Supporting Information

Chameleon-Like Behavior of the Directing Group in the Rh(III)-Catalyzed Regioselective C−H Amidation of Indole: An Experimental and Computational Study

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1. General Information

Catalytic reactions were carried out in Schlenk tubes under a nitrogen atmosphere using pre-dried glassware. *N*-methoxy-1H-indole-1-carboxamides (**1)** and 1,4,2-dioxazol-5-ones (**2)** were synthesized according to previously described procedures[1,2]. Other chemicals were obtained from commercial sources and were used without further purification. Column chromatography purifications were performed using 200–300 mesh silica gel. NMR spectra were mostly recorded for ^{1}H NMR at 500 MHz and for ^{13}C NMR at 125 MHz. DMSO-d_6 and $CDCl_3$ were used as solvent. Chemical shifts were referenced relative to residual solvent signal (DMSO-d_6, ^{1}H NMR: δ 2.50 ppm, ^{13}C NMR: δ 39.52 ppm; $CDCl_3$: ^{1}H NMR: δ 7.26 ppm, ^{13}C NMR: δ 77.16 ppm). The following abbreviations are used to describe peak patterns where appropriate: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Coupling constants (*J*) are reported in Hertz (Hz). HRMS were performed on Agilent Technologies 6224 TOF LC/MS apparatus (ESI).

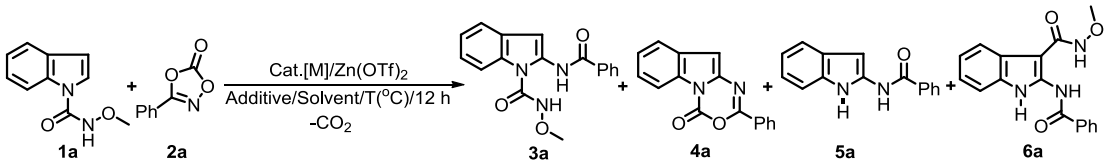
2. Experimental Section

2.1 Substrates preparation

The *N*-methoxy amide substituted indoles[1] and 3-substituted-1,4,2-dioxazol-5-ones[2] were prepared according to the methods in the references.

2.2 Preliminary optimization of reaction conditions

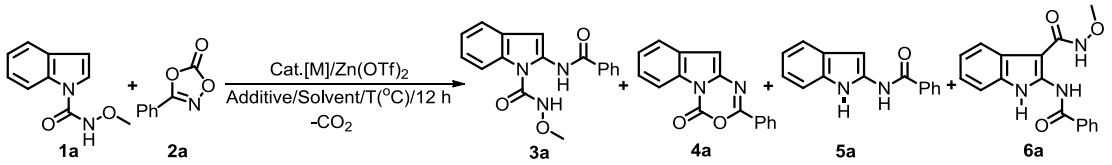
Table S1. Reaction **condition screening of 3a**



entry	cat. [M]	solvent	ligand	additive	T (℃)	yield (%)[a]			
						3a	**4a**	**5a**	**6a**
1	$[Cp^*RhCl_2]_2$	DCE	$Zn(OTf)_2$	CsOAc	r.t.	52	9	17	7
2	$[Cp^*RhCl_2]_2$	untreated THF	$Zn(OTf)_2$	CsOAc	r.t.	68	<5	21	<5
3	$[Cp^*RhCl_2]_2$	MeOH	$Zn(OTf)_2$	CsOAc	r.t.	32	<5	12	<5
4	$[Cp^*RhCl_2]_2$	TFE	$Zn(OTf)_2$	CsOAc	r.t.	23	<5	<5	<5
5	$[Cp^*RhCl_2]_2$	CH_3CN	$Zn(OTf)_2$	CsOAc	r.t.	29	<5	13	<5
6	$[Cp^*RhCl_2]_2$	DCM	$Zn(OTf)_2$	CsOAc	r.t.	55	8	15	<5
7	$[Cp^*RhCl_2]_2$	untreated THF	$Zn(OTf)_2$	KOAc	r.t.	76	<5	14	<5
8	**$[Cp^*RhCl_2]_2$**	**untreated THF**	**$Zn(OTf)_2$**	**NaOAc**	**r.t.**	**88**	**<5**	**<5**	**<5**
9	$[Cp^*RhCl_2]_2$	untreated THF	$Zn(OTf)_2$	$Cu(OAc)_2$	r.t.	<5	<5	<5	<5
10	$[Cp^*RhCl_2]_2$	THF/H_2O(10:1)	$Zn(OTf)_2$	NaOAc	r.t.	85	<5	<5	<5
11	$[Cp^*RhCl_2]_2$	untreated THF	$Zn(OTf)_2$	/	r.t.	<5	<5	<5	<5
12	$[Cp^*RhCl_2]_2$	untreated THF	$Zn(NTf_2)$	NaOAc	r.t.	85	<5	<5	<5
13	$[Cp^*RhCl_2]_2$	untreated THF	$AgNTf_2$	NaOAc	r.t.	74	<5	<5	<5
14	$[Cp^*RhCl_2]_2$	untreated THF	$AgSbF_6$	NaOAc	r.t.	83	<5	<5	<5
15	$[Cp^*RhCl_2]_2$	untreated THF	$AgBF_4$	NaOAc	r.t.	86	<5	<5	<5
16	$[Cp^*RhCl_2]_2$	untreated THF	Ag_2O	NaOAc	r.t.	72	<5	<5	<5
17	$[Cp^*RuCl_2]_2$	DCE	$Zn(OTf)_2$	CsOAc	r.t.	No reaction			
18	$[Cp^*IrCl_2]_2$	DCE	$Zn(OTf)_2$	CsOAc	r.t.	No reaction			
19	$Cp^*Co(CO)I_2$	DCE	$Zn(OTf)_2$	CsOAc	r.t.	No reaction			

The reaction was conducted with **1a** (0.2 mmol), **2a** (0.24 mmol), $[Cp^*RhCl_2]_2$ (5 mol%), ligand (30 mol%) and additive (0.2 mmol) in solvent (2 mL).

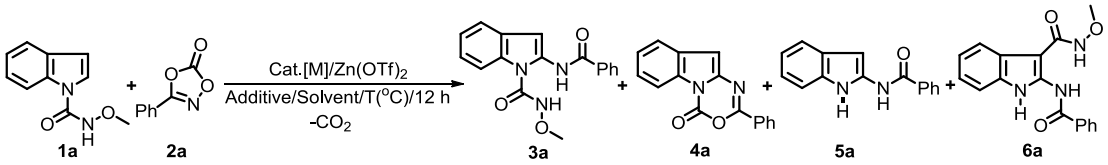
Table S2. Reaction condition screening of 4a



entry	cat. [M]	solvent	ligand	additive	T (℃)	yield (%)[a]			
						3a	**4a**	**5a**	**6a**
1	$[Cp^*RhCl_2]_2$	untreated THF	$Zn(OTf)_2$	CsOAc	r.t.	68	<5	21	<5
2	$[Cp^*RhCl_2]_2$	untreated THF	$Zn(OTf)_2$	CsOAc	60	<5	10	75	<5
3	$[Cp^*RhCl_2]_2$	untreated THF	$Zn(OTf)_2$	CsOAc	90	<5	8	73	<5
4	$[Cp^*RhCl_2]_2$	anhydrous THF	$Zn(OTf)_2$	CsOAc	60	<5	24	49	<5
5	$[Cp^*RhCl_2]_2$	anhydrous THF	$Zn(OTf)_2$	NaOAc	60	<5	34	44	<5
6	$[Cp^*RhCl_2]_2$	anhydrous THF	$Zn(OTf)_2$	NaOAc DDQ	60	<5	<5	<5	<5
7	$[Cp^*RhCl_2]_2$	anhydrous THF	$Zn(OTf)_2$	NaOAc PIFA	60	<5	<5	<5	<5
8	$[Cp^*RhCl_2]_2$	anhydrous THF	$Zn(OTf)_2$	NaOAc CAN	60	<5	<5	<5	<5
9	$[Cp^*RhCl_2]_2$	anhydrous THF	$Zn(OTf)_2$	NaOAc $K_2S_2O_8$	60	<5	75	<5	<5
10	$[Cp^*RhCl_2]_2$	anhydrous THF	/	NaOAc $K_2S_2O_8$	60	<5	78	<5	<5
11	$[Cp^*RhCl_2]_2$	anhydrous THF	/	NaOAc $2KHSO_5 \cdot KHSO_4 \cdot K_2SO_4$	60	<5	79	<5	<5
12	**$[Cp^*RhCl_2]_2$**	**anhydrous THF**	**/**	**NaOAc $KHSO_4$**	**60**	**<5**	**81**	**<5**	**<5**
13	$[Cp^*RhCl_2]_2$	anhydrous THF	/	$KHSO_4$	60	<5	<5	<5	<5

The reaction was conducted with **1a** (0.2 mmol), **2a** (0.24 mmol), $[Cp^*RhCl_2]_2$ (5 mol%), ligand (30 mol%) and additive (0.2 mmol) in solvent (2 mL).

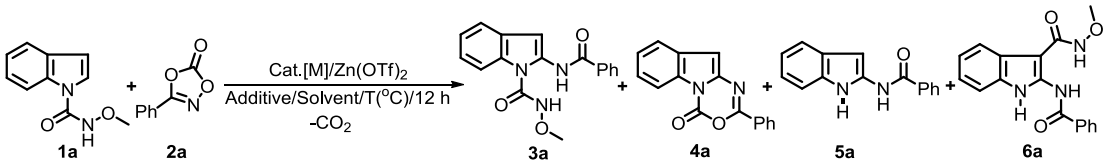
Table S3. Reaction condition screening of 5a



entry	cat. [M]	solvent	ligand	additive	T (℃)	yield (%)[a]			
						3a	**4a**	**5a**	**6a**
1	$[Cp^*RhCl_2]_2$	anhydrous THF	$Zn(OTf)_2$	CsOAc	60	<5	24	49	<5
2	$[Cp^*RhCl_2]_2$	untreated THF	$Zn(OTf)_2$	CsOAc	60	<5	10	75	<5
3	**$[Cp^*RhCl_2]_2$**	**THF/H_2O (10:1)**	$Zn(OTf)_2$	**CsOAc**	**60**	**<5**	**<5**	**85**	**<5**
4	$[Cp^*RhCl_2]_2$	THF/H_2O (5:1)	$Zn(OTf)_2$	CsOAc	60	<5	<5	82	<5
5	$[Cp^*RhCl_2]_2$	THF/H_2O (2:1)	$Zn(OTf)_2$	CsOAc	60	<5	<5	73	<5
6	$[Cp^*RhCl_2]_2$	THF/H_2O (1:1)	$Zn(OTf)_2$	CsOAc	60	<5	<5	61	<5
7	$[Cp^*RhCl_2]_2$	THF/H_2O (10:1)	/	CsOAc	60	<5	<5	78	<5
8	$[Cp^*RhCl_2]_2$	THF/H_2O (10:1)	$Zn(OTf)_2$	/	60	<5	<5	<5	<5

The reaction was conducted with **1a** (0.2 mmol), **2a** (0.24 mmol), $[Cp^*RhCl_2]_2$ (5 mol%), ligand (30 mol%) and additive (0.2 mmol) in solvent (2 mL).

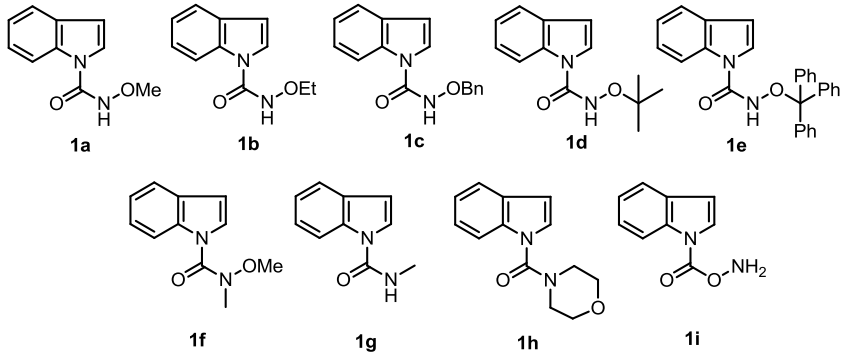
Table S4. Reaction condition screening of 6a



entry	cat. [M]	solvent	ligand	additive	T (℃)	yield (%)[a]			
						3a	**4a**	**5a**	**6a**
1	$[Cp^*RhCl_2]_2$	DCE	$Zn(OTf)_2$	CsOAc	r.t.	52	9	17	7
2	$[Cp^*RhCl_2]_2$	DCE	$Zn(OTf)_2$	CsOAc	60	<5	12	51	24
3	$[Cp^*RhCl_2]_2$	DCE	$Zn(OTf)_2$	CsOAc	95	<5	<5	25	48
4	**$[Cp^*RhCl_2]_2$**	**DCE**	$Zn(OTf)_2$	**CsOAc**	**130**	**<5**	**<5**	**<5**	**62**
5	$[Cp^*RhCl_2]_2$	DCE	/	CsOAc	130	<5	<5	<5	58
6	$[Cp^*RhCl_2]_2$	DCE	$Zn(OTf)_2$	/	130	<5	<5	<5	62

The reaction was conducted with **1a** (0.2 mmol), **2a** (0.24 mmol), $[Cp^*RhCl_2]_2$ (5 mol%), ligand (30 mol%) and additive (0.2 mmol) in solvent (2 mL).

Table S5. Reaction condition screening of directing groups



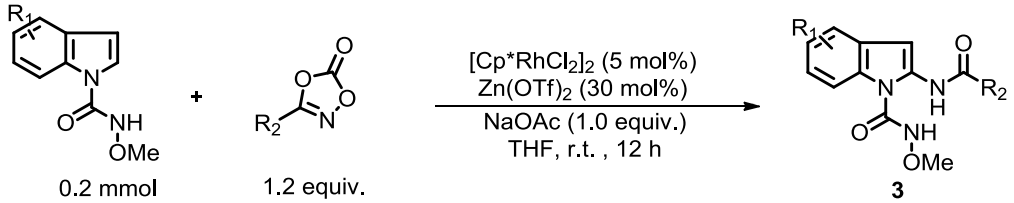
entry	Starting material	yield (%)[a]			
		3[b]	**4**[c]	**5**[d]	**6**[e]
1	**1a**	88	81	85	62
2	**1b**	77	61	76	59
3	**1c**	56	75	65	Not detected
4	**1d**	25	10	7	Not detected
5	**1e**			No reaction	
6	**1f**			No reaction	
7	**1g**			No reaction	
8	**1h**			No reaction	
9	**1i**			No reaction	

[a]isolated yield. [b]The reaction was conducted with **1** (0.2 mmol), **2** (0.24 mmol), $[Cp^*RhCl_2]_2$ (5 mol%), $Zn(OTf)_2$ (30 mol%), NaOAc (0.2 mmol), THF (2 mL), room temperature. [c]The reaction was conducted with **1** (0.2 mmol), **2** (0.24 mmol), $[Cp^*RhCl_2]_2$ (5 mol%), NaOAc (0.2 mmol), $KHSO_4$ (0.2 mmol), THF (2 mL), 60 °C. [d]The reaction was conducted with **1** (0.2 mmol), **2** (0.24 mmol), $[Cp^*RhCl_2]_2$ (5 mol%), $Zn(OTf)_2$ (30 mol%), CsOAc (0.2 mmol), THF (2 mL), H_2O (0.2 mL), 60 °C. [e]The reaction was conducted with **1** (0.2 mmol), **2** (0.24 mmol), $[Cp^*RhCl_2]_2$ (5 mol%), $Zn(OTf)_2$ (30 mol%), CsOAc (0.2 mmol), DCE (2 mL), 130 °C.

2.3 Synthesis and characterization of products 3, 4, 5 and 6

2.3.1 General procedure

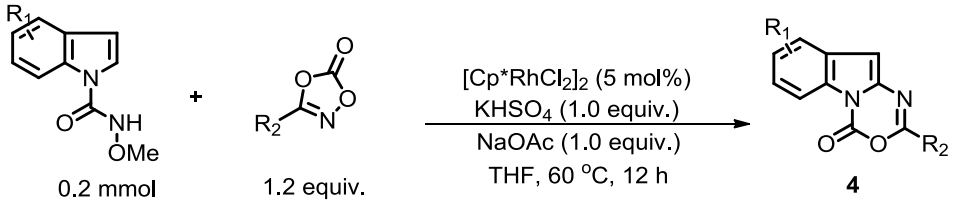
General procedure for product 3 (GP1)



A reaction tube (10 mL) with magnetic stir bar was charged with *N*-methoxy amide substituted

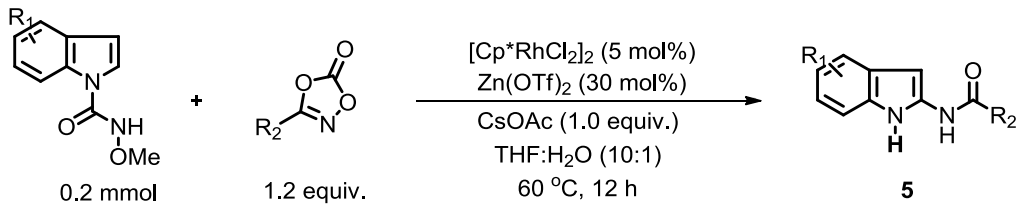
indole **1** (0.20 mmol), 1,4,2-dioxazol-5-one **2** (0.24 mmol), NaOAc (16 mg, 0.20 mmol), $[Cp^*RhCl_2]_2$ (6 mg, 0.010 mmol), $Zn(OTf)_2$ (22 mg, 0.060 mmol) and THF (2.0 mL). The reaction was allowed to stir at room temperature for 12 hours. Upon completion, the reaction mixture was evaporated to remove the solvent and directly loaded onto silica gel for flash column chromatography (PET/EtOAc) to afford the desired product **3**.

General procedure for product 4 (GP2)



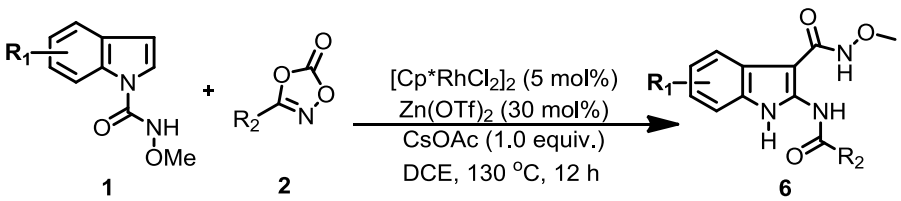
A 10 mL oven-dried Schlenk tube equipped with a magnetic stir bar was dried under vacuum. Then *N*-methoxy amide substituted indole **1** (0.20 mmol), 1,4,2-dioxazol-5-one **2** (0.24 mmol), $KHSO_4$ (27 mg, 0.20 mmol), NaOAc (16 mg, 0.20 mmol), $[Cp^*RhCl_2]_2$ (6 mg, 0.010 mmol) and anhydrous THF (2.0 mL) were added. The reaction was allowed to stir at 60 ℃ for 12 hours. After cooling to room temperature, the reaction mixture was evaporated to remove the solvent and directly loaded onto silica gel for flash column chromatography (PET/EtOAc) to afford the desired product **4**.

General procedure for product 5 (GP3)



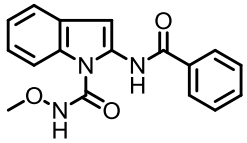
A reaction tube (10 mL) with magnetic stir bar was charged with *N*-methoxy amide substituted indole **1** (0.20 mmol), 1,4,2-dioxazol-5-one **2** (0.24 mmol), $Zn(OTf)_2$ (22 mg, 0.060 mmol), CsOAc (38 mg, 0.20 mmol) and $[Cp^*RhCl_2]_2$ (6 mg, 0.010 mmol), followed by the mixture of THF (2.0 mL) and H_2O (0.2 mL). The reaction was allowed to stir at 60 ℃ for 12 hours. After cooling to room temperature, the reaction mixture was evaporated to remove the solvent and directly loaded onto silica gel for flash column chromatography (PET/EtOAc) to afford the desired product **5**.

General procedure for product 6 (GP4)

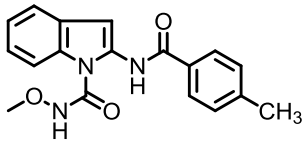


N-methoxy amide substituted indole **1** (0.20 mmol), 1,4,2-dioxazol-5-one **2** (0.24 mmol), $Zn(OTf)_2$ (22 mg, 0.060 mmol), CsOAc (38 mg, 0.20 mmol) and $[Cp^*RhCl_2]_2$ (6 mg, 0.010 mmol) were placed into a 10 mL Schlenk tube equipped with a septum under N_2 atmosphere. DCE (2.0 mL) was introduced via cannula. The reaction mixture was stirred at 130 ℃ for 12 h. After cooling to ambient temperature, the reaction mixture was evaporated to remove the solvent and directly loaded onto silica gel for flash column chromatography (PET/EtOAc) to afford the desired product **6**.

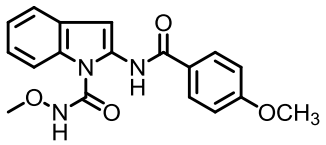
2.3.2 Characterization of Reaction Products



2-Benzamido-*N*-methoxy-1*H*-indole-1-carboxamide (3a): The title compound was obtained as a white solid in 92% yield according to the **GP1**. ^{1}H NMR (500 MHz, DMSO): δ 11.80 (1H, s), 10.83 (1H, s), 7.99 (2H, d, J = 7.0 Hz), 7.72 (1H, d, J = 8.0 Hz), 7.65 (1H, t, J = 7.5 Hz), 7.58 (3H, m), 7.23 (1H, td, J = 7.5, 1.0 Hz), 7.19 (1H, t, J = 7.5 Hz), 6.84 (1H, s), 3.77 (3H, s); ^{13}C NMR (125 MHz, DMSO): δ 164.5, 151.3, 133.6, 133.5, 132.2, 132.1, 128.7, 127.9, 127.5, 122.4, 122.1, 120.0, 112.8, 96.5, 63.5; HRMS (ESI) *m/z* calcd for $C_{17}H_{16}N_3O_3$ $[M+H]^+$ 310.1186, found 310.1187.

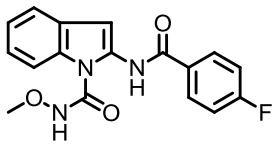


***N*-Methoxy-2-(4-methylbenzamido)-1*H*-indole-1-carboxamide (3b):** The title compound was obtained as a white solid in 76% yield according to the **GP1**. ^{1}H NMR (500 MHz, DMSO): δ 11.76 (1H, s), 10.74 (1H, s), 7.87 (2H, d, J = 8.0 Hz), 7.70 (1H, d, J = 8.0 Hz), 7.55 (1H, d, J = 8.0 Hz), 7.39 (2H, d, J = 8.0 Hz), 7.22 (1H, td, J = 7.5, 1.5 Hz), 7.17 (1H, td, J = 7.5, 1.0 Hz), 6.81 (1H, s), 3.75 (3H, s), 2.40 (3H, s); ^{13}C NMR (125 MHz, DMSO): δ 164.3, 151.4, 142.3, 133.7, 132.0, 130.8, 129.3, 127.9, 127.5, 122.3, 122.1, 119.9, 112.8, 96.4, 63.5, 21.1; HRMS (ESI) *m/z* calcd for $C_{18}H_{18}N_3O_3$ $[M+H]^+$ 324.1343, found 324.1345.

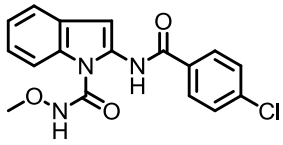


***N*-Methoxy-2-(4-methoxybenzamido)-1*H*-indole-1-carboxamide (3c):** The title compound was obtained as a white solid in 75% yield according to the **GP1**. ^{1}H NMR (500 MHz, DMSO): δ 11.76 (1H, s), 10.69 (1H, s), 7.95 (2H, d, J = 8.5 Hz), 7.70 (1H, d, J = 8.5 Hz), 7.55 (1H, d, J = 7.0 Hz), 7.22 (1H, td, J = 7.5, 1.5 Hz), 7.17 (1H, td, J = 7.5, 1.5 Hz), 7.12 (2H, d, J = 9.0 Hz), 6.80 (1H, s), 3.85 (3H, s), 3.75 (3H, s); ^{13}C NMR (125 MHz, DMSO): δ 163.9, 162.3, 151.4, 133.8,

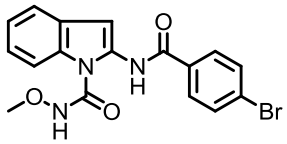
132.0, 129.5, 127.9, 125.7, 122.3, 122.1, 119.9, 114.0, 112.8, 96.2, 79.2, 63.5, 55.5; HRMS (ESI) *m/z* calcd for $C_{18}H_{18}N_3O_4$ $[M+H]^+$ 340.1292, found 340.1289.



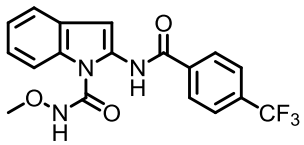
2-(4-Fluorobenzamido)-*N*-methoxy-1*H*-indole-1-carboxamide (3d): The title compound was obtained as a white solid in 89% yield according to the **GP1**. ^{1}H NMR (500 MHz, DMSO): δ 11.78 (1H, s), 10.82 (1H, s), 8.05 (2H, m), 7.71 (1H, d, J = 8.0 Hz), 7.56 (1H, d, J = 7.5 Hz), 7.43 (2H, t, J = 8.5 Hz), 7.23 (1H, td, J = 7.5, 1.0 Hz), 7.23 (1H, t, J = 7.0 Hz), 6.79 (1H, s), 3.75 (3H, s); ^{13}C NMR (125 MHz, DMSO): δ 164.4 (d, $^1J_{C\text{-}F}$ = 248.0 Hz), 163.7, 151.1, 133.3, 132.2, 130.4 (d, $^3J_{C\text{-}F}$ = 9.0 Hz), 130.2 (d, $^4J_{C\text{-}F}$ = 3.0 Hz), 127.8, 122.5, 122.1, 120.0, 115.7 (d, $^2J_{C\text{-}F}$ = 22.0 Hz), 112.7, 96.9, 63.5; HRMS (ESI) *m/z* calcd for $C_{17}H_{15}FN_3O_3$ $[M+H]^+$ 328.1092, found 328.1091.



2-(4-Chlorobenzamido)-*N*-methoxy-1*H*-indole-1-carboxamide (3e): The title compound was obtained as a white solid in 86% yield according to the **GP1**. ^{1}H NMR (500 MHz, DMSO): δ 11.78 (1H, s), 10.85 (1H, s), 7.98 (2H, d, J = 8.5 Hz), 7.69 (1H, d, J = 8.5 Hz), 7.67 (2H, d, J = 8.5 Hz), 7.56 (1H, d, J = 7.0 Hz), 7.23 (1H, td, J = 7.5, 1.5 Hz), 7.17 (1H, t, J = 7.5 Hz), 6.78 (1H, s), 3.73 (3H, s); ^{13}C NMR (125 MHz, DMSO): δ 163.7, 151.0, 137.0, 133.1, 132.4, 132.2, 129.5, 128.8, 127.7, 122.5, 122.1, 120.0, 112.7, 97.0, 63.5; HRMS (ESI) *m/z* calcd for $C_{17}H_{15}{}^{35}ClN_3O_3$ $[M+H]^+$ 344.0796, found 344.0797.

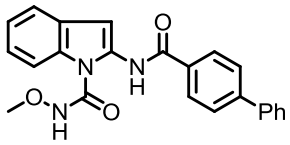


2-(4-Bromobenzamido)-*N*-methoxy-1*H*-indole-1-carboxamide (3f): The title compound was obtained as a white solid in 82% yield according to the **GP1**. ^{1}H NMR (500 MHz, DMSO): δ 11.79 (1H, s), 10.87 (1H, s), 7.91 (2H, d, J = 8.5 Hz), 7.81 (2H, d, J = 8.5 Hz), 7.71 (1H, d, J = 8.0 Hz), 7.56 (1H, d, J = 8.0 Hz), 7.23 (1H, td, J = 7.5, 1.0 Hz), 7.18 (1H, td, J = 7.5, 1.0 Hz), 6.80 (1H, s), 3.75 (3H, s); ^{13}C NMR (125 MHz, DMSO): δ 163.8, 151.0, 133.2, 132.7, 132.2, 131.8, 129.7, 127.7, 126.0, 122.5, 122.1, 120.0, 112.7, 97.0, 63.5; HRMS (ESI) *m/z* calcd for $C_{17}H_{15}{}^{79}BrN_3O_3$ $[M+H]^+$ 388.0291, found 388.0293.

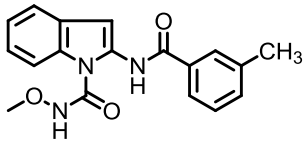


***N*-Methoxy-2-(4-(trifluoromethyl)benzamido)-1*H*-indole-1-carboxamide (3g):** The title

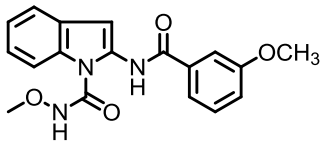
compound was obtained as a white solid in 87% yield according to the **GP1**. ^{1}H NMR (500 MHz, DMSO): δ 11.82 (1H, s), 11.00 (1H, s), 8.17 (2H, d, J = 8.0 Hz), 7.98 (2H, t, J = 8.0 Hz), 7.71 (1H, d, J = 8.5 Hz), 7.58 (1H, d, J = 7.5 Hz), 7.24 (1H, td, J = 7.5, 1.0 Hz), 7.19 (1H, t, J = 7.5, 1.0 Hz), 6.81 (1H, s), 3.75 (3H, s); ^{13}C NMR (125 MHz, DMSO): δ 163.7, 150.9, 137.4, 132.9, 132.3, 131.8 (q, $^{2}J_{C\text{-}F}$ = 32.0 Hz), 128.5, 127.6, 125.7 (q, $^{3}J_{C\text{-}F}$ = 4.0 Hz), 123.9 (q, $^{1}J_{C\text{-}F}$ = 271.0 Hz), 122.6, 122.1, 120.1, 112.7, 97.3, 63.5; HRMS (ESI) *m/z* calcd for $C_{18}H_{15}F_3N_3O_3$ $[M+H]^+$ 378.1060, found 378.1061.



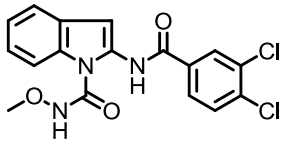
2-([1,1'-Biphenyl]-4-ylcarboxamido)-*N*-methoxy-1*H*-indole-1-carboxamide (3h): The title compound was obtained as a white solid in 56% yield according to the **GP1**. ^{1}H NMR (500 MHz, DMSO): δ 11.80 (1H, s), 10.87 (1H, s), 8.06 (2H, d, J = 8.5 Hz), 7.90 (2H, d, J = 8.0 Hz), 7.78 (2H, d, J = 7.0 Hz), 7.71 (1H, d, J = 8.0 Hz), 7.57 (1H, d, J = 8.0 Hz), 7.53 (2H, t, J = 7.5 Hz), 7.44 (1H, t, J = 7.5 Hz), 7.23 (1H, td, J = 7.5, 1.0 Hz), 7.18 (1H, td, J = 7.5, 1.0 Hz), 6.83 (1H, s), 3.76 (3H, s); ^{13}C NMR (125 MHz, DMSO): δ 164.1, 151.3, 143.6, 139.0, 133.5, 132.4, 132.1, 129.1, 128.3, 128.2, 127.8, 127.0, 126.9, 122.4, 122.1, 120.0, 112.8, 96.5, 63.5; HRMS (ESI) *m/z* calcd for $C_{23}H_{20}N_3O_3$ $[M+H]^+$ 386.1499, found 386.1497.



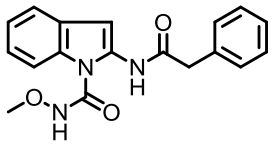
***N*-Methoxy-2-(3-methylbenzamido)-1*H*-indole-1-carboxamide (3i):** The title compound was obtained as a white solid in 79% yield according to the **GP1**. ^{1}H NMR (500 MHz, DMSO): δ 11.80 (1H, s), 10.79 (1H, s), 7.80 (1H, s), 7.77 (1H, d, J = 6.5 Hz), 7.72 (1H, d, J = 8.5 Hz), 7.57 (1H, d, J = 7.5 Hz), 7.46 (2H, m), 7.23 (1H, td, J = 7.5, 1.0 Hz), 7.19 (1H, t, J = 7.0 Hz), 6.83 (1H, s), 3.77 (3H, s), 2.42 (3H, s); ^{13}C NMR (125 MHz, DMSO): δ 164.6, 151.4, 138.1, 133.6, 133.6, 132.8, 132.0, 128.6, 128.1, 127.9, 124.6, 122.4, 122.1, 120.0, 112.8, 96.5, 63.5, 21.0; HRMS (ESI) *m/z* calcd for $C_{18}H_{18}N_3O_3$ $[M+H]^+$ 324.1343, found 324.1341.



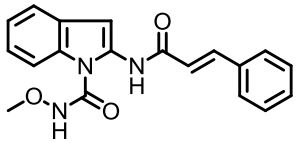
***N*-Methoxy-2-(3-methoxybenzamido)-1*H*-indole-1-carboxamide (3j):** The title compound was obtained as a white solid in 72% yield according to the **GP1**. ^{1}H NMR (500 MHz, DMSO): δ 11.79 (1H, s), 10.80 (1H, s), 7.72 (1H, d, J = 8.5 Hz), 7.55 (3H, m), 7.50 (1H, t, J = 7.5 Hz), 7.21 (3H, m), 6.82 (1H, s), 3.86 (3H, s), 3.77 (3H, s); ^{13}C NMR (125 MHz, DMSO): δ 164.3, 159.4, 151.3, 135.1, 133.5, 132.1, 129.9, 127.9, 122.4, 122.1, 120.0, 119.6, 117.8, 112.9, 112.8, 96.6, 63.5, 55.4; HRMS (ESI) *m/z* calcd for $C_{18}H_{18}N_3O_4$ $[M+H]^+$ 340.1292, found 340.1295.



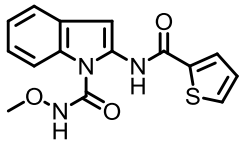
2-(3,4-Dichlorobenzamido)-*N*-methoxy-1*H*-indole-1-carboxamide (3k): The title compound was obtained as a white solid in 83% yield according to the **GP1**. ^{1}H NMR (500 MHz, DMSO): δ 11.78 (1H, s), 10.92 (1H, s), 8.20 (1H, d, J = 2.0 Hz), 7.93 (1H, dd, J = 8.0, 4.0 Hz), 7.88 (1H, d, J = 8.5 Hz), 7.70 (1H, d, J = 8.5 Hz), 7.56 (1H, d, J = 7.5 Hz), 7.23 (1H, td, J = 7.5, 1.0 Hz), 7.17 (1H, td, J = 7.5, 1.0 Hz), 6.74 (1H, s), 3.73 (3H, s); ^{13}C NMR (125 MHz, DMSO): δ 162.8, 150.6, 134.9, 134.0, 132.7, 132.5, 131.5, 131.1, 129.7, 127.9, 127.5, 122.6, 122.0, 120.1, 112.7, 97.5, 63.5; HRMS (ESI) *m/z* calcd for $C_{17}H_{14}{}^{35}Cl_2N_3O_3$ $[M+H]^+$ 378.0407, found 378.0411.



***N*-Methoxy-2-(2-phenylacetamido)-1*H*-indole-1-carboxamide (3l):** The title compound was obtained as a white solid in 67% yield according to the **GP1**. ^{1}H NMR (500 MHz, DMSO): δ 11.77 (1H, s), 10.29 (1H, s), 7.61 (1H, d, J = 7.5 Hz), 7.50 (1H, d, J = 7.0 Hz), 7.34 (3H, m), 7.29 (2H, m), 7.16 (2H, m), 6.68 (1H, s), 3.75 (2H, s), 3.74 (3H, s); ^{13}C NMR (125 MHz, DMSO): δ 168.8, 150.7, 135.3, 133.3, 129.4, 129.1, 128.4, 127.8, 126.7, 122.2, 122.0, 119.8, 112.4, 95.8, 63.5, 42.7; HRMS (ESI) *m/z* calcd for $C_{18}H_{18}N_3O_3$ $[M+H]^+$ 324.1343, found 324.1348.

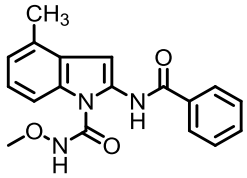


2-Cinnamamido-*N*-methoxy-1*H*-indole-1-carboxamide (3m): The title compound was obtained as a white solid in 63% yield according to the **GP1**. ^{1}H NMR (500 MHz, DMSO): δ 11.85 (1H, s), 10.40 (1H, s), 7.68 (2H, d, J = 7.0 Hz), 7.62 (2H, m), 7.54 (1H, d, J = 7.0 Hz), 7.44 (3H, m), 7.20 (1H, td, J = 7.5, 1.5 Hz), 7.16 (1H, td, J = 7.5, 1.0 Hz), 7.00 (1H, d, J = 16.0 Hz), 6.83 (1H, s), 3.80 (3H, s); ^{13}C NMR (125 MHz, DMSO): δ 163.1, 150.6, 141.0, 134.6, 133.5, 132.1, 130.0, 129.0, 128.0, 122.2, 122.0, 121.4, 119.9, 112.3, 95.8, 63.6; HRMS (ESI) *m/z* calcd for $C_{19}H_{18}N_3O_3$ $[M+H]^+$ 336.1343, found 336.1344.

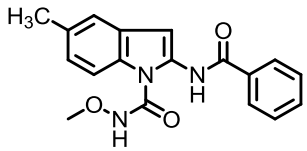


***N*-Methoxy-2-(thiophene-2-carboxamido)-1*H*-indole-1-carboxamide (3n):** The title compound was obtained as a white solid in 85% yield according to the **GP1**. ^{1}H NMR (500 MHz, DMSO): δ 11.74 (1H, s), 10.73 (1H, s), 7.92 (2H, m), 7.68 (1H, d, J = 8.0 Hz), 7.55 (1H, d, J = 7.5 Hz), 7.26 (1H, t, J = 4.0 Hz), 7.22 (1H, t, J = 7.5 Hz), 7.17 (1H, t, J = 7.5 Hz), 6.71 (1H, s), 3.74 (3H, s); ^{13}C NMR (125 MHz, DMSO): δ 159.4, 150.8, 138.7, 132.8, 132.5, 132.4, 129.7, 128.3, 127.6, 122.5,

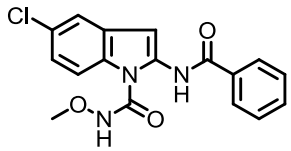
122.0, 120.0, 112.7, 97.2, 63.4; HRMS (ESI) *m/z* calcd for $C_{15}H_{14}N_3O_3S$ $[M+H]^+$ 316.0750, found 316.0752.



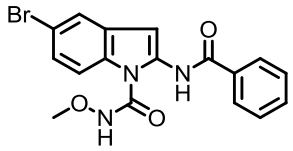
2-Benzamido-*N*-methoxy-4-methyl-1*H*-indole-1-carboxamide (3o): The title compound was obtained as a white solid in 81% yield according to the **GP1**. ^{1}H NMR (500 MHz, DMSO): δ 11.77 (1H, s), 10.80 (1H, s), 7.97 (2H, d, J = 7.0 Hz), 7.70 (1H, d, J = 8.0 Hz), 7.64 (1H, d, J = 7.5 Hz), 7.58 (2H, t, J = 7.5 Hz), 7.52 (1H, d, J = 8.5 Hz), 7.12 (1H, t, J = 7.5 Hz), 6.99 (1H, d, J = 7.5 Hz), 6.84 (1H, s), 3.75 (3H, s), 2.46 (3H, s); ^{13}C NMR (125 MHz, DMSO): δ 164.4, 151.3, 133.6, 133.0, 132.1, 131.7, 128.7, 127.5, 127.3, 122.4, 122.3, 118.2, 110.4, 95.1, 63.4, 18.3; HRMS (ESI) *m/z* calcd for $C_{18}H_{18}N_3O_3$ $[M+H]^+$ 324.1343, found 324.1347.



2-Benzamido-*N*-methoxy-5-methyl-1*H*-indole-1-carboxamide (3p): The title compound was obtained as a white solid in 75% yield according to the **GP1**. ^{1}H NMR (500 MHz, DMSO): δ 11.73 (1H, s), 10.83 (1H, s), 7.96 (2H, d, J = 7.0 Hz), 7.64 (1H, t, J = 7.0 Hz), 7.58 (3H, m), 7.34 (1H, s), 7.04 (1H, dd, J = 8.5, 1.0 Hz), 6.76 (1H, s), 3.74 (3H, s), 2.38 (3H, s); ^{13}C NMR (125 MHz, DMSO): δ 164.3, 151.7, 133.6, 132.2, 131.0, 130.2, 128.8, 128.1, 127.5, 123.7, 119.8, 112.6, 96.2, 63.4, 21.0; HRMS (ESI) *m/z* calcd for $C_{18}H_{18}N_3O_3$ $[M+H]^+$ 324.1343, found 324.1345.

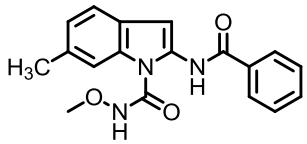


2-Benzamido-5-chloro-*N*-methoxy-1*H*-indole-1-carboxamide (3q): The title compound was obtained as a white solid in 82% yield according to the **GP1**. ^{1}H NMR (500 MHz, DMSO): δ 11.87 (1H, s), 10.87 (1H, s), 7.95 (2H, d, J = 7.0 Hz), 7.68 (1H, d, J = 9.0 Hz), 7.64 (2H, m), 7.58 (2H, t, J = 7.5 Hz), 7.23 (1H, dd, J = 8.5, 1.5 Hz), 6.80 (1H, s), 3.74 (3H, s); ^{13}C NMR (125 MHz, DMSO): δ 164.6, 150.8, 134.9, 133.5, 132.3, 130.7, 129.3, 128.7, 127.6, 126.5, 122.1, 119.2, 114.2, 95.8, 63.5; HRMS (ESI) *m/z* calcd for $C_{17}H_{15}{}^{35}ClN_3O_3$ $[M+H]^+$ 344.0796, found 344.0799.

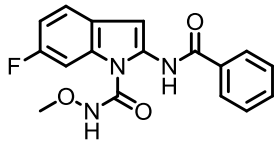


2-Benzamido-5-bromo-*N*-methoxy-1*H*-indole-1-carboxamide (3r): The title compound was obtained as a white solid in 86% yield according to the **GP1**. ^{1}H NMR (500 MHz, DMSO): δ

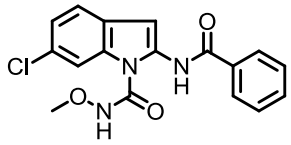
11.86 (1H, s), 10.87 (1H, s), 7.96 (2H, d, *J* = 7.5 Hz), 7.78 (1H, d, *J* = 2.0 Hz), 7.64 (2H, m), 7.58 (2H, t, *J* = 7.5 Hz), 7.34 (1H, dd, *J* = 9.0, 2.0 Hz), 6.79 (1H, s), 3.74 (3H, s); ^{13}C NMR (125 MHz, DMSO): δ 164.6, 150.7, 134.7, 133.5, 132.2, 131.0, 129.8, 128.7, 127.6, 124.7, 122.1, 114.6, 114.5, 95.7, 63.5; HRMS (ESI) *m/z* calcd for $C_{17}H_{15}{}^{79}BrN_3O_3$ $[M+H]^+$ 388.0291, found 388.0294.



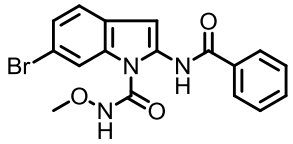
2-Benzamido-*N*-methoxy-6-methyl-1*H*-indole-1-carboxamide (3s): The title compound was obtained as a white solid in 63% yield according to the **GP1**. ^{1}H NMR (500 MHz, DMSO): δ 11.73 (1H, s), 10.76 (1H, s), 7.96 (2H, d, *J* = 7.5 Hz), 7.64 (1H, t, *J* = 7.0 Hz), 7.58 (2H, t, *J* = 7.5 Hz), 7.51 (1H, s), 7.44 (1H, d, *J* = 8.0 Hz), 6.75 (1H, s), 3.74 (3H, s), 2.43 (3H, s); ^{13}C NMR (125 MHz, DMSO): δ 164.5, 151.3, 133.6, 132.8, 132.4, 132.1, 131.6, 128.7, 127.5, 125.5, 123.5, 119.7, 112.9, 96.6, 63.5, 21.7; HRMS (ESI) *m/z* calcd for $C_{18}H_{18}N_3O_3$ $[M+H]^+$ 324.1343, found 324.1345.



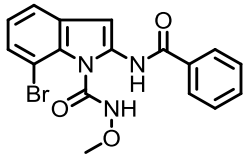
2-Benzamido-6-fluoro-*N*-methoxy-1*H*-indole-1-carboxamide (3t): The title compound was obtained as a white solid in 72% yield according to the **GP1**. ^{1}H NMR (500 MHz, DMSO): δ 11.81 (1H, s), 10.76 (1H, s), 7.98 (2H, d, *J* = 7.0 Hz), 7.64 (1H, t, *J* = 7.5 Hz), 7.58 (3H, m), 7.47 (1H, dd, *J* = 10.0, 2.0 Hz), 7.06 (1H, td, *J* = 9.0, 2.5 Hz), 6.78 (1H, s), 3.74 (3H, s); ^{13}C NMR (125 MHz, DMSO): δ 164.8, 159.0 (d, $^1J_{C\text{-}F}$ = 234.0 Hz), 150.7, 133.8 (d, $^4J_{C\text{-}F}$ = 4.0 Hz), 133.6, 132.3 (d, $^3J_{C\text{-}F}$ = 13.0 Hz), 132.2, 128.7, 127.6, 124.3, 121.1 (d, $^3J_{C\text{-}F}$ = 10.0 Hz), 110.1 (d, $^2J_{C\text{-}F}$ = 24.0 Hz), 99.9 (d, $^2J_{C\text{-}F}$ = 28.0 Hz), 96.8, 63.5; HRMS (ESI) *m/z* calcd for $C_{17}H_{15}FN_3O_3$ $[M+H]^+$ 328.1092, found 328.1093.



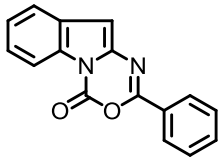
2-Benzamido-6-chloro-*N*-methoxy-1*H*-indole-1-carboxamide (3u): The title compound was obtained as a white solid in 77% yield according to the **GP1**. ^{1}H NMR (500 MHz, DMSO): δ 11.85 (1H, s), 10.83 (1H, s), 7.97 (2H, d, *J* = 7.5 Hz), 7.69 (1H, d, *J* = 1.0 Hz), 7.65 (1H, t, *J* = 7.5 Hz), 7.58 (3H, m), 7.22 (1H, dd, *J* = 8.5, 1.5 Hz), 6.81 (1H, s), 3.74 (3H, s); ^{13}C NMR (125 MHz, DMSO): δ 164.7, 150.6, 134.3, 133.5, 132.6, 132.3, 128.7, 127.6, 126.7, 126.6, 122.3, 121.3, 112.5, 96.5, 63.5; HRMS (ESI) *m/z* calcd for $C_{17}H_{15}{}^{35}ClN_3O_3$ $[M+H]^+$ 344.0796, found 344.0798.



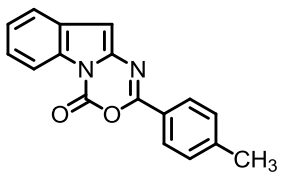
2-Benzamido-6-bromo-*N*-methoxy-1*H*-indole-1-carboxamide (3v): The title compound was obtained as a white solid in 79% yield according to the **GP1**. ^{1}H NMR (500 MHz, DMSO): δ 11.86 (1H, s), 10.83 (1H, s), 7.97 (2H, d, J = 7.0 Hz), 7.83 (1H, d, J = 1.0 Hz), 7.64 (1H, t, J = 7.5 Hz), 7.58 (2H, t, J = 7.5 Hz), 7.53 (1H, d, J = 8.0 Hz), 7.33 (1H, dd, J = 8.0, 1.5 Hz), 6.80 (1H, s), 3.74 (3H, s); ^{13}C NMR (125 MHz, DMSO): δ 164.7, 150.5, 134.1, 133.5, 132.9, 132.3, 128.7, 127.6, 126.9, 124.9, 121.7, 115.3, 114.7, 96.4, 63.5; HRMS (ESI) *m/z* calcd for $C_{17}H_{15}{}^{79}BrN_3O_3$ $[M+H]^+$ 388.0291, found 388.0295.



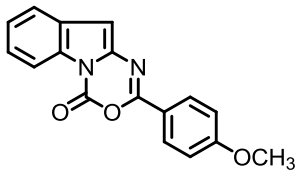
2-Benzamido-*N*-methoxy-7-methyl-1*H*-indole-1-carboxamide (3w): The title compound was obtained as a white solid in 57% yield according to the **GP1**. ^{1}H NMR (500 MHz, DMSO): δ 12.05 (1H, s), 10.38 (1H, s), 7.97 (2H, d, J = 7.0 Hz), 7.63 (2H, m), 7.57 (2H, t, J = 7.5 Hz), 7.44 (1H, d, J = 7.5 Hz), 7.11 (1H, t, J = 8.0 Hz), 6.73 (1H, s), 3.71 (3H, s); ^{13}C NMR (125 MHz, DMSO): δ 166.2, 148.2, 134.3, 133.3, 132.2, 131.3, 130.5, 128.6, 127.8, 126.8, 122.9, 119.8, 104.6, 99.7, 62.9; HRMS (ESI) *m/z* calcd for $C_{17}H_{15}{}^{79}BrN_3O_3$ $[M+H]^+$ 388.0291, found 388.0291.



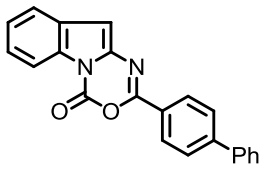
2-Phenyl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4a): The title compound was obtained as a yellow solid in 81% yield according to the **GP2**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.31 (1H, d, J = 8.5 Hz), 8.26 (2H, d, J = 7.5 Hz), 7.67 (1H, d, J = 7.5 Hz), 7.59 (1H, t, J = 7.5 Hz), 7.53 (2H, t, J = 7.5 Hz), 7.45 (1H, t, J = 7.5 Hz), 7.41 (1H, t, J = 7.5 Hz), 6.74 (1H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 152.9, 142.4, 138.0, 133.0, 131.1, 130.0, 129.0, 128.9, 128.4, 125.4, 125.4, 121.3, 115.5, 101.0; HR-MS (ESI) *m/z* calcd for $C_{16}H_{10}N_2O_2Na$ $[M+Na]^+$ 285.0634, found 285.0634.



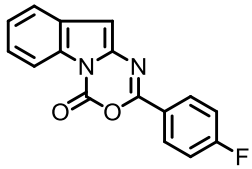
2-(p-Tolyl)-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4b): The title compound was obtained as a yellow solid in 75% yield according to the **GP2**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.30 (1H, d, J = 8.0 Hz), 8.14 (2H, d, J = 8.0 Hz), 7.66 (1H, d, J = 8.0 Hz), 7.44 (1H, t, J = 7.0 Hz), 7.40 (1H, t, J = 7.0 Hz), 7.32 (2H, d, J = 8.5 Hz), 6.70 (1H, s), 2.45 (3H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.1, 144.0, 142.5, 138.1, 131.0, 130.1, 129.8, 128.4, 126.1, 125.2, 125.2, 121.2, 115.5, 100.6, 21.9; HRMS (ESI) *m/z* calcd for $C_{17}H_{12}N_2O_2Na$ $[M+ Na]^+$ 299.0791, found 299.0790.



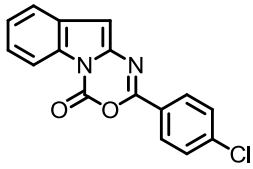
2-(4-Methoxyphenyl)-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4c): The title compound was obtained as a yellow solid in 72% yield according to the **GP2**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.29 (1H, d, J = 8.0 Hz), 8.20 (2H, d, J = 8.5 Hz), 7.65 (1H, d, J = 7.0 Hz), 7.41 (2H, m), 7.00 (2H, d, J = 4.0 Hz), 6.66 (1H, s), 3.90 (3H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 163.6, 152.9, 142.6, 138.3, 131.0, 130.4, 130.1, 125.0, 121.1, 115.4, 114.5, 100.0, 55.7; HRMS (ESI) *m/z* calcd for $C_{17}H_{12}N_2O_3Na$ $[M+Na]^+$ 315.0740, found 315.0742.



2-([1,1'-Biphenyl]-4-yl)-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4d): The title compound was obtained as a yellow solid in 91% yield according to the **GP2**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.24 (3H, d, J = 8.5 Hz), 7.76 (2H, m), 7.67 (3H, m), 7.45 (5H, m), 6.75 (1H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ152.8, 145.8, 142.5, 139.9, 138.1, 131.1, 130.1, 129.2, 128.9, 128.5, 127.6, 127.4, 125.4, 125.3, 121.3, 115.5, 101.0; HRMS (ESI) *m/z* calcd for $C_{22}H_{14}N_2O_2Na$ $[M+Na]^+$ 361.0947, found 361.0946.

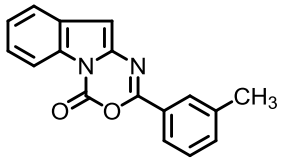


2-(4-Fluorophenyl)-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4e): The title compound was obtained as a yellow solid in 43% yield according to the **GP2**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.28 (3H, m), 7.67 (1H, d, J = 7.5 Hz), 7.44 (2H, m), 7.21 (2H, t, J = 8.5), 6.73 (1H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 166.85 (d, $^{1}J_{C\text{-}F}$ = 254.0 Hz), 152.0, 142.2, 137.8, 131.0, 130.8, 130.8, 130.0, 125.4 (d, $^{3}J_{C\text{-}F}$ = 7.0 Hz), 125.1 (d, $^{4}J_{C\text{-}F}$ = 3.0 Hz), 121.3, 116.4 (d, $^{2}J_{C\text{-}F}$ = 22.0 Hz), 115.5, 101.1; HRMS (ESI) *m/z* calcd for $C_{16}H_9FN_2O_2Na$ $[M+Na]^+$ 303.0540, found 303.0543.

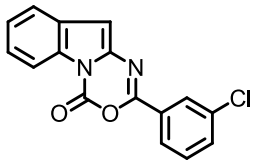


2-(4-Chlorophenyl)-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4f): The title compound was obtained as a yellow solid in 47% yield according to the **GP2**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.31 (1H, d, J = 7.5 Hz), 8.20 (2H, d, J = 8.5 Hz), 7.68 (1H, d, J = 7.5 Hz), 7.51 (2H, d, J = 8.5 Hz),

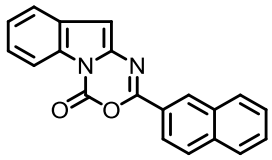
7.47 (1H, t, *J* = 7.0 Hz), 7.42 (1H, t, *J* = 7.5 Hz), 6.75 (1H, s); ^{13}C NMR (125 MHz, $CDCl_3$): *δ*152.0, 142.2, 139.5, 137.8, 131.1, 130.0, 129.6, 129.4, 127.4, 125.6, 125.4, 121.4, 115.5, 101.4; HRMS (ESI) *m/z* calcd for $C_{16}H_9{}^{35}ClN_2O_2Na$ $[M+Na]^+$ 319.0245, found 319.0245.



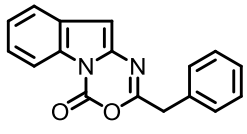
2-(m-Tolyl)-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4g): The title compound was obtained as a yellow solid in 75% yield according to the **GP2**. ^{1}H NMR (500 MHz, $CDCl_3$): *δ* 8.31 (1H, d, *J* = 8.0 Hz), 8.07 (2H, m), 7.67 (1H, d, *J* = 7.5 Hz), 7.42 (4H, m), 6.73 (1H, s), 2.46 (3H, s); ^{13}C NMR (125 MHz, $CDCl_3$): *δ* 153.1, 142.5, 138.9, 138.1, 133.9, 131.1, 130.0, 128.9, 128.8, 128.8, 125.6, 125.3, 121.2, 115.5, 100.9, 21.5; HRMS (ESI) *m/z* calcd for $C_{17}H_{12}N_2O_2Na$ $[M+Na]^+$ 299.0791, found 299.0791.



2-(3-Chlorophenyl)-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4h): The title compound was obtained as a yellow solid in 45% yield according to the **GP2**. ^{1}H NMR (500 MHz, $CDCl_3$): *δ* 8.28 (1H, d, *J* = 8.5 Hz), 8.22 (1H, t, *J* = 2.0 Hz), 8.11 (1H, m), 7.66 (1H, d, *J* = 8.0 Hz), 7.54 (1H, m), 7.45 (2H, m), 7.40 (1H, td, *J* = 7.5, 1.0 Hz), 6.74 (1H, s); ^{13}C NMR (125 MHz, $CDCl_3$): *δ* 151.5, 142.0, 137.6, 135.3, 132.9, 131.1, 130.6, 130.3, 129.9, 128.2, 126.3, 125.6, 125.4, 121.4, 115.5, 101.7; HRMS (ESI) *m/z* calcd for $C_{16}H_9{}^{35}ClN_2O_2Na$ $[M+Na]^+$ 319.0245, found 319.0248.

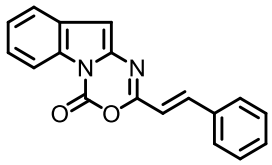


2-(Naphthalen-2-yl)-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4i): The title compound was obtained as a yellow solid in 62% yield according to the **GP2**. ^{1}H NMR (500 MHz, $CDCl_3$): *δ* 8.79 (1H, s), 8.34 (1H, d, *J* = 8.0 Hz), 7.30 (1H, dd, *J* = 8.5, 2.0 Hz), 8.01 (1H, d, *J* = 8.0 Hz), 7.96 (1H, d, *J* = 9.0 Hz), 7.90 (1H, d, *J* = 7.5 Hz), 7.69 (1H, d, *J* = 7.5 Hz), 7.60 (2H, m), 7.47 (1H, t, *J* = 8.0 Hz), 7.42 (1H, t, *J* = 7.0 Hz), 6.78 (1H, s); ^{13}C NMR (125 MHz, $CDCl_3$): *δ* 153.0, 142.5, 138.1, 135.6, 132.9, 131.1, 130.1, 129.7, 129.5, 128.9, 128.7, 128.0, 127.2, 126.0, 125.4, 125.3, 124.0, 121.3, 115.5, 101.2; HRMS (ESI) *m/z* calcd for $C_{20}H_{12}N_2O_2Na$ $[M+Na]^+$ 335.0791, found 335.0793.

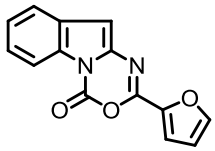


2-Benzyl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4j): The title compound was obtained as a

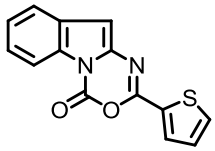
yellow solid in 49% yield according to the **GP2**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.87 (1H, d, J = 8.0 Hz), 7.68 (1H, d, J = 8.0 Hz), 7.48 (3H, m), 7.35 (2H, t, J = 7.5 Hz), 7.30 (2H, m), 7.12 (1H, s), 4.83 (2H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 159.1, 148.8, 135.9, 133.2, 132.4, 129.0, 129.0, 128.9, 128.7, 128.3, 124.3, 124.3, 113.5, 109.3, 42.7; HRMS (ESI) *m/z* calcd for $C_{17}H_{12}N_2O_2Na$ $[M+Na]^+$ 299.0791, found 299.0789.



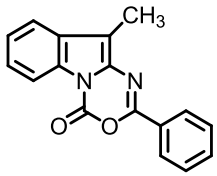
(*E*)-2-Styryl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4k): The title compound was obtained as a yellow solid in 59% yield according to the **GP2**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.29 (1H, d, J = 8.5 Hz), 7.82 (1H, d, J = 16.0 Hz), 7.66 (1H, d, J = 7.0 Hz), 7.60 (2H, dd, J = 8.0, 2.0 Hz), 7.42 (5H, m), 6.75 (1H, d, J = 16.0 Hz), 6.69 (1H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.0, 142.4, 142.3, 138.2, 134.7, 131.3, 130.7, 130.0, 129.3, 128.2, 125.5, 125.3, 121.3, 117.3, 115.5, 101.2; HRMS (ESI) *m/z* calcd for $C_{18}H_{12}N_2O_2Na$ $[M+Na]^+$ 311.0791, found 311.0795.



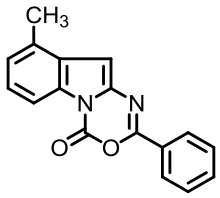
2-(Furan-2-yl)-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4l): The title compound was obtained as a yellow solid in 45% yield according to the **GP2**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.27 (1H, d, J = 8.5 Hz), 7.72 (1H, d, J = 1.0 Hz), 7.65 (1H, d, J = 7.5 Hz), 7.44 (1H, td, J = 7.5, 1.5 Hz), 7.40 (1H, td, J = 7.5, 1.5 Hz), 7.37 (1H, dd, J = 4.0, 0.5 Hz), 6.75 (1H, s), 6.65 (1H, m); ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.7, 145.3, 143.4, 141.7, 137.5, 131.2, 129.9, 125.5, 125.4, 121.3, 117.8, 115.4, 112.9, 101.5; HRMS (ESI) *m/z* calcd for $C_{14}H_8N_2O_3Na$ $[M+Na]^+$ 275.0427, found 275.0428.



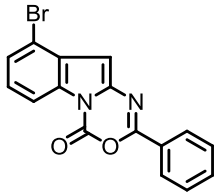
2-(Thiophen-2-yl)-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4m): The title compound was obtained as a yellow solid in 41% yield according to the **GP2**. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.28 (1H, d, J = 7.6 Hz), 7.95 (1H, d, J = 3.6 Hz), 7.65 (2H, d, J = 6.0 Hz), 7.44 (1H, t, J = 7.2 Hz), 7.39 (1H, t, J = 6.8 Hz), 7.19 (1H, t, J = 4.4 Hz), 6.68 (1H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.4, 142.0, 137.8, 133.1, 132.6, 132.2, 131.2, 130.0, 128.7, 125.3, 125.3, 121.2, 115.4, 100.7; HRMS (ESI) *m/z* calcd for $C_{14}H_8N_2O_2SNa$ $[M+Na]^+$ 291.0199, found 291.0200.



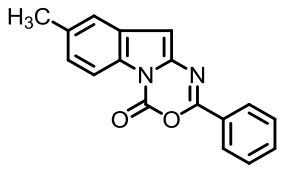
10-Methyl-2-phenyl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4n): The title compound was obtained as a yellow solid in 61% yield according to the **GP2**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.26 (3H, m), 7.61 (1H, d, J = 7.5 Hz), 7.56 (1H, t, J = 7.5 Hz), 7.51 (2H, t, J = 7.5 Hz), 7.42 (2H, m), 2.46 (3H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 151.5, 142.6, 134.1, 132.6, 131.3, 130.5, 129.2, 128.9, 128.1, 125.4, 124.9, 119.3, 115.3, 109.8, 7.93; HRMS (ESI) *m/z* calcd for $C_{17}H_{12}N_2O_2Na$ $[M+Na]^+$ 299.0791, found 299.0794.



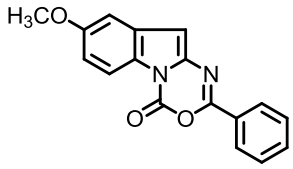
9-Methyl-2-phenyl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4o): The title compound was obtained as a yellow solid in 69% yield according to the **GP2**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.24 (2H, d, J = 7.5 Hz), 8.12 (1H, d, J = 8.0 Hz), 7.58 (1H, tt, J = 7.5, 2.0 Hz), 7.52 (2H, t, J = 7.5 Hz), 7.33 (1H, t, J = 8.0 Hz), 7.18 (1H, d, J = 7.5 Hz), 6.73 (1H, s), 2.57 (3H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 152.6, 142.4, 137.5, 132.9, 130.8, 130.8, 129.7, 129.0, 128.9, 128.3, 125.6, 125.4, 112.9, 99.6, 18.76; HRMS (ESI) *m/z* calcd for $C_{17}H_{12}N_2O_2Na$ $[M+Na]^+$ 299.0791, found 299.0792.



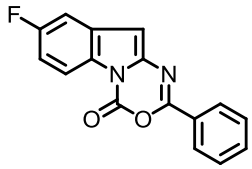
9-Bromo-2-phenyl-4H-[1,3,5]oxadiazino[3,4-a]indol-4-one (4p): The title compound was obtained as a yellow solid in 37% yield according to the **GP2**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.23 (3H, m), 7.60 (1H, t, J = 7.5 Hz), 7.53 (3H, m), 7.29 (1H, t, J = 8.0 Hz), 6.77 (1H, m); ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.4, 142.2, 138.3, 133.3, 131.2, 130.9, 129.1, 128.5, 128.5, 128.2, 126.2, 114.9, 114.4, 100.9; HRMS (ESI) *m/z* calcd for $C_{16}H_9{}^{79}BrN_2O_2Na$ $[M+Na]^+$ 362.9740, found 362.9742.



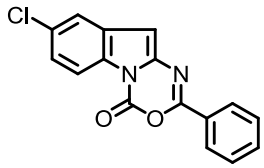
8-Methyl-2-phenyl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4q): The title compound was obtained as a yellow solid in 62% yield according to the **GP2**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.24 (2H, d, J = 7.0 Hz), 8.16 (1H, d, J = 8.0 Hz), 7.58 (1H, tt, J = 7.5, 1.5 Hz), 7.52 (2H, t, J = 7.0 Hz), 7.45 (1H, s), 7.25 (1H, m), 6.65 (1H, s), 2.48 (3H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 152.7, 142.4, 138.0, 135.1, 132.9, 130.2, 129.2, 129.0, 129.0, 128.3, 126.8, 121.1, 115.1, 100.8, 21.8; HRMS (ESI) *m/z* calcd for $C_{17}H_{12}N_2O_2Na$ $[M+Na]^+$ 299.0791, found 299.0791.



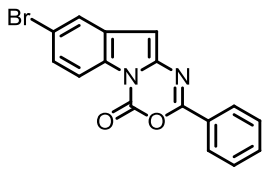
8-Methoxy-2-phenyl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4r): The title compound was obtained as a yellow solid in 60% yield according to the **GP2**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.25 (2H, d, J = 7.0 Hz), 8.18 (1H, d, J = 9.0 Hz), 7.59 (1H, tt, J = 7.0, 1.5 Hz), 7.52 (2H, t, J = 7.5 Hz), 7.11 (1H, d, J = 2.5 Hz), 7.05 (1H, dd, J = 9.0, 2.5 Hz), 6.67 (1H, s), 3.89 (3H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.8, 152.9, 142.3, 138.6, 133.0, 131.1, 129.0, 129.0, 128.3, 125.5, 116.3, 114.4, 103.6, 100.9, 55.8; HRMS (ESI) *m/z* calcd for $C_{17}H_{12}N_2O_3Na$ $[M+Na]^+$ 315.0740, found 315.0739.



8-Fluoro-2-phenyl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4s): The title compound was obtained as a yellow solid in 38% yield according to the **GP2**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.24 (3H, m), 7.60 (1H, tt, J = 7.5, 1.5 Hz), 7.52 (2H, t, J = 8.0 Hz), 7.31 (1H, dd, J = 9.0, 2.5 Hz), 7.15 (1H, td, J = 9.0, 2.5 Hz), 6.68 (1H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 160.7 (d, $^{1}J_{C\text{-}F}$ = 241.0 Hz), 153.4, 142.2, 139.3, 133.2, 131.1 (d, $^{3}J_{C\text{-}F}$ = 10.6 Hz), 129.0, 128.6, 128.4, 127.3, 116.6 (d, $^{3}J_{C\text{-}F}$ = 9.4 Hz), 113.3 (d, $^{2}J_{C\text{-}F}$ = 25.5 Hz), 106.9 (d, $^{2}J_{C\text{-}F}$ = 24.4 Hz), 100.7 (d, $^{4}J_{C\text{-}F}$ = 4.3 Hz); HRMS (ESI) *m/z* calcd for $C_{16}H_9FN_2O_2Na$ $[M+Na]^+$ 303.0540, found 303.0541.

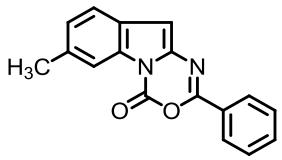


8-Chloro-2-phenyl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4t): The title compound was obtained as a yellow solid in 45% yield according to the **GP2**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.25 (2H, d, J = 7.5 Hz), 8.22 (1H, d, J = 9.0 Hz), 7.64 (1H, d, J = 1.5 Hz), 7.61 (1H, t, J = 7.5 Hz), 7.53 (2H, t, J = 7.5 Hz), 7.40 (1H, dd, J = 8.5, 2.0 Hz), 6.67 (1H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.5, 142.1, 139.1, 133.3, 131.2, 131.1, 129.3, 129.1, 128.6, 128.5, 125.6, 120.9, 116.5, 100.2; HRMS (ESI) *m/z* calcd for $C_{16}H_9{}^{35}ClN_2O_2Na$ $[M+Na]^+$ 319.0245, found 319.0246.

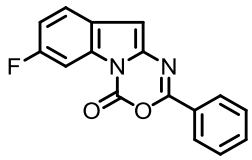


8-Bromo-2-phenyl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4u): The title compound was

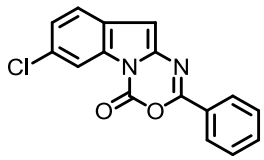
obtained as a yellow solid in 46% yield according to the **GP2**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.25 (2H, d, J = 7.5 Hz), 8.18 (1H, d, J = 8.5 Hz), 7.81 (1H, d, J = 1.5 Hz), 7.61 (1H, tt, J = 7.5, 1.5 Hz), 7.54 (3H, m), 6.67 (1H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.6, 142.2, 139.0, 133.3, 131.7, 129.7, 129.1, 128.6, 128.5, 128.3, 124.0, 118.9, 116.9, 100.1; HRMS (ESI) *m/z* calcd for $C_{16}H_9{}^{79}BrN_2O_2Na$ $[M+Na]^+$ 362.9740, found 362.9744.



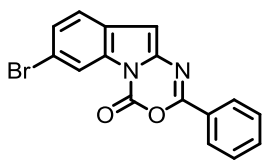
7-Methyl-2-phenyl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4v): The title compound was obtained as a yellow solid in 77% yield according to the **GP2**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.25 (2H, d, J = 8.5 Hz), 8.13 (1H, s), 7.59 (1H, t, J = 7.5 Hz), 7.53 (3H, m), 7.24 (1H, d, J = 8.0 Hz), 6.69 (1H, s), 2.55 (3H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 152.4, 142.6, 137.4, 135.8, 132.9, 131.4, 129.0, 128.9, 128.2, 127.6, 126.8, 120.9, 115.6, 101.0, 22.1; HRMS (ESI) *m/z* calcd for $C_{17}H_{12}N_2O_2Na$ $[M+Na]^+$ 299.0791, found 299.0790.



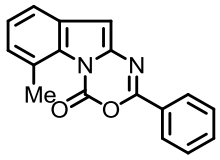
7-Fluoro-2-phenyl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4w): The title compound was obtained as a yellow solid in 51% yield according to the **GP2**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.24 (2H, d, J = 7.0 Hz), 8.03 (1H, dd, J = 9.0, 2.5 Hz), 7.60 (2H, m), 7.53 (2H, t, J = 7.5 Hz), 7.17 (1H, td, J = 9.0, 2.5 Hz), 6.71 (1H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 161.1 (d, $^{1}J_{C\text{-}F}$ = 242.4 Hz), 152.7, 142.3, 138.2 (d, $^{3}J_{C\text{-}F}$ = 4.0 Hz), 133.1, 131.2, 129.0, 128.7, 128.3, 126.2, 122.2 (d, $^{3}J_{C\text{-}F}$ = 9.5 Hz), 113.8 (d, $^{2}J_{C\text{-}F}$ = 25.4 Hz), 103.0 (d, $^{2}J_{C\text{-}F}$ = 28.1 Hz), 100.6 (d, $^{4}J_{C\text{-}F}$ = 1.8 Hz); HRMS (ESI) *m/z* calcd for $C_{16}H_9FN_2O_2Na$ $[M+Na]^+$ 303.0540, found 303.0538.



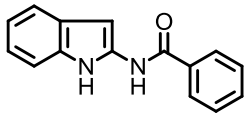
7-Chloro-2-phenyl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4x): The title compound was obtained as a yellow solid in 55% yield according to the **GP2**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.34 (1H, d, J = 2.0 Hz), 8.25 (2H, d, J = 7.5 Hz), 7.60 (2H, t, J = 8.0 Hz), 7.53 (2H, m), 7.39 (1H, dd, J = 8.5, 2.0 Hz), 6.71 (1H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.0, 142.2, 138.4, 133.3, 131.1, 129.1, 128.6, 128.4, 126.0, 122.1, 115.7, 111.1, 102.9, 100.6; HRMS (ESI) *m/z* calcd for $C_{16}H_9{}^{35}ClN_2O_2Na$ $[M+Na]^+$ 319.0245, found 319.0247.



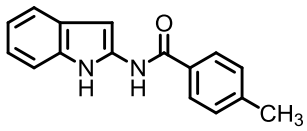
7-Bromo-2-phenyl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4y): The title compound was obtained as a yellow solid in 52% yield according to the **GP2**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.49 (1H, d, J = 2.0 Hz), 8.25 (2H, d, J = 7.0 Hz), 7.61 (1H, tt, J = 7.5, 1.5 Hz), 7.53 (4H, m), 6.70 (1H, d, J = 0.5 Hz); ^{13}C NMR (125 MHz, $CDCl_3$): δ153.1, 142.2, 138.3, 133.3, 131.5, 129.1, 128.8, 128.7, 128.6, 128.4, 122.4, 118.7, 118.5, 100.7; HRMS (ESI) *m/z* calcd for $C_{16}H_9{}^{79}BrN_2O_2Na$ $[M+Na]^+$ 362.9740, found 362.9741.



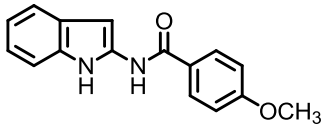
6-Methyl-2-phenyl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4z): The title compound was obtained as a yellow solid in 53% yield according to the **GP2**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.24 (2H, d, J = 7.5 Hz), 7.59 (1H, tt, J = 7.5, 1.5 Hz), 7.52 (2H, t, J = 7.5 Hz), 7.47 (1H, d, J = 7.5 Hz), 7.29 (1H, t, J = 7.5 Hz), 7.21 (1H, d, J = 7.5 Hz), 6.72 (1H, s), 2.88 (3H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 152.7, 142.7, 139.1, 132.9, 131.5, 130.9, 129.1, 129.0, 128.7, 128.2, 126.6, 125.7, 119.0, 102.4, 22.7; HRMS (ESI) *m/z* calcd for $C_{17}H_{12}N_2O_2Na$ $[M+Na]^+$ 299.0791, found 299.0793.



***N*-(1*H*-Indol-2-yl)benzamide (5a):** The title compound was obtained as a blue solid in 82% yield according to the **GP3**. ^{1}H NMR (500 MHz, DMSO): δ 11.06 (1H, s), 11.06 (1H, s), 8.03 (2H, d, J = 7 Hz), 7.63 (1H, t, J = 7.5 Hz), 7.57 (2H, t, J = 7.5 Hz), 7.46 (1H, d, J = 8 Hz), 7.42 (1H, d, J = 7 Hz), 6.99 (1H, td, J = 7.0, 1.5 Hz), 6.96 (1H, td, J = 7.5, 1.5 Hz), 6.28 (1H, d, J = 1.5 Hz); ^{13}C NMR (125 MHz, DMSO): δ 164.4, 135.3, 133.8, 132.7, 131.9, 128.6, 127.6, 127.0, 119.7, 119.2, 118.6, 111.3, 88.0; HRMS (ESI) *m/z* calcd for $C_{15}H_{13}N_2O$ $[M+H]^+$ 237.1022, found 237.1025.

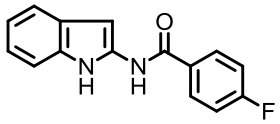


***N*-(1*H*-Indol-2-yl)-4-methylbenzamide (5b):** The title compound was obtained as a blue solid in 85% yield according to the **GP3**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.62 (1H, s), 8.42 (1H, s), 7.80 (2H, d, J = 8.0 Hz), 7.51 (1H, d, J = 7.5 Hz), 7.36 (1H, d, J = 8.0 Hz), 7.32 (2H, d, J = 7.5 Hz), 7.14 (1H, m), 7.11 (1H, td, J = 7.0, 1.0 Hz), 6.02 (1H, m), 2.44 (3H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.5, 143.4, 135.5, 132.6, 130.6, 129.8, 127.2, 126.8, 121.0, 120.4, 119.3, 111.1, 86.3, 21.7; HRMS (ESI) *m/z* calcd for $C_{16}H_{15}N_2O$ $[M+H]^+$ 251.1179, found 251.1180.

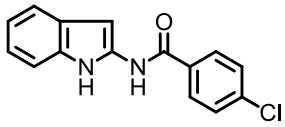


***N*-(1*H*-Indol-2-yl)-4-methoxybenzamide (5c):** The title compound was obtained as a blue solid

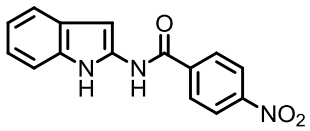
in 75% yield according to the **GP3**. ^{1}H NMR (500 MHz, DMSO): δ 11.04 (1H, s), 10.89 (1H, s), 8.02 (2H, d, J = 8.0 Hz), 7.44 (1H, d, J = 7.5 Hz), 7.40 (1H, d, J = 7.0 Hz), 7.10 (2H, d, J = 8.5 Hz), 6.97 (1H, m), 6.94 (1H, m), 6.24 (1H, s), 3.85 (3H, s); ^{13}C NMR (125 MHz, DMSO): δ 163.9, 162.2, 135.5, 132.6, 129.6, 127.1, 125.8, 119.5, 119.2, 118.6, 113.8, 111.2, 87.6, 55.4; HRMS (ESI) *m/z* calcd for $C_{16}H_{15}N_2O_2$ $[M+H]^+$ 267.1128, found 267.1124.



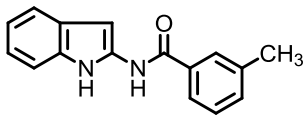
4-Fluoro-*N*-(1*H*-indol-2-yl)benzamide (5d): The title compound was obtained as a blue solid in 69% yield according to the **GP3**. ^{1}H NMR (500 MHz, DMSO): δ 11.09 (1H, s), 11.08 (1H, s), 8.10 (2H, m), 7.43 (4H, m), 6.97 (2H, m), 6.26 (1H, s); ^{13}C NMR (125 MHz, DMSO): δ 164.3 (d, $^{1}J_{C\text{-}F}$ = 248.0 Hz), 163.4, 135.1, 132.7, 130.3 (d, $^{3}J_{C\text{-}F}$ = 9.0 Hz), 130.2 (d, $^{4}J_{C\text{-}F}$ = 3.0 Hz), 127.0, 119.8, 119.3, 118.7, 115.6 (d, $^{2}J_{C\text{-}F}$ = 22.0 Hz), 111.4, 88.1; HRMS (ESI) *m/z* calcd for $C_{15}H_{12}FN_2O$ $[M+H]^+$ 255.0928, found 255.0931.



4-Chloro-*N*-(1*H*-indol-2-yl)benzamide (5e): The title compound was obtained as a blue solid in 66% yield according to the **GP3**. ^{1}H NMR (500 MHz, DMSO): δ 11.14 (1H, s), 11.07 (1H, s), 8.05 (2H, d, J = 8.5 Hz), 7.65 (2H, d, J = 8.5 Hz), 7.45 (1H, d, J = 7.5), 7.42 (1H, d, J = 7.0), 6.97 (2H, m) , 6.27 (1H, d, J = 1.5 Hz); ^{13}C NMR (125 MHz, DMSO): δ 163.8, 137.3, 135.5, 133.2, 132.9, 130.0, 129.1, 127.5, 120.3, 119.7, 119.2, 111.8, 88.7; HRMS (ESI) *m/z* calcd for $C_{15}H_{12}{}^{35}ClN_2O$ $[M+H]^+$ 271.0633, found 271.0638.

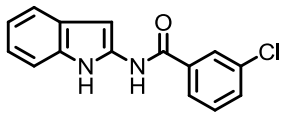


***N*-(1*H*-Indol-2-yl)-4-nitrobenzamide (5f):** The title compound was obtained as a red solid in 48% yield according to the **GP3**. ^{1}H NMR (500 MHz, DMSO): δ 11.41 (1H, s), 11.11 (1H, s), 8.41 (2H, d, J = 9.0 Hz), 8.25 (2H, d, J = 8.5 Hz), 7.47 (1H, d, J = 8.0 Hz), 7.44 (1H, d, J = 8.0 Hz), 7.01 (1H, td, J = 7.0, 1.0 Hz), 7.44 (1H, td, J = 7.5, 1.0 Hz), 6.32 (1H, d, J = 1.5 Hz); ^{13}C NMR (125 MHz, DMSO): δ 162.7, 149.4, 139.4, 134.6, 132.8, 129.2, 126.9, 123.8, 120.1, 119.4, 118.9, 111.5, 88.7; HRMS (ESI) *m/z* calcd for $C_{15}H_{12}N_3O_3$ $[M+H]^+$ 282.0873, found 282.0872.

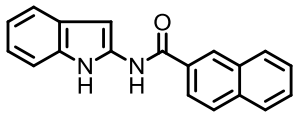


***N*-(1*H*-Indol-2-yl)-3-methylbenzamide (5g):** The title compound was obtained as a blue solid in 88% yield according to the **GP3**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.59 (1H, s), 8.56 (1H, s), 7.71

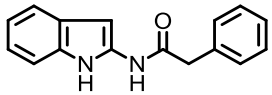
(1H, s), 7.67 (1H, d, *J* = 6.0 Hz), 7.51 (1H, d, *J* = 7.5 Hz), 7.36 (3H, m), 7.16 (1H, t, *J* = 8.0 Hz), 7.12 (1H, t, *J* = 7.5 Hz), 6.05 (1H, s), 2.43 (3H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.9, 139.1, 135.4, 133.4, 133.3, 132.6, 128.9, 127.9, 126.8, 124.2, 121.0, 120.4, 119.3, 111.1, 86.5, 21.5; HRMS (ESI) *m/z* calcd for $C_{16}H_{15}N_2O$ $[M+H]^+$ 251.1179, found 251.1172.



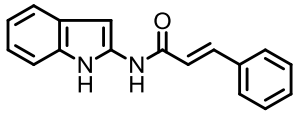
3-Chloro-*N*-(1*H*-indol-2-yl)benzamide (5h): The title compound was obtained as a blue solid in 78% yield according to the **GP3**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.48 (1H, s), 8.54 (1H, s), 7.88 (1H, s), 7.75 (1H, d, *J* = 8.0 Hz), 7.55 (1H, d, *J* = 8.0 Hz), 7.51 (1H, d, *J* = 7.5 Hz), 7.43 (1H, t, *J* = 7.5 Hz), 7.35 (1H, d, *J* = 7.5 Hz), 7.16 (1H, t, *J* = 6.5 Hz), 7.12 (1H, t, *J* = 7.5 Hz) , 6.06 (1H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 164.2, 135.4, 135.2, 134.8, 132.7, 132.6, 130.4, 127.6, 126.7, 125.2, 121.3, 120.5, 119.5, 111.1, 87.1; HRMS (ESI) *m/z* calcd for $C_{15}H_{12}{}^{35}ClN_2O$ $[M+H]^+$ 271.0633, found 271.0632.



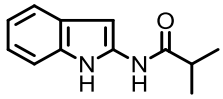
***N*-(1*H*-Indol-2-yl)-2-naphthamide (5i):** The title compound was obtained as a blue solid in 77% yield according to the **GP3**. ^{1}H NMR (500 MHz, DMSO): δ 11.25 (1H, s), 11.13 (1H, s), 8.65 (1H, s), 8.11 (3H, m), 8.03 (1H, d, *J* = 7.0 Hz), 7.66 (2H, m), 7.48 (1H, d, *J* = 8.0 Hz), 7.44 (1H, d, *J* = 7.0 Hz), 6.99 (2H, m), 6.32 (1H, d, *J* = 1.5 Hz); ^{13}C NMR (125 MHz, DMSO): δ 164.5, 135.3, 134.4, 132.7, 132.1, 131.1, 129.0, 128.2, 128.1, 128.0, 127.7, 127.1, 127.0, 124.2, 119.7, 119.3, 118.7, 111.4,88.0; HRMS (ESI) *m/z* calcd for $C_{19}H_{15}N_2O$ $[M+H]^+$ 287.1179, found 287.1173.



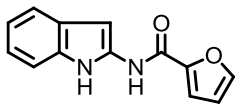
***N*-(1*H*-Indol-2-yl)-2-phenylacetamide (5j):** The title compound was obtained as a blue solid in 35% yield according to the **GP3**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.37 (1H, s), 7.74 (1H, s), 7.37 (7H, m), 7.10 (2H, m), 5.78 (1H, m), 3.78 (2H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 169.6, 134.9, 133.7, 132.5, 129.7, 129.5, 128.2, 126.4, 121.0, 120.4, 119.3, 111.0, 86.0, 44.3; HRMS (ESI) *m/z* calcd for $C_{16}H_{15}N_2O$ $[M+H]^+$ 251.1179, found 251.1175.



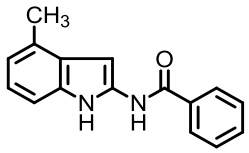
***N*-(1*H*-Indol-2-yl)cinnamamide (5k):** The title compound was obtained as a blue solid in 53% yield according to the **GP3**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.59 (1H, s), 8.56 (1H, s), 7.71 (1H, s), 7.67 (1H, d, *J* = 6.0 Hz), 7.51 (1H, d, *J* = 7.5 Hz), 7.36 (3H, m), 7.16 (1H, t, *J* = 8.0 Hz), 7.12 (1H, td, *J* = 7.5 Hz), 6.05 (1H, s), 2.43 (3H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.9, 139.1, 135.4, 133.4, 133.3, 132.6, 128.9, 127.9, 126.8, 124.2, 121.0, 120.4, 119.3, 111.1, 86.5, 21.5; HRMS (ESI) *m/z* calcd for $C_{17}H_{15}N_2O$ $[M+H]^+$ 263.1179, found 263.1182.



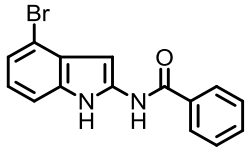
***N*-(1*H*-Indol-2-yl)isobutyramide (5l):** The title compound was obtained as a blue solid in 29% yield according to the **GP3**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.44 (1H, s), 7.99 (1H, s), 7.48 (1H, d, J = 10.0 Hz), 7.30 (1H, d, J = 10.5 Hz), 7.11 (2H, m), 5.91 (1H, s), 2.56 (1H, m), 1.28 (6H, d, J = 8.5 Hz); ^{13}C NMR (125 MHz, $CDCl_3$): δ 175.8, 135.3, 132.5, 126.7, 120.8, 120.3, 119.2, 111.0, 85.6, 36.3, 19.6; HRMS (ESI) *m/z* calcd for $C_{12}H_{15}N_2O$ $[M+H]^+$ 203.1179, found 203.1183.



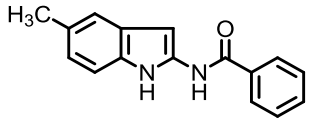
***N*-(1*H*-Indol-2-yl)furan-2-carboxamide (5m):** The title compound was obtained as a blue solid in 34% yield according to the **GP3**. ^{1}H NMR (500 MHz, DMSO): δ 11.01 (1H, s), 10.93 (1H, s), 7.99 (1H, s), 7.42 (2H, m), 7.37 (1H, d, J = 3.5 Hz), 6.97 (2H, m), 6.73 (1H, m), 6.30 (1H, d, J = 1.5 Hz); ^{13}C NMR (125 MHz, DMSO): δ 155.2, 147.0, 146.3, 134.5, 132.6, 127.1, 119.8, 119.3, 118.7, 115.2, 112.4, 111.3, 88.3; HRMS (ESI) *m/z* calcd for $C_{13}H_{11}N_2O_2$ $[M+H]^+$ 227.0815, found 227.0819.



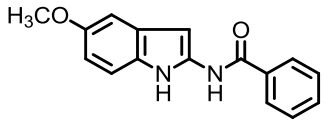
***N*-(4-Methyl-1*H*-indol-2-yl)benzamide (5n):** The title compound was obtained as a blue solid in 82% yield according to the **GP3**. ^{1}H NMR (500 MHz, DMSO): δ 11.06 (1H, s), 11.03 (1H, s), 8.03 (2H, d, J = 7.0 Hz), 7.63 (1H, tt, J = 7.5, 1.5 Hz), 7.58 (2H, t, J = 7.5 Hz), 7.29 (1H, d, J = 8.0 Hz), 6.90 (1H, t, J = 7.5 Hz), 6.77 (1H, d, J = 7.0 Hz), 6.31 (1H, d, J = 1.5 Hz), 2.43 (3H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 164.4, 134.7, 133.8, 132.2, 132.0, 128.6, 127.6, 127.3, 126.9, 119.9, 119.5, 109.1, 86.8, 18.6; HRMS (ESI) *m/z* calcd for $C_{16}H_{15}N_2O$ $[M+H]^+$ 251.1179, found 251.1182.



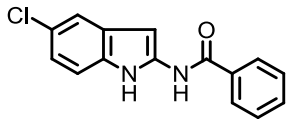
***N*-(4-Methyl-1*H*-indol-2-yl)benzamide (5o):** The title compound was obtained as a blue solid in 70% yield according to the **GP3**. ^{1}H NMR (500 MHz, DMSO): δ 11.44 (1H, s), 11.19 (1H, s), 8.04 (2H, d, J = 7.5 Hz), 7.64 (1H, t, J = 7.5 Hz), 7.58 (2H, t, J = 7.5 Hz), 7.50 (1H, d, J = 8.0 Hz), 7.18 (1H, d, J = 7.5 Hz), 6.94 (1H, t, J = 8.0 Hz), 6.29 (1H, d, J = 1.5 Hz); ^{13}C NMR (125 MHz, $CDCl_3$): δ 164.6, 136.1, 133.5, 133.1, 132.1, 128.6, 127.6, 127.6, 121.9, 120.8, 111.7, 111.0, 87.7; HRMS (ESI) *m/z* calcd for $C_{15}H_{12}{}^{79}BrN_2O$ $[M+H]^+$ 315.0128, found 315.0131.



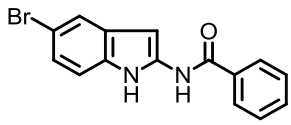
***N*-(5-Methyl-1*H*-indol-2-yl)benzamide (5p):** The title compound was obtained as a blue solid in 76% yield according to the **GP3**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.49 (1H, s), 8.47 (1H, s), 7.89 (2H, d, J = 8.0 Hz), 7.59 (1H, t, J = 7.5 Hz), 7.51 (2H, t, J = 7.5 Hz), 7.30 (1H, s), 7.25 (1H, d, J = 8.0 Hz), 6.97 (1H, d, J = 8.0 Hz), 5.96 (1H, s), 2.44 (3H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.5, 135.3, 133.5, 132.6, 130.9, 129.7, 129.1, 127.2, 127.0, 122.6, 119.2, 110.7, 86.1, 21.7; HRMS (ESI) *m/z* calcd for $C_{16}H_{15}N_2O$ $[M+H]^+$ 251.1179, found 251.1184.



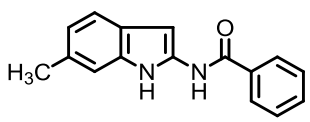
***N*-(5-Methoxy-1*H*-indol-2-yl)benzamide (5q):** The title compound was obtained as a blue solid in 85% yield according to the **GP3**. ^{1}H NMR (500 MHz, DMSO): δ 11.04 (1H, s), 10.93 (1H, s), 8.02 (2H, d, J = 7.0 Hz), 7.62 (1H, t, J = 7.5 Hz), 7.57 (2H, t, J = 7.5 Hz), 7.37 (1H, d, J = 8.5 Hz), 6.95 (1H, d, J = 2.5 Hz), 6.63 (1H, m), 6.22 (1H, d, J = 1.5 Hz), 3.74 (3H, s); ^{13}C NMR (125 MHz, DMSO): δ 153.6, 135.8, 133.8, 131.9, 128.5, 127.6, 127.6, 127.5, 112.0, 109.3, 101.0, 88.0; HRMS (ESI) *m/z* calcd for $C_{16}H_{15}N_2O_2$ $[M+H]^+$ 267.1128, found 267.1129.



***N*-(5-Chloro-1*H*-indol-2-yl)benzamide (5r):** The title compound was obtained as a blue solid in 69% yield according to the **GP3**. ^{1}H NMR (500 MHz, DMSO): δ 11.30 (1H, s), 11.16 (1H, s), 8.02 (2H, d, J = 7.0 Hz), 7.64 (1H, tt, J = 7.5, 1.5 Hz), 7.57 (2H, t, J = 7.5 Hz), 7.47 (1H, d, J = 8.5 Hz), 7.45 (1H, d, J = 2.0 Hz), 6.98 (1H, dd, J = 8.5, 2.0 Hz), 6.27 (1H, d, J = 1.5 Hz); ^{13}C NMR (125 MHz, DMSO): δ 164.6, 136.8, 133.6, 132.1, 131.2, 128.6, 128.4, 127.6, 123.8, 119.4, 117.7, 112.8, 87.6; HRMS (ESI) *m/z* calcd for $C_{15}H_{12}{}^{35}ClN_2O$ $[M+H]^+$ 271.0633, found 271.0635.

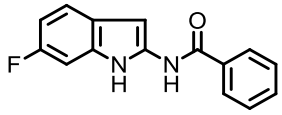


***N*-(5-Bromo-1*H*-indol-2-yl)benzamide (5s):** The title compound was obtained as a blue solid in 62% yield according to the **GP3**. ^{1}H NMR (500 MHz, DMSO): δ 11.32 (1H, s), 11.17 (1H, s), 8.03 (2H, d, J = 7.5 Hz), 7.63 (1H, tt, J = 7.5, 1.5 Hz), 7.60 (1H, d, J = 2.0 Hz), 7.57 (2H, t, J = 7.5 Hz), 7.43 (1H, d, J = 8.5 Hz), 7.10 (1H, dd, J = 8.5, 2.0 Hz), 6.28 (1H, d, J = 1.5 Hz); ^{13}C NMR (125 MHz, DMSO): δ 164.6, 136.6, 133.6, 132.1, 131.5, 129.1, 128.6, 127.6, 122.0, 120.7, 113.3, 111.8, 87.5; HRMS (ESI) *m/z* calcd for $C_{15}H_{12}{}^{79}BrN_2O$ $[M+H]^+$ 315.0128, found 315.0130.

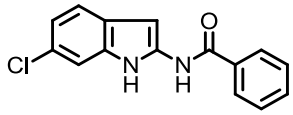


***N*-(6-Methyl-1*H*-indol-2-yl)benzamide (5t):** The title compound was obtained as a blue solid in

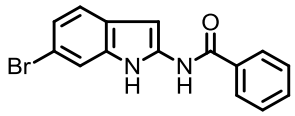
79% yield according to the **GP3**. ^{1}H NMR (500 MHz, DMSO): δ 10.99 (1H, s), 10.90 (1H, s), 8.01 (2H, d, J = 7.0 Hz), 7.62 (1H, tt, J = 7.5, 1.5 Hz), 7.57 (2H, t, J = 7.5 Hz), 7.29 (1H, d, J = 8.0 Hz), 7.24 (1H, s), 6.79 (1H, dd, J = 8.0, 1.0 Hz), 6.22 (1H, d, J = 1.5 Hz), 2.37 (3H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 164.3, 134.6, 133.8, 133.1, 131.9, 128.6, 128.6, 127.6, 124.9, 120.9, 118.4, 111.3, 88.0, 21.5; HRMS (ESI) *m/z* calcd for $C_{16}H_{15}N_2O$ $[M+H]^+$ 251.1179, found 251.1178.



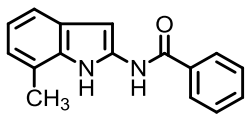
***N*-(6-Fluoro-1*H*-indol-2-yl)benzamide (5u):** The title compound was obtained as a blue solid in 45% yield according to the **GP3**. ^{1}H NMR (500 MHz, DMSO): δ 11.19 (1H, s), 11.07 (1H, s), 8.02 (2H, d, J = 7.0 Hz), 7.63 (1H, t, J = 7.5 Hz), 7.57 (2H, t, J = 7.5 Hz), 7.40 (1H, dd, J = 9.0, 5.5 Hz), 7.27 (1H, dd, J = 10.5, 2.5 Hz), 6.82 (1H, m), 6.28 (1H, d, J = 2.0 Hz); ^{13}C NMR (125 MHz, $CDCl_3$): δ 164.4, 157.9 (d, $^{1}J_{C\text{-}F}$ = 230.5 Hz), 135.7 (d, $^{4}J_{C\text{-}F}$ = 3.1 Hz), 133.7, 132.6 (d, $^{3}J_{C\text{-}F}$ = 13.1 Hz), 132.0, 128.54, 127.59, 123.70, 119.4 (d, $^{3}J_{C\text{-}F}$ = 9.8 Hz), 107.3 (d, $^{2}J_{C\text{-}F}$ = 23.6 Hz), 97.7 (d, $^{2}J_{C\text{-}F}$ = 26.0 Hz), 87.8; HRMS (ESI) *m/z* calcd for $C_{15}H_{12}FN_2O$ $[M+H]^+$ 255.0928, found 255.0930.



***N*-(6-Chloro-1*H*-indol-2-yl)benzamide (5v):** The title compound was obtained as a blue solid in 58% yield according to the **GP3**. ^{1}H NMR (500 MHz, DMSO): δ 11.27 (1H, s), 11.15 (1H, s), 8.03 (2H, d, J = 7.5 Hz), 7.63 (1H, tt, J = 7.0, 1.5 Hz), 7.57 (2H, t, J = 7.5 Hz), 7.54 (1H, d, J = 2.0 Hz), 7.42 (1H, d, J = 8.5 Hz), 6.97 (1H, dd, J = 8.5, 2.0 Hz), 6.30 (1H, d, J = 1.0 Hz); ^{13}C NMR (125 MHz, DMSO): δ 164.5, 136.2, 133.6, 133.2, 132.0, 128.6, 127.6, 125.8, 124.0, 119.8, 119.4, 111.1, 87.8; HRMS (ESI) *m/z* calcd for $C_{15}H_{12}{}^{35}ClN_2O$ $[M+H]^+$ 271.0633, found 271.0635.

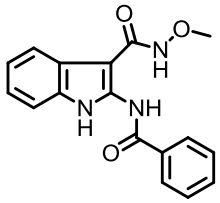


***N*-(6-Bromo-1*H*-indol-2-yl)benzamide (5w):** The title compound was obtained as a blue solid in 67% yield according to the **GP3**. ^{1}H NMR (500 MHz, DMSO): δ 11.27 (1H, s), 11.15 (1H, s), 8.03 (2H, d, J = 7.5 Hz), 7.68 (1H, d, J = 1.5 Hz), 7.63 (1H, tt, J = 7.5, 1.5 Hz), 7.57 (2H, t, J = 7.5 Hz), 7.38 (1H, d, J = 8.5 Hz), 7.08 (1H, dd, J = 8.5, 2.0 Hz), 6.30 (1H, d, J = 1.5 Hz); ^{13}C NMR (125 MHz, DMSO): δ 164.5, 136.1, 133.6, 133.6, 132.0, 128.6, 127.6, 126.1, 122.0, 120.3, 113.9, 111.9, 87.8; HRMS (ESI) *m/z* calcd for $C_{15}H_{12}{}^{79}BrN_2O$ $[M+H]^+$ 315.0128, found 315.0129.

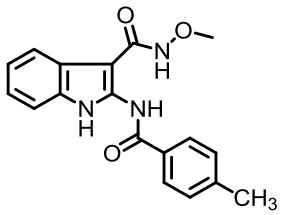


***N*-(7-Methyl-1*H*-indol-2-yl)benzamide (5x):** The title compound was obtained as a blue solid in 75% yield according to the **GP3**. ^{1}H NMR (500 MHz, DMSO): δ 10.79 (1H, s), 10.54 (1H, s),

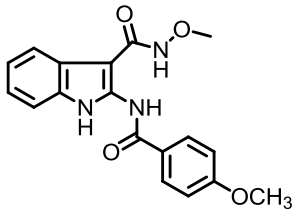
8.03 (2H, d, *J* = 7.0 Hz), 7.64 (1H, tt, *J* = 7.5, 1.5 Hz), 7.58 (2H, t, *J* = 7.5 Hz), 7.29 (1H, d, *J* = 8.0 Hz), 6.91 (1H, t, *J* = 7.5 Hz), 6.84 (1H, d, *J* = 7.5 Hz), 6.42 (1H, d, *J* = 1.5 Hz), 2.46 (3H, s); ^{13}C NMR (125 MHz, $CDCl_3$): *δ*164.4, 134.8, 133.6, 131.9, 131.5, 128.6, 127.4, 127.1, 120.8, 119.5, 119.4, 116.8, 89.6, 16.5; HRMS (ESI) *m/z* calcd for $C_{16}H_{15}N_2O$ $[M+H]^+$ 251.1179, found 251.1181.



2-Benzamido-*N*-methoxy-1*H*-indole-3-carboxamide (6a): The title compound was obtained as a white solid in 62% yield according to the **GP4**. ^{1}H NMR (500 MHz, $CDCl_3$): *δ* 12.20 (1H, s), 11.16 (1H, s), 8.53 (1H, s), 8.09 (2H, d, *J* = 8 Hz), 7.63 (1H, t, *J* = 7 Hz), 7.54 (2H, t, *J* = 7.5 Hz), 7.50 (1H, d, *J* = 7.5 Hz), 7.43 (1H, d, *J* = 7.5 Hz), 7.28 (1H, t, *J* = 7 Hz), 7.24 (1H, t, *J* = 7.5 Hz), 3.98 (3H, s); ^{13}C NMR (125 MHz, $CDCl_3$): *δ* 168.6, 166.3, 144.0, 133.3, 132.1, 132.1, 129.2, 127.8, 122.7, 122.4, 122.0, 118.2, 112.3, 89.6, 65.3; HRMS (ESI) *m/z* calcd for $C_{17}H_{16}N_3O_3$ $[M+H]^+$ 310.1186, found 310.1189.

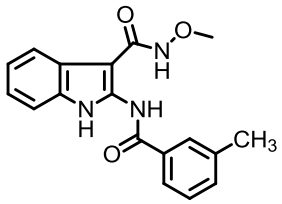


***N*-Methoxy-2-(4-methylbenzamido)-1*H*-indole-3-carboxamide (6b):** The title compound was obtained as a white solid in 59% yield according to the **GP4**. ^{1}H NMR (500 MHz, $CDCl_3$): *δ* 12.13 (1H, s), 11.17 (1H, s), 8.51 (1H, s), 7.97 (2H, d, *J* = 8.5 Hz), 7.49 (1H, d, *J* = 8 Hz), 7.42 (1H, d, *J* = 8 Hz), 7.33 (2H, d, *J* = 8.0 Hz), 7.28 (1H, d, *J* = 7.5 Hz), 7.23 (2H, t, *J* = 7.5 Hz), 3.98 (3H, s), 2.45 (3H, s); ^{13}C NMR (125 MHz, $CDCl_3$): *δ* 168.6, 166.3, 144.2, 144.2, 132.1, 129.9, 129.3, 127.9, 122.6, 122.4, 122.1, 118.1, 112.2, 89.5, 65.3, 21.8; HRMS (ESI) *m/z* calcd for $C_{18}H_{18}N_3O_3$ $[M+H]^+$ 324.1343, found 324.1348.

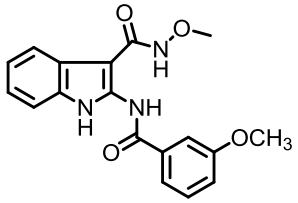


***N*-Methoxy-2-(4-methoxybenzamido)-1*H*-indole-3-carboxamide (6c):** The title compound was obtained as a white solid in 57% yield according to the **GP4**. ^{1}H NMR (500 MHz, $CDCl_3$): *δ* 12.09 (1H, s), 11.17 (1H, s), 8.49 (1H, s), 8.05 (2H, d, *J* = 8.5 Hz), 7.49 (1H, d, *J* = 8 Hz), 7.42 (1H, d, *J* = 7.5 Hz), 7.28 (1H, d, *J* = 7.5 Hz), 7.23 (1H, t, *J* = 7.5 Hz), 7.01 (2H, d, *J* = 8.5 Hz), 3.98 (3H, s), 3.90 (3H, s); ^{13}C NMR (125 MHz, $CDCl_3$): *δ* 168.7, 165.9, 163.7.0, 144.5, 132.1, 129.9, 124.4,

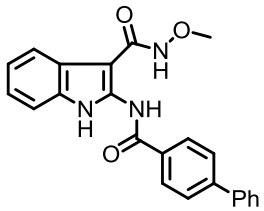
122.6, 122.3, 122.1, 118.1, 114.4, 112.2, 89.3, 65.3, 55.7; HRMS (ESI) *m/z* calcd for $C_{18}H_{18}N_3O_4$ $[M+H]^+$ 340.1292, found 340.1288.



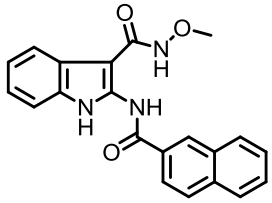
***N*-Methoxy-2-(3-methylbenzamido)-1*H*-indole-3-carboxamide (6d):** The title compound was obtained as a white solid in 65% yield according to the **GP4**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 12.09 (1H, s), 11.19 (1H, s), 8.55 (1H, s), 7.86 (2H, m), 7.50 (1H, d, *J* = 8 Hz), 7.42 (3H, m), 7.26 (1H, t, *J* = 7.0 Hz), 7.22 (1H, t, *J* = 7.0 Hz), 3.98 (3H, s), 2.48 (3H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 168.6, 166.6, 144.0, 139.1, 134.1, 132.1, 129.0, 128.3, 124.9, 122.6, 122.4, 122.0, 118.1, 112.2, 89.6, 66.3, 21.6; HRMS (ESI) *m/z* calcd for $C_{18}H_{18}N_3O_3$ $[M+H]^+$ 324.1343, found 324.1340.



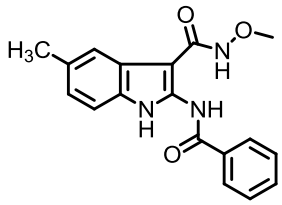
***N*-Methoxy-2-(3-methoxybenzamido)-1*H*-indole-3-carboxamide (6e):** The title compound was obtained as a white solid in 53% yield according to the **GP4**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 12.13 (1H, s), 11.14 (1H, s), 8.52 (1H, s), 7.61 (2H, m), 7.50 (1H, d, *J* = 7.5 Hz), 7.43 (2H, t, *J* = 8.5 Hz), 7.27 (1H, t, *J* = 7.5 Hz), 7.23 (1H, t, *J* = 7.5 Hz), 7.15 (1H, d, *J* = 8.5 Hz), 3.97 (3H, s), 3.90 (3H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 168.5, 166.3, 160.3, 143.9, 133.6, 132.1, 130.2, 122.6, 122.4, 122.0, 119.6, 119.5, 118.2, 113.0, 112.3, 89.7, 65.3, 55.7; HRMS (ESI) *m/z* calcd for $C_{18}H_{18}N_3O_4$ $[M+H]^+$ 340.1292, found 340.1296.



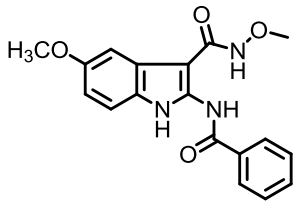
2-([1,1'-Biphenyl]-4-ylcarboxamido)-*N*-methoxy-1*H*-indole-3-carboxamide (6f): The title compound was obtained as a white solid in 38% yield according to the **GP4**. ^{1}H NMR (500 MHz, DMSO): δ 12.50 (1H, s), 12.33 (1H, s), 10.94 (1H, s), 8.10 (2H, d, *J* = 8.5 Hz), 7.97 (2H, d, *J* = 8.0 Hz), 7.79 (3H, m), 7.63 (1H, d, *J* = 8.5 Hz), 7.54 (2H, t, *J* = 7.5 Hz), 7.45 (1H, t, *J* = 7.5 Hz), 7.15 (2H, m), 3.79 (3H, s); ^{13}C NMR (125 MHz, DMSO): δ166.9, 163.6, 144.4, 141.7, 138.8, 132.6, 131.1, 129.2, 128.5, 127.9, 127.5, 127.0, 121.7, 121.3, 121.2, 119.2, 112.6, 99.5, 89.6, 63.5; HRMS (ESI) *m/z* calcd for $C_{23}H_{20}N_3O_3$ $[M+H]^+$ 386.1499, found 386.1501.



2-(2-Naphthamido)-*N*-methoxy-1*H*-indole-3-carboxamide (6g): The title compound was obtained as a white solid in 45% yield according to the **GP4**. ^{1}H NMR (500 MHz, DMSO): δ 12.53 (1H, s), 12.35 (1H, s), 10.96 (1H, s), 8.63 (1H, s), 8.20 (2H, t, J = 8.5 Hz), 8.06 (2H, m), 7.80 (1H, d, J = 7.0 Hz), 7.68 (3H, m), 7.16 (2H, m), 3.80 (3H, s); ^{13}C NMR (125 MHz, DMSO): δ 166.9, 164.1, 141.7, 134.8, 132.6, 132.2, 129.8, 129.3, 129.1, 128.6, 128.3, 127.8, 127.4, 123.1, 121.7, 121.4, 121.2, 119.2, 112.6, 89.8, 63.5; HRMS (ESI) *m/z* calcd for $C_{21}H_{18}N_3O_3$ $[M+H]^+$ 360.1343, found 360.1341.



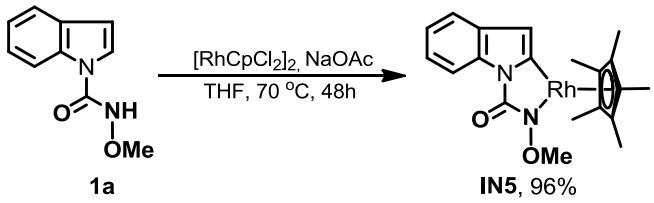
2-Benzamido-*N*-methoxy-5-methyl-1*H*-indole-3-carboxamide (6h): The title compound was obtained as a white solid in 67% yield according to the **GP4**. ^{1}H NMR (500 MHz, DMSO): δ 12.43 (1H, s), 12.18 (1H, s), 10.86 (1H, s), 8.01 (2H, d, J = 7.5 Hz), 7.72 (1H, t, J = 7.5 Hz), 7.66 (2H, t, J = 7.5 Hz), 7.60 (1H, s), 7.48 (1H, d, J = 8.0 Hz), 6.96 (1H, d, J = 8.0 Hz), 3.77 (3H, s), 2.41 (3H, s); ^{13}C NMR (125 MHz, DMSO): δ 167.0, 163.9, 141.6, 133.0, 132.4, 130.8, 130.0, 129.3, 127.2, 122.7, 121.8, 119.1, 112.3, 89.2, 63.5, 21.4; HRMS (ESI) *m/z* calcd for $C_{18}H_{18}N_3O_3$ $[M+H]^+$ 324.1343, found 324.1346.



2-Benzamido-*N*,5-dimethoxy-1*H*-indole-3-carboxamide (6i): The title compound was obtained as a white solid in 72% yield according to the **GP4**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 12.13 (1H, s), 11.02 (1H, s), 8.50 (1H, s), 8.05 (2H, d, J = 7.0 Hz), 7.60 (1H, t, J = 7.5 Hz), 7.52 (2H, t, J = 7.5 Hz), 7.30 (1H, d, J = 9.0 Hz), 6.96 (1H, d, J = 2.5 Hz), 6.83 (1H, dd, J = 8.5, 2.5 Hz), 3.97 (3H, s), 3.87 (3H, s); ^{13}C NMR (125 MHz, $CDCl_3$): δ 168.8, 166.2, 156.2, 144.3, 133.2, 132.1, 129.2, 129.1, 127.8, 127.0, 122.9, 119.8, 112.8, 110.0, 102.9, 89.8, 65.2, 56.2; HRMS (ESI) *m/z* calcd for $C_{18}H_{18}N_3O_4$ $[M+H]^+$ 340.1292, found 340.1299.

2.4 Mechanism study

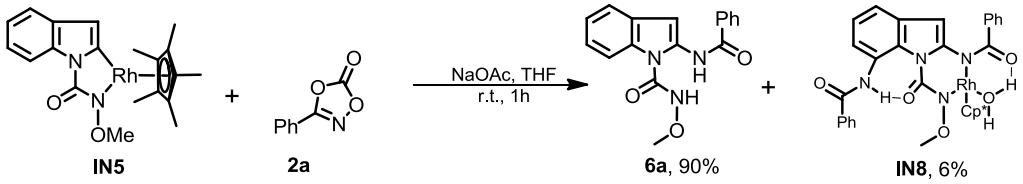
2.4.1 Preparation of the five-membered rhodacycle IN5



A 25 mL oven-dried Schlenk tube equipped with a magnetic stir bar was dried under vacuum. *N*-methoxy-1*H*-indole-1-carboxamide **1a** (230 mg, 1.2 mmol), $[Cp^*RhCl_2]_2$ (309 mg, 0.5 mmol) and NaOAc (164 mg, 2 mmol) were added to the tube, followed by the addition of THF (10 mL) under N_2. The Schlenk tube was sealed and stirred at 70 ^oC for 48 h. After cooling to ambient temperature, the reaction mixture was evaporated to remove the solvent and dissolved in dichloromethane (100 mL), then the mixture was filtered through Celite and evaporated to dryness. The solid obtained was washed with ether to remove excess **1a**. The solvent was then removed under vacuum. Analytically pure **IN5** (423 mg, 96% yield) was obtained by recrystallization using dichloromethane and ethyl acetate.

^1H NMR (500 MHz, CD_2Cl_2): 8.24 (2H, d, *J* = 8.0 Hz), 7.73 (1H, d, *J* = 8.0 Hz), 7.64 (2H, d, *J* = 7.5 Hz), 7.38 (1H, d, *J* = 8.0 Hz), 7.20 (2H, td, *J* = 7.5, 1.0 Hz), 7.16 (2H, td, *J* = 7.5, 1.0 Hz), 7.08 (1H, td, *J* = 8.0, 1.0 Hz), 6.92 (1H, td, *J* = 8.0, 1.0 Hz), 6.85 (1H, s), 6.55 (2H, s), 4.06 (6H, s), 3.82 (3H, s), 1.86 (15H, s), 0.93 (30H, s); ^{13}C NMR (125 MHz, CD_2Cl_2): δ 162.9, 140.6, 138.4, 138.1, 136.1, 124.2, 123.6, 122.0, 121.9, 120.4, 120.3, 113.8, 112.0, 110.3, 99.9, 99.9, 96.5, 96.5, 80.9, 80.8, 63.6, 62.1, 10.9, 8.2.

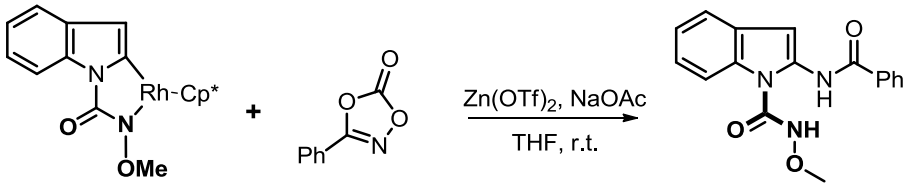
2.4.2 Preparation of the six-membered rhodacycle IN8



A 25 mL oven-dried Schlenk tube equipped with a magnetic stir bar was dried under vacuum. **IN5** (441 mg, 1 mmol), **2a** (245 mg, 1.5 mmol) and NaOAc (164 mg, 2 mmol) were added to the tube, followed by the addition of THF (10 mL) under N_2. The Schlenk tube was sealed and stirred at room temperature for 1 h. Upon completion, the reaction mixture was evaporated to remove the solvent and dissolved in dichloromethane (100 mL), then the mixture was filtered through Celite and evaporated to remove solvent. The solid obtained was washed with ether to remove excess **2a** and **6a**. The solvent was then removed under vacuum. Analytically pure **IN8** (33 mg, 6% yield) was obtained by recrystallization using dichloromethane and ethyl acetate. In8 was subjected for NMR and a trace amount of EtOAc was still remaining.

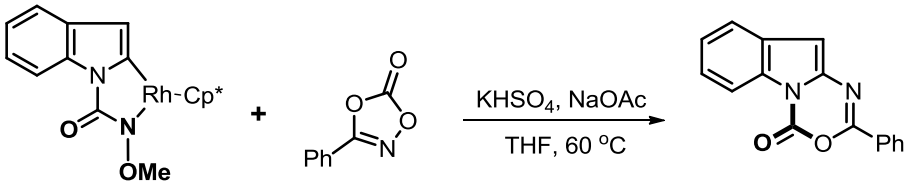
^1H NMR (500 MHz, CD_2Cl_2): 11.12 (1H, s), 8.21 (2H, m), 7.94 (1H, dd, *J* = 8.0, 1.0 Hz), 7.58 (3H, m), 7.30 (3H, m), 7.24 (2H, t, *J* = 7.5 Hz), 7.09 (1H, t, *J* = 7.5 Hz), 7.04 (1H, dd, *J* = 8.0, 1.0 Hz), 5.52 (1H, s), 3.71 (3H, s), 1.42 (15H, s); ^{13}C NMR (125 MHz, CD_2Cl_2): δ 178.5, 171.4 (EtOAc), 165.3, 159.1, 144.8, 138.1, 135.9, 131.9, 130.5, 130.0, 129.0, 128.4, 128.0, 127.9, 125.2, 124.8, 122.2, 117.5, 116.3, 96.7, 95.0, 94.9, 62.4, 60.8 (EtOAc), 21.3 (EtOAc), 14.5 (EtOAc), 8.8.

2.4.3 Reactions of IN5 and 2a leading to 3a, 4a, 5a and 6a



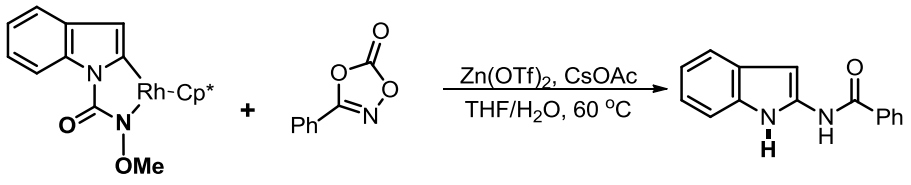
IN5 **2a** **3a**, 92%

A 10 mL reaction tube equipped with a magnetic stir bar was added **IN5** (44 mg, 0.1 mmol), **2a** (25 mg, 0.15 mmol), $Zn(OTf)_2$ (11 mg, 0.03 mmol), NaOAc (8 mg, 0.1 mmol) and THF (2 mL). The reaction was stirred at room temperature for 12 h. Upon completion, the reaction mixture was evaporated to remove the solvent and directly loaded onto silica gel for flash column chromatography (PET/EtOAc) to afford the desired product **3a** in 92% yield.



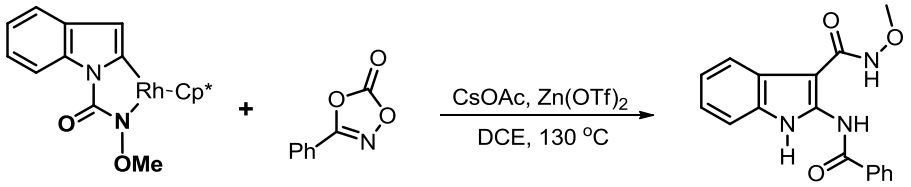
IN5 **2a** **4a**, 83%

A 10 mL oven-dried Schlenk tube equipped with a magnetic stir bar was dried under vacuum. **IN5** (44 mg, 0.1 mmol), **2a** (25 mg, 0.15 mmol), $KHSO_4$ (14 mg, 0.1 mmol) and NaOAc (8 mg, 0.1 mmol) were added to the tube, followed by the addition of anhydrous THF (2 mL). The Schlenk tube was sealed and stirred at 60 °C for 12 h. Upon completion, the reaction mixture was evaporated to remove the solvent and directly loaded onto silica gel for flash column chromatography (PET/EtOAc) to afford the desired product **4a** in 83% yield.



IN5 **2a** **5a**, 87%

A 10 mL Schlenk tube equipped with a magnetic stir bar was added **IN5** (44 mg, 0.1 mmol), **2a** (25 mg, 0.15 mmol), $Zn(OTf)_2$ (11 mg, 0.03 mmol), CsOAc (19 mg, 0.1 mmol), THF (2.0 mL) and H_2O (0.2 mL). The Schlenk tube was sealed and stirred at 60 °C for 12 h. Upon completion, the reaction mixture was evaporated to remove the solvent and directly loaded onto silica gel for flash column chromatography (PET/EtOAc) to afford the desired product **5a** in 87% yield.

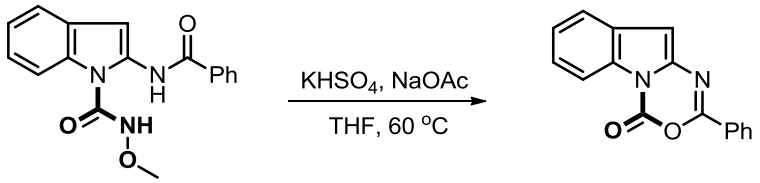


IN5 **2a** **6a**, 56%

A 10 mL oven-dried Schlenk tube equipped with a magnetic stir bar was dried under vacuum. **IN5**

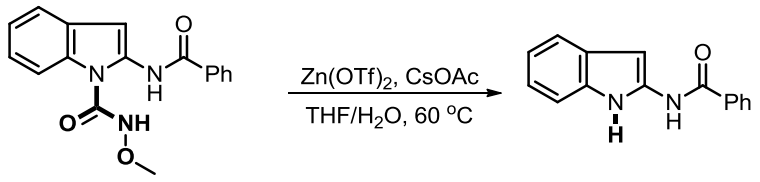
(44 mg, 0.1 mmol), **2a** (25 mg, 0.15 mmol), $Zn(OTf)_2$ (11 mg, 0.03 mmol) and CsOAc (19 mg, 0.1 mmol) were added to the tube, followed by the addition of DCE (2 mL) under N_2. The Schlenk tube was sealed and stirred at 130 ^oC for 12 h. Upon completion, the reaction mixture was evaporated to remove the solvent and directly loaded onto silica gel for flash column chromatography (PET/EtOAc) to afford the desired product **6a** in 56% yield.

2.4.4 Reactions of 3a and 2a leading to 4a, 5a and 6a



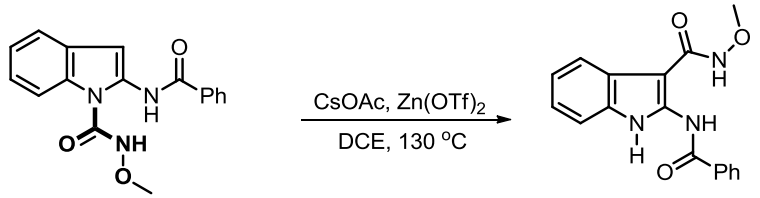
3a **4a**, 84%

A 10 mL oven-dried Schlenk tube equipped with a magnetic stir bar was dried under vacuum. **3a** (31 mg, 0.1 mmol), $KHSO_4$ (14 mg, 0.1 mmol) and NaOAc (8 mg, 0.1 mmol) were added to the tube, followed by the addition of anhydrous THF (2 mL). The Schlenk tube was sealed and stirred at 60 ^oC for 12 h. Upon completion, the reaction mixture was evaporated to remove the solvent and directly loaded onto silica gel for flash column chromatography (PET/EtOAc) to afford the desired product **4a** in 84% yield.



3a **5a**, 89%

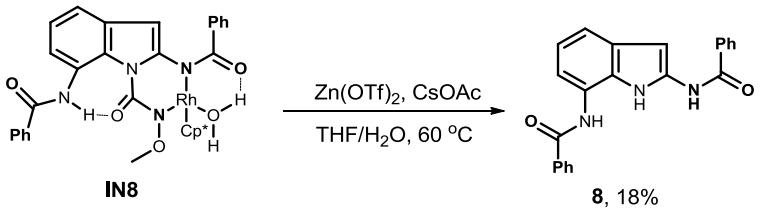
A 10 mL reaction tube equipped with a magnetic stir bar was added **3a** (31 mg, 0.1 mmol), $Zn(OTf)_2$ (11 mg, 0.03 mmol), CsOAc (19 mg, 0.1 mmol), THF (2.0 mL) and H_2O (0.2 mL). The Schlenk tube was sealed and stirred at 60 ^oC for 12 h. Upon completion, the reaction mixture was evaporated to remove the solvent and directly loaded onto silica gel for flash column chromatography (PET/EtOAc) to afford the desired product **5a** in 89% yield.



3a **6a**, 65%

A 10 mL oven-dried Schlenk tube equipped with a magnetic stir bar was dried under vacuum. **3a** (31 mg, 0.1 mmol), $Zn(OTf)_2$ (11 mg, 0.03 mmol) and CsOAc (19 mg, 0.1 mmol) were added to the tube, followed by the addition of DCE (2 mL) under N_2. The Schlenk tube was sealed and stirred at 130 ^oC for 12 h. Upon completion, the reaction mixture was evaporated to remove the solvent and directly loaded onto silica gel for flash column chromatography (PET/EtOAc) to afford the desired product **6a** in 65% yield.

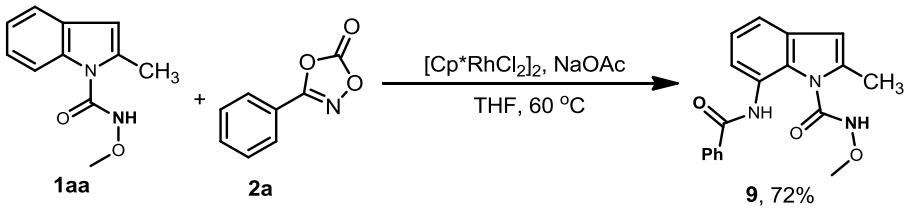
2.4.5 Reaction study using IN8 as starting material



A 10 mL oven-dried Schlenk tube equipped with a magnetic stir bar was dried under vacuum. **IN8** (68 mg, 0.1 mmol), $Zn(OTf)_2$ (11 mg, 0.03 mmol) and CsOAc (19 mg, 0.1 mmol) were added to the tube, followed by the mixture of THF (2.0 mL) and H_2O (0.2 mL) under N_2. The Schlenk tube was sealed and stirred at 60 °C for 12 h. Upon completion, the reaction mixture was evaporated to remove the solvent and directly loaded onto silica gel for flash column chromatography (PET/EtOAc) to afford the desired product **8** in 18% yield.

^{1}H NMR (500 MHz, DMSO): δ 11.11 (1H, s), 10.61 (1H, s), 10.52 (1H, s), 8.05 (2H, d, *J* = 7.0 Hz), 8.01 (2H, d, *J* = 7.0 Hz), 7.64 (2H, m), 7.58 (4H, m), 7.33 (1H, d, *J* = 7.5 Hz), 7.17 (1H, d, *J* = 7.5 Hz), 7.00 (1H, t, *J* = 7.5 Hz), 6.49 (1H, d, *J* = 2.0 Hz); ^{13}C NMR (125 MHz, DMSO): δ 165.5, 164.1, 135.4, 134.6, 133.6, 132.1, 129.5, 128.6, 128.5, 127.5, 125.1, 122.5, 119.4, 116.9, 114.4, 113.0, 106.0, 88.5; HRMS (ESI) *m/z* calcd for $C_{12}H_{18}N_3O_2$ $[M+H]^+$ 356.1394, found 356.1397.

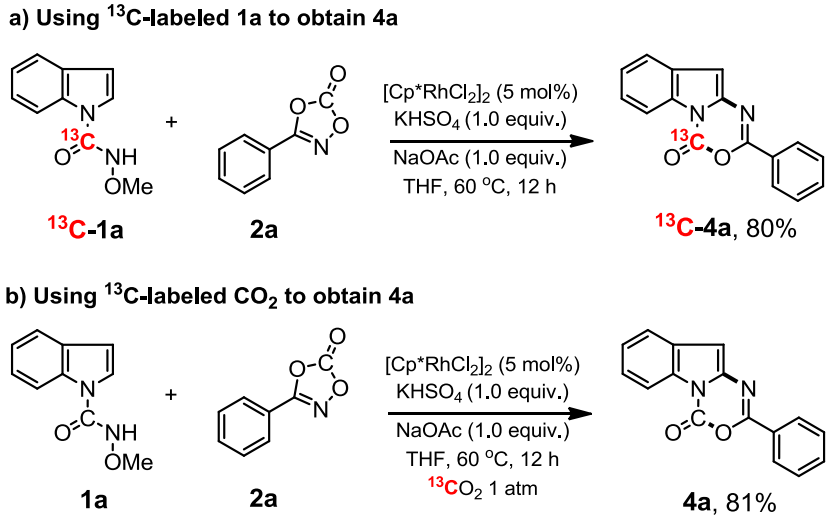
2.4.6 Study of C-H activation on C7 of indole



A reaction tube (10 mL) with magnetic stir bar was charged with **1aa** (41mg, 0.20 mmol), **2a** (39 mg, 0.24 mmol), NaOAc (16 mg, 0.20 mmol), $[Cp^*RhCl_2]_2$ (6 mg, 0.010 mmol) and anhydrous THF (2.0 mL). The reaction tube was sealed and allowed to stir at 60 ℃ for 12 hours. After cooling to room temperature, the reaction mixture was evaporated to remove the solvent and directly loaded onto silica gel for flash column chromatography (PET/EtOAc) to afford the desired product **9** in 72% yield.

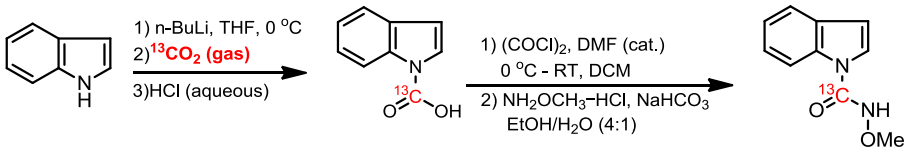
^{1}H NMR (500 MHz, DMSO): δ 11.95 (1H, s), 9.97 (1H, s), 8.00 (2H, d, *J* = 7.0 Hz), 7.59 (1H, t, *J* = 7.5 Hz), 7.53 (2H, t, *J* = 7.5 Hz), 7.40 (1H, d, *J* = 7.5 Hz), 7.19 (1H, d, *J* = 7.5 Hz), 7.13 (1H, t, *J* = 7.5 Hz), 6.41 (1H, s), 3.46 (3H, s), 2.41 (3H, s); ^{13}C NMR (125 MHz, DMSO): δ 165.3, 150.4, 136.4, 134.4, 131.6, 130.8, 130.5, 128.4, 127.6, 122.8, 121.2, 120.5, 117.7, 104.0, 63.1, 13.6; HRMS (ESI) *m/z* calcd for $C_{18}H_{18}N_3O_3$ $[M+H]^+$ 324.1343, found 324.1344.

2.4.7 ^{13}C Stable isotope labeling experiment for carbonyl source of 4



Scheme S1. ^{13}C labeling experiment identifying the carbonyl source in **4a**

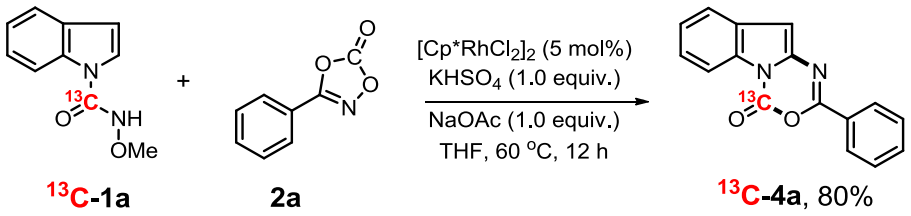
As shown in previous results, the newly installed amides at C2 will automatically couple with the directing group *N*-methoxy amide to smoothly afford the cyclized product **4**. However, the source of the carbonyl group of **4** is uncertain, since there are three possible paths to deliver **4**: (i) The *N*-carboxamide group of **1** could participate in the reaction to obtain **4**; (ii) **2** could also provide the carbonyl source for the assembly of **4**; (iii) CO_2, spontaneously produced from the decomposition of **2** or **1**, could also provide the carbonyl source by coupling with the DG-removed indole for the assembly of **4**. To address this uncertainty, a stable-isotope labeling experiment with ^{13}C was conducted to confirm the source of carbonyl in the newly cyclized product **4a**. $^{13}CO_2$ was used to synthesize the ^{13}C-labeled substrate **1a** (^{13}C-**1a**, Scheme S1a), which reacted with **2a** to achieve the product **4a**. LC-MS and ^{13}C NMR data (see Supporting Information) showed that the resulting **4a** had a ^{13}C-labeled carbonyl group (^{13}C-**4a**). Furthermore, we attempted the reaction of **1a** (Scheme S1b) and **2a** by supplying $^{13}CO_2$ to the system. However, the achieved product was not labeled with ^{13}C which indicated that CO_2 was not involved in this reaction. These results confirmed that the DG (*N*-carboxamide) in **1a** directly provides the carbonyl group for the cyclization of **2a** to produce **4a** (Scheme S1).



A 250 mL three-necked flask with a stir-bar was charged with indole (4.68g, 40mmol), which was then evacuated and backfilled with argon for three times. THF (120 mL) was added and the solution was cooled to 0 °C. *n*-BuLi (19.2 mL, 2.5 M in hexane) was then added over 30 min to the solution and the reaction was kept at 0 °C for another 30 min. Next, **$^{13}CO_2$** was bubbled to the reaction solution for 1 h at 0 °C and the solution was then quenched with H_2O (20 mL). The solution was transferred to a flask and evaporated to about 30 mL under vacuum. Aqueous HCl solution (6 M) was added to adjust the pH to 3 and the solution was extracted with ethyl acetate (60 mL × 3). The combined organic layer was dried over anhydrous Na_2SO_4 and concentrated to

afford the acid product 4.64 g (72% yield).

To a 250 mL flask charged with acid (1.61 g, 10 mmol) was added anhydrous DCM (20 mL) and DMF (0.1 mL), and cooled to 0 °C. $(COCl)_2$ (1.72 mL, 20 mmol) was added dropwise over 30 min, the solution was then warmed to room temperature and stirred for 2 h. Then the solvent was concentrated to afford the crude acyl chloride to be used for next step. To a 100 mL flask charged with methoxylamine hydrochloride (1.67 g, 20 mmol) was added EtOH (40 mL) and H_2O (10 mL), $NaHCO_3$ (3.36 g, 40 mmol) was then added and the solution was kept at 0 °C. Afterwards, the acyl chloride was added dropwise to the solution at 0 °C over 30 min, then the solution was warmed to room temperature and kept for 5 h. Then the solution was filtered and the filtrate was concentrated. The residue was subjected to flash column chromatography on silica gel using ethyl acetate/petroleum ether (v/v, 1:5) as eluent to give labeled *N*-(methoxy)-1*H*-indole-1-carboxamide **^{13}C-1a** as a pale yellow solid (0.9 g, 47% yield for two steps).[1]



N-methoxy amide substituted indole **^{13}C-1a** (0.20 mmol), 1,4,2-dioxazol-5-one **2a** (0.24 mmol), $KHSO_4$ (27 mg, 0.20 mmol), NaOAc (16 mg, 0.20 mmol) and $[Cp^*RhCl_2]_2$ (6 mg, 0.010 mmol) were placed into a 10 mL Schlenk tube equipped with a septum under N_2 atmosphere. THF (2.0 mL) was introduced via cannula. The reaction mixture was stirred at 60 ℃ for 12 h. After cooling to room temperature, the reaction mixture was evaporated to remove the solvent and directly loaded onto silica gel for flash column chromatography (n-hexane/EtOAc) to get the product **^{13}C-4a**.

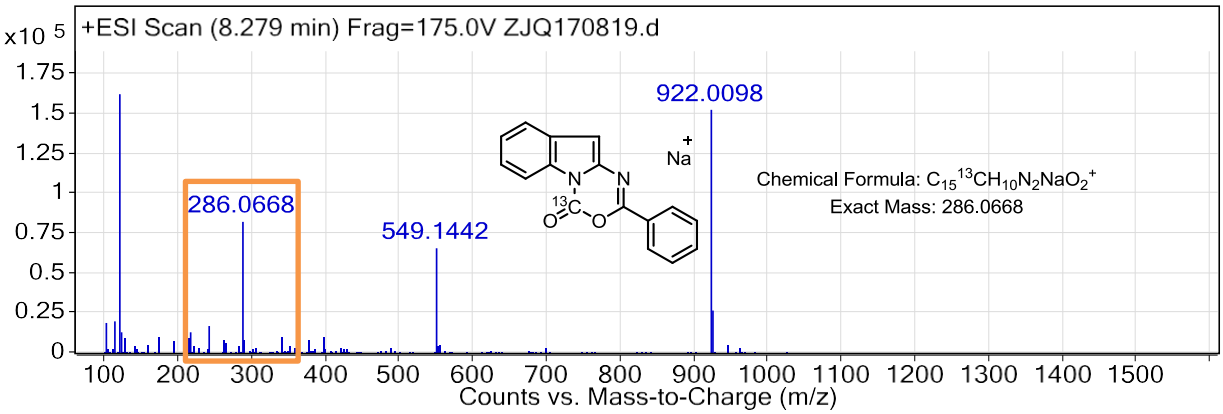


Figure S1. LC-Mass result of **^{13}C-4a** using **^{13}C-1a** as starting marerial. HR-MS (ESI) *m/z* calcd for $C_{15}{}^{13}CH_{10}N_2O_2Na$ $[M+Na]^+$ 286.0668, found 286.0668.

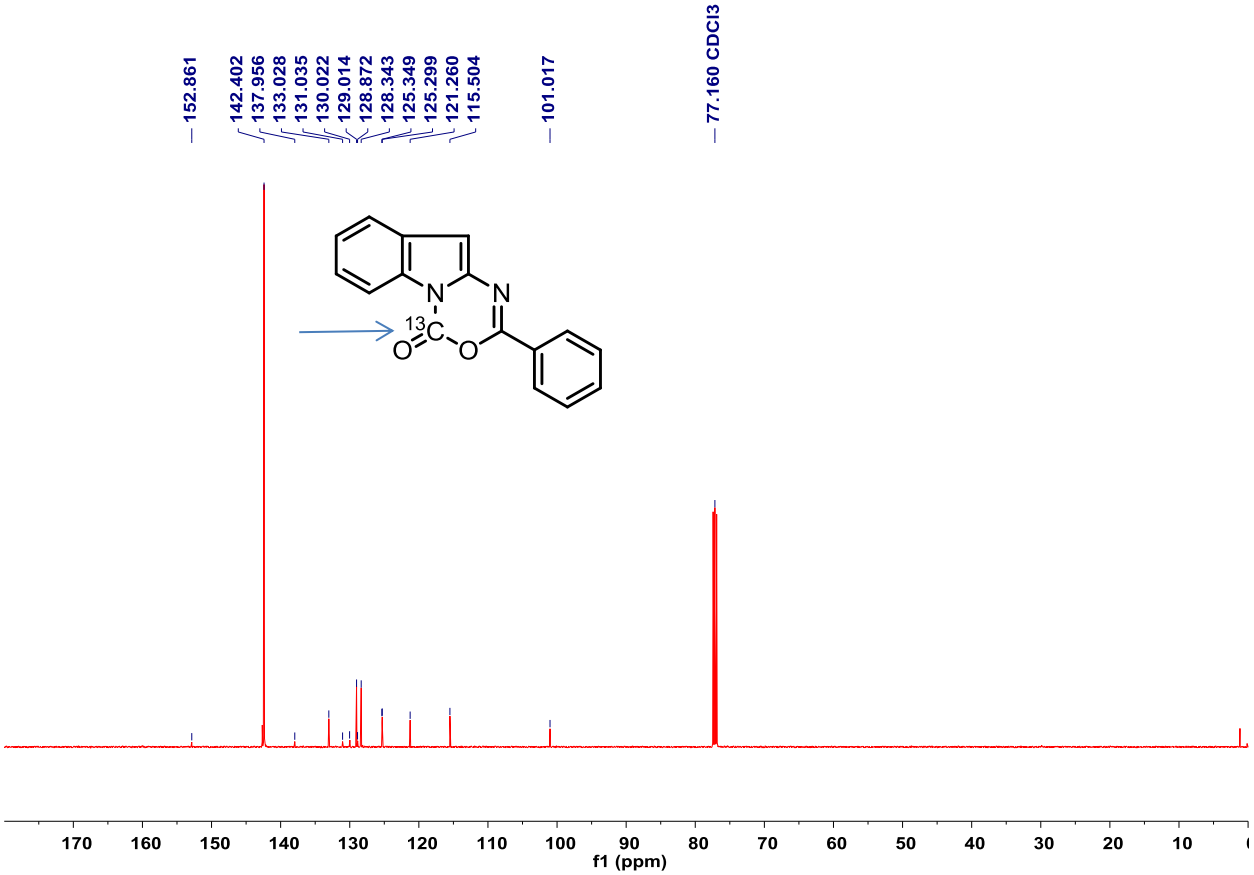
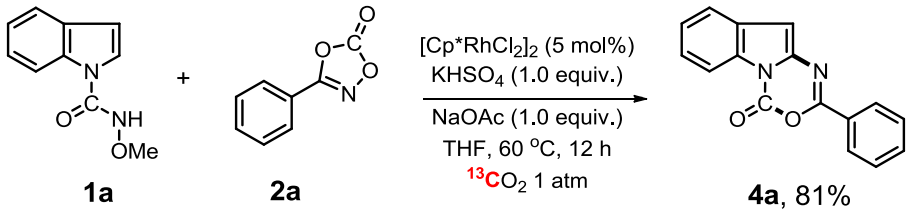


Figure S2. ^{13}C NMR spectra of product **^{13}C-4a** using **^{13}C-1a** as starting marerial.



N-methoxy amide substituted indole **1a** (0.20 mmol), 1,4,2-dioxazol-5-one **2a** (0.24 mmol), $KHSO_4$ (27 mg, 0.20 mmol), NaOAc (16 mg, 0.20 mmol) and $[Cp^*RhCl_2]_2$ (6 mg, 0.010 mmol) were placed into a 10 mL Schlenk tube equipped with a septum under **$^{13}CO_2$** atmosphere. THF (2.0 mL) was introduced via cannula. The reaction mixture was stirred at 60 ℃ for 12 h. After cooling to room temperature, the reaction mixture was evaporated to remove the solvent and directly loaded onto silica gel for flash column chromatography (n-hexane/EtOAc) to get the product **4a**.

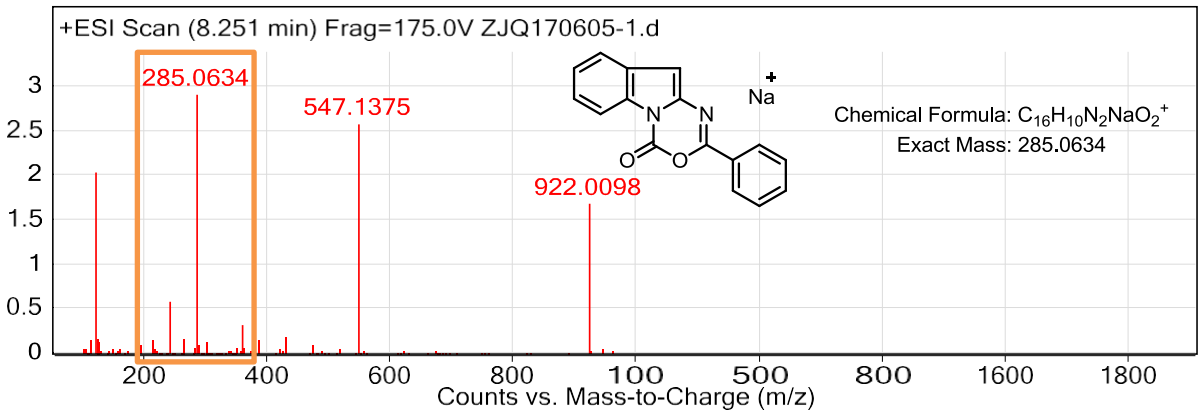


Figure S3. LC-Mass result of product **4a** under $^{13}CO_2$ atmosphere. HR-MS (ESI) *m/z* calcd for $C_{16}H_{10}N_2O_2Na$ $[M+Na]^+$ 285.0634, found 285.0634.

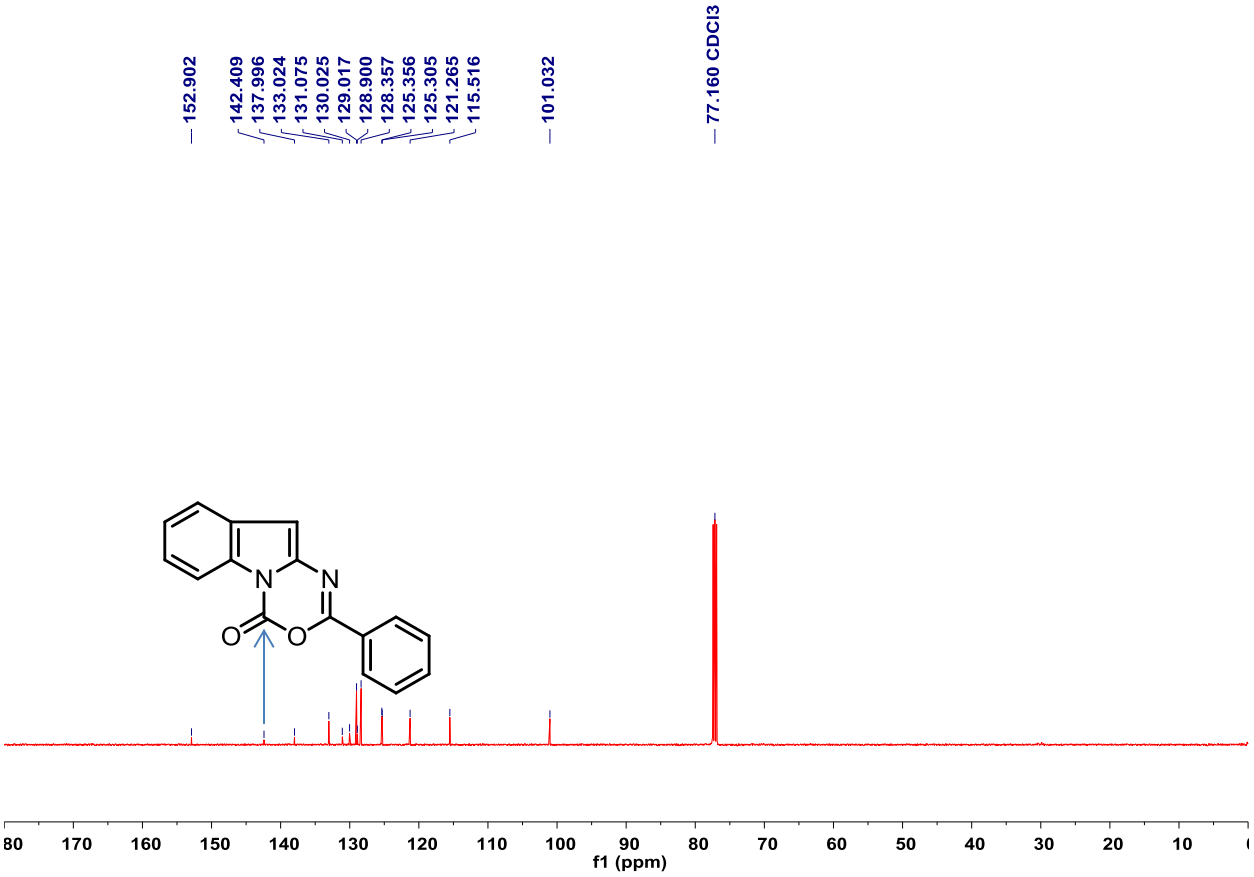
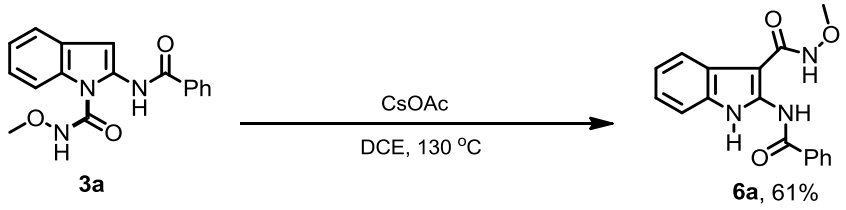


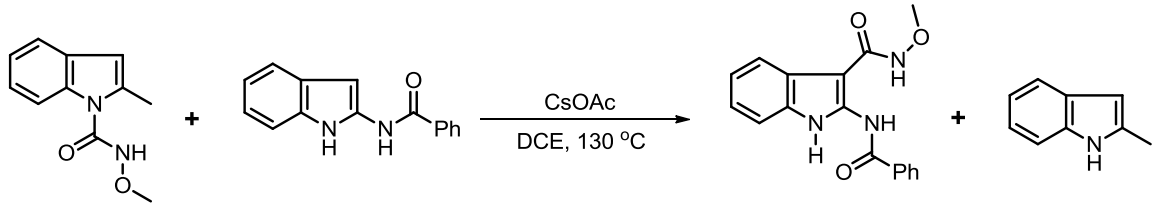
Figure S4. ^{13}C NMR spectra of product **4a** under $^{13}CO_2$ atmosphere.

2.4.8 Study on FG effect on DG elimination and migration



3a **6a**, 61%

A 10 mL oven-dried Schlenk tube equipped with a magnetic stir bar was dried under vacuum. **3a** (31 mg, 0.1 mmol), CsOAc (19 mg, 0.1 mmol) were added to the tube, followed by the addition of DCE (2 mL) under N_2. The Schlenk tube was sealed and stirred at 130 °C for 12 h. Upon completion, the reaction mixture was evaporated to remove the solvent and directly loaded onto silica gel for flash column chromatography (PET/EtOAc) to afford the desired product **6a** in 61% yield.

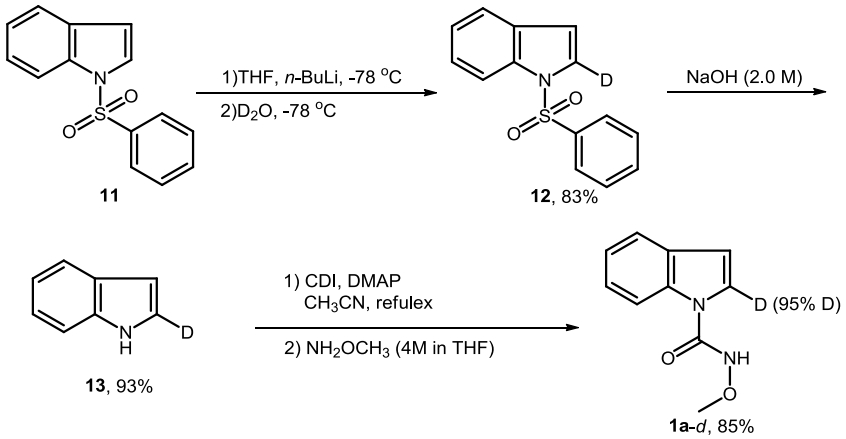


1aa **5a** **6a**, 53% **10**, 75%

A 10 mL oven-dried Schlenk tube equipped with a magnetic stir bar was dried under vacuum. **1aa** (20 mg, 0.1 mmol), **5a** (24 mg, 0.1 mmol), CsOAc (19 mg, 0.1 mmol) were added to the tube, followed by the addition of DCE (2 mL) under N_2. The Schlenk tube was sealed and stirred at 130 °C for 12 h. Upon completion, the reaction mixture was evaporated to remove the solvent and directly loaded onto silica gel for flash column chromatography (PET/EtOAc) to afford the products **6a** in 53% yield and **10** in 75% yield.

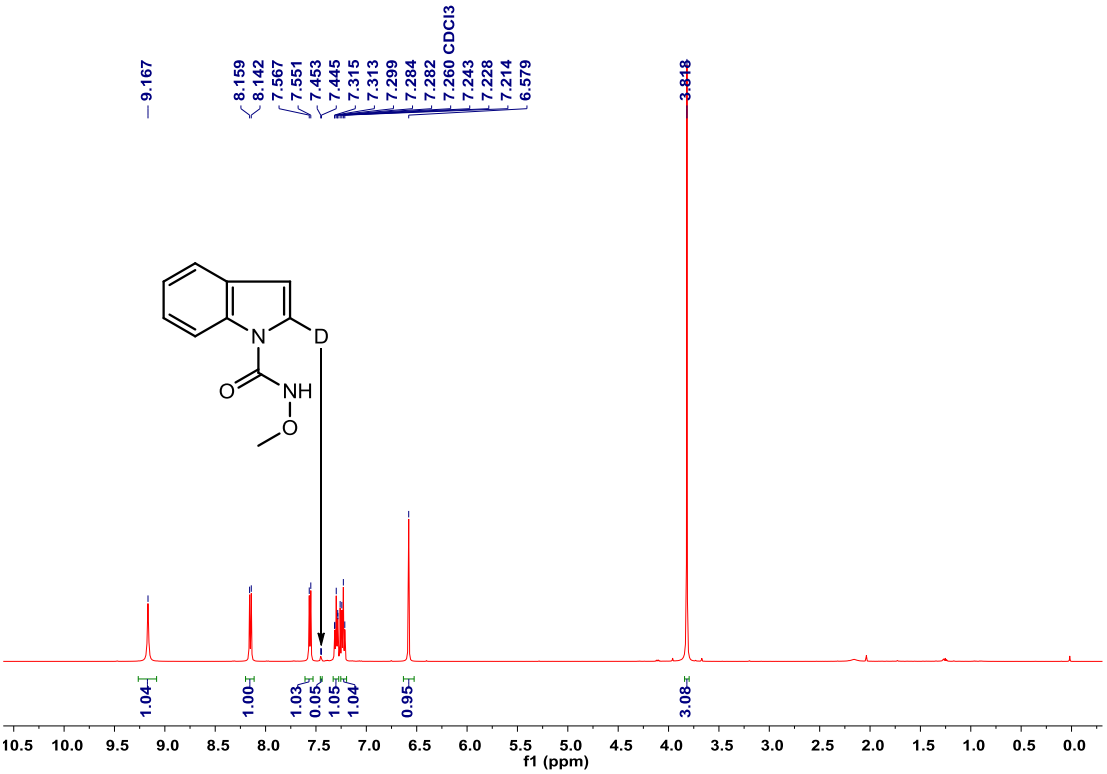
2.4.9 KIE experiments

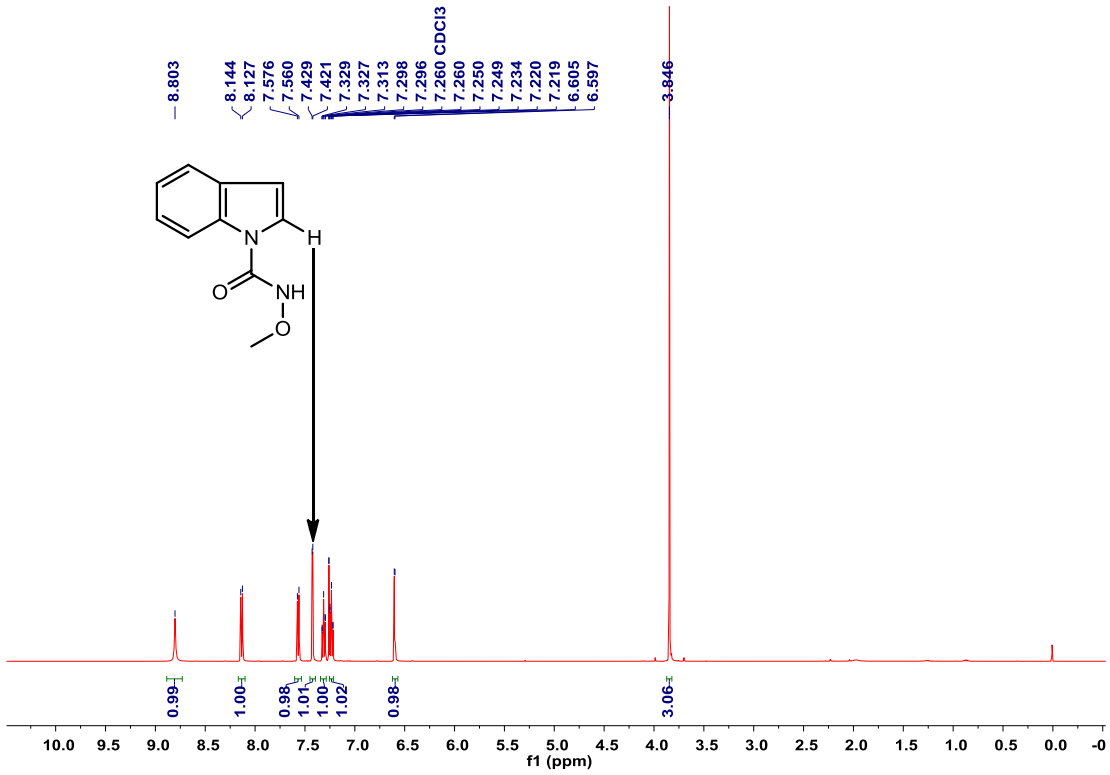
1) Reaction procedure for the preparation of Deuterium Labeled Compounds.[3]



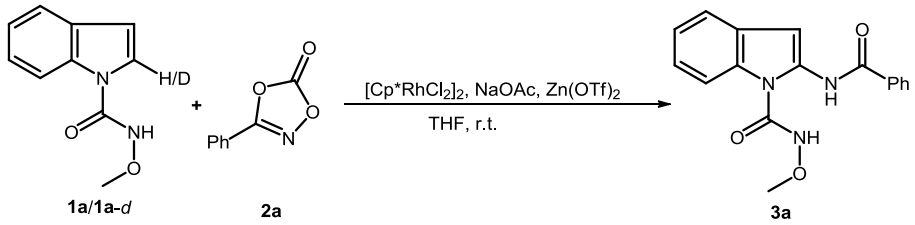
11 **12**, 83% **13**, 93% **1a**-*d*, 85%

Compound **1a**-*d*: a red solid. 85% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.17 (1H, s), 8.15 (1H, d, J = 8.5 Hz), 7.56 (1H, t, J = 8.0 Hz), **7.45 (0.05H, d, J = 4.0 Hz)**, 7.30 (1H, td, J = 8.0, 1.0 Hz), 7.23 (1H, t, J = 7.5 Hz), 6.58 (1H, s), 3.82 (3H, s).


9.167
8.159
8.142
7.567
7.551
7.453
7.445
7.315
7.313
7.299
7.284
7.282
7.260 CDCl3
7.243
7.228
7.214
6.579
3.818
D
N
O
NH
O
1.04
1.00
1.03
0.05
1.05
1.04
0.95
3.08
f1 (ppm)


8.803
8.144
8.127
7.576
7.560
7.429
7.421
7.329
7.327
7.313
7.298
7.296
7.260 CDCl3
7.260
7.250
7.249
7.234
7.220
7.219
6.605
6.597
3.846
H
N
O
NH
O
0.99
1.00
0.98
1.01
1.00
1.02
0.98
3.06
f1 (ppm)

2) kinetic isotope effect experiment



A reaction tube (10 mL) with magnetic stir bar was charged with **1a** or **1a**-*d* (96mg, 0.5 mmol), **2a** (98mg, 0.6 mmol), NaOAc (41 mg, 0.5 mmol), $[Cp^*RhCl_2]_2$ (15 mg, 0.025 mmol), $Zn(OTf)_2$ (54 mg, 0.15 mmol) and THF (3.0 mL). The reaction was allowed to stir at room temperature, the yield of **3a** was detected by HPLC after 10, 20, 35, 60 and 120 min.

Table S6. Yield of **3a** using **1a** or **1a**-*d* as starting material.

entry	Time (min)	yield (%)[a]	
		3a[b]	**3a**[c]
1	10	15	14
2	20	26	19
3	35	35	30
4	60	55	43
9	120	68	61

[a]HPLC yield. [b]1a using as starting material. [c]1a-d using as starting material.

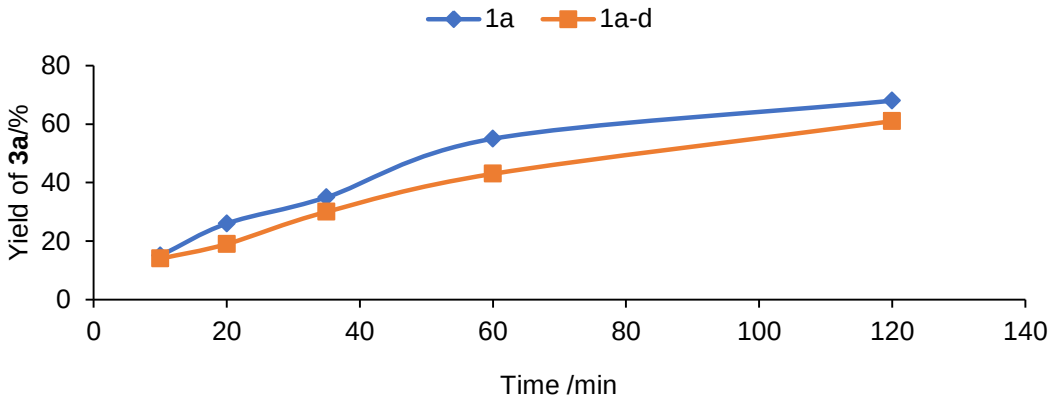


Figure S5. Rate profile for production of **3a** using **1a** or **1a**-*d* as starting material.

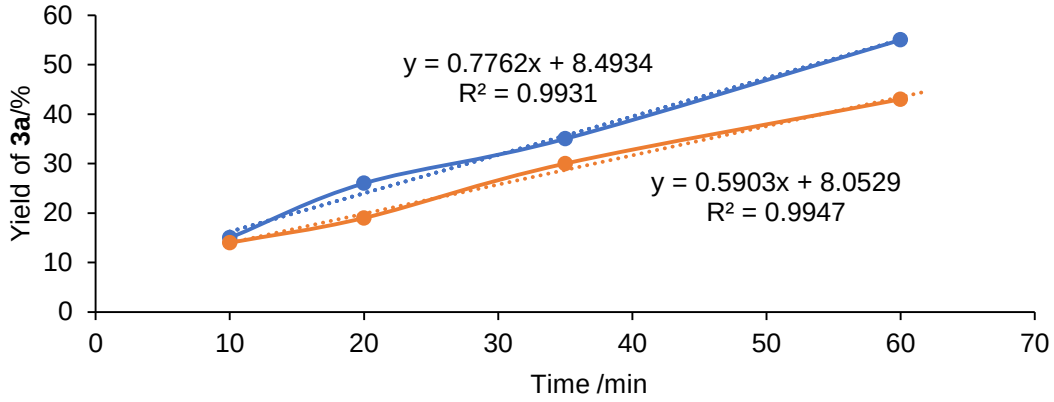


Figure S6. Rate profile at initial stage within 60 min.
KIE = K(**1a**)/K(**1a**-*d*) = 1.31

2.5 X-ray crystallographic data of IN5 and IN8

CIF files of **IN5** and **IN8** can be obtained from the Cambridge Crystallographic Data Centre using CCDC 1917713 and 1917709, respectively. Copies of the data can be obtained, free of charge, on application to the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK [fax: +44(1223)336033; e-mail: deposit@ccdc.cam.ac.uk].

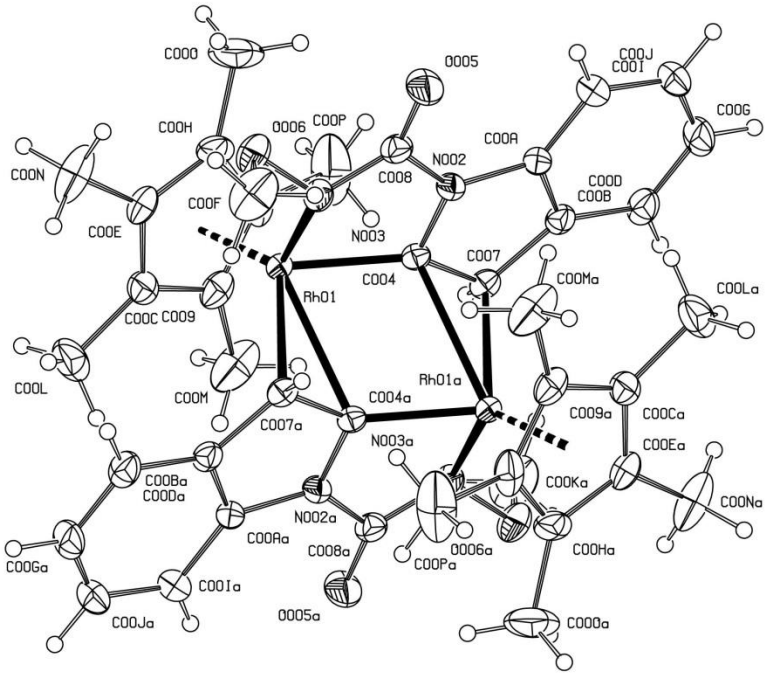


Figure S7. Molecular structure and atom numbering scheme for **IN5**.

Table S7. Crystal data and structure refinement for **IN5**.

Empirical formula	$C_{20}H_{23}N_2O_2Rh$
Formula weight	426.31
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	10.0187(4)
b/Å	15.9458(6)
c/Å	11.4017(4)
α/°	90
β/°	90.898(3)
γ/°	90
Volume/Å^3	1821.27(12)
Z	22
ρ_{calc}g/cm^3	1.555
μ/mm^{-1}	0.953
F(000)	872.0
Crystal size/mm^3	0.7 × 0.35 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.236 to 58.704
Index ranges	$-12 \leq h \leq 13$, $-21 \leq k \leq 20$, $-15 \leq l \leq 15$
Reflections collected	19482
Independent reflections	4483 [R_{int} = 0.0393, R_{sigma} = 0.0347]
Data/restraints/parameters	4483/0/232
Goodness-of-fit on F^2	1.111
Final R indexes [I>=2σ (I)]	R_1 = 0.0328, wR_2 = 0.0781
Final R indexes [all data]	R_1 = 0.0484, wR_2 = 0.0877
Largest diff. peak/hole / e Å^{-3}	0.65/-0.62

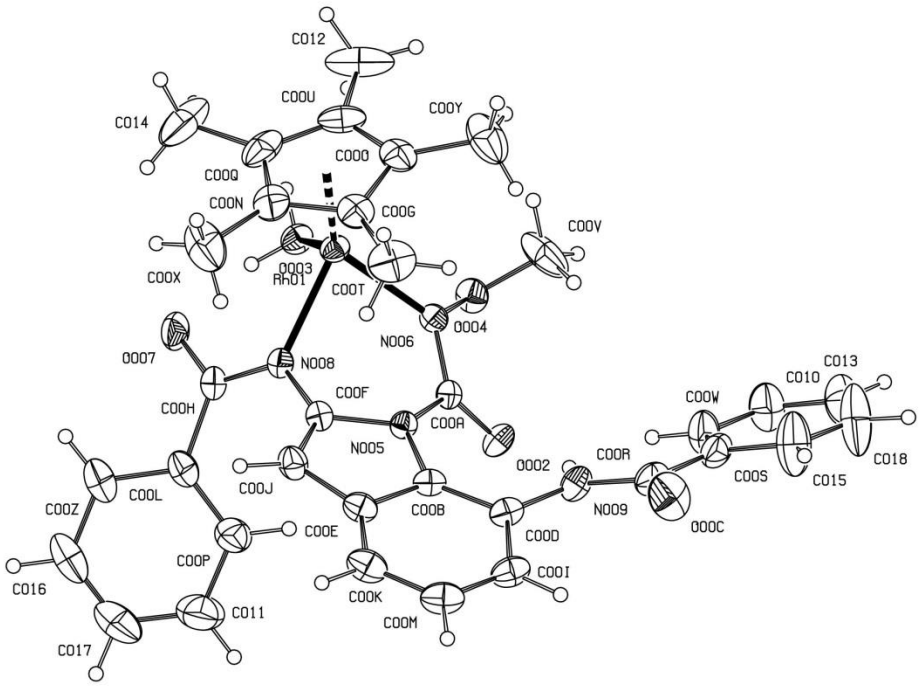
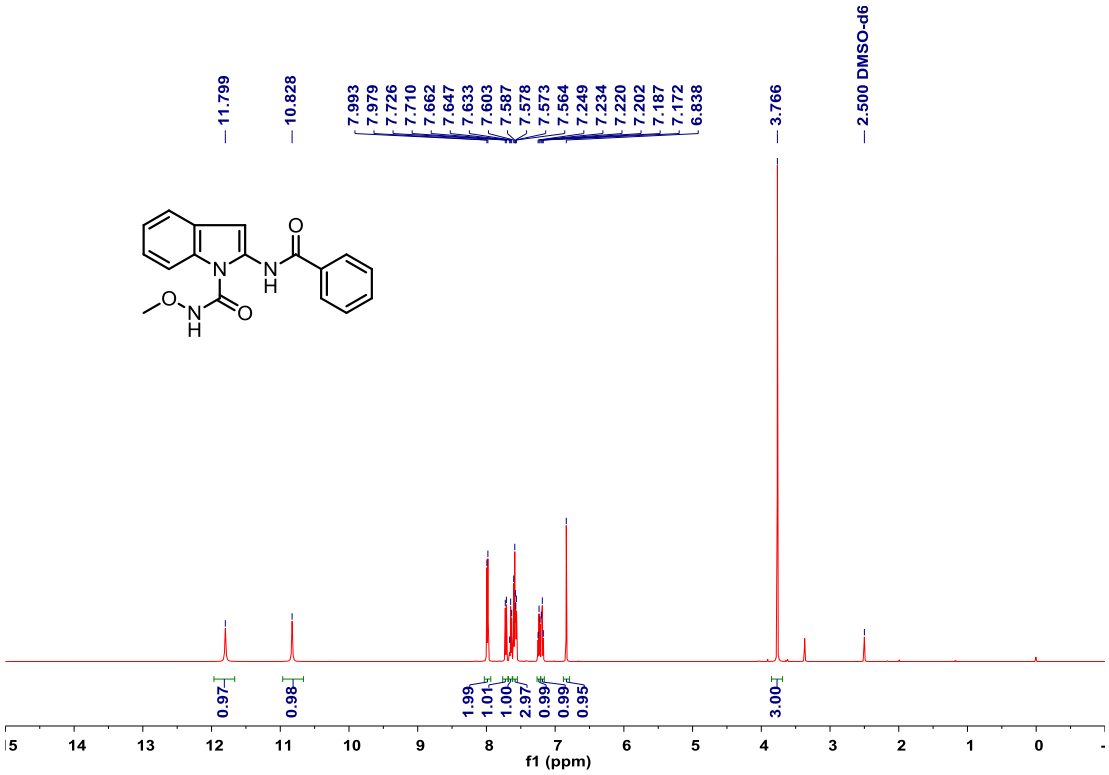


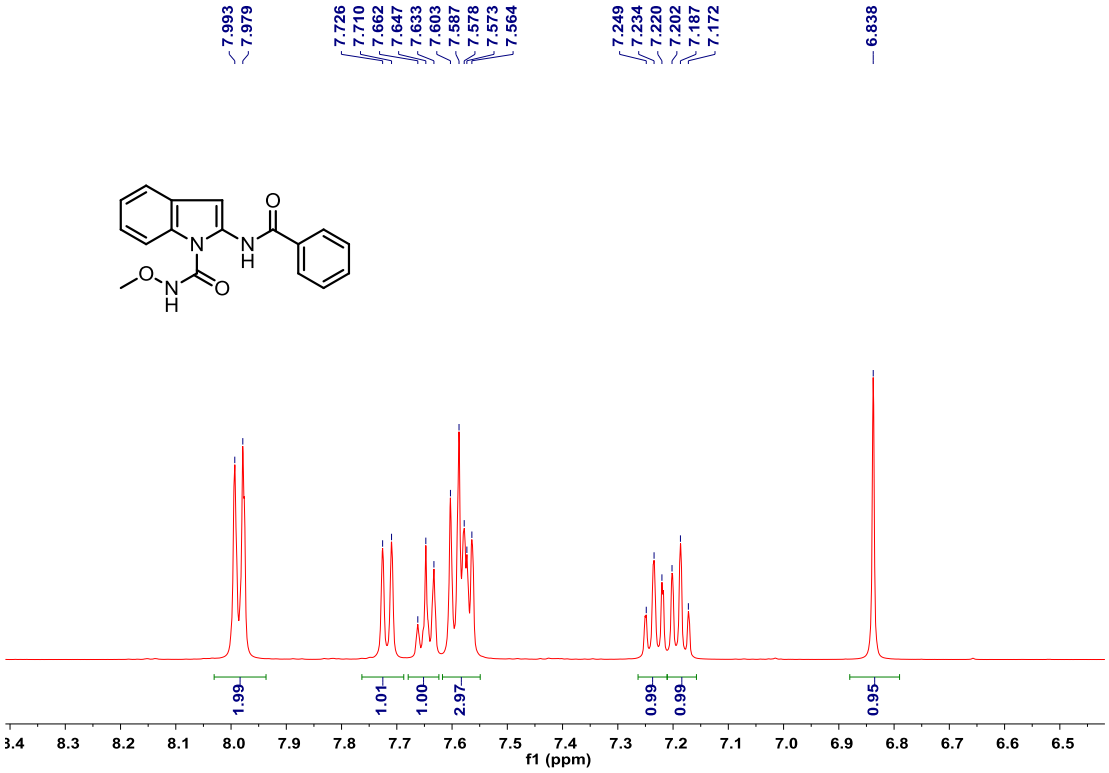
Figure S8. Molecular structure and atom numbering scheme for **IN8**.

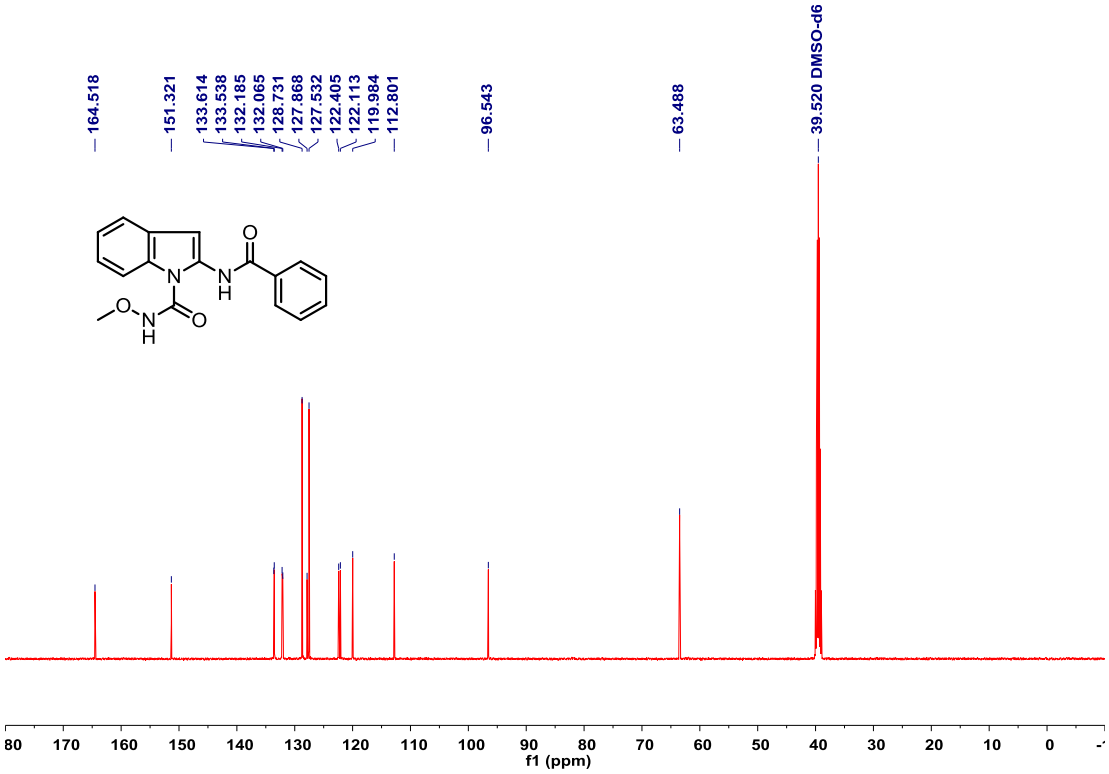
Table S8. Crystal data and structure refinement for **IN8**.

Empirical formula	$C_{34}H_{35}N_4O_5Rh$
Formula weight	682.57
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	10.2360(2)
b/Å	12.9813(3)
c/Å	14.3231(3)
α/°	94.366(2)
β/°	90.239(2)
γ/°	103.146(2)
Volume/Å^3	1847.50(7)
Z	22
ρ_{calc}g/cm^3	2.886
μ/mm^{-1}	4.828
F(000)	1474.0
Crystal size/mm^3	0.6 × 0.2 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.274 to 52.742
Index ranges	-12 ≤ h ≤ 12, -16 ≤ k ≤ 16, -17 ≤ l ≤ 17
Reflections collected	74811
Independent reflections	7533 [R_{int} = 0.0422, R_{sigma} = 0.0210]
Data/restraints/parameters	7533/0/404
Goodness-of-fit on F^2	1.046
Final R indexes [I>=2σ (I)]	R_1 = 0.0298, wR_2 = 0.0750
Final R indexes [all data]	R_1 = 0.0364, wR_2 = 0.0798
Largest diff. peak/hole / e Å^{-3}	0.63/-0.50

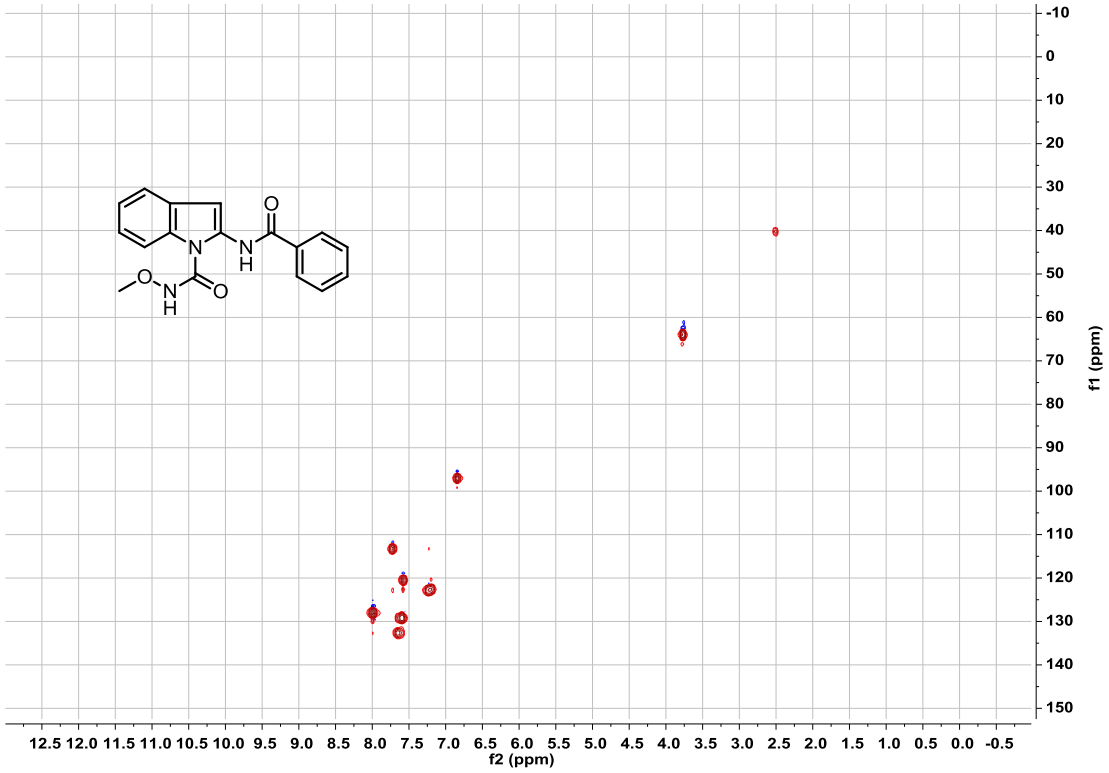
2.6 2D NMR spectra of 3a and 6a



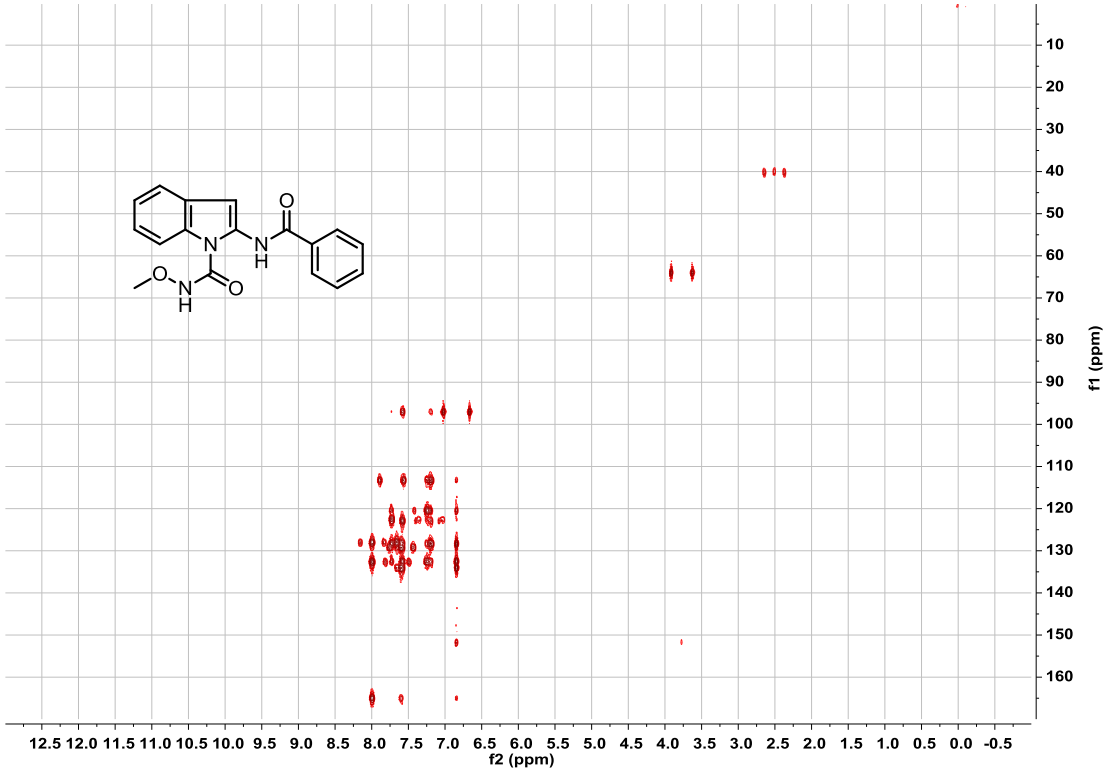


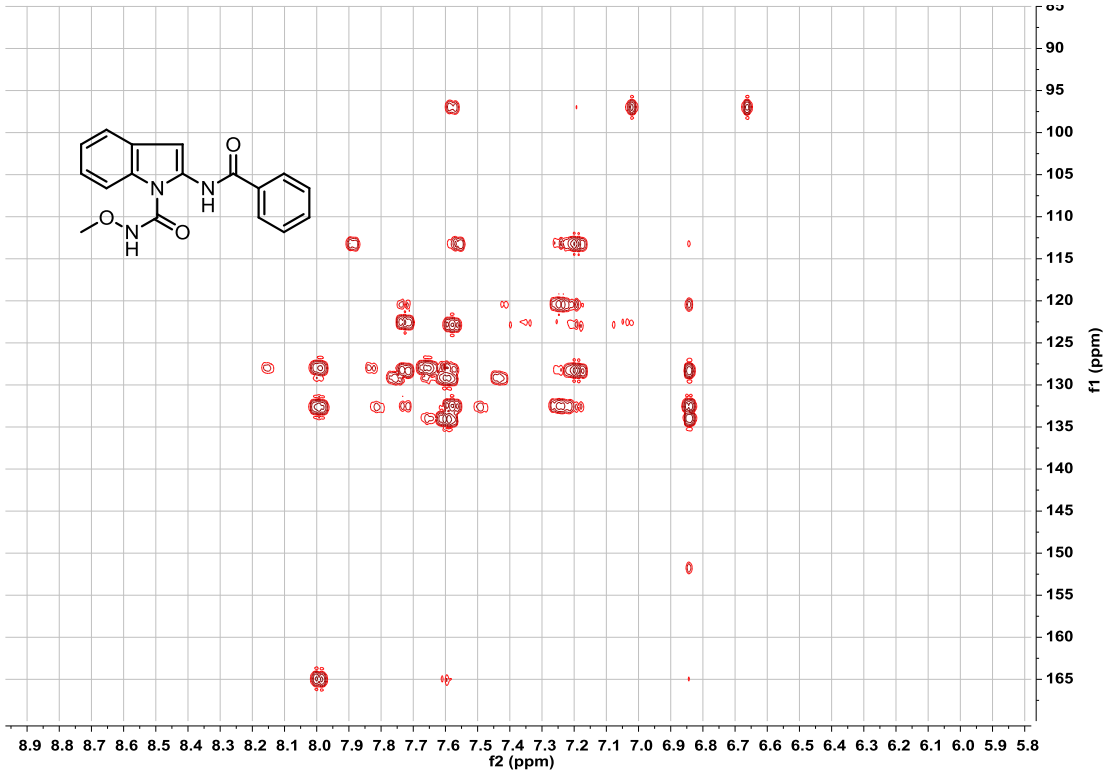

164.518
151.321
133.614
133.538
132.185
132.065
128.731
127.868
127.532
122.405
122.113
119.984
112.801
96.543
63.488
39.520 DMSO-d6
f1 (ppm)

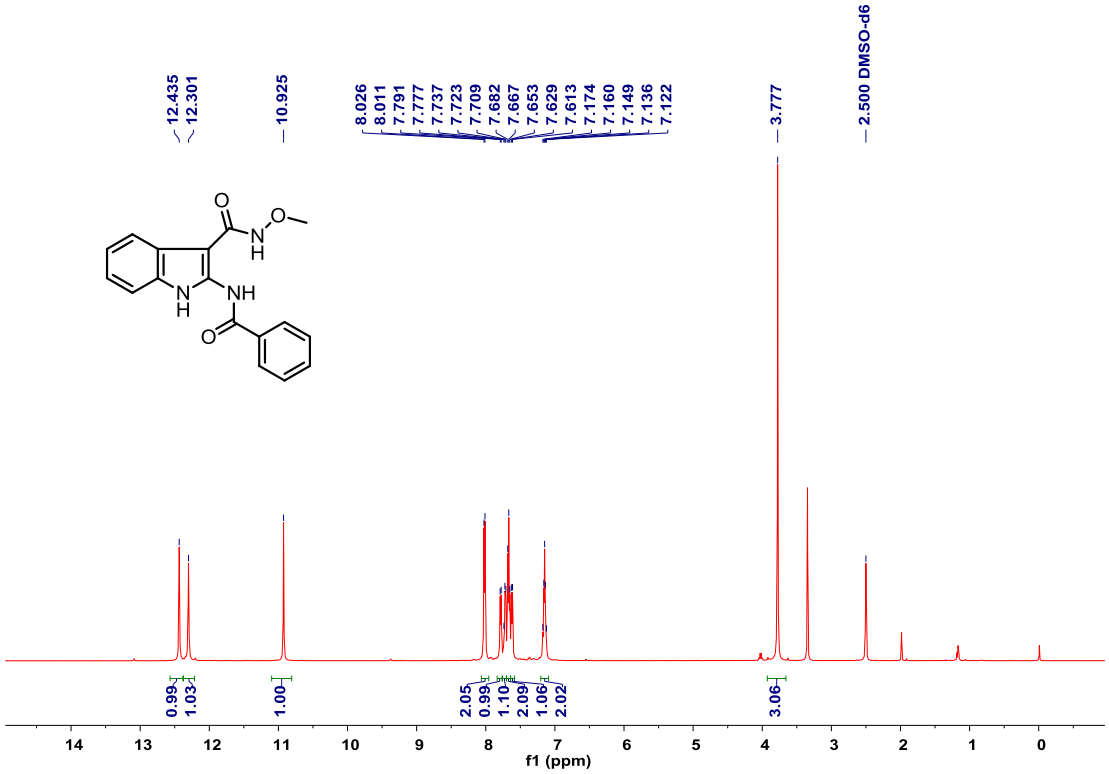
HSQC


f1 (ppm)
f2 (ppm)

HMBC



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10.925
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8.011
7.791
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7.653
7.629
7.613
7.174
7.160
7.149
7.136
7.122
3.777
2.500 DMSO-d6
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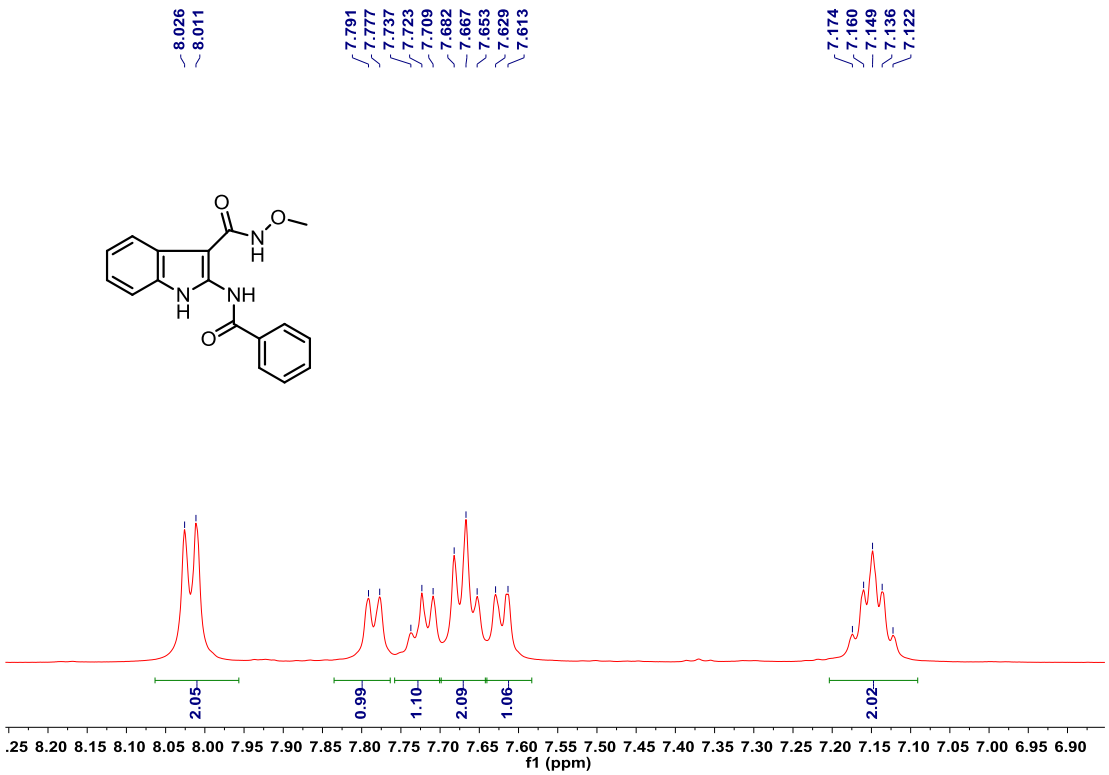
1.03
1.00
2.05
0.99
1.10
2.09
1.06
2.02
3.06
f1 (ppm)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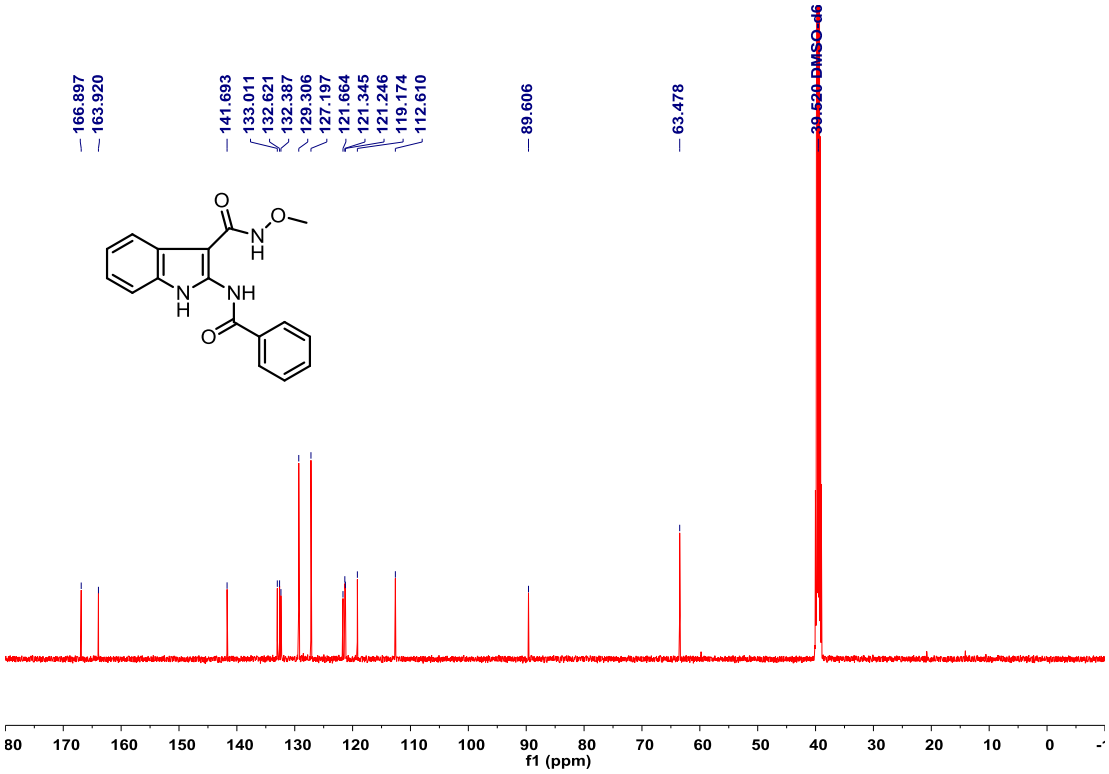
f1 (ppm)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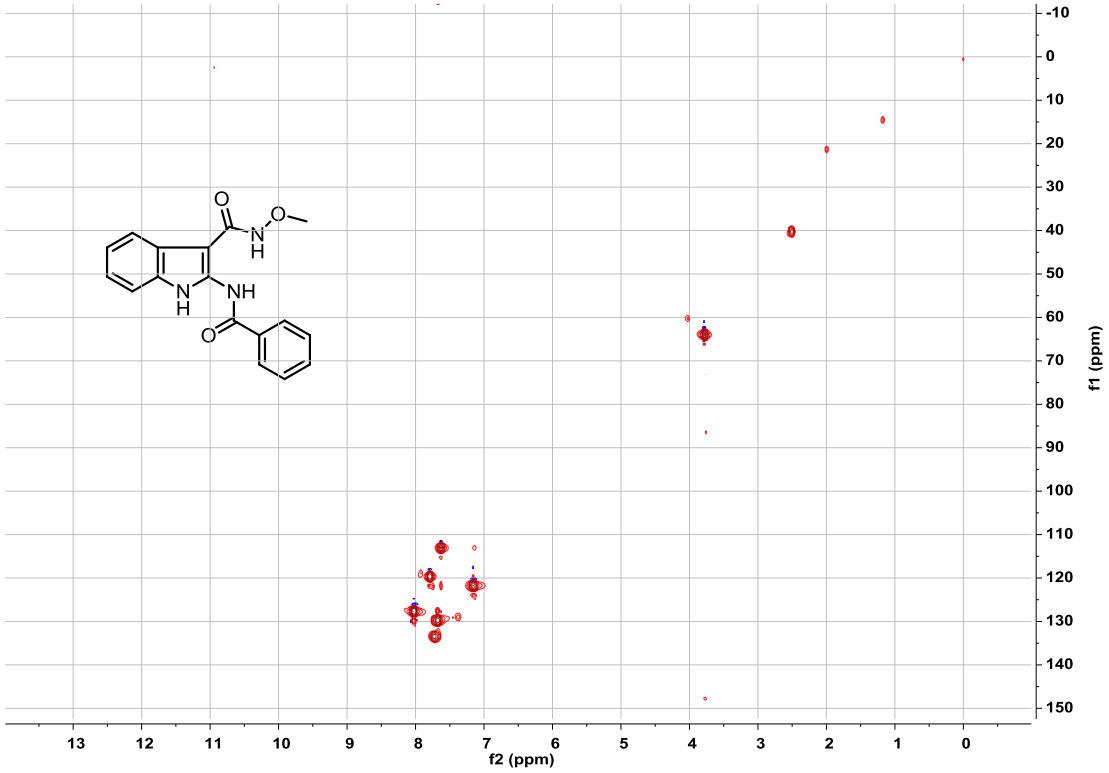
f2 (ppm)
f1 (ppm)

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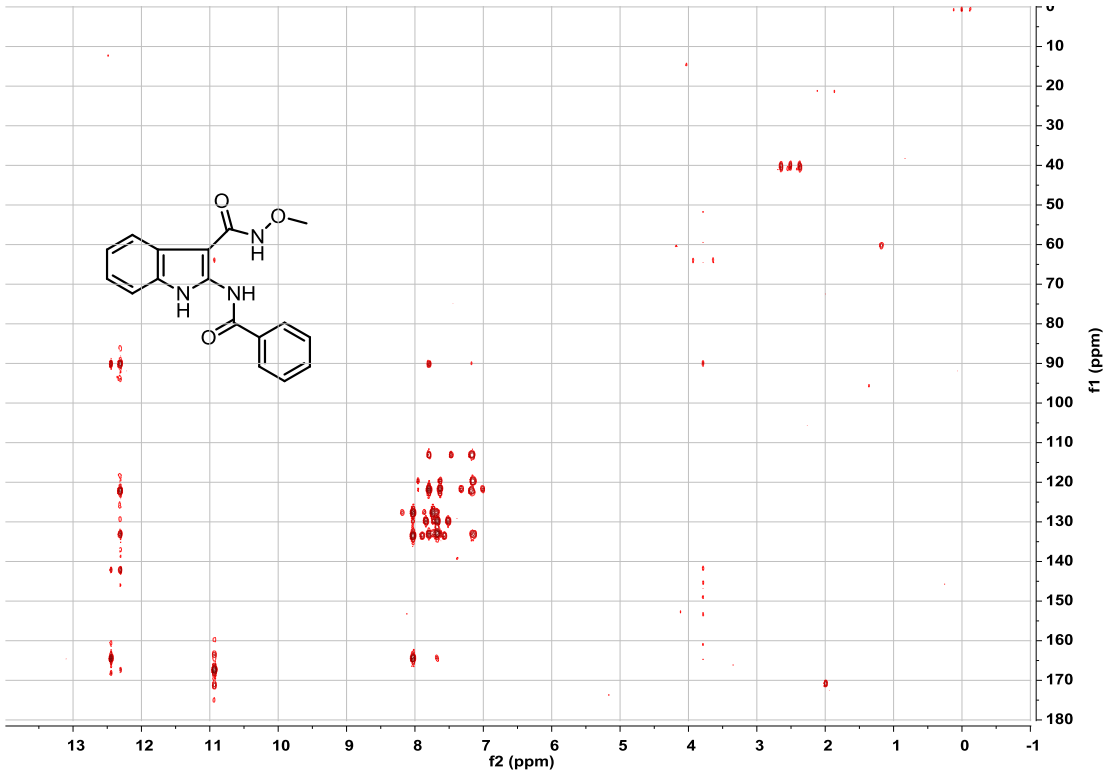

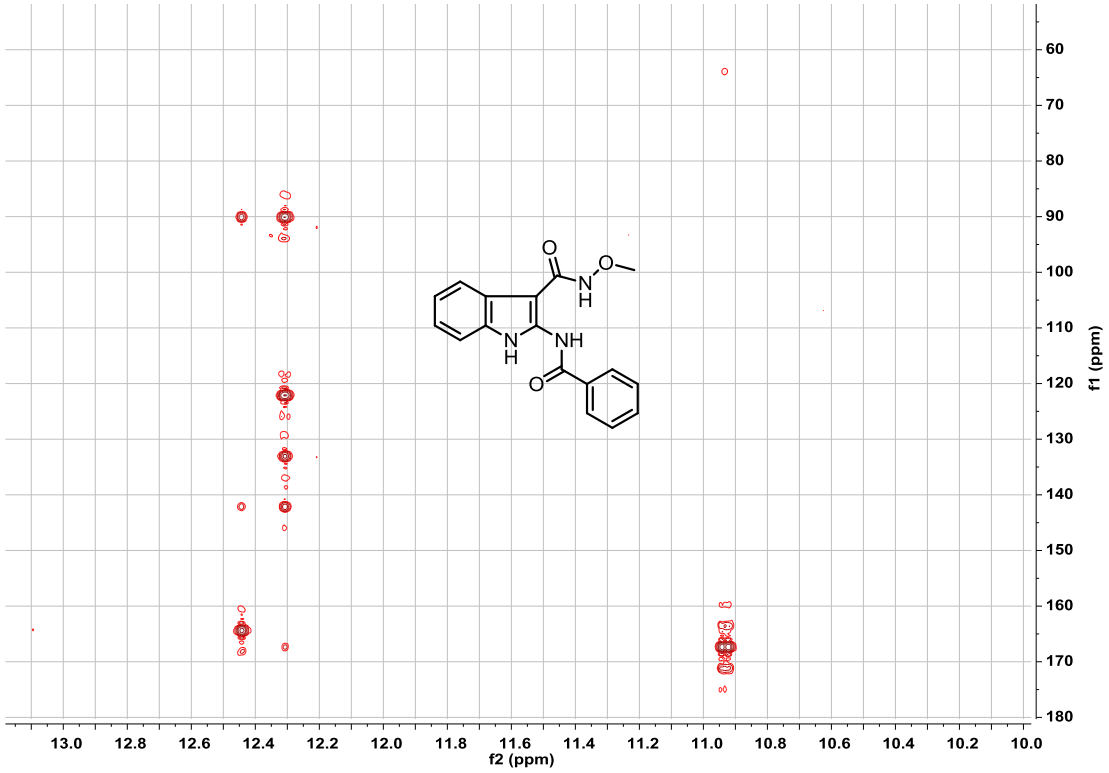

3. Computational Section

All species along free energy profiles were fully optimized by density functional theory (DFT) calculations at the M06 level.[4] The Rh and Cl atoms were described by the Lanl2dz basis set and effective core potential.[5] The 6-31G(d,p) basis set[6] was applied for the C, H, O and N atoms. In addition, polarization functions of Rh(ζ_f) = 1.350 and Cl(ζ_d) = 0.514 were added.[7] Frequencies were calculated at the same level of theory to obtain the thermodynamic corrections and to confirm whether the structures were minima (no imaginary frequency) or transition states (only one imaginary frequency). Intrinsic reaction coordinate (IRC) calculations[8] were conducted to confirm all transition-state structures that connected the proposed reactants and products. All calculations were conducted by using the Gaussian 09 suite of computational programs.[9] The solvation effect was examined by performing single-point self-consistent reaction field (SCRF) calculations based on the solvation model density (SMD) solvation model for gas-phase optimized structures.[10] Dichlororthane was used as the solvent based on experimental reaction conditions. The relative free energies corrected by solvation effects are used in further discussion.

Our experiments showed that no reaction occurred when only a catalytic amount of $[Cp^*RhCl_2]_2$ was used. Therefore, the presence of CsOAc as an additive is crucial for efficient transformation. We first consider the catalytic active species in these reactions. Calculations showed that the formation of $[Cp^*Rh(OAc)_2]$ from $[Cp^*RhCl_2]$ and CsOAc is exergonic by 1.6 kcal/mol; thus, we assumed that all three Rh(III) monomers, $[Cp^*RhCl_2]$, $[Cp^*RhCl(OAc)]$ and $[Cp^*Rh(OAc)_2]$, could be involved in the system. Calculations were performed to evaluate the reactivity of these monomers in promoting the processes of both **1a** and **2a** decompositions and benzamide N-H bond deprotonation/C-H bond activation. As shown in Figure S9, the decomposition of a five-membered ring of **2a** of the three possible Rh(III) complexes (**TS-1**) is difficult and the activation energies for CO_2 exclusion were calculated to be 56.8, 54.9 and 54.3 kcal/mol, respectively. High activation barriers indicated that the reaction cannot occur under the given reaction conditions.

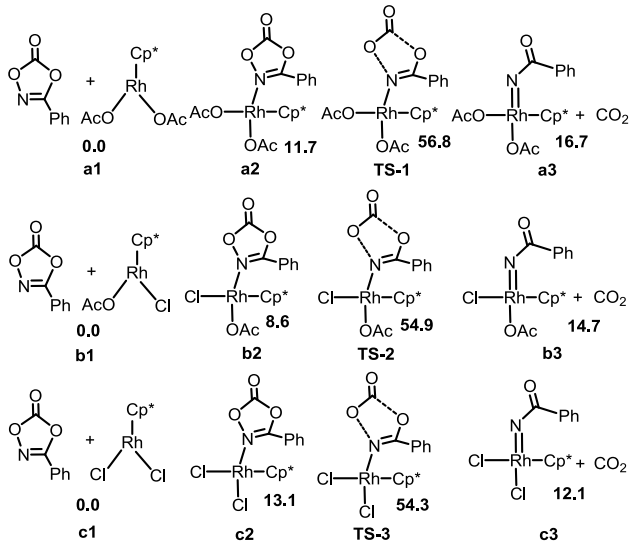

Figure S9. Relative Gibbs free energies (kcal/mol) for decomposition of substrate **2a** with Rh_{III} possible monomers.

Figure S10 shows the N-H bond deprotonation/C-H bond activation reaction of **1a** by [Cp*Rh(OAc)$_2$]. **IN1** is formed by the coordination of the N atom of of *N*-methoxyamide of **1a** to the Rh center, and this step is clearly endergonic by 18.7 kcal/mol. Subsequently, the deprotonation of the N-H bond by the acetate ligand is facile, with a low barrier of only 0.2 kcal/mol *via* the six-membered ring transition state **TSa,** and **IN2** is generated. Then, aromatic C-H bond activation occurs by concerted metalation–deprotonation (CMD) with a barrier (**TS1**) of 12.9 kcal/mol. The acetic acid molecule in **IN4** is coordinated to the Rh center, then dissociates to yield the 5-membered rhodacycle **IN5**. The energy of **IN5** is equal to that of the starting compounds, which indicates that the C-H activation in this reaction is reversible. However, much higher barriers of 45.9 kcal/mol and 24.5 kcal/mol (Figure S11 and S12) are found when using [Cp*RhCl$_2$ and [Cp*RhCl(OAc)], respectively, as catalysts. For the latter two processes, CMD is involved in four-membered ring transition states, where the chloride anion is the hydrogen acceptor. These results illustrate the importance of anion exchange to afford [Cp*Rh(OAc)$_2$] as an efficient catalyst for the N-H deprotonation and C-H activation steps.

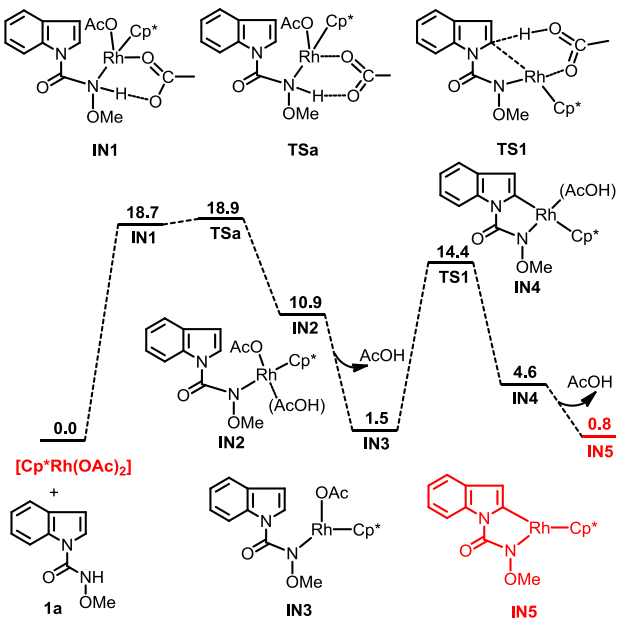

Figure S10. Relative Gibbs free energies (kcal/mol) for the generation of the 5-membered rhodacycle of **1a** through sequential N-H deprotonation/C-H activation catalyzed by [Cp*Rh(OAc)$_2$].

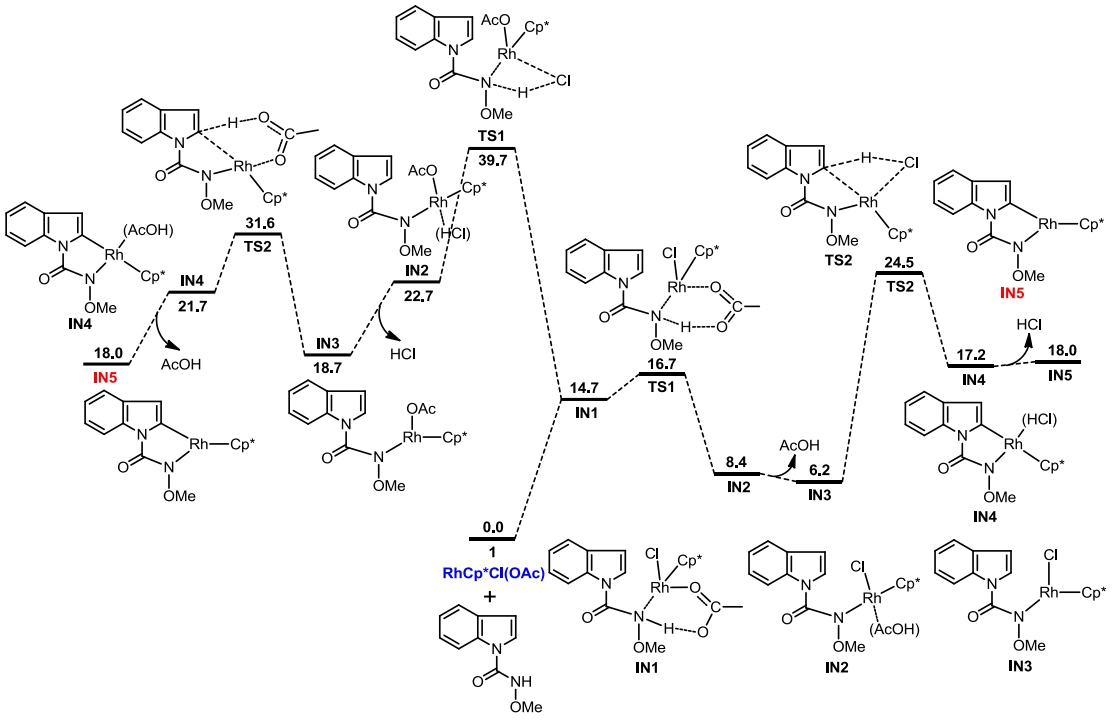

Figure S11. Relative Gibbs free energies (kcal/mol) for the generation of 5-membered ring rhodacycle through sequentil N−H deprotonation/C−H activation catalyzed by RhCp*Cl(OAc).

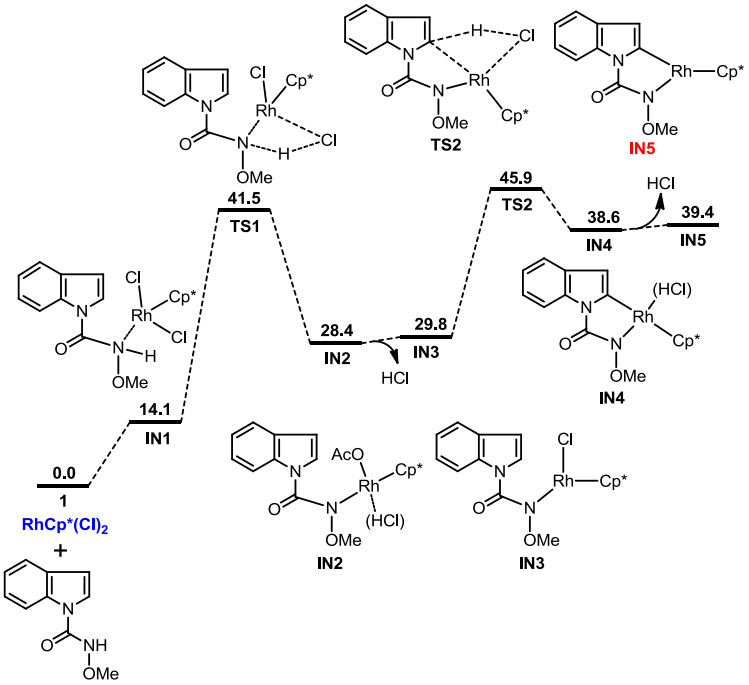

Figure S12. Relative Gibbs free energies (kcal/mol) for the generation of 5-membered ring rhodacycle through sequentil N−H deprotonation/C−H activation catalyzed by RhCp*$(Cl)_2$.

The calculations indicated that the C-H activation of the substrate by [Cp*Rh(OAc)$_2$] occurs more easily than the decomposition of the substrate with [Cp*RhCl$_2$]; as a result, **IN5** is generated (Figure S10). Compared to the difficult decomposition of the five-membered ring of **2a** substrate by Rh(III) catalysts (Figure S9), the reactions of the substrate **2a** with the intermediate **IN5** are much more facile (Figure S13). **IN6** is first formed with an endergonicity of only 4.4 kcal/mol, and an overall activation barrier of 14.9 kcal/mol from **1a** to **TS2** is required for CO_2 release. Therefore, the deprotonated substrate makes the Rh(III) center in **IN5** more electron-deficient than the free catalyst for the coordination of the substrate and stabilizes the Rh(V) intermediate (**IN7**) more efficiently. From **IN7**, C-N bond coupling occurs *via* **TS3** with a barrier of 13.6 kcal/mol. The direct reductive elimination product is impossible from the N(sp^3)-Rh(III)-N(sp^3) unit, with a barrier of 50 kcal/mol from **INX** to **TS4′**. Thus, **INX** is proposed as the favorable common intermediate for C-H amidation to deliver different final products based on reaction conditions.

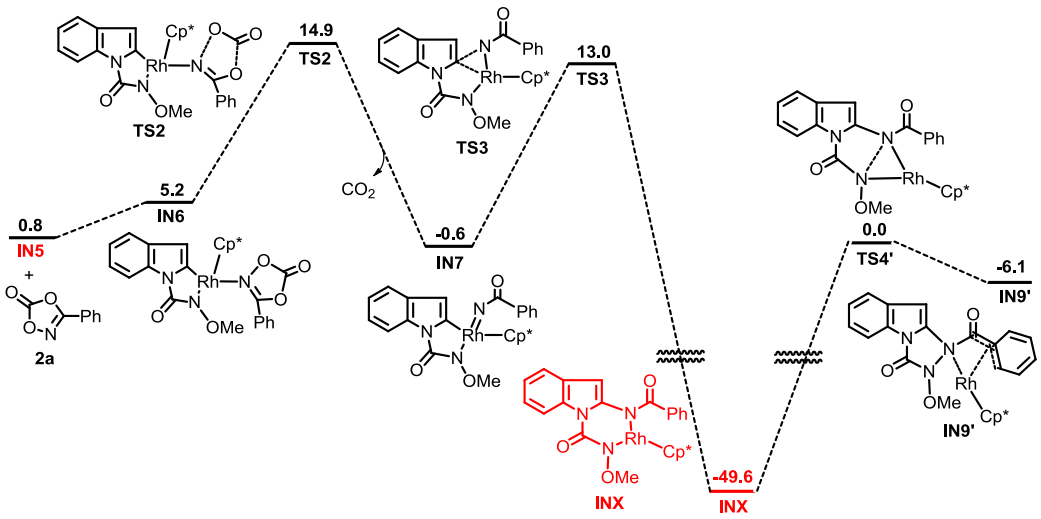

Figure S13. Relative Gibbs free energies (kcal/mol) for the generation of the 6-membered rhodacycle **INX** after intermediate **IN5** conjugating with **2a**.

We also consider the possibilities for the formation of products **3a** and the corresponding free energy profiles for the favoralble paths to obtain **3a** from **INX** are shown in Figure S14. The calculation results indicate that **INX** is more likely to go through **TS4** and **TS5** for the ultimate product **3a**.

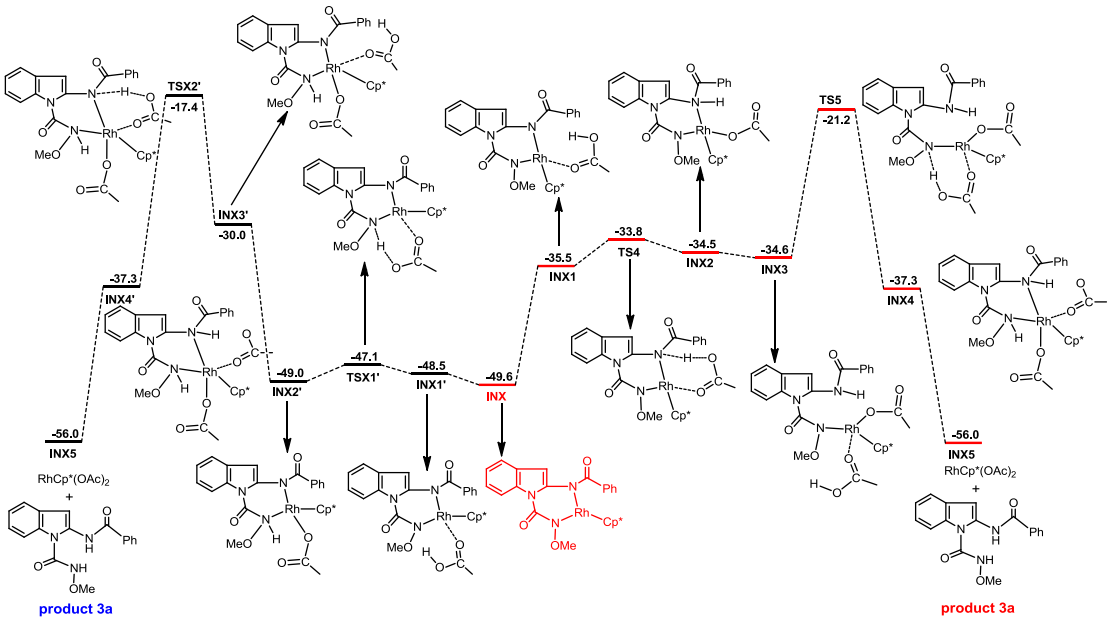

Figure S14. Relative Gibbs free energies (kcal/mol) for the generation of product **3a** from **INX**.

4. References

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5. NMR Spectra

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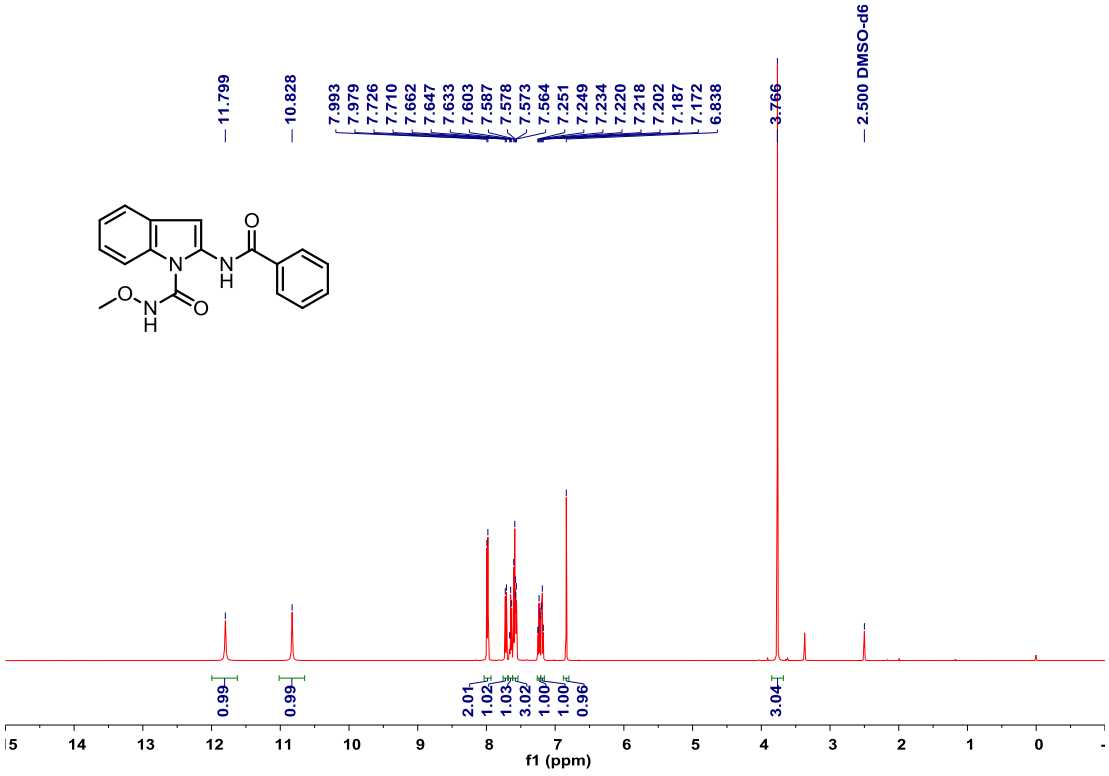

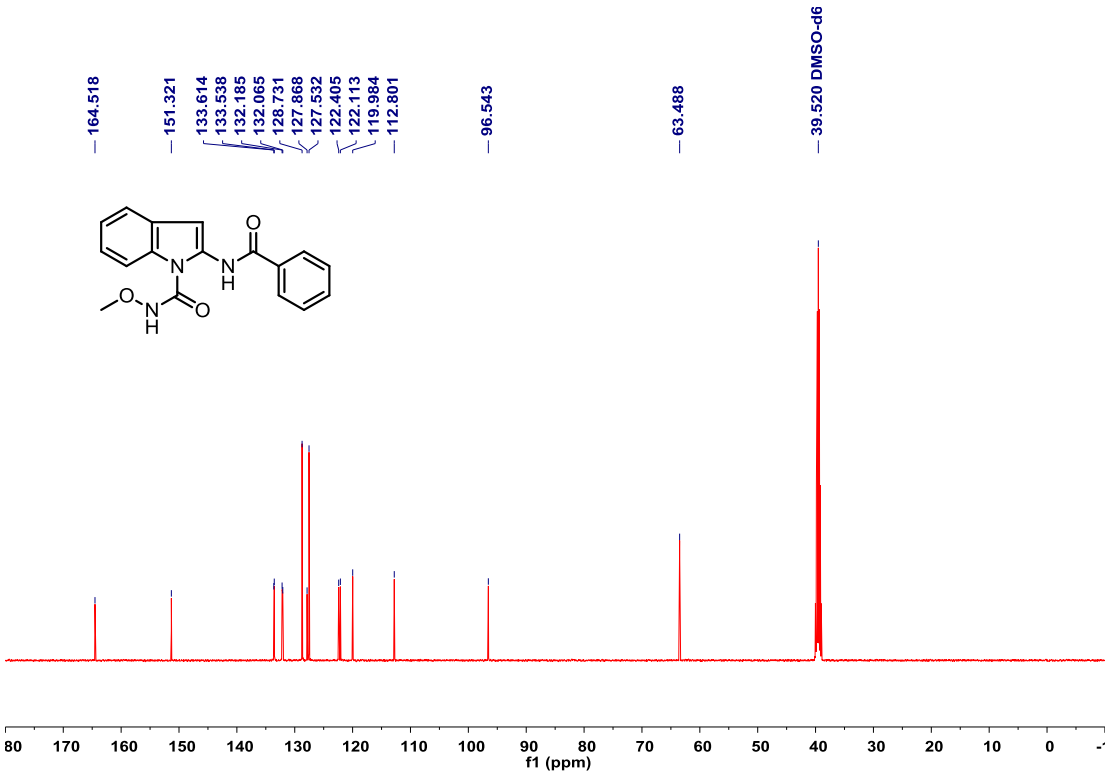

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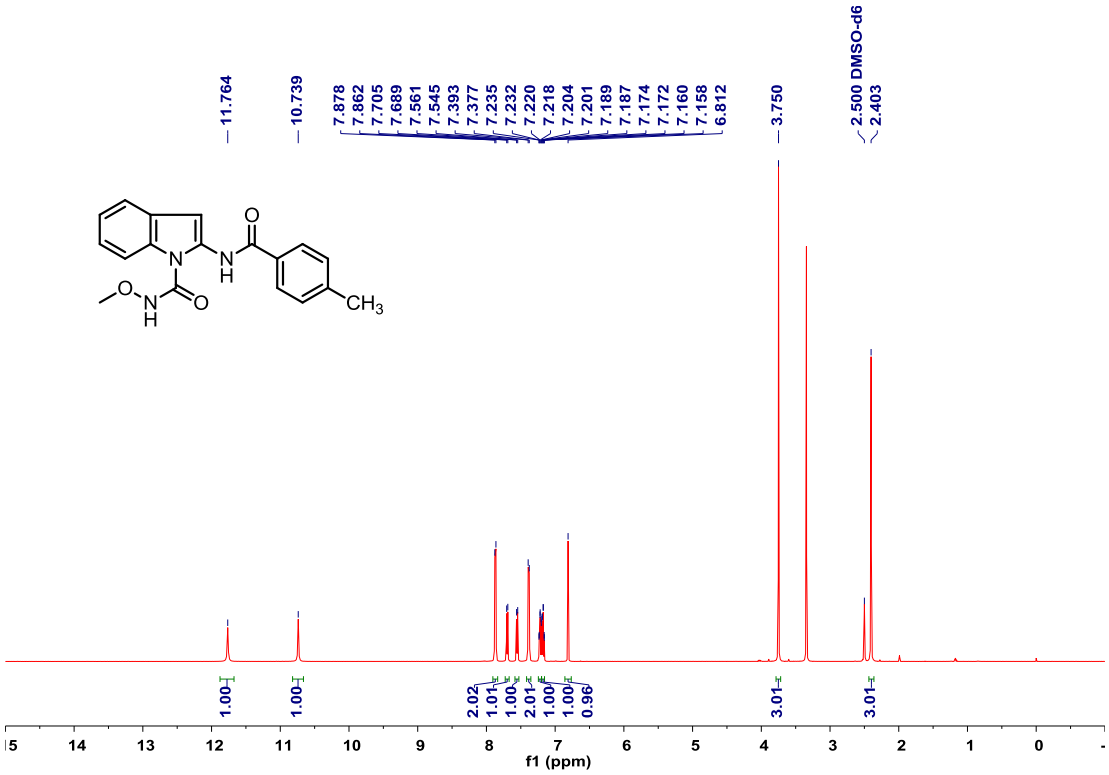

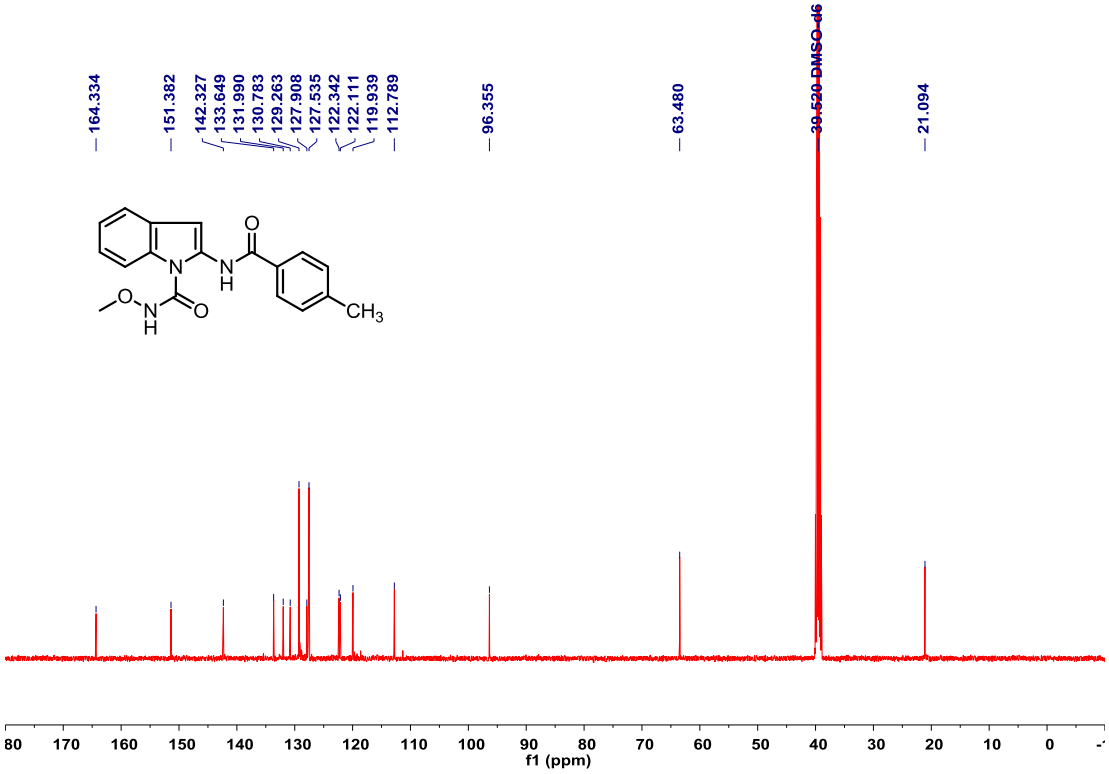

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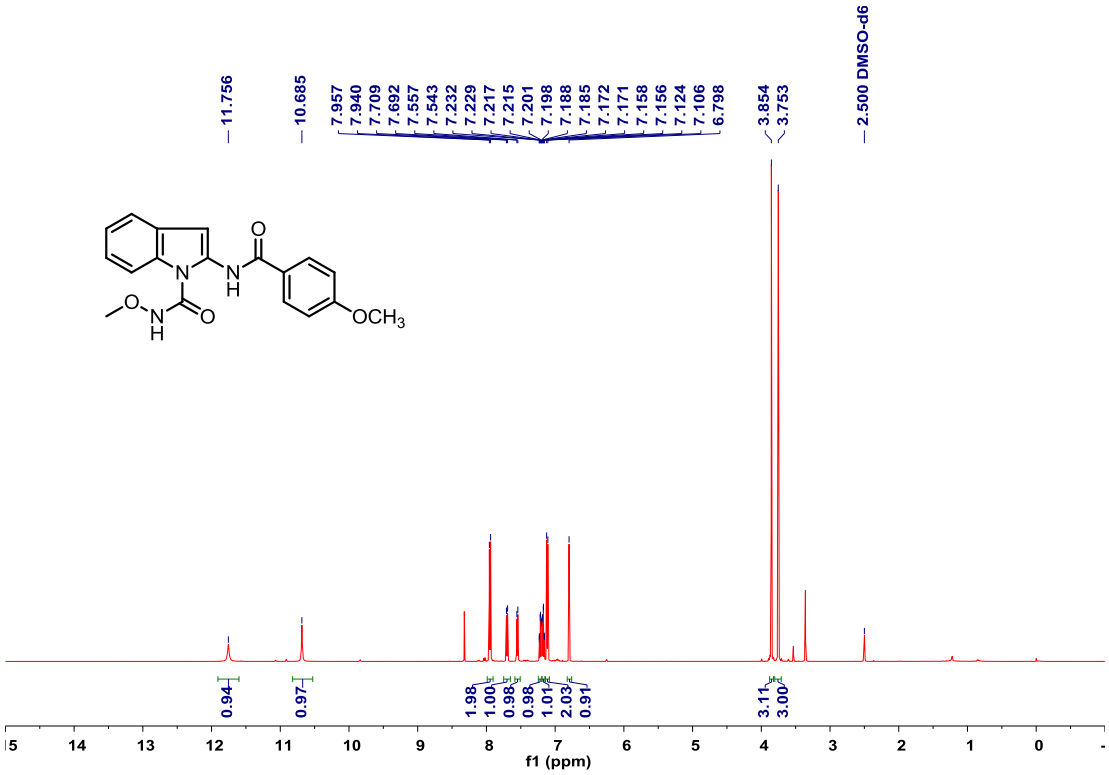

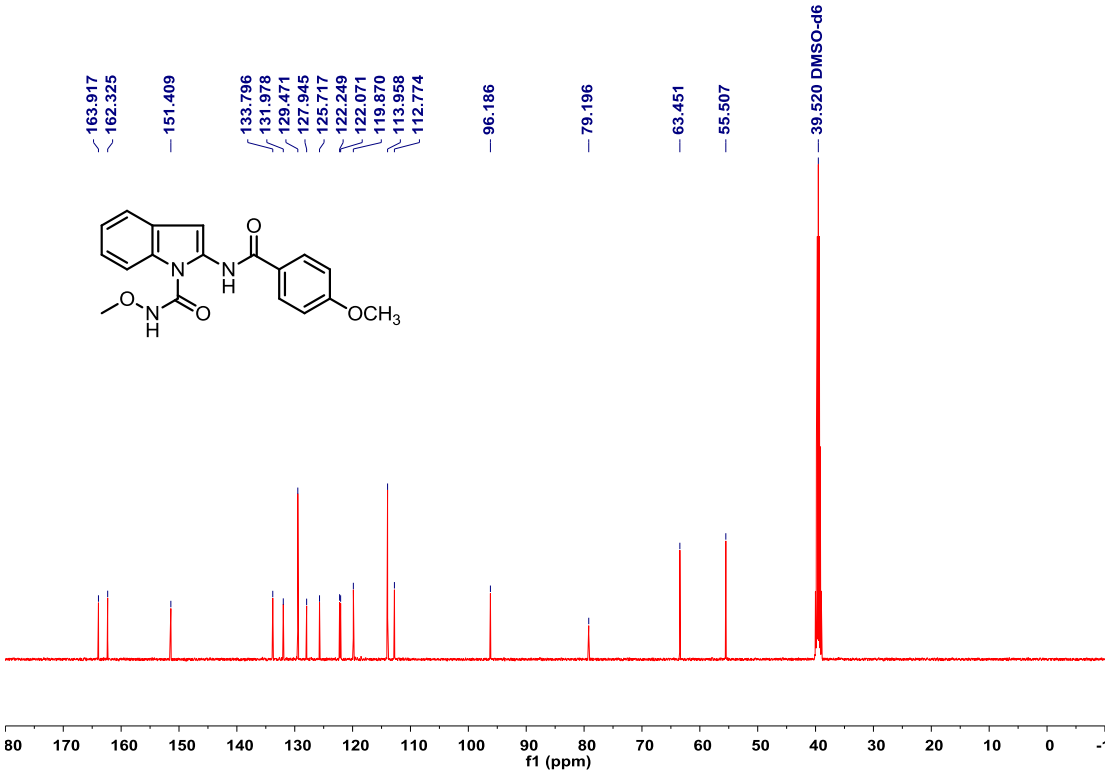

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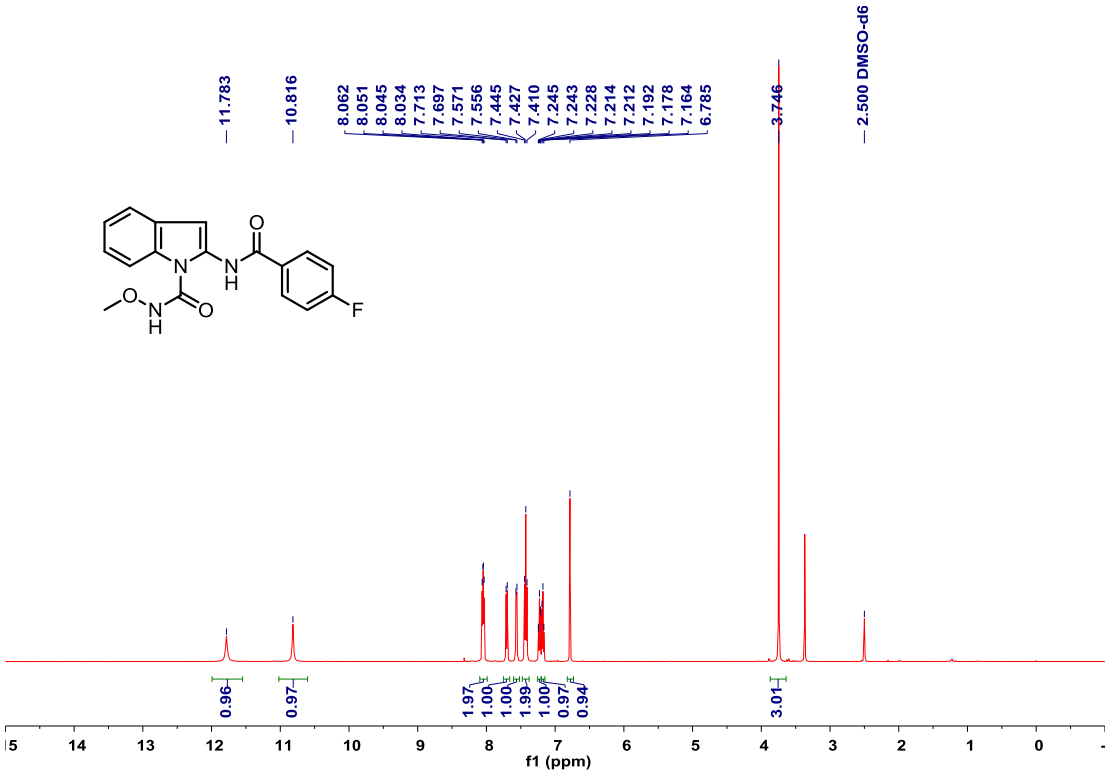

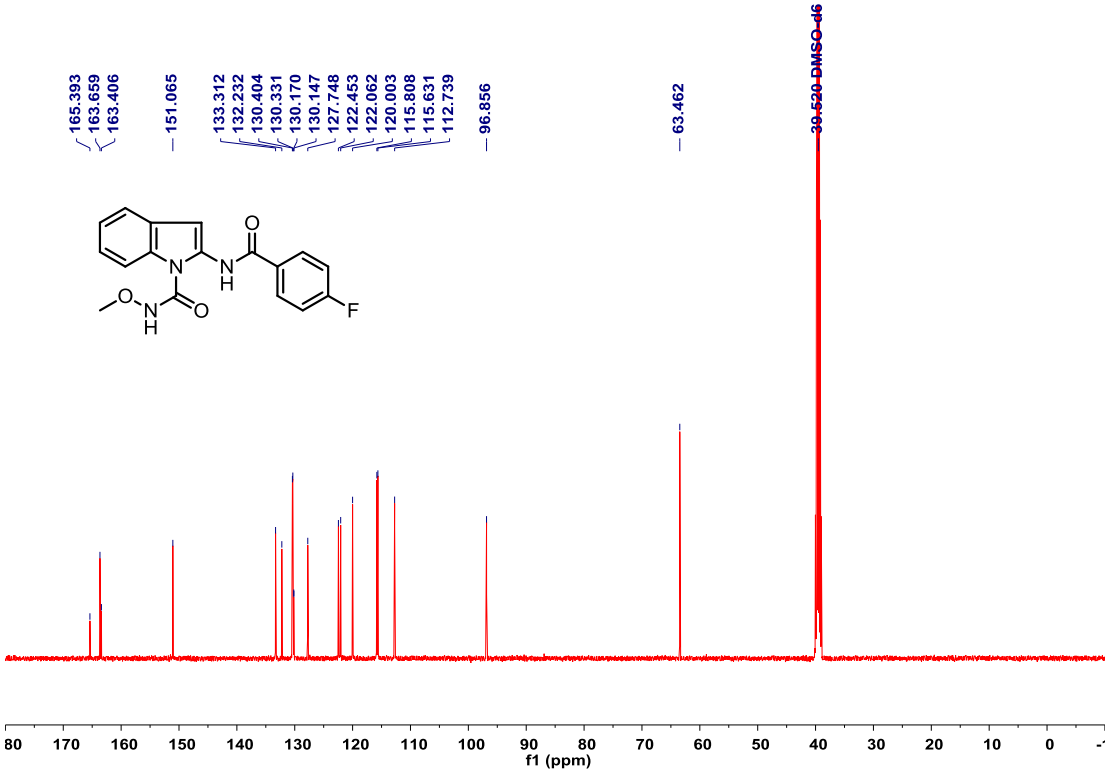

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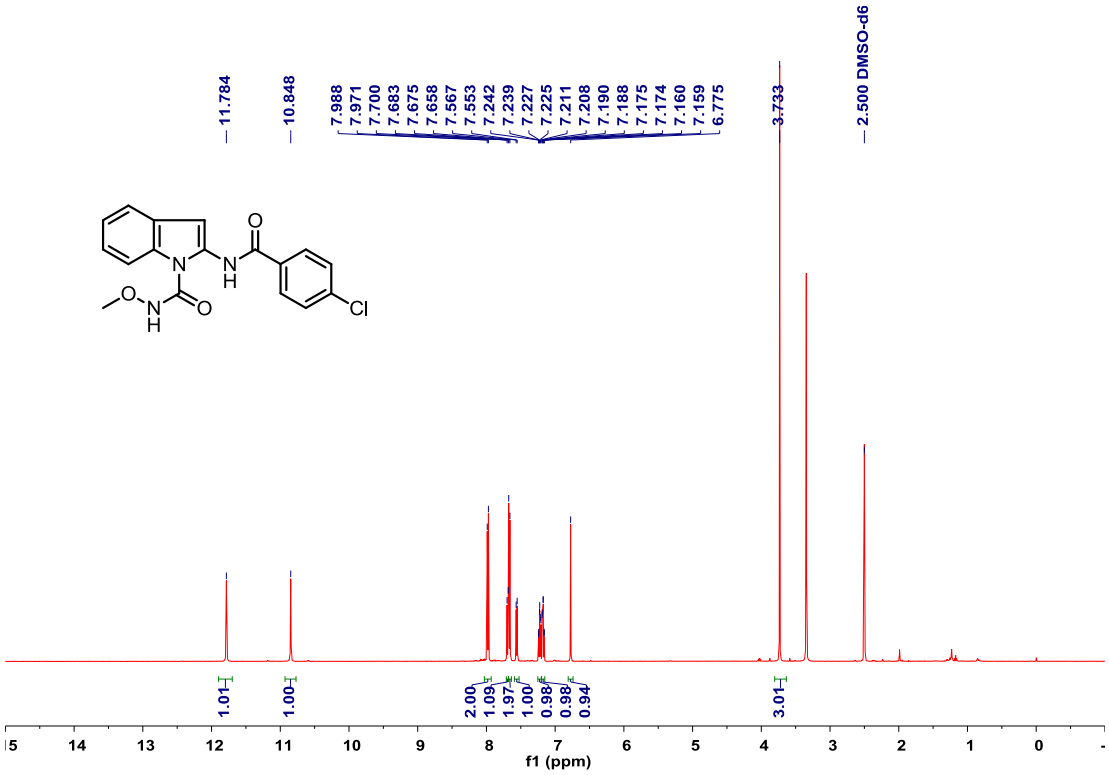

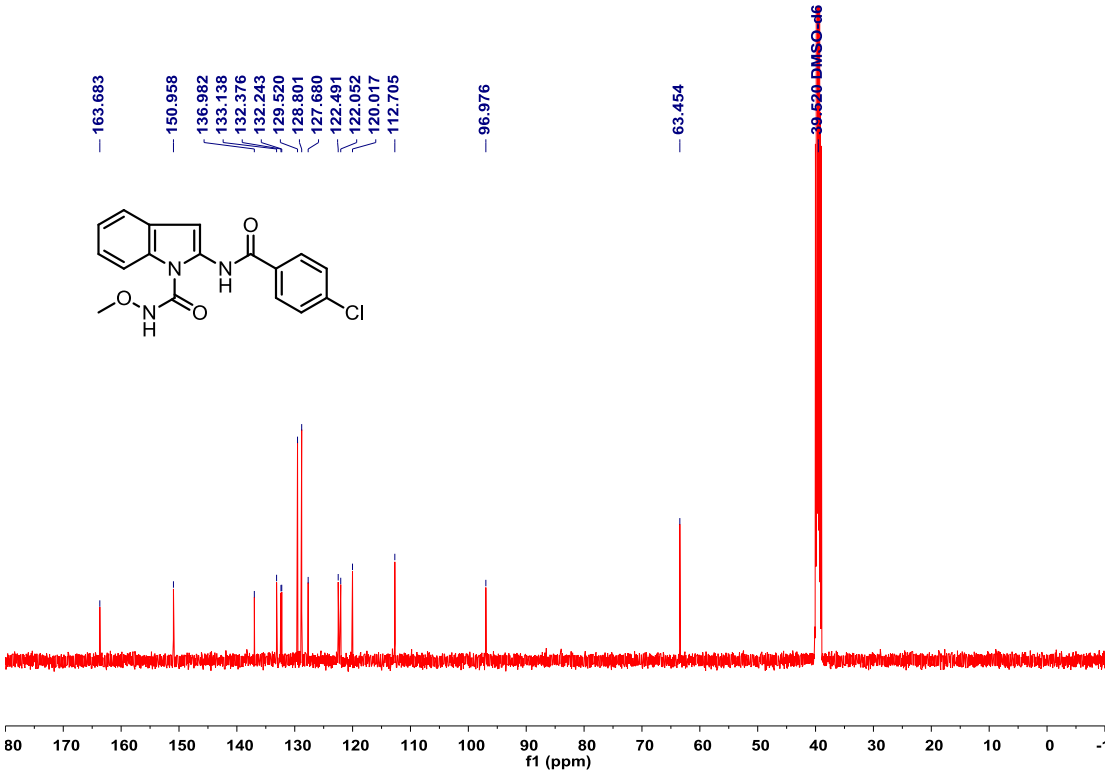

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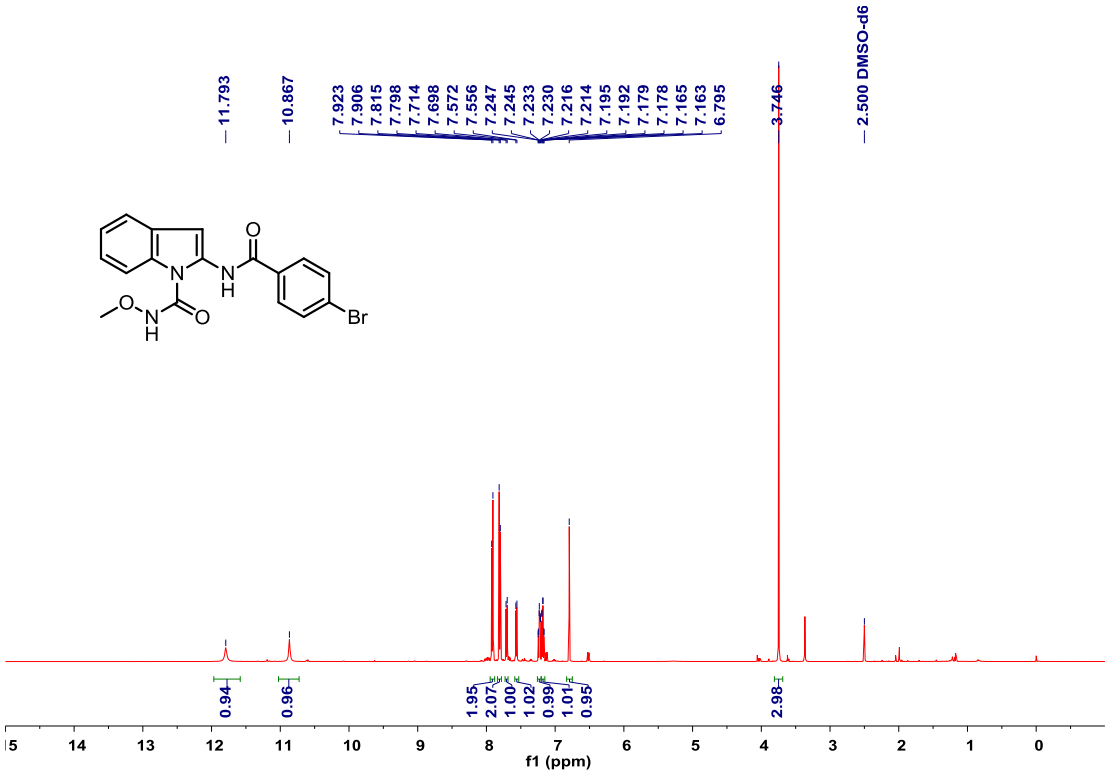

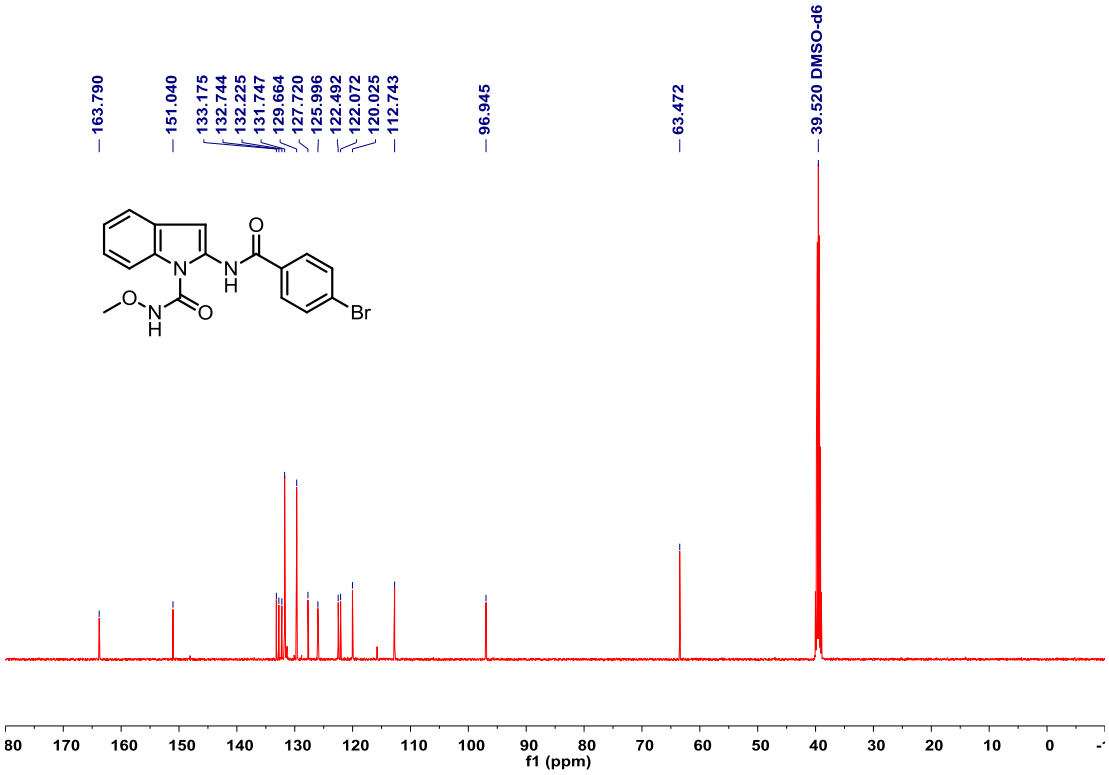

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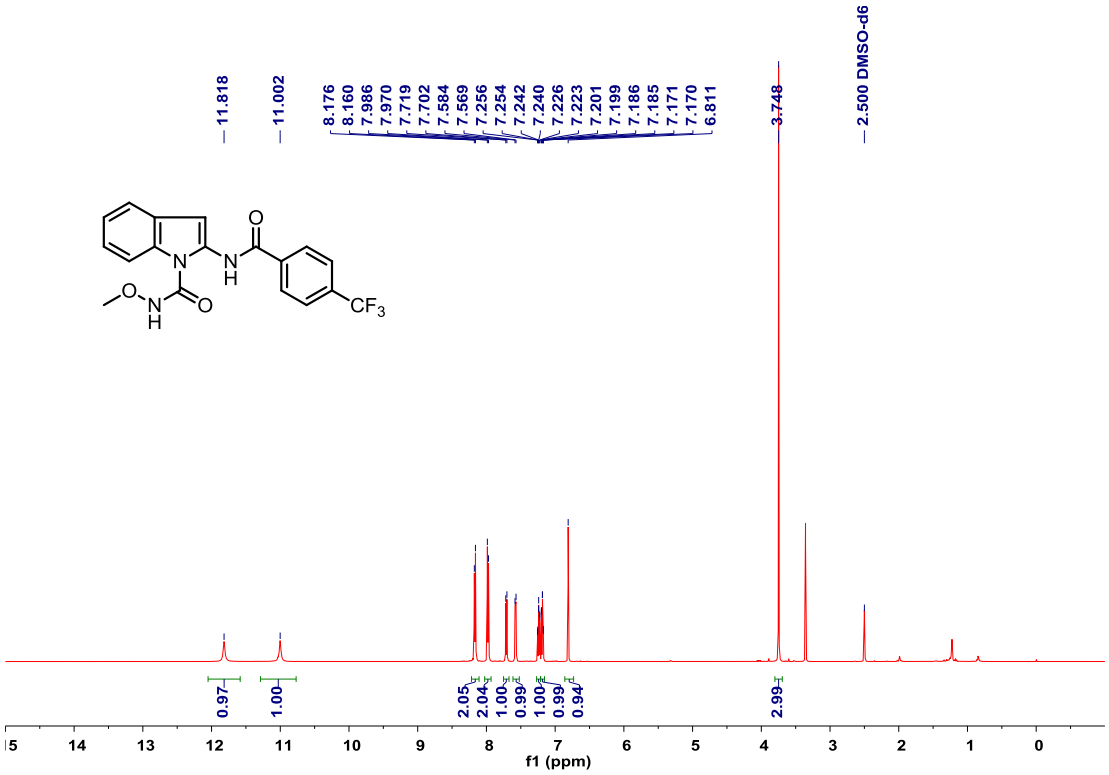

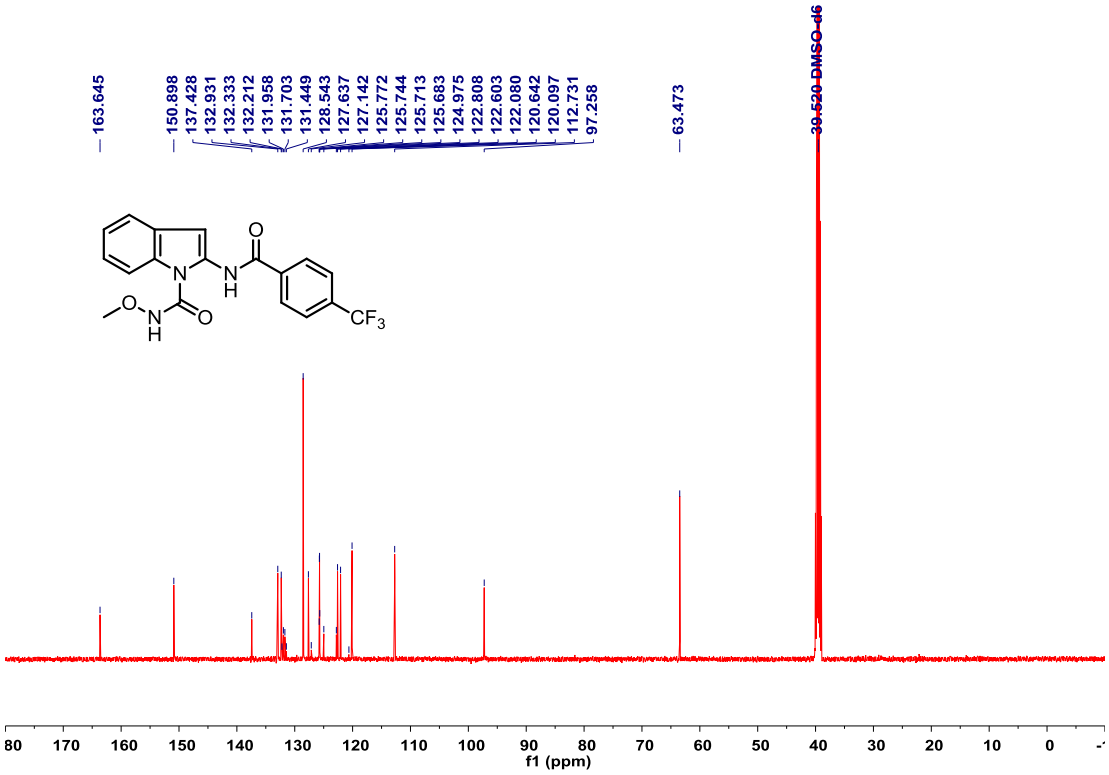

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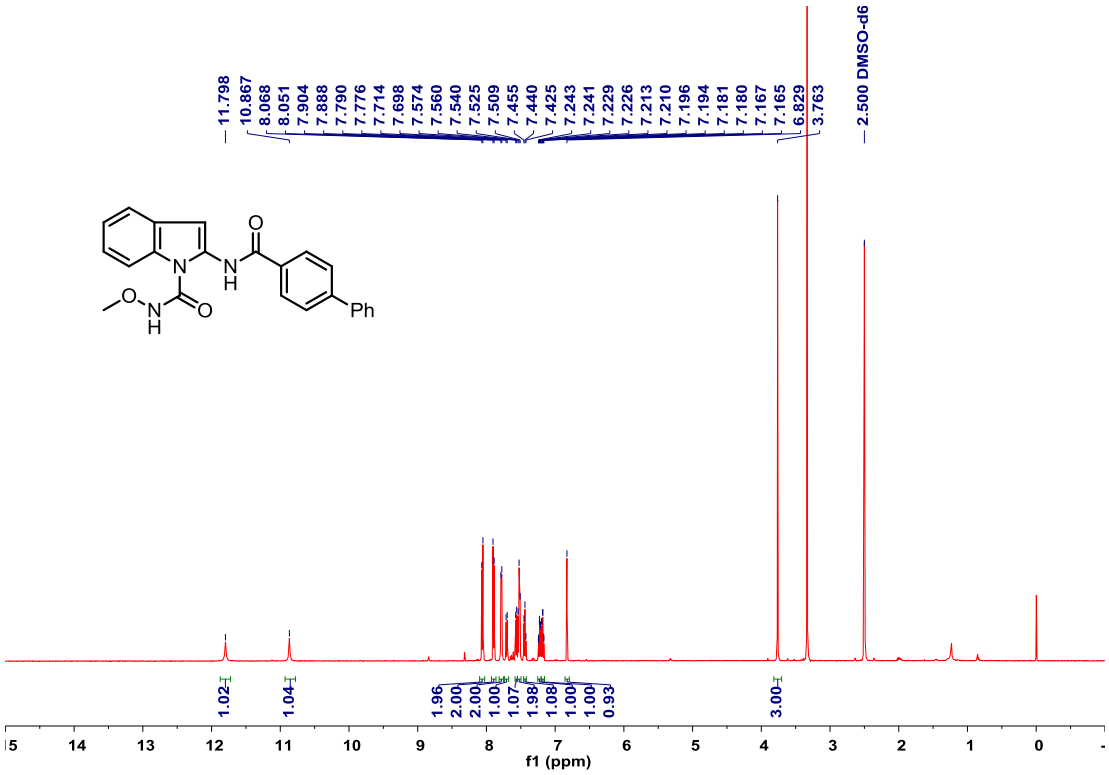
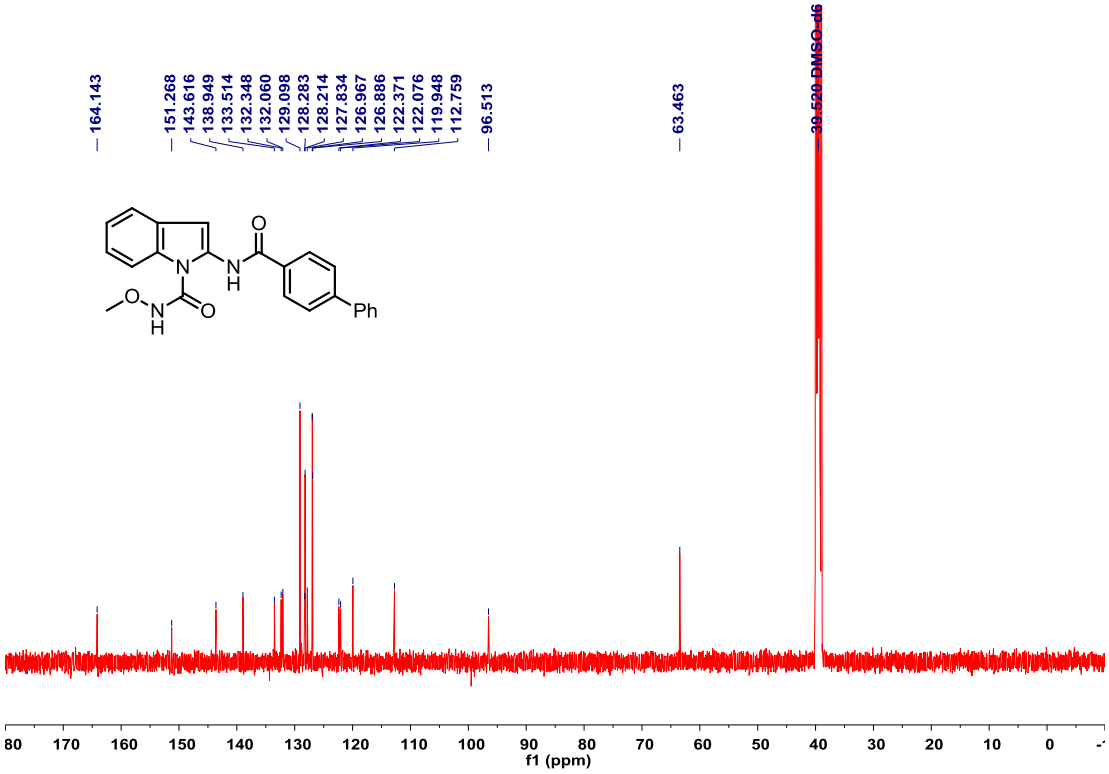
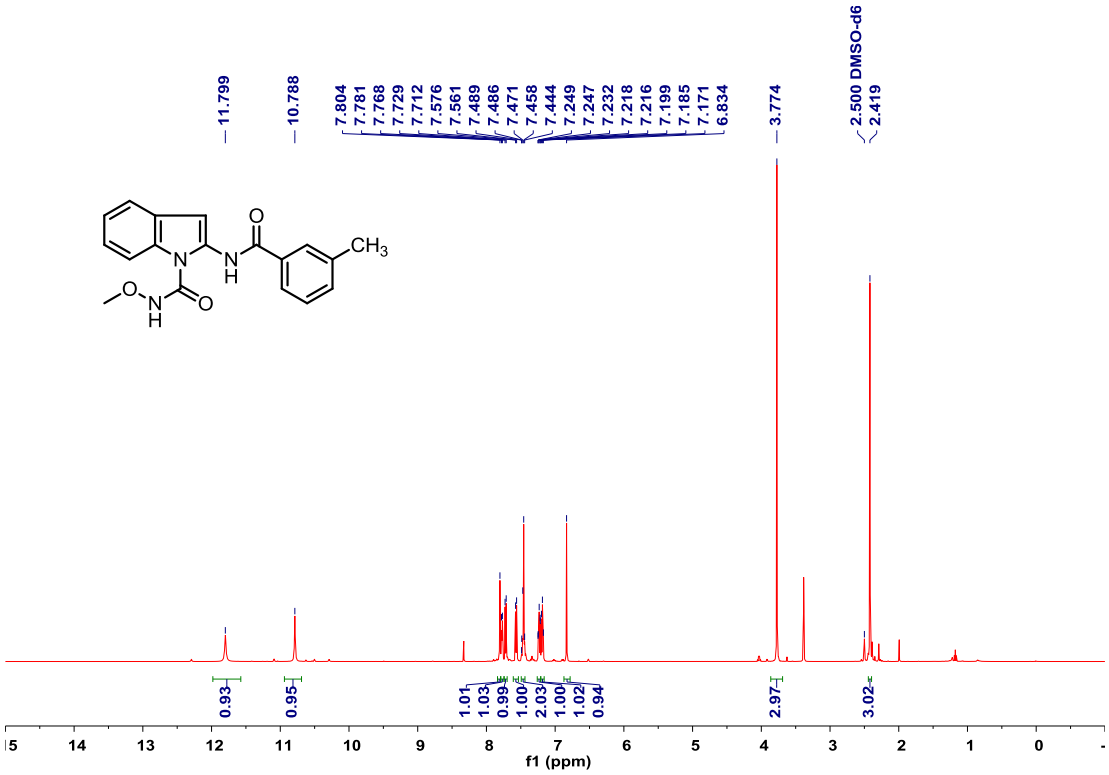
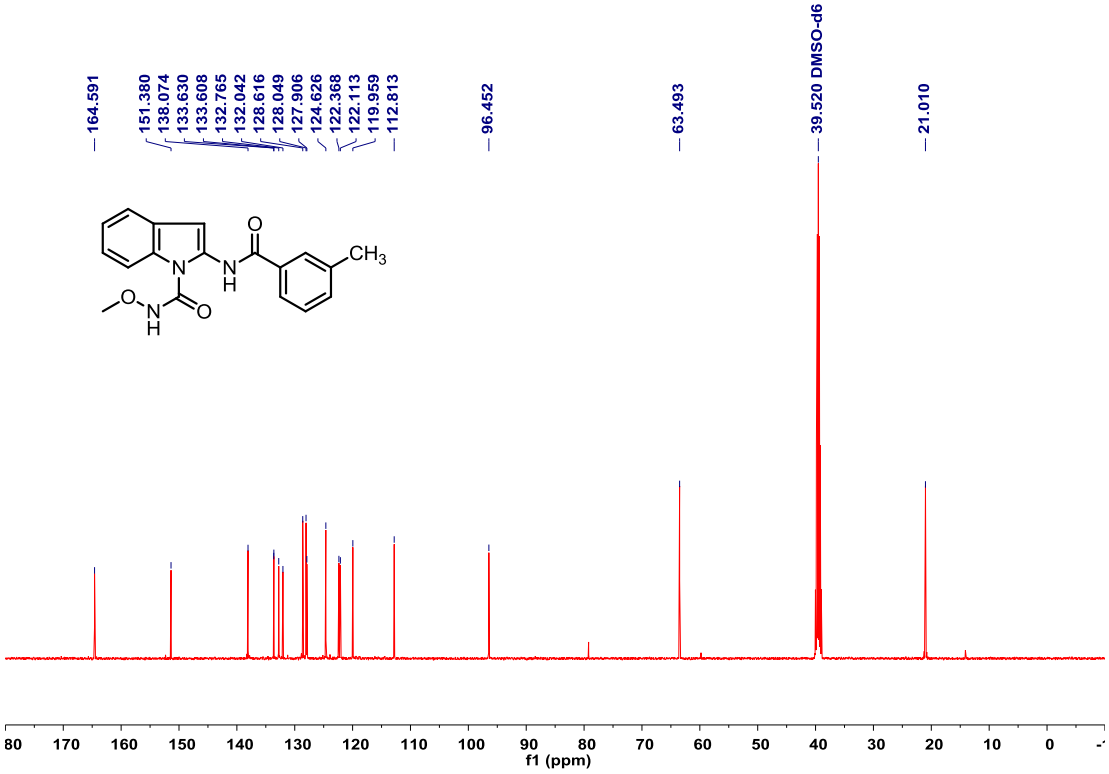


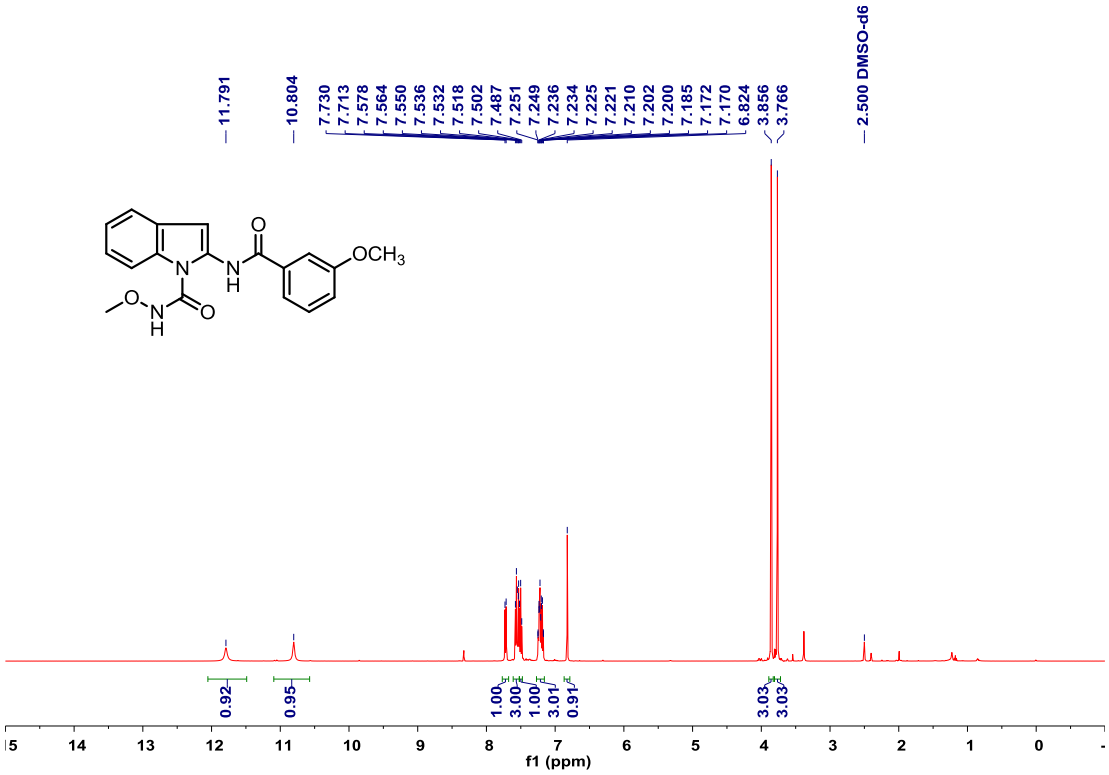


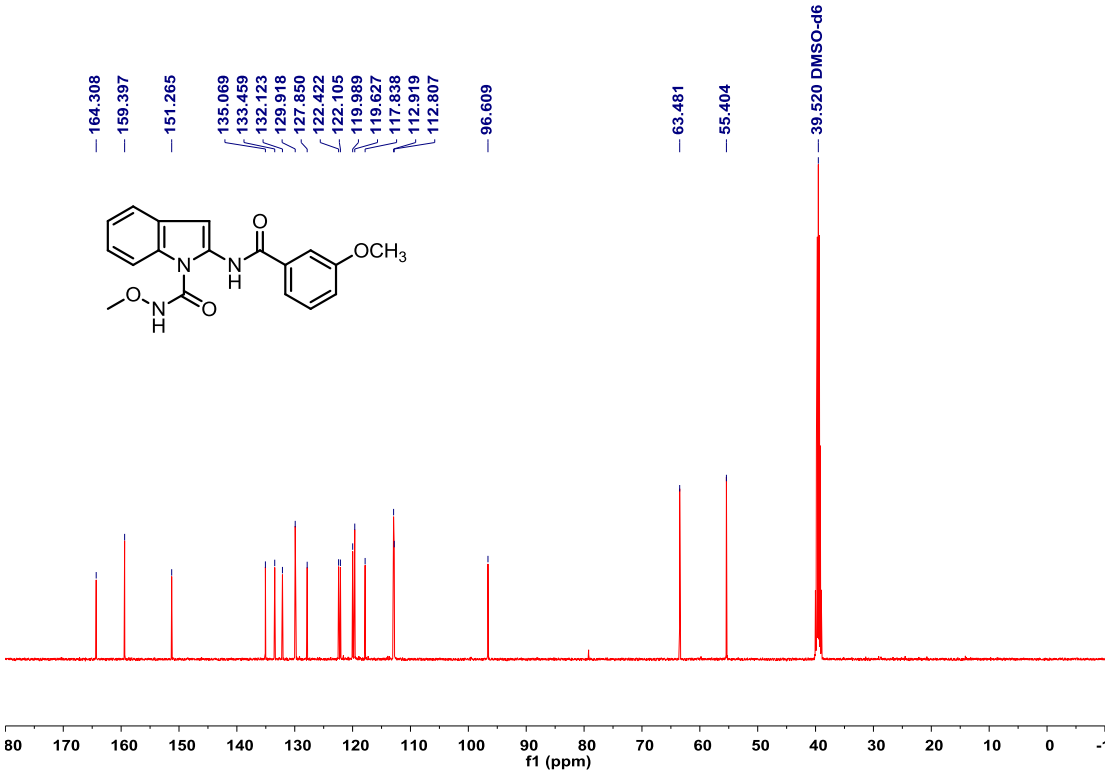
_N_-Methoxy-2-(3-methylbenzamido)-1_H_-indole-1-carboxamide (3i)



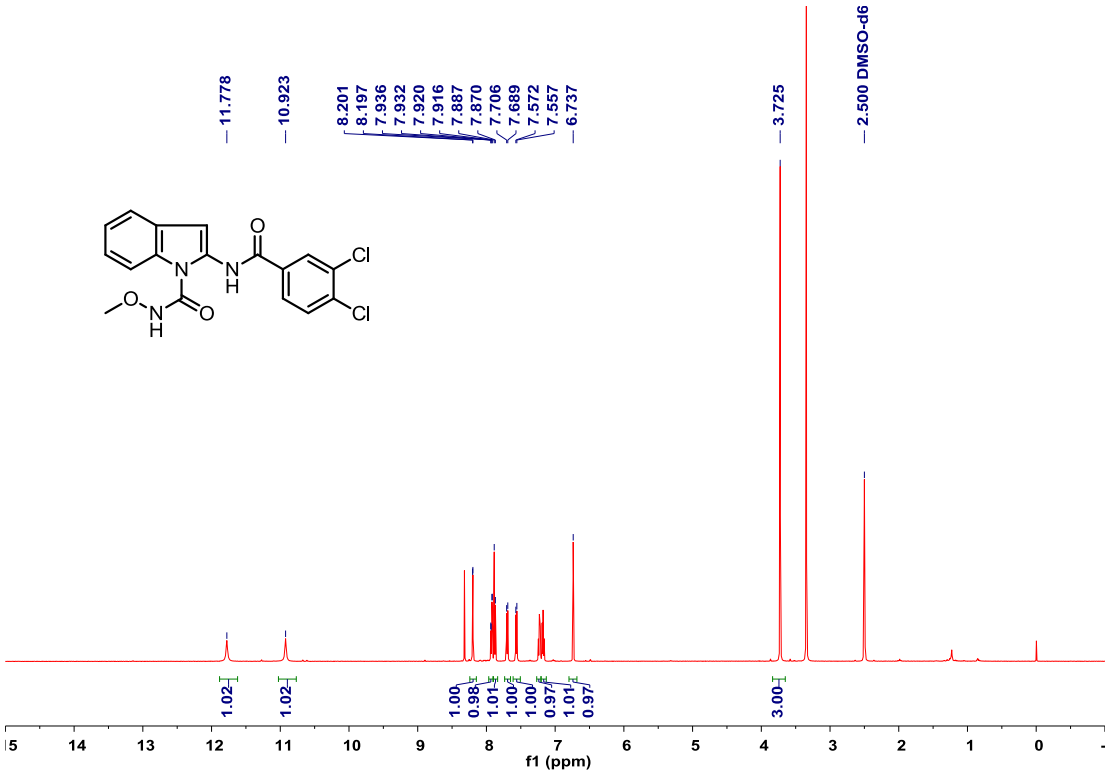


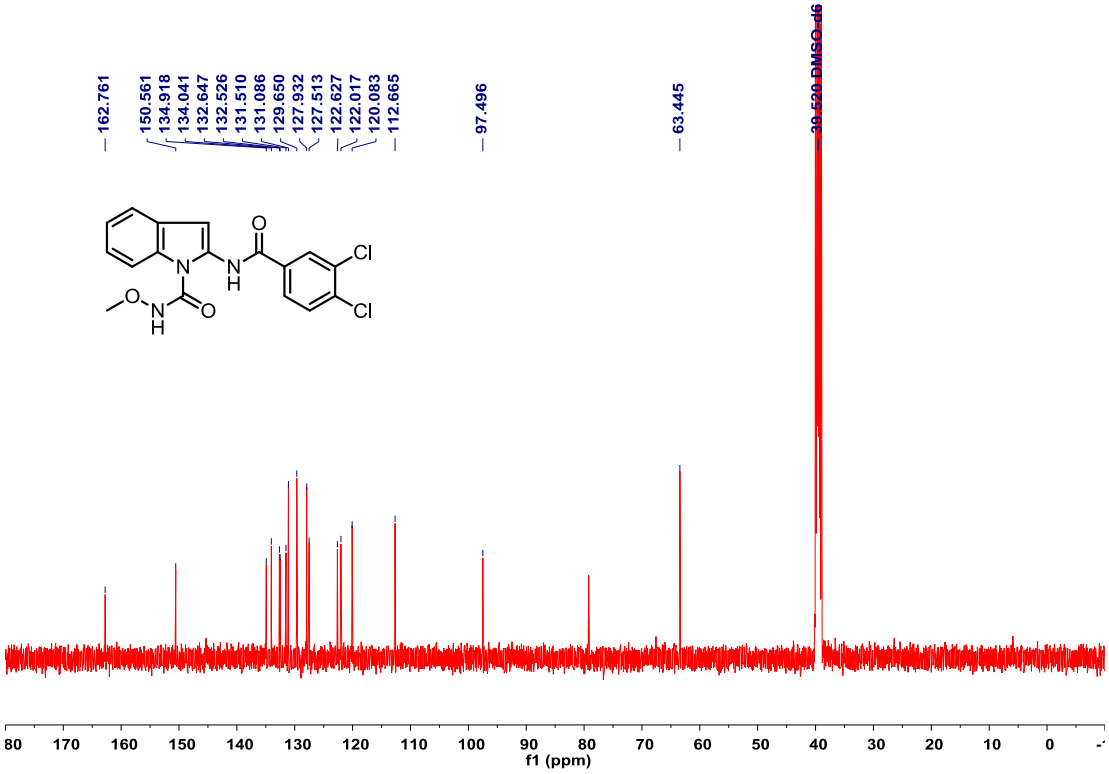
***N*-Methoxy-2-(3-methoxybenzamido)-1*H*-indole-1-carboxamide (3j)**



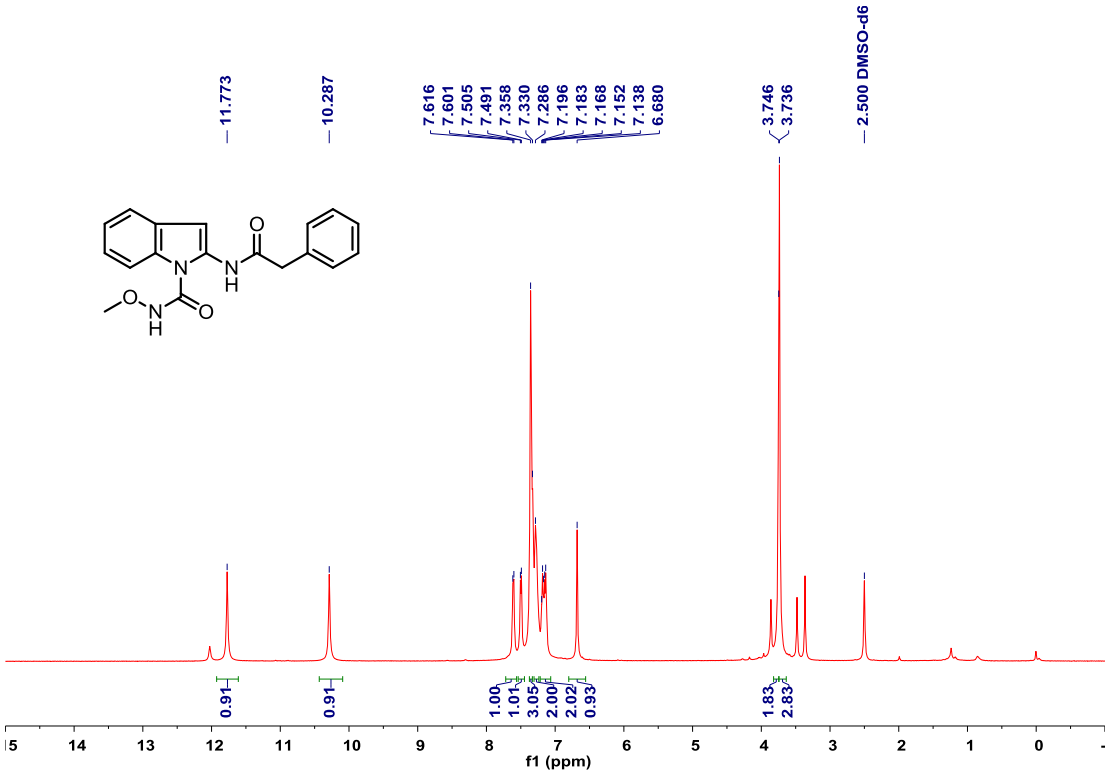


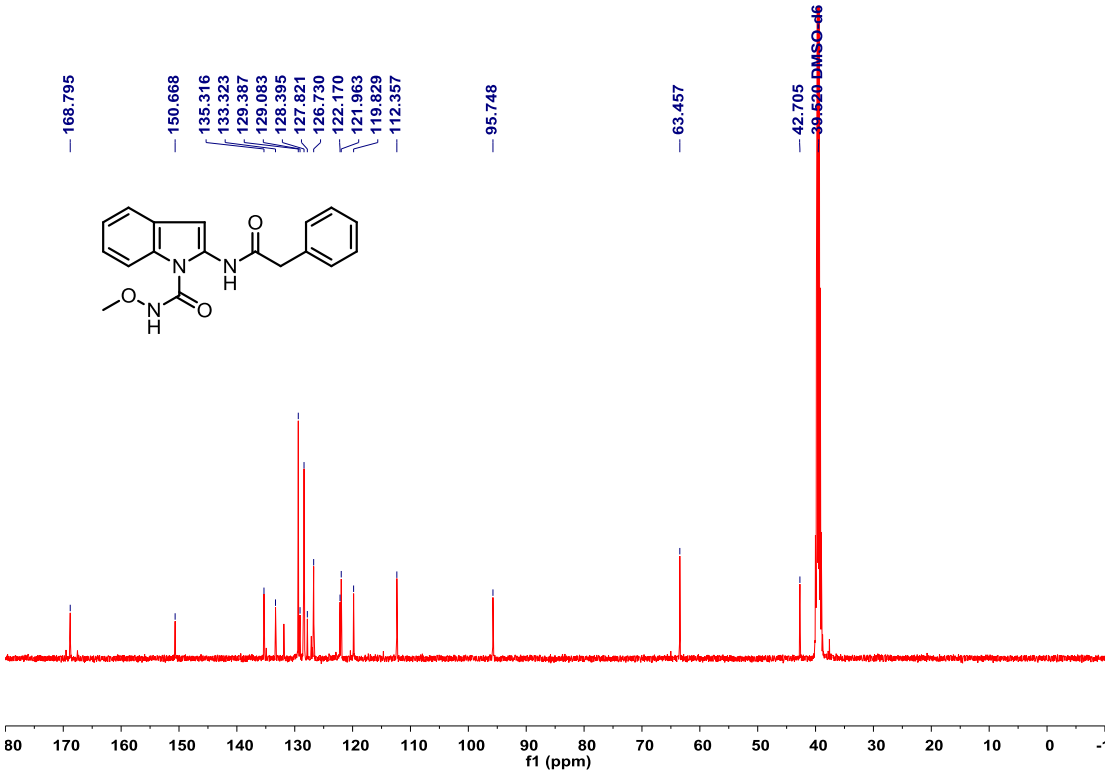
2-(3,4-Dichlorobenzamido)-*N*-methoxy-1*H*-indole-1-carboxamide (3k)



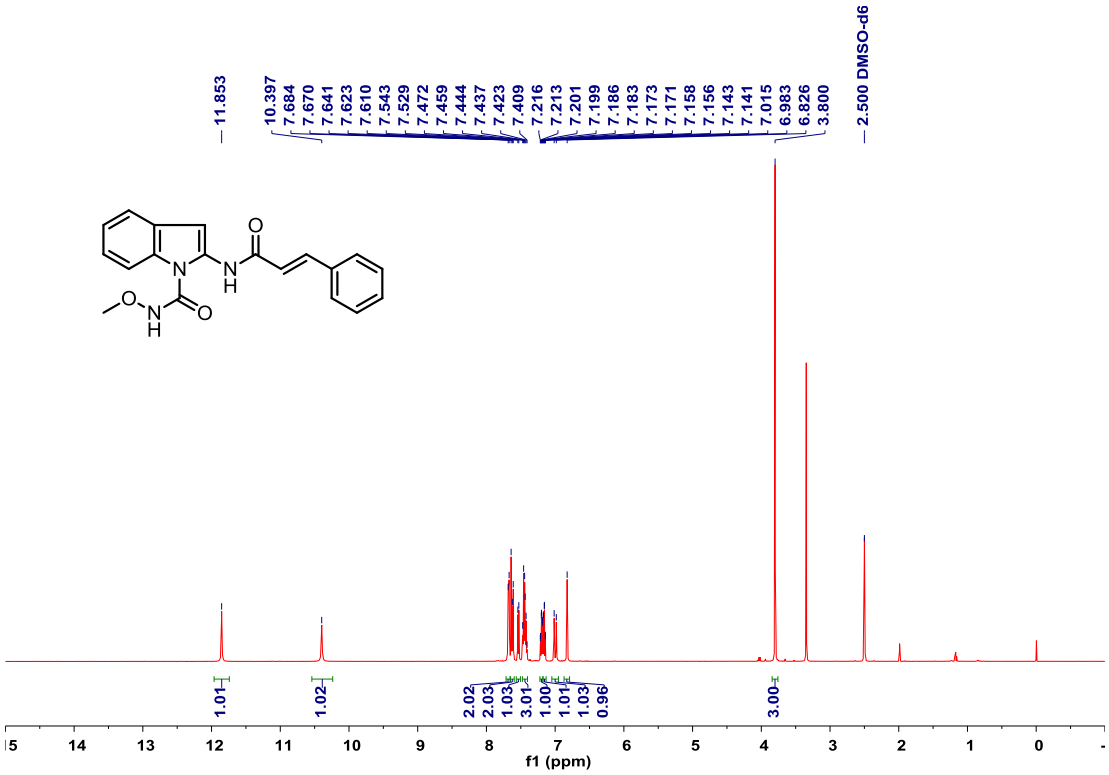


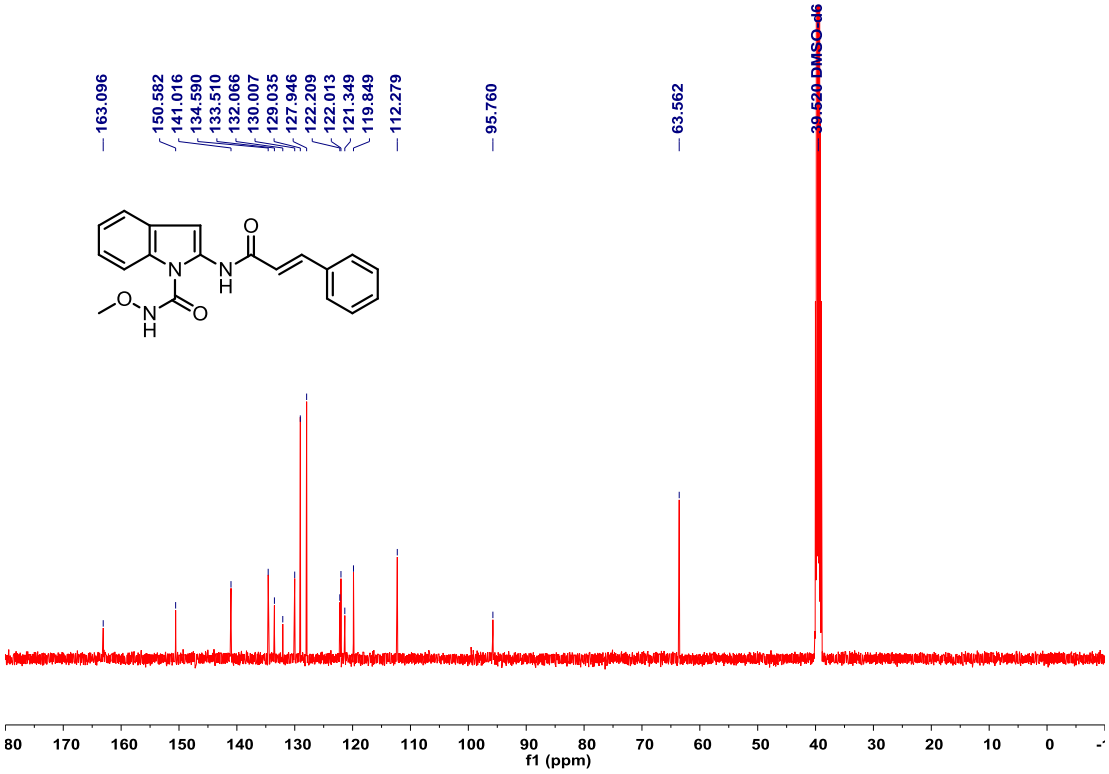
***N*-Methoxy-2-(2-phenylacetamido)-1*H*-indole-1-carboxamide (3l)**



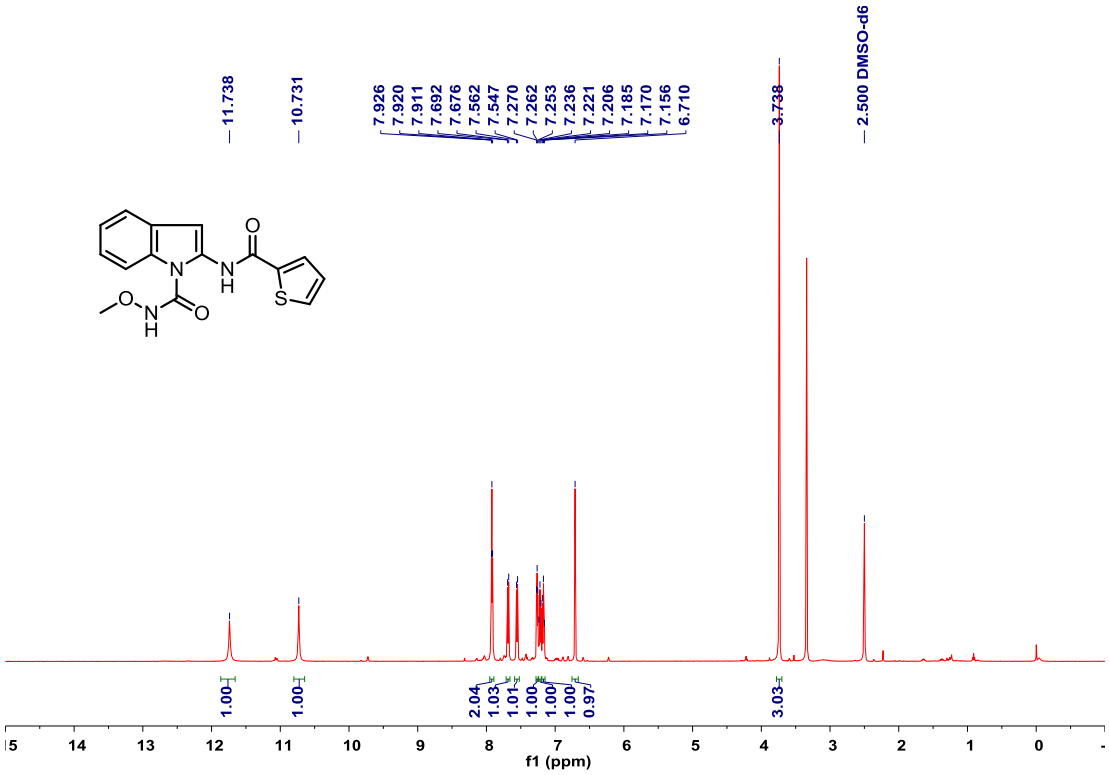


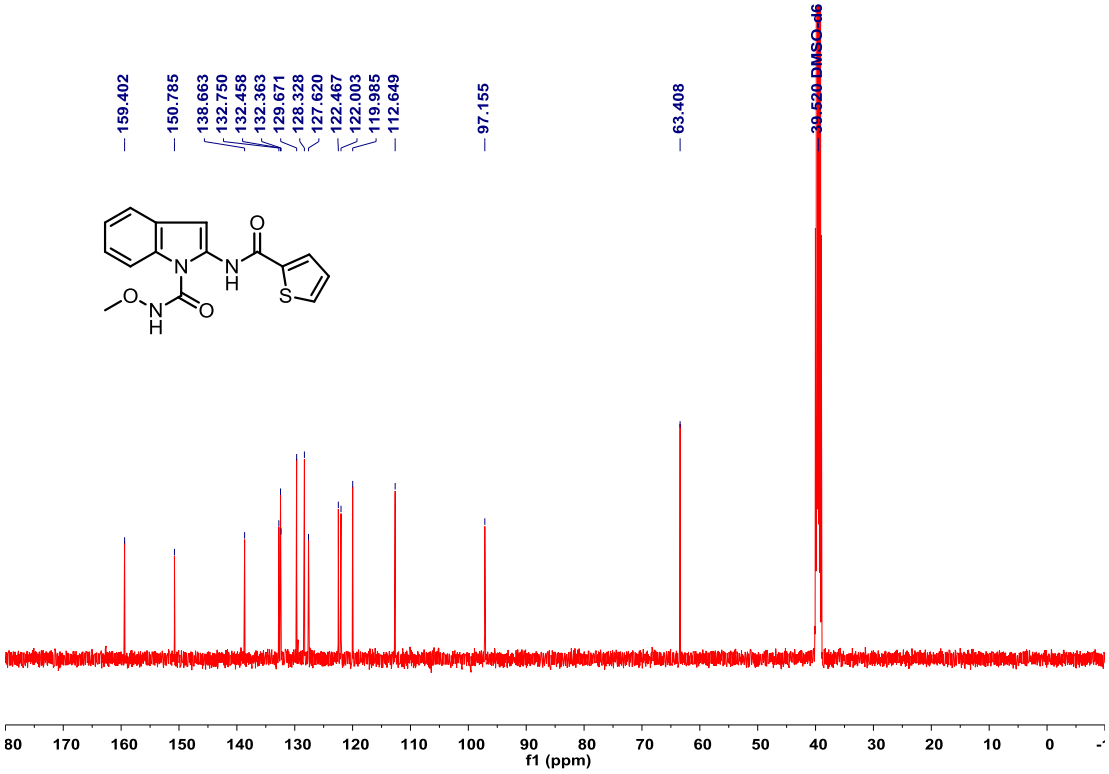
2-Cinnamamido-*N*-methoxy-1*H*-indole-1-carboxamide (3m)



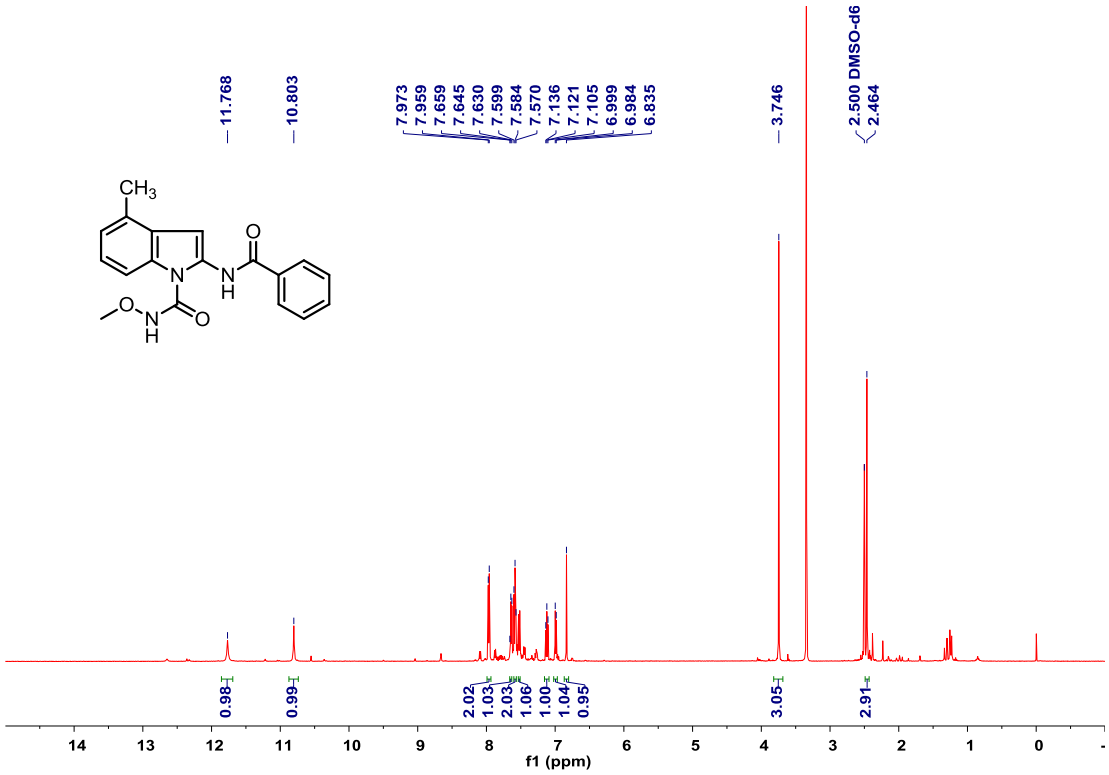


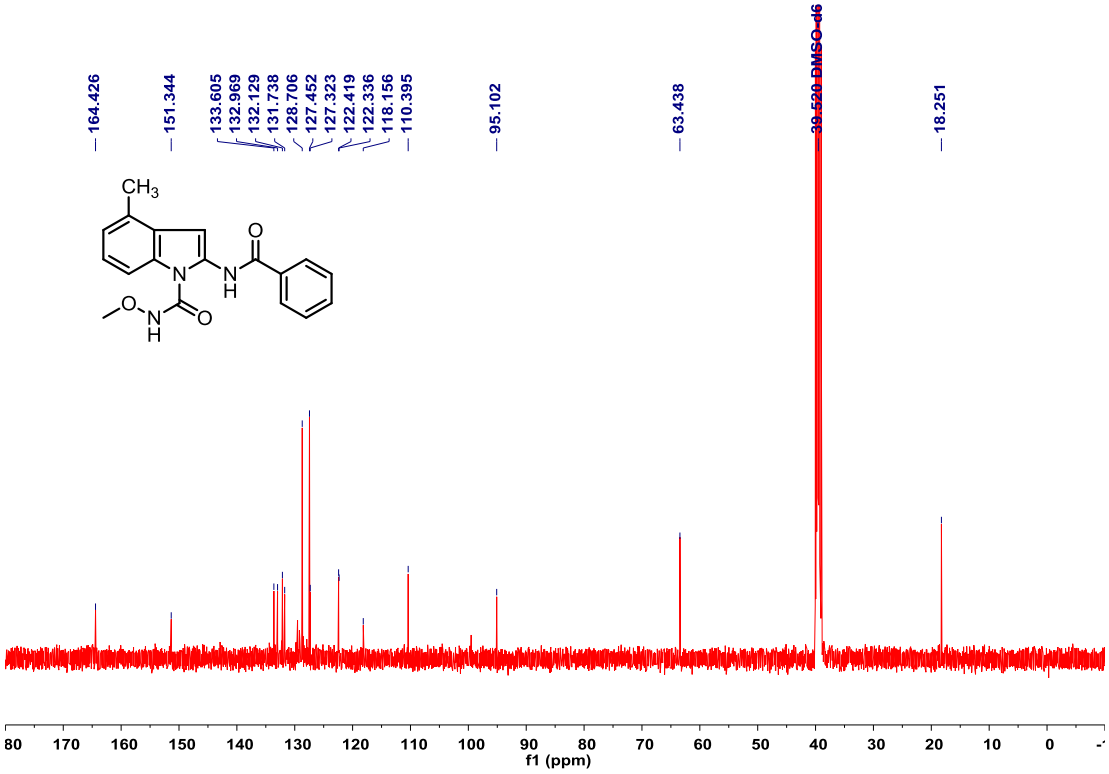
***N*-Methoxy-2-(thiophene-2-carboxamido)-1*H*-indole-1-carboxamide (3n)**



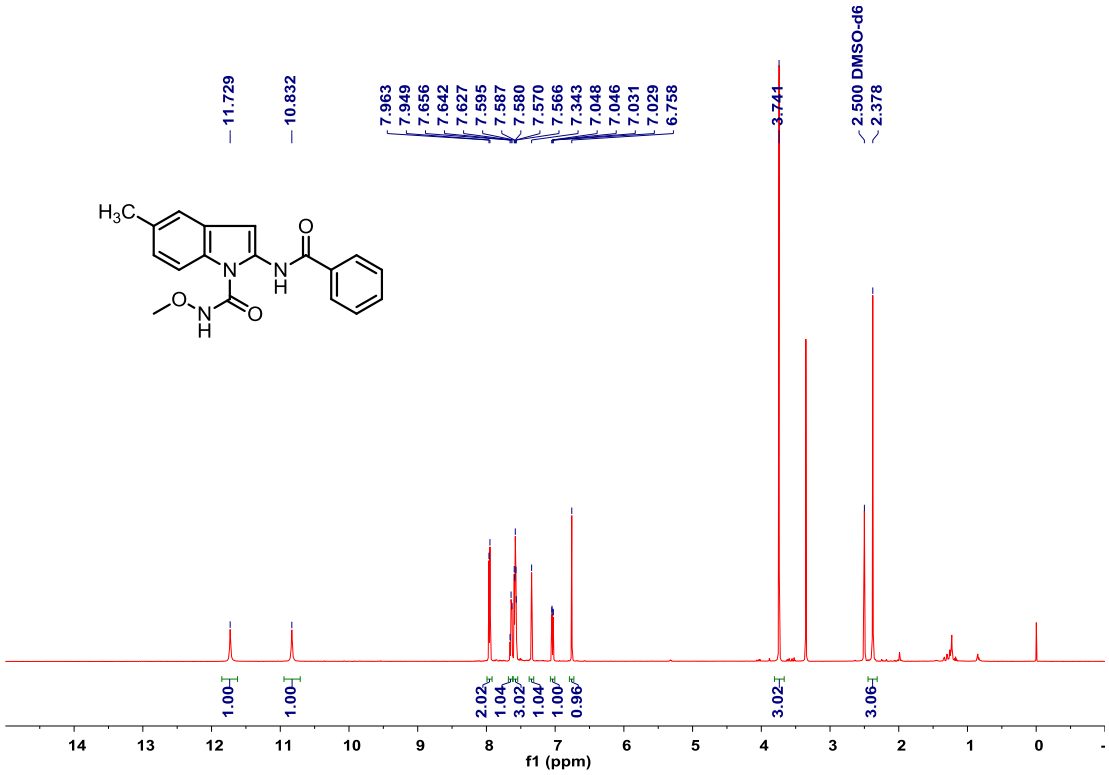


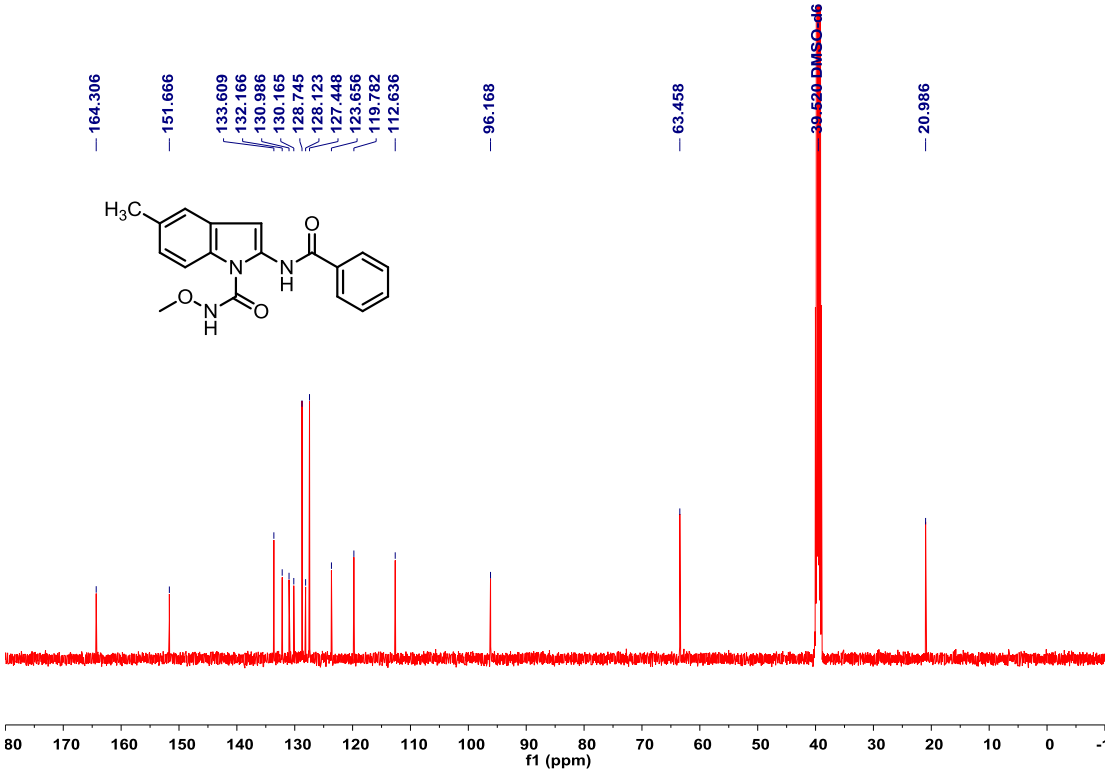
2-Benzamido-*N*-methoxy-4-methyl-1*H*-indole-1-carboxamide (3o)



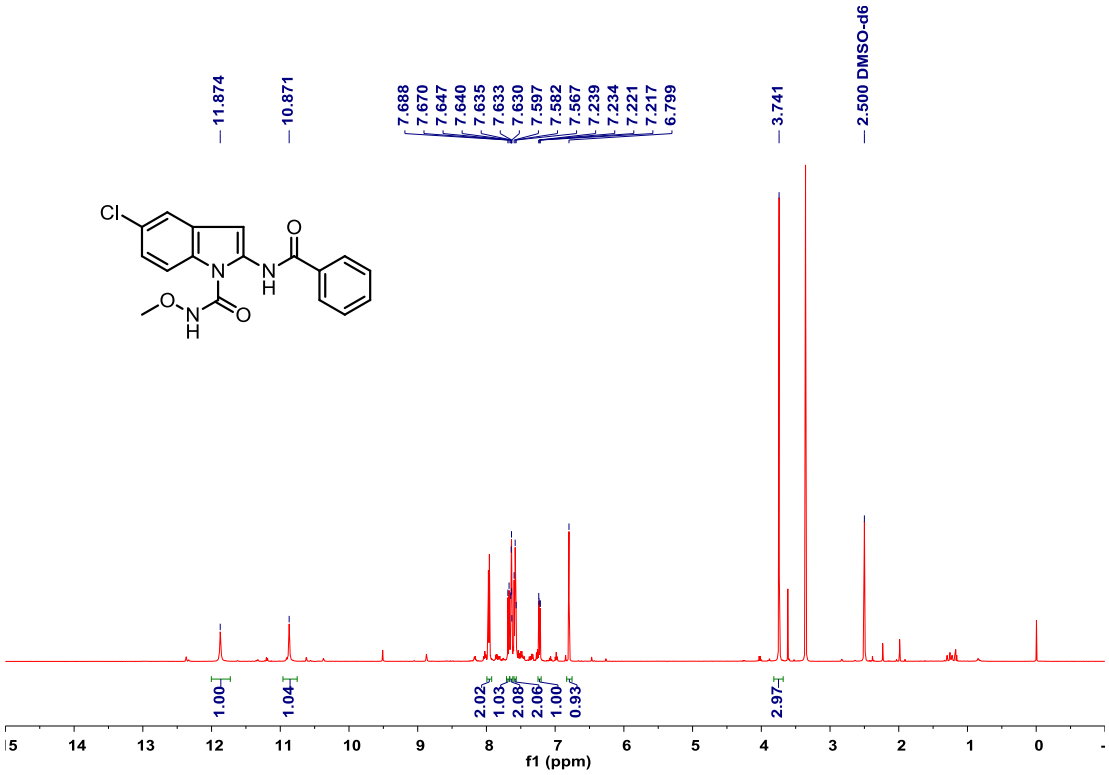


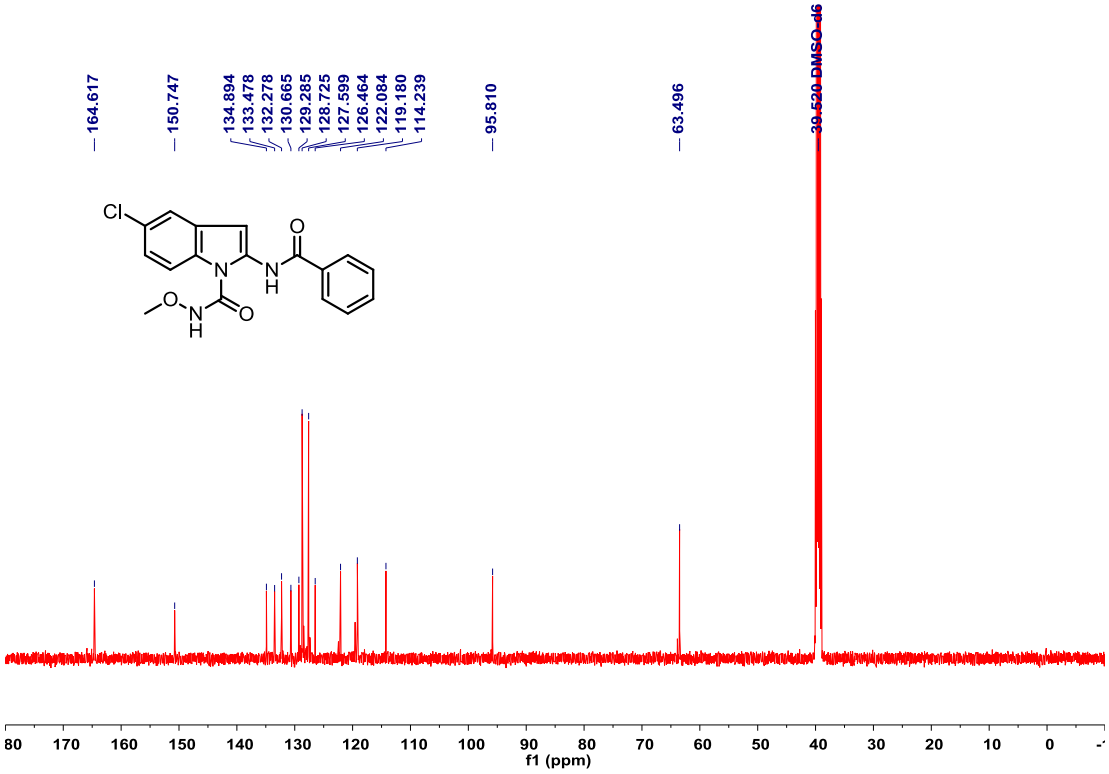
2-Benzamido-*N*-methoxy-5-methyl-1*H*-indole-1-carboxamide (3p)



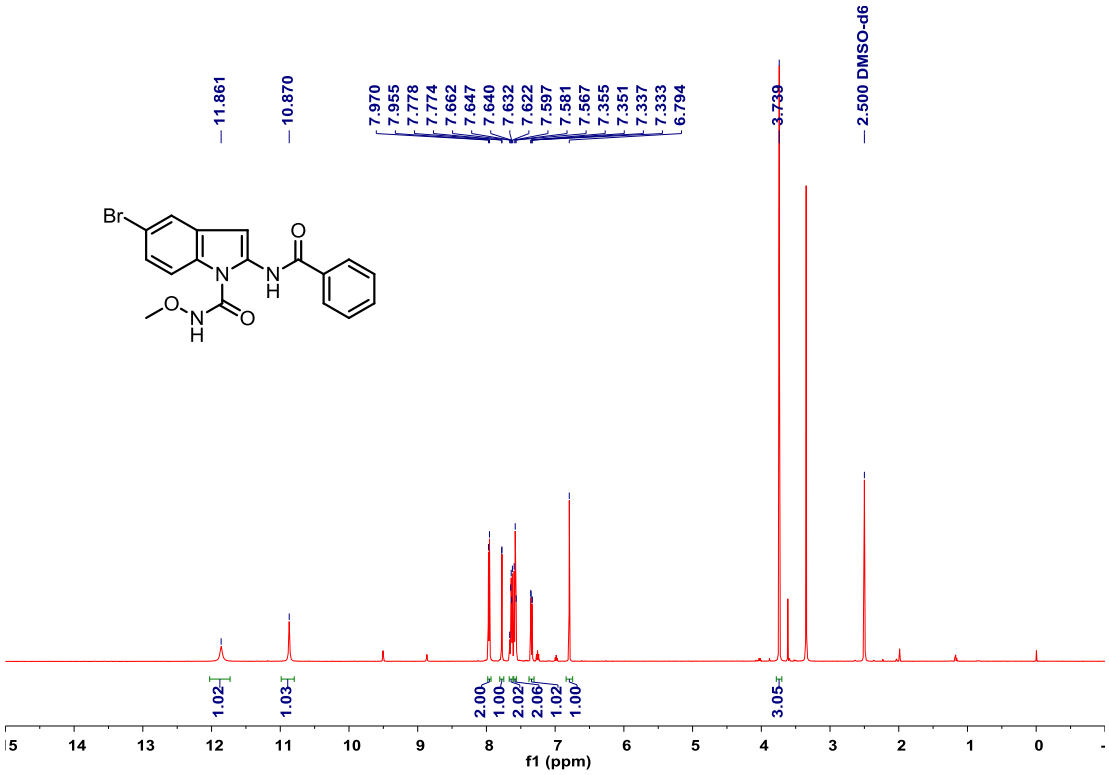


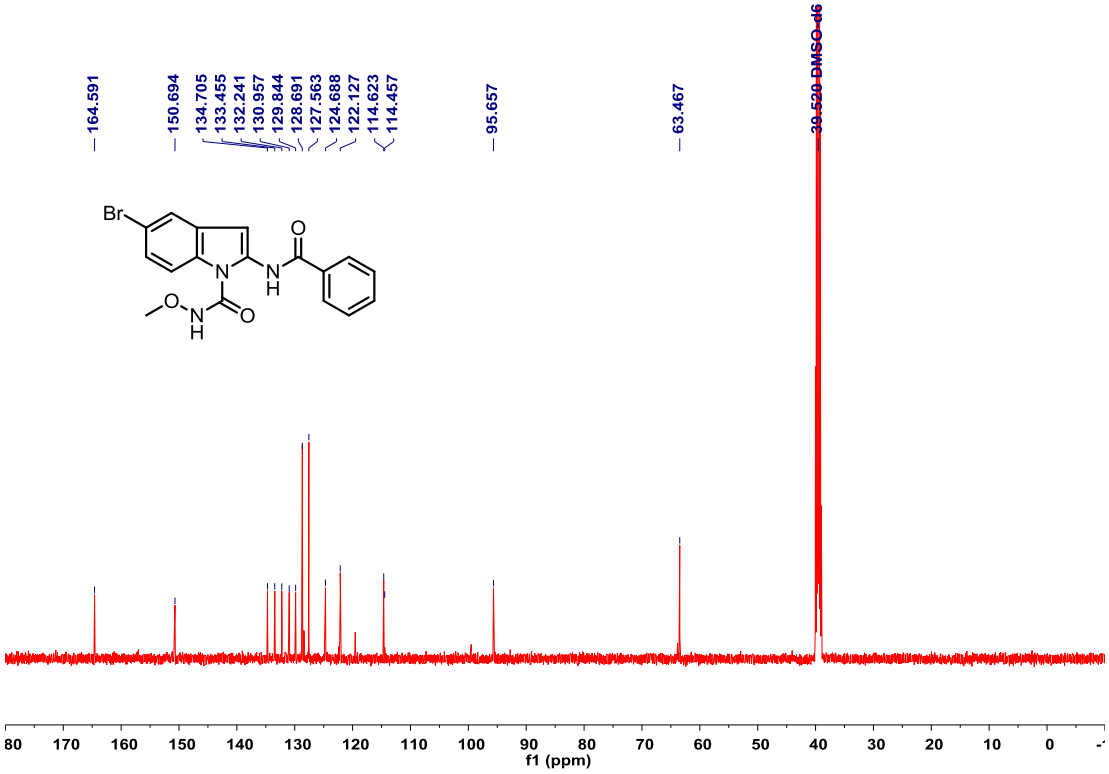
2-Benzamido-5-chloro-*N*-methoxy-1*H*-indole-1-carboxamide (3q)



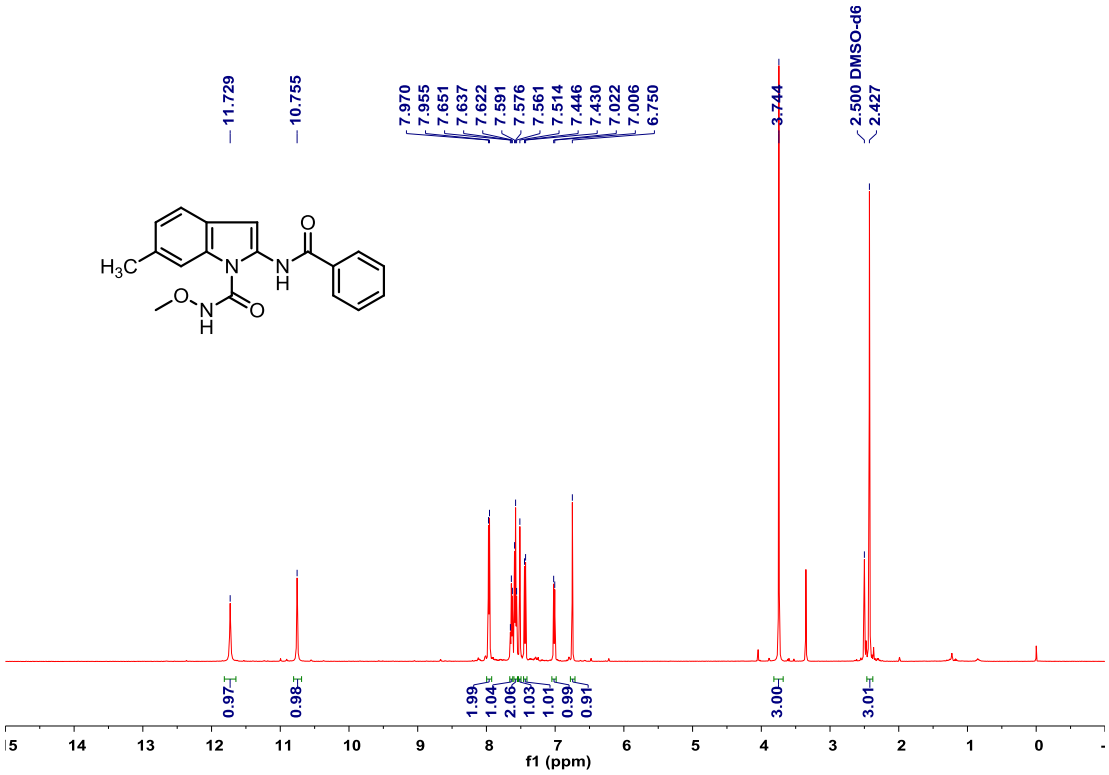


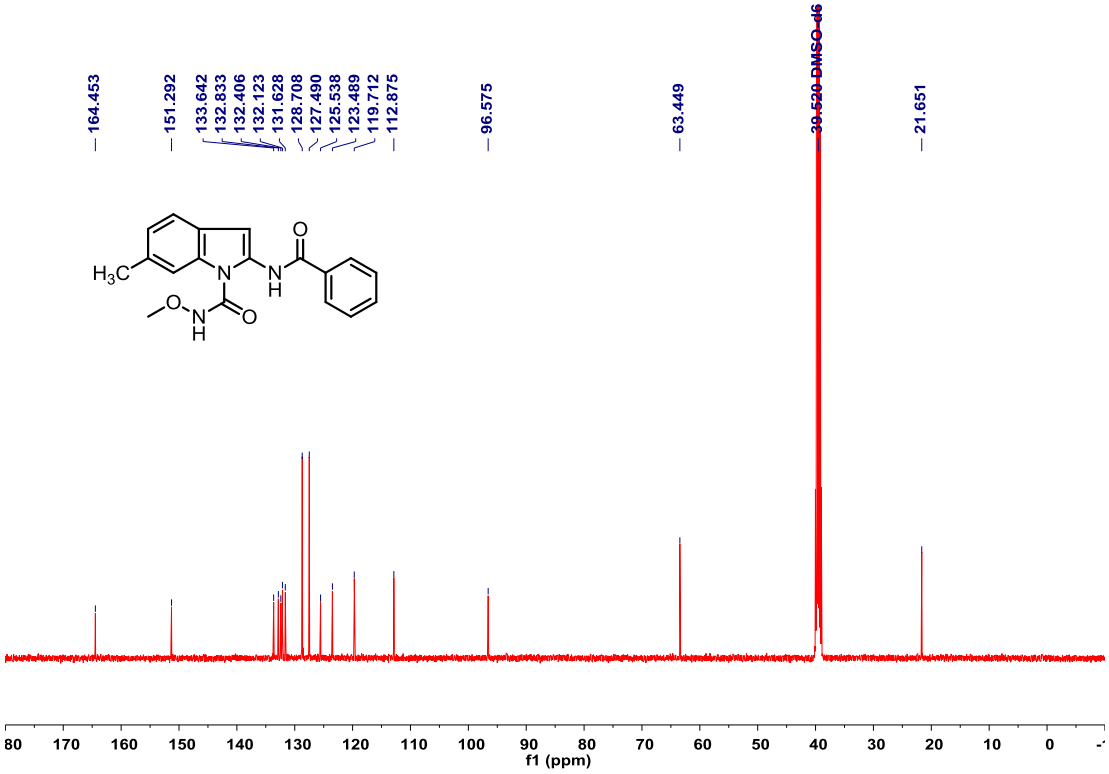
2-Benzamido-5-bromo-*N*-methoxy-1*H*-indole-1-carboxamide (3r)



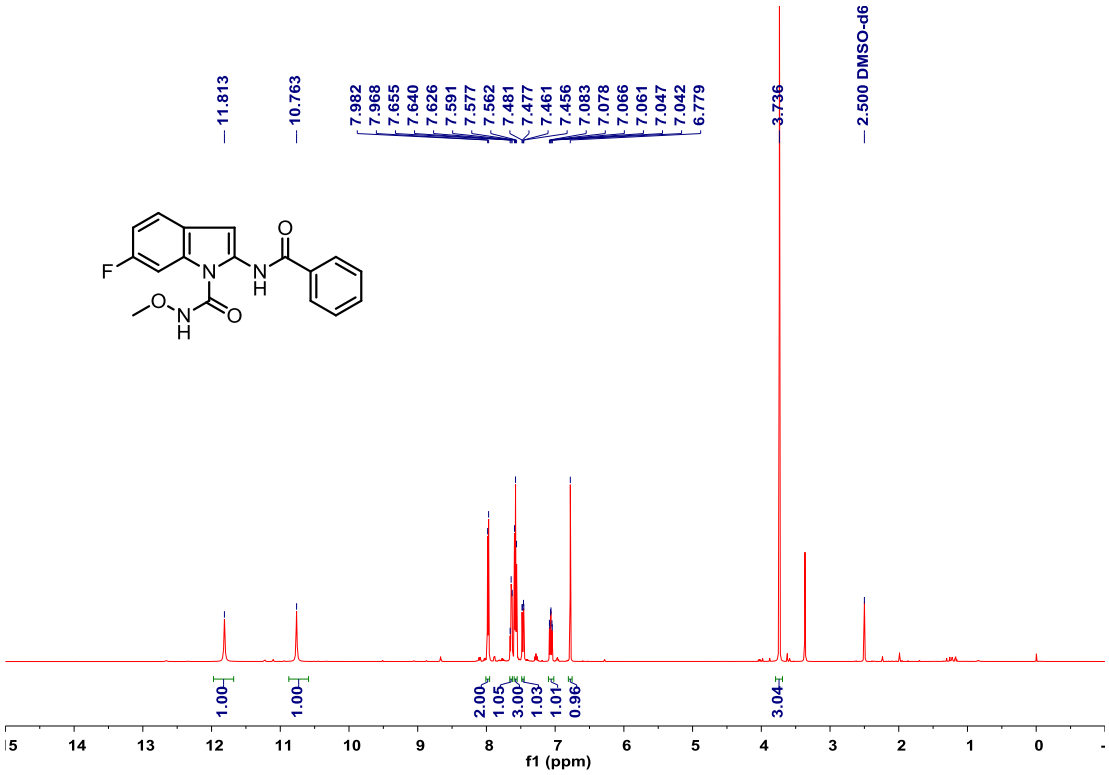


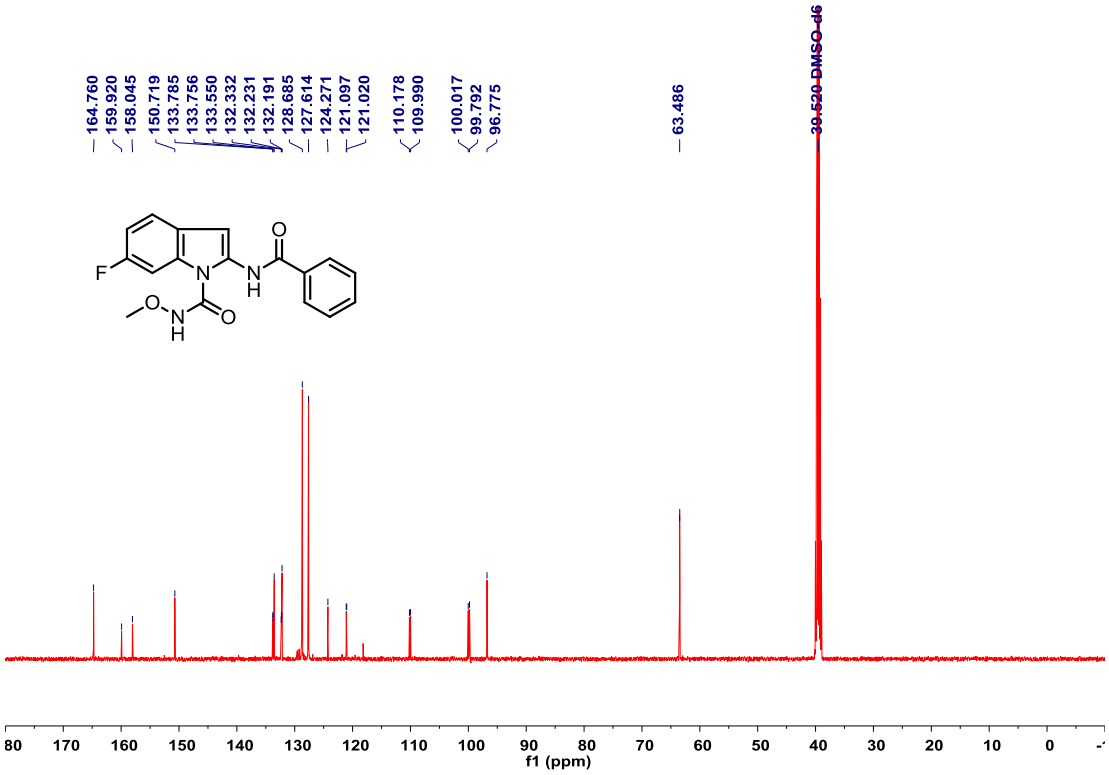
2-Benzamido-*N*-methoxy-6-methyl-1*H*-indole-1-carboxamide (3s)



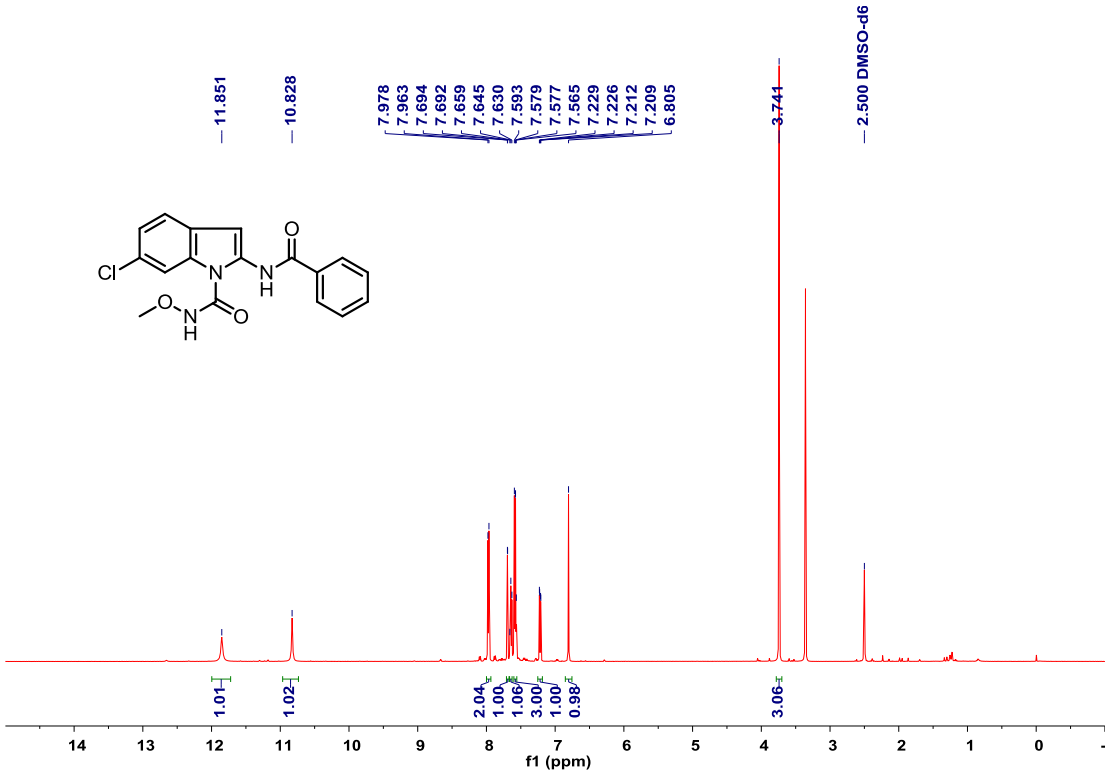


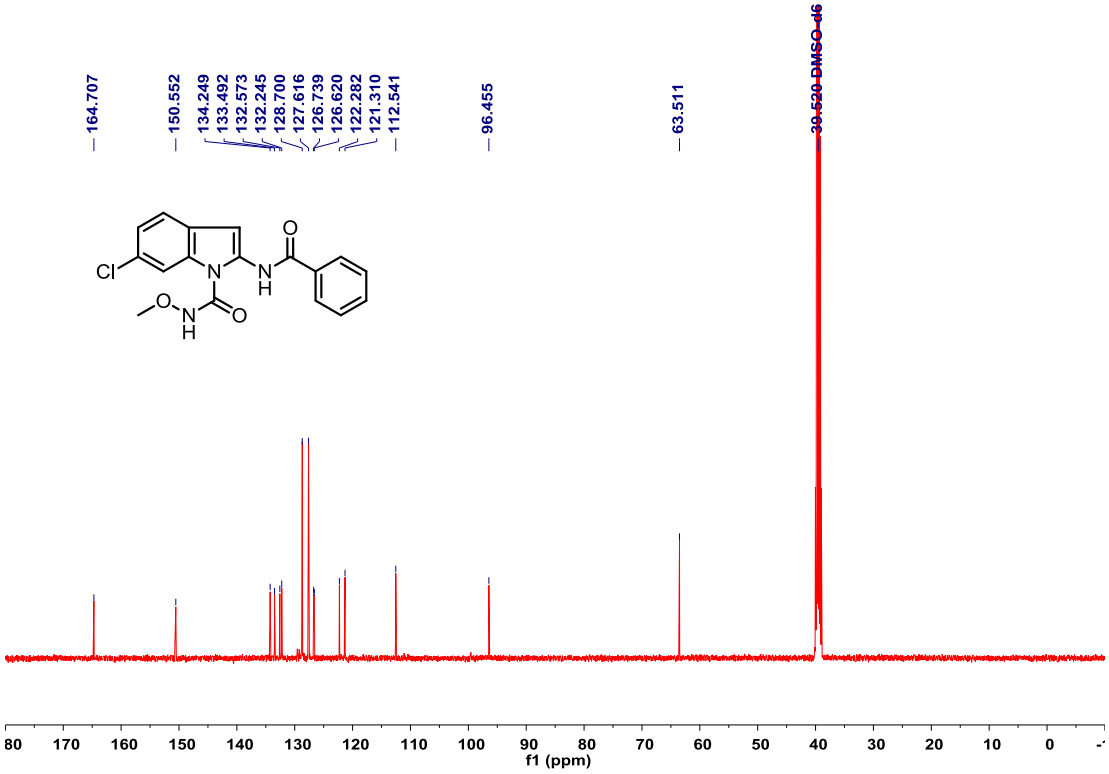
2-Benzamido-6-fluoro-*N*-methoxy-1*H*-indole-1-carboxamide (3t)



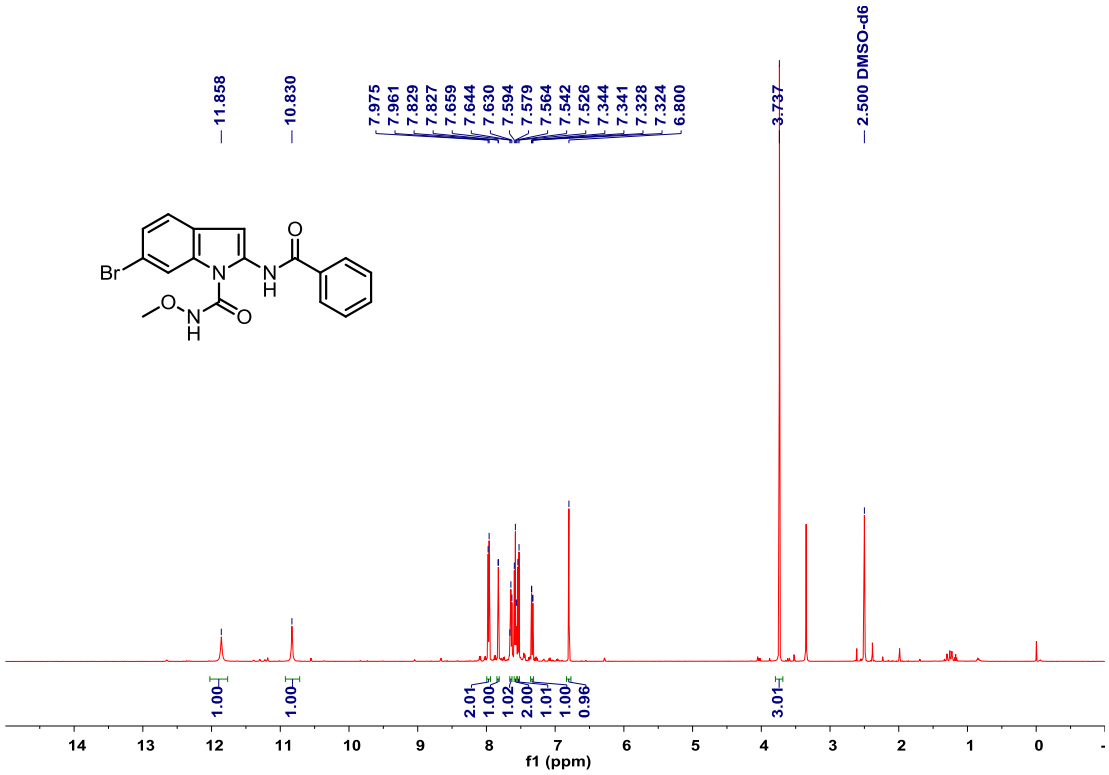


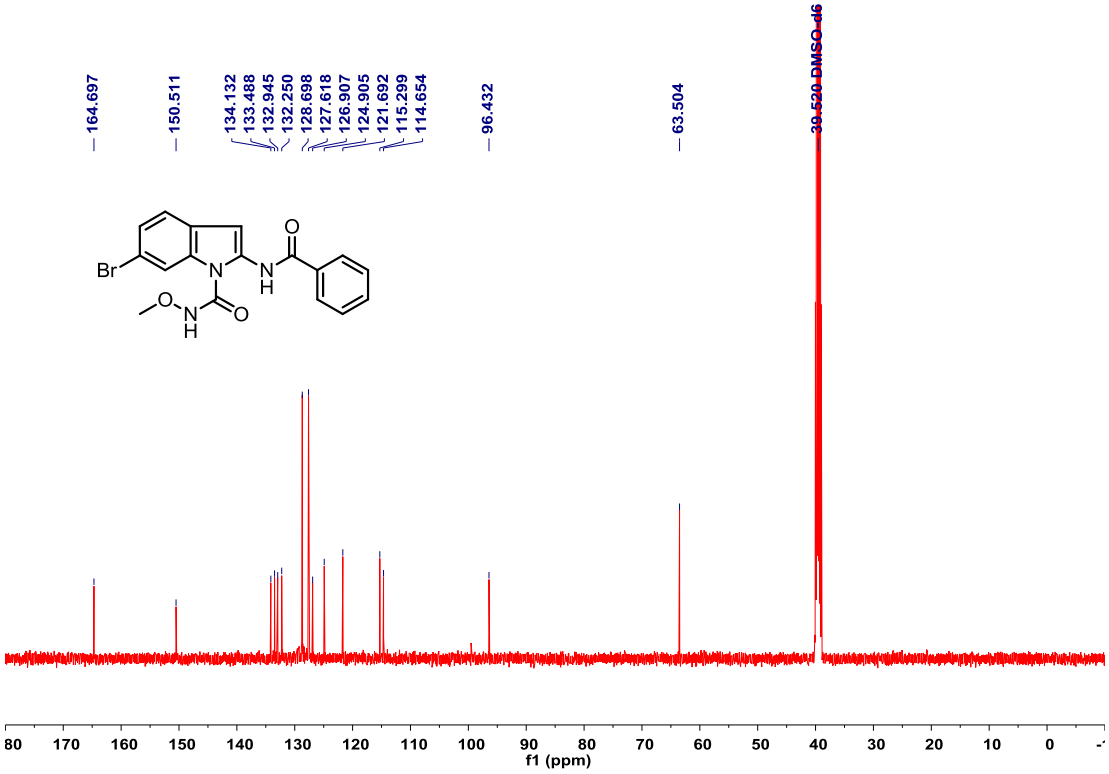
2-Benzamido-6-chloro-*N*-methoxy-1*H*-indole-1-carboxamide (3u)



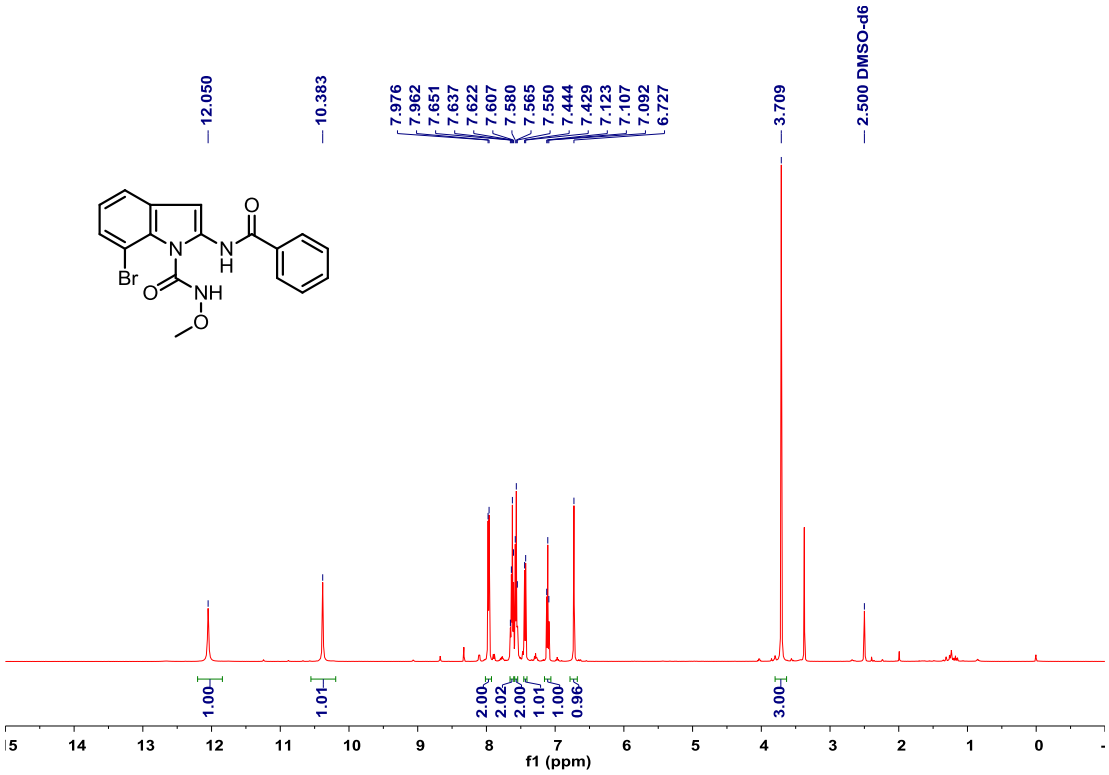


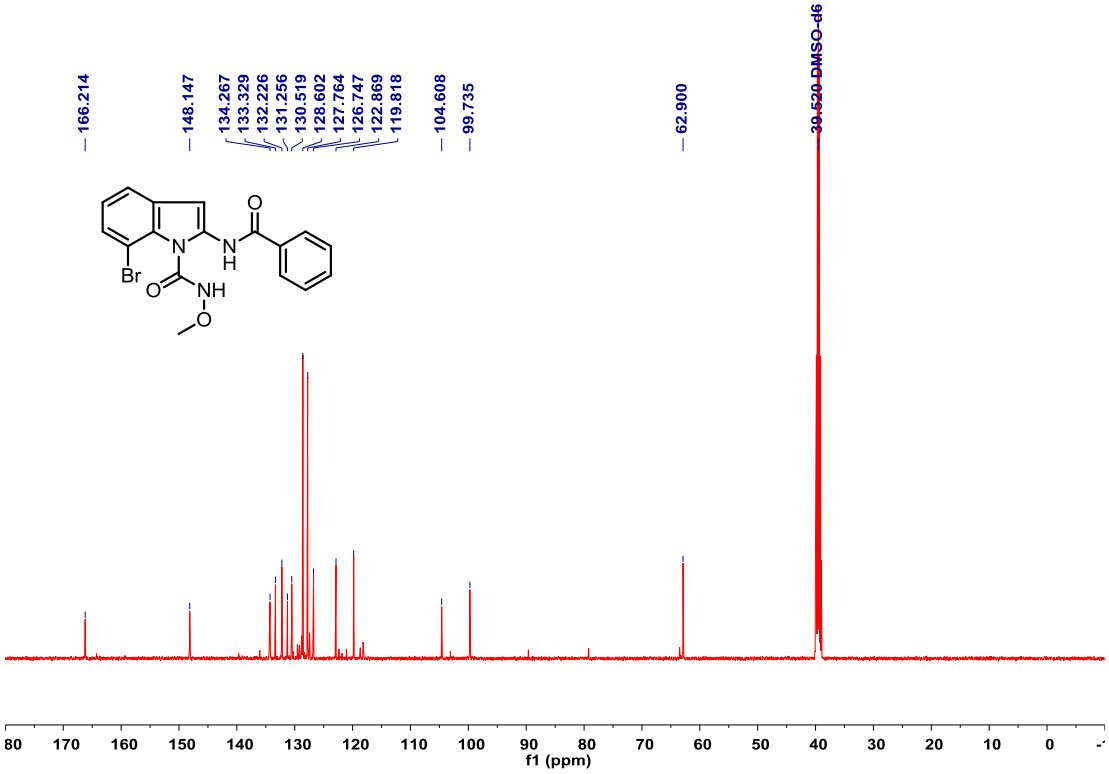
2-Benzamido-6-bromo-*N*-methoxy-1*H*-indole-1-carboxamide (3v)



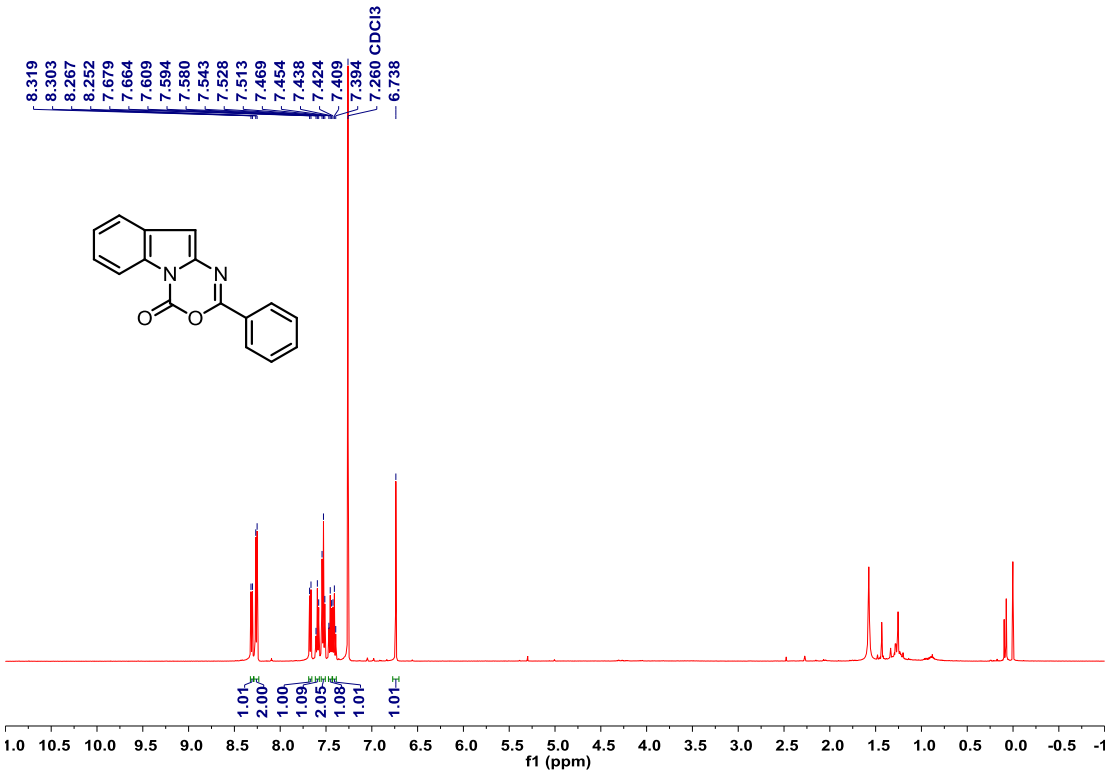


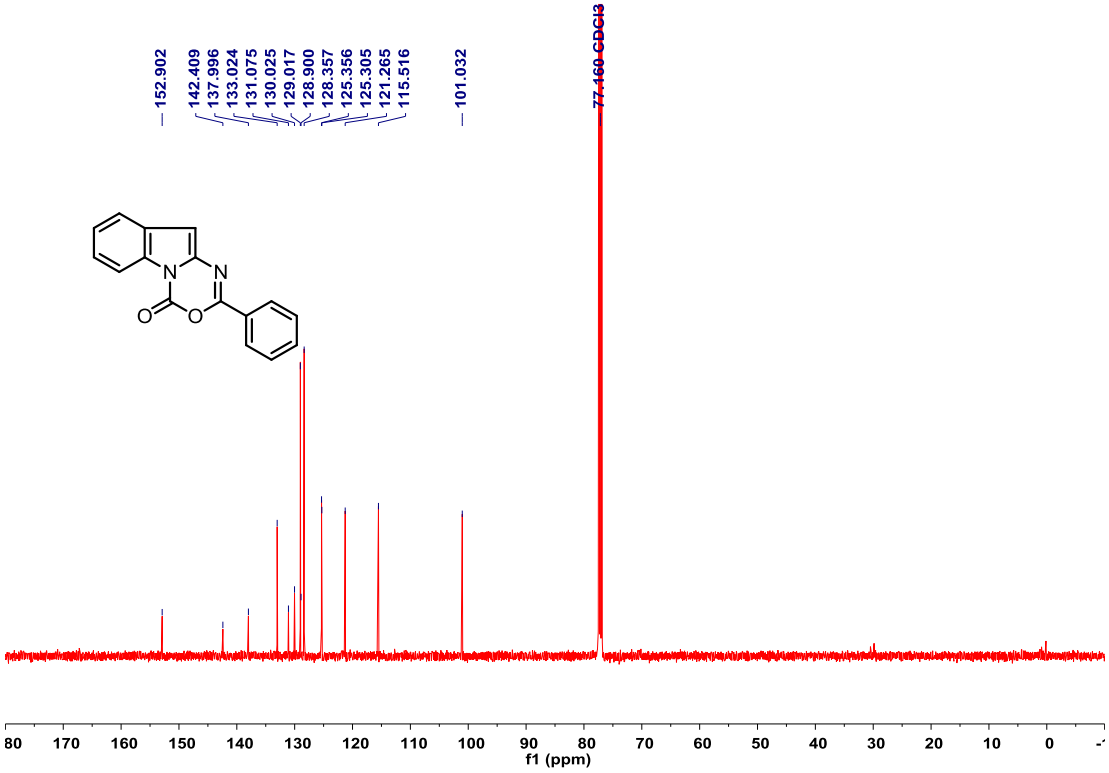
2-Benzamido-*N*-methoxy-7-methyl-1*H*-indole-1-carboxamide (3w)



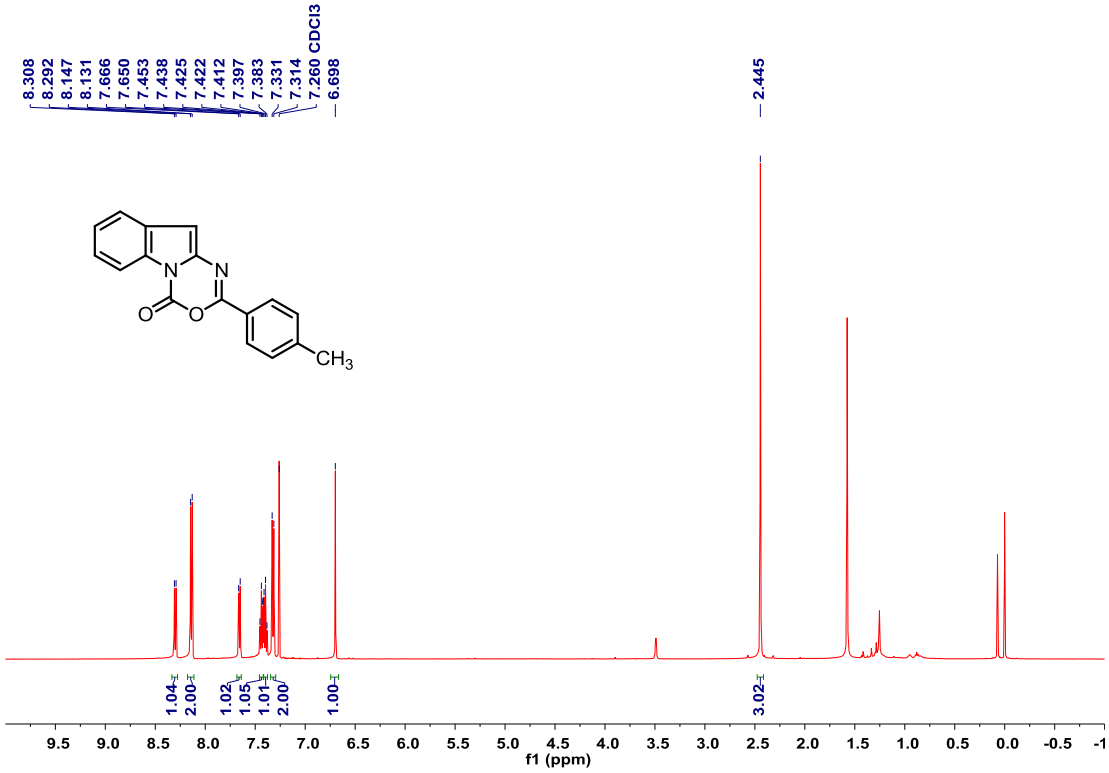


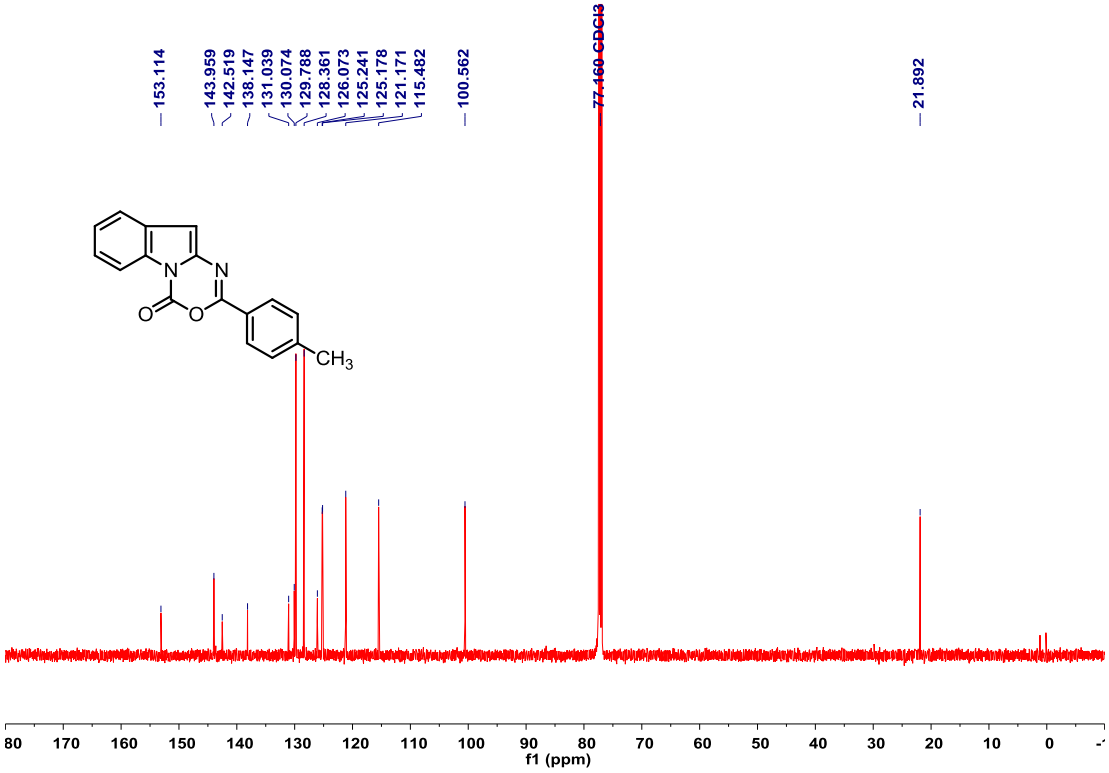
2-Phenyl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4a)



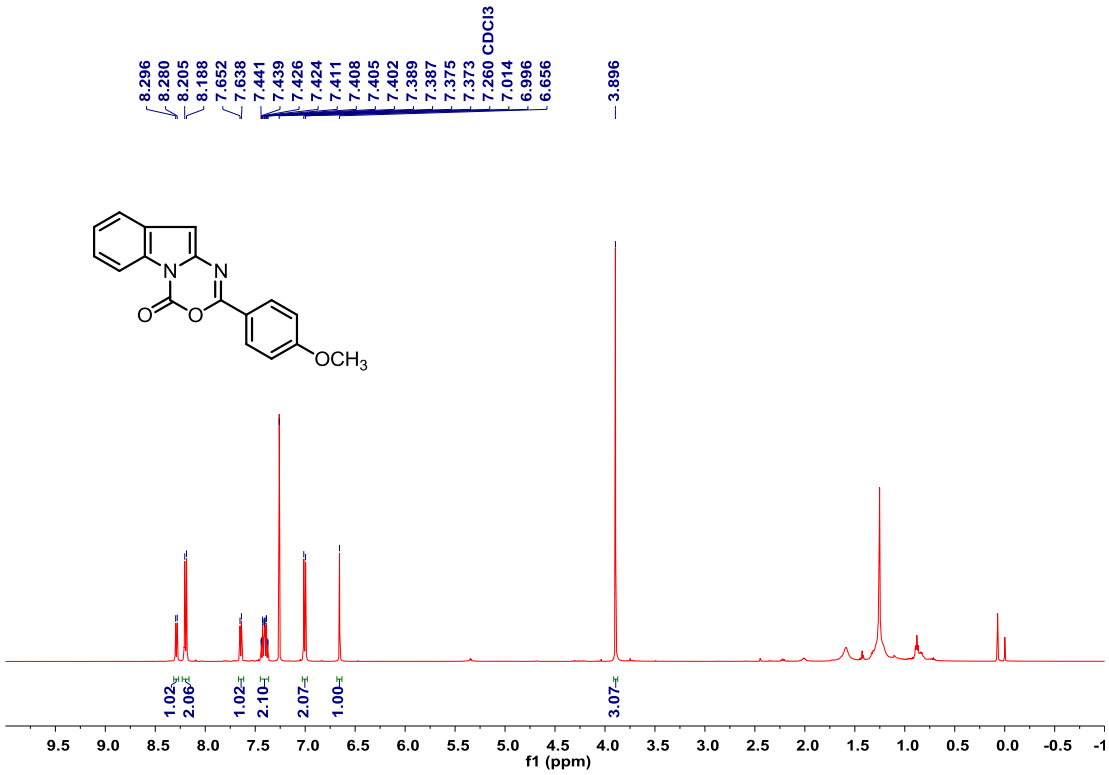


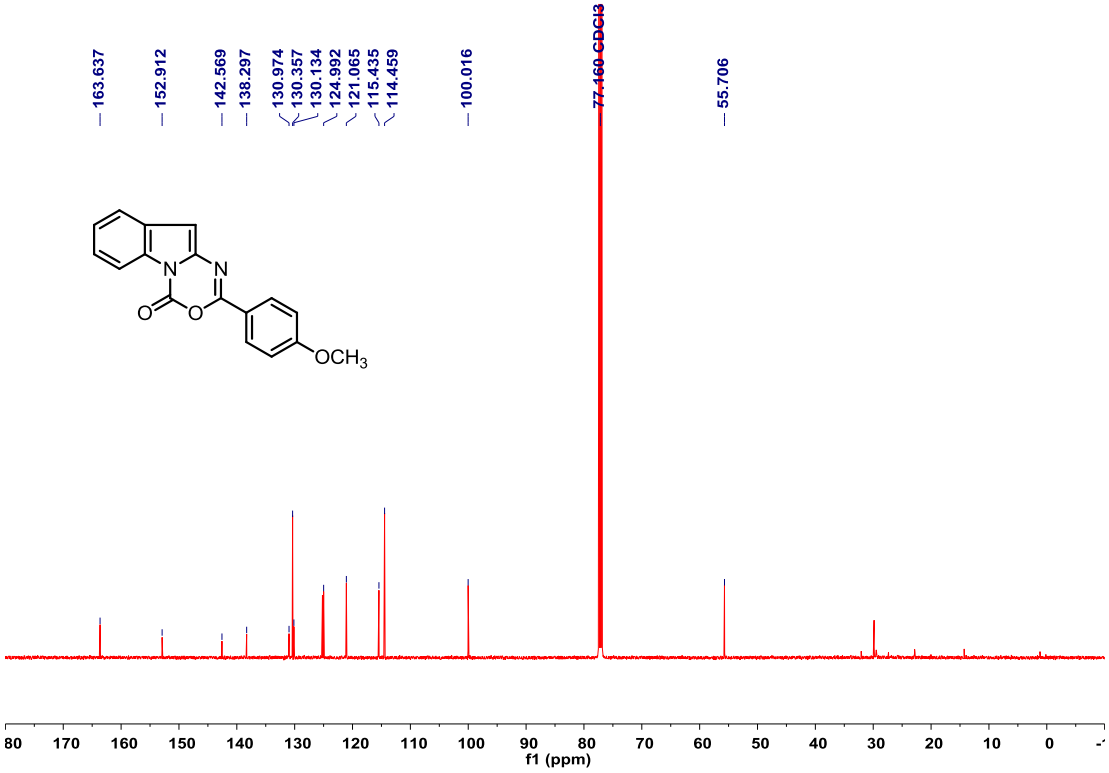
2-(p-Tolyl)-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4b)



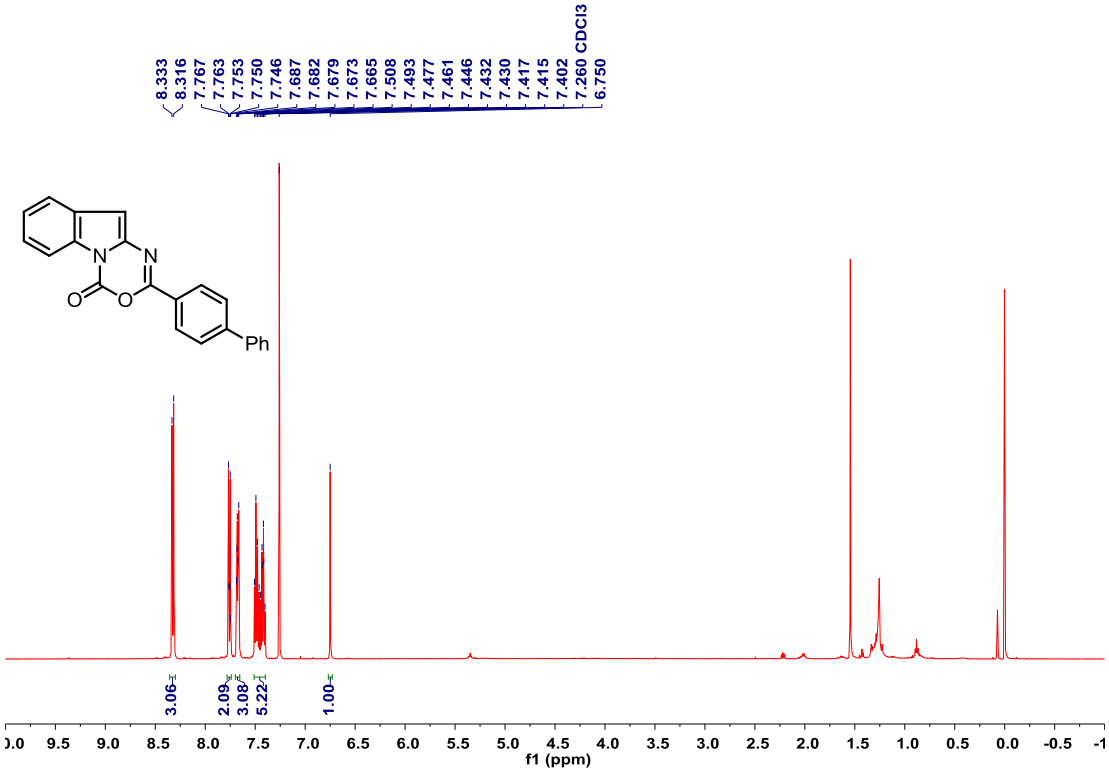


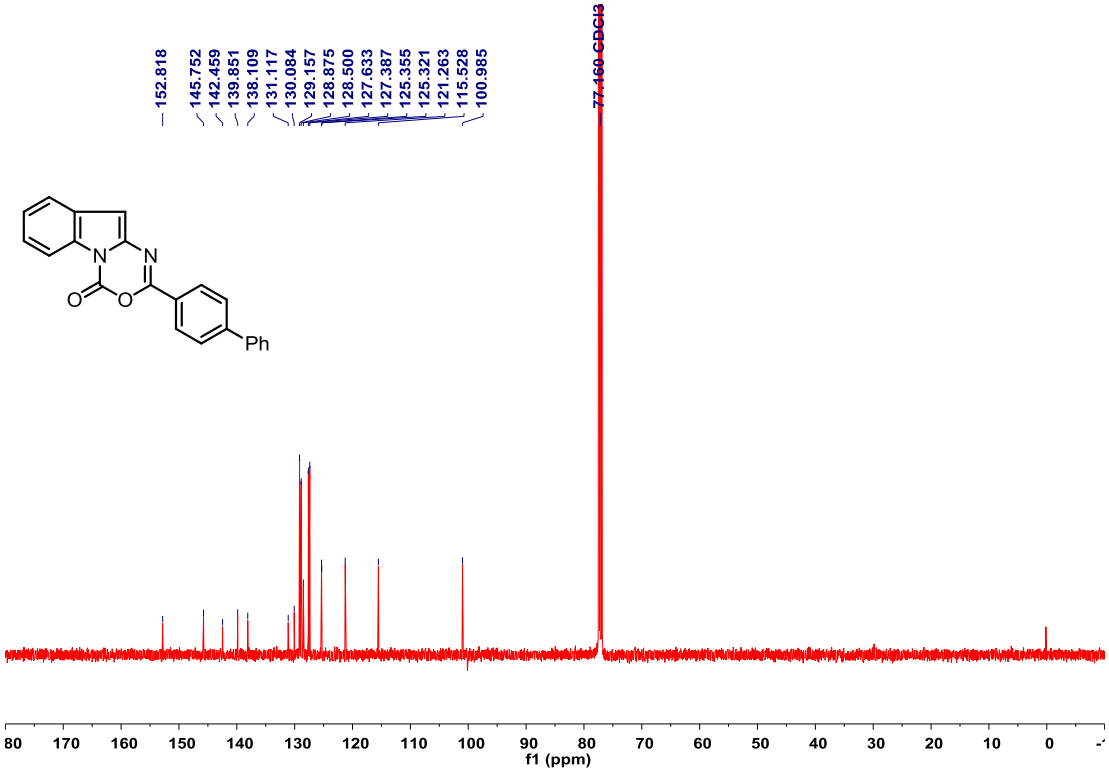
2-(4-Methoxyphenyl)-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4c)



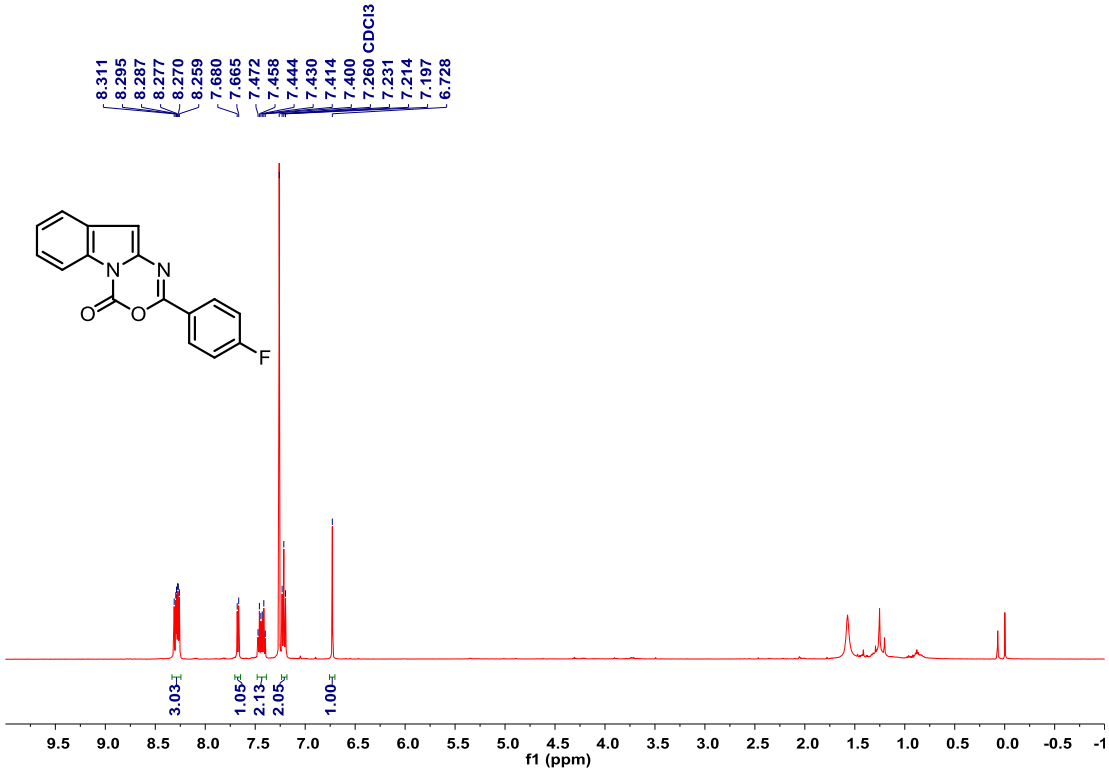


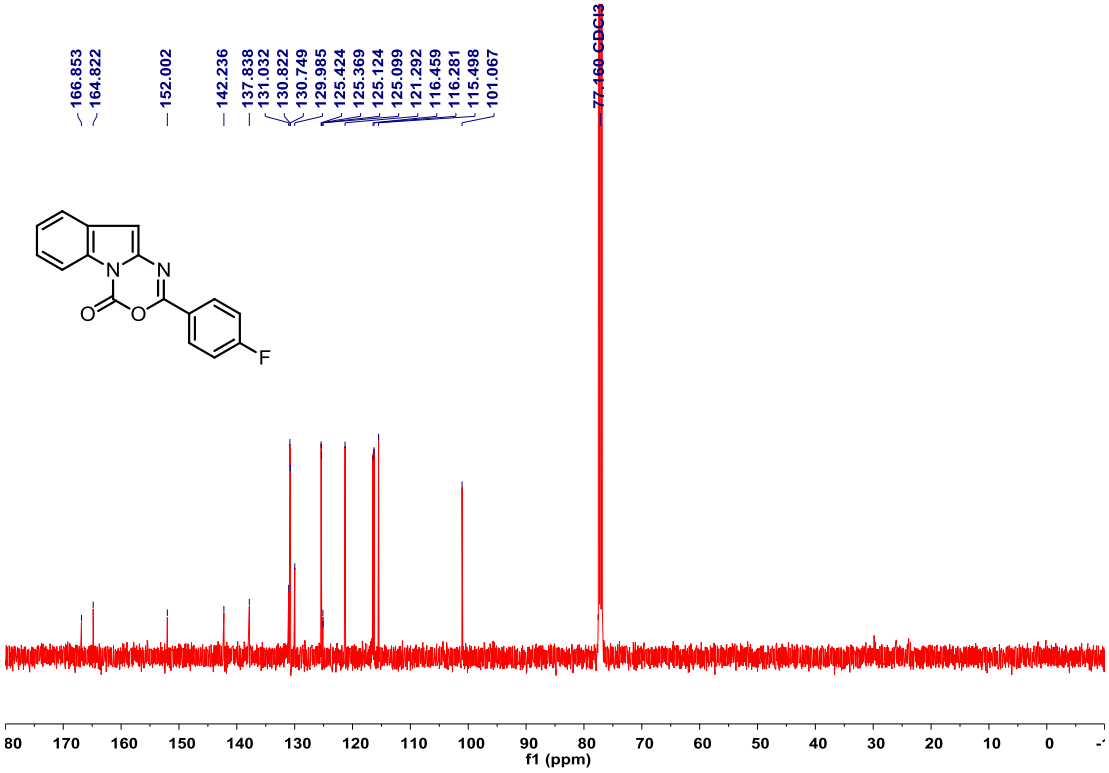
2-([1,1'-Biphenyl]-4-yl)-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4d)



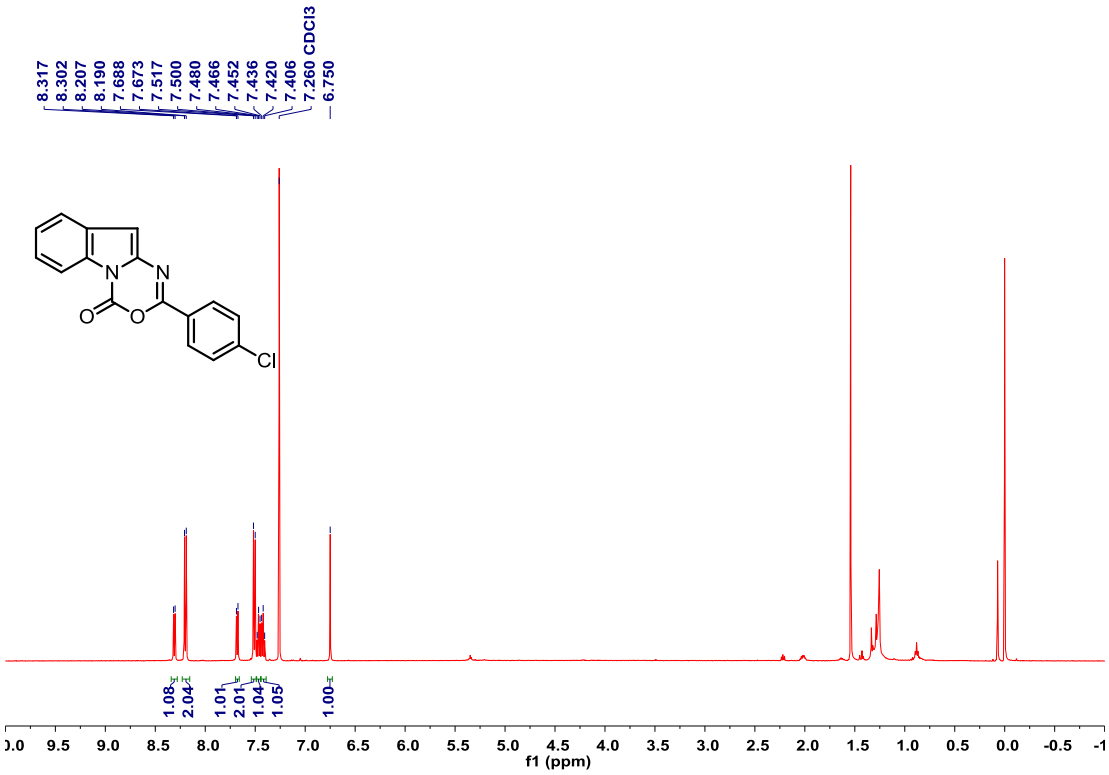


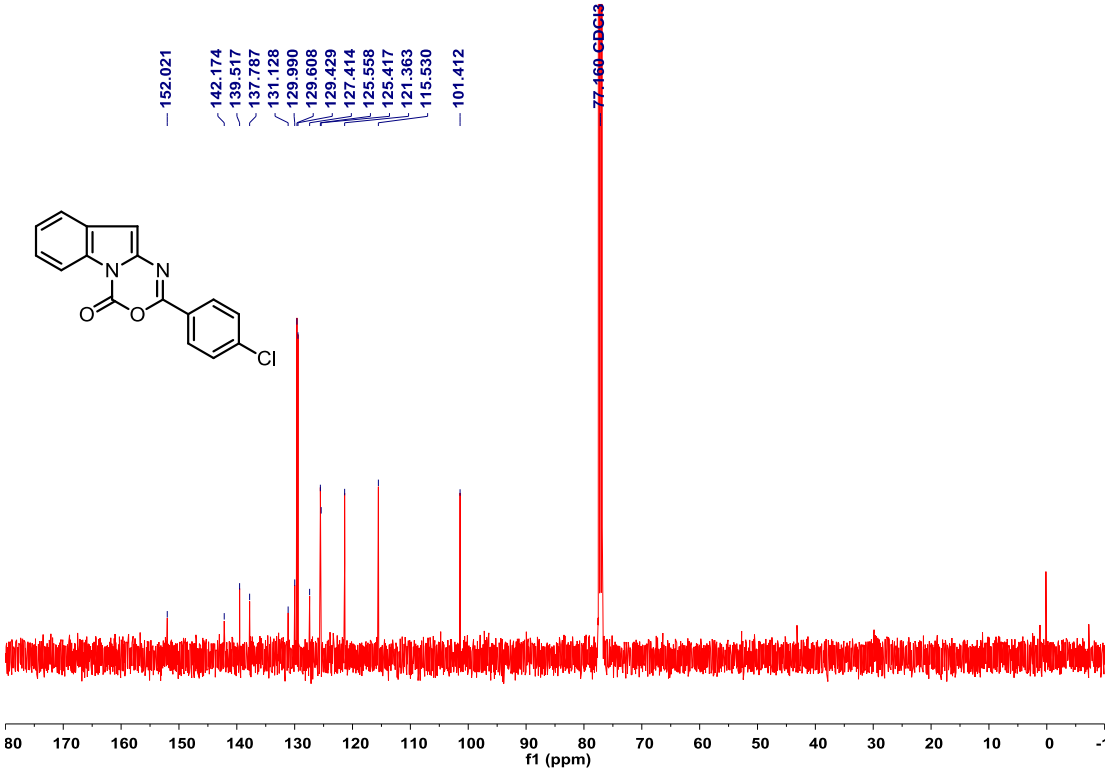
2-(4-Fluorophenyl)-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4e)



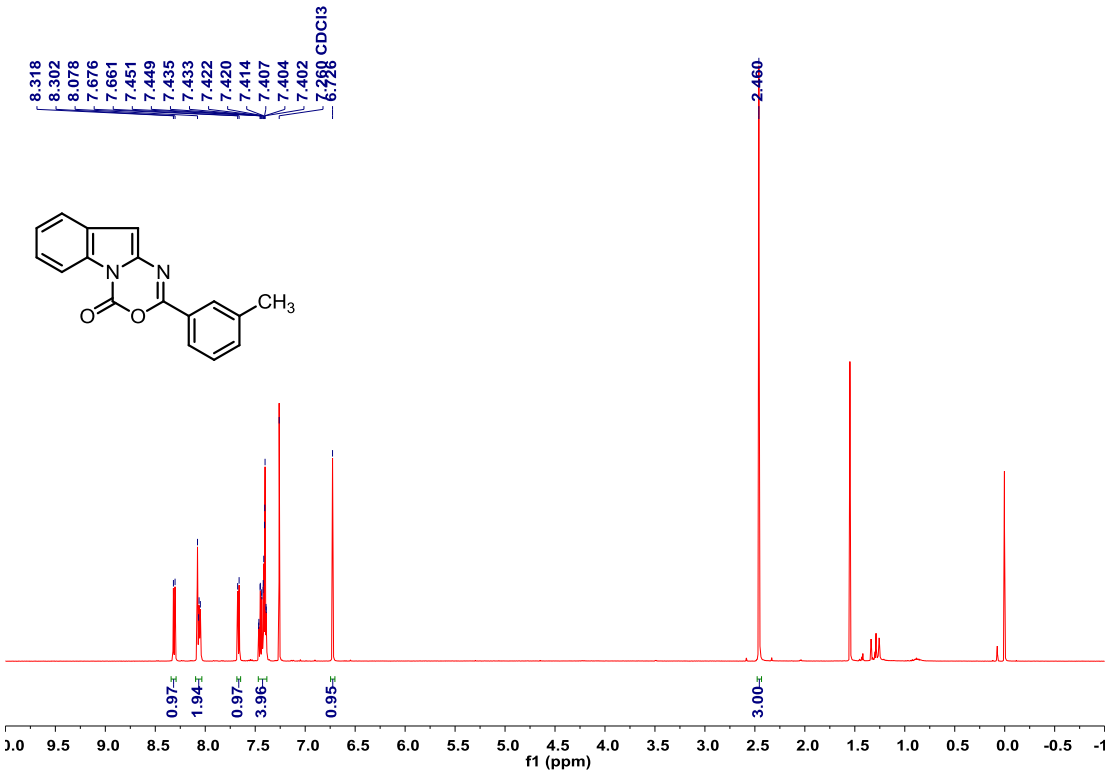


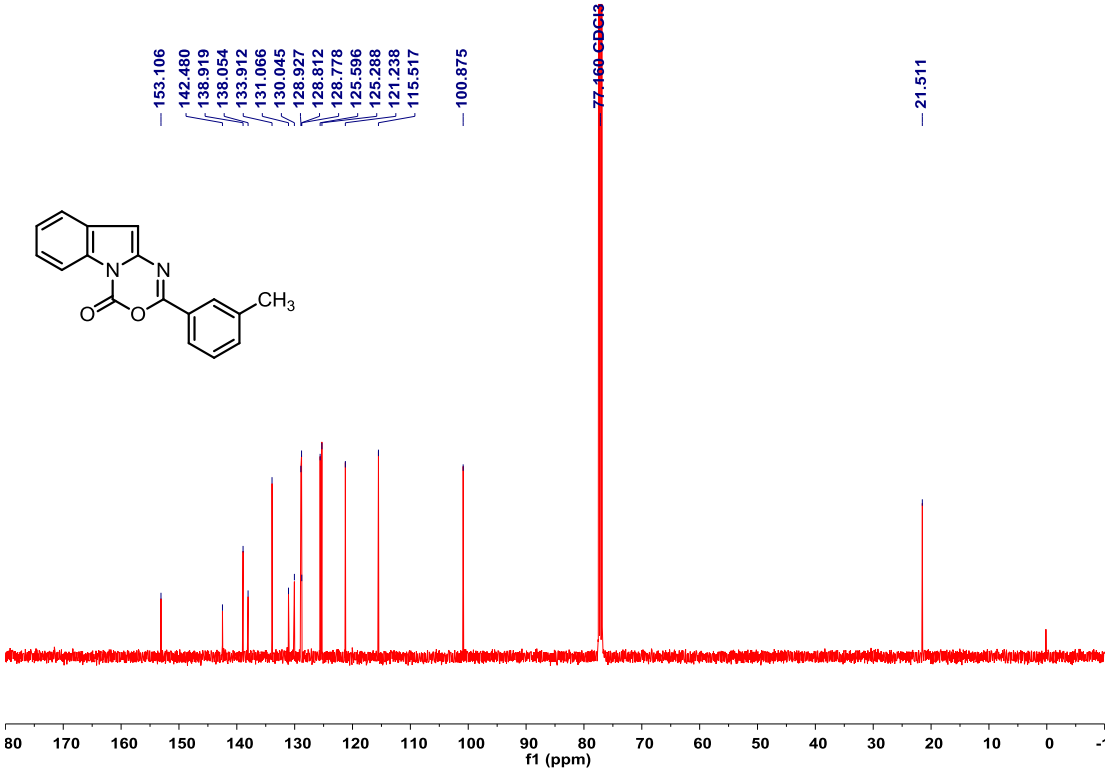
2-(4-Chlorophenyl)-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4f)



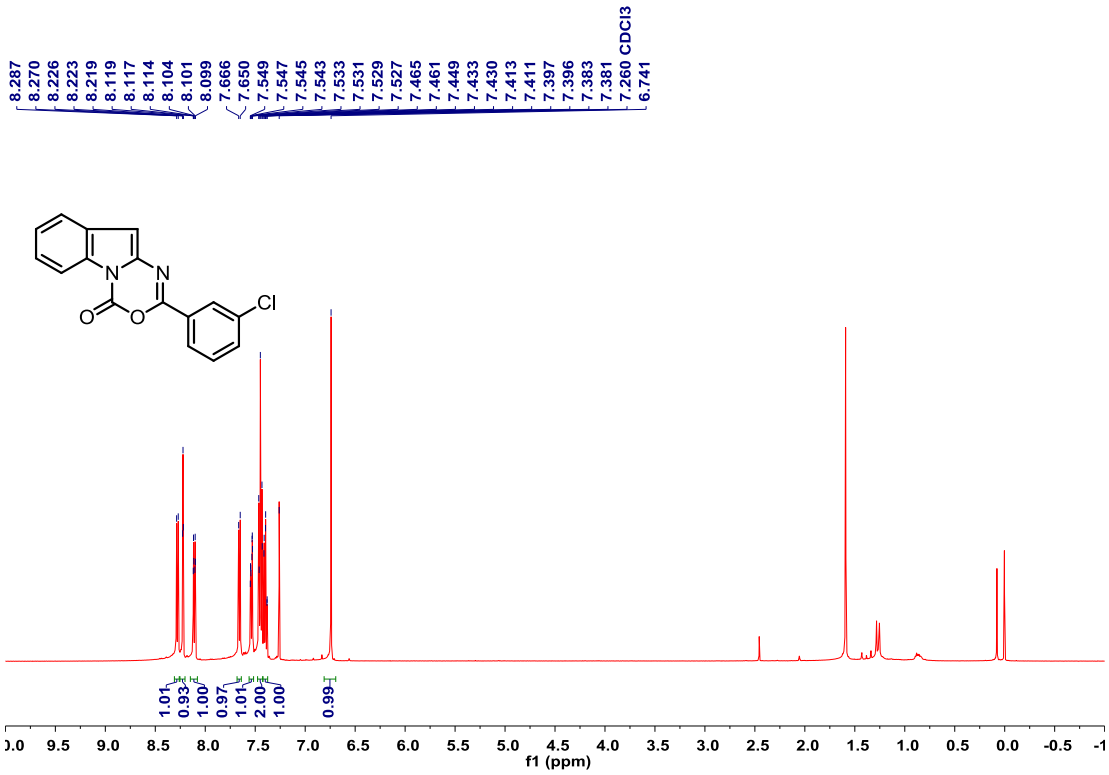


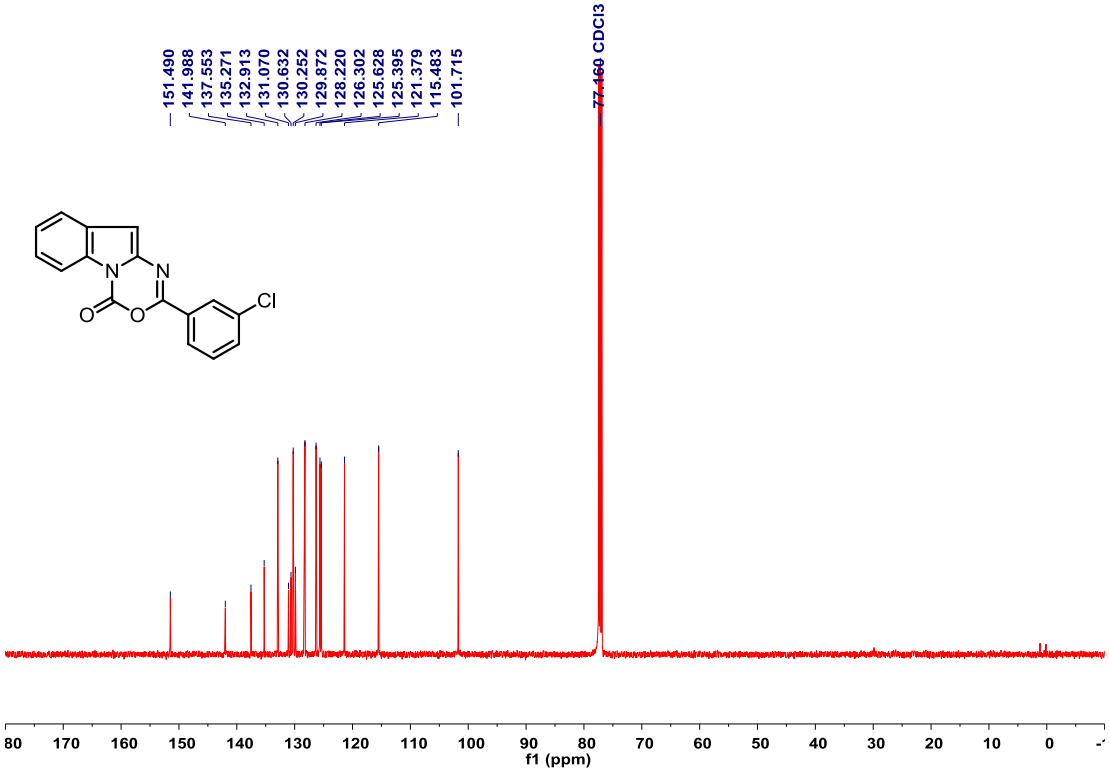
2-(m-Tolyl)-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4g)



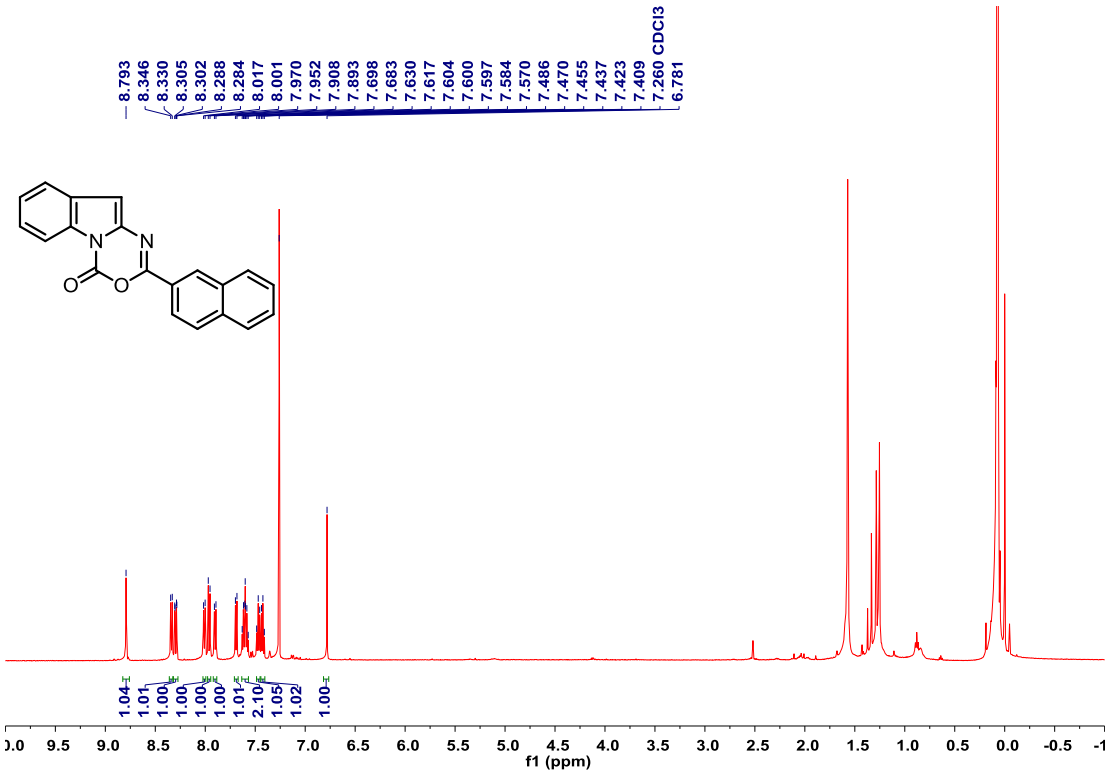


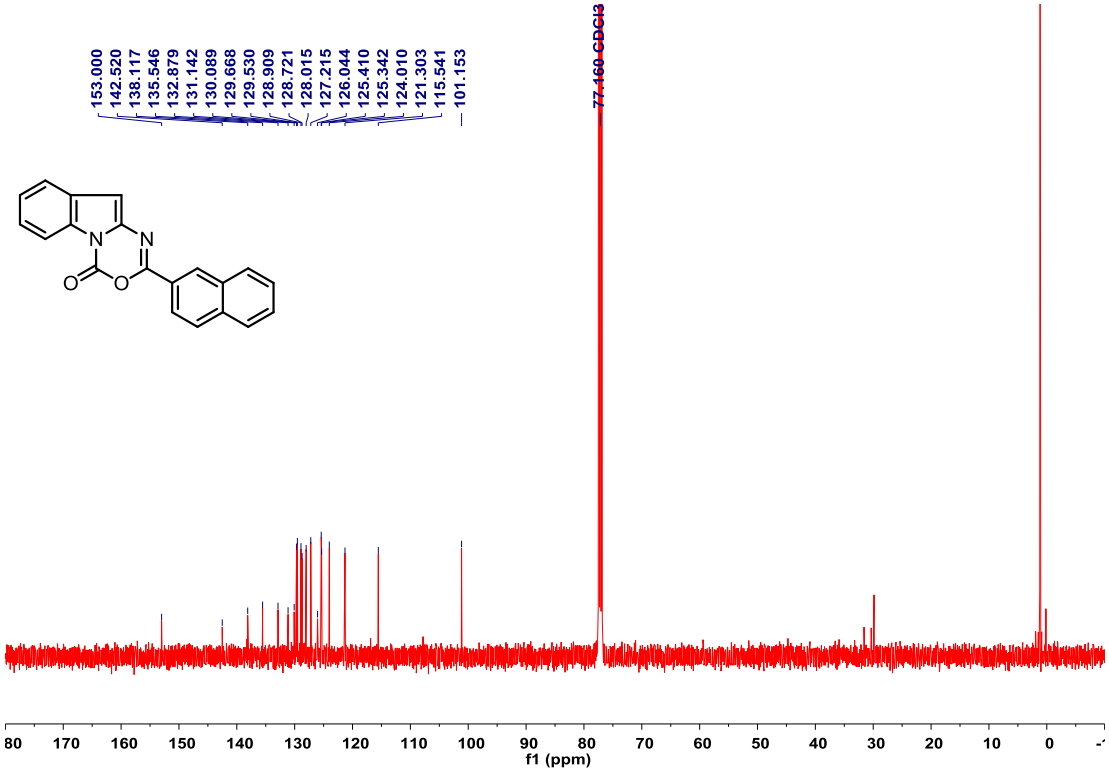
2-(3-Chlorophenyl)-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4h)



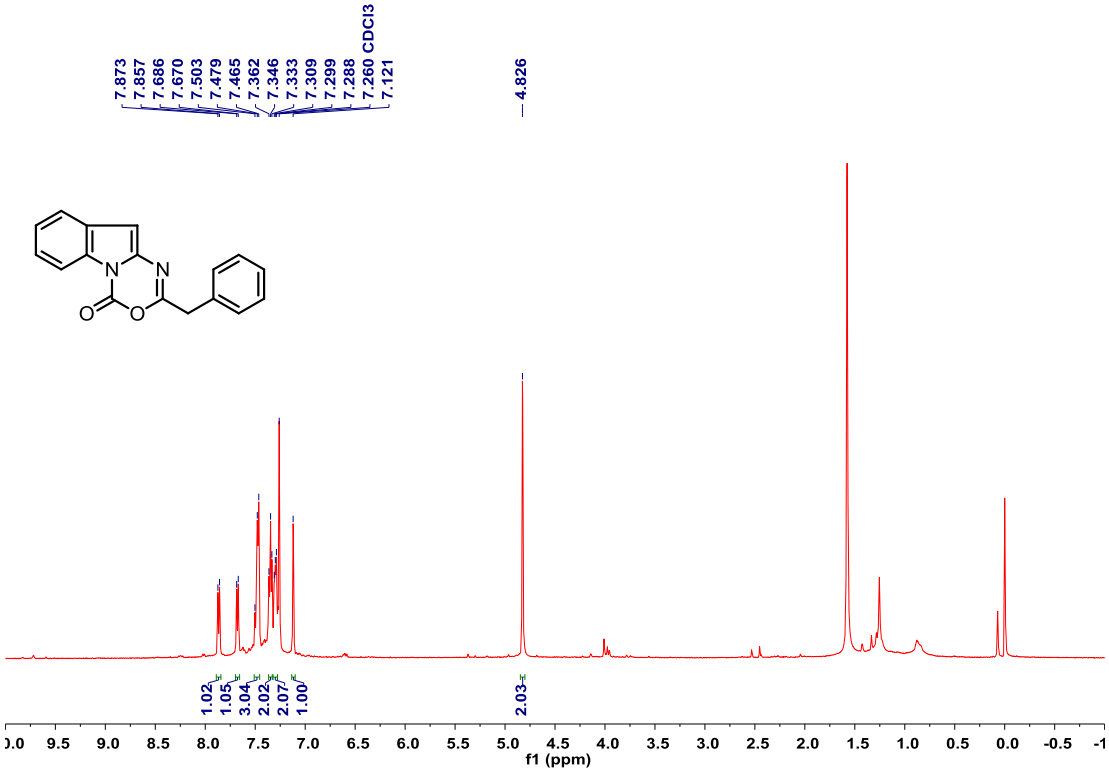


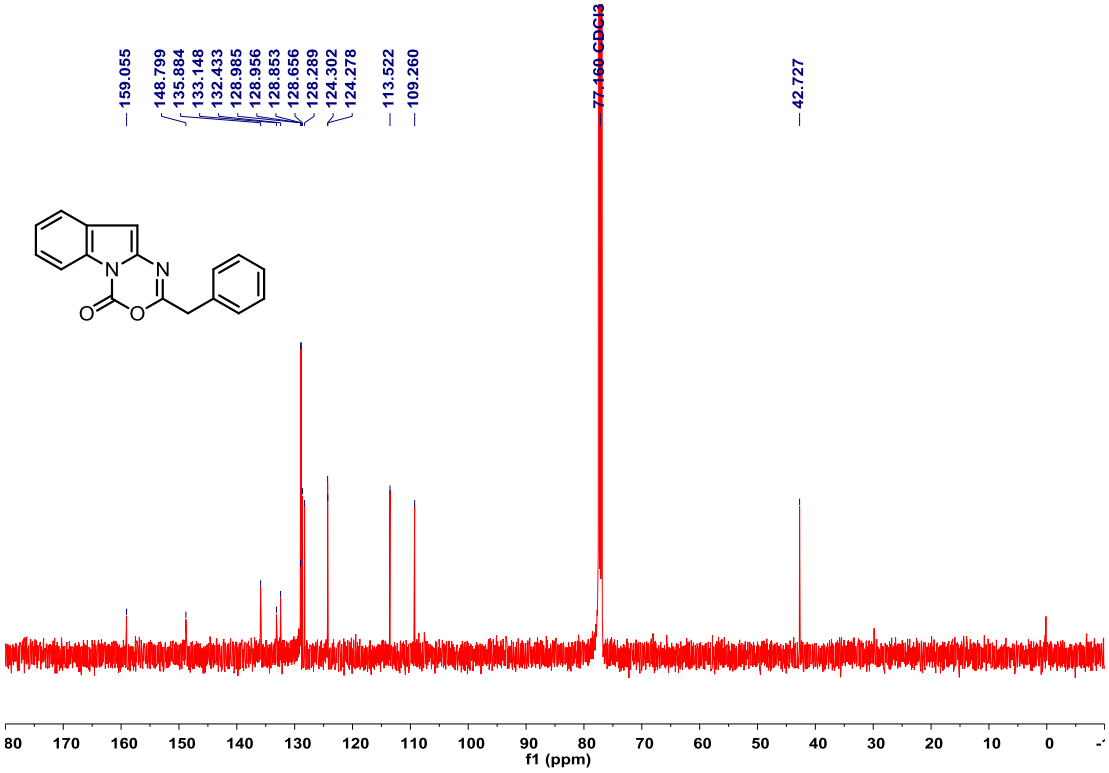
2-(Naphthalen-2-yl)-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4i)



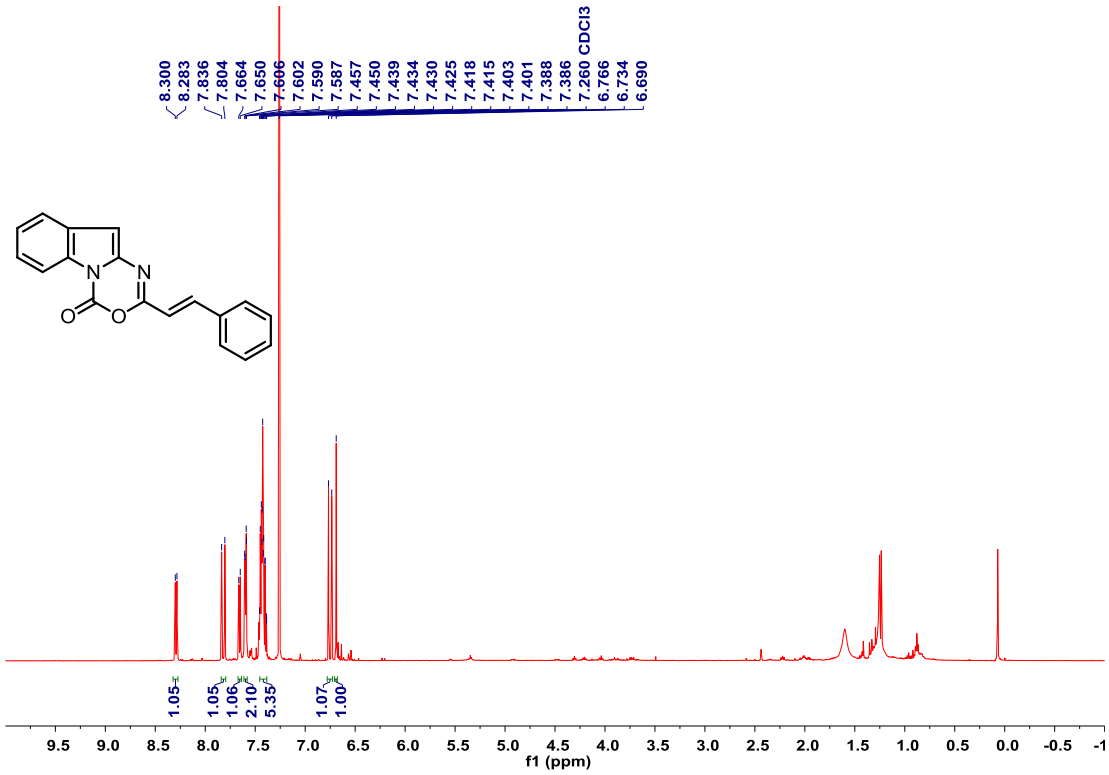


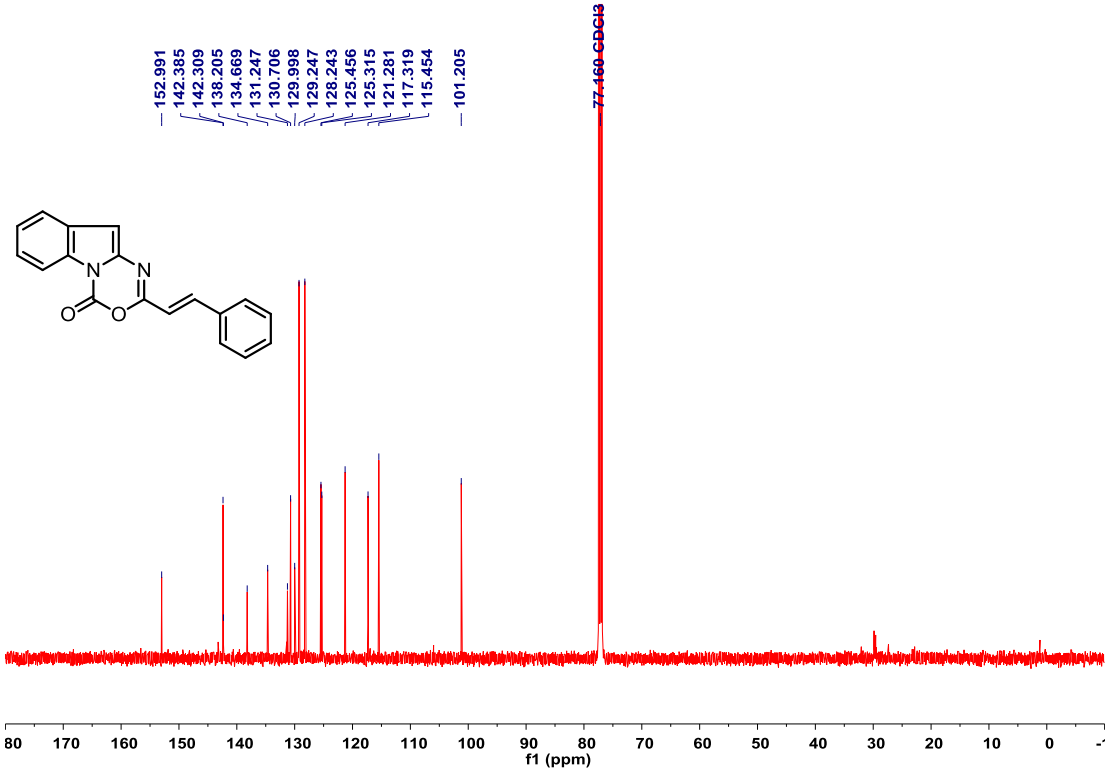
2-Benzyl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4j)



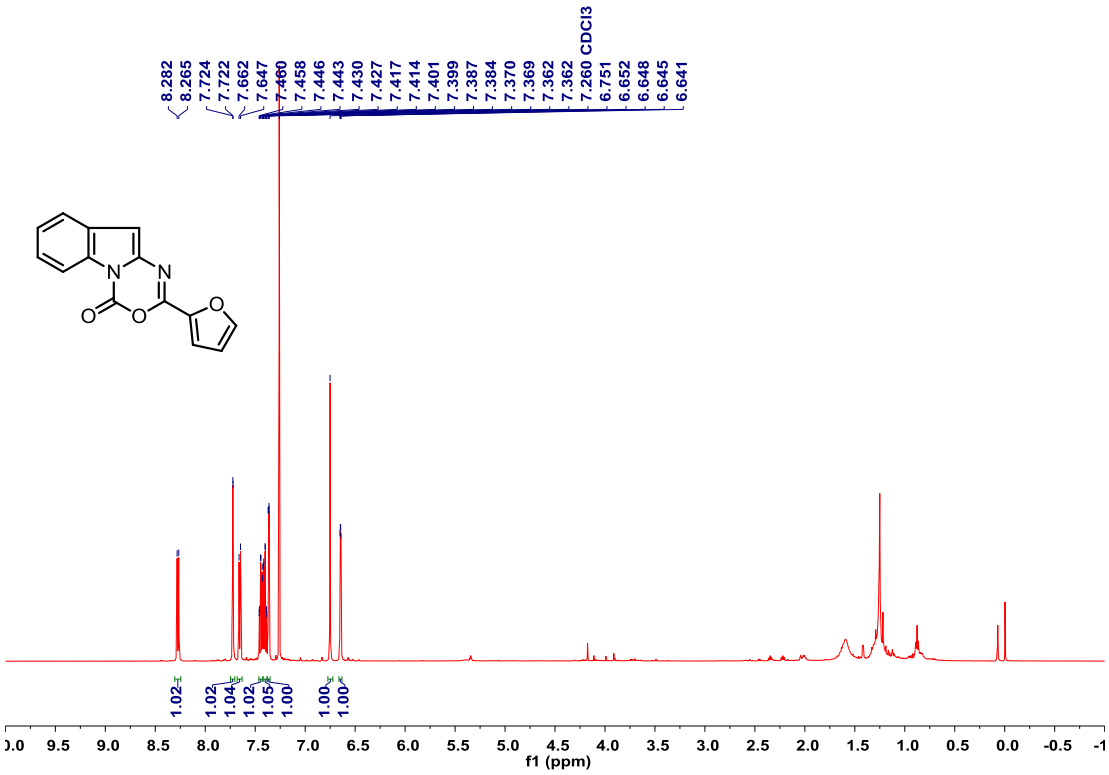


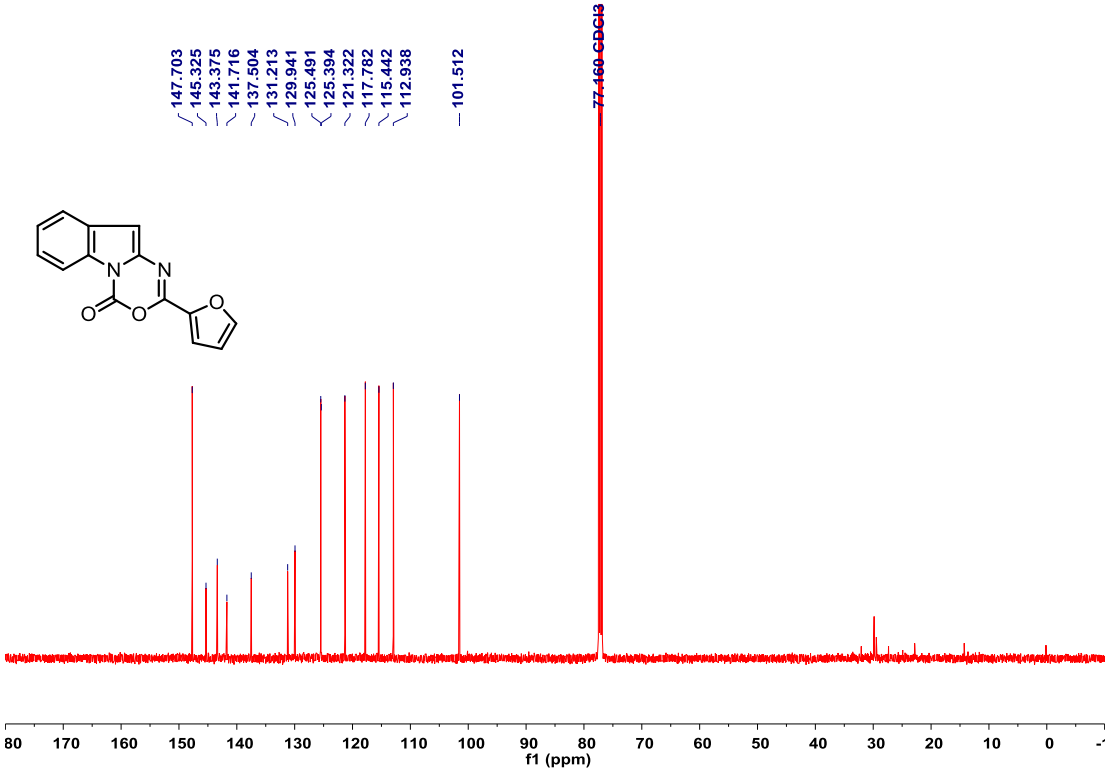
(*E*)-2-Styryl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4k)



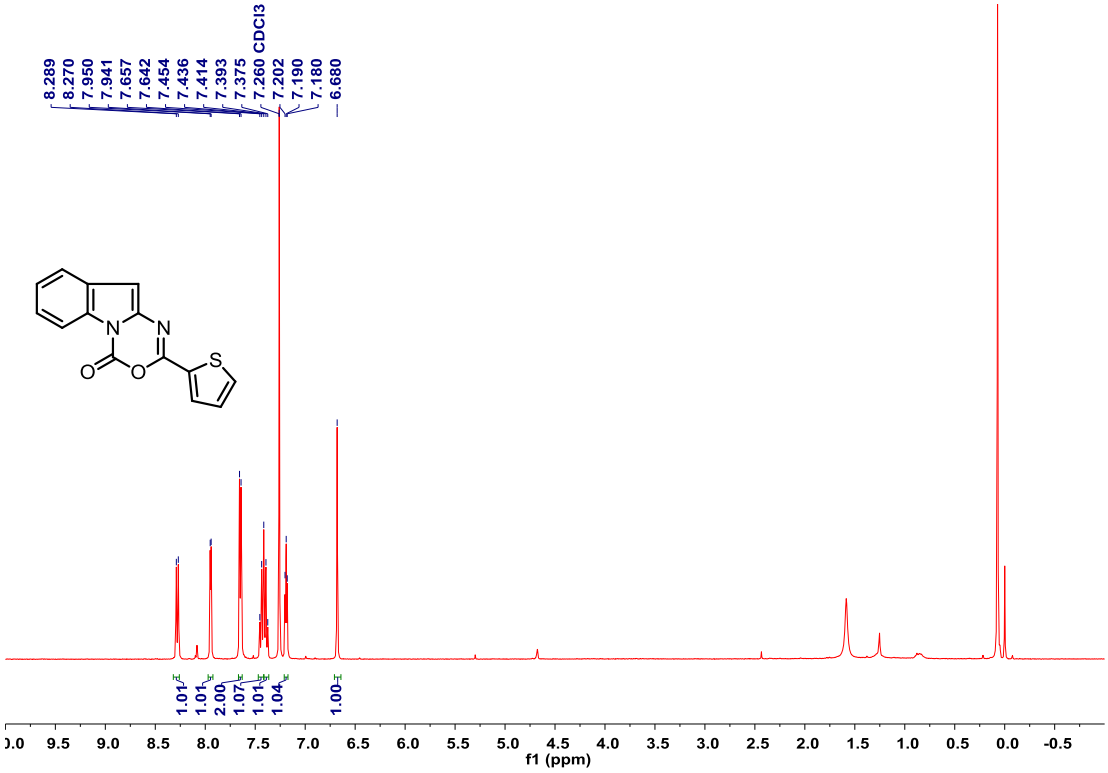


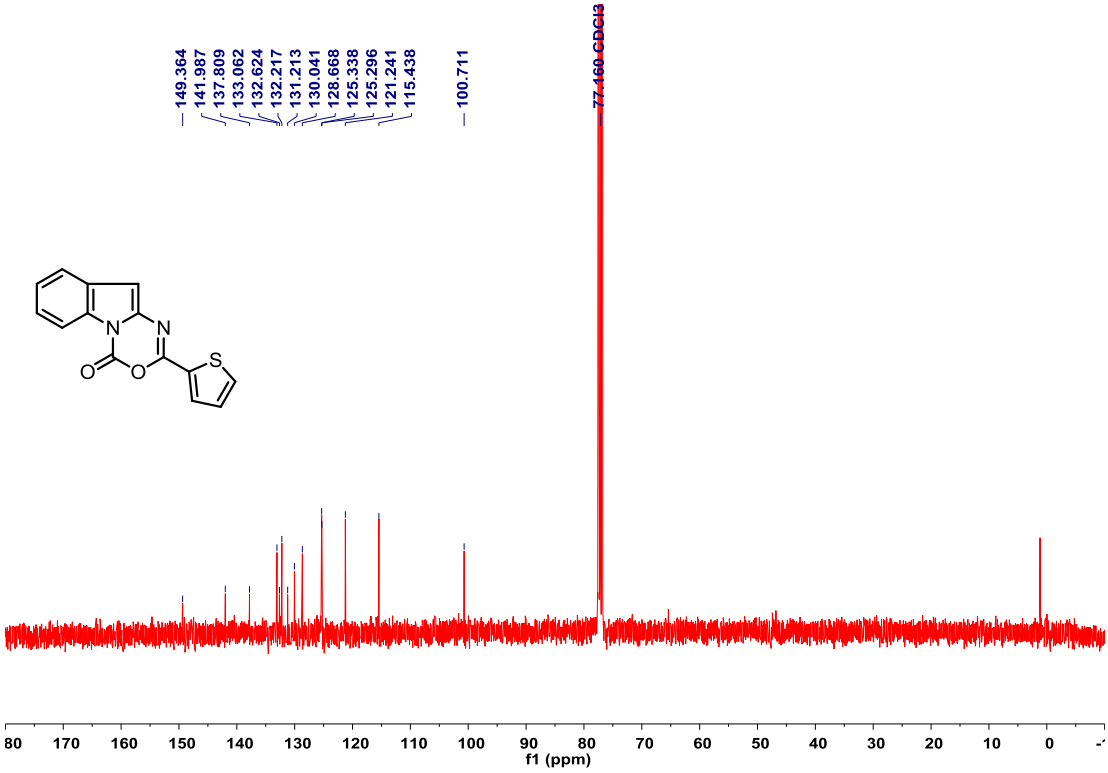
2-(Furan-2-yl)-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4l)



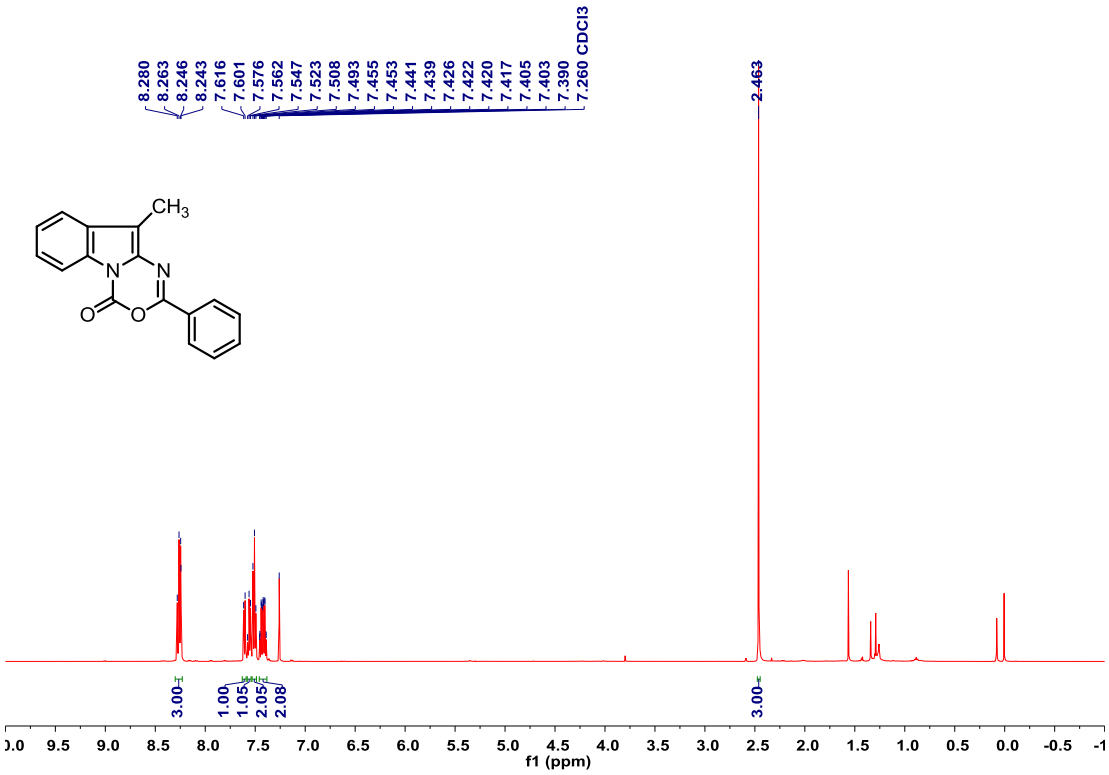


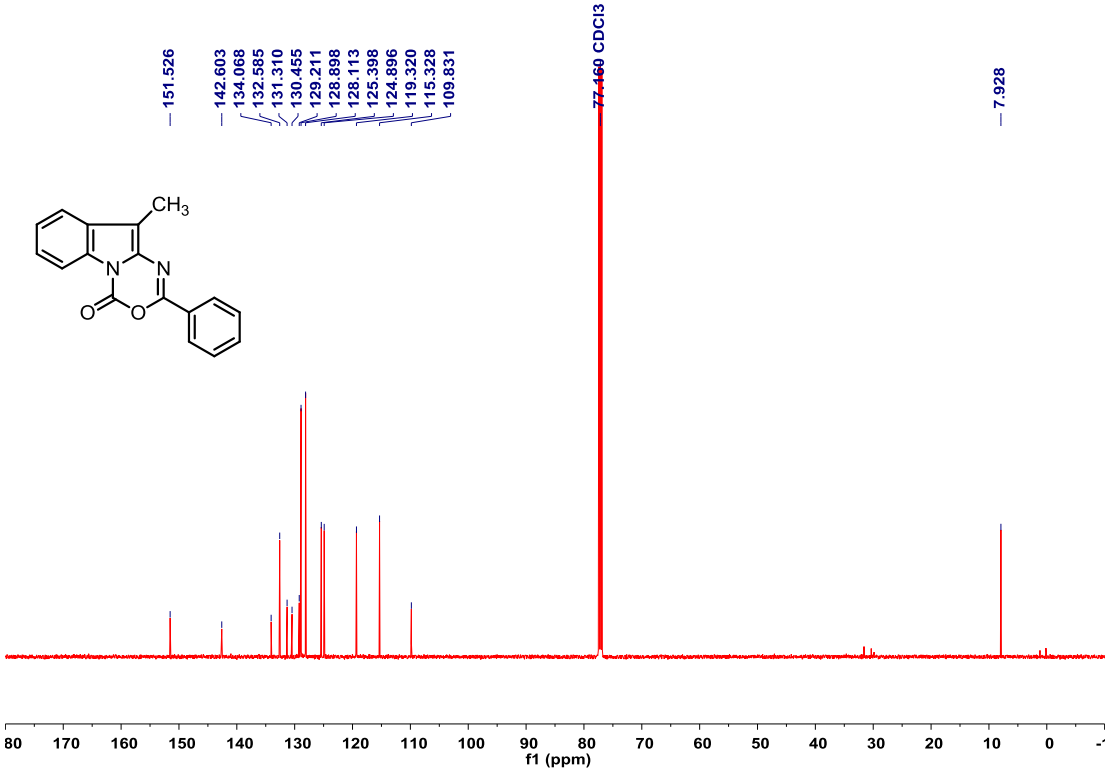
2-(Thiophen-2-yl)-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4m)



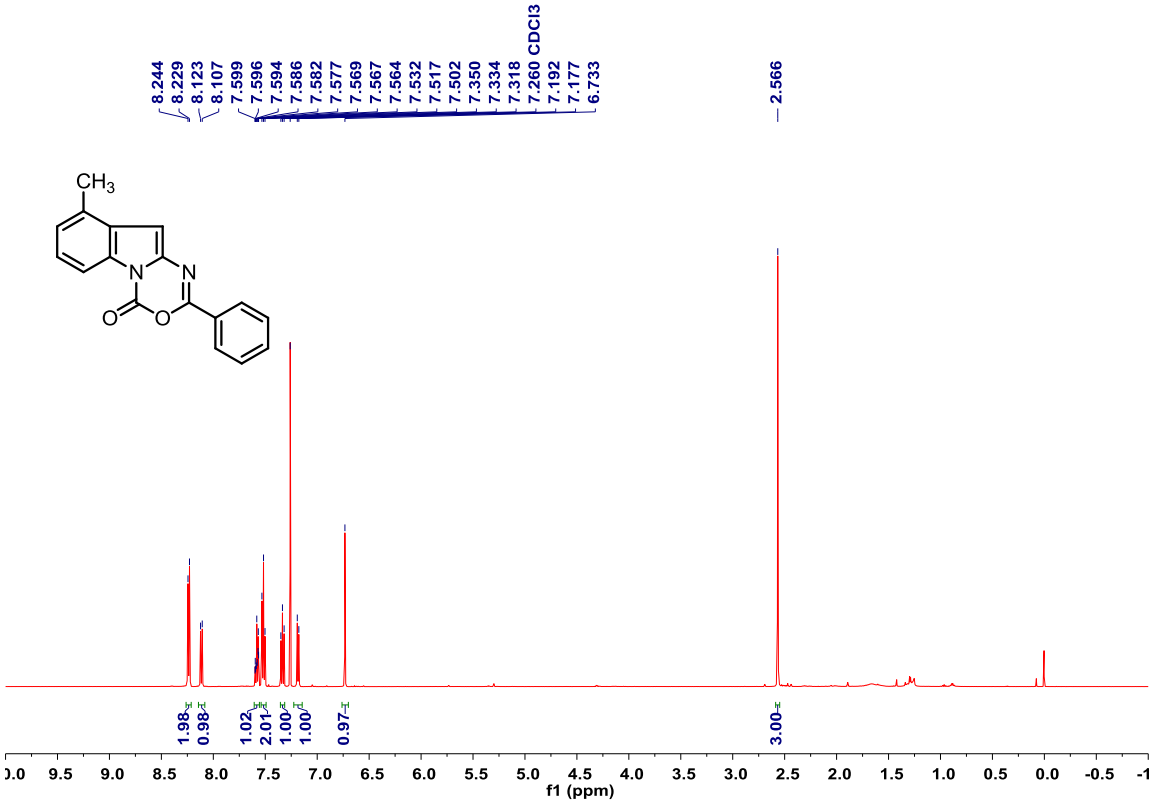


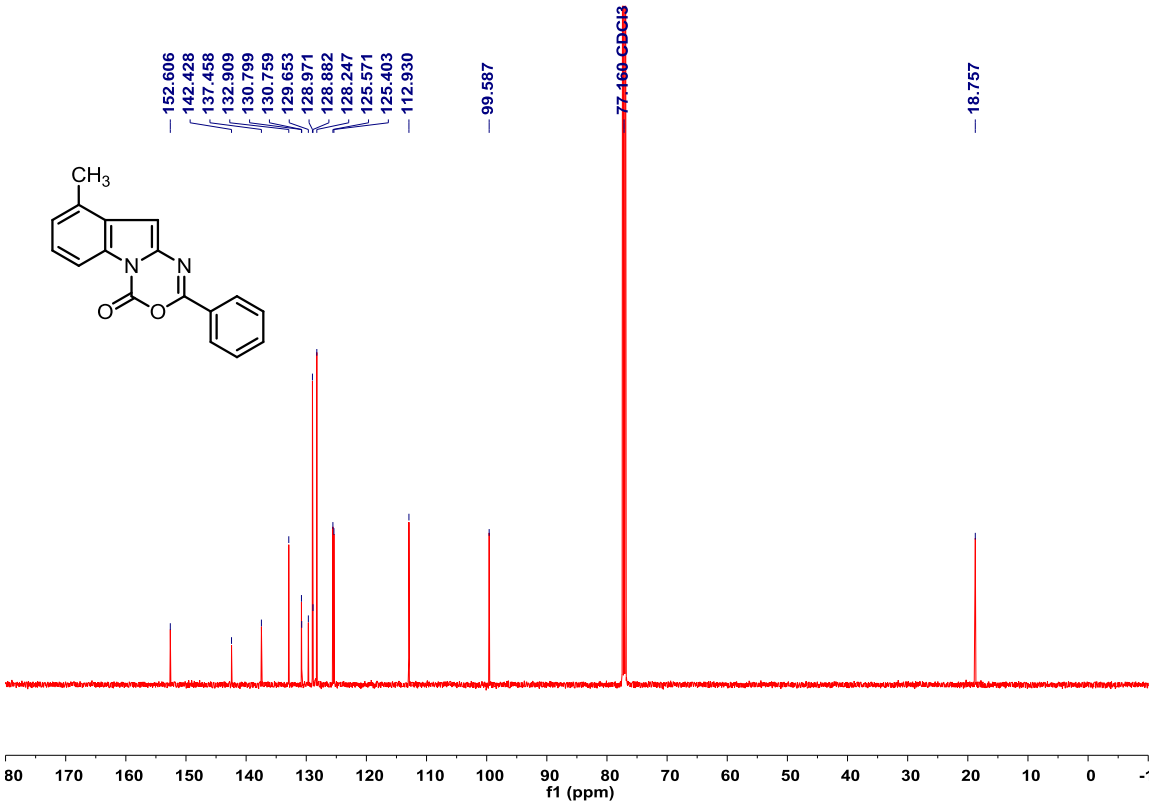
10-Methyl-2-phenyl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4n)



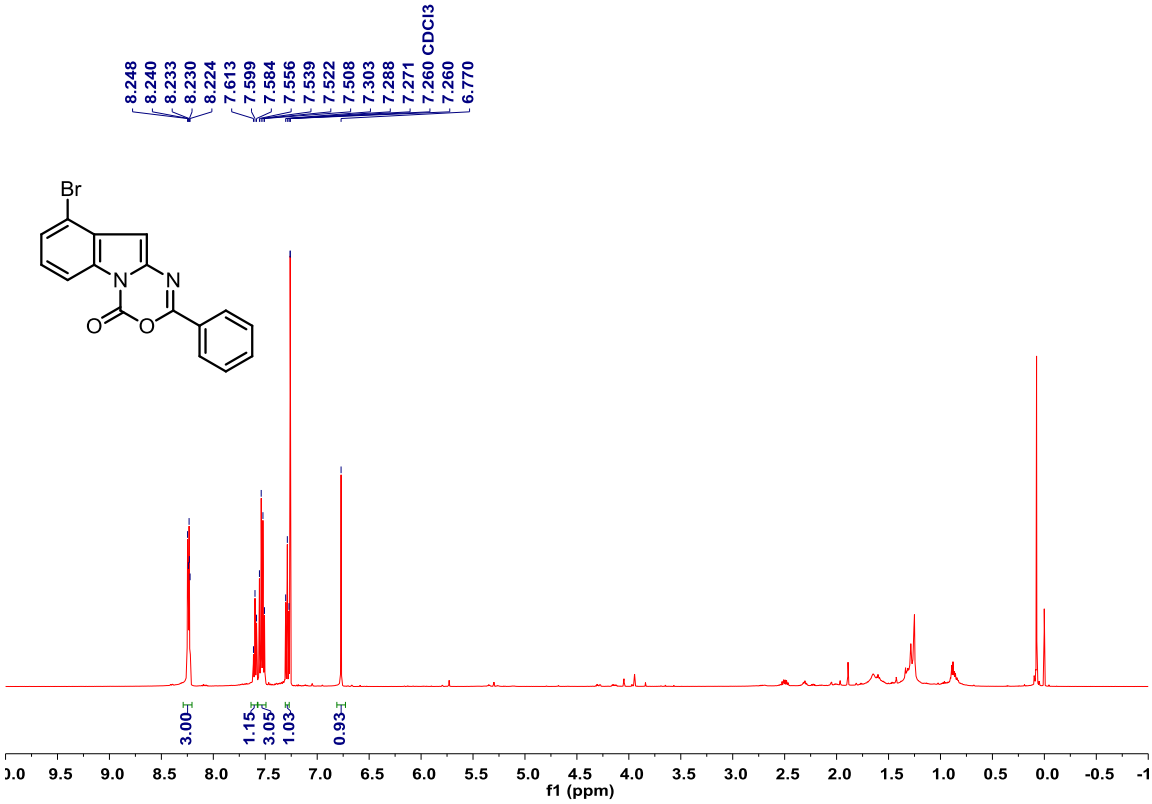


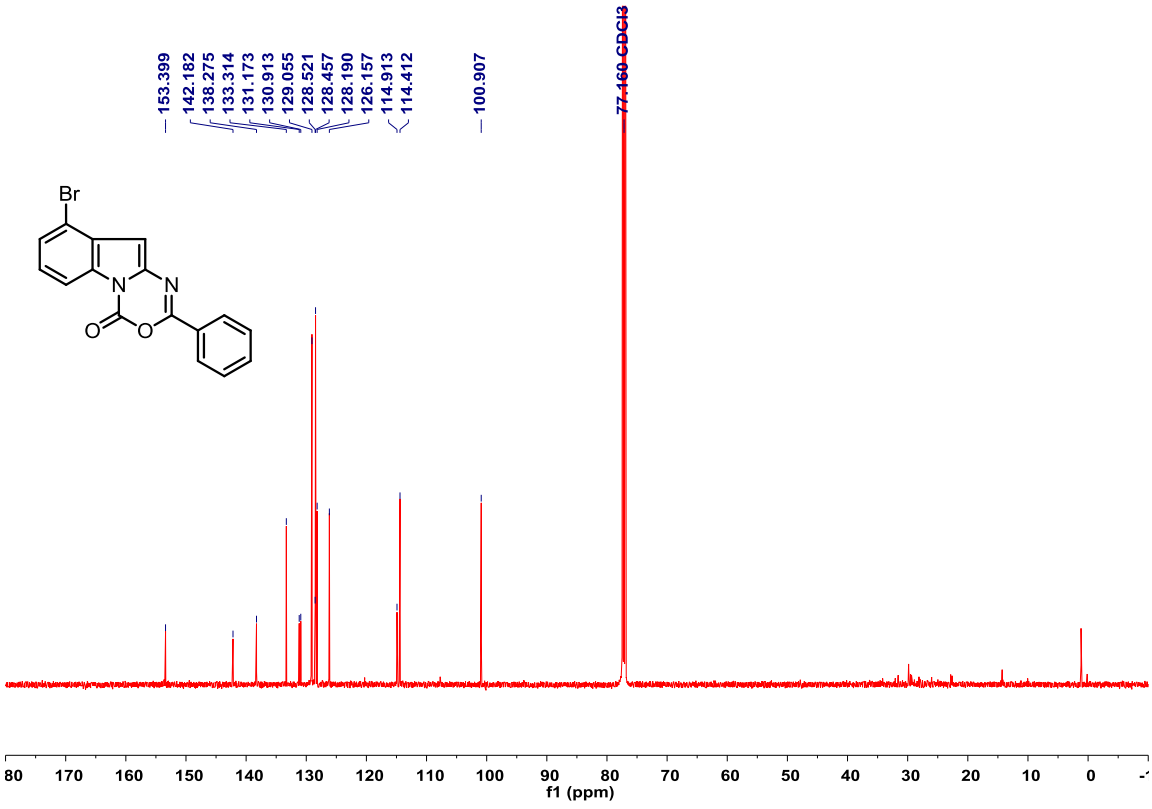
9-Methyl-2-phenyl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4o)



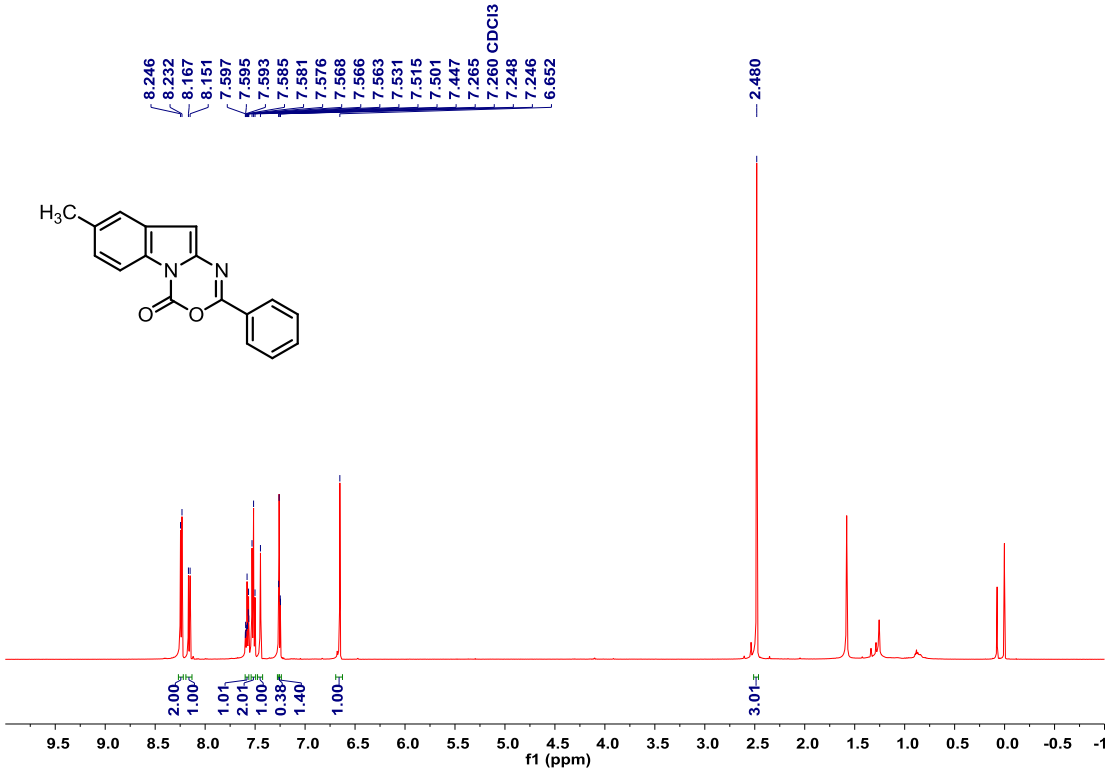


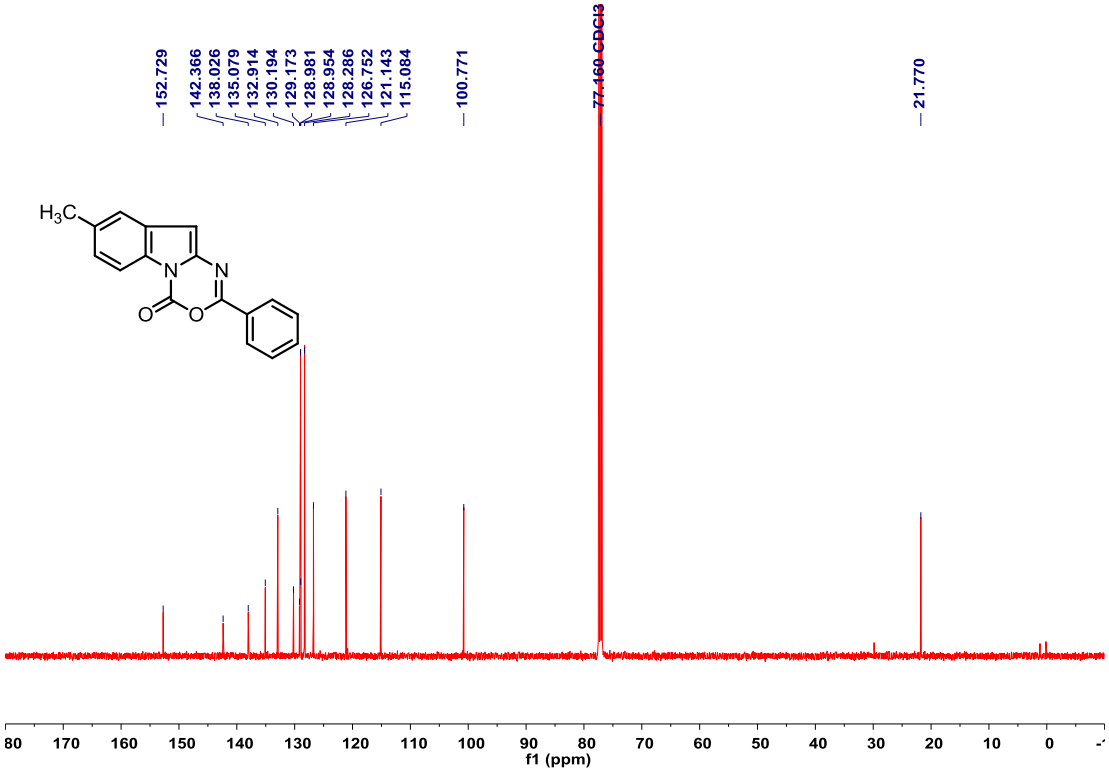
9-Bromo-2-phenyl-4H-[1,3,5]oxadiazino[3,4-a]indol-4-one (4p)



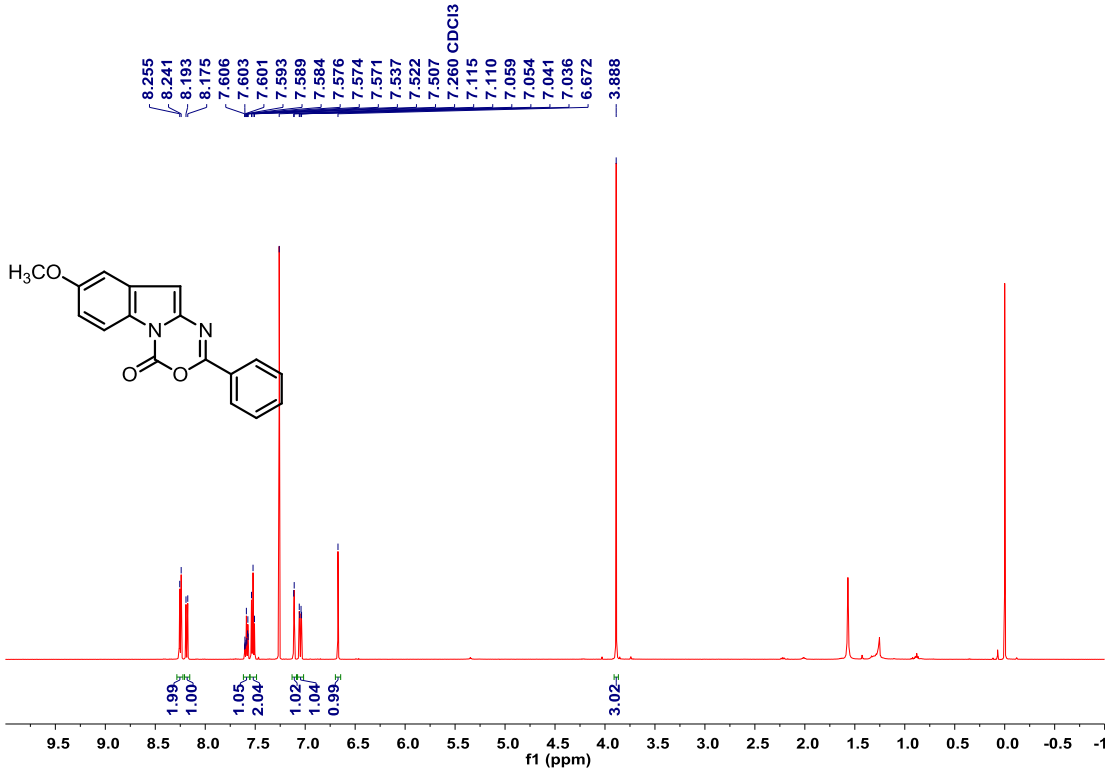


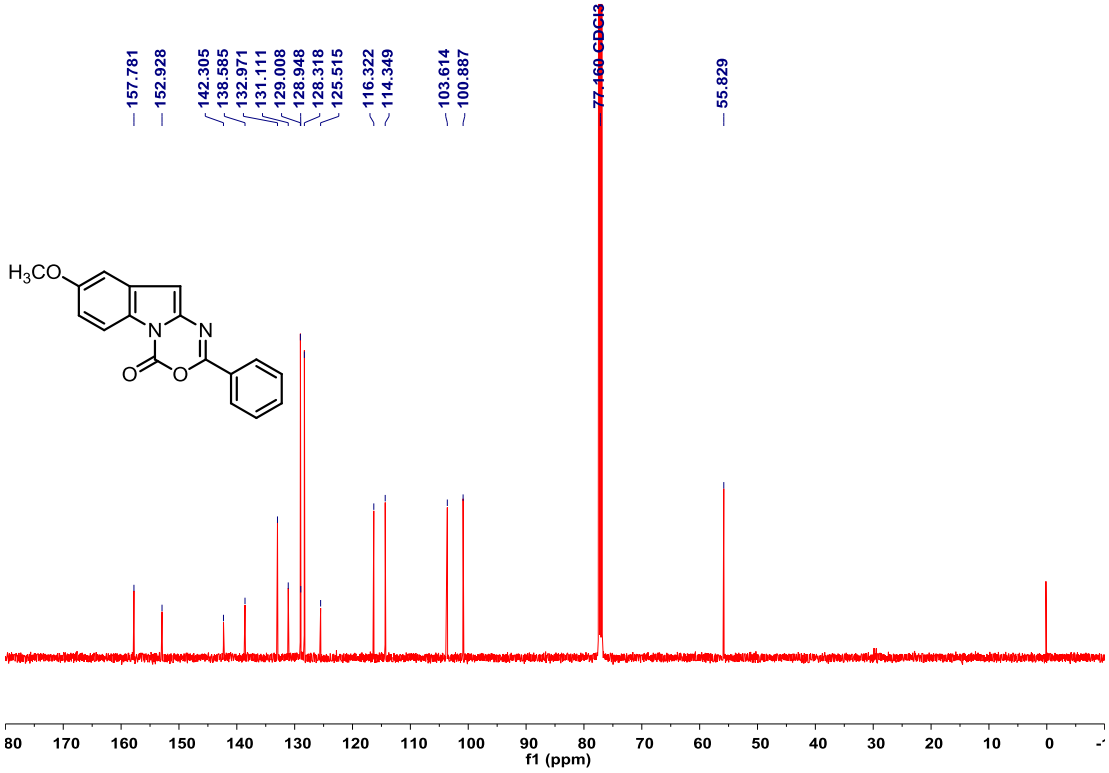
8-Methyl-2-phenyl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4q)



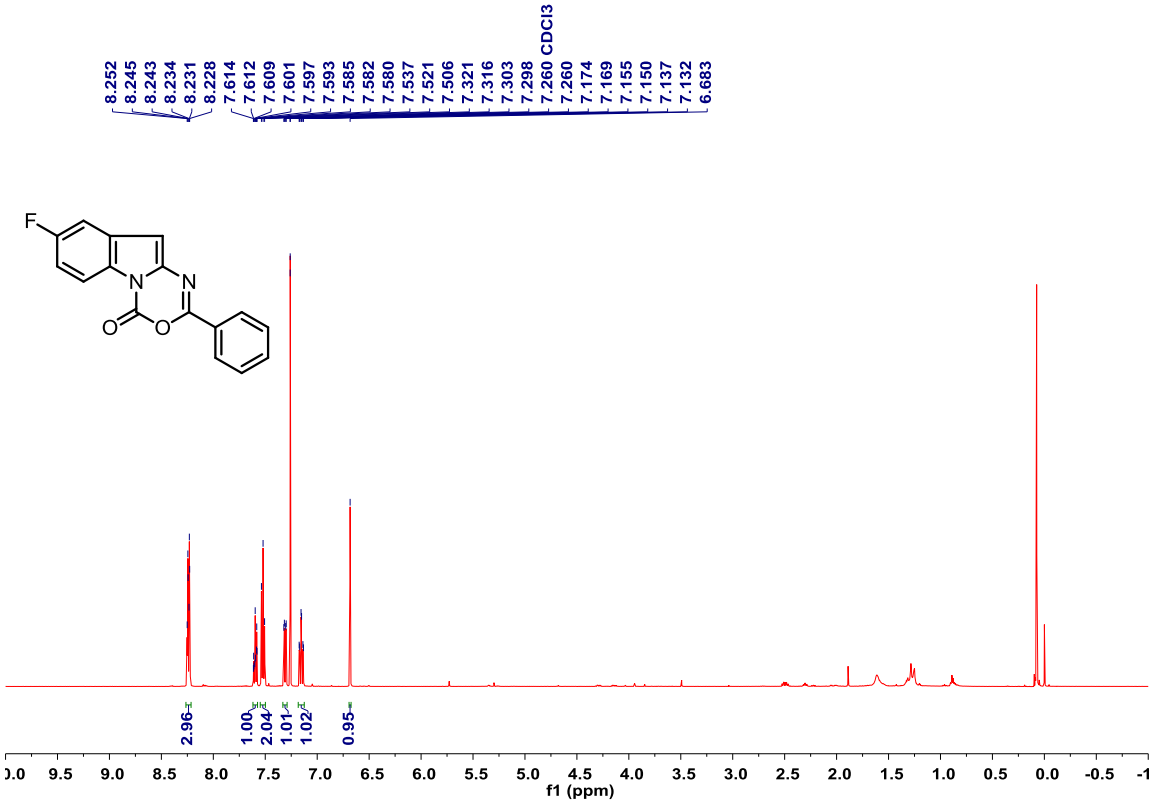


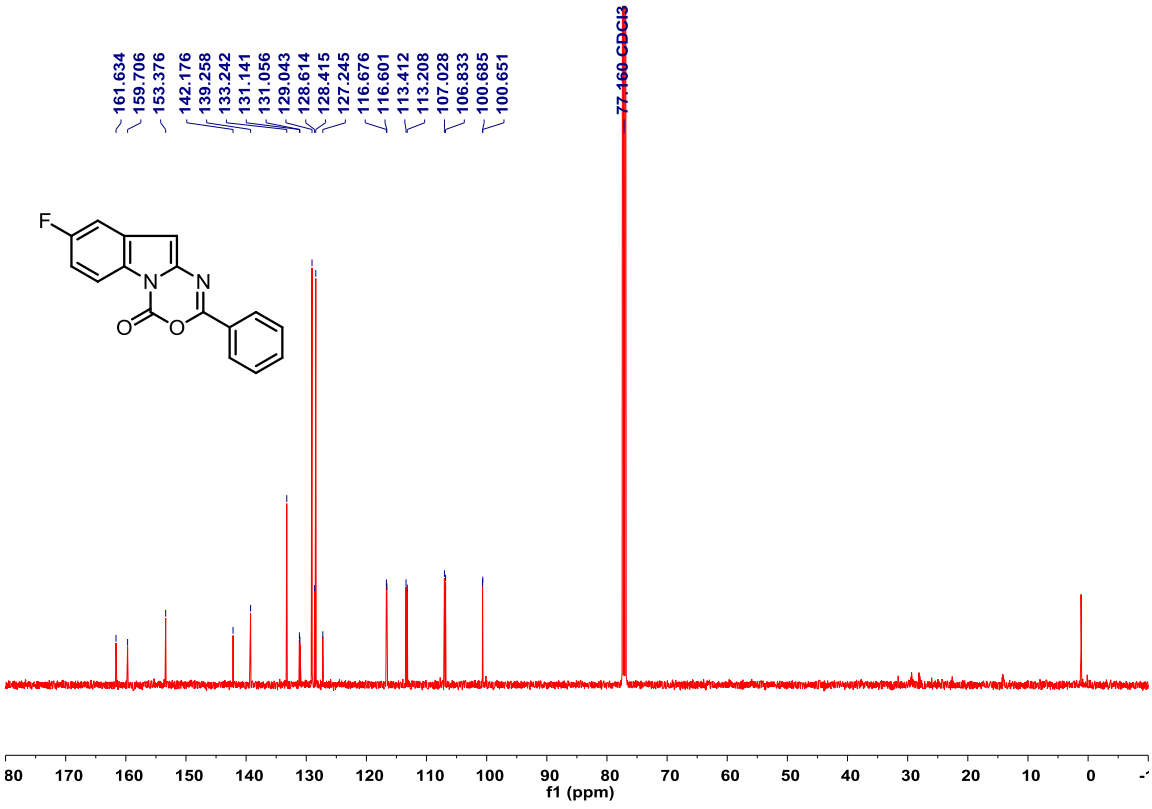
8-Methoxy-2-phenyl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4r)



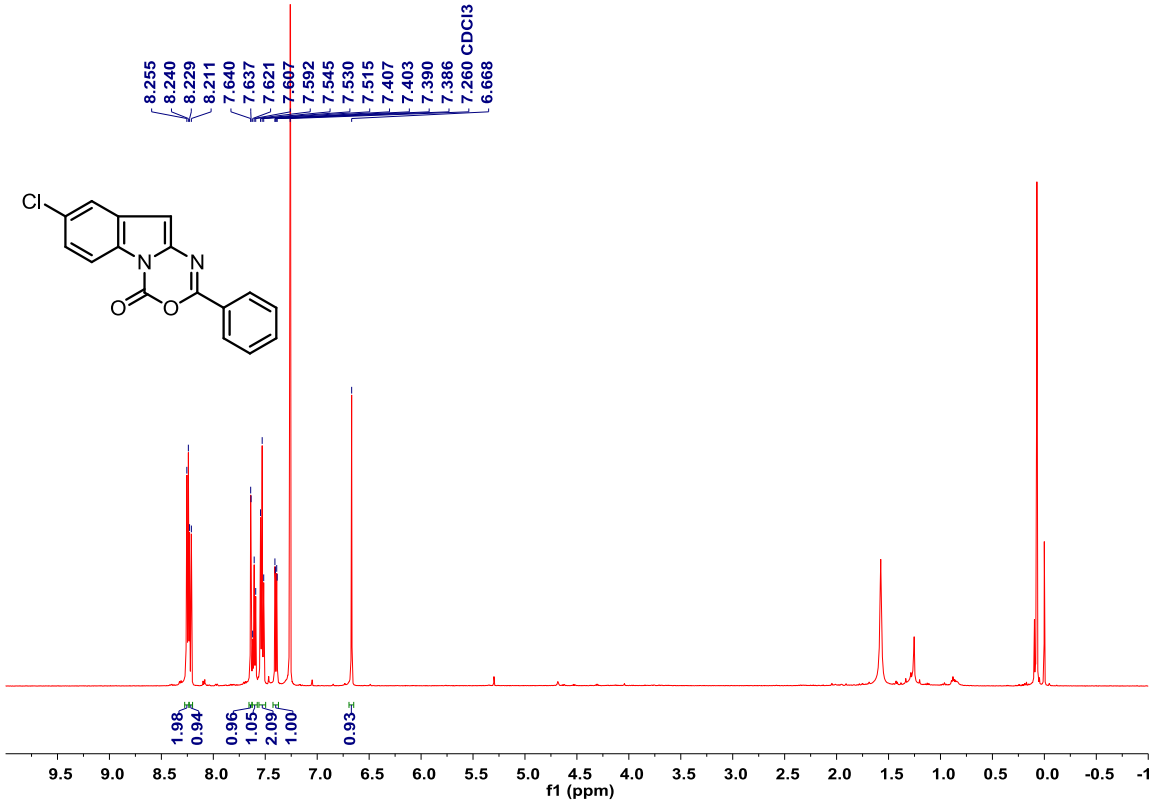


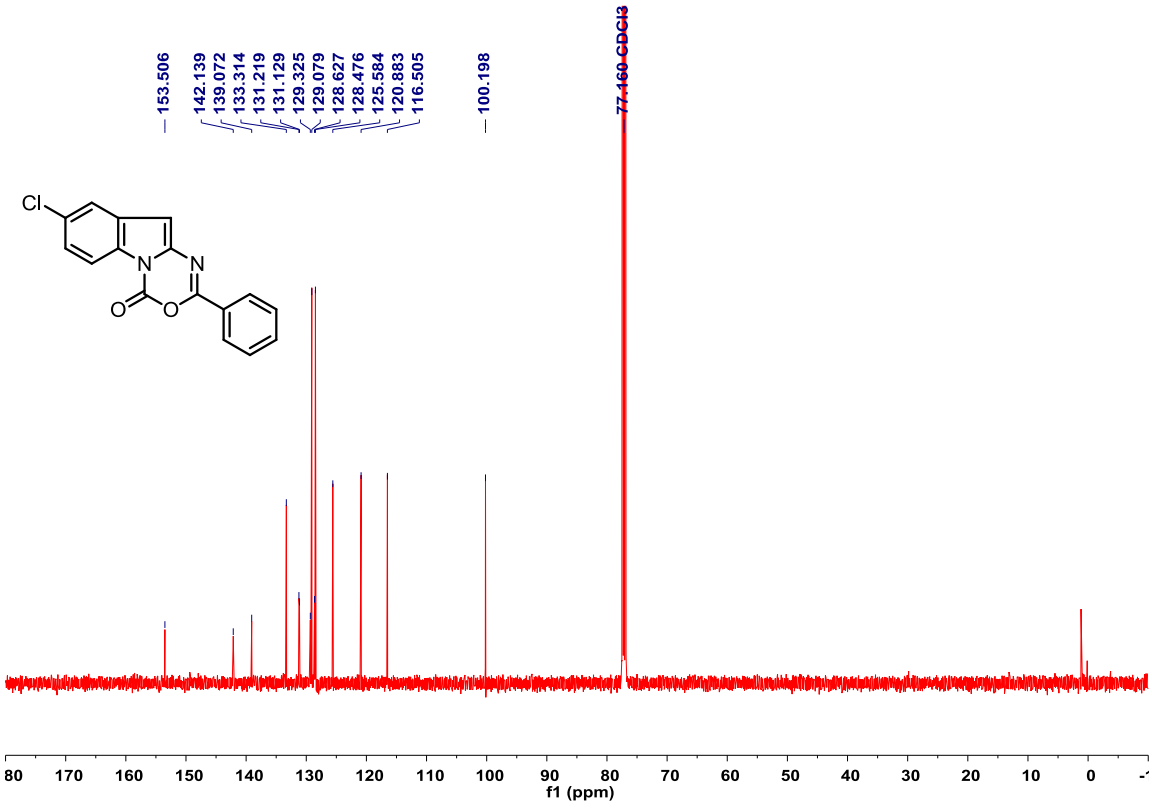
8-Fluoro-2-phenyl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4s)



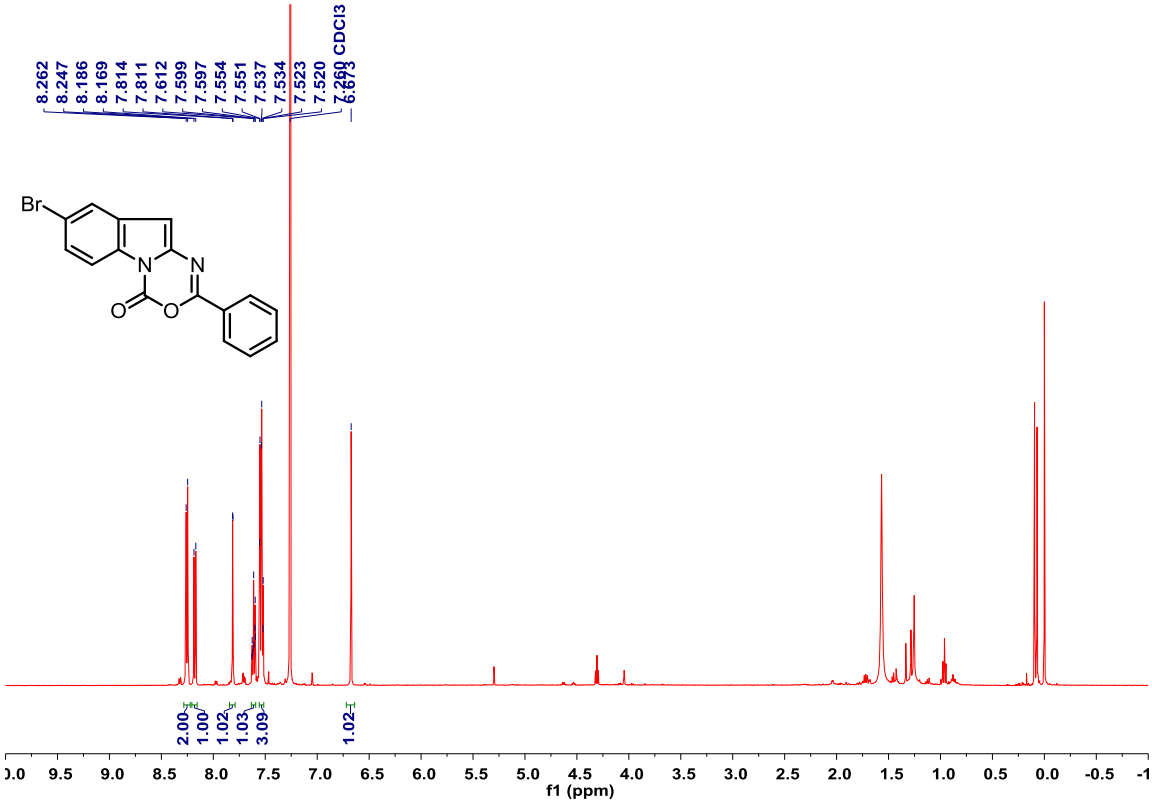


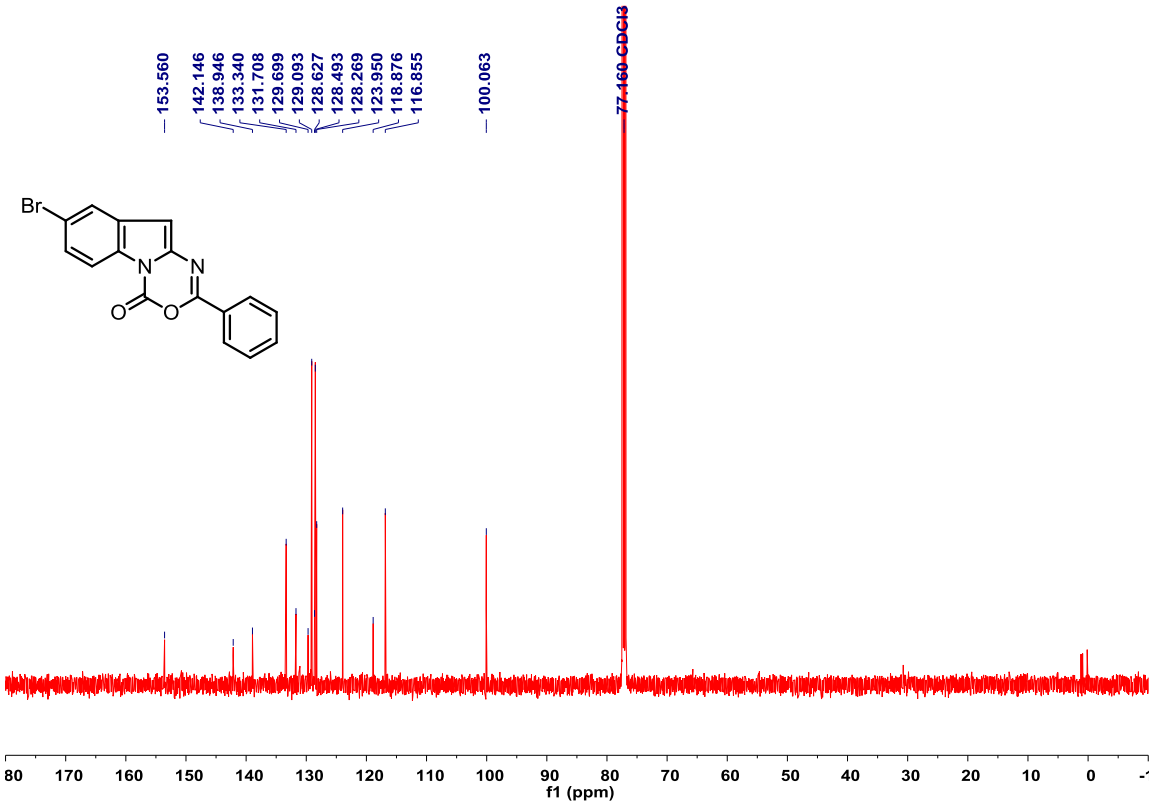
8-Chloro-2-phenyl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4t)



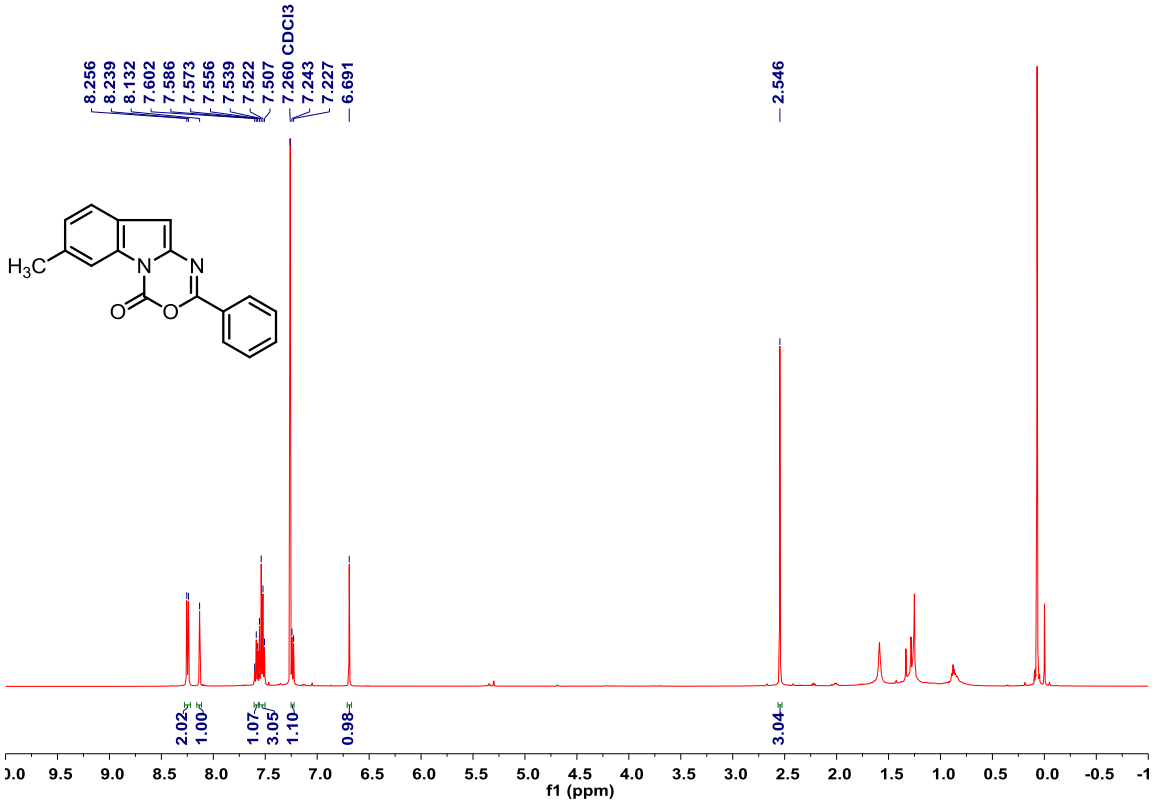


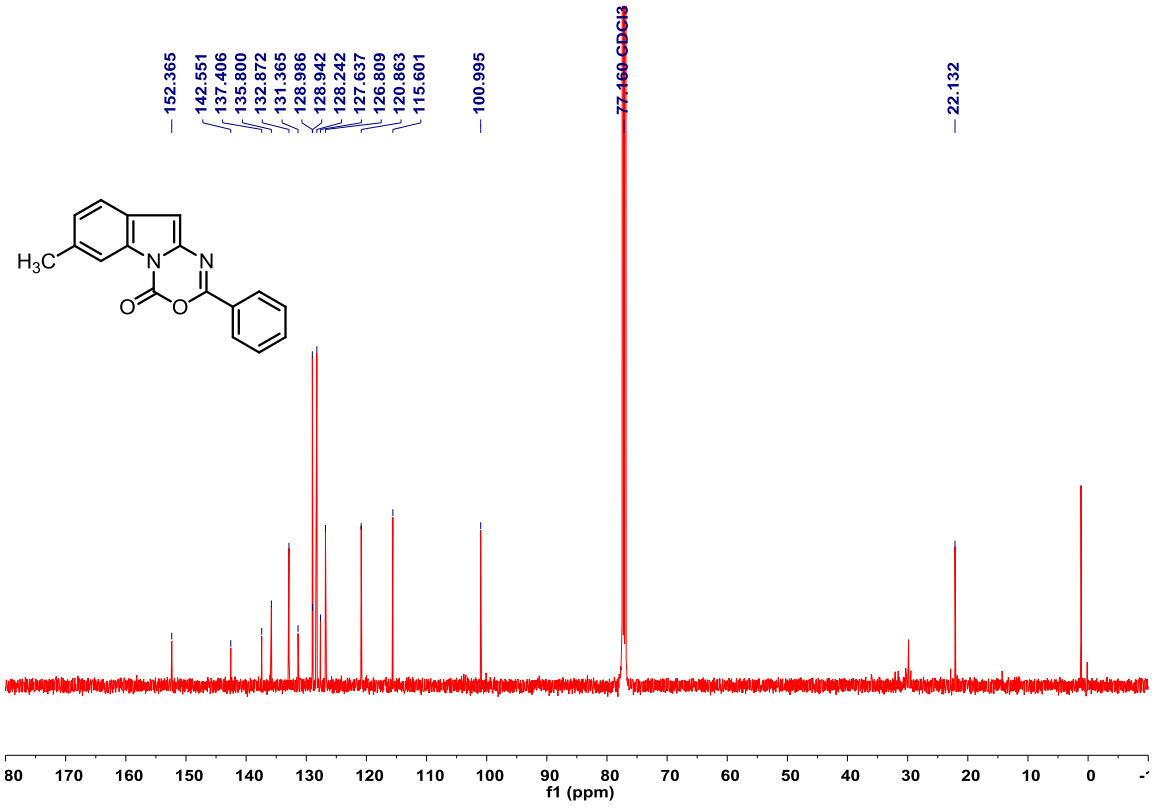
8-Bromo-2-phenyl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4u)



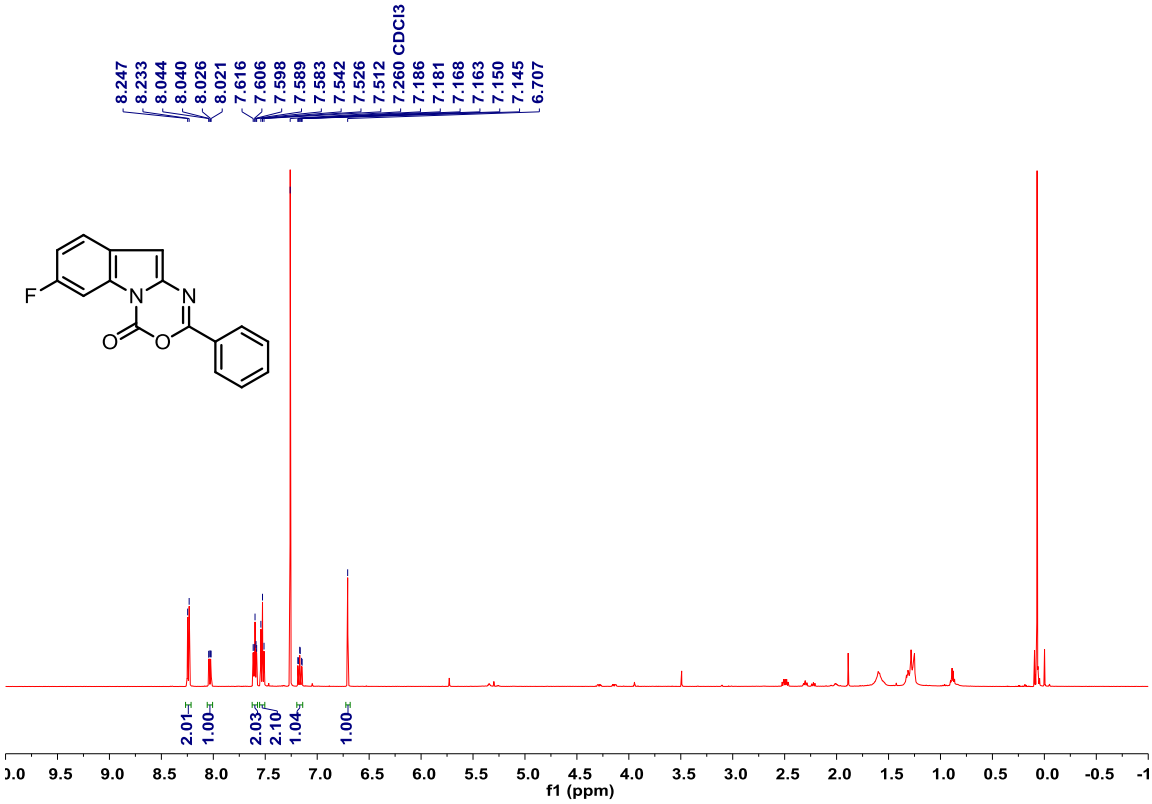


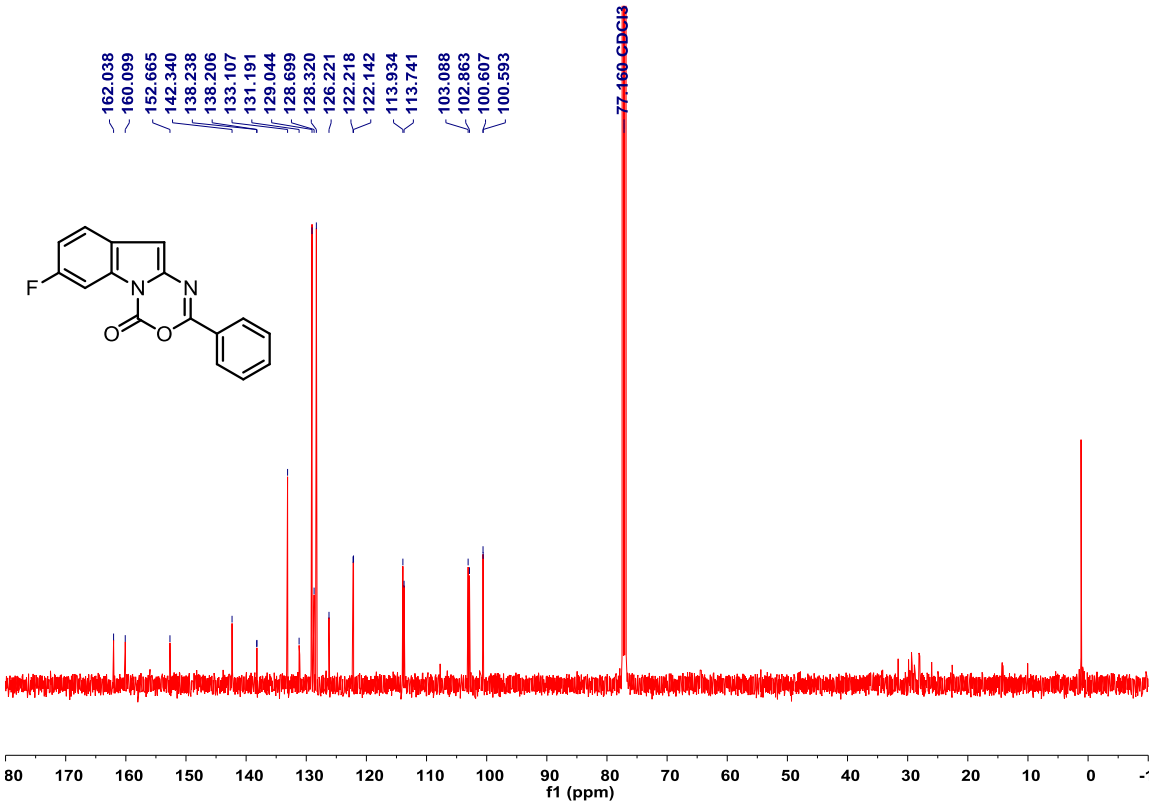
7-Methyl-2-phenyl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4v)



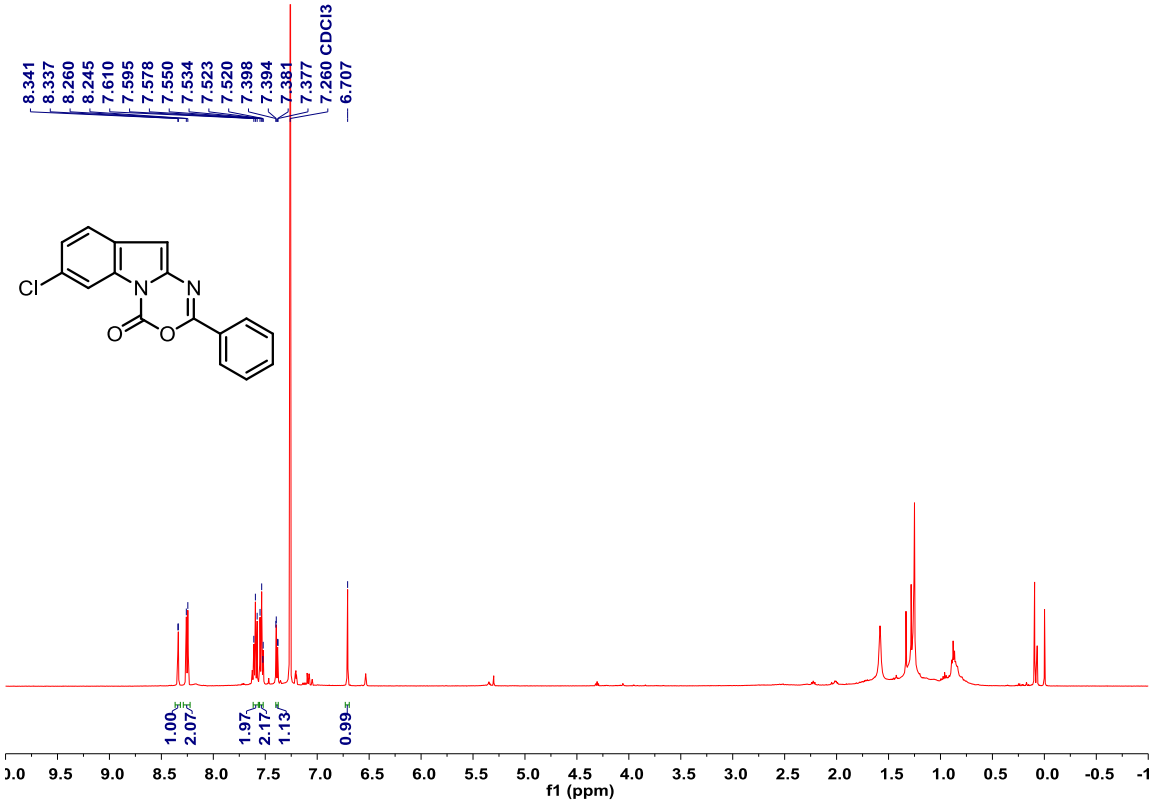


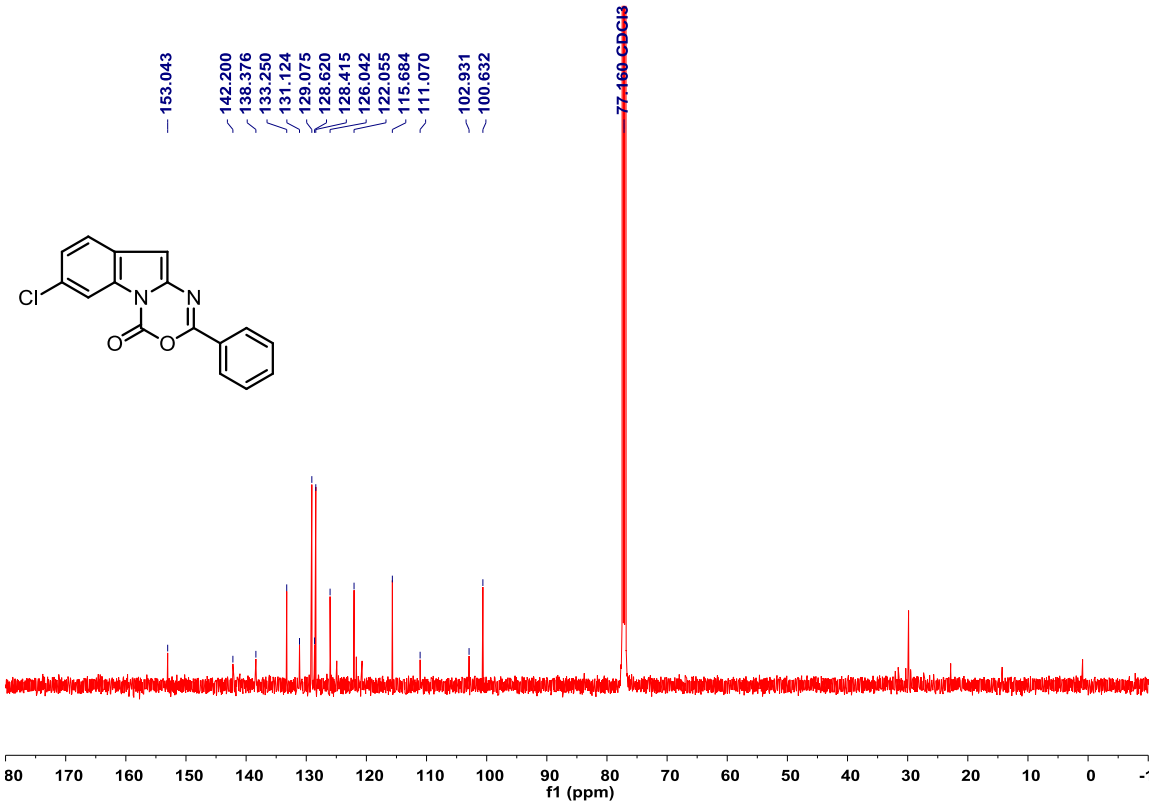
7-Fluoro-2-phenyl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4w)



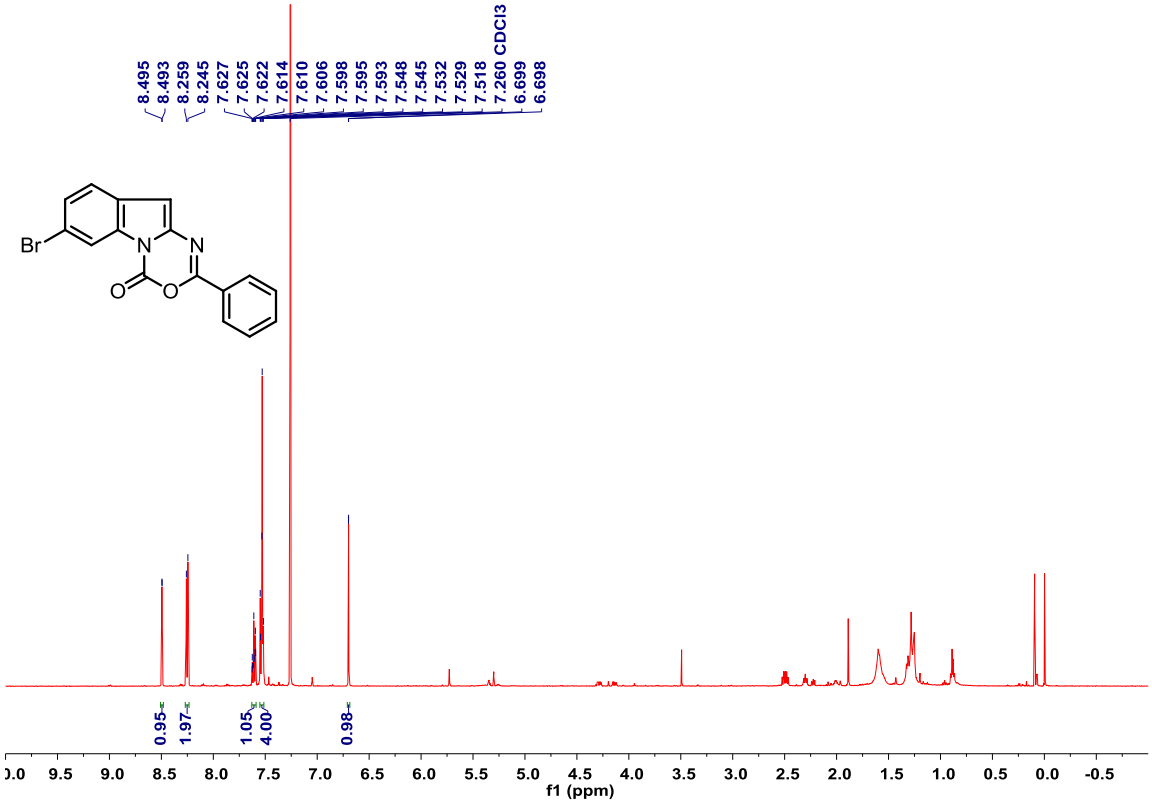


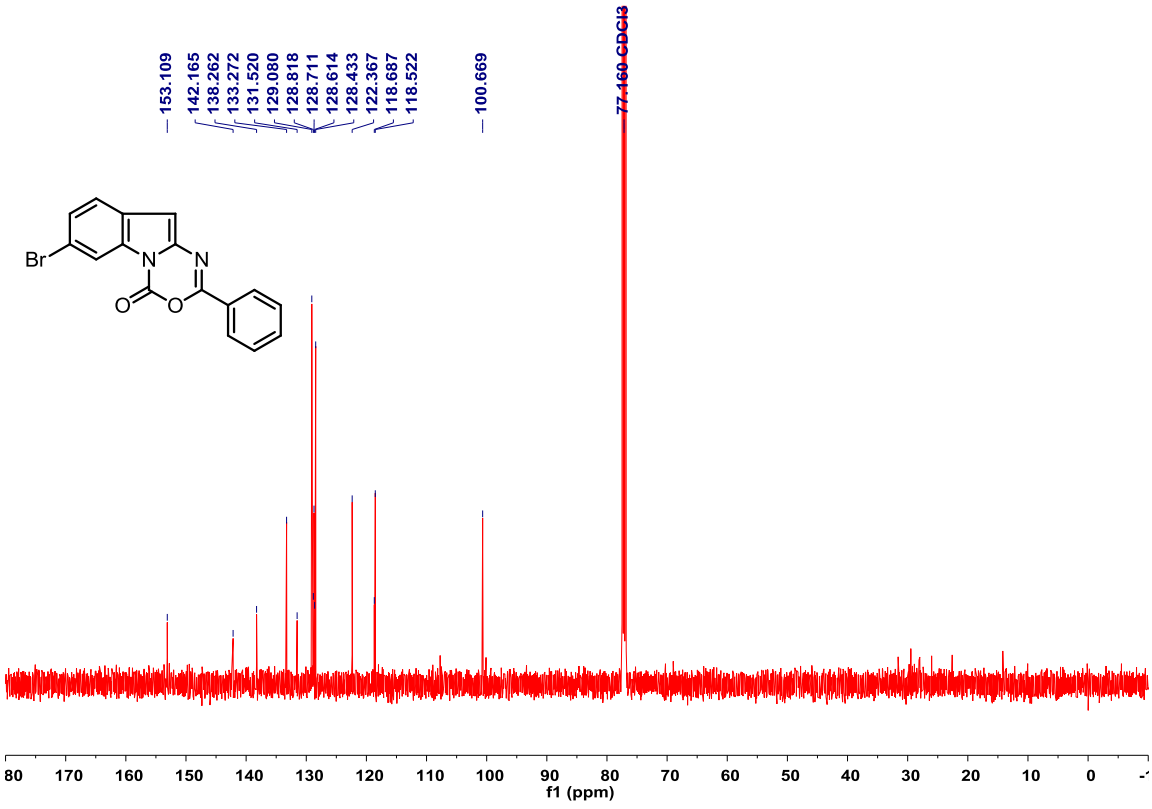
7-Chloro-2-phenyl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4x)



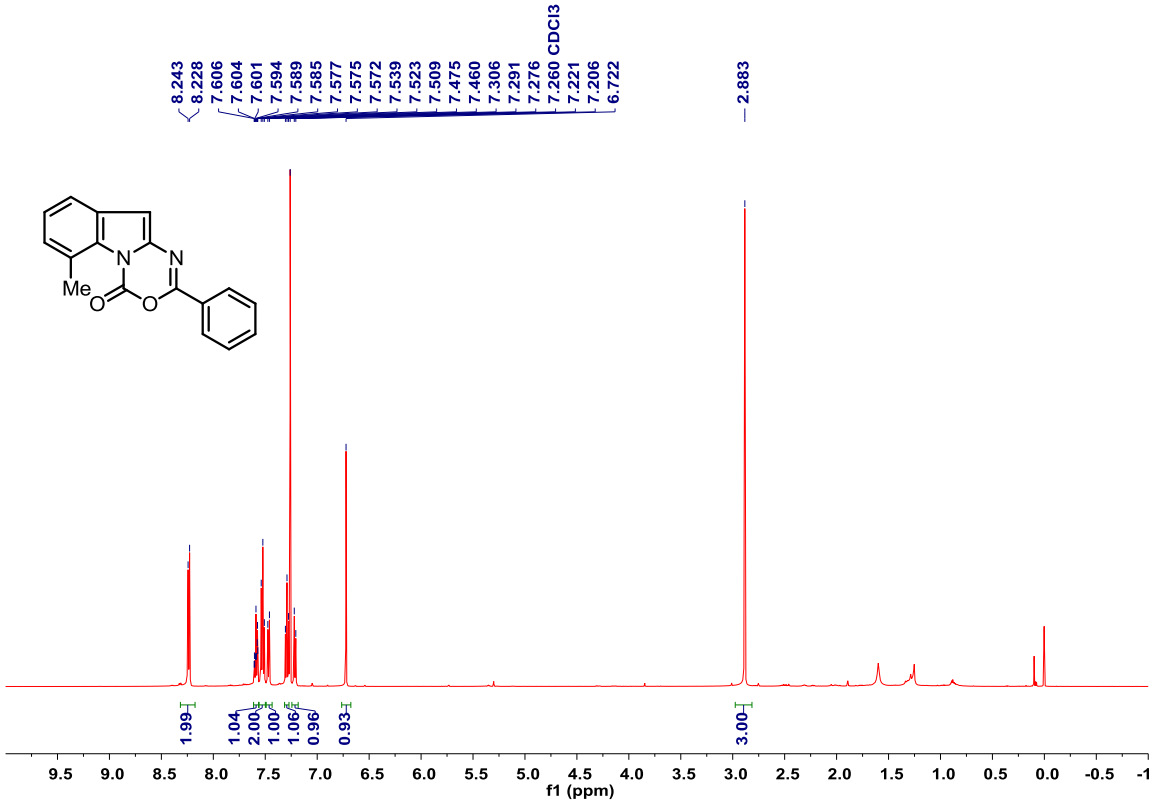


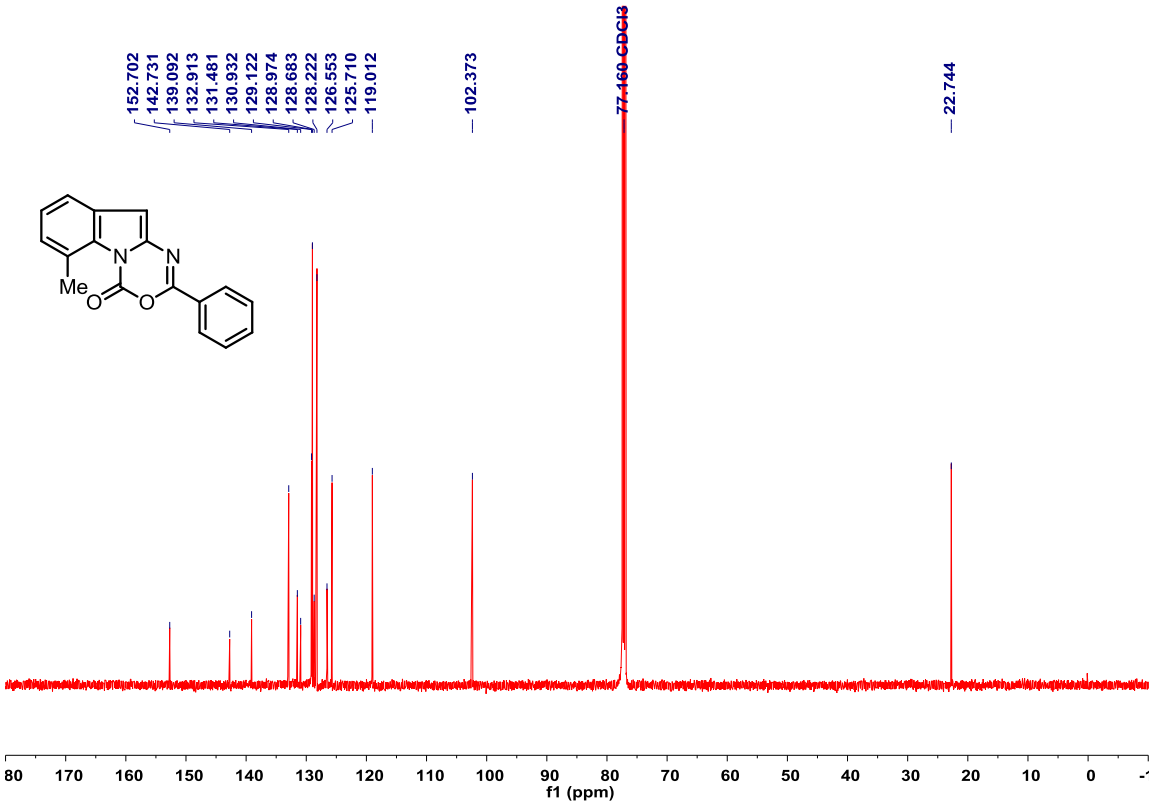
7-Bromo-2-phenyl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4y)



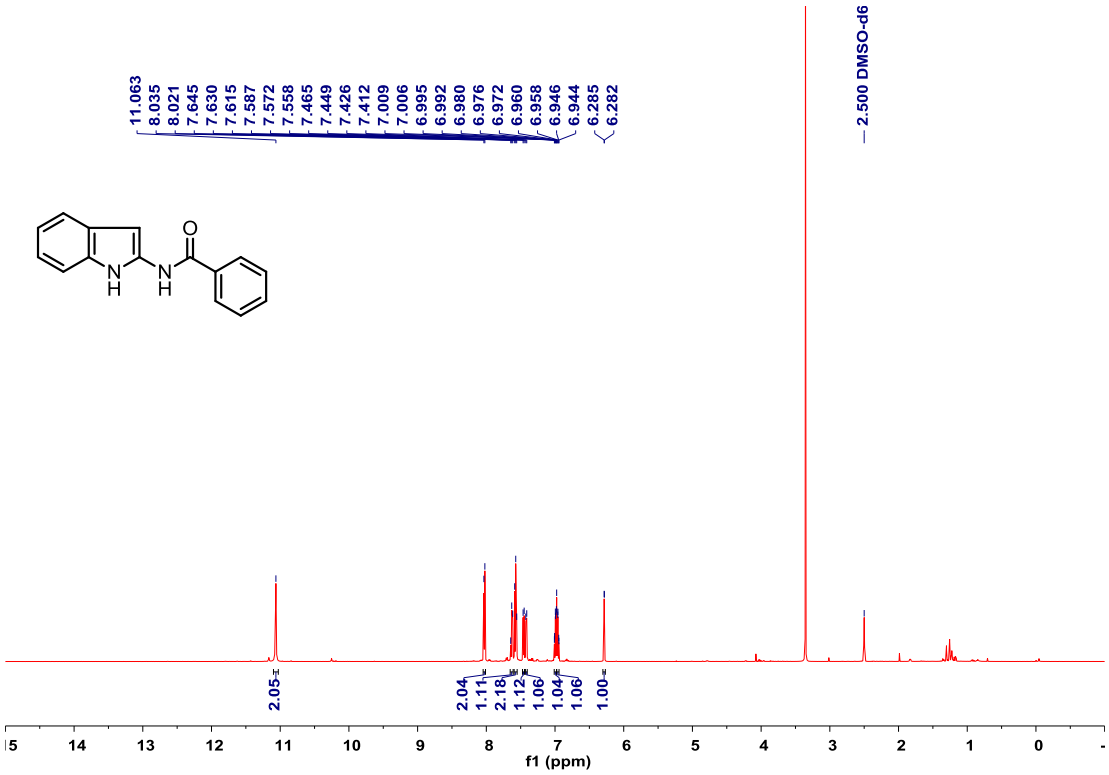


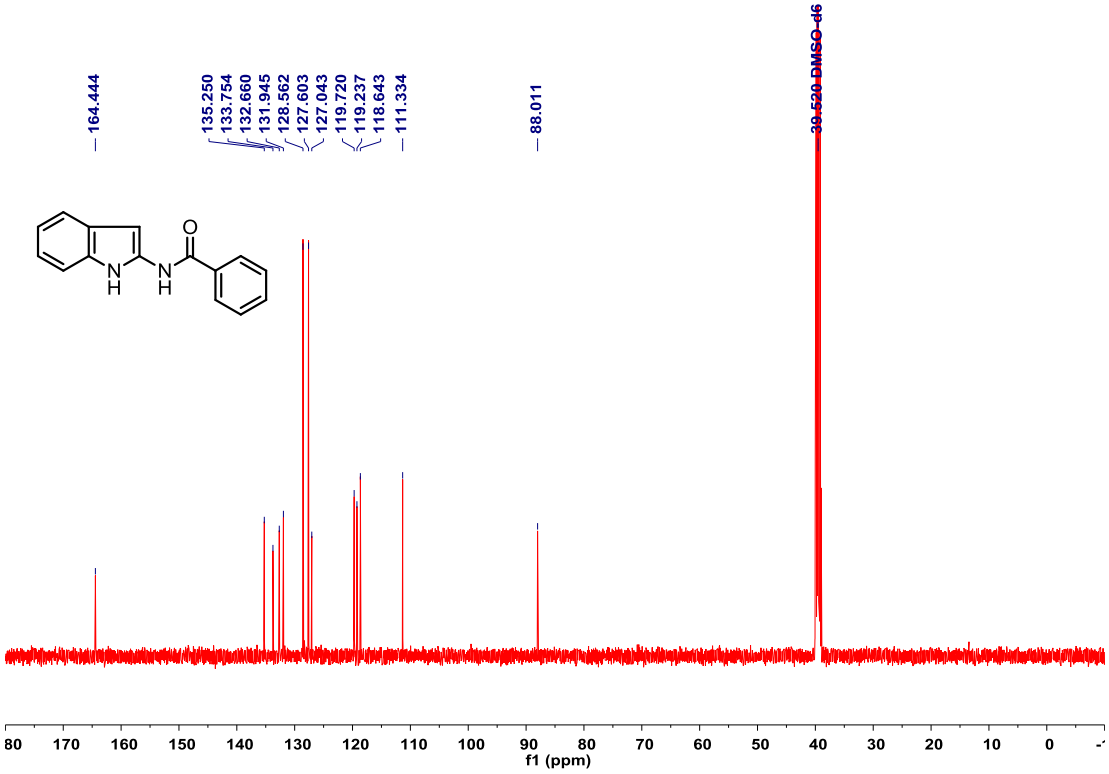
6-Methyl-2-phenyl-4*H*-[1,3,5]oxadiazino[3,4-a]indol-4-one (4z)



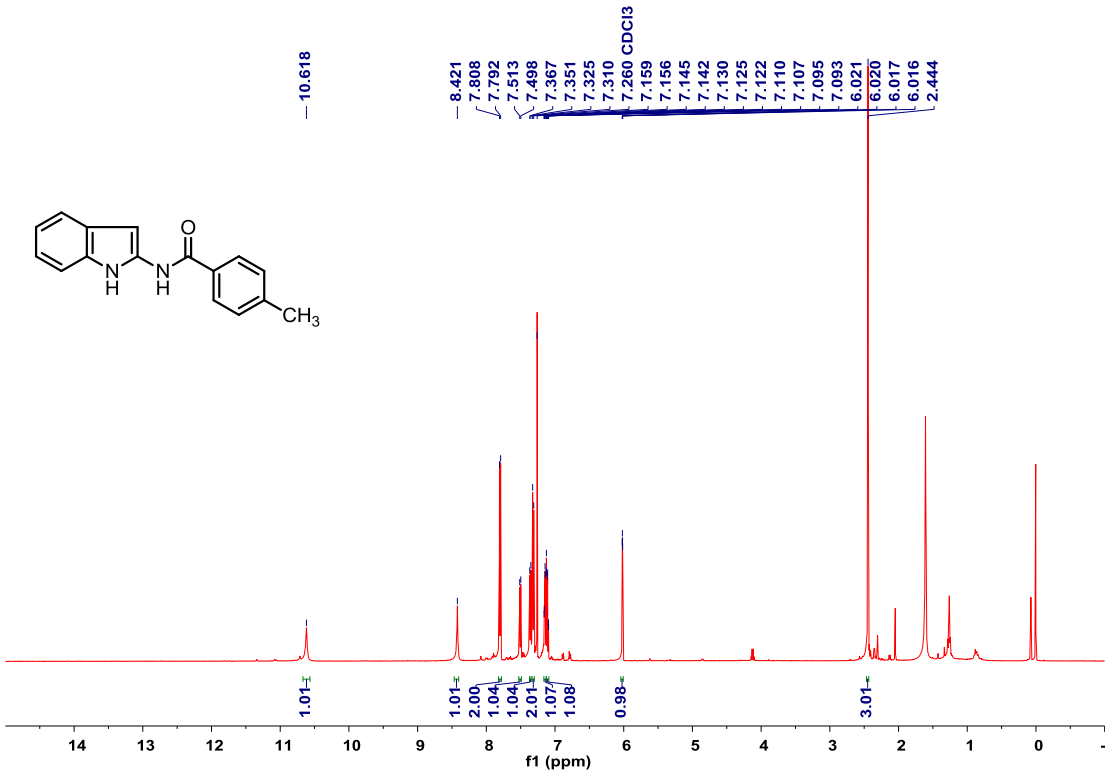


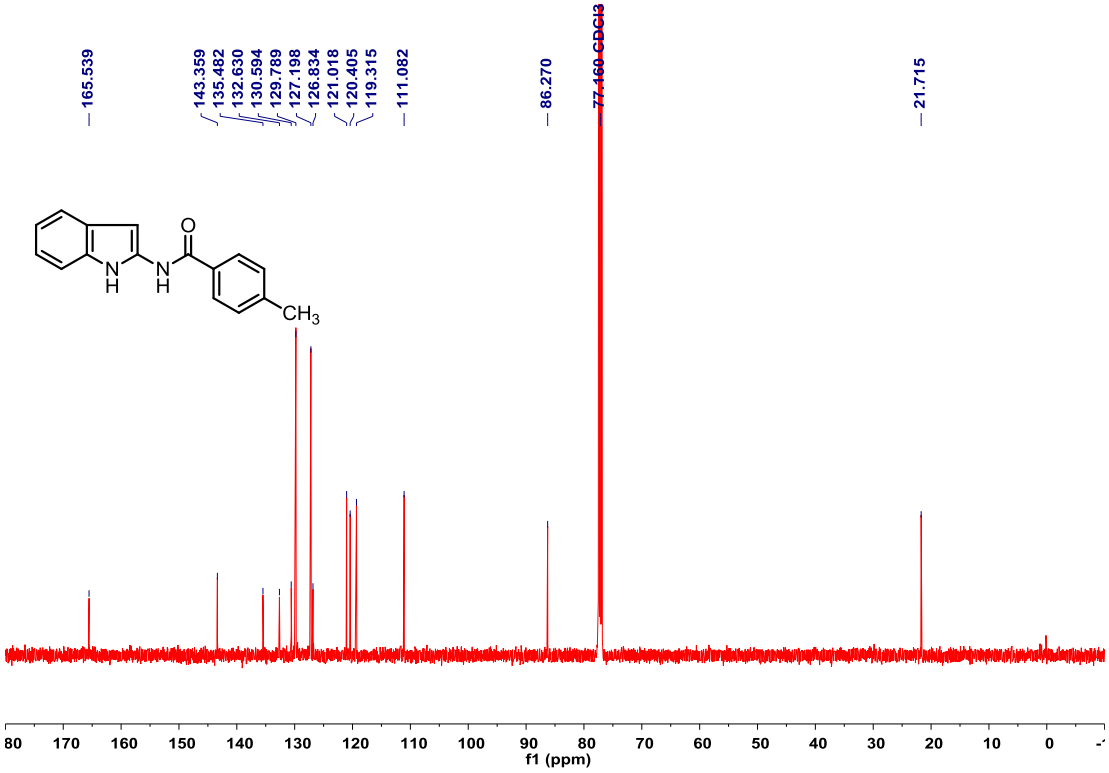
***N*-(1*H*-Indol-2-yl)benzamide (5a)**



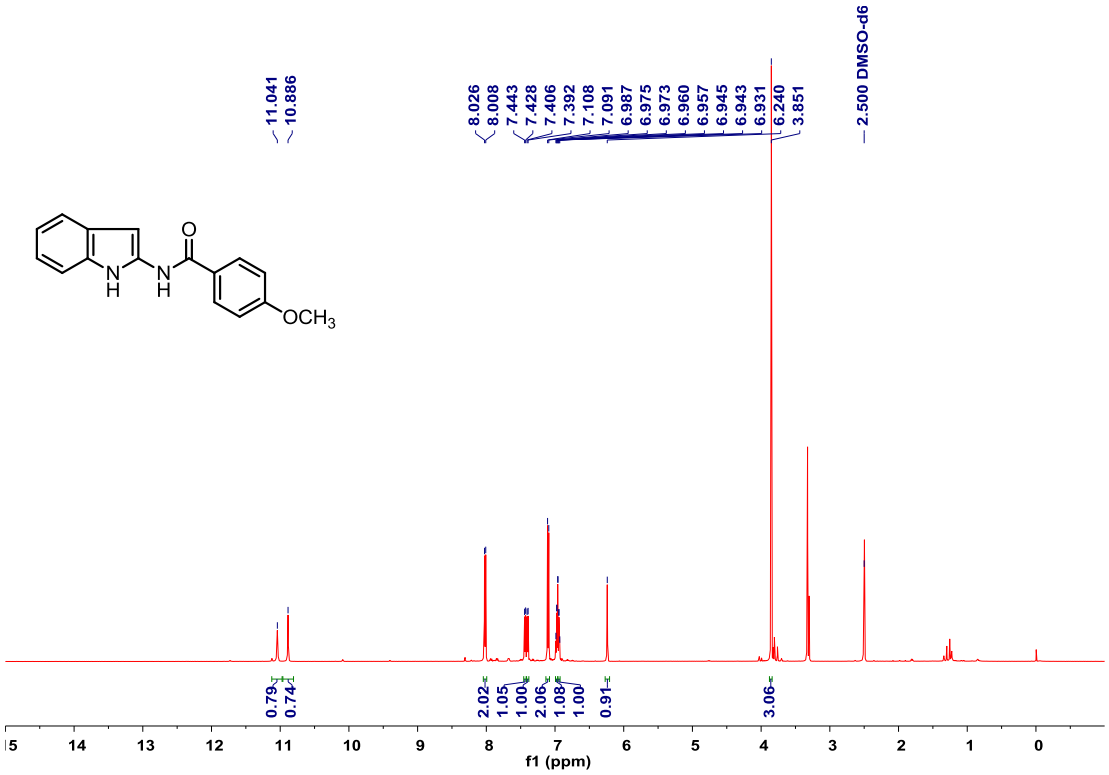


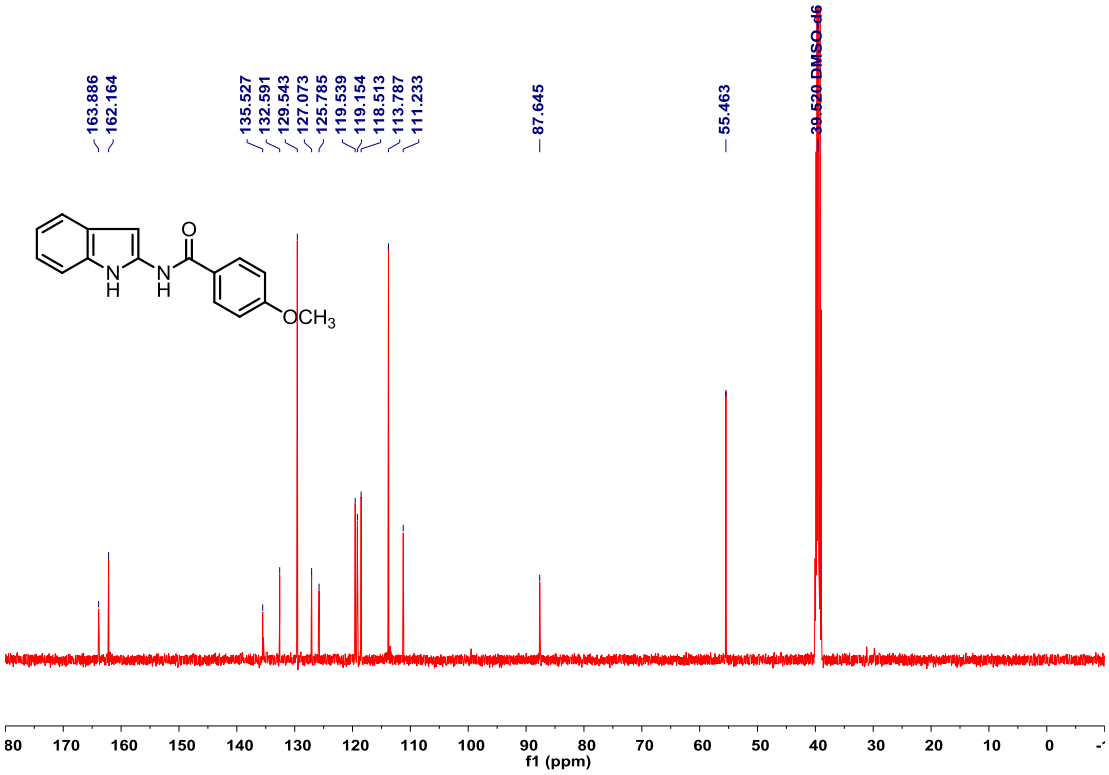
***N*-(1*H*-Indol-2-yl)-4-methylbenzamide (5b)**



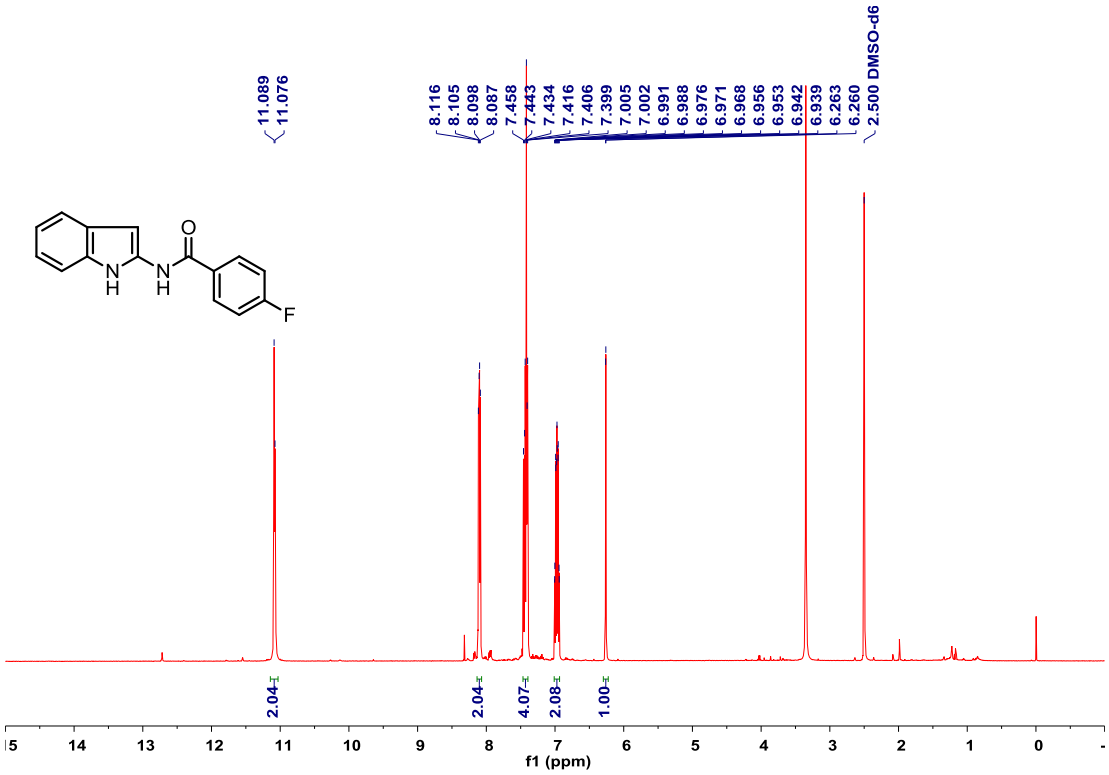


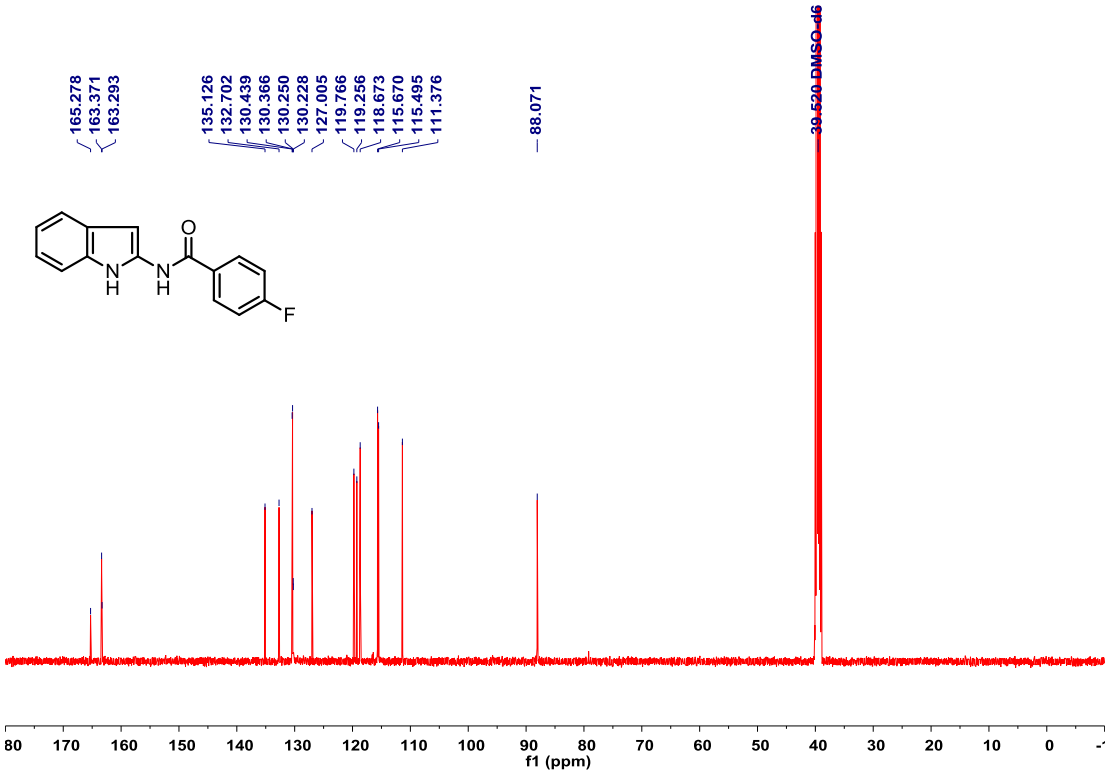
***N*-(1*H*-Indol-2-yl)-4-methoxybenzamide (5c)**



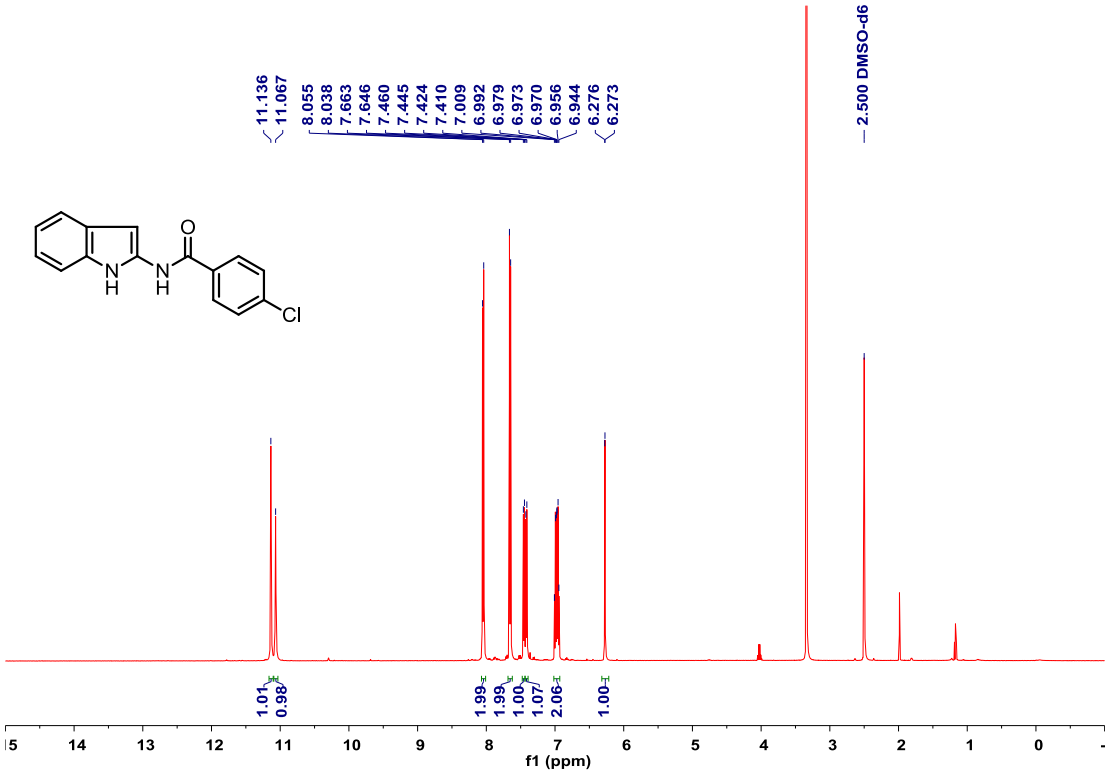


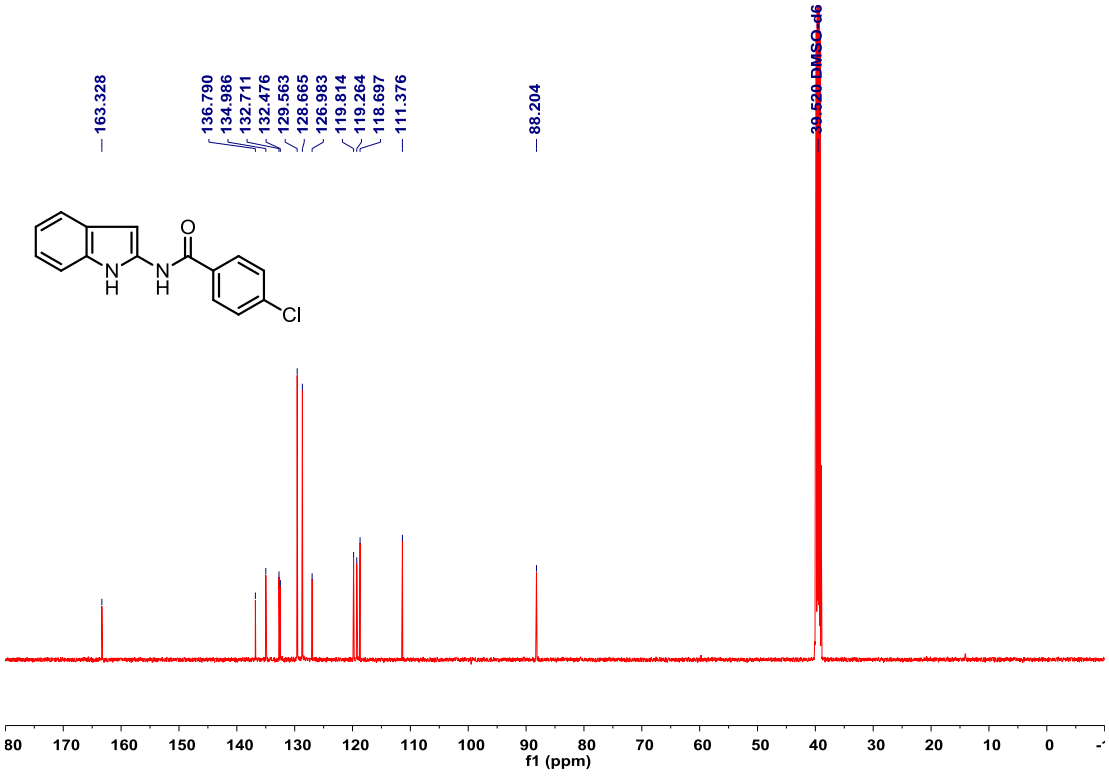
4-Fluoro-*N*-(1*H*-indol-2-yl)benzamide (5d)



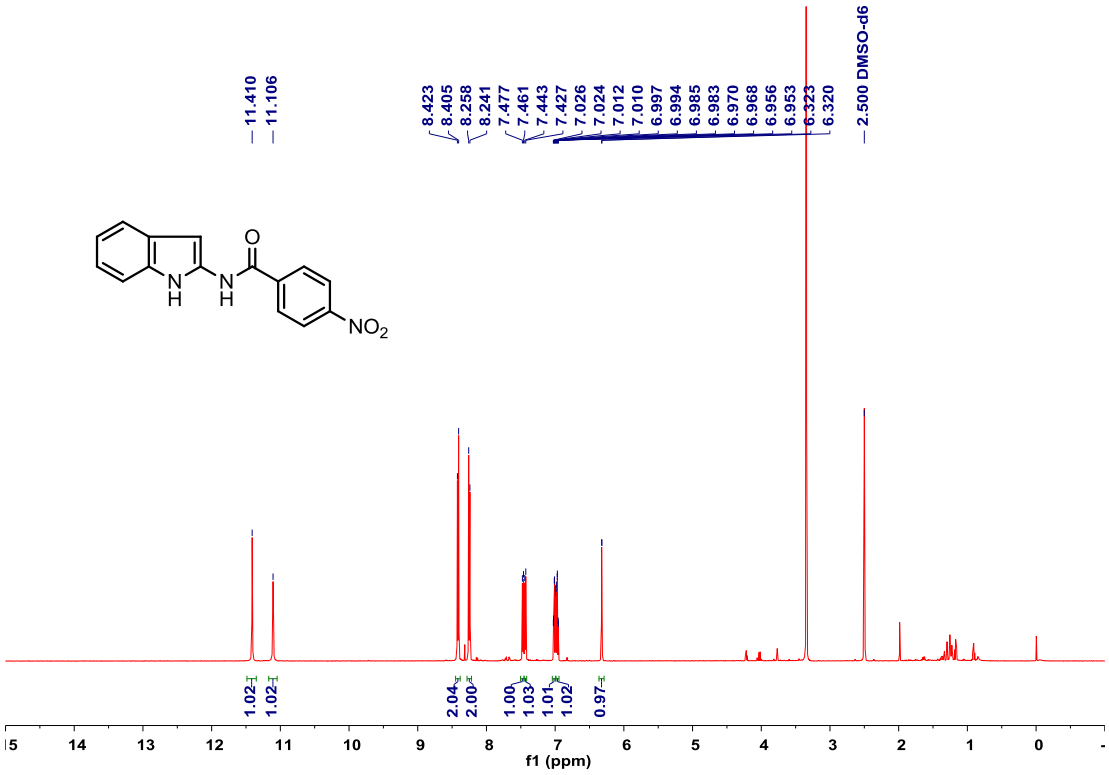


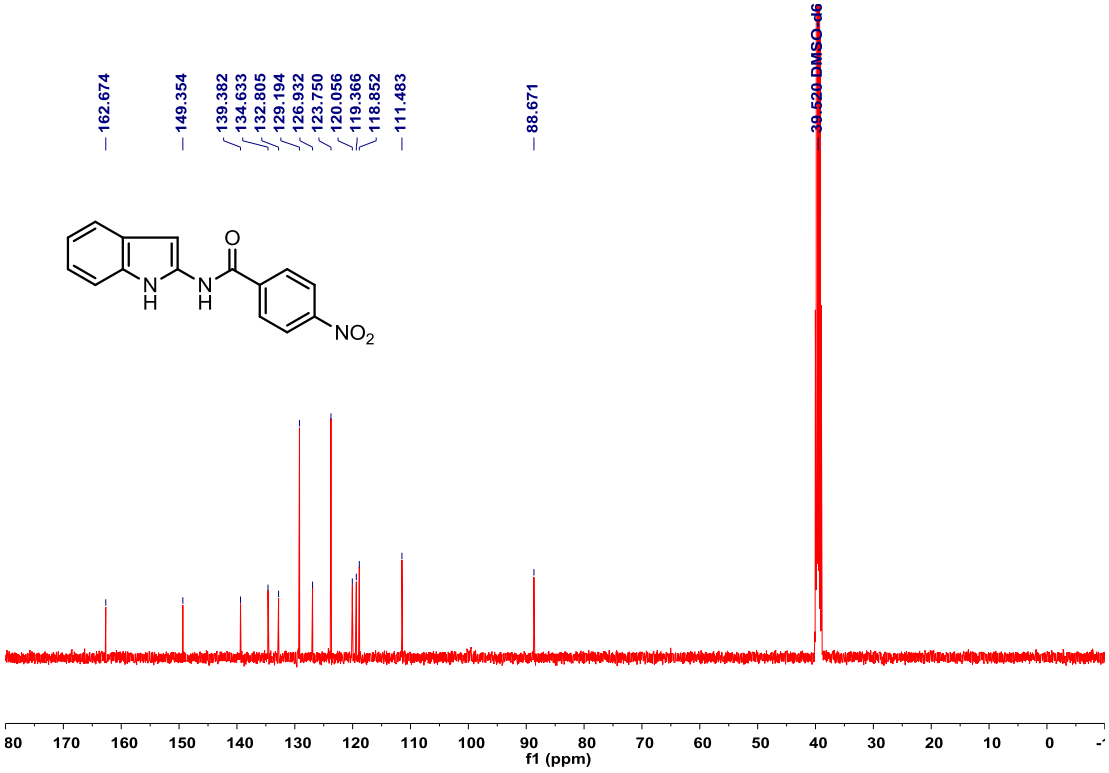
4-Chloro-*N*-(1*H*-indol-2-yl)benzamide (5e)



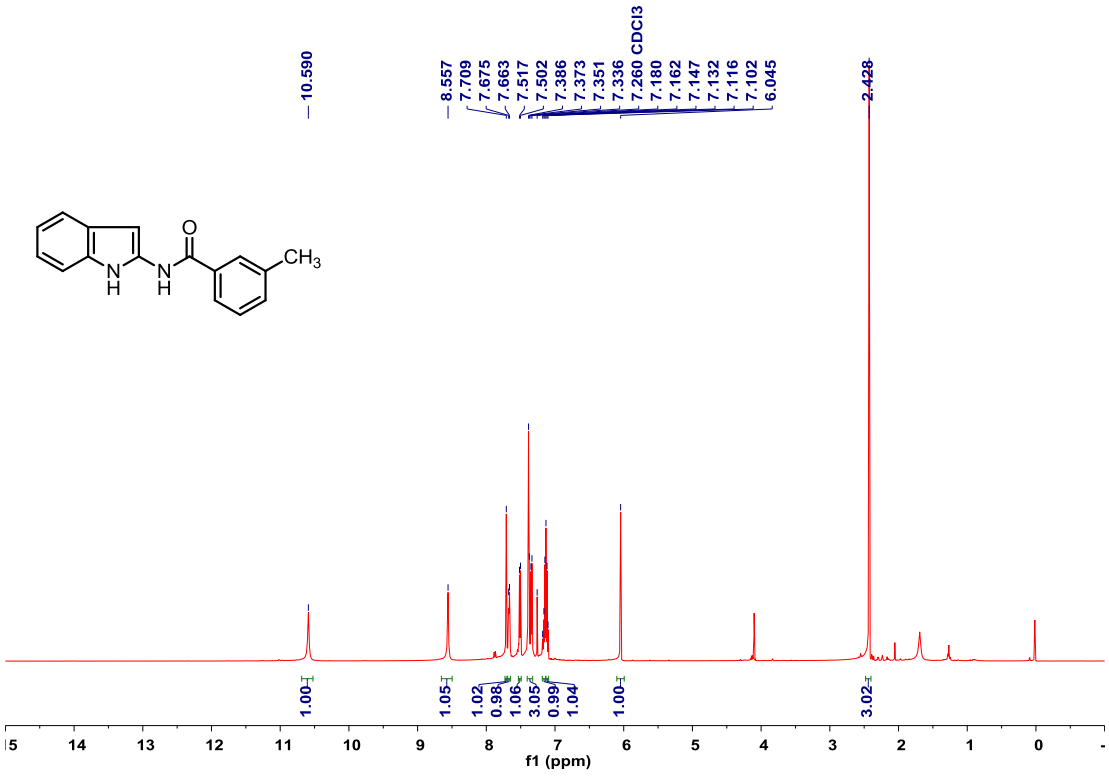


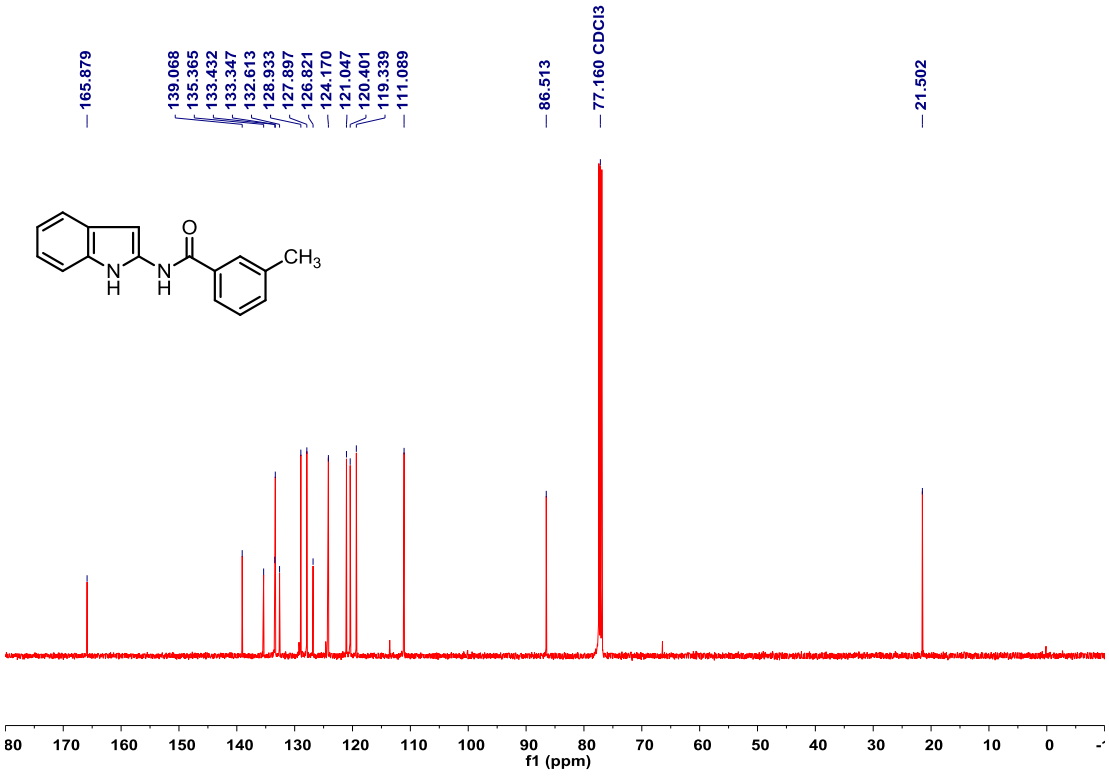
***N*-(1*H*-Indol-2-yl)-4-nitrobenzamide (5f)**



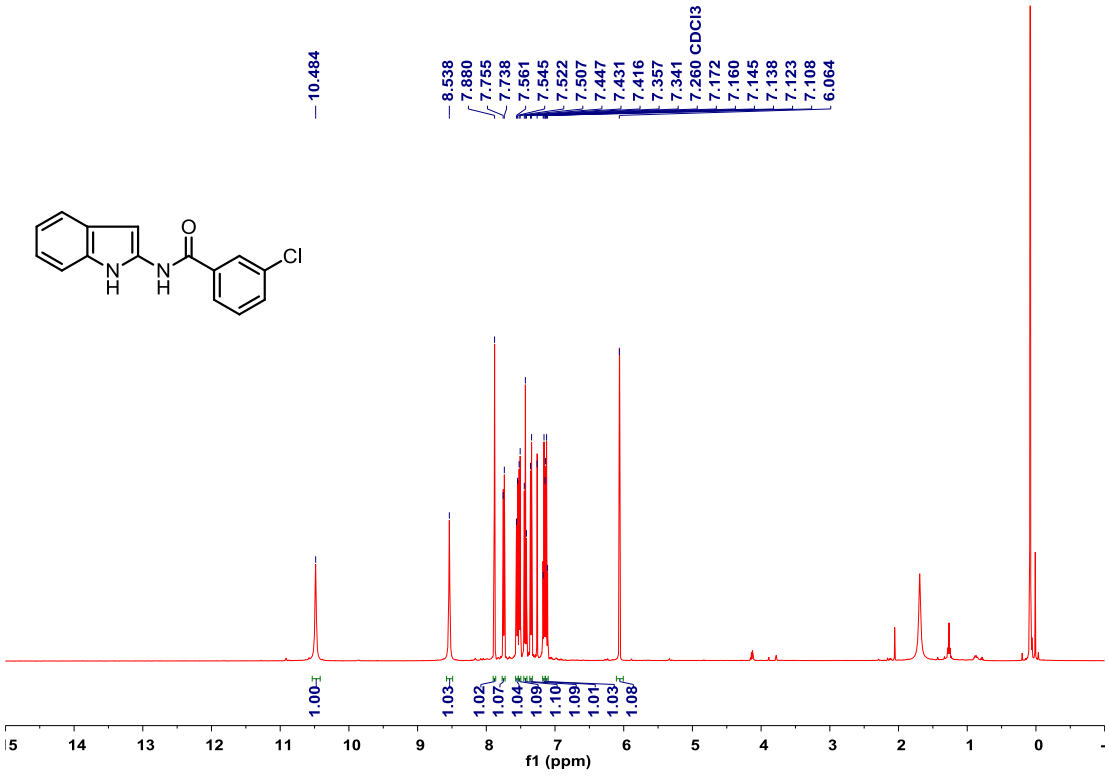


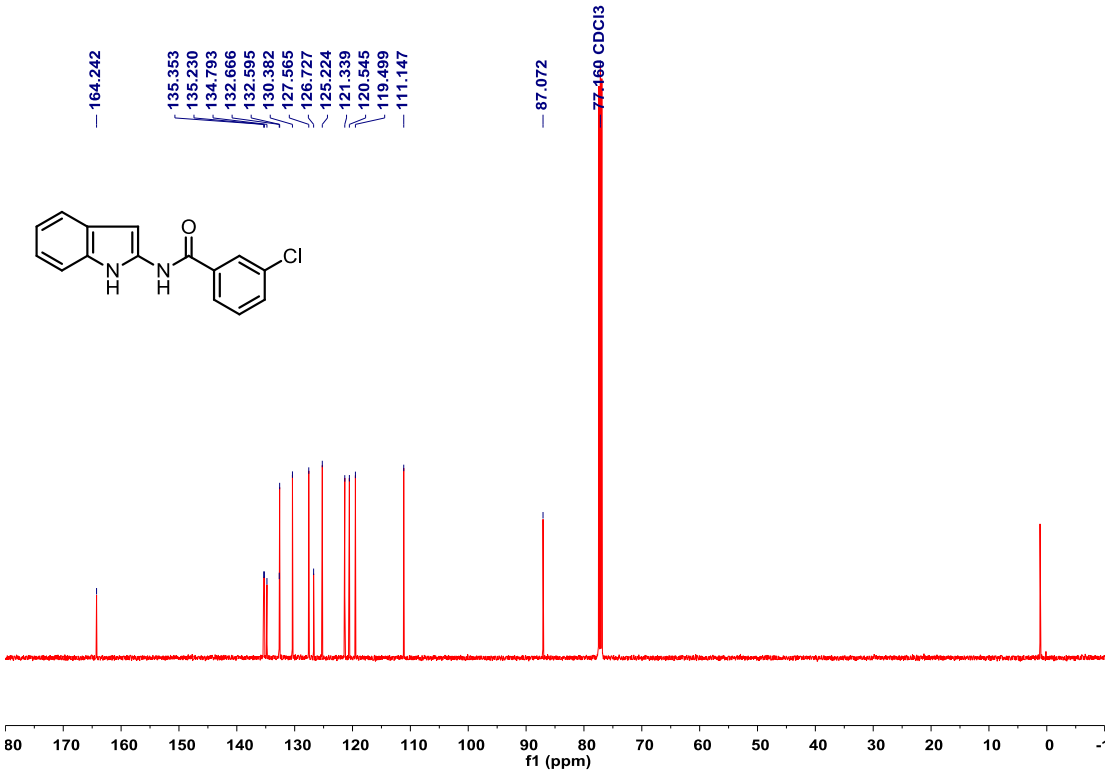
***N*-(1*H*-Indol-2-yl)-3-methylbenzamide (5g)**



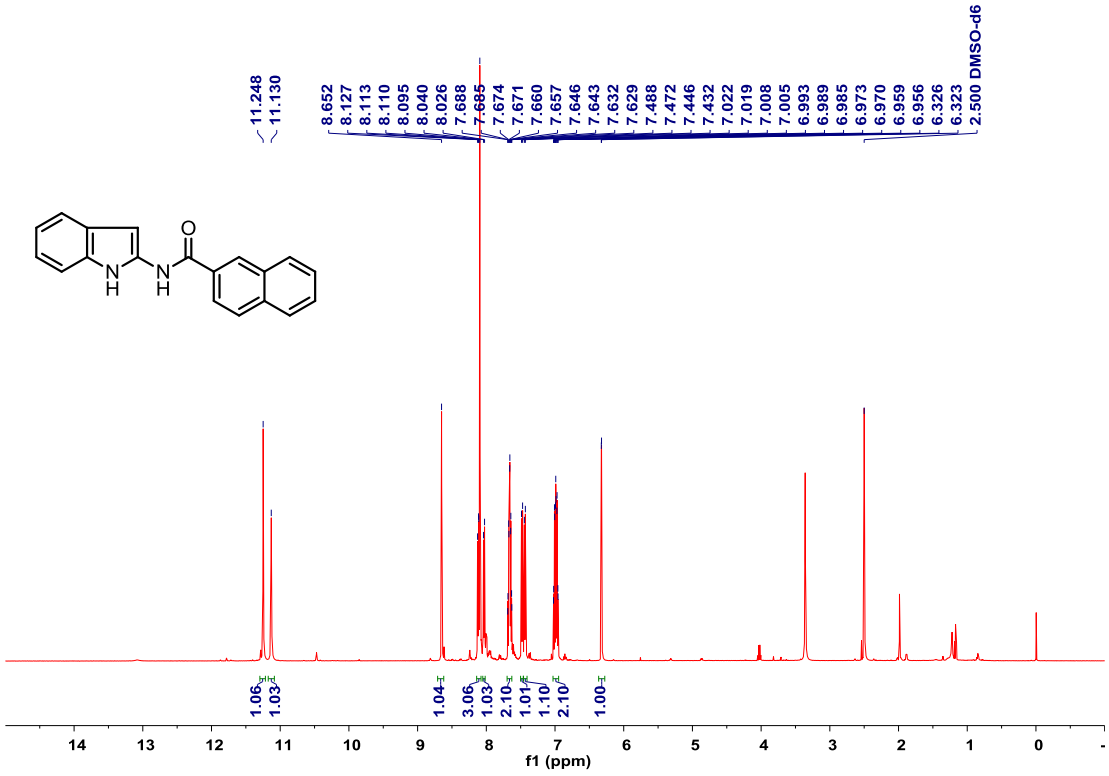


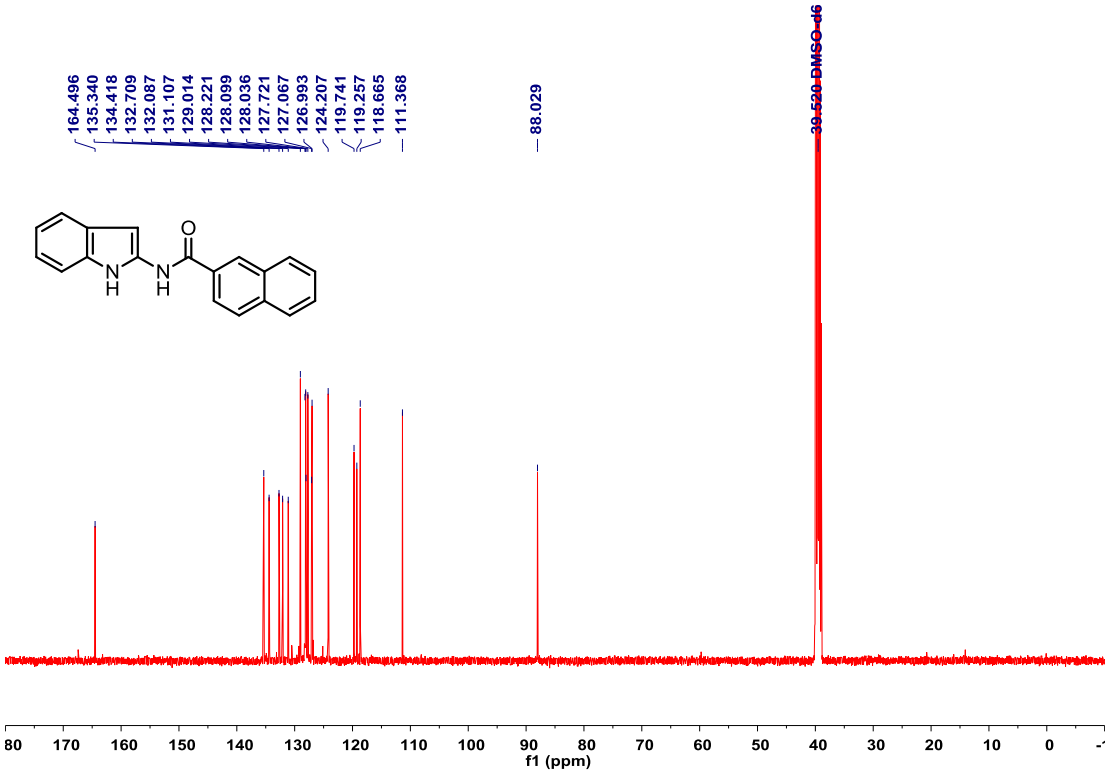
3-Chloro-*N*-(1*H*-indol-2-yl)benzamide (5h)



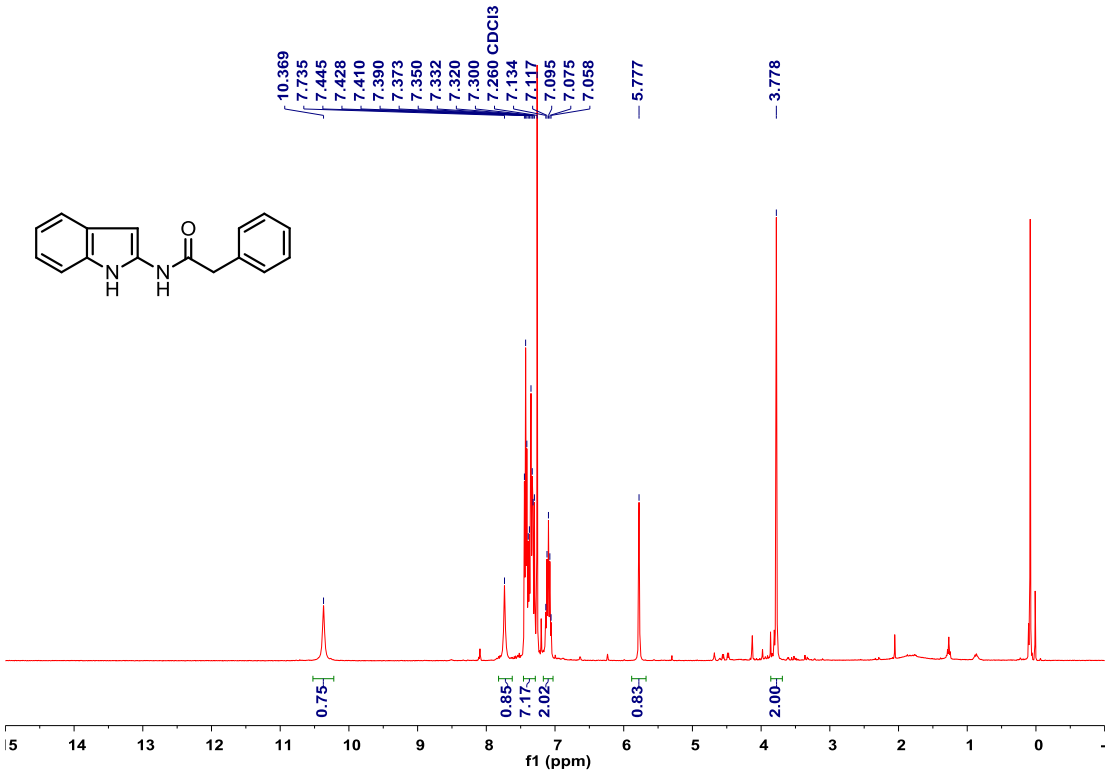


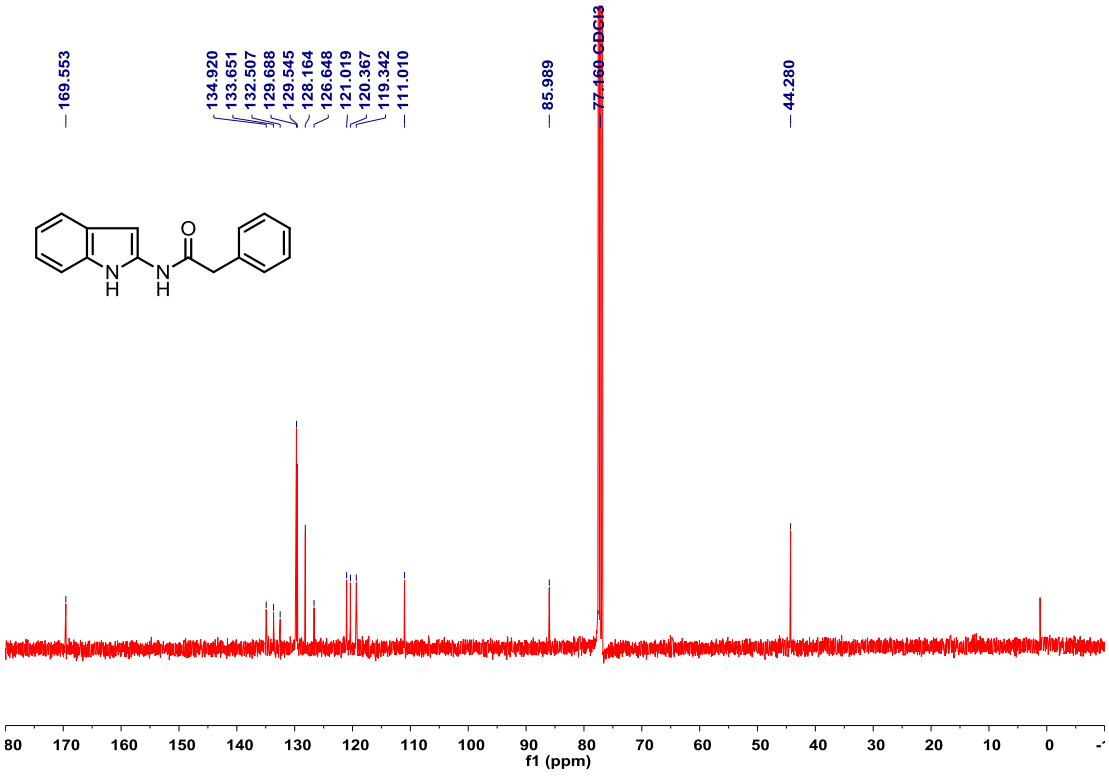
***N*-(1*H*-Indol-2-yl)-2-naphthamide (5i)**



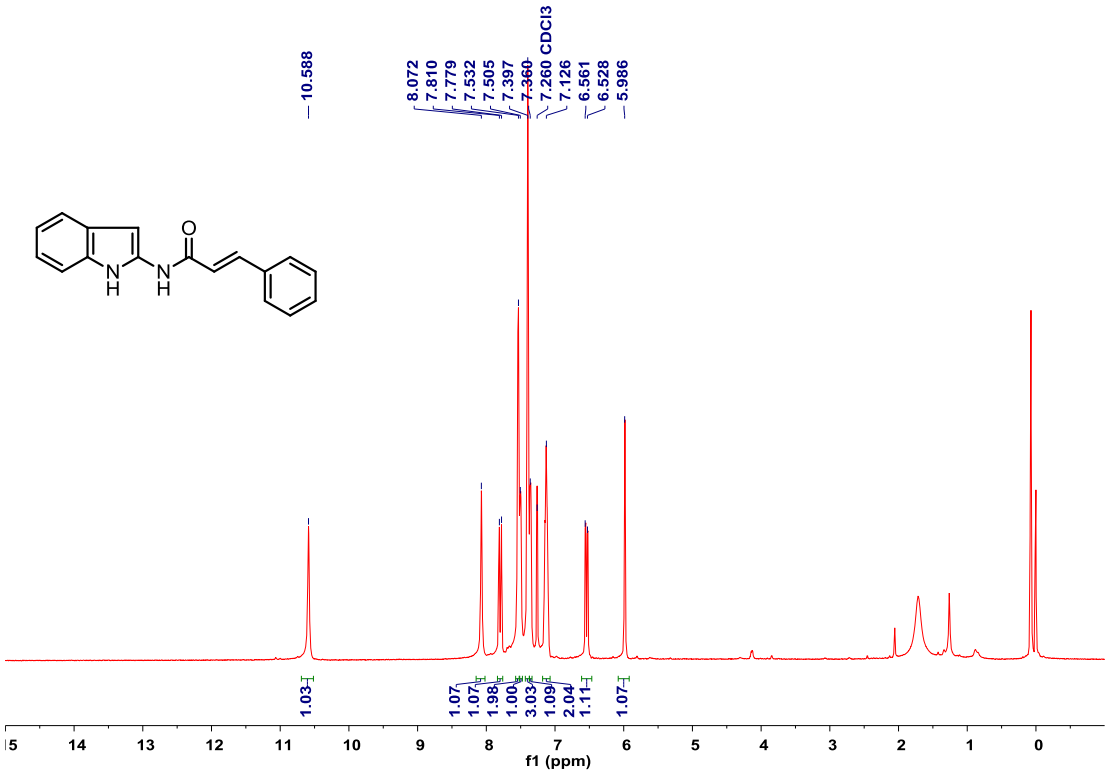


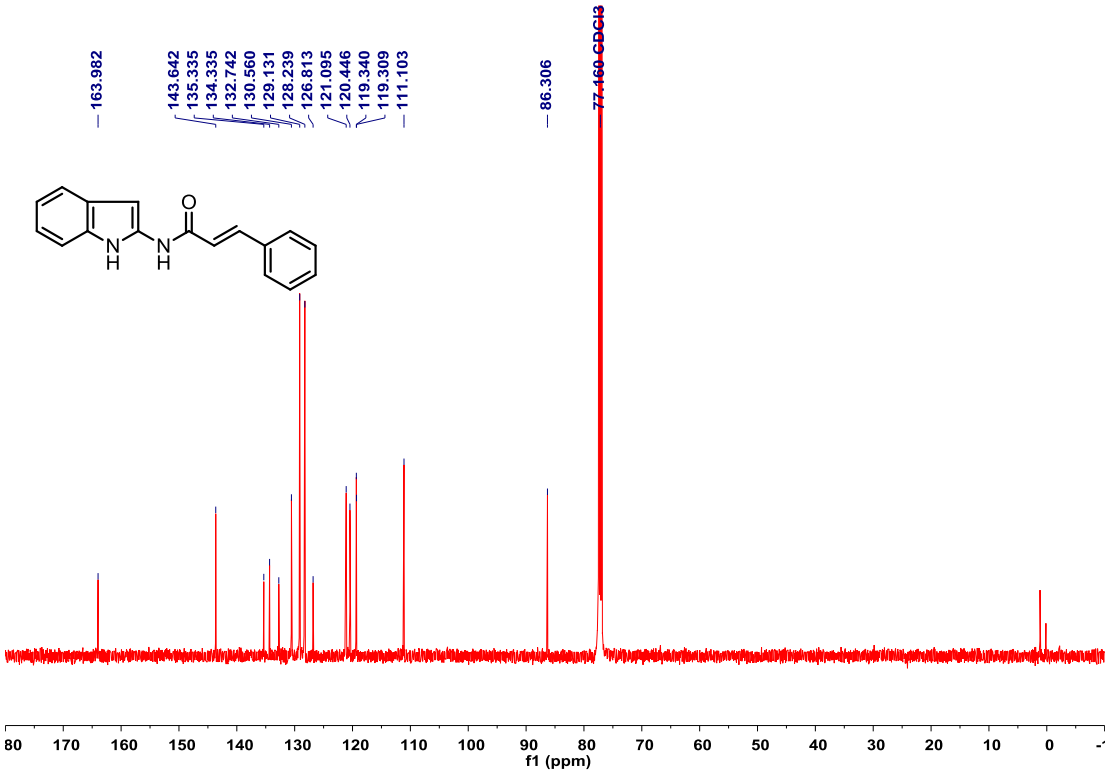
***N*-(1*H*-Indol-2-yl)-2-phenylacetamide (5j)**



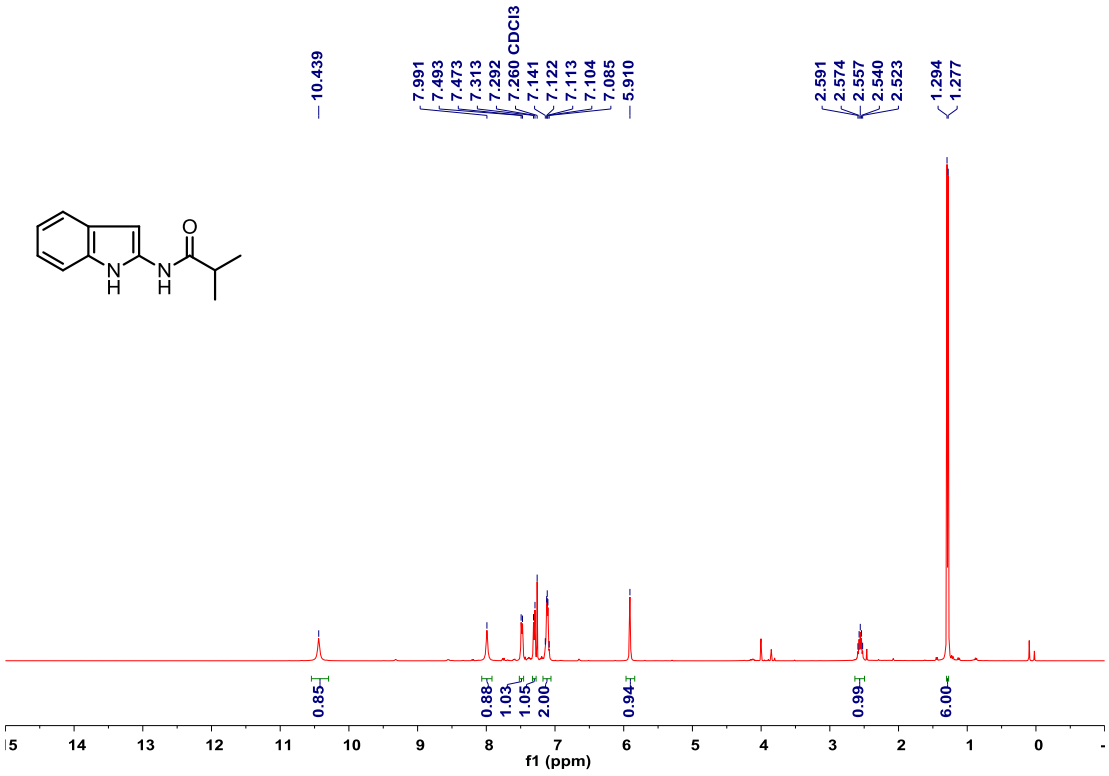


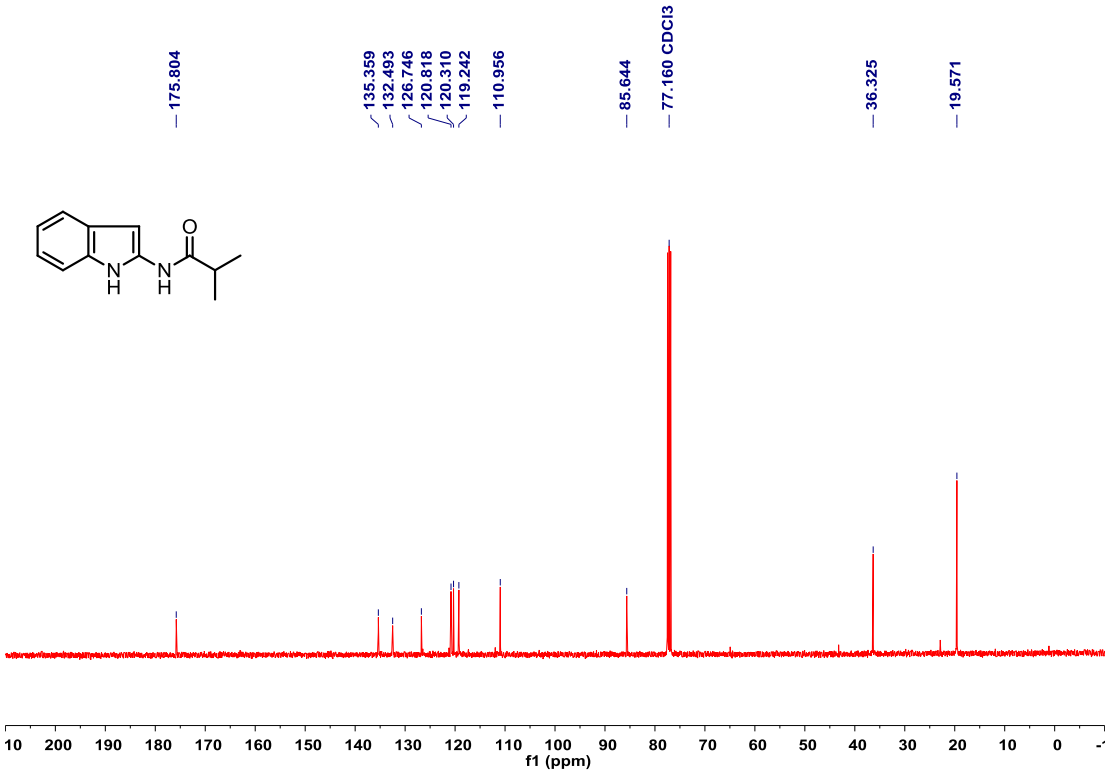
***N*-(1*H*-Indol-2-yl)cinnamamide (5k)**



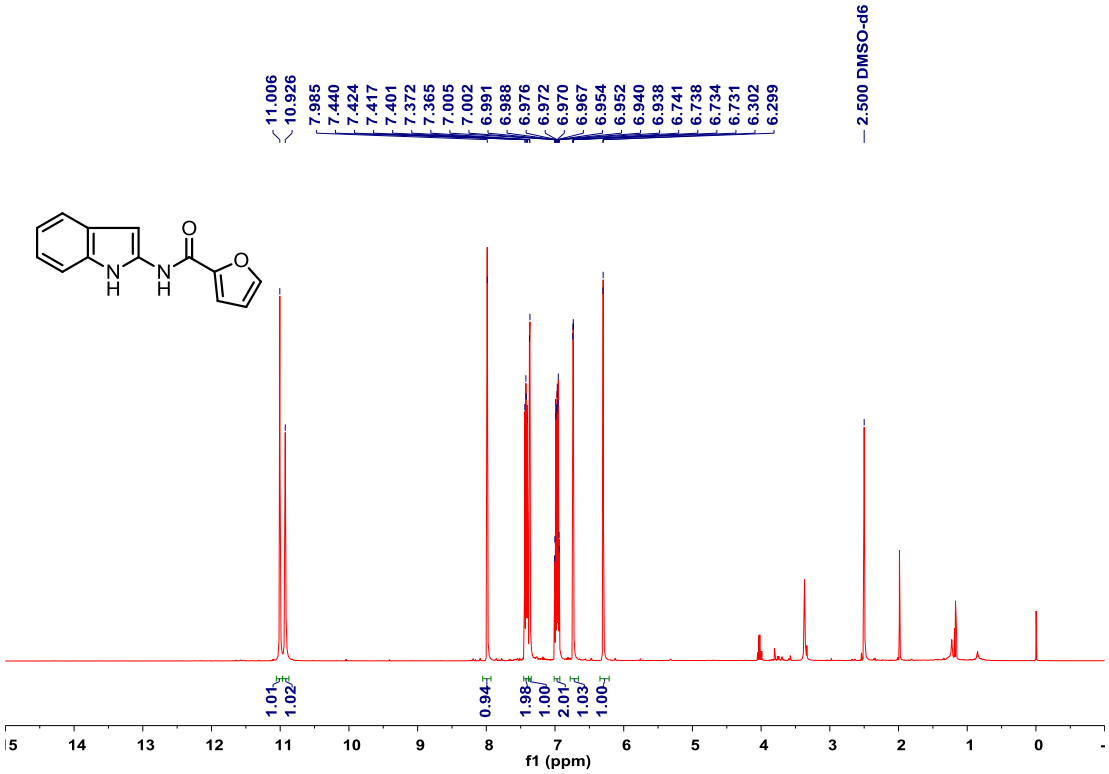


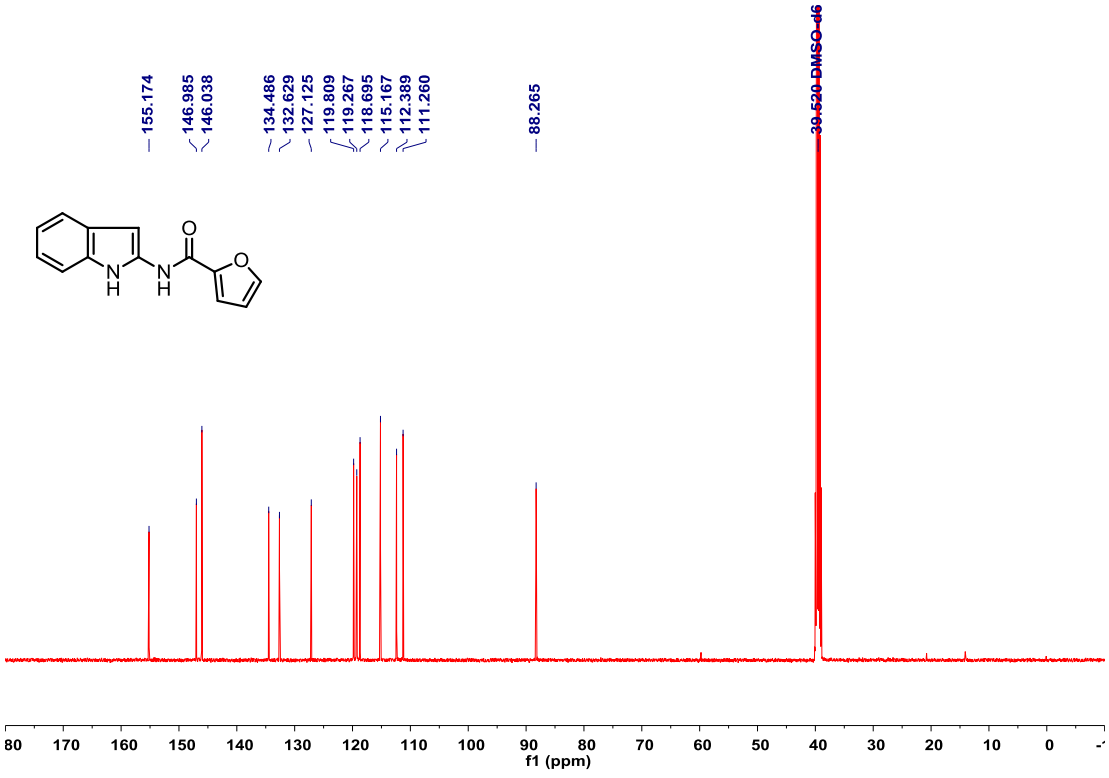
***N*-(1*H*-Indol-2-yl)isobutyramide (5l)**



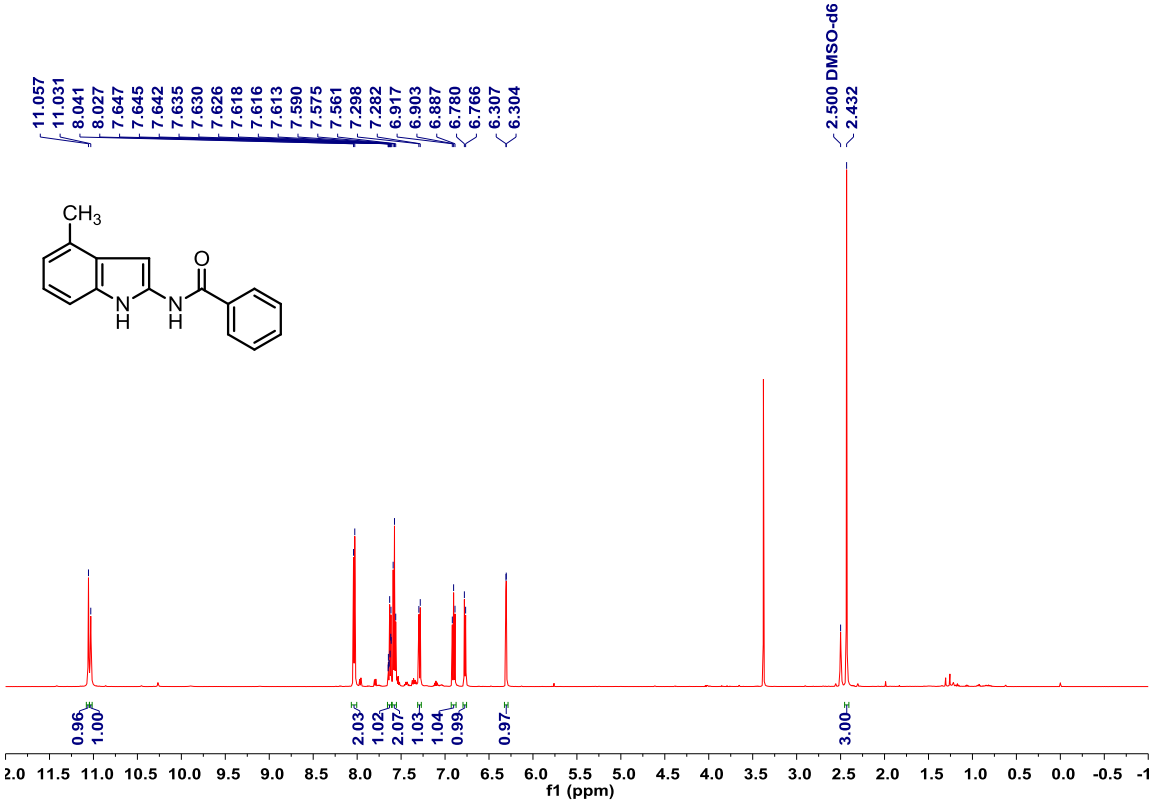


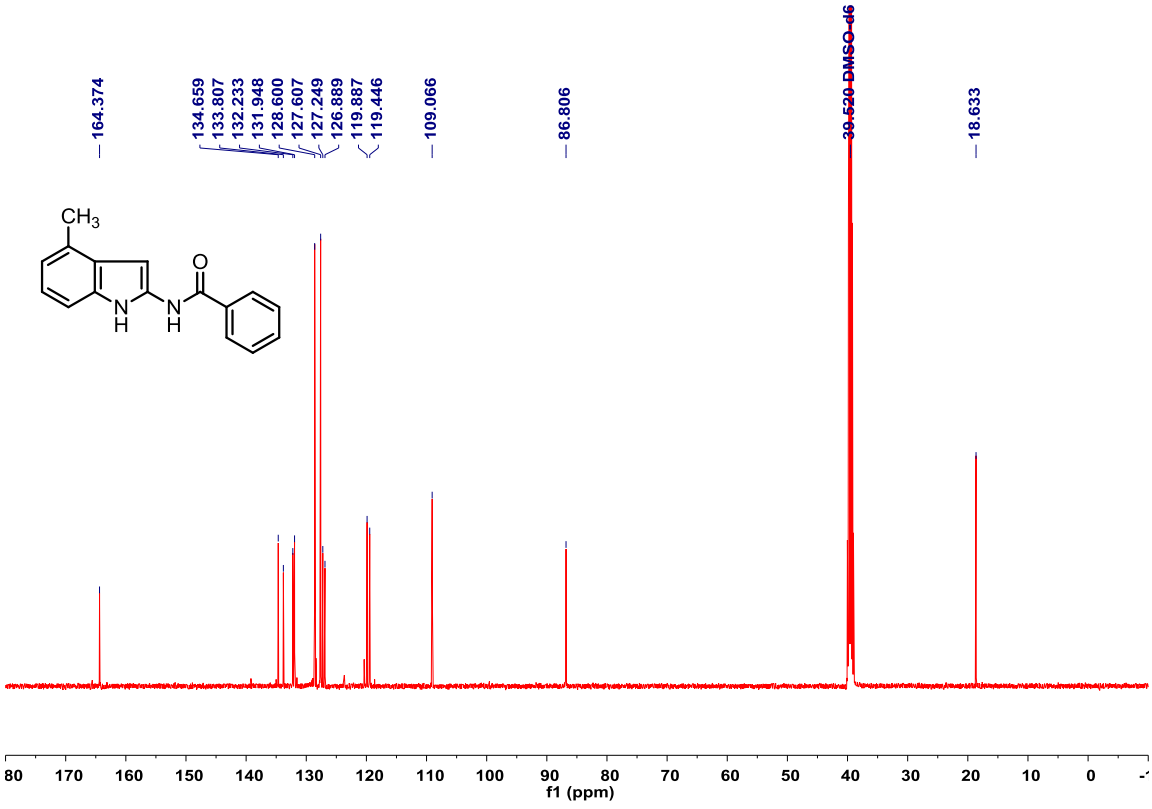
***N*-(1*H*-Indol-2-yl)furan-2-carboxamide (5m)**



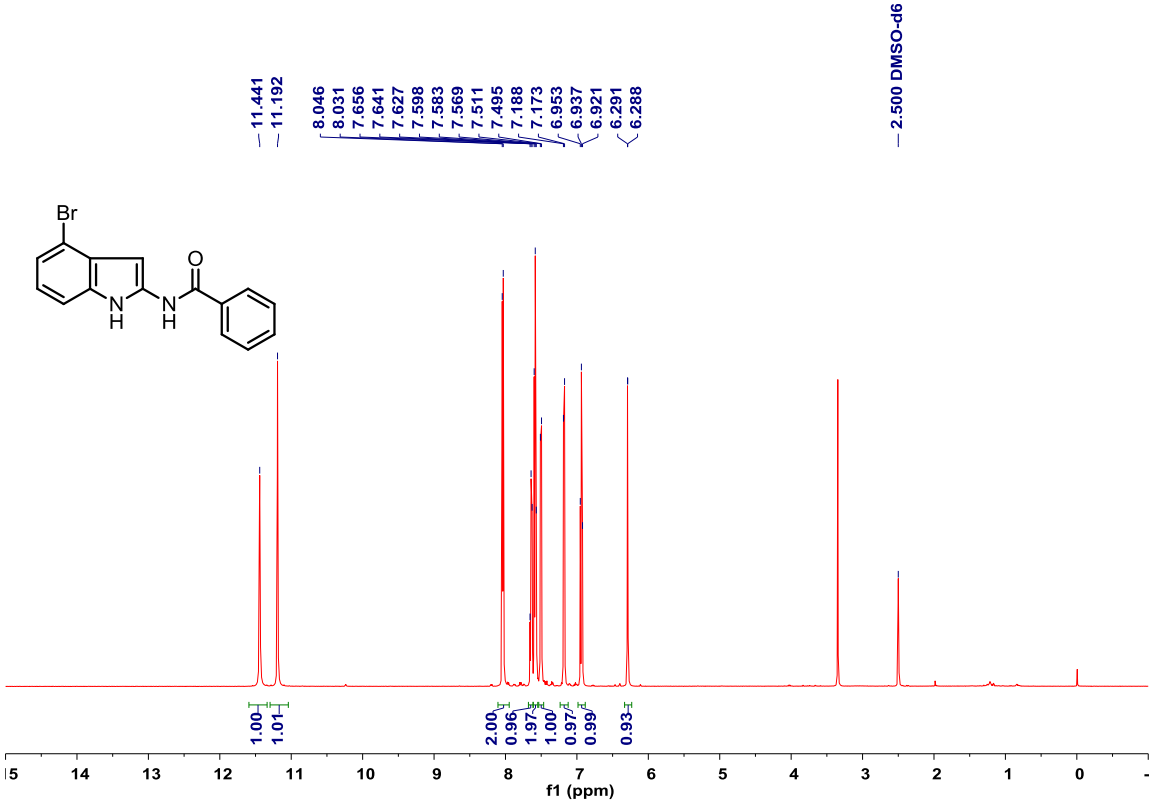


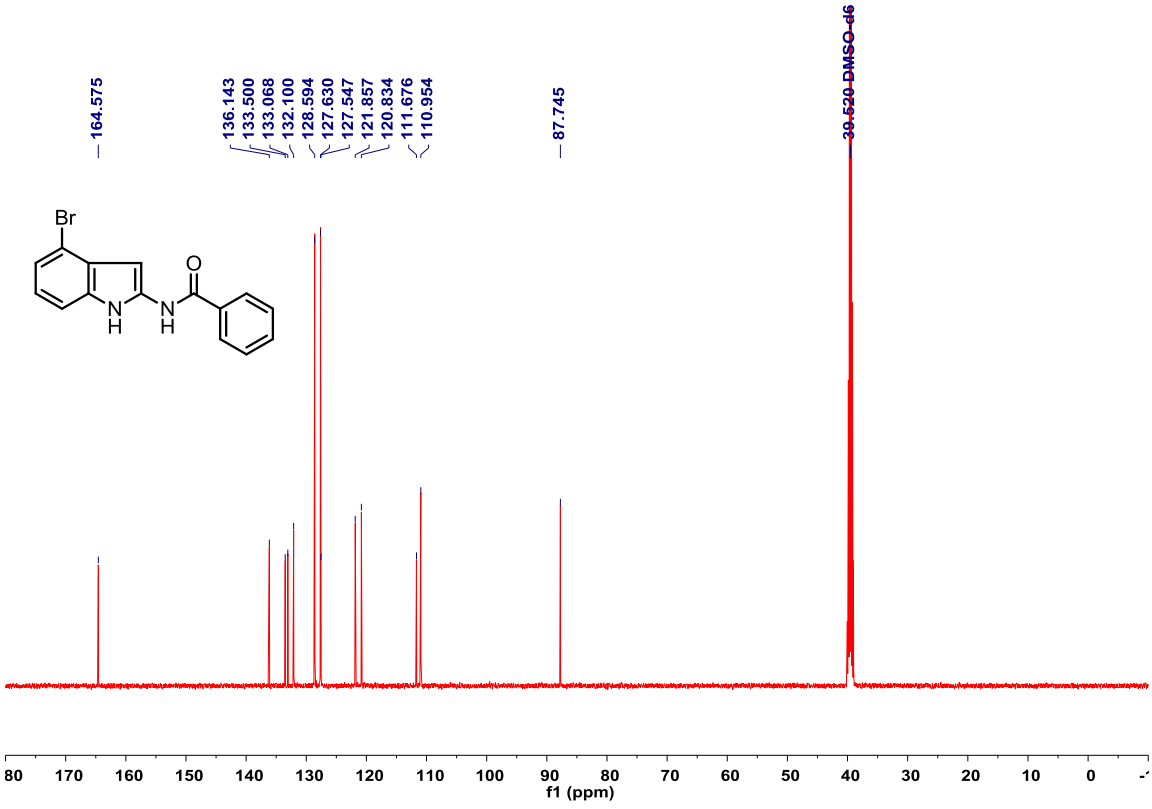
_N_-(4-Methyl-1_H_-indol-2-yl)benzamide (5n)



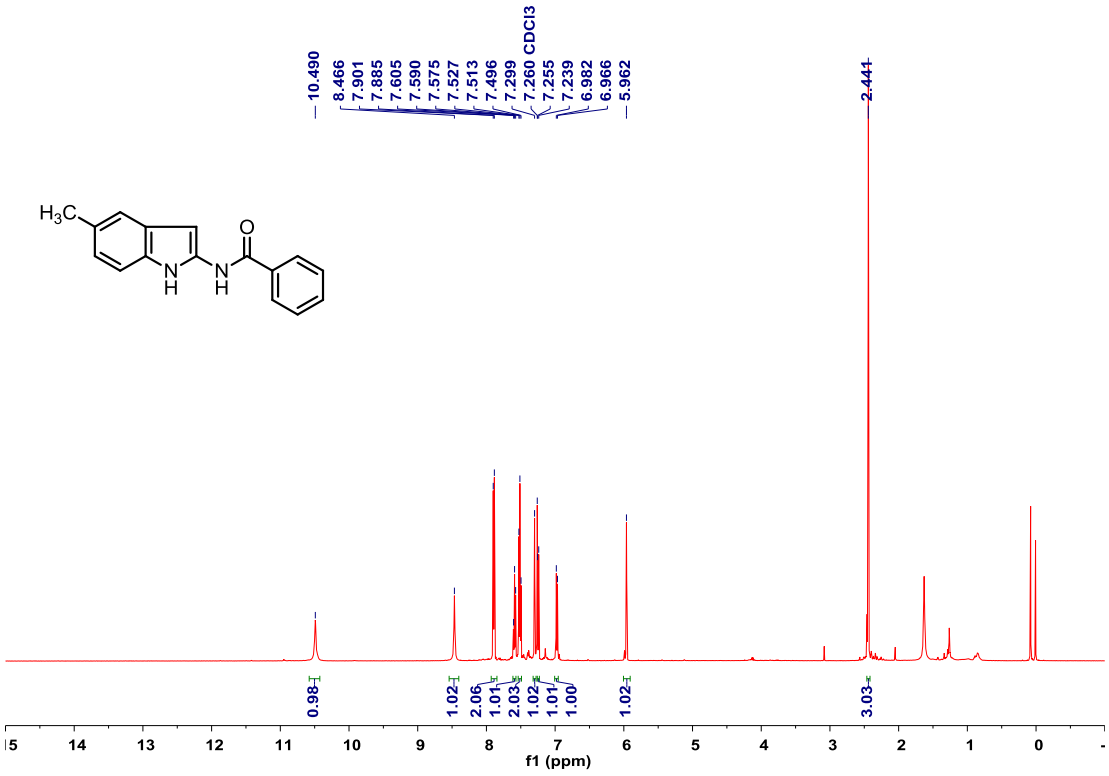


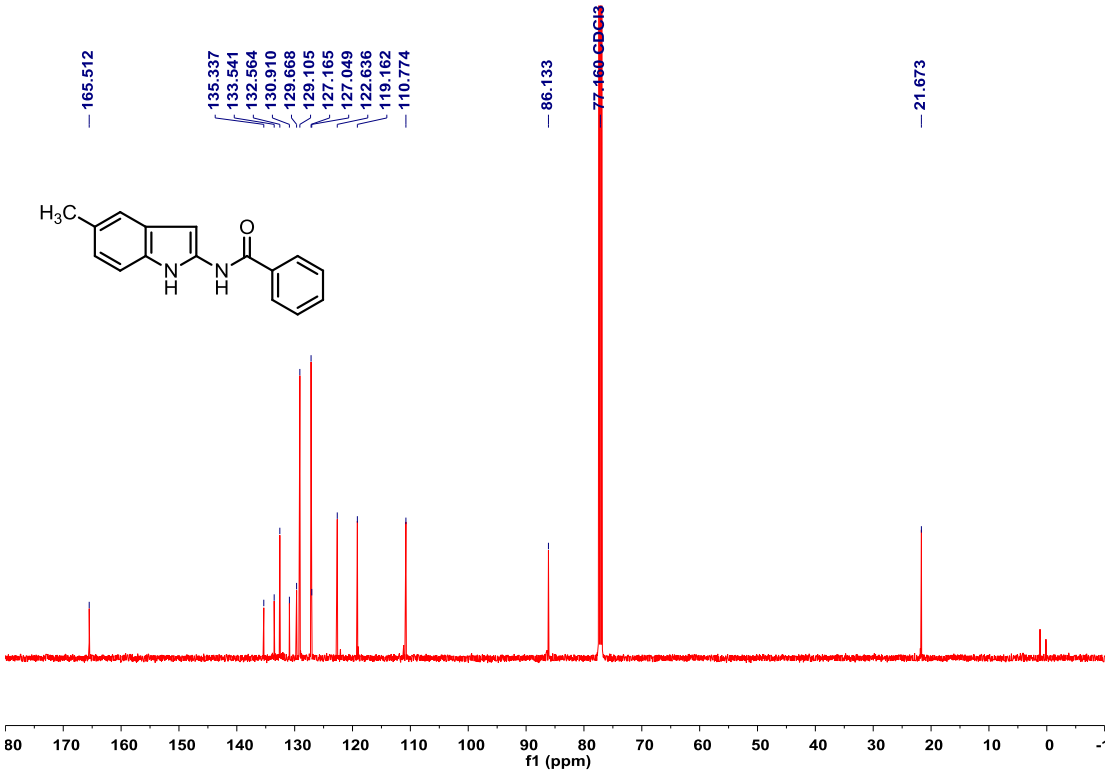
***N*-(4-Methyl-1*H*-indol-2-yl)benzamide (5o)**



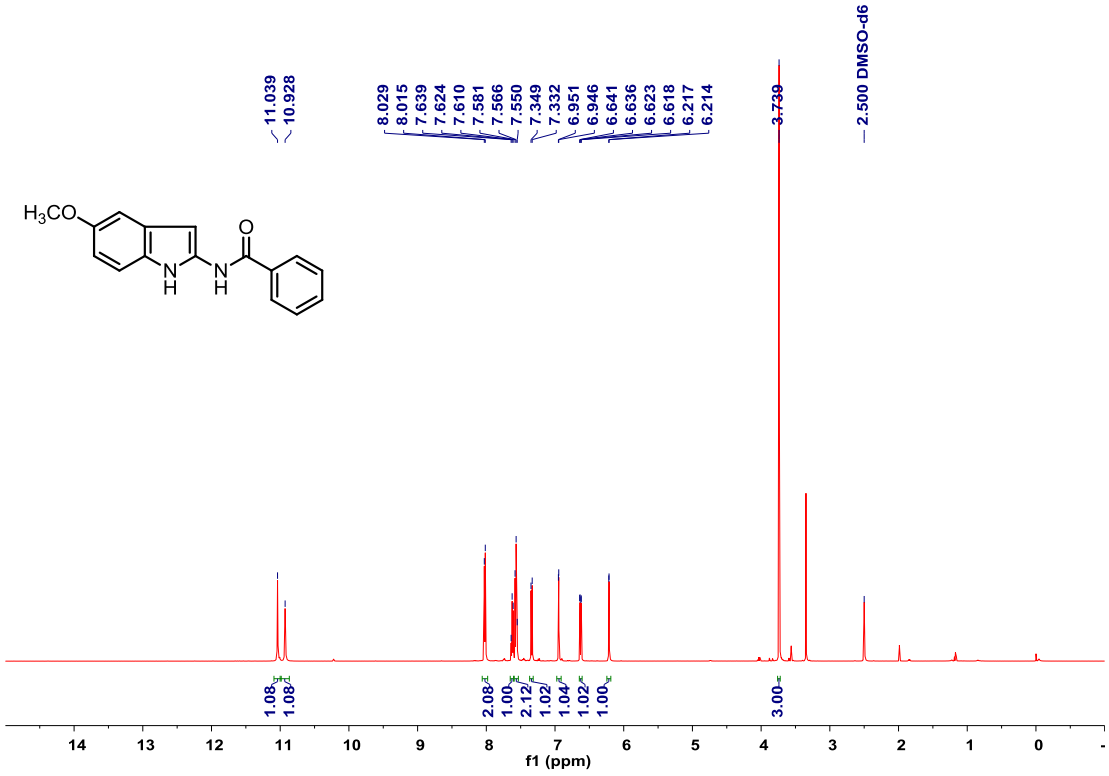


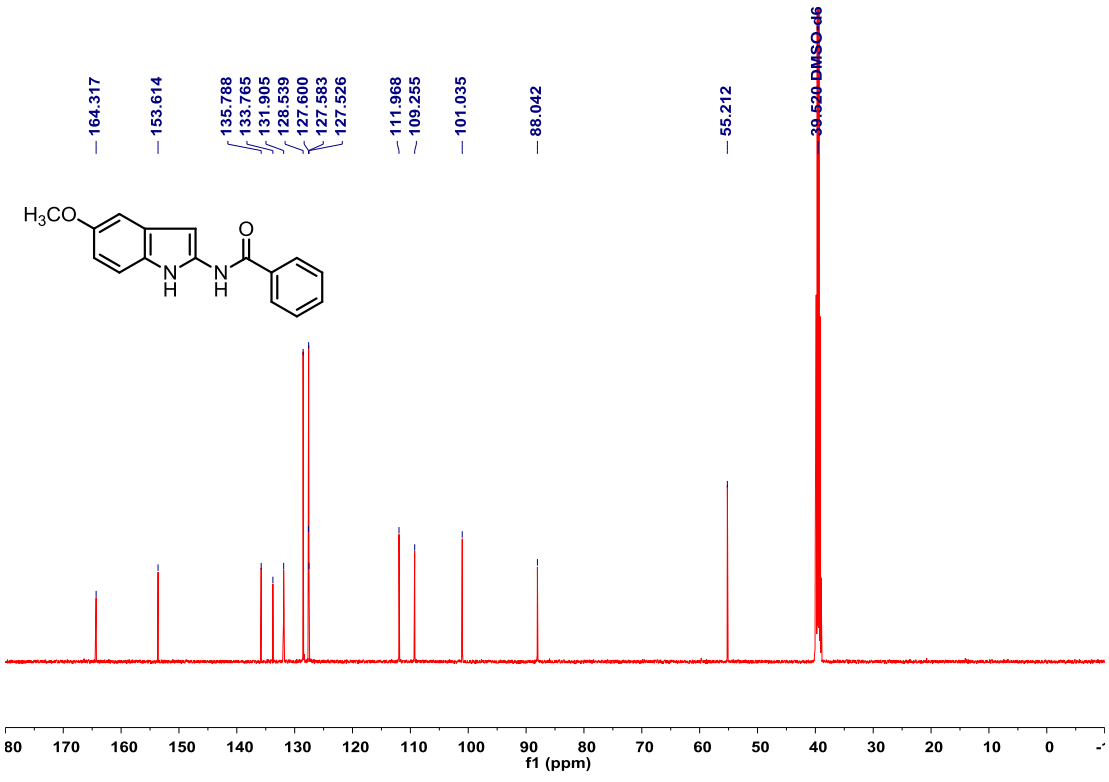
***N*-(5-Methyl-1*H*-indol-2-yl)benzamide (5p)**



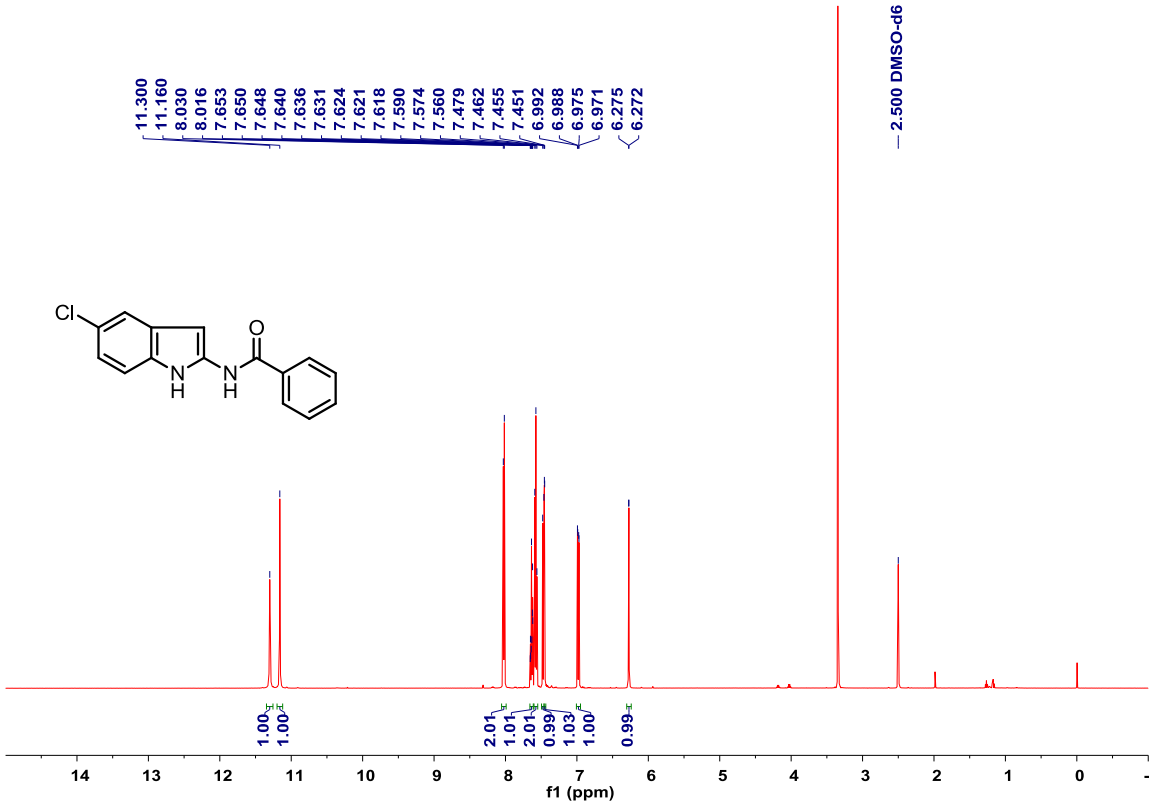


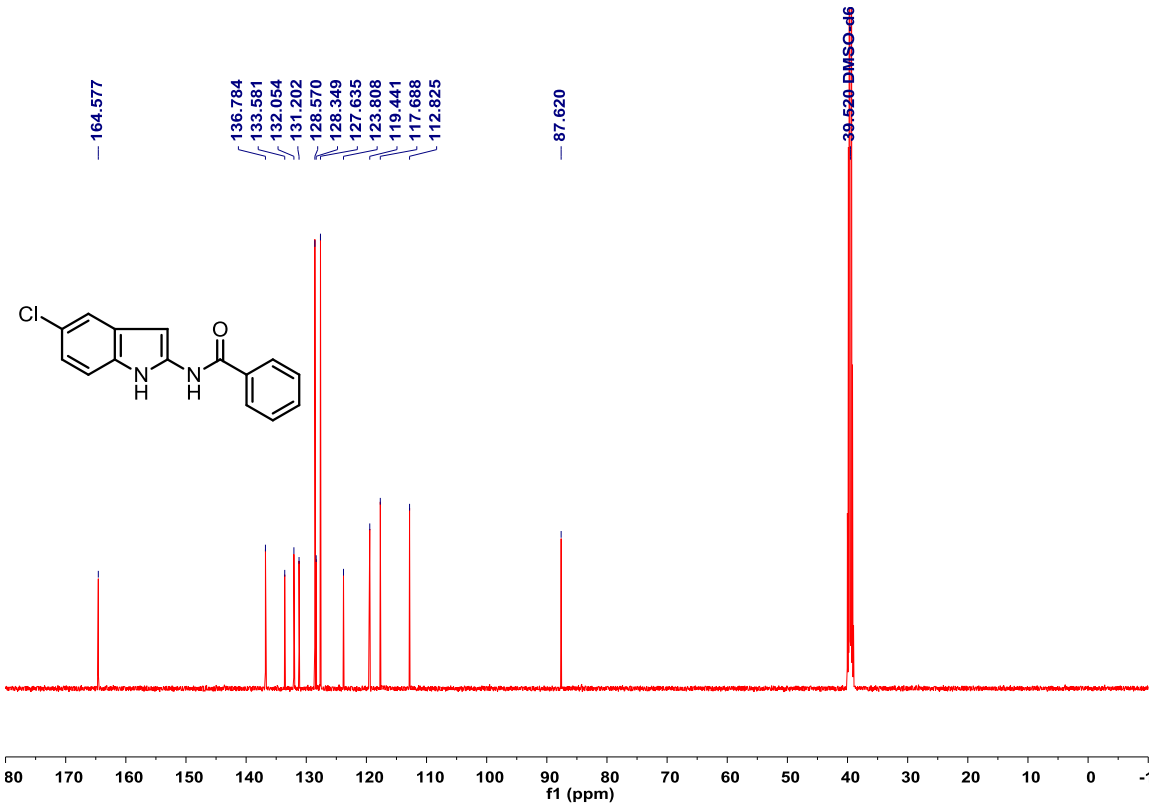
_N_-(5-Methoxy-1_H_-indol-2-yl)benzamide (5q)



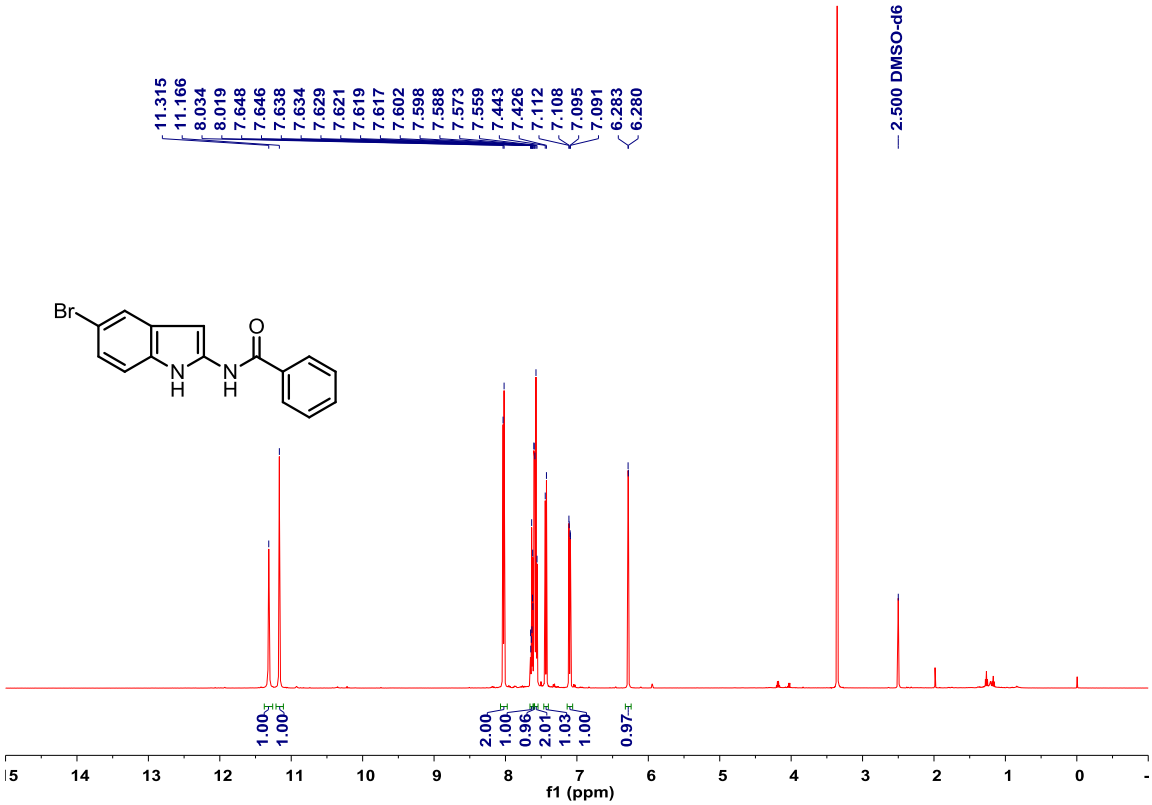


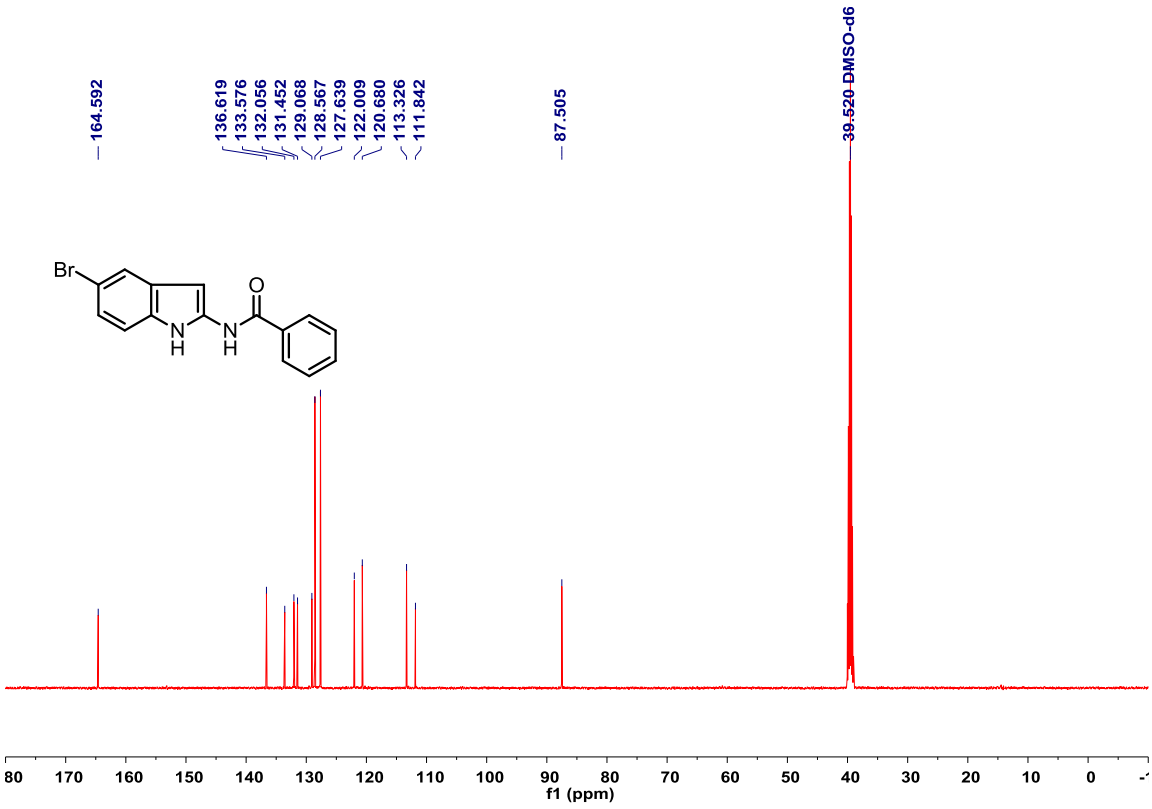
***N*-(5-Chloro-1*H*-indol-2-yl)benzamide (5r)**



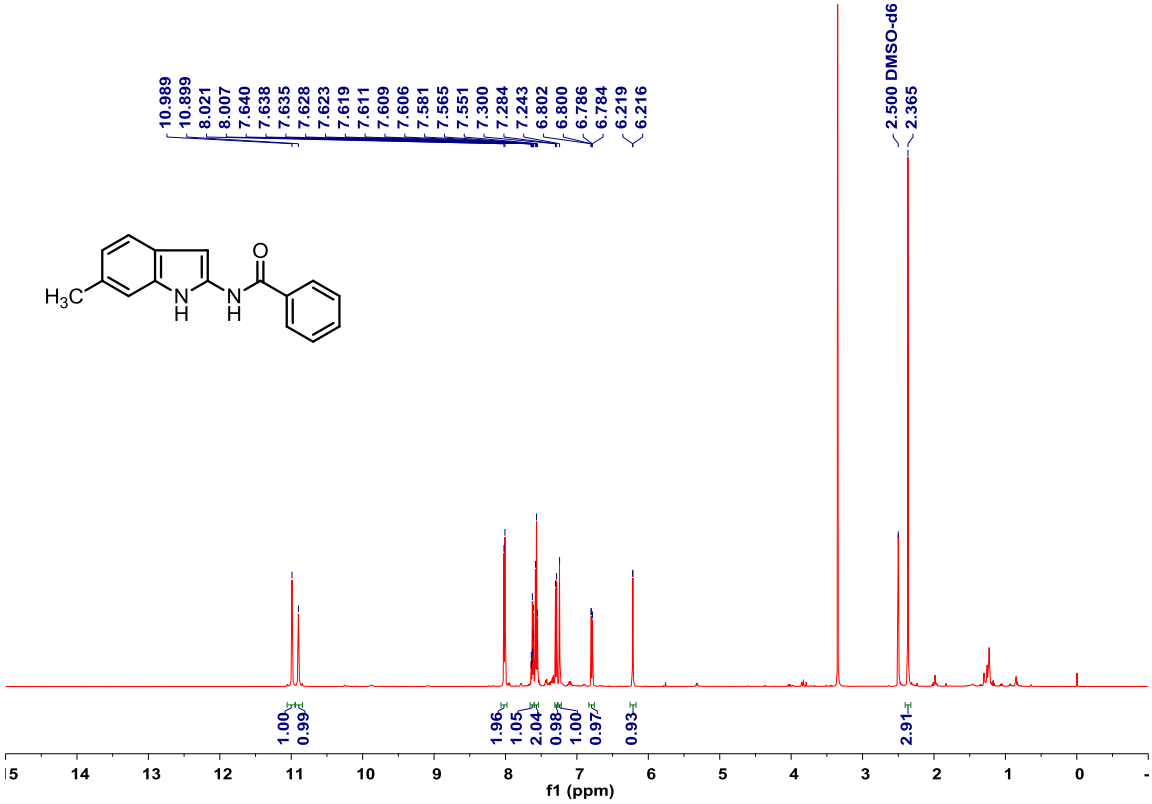


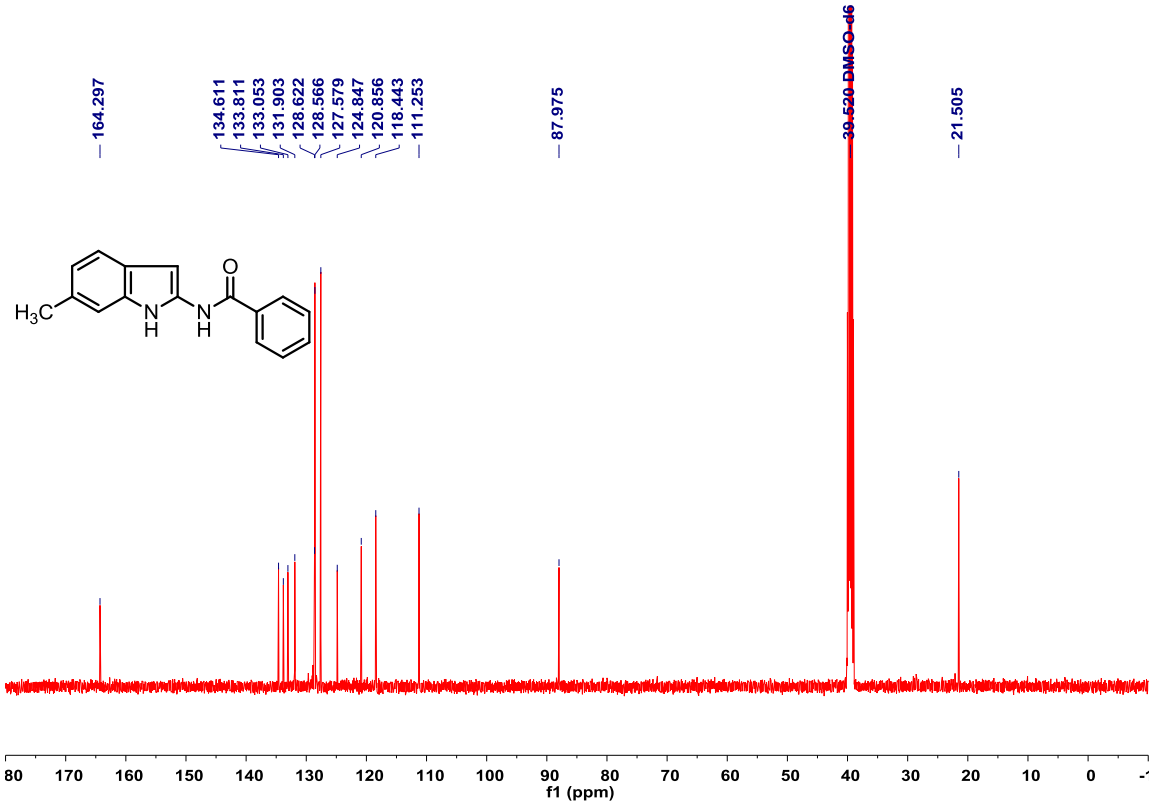
***N*-(5-Bromo-1*H*-indol-2-yl)benzamide (5s)**



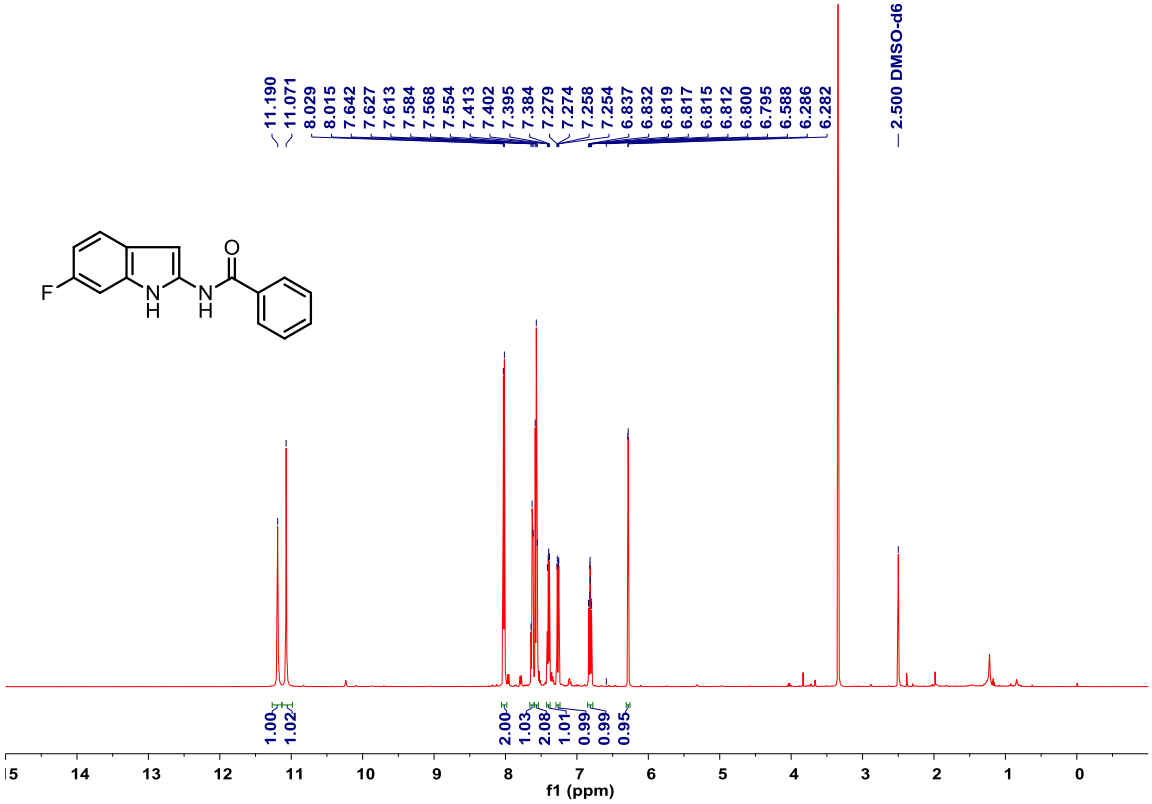


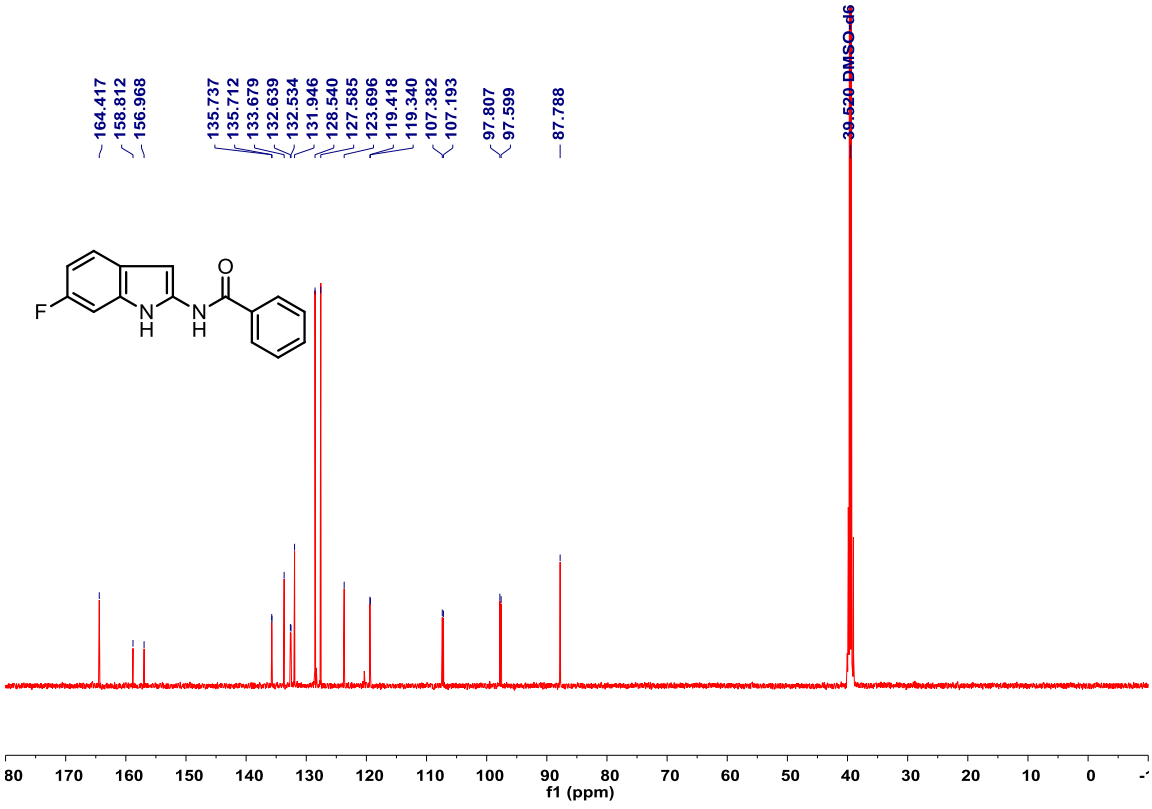
***N*-(6-Methyl-1*H*-indol-2-yl)benzamide (5t)**



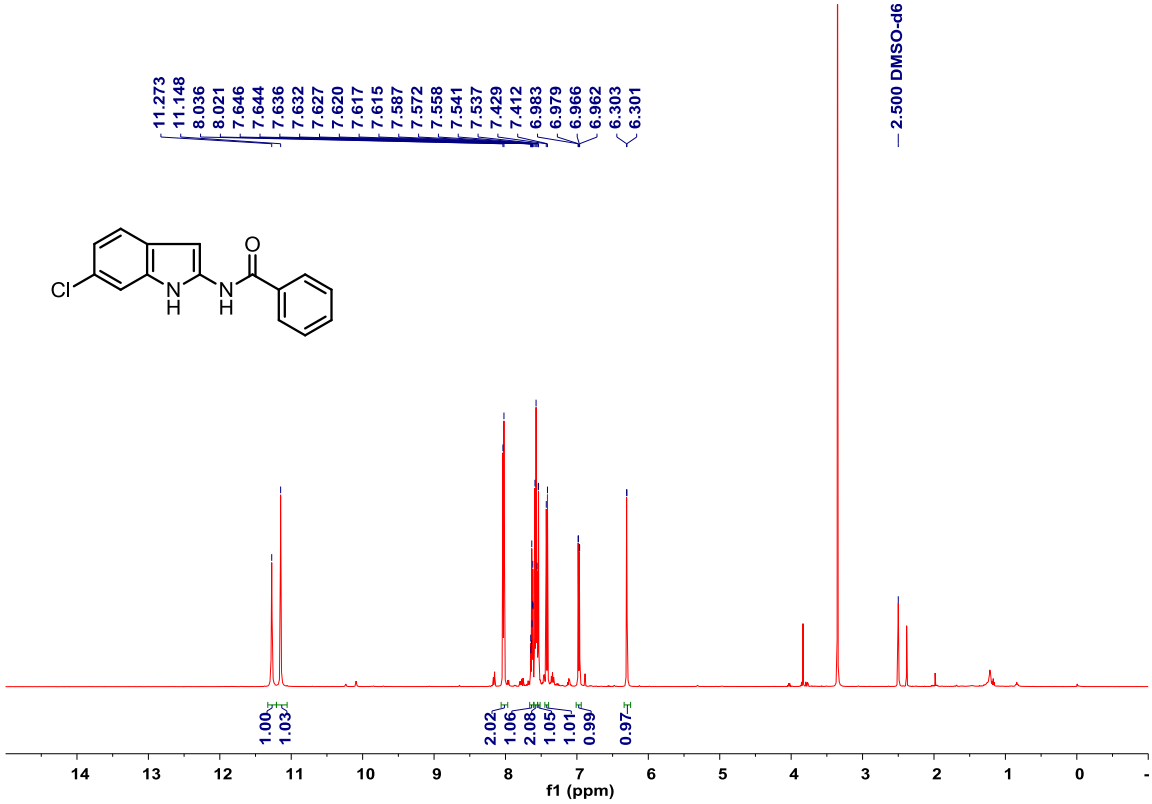


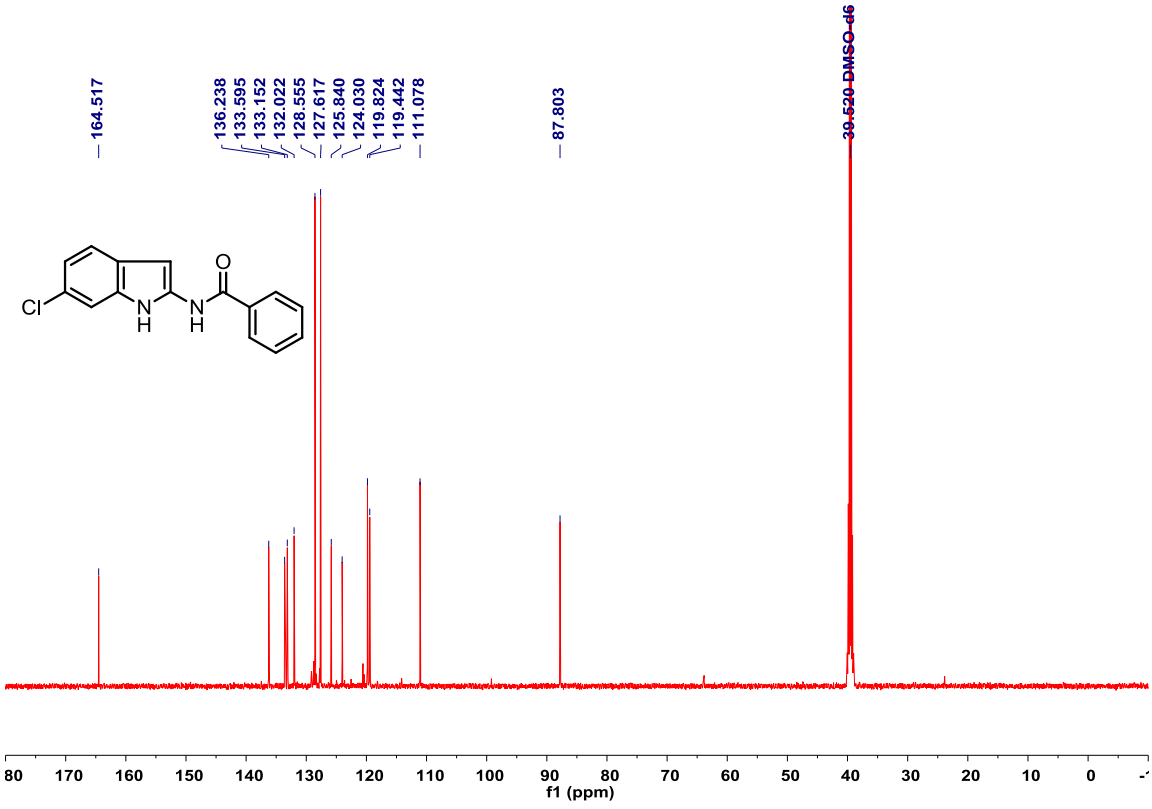
***N*-(6-Fluoro-1*H*-indol-2-yl)benzamide (5u)**



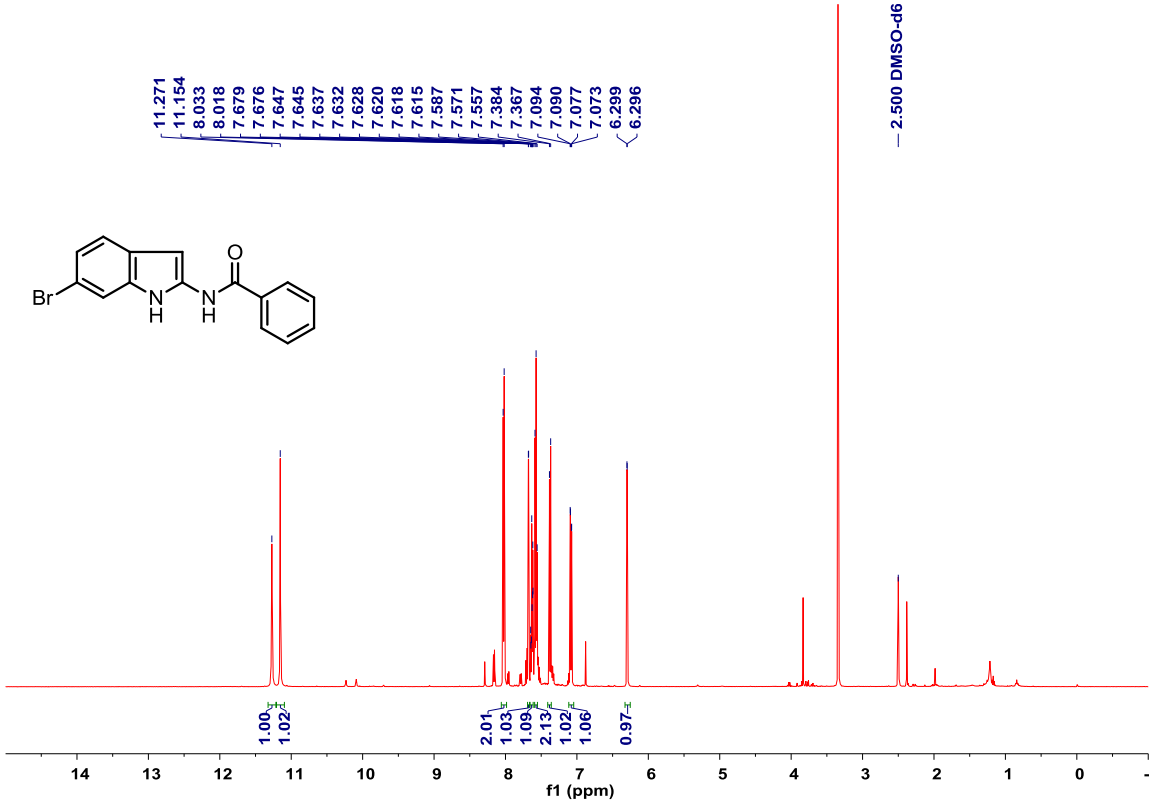


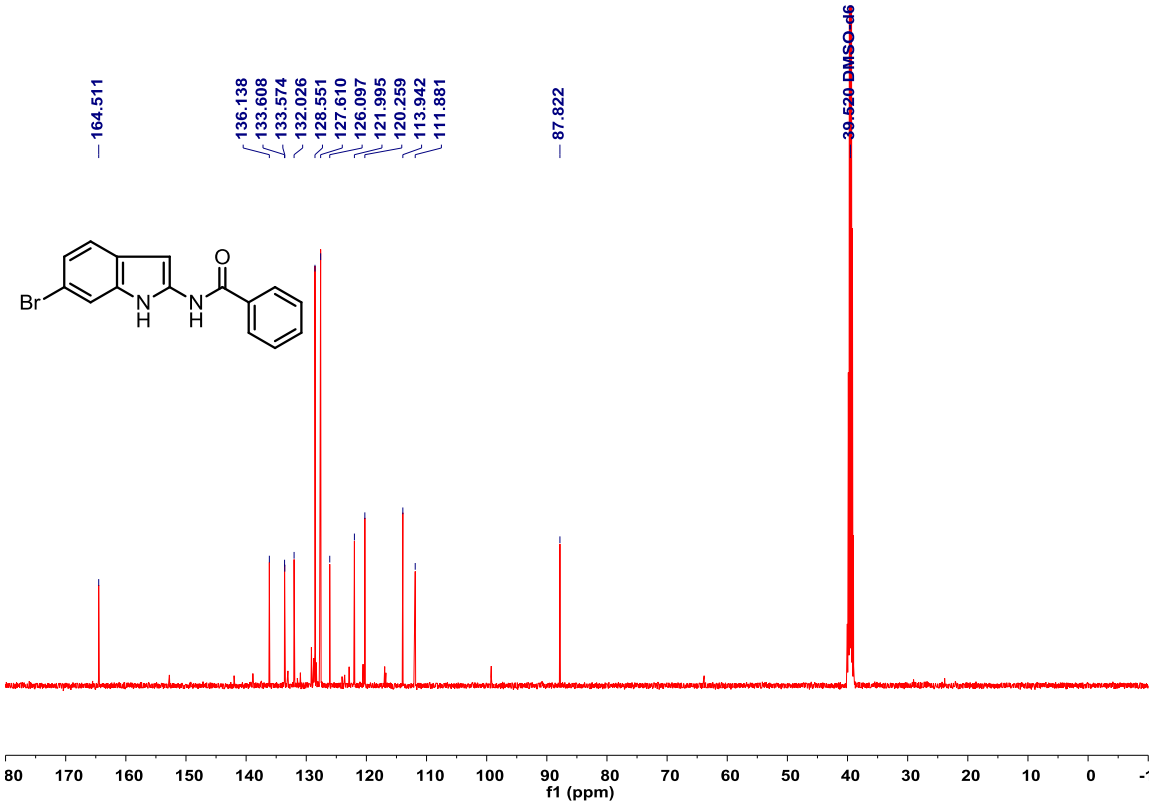
***N*-(6-Chloro-1*H*-indol-2-yl)benzamide (5v)**



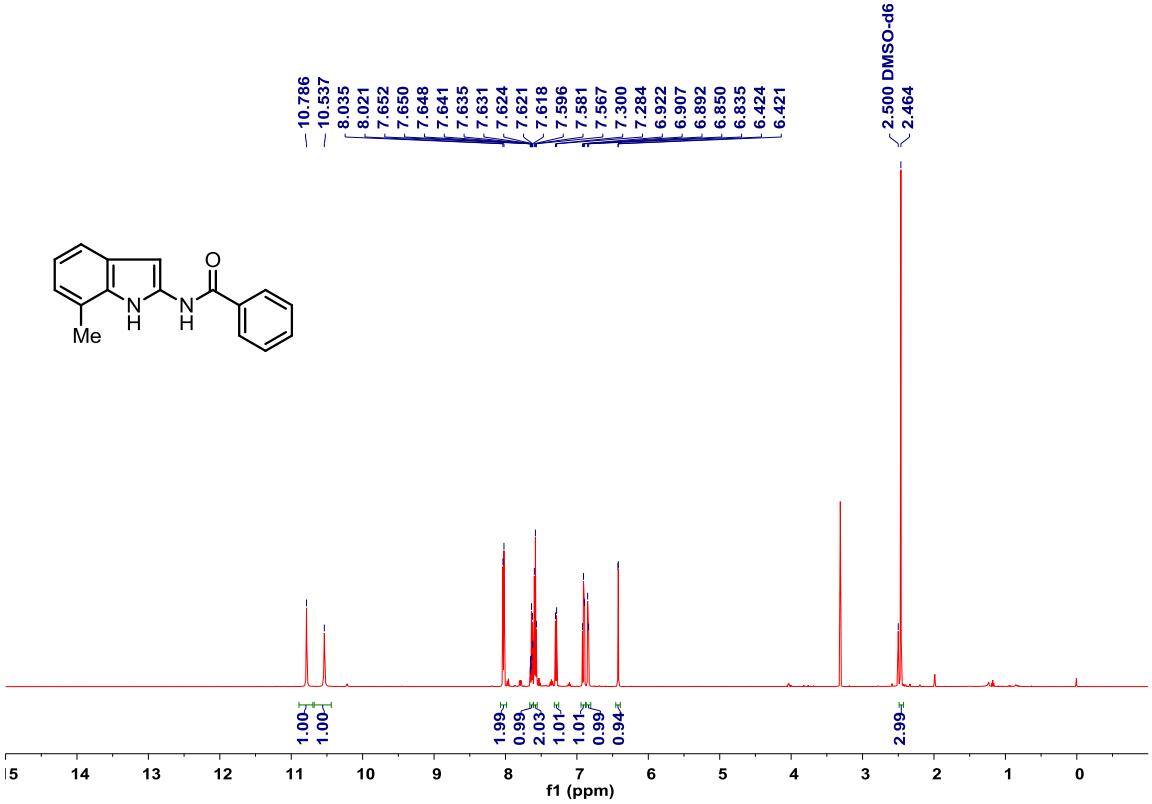


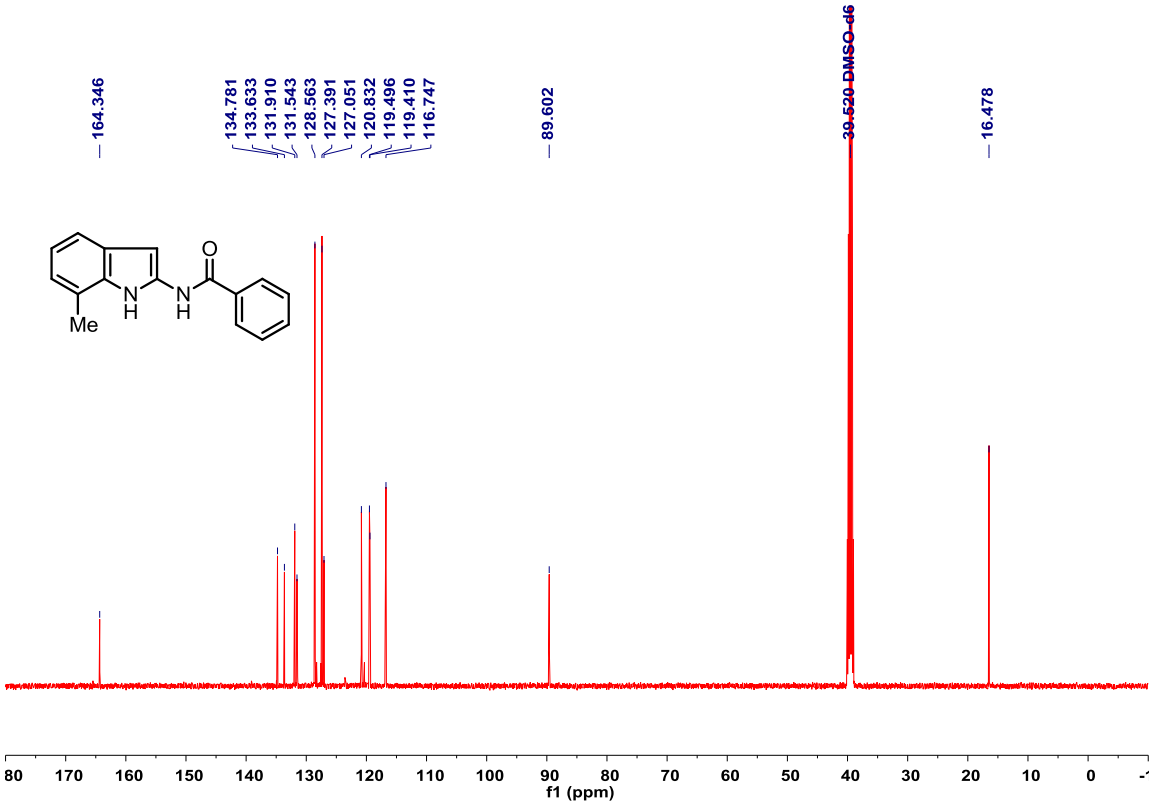
***N*-(6-Bromo-1*H*-indol-2-yl)benzamide (5w)**



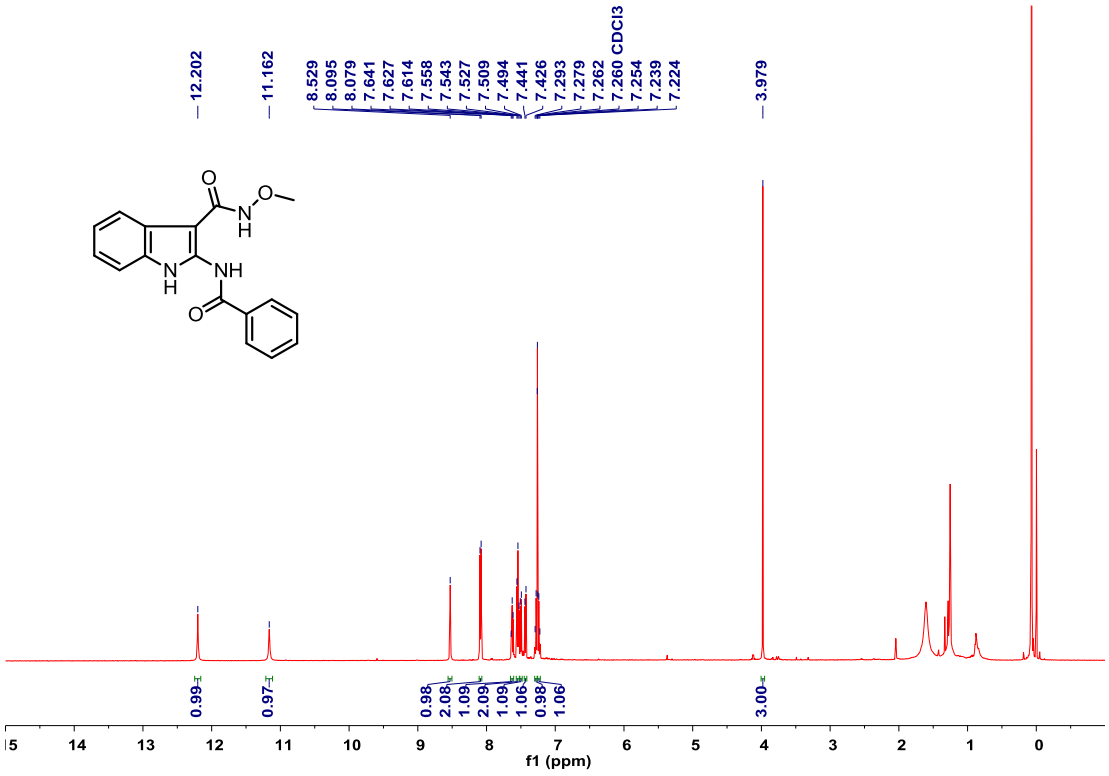


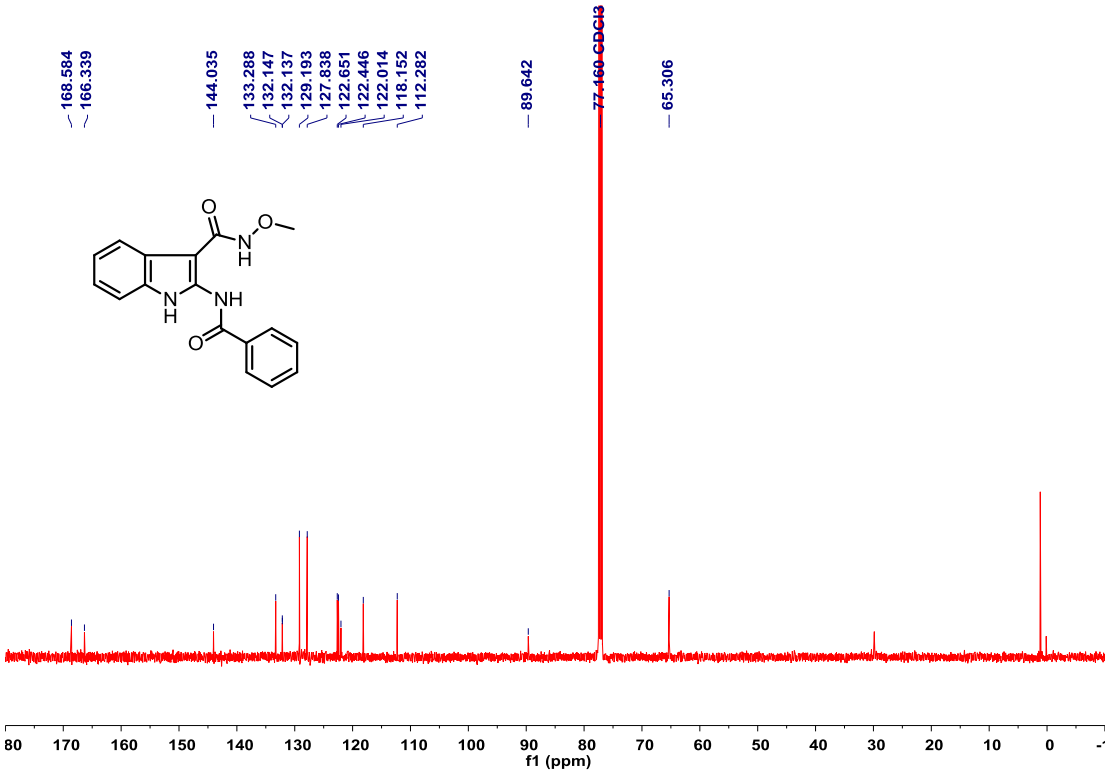
***N*-(7-Methyl-1*H*-indol-2-yl)benzamide (5x)**



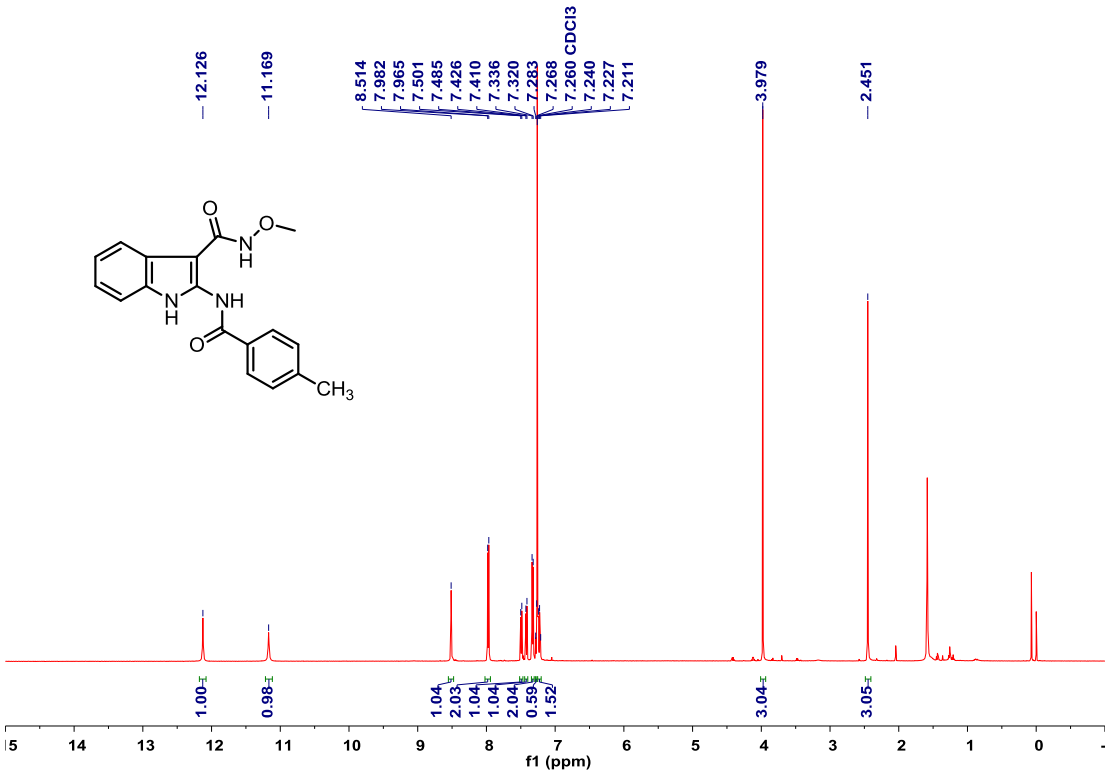


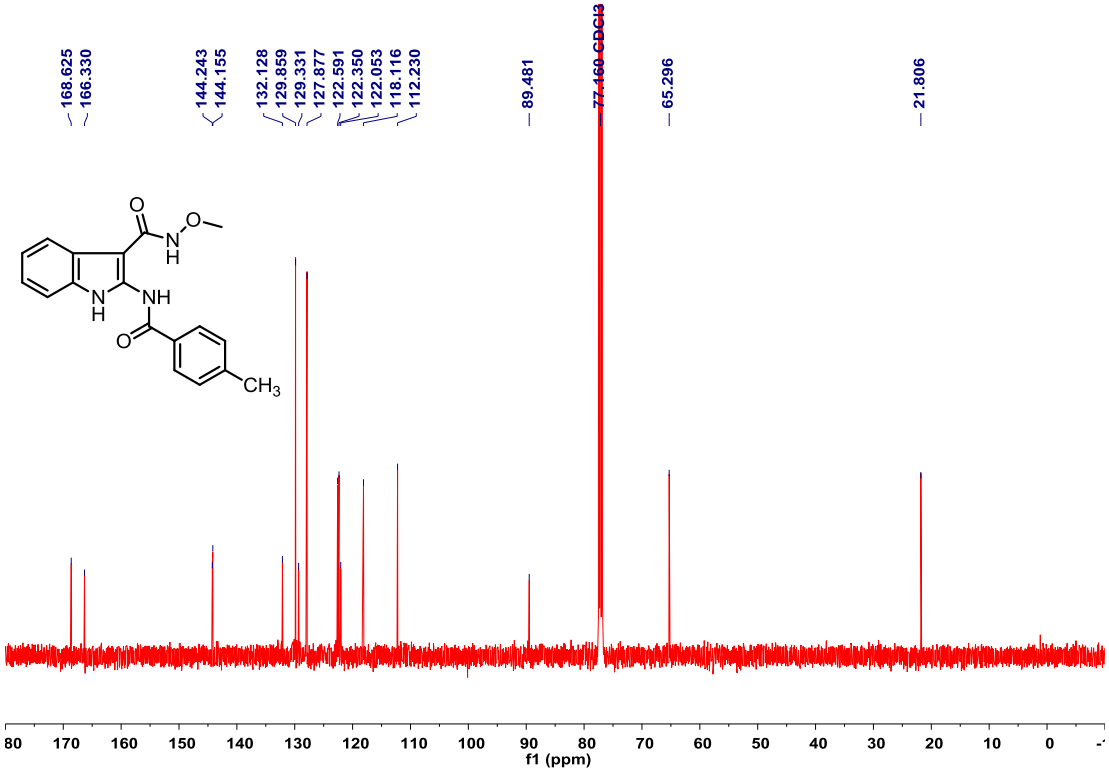
2-Benzamido-*N*-methoxy-1*H*-indole-3-carboxamide (6a)



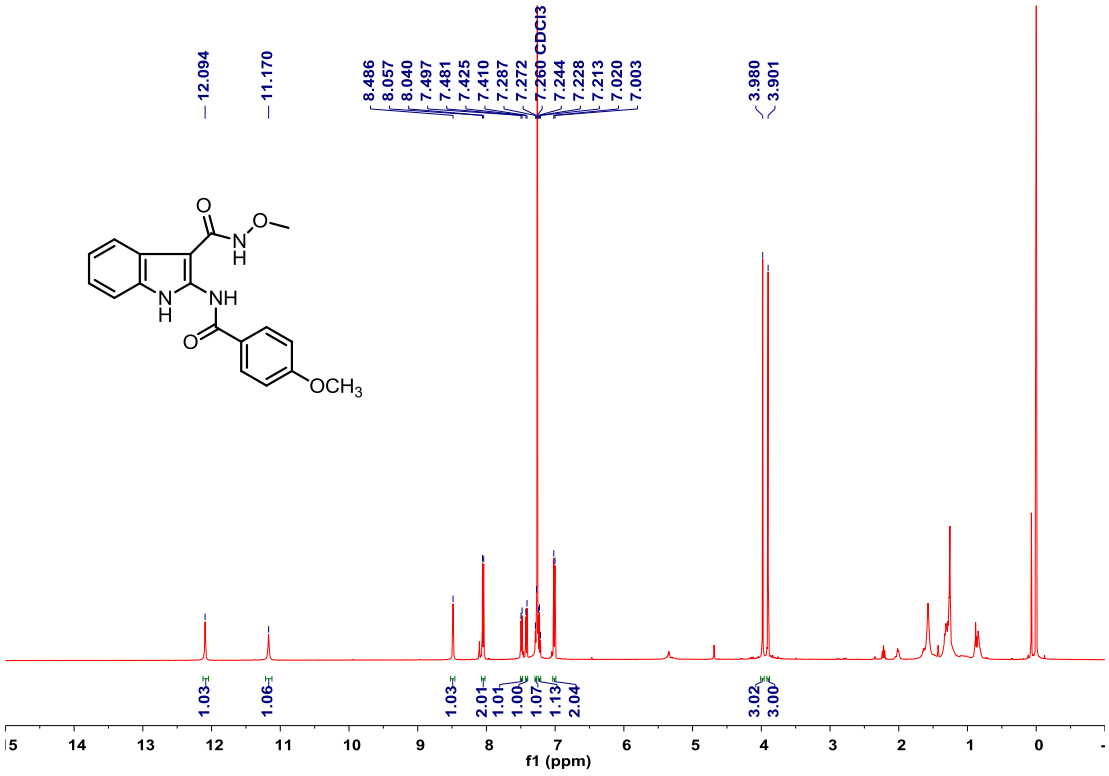


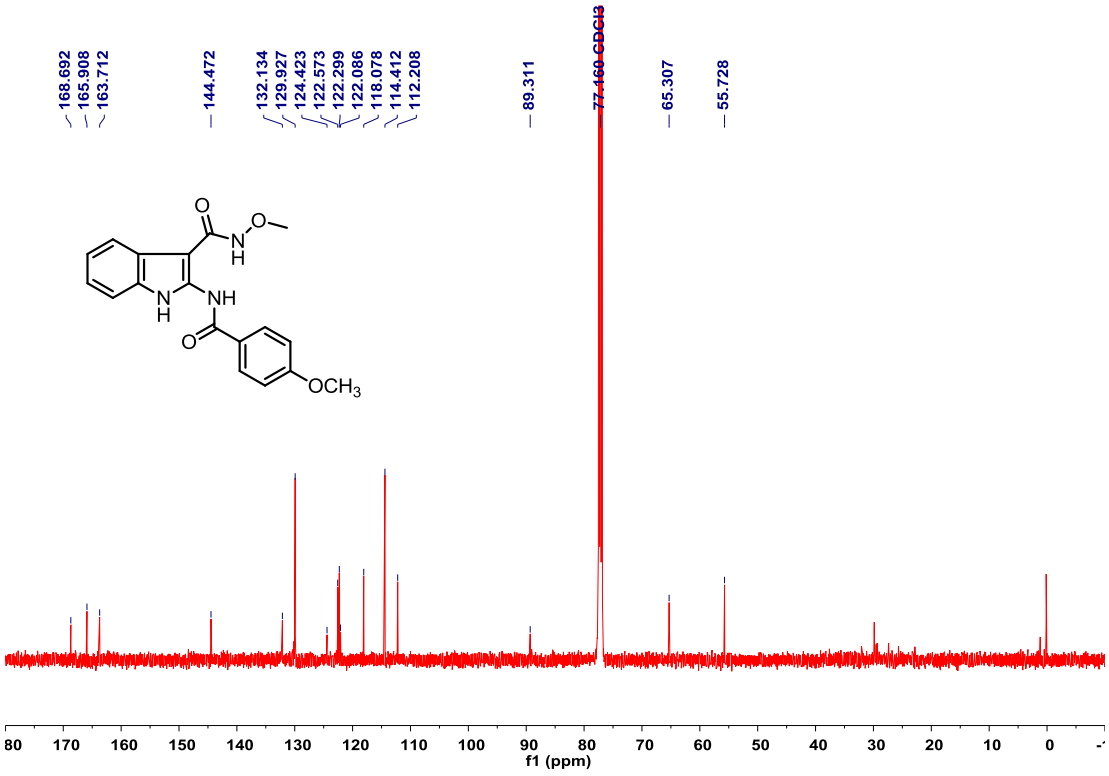
_N_-Methoxy-2-(4-methylbenzamido)-1_H_-indole-3-carboxamide (6b)



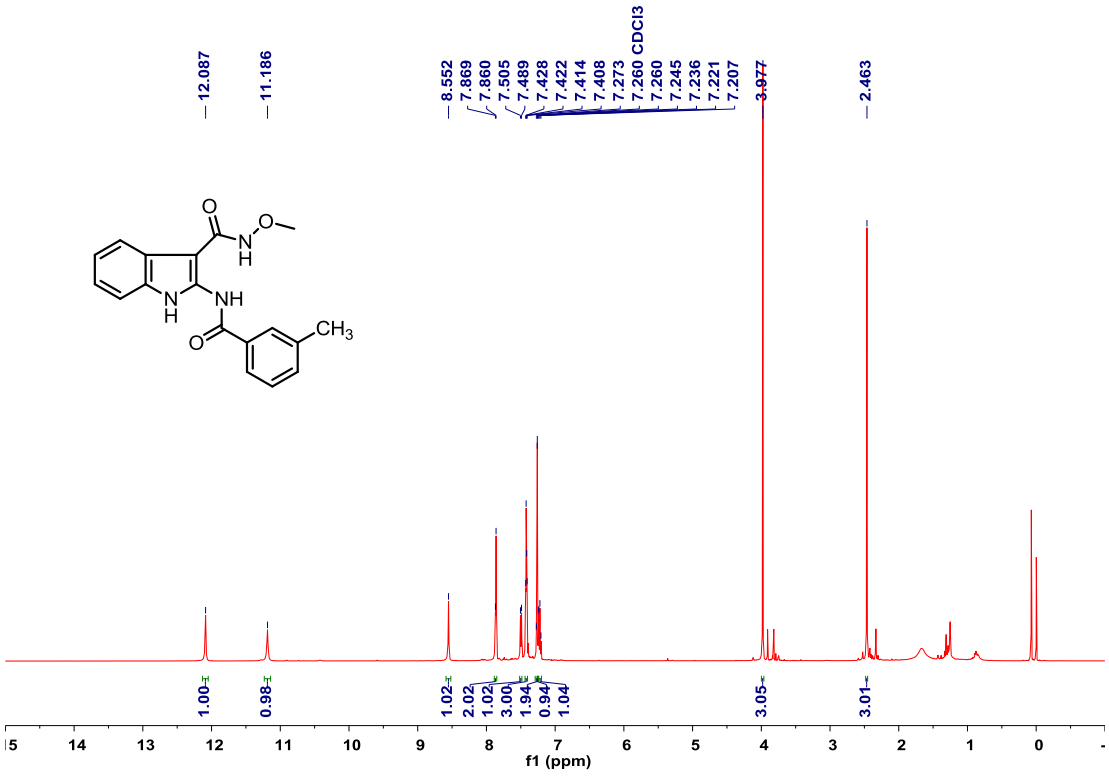


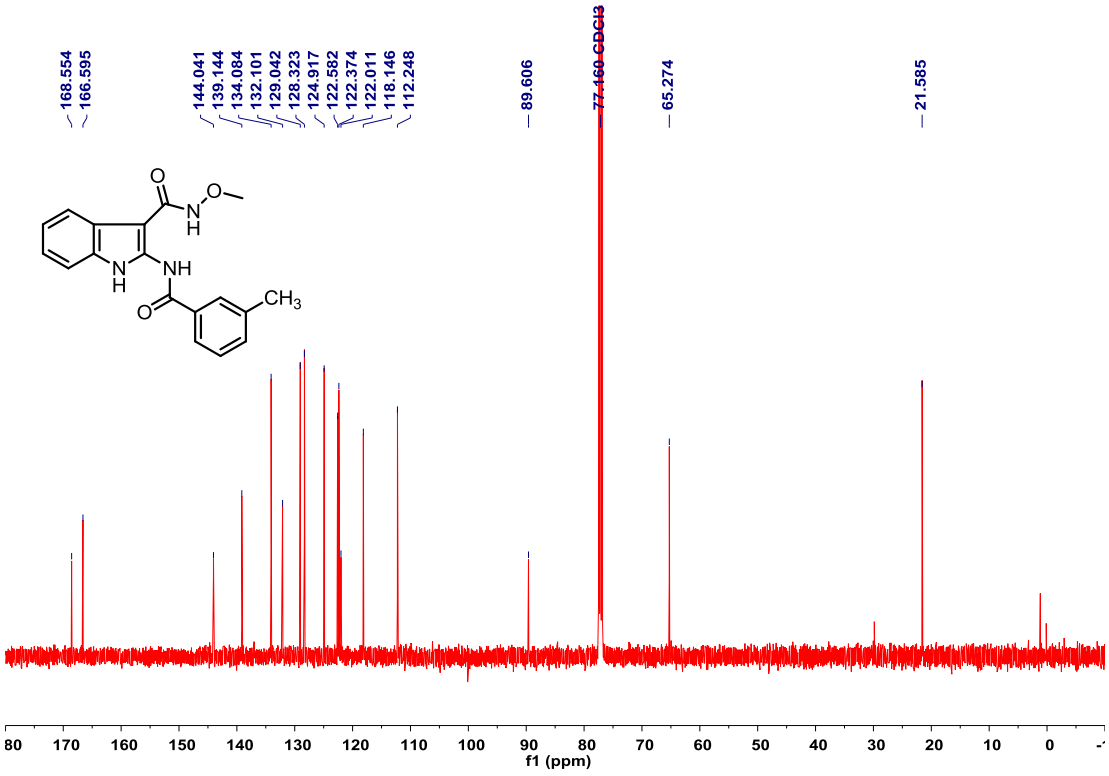
***N*-Methoxy-2-(4-methoxybenzamido)-1*H*-indole-3-carboxamide (6c)**



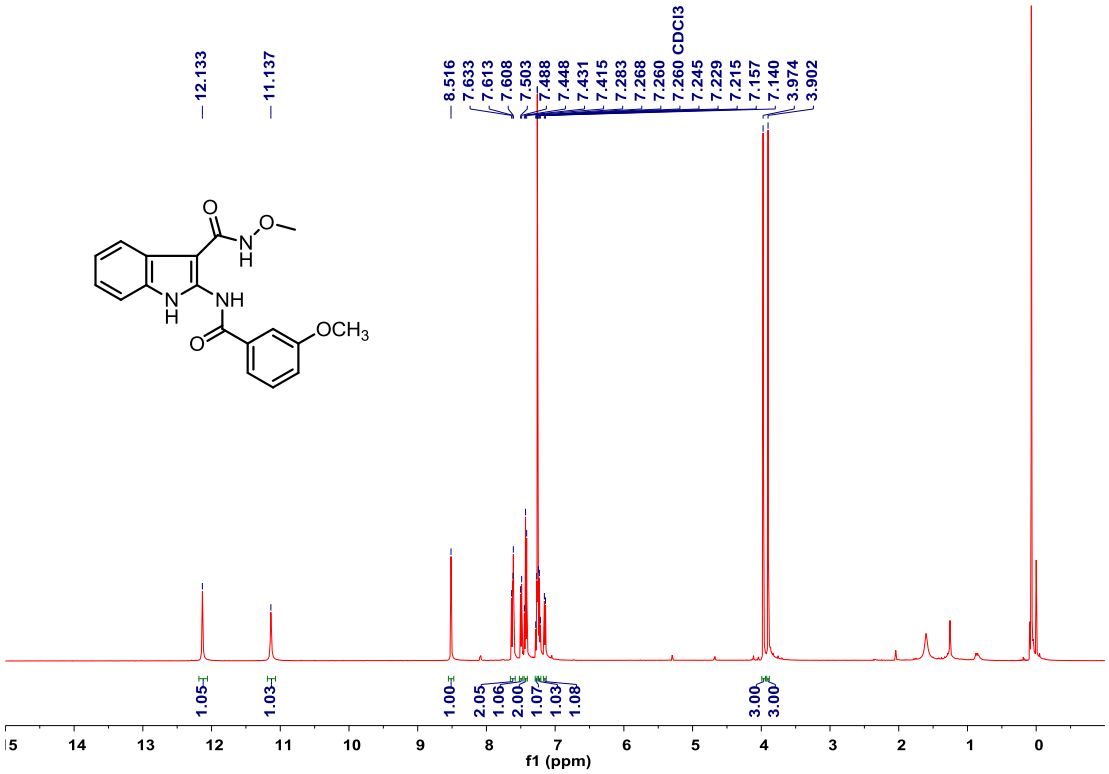


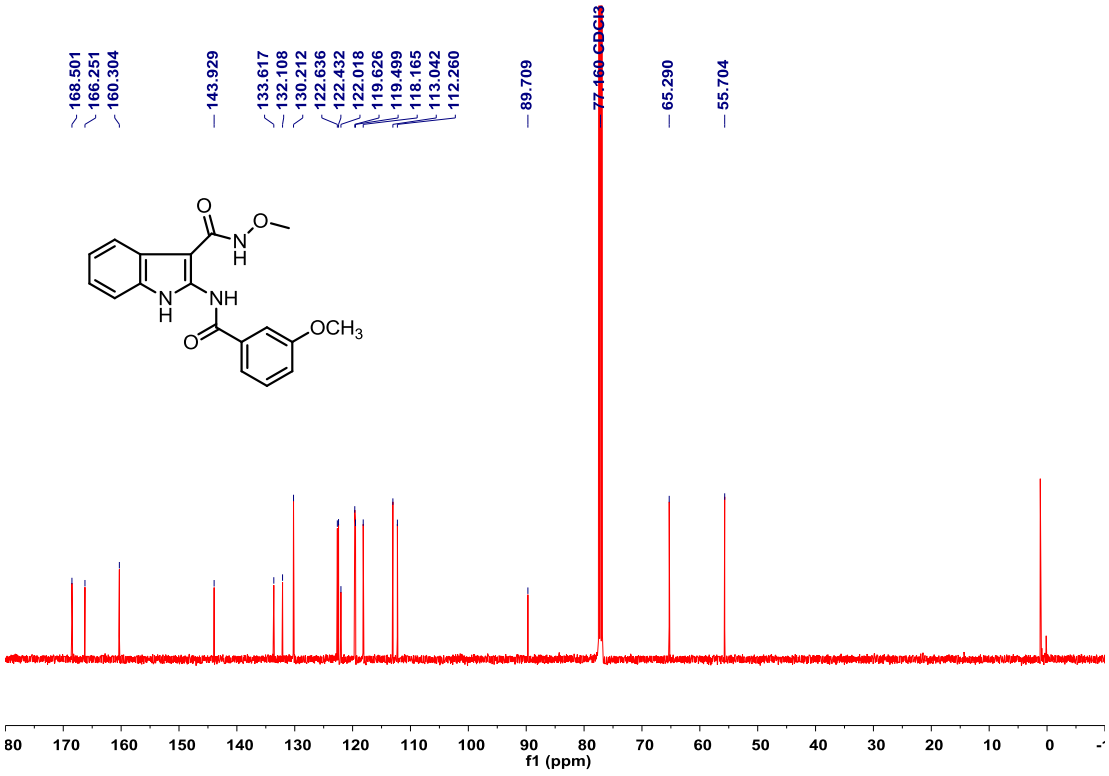
_N_-Methoxy-2-(3-methylbenzamido)-1_H_-indole-3-carboxamide (6d)



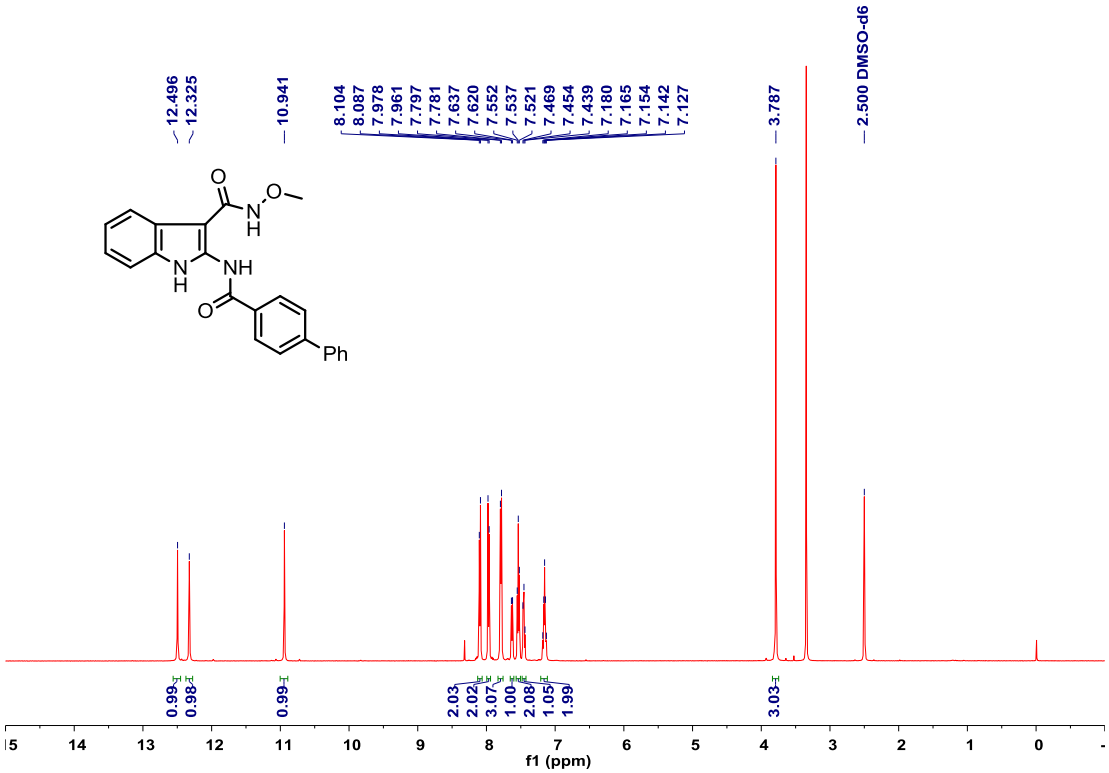


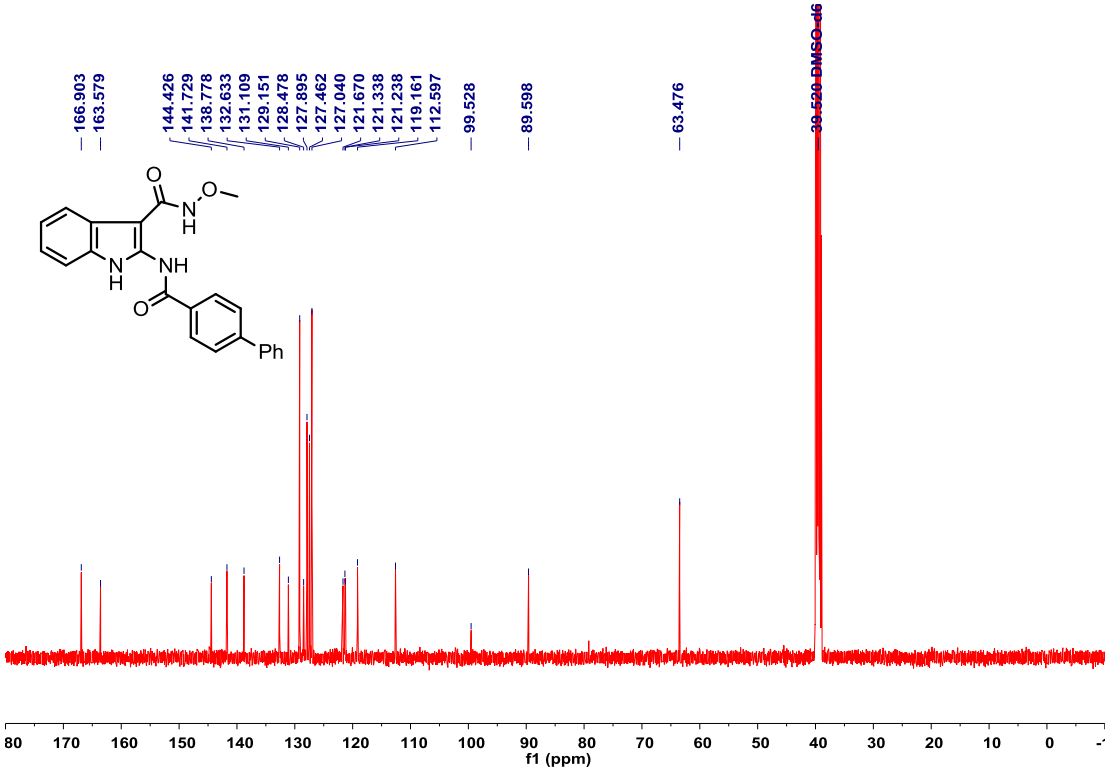
***N*-Methoxy-2-(3-methoxybenzamido)-1*H*-indole-3-carboxamide (6e)**



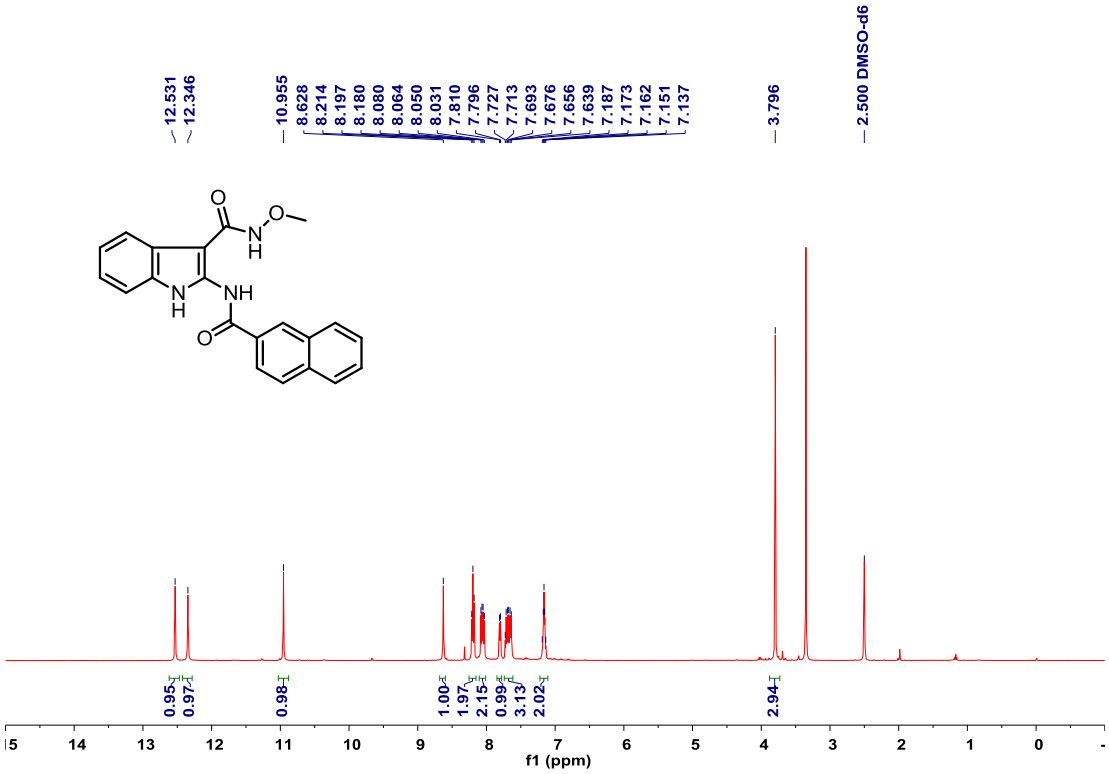


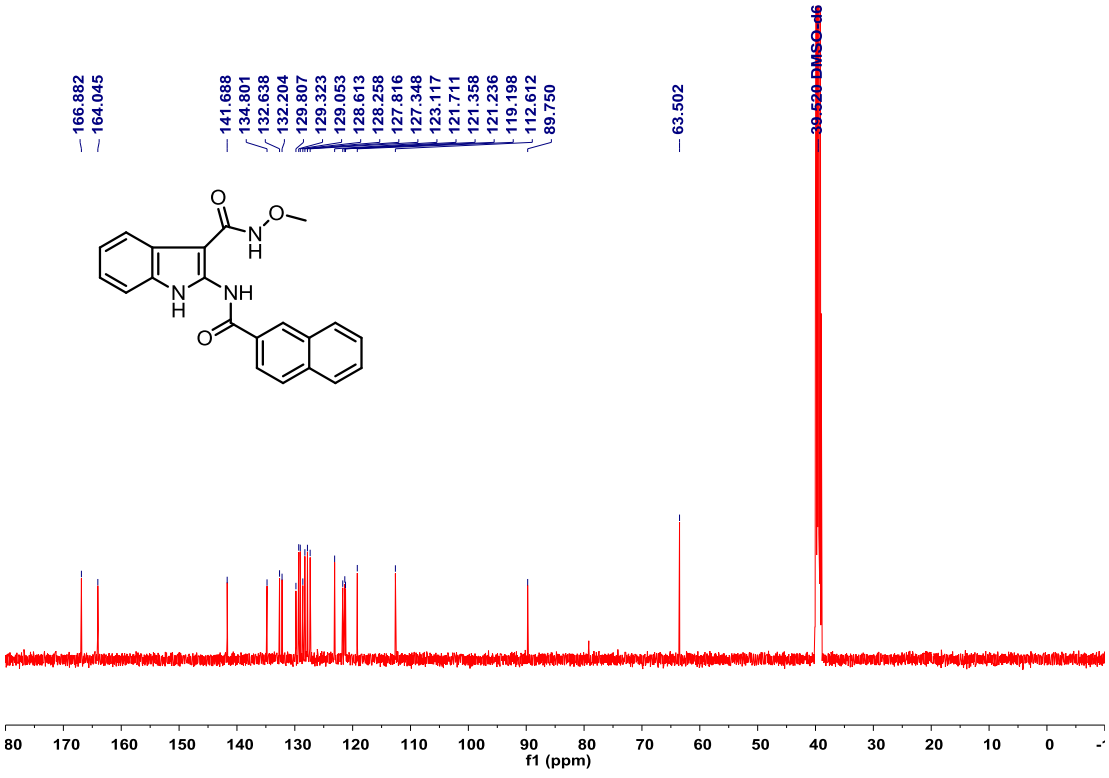
2-([1,1'-Biphenyl]-4-ylcarboxamido)-*N*-methoxy-1*H*-indole-3-carboxamide (6f)



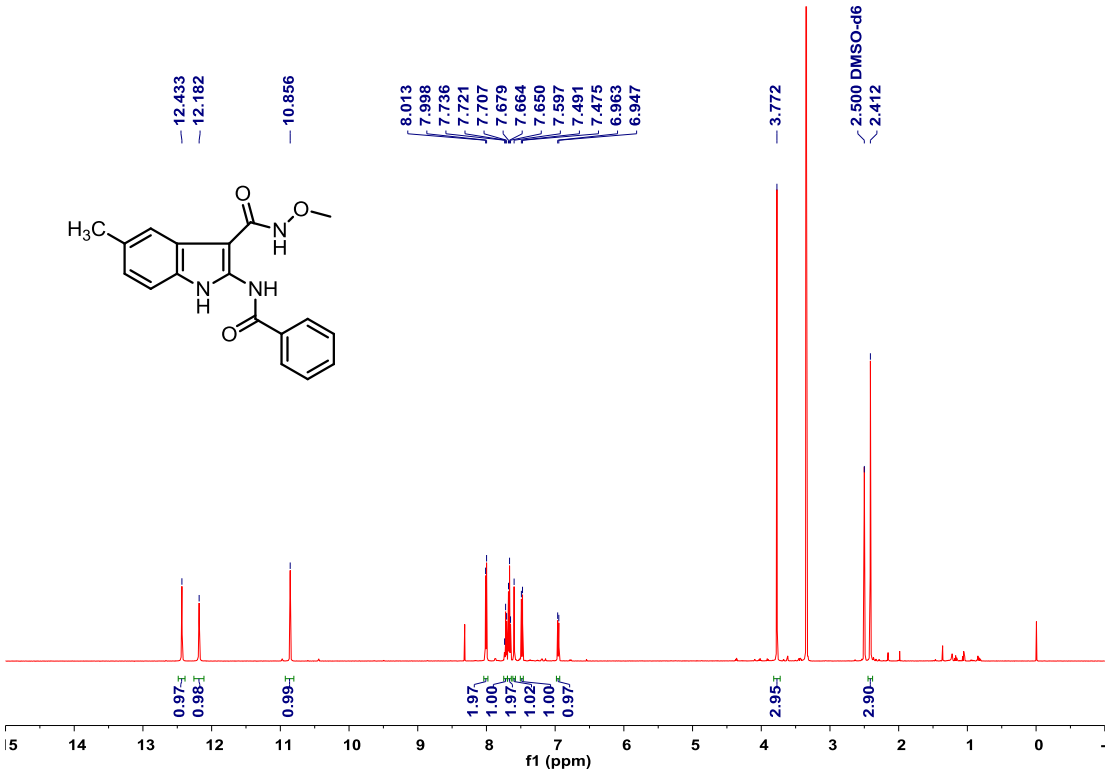


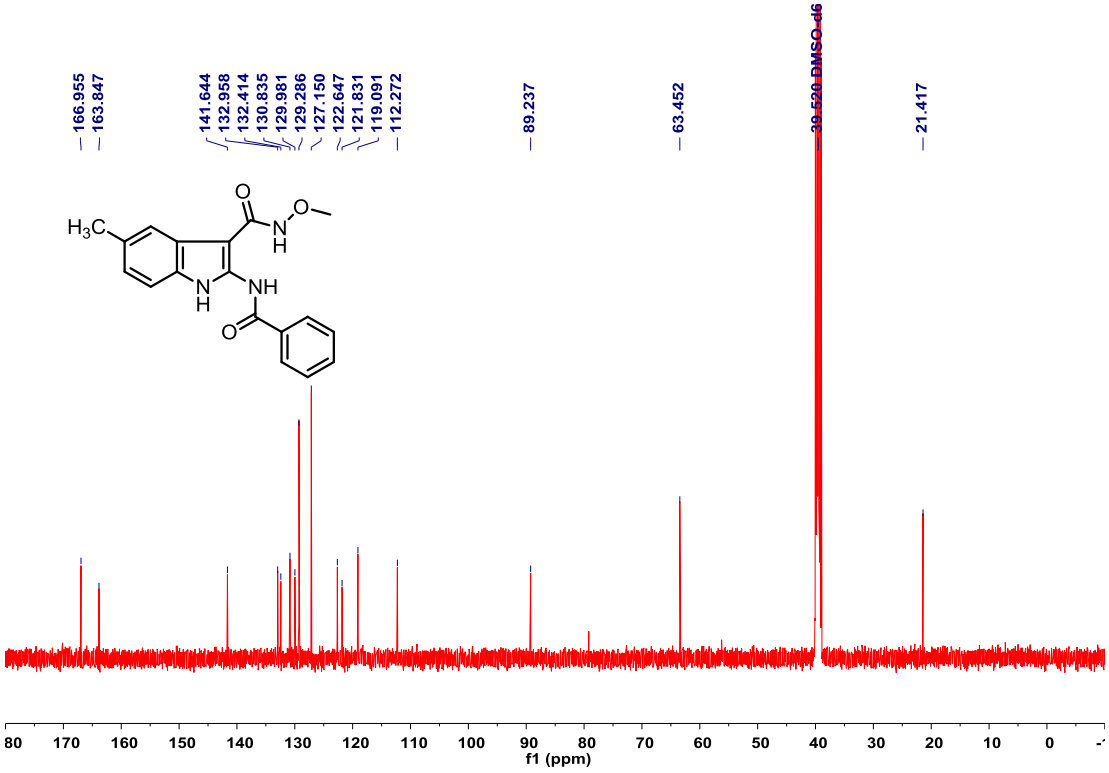
2-(2-Naphthamido)-*N*-methoxy-1*H*-indole-3-carboxamide (6g)



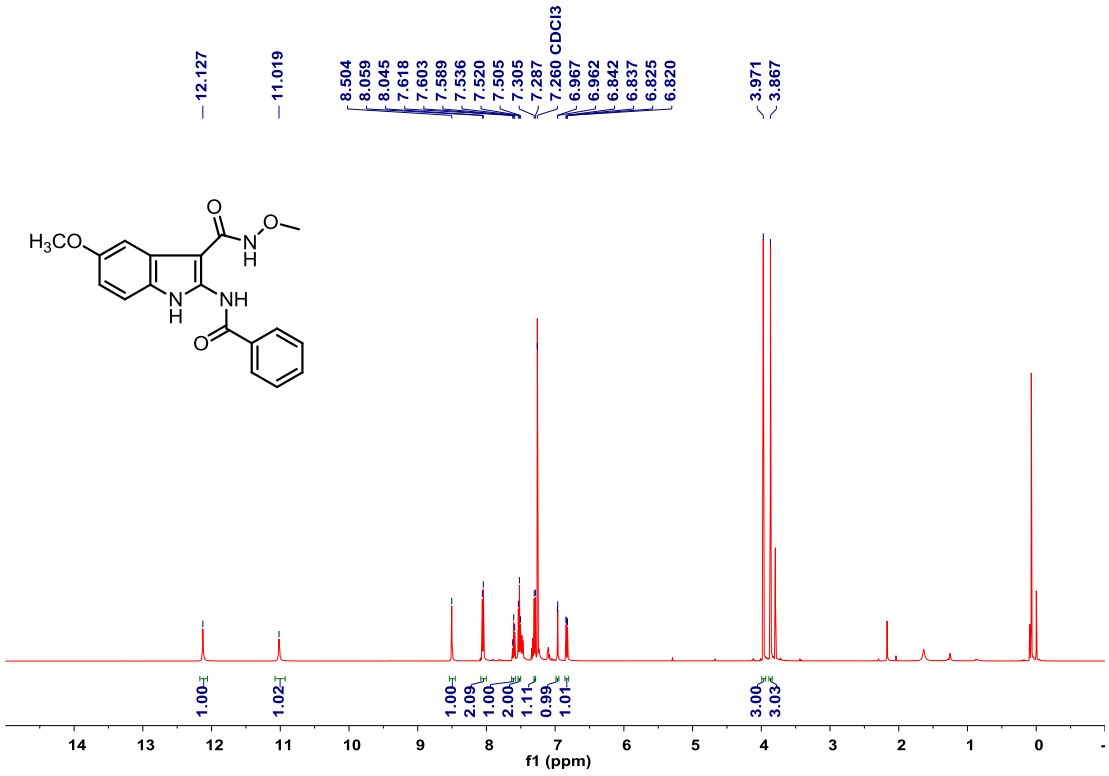


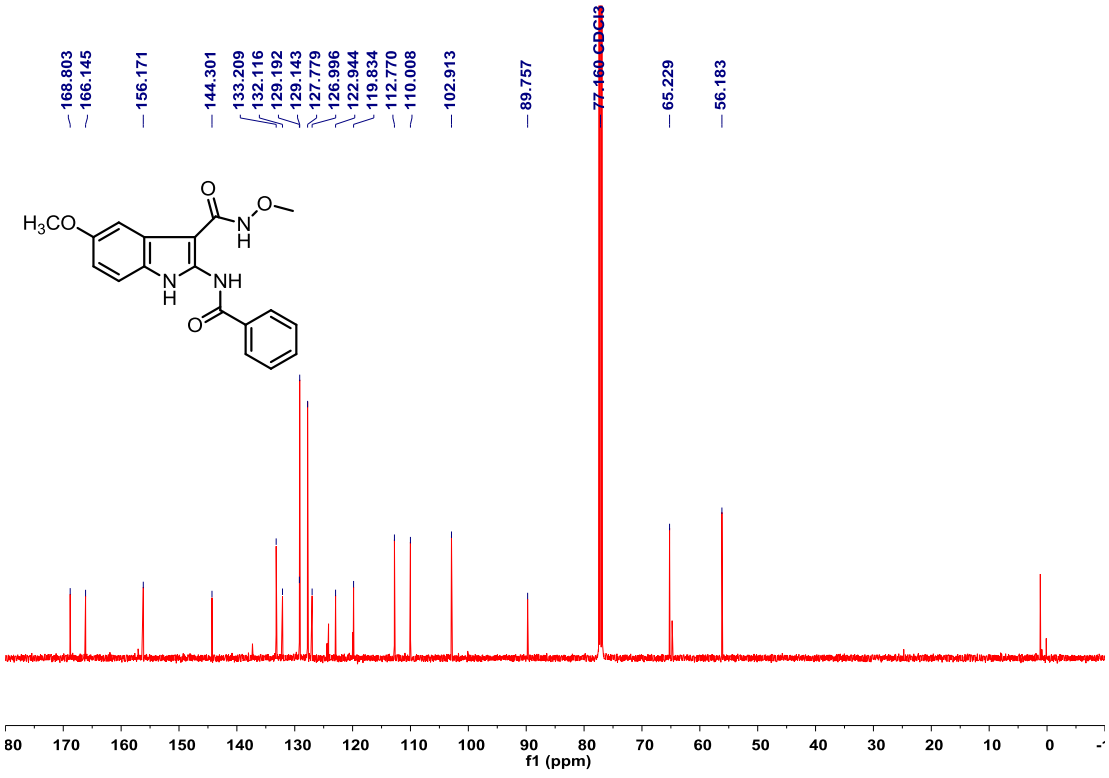
2-Benzamido-*N*-methoxy-5-methyl-1*H*-indole-3-carboxamide (6h)



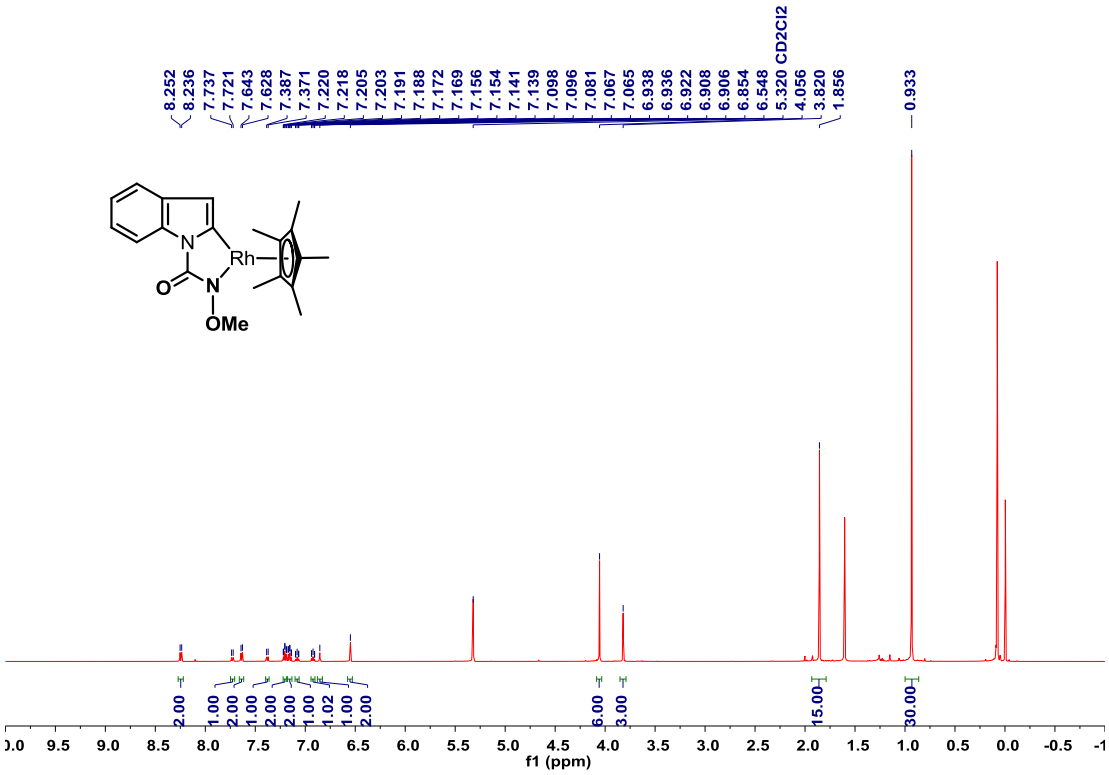


2-Benzamido-*N*,5-dimethoxy-1*H*-indole-3-carboxamide (6i)





IN5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7.188
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7.154
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7.096
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7.067
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6.936
6.922
6.908
6.906
6.854
6.548
5.320 CD2Cl2
4.056
3.820
1.856
0.933
Rh
N
O
N
OMe
2.00
1.00
2.00
1.00
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1.00
2.00
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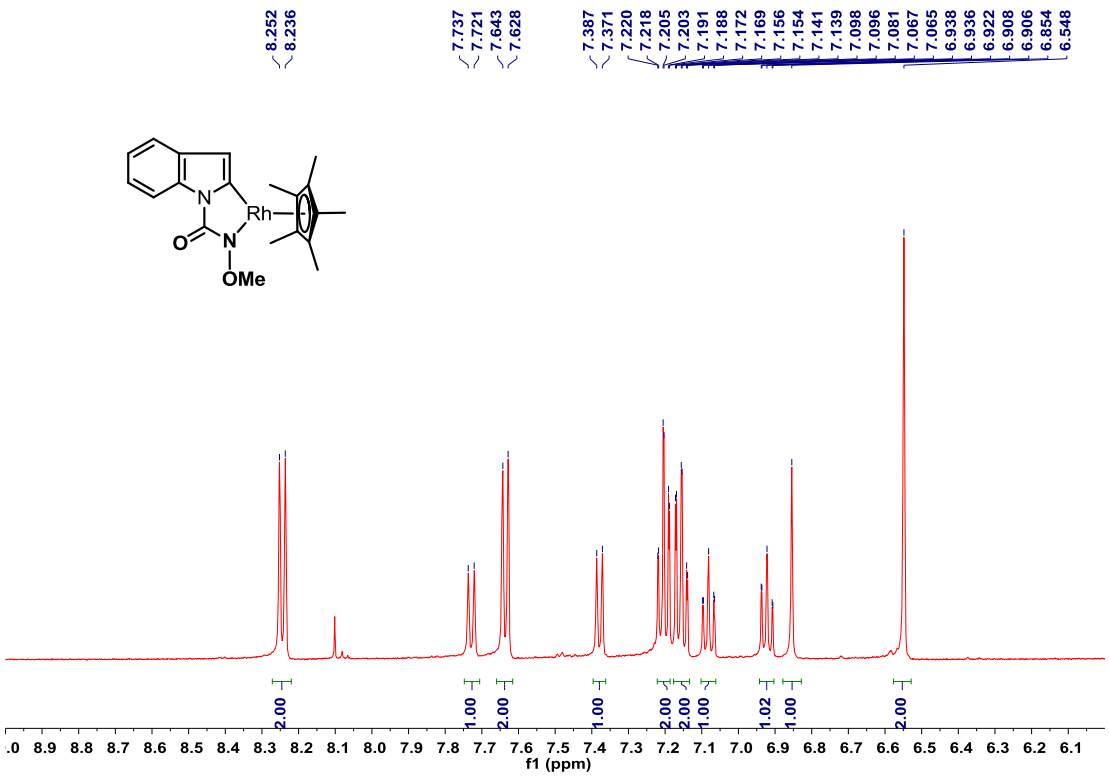
3.00
15.00
30.00
f1 (ppm)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6.548
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N
O
N
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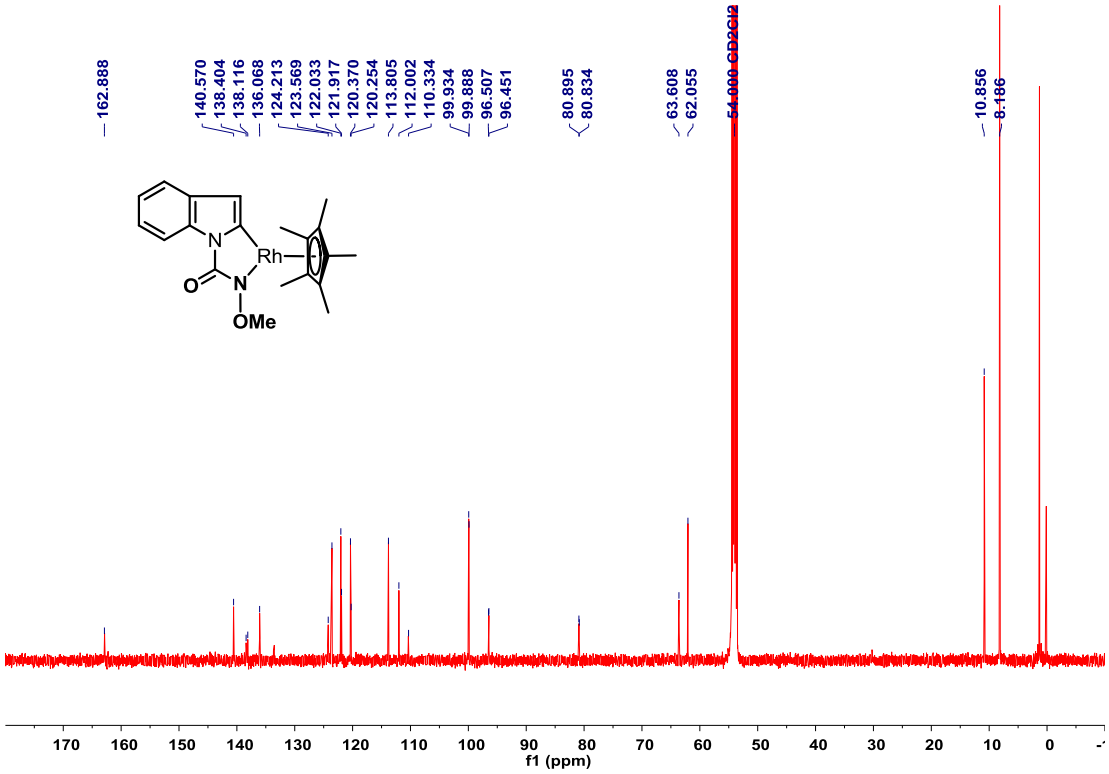
2.00
f1 (ppm)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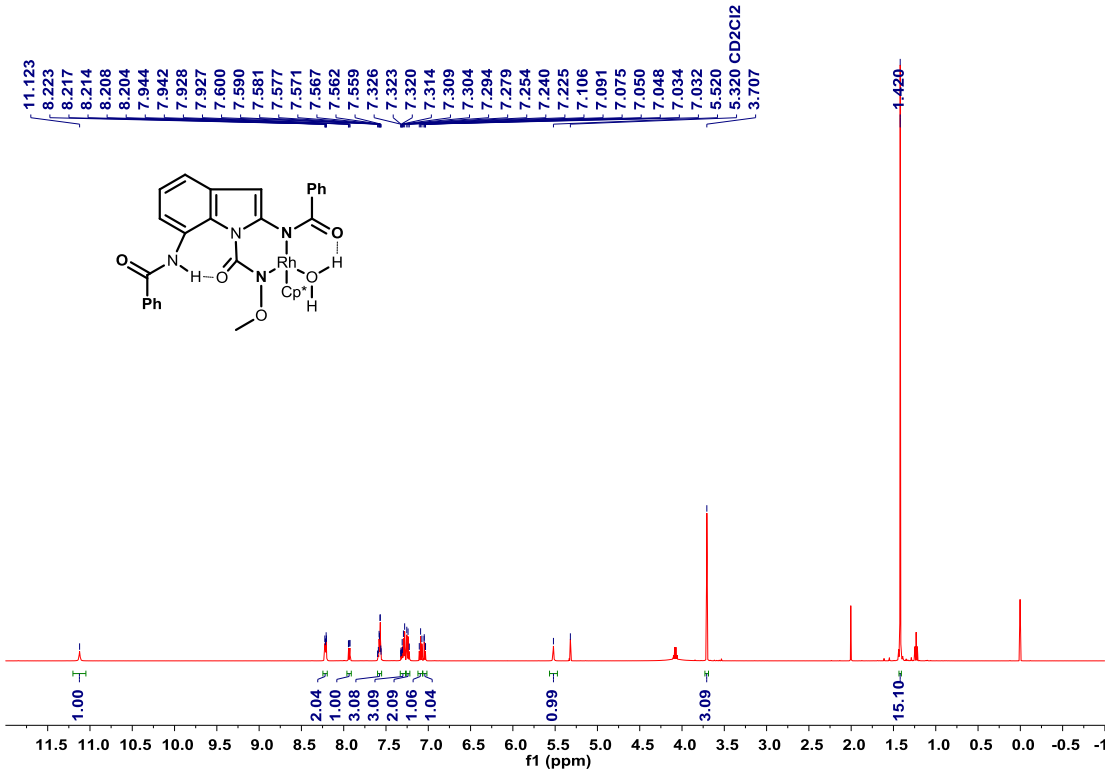
Rh
N
O
OMe
f1 (ppm)

IN8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7.106
7.091
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7.050
7.048
7.034
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5.520
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Ph
N
O
H
Rh
Cp*
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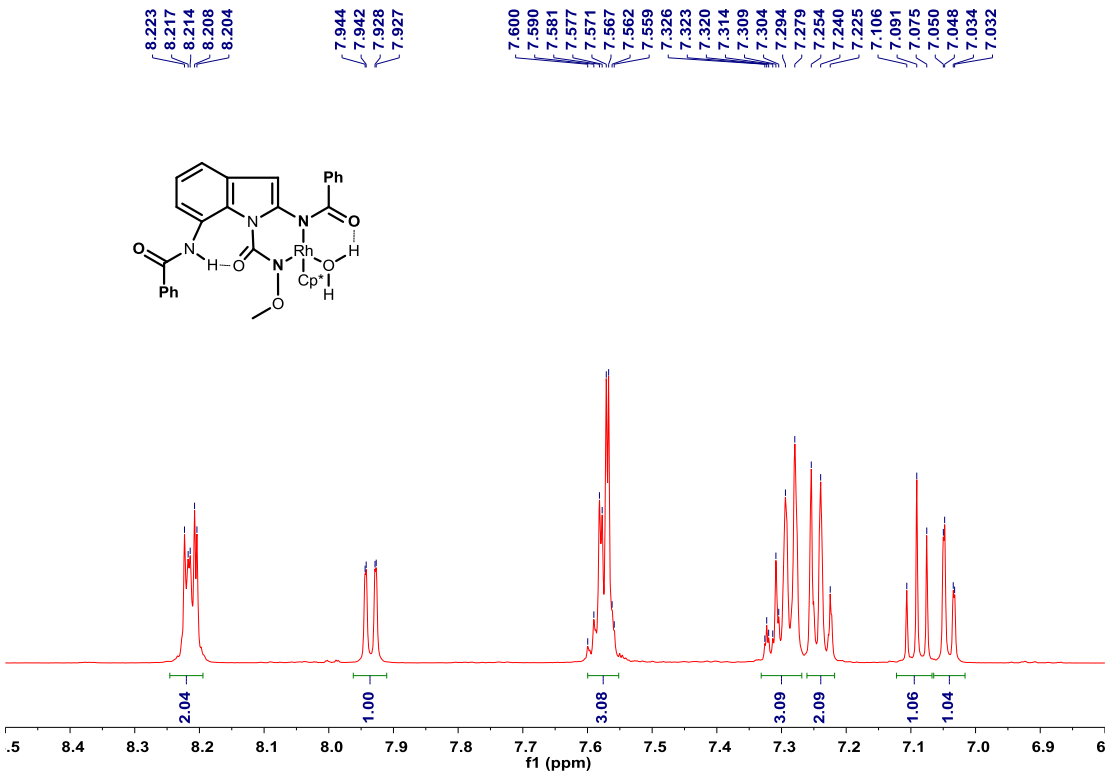
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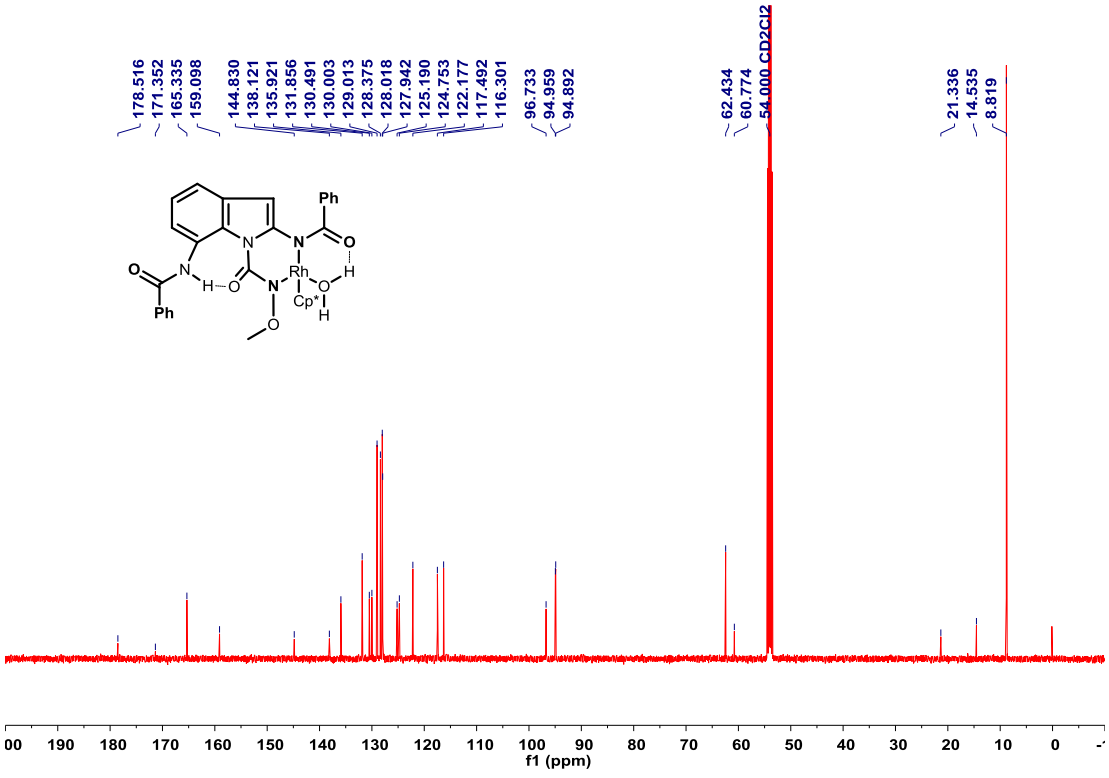
7.106
7.091
7.075
7.050
7.048
7.034
7.032
Ph
N
N
O
O
N
H
O
Rh
O
H
N
Cp*
Ph
O
H
2.04
1.00
3.08
3.09
2.09
1.06
1.04
f1 (ppm)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116.301
96.733
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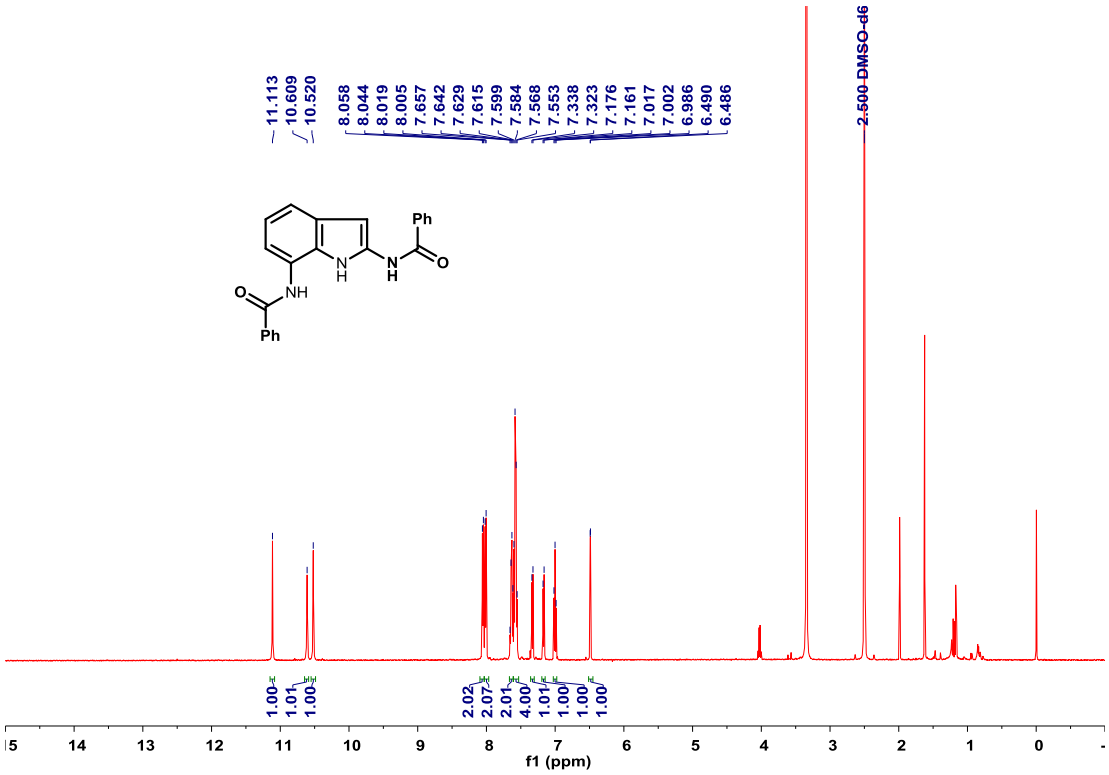
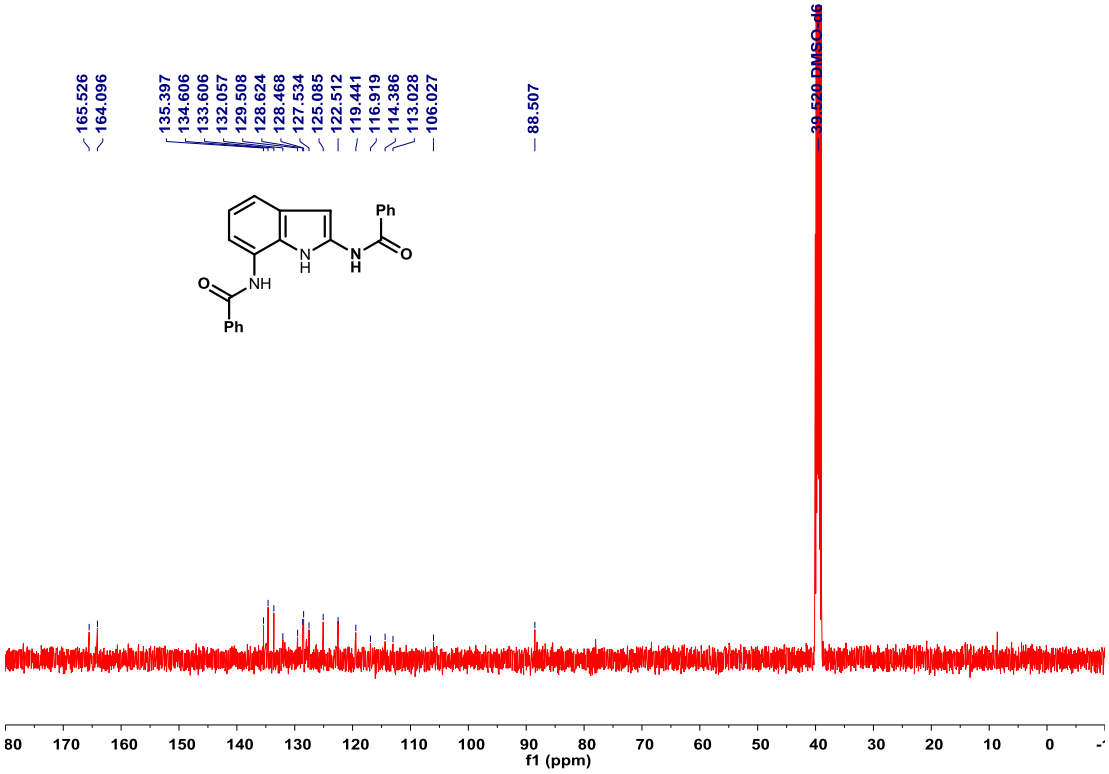
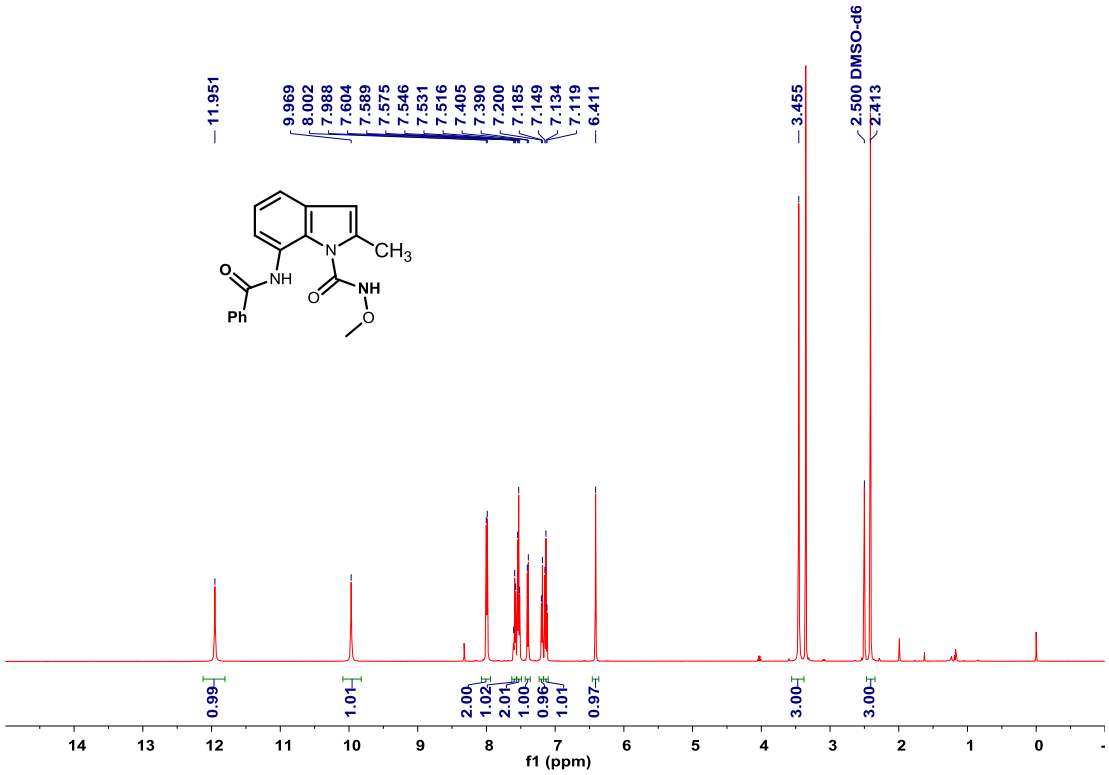
94.892
62.434
60.774
54.000 CD2Cl2
21.336
14.535
8.819
Ph
N
N
O
O
N
H
O
Rh
O
H
N
Cp*
Ph
O
H
f1 (ppm)

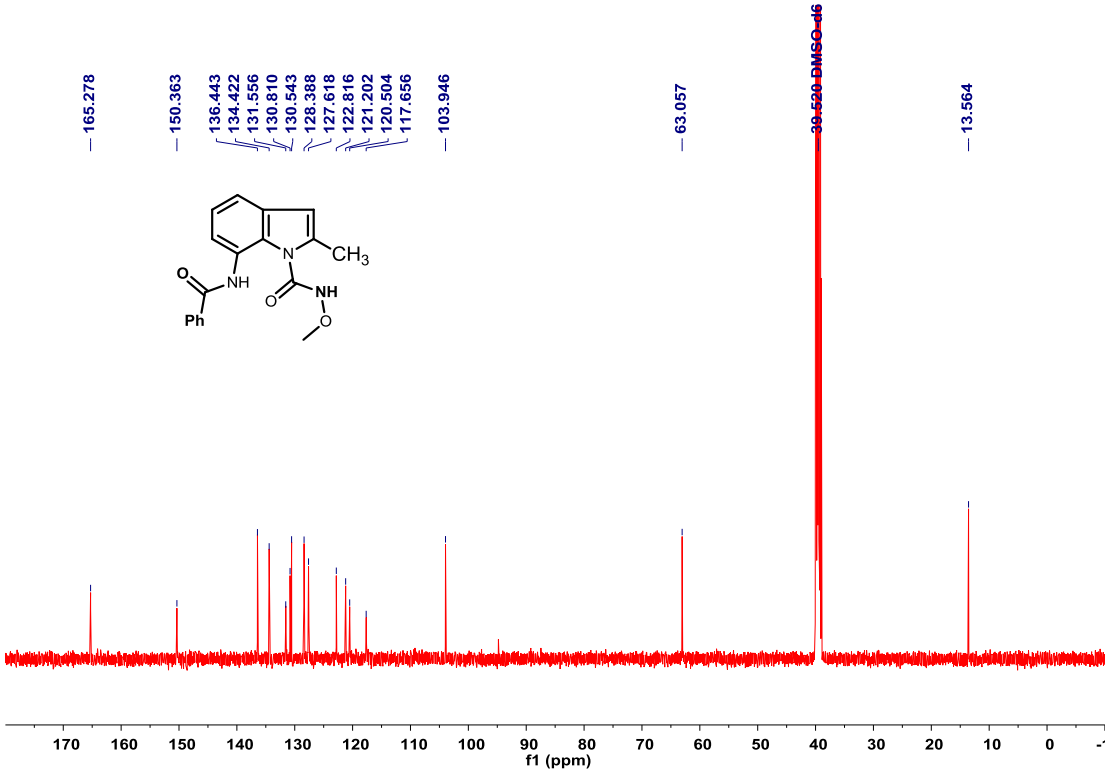
***N*,*N*'-(1*H*-Indole-2,7-diyl)dibenzamide (8)**





7-Benzamido-*N*-methoxy-2-methyl-1*H*-indole-1-carboxamide (9)





6. Cartesian coordinates and electronic energies for all of the calculated structures

a1(catalyst)
SCF done: -956.085482

C	1.184512	-1.671914	-0.110179
C	1.697934	-0.760793	-1.095510
C	2.182433	0.421127	-0.400800
C	1.918339	0.256022	0.988402
C	1.278674	-1.037182	1.170268
O	-0.663388	2.070635	-1.005244
O	-1.206667	1.557568	1.054354
C	-1.336525	2.307874	0.041932
C	-2.318207	3.437194	0.063543
H	-3.285681	3.059563	-0.286004
H	-2.447240	3.816581	1.080053
H	-2.000540	4.235214	-0.611894
Rh	0.054046	0.188730	-0.115449
C	2.757594	1.615277	-1.073710
H	3.779665	1.414085	-1.420195
H	2.153141	1.897976	-1.942995
H	2.786068	2.478960	-0.403118
C	1.776850	-0.988076	-2.562396
H	1.636907	-0.051281	-3.112346
H	2.753149	-1.403327	-2.847022
H	1.000840	-1.684185	-2.895843
C	0.604175	-3.015719	-0.364083
H	0.221114	-3.094690	-1.386707
H	1.368798	-3.791732	-0.225983
H	-0.229618	-3.201352	0.319305
C	0.799966	-1.608666	2.455133
H	-0.249279	-1.909534	2.345094
H	1.395993	-2.487212	2.735550
H	0.868038	-0.877288	3.265935
C	2.172699	1.233286	2.080355
H	1.274569	1.368251	2.693539
H	2.982522	0.887411	2.735538
H	2.452393	2.213667	1.683863
O	-1.770548	-0.517336	-0.811225
O	-2.005498	-1.855580	0.989395
C	-2.422306	-1.332423	-0.042993
C	-3.828159	-1.599857	-0.541358
H	-4.285988	-2.409054	0.031852
H	-4.426613	-0.689616	-0.425330

H	-3.819354	-1.844469	-1.607974

Substrate(five ring)
SCF done: -587.905808

C	-0.639869	0.277292	0.000015
C	-2.735033	-0.311726	0.000017
O	-1.451874	-0.807376	0.000083
O	-3.733317	-0.951881	0.000088
O	-2.621359	1.035977	-0.000130
N	-1.267267	1.401932	-0.000104
C	0.798216	0.089327	0.000021
C	1.332585	-1.200749	0.000027
C	1.640248	1.205811	0.000026
C	2.710312	-1.370873	-0.000129
H	0.666543	-2.058970	-0.000127
C	3.014008	1.024444	0.000120
H	1.206341	2.202316	0.000084
C	3.549574	-0.261737	0.000005
H	3.130718	-2.372630	-0.000290
H	3.671516	1.889366	0.000191
H	4.627904	-0.398105	-0.000064

a2
SCF done: -1732.617316

Rh	-1.039700	0.636968	0.081290
N	0.258078	-0.114492	1.519820
C	-1.901108	2.291240	1.042629
C	-2.001672	2.551269	-0.380974
C	-2.824724	1.539949	-0.936897
C	-3.367028	0.740084	0.161279
C	-2.847073	1.227026	1.366708
O	-0.228546	-0.424594	2.787735
C	1.524594	0.409134	1.595588
C	0.779730	1.221381	-0.568385
C	3.014225	1.426182	-0.174443
C	1.336204	1.689553	-1.727739
C	2.755965	1.827882	-1.507808
H	0.802963	1.909959	-2.646651
O	2.339976	0.303021	2.492442
C	-3.136612	0.754895	2.744898
H	-3.781441	-0.129579	2.743124
H	-2.205564	0.499129	3.263889
H	-3.644111	1.539503	3.321672
C	-4.351586	-0.368346	0.007496
H	-4.241057	-1.117769	0.799042
H	-5.378756	0.017023	0.058090

H	-4.242960	-0.882993	-0.951897
C	-3.200626	1.393734	-2.370103
H	-3.296949	0.340909	-2.651648
H	-4.161425	1.883208	-2.580674
H	-2.447079	1.841590	-3.026557
C	-1.374294	3.694437	-1.097622
H	-1.220104	3.477239	-2.159144
H	-2.021769	4.578943	-1.029267
H	-0.399304	3.953143	-0.674607
C	-1.172242	3.116141	2.045261
H	-0.307035	3.615746	1.596708
H	-1.827177	3.888051	2.472511
H	-0.802831	2.493087	2.866923
C	-0.422364	-1.813548	2.884534
H	0.524706	-2.352335	2.731321
H	-0.799720	-2.004943	3.894452
H	-1.167393	-2.163787	2.147407
N	1.789108	1.072126	0.378397
C	4.293349	1.413721	0.374748
H	4.441773	1.102303	1.404860
C	3.829431	2.237182	-2.306165
H	3.661645	2.554125	-3.333995
C	5.109337	2.224641	-1.770493
H	5.951573	2.537075	-2.384480
C	5.338994	1.815381	-0.448554
H	6.353931	1.819391	-0.056863
C	-0.230496	-2.536735	-0.947276
C	-2.141691	-3.011347	-1.903140
O	-0.984006	-3.561080	-1.416776
O	-3.059927	-3.592461	-2.378914
O	-2.027456	-1.675294	-1.732127
N	-0.819071	-1.387955	-1.070874
C	1.067546	-2.821970	-0.375753
C	2.100727	-1.888632	-0.494192
C	1.263543	-4.024906	0.313283
C	3.316415	-2.135793	0.127318
H	1.944876	-0.983322	-1.077275
C	2.484204	-4.262984	0.926938
H	0.456118	-4.749954	0.383012
C	3.501872	-3.314027	0.845349
H	4.113836	-1.400016	0.047852
H	2.642214	-5.187448	1.476101
H	4.452704	-3.499569	1.338842

TS-1

SCF done: -1732.581092

Rh	1.139567	-0.473332	-0.173265
N	0.522311	0.434855	1.597172
C	1.749119	-2.650911	-0.355154
C	2.084520	-1.971866	-1.577660
C	3.057977	-0.965077	-1.264961
C	3.299369	-0.993332	0.148673
C	2.473618	-2.030815	0.714322
O	1.460471	0.649192	2.588384
C	-0.702672	0.080893	2.119823
C	-0.802952	-1.043656	-0.028484
C	-2.784517	-0.887220	1.060374
C	-1.721170	-1.663609	-0.827502
C	-2.995485	-1.569443	-0.161532
H	-1.543045	-2.077138	-1.815219
O	-1.144541	0.338550	3.220591
C	2.413353	-2.397331	2.154880
H	3.247564	-3.055924	2.428637
H	2.457368	-1.500754	2.782206
H	1.478681	-2.916418	2.392123
C	4.234332	-0.114703	0.901086
H	3.837488	0.099829	1.899514
H	5.216073	-0.592160	1.021741
H	4.377593	0.840952	0.386337
C	3.695745	-0.035712	-2.235098
H	3.147318	-0.011180	-3.181730
H	3.728561	0.985696	-1.842423
H	4.723326	-0.356413	-2.449963
C	1.564305	-2.291410	-2.936821
H	1.300341	-1.378881	-3.484136
H	2.308832	-2.834156	-3.533938
H	0.666704	-2.915489	-2.881610
C	0.864398	-3.838782	-0.235275
H	-0.008351	-3.766307	-0.891208
H	1.421559	-4.746366	-0.501953
H	0.490295	-3.958846	0.785449
C	1.824293	2.020958	2.649230
H	0.928681	2.653308	2.683722
H	2.392890	2.137409	3.576407
H	2.452017	2.303894	1.794255
N	-1.428887	-0.594177	1.122924
C	-3.816236	-0.574772	1.939686
H	-3.605904	-0.055679	2.869894
C	-4.298447	-1.941486	-0.509251
H	-4.492389	-2.458727	-1.447614

C	-5.336855	-1.625813	0.354374
H	-6.355574	-1.906668	0.094809
C	-5.098562	-0.951500	1.562193
H	-5.935232	-0.722340	2.218481
C	-0.095911	2.161048	-0.893563
C	1.715579	3.511340	-0.234340
O	0.228400	3.345195	-0.475120
O	2.009386	4.549181	0.284059
O	2.320095	2.491768	-0.641983
N	0.749416	1.186517	-1.066452
C	-1.514627	1.921238	-1.214265
C	-1.879727	1.201959	-2.354301
C	-2.485703	2.391817	-0.325886
C	-3.223684	0.968936	-2.612562
H	-1.106772	0.840123	-3.029713
C	-3.824109	2.123064	-0.576584
H	-2.180876	2.942161	0.561399
C	-4.192349	1.415012	-1.718131
H	-3.515452	0.416713	-3.502630
H	-4.582402	2.460596	0.124915
H	-5.241811	1.198304	-1.903427

a3

SCF done: -1544.112250

Rh	1.174649	0.157336	-0.014352
N	0.634309	-0.831931	1.633507
C	3.139666	-1.135923	-0.019539
C	2.452033	-1.219862	-1.254573
C	2.422898	0.118156	-1.813108
C	3.217346	0.976566	-0.948930
C	3.613272	0.222488	0.166186
O	1.371231	-0.789564	2.792102
C	-0.506092	-1.608086	1.663480
C	-0.576861	-0.661563	-0.575013
C	-2.284308	-2.072158	-0.071491
C	-1.383257	-0.674680	-1.672186
C	-2.477266	-1.572406	-1.379577
H	-1.250546	-0.083701	-2.570867
O	-0.946254	-2.245744	2.596713
C	4.369012	0.677088	1.365090
H	4.484293	1.764489	1.383995
H	3.850939	0.375248	2.283995
H	5.370728	0.228408	1.396562
C	3.399776	2.427541	-1.187550
H	4.104894	2.874779	-0.481266

H	3.761742	2.615945	-2.205028
H	2.429615	2.939394	-1.078196
C	1.905362	0.512212	-3.152738
H	1.364276	1.464121	-3.105490
H	2.734837	0.610572	-3.867066
H	1.212699	-0.237725	-3.546617
C	1.883424	-2.449476	-1.871974
H	1.035565	-2.213825	-2.522156
H	2.641071	-2.973116	-2.469054
H	1.515718	-3.144359	-1.108697
C	3.404176	-2.252223	0.924294
H	2.730624	-3.096223	0.749576
H	4.435113	-2.611588	0.804682
H	3.271765	-1.931983	1.962246
C	0.979413	0.326372	3.578850
H	-0.064507	0.223714	3.902059
H	1.635969	0.327288	4.453212
H	1.106676	1.261840	3.012764
N	-1.105359	-1.502889	0.402297
C	-3.156849	-2.968031	0.535061
H	-2.969300	-3.322122	1.543953
C	-3.598831	-1.993896	-2.100102
H	-3.776711	-1.623772	-3.107751
C	-4.478145	-2.888545	-1.507136
H	-5.354421	-3.223370	-2.058113
C	-4.260008	-3.368691	-0.207744
H	-4.969338	-4.068381	0.228611
C	-0.654255	2.253345	-0.840175
O	-0.594279	2.437751	-2.056275
N	0.472133	1.850593	-0.161190
C	-1.855867	2.579119	-0.029674
C	-2.825506	3.410165	-0.592864
C	-2.040472	2.057918	1.253345
C	-3.969905	3.725708	0.126205
H	-2.659246	3.792164	-1.597336
C	-3.191064	2.368775	1.966853
H	-1.289453	1.393291	1.677808
C	-4.152154	3.205276	1.405726
H	-4.724567	4.376137	-0.309749
H	-3.342511	1.952270	2.959841
H	-5.051493	3.449301	1.966992

b1

SCF done: -742.679362

C	0.141487	1.746370	0.384987

C	1.123910	1.047803	1.178031
C	2.059486	0.380630	0.298443
C	1.597223	0.588564	-1.029924
C	0.414143	1.444427	-0.978303
Rh	0.064177	-0.427638	0.065583
C	3.238486	-0.419815	0.723201
H	4.125744	0.218648	0.821423
H	3.061725	-0.906749	1.687346
H	3.459306	-1.214333	0.004986
C	1.187544	1.043666	2.660427
H	1.592428	0.101173	3.041689
H	1.838428	1.855737	3.012338
H	0.197609	1.191776	3.102009
C	-0.937347	2.627907	0.901687
H	-1.338496	2.249905	1.848478
H	-0.551392	3.640462	1.080111
H	-1.771689	2.668283	0.198480
C	-0.371631	1.917917	-2.143670
H	-1.431856	1.684539	-1.982810
H	-0.268410	3.005733	-2.251358
H	-0.036930	1.451767	-3.074469
C	2.190463	0.042124	-2.277212
H	1.411186	-0.339805	-2.945234
H	2.742384	0.824576	-2.814400
H	2.875296	-0.783050	-2.066887
O	-1.844983	-1.040913	0.294755
O	-2.831033	0.786959	-0.585577
C	-2.870803	-0.308685	-0.033059
C	-4.182773	-0.971909	0.316392
H	-5.019457	-0.309319	0.086271
H	-4.279270	-1.902686	-0.251606
H	-4.194517	-1.245755	1.375866
Cl	0.621584	-2.691150	-0.088406

b2

SCF done: -1330.601224

C	-3.149264	-0.496528	-0.614291
C	-2.812597	-1.083733	0.669475
C	-2.325458	-0.021308	1.523713
C	-2.259986	1.173946	0.752349
C	-2.760762	0.871534	-0.579588
O	0.493729	-1.180421	1.092539
O	1.016593	0.868990	1.876193
C	1.148942	-0.361529	1.843575
C	2.174478	-1.055722	2.714403

H	2.880065	-1.595939	2.072941
H	2.709622	-0.329326	3.330045
H	1.684451	-1.799755	3.351209
Rh	-1.017274	-0.395091	-0.155969
C	-1.926319	-0.153222	2.947524
H	-2.776067	0.089260	3.599371
H	-1.602074	-1.173124	3.176334
H	-1.100520	0.525509	3.180894
C	-3.034432	-2.499034	1.063698
H	-2.259081	-2.836328	1.759615
H	-4.011154	-2.621667	1.551042
H	-2.997227	-3.155198	0.189443
C	-3.770092	-1.225137	-1.748613
H	-3.243380	-2.165964	-1.940803
H	-4.820424	-1.448032	-1.519195
H	-3.738406	-0.636835	-2.669567
C	-2.895086	1.841793	-1.698520
H	-2.795402	1.344224	-2.668150
H	-3.878529	2.328729	-1.666755
H	-2.129477	2.619458	-1.645209
C	-1.804446	2.488476	1.277864
H	-1.733741	3.247976	0.495309
H	-2.502299	2.852174	2.043206
H	-0.815297	2.376031	1.738978
C	1.946907	1.049794	-0.716613
C	1.160071	3.081483	-0.586712
O	2.298883	2.331013	-0.484862
O	1.053481	4.248000	-0.394070
O	0.186132	2.236609	-0.982433
N	0.689793	0.923436	-1.022837
C	2.974110	0.034604	-0.617091
C	4.188407	0.370279	-0.003645
C	2.756346	-1.254298	-1.114611
C	5.186498	-0.586103	0.103920
H	4.333129	1.370770	0.395082
C	3.763732	-2.201260	-0.997220
H	1.800916	-1.512569	-1.570829
C	4.974980	-1.869933	-0.394817
H	6.129395	-0.332280	0.581161
H	3.597862	-3.204823	-1.379546
H	5.759604	-2.618454	-0.309265
Cl	-0.538230	-2.156878	-1.748506

TS-2
SCF done: -1330.521347

C	-3.172910	0.021643	-0.672250
C	-2.908348	-1.235131	0.005952
C	-2.398841	-0.933476	1.329728
C	-2.219844	0.477319	1.406115
C	-2.718346	1.069705	0.167784
O	0.389213	-1.777322	0.072224
O	0.866564	-0.947666	2.112125
C	0.991480	-1.787753	1.218573
C	1.908877	-2.981208	1.386027
H	2.569084	-3.076826	0.516953
H	2.496457	-2.886065	2.302022
H	1.307660	-3.896485	1.431554
Rh	-1.059805	-0.299292	-0.251762
C	-2.096352	-1.923060	2.394833
H	-2.949803	-2.006554	3.080257
H	-1.909400	-2.916251	1.973603
H	-1.209989	-1.627777	2.963249
C	-3.197314	-2.584254	-0.542614
H	-2.468465	-3.317853	-0.183557
H	-4.199739	-2.921224	-0.245327
H	-3.146055	-2.574457	-1.635526
C	-3.772069	0.153676	-2.024631
H	-3.181576	-0.395675	-2.766875
H	-4.795288	-0.242950	-2.023666
H	-3.807825	1.198796	-2.342797
C	-2.788147	2.519241	-0.151575
H	-2.500941	2.705928	-1.191758
H	-3.812790	2.886119	-0.006779
H	-2.116356	3.104198	0.478513
C	-1.602801	1.216527	2.536746
H	-1.173283	2.160976	2.187841
H	-2.346546	1.438574	3.313011
H	-0.791381	0.622669	2.971557
C	1.859929	1.053390	-0.160419
C	1.688325	3.713664	0.261711
O	2.642960	2.968735	0.142212
O	1.275159	4.807661	0.443200
O	0.268357	2.642682	0.091054
N	0.721412	1.448841	-0.056617
C	2.908811	0.130104	-0.346896
C	3.899989	0.022453	0.643351
C	2.940812	-0.667376	-1.503056
C	4.931413	-0.883041	0.467414
H	3.841990	0.657644	1.522902

C	3.968767	-1.587076	-1.646596
H	2.136715	-0.577626	-2.233014
C	4.960928	-1.687281	-0.672716
H	5.709492	-0.973422	1.220259
H	3.999291	-2.224792	-2.525672
H	5.768324	-2.404639	-0.801688
Cl	-0.436610	-0.329832	-2.573581

b3

SCF done: -1142.063223

C	3.430130	-0.425815	0.126646
C	3.072350	0.809249	-0.547728
C	2.280746	1.607603	0.370695
C	2.053662	0.831037	1.539392
C	2.756248	-0.436209	1.379041
O	-0.272224	0.669429	-1.268355
O	-1.180874	1.662497	0.540241
C	-1.106413	1.448553	-0.677878
C	-2.084765	2.099924	-1.637097
H	-2.797785	1.346250	-1.991276
H	-2.633523	2.905401	-1.141505
H	-1.559349	2.480877	-2.517595
Rh	1.292355	-0.228947	-0.196427
C	1.757979	2.974993	0.117153
H	2.458086	3.724861	0.508646
H	1.633794	3.161062	-0.954629
H	0.784498	3.115153	0.597908
C	3.534338	1.215320	-1.899907
H	2.790335	1.848327	-2.393766
H	4.477982	1.774855	-1.842143
H	3.690429	0.336577	-2.532878
C	4.292341	-1.488772	-0.452223
H	3.859870	-1.869537	-1.385693
H	5.293661	-1.091502	-0.660886
H	4.396410	-2.335811	0.231020
C	2.729100	-1.545223	2.367920
H	3.119125	-2.472435	1.939238
H	3.326615	-1.293401	3.253657
H	1.702746	-1.741826	2.697138
C	1.226867	1.234089	2.707525
H	1.039429	0.384349	3.370364
H	1.730855	2.015874	3.290586
H	0.258594	1.614919	2.361437
C	-2.571392	-1.144753	0.545761
O	-0.271622	-1.469710	1.075440

N	-1.451393	-1.294500	0.806580
C	-3.915193	-0.720442	0.328621
C	-4.242933	0.621194	0.580795
C	-4.886329	-1.620232	-0.126524
C	-5.548158	1.045118	0.374794
H	-3.455748	1.302855	0.904871
C	-6.186762	-1.178389	-0.323664
H	-4.610822	-2.652973	-0.323812
C	-6.518045	0.150811	-0.072508
H	-5.809957	2.083288	0.563804
H	-6.943874	-1.872894	-0.678425
H	-7.538214	0.492760	-0.230173
Cl	1.185045	-1.979941	-1.815072

c1

SCF done: -529.278108

C	-1.267053	1.258272	0.152370
C	-0.259766	1.258680	1.179219
C	1.051730	1.324946	0.556507
C	0.854473	1.286252	-0.850473
C	-0.582403	1.218892	-1.100550
Rh	0.018584	-0.504296	0.012125
C	2.353860	1.364058	1.271977
H	2.642534	2.396972	1.504628
H	2.307151	0.804033	2.211278
H	3.146471	0.907590	0.672425
C	-0.517692	1.214397	2.640129
H	0.320897	0.765344	3.179995
H	-0.668267	2.228886	3.033395
H	-1.412657	0.626343	2.864976
C	-2.739298	1.223226	0.351806
H	-2.997742	0.830058	1.339241
H	-3.169681	2.228438	0.259905
H	-3.221781	0.572170	-0.383628
C	-1.215367	1.134990	-2.440817
H	-2.166027	0.595485	-2.397009
H	-1.409353	2.140862	-2.837213
H	-0.568834	0.613799	-3.153390
C	1.903332	1.282964	-1.902264
H	1.656696	0.576767	-2.701881
H	2.005931	2.279713	-2.351089
H	2.873869	0.986645	-1.496063
Cl	1.760376	-2.041067	0.014148
Cl	-1.623103	-2.150689	0.018875

c2

SCF done: -1330.601224

C	-3.149264	-0.496528	-0.614291
C	-2.812597	-1.083733	0.669475
C	-2.325458	-0.021308	1.523713
C	-2.259986	1.173946	0.752349
C	-2.760762	0.871534	-0.579588
O	0.493729	-1.180421	1.092539
O	1.016593	0.868990	1.876193
C	1.148942	-0.361529	1.843575
C	2.174478	-1.055722	2.714403
H	2.880065	-1.595939	2.072941
H	2.709622	-0.329326	3.330045
H	1.684451	-1.799755	3.351209
Rh	-1.017274	-0.395091	-0.155969
C	-1.926319	-0.153222	2.947524
H	-2.776067	0.089260	3.599371
H	-1.602074	-1.173124	3.176334
H	-1.100520	0.525509	3.180894
C	-3.034432	-2.499034	1.063698
H	-2.259081	-2.836328	1.759615
H	-4.011154	-2.621667	1.551042
H	-2.997227	-3.155198	0.189443
C	-3.770092	-1.225137	-1.748613
H	-3.243380	-2.165964	-1.940803
H	-4.820424	-1.448032	-1.519195
H	-3.738406	-0.636835	-2.669567
C	-2.895086	1.841793	-1.698520
H	-2.795402	1.344224	-2.668150
H	-3.878529	2.328729	-1.666755
H	-2.129477	2.619458	-1.645209
C	-1.804446	2.488476	1.277864
H	-1.733741	3.247976	0.495309
H	-2.502299	2.852174	2.043206
H	-0.815297	2.376031	1.738978
C	1.946907	1.049794	-0.716613
C	1.160071	3.081483	-0.586712
O	2.298883	2.331013	-0.484862
O	1.053481	4.248000	-0.394070
O	0.186132	2.236609	-0.982433
N	0.689793	0.923436	-1.022837
C	2.974110	0.034604	-0.617091
C	4.188407	0.370279	-0.003645
C	2.756346	-1.254298	-1.114611
C	5.186498	-0.586103	0.103920
H	4.333129	1.370770	0.395082

C	3.763732	-2.201260	-0.997220
H	1.800916	-1.512569	-1.570829
C	4.974980	-1.869933	-0.394817
H	6.129395	-0.332280	0.581161
H	3.597862	-3.204823	-1.379546
H	5.759604	-2.618454	-0.309265
Cl	-0.538230	-2.156878	-1.748506

TS-3

SCF done: -1330.521347

C	-3.172910	0.021643	-0.672250
C	-2.908348	-1.235131	0.005952
C	-2.398841	-0.933476	1.329728
C	-2.219844	0.477319	1.406115
C	-2.718346	1.069705	0.167784
O	0.389213	-1.777322	0.072224
O	0.866564	-0.947666	2.112125
C	0.991480	-1.787753	1.218573
C	1.908877	-2.981208	1.386027
H	2.569084	-3.076826	0.516953
H	2.496457	-2.886065	2.302022
H	1.307660	-3.896485	1.431554
Rh	-1.059805	-0.299292	-0.251762
C	-2.096352	-1.923060	2.394833
H	-2.949803	-2.006554	3.080257
H	-1.909400	-2.916251	1.973603
H	-1.209989	-1.627777	2.963249
C	-3.197314	-2.584254	-0.542614
H	-2.468465	-3.317853	-0.183557
H	-4.199739	-2.921224	-0.245327
H	-3.146055	-2.574457	-1.635526
C	-3.772069	0.153676	-2.024631
H	-3.181576	-0.395675	-2.766875
H	-4.795288	-0.242950	-2.023666
H	-3.807825	1.198796	-2.342797
C	-2.788147	2.519241	-0.151575
H	-2.500941	2.705928	-1.191758
H	-3.812790	2.886119	-0.006779
H	-2.116356	3.104198	0.478513
C	-1.602801	1.216527	2.536746
H	-1.173283	2.160976	2.187841
H	-2.346546	1.438574	3.313011
H	-0.791381	0.622669	2.971557
C	1.859929	1.053390	-0.160419
C	1.688325	3.713664	0.261711

O	2.642960	2.968735	0.142212
O	1.275159	4.807661	0.443200
O	0.268357	2.642682	0.091054
N	0.721412	1.448841	-0.056617
C	2.908811	0.130104	-0.346896
C	3.899989	0.022453	0.643351
C	2.940812	-0.667376	-1.503056
C	4.931413	-0.883041	0.467414
H	3.841990	0.657644	1.522902
C	3.968767	-1.587076	-1.646596
H	2.136715	-0.577626	-2.233014
C	4.960928	-1.687281	-0.672716
H	5.709492	-0.973422	1.220259
H	3.999291	-2.224792	-2.525672
H	5.768324	-2.404639	-0.801688
Cl	-0.436610	-0.329832	-2.573581

c3

SCF done: -1142.063223

C	3.430130	-0.425815	0.126646
C	3.072350	0.809249	-0.547728
C	2.280746	1.607603	0.370695
C	2.053662	0.831037	1.539392
C	2.756248	-0.436209	1.379041
O	-0.272224	0.669429	-1.268355
O	-1.180874	1.662497	0.540241
C	-1.106413	1.448553	-0.677878
C	-2.084765	2.099924	-1.637097
H	-2.797785	1.346250	-1.991276
H	-2.633523	2.905401	-1.141505
H	-1.559349	2.480877	-2.517595
Rh	1.292355	-0.228947	-0.196427
C	1.757979	2.974993	0.117153
H	2.458086	3.724861	0.508646
H	1.633794	3.161062	-0.954629
H	0.784498	3.115153	0.597908
C	3.534338	1.215320	-1.899907
H	2.790335	1.848327	-2.393766
H	4.477982	1.774855	-1.842143
H	3.690429	0.336577	-2.532878
C	4.292341	-1.488772	-0.452223
H	3.859870	-1.869537	-1.385693
H	5.293661	-1.091502	-0.660886
H	4.396410	-2.335811	0.231020
C	2.729100	-1.545223	2.367920

H	3.119125	-2.472435	1.939238
H	3.326615	-1.293401	3.253657
H	1.702746	-1.741826	2.697138
C	1.226867	1.234089	2.707525
H	1.039429	0.384349	3.370364
H	1.730855	2.015874	3.290586
H	0.258594	1.614919	2.361437
C	-2.571392	-1.144753	0.545761
O	-0.271622	-1.469710	1.075440
N	-1.451393	-1.294500	0.806580
C	-3.915193	-0.720442	0.328621
C	-4.242933	0.621194	0.580795
C	-4.886329	-1.620232	-0.126524
C	-5.548158	1.045118	0.374794
H	-3.455748	1.302855	0.904871
C	-6.186762	-1.178389	-0.323664
H	-4.610822	-2.652973	-0.323812
C	-6.518045	0.150811	-0.072508
H	-5.809957	2.083288	0.563804
H	-6.943874	-1.872894	-0.678425
H	-7.538214	0.492760	-0.230173
Cl	1.185045	-1.979941	-1.815072

substrate
SCF done: -646.574049

N	-2.464644	0.548801	-0.304796
C	-1.371970	-0.280810	-0.049588
O	-1.456396	-1.467796	0.151353
O	-3.624308	-0.141532	-0.628651
H	-2.319334	1.275492	-0.997781
C	-4.392452	-0.355402	0.544824
H	-4.631733	0.594530	1.039554
H	-5.311212	-0.839531	0.205284
H	-3.867764	-1.018487	1.242685
N	-0.170300	0.435372	0.021250
C	-0.017987	1.825928	0.088209
C	1.106685	-0.141398	0.012199
C	1.298522	2.143594	0.106489
H	-0.884628	2.466260	0.179466
C	2.041054	0.914719	0.051719
H	1.707502	3.143254	0.175270
C	3.408527	0.624350	0.039850
H	4.140913	1.427900	0.072482
C	1.497746	-1.476783	-0.045419
H	0.762356	-2.272427	-0.068566

C	3.806803	-0.700069	-0.013122
H	4.866033	-0.945500	-0.020773
C	2.860886	-1.734133	-0.056636
H	3.201229	-2.766052	-0.095569

IN1(2Cl)
SCF done: -1175.860837

N	-0.617821	1.111144	0.766635
C	3.028622	-0.654405	-1.022240
C	3.296049	0.016779	0.235980
C	2.542813	-0.648321	1.247092
C	1.815710	-1.739990	0.635902
C	2.164989	-1.777241	-0.751007
Rh	1.182529	0.112015	-0.340576
C	-1.246198	0.137280	1.601794
O	-0.742691	-0.215058	2.646760
O	-0.562883	2.346144	1.440567
H	-1.120609	1.284774	-0.108489
C	2.519896	-0.352190	2.702521
H	1.489897	-0.322224	3.078196
H	3.051836	-1.145268	3.244971
H	3.007636	0.598650	2.935537
C	0.949870	-2.714481	1.352075
H	1.542609	-3.551738	1.744903
H	0.437562	-2.238557	2.196318
H	0.187694	-3.127222	0.681178
C	1.709759	-2.792169	-1.733334
H	2.339871	-3.688137	-1.651883
H	0.668343	-3.076057	-1.557460
H	1.772062	-2.416053	-2.757418
C	3.620901	-0.295980	-2.337138
H	4.572396	-0.822680	-2.492055
H	2.943096	-0.556928	-3.156148
H	3.799812	0.781132	-2.399709
C	4.197559	1.188350	0.389252
H	5.228202	0.916805	0.128307
H	3.876375	2.001284	-0.275047
H	4.196961	1.569185	1.414888
C	0.689289	2.580629	2.061236
H	1.500105	2.499534	1.327257
H	0.625464	3.609958	2.423058
H	0.845307	1.902658	2.909237
N	-2.407757	-0.412045	1.099400
C	-2.782891	-1.728936	1.403262
C	-3.365024	0.126688	0.218635

C	-3.900729	-2.052263	0.716182
H	-2.171146	-2.298328	2.089531
C	-4.301431	-0.893868	-0.039957
H	-4.404256	-3.010073	0.738939
C	-5.391855	-0.631492	-0.871416
H	-6.121468	-1.410593	-1.080707
C	-3.526277	1.417541	-0.277169
H	-2.859578	2.236686	-0.016932
C	-5.533110	0.638013	-1.408424
H	-6.375896	0.858375	-2.058850
C	-4.616087	1.651239	-1.104966
H	-4.759972	2.646907	-1.516262
Cl	1.380448	2.296387	-1.365014
Cl	-0.621248	-0.477342	-1.834161

TS1(2Cl)
SCF done: -1175.810714

N	-0.319290	1.029470	-1.177476
C	2.854786	-0.975348	1.027309
C	2.564529	0.399394	1.356744
C	1.226628	0.460327	1.922914
C	0.649094	-0.835773	1.812453
C	1.662688	-1.717247	1.252945
Rh	1.241752	-0.142493	-0.187254
C	-1.061743	1.843999	-0.317213
O	-0.831431	3.008497	-0.045204
O	0.098961	1.761313	-2.297773
H	-0.591575	-0.577911	-1.722886
C	0.649965	1.686606	2.530050
H	-0.302215	1.476458	3.023974
H	1.343014	2.087260	3.280180
H	0.477009	2.473855	1.781695
C	-0.709644	-1.276735	2.224562
H	-0.651031	-1.935306	3.101063
H	-1.359792	-0.431250	2.469714
H	-1.200974	-1.837274	1.419375
C	1.498540	-3.168275	0.986642
H	1.895582	-3.748045	1.831483
H	0.448300	-3.438790	0.849566
H	2.046534	-3.465660	0.086548
C	4.138436	-1.529118	0.522518
H	4.862505	-0.737234	0.316229
H	4.572111	-2.208863	1.267596
H	3.993343	-2.081233	-0.412019
C	3.503785	1.545443	1.265613

H	4.139859	1.591653	2.160408
H	4.149081	1.454550	0.386641
H	2.958829	2.492136	1.188642
C	1.073870	2.769776	-2.076477
H	1.805272	2.441795	-1.326116
H	1.590112	2.884504	-3.034235
H	0.618718	3.713990	-1.761884
N	-2.148249	1.197569	0.325142
C	-2.608763	1.639574	1.566064
C	-3.051661	0.233510	-0.146192
C	-3.693719	0.919822	1.948038
H	-2.096753	2.460864	2.048072
C	-4.003201	0.014208	0.876682
H	-4.243473	1.039044	2.873125
C	-5.041938	-0.899996	0.671600
H	-5.773526	-1.082376	1.456158
C	-3.195235	-0.346042	-1.404531
H	-2.535282	-0.088111	-2.226278
C	-5.141192	-1.533618	-0.555182
H	-5.945625	-2.243270	-0.733855
C	-4.238953	-1.240319	-1.587671
H	-4.364095	-1.711015	-2.559714
Cl	2.663939	-0.068304	-2.093249
Cl	-0.372167	-1.920312	-1.782522

IN2(2Cl)

SCF done: -1175.832484

N	-0.194838	1.338214	-1.345178
C	2.225616	-0.639384	1.507092
C	2.194375	0.802056	1.521415
C	0.838814	1.228556	1.855694
C	0.049214	0.057733	1.996003
C	0.904109	-1.092587	1.752968
Rh	0.924972	0.237435	-0.053729
C	-1.338972	2.035061	-1.021382
O	-1.572738	3.208409	-1.235654
O	0.437951	1.947499	-2.422894
H	1.701779	-2.471815	-1.684705
C	0.379993	2.632247	2.032715
H	-0.686130	2.737510	1.803311
H	0.537149	2.964460	3.067236
H	0.924409	3.317372	1.374706
C	-1.349115	-0.026292	2.481835
H	-1.341617	-0.109847	3.577651
H	-1.938730	0.857283	2.218006
H	-1.866571	-0.905459	2.084942
C	0.432247	-2.496891	1.803990
H	0.172993	-2.759878	2.838967
H	-0.468274	-2.630867	1.191453
H	1.184662	-3.198637	1.435950
C	3.413619	-1.492960	1.236609
H	3.854251	-1.843397	2.178961
H	3.146016	-2.369799	0.636292
H	4.180874	-0.945100	0.683296
C	3.365849	1.690934	1.314732
H	3.989802	1.710434	2.218525
H	3.986172	1.338573	0.483976
H	3.059429	2.718028	1.095048
C	1.346724	2.952064	-2.025513
H	2.169053	2.518750	-1.432730

H	1.759397	3.358722	-2.952764
H	0.841175	3.749752	-1.466087
N	-2.321473	1.225849	-0.385001
C	-3.391190	1.818596	0.279771
C	-2.570355	-0.151270	-0.469790
C	-4.283879	0.872734	0.669657
H	-3.399608	2.895544	0.380930
C	-3.788504	-0.393743	0.210957
H	-5.201548	1.048567	1.216379
C	-4.260020	-1.704895	0.342820
H	-5.189242	-1.899869	0.874719
C	-1.856229	-1.190545	-1.071552
H	-0.958024	-1.000763	-1.653668
C	-3.528994	-2.741117	-0.214415
H	-3.881693	-3.765388	-0.118125
C	-2.347670	-2.481471	-0.926093
H	-1.794105	-3.301196	-1.379778
Cl	2.345390	-0.438071	-1.852282
Cl	1.282453	-3.677588	-1.355961

IN3(2Cl)
SCF done: -1160.278451

N	0.027258	1.530339	-0.976257
C	2.434183	-1.355047	0.840355
C	2.191063	-0.076964	1.481198
C	0.815225	-0.029952	1.925148
C	0.197936	-1.231206	1.487503
C	1.196031	-2.036808	0.788091
Rh	1.008711	-0.126495	-0.265946
C	-0.929921	2.205555	-0.263531
O	-0.949493	3.385738	0.034845
O	0.732715	2.413653	-1.788964
C	0.213901	1.085886	2.706456
H	-0.857077	0.931751	2.867232
H	0.697445	1.174033	3.687805
H	0.329958	2.049681	2.191792
C	-1.180684	-1.703762	1.758411
H	-1.135718	-2.519198	2.494269
H	-1.824685	-0.916542	2.160104
H	-1.658679	-2.103316	0.856412
C	0.903269	-3.342154	0.142627
H	-0.047434	-3.294626	-0.401461
H	1.681978	-3.617925	-0.573419
H	0.819280	-4.140350	0.892373
C	3.738553	-1.799006	0.284145
H	4.393668	-2.161288	1.086971
H	3.609673	-2.601231	-0.446651
H	4.247538	-0.978954	-0.232684
C	3.213778	0.962070	1.758716
H	3.651484	0.797954	2.753686
H	4.027142	0.932834	1.027130
H	2.776719	1.965625	1.747601
C	1.844907	2.978120	-1.133062
H	2.611228	2.210827	-0.931115

H	2.259681	3.714142	-1.827487
H	1.545081	3.482891	-0.203787
N	-2.006259	1.360964	0.141167
C	-2.858789	1.745230	1.167016
C	-2.522392	0.198818	-0.443726
C	-3.872879	0.849112	1.297302
H	-2.644251	2.664876	1.695530
C	-3.688161	-0.148453	0.281420
H	-4.678528	0.897665	2.018841
C	-4.394498	-1.307938	-0.058646
H	-5.286702	-1.587737	0.498277
C	-2.084360	-0.561731	-1.530877
H	-1.219518	-0.265425	-2.116480
C	-3.942603	-2.084065	-1.113220
H	-4.482457	-2.986767	-1.390565
C	-2.806588	-1.705260	-1.845756
H	-2.487430	-2.310501	-2.691374
Cl	1.944647	-0.478531	-2.382017

TS2(2Cl)
SCF done: -1160.245376

Rh	0.900622	-0.076475	-0.044422
N	0.017800	1.737805	-0.052306
C	1.909339	-0.461149	1.760408
C	1.645822	-1.747994	1.133440
C	2.330673	-1.767151	-0.104746
C	3.089568	-0.524916	-0.217270
C	2.875826	0.249256	0.944238
O	0.718156	2.878655	0.296426
C	-1.339546	1.883570	0.081470
C	-1.127622	-0.534778	-0.222142
C	-3.251800	0.241885	0.068197
C	-1.968138	-1.633035	-0.199254
H	-0.537760	-0.559613	-1.609031
C	-3.309951	-1.172102	-0.033914
H	-1.655060	-2.661866	-0.347986
O	-1.981689	2.896607	0.266225
C	3.448534	1.578638	1.286225
H	2.650851	2.324681	1.396855
H	4.008506	1.529088	2.228677
H	4.133098	1.934437	0.509987
C	3.905350	-0.162332	-1.406363
H	4.343502	0.835040	-1.307537
H	4.720745	-0.883036	-1.550957
H	3.289487	-0.171968	-2.314185

C	2.326420	-2.852514	-1.122405
H	3.176818	-3.533245	-0.982109
H	1.406938	-3.445742	-1.069201
H	2.382902	-2.438559	-2.134182
C	0.803860	-2.824976	1.721306
H	0.506423	-3.559685	0.966854
H	1.356485	-3.358429	2.505761
H	-0.109663	-2.418227	2.167193
C	1.419693	-0.006996	3.087683
H	0.494822	-0.519591	3.369531
H	2.169177	-0.206458	3.866370
H	1.221046	1.070543	3.080108
C	1.272936	3.447141	-0.875007
H	0.480422	3.778781	-1.557928
H	1.869599	4.305030	-0.549063
H	1.915487	2.717618	-1.394980
N	-1.926988	0.601765	-0.051481
C	-4.554302	-1.816168	0.041655
H	-4.620027	-2.899073	-0.041252
C	-4.393973	1.022692	0.254015
H	-4.312721	2.102000	0.330444
C	-5.687668	-1.048094	0.226800
H	-6.661478	-1.527947	0.291817
C	-5.603993	0.353389	0.332287
H	-6.516845	0.927163	0.476672
Cl	0.263861	-0.342638	-2.861606

IN4(2Cl)
SCF done: -1160.256841

Rh	0.967540	-0.064256	0.260033
N	0.114937	1.674148	0.506780
C	2.220380	-1.677213	0.985842
C	2.008265	-1.883928	-0.402371
C	2.540855	-0.733395	-1.093303
C	3.177707	0.136799	-0.134549
C	2.951048	-0.418695	1.145073
O	0.817596	2.857103	0.625237
C	-1.265755	1.822547	0.610130
C	-1.005877	-0.561690	0.307681
C	-3.170013	0.172557	0.476894
C	-1.824202	-1.657874	0.158659
H	-0.990728	-0.338937	-1.813062
C	-3.192638	-1.226728	0.264309
H	-1.492443	-2.675057	-0.025178
O	-1.889403	2.852194	0.749830

C	3.358230	0.198628	2.434648
H	3.184957	1.280902	2.417775
H	2.797981	-0.216003	3.277685
H	4.426479	0.031390	2.627396
C	3.894116	1.410326	-0.422343
H	3.678688	2.167072	0.340280
H	4.981235	1.258257	-0.446185
H	3.598792	1.828030	-1.390146
C	2.506330	-0.519755	-2.562060
H	2.427355	0.544023	-2.810034
H	3.425516	-0.907473	-3.022923
H	1.653155	-1.024209	-3.025735
C	1.348560	-3.051487	-1.051596
H	0.698098	-2.740857	-1.877400
H	2.091335	-3.750220	-1.457948
H	0.729649	-3.606607	-0.339079
C	1.813448	-2.581768	2.094340
H	0.940178	-3.179774	1.815877
H	2.626185	-3.268345	2.366434
H	1.540508	-2.013251	2.989461
C	0.862157	3.514738	-0.630881
H	-0.135624	3.854543	-0.933907
H	1.523933	4.375817	-0.501419
H	1.269443	2.838713	-1.400547
N	-1.833609	0.546707	0.504797
C	-4.425653	-1.883982	0.192370
H	-4.469298	-2.958967	0.028884
C	-4.327907	0.928756	0.616459
H	-4.269483	2.000757	0.774202
C	-5.586652	-1.139780	0.331041
H	-6.553734	-1.634544	0.275951
C	-5.536076	0.246949	0.539097
H	-6.465489	0.802830	0.641050
Cl	-1.072282	0.143121	-3.026539

IN5

SCF done: -1144.705687

Rh	0.866073	-0.057370	-0.001769
N	0.018298	1.702212	0.140896
C	2.414818	-0.864941	1.246600
C	1.896515	-1.940974	0.431630
C	2.128842	-1.583873	-0.919517
C	2.881504	-0.328764	-0.934513
C	3.087897	0.091122	0.394846
O	0.716746	2.872658	0.379864
C	-1.363357	1.858381	0.198292

C	-1.098284	-0.533485	-0.001978
C	-3.264270	0.205538	0.038176
C	-1.904835	-1.637276	-0.125546
C	-3.276701	-1.203331	-0.105369
H	-1.563816	-2.663112	-0.224001
O	-1.985392	2.895086	0.293845
C	3.748073	1.340853	0.872467
H	4.318622	1.821377	0.071516
H	3.005365	2.067753	1.228816
H	4.444647	1.131553	1.693160
C	3.316828	0.356147	-2.180604
H	3.710313	1.356809	-1.978945
H	4.099942	-0.222124	-2.689435
H	2.481028	0.461220	-2.882426
C	1.748811	-2.358335	-2.132001
H	1.498501	-1.691932	-2.964210
H	2.569616	-3.010033	-2.461350
H	0.871237	-2.985103	-1.944038
C	1.229167	-3.169442	0.944571
H	0.647555	-3.663411	0.159587
H	1.966294	-3.893489	1.315823
H	0.540427	-2.937888	1.764233
C	2.366514	-0.791570	2.729087
H	1.513333	-1.346497	3.130859
H	3.281782	-1.218308	3.163583
H	2.286503	0.246003	3.070074
C	0.970248	3.543706	-0.838648
H	0.033194	3.856579	-1.316153
H	1.565735	4.425263	-0.583819
H	1.538996	2.897208	-1.527502
N	-1.929370	0.583030	0.103053
C	-4.426010	0.965019	0.091573
H	-4.373210	2.043512	0.201636
C	-4.506352	-1.863711	-0.194080
H	-4.544420	-2.945875	-0.304599
C	-5.673370	-1.115591	-0.141473
H	-6.637167	-1.615423	-0.210761
C	-5.632141	0.278973	-0.001217
H	-6.564461	0.838247	0.036471

HCl
SCF done: -15.534842

Cl	0.000000	0.000000	0.071315
H	0.000000	0.000000	-1.212348

IN1(2OAc)
SCF done: -1602.663292

N	0.357338	0.554948	-1.500890
C	-2.948114	-0.828793	1.129867
C	-2.761736	-1.446238	-0.150683
C	-1.555534	-2.242228	-0.082980
C	-0.967232	-2.072367	1.201190
C	-1.826433	-1.182367	1.957188
O	1.225977	2.377901	0.343079
O	0.559707	0.572819	1.504334
C	1.183390	1.694250	1.372097
C	1.952484	2.114925	2.601757
H	1.270294	2.230599	3.450780
H	2.668894	1.328298	2.864759
H	2.484915	3.050437	2.417895
Rh	-1.090181	-0.094303	0.296559
C	1.134194	-0.555469	-1.894170
O	0.805097	-1.289219	-2.800733
O	-0.185025	1.231297	-2.597956
H	0.777390	1.296387	-0.877966
C	-1.083820	-3.119466	-1.183975
H	-0.181048	-3.669875	-0.903780
H	-1.863901	-3.852825	-1.424957
H	-0.858542	-2.556207	-2.098802
C	0.298088	-2.641460	1.735372
H	0.110327	-3.186270	2.669264
H	0.773264	-3.327889	1.029227
H	1.009271	-1.832166	1.951678
C	-1.555759	-0.749869	3.350813
H	-1.627626	-1.602530	4.038692
H	-0.542386	-0.334292	3.415320
H	-2.262330	0.015956	3.681757
C	-4.096774	0.016415	1.541697
H	-4.863339	-0.608403	2.019338
H	-3.786945	0.779490	2.262960
H	-4.529207	0.529920	0.680252
C	-3.729647	-1.437257	-1.278348
H	-4.536976	-2.159233	-1.093178
H	-4.162531	-0.439535	-1.398181
H	-3.243546	-1.717785	-2.218692
O	-3.498585	1.720599	-0.982021
O	-1.591600	1.913011	0.211275
C	-2.618475	2.377368	-0.422569
C	-2.629616	3.890352	-0.456784
H	-2.444037	4.301440	0.539537

H	-1.808008	4.227299	-1.098424
H	-3.578744	4.257240	-0.853319
C	-1.382611	0.650626	-3.098665
H	-2.137628	0.576399	-2.307591
H	-1.734619	1.364592	-3.847925
H	-1.191533	-0.319510	-3.570218
N	2.239624	-0.855708	-1.086172
C	2.576742	-2.189930	-0.836564
C	3.276826	-0.049760	-0.582946
C	3.718018	-2.254625	-0.111369
H	1.935190	-2.968030	-1.227863
C	4.193129	-0.909379	0.062008
H	4.194298	-3.158903	0.245489
C	5.350929	-0.377082	0.638556
H	6.060807	-1.029165	1.142992
C	3.541938	1.305350	-0.755571
H	2.875324	1.961371	-1.303813
C	5.587551	0.982382	0.523677
H	6.485420	1.413120	0.960791
C	4.699425	1.808096	-0.179369
H	4.920625	2.866918	-0.286948

TSa(2OAc)
SCF done: -1602.660742

N	0.182980	0.134728	-1.724451
C	-2.053135	-0.991416	1.934900
C	-1.706944	-2.001069	0.964144
C	-0.272430	-2.123930	0.954955
C	0.279275	-1.170426	1.866696
C	-0.830806	-0.474911	2.478690
O	0.131199	2.599842	-1.337524
O	-0.184695	1.947870	0.783563
C	-0.178987	2.820207	-0.134124
C	-0.567445	4.219860	0.244693
H	-1.661109	4.278515	0.189642
H	-0.270975	4.442964	1.272531
H	-0.145880	4.946188	-0.453344
Rh	-0.876220	-0.080187	0.380154
C	1.202987	-0.774291	-2.062386
O	1.051619	-1.653007	-2.885427
O	-0.744663	0.195090	-2.779935
H	0.315057	1.298825	-1.531685
C	0.461504	-3.120181	0.133287
H	1.544080	-3.044710	0.269051
H	0.146863	-4.131761	0.419734

H	0.247558	-3.004415	-0.938361
C	1.710922	-0.940795	2.203191
H	1.899941	-1.186439	3.256233
H	2.379395	-1.552916	1.589076
H	1.994078	0.108343	2.044847
C	-0.714083	0.597943	3.496863
H	0.264729	1.082412	3.449781
H	-1.473868	1.370470	3.343992
H	-0.847408	0.177856	4.502725
C	-3.421512	-0.577739	2.337453
H	-3.731556	-1.135013	3.231916
H	-3.448582	0.489567	2.582332
H	-4.135504	-0.752411	1.528340
C	-2.649276	-2.890695	0.238268
H	-2.978116	-3.706177	0.897329
H	-3.519489	-2.322162	-0.099868
H	-2.170958	-3.342916	-0.636963
O	-4.085531	-0.303229	-0.677381
O	-2.332921	1.112647	-0.530220
C	-3.531473	0.777590	-0.877032
C	-4.231626	1.887969	-1.633761
H	-4.241666	2.806847	-1.038949
H	-3.664870	2.105971	-2.546022
H	-5.252880	1.596117	-1.887330
C	-1.658501	-0.887506	-2.826944
H	-2.083770	-1.086178	-1.834886
H	-2.468094	-0.542189	-3.477679
H	-1.199617	-1.790048	-3.243123
N	2.420199	-0.742158	-1.336598
C	3.192154	-1.912741	-1.335156
C	3.109695	0.216164	-0.571690
C	4.289703	-1.756521	-0.559107
H	2.848739	-2.754725	-1.918378
C	4.268539	-0.412531	-0.056826
H	5.051409	-2.504242	-0.378486
C	5.142271	0.299963	0.768565
H	6.029935	-0.184356	1.170394
C	2.867581	1.566258	-0.346651
H	2.045536	2.087427	-0.819091
C	4.866541	1.628721	1.045343
H	5.535671	2.200943	1.683657
C	3.749488	2.254146	0.476986
H	3.572279	3.310515	0.666240

IN2(2OAc)

SCF done: -1373.695679

Rh	1.226783	-0.150036	-0.085913
N	0.195804	1.576382	0.532768
C	0.161542	-2.022470	0.035184
C	1.476246	-2.269090	-0.540946
C	2.454093	-1.874429	0.404356
C	1.755728	-1.352667	1.573151
C	0.346236	-1.523007	1.364947
O	2.842445	1.264822	-0.545156
O	1.399008	0.771714	-2.116562
C	2.381371	1.459693	-1.709111
C	2.964586	2.530661	-2.576538
H	2.847005	2.277366	-3.632725
H	2.420388	3.463611	-2.389598
H	4.016488	2.695952	-2.332350
O	0.928061	2.019991	1.653826
C	-1.134019	1.524739	0.868819
O	-1.641188	1.846318	1.929628
C	-0.707468	-1.208728	2.364855
H	-0.568203	-0.220154	2.818049
H	-1.708481	-1.221836	1.922022
H	-0.680979	-1.955954	3.168763
C	2.381642	-0.786130	2.796485
H	1.873239	0.142127	3.081617
H	2.319112	-1.492296	3.635012
H	3.435955	-0.547655	2.626531
C	3.932153	-1.876959	0.242568
H	4.343694	-0.876134	0.418851
H	4.398689	-2.566912	0.957064
H	4.226806	-2.182626	-0.765302
C	1.688011	-2.781301	-1.919903
H	2.736186	-2.712328	-2.223714
H	1.376418	-3.831048	-1.997240
H	1.094873	-2.201407	-2.636673
C	-1.121416	-2.367448	-0.630766
H	-1.164658	-1.957035	-1.646471
H	-1.231594	-3.457946	-0.700804
H	-1.986049	-1.970897	-0.089292
C	1.261358	3.378532	1.479056
H	0.358444	4.005613	1.462794
H	1.876524	3.655380	2.340890
H	1.836666	3.526699	0.554665
N	-1.946502	1.048420	-0.200059
C	-3.213804	0.489986	-0.035710
C	-1.634376	1.031515	-1.556543

C	-3.674134	0.102987	-1.317061
C	-2.656602	0.472375	-2.259025
H	-0.684697	1.422666	-1.897298
H	-2.692064	0.349669	-3.334289
C	-3.962838	0.257618	1.119432
H	-3.601995	0.596580	2.084902
C	-4.912677	-0.537530	-1.435509
H	-5.280711	-0.842024	-2.413594
C	-5.655796	-0.779218	-0.291837
H	-6.620362	-1.276246	-0.370314
C	-5.184005	-0.384433	0.969329
H	-5.792628	-0.576086	1.850338

IN3(2OAc)
SCF done: -1373.693313

Rh	0.921100	-0.169142	-0.074526
N	0.032188	1.249168	1.136806
C	1.772248	-1.666252	1.127726
C	1.585256	-2.241158	-0.193004
C	2.373343	-1.483676	-1.093452
C	3.172953	-0.535714	-0.317619
C	2.849026	-0.684424	1.037824
O	0.917392	1.529320	-1.698500
O	-1.284235	1.747738	-2.108821
C	-0.044367	2.183794	-2.088111
C	0.083026	3.586694	-2.585849
H	-0.470053	3.714829	-3.520079
H	-0.367028	4.258202	-1.846338
H	1.133941	3.845518	-2.717916
O	0.793076	1.877946	2.118516
C	-1.256908	1.038545	1.562620
C	-1.058435	-0.558592	-0.259196
C	-3.188841	-0.165134	0.457403
C	-1.896456	-1.251821	-1.101512
H	-1.328422	0.826671	-1.750210
C	-3.253661	-1.024997	-0.664331
H	-1.588297	-1.874858	-1.935659
O	-1.858233	1.554311	2.482714
C	3.398841	0.050255	2.206607
H	4.172868	0.764992	1.909741
H	2.602789	0.605635	2.718471
H	3.843874	-0.647860	2.927263
C	4.120140	0.437048	-0.927108
H	4.598400	1.063616	-0.168032
H	4.910958	-0.077836	-1.488127

H	3.595864	1.101283	-1.625836
C	2.458958	-1.638487	-2.571539
H	2.549176	-0.660574	-3.057659
H	3.331161	-2.238864	-2.864857
H	1.564629	-2.125350	-2.974782
C	0.733549	-3.419697	-0.508655
H	0.419603	-3.428390	-1.557329
H	1.291489	-4.346919	-0.322039
H	-0.171778	-3.441243	0.105196
C	1.157784	-2.137833	2.398703
H	0.174882	-2.586438	2.220967
H	1.790594	-2.885903	2.896148
H	1.016253	-1.300522	3.091635
C	1.450479	2.983462	1.546058
H	0.727975	3.703336	1.135864
H	2.024176	3.452517	2.351671
H	2.135798	2.670270	0.740480
N	-1.843596	0.098479	0.681847
C	-4.322961	0.273567	1.134856
H	-4.227969	0.931976	1.992404
C	-4.505489	-1.459333	-1.113124
H	-4.583622	-2.122568	-1.972665
C	-5.641524	-1.028574	-0.444669
H	-6.621142	-1.359820	-0.782941
C	-5.550197	-0.172069	0.663166
H	-6.460370	0.147992	1.165675

TS1(2OAc)
SCF done: -1373.671548

Rh	0.892302	-0.227696	-0.122311
N	0.257892	1.465684	0.919079
C	0.294876	-2.182468	0.589244
C	1.157589	-2.384812	-0.560766
C	2.423676	-1.816895	-0.249827
C	2.366567	-1.257433	1.083859
C	1.060682	-1.533404	1.614843
O	2.121478	1.143626	-1.259184
O	0.363647	2.085777	-2.285089
C	1.589301	2.013219	-2.009840
C	2.503819	3.060952	-2.585831
H	2.078572	3.489147	-3.495626
H	2.609825	3.861896	-1.844503
H	3.496525	2.646464	-2.775977
O	1.016695	1.855484	2.016247
C	-1.080695	1.470227	1.203795

C	-1.059879	0.310240	-0.985442
C	-3.087954	0.499918	0.053547
C	-1.986478	-0.393044	-1.737235
H	-0.296774	1.131954	-1.626539
C	-3.263616	-0.282157	-1.120171
H	-1.773551	-0.881559	-2.682859
O	-1.666895	1.909514	2.173327
C	0.584357	-1.161324	2.972762
H	0.945638	-0.166562	3.254170
H	-0.508548	-1.140811	3.027836
H	0.947026	-1.884972	3.714502
C	3.462154	-0.539644	1.789124
H	3.045531	0.242168	2.436592
H	4.062847	-1.216786	2.411307
H	4.132671	-0.054931	1.070778
C	3.605064	-1.711285	-1.146636
H	3.842725	-0.656780	-1.334505
H	4.482914	-2.182618	-0.687653
H	3.426289	-2.193188	-2.111766
C	0.775970	-3.099471	-1.810189
H	1.376431	-2.770399	-2.664081
H	0.911109	-4.184152	-1.702589
H	-0.274699	-2.921041	-2.060728
C	-1.101822	-2.676149	0.733012
H	-1.601151	-2.754644	-0.237055
H	-1.114894	-3.665672	1.208590
H	-1.704027	-1.999371	1.349158
C	1.895733	2.887784	1.612742
H	1.333364	3.766659	1.269609
H	2.484577	3.149080	2.497828
H	2.560456	2.545440	0.806038
N	-1.761639	0.852934	0.114759
C	-4.543430	-0.767190	-1.440620
H	-4.697431	-1.357005	-2.342091
C	-4.151606	0.790553	0.916244
H	-3.985565	1.390222	1.804628
C	-5.592843	-0.480296	-0.592061
H	-6.590676	-0.847213	-0.821427
C	-5.393430	0.288819	0.573281
H	-6.244171	0.498636	1.218076

IN4(2OAc)

SCF done: -1144.705687

Rh	0.866073	-0.057370	-0.001769
N	0.018298	1.702212	0.140896

C	2.414818	-0.864941	1.246600
C	1.896515	-1.940974	0.431630
C	2.128842	-1.583873	-0.919517
C	2.881504	-0.328764	-0.934513
C	3.087897	0.091122	0.394846
O	0.716746	2.872658	0.379864
C	-1.363357	1.858381	0.198292
C	-1.098284	-0.533485	-0.001978
C	-3.264270	0.205538	0.038176
C	-1.904835	-1.637276	-0.125546
C	-3.276701	-1.203331	-0.105369
H	-1.563816	-2.663112	-0.224001
O	-1.985392	2.895086	0.293845
C	3.748073	1.340853	0.872467
H	4.318622	1.821377	0.071516
H	3.005365	2.067753	1.228816
H	4.444647	1.131553	1.693160
C	3.316828	0.356147	-2.180604
H	3.710313	1.356809	-1.978945
H	4.099942	-0.222124	-2.689435
H	2.481028	0.461220	-2.882426
C	1.748811	-2.358335	-2.132001
H	1.498501	-1.691932	-2.964210
H	2.569616	-3.010033	-2.461350
H	0.871237	-2.985103	-1.944038
C	1.229167	-3.169442	0.944571
H	0.647555	-3.663411	0.159587
H	1.966294	-3.893489	1.315823
H	0.540427	-2.937888	1.764233
C	2.366514	-0.791570	2.729087
H	1.513333	-1.346497	3.130859
H	3.281782	-1.218308	3.163583
H	2.286503	0.246003	3.070074
C	0.970248	3.543706	-0.838648
H	0.033194	3.856579	-1.316153
H	1.565735	4.425263	-0.583819
H	1.538996	2.897208	-1.527502
N	-1.929370	0.583030	0.103053
C	-4.426010	0.965019	0.091573
H	-4.373210	2.043512	0.201636
C	-4.506352	-1.863711	-0.194080
H	-4.544420	-2.945875	-0.304599
C	-5.673370	-1.115591	-0.141473
H	-6.637167	-1.615423	-0.210761

C	-5.632141	0.278973	-0.001217
H	-6.564461	0.838247	0.036471

IN1(ClOAc)
SCF done: -1389.259355

N	0.330498	-0.526803	-1.637592
C	-3.191335	0.378861	0.902730
C	-2.980938	-0.942271	0.388277
C	-1.885637	-1.534236	1.121917
C	-1.356467	-0.555154	2.011680
C	-2.157413	0.644806	1.867699
O	1.316181	1.999942	-1.407307
O	0.405186	1.538728	0.593221
C	1.160179	2.220379	-0.201882
C	1.926937	3.325183	0.483280
H	1.232030	4.034811	0.944235
H	2.537713	2.894372	1.284827
H	2.570119	3.840889	-0.232722
Rh	-1.219331	0.294461	0.002064
C	0.964530	-1.674243	-1.118849
O	0.566815	-2.794104	-1.357139
O	-0.090433	-0.744921	-2.952863
H	0.823897	0.406040	-1.625591
C	-1.464426	-2.949957	0.977557
H	-0.692286	-3.216040	1.705262
H	-2.327198	-3.606116	1.149320
H	-1.074947	-3.167931	-0.026062
C	-0.185668	-0.669311	2.919856
H	-0.482875	-0.524128	3.966214
H	0.306386	-1.642038	2.831005
H	0.558169	0.097801	2.664397
C	-1.937879	1.902002	2.624468
H	-2.232530	1.777787	3.674815
H	-0.878279	2.177498	2.588233
H	-2.512768	2.729222	2.199172
C	-4.292947	1.292472	0.514183
H	-5.195130	1.037437	1.086901
H	-4.039203	2.337219	0.709935
H	-4.517117	1.211885	-0.552633
C	-3.860250	-1.650694	-0.579159
H	-4.707904	-2.120436	-0.061272
H	-4.266896	-0.959779	-1.325211
H	-3.317992	-2.438974	-1.111426
C	-1.412745	-1.243495	-3.042521
H	-2.124157	-0.527939	-2.611223

H	-1.596532	-1.336924	-4.115963
H	-1.497514	-2.230805	-2.570514
N	1.994986	-1.449072	-0.195769
C	2.148025	-2.305175	0.898780
C	3.088270	-0.564708	-0.206834
C	3.226913	-1.936986	1.629805
H	1.439723	-3.112240	1.028593
C	3.852027	-0.835891	0.949357
H	3.567890	-2.408979	2.542480
C	5.028565	-0.115962	1.182666
H	5.622674	-0.311684	2.072724
C	3.526261	0.325530	-1.182841
H	2.979713	0.492365	-2.104225
C	5.434671	0.818769	0.245052
H	6.349487	1.384045	0.406982
C	4.698614	1.022527	-0.930698
H	5.054334	1.735341	-1.670361
Cl	-1.914412	1.900932	-1.637746

TS1(ClOAc)
SCF done: -1389.257270

N	0.145083	-0.267894	-1.769576
C	-2.545931	-0.296683	1.723972
C	-2.258094	-1.513467	0.998713
C	-0.869146	-1.826611	1.198502
C	-0.273309	-0.774184	1.970512
C	-1.322022	0.161706	2.306675
O	0.278871	2.216102	-1.983292
O	-0.273488	2.093682	0.181078
C	-0.105323	2.736052	-0.901195
C	-0.394015	4.206175	-0.878668
H	-1.473404	4.317062	-1.038062
H	-0.151439	4.637039	0.095834
H	0.134241	4.723031	-1.682353
Rh	-1.115898	0.102473	0.154262
C	1.112205	-1.293619	-1.727346
O	0.978326	-2.342720	-2.321737
O	-0.609003	-0.414971	-2.949327
H	0.366405	0.897294	-1.840715
C	-0.214096	-3.062907	0.698666
H	0.847725	-3.090530	0.957899
H	-0.699065	-3.940602	1.144653
H	-0.295641	-3.160094	-0.392270
C	1.129863	-0.652880	2.445729
H	1.191991	-0.868360	3.521073

H	1.807825	-1.334609	1.922976
H	1.503737	0.366368	2.285574
C	-1.113824	1.408706	3.085129
H	-0.561574	1.195962	4.008168
H	-0.529893	2.123301	2.489943
H	-2.062226	1.882795	3.350580
C	-3.885243	0.327249	1.861842
H	-4.440344	-0.160152	2.674819
H	-3.808696	1.395455	2.082241
H	-4.455826	0.233362	0.933844
C	-3.260962	-2.364746	0.306105
H	-3.807787	-2.981685	1.032112
H	-3.991056	-1.751973	-0.233063
H	-2.784203	-3.036542	-0.414671
C	-1.640533	-1.382363	-2.881503
H	-2.316394	-1.166516	-2.045281
H	-2.195243	-1.248755	-3.814171
H	-1.240860	-2.401340	-2.831175
N	2.232811	-1.148318	-0.873373
C	2.875065	-2.325299	-0.462106
C	2.944319	-0.067432	-0.318961
C	3.900694	-2.039360	0.373500
H	2.509021	-3.268351	-0.841446
C	3.971871	-0.610813	0.487620
H	4.558165	-2.759983	0.842879
C	4.828077	0.237991	1.194492
H	5.611740	-0.178408	1.824045
C	2.829903	1.305527	-0.504251
H	2.119397	1.733029	-1.198973
C	4.670990	1.607555	1.062028
H	5.328427	2.284116	1.603012
C	3.693555	2.129314	0.205397
H	3.613855	3.206250	0.075456
Cl	-2.861803	1.163460	-1.166880

IN2(ClOAc)
SCF done: -1389.270070

N	-0.119758	-0.105486	1.624215
C	2.271217	-0.638902	-1.894859
C	2.033093	-1.753317	-0.998707
C	0.620238	-2.027503	-0.986151
C	-0.026130	-1.063237	-1.829916
C	1.002483	-0.200072	-2.366266
O	0.847880	2.770596	1.903079
O	0.598375	2.162708	-0.262353

C	0.643189	3.004626	0.637462
C	0.411464	4.453922	0.349249
H	1.283752	5.034192	0.664747
H	0.221903	4.604021	-0.713937
H	-0.442180	4.805121	0.938173
Rh	1.040174	-0.057734	-0.184826
C	-1.115477	-0.983110	1.954177
O	-1.167355	-1.733002	2.915167
O	0.644355	0.200357	2.769277
H	1.027440	1.815759	2.115756
C	-0.019061	-3.156710	-0.256825
H	-1.104286	-3.148792	-0.390188
H	0.366880	-4.113751	-0.629648
H	0.180090	-3.111723	0.822117
C	-1.442517	-1.034397	-2.273574
H	-1.506210	-1.415208	-3.302644
H	-2.095170	-1.648393	-1.646113
H	-1.843051	-0.014543	-2.274251
C	0.720174	0.980516	-3.220864
H	-0.108801	1.560384	-2.797129
H	1.587072	1.642886	-3.290949
H	0.435829	0.667427	-4.233884
C	3.605873	-0.099445	-2.259489
H	4.110812	-0.784552	-2.953454
H	3.522890	0.876508	-2.746492
H	4.230870	0.028373	-1.370120
C	3.086422	-2.535654	-0.301588
H	3.655120	-3.132616	-1.027189
H	3.783179	-1.868028	0.217988
H	2.651112	-3.217816	0.435005
C	1.517603	-0.835320	3.213828
H	2.056241	-1.272264	2.362954
H	2.247158	-0.343589	3.863162
H	0.954097	-1.597193	3.756851
N	-2.219123	-0.983970	1.040461
C	-3.052086	-2.091584	0.945730
C	-2.817886	0.061825	0.338846
C	-4.121270	-1.813828	0.151364
H	-2.786960	-2.984226	1.497111
C	-4.002723	-0.441166	-0.249457
H	-4.918713	-2.499034	-0.106551
C	-4.775608	0.399938	-1.059160
H	-5.683119	0.026064	-1.529328
C	-2.435678	1.392026	0.194923

H	-1.554858	1.754028	0.707418
C	-4.371002	1.711977	-1.244333
H	-4.961947	2.375214	-1.872183
C	-3.218663	2.205228	-0.610492
H	-2.938455	3.248670	-0.743993
Cl	3.101509	0.736306	0.935674

IN3(ClOAc)
SCF done: -1160.278451

N	0.027258	1.530339	-0.976257
C	2.434183	-1.355047	0.840355
C	2.191063	-0.076964	1.481198
C	0.815225	-0.029952	1.925148
C	0.197936	-1.231206	1.487503
C	1.196031	-2.036808	0.788091
Rh	1.008711	-0.126495	-0.265946
C	-0.929921	2.205555	-0.263531
O	-0.949493	3.385738	0.034845
O	0.732715	2.413653	-1.788964
C	0.213901	1.085886	2.706456
H	-0.857077	0.931751	2.867232
H	0.697445	1.174033	3.687805
H	0.329958	2.049681	2.191792
C	-1.180684	-1.703762	1.758411
H	-1.135718	-2.519198	2.494269
H	-1.824685	-0.916542	2.160104
H	-1.658679	-2.103316	0.856412
C	0.903269	-3.342154	0.142627
H	-0.047434	-3.294626	-0.401461
H	1.681978	-3.617925	-0.573419
H	0.819280	-4.140350	0.892373
C	3.738553	-1.799006	0.284145
H	4.393668	-2.161288	1.086971
H	3.609673	-2.601231	-0.446651
H	4.247538	-0.978954	-0.232684
C	3.213778	0.962070	1.758716
H	3.651484	0.797954	2.753686
H	4.027142	0.932834	1.027130
H	2.776719	1.965625	1.747601
C	1.844907	2.978120	-1.133062
H	2.611228	2.210827	-0.931115
H	2.259681	3.714142	-1.827487
H	1.545081	3.482891	-0.203787
N	-2.006259	1.360964	0.141167
C	-2.858789	1.745230	1.167016

C	-2.522392	0.198818	-0.443726
C	-3.872879	0.849112	1.297302
H	-2.644251	2.664876	1.695530
C	-3.688161	-0.148453	0.281420
H	-4.678528	0.897665	2.018841
C	-4.394498	-1.307938	-0.058646
H	-5.286702	-1.587737	0.498277
C	-2.084360	-0.561731	-1.530877
H	-1.219518	-0.265425	-2.116480
C	-3.942603	-2.084065	-1.113220
H	-4.482457	-2.986767	-1.390565
C	-2.806588	-1.705260	-1.845756
H	-2.487430	-2.310501	-2.691374
Cl	1.944647	-0.478531	-2.382017

TS2(ClOAc)
SCF done: - -1160.245376

Rh	0.900622	-0.076475	-0.044422
N	0.017800	1.737805	-0.052306
C	1.909339	-0.461149	1.760408
C	1.645822	-1.747994	1.133440
C	2.330673	-1.767151	-0.104746
C	3.089568	-0.524916	-0.217270
C	2.875826	0.249256	0.944238
O	0.718156	2.878655	0.296426
C	-1.339546	1.883570	0.081470
C	-1.127622	-0.534778	-0.222142
C	-3.251800	0.241885	0.068197
C	-1.968138	-1.633035	-0.199254
H	-0.537760	-0.559613	-1.609031
C	-3.309951	-1.172102	-0.033914
H	-1.655060	-2.661866	-0.347986
O	-1.981689	2.896607	0.266225
C	3.448534	1.578638	1.286225
H	2.650851	2.324681	1.396855
H	4.008506	1.529088	2.228677
H	4.133098	1.934437	0.509987
C	3.905350	-0.162332	-1.406363
H	4.343502	0.835040	-1.307537
H	4.720745	-0.883036	-1.550957
H	3.289487	-0.171968	-2.314185
C	2.326420	-2.852514	-1.122405
H	3.176818	-3.533245	-0.982109
H	1.406938	-3.445742	-1.069201
H	2.382902	-2.438559	-2.134182

C	0.803860	-2.824976	1.721306
H	0.506423	-3.559685	0.966854
H	1.356485	-3.358429	2.505761
H	-0.109663	-2.418227	2.167193
C	1.419693	-0.006996	3.087683
H	0.494822	-0.519591	3.369531
H	2.169177	-0.206458	3.866370
H	1.221046	1.070543	3.080108
C	1.272936	3.447141	-0.875007
H	0.480422	3.778781	-1.557928
H	1.869599	4.305030	-0.549063
H	1.915487	2.717618	-1.394980
N	-1.926988	0.601765	-0.051481
C	-4.554302	-1.816168	0.041655
H	-4.620027	-2.899073	-0.041252
C	-4.393973	1.022692	0.254015
H	-4.312721	2.102000	0.330444
C	-5.687668	-1.048094	0.226800
H	-6.661478	-1.527947	0.291817
C	-5.603993	0.353389	0.332287
H	-6.516845	0.927163	0.476672
Cl	0.263861	-0.342638	-2.861606

IN4(ClOAc)
SCF done: -1160.256841

C	-6.054100	-3.975200	0.006100
Rh	0.967540	-0.064256	0.260033
N	0.114937	1.674148	0.506780
C	2.220380	-1.677213	0.985842
C	2.008265	-1.883928	-0.402371
C	2.540855	-0.733395	-1.093303
C	3.177707	0.136799	-0.134549
C	2.951048	-0.418695	1.145073
O	0.817596	2.857103	0.625237
C	-1.265755	1.822547	0.610130
C	-1.005877	-0.561690	0.307681
C	-3.170013	0.172557	0.476894
C	-1.824202	-1.657874	0.158659
H	-0.990728	-0.338937	-1.813062
C	-3.192638	-1.226728	0.264309
H	-1.492443	-2.675057	-0.025178
O	-1.889403	2.852194	0.749830
C	3.358230	0.198628	2.434648
H	3.184957	1.280902	2.417775
H	2.797981	-0.216003	3.277685

H	4.426479	0.031390	2.627396
C	3.894116	1.410326	-0.422343
H	3.678688	2.167072	0.340280
H	4.981235	1.258257	-0.446185
H	3.598792	1.828030	-1.390146
C	2.506330	-0.519755	-2.562060
H	2.427355	0.544023	-2.810034
H	3.425516	-0.907473	-3.022923
H	1.653155	-1.024209	-3.025735
C	1.348560	-3.051487	-1.051596
H	0.698098	-2.740857	-1.877400
H	2.091335	-3.750220	-1.457948
H	0.729649	-3.606607	-0.339079
C	1.813448	-2.581768	2.094340
H	0.940178	-3.179774	1.815877
H	2.626185	-3.268345	2.366434
H	1.540508	-2.013251	2.989461
C	0.862157	3.514738	-0.630881
H	-0.135624	3.854543	-0.933907
H	1.523933	4.375817	-0.501419
H	1.269443	2.838713	-1.400547
N	-1.833609	0.546707	0.504797
C	-4.425653	-1.883982	0.192370
H	-4.469298	-2.958967	0.028884
C	-4.327907	0.928756	0.616459
H	-4.269483	2.000757	0.774202
C	-5.586652	-1.139780	0.331041
H	-6.553734	-1.634544	0.275951
C	-5.536076	0.246949	0.539097
H	-6.465489	0.802830	0.641050
Cl	-1.072282	0.143121	-3.026539

TS1(OAcCl)
SCF done: -1389.215134

N	-0.400737	1.114175	0.917230
C	2.562820	-1.526777	-0.884842
C	2.243744	-1.715614	0.510637
C	0.863896	-2.160022	0.605309
C	0.304267	-2.124883	-0.698463
C	1.365815	-1.742541	-1.621740
Rh	1.037157	-0.122883	-0.217873
C	-1.210768	0.397000	1.794130
O	-0.993915	0.165116	2.970749
O	0.190002	2.195711	1.588733
H	-0.721961	1.483178	-0.779943

C	0.230437	-2.599140	1.874205
H	-0.741564	-3.065727	1.693345
H	0.872776	-3.339123	2.366773
H	0.085994	-1.763741	2.575362
C	-1.088227	-2.450938	-1.107876
H	-1.112010	-3.385778	-1.683126
H	-1.756712	-2.556397	-0.247493
H	-1.505437	-1.657561	-1.740014
C	1.223426	-1.619674	-3.094962
H	1.636644	-2.511832	-3.584628
H	0.176812	-1.519553	-3.393635
H	1.767415	-0.747829	-3.472868
C	3.893105	-1.168979	-1.441977
H	4.483112	-2.077490	-1.622747
H	3.792554	-0.641459	-2.396236
H	4.436864	-0.516130	-0.752523
C	3.192382	-1.624580	1.645463
H	3.813423	-2.530518	1.687132
H	3.837334	-0.748796	1.519015
H	2.659659	-1.531110	2.597437
O	3.965657	1.212697	0.586797
O	2.025937	1.658423	-0.471563
C	3.209891	1.953982	-0.041264
C	3.585477	3.386691	-0.345858
H	3.377359	3.625335	-1.392790
H	2.955998	4.046319	0.262537
H	4.636701	3.566484	-0.111485
C	1.226387	1.870368	2.502230
H	1.914999	1.130552	2.068189
H	1.778307	2.804458	2.653915
H	0.833179	1.499762	3.453846
N	-2.377459	-0.141631	1.193708
C	-2.961419	-1.312994	1.674123
C	-3.264214	0.429104	0.270167
C	-4.118402	-1.567086	1.011690
H	-2.475099	-1.843852	2.480667
C	-4.342247	-0.471043	0.110121
H	-4.768979	-2.418077	1.168832
C	-5.396372	-0.140331	-0.748988
H	-6.226189	-0.830275	-0.887838
C	-3.279534	1.693073	-0.315822
H	-2.502121	2.422345	-0.108299
C	-5.379676	1.089243	-1.384678
H	-6.195149	1.365651	-2.048939

C	-4.341343	2.002685	-1.151132
H	-4.371296	2.980730	-1.625048
Cl	-0.619141	1.296561	-2.118371

IN2(OAcCl)
SCF done: -1389.241364

N	0.075480	-1.343380	-1.232773
C	-1.727171	0.500702	2.060509
C	-1.489031	-0.930168	2.048260
C	-0.054024	-1.156681	2.110150
C	0.569990	0.116469	2.120145
C	-0.468982	1.143047	2.064906
Rh	-0.635882	-0.154335	0.286044
C	1.259895	-2.011865	-1.319285
O	1.471562	-3.116109	-1.784002
O	-0.883009	-1.865670	-2.095596
H	-1.568898	2.271920	-1.307185
C	0.618989	-2.483286	2.156629
H	1.632835	-2.427817	1.744268
H	0.690209	-2.851854	3.187838
H	0.068169	-3.225664	1.568609
C	2.009780	0.418105	2.295415
H	2.189972	0.645867	3.355991
H	2.656200	-0.419456	2.016572
H	2.314171	1.295497	1.715723
C	-0.188905	2.601138	2.047240
H	0.250944	2.908628	3.005810
H	0.524543	2.860045	1.254483
H	-1.094390	3.188670	1.877288
C	-3.067145	1.140669	1.983896
H	-3.486149	1.285008	2.988151
H	-3.012432	2.118067	1.493384
H	-3.751766	0.516917	1.401572
C	-2.561656	-1.953312	2.059593
H	-3.151924	-1.859920	2.981406
H	-3.233375	-1.791612	1.205848
H	-2.158195	-2.968705	2.013345
O	-3.549259	-0.712586	-0.720782
O	-1.857555	0.683967	-1.183575
C	-3.020531	0.135231	-1.429893
C	-3.646749	0.628145	-2.706946
H	-3.535107	1.712483	-2.810498
H	-3.111319	0.163916	-3.543021
H	-4.700045	0.345911	-2.751465
C	-1.491797	-3.036508	-1.576162

H	-1.927919	-2.836701	-0.586977
H	-2.302358	-3.279426	-2.268701
H	-0.773650	-3.862722	-1.525596
N	2.350910	-1.249843	-0.790209
C	3.511498	-1.875762	-0.358244
C	2.583580	0.127424	-0.823349
C	4.462251	-0.949979	-0.059804
H	3.533411	-2.957402	-0.333546
C	3.901966	0.338374	-0.349431
H	5.458435	-1.154029	0.311427
C	4.389290	1.644609	-0.224216
H	5.398342	1.817677	0.145174
C	1.772534	1.194169	-1.222901
H	0.789437	1.037383	-1.661814
C	3.572258	2.705319	-0.581381
H	3.939892	3.725056	-0.491952
C	2.281462	2.479531	-1.084642
H	1.658895	3.319932	-1.385556
Cl	-1.319230	3.585347	-1.253116

IN3(OAcCl)
SCF done: -1373.695679

Rh	1.226783	-0.150036	-0.085913
N	0.195804	1.576382	0.532768
C	0.161542	-2.022470	0.035184
C	1.476246	-2.269090	-0.540946
C	2.454093	-1.874429	0.404356
C	1.755728	-1.352667	1.573151
C	0.346236	-1.523007	1.364947
O	2.842445	1.264822	-0.545156
O	1.399008	0.771714	-2.116562
C	2.381371	1.459693	-1.709111
C	2.964586	2.530661	-2.576538
H	2.847005	2.277366	-3.632725
H	2.420388	3.463611	-2.389598
H	4.016488	2.695952	-2.332350
O	0.928061	2.019991	1.653826
C	-1.134019	1.524739	0.868819
O	-1.641188	1.846318	1.929628
C	-0.707468	-1.208728	2.364855
H	-0.568203	-0.220154	2.818049
H	-1.708481	-1.221836	1.922022
H	-0.680979	-1.955954	3.168763
C	2.381642	-0.786130	2.796485
H	1.873239	0.142127	3.081617

H	2.319112	-1.492296	3.635012
H	3.435955	-0.547655	2.626531
C	3.932153	-1.876959	0.242568
H	4.343694	-0.876134	0.418851
H	4.398689	-2.566912	0.957064
H	4.226806	-2.182626	-0.765302
C	1.688011	-2.781301	-1.919903
H	2.736186	-2.712328	-2.223714
H	1.376418	-3.831048	-1.997240
H	1.094873	-2.201407	-2.636673
C	-1.121416	-2.367448	-0.630766
H	-1.164658	-1.957035	-1.646471
H	-1.231594	-3.457946	-0.700804
H	-1.986049	-1.970897	-0.089292
C	1.261358	3.378532	1.479056
H	0.358444	4.005613	1.462794
H	1.876524	3.655380	2.340890
H	1.836666	3.526699	0.554665
N	-1.946502	1.048420	-0.200059
C	-3.213804	0.489986	-0.035710
C	-1.634376	1.031515	-1.556543
C	-3.674134	0.102987	-1.317061
C	-2.656602	0.472375	-2.259025
H	-0.684697	1.422666	-1.897298
H	-2.692064	0.349669	-3.334289
C	-3.962838	0.257618	1.119432
H	-3.601995	0.596580	2.084902
C	-4.912677	-0.537530	-1.435509
H	-5.280711	-0.842024	-2.413594
C	-5.655796	-0.779218	-0.291837
H	-6.620362	-1.276246	-0.370314
C	-5.184005	-0.384433	0.969329
H	-5.792628	-0.576086	1.850338

TS2(OAcCl)
SCF done: -1373.671548

Rh	0.892302	-0.227696	-0.122311
N	0.257892	1.465684	0.919079
C	0.294876	-2.182468	0.589244
C	1.157589	-2.384812	-0.560766
C	2.423676	-1.816895	-0.249827
C	2.366567	-1.257433	1.083859
C	1.060682	-1.533404	1.614843
O	2.121478	1.143626	-1.259184
O	0.363647	2.085777	-2.285089

C	1.589301	2.013219	-2.009840
C	2.503819	3.060952	-2.585831
H	2.078572	3.489147	-3.495626
H	2.609825	3.861896	-1.844503
H	3.496525	2.646464	-2.775977
O	1.016695	1.855484	2.016247
C	-1.080695	1.470227	1.203795
C	-1.059879	0.310240	-0.985442
C	-3.087954	0.499918	0.053547
C	-1.986478	-0.393044	-1.737235
H	-0.296774	1.131954	-1.626539
C	-3.263616	-0.282157	-1.120171
H	-1.773551	-0.881559	-2.682859
O	-1.666895	1.909514	2.173327
C	0.584357	-1.161324	2.972762
H	0.945638	-0.166562	3.254170
H	-0.508548	-1.140811	3.027836
H	0.947026	-1.884972	3.714502
C	3.462154	-0.539644	1.789124
H	3.045531	0.242168	2.436592
H	4.062847	-1.216786	2.411307
H	4.132671	-0.054931	1.070778
C	3.605064	-1.711285	-1.146636
H	3.842725	-0.656780	-1.334505
H	4.482914	-2.182618	-0.687653
H	3.426289	-2.193188	-2.111766
C	0.775970	-3.099471	-1.810189
H	1.376431	-2.770399	-2.664081
H	0.911109	-4.184152	-1.702589
H	-0.274699	-2.921041	-2.060728
C	-1.101822	-2.676149	0.733012
H	-1.601151	-2.754644	-0.237055
H	-1.114894	-3.665672	1.208590
H	-1.704027	-1.999371	1.349158
C	1.895733	2.887784	1.612742
H	1.333364	3.766659	1.269609
H	2.484577	3.149080	2.497828
H	2.560456	2.545440	0.806038
N	-1.761639	0.852934	0.114759
C	-4.543430	-0.767190	-1.440620
H	-4.697431	-1.357005	-2.342091
C	-4.151606	0.790553	0.916244
H	-3.985565	1.390222	1.804628
C	-5.592843	-0.480296	-0.592061

H	-6.590676	-0.847213	-0.821427
C	-5.393430	0.288819	0.573281
H	-6.244171	0.498636	1.218076

IN4(OAcCl)
SCF done: -1373.693313

Rh	0.921100	-0.169142	-0.074526
N	0.032188	1.249168	1.136806
C	1.772248	-1.666252	1.127726
C	1.585256	-2.241158	-0.193004
C	2.373343	-1.483676	-1.093452
C	3.172953	-0.535714	-0.317619
C	2.849026	-0.684424	1.037824
O	0.917392	1.529320	-1.698500
O	-1.284235	1.747738	-2.108821
C	-0.044367	2.183794	-2.088111
C	0.083026	3.586694	-2.585849
H	-0.470053	3.714829	-3.520079
H	-0.367028	4.258202	-1.846338
H	1.133941	3.845518	-2.717916
O	0.793076	1.877946	2.118516
C	-1.256908	1.038545	1.562620
C	-1.058435	-0.558592	-0.259196
C	-3.188841	-0.165134	0.457403
C	-1.896456	-1.251821	-1.101512
H	-1.328422	0.826671	-1.750210
C	-3.253661	-1.024997	-0.664331
H	-1.588297	-1.874858	-1.935659
O	-1.858233	1.554311	2.482714
C	3.398841	0.050255	2.206607
H	4.172868	0.764992	1.909741
H	2.602789	0.605635	2.718471
H	3.843874	-0.647860	2.927263
C	4.120140	0.437048	-0.927108
H	4.598400	1.063616	-0.168032
H	4.910958	-0.077836	-1.488127
H	3.595864	1.101283	-1.625836
C	2.458958	-1.638487	-2.571539
H	2.549176	-0.660574	-3.057659
H	3.331161	-2.238864	-2.864857
H	1.564629	-2.125350	-2.974782
C	0.733549	-3.419697	-0.508655
H	0.419603	-3.428390	-1.557329
H	1.291489	-4.346919	-0.322039
H	-0.171778	-3.441243	0.105196

C	1.157784	-2.137833	2.398703
H	0.174882	-2.586438	2.220967
H	1.790594	-2.885903	2.896148
H	1.016253	-1.300522	3.091635
C	1.450479	2.983462	1.546058
H	0.727975	3.703336	1.135864
H	2.024176	3.452517	2.351671
H	2.135798	2.670270	0.740480
N	-1.843596	0.098479	0.681847
C	-4.322961	0.273567	1.134856
H	-4.227969	0.931976	1.992404
C	-4.505489	-1.459333	-1.113124
H	-4.583622	-2.122568	-1.972665
C	-5.641524	-1.028574	-0.444669
H	-6.621142	-1.359820	-0.782941
C	-5.550197	-0.172069	0.663166
H	-6.460370	0.147992	1.165675

IN6
SCF done: -1732.617316

Rh	-1.039700	0.636968	0.081290
N	0.258078	-0.114492	1.519820
C	-1.901108	2.291240	1.042629
C	-2.001672	2.551269	-0.380974
C	-2.824724	1.539949	-0.936897
C	-3.367028	0.740084	0.161279
C	-2.847073	1.227026	1.366708
O	-0.228546	-0.424594	2.787735
C	1.524594	0.409134	1.595588
C	0.779730	1.221381	-0.568385
C	3.014225	1.426182	-0.174443
C	1.336204	1.689553	-1.727739
C	2.755965	1.827882	-1.507808
H	0.802963	1.909959	-2.646651
O	2.339976	0.303021	2.492442
C	-3.136612	0.754895	2.744898
H	-3.781441	-0.129579	2.743124
H	-2.205564	0.499129	3.263889
H	-3.644111	1.539503	3.321672
C	-4.351586	-0.368346	0.007496
H	-4.241057	-1.117769	0.799042
H	-5.378756	0.017023	0.058090
H	-4.242960	-0.882993	-0.951897
C	-3.200626	1.393734	-2.370103
H	-3.296949	0.340909	-2.651648

H	-4.161425	1.883208	-2.580674
H	-2.447079	1.841590	-3.026557
C	-1.374294	3.694437	-1.097622
H	-1.220104	3.477239	-2.159144
H	-2.021769	4.578943	-1.029267
H	-0.399304	3.953143	-0.674607
C	-1.172242	3.116141	2.045261
H	-0.307035	3.615746	1.596708
H	-1.827177	3.888051	2.472511
H	-0.802831	2.493087	2.866923
C	-0.422364	-1.813548	2.884534
H	0.524706	-2.352335	2.731321
H	-0.799720	-2.004943	3.894452
H	-1.167393	-2.163787	2.147407
N	1.789108	1.072126	0.378397
C	4.293349	1.413721	0.374748
H	4.441773	1.102303	1.404860
C	3.829431	2.237182	-2.306165
H	3.661645	2.554125	-3.333995
C	5.109337	2.224641	-1.770493
H	5.951573	2.537075	-2.384480
C	5.338994	1.815381	-0.448554
H	6.353931	1.819391	-0.056863
C	-0.230496	-2.536735	-0.947276
C	-2.141691	-3.011347	-1.903140
O	-0.984006	-3.561080	-1.416776
O	-3.059927	-3.592461	-2.378914
O	-2.027456	-1.675294	-1.732127
N	-0.819071	-1.387955	-1.070874
C	1.067546	-2.821970	-0.375753
C	2.100727	-1.888632	-0.494192
C	1.263543	-4.024906	0.313283
C	3.316415	-2.135793	0.127318
H	1.944876	-0.983322	-1.077275
C	2.484204	-4.262984	0.926938
H	0.456118	-4.749954	0.383012
C	3.501872	-3.314027	0.845349
H	4.113836	-1.400016	0.047852
H	2.642214	-5.187448	1.476101
H	4.452704	-3.499569	1.338842

TS2

SCF done: -1732.581092

Rh	1.139567	-0.473332	-0.173265
N	0.522311	0.434855	1.597172

C	1.749119	-2.650911	-0.355154
C	2.084520	-1.971866	-1.577660
C	3.057977	-0.965077	-1.264961
C	3.299369	-0.993332	0.148673
C	2.473618	-2.030815	0.714322
O	1.460471	0.649192	2.588384
C	-0.702672	0.080893	2.119823
C	-0.802952	-1.043656	-0.028484
C	-2.784517	-0.887220	1.060374
C	-1.721170	-1.663609	-0.827502
C	-2.995485	-1.569443	-0.161532
H	-1.543045	-2.077138	-1.815219
O	-1.144541	0.338550	3.220591
C	2.413353	-2.397331	2.154880
H	3.247564	-3.055924	2.428637
H	2.457368	-1.500754	2.782206
H	1.478681	-2.916418	2.392123
C	4.234332	-0.114703	0.901086
H	3.837488	0.099829	1.899514
H	5.216073	-0.592160	1.021741
H	4.377593	0.840952	0.386337
C	3.695745	-0.035712	-2.235098
H	3.147318	-0.011180	-3.181730
H	3.728561	0.985696	-1.842423
H	4.723326	-0.356413	-2.449963
C	1.564305	-2.291410	-2.936821
H	1.300341	-1.378881	-3.484136
H	2.308832	-2.834156	-3.533938
H	0.666704	-2.915489	-2.881610
C	0.864398	-3.838782	-0.235275
H	-0.008351	-3.766307	-0.891208
H	1.421559	-4.746366	-0.501953
H	0.490295	-3.958846	0.785449
C	1.824293	2.020958	2.649230
H	0.928681	2.653308	2.683722
H	2.392890	2.137409	3.576407
H	2.452017	2.303894	1.794255
N	-1.428887	-0.594177	1.122924
C	-3.816236	-0.574772	1.939686
H	-3.605904	-0.055679	2.869894
C	-4.298447	-1.941486	-0.509251
H	-4.492389	-2.458727	-1.447614
C	-5.336855	-1.625813	0.354374
H	-6.355574	-1.906668	0.094809

C	-5.098562	-0.951500	1.562193
H	-5.935232	-0.722340	2.218481
C	-0.095911	2.161048	-0.893563
C	1.715579	3.511340	-0.234340
O	0.228400	3.345195	-0.475120
O	2.009386	4.549181	0.284059
O	2.320095	2.491768	-0.641983
N	0.749416	1.186517	-1.066452
C	-1.514627	1.921238	-1.214265
C	-1.879727	1.201959	-2.354301
C	-2.485703	2.391817	-0.325886
C	-3.223684	0.968936	-2.612562
H	-1.106772	0.840123	-3.029713
C	-3.824109	2.123064	-0.576584
H	-2.180876	2.942161	0.561399
C	-4.192349	1.415012	-1.718131
H	-3.515452	0.416713	-3.502630
H	-4.582402	2.460596	0.124915
H	-5.241811	1.198304	-1.903427

IN7
SCF done: -1544.112250

Rh	1.1746490	0.157336	-0.014352
N	0.6343090	-0.831931	1.633507
C	3.1396660	-1.135923	-0.019539
C	2.4520330	-1.219862	-1.254573
C	2.4228980	0.118156	-1.813108
C	3.2173460	0.976566	-0.948930
C	3.6132720	0.222488	0.166186
O	1.3712310	-0.789564	2.792102
C	-0.5060920	-1.608086	1.663480
C	-0.5768610	-0.661563	-0.575013
C	-2.2843080	-2.072158	-0.071491
C	-1.3832570	-0.674680	-1.672186
C	-2.4772660	-1.572406	-1.379577
H	-1.2505460	-0.083701	-2.570867
O	-0.9462540	-2.245744	2.596713
C	4.3690120	0.677088	1.365090
H	4.4842930	1.764489	1.383995
H	3.8509390	0.375248	2.283995
H	5.3707280	0.228408	1.396562
C	3.3997760	2.427541	-1.187550
H	4.1048940	2.874779	-0.481266
H	3.7617420	2.615945	-2.205028
H	2.4296150	2.939394	-1.078196

C	1.9053620	0.512212	-3.152738
H	1.3642760	1.464121	-3.105490
H	2.7348370	0.610572	-3.867066
H	1.2126990	-0.237725	-3.546617
C	1.8834240	-2.449476	-1.871974
H	1.0355650	-2.213825	-2.522156
H	2.6410710	-2.973116	-2.469054
H	1.5157180	-3.144359	-1.108697
C	3.4041760	-2.252223	0.924294
H	2.7306240	-3.096223	0.749576
H	4.4351130	-2.611588	0.804682
H	3.2717650	-1.931983	1.962246
C	0.9794130	0.326372	3.578850
H	-0.0645070	0.223714	3.902059
H	1.6359690	0.327288	4.453212
H	1.1066760	1.261840	3.012764
N	-1.1053590	-1.502889	0.402297
C	-3.1568490	-2.968031	0.535061
H	-2.9693000	-3.322122	1.543953
C	-3.5988310	-1.993896	-2.100102
H	-3.7767110	-1.623772	-3.107751
C	-4.4781450	-2.888545	-1.507136
H	-5.3544210	-3.223370	-2.058113
C	-4.2600080	-3.368691	-0.207744
H	-4.9693380	-4.068381	0.228611
C	-0.6542550	2.253345	-0.840175
O	-0.5942790	2.437751	-2.056275
N	0.4721330	1.850593	-0.161190
C	-1.8558670	2.579119	-0.029674
C	-2.8255060	3.410165	-0.592864
C	-2.0404720	2.057918	1.253345
C	-3.9699050	3.725708	0.126205
H	-2.6592460	3.792164	-1.597336
C	-3.1910640	2.368775	1.966853
H	-1.2894530	1.393291	1.677808
C	-4.1521540	3.205276	1.405726
H	-4.7245670	4.376137	-0.309749
H	-3.3425110	1.952270	2.959841
H	-5.0514930	3.449301	1.966992

TS3

SCF done: -1544.093585

Rh	-1.446591	0.067801	-0.189756
N	-0.464459	-1.170640	1.142380
C	-3.100458	0.748054	1.160367

C	-2.617499	1.881152	0.448207
C	-2.831272	1.651274	-0.966204
C	-3.469326	0.382497	-1.111411
C	-3.606432	-0.199562	0.197874
O	-1.166736	-2.098785	1.884156
C	0.735204	-0.811305	1.671754
C	0.431728	0.906147	-0.035044
C	2.443795	0.944745	0.977145
C	1.133103	1.918047	-0.640758
C	2.412117	1.979650	0.007103
H	0.793131	2.514249	-1.480243
O	1.373765	-1.330987	2.566249
C	-4.206467	-1.517577	0.540632
H	-4.274153	-2.169903	-0.335731
H	-3.591829	-2.027630	1.291847
H	-5.217480	-1.399387	0.953249
C	-3.865152	-0.244019	-2.401550
H	-3.795546	-1.335305	-2.353680
H	-4.898092	0.019635	-2.663913
H	-3.215423	0.088846	-3.217357
C	-2.494372	2.581880	-2.080319
H	-1.980151	2.054336	-2.892774
H	-3.396675	3.044007	-2.501567
H	-1.837098	3.388462	-1.741427
C	-2.014941	3.101817	1.050466
H	-1.282019	3.562600	0.381255
H	-2.790039	3.847028	1.271429
H	-1.494535	2.869330	1.984859
C	-3.076316	0.529081	2.632509
H	-2.351663	1.184365	3.125347
H	-4.062669	0.724452	3.073456
H	-2.796418	-0.504084	2.864820
C	-1.023149	-3.384754	1.296338
H	0.024202	-3.711397	1.343233
H	-1.647218	-4.058789	1.891408
H	-1.351414	-3.375149	0.248083
N	1.207923	0.311627	0.932505
C	3.554528	0.697768	1.775515
H	3.535935	-0.102752	2.508167
C	3.548332	2.780097	-0.169073
H	3.551083	3.578067	-0.909118
C	4.666097	2.530374	0.610411
H	5.557842	3.140290	0.483892
C	4.666347	1.504832	1.570356

H	5.560664	1.335313	2.165935
C	0.532937	-1.629138	-1.569265
O	0.003882	-2.727998	-1.734888
N	-0.344511	-0.575085	-1.616790
C	1.996273	-1.452241	-1.436794
C	2.697174	-0.454390	-2.114543
C	2.676788	-2.344669	-0.604203
C	4.072636	-0.344306	-1.948721
H	2.161483	0.227142	-2.771536
C	4.045180	-2.209524	-0.416633
H	2.113020	-3.121230	-0.090889
C	4.742973	-1.208471	-1.088323
H	4.619646	0.435046	-2.474250
H	4.568454	-2.883691	0.256809
H	5.814640	-1.098786	-0.938124

INX
SCF done: -1544.195919

Rh	-0.676254	0.680435	-0.162109
N	0.692422	1.407345	1.050371
C	-1.125281	2.321267	-1.476683
C	-1.055544	1.064778	-2.209129
C	-2.170004	0.245692	-1.811257
C	-2.847239	0.928573	-0.770570
C	-2.204119	2.217314	-0.561062
O	0.460550	2.725543	1.448509
C	2.043173	1.100247	1.172906
C	1.677668	-1.116290	-0.046979
C	3.810723	-0.390285	0.318676
C	2.511393	-2.035967	-0.626053
C	3.854660	-1.603270	-0.403567
H	2.180323	-2.927372	-1.136965
O	2.829110	1.805019	1.776507
C	-2.633463	3.265498	0.401988
H	-3.176115	2.831731	1.248691
H	-1.761275	3.797207	0.796828
H	-3.295517	3.998947	-0.077153
C	-4.034575	0.454174	-0.016778
H	-3.940473	0.678103	1.051924
H	-4.939495	0.959863	-0.380346
H	-4.180151	-0.626073	-0.114116
C	-2.524391	-1.053648	-2.445715
H	-3.381123	-1.522950	-1.954528
H	-2.785410	-0.891422	-3.499491
H	-1.695069	-1.772846	-2.418759

C	-0.053559	0.679403	-3.235946
H	0.238279	-0.371925	-3.117987
H	-0.464538	0.803160	-4.247502
H	0.854209	1.285509	-3.161803
C	-0.213644	3.486555	-1.620831
H	0.711001	3.213466	-2.138253
H	-0.699592	4.284182	-2.197583
H	0.060208	3.886759	-0.638762
C	0.069578	2.744561	2.808283
H	0.885875	2.399634	3.453692
H	-0.165651	3.787993	3.041852
H	-0.823508	2.117566	2.964357
N	2.455574	-0.078282	0.529582
C	4.970323	0.295088	0.672187
H	4.918884	1.219866	1.232969
C	5.091997	-2.142081	-0.771089
H	5.135030	-3.076900	-1.326581
C	6.249594	-1.468212	-0.416585
H	7.219085	-1.878229	-0.692195
C	6.186044	-0.263525	0.294810
H	7.106798	0.248164	0.566368
C	-0.432185	-2.212660	-0.186379
O	-0.132046	-3.048339	-1.032029
N	0.317334	-1.102120	0.155169
C	-1.698665	-2.361384	0.605559
C	-1.902673	-1.706357	1.825418
C	-2.676113	-3.242930	0.135290
C	-3.079589	-1.904245	2.540360
H	-1.120997	-1.059033	2.217713
C	-3.859569	-3.425315	0.839886
H	-2.479522	-3.781124	-0.789631
C	-4.064742	-2.752976	2.044051
H	-3.222615	-1.402740	3.495236
H	-4.618494	-4.105756	0.459940
H	-4.985747	-2.905749	2.602475

TS4′
SCF done: -1544.115367

Rh	1.103861	0.763204	-0.165944
N	-0.280686	0.307453	-1.588391
C	0.658175	2.311166	1.195490
C	0.065432	1.102459	1.738600
C	1.116537	0.178229	1.985299
C	2.374109	0.834657	1.657822
C	2.100684	2.148107	1.201932

O	0.640671	1.848454	-1.906588
C	-1.604596	0.767789	-1.304220
C	-1.942788	-1.512590	-0.474597
C	-3.767849	-0.128925	-0.421748
C	-2.928632	-2.201951	0.182343
C	-4.090488	-1.353857	0.213086
H	-2.823040	-3.202116	0.576554
O	-1.997307	1.912373	-1.447964
C	3.074640	3.171917	0.734790
H	4.047570	2.724916	0.509746
H	2.716289	3.666452	-0.175755
H	3.229048	3.948244	1.495360
C	3.708125	0.203064	1.814291
H	4.001454	0.202705	2.872651
H	3.698932	-0.839821	1.475866
H	4.481793	0.732061	1.249421
C	0.958624	-1.159403	2.613806
H	1.831405	-1.795165	2.437306
H	0.838418	-1.046042	3.699827
H	0.084211	-1.700187	2.231870
C	-1.380740	0.886205	1.985726
H	-1.664216	-0.162949	1.838626
H	-1.623633	1.156120	3.022543
H	-2.001838	1.506241	1.329909
C	-0.096863	3.524513	0.796874
H	-0.915647	3.266670	0.112393
H	-0.528320	4.007916	1.683443
H	0.546691	4.247352	0.288595
C	1.386541	1.672315	-3.081103
H	0.913125	2.242204	-3.892055
H	2.413571	2.044374	-2.936783
H	1.433031	0.619073	-3.392150
N	-2.436286	-0.243707	-0.844976
C	-4.667833	0.920628	-0.536717
H	-4.379954	1.844155	-1.027757
C	-5.376484	-1.514561	0.735101
H	-5.655454	-2.446200	1.223479
C	-6.288023	-0.471713	0.622240
H	-7.291296	-0.592318	1.026189
C	-5.939919	0.730484	-0.001977
H	-6.673534	1.529862	-0.077259
C	0.139991	-2.592979	-0.241979
O	-0.223940	-3.461039	0.560020
N	-0.650451	-1.674711	-0.833022

C	1.605233	-2.434820	-0.553182
C	2.081656	-1.525989	-1.511952
C	2.525095	-3.181502	0.182346
C	3.454357	-1.340966	-1.692869
H	1.364238	-1.044588	-2.170007
C	3.892802	-3.005867	-0.010243
H	2.131323	-3.897595	0.901227
C	4.363304	-2.074922	-0.936902
H	3.809385	-0.645195	-2.451742
H	4.599822	-3.600561	0.565011
H	5.432918	-1.940240	-1.081590

IN9′

SCF done: -1544.126165

Rh	-1.176462	0.301171	0.152037
N	0.865327	-2.085206	0.601835
C	-1.676169	1.871709	1.710246
C	-0.482853	2.218900	1.021611
C	-0.804488	2.531752	-0.373195
C	-2.163512	2.255948	-0.561110
C	-2.695617	1.765940	0.706014
O	1.220819	-3.251558	-0.143574
C	2.160996	-1.697029	1.194070
C	1.790986	-0.426001	-0.670438
C	3.859669	-0.040416	0.173661
C	2.374055	0.401846	-1.566716
C	3.702536	0.667488	-1.041502
H	1.942783	0.751894	-2.493544
O	2.646951	-2.225988	2.151941
C	-4.139877	1.500293	0.943756
H	-4.593751	0.953157	0.109091
H	-4.303858	0.908379	1.850117
H	-4.685908	2.447749	1.055422
C	-2.959444	2.349254	-1.815369
H	-3.749940	3.108280	-1.735727
H	-2.331781	2.609266	-2.673600
H	-3.448024	1.390125	-2.040752
C	0.159367	3.056283	-1.379582
H	-0.098040	2.727046	-2.393519
H	0.183730	4.154759	-1.379728
H	1.179076	2.710457	-1.174752
C	0.865529	2.395421	1.631808
H	1.665811	2.162614	0.918437
H	1.019782	3.433293	1.958016
H	0.999816	1.749501	2.506813

C	-1.837084	1.604350	3.167407
H	-0.901292	1.256991	3.618737
H	-2.153221	2.502861	3.716602
H	-2.589888	0.828202	3.349868
C	0.524171	-4.365081	0.393506
H	-0.562051	-4.226137	0.318028
H	0.831706	-5.216739	-0.218249
H	0.809480	-4.538043	1.438101
N	2.651830	-0.709241	0.382996
C	5.019114	-0.029573	0.928945
H	5.091814	-0.600983	1.850185
C	4.777153	1.429617	-1.502010
H	4.700349	1.986603	-2.432969
C	5.946945	1.459866	-0.751476
H	6.788252	2.053631	-1.101254
C	6.070498	0.742066	0.443626
H	7.001989	0.786171	1.002066
C	-0.410742	-1.298383	-1.453822
O	-0.057789	-1.135324	-2.606091
N	0.566491	-1.047821	-0.354910
C	-1.754113	-1.520309	-0.934666
C	-2.036648	-1.712186	0.471945
C	-2.835453	-1.483183	-1.874359
C	-3.408912	-1.821626	0.854990
H	-1.291850	-2.134831	1.141400
C	-4.127134	-1.583072	-1.445908
H	-2.584571	-1.368650	-2.926694
C	-4.420916	-1.741501	-0.059955
H	-3.635324	-1.998808	1.905709
H	-4.941252	-1.554970	-2.167130
H	-5.456769	-1.829907	0.261131

INX1

SCF done: -1773.168253

Rh	1.428647	-0.221264	0.026332
N	0.125394	0.282168	1.583940
C	1.265341	-2.339190	-0.471842
C	2.157141	-1.729998	-1.442535
C	3.267404	-1.206074	-0.741841
C	3.069018	-1.460699	0.681275
C	1.868493	-2.214378	0.830595
O	0.763758	0.250330	2.825235
C	-1.040706	-0.446084	1.641259
C	-1.255103	-0.089019	-0.880776
C	-2.727570	-1.495395	0.125766

C	-1.998467	-0.647509	-1.878623
C	-2.951992	-1.529266	-1.271813
H	-1.909051	-0.391838	-2.928606
O	-1.551524	-0.923394	2.637458
C	1.317357	-2.739146	2.106924
H	1.441965	-2.013264	2.916839
H	0.245675	-2.951625	2.035172
H	1.832578	-3.668010	2.383760
C	3.969585	-1.029147	1.784018
H	3.387150	-0.843234	2.693442
H	4.730259	-1.788359	2.009076
H	4.484880	-0.097159	1.528901
C	4.455553	-0.521694	-1.314780
H	4.751150	0.339544	-0.706585
H	5.309161	-1.211646	-1.341614
H	4.275910	-0.170673	-2.335190
C	1.874976	-1.665054	-2.901450
H	2.510254	-0.931417	-3.407379
H	2.032501	-2.640366	-3.380516
H	0.828457	-1.381221	-3.073711
C	0.077398	-3.156819	-0.821142
H	-0.501767	-2.695133	-1.627862
H	0.404298	-4.147674	-1.165299
H	-0.596442	-3.300555	0.028855
C	1.221637	1.554792	3.125201
H	0.381487	2.257276	3.206071
H	1.731837	1.477411	4.090447
H	1.917417	1.917616	2.356400
N	-1.667227	-0.610894	0.362878
C	-3.475350	-2.278279	1.003069
H	-3.289347	-2.236088	2.069438
C	-3.953785	-2.352418	-1.791942
H	-4.135378	-2.382249	-2.864828
C	-4.707387	-3.125103	-0.921365
H	-5.493968	-3.767503	-1.311369
C	-4.465072	-3.087892	0.457085
H	-5.068401	-3.702045	1.122138
C	-0.554540	2.118684	-0.465518
O	0.282675	2.981440	-0.233241
N	-0.229338	0.851172	-0.945815
C	-1.999353	2.476779	-0.250398
C	-2.971128	2.376948	-1.246742
C	-2.342733	3.023113	0.987327
C	-4.272029	2.800778	-0.999573

H	-2.705417	1.977395	-2.222198
C	-3.648585	3.421727	1.241578
H	-1.570249	3.127022	1.746472
C	-4.616481	3.311913	0.247487
H	-5.021141	2.726773	-1.784672
H	-3.910496	3.825933	2.216753
H	-5.638432	3.628757	0.443401
C	3.410795	3.648029	-1.057348
H	3.848641	3.789163	-2.048430
H	4.168651	3.707179	-0.275039
H	2.670404	4.440533	-0.897191
C	2.668670	2.360764	-0.975448
O	2.652376	1.686172	0.055263
O	2.078183	2.021810	-2.103297
H	1.334248	1.392199	-1.910649

TS4

SCF done: -1773.161564

Rh	1.465109	-0.148703	0.122249
N	0.001608	0.556234	1.494890
C	1.295012	-2.334371	0.149806
C	2.030262	-1.968365	-1.046916
C	3.199777	-1.272312	-0.657828
C	3.197504	-1.183089	0.796196
C	2.050033	-1.890928	1.286407
O	0.507506	0.692214	2.791541
C	1.081935	-0.285708	1.526973
C	1.168150	-0.126275	-1.028552
C	2.658361	-1.486920	-0.008656
C	1.803791	-0.800449	-2.027353
C	2.764324	-1.667874	-1.408410
H	1.657040	-0.620999	-3.086389
O	1.581923	-0.803766	2.510857
C	1.673704	-2.124417	2.704238
H	2.183167	-1.431118	3.377717
H	0.597533	-1.992916	2.867070
H	1.942687	-3.150136	2.990539
C	4.239378	-0.501684	1.608716
H	3.900520	-0.348050	2.637900
H	5.164270	-1.092699	1.638276
H	4.476339	0.481090	1.185621
C	4.257160	-0.729602	-1.552301
H	4.798958	0.091484	-1.072439
H	4.988872	-1.509257	-1.800780
H	3.833422	-0.347545	-2.486280

C	1.563137	-2.233747	-2.430504
H	2.174028	-1.711629	-3.171897
H	1.592928	-3.309095	-2.648661
H	0.519677	-1.907895	-2.553761
C	0.100512	-3.217383	0.207069
H	0.518249	-3.139609	-0.692763
H	0.422804	-4.263945	0.299379
H	0.531573	-2.990333	1.072167
C	1.187692	1.926839	2.858017
H	0.509856	2.770482	2.668680
H	1.588511	1.994996	3.873574
H	2.005348	1.973411	2.122711
N	1.641388	-0.550032	0.225346
C	3.470477	-2.191071	0.878837
H	3.377028	-2.038898	1.947150
C	3.699558	-2.569593	-1.923578
H	3.788520	-2.710934	-2.999038
C	4.508838	-3.270654	-1.043623
H	5.244190	-3.973551	-1.428870
C	4.391433	-3.080415	0.338933
H	5.039041	-3.638632	1.011371
C	0.600074	2.173992	-0.632662
O	0.193462	3.089330	-0.579326
N	0.204830	0.882701	-1.095462
C	2.032925	2.413014	-0.265697
C	3.094911	2.145956	-1.131478
C	2.284235	3.040791	0.955526
C	4.394076	2.476852	-0.762755
H	2.908707	1.686207	-2.098480
C	3.583901	3.353061	1.329502
H	1.444941	3.263150	1.610117
C	4.642138	3.069258	0.470853
H	5.215619	2.268364	-1.443926
H	3.771421	3.821361	2.292831
H	5.661097	3.314668	0.761483
C	3.302648	3.260010	-1.891311
H	3.612764	3.191585	-2.936822
H	4.162843	3.395074	-1.231898
H	2.644457	4.130286	-1.785624
C	2.497302	2.058894	-1.496709
O	2.558898	1.692741	-0.289020
O	1.800988	1.495526	-2.400699
H	0.699411	1.033177	-1.876839

INX2

SCF done: -1773.170271

Rh	-1.270968	-0.295536	0.115028
N	0.541226	-0.149994	1.220060
C	-2.815002	1.131418	0.773539
C	-3.293594	0.406093	-0.390066
C	-3.331005	-0.976366	-0.070764
C	-2.863903	-1.129333	1.296716
C	-2.605427	0.178734	1.820841
O	0.536820	-0.742264	2.479579
C	1.532137	0.758910	1.075338
C	0.852824	0.440390	-1.243022
C	0.731276	2.519846	-0.414020
C	-0.303646	1.005061	-1.795483
C	-0.291165	2.396331	-1.373583
H	-0.797367	0.597245	-2.671736
O	2.377296	1.158384	1.841163
C	-2.173555	0.481723	3.207827
H	-2.978460	0.235616	3.912354
H	-1.286690	-0.105283	3.468711
H	-1.924491	1.539418	3.329862
C	-2.727747	-2.420090	2.020038
H	-2.277092	-2.274780	3.006467
H	-3.705096	-2.901055	2.156527
H	-2.083572	-3.100970	1.448250
C	-3.791547	-2.073507	-0.962961
H	-3.501712	-3.050195	-0.563317
H	-4.885225	-2.056192	-1.058027
H	-3.354564	-1.982121	-1.963246
C	-3.724005	0.991865	-1.686339
H	-3.506618	0.310185	-2.516275
H	-4.806439	1.177590	-1.680484
H	-3.225349	1.945821	-1.884142
C	-2.749930	2.605442	0.954630
H	-2.764821	3.139156	0.002151
H	-3.604414	2.951004	1.552058
H	-1.832924	2.901889	1.477119
C	1.221389	-1.984425	2.416556
H	2.297352	-1.817250	2.267957
H	1.063803	-2.467812	3.386135
H	0.817357	-2.604471	1.605430
N	1.421609	1.293283	-0.305507
C	0.980378	3.696699	0.270179
H	1.759642	3.737932	1.026828
C	-1.004732	3.532869	-1.750207
H	-1.749850	3.487259	-2.543702

C	-0.731569	4.738703	-1.105920
H	-1.273242	5.635807	-1.397162
C	0.226592	4.813602	-0.091907
H	0.412265	5.765025	0.400760
C	2.493357	-1.468394	-1.154133
O	2.448036	-2.679661	-1.268532
N	1.447885	-0.702587	-1.692653
C	3.664504	-0.781468	-0.558464
C	4.126584	0.454680	-1.013225
C	4.371495	-1.461900	0.435912
C	5.262296	1.020025	-0.449010
H	3.603543	0.966777	-1.816274
C	5.489711	-0.883107	1.017148
H	4.023532	-2.446894	0.739227
C	5.931985	0.361663	0.577314
H	5.623661	1.980379	-0.808375
H	6.022226	-1.403717	1.809212
H	6.809912	0.816516	1.030660
C	-0.485334	-4.273454	-1.602005
H	-0.852532	-4.657815	-2.556379
H	-0.961524	-4.792588	-0.764034
H	0.595569	-4.446340	-1.537743
C	-0.693830	-2.781778	-1.513992
O	-0.623303	-2.308632	-0.322213
O	-0.852972	-2.102004	-2.542521
H	0.783407	-1.273898	-2.233801

INX3

SCF done: -1773.156154

Rh	1.697598	-0.327598	0.019210
N	-0.203483	-0.923591	-0.708025
C	2.726782	1.532375	-0.403068
C	3.611807	0.664205	0.355072
C	3.797643	-0.517748	-0.402104
C	3.019346	-0.388691	-1.635730
C	2.400768	0.903715	-1.650301
O	0.027385	-1.705406	-1.866668
C	-1.037871	0.116900	-1.001536
C	-1.397495	0.523225	1.508748
C	-1.180618	2.309079	0.140999
C	-1.277178	1.616440	2.321845
C	-1.120067	2.763377	1.480411
H	-1.390341	1.598083	3.398233
O	-1.544658	0.413748	-2.067747
C	1.549743	1.450792	-2.742568

H	2.151625	1.639794	-3.640240
H	0.737822	0.761339	-3.007513
H	1.082856	2.393936	-2.441602
C	2.941457	-1.400872	-2.716152
H	2.036392	-1.260849	-3.311300
H	3.821554	-1.324724	-3.369077
H	2.905311	-2.416337	-2.307301
C	4.590073	-1.709886	-0.008039
H	4.214937	-2.614910	-0.495122
H	5.640834	-1.585188	-0.300397
H	4.554530	-1.871347	1.073949
C	4.140529	0.960009	1.712461
H	4.492743	0.051829	2.209187
H	4.973719	1.672832	1.666521
H	3.361173	1.393754	2.349006
C	2.264083	2.850807	0.087030
H	1.956147	2.791077	1.137746
H	3.088113	3.575289	0.028354
H	1.415685	3.236169	-0.484846
C	-1.016916	-2.652631	-2.018759
H	-1.965972	-2.158791	-2.269048
H	-0.715270	-3.301028	-2.847153
H	-1.145874	-3.244087	-1.101246
N	-1.280381	0.920978	0.169016
C	-1.135442	3.182964	-0.944111
H	-1.250972	2.808259	-1.956723
C	-0.973802	4.134712	1.725605
H	-0.928691	4.506632	2.747351
C	-0.899852	5.007259	0.650583
H	-0.794480	6.074940	0.830643
C	-0.987768	4.537338	-0.669171
H	-0.961445	5.247197	-1.492984
C	-2.510287	-1.675065	1.200106
O	-2.346221	-2.876635	1.331475
N	-1.689446	-0.783050	1.872938
C	-3.624134	-1.138526	0.357540
C	-4.176315	0.138155	0.494238
C	-4.163339	-2.016062	-0.586702
C	-5.221892	0.538236	-0.329111
H	-3.798051	0.825126	1.248445
C	-5.199845	-1.612217	-1.415884
H	-3.751165	-3.020846	-0.642747
C	-5.725692	-0.329352	-1.292751
H	-5.644439	1.533757	-0.216187

H	-5.603281	-2.299722	-2.155823
H	-6.536751	-0.008112	-1.942667
C	1.117437	-3.575532	1.077833
H	0.503533	-4.435002	1.353122
H	2.176051	-3.864999	1.083900
H	0.866153	-3.242642	0.063516
C	0.895565	-2.450419	2.058112
O	1.449680	-1.301223	1.745098
O	0.280024	-2.598143	3.101547
H	-1.041204	-1.254136	2.512859

TS5

SCF done: -2002.155570

Rh	1.859225	-0.053189	-0.217766
N	-0.235245	-0.649396	-0.828977
C	2.320697	1.821430	-1.160734
C	3.281390	1.579511	-0.118783
C	3.951103	0.347228	-0.411180
C	3.436586	-0.145557	-1.680775
C	2.472569	0.785463	-2.160248
O	-0.002918	-1.285636	-2.066731
C	-1.067780	0.473494	-1.013488
C	-1.881291	0.501557	1.411982
C	-1.922537	2.428445	0.198132
C	-2.254830	1.490839	2.261579
C	-2.273136	2.722415	1.533809
H	-2.539528	1.327073	3.293066
O	-1.254453	0.968335	-2.110727
C	1.726170	0.741395	-3.441024
H	1.897252	-0.195004	-3.977285
H	0.646889	0.841973	-3.274754
H	2.059670	1.571802	-4.077955
C	3.860373	-1.413415	-2.328787
H	3.113047	-1.755314	-3.050874
H	4.817600	-1.287893	-2.851574
H	3.981044	-2.203493	-1.580374
C	5.015668	-0.327063	0.376071
H	4.750749	-1.374689	0.561666
H	5.965883	-0.312762	-0.173242
H	5.173787	0.152913	1.346063
C	3.433306	2.439386	1.083991
H	4.293463	2.145091	1.692369
H	3.566577	3.486560	0.787964
H	2.530305	2.373626	1.705543
C	1.424022	3.000620	-1.258412

H	1.067729	3.315055	-0.270713
H	1.944409	3.850710	-1.720736
H	0.544720	2.768904	-1.867977
C	-1.120698	-2.087743	-2.428405
H	-2.025229	-1.478760	-2.563812
H	-0.849198	-2.548403	-3.382021
H	-1.303856	-2.868440	-1.678665
N	-1.602903	1.056265	0.136934
C	-1.946433	3.409913	-0.791499
H	-1.743110	3.161917	-1.826520
C	-2.607314	4.031276	1.891751
H	-2.876164	4.262962	2.920164
C	-2.599419	5.016352	0.917446
H	-2.861339	6.038965	1.179851
C	-2.278130	4.704361	-0.409050
H	-2.306653	5.485372	-1.165549
C	-2.680115	-1.868693	1.350936
O	-2.606183	-2.951205	1.903013
N	-1.811549	-0.853084	1.701044
C	-3.640582	-1.660217	0.216288
C	-4.266756	-0.454377	-0.113094
C	-3.937463	-2.804398	-0.531886
C	-5.140327	-0.392229	-1.194189
H	-4.097876	0.438173	0.483450
C	-4.799665	-2.738545	-1.617306
H	-3.470396	-3.740178	-0.232640
C	-5.399273	-1.527367	-1.955179
H	-5.623641	0.550891	-1.437793
H	-5.011886	-3.633846	-2.197657
H	-6.076546	-1.471010	-2.804593
C	2.705299	-0.519779	3.152807
H	2.762184	-0.832922	4.197462
H	3.264273	0.412774	3.015561
H	3.164320	-1.292742	2.524575
C	1.254956	-0.366977	2.746460
O	0.982142	0.290933	1.657180
O	0.380983	-0.854320	3.463904
H	-1.148704	-1.085252	2.458177
H	-0.275939	-1.558569	-0.054958
O	2.127655	-2.078520	0.476805
O	-0.023363	-2.725307	0.464461
C	1.186840	-2.886025	0.759513
C	1.553240	-4.099467	1.562932
H	1.348300	-3.861822	2.614214

H	0.919213	-4.945232	1.288402
H	2.611660	-4.346644	1.456420

INX4
SCF done: -2002.160704

Rh	1.901009	0.000760	-0.172296
N	-0.233567	-0.558165	-0.833066
C	2.327114	1.908791	-1.102371
C	3.233410	1.698160	-0.014967
C	3.964352	0.484551	-0.273706
C	3.546949	-0.015394	-1.573285
C	2.559686	0.868929	-2.088018
O	-0.001095	-1.262576	-2.014223
C	-1.081810	0.559942	-1.056187
C	-1.986857	0.541824	1.333343
C	-2.115531	2.457466	0.092285
C	-2.481963	1.506612	2.145499
C	-2.562540	2.728433	1.402263
H	-2.789902	1.334001	3.168928
O	-1.180015	1.054629	-2.161146
C	1.863445	0.783053	-3.395445
H	2.122432	-0.131925	-3.933958
H	0.775561	0.800840	-3.266512
H	2.150327	1.642221	-4.016340
C	4.048252	-1.273953	-2.183347
H	3.506124	-1.516983	-3.101455
H	5.116831	-1.197650	-2.421153
H	3.906695	-2.106053	-1.482652
C	5.022990	-0.141956	0.558692
H	4.834037	-1.215553	0.671822
H	6.006178	-0.018129	0.085771
H	5.069470	0.296477	1.559496
C	3.313938	2.562168	1.191401
H	4.018533	2.167629	1.929026
H	3.642532	3.571445	0.913397
H	2.331952	2.645627	1.672457
C	1.395970	3.056482	-1.253398
H	0.973559	3.359886	-0.288630
H	1.914377	3.924988	-1.682537
H	0.563309	2.800932	-1.916338
C	-1.109989	-2.101402	-2.326889
H	-2.027701	-1.511877	-2.458182
H	-0.847704	-2.583129	-3.271853
H	-1.247936	-2.858059	-1.545380
N	-1.696393	1.108957	0.058864

C	-2.131462	3.434407	-0.900955
H	-1.835316	3.203461	-1.917248
C	-3.005989	4.011032	1.732500
H	-3.349695	4.226045	2.741838
C	-3.003387	4.992958	0.754372
H	-3.348503	5.996016	0.994379
C	-2.574630	4.703378	-0.546040
H	-2.600803	5.482129	-1.304762
C	-2.649929	-1.866539	1.437271
O	-2.564063	-2.861896	2.128028
N	-1.787889	-0.796560	1.649955
C	-3.581643	-1.833770	0.261440
C	-4.247677	-0.706693	-0.228325
C	-3.784146	-3.068702	-0.363561
C	-5.068515	-0.812049	-1.347882
H	-4.151457	0.254294	0.270790
C	-4.590897	-3.168863	-1.488399
H	-3.282471	-3.937938	0.055680
C	-5.230178	-2.036387	-1.987843
H	-5.586026	0.070121	-1.717123
H	-4.727204	-4.132773	-1.973793
H	-5.864283	-2.110132	-2.868593
C	2.596915	-0.612383	3.164984
H	2.644247	-0.971535	4.194816
H	3.222443	0.282579	3.060022
H	2.989688	-1.377095	2.485046
C	1.164528	-0.304173	2.795561
O	0.933878	0.277824	1.655342
O	0.254755	-0.581571	3.576069
H	-1.153916	-0.923628	2.458383
H	-0.413327	-1.232108	-0.054831
O	2.248693	-2.036901	0.342988
O	0.141621	-2.836061	0.478320
C	1.363969	-2.946698	0.595192
C	1.959611	-4.234027	1.120190
H	1.237270	-5.047640	1.030238
H	2.889760	-4.481836	0.600987
H	2.196351	-4.097237	2.182040

INX1’

SCF done: -1773.190458

Rh	-0.506493	-0.649895	0.431316
N	0.542222	-1.182976	-1.327951
C	0.356766	-2.180502	1.748631
C	0.661165	-0.850501	2.223635

C	-0.586707	-0.218867	2.613226
C	-1.642354	-1.096320	2.254281
C	-1.060489	-2.311553	1.704342
O	0.250642	-2.552094	-1.565000
C	1.914943	-1.015434	-1.141888
C	1.498322	1.377439	-0.327128
C	3.654288	0.665524	-0.665909
C	2.328944	2.404398	0.039849
C	3.679744	1.989786	-0.182305
H	1.992518	3.351372	0.432344
O	2.738639	-1.898702	-1.305682
C	-1.802806	-3.508418	1.227748
H	-2.853218	-3.272505	1.033793
H	-1.362479	-3.882753	0.296884
H	-1.768669	-4.316227	1.971186
C	-3.103821	-0.848033	2.361269
H	-3.576697	-0.948649	1.375719
H	-3.573683	-1.568500	3.042617
H	-3.313545	0.160620	2.727298
C	-0.675017	1.100685	3.286832
H	-1.714304	1.408207	3.439277
H	-0.194526	1.042311	4.272431
H	-0.169767	1.892795	2.716042
C	2.010348	-0.283855	2.483498
H	2.058200	0.776974	2.206665
H	2.253252	-0.363228	3.551979
H	2.791510	-0.804723	1.919864
C	1.325999	-3.227979	1.333797
H	2.360902	-2.889900	1.428016
H	1.193635	-4.119447	1.960189
H	1.169681	-3.511323	0.286534
C	0.522947	-2.910232	-2.911068
H	1.598885	-2.897629	-3.114710
H	0.140208	-3.929046	-3.024089
H	-0.002554	-2.247567	-3.611726
N	2.298982	0.284267	-0.769516
C	4.826263	-0.028070	-0.952368
H	4.796574	-1.046379	-1.318357
C	4.904170	2.632838	0.014661
H	4.928164	3.655447	0.386067
C	6.076295	1.948970	-0.272919
H	7.037793	2.437001	-0.127087
C	6.033690	0.635759	-0.750486
H	6.962393	0.114284	-0.972075

C	-0.614702	2.299179	0.179782
O	-0.199478	3.167439	0.945998
N	0.121035	1.276557	-0.382849
C	-2.057843	2.335943	-0.220456
C	-2.433448	2.282135	-1.562653
C	-3.031854	2.549289	0.754864
C	-3.773237	2.403654	-1.918166
H	-1.667004	2.145655	-2.322363
C	-4.374541	2.623581	0.405219
H	-2.715588	2.666761	1.790624
C	-4.748023	2.548821	-0.934802
H	-4.058067	2.387814	-2.968929
H	-5.130898	2.763112	1.174880
H	-5.796604	2.628897	-1.213385
H	-0.604715	-0.428656	-2.302240
O	-2.364497	-0.817762	-0.810632
O	-1.473738	-0.401578	-2.828682
C	-2.465350	-0.691929	-2.034904
C	-3.770373	-0.904106	-2.730536
H	-3.860780	-0.226730	-3.582925
H	-3.800133	-1.930585	-3.113227
H	-4.596422	-0.758706	-2.032611

TSX1'

SCF done: -1773.187174

Rh	0.530901	0.789603	0.392844
N	-0.584520	1.103953	-1.432995
C	-0.640197	2.072572	1.692657
C	-0.374688	0.837519	2.372405
C	1.059252	0.709897	2.523136
C	1.663041	1.866573	1.935837
C	0.627522	2.700094	1.392240
O	-0.404759	2.453407	-1.789043
C	-1.968464	0.815183	-1.285927
C	-1.412743	-1.393207	-0.129468
C	-3.610319	-0.865593	-0.585557
C	-2.192587	-2.395725	0.379524
C	-3.561708	-2.101205	0.091054
H	-1.812534	-3.249362	0.920864
O	-2.823217	1.622690	-1.587804
C	0.842886	4.000987	0.704334
H	1.734931	3.957600	0.068929
H	-0.001909	4.251125	0.057172
H	0.979763	4.813713	1.430491
C	3.118634	2.131833	1.799308

H	3.343871	3.179326	2.029633
H	3.709099	1.498232	2.466695
H	3.437639	1.930052	0.767275
C	1.746712	-0.382538	3.257416
H	2.796147	-0.466976	2.957012
H	1.715488	-0.190387	4.338410
H	1.261947	-1.349756	3.073761
C	-1.357616	-0.139784	2.905439
H	-1.023138	-1.167644	2.713604
H	-1.461430	-0.007467	3.990868
H	-2.347065	-0.024148	2.452382
C	-1.975234	2.633512	1.356240
H	-2.754631	1.864472	1.345376
H	-2.259647	3.388176	2.101056
H	-1.975759	3.110919	0.370353
C	-0.626198	2.677447	-3.179766
H	-1.677440	2.521880	-3.440913
H	-0.360975	3.725917	-3.339955
H	0.025090	2.039367	-3.789005
N	-2.271478	-0.424917	-0.741576
C	-4.814197	-0.293486	-0.978742
H	-4.840507	0.657964	-1.493813
C	-4.748024	-2.780039	0.375020
H	-4.717689	-3.734841	0.895950
C	-5.954668	-2.218581	-0.019404
H	-6.886910	-2.737650	0.193179
C	-5.984557	-0.991434	-0.686499
H	-6.938742	-0.566340	-0.989353
C	0.728610	-2.117264	0.519349
O	0.373793	-2.700928	1.544770
N	-0.050083	-1.241318	-0.225116
C	2.098484	-2.364225	-0.023337
C	2.329812	-2.399193	-1.398979
C	3.133444	-2.693890	0.854591
C	3.588248	-2.734081	-1.887764
H	1.514106	-2.160225	-2.076273
C	4.399115	-2.994106	0.367303
H	2.923925	-2.724521	1.921548
C	4.628579	-3.015203	-1.006657
H	3.756913	-2.773262	-2.962263
H	5.205383	-3.231537	1.057971
H	5.614924	-3.268212	-1.389920
H	0.178298	0.493807	-2.111767
O	2.273030	0.782977	-0.877803

O	1.270272	0.231925	-2.810453
C	2.285734	0.510700	-2.114330
C	3.625891	0.552269	-2.795758
H	4.384934	0.102931	-2.149604
H	3.581885	0.029298	-3.753724
H	3.904526	1.596614	-2.975445

INX2'

SCF done: -1773.190082

Rh	-0.560941	-0.631652	0.462306
N	0.603900	-1.309443	-1.235372
C	0.215182	-2.051335	1.933749
C	0.481346	-0.704742	2.366073
C	-0.791313	-0.053454	2.583855
C	-1.824566	-0.960900	2.195644
C	-1.202545	-2.201323	1.780933
O	0.329044	-2.660383	-1.446637
C	2.004209	-1.088475	-1.003670
C	1.541892	1.340222	-0.361412
C	3.719118	0.604747	-0.639022
C	2.380080	2.374227	-0.039274
C	3.734320	1.950250	-0.229515
H	2.044663	3.339724	0.304970
O	2.784962	-2.013818	-1.008669
C	-1.915293	-3.420931	1.318753
H	-2.808936	-3.152298	0.746052
H	-1.272508	-4.023117	0.668760
H	-2.227169	-4.044530	2.167464
C	-3.285934	-0.696552	2.141686
H	-3.622549	-0.723587	1.095264
H	-3.840014	-1.458497	2.703213
H	-3.536105	0.286384	2.550759
C	-0.943392	1.300396	3.168738
H	-1.985719	1.631836	3.160151
H	-0.599478	1.284289	4.211559
H	-0.347876	2.051555	2.632838
C	1.805075	-0.098106	2.671564
H	1.841930	0.948733	2.343981
H	2.004275	-0.120535	3.751308
H	2.622789	-0.625026	2.167681
C	1.222440	-3.105154	1.641601
H	2.243885	-2.732346	1.752999
H	1.085878	-3.947869	2.330939
H	1.121887	-3.479206	0.615742
C	0.639926	-3.060166	-2.783759

H	1.716342	-2.993743	-2.972351
H	0.323155	-4.104017	-2.842110
H	0.067079	-2.458599	-3.498388
N	2.357595	0.217962	-0.742462
C	4.887068	-0.103420	-0.889650
H	4.861998	-1.141650	-1.196743
C	4.955840	2.606148	-0.066878
H	4.977590	3.647283	0.247807
C	6.130083	1.909638	-0.318728
H	7.089676	2.407960	-0.198939
C	6.094144	0.573667	-0.725056
H	7.024457	0.044685	-0.918451
C	-0.561735	2.302130	0.047610
O	-0.128292	3.183476	0.789529
N	0.172786	1.234789	-0.445401
C	-1.989970	2.363847	-0.382319
C	-2.370299	2.058927	-1.687798
C	-2.940298	2.860153	0.512745
C	-3.693135	2.221963	-2.084851
H	-1.623889	1.684929	-2.383499
C	-4.268721	2.987341	0.127786
H	-2.614942	3.157817	1.508341
C	-4.647196	2.668139	-1.174822
H	-3.979395	1.993752	-3.110067
H	-5.007801	3.357273	0.835430
H	-5.683759	2.784843	-1.484262
H	0.088593	-0.753593	-1.971450
O	-2.264891	-0.823628	-0.815821
O	-1.354963	-0.702878	-2.876101
C	-2.305371	-0.887181	-2.095343
C	-3.667606	-1.237856	-2.651379
H	-3.710563	-1.010801	-3.719133
H	-3.847181	-2.309933	-2.509773
H	-4.450880	-0.695893	-2.113179

INX3’

SCF done: -2002.150038

Rh	-0.803448	-0.693330	0.704065
N	1.447436	-1.185531	-1.939140
C	0.675163	-2.039201	1.555194
C	0.394911	-0.993465	2.513092
C	-0.989535	-1.066502	2.835006
C	-1.584981	-2.163467	2.089119
C	-0.547205	-2.765498	1.317090
O	1.332061	-2.533458	-2.223347

C	2.618954	-0.813381	-1.358398
C	1.572079	1.216132	-0.117975
C	3.842721	0.971221	-0.198032
C	2.119713	2.219729	0.626643
C	3.540677	2.099093	0.594538
H	1.537640	2.981926	1.134672
O	3.621473	-1.502160	-1.432588
C	-0.648130	-3.939815	0.415622
H	-1.685408	-4.155372	0.153779
H	-0.088513	-3.755824	-0.510775
H	-0.203535	-4.816544	0.906261
C	-3.006319	-2.593320	2.128027
H	-3.361049	-2.764262	1.105634
H	-3.113899	-3.518369	2.709419
H	-3.643724	-1.831040	2.585578
C	-1.703221	-0.211408	3.818983
H	-2.770059	-0.137343	3.586717
H	-1.613988	-0.648505	4.822036
H	-1.285596	0.799949	3.857701
C	1.394923	-0.054418	3.080274
H	0.926988	0.866942	3.443166
H	1.920841	-0.523143	3.922467
H	2.142837	0.235688	2.334702
C	2.014609	-2.473515	1.091915
H	2.764751	-1.680866	1.162336
H	2.353615	-3.300632	1.732591
H	2.001272	-2.844977	0.062259
C	1.839467	-2.806544	-3.524850
H	2.916221	-2.611456	-3.563575
H	1.644178	-3.868419	-3.700546
H	1.318055	-2.201221	-4.277308
N	2.625314	0.414181	-0.647403
C	5.165728	0.595667	-0.437500
H	5.395998	-0.269520	-1.044700
C	4.569605	2.854844	1.165328
H	4.332944	3.724847	1.774805
C	5.881589	2.481291	0.931483
H	6.695868	3.057575	1.365158
C	6.169441	1.365029	0.135843
H	7.206307	1.088172	-0.041650
C	-0.263420	1.448513	-1.555130
O	0.419495	1.379421	-2.561602
N	0.190084	1.058450	-0.280764
C	-1.601423	2.121504	-1.634378

C	-2.669063	1.565258	-2.336114
C	-1.715265	3.414512	-1.120896
C	-3.857784	2.271562	-2.471601
H	-2.562684	0.566889	-2.750199
C	-2.895760	4.133937	-1.283809
H	-0.869822	3.860841	-0.598332
C	-3.975003	3.556181	-1.946387
H	-4.695171	1.820091	-2.998529
H	-2.969656	5.147894	-0.895377
H	-4.902840	4.111336	-2.066325
H	0.533044	-0.749483	-1.835832
O	-1.253812	-1.037739	-1.312307
O	-2.940273	-2.506068	-1.034129
C	-2.110054	-1.927811	-1.724215
C	-1.946511	-2.240177	-3.196670
H	-1.194862	-3.035846	-3.280406
H	-2.885580	-2.600656	-3.622753
H	-1.566348	-1.377456	-3.755161
H	-0.661485	1.871501	0.946226
O	-2.643893	0.655235	0.883250
O	-1.328368	2.338287	1.567452
C	-2.494891	1.758142	1.414880
C	-3.650701	2.541043	1.939816
H	-3.910594	3.299280	1.191169
H	-4.511107	1.888468	2.096046
H	-3.374665	3.060728	2.861761

TSX2’

SCF done: -2002.128289

Rh	-0.779707	-0.674067	0.722234
N	1.340245	-1.267655	-1.791985
C	0.858904	-1.953880	1.564685
C	0.509036	-0.908308	2.521491
C	-0.866574	-1.082635	2.880499
C	-1.397739	-2.221042	2.132172
C	-0.314789	-2.762364	1.346274
O	1.399654	-2.665114	-2.116285
C	2.530590	-0.732766	-1.423638
C	1.464718	1.300172	-0.152753
C	3.736447	1.088549	-0.280364
C	2.002537	2.318862	0.579964
C	3.427423	2.212824	0.526459
H	1.416615	3.065697	1.099910
O	3.603909	-1.296306	-1.648953
C	-0.390126	-3.928793	0.421696

H	-1.417946	-4.069821	0.072484
H	0.255881	-3.765386	-0.451609
H	-0.052817	-4.837947	0.942155
C	-2.794015	-2.742862	2.159778
H	-3.183902	-2.746118	1.131850
H	-2.812650	-3.767946	2.557778
H	-3.439629	-2.115237	2.783376
C	-1.653920	-0.255363	3.838014
H	-2.671846	-0.101059	3.459746
H	-1.717603	-0.767336	4.808986
H	-1.189289	0.725500	3.989851
C	1.420348	0.151557	3.039271
H	0.878989	1.099212	3.162268
H	1.841505	-0.145874	4.010631
H	2.244756	0.342005	2.343541
C	2.229674	-2.289257	1.090206
H	2.882270	-1.409350	1.068674
H	2.675142	-3.016063	1.787740
H	2.220084	-2.739911	0.091584
C	1.934393	-2.826177	-3.477185
H	2.976936	-2.503332	-3.494947
H	1.851534	-3.898901	-3.676201
H	1.330272	-2.252818	-4.190462
N	2.512913	0.506755	-0.705467
C	5.067012	0.735881	-0.518709
H	5.297911	-0.125458	-1.125315
C	4.446871	2.982336	1.093883
H	4.200910	3.843193	1.710474
C	5.763847	2.629260	0.851093
H	6.571590	3.216144	1.280272
C	6.063560	1.516563	0.051793
H	7.102536	1.252647	-0.127197
C	-0.464610	1.359547	-1.596165
O	0.160728	1.090647	-2.611866
N	0.067421	1.133385	-0.275903
C	-1.783866	2.058935	-1.607205
C	-2.908706	1.460649	-2.168947
C	-1.838492	3.389022	-1.182390
C	-4.096189	2.175797	-2.276183
H	-2.847715	0.423187	-2.478420
C	-3.020590	4.112489	-1.315849
H	-0.954077	3.856240	-0.754767
C	-4.151936	3.504515	-1.857547
H	-4.978088	1.697907	-2.693951

H	-3.056561	5.152374	-1.002244
H	-5.075779	4.068361	-1.958183
H	0.359277	-0.955327	-1.700179
O	-1.266225	-1.030248	-1.246414
O	-2.878673	-2.616782	-0.950642
C	-2.055224	-2.027549	-1.652835
C	-1.736147	-2.381030	-3.093986
H	-0.757188	-2.880496	-3.066692
H	-2.492565	-3.047117	-3.513488
H	-1.624005	-1.469612	-3.693268
H	-0.510201	1.731588	0.589260
O	-2.561580	0.485254	0.942405
O	-1.225081	2.244393	1.405334
C	-2.384512	1.680520	1.370640
C	-3.584396	2.463668	1.813583
H	-3.936049	3.049982	0.952192
H	-4.383644	1.789309	2.130555
H	-3.304910	3.157882	2.611453

INX4'
SCF done: -2002.164027

Rh	0.926285	-0.944536	-0.586283
N	-1.308203	-0.888825	1.894775
C	-0.681099	-2.387628	-1.100804
C	-0.308919	-1.597127	-2.264589
C	1.062806	-1.833106	-2.544904
C	1.580963	-2.714757	-1.515173
C	0.475328	-3.074997	-0.644794
O	-1.200972	-1.884383	2.840150
C	-2.563308	-0.413118	1.666002
C	-1.700989	1.267157	-0.109386
C	-3.924809	0.886269	0.070909
C	-2.293084	1.951874	-1.124535
C	-3.699744	1.722387	-1.044235
H	-1.755601	2.563473	-1.841701
O	-3.554834	-0.880599	2.186804
C	0.537246	-3.988415	0.524954
H	1.561617	-4.082089	0.893319
H	-0.079066	-3.609211	1.349218
H	0.159687	-4.981358	0.245979
C	2.963618	-3.242029	-1.426474
H	3.299417	-3.231083	-0.384769
H	3.000105	-4.270373	-1.811434
H	3.657024	-2.632587	-2.013294
C	1.839362	-1.259049	-3.673656

H	2.905654	-1.209140	-3.432379
H	1.725230	-1.883251	-4.569176
H	1.498246	-0.246407	-3.909613
C	-1.219327	-0.729445	-3.054563
H	-0.692578	0.157555	-3.422660
H	-1.611675	-1.282451	-3.918521
H	-2.072913	-0.383415	-2.461744
C	-2.061827	-2.568729	-0.584130
H	-2.685416	-1.679612	-0.728335
H	-2.540665	-3.388592	-1.137440
H	-2.074023	-2.825754	0.478728
C	-1.314918	-1.348706	4.157709
H	-2.330808	-0.981728	4.339021
H	-1.091791	-2.178271	4.833856
H	-0.587937	-0.538178	4.305157
N	-2.669847	0.583944	0.651453
C	-5.217083	0.494067	0.425897
H	-5.389424	-0.139287	1.284979
C	-4.774864	2.168662	-1.818984
H	-4.597756	2.815623	-2.675539
C	-6.055224	1.776459	-1.470825
H	-6.905156	2.113999	-2.059521
C	-6.266622	0.948991	-0.360496
H	-7.280380	0.654461	-0.098934
C	0.234554	1.861704	1.257366
O	-0.288247	1.716984	2.343022
N	-0.304799	1.259098	0.091707
C	1.454672	2.684621	1.063457
C	2.503513	2.556396	1.974078
C	1.505917	3.664231	0.070496
C	3.613063	3.383210	1.872470
H	2.436612	1.796392	2.748356
C	2.603336	4.515440	-0.005186
H	0.685928	3.769543	-0.637368
C	3.659298	4.369448	0.888705
H	4.439825	3.268200	2.568971
H	2.635298	5.289218	-0.768522
H	4.522146	5.028276	0.821828
H	-0.444688	-0.352766	1.818540
O	1.401261	-0.679476	1.432312
O	2.986925	-2.271335	1.548953
C	2.264580	-1.421727	2.056792
C	2.279999	-1.186595	3.552556
H	1.626226	-1.937462	4.013561

H	3.288573	-1.331224	3.947368
H	1.897213	-0.196264	3.821221
H	0.169309	1.527620	-0.792042
O	2.527929	0.388121	-0.947233
O	1.220462	1.657195	-2.259011
C	2.330965	1.330081	-1.793795
C	3.585520	2.049704	-2.223283
H	4.187759	2.297271	-1.343484
H	4.186099	1.384411	-2.854609
H	3.337308	2.955335	-2.781291

TSC7

SCF done: -1373.669480

Rh	0.620809	0.261654	-0.054134
N	0.142790	-1.795080	0.005106
C	-0.120682	1.359332	-1.762175
C	0.681025	2.279536	-0.974953
C	2.002610	1.759829	-0.920402
C	2.046304	0.524092	-1.671176
C	0.741952	0.309042	-2.229685
O	1.968457	-0.071698	1.608512
O	0.310237	-0.585337	3.020054
C	1.527225	-0.450604	2.733344
C	2.541586	-0.804562	3.786952
H	2.148774	-0.589232	4.783048
H	2.731455	-1.882893	3.728184
H	3.484448	-0.280473	3.616950
O	1.185533	-2.554438	-0.546895
C	-1.033409	-2.272828	-0.493764
C	-3.435949	-1.772077	-0.630803
C	-2.243987	-0.267725	0.540267
C	-4.324863	-0.813156	-0.256417
H	-3.556842	-2.685016	-1.197399
C	-3.591329	0.168570	0.490729
H	-5.382853	-0.801436	-0.484548
O	-1.219352	-3.282337	-1.147612
C	0.354294	-0.825314	-3.109619
H	0.809302	-1.763395	-2.775059
H	-0.729699	-0.976994	-3.128337
H	0.683653	-0.629808	-4.138575
C	3.241716	-0.342958	-1.850568
H	2.943272	-1.393713	-1.932205
H	3.809602	-0.070440	-2.750535
H	3.913726	-0.256144	-0.989107

C	3.156559	2.312346	-0.163505
H	3.497974	1.586367	0.585395
H	3.994844	2.525898	-0.838255
H	2.895121	3.237489	0.357607
C	0.205027	3.565314	-0.395135
H	0.782599	3.844641	0.492407
H	0.298756	4.378088	-1.127723
H	-0.845541	3.503127	-0.093351
C	-1.548444	1.550516	-2.137188
H	-2.087333	2.128898	-1.379960
H	-1.629010	2.085763	-3.092723
H	-2.068115	0.591935	-2.243313
C	2.014987	-3.067525	0.472939
H	1.419794	-3.571704	1.245989
H	2.671513	-3.795817	-0.014402
H	2.622396	-2.274557	0.931525
N	-2.167028	-1.455607	-0.162142
C	-3.921777	1.387120	1.089687
H	-4.948835	1.747437	1.068283
C	-1.215628	0.451710	1.169948
H	-0.400438	-0.147290	1.982584
C	-2.926766	2.130938	1.718528
H	-3.182924	3.070808	2.203503
C	-1.608369	1.668778	1.753466
H	-0.853886	2.247075	2.290013

TSC2

SCF done: -1373.671854

Rh	0.627721	-0.079427	0.003677
N	0.207934	-1.809117	1.131946
C	-0.374819	0.166926	-1.999960
C	0.572791	1.260821	-1.822530
C	1.876529	0.684558	-1.696139
C	1.753374	-0.761092	-1.752284
C	0.354789	-1.072243	-1.966743
O	2.105917	0.624486	1.372089
O	1.270894	2.759576	1.403403
C	2.178618	1.886064	1.628662
C	3.465443	2.376607	2.254105
H	3.829833	3.241926	1.688379
H	3.260529	2.714789	3.277883
H	4.212358	1.580662	2.269562
O	0.859886	-3.026968	0.682537
C	-1.171873	-1.994476	1.250451

C	-0.665161	0.301216	1.816900
C	-2.727417	-0.058299	0.954194
C	-1.012491	1.522707	1.221574
H	0.089705	0.119271	2.570874
C	-2.360364	1.299967	0.714745
H	0.102581	2.387701	1.267846
O	-1.878452	-2.971289	1.069014
C	-0.207241	-2.442993	-2.122925
H	0.223262	-3.105395	-1.363526
H	-1.294944	-2.443189	-1.986817
H	0.024818	-2.835438	-3.123687
C	2.861685	-1.754161	-1.671566
H	2.495773	-2.665589	-1.185303
H	3.233904	-2.014273	-2.673904
H	3.698666	-1.359723	-1.081400
C	3.156692	1.413361	-1.463669
H	3.709047	0.955784	-0.631944
H	3.786421	1.369672	-2.363775
H	2.973647	2.466409	-1.219459
C	0.250005	2.719103	-1.824926
H	0.773005	3.229888	-1.008023
H	0.539462	3.180918	-2.780160
H	-0.825533	2.872896	-1.680920
C	-1.820787	0.308977	-2.309686
H	-2.269841	1.140779	-1.759026
H	-1.948786	0.491876	-3.387531
H	-2.376130	-0.596900	-2.040087
C	2.048266	-3.161494	1.510932
H	1.774219	-3.284134	2.565105
H	2.557674	-4.058374	1.141949
H	2.693662	-2.279322	1.400247
N	-1.683872	-0.687103	1.639950
C	-3.272999	2.148760	0.080796
H	-3.019677	3.195654	-0.075073
C	-3.929626	-0.586185	0.499672
H	-4.157892	-1.634936	0.659672
C	-4.498933	1.636710	-0.330116
H	-5.224416	2.287045	-0.811632
C	-4.812214	0.281448	-0.136927
H	-5.772541	-0.095747	-0.479078