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Rh(II)-Catalysed N^2-Selective Arylation of Benzotriazoles and Indazoles using Quinoid Carbenes via 1,5-H Shift

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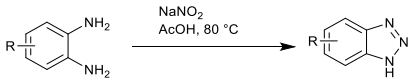
Experimental Section

General information: All commercially available compounds were used without further purification. Solvents for elution in column were distilled. Analytical thin layer chromatography (TLC) was performed on pre-coated silica gel 60 F254. Visualization on TLC was achieved using UV light (254 nm). Column chromatography was undertaken on silica gel (230-400 mesh). ^{1}H and ^{13}C NMR spectra were recorded on BRUKER ULTRA SHIELD and BRUKER ASCEND (400 MHz and 500 MHz) instruments. Chemical shifts were quoted in parts per million (ppm) referenced to the appropriate solvent peak or 0.0 ppm for tetramethylsilane. The following abbreviations were used to describe peak splitting patterns when appropriate: br= broad, s= singlet, d= doublet, t= triplet, q= quartet, dd= doublet of doublet, td= triplet of doublet, ddd= doublet of doublet of doublet, m= multiplet. Coupling constants, *J*, were reported in hertz unit (Hz). ^{13}C NMR spectra were fully decoupled by broad band proton decoupling. Chemical shifts were reported in ppm referenced to the centre of a triplet at 77.16 ppm of $CDCl_3$. Infrared (IR) spectra were recorded using Spectrum BX FTIR instrument from Perkin Elmer. Frequencies are given in reciprocal centimeters (cm^{-1}) and only selected absorbance peaks are reported. High-resolution mass spectra were obtained from Agilent AdvanceBio 6545XT LC/Q-TOF (1260 Infinity II). LC-MS were obtained from Agilent Technologies A6120BW (single quadruple mass analyzer). Materials were obtained from commercial suppliers or prepared according to standard procedures unless otherwise noted.

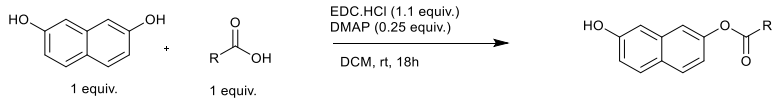
1. General procedure for the synthesis of starting materials:

1.1 General procedure for the synthesis of Benzotriazole[1]:

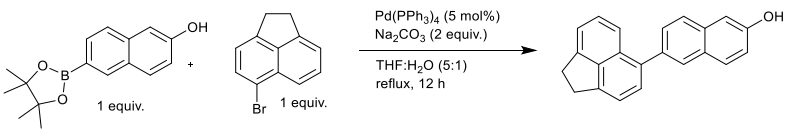


Aqueous $NaNO_2$ solution (25 mL, 1 M) was added to a solution of aryl-1,2-diamine (5 mmol) in acetic acid (10 mL). The solution stirred at 80 °C for 1 hour. After cooling to room temperature pH value of the reaction mixture was adjusted to 4.4-4.6 by adding 40% NaOH aqueous solution and 1 M HCl dropwise. The precipitated residue was collected by filtration. The precipitated residue was washed by 5% ice cold NaCl aqueous solution. The precipitate was recrystallized with (CH_2Cl_2/CH_3OH).

1.2 General procedure for the preparation of biologically relevant naphthol



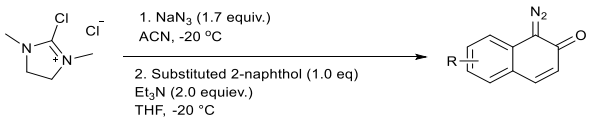
To a solution of carboxylic acid compound (1.0 equiv) and 2,7-dihydroxynapthalene (1.0 equiv) in CH_2Cl_2 (38 mL, 0.5 M), EDC.HCl (4.04 g, 21.1 mmol, 1.1 equiv) and DMAP (586.4 mg, 4.8 mmol, 0.25 equiv) were added under N_2 flow. The reaction mixture was stirred for 18 h at room temperature. The resulting mixture was quenched with saturated $NaHCO_3$ solution (20 mL) and extracted with CH_2Cl_2 (60 mL ×3), washed with brine (50 mL×1). The combined organic layer was dried over Na_2SO_4. After removal of the solvent, the resulting crude mixture was purified by silica gel column chromatography using 20% ethylacetate in hexane to give the desired product.



6-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)naphthalen-2-ol was prepared from previous reported procedure[2] starting from 6-bromo-2-naphthol. Next this naphthol (1 equiv.) and aromatic halide (1 equiv.) was taken in a round bottom flask followed by sodium carbonate (2 equiv.), tetrakis(triphenylphosphine)palladium (5 mol%) and THF:water (5:1) was added

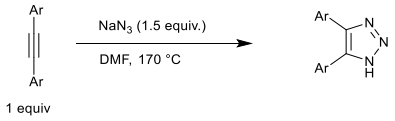
under nitrogen atmosphere. The system was degassed for 20 minutes and refluxed for 12 hours. The progress of reaction was monitored by TLC. After completion it was extracted with ethylacetate. The combined organic layers were dried over anhydrous Na_2SO_4. After removal of the solvent, the resulting crude mixture was purified by silica gel column chromatography using 20% ethylacetate in hexane to give the desired product with 82% yield.

1.3 General procedure for the preparation of diazonaphthoquinones[3]:



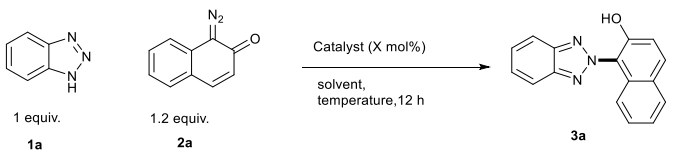
To a solution of 2-chloro-1,3-dimethylimidazoliniumchloride (228 mg, 1.35 mmol) in acetonitrile (2.0 mL), sodium azide (99.4 mg, 1.5 mmol) was added at -20 °C and the mixture was stirred for 30 min. A mixture of 2-naphthol (130 mg, 0.90 mmol) and triethylamine (0.25 mL, 1.8 mmol) in THF (4.0 mL) were added to the reaction mixture and was stirred for 20 min. The reaction was quenched with water and organic parts were extracted with CH_2Cl_2 (3 x 15 mL). The combined extracts were washed with water and brine, and then dried over anhydrous Na_2SO_4. The solvent was removed in vacuum to afford crude compounds. The crude materials were purified by flash column chromatography to give pure diazonaphthoquinone (80 – 90% yield).

1.4 General procedure for the preparation of 4,5-diaryl-1*H*-1,2,3-triazole[4]



Diarylacetylene (2 mmol, 1 equiv.) and sodium azide (3 mmol, 1.5 equiv.) were taken in 5 ml dry DMF in a sealed tube and it was heated at 170 °C for 5 hours in oil bath. The reaction was quenched with water and extracted with ethyl acetate. The organic layer was removed in vacuum and purified by column chromatography using 20 % ethyl acetate in hexane.

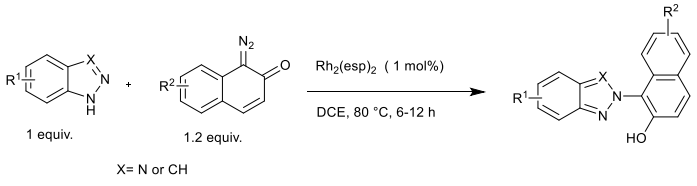
1.3 Table 1: Reaction optimisation



SL No.	Catalyst (XX mol%)	Sovent	Temperature (^oC)	$N^2:N^{1c}$	Yield[a] (%)
1	$Cu(OAc)_2$ (10)	DCE	50-90	-	trace
2	$CuBr_2$ (10)	DCE	50-90	-	trace
3	CuI (10)	DCE	50-90	-	trace
4	$Cu(OTf)_2$ (10)	DCE	50-90	-	trace
5	$Rh_2(Oct)_4$ (1)	DCE	50-90	-	trace
6	$Rh_2(OAc)_4$ (1)	DCE	50-90	-	n.d.
7	Ru(*p*-cymene)$Cl_2)_2$ (5)	DCE	50-90	-	n.d.
8	$Rh_2(esp)_2$ (1)	DCE	50	>99:1	48
9	$Rh_2(esp)_2$ (1)	Toluene	50	>99:1	38
10	$Rh_2(esp)_2$ (1)	Acetonitrile	50	4:3	33
11	$Rh_2(esp)_2$ (1)	Dioxane	50	5:1	26
12	$Rh_2(esp)_2$ (1)	MeOH	50	-	n.d.
13	$Rh_2(esp)_2$ (1)	DCM	50	>99:1	36
14	$Rh_2(esp)_2$ (1)	Chloroform	50	>99:1	42
15	$Rh_2(esp)_2$ (1)	DCE	40	>99:1	41
16	$Rh_2(esp)_2$ (1)	DCE	60	>99:1	73
17	$Rh_2(esp)_2$ (1)	DCE	70	>99:1	83
18	$Rh_2(esp)_2$ (1)	DCE	80	>99:1	91 (86)[b]
19	$Rh_2(esp)_2$ (1)	DCE	90	>99:1	84

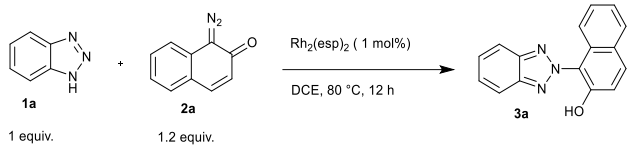
Reaction conditions **1a** (0.1 mmol), **2a** (0.12 mmol), solvent 1 ml; [a]Yield was calculated by ^1H NMR using 1,3,5 trimethoxybenzene as standard; [b]isolated yield. [c]Determined by ^1H NMR analysis.

1.4.1 General procedure for rhodium(II) catalyzed N^2- selective arylation of benzotriazole and indazole using diazonaphthoquinone:



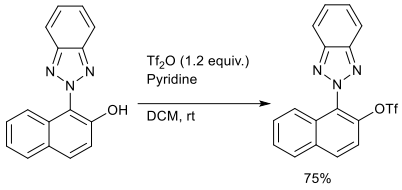
In a 10 mL screw cap vial equipped with magnetic stirring bar, benzotriazole or indazole derivatives (0.20 mmol), $Rh_2(esp)_2$ (0.002 mmol, 1 mol%), and diazonaphthoquinone (0.24 mmol) were taken in a 2 ml dry 1,2-dicholroethane solvent. The reaction mixture was stirred at 80 °C temperature in an oil bath for 6 -12 h. The progress of reaction was checked by thin layer chromatography using 20 % ethylacetate in hexane. After the completion, the reaction mixture was purified directly through silica gel column chromatography with 10 to 20 % ethyl acetate/hexane as eluent to give the desired product.

1.4.2 Scale up synthesis:



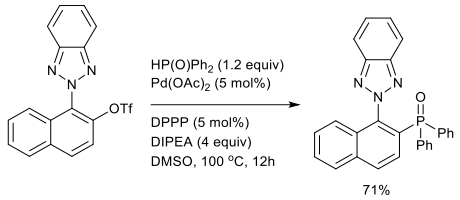
In a 10 mL screw cap vial equipped with magnetic stirring bar benzotriazole (5 mmol, 595 mg), $Rh_2(esp)_2$ (0.05 mmol, 1 mol%), and diazonaphthoquinone (6 mmol) were taken in a 20 ml dry 1,2-dicholroethane solvent. The reaction mixture was stirred at 80 °C temperature in an oil bath for 12 h. The progress of reaction was checked by thin layer chromatography using 20 % ethylacetate in hexane. After the completion, the reaction mixture was purified directly through silica gel column chromatography with 10 to 20 % ethyl acetate/hexane as eluent to give the desired product **3a**.

1.4.3 Synthesis of 1-(2*H*-benzo[*d*][1,2,3]triazol-2-yl)naphthalen-2-yl trifluoromethanesulfonate (6):



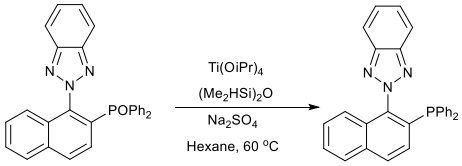
To a solution of 1-(2*H*-benzo[*d*][1,2,3]triazol-2-yl)naphthalen-2-ol (130.64 mg, 0.5 mmol) in dry CH_2Cl_2, pyridine (80 µL, 2.0 equiv.) was added and the solution was cooled to 0 ºC. Next, triflic anhydride (252 µL, 1.5 equiv.) was added dropwise and stirred for 8h at room temperature. After completion of the reaction time, the reaction mixture was concentrated under reduced pressure. The crude product was purified by flash column chromatography to obtain a quantitative yield of triflated product **6** (147.5 mg, 75%).

1.4.4 Synthesis of (1-(2*H*-benzo[*d*][1,2,3]triazol-2-yl)naphthalen-2-yl)diphenylphosphine oxide (8):



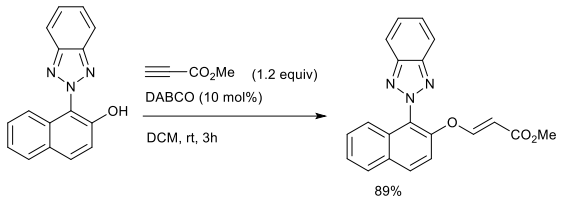
In a 10 mL round bottom flask 1-(2*H*-benzo[*d*][1,2,3]triazol-2-yl)naphthalen-2-yl trifluoromethanesulfonate **6** (78.67 mg, 0.2 mmol) was dissolved in dry DMSO (2 ml). Next, $Pd(OAc)_2$ (2.24 mg, 5 mol%) and DPPP (diphenyl phosphinopropane) (4.12 mg, 5 mol%) were added to the reaction mixture. After that, $^{i}Pr_2NEt$ (139 μL, 4.0 equiv.) and diphenylphosphine oxide [$HP(O)Ph_2$] (44 mg, 1.1 equiv.) were added sequentially to the reaction mixture. The resulting solution was stirred for 12 h under nitrogen atmosphere at 100 ºC in a pre-heated oil bath. On completion of reaction time, solvent was removed under reduced pressure and crude residue was purified via flash column chromatography on silica gel to obtain the desired phosphine oxide product **8** in 71% (63.2 mg) isolated yield.

1.4.5 Synthesis of 2-(2-(diphenylphosphaneyl)naphthalen-1-yl)-2H-benzo[*d*][1,2,3]triazole (11):



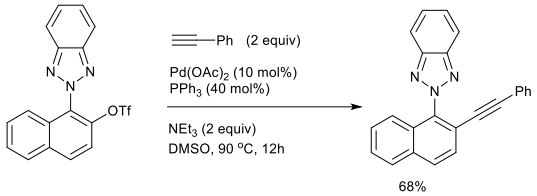
An oven dried 25 ml round bottom flask charged with a stir bar, phosphine oxide (**8**, 0.2 mmol, 1.0 equiv), anhydrous Na_2SO_4 (20 wt%), and hexanes (2 mL), followed by tetramethyldisiloxane (0.6 mmol, 3.0 equiv) and $Ti(OiPr)_4$ (0.40 mmol, 2.0 equiv) were added. The heterogeneous mixture was stirred at 60 ºC overnight (12 h) under N_2. Upon completion of the reaction, as determined by TLC, the reaction mixture was passed through a plug of silica, washed with 10% EtOAc in hexanes, and concentrated in vacuo. The residue was then dissolved in THF and stirred vigorously with NaOH (3 M aq.) at 0 ºC overnight. The mixture was then dried over Na_2SO_4, and purified by silica gel chromatography (5% EtOAc in hexanes) to obtain the pure phosphine product **11** in 64% yield (54.9 mg).

1.4.6 Synthesis of methyl (*E*)-3-((1-(2*H*-benzo[*d*][1,2,3]triazol-2-yl)naphthalen-2-yl)oxy)acrylate (10):



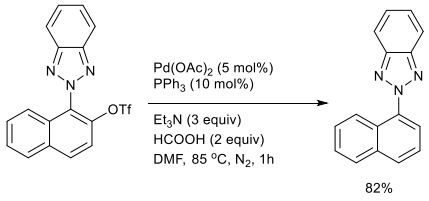
In an oven dried 25 mL round bottom flask, 1-(2*H*-benzo[*d*][1,2,3]triazol-2-yl)naphthalen-2-ol **3a** (0.2 mmol) was dissolved in 5 ml dry DCM. Then 10 mol% of DABCO and methyl propiolate (1.2 equiv.) were added. The reaction mixture was allowed to stir at room temperature for 3h under the nitrogen atmosphere. The solvent was evaporated under reduced pressure. The residue was purified by silica gel column chromatography using 40% ethyl acetate in hexane as eluent to afford the desired product **10** in 70% yield (61.5 mg).

1.4.7 Synthesis of 2-(2-(phenylethynyl)naphthalen-1-yl)-2*H*-benzo[*d*][1,2,3]triazole (9):



To a dry 25 mL round bottom flask was charged with 1-(2*H*-benzo[*d*][1,2,3]triazol-2-yl)naphthalen-2-yl trifluoromethanesulfonate **6** (78.67 mg, 0.2 mmol) in DMSO solvent. After that phenylacetylene (40.8 mg, 0.4 mmol, 2.0 equiv.), Et_3N (56 µL, 0.4 mmol, 2.0 equiv.), $Pd(OAc)_2$ (9.0 mg, 0.04 mmol, 10 mol%) and PPh_3 (42.0 mg, 0.16 mmol, 40 mol%) were added to the reaction mixture under argon atmosphere. The mixture was stirred at 90 °C in a pre-heated oil bath for 12 h until the starting material disappeared (monitored by TLC). Then, the solvent was removed under reduced pressure and the crude product was purified by silica gel column chromatography using 20% ethyl acetate in hexane to afford the title compound **9** as white solid in 68% yield (46.9 mg).

1.4.8 Synthesis of 2-(naphthalen-1-yl)-2*H*-benzo[*d*][1,2,3]triazole (7):

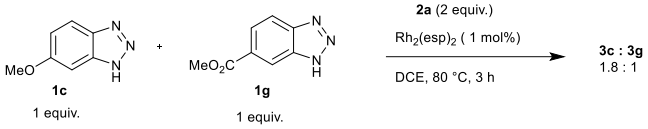


To a dry 25 mL round bottom flask was charged with 1-(2*H*-benzo[*d*][1,2,3]triazol-2-yl)naphthalen-2-yl trifluoromethanesulfonate **6** (78.67 mg, 0.2 mmol) DMF solvent. Then the

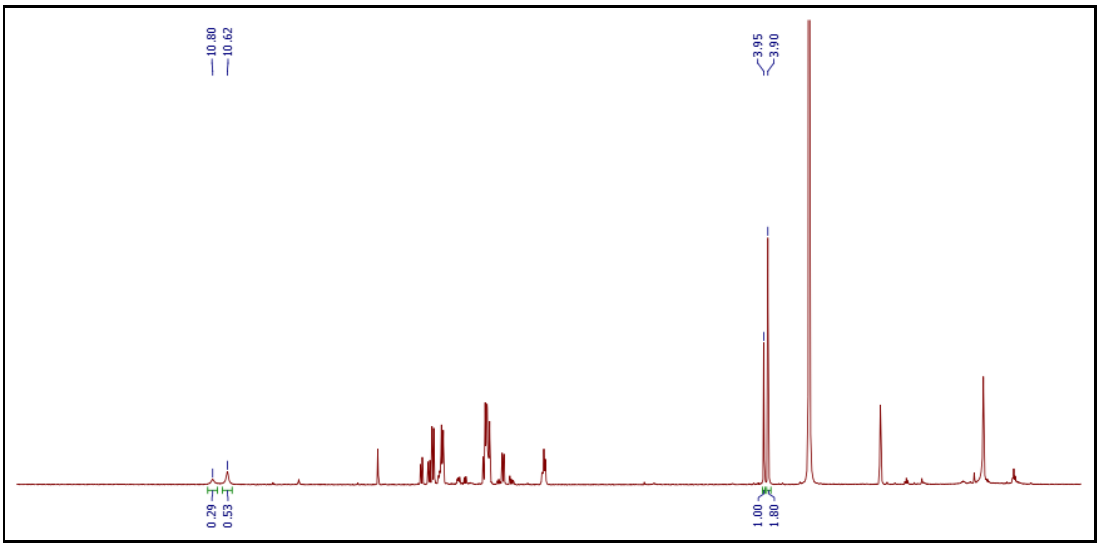
solution was treated with $Pd(OAc)_2$ (5 mol%), PPh_3 (10 mol%), triethylamine (3 equiv), and formic acid (2 equiv) and the temperature was slowly raised to 85 ^oC. After 1h, the reaction mixture cooled to room temperature and diluted with ethyl acetate. The organic layer was washed three times with water and dried with sodium sulfate. Then, the solvent was removed under reduced pressure and the crude product was purified by silica gel column chromatography using 20% ethyl acetate in hexane to get the desired product **7** in 82% yield (41.7 mg).

1.5 Kinetic experiments

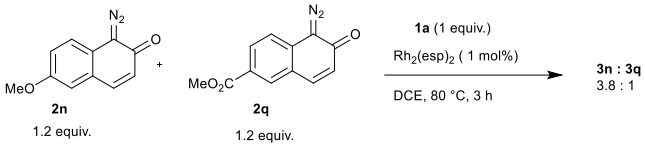
1.5.1 Kinetic experiments with electronically variable benzotriazole derivative:



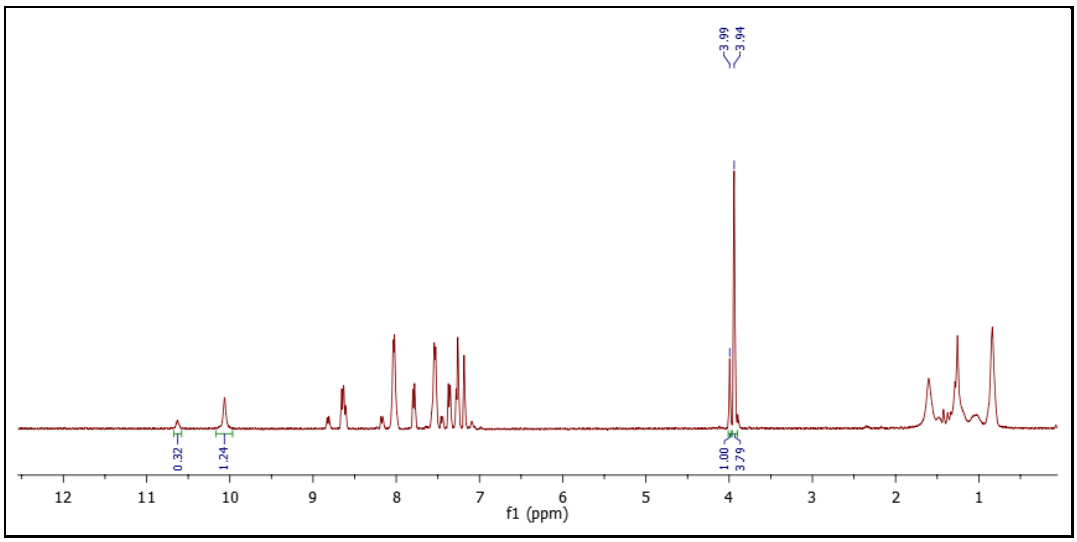
To an oven-dried 10 mL screw cap vial equipped with a magnetic stirring bar **1c** (0.1 mmol) and **1g** (0.1 mmol) were taken in 2 ml DCE. Then $Rh_2(esp)_2$ (0.001 mmol, 1 mol%), and diazonaphthoquinone (0.12 mmol) were added subsequently. Next it was stirred for 3 hours at 80 °C in oil bath. After cooling to room temperature, the solvent was removed under reduced pressure, and filtered through silica gel column chromatography using an 20% ethylacetate in hexane mixture as the eluent and product ratio was monitored via ^1H NMR spectroscopy of crude product mixture (**3c** : **3g** = 1.8:1) in DMSO-D_6.



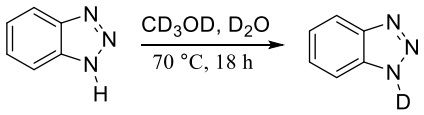
1.5.2 Kinetic experiments with electronically variable diazonaphthoquinone derivative:



To an oven-dried 10 mL screw cap vial equipped with a magnetic stirring bar **2n** (0.12 mmol) and **2q** (0.12 mmol) were taken in 2 ml DCE. Then $Rh_2(esp)_2$ (0.001 mmol, 1 mol%), and benzotriazole (0.1 mmol) were added subsequently. Next it was stirred for 3 hours at 80 °C in oil bath. After cooling to room temperature, the solvent was removed under reduced pressure, and filtered through silica gel column chromatography using an 20% ethylacetate in hexane mixture as the eluent and product ratio was monitored via ^{1}H NMR spectroscopy of crude product mixture (**3n** : **3q** = 3.8:1) in $CDCl_3$.

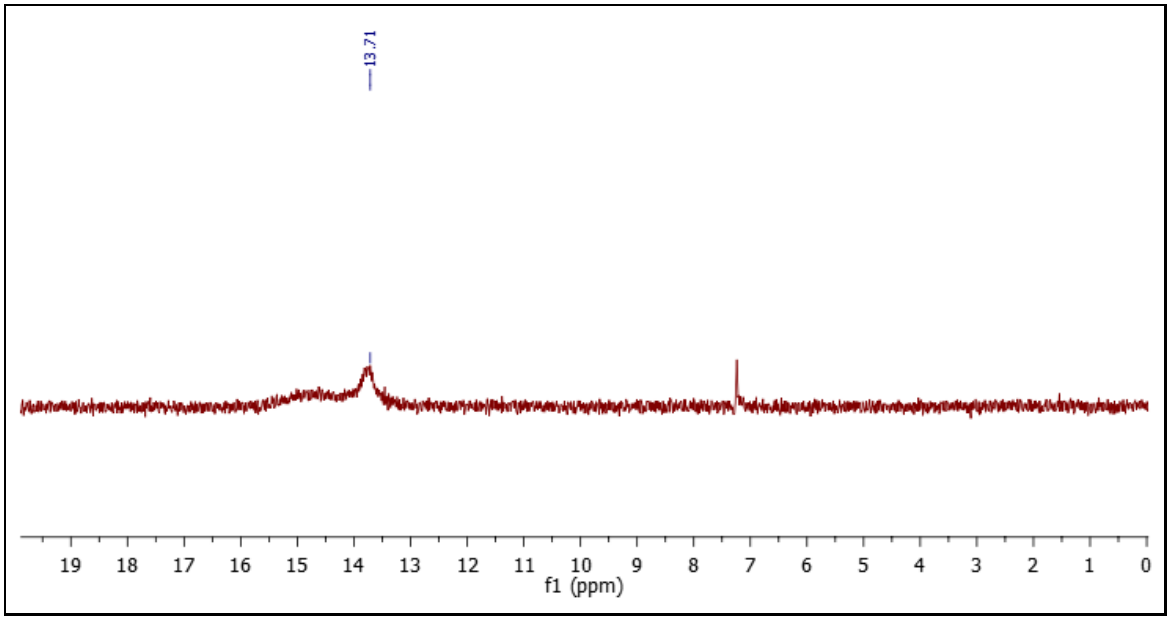


1.5.3 Synthesis of deuterated benzotriazole substrate:

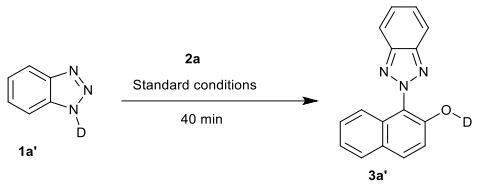


297.8 mg 1H-benzotriazole (2.50 mmol, 1.0 equiv) was dissolved in 1.5 mL deuteromethanol-d4 at room temperature. Then 0.25 mL D_2O was added to mixuter. The mixture was stirred at 70°C for 18 hours. the mixture under was concentrated under reduced pressure to obtain 1*D*-benzotriazole. HRMS: Calculated for $[M]^+$ $C_6H_4DN_3$; 120.0546, found 120.0550.

^{2}H NMR (92 MHz, $CHCl_3$) of deuterated benzotriazole substrate:

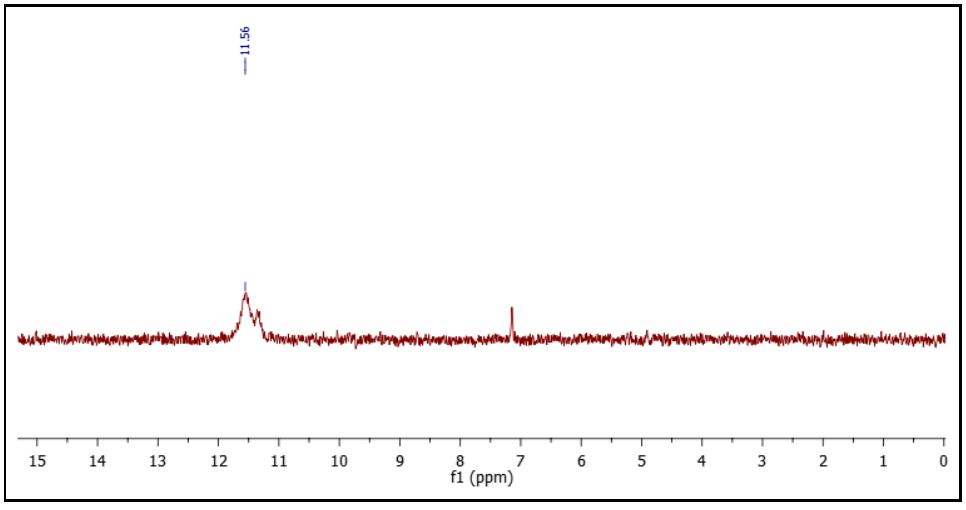


1.5.4 Kinetic experiments with deuterated benzotriazole substrate:

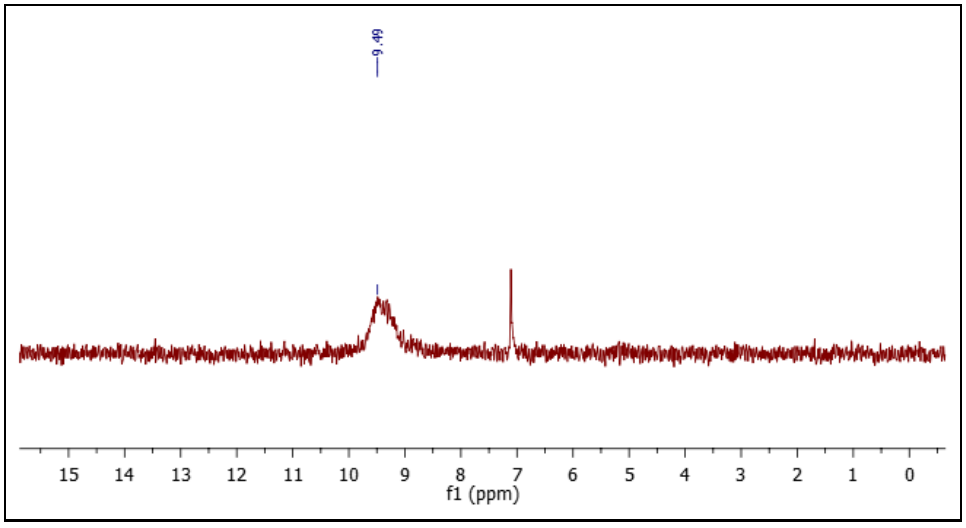


In NMR tube deuterated benzotriazole(**1a'**) (0.05 mmol), $Rh_2(esp)_2$ (0.0005 mmol, 1 mol%), and diazonaphthoquinone(**2a**) (0.06 mmol) were taken in a 0.6 ml dry chloroform solvent. And a ^2H NMR was recorded at room temperature. Next the reaction mixture was stirred at 60 °C temperature in a water bath for 40 minutes. Then the NMR tube was cooled to room temperature and again ^2H NMR was recorded.

^{2}H NMR (92 MHz, $CHCl_3$) of reaction mixture (time: 0 min)



^{2}H NMR (92 MHz, $CHCl_3$) of reaction mixture (time: 40 min)



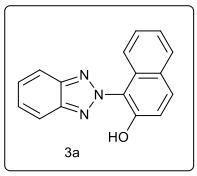
2 X-ray crystallographic data:

2.1 X-ray crystallographic data of compound 3a:

The crystal structures have been deposited at the Cambridge Crystallographic Data Centre. CCDC No of **3a** is 2264523. The structure solution and refinement were processed by SHELXTL.

2.2 Method of crystallization of compound 3a: Compound **3a** was dissolved in a minimum volume of chloroform and kept at room temperature for slow evaporation. Needle -shaped white colour crystal was formed and was subjected to single crystal x-ray analysis.

2.3 Single crystal x-ray data of compound 3a (CCDC No: 2264523):



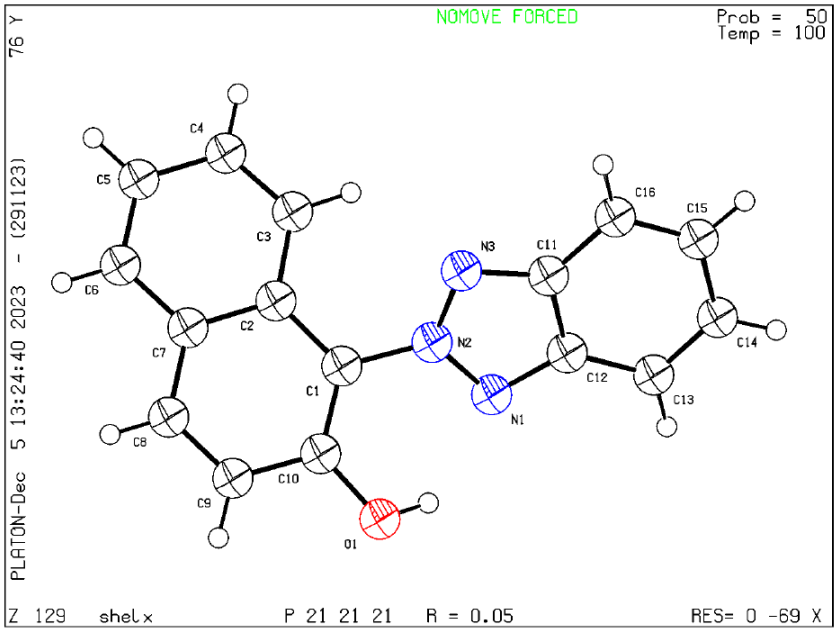


Figure: S1 ORTEP view of the molecular structure of **3a** with thermal ellipsoids drawn at the 50% probability level.

2.4 Crystal data and structure refinement for compound 3a (CCDC no: 2264523)

Datablock: shelx

Bond precision:	C-C = 0.0030 A		Wavelength=0.71073
Cell:	a=3.74100	b=17.18700	c=18.37100
	alpha=90	beta=90	gamma=90
Temperature:	100 K		
	Calculated		Reported
Volume	1181.192		1181
Space group	P 21 21 21		P 21 21 21
Hall group	P 2ac 2ab		P 2ac 2ab
Moiety formula	C16 H11 N3 O		?
Sum formula	C16 H11 N3 O		C8 H5.50 N1.50 O0.50
Mr	261.28		130.64
Dx,g cm-3	1.469		1.469
Z	4		8
Mu (mm-1)	0.096		0.096
F000	544.0		544.0
F000'	544.21		
h,k,lmax			5,24,24
Nref			3590
Tmin,Tmax	0.983,0.989		
Tmin'	0.982		
Correction method= Not given			
Data completeness=		Theta(max)= 31.113	
R(reflections)= 0.0502(2988)			wR2(reflections)= 0.1296(3590)
S = 1.035	Npar= 85		

2.5 X-ray crystallographic data of compound 5a:

The crystal structures have been deposited at the Cambridge Crystallographic Data Centre. CCDC No of **5a** is 2264605. The structure solution and refinement were processed by SHELXTL.

2.6 Method of crystallization of compound 5a: Compound **5a** was dissolved in a minimum volume of DMSO and kept at room temperature for slow evaporation. Needle -shaped white colour crystal was formed and was subjected to single crystal x-ray analysis.

2.7 Single crystal x-ray data of compound 5a (CCDC No: 2264605)

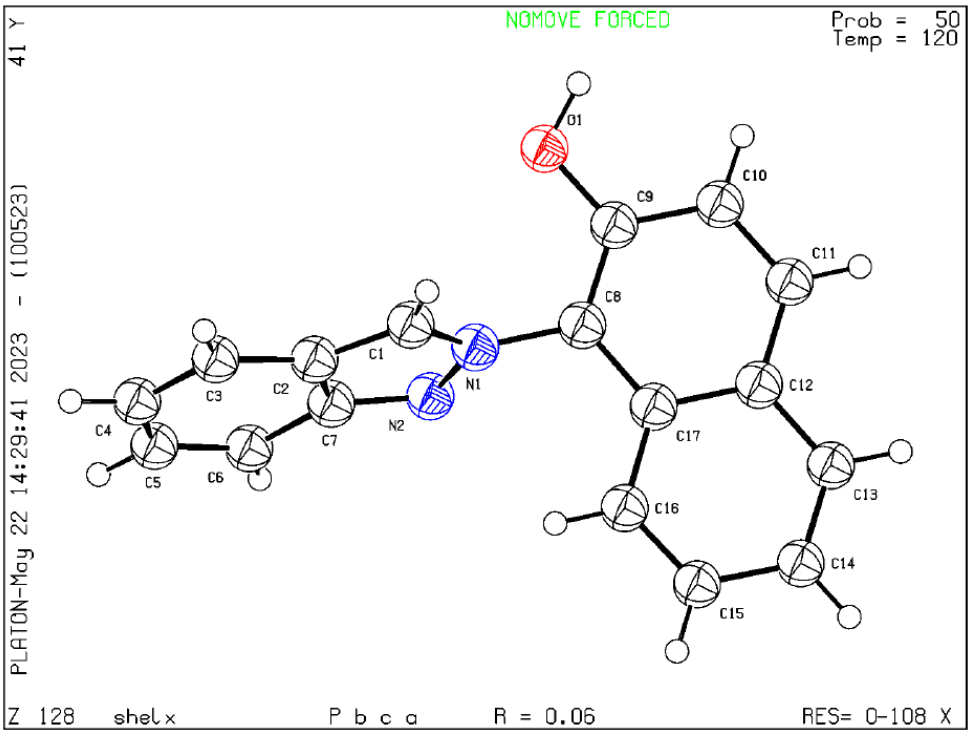


Figure: S2 ORTEP view of the molecular structure of **5a** with thermal ellipsoids drawn at the 50% probability level.

2.8 Crystal data and structure refinement for compound 5a (CCDC no: 2264605)

Datablock: shelx

Bond precision:	C-C = 0.0021 A		Wavelength=0.71073
Cell:	a=11.511(4)	b=10.247(3)	c=21.356(7)
	alpha=90	beta=90	gamma=90
Temperature: 120 K			
	Calculated		Reported
Volume	2519.0(14)		2519.0(13)
Space group	P b c a		P b c a
Hall group	-P 2ac 2ab		-P 2ac 2ab
Moiety formula	C17 H12 N2 O		?
Sum formula	C17 H12 N2 O		C17 H12 N2 O
Mr	260.29		260.29
Dx,g cm-3	1.373		1.373
Z	8		8
Mu (mm-1)	0.087		0.087
F000	1088.0		1088.0
F000'	1088.43		
h,k,lmax	16,14,30		16,14,30
Nref	3682		3674
Tmin,Tmax	0.984,0.990		
Tmin'	0.984		
Correction method= Not given			
Data completeness= 0.998		Theta(max)= 30.037	
R(reflections)= 0.0599(3013)			wR2(reflections)= 0.1658(3674)
S = 1.038	Npar= 83		

3. Computational Details.

All calculations were conducted using the Gaussian16 suite of programs.[5] We have used B3LYP functional[6] in combination with Grimme's empirical GD3 dispersion correction,[7] Def2SVP basis set[8] and W06 density fitting[9] to optimize possible intermediates and transition states in gas phase. Frequency analysis of each intermediate and transition states have been done at the same level of theory in gas phase. Furthermore, harmonic frequency calculations at the same level of theory enabled us to characterize transition states (with one imaginary normal mode) and intermediates (all real normal modes). Solution phase energy of intermediates and transition states are obtained at B3LYP-D3/Def2TZVP level of theory using CPCM solvent model[10] with the dielectric constant of dichloroethane, $C_2H_4Cl_2$ (ε=10.125) on the gas phase optimized geometries. All relative free energies in this article are calculated at B3LYP-D3/Def2TZVP/CPCM//B3LYP-D3/Def2SVP/W06 level of theory.

3.1 Methodology adapted for determination of free energy barrier in solution phase.

The thermodynamic parameter obtained after gas phase optimization and frequency analysis is listed below –

H_{corr} = Enthalpic correction obtained from gas phase harmonic frequency computation.

G_{corr} = Free energy correction obtained from gas phase harmonic frequency computation.

After single point calculation on the gas phase optimized geometry of intermediates and transition states in presence of polarizable continuum with dielectric constant of 10.125, the thermodynamic parameter obtained is given below –

E(CPCM)= Soln. phase energy obtained after single point energy calculation using CPCM solvent model.

We have determined solution phase free energy of each solute by the approximation mentioned Below-

$G^{0.5}_{(CPCM)} = E\ (CPCM) + H_{corr} + 0.5\ (G_{corr} - H_{corr})$, where $G^{0.5}_{(CPCM)}$ is corrected solution phase free energy.

using those solution phase corrected free energies we have determined free energy activation barriers and free energy change of each step.

$\Delta G^{\#}_{0.5} = G^{0.5}_{(CPCM)}\ (Ts) - G^{0.5}_{(CPCM)}\ (r)$

$\Delta G_{0.5} = G^{0.5}_{(CPCM)}\ (p) - G^{0.5}_{(CPCM)}\ (r)$

where,

$\Delta G^{\#}_{0.5}$ = free energy activation barrier.

$\Delta G_{0.5}$ = Free energy change of a reaction step.

Ts = transition state of a reaction step.

P = product of a reaction step.

and r = reactant of a reaction step.

3.2 Justification for the methodology adapted for free energy barrier determination.

Admittedly getting accurate free energy estimates for solution phase reactions is always challenging and at times questionable with quantum chemistry. Several recipes are used and its common to find questions being raised on their accuracy. Our general philosophy is that we always use the empirical correction to the entropy estimates derived from quantum chemistry. It must be noted that generally the entropy computation in quantum chemical computations follows from frequency computations which computes entropy through Sakur-Tetrode

Equation which essentially uses an ideal gas model, where each particle is considered to behave in a non-interacting ideal way.[11] It has been shown experimentally that the entropic reduction of noble gases is about 50% when they are dissolved in solution phase. This forms the basis for Wertz's approximation that there is reduction of entropy when a species is moved from gas phase to liquid phase.[12] One can easily see that this arises from substantial loss of translational freedom within a liquid. Hence, it has evolved as a general practice that a 50% scaling factor to gas phase entropy of a species is applied to estimate the solvent phase entropy. This reduction shows a marked effect for reaction free energy changes which involve association and in free energy activation barriers where the transition states are formed through associative pathways. Thus, we have adapted the empirical approximation to the entropy which uses a 50% scaling factor to entropic contribution to free energy estimated through the Sakur-Tetrode equation (assuming the species to behave as an ideal gas) for obtaining the entropic contribution to free energy in solution phase.[12]

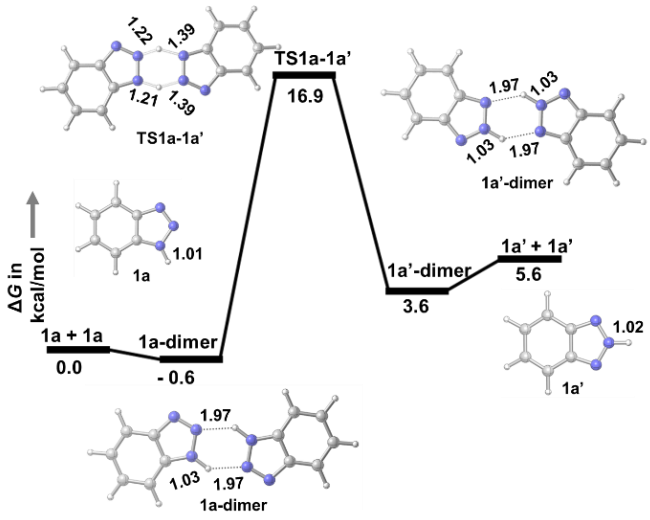


Figure S3. Relative Gibbs free energy profile at B3LYP-D3/Def2TZVP/CPCM($C_2H_4Cl_2$, ε=10.125) in kcal/mol. Optimized geometries at B3LYP-D3/Def2SVP/W06 level of theory are shown. Distances shown are in units of Å. Color codes: Rh (purple), N (blue), C (grey), H (white), O (red).

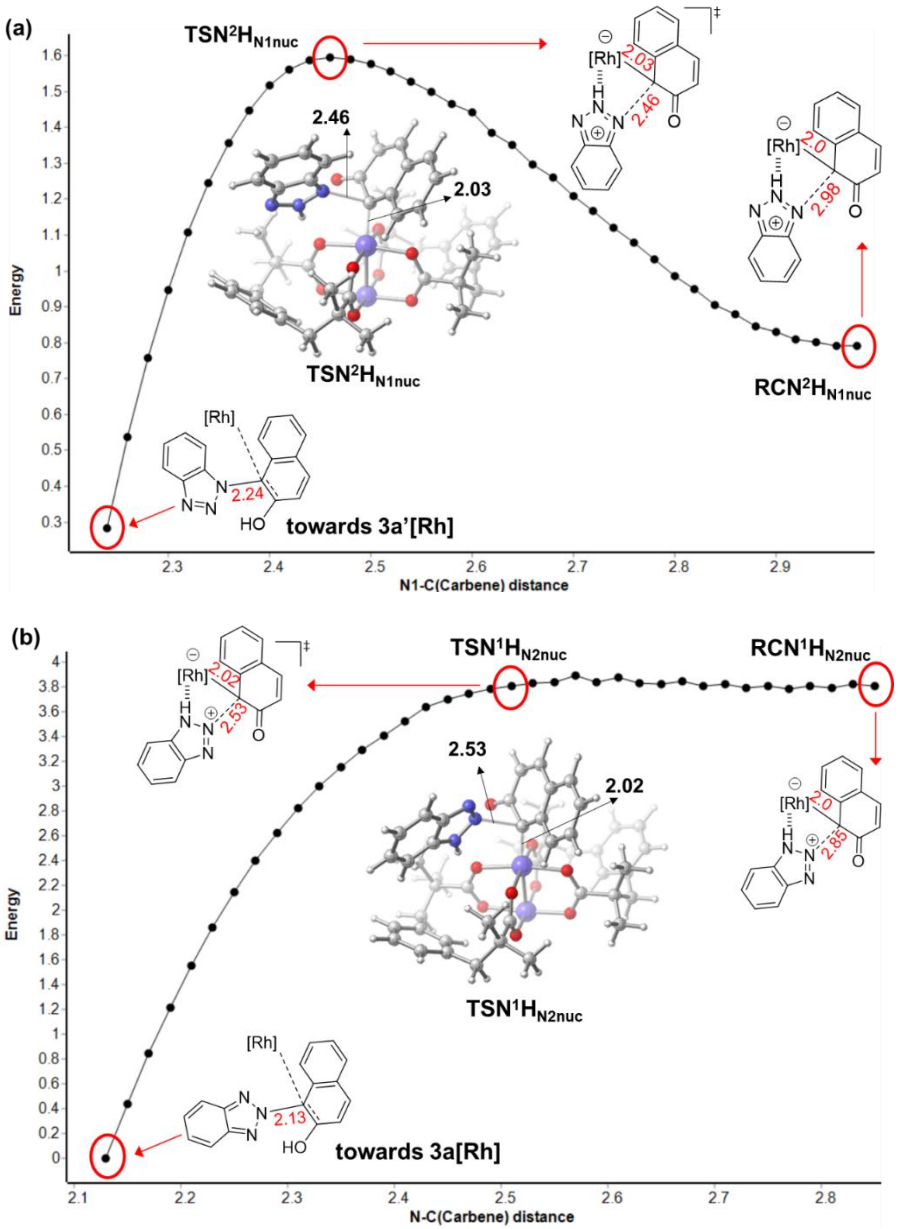


Figure S4. Linear transit scans of N-C(Carbene) distance in units of Å against electronic energy in units of kcal/mol starting from local reactant complexes (a) **RCN^{2}H$_{N1nuc}$** and (b) **RCN^{1}H$_{N2nuc}$** leading to products **3a'[Rh]** (unobserved) and **3a[Rh]** (observed) on nucleophilic attack and 1,3 H shift. Distances shown are in units of Å. Color codes: Rh (purple), N (blue), C (grey), H (white), O (red). The local intermediates **RCN^{2}H$_{N1nuc}$** and **RCN^{1}H$_{N2nuc}$** were identified at B3LYP/6-31G(d)/LanL2DZ+f (1.350) with Gaussian 09 suite of programs after repeated attempts failed with Gaussian 16. Linear transit scans and frequency calculations were also conducted at this level of theory followed by single point energy calculations in the solvent phase at B3LYP-D3/Def2TZVP/CPCM for the crucial stationary states along the surface. Notably, in both these reactant complexes, the esp ligand was re-oriented to a sterically less hindered conformer that opens up the coordination site on the metal coordinated to napthalone.

In fact, neither the reactant complexes nor the transition states are identified when the phenyl groups of $(esp)_2$ are in parallel fashion as in **RC1**.

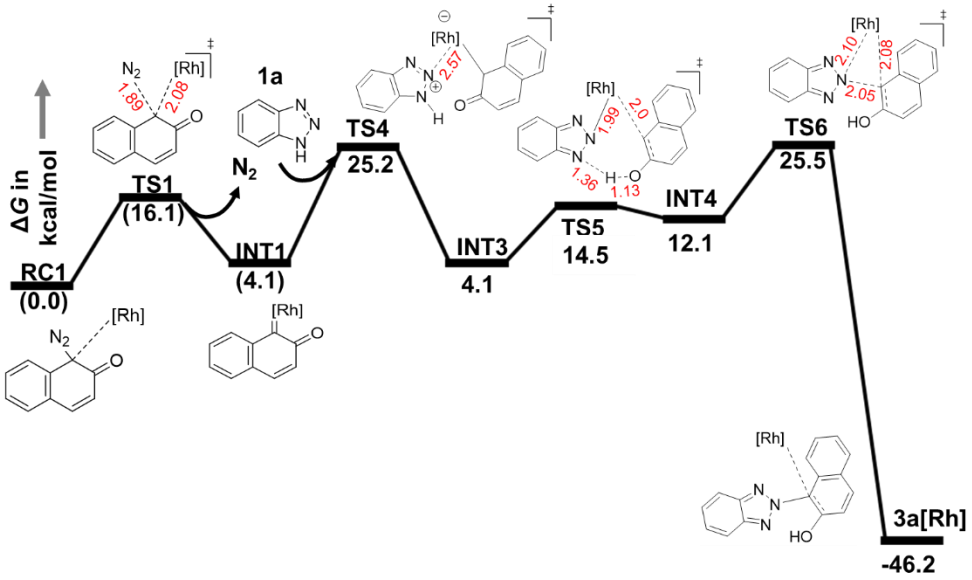
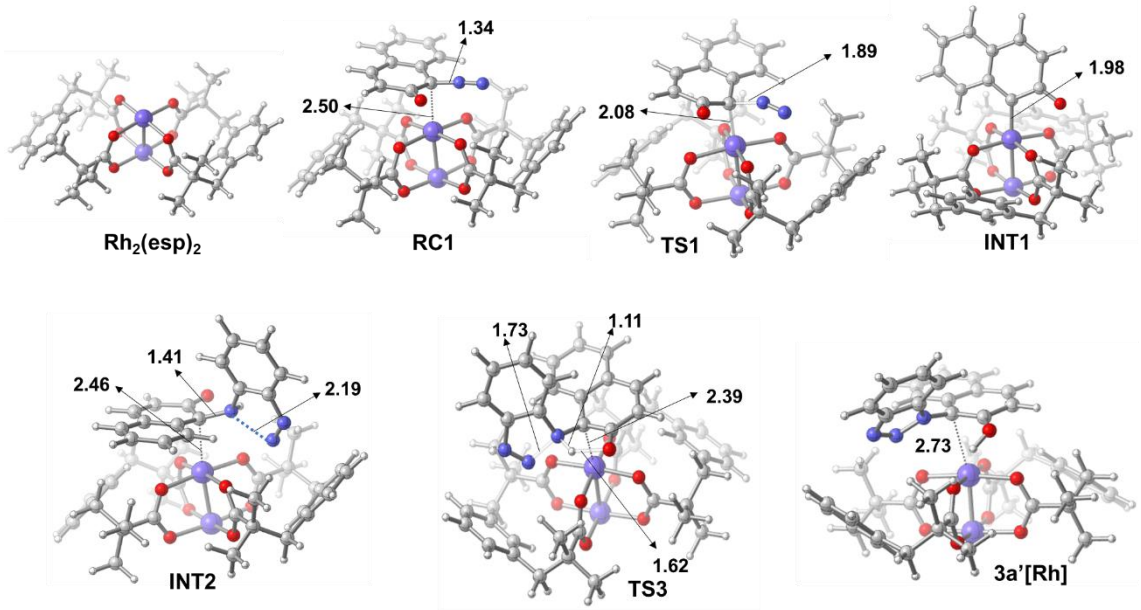


Figure S5. Relative Gibbs free energy profile at B3LYP-D3/Def2TZVP/CPCM in kcal/mol for migratory insertion pathway. Distances shown are in units of Å.



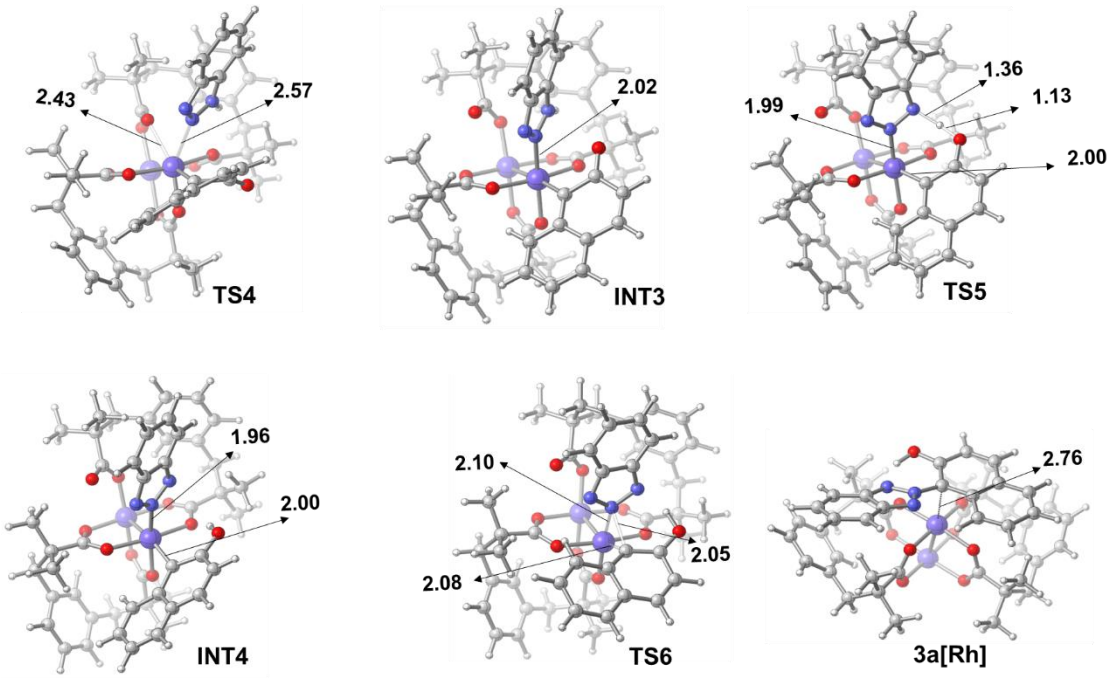


Figure S6. Optimized geometries of intermediates and transition states. Distances shown are in units of Å.

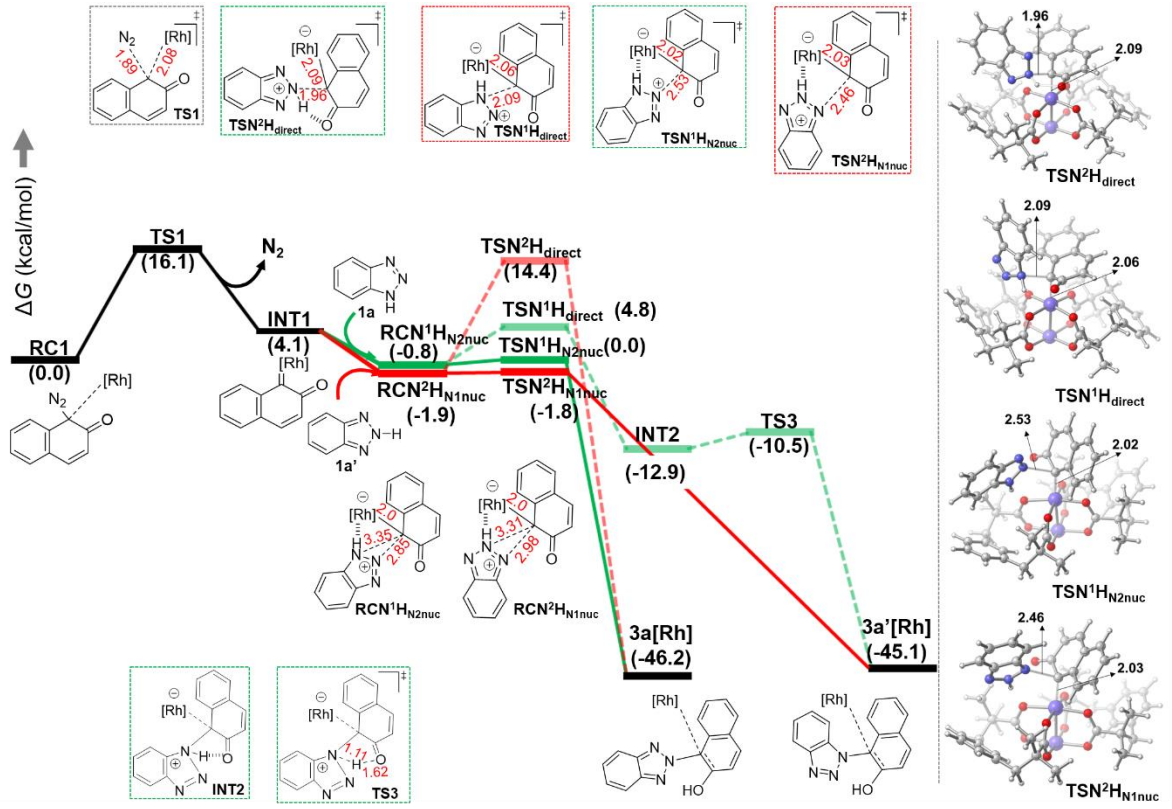


Figure S7. Relative Gibbs free energy profile at B3LYP-D3/Def2TZVP/CPCM in kcal/mol. Reaction paths with **1a** (N^1 tautomer) and **1a'** (N^2 tautomer) are shown in green and red profiles, respectively. Optimized geometries at B3LYP-D3/Def2SVP/W06 level of theory are

shown. Distances shown are in units of Å. Color codes: Rh (purple), N (blue), C (grey), H (white), O (red).

To get more insight into the reaction mechanism, DFT calculations were performed at B3LYP-D3/Def2TZVP/CPCM level of theory. The relevant steps of the catalytic cycle with the potential energies of transition states and intermediates are represented in Figure S7. We hypothesize that the rhodium-carbenoid species **INT1** is formed from the extrusion of N_2 from **2a** on coordination of the Rh(II)-catalyst with an energy barrier of 16.1 kcal/mol (see Figure S7). This N_2 extrusion step is endoergic by 4.1 kcal/mol, like predictions by Hansen and others.[13] Next, we wanted to check the selective insertion of N1 or N2 centre to quinoid carbene. We identified two reactant complexes **RCN^{1}H$_{N2nuc}$** (**INT1**+**1a)** and **RCN^{2}H$_{N1nuc}$** (**INT1**+**1a'**) on introduction of 1H-benzotriazole (**1a**) and 2H-benzotriazole (**1a'**) in the vicinity of the rhodium-carbenoid species **INT1**, displaying weak hydrogen bonding interactions between -NH of the substrate and carboxylate groups of the catalyst. Notably, as shown in Figure S3, the tautomerism of 1H-benzotriazole (**1a**) to 2H-benzotriazole (**1a'**) proceeds through a dimerization step, occurring at an energetic expense of 17.5 kcal/mol, with an overall endergonicity of >5 kcal/mol for the 2H-tautomer. This suggests the greater abundance of **1a** over **1a'** in an equilibrium mixture. Nevertheless, we explored both 1H and 2H direct nucleophilic attacks on the metal-carbenoid centre. While the 2H tautomer direct attack through **TSN^{2}H$_{direct}$** is a concerted process of nucleophilic addition and proton exchange, the 1H tautomer direct attack leads to a step-wise process via **TSN^{1}H$_{direct}$** and **TS3**. Notably, the 1H direct attack takes place at effective barriers of 5.6 and 2.4 kcal/mol for the nucleophilic addition and proton transfer steps, respectively. However, **TSN^{2}H$_{direct}$** occurring through a reasonable energetic expense of 16.3 kcal/mol cannot be ruled out under the experimental conditions, albeit the preference for a 1H direct attack is greater. Thereafter, we explored the possibility of N2 attack with 1H tautomer (**TSN^{1}H$_{N2nuc}$**, 0.8 kcal/mol) and N1 attack with 2H tautomer (**TSN^{2}H$_{N1nuc}$**, 0.15 kcal/mol). Interestingly, these led to almost barrierless reaction steps with reference to the preceding reactant complexes, **RCN^{1}H$_{N2nuc}$** and **RCN^{2}H$_{N1nuc}$** respectively (Figure S7). Perhaps, the DFT computed relative Gibbs free energies are underestimated for both these transition states.

To understand the kinetic origin of observed regioselectivity from electronic energy, ΔE (i.e. not accounting for the entropic effect), we have conducted linear transit scans starting from the two different reactant complexes, **RCN^{1}H$_{N2nuc}$** (**INT1**+**1a)** and **RCN^{2}H$_{N1nuc}$** (**INT1**+**1a'**) and varying the corresponding N-C(carbene) distance starting ~ 3 to ~ 2.2 Å (Figure S4).

Interestingly, a careful investigation of the linear transit scans of N-C(carbene) distance versus total electronic energy from the corresponding local intermediates such as **RCN^{1}H$_{N2nuc}$** for N2 nucleophilic attack (Figure S4b), led to **3a[Rh]**, and **RCN^{2}H$_{N1nuc}$** for N1 nucleophilic attack (Figure S4a), leading to **3a'[Rh]**, reveals that while **TSN^{1}H$_{N2nuc}$** shows $\Delta E^{\ddagger}$ = 0.0 kcal/mol w.r.t **RCN^{1}H$_{N2nuc}$** (Figure S4b), **TSN^{2}H$_{N1nuc}$** must overcome $\Delta E^{\ddagger}$ = 0.8 kcal/mol w.r.t **RCN^{2}H$_{N1nuc}$** (Figure S4a). Hence, the relative total energy barrier difference in between the two transition states is slightly less to explain the observed regio-selectivity. Furthermore, as shown in Figure S7, the C-N distances in **TSN^{1}H$_{N2nuc}$** (2.53 Å) and **TSN^{2}H$_{N1nuc}$** (2.46 Å) are apparently much longer than those found in **TSN^{1}H$_{direct}$** (2.09 Å) and **TSN^{2}H$_{direct}$** (1.96 Å), indicating that the two most favourable transition states are observed at an early stage.

However, the computed $\Delta G^{\ddagger}$ and $\Delta E^{\ddagger}$ for **TSN^{1}H$_{N2nuc}$** and **TSN^{2}H$_{N1nuc}$** are not conclusive about the observed experimental selectivity. Perhaps, the relative greater stability of the 1H tautomer (2H-tautomer is thermodynamically less stable by >5 kcal/mol than 1H-tautomer), as well as the kinetic expense of 17.5 kcal/mol (Figure S4) required in the isomerisation of **1a** to **1a'** is the governing factor in the observed selectivity of **3a[Rh]** generated through **TSN^{1}H$_{N2nuc}$**. In fact, **3a[Rh]** is also thermodynamically more stable than the regio-isomer, **3a'[Rh]**. Hence, one may argue that N2 selectivity is both kinetically and thermodynamically controlled in the abundance of 1H tautomer. Additionally, the steric factor might also play an important role in achieving N2-selectivity. Indeed, the insertion of the N2 centre of the 1H-tautomer to rhodium in the quinoid carbene centre and subsequent proton shifts demonstrates an overall barrier greater than 25 kcal/mol, indicating that classical migratory insertion might not be a possibility in this reaction (Figure S5). Further, the observation of weak H-bonding between the N1H functionality with the carboxylate groups of esp ligand in **TSN^{1}H$_{N2nuc}$** (1.93 Å, Figure S4) leading to favourable N2 attack might explain the necessity of an unsubstituted -NH (Scheme 5e, main text).

3.3 XYZ coordinates of optimized geometries

Rh$_2$(esp)$_2$

Rh	-0.02836900	0.00011000	-1.19016600
O	-1.46368400	-1.45070900	-1.09823800
C	-1.84136300	-1.88299400	0.03040500
O	-1.40000300	-1.47194800	1.14898500
Rh	0.02837700	0.00011000	1.19023500
O	-1.40013100	1.47207300	1.14898600
C	-1.84142500	1.88315800	0.03039100
O	-1.46356200	1.45103100	-1.09824800
O	1.46363900	-1.45076600	1.09831000
C	1.84133000	-1.88304500	-0.03032600
O	1.39998400	-1.47199200	-1.14891600
O	1.46358000	1.45103700	1.09830300
C	1.84147100	1.88312900	-0.03034100
O	1.40017800	1.47203300	-1.14893300
C	-2.89833200	2.99296100	0.06654500
C	2.89837800	2.99292200	-0.06651200
C	2.89807000	-2.99299500	-0.06650700
C	-2.89812400	-2.99293100	0.06654600
C	-3.37323000	-3.33060900	-1.35214700
H	-2.53502800	-3.67872900	-1.97235700
H	-4.13187300	-4.12834400	-1.30971900
H	-3.81236700	-2.45489100	-1.84852300
C	-2.24063300	4.22955900	0.71486800

H	-2.96914400	5.05352600	0.77646800
H	-1.88155000	3.99996500	1.72835100
H	-1.38403500	4.57731800	0.11499100
C	2.24061300	4.22953800	-0.71473900
H	1.88149300	4.00000000	-1.72822500
H	1.38402600	4.57724500	-0.11481400
H	2.96907900	5.05354800	-0.77632700
C	2.24013700	-4.22952400	-0.71471900
H	1.38352200	-4.57712700	-0.11477300
H	1.88102000	-3.99994400	-1.72819500
H	2.96849600	-5.05362700	-0.77632600
C	4.08514300	2.52086200	-0.96603800
C	4.08489000	-2.52108100	-0.96604600
H	3.70701500	-2.41178200	-1.99340300
H	4.82772000	-3.33544300	-0.97547000
C	3.37328400	-3.33065400	1.35214200
H	2.53514200	-3.67878000	1.97243500
H	4.13193100	-4.12838300	1.30967100
H	3.81246100	-2.45492200	1.84845800
C	3.37361200	3.33052600	1.35214400
H	2.53551200	3.67879200	1.97241300
H	3.81264200	2.45473100	1.84847900
H	4.13238600	4.12813500	1.30967800
C	4.73483100	-1.22721700	-0.52785900
C	4.21889900	-0.00011500	-0.97007800
C	5.82591700	-1.21243800	0.35450800
C	4.73495100	1.22693100	-0.52784700
H	3.37836800	-0.00006800	-1.66461900
C	6.37136500	-0.00022800	0.78550600
H	6.25340500	-2.15686400	0.70205500
C	5.82603500	1.21203900	0.35452200
H	7.22787200	-0.00027600	1.46483900
H	6.25361100	2.15642100	0.70207800
H	3.70726400	2.41159600	-1.99339600
H	4.82806300	3.33514400	-0.97547200
C	-2.24021300	-4.22948100	0.71478100
H	-2.96858600	-5.05357200	0.77632400
H	-1.38356700	-4.57705600	0.11486600
H	-1.88116400	-3.99988700	1.72827700
C	-4.08519100	2.52087800	0.96593300
H	-3.70746000	2.41165400	1.99334700
H	-4.82815500	3.33512400	0.97523900
C	-3.37345400	3.33061400	-1.35212800
H	-2.53530800	3.67889900	-1.97232600
H	-3.81244500	2.45483000	-1.84852900
H	-4.13223900	4.12821500	-1.30970600
C	-4.73495500	1.22692800	0.52770400
C	-4.21896500	-0.00011400	0.96999900
C	-5.82596400	1.21204500	-0.35475600
C	-4.73489700	-1.22721700	0.52777000
H	-3.37848700	-0.00006500	1.66459900
C	-6.37129000	-0.00021200	-0.78575300
H	-6.25348000	2.15643200	-0.70238200
C	-5.82590600	-1.21242900	-0.35467200
H	-7.22773900	-0.00024300	-1.46515700
H	-6.25338500	-2.15685200	-0.70223600
C	-4.08501700	-2.52106500	0.96596600
H	-4.82785800	-3.33541300	0.97532500
H	-3.70733600	-2.41175300	1.99338000

1b

C	-3.23447600	-0.09434000	-0.00001300
C	-2.43215100	1.04158400	-0.00004100
C	-1.02687600	0.93924400	-0.00002400
C	-0.42804800	-0.35098400	0.00002900
C	-1.25098000	-1.49361600	0.00007800
C	-2.63690100	-1.36493900	0.00005100
H	-0.67769400	3.09096400	-0.00002500
H	-4.32254300	0.00082500	-0.00002700
H	-2.88700900	2.03593900	-0.00007200
C	-0.17942000	2.11655800	-0.00001000
C	1.02513800	-0.40104500	0.00006500
H	-0.80067700	-2.48965700	0.00013500
H	-3.26079400	-2.26210000	0.00008500
C	1.91692700	0.79190300	-0.00004300
C	1.17613200	2.06052200	0.00003400
H	1.79258700	2.96204700	0.00008200
N	1.65605400	-1.55941000	0.00013400
N	2.27000900	-2.50802900	-0.00045600
O	3.13720300	0.70809100	0.00016500

RC1

Rh	0.19394900	-0.70735600	-1.85550000
O	1.54496100	0.81919700	-2.16696000
C	1.88710800	1.57062100	-1.20689900
O	1.47227800	1.46222900	-0.01273500
Rh	0.10399400	0.00576100	0.43368400
O	1.61211500	-1.29390500	0.83544200
C	2.06804500	-2.03793300	-0.08268500
O	1.68849000	-2.01272900	-1.29216100
O	-1.39847800	1.29310500	-0.11578800
C	-1.78994200	1.32160900	-1.32401000
O	-1.32007700	0.61082400	-2.25828800
O	-1.23770700	-1.50191300	0.75134900
C	-1.58824700	-2.25850900	-0.20646000
O	-1.17401500	-2.16134600	-1.39690300
C	3.15998900	-3.04145100	0.30242800
C	-2.57711500	-3.37386000	0.14848400
C	-2.90883000	2.31751900	-1.65256500
C	2.88060900	2.69588900	-1.52230000
C	2.24115900	3.59507100	-2.59999400
H	1.31026600	4.05223200	-2.22688800
H	2.93398700	4.40671700	-2.87363700
H	2.00096600	3.01600500	-3.50279200
C	3.47783300	-2.93560200	1.80031900
H	4.23717500	-3.68604700	2.07267100
H	3.86183400	-1.93973100	2.05946900
H	2.57619400	-3.10461400	2.40608900
C	-2.98128300	-4.15857700	-1.10470300
H	-3.46253200	-3.50830600	-1.84800500
H	-2.10082900	-4.61258600	-1.58119700
H	-3.68454800	-4.96144300	-0.83129300
C	-3.35151000	2.17195100	-3.11308700
H	-2.51165300	2.36355300	-3.79590300
H	-3.72411000	1.15994000	-3.32158300
H	-4.15378900	2.89451800	-3.33296300
C	-2.34063500	3.73081200	-1.40285400
H	-1.48549000	3.93092000	-2.06879600
H	-3.11391700	4.48901900	-1.60589800
H	-2.00286800	3.83901200	-0.36281800
C	-1.86465200	-4.29853500	1.15976900
H	-0.97883800	-4.76746800	0.70162200
H	-1.53377300	-3.73522300	2.04472000
H	-2.54671300	-5.10209900	1.48046600

C	4.17879600	2.05038700	-2.10366900
H	4.88932300	2.86951700	-2.30274000
H	3.92237000	1.59782500	-3.07293800
C	3.18362900	3.52014400	-0.26443000
H	3.91257800	4.31083900	-0.50264900
H	2.26840500	3.99756200	0.11461800
H	3.59692800	2.89414800	0.53800300
C	4.81974200	1.00585300	-1.21669800
C	5.78698600	1.34558800	-0.25833600
C	4.42123500	-0.33543600	-1.31598300
C	6.32853100	0.36599700	0.57819300
H	6.12367000	2.38243900	-0.17312800
C	4.93942000	-1.32997500	-0.47303200
H	3.67267500	-0.61087500	-2.06030900
C	5.90538200	-0.96178200	0.47599700
H	7.08858400	0.63918600	1.31496500
H	6.33201700	-1.72199800	1.13576800
C	4.42141200	-2.74802600	-0.57093400
H	5.20369700	-3.46122700	-0.26359100
H	4.16700000	-2.97230700	-1.61767200
C	2.63307000	-4.45224000	-0.02997300
H	1.73619600	-4.68329600	0.56701500
H	2.37066500	-4.53508300	-1.09438900
H	3.40151700	-5.20569100	0.20522500
C	0.17103800	0.70442300	2.82978700
C	-0.48277900	2.01391300	2.70245200
C	-0.51195400	-0.51397100	3.39603100
C	0.19589600	3.18207000	2.32239900
C	-1.88290300	2.05318200	2.92455900
C	-1.96204800	-0.34360200	3.52601800
C	-0.50020800	4.37859800	2.17150200
H	1.26522200	3.14379700	2.11156900
C	-2.56558200	3.27312500	2.75847000
C	-2.58128800	0.84280600	3.31467400
H	-2.50902900	-1.23540800	3.83584500
C	-1.88553000	4.42890000	2.38836200
H	0.03984500	5.27996900	1.87161800
H	-3.64543700	3.29924300	2.92680900
H	-3.66560000	0.91094600	3.44262900
H	-2.42788800	5.36835100	2.26139300
O	0.09251000	-1.52896800	3.69875000
N	1.50810600	0.65621700	2.91517100
N	2.61949900	0.52061500	2.97704200
C	-4.09698000	2.07205900	-0.66879500
H	-3.74278800	2.30441600	0.34597700
H	-4.88230700	2.80434200	-0.91886400
C	-4.66425700	0.66979700	-0.69964900
C	-4.09078300	-0.33673300	0.09187000
C	-5.73226200	0.32698800	-1.54307200
C	-4.52778800	-1.66898400	0.03359300
H	-3.26542400	-0.08142600	0.75537400
C	-6.19878700	-0.98920700	-1.59578700
H	-6.20229100	1.09712400	-2.16082300
C	-5.59674300	-1.98314900	-0.81948200
H	-7.03680300	-1.24338600	-2.25025800
H	-5.96181000	-3.01247800	-0.87259000
C	-3.82022300	-2.73251100	0.84431800
H	-4.51648900	-3.55262900	1.08443500
H	-3.48280900	-2.29963100	1.79706200

TS1

Rh	0.22325600	-0.71970600	-1.86619400
O	-1.14900300	-2.17480000	-1.39893000
C	-1.56533000	-2.27388800	-0.21433900
O	-1.22158800	-1.51969700	0.75235900
Rh	0.10128200	0.01916900	0.45768400
O	-1.40678800	1.27861800	-0.14152100
C	-1.78469500	1.29980400	-1.35710700
O	-1.30115300	0.59575700	-2.28349300
O	1.62552600	-1.26985500	0.86120900
C	2.08598700	-2.02226700	-0.05146000
O	1.71781400	-2.01230900	-1.26066800
O	1.46655200	1.47790900	-0.01662400
C	1.89368900	1.57539800	-1.21048500
O	1.57029100	0.81703800	-2.16590900
C	-2.90981100	2.29073500	-1.68427400
C	2.88646200	2.70518800	-1.51942100
C	3.17902600	-3.01923600	0.35412500
C	-2.55638700	-3.39031200	0.13805100
C	-2.96036500	-4.16742300	-1.12011100
H	-2.08012200	-4.62166900	-1.59662500
H	-3.66744000	-4.96905900	-0.85269100
H	-3.43665100	-3.51148700	-1.86143900
C	-2.34750900	3.70743500	-1.43989000
H	-3.12321000	4.46201000	-1.64733500
H	-2.01223200	3.82197100	-0.39927900
H	-1.49176600	3.90820700	-2.10487600
C	2.25734400	3.59172000	-2.61336800
H	2.03052700	3.00265500	-3.51308300
H	1.31986600	4.04859700	-2.25661000
H	2.95026300	4.40361400	-2.88628000
C	2.66205000	-4.43392000	0.02342700
H	1.76127100	-4.66699800	0.61383600
H	2.40841700	-4.52166700	-1.04263500
H	3.43201200	-5.18296800	0.26786500
C	4.19466600	2.06063700	-2.07850500
C	4.44787800	-2.72439800	-0.50774900
H	4.20522100	-2.95639500	-1.55552900
H	5.23145500	-3.43075600	-0.18794300
C	3.48347600	-2.90638300	1.85397500
H	2.57684300	-3.07065100	2.45336400
H	4.23947400	-3.65636300	2.13695100
H	3.86799600	-1.91053800	2.11161800
C	3.17192000	3.54288100	-0.26653300
H	2.25296500	4.02883000	0.09266800
H	3.57238400	2.92643700	0.54947500
H	3.90534400	4.33014200	-0.50243300
C	4.95584500	-1.30253300	-0.41342600
C	4.43996800	-0.31707400	-1.26840600
C	5.90967300	-0.92179700	0.54298800
C	4.82980600	1.02716300	-1.17464800
H	3.70081500	-0.60227600	-2.01849300
C	6.32289800	0.40942200	0.64103400
H	6.33480500	-1.67505500	1.21168900
C	5.78426000	1.37973600	-0.20806600
H	7.07335000	0.69249300	1.38392600
H	6.11379300	2.41921000	-0.12678200
H	3.95174100	1.59776000	-3.04628900
H	4.90408600	2.88100500	-2.27666000
C	-1.84624000	-4.32401600	1.14181500
H	-2.52651600	-5.13394500	1.45010700
H	-0.95567300	-4.78388400	0.68383500
H	-1.52349000	-3.77057800	2.03581600
C	-3.35414300	2.13795800	-3.14337300

H	-2.51557600	2.32918100	-3.82782000
H	-3.72254800	1.12334300	-3.34680700
H	-4.15967400	2.85624000	-3.36562800
C	-0.05711300	0.64795600	2.43279900
C	-0.63773600	1.97730200	2.57471800
C	-0.50983500	-0.46484700	3.31541400
C	-0.01251700	3.16556500	2.17050900
C	-2.00721800	1.99568900	2.96703300
C	-1.96955000	-0.40529500	3.54241100
C	-0.72163700	4.36548400	2.16784000
H	1.02486400	3.13396800	1.83958700
C	-2.71196300	3.20930900	2.91192500
C	-2.64454000	0.75935900	3.40525100
H	-2.42979500	-1.31239600	3.93845300
C	-2.07655100	4.38864400	2.52515100
H	-0.22037600	5.28696500	1.86222200
H	-3.77049400	3.21899900	3.18489100
H	-3.70654800	0.80615500	3.66334400
H	-2.63596900	5.32639000	2.49627800
O	0.20481400	-1.34552600	3.75980800
N	1.76750000	0.74829100	2.92367200
N	2.84737700	0.67450300	2.70969800
C	-4.09469600	2.04565400	-0.69619200
H	-3.73984900	2.28494700	0.31705300
H	-4.88373700	2.77319200	-0.94862000
C	-4.65718900	0.64131900	-0.71792800
C	-4.08065600	-0.35941500	0.07890900
C	-5.72462800	0.29089100	-1.55894600
C	-4.51290100	-1.69342400	0.02643600
H	-3.25613800	-0.09833600	0.74114000
C	-6.18762900	-1.02677400	-1.60456600
H	-6.19683400	1.05643300	-2.18073400
C	-5.58175600	-2.01495500	-0.82407700
H	-7.02520000	-1.28673200	-2.25734200
H	-5.94281500	-3.04591200	-0.87272500
C	-3.79930400	-2.75263400	0.83750400
H	-3.46083000	-2.31677200	1.78877700
H	-4.49237500	-3.57471600	1.08055100

INT1

Rh	-0.12267100	-1.04671300	-1.69900300
O	-1.56352800	-2.25921200	-0.87268600
C	-1.95576700	-2.04560200	0.31090400
O	-1.54579500	-1.11183800	1.06271200
Rh	-0.04887200	0.13230200	0.46661600
O	-1.48099700	1.39344200	-0.29210100
C	-1.90849000	1.24260900	-1.48131800
O	-1.53567200	0.34131000	-2.27962900
O	1.36806800	-1.24156400	0.99839900
C	1.71982100	-2.17423900	0.20763300
O	1.29280400	-2.33517200	-0.96621800
O	1.40904300	1.31746200	-0.37242300
C	1.79650800	1.12327100	-1.57322700
O	1.35284700	0.23582900	-2.34457100
C	-2.95337200	2.24764300	-1.98667000
C	2.87993900	2.08292800	-2.08584600
C	2.73844900	-3.16949700	0.77718200
C	-3.01414100	-2.99339500	0.89009900
C	-2.40906400	-4.41244200	0.88242800
H	-1.51622700	-4.45760500	1.52653300
H	-3.14434100	-5.13682300	1.26780300
H	-2.11724500	-4.71127300	-0.13453800
C	-3.33098200	3.24566700	-0.88459500
H	-4.08844200	3.95006400	-1.26393600
H	-3.73679900	2.73557000	-0.00090400
H	-2.45379300	3.82389700	-0.55943700
C	3.30824200	1.69189000	-3.50535800
H	3.70981300	0.67020500	-3.53564300
H	2.45372700	1.73172700	-4.19567000
H	4.08388400	2.38659700	-3.86559200
C	3.15797400	-4.18039400	-0.29656700
H	2.28767300	-4.74377900	-0.66169700
H	3.61581600	-3.68229200	-1.16198800
H	3.88482500	-4.89254700	0.12608400
C	2.05001500	-3.89081600	1.95619600
H	1.18058300	-4.46842000	1.60274800
H	2.75453000	-4.59255700	2.43080800
H	1.69592100	-3.17035700	2.70780400
C	2.27207300	3.50175100	-2.08637400
H	1.39121100	3.55088700	-2.74716400
H	1.96370100	3.79880800	-1.07328800
H	3.01326200	4.22903000	-2.45419700
C	-4.26216100	-2.96652800	-0.04821100
H	-5.01103400	-3.64953400	0.38536500
H	-3.96133900	-3.38447400	-1.02053700
C	-3.37673900	-2.58404000	2.32353900
H	-4.11581700	-3.28985800	2.73594000
H	-2.48392700	-2.58607400	2.96462700
H	-3.80198200	-1.57184100	2.35631300
C	-4.86508000	-1.59468900	-0.25545500
C	-5.89544900	-1.11093300	0.56516100
C	-4.36293000	-0.75357600	-1.25991600
C	-6.39685800	0.18106100	0.38587500
H	-6.30974700	-1.75311800	1.34712200
C	-4.83506500	0.55515300	-1.43861100
H	-3.56795100	-1.12257200	-1.90910900
C	-5.86662200	1.01244700	-0.60418600
H	-7.20697700	0.54360900	1.02428800
H	-6.25984500	2.02442100	-0.73480200
C	-4.20246100	1.45090500	-2.48104200
H	-4.93648200	2.18955500	-2.84308900
H	-3.89357800	0.84539200	-3.34593600
C	-2.32757700	2.99177500	-3.18463900
H	-1.42950400	3.55055800	-2.87361700
H	-2.03603800	2.28730600	-3.97656600
H	-3.04933900	3.71313400	-3.59986000
C	0.13117000	1.03208000	2.21768300
C	0.30888100	2.44673700	2.40645000
C	0.24261900	0.14254500	3.44432400
C	0.14432700	3.36536400	1.33353300
C	0.68194600	2.97690200	3.69183500
C	0.65193500	0.75698600	4.72338200
C	0.34176800	4.73151100	1.51122600
H	-0.15422500	2.98567900	0.36253000
C	0.88308100	4.35324800	3.84389500
C	0.85513200	2.08521800	4.82916800
H	0.76009600	0.07309000	5.56796300
C	0.71638600	5.22781200	2.76479300
H	0.20399300	5.41247100	0.66834700
H	1.17367800	4.74497500	4.82225700
H	1.14888200	2.53129100	5.78403000
H	0.87719900	6.29970800	2.90578500
O	0.00725500	-1.05689200	3.39641100
C	3.96627500	-2.37128400	1.32042100

H	3.62463100	-1.77090000	2.17645300
H	4.68993400	-3.10811900	1.70610100
C	4.63266800	-1.46876300	0.30501200
C	4.16826900	-0.15800700	0.11958800
C	5.68464000	-1.92256100	-0.50574600
C	4.69141300	0.68437500	-0.87245900
H	3.35823500	0.20854800	0.74992600
C	6.23990200	-1.08799300	-1.47928300
H	6.07282100	-2.93564300	-0.37002400
C	5.74186700	0.20390900	-1.66918800
H	7.06496500	-1.44883500	-2.09917200
H	6.17447300	0.84658000	-2.44083200
C	4.08782100	2.05377400	-1.09597600
H	4.85058500	2.74410700	-1.49253600
H	3.74524300	2.46417300	-0.13440100

N_2

N	0.00000000	0.00000000	0.55024100
N	0.00000000	0.00000000	-0.55024100

1a

C	-0.273744000	0.695331000	0.000143000
H	-2.063152000	1.899788000	0.001571000
C	-0.275337000	-0.715374000	0.000109000
C	0.913096000	1.443016000	-0.000041000
C	0.932395000	-1.431810000	0.000030000
C	2.095804000	0.717334000	-0.000019000
H	0.912899000	2.528135000	-0.000087000
C	2.108621000	-0.699055000	0.000003000
H	0.929131000	-2.516527000	-0.000063000
H	3.041932000	1.250533000	-0.000072000
H	3.063923000	-1.214686000	-0.000054000
N	-2.367184000	-0.130876000	-0.000036000
N	-1.584534000	-1.157327000	-0.000003000
N	-1.603958000	1.001933000	-0.000339000

1a-dimer

C	2.00934900	2.12787100	0.00000000
C	3.20147100	1.36198900	0.00000000
C	4.46019700	1.99305700	0.00000000
C	4.47675600	3.37972900	0.00000000
C	3.27430300	4.13659200	0.00000000
C	2.02343000	3.53413800	0.00000000
H	5.37630400	1.39998300	0.00000000
H	5.43227400	3.90941000	0.00000000
H	3.33899800	5.22758400	0.00000000
H	1.10268800	4.12002300	0.00000000
H	-0.00007400	1.23515600	0.00000000
N	2.86188100	0.02930300	0.00000000
N	1.57696500	-0.05110500	0.00000000
N	1.02988400	1.18370700	0.00000000
H	0.00000000	-1.23360000	0.00000000
C	-2.00924400	-2.12735300	0.00000000
C	-3.20190900	-1.36231500	0.00000000
C	-2.02238000	-3.53361200	0.00000000
C	-4.46019800	-1.99426000	0.00000000
C	-3.27281700	-4.13694500	0.00000000
H	-1.10122200	-4.11885400	0.00000000
C	-4.47581700	-3.38091700	0.00000000
H	-5.37665500	-1.40171900	0.00000000
H	-3.33680500	-5.22797500	0.00000000
H	-5.43092500	-3.91133300	0.00000000
N	-1.03031700	-1.18243100	0.00000000
N	-1.57852300	0.05183000	0.00000000
N	-2.86323800	-0.02937900	0.00000000

TS1a-1a'

C	2.63668300	0.82397600	0.00000000
C	3.27594800	-0.44928800	0.00000000
C	4.68435000	-0.55353600	0.00000000
C	5.40802300	0.62602300	0.00000000
C	4.76378800	1.89721200	0.00000000
C	3.38472300	2.02178100	0.00000000
H	5.16820200	-1.53200900	0.00000000
H	6.50026100	0.59068100	0.00000000
H	5.38238200	2.79848100	0.00000000
H	2.89537100	2.99763400	0.00000000
H	0.00000000	1.05022200	0.00000000
N	2.30959900	-1.41279300	0.00000000
N	1.17976300	-0.77314000	0.00000000
N	1.30553100	0.56775000	0.00000000
H	-0.18693900	-1.03383700	0.00000000
C	-2.63578000	-0.82971600	0.00000000
C	-3.26946600	0.44736800	0.00000000
C	-3.38192500	-2.02729800	0.00000000
C	-4.67774100	0.55678200	0.00000000
C	-4.75958100	-1.89485900	0.00000000
H	-2.89431700	-3.00330800	0.00000000
C	-5.40117200	-0.62153400	0.00000000
H	-5.15797100	1.53654200	0.00000000
H	-5.38112800	-2.79370500	0.00000000
H	-6.49301800	-0.58495000	0.00000000
N	-1.30747800	-0.56506900	0.00000000
N	-1.18298200	0.77016600	0.00000000
N	-2.30442400	1.41205500	0.00000000

1a'

C	0.00000000	0.71650800	0.28552500
C	0.00000000	-0.71650800	0.28552500
C	0.00000000	1.44725900	-0.92966500
C	0.00000000	-1.44725900	-0.92966500
C	0.00000000	0.71589300	-2.09884000
H	0.00000000	2.53859300	-0.92502700
C	0.00000000	-0.71589300	-2.09884000
H	0.00000000	-2.53859300	-0.92502700
H	0.00000000	1.23641200	-3.05991700
H	0.00000000	-1.23641200	-3.05991700
N	0.00000000	1.13657500	1.56863600
N	0.00000000	0.00000000	2.23857300
N	0.00000000	-1.13657500	1.56863600
H	0.00000000	0.00000000	3.25472000

RCN^1H_{N2nuc}

Rh	0.980146000	-2.094048000	0.760387000
O	2.397405000	-2.297238000	-0.724373000
C	2.538705000	-1.348971000	-1.556297000
O	1.882683000	-0.256673000	-1.556988000
Rh	0.425710000	0.131858000	-0.141028000
O	1.901129000	0.858757000	1.112815000
C	2.529013000	0.079102000	1.907732000
O	2.354503000	-1.170996000	2.006023000
O	-1.093148000	-0.821347000	-1.240191000

C	-1.151397000	-2.100704000	-1.245780000
O	-0.409856000	-2.866637000	-0.563677000
O	-1.002973000	0.279677000	1.374496000
C	-1.173949000	-0.704478000	2.175457000
O	-0.486681000	-1.766972000	2.190480000
C	3.575900000	0.718845000	2.843480000
C	-2.283301000	-0.581888000	3.241934000
C	-2.173947000	-2.792173000	-2.172650000
C	3.580926000	-1.540035000	-2.676839000
C	3.124458000	-2.747595000	-3.526877000
H	2.162977000	-2.543594000	-4.009670000
H	3.859625000	-2.947553000	-4.313834000
H	3.017575000	-3.643890000	-2.911080000
C	3.692951000	2.231123000	2.602130000
H	4.425811000	2.656654000	3.296938000
H	4.014826000	2.452447000	1.582703000
H	2.736061000	2.732809000	2.765184000
C	-1.564877000	-0.370787000	4.596740000
H	-0.888815000	-1.201207000	4.816228000
H	-0.981098000	0.556128000	4.590046000
H	-2.301704000	-0.296759000	5.403687000
C	-1.352182000	-3.559617000	-3.236086000
H	-0.767863000	-2.866726000	-3.850450000
H	-0.666937000	-4.268162000	-2.765169000
H	-2.027425000	-4.110218000	-3.899743000
C	-3.089548000	-1.920765000	3.325143000
C	-3.002674000	-3.831047000	-1.345217000
H	-2.305721000	-4.583820000	-0.964693000
H	-3.673543000	-4.337902000	-2.048846000
C	-3.092126000	-1.782272000	-2.874254000
H	-2.511021000	-1.024748000	-3.405205000
H	-3.722601000	-2.304968000	-3.601733000
H	-3.757624000	-1.277702000	-2.169637000
C	-3.212769000	0.606900000	2.957078000
H	-2.655777000	1.546323000	2.928952000
H	-3.732316000	0.499278000	2.002639000
H	-3.967304000	0.680827000	3.748114000
C	-3.808034000	-3.261104000	-0.193600000
C	-3.169818000	-2.931704000	1.009587000
C	-5.189210000	-3.041382000	-0.292780000
C	-3.847886000	-2.325381000	2.075109000
H	-2.115221000	-3.149057000	1.119362000
C	-5.895084000	-2.489624000	0.779359000
H	-5.715319000	-3.316020000	-1.203884000
C	-5.228059000	-2.115638000	1.948117000
H	-6.969696000	-2.346326000	0.701336000
H	-5.784172000	-1.671465000	2.769911000
H	-2.387448000	-2.714903000	3.595469000
H	-3.793625000	-1.814325000	4.158961000
C	4.966847000	-1.883227000	-2.035203000
H	5.675359000	-2.017220000	-2.861369000
H	4.872107000	-2.849352000	-1.530186000
C	3.675865000	-0.288497000	-3.562774000
H	4.387595000	-0.468902000	-4.376432000
H	2.704671000	-0.044545000	-3.999340000
H	4.015489000	0.580904000	-2.995533000
C	5.501735000	-0.857586000	-1.057477000
C	6.383325000	0.157797000	-1.452746000
C	5.096182000	-0.900236000	0.282246000
C	6.826115000	1.107857000	-0.530755000
H	6.731340000	0.199455000	-2.481856000
C	5.498022000	0.065677000	1.212690000
H	4.435071000	-1.697056000	0.604679000
C	6.380508000	1.069799000	0.791478000
H	7.520921000	1.882269000	-0.844617000
H	6.726504000	1.816991000	1.501385000
C	4.955517000	0.011642000	2.625704000
H	5.664897000	0.480701000	3.318191000
H	4.847577000	-1.033212000	2.932161000
C	3.118717000	0.452916000	4.295833000
H	2.157115000	0.936457000	4.500362000
H	3.009668000	-0.617901000	4.482939000
H	3.853803000	0.859469000	4.998749000
C	0.202695000	1.963150000	-0.932265000
C	0.271432000	3.192859000	-0.199832000
C	0.252795000	2.062367000	-2.452344000
C	0.075990000	3.214008000	1.203783000
C	0.535175000	4.434658000	-0.869468000
C	0.582498000	3.361360000	-3.066705000
C	0.136363000	4.403796000	1.920611000
H	-0.147403000	2.282799000	1.705174000
C	0.616259000	5.613078000	-0.126000000
C	0.712236000	4.467560000	-2.313654000
H	0.670681000	3.374107000	-4.148209000
C	0.415288000	5.601611000	1.256725000
H	-0.031456000	4.401388000	2.993035000
H	0.825774000	6.549669000	-0.635244000
H	0.926277000	5.431097000	-2.769835000
H	0.472351000	6.531978000	1.814711000
O	0.028290000	1.084012000	-3.155752000
C	-4.392760000	1.715909000	-1.046356000
H	-2.539665000	0.609253000	-1.341725000
C	-4.518305000	3.110160000	-1.231873000
C	-5.471971000	0.918520000	-0.632679000
C	-5.746089000	3.757384000	-1.011847000
C	-6.673861000	1.576353000	-0.418981000
H	-5.375912000	-0.150007000	-0.478831000
C	-6.813770000	2.974513000	-0.605899000
H	-5.838857000	4.828422000	-1.157348000
H	-7.537280000	1.001893000	-0.095849000
H	-7.780347000	3.434503000	-0.423792000
N	-2.464632000	2.625156000	-1.697202000
N	-3.297039000	3.612495000	-1.628590000
N	-3.086285000	1.471520000	-1.354609000

RCN^{2}H$_{\mathbf{N1nuc}}$

Rh	1.171424000	-2.082866000	0.740904000
O	2.587057000	-2.117088000	-0.762086000
C	2.613197000	-1.158317000	-1.592831000
O	1.839477000	-0.145366000	-1.582893000
Rh	0.379520000	0.077593000	-0.131132000
O	1.788225000	0.950866000	1.108736000
C	2.506126000	0.233924000	1.886652000
O	2.456169000	-1.027300000	1.980125000
O	-1.019963000	-1.027654000	-1.236987000
C	-0.952730000	-2.307806000	-1.251803000
O	-0.138530000	-2.996250000	-0.570190000
O	-1.026768000	0.062861000	1.400684000
C	-1.090021000	-0.937770000	2.197643000
O	-0.306162000	-1.931142000	2.188302000
C	3.504741000	0.966812000	2.806813000
C	-2.186091000	-0.916116000	3.283025000
C	-1.902464000	-3.085223000	-2.186461000
C	3.656676000	-1.235855000	-2.725216000

C	3.297317000	-2.464059000	-3.592637000
H	2.314377000	-2.338846000	-4.058786000
H	4.035402000	-2.583842000	-4.393122000
H	3.280172000	-3.377314000	-2.992818000
C	3.488507000	2.482035000	2.557870000
H	4.191625000	2.972489000	3.240429000
H	3.776672000	2.724717000	1.533222000
H	2.494122000	2.899248000	2.733614000
C	-1.465589000	-0.711150000	4.636833000
H	-0.741099000	-1.508446000	4.821634000
H	-0.935466000	0.247456000	4.658994000
H	-2.197518000	-0.707541000	5.451617000
C	-1.009464000	-3.814632000	-3.218024000
H	-0.461939000	-3.096107000	-3.837199000
H	-0.286391000	-4.466008000	-2.721692000
H	-1.633238000	-4.422567000	-3.881945000
C	-2.914646000	-2.300644000	3.322520000
C	-2.675426000	-4.161115000	-1.351347000
H	-1.940108000	-4.865601000	-0.950841000
H	-3.306345000	-4.715889000	-2.055948000
C	-2.877084000	-2.153326000	-2.920792000
H	-2.339196000	-1.372548000	-3.464761000
H	-3.456676000	-2.734806000	-3.646391000
H	-3.584952000	-1.678679000	-2.237377000
C	-3.186976000	0.224965000	3.045357000
H	-2.688585000	1.197497000	3.063247000
H	-3.694433000	0.124797000	2.083784000
H	-3.943691000	0.217317000	3.837774000
C	-3.521976000	-3.611560000	-0.221443000
C	-2.924253000	-3.306391000	1.007977000
C	-4.891660000	-3.360624000	-0.375345000
C	-3.635077000	-2.698392000	2.049913000
H	-1.874677000	-3.533921000	1.152970000
C	-5.627509000	-2.797423000	0.667913000
H	-5.383391000	-3.606841000	-1.313123000
C	-5.003374000	-2.456369000	1.868173000
H	-6.691185000	-2.615542000	0.541036000
H	-5.581981000	-2.004166000	2.669921000
H	-2.171556000	-3.062623000	3.575678000
H	-3.628950000	-2.256431000	4.153575000
C	5.073763000	-1.468597000	-2.102826000
H	5.781530000	-1.531770000	-2.938095000
H	5.066715000	-2.445823000	-1.610621000
C	3.632371000	0.034680000	-3.588637000
H	4.349849000	-0.067880000	-4.410548000
H	2.639563000	0.198669000	-4.013809000
H	3.899526000	0.920388000	-3.007923000
C	5.531618000	-0.413996000	-1.116520000
C	6.326093000	0.672920000	-1.506255000
C	5.139359000	-0.502042000	0.225209000
C	6.696240000	1.647067000	-0.577467000
H	6.663584000	0.751757000	-2.536721000
C	5.466248000	0.485265000	1.162403000
H	4.547480000	-1.352756000	0.543637000
C	6.262117000	1.561358000	0.746243000
H	7.325105000	2.477450000	-0.887250000
H	6.550037000	2.327788000	1.461547000
C	4.937258000	0.377719000	2.577706000
H	5.609322000	0.900545000	3.268922000
H	4.916959000	-0.673887000	2.878932000
C	3.087409000	0.669910000	4.265466000
H	2.090834000	1.071725000	4.478966000
H	3.071585000	-0.405403000	4.458255000
H	3.793365000	1.140445000	4.958237000
C	-0.054092000	1.885648000	-0.880833000
C	-0.089560000	3.104118000	-0.126311000
C	-0.055308000	2.019573000	-2.395140000
C	-0.281300000	3.085863000	1.277314000
C	0.083203000	4.373689000	-0.773389000
C	0.199406000	3.344486000	-2.989925000
C	-0.307497000	4.264762000	2.015335000
H	-0.435937000	2.131619000	1.761291000
C	0.082465000	5.541388000	-0.008956000
C	0.259059000	4.443581000	-2.217260000
H	0.281734000	3.381197000	-4.071404000
C	-0.115477000	5.491065000	1.374128000
H	-0.473017000	4.230421000	3.087523000
H	0.230670000	6.499210000	-0.500374000
H	0.412560000	5.426664000	-2.656400000
H	-0.121505000	6.412715000	1.949137000
O	-0.267716000	1.048514000	-3.113336000
C	-4.133553000	2.804941000	-1.272525000
C	-5.055983000	1.793457000	-0.872387000
C	-4.521958000	4.162833000	-1.337423000
C	-6.388904000	2.116430000	-0.529651000
C	-5.824844000	4.457449000	-0.997380000
H	-3.819391000	4.931187000	-1.642747000
C	-6.748766000	3.445205000	-0.598059000
H	-7.088472000	1.344345000	-0.227486000
H	-6.167210000	5.487706000	-1.032625000
H	-7.762724000	3.739376000	-0.343066000
N	-3.200270000	0.930655000	-1.297041000
N	-4.415796000	0.598888000	-0.898993000
N	-2.947120000	2.208782000	-1.541159000
H	-2.467186000	0.219620000	-1.395001000

TSN^{1}H$_{direct}$

Rh	0.96688300	-2.24672600	-0.62068600
O	-0.43722200	-3.03287600	0.69560500
C	-1.17983500	-2.25947100	1.35819100
O	-1.16623800	-0.98956500	1.27855500
Rh	0.18707200	-0.03742500	0.08066400
O	-1.06469300	-0.09259200	-1.54469500
C	-1.11066000	-1.11616100	-2.29010000
O	-0.41469000	-2.16222400	-2.14309000
O	1.54265300	-0.17969900	1.61761000
C	2.30591600	-1.19312800	1.71717000
O	2.30935100	-2.18168200	0.93724800
O	1.59372800	0.76893800	-1.15396600
C	2.33899900	0.00403800	-1.84815900
O	2.30717000	-1.25537100	-1.83647100
C	-2.09295300	-1.09166500	-3.47016900
C	3.32994200	0.72202800	-2.77333600
C	3.27270500	-1.17489800	2.90829700
C	-2.18612200	-2.88278700	2.33352100
C	-1.39906300	-3.76258700	3.32446100
H	-0.70233200	-3.15195000	3.92123300
H	-2.09324100	-4.26390900	4.01761900
H	-0.81649100	-4.52752200	2.79195500
C	-2.85715700	0.23745800	-3.52120700
H	-3.56782600	0.22465200	-4.36310000
H	-3.41311500	0.42304100	-2.59323600
H	-2.16168800	1.07565300	-3.67381400
C	4.24759800	-0.29011800	-3.46814600

H	4.82330400	-0.87612000	-2.73887800
H	3.66053800	-0.99735100	-4.07103200
H	4.95186300	0.23708900	-4.13169800
C	4.18475200	-2.40656100	2.87951900
H	3.59171300	-3.33095100	2.92616800
H	4.78131900	-2.44288500	1.95789900
H	4.86944400	-2.38495200	3.74264300
C	2.41100200	-1.17150500	4.18948600
H	1.80691900	-2.09104500	4.25473700
H	3.05867500	-1.12711200	5.07980000
H	1.72631300	-0.31068800	4.20160200
C	2.49392900	1.49521300	-3.81616200
H	1.88473200	0.80266500	-4.41939500
H	1.81802500	2.21144600	-3.32635000
H	3.16005800	2.04577800	-4.49979400
C	-3.16061700	-3.78275400	1.50796300
H	-3.90700300	-4.18652400	2.21194700
H	-2.58249300	-4.63485000	1.12043400
C	-2.95105800	-1.78961600	3.09328100
H	-3.64331200	-2.25145100	3.81488400
H	-2.25842400	-1.13588500	3.64387500
H	-3.54086800	-1.16596200	2.40738000
C	-3.84815100	-3.07913600	0.35843200
C	-5.07411800	-2.41659400	0.52420400
C	-3.23629200	-3.04318600	-0.90288000
C	-5.65787100	-1.73061600	-0.54362400
H	-5.57741500	-2.44433700	1.49469700
C	-3.80219500	-2.35181600	-1.98386300
H	-2.28179500	-3.55309200	-1.04361200
C	-5.02640100	-1.69547600	-1.78873100
H	-6.61301600	-1.21763200	-0.40454100
H	-5.48925600	-1.15463800	-2.61821600
C	-3.07170800	-2.29778900	-3.30734100
H	-3.79413300	-2.24506900	-4.13865200
H	-2.48996100	-3.22215600	-3.43820800
C	-1.27573900	-1.28230700	-4.76372700
H	-0.56522000	-0.45124700	-4.90332100
H	-0.70406500	-2.22066700	-4.73355500
H	-1.94874800	-1.30478600	-5.63587500
C	-0.50904600	1.79780400	0.71983900
C	-0.40882400	2.85769900	-0.26508700
C	-0.04186100	2.00821900	2.11013600
C	-1.14811100	2.91360700	-1.45918700
C	0.66843600	3.77687700	-0.06663800
C	1.14768000	2.87141500	2.17718600
C	-0.84869800	3.86842000	-2.42887400
H	-1.93516400	2.18697400	-1.63183500
C	0.97721400	4.69847300	-1.08122600
C	1.44319800	3.71822400	1.16178500
H	1.68965800	2.87100400	3.12481000
C	0.22134500	4.75576300	-2.25063500
H	-1.44157000	3.90244200	-3.34616300
H	1.82446800	5.37505500	-0.93991400
H	2.27937900	4.41635800	1.26387200
H	0.46860600	5.48343100	-3.02702800
O	-0.54573600	1.49269200	3.10633400
C	4.10087700	0.14911700	2.85835200
H	3.40349000	0.98501500	3.01465800
H	4.79187200	0.13280800	3.71725800
C	4.86996700	0.37185600	1.57478200
C	4.24855000	1.00161100	0.48571000
C	6.19014000	-0.07842500	1.42067700
C	4.89196500	1.15251000	-0.75211400
H	3.22656500	1.36251600	0.59784300
C	6.85797400	0.08925600	0.20474000
H	6.69832200	-0.56097300	2.26001400
C	6.21202100	0.69279200	-0.87749000
H	7.88936600	-0.25736800	0.09823600
H	6.73743700	0.81070800	-1.82916200
C	4.14693200	1.74976500	-1.92585500
H	4.85414300	2.24620800	-2.61076300
H	3.44620100	2.51716500	-1.56460600
C	-4.10975600	2.84792400	0.71354500
C	-3.12363200	2.58715500	1.67916100
C	-4.91928900	3.98651600	0.77981100
C	-2.91434300	3.43622600	2.76841000
C	-4.71022300	4.84611900	1.85615400
H	-5.67879700	4.17460100	0.01947800
C	-3.72995700	4.56794300	2.83375000
H	-2.16157100	3.21553800	3.52317200
H	-5.31831800	5.74826800	1.95403600
H	-3.60672300	5.25916600	3.67105300
N	-2.50222300	1.41992400	1.22474700
N	-3.22802400	0.95033900	0.10819900
N	-4.11654300	1.79254000	-0.19940400
H	-2.14966400	0.66519800	1.83656000

INT2

Rh	-0.87358100	-1.96536900	1.11415900
O	0.49002800	-3.04971400	0.00516000
C	1.15628100	-2.47020800	-0.90373900
O	1.06932800	-1.24537300	-1.20616100
Rh	-0.21823700	-0.03028700	-0.18479600
O	1.19870000	0.36589300	1.26564100
C	1.27944300	-0.39442400	2.27461000
O	0.57120000	-1.42501500	2.47531900
O	-1.68222900	-0.57278300	-1.50907200
C	-2.38988600	-1.60605600	-1.30630500
O	-2.29020000	-2.37425000	-0.30813300
O	-1.56311000	1.05161600	0.92818400
C	-2.25701200	0.47103100	1.81922100
O	-2.19536900	-0.75745400	2.11008100
C	2.31254400	-0.06008900	3.36186300
C	-3.23176100	1.35978100	2.60365100
C	-3.42701400	-1.92846300	-2.38901800
C	2.14505200	-3.33081000	-1.70209300
C	1.32331700	-4.41010200	-2.43676200
H	0.62092300	-3.94646200	-3.14793900
H	1.99329200	-5.07643300	-3.00356000
H	0.74375100	-5.01431200	-1.72424800
C	3.11081800	1.19858200	3.00202800
H	3.81723700	1.43611000	3.81347000
H	3.68437200	1.06174500	2.07711400
H	2.43898400	2.05720900	2.86210600
C	-4.06151900	0.52049100	3.58202700
H	-4.64457600	-0.24860800	3.05770700
H	-3.41047200	0.00756300	4.30418500
H	-4.75592400	1.17205000	4.13683400
C	-4.27269400	-3.14143900	-1.98510500
H	-3.63788700	-4.02555100	-1.83108500
H	-4.81683600	-2.95706600	-1.04860900
H	-5.00341200	-3.36796300	-2.77827300
C	-2.64241900	-2.22266800	-3.68612300
H	-2.00456800	-3.11277400	-3.56098100

H	-3.34223000	-2.41993400	-4.51417800
H	-1.99574200	-1.37473000	-3.95626500
C	-2.38231800	2.39450200	3.37141700
H	-1.71034200	1.89300100	4.08694800
H	-1.76957400	2.98929800	2.67990000
H	-3.03803100	3.07364700	3.94004200
C	3.11782800	-4.02892400	-0.69925900
H	3.82314000	-4.63136800	-1.29516800
H	2.52470800	-4.72779700	-0.09108300
C	2.91043500	-2.47445900	-2.71957700
H	3.57790300	-3.11421700	-3.31903300
H	2.21512700	-1.95586000	-3.39528700
H	3.52349400	-1.71415000	-2.21716300
C	3.88127400	-3.09736100	0.21845600
C	5.16288300	-2.62657600	-0.10713500
C	3.30199300	-2.66787700	1.42195300
C	5.83367500	-1.74817100	0.74810600
H	5.64146800	-2.95911300	-1.03253500
C	3.94824100	-1.76703800	2.28221000
H	2.31177800	-3.03585600	1.69093200
C	5.22951700	-1.31468100	1.93143800
H	6.83668700	-1.39770200	0.48960200
H	5.75973400	-0.62513600	2.59445900
C	3.25283900	-1.29470000	3.54153300
H	3.99924800	-1.02853000	4.30816700
H	2.64657600	-2.11737100	3.94832700
C	1.53817300	0.17426100	4.67549200
H	0.85624000	1.03453900	4.57780200
H	0.93995600	-0.70868000	4.94069300
H	2.24079200	0.38675500	5.49728900
C	0.67221600	1.82193600	-1.53008000
C	0.27798200	2.90169100	-0.64627400
C	-0.11422700	1.46377400	-2.72961700
C	1.07018200	3.34236300	0.43553000
C	-0.99485100	3.51014500	-0.85771500
C	-1.42548700	2.09903300	-2.83230200
C	0.62586800	4.35534600	1.27607200
H	2.01848700	2.84675900	0.63820500
C	-1.42357500	4.53272200	0.01112500
C	-1.81683200	3.06492900	-1.96121200
H	-2.04936200	1.78925300	-3.67212800
C	-0.62608100	4.96000700	1.06661300
H	1.25227800	4.67377700	2.11353800
H	-2.40265000	4.98972200	-0.15790100
H	-2.79615900	3.53739000	-2.08354800
H	-0.97309400	5.75241800	1.73366500
O	0.35504100	0.70318200	-3.58825200
C	-4.31878900	-0.66686500	-2.61815700
H	-3.67748300	0.12294500	-3.03436300
H	-5.06024600	-0.92922400	-3.39072200
C	-5.01812900	-0.14269100	-1.38307200
C	-4.35602400	0.75567900	-0.53242700
C	-6.31224500	-0.55922100	-1.03539700
C	-4.93493700	1.21633200	0.65941200
H	-3.35306200	1.08858100	-0.79589700
C	-6.91573700	-0.09203200	0.13549600
H	-6.85172000	-1.25046000	-1.68883200
C	-6.23084100	0.78445900	0.98145500
H	-7.92786100	-0.41620500	0.39232100
H	-6.70628200	1.13883900	1.90026600
C	-4.14385300	2.11446300	1.58496200
H	-4.82712500	2.75250400	2.16970700
H	-3.49960700	2.77938600	0.99156100
C	4.27311400	2.19662800	-1.29592500
C	3.01958400	2.44498800	-1.88032800
C	5.34664900	3.07861500	-1.37501900
C	2.83920000	3.65271400	-2.55681100
C	5.14686900	4.27968700	-2.05754500
H	6.29546400	2.82770300	-0.89866500
C	3.90135300	4.55796400	-2.64111700
H	1.86955700	3.86422200	-3.01130400
H	5.95884000	5.00597900	-2.12928800
H	3.75571400	5.49962500	-3.17547500
N	2.02654300	1.46229500	-1.69258000
N	3.39295700	0.24714200	-0.48322100
N	4.30975400	0.95393800	-0.60557400
H	2.02181600	0.72300100	-2.42448400

TS3

Rh	-0.92521800	-2.01914200	1.04335700
O	0.43063200	-3.08769000	-0.09454700
C	1.12109800	-2.48332800	-0.96791800
O	1.06805900	-1.24370700	-1.21330700
Rh	-0.20414800	-0.04606700	-0.16352600
O	1.16116000	0.27507700	1.34410600
C	1.22923700	-0.54011600	2.31044500
O	0.51251600	-1.57470400	2.44792200
O	-1.64298000	-0.51421200	-1.55320800
C	-2.38613700	-1.53074000	-1.39234000
O	-2.32929200	-2.32984000	-0.41645600
O	-1.55829700	1.01945100	0.95580400
C	-2.27488500	0.41939200	1.81598800
O	-2.23590600	-0.81808700	2.06673000
C	2.25838900	-0.26662400	3.41728600
C	-3.24818200	1.29808500	2.61372200
C	-3.41588200	-1.79026900	-2.49978800
C	2.10252700	-3.32193900	-1.79729400
C	1.27782300	-4.36655000	-2.57605100
H	0.58052700	-3.87214800	-3.27150800
H	1.94633200	-5.01401600	-3.16600000
H	0.69220400	-4.99494000	-1.88980900
C	3.06768900	1.00080100	3.11614300
H	3.79087400	1.18218300	3.92741800
H	3.62050700	0.91044400	2.17238800
H	2.40430100	1.87405400	3.04054300
C	-4.11990800	0.43932700	3.53718900
H	-4.70853900	-0.29287100	2.96799900
H	-3.49799700	-0.11910300	4.25111700
H	-4.81168300	1.08380000	4.10347000
C	-4.30360900	-2.98807100	-2.14315100
H	-3.69810700	-3.89575900	-2.00996000
H	-4.85238900	-2.81593100	-1.20719800
H	-5.03172400	-3.16709700	-2.95076300
C	-2.62297000	-2.07394300	-3.79365600
H	-2.00766700	-2.98140800	-3.68190900
H	-3.31645600	-2.23471400	-4.63478000
H	-1.95342300	-1.23594800	-4.03701800
C	-2.39318900	2.27946000	3.44319100
H	-1.74966300	1.73255100	4.15146200
H	-1.75082200	2.88779400	2.79130200
H	-3.04592200	2.95002100	4.02530400
C	3.06640100	-4.06194000	-0.81664000
H	3.77452500	-4.64272200	-1.43063000
H	2.46818200	-4.78187800	-0.23869900

C	2.87866000	-2.42881600	-2.77465800
H	3.55935500	-3.04512000	-3.38388000
H	2.19079200	-1.89266200	-3.44415400
H	3.47533300	-1.67921200	-2.23724300
C	3.82240100	-3.16217700	0.13719000
C	5.08912300	-2.64834500	-0.18100100
C	3.24516600	-2.79756000	1.36244100
C	5.74779600	-1.79035900	0.70308000
H	5.56436600	-2.92911700	-1.12501900
C	3.88251800	-1.92287900	2.25528500
H	2.26283000	-3.19365100	1.62174500
C	5.14851200	-1.42569500	1.91132300
H	6.73736900	-1.40167400	0.44805900
H	5.66971600	-0.75224700	2.59734000
C	3.18896000	-1.51530600	3.53730800
H	3.93528200	-1.29276400	4.31790500
H	2.57680600	-2.35393800	3.90031100
C	1.48230600	-0.09109800	4.73853100
H	0.80558700	0.77697900	4.68129800
H	0.87838600	-0.98235700	4.95992600
H	2.18425800	0.07737300	5.57107000
C	0.75842900	1.80835800	-1.31937900
C	0.38233800	2.89119000	-0.43630300
C	0.05771400	1.55898200	-2.57549300
C	1.15746400	3.30487400	0.66495000
C	-0.87379400	3.52286600	-0.67925300
C	-1.23975500	2.18882400	-2.72637400
C	0.70499000	4.31296000	1.50700900
H	2.09908200	2.79895600	0.87542700
C	-1.31495200	4.53402100	0.19948100
C	-1.65606300	3.12274100	-1.82605600
H	-1.82716700	1.92807300	-3.60738000
C	-0.53851200	4.93129500	1.28036500
H	1.31697700	4.61716800	2.36018100
H	-2.28344600	5.00686900	0.01419800
H	-2.62341700	3.61259000	-1.97167500
H	-0.89243400	5.71514000	1.95377800
O	0.63648000	0.86754300	-3.44864900
C	-4.26583600	-0.49628700	-2.70528500
H	-3.59246800	0.28914400	-3.07762300
H	-4.99519400	-0.70944700	-3.50409900
C	-4.98087000	0.00282500	-1.46872400
C	-4.31478500	0.84692500	-0.56727500
C	-6.29481500	-0.38827200	-1.16923600
C	-4.90989900	1.27760800	0.62798000
H	-3.29558600	1.15824300	-0.79179100
C	-6.91365500	0.04999800	0.00471300
H	-6.83706800	-1.03753100	-1.86220300
C	-6.22520300	0.87168600	0.90128900
H	-7.94063700	-0.25413300	0.22429700
H	-6.71301000	1.20309200	1.82217500
C	-4.11842000	2.11606200	1.60770500
H	-4.79966400	2.74620900	2.20322200
H	-3.44525500	2.78901400	1.05711800
C	4.27647500	2.31008000	-1.21571900
C	3.05465100	2.55025300	-1.85139100
C	5.34809300	3.19544400	-1.29317400
C	2.85134300	3.70968900	-2.58820400
C	5.15031600	4.36036900	-2.03967600
H	6.28748100	2.97892600	-0.78283500
C	3.92119800	4.60991100	-2.67463900
H	1.89130900	3.90173800	-3.06913800
H	5.95806200	5.09002800	-2.12605900
H	3.79381800	5.53138400	-3.24734200
N	2.15470700	1.48304100	-1.59041100
N	3.15371700	0.50048900	-0.57499800
N	4.20276100	1.08737600	-0.51788500
H	1.94790500	0.87573000	-2.49049900

TSN^{2}H$_{direct}$

Rh	0.91732900	1.82954800	1.33638700
O	-0.40140400	3.05891600	0.31482400
C	-1.04023100	2.60533200	-0.67763900
O	-0.94721000	1.42624300	-1.13382400
Rh	0.25304900	0.06094800	-0.21660000
O	-1.20845900	-0.43699700	1.14640200
C	-1.29770600	0.19305400	2.24240000
O	-0.57661800	1.17181400	2.58917300
O	1.78374200	0.71249700	-1.42033000
C	2.50970300	1.69731100	-1.07104000
O	2.38808400	2.34864400	-0.00010400
O	1.52025200	-1.17983000	0.81190300
C	2.20068100	-0.73100300	1.78961700
O	2.17536800	0.45481600	2.21513600
C	-2.37061900	-0.26056100	3.24447100
C	3.10296200	-1.75599900	2.49010100
C	3.60042100	2.10256900	-2.07090400
C	-2.00712000	3.55439500	-1.39894200
C	-1.16633800	4.70139300	-1.99556300
H	-0.44405300	4.31270900	-2.73144100
H	-1.82130500	5.42330300	-2.50935100
H	-0.60727100	5.22901100	-1.20931600
C	-3.16862500	-1.44548600	2.68926200
H	-3.96242300	-1.73087300	3.39788300
H	-3.62806600	-1.19790800	1.72482200
H	-2.51431900	-2.31555000	2.53594500
C	3.91248500	-1.08653900	3.60629100
H	4.54832300	-0.28175200	3.21332600
H	3.24485400	-0.64267700	4.35848200
H	4.55378400	-1.83270600	4.10262100
C	4.46536300	3.22972400	-1.49528600
H	3.85247700	4.11324000	-1.26734900
H	4.95929400	2.92063500	-0.56395300
H	5.23842300	3.51760400	-2.22588300
C	2.88301400	2.57429800	-3.35414100
H	2.26104300	3.46063500	-3.14902800
H	3.62428900	2.84952300	-4.12154300
H	2.23077600	1.78416400	-3.75439500
C	2.18178800	-2.84837000	3.07394900
H	1.49262000	-2.41988100	3.81979000
H	1.58272400	-3.32183300	2.28270600
H	2.78518500	-3.62263200	3.57466100
C	-2.99708900	4.14651600	-0.34751500
H	-3.67606200	4.82683000	-0.88745400
H	-2.41279900	4.75809400	0.35580200
C	-2.75874600	2.81109100	-2.51165300
H	-3.45661200	3.49927200	-3.01526000
H	-2.05521400	2.41990900	-3.26117100
H	-3.32654700	1.96194100	-2.10749600
C	-3.79928700	3.12456700	0.42876000
C	-5.06621400	2.69977700	0.00046700
C	-3.26897600	2.56148100	1.59878200
C	-5.77551000	1.74177500	0.72985000
H	-5.50479400	3.13178100	-0.90305900

C	-3.95173100	1.57779100	2.32906100
H	-2.28794100	2.88941100	1.94348600
C	-5.22159100	1.17939100	1.88401700
H	-6.77068200	1.43372900	0.39706200
H	-5.78306800	0.43211000	2.45256100
C	-3.30187800	0.95648000	3.54573600
H	-4.07295400	0.61163000	4.25439100
H	-2.69907900	1.71728800	4.06313900
C	-1.64990300	-0.67237000	4.54398900
H	-0.96717800	-1.51794300	4.36062100
H	-1.06007500	0.16279300	4.94725800
H	-2.38550800	-0.98621400	5.30201300
C	-0.30446600	-1.43299800	-1.56445300
C	-0.22819500	-2.75839200	-0.98215800
C	0.35010500	-1.13655300	-2.85804100
C	-1.10725000	-3.24120100	-0.00022300
C	0.93227100	-3.51378000	-1.32466800
C	1.58933100	-1.88743100	-3.06750800
C	-0.85665700	-4.46066300	0.62547600
H	-1.96299000	-2.63564800	0.28737600
C	1.18519200	-4.71827000	-0.64540700
C	1.83059200	-3.01530400	-2.35313500
H	2.23329700	-1.55649700	-3.88377800
C	0.29637400	-5.19644500	0.31538500
H	-1.55342400	-4.82972400	1.38221500
H	2.09214100	-5.28043600	-0.88413200
H	2.72375200	-3.60853100	-2.57050600
H	0.50212100	-6.13777900	0.83005600
O	-0.09255400	-0.30027600	-3.64995300
C	4.46065400	0.84406900	-2.41157100
H	3.81308900	0.13063500	-2.94127600
H	5.24125400	1.16648500	-3.12015100
C	5.09164400	0.15686600	-1.22042700
C	4.37330800	-0.81791300	-0.51146000
C	6.37736100	0.49499700	-0.77114100
C	4.88733300	-1.42957100	0.64158800
H	3.37630300	-1.09154200	-0.85426100
C	6.91701600	-0.12177600	0.36087000
H	6.96050100	1.24354000	-1.31453000
C	6.17588900	-1.07260500	1.06765000
H	7.92305600	0.14322300	0.69694900
H	6.60156600	-1.54437900	1.95754800
C	4.03608800	-2.40834600	1.42017500
H	4.67762800	-3.13414100	1.94686400
H	3.40004300	-2.97646000	0.72500300
H	-1.59681000	-0.29327900	-2.79707500
C	-3.59065800	-2.53078500	-2.36148000
C	-3.94809000	-1.56353500	-1.33546800
C	-4.42035400	-3.66648400	-2.61523600
C	-5.14775200	-1.71246500	-0.57504000
C	-5.55710100	-3.78213400	-1.85887800
H	-4.14411100	-4.39478400	-3.37876000
C	-5.91951300	-2.81111400	-0.85027400
H	-5.41639500	-0.96864400	0.17399500
H	-6.22425600	-4.63334900	-2.01579400
H	-6.84724900	-2.96968000	-0.29494400
N	-2.10927700	-1.02593900	-2.22050900
N	-3.01930900	-0.62604800	-1.28997400
N	-2.46596100	-2.14548300	-2.93134600

RCN^{1}H$_{N2nuc}$

Rh	0.980146000	-2.094048000	0.760387000
O	2.397405000	-2.297238000	-0.724373000
C	2.538705000	-1.348971000	-1.556297000
O	1.882683000	-0.256673000	-1.556988000
Rh	0.425710000	0.131858000	-0.141028000
O	1.901129000	0.858757000	1.112815000
C	2.529013000	0.079102000	1.907732000
O	2.354503000	-1.170996000	2.006023000
O	-1.093148000	-0.821347000	-1.240191000
C	-1.151397000	-2.100704000	-1.245780000
O	-0.409856000	-2.866637000	-0.563677000
O	-1.002973000	0.279677000	1.374496000
C	-1.173949000	-0.704478000	2.175457000
O	-0.486681000	-1.766972000	2.190480000
C	3.575900000	0.718845000	2.843480000
C	-2.283301000	-0.581888000	3.241934000
C	-2.173947000	-2.792173000	-2.172650000
C	3.580926000	-1.540035000	-2.676839000
C	3.124458000	-2.747595000	-3.526877000
H	2.162977000	-2.543594000	-4.009670000
H	3.859625000	-2.947553000	-4.313834000
H	3.017575000	-3.643890000	-2.911080000
C	3.692951000	2.231123000	2.602130000
H	4.425811000	2.656654000	3.296938000
H	4.014826000	2.452447000	1.582703000
H	2.736061000	2.732809000	2.765184000
C	-1.564877000	-0.370787000	4.596740000
H	-0.888815000	-1.201207000	4.816228000
H	-0.981098000	0.556128000	4.590046000
H	-2.301704000	-0.296759000	5.403687000
C	-1.352182000	-3.559617000	-3.236086000
H	-0.767863000	-2.866726000	-3.850450000
H	-0.666937000	-4.268162000	-2.765169000
H	-2.027425000	-4.110218000	-3.899743000
C	-3.089548000	-1.920765000	3.325143000
C	-3.002674000	-3.831047000	-1.345217000
H	-2.305721000	-4.583820000	-0.964693000
H	-3.673543000	-4.337902000	-2.048846000
C	-3.092126000	-1.782272000	-2.874254000
H	-2.511021000	-1.024748000	-3.405205000
H	-3.722601000	-2.304968000	-3.601733000
H	-3.757624000	-1.277702000	-2.169637000
C	-3.212769000	0.606900000	2.957078000
H	-2.655777000	1.546323000	2.928952000
H	-3.732316000	0.499278000	2.002639000
H	-3.967304000	0.680827000	3.748114000
C	-3.808034000	-3.261104000	-0.193600000
C	-3.169818000	-2.931704000	1.009587000
C	-5.189210000	-3.041382000	-0.292780000
C	-3.847886000	-2.325381000	2.075109000
H	-2.115221000	-3.149057000	1.119362000
C	-5.895084000	-2.489624000	0.779359000
H	-5.715319000	-3.316020000	-1.203884000
C	-5.228059000	-2.115638000	1.948117000
H	-6.969696000	-2.346326000	0.701336000
H	-5.784172000	-1.671465000	2.769911000
H	-2.387448000	-2.714903000	3.595469000
H	-3.793625000	-1.814325000	4.158961000
C	4.966847000	-1.883227000	-2.035203000
H	5.675359000	-2.017220000	-2.861369000
H	4.872107000	-2.849352000	-1.530186000
C	3.675865000	-0.288497000	-3.562774000
H	4.387595000	-0.468902000	-4.376432000

H	2.704671000	-0.044545000	-3.999340000
H	4.015489000	0.580904000	-2.995533000
C	5.501735000	-0.857586000	-1.057477000
C	6.383325000	0.157797000	-1.452746000
C	5.096182000	-0.900236000	0.282246000
C	6.826115000	1.107857000	-0.530755000
H	6.731340000	0.199455000	-2.481856000
C	5.498022000	0.065677000	1.212690000
H	4.435071000	-1.697056000	0.604679000
C	6.380508000	1.069799000	0.791478000
H	7.520921000	1.882269000	-0.844617000
H	6.726504000	1.816991000	1.501385000
C	4.955517000	0.011642000	2.625704000
H	5.664897000	0.480701000	3.318191000
H	4.847577000	-1.033212000	2.932161000
C	3.118717000	0.452916000	4.295833000
H	2.157115000	0.936457000	4.500362000
H	3.009668000	-0.617901000	4.482939000
H	3.853803000	0.859469000	4.998749000
C	0.202695000	1.963150000	-0.932265000
C	0.271432000	3.192859000	-0.199832000
C	0.252795000	2.062367000	-2.452344000
C	0.075990000	3.214008000	1.203783000
C	0.535175000	4.434658000	-0.869468000
C	0.582498000	3.361360000	-3.066705000
C	0.136363000	4.403796000	1.920611000
H	-0.147403000	2.282799000	1.705174000
C	0.616259000	5.613078000	-0.126000000
C	0.712236000	4.467560000	-2.313654000
H	0.670681000	3.374107000	-4.148209000
C	0.415288000	5.601611000	1.256725000
H	-0.031456000	4.401388000	2.993035000
H	0.825774000	6.549669000	-0.635244000
H	0.926277000	5.431097000	-2.769835000
H	0.472351000	6.531978000	1.814711000
O	0.028290000	1.084012000	-3.155752000
C	-4.392760000	1.715909000	-1.046356000
H	-2.539665000	0.609253000	-1.341725000
C	-4.518305000	3.110160000	-1.231873000
C	-5.471971000	0.918520000	-0.632679000
C	-5.746089000	3.757384000	-1.011847000
C	-6.673861000	1.576353000	-0.418981000
H	-5.375912000	-0.150007000	-0.478831000
C	-6.813770000	2.974513000	-0.605899000
H	-5.838857000	4.828422000	-1.157348000
H	-7.537280000	1.001893000	-0.095849000
H	-7.780347000	3.434503000	-0.423792000
N	-2.464632000	2.625156000	-1.697202000
N	-3.297039000	3.612495000	-1.628590000
N	-3.086285000	1.471520000	-1.354609000

TSN^{1}H$_{N2nuc}$

Rh	0.890742000	-2.076896000	0.864273000
O	2.302912000	-2.378876000	-0.613606000
C	2.469616000	-1.473998000	-1.487827000
O	1.840684000	-0.367155000	-1.542419000
Rh	0.388634000	0.114407000	-0.152545000
O	1.868627000	0.871226000	1.078599000
C	2.481947000	0.116518000	1.907412000
O	2.284129000	-1.124658000	2.061980000
O	-1.131813000	-0.882987000	-1.228546000
C	-1.220176000	-2.159239000	-1.156632000
O	-0.511354000	-2.897836000	-0.414413000
O	-1.045218000	0.363909000	1.346289000
C	-1.235900000	-0.571157000	2.198805000
O	-0.572705000	-1.646812000	2.272342000
C	3.542529000	0.775977000	2.813844000
C	-2.345492000	-0.366068000	3.252414000
C	-2.241534000	-2.882661000	-2.060343000
C	3.510499000	-1.742017000	-2.594022000
C	3.029525000	-2.977752000	-3.387938000
H	2.073435000	-2.775753000	-3.882256000
H	3.761166000	-3.230698000	-4.162926000
H	2.902075000	-3.841639000	-2.731107000
C	3.696453000	2.271292000	2.500373000
H	4.442227000	2.711032000	3.172302000
H	4.019679000	2.435777000	1.470645000
H	2.752943000	2.803784000	2.641145000
C	-1.630423000	-0.132071000	4.604704000
H	-0.988275000	-0.978958000	4.859840000
H	-1.011145000	0.770812000	4.568994000
H	-2.369465000	0.000138000	5.402152000
C	-1.422390000	-3.753311000	-3.042698000
H	-0.796956000	-3.128470000	-3.688697000
H	-0.775359000	-4.448357000	-2.502860000
H	-2.099526000	-4.327720000	-3.683820000
C	-3.204139000	-1.668704000	3.377181000
C	-3.126576000	-3.830019000	-1.182034000
H	-2.468137000	-4.584651000	-0.741505000
H	-3.808237000	-4.353114000	-1.863015000
C	-3.106377000	-1.896335000	-2.856575000
H	-2.487092000	-1.195504000	-3.421364000
H	-3.736126000	-2.448436000	-3.562673000
H	-3.772351000	-1.323560000	-2.206449000
C	-3.227981000	0.844232000	2.914051000
H	-2.636806000	1.761070000	2.854997000
H	-3.742595000	0.717616000	1.959217000
H	-3.985651000	0.976453000	3.694529000
C	-3.921725000	-3.153210000	-0.082769000
C	-3.289787000	-2.789560000	1.113888000
C	-5.288002000	-2.870690000	-0.223358000
C	-3.957273000	-2.095236000	2.131546000
H	-2.248281000	-3.048989000	1.256645000
C	-5.984148000	-2.223842000	0.800795000
H	-5.810975000	-3.172635000	-1.127761000
C	-5.321566000	-1.821736000	1.962478000
H	-7.048323000	-2.030944000	0.692277000
H	-5.869868000	-1.306450000	2.747085000
H	-2.537528000	-2.477297000	3.690942000
H	-3.916406000	-1.501217000	4.193880000
C	4.886472000	-2.085415000	-1.931897000
H	5.594262000	-2.274643000	-2.747843000
H	4.768800000	-3.023940000	-1.381673000
C	3.636313000	-0.535913000	-3.537522000
H	4.349177000	-0.768158000	-4.336928000
H	2.672814000	-0.293362000	-3.991685000
H	3.989827000	0.352176000	-3.009147000
C	5.441718000	-1.026835000	-1.001721000
C	6.346462000	-0.050851000	-1.441186000
C	5.031616000	-0.997663000	0.336995000
C	6.807618000	0.931436000	-0.563021000
H	6.697726000	-0.065074000	-2.469926000
C	5.452461000	0.001481000	1.222896000
H	4.351236000	-1.763320000	0.693251000

C	6.358021000	0.964985000	0.757961000
H	7.519955000	1.675134000	-0.910208000
H	6.718550000	1.737333000	1.432913000
C	4.905322000	0.026339000	2.634801000
H	5.624164000	0.510585000	3.306822000
H	4.772172000	-1.000145000	2.989755000
C	3.076888000	0.591205000	4.276039000
H	2.125563000	1.104656000	4.453543000
H	2.944391000	-0.466685000	4.514301000
H	3.819165000	1.015484000	4.960753000
C	0.202702000	1.927200000	-1.032994000
C	0.385340000	3.180461000	-0.343532000
C	0.311616000	1.950401000	-2.555478000
C	0.141248000	3.283769000	1.043636000
C	0.818486000	4.346929000	-1.049304000
C	0.814940000	3.175584000	-3.202554000
C	0.316062000	4.490193000	1.715683000
H	-0.211573000	2.407117000	1.570070000
C	1.019244000	5.539754000	-0.351108000
C	1.044513000	4.291655000	-2.487384000
H	0.942014000	3.133810000	-4.279582000
C	0.765698000	5.615285000	1.020498000
H	0.107138000	4.554270000	2.779097000
H	1.363644000	6.419159000	-0.888514000
H	1.383834000	5.202896000	-2.974661000
H	0.916161000	6.555089000	1.544130000
O	-0.007292000	0.978031000	-3.228479000
C	-4.294289000	1.725905000	-1.145724000
H	-2.526187000	0.445197000	-1.325356000
C	-4.250361000	3.136024000	-1.225743000
C	-5.492761000	1.029383000	-0.919565000
C	-5.420855000	3.902345000	-1.090173000
C	-6.635010000	1.803316000	-0.786224000
H	-5.524679000	-0.050721000	-0.836364000
C	-6.604465000	3.218440000	-0.872186000
H	-5.383009000	4.984490000	-1.154837000
H	-7.586320000	1.310685000	-0.607112000
H	-7.532507000	3.770843000	-0.760522000
N	-2.227425000	2.450952000	-1.503169000
N	-2.944929000	3.522703000	-1.440689000
N	-2.994343000	1.355359000	-1.331735000

RCN^2H_{N1nuc}

Rh	1.171424000	-2.082866000	0.740904000
O	2.587057000	-2.117088000	-0.762086000
C	2.613197000	-1.158317000	-1.592831000
O	1.839477000	-0.145366000	-1.582893000
Rh	0.379520000	0.077593000	-0.131132000
O	1.788225000	0.950866000	1.108736000
C	2.506126000	0.233924000	1.886652000
O	2.456169000	-1.027300000	1.980125000
O	-1.019963000	-1.027654000	-1.236987000
C	-0.952730000	-2.307806000	-1.251803000
O	-0.138530000	-2.996250000	-0.570190000
O	-1.026768000	0.062861000	1.400684000
C	-1.090021000	-0.937770000	2.197643000
O	-0.306162000	-1.931142000	2.188302000
C	3.504741000	0.966812000	2.806813000
C	-2.186091000	-0.916116000	3.283025000
C	-1.902464000	-3.085223000	-2.186461000
C	3.656676000	-1.235855000	-2.725216000
C	3.297317000	-2.464059000	-3.592637000
H	2.314377000	-2.338846000	-4.058786000
H	4.035402000	-2.583842000	-4.393122000
H	3.280172000	-3.377314000	-2.992818000
C	3.488507000	2.482035000	2.557870000
H	4.191625000	2.972489000	3.240429000
H	3.776672000	2.724717000	1.533222000
H	2.494122000	2.899248000	2.733614000
C	-1.465589000	-0.711150000	4.636833000
H	-0.741099000	-1.508446000	4.821634000
H	-0.935466000	0.247456000	4.658994000
H	-2.197518000	-0.707541000	5.451617000
C	-1.009464000	-3.814632000	-3.218024000
H	-0.461939000	-3.096107000	-3.837199000
H	-0.286391000	-4.466008000	-2.721692000
H	-1.633238000	-4.422567000	-3.881945000
C	-2.914646000	-2.300644000	3.322520000
C	-2.675426000	-4.161115000	-1.351347000
H	-1.940108000	-4.865601000	-0.950841000
H	-3.306345000	-4.715889000	-2.055948000
C	-2.877084000	-2.153326000	-2.920792000
H	-2.339196000	-1.372548000	-3.464761000
H	-3.456676000	-2.734806000	-3.646391000
H	-3.584952000	-1.678679000	-2.237377000
C	-3.186976000	0.224965000	3.045357000
H	-2.688585000	1.197497000	3.063247000
H	-3.694433000	0.124797000	2.083784000
H	-3.943691000	0.217317000	3.837774000
C	-3.521976000	-3.611560000	-0.221443000
C	-2.924253000	-3.306391000	1.007977000
C	-4.891660000	-3.360624000	-0.375345000
C	-3.635077000	-2.698392000	2.049913000
H	-1.874677000	-3.533921000	1.152970000
C	-5.627509000	-2.797423000	0.667913000
H	-5.383391000	-3.606841000	-1.313123000
C	-5.003374000	-2.456369000	1.868173000
H	-6.691185000	-2.615542000	0.541036000
H	-5.581981000	-2.004166000	2.669921000
H	-2.171556000	-3.062623000	3.575678000
H	-3.628950000	-2.256431000	4.153575000
C	5.073763000	-1.468597000	-2.102826000
H	5.781530000	-1.531770000	-2.938095000
H	5.066715000	-2.445823000	-1.610621000
C	3.632371000	0.034680000	-3.588637000
H	4.349849000	-0.067880000	-4.410548000
H	2.639563000	0.198669000	-4.013809000
H	3.899526000	0.920388000	-3.007923000
C	5.531618000	-0.413996000	-1.116520000
C	6.326093000	0.672920000	-1.506255000
C	5.139359000	-0.502042000	0.225209000
C	6.696240000	1.647067000	-0.577467000
H	6.663584000	0.751757000	-2.536721000
C	5.466248000	0.485265000	1.162403000
H	4.547480000	-1.352756000	0.543637000
C	6.262117000	1.561358000	0.746243000
H	7.325105000	2.477450000	-0.887250000
H	6.550037000	2.327788000	1.461547000
C	4.937258000	0.377719000	2.577706000
H	5.609322000	0.900545000	3.268922000
H	4.916959000	-0.673887000	2.878932000
C	3.087409000	0.669910000	4.265466000
H	2.090834000	1.071725000	4.478966000
H	3.071585000	-0.405403000	4.458255000

H	3.793365000	1.140445000	4.958237000
C	-0.054092000	1.885648000	-0.880833000
C	-0.089560000	3.104118000	-0.126311000
C	-0.055308000	2.019573000	-2.395140000
C	-0.281300000	3.085863000	1.277314000
C	0.083203000	4.373689000	-0.773389000
C	0.199406000	3.344486000	-2.989925000
C	-0.307497000	4.264762000	2.015335000
H	-0.435937000	2.131619000	1.761291000
C	0.082465000	5.541388000	-0.008956000
C	0.259059000	4.443581000	-2.217260000
H	0.281734000	3.381197000	-4.071404000
C	-0.115477000	5.491065000	1.374128000
H	-0.473017000	4.230421000	3.087523000
H	0.230670000	6.499210000	-0.500374000
H	0.412560000	5.426664000	-2.656400000
H	-0.121505000	6.412715000	1.949137000
O	-0.267716000	1.048514000	-3.113336000
C	-4.133553000	2.804941000	-1.272525000
C	-5.055983000	1.793457000	-0.872387000
C	-4.521958000	4.162833000	-1.337423000
C	-6.388904000	2.116430000	-0.529651000
C	-5.824844000	4.457449000	-0.997380000
H	-3.819391000	4.931187000	-1.642747000
C	-6.748766000	3.445205000	-0.598059000
H	-7.088472000	1.344345000	-0.227486000
H	-6.167210000	5.487706000	-1.032625000
H	-7.762724000	3.739376000	-0.343066000
N	-3.200270000	0.930655000	-1.297041000
N	-4.415796000	0.598888000	-0.898993000
N	-2.947120000	2.208782000	-1.541159000
H	-2.467186000	0.219620000	-1.395001000

TSN^{2}H$_{N1nuc}$

Rh	0.964124000	-2.096162000	0.904380000
O	2.380327000	-2.310519000	-0.589157000
C	2.475389000	-1.411574000	-1.479414000
O	1.768704000	-0.352149000	-1.544916000
Rh	0.296117000	0.027495000	-0.140256000
O	1.705387000	0.924335000	1.080353000
C	2.392407000	0.229351000	1.903257000
O	2.296096000	-1.022375000	2.070602000
O	-1.092515000	-1.122025000	-1.242895000
C	-1.115784000	-2.397567000	-1.116678000
O	-0.382606000	-3.059290000	-0.327178000
O	-1.137861000	0.192858000	1.359617000
C	-1.236511000	-0.722287000	2.248106000
O	-0.505140000	-1.752967000	2.327474000
C	3.413069000	0.978839000	2.784795000
C	-2.320031000	-0.552195000	3.333130000
C	-2.079700000	-3.212979000	-2.003472000
C	3.524796000	-1.624924000	-2.588882000
C	3.129389000	-2.906333000	-3.357373000
H	2.159492000	-2.782308000	-3.850615000
H	3.874009000	-3.121315000	-4.131412000
H	3.066166000	-3.764553000	-2.684051000
C	3.453923000	2.475939000	2.444320000
H	4.172851000	2.980435000	3.099838000
H	3.753707000	2.645785000	1.408309000
H	2.475528000	2.940168000	2.587853000
C	-1.586306000	-0.365416000	4.681614000
H	-0.931968000	-1.214688000	4.892639000
H	-0.976521000	0.544812000	4.674531000
H	-2.315079000	-0.273448000	5.494119000
C	-1.206570000	-4.142711000	-2.878737000
H	-0.572975000	-3.560344000	-3.556213000
H	-0.563129000	-4.774181000	-2.262098000
H	-1.848582000	-4.785142000	-3.490561000
C	-3.174326000	-1.861318000	3.418519000
C	-2.983795000	-4.104650000	-1.085573000
H	-2.336933000	-4.830815000	-0.584127000
H	-3.650680000	-4.667944000	-1.749006000
C	-2.933962000	-2.314958000	-2.910121000
H	-2.306742000	-1.650463000	-3.510609000
H	-3.515386000	-2.941233000	-3.595545000
H	-3.644597000	-1.707626000	-2.344287000
C	-3.211338000	0.666995000	3.052955000
H	-2.625770000	1.589926000	3.036871000
H	-3.728317000	0.581005000	2.095273000
H	-3.964212000	0.759545000	3.843742000
C	-3.795852000	-3.355472000	-0.049023000
C	-3.212598000	-3.024024000	1.180754000
C	-5.118221000	-2.957563000	-0.286630000
C	-3.886654000	-2.261717000	2.142635000
H	-2.201642000	-3.355613000	1.389015000
C	-5.821063000	-2.232501000	0.676657000
H	-5.600842000	-3.220199000	-1.224483000
C	-5.208497000	-1.877169000	1.879082000
H	-6.849661000	-1.938650000	0.486713000
H	-5.761739000	-1.305205000	2.619902000
H	-2.510763000	-2.672012000	3.733459000
H	-3.905714000	-1.710755000	4.221795000
C	4.925633000	-1.857846000	-1.930700000
H	5.640336000	-2.010404000	-2.748281000
H	4.877223000	-2.793077000	-1.364778000
C	3.557866000	-0.430278000	-3.554341000
H	4.284844000	-0.622496000	-4.351613000
H	2.578309000	-0.271623000	-4.011731000
H	3.842507000	0.492104000	-3.043552000
C	5.410096000	-0.747744000	-1.021195000
C	6.245455000	0.279183000	-1.481318000
C	5.004166000	-0.723581000	0.318956000
C	6.643089000	1.304932000	-0.621950000
H	6.593671000	0.270251000	-2.511202000
C	5.360836000	0.316169000	1.186252000
H	4.379197000	-1.527325000	0.692115000
C	6.197666000	1.330337000	0.700628000
H	7.303343000	2.088167000	-0.984818000
H	6.509256000	2.135304000	1.361633000
C	4.824159000	0.326244000	2.602552000
H	5.512767000	0.871928000	3.258927000
H	4.767487000	-0.700744000	2.975505000
C	2.977780000	0.788019000	4.255665000
H	1.995013000	1.237370000	4.435779000
H	2.922289000	-0.271927000	4.514626000
H	3.696212000	1.275433000	4.923603000
C	-0.062896000	1.818493000	-1.028291000
C	0.099844000	3.082241000	-0.339718000
C	0.070794000	1.834137000	-2.541415000
C	-0.251655000	3.220075000	1.017258000
C	0.665048000	4.200908000	-1.022949000
C	0.773983000	2.978957000	-3.149936000
C	-0.079270000	4.433585000	1.679408000
H	-0.683879000	2.365563000	1.522914000

C	0.870149000	5.397617000	-0.329210000
C	1.025832000	4.089908000	-2.431908000
H	0.985954000	2.907239000	-4.211940000
C	0.490762000	5.519522000	1.009556000
H	-0.377261000	4.530735000	2.718899000
H	1.322529000	6.240584000	-0.844880000
H	1.480579000	4.959743000	-2.900813000
H	0.645021000	6.460774000	1.529262000
O	-0.381767000	0.932135000	-3.236652000
C	-3.566211000	2.876132000	-1.188947000
C	-4.729690000	2.073124000	-1.377032000
C	-3.666403000	4.257439000	-0.906415000
C	-6.023503000	2.634447000	-1.288473000
C	-4.938240000	4.782776000	-0.820379000
H	-2.781792000	4.868615000	-0.763804000
C	-6.103954000	3.981875000	-1.009746000
H	-6.906301000	2.021472000	-1.435487000
H	-5.065064000	5.839402000	-0.603206000
H	-7.077941000	4.455644000	-0.931003000
N	-3.023687000	0.883285000	-1.595641000
N	-4.337002000	0.799118000	-1.631892000
N	-2.490074000	2.066784000	-1.342553000
H	-2.409946000	0.063202000	-1.697797000

TS4

Rh	0.25680300	-2.31410800	-0.10561800
O	1.80903900	-2.32110300	-1.45243200
C	2.18426700	-1.20848700	-1.88311700
O	1.67203100	-0.09365800	-1.54288400
Rh	0.18241000	0.24489100	-0.15971400
O	1.54983100	0.20385500	1.35482600
C	1.87638300	-0.90436900	1.88802300
O	1.53689600	-2.05369900	1.49172600
O	-1.36606700	-0.08312400	-1.51276600
C	-1.64974800	-1.24012500	-1.97979900
O	-1.08347300	-2.31402400	-1.65597000
O	-1.16180400	-0.45510300	1.76078500
C	-1.60081800	-1.61426300	1.91449100
O	-1.24362200	-2.60344600	1.19684800
C	2.79351100	-0.84580800	3.11877500
C	-2.65130100	-1.87434700	3.00772000
C	-2.76956700	-1.29340400	-3.02917500
C	3.34356500	-1.15613100	-2.88615000
C	2.89742200	-1.93973100	-4.13763900
H	2.02566300	-1.45921500	-4.60927200
H	3.71520400	-1.96247900	-4.87529200
H	2.62536600	-2.97330300	-3.87993500
C	3.11843700	0.60268400	3.50133100
H	3.75089700	0.61456300	4.40346100
H	3.64623400	1.12771700	2.69630800
H	2.19822700	1.16670800	3.70919400
C	-2.91221200	-3.37623700	3.17312300
H	-3.27390600	-3.82728500	2.23971300
H	-1.98932600	-3.90197600	3.45924400
H	-3.66541600	-3.54168000	3.96100000
C	-3.02600200	-2.74418600	-3.45675300
H	-2.11869600	-3.18932900	-3.88854400
H	-3.32989800	-3.36734400	-2.60480900
H	-3.82414200	-2.77069600	-4.21584200
C	-2.31384200	-0.44759600	-4.23690500
H	-1.40839200	-0.88013500	-4.69179800
H	-3.10526100	-0.43573400	-5.00353400
H	-2.07630700	0.58274200	-3.93974900
C	-2.12607300	-1.27229400	4.32452700
H	-1.20371200	-1.78241000	4.64465500
H	-1.90225200	-0.20289500	4.20293100
H	-2.87529000	-1.39264800	5.12356300
C	4.56635100	-1.88290400	-2.24038500
H	5.38613400	-1.84747100	-2.97621300
H	4.29527300	-2.94043100	-2.10441400
C	3.68606400	0.29138200	-3.26118100
H	4.51076200	0.29809400	-3.99143300
H	2.81793600	0.79564100	-3.70901300
H	3.99376000	0.87712900	-2.38470900
C	5.03295000	-1.31190200	-0.91848800
C	6.04368100	-0.34025800	-0.85340900
C	4.44123900	-1.73884900	0.28032200
C	6.44571500	0.18001200	0.37954700
H	6.52685400	0.00076800	-1.77284300
C	4.80865900	-1.20511600	1.52592200
H	3.66435300	-2.50318900	0.24333200
C	5.82878100	-0.24202200	1.56077500
H	7.24694400	0.92283600	0.41955400
H	6.14502300	0.17485200	2.52075100
C	4.09088700	-1.65046300	2.78167700
H	4.76191900	-1.56662200	3.65205400
H	3.81295700	-2.71015100	2.68295000
C	2.05535100	-1.54257600	4.27960100
H	1.13243300	-0.99808500	4.53255900
H	1.78522300	-2.57427300	4.01331000
H	2.69783900	-1.56351800	5.17430200
C	0.73501000	2.03106000	-0.80227500
C	1.88988900	2.73988600	-0.32096600
C	-0.08714800	2.68053200	-1.84725300
C	3.10229100	2.15721100	0.11652400
C	1.76697400	4.17378000	-0.26042700
C	-0.28201400	4.12412200	-1.59444100
C	4.12372500	2.94508600	0.63930500
H	3.24935200	1.08717300	0.00989000
C	2.78770400	4.93174500	0.33119300
C	0.60673900	4.81776400	-0.84709800
H	-1.09847200	4.59872600	-2.14339100
C	3.96223100	4.32903800	0.77977100
H	5.05283000	2.46358500	0.94581500
H	2.65812200	6.01430300	0.41438300
H	0.51131400	5.90174800	-0.73530600
H	4.75681600	4.93559000	1.22056200
O	-0.61466300	2.12354900	-2.80564600
C	-2.72392500	3.58766700	1.25292100
C	-3.24283100	3.21633400	-0.01185800
H	-2.46678600	1.52602300	-1.17156700
C	-3.22756400	4.71229000	1.93133300
C	-4.26646400	3.93936900	-0.64543100
C	-4.23857900	5.43050800	1.30814000
H	-2.82765000	4.99556100	2.90632200
C	-4.74790000	5.04873500	0.03880200
H	-4.65979400	3.64646600	-1.62020900
H	-4.65779800	6.31117500	1.80030400
H	-5.54422000	5.64680500	-0.41110800
N	-2.52051000	2.10849200	-0.33190200
N	-1.63206000	1.84154400	0.64345700
N	-1.73058300	2.69607600	1.59471000
C	-4.06472200	-0.66265000	-2.42976500
H	-3.87671000	0.40645000	-2.24510700

H	-4.83222700	-0.70343100	-3.21951400
C	-4.59702900	-1.31167800	-1.16942700
C	-4.08938500	-0.95340100	0.08744500
C	-5.60118000	-2.29055400	-1.22462700
C	-4.55460600	-1.53336000	1.27583000
H	-3.30453500	-0.20405800	0.15594600
C	-6.07680700	-2.88400000	-0.05237200
H	-6.01807000	-2.58367500	-2.19212800
C	-5.55956500	-2.50805000	1.19033000
H	-6.86322300	-3.64143000	-0.10757100
H	-5.94223800	-2.97151200	2.10373000
C	-3.95527400	-1.11758800	2.60060700
H	-3.72083600	-0.04212200	2.57498500
H	-4.68978100	-1.27269600	3.40815400

INT3

Rh	0.49494300	-0.13113300	-1.62878400
O	-1.25169700	-0.98918600	-2.32594200
C	-2.10536800	-1.46152200	-1.53440900
O	-2.01122600	-1.40707400	-0.27082200
Rh	-0.54894300	-0.28192300	0.65991100
O	-1.48583600	1.45771800	0.16542600
C	-1.11737400	2.13624800	-0.85274900
O	-0.36190200	1.72641800	-1.76881400
O	0.66130900	-1.95698000	0.87670400
C	1.20561100	-2.51058100	-0.14441100
O	1.23716200	-2.02142600	-1.29761600
O	2.11030300	2.55937400	-0.34028800
C	2.76169600	1.72594100	-0.95872700
O	2.34465900	0.55715800	-1.33775400
C	-1.68663200	3.55316700	-0.97378900
C	4.23498800	1.99409200	-1.36928300
C	1.90832800	-3.85349600	0.09610800
C	-3.33519600	-2.15641200	-2.13449400
C	-2.83222300	-3.41578200	-2.87042000
H	-2.35804200	-4.11762500	-2.16573900
H	-3.67678000	-3.93450300	-3.35178800
H	-2.09420700	-3.15188800	-3.64152500
C	-2.41409300	3.95310100	0.31676400
H	-2.78640700	4.98641200	0.22793400
H	-3.26633200	3.29200100	0.52584600
H	-1.72925400	3.89331000	1.17463400
C	4.34490600	1.85587700	-2.89747300
H	4.05611400	0.84838600	-3.22465800
H	3.68098500	2.57997200	-3.39661500
H	5.37699500	2.05612200	-3.23195600
C	1.89071800	-4.67419400	-1.20253800
H	0.85522400	-4.90018000	-1.50164600
H	2.36485300	-4.12988300	-2.02814300
H	2.42044400	-5.62814900	-1.05000400
C	1.19565300	-4.62244000	1.22203400
H	0.14985600	-4.83495200	0.94993600
H	1.70475000	-5.58260600	1.40180300
H	1.18786500	-4.04396700	2.15619900
C	4.61752300	3.41701300	-0.93744200
H	3.94413600	4.15463000	-1.39686400
H	4.53056400	3.53532500	0.15288600
H	5.65285400	3.64765100	-1.23833200
C	-3.98882200	-1.19358800	-3.17569200
H	-4.88053800	-1.70505500	-3.57414800
H	-3.28252900	-1.07241000	-4.00989600
C	-4.33284500	-2.54863900	-1.03782700
H	-5.20097300	-3.05667700	-1.48757300
H	-3.86793700	-3.22856800	-0.30991700
H	-4.68998900	-1.67059300	-0.48409700
C	-4.36885100	0.17307200	-2.64740100
C	-5.63398000	0.42799900	-2.09476500
C	-3.43972500	1.22323600	-2.69179800
C	-5.94509300	1.69621400	-1.59516300
H	-6.38262500	-0.36837800	-2.06661800
C	-3.72491400	2.49736400	-2.17713100
H	-2.45737000	1.03780800	-3.12813800
C	-4.99546300	2.72236000	-1.62545400
H	-6.93999400	1.88931100	-1.18389600
H	-5.24606300	3.71043200	-1.23021100
C	-2.65735500	3.56921600	-2.19931300
H	-3.11894500	4.56941100	-2.23999900
H	-2.04982900	3.45263800	-3.10938200
C	-0.50817100	4.51093300	-1.23848400
H	0.23546100	4.44527600	-0.43108000
H	0.00743500	4.24703200	-2.17197600
H	-0.87814200	5.54634300	-1.31257200
C	-1.54303700	-0.67121400	2.34882600
C	-2.96826700	-0.58933700	2.48543000
C	-0.77311900	-1.31331900	3.48150300
C	-3.76928600	0.11733000	1.54538200
C	-3.63882000	-1.23913200	3.58332800
C	-1.52330200	-2.02117300	4.53267700
C	-5.15273500	0.18912100	1.68110000
H	-3.28721700	0.62303100	0.71392700
C	-5.03125600	-1.16809000	3.68742500
C	-2.87064600	-1.97372300	4.57580000
H	-0.92418900	-2.54112900	5.28314700
C	-5.78678100	-0.45782900	2.74667800
H	-5.73039900	0.74343900	0.94015100
H	-5.53095100	-1.67392800	4.51791400
H	-3.42162300	-2.47666700	5.37613100
H	-6.87413100	-0.41203100	2.84860800
O	0.45163300	-1.25229800	3.54612400
C	1.86251400	2.42433400	2.59286400
C	2.75298900	1.32461700	2.52434700
H	2.15962000	-0.63567000	1.78605200
C	2.27539700	3.64938200	3.14652300
C	4.06711500	1.38894600	3.01457300
C	3.57541300	3.72088700	3.62256100
H	1.59335800	4.49989200	3.17994000
C	4.45419100	2.60571700	3.56007000
H	4.74583900	0.53693900	2.95977700
H	3.94186000	4.65497700	4.05406500
H	5.46928200	2.71326700	3.94979600
N	2.02701300	0.36664400	1.89578900
N	0.80522600	0.84573100	1.63481300
N	0.66802900	2.05581500	2.03815000
C	3.37801700	-3.55620300	0.55861800
H	3.32528700	-3.08495300	1.55437600
H	3.86003200	-4.53750200	0.70558900
C	4.22594700	-2.70005300	-0.35602800
C	4.35854400	-1.32780500	-0.11677800
C	4.89187900	-3.24233700	-1.46686500
C	5.09531200	-0.47612000	-0.94991000
H	3.86672400	-0.89312100	0.75201300
C	5.64314800	-2.41879900	-2.30791200
H	4.82994800	-4.31489400	-1.66721600
C	5.74377400	-1.04767200	-2.05414100

H	6.16447100	-2.85121500	-3.16614500
H	6.34194400	-0.41530200	-2.71505600
C	5.20432200	1.00136000	-0.64561000
H	5.08571900	1.15777500	0.43856500
H	6.22796600	1.33258900	-0.89186100

TS5

Rh	0.33691400	0.57927900	-1.56503800
O	-1.38409600	-0.05208400	-2.48854400
C	-2.21878900	-0.75811500	-1.85660800
O	-2.08524200	-1.09353300	-0.64633800
Rh	-0.50241200	-0.44016700	0.55759900
O	-1.43213600	1.33046000	0.91519200
C	-1.24738600	2.32586300	0.13581300
O	-0.62209200	2.28471100	-0.95411800
O	0.55990700	-2.09435100	-0.04076500
C	1.13877300	-2.15969800	-1.17562000
O	1.17363300	-1.23686200	-2.02934300
O	1.95327400	3.21778000	-0.19313300
C	2.61831800	2.31900400	-0.66967500
O	2.15638600	1.16034900	-1.10161000
C	-1.87168200	3.65956500	0.55413100
C	4.15112600	2.44051300	-0.85881300
C	1.87234800	-3.47150500	-1.46982400
C	-3.46417100	-1.24149300	-2.61008400
C	-2.98136300	-2.13196100	-3.77344300
H	-2.45001000	-3.01923200	-3.39338000
H	-3.84413000	-2.47893400	-4.36408200
H	-2.29911700	-1.57995500	-4.43554500
C	-2.57935000	3.52633700	1.90924400
H	-3.00669000	4.49945100	2.19930900
H	-3.39057900	2.78591400	1.87884400
H	-1.86861300	3.21028100	2.68563100
C	4.44409300	2.41677800	-2.36984000
H	4.10294100	1.47752800	-2.82556800
H	3.93256600	3.25452400	-2.87090200
H	5.52534200	2.52073100	-2.55698000
C	2.17281900	-3.58895000	-2.96897400
H	1.23961300	-3.61161900	-3.55241200
H	2.77326400	-2.74289400	-3.32605600
H	2.72644700	-4.52104300	-3.16493700
C	1.00121600	-4.65153100	-0.99992800
H	0.03134100	-4.65863100	-1.52275900
H	1.51252600	-5.60247400	-1.21739900
H	0.80693900	-4.59401200	0.07996000
C	4.60600400	3.77861800	-0.25675100
H	4.03938600	4.61527000	-0.68832600
H	4.44023700	3.79544400	0.83103500
H	5.67952700	3.93783600	-0.44868700
C	-4.19849000	0.00498700	-3.19787900
H	-5.10201900	-0.36367200	-3.71054900
H	-3.54682000	0.44900000	-3.96484700
C	-4.38421300	-2.03952400	-1.67774200
H	-5.26790100	-2.38750500	-2.23599300
H	-3.86192000	-2.91589500	-1.26807100
H	-4.72278400	-1.43314900	-0.82758400
C	-4.57007800	1.06660800	-2.18583300
C	-5.80675200	1.05762300	-1.52247900
C	-3.65461500	2.08293900	-1.87436000
C	-6.10552700	2.03829800	-0.57190400
H	-6.54319500	0.28527700	-1.76008100
C	-3.92523400	3.06236200	-0.90677700
H	-2.69518200	2.10543300	-2.39230600
C	-5.16981600	3.02871400	-0.25807400
H	-7.07937200	2.03396000	-0.07430600
H	-5.41121500	3.79079700	0.48766400
C	-2.87152200	4.09287100	-0.56564600
H	-3.34690800	5.02991100	-0.23305300
H	-2.28476200	4.32544100	-1.46648100
C	-0.73299700	4.69470800	0.65124100
H	0.00038500	4.39179300	1.41191800
H	-0.18756100	4.77393000	-0.29772300
H	-1.15139600	5.67758400	0.92239000
C	-1.38810100	-1.60366700	1.93158700
C	-2.81459200	-1.58224700	2.14403200
C	-0.63921600	-2.71663700	2.53070500
C	-3.63793400	-0.51398500	1.69217200
C	-3.46932000	-2.66186800	2.83413800
C	-1.33553200	-3.79151800	3.18366900
C	-5.01285900	-0.50755400	1.90846800
H	-3.18649000	0.32149900	1.16828500
C	-4.85940600	-2.63687000	3.03618800
C	-2.68908900	-3.76819200	3.31843500
H	-0.72335100	-4.60915600	3.56828000
C	-5.63291800	-1.57052700	2.57650300
H	-5.59934400	0.33483700	1.53774100
H	-5.33171600	-3.46832900	3.56643700
H	-3.20644300	-4.59318300	3.81609800
H	-6.71318100	-1.56674300	2.74042300
O	0.64417600	-2.81838100	2.53995400
C	2.36987900	1.42603500	2.72155200
C	2.79047000	0.07159100	2.86538300
C	3.14088100	2.49201200	3.23351700
C	3.98763800	-0.25712800	3.53767500
C	4.31329000	2.15771100	3.88677300
H	2.82136100	3.52455500	3.08787900
C	4.72814300	0.80031600	4.03720500
H	4.31774500	-1.29240800	3.63609100
H	4.95072000	2.94785100	4.29056700
H	5.66874400	0.59591500	4.55475900
N	1.87262000	-0.68088600	2.21066100
N	0.97855600	0.18972400	1.72520800
N	1.21363400	1.43513900	2.01019200
H	1.25293300	-1.93744100	2.29887300
C	3.18823300	-3.45615500	-0.62151000
H	2.89872300	-3.36161800	0.43695600
H	3.65248900	-4.44900200	-0.74134000
C	4.18877000	-2.38046500	-0.98099600
C	4.08279200	-1.09490100	-0.43099500
C	5.23136400	-2.64206400	-1.88290100
C	4.99141000	-0.07484100	-0.74508100
H	3.27094900	-0.88101400	0.26200000
C	6.14395800	-1.63889600	-2.21545000
H	5.33246800	-3.63989200	-2.31917100
C	6.02808300	-0.36908300	-1.64544400
H	6.95940900	-1.85158100	-2.91206300
H	6.76081700	0.40359600	-1.89337800
C	4.90468200	1.29296000	-0.10353900
H	5.93609500	1.65256900	0.04751000
H	4.47097300	1.20361800	0.90377600

INT4

Rh	-0.38186200	-1.09789200	1.32838100
O	1.25557300	-2.33638400	1.34863900

C	2.02044100	-2.27939800	0.34474800
O	1.83628400	-1.50037200	-0.63201400
Rh	0.38270100	0.08066700	-0.72488100
O	1.46576900	1.26454300	0.50567500
C	1.32113500	1.19281600	1.76808200
O	0.65473200	0.30994400	2.37835700
O	-0.86434000	-1.28508500	-1.68829000
C	-1.45343900	-2.25249500	-1.08152000
O	-1.37219400	-2.45636900	0.15069700
O	-1.69023800	1.93886100	1.79047800
C	-2.42438900	0.98012200	1.95677600
O	-2.12026000	-0.25893500	1.64572200
C	2.04187600	2.24687700	2.60970700
C	-3.84983200	1.11245700	2.53739300
C	-2.32067500	-3.18445700	-1.92844100
C	3.23359800	-3.21797600	0.32585200
C	2.69102600	-4.66001700	0.23861200
H	2.12886300	-4.81111400	-0.69680600
H	3.52671200	-5.37763700	0.25267800
H	2.02244700	-4.88173300	1.08296800
C	2.79735500	3.22867800	1.70413500
H	3.28958800	3.99625800	2.32235700
H	3.56158400	2.72042000	1.10028400
H	2.10218000	3.72064500	1.00963000
C	-4.04532700	0.08459800	3.66409600
H	-3.92651600	-0.94164300	3.29234800
H	-3.31151100	0.24748700	4.47004800
H	-5.05346300	0.18383300	4.09946300
C	-2.53123900	-4.51097500	-1.18447300
H	-1.57046500	-5.02306500	-1.02124400
H	-2.99984100	-4.35233800	-0.20558000
H	-3.17766900	-5.17163000	-1.78321800
C	-1.63624800	-3.44337100	-3.28378100
H	-0.64412400	-3.90136400	-3.14460200
H	-2.24968600	-4.13636300	-3.87995200
H	-1.50542200	-2.52092000	-3.86636400
C	-4.01594700	2.53906500	3.08181100
H	-3.26348400	2.75165300	3.85583000
H	-3.88284900	3.28292300	2.28324200
H	-5.01761300	2.66553300	3.52341200
C	4.00998200	-3.05318800	1.67136900
H	4.87344300	-3.73700700	1.62976700
H	3.35532600	-3.40470400	2.48230300
C	4.13598200	-2.91804500	-0.87715000
H	4.98801300	-3.61627200	-0.88528300
H	3.58299300	-3.02998500	-1.82040900
H	4.52851100	-1.89294100	-0.84524700
C	4.48036100	-1.64853200	1.98599500
C	5.76088200	-1.20086400	1.62500500
C	3.62703700	-0.75404800	2.65032600
C	6.16303500	0.10477800	1.92178800
H	6.45141100	-1.88306900	1.12185700
C	3.99905600	0.57098500	2.92703800
H	2.63901200	-1.09809600	2.95542300
C	5.28619700	0.98990100	2.55626900
H	7.17018800	0.43618500	1.65438100
H	5.60606800	2.01204500	2.77560900
C	3.01149800	1.50843700	3.58799100
H	3.54703000	2.28386700	4.15927100
H	2.39884100	0.94072200	4.30404100
C	0.96479000	2.99457600	3.42362600
H	0.22114900	3.45226500	2.75586600
H	0.42655900	2.30451100	4.08836200
H	1.44088600	3.77989000	4.03236600
C	1.41680200	0.46743400	-2.40042000
C	2.79318700	0.88666900	-2.38004100
C	0.68881200	0.48089700	-3.63116700
C	3.66311500	0.76363800	-1.26362700
C	3.33043800	1.52193700	-3.55774600
C	1.23636300	1.16924400	-4.75477300
C	4.96226200	1.25192800	-1.29751800
H	3.32053100	0.26026500	-0.36874300
C	4.65023600	2.02438500	-3.55632300
C	2.51133700	1.65820800	-4.72041600
H	0.60316900	1.24518100	-5.64073200
C	5.46522200	1.89204900	-2.44202600
H	5.58743900	1.12856000	-0.41260100
H	5.01764800	2.53004400	-4.45343400
H	2.93127700	2.14961100	-5.60204400
H	6.48574100	2.28163500	-2.45413100
O	-0.51553500	-0.01688100	-3.82512200
C	-1.67532700	3.49756100	-0.99688600
C	-2.68236300	2.55477400	-1.38858400
C	-1.96860100	4.87795600	-0.90210400
C	-4.00398700	2.97351300	-1.69160400
C	-3.26204800	5.26515500	-1.19366800
H	-1.20197000	5.59312100	-0.59916200
C	-4.26935200	4.32274900	-1.58484000
H	-4.76700300	2.25121400	-1.98716100
H	-3.53695400	6.32072500	-1.12358300
H	-5.27424400	4.69395400	-1.80148100
N	-2.12360600	1.33352500	-1.37655100
N	-0.86702300	1.55752500	-0.98356100
N	-0.53797600	2.81235000	-0.76346900
H	-0.83423200	-0.55250100	-3.04590300
C	-3.68419000	-2.45287500	-2.18174700
H	-3.47369200	-1.53745100	-2.75698200
H	-4.27050900	-3.11681700	-2.83880700
C	-4.49406800	-2.09875400	-0.95254300
C	-4.33046200	-0.84712700	-0.34442400
C	-5.41312500	-3.00301700	-0.39731600
C	-5.06071800	-0.47298500	0.79329000
H	-3.60731300	-0.14733300	-0.76524400
C	-6.14057100	-2.65430600	0.74292000
H	-5.56695400	-3.97944800	-0.86521500
C	-5.96857700	-1.39783100	1.33128900
H	-6.85882300	-3.36065500	1.16796500
H	-6.55756400	-1.12663500	2.21195200
C	-4.90448100	0.90608100	1.39838000
H	-5.87594000	1.20977000	1.82414200
H	-4.67699600	1.63191900	0.60263600

TS6

Rh	0.30142000	-1.17616900	-1.17127600
O	-1.29495500	-2.48084300	-0.95778000
C	-2.10797700	-2.40154100	-0.00143400
O	-2.04366800	-1.50103500	0.89099400
Rh	-0.66467200	-0.03684900	0.82448000
O	-1.82858800	0.98030200	-0.55404100
C	-1.62177900	0.86048600	-1.80440100
O	-0.83847000	0.02944400	-2.34202300
O	0.58593700	-1.27197000	1.89590000
C	1.31520900	-2.15457700	1.33497500
O	1.36868400	-2.37083400	0.09638400

O	1.54223700	1.77276500	-2.24958400
C	2.29765200	0.81370800	-2.18960900
O	2.03272200	-0.34087400	-1.65142900
C	-2.40022700	1.76822200	-2.76747900
C	3.73759200	0.86436800	-2.76651700
C	2.23143800	-2.97994300	2.24285200
C	-3.21927600	-3.44859100	0.10699900
C	-2.53474300	-4.80855900	0.36069300
H	-1.97845000	-4.79725900	1.31170600
H	-3.29414400	-5.60436800	0.41960100
H	-1.83068100	-5.05263500	-0.44790500
C	-3.25409500	2.79005600	-2.00813800
H	-3.86356300	3.36552600	-2.72293100
H	-3.92065600	2.30942300	-1.28035500
H	-2.61227000	3.49939800	-1.46726300
C	3.89811300	-0.26445900	-3.79849600
H	3.74685700	-1.24832100	-3.33499900
H	3.16521500	-0.14975000	-4.61356600
H	4.90661200	-0.23777900	-4.24431000
C	2.40658600	-4.38737600	1.65268700
H	1.43967900	-4.91373100	1.61376200
H	2.81211900	-4.34772400	0.63424200
H	3.09100400	-4.97499700	2.28515200
C	1.63672000	-3.06212000	3.65871700
H	0.64583200	-3.54242100	3.64128900
H	2.29678000	-3.66131800	4.30567600
H	1.51973100	-2.06226100	4.09810300
C	3.94538700	2.23045100	-3.43636200
H	3.19527400	2.39582400	-4.22301400
H	3.83673800	3.04662000	-2.70680600
H	4.94956600	2.28883900	-3.88734200
C	-3.97874400	-3.51008600	-1.25633300
H	-4.78232300	-4.25627100	-1.14352100
H	-3.28069000	-3.89498400	-2.01437000
C	-4.17012200	-3.11004800	1.26244400
H	-4.96207200	-3.87308000	1.32696200
H	-3.62998500	-3.08643800	2.21967600
H	-4.64055400	-2.12755700	1.12119200
C	-4.55094600	-2.19089400	-1.72634900
C	-5.84332200	-1.77569900	-1.36964500
C	-3.76689900	-1.32997800	-2.50758000
C	-6.32284800	-0.52788300	-1.77742700
H	-6.47964700	-2.43649400	-0.77464800
C	-4.22072100	-0.06439700	-2.90603500
H	-2.76365500	-1.64496800	-2.79680900
C	-5.51587100	0.32641600	-2.53390700
H	-7.33479300	-0.21843100	-1.50263200
H	-5.89584400	1.30359900	-2.84394200
C	-3.29370500	0.85480800	-3.66831000
H	-3.87050900	1.51725200	-4.33439100
H	-2.62572800	0.25428800	-4.30306600
C	-1.36804500	2.49937100	-3.65078200
H	-0.66210100	3.07322700	-3.03332000
H	-0.77168000	1.78417900	-4.23270100
H	-1.88874200	3.18286400	-4.34094000
C	-0.73370700	1.33269300	2.39354200
C	-1.86652500	2.22641300	2.42605400
C	-0.05920700	0.95244700	3.59065100
C	-2.34773000	3.01003200	1.35350400
C	-2.58779800	2.26893200	3.67382900
C	-0.84285100	0.97205700	4.78491400
C	-3.50726900	3.75672100	1.48535300
H	-1.77647100	3.02952800	0.43409800
C	-3.78978700	3.01312200	3.75775100
C	-2.06142300	1.59369500	4.81551600
H	-0.38956600	0.52187100	5.67013800
C	-4.25071700	3.74842400	2.68156300
H	-3.84800300	4.35442700	0.63678400
H	-4.34208300	3.00136600	4.70120600
H	-2.62783600	1.62877700	5.74968600
H	-5.17461700	4.32559100	2.76116300
O	1.17804200	0.54573800	3.69779200
C	1.63532800	3.33942100	0.19628900
C	2.55109000	2.56569700	0.98286100
C	2.04964000	4.53421900	-0.44445000
C	3.89256500	2.98511700	1.17306100
C	3.35718200	4.92169800	-0.25410300
H	1.35656200	5.09531700	-1.07183000
C	4.26604300	4.15771600	0.55180300
H	4.59018400	2.39128700	1.76519000
H	3.72713800	5.83068800	-0.73411800
H	5.29214100	4.51762600	0.66026300
N	1.89139400	1.47887000	1.40990100
N	0.64197600	1.60863100	0.90240300
N	0.45340200	2.71108800	0.19075800
H	1.66654100	0.71568100	2.82461400
C	3.60398800	-2.22392800	2.32952200
H	3.41521500	-1.24878500	2.80599200
H	4.22616800	-2.80150600	3.03387400
C	4.36483800	-2.01601300	1.03785900
C	4.22054300	-0.82622100	0.31230400
C	5.23363000	-3.00089600	0.54151600
C	4.91670800	-0.58906200	-0.88225300
H	3.53326700	-0.06605600	0.68204000
C	5.92618700	-2.79252700	-0.65288100
H	5.37530200	-3.93074900	1.09902100
C	5.77282400	-1.59446600	-1.35628700
H	6.60409200	-3.56265300	-1.03088800
H	6.33579400	-1.43163800	-2.27943400
C	4.78843600	0.72899400	-1.61614800
H	5.76790000	0.96675200	-2.06576100
H	4.58614700	1.53022800	-0.88991800

3a[Rh]

Rh	0.42043600	-1.46905200	1.71212100
O	2.02118200	-2.37963900	0.80932900
C	2.39171100	-1.98130300	-0.33687400
O	1.85990200	-1.03196700	-0.98371400
Rh	0.24428400	-0.03984700	-0.20425800
O	1.47657700	1.28369700	0.77376600
C	1.87914200	1.01437500	1.94227600
O	1.62456600	-0.05786200	2.57442700
O	-0.98465700	-1.44910000	-1.02965100
C	-1.24147200	-2.51977500	-0.39636600
O	-0.80963700	-2.79864300	0.75874600
O	-1.35586400	0.87010900	0.72341800
C	-1.71155700	0.46934400	1.87689000
O	-1.18092100	-0.49017400	2.50679000
C	2.74636100	2.04638900	2.67484000
C	-2.86968100	1.21294300	2.55357200
C	-2.14043400	-3.53462000	-1.11105800
C	3.57749500	-2.72011400	-0.97160400
C	3.19254400	-4.20857900	-1.09152500
H	2.32135000	-4.33519400	-1.75462800

H	4.03121600	-4.78158400	-1.51818500
H	2.93988000	-4.63038800	-0.10852000
C	2.94557800	3.29428000	1.81057400
H	3.56325900	4.02909300	2.35167300
H	3.43386500	3.04743600	0.86062200
H	1.97981700	3.75781900	1.56594700
C	-3.12842500	0.64183400	3.95322500
H	-3.40400500	-0.42050000	3.90660800
H	-2.23225100	0.72522200	4.58464600
H	-3.94895000	1.19829800	4.43393400
C	-2.34170200	-4.78145500	-0.24201500
H	-1.37873500	-5.26605700	-0.02545300
H	-2.80931100	-4.52983600	0.71946600
H	-2.98540600	-5.50324500	-0.76983300
C	-1.45200400	-3.90549900	-2.44171200
H	-0.47124500	-4.37355900	-2.25687800
H	-2.07274900	-4.62715600	-2.99649500
H	-1.30094200	-3.01220200	-3.06474400
C	-2.47814300	2.70213200	2.64314500
H	-1.58565600	2.83511100	3.27597600
H	-2.25881700	3.10961600	1.64633900
H	-3.30221200	3.28167300	3.08871700
C	4.80494000	-2.58693400	-0.01443000
H	5.65718000	-3.08369000	-0.50682700
H	4.58137900	-3.15372300	0.90142000
C	3.89531300	-2.14620000	-2.35623700
H	4.74675900	-2.68791500	-2.79822700
H	3.02975900	-2.24472600	-3.02566500
H	4.14675200	-1.07973700	-2.29552200
C	5.16732500	-1.16541200	0.35400700
C	6.05245600	-0.40013500	-0.42105500
C	4.57913800	-0.56805000	1.47790500
C	6.32655200	0.92677400	-0.07864600
H	6.53584400	-0.84935300	-1.29286600
C	4.83093500	0.76574500	1.83042000
H	3.88890200	-1.15389900	2.08665300
C	5.71834800	1.50856900	1.03689700
H	7.02437100	1.51157800	-0.68399900
H	5.93937300	2.54663900	1.29893300
C	4.11554700	1.37524800	3.01543800
H	4.74701900	2.14498900	3.48888100
H	3.93160700	0.59479300	3.76854100
C	2.02829700	2.41792900	3.98789200
H	1.05312600	2.88766500	3.78018300
H	1.85563200	1.52818300	4.60970900
H	2.63690400	3.13717500	4.55890500
C	-0.26883600	1.43912600	-2.54134200
C	0.96733900	2.18453200	-2.32523700
C	-0.26557400	0.29030600	-3.38742000
C	1.08452200	3.38754300	-1.57642700
C	2.17343900	1.66336800	-2.91028900
C	0.95587100	-0.16690400	-3.94681100
C	2.30328100	4.02320800	-1.42497500
H	0.19975300	3.81078800	-1.11712300
C	3.41239100	2.31991000	-2.69917300
C	2.12639300	0.49530600	-3.71921300
H	0.90300200	-1.06364500	-4.56516100
C	3.48633100	3.48889100	-1.97220600
H	2.34547400	4.94809400	-0.84493300
H	4.31257400	1.87705800	-3.13285600
H	3.05481100	0.12853700	-4.16069900
H	4.44511300	3.98879300	-1.81764200
O	-1.33867600	-0.41139900	-3.72176000
C	-3.07781000	3.17733500	-1.35343600
C	-3.66356200	1.98987100	-1.88058700
C	-3.87407900	4.17661900	-0.74646200
C	-5.05766100	1.76368900	-1.81702900
C	-5.23517100	3.94314500	-0.69222700
H	-3.42126200	5.08159800	-0.33881700
C	-5.81872600	2.75143200	-1.22103000
H	-5.49735800	0.84298000	-2.20170300
H	-5.89016600	4.68454100	-0.22849900
H	-6.89999000	2.61783500	-1.13942900
N	-2.66160200	1.23120900	-2.36131700
N	-1.54971400	1.94800100	-2.13509300
N	-1.74422900	3.10821000	-1.53888600
H	-2.12578800	-0.00922500	-3.25385100
C	-3.50315000	-2.84124200	-1.43159100
H	-3.30623100	-2.05026400	-2.16990100
H	-4.14343700	-3.59392800	-1.92021000
C	-4.21487400	-2.24257200	-0.23864200
C	-3.92376300	-0.92781900	0.15041400
C	-5.14551700	-2.97104700	0.51808700
C	-4.51871700	-0.33118200	1.27182100
H	-3.20259500	-0.35735200	-0.43195600
C	-5.75539200	-2.39200400	1.63451200
H	-5.39782600	-3.99458700	0.22773100
C	-5.44334600	-1.08241400	2.01226700
H	-6.48358100	-2.96560100	2.21419100
H	-5.92817000	-0.63607400	2.88494400
C	-4.13893000	1.08085200	1.65621200
H	-3.96771100	1.66676400	0.74611300
H	-4.97002800	1.56488700	2.19428300

3a[Rh] (conformer 2)

Rh	-0.74753000	-1.22701900	1.82566100
O	0.70917700	-2.56583100	1.27777800
C	1.33871900	-2.39609600	0.19038000
O	1.16255600	-1.43033600	-0.61000700
Rh	-0.27989700	-0.03676200	-0.20609800
O	1.06737500	1.09624100	0.83691800
C	1.22123300	0.89005400	2.07687700
O	0.61784200	-0.00109000	2.74868200
O	-1.64636300	-1.26506600	-1.11556400
C	-2.26285600	-2.14753100	-0.44318500
O	-2.10570500	-2.35980300	0.79316200
O	-1.75777800	1.28106400	0.34718500
C	-2.39771900	1.09789700	1.42895800
O	-2.19664000	0.14867600	2.24033700
C	2.21060500	1.77831700	2.84091800
C	-3.48161800	2.12682300	1.77255500
C	-3.25413500	-3.01862500	-1.22360500
C	2.39183200	-3.45087900	-0.16861900
C	1.67140500	-4.80991100	-0.27989900
H	0.92343900	-4.78986500	-1.08902100
H	2.39950200	-5.60435700	-0.50901100
H	1.15720300	-5.06155600	0.65850800
C	2.87208600	2.78974200	1.89748600
H	3.58431800	3.41333200	2.46122200
H	3.40677000	2.28970300	1.08085600
H	2.11780400	3.44624700	1.44156400
C	-4.24943900	1.70400000	3.03073300
H	-4.73734900	0.72902500	2.89687800
H	-3.57177600	1.62108600	3.89212300

H	-5.02203600	2.45433300	3.26373500
C	-4.00144300	-3.96792900	-0.28001600
H	-3.29786900	-4.62961900	0.24480300
H	-4.56709000	-3.41393300	0.48138500
H	-4.70440700	-4.59034200	-0.85662900
C	-2.43023800	-3.82293200	-2.25231300
H	-1.71393600	-4.48836300	-1.74378300
H	-3.09858200	-4.44804400	-2.86576300
H	-1.86294900	-3.15205600	-2.91395600
C	-2.76259400	3.47111500	2.01278400
H	-2.06961900	3.39506200	2.86643300
H	-2.18903000	3.77165700	1.12589800
H	-3.49994100	4.25715200	2.24202400
C	3.42959300	-3.51672800	0.99743900
H	4.19550900	-4.25594300	0.71050700
H	2.91268700	-3.90952200	1.88548600
C	3.07183200	-3.10344700	-1.49746600
H	3.81849800	-3.87408300	-1.74749300
H	2.33448000	-3.05243400	-2.31137600
H	3.57340300	-2.13038700	-1.44131500
C	4.08211400	-2.19534800	1.34074100
C	5.27373800	-1.78093600	0.72725000
C	3.47431100	-1.33240500	2.26531500
C	5.82873600	-0.53519900	1.02853400
H	5.77106600	-2.43846900	0.00930800
C	4.00501000	-0.06867100	2.56436200
H	2.55085300	-1.64619400	2.75334100
C	5.19685500	0.31959600	1.93397500
H	6.75667800	-0.22343000	0.54552700
H	5.63405800	1.29670400	2.15564600
C	3.27308600	0.85285500	3.51493700
H	3.99011400	1.50699100	4.03778200
H	2.75936200	0.25293200	4.28058500
C	1.41914500	2.51760600	3.93918300
H	0.64774600	3.16705300	3.49442900
H	0.92241800	1.80621000	4.61415100
H	2.09867100	3.15174200	4.53072000
C	0.54755600	1.36246600	-2.32968600
C	-0.21293000	2.56500000	-1.99644600
C	-0.05879200	0.33387100	-3.10984900
C	0.26192100	3.62556700	-1.18044200
C	-1.55843000	2.66656700	-2.48413800
C	-1.41412400	0.47535900	-3.52954100
C	-0.52587300	4.73190800	-0.91040900
H	1.25976600	3.56061500	-0.76496200
C	-2.33511400	3.81640100	-2.19660000
C	-2.12392000	1.60412400	-3.25023300
H	-1.83268300	-0.35380300	-4.09954900
C	-1.83091600	4.84615400	-1.42839800
H	-0.12224000	5.52553700	-0.27632200
H	-3.35239700	3.86601600	-2.59355900
H	-3.15523400	1.70063400	-3.59795900
H	-2.43951800	5.72650700	-1.20959100
O	0.54867000	-0.77002200	-3.51310600
C	-4.24232400	-2.08321900	-1.99091000
H	-3.65833800	-1.51164800	-2.72700700
H	-4.93402300	-2.73223600	-2.55264600
C	-5.02231900	-1.12685400	-1.11542800
C	-4.46671900	0.11146500	-0.75900300
C	-6.28498400	-1.46363100	-0.60412000
C	-5.11692700	0.99391300	0.11718300
H	-3.49036700	0.38600400	-1.15638500
C	-6.96083100	-0.58573600	0.24751900
H	-6.74219400	-2.41857100	-0.87751500
C	-6.37867200	0.63094200	0.61291000
H	-7.94797200	-0.85408400	0.63326700
H	-6.90865800	1.30761400	1.28886800
C	-4.43584000	2.27499100	0.54596900
H	-5.19005200	3.03427100	0.81069100
H	-3.84457000	2.67687600	-0.28835900
H	1.50618300	-0.71793600	-3.22255700
C	3.95454400	0.55522400	-2.37139500
C	3.97262400	1.82843300	-1.72943200
C	5.15426300	-0.13934600	-2.65683400
C	5.19062600	2.43682300	-1.34283800
C	6.33261900	0.47731800	-2.28485600
H	5.13937000	-1.11037500	-3.15315300
C	6.35189000	1.74856800	-1.63275300
H	5.19645400	3.40858700	-0.84710500
H	7.28429700	-0.01978200	-2.48834800
H	7.31707000	2.18069400	-1.35772000
N	1.97548000	1.30532700	-2.16285700
N	2.70287800	2.26359400	-1.62095100
N	2.66889500	0.25505900	-2.62528200

3a'[Rh]

Rh	-0.92110900	-0.29508500	-2.19256200
O	0.69531800	0.89938700	-2.69355400
C	1.44119800	1.38502700	-1.79723500
O	1.28028800	1.19826700	-0.54699700
Rh	-0.28222500	0.03382800	0.09151000
O	0.78184900	-1.70227500	-0.05002100
C	0.83963500	-2.32509200	-1.14685000
O	0.24625800	-1.97326300	-2.21525100
O	-1.44580600	1.73021700	0.05384900
C	-2.09350700	2.04256900	-0.99154500
O	-2.08081500	1.38904900	-2.07325600
O	-1.87116600	-1.11185000	0.63387000
C	-2.62371600	-1.60617200	-0.26247400
O	-2.48048600	-1.43622600	-1.50798500
C	1.67836100	-3.60647000	-1.20588200
C	-3.77486600	-2.48410200	0.23920100
C	-2.92859000	3.32529800	-0.90930400
C	2.61624500	2.26053000	-2.24499000
C	2.02853000	3.48757800	-2.97214300
H	1.39466600	4.08088900	-2.29303000
H	2.84266200	4.13681700	-3.33125200
H	1.41740600	3.17967100	-3.83263200
C	2.38665500	-3.84596000	0.13351700
H	2.99944600	-4.75952000	0.07030000
H	3.02847100	-2.99778300	0.40403500
H	1.65136300	-3.97250900	0.94095400
C	-4.66622800	-2.92697400	-0.92659600
H	-5.09889900	-2.06515100	-1.45262100
H	-4.08826600	-3.50735400	-1.65971400
H	-5.48718100	-3.55762800	-0.54952200
C	-3.72347000	3.53833600	-2.20264800
H	-3.04843500	3.61911600	-3.06646200
H	-4.40900400	2.70181700	-2.39472400
H	-4.31238400	4.46669400	-2.13027600
C	-1.93986700	4.49029300	-0.68681700
H	-1.25360500	4.58801200	-1.54375600
H	-2.49078300	5.43873700	-0.58367600
H	-1.33740900	4.32738500	0.21894100

C	-3.13717400	-3.71152800	0.92594800
H	-2.53748500	-4.29324900	0.20735500
H	-2.48136200	-3.40371600	1.75314400
H	-3.92547400	-4.37084900	1.32329200
C	3.48152300	1.43627700	-3.25182000
H	4.32292700	2.08012800	-3.55640000
H	2.86988100	1.25295300	-4.14762100
C	3.45209400	2.70848500	-1.03816300
H	4.31588500	3.29837400	-1.38218200
H	2.86526000	3.34682500	-0.36000900
H	3.82534700	1.85104200	-0.46394100
C	3.99742100	0.11934600	-2.71404900
C	5.23110000	0.02733900	-2.05287800
C	3.21571900	-1.03898900	-2.83303700
C	5.65567600	-1.18925900	-1.51604300
H	5.86013200	0.91626000	-1.95377700
C	3.61794900	-2.26577800	-2.28434000
H	2.25902500	-0.98166200	-3.35306800
C	4.85490700	-2.32733400	-1.62653200
H	6.61348800	-1.24879700	-0.99393200
H	5.19010300	-3.27276600	-1.19215400
C	2.70547600	-3.46942300	-2.37477400
H	3.30195100	-4.39640100	-2.39031400
H	2.14013300	-3.42916600	-3.31772500
C	0.71739200	-4.77231900	-1.51828200
H	-0.03375900	-4.88378200	-0.71942400
H	0.18888600	-4.60652100	-2.46821100
H	1.28151900	-5.71608200	-1.58812900
C	0.97581200	0.33758900	2.50089300
C	0.36945600	-0.81723600	3.12293100
C	0.25988400	1.54539300	2.39866400
C	1.01168500	-2.07905600	3.19904100
C	-0.95333800	-0.68390600	3.65903200
C	-1.02370500	1.66365100	3.00235600
C	0.36323800	-3.16401100	3.75905800
H	2.00666200	-2.19527400	2.77444100
C	-1.58900100	-1.81860100	4.22539600
C	-1.60481900	0.58427500	3.61299400
H	-1.52804200	2.62574000	2.91738400
C	-0.94863600	-3.04082400	4.27133500
H	0.87074700	-4.13118100	3.79626900
H	-2.60240200	-1.70719700	4.62014500
H	-2.60425200	0.67656600	4.04509700
H	-1.45082700	-3.91027500	4.70216000
O	0.76462300	2.64298300	1.80021300
C	-3.87410200	3.22442300	0.33027100
H	-3.24380600	3.20374200	1.23127900
H	-4.46401100	4.15494800	0.36528400
C	-4.79452300	2.02359100	0.33322200
C	-4.35205900	0.80085100	0.86067700
C	-6.08116900	2.08370000	-0.22363300
C	-5.14026100	-0.35905100	0.81009600
H	-3.35723400	0.74428200	1.30180800
C	-6.89173600	0.94595500	-0.25768600
H	-6.45129000	3.02911800	-0.62955900
C	-6.42309300	-0.26940200	0.24811400
H	-7.89607400	1.00621900	-0.68525200
H	-7.05946500	-1.15769100	0.20899700
C	-4.58337900	-1.67608400	1.30466700
H	-5.40172700	-2.32723300	1.65334100
H	-3.91823600	-1.49673000	2.16220600
C	4.50929900	0.83757100	2.08881600
C	3.29681300	1.28810300	2.65037600
C	5.71359100	1.52692000	2.30981300
C	3.23874700	2.42678200	3.47028500
C	5.65942300	2.66025400	3.10963500
H	6.64345600	1.16877600	1.86484500
C	4.43819200	3.09679500	3.68345900
H	2.30324900	2.77525800	3.90526900
H	6.57098200	3.22873200	3.30833800
H	4.44023000	3.99038600	4.31263500
N	2.36851400	0.37140700	2.20192900
N	3.00196400	-0.57121800	1.43203600
N	4.25140900	-0.30621100	1.36493000
H	1.30113700	2.37227600	1.02754600

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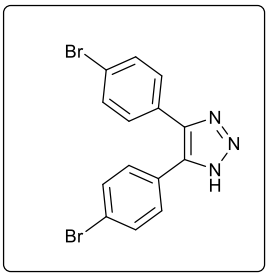
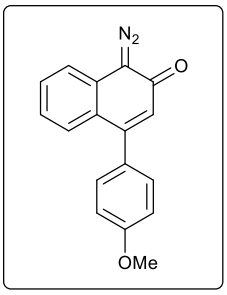
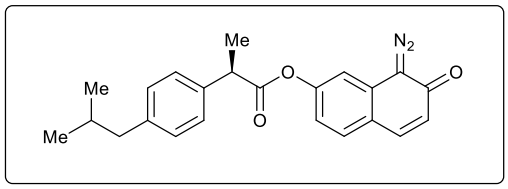
2 Analytical data:



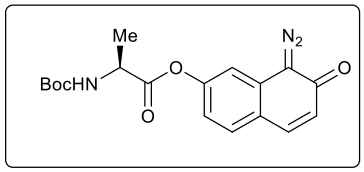
4,5-Bis(4-bromophenyl)-1*H*-1,2,3-triazole (1j); Eluent: 20% ethyl acetate in hexane. White solid. Yield 56%, 421 mg. ^{1}H NMR (400 MHz, DMSO-D_6) δ 7.62 (d, *J* = 6.0 Hz, 4H), 7.43 (d, *J* = 8.0 Hz, 4H). ^{13}C NMR (100 MHz, DMSO-D_6) δ 142.3, 131.9, 130.0, 121.8, 99.5. FT-IR: $\tilde{\nu}$ = 3154, 2916, 1596, 1501, 1452, 1391, 1283, 1202 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{14}H_{14}Br_2N_3$; 377.9236, found 377.9243.



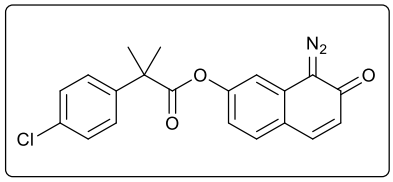
1-Diazo-4-(4-methoxyphenyl)naphthalen-2(1*H*)-one (2t); Eluent: 20% ethyl acetate in hexane. White solid. Yield 78%, 193.7 mg. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.1 Hz, 1H), 7.50 (t, *J* = 7.6 Hz, 1H), 7.33-7.31(m, 3H), 7.20 (m, 1H), 7.00 (d, *J* = 8.7 Hz, 2H), 6.61 (d, *J* = 1.5 Hz, 1H), 3.87 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 179.4, 160.2, 152.4, 130.4, 130.2, 129.7, 129.4, 127.9, 126.1, 124.5, 120.1, 114.1, 55.5. FT-IR: $\tilde{\nu}$ = 2926, 2838, 2092, 1607, 1509, 1477, 1370, 1283, 1248 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{17}H_{13}N_2O_2$; 277.0972, found 277.0980.



8-Diazo-7-*oxo*-7,8-dihydronaphthalen-2-yl (*R*)-2-(4-isobutylphenyl)propanoate (2v); Eluent: 30% ethyl acetate in hexane. Brown solid. Yield 65%, 219.3 mg. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.89 (dd, *J* = 9.8, 2.6 Hz, 1H), 7.84 (dd, *J* = 8.4, 2.3 Hz, 1H), 7.65 (d, *J* = 8.1 Hz, 2H), 7.51 (d, *J* = 8.1 Hz, 2H), 7.23 (m, 1H), 6.94 (dd, *J* = 9.8, 1.9 Hz, 1H), 4.31 (q, *J* = 7.1 Hz, 1H), 2.83 (d, *J* = 7.2 Hz, 2H), 2.22 (m, 1H), 1.98 (d, *J* = 7.2 Hz, 3H), 1.27 (s, 3H), 1.26 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 179.8, 173.0, 152.3, 141.2, 139.7, 136.9, 131.2, 129.7, 128.7, 127.3, 125.6, 123.3, 118.6, 112.4, 45.4, 45.1, 30.2, 22.5, 18.5. FT-IR: $\tilde{\nu}$ = 2955, 2873, 1096, 1755, 1622, 1462, 1396, 1307, 1215 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{23}H_{23}N_2O_3$; 375.1703, found 375.1710.

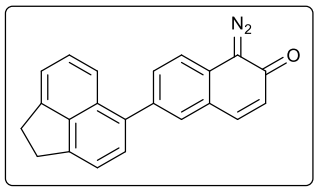


8-Diazo-7-*oxo*-7,8-dihydronaphthalen-2-yl (*tert*-butoxycarbonyl)-*L*-alaninate (2w); Eluent: 40% ethyl acetate in hexane. Brown solid. Yield 63%, 203 mg. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 (d, *J* = 9.8 Hz, 1H), 7.55 (d, *J* = 8.4 Hz, 1H), 7.03 (s, 1H), 6.99 (dd, *J* = 8.4, 1.5 Hz, 1H), 6.62 (dd, *J* = 9.8, 0.7 Hz, 1H), 5.16 (s, 1H), 4.52 (s, 1H), 1.56 (d, *J* = 7.3 Hz, 3H), 1.46 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 179.8, 171.9, 155.4, 151.9, 139.7, 131.4, 128.9, 125.8, 123.6, 118.5, 112.4, 80.5, 45.2, 28.4, 18.2. FT-IR: $\tilde{\nu}$ = 3312, 2980, 2098, 1765, 1699, 1620, 1574, 1517, 1454, 1367, 1296 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{18}H_{20}N_3O_5$; 358.1397, found 358.1414.

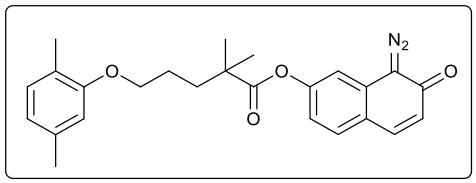


8-Diazo-7-*oxo*-7,8-dihydronaphthalen-2-yl 2-(4-chlorophenyl)-2-methylpropanoate (2x); Eluent: 30% ethyl acetate in hexane. Brown solid. Yield 73%, 241 mg. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.62 (d, *J* = 9.8 Hz, 1H), 7.57 (d, *J* = 8.4 Hz, 1H), 7.29 – 7.24 (m, 2H), 6.95 – 6.88

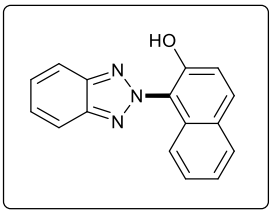
(m, 4H), 6.65 (d, *J* = 9.8 Hz, 1H), 1.77 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 179.7, 172.5, 154.1, 151.8, 139.7, 131.5, 129.5, 129.0, 128.0, 126.0, 123.7, 120.7, 118.4, 112.2, 79.9, 25.5. FT-IR: $\tilde{\nu}$ = 2994, 2938, 2106, 1756, 1595, 1488, 1385, 1237 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{20}H_{16}ClN_2O_3$; 367.0844, found 367.0853.



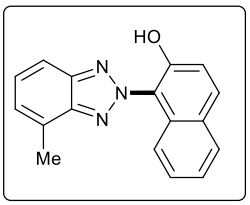
1-Diazo-6-(1,2-dihydroacenaphthylen-5-yl)naphthalen-2(1H)-one (2y); Eluent: 20% ethyl acetate in hexane. Brown solid. Yield 74%, 215 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (s, 1H), 7.73 (m, 1H), 7.67 (dd, *J* = 9.0, 4.3 Hz, 2H), 7.50 – 7.43 (m, 2H), 7.37 (t, *J* = 7.6 Hz, 3H), 6.72 (m, 1H), 3.47 (s, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 180.4, 146.6, 146.4, 140.8, 139.8, 137.5, 134.2, 131.7, 131.1, 129.8, 128.9, 128.5, 126.1, 126.0, 125.9, 120.4, 119.9, 119.8, 119.3, 30.7, 30.2. FT-IR: $\tilde{\nu}$ = 3028, 2919, 2093, 1713, 1600, 1544, 1482, 1422, 1379, 1296, 1258, 1205 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{22}H_{15}N_2O$; 323.1179 found 323.1183.



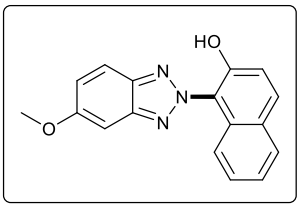
8-Diazo-7-*oxo*-7,8-dihydronaphthalen-2-yl 5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoate (2z); Eluent: 30% ethyl acetate in hexane. Brown solid. Yield 71%, 267 mg. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (d, *J* = 9.8 Hz, 1H), 7.79 (d, *J* = 8.4 Hz, 1H), 7.24 (dd, *J* = 8.1, 4.8 Hz, 2H), 7.20 (dd, *J* = 8.4, 2.1 Hz, 1H), 6.92 (d, *J* = 7.5 Hz, 1H), 6.88 (d, *J* = 9.6 Hz, 2H), 4.26 (t, *J* = 5.6 Hz, 2H), 3.97 (s, 1H), 2.56 (s, 3H), 2.43 (s, 3H), 2.21 – 2.12 (m, 4H), 1.67 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 179.83, 176.1, 156.9, 152.4, 139.8, 136.6, 131.3, 130.5, 128.8, 125.5, 123.6, 123.3, 121.0, 118.7, 112.5, 112.1, 67.8, 43.5, 42.7, 37.1, 25.4, 25.2, 21.4, 15.8. FT-IR: $\tilde{\nu}$ = 2925, 2096, 1750, 1662, 1509, 1394, 1255 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{25}H_{27}N_2O_4$; 419.1965 found 419.1975.



1-(2*H*-Benzo[*d*][1,2,3]triazol-2-yl)naphthalen-2-ol (3a); Eluent: 20% ethyl acetate in hexane. Yield 86%, 44.9 mg. White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.20 (s, 1H), 8.71 (d, *J* = 8.7 Hz, 1H), 8.04 (dd, *J* = 6.5, 3.1 Hz, 2H), 7.91-7.86 (m, 2H), 7.60 (t, *J* = 7.8 Hz, 1H), 7.54 (dd, *J* = 6.6, 3.0 Hz, 2H), 7.45 (t, *J* = 7.5 Hz, 1H), 7.39 (d, *J* = 8.9 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.2, 143.7, 132.0, 129.3, 128.5, 128.3, 127.9, 127.5, 124.5, 122.8, 119.9, 119.3, 118.1. FT-IR: $\tilde{\nu}$ = 3167, 2921, 1603, 1527, 1461, 1408, 1340, 1232 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{16}H_{12}N_3O$; 262.0975, found 262.0982.

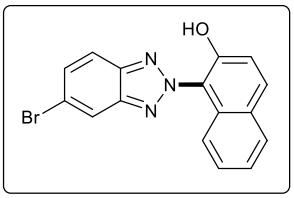


1-(4-Methyl-2*H*-benzo[*d*][1,2,3]triazol-2-yl)naphthalen-2-ol (3b); Eluent: 20% ethyl acetate in hexane. White solid. Yield 56%, 30.8 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.18 (s, 1H), 8.69 (d, *J* = 8.6 Hz, 1H), 7.92 – 7.82 (m, 3H), 7.60 (t, *J* = 7.7 Hz, 1H), 7.48 – 7.33 (m, 4H), 7.28 (d, *J* = 6.7 Hz, 1H), 2.78 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 149.2, 144.3, 143.7, 131.9, 129.3, 128.8, 128.5, 128.3, 128.1, 127.6, 126.9, 124.5, 122.8, 119.2, 115.3, 17.4. FT-IR: $\tilde{\nu}$ = 2924, 2853, 1629, 1515, 1466, 1378, 1288, 1233 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{17}H_{14}N_3O$; 276.1131, found 276.1135.

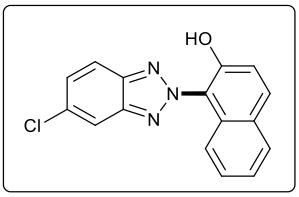


1-(5-Methoxy-2*H*-benzo[*d*][1,2,3]triazol-2-yl)naphthalen-2-ol (3c); Eluent: 20% ethyl acetate in hexane. White solid. Yield 87%, 50.6 mg. ^{1}H NMR (600 MHz, DMSO-D_6) δ 10.62 (s, 1H), 8.07 (d, *J* = 9.0 Hz, 1H), 7.95 (t, *J* = 7.5 Hz, 2H), 7.44 – 7.33 (m, 4H), 7.20 (d, *J* = 9.2 Hz, 1H), 6.67 (d, *J* = 8.0 Hz, 1H), 3.90 (s, 3H). ^{13}C NMR (150 MHz, DMSO-D_6) δ 158.6, 151.4, 145.3, 140.5, 131.7, 131.2, 128.1, 128.0, 127.3, 123.8, 121.7, 120.9, 120.3, 119.2, 118.5,

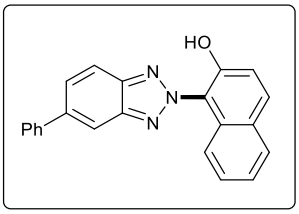
95.3, 55.7. FT-IR: $\tilde{\nu}$ = 2978, 1622, 1541, 1374, 1253, 1219 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{17}H_{14}N_3O_2$; 292.1081, found 292.1087.



1-(5-Bromo-2*H*-benzo[*d*][1,2,3]triazol-2-yl)naphthalen-2-ol (3d); Eluent: 10% ethyl acetate in hexane. White solid. Yield 81%, 54.9 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.02 (s, 1H), 8.62 (d, *J* = 8.7 Hz, 1H), 8.21 (s, 1H), 7.94 – 7.88 (m, 2H), 7.86 (d, *J* = 8.1 Hz, 1H), 7.63 – 7.56 (m, 2H), 7.45 (t, *J* = 7.5 Hz, 1H), 7.37 (d, *J* = 9.0 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.4, 144.6, 142.4, 132.4, 131.8, 129.3, 128.6, 128.4, 127.5, 124.6, 122.7, 121.7, 120.5, 119.8, 119.4, 119.3. FT-IR: $\tilde{\nu}$ = 2923, 1602, 1525, 1470, 1401, 1339, 1229 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{16}H_{11}BrN_3O$; 340.0080, found 340.0081.

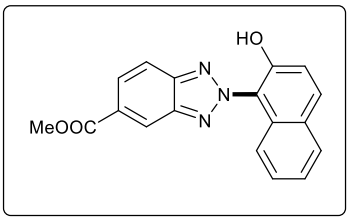


1-(5-Chloro-2*H*-benzo[*d*][1,2,3]triazol-2-yl)naphthalen-2-ol (3e); Eluent: 20% ethyl acetate in hexane. White solid. Yield 79%, 46.6 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.01 (s, 1H), 8.63 (d, *J* = 8.7 Hz, 1H), 8.03 (s, 1H), 7.98 (d, *J* = 9.1 Hz, 1H), 7.92 – 86 (m, 2H), 7.60 (t, *J* = 7.8 Hz, 1H), 7.50 – 7.44 (m, 2H), 7.38 (d, *J* = 8.9 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.3, 144.0, 142.2, 133.9, 132.4, 129.5, 129.3, 128.6, 128.5, 127.4, 124.6, 122.6, 119.7, 119.3, 119.2, 117.1. FT-IR: $\tilde{\nu}$ = 3104, 2918, 1626, 1528, 1470, 1403, 1346, 1231, 1159 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{16}H_{11}ClN_3O$; 296.0585, found 296.0586.

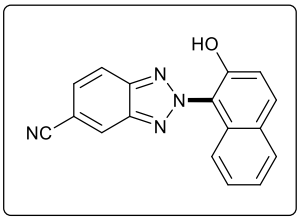


1-(5-Phenyl-2*H*-benzo[*d*][1,2,3]triazol-2-yl)naphthalen-2-ol (3f); Eluent: 10% ethyl acetate in hexane. White solid. Yield 78%, 52.6 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.28 (s, 1H), 8.74 (d, *J* = 8.7 Hz, 1H), 8.19 (s, 1H), 8.10 (d, *J* = 8.6 Hz, 1H), 7.92 – 7.86 (m, 2H), 7.82 (dd, *J* =

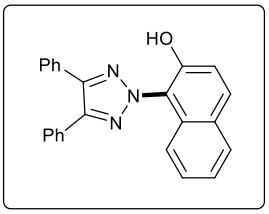
8.9, 1.2 Hz, 1H), 7.73 (d, *J* = 7.1 Hz, 2H), 7.62 (t, *J* = 7.3 Hz, 1H), 7.53 (t, *J* = 7.5 Hz, 2H), 7.49 – 7.38 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.3, 144.3, 143.2, 141.3, 140.7, 132.1, 129.3, 129.2, 128.7, 128.5, 128.3, 128.1, 127.7, 127.5, 124.5, 122.8, 119.9, 119.3, 118.3, 115.3. FT-IR: $\tilde{\nu}$ = 2924, 2853, 1627, 1468, 1377, 1287, 1215 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{22}H_{16}N_3O$; 338.1288, found 338.1295.



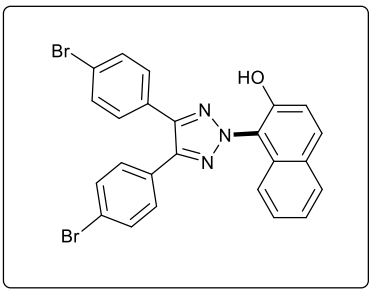
Methyl 2-(2-hydroxynaphthalen-1-yl)-2*H*-benzo[*d*][1,2,3]triazole-5-carboxylate (3g); Eluent: 20% ethyl acetate in hexane. White solid. Yield 72%, 45.9 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.14 (s, 1H), 8.79 (s, 1H), 8.64 (d, *J* = 8.7 Hz, 1H), 8.15 (d, *J* = 9.0 Hz, 1H), 8.04 (d, *J* = 9.0 Hz, 1H), 7.90 (d, *J* = 8.9 Hz, 1H), 7.86 (d, *J* = 8.1 Hz, 1H), 7.60 (m, 1H), 7.45 (t, *J* = 7.5 Hz, 1H), 7.38 (d, *J* = 9.0 Hz, 1H), 4.01 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.6, 149.6, 145.4, 143.1, 132.6, 129.7, 129.3, 128.6, 128.5, 127.8, 127.5, 124.7, 122.7, 121.6, 119.8, 119.3, 118.0, 52.7. FT-IR: $\tilde{\nu}$ = 2922, 2844, 1724, 1579, 1472, 1401, 1322, 1231 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{18}H_{14}N_3O_3$; 320.1030, found 320.1034.



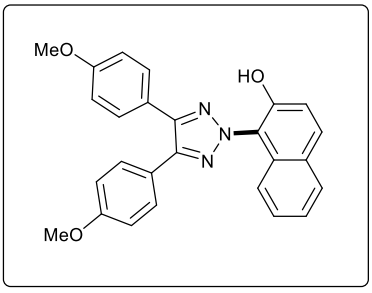
2-(2-Hydroxynaphthalen-1-yl)-2*H*-benzo[*d*][1,2,3]triazole-5-carbonitrile (3h); Eluent: 20% ethyl acetate in hexane. White solid. Yield 68%, 38.9 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.94 (s, 1H), 8.59 (d, *J* = 8.7 Hz, 1H), 8.46 (s, 1H), 8.13 (d, *J* = 8.8 Hz, 1H), 7.94 (d, *J* = 9.0 Hz, 1H), 7.88 (d, *J* = 8.1 Hz, 1H), 7.68 (dd, *J* = 8.8, 1.2 Hz, 1H), 7.61 (m, 1H), 7.48 (t, *J* = 7.3 Hz, 1H), 7.38 (d, *J* = 9.0 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.7, 144.5, 142.5, 133.1, 129.3, 128.8, 128.7, 128.7, 127.4, 125.1, 124.9, 122.4, 119.7, 119.6, 119.3, 118.5, 111.4. FT-IR: $\tilde{\nu}$ = 2923, 2845, 2228, 1628, 1517, 1470, 1408, 1357, 1288, 1218 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{17}H_{11}N_4O$; 287.0927, found 287.0928.



1-(4,5-Diphenyl-2*H*-1,2,3-triazol-2-yl)naphthalen-2-ol (3i); Eluent: 20% ethyl acetate in hexane. White solid. Yield 42%, 30.5 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.52 (s, 1H), 8.65 (d, *J* = 8.7 Hz, 1H), 7.85 (d, *J* = 8.7 Hz, 2H), 7.69 (dd, *J* = 6.4, 2.8 Hz, 4H), 7.58 – 7.53 (m, 1H), 7.46 – 7.43 (m, 6H), 7.36 (d, *J* = 8.9 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.3, 145.1, 130.9, 130.1, 129.4, 129.2, 128.9, 128.7, 128.4, 127.9, 127.6, 124.3, 123.0, 119.5, 119.2. FT-IR: $\tilde{\nu}$ = 2923, 2852, 1629, 1462, 1377, 1289, 1213 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{24}H_{18}N_3O$; 364.1444, found 364.1459.

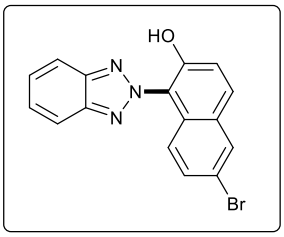


1-(4,5-Bis(4-bromophenyl)-2*H*-1,2,3-triazol-2-yl)naphthalen-2-ol (3j); Eluent: 20% ethyl acetate in hexane. White solid. Yield 39%,40.5 mg. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.22 (s, 1H), 8.53 (d, *J* = 8.7 Hz, 1H), 7.85 (dd, *J* = 8.5, 4.3 Hz, 2H), 7.58 (t, *J* = 7.8 Hz, 4H), 7.54 (d, *J* = 8.5 Hz, 5H), 7.43 (t, *J* = 7.5 Hz, 1H), 7.36 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.2, 144.1, 132.3, 131.2, 130.1, 129.4, 128.7, 128.5, 128.1, 127.4, 124.5, 123.8, 122.7, 119.3, 119.1. FT-IR: $\tilde{\nu}$ = 2924, 2853, 1627, 1464, 1393, 1284, 1214 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{24}H_{16}Br_2N_3O$; 519.9655, found 519.9673.

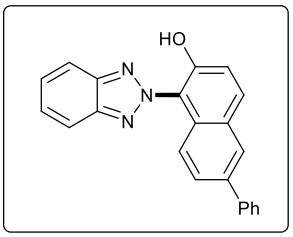


1-(4,5-Bis(4-methoxyphenyl)-2*H*-1,2,3-triazol-2-yl)naphthalen-2-ol (3k); Eluent: 20% ethyl acetate in hexane. White solid. Yield 45%, 38.0 mg. ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.60

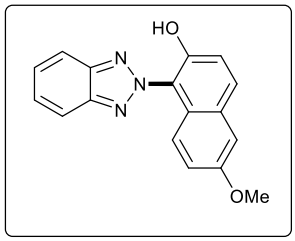
(s, 1H), 8.66 (d, *J* = 8.6 Hz, 1H), 7.82 (d, *J* = 6.4 Hz, 2H), 7.64 – 7.60 (m, 3H), 7.56 – 7.52 (m, 2H), 7.41 (m, 1H), 7.35 (d, *J* = 8.9 Hz, 1H), 7.26 (s, 2H), 7.02 – 6.92 (m, 4H), 3.87 (s, 6H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 160.3, 148.1, 144.6, 130.6, 130.0, 129.4, 128.4, 127.8, 127.5, 124.3, 123.1, 122.6, 119.2, 114.3, 57.8, 55.5. FT-IR: $\tilde{\nu}$ = 2924, 2853, 1712, 1613, 1664, 1378,1250, 1178 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{26}H_{22}N_3O_3$; 424.1656, found 424.1659.



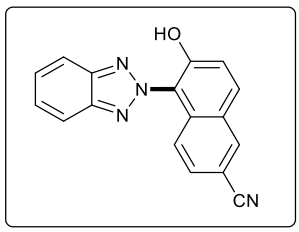
1-(2*H*-Benzo[*d*][1,2,3]triazol-2-yl)-6-bromonaphthalen-2-ol (3l); Eluent: 20% ethyl acetate in hexane. White solid. Yield 85%, 57.6 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.49 (s, 1H), 8.68 (d, *J* = 9.2 Hz, 1H), 8.04-8.00 (m, 3H), 7.79 (d, *J* = 9.0 Hz, 1H), 7.64 (d, *J* = 9.3 Hz, 1H), 7.59 – 7.51 (m, 2H), 7.40 (d, *J* = 9.0 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.6, 143.6, 131.4, 130.9, 130.5, 130.4, 128.1, 126.1, 125.0, 120.6, 119.9, 118.2, 118.1. FT-IR: $\tilde{\nu}$ = 2922, 2862, 1592, 1517, 1466, 1394, 1343, 1239 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{16}H_{11}BrN_3O$; 340.0080, found 340.0079.



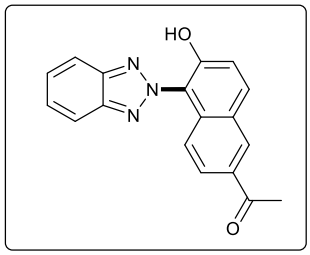
1-(2*H*-Benzo[*d*][1,2,3]triazol-2-yl)-6-phenylnaphthalen-2-ol (3m); Eluent: 20% ethyl acetate in hexane. White solid. Yield 83%, 55.9 mg. ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.41 (d, *J* = 0.7 Hz, 1H), 8.84 (d, *J* = 9.0 Hz, 1H), 8.05 (dd, *J* = 6.5, 2.9 Hz, 3H), 7.94 (d, *J* = 8.9 Hz, 1H), 7.87 (dd, *J* = 9.0, 1.8 Hz, 1H), 7.74 (d, *J* = 7.3 Hz, 2H), 7.58 – 7.52 (m, 2H), 7.50 (t, *J* = 7.7 Hz, 2H), 7.44 – 7.38 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.4, 143.6, 140.6, 137.2, 132.2, 129.7, 129.0, 127.9, 127.8, 127.6, 127.3, 126.6, 126.3, 123.6, 119.8, 119.8, 118.1. FT-IR: $\tilde{\nu}$ = 2923, 2851, 1601, 1495, 1437, 1394, 1341, 1241 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{22}H_{16}N_3O$; 338.1288, found 338.1294.



1-(2*H*-Benzo[*d*][1,2,3]triazol-2-yl)-6-methoxynaphthalen-2-ol (3n); Eluent: 20% ethyl acetate in hexane. White solid. Yield 89%, 51.8 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.07 (s, 1H), 8.64 (d, *J* = 9.4 Hz, 1H), 8.03 (dd, *J* = 6.8, 2.4 Hz, 2H), 7.78 (d, *J* = 8.9 Hz, 1H), 7.53 (dd, *J* = 6.8, 2.4 Hz, 2H), 7.36 (d, *J* = 8.9 Hz, 1H), 7.27 (d, *J* = 8.7 Hz, 1H), 7.18 (s, 1H), 3.94 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.6, 147.6, 143.7, 130.7, 130.6, 127.8, 124.7, 122.7, 120.4, 120.3, 119.8, 118.1, 107.2, 55.5. FT-IR: $\tilde{\nu}$ = 2973, 2844, 1647, 1541, 1473, 1391, 1321, 1265 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{17}H_{14}N_3O_2$; 292.1081, found 292.1082.

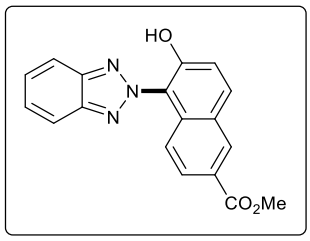


5-(2*H*-Benzo[*d*][1,2,3]triazol-2-yl)-6-hydroxy-2-naphthonitrile (3o); Eluent: 20% ethyl acetate in hexane. White solid. Yield 71%, 40.6 mg. ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.88 (s, 1H), 8.95 (d, *J* = 9.0 Hz, 1H), 8.23 (d, *J* = 1.4 Hz, 1H), 8.04 (dd, *J* = 6.6, 3.1 Hz, 2H), 7.94 (d, *J* = 9.0 Hz, 1H), 7.73 (dd, *J* = 9.0, 1.7 Hz, 1H), 7.57 (dd, *J* = 6.6, 3.1 Hz, 2H), 7.51 (d, *J* = 9.0 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.9, 143.6, 134.3, 132.2, 129.2, 128.8, 128.4, 128.1, 124.6, 121.5, 119.8, 119.1, 118.1, 108.0. FT-IR: $\tilde{\nu}$ = 2915, 2850, 2223, 1730, 1620, 1478, 1394, 1342, 1234 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{17}H_{11}N_4O$; 287.0927, found 287.0925.

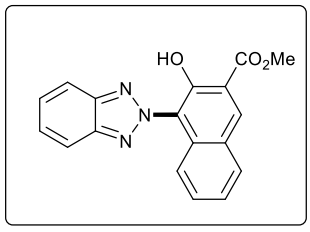


1-(5-(2*H*-Benzo[*d*][1,2,3]triazol-2-yl)-6-hydroxynaphthalen-2-yl)ethan-1-one (3p); Eluent: 20% ethyl acetate in hexane. White solid. Yield 67%, 40.6 mg. ^{1}H NMR (400 MHz, DMSO-D_6) δ 11.26 (s, 1H), 8.71 (s, 1H), 8.30 (d, *J* = 9.0 Hz, 1H), 8.11 – 8.03 (m, 2H), 7.94 –

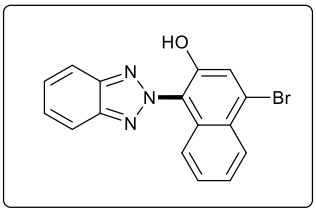
7.84 (m, 2H), 7.61 – 7.49 (m, 3H), 7.46 – 7.40 (m, 1H), 6.76 (d, *J* = 8.8 Hz, 1H), 2.66 (s, 3H). ^{13}C NMR (125 MHz, DMSO-D_6) δ 197.4, 153.9, 144.5, 133.8, 133.3, 132.3, 130.8, 127.2, 126.3, 126.0, 125.5, 121.1, 120.7, 119.5, 118.4, 26.6. FT-IR: $\tilde{\nu}$ = 2923, 2853, 1639, 1614, 1442, 1364, 1294, 1260, 1197 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{18}H_{14}N_3O_2$; 304.1081, found 304.1085.



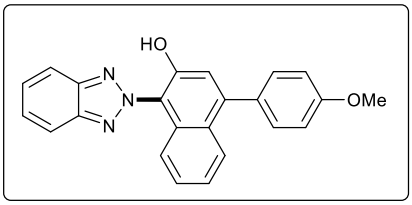
Methyl 5-(2*H*-benzo[*d*][1,2,3]triazol-2-yl)-6-hydroxy-2-naphthoate (3q); Eluent: 20% ethyl acetate in hexane. White solid. Yield 74%, 47.2 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.62 (s, 1H), 8.80 (d, *J* = 9.1 Hz, 1H), 8.59 (d, *J* = 1.3 Hz, 1H), 8.16 (dd, *J* = 9.1, 1.6 Hz, 1H), 8.03 (dd, *J* = 6.5, 3.1 Hz, 2H), 7.99 (d, *J* = 9.0 Hz, 1H), 7.55 (dd, *J* = 6.6, 3.0 Hz, 2H), 7.44 (d, *J* = 9.0 Hz, 1H), 3.99 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.0, 151.3, 143.7, 133.3, 131.4, 129.9, 128.4, 128.1, 127.7, 126.1, 123.3, 120.3, 119.9, 118.1, 52.4. FT-IR: $\tilde{\nu}$ = cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{18}H_{14}N_3O_3$; 320.1030, found 320.1036.



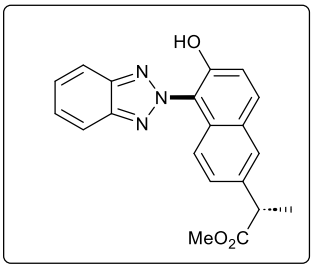
Methyl 4-(2*H*-benzo[*d*][1,2,3]triazol-2-yl)-3-hydroxy-2-naphthoate (3r); Eluent: 20% ethyl acetate in hexane. White solid. Yield 72%, 45.9 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.10 (s, 1H), 8.72 (s, 1H), 8.11 – 7.99 (m, 2H), 7.90 (s, 1H), 7.56 – 7.46 (m, 3H), 7.41 (s, 1H), 7.03 (d, *J* = 8.2 Hz, 1H), 4.06 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 169.8, 152.7, 145.2, 134.9, 134.4, 131.3, 129.6, 127.2, 126.5, 125.2, 122.8, 121.4, 118.8, 114.3, 53.2. FT-IR: $\tilde{\nu}$ = 2924, 2854, 1688, 1635, 1513, 1454, 1328, 1224, 1158 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{18}H_{14}N_3O_3$; 320.1030, found 320.1038.



1-(2*H*-Benzo[*d*][1,2,3]triazol-2-yl)-4-bromonaphthalen-2-ol (3s); Eluent: 10% ethyl acetate in hexane. White solid. Yield 72%, 48.8 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.20 (s, 1H), 8.67 (d, *J* = 8.6 Hz, 1H), 8.27 (d, *J* = 8.4 Hz, 1H), 8.01 (dd, *J* = 6.5, 2.8 Hz, 2H), 7.74 (s, 1H), 7.62 (t, *J* = 7.7 Hz, 1H), 7.57 – 7.50 (m, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.8, 143.8, 128.9, 128.2, 128.1, 127.8, 127.8, 125.9, 125.7, 123.4, 123.3, 119.8, 118.1. FT-IR: $\tilde{\nu}$ = 2920, 2851, 1594, 15191458, 1370, 1327, 1225 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{16}H_{11}BrN_3O$; 340.0080, found 340.0082.

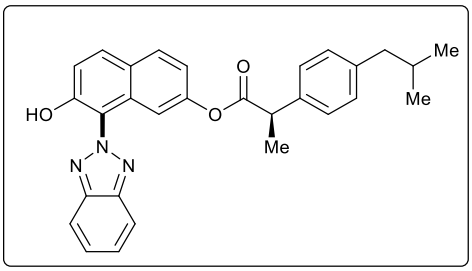


1-(2*H*-Benzo[*d*][1,2,3]triazol-2-yl)-4-(4-methoxyphenyl)naphthalen-2-ol (3t); Eluent: 10% ethyl acetate in hexane. White solid. Yield 79%, 57.9 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.03 (s, 1H), 8.68 (d, *J* = 8.7 Hz, 1H), 8.08 – 8.01 (m, 2H), 7.92 (d, *J* = 8.5 Hz, 1H), 7.62 – 7.53 (m, 3H), 7.47 (d, *J* = 8.2 Hz, 2H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.34 (s, 1H), 7.06 (d, *J* = 8.1 Hz, 2H), 3.92 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.7, 148.5, 144.3, 143.9, 132.1, 131.2, 128.3, 128.11, 128.07, 127.9, 126.9, 124.5, 123.0, 120.0, 119.3, 118.2, 114.1, 55.6. FT-IR: $\tilde{\nu}$ = 2926, 2853, 1608, 1512, 1463, 1366, 1295, 1248 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{23}H_{18}N_3O_2$; 368.1394, found 368.1408.

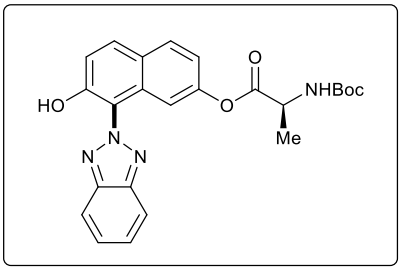


Methyl (*S*)-2-(5-(2*H*-benzo[*d*][1,2,3]triazol-2-yl)-6-hydroxynaphthalen-2-yl)propanoate (3u); Eluent: 20% ethyl acetate in hexane. White solid. Yield 76%, 52.7 mg. ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.27 (s, 1H), 8.69 (d, *J* = 8.9 Hz, 1H), 8.06 – 8.00 (m, 2H), 7.86 (d, *J* = 8.9

Hz, 1H), 7.76 (d, *J* = 1.7 Hz, 1H), 7.57 – 7.51 (m, 3H), 7.38 (d, *J* = 8.9 Hz, 1H), 3.90 (q, *J* = 7.1 Hz, 1H), 3.68 (s, 3H), 1.60 (d, *J* = 7.1 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 175.0, 149.2, 143.7, 136.6, 131.9, 129.4, 128.2, 127.9, 126.8, 126.6, 123.4, 119.8, 119.6, 118.1, 52.3, 45.3, 18.6. FT-IR: $\tilde{\nu}$ = 2923, 2851, 1732, 1609, 1455, 1377, 1196 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{20}H_{18}N_3O_3$; 348.1343, found 348.1356.

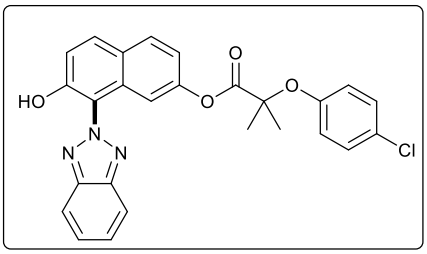


8-(2*H*-Benzo[*d*][1,2,3]triazol-2-yl)-7-hydroxynaphthalen-2-yl (R)-2-(4-isobutylphenyl)propanoate (3v); Eluent: 20% ethyl acetate in hexane. White solid. Yield 71%, 66 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.55 (s, 1H), 8.48 (s, 1H), 8.02 (dd, *J* = 6.5, 2.9 Hz, 2H), 7.86-7.80 (m, 2H), 7.54 (dd, *J* = 6.5, 2.8 Hz, 2H), 7.36-7.31 (m, 4H), 7.15 (t, *J* = 9.6 Hz, 3H), 3.99 (q, *J* = 7.1 Hz, 1H), 2.47 (d, *J* = 7.6 Hz, 3H), 1.86 (dd, *J* = 13.0, 6.5 Hz, 1H), 1.62 (d, *J* = 7.6 Hz, 4H), 0.90 (d, *J* = 6.8 Hz, 8H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 173.5, 151.0, 150.0, 143.5, 141.0, 137.4, 131.7, 129.9, 129.69, 129.66, 129.3, 127.9, 127.4, 119.6, 119.2, 118.1, 114.5, 109.4, 45.5, 45.2, 30.3, 22.5, 18.7. FT-IR: $\tilde{\nu}$ = 2958, 2921, 1734, 1628, 1450, 1341, 1263, 1197 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{29}H_{28}N_3O_3$; 466.2125, found 466.2138.

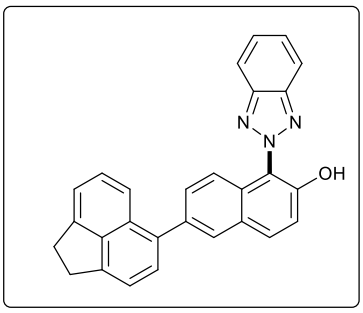


8-(2*H*-Benzo[*d*][1,2,3]triazol-2-yl)-7-hydroxynaphthalen-2-yl (*tert*-butoxycarbonyl)-*L*-alaninate (3w); Eluent: 20% ethyl acetate in hexane. White solid. Yield 53%, 47.5 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.57 (s, 1H), 8.55 (s, 1H), 8.07 – 8.00 (m, 2H), 7.92 – 7.85 (m, 2H), 7.57 – 7.51 (m, 2H), 7.38 (d, *J* = 9.0 Hz, 1H), 7.23 (d, *J* = 8.6 Hz, 1H), 5.12 (s, 1H), 4.61 (s, 1H), 1.59 (d, *J* = 7.1 Hz, 3H), 1.45 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.6, 150.1, 143.6, 131.8, 130.1, 128.2, 128.0, 127.8, 127.4, 119.7, 119.44, 119.36, 118.1, 118.0, 114.5,

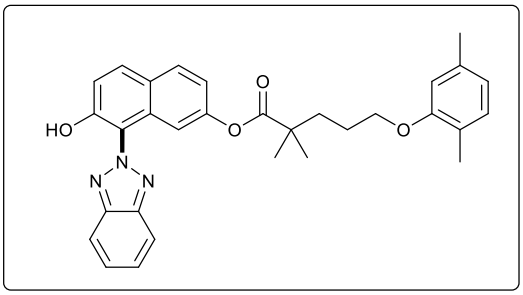
80.3, 49.7, 28.5, 18.7. FT-IR: $\tilde{\nu}$ = 2925, 2854, 1763, 1708, 1636, 1513, 1456, 1367, 1272, 1214 cm^{-1}. HRMS: Calculated for $[M+NH_4]^+$ $C_{24}H_{28}N_5O_5$; 466.2085, found 466.2096.



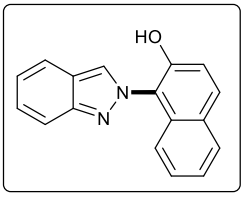
8-(2*H*-Benzo[*d*][1,2,3]triazol-2-yl)-7-hydroxynaphthalen-2-yl 2-(4-chlorophenoxy)-2-methylpropanoate (3x); Eluent: 20% ethyl acetate in hexane. White solid. Yield 73%, 69 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.63 (s, 1H), 8.51 (s, 1H), 8.02 (dd, *J* = 6.6, 3.0 Hz, 2H), 7.88 (dd, *J* = 8.8, 4.9 Hz, 2H), 7.56 (dd, *J* = 6.6, 3.1 Hz, 2H), 7.38 (d, *J* = 9.0 Hz, 1H), 7.20 (t, *J* = 6.1 Hz, 2H), 7.14 (dd, *J* = 8.8, 2.2 Hz, 1H), 6.95 (dd, *J* = 6.1, 2.6 Hz, 2H), 1.76 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 172.9, 154.5, 154.2, 150.6, 150.2, 143.5, 131.8, 130.2, 129.5, 129.4, 128.1, 120.9, 120.8, 119.6, 119.2, 118.1, 114.6, 109.5, 79.8, 25.5. FT-IR: $\tilde{\nu}$ = 2925, 2854, 1755, 1633, 1489, 1385, 1236 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{26}H_{21}ClN_3O_4$; 474.1215, found 474.1230.



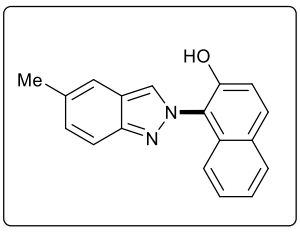
1-(2*H*-Benzo[*d*][1,2,3]triazol-2-yl)-6-(1,2-dihydroacenaphthylen-5-yl)naphthalen-2-ol (3y); Eluent: 20% ethyl acetate in hexane. White solid. Yield 71%, 58.6 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.38 (s, 1H), 8.86 (d, *J* = 8.9 Hz, 1H), 8.09 – 8.01 (m, 3H), 7.96 (d, *J* = 8.9 Hz, 1H), 7.85 (d, *J* = 8.9 Hz, 1H), 7.79 (d, *J* = 8.3 Hz, 1H), 7.59 – 7.51 (m, 3H), 7.46 (t, *J* = 8.2 Hz, 2H), 7.39 (d, *J* = 6.9 Hz, 1H), 7.34 (d, *J* = 6.7 Hz, 1H), 3.48 (s, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.2, 146.4, 146.0, 143.7, 139.8, 136.7, 135.0, 132.2, 130.6, 130.0, 129.5, 129.0, 128.9, 128.3, 127.9, 126.5, 122.9, 120.9, 119.9, 119.6, 119.3, 118.1, 30.7, 30.2. FT-IR: $\tilde{\nu}$ = 2923, 2853, 1607, 1464, 1362, 1269, 1216 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{28}H_{20}N_3O$; 414.1601, found 414.1614.



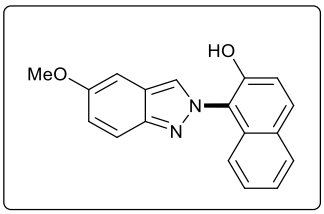
8-(2*H*-Benzo[*d*][1,2,3]triazol-2-yl)-7-hydroxynaphthalen-2-yl 5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoate (3z); Eluent: 20% ethyl acetate in hexane. White solid. Yield 48.8 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.57 (s, 1H), 8.53 (s, 1H), 7.98 (dd, *J* = 6.6, 3.0 Hz, 2H), 7.87 (t, *J* = 9.5 Hz, 2H), 7.49 (dd, *J* = 6.5, 3.0 Hz, 2H), 7.37 (d, *J* = 8.9 Hz, 1H), 7.17 (dd, *J* = 8.7, 2.1 Hz, 1H), 7.07 – 6.95 (m, 2H), 6.67 (d, *J* = 7.5 Hz, 1H), 6.62 (s, 1H), 3.99 (s, 2H), 2.31 (s, 3H), 2.15 (s, 3H), 1.93 (d, *J* = 2.1 Hz, 4H), 1.41 (s, 6H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 176.7, 157.0, 151.2, 150.0, 143.5, 136.6, 131.8, 130.5, 130.0, 128.2, 127.9, 127.2, 123.7, 120.9, 119.8, 119.6, 119.2, 118.0, 114.5, 112.1, 67.9, 42.7, 37.4, 25.5, 25.3, 21.5, 15.9. FT-IR: $\tilde{\nu}$ = 2925, 2855, 1748, 1628, 1510, 1454, 152, 1265 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{31}H_{32}N_3O_4$; 510.2384, found 510.2408.



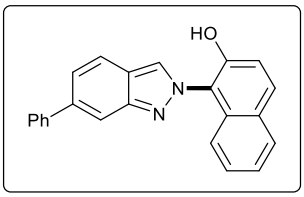
1-(2*H*-Indazol-2-yl)naphthalen-2-ol (5a); Eluent: 20% ethyl acetate in hexane. White solid. Yield 81%, 42.1 mg. ^{1}H NMR (400 MHz, DMSO-D_6) δ 10.46 (s, 1H), 8.57 (d, *J* = 0.8 Hz, 1H), 8.01 (d, *J* = 8.9 Hz, 1H), 7.93 (dd, *J* = 6.8, 2.4 Hz, 1H), 7.82 (d, *J* = 8.4 Hz, 1H), 7.72 (dd, *J* = 8.8, 0.8 Hz, 1H), 7.42 – 7.32 (m, 4H), 7.15 (m, 1H), 6.85 (m, 1H). ^{13}C NMR (125 MHz, DMSO-D_6) δ 150.6, 148.6, 131.5, 130.6, 127.7, 127.64, 127.55, 127.4, 125.9, 123.5, 121.6, 121.3, 120.9, 120.8, 120.6, 118.4, 117.3. FT-IR: $\tilde{\nu}$ = 2925, 2854, 1634, 1510, 1443, 1355, 1288, 1231, 1148 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{17}H_{23}N_2O$; 261.1022, found 261.1025.



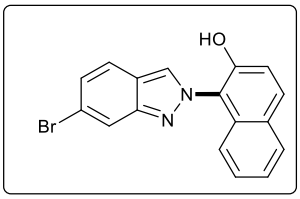
1-(5-Methyl-2*H*-indazol-2-yl)naphthalen-2-ol (5b); Eluent: 20% ethyl acetate in hexane. White solid. Yield 77%, 42.2 mg. ^{1}H NMR (400 MHz, DMSO-D_6) δ 10.45 (s, 1H), 8.42 (s, 1H), 7.99 (d, *J* = 9.0 Hz, 1H), 7.92 (m, 1H), 7.63 (d, *J* = 8.7 Hz, 1H), 7.55 (s, 1H), 7.41 – 7.32 (m, 3H), 7.18 (d, *J* = 8.8 Hz, 1H), 6.86 (d, *J* = 6.9 Hz, 1H), 2.42 (s, 3H). ^{13}C NMR (125 MHz, DMSO-D_6) δ 150.6, 147.6, 131.6, 130.7, 130.2, 128.8, 127.8, 127.6, 127.4, 126.7, 123.5, 121.9, 121.0, 120.7, 118.8, 118.4, 117.2, 21.4. FT-IR: $\tilde{\nu}$ = 2979, 1664, 1624, 1374, 1248 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{18}H_{15}N_2O$; 275.1179, found 275.1177.



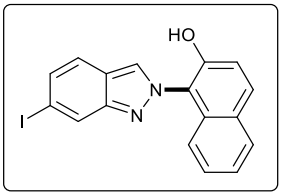
1-(5-Methoxy-2*H*-indazol-2-yl)naphthalen-2-ol (5c); Eluent: 20% ethyl acetate in hexane. White solid. Yield 82%, 47.6 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.45 (s, 1H), 8.34 (s, 1H), 7.98 – 7.83 (m, 3H), 7.75 (d, *J* = 9.2 Hz, 1H), 7.52 (m, 1H), 7.44 (m, 1H), 7.39 (d, *J* = 8.9 Hz, 1H), 7.17 (dd, *J* = 9.4, 2.1 Hz, 1H), 7.04 (s, 1H), 3.92 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 155.9, 149.3, 146.4, 130.6, 129.1, 128.7, 128.2, 127.9, 125.9, 124.1, 122.9, 122.2, 120.9, 119.9, 119.2, 118.8, 96.6, 55.6. FT-IR: $\tilde{\nu}$ = 2924, 2853, 1715, 1516, 1397, 1351, 1307, 1266, 1215, 1146 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{18}H_{15}N_2O_2$; 291.1128, found 291.1105.



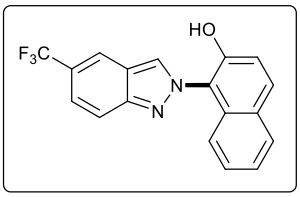
1-(6-Phenyl-2*H*-indazol-2-yl)naphthalen-2-ol (5d); Eluent: 20% ethyl acetate in hexane. White solid. Yield 70%, 47.0 mg. ^{1}H NMR (400 MHz, DMSO-D_6) δ 10.53 (s, 1H), 8.59 (s, 1H), 8.01 (d, *J* = 9.1 Hz, 1H), 7.97 – 7.90 (m, 3H), 7.79 (d, *J* = 7.3 Hz, 2H), 7.52-7.46 (m, 3H), 7.43 – 7.35 (m, 4H), 6.92 (d, *J* = 7.4 Hz, 1H). ^{13}C NMR (125 MHz, DMSO-D_6) δ 150.7, 149.2, 141.0, 138.2, 131.5, 130.8, 129.0, 127.93, 127.85, 127.7, 127.5, 127.4, 127.1, 123.6, 121.63, 121.57, 121.03, 120.99, 120.7, 118.5, 114.7. FT-IR: $\tilde{\nu}$ = 2924, 2856, 1620, 1497, 1364, 1265 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{23}H_{17}N_2O$; 337.1335, found 337.1338.



1-(6-Bromo-2*H*-indazol-2-yl)naphthalen-2-ol (5e); Eluent: 20% ethyl acetate in hexane. White solid. Yield 74%, 50 mg. ^{1}H NMR (500 MHz, DMSO-D_6) δ 10.51 (s, 1H), 8.65 (d, *J* = 0.6 Hz, 1H), 8.03 – 7.98 (m, 2H), 7.93 (m, 1H), 7.82 (d, *J* = 8.8 Hz, 1H), 7.41 – 7.35 (m, 3H), 7.24 (dd, *J* = 8.9, 1.6 Hz, 1H), 6.87 (d, *J* = 7.9 Hz, 1H). ^{13}C NMR (125 MHz, DMSO-D_6) δ 150.6, 149.2, 131.3, 131.0, 128.9, 127.84, 127.76, 127.4, 124.7, 123.6, 123.2, 120.8, 120.28, 120.26, 119.5, 119.4, 118.4. FT-IR: $\tilde{\nu}$ = 2934, 2851, 1622, 1517, 1493, 1444, 1382, 1291, 1251 cm^{-1}.HRMS: Calculated for $[M+H]^+$ $C_{17}H_{12}BrN_2O$; 339.0128, found 339.0119.

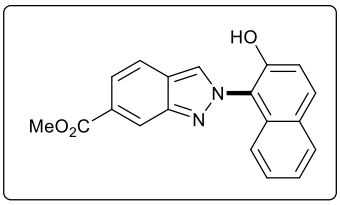


1-(6-Iodo-2*H*-indazol-2-yl)naphthalen-2-ol (5f); Eluent: Eluent: 20% ethyl acetate in hexane. White solid. Yield 71%, 54.7 mg. ^{1}H NMR (400 MHz, DMSO-D_6) δ 10.51 (s, 1H), 8.62 (s, 1H), 8.20 (s, 1H), 8.01 (d, *J* = 8.9 Hz, 1H), 7.93 (d, *J* = 5.6 Hz, 1H), 7.68 (d, *J* = 8.7 Hz, 1H), 7.38 (d, *J* = 8.7 Hz, 4H), 6.86 (d, *J* = 6.5 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-D_6) δ 150.7, 150.0, 131.3, 131.0, 129.7, 128.8, 127.9, 127.8, 127.4, 126.1, 123.7, 123.1, 120.9, 120.5, 120.3, 118.4, 92.2. FT-IR: $\tilde{\nu}$ = 2926, 2854, 1624, 1509, 1372, 1267 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{17}H_{12}IN_2O$; 386.9989, found 386.9987.

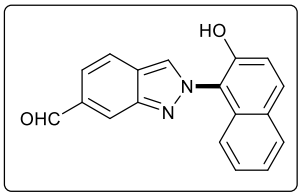


1-(5-(Trifluoromethyl)-2*H*-indazol-2-yl)naphthalen-2-ol (5g); Eluent: 20% ethyl acetate in hexane. White solid. Yield 63%, 41.3 mg. ^{1}H NMR (400 MHz, DMSO-D_6) δ 10.59 (s, 1H), 8.85 (s, 1H), 8.35 (s, 1H), 8.03 (d, *J* = 9.0 Hz, 1H), 7.95 (d, *J* = 9.3 Hz, 2H), 7.56 (d, *J* = 9.1 Hz, 1H), 7.43 – 7.34 (m, 3H), 6.89 (d, *J* = 8.2 Hz, 1H). ^{13}C NMR (125 MHz, DMSO-D_6) δ 150.6, 148.8, 131.1, 131.1, 130.6, 127.8, 127.8, 127.4, 126.0, 122.2, 121.9, 121.4, 121.4, 120.7,

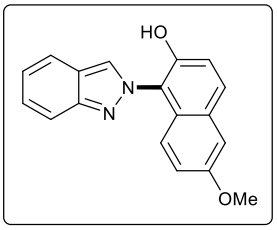
120.4 (q, *J* = 4.9 Hz), 120.2, 119.0, 118.4. FT-IR: $\tilde{\nu}$ = 2917, 1715, 1625, 1542, 1426, 1329, 1250 cm^{-1}. HRMS: Calculated for $[M+H]^+C_{18}H_{12}F_3N_2O$; 329.0896, found 329.0903.



Methyl 2-(2-hydroxynaphthalen-1-yl)-2*H*-indazole-6-carboxylate (5h); Eluent: 20% ethyl acetate in hexane. White solid. Yield 62%, 39.4 mg. ^1H NMR (400 MHz, $CDCl_3$) δ 9.40 (s, 1H), 8.56 (s, 1H), 8.48 (s, 1H), 7.90 – 7.82 (m, 4H), 7.79 (d, *J* = 8.6 Hz, 1H), 7.51 (m, 1H), 7.42 (t, *J* = 7.5 Hz, 1H), 7.32 (d, *J* = 9.0 Hz, 1H), 4.00 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.3, 149.6, 148.7, 131.3, 129.6, 129.1, 128.8, 128.28, 128.25, 127.3, 124.4, 124.0, 122.6, 121.0, 120.8, 120.6, 119.8, 119.3, 52.5. FT-IR: $\tilde{\nu}$ = 2925, 2854, 1717, 1630, 1503, 1439, 1318, 1242 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{19}H_{15}N_2O_3$; 319.1077, found 319.1083.

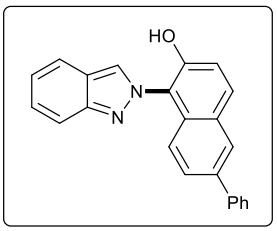


2-(2-Hydroxynaphthalen-1-yl)-2*H*-indazole-6-carbaldehyde (5i); Eluent: 30% ethyl acetate in hexane. White solid. Yield 53%, 30.5 mg. ^1H NMR (500 MHz, $CDCl_3$) δ 10.11 (s, 1H), 8.49 (s, 1H), 8.29 (s, 1H), 7.90-7.87 (m, 3H), 7.72 (d, *J* = 8.6 Hz, 2H), 7.51 (m, 1H), 7.43 (t, *J* = 7.5 Hz, 1H), 7.33 (d, *J* = 9.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.3, 149.8, 148.1, 136.5, 131.7, 129.0, 128.8, 128.49, 128.45, 128.2, 124.7, 124.5, 121.9, 120.4, 119.9, 119.3, 119.2. FT-IR: $\tilde{\nu}$ = 2924, 2853, 1691, 1629, 1556, 1501, 1442, 1355, 186, 1214 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{18}H_{13}N_2O_2$; 289.0972, found 289.0974.

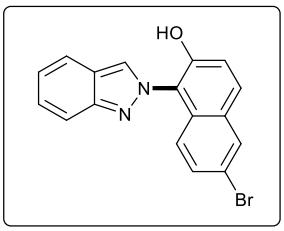


1-(2*H*-Indazol-2-yl)-6-methoxynaphthalen-2-ol (5j); Eluent: Eluent: 20% ethyl acetate in hexane. White solid. Yield 82%, 47.5 mg. ^1H NMR (500 MHz, DMSO-D_6) δ 10.17 (s, 1H),

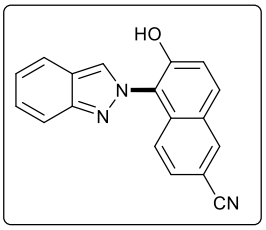
8.54 (s, 1H), 7.89 (d, *J* = 9.0 Hz, 1H), 7.82 (d, *J* = 8.4 Hz, 1H), 7.72 (d, *J* = 8.7 Hz, 1H), 7.35 (m, 3H), 7.13 (m, 1H), 7.06 (dd, *J* = 9.2, 2.5 Hz, 1H), 6.82 (d, *J* = 9.2 Hz, 1H), 3.84 (s, 3H). ^{13}C NMR (125 MHz, DMSO-D_6) δ 155.6, 148.7, 148.6, 129.4, 128.6, 127.8, 126.7, 126.0, 122.7, 121.6, 121.4, 121.0, 120.9, 120.0, 118.9, 117.4, 106.4, 55.3. FT-IR: $\tilde{\nu}$ = 3062, 2935, 1610, 1513, 1408, 1379, 1241 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{18}H_{15}N_2O_2$; 291.1128, found 291.1131.



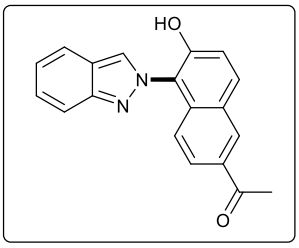
1-(2*H*-Indazol-2-yl)-6-phenylnaphthalen-2-ol (5k); Eluent: 20% ethyl acetate in hexane. White solid. Yield 78%, 52.4 mg. ^{1}H NMR (500 MHz, DMSO-D_6) δ 10.54 (s, 1H), 8.62 (d, *J* = 0.5 Hz, 1H), 8.28 (d, *J* = 1.6 Hz, 1H), 8.12 (d, *J* = 9.0 Hz, 1H), 7.88 (d, *J* = 8.5 Hz, 1H), 7.80 – 7.77 (m, 4H), 7.55 – 7.49 (m, 2H), 7.47 (d, *J* = 9.0 Hz, 1H), 7.39 (dd, *J* = 8.6, 7.6 Hz, 2H), 7.19 (dd, *J* = 5.4, 2.2 Hz, 1H), 7.03 (d, *J* = 8.8 Hz, 1H). ^{13}C NMR (125 MHz, DMSO-D_6) δ 150.8, 148.6, 139.7, 135.2, 131.2, 130.7, 129.01, 128.95, 127.8, 126.7, 126.6, 126.0, 125.2, 121.9, 121.7, 121.4, 121.0, 120.6, 119.0, 117.4, 108.5. FT-IR: $\tilde{\nu}$ = 2928, 2853, 1619, 1520, 1415, 1378, 1248 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{23}H_{17}N_2O$; 337.1335, found 337.1346.



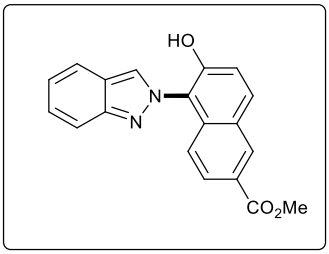
6-Bromo-1-(2*H*-indazol-2-yl)naphthalen-2-ol (5l); Eluent: 20% ethyl acetate in hexane. White solid. Yield 76%, 51.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.67 (s, 1H), 8.39 (s, 1H), 8.02 (d, *J* = 1.6 Hz, 1H), 7.80 (t, *J* = 7.6 Hz, 2H), 7.74 – 7.71 (m, 2H), 7.56 (dd, *J* = 9.1, 1.8 Hz, 1H), 7.43 (m, 1H), 7.34 (d, *J* = 8.9 Hz, 1H), 7.22 (dd, *J* = 8.2, 7.0 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.8, 149.6, 131.2, 130.7, 130.2, 129.8, 128.0, 126.9, 123.2, 122.7, 122.1, 120.7, 120.6, 120.0, 117.8, 117.4. FT-IR: $\tilde{\nu}$ = 2923, 2865, 1629, 1579, 1501, 1357, 1286, 1230 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{17}H_{12}BrN_2O$; 339.1028, found 339.1040.



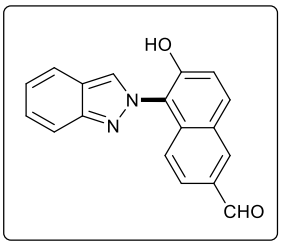
6-Hydroxy-5-(2*H*-indazol-2-yl)-2-naphthonitrile (5m); Eluent: 20% ethyl acetate in hexane. White solid. Yield 64%, 36.5 mg. ^{1}H NMR (400 MHz, DMSO-D_6) δ 11.17 (s, 1H), 8.62-8.60 (m, 2H), 8.16 (d, *J* = 9.0 Hz, 1H), 7.83 (d, *J* = 8.4 Hz, 1H), 7.73 (d, *J* = 8.4 Hz, 1H), 7.66 (d, *J* = 8.8 Hz, 1H), 7.55 (d, *J* = 9.0 Hz, 1H), 7.39 – 7.29 (m, 1H), 7.18 – 7.09 (m, 1H), 6.99 (d, *J* = 8.8 Hz, 1H). ^{13}C NMR (125 MHz, DMSO-D_6) δ 153.5, 148.7, 134.2, 133.1, 131.6, 128.2, 127.9, 126.2, 126.1, 122.5, 121.6, 121.5, 120.9, 120.7, 120.2, 119.1, 117.3, 105.7. FT-IR: $\tilde{\nu}$ = 2981, 2666, 2254, 1629, 1580, 1510, 1391, 1321, 1248 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{18}H_{12}N_3O$; 286.0975, found 286.0978.



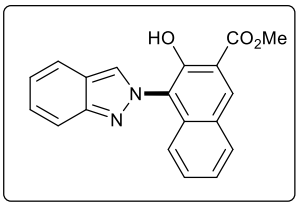
1-(6-Hydroxy-5-(2*H*-indazol-2-yl)naphthalen-2-yl)ethan-1-one (5n); Eluent: 20% ethyl acetate in hexane. White solid. Yield 63%, 38 mg. ^{1}H NMR (400 MHz, DMSO-D_6) δ 10.94 (s, 1H), 8.69 (s, 1H), 8.60 (s, 1H), 8.22 (d, *J* = 8.8 Hz, 1H), 7.88 – 7.82 (m, 2H), 7.73 (d, *J* = 8.7 Hz, 1H), 7.49 (d, *J* = 8.9 Hz, 1H), 7.34 (d, *J* = 7.8 Hz, 1H), 7.14 (m, 1H), 6.96 (d, *J* = 8.9 Hz, 1H), 2.66 (s, 3H). ^{13}C NMR (125 MHz, DMSO-D_6) δ 197.4, 153.3, 148.7, 133.8, 132.6, 132.0, 130.6, 127.8, 126.4, 126.1, 125.4, 121.7, 121.5, 121.4, 121.0, 120.8, 119.4, 117.4. FT-IR: $\tilde{\nu}$ = 2981, 2865, 1706, 1624, 1570, 1514, 1352, 1310, 1244 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{19}H_{15}N_2O_2$; 303.1128, found 303.1133.



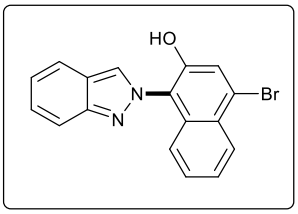
Methyl 6-hydroxy-5-(2*H*-indazol-2-yl)-2-naphthoate (5o); Eluent: Eluent: 20% ethyl acetate in hexane. White solid. Yield 68%, 43.2 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.96 (s, 1H), 8.62 (s, 1H), 8.45 (s, 1H), 8.09 (d, *J* = 8.4 Hz, 1H), 7.98-7.91 (m, 2H), 7.81 (d, *J* = 5.7 Hz, 2H), 7.47-7.40 (m, 2H), 7.23 (d, *J* = 7.5 Hz, 1H), 3.99 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.0, 151.7, 149.6, 132.2, 131.8, 130.4, 128.2, 128.1, 127.6, 127.0, 125.9, 123.2, 122.2, 121.0, 120.7, 120.3, 119.9, 117.4, 52.4. FT-IR: $\tilde{\nu}$ = 2923, 2854, 1726, 1579, 1467, 1378, 1291, 1206 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{19}H_{15}N_2O_3$; 319.1077, found 319.1082.



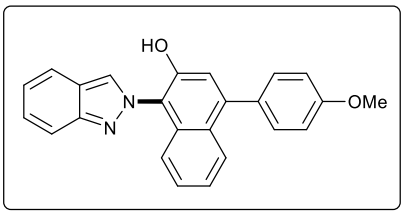
6-Hydroxy-5-(2*H*-indazol-2-yl)-2-naphthaldehyde (5p); Eluent: 20% ethyl acetate in hexane. White solid. Yield 53%, 30.5 mg. ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.14 (s, 1H), 8.44 (s, 1H), 8.35 (s, 1H), 7.98 (d, *J* = 9.0 Hz, 2H), 7.87 – 7.79 (m, 3H), 7.49 (dd, *J* = 8.8, 5.8 Hz, 2H), 7.31 – 7.26 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 191.6, 153.1, 148.3, 134.7, 132.9, 132.6, 131.8, 129.0, 128.0, 127.9, 125.5, 123.7, 121.9, 121.6, 120.9, 120.6, 119.4, 116.7. FT-IR: $\tilde{\nu}$ = 2922, 2865, 1687, 1621, 1580, 1474, 1391, 1308, 1249 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{18}H_{13}N_2O_2$; 289.0978, found 289.0973.



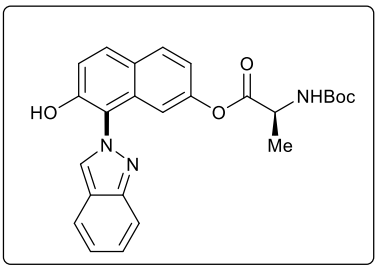
Methyl 3-hydroxy-4-(2*H*-indazol-2-yl)-2-naphthoate (5q); Eluent: 20% ethyl acetate in hexane. White solid.Yield 65%, 41.3 mg. ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.97 (s, 1H), 8.69 (s, 1H), 8.25 (s, 1H), 7.90 (d, *J* = 8.2 Hz, 1H), 7.86 (d, *J* = 8.8 Hz, 1H), 7.80 (d, *J* = 8.5 Hz, 1H), 7.50 (t, *J* = 7.7 Hz, 1H), 7.43 – 7.35 (m, 2H), 7.22 – 7.15 (m, 2H), 4.07 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.1, 152.1, 149.9, 134.9, 134.1, 131.1, 129.5, 127.0, 126.7, 126.6, 125.1, 122.4, 122.3, 122.1, 122.0, 120.7, 118.3, 114.3, 53.1. FT-IR: $\tilde{\nu}$ = 2924, 2854, 1683, 1628, 1578, 1510, 1440, 1326, 1210 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{19}H_{15}N_2O_3$; 319.1077, found 319.1087.



4-Bromo-1-(2*H*-indazol-2-yl)naphthalen-2-ol (5r); Eluent: 20% ethyl acetate in hexane. White solid. Yield 74%, 50 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.76 (s, 1H), 8.40 (s, 1H), 8.27 (d, *J* = 8.3 Hz, 1H), 7.85 – 7.74 (m, 3H), 7.66 (s, 1H), 7.59 – 7.48 (m, 2H), 7.42 (t, *J* = 7.7 Hz, 1H), 7.22 (t, *J* = 7.6 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.6, 149.3, 129.0, 128.8, 128.1, 128.0, 127.7, 127.2, 125.5, 124.6, 123.4, 123.2, 122.1, 121.3, 120.7, 119.9, 117.4. FT-IR: $\tilde{\nu}$ = 2924, 2853, 1629, 1508, 1418, 1359, 1275, 1231 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{17}H_{12}BrN_2O$; 339.0128, found 339.0125.

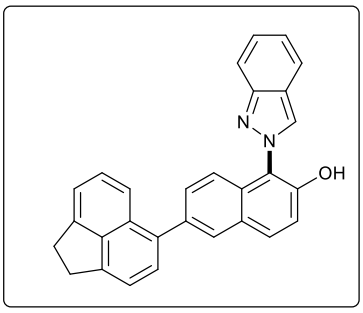


1-(2*H*-Indazol-2-yl)-4-(4-methoxyphenyl)naphthalen-2-ol (5s); Eluent: Eluent: 20% ethyl acetate in hexane. White solid. Yield 79%, 57.8 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (s, 1H), 7.94 (d, *J* = 8.5 Hz, 1H), 7.90 – 7.78 (m, 3H), 7.54-7.48 (m, 2H), 7.46 – 7.32 (m, 5H), 7.05 (d, *J* = 7.8 Hz, 3H), 3.93 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.5, 149.1, 143.4, 131.9, 131.2, 129.0, 128.3, 128.0, 127.7, 127.2, 126.9, 124.1, 123.7, 123.2, 121.9, 120.9, 120.8, 120.0, 117.0, 114.0, 113.9, 55.6. FT-IR: $\tilde{\nu}$ = 2927, 2853, 1609, 1510, 1463, 1393, 1247 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{24}H_{29}N_2O_2$; 367.1441, found 367.1449.

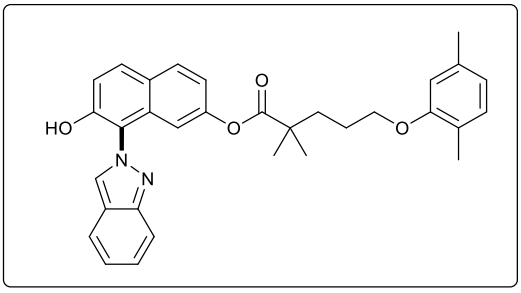


7-Hydroxy-8-(2*H*-indazol-2-yl)naphthalen-2-yl (*tert*-butoxycarbonyl)-*L*-alaninate (5t); Eluent: Eluent: 20% ethyl acetate in hexane. White solid. Yield 51%, 45.6 mg. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.34 (s, 1H), 7.77 (dd, *J* = 8.3, 5.4 Hz, 2H), 7.71 (d, *J* = 8.9 Hz, 1H), 7.65 (d, *J* = 8.6 Hz, 1H), 7.42 – 7.37 (m, 1H), 7.33 (d, *J* = 8.8 Hz, 1H), 7.28 (s, 1H), 7.22 – 7.17 (m,

3H), 7.09 (d, *J* = 8.2 Hz, 1H), 4.97 (s, 1H), 4.44 (s, 1H), 1.46 (d, *J* = 7.2 Hz, 3H), 1.34 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 172.2, 155.3, 151.2, 150.5, 132.1, 131.3, 130.5, 129.4, 129.1, 128.2, 126.8, 123.5, 121.8, 121.1, 119.3, 119.3, 119.1, 116.4, 111.8, 80.4, 31.1, 28.4, 18.5. FT-IR: $\tilde{\nu}$ = 3314, 2979, 2929, 1764, 1696, 1634, 1512, 1453, 1368, 1251 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{25}H_{26}N_3O_5$; 448.1867, found 448.1877.

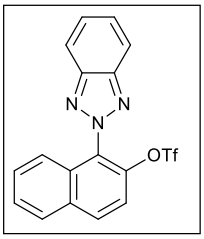


6-(1,2-Dihydroacenaphthylen-5-yl)-1-(2*H*-indazol-2-yl)naphthalen-2-ol (5u); Eluent: 20% ethyl acetate in hexane. White solid. Yield 71%, 58.5 mg. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.38 (s, 1H), 7.89 (d, *J* = 1.4 Hz, 1H), 7.77 (t, *J* = 9.5 Hz, 2H), 7.68 (t, *J* = 8.1 Hz, 2H), 7.60 (d, *J* = 8.6 Hz, 2H), 7.37 (d, *J* = 7.0 Hz, 1H), 7.32-7.28 (m, 3H), 7.24-7.19 (m, 3H), 7.10 (d, *J* = 5.7 Hz, 1H), 3.32 (s, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.4, 146.5, 146.1, 140.0, 136.4, 134.9, 130.9, 130.4, 130.1, 129.9, 129.3, 129.1, 129.0, 128.4, 128.2, 127.9, 127.1, 127.0, 126.4, 123.0, 122.1, 120.8, 120.7, 119.7, 119.6, 119.4, 117.4, 30.7, 30.2. FT-IR: $\tilde{\nu}$ = 2924, 2854, 1632, 1607, 1487, 1358, 1291, 1231 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{29}H_{21}N_2O$; 413.1648, found 413.1661.

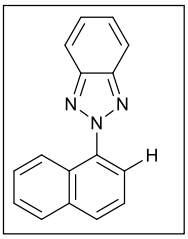


7-Hydroxy-8-(2*H*-indazol-2-yl)naphthalen-2-yl 5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoate (5v); Eluent: 20% ethyl acetate in hexane. White solid. Yield 46%, 46.7 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (s, 1H), 8.10 (s, 1H), 7.85 (t, *J* = 8.8 Hz, 2H), 7.80 – 7.76 (m, 2H), 7.49 (d, *J* = 8.3 Hz, 2H), 7.22 – 7.16 (m, 2H), 7.11 (dd, *J* = 8.8, 2.1 Hz, 1H), 6.99 (d, *J* = 7.5 Hz, 1H), 6.66 (d, *J* = 7.4 Hz, 1H), 6.60 (s, 1H), 3.96 (d, *J* = 5.4 Hz, 2H), 2.30 (s, 3H), 2.13 (s, 3H), 1.88 (s, 4H), 1.37 (s, 6H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 176.6, 157.0, 150.9, 150.3, 149.5, 136.6, 130.7, 130.5, 130.3, 127.8, 127.0, 126.9, 123.7, 122.9, 122.1, 121.2,

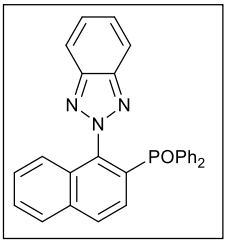
120.9, 120.8, 119.4, 119.0, 117.4, 112.2, 112.1, 109.9, 67.8, 42.7, 37.3, 25.4, 25.2, 21.5, 15.9. FT-IR: $\tilde{\nu}$ = 2955, 2925, 2855, 1748, 1628, 1510, 1454, 1352, 1265 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{32}H_{33}N_2O_4$; 509.2435, found 509.2451.



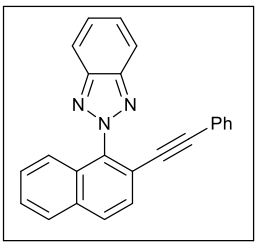
1-(2*H*-Benzo[*d*][1,2,3]triazol-2-yl)naphthalen-2-yl trifluoromethanesulfonate (6): Eluent: 10% ethyl acetate in hexane. White solid. Yield 75%, 147.5 mg. ^1H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 9.1 Hz, 1H), 8.12 – 7.95 (m, 3H), 7.67 – 7.46 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 145.3, 142.1, 132.7, 132.5, 130.1, 129.8, 129.3, 128.1, 128.0, 127.7, 123.5, 119.6, 119.4, 118.6(q, J= 320 Hz). ^{19}F NMR (470 MHz, $CDCl_3$) δ -73.79. FT-IR: $\tilde{\nu}$ = 2962, 1603, 1479, 1428, 1214, 1136 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{17}H_{11}F_3N_3O_3S$; 394.0468, found 394.0469.



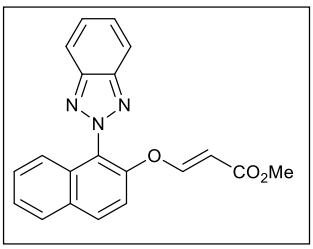
2-(Naphthalen-1-yl)-2*H*-benzo[*d*][1,2,3]triazole (7); Eluent: 10% ethyl acetate in hexane. White solid. Yield 82%, 40.2 mg. ^1H NMR (500 MHz, $CDCl_3$) δ 8.23 (dd, *J* = 6.2, 3.4 Hz, 1H), 8.05 (dd, *J* = 6.6, 3.3 Hz, 3H), 8.00 – 7.95 (m, 2H), 7.66 – 7.56 (m, 3H), 7.50 (dd, *J* = 6.5, 3.0 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 145.2, 137.6, 134.5, 130.5, 128.4, 127.9, 127.8, 127.3, 127.0, 125.1, 124.1, 123.5, 118.6. FT-IR: $\tilde{\nu}$ = 3049, 2925, 1597, 1512, 1466, 1388, 1336, 1294, 1208 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{16}H_{12}N_3$; 246.1026, found 246.1027.



(1-(2*H*-Benzo[*d*][1,2,3]triazol-2-yl)naphthalen-2-yl)diphenylphosphine oxide (8); Eluent: 50% ethyl acetate in hexane. White solid. Yield 71%, 63.2 mg. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.23 – 8.11 (m, 2H), 7.99 (d, *J* = 8.3 Hz, 1H), 7.74 – 7.54 (m, 7H), 7.44 (t, *J* = 7.7 Hz, 1H), 7.38 – 7.30 (m, 2H), 7.29 – 7.23 (m, 2H), 7.17 (t, *J* = 6.8 Hz, 4H), 6.86 (d, *J* = 8.6 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 144.3, 140.0 (d, *J* = 3.4 Hz), 135.6 (d, *J* = 1.9 Hz), 132.0 (d, *J* = 10.4 Hz), 131.6 (d, *J* = 2.8 Hz), 130.3 (d, *J* = 7.7 Hz), 129.5, 128.9 (d, *J* = 34.8 Hz), 128.5 (d, *J* = 7.5 Hz), 128.0, 127.8 (d, *J* = 12.7 Hz), 127.1, 123.6, 118.7. ^{31}P NMR (202 MHz, $CDCl_3$) δ 28.54. FT-IR: $\tilde{\nu}$ = 3058, 2972, 1571, 1501, 1437, 1376, 1271 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{28}H_{21}N_3OP$; 446.1417, found 446.1429.

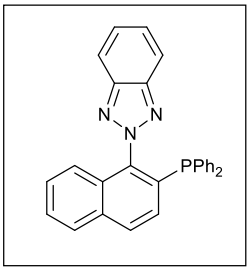


2-(2-(Phenylethynyl)naphthalen-1-yl)-2*H*-benzo[*d*][1,2,3]triazole (9); Eluent: 10% ethyl acetate in hexane. White solid. Yield 68%, 46.9 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (dd, *J* = 6.6, 3.1 Hz, 2H), 8.04 (d, *J* = 8.5 Hz, 1H), 7.94 (d, *J* = 8.1 Hz, 1H), 7.75 (d, *J* = 8.6 Hz, 1H), 7.61 – 7.45 (m, 4H), 7.27 (d, *J* = 8.1 Hz, 1H), 7.24 – 7.14 (m, 3H), 7.09 – 6.99 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 145.1, 139.4, 133.4, 131.7, 130.4, 129.8, 128.8, 128.5, 128.3, 128.1, 128.1, 127.6, 127.3, 122.9, 122.5, 120.2, 118.8, 95.7, 85.1. FT-IR: $\tilde{\nu}$ = 3060, 2924, 2851, 2210, 1600, 1505, 1443, 1377, 1269 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{24}H_{16}N_3$; 346.1339, found 346.1342.



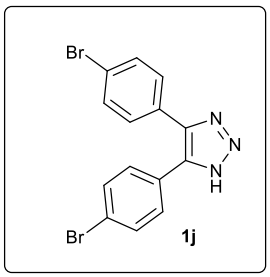
Methyl (*E*)-3-((1-(2*H*-benzo[*d*][1,2,3]triazol-2-yl)naphthalen-2-yl)oxy)acrylate (10); Eluent: 20% ethyl acetate in hexane. White solid. Yield 89%, 61.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 9.0 Hz, 1H), 8.02 (dd, *J* = 6.6, 3.0 Hz, 2H), 7.94 (d, *J* = 7.9 Hz, 1H), 7.69 (d, *J* = 12.2 Hz, 1H), 7.57 – 7.42 (m, 5H), 7.19 (d, *J* = 8.2 Hz, 1H), 5.46 (d, *J* = 12.2 Hz, 1H), 3.65 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.9, 158.5, 148.7, 145.2, 132.6, 131.2, 130.8,

128.9, 128.1, 127.4, 127.3, 126.7, 122.5, 118.7, 118.1, 103.5, 51.4. FT-IR: $\tilde{\nu}$ = 3075, 2953, 1713, 1626, 1479, 1436, 1381, 1231 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{20}H_{16}N_3O_3$; 346.1186, found 346.1189.

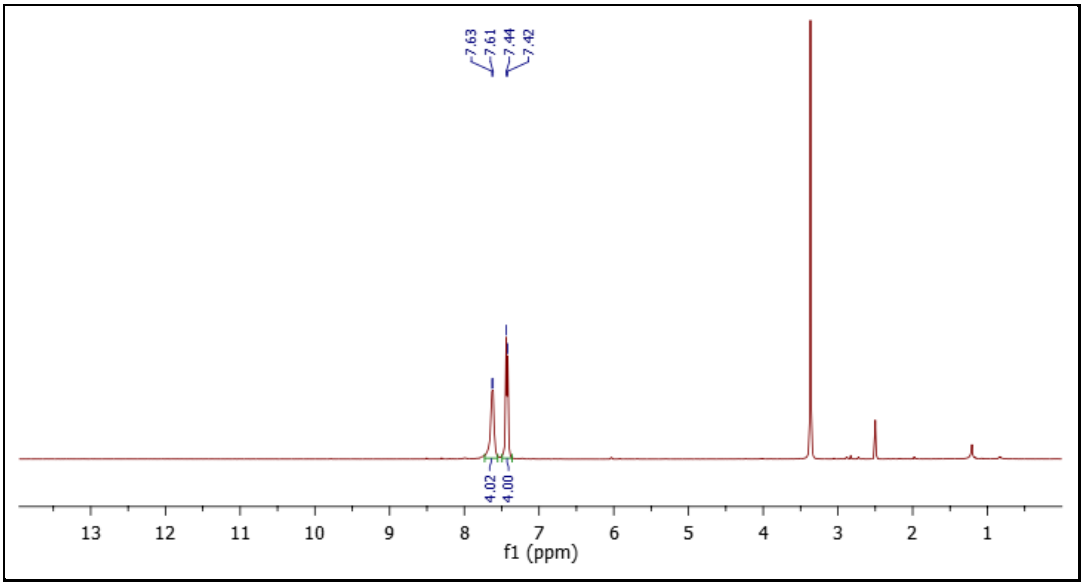


2-(2-(Diphenylphosphaneyl)naphthalen-1-yl)-2H-benzo[*d*][1,2,3]triazole (11); Eluent: 5% ethyl acetate in hexane. White solid. Yield 64%, 54.9 mg. ^{1}H NMR (400 MHz, CDCl3) δ 7.95 – 7.90 (m, 4H), 7.55 (t, *J* = 7.5 Hz, 1H), 7.50 – 7.39 (m, 3H), 7.36 – 7.24 (m, 11H), 7.15 (d, *J* = 8.5 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.7, 142.1 (d, *J* = 23.2 Hz), 136.2 (d, *J* = 10.9 Hz), 134.6 (d, *J* = 21.8 Hz), 134.1, 134.0, 133.8, 130.3, 130.0 (d, *J* = 3.2 Hz), 129.5, 128.9, 128.5 (d, *J* = 7.1 Hz), 128.2, 127.8 (d, *J* = 20.6 Hz), 127.1, 123.2 (d, *J* = 1.8 Hz), 118.8; FT-IR: $\tilde{\nu}$ = 3055, 3003, 2925, 2856, 1569, 1480, 1434, 1370, 1270, 1217 cm^{-1}. HRMS: calculated for $[C_{29}H_{20}N_3P]^+$ 430.1468 ; found 430.1461.

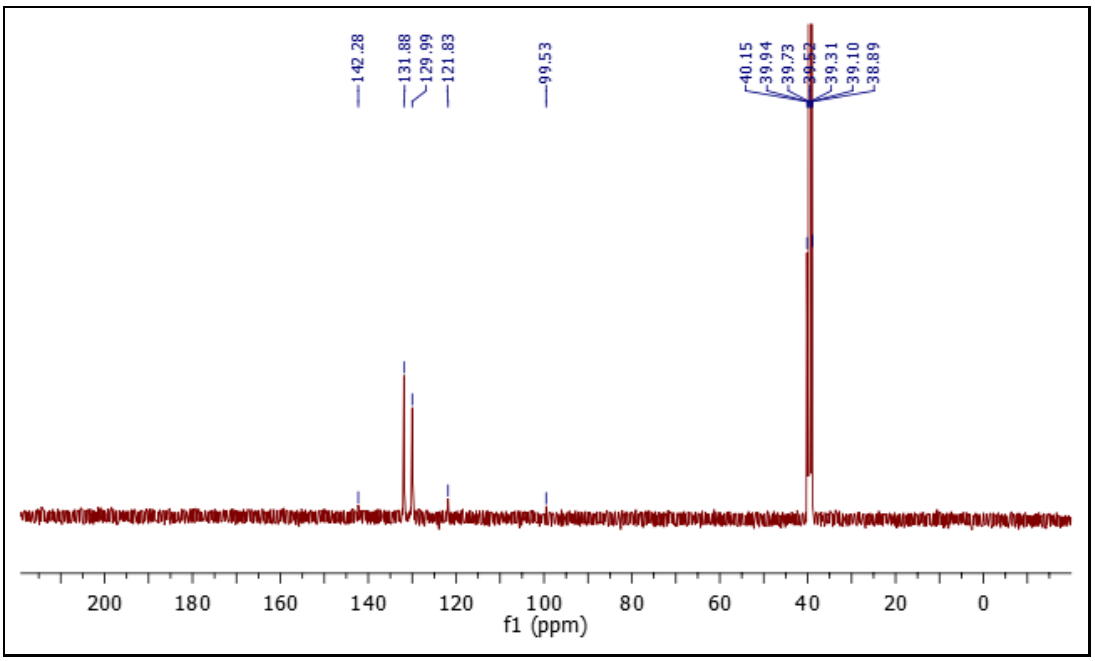
NMR Spectrum

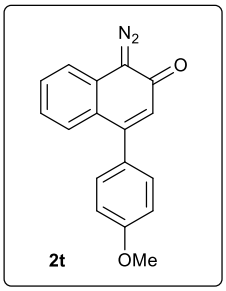


^{1}H NMR (400 MHz, DMSO-D$_6$)

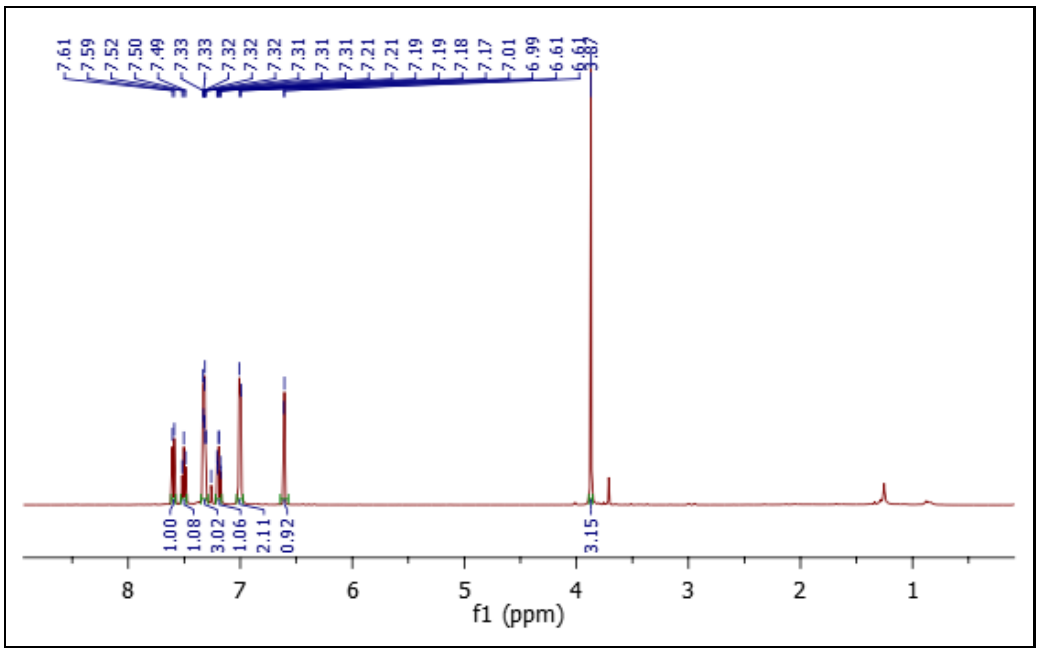


^{13}C NMR (100 MHz, DMSO-D$_6$)

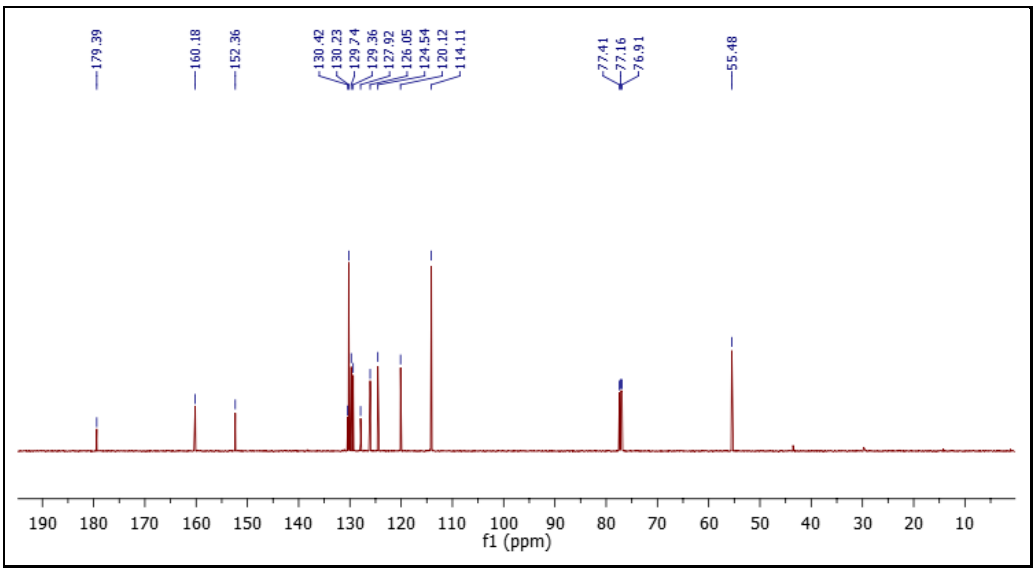


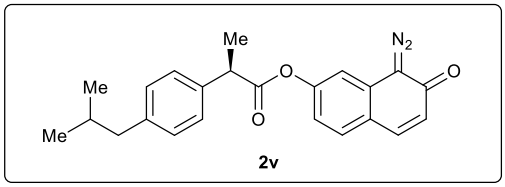


^{1}H NMR (500 MHz, $CDCl_3$)

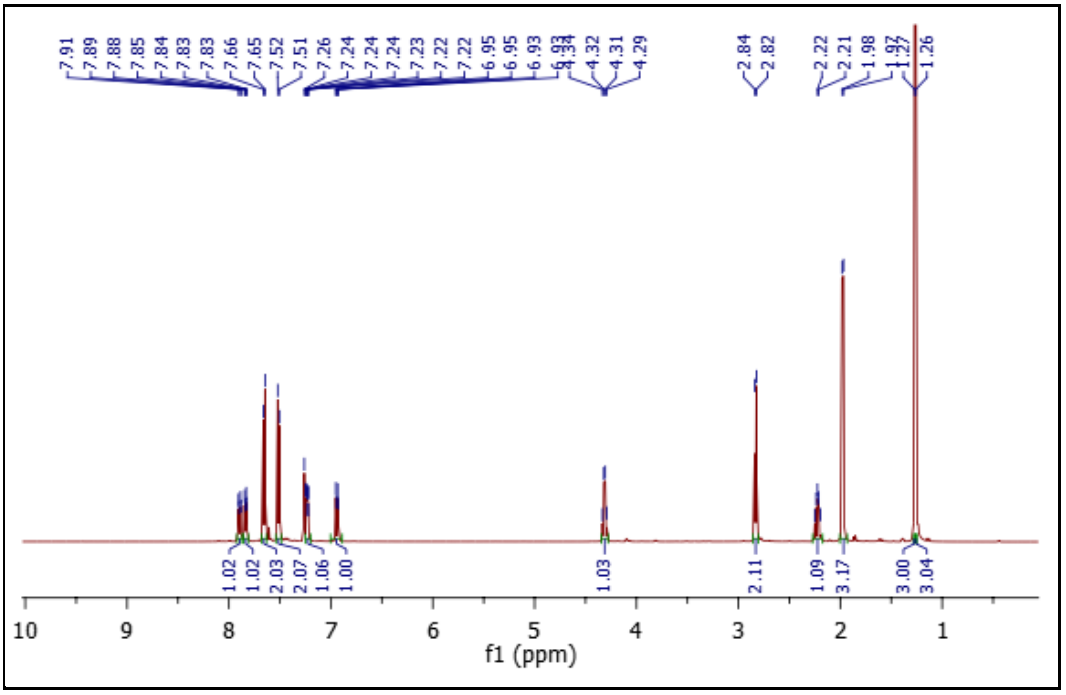


^{13}C NMR (125 MHz, $CDCl_3$)

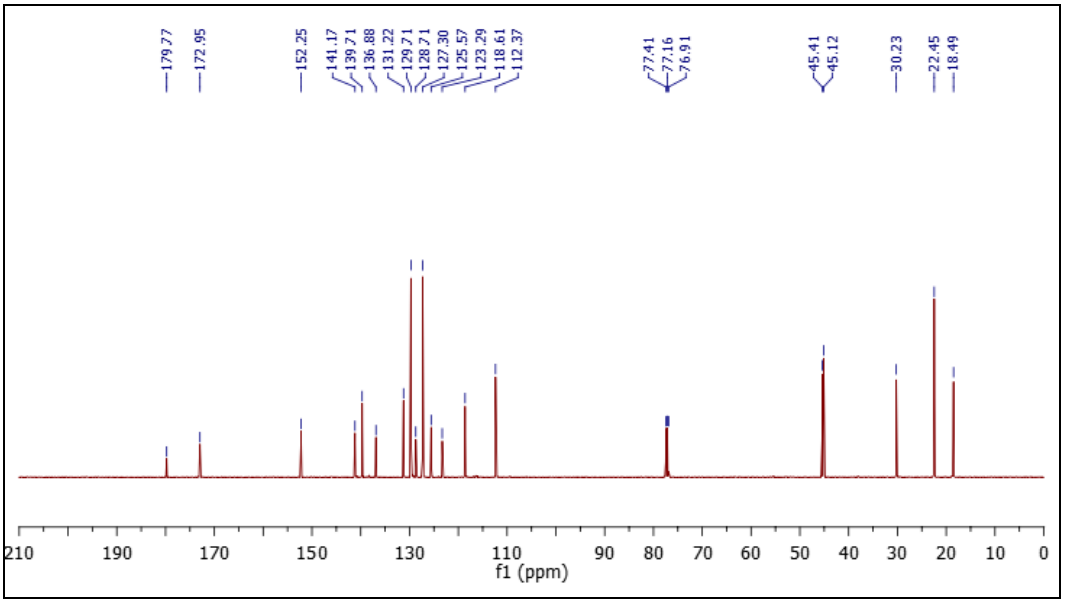


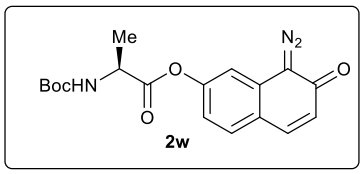


^{1}H NMR (500 MHz, $CDCl_3$)



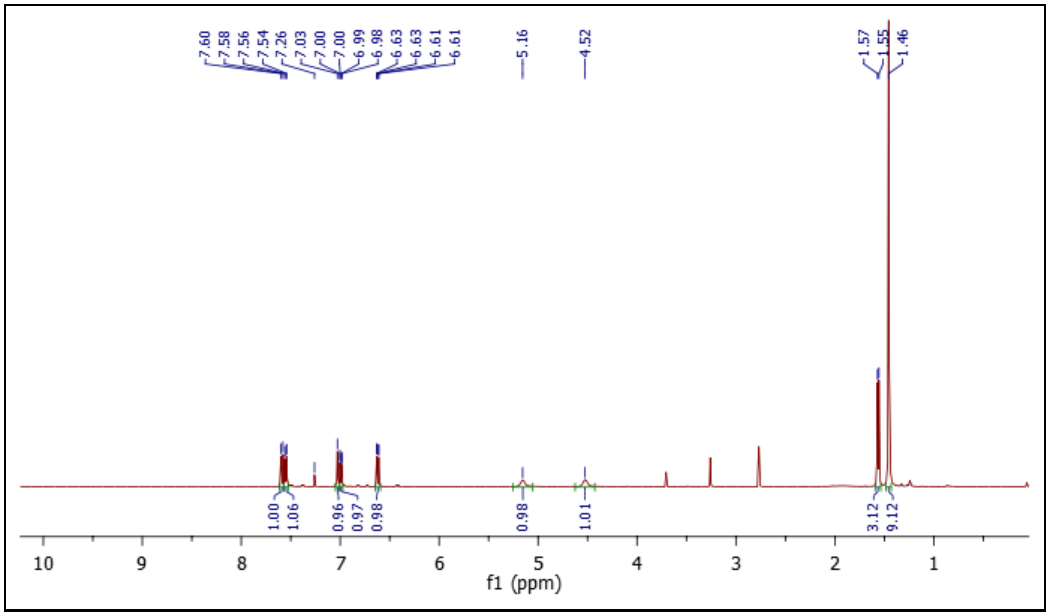
^{13}C NMR (125 MHz, $CDCl_3$)



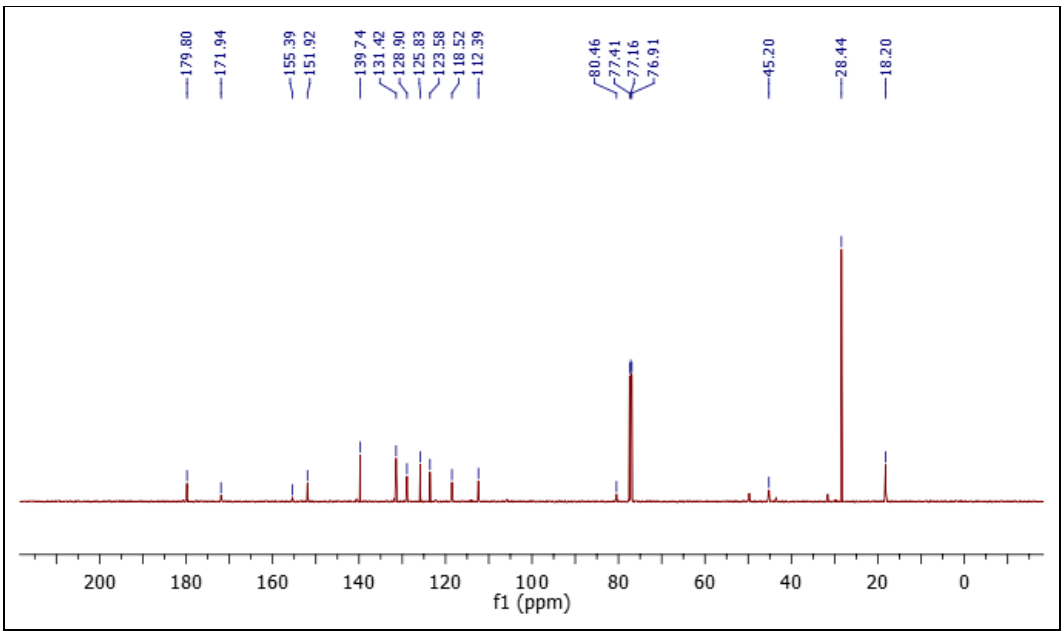


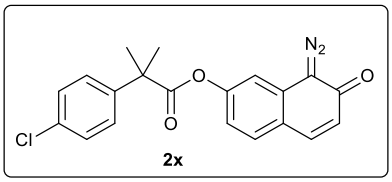
2w

^{1}H NMR (500 MHz, $CDCl_3$)



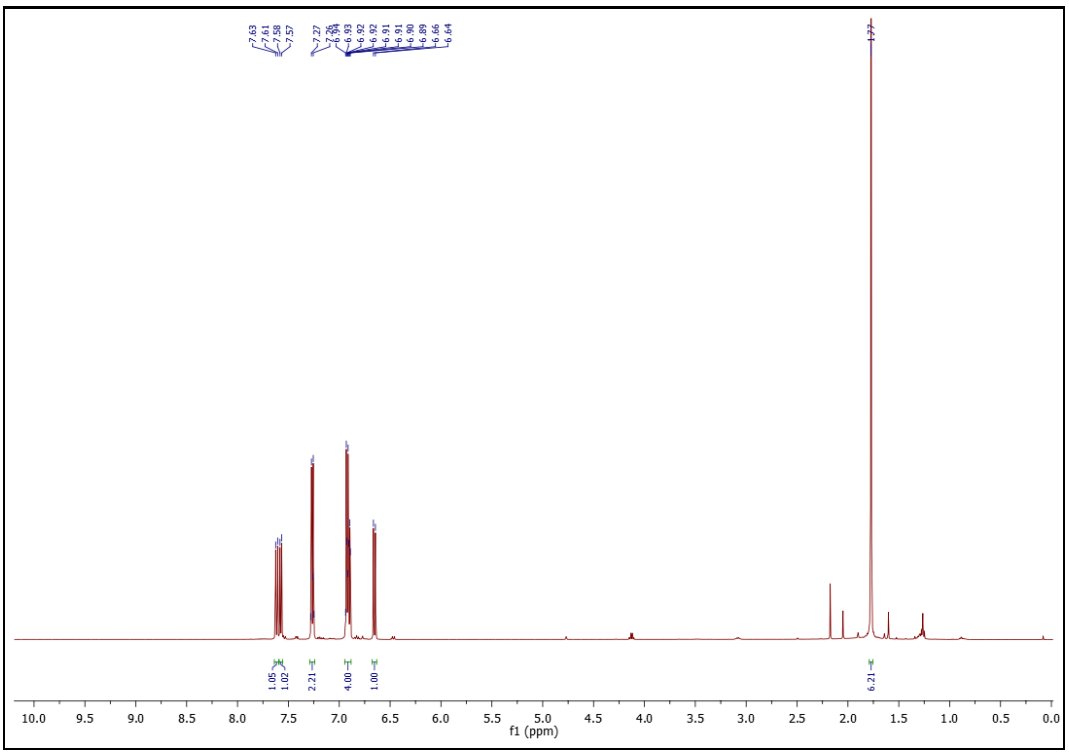
^{13}C NMR (125 MHz, $CDCl_3$)



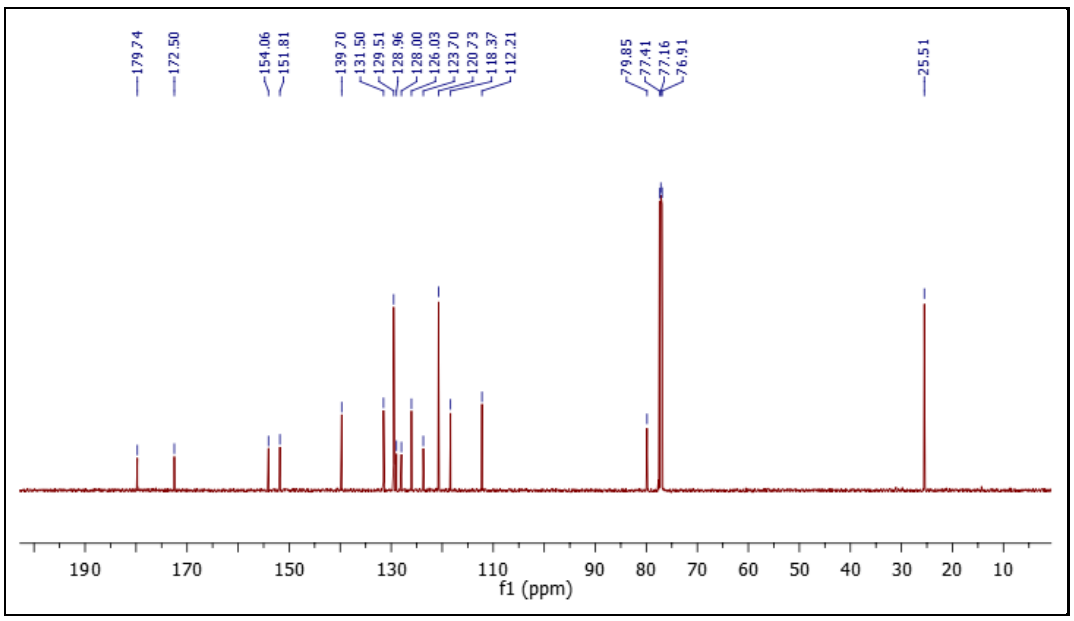


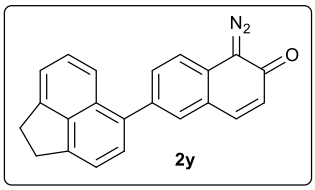
2x

^{1}H NMR (500 MHz, $CDCl_3$)

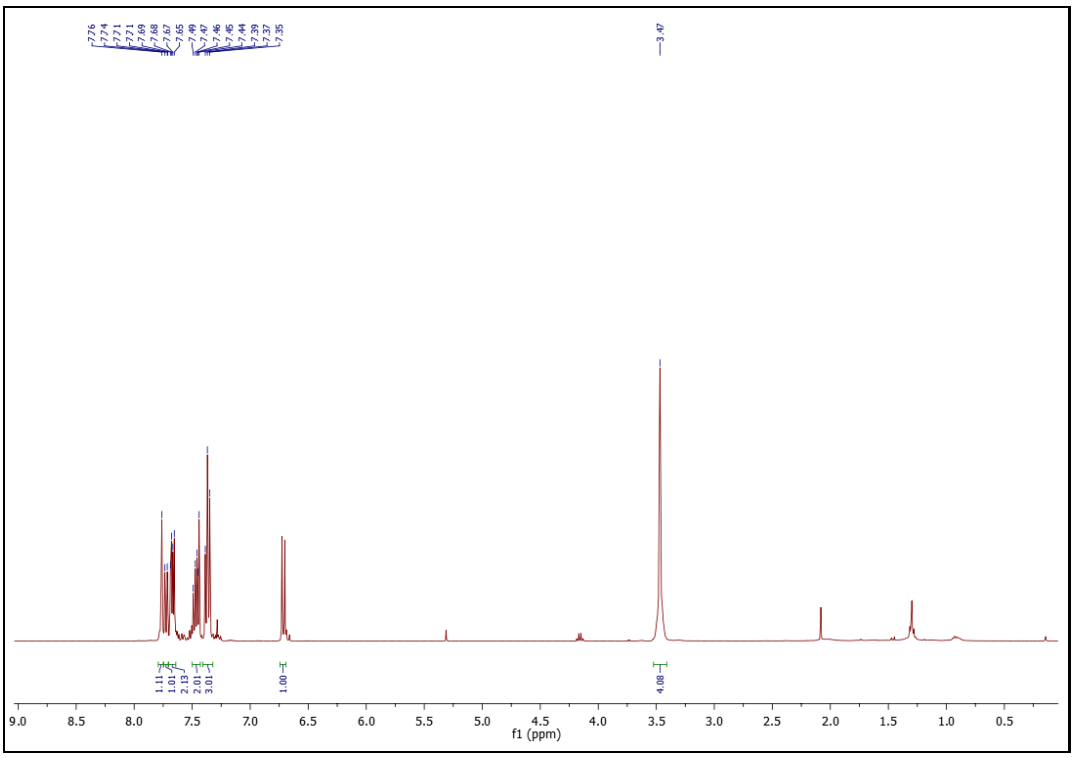


^{13}C NMR (125 MHz, $CDCl_3$)

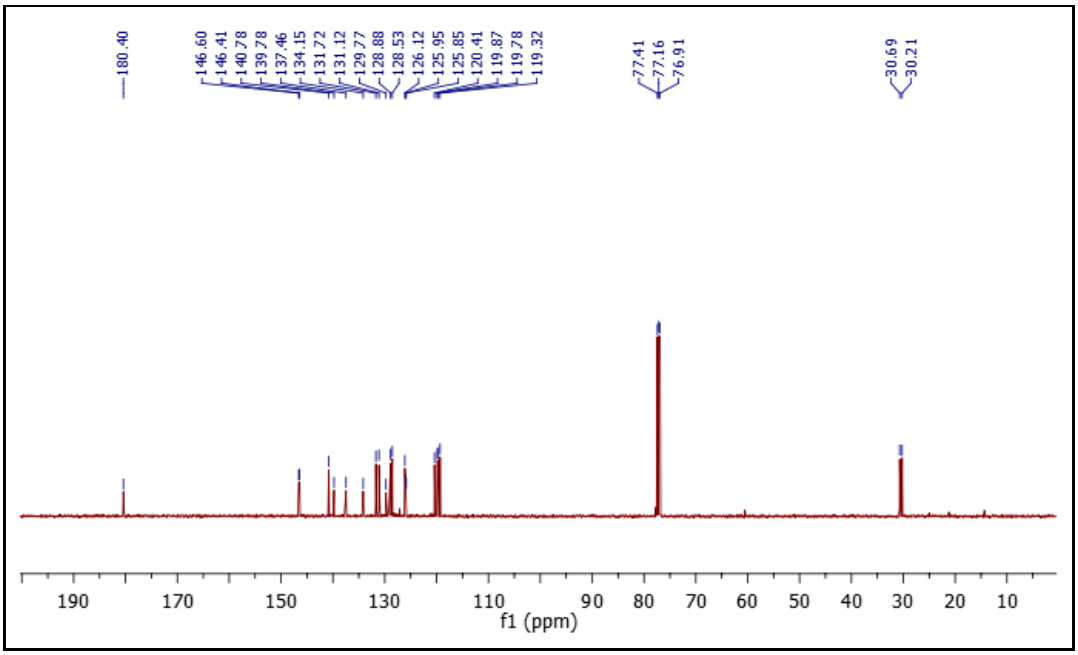


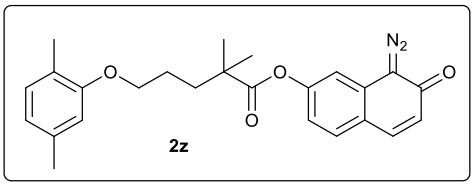


^{1}H NMR (400 MHz, $CDCl_3$)



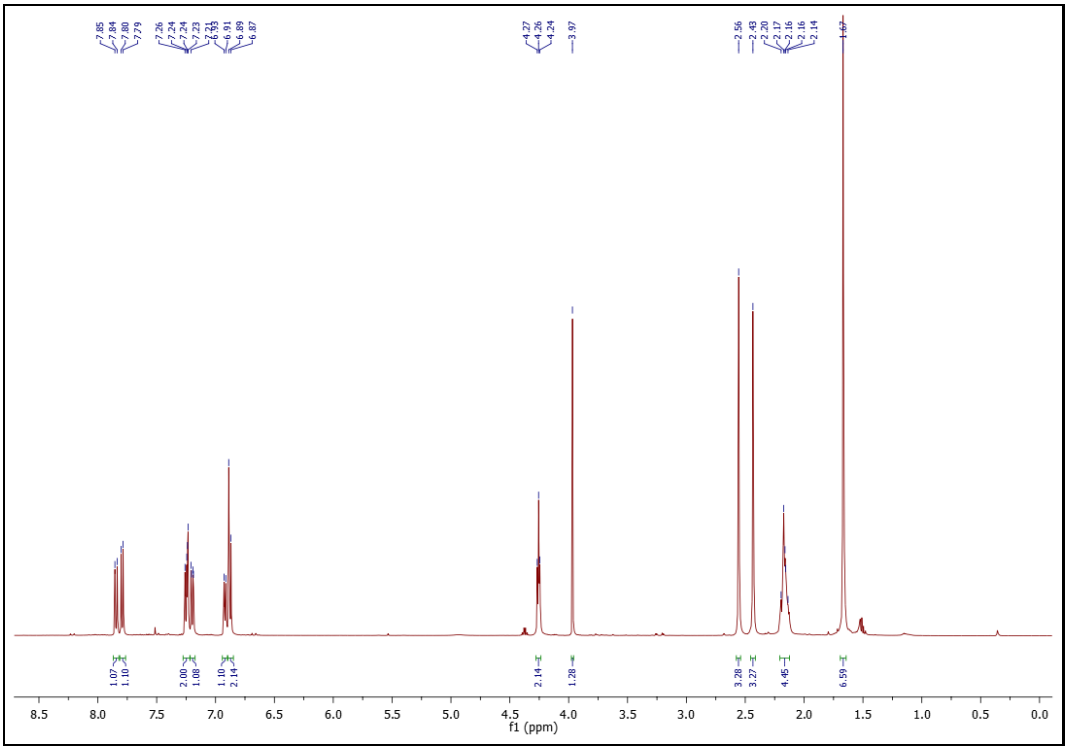
^{13}C NMR (125 MHz, $CDCl_3$)



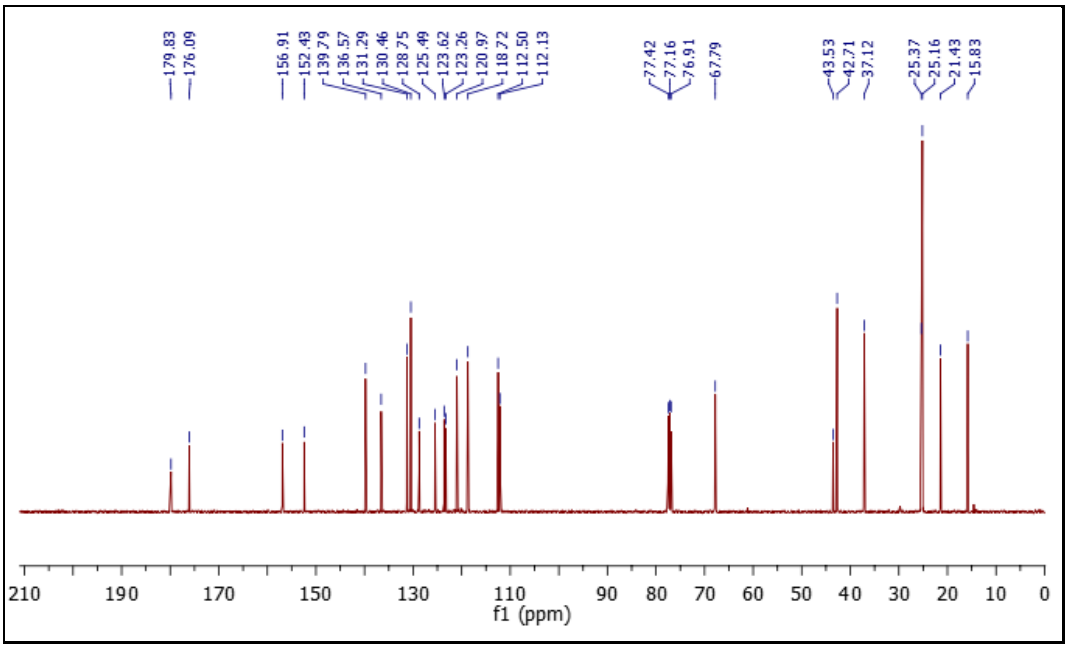


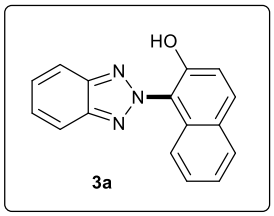
2z

^{1}H NMR (500 MHz, $CDCl_3$)

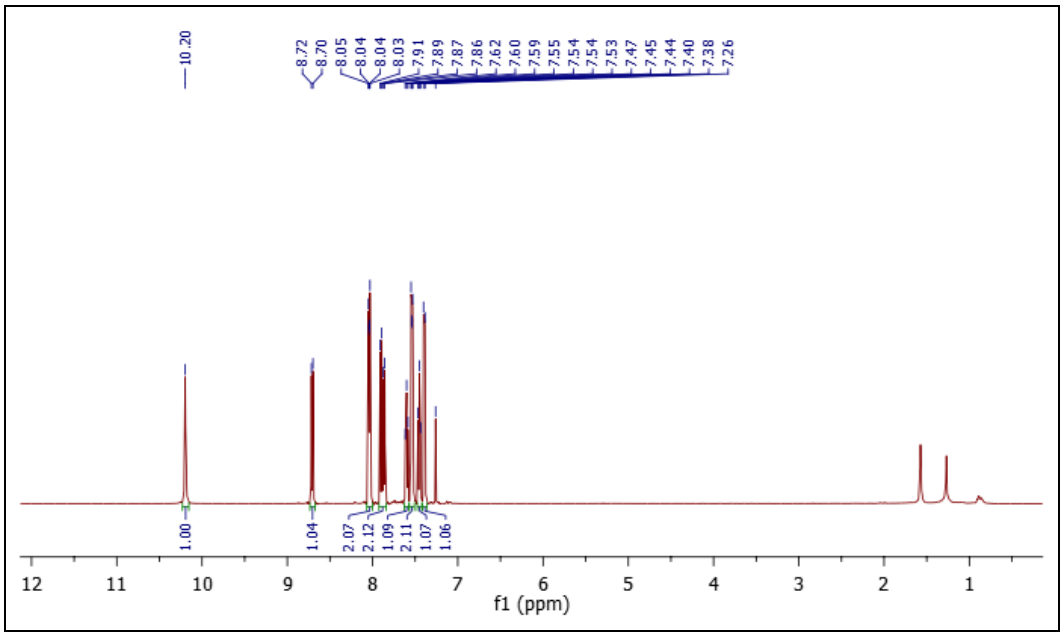


^{13}C NMR (125 MHz, $CDCl_3$)

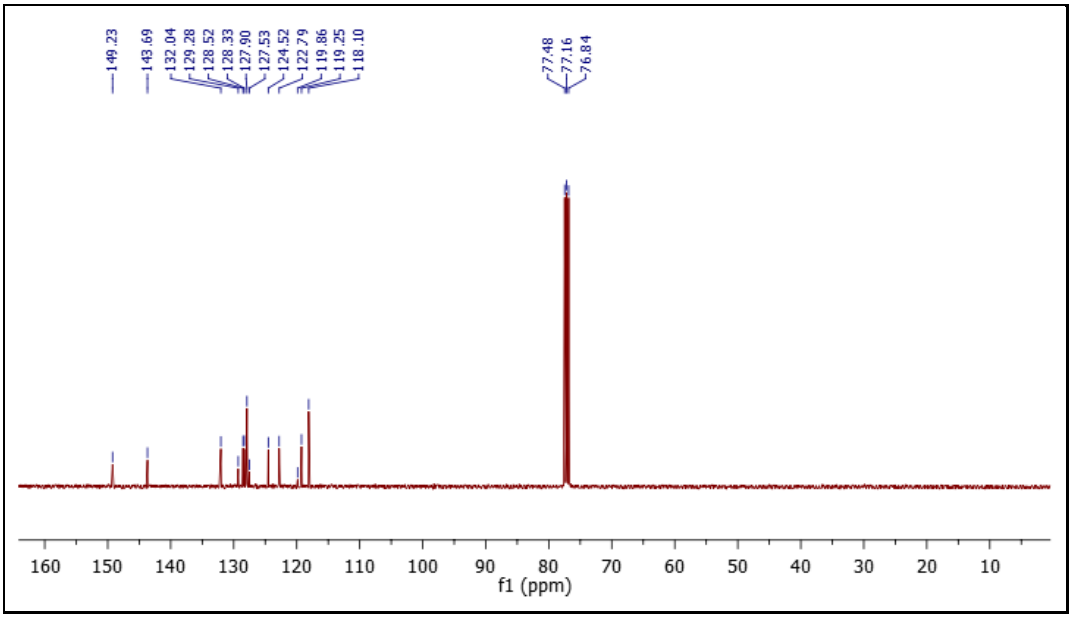


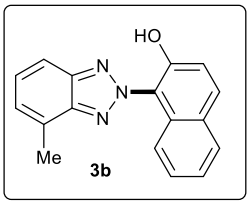


^{1}H NMR (500 MHz, $CDCl_3$)



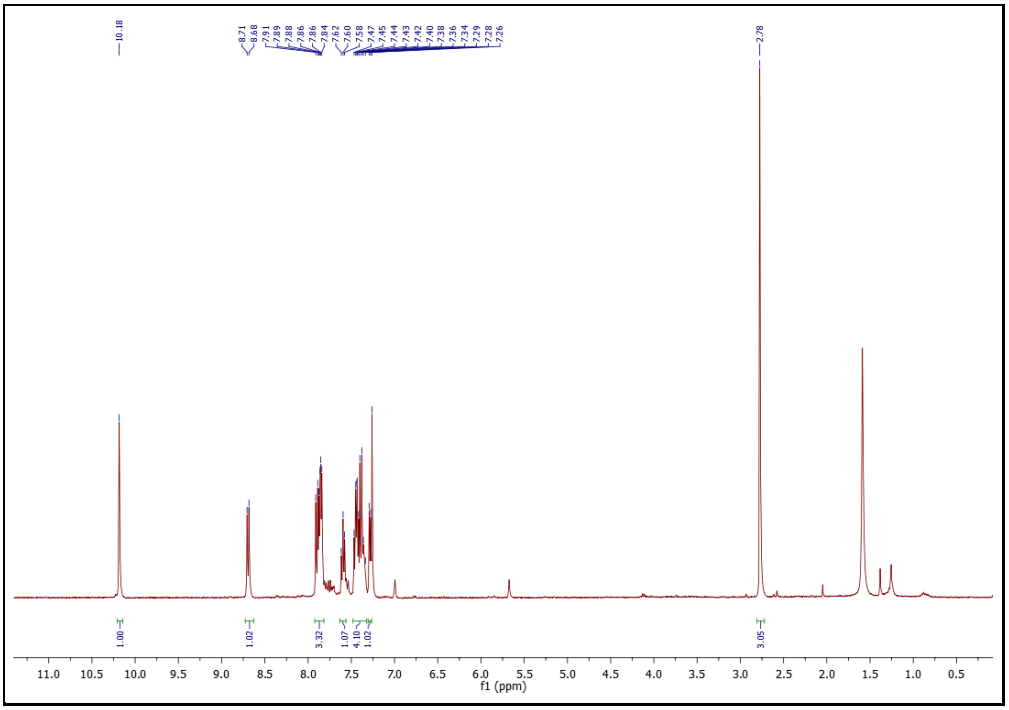
^{13}C NMR (100 MHz, $CDCl_3$)



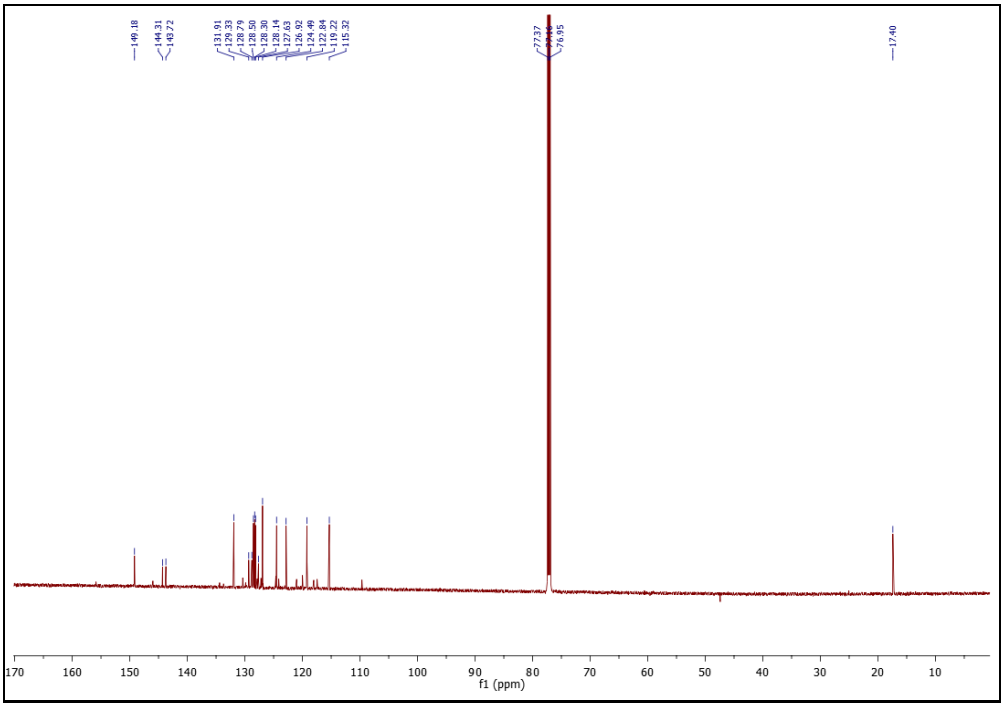


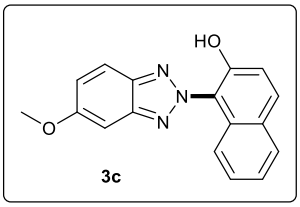
3b

^{1}H NMR (400 MHz, $CDCl_3$)



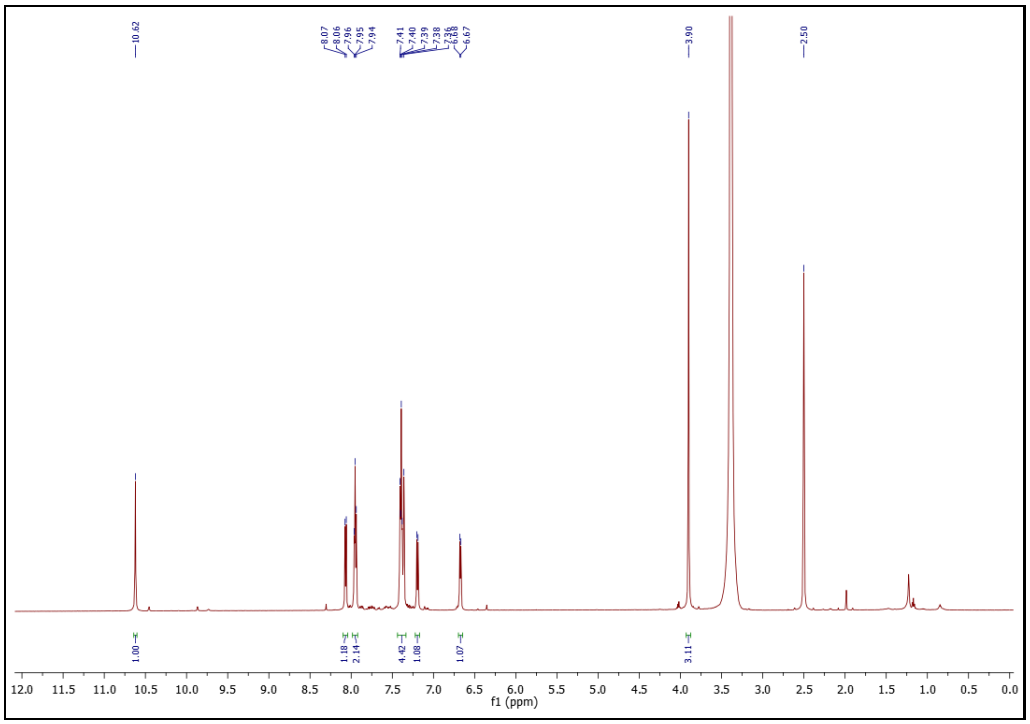
^{13}C NMR (150 MHz, $CDCl_3$)



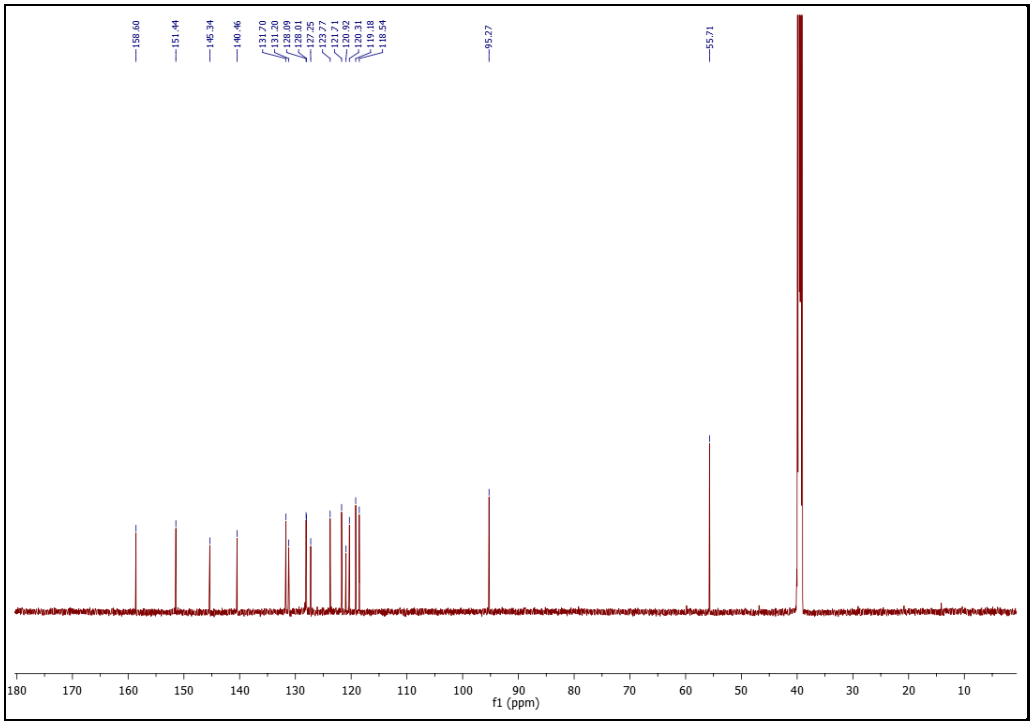


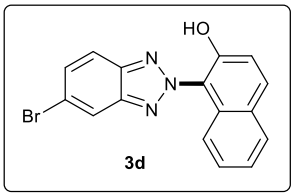
3c

^{1}H NMR (600 MHz, DMSO-D$_6$)



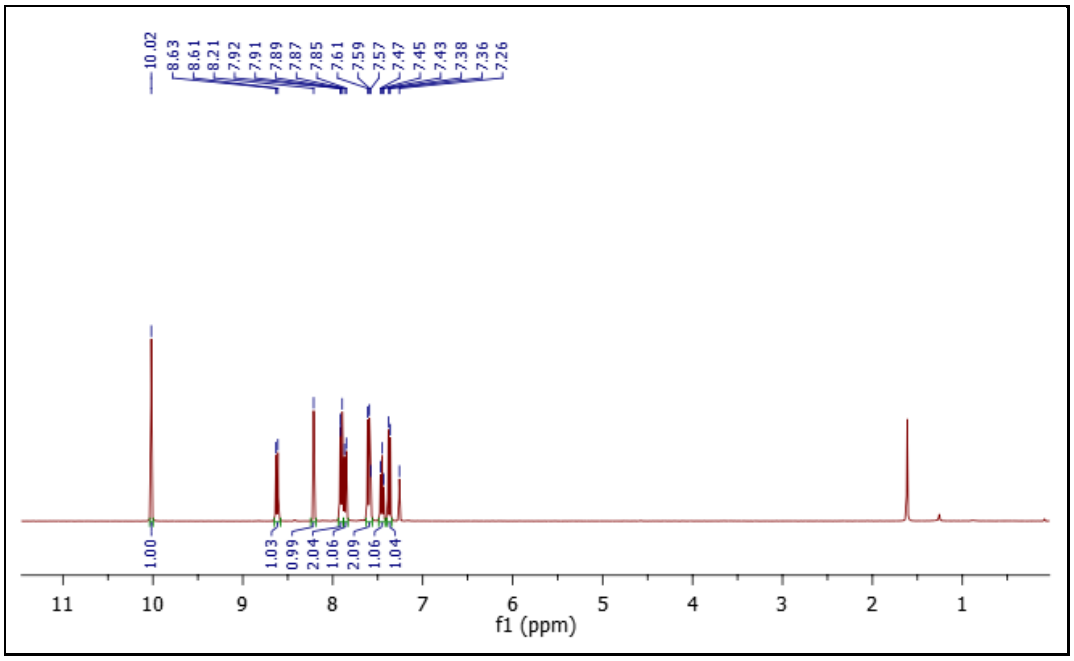
^{1}H NMR (600 MHz, DMSO-D$_6$)



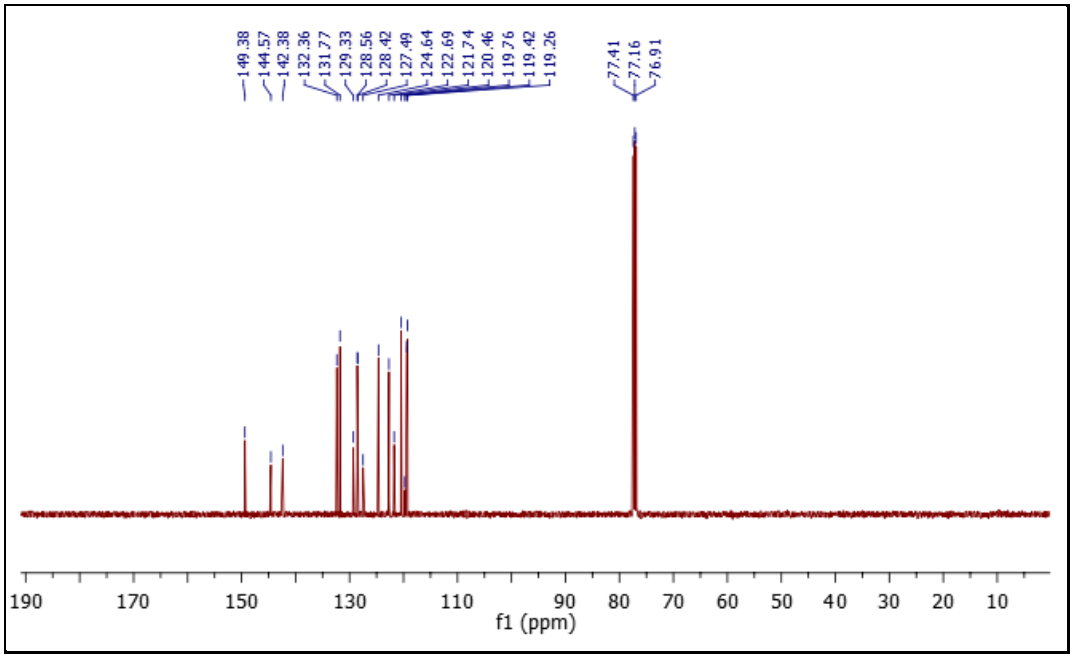


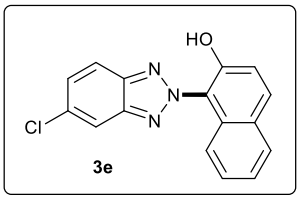
3d

^{1}H NMR (400 MHz, $CDCl_3$)



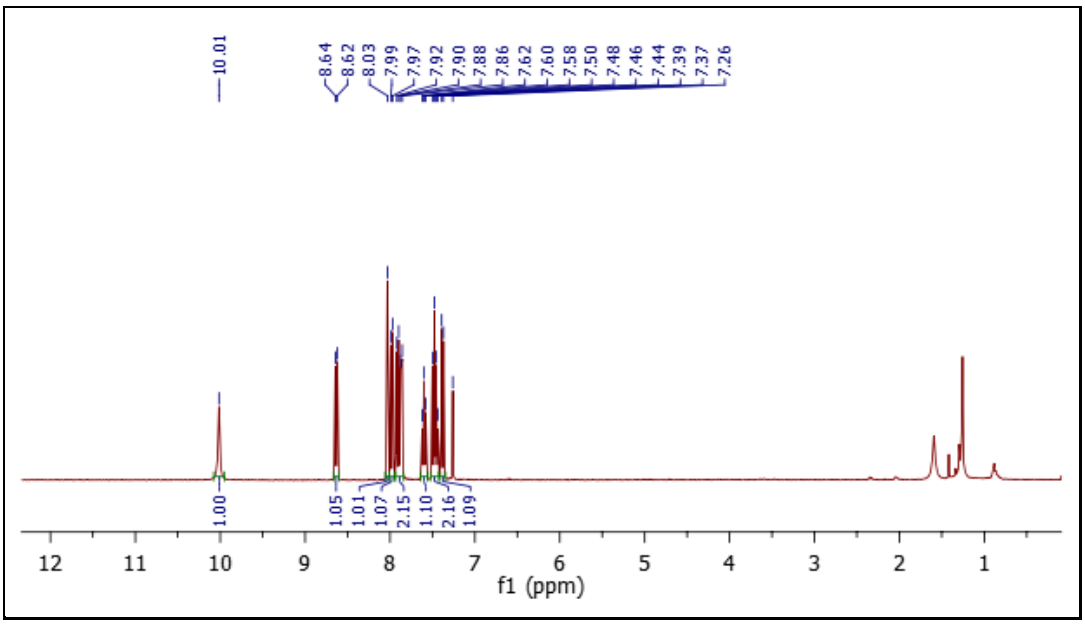
^{13}C NMR (125 MHz, $CDCl_3$)



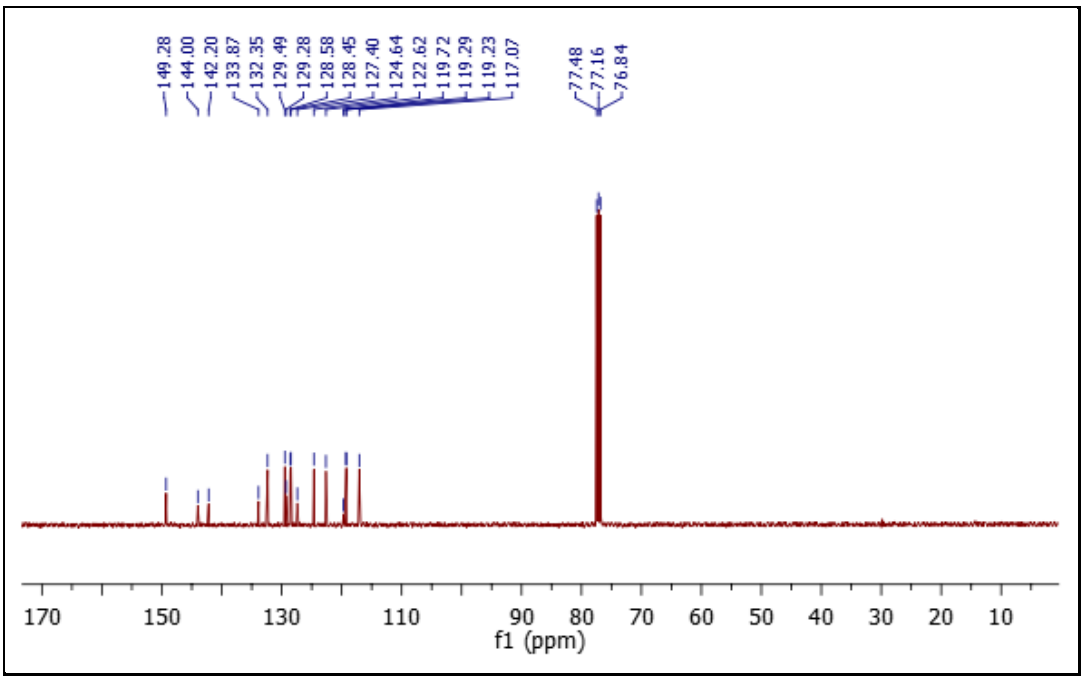


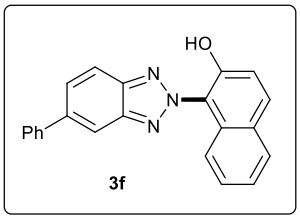
3e

^{1}H NMR (400 MHz, $CDCl_3$)



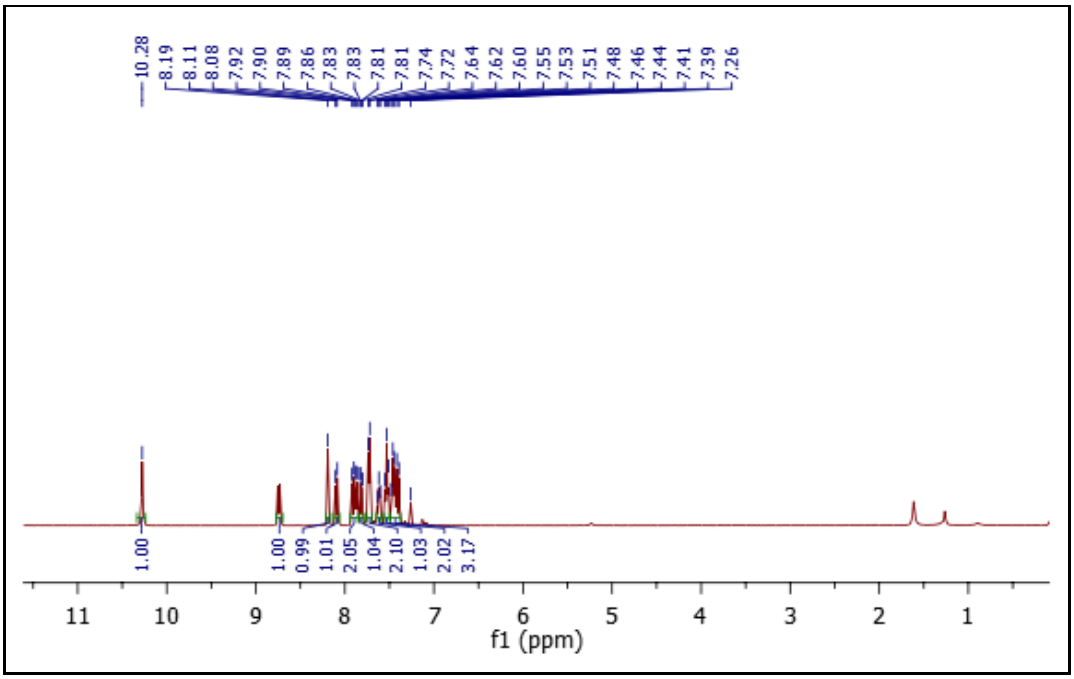
^{13}C NMR (100 MHz, $CDCl_3$)



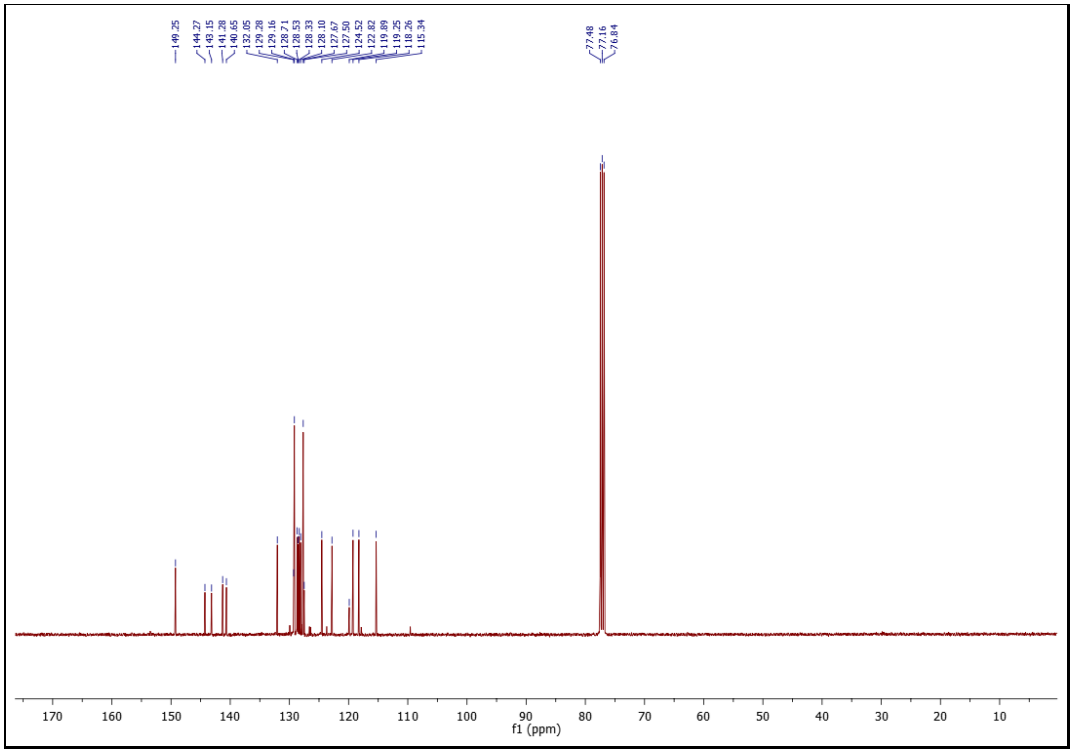


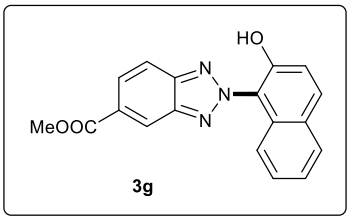
3f

^{1}H NMR (400 MHz, $CDCl_3$)



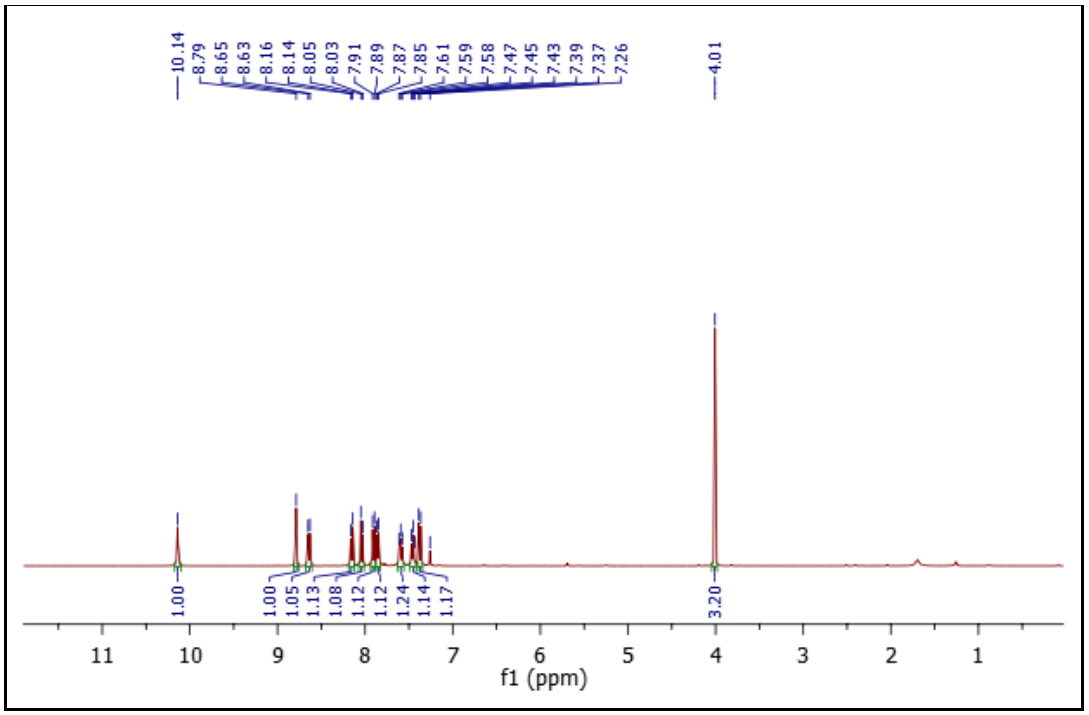
^{13}C NMR (125 MHz, $CDCl_3$)



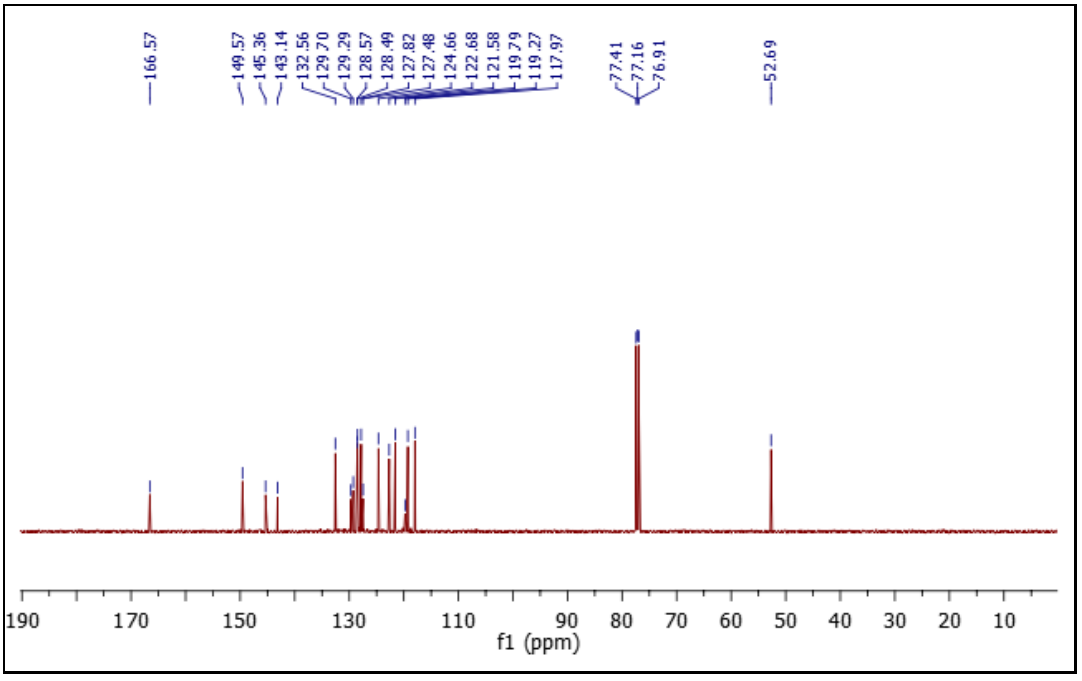


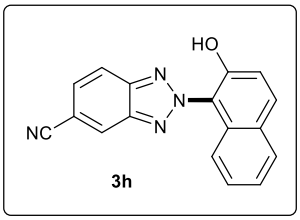
3g

^{1}H NMR (400 MHz, $CDCl_3$)



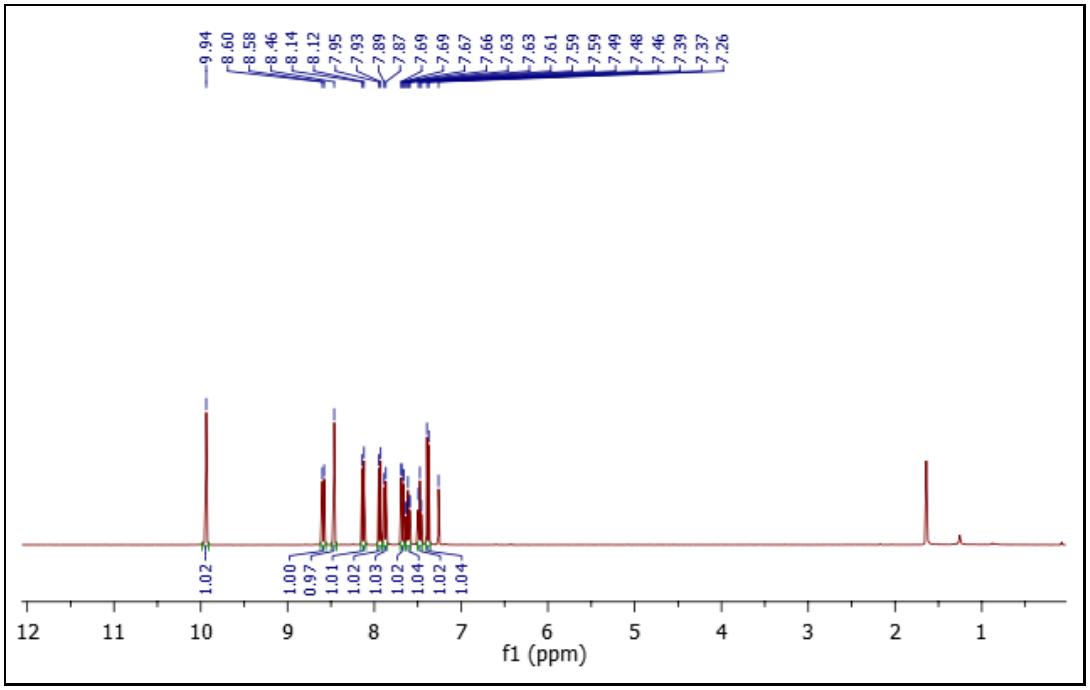
^{13}C NMR (125 MHz, $CDCl_3$)



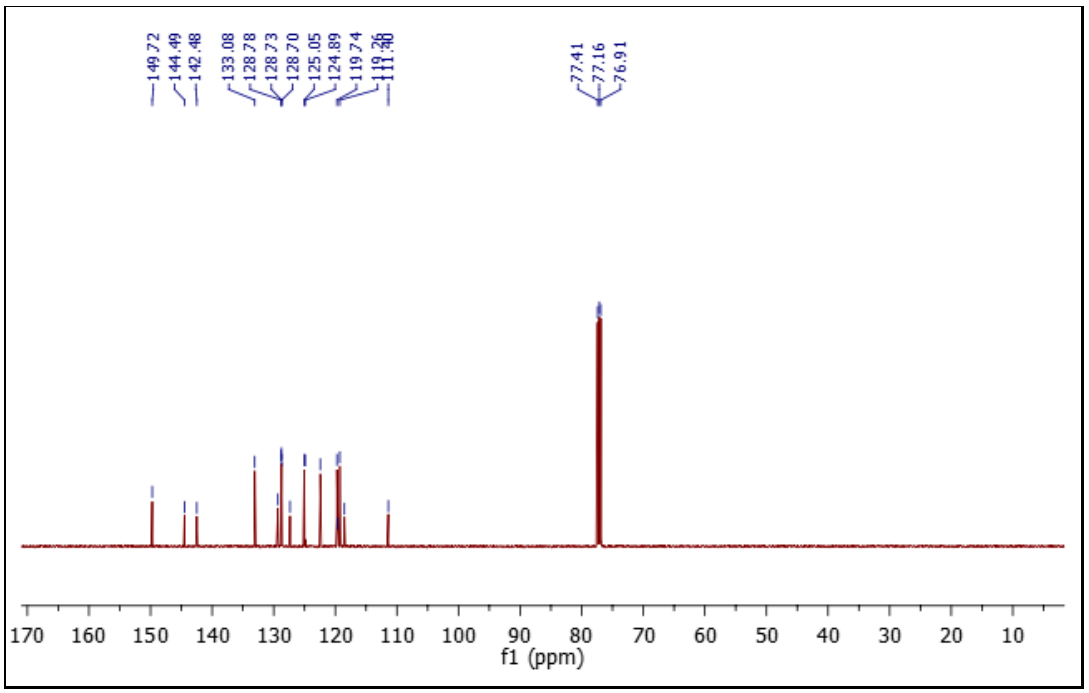


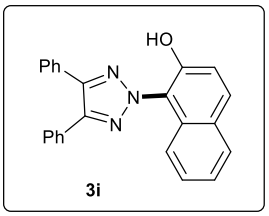
3h

^{1}H NMR (400 MHz, $CDCl_3$)



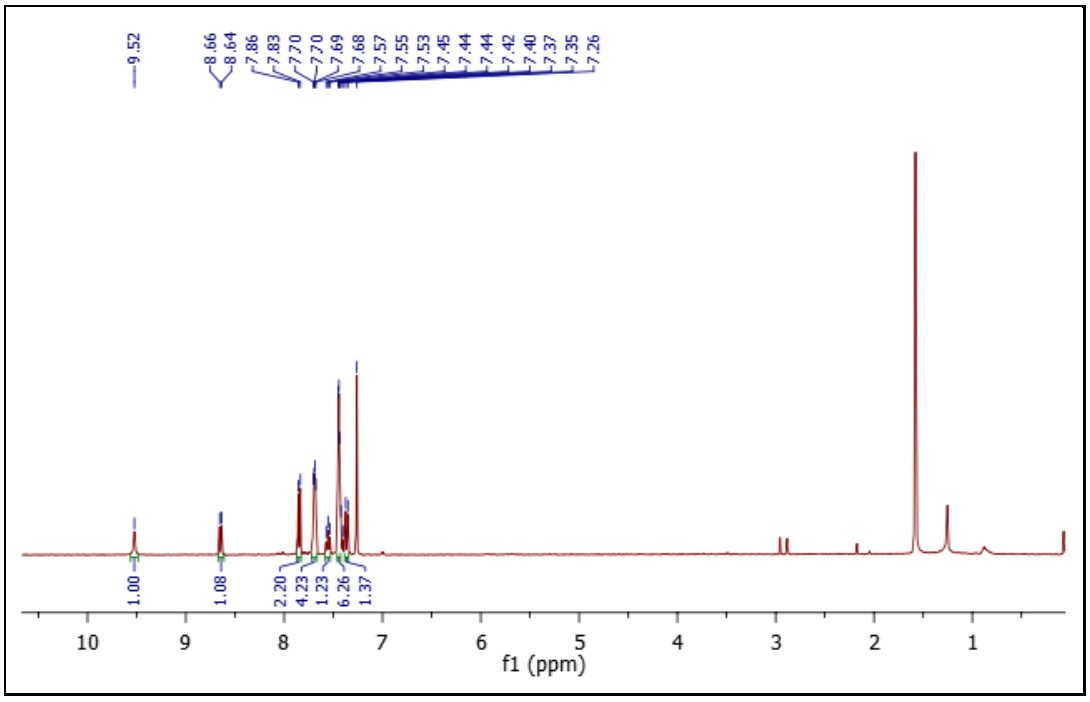
^{13}C NMR (125 MHz, $CDCl_3$)



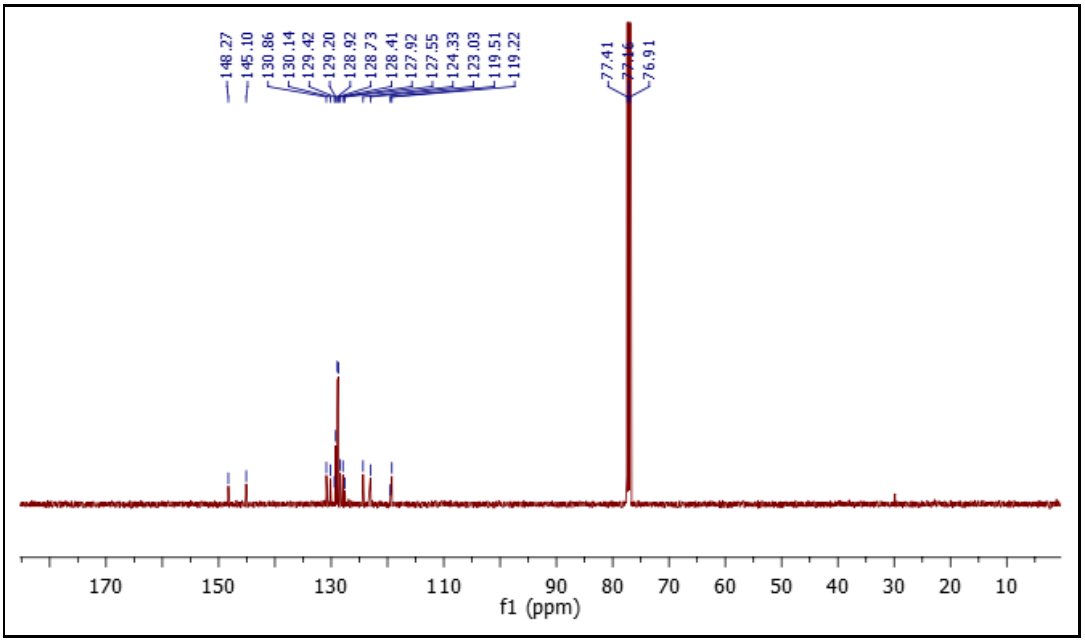


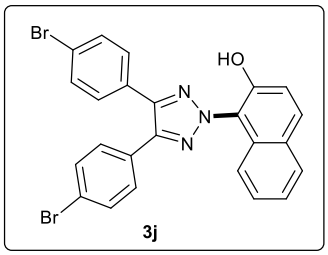
3i

^{1}H NMR (400 MHz, $CDCl_3$)



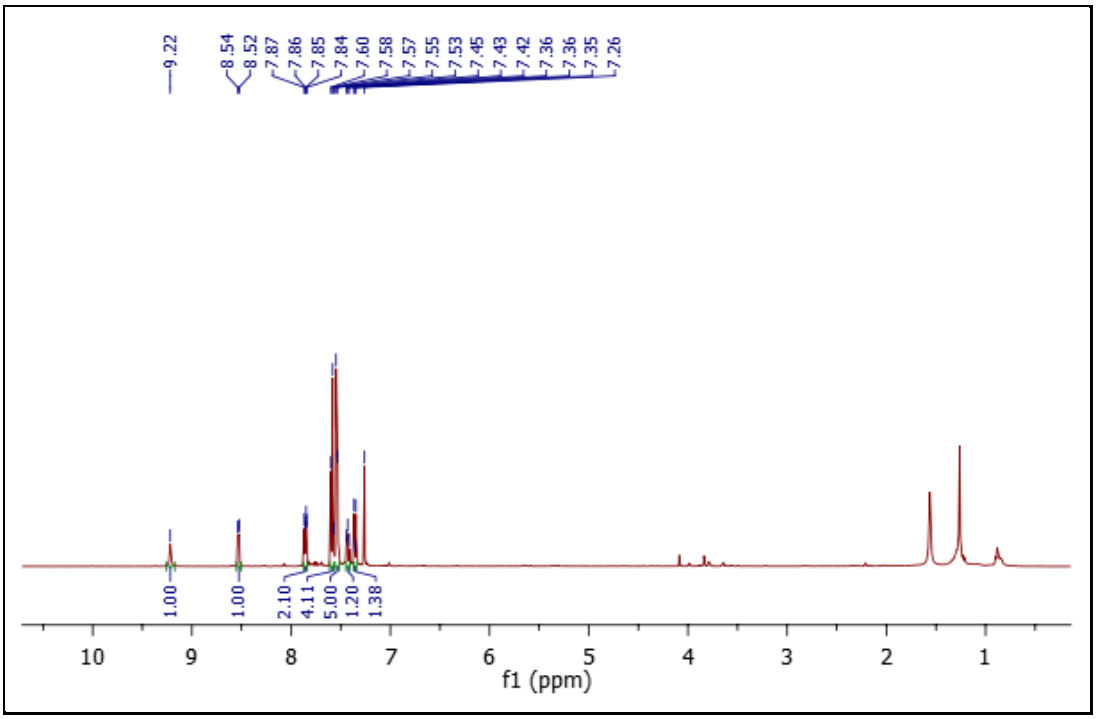
^{13}C NMR (125 MHz, $CDCl_3$)



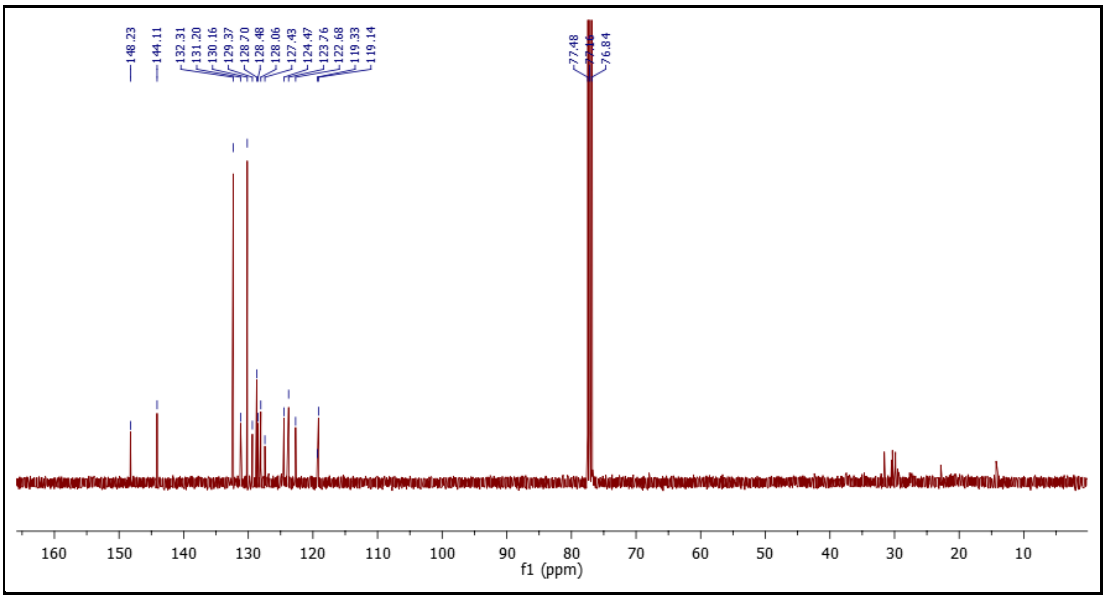


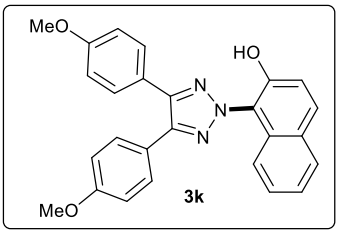
3j

^{1}H NMR (500 MHz, $CDCl_3$)

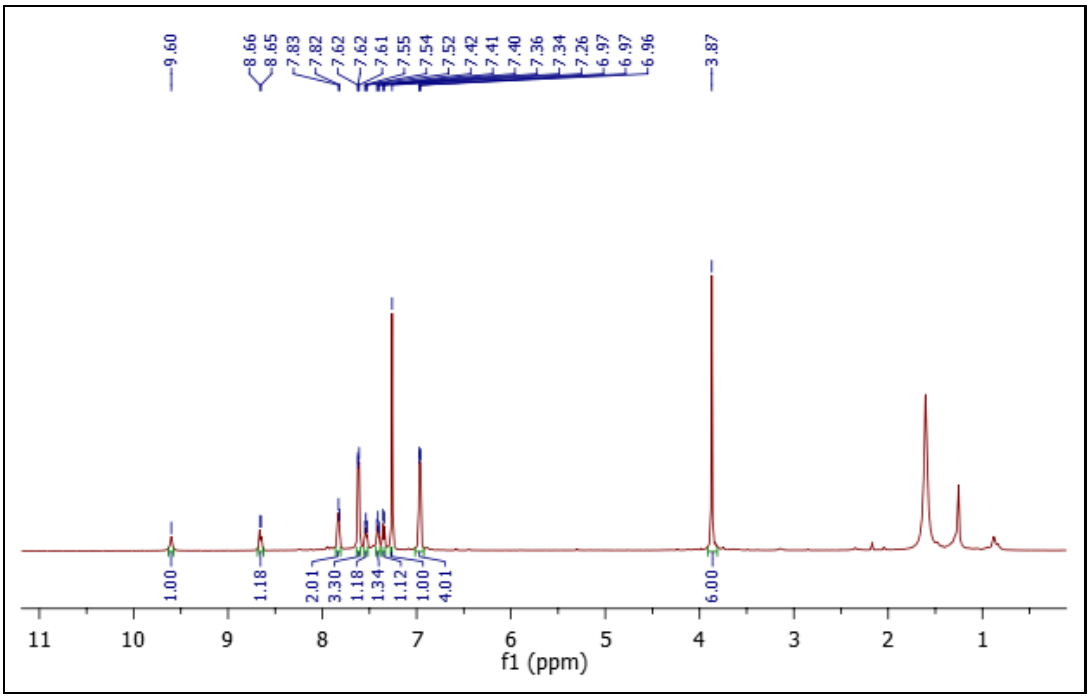


^{13}C NMR (100 MHz, $CDCl_3$)

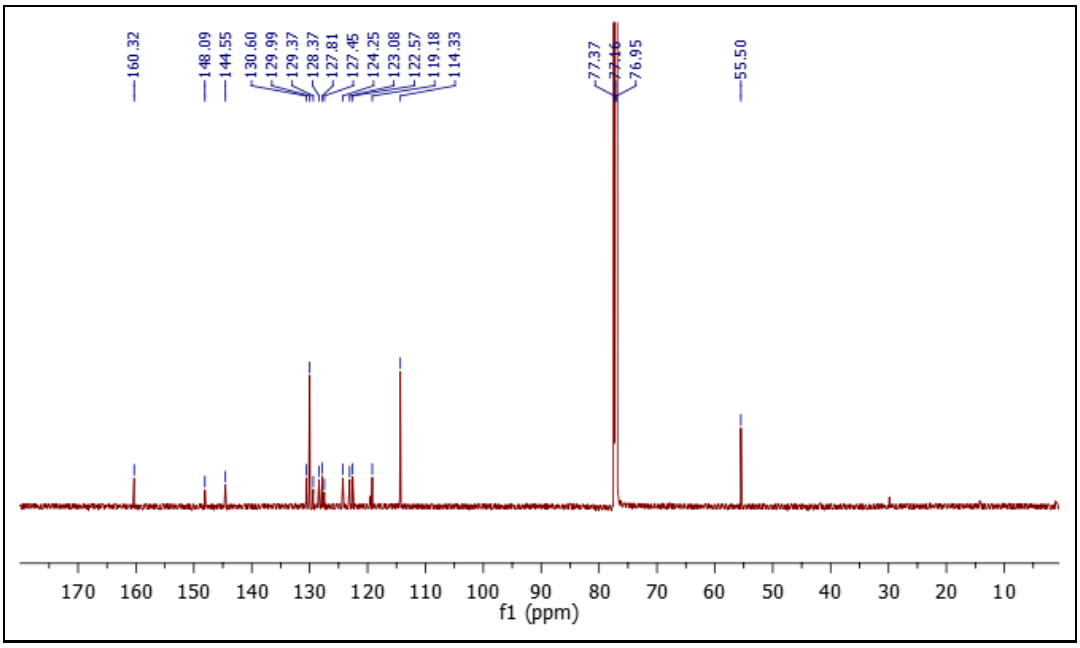


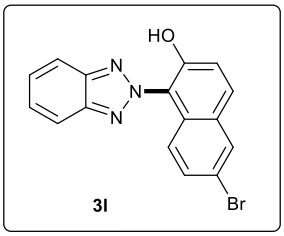


^{1}H NMR (600 MHz, $CDCl_3$)



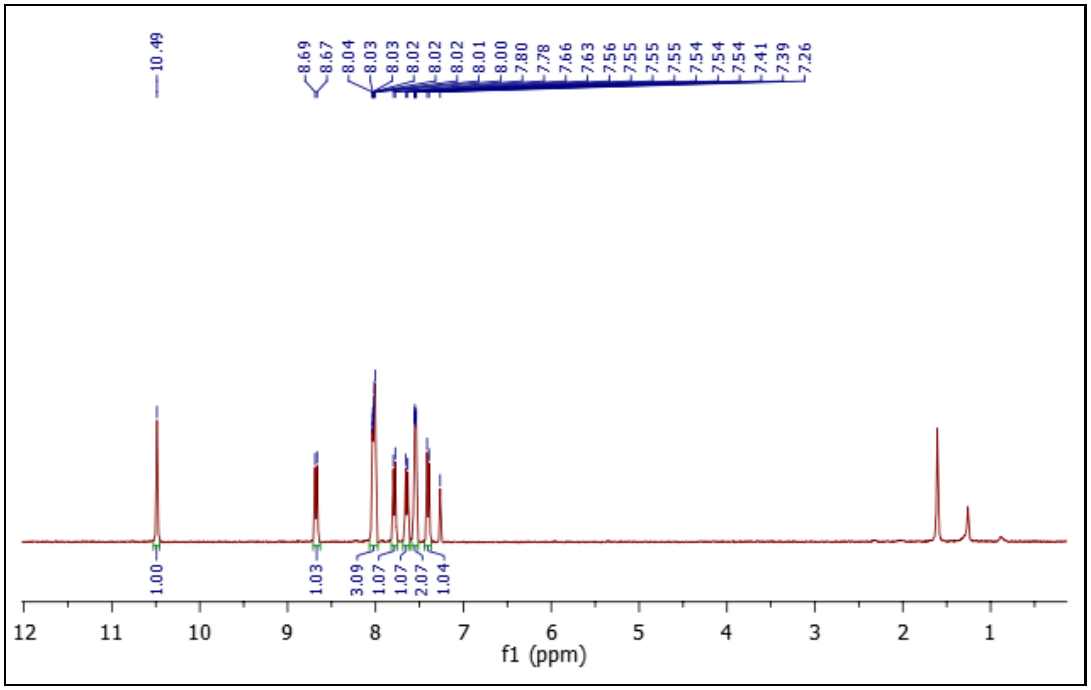
^{13}C NMR (150 MHz, $CDCl_3$)



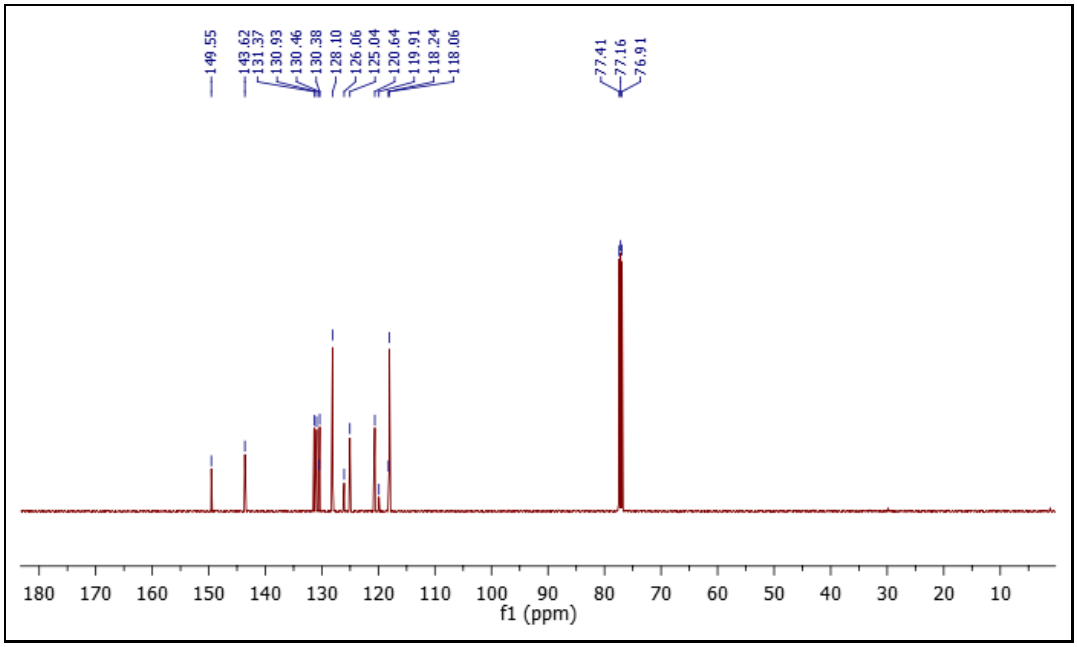


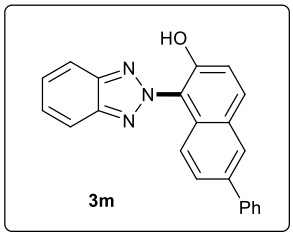
3l

^{1}H NMR (400 MHz, $CDCl_3$)

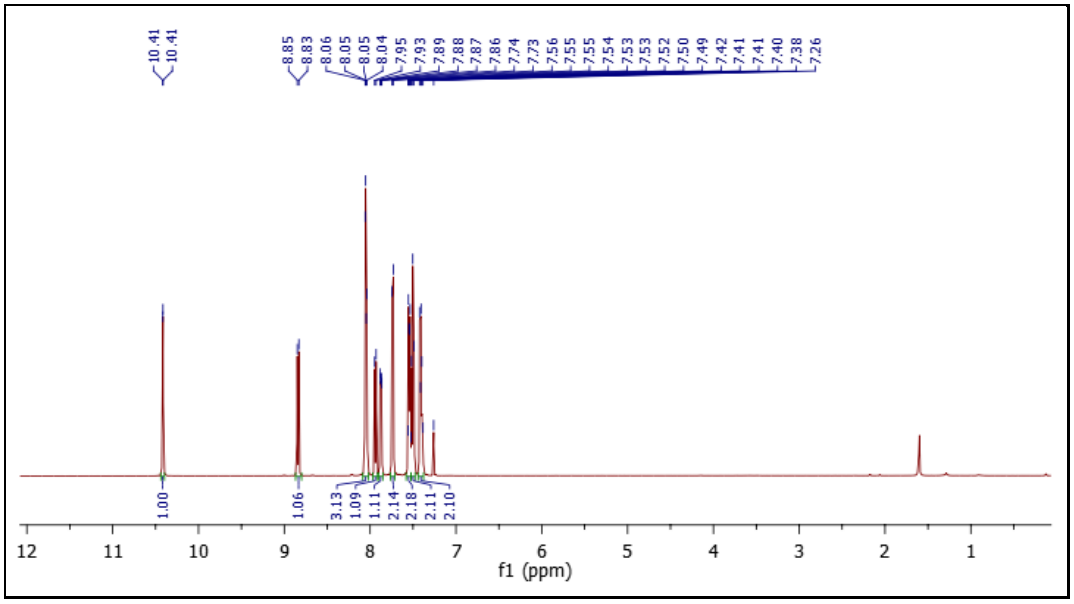


^{13}C NMR (125 MHz, $CDCl_3$)

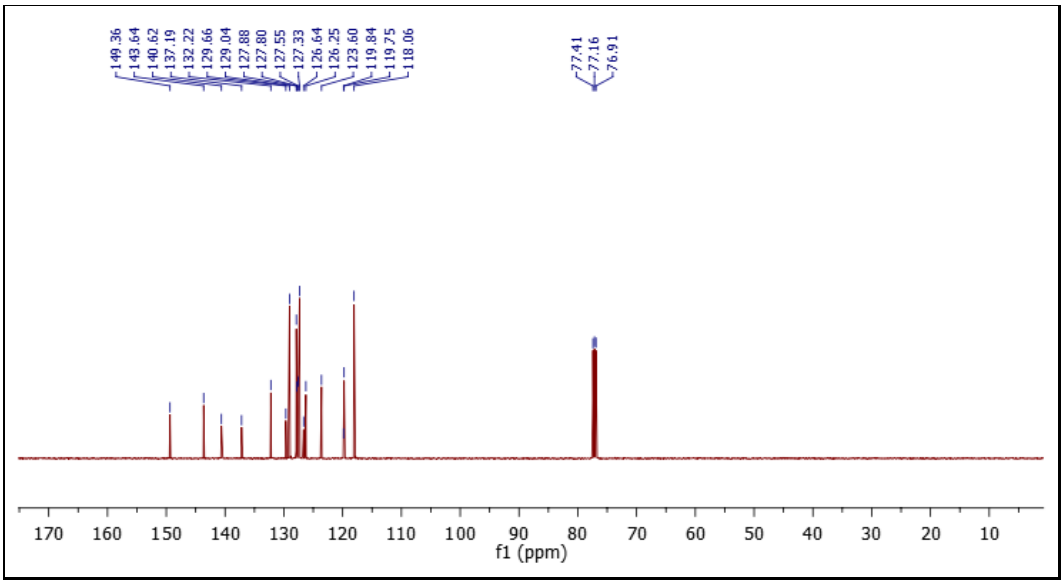


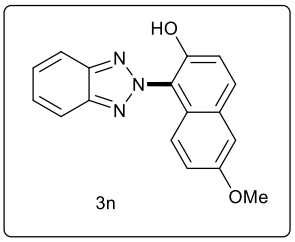


^{1}H NMR (500 MHz, $CDCl_3$)

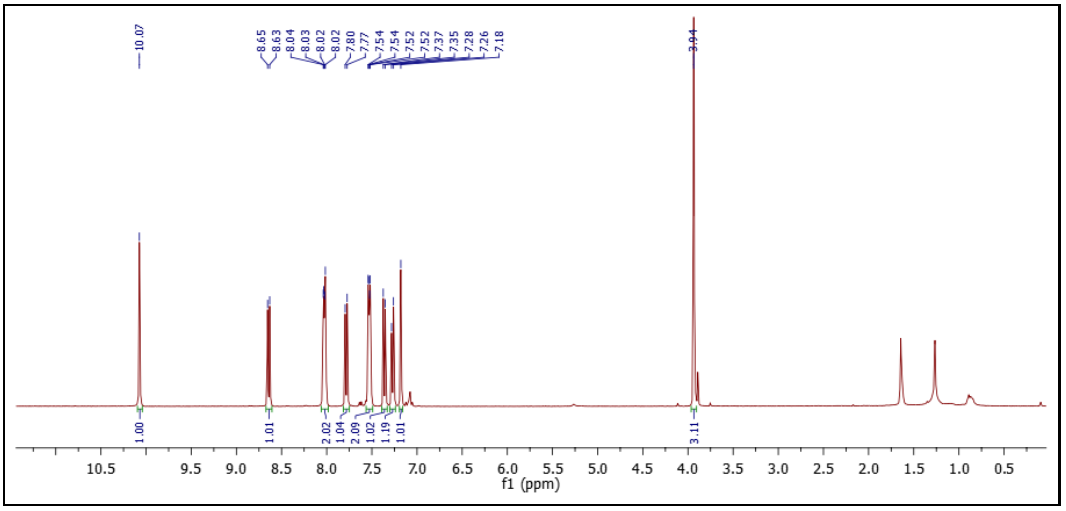


^{13}C NMR (125 MHz, $CDCl_3$)

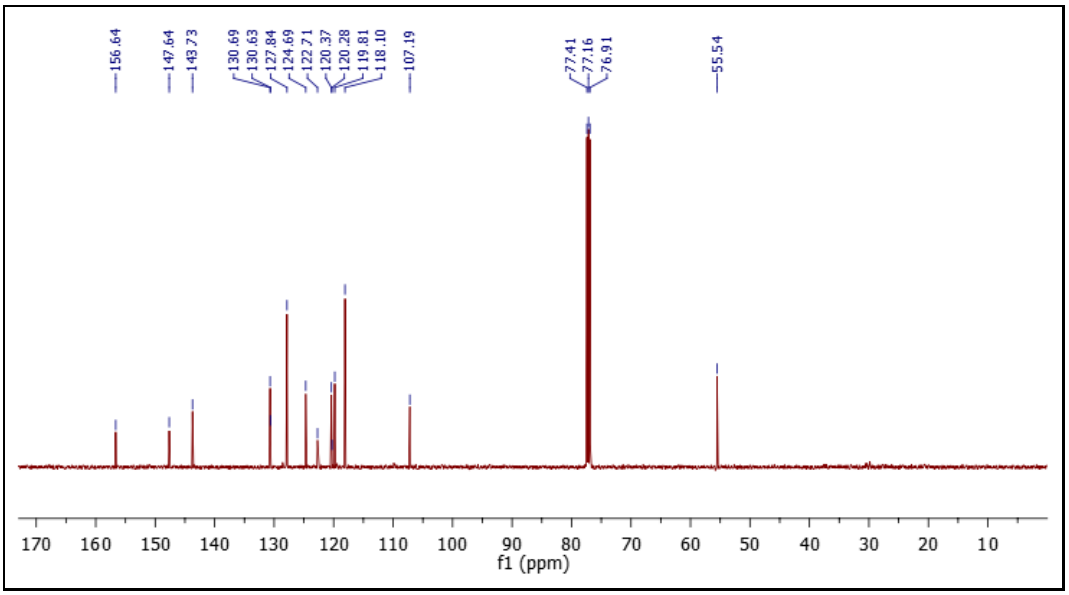


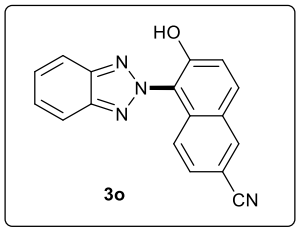


^{1}H NMR (400 MHz, $CDCl_3$)



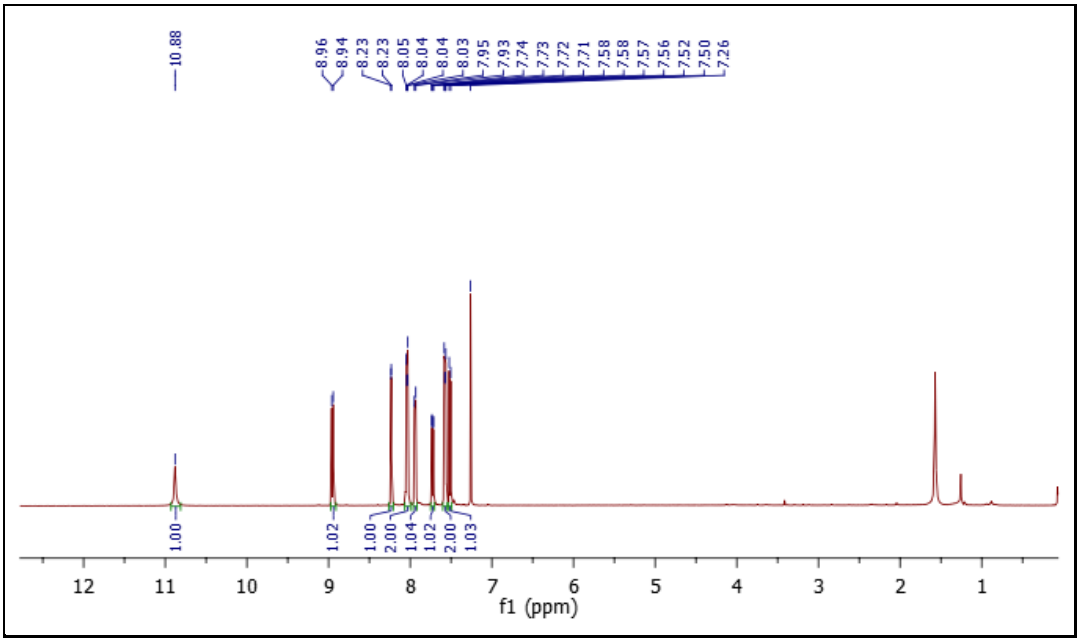
^{13}C NMR (125 MHz, $CDCl_3$)



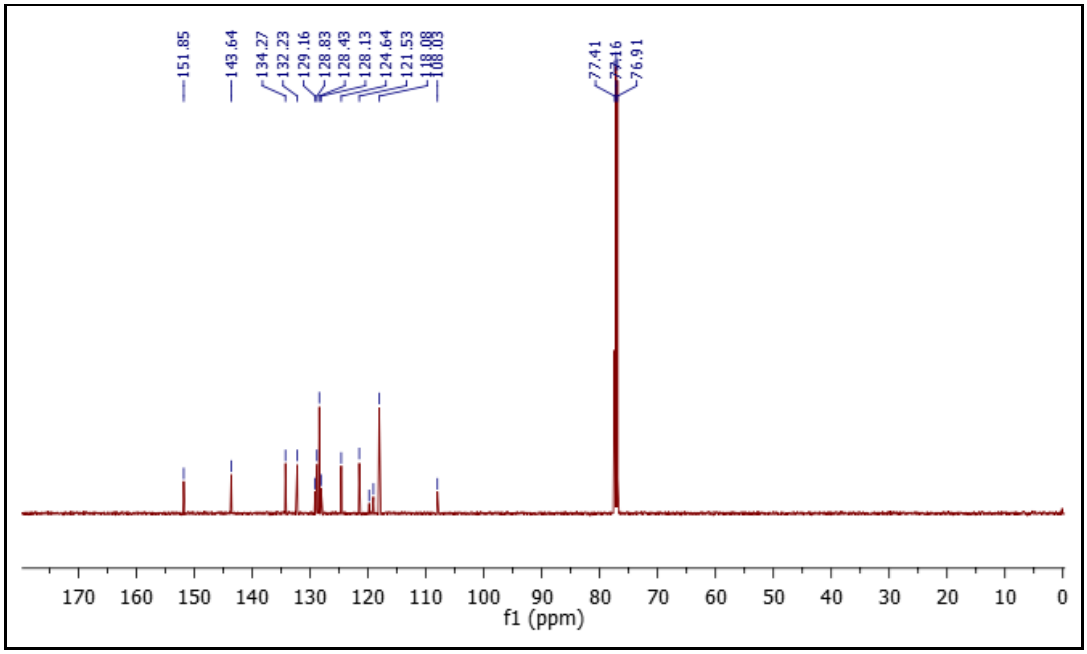


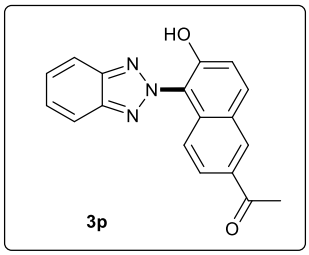
3o

^{1}H NMR (500 MHz, $CDCl_3$)

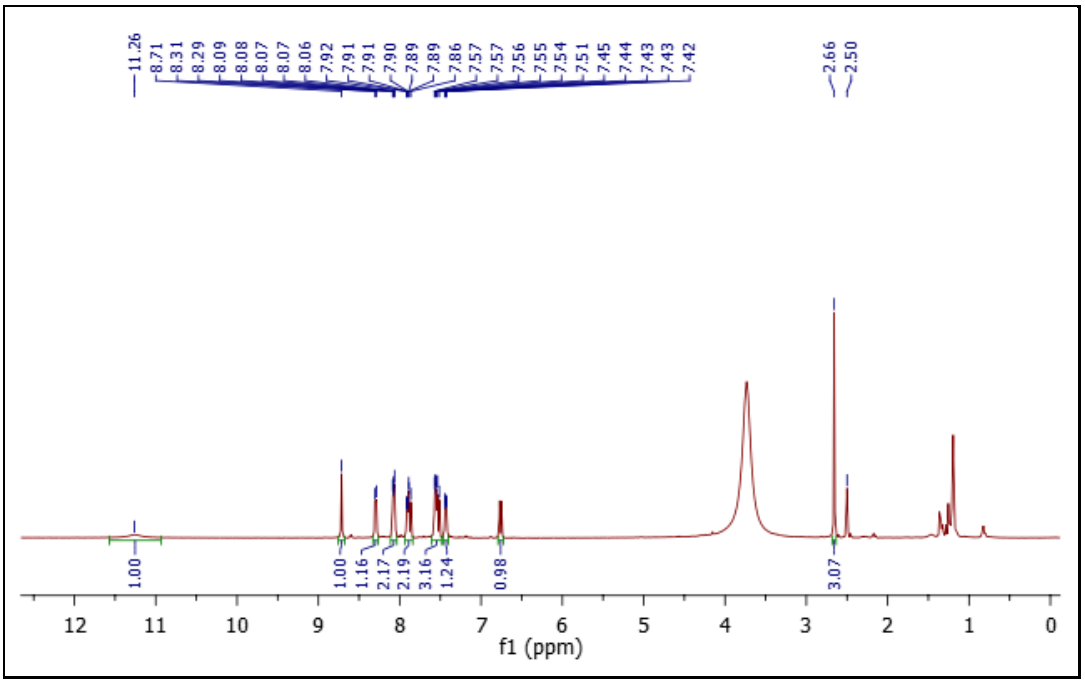


^{13}C NMR (125 MHz, $CDCl_3$)

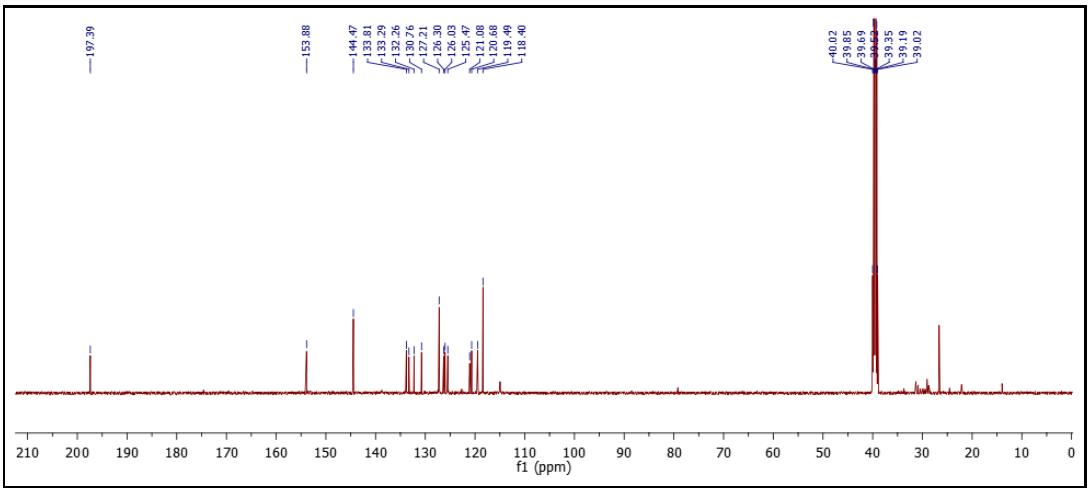


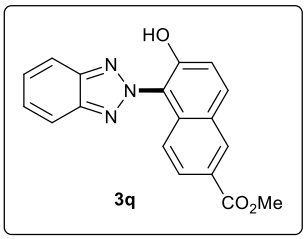


^{1}H NMR (400 MHz, DMSO-D$_6$)

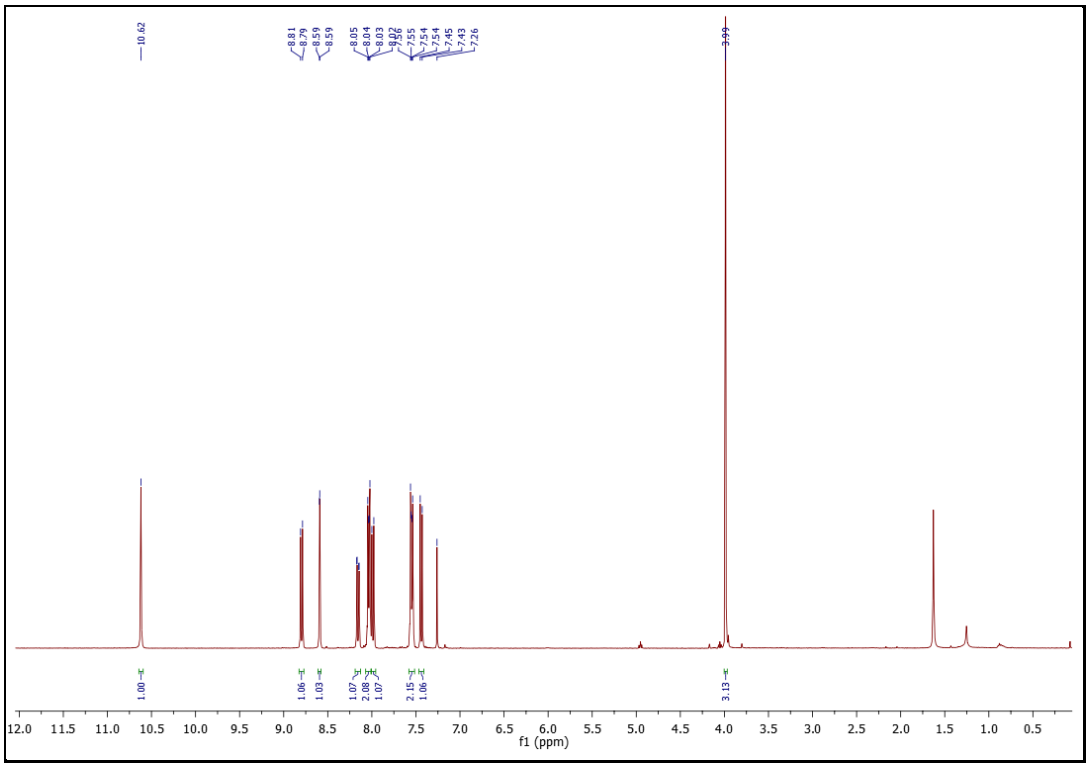


^{13}C NMR (125 MHz, DMSO-D$_6$)

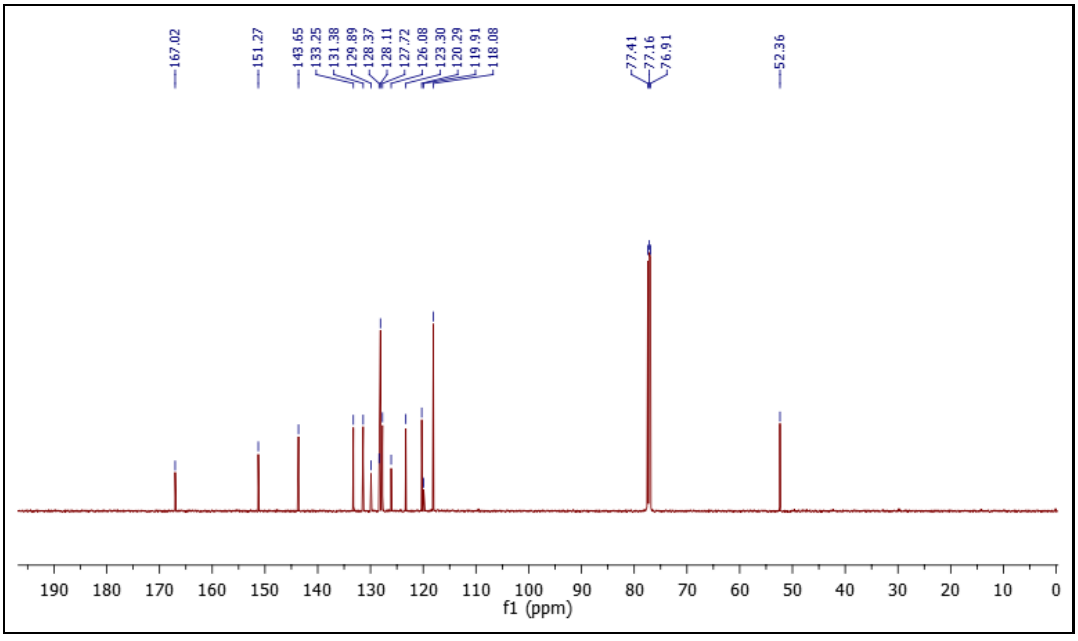


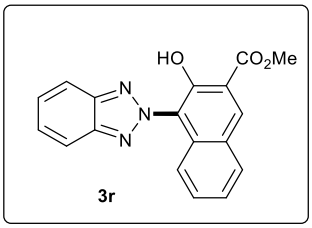


^{1}H NMR (400 MHz, $CDCl_3$)

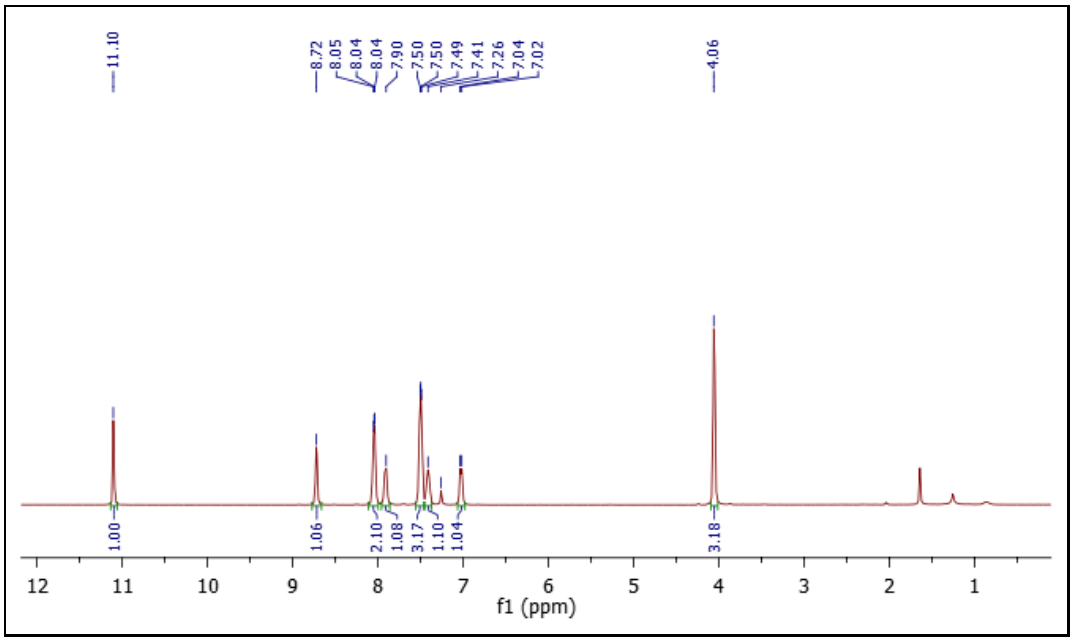


^{13}C NMR (125 MHz, $CDCl_3$)

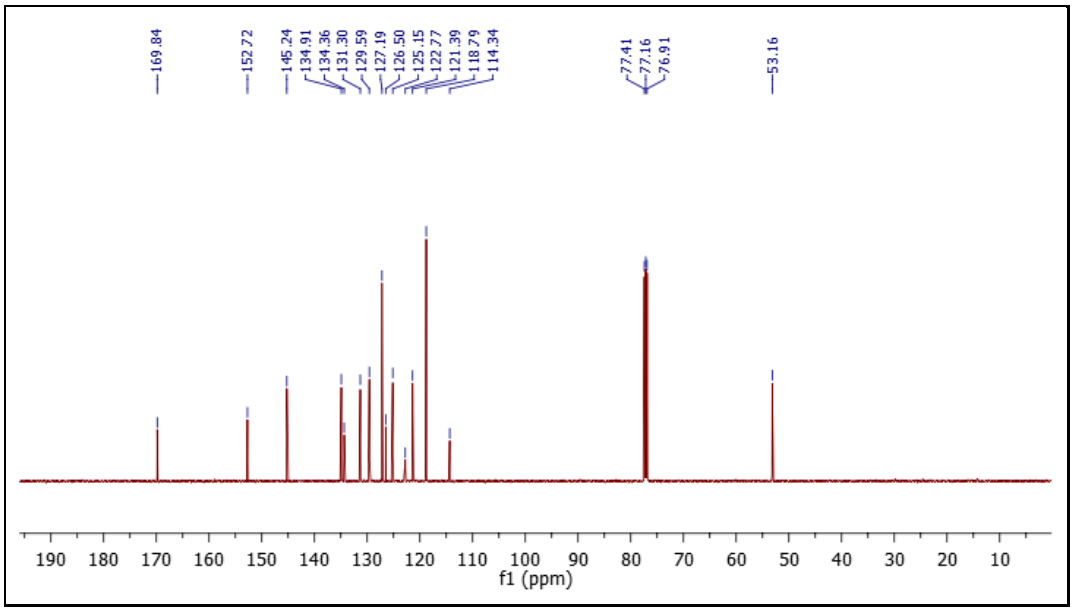


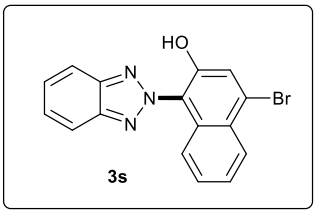


^{1}H NMR (400 MHz, $CDCl_3$)



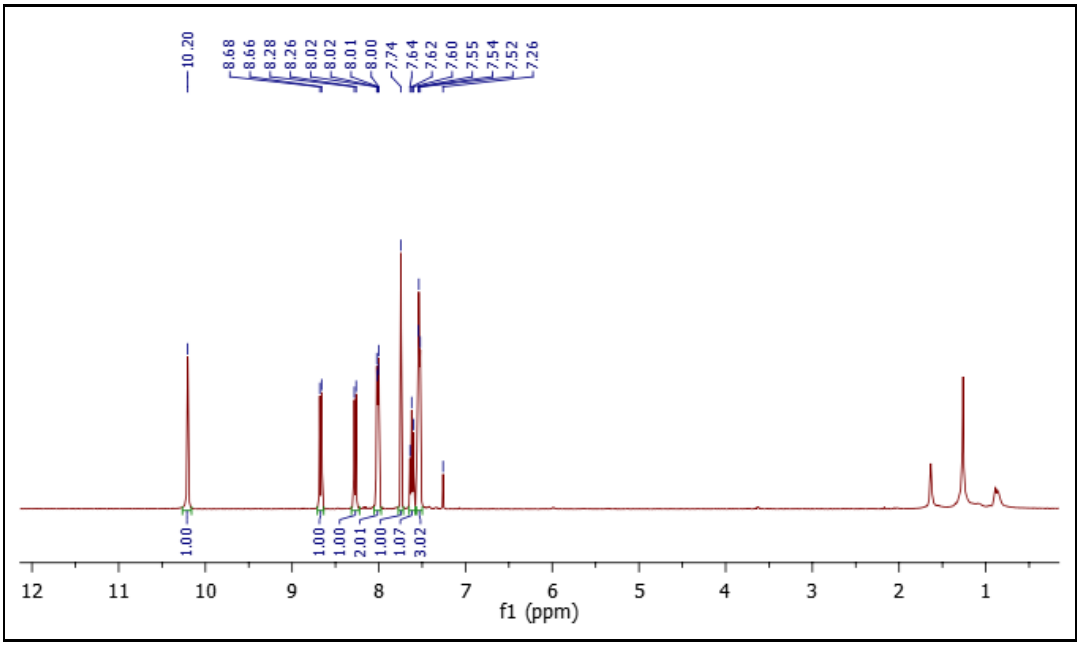
^{13}C NMR (125 MHz, $CDCl_3$)



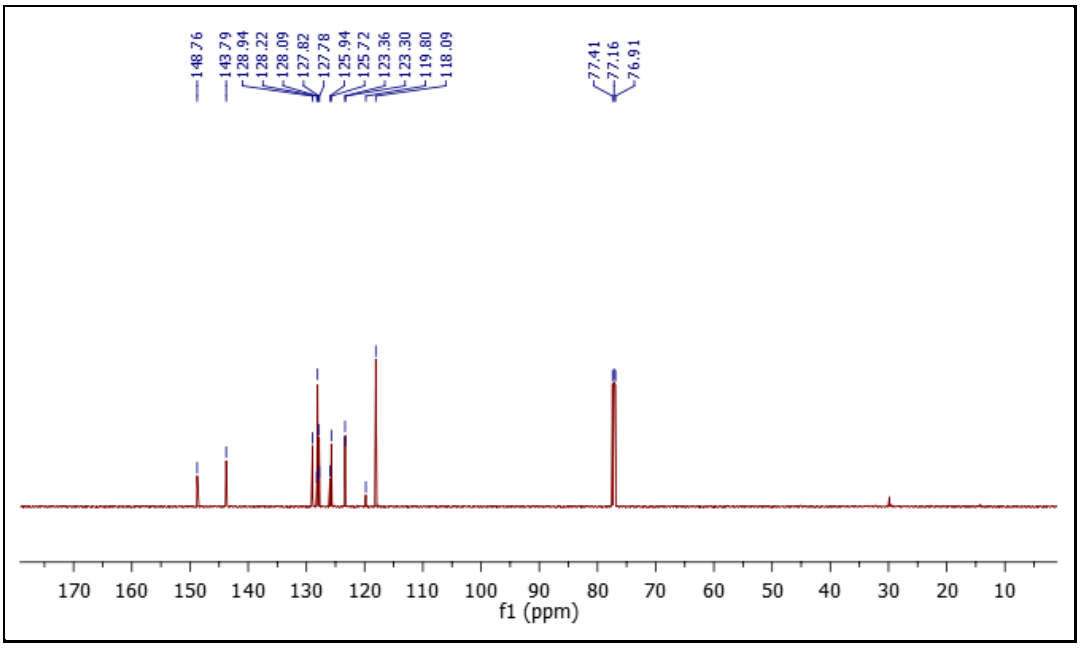


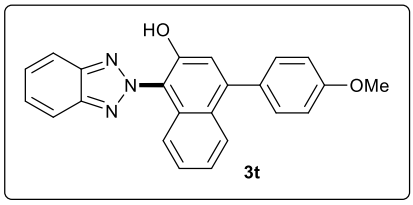
3s

^{1}H NMR (400 MHz, $CDCl_3$)



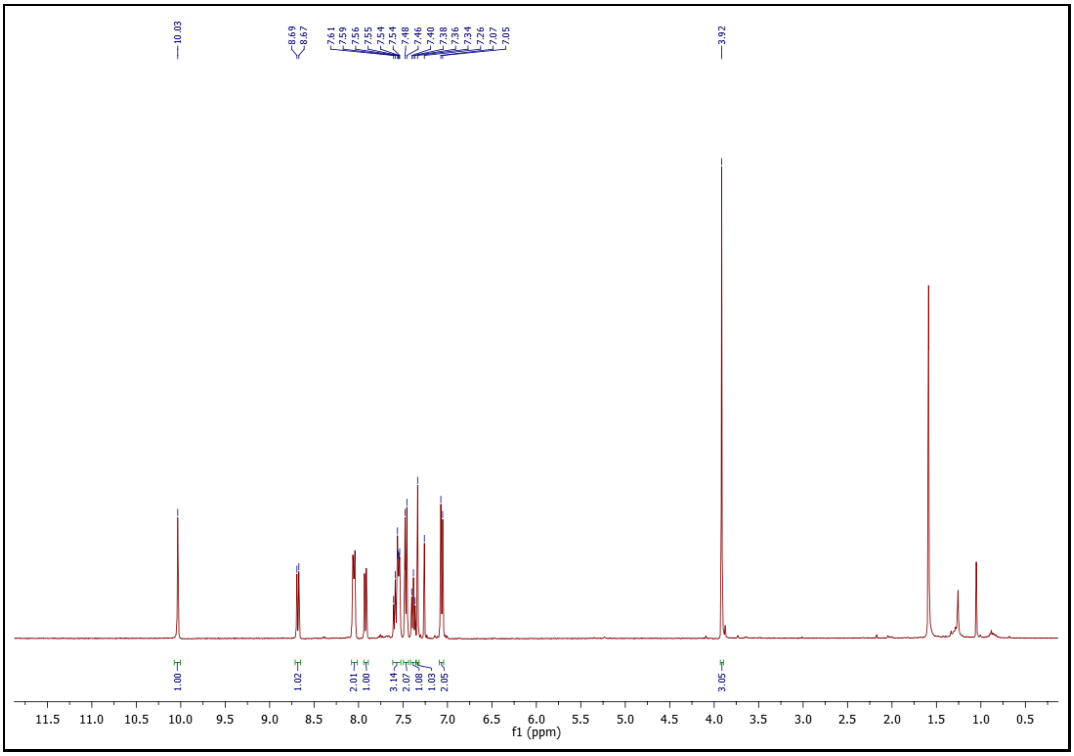
^{13}C NMR (125 MHz, $CDCl_3$)



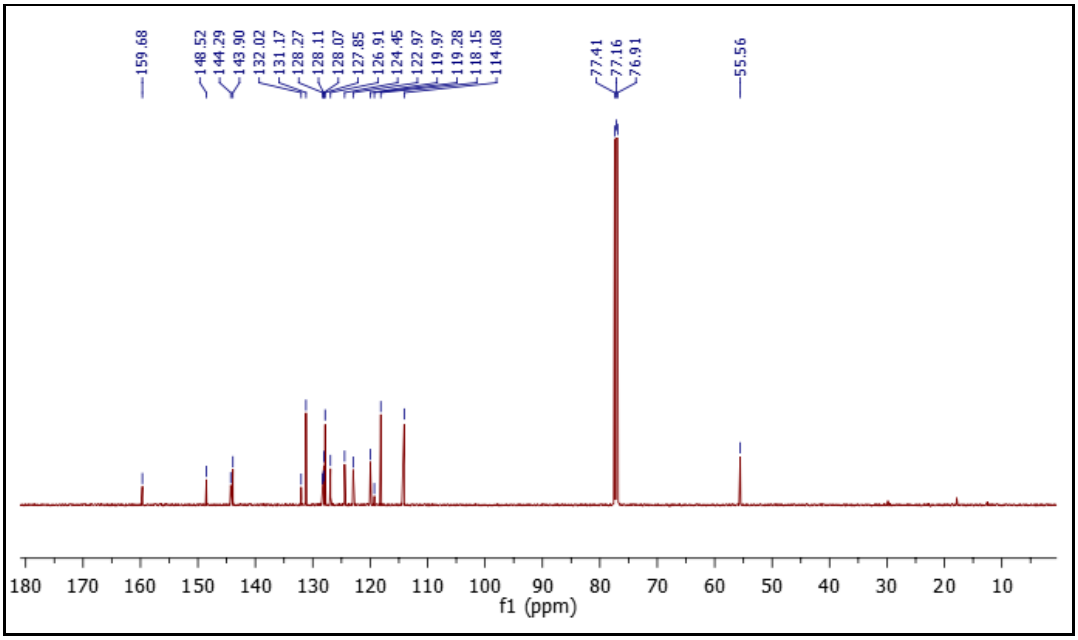


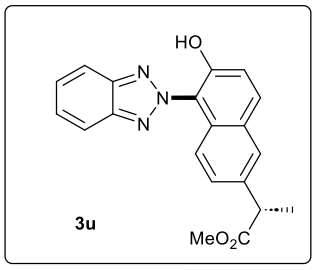
3t

^{1}H NMR (400 MHz, $CDCl_3$)

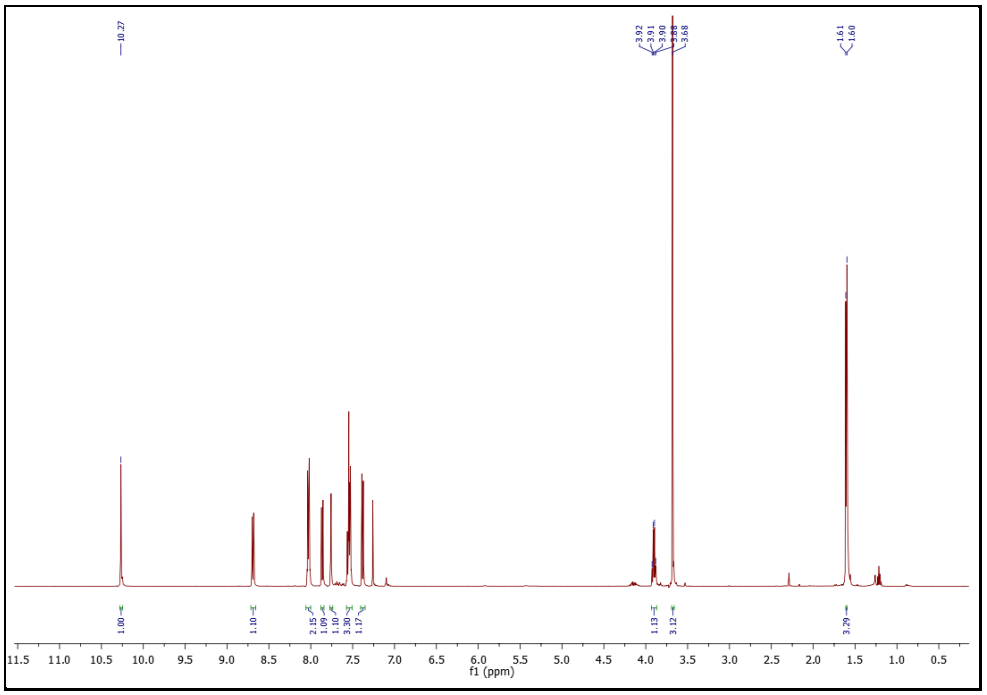


^{13}C NMR (125 MHz, $CDCl_3$)

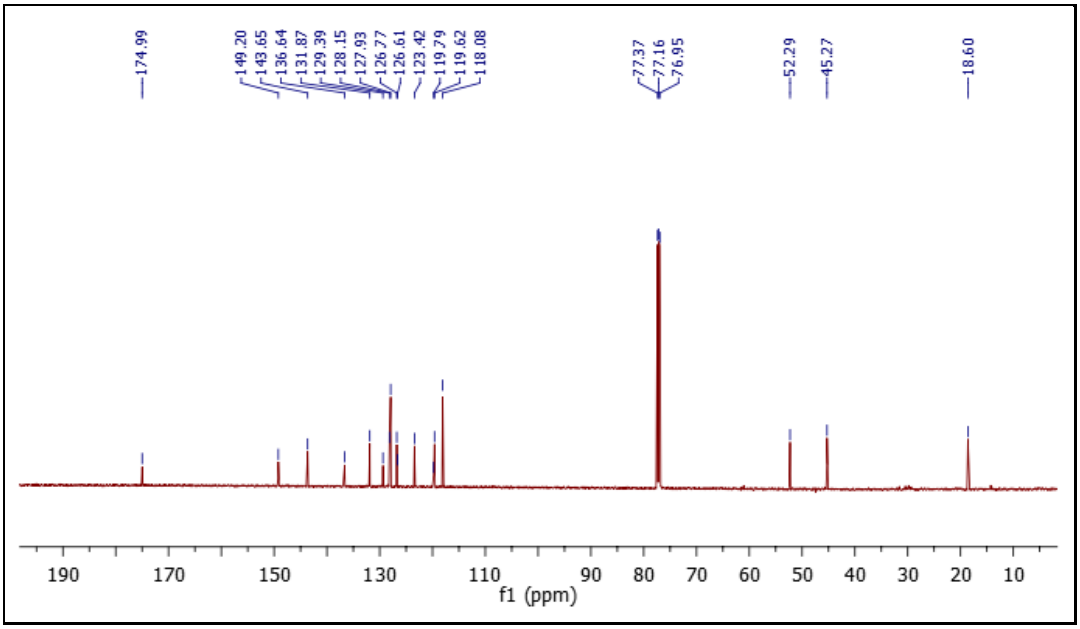


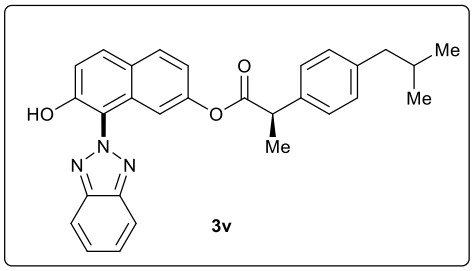


^{1}H NMR (500 MHz, $CDCl_3$)

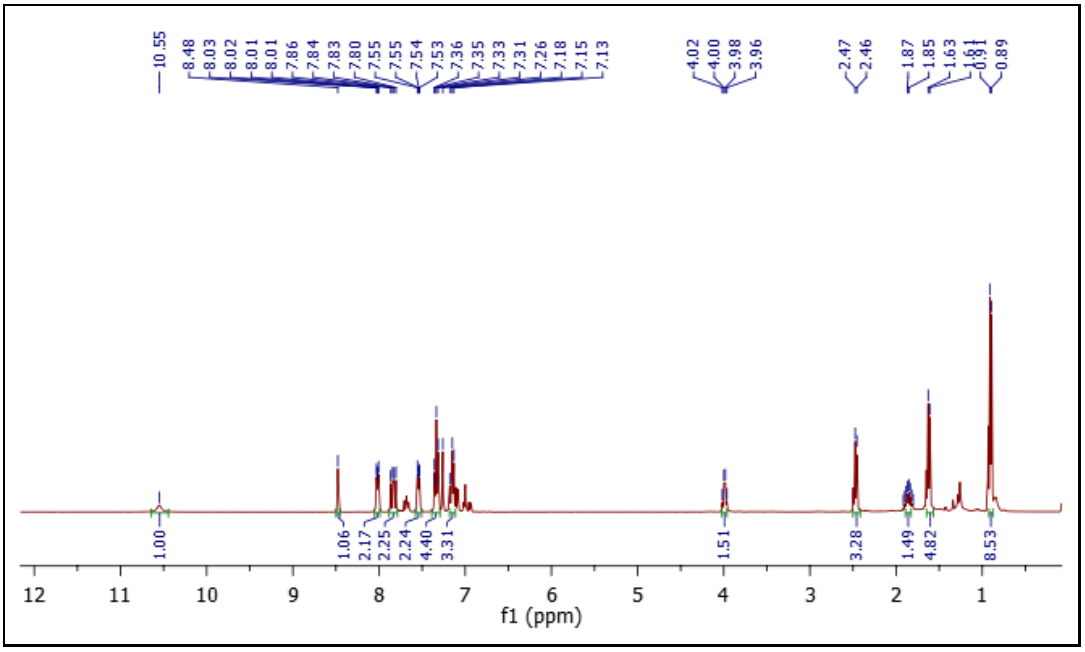


^{13}C NMR (150 MHz, $CDCl_3$)

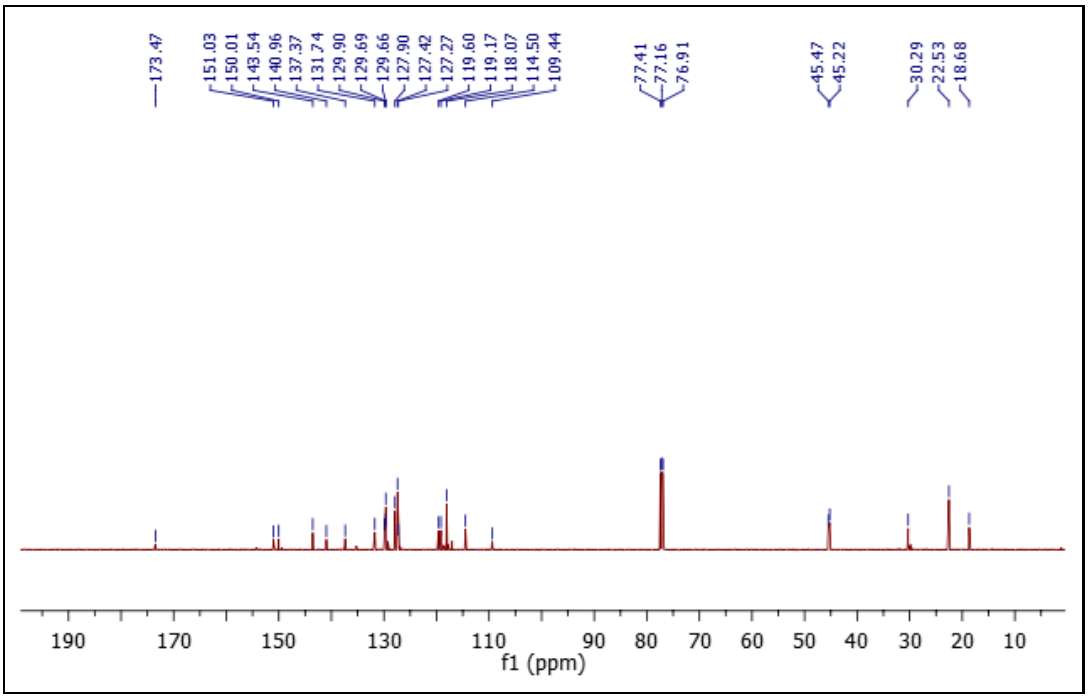


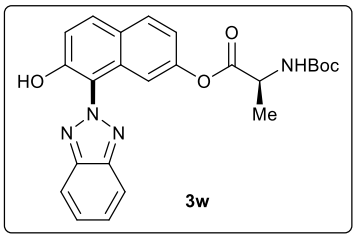


. ^{1}H NMR (400 MHz, $CDCl_3$)

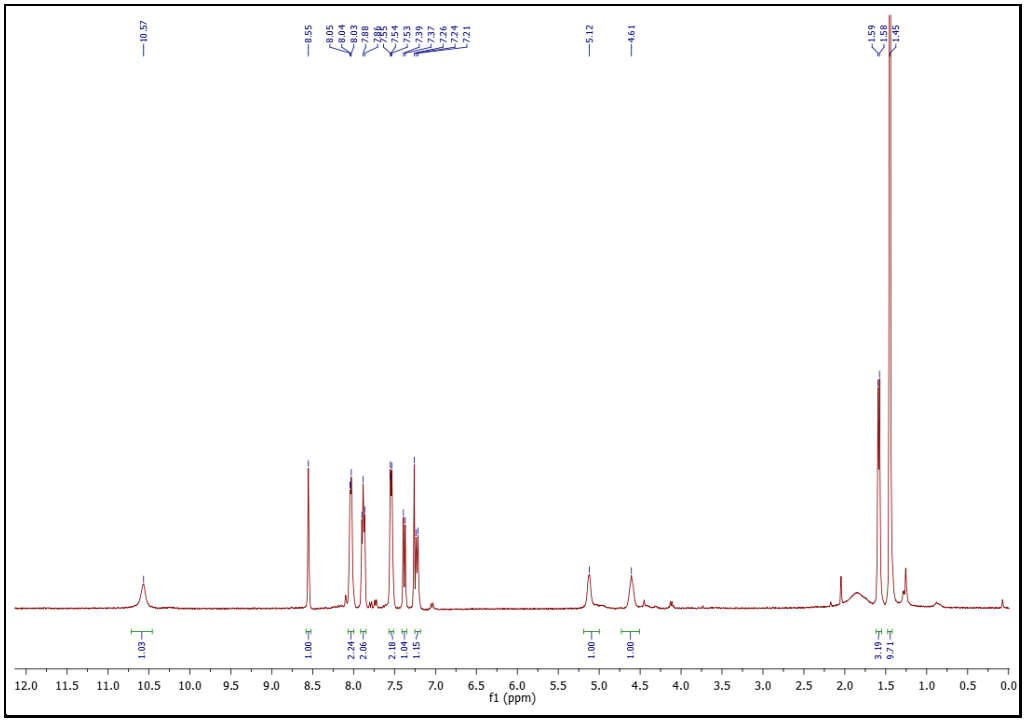


^{13}C NMR (125 MHz, $CDCl_3$)

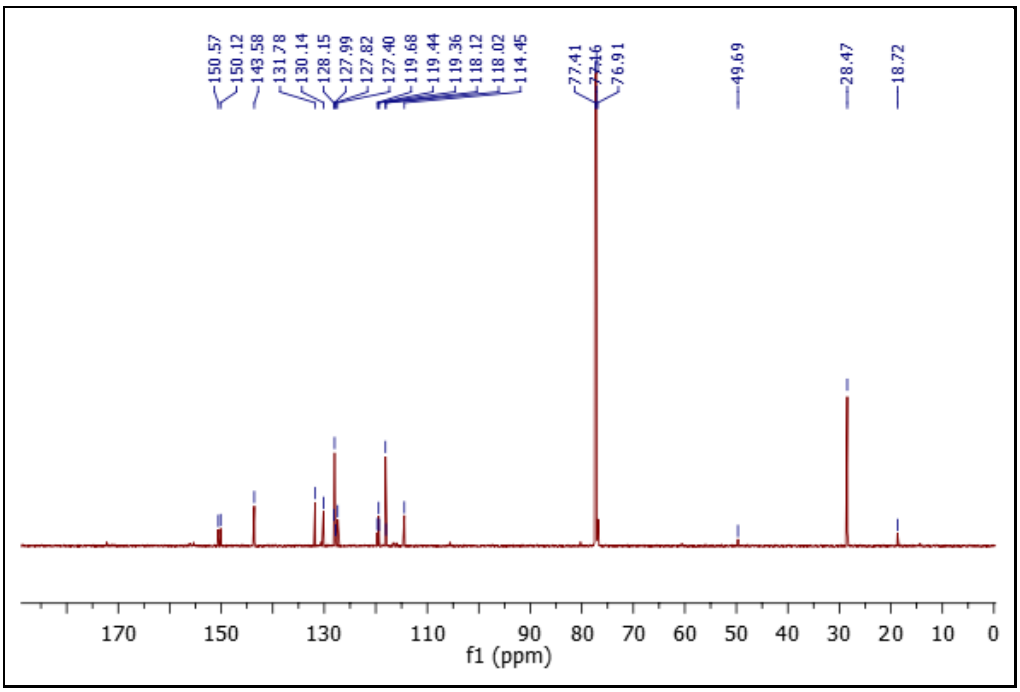


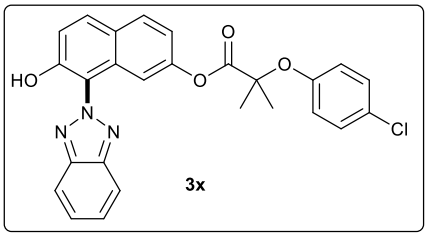


^{1}H NMR (400 MHz, $CDCl_3$)

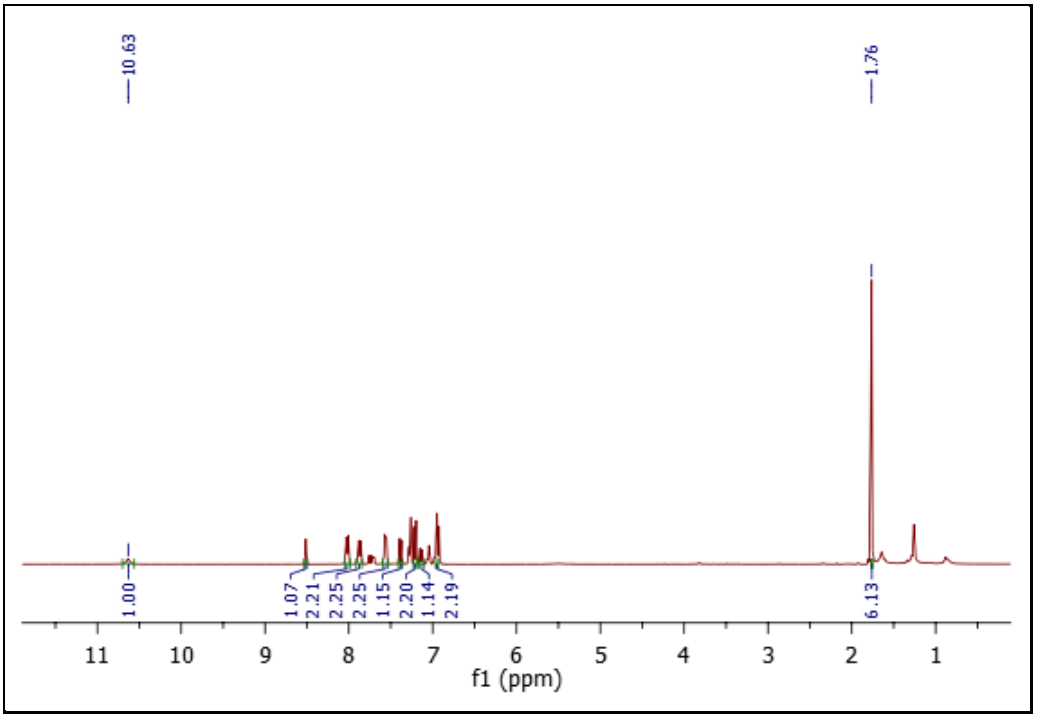


^{13}C NMR (125 MHz, $CDCl_3$)

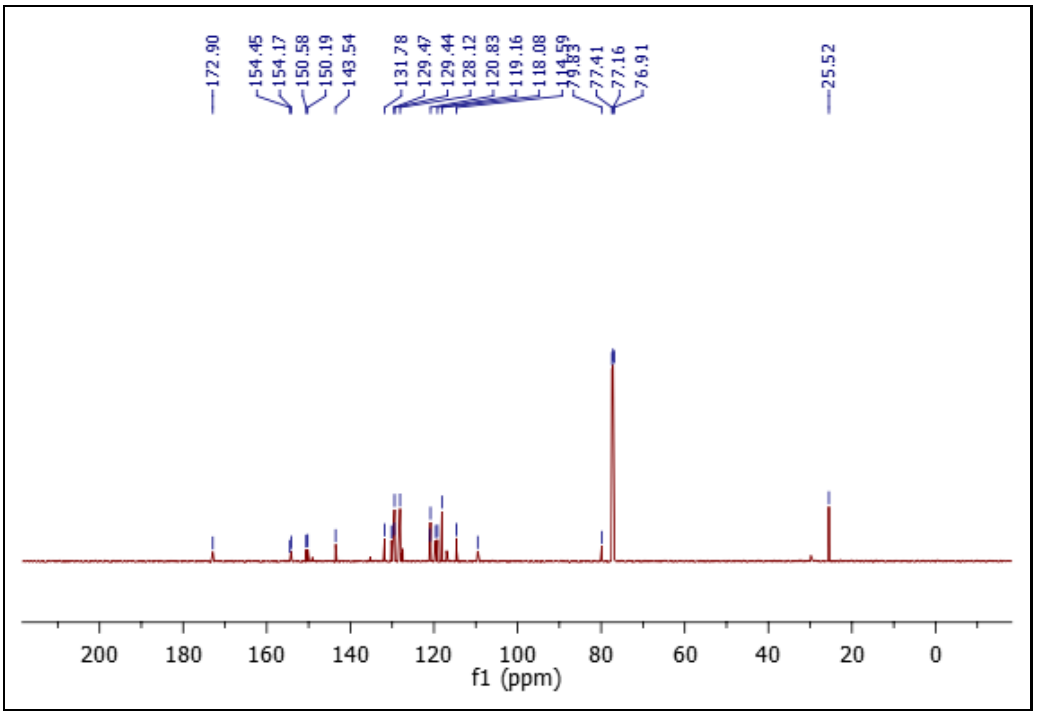


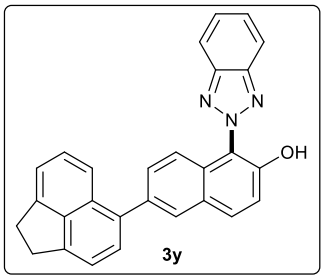


^{1}H NMR (400 MHz, $CDCl_3$)



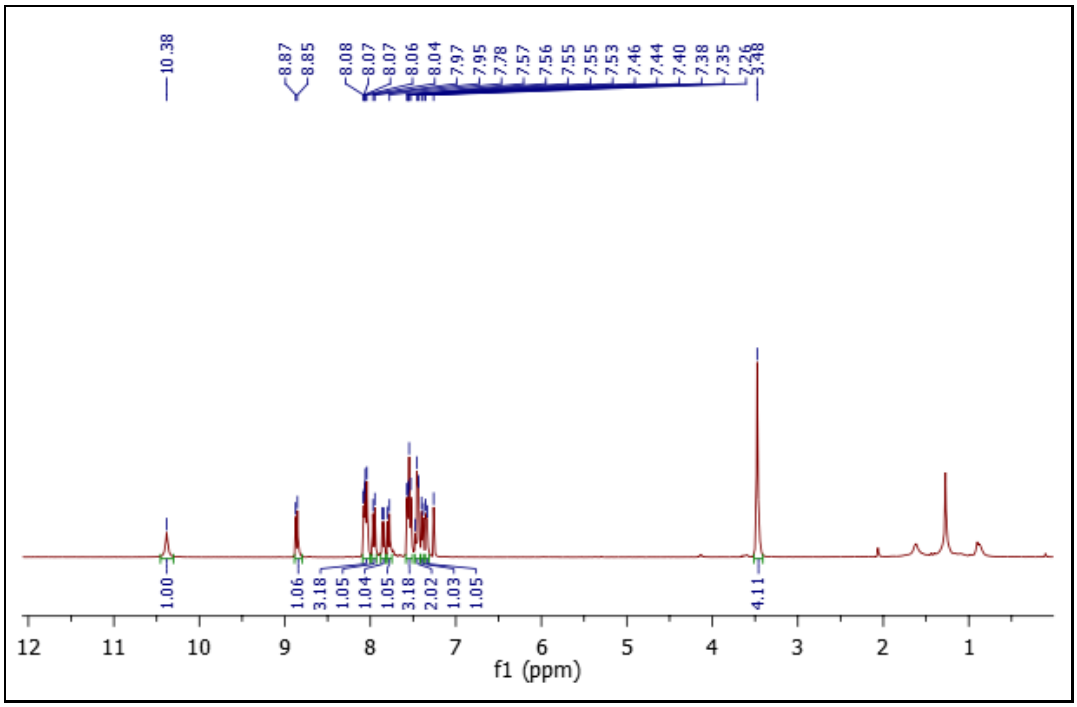
^{13}C NMR (125 MHz, $CDCl_3$)



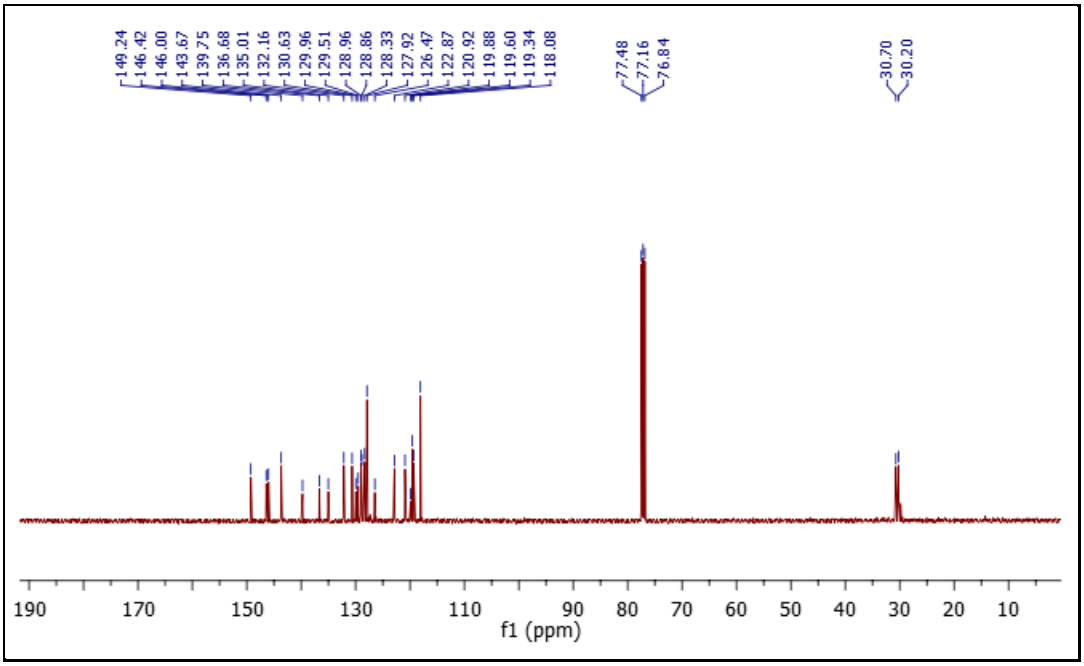


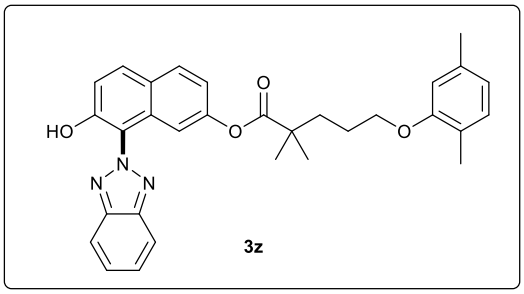
3y

^{1}H NMR (400 MHz, $CDCl_3$)

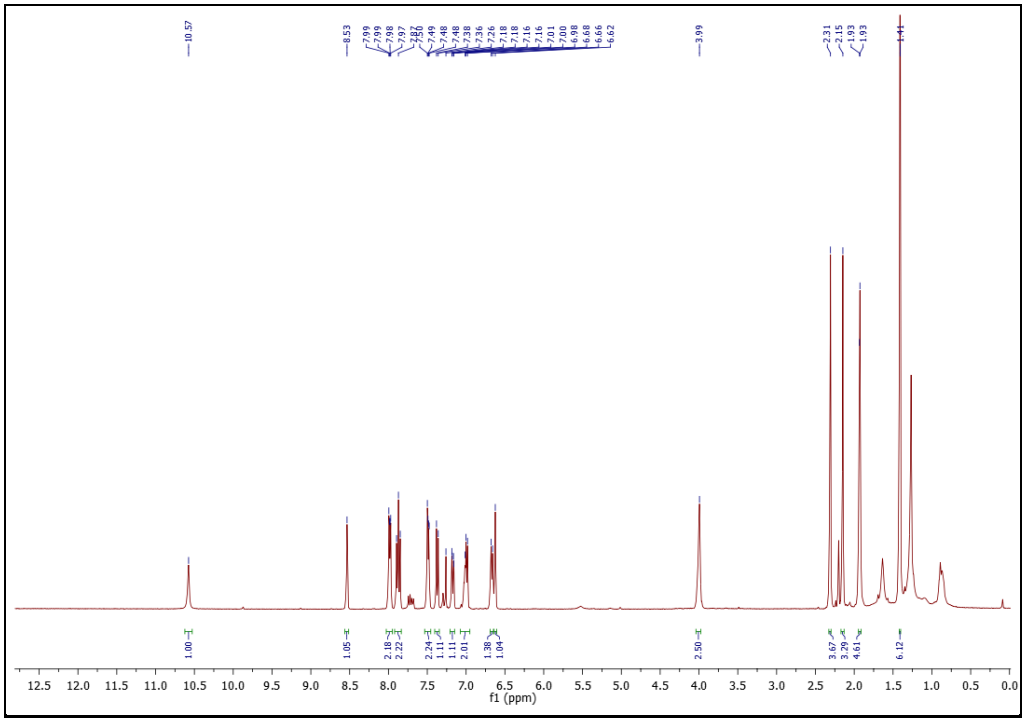


^{13}C NMR (100 MHz, $CDCl_3$)

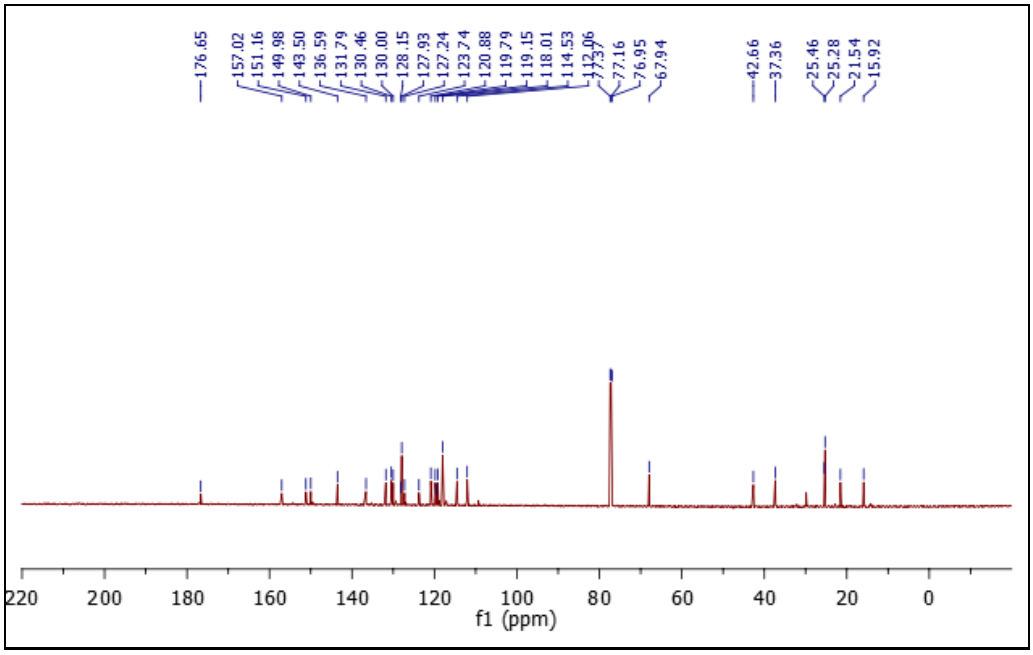


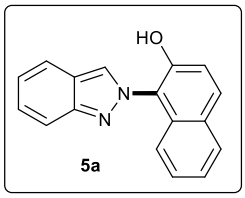


^{1}H NMR (400 MHz, $CDCl_3$)

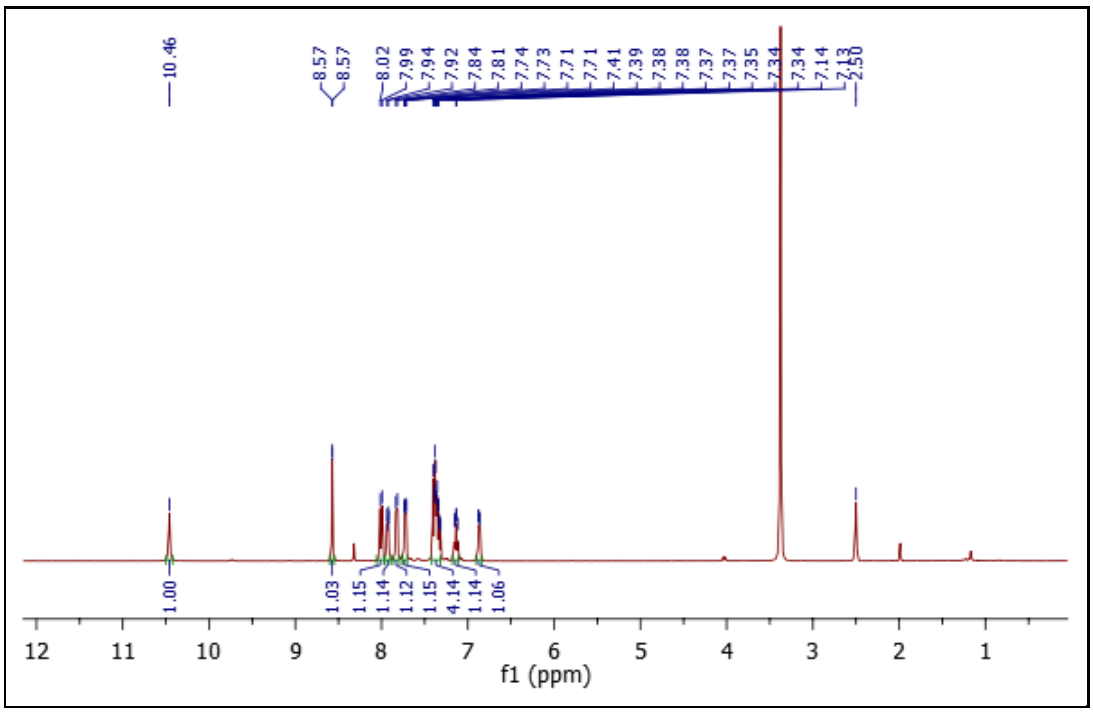


^{13}C NMR (150 MHz, $CDCl_3$)

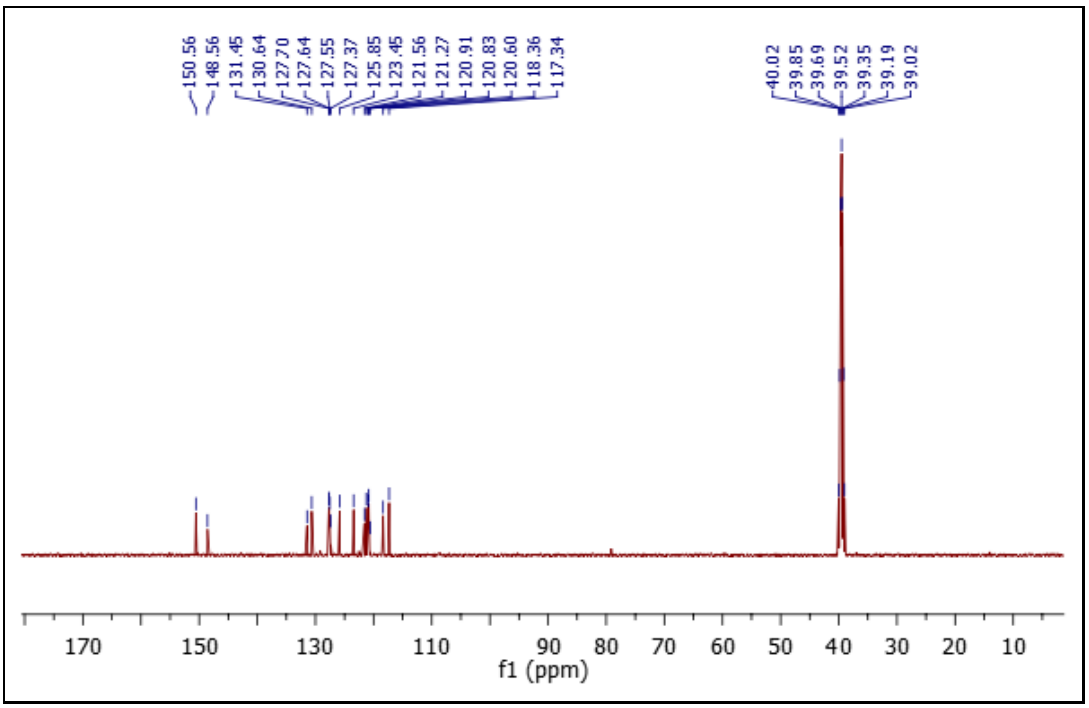


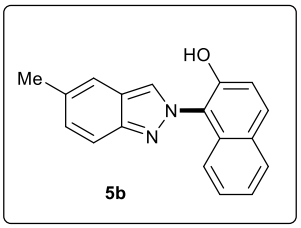


^{1}H NMR (400 MHz, DMSO-D$_6$)

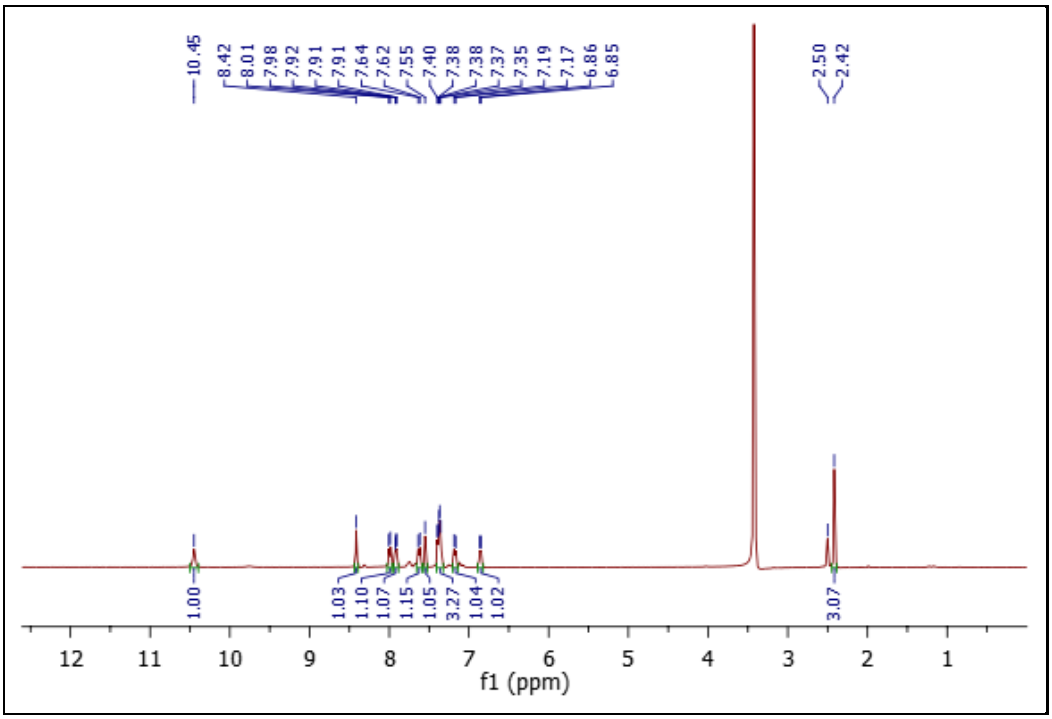


^{13}C NMR (125 MHz, DMSO-D$_6$)

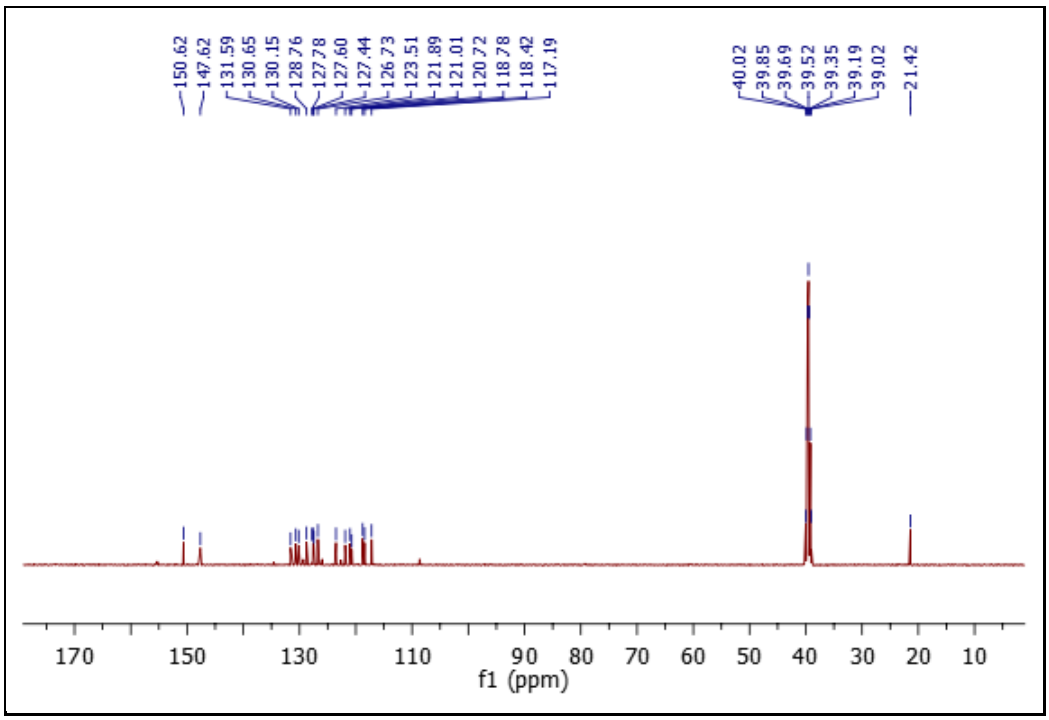


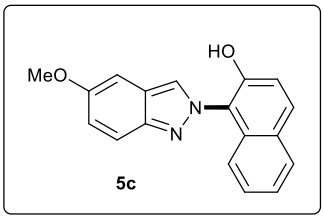


^{1}H NMR (400 MHz, DMSO-D$_6$)

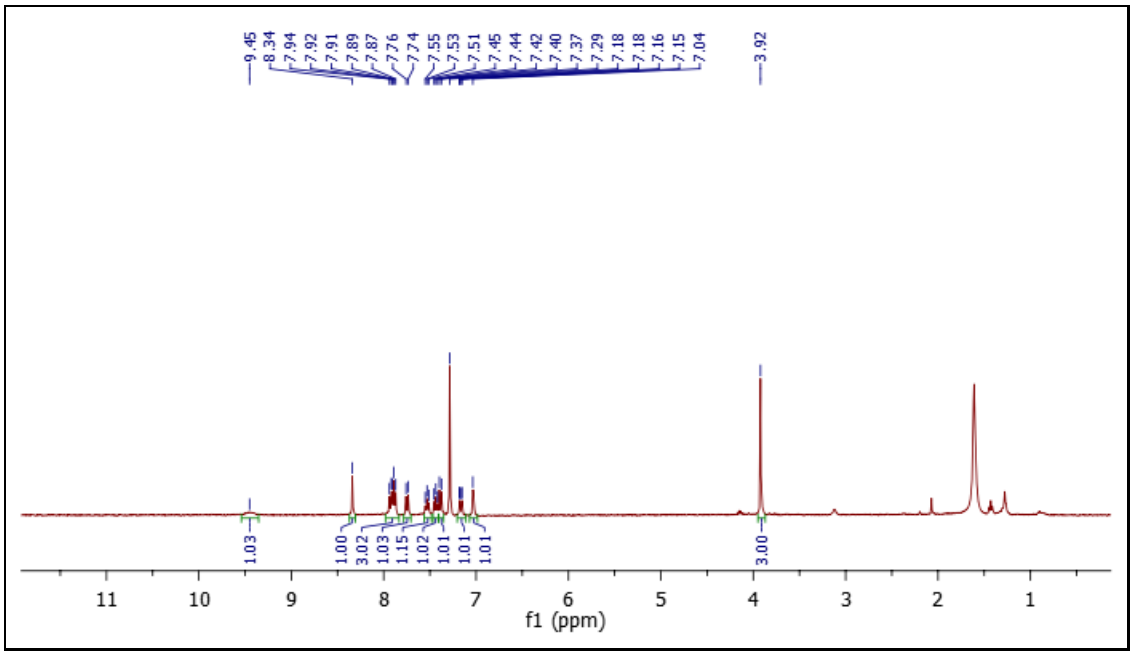


^{13}C NMR (125 MHz, DMSO-D$_6$)

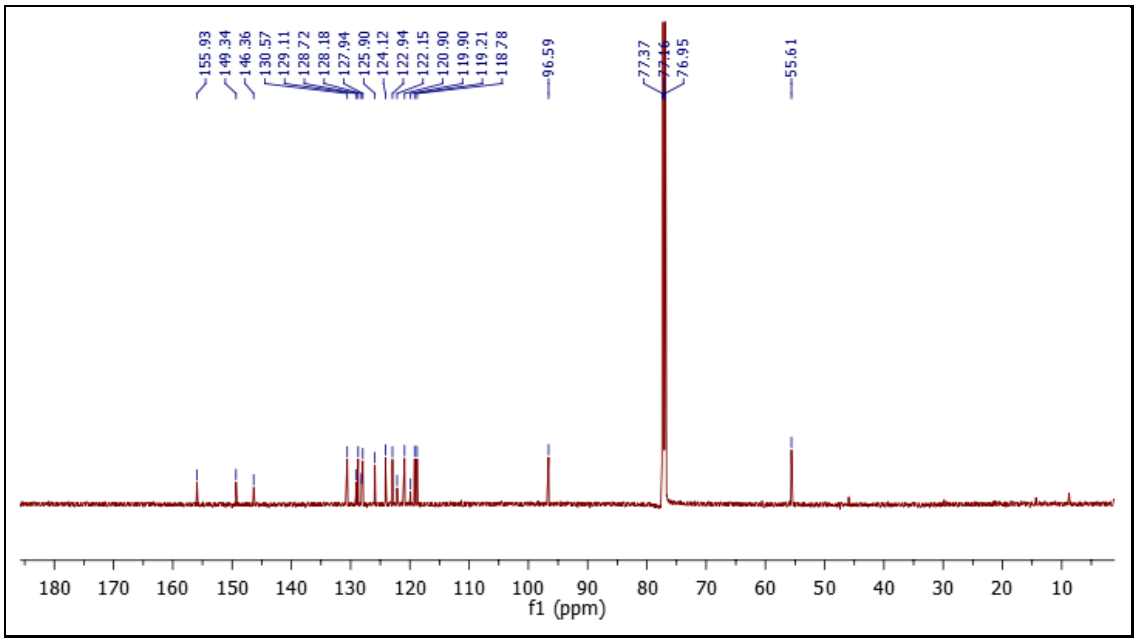


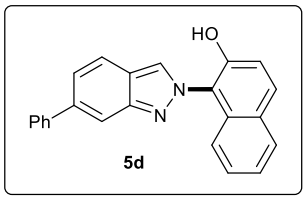


^{1}H NMR (400 MHz, $CDCl_3$)



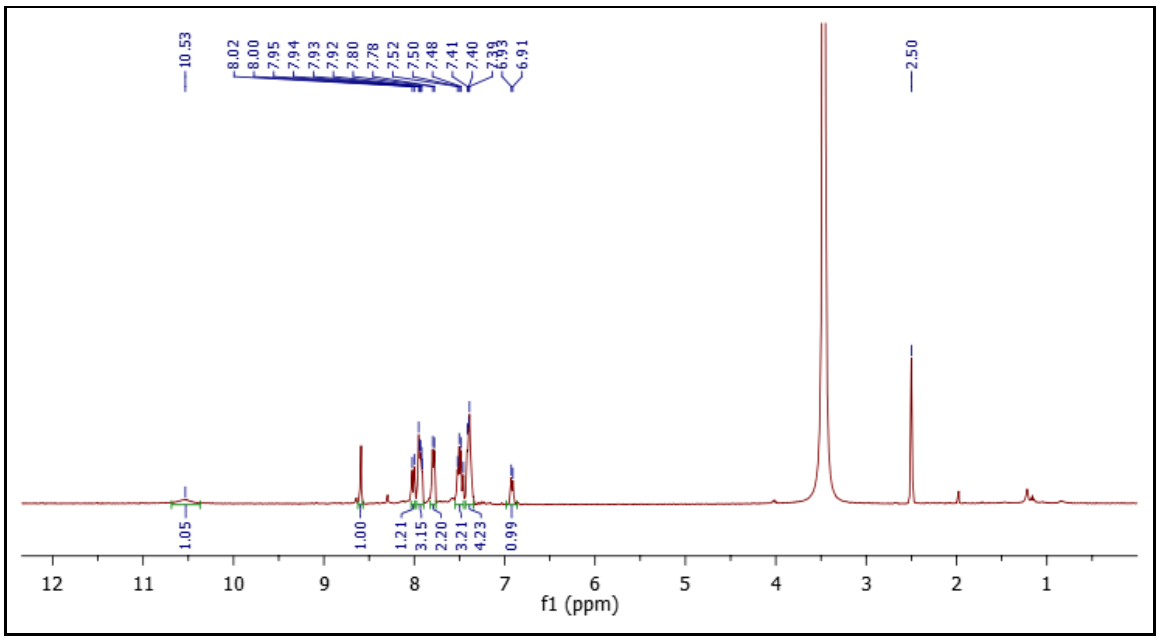
^{13}C NMR (150 MHz, $CDCl_3$)



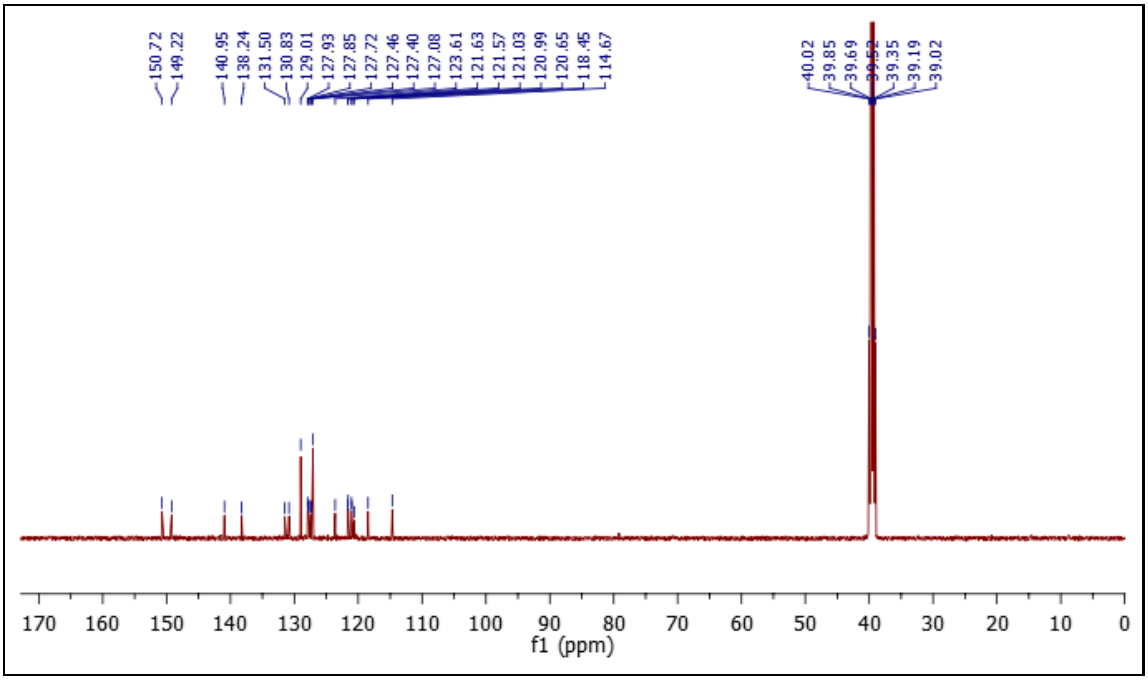


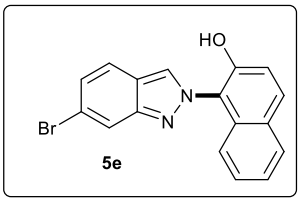
5d

^{1}H NMR (400 MHz, DMSO-D$_6$)

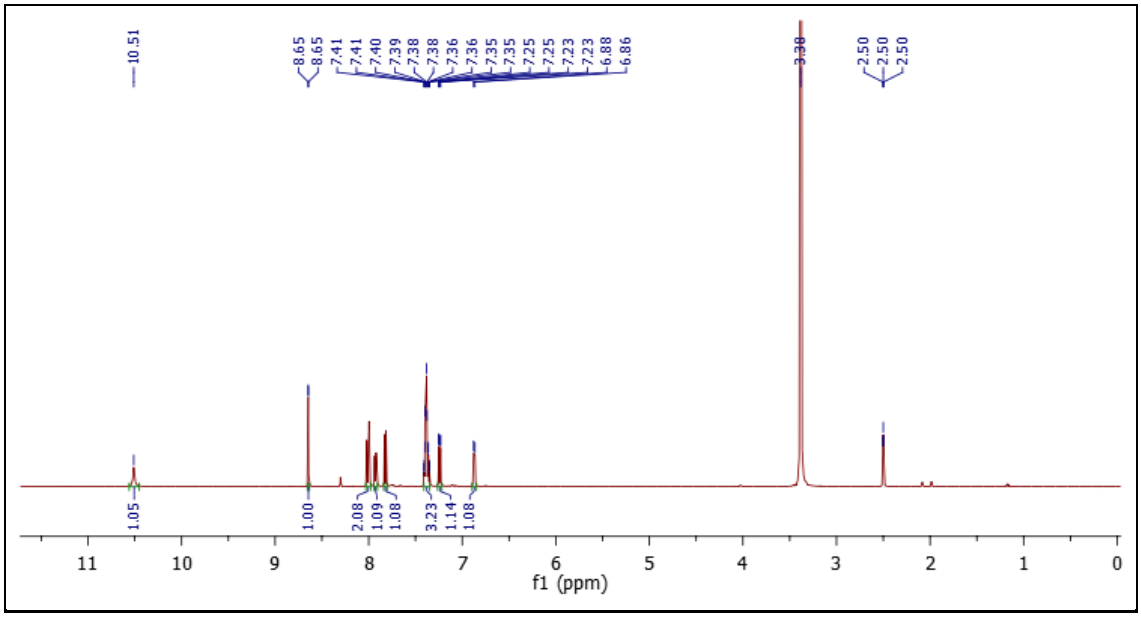


^{13}C NMR (125 MHz, DMSO-D$_6$)

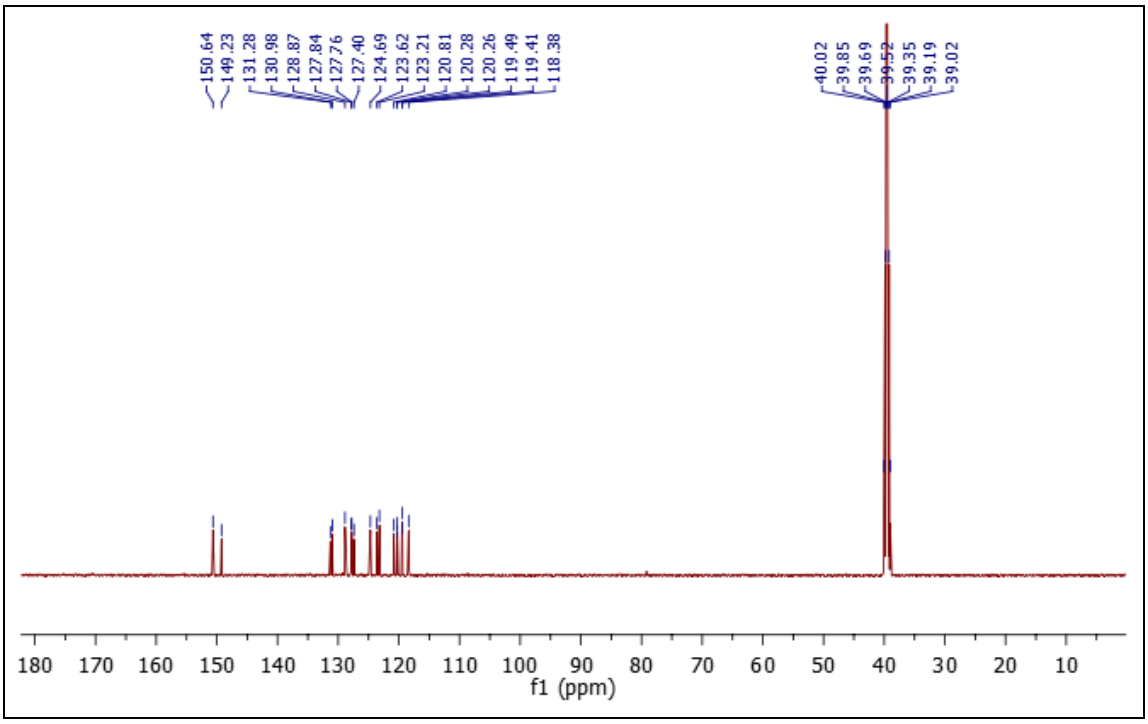


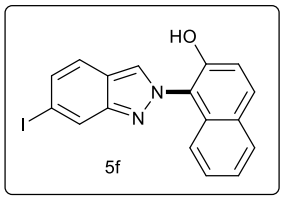


^{1}H NMR (500 MHz, DMSO-D$_6$)

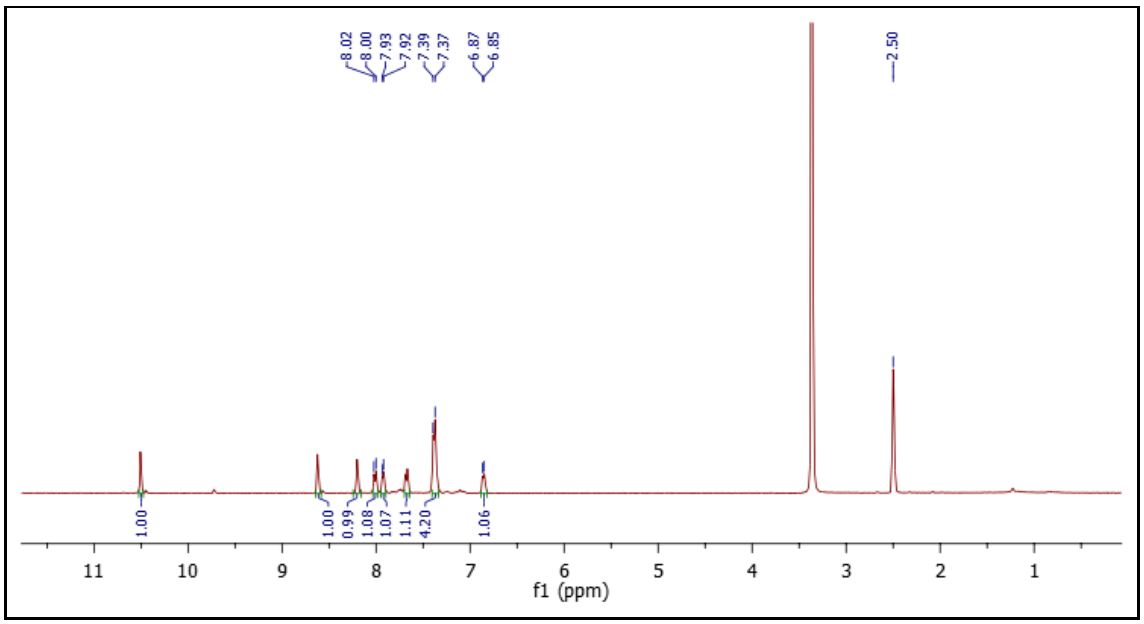


^{13}C NMR (125 MHz, DMSO-D$_6$)

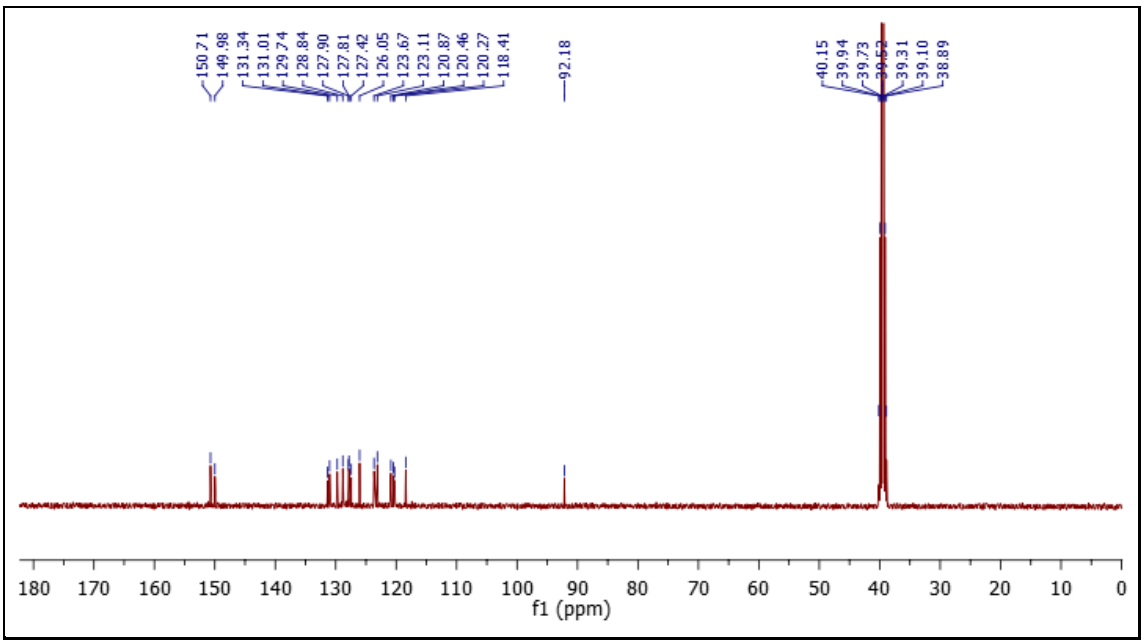


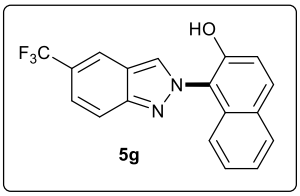


^{1}H NMR (400 MHz, DMSO-D$_6$)



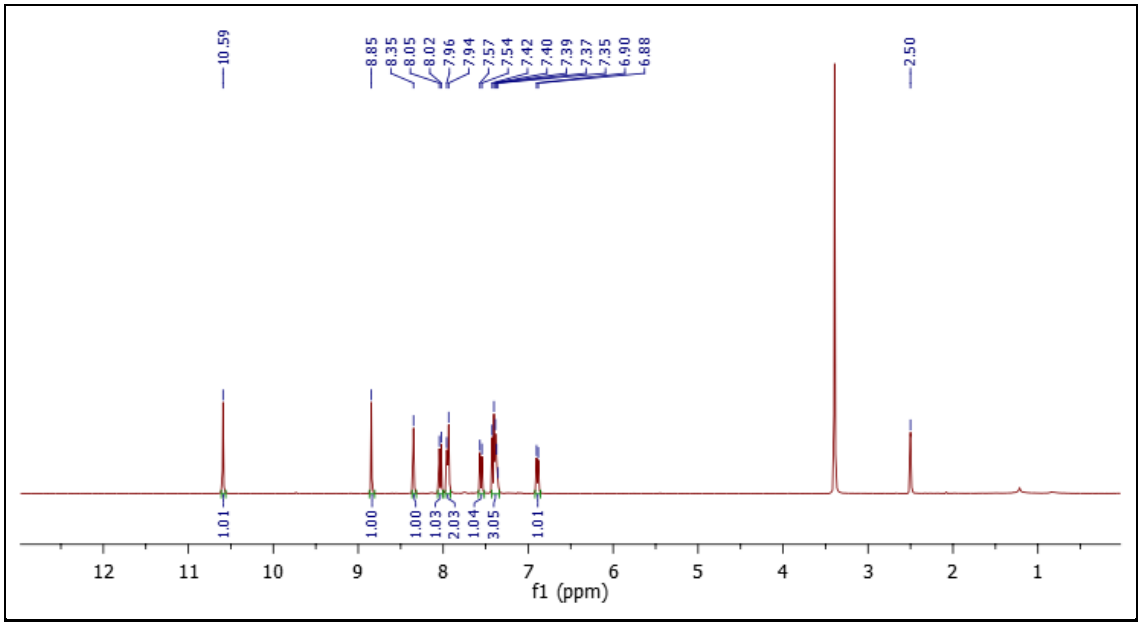
^{13}C NMR (100 MHz, DMSO-D$_6$)



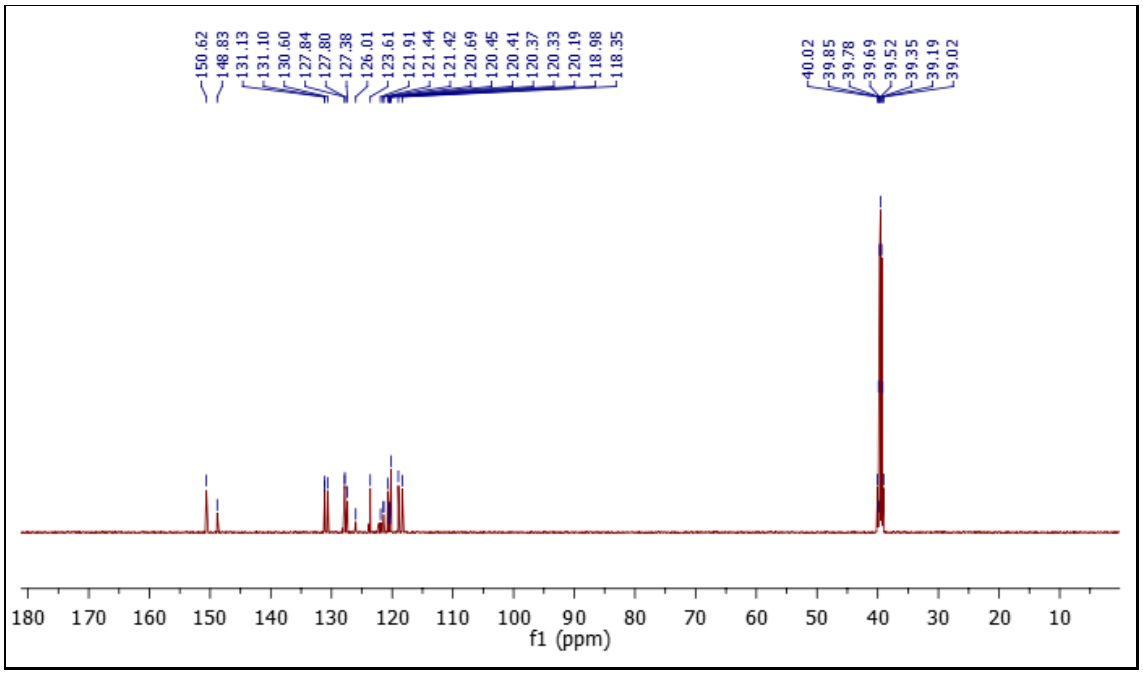


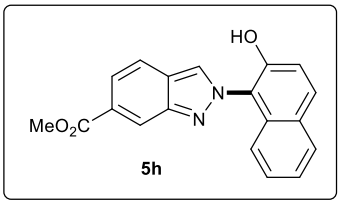
5g

^{1}H NMR (400 MHz, DMSO-D$_6$)



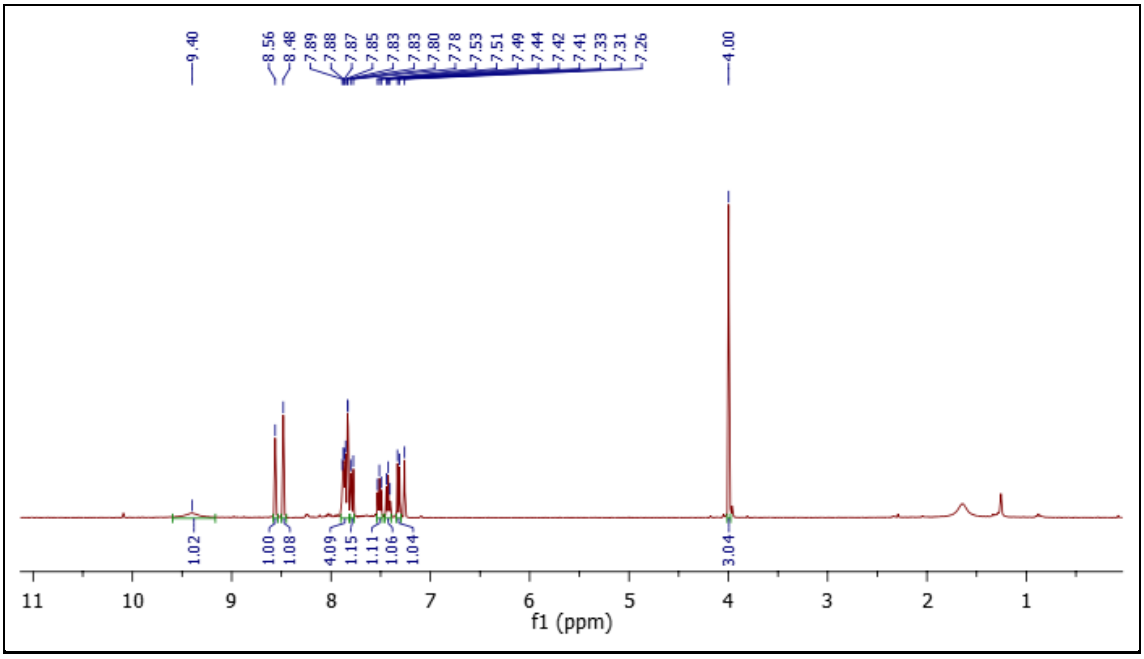
^{13}C NMR (125 MHz, DMSO-D$_6$)



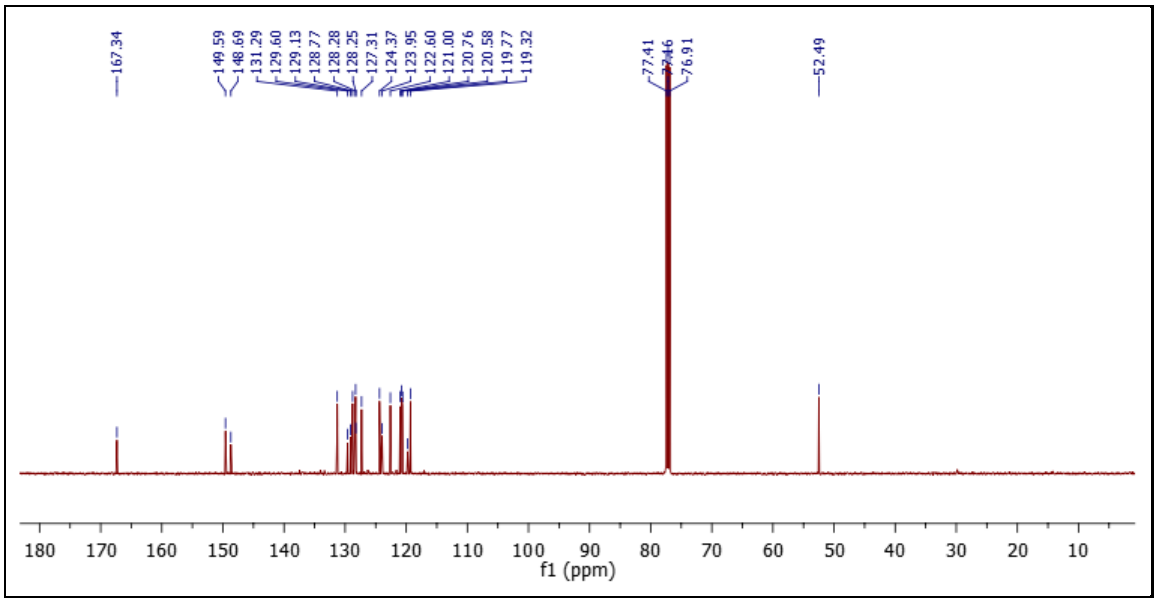


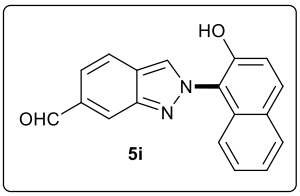
5h

^{1}H NMR (400 MHz, $CDCl_3$)



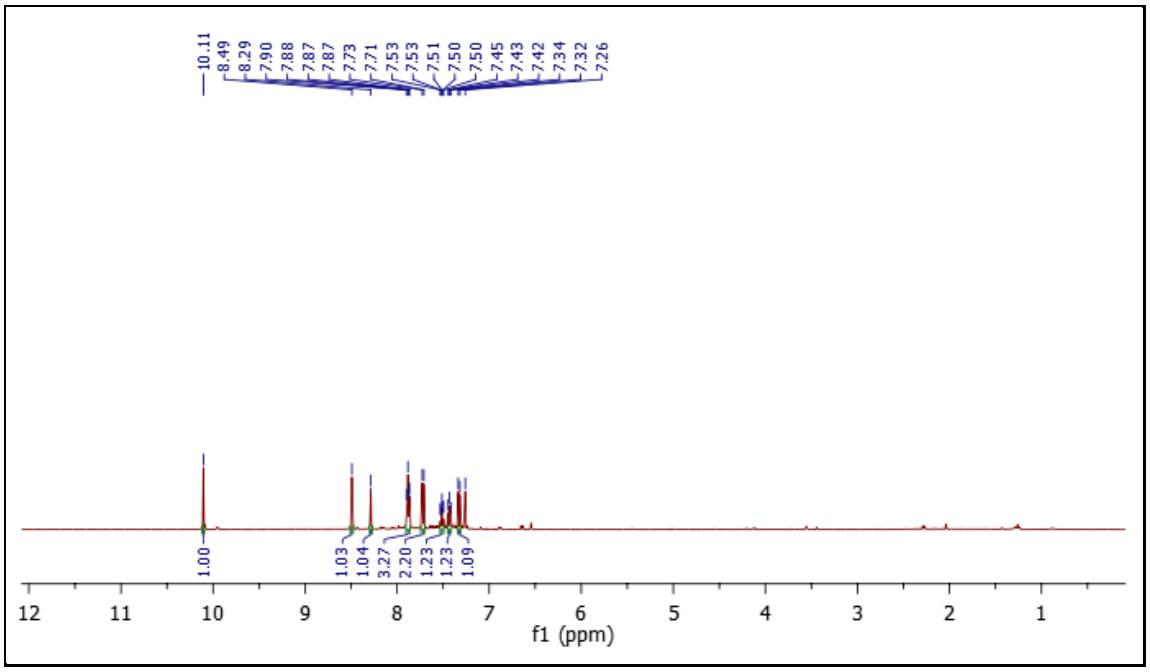
^{13}C NMR (125 MHz, $CDCl_3$)



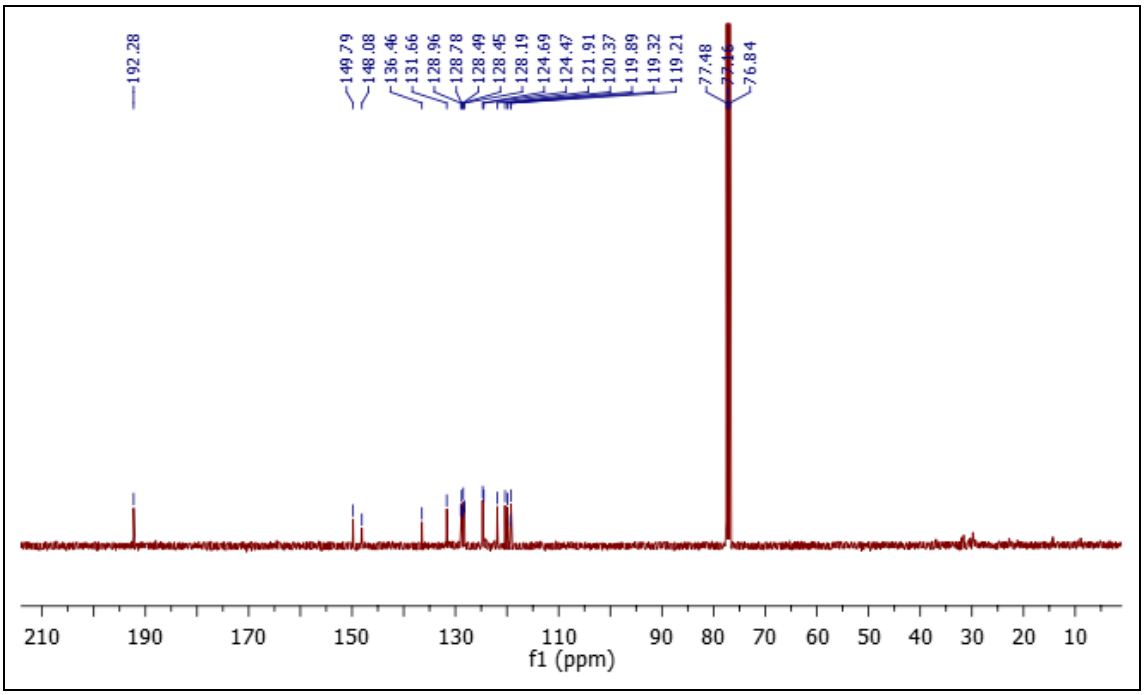


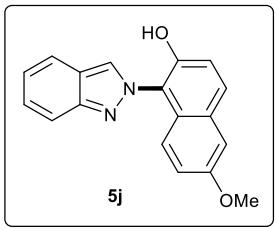
5i

^{1}H NMR (500 MHz, $CDCl_3$)



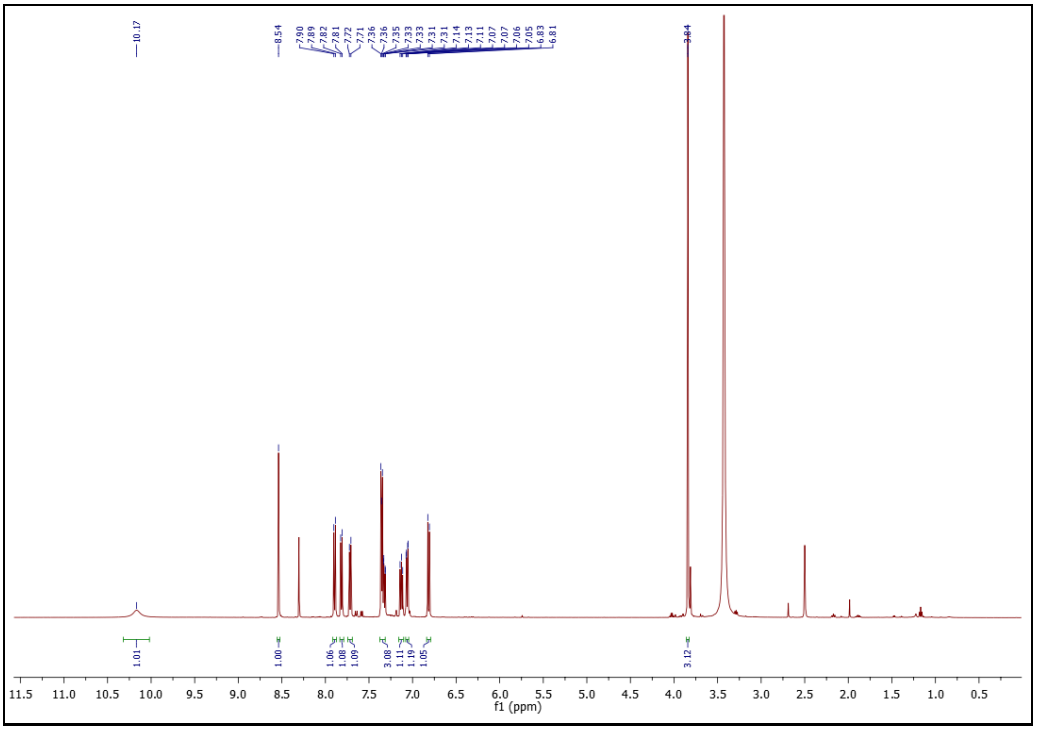
^{13}C NMR (100 MHz, $CDCl_3$)



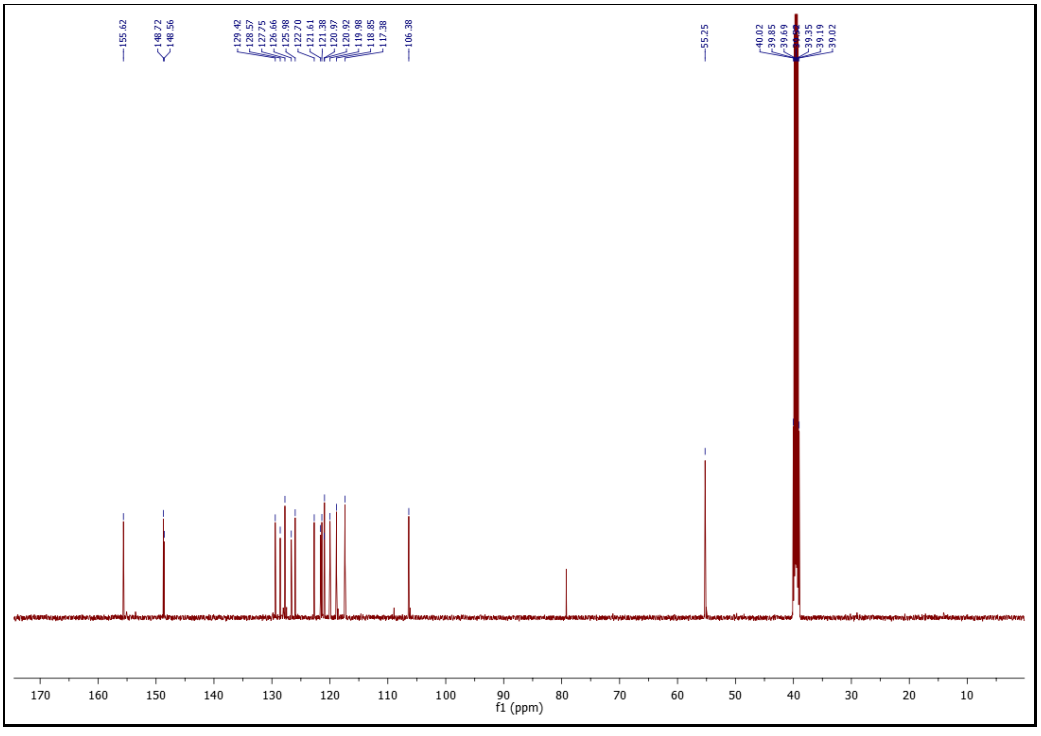


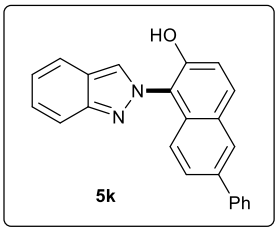
5j

^{1}H NMR (500 MHz, DMSO-D$_6$)

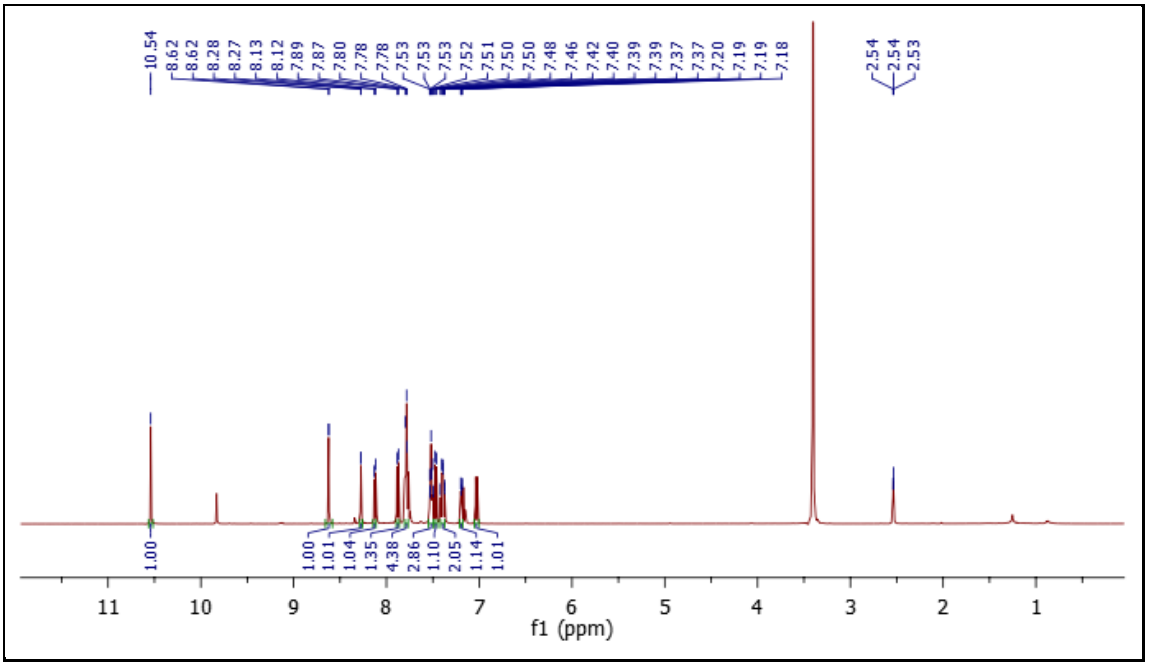


^{13}C NMR (125 MHz, DMSO-D$_6$)

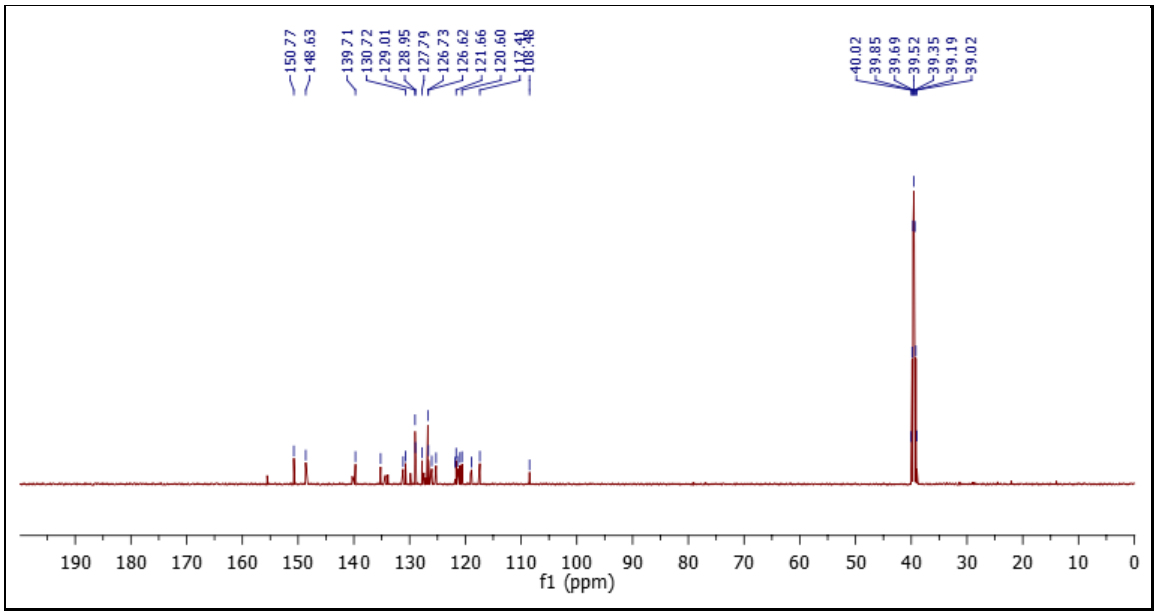


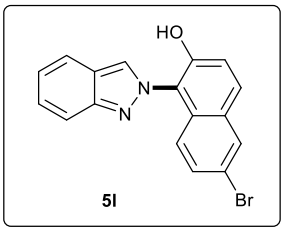


^{1}H NMR (500 MHz, DMSO-D$_6$)

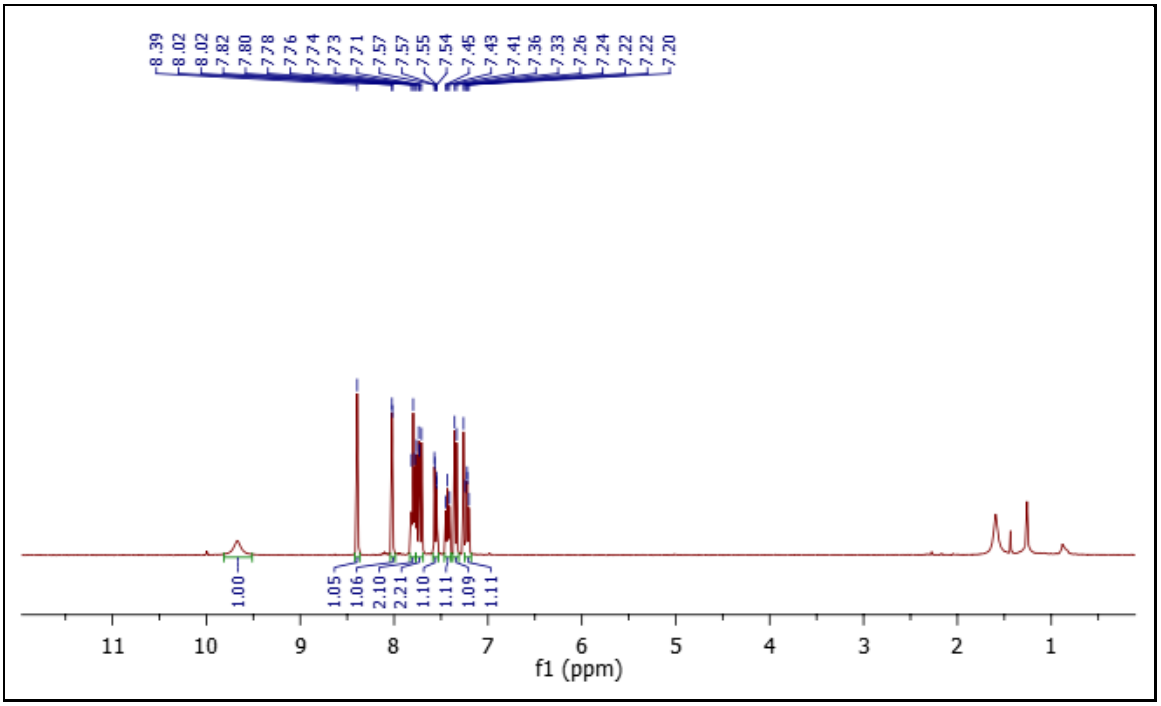


^{13}C NMR (125 MHz, DMSO-D$_6$)

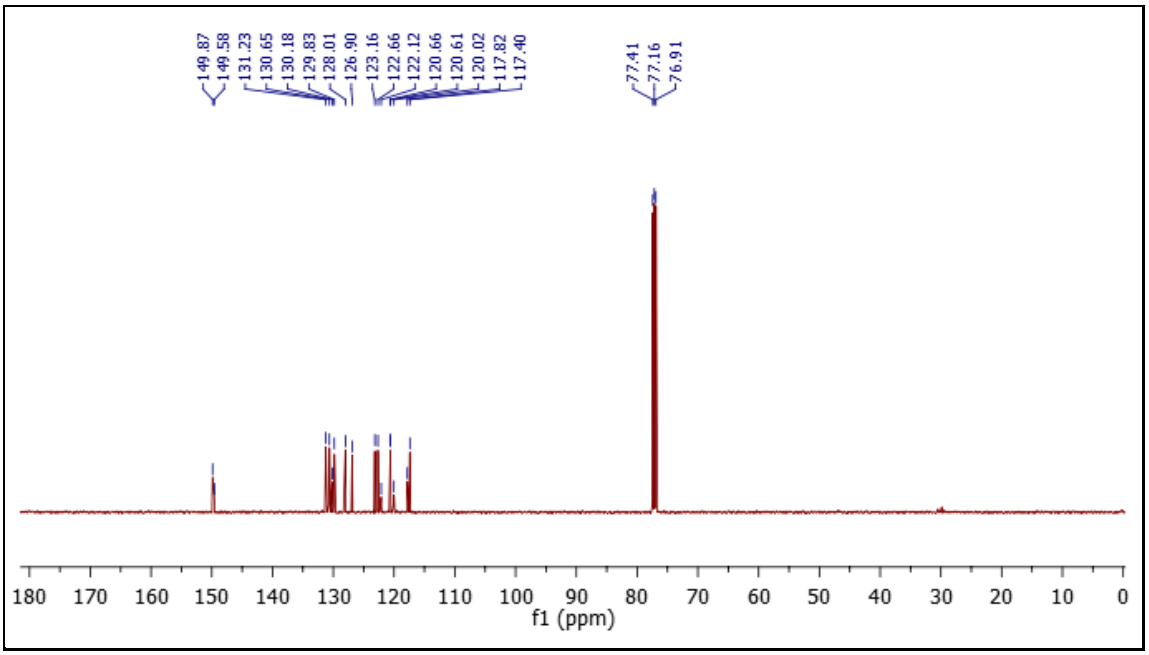


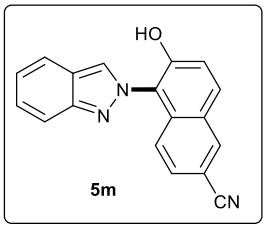


^{1}H NMR (400 MHz, $CDCl_3$)

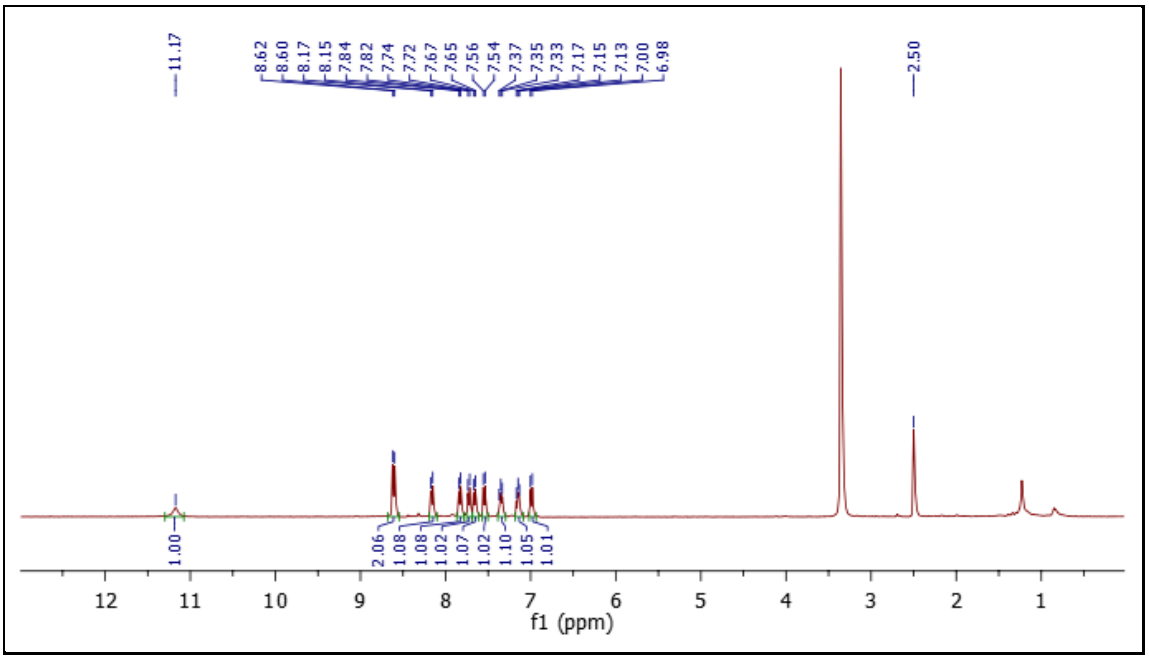


^{13}C NMR (125 MHz, $CDCl_3$)

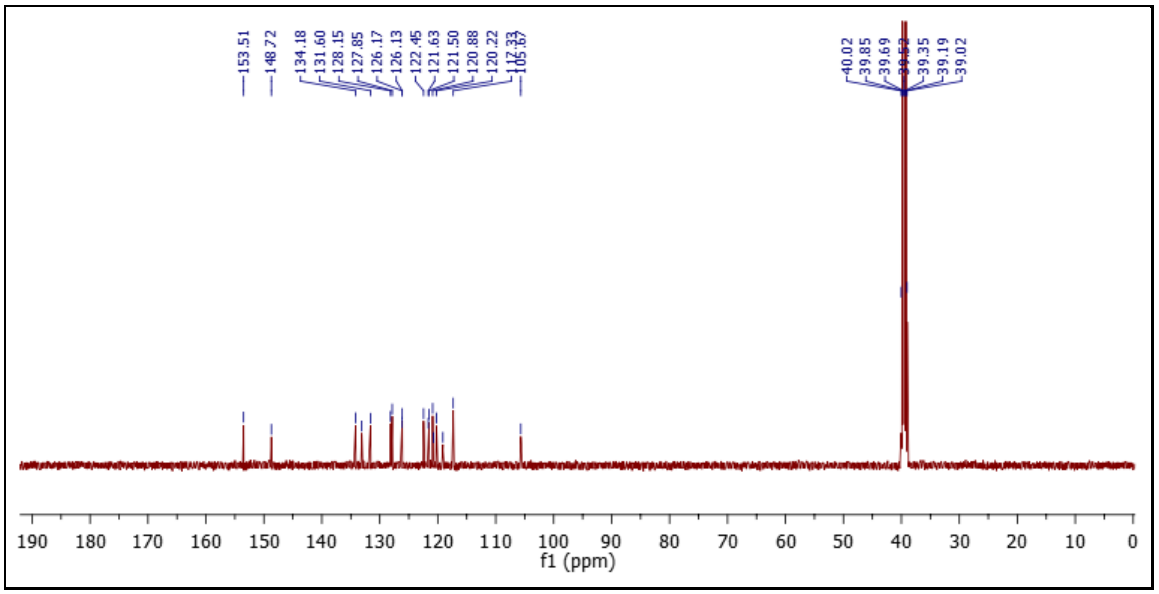


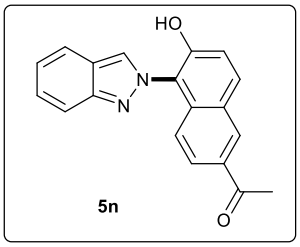


^{1}H NMR (400 MHz, DMSO-D$_6$)



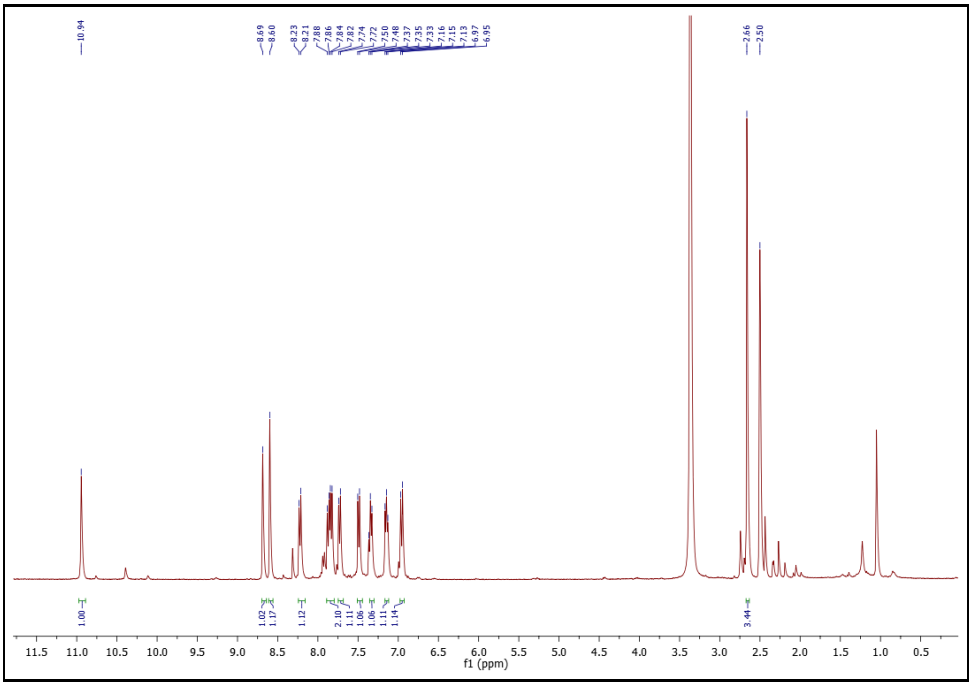
^{13}C NMR (125 MHz, DMSO-D$_6$)



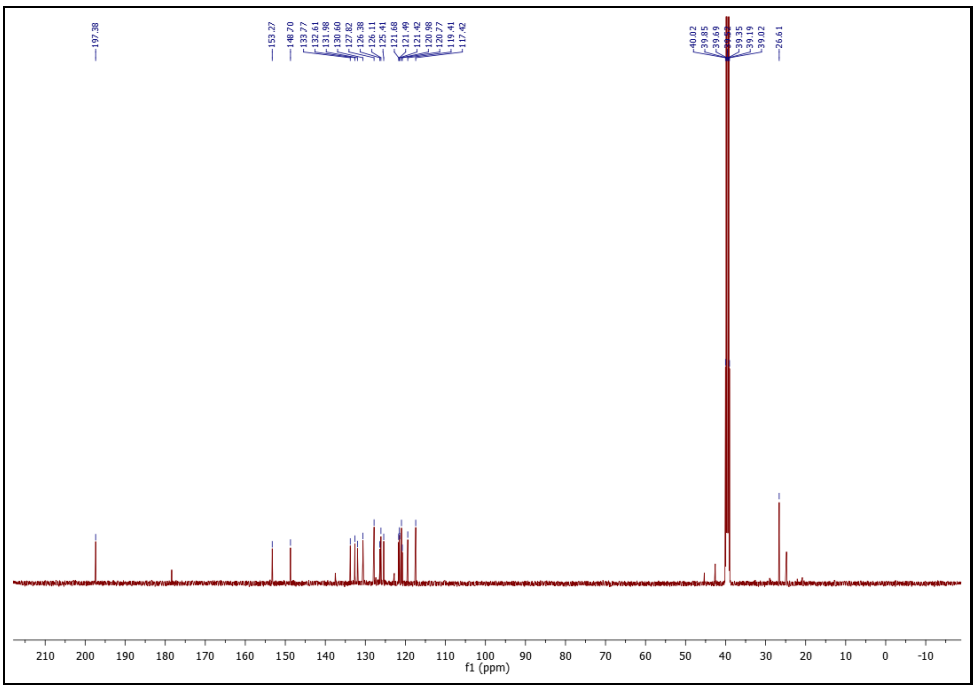


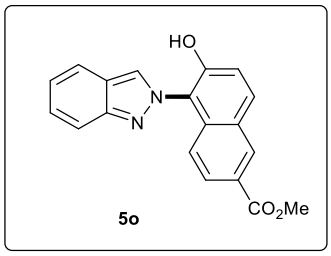
5n

^{1}H NMR (400 MHz, DMSO-D$_6$)



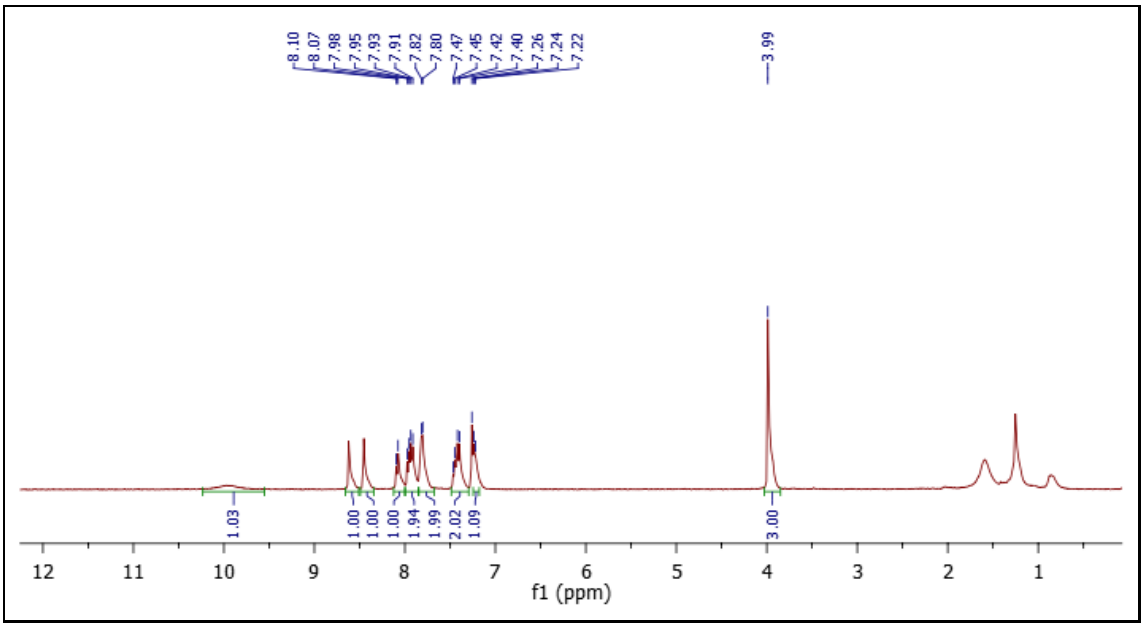
^{13}C NMR (125 MHz, DMSO-D$_6$)



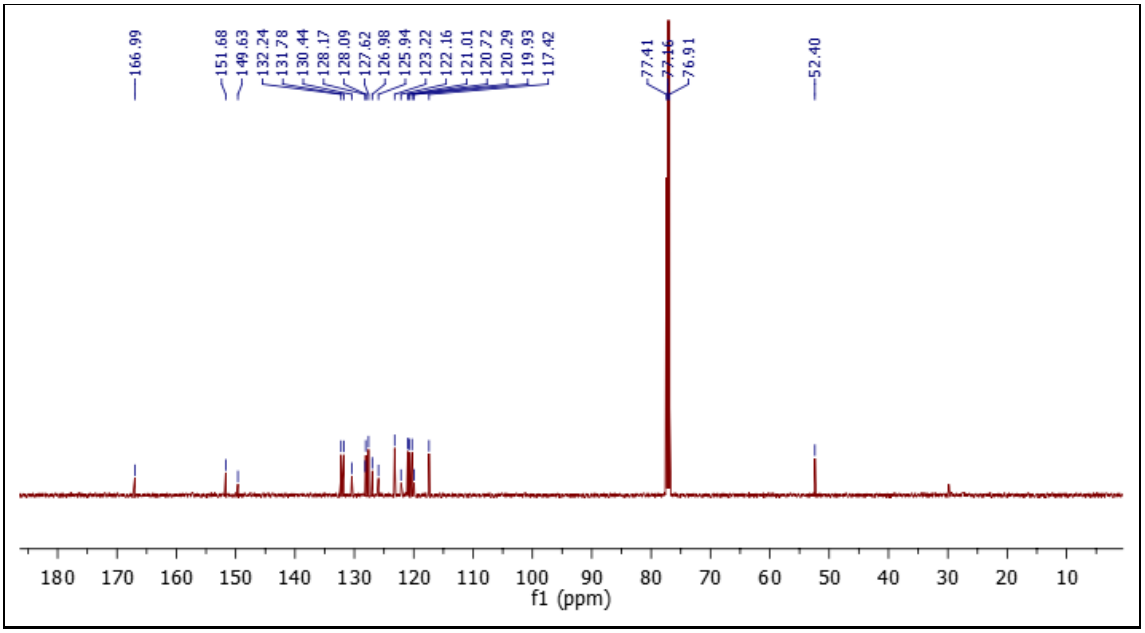


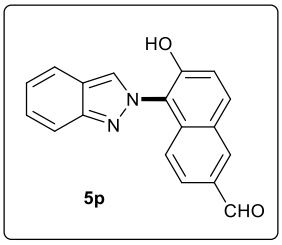
5o

^{1}H NMR (400 MHz, $CDCl_3$)

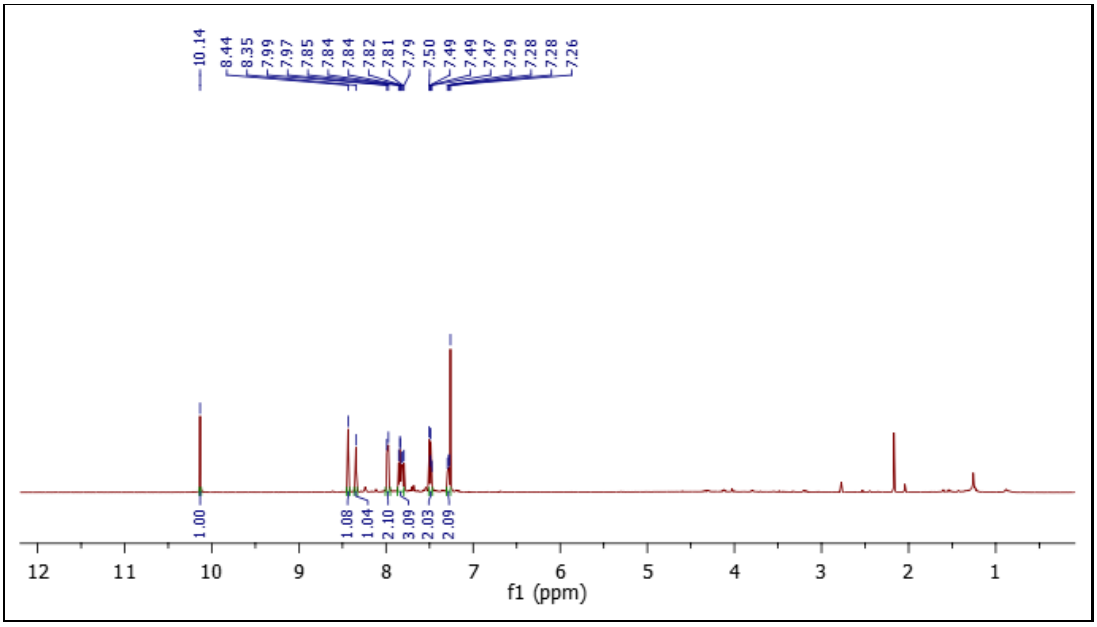


^{13}C NMR (125 MHz, $CDCl_3$)

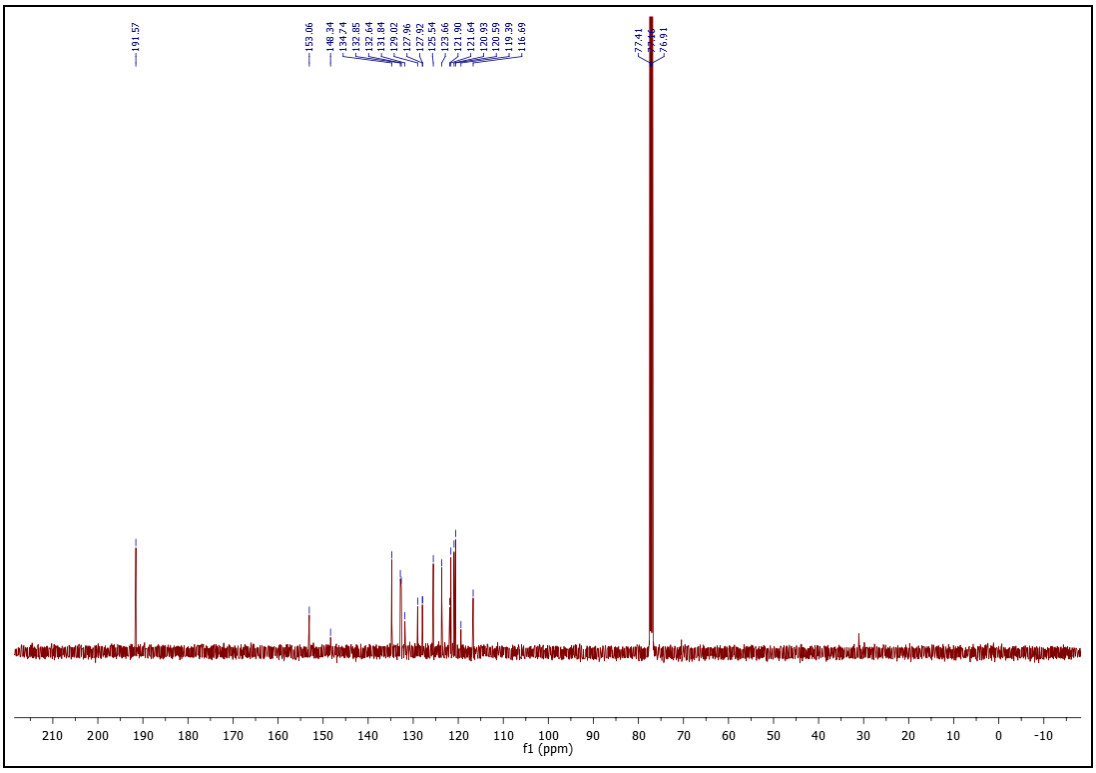


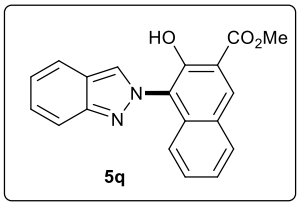


^{1}H NMR (500 MHz, $CDCl_3$)

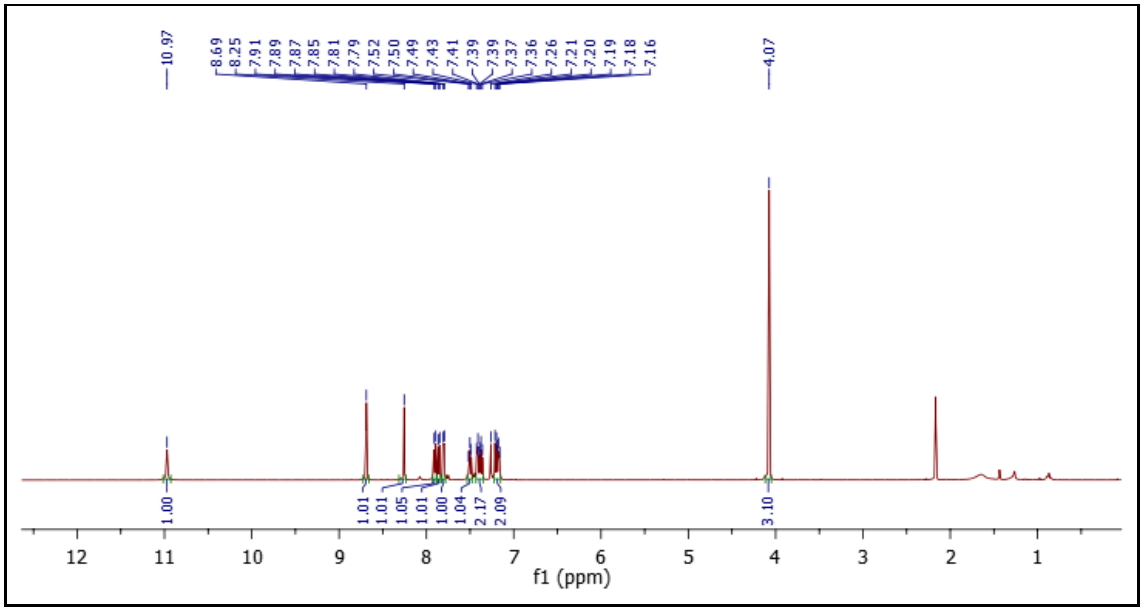


^{13}C NMR (125 MHz, $CDCl_3$)

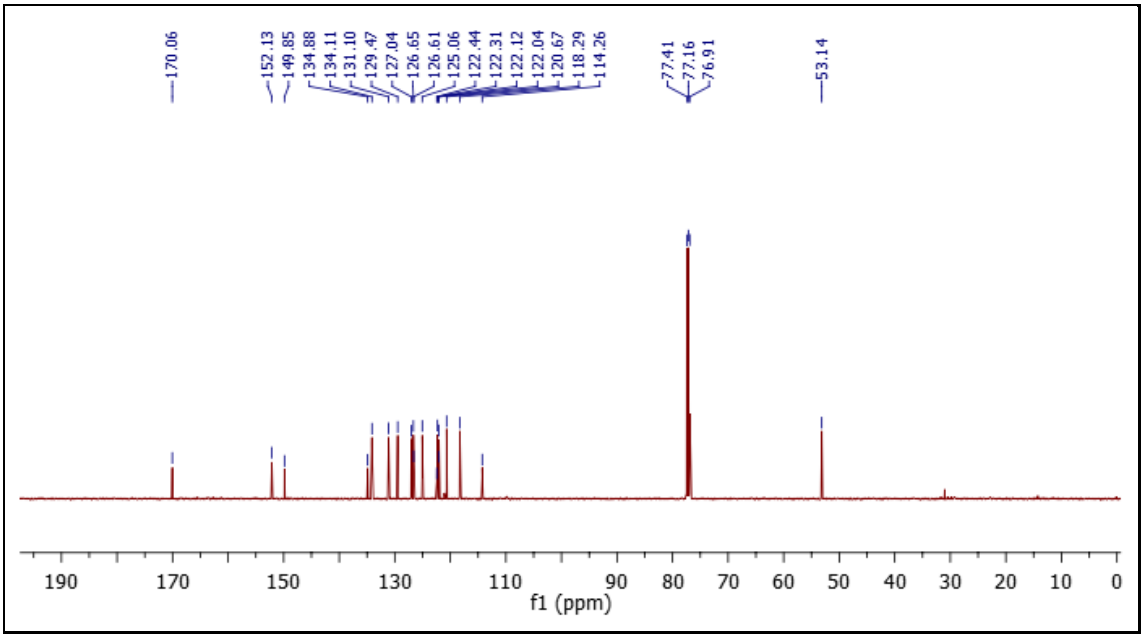


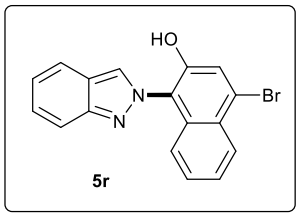


^{1}H NMR (500 MHz, $CDCl_3$)



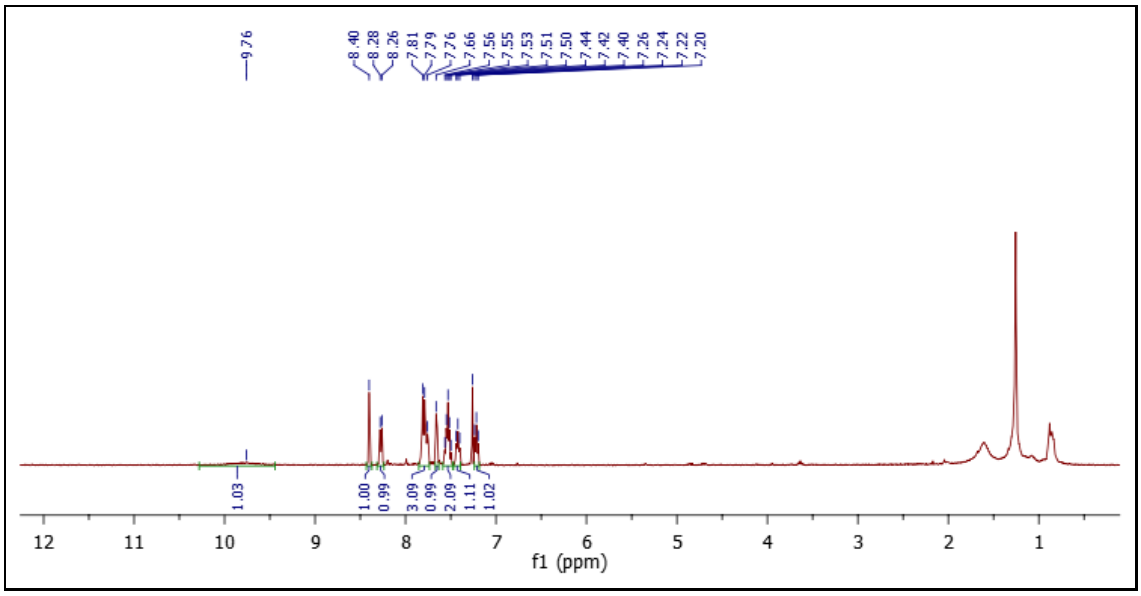
^{13}C NMR (125 MHz, $CDCl_3$)



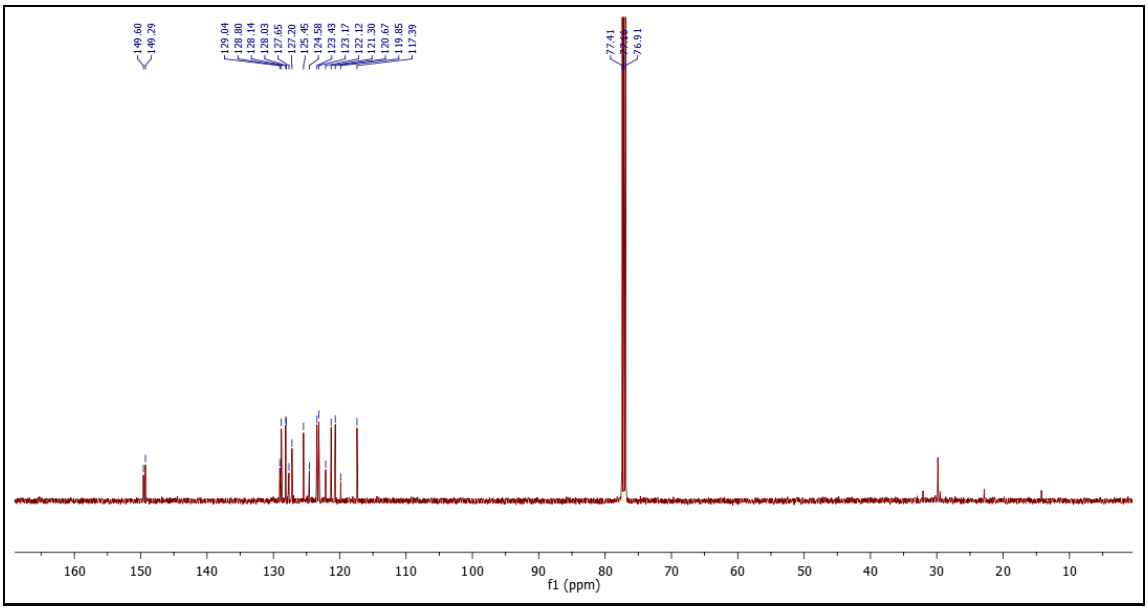


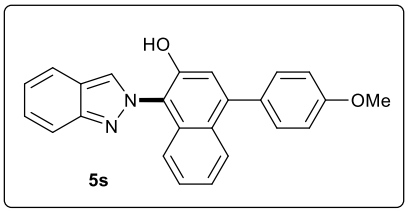
5r

^{1}H NMR (400 MHz, $CDCl_3$)

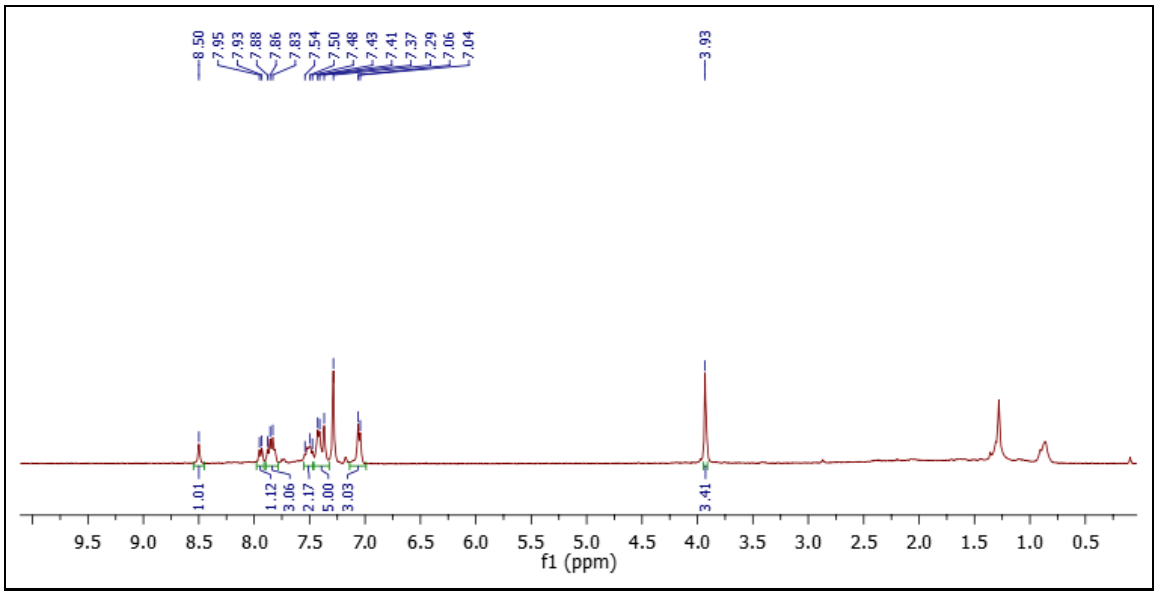


^{13}C NMR (125 MHz, $CDCl_3$)

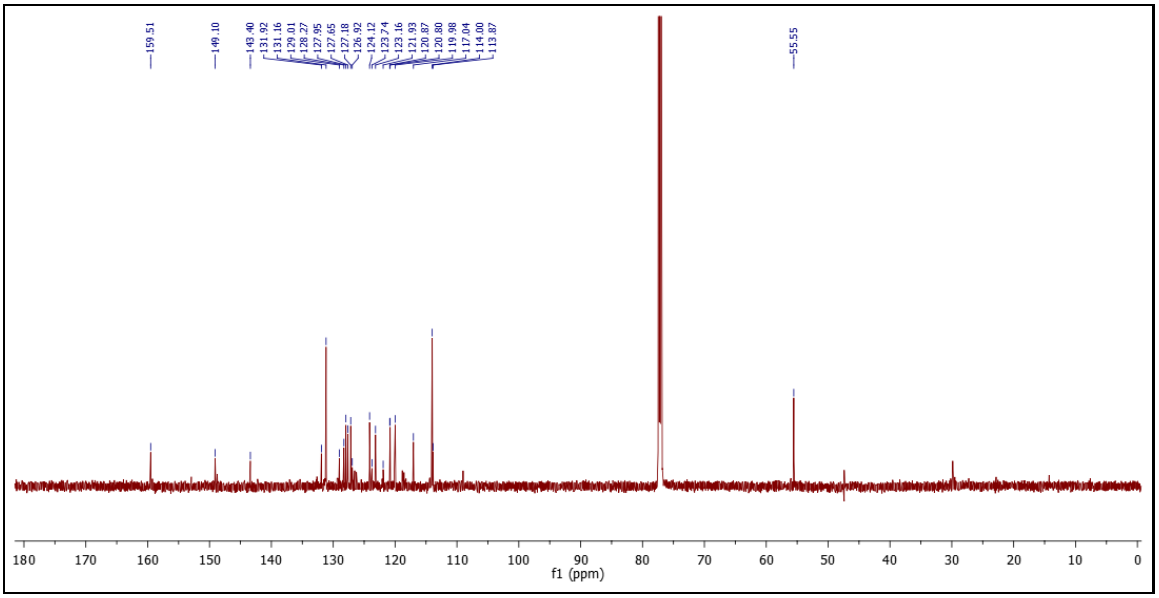


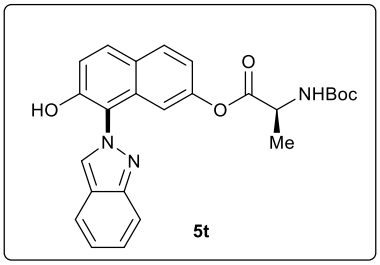


^{1}H NMR (400 MHz, $CDCl_3$)

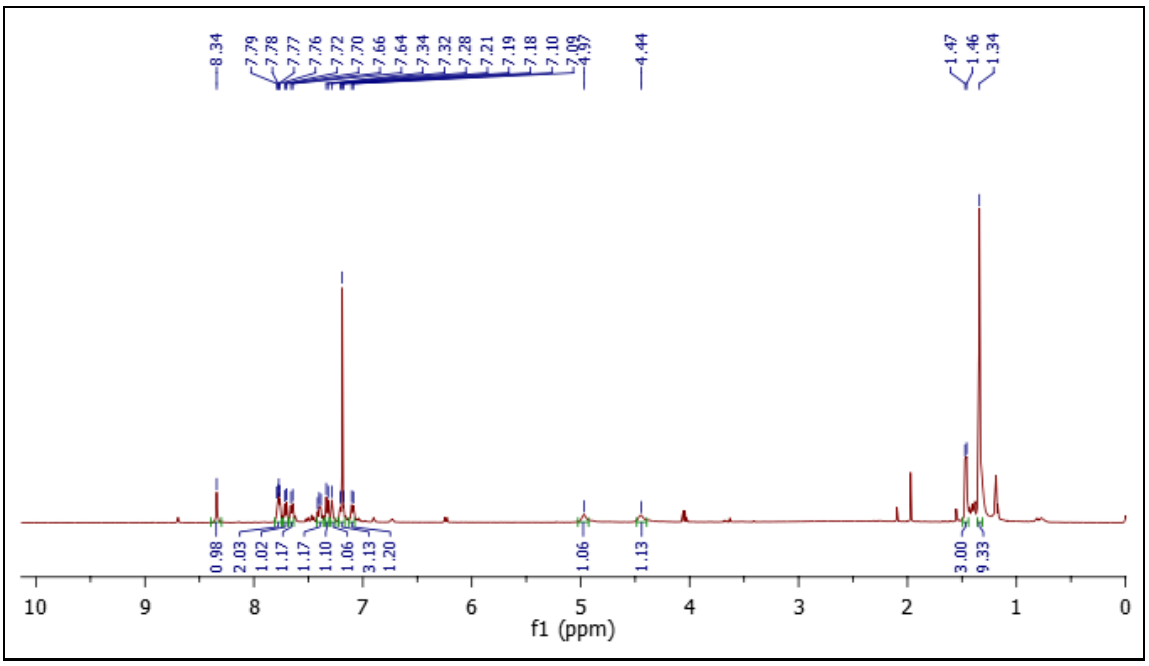


^{13}C NMR (150 MHz, $CDCl_3$)

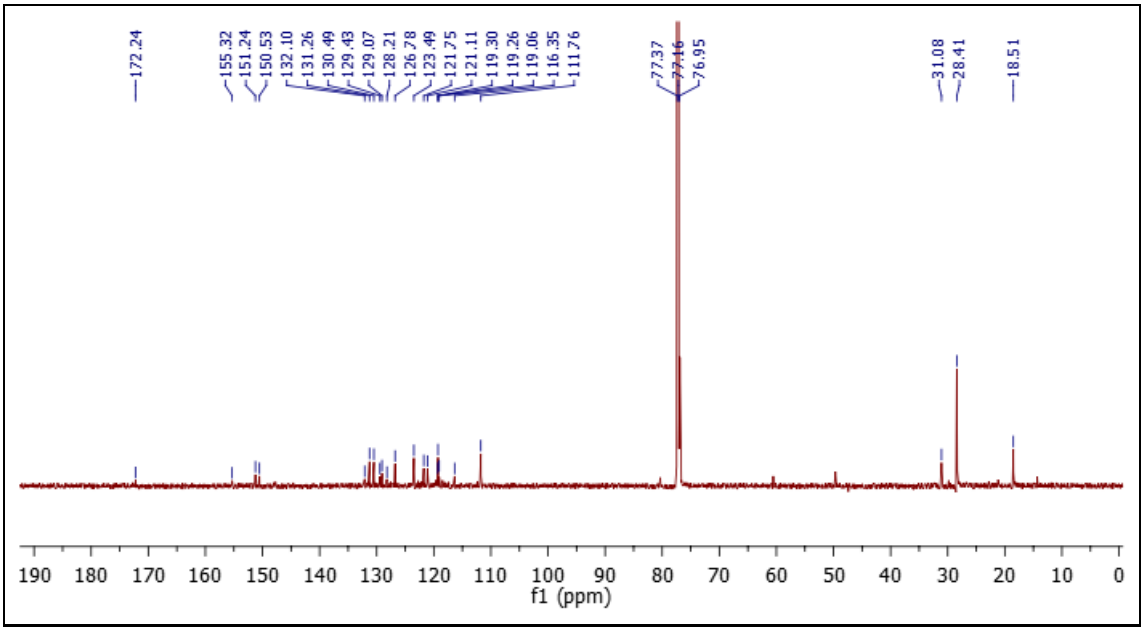


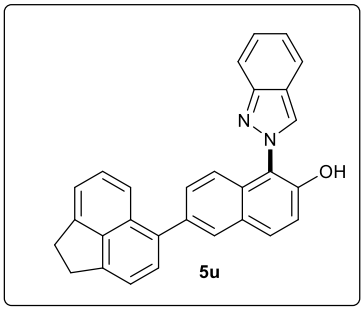


^{1}H NMR (500 MHz, $CDCl_3$)

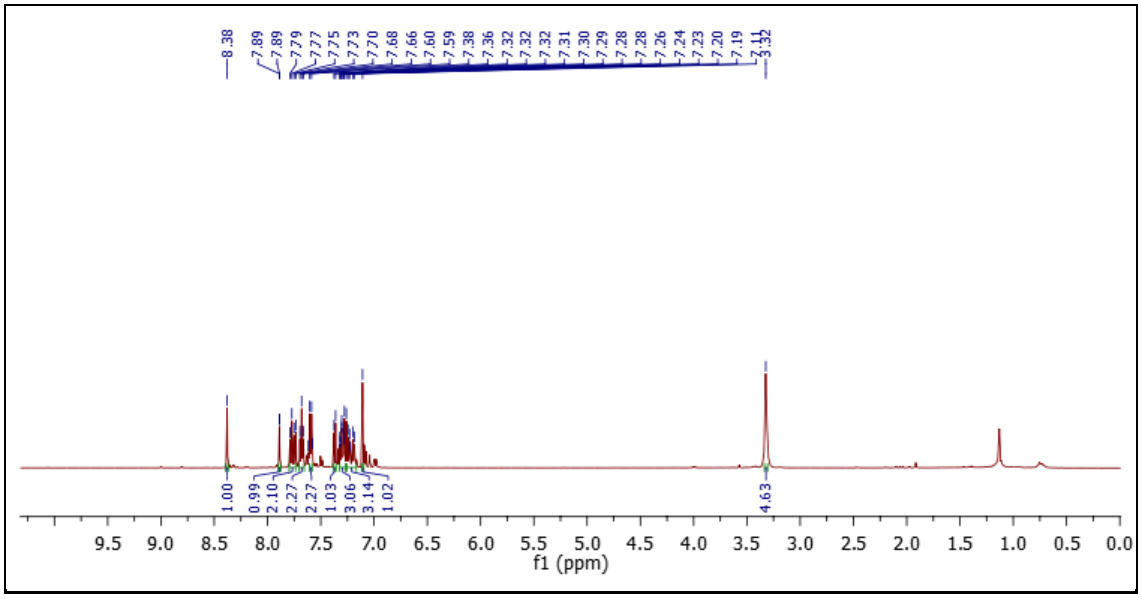


^{13}C NMR (150 MHz, $CDCl_3$)

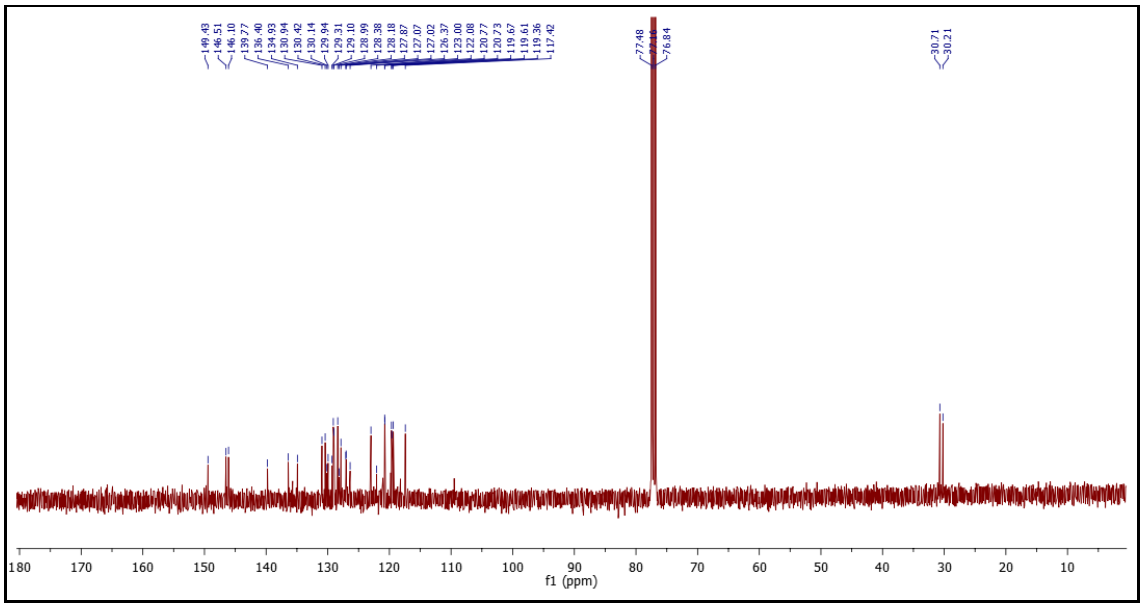


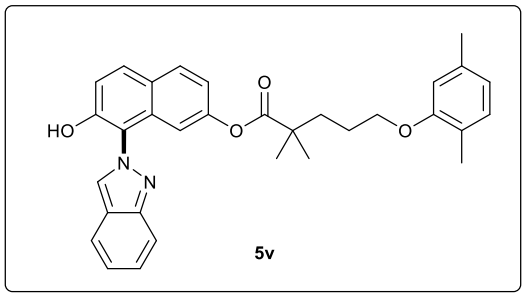


^{1}H NMR (500 MHz, $CDCl_3$)



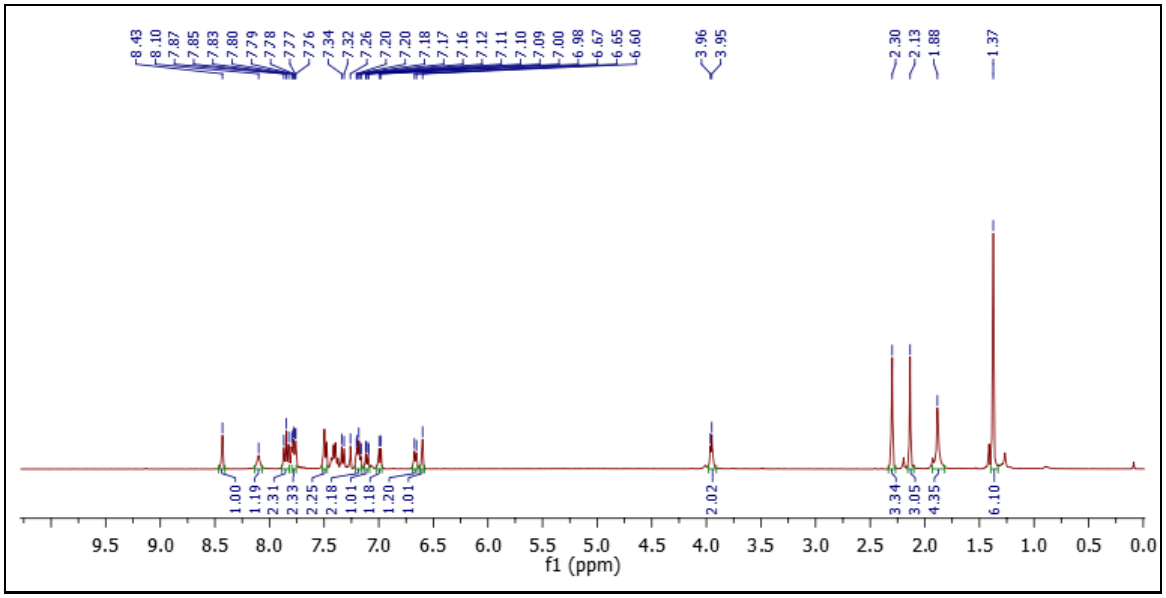
^{13}C NMR (100 MHz, $CDCl_3$)



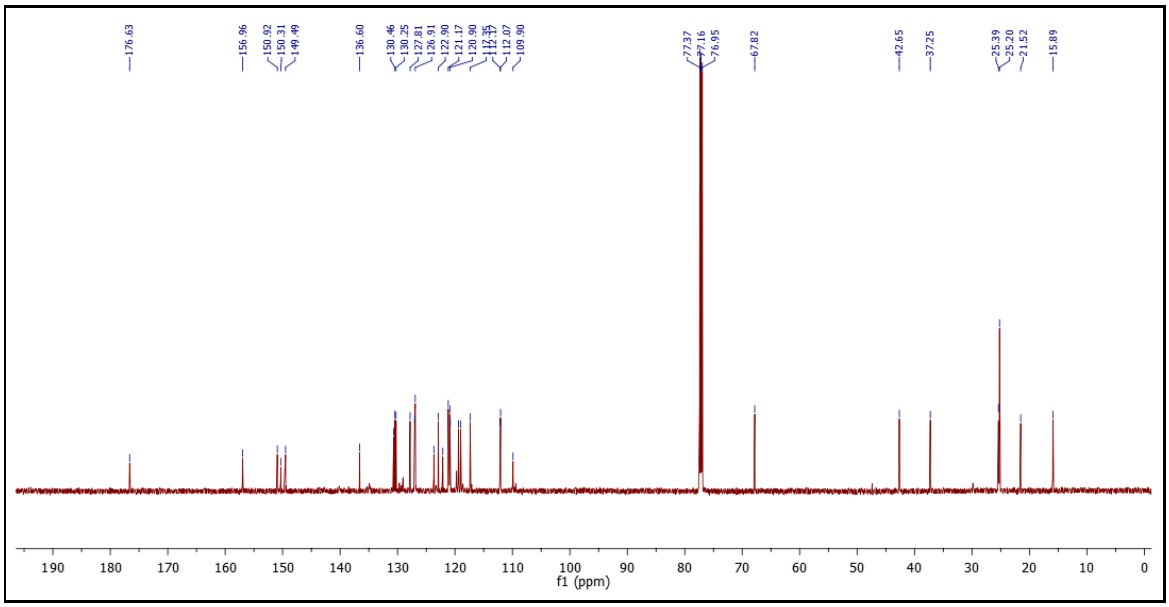


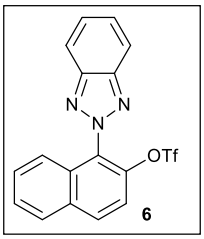
5v

^{1}H NMR (400 MHz, $CDCl_3$)

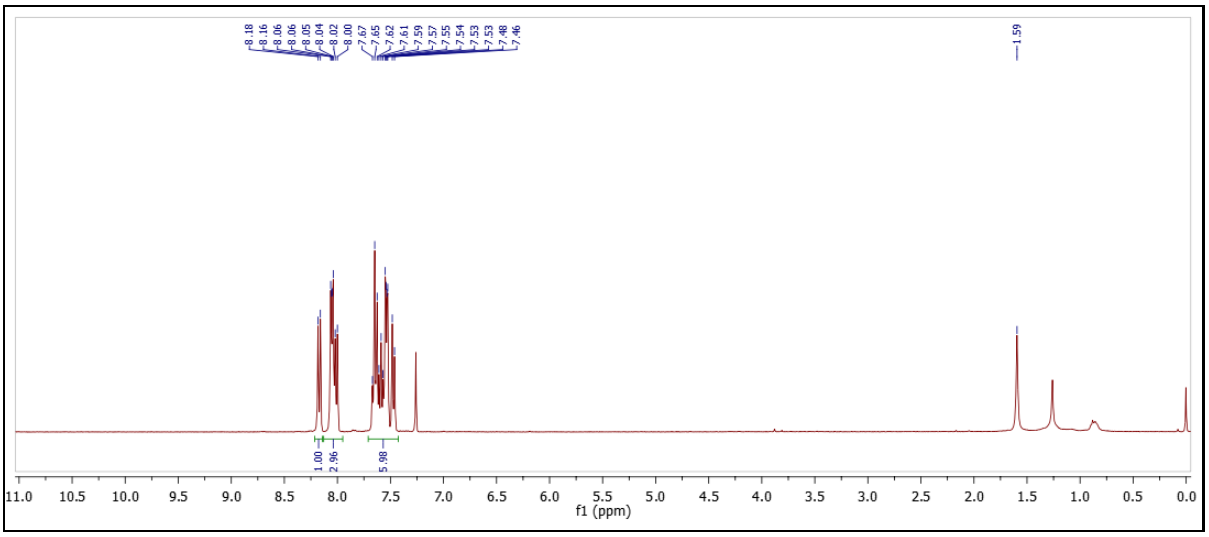


^{13}C NMR (150 MHz, $CDCl_3$)

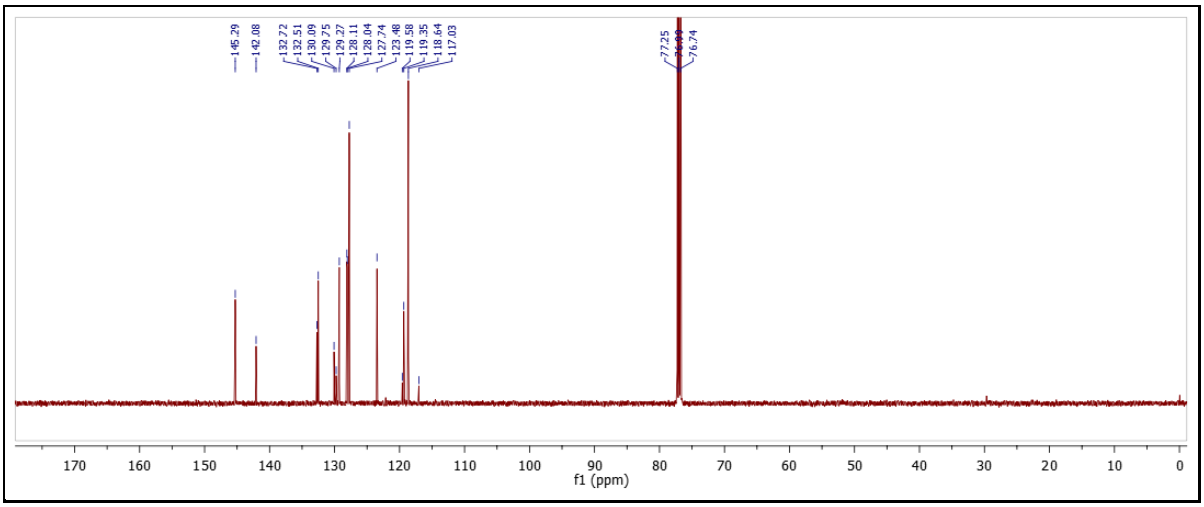




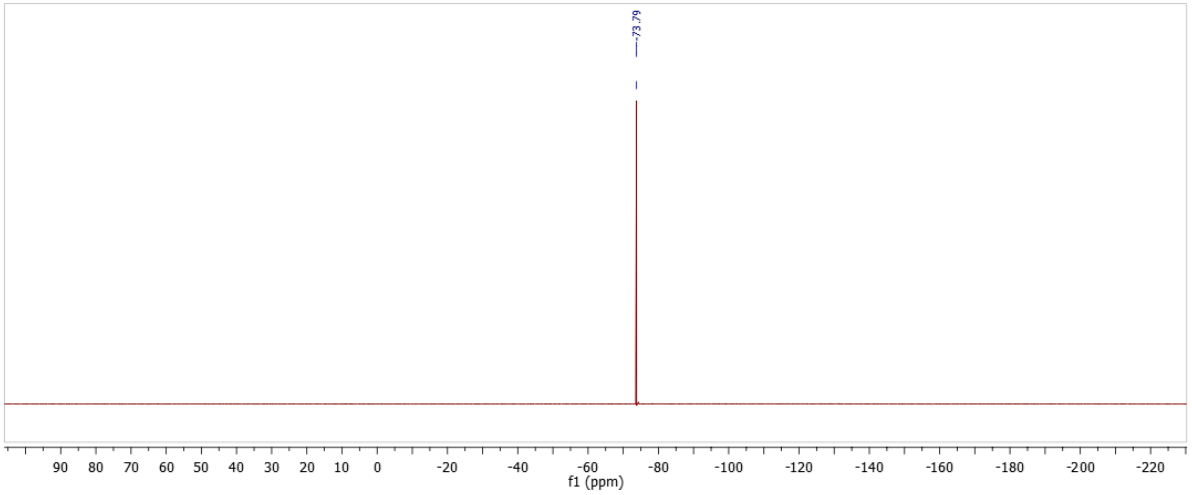
^{1}H NMR (400 MHz, $CDCl_3$)

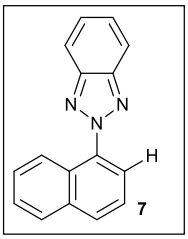


^{13}C NMR (125 MHz, $CDCl_3$)

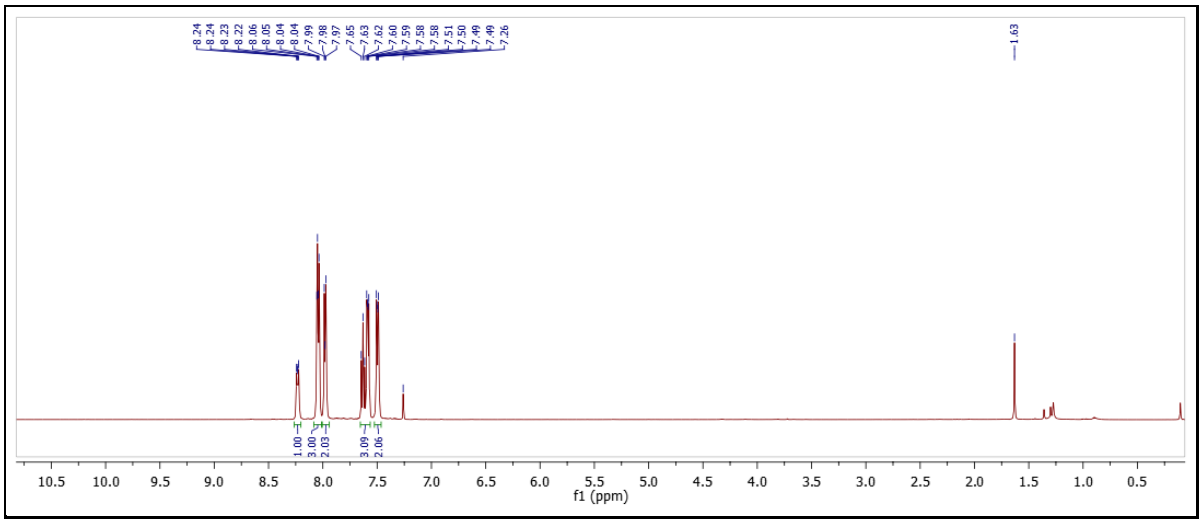


^{19}F NMR (470 MHz, $CDCl_3$)

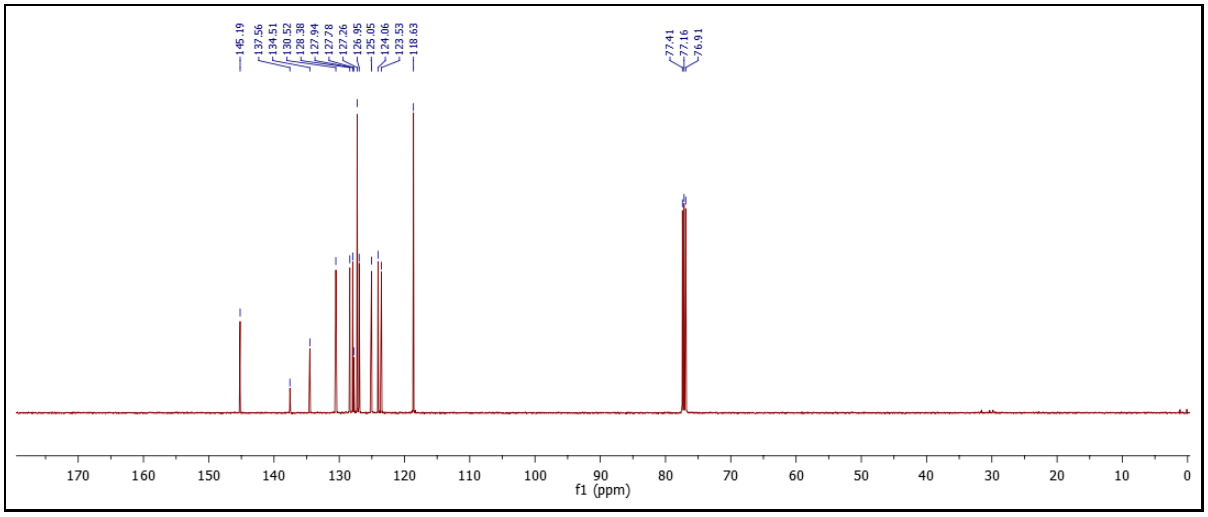


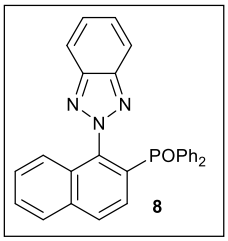


^{1}H NMR (500 MHz, $CDCl_3$)

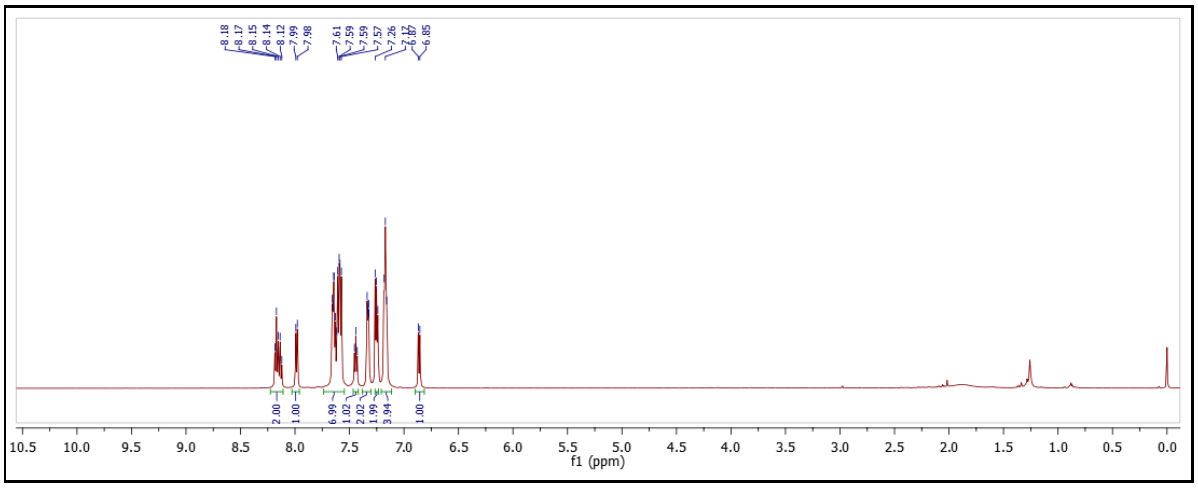


^{13}C NMR (125 MHz, $CDCl_3$)

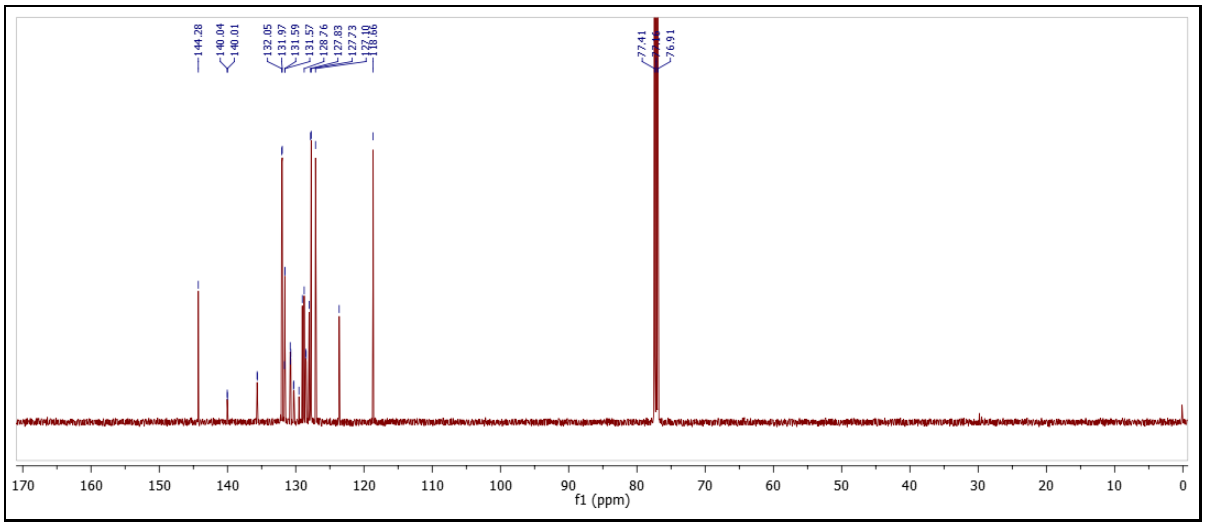


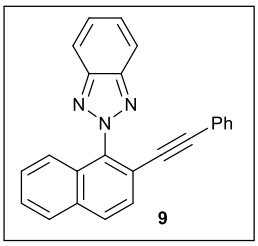


^{1}H NMR (600 MHz, $CDCl_3$)

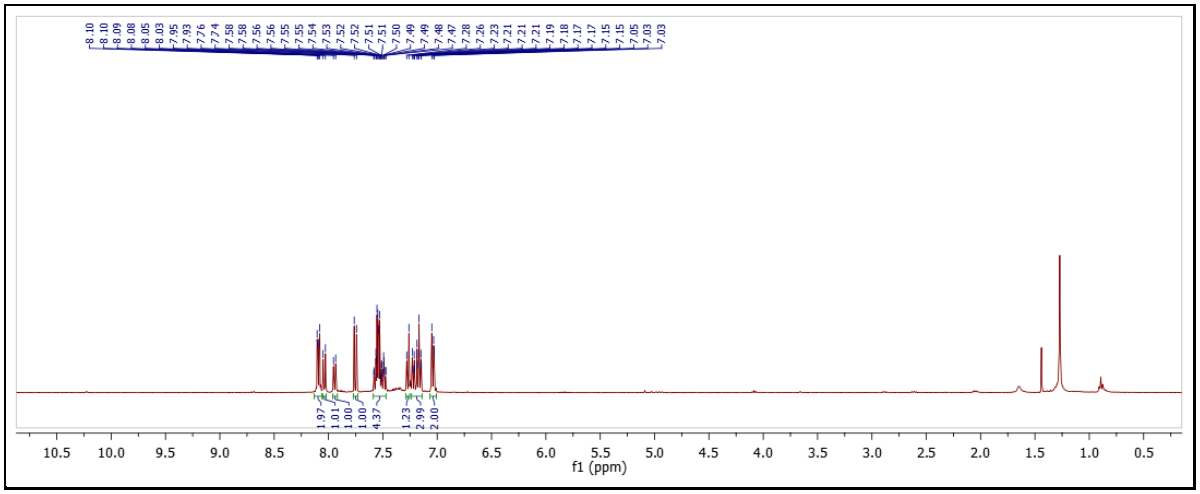


^{13}C NMR (125 MHz, $CDCl_3$)

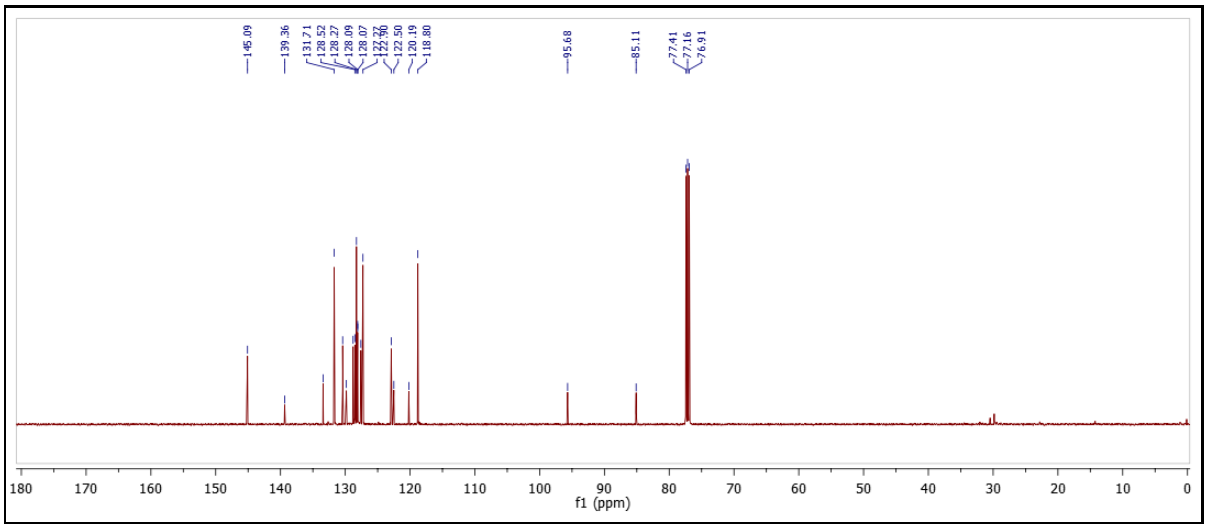


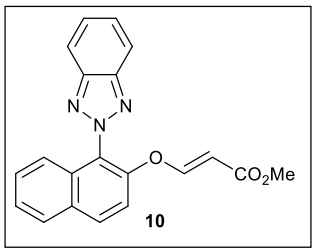


^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (125 MHz, $CDCl_3$)





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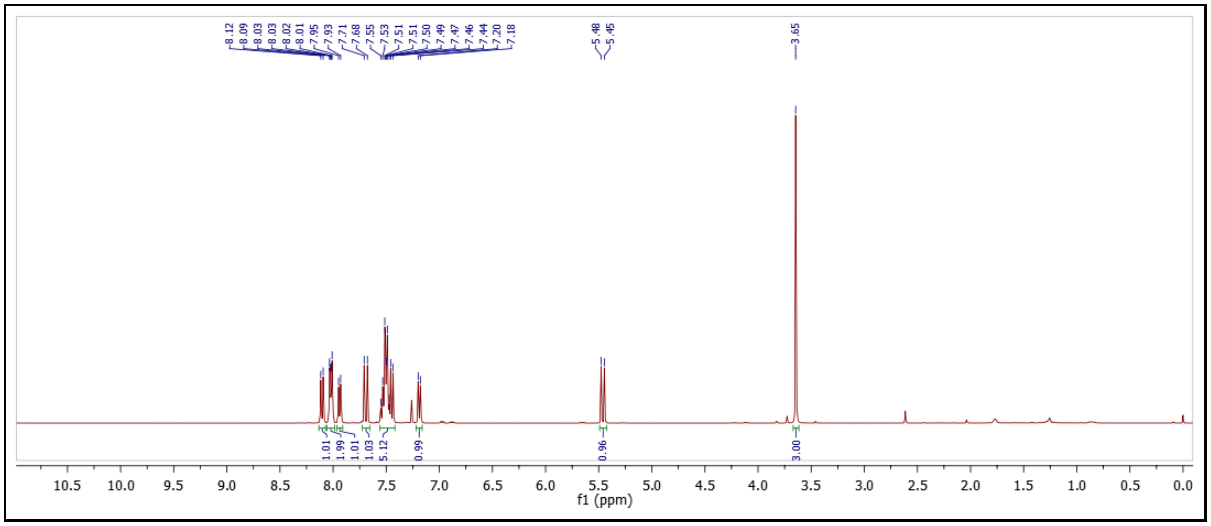
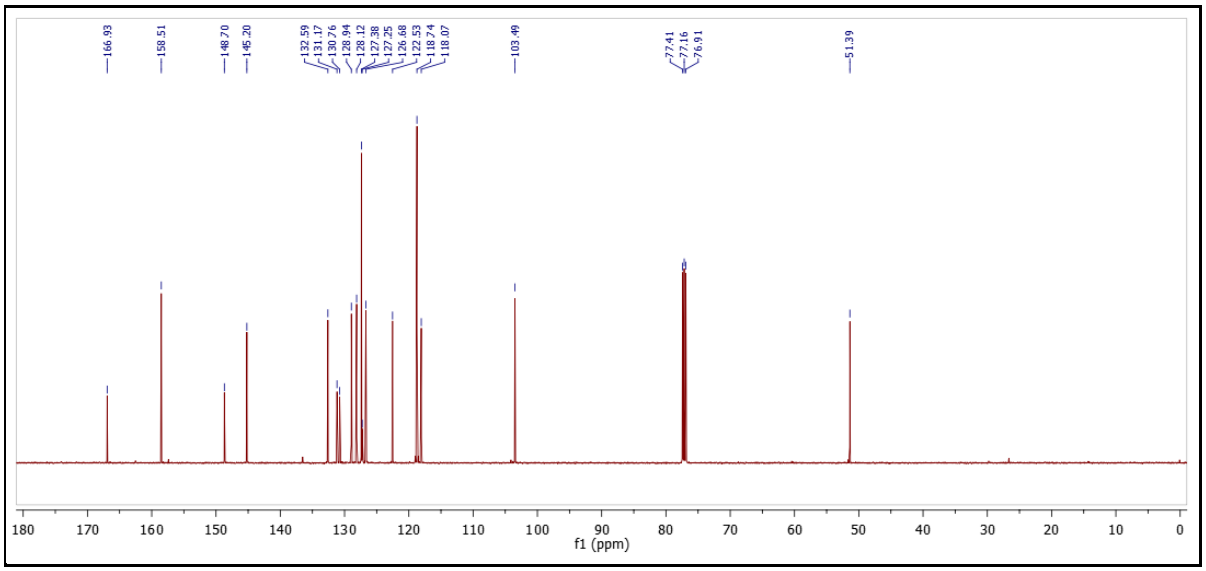
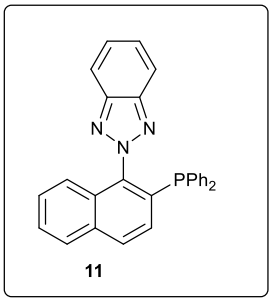
^{1}H NMR (400 MHz, $CDCl_3$)



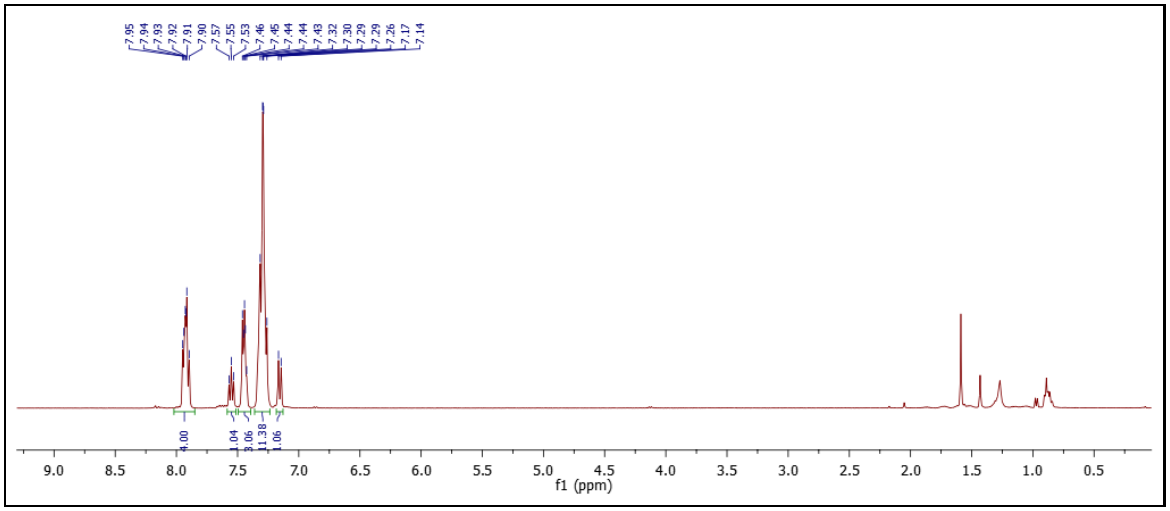
^{13}C NMR (125 MHz, $CDCl_3$)





11

^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (100 MHz, $CDCl_3$)