Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Diverse reactivity of isatin based N, N'-cyclic azomethine imine dipoles with arynes: Synthesis of 1'-methyl-2'-oxospiro [indene-1,3'-indolines] and 3-aryl-3-pyrazol-2-oxindoles

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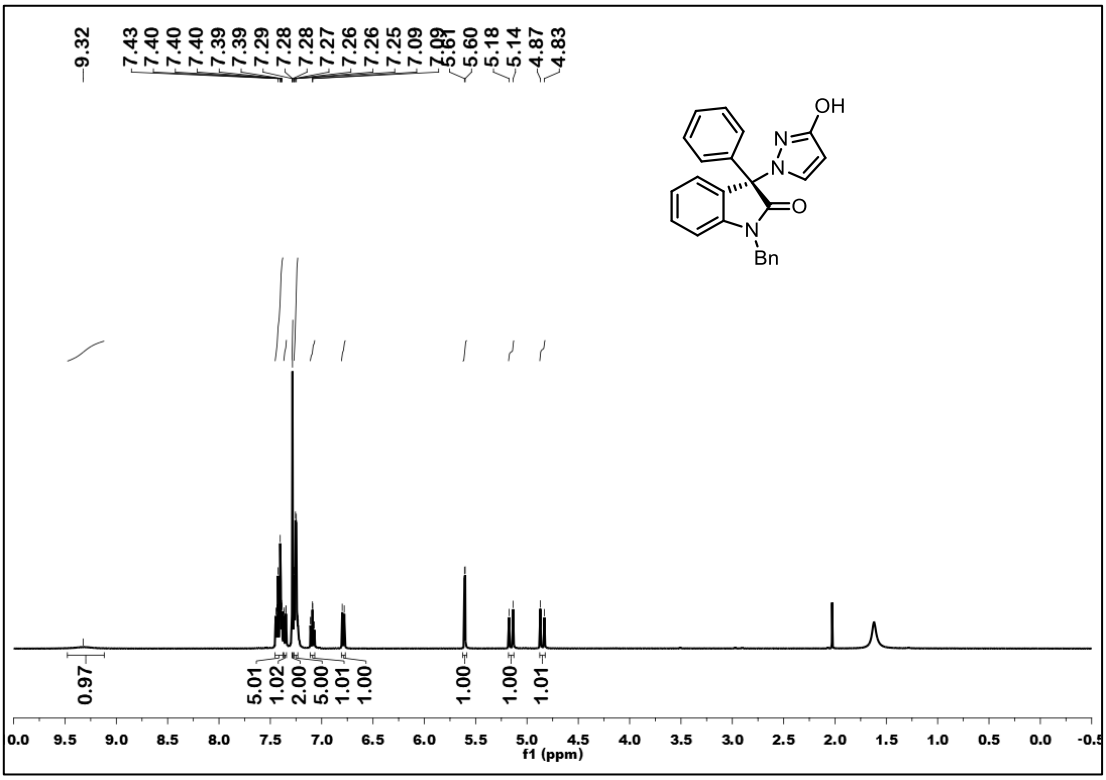

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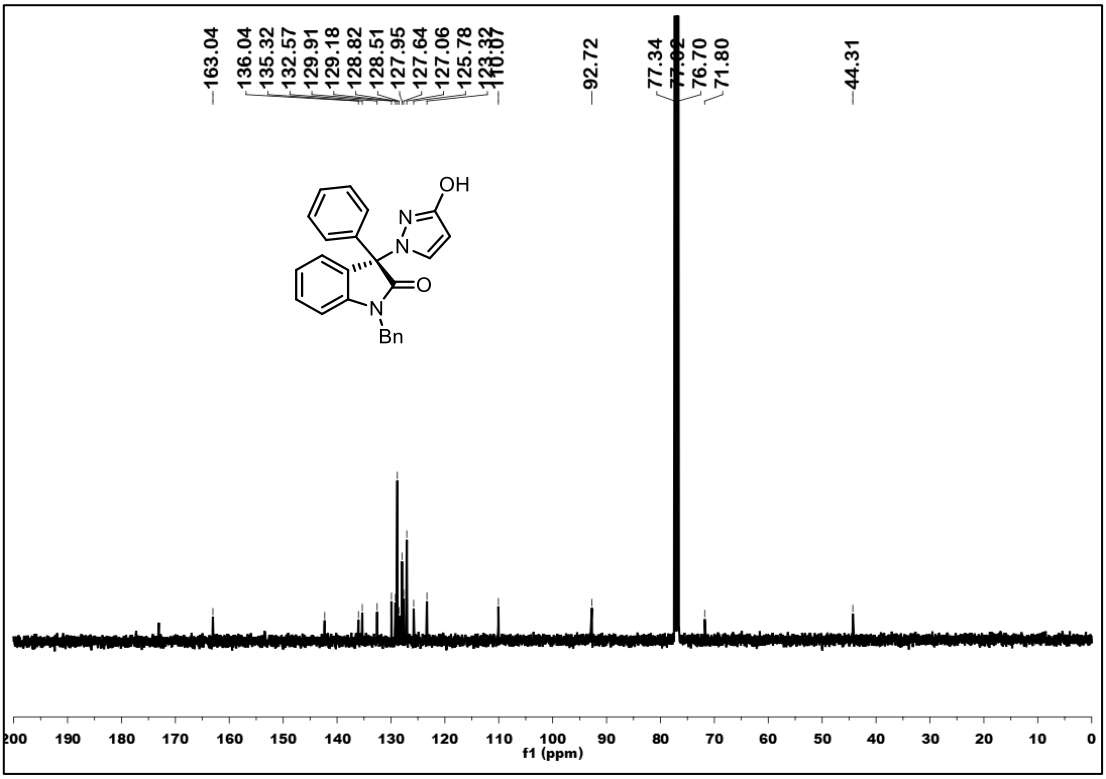

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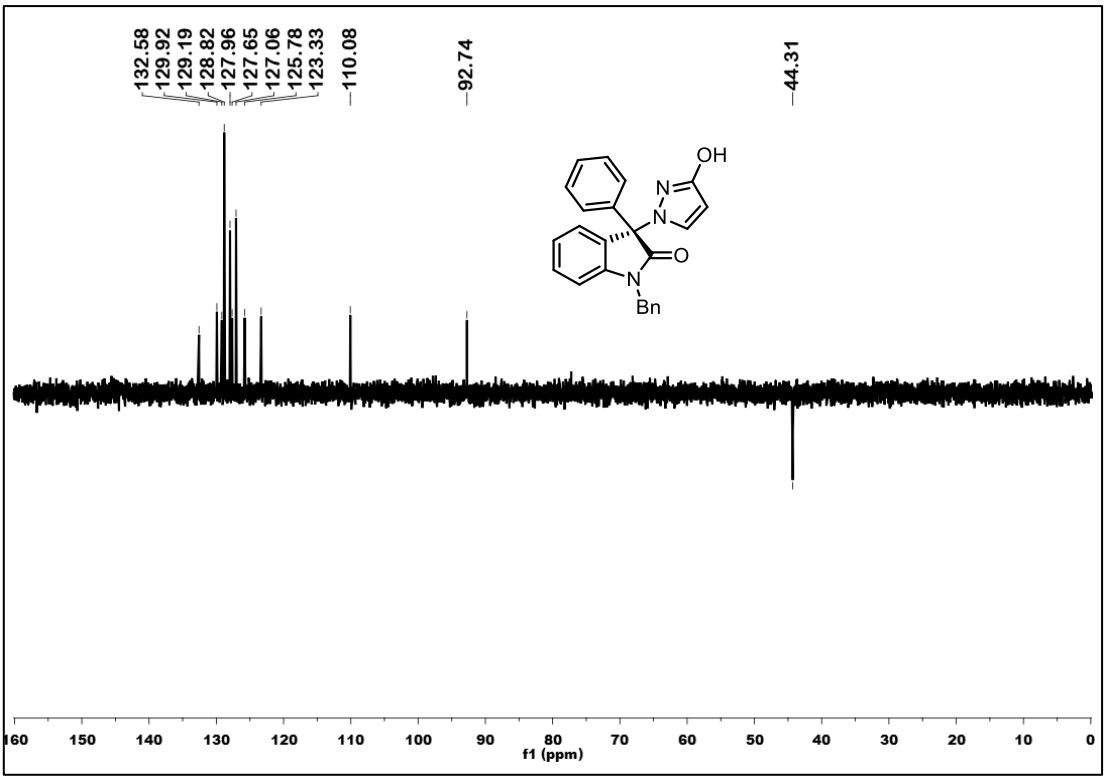

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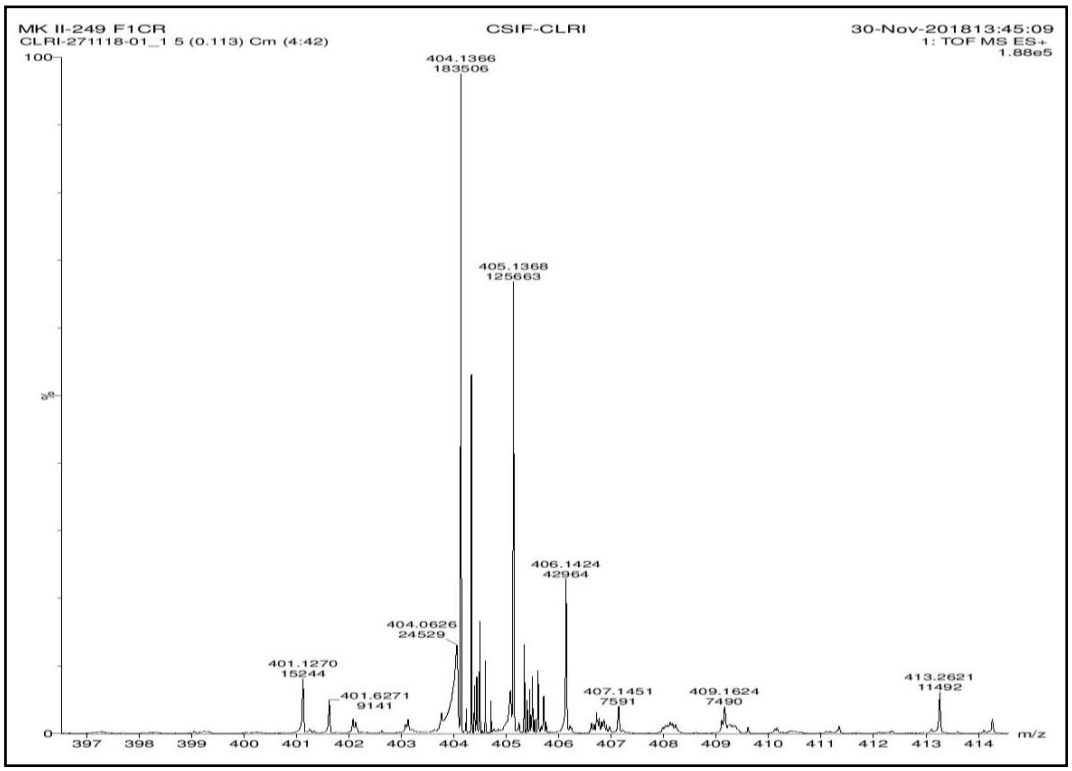

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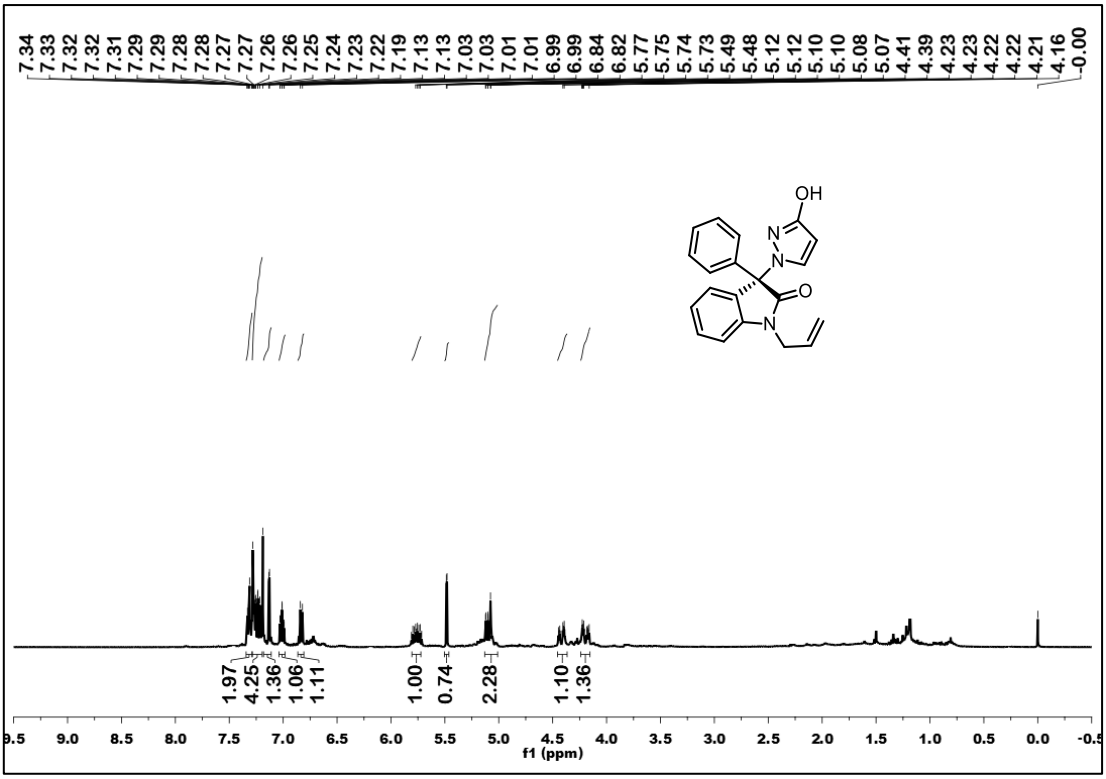

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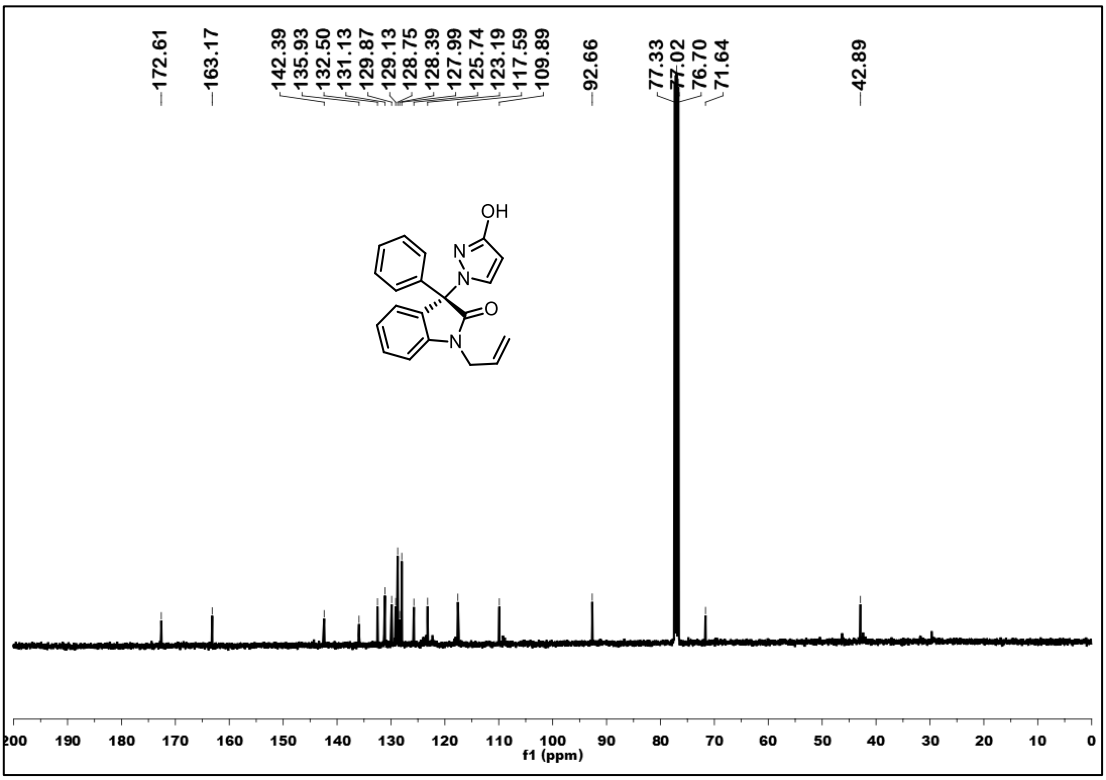

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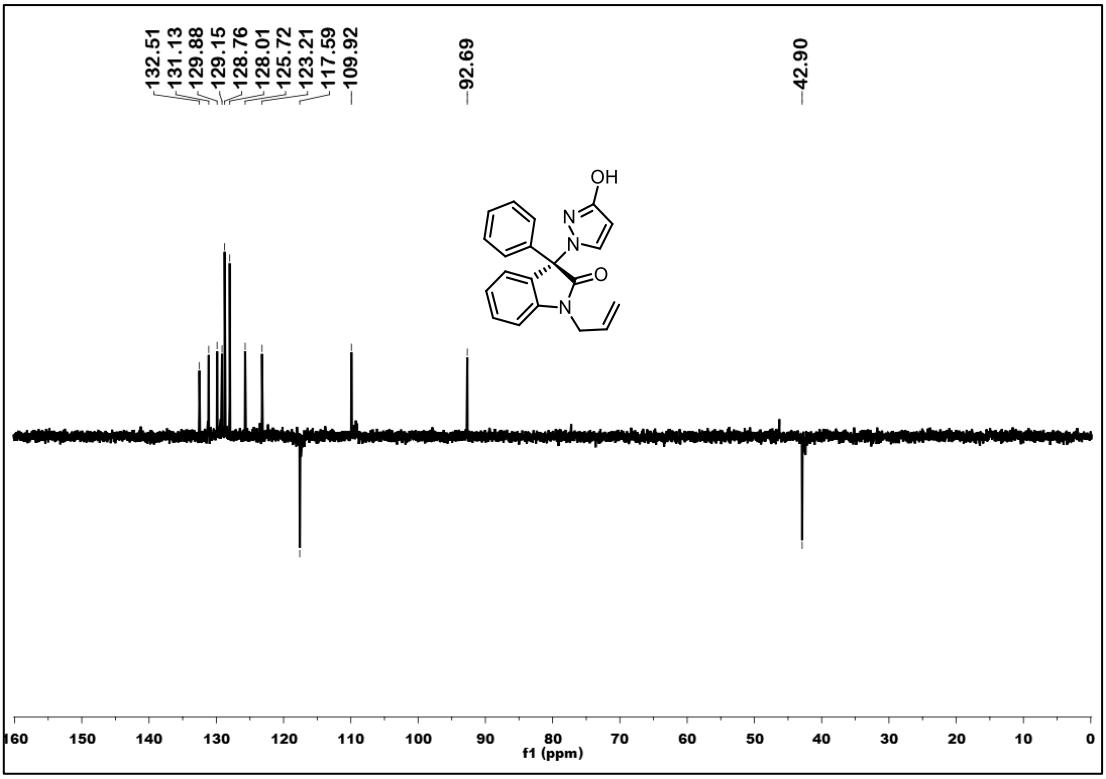

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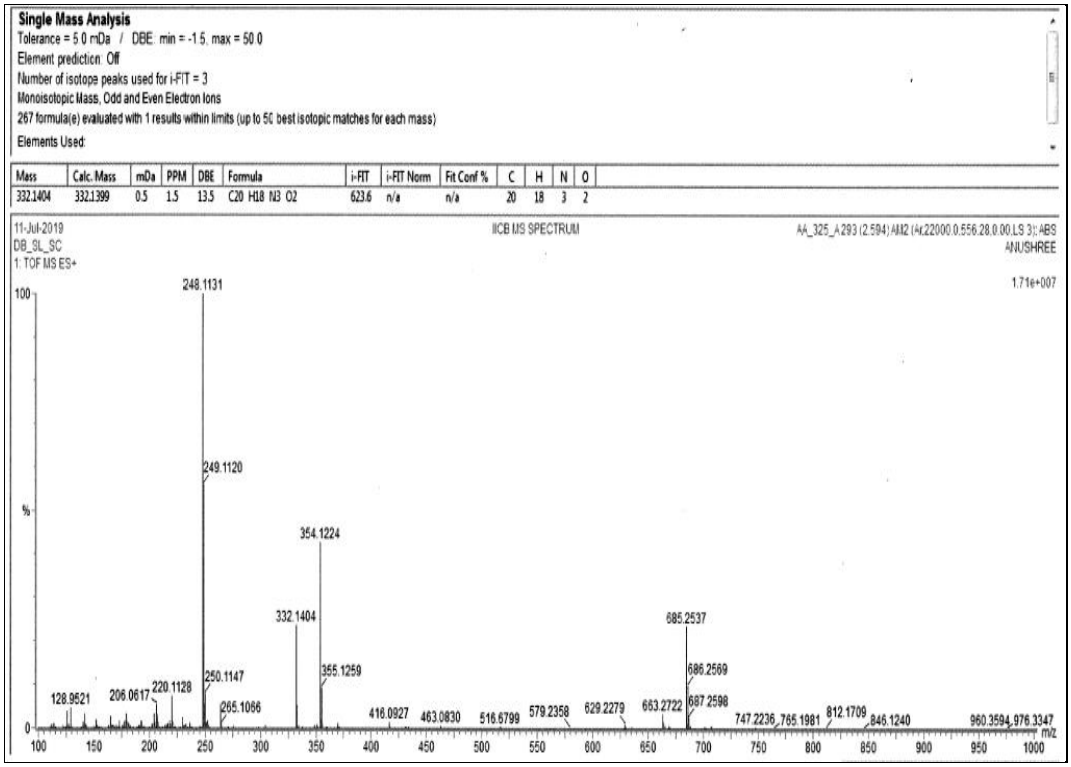

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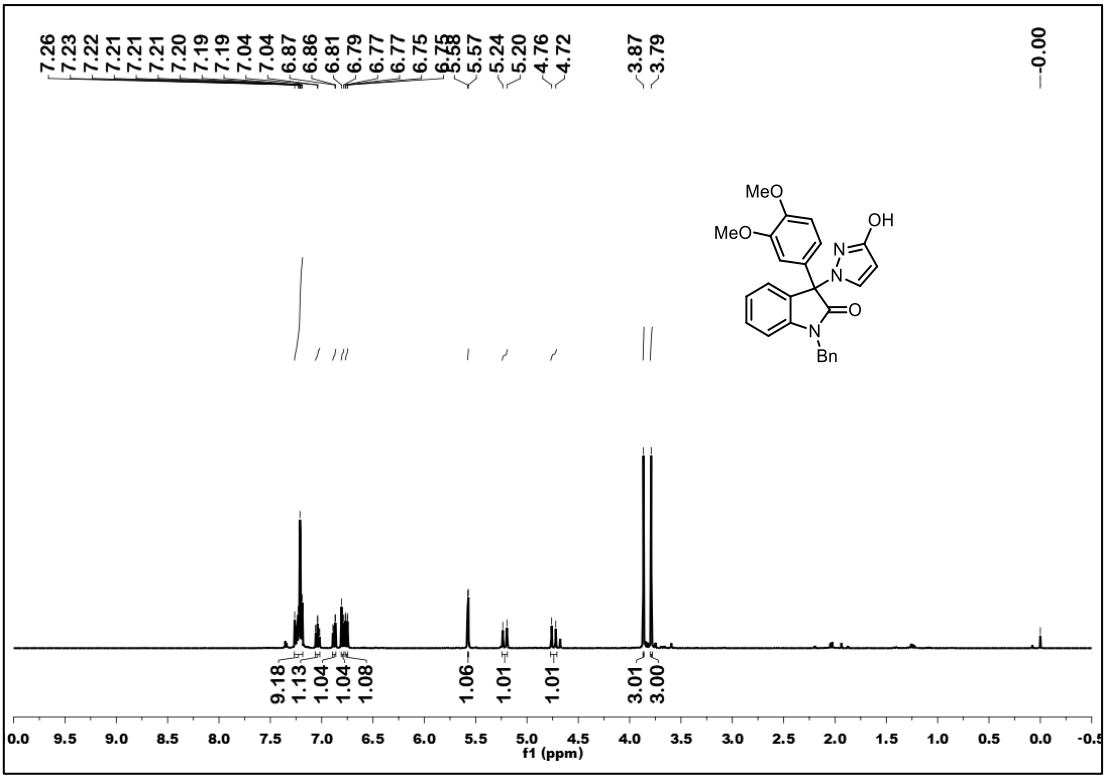

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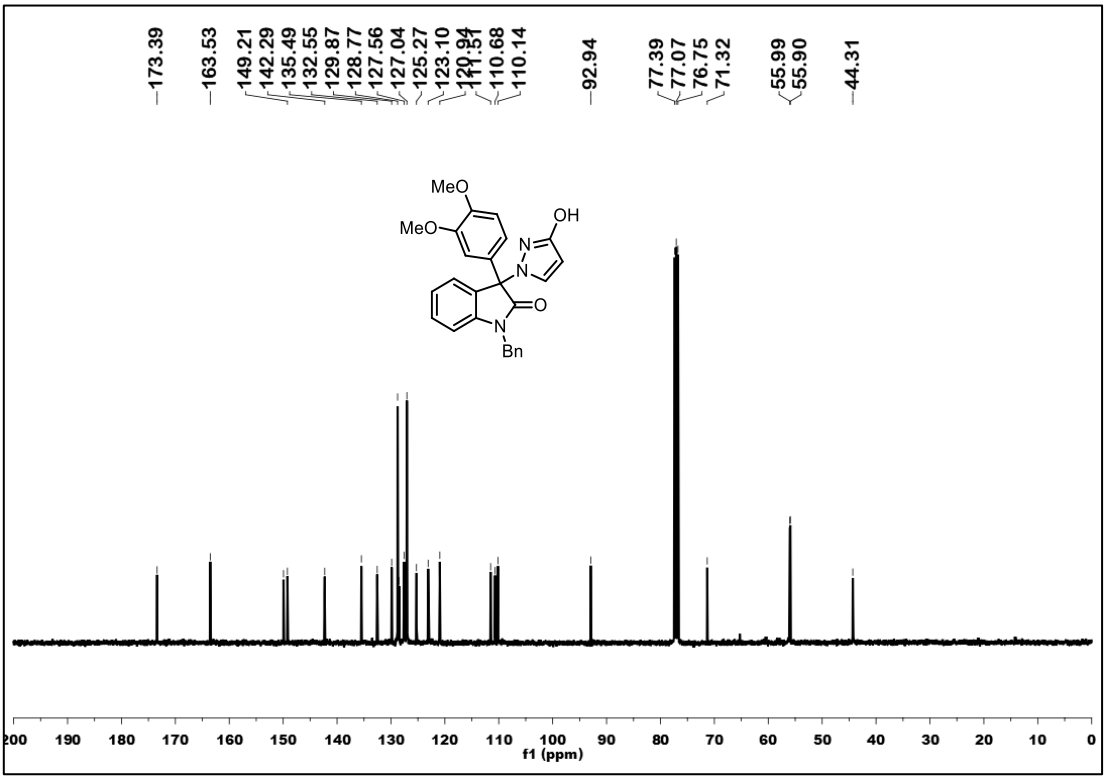

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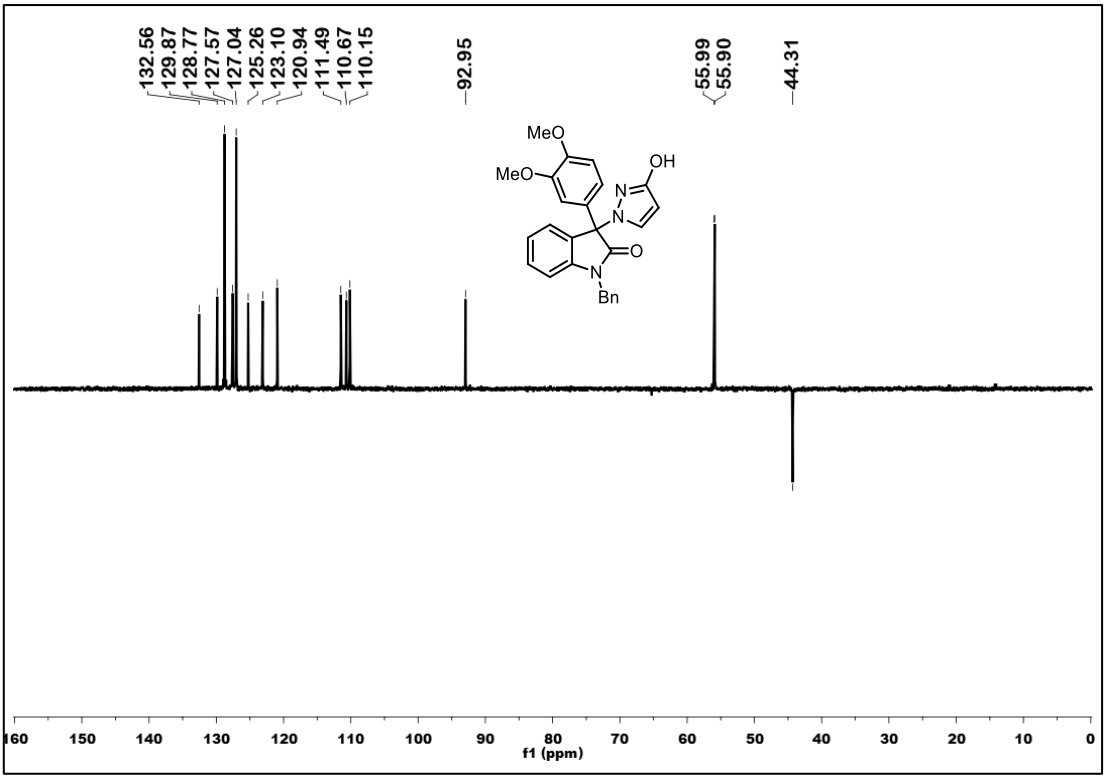

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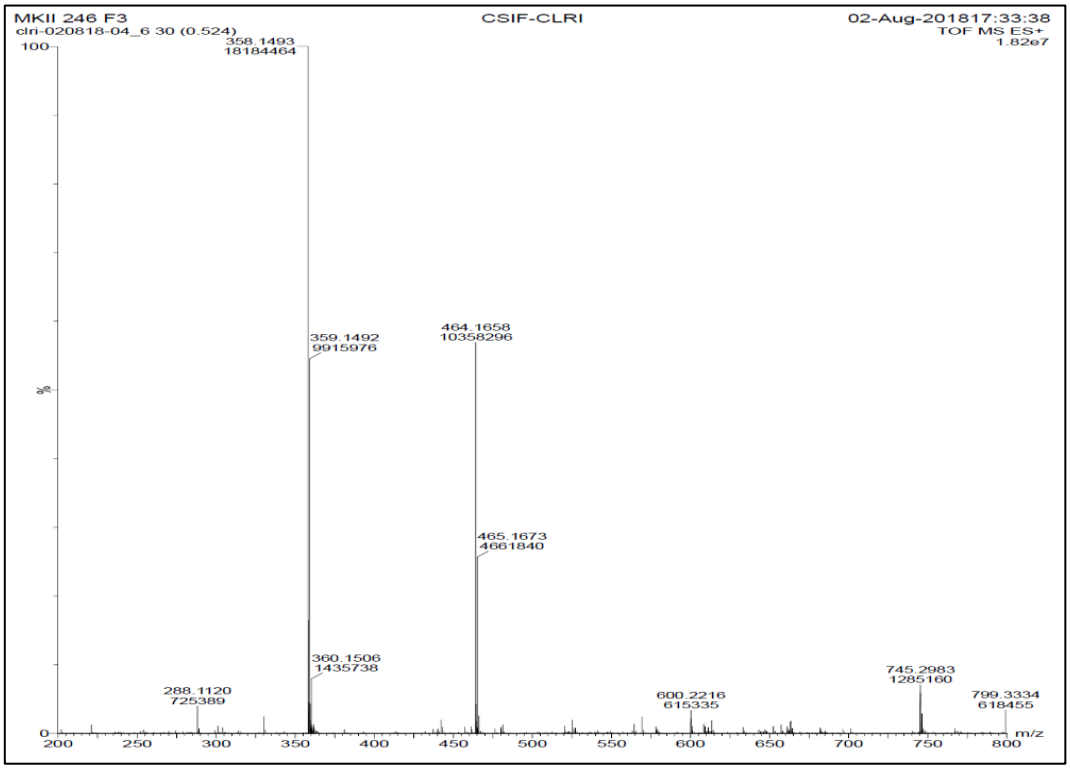

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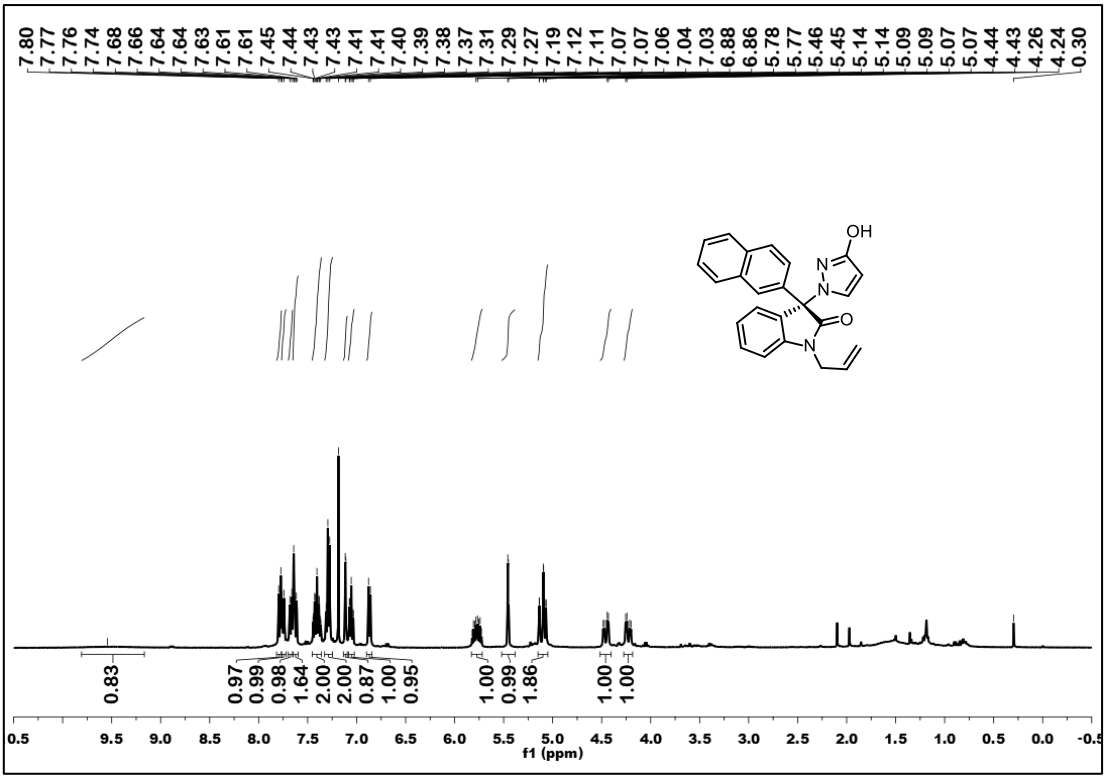

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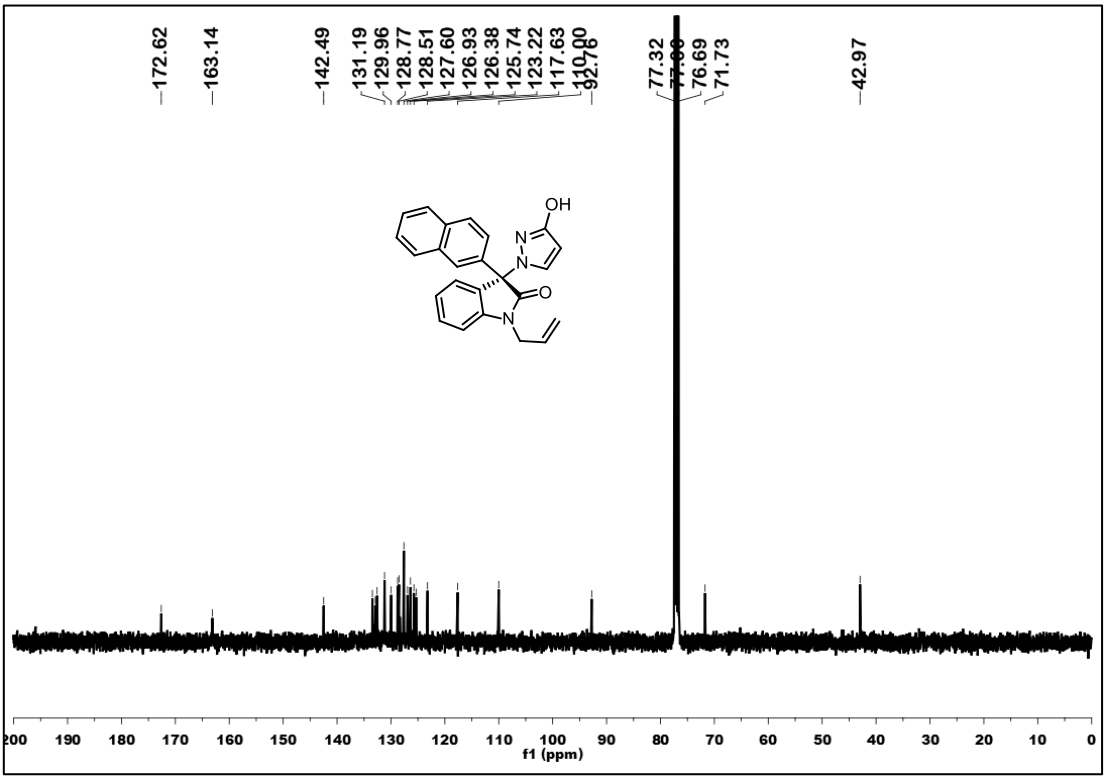

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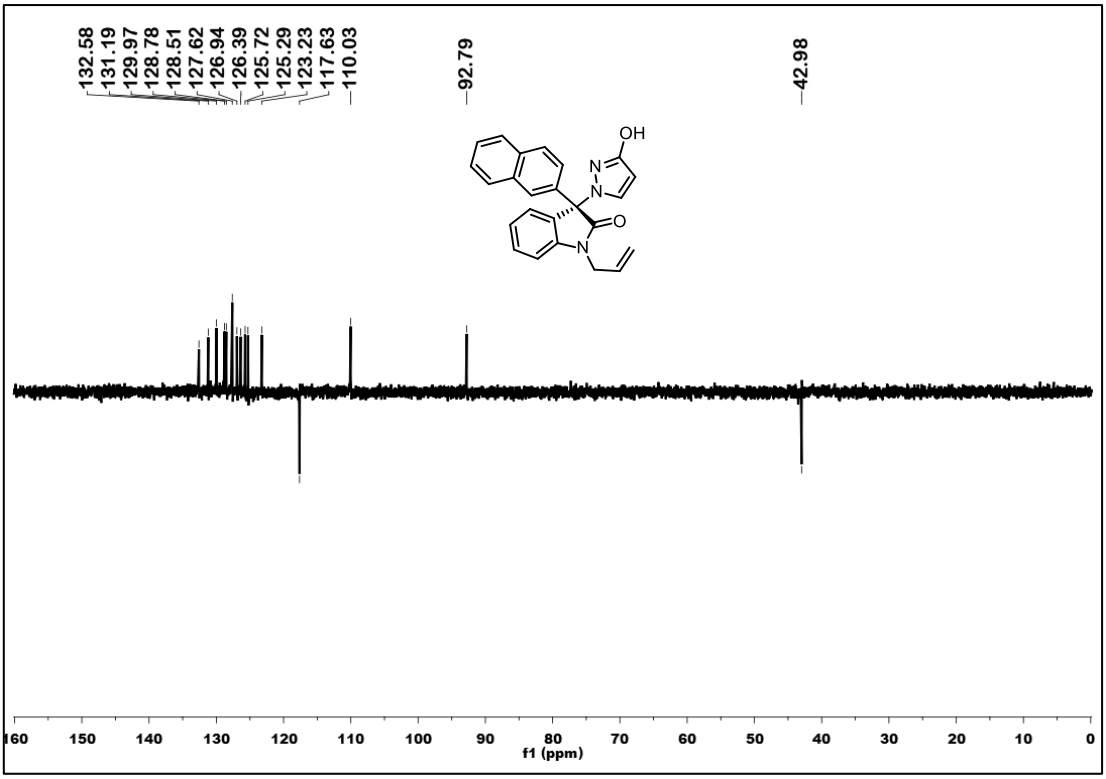

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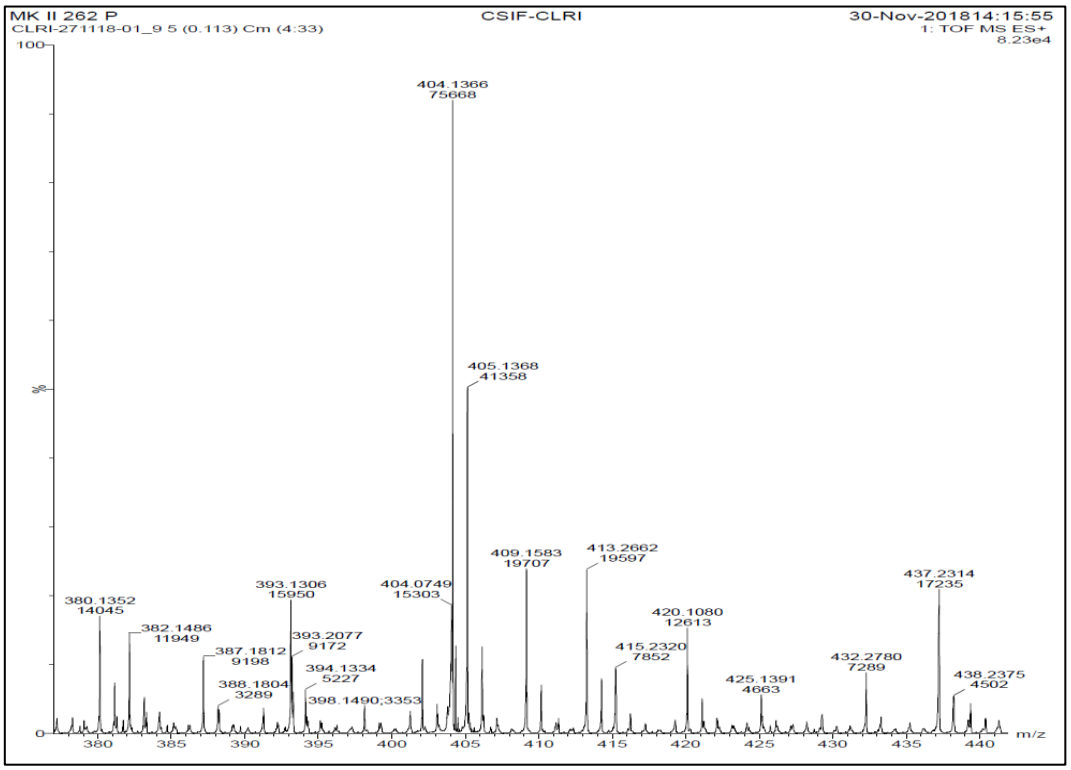

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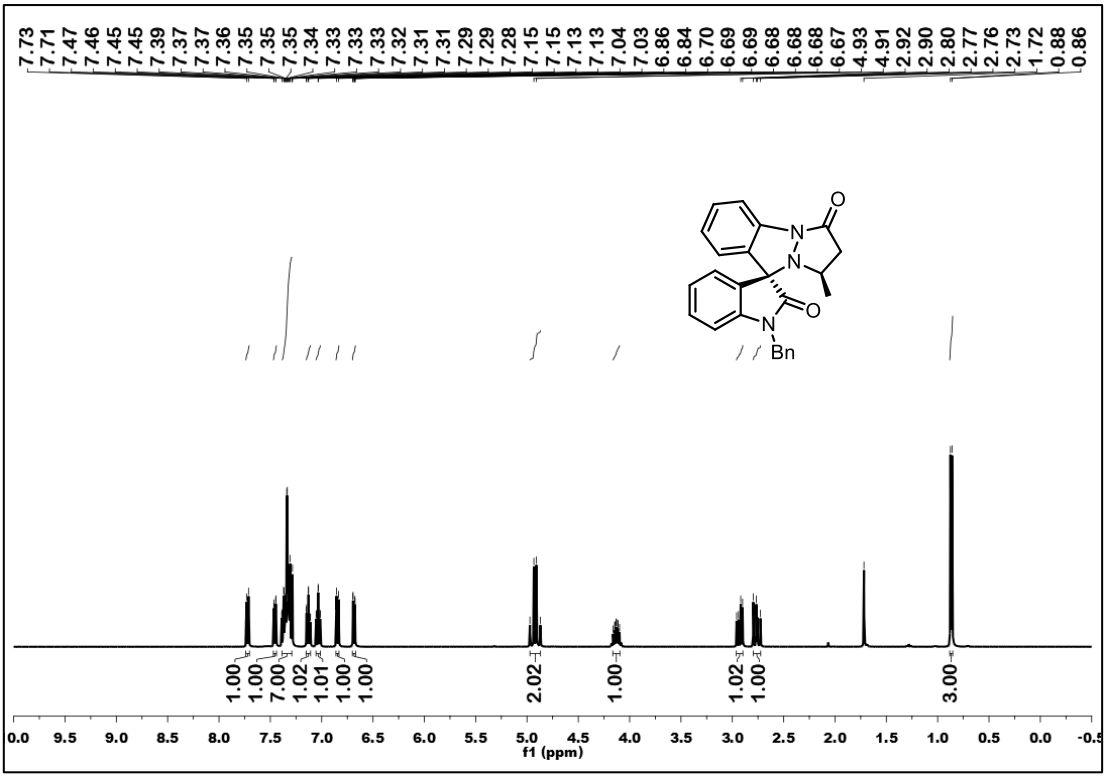

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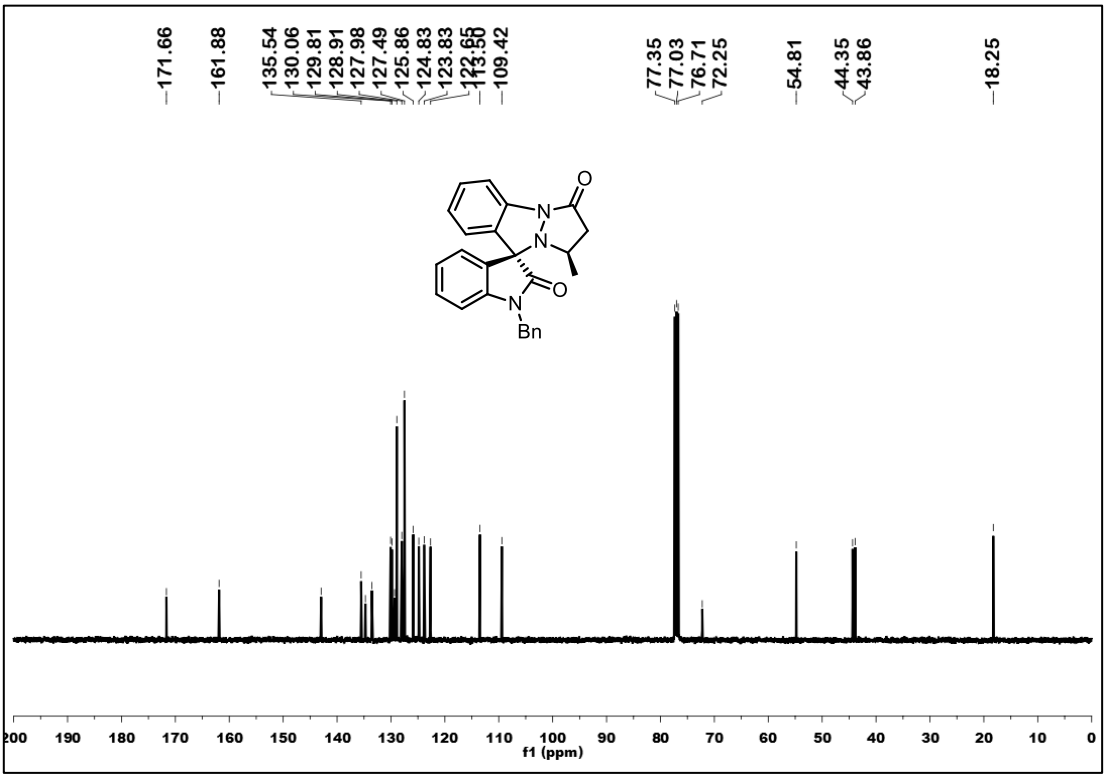

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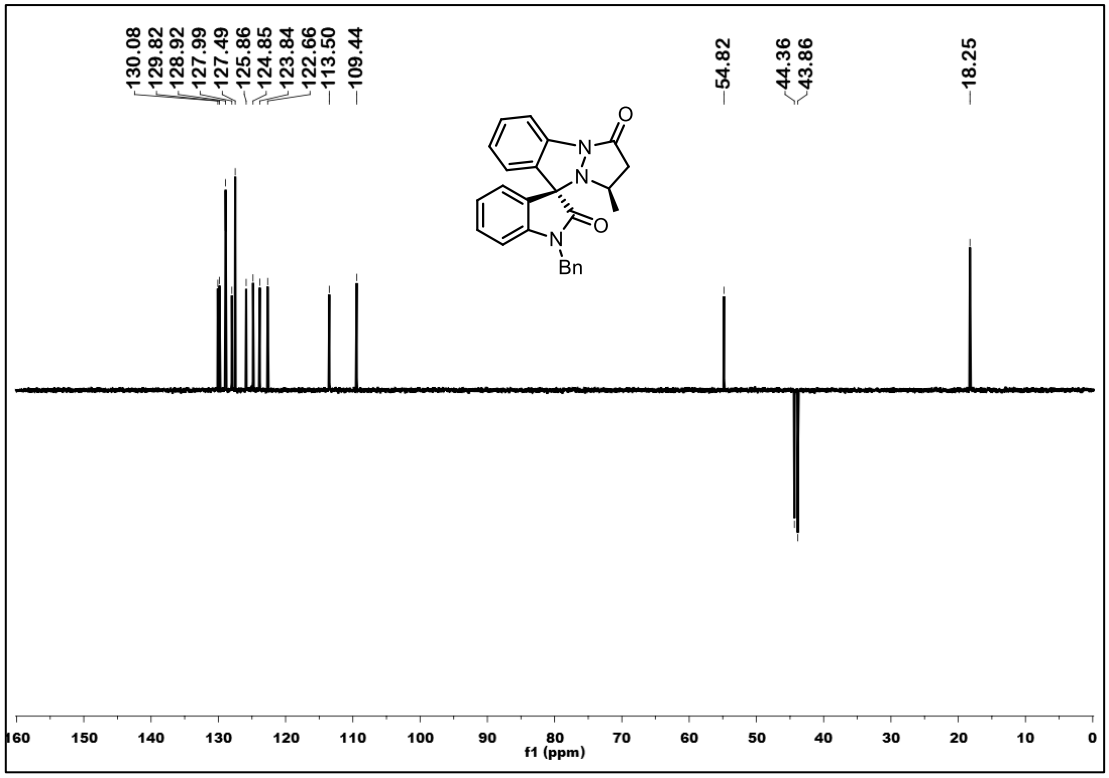

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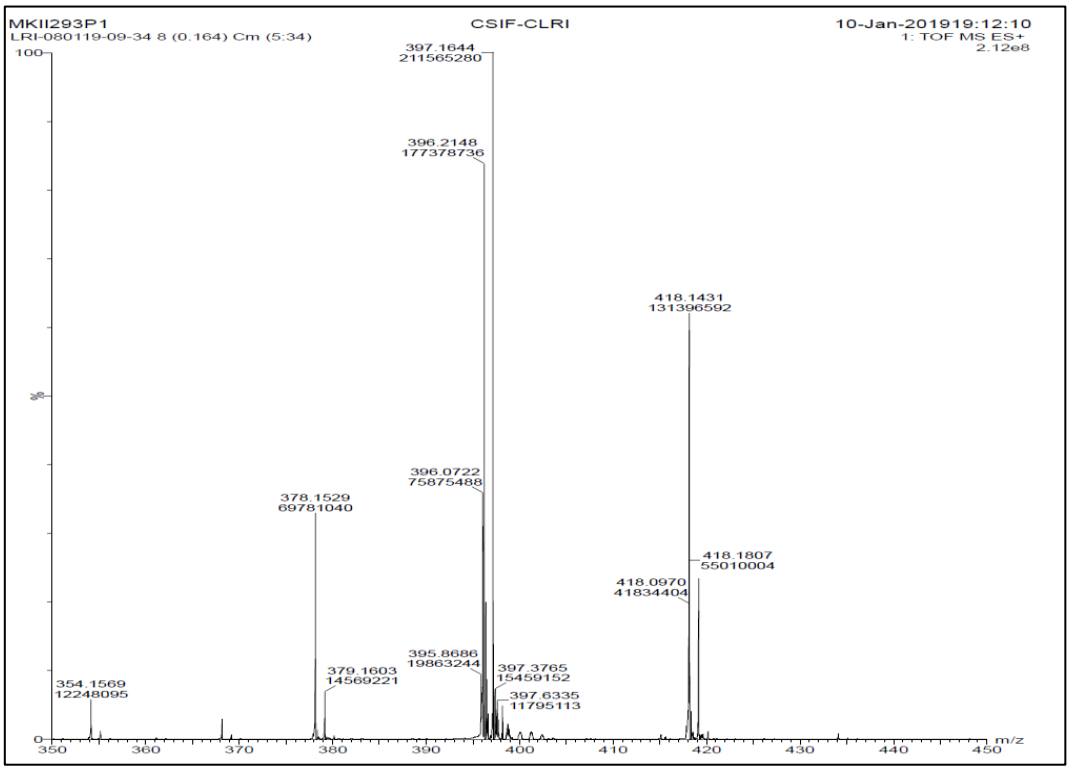

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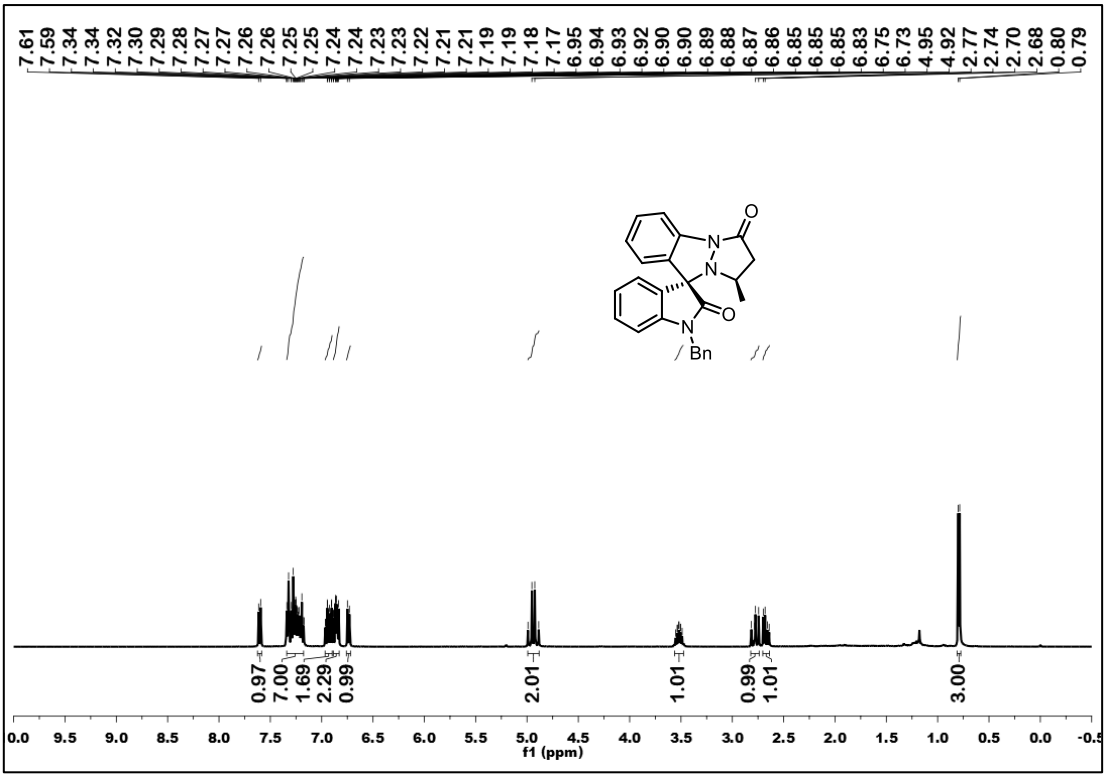

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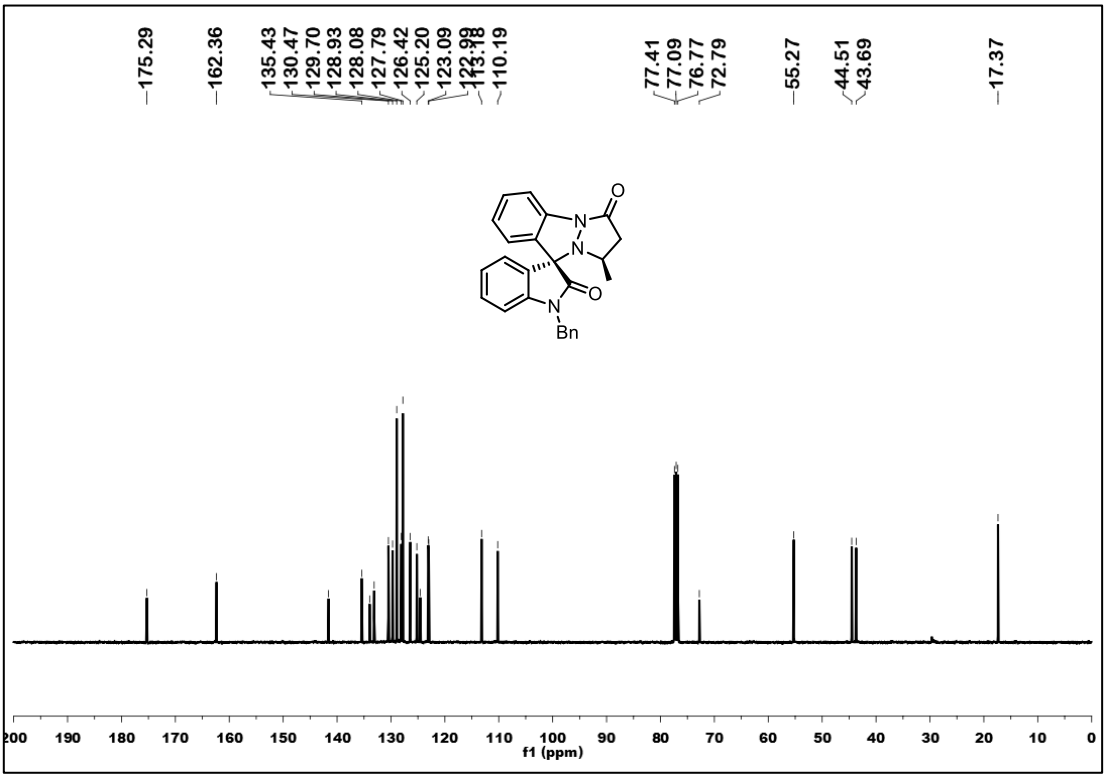

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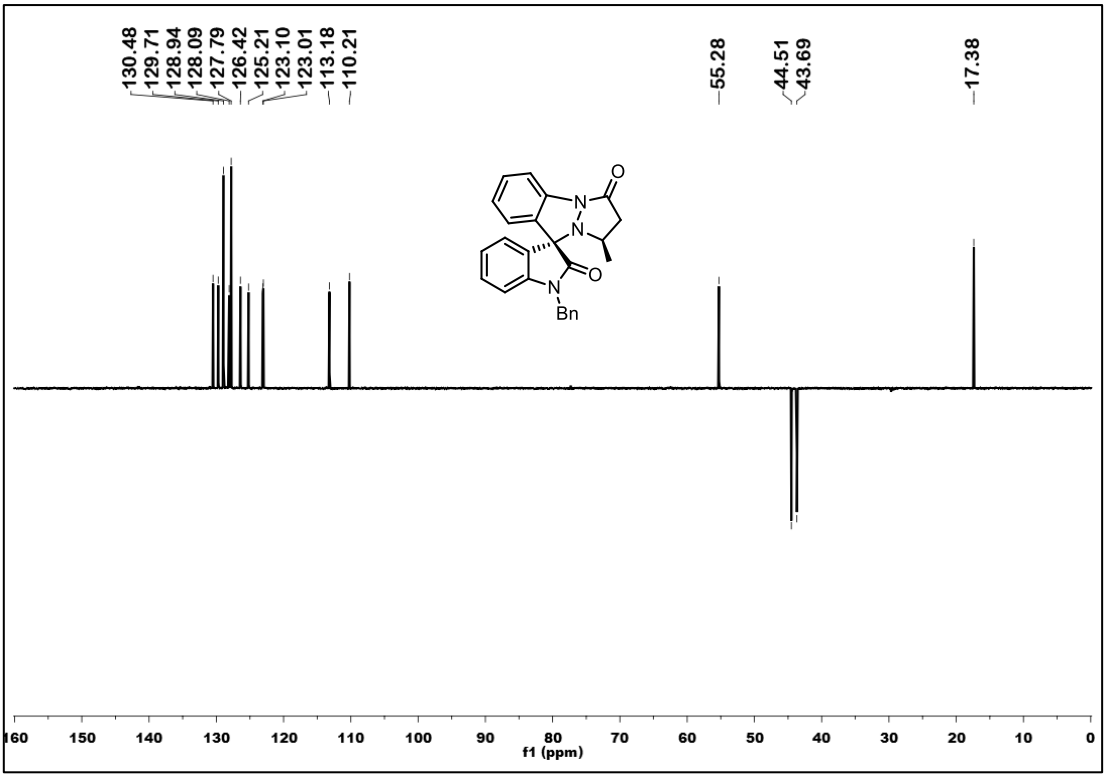

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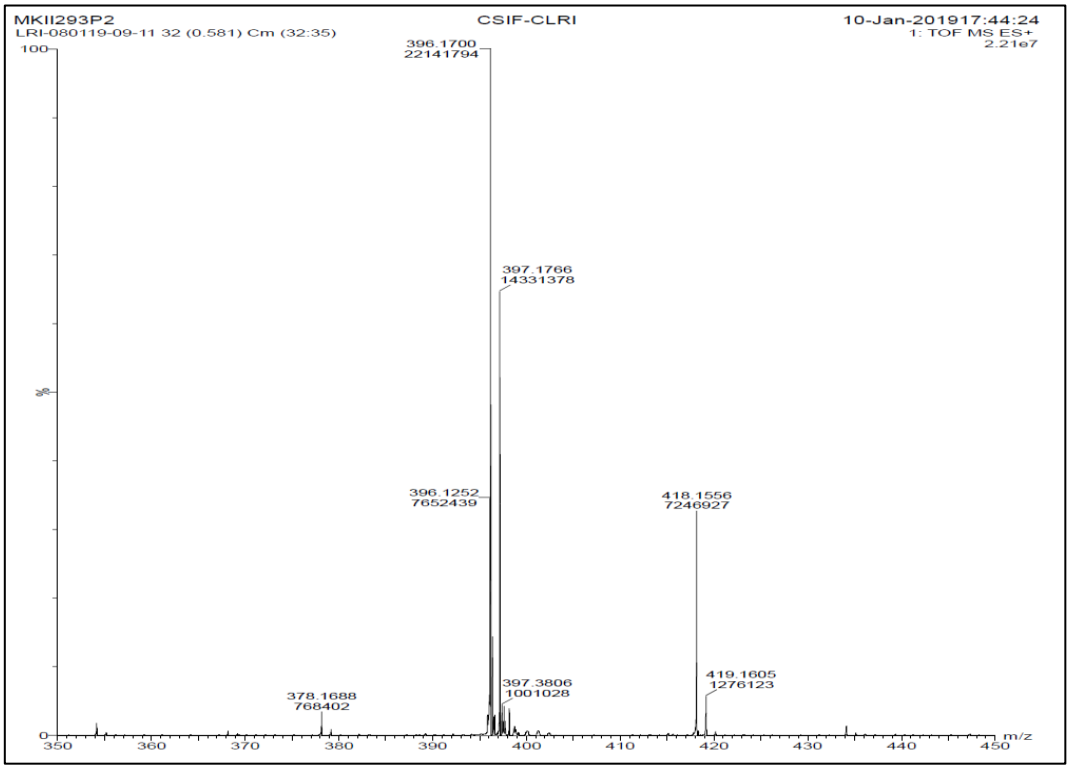

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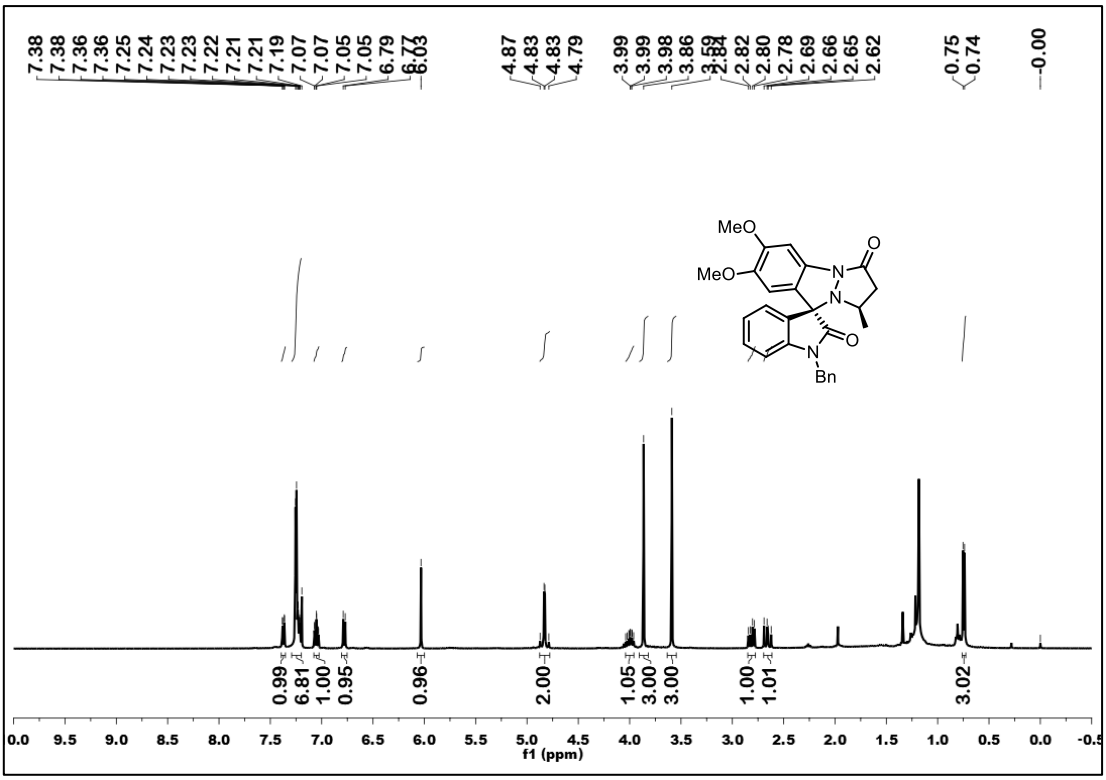

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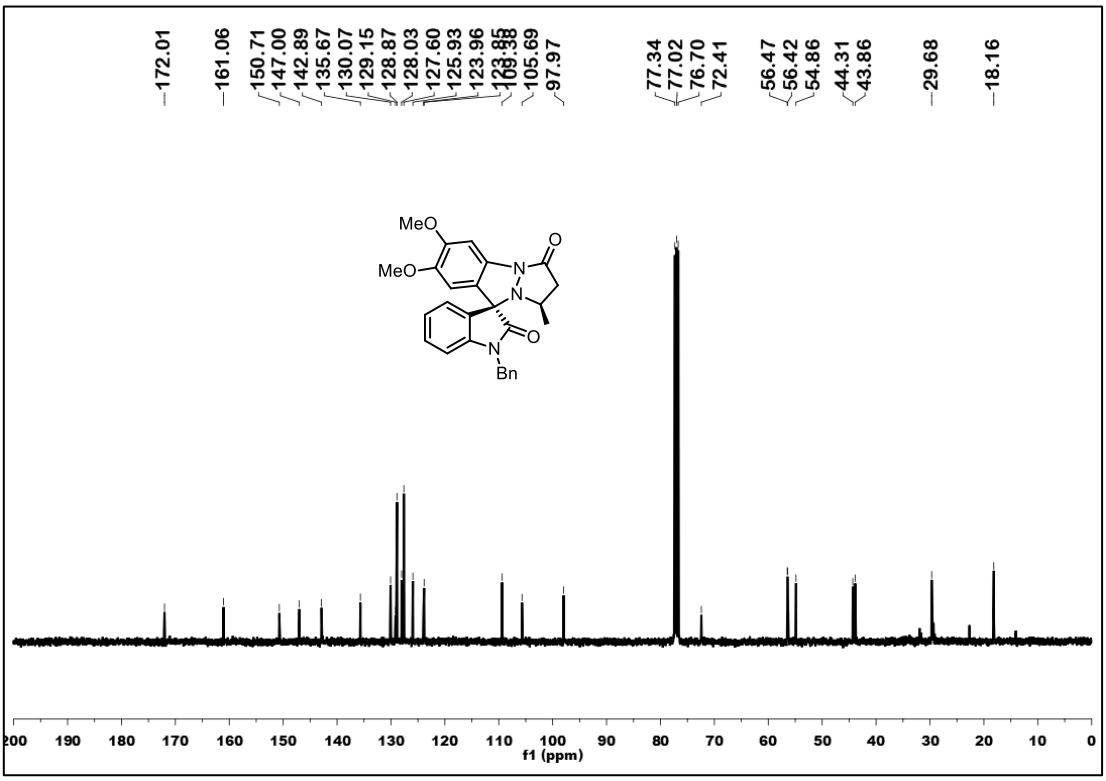

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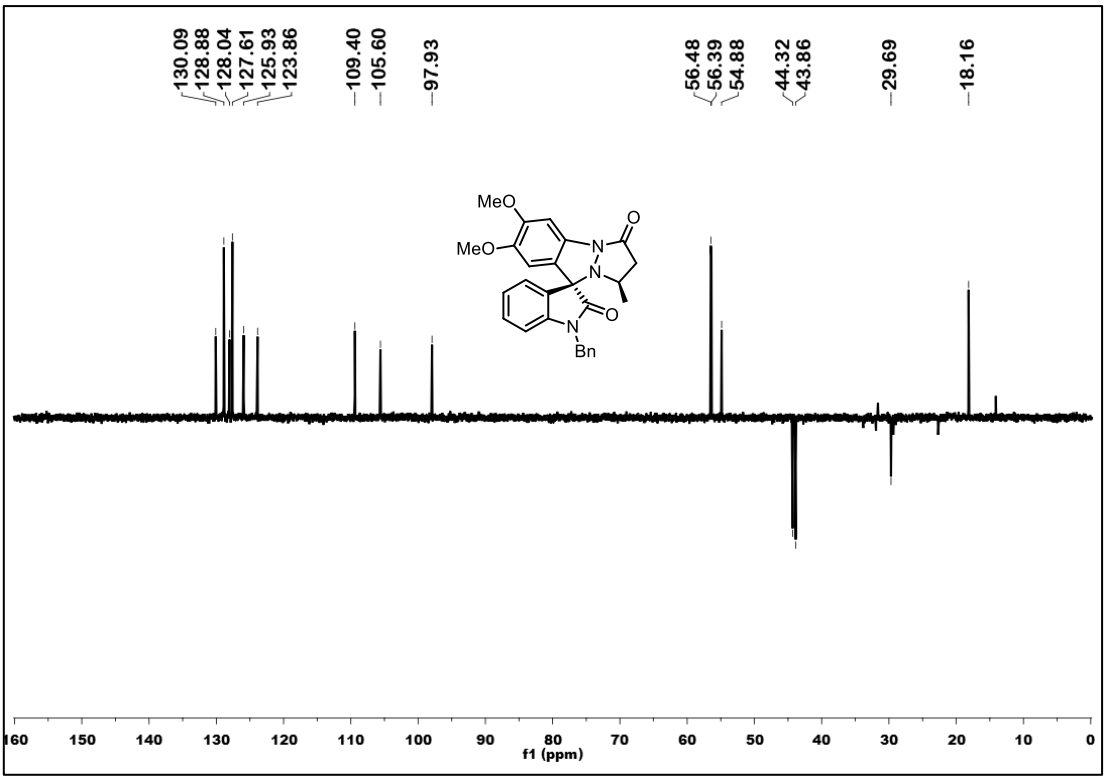

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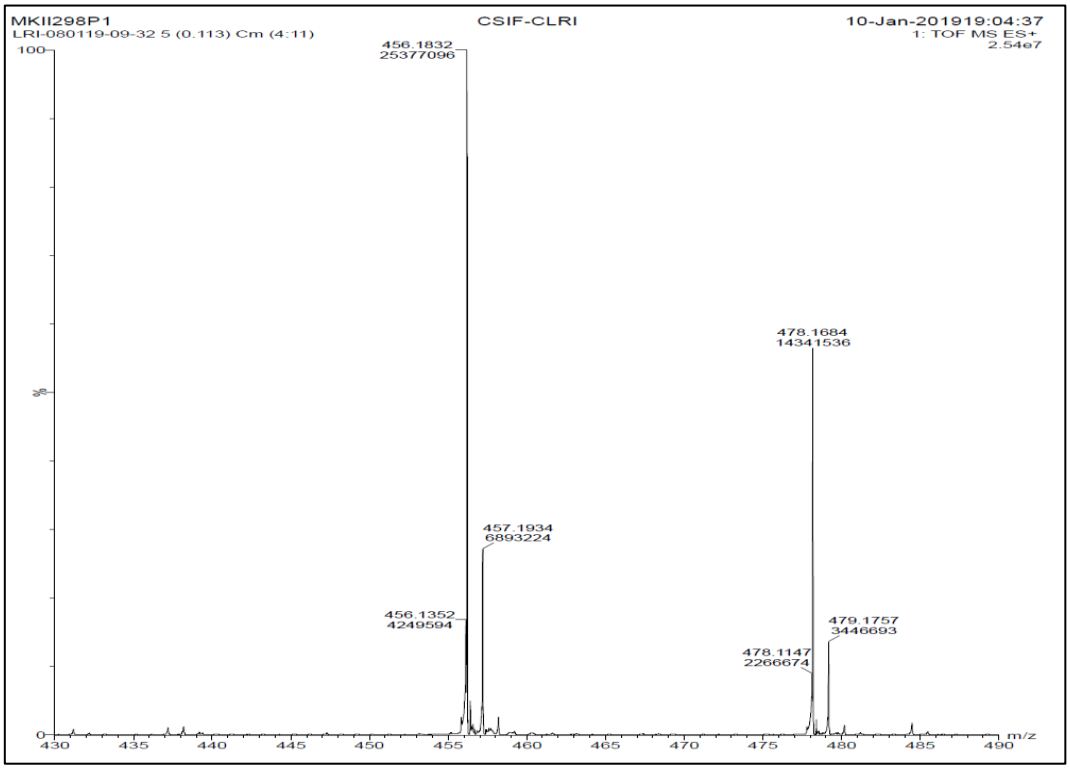

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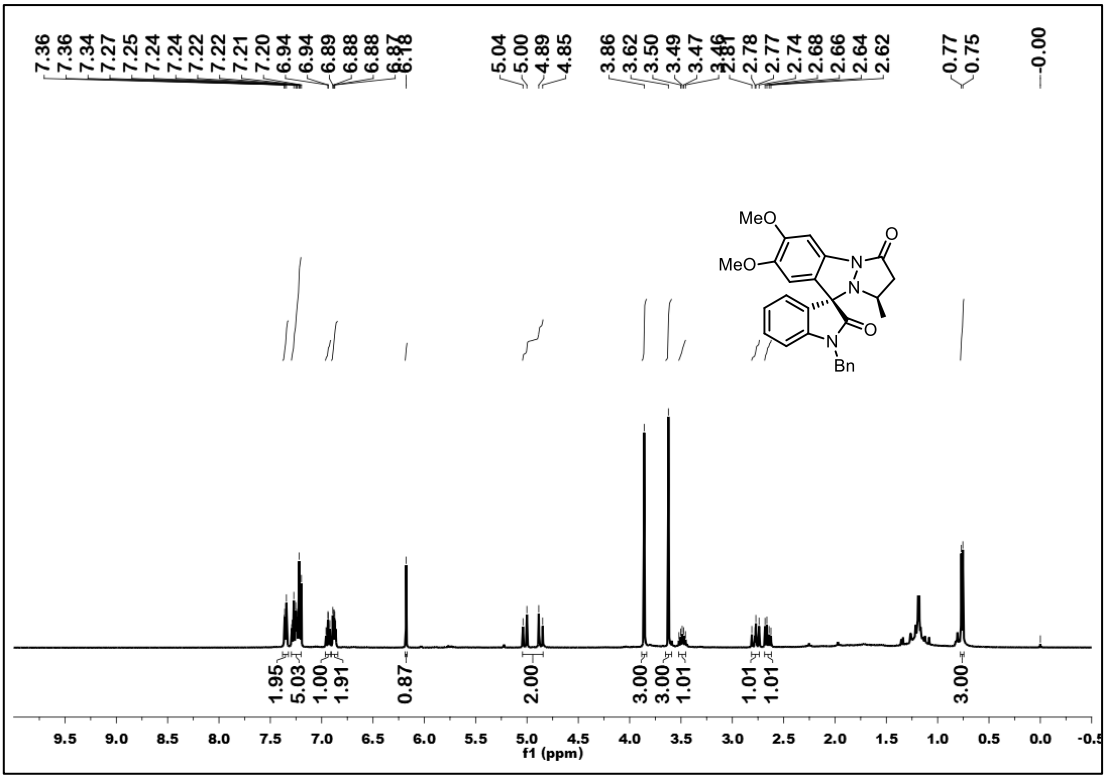

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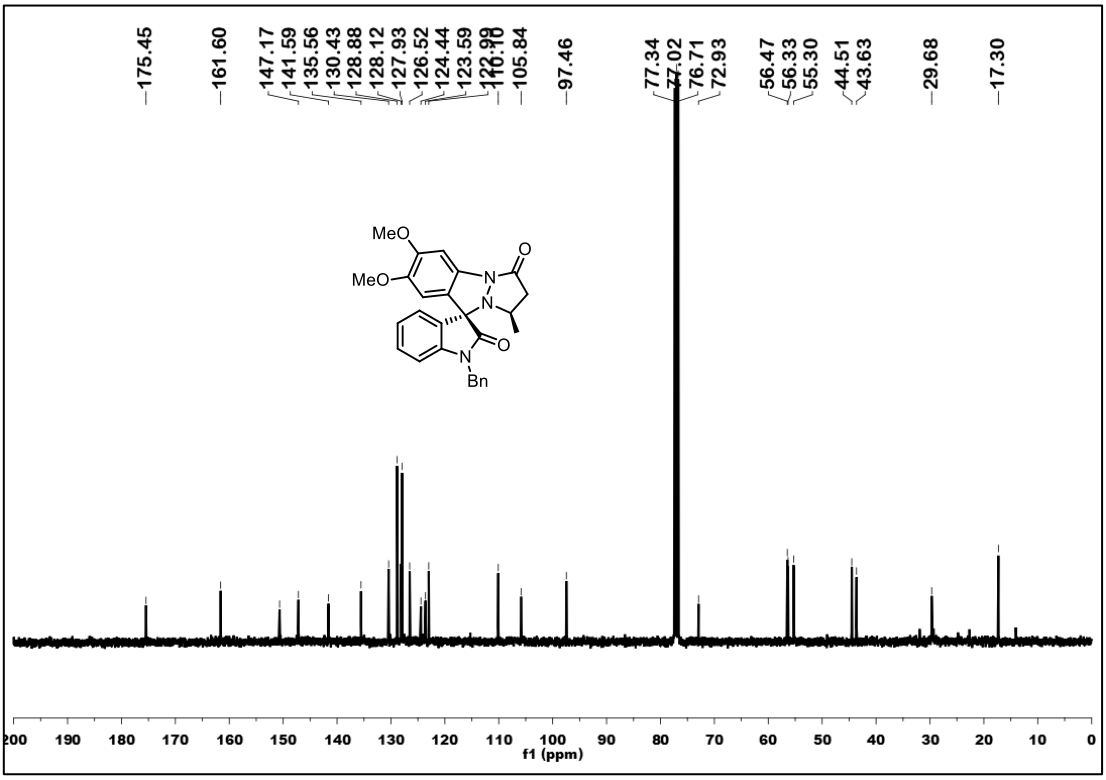

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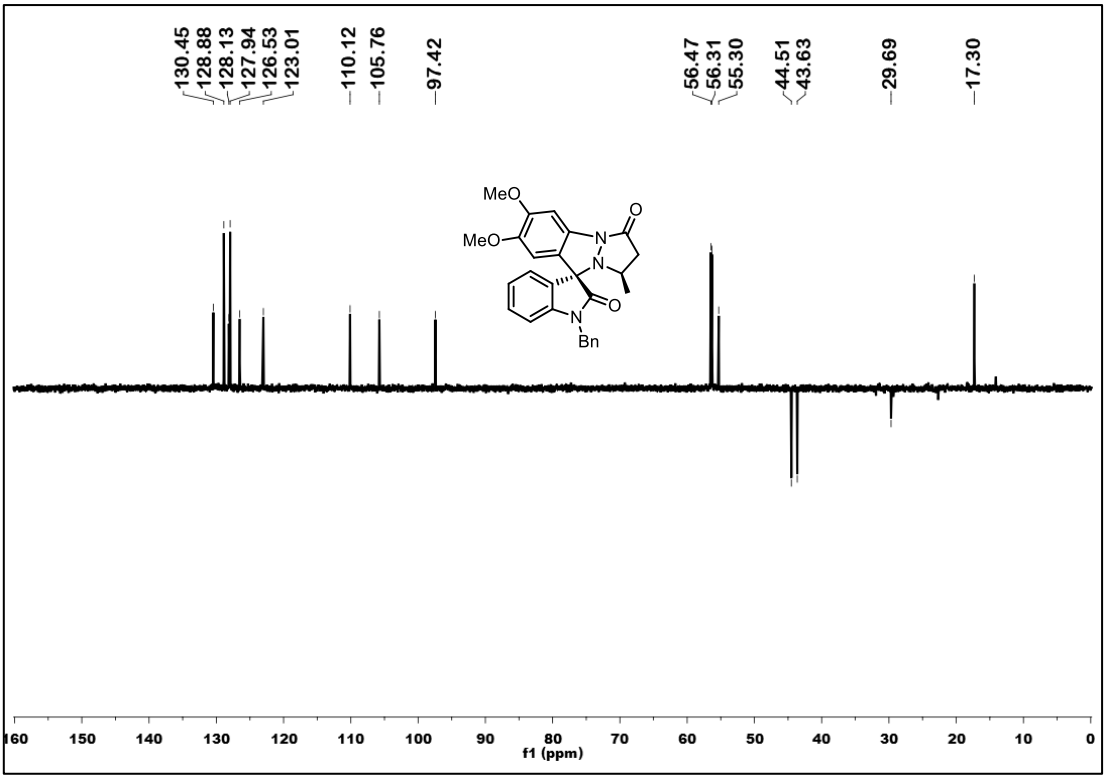

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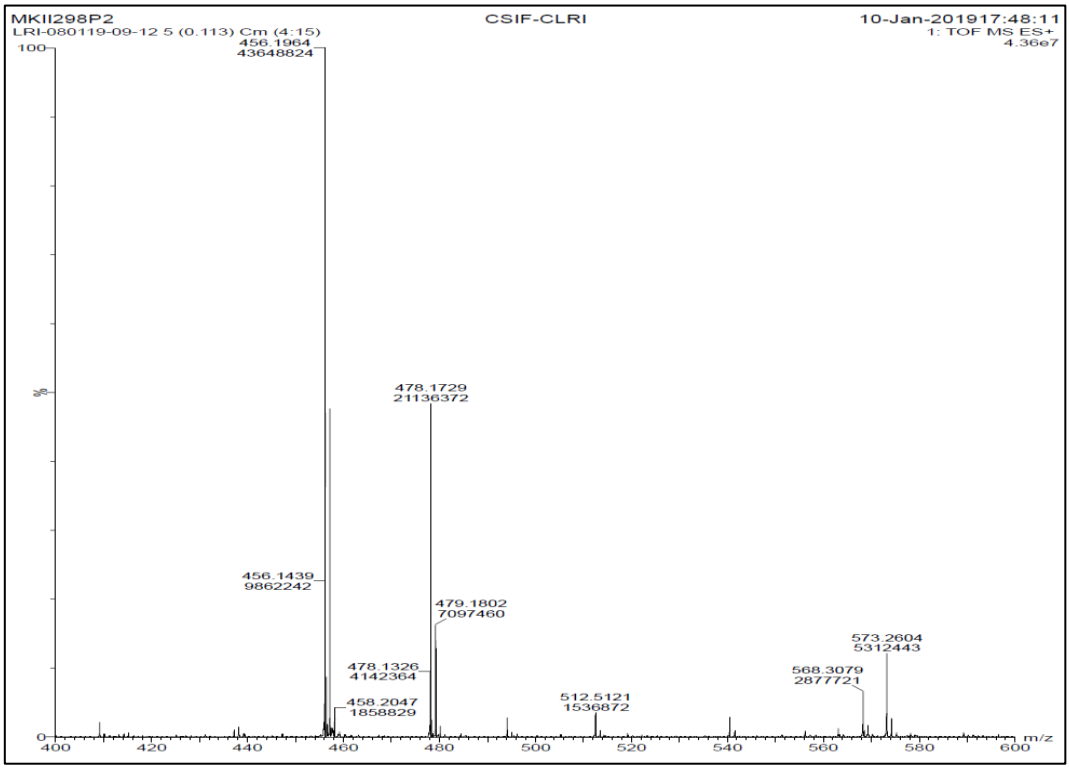

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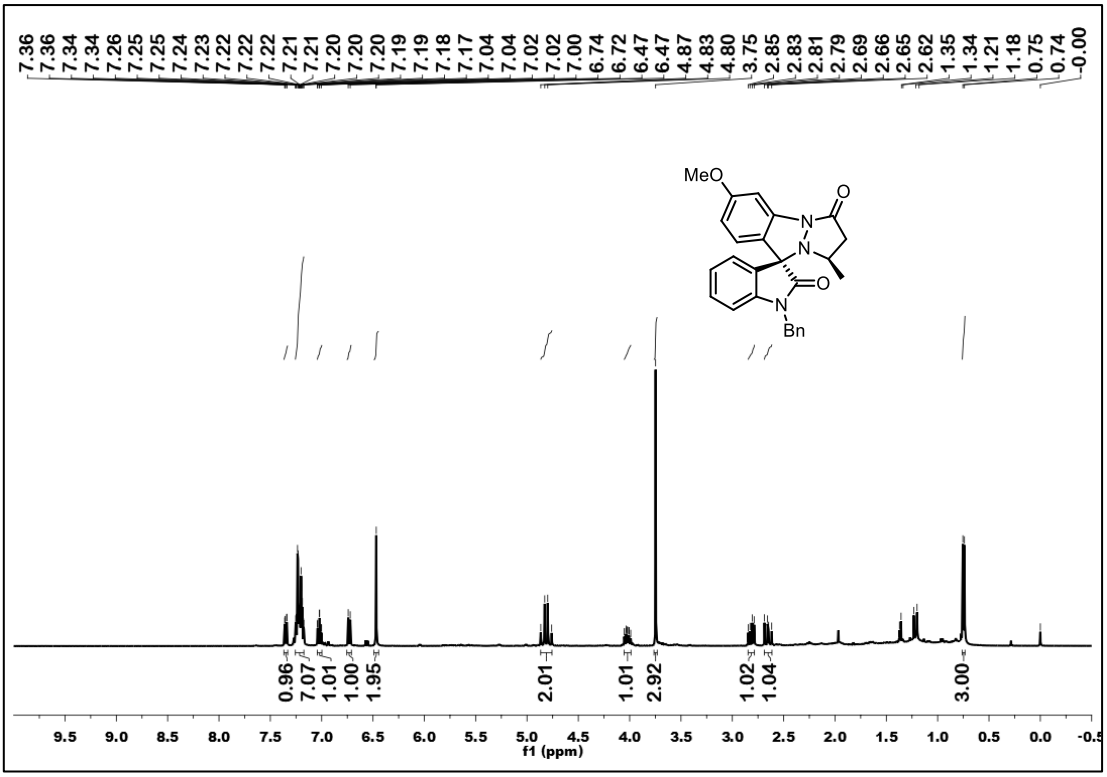

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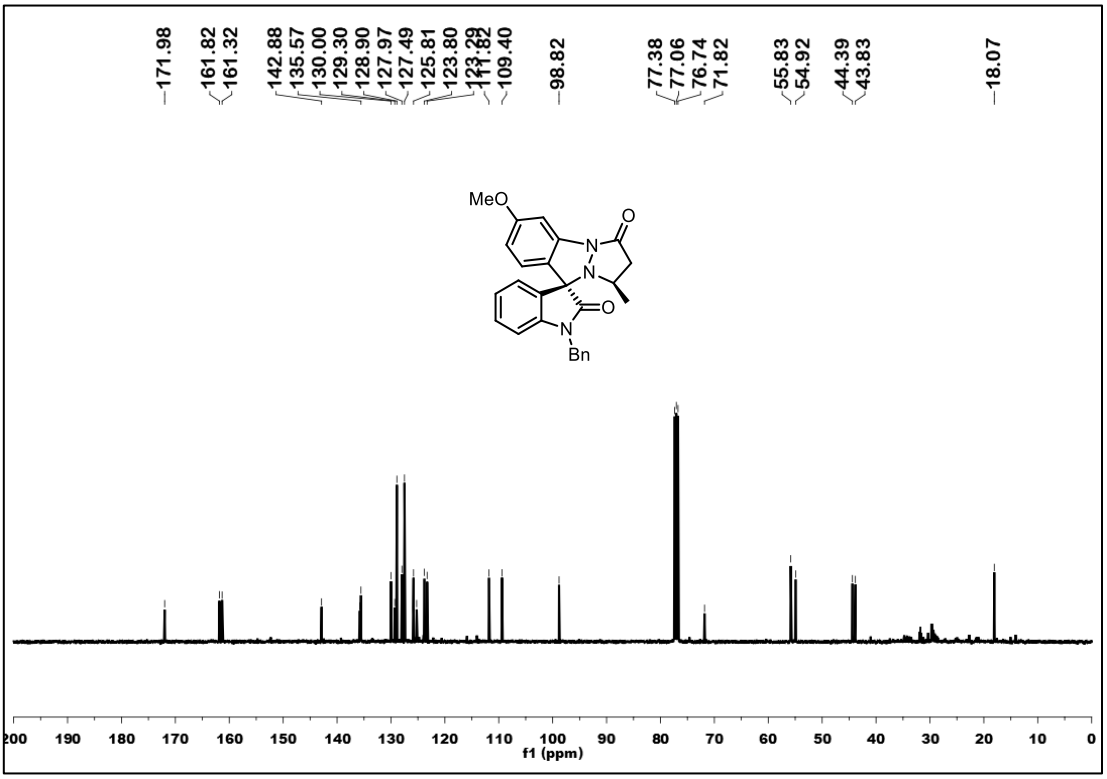

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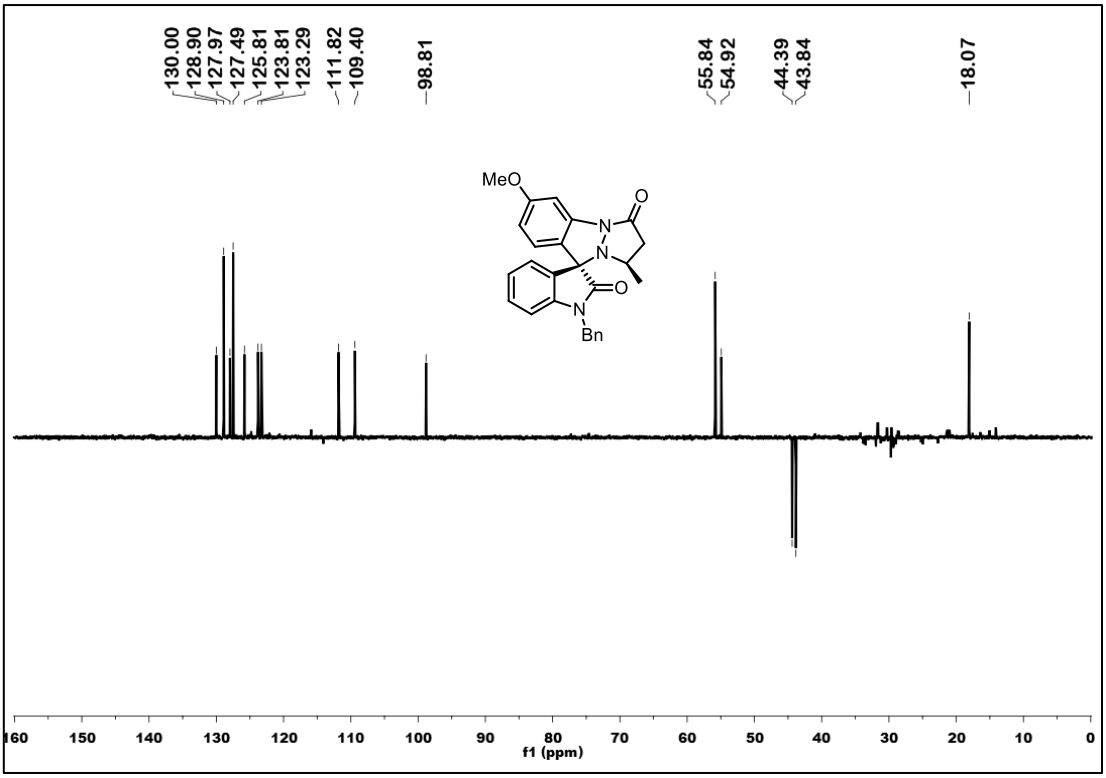

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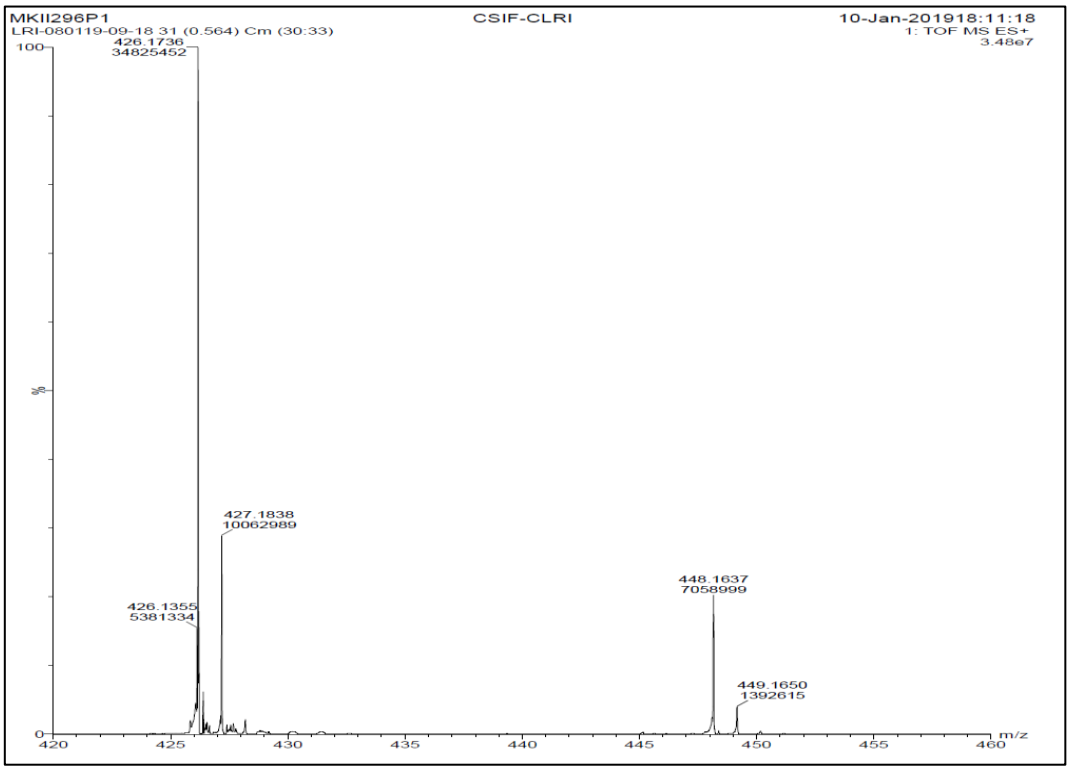

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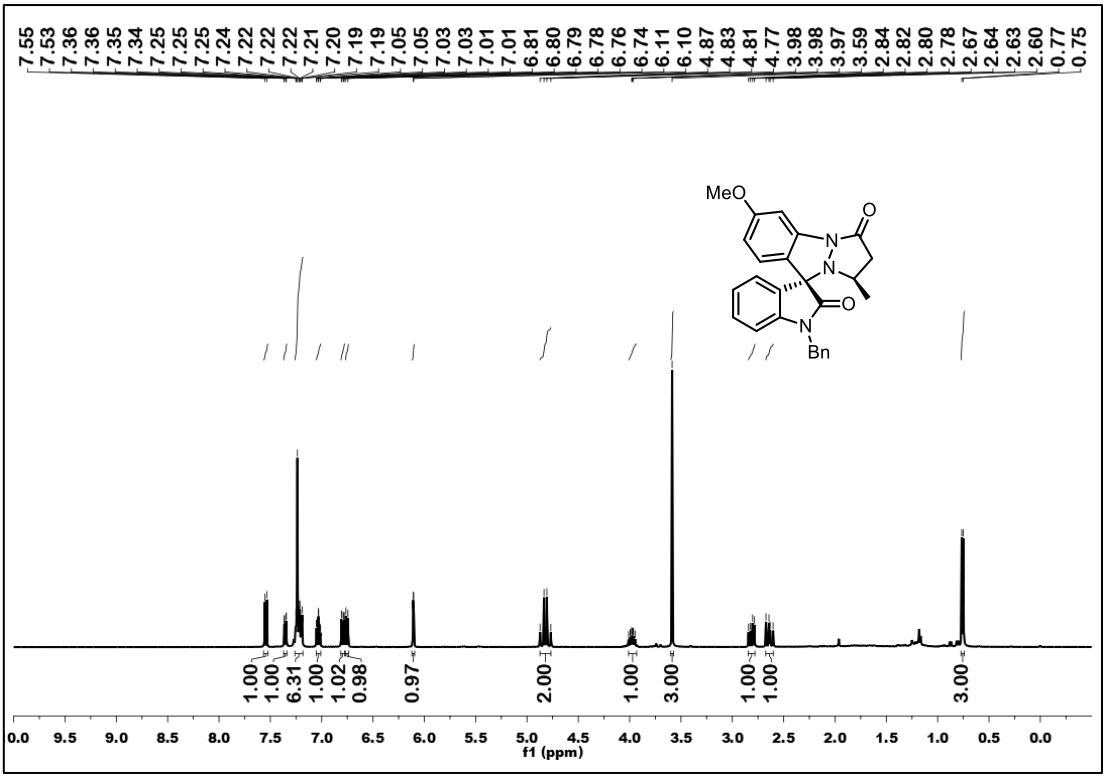

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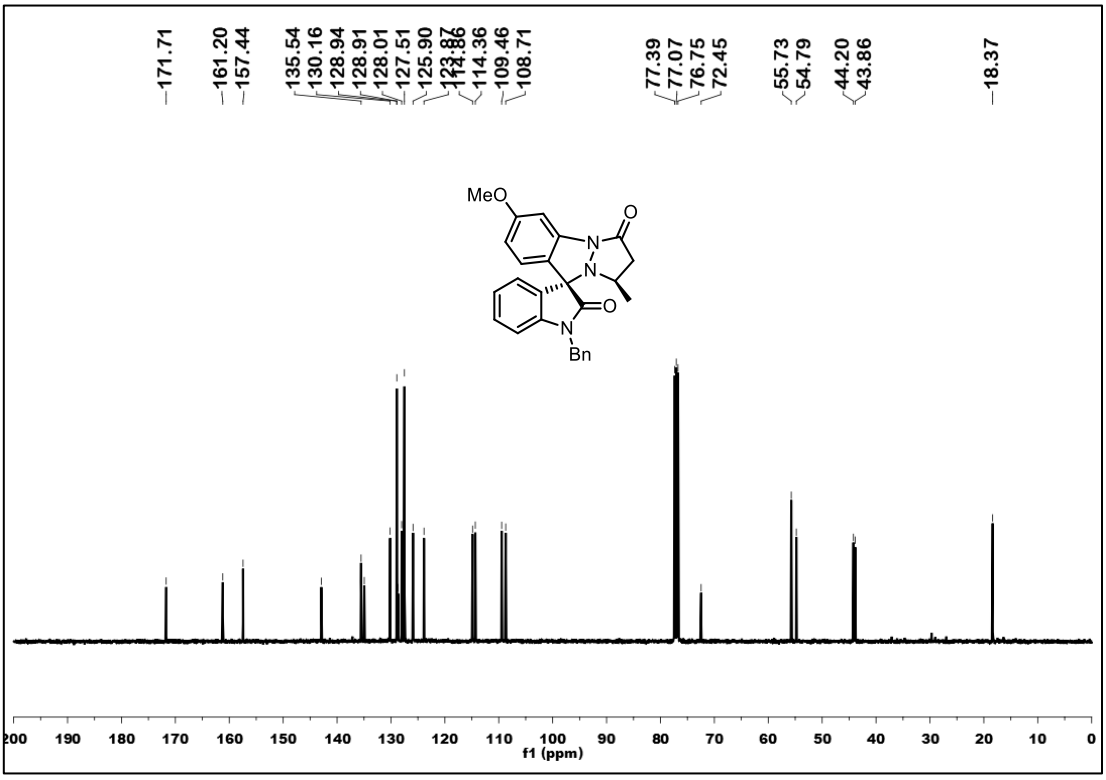

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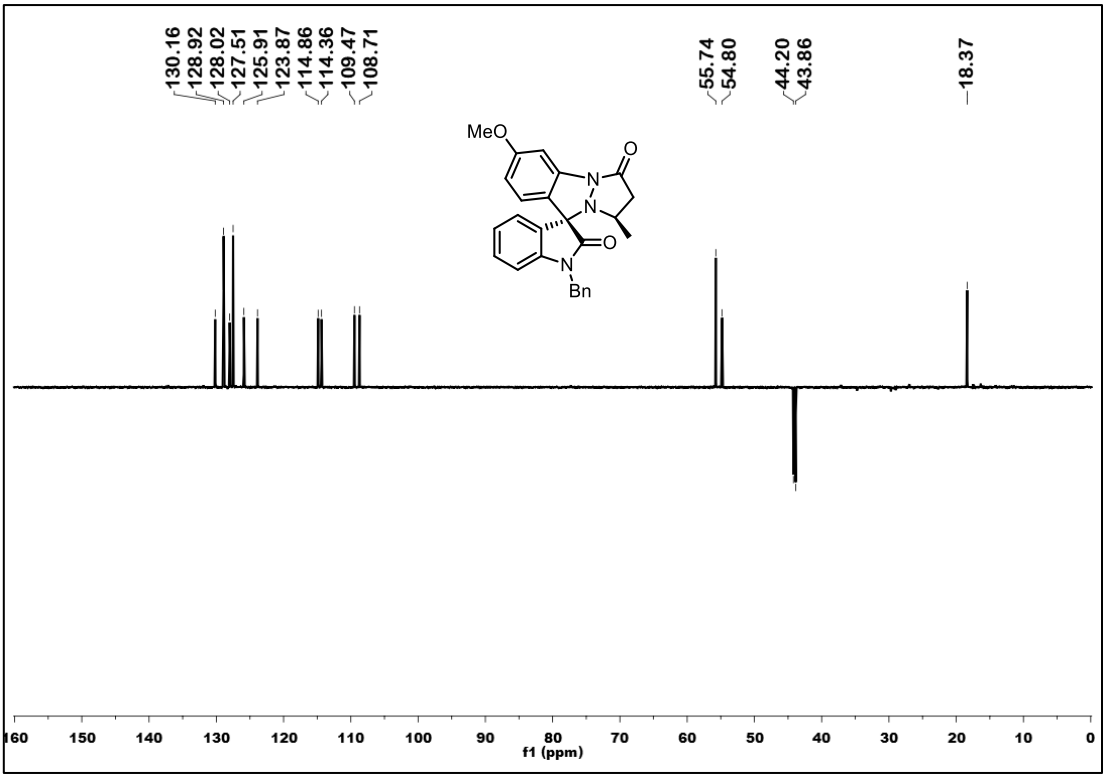

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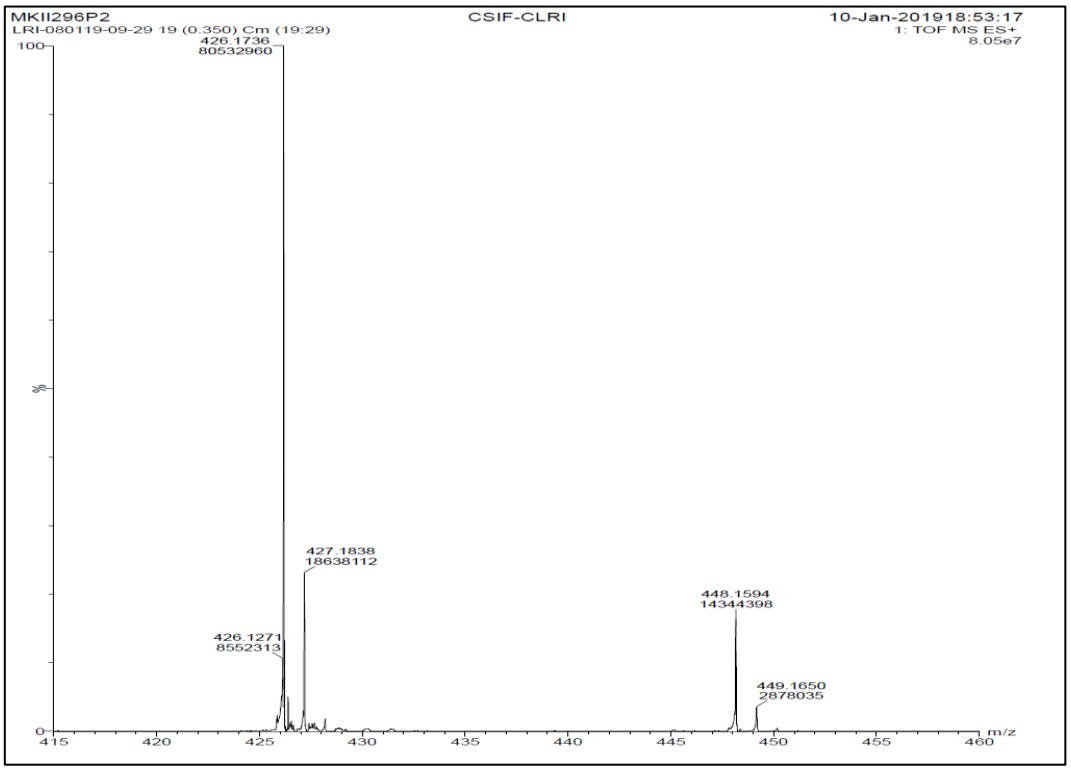

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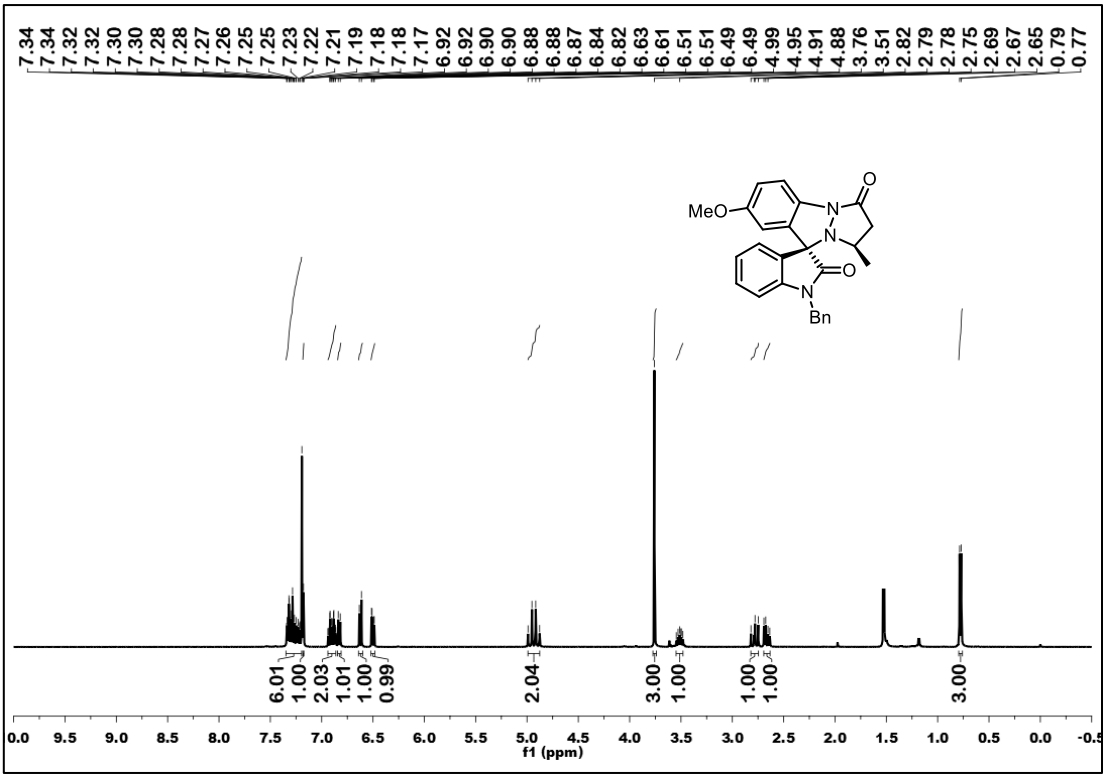

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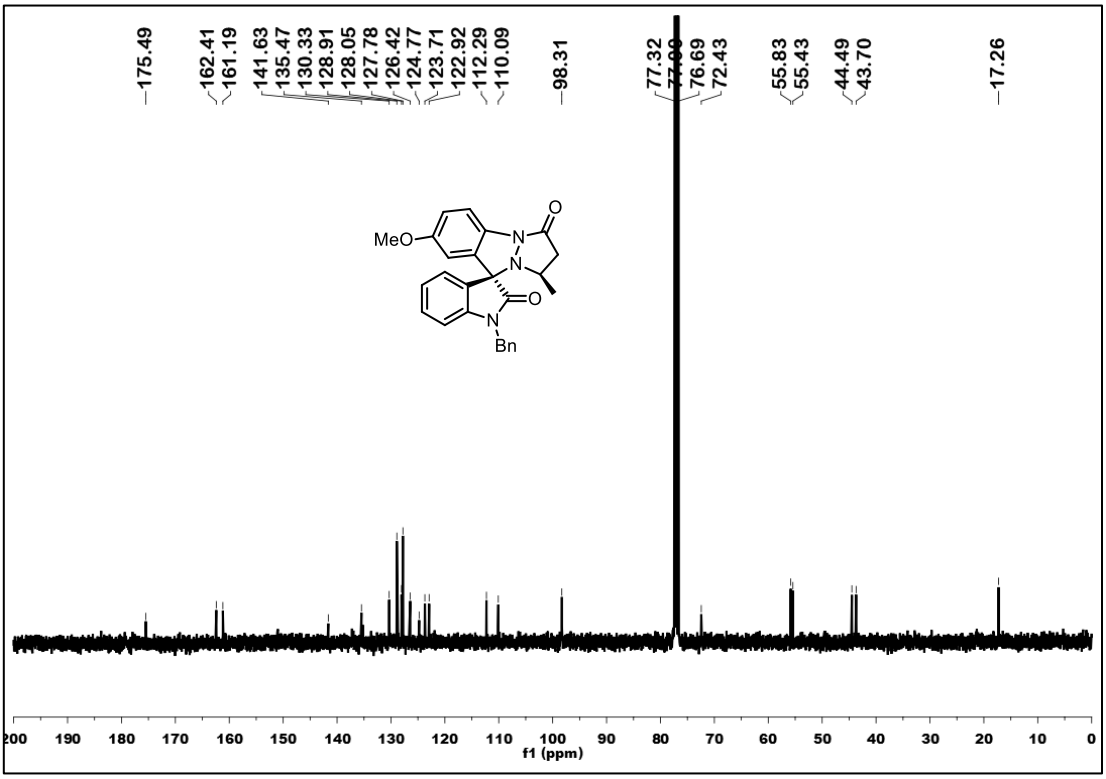

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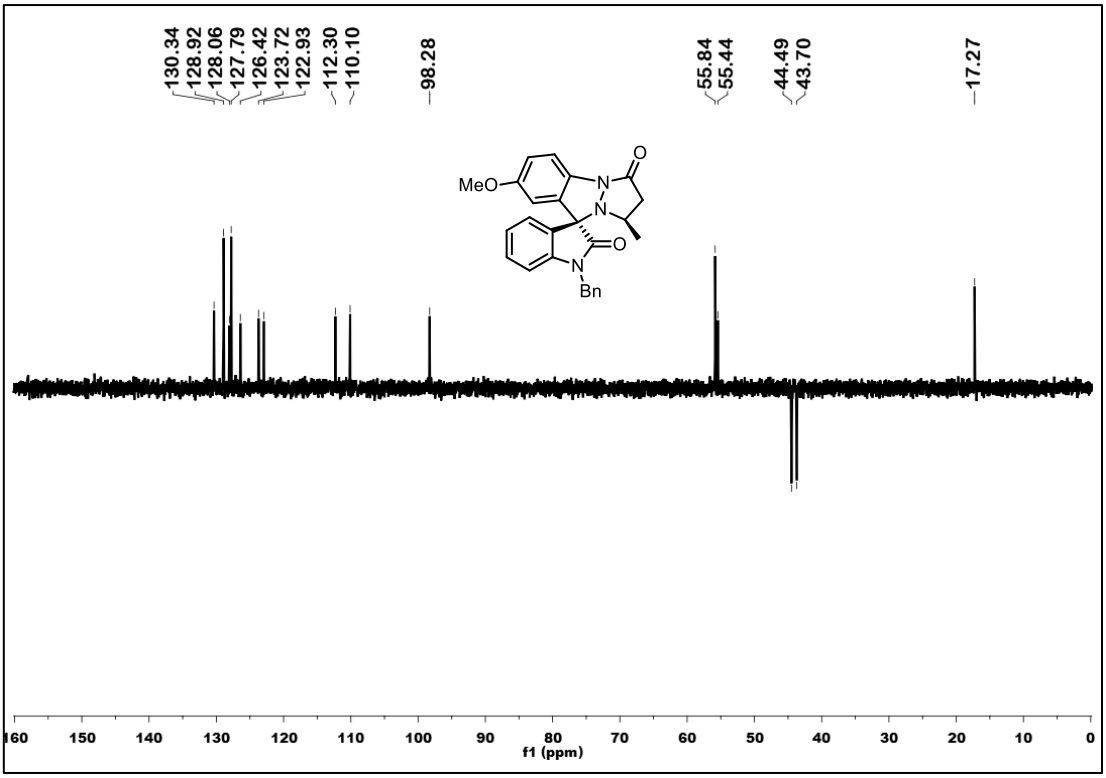

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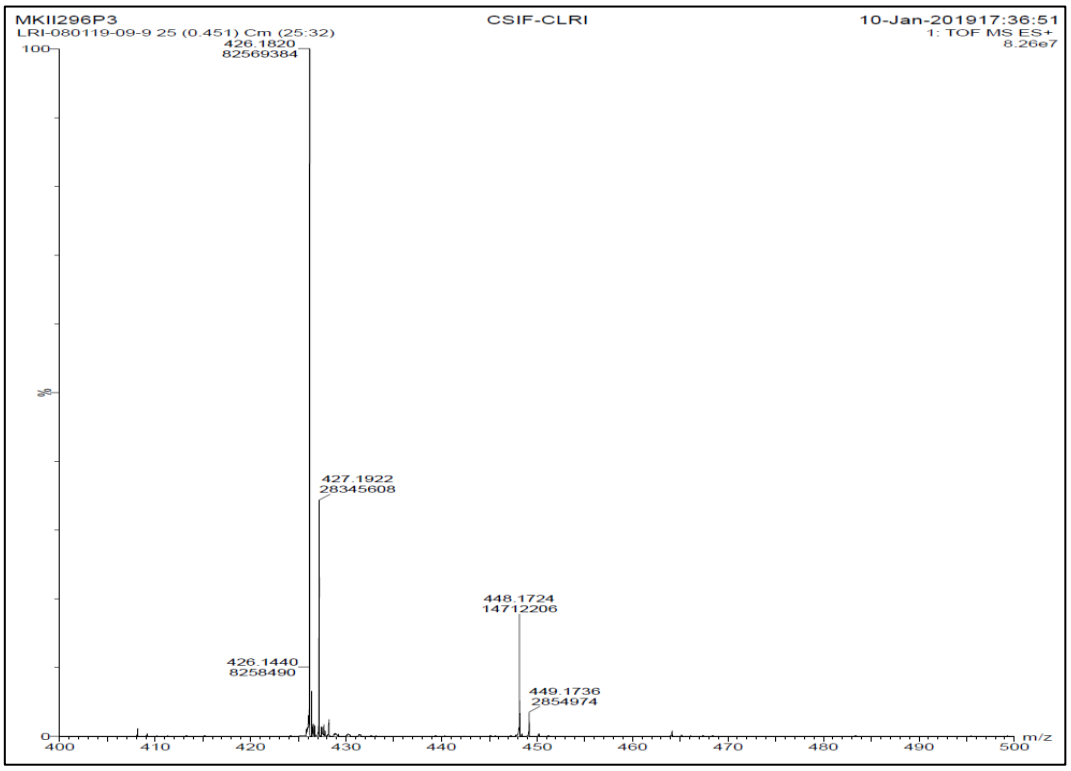

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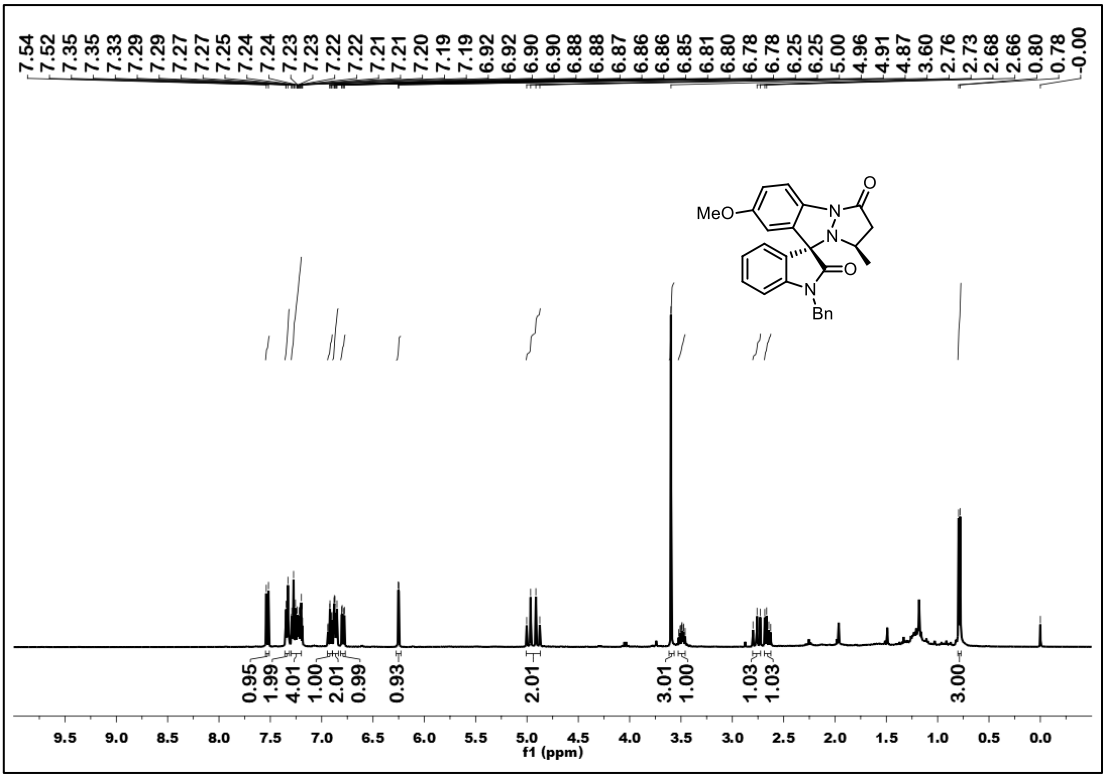

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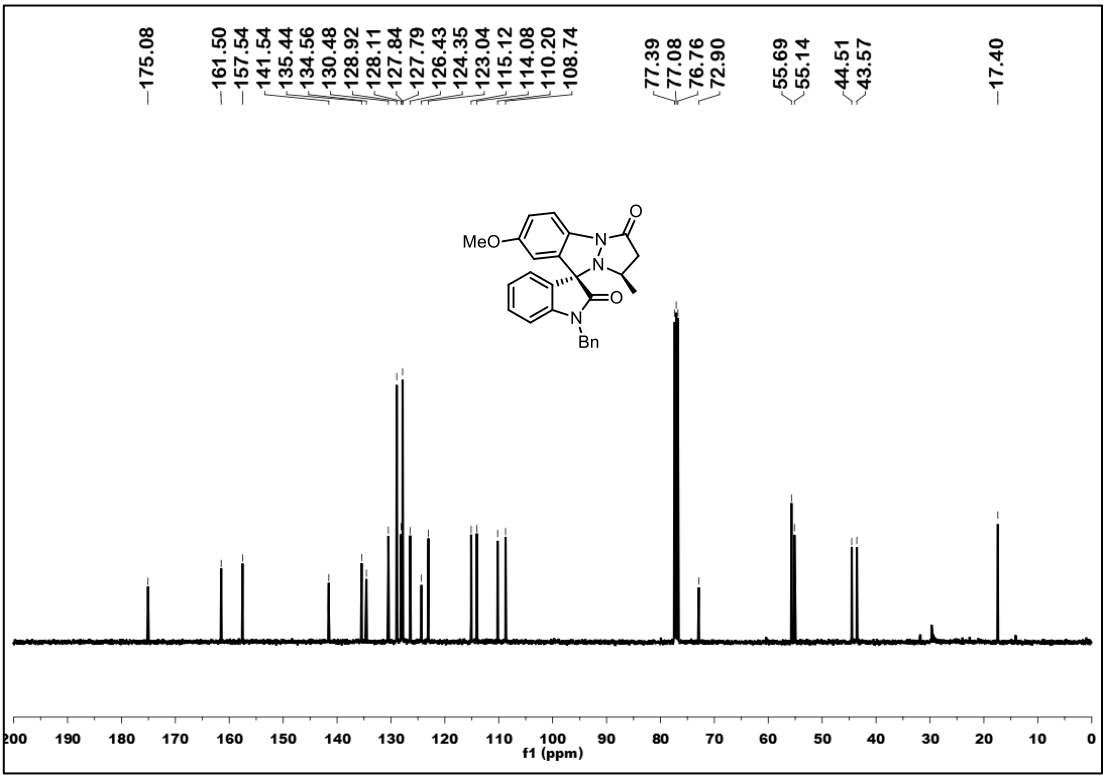

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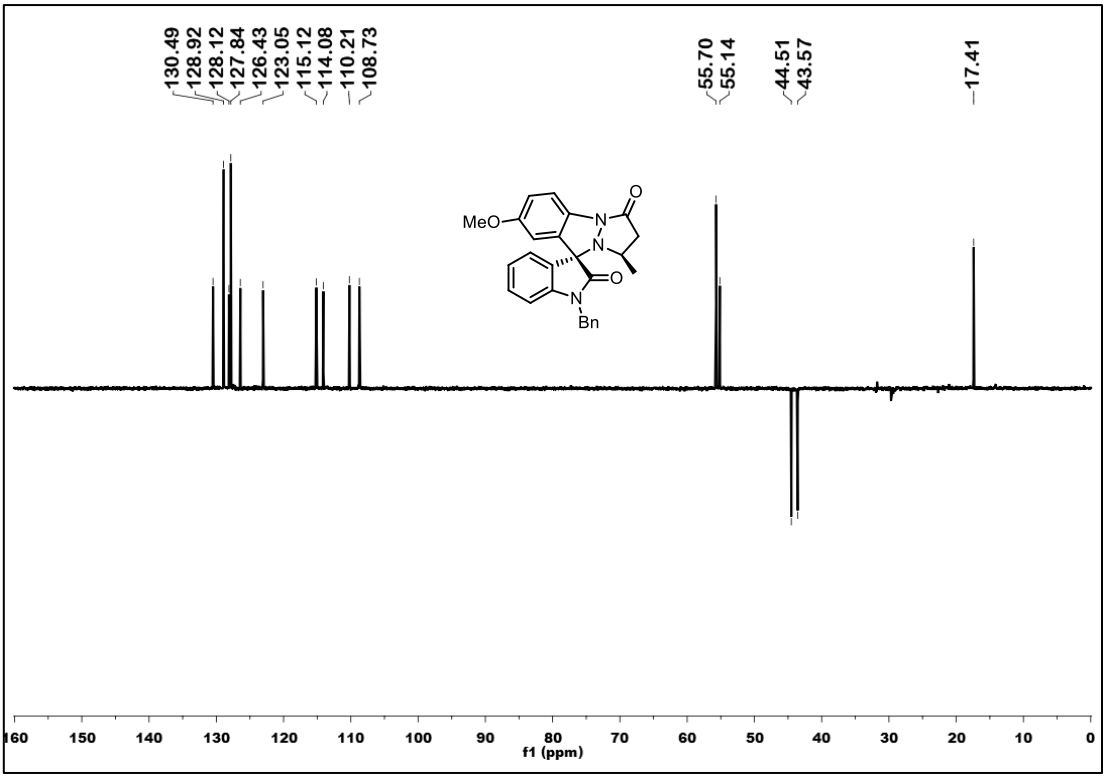

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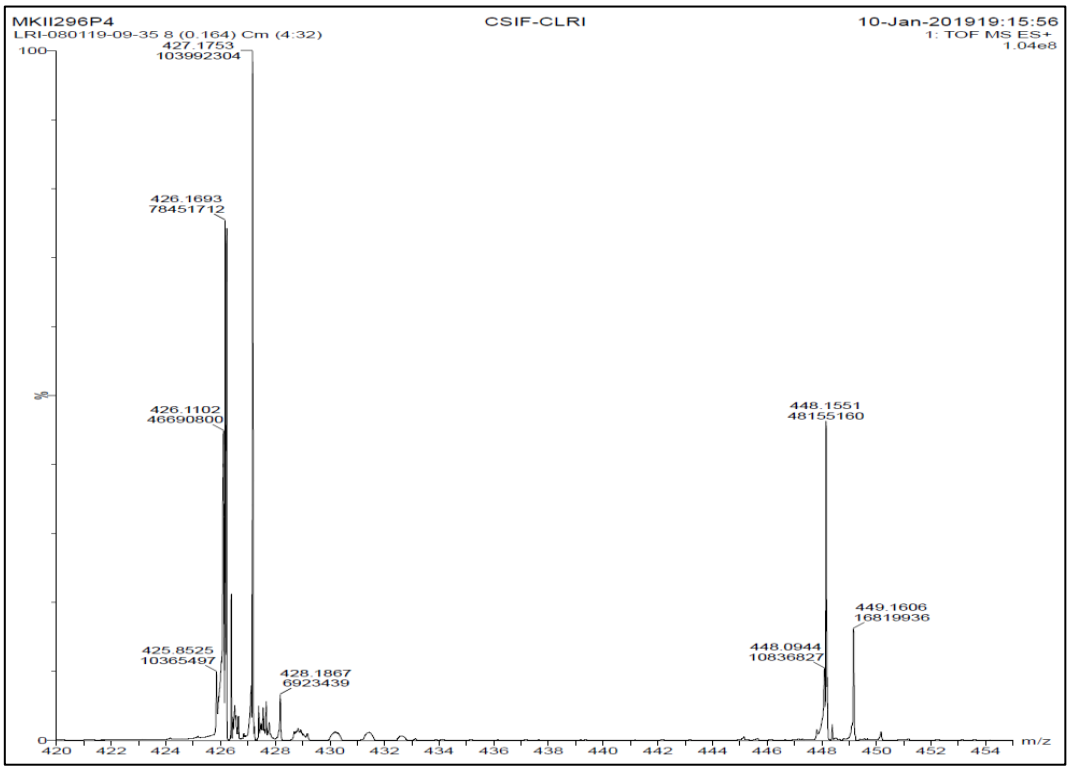

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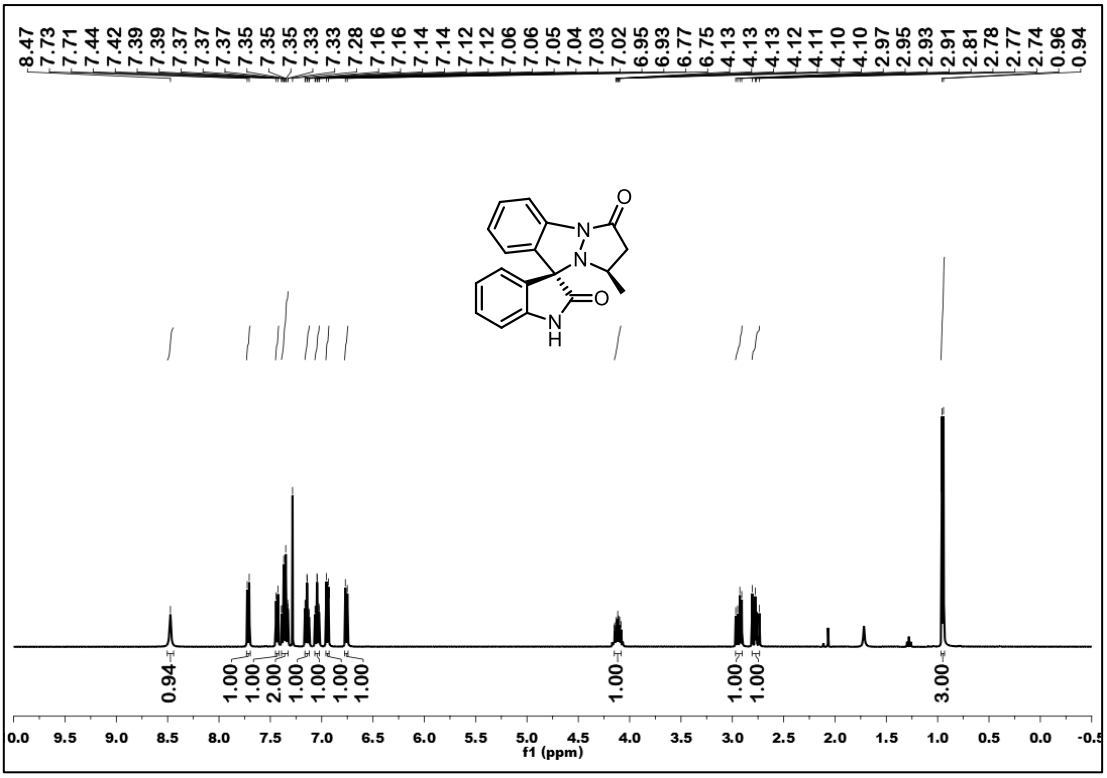

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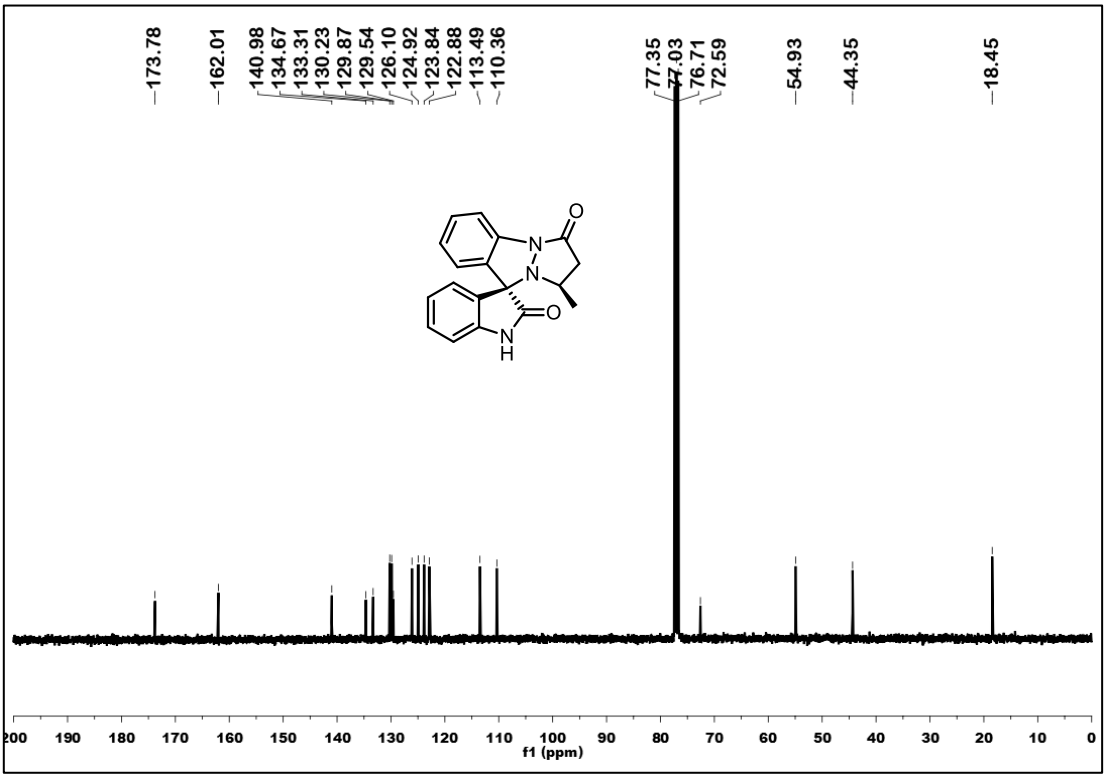

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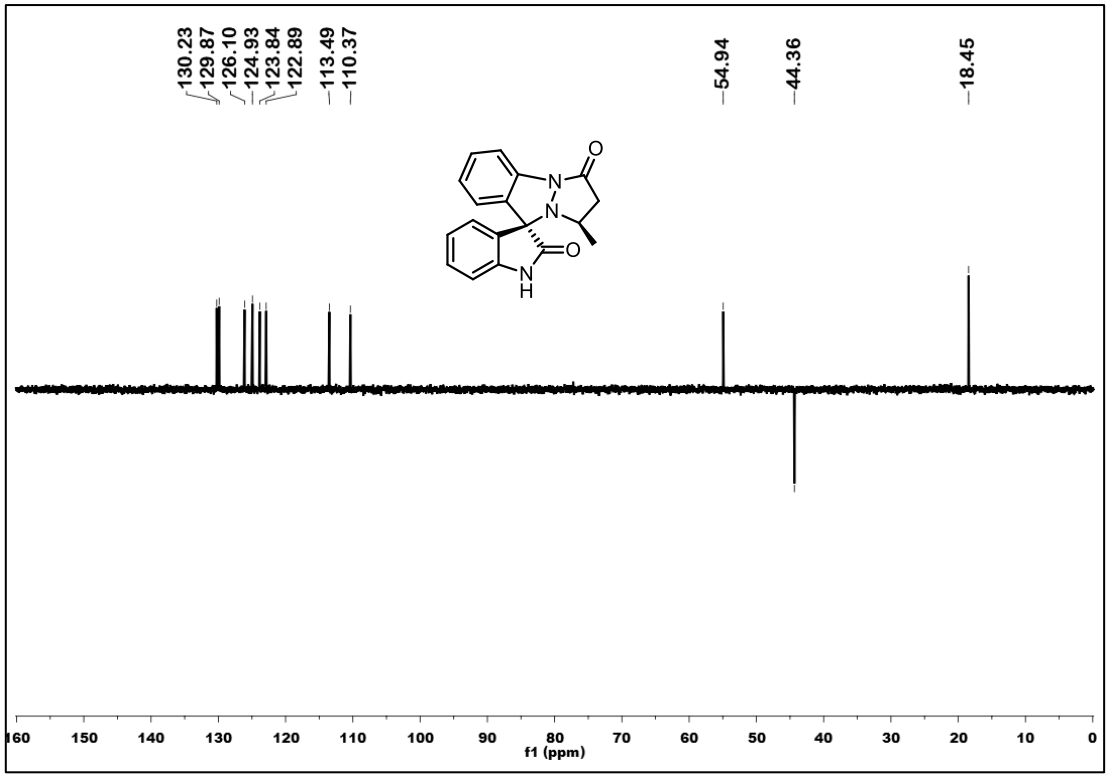

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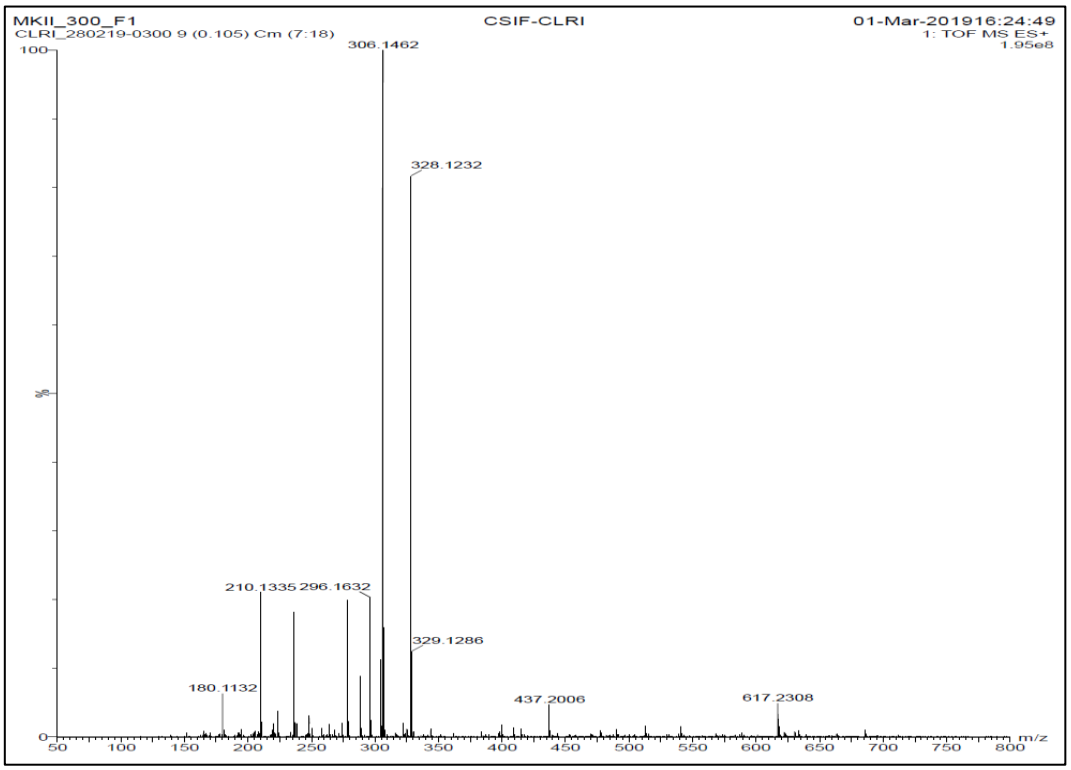

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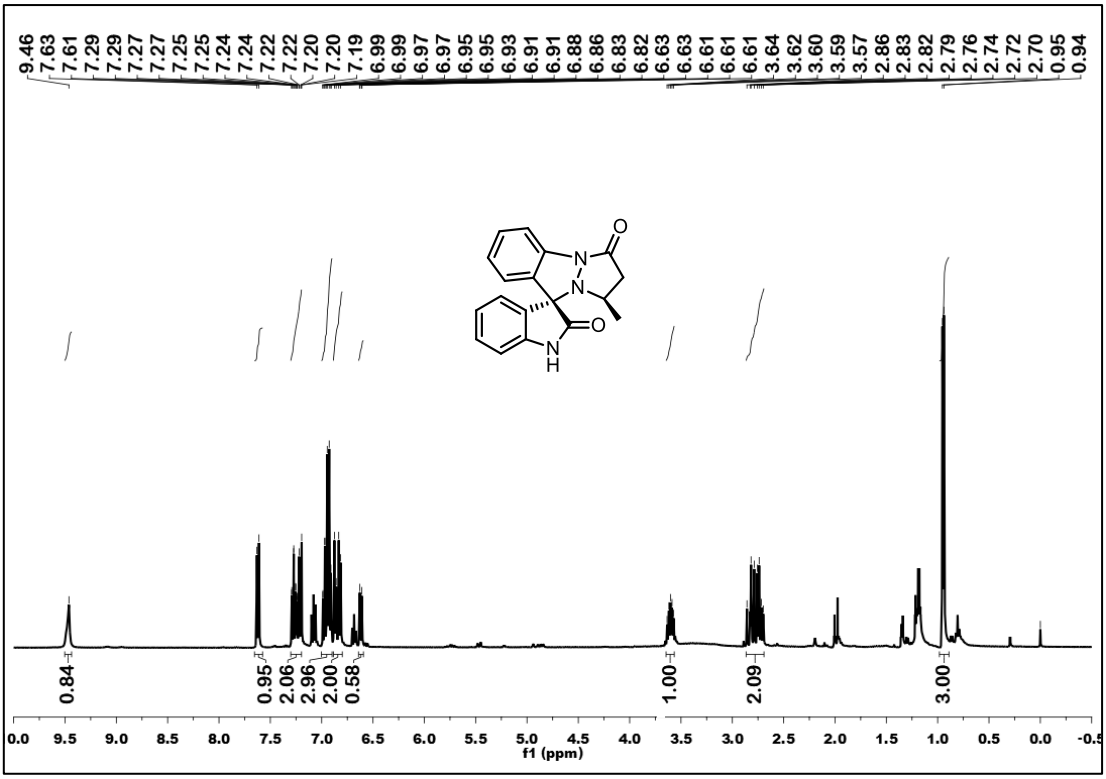

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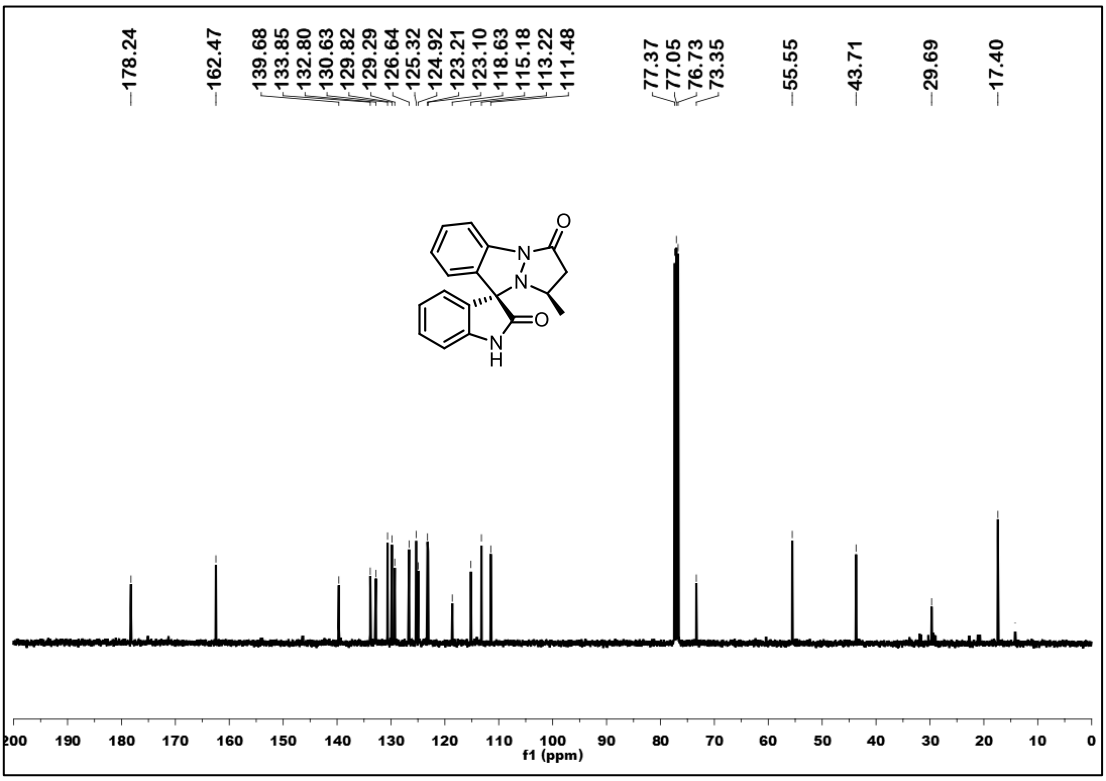
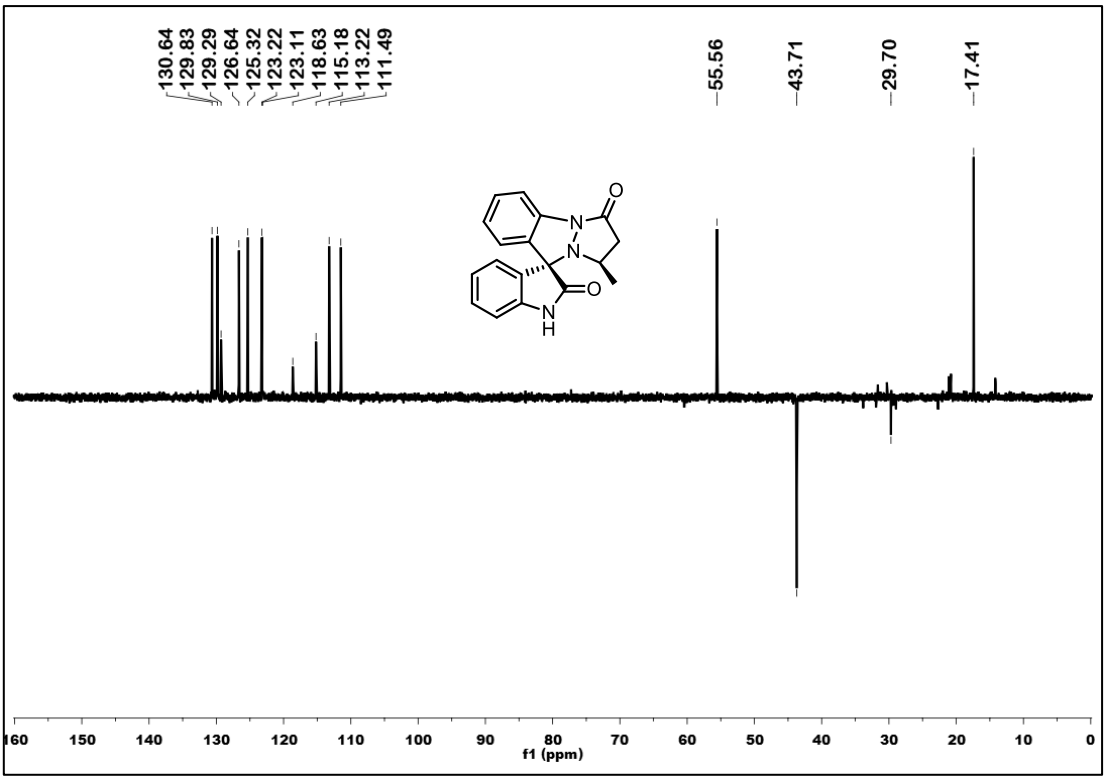
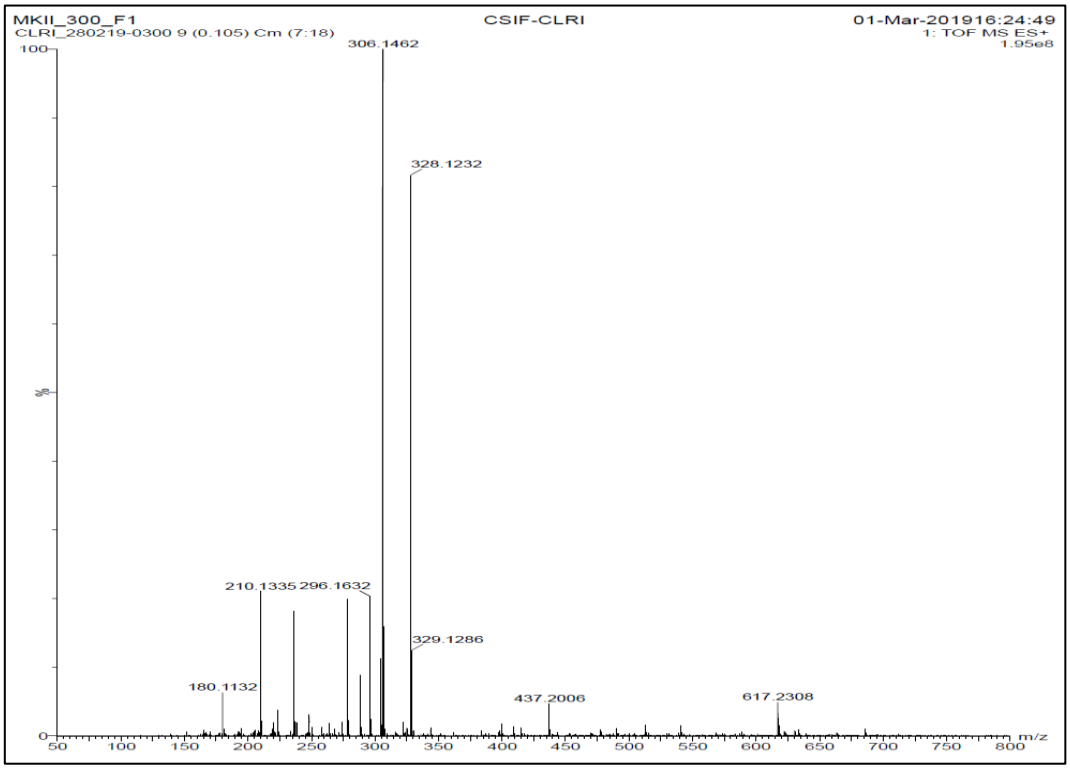


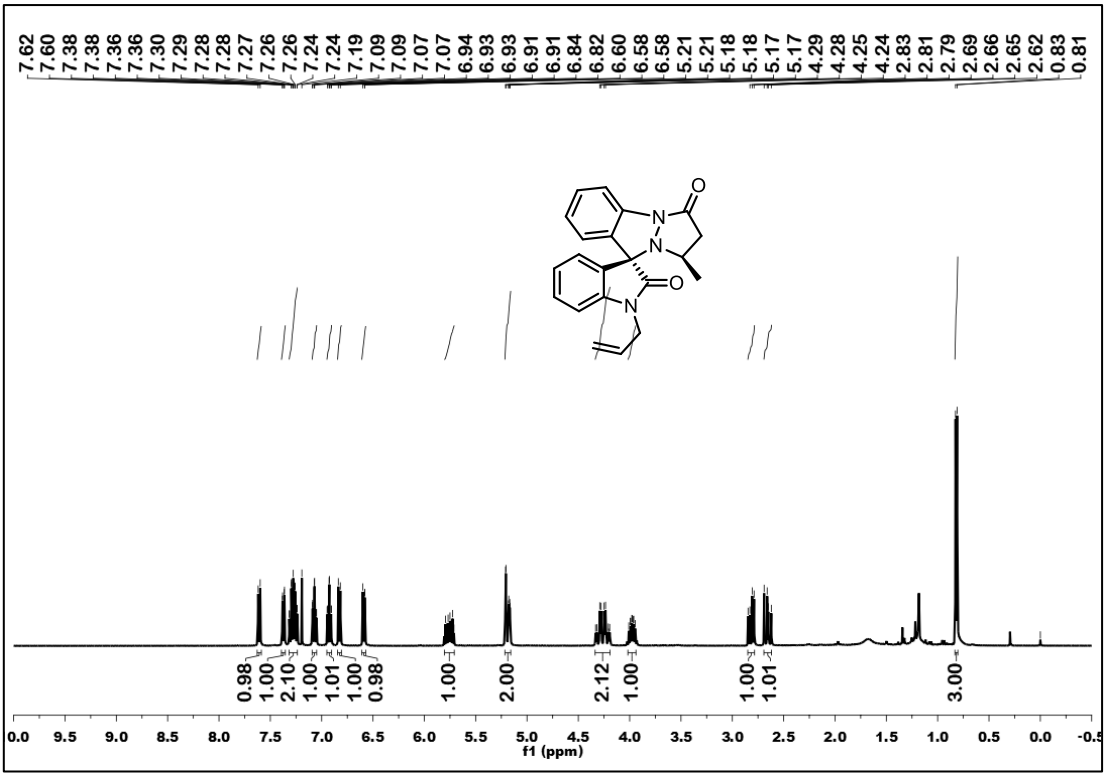
^{13}C NMR spectrum of compound **5e**



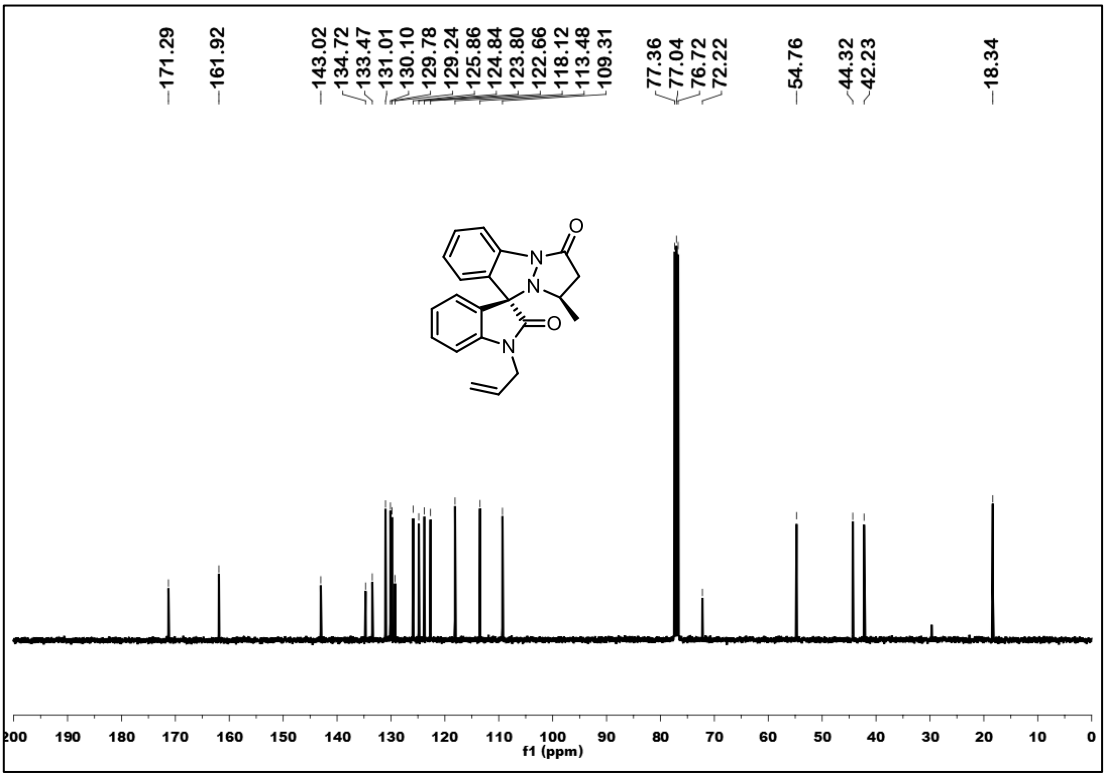
DEPT- 135 NMR spectrum of compound **5e**



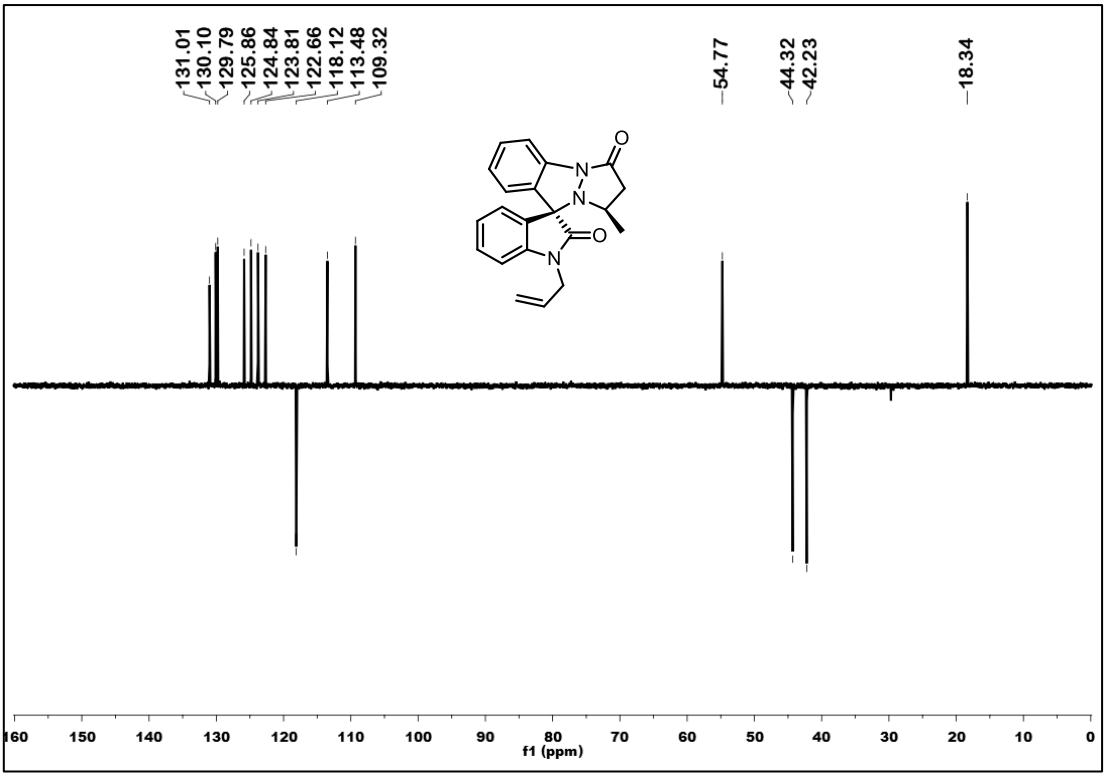
HRMS-Mass spectrum of compound **5e**



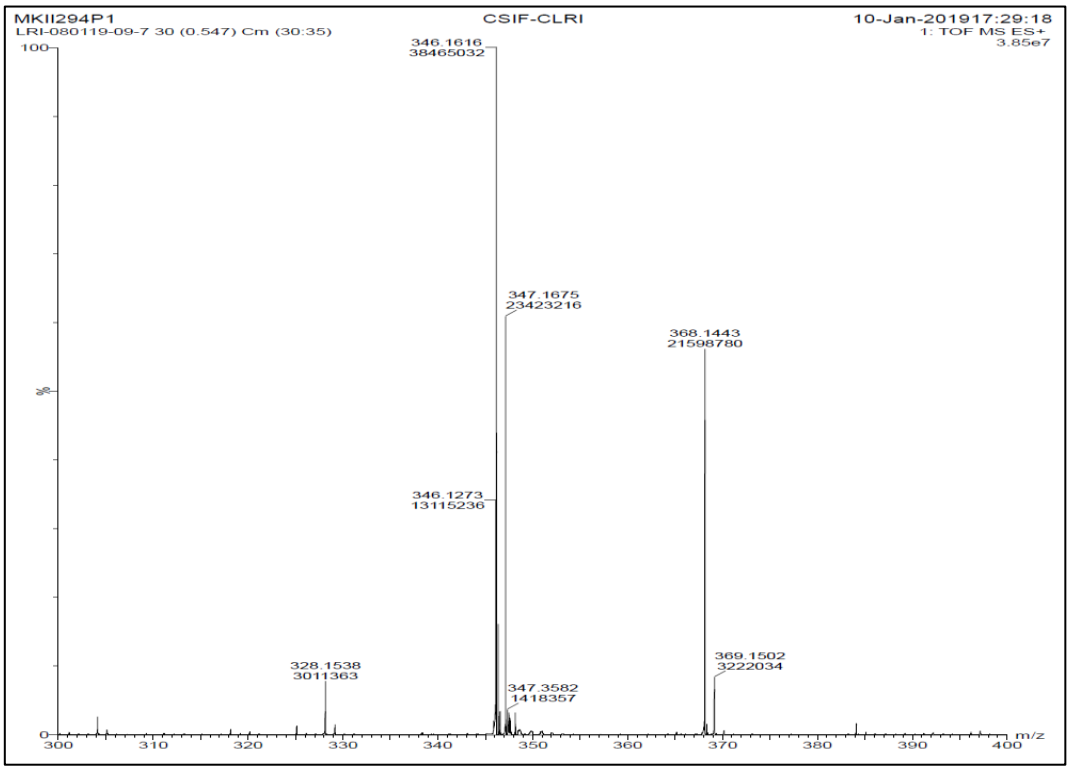
^{1}H NMR spectrum of compound **4f**



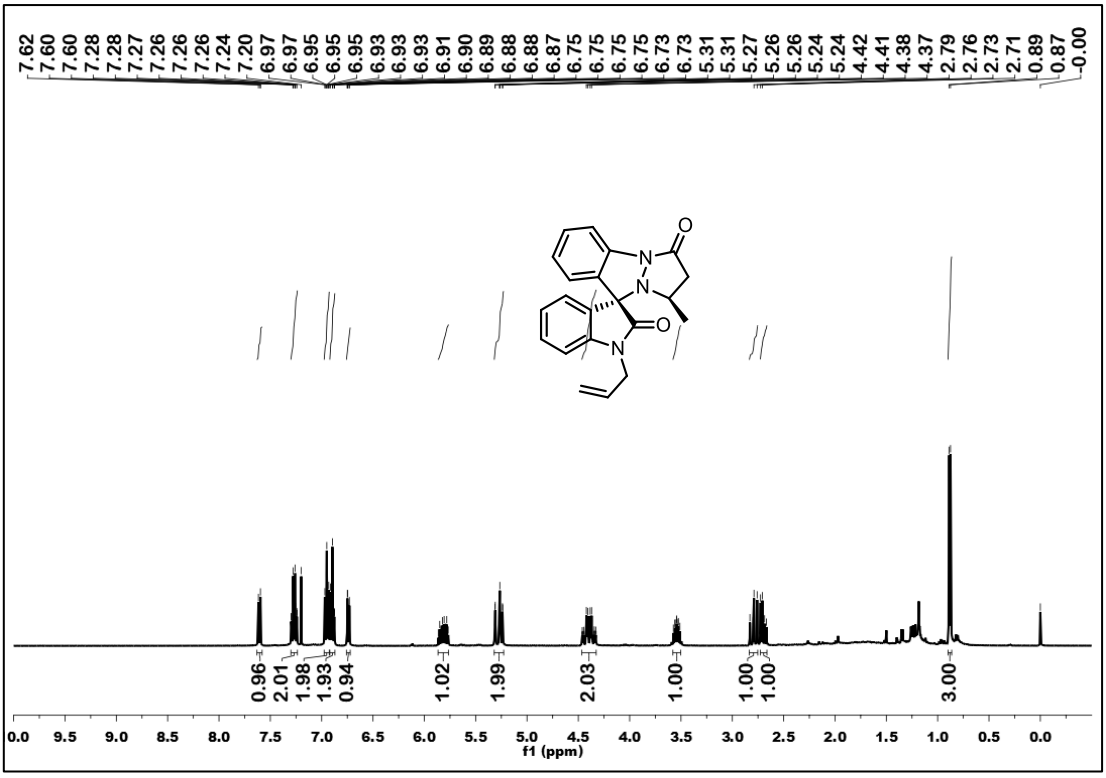
^{13}C NMR spectrum of compound **4f**



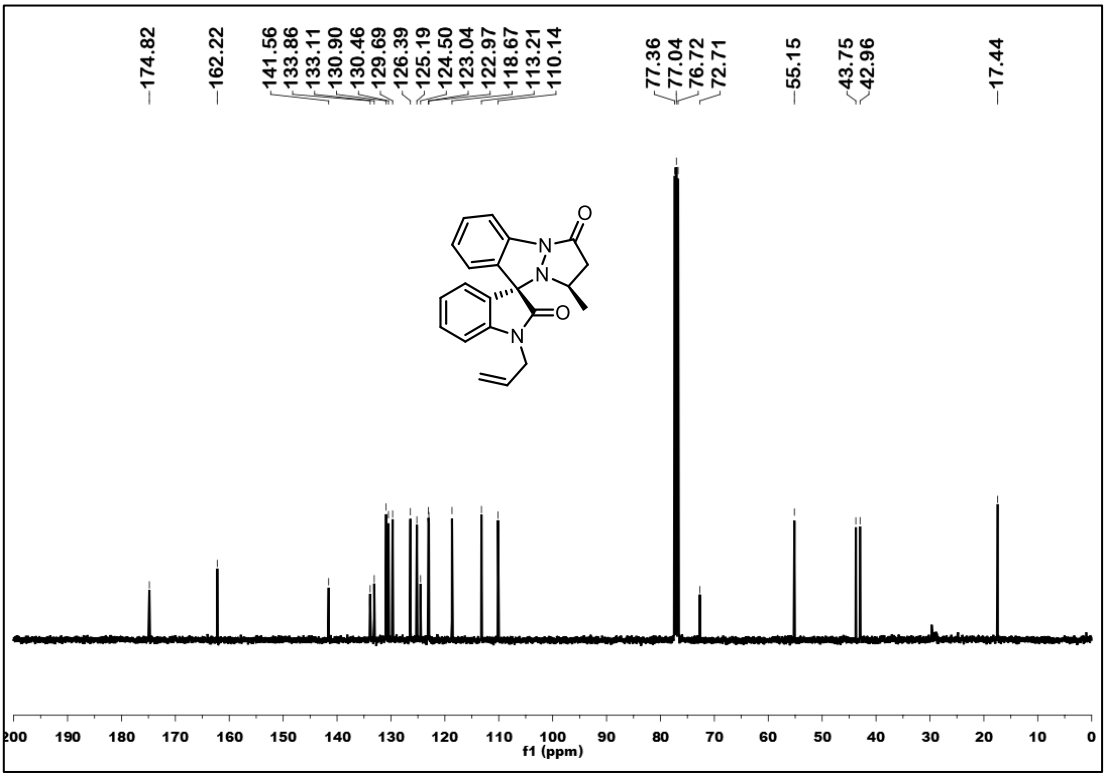
DEPT- 135 NMR spectrum of compound **4f**



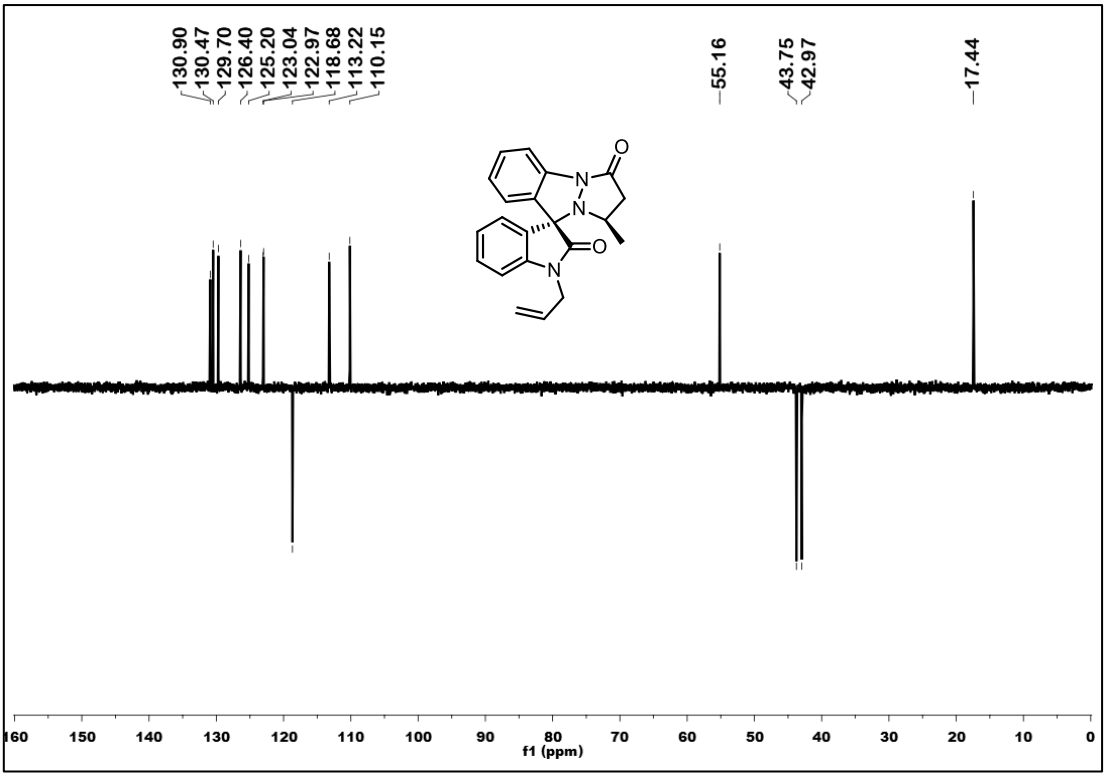
HRMS-Mass spectrum of compound **4f**



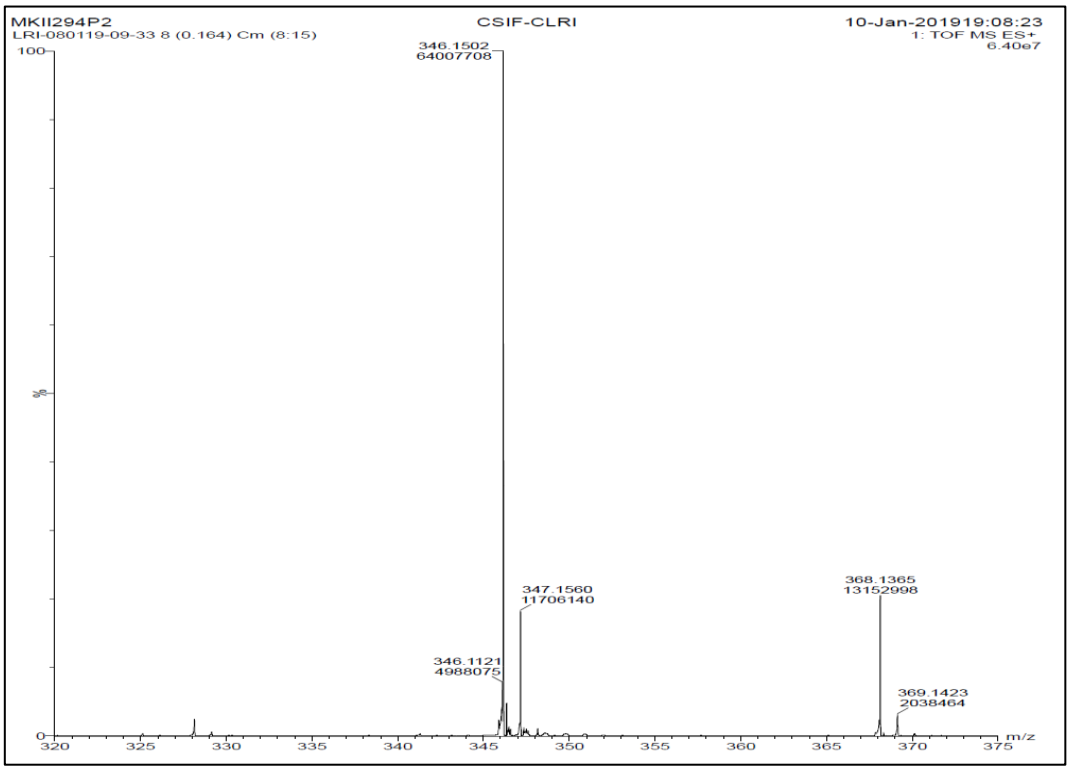
^{1}H NMR spectrum of compound **5f**



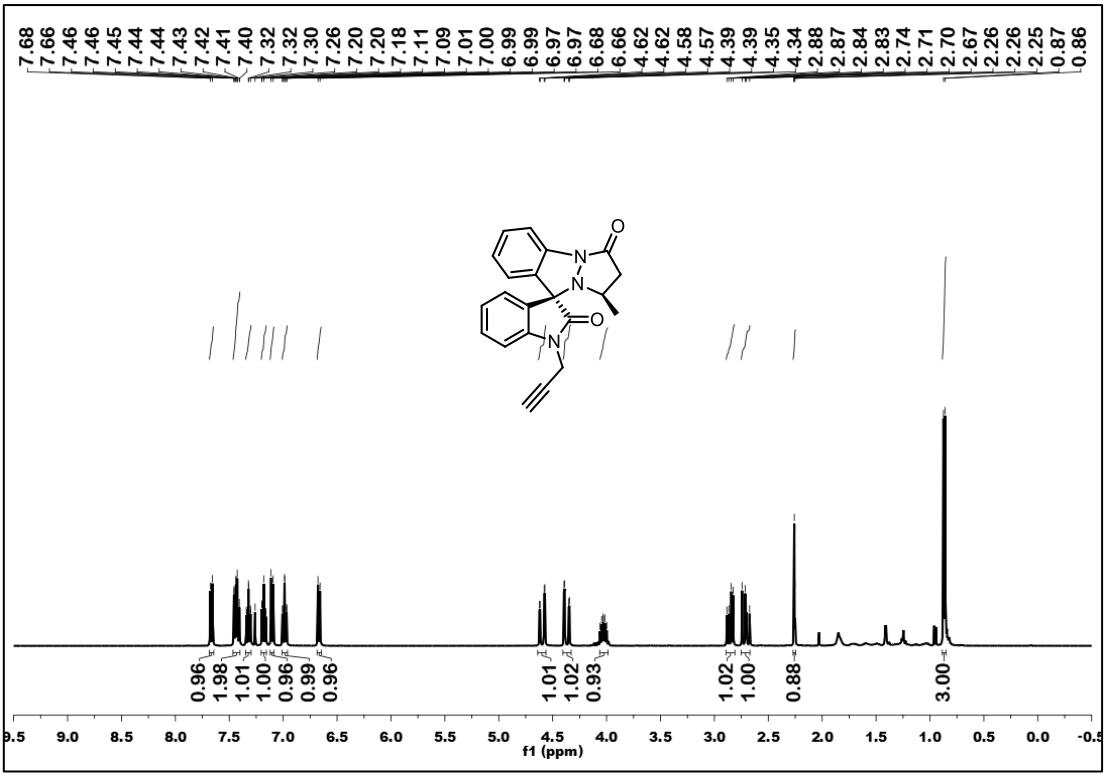
^{13}C NMR spectrum of compound **5f**



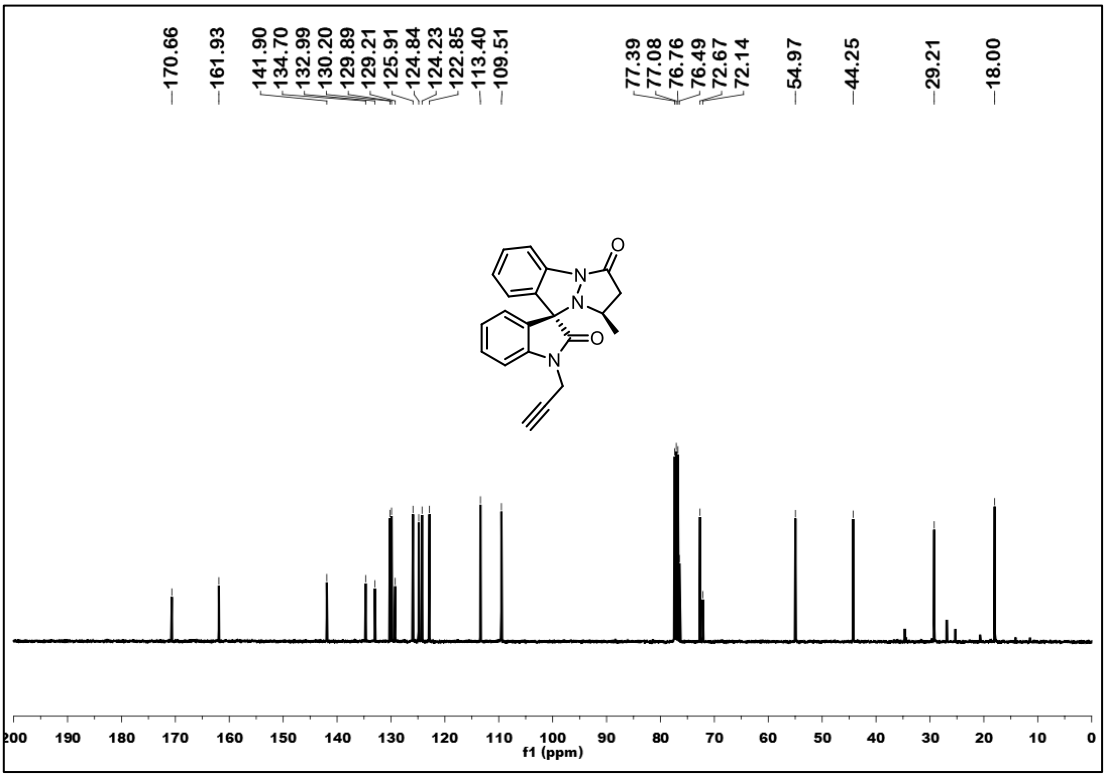
DEPT- 135 NMR spectrum of compound **5f**



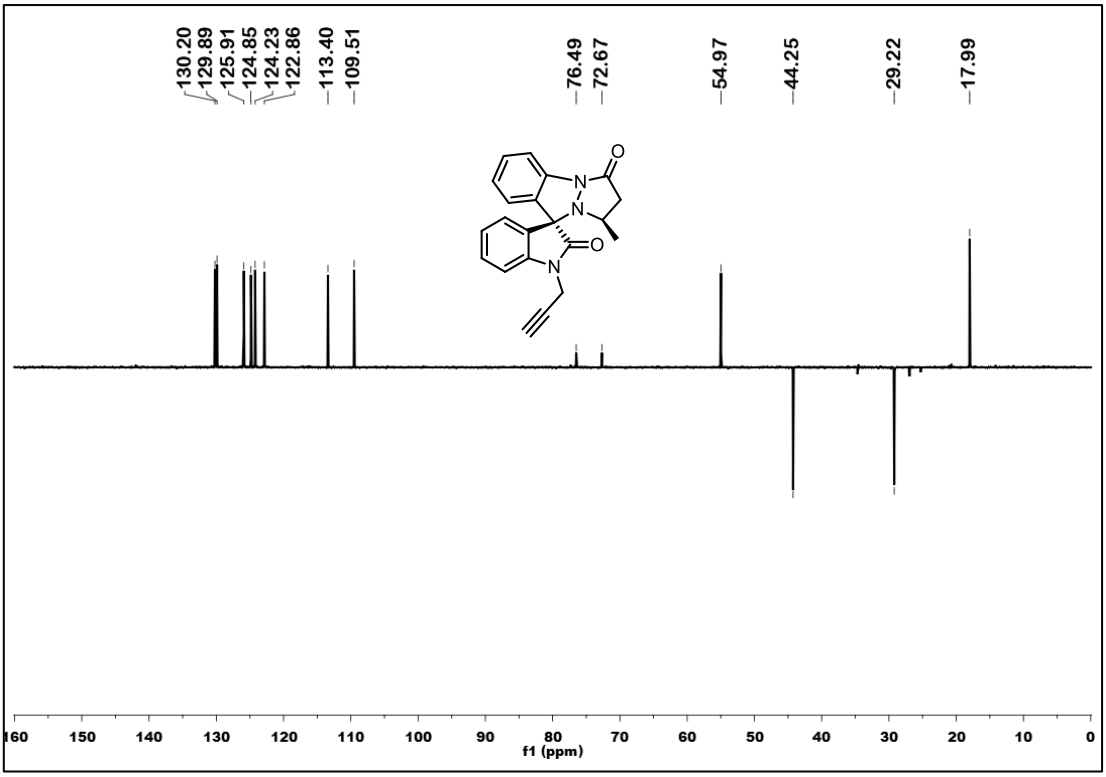
HRMS-Mass spectrum of compound **5f**



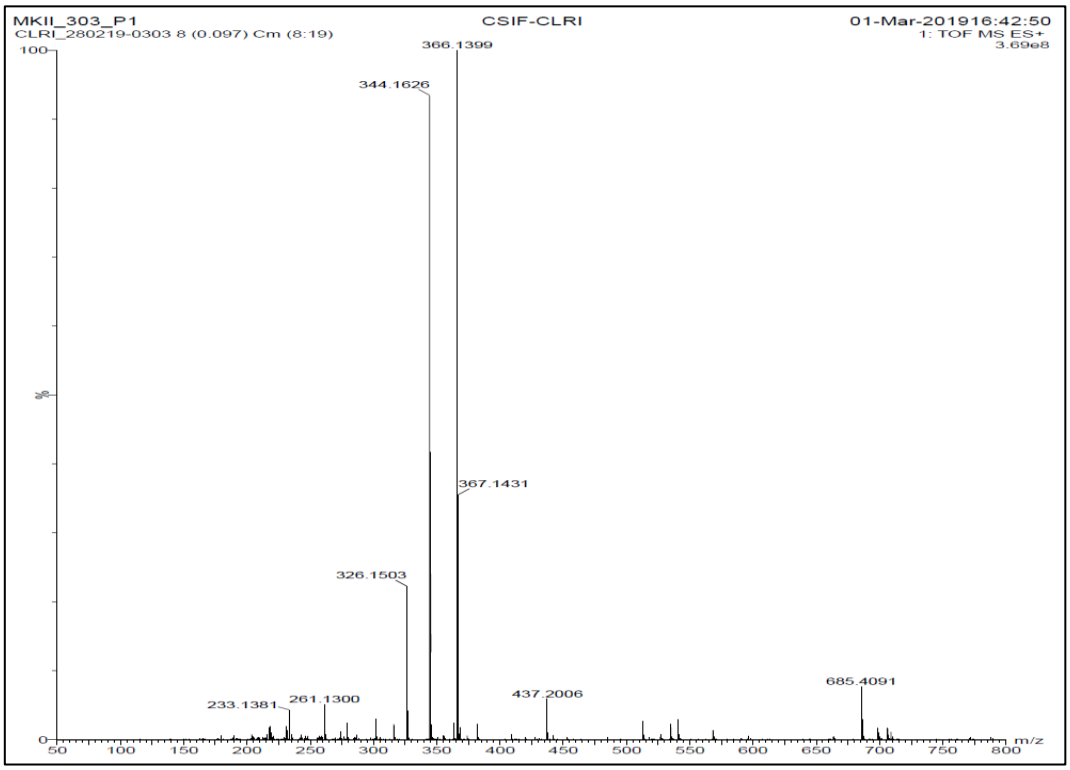
^{1}H NMR spectrum of compound **4g**



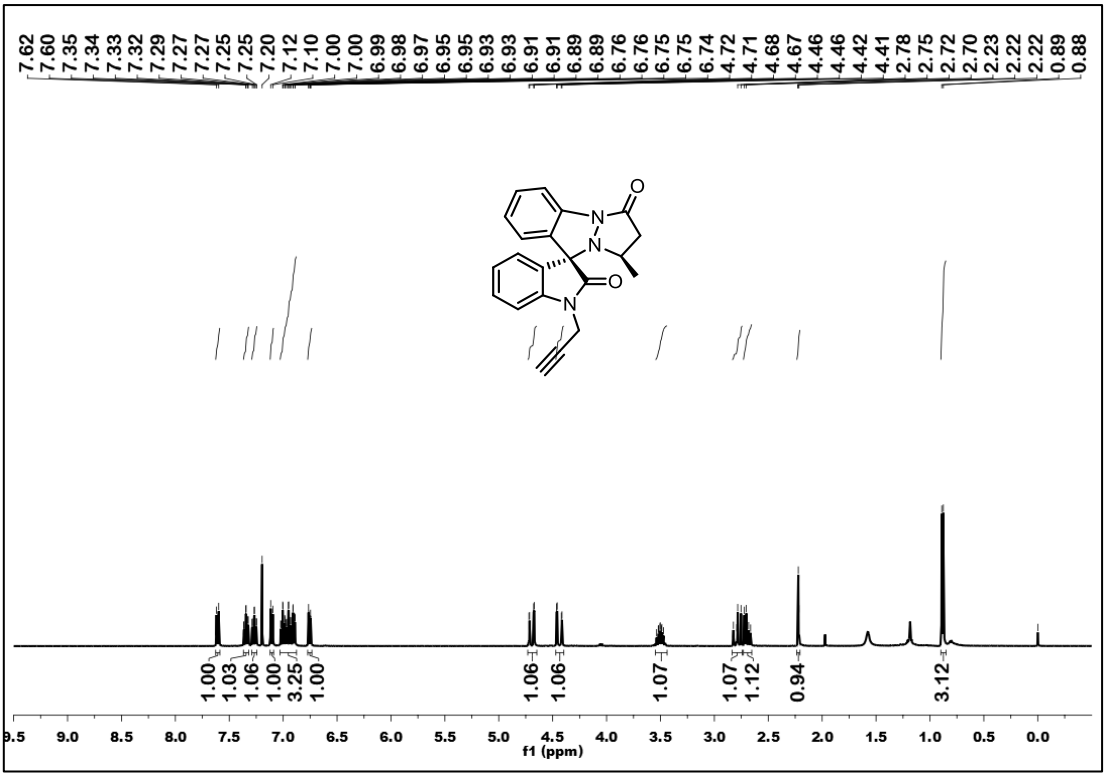
^{13}C NMR spectrum of compound **4g**



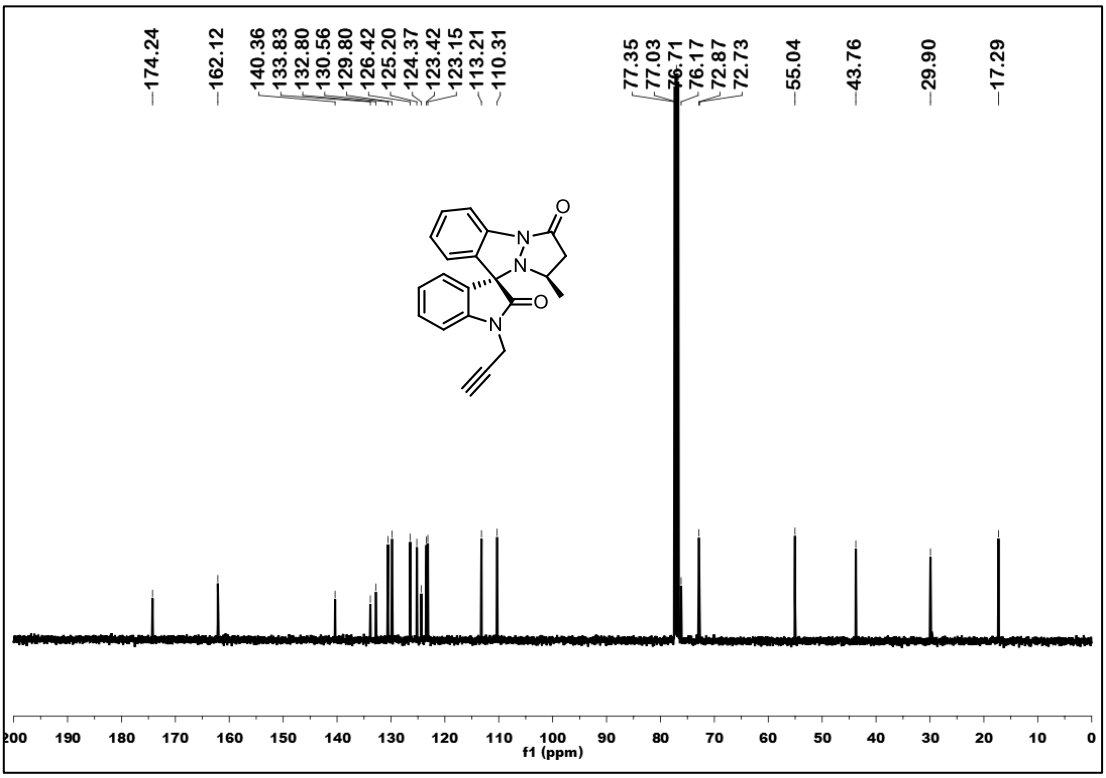
DEPT- 135 NMR spectrum of compound **4g**



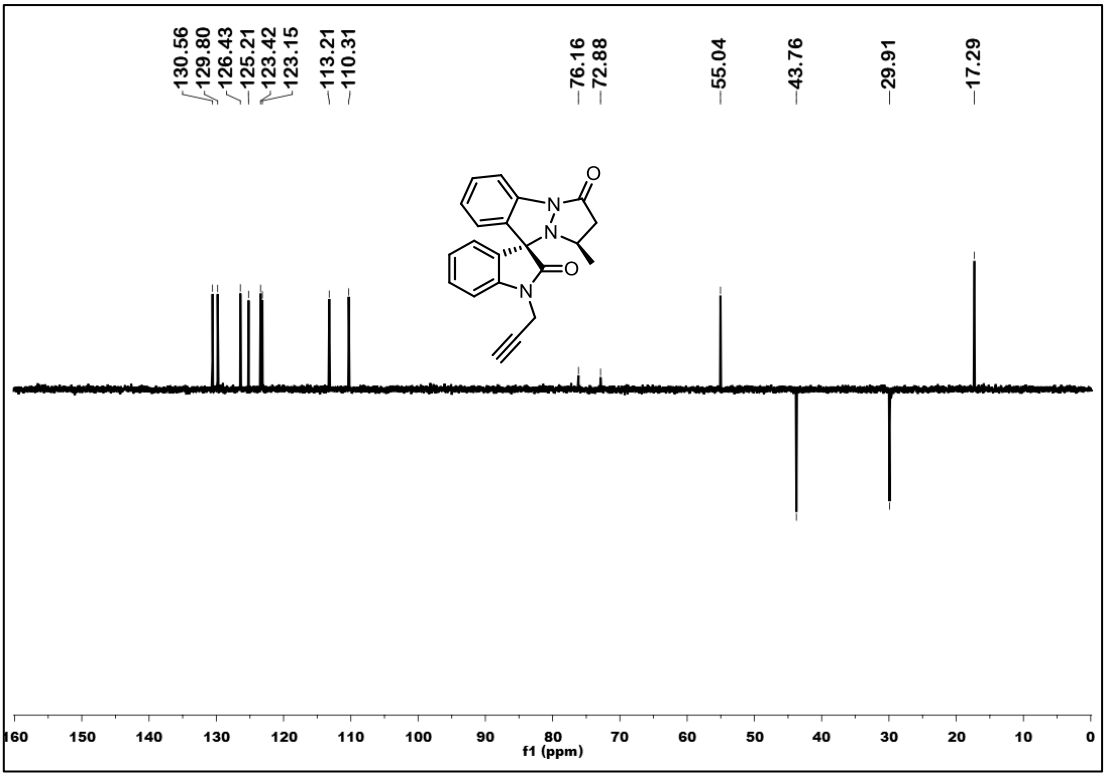
HRMS-Mass spectrum of compound **4g**



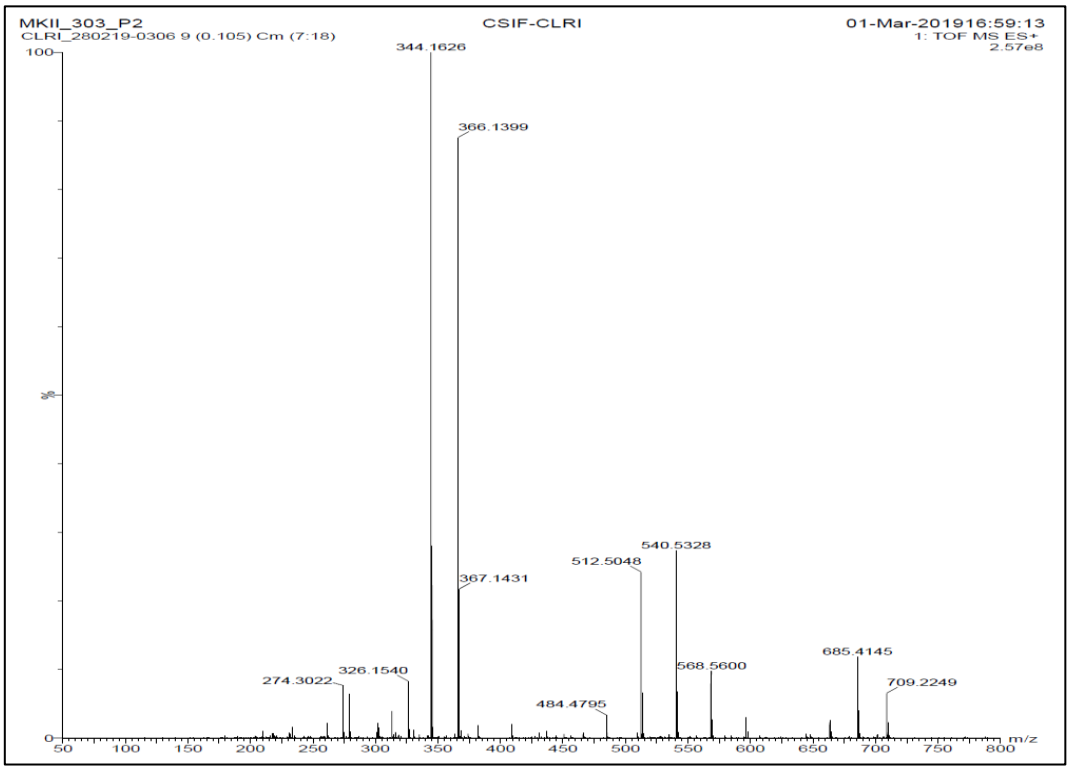
^{1}H NMR spectrum of compound **5g**



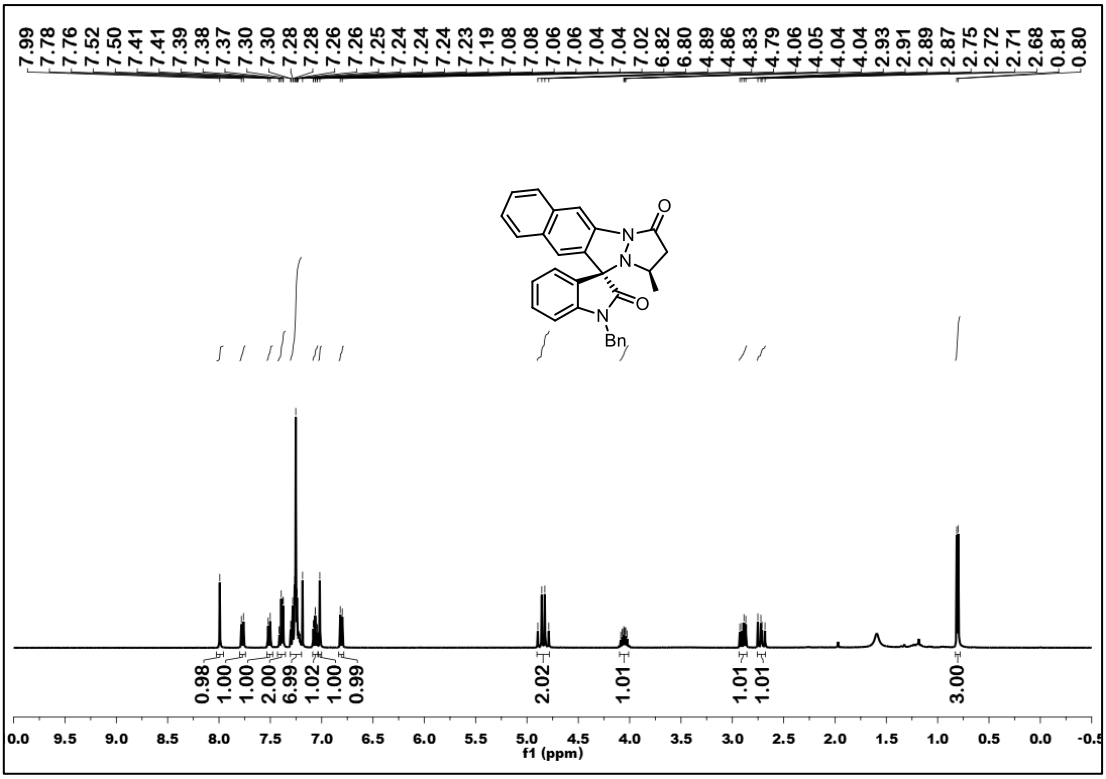
^{13}C NMR spectrum of compound **5g**



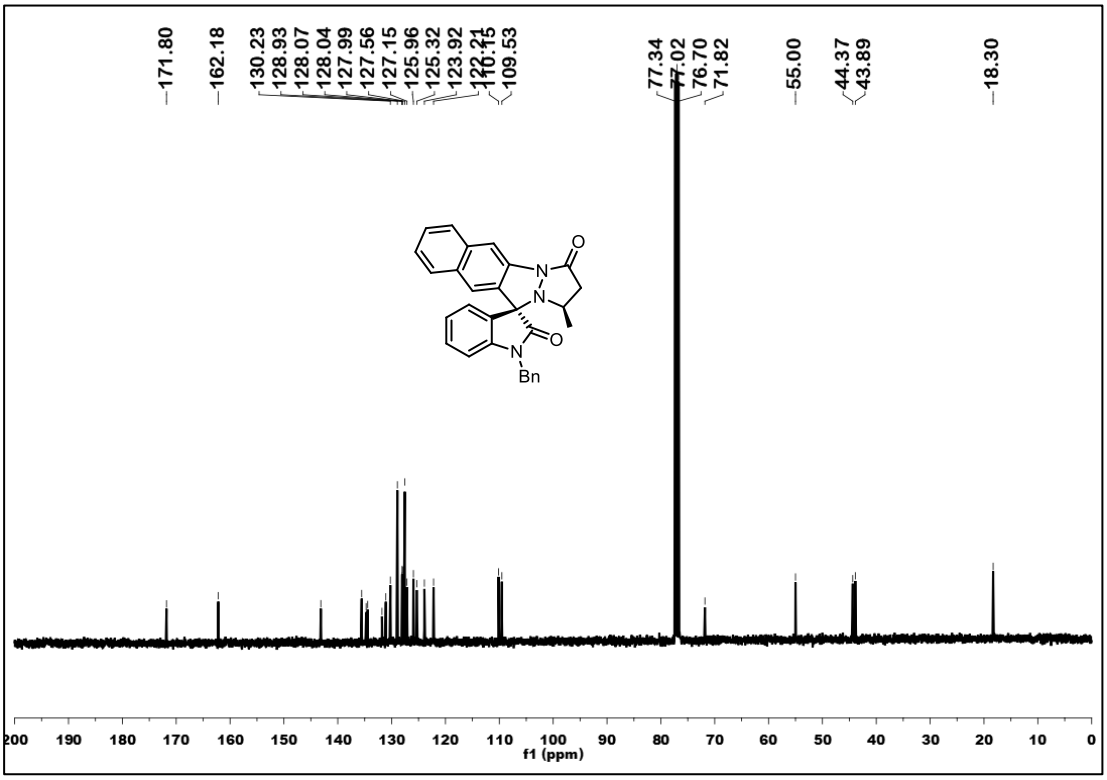
DEPT- 135 NMR spectrum of compound **5g**



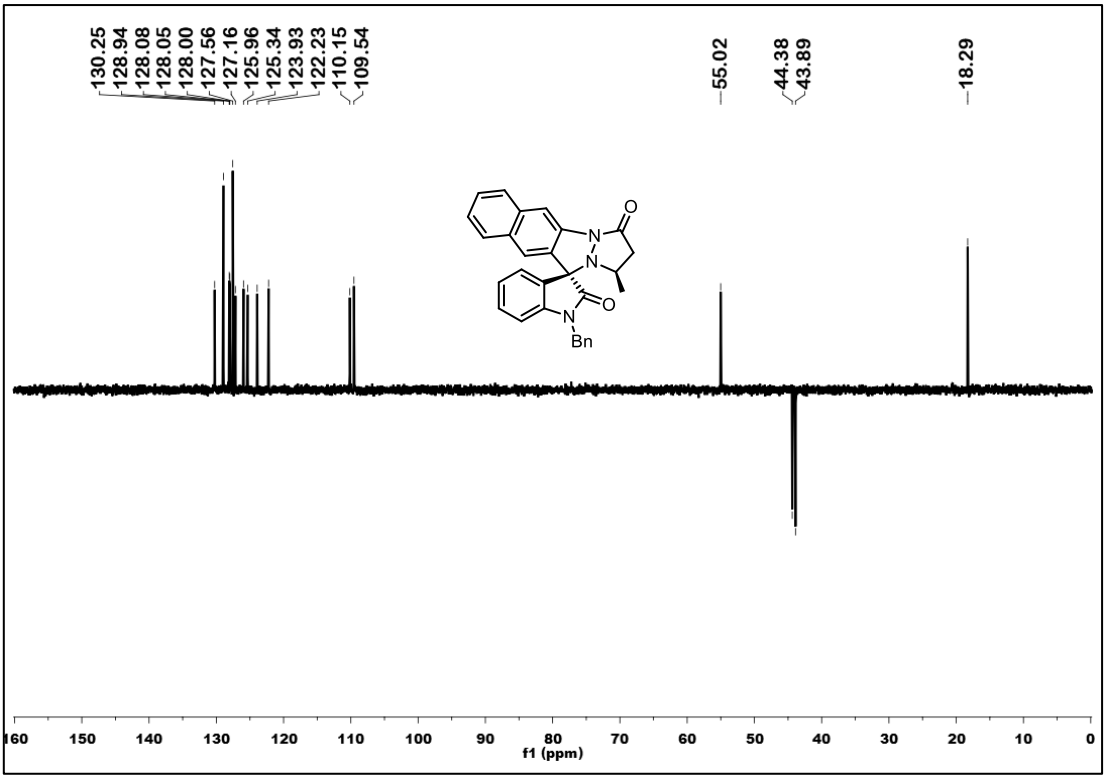
HRMS-Mass spectrum of compound **5g**



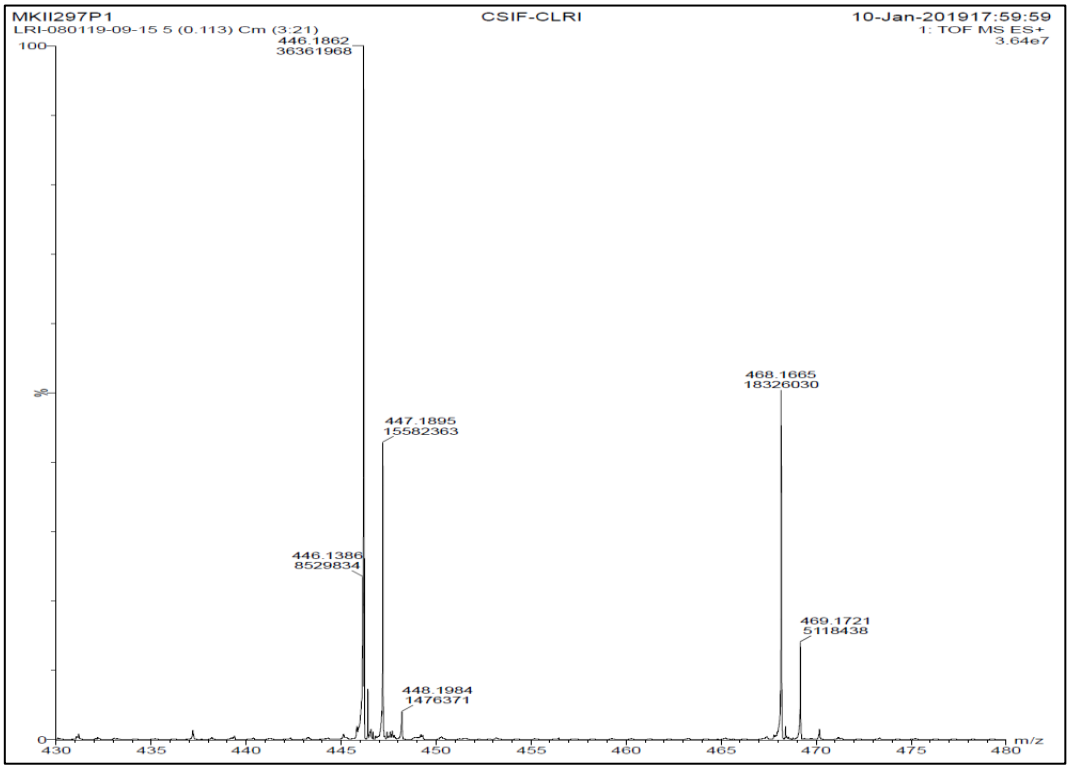
^{1}H NMR spectrum of compound **4h**



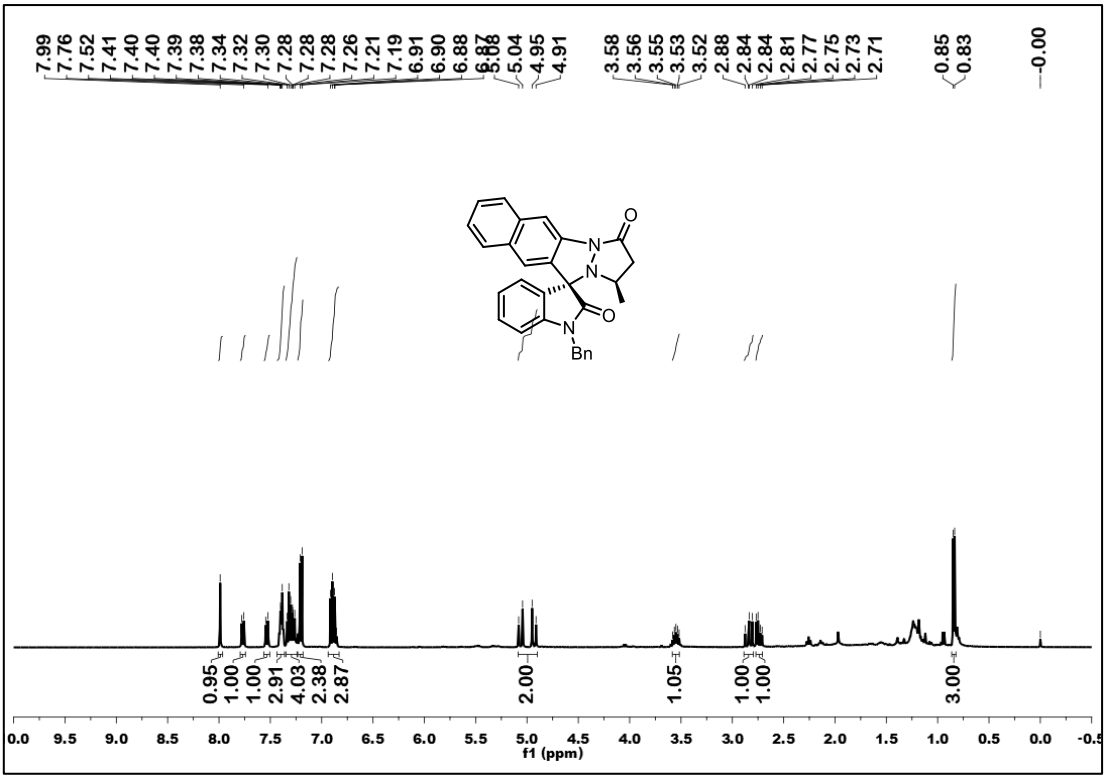
^{13}C NMR spectrum of compound **4h**



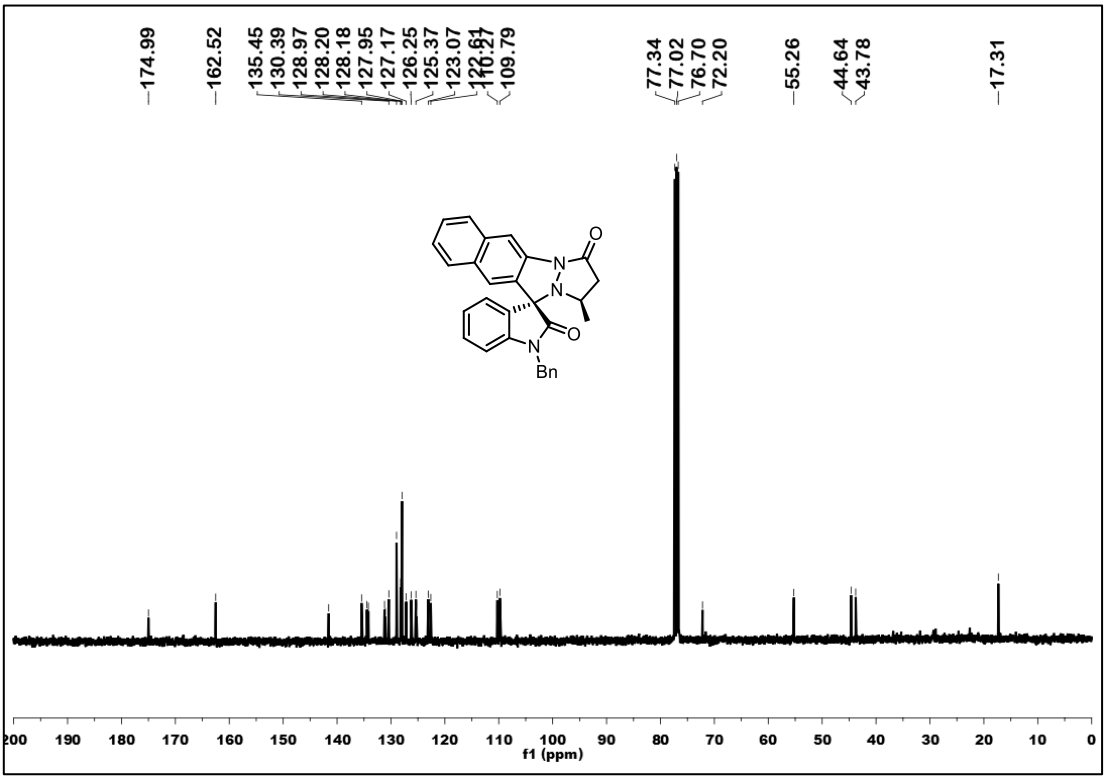
DEPT- 135 NMR spectrum of compound **4h**



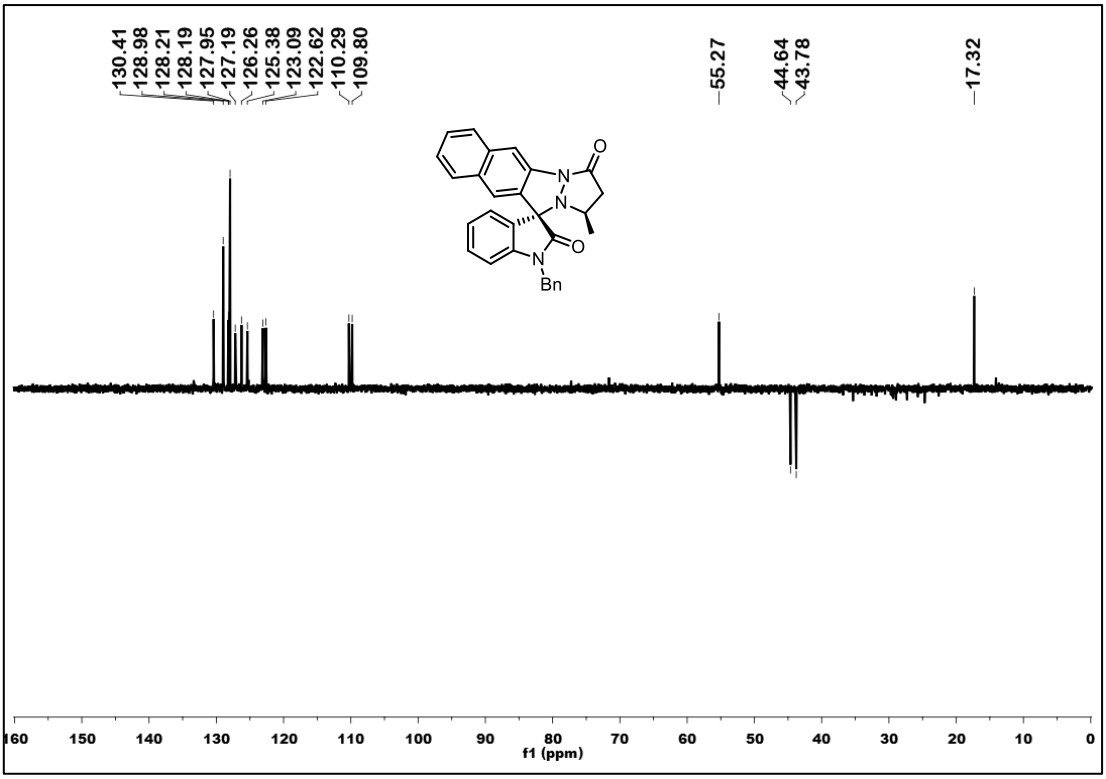
HRMS-Mass spectrum of compound **4h**



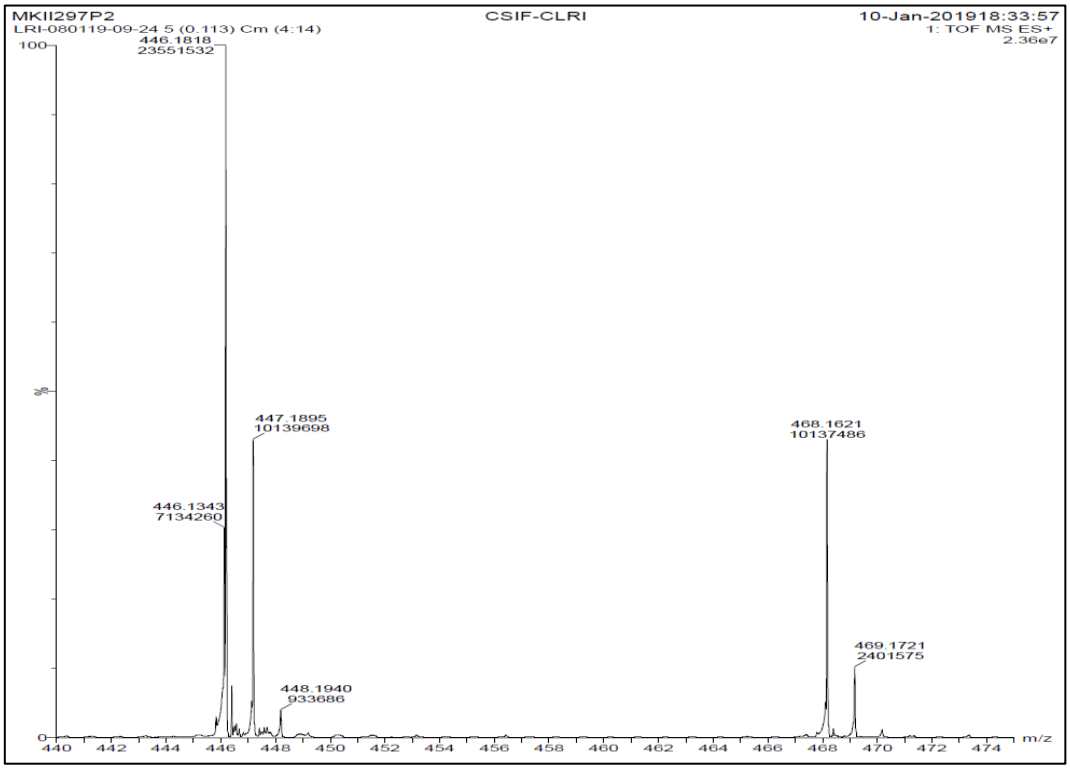
^{1}H NMR spectrum of compound **5h**



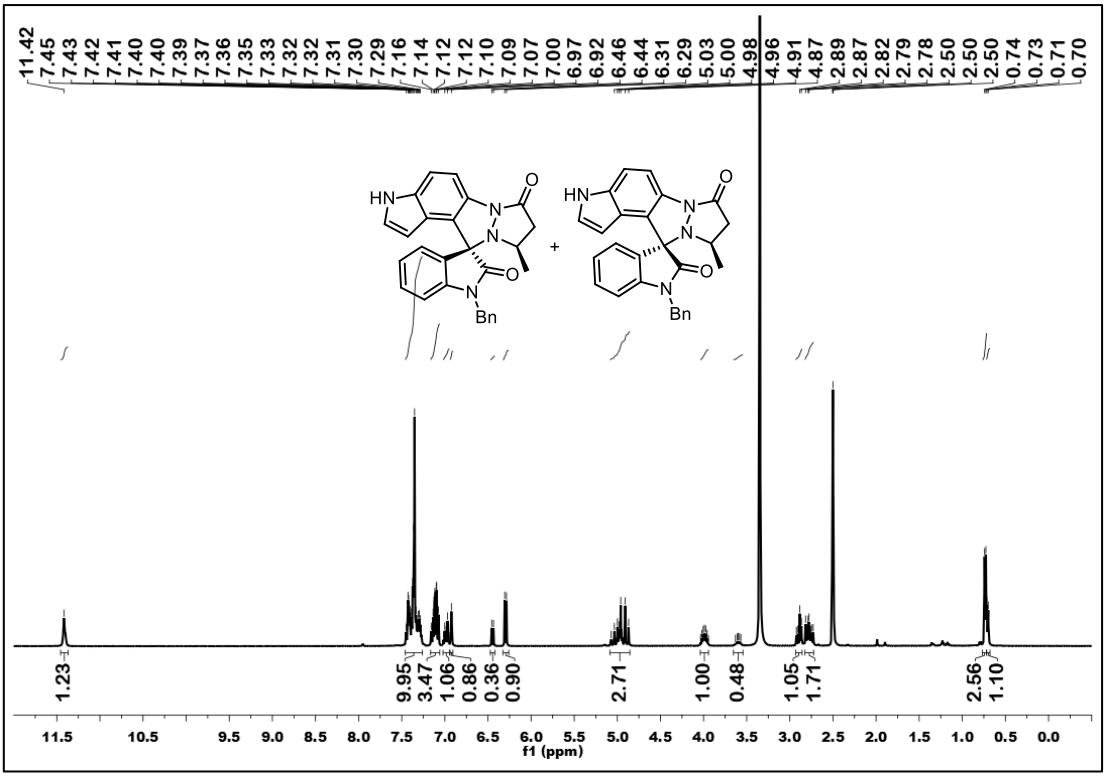
^{13}C NMR spectrum of compound **5h**



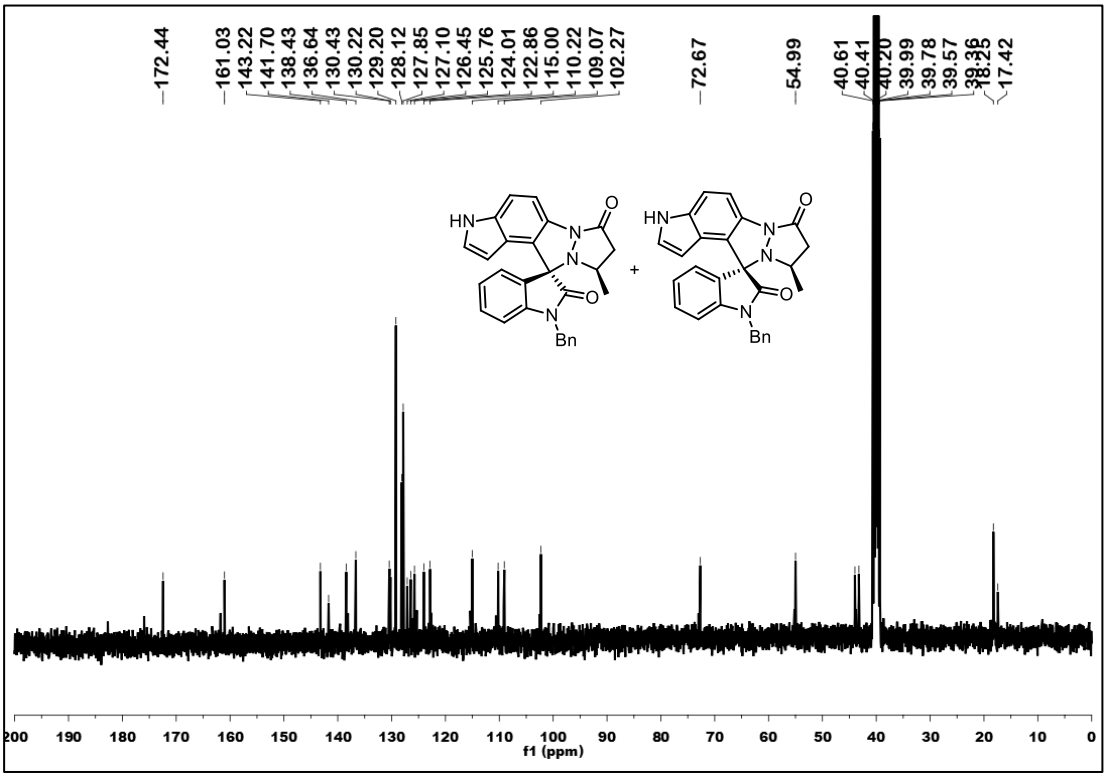
DEPT- 135 NMR spectrum of compound **5h**



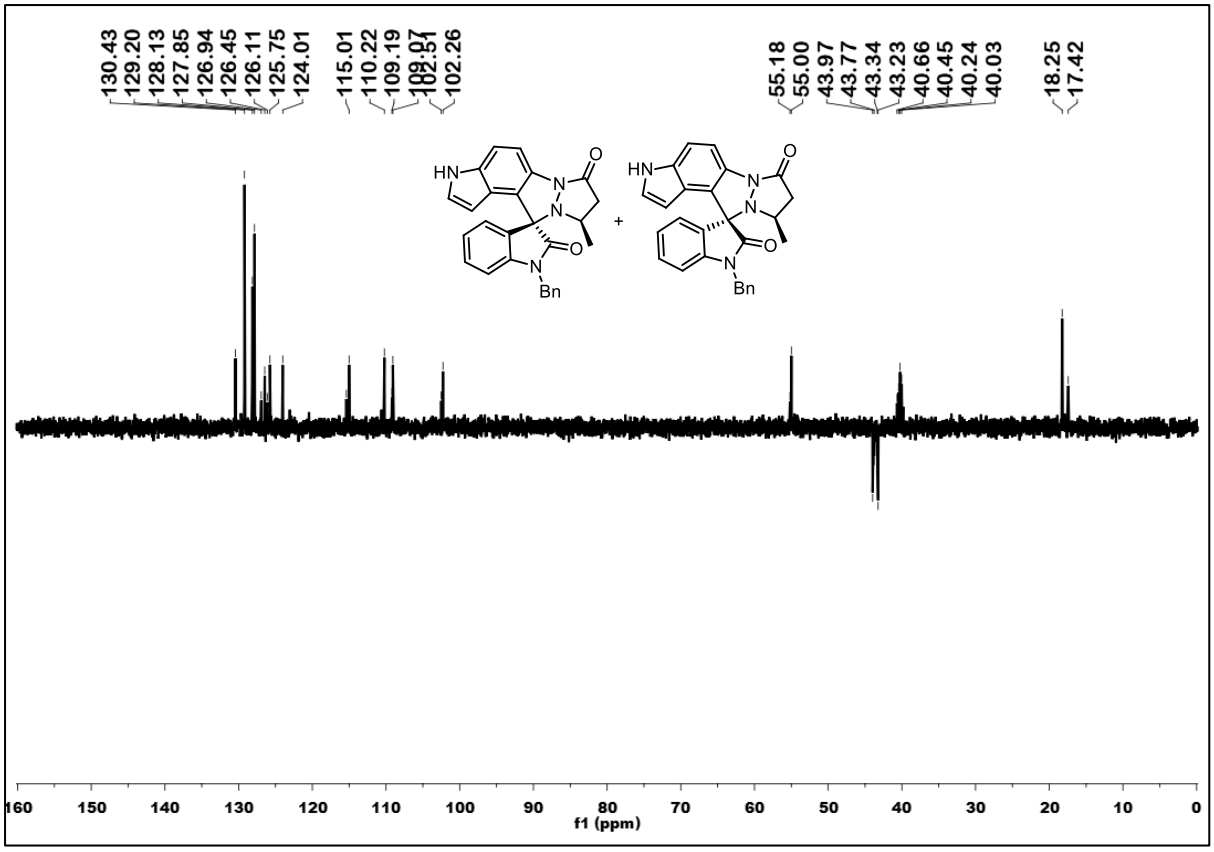
HRMS-Mass spectrum of compound **5h**



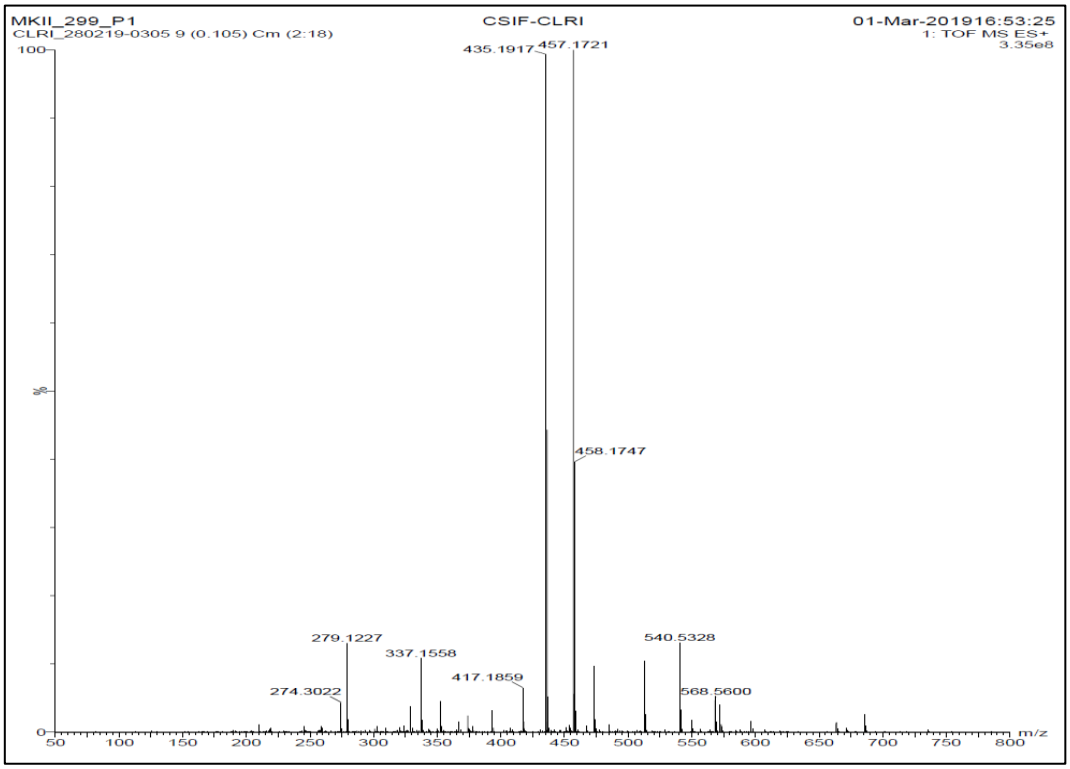
^{1}H NMR spectrum of column inseparable mixture of compounds **4i** and **5i**



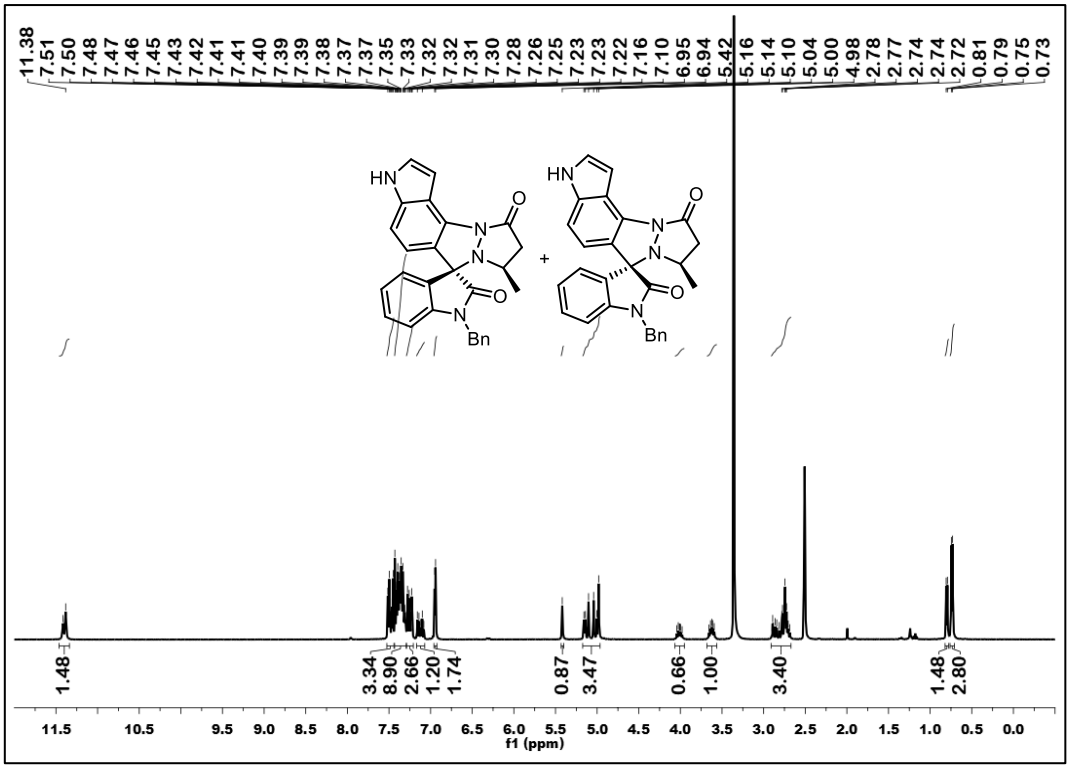
^{13}C NMR spectrum of column inseparable mixture of compounds **4i** and **5i**



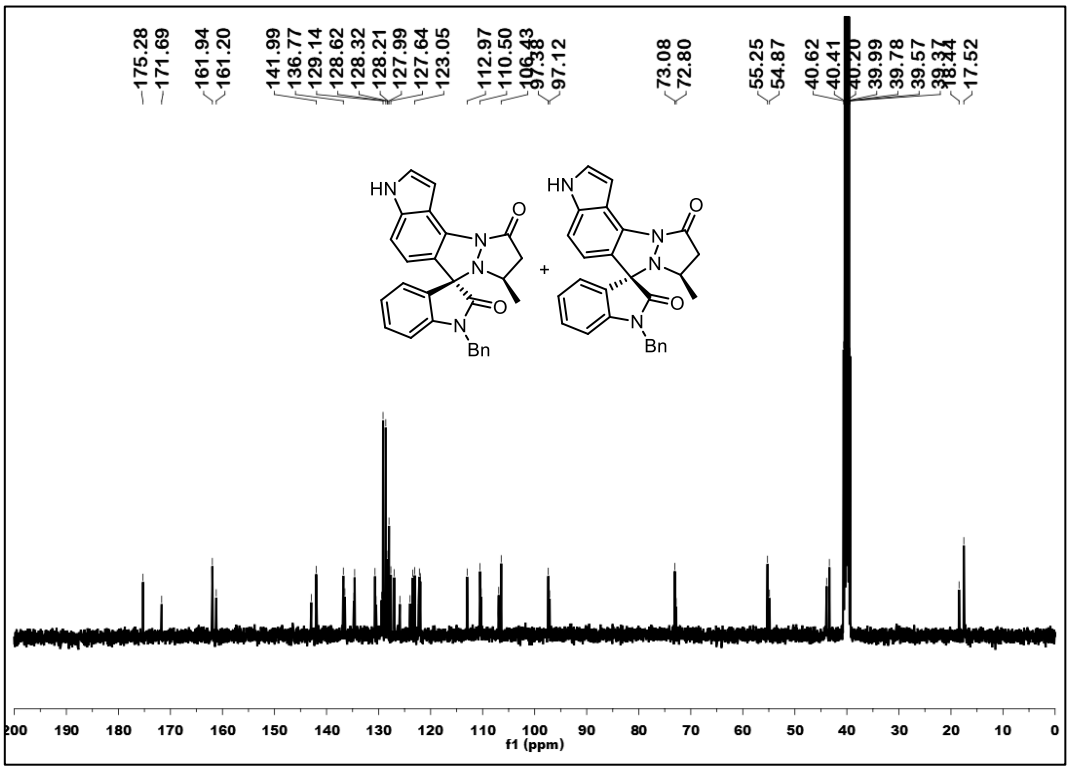
DEPT- 135 NMR spectrum of column inseparable mixture of compounds **4i** and **5i**



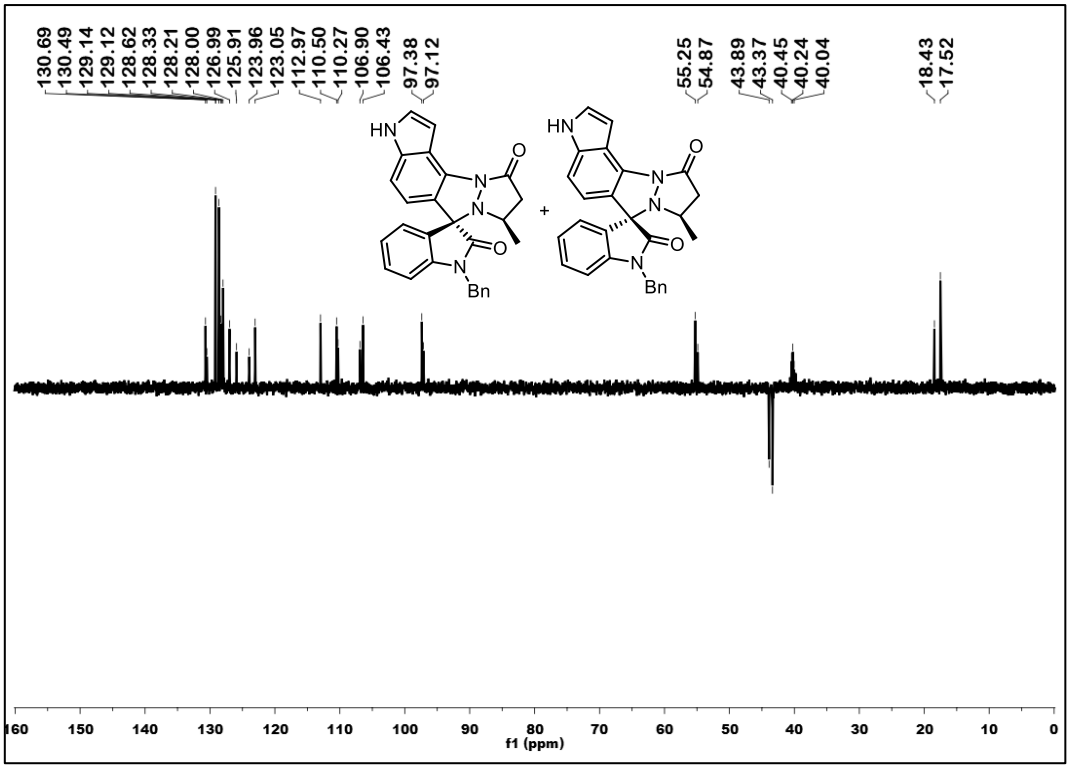
HRMS-Mass spectrum of column inseparable mixture of compounds **4i** and **5i**



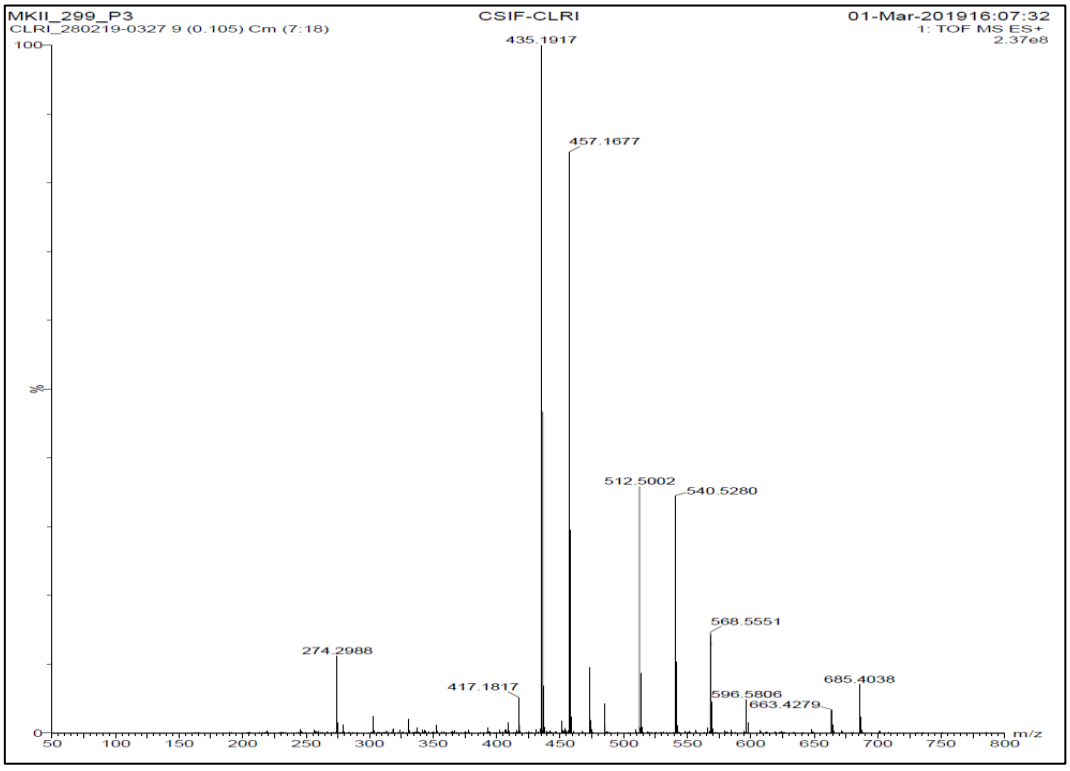
^{1}H NMR spectrum of column inseparable mixture of compounds **4j** and **5j**



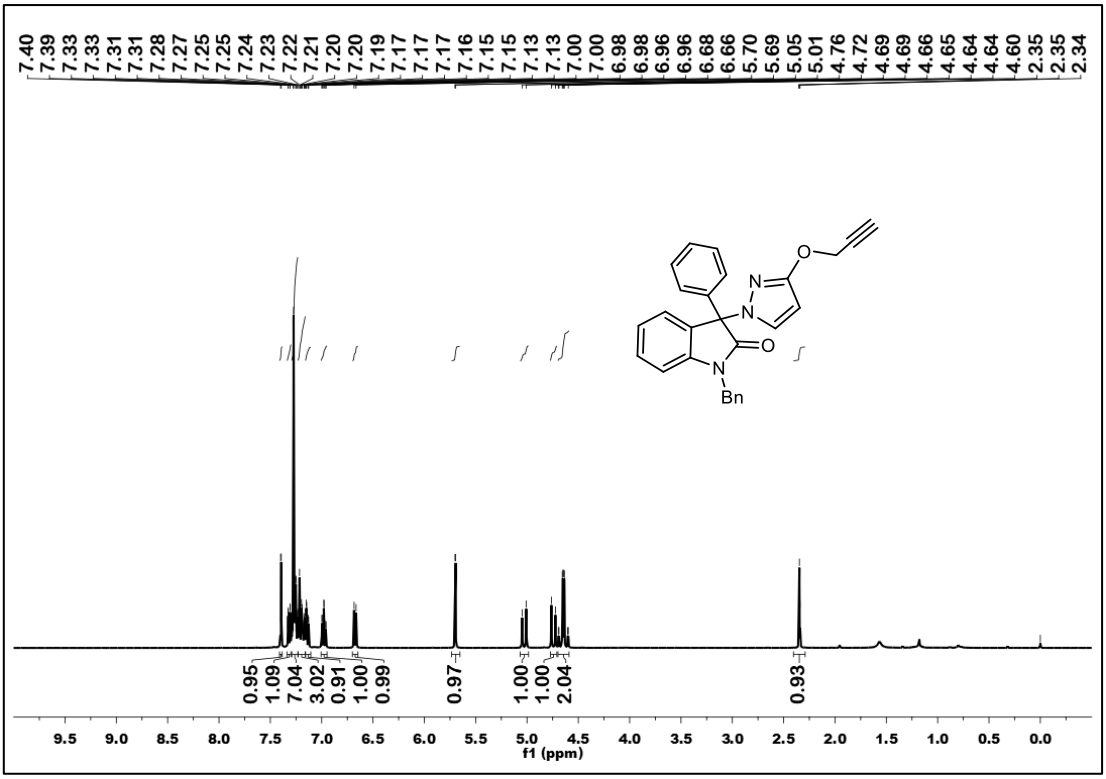
^{13}C NMR spectrum of column inseparable mixture of compounds **4j** and **5j**



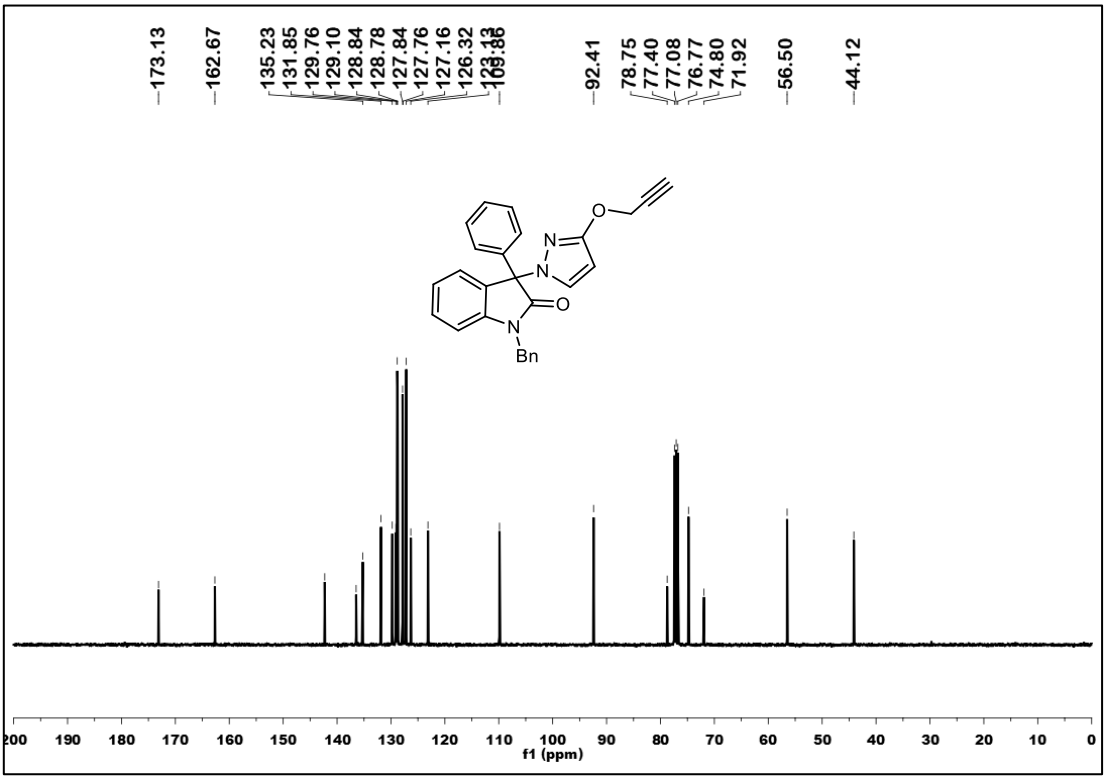
DEPT- 135 NMR spectrum of column inseparable mixture of compounds **4j** and **5j**



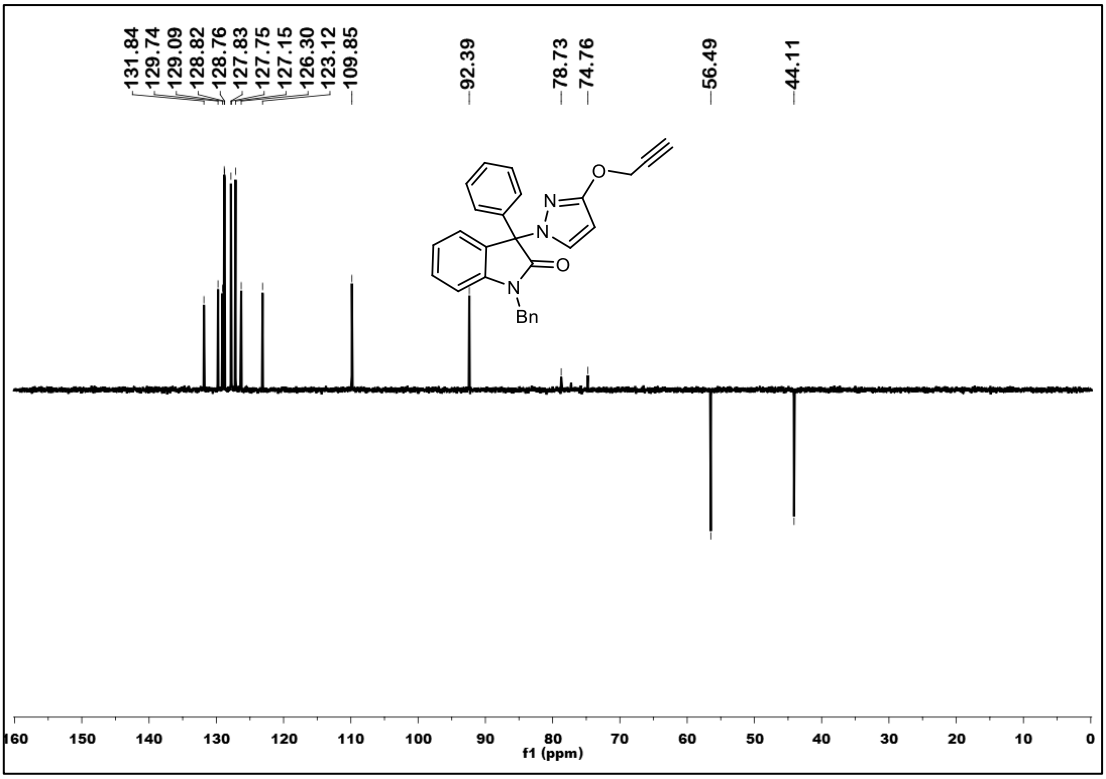
HRMS-Mass spectrum of column inseparable mixture of compounds **4j** and **5j**



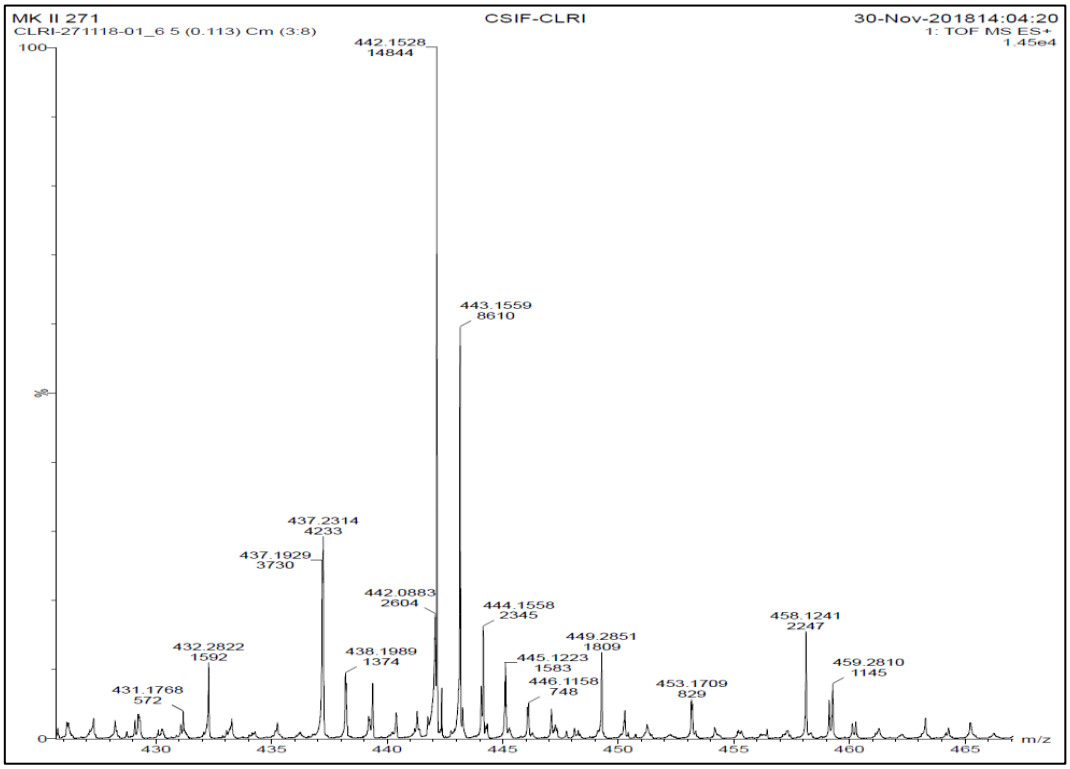
^{1}H NMR spectrum of compound **6**



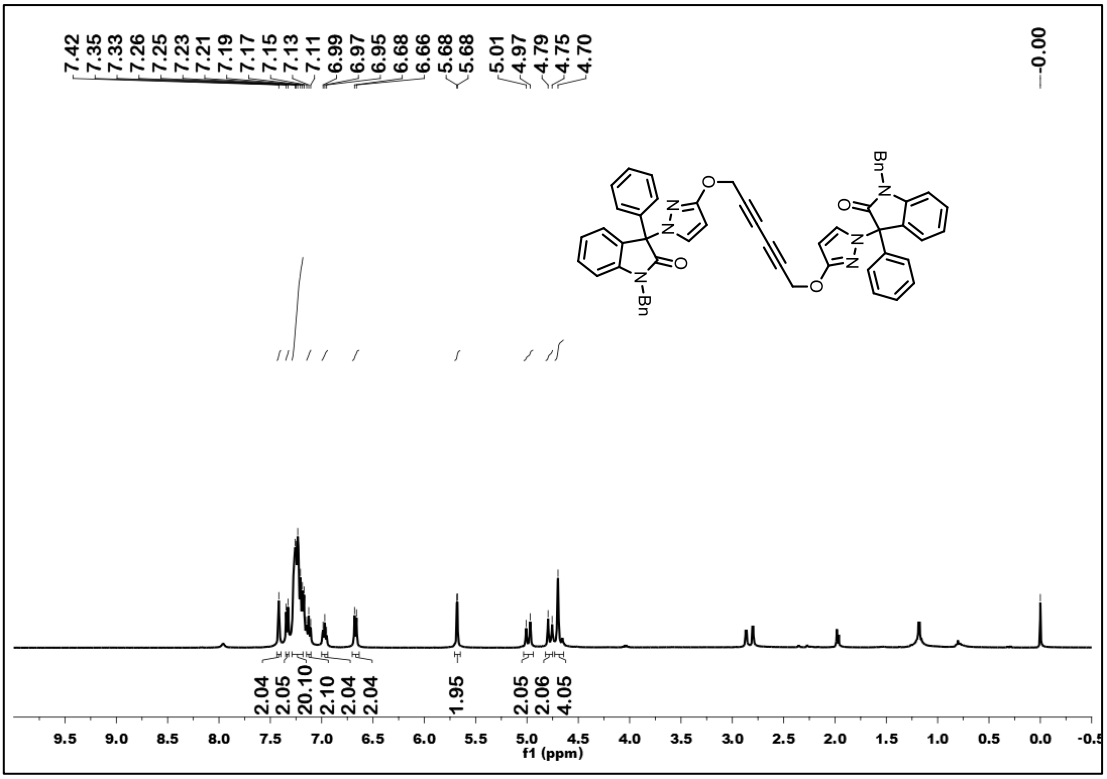
^{13}C NMR spectrum of compound **6**



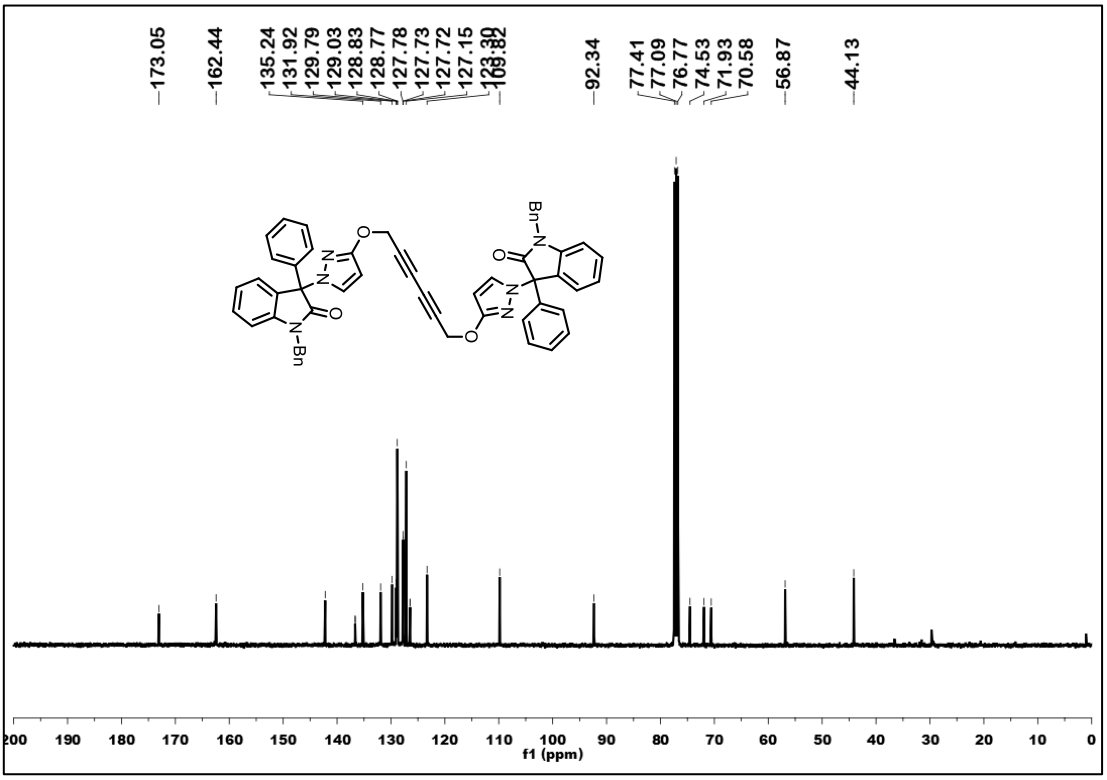
DEPT- 135 NMR spectrum of compound **6**



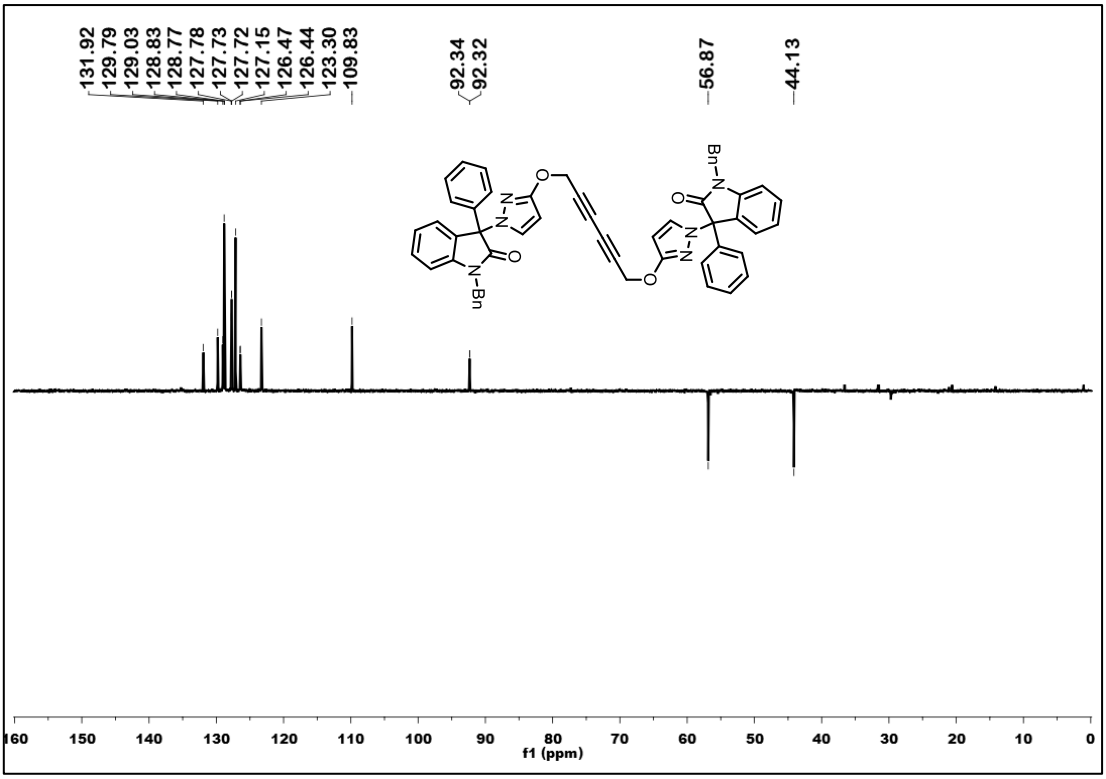
HRMS-Mass spectrum of compound **6**



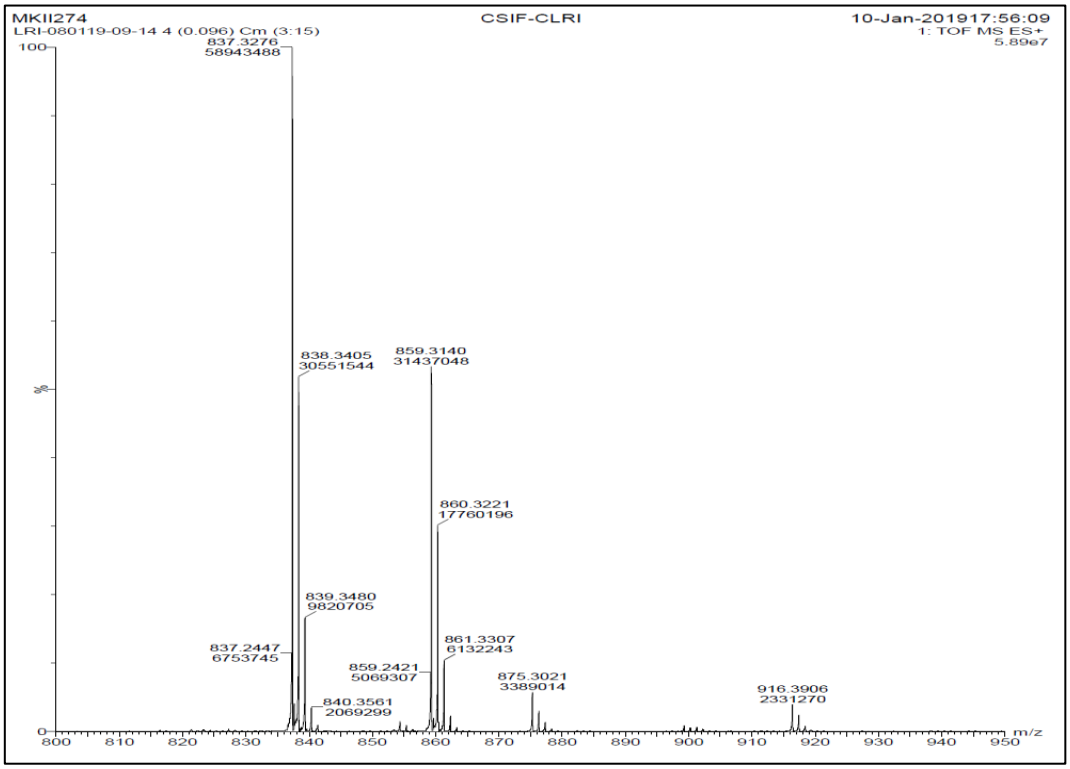
^{1}H NMR spectrum of compound **7**



^{13}C NMR spectrum of compound **7**



DEPT- 135 NMR spectrum of compound **7**



HRMS-Mass spectrum of compound **7**

2. Crystallographic data

Crystallographic data of compound 3a (CCDC No. 1874879)

Empirical formula :	C_{24} H_{19} N_3 O_2
Formula weight :	381.42
Temperature :	296(2) K
Wavelength :	0.71073 Å
Crystal system :	Monoclinic
Space group :	$P2_1/c$
Unit cell dimensions	
a = 12.1075(9) Å	α= 90°.
b = 15.3568(12) Å	β= 104.326(3)°.
c = 10.8188(7) Å	γ = 90°.
Volume:	1949.0(2) $Å^3$
Z:	4
Density (calculated):	1.300 Mg/m^3
Absorption coefficient:	0.084 mm^{-1}
F(000):	800
Crystal size:	0.150 x 0.150 x 0.100 mm^3
Theta range for data collection:	2.185 to 24.997°.
Index ranges:	-14<=h<=14, -18<=k<=18, -11<=l<=12
Reflections collected:	28245
Independent reflections:	3438 [R(int) = 0.0763]
Completeness to theta	24.997°: 99.9 %
Absorption correction:	Semi-empirical from equivalents
Max. and min. transmission:	0.7451 and 0.7021
Refinement method:	Full-matrix least-squares on F^2
Data / restraints / parameters:	3438 / 0 / 263
Goodness-of-fit on F^2:	1.041
R1 = 0.0437	wR2 = 0.0890
R indices (all data):	R1 = 0.1136, wR2 = 0.1218
Extinction coefficient:	0.0049(8)
Largest diff. peak and hole:	0.144 and -0.154 $e.Å^{-3}$

Crystallographic data of compound 4a (CCDC No. 1896309)

Empirical formula :	C_{25} H_{21} N_3 O_2
Formula weight :	395.45
Temperature :	296(2) K
Wavelength :	0.71073 Å
Space group :	P 21/n
Unit cell dimensions	

a=8.7600(3)	b=23.4233(8)	c=10.4245(3)
alpha=90	beta=109.446(2)	gamma=90
Volume:	2016.97(12) $Å^3$	
Z:	4	
Density (reported):	1.302 Mg/m^3	
Absorption coefficient:	0.084mm^{-1}	
F(000):	832.0	
Index ranges h,k,lmax =	10,27,12	
R(reflections)=	0.0422(2858)	
Data completeness=	0.999	
AbsCorr =	MULTI-SCAN	
Max. and min. transmission:	0.655 and 0.746	
Refinement method:	Full-matrix least-squares on F^2	
wR2(reflections)=	0.1006(3559)	
S = 1.054 ; Npar=273		

Crystallographic data of compound 5a (CCDC No. 1896310)

Empirical formula :	C_{25} H_{21} N_3 O_2	
Formula weight :	395.45	
Temperature :	296(2) K	
Wavelength :	0.71073Å	
Space group :	P 21/c	
Unit cell dimensions		
a=13.6544(5)	b=10.6301(4)	c=28.4877(11)
alpha=90	beta=100.3055(16)	gamma=90
Volume:	4068.2(3) $Å^3$	
Z:	8	
Density (reported):	1.291Mg/m^3	
Absorption coefficient:	0.083 mm^{-1}	
F(000):	1664.0	
Index ranges h,k,lmax =	16,12,33	
R(reflections)=	0.0463(4667)	
Data completeness=	0.999	
AbsCorr =	MULTI-SCAN	
Max. and min. transmission:	0.652 and 0.745	
Refinement method:	Full-matrix least-squares on F^2	
wR2(reflections)=	0.1138(6943)	
S = 1.029; Npar= 543		

3. Computational Details

Quantum chemical computations were carried out with the meta-GGA functional of the Minnesota family M08-HX[1] functional in conjunction with the def2SVP[2] basis set. Various functionals starting with traditional B3LYP[3], M062X[4], ωB97XD[5], LC-ωPBE[6], and M06-L[7], were tested along with 6-31G(d)[8] and def2-SVP basis sets however, we could not locate the transition states. The calculations with M08-HX method were successful in obtaining all the desired transition states. M08-HX functional is an improved version of M06-2X functional and has the best performance particularly, in handling main-group reaction thermochemistry, kinetics, atomization energies, electron affinities and noncovalent interaction energies.[1] Standard convergence criteria and an ultrafine integration grid were used. For better results, single point calculations were carried out at M08-HX/def2TZVP level of theory on optimized geometries. All the thermodynamic data were computed at 298.15 K and 1 atm. Solvent effects were included through the calculations based on polarizable continuum model (PCM) using acetonitrile as solvent medium at the same level of theory. All the optimized geometries were verified as minima or first order saddle points by the harmonic vibrational frequency analysis and thermal and zero point energy (ZPE) corrections were also included. As in the standard practice, the presence of one imaginary frequency criteria was used for the characterization of transition states (TS). Further, intrinsic reaction coordinate (IRC)[9] calculations confirmed the nature of the transition states and provided the information that, they were connected to the respective minima (reactant and product). All the calculations were performed using G16 (Revision A.03) suite of program[10].

Cycloaddition reactions of **1a** and **1f** with **2a** have been investigated by using state of the art DFT methods. Two possible reactions like 1,3 dipolar cycloaddition reaction and arylation reactions have been unraveled. Arylation reaction involves formation of C-C bond and hydrogen abstraction in a concerted fashion. Whereas the 1,3 dipolar cycloaddition

reaction involves formation of two new C-C bonds. The atom labeling of the substrates is shown in Figures 1. While the labeling the transition states, "A" denotes the arylation and "C" accounts for cycloaddition reaction. The complete energy profile of the **1a/1f** reaction with **2a** is depicted in Figure 2. It is clear from the figure that, arylation reaction between **1a** and **2a** proceeds through a transition state $\mathbf{T1^{A}_{1a2a}}$ of activation barrier 5.39 kcal/mol followed by the keto-enol tautomerisation to lead final product **3a** (-92.27 kcal/mol). Whereas, in the case of aryalation reaction between **1f** and **2a** witnesses an activation barrier of 13.39 kcal/mol ($\mathbf{T1^{A}_{1f2a}}$) which is 8.00 kcal/mol higher than $\mathbf{T1^{A}_{1a2a}}$. Therefore, arylation reaction of **2a** with **1a** is more feasible than arylation with **1f** by 8.00 kcal/mol.

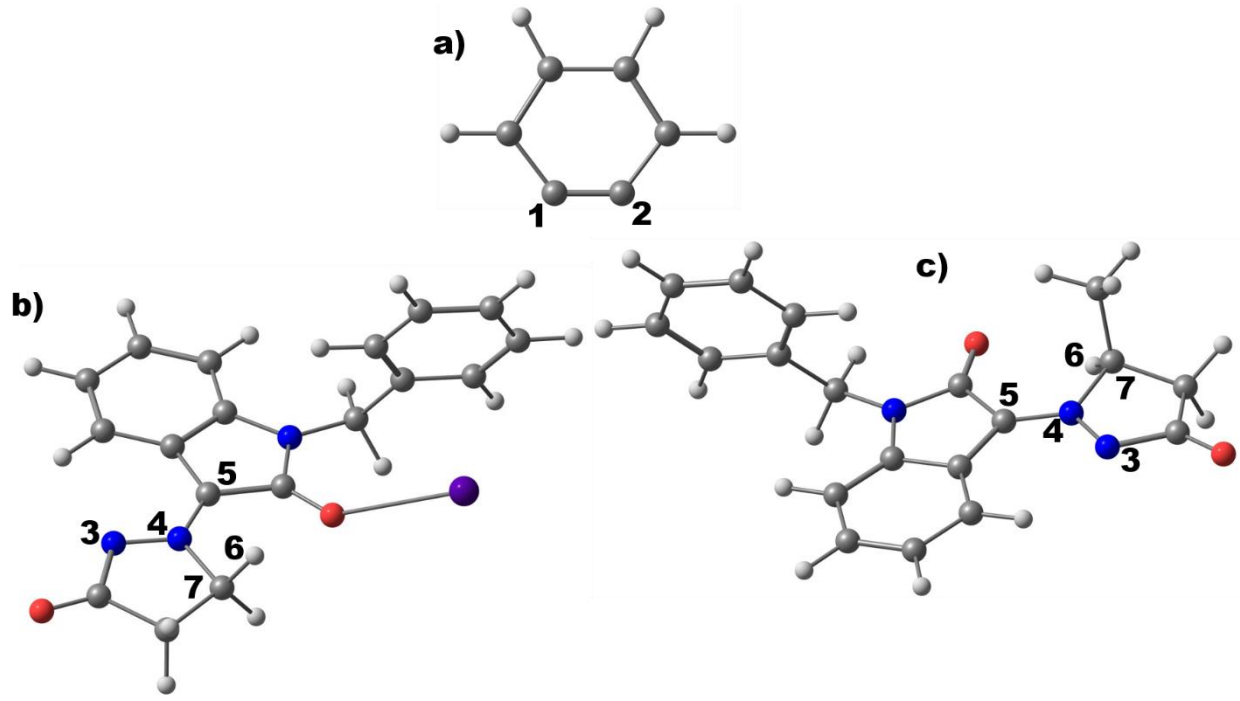


Figure 1 Substrates investigated for DFT calculations. a) Benzyne-**2a**, b) **1a** and c) **1f**.

In the case of 1,3 dipolar cycloaddition reaction, cycloaddition of **2a** with **1a** proceeds through a transition state $\mathbf{T^{C}_{1a2a}}$ with an activation barrier of 7.82 kcal/mol whereas the same with **1f** results two isomers **4a** and **5a**. Formation of **4a** is observed via the transition state $\mathbf{T^{C}_{1f2a4a}}$ with activation barrier of 3.83 kcal/mol and the formation of **5a** witnesses an activation barrier of 3.48 kcal/mol ($\mathbf{T^{C}_{1f2a5a}}$). Even though the activation barrier associated with the formation of **5a** is lower, the thermodynamic stability of **4a** (-89.43 kcal/mol) drives the reaction towards its

formation rather than **5a** (-83.80 kcal/mol) formation. Hence, the cycloaddition reaction of **2a** with **1f** is more feasible to form **4a**.

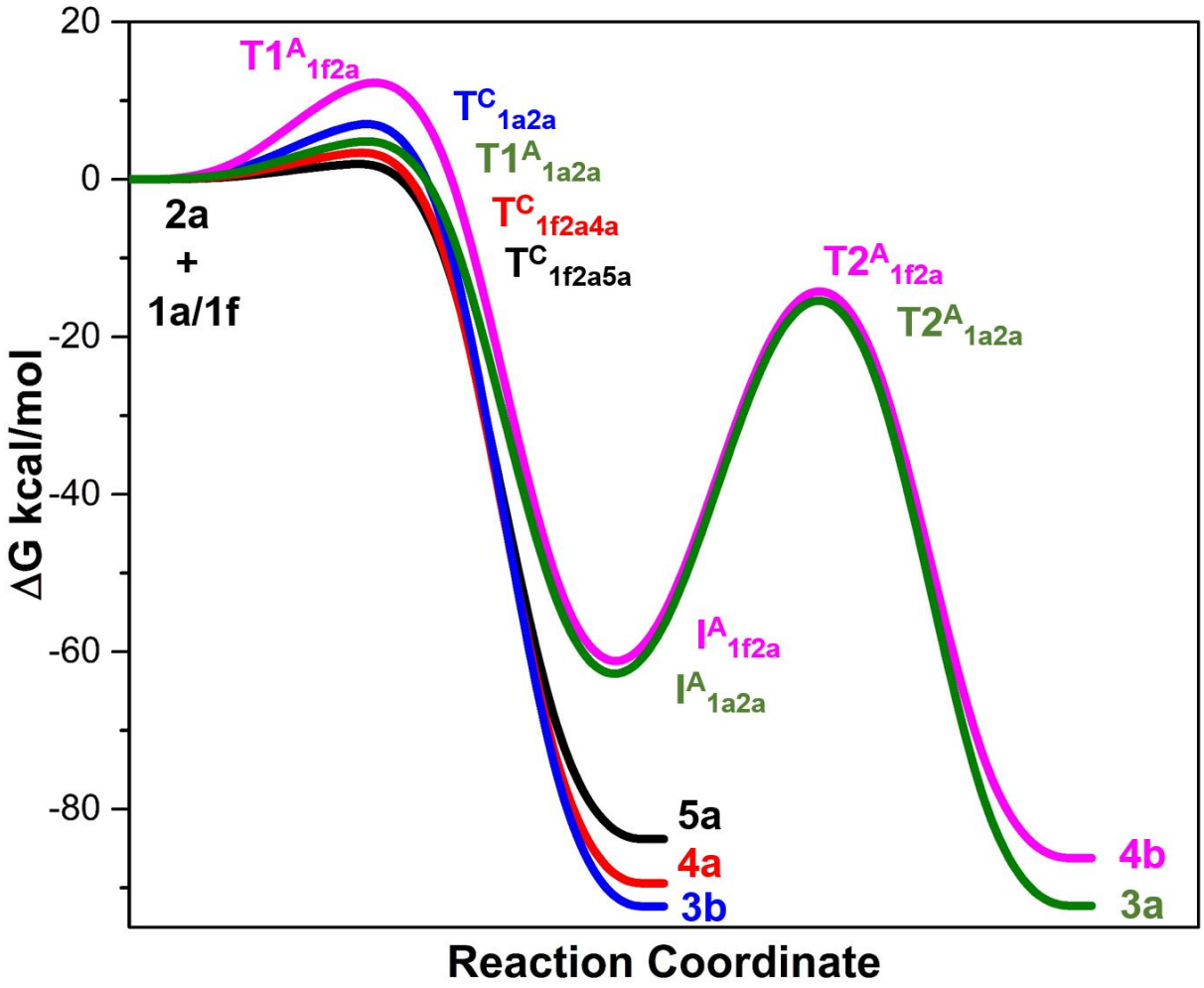


Figure 2 Complete reaction profile of reaction of **2a** with **1a**Cs/**1f**.

To get the further insights, we have carried out the NBO[11] analysis at the same level of theory. NBO charge on C5 of **1f** in $\mathbf{T1^{A}_{1f2a}}$ is -0.070 whereas the same on C5 of **1a** in $\mathbf{T1^{A}_{1a2a}}$ is -0.256 |e|. Which indicates that, C7-H6 bond in $\mathbf{T1^{A}_{1a2a}}$ is more polarized than C7-H6 bond of $\mathbf{T1^{A}_{1f2a}}$. Further, it is well known that secondary carbanions are more stable than the tertiary carbanions hence, the formation of secondary carbanions (C7 of $\mathbf{T1^{A}_{1a2a}}$) are more preferred than the tertiary carbanions (C7 of $\mathbf{T1^{A}_{1f2a}}$). Therefore, $\mathbf{T1^{A}_{1a2a}}$ witnesses less activation barrier when compared to $\mathbf{T1^{A}_{1f2a}}$. Hence, arylation reaction is more feasible with **1a** rather than **1f**. In the case of cycloaddition reactions, careful observation of geometries of transition states reveal

that, the newly forming bond lengths of C2-N3 and C1-C5 are 2.37 Å and 2.78 Å, respectively in $\mathbf{T^{C}_{1a2a}}$ whereas the same in $\mathbf{T^{C}_{1f2a4a}}$ are 2.37 Å and 2.87 Å, respectively. This indicates that, $\mathbf{T^{C}_{1f2a4a}}$ is more asynchronous than $\mathbf{T^{C}_{1a2a}}$. The high activation barrier of $\mathbf{T^{C}_{1a2a}}$ may be attributed to the high repulsions between reactants due to smaller interaction distances. Hence, it is also evident from the results that, smaller the distance between two reacting substrates in the transition state, larger the activation barrier. From the distortion-interaction analysis[12,13], it is clear that **1a** of $\mathbf{T^{C}_{1a2a}}$ is distorted more hence; the activation barrier is governed by the distortion energy. On the other hand, in the case of $\mathbf{T^{C}_{1f2a}}$, **1f** experiences lesser distortions resulting lower activation barrier. The distortion interaction values are tabulated as Table 1 and the optimized geometries of all the transition states are given in Figures 3 and 4.

Table 1. Distortion/Interaction analysis

TS	Distortion (E_D kcal/mol)			Interaction (E_I kcal/mol)	E_D+E_I kcal/mol
	R1	R2	E_D		
$T1^{A}_{1a2a}$	4.35	0.96	5.31	-0.12	5.19
$T1^{A}_{1f2a4a}$	2.06	0.83	2.89	0.65	3.54

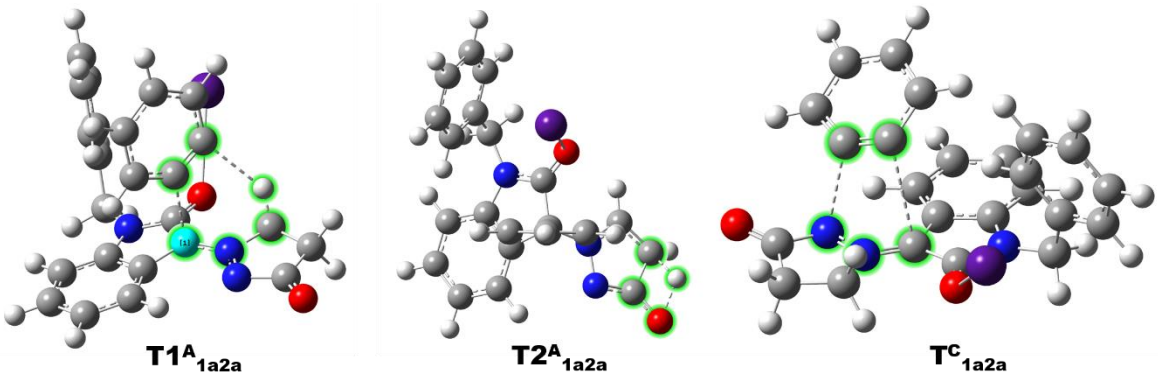


Figure 3. Geometries of transition states involved in reaction of **2a** with **1a**.

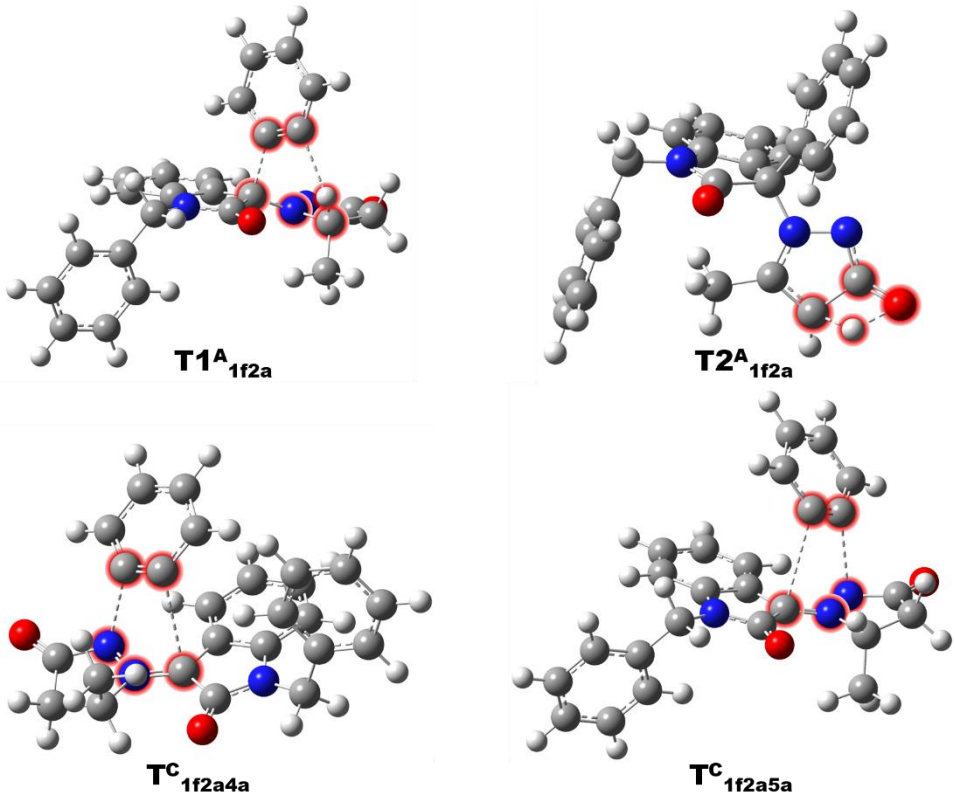


Figure 4 Geometries of transition states involved in reaction of **2a** with **1f**.

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Table 2 Cartesian Coordinates of geometries.

1aCs$^+$				**1f**			
C	-2.60438200	1.35155800	-0.06591800	C	-0.65520300	1.31819200	-0.15517300
C	-1.53046600	2.20675000	-0.40057600	C	0.68821900	1.10853200	-0.54875100
C	-1.66118200	3.58711100	-0.38207700	C	1.62066600	2.13663800	-0.54094200
C	-2.91118900	4.11029900	-0.02267600	C	1.17779000	3.40316100	-0.13252300
C	-3.98299100	3.27660500	0.30603100	C	-0.14572100	3.62466200	0.25599700
C	-3.84556400	1.88464400	0.29017400	C	-1.08196900	2.58334600	0.25087000
C	-2.09051200	0.00419100	-0.19633300	C	-1.30854100	0.03300600	-0.29230800
C	-0.67615400	0.08801900	-0.59701300	C	-0.29971200	-0.94888600	-0.79217800
H	-0.83132800	4.25532900	-0.63316300	H	2.66184100	1.96146500	-0.83122000
H	-3.04488500	5.19689200	0.00003900	H	1.89107400	4.23445400	-0.11591600
H	-4.94547900	3.71889900	0.58122000	H	-0.45624200	4.62614000	0.57037800
H	-4.67341500	1.21804100	0.54538400	H	-2.12284800	2.73187100	0.55027400
N	-2.75993100	-1.12617000	-0.02039100	N	-2.57564500	-0.24340400	-0.07001300
C	-2.12815900	-2.47551500	-0.22758100	C	-3.14560500	-1.64107900	-0.18896800
C	-3.29080000	-3.41426000	0.00583800	C	-4.63047300	-1.33032300	-0.20882200
C	-4.43477300	-2.47438500	0.40881400	C	-4.69500500	0.09484200	0.35293200
H	-3.12049800	-4.14448300	0.81163200	H	-5.23150800	-2.01259200	0.41118100
N	-3.99342300	-1.14186900	0.33283500	N	-3.42240700	0.65683400	0.32821400
O	-5.53621200	-2.79216600	0.73311900	O	-5.68187400	0.66656800	0.72269500
O	0.15493200	-0.80612900	-0.78511300	O	-0.42723600	-2.12643200	-1.05587800
N	-0.40453700	1.42450500	-0.72041300	N	0.87062000	-0.22590900	-0.91639100
H	-3.59048400	-3.97167200	-0.89591000	H	-5.05504700	-1.32567900	-1.22725100
H	-1.69166600	-2.48977300	-1.23757700	H	-2.74163800	-2.07868500	-1.11403300
H	-1.30425100	-2.56440700	0.49715400	C	2.09951300	-0.79893700	-1.40230400
C	0.87001800	1.90713700	-1.18508500	H	2.41144700	-0.28411700	-2.33236600
H	0.76862400	2.98585200	-1.39531100	H	1.85603000	-1.84396700	-1.66970500
H	1.11068600	1.42257800	-2.15075000	C	3.23088500	-0.75703900	-0.39171500
C	2.01048200	1.67484800	-0.21011300	C	2.97535900	-0.79547000	0.98291000
C	1.77544300	1.40815100	1.14450000	C	4.55632200	-0.69712700	-0.83575700
C	3.33361900	1.73308100	-0.67295900	C	4.02893300	-0.78406600	1.89763700
C	2.84536300	1.18898400	2.01938200	H	1.93846900	-0.82625800	1.33980900
H	0.74454900	1.38146600	1.52005000	C	5.61120700	-0.69013600	0.07760800
C	4.40396200	1.52038400	0.20071300	H	4.76473600	-0.65444700	-1.91233100
H	3.52980200	1.96088400	-1.72892200	C	5.34943200	-0.73377900	1.44795700
C	4.16209100	1.23895900	1.55035100	H	3.81559500	-0.81163400	2.97177700
H	2.64842800	0.99776700	3.08046500	H	6.64439700	-0.64390700	-0.28371000
H	5.43291000	1.58984700	-0.17037800	H	6.17581600	-0.72251600	2.16676600
H	4.99943100	1.08635500	2.24025100	C	-2.70472300	-2.45562200	1.02190200
Cs	2.83007700	-1.65185200	-0.17427800	H	-1.61298500	-2.59360400	1.02845000
				H	-3.02794100	-1.95818800	1.95340500
				H	-3.17453300	-3.45156100	0.97705200
T1$^{A}_{1a2a}$				**I$^{A}_{1a2a}$**			
C	-2.44340400	1.43410100	-0.37020200	C	2.34128800	1.40795800	0.15893900
C	-1.40964100	2.31547600	-0.75616900	C	1.34215800	2.25866400	0.64288100
C	-1.52610600	3.68883300	-0.59063000	C	1.57370000	3.61051900	0.85607000
C	-2.72377400	4.17444900	-0.04803000	C	2.85579900	4.09360700	0.55993700
C	-3.76334500	3.31350800	0.31281100	C	3.85710300	3.25342200	0.06957600

C	-3.63413000	1.92742600	0.16176700	C	3.60854200	1.88955400	-0.13566300
C	-1.91281600	0.09061700	-0.57473100	C	1.78054000	0.00618900	0.06182300
C	-0.59409500	0.23341200	-1.26340200	C	0.30573600	0.21895700	0.49377600
H	-0.72314300	4.37666800	-0.87364100	H	0.79983500	4.28558200	1.23446600
H	-2.84482500	5.25421500	0.08873800	H	3.07064000	5.15603500	0.71625600
H	-4.68993200	3.72675800	0.72315400	H	4.84620900	3.66380300	-0.15618600
H	-4.43276500	1.23965000	0.45263100	H	4.37004000	1.20704600	-0.52868600
N	-2.65178500	-1.04106600	-0.62868700	N	1.86498900	-0.46826400	-1.33245300
C	-2.04201700	-2.33418900	-1.01857200	C	0.85837400	-0.67474500	-2.14455500
C	-3.21199500	-3.28661100	-0.90759400	C	1.45385200	-1.08847300	-3.43831700
C	-4.32670800	-2.41370100	-0.32886900	C	2.96832900	-1.04682800	-3.09785200
H	-3.03162300	-4.13939600	-0.23527200	H	1.22968800	-0.39676500	-4.27068000
N	-3.85495600	-1.07627800	-0.22052200	N	3.09700300	-0.65249900	-1.77429400
O	-5.42186300	-2.74360100	-0.00494800	O	3.86342200	-1.30729400	-3.85108200
O	0.16308100	-0.62687300	-1.68369900	O	-0.56496500	-0.63042100	0.55178500
N	-0.33851000	1.57799900	-1.28352200	N	0.14859000	1.52004800	0.83960100
H	-3.53967500	-3.68834900	-1.88031400	H	1.15769700	-2.10101500	-3.76660600
H	-1.58272700	-2.21869100	-2.01174700	H	1.63382400	-2.70509600	-0.12115400
H	-1.21698700	-2.49101100	-0.28305700	C	-1.08683300	2.01268800	1.40164100
C	0.91414500	2.09100400	-1.78418100	H	-0.94431300	3.07839000	1.64924700
H	0.79844300	3.17591200	-1.95230100	H	-1.28671900	1.49131800	2.35760000
H	1.11482600	1.63467800	-2.77048100	C	-2.28747900	1.85882900	0.48448300
C	2.08237300	1.82040500	-0.85097400	C	-2.14733300	1.71627100	-0.90172900
C	1.88818700	1.69395600	0.53092800	C	-3.57543700	1.89086100	1.03648700
C	3.38080800	1.71534500	-1.36846200	C	-3.27460900	1.59950500	-1.72018900
C	2.97267300	1.45708700	1.38118100	H	-1.14424900	1.71017600	-1.34823400
H	0.88023500	1.78388900	0.95434000	C	-4.70466300	1.78401400	0.21921800
C	4.46769300	1.48786900	-0.51914500	H	-3.69814000	2.01968500	2.11978600
H	3.54583000	1.82367100	-2.44814100	C	-4.55734200	1.63133700	-1.16340600
C	4.26585000	1.35277900	0.85909700	H	-3.15051600	1.50741100	-2.80526200
H	2.79977700	1.36885200	2.46032900	H	-5.70536900	1.83854200	0.66307500
H	5.48023200	1.42905600	-0.93456200	H	-5.44052900	1.56555300	-1.80848200
H	5.11930700	1.18854000	1.52647500	C	2.40317200	-1.02079800	1.00415000
Cs	2.67596100	-1.69035900	-0.40248500	C	2.18426500	-2.38340600	0.77168900
C	0.46759600	-0.56805700	3.56816500	C	3.11508400	-0.61150200	2.13324800
C	0.57794100	-1.55858600	2.58001800	C	2.69171600	-3.33098600	1.65663900
C	-0.16579600	-1.35555400	1.40529900	C	3.61477700	-1.56546200	3.02357700
C	-0.90369600	-0.30340200	1.32452700	H	3.29564500	0.45431700	2.31424300
C	-1.12840500	0.72588000	2.22681400	C	3.40676100	-2.92294500	2.78645300
C	-0.37133700	0.54697900	3.39647500	H	2.54028500	-4.39748400	1.45887900
H	1.02440200	-0.67512300	4.50683400	H	4.18147900	-1.24093600	3.90257900
H	1.20497300	-2.44273500	2.76809300	H	3.81139500	-3.66938400	3.47817600
H	-1.79912500	1.58050700	2.08734900	Cs	-3.34398900	-1.59509500	0.18985200
H	-0.45808100	1.28768600	4.19985800	H	-0.17423000	-0.55362300	-1.81973600

$T2^{A}_{1a2a}$				**3a**			
C	-1.95607600	1.55720200	0.47036100	C	-1.95310600	1.54596800	0.45340200
C	-1.04691600	2.48753300	-0.04973800	C	-1.04286700	2.47964200	-0.05774300
C	-1.06993000	3.82310200	0.32826300	C	-1.07147300	3.81505400	0.32164400
C	-2.06010300	4.21083900	1.24272900	C	-2.06936400	4.19986300	1.22882500
C	-2.98015600	3.29434800	1.75419600	C	-2.99269000	3.28084800	1.72969000
C	-2.93260500	1.94496700	1.37545700	C	-2.93942500	1.93249200	1.34755600
C	-1.61449800	0.19101000	-0.08706000	C	-1.61003200	0.17858500	-0.10369000
C	-0.45784100	0.52251000	-1.06758200	C	-0.44689600	0.51519200	-1.07482100
H	-0.35908600	4.55427500	-0.06980200	H	-0.35928900	4.54825800	-0.07042900
H	-2.11052300	5.25894100	1.55632600	H	-2.12402700	5.24729900	1.54394500
H	-3.74465100	3.63143900	2.46101500	H	-3.76451200	3.61576200	2.42961800
H	-3.64245400	1.20592400	1.76215600	H	-3.65420200	1.19216500	1.72277200

N	-2.73976200	-0.42340400	-0.77169600	N	-2.71039300	-0.45263500	-0.79407800
C	-2.84033500	-0.79781900	-2.03984100	C	-2.81030100	-0.88024500	-2.07505500
C	-4.14309100	-1.33774700	-2.19984600	C	-4.05227800	-1.47329800	-2.19386400
C	-4.68085500	-1.28528200	-0.81623400	C	-4.61968000	-1.34376800	-0.89571100
H	-4.81106100	-2.42502000	-1.72114700	N	-3.79730200	-0.73404200	-0.06589600
N	-3.80780300	-0.71158100	0.01349800	O	-5.81309600	-1.74914800	-0.45213400
O	-5.64666500	-2.07497900	-0.58426800	O	0.18010800	-0.27874700	-1.74900800
O	0.15668900	-0.27782800	-1.74594600	N	-0.16341900	1.83455100	-0.95606200
N	-0.17285400	1.84009000	-0.95292300	H	-6.32418500	-2.12573900	-1.17357200
H	-4.74790900	-1.19778000	-3.10240500	H	-2.00175900	-0.74737400	-2.79449800
H	-1.77347800	-2.55798400	-0.01374100	H	-1.76187300	-2.55319600	-0.02019100
C	1.00001800	2.39407500	-1.59794700	C	1.00905200	2.39095700	-1.59736400
H	0.92834000	3.49452600	-1.56171500	H	0.93493300	3.49134900	-1.56213900
H	0.99160500	2.09818200	-2.66130500	H	1.00523600	2.09415200	-2.66055000
C	2.27914400	1.91159900	-0.93690400	C	2.28809400	1.91311800	-0.93268500
C	2.38702300	1.89934800	0.46172500	C	2.39272500	1.90441500	0.46622200
C	3.36686600	1.48612900	-1.70830300	C	3.37805100	1.48592800	-1.69996900
C	3.56718600	1.47554900	1.07823100	C	3.57120500	1.48206600	1.08684500
H	1.54575700	2.25190700	1.07409800	H	1.54896000	2.25720400	1.07494400
C	4.55099000	1.06556000	-1.09361200	C	4.56056400	1.06665500	-1.08128300
H	3.29095800	1.49471700	-2.80265700	H	3.30426600	1.49094200	-2.79447900
C	4.65372200	1.05836600	0.30092900	C	4.65974100	1.06267200	0.31351500
H	3.64951800	1.49628200	2.17084600	H	3.65034100	1.50484900	2.17965700
H	5.40393400	0.75722400	-1.70892600	H	5.41491300	0.75632300	-1.69366600
H	5.58891400	0.75097500	0.78243100	H	5.59344200	0.75578800	0.79822000
Cs	2.34155300	-1.73426200	-0.21812700	C	-1.12919900	-2.15418100	0.78234500
C	0.27981300	-2.51578100	2.71833000	C	-0.99298600	-0.76837200	0.93370700
C	-0.50550000	-3.02246800	1.67667000	C	-0.49397200	-3.02062600	1.67610000
C	-1.14068900	-2.15407100	0.78531200	C	-0.21413300	-0.25961500	1.98073900
C	-1.00672300	-0.76895600	0.94094000	C	0.29030100	-2.51191700	2.71774200
C	-0.22592600	-0.26203100	1.98710200	H	-0.63429300	-4.10276700	1.57388200
C	0.41826900	-1.13324300	2.87129900	C	0.42812500	-1.12880500	2.86843900
H	0.75495800	-3.19897200	3.43127000	H	-0.14131100	0.82617600	2.12447400
H	-0.64830600	-4.10401700	1.57282900	H	0.76543600	-3.19353400	3.43225900
H	-0.15334000	0.82324500	2.13386100	H	1.01232600	-0.72199500	3.70155900
H	1.00361200	-0.72780100	3.70418500	H	-4.48988100	-1.92390500	-3.08398500
H	-2.04020000	-0.60337000	-2.75764700	Cs	2.34455400	-1.72726300	-0.21043500
	T^{C}_{1a2a}				**3b**		
C	1.99537100	-0.98527100	-1.31137200	C	-2.42229000	1.49329700	0.35987200
C	0.92799200	-1.87497000	-1.55766500	C	-1.64313100	2.50908900	-0.21565200
C	1.11420500	-3.24835100	-1.60049800	C	-1.92949300	3.85182400	-0.00881300
C	2.41633300	-3.72700800	-1.39853200	C	-3.04451100	4.15520800	0.78586600
C	3.48307700	-2.85706000	-1.15879100	C	-3.83712800	3.15226300	1.34671500
C	3.28759700	-1.47297800	-1.11022600	C	-3.52485600	1.80130000	1.13969700
C	1.39891000	0.33720200	-1.25468000	C	-1.80225500	0.16473000	0.01916000
C	-0.06119300	0.19277500	-1.47210800	C	-0.68356000	0.58082900	-0.97695200
H	0.28598700	-3.94194900	-1.77703900	H	-1.32745500	4.65112100	-0.45245800
H	2.59534200	-4.80698800	-1.42672300	H	-3.29944300	5.20564100	0.96178400
H	4.48672800	-3.26423100	-1.00196900	H	-4.70621200	3.42417800	1.95369300
H	4.10800300	-0.77974700	-0.90407400	H	-4.13199200	0.99967100	1.57484500
N	1.99720200	1.48083600	-0.99677100	N	-2.69517300	-0.89676700	-0.43985900
C	1.26428200	2.77419600	-0.85286400	C	-3.04781400	-1.02867500	-1.86256100
C	2.39379800	3.75631300	-0.61861900	C	-3.22798300	-2.54409900	-2.03092100
C	3.57749000	2.83878000	-0.29744700	C	-2.24294000	-3.12956600	-1.02274900
H	2.22093900	4.45091300	0.21607500	H	-3.01952800	-2.91352900	-3.04533600
N	3.24142500	1.51969300	-0.64248400	N	-2.02228300	-2.11437600	-0.12717800
O	4.62935000	3.14848700	0.17572000	O	-1.73624500	-4.21855600	-0.95860900

O	-0.95341700	1.03510600	-1.42865700	O	0.06863200	-0.17679600	-1.56557600
N	-0.26693000	-1.14227400	-1.68938700	N	-0.61238700	1.93201600	-0.99553300
H	2.63827700	4.35145500	-1.51466100	H	-4.24408900	-2.87279800	-1.74695800
H	0.64205400	2.93409400	-1.74464400	H	-3.95788800	-0.44827100	-2.07802400
C	-1.59147700	-1.68565700	-1.81873400	H	-2.22539400	-0.67353900	-2.51755900
H	-1.51168700	-2.70685400	-2.23027700	C	0.49854800	2.59799700	-1.64649600
H	-2.14756900	-1.08837900	-2.56481800	H	0.31619200	3.68566000	-1.62032400
C	-2.35601900	-1.70103700	-0.50453200	H	0.53252400	2.29415300	-2.70755600
C	-1.70280500	-1.48032300	0.71449600	C	1.81306700	2.25451300	-0.96556500
C	-3.73966100	-1.92871000	-0.50469100	C	1.91057500	2.30743200	0.43242200
C	-2.42201200	-1.48461900	1.91437900	C	2.93703400	1.88447000	-1.71315300
H	-0.61932700	-1.29900400	0.72791600	C	3.11479800	2.00312800	1.07330200
C	-4.45931400	-1.93308900	0.69305700	H	1.03766500	2.61752000	1.02321900
H	-4.25963600	-2.11662100	-1.45309400	C	4.14584400	1.58525200	-1.07513800
C	-3.80206300	-1.70741600	1.90825900	H	2.86928400	1.83913100	-2.80703700
H	-1.89406300	-1.32369800	2.86209600	C	4.23758600	1.64246600	0.31927400
H	-5.53726600	-2.13060900	0.68034900	H	3.18642300	2.07538200	2.16456000
H	-4.36242300	-1.72819400	2.84952200	H	5.02535700	1.32044900	-1.67313600
C	4.00954100	-0.98485200	2.76259700	H	5.19017900	1.42969400	0.81753200
C	4.06267800	0.24020400	2.07028400	Cs	2.25517100	-1.32493100	-0.06737100
C	2.81063400	0.50835100	1.56122600	C	0.32814500	-2.34762100	2.73709600
C	1.70774900	-0.10360100	1.60303900	C	-0.46448800	-2.85699700	1.69692800
C	1.60778800	-1.31672900	2.29890900	C	-1.15875300	-1.92539800	0.92214900
C	2.82228300	-1.73835700	2.86778500	C	-1.05424800	-0.54204000	1.15263100
H	4.92599200	-1.36715400	3.22778500	C	-0.27508500	-0.05018500	2.18753500
H	4.96424600	0.84982800	1.95219400	C	0.42129300	-0.97241400	2.99043600
H	0.70203900	-1.92845500	2.40259200	H	0.86192400	-3.04954700	3.38827600
H	2.85124800	-2.69074100	3.40976300	H	-0.57066000	-3.92882200	1.50388900
Cs	-3.40672400	1.58099500	0.21804200	H	-0.22650300	1.02765800	2.38802800
H	0.60048500	2.64832100	0.02102600	H	1.01488100	-0.61663100	3.83893700

$T1^{A}_{1f2a}$				I^{A}_{1f2a}			
C	-0.14847500	0.19201800	1.32134300	C	-0.57455700	0.94147100	1.14152100
C	1.10532200	0.65824800	0.87611600	C	0.56063500	1.68048100	0.77744600
C	2.02646000	1.22967000	1.74580800	C	1.13803000	2.58470600	1.66388400
C	1.66420900	1.32353900	3.09596600	C	0.55144300	2.71497500	2.93050300
C	0.43093400	0.85417200	3.55223600	C	-0.56755200	1.96686700	3.30142100
C	-0.49441700	0.28408800	2.66689100	C	-1.14736700	1.06583500	2.39634600
C	-0.87059200	-0.25595500	0.11646800	C	-0.98524000	0.08738400	-0.03126300
C	0.13472100	-0.18849600	-1.02620700	C	0.17955200	0.32961900	-1.03630000
H	3.00251000	1.57556600	1.39020600	H	2.01765900	3.17713700	1.39193900
H	2.37027800	1.76737500	3.80628100	H	0.98892400	3.42043000	3.64540300
H	0.18044300	0.93274700	4.61488100	H	-0.99526800	2.08723900	4.30158800
H	-1.46644600	-0.08224700	3.00618700	H	-2.02971200	0.46443900	2.64839600
N	-1.86253900	-1.19110600	0.16952500	N	-1.10858700	-1.32199800	0.38544600
C	-2.42250900	-1.79314700	-1.05942200	C	-0.14084300	-2.19624500	0.48711300
C	-3.79445300	-2.23108800	-0.56703900	C	-0.77633500	-3.42053500	1.04513900
C	-3.68103800	-2.11171700	0.95057700	C	-2.23941300	-2.96198500	1.24989700
H	-4.06545600	-3.25634200	-0.86120200	H	-0.31777400	-3.73837600	1.99891000
N	-2.52537100	-1.37300500	1.25555200	N	-2.34058400	-1.66751500	0.81330500
O	-4.45191600	-2.50896800	1.77521000	O	-3.12309500	-3.64118900	1.71368000
O	0.00805500	-0.53273000	-2.17414200	O	0.35591700	-0.22748400	-2.08780700
N	1.23889700	0.44206300	-0.49539000	N	0.94857300	1.34673900	-0.52694800
H	-4.59473300	-1.54943800	-0.90323800	H	-0.72597700	-4.28324200	0.35557300
H	-2.45303900	-0.93129100	-1.78594400	H	-2.19906300	-1.14974200	-2.09576000
C	2.38391200	0.80720400	-1.29094600	C	2.17307100	1.75396900	-1.19459800

H	2.53526000	1.90315900	-1.24215500	H	2.45349800	2.75427300	-0.82362200
H	2.11385400	0.55683400	-2.33346900	H	1.94888000	1.83900200	-2.27156800
C	3.65960100	0.09271400	-0.88462500	C	3.27224300	0.73659800	-0.96504600
C	3.62458000	-1.18597800	-0.31878200	C	3.52237700	-0.25033200	-1.92533800
C	4.89754500	0.71037400	-1.09339100	C	3.96971000	0.70396500	0.24969300
C	4.80886800	-1.83945900	0.02367900	C	4.45189000	-1.26064500	-1.67180900
H	2.65783000	-1.67201900	-0.13795200	H	2.95622200	-0.23622100	-2.86432300
C	6.08303200	0.05631600	-0.75581500	C	4.89400300	-0.30953200	0.50590000
H	4.93290000	1.71796800	-1.52670300	H	3.78173600	1.47434200	1.00820100
C	6.04107900	-1.22145600	-0.19562500	C	5.13370200	-1.29566400	-0.45396300
H	4.76804100	-2.83960600	0.46875300	H	4.64061100	-2.02964500	-2.42895500
H	7.04562700	0.55092000	-0.92588100	H	5.43308200	-0.32812500	1.45933600
H	6.97017500	-1.73427400	0.07555800	H	5.86008500	-2.09088400	-0.25357400
C	-1.57502100	-2.95818200	-1.56620200	C	1.30997100	-1.98785000	0.20655800
H	-0.54722500	-2.65797600	-1.80701800	H	1.53988000	-2.06880200	-0.87078400
H	-1.56728600	-3.76688500	-0.81369600	H	1.67125300	-1.00091200	0.55016200
H	-2.03699100	-3.34922000	-2.48714000	H	1.88813200	-2.75698800	0.74171700
C	-1.91694300	1.28942800	-0.50293700	C	-2.25052100	0.54672400	-0.75576600
C	-2.60803800	1.17022200	-1.59665800	C	-2.71684200	-0.22052800	-1.83147200
C	-1.82558500	2.41918600	0.30893600	C	-2.89123400	1.73968300	-0.42368400
C	-3.36508500	2.22870600	-2.09740500	C	-3.82906000	0.19733900	-2.55350900
C	-2.58074900	3.50109500	-0.16160100	C	-4.00647900	2.15893100	-1.15592600
H	-1.22629000	2.48876100	1.22390200	H	-2.52820100	2.34568000	0.41355000
C	-3.33927900	3.40877300	-1.34012800	C	-4.47794800	1.38998000	-2.21650900
H	-3.95868000	2.17455600	-3.01904700	H	-4.19670000	-0.41263400	-3.38547000
H	-2.57451100	4.43940400	0.40470100	H	-4.50971300	3.09372400	-0.88665800
H	-3.92074400	4.27825200	-1.67080100	H	-5.35536700	1.71685600	-2.78510000

$T2^{A}_{1f2a}$				**4b**			
C	0.56467300	-0.98726000	1.14088900	C	-0.57258900	0.90000000	1.18406800
C	-0.56212000	-1.71658500	0.73278500	C	0.57080800	1.64280200	0.85368900
C	-1.15802400	-2.64578200	1.58063200	C	1.16873000	2.48957700	1.78272500
C	-0.59832900	-2.81377300	2.85489000	C	0.59289700	2.56307000	3.05900900
C	0.51157500	-2.07619400	3.27107100	C	-0.53324300	1.81133600	3.39818000
C	1.10784100	-1.14843300	2.40452800	C	-1.12829300	0.96551300	2.45018300
C	0.99854700	-0.09420700	0.00341400	C	-0.99684200	0.09324100	-0.02182000
C	-0.15276600	-0.30461900	-1.02656600	C	0.16981000	0.37980400	-1.01811700
H	-2.03243200	-3.22867900	1.27348500	H	2.05729200	3.08007900	1.53644600
H	-1.05027900	-3.53978500	3.53951400	H	1.04606100	3.22306000	3.80684600
H	0.91800900	-2.22486500	4.27629600	H	-0.95184000	1.88309600	4.40693900
H	1.98363600	-0.55750100	2.69995100	H	-2.01395400	0.36243500	2.68608100
N	1.10876700	1.30057800	0.43365000	N	-1.11466800	-1.32580700	0.27460900
C	0.11612900	2.16391300	0.63920100	C	-0.10892600	-2.20123500	0.54453400
C	0.70973100	3.31501600	1.23112100	C	-0.72221900	-3.35283600	1.00784400
C	2.14702200	2.95735200	1.27880600	C	-2.10652600	-3.03955800	1.00267200
H	0.19673300	3.91266100	1.99143600	N	-2.32811600	-1.81763800	0.57946700
N	2.34898500	1.74023000	0.79696500	O	-3.14457200	-3.81506300	1.36487700
O	2.94420200	3.95146700	1.40322800	O	0.34526500	-0.12937600	-2.09348900
O	-0.31908700	0.29481100	-2.05575000	N	0.95075500	1.36611900	-0.46489000
N	-0.92689500	-1.34118200	-0.56646300	H	-2.81252700	-4.67043400	1.64705600
H	1.63788200	4.24393200	0.85940300	H	-2.21994600	-1.00619700	-2.14851600
H	2.25503900	1.17473700	-2.01746100	C	2.17384100	1.79368700	-1.12009700
C	-2.14159700	-1.72241400	-1.26679500	H	2.47076900	2.76842600	-0.69718000
H	-2.43520800	-2.72979700	-0.92651100	H	1.94133300	1.94113200	-2.18872300
H	-1.89856500	-1.78237300	-2.34140200	C	3.26618900	0.75535600	-0.96178900
C	-3.23960500	-0.70462600	-1.03303800	C	3.49951700	-0.17461200	-1.98143700

C	-3.47809700	0.29704900	-1.98101000	C	3.98026200	0.64998500	0.23873600
C	-3.95150000	-0.69047000	0.17348300	C	4.42890800	-1.20036100	-1.80038100
C	-4.40994100	1.30413700	-1.72293500	H	2.91783800	-0.10611700	-2.90830700
H	-2.90037800	0.29793400	-2.91292600	C	4.90396900	-0.37953700	0.42274000
C	-4.87740800	0.32025200	0.43483100	H	3.80419000	1.37486600	1.04376100
H	-3.77323300	-1.47320000	0.92187000	C	5.12754800	-1.30805100	-0.59655700
C	-5.10556100	1.32111800	-0.51261000	H	4.60239500	-1.92552500	-2.60297900
H	-4.58853700	2.08523500	-2.47000000	H	5.45522100	-0.45611500	1.36634100
H	-5.42765000	0.32461700	1.38207300	H	5.85325200	-2.11609100	-0.45284000
H	-5.83333800	2.11404500	-0.30827600	C	1.34707000	-1.89524300	0.39244300
C	-1.33590800	1.86806200	0.45609100	H	1.64213700	-1.78769400	-0.66564700
H	-1.61995600	1.88942100	-0.61066400	H	1.62559800	-0.96317500	0.91929300
H	-1.61192000	0.87738000	0.86103000	H	1.93687300	-2.71304900	0.83303600
H	-1.92744300	2.63022600	0.98444200	C	-2.25597700	0.61298600	-0.72052500
C	2.26888500	-0.55222500	-0.71704300	C	-2.73092800	-0.08838100	-1.83746800
C	2.75801600	0.23321200	-1.76981100	C	-2.88700100	1.79239400	-0.32433500
C	2.89312800	-1.75957200	-0.40384600	C	-3.83601100	0.38249000	-2.53803100
C	3.87325100	-0.18280800	-2.48833000	C	-3.99707600	2.26351500	-1.03308500
C	4.01257300	-2.17569900	-1.13166100	H	-2.51773600	2.34891600	0.54411100
H	2.51281500	-2.38118000	0.41408900	C	-4.47432400	1.56055800	-2.13621800
C	4.50506500	-1.38964200	-2.16986300	H	-4.20613800	-0.17484100	-3.40527800
H	4.25723900	0.44092400	-3.30252100	H	-4.49070400	3.18747000	-0.71284800
H	4.50176400	-3.12194900	-0.87685200	H	-5.34649500	1.92859400	-2.68772100
H	5.38542900	-1.71420700	-2.73526700	H	-0.23252200	-4.28102500	1.30294800

T^{C}_{1f2a4a}				**4a**			
C	0.39529500	0.25925000	1.51168000	C	-0.12097500	-1.39683300	-0.90050100
C	-0.99533500	0.05296800	1.64406300	C	1.09402100	-1.59381300	-0.22841700
C	-1.83617100	1.03627300	2.14721200	C	2.08443200	-2.42286600	-0.74400800
C	-1.24679800	2.24234900	2.54976300	C	1.81778700	-3.06256600	-1.96270500
C	0.13180300	2.44943900	2.44875700	C	0.61186100	-2.87171600	-2.63950000
C	0.97084500	1.46116100	1.92298000	C	-0.37217000	-2.02502600	-2.10747800
C	0.90032600	-0.92949900	0.84220800	C	-0.96383200	-0.43026600	-0.10648900
C	-0.24153100	-1.88957200	0.68405300	C	-0.02802800	-0.09549600	1.09649600
H	-2.91832500	0.88049800	2.20928200	H	3.04151600	-2.55712300	-0.22981900
H	-1.88478100	3.03904600	2.94761100	H	2.57965900	-3.72097500	-2.39426200
H	0.56077600	3.40351200	2.77095500	H	0.43767800	-3.38063200	-3.59283900
H	2.04620800	1.61954900	1.80151300	H	-1.31970800	-1.84754100	-2.62882700
N	2.11804000	-1.16311600	0.41669000	N	-1.37623400	0.75132100	-0.88012200
C	2.52658100	-2.39180100	-0.36152400	C	-0.57413600	1.98453900	-0.90031500
C	4.04026100	-2.24735000	-0.30331900	C	-1.64944200	3.01455800	-1.27931400
C	4.21787000	-0.74529600	-0.06651500	C	-2.90585400	2.47975500	-0.58420500
H	4.54809700	-2.55600600	-1.22904200	H	-1.82958700	3.01709300	-2.37150000
N	3.03070400	-0.23016200	0.45616900	N	-2.62980500	1.16436600	-0.35314900
O	5.20098200	-0.08794600	-0.26538900	O	-3.93086800	3.04678900	-0.29982300
O	-0.24591700	-3.00961700	0.22211000	O	-0.25276900	0.69488000	1.97734200
N	-1.33910100	-1.21756000	1.17400800	N	1.11879600	-0.83935200	0.95145000
H	4.48966400	-2.79565100	0.54298500	H	-1.42820900	4.04246000	-0.95619800
H	2.11223200	-3.26486200	0.16373600	H	-0.23047700	2.22246700	0.13145900
C	-2.68173200	-1.71926800	1.04597300	C	2.24969600	-0.72211800	1.84332700
H	-3.19730500	-1.67124500	2.02400300	H	2.61651100	-1.73115900	2.10808900
H	-2.58214900	-2.78640000	0.77441600	H	1.86157800	-0.24598600	2.76170500
C	-3.48440400	-0.97794600	-0.00926800	C	3.36442600	0.11198600	1.24298400
C	-2.84816200	-0.40028700	-1.11412800	C	3.08952700	1.42145200	0.82551900
C	-4.87569800	-0.88859700	0.10013200	C	4.65485700	-0.39829600	1.08560300
C	-3.59682500	0.24481200	-2.09952900	C	4.09129800	2.20298500	0.25315800
H	-1.75305400	-0.44873200	-1.20155000	H	2.07788000	1.82727800	0.96898500
C	-5.62483300	-0.24340200	-0.88507100	C	5.66164900	0.38516900	0.51504800

H	-5.38001600	-1.33059700	0.96887800	H	4.87684600	-1.42185500	1.41503500
C	-4.98641500	0.32440000	-1.98862100	C	5.38036800	1.68472600	0.09556400
H	-3.08837400	0.68918700	-2.96310300	H	3.86966700	3.22755600	-0.06562000
H	-6.71412300	-0.17979600	-0.78713300	H	6.67027000	-0.02499300	0.39473500
H	-5.57202400	0.83324300	-2.76184600	H	6.16772800	2.29925400	-0.35415600
C	1.82235100	3.51906500	-1.20863100	C	0.61077500	1.85043600	-1.83808900
C	2.72299100	2.45383500	-1.02029100	H	1.29915500	1.05503300	-1.49590200
C	2.03689400	1.25952300	-1.09315700	H	0.26817100	1.59306200	-2.85492100
C	0.81678300	0.99669000	-1.29394000	H	1.18401000	2.79215500	-1.87880600
C	-0.11536700	2.01853800	-1.50239100	C	-3.24046200	0.11094700	0.29584000
C	0.44620400	3.30615000	-1.43374200	C	-2.30712800	-0.92856000	0.41345300
H	2.20128200	4.54751800	-1.16848700	C	-4.54287900	-0.00308000	0.77568000
H	3.79353700	2.57571400	-0.82619800	C	-2.66303900	-2.13015700	1.00450800
H	-1.19068300	1.87914200	-1.67160000	C	-4.88716500	-1.21795700	1.37712800
H	-0.20823900	4.17816800	-1.55074300	H	-5.24274700	0.83099400	0.67541700
C	1.98256600	-2.30419100	-1.78357500	C	-3.97212600	-2.27064600	1.48524200
H	2.30806800	-3.19870600	-2.33950700	H	-1.93727100	-2.94773900	1.09056400
H	0.88265000	-2.27443200	-1.79198100	H	-5.90301600	-1.34872700	1.76592000
H	2.37352700	-1.40625100	-2.29275000	H	-4.28063500	-3.21125300	1.95238000
	T^{C}_{1f2a5a}				**5a**		
C	-0.14713900	0.50849800	0.76141900	C	0.04204600	-1.40921900	1.01821500
C	1.11098400	0.83485900	0.20631000	C	-1.16197700	-1.62085200	0.33128100
C	1.80061700	1.98050600	0.57968200	C	-2.16802200	-2.42202100	0.86136100
C	1.19371300	2.81535400	1.52819700	C	-1.91874800	-3.03568400	2.09677400
C	-0.05389100	2.50944700	2.07802600	C	-0.71178100	-2.85205600	2.77424500
C	-0.74231100	1.35054300	1.70110900	C	0.28331800	-2.02363000	2.23460700
C	-0.55495800	-0.72320200	0.10956700	C	0.88027800	-0.43946200	0.23009800
C	0.53161900	-1.12194000	-0.84400200	C	0.02820500	-0.24508100	-1.07161600
H	2.78211700	2.21604400	0.15522500	H	-3.11989900	-2.56334200	0.33937100
H	1.71336300	3.72705100	1.84268700	H	-2.69247100	-3.67359300	2.53796400
H	-0.50099800	3.18537800	2.81373600	H	-0.54724400	-3.34956600	3.73529800
H	-1.72358300	1.09633000	2.11157400	H	1.23498600	-1.85240300	2.75045000
N	-1.67058000	-1.39150300	0.28463300	N	2.28702500	-0.79804200	0.12150000
C	-2.01819500	-2.64611600	-0.47454200	C	2.89102700	-1.77286700	-0.80170800
C	-3.52760900	-2.67583400	-0.29538600	C	4.35395300	-1.27939300	-0.80733700
C	-3.77587700	-1.67631100	0.83531000	C	4.25758700	0.22836700	-0.55691900
H	-3.92187700	-3.66860200	-0.02909700	H	4.88744000	-1.48956500	-1.74721600
N	-2.61356100	-0.93653200	1.05980100	N	2.99578700	0.41600500	-0.08310100
O	-4.80970500	-1.48839100	1.41405600	O	5.09579200	1.08308900	-0.70255900
O	0.60069600	-2.08546500	-1.57593900	O	0.28750300	0.46512900	-2.00855700
N	1.48723700	-0.13486000	-0.72705600	N	-1.14387100	-0.94342900	-0.89401200
H	-4.06654200	-2.31398500	-1.18759800	H	4.93758800	-1.71308700	0.02454700
H	-1.68306500	-2.49021100	-1.51195900	H	2.80860200	-2.76878100	-0.33170900
C	2.70070500	-0.12092600	-1.50255700	C	0.44142900	3.11285200	1.70382200
H	2.73238400	0.78915400	-2.13350400	C	0.06880100	1.79229700	1.41320000
H	2.63113600	-0.99076500	-2.18177500	C	1.00527100	0.97356800	0.80383800
C	3.96035200	-0.20216500	-0.65990300	C	2.28255600	1.45446100	0.48453400
C	3.96405000	-0.86076900	0.57401700	C	2.66911700	2.76367400	0.75736000
C	5.14691300	0.37386500	-1.12662400	C	1.71693000	3.58353200	1.37316900
C	5.13738600	-0.94961200	1.32379300	H	-0.27238900	3.78268400	2.19394300
H	3.03459600	-1.30151600	0.95508900	H	-0.93246200	1.41386800	1.65838600
C	6.32230600	0.28193800	-0.38015800	H	3.67294400	3.10979600	0.49605100
H	5.14976600	0.90244600	-2.08833400	H	1.98236200	4.62018500	1.60795400
C	6.32008200	-0.38087600	0.84821900	C	-2.27501600	-0.80372400	-1.78346000
H	5.12625900	-1.46534300	2.29021400	H	-2.71516500	-1.79758900	-1.98558500
H	7.24462100	0.73660200	-0.75804800	H	-1.86724300	-0.40855900	-2.73102700

H	7.24014000	-0.44911900	1.43861200	C	-3.31405000	0.14231000	-1.21409400
C	-1.29269500	-3.83184300	0.15001800	C	-2.92824800	1.44425300	-0.86264000
H	-0.20202300	-3.71807800	0.05580400	C	-4.63630600	-0.25816200	-1.01258500
H	-1.56994900	-3.93386600	1.21392300	C	-3.85694400	2.32688500	-0.31439000
H	-1.58631200	-4.75415200	-0.37717100	H	-1.89166800	1.76618800	-1.03691600
C	-3.93169900	3.01204100	-0.46281300	C	-5.56892300	0.62805200	-0.46612800
C	-4.13928600	1.71491700	0.04605700	H	-4.94276200	-1.27582900	-1.28807700
C	-3.23717500	0.85180600	-0.54113400	C	-5.17968000	1.91966400	-0.11407000
C	-2.32912400	1.04504300	-1.39148700	H	-3.54874700	3.34367600	-0.04709200
C	-2.09019200	2.30121000	-1.94934500	H	-6.60381200	0.30392400	-0.31105900
C	-2.93863000	3.29394300	-1.42430800	H	-5.90879700	2.61444500	0.31679400
H	-4.56131100	3.83183700	-0.09610400	C	2.30186500	-1.81686100	-2.20963000
H	-4.89881000	1.45834700	0.79189600	H	1.25722700	-2.17401400	-2.20139800
H	-1.32712000	2.53886300	-2.69937300	H	2.31994100	-0.82091900	-2.68379700
H	-2.82207000	4.32844200	-1.76916600	H	2.88649400	-2.52042100	-2.82622600