Experimental and computational investigation of α-amylase catalysed Friedel−Crafts reaction on isatin to access symmetrical and unsymmetrical 3,3',3''–trisindoles

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General Procedures:

Procedure for control experiments:

To investigate the role of enzyme in the reaction, five distinct control reactions were set up. Five teflon tubes were taken for the experiments, and each tube was equipped with magnetic beads. Subsequently, a volume of 4.25 ml of water was added to each tube, following this, the catalyst (α-amylase, denatured amylase, and BSA) with the concentration of 3 mg/ml were added into the different reaction tubes. Next, additives like starch (0.032 mmol, 0.3 equiv.) and urea (0.75 mmol, 1 equiv.) were added into two reaction tubes. Then, the reactants, isatin (0.68 mmol, 1 equivalent), indole (0.675 mmol, 1 equivalent), and 5-methoxyindole (0.680 mmol, 1 equivalent), were subsequently dissolved in 0.75 ml of DMSO and added to the reaction vials. The resultant reaction mixture was subjected to gentle stirring at a temperature of 50^{o}C for a duration of 12 hours. The mixture was extracted using ethyl acetate and the volatiles were evaporated under high vacuum conditions. The resulting crude mixture was then subjected to purification via column chromatography, utilizing silica (mesh size 60-120) as the stationary phase and a mobile phase consisting of a mixture of ethyl acetate and hexane. This purification process aimed to obtain both 3,3',3"–trisindoles or 3-hydroxy bisindoles.

Procedure for hammett studies:

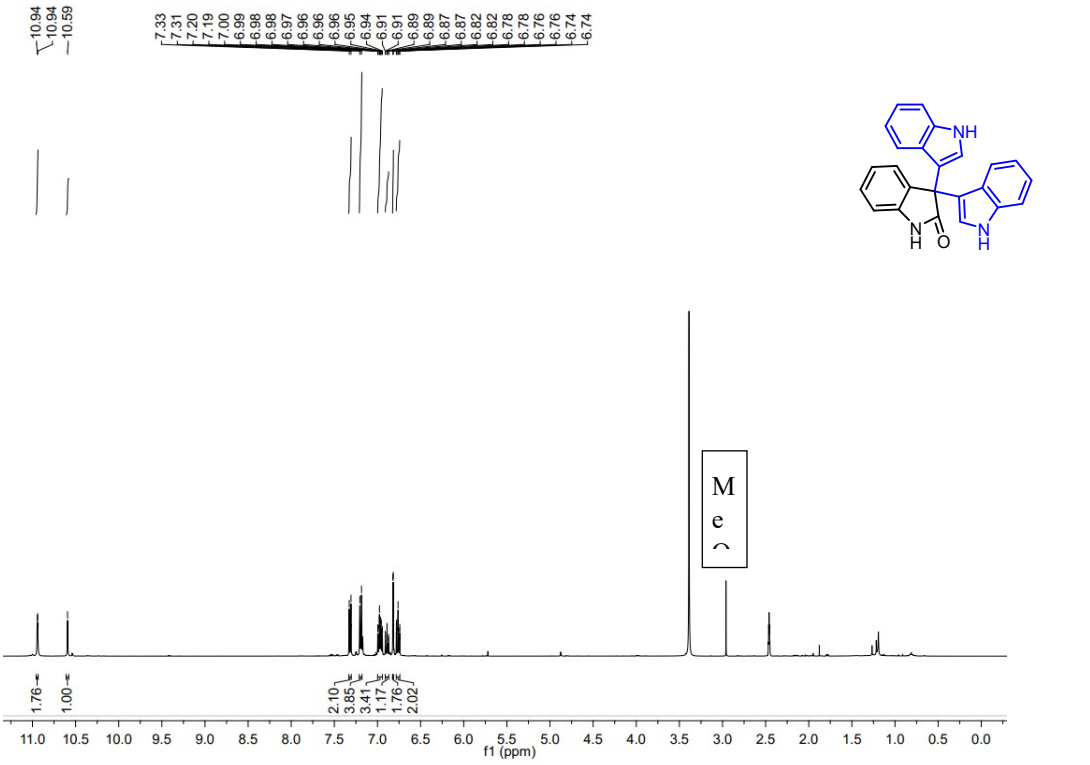
In a Teflon tube having a stirrer, 4.25 ml of deionized water, 3 mg/ml of the enzyme (α-amylase from *Aspergillus oryzae* were added. Afterwards, the reactants, isatin (0.68 mmol, 1.0 equiv.), substituted isatin (0.68 mmol, 1.0 equiv.) and indole (1.35 mmol, 2.0 equiv.) were dissolved in 0.75 ml of dimethyl sulfoxide (DMSO) and subsequently introduced into the reaction tube. The resulting reaction mixture was subjected to gentle stirring at a temperature of 50^{o}C for a duration of 12 hours. Then the mixture underwent extraction using ethyl acetate (3x10 ml) followed by the evaporation of volatiles under high vacuum conditions. The resulting crude mixture was then subjected to purification via column chromatography, utilizing silica (mesh size 60-120) as the stationary phase and a mobile phase consisting of a mixture of ethyl acetate and hexane. This process allowed for the separate isolation of substituted and unsubstituted 3,3',3"–trisindoles, and the yields of these isolated compounds were determined.

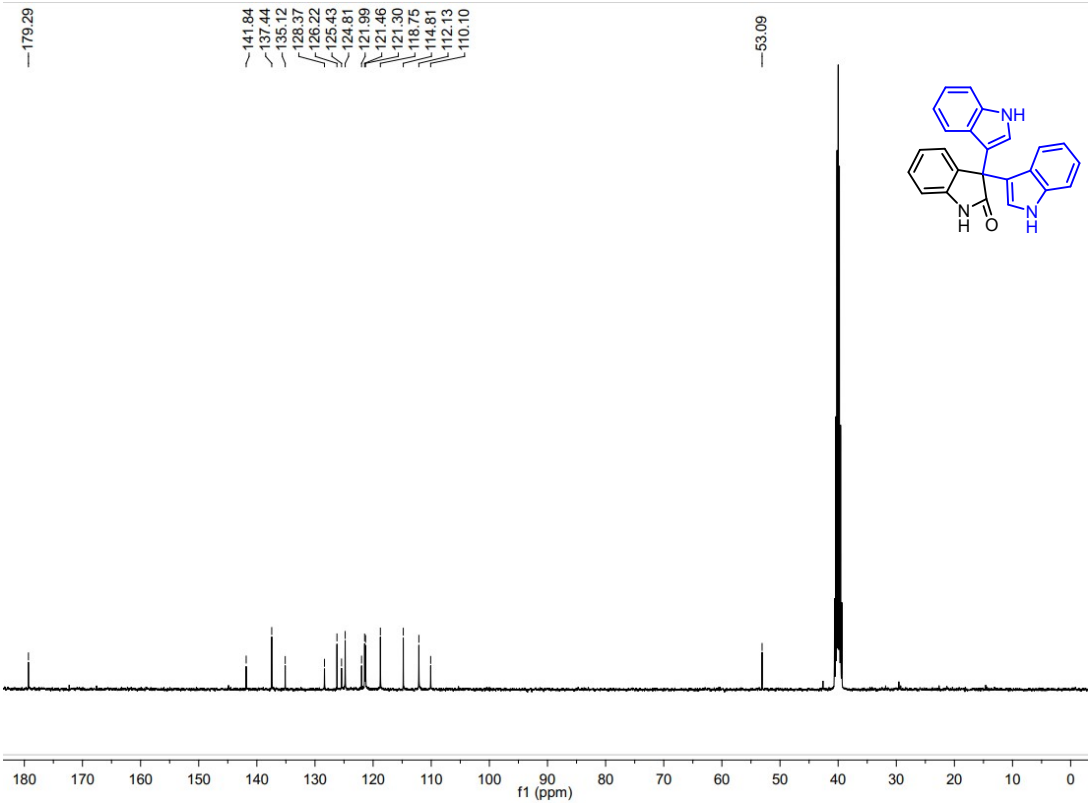
Procedure for scale-up reactions:

In the context of scaling up a reaction, a round-bottom flask with a volume of 100 mL was taken. In this experimental setup, a stirrer bar was placed inside the flask and then filled with 42.5 ml of deionized water and enzyme (α-amylase from *Aspergillus oryzae)* with a concentration of 3 mg/ml. Furthermore, the reactants, isatin (6.80 mmol, 1.0 equiv.) and indole (13.5 mmol, 2.0 equiv.), were solubilized in 7.5 ml of dimethyl sulfoxide (DMSO) and introduced into a round-bottom flask, which was properly sealed using a rubber septum and paraffin film. The reaction mixture obtained was subjected to continous stirring at a temperature of 50^{o}C for a period of 12 hours. After the completion of the reaction, the mixture was subjected to extraction using ethyl acetate. Following this, the volatile substances underwent evaporation under conditions of high vacuum. The crude mixture obtained was subsequently purified using column chromatography, employing silica (mesh size 60-120) as the stationary phase and a mobile phase of ethyl acetate and hexane. The purification procedure thus acquired 3,3',3''–trisindoles product.

^{1}H and ^{13}C-NMR Spectra of Synthesized compounds (3a-3o) and (4a-4s):

^{1}H and ^{13}C-NMR spectra of 3a





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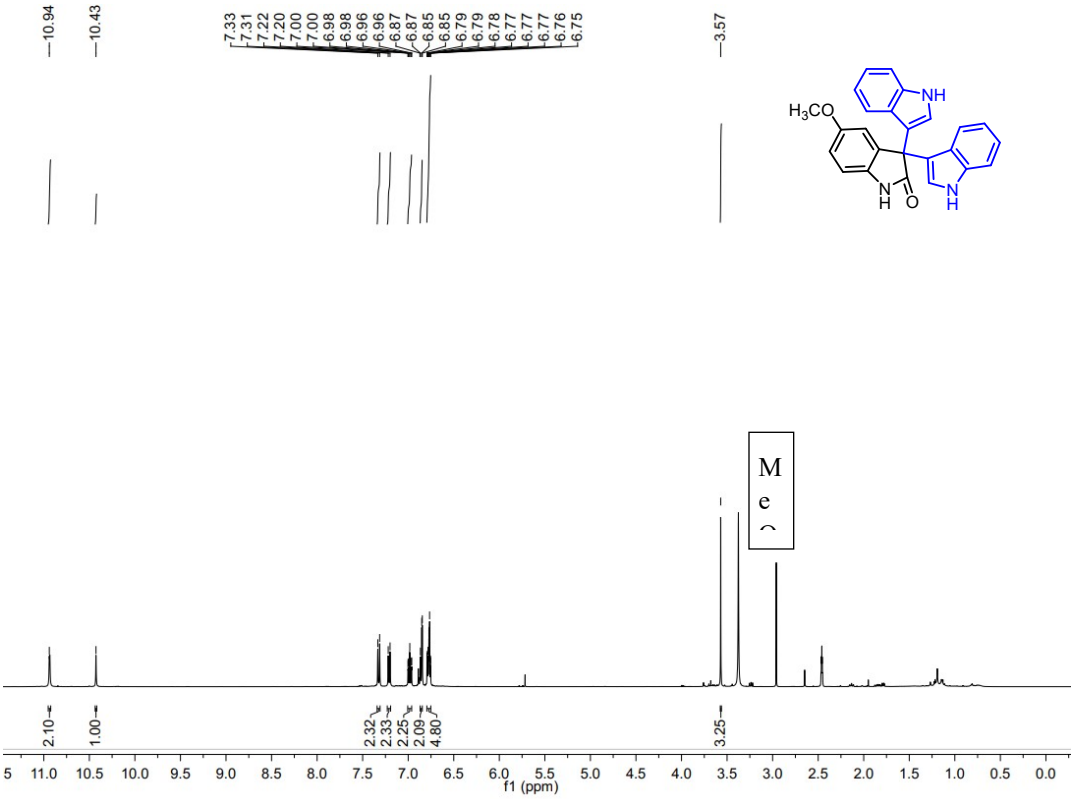

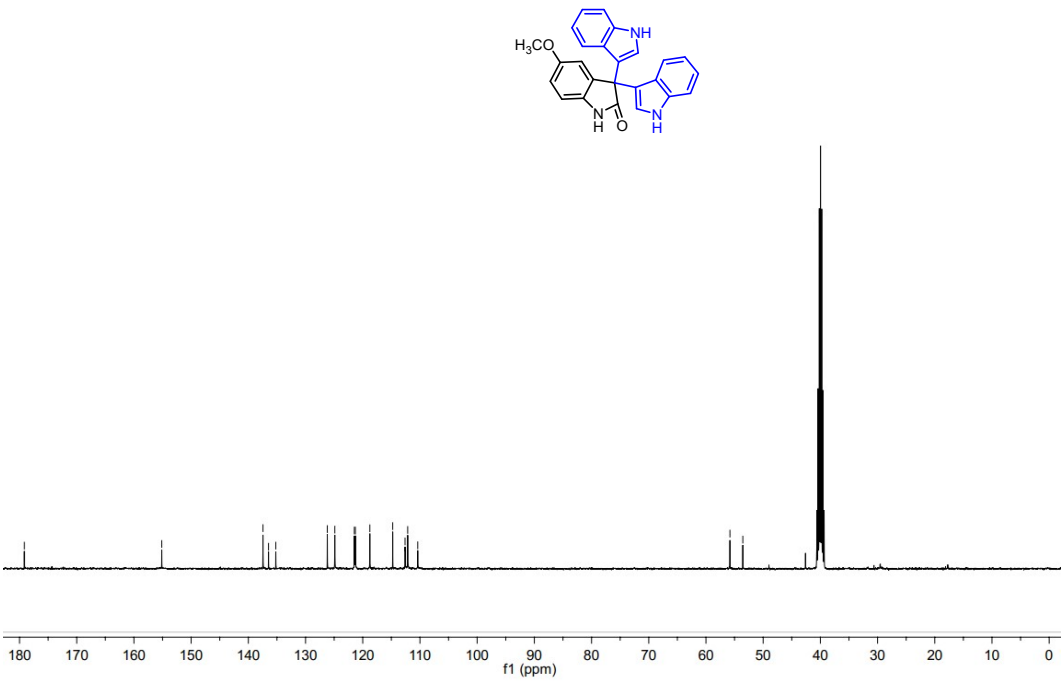

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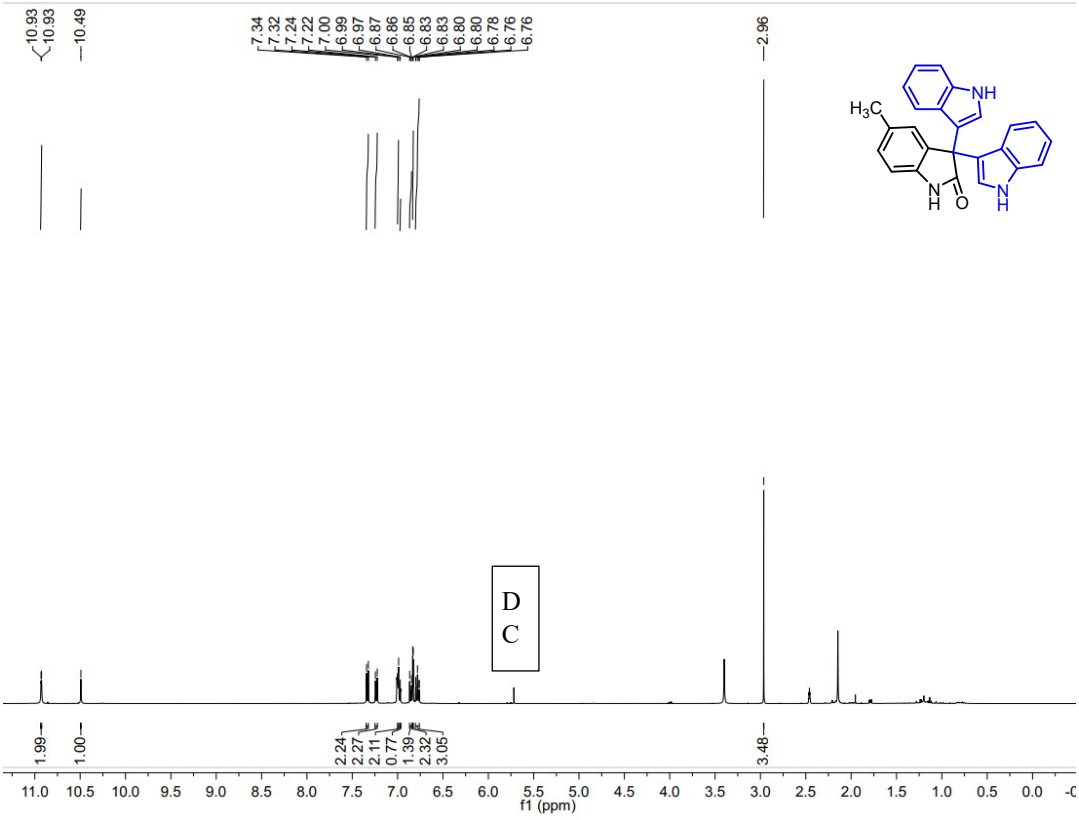

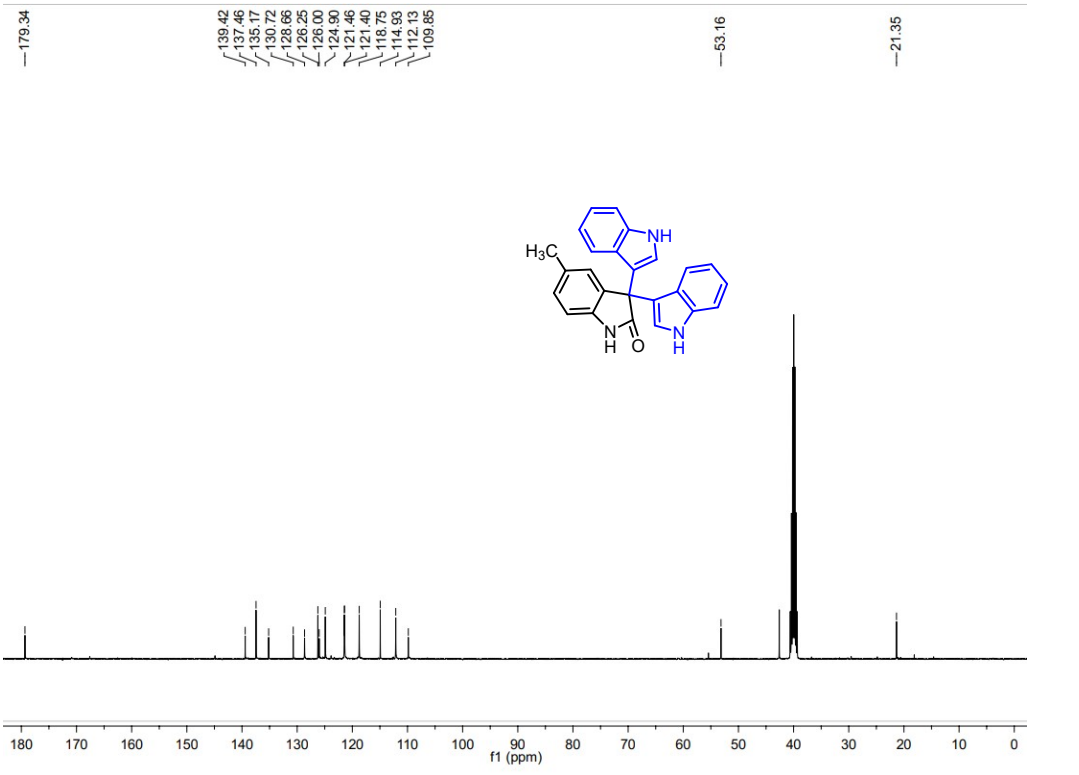

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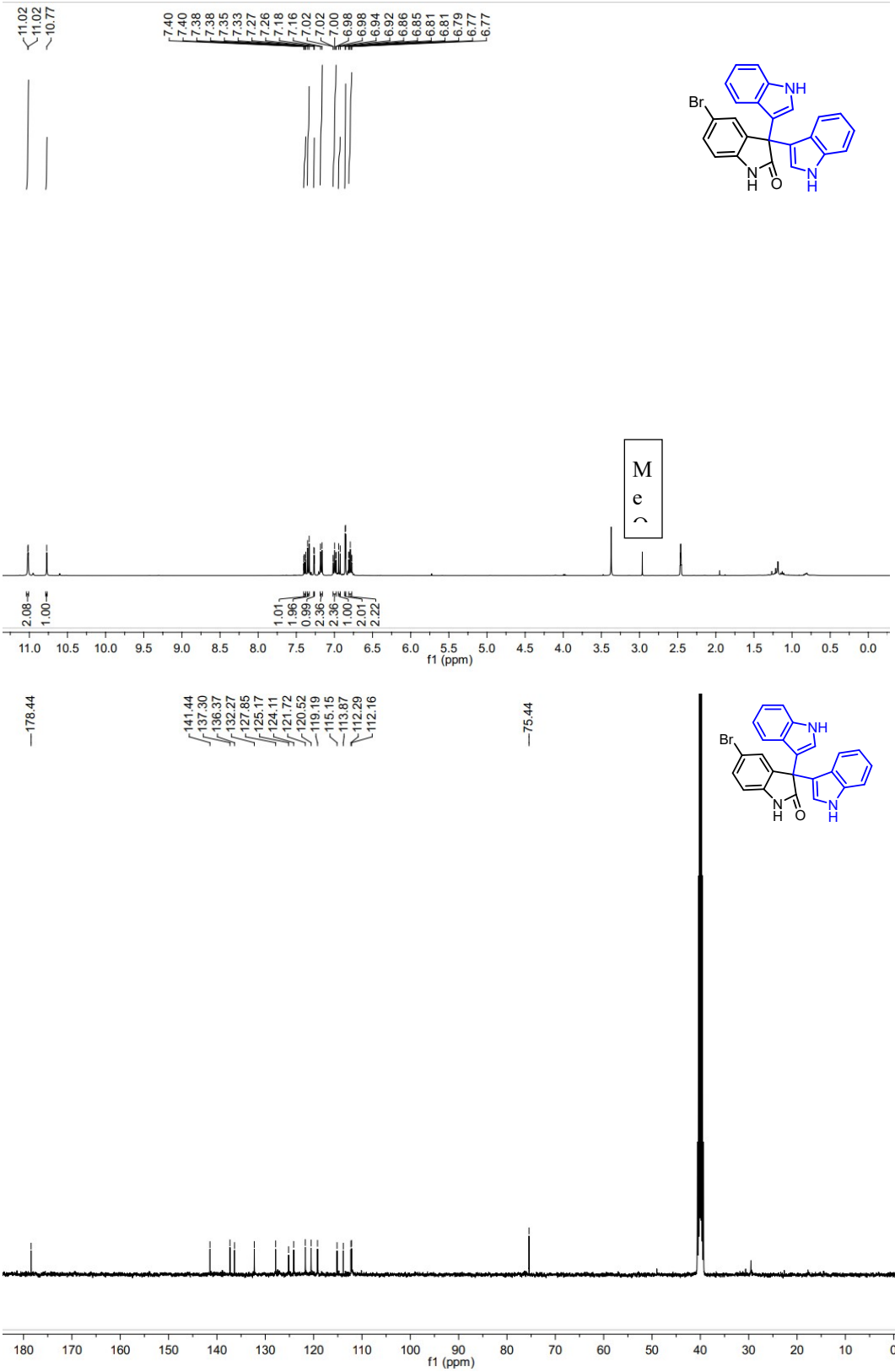

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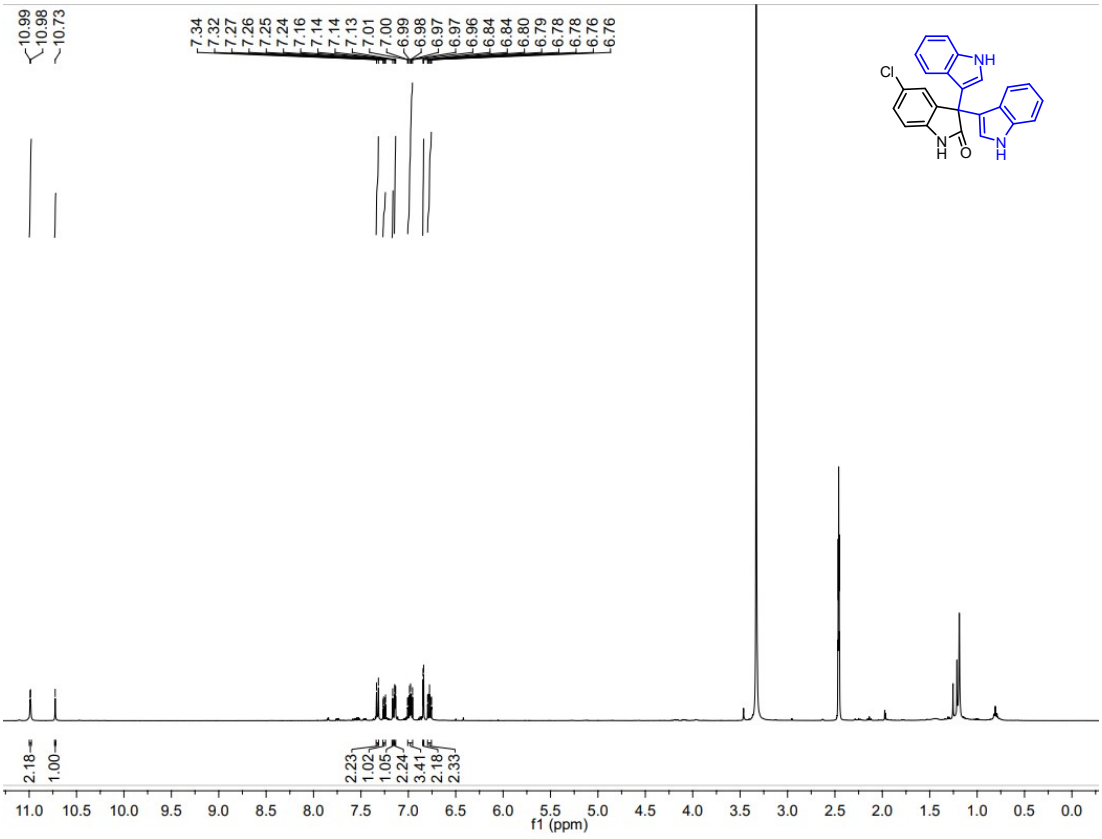
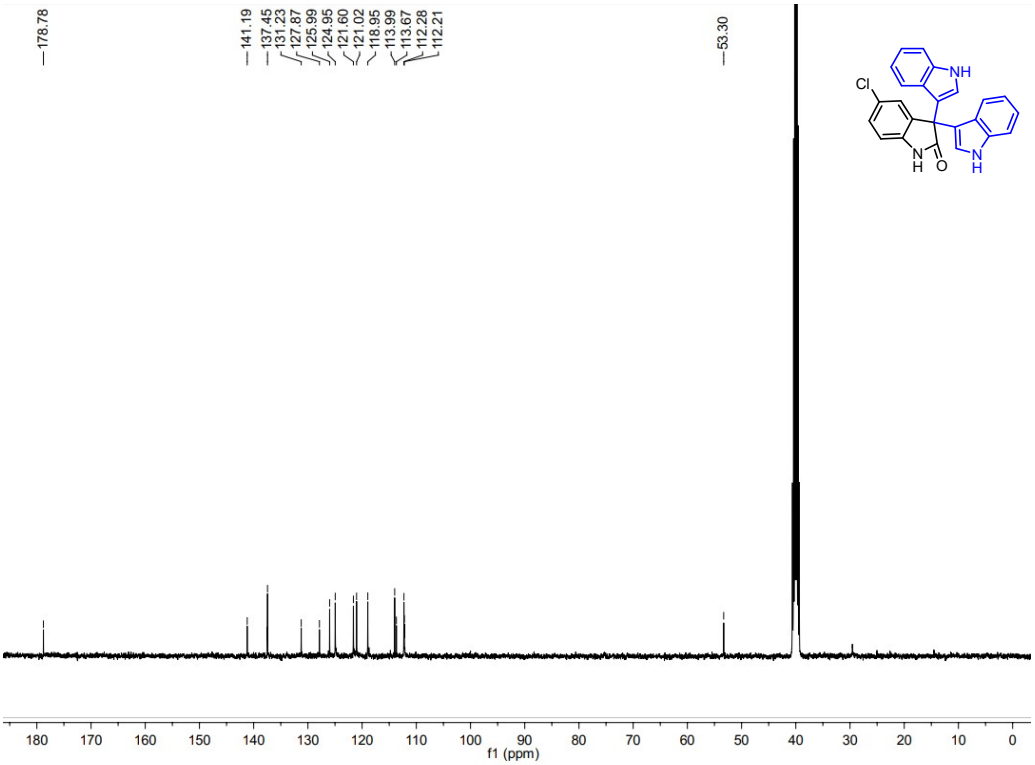
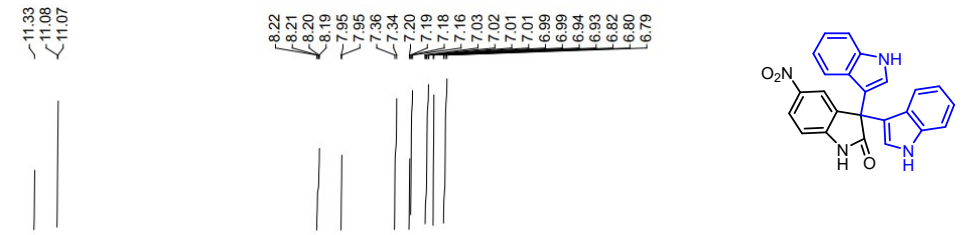
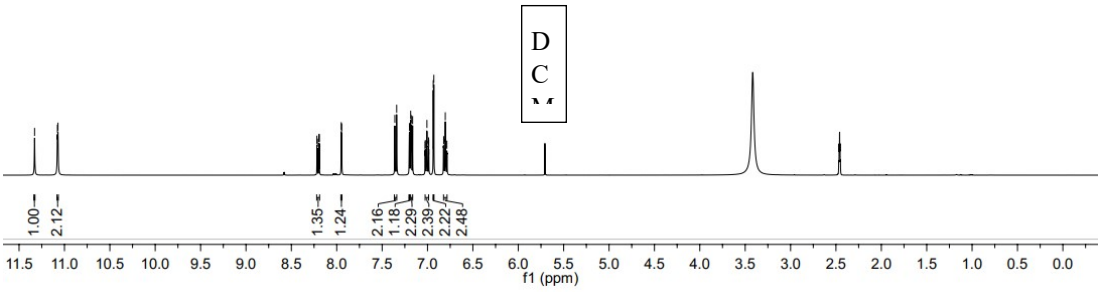
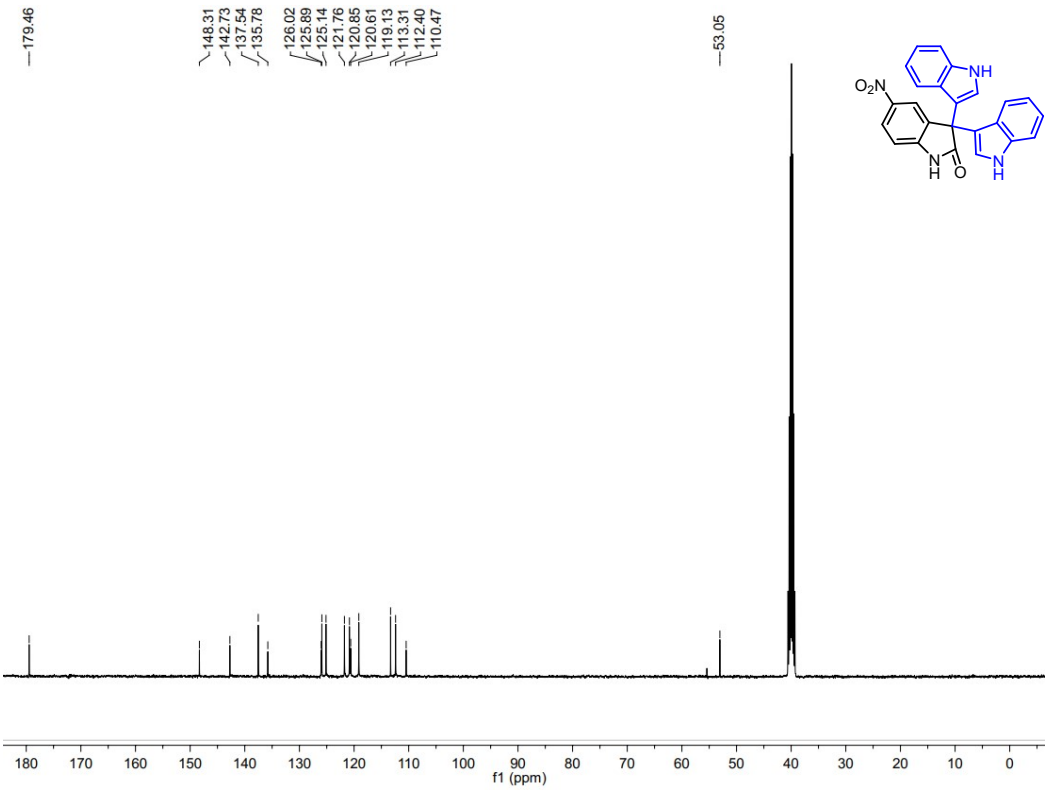




^{1}H and ^{13}C-NMR spectra of 3f







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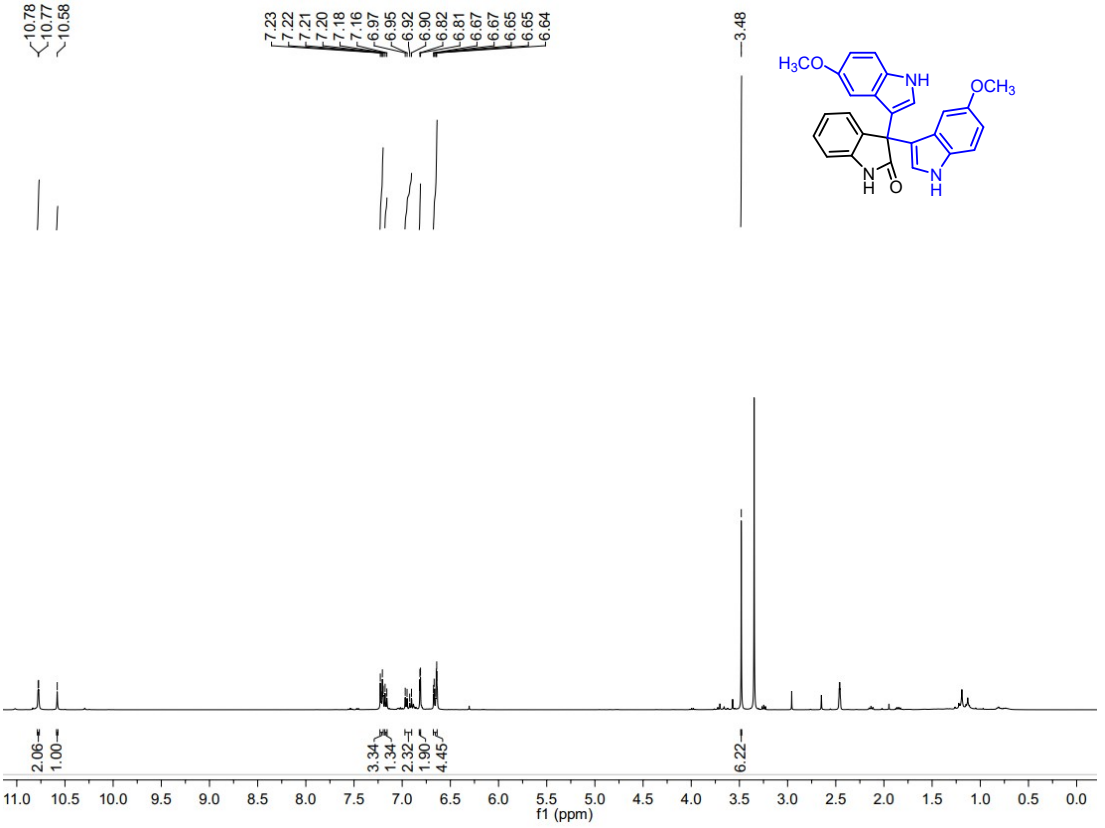
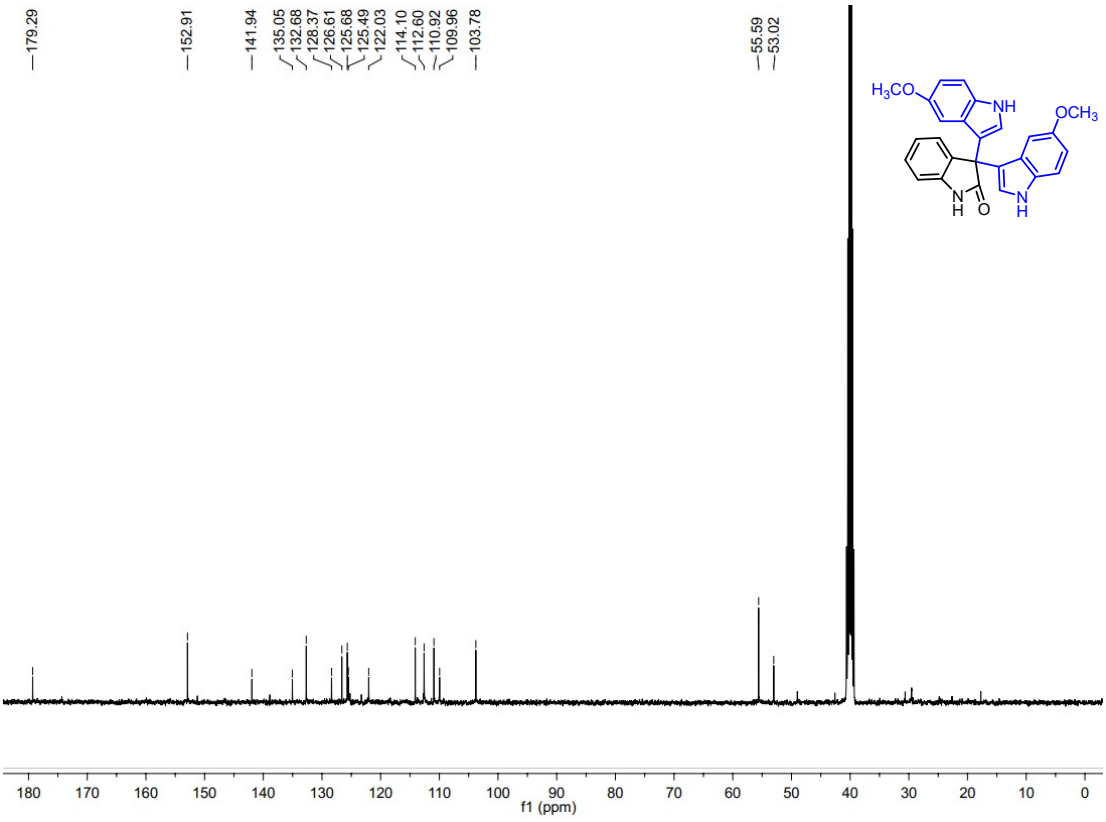
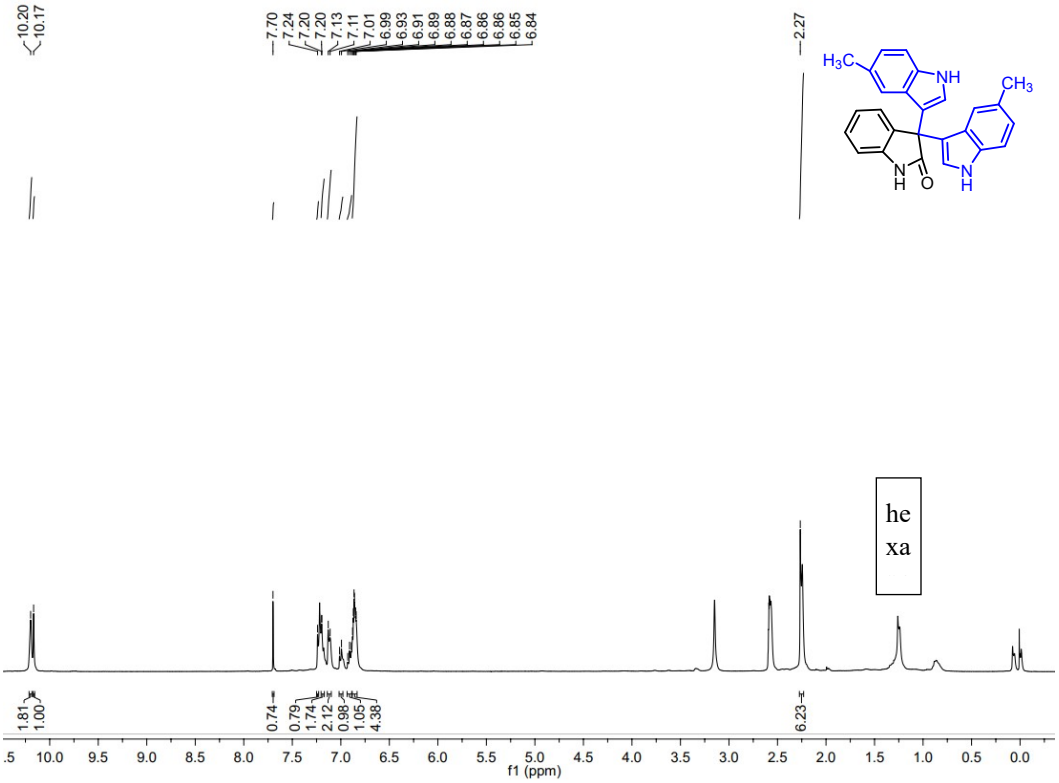
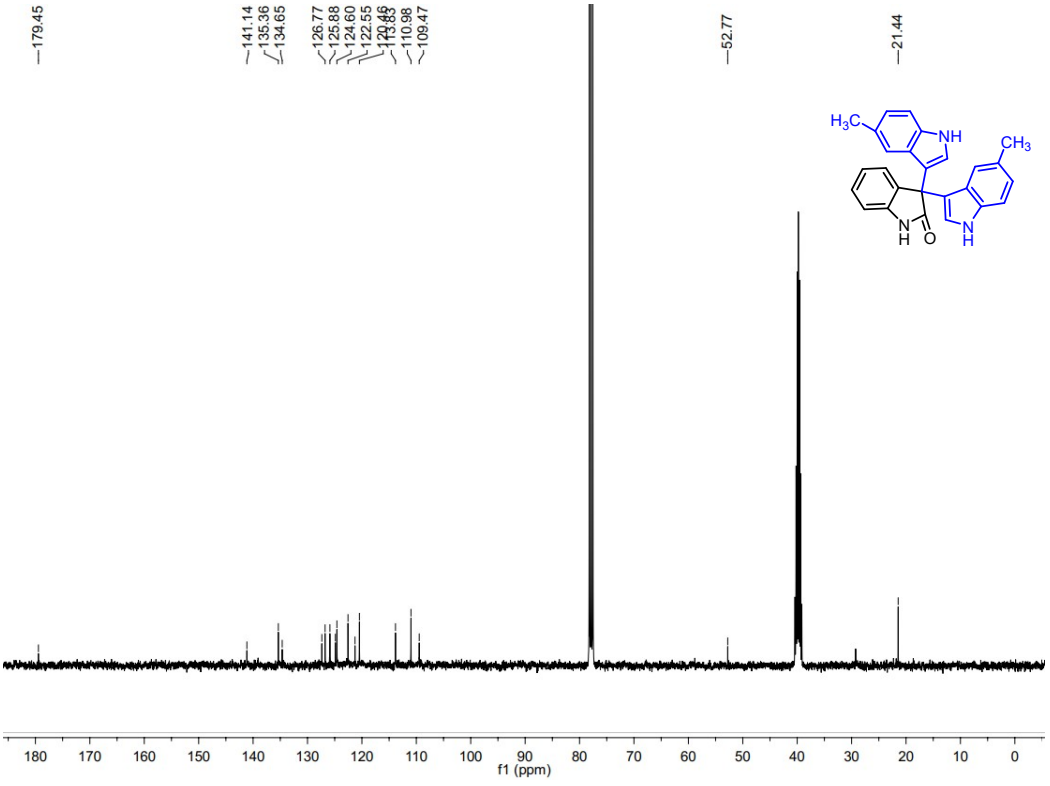


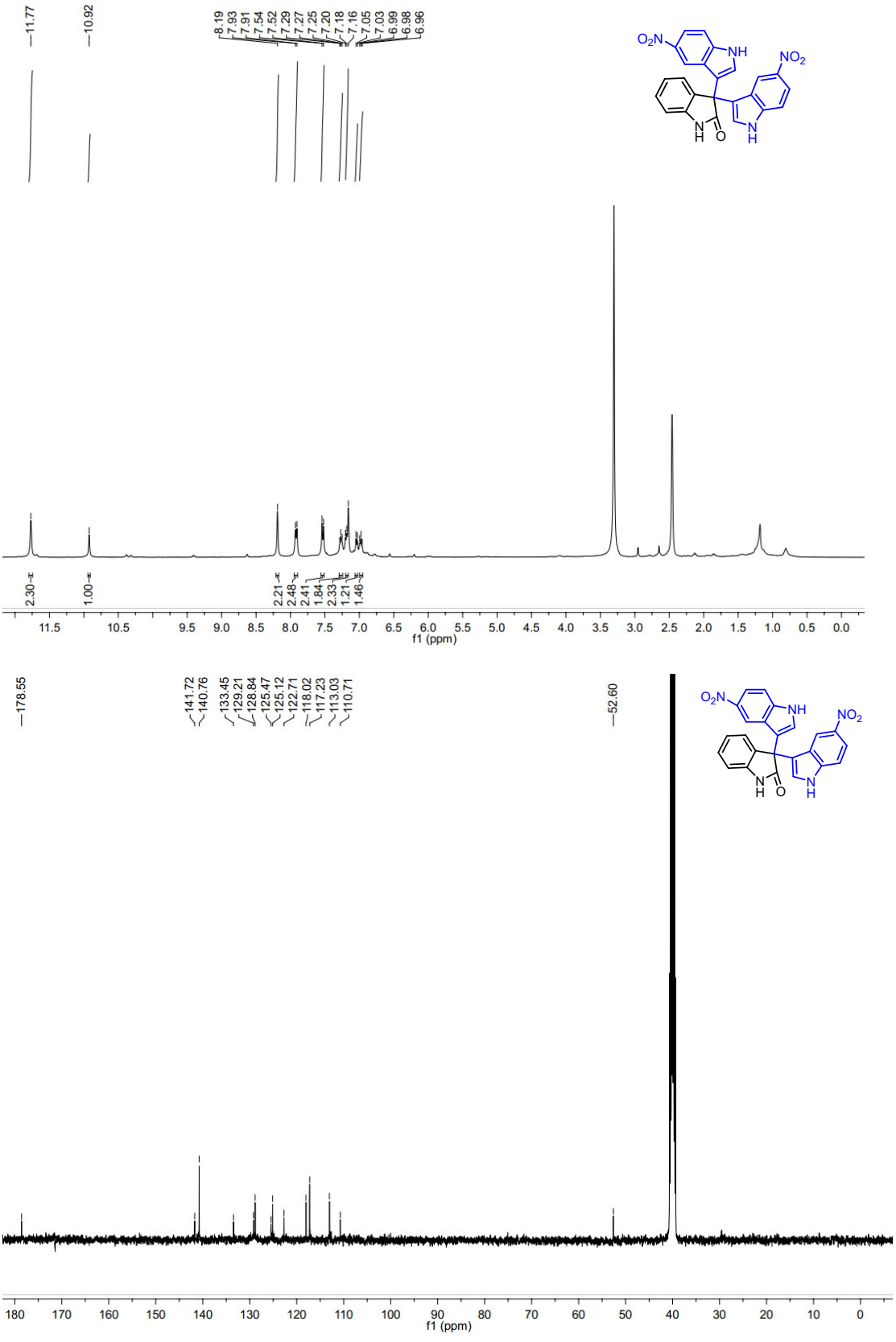


^{1}H and ^{13}C-NMR spectra of 3h

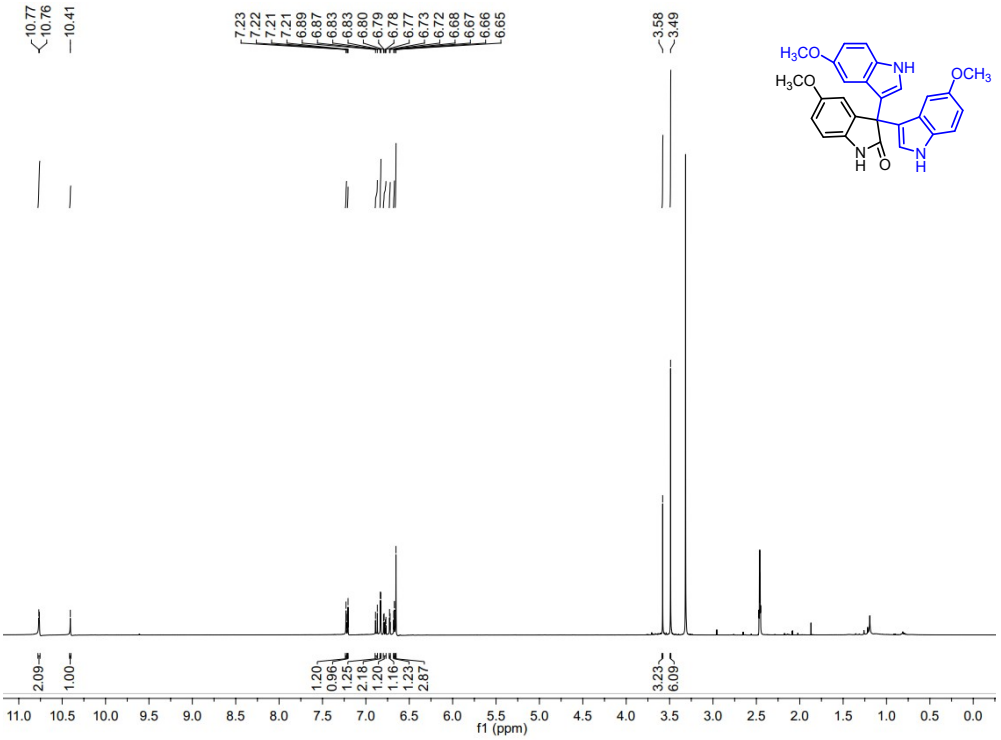


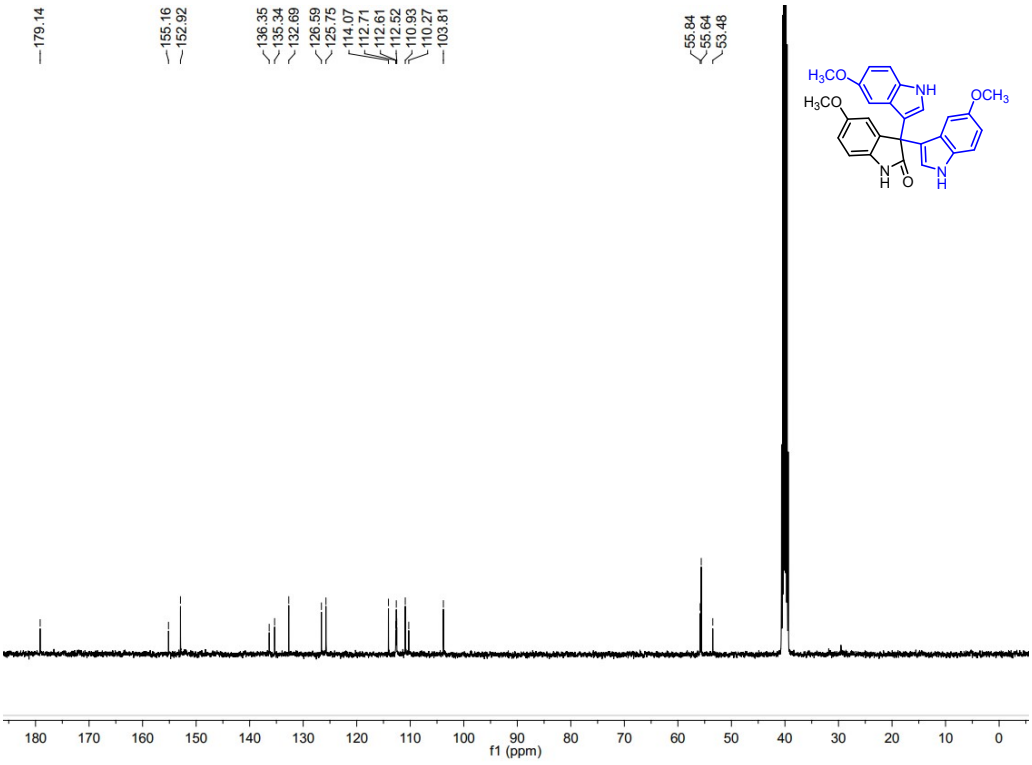


^{1}H and ^{13}C-NMR spectra of 3i



^{1}H and ^{13}C-NMR spectra of 3j





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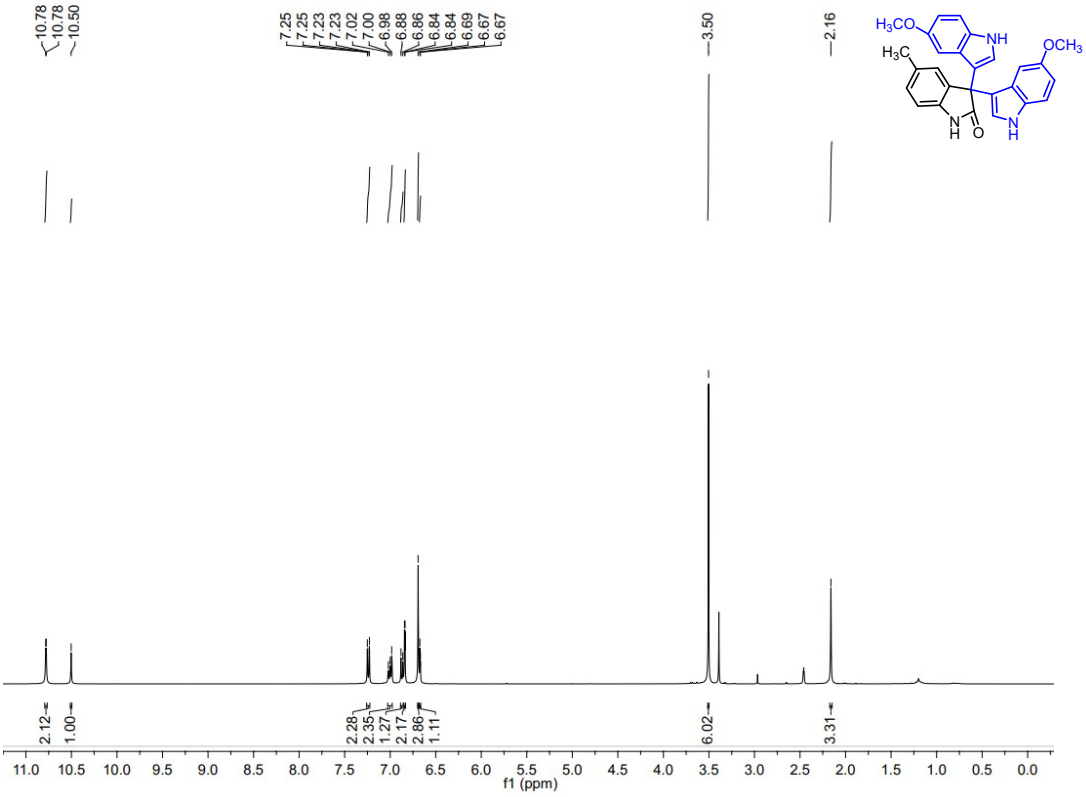
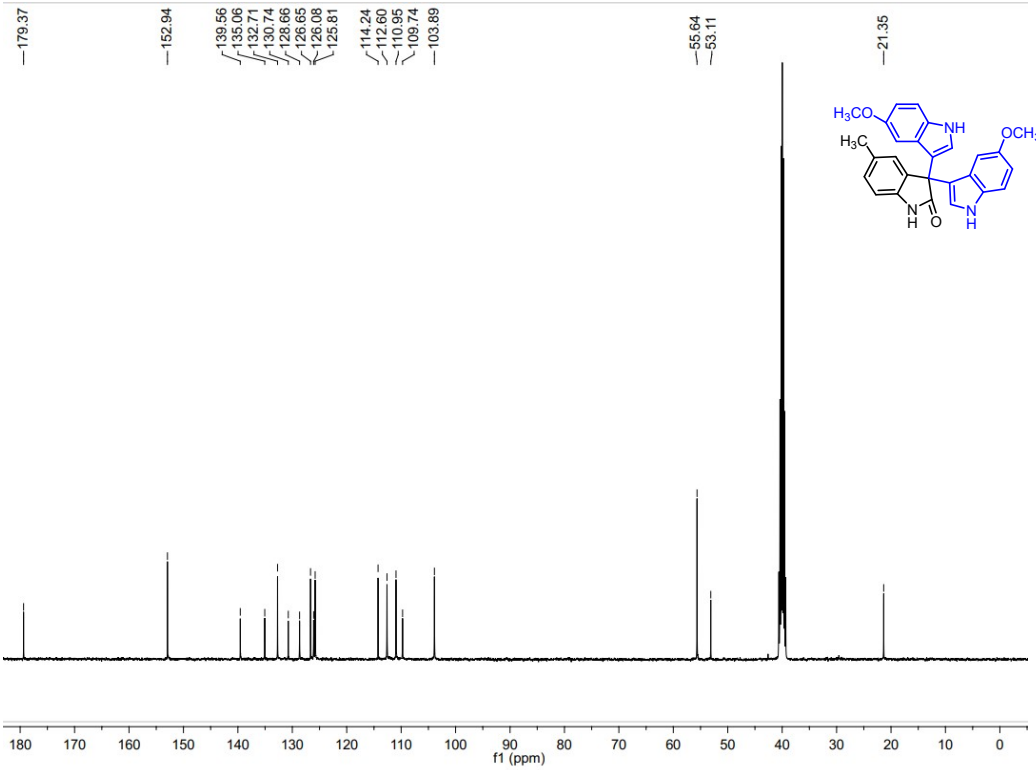
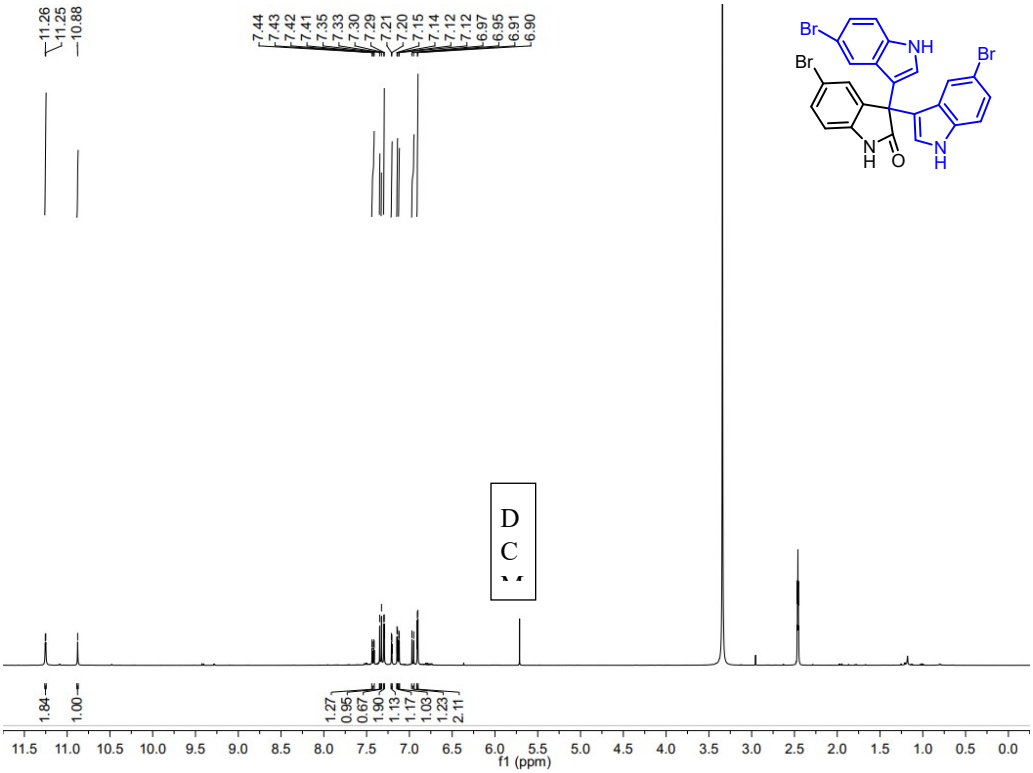
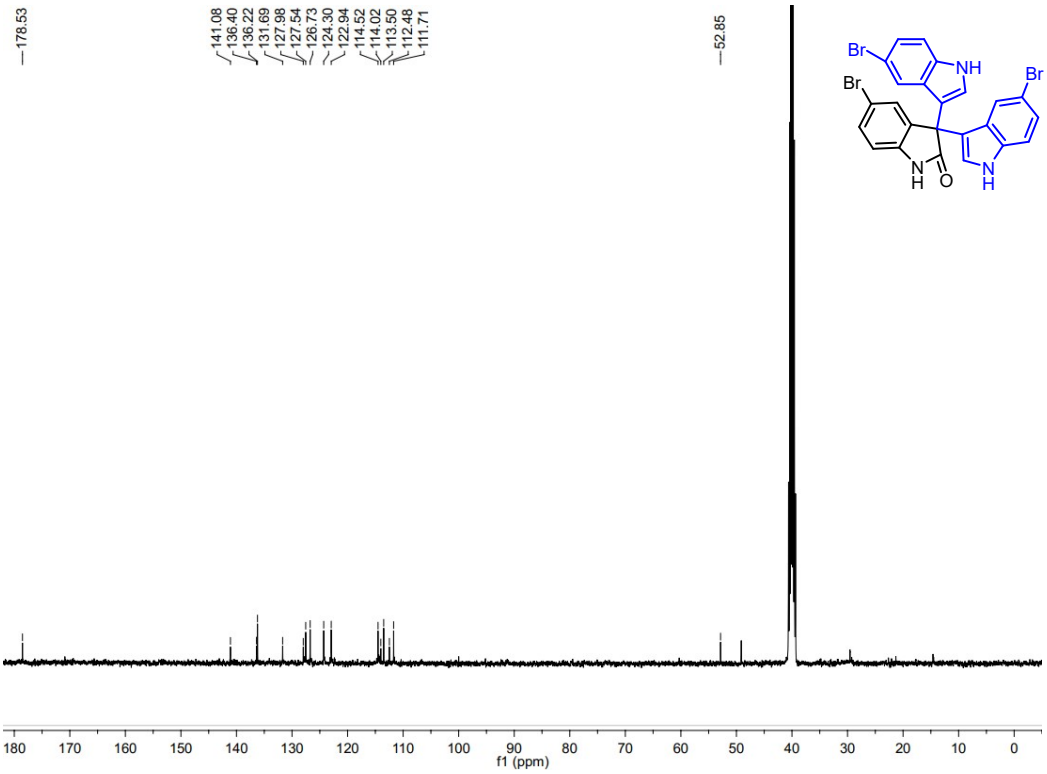


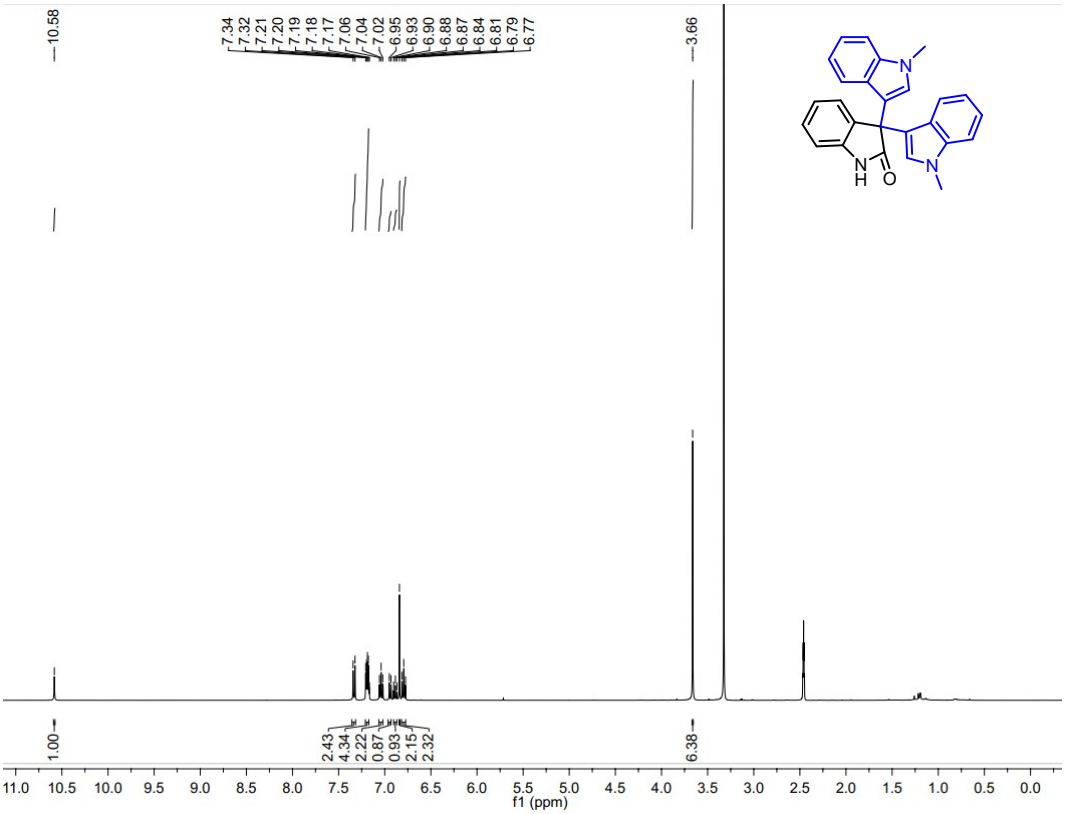


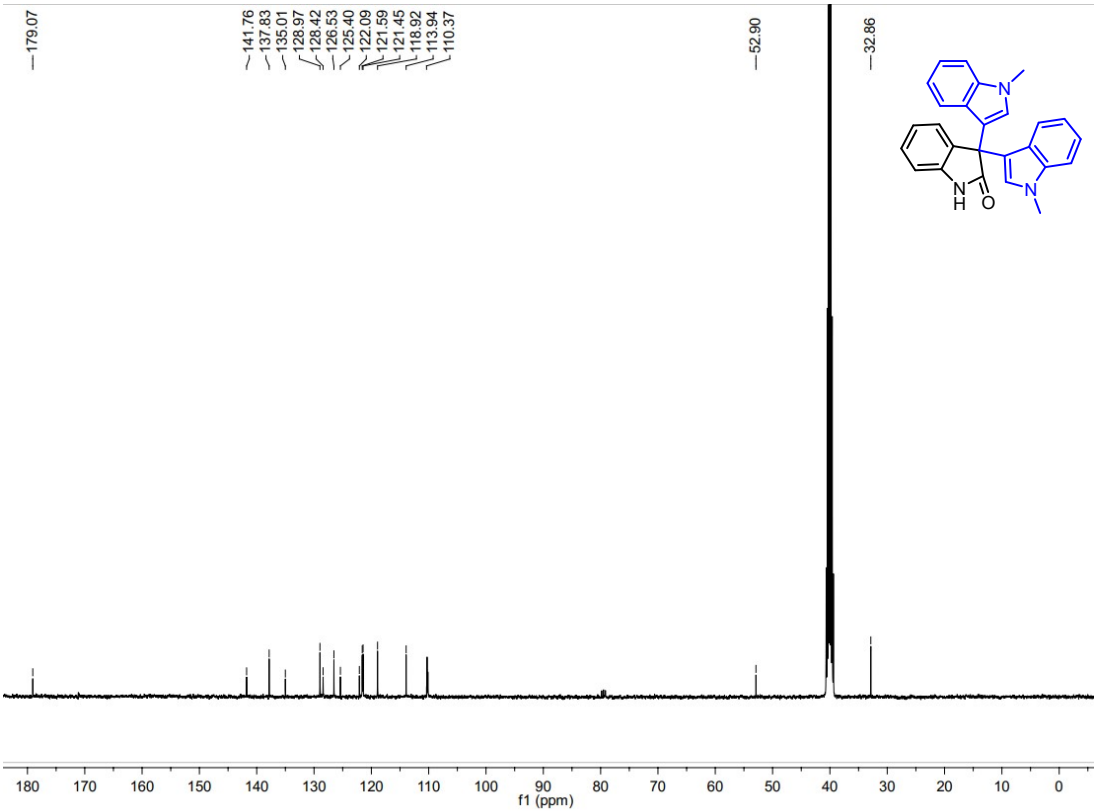
^{1}H and ^{13}C-NMR spectra of 3l



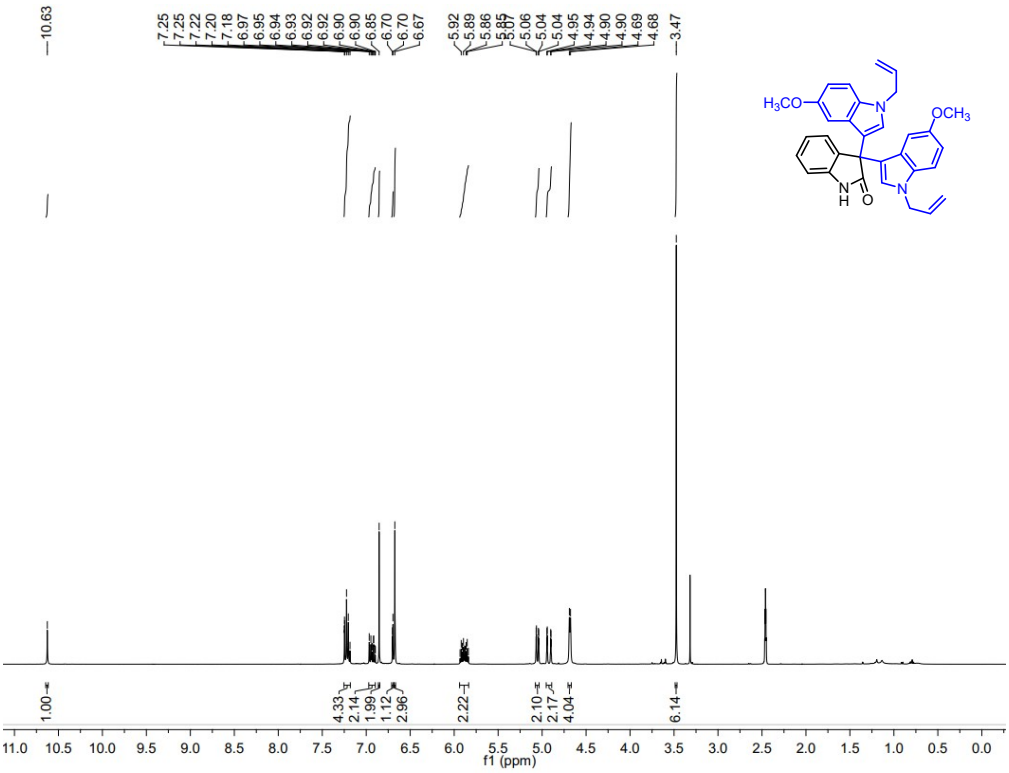


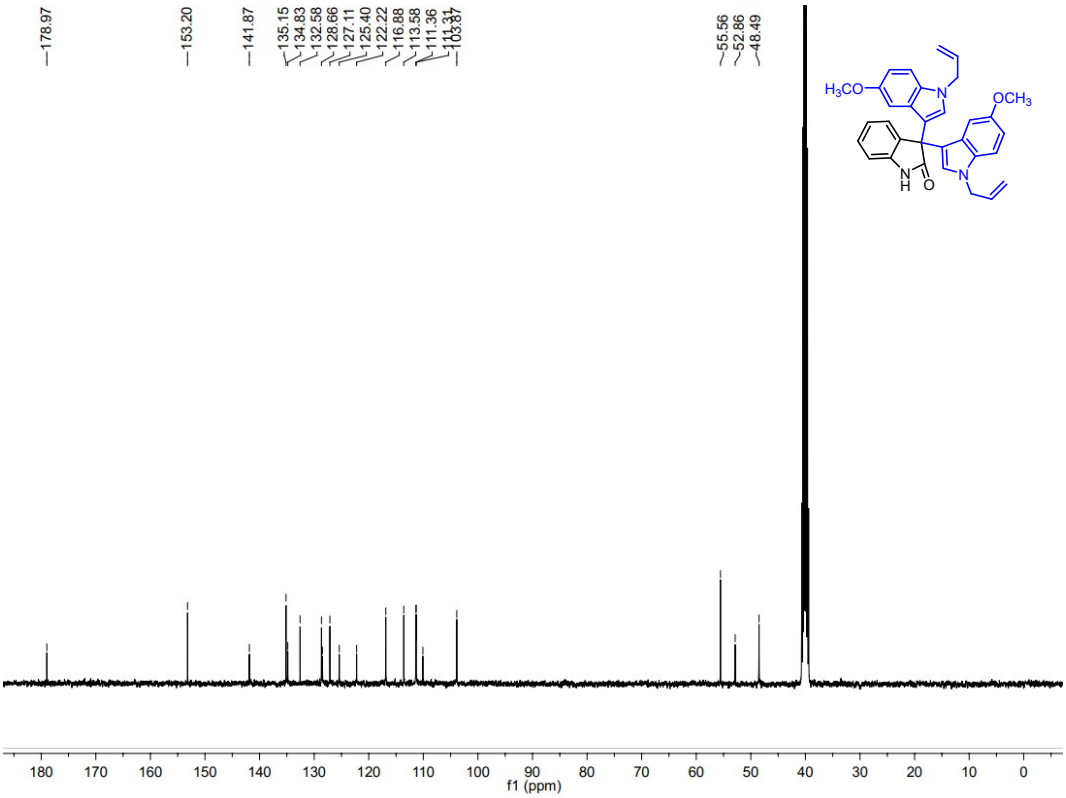
^{1}H and ^{13}C-NMR spectra of 3n



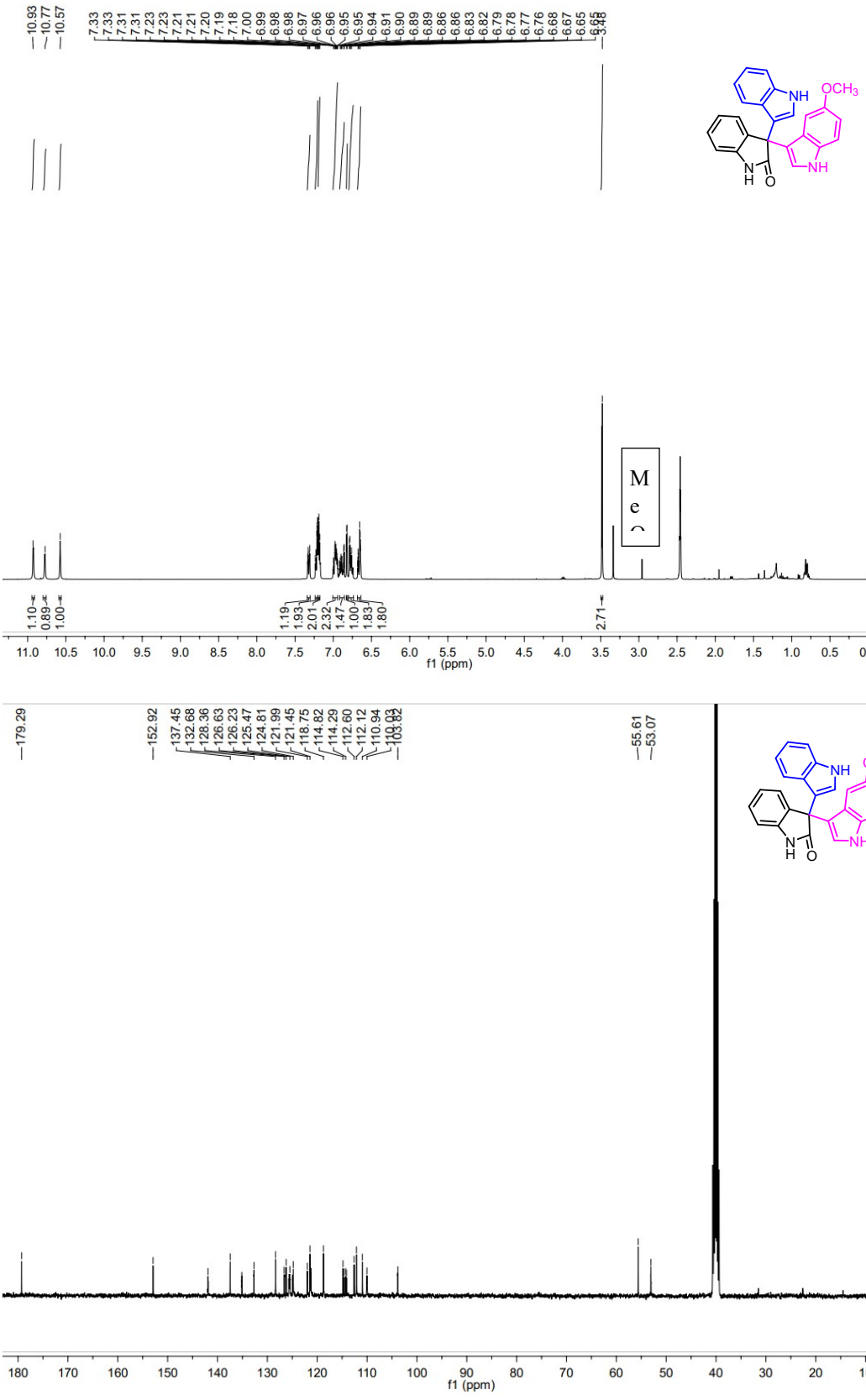


^{1}H and ^{13}C-NMR spectra of 3o





^{1}H and ^{13}C-NMR spectra of 4a



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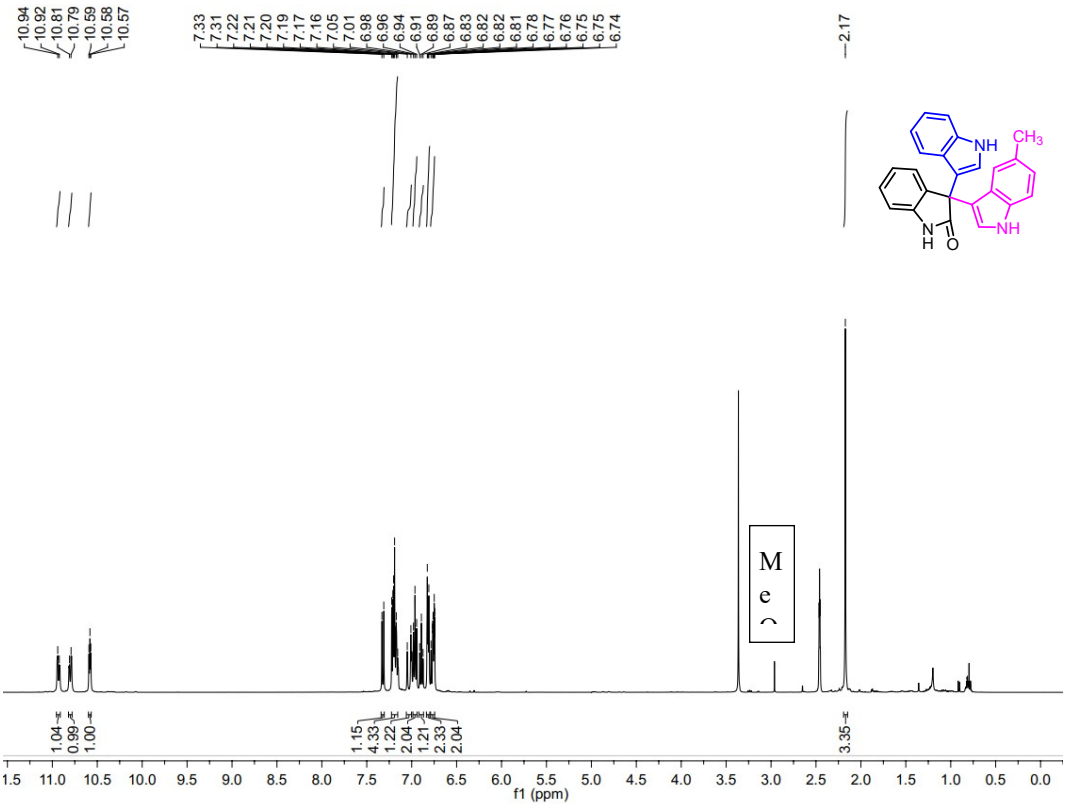
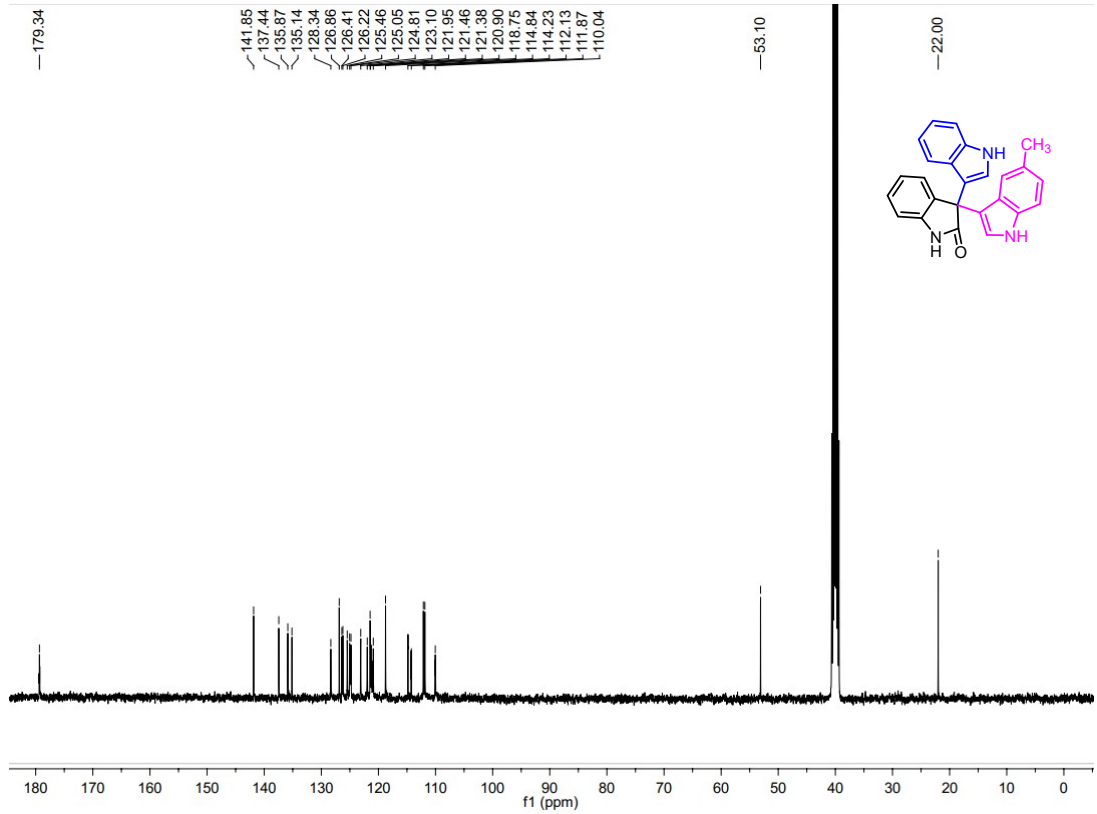
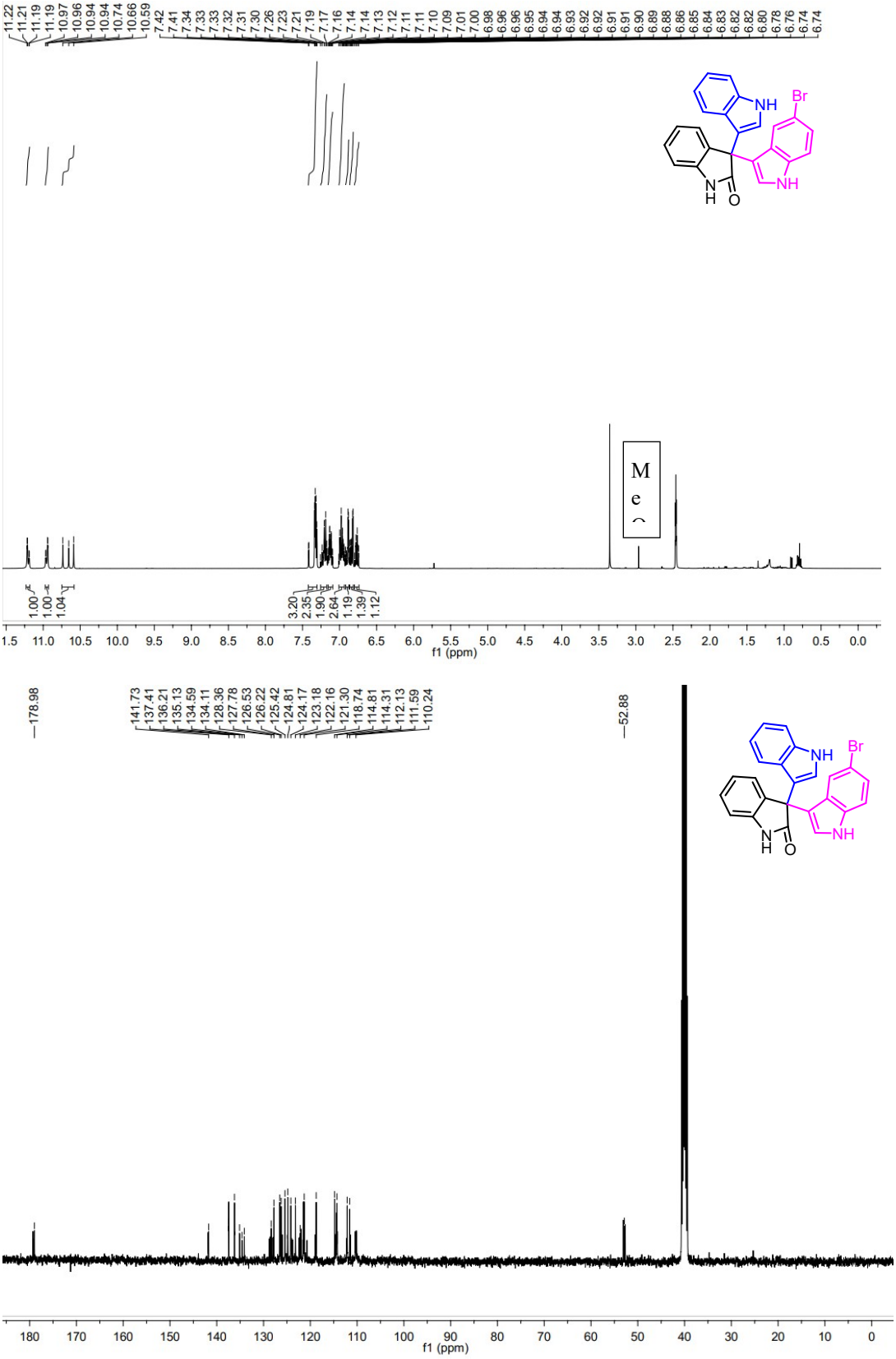




^{1}H and ^{13}C-NMR spectra of 4c



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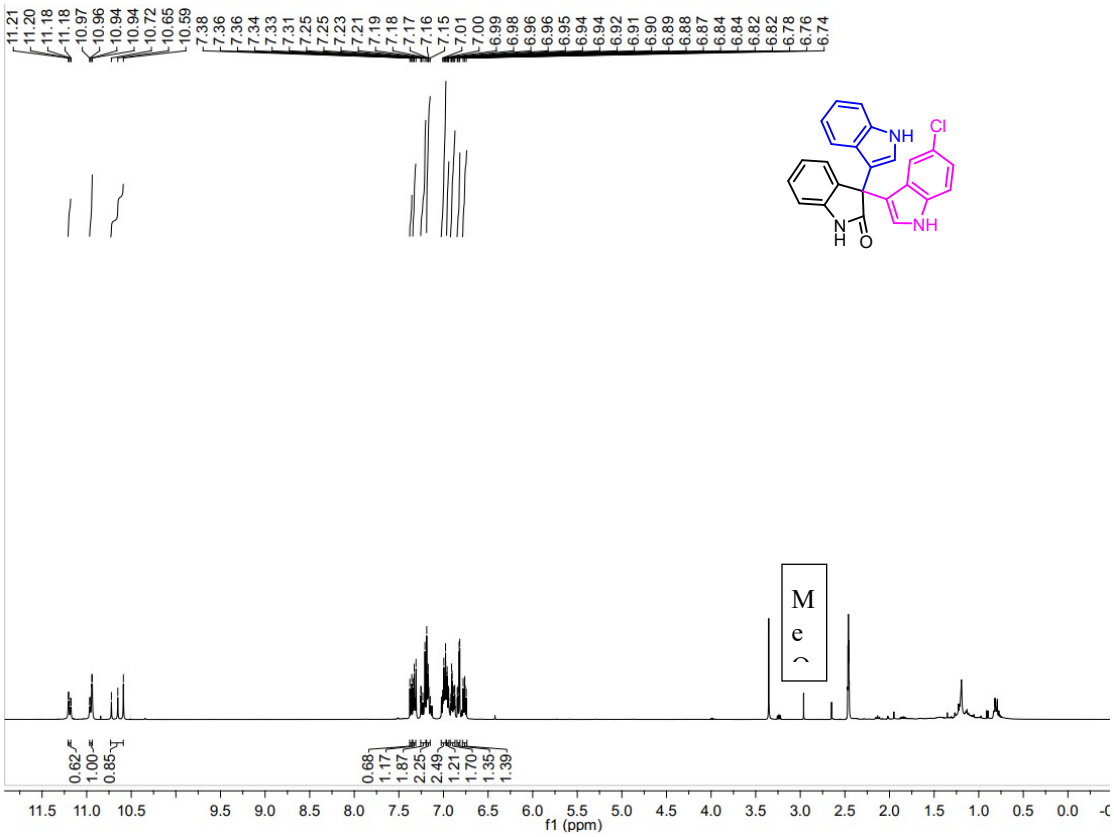
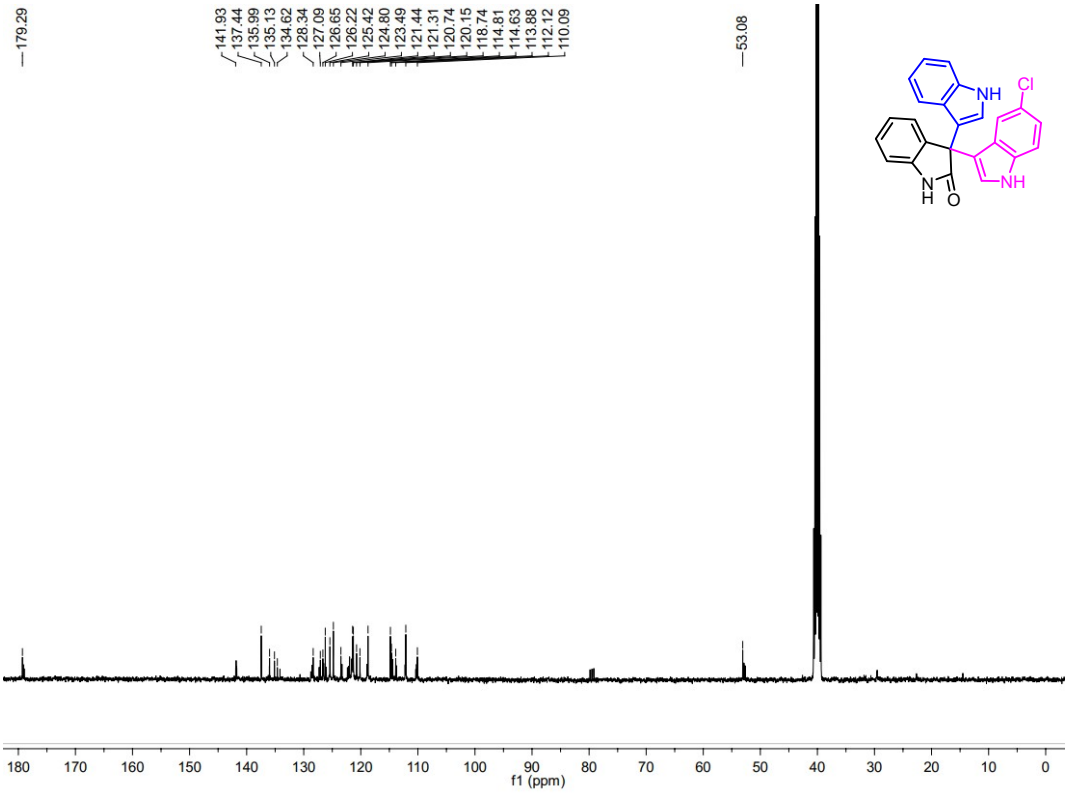
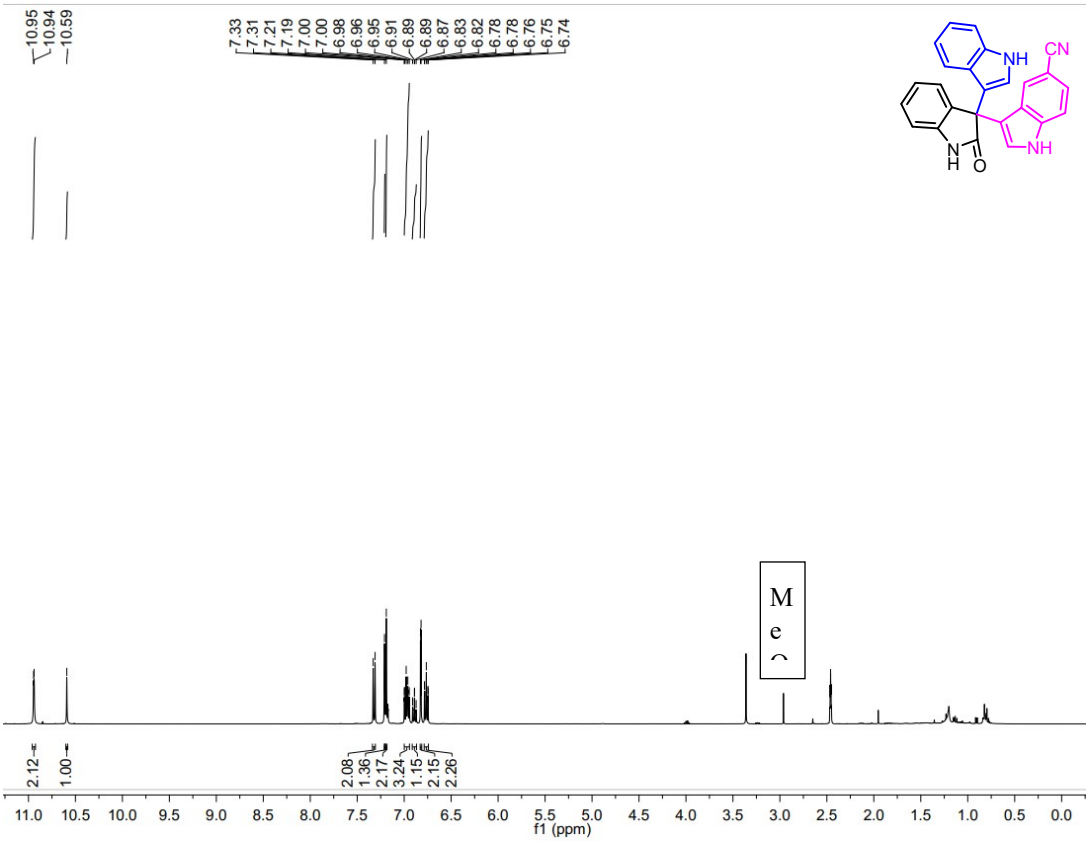
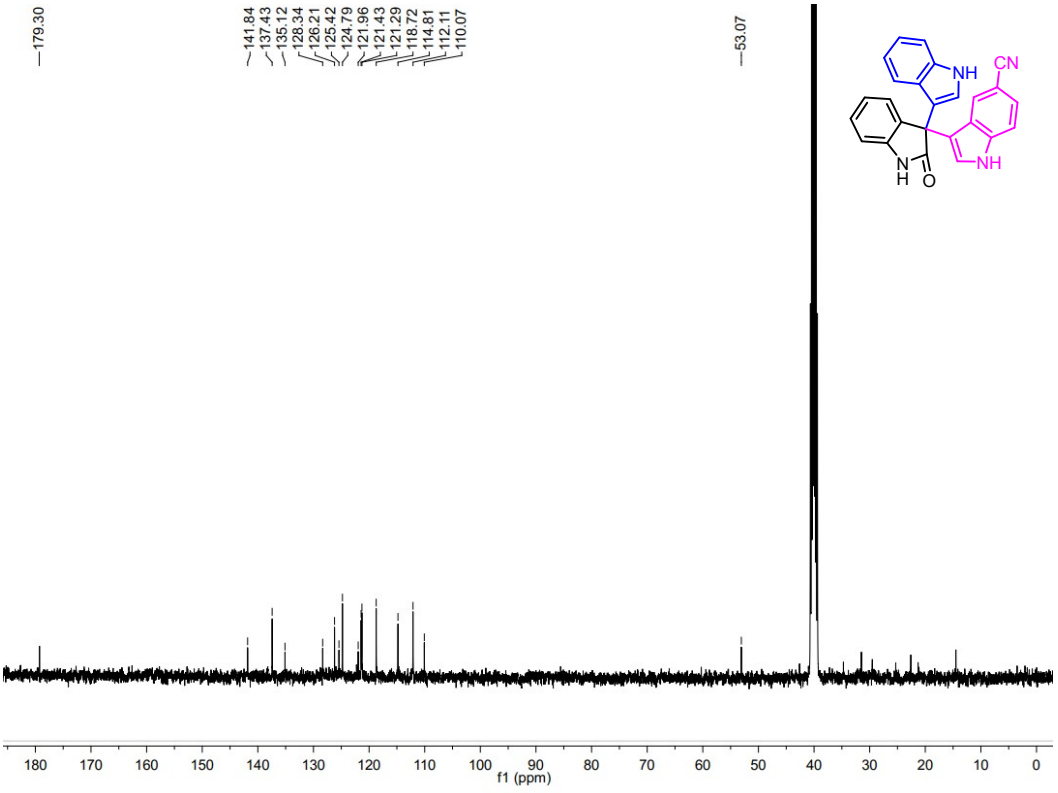




^{1}H and ^{13}C-NMR spectra of 4e





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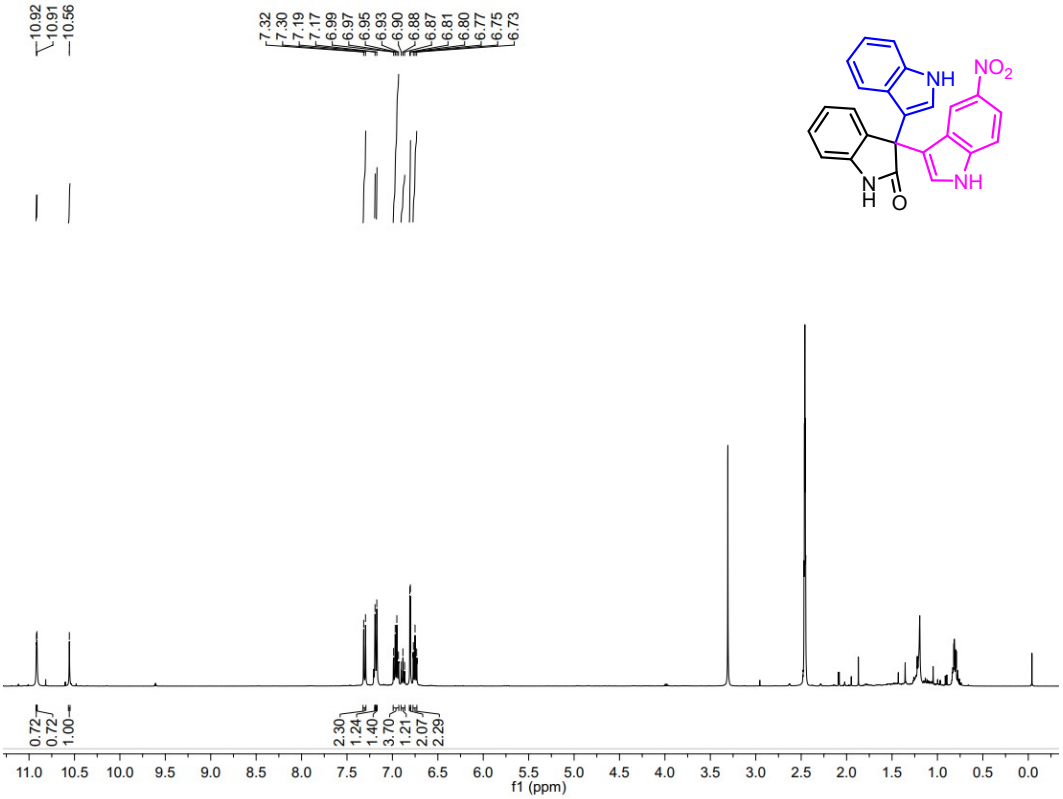

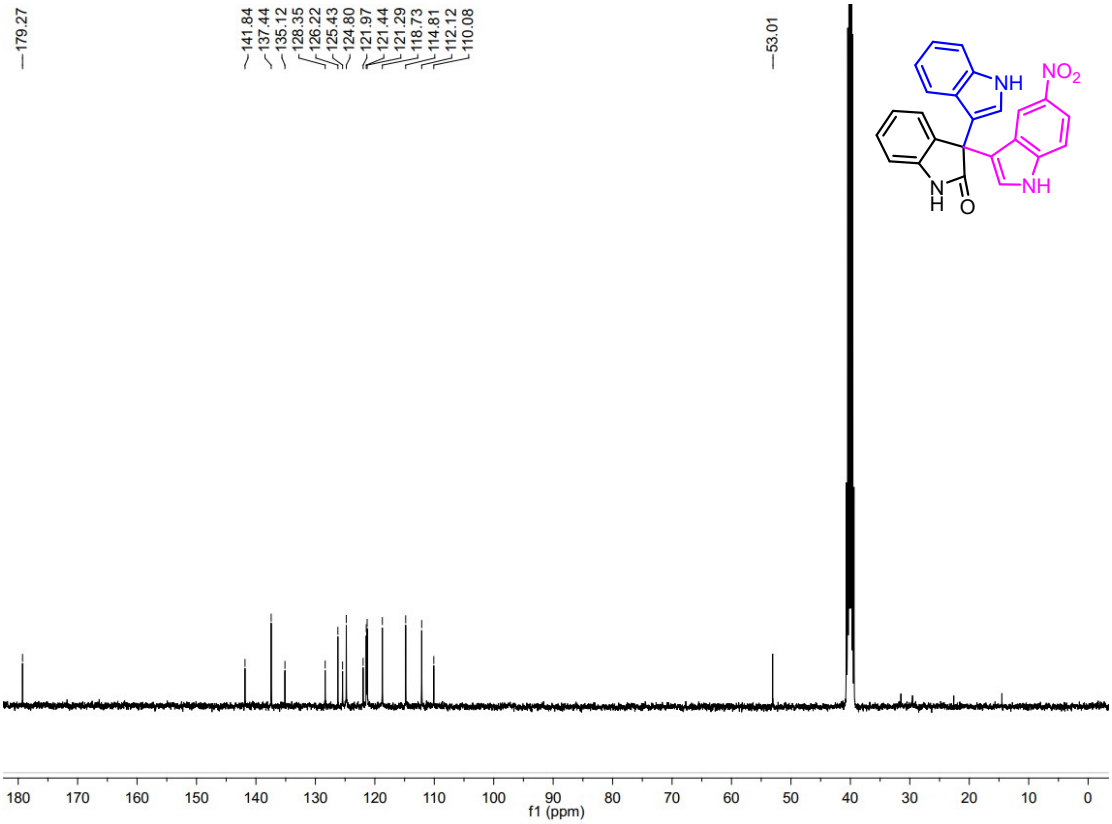

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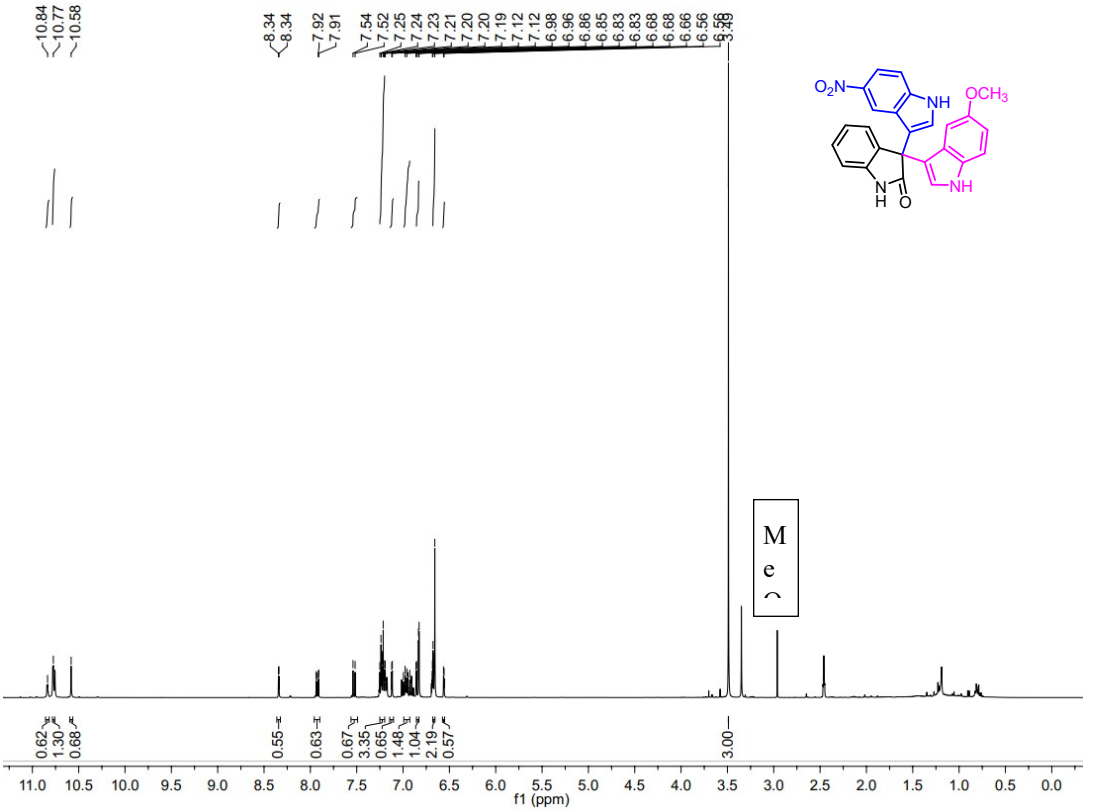
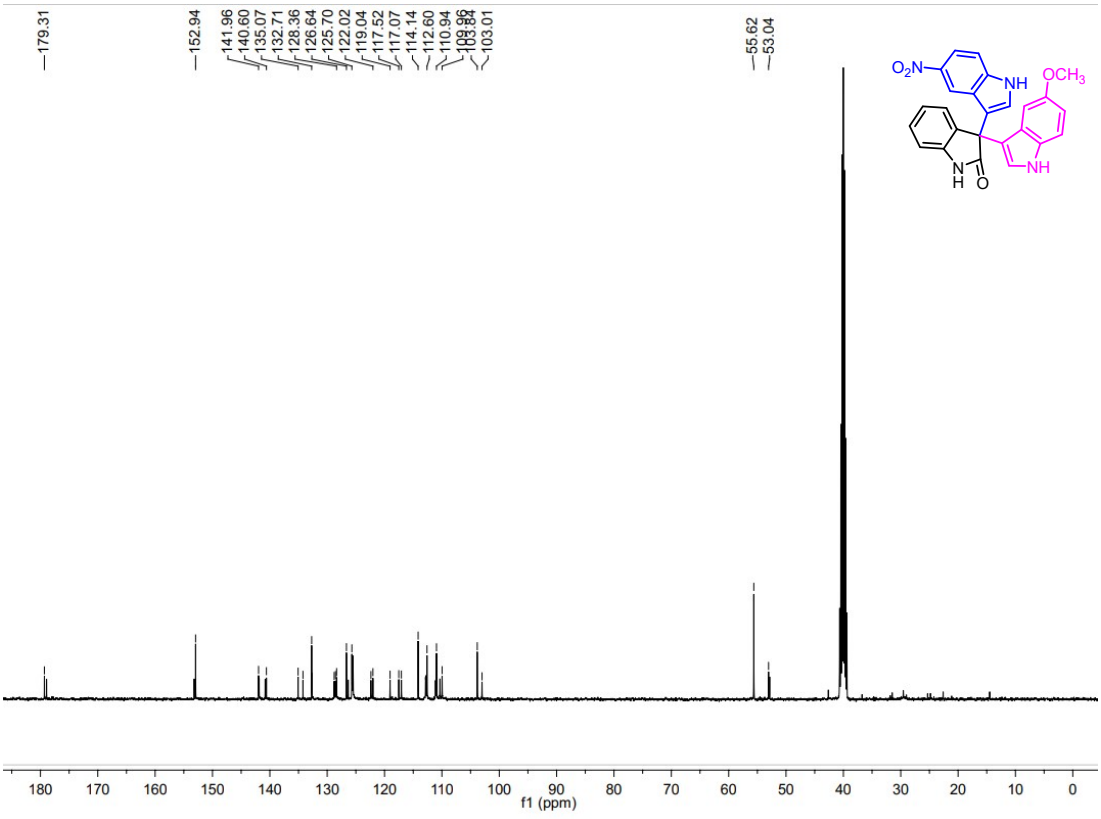
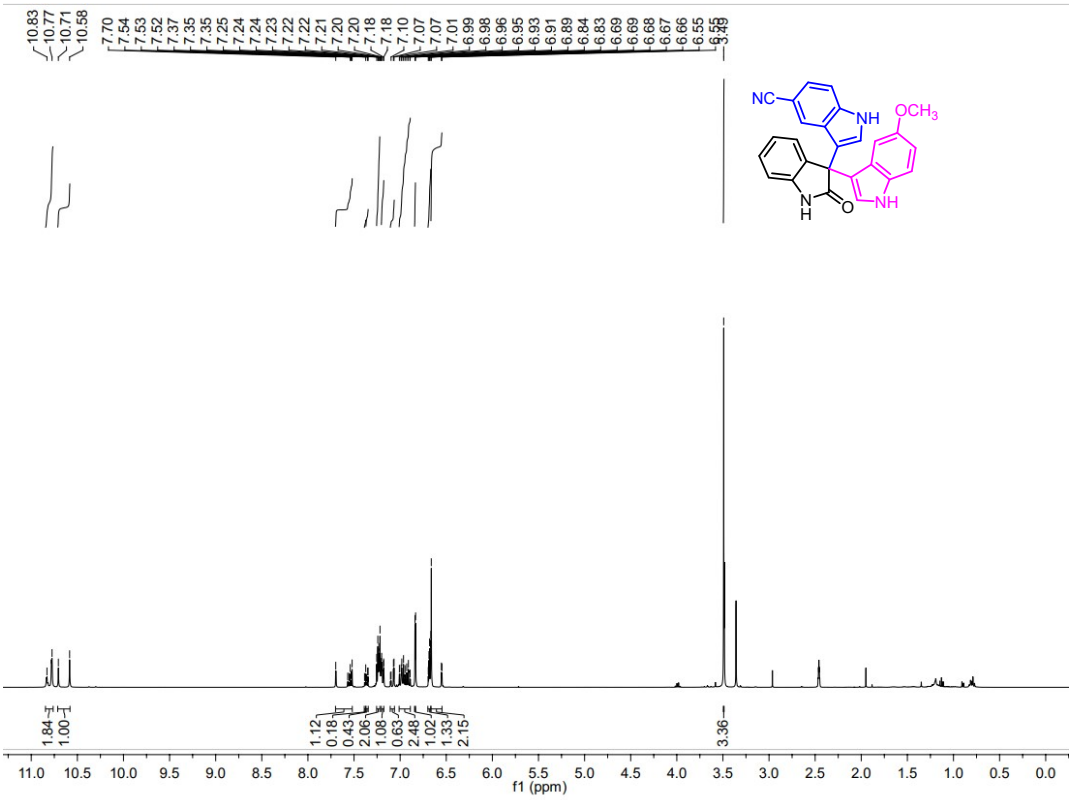
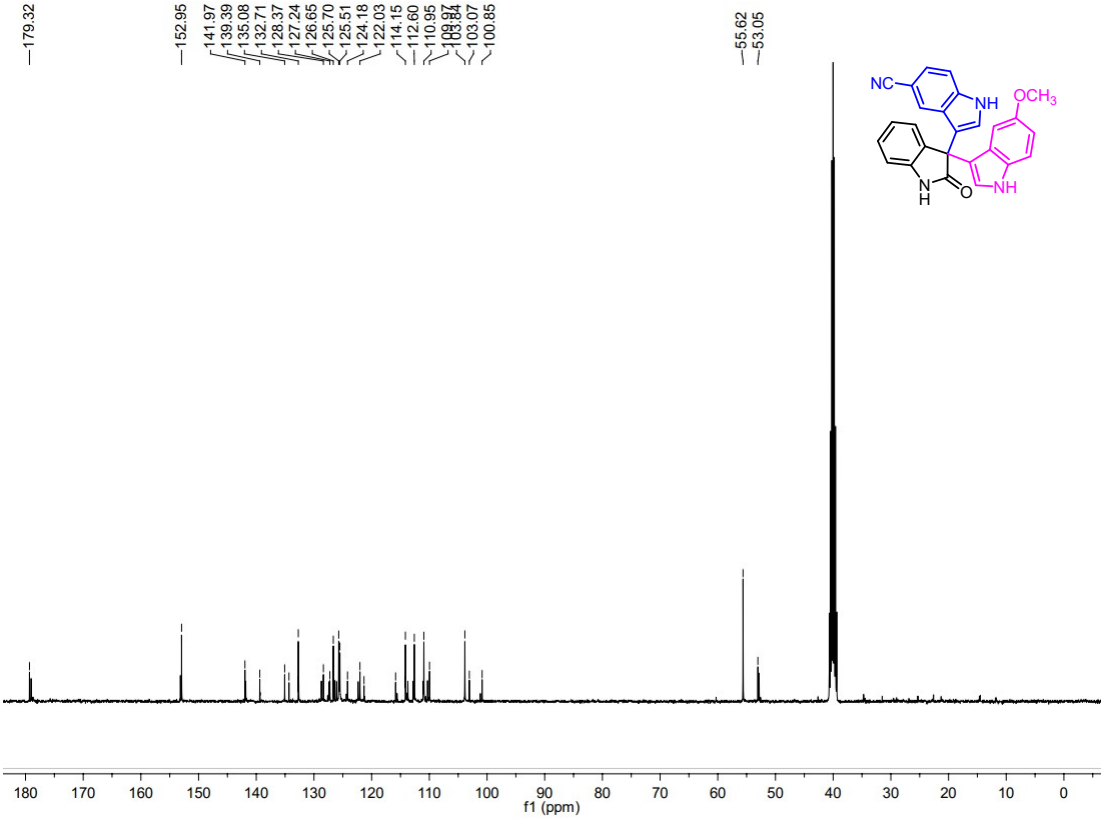




^{1}H and ^{13}C-NMR spectra of 4h





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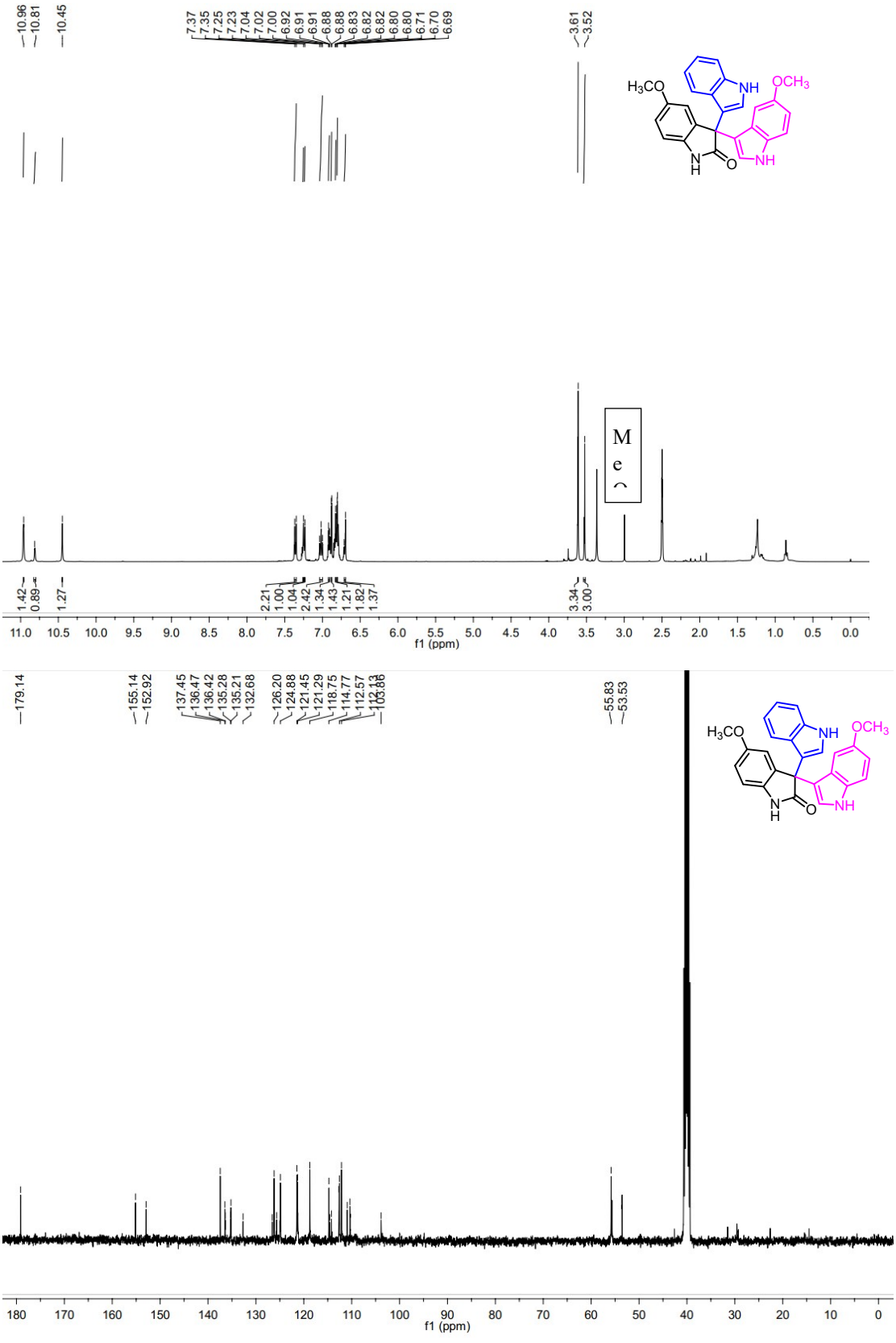

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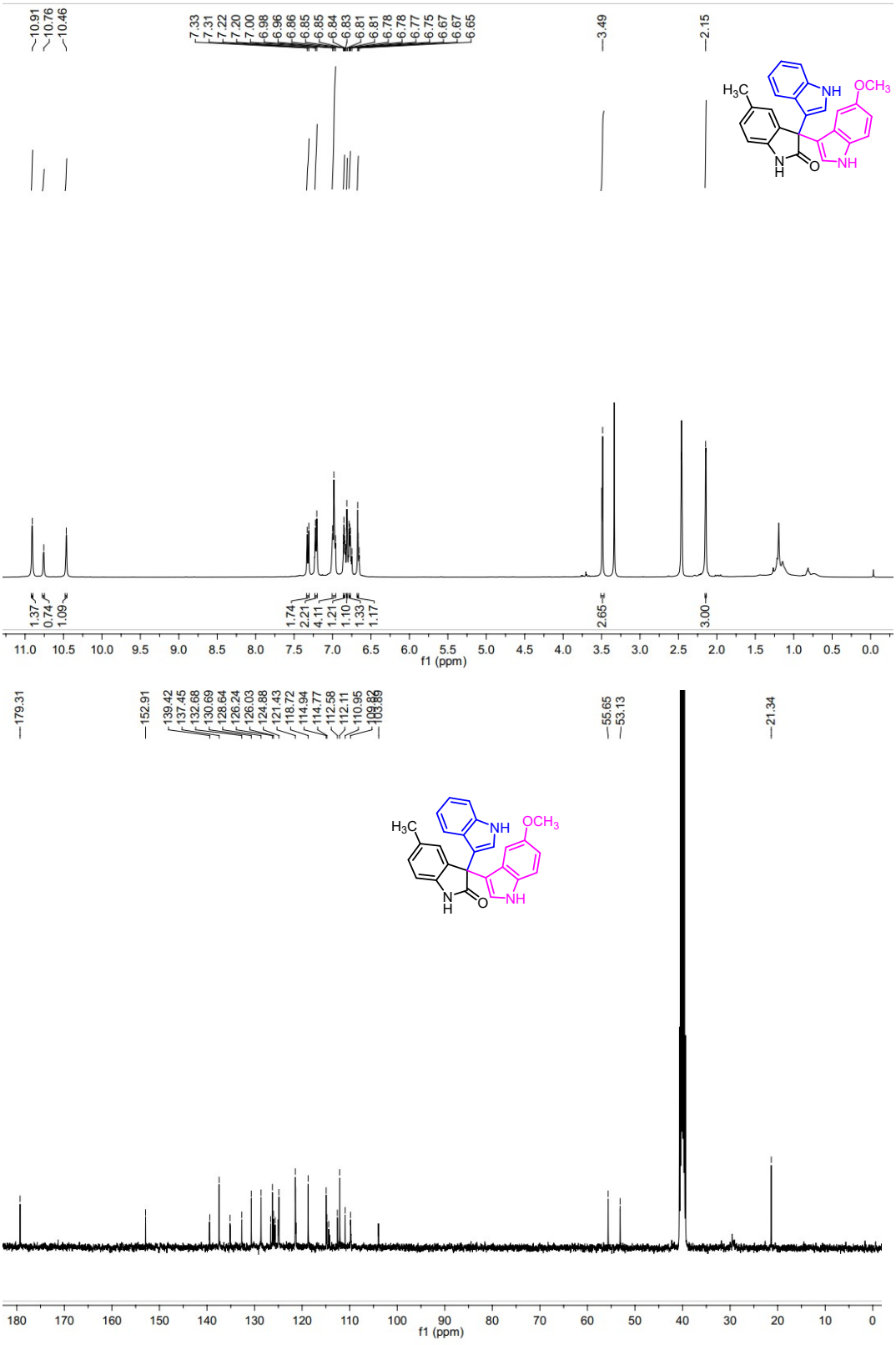

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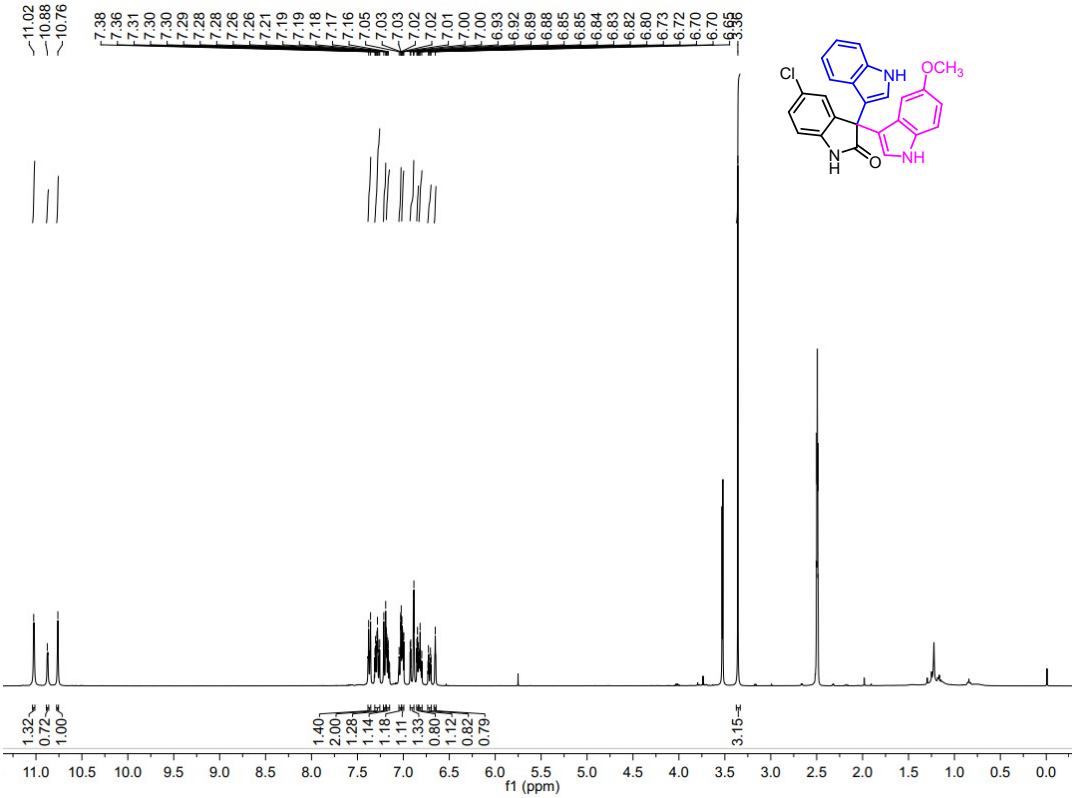
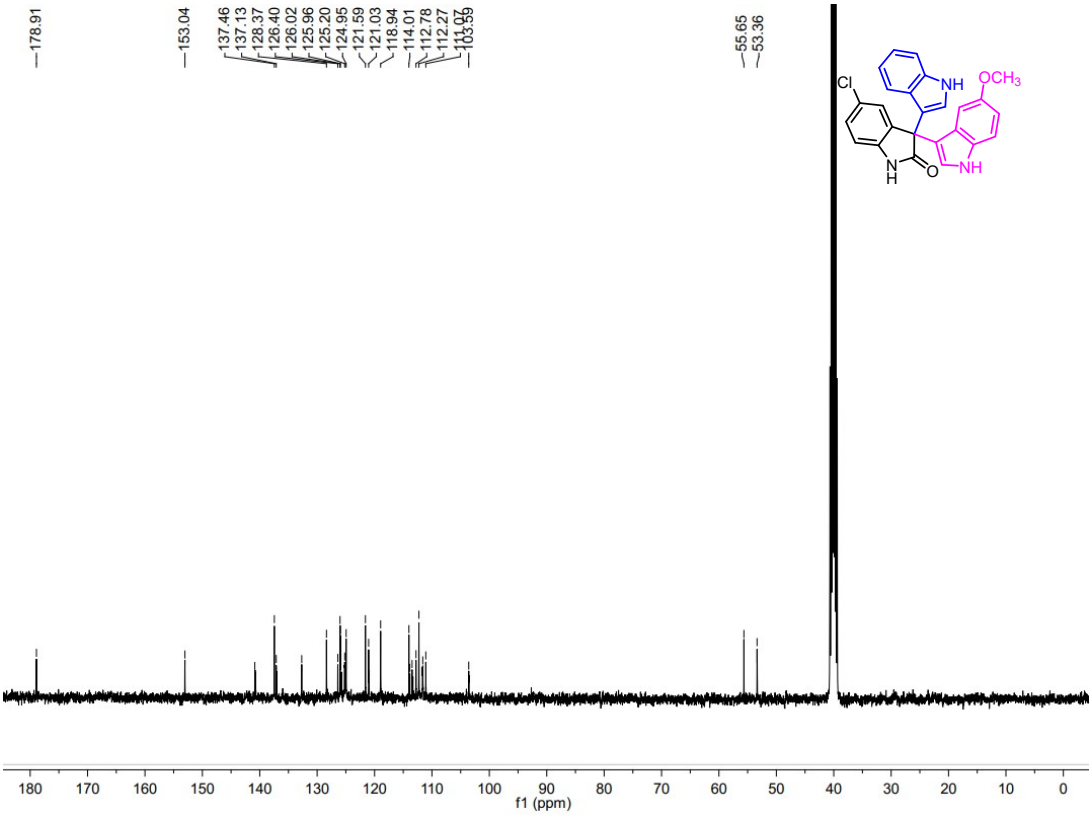
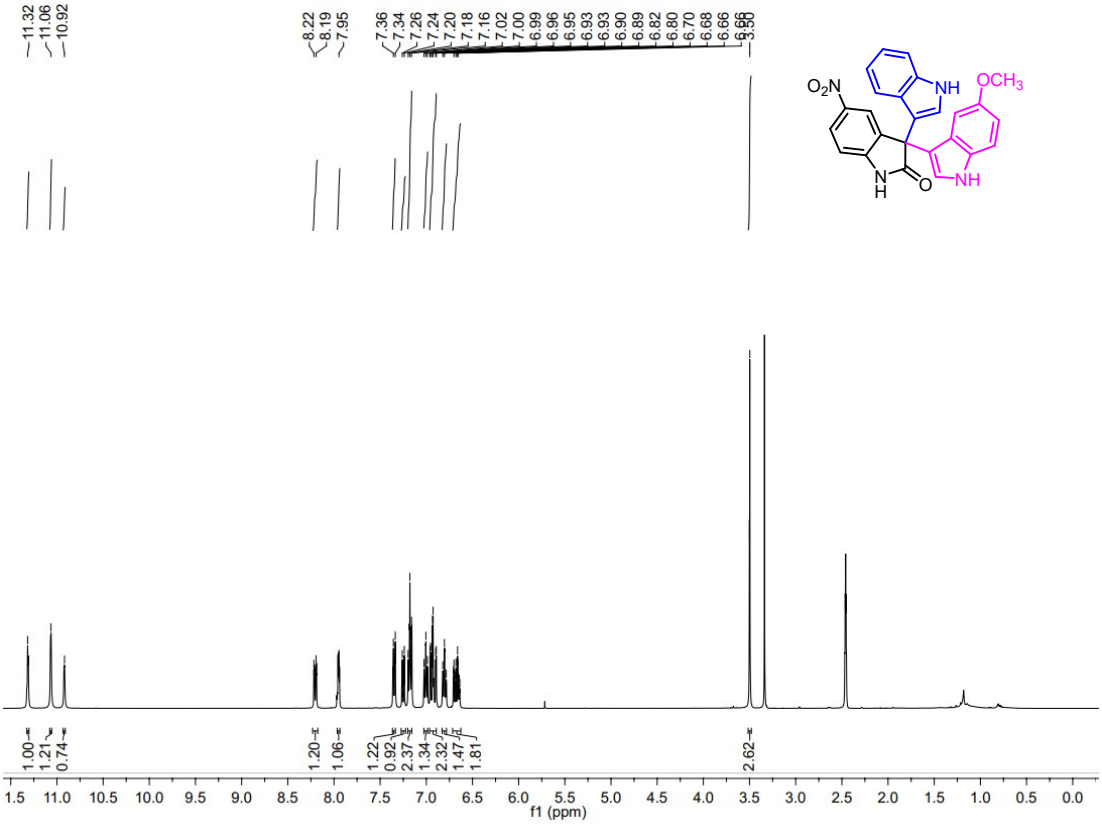
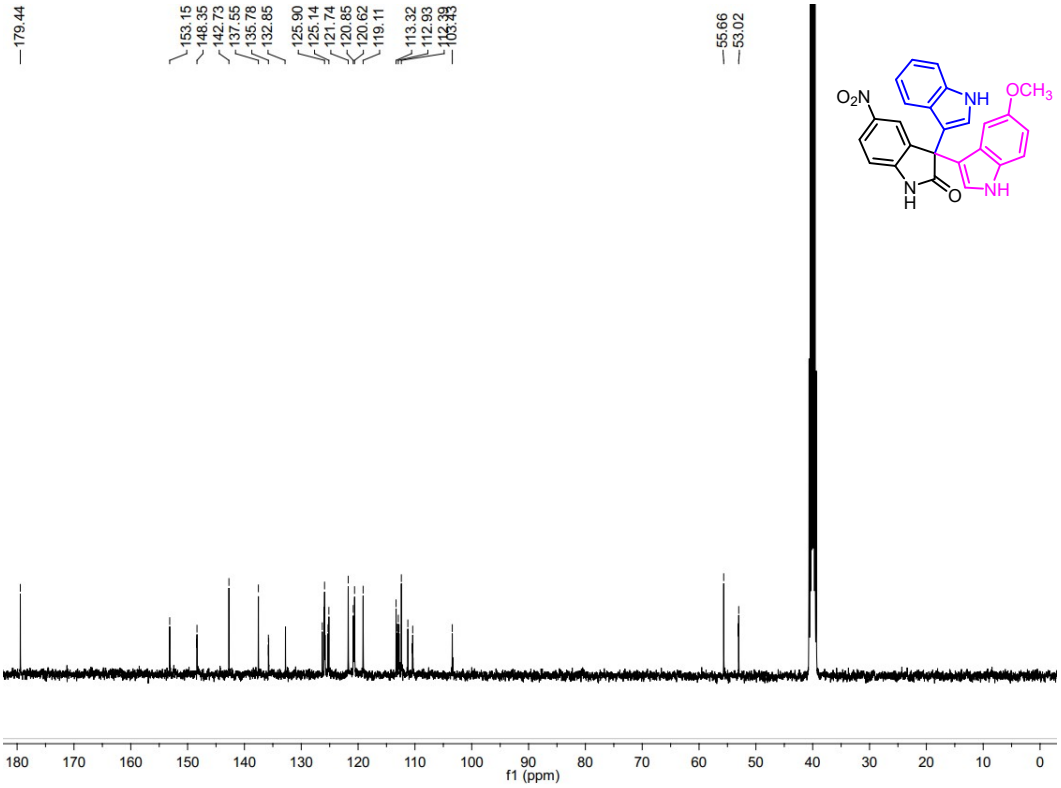


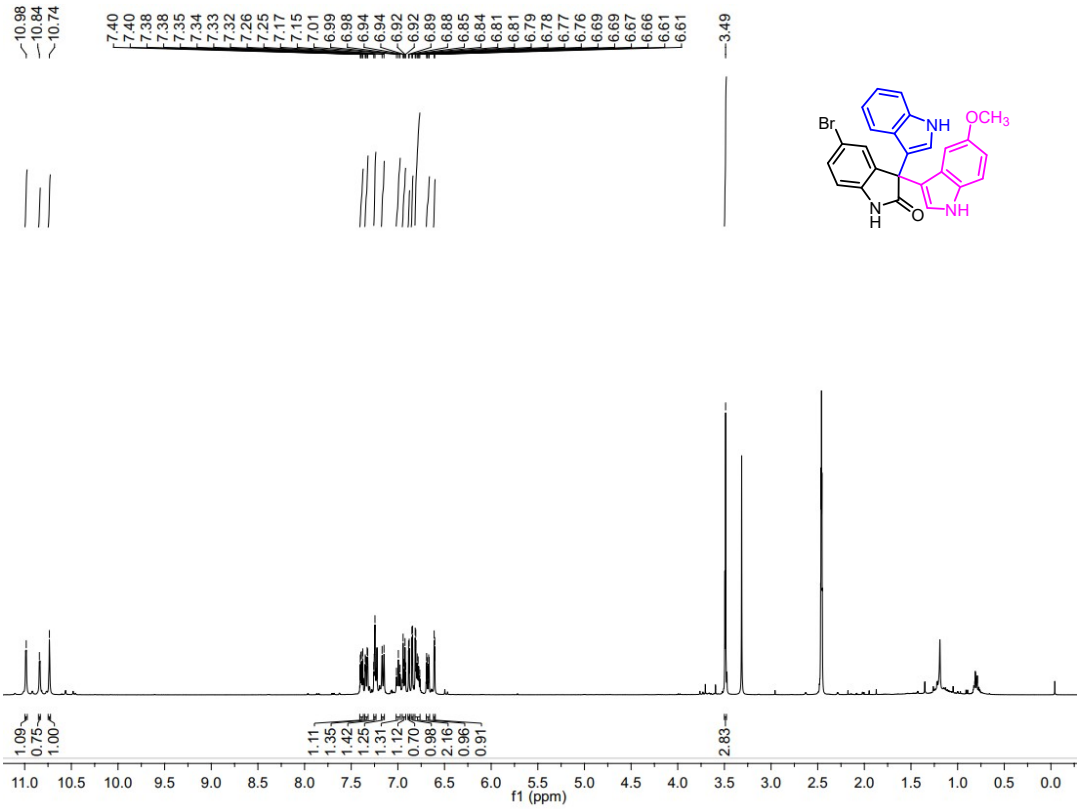


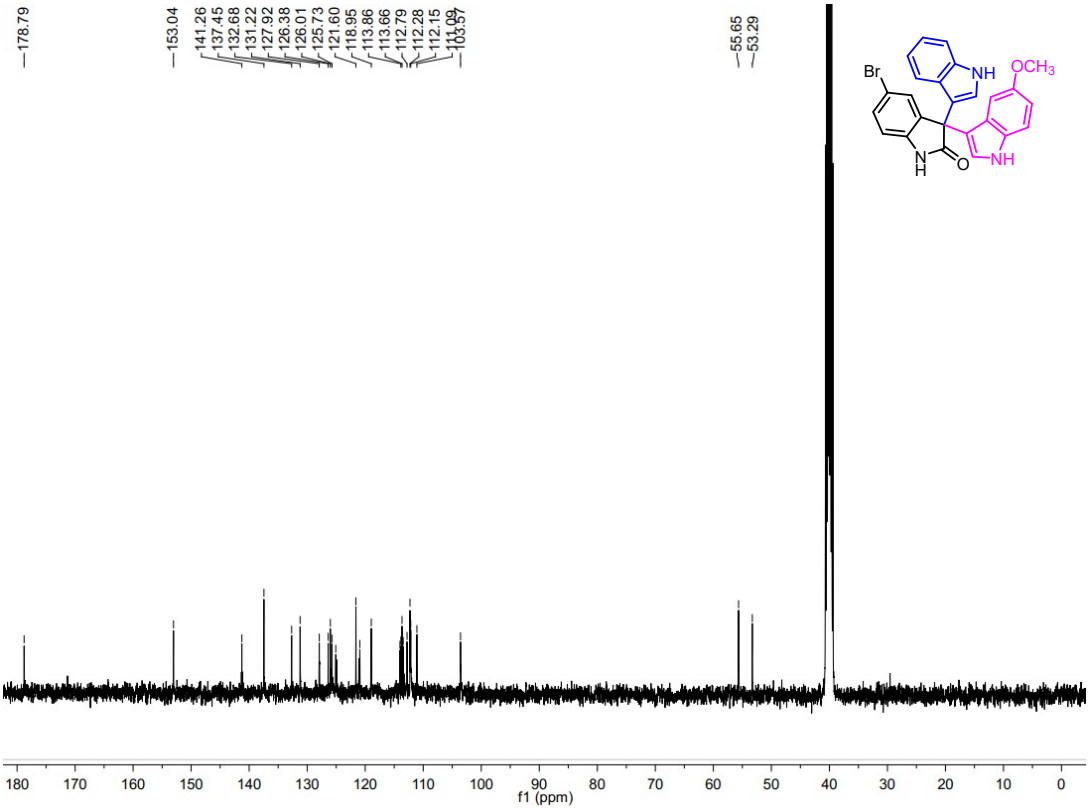
^{1}H and ^{13}C-NMR spectra of 4l



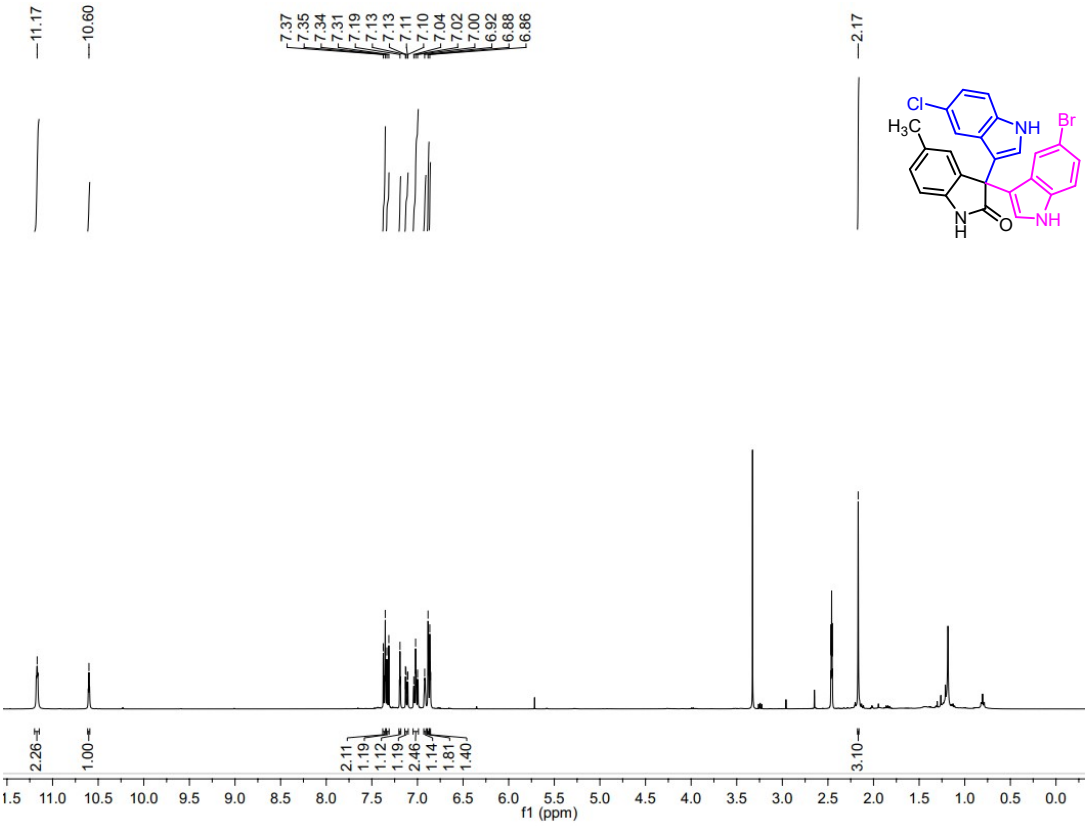


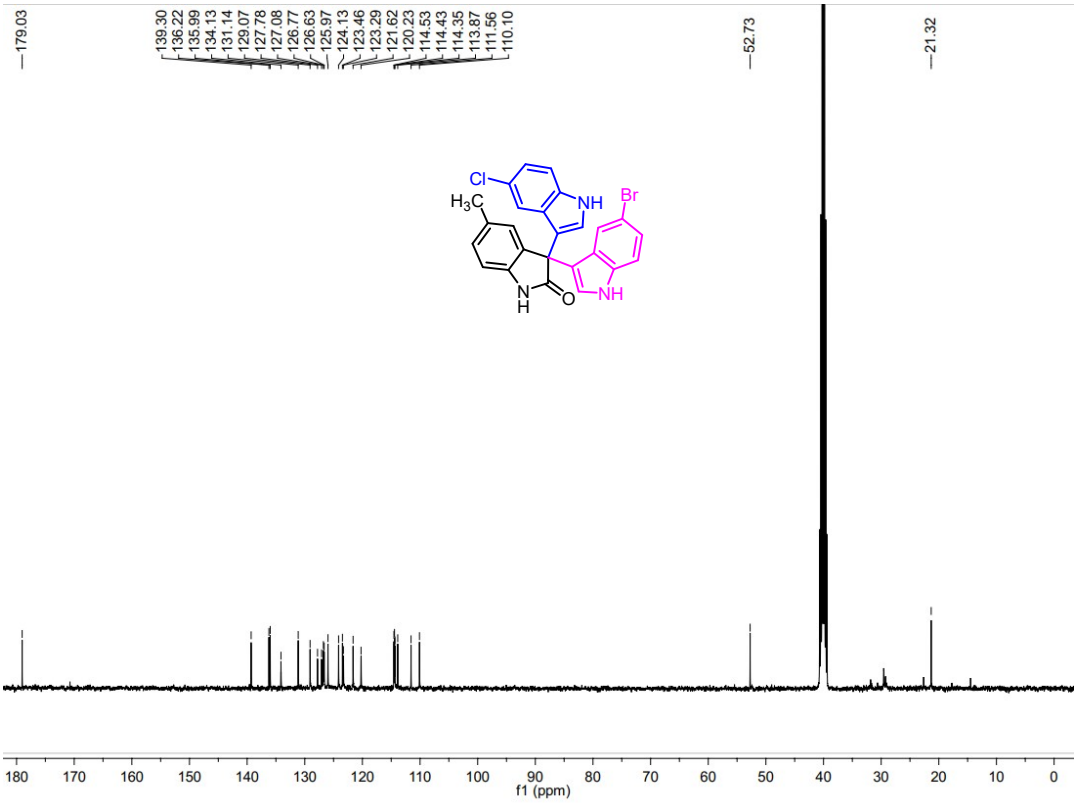
^{1}H and ^{13}C-NMR spectra of 4m



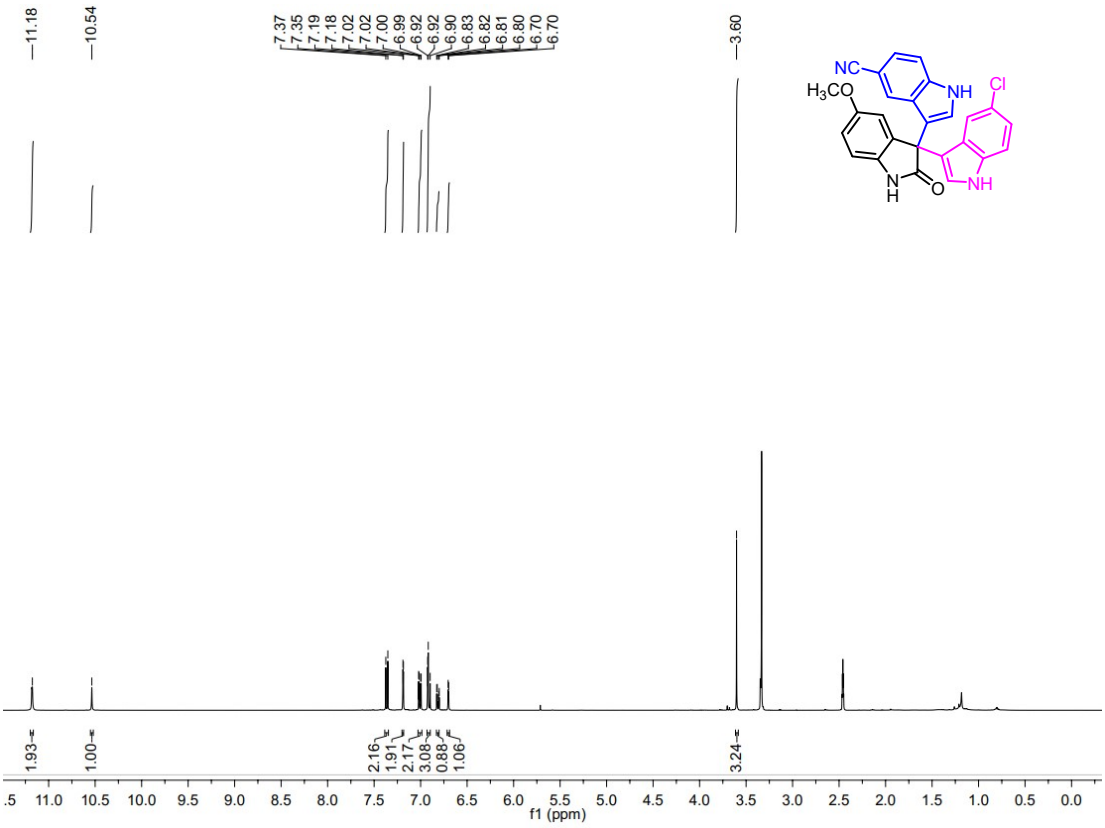


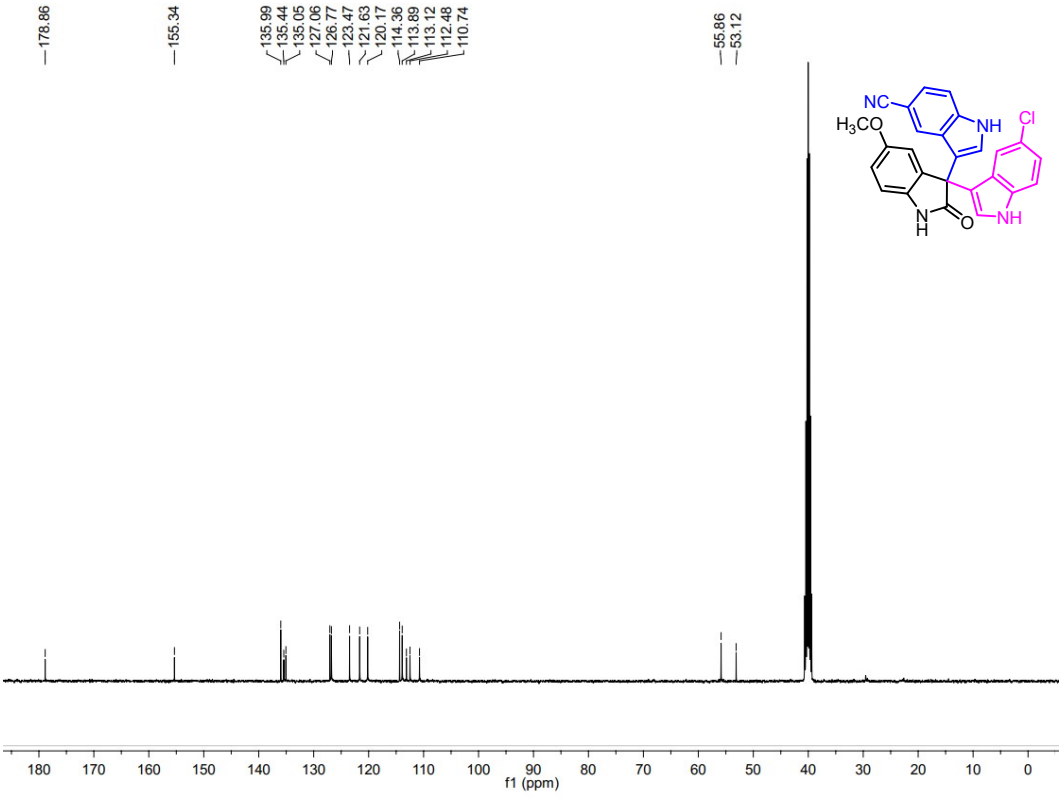
^{1}H and ^{13}C-NMR spectra of 4n



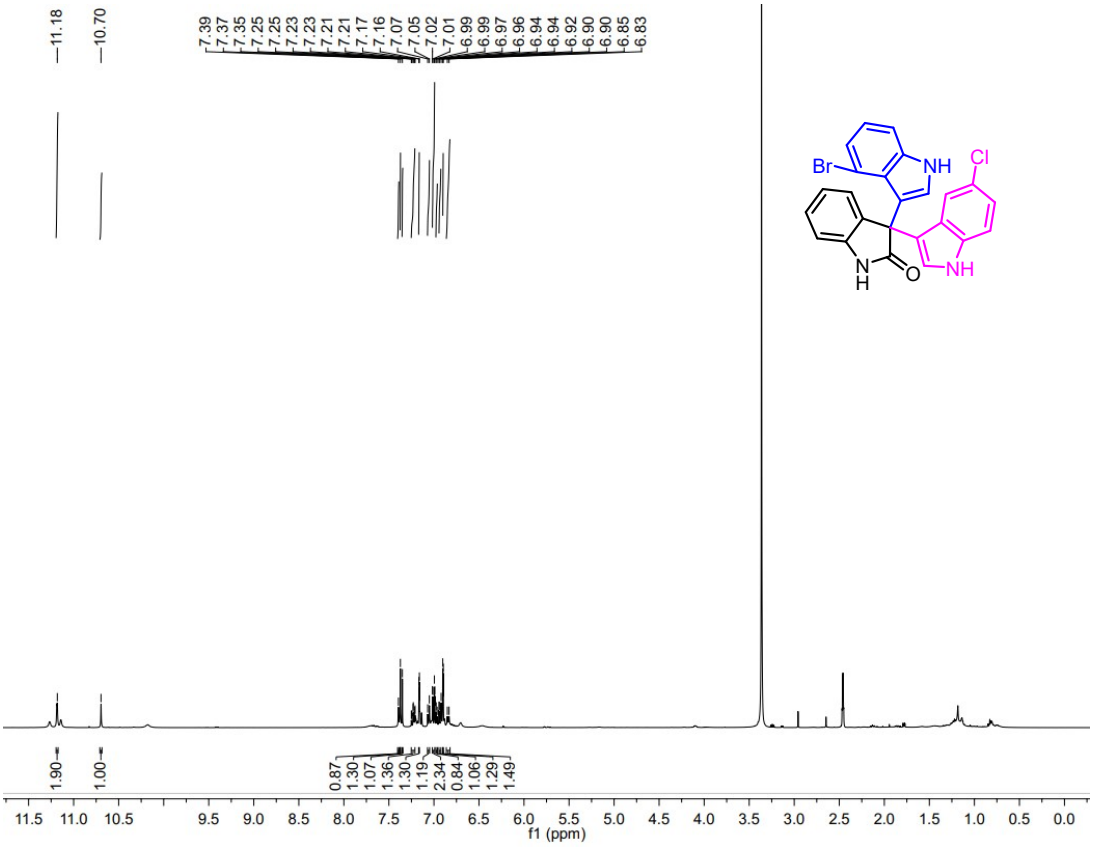


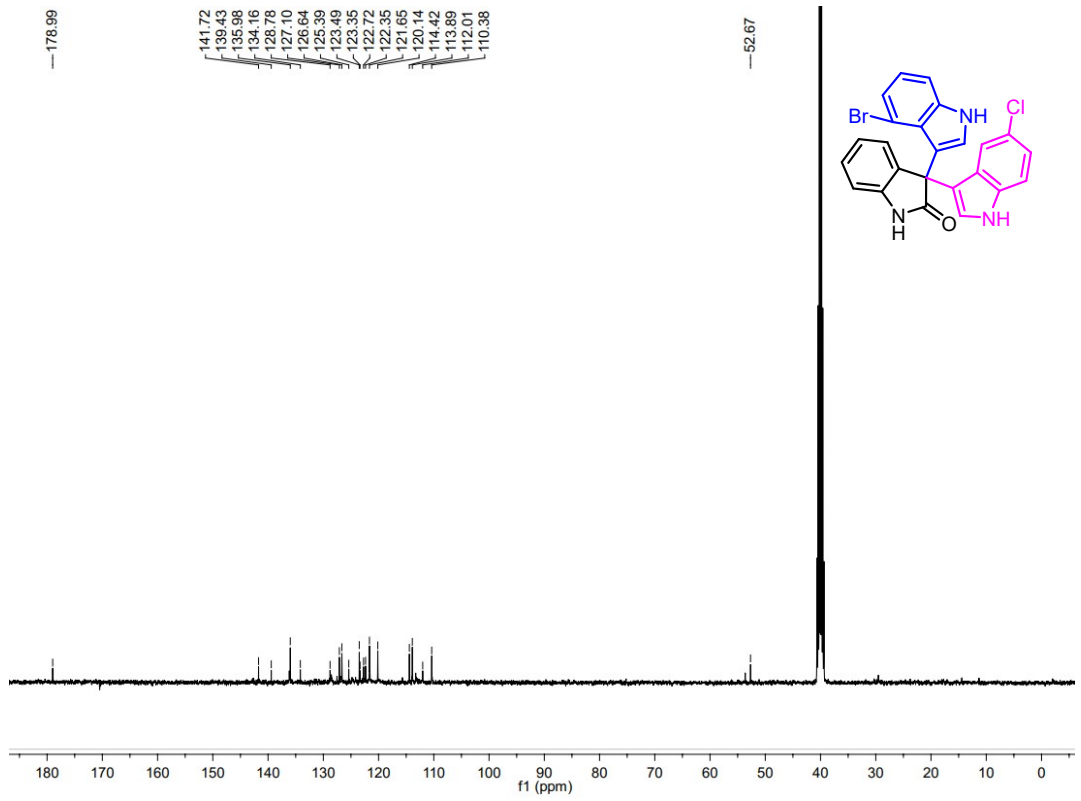
^{1}H and ^{13}C-NMR spectra of 4o



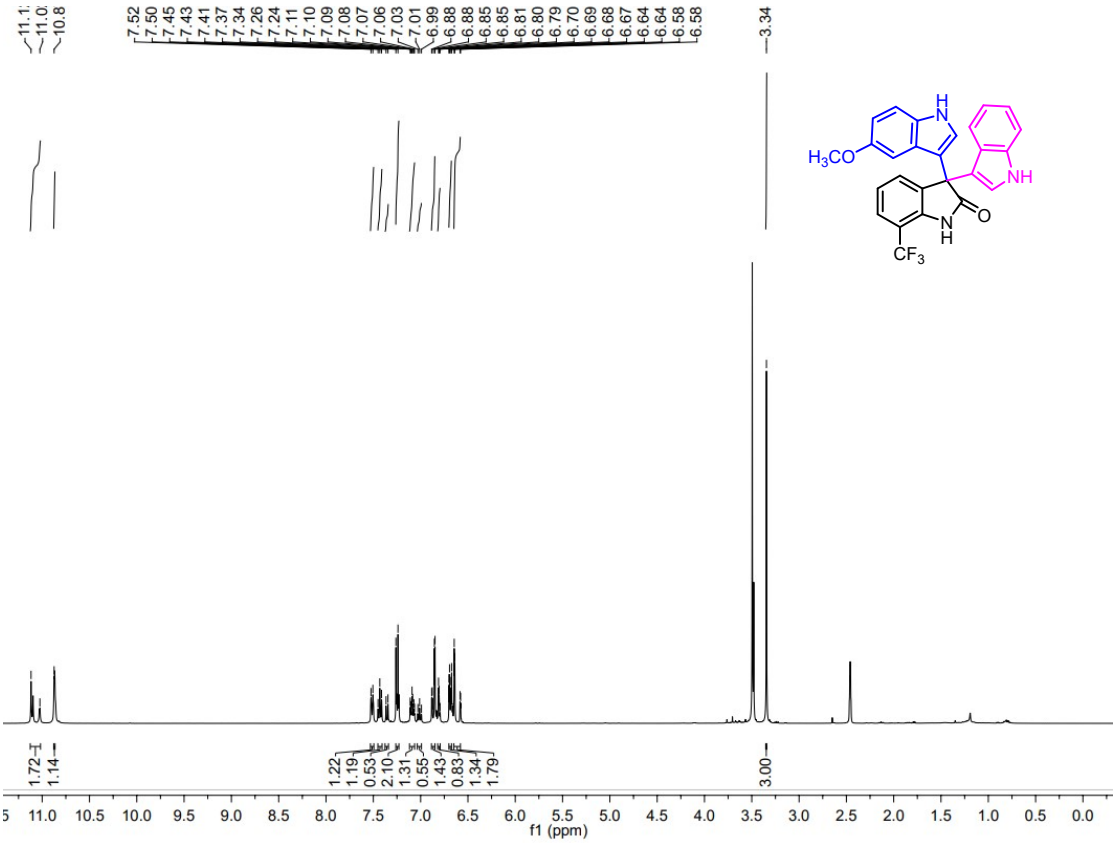


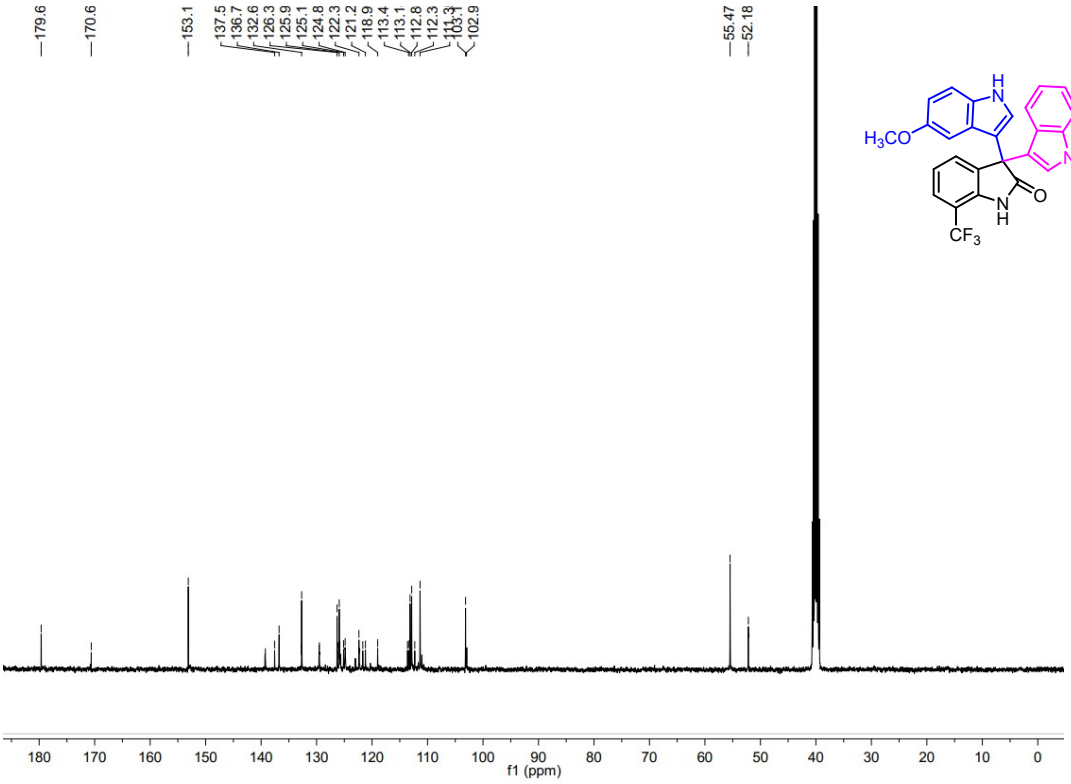
^{1}H and ^{13}C-NMR spectra of 4p



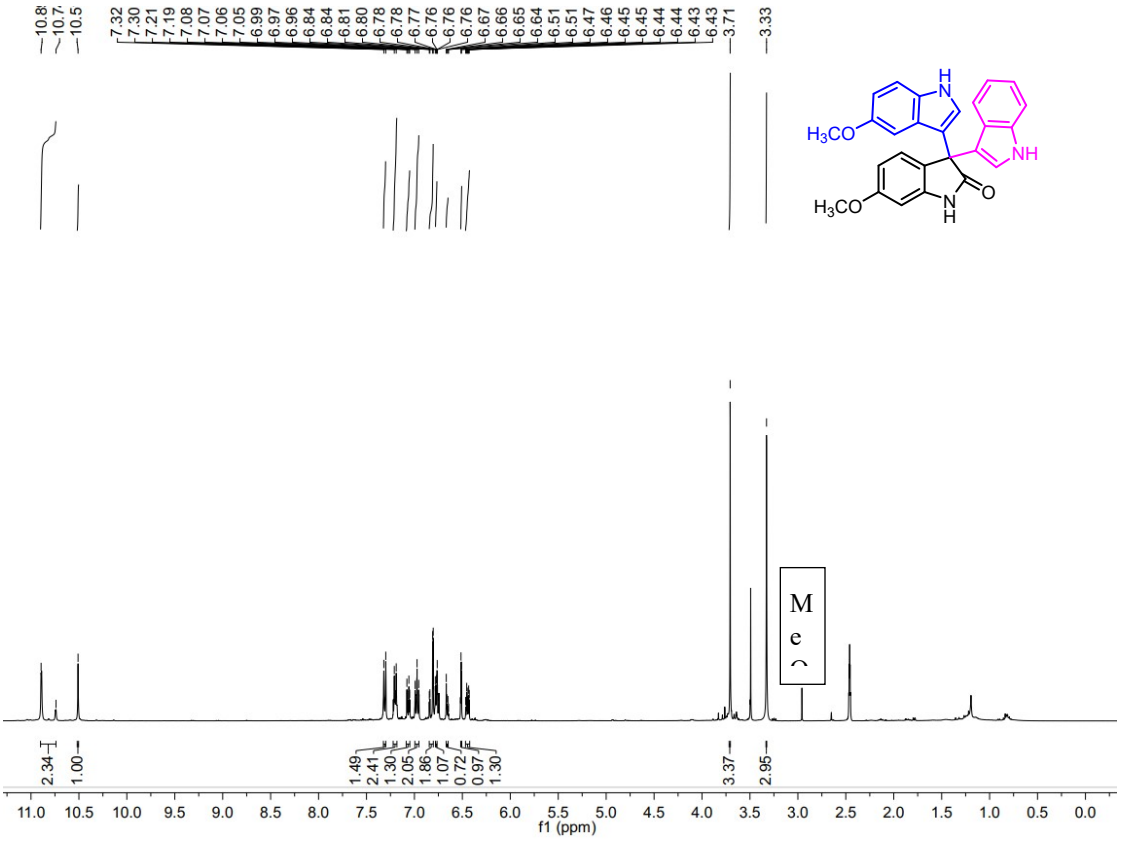


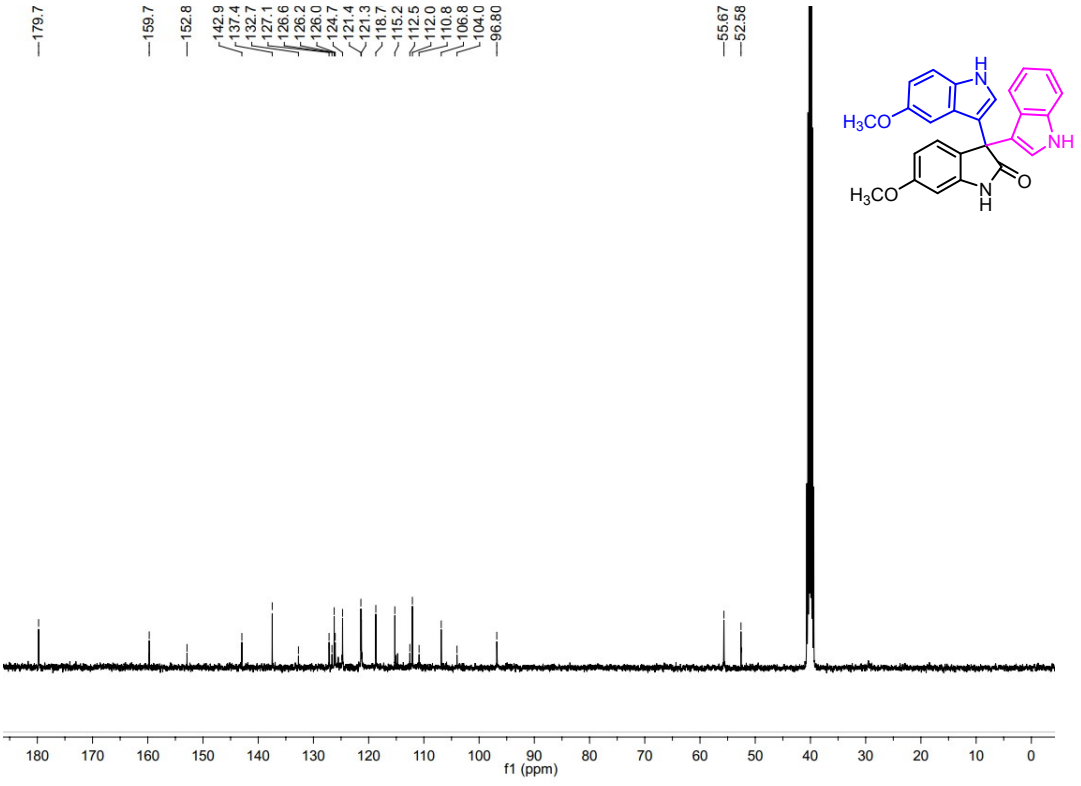
^{1}H and ^{13}C-NMR spectra of 4q



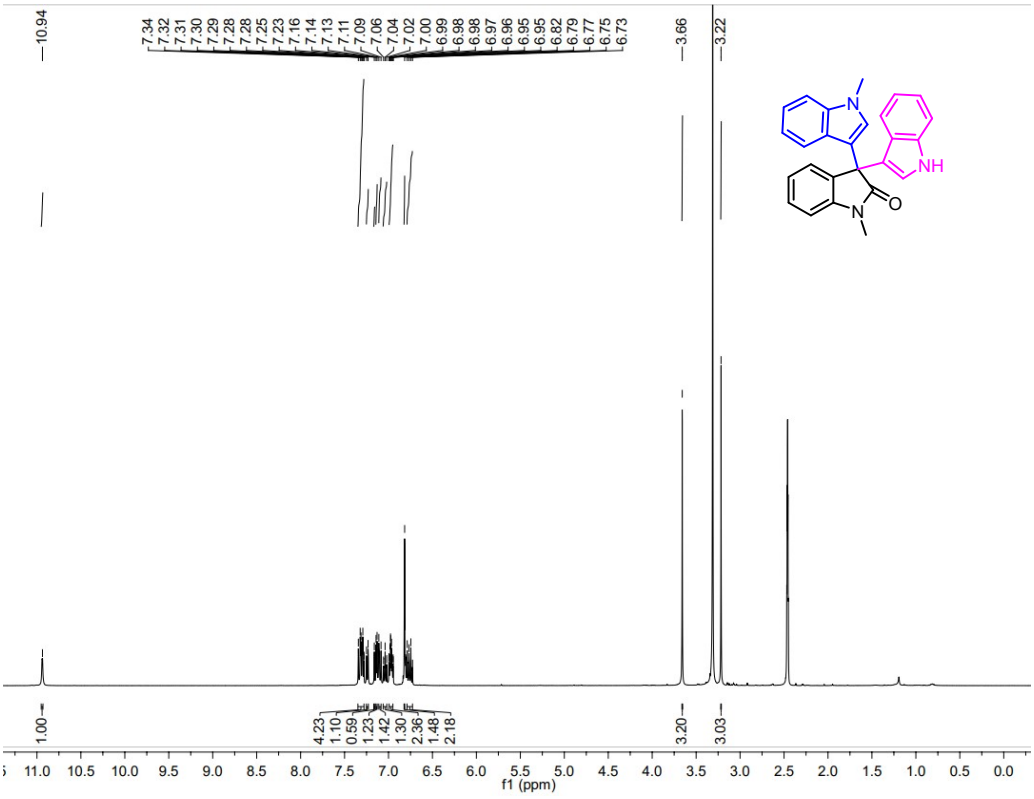


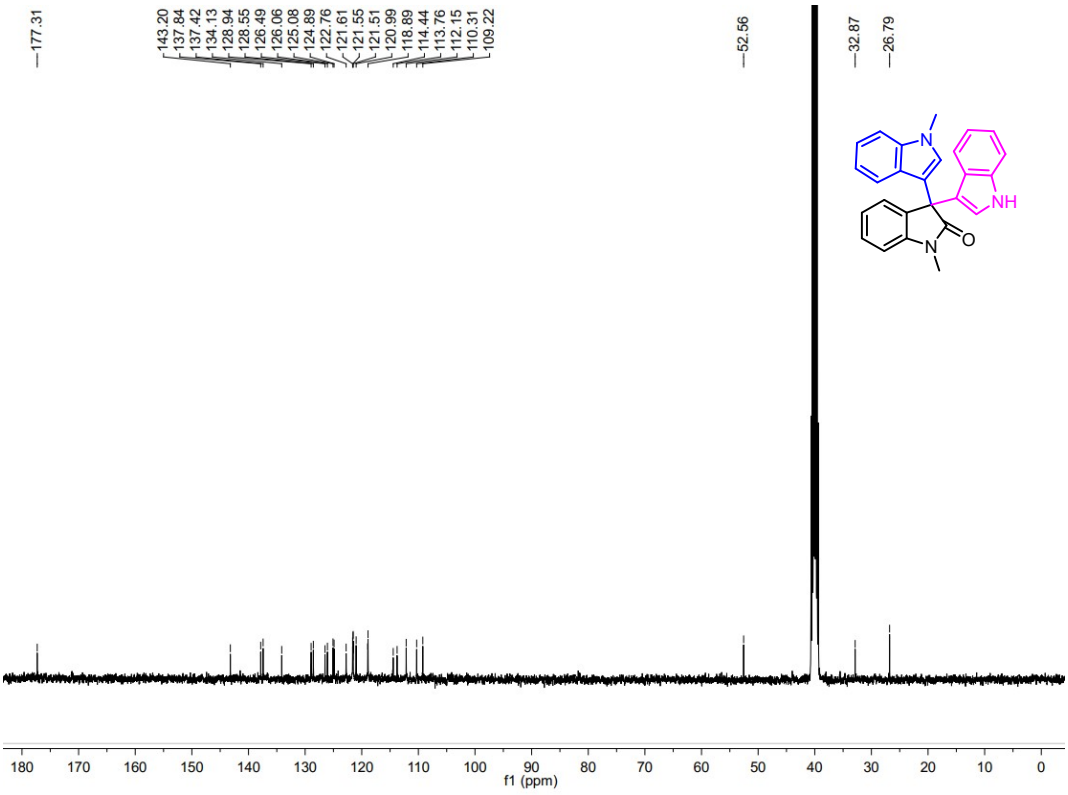
^{1}H and ^{13}C-NMR spectra of 4r





^{1}H and ^{13}C-NMR spectra of 4s





Computational Details:

Molecular docking:

The PDB of hydrolase α-amylase from *Aspergillus oryzae* (PDB id: 6TAA, EC 3.2.1.1)[1] having resolution 2.1Å was collected from the RCSB protein data bank. The substrates indole, isatin, and intermediates involved in the mechanism were optimized with the B3LYP/6-31+G** level of theory using Gaussian 16[2] in the gas phase. The enzyme 6TAA consists of a single polypeptide chain of 476 amino-acid residues. The pocket containing amino-acids Glu162, Asp175, Asp206, His210, and Glu230 were predicted as the active site by the web version of SCFBio program[3] . The substrates were docked using AutoDock Vina program[4]. The interactions and orientation of the substrates at the active site of the protein were visualized by PyMOL[5]. In order to accurately forecast all possible interactions, we have not established any constraints in this work.

Molecular Dynamics:

We then proceed to molecular dynamics simulation with the most favorable orientation predicted from docking analysis. The protonation states of the titratable residues Glu, His, and Asp of enzymes were assigned based on pKa values obtained from the PROPKA software[6]. The missing hydrogen atoms were added using the Leap module of AMBER 20[7]. For all substrates, the general AMBER force field (GAFF)[8] was employed. The complexes were solvated in a TIP3P explicit water box [9] with a minimum cutoff of 10 Å from the protein border was used to solvate the resultant system, overall was neutralized by adding twenty-three Na^+ ions. The Amber ff99SB force field[10] for the protein was used in all MD simulations. The energy of the system was minimized by 1000 steps of steepest descent 5000 steps of conjugate gradients. The minimized system was heated to room temperature under the canonical ensemble with a weak restraint of 5 Å, followed by 1 ns of density equilibration under isothermal–isobaric ensemble at the target temperature and pressure of 300K and 1.0 atm using Langevin[11] dynamics and the Berendsen barostat[12] with collision frequency of 2 ps and a pressure-relaxation time of 1 ps. Finally, the system underwent 50 ns of MD simulations with the GPU version of the AMBER 20[7]. The covalent bonds containing hydrogen atoms were constrained using SHAKE[13], and particle mesh Ewald (PME)[14] was used to compute long-range electrostatic interactions. We have used an integration step of 2 fs during the entire MD simulations. The trajectory and RMSD were analysed by the CPPTRAJ[15] module of

AMBER and the favorable orientation and interaction of protein-substrate complex were visualized using VMD [16].

RMSD Analysis:

In this work, mass weighted RMSD using the first frame as a reference has been plotted for the protein backbone along with substates using QtGrace[17]. The figures S1 and S2 represent the standard deviation with respect to the first frame throughout the trajectory for 50 ns MD stimulation. The X axis is the frame number, and the Y axis is the coordinate RMSD to the first frame (Å). At frame 1300, the RMSD jumps up quickly this corresponds to the release of harmonic restraints on the protein backbone. However, overall RMSD distribution exists within the range of ~1.8 Å.

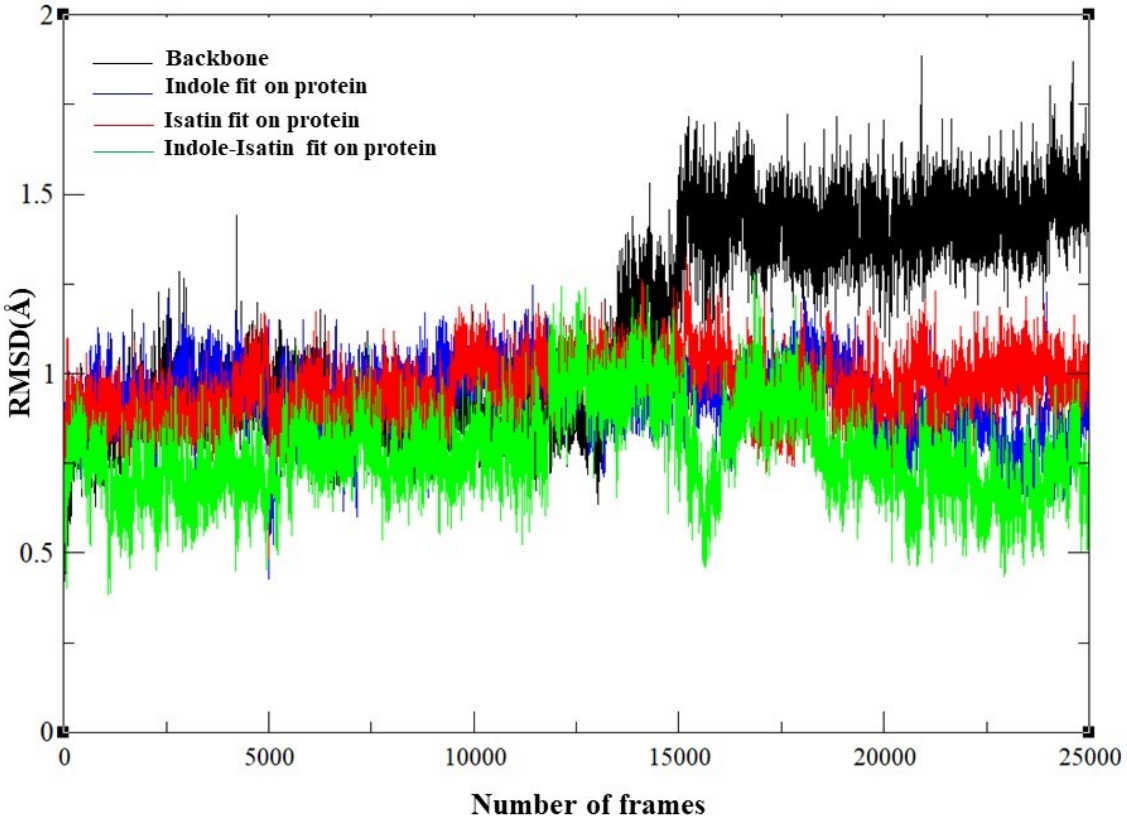


Figure S1: RMSD of α-amylase *Aspergillus oryzae* with substrate indole, isatin both indole and isatin respectively.

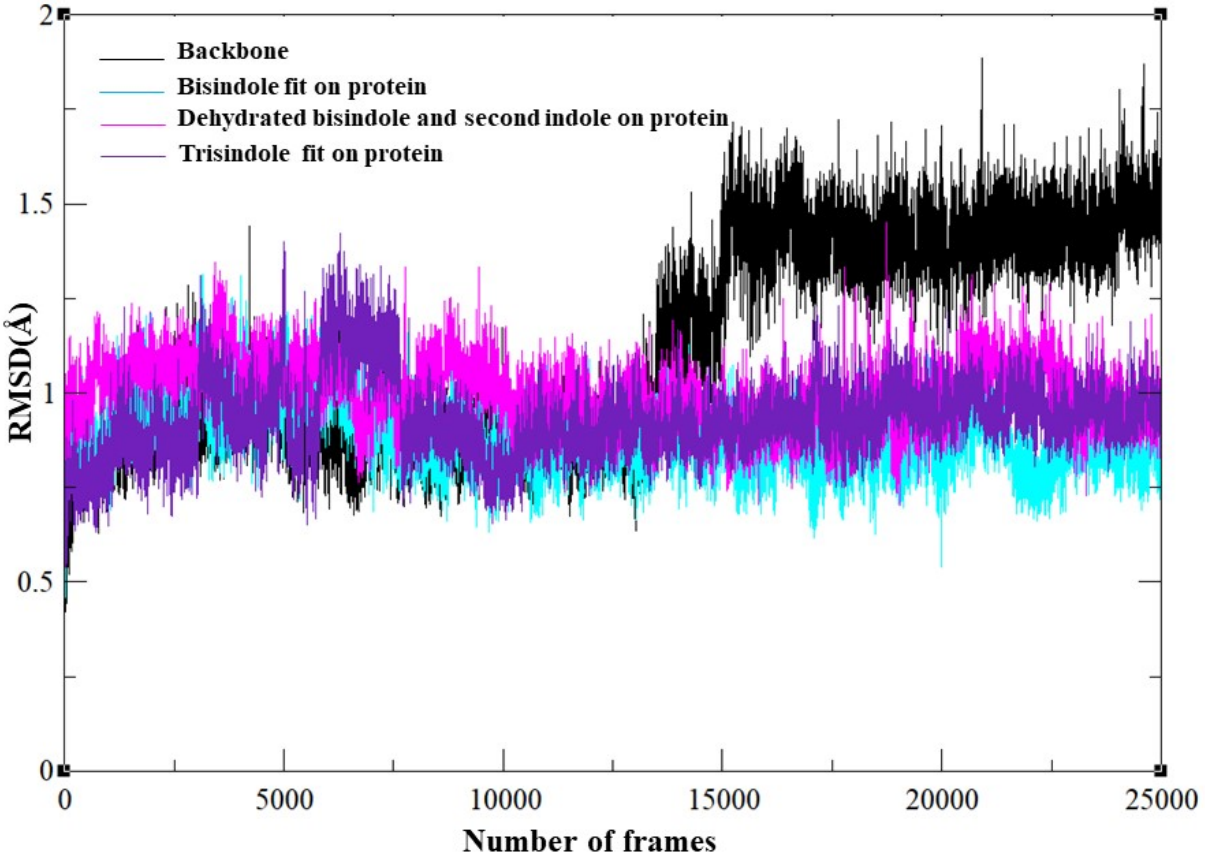


Figure S2: RMSD of α-amylase *Aspergillus oryzae* with bisindole, dehydrated bisindole with second indole, and product trisindole respectively.

DFT Study:

The geometry optimization for reactants, transition structure, and major product were done by DFT-B3LYP method which uses Becke's three parameter hybrid exchange correlation functional along with the Lee, Yang and Parr (LYP) correlation functional[18] using Pople's double zeta 6-31+G(d,p) basis set [19] by Gaussian 16[2] package. Frequency calculations were carried out at the same level of theory. The transition structures were located through a combination of scans of bond distance and dihedral angle for C-C bond formation.

PES

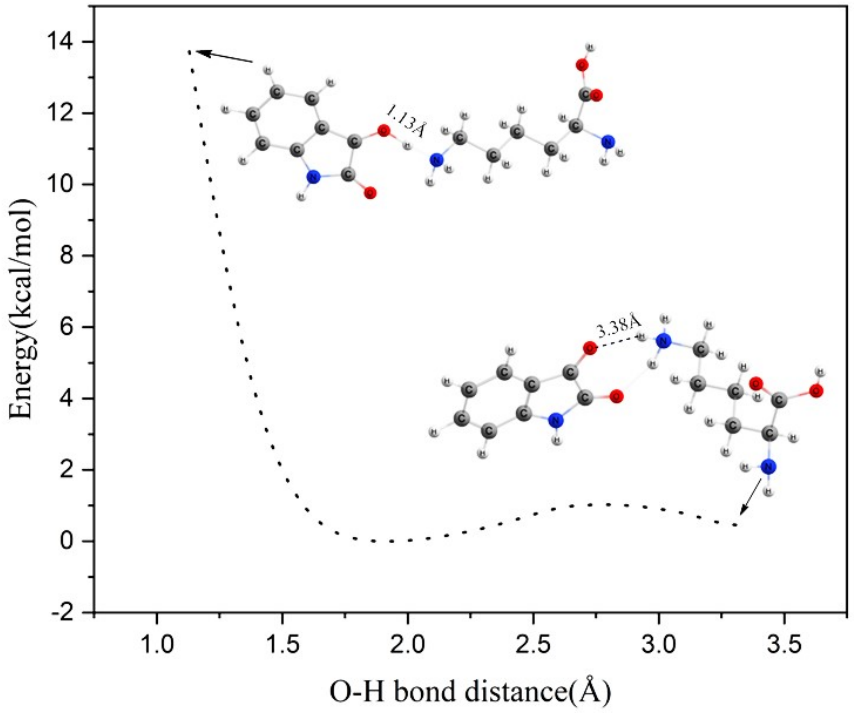


Figure S3: Relaxed potential energy surface scan for O-H proton abstraction from Lysine to isatin.

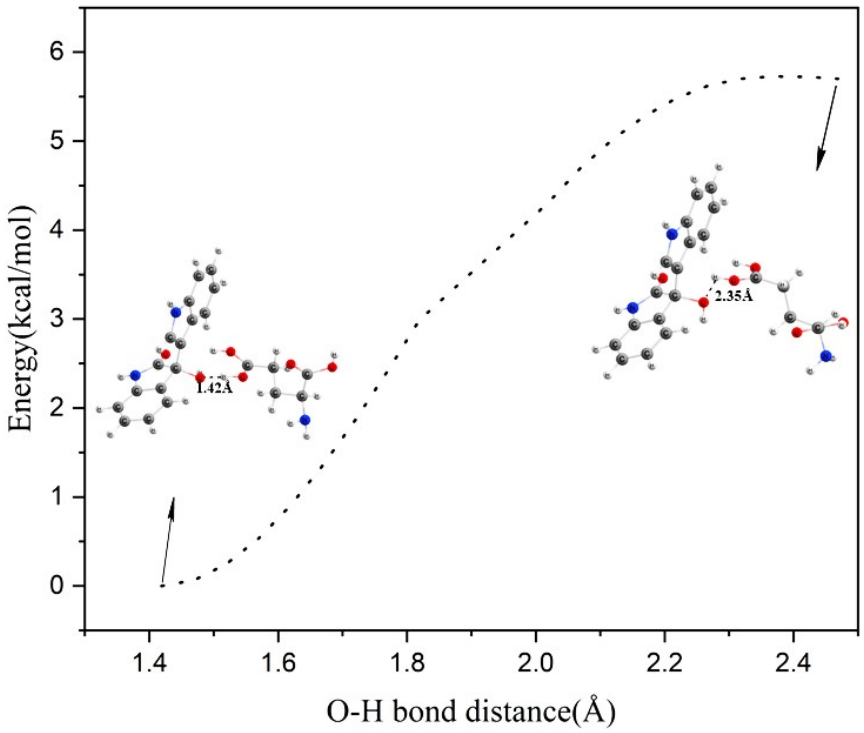


Figure S4: Relaxed potential energy surface for O-H bond distance between bisindole-intermediate(D) with Glutamic acid.

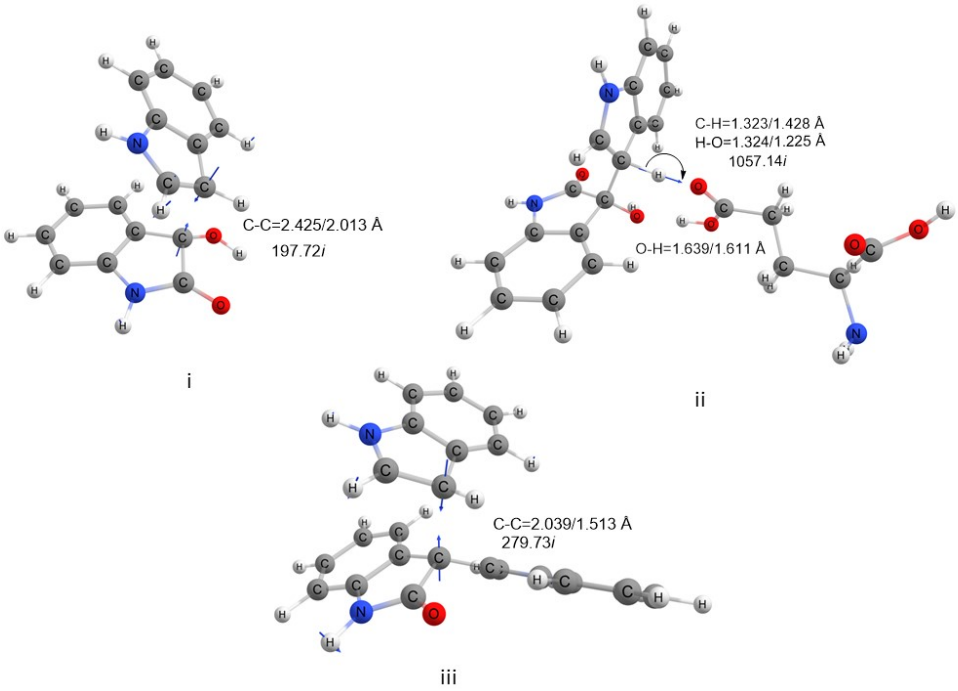


Figure S5: TS1, TS2, TS3 with imaginary frequency respectively.

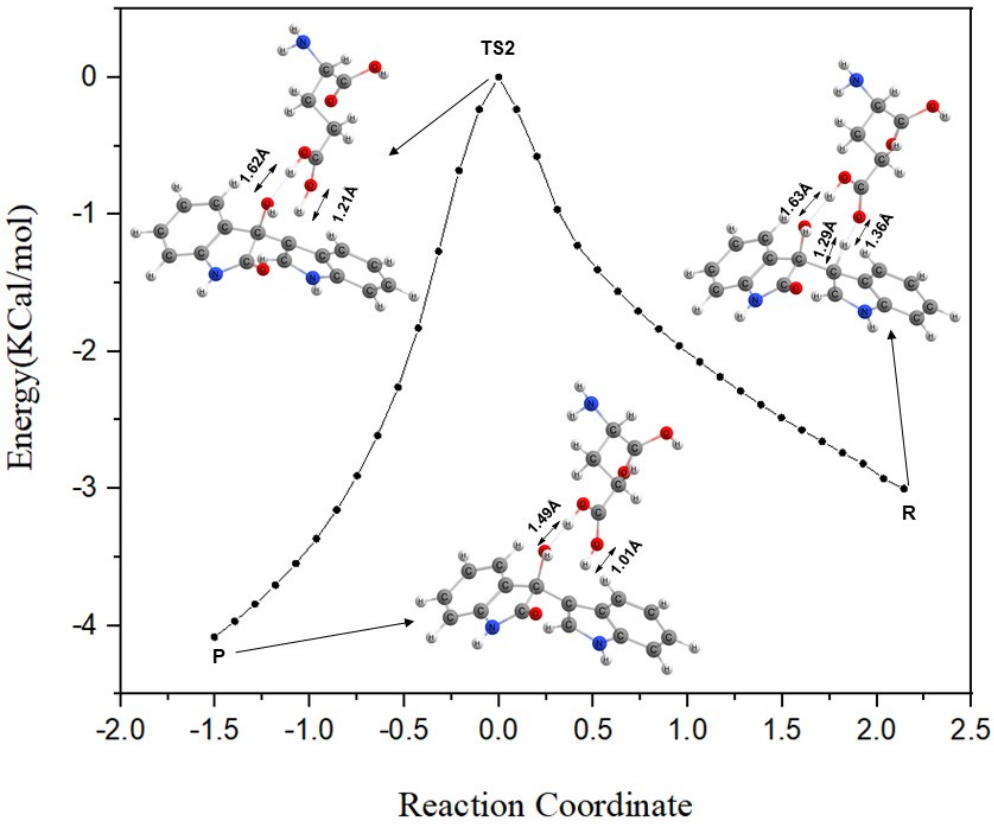


Figure S6: Intrinsic Reaction Coordinate for TS2

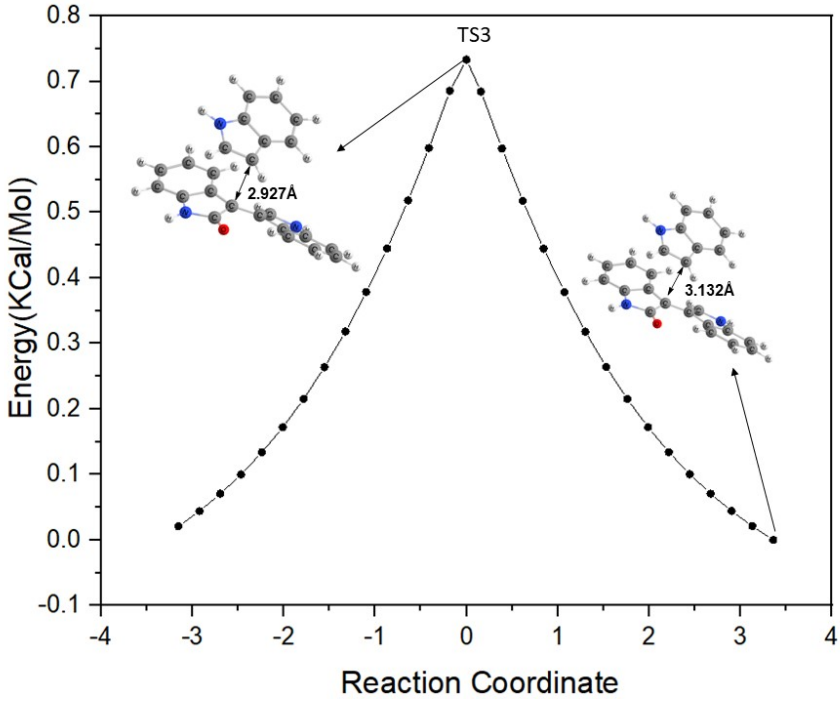


Figure S7: Intrinsic Reaction Coordinate for TS3

File Name	ZPE	E	E + ZPE	Δ(E+ZPE) in au	Δ(E+ZPE) in kcal	G(298K)	ΔG in au	ΔG in kcal
LYS	0.225848	-497.4378898	-497.2120418			-497.252069		
LYS-H (deprotonated)	0.210954	-497.0755796	-496.8646256			-496.904218		
1a	0.115118	-513.0949378	-512.9798198			-513.012869		
A	0.127589	-513.4213953	-513.2938063			-513.32696		
2a	0.129619	-363.8450759	-363.7154569			-363.745786		
IM1	0.258498	-877.2942721	-877.0357741			-877.081578		
TS1	0.259213	-877.29102	-877.031807			-877.075036		
B	0.260832	-877.3046862	-877.0438542			-877.08674		
GLU	0.151636	-551.6711258	-551.5194898			-551.558348		
C	0.413474	-1428.991104	-1428.57763			-1428.642376		
TS2	0.409055	-1428.981664	-1428.572609			-1428.635006		
D	0.412431	-1428.99161	-1428.579179			-1428.642269		
E	0.543175	-1792.852906	-1792.309731			-1792.383945		
F	0.364336	-1164.737186	-1164.37285			-1164.427753		
TS3	0.36541	-1164.724847	-1164.359437			-1164.409066		
H2O	0.021288	-76.4340489	-76.4127609			-76.430409		
G	0.366694	-1164.733256	-1164.366562			-1164.41654		
3a	0.353568	-1164.369176	-1164.015608			-1164.065711		

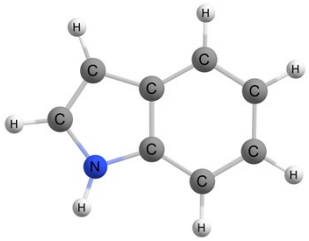
Atom Balance	ZPE	E	E + ZPE	Δ(E+ZPE) in au	Δ(E+ZPE) in kcal	G(298K)	ΔG in au	ΔG in kcal
1a+2a+LYS	0.470585	-1374.377904	-1373.907319	0	0	-1374.010724	0	0
IM1+LYS-(H)	0.469452	-1374.369852	-1373.9004	0.0069188	4.341547	-1373.985796	0.024928	15.64232
TS1+LYS-(H)	0.470167	-1374.3666	-1373.896433	0.0108859	6.83090225	-1373.979254	0.03147	19.747425
B+LYS-(H)	0.471786	-1373.90848	-1373.90848	-0.0011613	-0.72871575	-1373.990958	0.019766	12.403165
1a+2a+LYS +GLU	0.622221	-1926.049029	-1925.426808	0	0	-1925.569072	0	0
C+LYS-(H)	0.624428	-1926.066683	-1925.442255	-0.0154469	-9.69292975	-1925.546594	0.022478	14.104945
TS2+LYS-(H)	0.620009	-1926.057244	-1925.437235	-0.0104264	-6.542566	-1925.539224	0.029848	18.72962
D+LYS-(H)	0.623385	-1926.06719	-1925.443805	-0.0169962	-10.6651155	-1925.546487	0.022585	14.1720875
1a+2a+LYS +GLU +2a	0.75184	-2289.894105	-2289.142265	0	0	-2289.314858	0	0
E+LYS-(H)	0.754129	-2289.928485	-2289.174356	-0.0320912	-20.137228	-2289.288163	0.026695	16.7511125
F+LYS-(H)+H2O +GLU	0.748214	-2289.917941	-2289.169727	-0.0274615	-17.23209125	-2289.320728	-0.00587	-3.683425

1a+2a+LYS +GLU +2a - H2O	0.730552	-2213.460056	-2212.729504	0	0	-2212.884449	0	0
TS3 +LYS-H+GLU	0.728	-2213.471553	-2212.743553	-0.0140484	-8.815371	-2212.871632	0.012817	8.0426675
G + LYS-H + GLU	0.729284	-2213.479962	-2212.750678	-0.0211733	-13.28624575	-2212.879106	0.005343	3.3527325
1a + 2*2a	0.374356	-1240.78509	-1240.410734	0	0	-1240.504441	0	0
3a + H2O	0.374856	-1240.803225	-1240.428369	-0.0176351	-11.06602525	-1240.49612	0.008321	5.2214275

Table S1: All-point atom balance

Optimized Cartesian Coordinates and electronic energies

2a

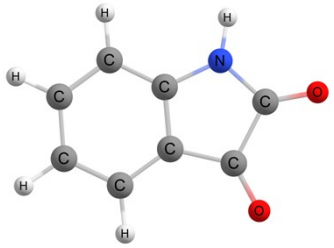


Zero-point correction= 0.129619 (Hartree/Particle)
Thermal correction to Energy= 0.135937
Thermal correction to Enthalpy= 0.136882
Thermal correction to Gibbs Free Energy= 0.099290
Sum of electronic and zero-point Energies= -363.715457
Sum of electronic and thermal Energies= -363.709139
Sum of electronic and thermal Enthalpies= -363.708194
Sum of electronic and thermal Free Energies= -363.745786

C	0.249870000	0.751732000	0.000060000
C	0.248458000	-0.672330000	0.000123000
C	-0.935389000	-1.420319000	0.000319000
C	-2.137728000	-0.719888000	-0.000375000
C	-2.161649000	0.692424000	-0.000054000
C	-0.983634000	1.430471000	0.000125000

C	1.626518000	1.168480000	-0.000090000
H	-0.919568000	-2.506855000	0.000287000
H	-3.074568000	-1.269242000	-0.000752000
H	-3.118430000	1.206340000	0.000364000
H	-1.012642000	2.516651000	0.000523000
H	2.000266000	2.182686000	-0.000054000
N	1.568429000	-1.081736000	-0.000096000
H	1.883688000	-2.038384000	0.000738000
C	2.392707000	0.030273000	-0.000117000
H	3.467333000	-0.084102000	-0.000376000

1a

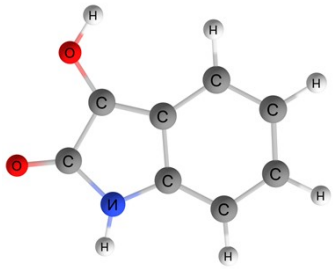


Zero-point correction=	0.115118 (Hartree/Particle)
Thermal correction to Energy=	0.123147
Thermal correction to Enthalpy=	0.124091
Thermal correction to Gibbs Free Energy=	0.082069
Sum of electronic and zero-point Energies=	-512.979820
Sum of electronic and thermal Energies=	-512.971791
Sum of electronic and thermal Enthalpies=	-512.970847
Sum of electronic and thermal Free Energies=	-513.012869

C	0.254974000	0.580713000	-0.000066000
C	0.381456000	-0.823594000	0.000162000
C	1.630779000	-1.432441000	0.000052000
C	2.757848000	-0.597363000	-0.000100000
C	2.645567000	0.800154000	0.000138000
C	1.382593000	1.399713000	0.000311000

C	-1.181163000	0.902592000	-0.000110000
H	1.737352000	-2.512740000	0.000212000
H	3.744611000	-1.051209000	0.000325000
H	3.540860000	1.412978000	-0.000223000
H	1.266528000	2.479222000	0.000430000
N	-0.886357000	-1.427483000	-0.000460000
H	-1.056067000	-2.423480000	0.000202000
C	-1.909121000	-0.493726000	-0.000921000
O	-3.100041000	-0.713409000	0.000889000

A

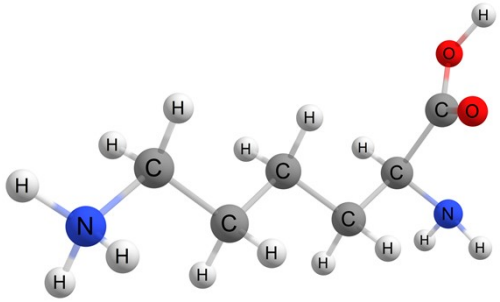


Zero-point correction=	0.127589 (Hartree/Particle)
Thermal correction to Energy=	0.135852
Thermal correction to Enthalpy=	0.136796
Thermal correction to Gibbs Free Energy=	0.094436
Sum of electronic and zero-point Energies=	-513.293806
Sum of electronic and thermal Energies=	-513.285543
Sum of electronic and thermal Enthalpies=	-513.284599
Sum of electronic and thermal Free Energies=	-513.326960

C	0.241754000	0.563634000	0.000575000
C	0.413520000	-0.871483000	0.000352000
C	1.687175000	-1.429630000	-0.000157000
C	2.772137000	-0.551541000	-0.000556000
C	2.628206000	0.863358000	-0.000314000
C	1.374932000	1.429241000	0.000391000
C	-1.128763000	0.786757000	0.000101000
H	1.837691000	-2.503551000	-0.000148000
H	3.774931000	-0.969035000	-0.001052000

H	3.514199000	1.487761000	-0.000559000
H	1.254040000	2.508382000	0.000811000
N	-0.808943000	-1.508107000	0.001257000
H	-0.962763000	-2.508953000	-0.002037000
C	-1.848366000	-0.580912000	-0.000009000
O	-3.032582000	-0.772242000	-0.000736000
O	-1.870239000	1.847035000	-0.000217000
H	-1.376502000	2.687254000	-0.000487000

Lys

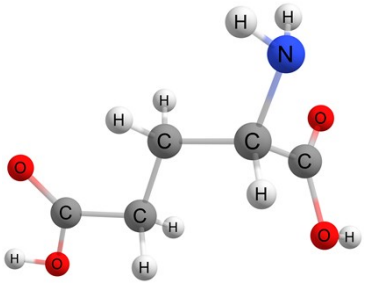


Zero-point correction=	0.225848 (Hartree/Particle)
Thermal correction to Energy=	0.238274
Thermal correction to Enthalpy=	0.239218
Thermal correction to Gibbs Free Energy=	0.185821
Sum of electronic and zero-point Energies=	-497.212041
Sum of electronic and thermal Energies=	-497.199616
Sum of electronic and thermal Enthalpies=	-497.198672
Sum of electronic and thermal Free Energies=	-497.252069

N	2.840787000	1.552815000	-0.157005000
H	2.759569000	1.723951000	-1.155030000
C	1.788051000	0.672924000	0.344334000
H	1.856340000	0.678192000	1.437538000
C	0.361575000	1.049120000	-0.104644000
C	2.149330000	-0.739126000	-0.132368000
H	0.179526000	2.089381000	0.192675000
H	0.331941000	1.008923000	-1.200227000
C	-0.736809000	0.139337000	0.468244000

O	1.751334000	-1.232117000	-1.170243000
H	-0.497923000	-0.905089000	0.236433000
H	-0.768983000	0.232121000	1.561933000
C	-2.121776000	0.469352000	-0.118437000
H	-2.394513000	1.504604000	0.128256000
H	-2.069615000	0.394076000	-1.213205000
C	-3.184212000	-0.486711000	0.408799000
H	-2.960703000	-1.528231000	0.166083000
H	-3.333651000	-0.397526000	1.487394000
N	-4.546356000	-0.192680000	-0.229695000
H	-4.499628000	-0.290464000	-1.250117000
H	-5.276964000	-0.826700000	0.111788000
H	-4.846950000	0.767688000	-0.029738000
H	2.873296000	2.438806000	0.335289000
O	2.975280000	-1.370670000	0.718453000
H	3.237378000	-2.217752000	0.316582000

Glu

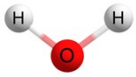


Zero-point correction=	0.151636 (Hartree/Particle)
Thermal correction to Energy=	0.162581
Thermal correction to Enthalpy=	0.163526
Thermal correction to Gibbs Free Energy=	0.112778
Sum of electronic and zero-point Energies=	-551.519490
Sum of electronic and thermal Energies=	-551.508544
Sum of electronic and thermal Enthalpies=	-551.507600
Sum of electronic and thermal Free Energies=	-551.558348

N	-2.235826000	1.750222000	-0.316234000
H	-2.454894000	1.843824000	0.672957000

C	-1.338557000	0.616441000	-0.530126000
H	-1.285768000	0.413413000	-1.605564000
C	0.099276000	0.826529000	0.012267000
C	-1.978608000	-0.591441000	0.142317000
H	0.487775000	1.747864000	-0.434793000
H	0.047971000	1.001472000	1.093067000
C	1.066989000	-0.320762000	-0.292137000
O	-2.486357000	-0.575265000	1.243554000
H	0.798362000	-1.243013000	0.234032000
H	1.049275000	-0.578490000	-1.360039000
C	2.500280000	0.014797000	0.056647000
O	2.927546000	1.110140000	0.354866000
H	-1.806708000	2.614647000	-0.633629000
O	-1.889000000	-1.716578000	-0.605604000
H	-2.296955000	-2.437373000	-0.094165000
O	3.299377000	-1.080286000	-0.016539000
H	4.202914000	-0.791373000	0.197741000

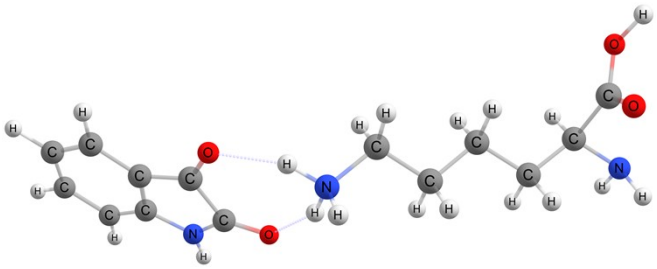
water



Zero-point correction=	0.021288 (Hartree/Particle)
Thermal correction to Energy=	0.024124
Thermal correction to Enthalpy=	0.025068
Thermal correction to Gibbs Free Energy=	0.003640
Sum of electronic and zero-point Energies=	-76.412761
Sum of electronic and thermal Energies=	-76.409925
Sum of electronic and thermal Enthalpies=	-76.408981
Sum of electronic and thermal Free Energies=	-76.430409

O	0.000000000	0.000000000	0.116490000
H	0.000000000	0.769490000	-0.465961000
H	0.000000000	-0.769490000	-0.465961000

Lys-1a complex

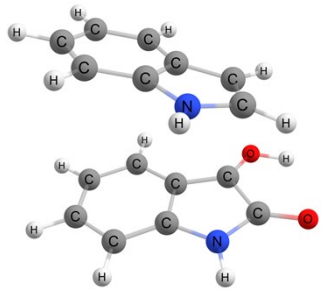


Zero-point correction=	0.342595 (Hartree/Particle)
Thermal correction to Energy=	0.364569
Thermal correction to Enthalpy=	0.365513
Thermal correction to Gibbs Free Energy=	0.285866
Sum of electronic and zero-point Energies=	-1010.241705
Sum of electronic and thermal Energies=	-1010.219731
Sum of electronic and thermal Enthalpies=	-1010.218787
Sum of electronic and thermal Free Energies=	-1010.298434

C	-4.786523000	-0.530057000	0.071657000
C	-5.185008000	0.812518000	0.255623000
C	-6.476667000	1.140866000	0.623267000
C	-7.379449000	0.077998000	0.806763000
C	-7.002555000	-1.260935000	0.628800000
C	-5.695214000	-1.577811000	0.257491000
C	-3.386809000	-0.521874000	-0.307316000
H	-6.791132000	2.169328000	0.766414000
H	-8.400586000	0.307040000	1.095526000
H	-7.731554000	-2.049139000	0.780748000
H	-5.380422000	-2.606379000	0.113563000
N	-4.092957000	1.683891000	0.009609000
H	-4.128913000	2.693607000	0.073676000
C	-2.975536000	0.995609000	-0.333244000
O	-1.866792000	1.444276000	-0.608798000
O	-2.605896000	-1.428060000	-0.570497000
N	7.079492000	1.643779000	0.370709000
H	7.272288000	1.720019000	-0.624367000

C	5.988882000	0.706530000	0.641033000
H	5.773497000	0.759126000	1.713253000
C	4.701936000	0.951317000	-0.172277000
C	6.556957000	-0.684271000	0.346421000
H	4.382970000	1.985376000	0.011463000
H	4.952759000	0.870118000	-1.237041000
C	3.555205000	-0.015079000	0.160710000
O	6.629012000	-1.167887000	-0.765507000
H	3.893571000	-1.047617000	0.007994000
H	3.284967000	0.079059000	1.221345000
C	2.312213000	0.233852000	-0.708815000
H	1.941068000	1.254529000	-0.546627000
H	2.595167000	0.157696000	-1.767964000
C	1.202173000	-0.768769000	-0.407575000
H	1.528879000	-1.797325000	-0.580851000
H	0.848476000	-0.688895000	0.623366000
N	-0.002371000	-0.536165000	-1.287390000
H	0.244543000	-0.597981000	-2.278175000
H	-0.779184000	-1.194475000	-1.093994000
H	-0.452460000	0.386266000	-1.111714000
H	6.886180000	2.567948000	0.742672000
O	6.991292000	-1.313426000	1.455306000
H	7.412179000	-2.147419000	1.180942000

IM1

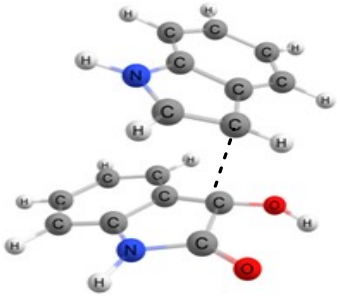


Zero-point correction=	0.258498 (Hartree/Particle)
Thermal correction to Energy=	0.274934
Thermal correction to Enthalpy=	0.275879
Thermal correction to Gibbs Free Energy=	0.212694
Sum of electronic and zero-point Energies=	-877.035774
Sum of electronic and thermal Energies=	-877.019338
Sum of electronic and thermal Enthalpies=	-877.018394
Sum of electronic and thermal Free Energies=	-877.081578

C	1.024503000	0.973472000	0.671171000
C	1.319602000	1.292924000	-0.697885000
C	0.669148000	2.332847000	-1.338191000
C	-0.287487000	3.047262000	-0.599056000
C	-0.590700000	2.749287000	0.745627000
C	0.058462000	1.712512000	1.394756000
C	1.859343000	-0.094182000	1.004937000
H	0.889354000	2.599175000	-2.366428000
H	-0.805430000	3.870240000	-1.082340000
H	-1.334343000	3.339871000	1.268333000
H	-0.149447000	1.472488000	2.431310000
N	2.313073000	0.440209000	-1.187289000
H	2.771877000	0.519057000	-2.085115000
C	2.728038000	-0.428122000	-0.197199000
O	3.616016000	-1.256055000	-0.196622000
O	2.085898000	-0.638012000	2.167354000
H	2.807609000	-1.296970000	2.087610000
C	-1.342284000	-1.403724000	0.403505000
C	-1.666163000	-1.021479000	-0.926812000

C	-2.795814000	-0.267095000	-1.237846000
C	-3.623877000	0.108521000	-0.175323000
C	-3.326047000	-0.254941000	1.151591000
C	-2.190569000	-1.004321000	1.454643000
C	-0.130869000	-2.167556000	0.335325000
H	-3.039812000	0.005652000	-2.260094000
H	-4.522245000	0.681459000	-0.381795000
H	-4.000992000	0.042661000	1.947597000
H	-1.980041000	-1.300749000	2.478038000
H	0.359544000	-2.688487000	1.145089000
N	-0.676659000	-1.547826000	-1.756284000
H	-0.683259000	-1.511805000	-2.765555000
C	0.224041000	-2.249267000	-1.006901000
H	1.041009000	-2.783563000	-1.471552000

TS1

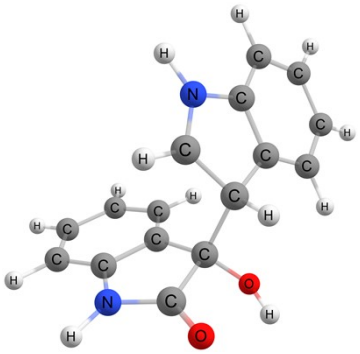


Zero-point correction=	0.259213 (Hartree/Particle)
Thermal correction to Energy=	0.274420
Thermal correction to Enthalpy=	0.275364
Thermal correction to Gibbs Free Energy=	0.215984
Sum of electronic and zero-point Energies=	-877.031807
Sum of electronic and thermal Energies=	-877.016600
Sum of electronic and thermal Enthalpies=	-877.015656
Sum of electronic and thermal Free Energies=	-877.075036

C	-1.125517000	0.465088000	-0.671815000
C	-2.232001000	0.686193000	0.188471000
C	-2.664609000	1.968082000	0.490471000
C	-1.970396000	3.038184000	-0.095957000

C	-0.881456000	2.835143000	-0.957412000
C	-0.447924000	1.542791000	-1.254084000
C	-0.982959000	-0.963726000	-0.796026000
H	-3.520509000	2.144897000	1.133617000
H	-2.297782000	4.051342000	0.115825000
H	-0.381447000	3.688973000	-1.401237000
H	0.387710000	1.369858000	-1.923672000
N	-2.777114000	-0.546518000	0.600730000
H	-3.650935000	-0.659811000	1.098841000
C	-2.152318000	-1.593505000	-0.037803000
O	-2.430558000	-2.775838000	-0.055893000
O	-0.531586000	-1.566403000	-1.884643000
H	-0.825617000	-2.499515000	-1.885145000
C	1.757440000	-0.910812000	0.164655000
C	1.967928000	0.154646000	1.067431000
C	2.997067000	1.082203000	0.930660000
C	3.844387000	0.916933000	-0.167060000
C	3.658259000	-0.135592000	-1.081401000
C	2.618687000	-1.055922000	-0.929706000
C	0.580765000	-1.636314000	0.628436000
H	3.145773000	1.888692000	1.641646000
H	4.667866000	1.608669000	-0.310694000
H	4.344522000	-0.239408000	-1.915517000
H	2.494165000	-1.870119000	-1.635614000
H	0.346818000	-2.669673000	0.406329000
N	0.991761000	0.037619000	2.074951000
H	0.904036000	0.660300000	2.868771000
C	0.222031000	-1.035903000	1.861836000
H	-0.556278000	-1.318919000	2.557183000

B

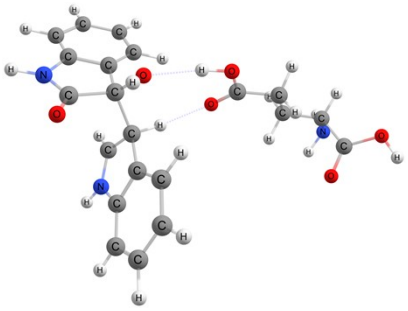


Zero-point correction=	0.260832 (Hartree/Particle)
Thermal correction to Energy=	0.276049
Thermal correction to Enthalpy=	0.276993
Thermal correction to Gibbs Free Energy=	0.217946
Sum of electronic and zero-point Energies=	-877.043854
Sum of electronic and thermal Energies=	-877.028638
Sum of electronic and thermal Enthalpies=	-877.027693
Sum of electronic and thermal Free Energies=	-877.086740

C	-1.268461000	0.451361000	-0.438225000
C	-2.546452000	0.405083000	0.144868000
C	-3.298843000	1.551339000	0.363233000
C	-2.740050000	2.774401000	-0.034449000
C	-1.476517000	2.837429000	-0.630201000
C	-0.729872000	1.668861000	-0.839594000
C	-0.742265000	-0.962053000	-0.538155000
H	-4.287422000	1.507528000	0.809004000
H	-3.308706000	3.686793000	0.114455000
H	-1.076901000	3.795357000	-0.945734000
H	0.237879000	1.715003000	-1.328349000
N	-2.892317000	-0.936173000	0.436156000
H	-3.805024000	-1.247386000	0.745309000
C	-1.925765000	-1.808744000	0.024558000
O	-1.927590000	-3.026845000	0.057976000
O	-0.459141000	-1.348761000	-1.859598000
H	-0.645170000	-2.299332000	-1.954647000
C	1.815531000	-0.569646000	-0.068674000

C	2.300609000	0.168922000	1.021258000
C	3.470151000	0.919516000	1.003258000
C	4.181193000	0.913906000	-0.199515000
C	3.721721000	0.184739000	-1.307371000
C	2.539095000	-0.565933000	-1.257670000
C	0.536794000	-1.254334000	0.354504000
H	3.818956000	1.476166000	1.867048000
H	5.103384000	1.480049000	-0.275085000
H	4.298906000	0.200854000	-2.226174000
H	2.193114000	-1.119440000	-2.122291000
H	0.626959000	-2.354273000	0.357577000
N	1.385165000	-0.018908000	2.092808000
H	1.491844000	0.409629000	3.009677000
C	0.394314000	-0.800076000	1.766852000
H	-0.391006000	-1.049157000	2.471372000

C



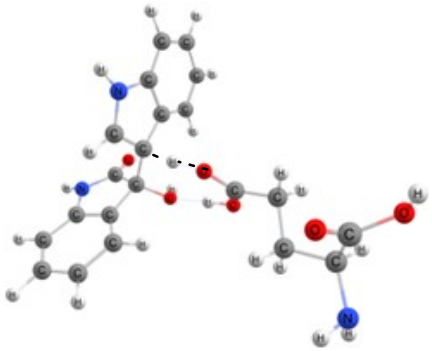
Zero-point correction=	0.413474 (Hartree/Particle)
Thermal correction to Energy=	0.441578
Thermal correction to Enthalpy=	0.442522
Thermal correction to Gibbs Free Energy=	0.348728
Sum of electronic and zero-point Energies=	-1428.577629
Sum of electronic and thermal Energies=	-1428.549526
Sum of electronic and thermal Enthalpies=	-1428.548582
Sum of electronic and thermal Free Energies=	-1428.642376

N	6.195893000	-1.461981000	1.721503000
H	5.825740000	-0.849127000	2.443004000
C	5.537133000	-1.235533000	0.433490000

H	5.895715000	-2.008473000	-0.253952000
C	3.997164000	-1.235926000	0.486148000
C	6.062914000	0.112454000	-0.067192000
H	3.672430000	-2.182727000	0.932004000
H	3.671145000	-0.434566000	1.156691000
C	3.341402000	-1.055813000	-0.885808000
O	5.628190000	1.189112000	0.291658000
H	3.694879000	-0.139352000	-1.376784000
H	3.594724000	-1.873147000	-1.572762000
C	1.837483000	-0.952273000	-0.835529000
O	1.164959000	-0.932473000	0.191058000
H	6.102568000	-2.425253000	2.027099000
O	7.080290000	-0.018919000	-0.939191000
H	7.409643000	0.871918000	-1.152961000
O	1.287971000	-0.866043000	-2.054069000
H	0.312889000	-0.778200000	-1.971690000
C	-2.613615000	-1.657632000	-0.120981000
C	-4.011728000	-1.778306000	-0.064392000
C	-4.633001000	-2.933583000	0.390424000
C	-3.806339000	-3.993007000	0.792664000
C	-2.412712000	-3.886564000	0.748193000
C	-1.802083000	-2.708263000	0.294409000
C	-2.273912000	-0.279143000	-0.638003000
H	-5.713992000	-3.023280000	0.426778000
H	-4.262772000	-4.912859000	1.144264000
H	-1.798196000	-4.722836000	1.064154000
H	-0.720657000	-2.618329000	0.264327000
N	-4.612476000	-0.580704000	-0.519214000
H	-5.599126000	-0.465035000	-0.714818000
C	-3.680509000	0.315394000	-0.963330000
O	-3.859010000	1.367619000	-1.550288000
C	-1.200932000	2.036340000	0.147225000

C	-1.646090000	2.795712000	1.240188000
C	-1.507209000	4.174624000	1.350473000
C	-0.875207000	4.813624000	0.282627000
C	-0.402501000	4.081248000	-0.817548000
C	-0.549742000	2.691364000	-0.894618000
C	-1.496909000	0.581831000	0.434358000
H	-1.860784000	4.727300000	2.214892000
H	-0.739446000	5.889393000	0.309353000
H	0.095490000	4.605752000	-1.626413000
H	-0.155357000	2.147821000	-1.745270000
H	-0.543277000	0.018306000	0.557602000
N	-2.217178000	1.889316000	2.172301000
H	-2.611080000	2.171855000	3.066557000
C	-2.160107000	0.651988000	1.759247000
H	-2.551800000	-0.168873000	2.347963000
O	-1.509671000	-0.289647000	-1.836199000
H	-1.845247000	0.414894000	-2.418185000

TS2

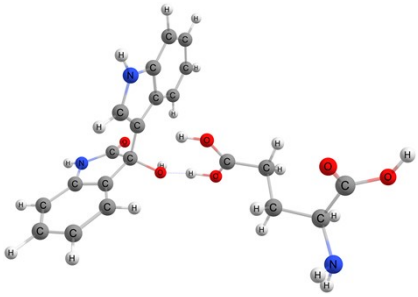


Zero-point correction=	0.409055 (Hartree/Particle)
Thermal correction to Energy=	0.436278
Thermal correction to Enthalpy=	0.437223
Thermal correction to Gibbs Free Energy=	0.346658
Sum of electronic and zero-point Energies=	-1428.572609
Sum of electronic and thermal Energies=	-1428.545386
Sum of electronic and thermal Enthalpies=	-1428.544441
Sum of electronic and thermal Free Energies=	-1428.635006

N	6.240625000	-1.718450000	-0.824406000
H	5.931103000	-2.448521000	-0.189306000
C	5.469339000	-0.489163000	-0.674264000
H	5.808513000	0.207806000	-1.447389000
C	3.939862000	-0.679000000	-0.766562000
C	5.859882000	0.087939000	0.689794000
H	3.713652000	-1.170221000	-1.718495000
H	3.626580000	-1.342191000	0.047219000
C	3.161803000	0.659905000	-0.674317000
O	5.373245000	-0.276103000	1.741392000
H	3.372626000	1.161904000	0.271861000
H	3.448479000	1.312140000	-1.506565000
C	1.685823000	0.428761000	-0.750984000
O	0.972652000	0.474015000	0.285862000
H	6.230448000	-2.068566000	-1.776469000
O	6.816846000	1.027793000	0.597963000
H	7.072993000	1.289590000	1.500238000
O	1.212074000	0.146905000	-1.932789000
H	0.230168000	-0.073043000	-1.923926000
C	-2.008291000	-1.977262000	-0.035354000
C	-3.313289000	-2.479697000	0.097152000
C	-3.571261000	-3.713481000	0.680189000
C	-2.471730000	-4.457913000	1.130356000
C	-1.165545000	-3.974686000	1.004398000
C	-0.926832000	-2.720209000	0.424584000
C	-2.089328000	-0.597492000	-0.651481000
H	-4.582072000	-4.096300000	0.777616000
H	-2.642302000	-5.429918000	1.582110000
H	-0.332115000	-4.574041000	1.355023000
H	0.089168000	-2.348565000	0.331205000
N	-4.237961000	-1.558562000	-0.444852000
H	-5.213418000	-1.759824000	-0.626269000

C	-3.600494000	-0.507776000	-1.041469000
O	-4.054787000	0.327554000	-1.801704000
C	-1.859888000	1.976856000	0.082073000
C	-1.916732000	2.591572000	1.351056000
C	-2.007926000	3.970950000	1.539503000
C	-2.056496000	4.755109000	0.390904000
C	-2.010936000	4.169849000	-0.889008000
C	-1.904904000	2.790894000	-1.057842000
C	-1.676143000	0.521244000	0.316856000
H	-2.043198000	4.413024000	2.530134000
H	-2.135800000	5.833156000	0.483241000
H	-2.066001000	4.808511000	-1.764564000
H	-1.887355000	2.368326000	-2.055066000
H	-0.302962000	0.444174000	0.280972000
N	-1.870764000	1.570273000	2.312682000
H	-1.855369000	1.722921000	3.314019000
C	-1.786213000	0.372848000	1.733138000
H	-1.743856000	-0.536556000	2.317126000
O	-1.347214000	-0.463457000	-1.883359000
H	-1.929312000	-0.035777000	-2.537925000

D



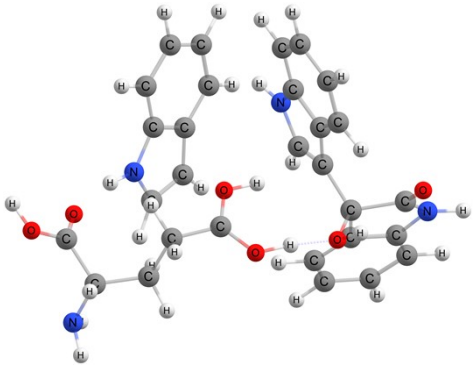
Zero-point correction=	0.412431 (Hartree/Particle)
Thermal correction to Energy=	0.440041
Thermal correction to Enthalpy=	0.440986
Thermal correction to Gibbs Free Energy=	0.349341
Sum of electronic and zero-point Energies=	-1428.579179
Sum of electronic and thermal Energies=	-1428.551568
Sum of electronic and thermal Enthalpies=	-1428.550624

Sum of electronic and thermal Free Energies= -1428.642269

N	6.040029000	-2.379055000	-0.493700000
H	5.715153000	-2.880231000	0.327615000
C	5.420907000	-1.069500000	-0.641412000
H	5.752102000	-0.656288000	-1.599814000
C	3.877140000	-1.090247000	-0.577199000
C	5.995261000	-0.190781000	0.476299000
H	3.512354000	-1.778986000	-1.346073000
H	3.577131000	-1.470549000	0.404717000
C	3.253050000	0.318915000	-0.798990000
O	5.506237000	-0.103545000	1.585030000
H	3.601426000	1.007738000	-0.026735000
H	3.524086000	0.695913000	-1.789640000
C	1.771171000	0.244746000	-0.725500000
O	1.220851000	0.510067000	0.417455000
H	5.937496000	-2.960812000	-1.317803000
O	7.109620000	0.453859000	0.097391000
H	7.469415000	0.925544000	0.869644000
O	1.112071000	-0.112152000	-1.753943000
H	0.056058000	-0.226337000	-1.684926000
C	-2.433184000	-1.801983000	0.033248000
C	-3.804893000	-2.103746000	0.009919000
C	-4.311297000	-3.269024000	0.570016000
C	-3.396546000	-4.156390000	1.154040000
C	-2.026334000	-3.878146000	1.176698000
C	-1.537224000	-2.687575000	0.620183000
C	-2.237089000	-0.439281000	-0.589954000
H	-5.372639000	-3.494463000	0.550529000
H	-3.763064000	-5.079471000	1.591655000
H	-1.338895000	-4.587049000	1.625762000
H	-0.471513000	-2.477050000	0.640997000

N	-4.509295000	-1.078270000	-0.659923000
H	-5.473656000	-1.143183000	-0.960745000
C	-3.651805000	-0.163409000	-1.197452000
O	-3.865956000	0.677518000	-2.052691000
C	-1.652673000	2.062474000	0.128187000
C	-1.415039000	2.672602000	1.388467000
C	-1.177493000	4.043795000	1.536969000
C	-1.191846000	4.818001000	0.383721000
C	-1.440042000	4.240348000	-0.880288000
C	-1.668882000	2.877493000	-1.022374000
C	-1.816483000	0.635015000	0.384188000
H	-0.997116000	4.485647000	2.512019000
H	-1.019652000	5.886927000	0.456652000
H	-1.465664000	4.878435000	-1.757768000
H	-1.899521000	2.465301000	-1.997735000
H	0.220716000	0.470245000	0.432974000
N	-1.469950000	1.675323000	2.352175000
H	-1.332062000	1.813650000	3.343105000
C	-1.717533000	0.470378000	1.763350000
H	-1.826454000	-0.427396000	2.353976000
O	-1.342642000	-0.453967000	-1.756320000
H	-1.787623000	0.050080000	-2.466345000

E



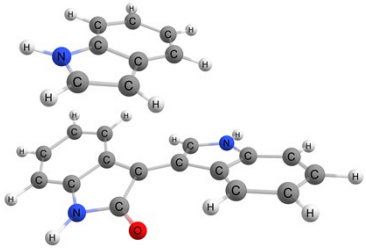
Zero-point correction=	0.543175 (Hartree/Particle)
Thermal correction to Energy=	0.578908
Thermal correction to Enthalpy=	0.579852
Thermal correction to Gibbs Free Energy=	0.468961
Sum of electronic and zero-point Energies=	-1792.309731
Sum of electronic and thermal Energies=	-1792.273997
Sum of electronic and thermal Enthalpies=	-1792.273053
Sum of electronic and thermal Free Energies=	-1792.383945

N	5.308358000	-3.449689000	0.187700000
H	5.002930000	-3.219878000	1.128228000
C	4.658379000	-2.644606000	-0.837831000
H	4.923778000	-3.074254000	-1.808790000
C	3.124306000	-2.544717000	-0.698388000
C	5.305921000	-1.257379000	-0.749991000
H	2.717166000	-3.558193000	-0.630612000
H	2.897604000	-2.021569000	0.236851000
C	2.460303000	-1.799589000	-1.891886000
O	4.943528000	-0.383028000	0.019097000
H	2.953689000	-0.840563000	-2.066582000
H	2.514636000	-2.411256000	-2.796406000
C	1.027850000	-1.522986000	-1.589624000
O	0.761392000	-0.372763000	-1.065871000
H	5.212696000	-4.446150000	0.027130000
O	6.335726000	-1.116950000	-1.589848000
H	6.762642000	-0.256670000	-1.426009000
O	0.155584000	-2.422093000	-1.806670000
H	-0.871705000	-2.234088000	-1.546808000

C	-2.839483000	-1.563226000	1.093784000
C	-4.175239000	-1.524885000	1.527424000
C	-4.533270000	-1.819551000	2.836071000
C	-3.507821000	-2.179723000	3.721478000
C	-2.174338000	-2.234459000	3.305000000
C	-1.831735000	-1.915634000	1.983140000
C	-2.798086000	-1.121935000	-0.351004000
H	-5.567141000	-1.784218000	3.163988000
H	-3.759289000	-2.424381000	4.748561000
H	-1.400702000	-2.523959000	4.008180000
H	-0.792757000	-1.953910000	1.668572000
N	-5.018300000	-1.174798000	0.449482000
H	-6.027528000	-1.251424000	0.458910000
C	-4.317070000	-1.103906000	-0.718747000
O	-4.736561000	-1.108989000	-1.863039000
C	-2.076884000	0.990840000	-1.813131000
C	-1.470001000	2.230203000	-1.473960000
C	-1.212439000	3.231418000	-2.418208000
C	-1.586800000	2.978179000	-3.731592000
C	-2.203641000	1.760711000	-4.092767000
C	-2.451908000	0.766887000	-3.153924000
C	-2.131691000	0.211853000	-0.579379000
H	-0.745294000	4.167846000	-2.131505000
H	-1.411490000	3.732572000	-4.491889000
H	-2.502707000	1.604243000	-5.124339000
H	-2.965930000	-0.140925000	-3.447434000
H	-0.205952000	-0.208335000	-0.839574000
N	-1.213707000	2.217213000	-0.111815000
H	-0.724420000	2.942062000	0.408454000
C	-1.611721000	1.033663000	0.422546000
H	-1.500295000	0.840551000	1.479211000
O	-2.231590000	-2.145344000	-1.251208000

H	-2.818947000	-2.197205000	-2.031399000
C	1.306157000	2.410011000	2.622218000
C	2.280364000	2.263771000	1.588899000
C	2.450482000	3.223590000	0.581933000
C	1.631628000	4.348950000	0.617129000
C	0.659013000	4.516582000	1.631556000
C	0.491243000	3.559725000	2.631131000
C	1.431496000	1.261221000	3.476616000
H	3.207180000	3.105966000	-0.188095000
H	1.755731000	5.122728000	-0.134517000
H	0.057997000	5.421199000	1.647357000
H	-0.240328000	3.711068000	3.420249000
H	0.872169000	1.053946000	4.378069000
N	2.950022000	1.080506000	1.817375000
H	3.705056000	0.704872000	1.255441000
C	2.441529000	0.487888000	2.956507000
H	2.862691000	-0.436707000	3.325873000

F

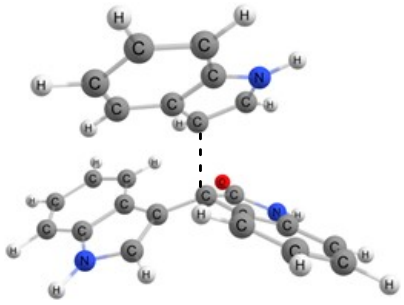


Zero-point correction=	0.364336 (Hartree/Particle)
Thermal correction to Energy=	0.386536
Thermal correction to Enthalpy=	0.387480
Thermal correction to Gibbs Free Energy=	0.309434
Sum of electronic and zero-point Energies=	-1164.372850
Sum of electronic and thermal Energies=	-1164.350651
Sum of electronic and thermal Enthalpies=	-1164.349706
Sum of electronic and thermal Free Energies=	-1164.427753

C	-1.262346000	1.271903000	0.811804000
C	-1.953292000	2.396567000	0.272259000
C	-3.270929000	2.684032000	0.602947000
C	-3.924654000	1.806774000	1.474923000
C	-3.289141000	0.656358000	1.976873000
C	-1.970076000	0.376611000	1.641169000
C	0.081721000	1.297916000	0.302145000
H	-3.778665000	3.553993000	0.199876000
H	-4.954437000	2.009750000	1.752489000
H	-3.840422000	-0.026381000	2.614042000
H	-1.520949000	-0.550485000	1.977056000
N	-1.109874000	3.082700000	-0.590466000
H	-1.348990000	3.896645000	-1.139778000
C	0.122767000	2.463587000	-0.691057000
O	1.037075000	2.829449000	-1.403161000
C	2.576134000	0.467230000	0.183435000
C	3.292065000	-0.358406000	1.082305000
C	4.619322000	-0.733523000	0.911472000
C	5.264702000	-0.256332000	-0.232141000
C	4.584005000	0.556069000	-1.149685000
C	3.248065000	0.925564000	-0.959561000
C	1.209212000	0.587477000	0.719714000
H	5.131225000	-1.369110000	1.627202000
H	6.302011000	-0.519988000	-0.409566000
H	5.106826000	0.915966000	-2.029806000
H	2.750035000	1.571474000	-1.667854000
N	2.419358000	-0.706545000	2.125712000
H	2.679734000	-1.253058000	2.937726000
C	1.212570000	-0.186825000	1.923464000
H	0.428991000	-0.303342000	2.655402000
C	-0.682087000	-1.851161000	-1.150374000
C	-2.097737000	-2.001207000	-1.163703000

C	-2.763748000	-2.919147000	-0.347317000
C	-1.987268000	-3.695965000	0.511993000
C	-0.583909000	-3.561836000	0.550797000
C	0.076019000	-2.650061000	-0.272419000
C	-0.358706000	-0.840360000	-2.117306000
H	-3.843052000	-3.034381000	-0.383169000
H	-2.470976000	-4.428757000	1.150168000
H	-0.009802000	-4.203928000	1.212313000
H	1.160556000	-2.587885000	-0.271529000
H	0.625010000	-0.500697000	-2.407951000
N	-2.592908000	-1.109404000	-2.102029000
H	-3.560909000	-1.025427000	-2.373832000
C	-1.549304000	-0.425878000	-2.679535000
H	-1.729130000	0.296457000	-3.463217000

TS3



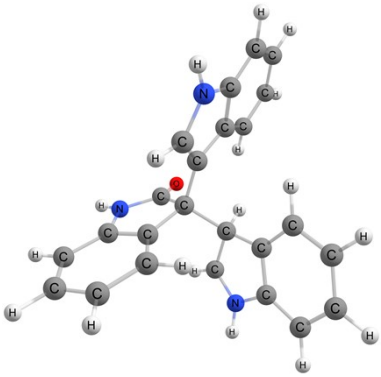
Zero-point correction=	0.365410 (Hartree/Particle)
Thermal correction to Energy=	0.386044
Thermal correction to Enthalpy=	0.386988
Thermal correction to Gibbs Free Energy=	0.315781
Sum of electronic and zero-point Energies=	-1164.359438
Sum of electronic and thermal Energies=	-1164.338803
Sum of electronic and thermal Enthalpies=	-1164.337859
Sum of electronic and thermal Free Energies=	-1164.409066

C	1.350964000	-1.124828000	0.580129000
C	1.918896000	-2.337762000	0.135669000
C	3.114758000	-2.826468000	0.646240000
C	3.764928000	-2.058714000	1.622108000

C	3.235745000	-0.838430000	2.057668000
C	2.026978000	-0.362067000	1.535079000
C	0.071017000	-0.921818000	-0.142997000
H	3.531599000	-3.769971000	0.308540000
H	4.698747000	-2.419084000	2.042070000
H	3.766123000	-0.256040000	2.803677000
H	1.636152000	0.597073000	1.858451000
N	1.100524000	-2.894895000	-0.854751000
H	1.274513000	-3.759807000	-1.349453000
C	-0.004289000	-2.114808000	-1.122714000
O	-0.837483000	-2.328465000	-1.982919000
C	-2.502643000	-0.374489000	0.087647000
C	-3.276910000	0.021949000	1.208104000
C	-4.643211000	0.294036000	1.141044000
C	-5.254061000	0.169094000	-0.104885000
C	-4.514225000	-0.222171000	-1.235535000
C	-3.150556000	-0.500238000	-1.155659000
C	-1.132925000	-0.540762000	0.565720000
H	-5.207999000	0.589894000	2.019784000
H	-6.316106000	0.369648000	-0.201363000
H	-5.020033000	-0.326240000	-2.190046000
H	-2.614724000	-0.854299000	-2.026757000
N	-2.423944000	0.075257000	2.309005000
H	-2.711640000	0.268109000	3.258202000
C	-1.164759000	-0.245458000	1.935645000
H	-0.369298000	-0.298272000	2.662608000
C	0.643556000	1.791986000	-0.820079000
C	2.015484000	2.049289000	-1.020178000
C	2.684136000	3.131517000	-0.456513000
C	1.921789000	3.989139000	0.340446000
C	0.550895000	3.760743000	0.550886000
C	-0.101935000	2.664631000	-0.021793000

C	0.319651000	0.550971000	-1.531378000
H	3.740253000	3.312166000	-0.629811000
H	2.395488000	4.853230000	0.794577000
H	-0.013447000	4.458971000	1.160747000
H	-1.164690000	2.510083000	0.130327000
H	-0.646034000	0.355108000	-1.983738000
N	2.498892000	1.047864000	-1.885158000
H	3.457493000	0.973840000	-2.204090000
C	1.517591000	0.215762000	-2.236236000
H	1.689918000	-0.600900000	-2.924561000

G



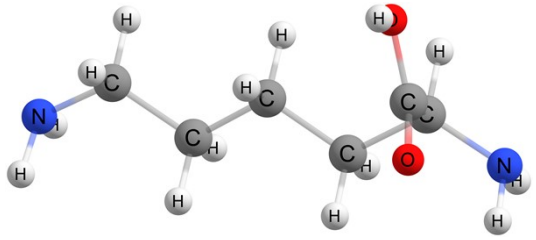
Zero-point correction=	0.366694 (Hartree/Particle)
Thermal correction to Energy=	0.387503
Thermal correction to Enthalpy=	0.388447
Thermal correction to Gibbs Free Energy=	0.316716
Sum of electronic and zero-point Energies=	-1164.366563
Sum of electronic and thermal Energies=	-1164.345754
Sum of electronic and thermal Enthalpies=	-1164.344809
Sum of electronic and thermal Free Energies=	-1164.416540

C	1.480575000	-1.178818000	0.353580000
C	1.871460000	-2.440628000	-0.127094000
C	2.948097000	-3.136858000	0.410520000
C	3.654391000	-2.530803000	1.458081000
C	3.288972000	-1.271504000	1.943595000
C	2.191971000	-0.589609000	1.394760000

C	0.247129000	-0.725027000	-0.414380000
H	3.235085000	-4.114179000	0.035520000
H	4.498916000	-3.052022000	1.897658000
H	3.851035000	-0.821844000	2.755534000
H	1.901041000	0.379459000	1.788851000
N	1.036959000	-2.813789000	-1.194519000
H	1.132650000	-3.654671000	-1.749031000
C	0.135318000	-1.830055000	-1.517230000
O	-0.582883000	-1.793613000	-2.500319000
C	-2.368494000	-0.421488000	-0.003824000
C	-3.175290000	-0.471874000	1.166207000
C	-4.554707000	-0.242560000	1.149295000
C	-5.139167000	0.047580000	-0.078926000
C	-4.367084000	0.092892000	-1.257703000
C	-2.996913000	-0.145969000	-1.236839000
C	-1.007558000	-0.696578000	0.421574000
H	-5.147890000	-0.293796000	2.057400000
H	-6.207940000	0.228358000	-0.132265000
H	-4.856864000	0.297184000	-2.204498000
H	-2.440381000	-0.175827000	-2.166277000
N	-2.344251000	-0.777717000	2.231620000
H	-2.645097000	-0.925154000	3.183379000
C	-1.056671000	-0.912183000	1.787594000
H	-0.260515000	-1.158235000	2.473507000
C	0.584878000	1.922008000	-0.376883000
C	1.792448000	2.539743000	-0.736284000
C	2.254183000	3.734719000	-0.197691000
C	1.432954000	4.333226000	0.761387000
C	0.213872000	3.746535000	1.133913000
C	-0.227250000	2.541906000	0.569777000
C	0.433450000	0.661461000	-1.193438000
H	3.192220000	4.186589000	-0.503781000

H	1.739939000	5.268935000	1.216332000
H	-0.407072000	4.243099000	1.872559000
H	-1.178987000	2.110875000	0.856699000
H	-0.435238000	0.704473000	-1.870835000
N	2.394888000	1.729606000	-1.736180000
H	3.286781000	1.940069000	-2.176591000
C	1.666396000	0.683438000	-2.021530000
H	1.974471000	-0.038449000	-2.768818000

LYS -H (Deprotonated)

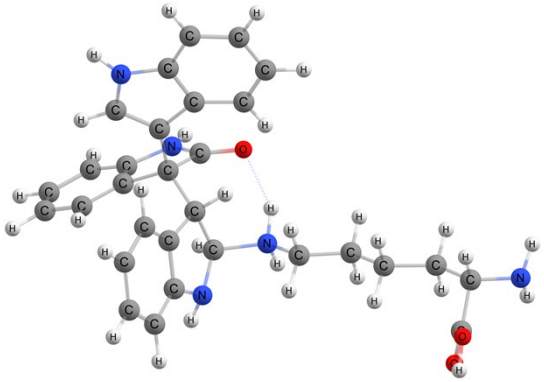


Zero-point correction=	0.210954 (Hartree/Particle)
Thermal correction to Energy=	0.223155
Thermal correction to Enthalpy=	0.224100
Thermal correction to Gibbs Free Energy=	0.171361
Sum of electronic and zero-point Energies=	-496.864625
Sum of electronic and thermal Energies=	-496.852424
Sum of electronic and thermal Enthalpies=	-496.851480
Sum of electronic and thermal Free Energies=	-496.904218

N	-2.769690000	1.620407000	-0.176488000
H	-2.945554000	1.651789000	0.825397000
C	-1.730555000	0.631710000	-0.473426000
H	-1.676952000	0.504990000	-1.559797000
C	-0.321252000	0.990400000	0.064115000
C	-2.195509000	-0.686628000	0.131349000
H	-0.075047000	1.984552000	-0.333849000
H	-0.385969000	1.093531000	1.155359000
C	0.795254000	0.005119000	-0.309126000
O	-2.598778000	-0.812085000	1.269179000
H	0.579012000	-0.982934000	0.118756000

H	0.810773000	-0.132702000	-1.399547000
C	2.181053000	0.464277000	0.166165000
H	2.411951000	1.448506000	-0.267611000
H	2.168259000	0.602921000	1.257138000
C	3.304548000	-0.520339000	-0.200747000
H	3.081867000	-1.504487000	0.231024000
H	3.324037000	-0.661962000	-1.289013000
N	4.657475000	-0.148551000	0.221198000
H	4.711882000	-0.049386000	1.231809000
H	4.936859000	0.740895000	-0.184939000
H	-2.478723000	2.546113000	-0.478118000
O	-2.087825000	-1.728878000	-0.724294000
H	-2.385302000	-2.524338000	-0.248631000

H



Zero-point correction=	0.584137 (Hartree/Particle)
Thermal correction to Energy=	0.617454
Thermal correction to Enthalpy=	0.618399
Thermal correction to Gibbs Free Energy=	0.515062
Sum of electronic and zero-point Energies=	-1661.255577
Sum of electronic and thermal Energies=	-1661.222260
Sum of electronic and thermal Enthalpies=	-1661.221316
Sum of electronic and thermal Free Energies=	-1661.324653

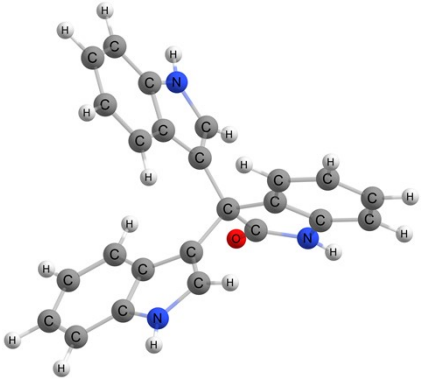
C	-3.416570000	-1.007086000	-0.806511000
C	-3.777024000	-0.995310000	-2.164156000
C	-4.838227000	-1.736333000	-2.666605000
C	-5.552193000	-2.532735000	-1.760247000

C	-5.203127000	-2.573373000	-0.407502000
C	-4.135703000	-1.802970000	0.080577000
C	-2.278941000	-0.012895000	-0.592511000
H	-5.105737000	-1.707630000	-3.718253000
H	-6.385916000	-3.127438000	-2.119768000
H	-5.764523000	-3.203234000	0.274890000
H	-3.879834000	-1.830450000	1.134263000
N	-2.878793000	-0.167008000	-2.873845000
H	-2.844133000	-0.072788000	-3.881102000
C	-1.882296000	0.291184000	-2.069601000
O	-0.815727000	0.782444000	-2.455406000
C	-2.062874000	2.521021000	0.252705000
C	-2.951788000	3.395727000	0.938134000
C	-2.599181000	4.696141000	1.316630000
C	-1.320938000	5.134196000	0.993187000
C	-0.423306000	4.297345000	0.297550000
C	-0.779799000	3.007335000	-0.077683000
C	-2.783089000	1.276189000	0.047812000
H	-3.299657000	5.340697000	1.839279000
H	-1.013327000	6.137789000	1.268905000
H	0.559975000	4.676923000	0.037111000
H	-0.091954000	2.406341000	-0.661076000
N	-4.143119000	2.718829000	1.118040000
H	-4.969405000	3.095579000	1.556918000
C	-4.042833000	1.460268000	0.580748000
H	-4.878253000	0.778251000	0.621667000
C	-1.133120000	-1.135818000	1.521285000
C	-0.513762000	-2.390157000	1.548398000
C	-0.460855000	-3.163814000	2.704212000
C	-1.049947000	-2.642980000	3.862308000
C	-1.646909000	-1.377133000	3.860403000
C	-1.682954000	-0.609299000	2.689579000

C	-0.997375000	-0.537427000	0.136097000
H	0.025830000	-4.134293000	2.713033000
H	-1.027819000	-3.226420000	4.777395000
H	-2.080036000	-0.983983000	4.774342000
H	-2.138655000	0.374736000	2.690787000
H	-0.331945000	0.329837000	0.186391000
N	0.059390000	-2.709433000	0.283369000
H	-0.071534000	-3.662358000	-0.036266000
C	-0.280521000	-1.677341000	-0.651247000
H	-0.882225000	-2.052155000	-1.486136000
N	8.232774000	1.112622000	-1.204931000
H	8.441989000	0.427306000	-1.925970000
C	7.047362000	0.738600000	-0.432291000
H	6.828944000	1.566998000	0.249444000
C	5.800088000	0.400049000	-1.273143000
C	7.469956000	-0.464433000	0.414519000
H	5.591166000	1.261198000	-1.920919000
H	6.049305000	-0.446643000	-1.924631000
C	4.554953000	0.060211000	-0.440373000
O	7.517020000	-1.605303000	0.000188000
H	4.780819000	-0.778984000	0.229429000
H	4.289296000	0.914360000	0.197192000
C	3.351117000	-0.316798000	-1.319002000
H	3.094620000	0.522740000	-1.978633000
H	3.632723000	-1.160091000	-1.965449000
C	2.138818000	-0.704982000	-0.473326000
H	2.344948000	-1.560349000	0.172778000
H	1.801148000	0.127196000	0.147466000
N	0.979075000	-1.105871000	-1.353092000
H	1.318827000	-1.798686000	-2.026392000
H	0.626359000	-0.291571000	-1.899242000
H	8.129667000	2.025323000	-1.636641000

O	7.807358000	-0.121764000	1.673007000
H	8.141055000	-0.919465000	2.120440000

3a



Zero-point correction=	0.353568 (Hartree/Particle)
Thermal correction to Energy=	0.374604
Thermal correction to Enthalpy=	0.375548
Thermal correction to Gibbs Free Energy=	0.303465
Sum of electronic and zero-point Energies=	-1164.015607
Sum of electronic and thermal Energies=	-1163.994572
Sum of electronic and thermal Enthalpies=	-1163.993628
Sum of electronic and thermal Free Energies=	-1164.065711

C	-2.099061000	-0.353980000	-0.240443000
C	-3.009442000	-1.130481000	0.493337000
C	-4.331555000	-1.302248000	0.095258000
C	-4.745357000	-0.659772000	-1.079617000
C	-3.858351000	0.130389000	-1.816084000
C	-2.527719000	0.287614000	-1.395647000
C	-0.733008000	-0.377723000	0.453959000
H	-5.022740000	-1.906352000	0.675668000
H	-5.772273000	-0.774102000	-1.414119000
H	-4.200007000	0.631077000	-2.716731000
H	-1.846849000	0.912584000	-1.963985000
N	-2.370808000	-1.636539000	1.631937000
H	-2.807229000	-2.194798000	2.352133000
C	-1.071457000	-1.189543000	1.753985000
O	-0.343883000	-1.409249000	2.705798000

C	1.676257000	-1.423905000	0.000731000
C	2.216853000	-2.252560000	-1.020456000
C	3.552180000	-2.674283000	-1.022926000
C	4.357660000	-2.253808000	0.029860000
C	3.842023000	-1.437301000	1.059940000
C	2.515794000	-1.021817000	1.057414000
C	0.287080000	-1.192284000	-0.336248000
H	3.944092000	-3.306870000	-1.814758000
H	5.398658000	-2.562086000	0.061730000
H	4.495589000	-1.133341000	1.872327000
H	2.123348000	-0.413187000	1.863240000
N	1.200408000	-2.516009000	-1.918969000
H	1.285855000	-3.073185000	-2.753718000
C	0.046864000	-1.881068000	-1.503404000
H	-0.863098000	-1.963185000	-2.078713000
C	0.369300000	1.981990000	-0.083640000
C	0.598296000	3.161748000	0.679262000
C	1.178724000	4.313076000	0.134216000
C	1.541256000	4.277560000	-1.208184000
C	1.334140000	3.117765000	-1.985353000
C	0.757405000	1.976858000	-1.438408000
C	-0.234084000	1.013844000	0.807343000
H	1.342972000	5.201772000	0.737487000
H	1.995547000	5.152954000	-1.662790000
H	1.639759000	3.115586000	-3.027571000
H	0.627121000	1.086194000	-2.043887000
N	0.154777000	2.913309000	1.962618000
H	0.233271000	3.546363000	2.742176000
C	-0.333638000	1.623777000	2.035686000
H	-0.694550000	1.226164000	2.972549000

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