 4:1): 0.21. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (dd, *J* = 7.9, 1.2 Hz, 1H), 8.24 (d, *J* = 8.0 Hz, 1H), 8.01 (td, *J* = 8.3, 7.8, 1.4 Hz, 1H), 7.89 – 7.83 (m, 1H), 7.58 – 7.40 (m, 4H), 3.77 (s, 2H), 1.87 – 1.79 (m, 1H), 0.86 (p, *J* = 3.8, 3.3 Hz, 2H), 0.73 (p, *J* = 7.5, 3.7 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 207.04, 155.27, 143.83, 138.03, 135.28, 132.94, 132.48, 131.79, 130.16, 128.70, 128.54, 128.46, 125.59, 120.30, 46.93, 20.09, 11.78. ESI-MS: calculated $C_{18}H_{16}N_3O_2$ $[M+H]^+$ 306.1237; Found 306.1229.

3-(2-(2-(adamantan-1-yl)-2-oxoethyl)phenyl)benzo[*d*][1,2,3]triazin-4(3*H*)-one (4am)



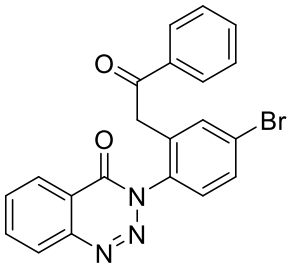
Following the above procedure 4, the product **4am** was obtained in 43 % yield (34.5 mg, 0.086 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 8:1 v/v). Rf (Petroleum ether/EtOAc 8:1): 0.24. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (dd, *J* = 7.9, 1.0 Hz, 1H), 8.23 (d, *J* = 7.7 Hz, 1H), 8.00 (td, *J* = 8.2, 7.8, 1.4 Hz, 1H), 7.90 – 7.81 (m, 1H), 7.52 – 7.40 (m, 3H), 7.38 – 7.33 (m, 1H), 3.77 (s, 2H), 1.87 (s, 3H), 1.66 – 1.57 (m, 9H), 1.52 (d, *J* = 11.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 210.80, 155.24, 143.86, 137.92, 135.33, 132.94, 132.77, 132.35, 129.85, 128.67, 128.33, 128.16, 125.65, 120.42, 46.73, 39.55, 38.75, 38.22, 36.44, 27.91. ESI-MS: calculated $C_{25}H_{26}N_3O_2$ $[M+H]^+$ 400.2020; Found 400.2021.

3-(2-(3,3-dimethyl-2-oxobutyl)phenyl)benzo[*d*][1,2,3]triazin-4(3*H*)-one (4an)



Following the above procedure 4, the product **4an** was obtained in 36 % yield (23.3 mg, 0.072 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 8:1 v/v). Rf (Petroleum ether/EtOAc 8:1): 0.26. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (dd, *J* = 7.9, 1.1 Hz, 1H), 8.23 (d, *J* = 7.7 Hz, 1H), 8.01 (td, *J* = 8.2, 7.8, 1.4 Hz, 1H), 7.89 – 7.80 (m, 1H), 7.55 – 7.33 (m, 4H), 3.82 (s, 2H), 0.96 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 211.04, 155.16, 143.75, 137.85, 135.26, 132.89, 132.60, 132.16, 129.78, 128.63, 128.26, 128.14, 125.57, 120.26, 44.45, 39.82, 26.39. ESI-MS: calculated $C_{19}H_{20}N_3O_2$ $[M+H]^+$ 322.1550; Found 322.1546.

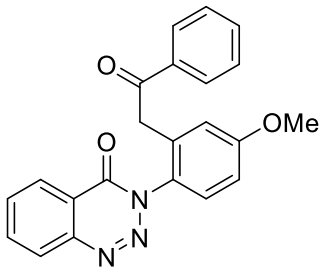
3-(4-bromo-2-(2-oxo-2-phenylethyl)phenyl)benzo[*d*][1,2,3]triazin-4(3*H*)-one (4ba)



Following the above procedure 4, the product **4ba** was obtained in 53 % yield (44.8 mg, 0.106 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 4:1 v/v). Rf (Petroleum ether/EtOAc 4:1): 0.24. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, *J* = 7.9 Hz, 1H), 8.14 (d, *J* = 8.1 Hz, 1H), 7.96 (t, *J* = 7.7 Hz,

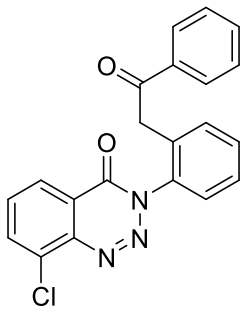
1H), 7.79 (dd, *J* = 19.8, 7.8 Hz, 3H), 7.61 (d, *J* = 9.6 Hz, 2H), 7.43 (t, *J* = 7.4 Hz, 1H), 7.36 – 7.18 (m, 3H), 4.22 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.68, 155.18, 143.65, 137.00, 136.13, 135.39, 135.04, 134.79, 133.45, 133.07, 131.57, 130.02, 128.78, 128.65, 128.36, 125.62, 124.00, 120.09, 41.29. ESI-MS: calculated $C_{21}H_{15}N_3O_2Br$ $[M+H]^+$ 420.0342; Found 420.0342.

3-(4-methoxy-2-(2-oxo-2-phenylethyl)phenyl)benzo[*d*][1,2,3]triazin-4(3*H*)-one (4ca)



Following the above procedure 4, the product **4ca** was obtained in 32 % yield (24.1 mg, 0.064 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 4:1 v/v). Rf (Petroleum ether/EtOAc 4:1): 0.27. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (dd, *J* = 7.9, 1.2 Hz, 1H), 8.15 (d, *J* = 8.1 Hz, 1H), 7.99 – 7.91 (m, 1H), 7.84 – 7.75 (m, 3H), 7.42 (t, *J* = 7.4 Hz, 1H), 7.35 (d, *J* = 8.3 Hz, 1H), 7.29 (t, *J* = 7.8 Hz, 2H), 7.02 – 6.94 (m, 2H), 4.18 (s, 2H), 3.84 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.50, 160.54, 155.60, 143.81, 136.35, 135.19, 134.30, 133.27, 132.84, 130.67, 129.62, 128.68, 128.60, 128.51, 125.66, 120.29, 116.91, 113.57, 55.71, 41.78. ESI-MS: calculated $C_{22}H_{18}N_3O_3$ $[M+H]^+$ 372.1343; Found 372.1338.

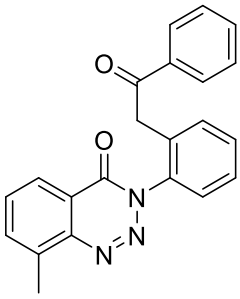
8-chloro-3-(2-(2-oxo-2-phenylethyl)phenyl)benzo[*d*][1,2,3]triazin-4(3*H*)-one (4da)



Following the above procedure 4, the product **4da** was obtained in 46 % yield (34.6 mg, 0.092 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 4:1 v/v). Rf (Petroleum ether/EtOAc 4:1): 0.20. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.97 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.78 (dd, *J* = 8.3, 1.2 Hz, 2H), 7.71 (t, *J* = 7.9 Hz, 1H), δ 7.52 – 7.38 (m, 5H), 7.34 – 7.27 (m, 2H)., 4.25 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.45, 154.43, 140.23, 137.61, 136.29, 135.88, 134.01, 133.28, 133.15, 133.07, 132.95, 131.88, 130.35, 128.57, 128.47, 128.45, 124.38, 122.08, 41.58.

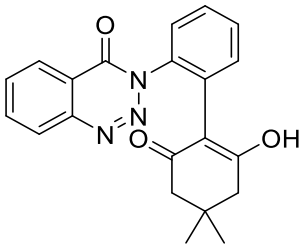
ESI-MS: calculated $C_{21}H_{15}N_3O_2Cl$ $[M+H]^+$ 376.0847; Found 376.0849.

8-methyl-3-(2-(2-oxo-2-phenylethyl)phenyl)benzo[*d*][1,2,3]triazin-4(3*H*)-one (4ea)



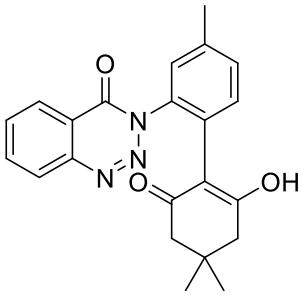
Following the above procedure 4, the product **4ea** was obtained in 41 % yield (29.1 mg, 0.082 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 8:1 v/v). Rf (Petroleum ether/EtOAc 8:1): 0.25. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (d, *J* = 7.0 Hz, 1H), 7.83 – 7.78 (m, 2H), 7.78 – 7.73 (m, 1H), 7.68 (t, *J* = 7.6 Hz, 1H), 7.52 – 7.39 (m, 5H), 7.33 – 7.27 (m, 2H), 4.24 (s, 2H), 2.83 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.68, 155.67, 142.16, 138.48, 138.02, 136.44, 136.34, 133.18, 133.07, 132.65, 131.64, 130.34, 130.09, 128.54, 128.52, 128.40, 123.26, 120.38, 41.59, 17.35. ESI-MS: calculated $C_{22}H_{18}N_3O_2$ $[M+H]^+$ 356.1394; Found 356.1386.

3-(6'-hydroxy-4',4'-dimethyl-2'-oxo-2',3',4',5'-tetrahydro-[1,1'-biphenyl]-2-yl)benzo[*d*][1,2,3] triazin-4(3*H*)-one (5aa)



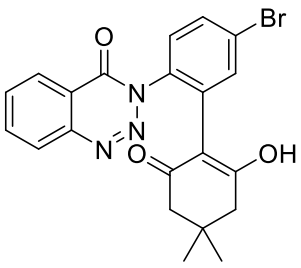
Following the above procedure 5, the product **5aa** was obtained in 81 % yield (58.5 mg, 0.162 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 1:1 v/v). Rf (Petroleum ether/EtOAc 1:1): 0.20. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, *J* = 7.4 Hz, 1H), 8.18 (d, *J* = 8.1 Hz, 1H), 8.02 – 7.93 (m, 1H), 7.81 (t, *J* = 7.5 Hz, 1H), 7.60 – 7.52 (m, 3H), 7.39 – 7.32 (m, 1H), 2.55 – 1.88 (m, 4H), 1.02 (s, 3H), 0.72 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.69, 171.30, 155.71, 143.66, 138.86, 135.29, 133.06, 132.75, 130.28, 130.24, 129.61, 128.62, 128.49, 125.46, 119.87, 113.59, 50.32, 42.28, 31.46, 28.46, 27.57. ESI-MS: calculated $C_{21}H_{20}N_3O_3$ $[M+H]^+$ 362.1499; Found 362.1493.

5,5-dimethyl-2-(2-methyl-6-(4-oxobenzo[*d*][1,2,3]triazin-3(4*H*)-yl)phenyl)cyclohexane-1,3-dione (5ba)



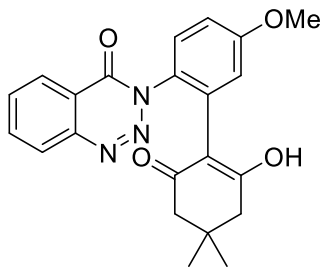
Following the above procedure 5, the product **5ba** was obtained in 82 % yield (61.4 mg, 0.164 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 1:1 v/v). Rf (Petroleum ether/EtOAc 1:1): 0.27. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 7.9 Hz, 1H), 8.13 (d, *J* = 8.1 Hz, 1H), 7.93 (t, *J* = 7.7 Hz, 1H), 7.77 (t, *J* = 7.6 Hz, 1H), 7.31 (d, *J* = 9.6 Hz, 2H), 7.20 (d, *J* = 7.7 Hz, 1H), 2.39 (s, 3H), 2.15 (d, *J* = 62.8 Hz, 4H), 0.98 (s, 3H), 0.70 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 154.11, 143.02, 137.91, 136.44, 135.41, 132.81, 132.77, 128.96, 128.91, 127.93, 127.88, 124.95, 120.08, 111.66, 30.94, 28.92, 26.61, 20.58. ESI-MS: calculated $C_{22}H_{22}N_3O_3$ $[M+H]^+$ 376.1656; Found 376.1652.

3-(5-bromo-6'-hydroxy-4',4'-dimethyl-2'-oxo-2',3',4',5'-tetrahydro-[1,1'-biphenyl]-2-yl)benzo[*d*][1,2,3]triazin-4(3*H*)-one (5ca)



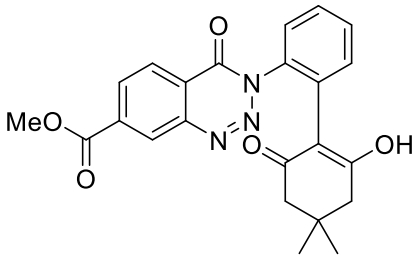
Following the above procedure 5, the product **5ca** was obtained in 68 % yield (60.2 mg, 0.136 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 1:1 v/v). Rf (Petroleum ether/EtOAc 1:1): 0.23. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.24 (d, *J* = 7.9 Hz, 1H), 8.06 (d, *J* = 8.1 Hz, 1H), 7.90 (t, *J* = 7.7 Hz, 1H), 7.74 (t, *J* = 7.6 Hz, 1H), 7.53 (d, *J* = 10.2 Hz, 1H), 7.44 (s, 1H), 7.34 (d, *J* = 8.4 Hz, 1H), 3.49 (s, 1H), 2.17 (s, 2H), 2.00 (d, *J* = 15.5 Hz, 2H), 0.93 (s, 3H), 0.70 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 145.76, 133.91, 127.71, 126.48, 125.84, 123.78, 123.29, 121.75, 119.66, 118.74, 115.86, 113.53, 110.50, 102.51, 21.82, 19.01, 17.88, 17.35. ESI-MS: calculated $C_{21}H_{19}N_3O_3Br$ $[M+H]^+$ 440.0604; Found 440.0602.

3-(6'-hydroxy-5-methoxy-4',4'-dimethyl-2'-oxo-2',3',4',5'-tetrahydro-[1,1'-biphenyl]-2-yl)benzo[*d*][1,2,3]triazin-4(3*H*)-one (5da)



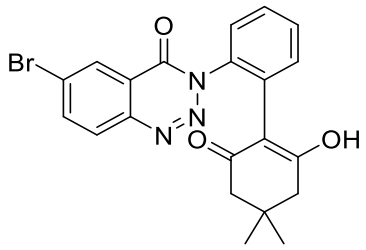
Following the above procedure 5, the product **5da** was obtained in 69 % yield (54.2 mg, 0.138 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 1:1 v/v). Rf (Petroleum ether/EtOAc 1:1): 0.24. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 7.9 Hz, 1H), 8.16 (d, *J* = 8.1 Hz, 1H), 7.96 (t, *J* = 7.7 Hz, 1H), 7.80 (t, *J* = 7.6 Hz, 1H), 7.44 (d, *J* = 8.7 Hz, 1H), 7.05 (dd, *J* = 8.6, 2.5 Hz, 1H), 6.84 (d, *J* = 2.7 Hz, 1H), 3.84 (s, 3H), 2.27 – 1.96 (m, 4H), 1.01 (s, 3H), 0.71 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 158.71, 154.29, 143.03, 135.34, 133.39, 132.69, 131.25, 128.67, 127.84, 124.96, 120.08, 117.87, 112.42, 111.80, 55.42, 46.24, 30.91, 28.97, 26.51. ESI-MS: calculated $C_{22}H_{22}N_3O_4$ $[M+H]^+$ 392.1605; Found 392.1602.

methyl 3-(6'-hydroxy-4',4'-dimethyl-2'-oxo-2',3',4',5'-tetrahydro-[1,1'-biphenyl]-2-yl)-4-oxo-3,4-dihydrobenzo[*d*][1,2,3]triazine-7-carboxylate (5ea)



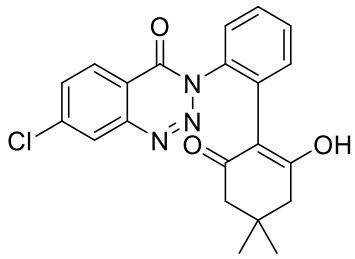
Following the above procedure 5, the product **5ea** was obtained in 77 % yield (64.8 mg, 0.154 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 1:1 v/v). Rf (Petroleum ether/EtOAc 1:1): 0.21. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.81 (s, 1H), 8.41 (s, 2H), 7.57 (s, 3H), 7.44 – 7.32 (m, 1H), 4.03 (s, 3H), 2.20 (d, *J* = 62.4 Hz, 4H), 1.02 (s, 3H), 0.74 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 195.71, 171.43, 165.16, 154.98, 143.53, 138.63, 136.45, 133.15, 132.66, 130.40, 130.29, 130.25, 129.56, 128.39, 126.11, 122.84, 113.49, 53.18, 50.38, 42.44, 31.53, 28.61, 27.65. ESI-MS: calculated $C_{23}H_{22}N_3O_5$ $[M+H]^+$ 420.1554; Found 420.1552.

6-bromo-3-(6'-hydroxy-4',4'-dimethyl-2'-oxo-2',3',4',5'-tetrahydro-[1,1'-biphenyl]-2-yl)benzo[*d*][1,2,3]triazin-4(3*H*)-one (5fa)



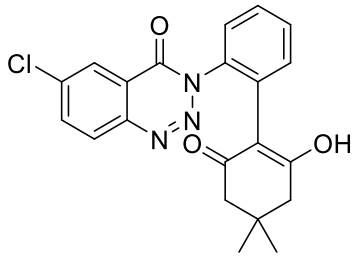
Following the above procedure 5, the product **5fa** was obtained in 77 % yield (68.1 mg, 0.154 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 1:1 v/v). Rf (Petroleum ether/EtOAc 1:1): 0.26. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (s, 1H), 8.05 (s, 2H), 7.62 – 7.52 (m, 3H), 7.38 – 7.32 (m, 1H), 2.64 – 1.84 (m, 4H), 1.04 (s, 3H), 0.77 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.55, 171.14, 154.42, 142.29, 138.68, 138.66, 133.02, 130.53, 130.26, 130.00, 129.78, 128.49, 128.22, 127.45, 121.12, 113.53, 50.35, 42.24, 31.49, 28.38, 27.67. ESI-MS: calculated $C_{21}H_{19}N_3O_3Br$ $[M+H]^+$ 440.0604; Found 440.0602.

2-(2-(7-chloro-4-oxobenzo[*d*][1,2,3]triazin-3(4*H*)-yl)phenyl)-5,5-dimethylcyclohexane-1,3-dione (5ga)



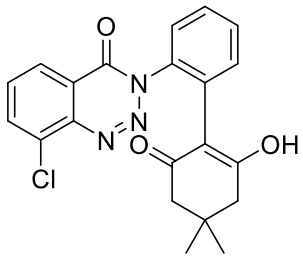
Following the above procedure 5, the product **5ga** was obtained in 94 % yield (74.6 mg, 0.188 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 1:1 v/v). Rf (Petroleum ether/EtOAc 1:1): 0.22. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, *J* = 9.9 Hz, 1H), 8.14 (s, 1H), 7.75 (d, *J* = 8.5 Hz, 1H), 7.60 – 7.49 (m, 3H), 7.38 – 7.32 (m, 1H), 2.20 (dd, *J* = 71.3, 15.7 Hz, 4H), 1.03 (s, 3H), 0.76 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.94, 144.35, 141.69, 138.55, 133.30, 133.13, 130.35, 130.20, 129.50, 128.37, 128.00, 127.25, 118.45, 113.44, 31.53, 28.54, 27.68. ESI-MS: calculated $C_{21}H_{19}N_3O_3Cl$ $[M+H]^+$ 396.1109; Found 396.1107.

2-(2-(6-chloro-4-oxobenzo[*d*][1,2,3]triazin-3(4*H*)-yl)phenyl)-5,5-dimethylcyclohexane-1,3-dione (5ha)



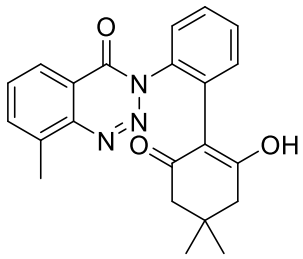
Following the above procedure 5, the product **5ha** was obtained in 79 % yield (62.4 mg, 0.158 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 1:1 v/v). Rf (Petroleum ether/EtOAc 1:1): 0.23. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, *J* = 2.3 Hz, 1H), 8.12 (d, *J* = 8.7 Hz, 1H), 7.89 (dd, *J* = 8.7, 2.3 Hz, 1H), 7.60 – 7.50 (m, 3H), 7.38 – 7.31 (m, 1H), 2.19 (d, *J* = 18.4 Hz, 4H), 1.03 (s, 3H), 0.76 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.62, 142.06, 139.21, 138.67, 135.88, 133.12, 130.49, 130.35, 130.15, 129.70, 128.49, 125.10, 121.16, 113.55, 31.56, 28.48, 27.72. ESI-MS: calculated $C_{21}H_{19}N_3O_3Cl$ $[M+H]^+$ 396.1109; Found 396.1106.

8-chloro-3-(6'-hydroxy-4',*4*'-dimethyl-2'-oxo-2',3',4',5'-tetrahydro-[1,1'-biphenyl]-2-yl)benzo[*d*][1,2,3]triazin-4(3*H*)-one (5ia)



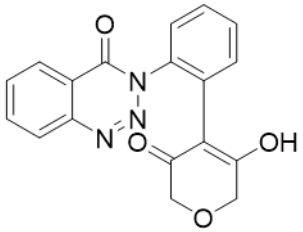
Following the above procedure 5, the product **5ia** was obtained in 67 % yield (52.8 mg, 0.134 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 1:1 v/v). Rf (Petroleum ether/EtOAc 1:1): 0.26. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 7.9 Hz, 1H), 7.99 (d, *J* = 7.9 Hz, 1H), 7.75 – 7.68 (m, 1H), 7.55 (s, 3H), 7.39 – 7.31 (m, 1H), 2.58 – 1.92 (m, 4H), 1.04 (s, 3H), 0.78 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.63, 171.39, 154.75, 140.18, 138.70, 135.97, 133.98, 133.13, 132.97, 130.51, 130.04, 129.65, 128.47, 124.37, 121.88, 113.58, 50.42, 42.36, 31.59, 28.57, 27.74. ESI-MS: calculated $C_{21}H_{19}N_3O_3Cl$ $[M+H]^+$ 396.1109; Found 396.1109.

3-(6'-hydroxy-4',4'-dimethyl-2'-oxo-2',3',4',5'-tetrahydro-[1,1'-biphenyl]-2-yl)-8-methylbenzo[*d*][1,2,3]triazin-4(3*H*)-one (5ja)



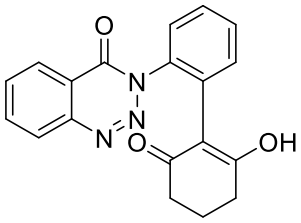
Following the above procedure 5, the product **5ja** was obtained in 70 % yield (52.8 mg, 0.140 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 1:1 v/v). Rf (Petroleum ether/EtOAc 1:1): 0.24. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, *J* = 7.7 Hz, 1H), 7.75 (d, *J* = 7.2 Hz, 1H), 7.66 (t, *J* = 7.6 Hz, 1H), 7.56 – 7.43 (m, 3H), 7.36 – 7.30 (m, 1H), 2.83 (s, 3H), 2.37 (d, *J* = 15.7 Hz, 1H), 2.17 (dd, *J* = 16.8, 7.9 Hz, 2H), 2.00 (d, *J* = 16.1 Hz, 1H), 1.00 (s, 3H), 0.73 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.94, 171.63, 155.99, 142.01, 138.92, 138.35, 136.34, 133.03, 132.44, 130.47, 130.02, 129.32, 128.33, 123.05, 119.97, 113.62, 50.34, 42.44, 31.48, 28.59, 27.51, 17.29. ESI-MS: calculated $C_{22}H_{22}N_3O_3$ $[M+H]^+$ 376.1656; Found 376.1653.

4-(2-(4-oxobenzo[*d*][1,2,3]triazin-3(4*H*)-yl)phenyl)-2*H*-pyran-3,5(4*H*,6*H*)-dione (5ab)



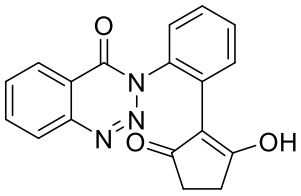
Following the above procedure 5, the product **5ab** was obtained in 84 % yield (56.3 mg, 0.168 mmol) as a yellow solid after column chromatography (eluent = Dichloromethane/Methanol 20:1 v/v). Rf (Dichloromethane/Methanol 20:1): 0.23. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.25 (d, *J* = 7.8 Hz, 1H), 8.15 (d, *J* = 8.6 Hz, 1H), 8.05 (t, *J* = 7.7 Hz, 1H), 7.89 (t, *J* = 7.8 Hz, 1H), 7.50 (d, *J* = 7.6 Hz, 1H), 7.46 – 7.29 (m, 3H), 3.81 (s, 4H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 154.19, 142.95, 137.89, 135.44, 132.87, 132.86, 129.90, 128.31, 128.00, 127.74, 127.32, 124.98, 120.07, 110.21, 68.03. ESI-MS: calculated $C_{18}H_{14}N_3O_4$ $[M+H]^+$ 336.0979; Found 336.0974.

3-(6'-hydroxy-2'-oxo-2',3',4',5'-tetrahydro-[1,1'-biphenyl]-2-yl)benzo[*d*][1,2,3]triazin-4(3*H*)-one (5ac)



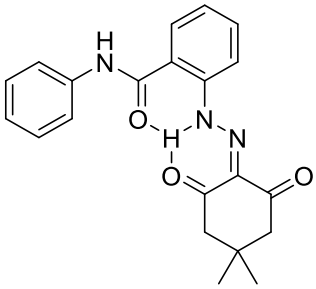
Following the above procedure 5, the product **5ac** was obtained in 85 % yield (56.9 mg, 0.170 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 1:3 v/v). Rf (Petroleum ether/EtOAc 1:3): 0.24. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, 1H), 8.18 (d, *J* = 8.0 Hz, 1H), 8.02 – 7.95 (m, 1H), 7.87 – 7.79 (m, 1H), 7.55 (d, *J* = 3.1 Hz, 3H), 7.38 – 7.32 (m, 1H), 4.59 (s, 1H), 2.49 – 2.32 (m, 2H), 2.28 – 2.09 (m, 2H), 1.97 – 1.81 (m, 1H), 1.79 – 1.65 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.74, 143.68, 138.78, 135.41, 133.11, 132.91, 130.28, 130.17, 129.62, 128.71, 128.42, 125.53, 119.85, 114.78, 32.61, 32.56, 20.42. ESI-MS: calculated $C_{19}H_{16}N_3O_3$ $[M+H]^+$ 334.1186; Found 334.1176.

3-(2-(2-hydroxy-5-oxocyclopent-1-en-1-yl)phenyl)benzo[*d*][1,2,3]triazin-4(3*H*)-one (5ad)



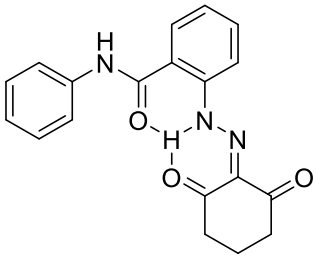
Following the above procedure 5, the product **5ad** was obtained in 99 % yield (63.2 mg, 0.198 mmol) as a yellow solid after column chromatography (eluent = Dichloromethane/Methanol 20:1 v/v). Rf (Dichloromethane/Methanol 20:1): 0.21. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.28 – 8.24 (dd, 1H), 8.14 (d, *J* = 7.7 Hz, 1H), 8.04 (td, *J* = 8.2, 7.8, 1.4 Hz, 1H), 7.91 – 7.86 (m, 1H), 7.60 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.48 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.43 (td, *J* = 7.6, 1.4 Hz, 1H), 7.34 (td, *J* = 7.6, 1.5 Hz, 1H), 3.67 (s, 1H), 2.03 (s, 4H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 154.55, 142.99, 136.75, 135.31, 132.76, 131.32, 129.28, 128.44, 128.13, 128.01, 127.07, 124.88, 120.41, 113.26, 30.34, 26.38. ESI-MS: calculated $C_{18}H_{14}N_3O_3$ $[M+H]^+$ 320.1030; Found 320.1027.

2-(2-(4,4-dimethyl-2,6-dioxocyclohexylidene)hydrazineyl)-*N*-phenylbenzamide (6aa)



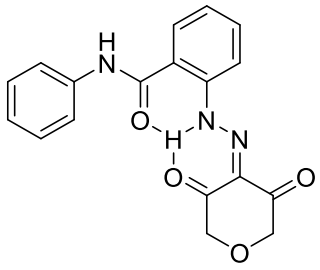
Following the above procedure 6, the product **6aa** was obtained in 83 % yield (60.3 mg, 0.166 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 2:1 v/v). Rf (Petroleum ether/EtOAc 2:1): 0.27. ^{1}H NMR (400 MHz, DMSO-d_6) δ 15.57 (s, 1H), 10.58 (s, 1H), 8.00 (d, J = 8.2 Hz, 1H), 7.92 (d, J = 7.0 Hz, 1H), 7.76 (d, J = 7.7 Hz, 2H), 7.69 (t, J = 7.7 Hz, 1H), 7.43 – 7.34 (m, 3H), 7.16 (t, J = 7.4 Hz, 1H), 2.60 (d, J = 17.7 Hz, 4H), 1.02 (s, 6H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 196.05, 193.11, 165.68, 141.54, 138.60, 132.85, 131.19, 129.06, 128.72, 125.22, 124.27, 122.57, 120.78, 116.50, 52.13, 51.80, 30.17, 28.04. ESI-MS: calculated $C_{21}H_{22}N_3O_3$ $[M+H]^+$ 364.1656; Found 364.1647.

2-(2-(2,6-dioxocyclohexylidene)hydrazineyl)-*N*-phenylbenzamide (6ab)



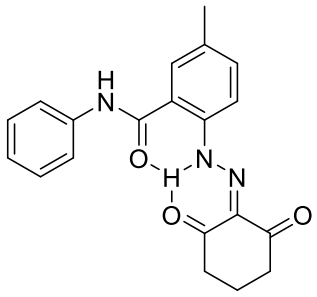
Following the above procedure 6, the product **6ab** was obtained in 83 % yield (55.8 mg, 0.166 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 2:1 v/v). Rf (Petroleum ether/EtOAc 2:1): 0.28. ^{1}H NMR (400 MHz, DMSO-d_6) δ 15.53 (s, 1H), 10.58 (s, 1H), 7.98 (d, *J* = 8.1 Hz, 1H), 7.91 (dd, *J* = 7.8, 1.1 Hz, 1H), 7.76 (d, *J* = 7.6 Hz, 2H), 7.73 – 7.66 (m, 1H), 7.44 – 7.33 (m, 3H), 7.15 (t, *J* = 7.4 Hz, 1H), 2.66 (t, *J* = 6.3 Hz, 2H), 2.63 – 2.59 (t, 2H), 2.01 – 1.91 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 196.76, 193.63, 165.68, 141.57, 138.63, 132.85, 132.51, 129.04, 128.74, 125.15, 124.27, 122.65, 120.75, 116.49, 38.79, 38.62, 17.69. ESI-MS: calculated $C_{19}H_{18}N_3O_3$ $[M+H]^+$ 336.1343; Found 336.1347.

2-(2-(3,5-dioxotetrahydro-4*H*-pyran-4-ylidene)hydrazineyl)-*N*-phenylbenzamide (6ac)



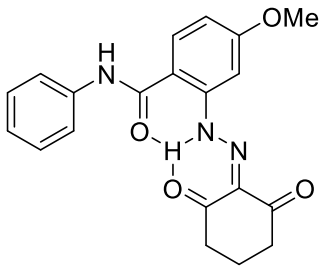
Following the above procedure 6, the product **6ac** was obtained in 39 % yield (26.3 mg, 0.078 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 2:1 v/v). Rf (Petroleum ether/EtOAc 2:1): 0.23. ^{1}H NMR (400 MHz, DMSO-d_6) δ 15.45 (s, 1H), 10.62 (s, 1H), 7.99 (dd, *J* = 15.1, 8.1 Hz, 2H), 7.76 (d, *J* = 8.2 Hz, 2H), 7.71 (d, *J* = 7.9 Hz, 1H), 7.45 (d, *J* = 7.6 Hz, 1H), 7.40 (t, *J* = 7.8 Hz, 2H), 7.16 (t, *J* = 7.2 Hz, 1H), 4.37 (d, *J* = 13.9 Hz, 4H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 192.91, 191.13, 165.65, 141.28, 138.52, 133.05, 130.62, 129.14, 128.76, 125.92, 124.38, 122.68, 120.89, 116.71, 73.21, 72.45. ESI-MS: calculated $C_{18}H_{15}N_3O_4Na$ $[M+Na]^+$ 360.0955; Found 360.0958.

2-(2-(2,6-dioxocyclohexylidene)hydrazineyl)-5-methyl-*N*-phenylbenzamide (6bb)



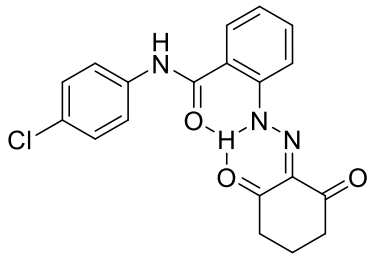
Following the above procedure 6, the product **6bb** was obtained in 96 % yield (67.1 mg, 0.192 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 2:1 v/v). Rf (Petroleum ether/EtOAc 2:1): 0.20. ^{1}H NMR (400 MHz, DMSO-d_6) δ 15.53 (s, 1H), 10.48 (s, 1H), 7.98 (d, J = 8.1 Hz, 1H), 7.92 – 7.86 (m, 1H), 7.70 – 7.64 (m, 1H), 7.59 (s, 1H), 7.56 (d, J = 8.2 Hz, 1H), 7.41 – 7.33 (m, 1H), 7.27 (t, J = 7.8 Hz, 1H), 6.97 (d, J = 7.2 Hz, 1H), 2.77 – 2.54 (m, 4H), 2.33 (s, 3H), 2.05 – 1.84 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 196.31, 193.25, 165.25, 141.21, 138.18, 137.52, 132.40, 132.11, 128.64, 128.19, 124.76, 124.59, 122.30, 120.89, 117.61, 116.15, 38.41, 38.24, 20.91, 17.34. ESI-MS: calculated $C_{20}H_{19}N_3O_3Na$ $[M+Na]^+$ 372.1324; Found 372.1322.

2-(2-(2,6-dioxocyclohexylidene)hydrazineyl)-4-methoxy-*N*-phenylbenzamide (6cb)



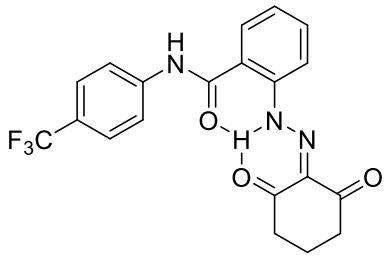
Following the above procedure 6, the product **6cb** was obtained in 78 % yield (57.2 mg, 0.156 mmol) as a yellow solid after column chromatography (eluent = Dichloromethane/Methanol 80:1 v/v). Rf (Dichloromethane/Methanol 80:1): 0.23. ^{1}H NMR (400 MHz, DMSO-d_6) δ 15.55 (s, 1H), 10.44 (s, 1H), 7.98 (d, J = 8.0 Hz, 1H), 7.92 – 7.87 (m, 1H), 7.71 – 7.64 (m, 3H), 7.39 – 7.34 (m, 1H), 6.99 – 6.94 (m, 2H), 3.76 (s, 3H), 2.70 – 2.57 (m, 4H), 2.01 – 1.89 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 196.24, 193.23, 164.86, 155.59, 141.18, 132.28, 132.08, 131.24, 128.48, 124.75, 122.31, 121.99, 116.10, 113.47, 54.88, 38.41, 38.24, 17.33. ESI-MS: calculated $C_{20}H_{19}N_3O_4Na$ $[M+Na]^+$ 388.1273; Found 388.1274.

***N*-(4-chlorophenyl)-2-(2-(2,6-dioxocyclohexylidene)hydrazineyl)benzamide (6db)**



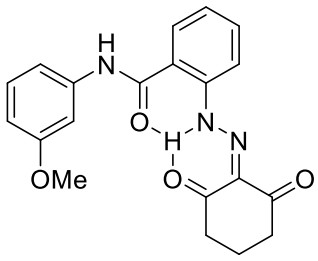
Following the above procedure 6, the product **6db** was obtained in 45 % yield (33.3 mg, 0.090 mmol) as a yellow solid after column chromatography (eluent = Dichloromethane/Methanol 80:1 v/v). Rf (Dichloromethane/Methanol 80:1): 0.21. ^{1}H NMR (400 MHz, DMSO-d_6) δ 15.42 (s, 1H), 10.59 (s, 1H), 7.96 (d, J = 8.5 Hz, 1H), 7.91 (d, J = 2.1 Hz, 1H), 7.74 (d, J = 7.7 Hz, 2H), 7.47 – 7.35 (m, 3H), 7.16 (t, J = 7.4 Hz, 1H), 2.74 – 2.54 (m, 4H), 2.05 – 1.89 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 196.62, 193.36, 164.51, 142.93, 138.06, 137.11, 132.66, 130.65, 128.38, 124.03, 123.98, 120.49, 120.27, 115.32, 38.44, 38.34, 17.14. ESI-MS: calculated $C_{19}H_{16}N_3O_3NaCl$ $[M+Na]^+$ 392.0778; Found 392.0771.

2-(2-(2,6-dioxocyclohexylidene)hydrazineyl)-*N*-(4-(trifluoromethyl)phenyl)benzamide (6eb)



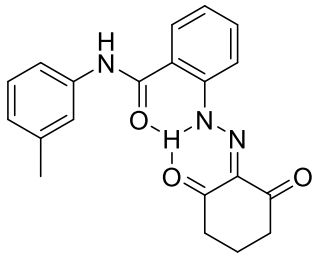
Following the above procedure 6, the product **6eb** was obtained in 74 % yield (59.7 mg, 0.148 mmol) as a yellow solid after column chromatography (eluent = Dichloromethane/Methanol 80:1 v/v). Rf (Dichloromethane/Methanol 80:1): 0.24. ^{1}H NMR (400 MHz, DMSO-d_6) δ 15.40 (s, 1H), 10.75 (s, 1H), 8.18 – 8.15 (m, 1H), 8.12 (d, *J* = 8.1 Hz, 1H), 7.76 (d, *J* = 7.6 Hz, 2H), 7.74 – 7.70 (m, 1H), 7.41 (t, *J* = 7.9 Hz, 2H), 7.18 (t, *J* = 7.4 Hz, 1H), 2.72 – 2.60 (m, 4H), 2.01 – 1.92 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 196.95, 193.38, 164.24, 141.99, 137.97, 132.10 (d, *J* = 32.3 Hz), 131.56 (d, *J* = 269.0 Hz), 128.45, 125.18, 124.51, 124.22, 121.80, 120.44, 112.18, 38.46, 38.38, 17.11. ^{19}F NMR (376 MHz, DMSO-d_6) δ -61.92. ESI-MS: calculated $C_{20}H_{16}N_3O_3F_3Na$ $[M+Na]^+$ 426.1041; Found 426.1044.

2-(2-(2,6-dioxocyclohexylidene)hydrazineyl)-*N*-(3-methoxyphenyl)benzamide (6fb)



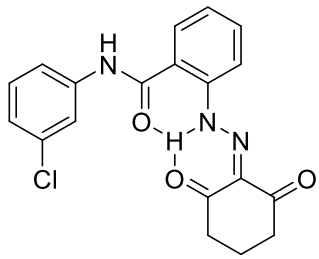
Following the above procedure 6, the product **6fb** was obtained in 87 % yield (63.6 mg, 0.174 mmol) as a yellow solid after column chromatography (eluent = Dichloromethane/Methanol 80:1 v/v). Rf (Dichloromethane/Methanol 80:1): 0.23. ^{1}H NMR (400 MHz, DMSO-d_6) δ 15.63 (s, 1H), 10.60 (s, 1H), 7.90 (d, *J* = 9.1 Hz, 1H), 7.75 (d, *J* = 7.9 Hz, 2H), 7.44 (d, *J* = 2.7 Hz, 1H), 7.39 (t, *J* = 7.8 Hz, 2H), 7.30 (dd, *J* = 9.1, 2.7 Hz, 1H), 7.16 (t, *J* = 7.3 Hz, 1H), 3.88 (s, 3H), 2.67 – 2.54 (m, 4H), 1.98 – 1.89 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 196.00, 193.18, 164.93, 156.50, 138.15, 134.40, 131.41, 128.38, 124.03, 123.74, 120.58, 118.54, 118.11, 113.24, 55.52, 38.36, 38.08, 17.58. ESI-MS: calculated $C_{20}H_{19}N_3O_4Na$ $[M+Na]^+$ 388.1273; Found 388.1277.

2-(2-(2,6-dioxocyclohexylidene)hydrazineyl)-*N*-(m-tolyl)benzamide (6gb)



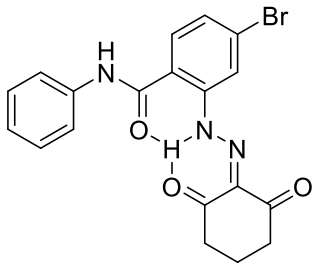
Following the above procedure 6, the product **6gb** was obtained in 94 % yield (65.7 mg, 0.188 mmol) as a yellow solid after column chromatography (eluent = Dichloromethane/Methanol 80:1 v/v). Rf (Dichloromethane/Methanol 80:1): 0.20. ^{1}H NMR (400 MHz, DMSO-d_6) δ 15.16 (s, 1H), 10.46 (s, 1H), 7.68 (d, *J* = 7.8 Hz, 2H), 7.57 (d, *J* = 7.4 Hz, 1H), 7.49 (d, *J* = 7.4 Hz, 1H), 7.38 – 7.30 (m, 3H), 7.10 (t, *J* = 7.4 Hz, 1H), 2.63 (t, *J* = 6.3 Hz, 2H), 2.54 – 2.49 (m, 2H), 2.48 (s, 3H), 1.93 – 1.82 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 196.61, 192.58, 165.42, 138.48, 137.66, 133.95, 131.82, 130.50, 128.46, 128.23, 126.49, 125.88, 123.48, 119.90, 38.16, 38.08, 19.30, 17.46. ESI-MS: calculated $C_{20}H_{19}N_3O_3Na$ $[M+Na]^+$ 372.1324; Found 372.1327.

***N*-(3-chlorophenyl)-2-(2-(2,6-dioxocyclohexylidene)hydrazineyl)benzamide (6hb)**



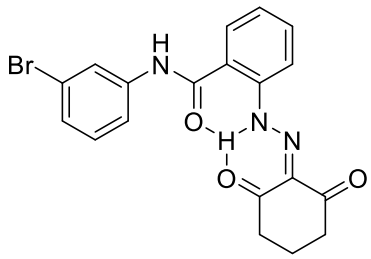
Following the above procedure 6, the product **6hb** was obtained in 78 % yield (57.7 mg, 0.156 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 4:1 v/v). Rf (Petroleum ether/EtOAc 4:1): 0.27. ^{1}H NMR (400 MHz, DMSO-d_6) δ 15.44 (s, 1H), 10.62 (s, 1H), 7.99 (d, *J* = 2.3 Hz, 1H), 7.95 (d, *J* = 9.0 Hz, 1H), 7.78 – 7.71 (m, 3H), 7.40 (t, *J* = 7.9 Hz, 2H), 7.17 (t, *J* = 7.4 Hz, 1H), 2.70 – 2.58 (m, 4H), 2.02 – 1.88 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 196.51, 193.25, 163.98, 140.27, 138.01, 132.36, 132.28, 128.63, 128.38, 128.22, 124.09, 123.17, 120.47, 117.94, 38.41, 38.28, 17.24. ESI-MS: calculated $C_{19}H_{16}N_3O_3NaCl$ $[M+Na]^+$ 392.0778; Found 392.0782.

4-bromo-2-(2-(2,6-dioxocyclohexylidene)hydrazineyl)-*N*-phenylbenzamide (6ib)



Following the above procedure 6, the product **6ib** was obtained in 70 % yield (58.0 mg, 0.140 mmol) as a yellow solid after column chromatography (eluent = Dichloromethane/Methanol 80:1 v/v). Rf (Dichloromethane/Methanol 80:1): 0.25. ^{1}H NMR (400 MHz, DMSO-d_6) δ 15.51 (s, 1H), 10.67 (s, 1H), 7.98 (d, *J* = 8.3 Hz, 1H), 7.92 – 7.88 (m, 1H), 7.75 (d, *J* = 8.9 Hz, 2H), 7.69 (t, *J* = 7.7 Hz, 1H), 7.58 (d, *J* = 8.8 Hz, 2H), 7.40 – 7.35 (m, 1H), 2.70 – 2.58 (m, 4H), 2.00 – 1.92 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 196.46, 193.32, 165.43, 141.26, 137.70, 132.67, 132.20, 131.25, 128.71, 124.80, 122.27, 121.97, 116.20, 115.69, 38.44, 38.27, 17.35. ESI-MS: calculated $C_{19}H_{16}N_3O_3NaBr$ $[M+Na]^+$ 436.0273; Found 436.0271.

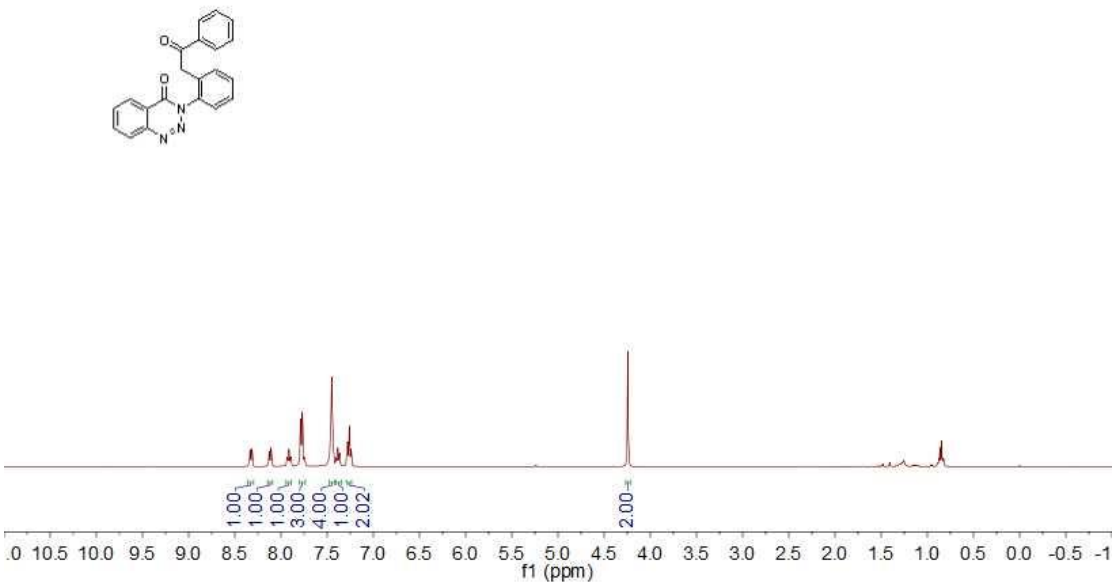
***N*-(3-bromophenyl)-2-(2-(2,6-dioxocyclohexylidene)hydrazineyl)benzamide (6jb)**



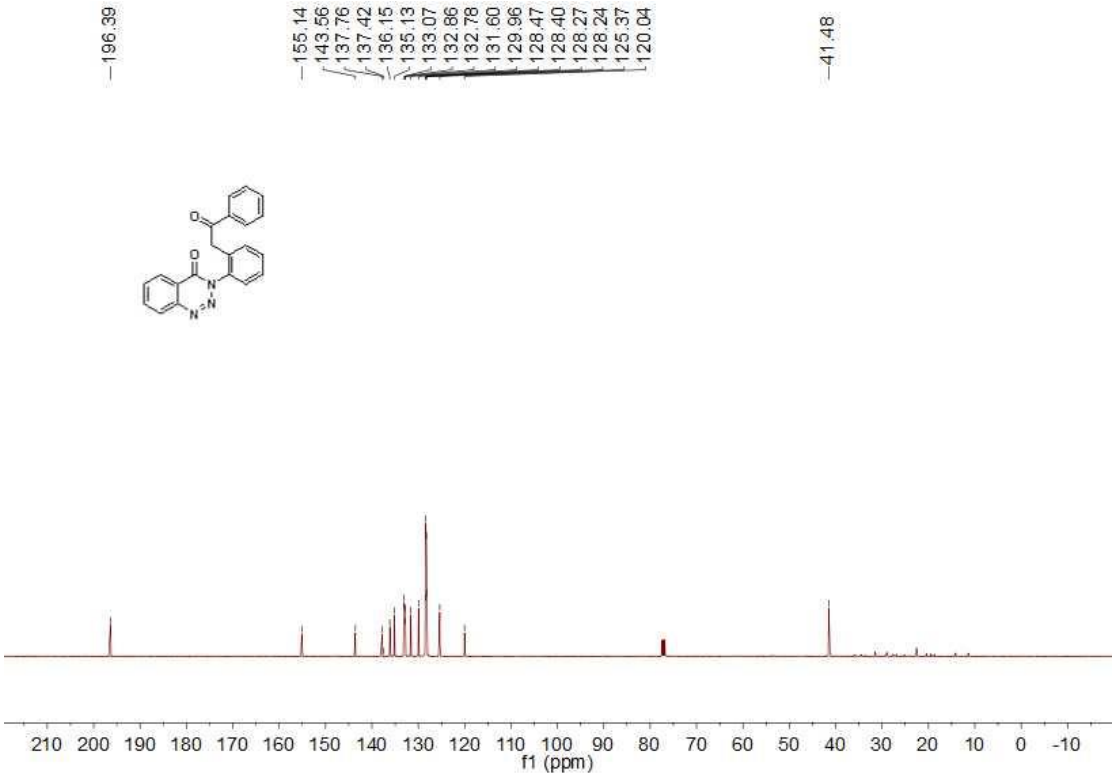
Following the above procedure 6, the product **6jb** was obtained in 83 % yield (68.7 mg, 0.166 mmol) as a yellow solid after column chromatography (eluent = Petroleum ether/EtOAc 4:1 v/v). Rf (Petroleum ether/EtOAc 4:1): 0.23. ^{1}H NMR (400 MHz, DMSO-d_6) δ 15.43 (s, 1H), 10.63 (s, 1H), 8.10 (d, *J* = 1.9 Hz, 1H), 7.92 – 7.84 (m, 2H), 7.75 (d, *J* = 7.7 Hz, 2H), 7.40 (t, *J* = 7.9 Hz, 2H), 7.17 (t, *J* = 7.4 Hz, 1H), 2.74 – 2.55 (m, 4H), 2.03 – 1.90 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 196.59, 193.29, 163.92, 140.66, 138.02, 135.18, 132.42, 131.00, 128.40, 124.11, 123.50, 120.49, 118.17, 116.77, 38.42, 38.30, 17.23. ESI-MS: calculated $C_{19}H_{16}N_3O_3NaBr$ $[M+Na]^+$ 436.0273; Found 436.0269.

8. NMR Spectra for New Compounds

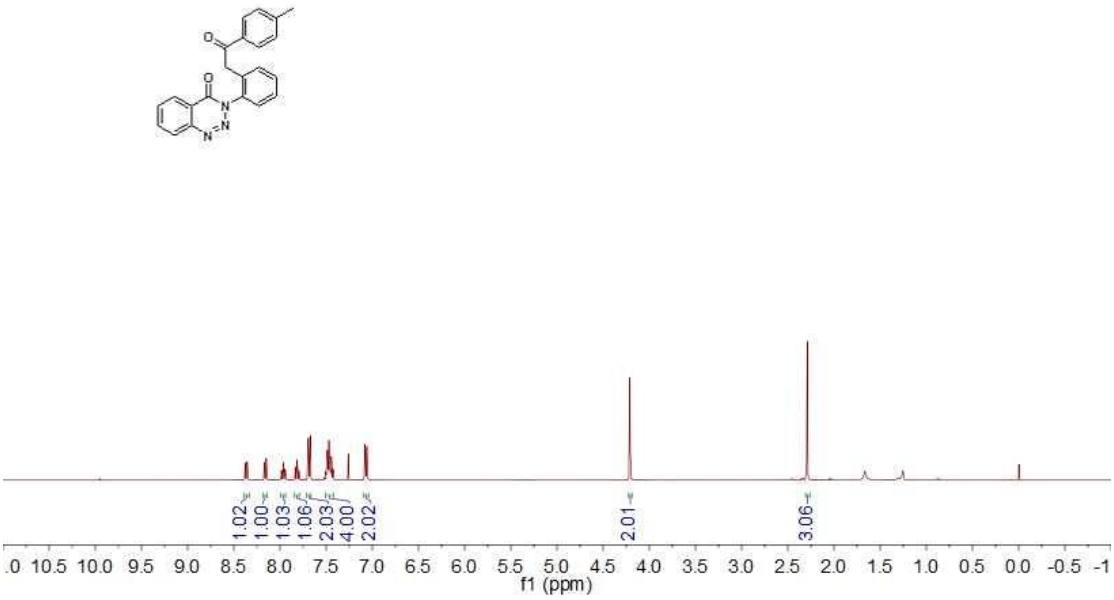
^{1}H NMR (400 MHz, $CDCl_3$) Spectra of **4aa**



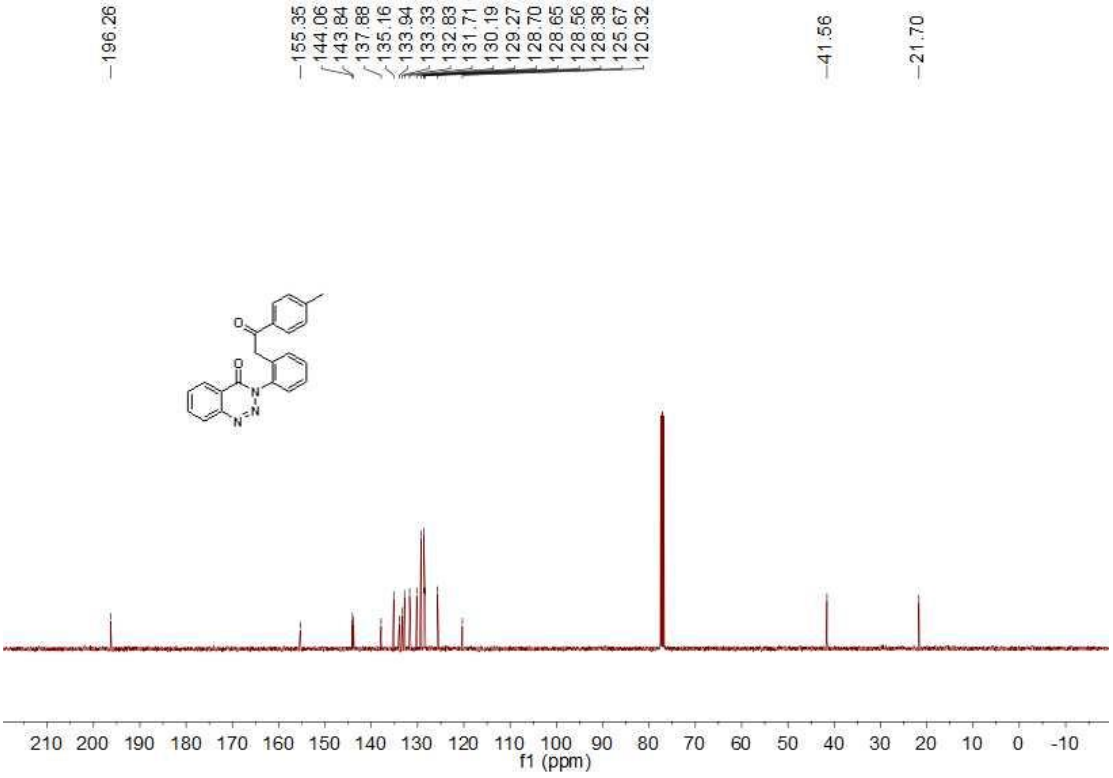
^{13}C NMR (101 MHz, $CDCl_3$) Spectra of **4aa**



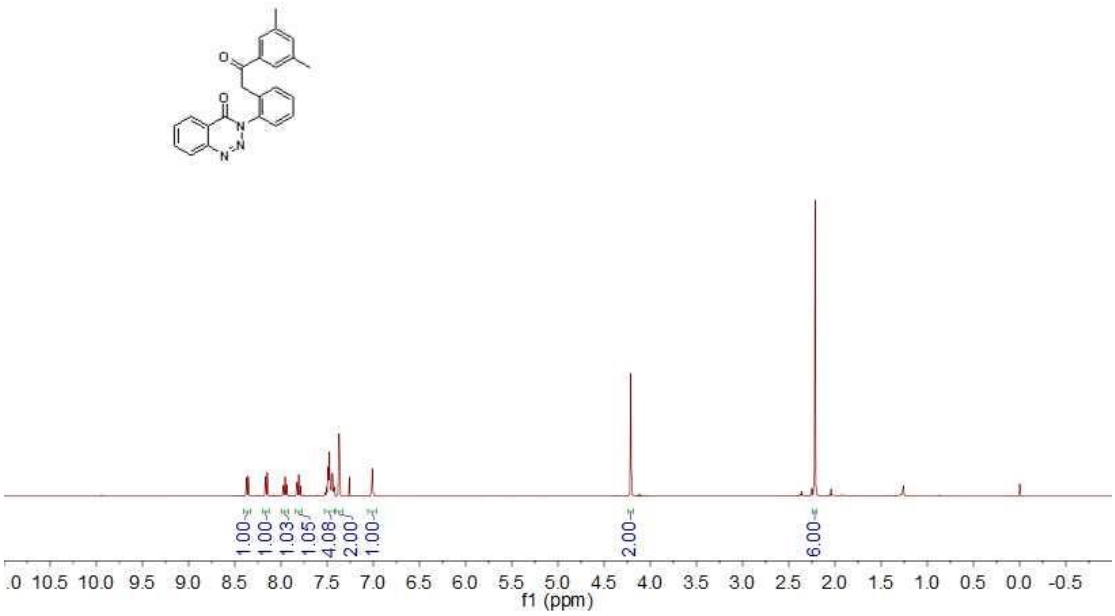
^{1}H NMR (400 MHz, $CDCl_3$) Spectra of **4ab**



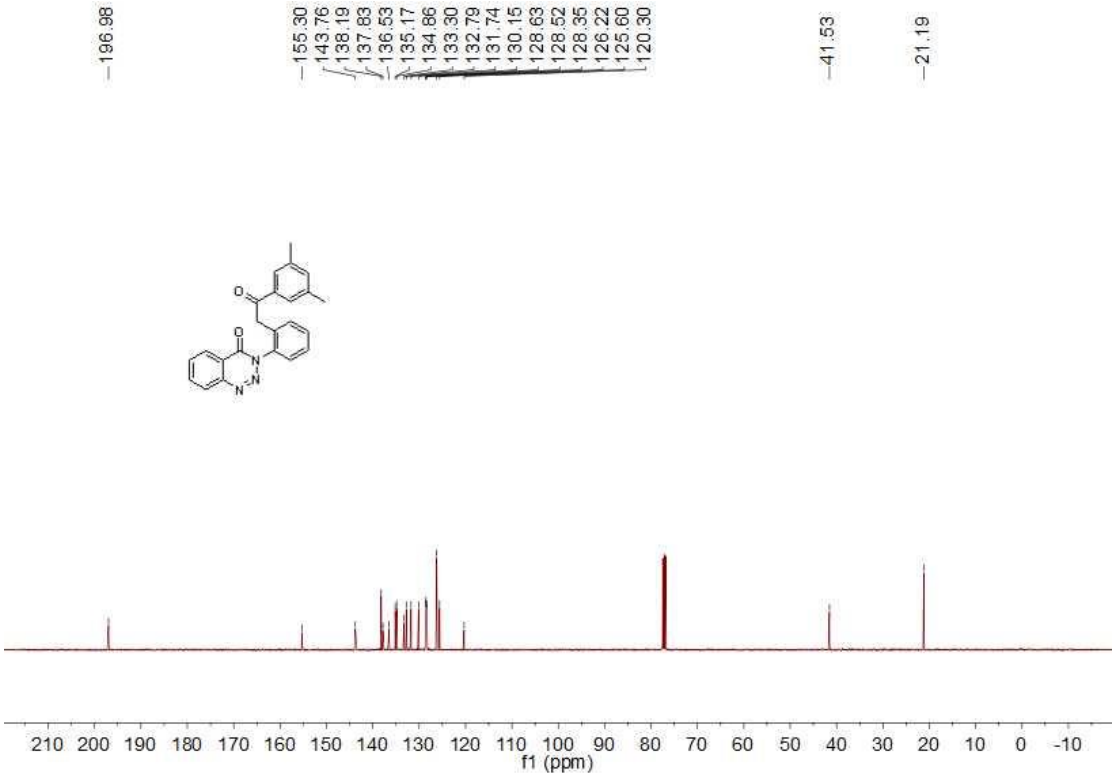
^{13}C NMR (101 MHz, $CDCl_3$) Spectra of **4ab**



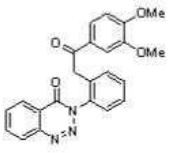
^{1}H NMR (400 MHz, $CDCl_3$) Spectra of **4ac**

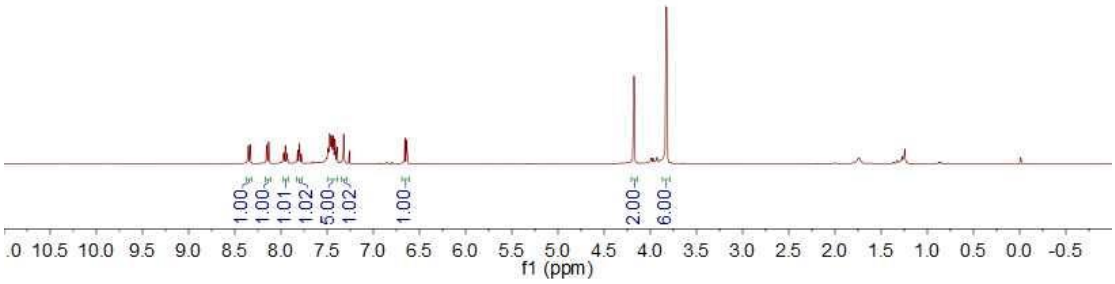


^{13}C NMR (101 MHz, $CDCl_3$) Spectra of **4ac**

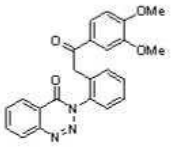


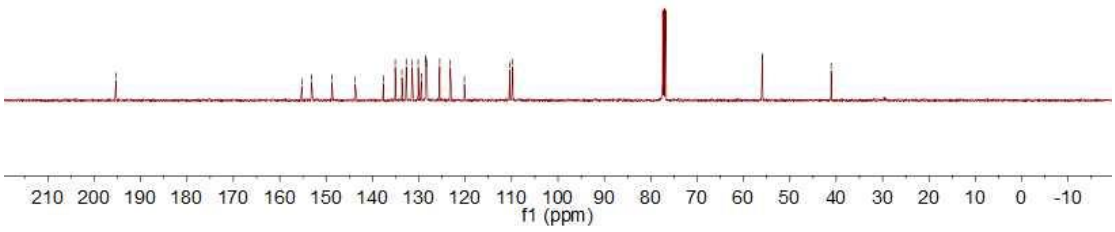
^{1}H NMR (400 MHz, $CDCl_3$) Spectra of **4ad**



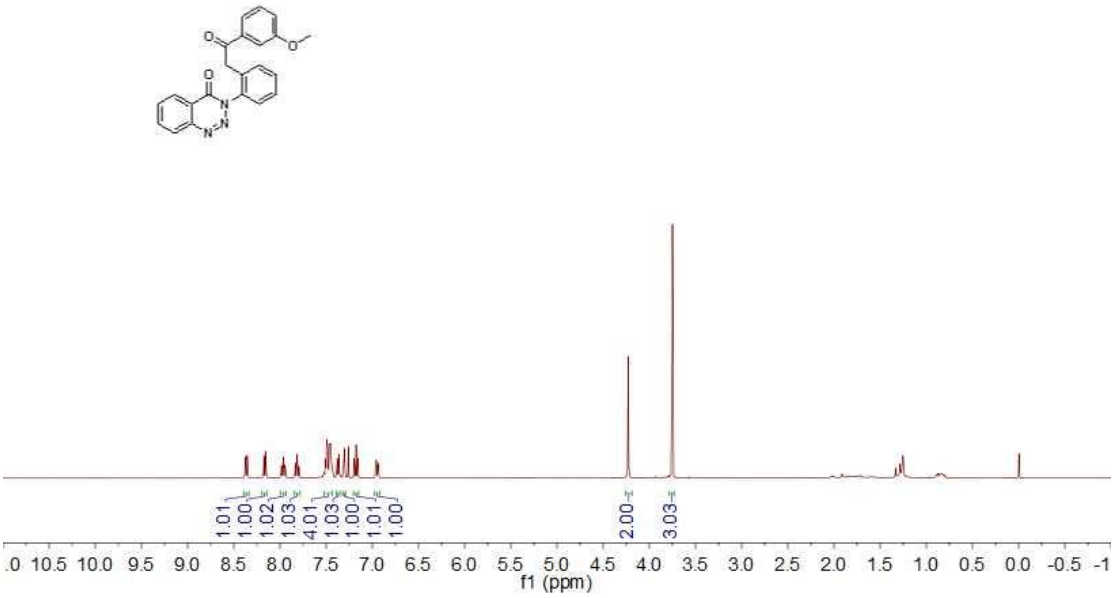


^{13}C NMR (101 MHz, $CDCl_3$) Spectra of **4ad**

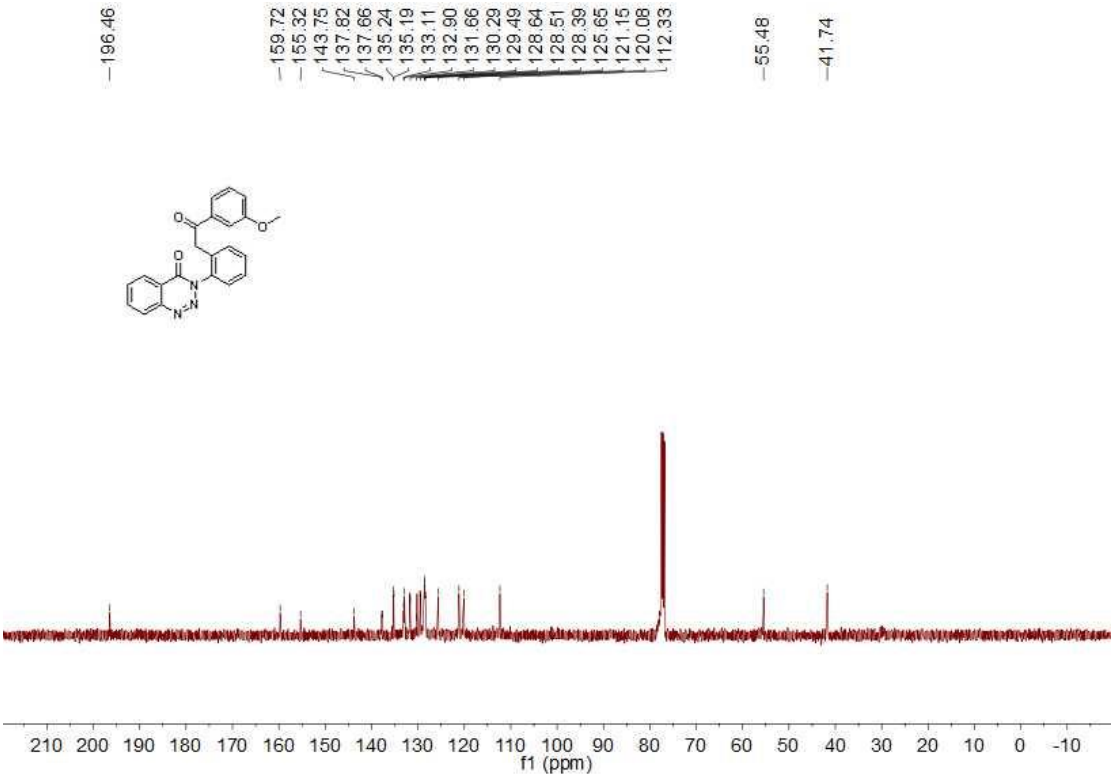




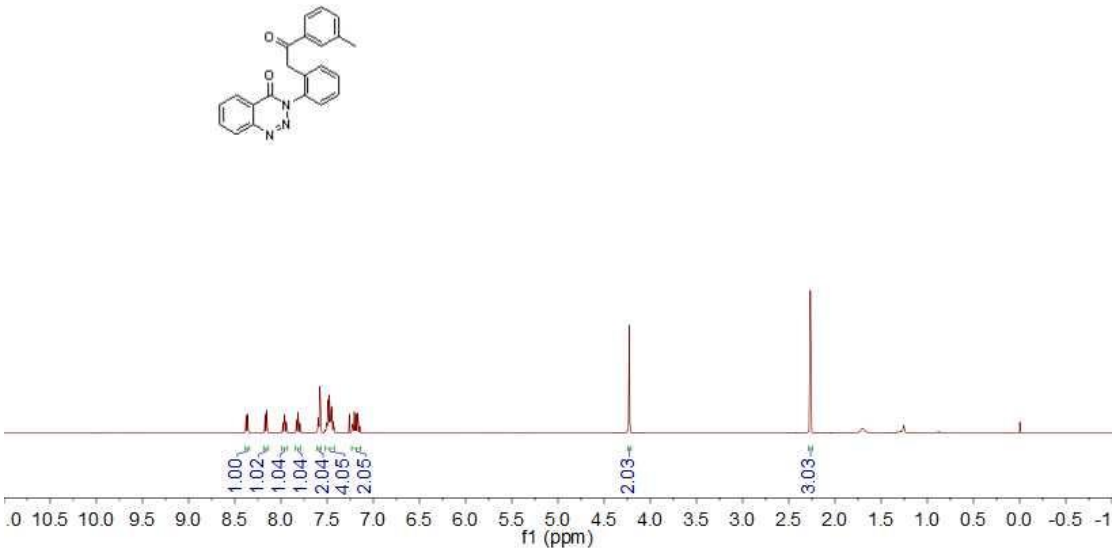
^{1}H NMR (400 MHz, $CDCl_3$) Spectra of **4ae**



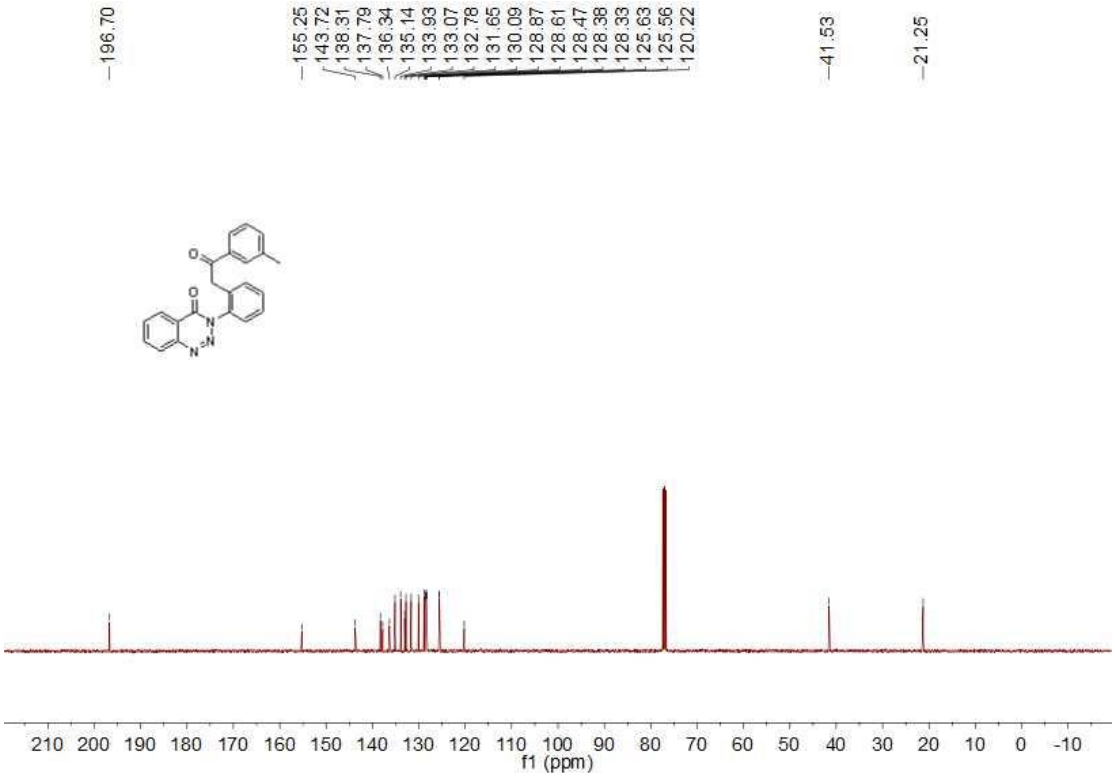
^{13}C NMR (101 MHz, $CDCl_3$) Spectra of **4ae**



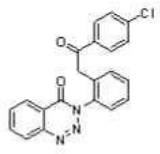
^{1}H NMR (400 MHz, $CDCl_3$) Spectra of **4af**

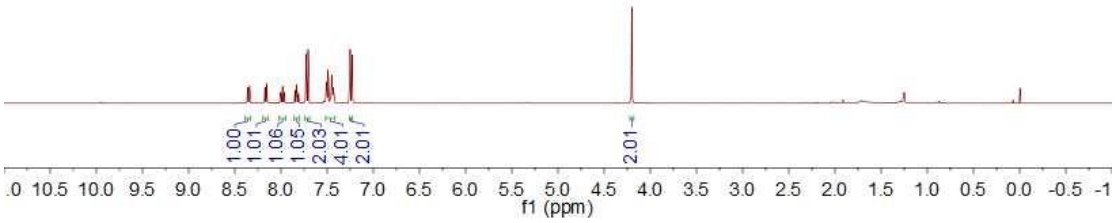


^{13}C NMR (101 MHz, $CDCl_3$) Spectra of **4af**

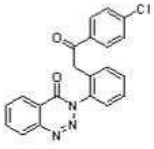


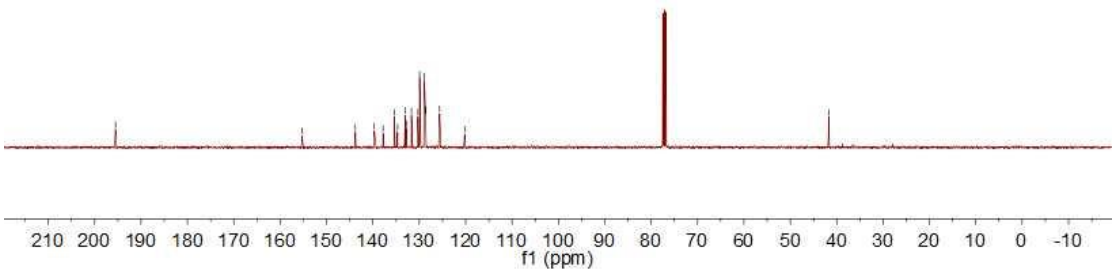
^{1}H NMR (400 MHz, $CDCl_3$) Spectra of **4ag**



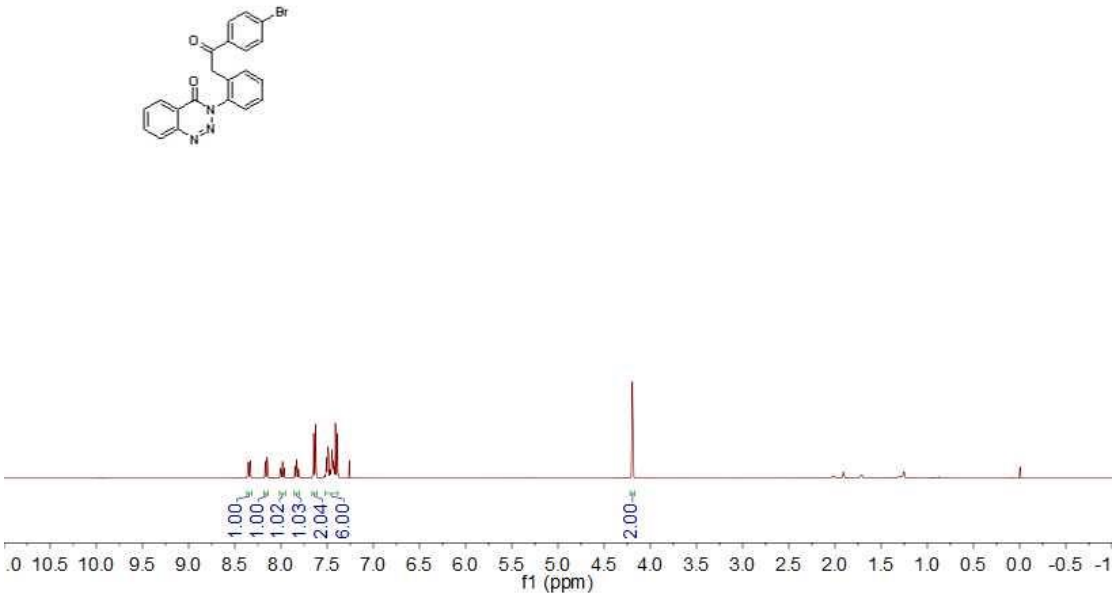


^{13}C NMR (101 MHz, $CDCl_3$) Spectra of **4ag**

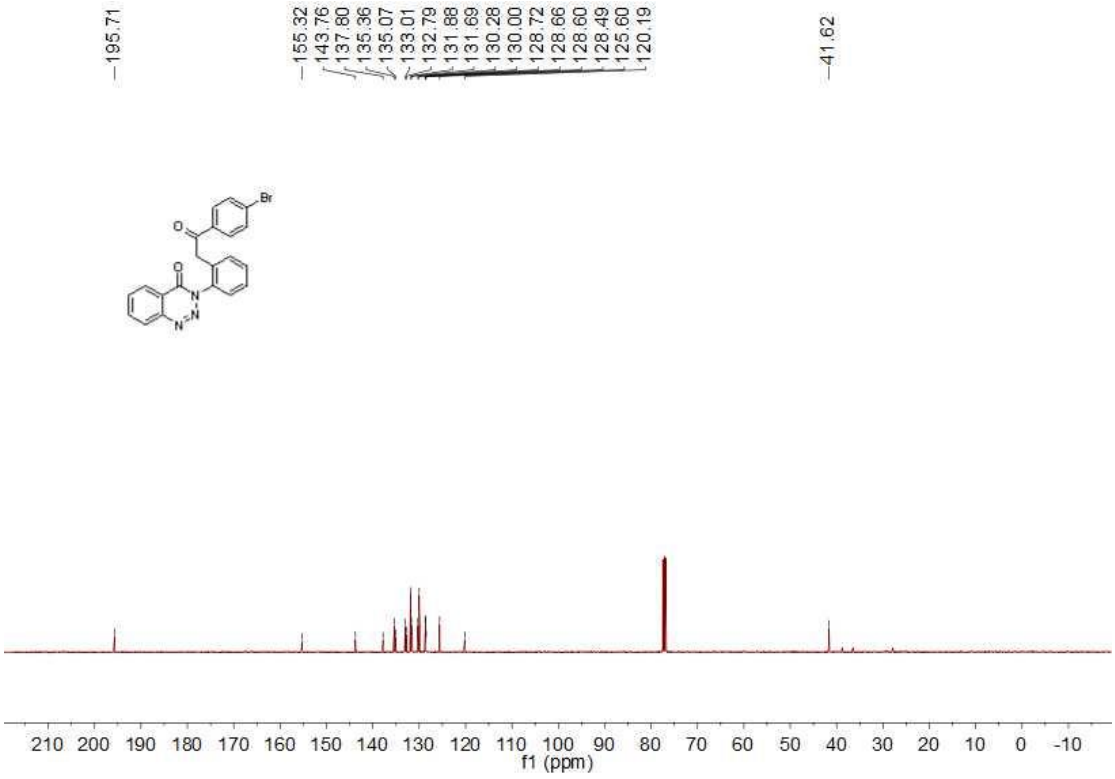




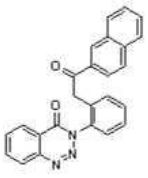
^{1}H NMR (400 MHz, $CDCl_3$) Spectra of **4ah**

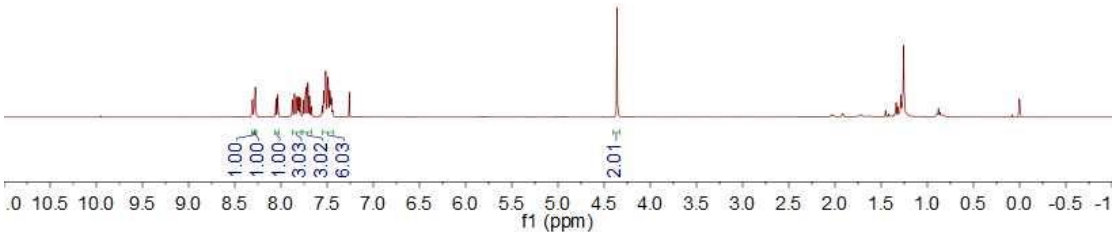


^{13}C NMR (101 MHz, $CDCl_3$) Spectra of **4ah**

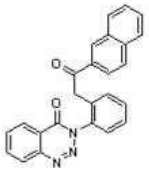


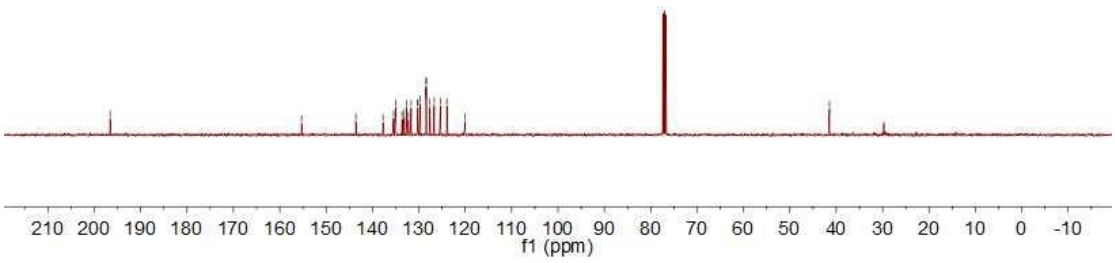
^{1}H NMR (400 MHz, $CDCl_3$) Spectra of **4ai**



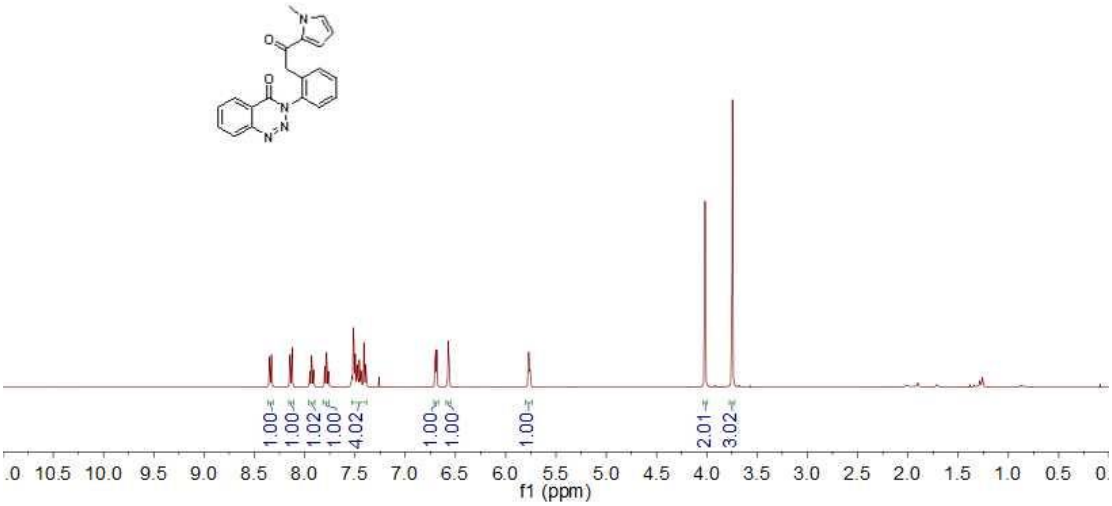


^{13}C NMR (101 MHz, $CDCl_3$) Spectra of **4ai**

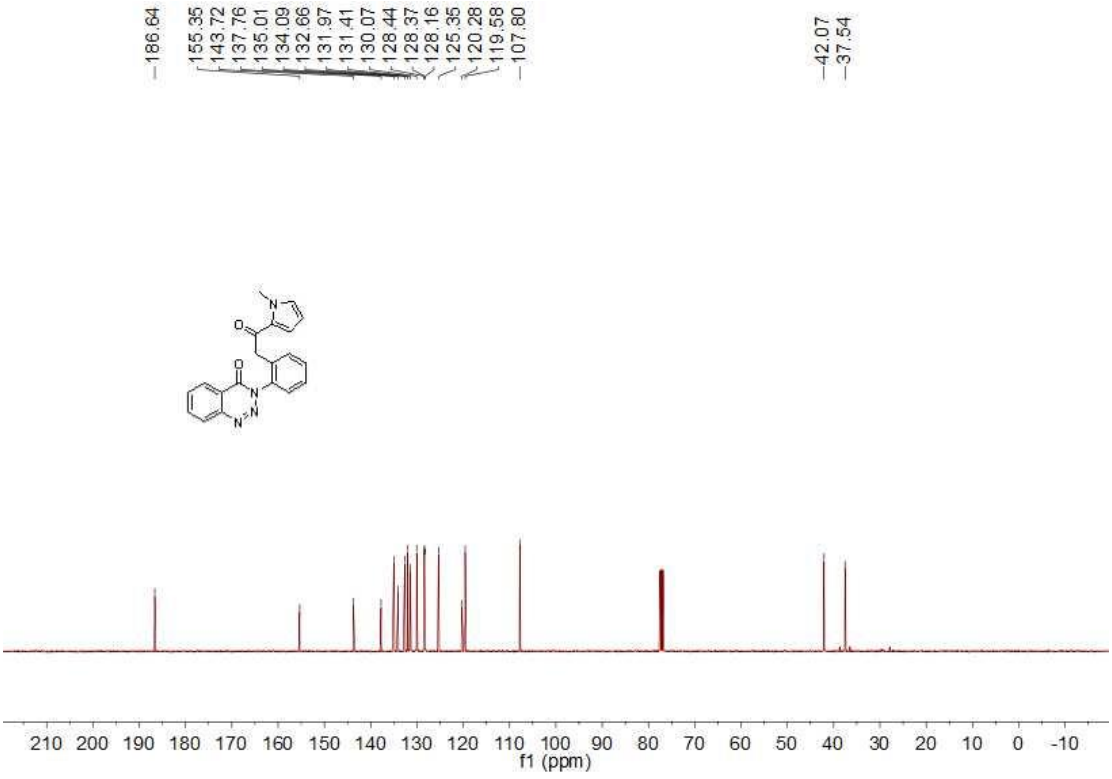




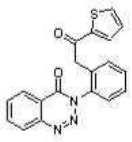
^{1}H NMR (400 MHz, $CDCl_3$) Spectra of **4aj**

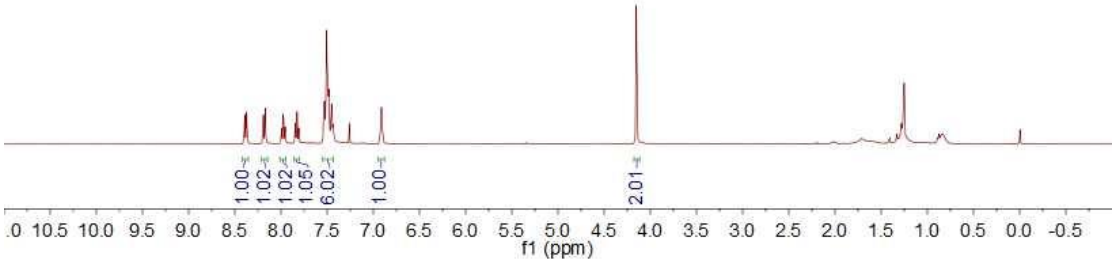


^{13}C NMR (101 MHz, $CDCl_3$) Spectra of **4aj**

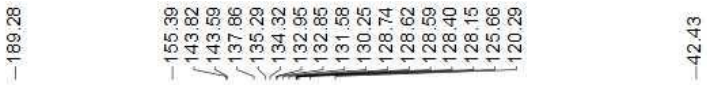


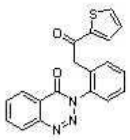
^{1}H NMR (400 MHz, $CDCl_3$) Spectra of **4ak**

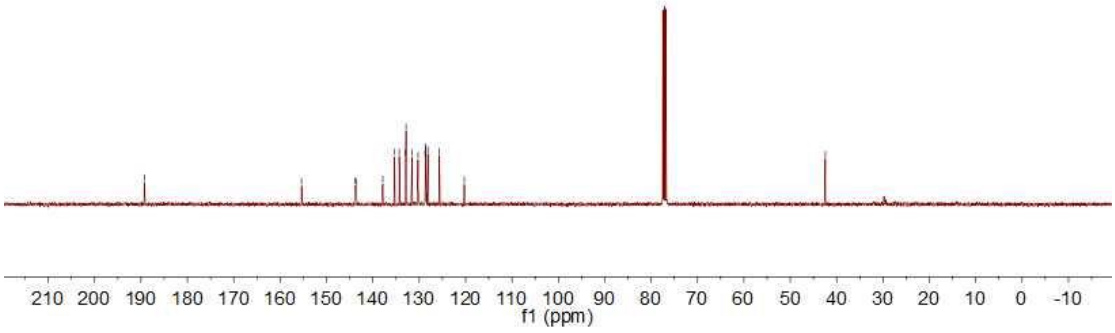




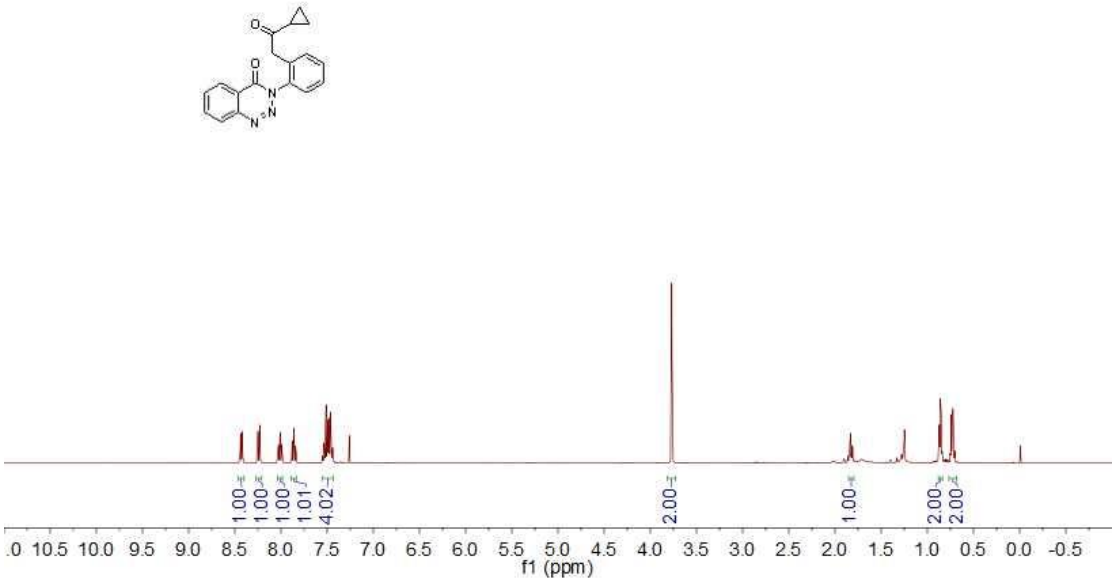
^{13}C NMR (101 MHz, $CDCl_3$) Spectra of **4ak**



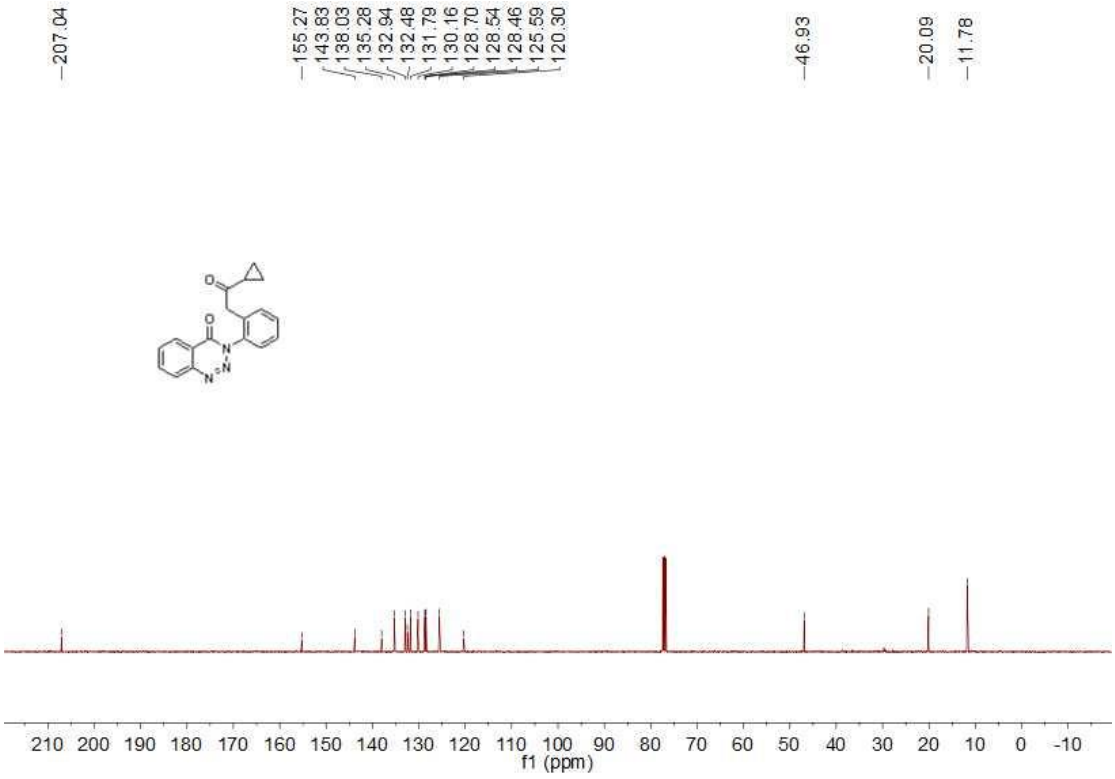




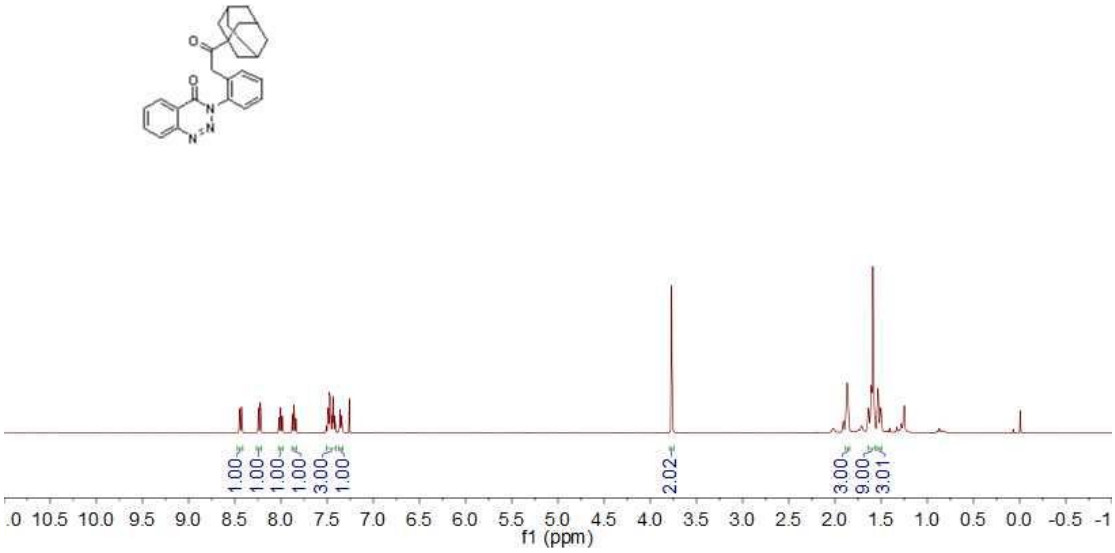
^{1}H NMR (400 MHz, $CDCl_3$) Spectra of **4al**



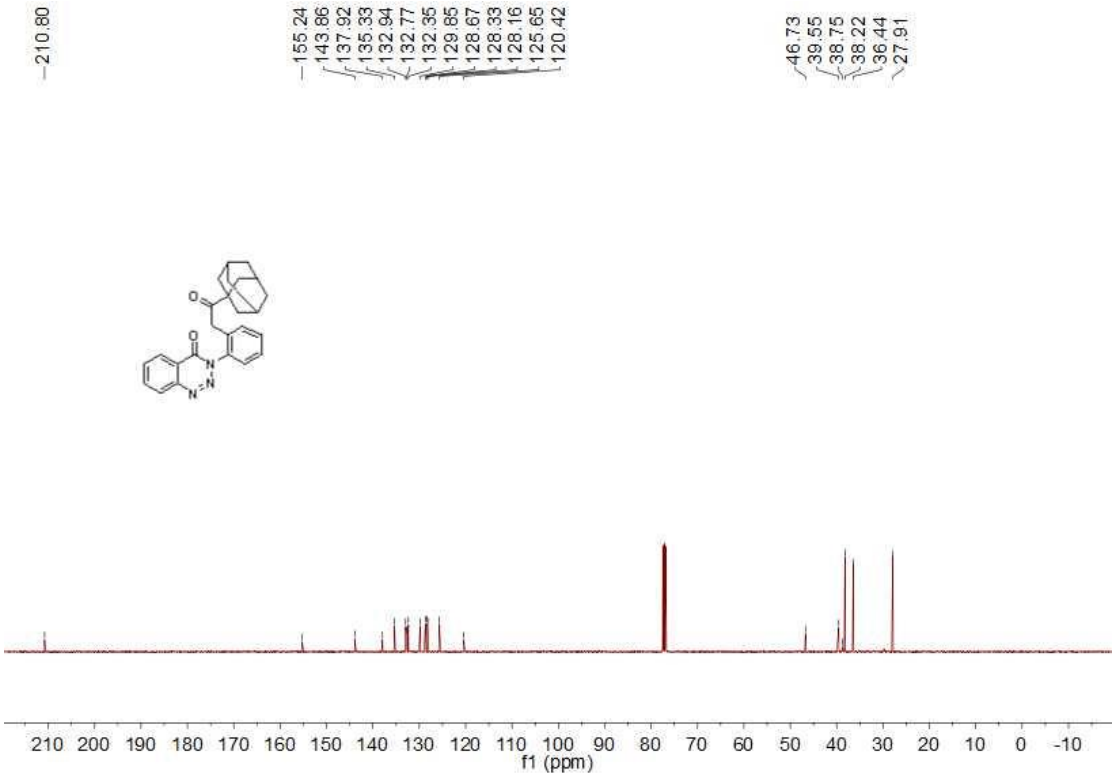
^{13}C NMR (101 MHz, $CDCl_3$) Spectra of **4al**



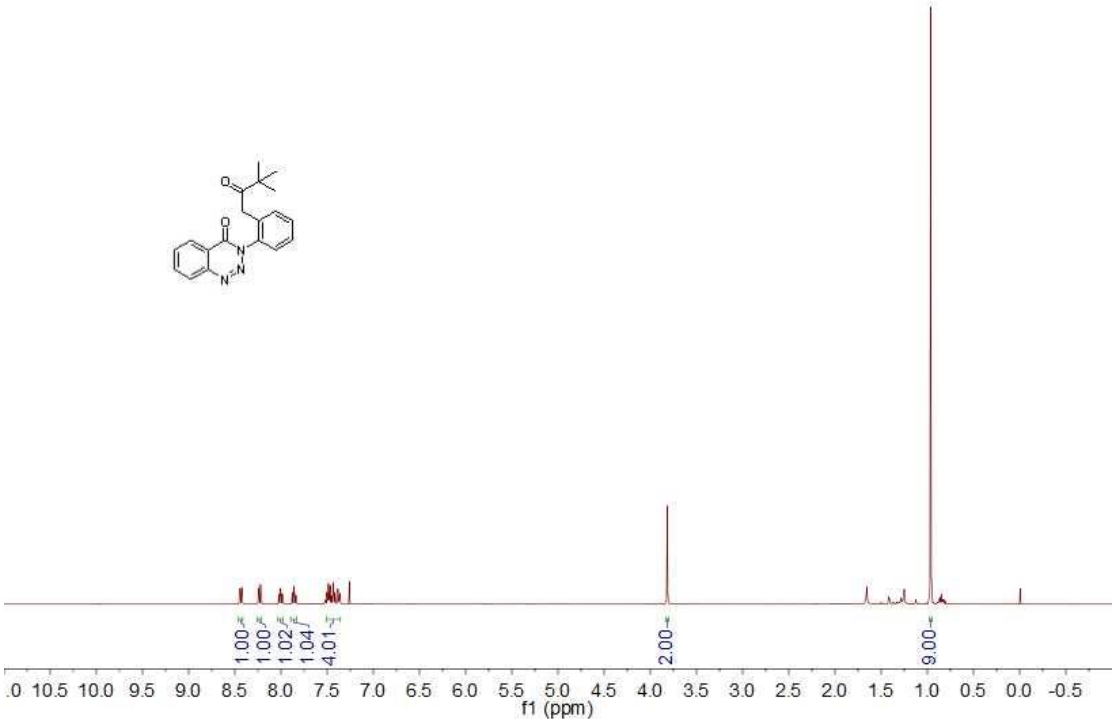
^{1}H NMR (400 MHz, $CDCl_3$) Spectra of **4am**



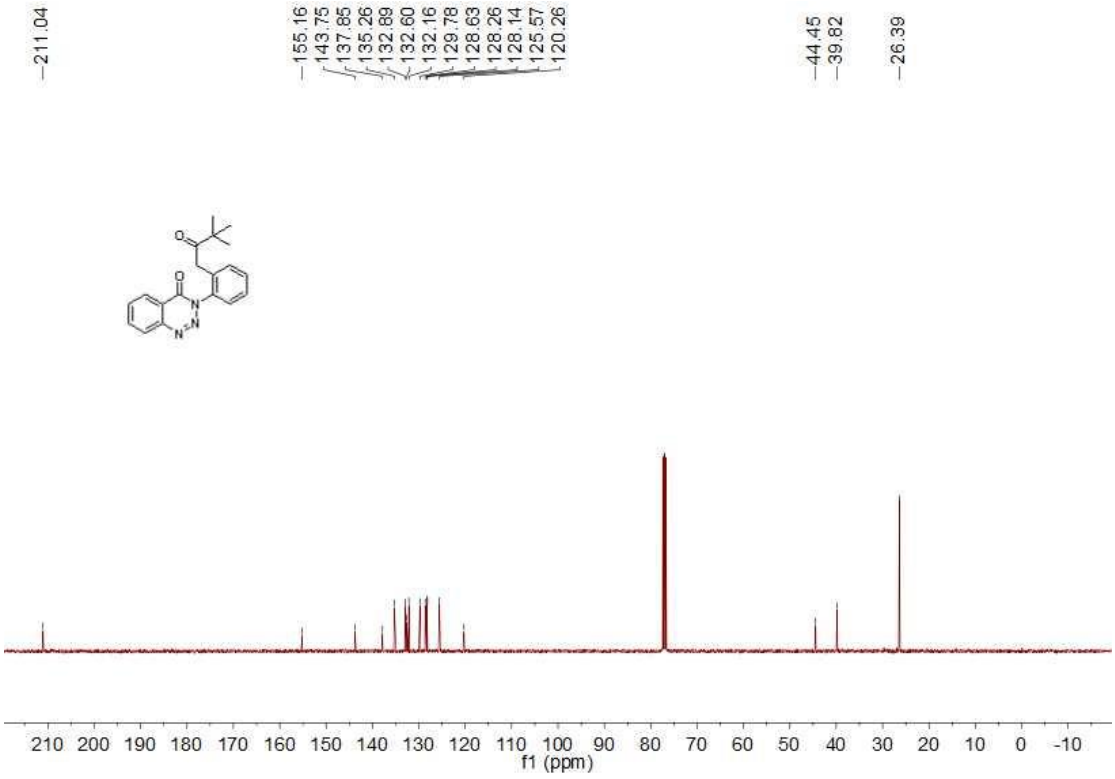
^{13}C NMR (101 MHz, $CDCl_3$) Spectra of **4am**



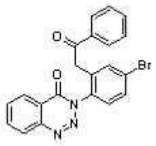
^{1}H NMR (400 MHz, $CDCl_3$) Spectra of **4an**

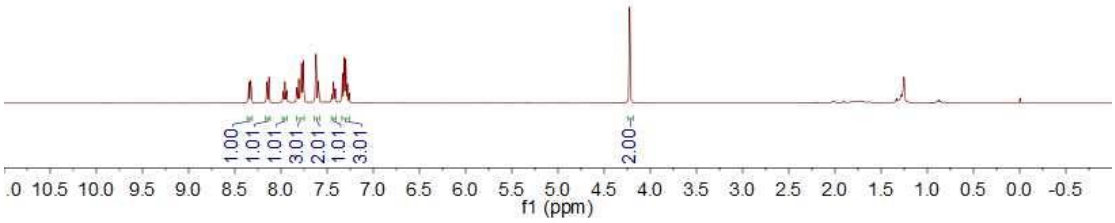


^{13}C NMR (101 MHz, $CDCl_3$) Spectra of **4an**

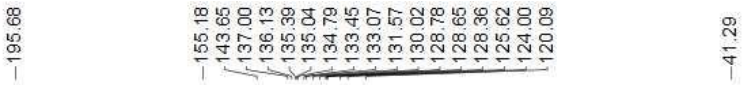


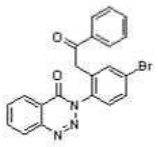
^{1}H NMR (400 MHz, $CDCl_3$) Spectra of **4ba**

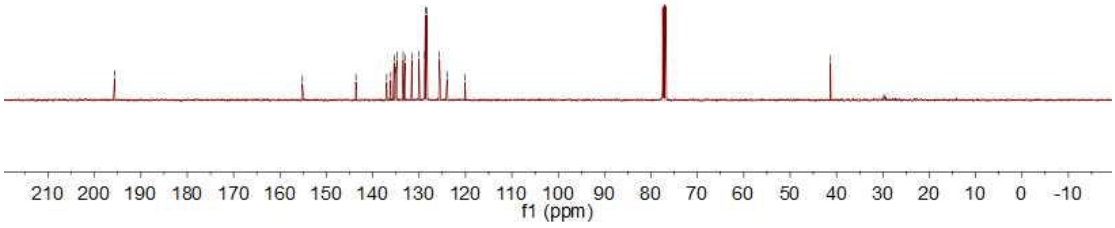




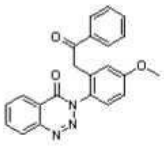
^{13}C NMR (101 MHz, $CDCl_3$) Spectra of **4ba**

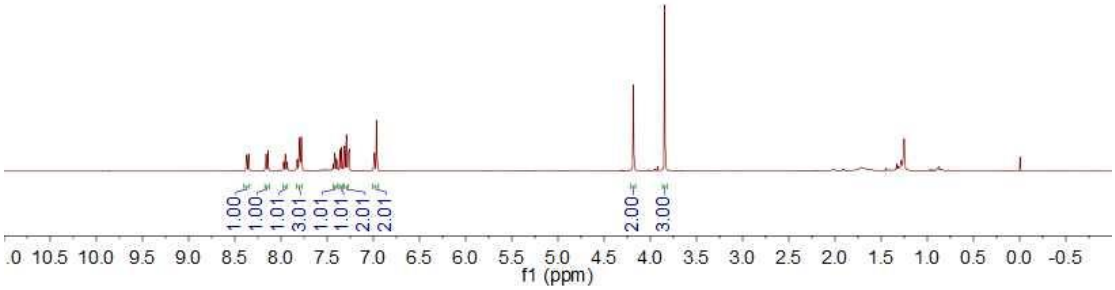




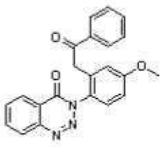


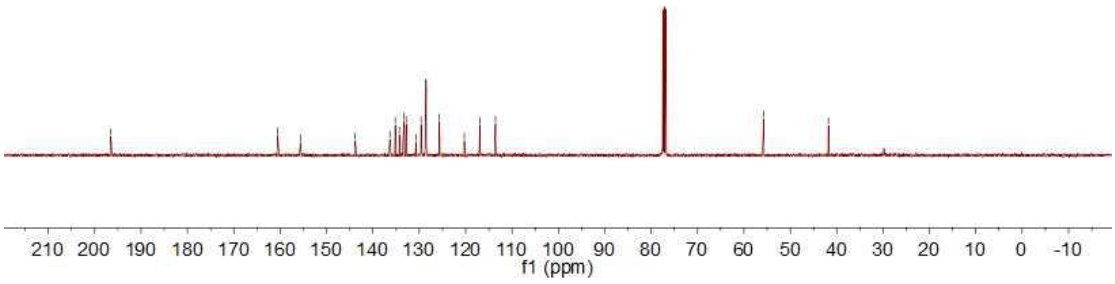
^{1}H NMR (400 MHz, $CDCl_3$) Spectra of **4ca**



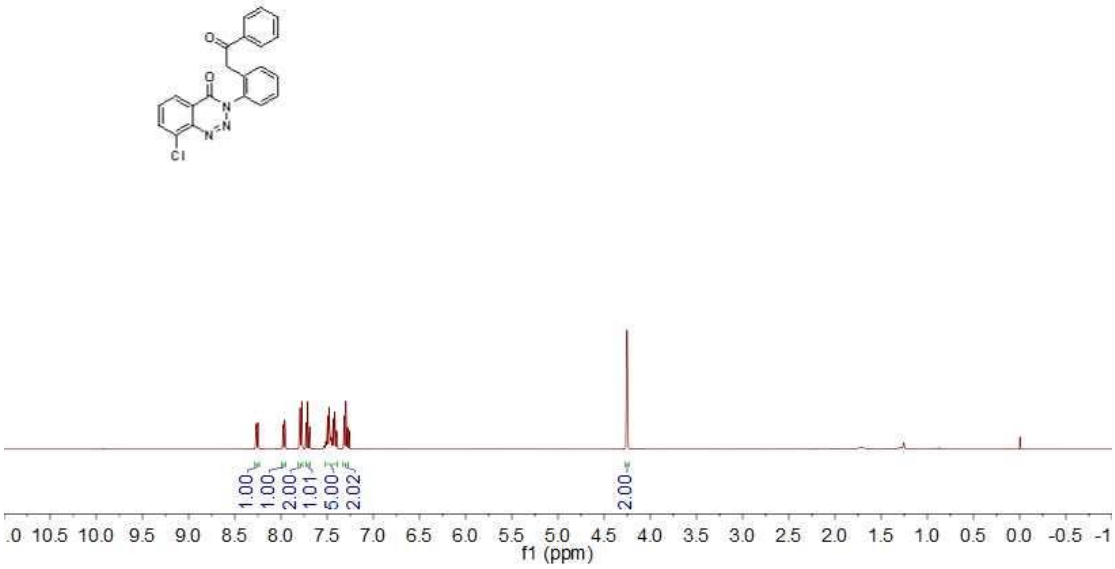


^{13}C NMR (101 MHz, $CDCl_3$) Spectra of **4ca**

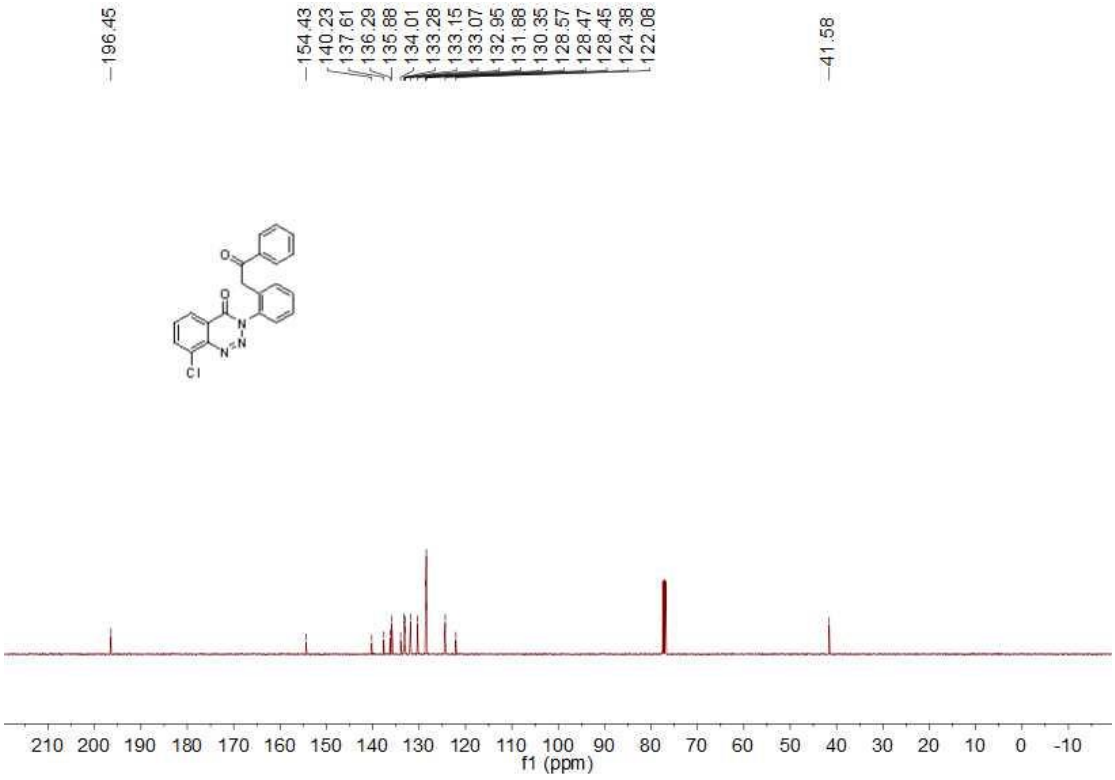




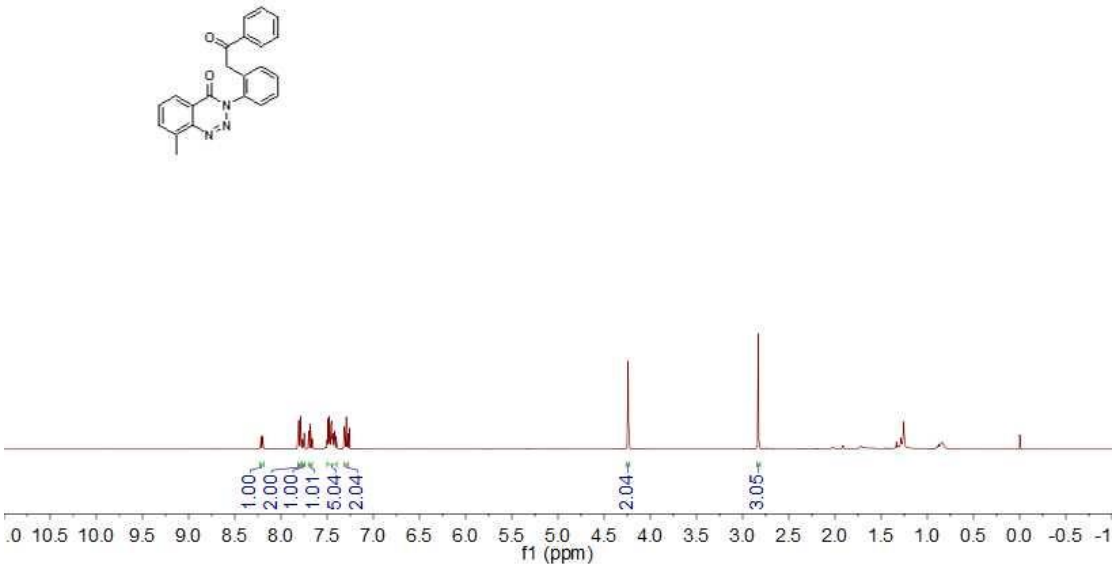
^{1}H NMR (400 MHz, $CDCl_3$) Spectra of **4da**



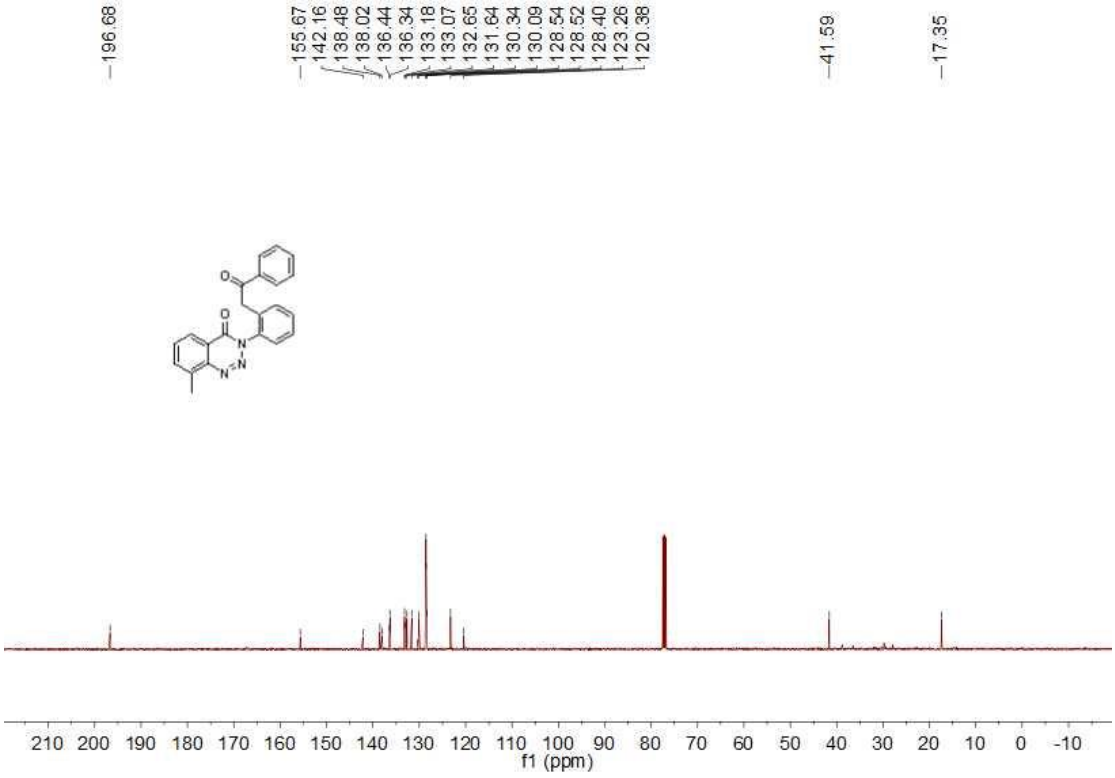
^{13}C NMR (101 MHz, $CDCl_3$) Spectra of **4da**



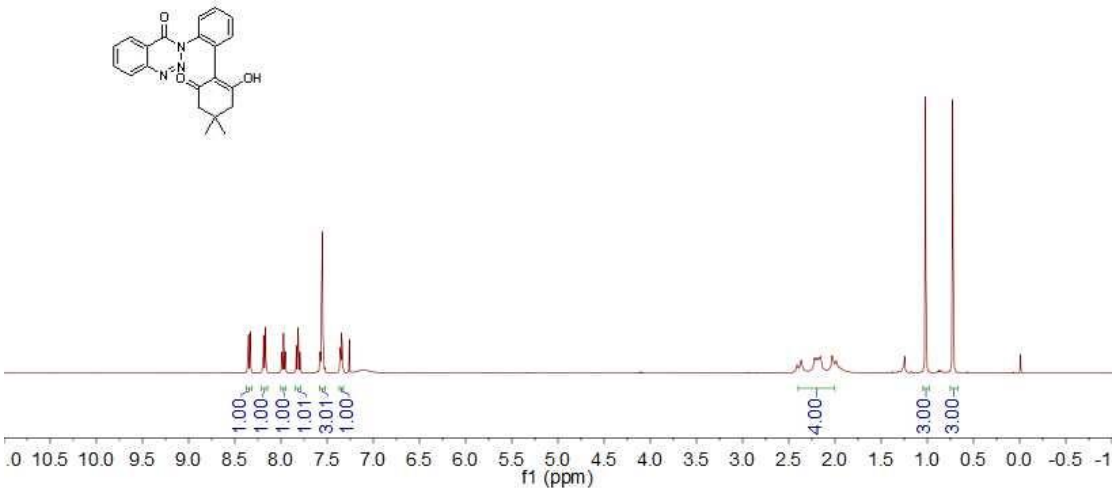
^{1}H NMR (400 MHz, $CDCl_3$) Spectra of **4ea**



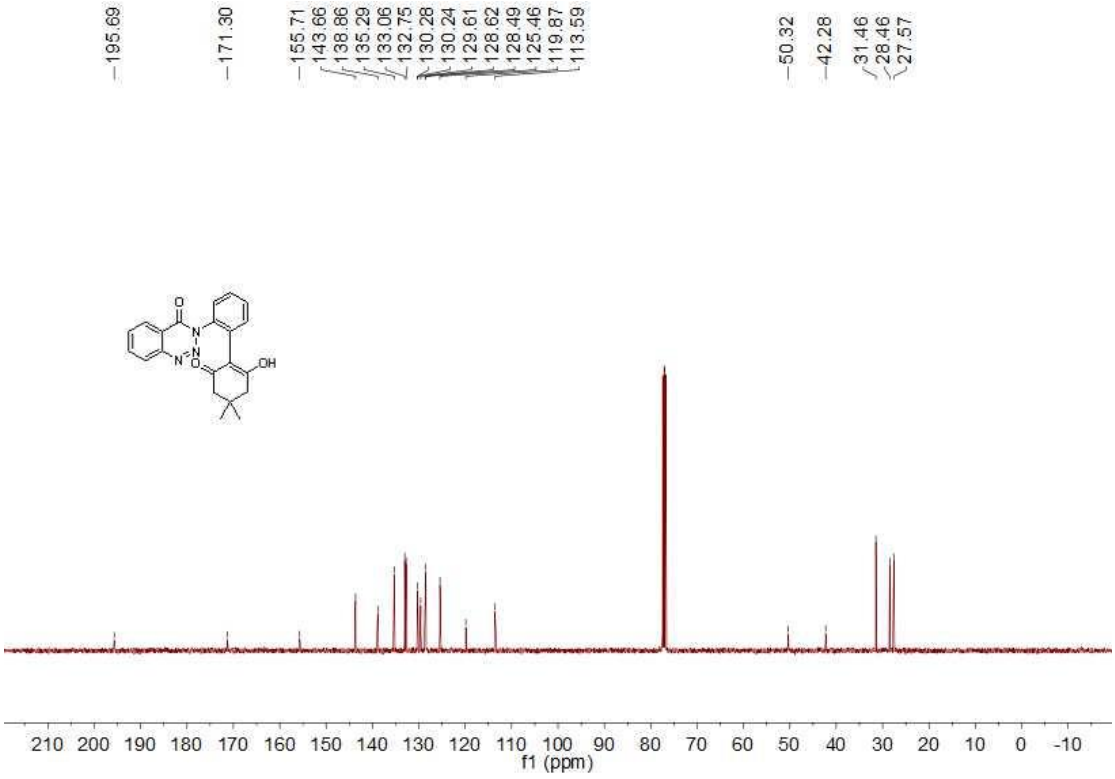
^{13}C NMR (101 MHz, $CDCl_3$) Spectra of **4ea**



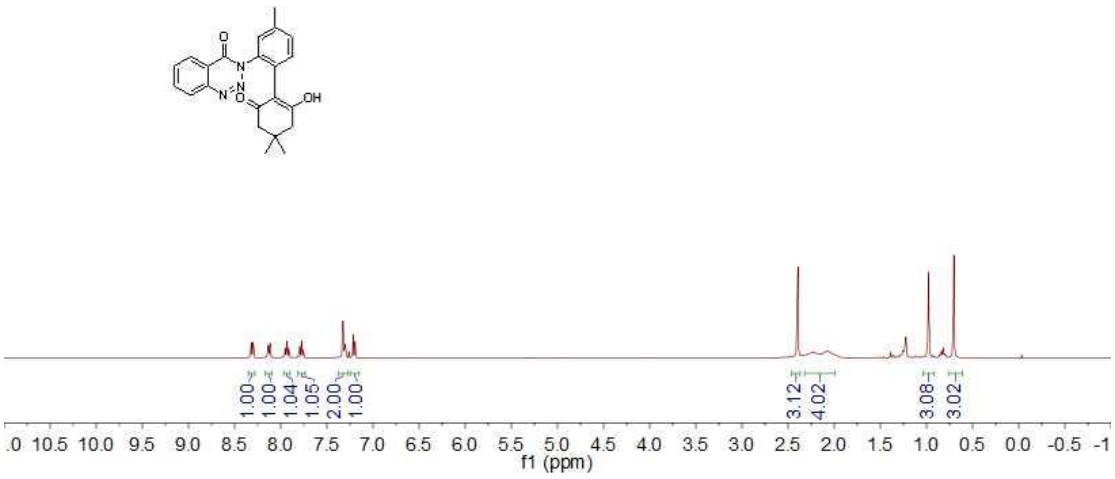
^{1}H NMR (400 MHz, $CDCl_3$) Spectra of **5aa**



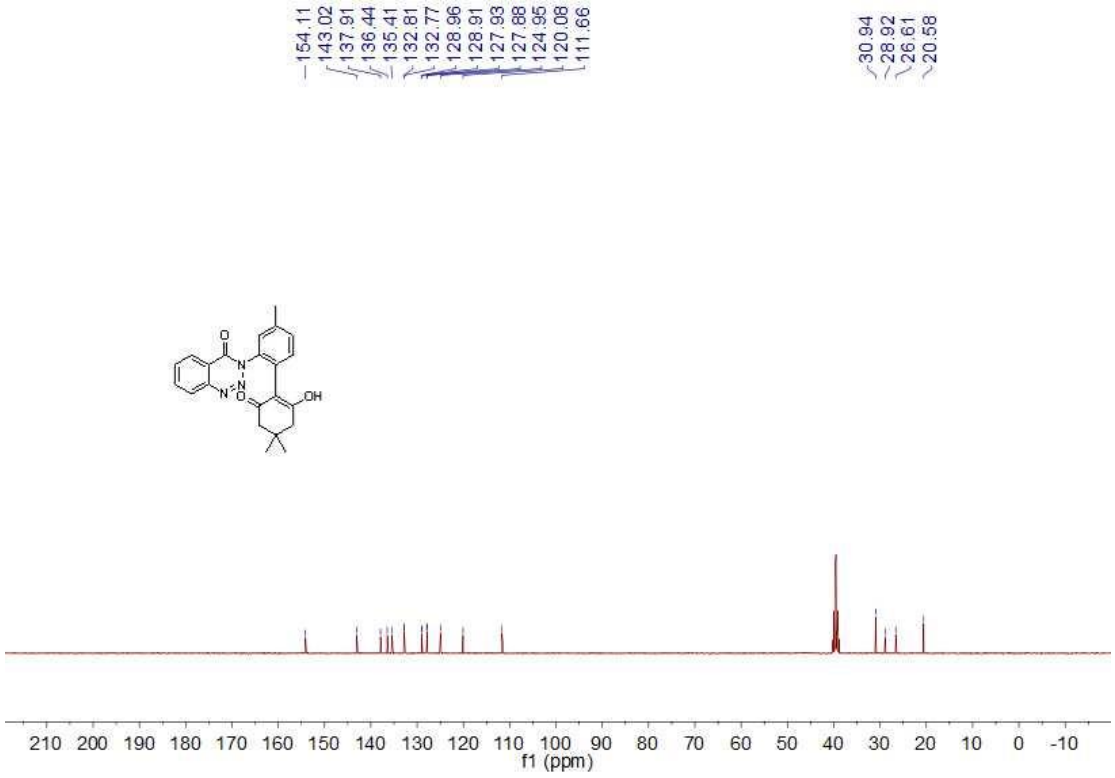
^{13}C NMR (101 MHz, $CDCl_3$) Spectra of **5aa**



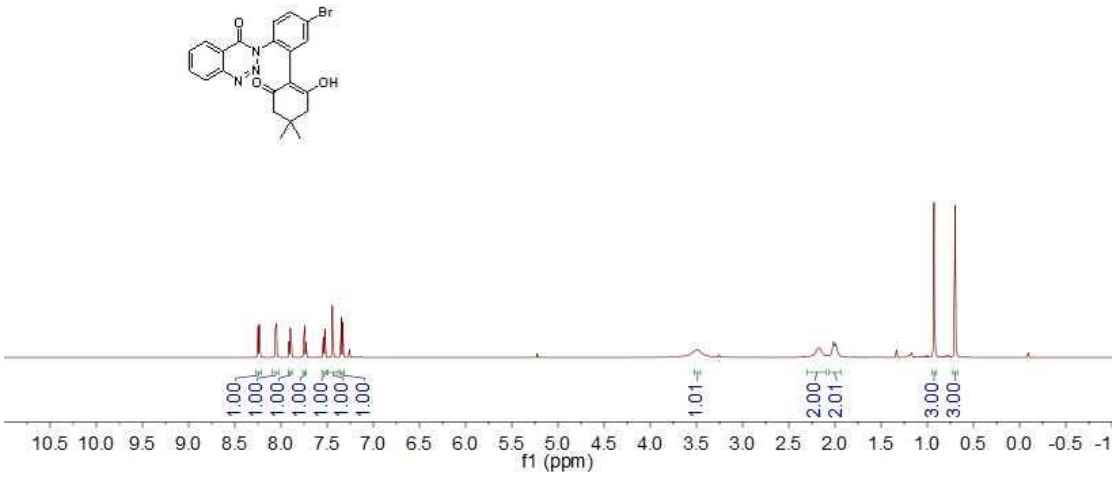
^{1}H NMR (400 MHz, $CDCl_3$) Spectra of **5ba**



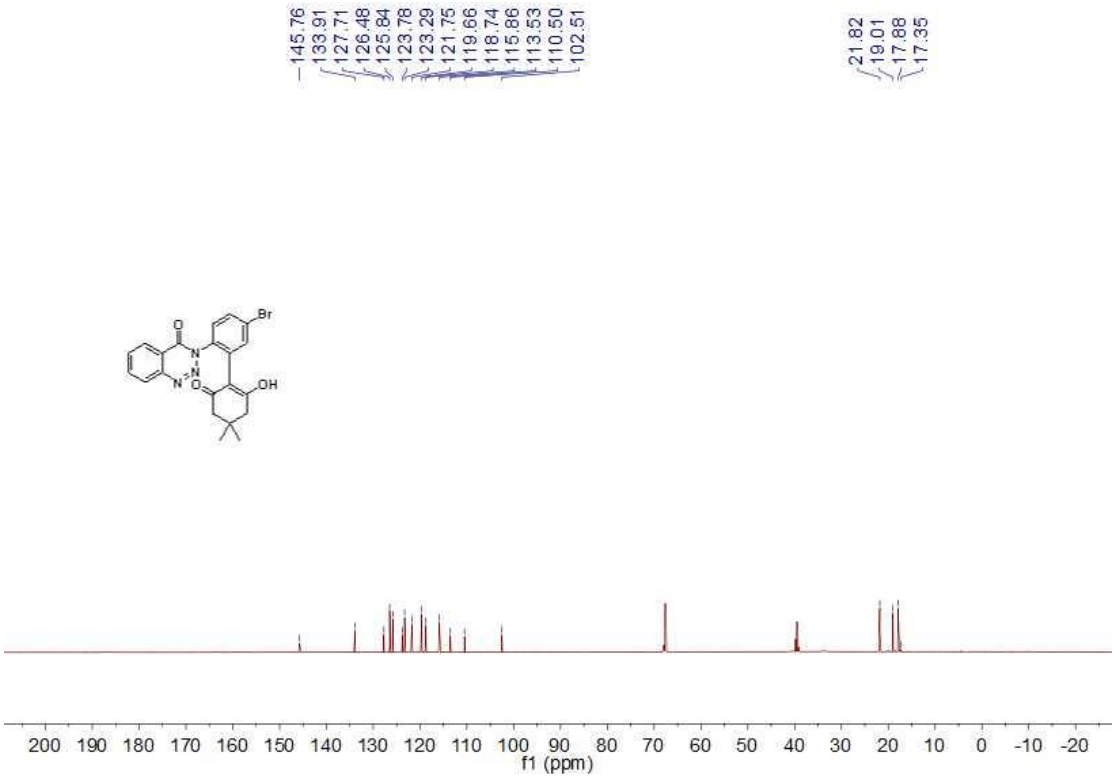
^{13}C NMR (101 MHz, DMSO-d_6) Spectra of **5ba**



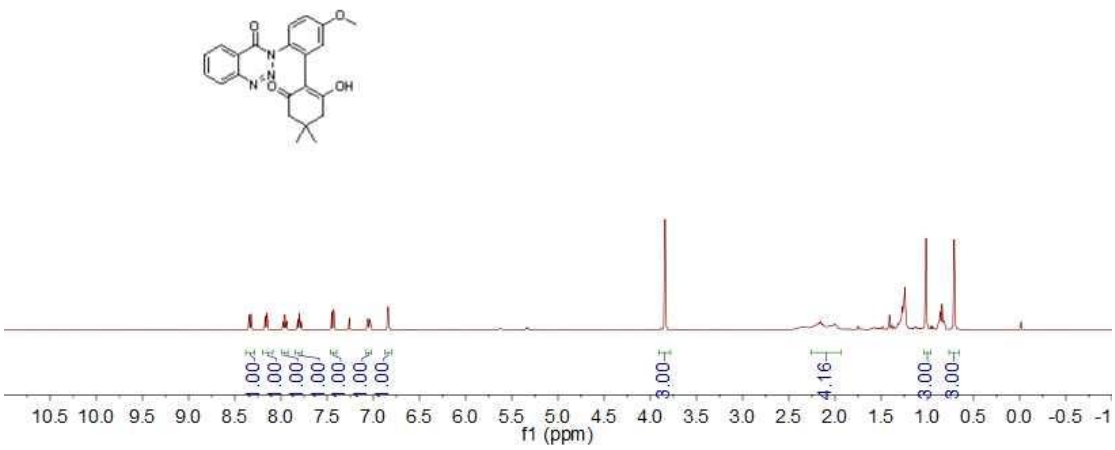
^{1}H NMR (600 MHz, $CDCl_3$) Spectra of **5ca**



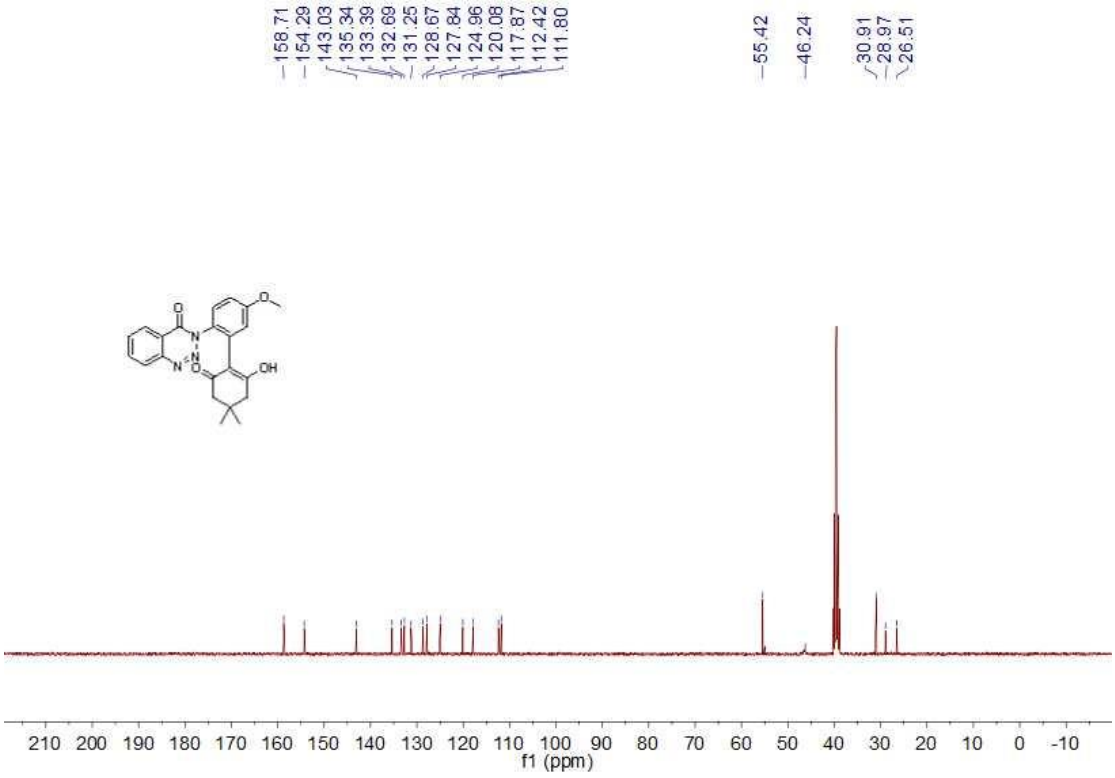
^{13}C NMR (151 MHz, $CDCl_3$) Spectra of **5ca**



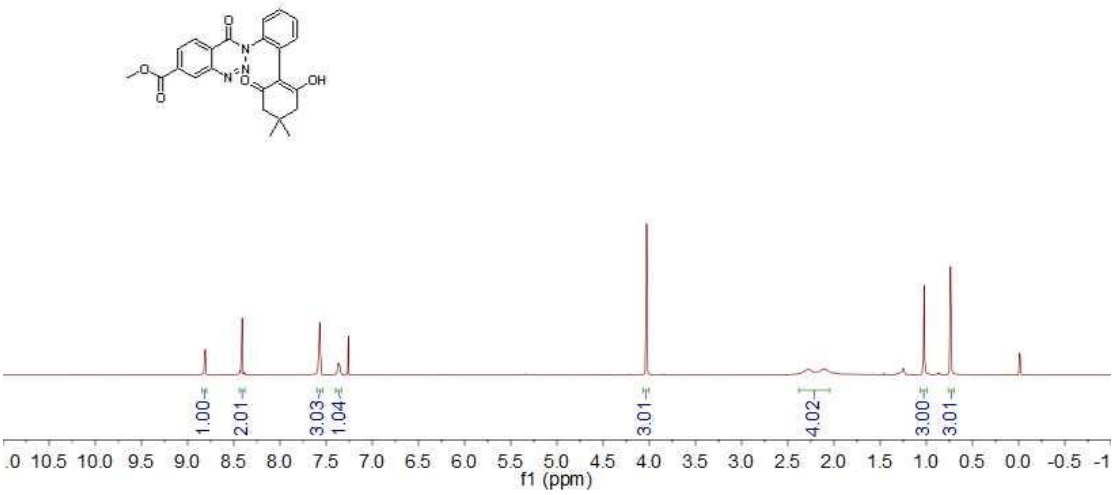
^{1}H NMR (400 MHz, $CDCl_3$) Spectra of **5da**



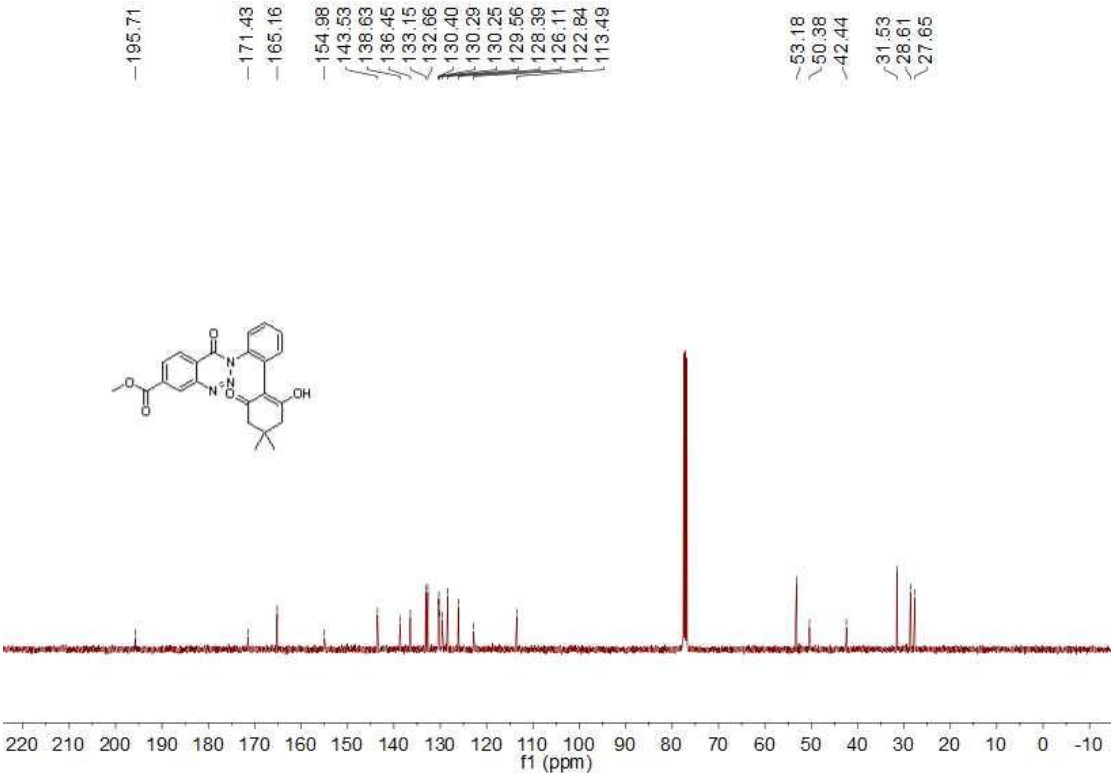
^{13}C NMR (101 MHz, DMSO-d_6) Spectra of **5da**



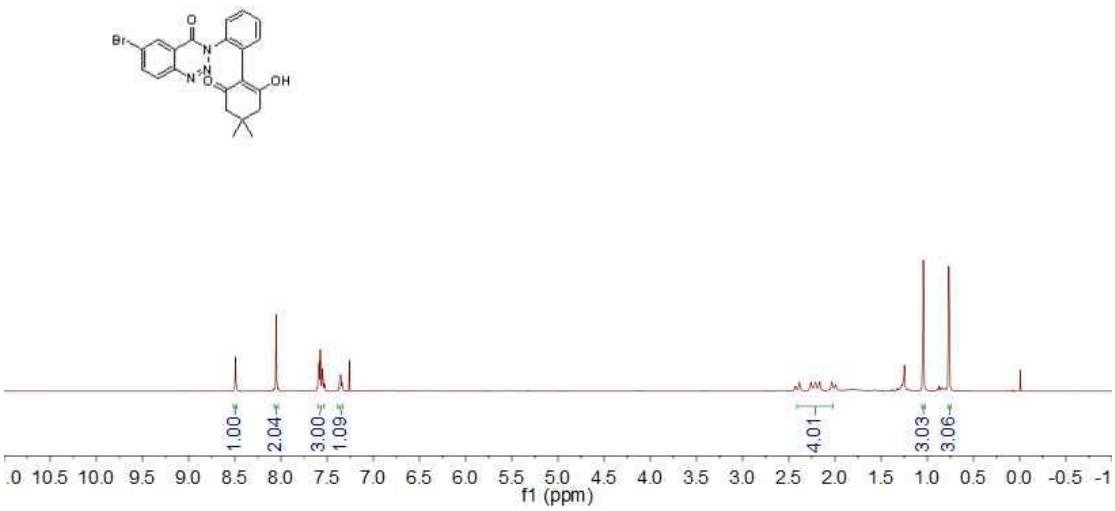
^{1}H NMR (400 MHz, $CDCl_3$) Spectra of **5ea**



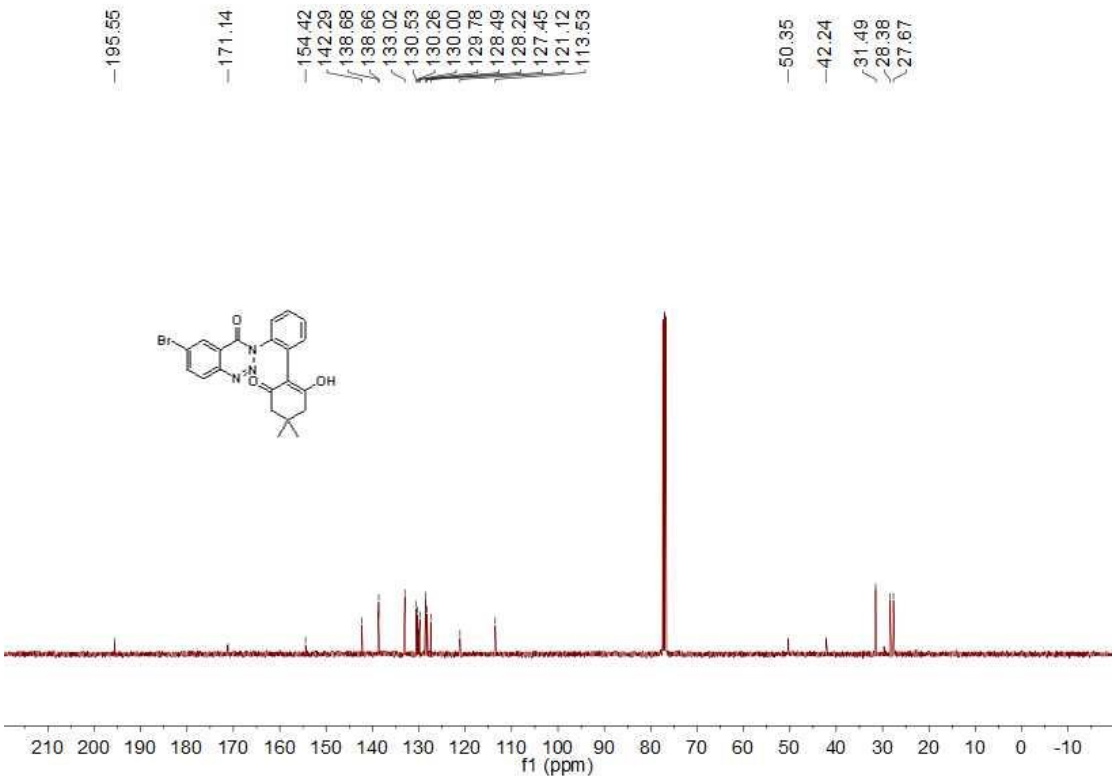
^{13}C NMR (101 MHz, DMSO-d_6) Spectra of **5ea**



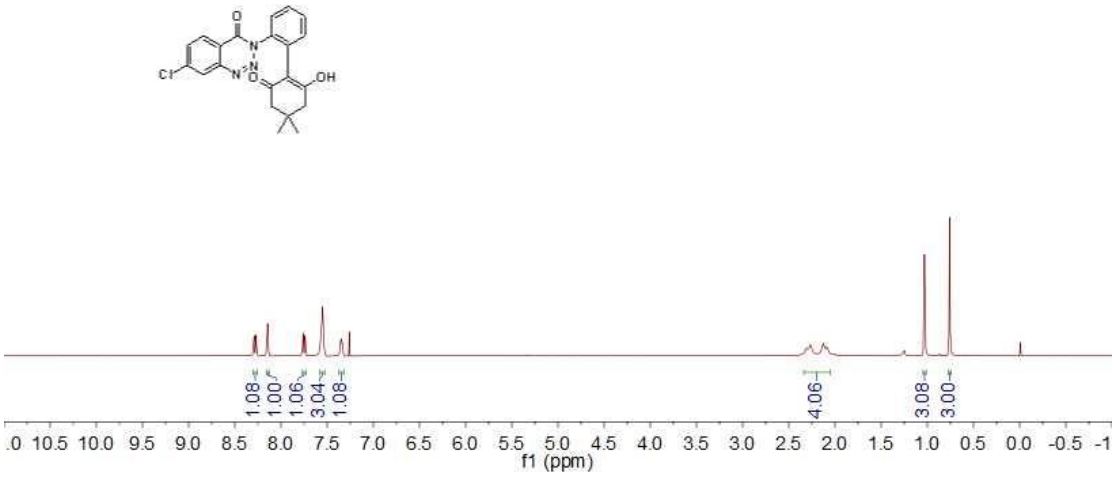
^{1}H NMR (400 MHz, $CDCl_3$) Spectra of **5fa**



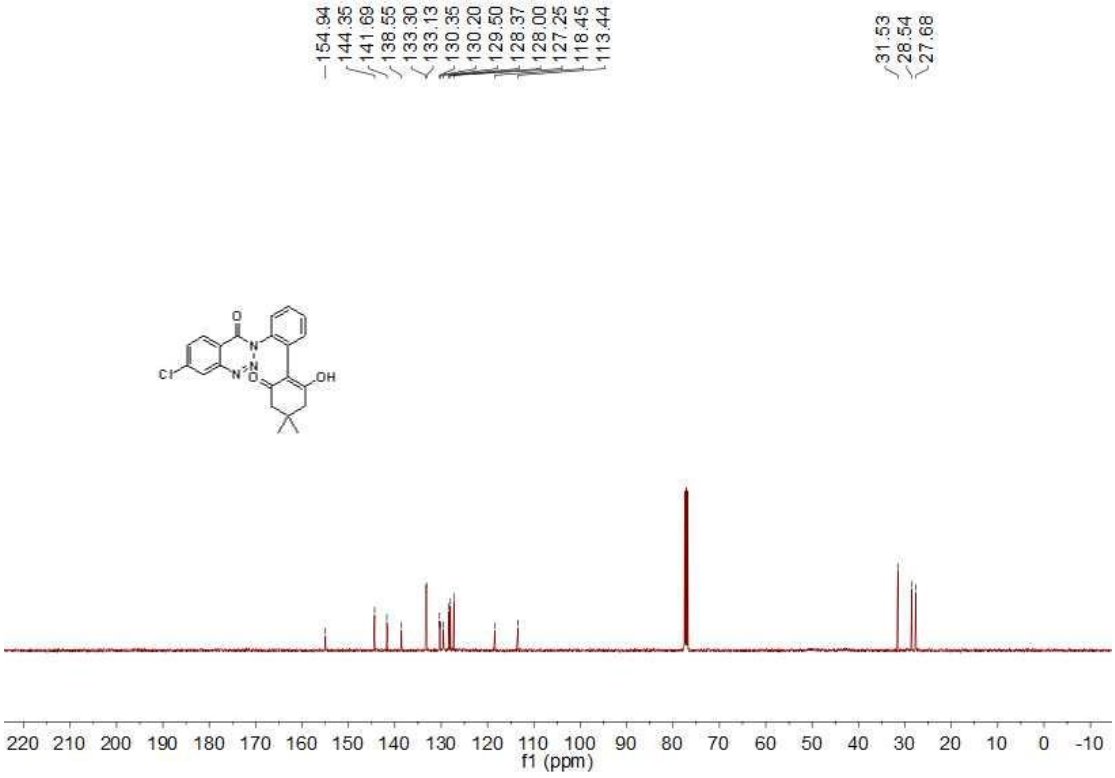
^{13}C NMR (101 MHz, $CDCl_3$) Spectra of **5fa**



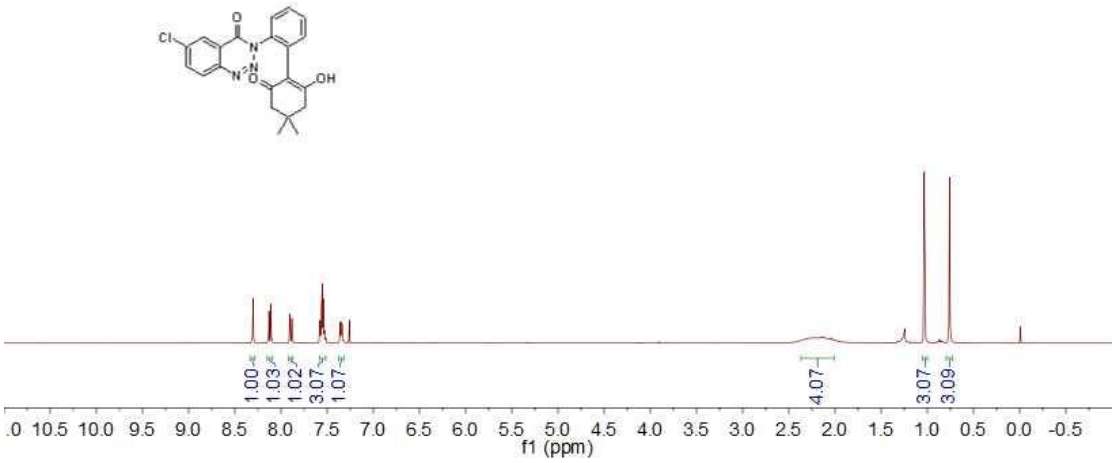
^{1}H NMR (400 MHz, $CDCl_3$) Spectra of **5ga**



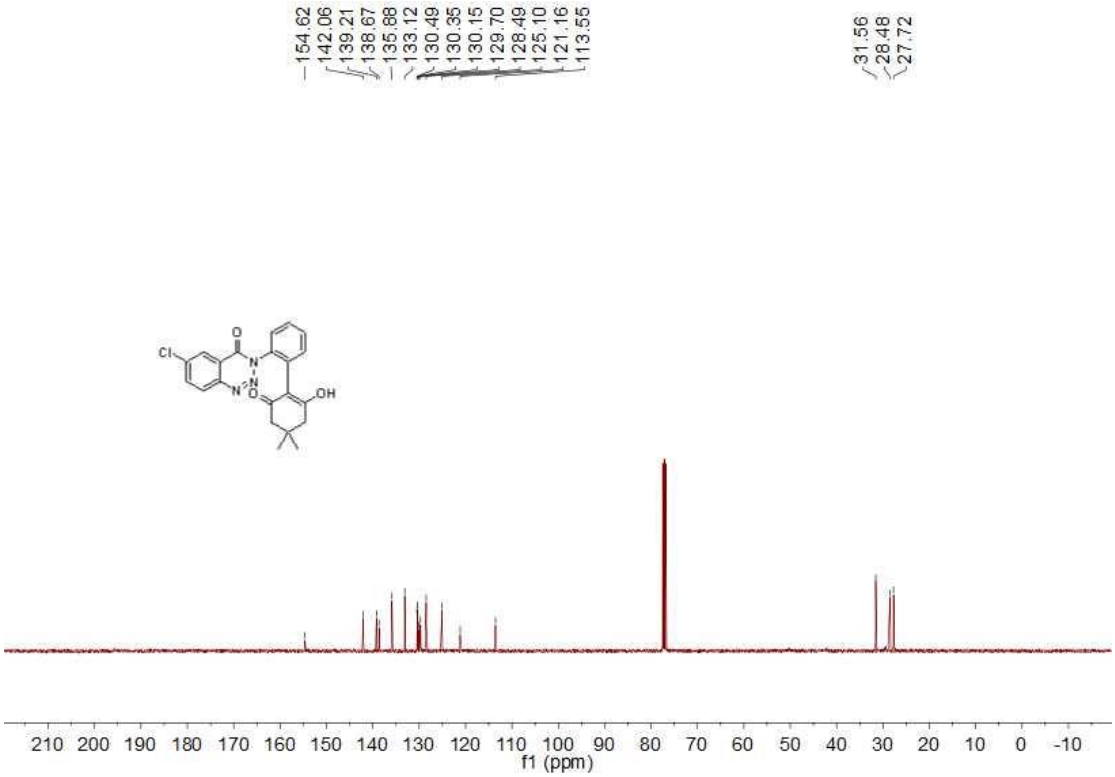
^{13}C NMR (101 MHz, $CDCl_3$) Spectra of **5ga**



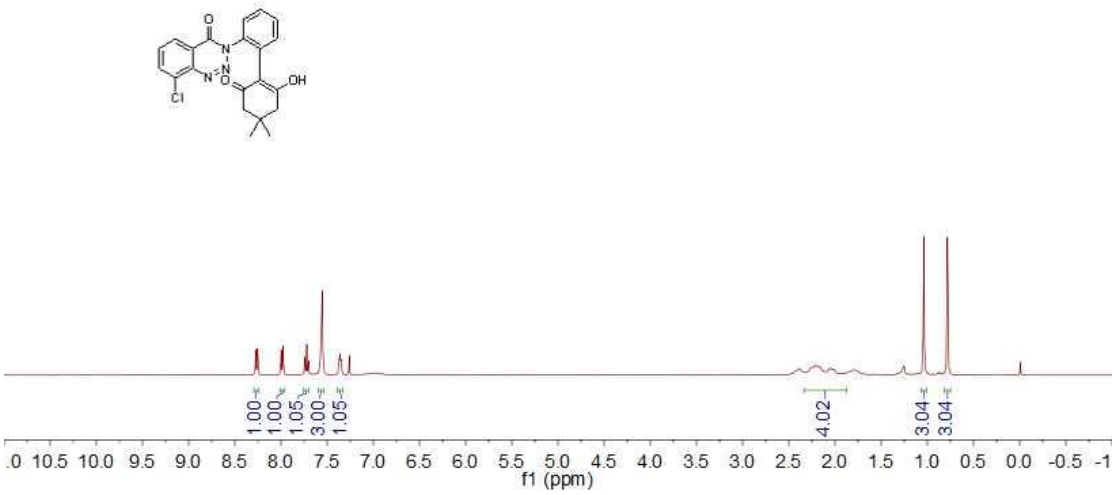
^{1}H NMR (400 MHz, $CDCl_3$) Spectra of **5ha**



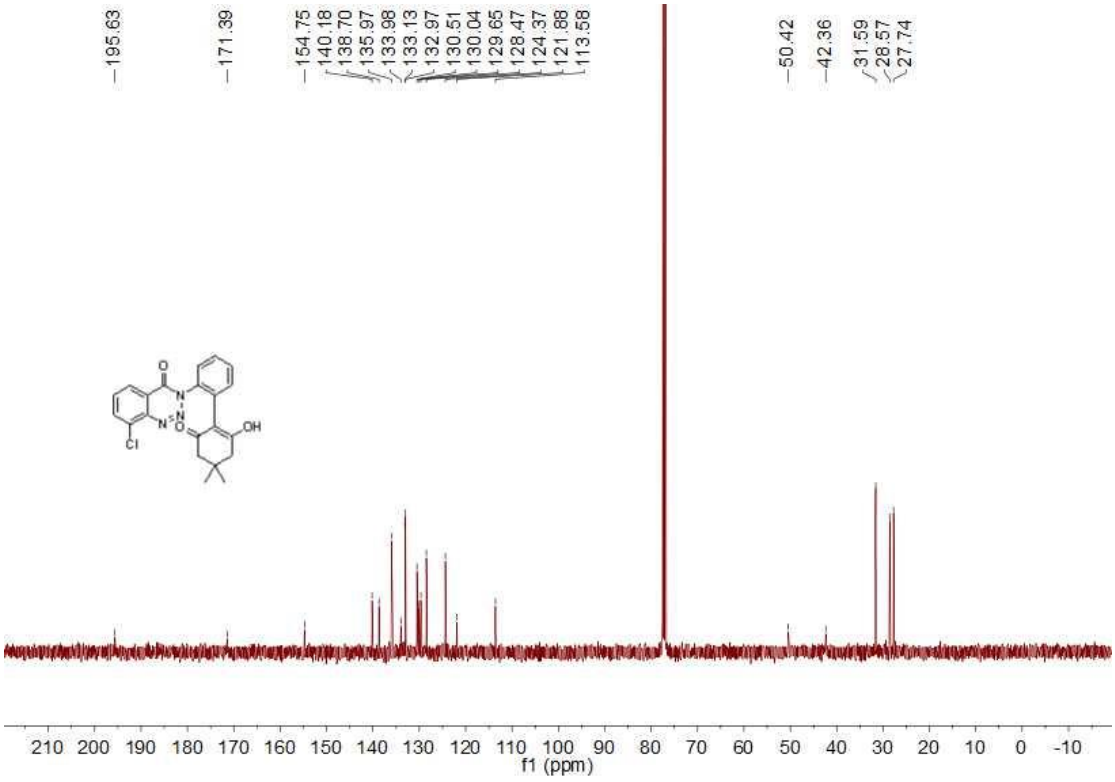
^{13}C NMR (101 MHz, $CDCl_3$) Spectra of **5ha**



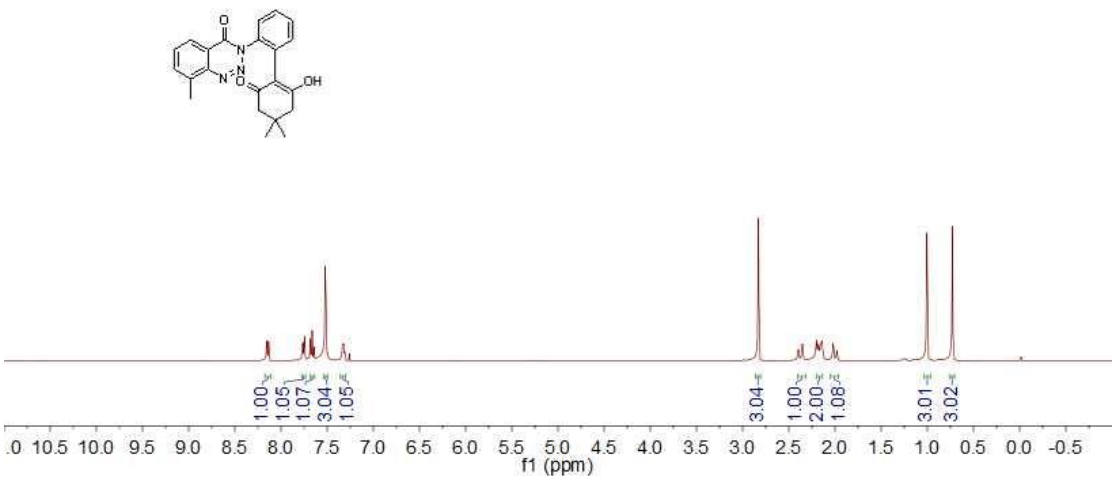
^{1}H NMR (400 MHz, $CDCl_3$) Spectra of **5ia**



^{13}C NMR (101 MHz, $CDCl_3$) Spectra of **5ia**



^{1}H NMR (400 MHz, $CDCl_3$) Spectra of **5ja**



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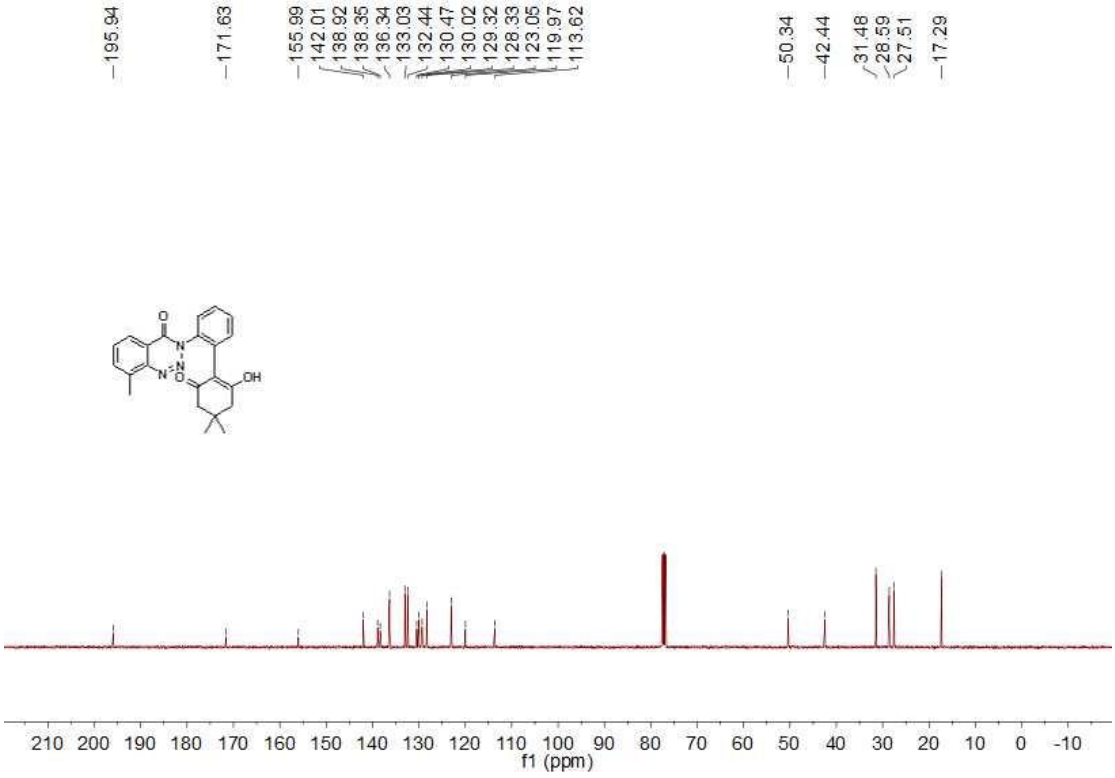
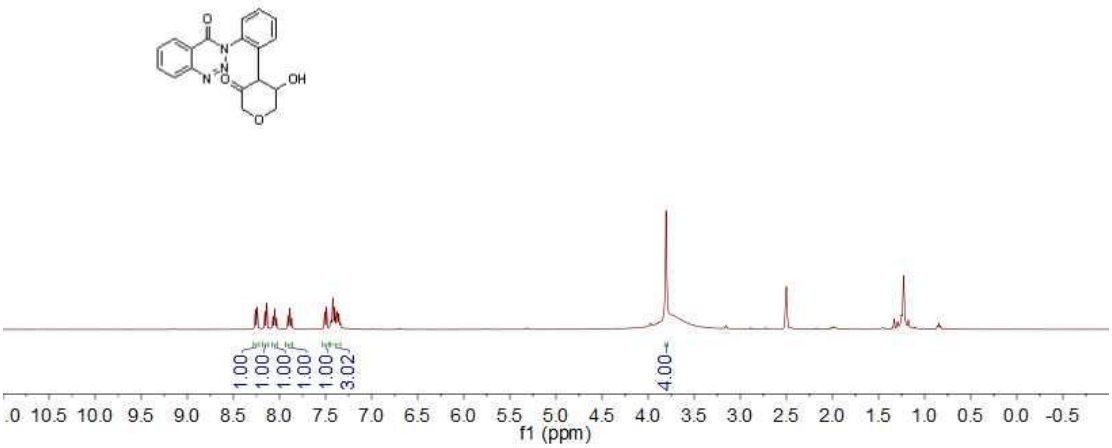
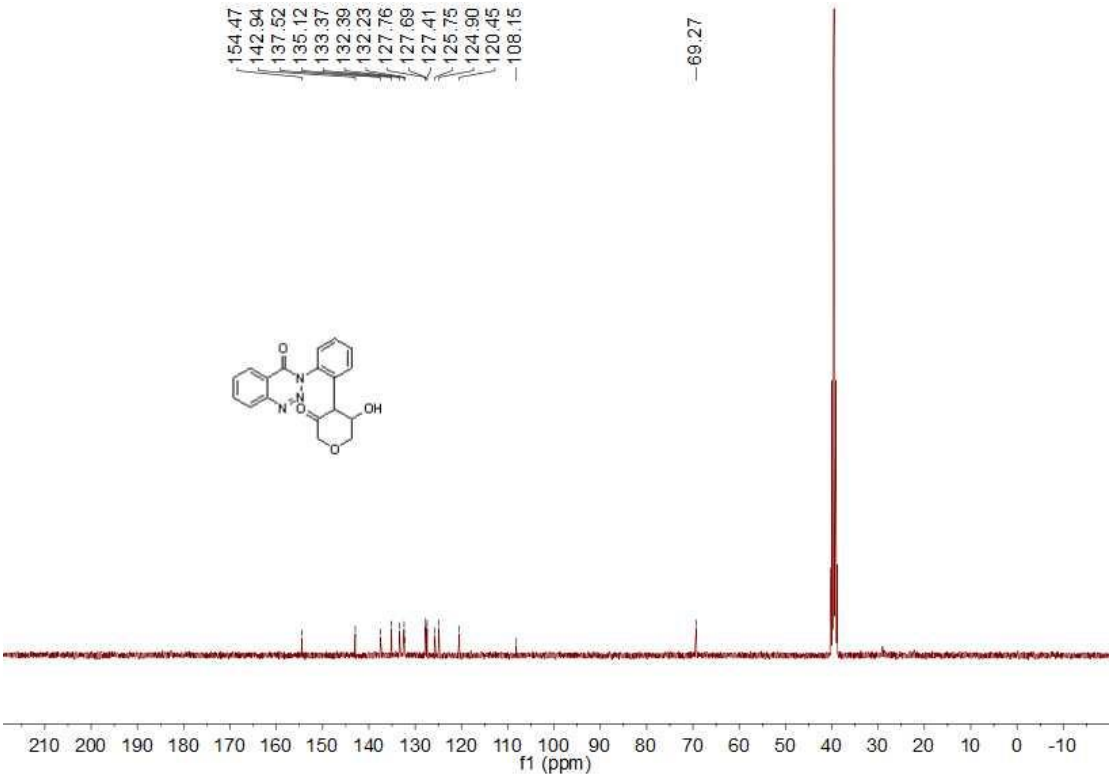


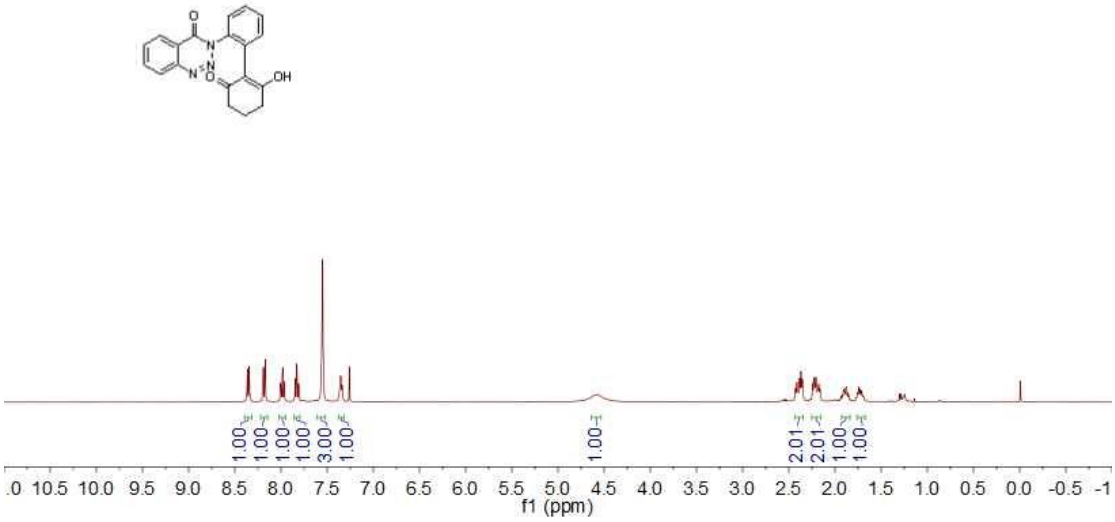
^{1}H NMR (400 MHz, DMSO-d_6) Spectra of **5ab**



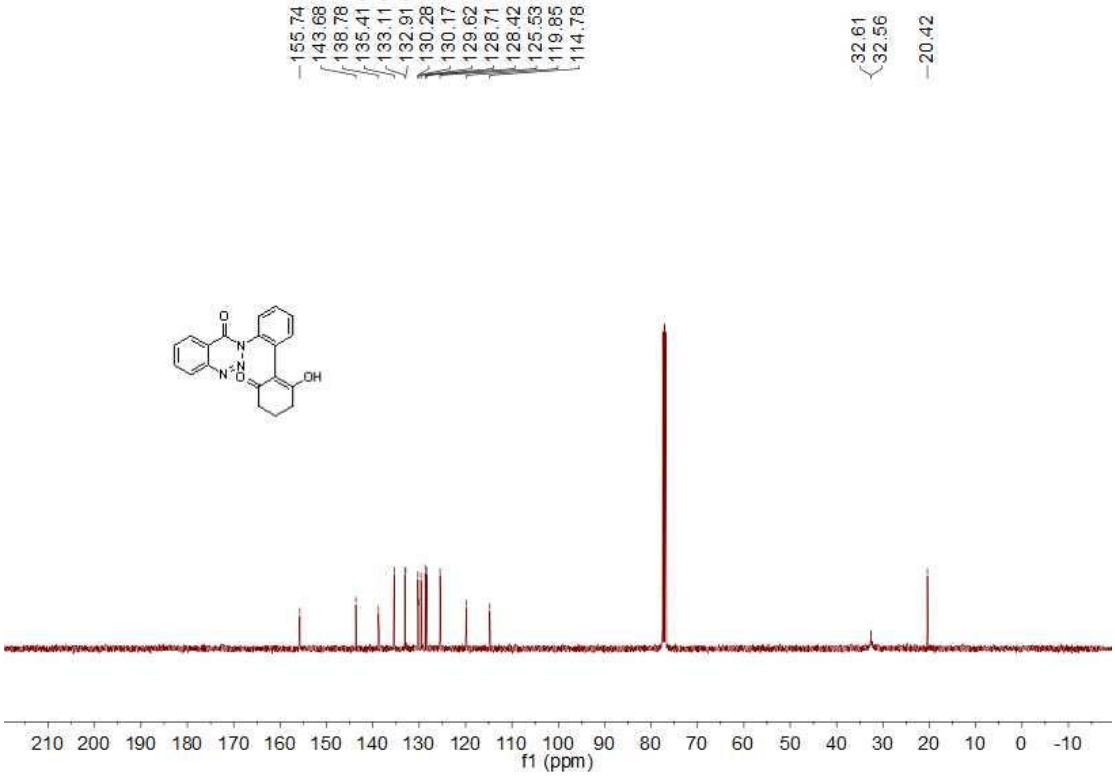
^{13}C NMR (101 MHz, DMSO-d_6) Spectra of **5ab**



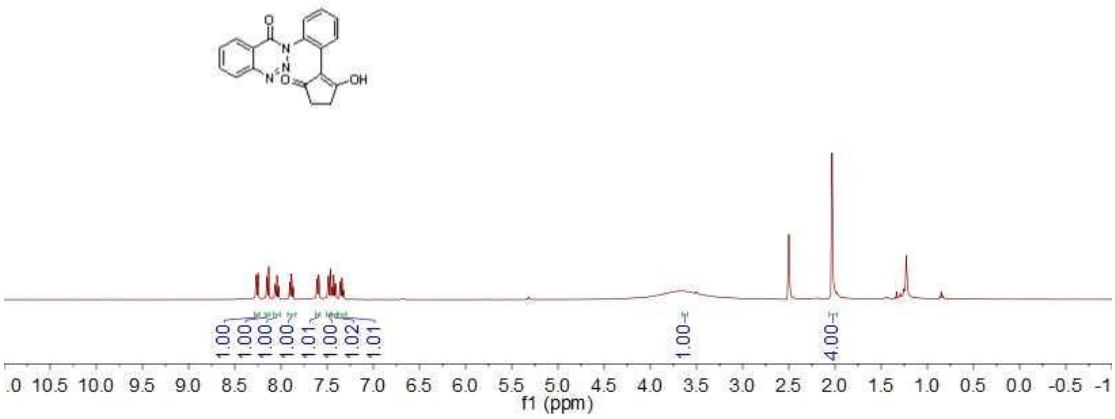
^{1}H NMR (400 MHz, $CDCl_3$) Spectra of **5ac**



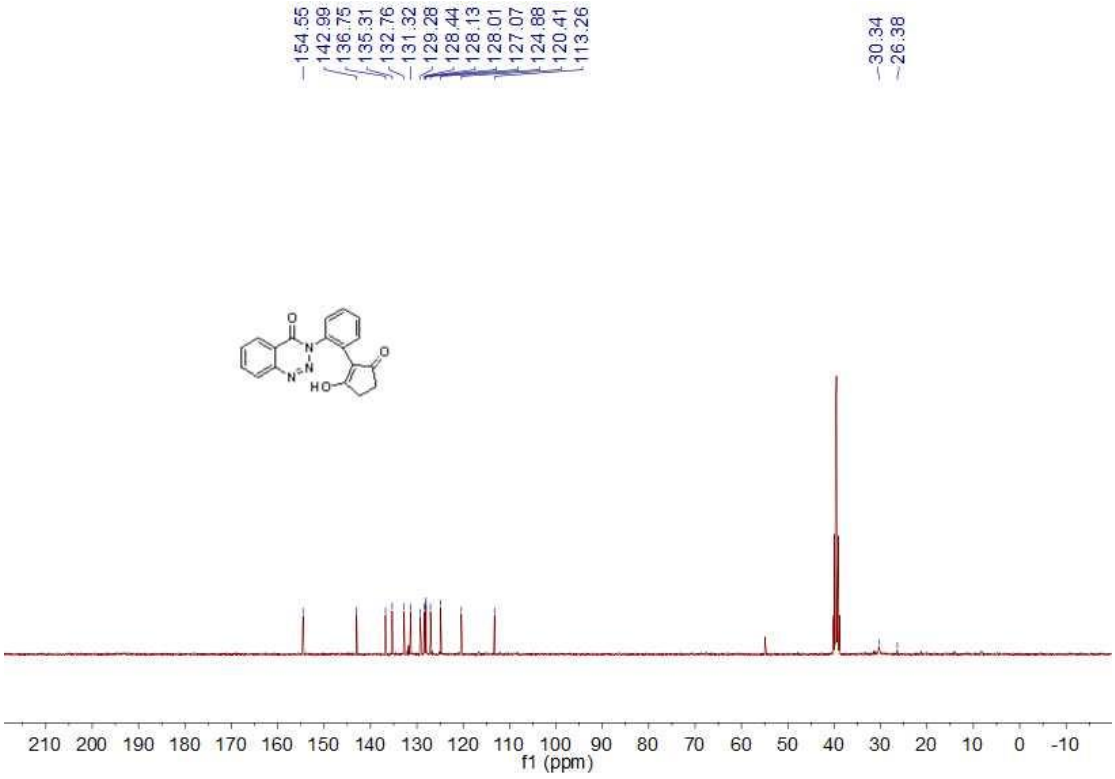
^{13}C NMR (101 MHz, $CDCl_3$) Spectra of **5ac**



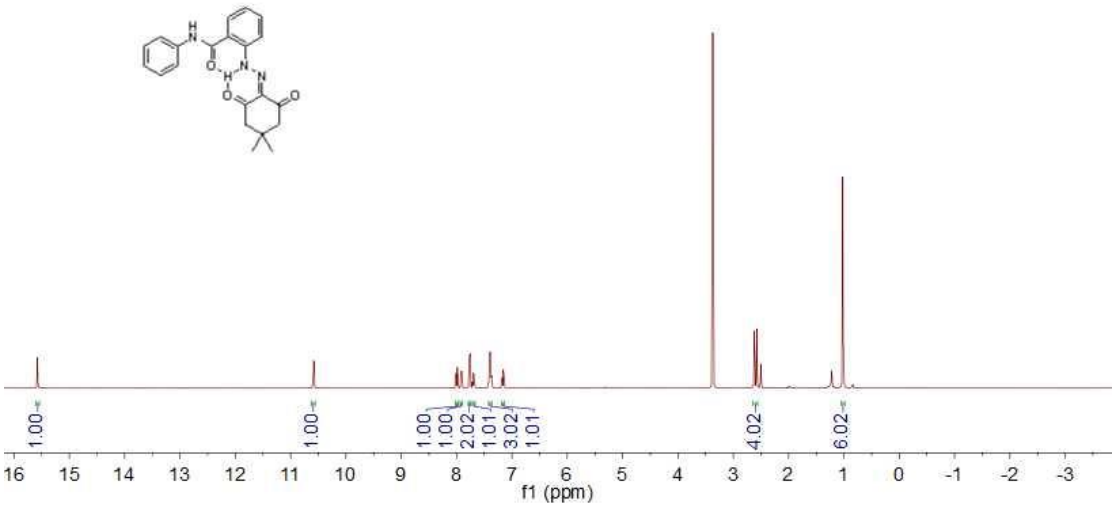
^{1}H NMR (400 MHz, DMSO-d_6) Spectra of **5ad**



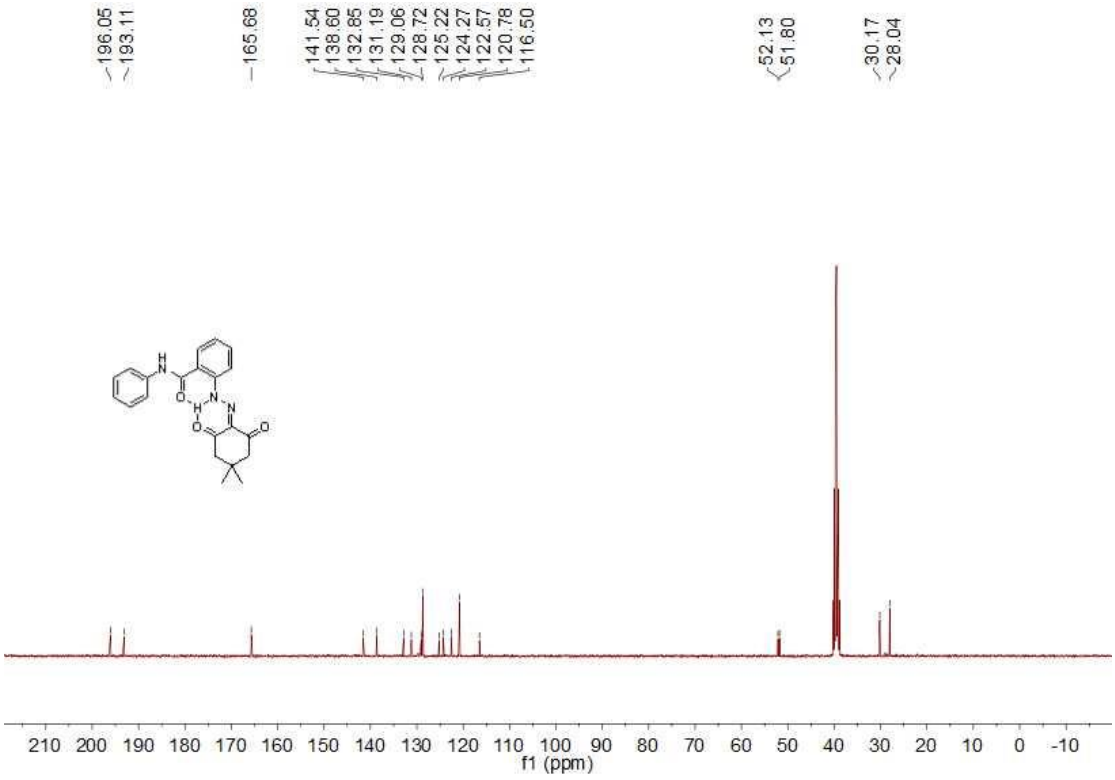
^{13}C NMR (101 MHz, DMSO-d_6) Spectra of **5ad**



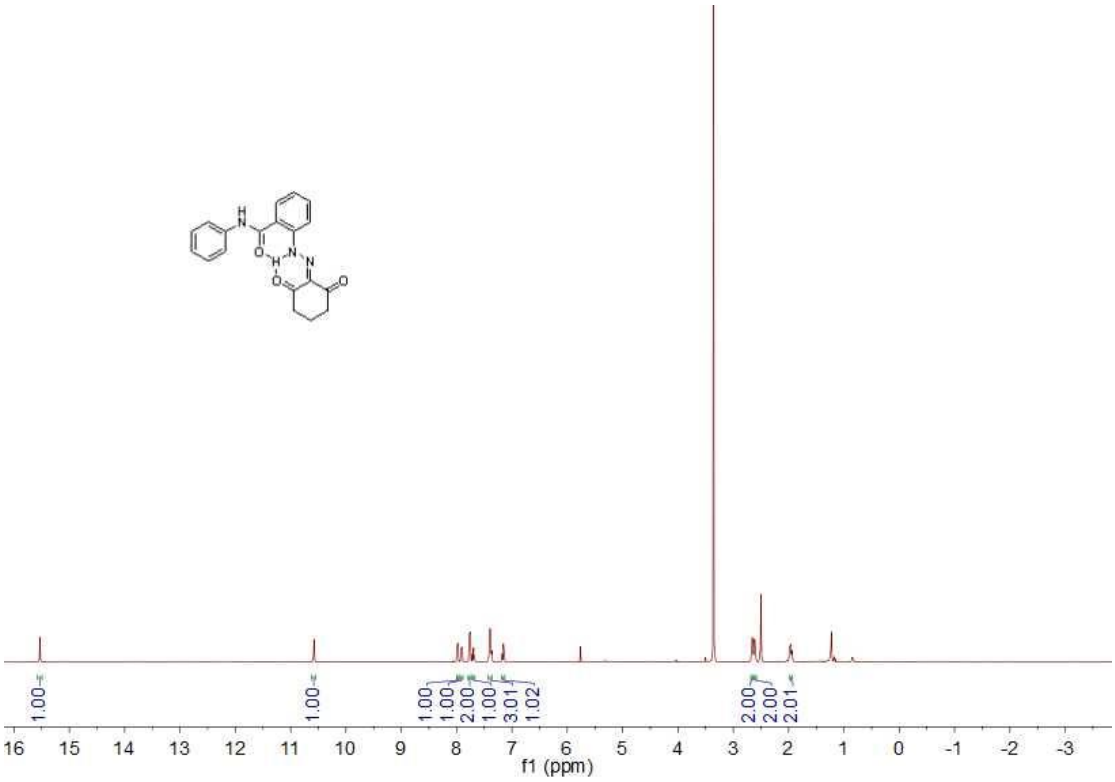
^{1}H NMR (400 MHz, DMSO-d_6) Spectra of **6aa**



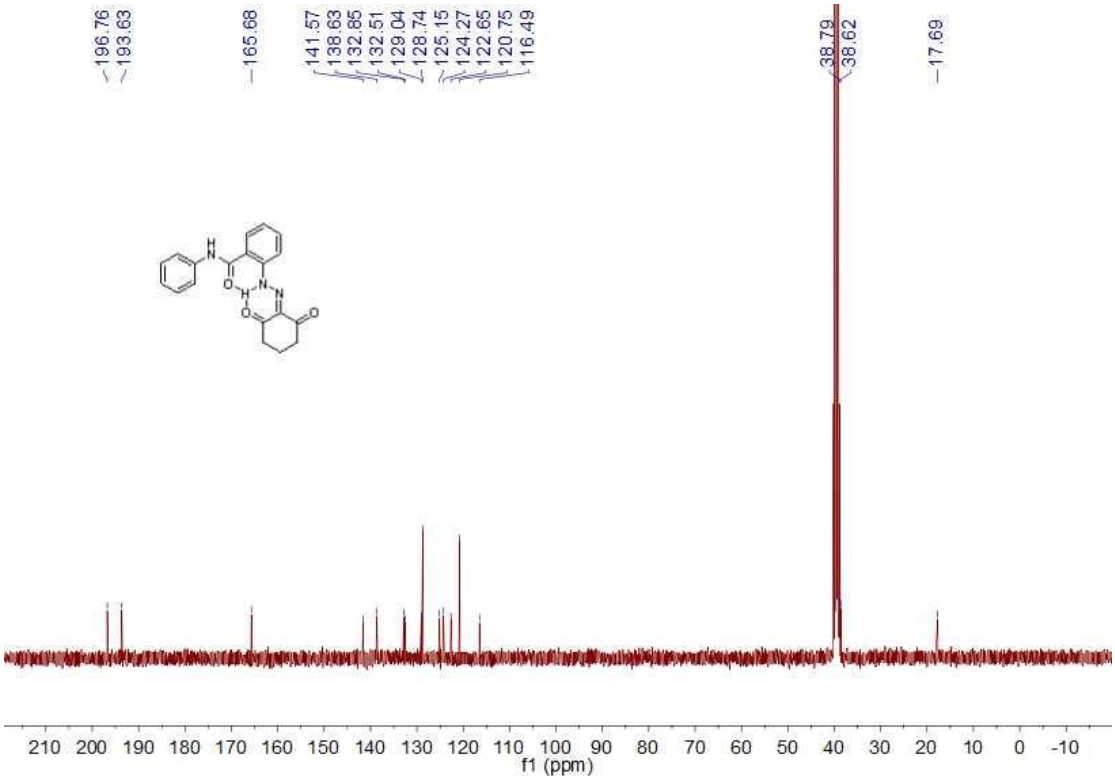
^{13}C NMR (101 MHz, DMSO-d_6) Spectra of **6aa**



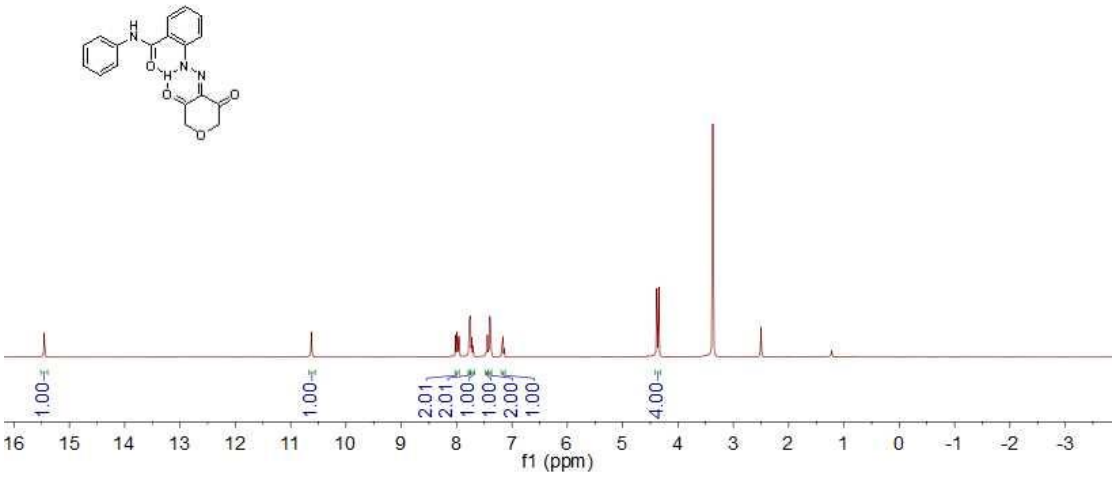
^{1}H NMR (400 MHz, DMSO-d_6) Spectra of **6ab**



^{13}C NMR (101 MHz, DMSO-d_6) Spectra of **6ab**



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



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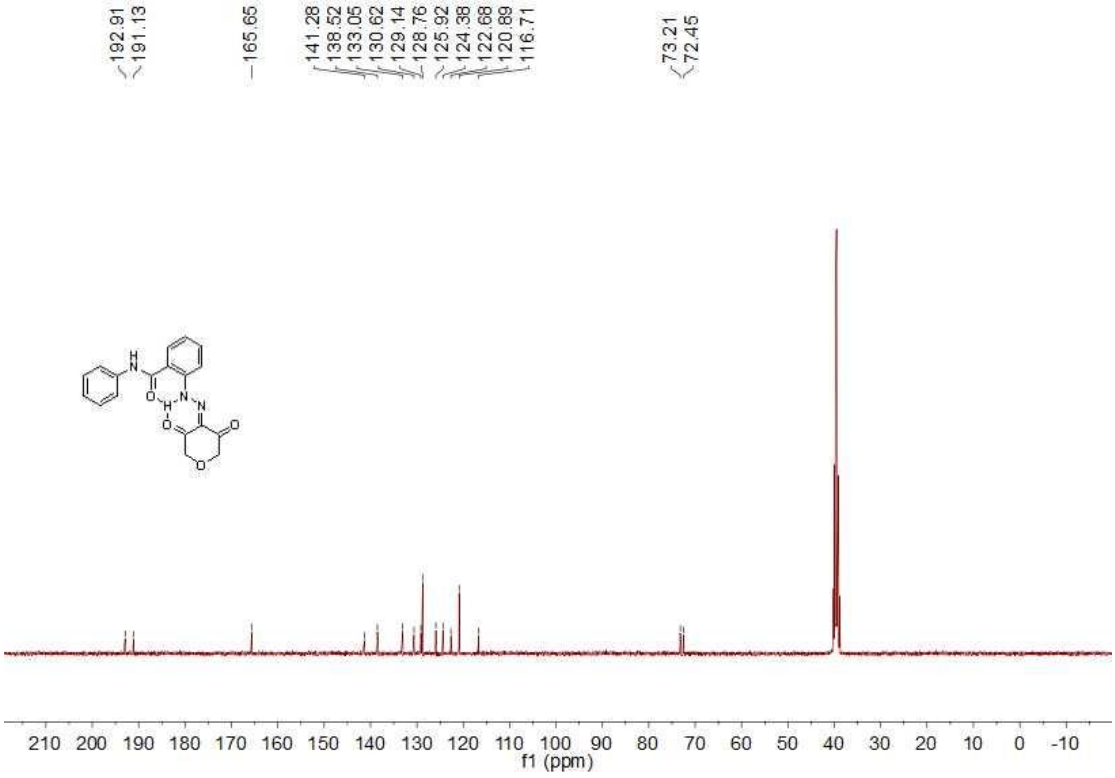
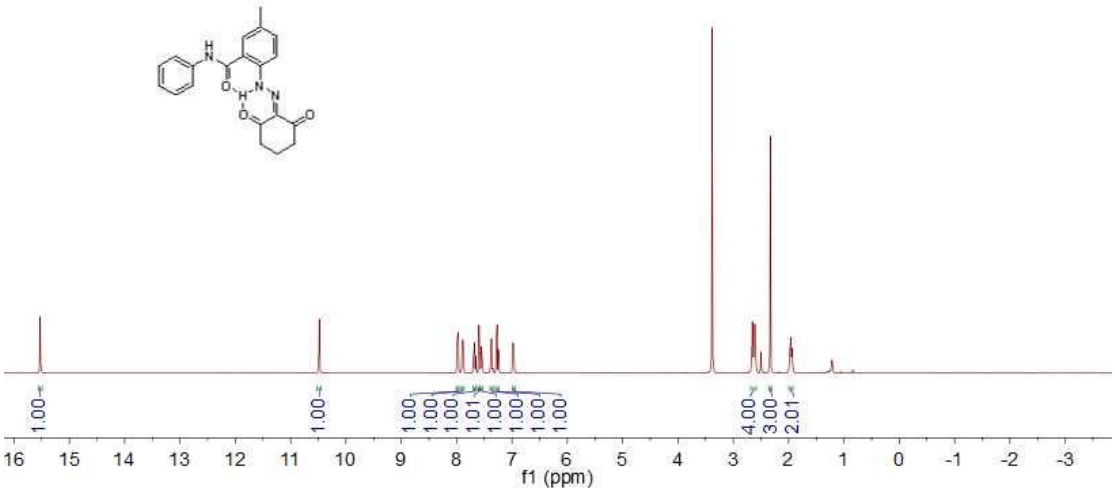
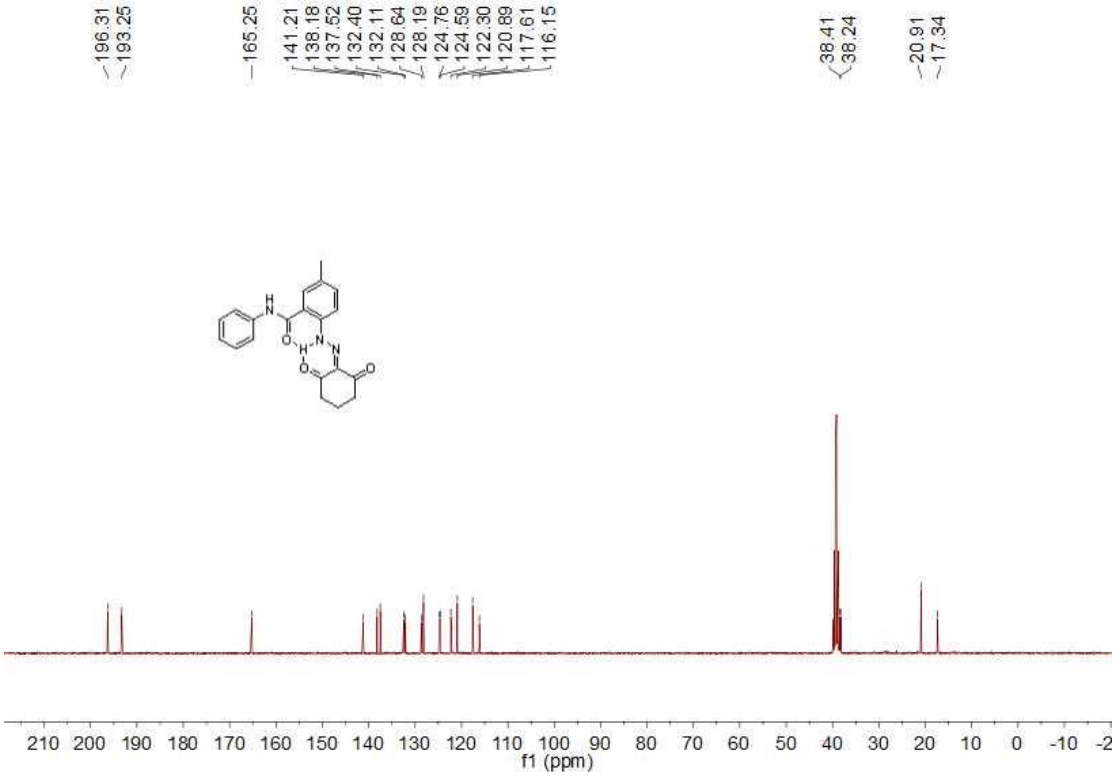


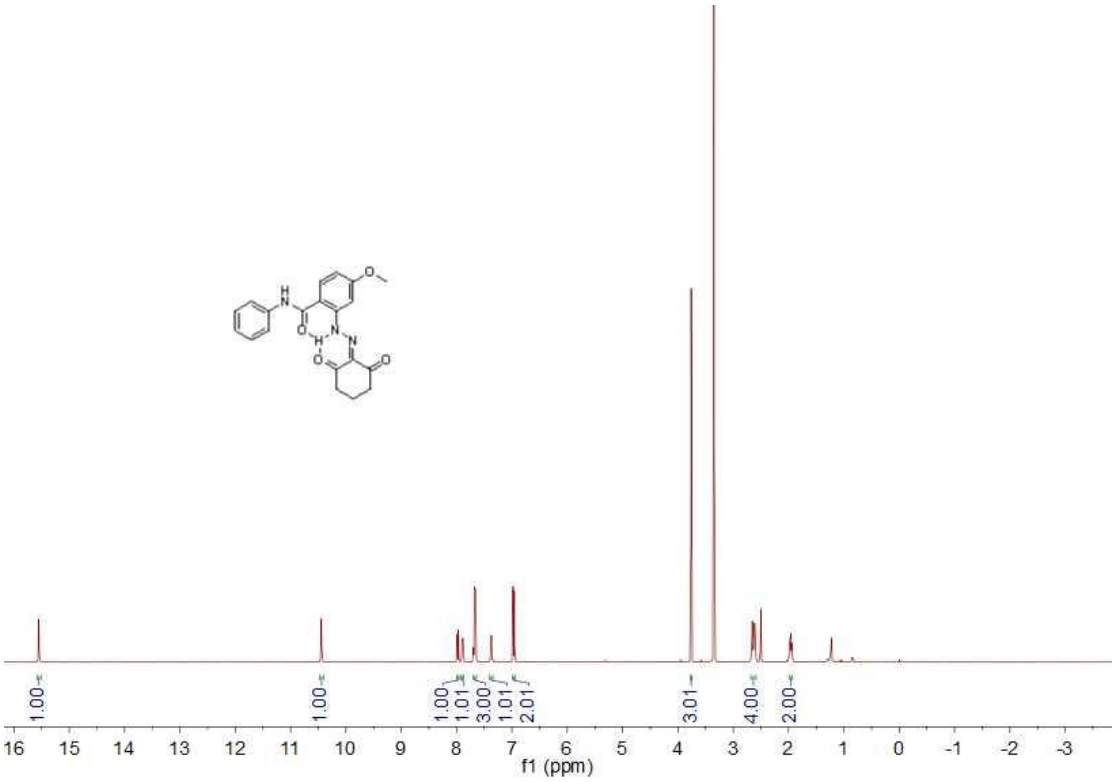
^{1}H NMR (400 MHz, DMSO-d_6) Spectra of **6bb**



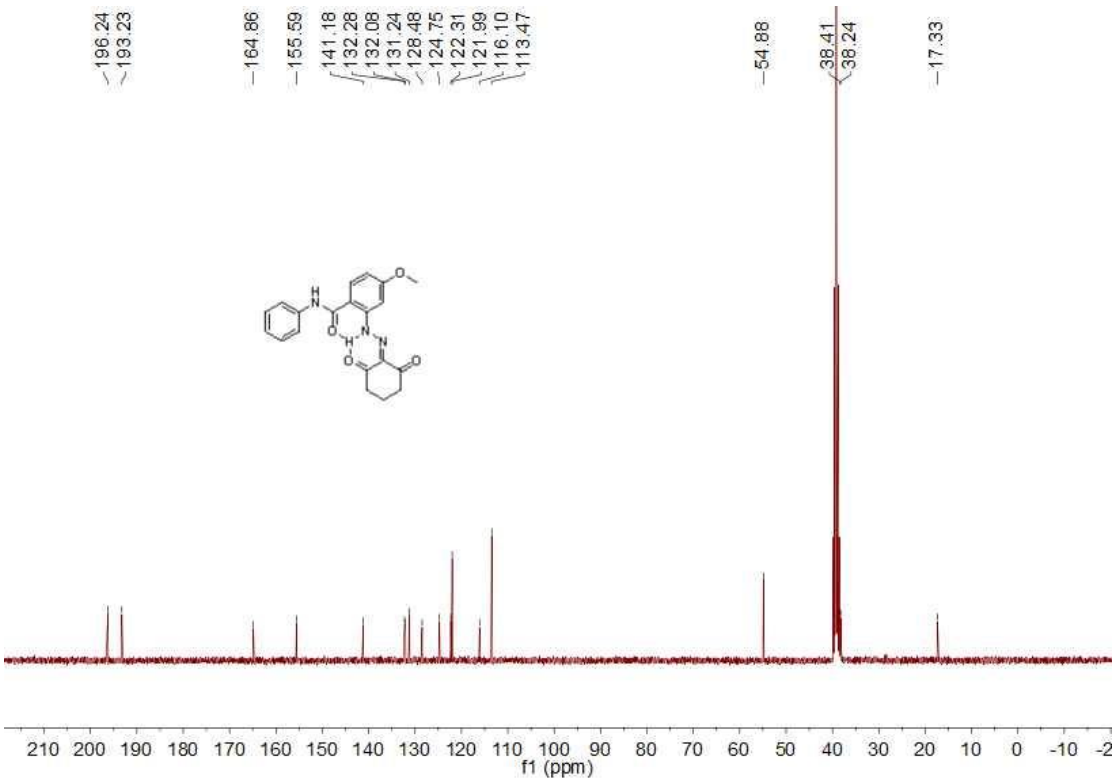
^{13}C NMR (101 MHz, DMSO-d_6) Spectra of **6bb**



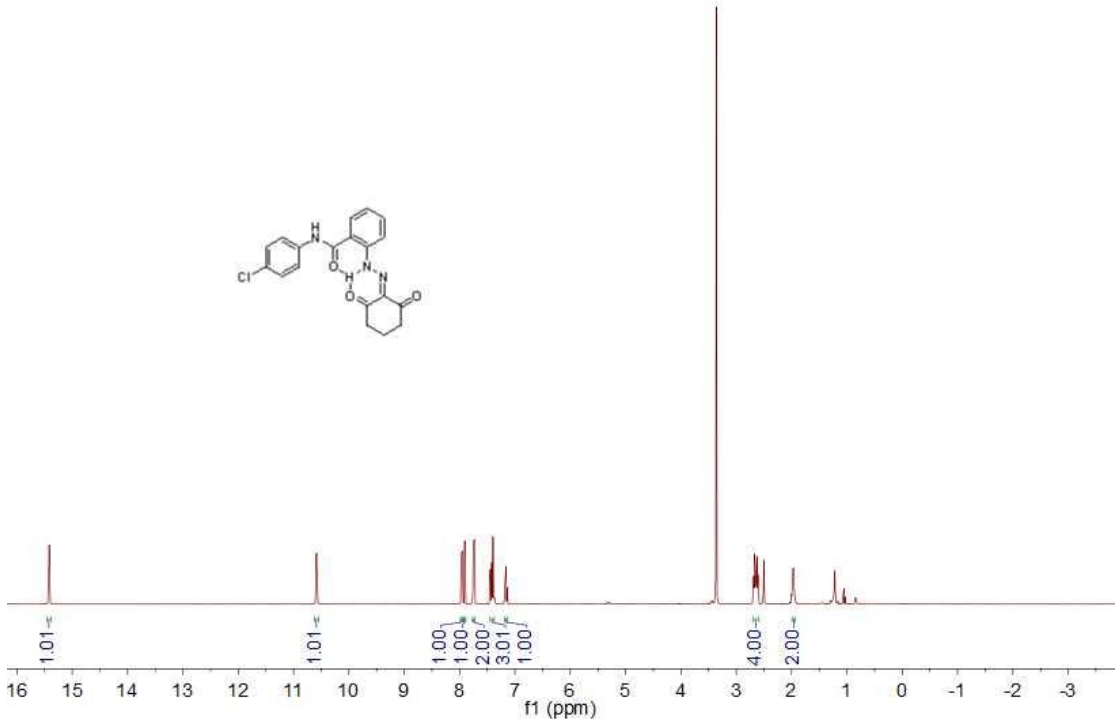
^{1}H NMR (400 MHz, DMSO-d_6) Spectra of **6cb**



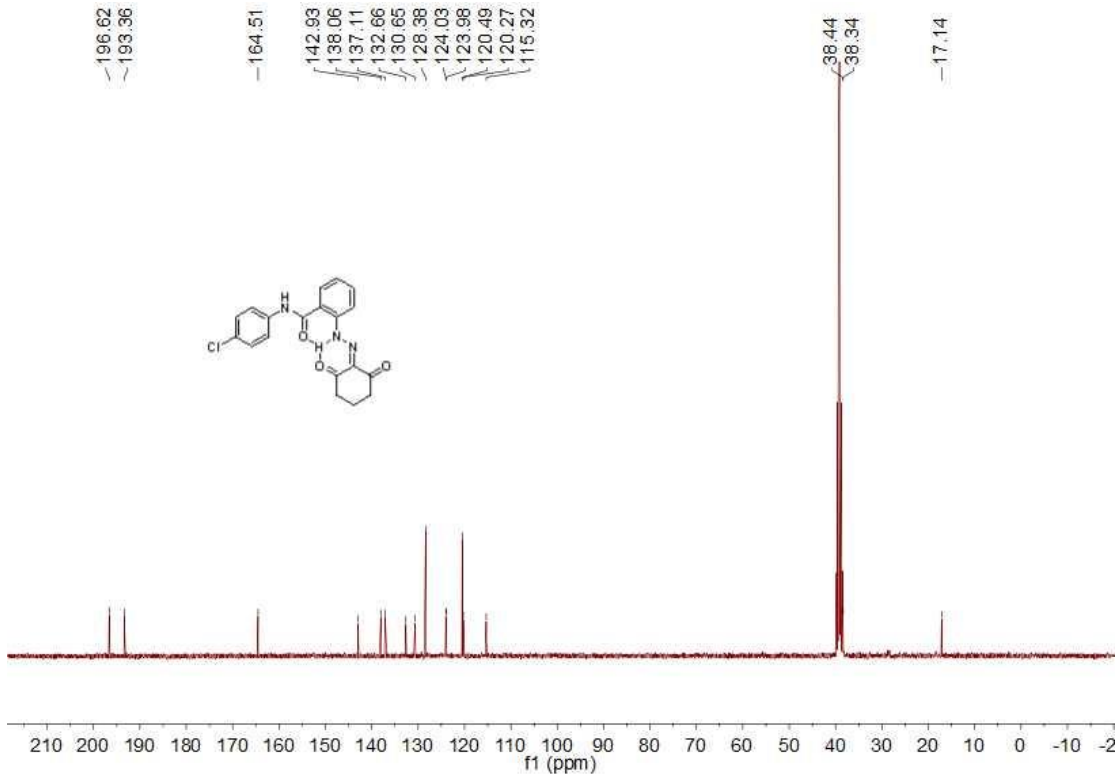
^{13}C NMR (101 MHz, DMSO-d_6) Spectra of **6cb**



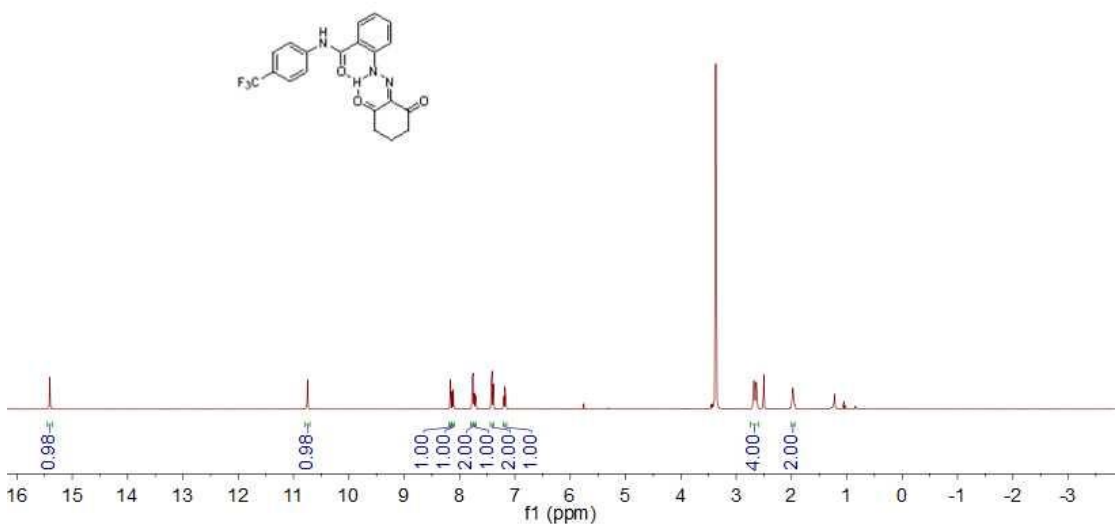
^{1}H NMR (400 MHz, DMSO-d_6) Spectra of **6db**



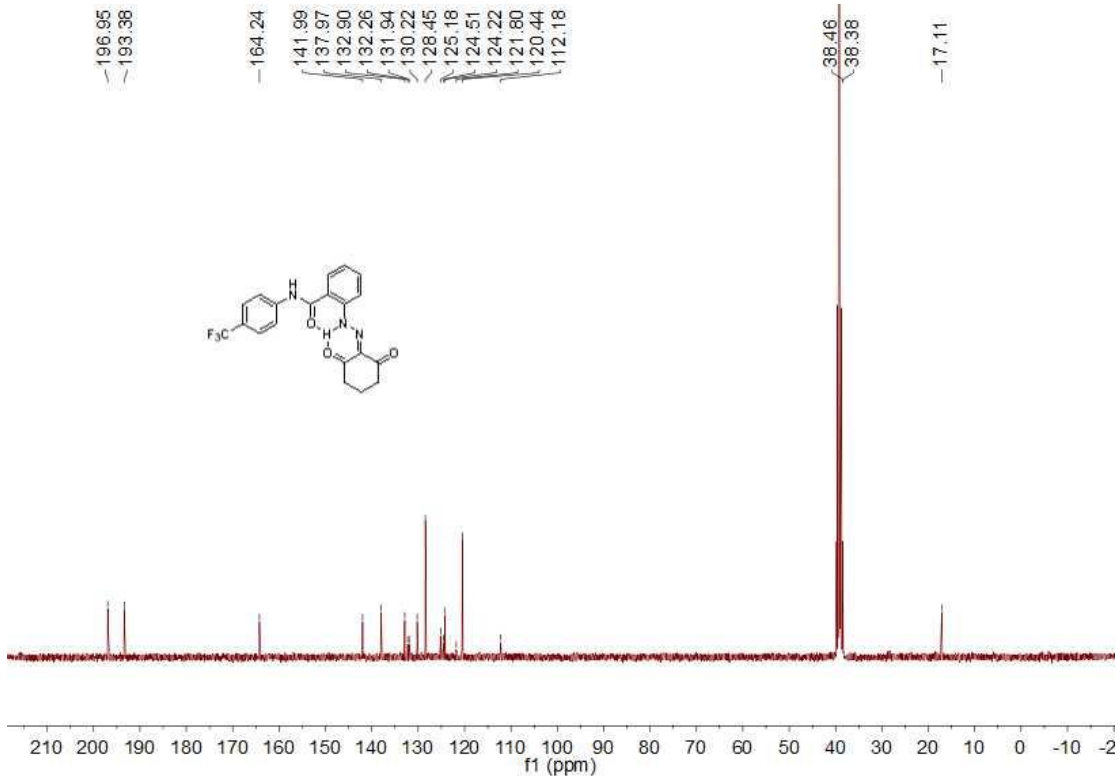
^{13}C NMR (101 MHz, DMSO-d_6) Spectra of **6db**



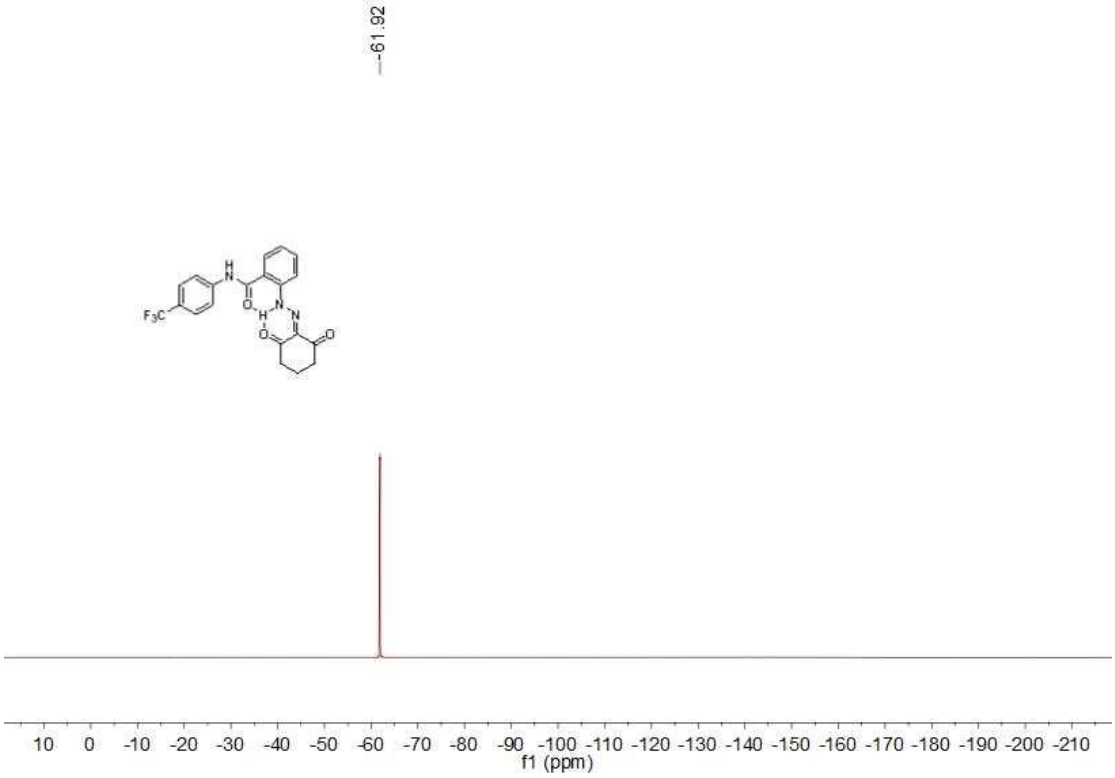
^{1}H NMR (400 MHz, DMSO-d_6) Spectra of **6eb**



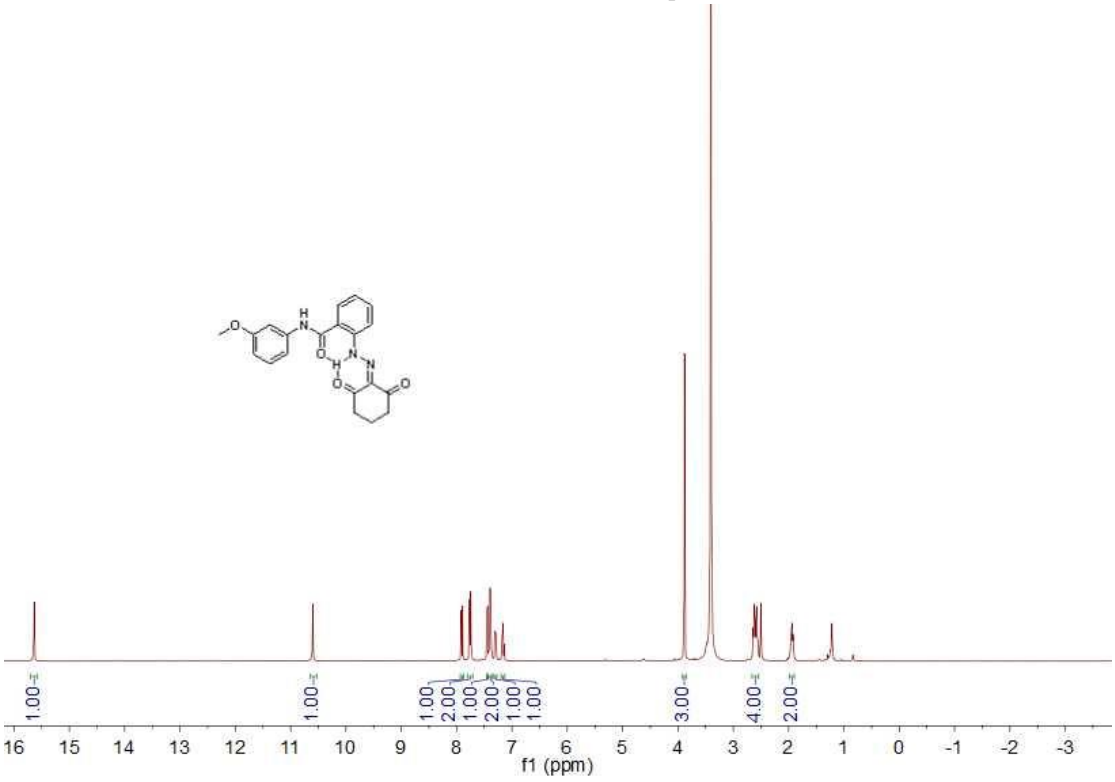
^{13}C NMR (101 MHz, DMSO-d_6) Spectra of **6eb**



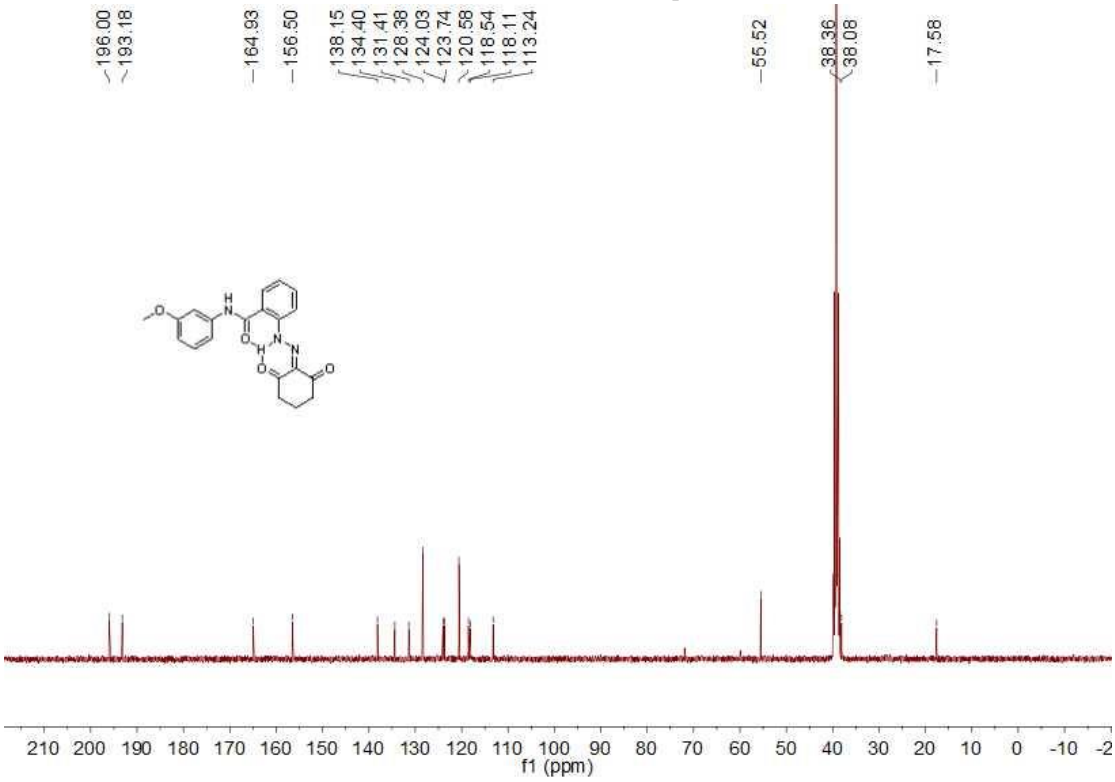
^{19}F NMR (376 MHz, DMSO-d_6) Spectra of **6eb**



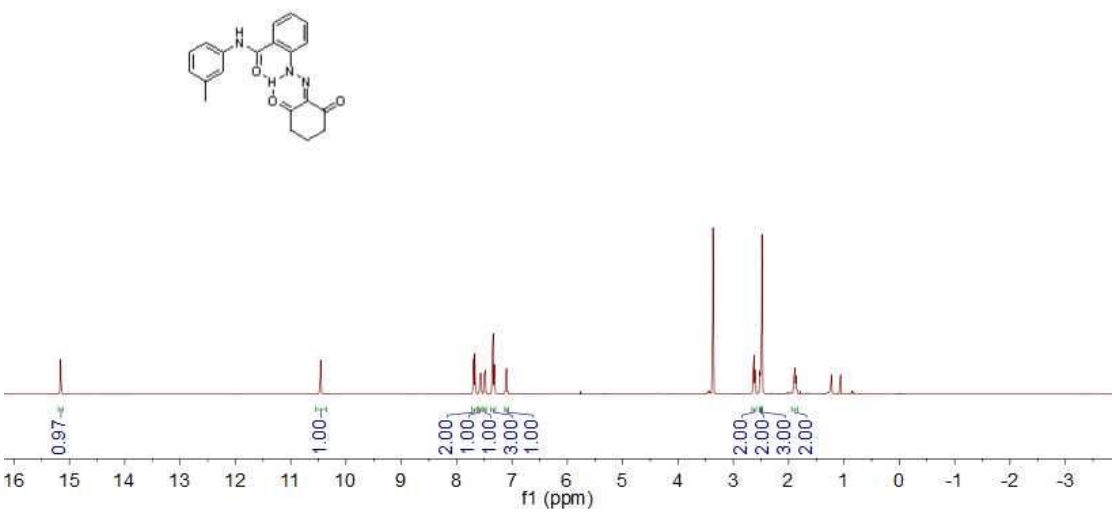
^{1}H NMR (400 MHz, DMSO-d_6) Spectra of **6fb**



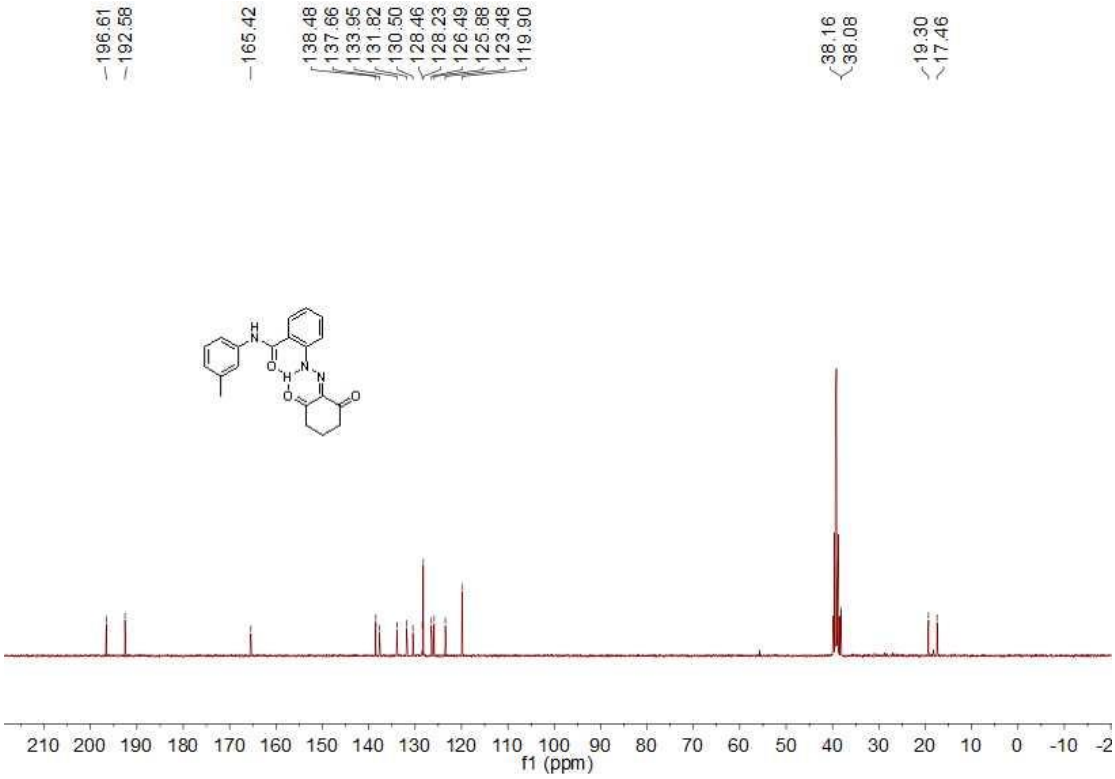
^{13}C NMR (101 MHz, DMSO-d_6) Spectra of **6fb**



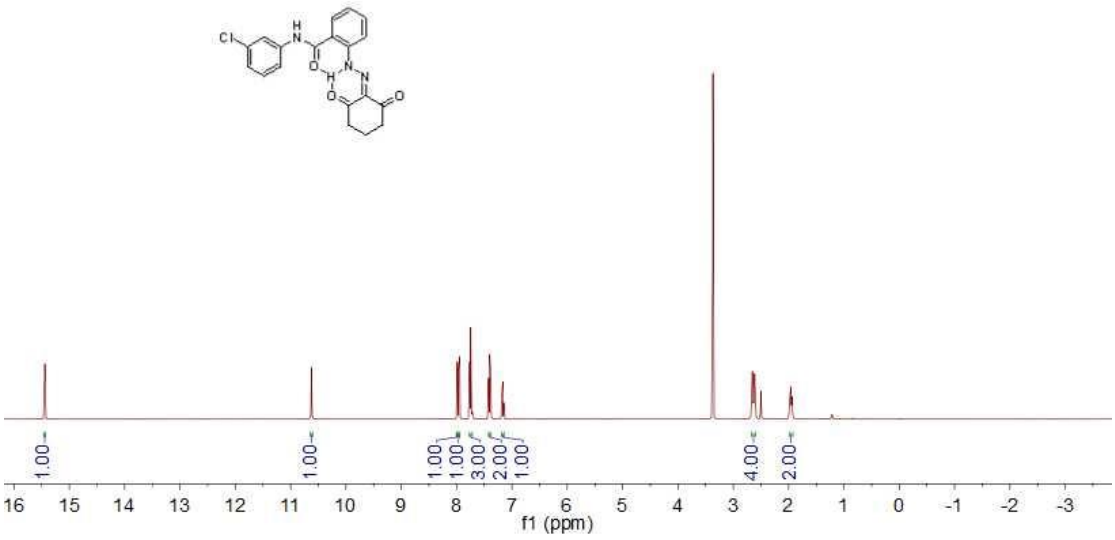
^{1}H NMR (400 MHz, DMSO-d_6) Spectra of **6gb**



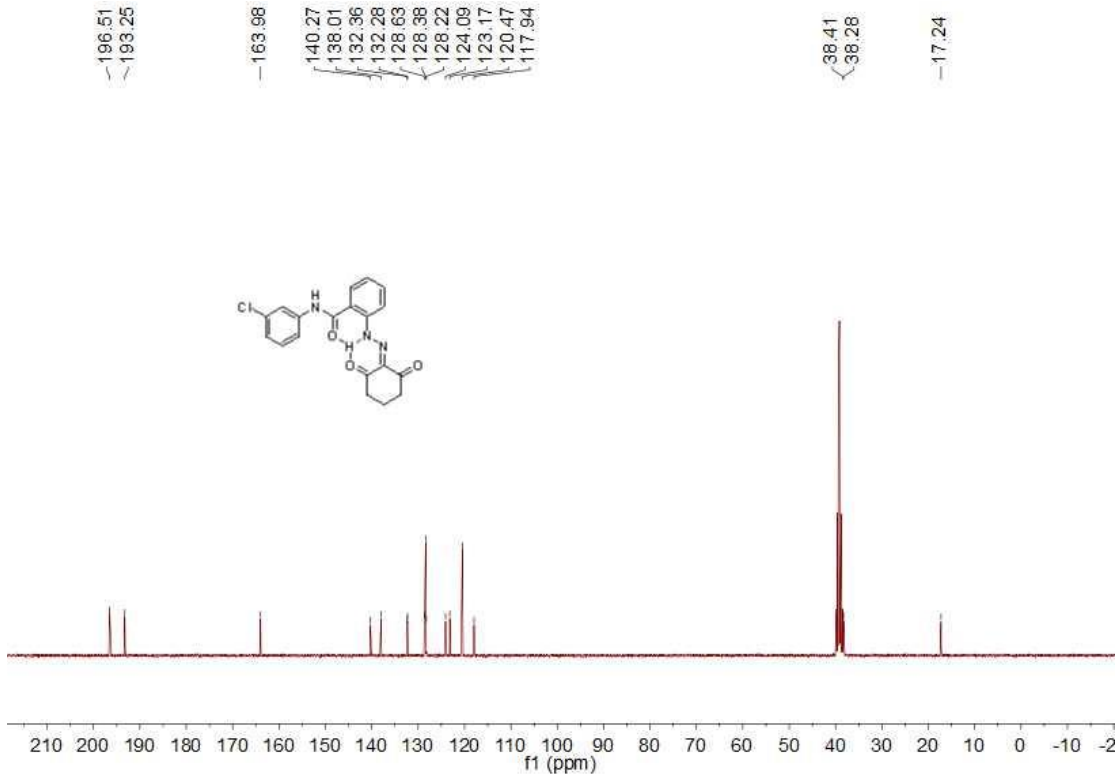
^{13}C NMR (101 MHz, DMSO-d_6) Spectra of **6gb**



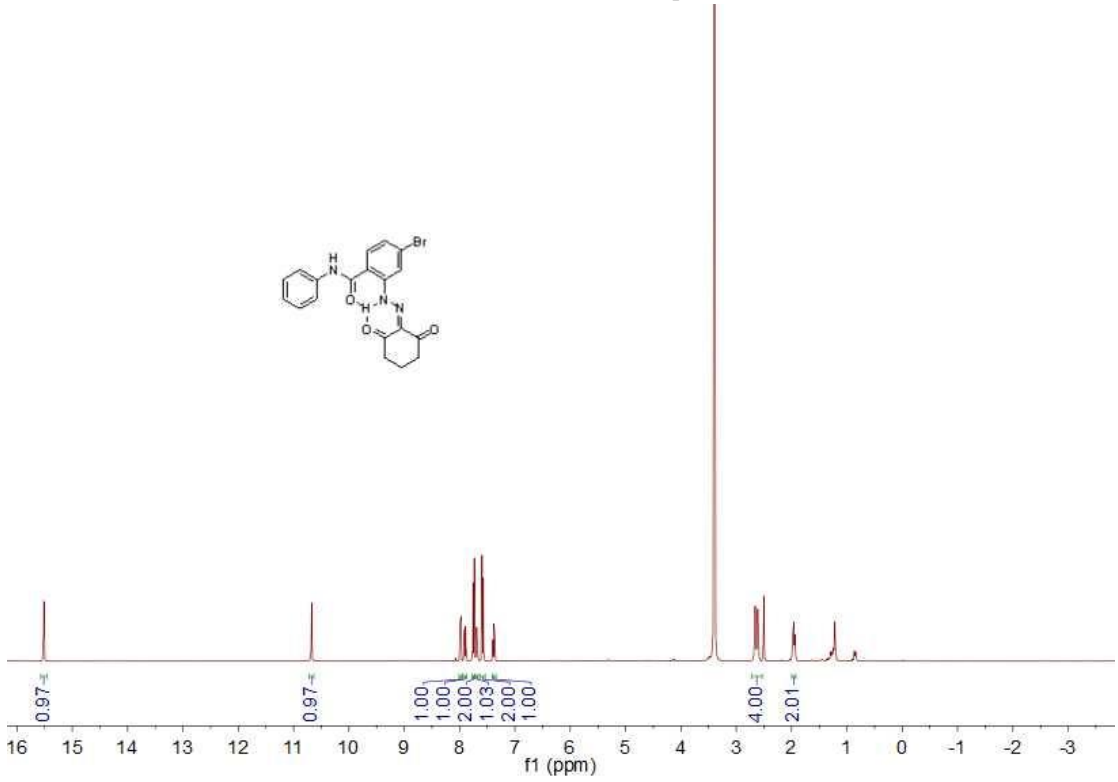
^{1}H NMR (400 MHz, DMSO-d_6) Spectra of **6hb**



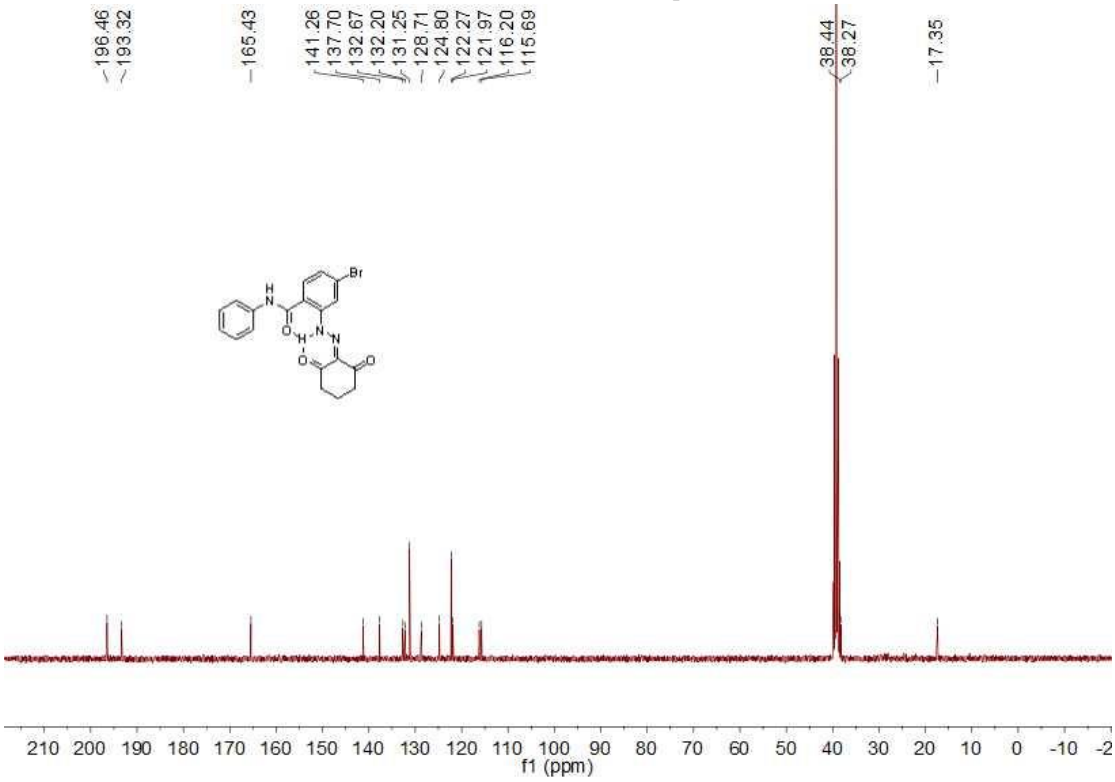
^{13}C NMR (101 MHz, DMSO-d_6) Spectra of **6hb**



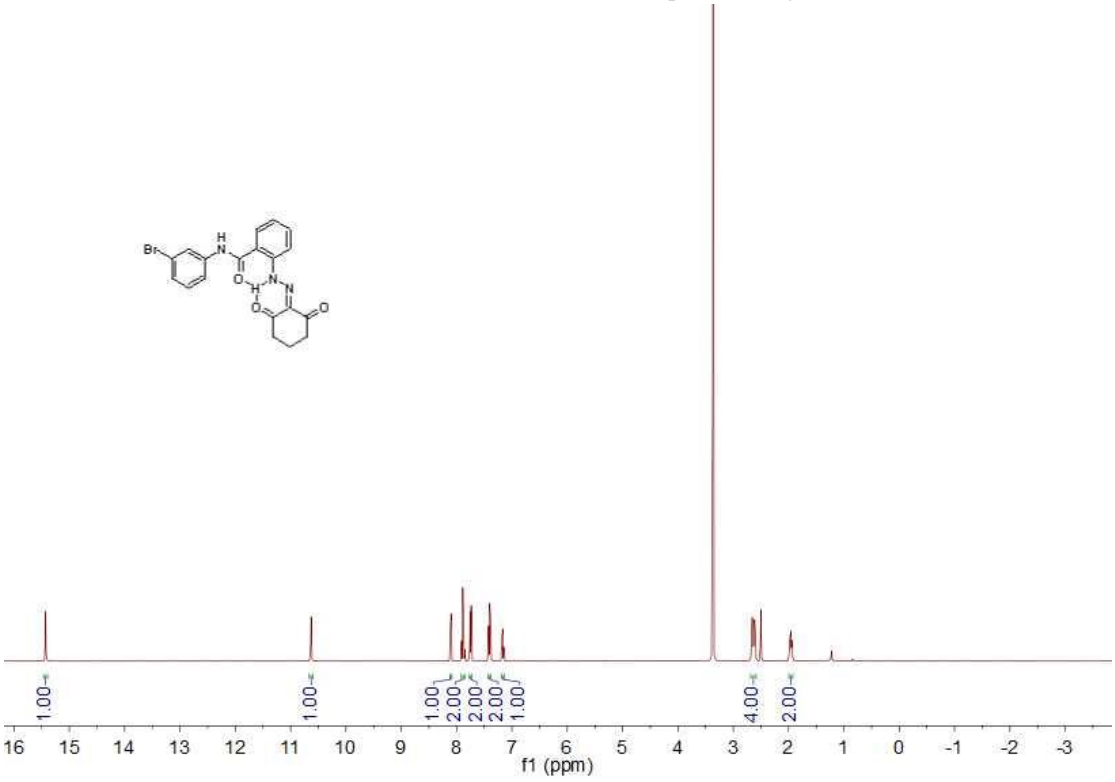
^{1}H NMR (400 MHz, DMSO-d_6) Spectra of **6ib**



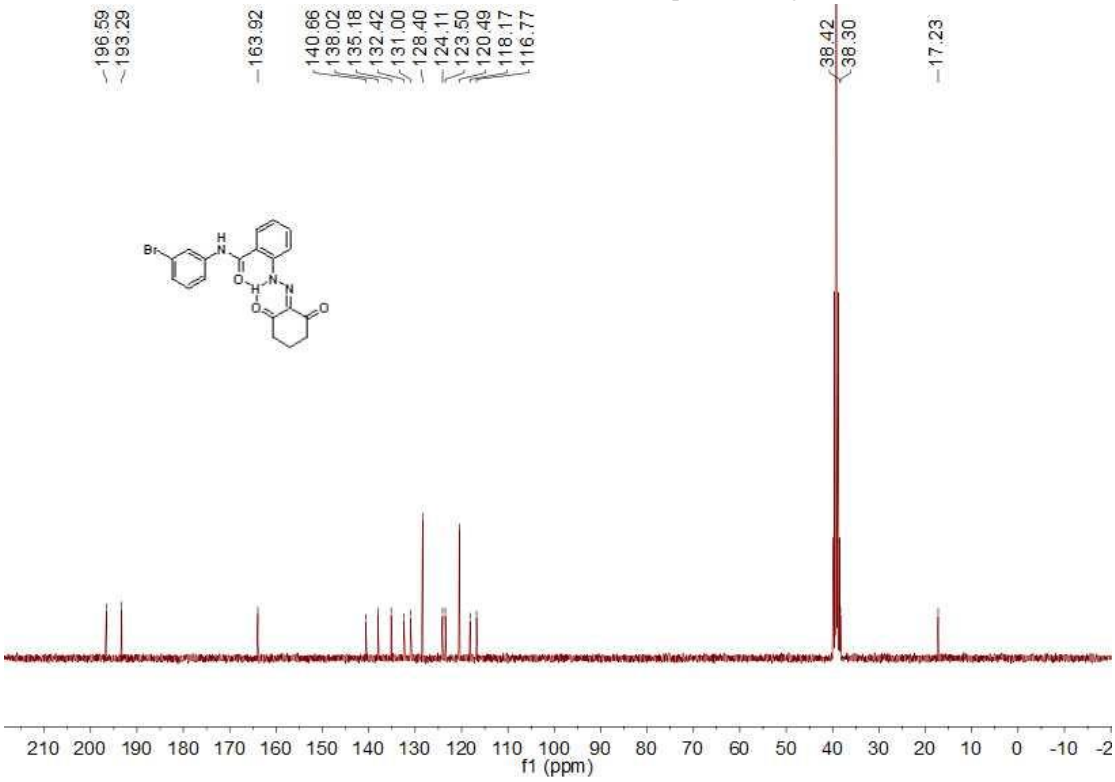
^{13}C NMR (101 MHz, DMSO-d_6) Spectra of **6ib**



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



^{13}C NMR (101 MHz, DMSO-d_6) Spectra of **6jb**



9. Reference

[1] Wang, H.; Yu, S. *Org. Lett.* **2015**, *17*, 4272-4275.

[2] S.-S. Zhang, H. Xie, B. Shu, T. Che, X.-T. Wang, D.-M. Peng, F. Yang, L.-Y. Zhang. *Chem. Commun*., **2020**, *56*, 423-426.

[3] F. Wu, L. Xiao, H. Xie, et al. *Org. Biomol. Chem.*, **2022**, *20*, 5055-5059.