Synthesis of Dimeric Indoles from Friedel–Crafts Reaction of Indoles with Ketones Catalysed by a Bronsted Acid Ionic Liquid and Their Interactions with BSA and DNA

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Experimental Section

Materials and Methods

Indole, substituted indoles, isatin, substituted isatins, Acenaphthoquinone, Phenanthrenequinone, cyclohexanone, dibromo alkanes, imidazole, and 2-chloro acetic acid, were acquired from Sigma-Aldrich, and all organic solvents were developed from commercial suppliers and used without any further purification. Analytical thin-layer chromatography (TLC) was performed using 0.25-mm silica gel-coated Kieselgel 60 F254 plates. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra were recorded on a Bruker AVANCE III 400 MHz spectrometer. Chemical shifts and coupling constants are stated in parts per million (ppm) and Hertz (Hz) respectively using tetra-methyl silane (TMS) as an internal standard and the solvent resonance at (DMSO-d_6: ^{1}H NMR 400 MHz and ^{13}C NMR 100 MHz): δ 2.49 and 39.7 ppm; The peak multiplicities are denoted as s (singlet), d (doublet), dd (doublet of doublet), m (multiplet), dt (doublet of triplet), and t (triplet). The FT-IR spectra were recorded utilising the Perkin-Elmer RX-I FTIR spectrometer in ATR mode. The UV-Vis absorption spectra were acquired using the JASCO V-670 spectrophotometer, operating at room temperature, with the solvent being DMSO and acetonitrile. JASCO fluorescence spectrophotometer (FP8200) equipped with a xenon and helium lamp using 1 cm quartz cell was utilized to measure emission fluorescence spectra by excitation at their respective absorption maxima.

General Procedure for the Synthesis of ***1,3-bis(carboxymethyl)imidazolium chloride*** [BCMIM][Cl] ionic liquid **4**.[1,2]

1 equivalent (5.0 g) of imidazole **1** was reacted with 2 equivalents (13.9 g) of chloroacetic acid **2** in the presence of 1.2 equivalents (3.6 g) of NaOH in acetonitrile under reflux conditions for a duration of 18 hours, resulting in the formation of **3**. Subsequently, the crude ionic liquid **3** was subjected to a reaction with cold concentrated hydrochloric acid at ambient temperature for a period of 24 h. The precipitate obtained was filtered and subjected to thorough washing using acetonitrile (3 X 30 mL). The concentration of the cumulative filtrates, followed by dichloromethane and ether wash yielded the desired 1,3-bis(carboxymethyl)imidazolium chloride [BCMIM][Cl] ionic liquid **4** as white solid with 95% yield (14.9 g). The formed product was further characterized by ^{1}H, ^{13}C NMR and FT-IR spectral techniques.

Representative General Procedure for the Synthesis of ***1H,1''H-[3,3':3',3''-terindol]-2'(1'H)-one*** **7aa**.

To a dried 25-mL round bottom flask, indole **5a** (0.24 g, 2 equiv, 2.04 mmol), isatin **6a** (0.15 g, 1 equiv, 1.02 mmol), and 4 mol% of [BCMIM][Cl] ionic liquid **4** were sequentially added to 5 mL of aqueous ethanol (1:1 *v/v*) and stirred at 80 ºC under reflux conditions for 30 min. The progress of reaction was scrutinized by TLC. After, the completion of the reaction the resultant solid precipitate was filtered out and then washed with ether (10 mL X 2) and hexane without any additional column chromatography to obtain the desired product **7aa** in 95% yield (0.35 g). The furnished products were subjected to characterization using ^{1}H NMR, ^{13}C NMR, FT-IR and HRMS spectra techniques and were found to be similar to those reported in the literature.

Representative General Procedure for the Synthesis of ***1',1''''-(propane-1,3-diyl)bis(([3,3':3',3''-terindolin]-2'-one))*** **10aa**.

To a dried 25-mL round bottom flask, indole **5a** (0.21 g, 4 equiv, 1.79 mmol), bis-isatin **9a** (0.15 g, 1 equiv, 0.45 mmol), and 4 mol% of [BCMIM][Cl] ionic liquid **4** were sequentially added to 5 mL of aqueous ethanol (1:1 *v/v*) and stirred at 80 ºC under reflux conditions for 1.5 h. The progress of reaction was scrutinized by TLC. After, the completion of the reaction the resultant solid precipitate was filtered out and then washed with ether (10 mL X 2) and hexane without any additional column chromatography to obtain the desired product **10aa** in 94% yield (0.32 g). The furnished products were subjected to characterization using ^{1}H NMR, ^{13}C NMR, FT-IR and HRMS spectra techniques.

General information

UV-Vis and FL studies

The molar extinction coefficient (ε) was estimated using Beer-Lambert's law using equation 1.

$$A = \varepsilon cl \qquad \ldots\ldots\ldots\ldots \text{(eqn. i)}$$

where, A - absorbance*, ε - molar adsorption coefficient, c - concentration of the sample, and l - distance travelled by the light through the sample.*

The Stoke's Shift was determined using the following equation (ii):

$$\Delta\bar{\upsilon} = 10^{7} / \lambda_{\max(\text{absorption})} - 10^{7} / \lambda_{\max(\text{emission})} \qquad \ldots\ldots\ldots \text{(eqn. ii)}$$

Computational details

Calculations employing density functional theory (DFT) were executed to gain insight into both the structural and functional characteristics. The computations were carried out using Gaussian 16W software, employing the density functional theory (DFT) methodology.[3] The configurations of compounds in the gaseous phase were refined utilizing Becke's three-parameter and Lee–Yang–Parr functional (B3LYP).[4] Throughout all computations, the B3LYP functional was coupled with the 6-31G (d, p) basis set.[5] TD-DFT single-point calculations were performed at the B3LYP/6-31G (d, p) level of theory on the optimized configurations in the gaseous phase. The molecular visualization tool Gauss View 6.1 facilitated the determination of electronic structures and frontier molecular orbital architectures.[6]

Molecular docking studies with protein BSA

To investigate binding interactions and affinities, the 3D structures of the produced derivatives 7 were docked with the BSA protein target. This study made use of MGL TOOL 1.5.7 and the AutoDock Vina algorithm (ADT).[7] The crystal structure of BSA (PDB ID 4F5S) was acquired from the Protein Data Bank (www.rcsb.org/pdb).[8,9] After obtaining the protein, Gasteiger charges and polar hydrogens were included, while water molecules were removed to avoid unwanted interactions. In addition, we performed optimization of rotatable bonds. The ligands, which were optimized using Gaussian 6.1, were saved in PDB format. AutoDock Tools were subsequently utilized to create distinct files for the protein and ligands. A binding site was delineated by constructing a grid box around the active residue sites of the protein, with a spacing of 0.375 Å. The grid dimensions were set to 80 × 80 × 80 points, with coordinates established at 72.821, 26.360, and 91.719 Å in the X, Y, and Z directions, respectively. The files were converted to pdbqt format in the last stage. By employing an exhaustiveness value of eight, AutoDock produced a total of nine significant conformers for each ligand and protein separately. The orientation of each conformer was evaluated using PyMOL, a molecular graphics application (The PyMOL Molecular Graphics System, Version 2.0, Schrödinger, LLC). The most favorable binding configuration was selected for each docking situation, based on the docked conformation with the lowest energy as calculated by the AutoDock scoring technique. In addition, BIOVIA DSV was used to improve the imaging of the docked ligand complexes for the investigation of numerous molecular interactions.[10]

Molecular docking studies with DNA

The binding affinities of the synthesized derivatives **7** for DNA were predicted by performing molecular docking using AUTODOCK 4.2 and MGL TOOL 1.5.7. The DNA structure with the PDB id 1BNA was obtained from the Protein Data Bank (www.rcsb.org/pdb) at a resolution of 1.60 Å.[11] The water molecules were removed and Gasteiger charges were incorporated. The synthesized derivatives **7** were generated using ChemDraw 21.0.0 and then converted to PDB format using openbabel. Later, the target (DNA) and ligands were created using AutoDock Tools to generate the necessary files. Subsequently, the ligands were positioned into the DNA constructs using certain grid parameters located at their centers. A total of fifty orientations were produced for each ligand. The results, which include the surface analyses of the graphical representations, are displayed using PyMOL (PyMOL Molecular Graphics System, Version 1.3, Schrodinger, LLC). The binding mode chosen for each docking scenario was the docked conformation with the lowest energy, as determined by the Autodock scoring system.

Protein binding studies

Most proteins found in blood plasma are serum albumin proteins, which play a critical role in the transportation and metabolism of drugs. The ligands' interactions with BSA were investigated by intrinsic tryptophan emission quenching assays. The emission intensity of BSA at a wavelength of 342 nm drops gradually as the concentration of ligands increases, providing evidence that the ligands are interacting with BSA. The ligand solutions were gradually introduced into a solution of BSA (2 μM) in a 5 mM Tris–HCl/NaCl buffer (pH 7.2). The reduction in the emission signals at 342 nm (λ_{ex} = 295 nm) was then measured. The quenching constant (K_{BSA}) was determined by applying the Stern-Volmer equation. The Stern-Volmer plots were constructed by plotting the ratio of I_0/I against the concentration of the ligand. The corrected fluorescence data was used, considering the impact of dilution. The data were linearly fitted using equation (iii):

$$I_0/I = 1 + K_{BSA}[Q] = 1 + K_q\tau_0[Q] \qquad \text{.....eqn (iii)}$$

where, $\mathbf{I_0}$ and **I** - emission intensities of BSA in absence and presence of quencher with concentration [Q], respectively,

$\boldsymbol{K_q}$ - quenching rate constant, and

$\boldsymbol{\tau_0}$ - average lifetime of tryptophan in BSA without quencher (reported as 1 x 10^{-8} s). The quenching constant (K_{BSA}) was deduced using Origin Pro 2022 software.

For static quenching interactions, the binding constant (K) and the number of binding sites (n) was determined using

the Scatchard equation (iv):[7]

$$\log \frac{I_0 - I}{I} = \log k + n\log[Q] \quad \text{……. eqn (iv)}$$

DNA binding studies

The DNA binding assay was performed by using UV-vis spectroscopy with ligands **7af**, **7ai**, **7aj**, and **7ak**, at concentration 4×10^{-5} M in Tris-HCl buffer (pH 7.2).[12] DNA solution with concentration 2.87×10^{-4} M was prepared. Later, the absorption was recorded by an incremental addition of DNA (20-100 μM) to each ligand. The intrinsic DNA binding constant (K_b) was determined using the equation eq.(v)

$$\frac{[DNA]}{\varepsilon_a - \varepsilon_f} = \frac{[DNA]}{\varepsilon_b - \varepsilon_f} + \frac{[DNA]}{K_b\,(\varepsilon_a - \varepsilon_f)} \quad \text{……. eqn (v)}$$

Where, [DNA] - concentration of DNA in the base pairs, ε_a - apparent extinction coefficient observed for the ligand, ε_b - extinction coefficient of the ligand when fully bound to DNA, ε_f is the extinction of the ligand in its free form. The liner plot data $[DNA]/(\varepsilon_a - \varepsilon_f)$ vs. [DNA] was obtained using Origin Lab version 8.5. The intrinsic binding constant (K_b) value is the ratio of slope to the intercept of the linear fit.

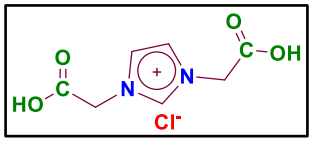
Ethidium bromide displacement assay

The EtBr displacement experiments were conducted to elucidate the binding mechanism between each ligand and DNA.[13] The incorporation of EtBr into DNA results in a strong fluorescence emission because of the generation of EtBr-DNA complex. When the ligand molecule inserts itself between the base pairs of DNA, the amount of binding locations on DNA that are accessible to EtBr reduces, leading to a decrease in the fluorescence intensity. The value of K_{SV} (Stern-Volmer quenching constant) was calculated from the following eq. (vi):

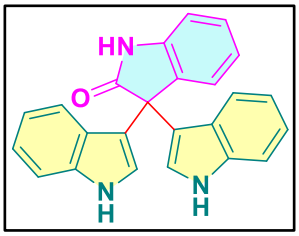
$$I_0/I = 1 + K_{sv}[Q] \quad \text{……. eqn (vi)}$$

where, $\mathbf{I_0}$ and **I** - emission intensities of EtBr-DNA in absence and presence of ligand with concentration [Q], respectively.

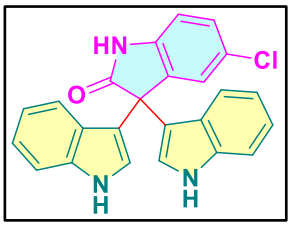
Spectral characterization data



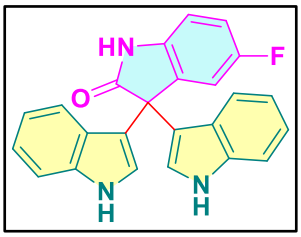
1,3-bis(carboxymethyl)imidazolium chloride [BCMIM][Cl] **4**.[1,2] White **solid**; **Yield**: 95% (14.9011g); **mp (ºC):** 225-227 [226-228];[1,2] **FT-IR (ATR mode, cm^{-1})**: 2869, 1730, 1564, 1403, 1171, 753, 652. **^{1}H NMR (400 MHz, D$_2$O, ppm)** δ 8.93 (s, 1H), 7.56 (d, *J* = 1.4 Hz, 2H), 5.14 (s, 4H). **^{13}C NMR (100 MHz, D$_2$O, ppm)** δ 169.97, 138.21, 123.55, 50.36. **DEPT-135 NMR (100 MHz, D$_2$O, ppm)** δ 138.2, 123.5, 50.4;



1H,1''H-[3,3':3',3''-terindol]-2'(1'H)-one ***7aa***. Beige-cream **solid**; **Yield**: 95%; **mp (ºC)**: >300 [312];[14,15] **FT-IR (ATR, cm^{-1})**: 3381, 3312, 1705, 1614, 1467, 1247, 1173, 738, 608, 553; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** δ 10.86 (s, 2H), 10.50 (s, 1H), 7.28 (d, *J* = 8.1 Hz, 2H), 7.16 (d, *J* = 7.8 Hz, 4H), 6.96 – 6.91 (m, 3H), 6.85 (t, *J* = 7.5 Hz, 1H), 6.78 (s, 2H), 6.72 (t, *J* = 7.5 Hz, 2H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** δ 179.2, 141.8, 137.4, 135.1, 128.3, 126.18, 125.4, 124.7, 121.9, 121.4, 121.2, 118.7, 114.8, 112.1, 110.0, 53.0.

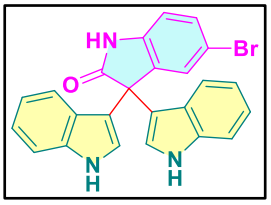


5'-chloro-1H,1''H-[3,3':3',3''-terindol]-2'(1'H)-one ***7ab***. Peachy-pink **solid**; **Yield**: 94%; **mp (ºC)**: 293-295 [294-296];[16] **FT-IR (ATR, cm^{-1})**:3347, 1700, 1476, 1171, 1104, 734, 642, 550, 491, 426; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** δ 10.99 (s, 1H), 8.36 (d, *J* = 8.1 Hz, 1H), 8.02 – 7.99 (m, 2H), 7.90 (t, *J* = 7.5 Hz, 1H), 7.70 (t, *J* = 7.6 Hz, 1H), 7.55 (d, *J* = 6.9 Hz, 1H), 7.35 (d, *J* = 8.1 Hz, 2H), 7.02 – 6.98 (m, 4H), 6.85 (d, *J* = 2.0 Hz, 2H), 6.74 (t, *J* = 7.5 Hz, 2H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** δ 203.1, 144.3, 140.1, 137.4, 132.5, 131.9, 130.9, 129.5, 129.3, 126.2, 125.1, 124.6, 122.7, 122.2, 121.3, 121.1, 118.8, 115.3, 114.9, 112.1, 58.1.

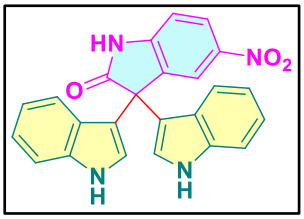


5'-fluoro-1H,1''H-[3,3':3',3''-terindol]-2'(1'H)-one ***7ac***. Off-white **solid**; **Yield**: 95%; **mp (ºC)**: 291-293 [289-290];[17] **FT-IR (ATR, cm^{-1})**: 3436, 3387, 3315, 1695, 1480, 1173, 734, 677, 575, 505, 428;**^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** δ 11.01 (d, *J* = 1.5 Hz, 2H), 10.64 (s, 1H), 7.37 (d, *J* = 8.1 Hz, 2H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.11 – 6.97 (m, 6H), 6.90 (d, J = 2.4 Hz, 2H), 6.82 (t, *J* = 7.4 Hz, 2H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** δ 179.1, 158.3 (d, $J_{C\text{-}F}$ = 231.6 Hz, *ipso*-C), 138.0, 137.4, 136.8 (d, $J_{C\text{-}F}$ = 8.3

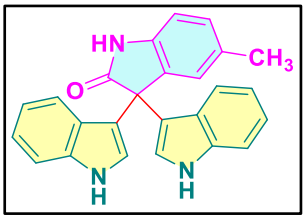
Hz), 126.0, 124.9, 121.5, 121.1, 118.8, 114.7 (d, $J_{C\text{-}F}$ = 23.7 Hz), 114.1, 112.9 (d, $J_{C\text{-}F}$ = 24.7 Hz), 112.1, 110.8 (d, $J_{C\text{-}F}$ = 7.9 Hz), 53.6.



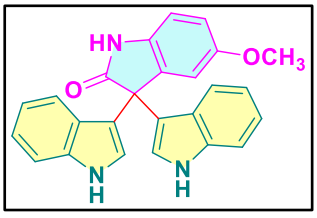
5'-bromo-1H,1''H-[3,3':3',3''-terindol]-2'(1'H)-one ***7ad***. Beige-cream **solid**; **Yield**: 93%**; mp (°C)**: >300 [310-312];[14] **FT-IR (ATR, cm^{-1})**: 3353, 1690, 1472, 1104, 814, 737, 637, 547, 491, 427; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** δ 11.03 (d, *J* = 1.7 Hz, 2H), 10.77 (s, 1H), 7.44 – 7.42 (m, 1H), 7.38 (d, *J* = 8.1 Hz, 2H), 7.31 (d, *J* = 1.8 Hz, 1H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.04 (t, *J* = 7.3 Hz, 2H), 6.98 (d, *J* = 8.3 Hz, 1H), 6.90 (d, *J* = 2.5 Hz, 2H), 6.83 (t, *J* = 7.5 Hz, 2H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** δ 178.7, 141.2, 137.5, 137.4, 131.2, 127.8, 125.9, 124.9, 121.6, 120.9, 118.9, 113.9, 113.6, 112.2, 112.2, 53.3.



5'-nitro-1H,1''H-[3,3':3',3''-terindol]-2'(1'H)-one ***7ae***. Coral-red **solid**; **Yield**: 94%; **mp (°C)**: >300 [293-295];[18] **FT-IR (ATR, cm^{-1})**: 3382, 1706, 1619, 1533, 1340, 1090, 832, 744, 546; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** δ 11.34 (s, 1H), 11.10 (s, 2H), 8.25 (dd, *J* = 8.6, 2.2 Hz, 1H), 7.98 (d, *J* = 2.1 Hz, 1H), 7.39 (d, *J* = 8.1 Hz, 2H), 7.24 – 7.20 (m, 3H), 7.05 (t, *J* = 7.5 Hz, 2H), 6.97 (d, *J* = 2.2 Hz, 2H), 6.84 (t, *J* = 7.5 Hz, 2H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** δ 179.4, 148.3, 142.7, 137.5, 135.7, 125.9, 125.9, 125.1, 121.7, 120.8, 120.6, 119.0, 113.3, 112.3, 110.4, 53.0.

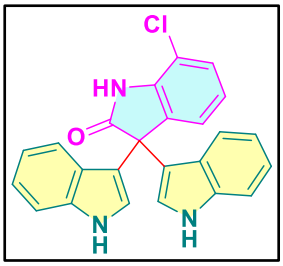


5'-methyl-1H,1''H-[3,3':3',3''-terindol]-2'(1'H)-one ***7af***. Apricot-pink **solid**; **Yield**: 93%; **mp (°C)**: >300 [321-322];[19] **FT-IR (ATR, cm^{-1})**: 3377, 3317, 1704, 1488, 1191, 1101, 737, 574, 425; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** δ 10.94 (d, *J* = 1.8 Hz, 2H), 10.49 (s, 1H), 7.36 (d, *J* = 8.1 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 2H), 7.05 – 7.00 (m, 4H), 6.89 – 6.78 (m, 5H), 2.19 (s, 3H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** δ 179.2, 139.4, 137.4, 135.1, 130.7, 128.6, 126.2, 125.9, 124.8, 121.37, 121.3, 118.7, 114.9, 112.0, 109.8, 53.1, 21.3.

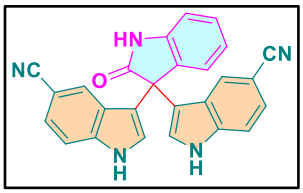


5'-methoxy-1H,1''H-[3,3':3',3''-terindol]-2'(1'H)-one ***7ag***. Light-brown **solid**; **Yield**: 93%; **mp (°C)**: 292-294 [301-303];[18,20] **FT-IR (ATR, cm^{-1})**: 3359, 1685, 1487, 1199, 1016, 787, 740, 590, 424; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** δ 10.95 (s, 2H), 10.44 (s, 1H), 7.35 (d, *J* = 8.1 Hz, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.02 (t, *J* = 7.5 Hz, 2H), 6.92 – 6.87(m, 3H), 6.82 – 6.79 (m, 4H), 3.61 (s, 3H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** δ 179.1, 155.1,

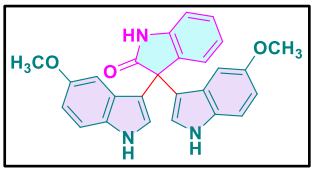
137.4, 136.4, 135.2, 126.1, 124.8, 121.4, 121.2, 118.7, 114.7, 112.6, 112.5, 112.1, 110.3, 55.8, 53.5.



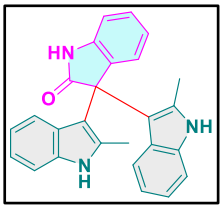
7'-chloro-1H,1''H-[3,3':3',3''-terindol]-2'(1'H)-one ***7ah***. Pale-pink **solid**; **Yield**: 92%; **mp (ºC)**: 290-292 [288-289];[21] **FT-IR (ATR, cm^{-1})**: 3414, 1724, 740, 483; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** δ 11.05 (s, 1H), 11.03 (d, *J* = 1.6 Hz, 2H), 7.37 (d, *J* = 8.1 Hz, 2H), 7.32 (d, *J* = 8.1 Hz, 1H), 7.23 7.19 (m, 3H), 7.03 (t, *J* = 7.5 Hz, 2H), 6.97 (t, *J* = 7.8 Hz, 1H), 6.87 (d, *J* = 2.4 Hz, 2H), 6.82 (t, *J* = 7.5 Hz, 2H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** δ 179.1, 155.1, 137.4, 136.4, 135.2, 126.1, 124.8, 121.4, 121.2, 118.7, 114.7, 112.6, 112.5, 112.1, 110.3, 55.8, 53.5.



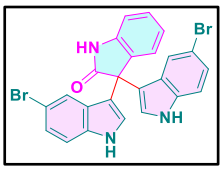
2'-oxo-1',2'-dihydro-1H,1''H-[3,3':3',3''-terindole]-5,5''-dicarbonitrile ***7ba***.Lemom-yellow **solid**; **Yield**: 90%; **mp (ºC)**: >300 [303-305];[22] **FT-IR (ATR, cm^{-1})**:1720, 1600, 1280, 1010, 831, 776, 410; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** 11.66 (d, *J* = 1.5 Hz, 2H), 10.84 (s, 1H), 7.59 – 7.57 (m, 4H), 7.41 (dd, *J* = 8.6, 1.3 Hz, 2H), 7.33 – 7.26 (m, 2H), 7.12 (d, *J* = 2.4 Hz, 2H), 7.08 – 6.99 (m, 2H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** 178.7, 141.6, 139.3, 133.6, 129.0, 127.5, 126.2, 125.7, 125.5, 124.3, 122.6, 121.1, 115.5, 113.9, 110.6, 101.1, 52.5.



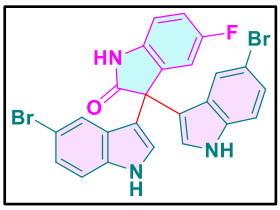
5,5''-dimethoxy-1H,1''H-[3,3':3',3''-terindol]-2'(1'H)-one ***7ca***. Off-white solid **solid**; **Yield**: 88%; **mp (ºC)**: 291-293 [290-293];[23] **FT-IR (ATR, cm^{-1})**: 3386, 3314, 1683, 1474, 1207, 1019, 804, 759, 645; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** 10.80 (d, *J* = 1.6 Hz, 2H), 10.61 (s, 1H), 7.27 – 7.21 (m, 4H), 7.01 (d, *J* = 7.6 Hz, 1H), 6.95 (t, *J* = 7.5 Hz, 1H), 6.87 (d, *J* = 2.4 Hz, 2H), 6.72 – 6.70 (m, 4H), 3.53 (s, 6H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** 179.3, 152.9, 141.9, 135.0, 132.7, 128.3, 126.6, 125.7, 125.4, 121.9, 114.1, 112.6, 110.9, 109.9, 103.8, 55.6, 53.0.



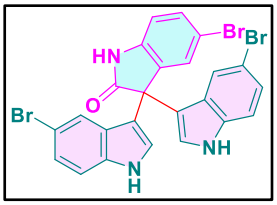
2,2''-dimethyl-1H,1''H-[3,3':3',3''-terindol]-2'(1'H)-one ***7da***. Off-white **solid**; **Yield**: 90%; **mp (ºC)**: 296-298 [286-287];[14,21,24] **FT-IR (ATR, cm^{-1})**: 3394, 1704, 1621, 1471, 1304,1070, 923, 752, 608, 521; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** δ 10.87 (s, 2H), 10.33 (s, 1H), 7.20 – 6.27 (m, 12H), 3.38 (s, 6H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** δ 179.1, 142.0, 135.3, 134.6, 133.9, 129.5, 127.1, 125.4, 122.2, 120.3, 119.6, 118.6, 110.7, 110.1, 109.9, 76.3, 13.8.



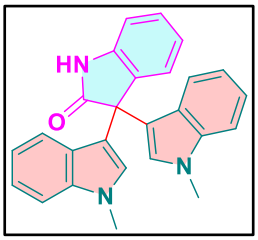
5,5''-dibromo-1H,1''H-[3,3':3',3''-terindol]-2'(1'H)-one ***7ea***. White **solid**; **Yield**: 93%; **mp (°C)**: >300 [320-321];[14,21] **FT-IR (ATR, cm^{-1})**: 3418, 3269, 1713, 1468, 1099, 885, 798, 750, 548, 486; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** δ 11.16 (d, *J* = 1.8 Hz, 2H), 10.67 (s, 1H), 7.30 – 7.28 (m, 4H), 7.22 – 7.18 (m, 1H), 7.11 – 7.07 (m, 3H), 6.96 – 6.90 (m, 2H), 6.84 (d, *J* = 2.5 Hz, 2H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** δ 178.91, 141.68, 136.16, 134.06, 128.74, 127.73, 126.46, 125.35, 124.10, 123.13, 122.30, 114.31, 114.27, 111.53, 110.31, 52.62.



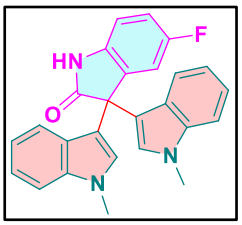
5,5''-dibromo-5'-fluoro-1H,1''H-[3,3':3',3''-terindol]-2'(1'H)-one ***7ec***. White **solid**; **Yield**: 94%; **mp (°C)**: >300 [332-224];[25] **FT-IR (ATR, cm^{-1})**: 3387, 3306, 1690, 1483, 1452, 1174, 885, 793, 588; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** 11.28 (d, *J* = 1.8 Hz, 2H), 10.79 (s, 1H), 7.39 – 7.37 (m, 4H), 7.19 – 7.10 (m, 3H), 7.05 – 6.99 (m, 2H), 6.97 (d, *J* = 2.5 Hz, 2H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** 178.9, 158.45 (d, $J_{C\text{-}F}$ = 238.3 Hz, *ipso*-C), 137.9, 136.2, 135.7 (d, $J_{C\text{-}F}$ = 7.4 Hz), 127.6, 126.6, 124.2, 122.9, 115.2 (d, $J_{C\text{-}F}$ = 23.4 Hz), 114.4, 113.7, 112.9 (d, $J_{C\text{-}F}$ = 24.6 Hz), 111.6, 111.2 (d, $J_{C\text{-}F}$ = 8.5 Hz), 53.1.



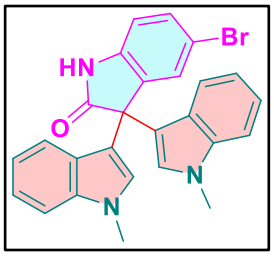
5,5',5''-tribromo-1H,1''H-[3,3':3',3''-terindol]-2'(1'H)-one ***7ed***. Merino-white **solid**; **Yield**: 92%; **mp (°C)**: >300 [>300];[21] **FT-IR (ATR, cm^{-1})**: 3374, 1694, 1453, 1168, 1104, 884, 796, 623, 551, 513. **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** δ 11.29 (d, *J* = 1.9 Hz, 2H), 10.91 (s, 1H), 7.47 (dd, *J* = 8.3, 1.9 Hz, 1H), 7.40 7.36 (m, 4H), 7.26 (d, *J* = 1.8 Hz, 1H), 7.18 (dd, *J* = 8.6, 1.8 Hz, 2H), 7.01 (d, *J* = 8.3 Hz, 1H), 6.96 (d, *J* = 2.5 Hz, 2H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** δ 178.5, 141.1, 136.4, 136.2, 131.6, 127.9, 127.5, 126.7, 124.7, 124.3, 123.3, 122.9, 114.5, 113.9, 113.5, 112.4, 111.7, 52.8.



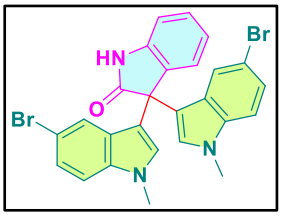
1,1''-dimethyl-1H,1''H-[3,3':3',3''-terindol]-2'(1'H)-one ***7fa***. Biege-white **solid**; **Yield**: 91%; **mp (°C)**: >300 [>300];[20] **FT-IR (ATR, cm^{-1})**: 1697, 1470, 1330, 1208, 735, 681, 633, 427; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** δ 10.64 (s, 1H), 7.38 (d, *J* = 8.2 Hz, 2H), 7.27 – 7.22 (m, 4H), 7.09 (t, *J* = 7.4 Hz, 2H), 7.00 (d, *J* = 7.6 Hz, 1H), 6.95 (d, *J* = 7.4 Hz, 1H), 6.94 – 6.90 (m, 2H), 6.85 (t, *J* = 7.5 Hz, 2H), 3.70 (s, 6H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** δ 179.0, 141.7, 137.8, 134.9, 128.9, 128.4, 126.5, 125.4, 122.1, 121.6, 121.4, 1189, 113.9, 110.2, 110.1, 52.9, 32.8.



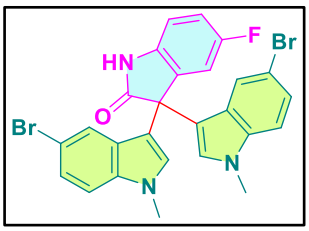
5'-fluoro-1,1''-dimethyl-1H,1''H-[3,3':3',3''-terindol]-2'(1'H)-one ***7fb***. White **solid**; **Yield**: 92%; **mp (°C)**: >300 [>300];[20] **FT-IR (ATR, cm^{-1})**: 3365, 1685, 1480, 1179, 865, 795, 746, 673, 594, 432; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** δ 10.66 (s, 1H), 7.39 (d, *J* = 8.2 Hz, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.11 – 7.03 (m, 4H), 6.99 – 6.96 (m, 1H), 6.94 (s, 2H), 6.86 (t, *J* = 7.5 Hz, 2H), 3.72 (s, 6H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** δ 178.9, 158.3 (d, $J_{C\text{-}F}$ = 241.5 Hz, *ipso*-C), 137.9, 137.8, 136.6 (d, $J_{C\text{-}F}$ = 7.4 Hz), 129.1, 126.3, 121.6, 121.2, 119.0, 114.8 (d, $J_{C\text{-}F}$ = 23.3 Hz),113.2, 112.9 (d, $J_{C\text{-}F}$ = 24.0 Hz), 110.9 (d, $J_{C\text{-}F}$ = 8.1 Hz), 110.3, 53.4, 32.8.



5'-bromo-1,1''-dimethyl-1H,1''H-[3,3':3',3''-terindol]-2'(1'H)-one ***7fd***. Ivory-cream **solid**; **Yield**: 91%; **mp (°C)**: >300 [325-327];[24,26] **FT-IR (ATR, cm^{-1})**: 1715, 1613, 1471, 750, 732, 554, 431; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** δ 10.71 (s, 1H), 7.34 – 7.31 (m, 3H), 7.24 (d, *J* = 1.6 Hz, 1H), 7.14 (d, *J* = 8.0 Hz, 2H), 7.04 – 7.00 (m, 2H), 6.91 – 6.86 (m, 3H), 6.79 (t, *J* = 7.5 Hz, 2H), 3.64 (s, 6H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** δ 178.5, 141.1, 137.8, 137.3, 131.3, 129.0, 127.8, 126.3, 121.7, 121.2, 119.1, 113.7, 113.1, 112.2, 110.4, 53.1, 32.8.

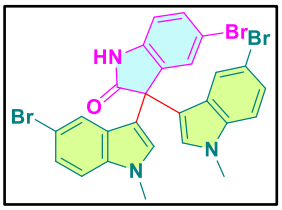


5,5''-dibromo-1,1''-dimethyl-1H,1''H-[3,3':3',3''-terindol]-2'(1'H)-one ***7ga***. White **solid**; **Yield**: 95%; **mp (°C)**: >300; **FT-IR (ATR, cm^{-1})**: 3385, 1721, 1468, 1193, 788, 768, 660, 565, 542; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** δ 10.76 (s, 1H), 7.41 – 7.37 (m, 4H), 7.27 (t, *J* = 7.6 Hz, 1H), 7.22 (dd, *J* = 8.7, 1.8 Hz, 2H), 7.17 (d, *J* = 7.3 Hz, 1H), 7.03 – 6.96 (m, 2H), 6.96 (s, 2H), 3.72 (s, 6H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** δ 178.7, 141.6, 136.6, 133.9, 130.6, 128.8, 127.9, 125.4, 124.2, 123.2, 122.4, 113.3, 112.7, 111.9, 110.3, 52.5, 33.1. **HRMS(ESI)**: Calcd. for $C_{26}H_{19}Br_2N_3O$ $[M+H]^+$ m/z: 547.9973; Found, $[M+H]^+$: 547.9972.

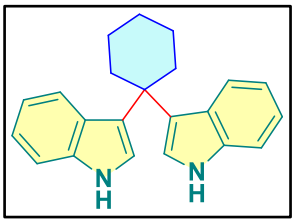


5,5''-dibromo-5'-fluoro-1,1''-dimethyl-1H,1''H-[3,3':3',3''-terindol]-2'(1'H)-one ***7gc***. White **solid**; **Yield**: 89%; **mp (°C)**: >300; **FT-IR (ATR, cm^{-1})**: 3387, 3306, 1690, 1483, 1452, 1174, 885, 793, 588; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** 10.80 (s, 1H), 7.43 (s, 1H), 7.40 – 7.39 (m, 3H), 7.24 (dd, *J* = 8.7, 1.8 Hz, 2H), 7.13 (td, *J* = 9.1, 2.6 Hz, 1H), 7.04 – 6.98 (m, 4H), 3.73 (s, 6H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** 178.7, 158.5 (d, $J_{C\text{-}F}$ = 238.7 Hz, *ipso*-C), 137.8, 136.6, 135.6 (d, $J_{C\text{-}F}$ = 7.6 Hz), 130.8, 127.7, 124.3, 123.1, 115.3 (d, $J_{C\text{-}F}$ = 23.7

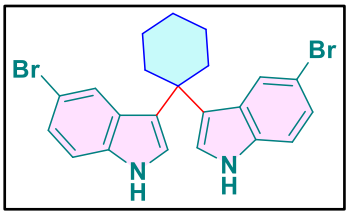
Hz), 113.2, 112.9, 112.7 (d, $J_{C\text{-}F}$ = 4.4 Hz), 111.7 (d, $J_{C\text{-}F}$ = 8.2 Hz), 111.2, 52.9, 33.1. **HRMS(ESI)**: Calcd. for $C_{26}H_{18}Br_2FN_3O$ $[M+H]^+$ m/z: 565.9879; Found, $[M+H]^+$: 565.9881.



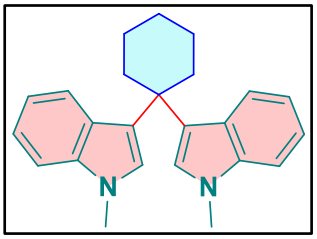
5,5',5''-tribromo-1,1''-dimethyl-1H,1''H-[3,3':3',3''-terindol]-2'(1'H)-one ***7gd***. White **solid**; **Yield**: 93%; **mp (°C)**: >300; **FT-IR (ATR, cm^{-1})**: 1725, 1471, 1285, 1201, 870, 820, 788, 688, 545; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** δ 10.92 (s, 1H), 7.45 – 7.37 (m, 5H), 7.25 – 7.23 (m, 3H), 7.01 6.99 (m, 3H), 3.73 (s, 1H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** δ 178.3, 140.9, 136.7, 136.3, 131.7, 130.7, 127.9, 127.7, 124.3, 123.0, 114.1, 112.8, 112.5, 112.4, 111.9, 52.7, 33.1. **HRMS(ESI)**: Calcd. for $C_{26}H_{18}Br_3N_3O$ $[M+H]^+$ m/z: 625.9078; Found, $[M+H]^+$: 625.9080.



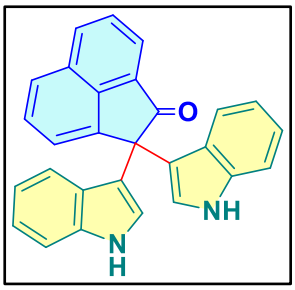
3,3'-(cyclohexane-1,1-diyl)bis(1H-indole) ***7ai***. Tortilla **solid**; **Yield**: 86%; **mp (°C)**: 121-123 [76-78];[27] **FT-IR (ATR, cm^{-1})**: 3406, 2289, 2930, 1454, 1414, 1334, 1099, 738, 581, 493, 456; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** δ 10.74 (s, 2H), 7.36 (d, J = 8.0 Hz, 2H), 7.32 (s, 2H), 7.26 (d, J = 8.1 Hz, 2H), 6.90 (t, J = 7.4 Hz, 2H), 6.70 (t, J = 7.4 Hz, 2H), 2.51 – 2.45 (m, 5H), 1.60 (s, 3H), 1.52 (s, 2H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** δ 137.4, 126.4, 122.6, 122.5, 121.0, 120.5, 117.9, 111.7, 39.0, 37.1, 26.9, 23.1.



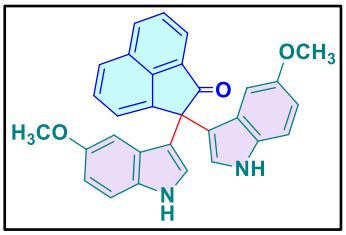
3,3'-(cyclohexane-1,1-diyl)bis(5-bromo-1H-indole) ***7ei***. Dark-yellow **solid**; **Yield**: 81%; **mp (°C)**: 225-227 [223-224];[25] **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** 11.10 (s, 2H), 7.48 (d, J = 31.9 Hz, 4H), 7.31 (s, 2H), 7.08 (s, 2H), 2.39 (s, 4H), 1.58 – 1.49 (m, 6H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** 136.2, 128.1, 124.3, 123.3, 122.8, 122.0, 113.9, 110.9, 38.7, 37.2, 26.8, 22.9.



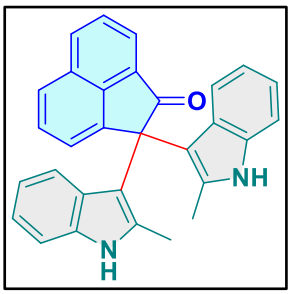
3,3'-(cyclohexane-1,1-diyl)bis(1-methyl-1H-indole) ***7fi***. Cream-white **solid**; **Yield**: 92%; **mp (°C)**: 211-213 [206-208];[28] **FT-IR (ATR, cm^{-1})**: 2938, 1484, 1329, 1245, 816, 740, 561, 434; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** 7.37 (d, J = 8.0 Hz, 2H), 7.30 (s, 2H), 7.27 (d, J = 8.2 Hz, 2H), 6.96 (t, J = 7.5 Hz, 2H), 6.74 (t, J = 7.5 Hz, 2H), 3.74 (s, 6H), 2.42 – 2.40 (m, 4H), 1.58 – 1.49 (m, 6H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** 137.7, 127.2, 126.7, 121.6, 121.1, 120.7, 118.1, 109.9, 39.0, 37.2, 32.8, 26.8, 22.9.



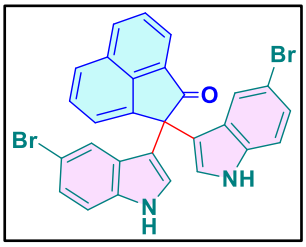
2,2-di(1H-indol-3-yl)acenaphthylen-1(2H)-one ***7aj***. Lemon-yellow **solid**; **Yield**: 93%; **mp (ºC)**: 241-243 [242-244];[16] **FT-IR (ATR, cm^{-1})**: 3416, 3357, 1682, 1339, 1101, 778, 737, 555; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** δ 10.99 (s, 1H), 8.36 (d, *J* = 8.1 Hz, 1H), 8.02 – 7.99 (m, 2H), 7.90 (t, *J* = 7.5 Hz, 1H), 7.70 (t, *J* = 7.6 Hz, 1H), 7.55 (d, *J* = 6.9 Hz, 1H), 7.35 (d, *J* = 8.1 Hz, 2H), 7.02 – 6.98 (m, 4H), 6.85 (d, *J* = 2.0 Hz, 2H), 6.74 (t, *J* = 7.5 Hz, 2H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** δ 203.1, 144.3, 140.1, 137.4, 132.5, 131.9, 130.9, 129.5, 129.3, 126.2, 125.1, 124.6, 122.7, 122.2, 121.5, 121.1, 118.8, 115.3, 114.9, 112.2, 58.1.



2,2-bis(5-methoxy-1H-indol-3-yl)acenaphthylen-1(2H)-one ***7cj***. Lemon-yellow **solid**; **Yield**: 90%; **mp (ºC)**: 281-283 [284-286];[16] **FT-IR (ATR, cm^{-1})**: 3395, 3367, 1698, 1481, 1231, 1028, 777, 613, 512; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** 10.80 (s, 2H), 8.36 (d, *J* = 8.1 Hz, 1H), 8.02 – 8.00 (m, 2H), 7.89 (t, *J* = 7.5 Hz, 1H), 7.70 (t, *J* = 7.6 Hz, 1H), 7.54 (d, *J* = 6.9 Hz, 1H), 7.24 (d, *J* = 8.8 Hz, 2H), 6.86 (s, 2H), 6.67 (d, *J* = 8.8 Hz, 2H), 6.42 (s, 2H), 3.40 (s, 6H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** 203.2, 152.9, 144.3, 140.2, 132.7, 132.5, 132.2, 130.9, 129.5, 129.3, 126.7, 125.9, 124.5, 122.5, 122.2, 114.7, 112.6, 110.9, 103.7, 58.1, 55.5.

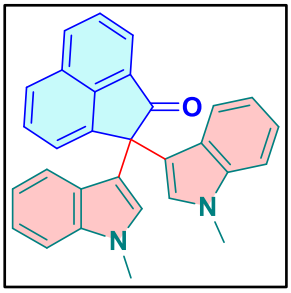


2,2-bis(2-methyl-1H-indol-3-yl)acenaphthylen-1(2H)-one ***7dj***. Tortilla-brown **solid**; **Yield**: 92%; **mp (ºC)**: 291-293 [292-293];[29] **FT-IR (ATR, cm^{-1})**: 3383, 3340, 1712, 1459, 1022, 781, 741, 521; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** 10.84 (d, *J* = 9.7 Hz, 2H), 8.27 (d, *J* = 8.1 Hz, 1H), 7.96 – 7.95 (m, 2H), 7.80 (t, *J* = 7.6 Hz, 1H), 7.60 – 7.56 (m, 1H), 7.36 (d, *J* = 7.0 Hz, 1H), 7.15 – 7.12 (m, 2H), 6.83 – 6.77 (m, 2H), 6.54 – 6.44 (m, 3H), 6.25 (d, *J* = 8.1 Hz, 1H), 1.77 (s, 3H), 1.71 (s, 3H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** δ 202.5, 144.5, 140.3, 135.5, 135.5, 134.2, 134.1, 133.9, 133.8, 133.2, 132.1, 130.8, 129.4, 129.2, 128.1, 127.8, 124.6, 122.8, 122.3, 120.3, 120.2, 120.0, 119.91, 118.5, 118.4, 111.4, 110.9, 110.5, 57.9, 13.89, 13.8.

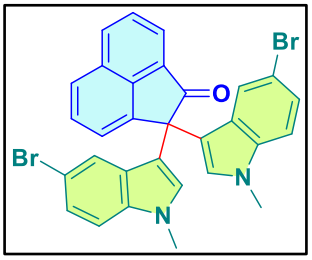


2,2-bis(5-bromo-1H-indol-3-yl)acenaphthylen-1(2H)-one ***7ej***. Light-yellow **solid**; **Yield**: 91%; **mp (ºC)**: >300 [>300];[29] **FT-IR (ATR, cm^{-1})**: 3428, 3338, 1076, 1455, 1093, 782, 663, 605, 460, 418; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** δ 11.28 (s, 2H), 8.39 (s, 1H), 8.06

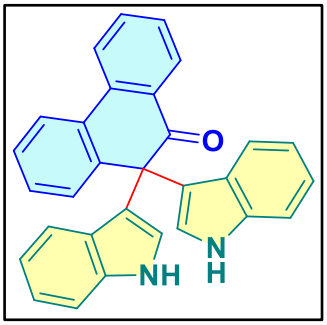
– 8.04 (m, 2H), 7.92 (t, *J* = 7.6 Hz, 1H), 7.74 (t, *J* = 7.6 Hz, 1H), 7.54 (d, *J* = 6.9 Hz, 1H), 7.37 (d, *J* = 9.1 Hz, 2H), 7.15 (d, *J* = 6.3 Hz, 4H), 6.95 (d, *J* = 2.3 Hz, 2H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** δ 202.8, 143.3, 140.0, 136.2, 132.9, 131.5, 130.9, 129.6, 129.5, 127.9, 126.8, 124.9, 124.2, 123.1, 122.9, 122.3, 114.7, 114.4, 111.6, 57.7.



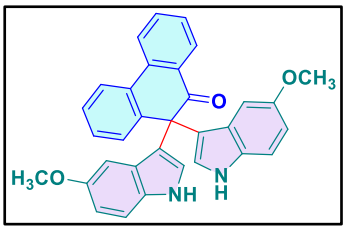
2,2-bis(1-methyl-1H-indol-3-yl)acenaphthylen-1(2H)-one ***7fj***. Light-yellow **solid**; **Yield**: 87%; **mp (°C)**: >300 [>300];[29] **FT-IR (ATR, cm^{-1})**:1715, 1463, 1330, 977, 785, 735, 560, 431; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** δ 8.36 (d, *J* = 8.0 Hz, 1H), 8.01 (d, *J* = 7.6 Hz, 2H), 7.90 (t, *J* = 7.5 Hz, 2H), 7.69 (t, *J* = 7.6 Hz, 1H), 7.56 (d, *J* = 6.8 Hz, 1H), 7.37 (d, *J* = 8.1 Hz, 2H), 7.06 (dd, *J* = 14.6, 7.6 Hz, 6H), 6.88 (s, 3H), 6.79 (t, *J* = 7.4 Hz, 3H), 3.67 (s, 11H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** δ 202.9, 144.2, 139.9, 137.8, 132.6, 131.9, 130.9, 129.6, 129.4, 129.3, 126.6, 124.6, 122.8, 122.2, 121.6, 121.2, 119.0, 114.4, 110.3, 57.9, 32.8.



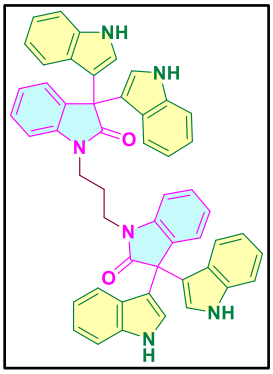
2,2-bis(5-bromo-1-methyl-1H-indol-3-yl)acenaphthylen-1(2H)-one ***7gj***. Pastel-cream **solid**; **Yield**: 94%; **mp (°C)**: >300; **FT-IR (ATR, cm^{-1})**: 1724, 1473, 1283, 1208, 826, 793, 423; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** 8.40 (d, *J* = 8.1 Hz, 1H), 8.06 – 8.04 (m, 2H), 7.94 – 7.90 (m, 1H), 7.76 – 7.72 (m, 1H), 7.53 (d, *J* = 6.9 Hz, 1H), 7.40 (d, *J* = 8.7 Hz, 2H), 7.21 (dd, *J* = 8.7, 1.8 Hz, 2H), 7.15 (d, *J* = 1.6 Hz), 6.98 (s, 2H), 3.69 (s, 6H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** δ 202.6, 143.1, 139.9, 136.7, 132.9, 131.4, 130.9, 130.9, 129.7, 129.6, 128.0, 124.9, 124.3, 123.2, 123.0, 122.3, 113.7, 112.8, 111.9, 57.6, 33.1. **HRMS(ESI)**: Calcd. for $C_{30}H_{20}Br_2N_2O$ $[M+H]^+$ m/z: 583.0021; Found, $[M+H]^+$: 583.0026.



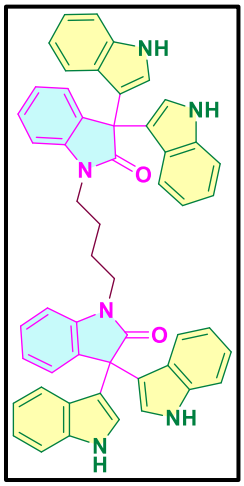
10,10-di(1H-indol-3-yl)phenanthren-9(10H)-one ***7gk***. Yellow **solid**; **Yield**: 87%; **mp (°C)**: >300; **FT-IR (ATR, cm^{-1})**: 3333, 1671, 1560, 1449, 1267, 1102, 733, 630, 459; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** 10.92 (s, 2H), 8.24 (dd, *J* = 21.3, 7.5 Hz, 2H), 7.72 – 7.65 (m, 2H), 7.46 (t, *J* = 6.9 Hz, 2H), 7.35 (d, *J* = 7.7 Hz, 1H), 7.03 (t, *J* = 7.0 Hz, 1H), 6.93 (t, *J* = 9.8 Hz, 1H), 6.81 (t, *J* = 7.1 Hz, 1H), 6.43 (s, 1H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** 178.7, 159.6, 157.3, 137.8, 136.6, 135.6, 135.6, 130.8, 127.7, 124.3, 123.1, 115.4, 115.2, 113.2, 112.9, 112.7, 112.7, 111.9, 111.3, 111.2, 52.9, 33.1. **HRMS(ESI)**: Calcd. for $C_{30}H_{20}N_2O$ $[M+Na]^+$ m/z: 447.1473; Found, $[M+Na]^+$: 447.1475.



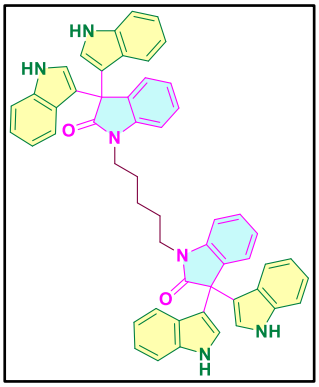
10,10-bis(5-methoxy-1H-indol-3-yl)phenanthren-9(10H)-one ***7ck***. Lemon-yellow **solid**; **Yield**: 91%; **mp (ºC)**: >300; **FT-IR (ATR, cm^{-1})**: 1720, 1600, 1280, 1010, 894, 831, 776; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** 10.78 (s, 2H), 8.23 (dd, *J* = 24.8, 7.9 Hz, 2H), 7.74 (d, *J* = 7.6 Hz, 1H), 7.66 (t, *J* = 7.5 Hz, 1H), 7.47 (t, *J* = 7.4 Hz, 1H), 7.35 (t, *J* = 7.4 Hz, 1H), 7.27 – 7.25 (m, 3H), 6.94 (d, *J* = 7.6 Hz, 1H), 6.71 (d, *J* = 7.2 Hz, 2H), 6.45 (s, 2H), 6.36 (s, 2H), 3.50 (s, 6H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** 196.7, 153.1, 141.3, 136.6, 134.5, 132.7, 130.7, 130.4, 130.2, 129.3, 128.8, 128.3, 127.9, 127.4, 126.8, 124.6, 123.7, 115.1, 112.8, 110.8, 103.8, 57.1, 55.8. **HRMS(ESI)**: Calcd. for $C_{32}H_{24}N_2O_3$ $[M+Na]^+$ m/z: 507.1685; Found, $[M+Na]^+$: 507.1685.



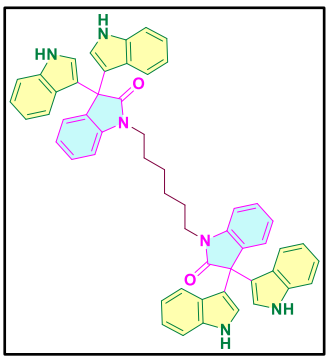
1',1''''-(propane-1,3-diyl)bis(([3,3':3',3''-terindolin]-2'-one)) ***10aa***. Brick-red **solid**; **Yield**: 94%; **mp (ºC)**: >300; **FT-IR (ATR, cm^{-1})**: 3402, 1693, 1338, 1090, 734; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** 10.90 (d, *J* = 1.8 Hz, 4H), 7.28 (d, *J* = 8.1 Hz, 4H), 7.22 (d, *J* = 7.0 Hz, 2H), 7.15 – 7.08 (m, 6H), 6.95 – 6.89 (m, 8H), 6.78 (d, *J* = 2.4 Hz, 2H), 6.69 (t, *J* = 7.5 Hz, 4H), 1.98 – 1.92 (m, 4H), 1.10 (t, *J* = 7.1 Hz, 2H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** 177.4, 142.2, 137.4, 134.3, 128.5, 126.1, 125.3, 124.8, 122.6, 121.5, 121.1, 118.8, 114.4, 112.1, 60.2, 37.9, 21.2. **HRMS(ESI)**: Calcd. for $C_{51}H_{38}N_6O_2$ $[M+Na]^+$ m/z: 789.2954; Found, $[M+Na]^+$: 789.2955.



1',1''''-(butane-1,4-diyl)bis(([3,3':3',3''-terindolin]-2'-one)) ***10ab***. Sand-brown **solid**; **Yield**: 91%; **mp (ºC)**: >300; **FT-IR (ATR, cm^{-1})**: 3363, 1676, 1609, 1359, 1100, 740, 615, 427; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** 10.96 (s, 4H), 7.37 – 7.14 (m, 15H), 7.01 (s, 6H), 6.87 – 6.79 (m, 7H), 3.83 (s, 4H), 1.76 (s, 4H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** 177.36, 142.41, 137.40, 134.32, 128.44, 126.12, 125.18, 124.72, 122.49, 121.44, 121.13, 118.80, 114.57, 112.12, 109.30, 52.65, 25.16. **HRMS(ESI)**: Calcd. for $C_{52}H_{40}N_6O_2$ $[M+H]^+$ m/z: 781.3291; Found, $[M+H]^+$: 781.3291.



1',1''''-(pentane-1,5-diyl)bis(([3,3':3',3''-terindolin]-2'-one)) ***10ac***. Pale-sand brown **solid**; **Yield**: 85%; **mp (°C)**: >300 [>300];[24] **FT-IR (ATR, cm^{-1})**: 3342, 1665, 1607, 1466, 1095, 741, 476; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** 10.97 (s, 4H), 7.36 – 7.27 (m, 9H), 7.16 (d, *J* = 8.1 Hz, 4H), 7.03 – 6.98 (m, 7H), 6.86 – 6.85 (m, 4H), 6.79 (t, *J* = 7.4 Hz, 4H), 1.71 – 1.61 (m, 6H), 1.38 – 1.23 (m, 4H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** 177.3, 158.5, 151.1, 142.4, 137.4, 134.3, 128.4, 126.1, 124.8, 121.4, 121.1, 118.8, 114.6, 112.1, 109.3, 52.7, 26.9, 23.9. **DEPT-135 NMR (100 MHz, DMSO-d$_6$, ppm)** 138.7, 128.5, 124.8, 122.5, 121.4, 121.1, 118.8, 112.1, 109.3, 39.6, 26.9, 23.9.



1',1''''-(hexane-1,6-diyl)bis(([3,3':3',3''-terindolin]-2'-one)) ***10ad.*** Brick-red **solid**; **Yield**: 92%; **mp (°C)**: 284-286 [283-285];[24] **FT-IR (ATR, cm^{-1})**: 3359, 1665, 1608, 1464, 1367, 1100, 734, 651 607; **^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)** 10.95 (s, 4H), 7.34 – 7.30 (m, 8H), 7.16 – 7.14 (m, 6H), 6.99 – 6.98 (m, 6H), 6.84 (s, 4H), 6.75 (s, 4H), 3.70 (s, 4H), 1.59 (s, 4H), 1.32 (s, 4H). **^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)** 177.3, 142.5, 137.4, 134.3, 128.4, 126.1, 125.2, 124.8, 122.4, 121.1, 118.7, 114.5, 112.1, 109.3, 52.7, 27.4, 26.6. **DEPT-135 NMR (100 MHz, DMSO-d$_6$, ppm)** 128.4, 125.2, 124.8, 122.5, 121.4, 121.1, 118.7, 112.1, 109.3, 39.9, 27.4, 26.6.

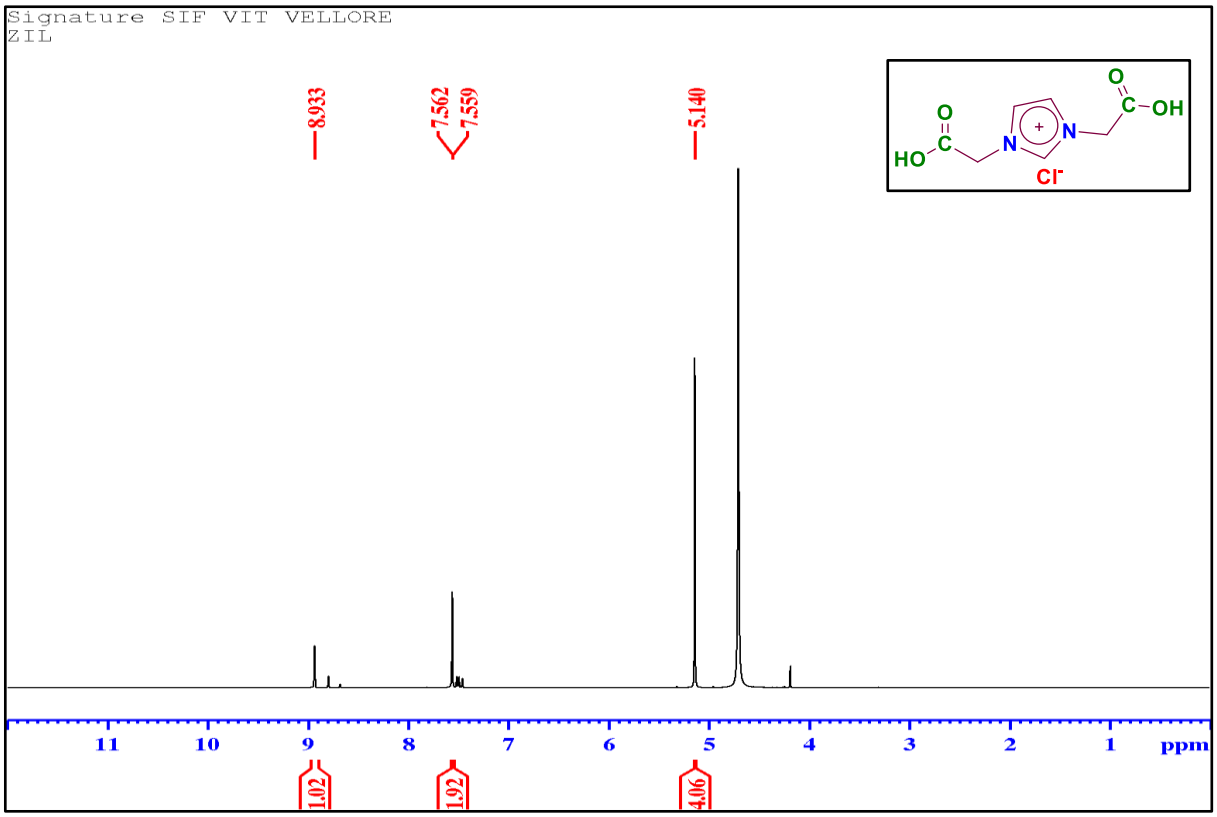


Fig. S1 ^{1}H NMR spectrum (400 MHz) of **4** in D_2O.

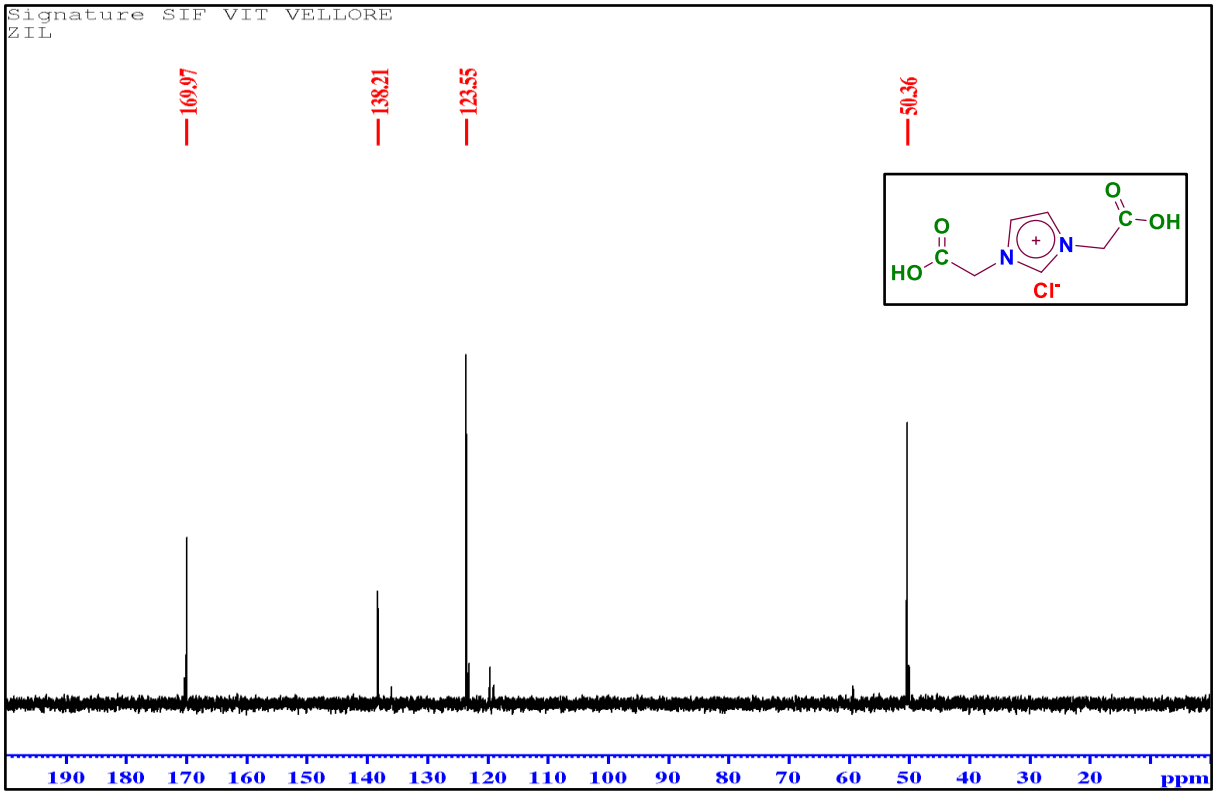


Fig. S2 ^{13}C NMR spectrum (100 MHz) of **4** in D_2O.

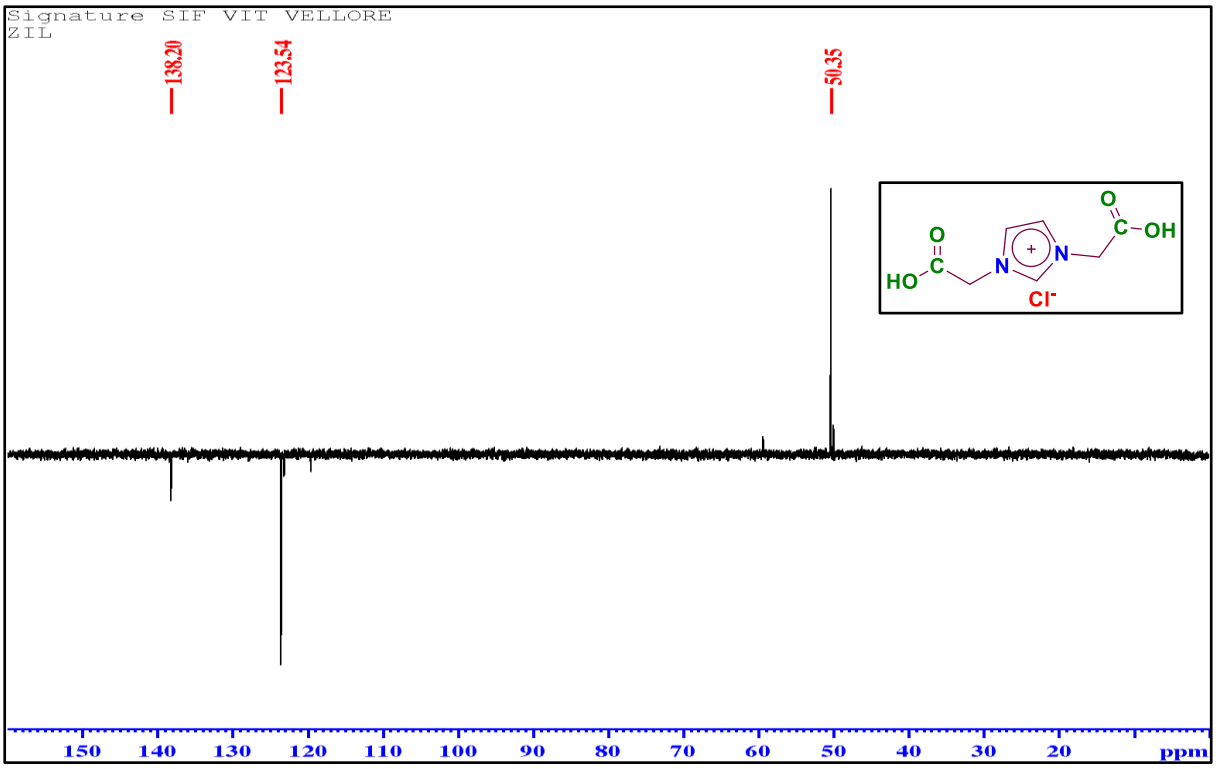


Fig. S3 DEPT-135 spectrum of (100 MHz) **4** in D_2O.

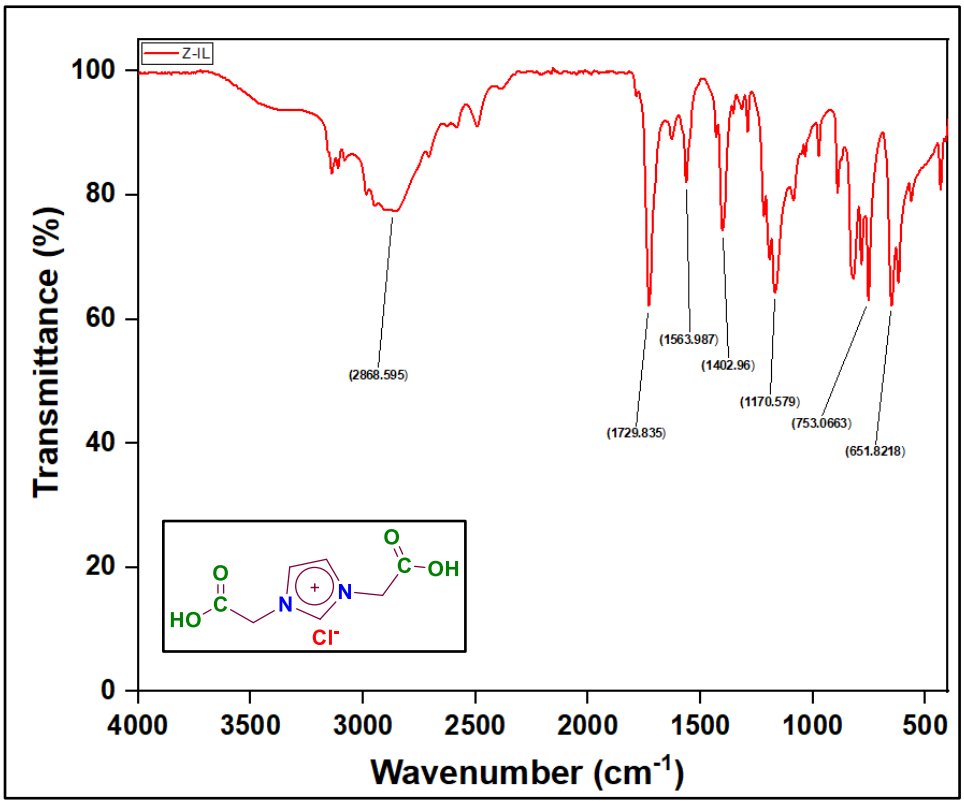


Fig. S4 FT-IR spectrum of **4**.

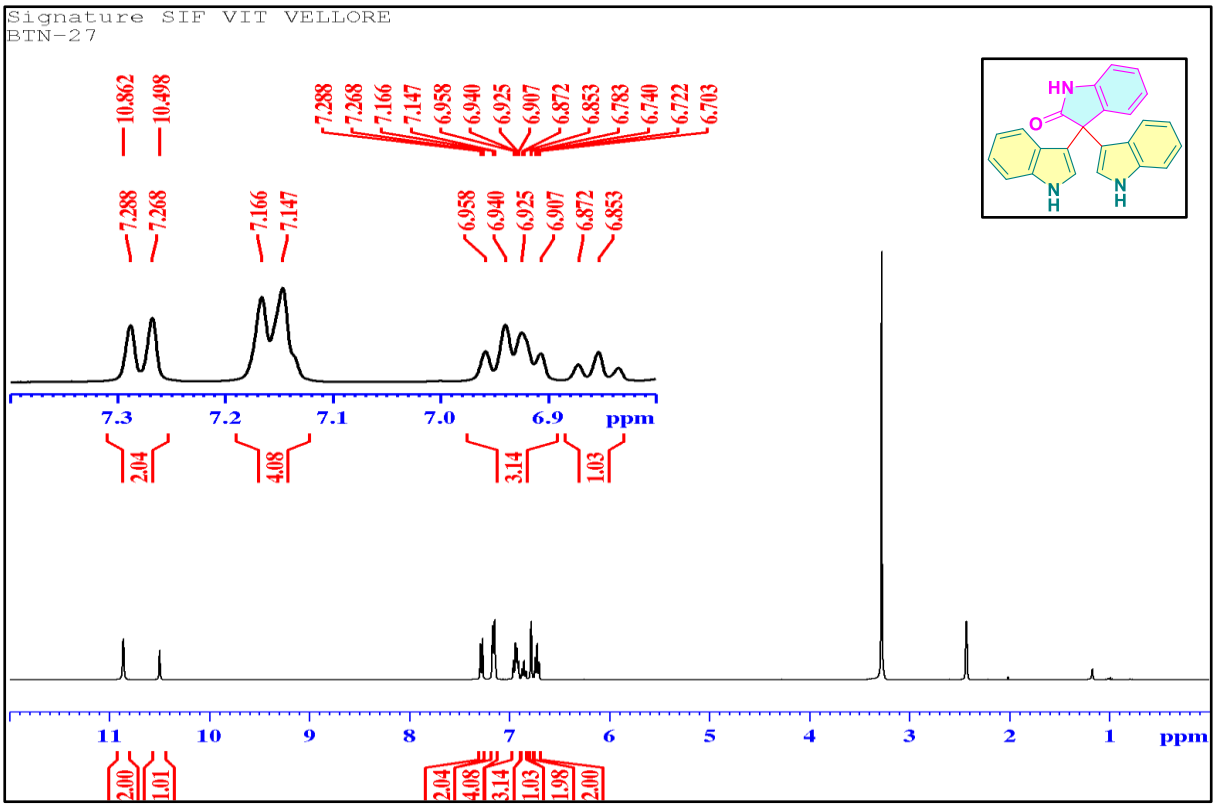


Fig. S5 ^{1}H NMR spectrum (400 MHz) of **7aa** in DMSO-d_6.

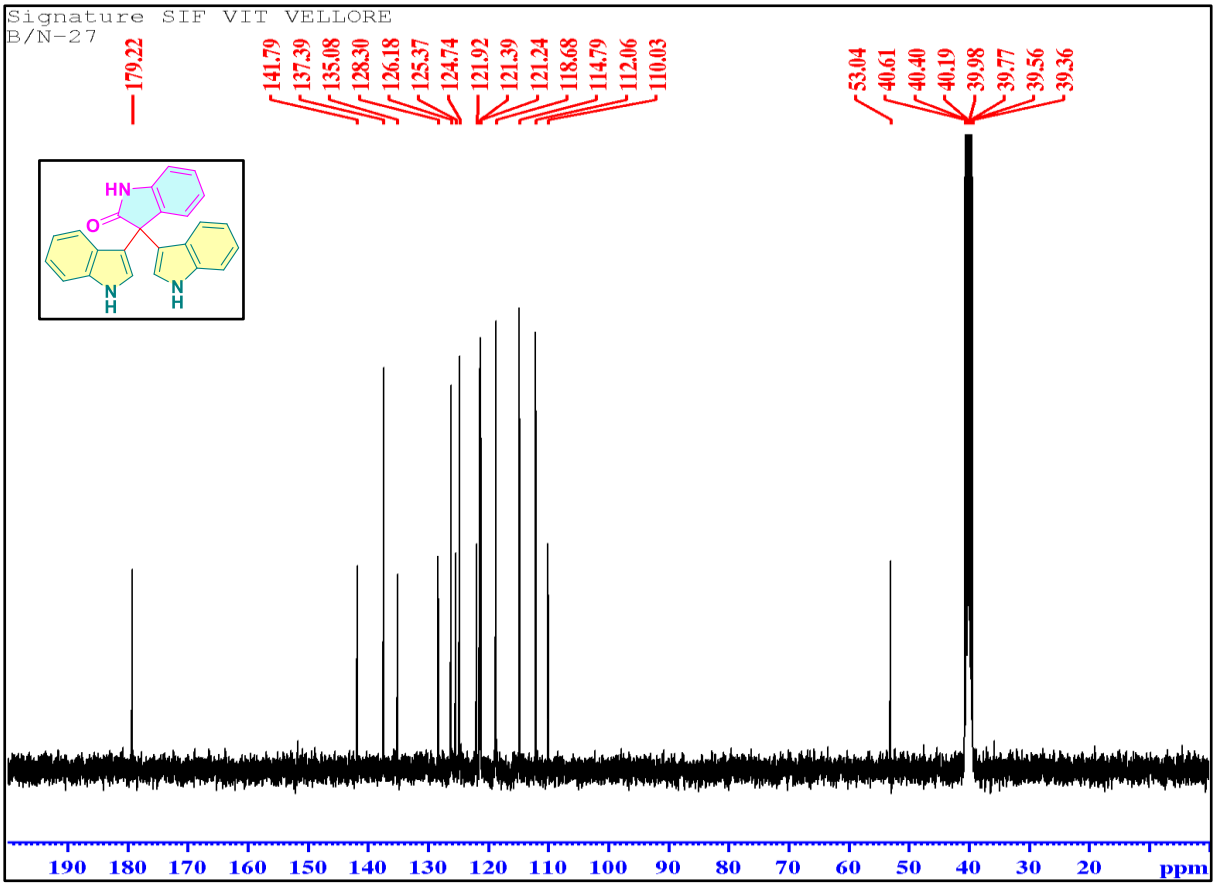


Fig. S6 ^{13}C NMR spectrum (100 MHz) of **7aa** in DMSO-d_6.

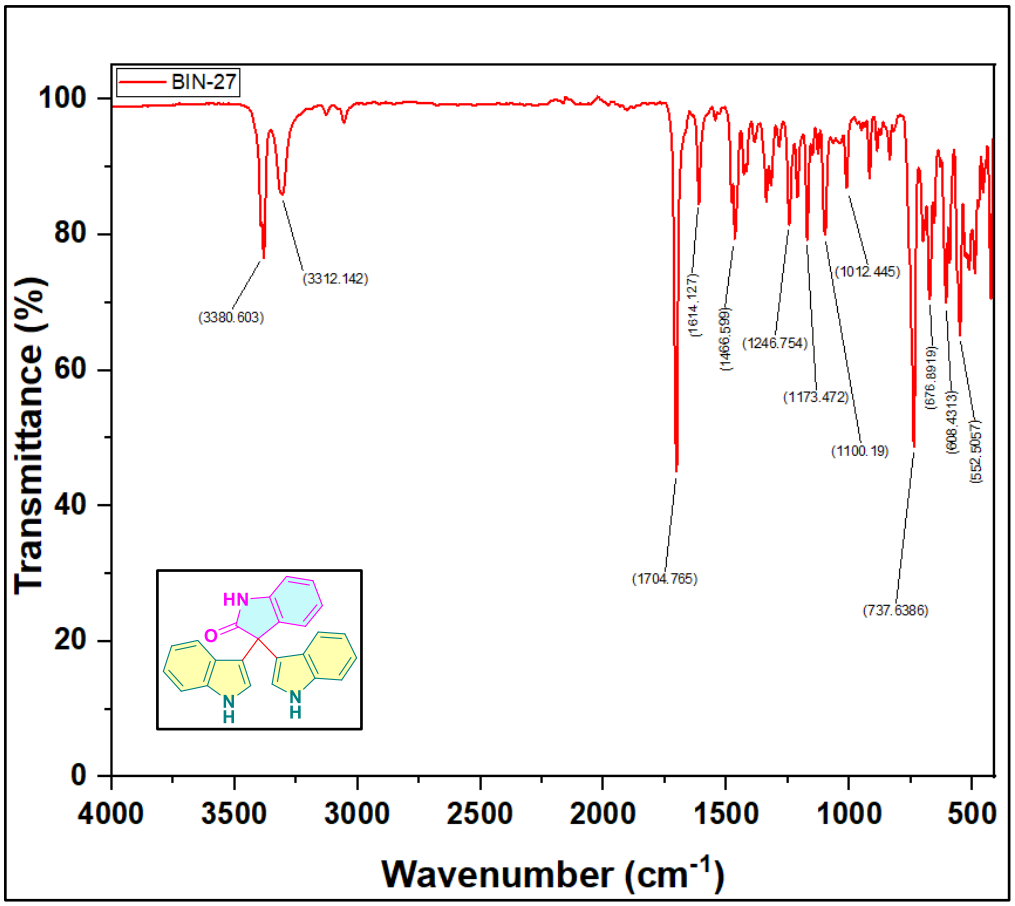


Fig. S7 FT-IR spectrum of **7aa**.

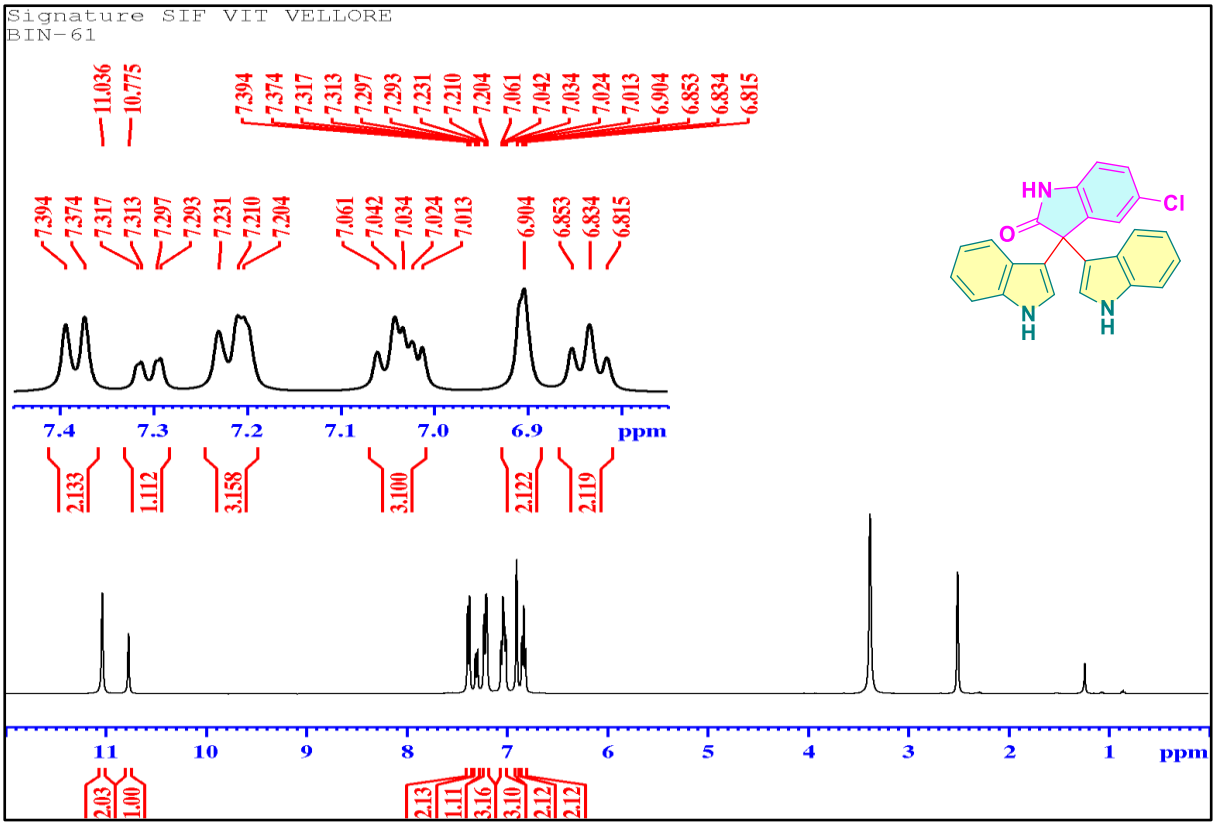


Fig. S8 ^{1}H NMR spectrum (400 MHz) of **7ab** in DMSO-d$_6$.

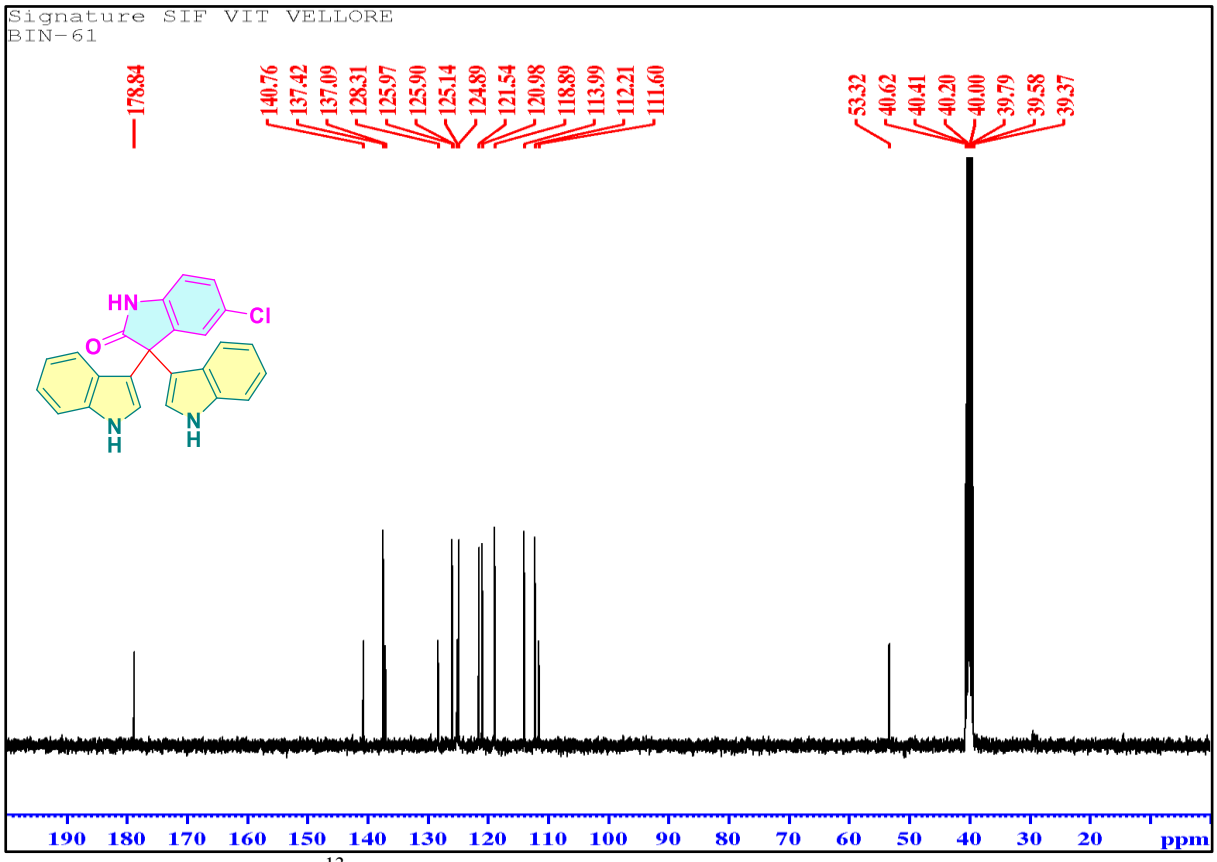


Fig. S9 ^{13}C NMR spectrum (100 MHz) of **7ab** in DMSO-d$_6$.

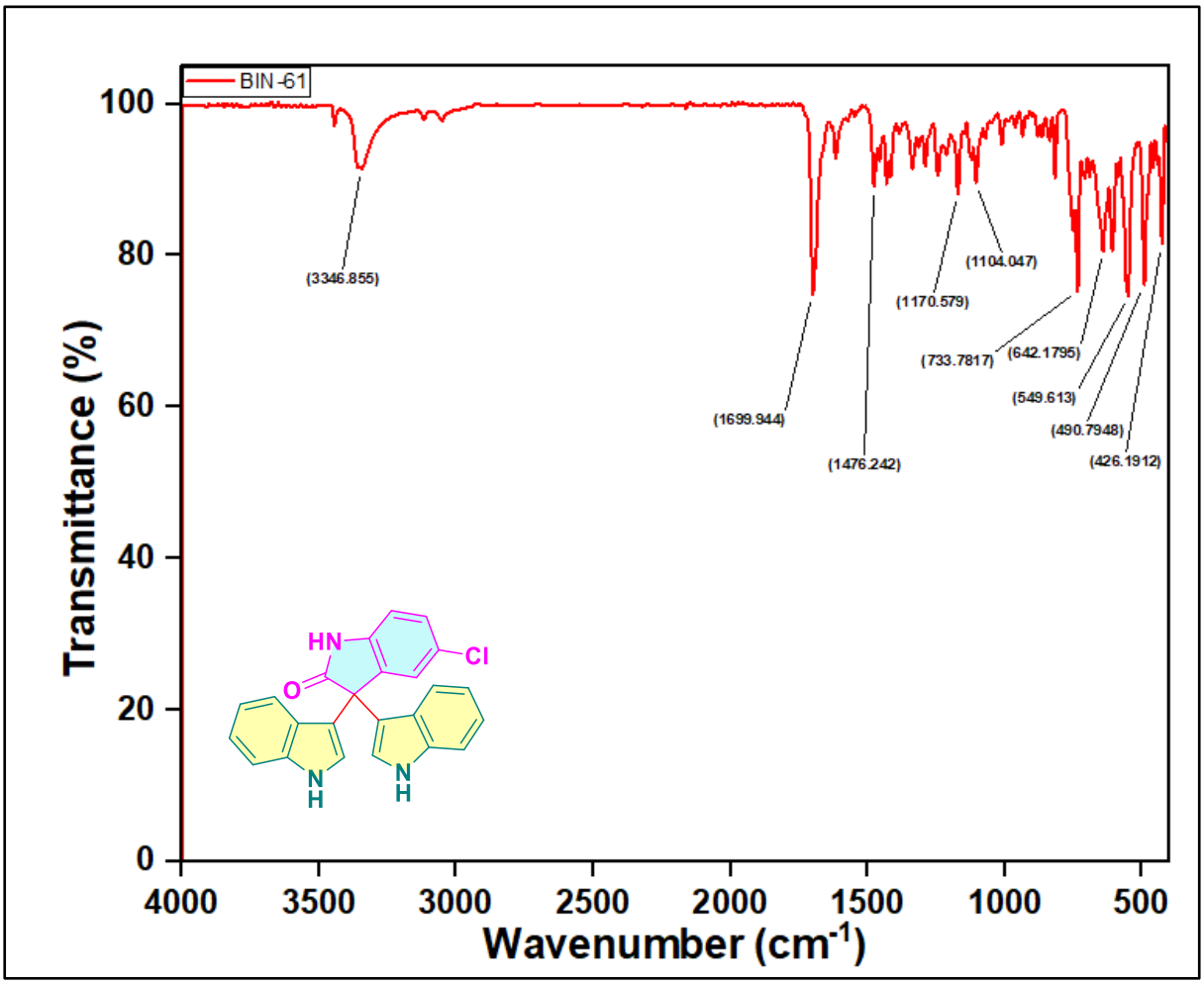


Fig. S10 FT-IR spectrum of **7ab**.

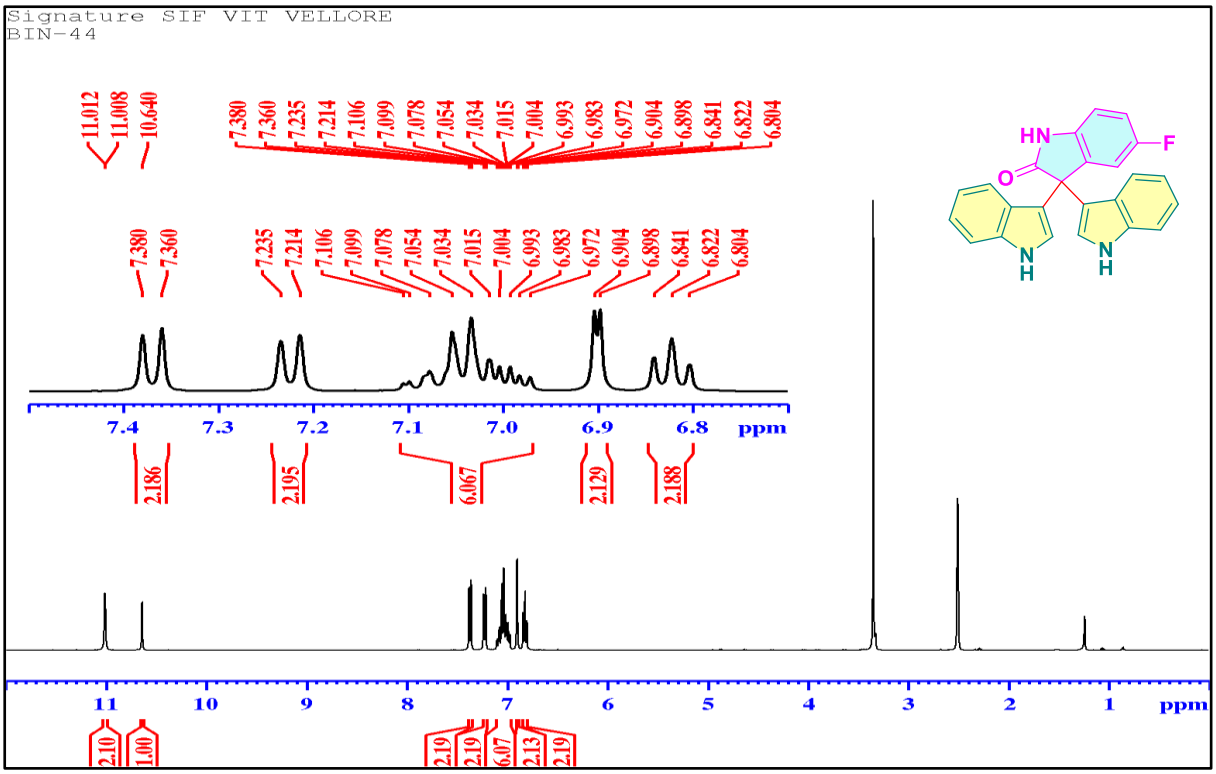


Fig. S11 ^{1}H NMR spectrum (400 MHz) of **7ac** in DMSO-d_6.

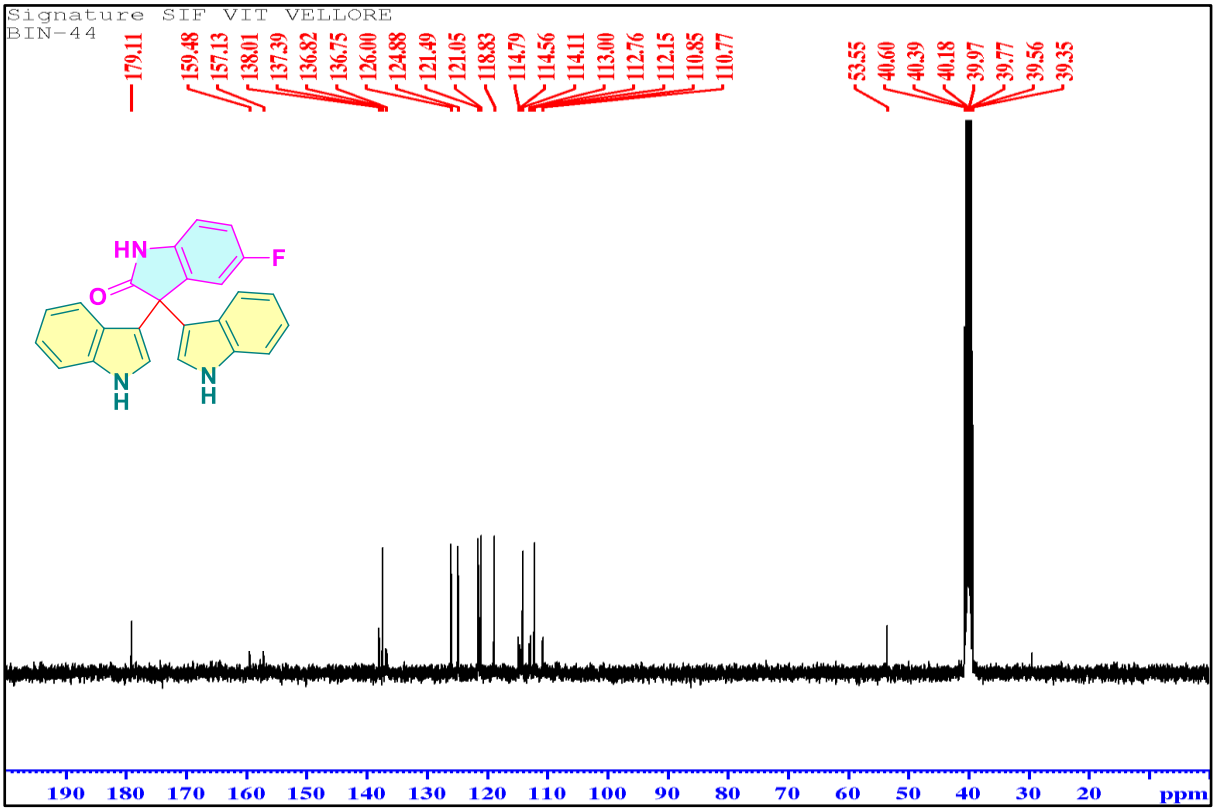


Fig. S12 ^{13}C NMR spectrum (100 MHz) of **7ac** in DMSO-d_6.

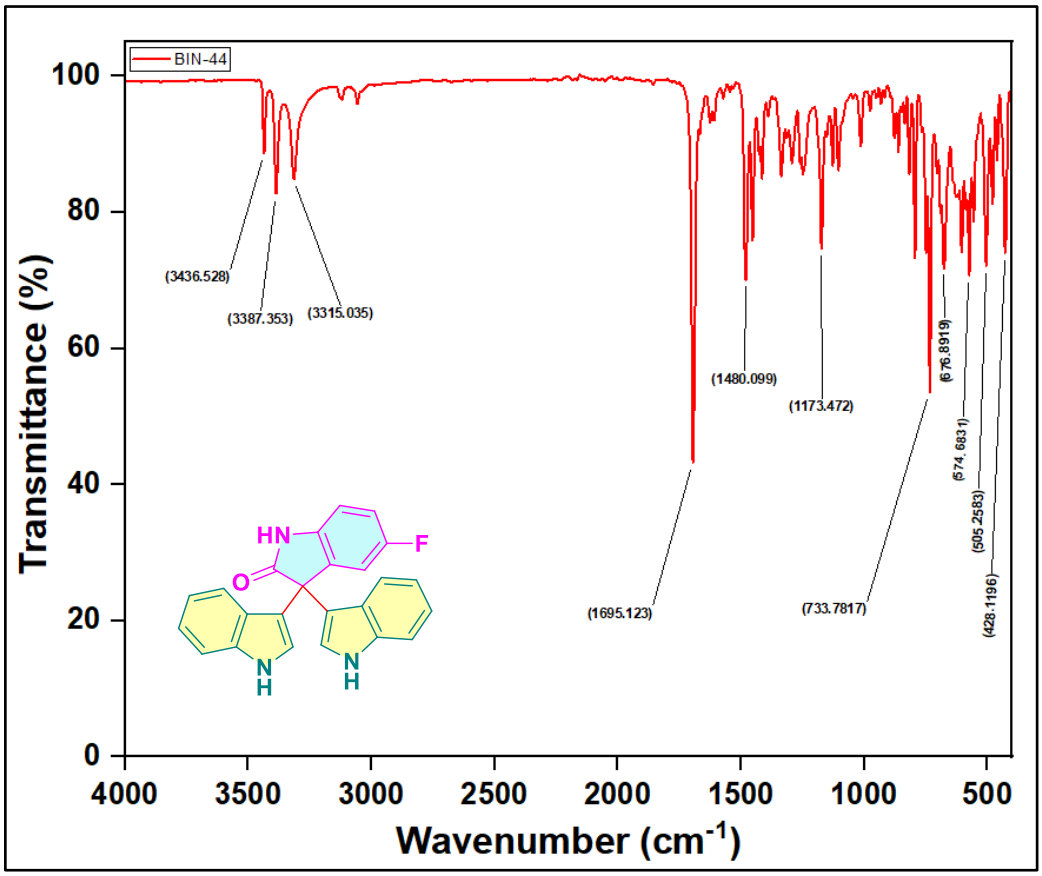


Fig. S13 FT-IR spectrum of **7ac**.

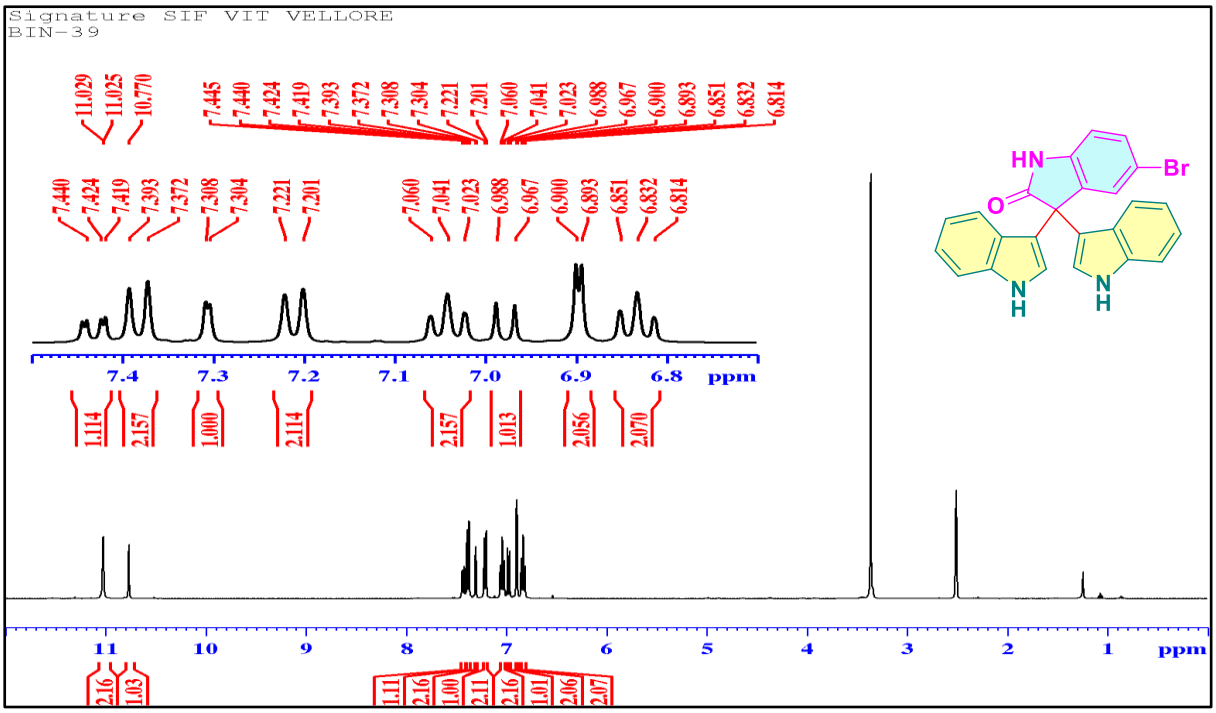


Fig. S14 ^{1}H NMR spectrum (400 MHz) of **7ad** in DMSO-d_6.

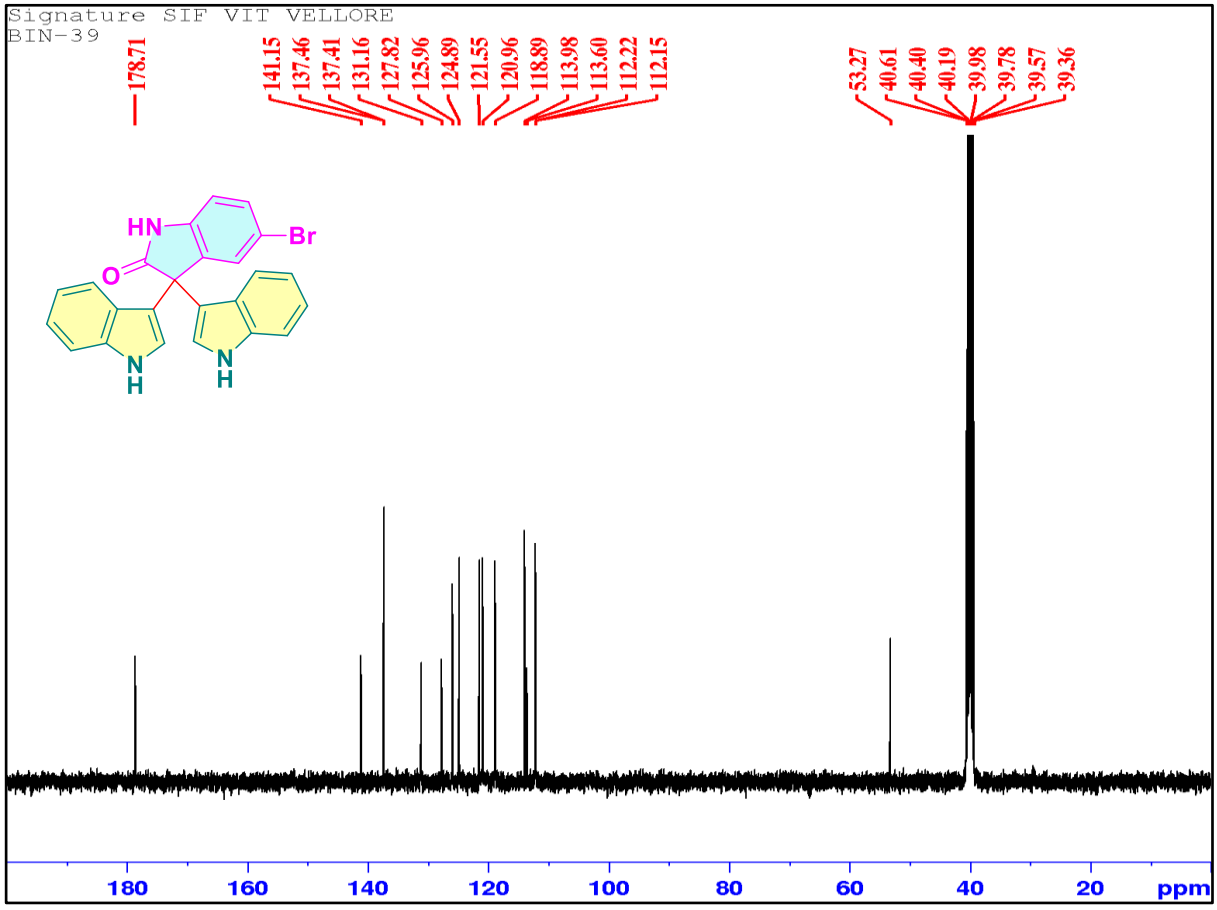


Fig. S15 ^{13}C NMR spectrum (100 MHz) of **7ad** in DMSO-d_6.

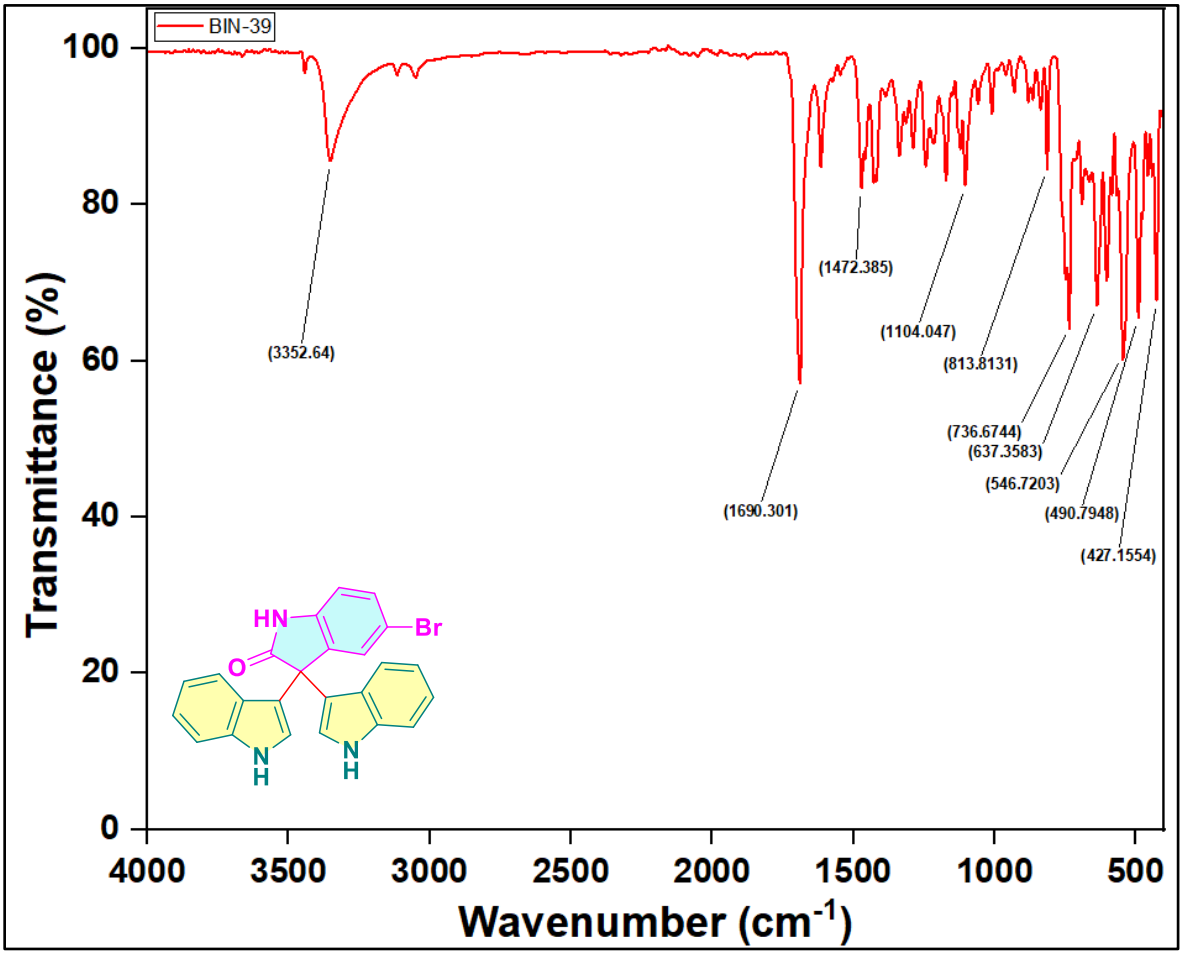


Fig. S16 FT-IR spectrum of **7ad**.

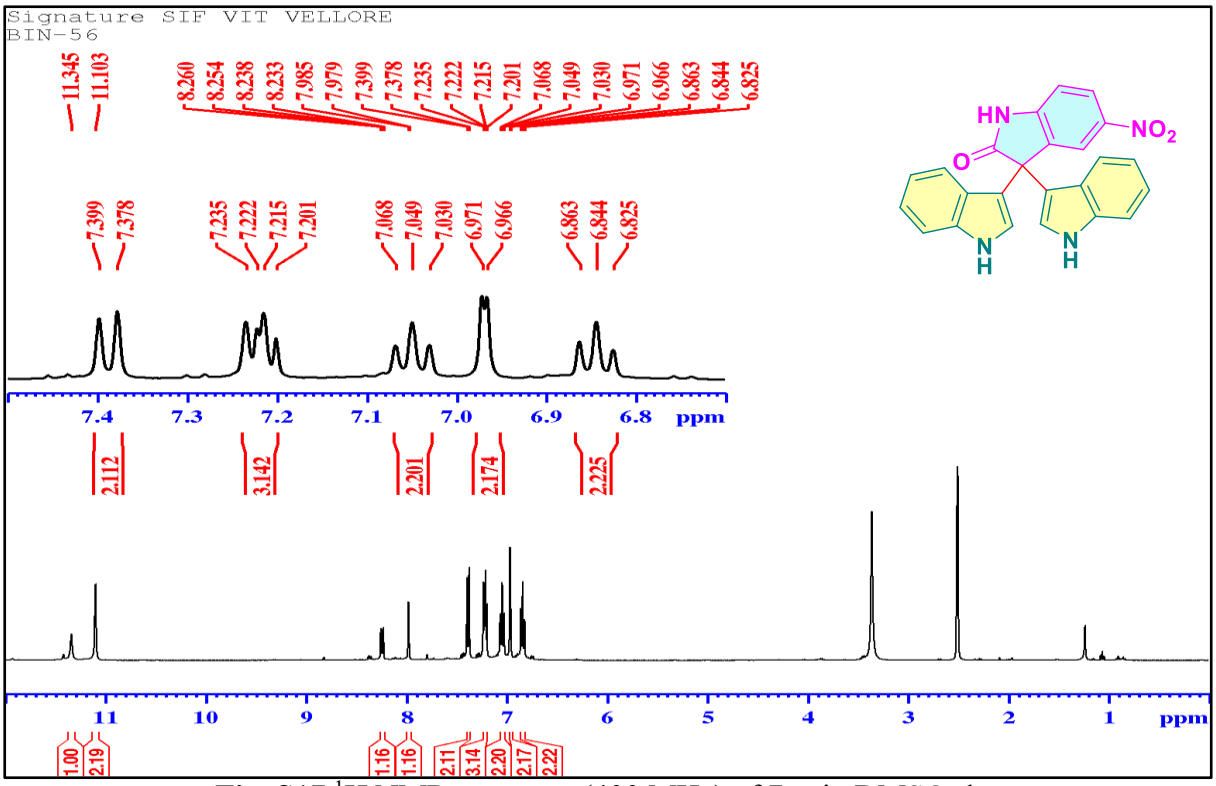


Fig. S17 ^{1}H NMR spectrum (400 MHz) of **7ae** in DMSO-d_6.

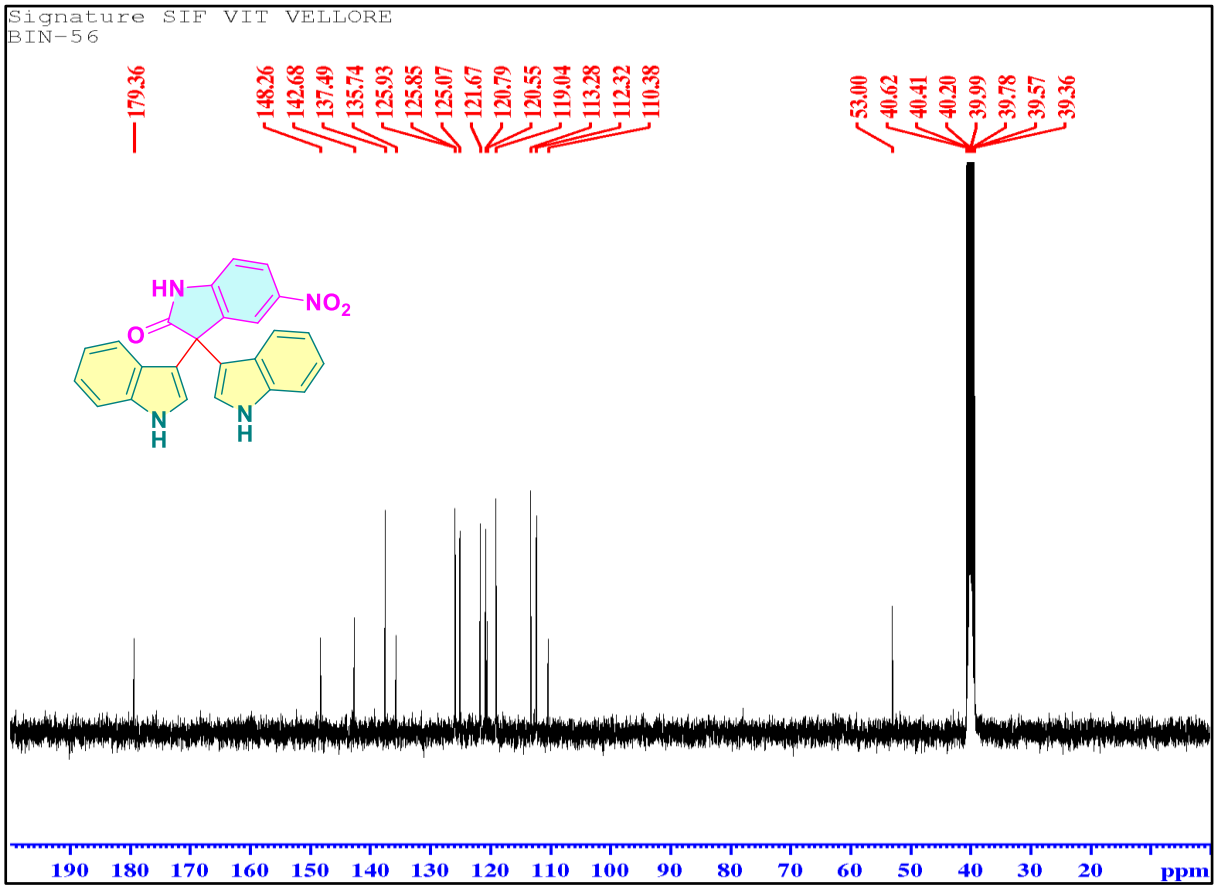


Fig. S18 ^{13}C NMR spectrum (100 MHz) of **7ae** in DMSO-d_6.

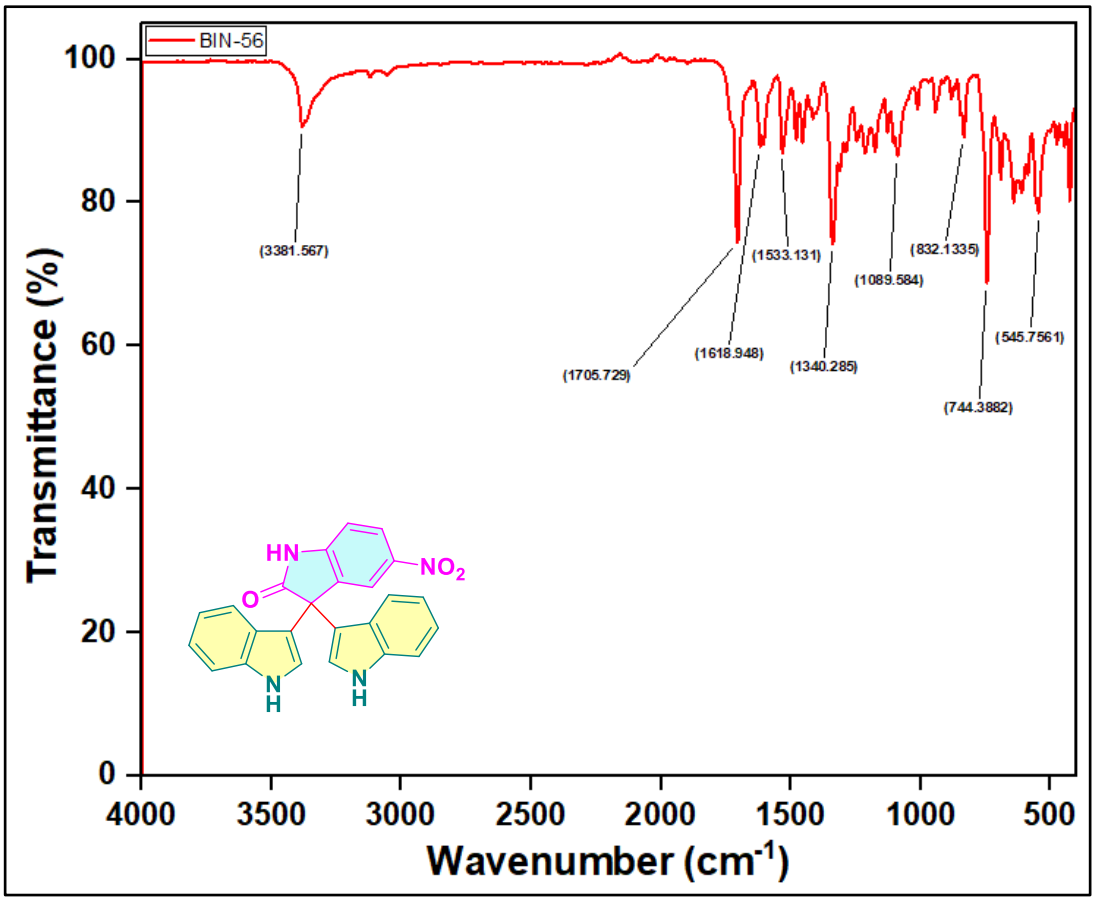


Fig. S19 FT-IR spectrum of **7ae**.

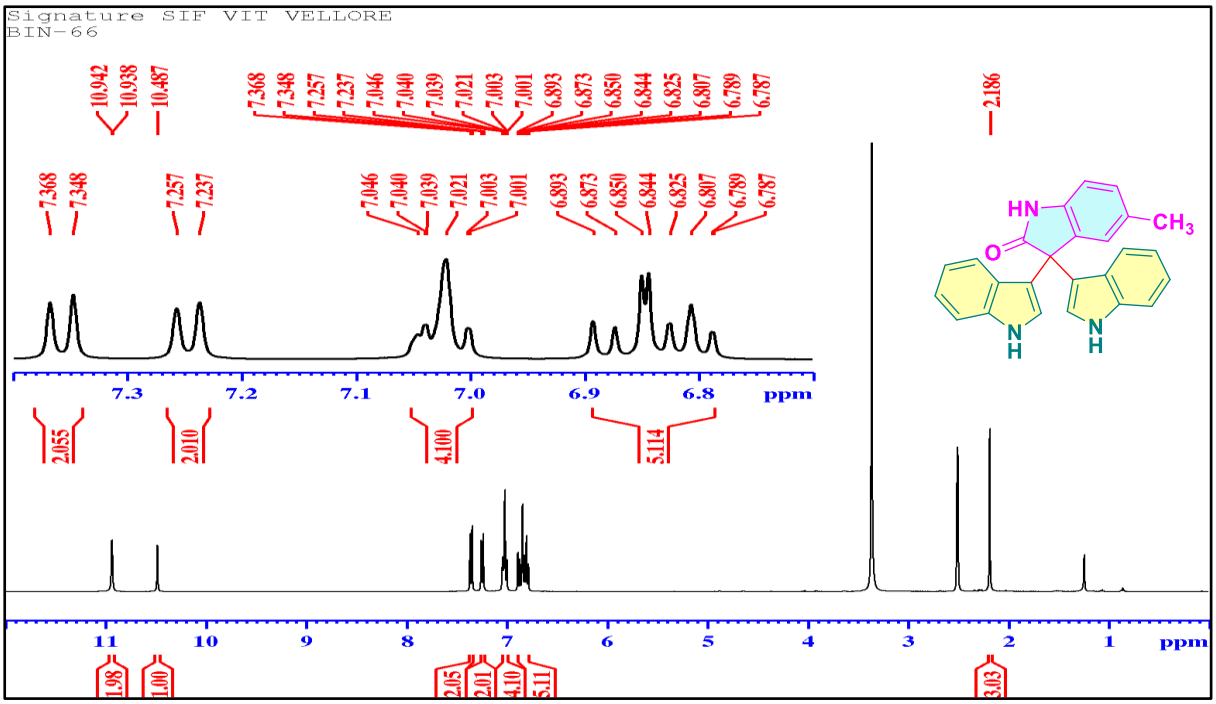


Fig. S20 ^{1}H NMR spectrum (400 MHz) of **7af** in DMSO-d_6.

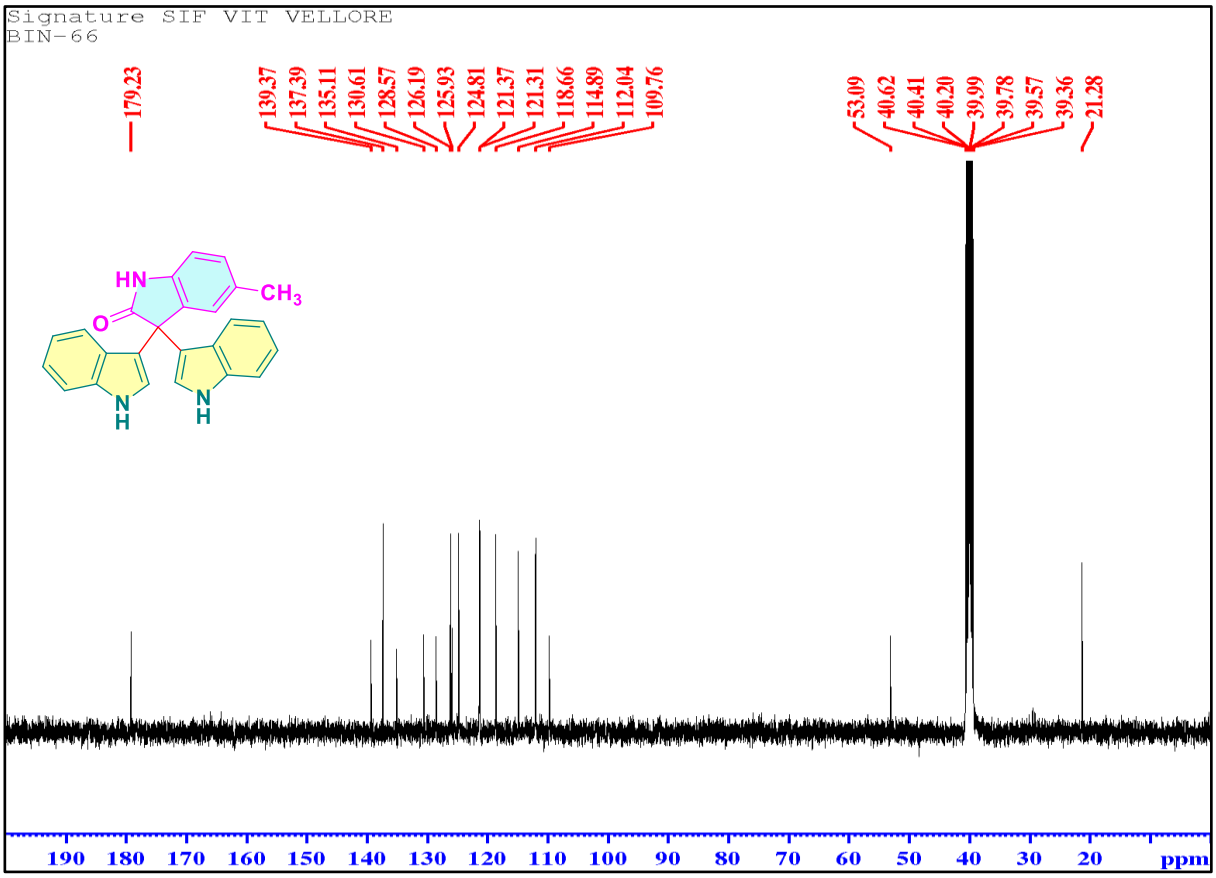


Fig. S21 ^{13}C NMR spectrum (100 MHz) of **7af** in DMSO-d_6.

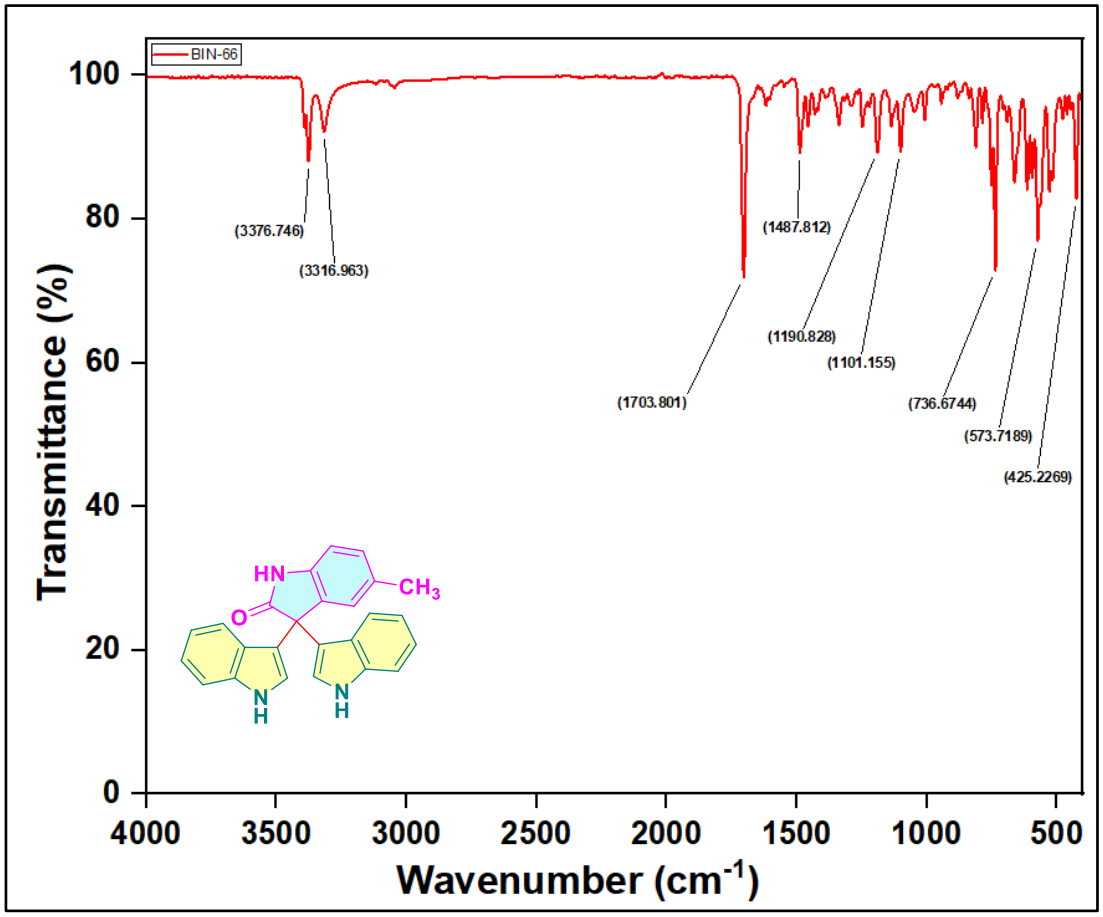


Fig. S22 FT-IR spectrum of **7af**.

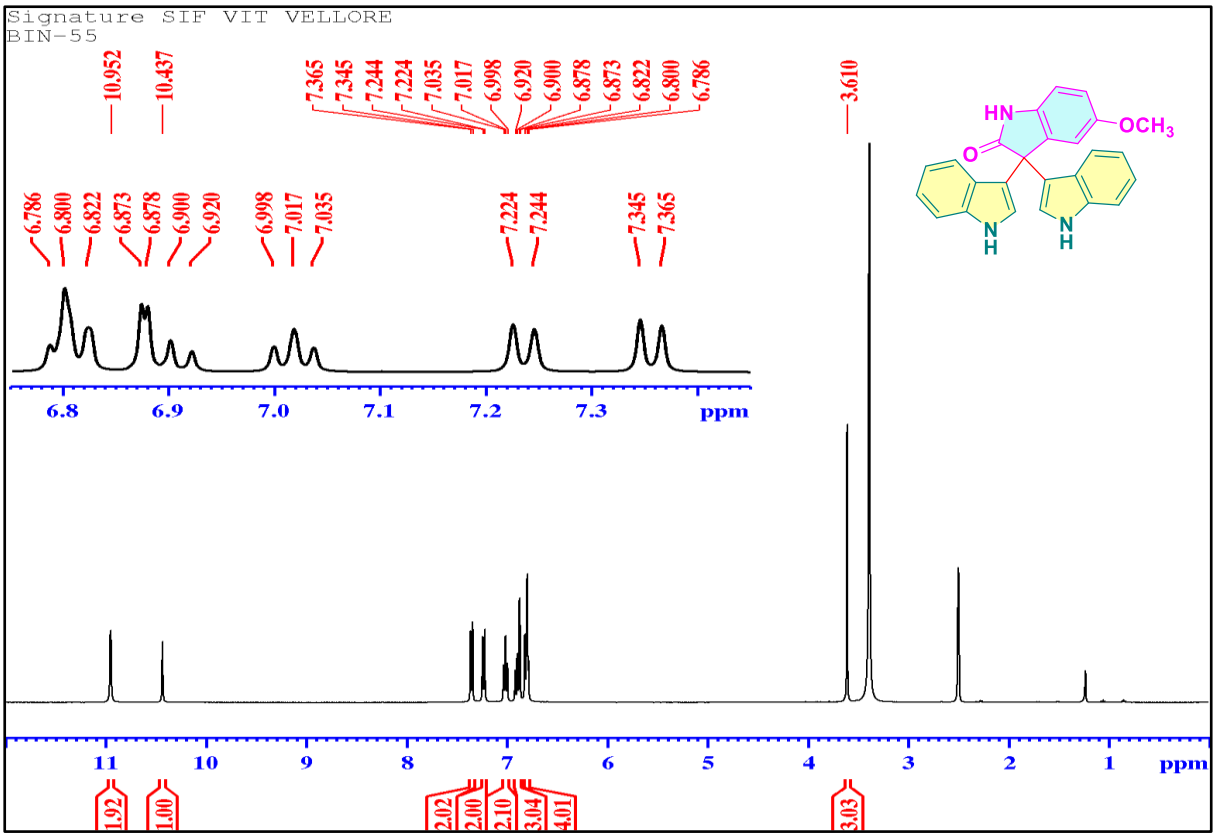


Fig. S23 ^{1}H NMR spectrum (400 MHz) of **7ag** in DMSO-d_6.

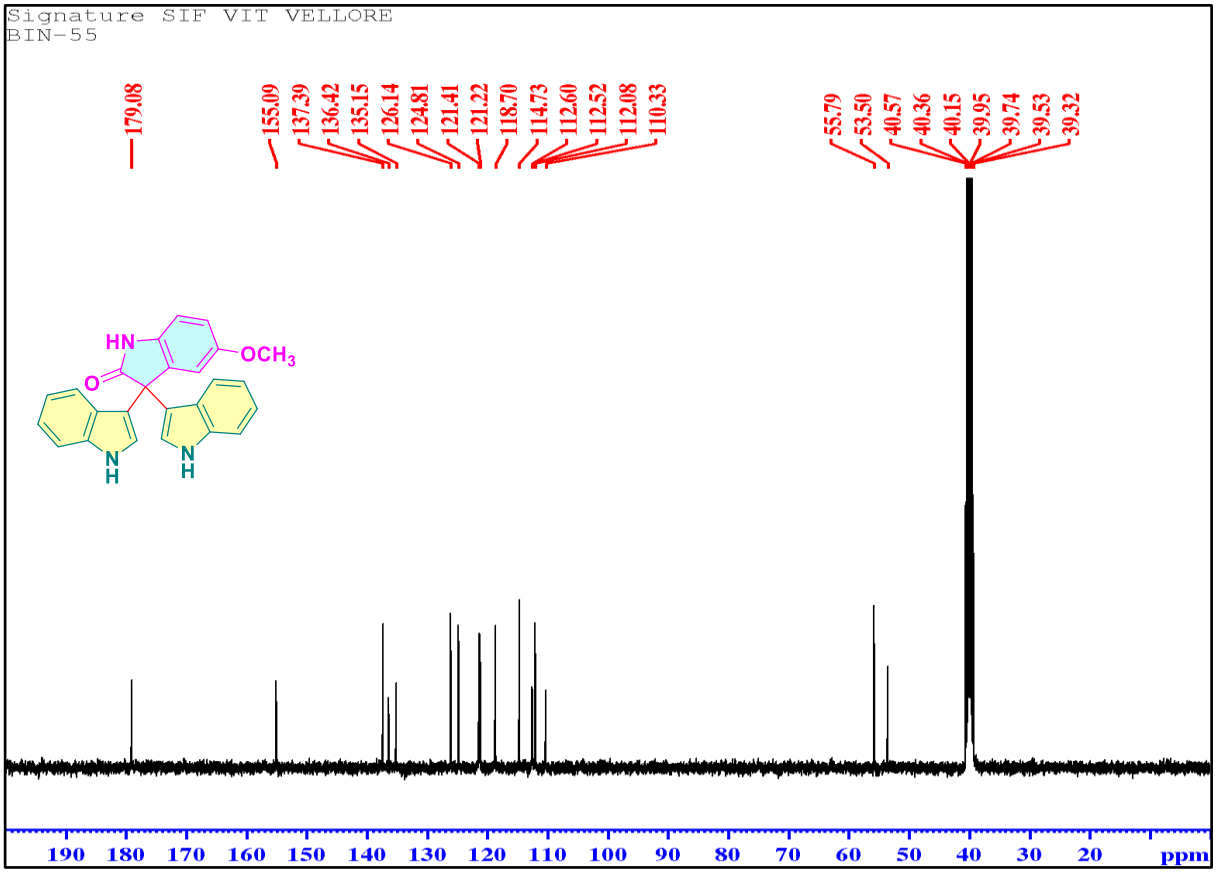


Fig. S24 ^{13}C NMR spectrum (100 MHz) of **7ag** in DMSO-d_6.

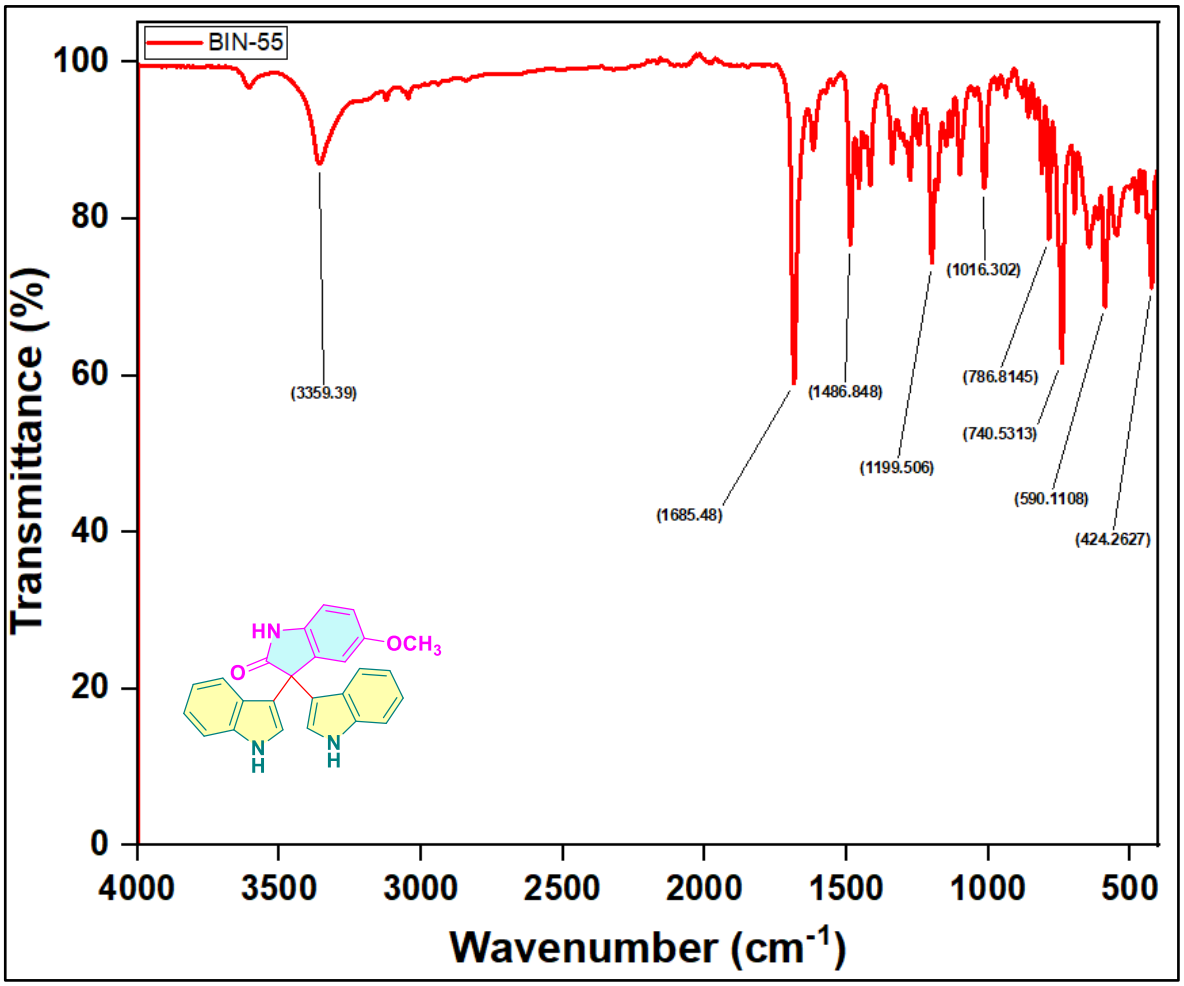


Fig. S25 FT-IR spectrum of **7ag**.

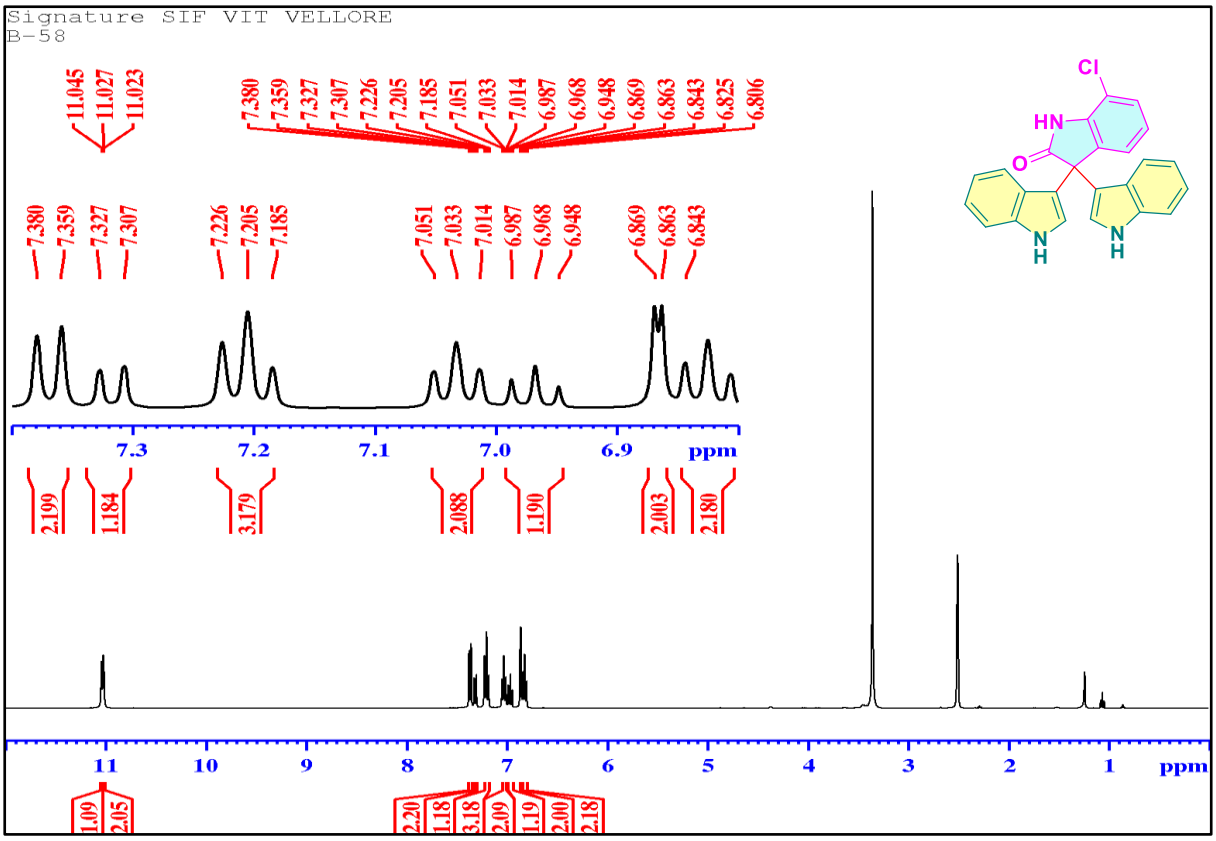


Fig. S26 ^{1}H NMR spectrum (400 MHz) of **7ah** in DMSO-d_6.

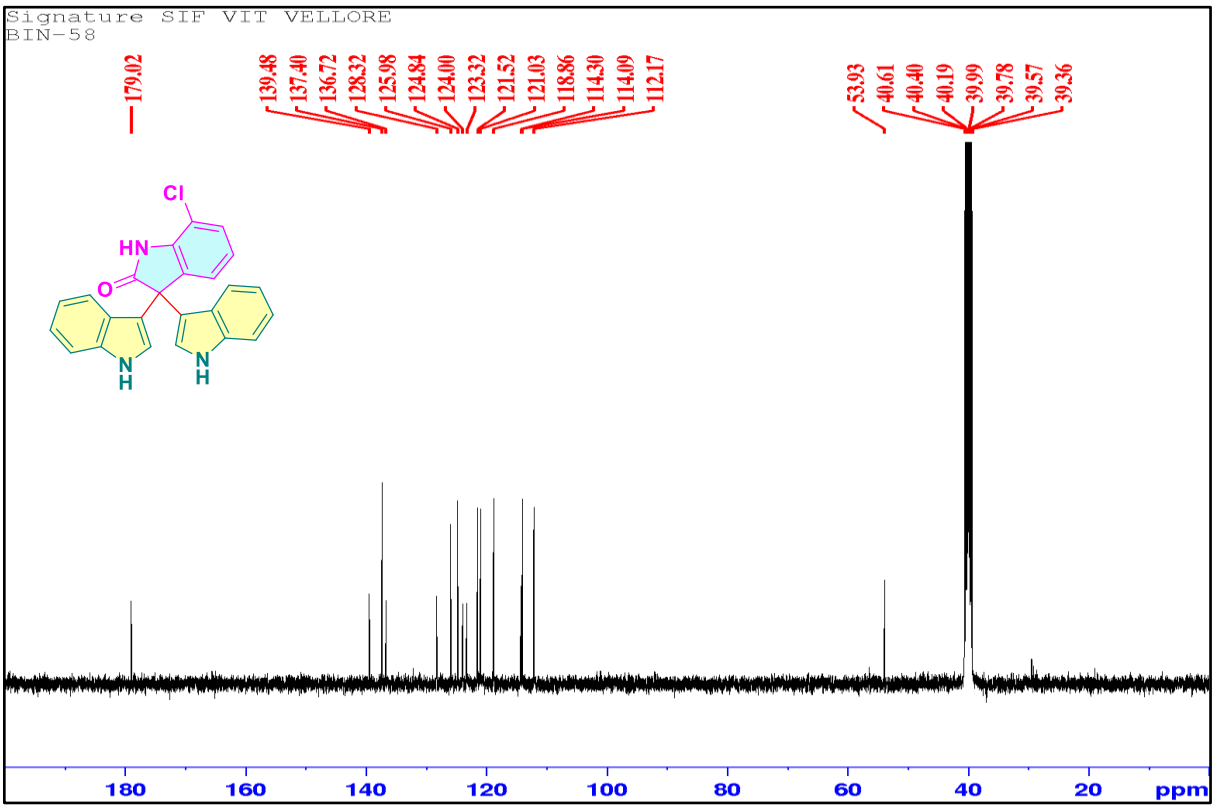


Fig. S27 ^{13}C NMR spectrum (100 MHz) of **7ah** in DMSO-d_6.

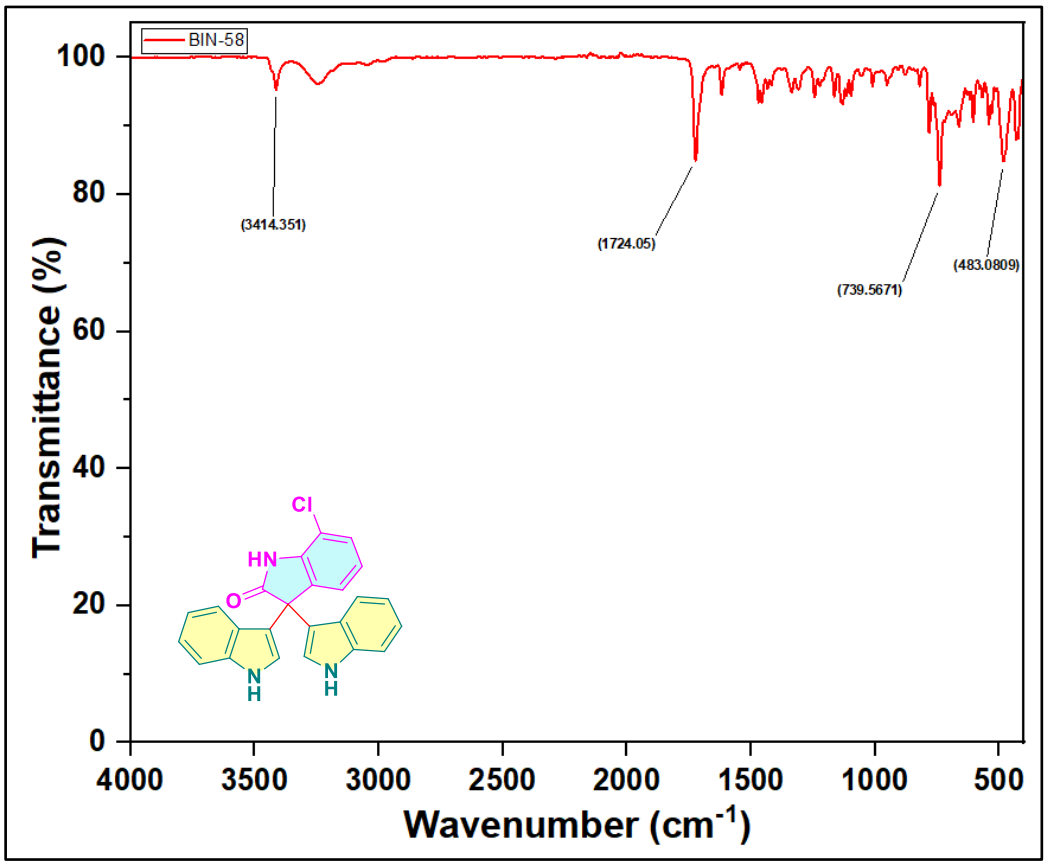


Fig. S28 FT-IR spectrum of **7ah**.

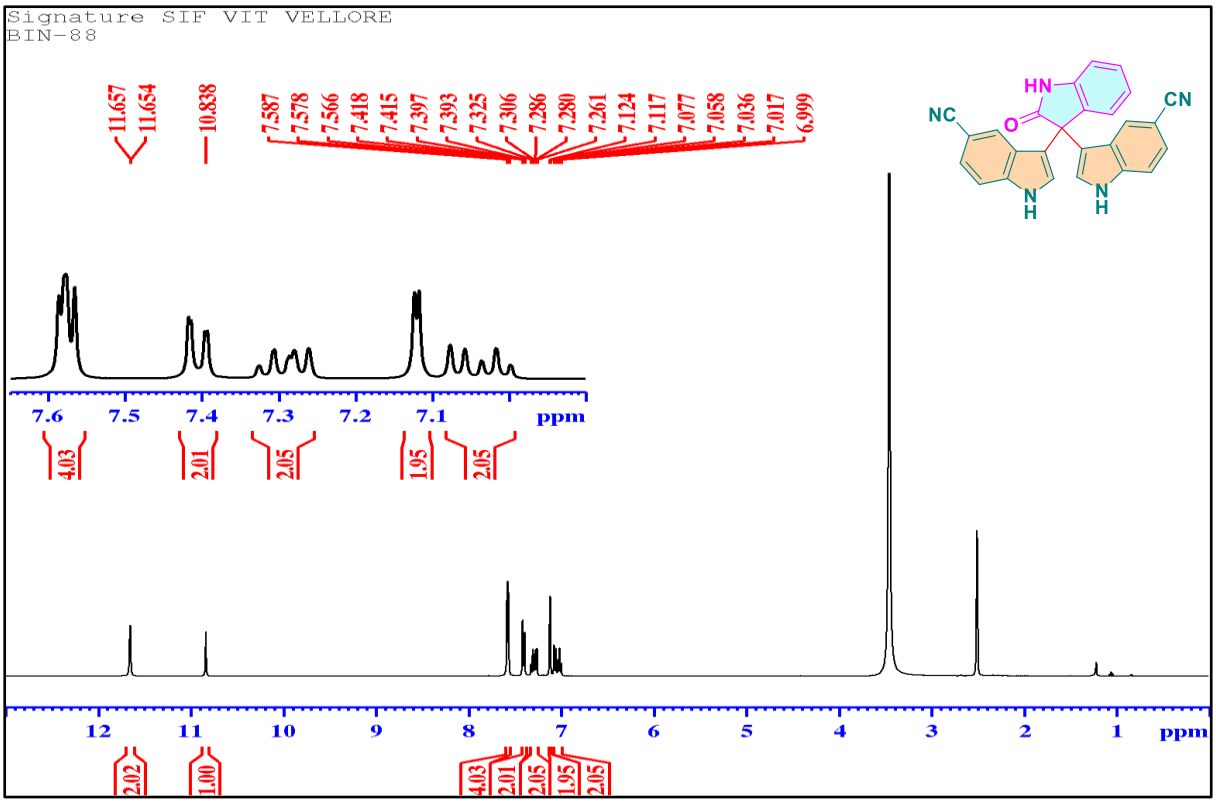


Fig. S29 ^{1}H NMR spectrum (400 MHz) of **7ba** in DMSO-d_6.

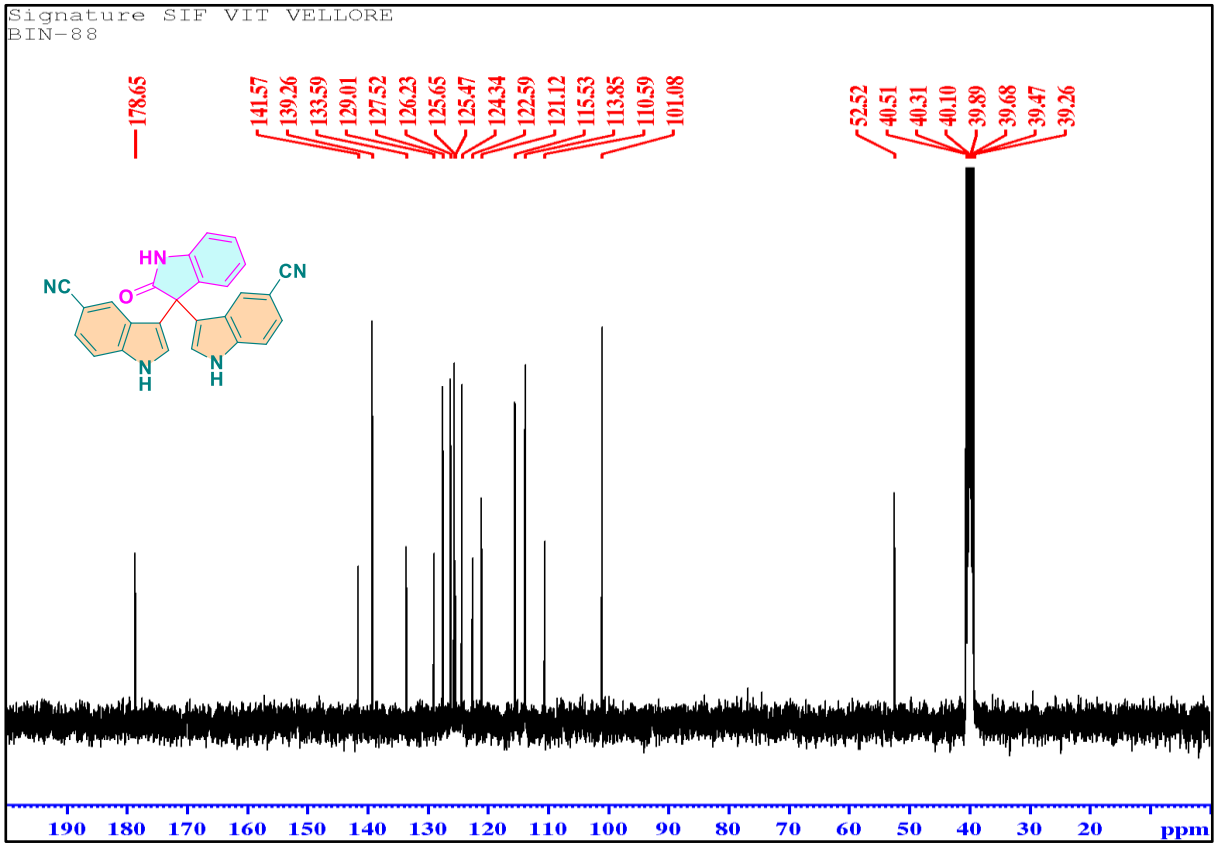


Fig. S30 ^{13}C NMR spectrum (100 MHz) of **7ba** in DMSO-d_6.

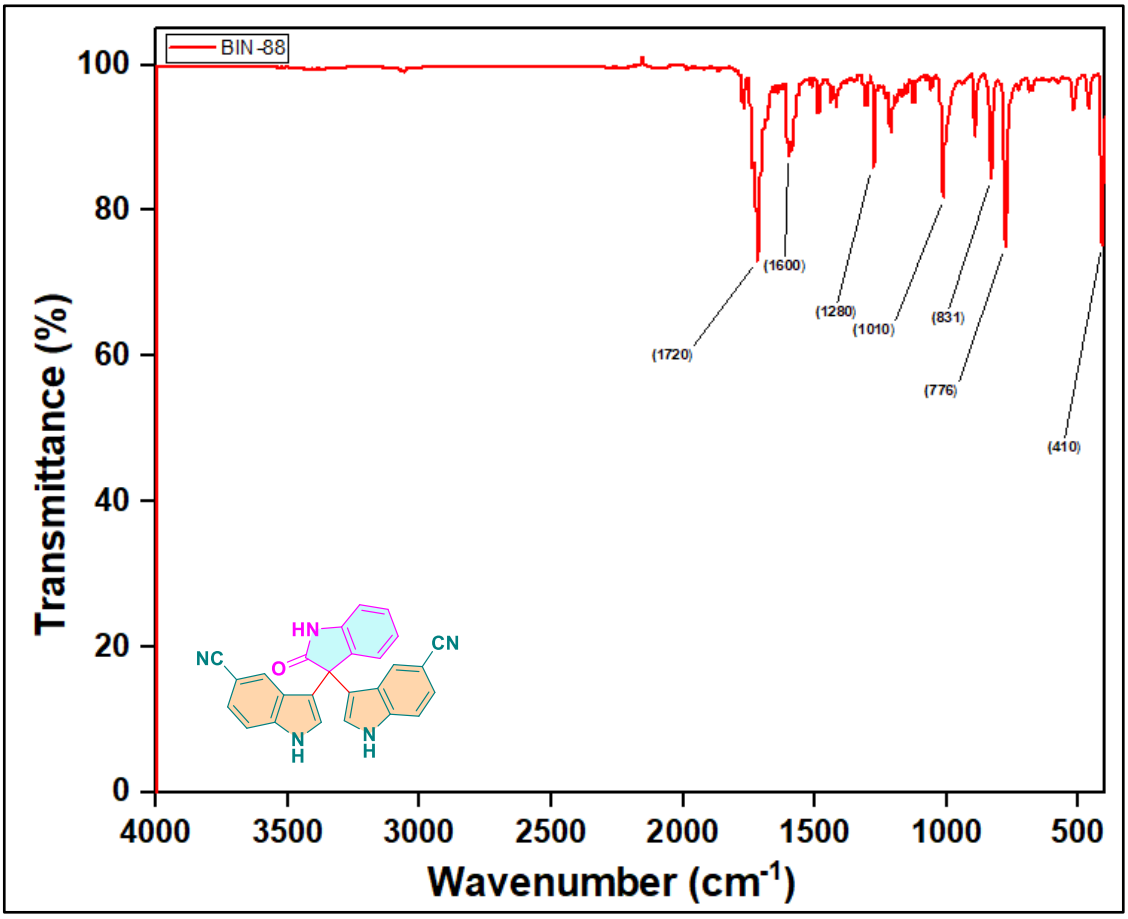


Fig. S31 FT-IR spectrum of **7ba**.

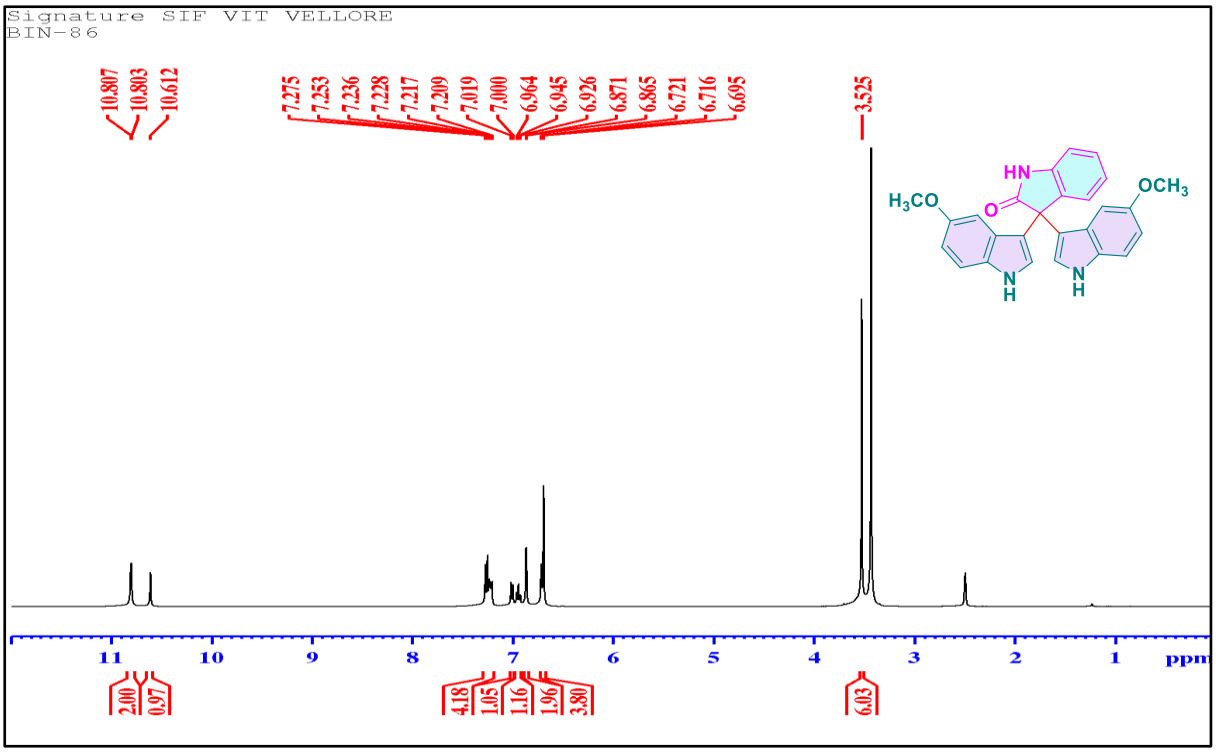


Fig. S32 ^{1}H NMR spectrum (400 MHz) of **7ca** in DMSO-d_6.

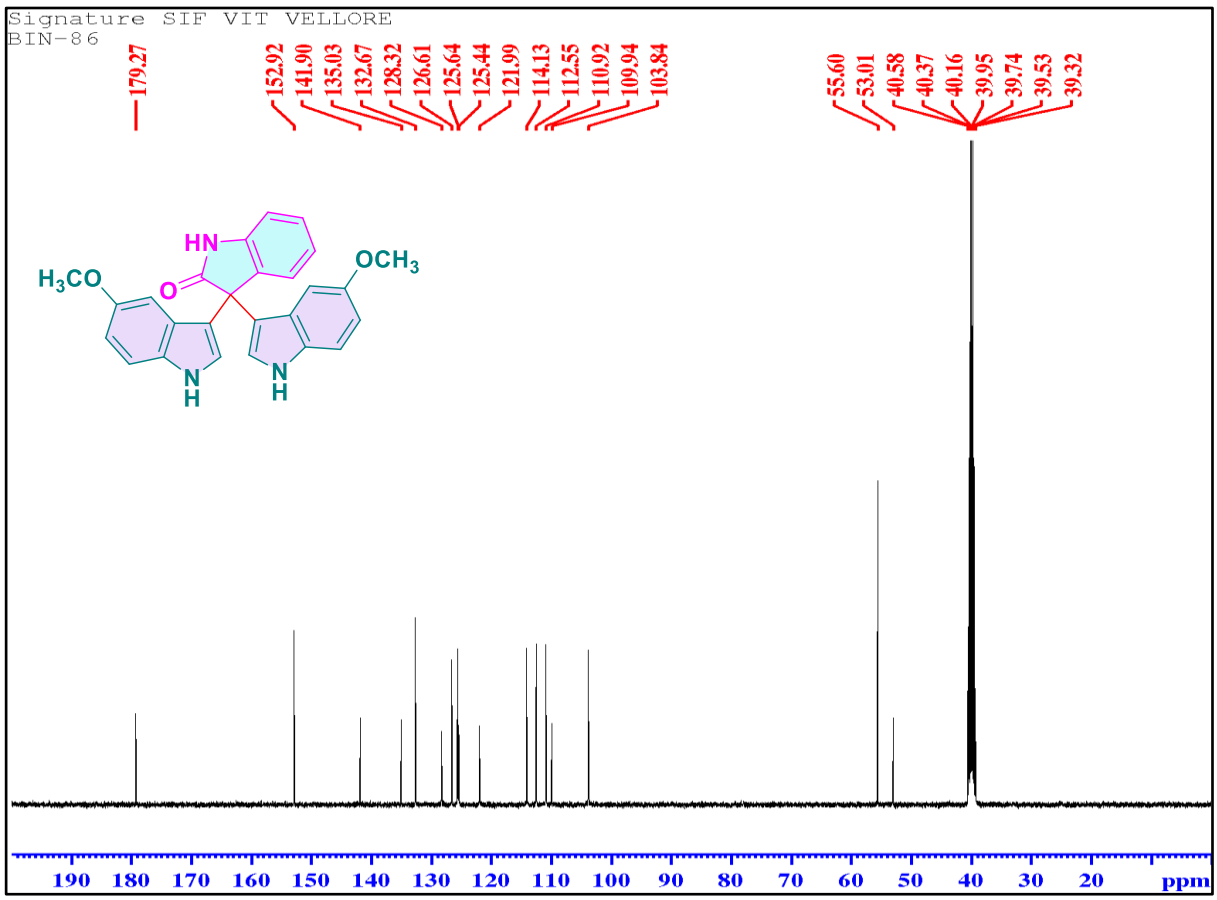


Fig. S33 ^{13}C NMR spectrum (100 MHz) of **7ca** in DMSO-d_6.

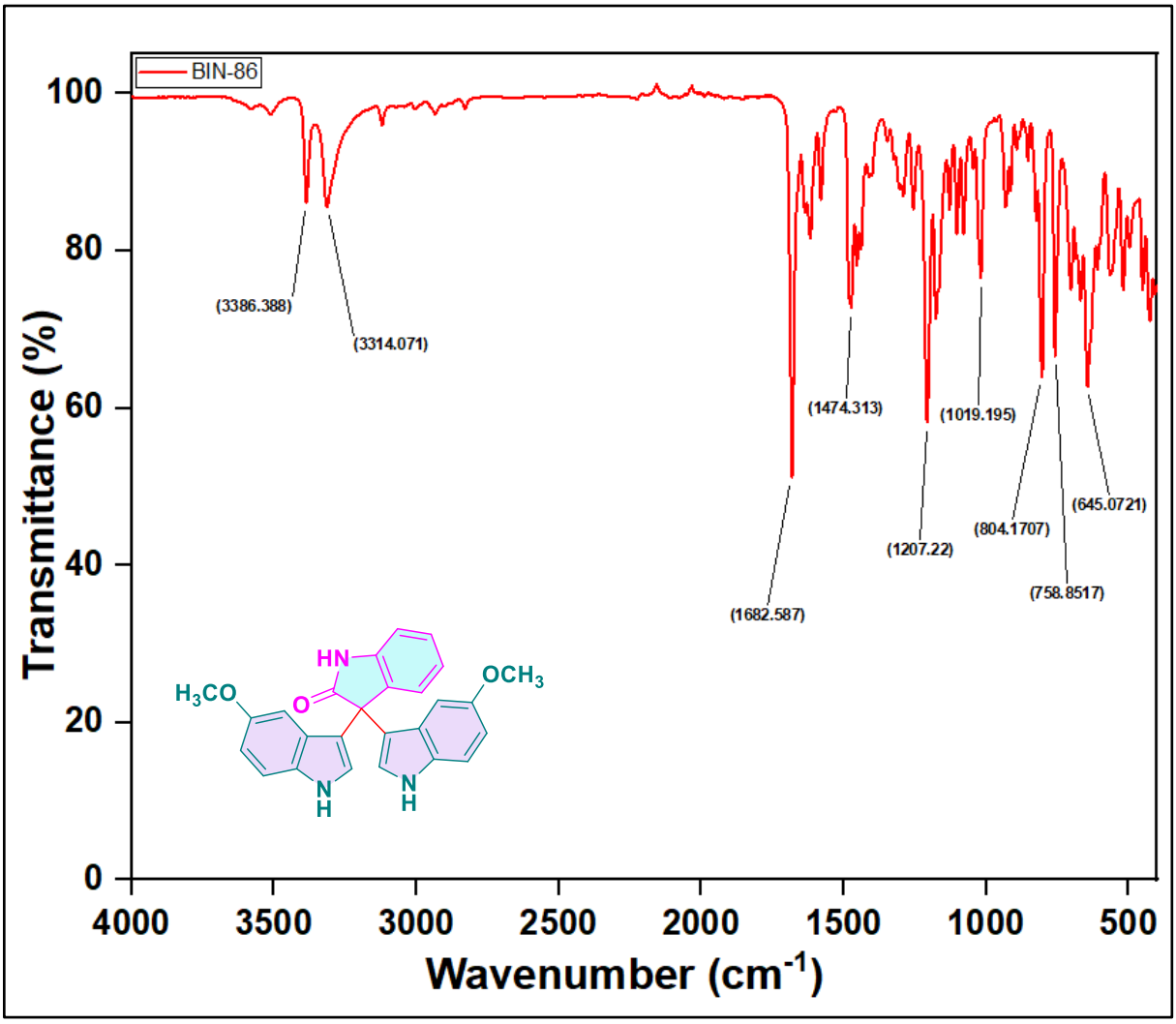


Fig. S34 FT-IR spectrum of **7ca**.

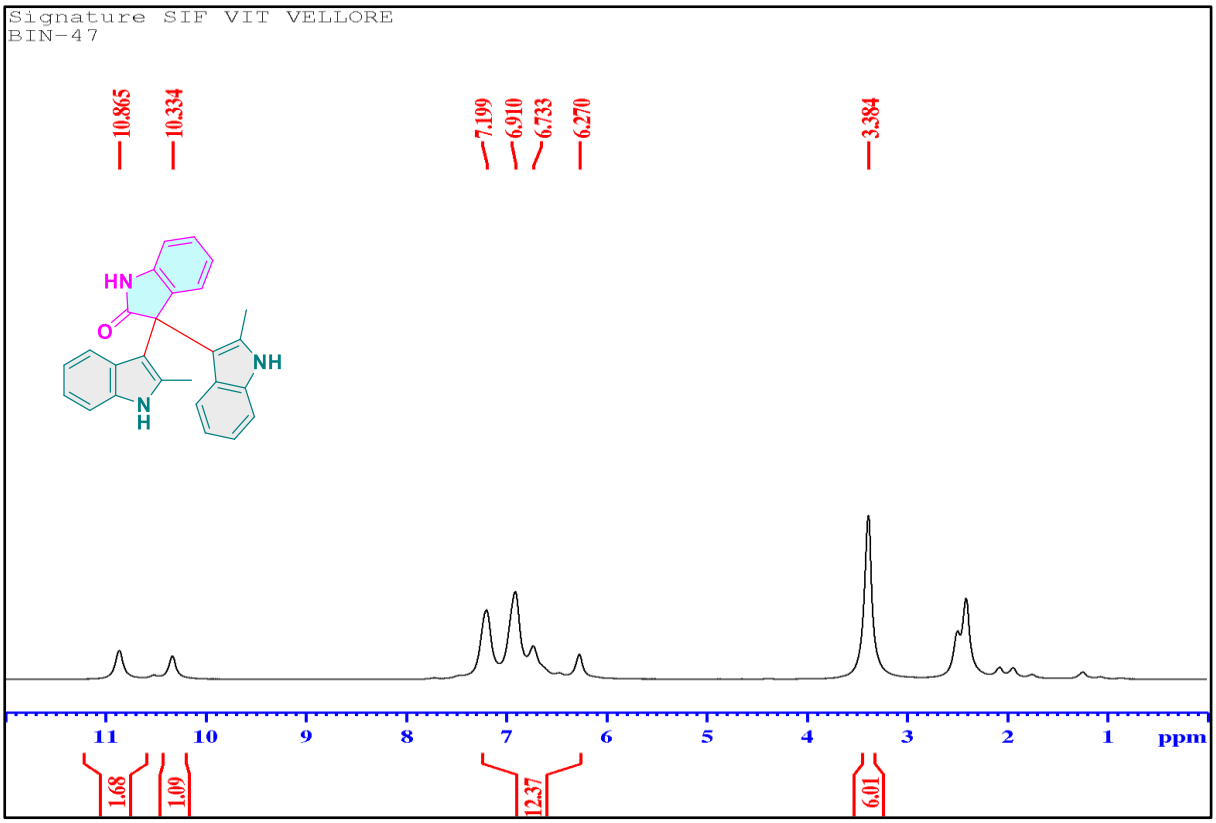


Fig. S35 ^{1}H NMR spectrum (400 MHz) of **7da** in DMSO-d_6.

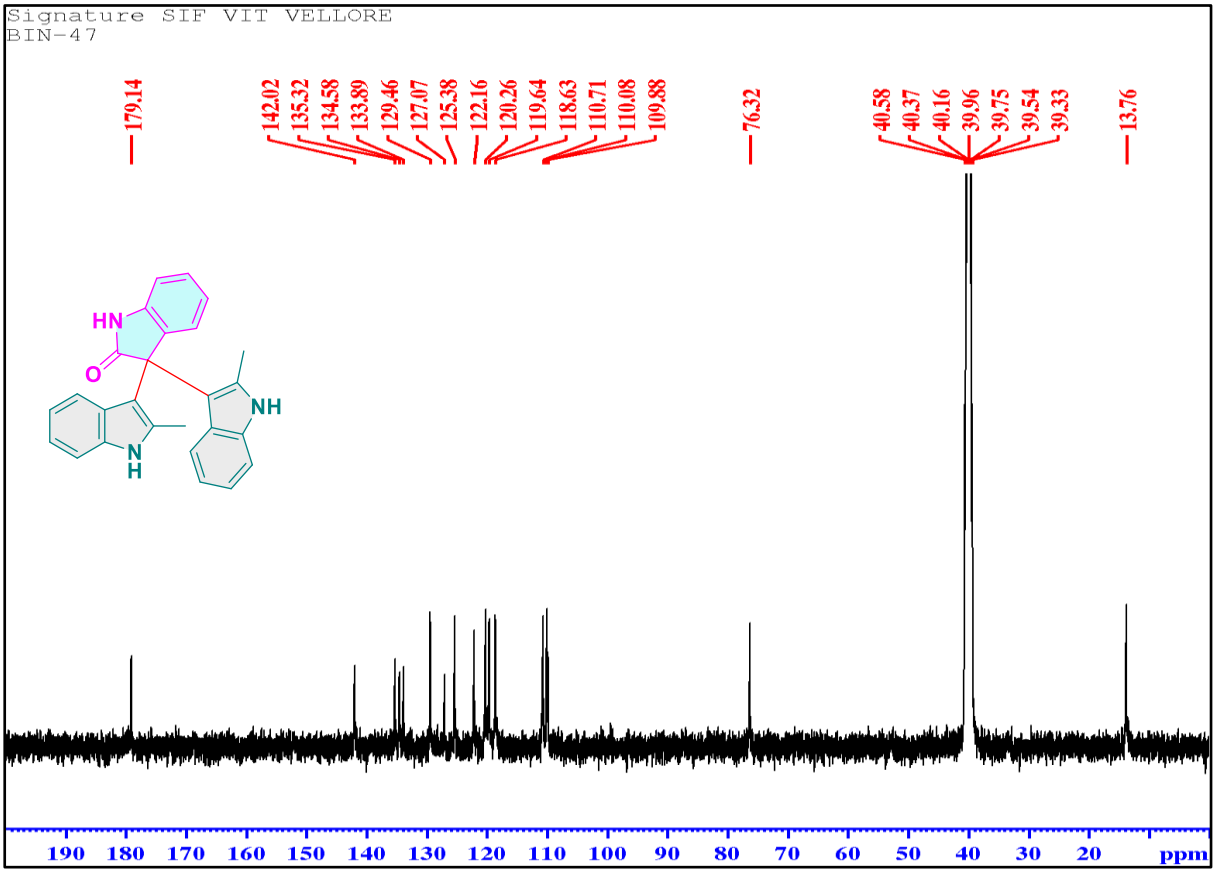


Fig. S36 ^{13}C NMR spectrum (100 MHz) of **7da** in DMSO-d_6.

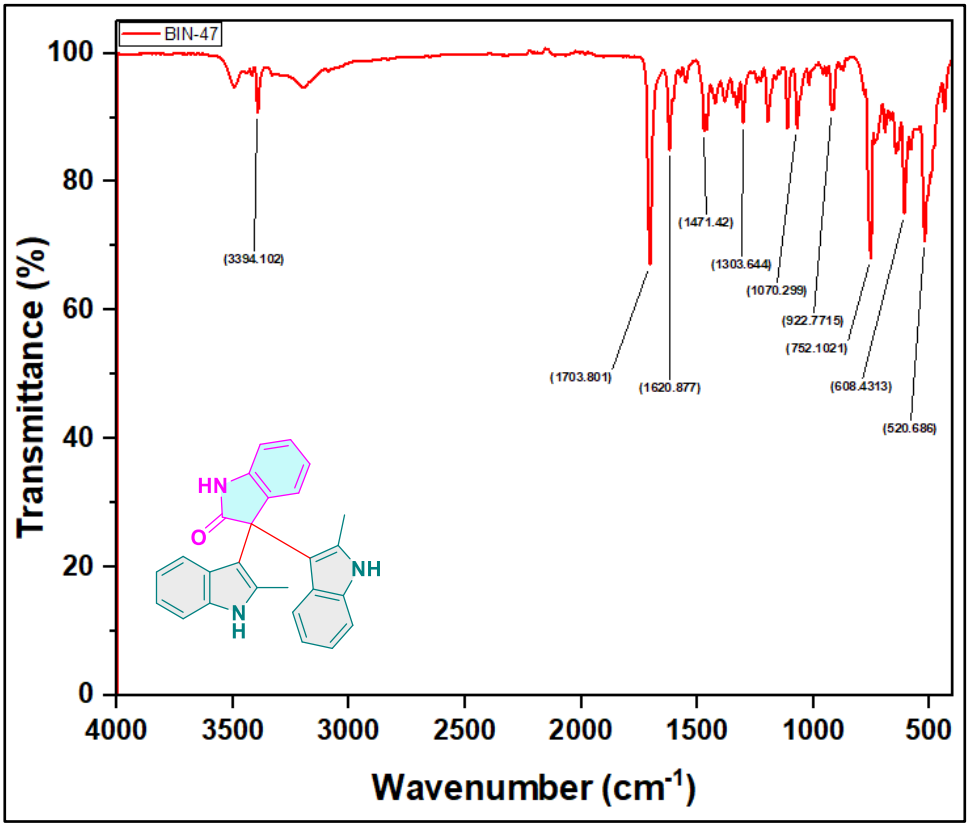


Fig. S37 FT-IR spectrum of **7da**.

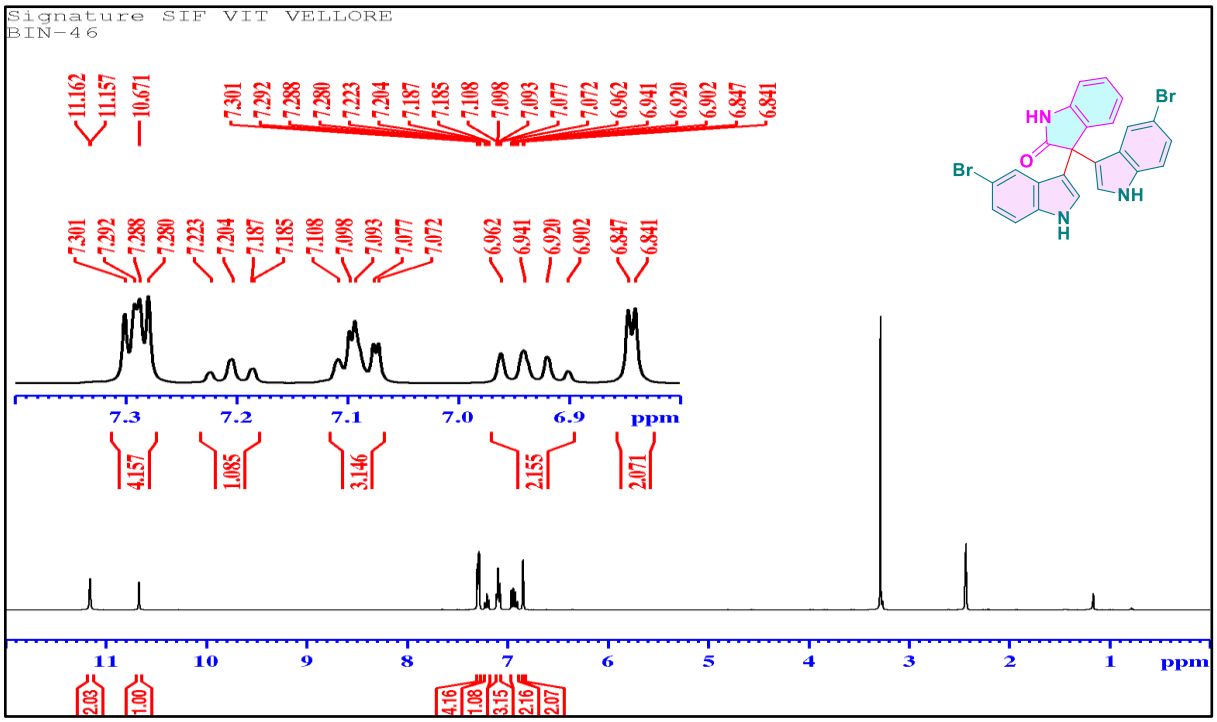


Fig. S38 ^{1}H NMR spectrum (400 MHz) of **7ea** in DMSO-d_6.

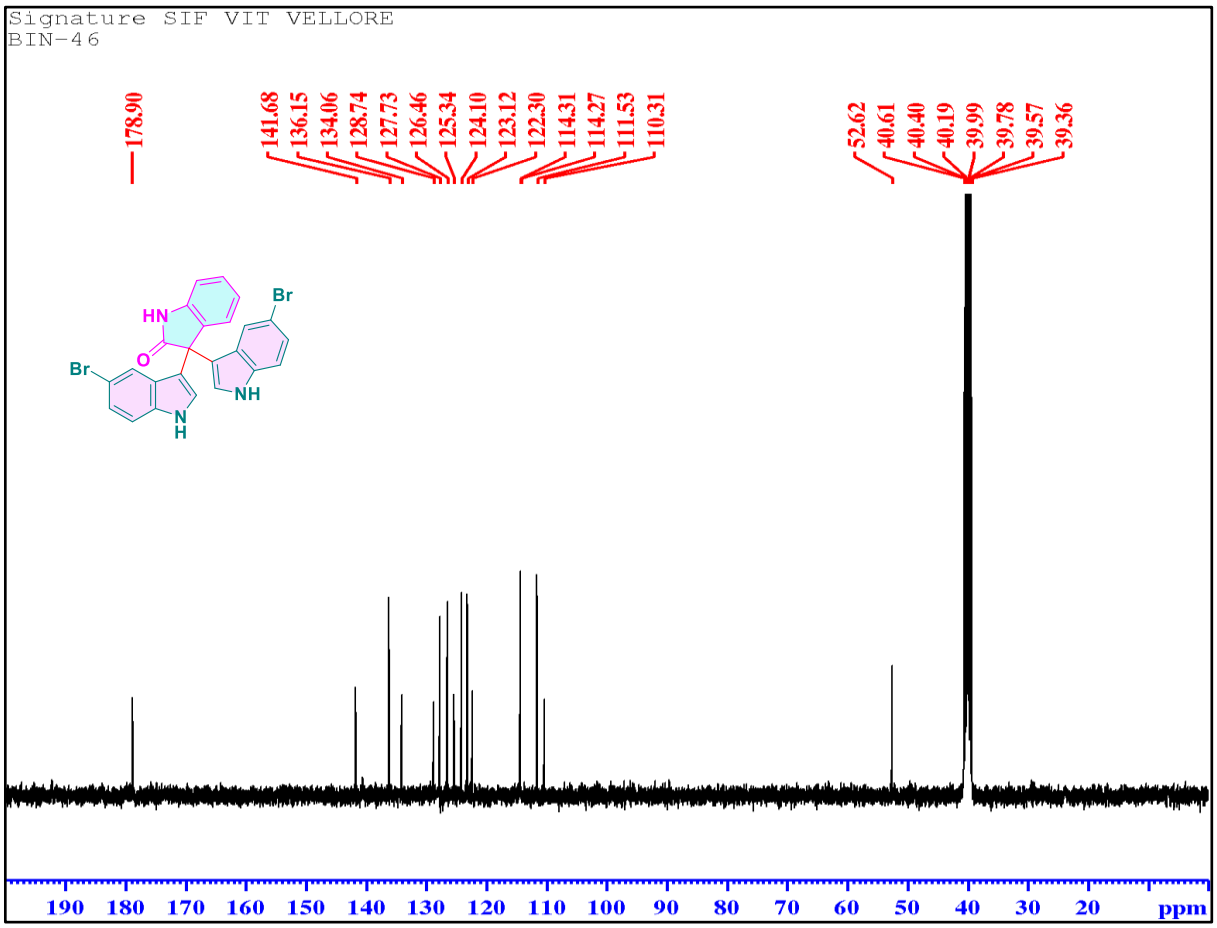


Fig. S39 ^{13}C NMR spectrum (100 MHz) of **7ea** in DMSO-d_6.

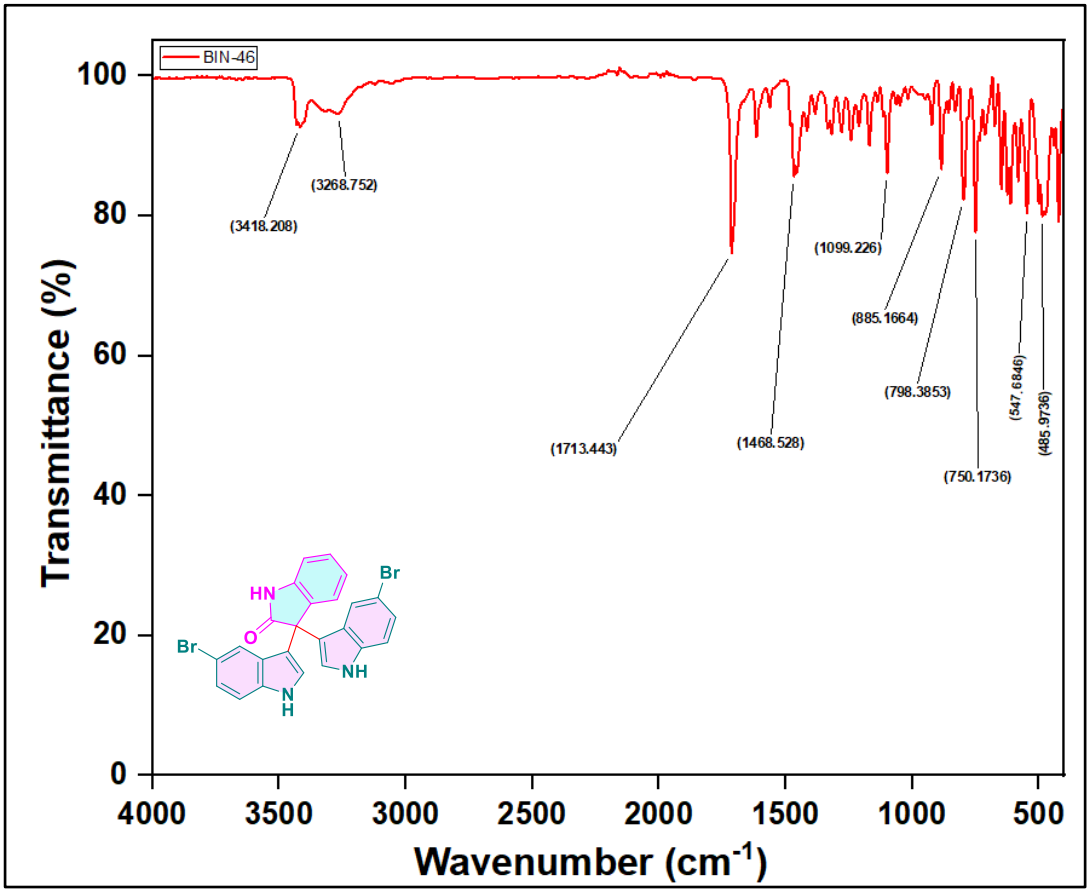


Fig. S40 FT-IR spectrum of **7ea**.

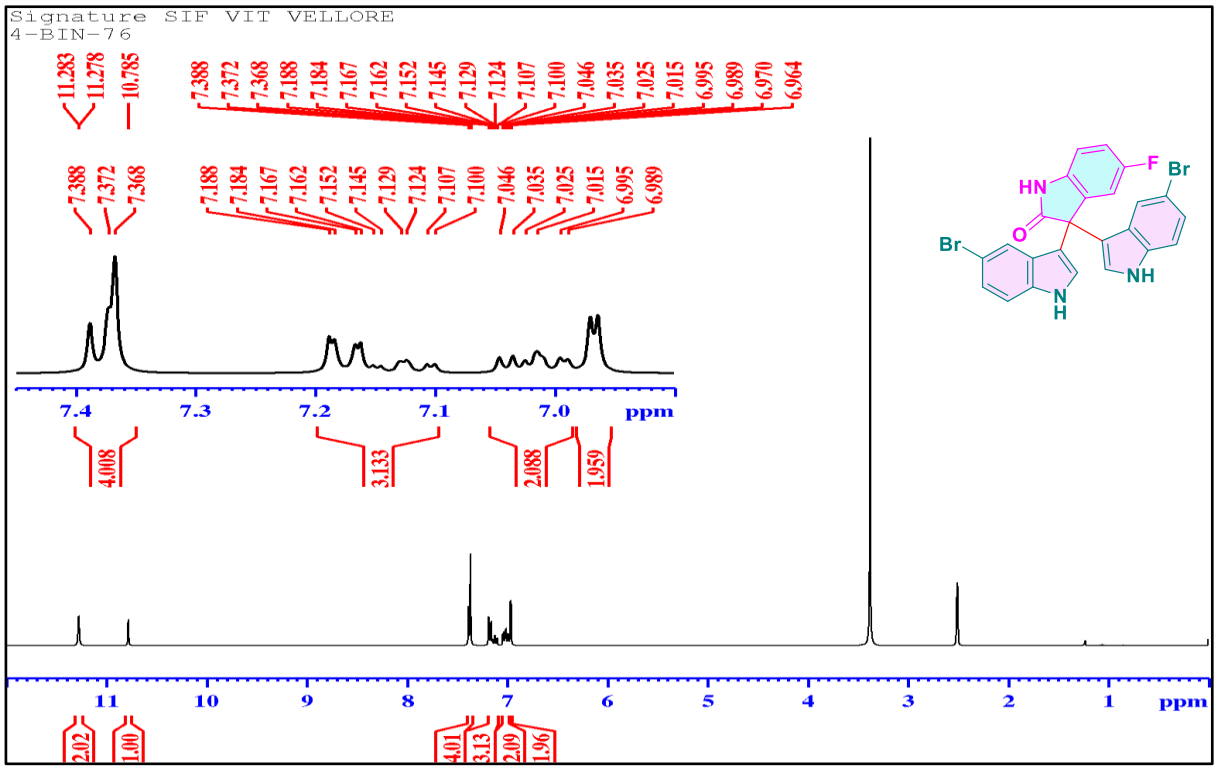


Fig. S41 ^{1}H NMR spectrum (400 MHz) of **7ec** in DMSO-d_6.

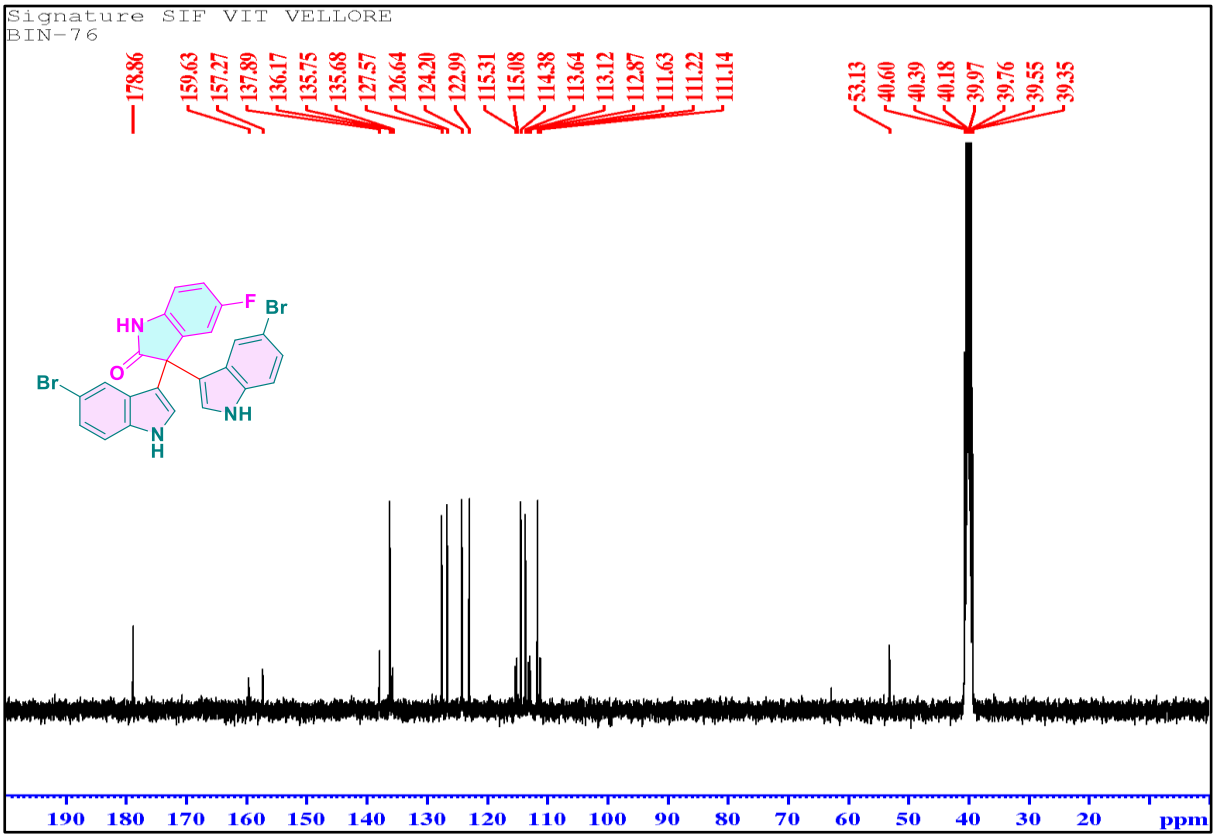


Fig. S42 ^{13}C NMR spectrum (100 MHz) of **7ec** in DMSO-d_6.

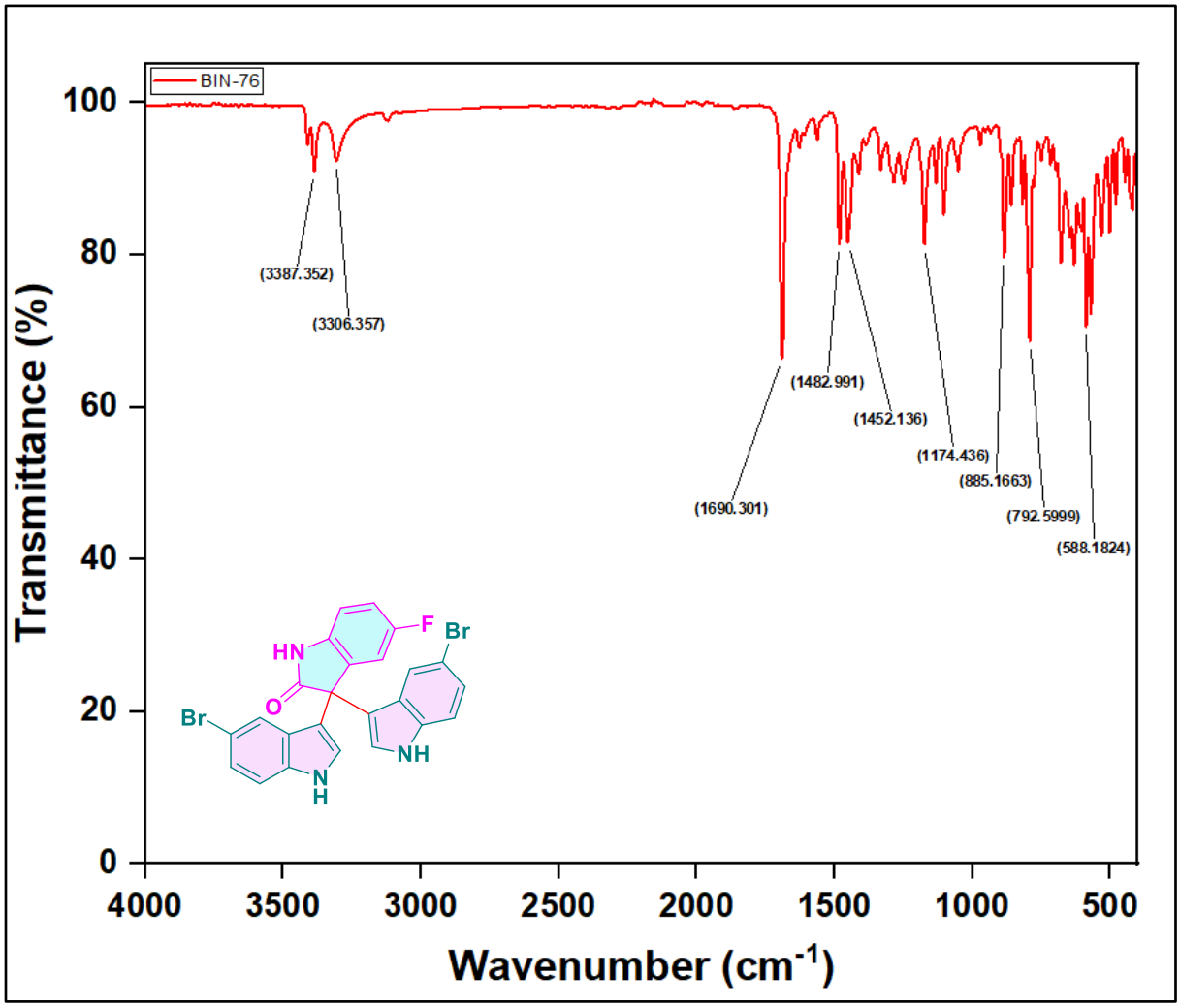


Fig. S43 FT-IR spectrum of **7ec**.

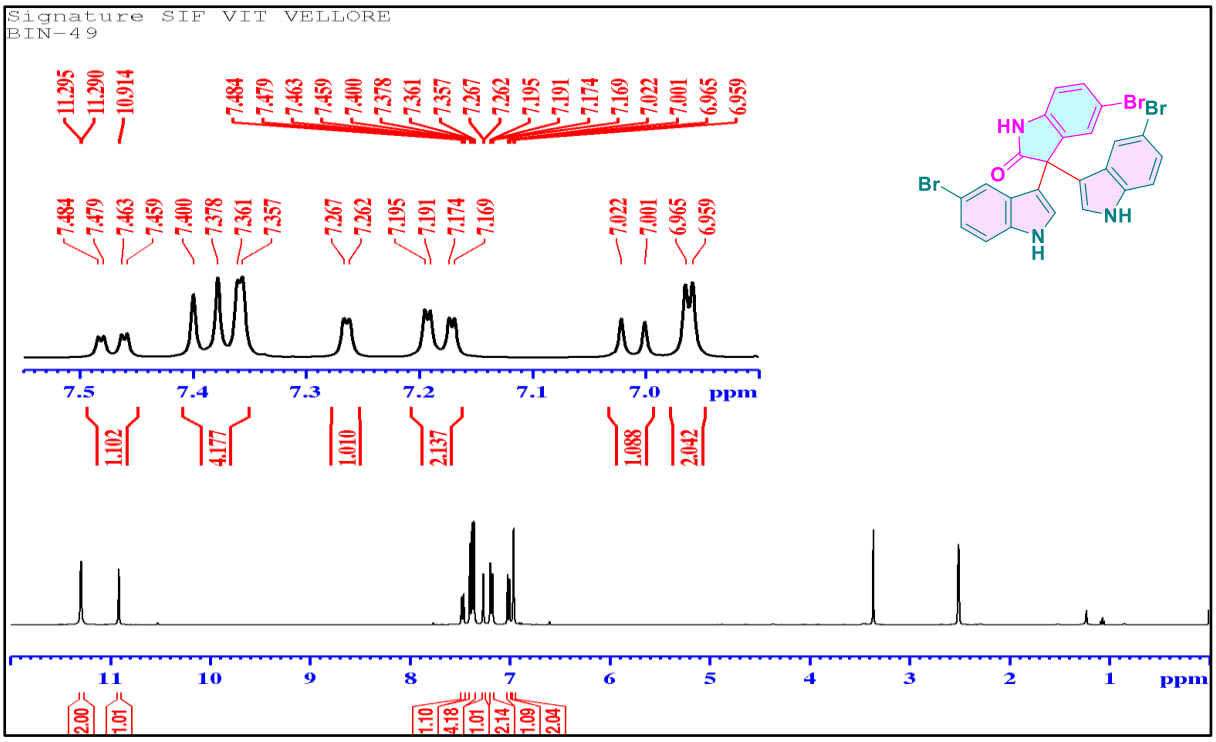


Fig. S44 ^{1}H NMR spectrum (400 MHz) of **7ed** in DMSO-d_6.

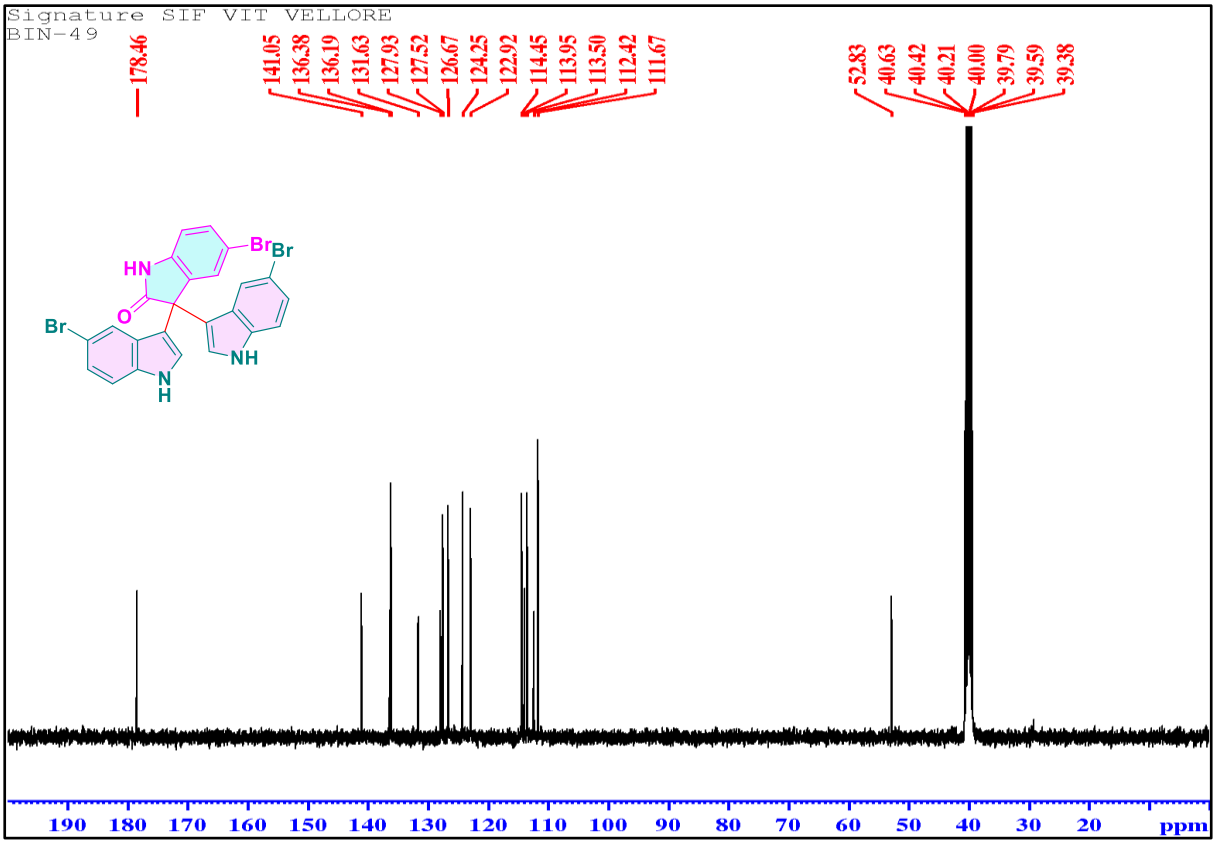


Fig. S45 ^{13}C NMR spectrum (100 MHz) of **7ed** in DMSO-d_6.

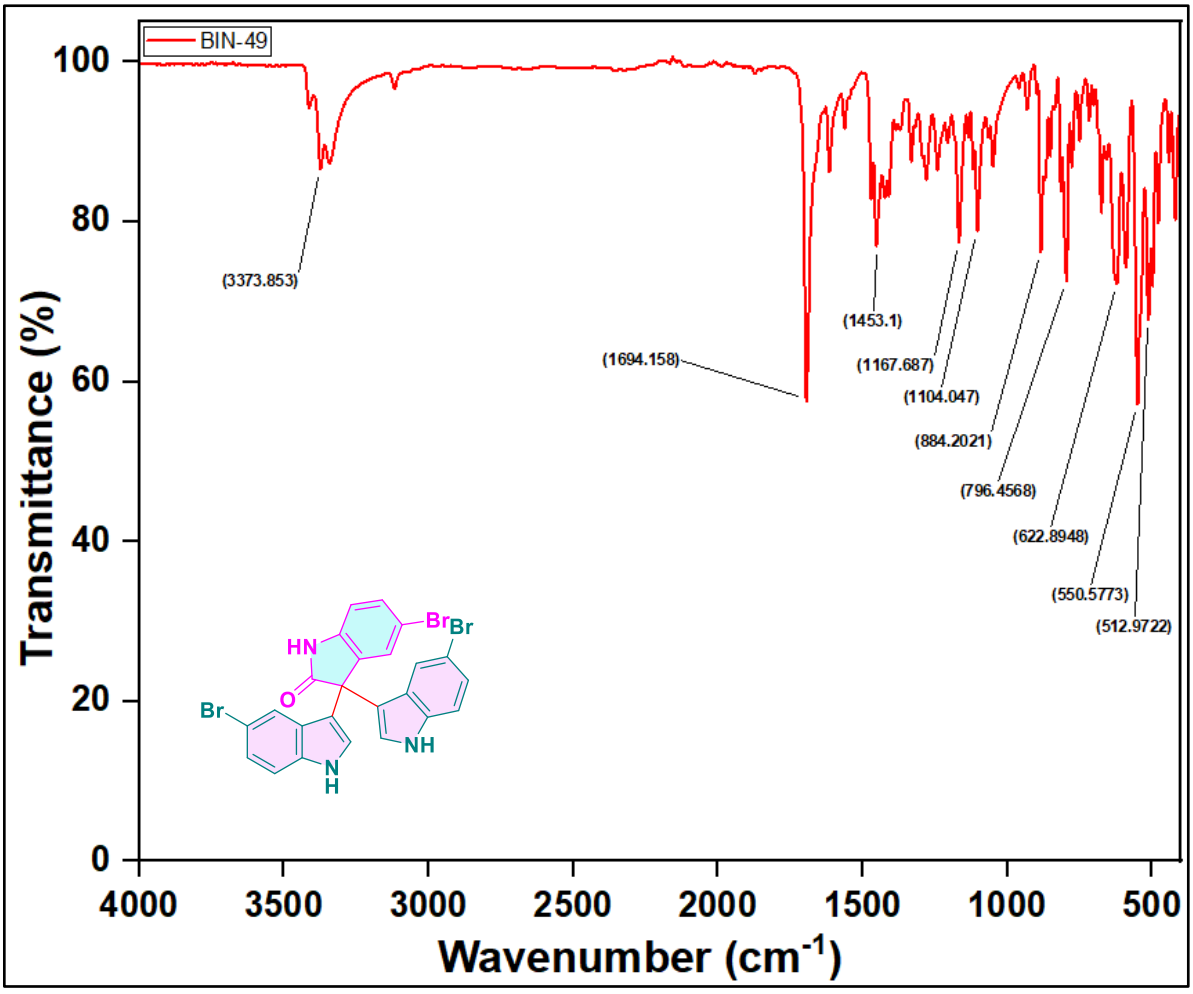


Fig. S46 FT-IR spectrum of **7ed**.

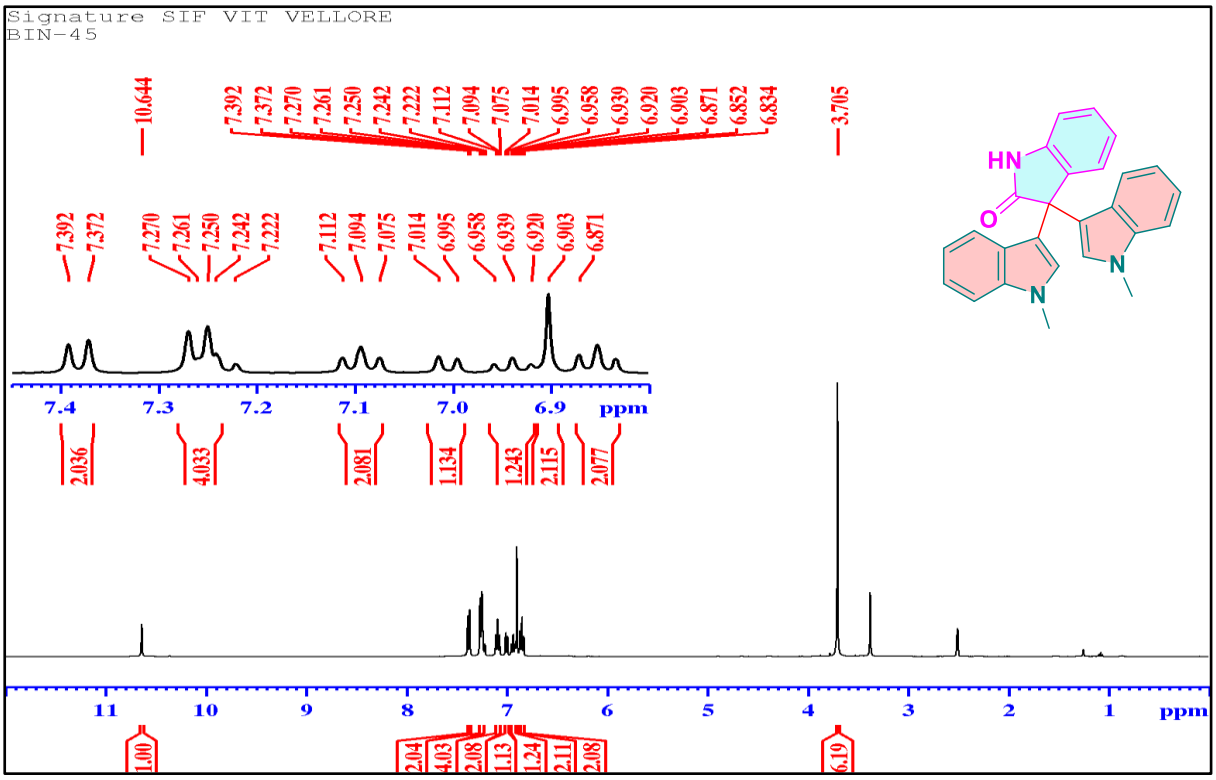


Fig. S47 ^{1}H NMR spectrum (400 MHz) of **7fa** in DMSO-d_6.

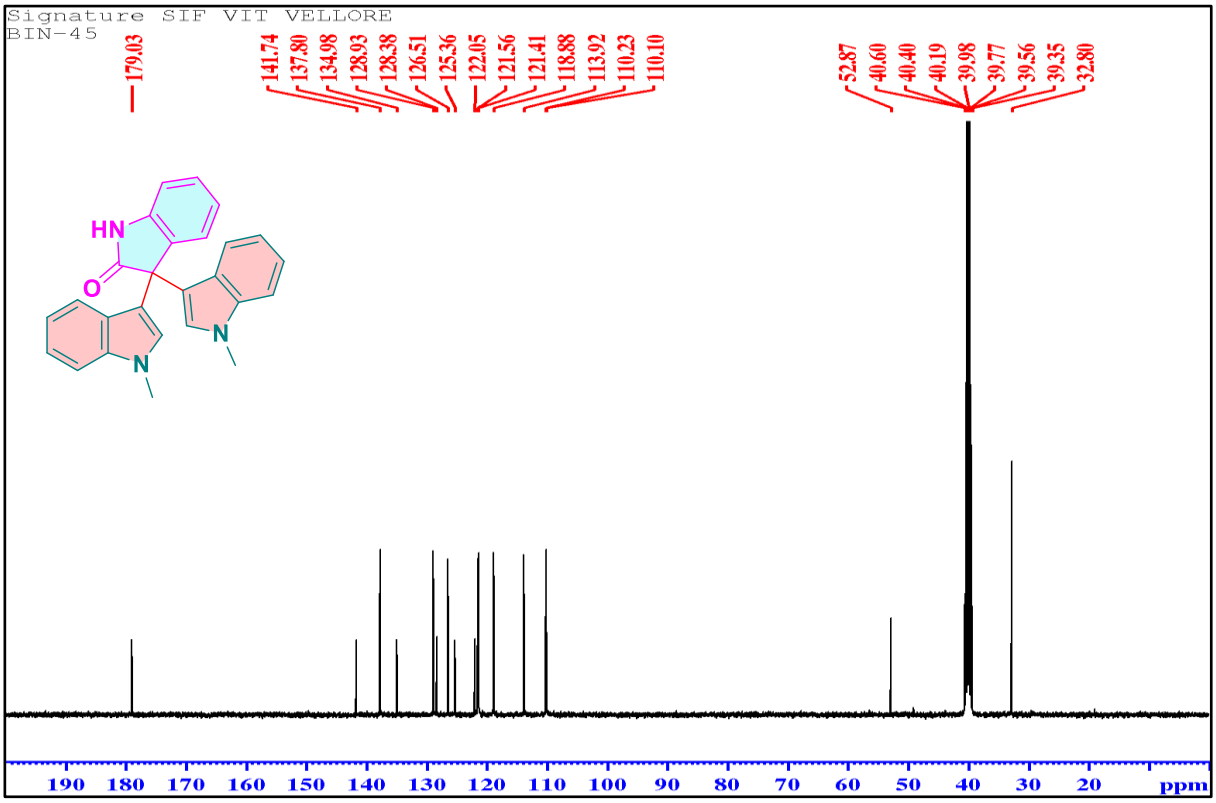


Fig. S48 ^{13}C NMR spectrum (100 MHz) of **7fa** in DMSO-d_6.

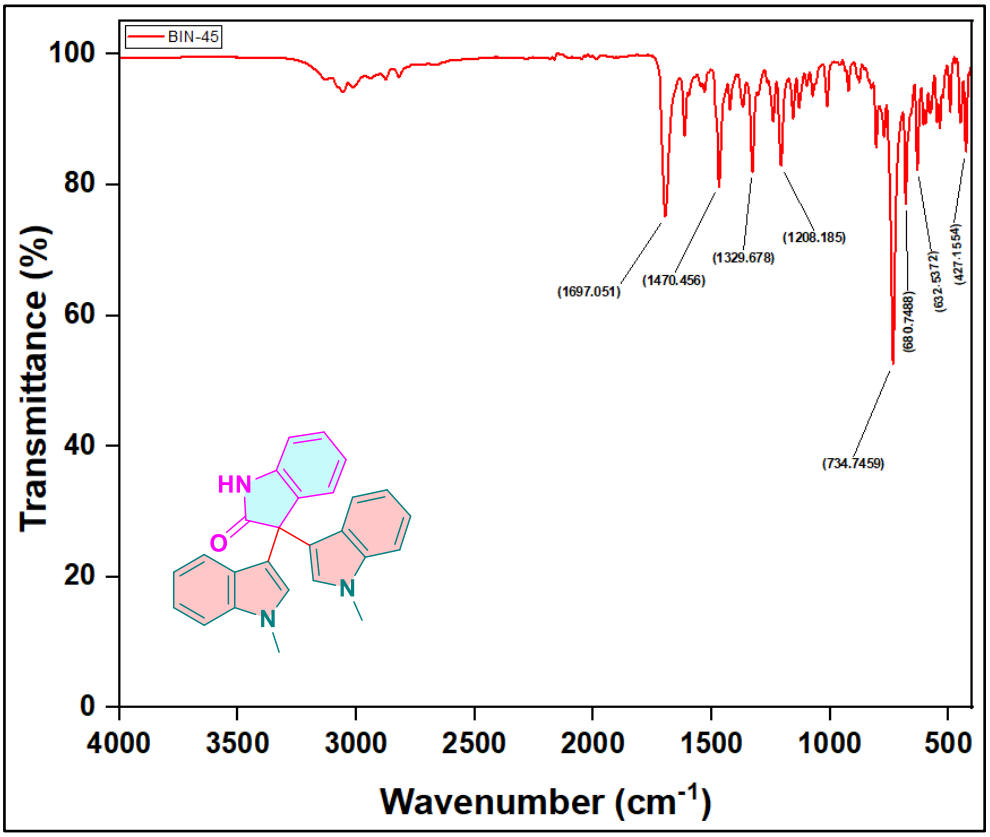


Fig. S49 FT-IR spectrum of **7fa**.

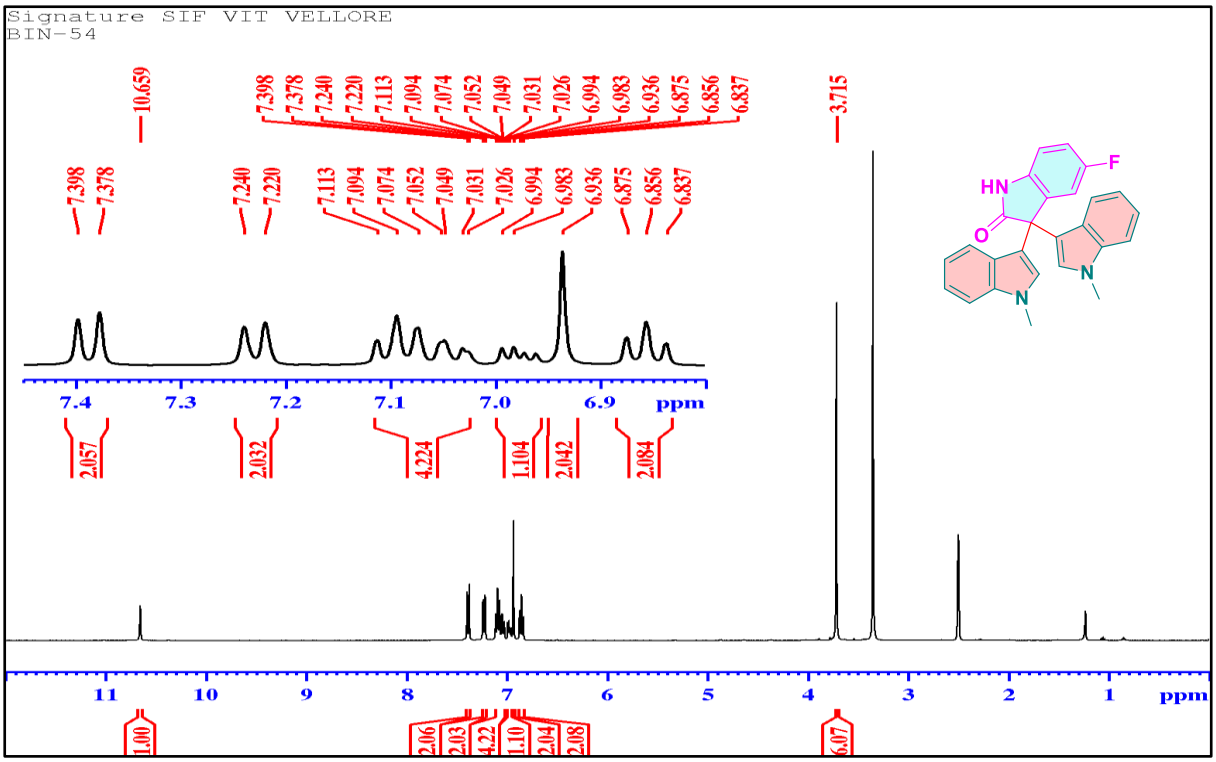


Fig. S50 ^{1}H NMR spectrum (400 MHz) of **7fb** in DMSO-d_6.

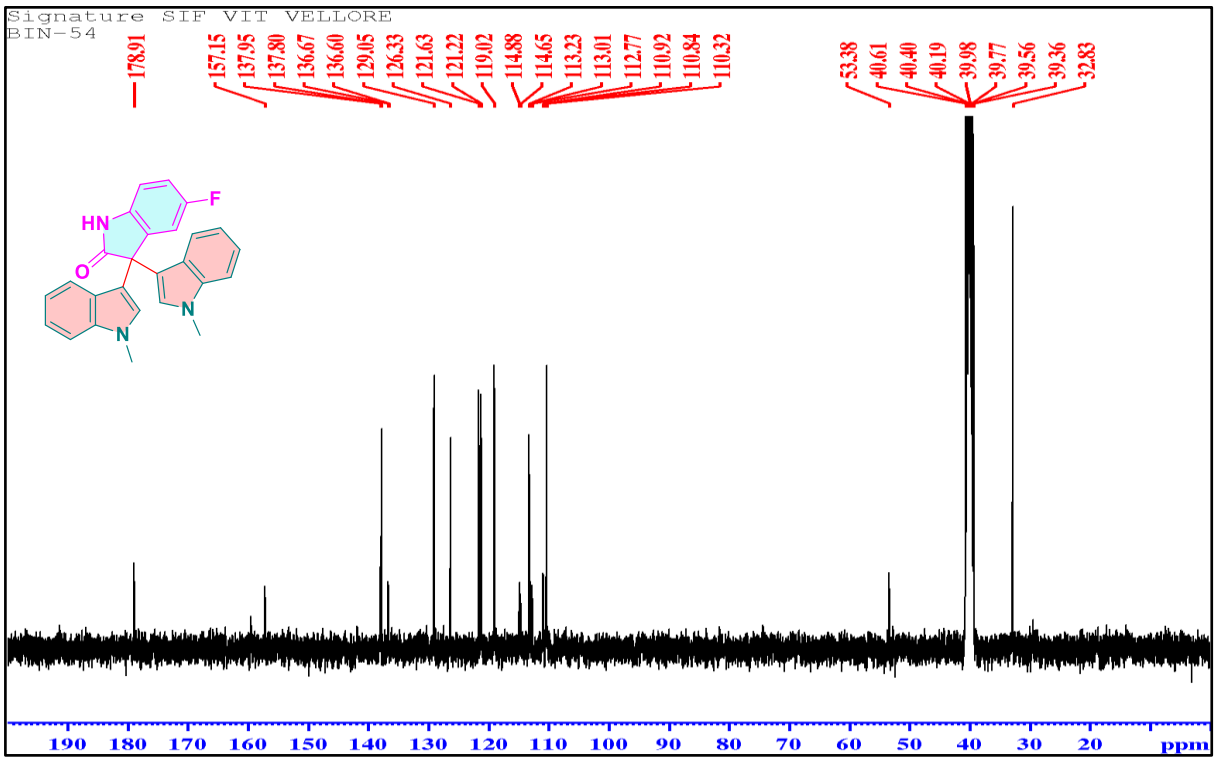


Fig. S51 ^{13}C NMR spectrum (100 MHz) of **7fb** in DMSO-d_6.

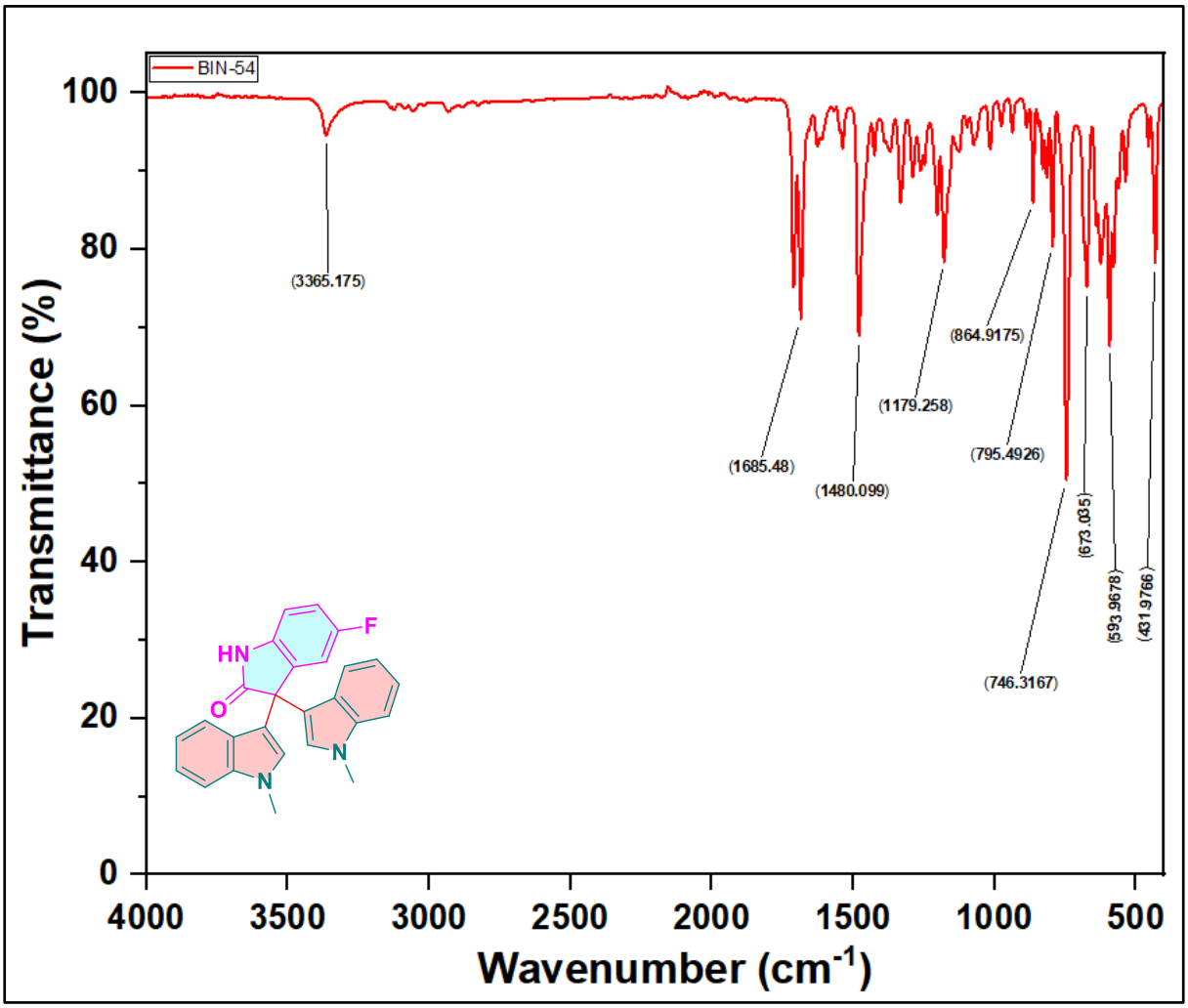


Fig. S52 FT-IR spectrum of **7fb**.

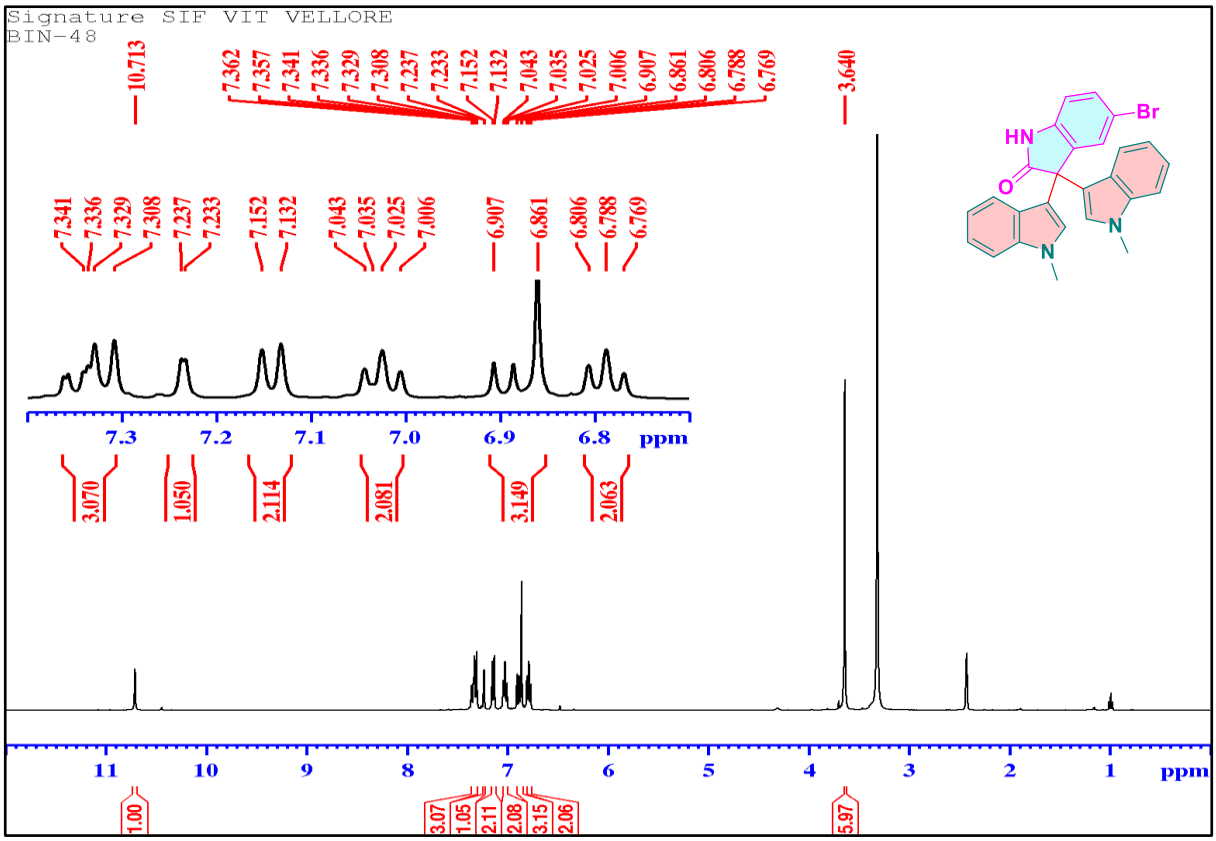


Fig. S53 ^{1}H NMR spectrum (400 MHz) of **7fd** in DMSO-d_6.

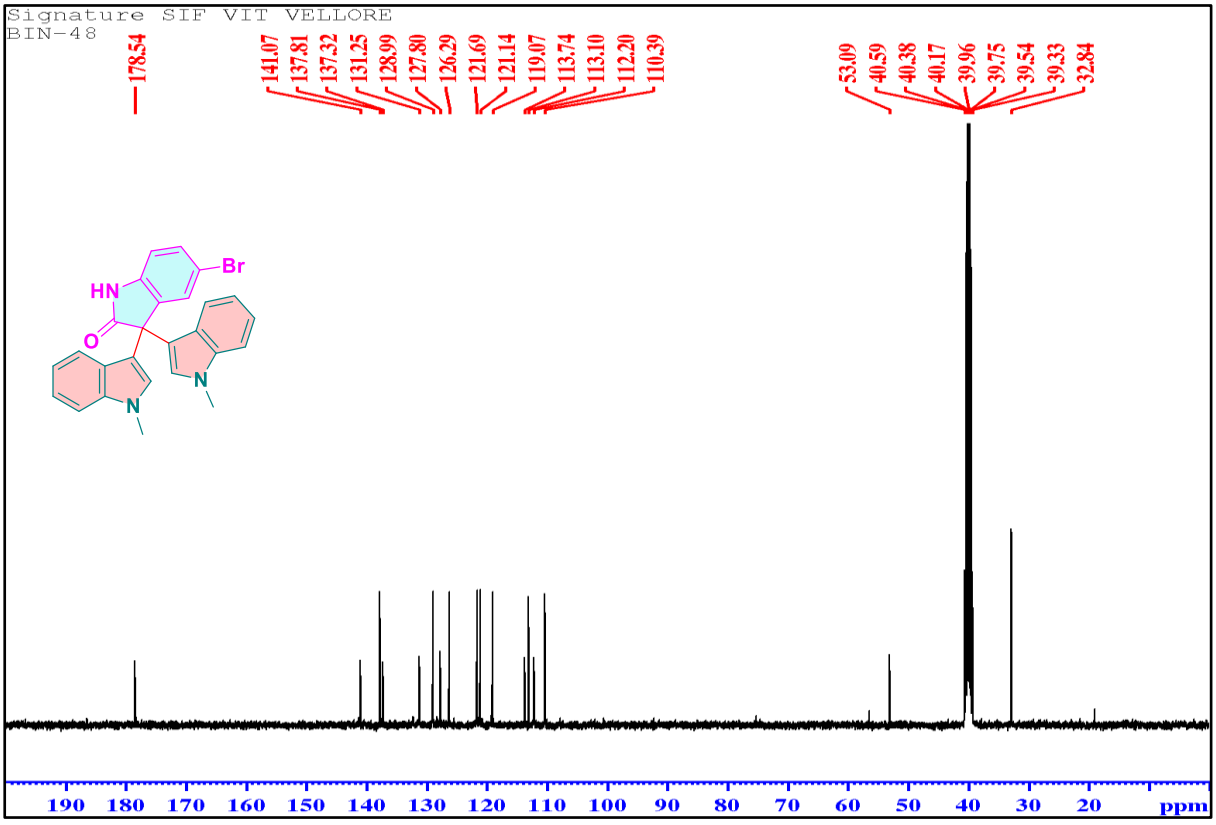


Fig. S54 ^{13}C NMR spectrum (100 MHz) of **7fd** in DMSO-d_6.

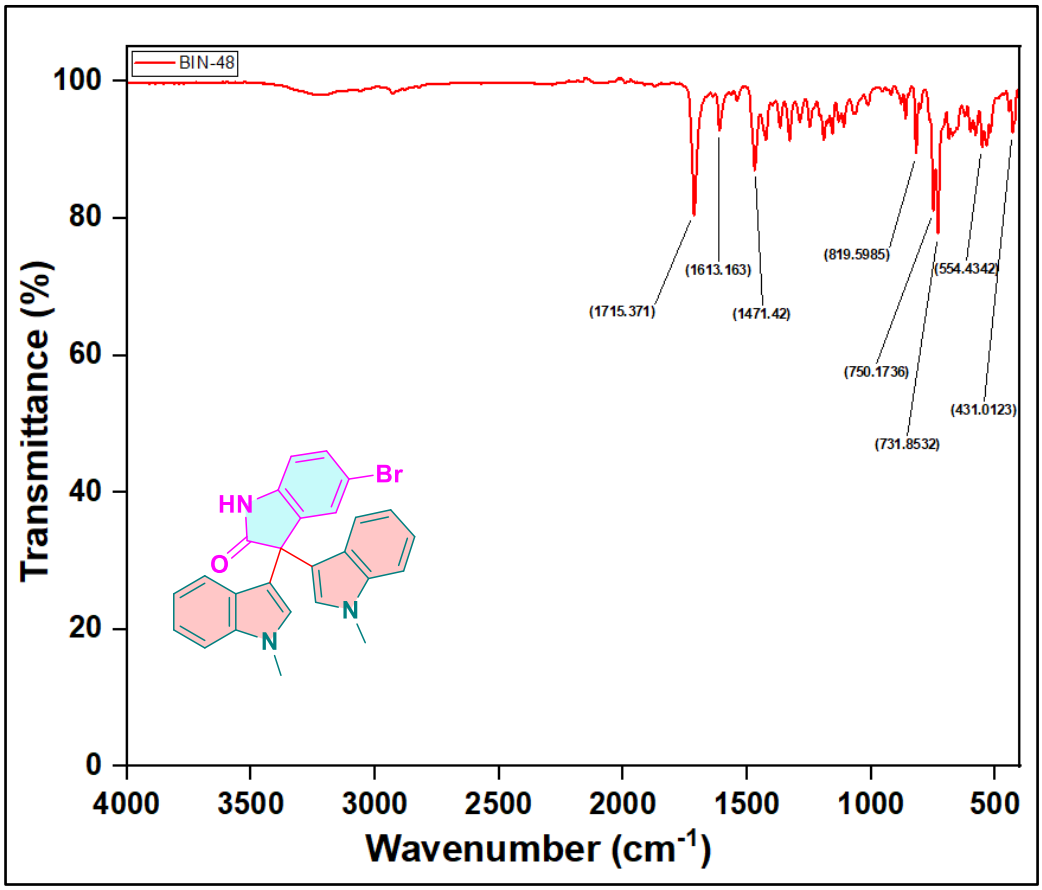


Fig. S55 FT-IR spectrum of **7fd**.

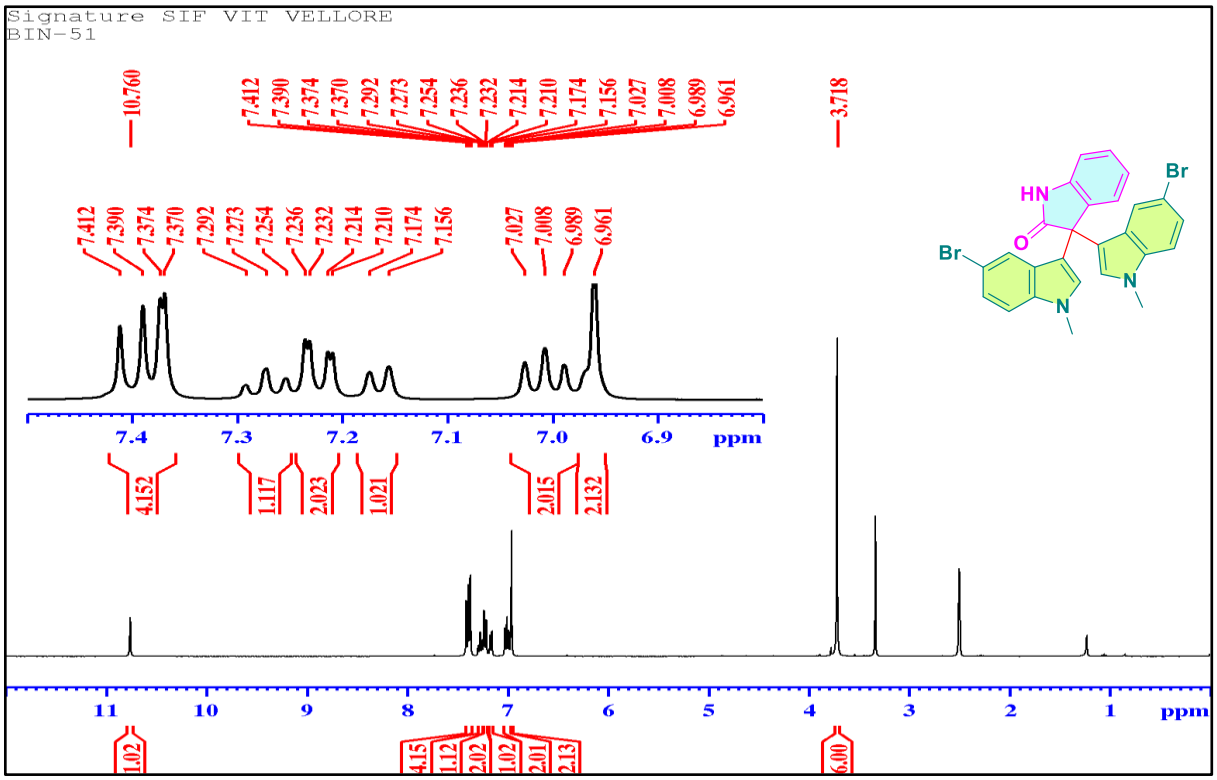


Fig. S56 ^{1}H NMR spectrum (400 MHz) of **7ga** in DMSO-d_6.

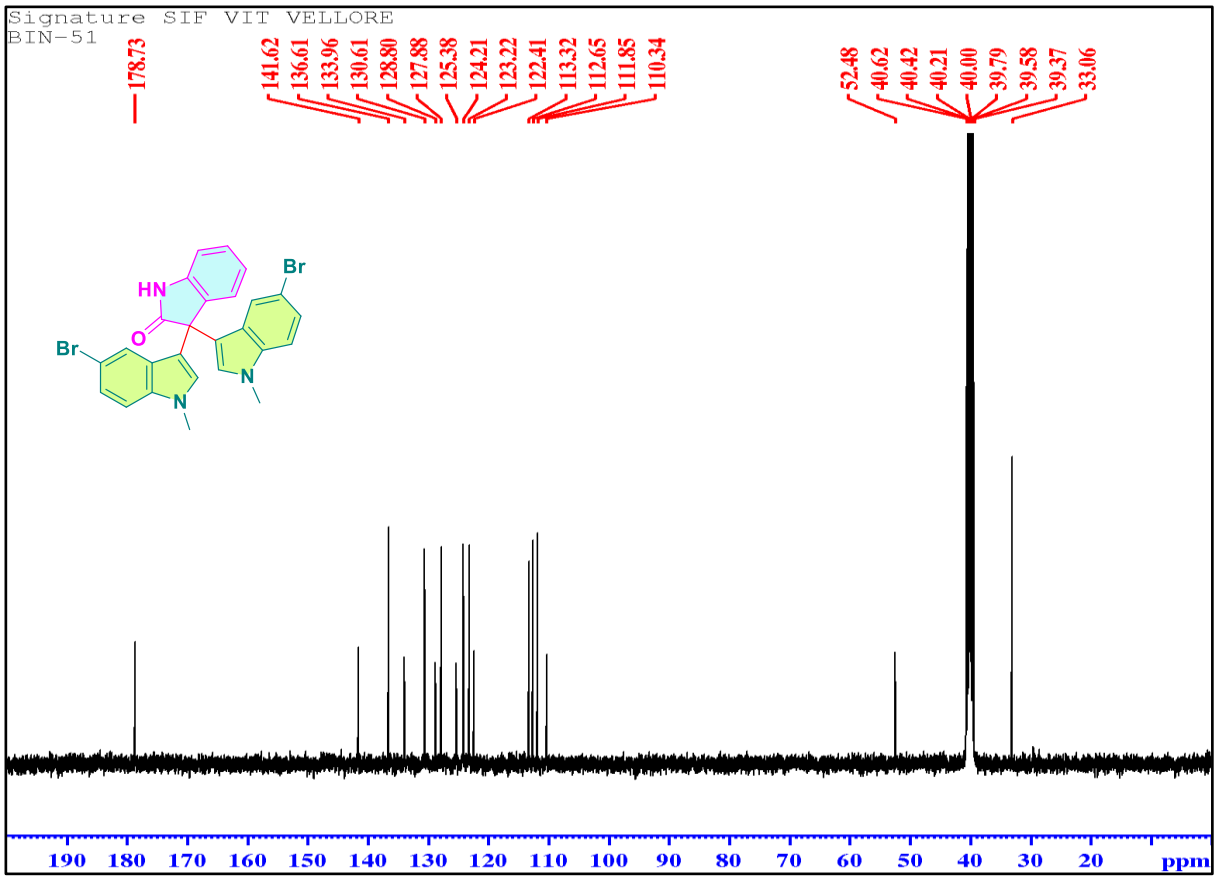


Fig. S57 ^{13}C NMR spectrum (100 MHz) of **7ga** in DMSO-d_6.

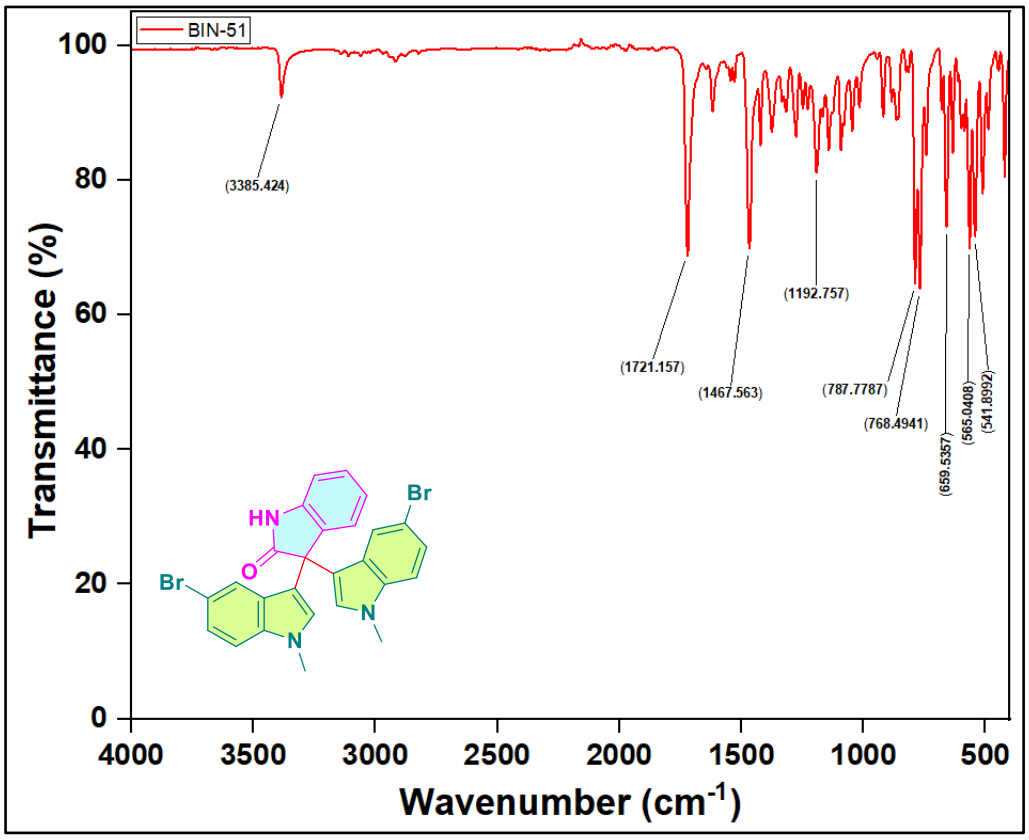


Fig. S58 FT-IR spectrum of **7ga**.

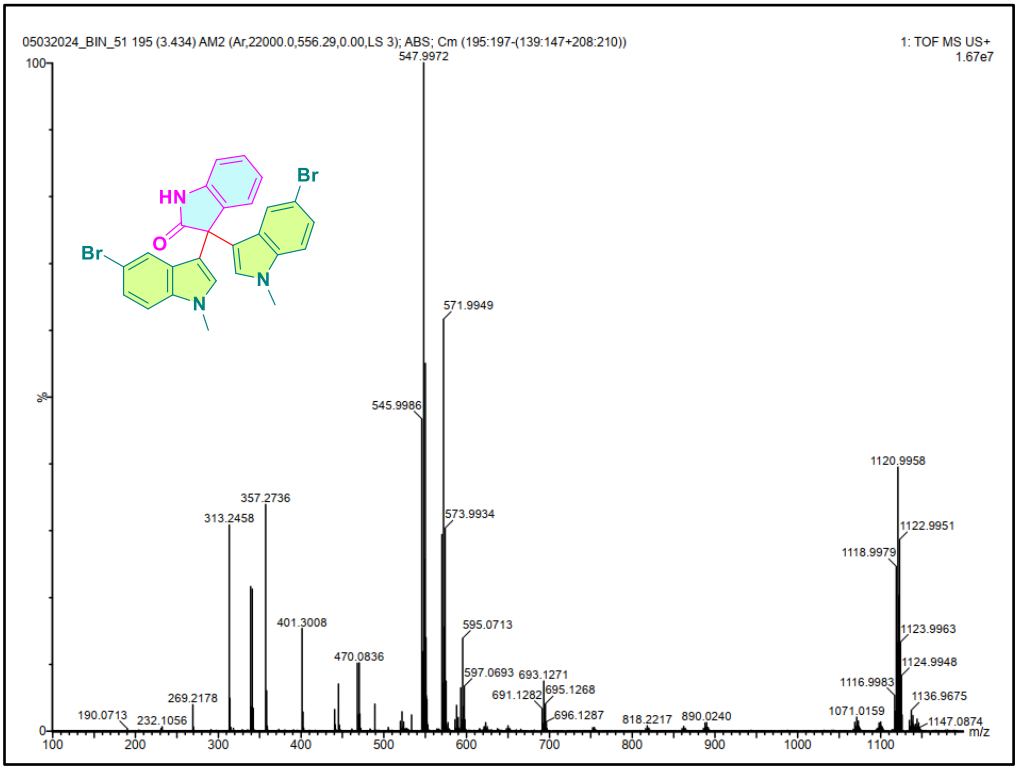


Fig. S59 HR-MS spectrum of **7ga**.

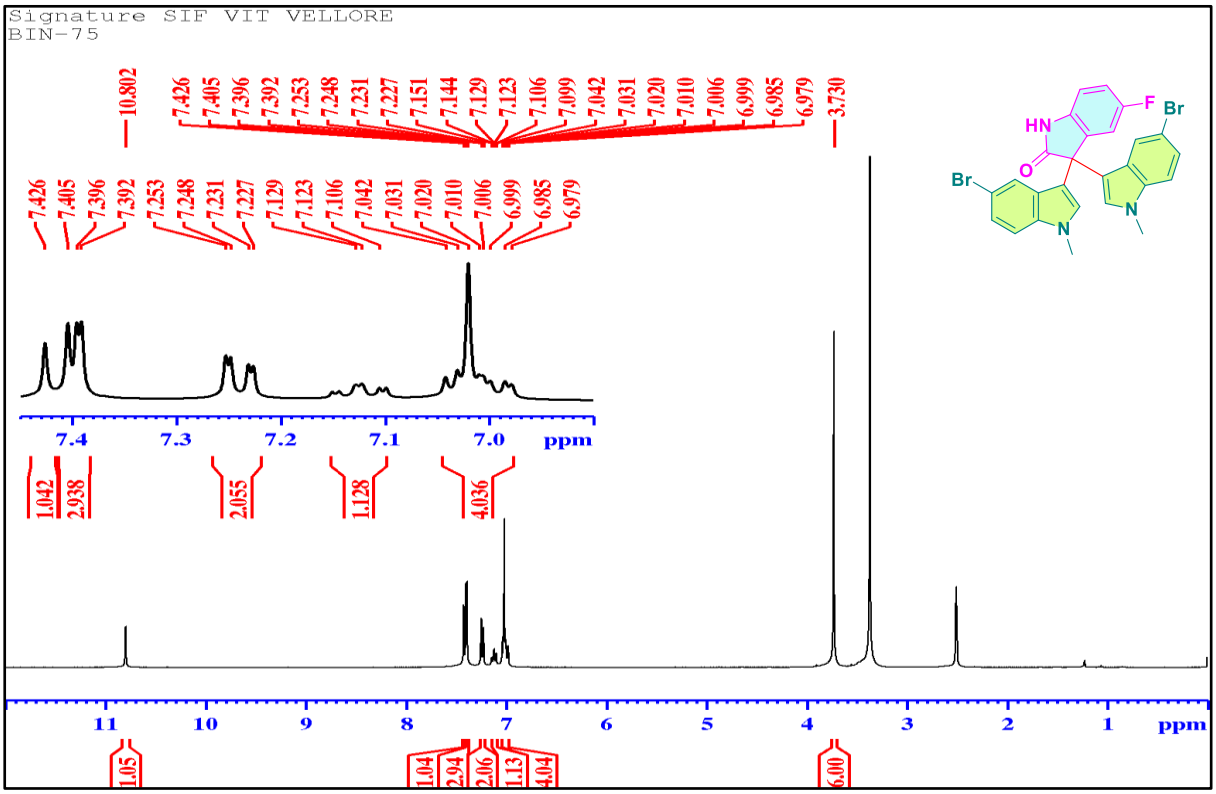


Fig. S60 ^{1}H NMR spectrum (400 MHz) of **7gc** in DMSO-d_6.

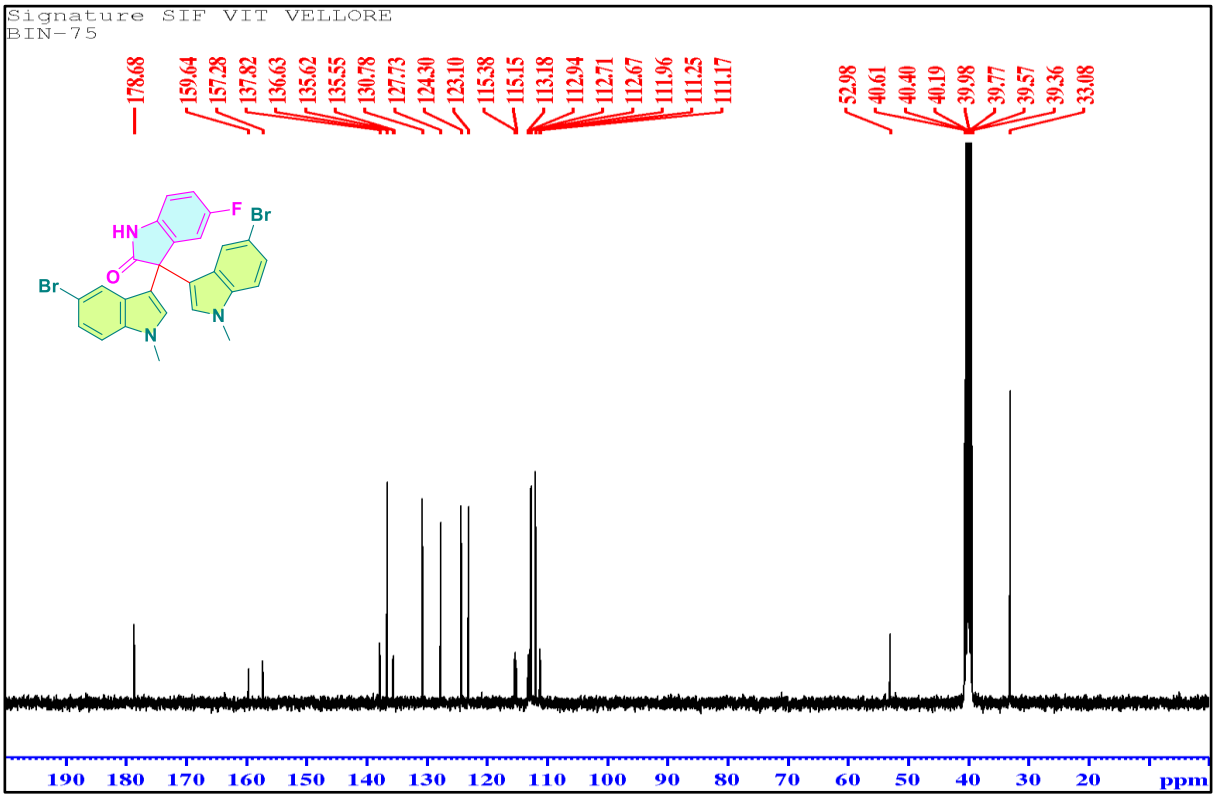


Fig. S61 ^{13}C NMR spectrum (100 MHz) of **7gc** in DMSO-d_6.

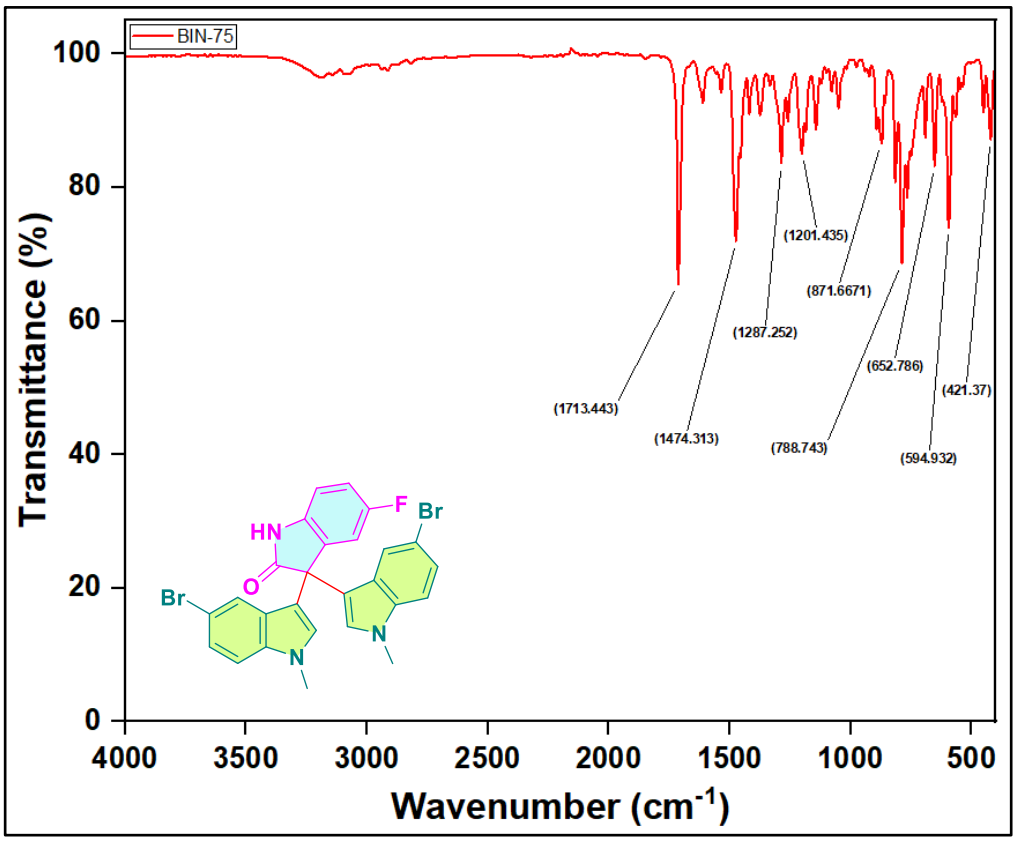


Fig. S62 FT-IR spectrum of **7gc**.

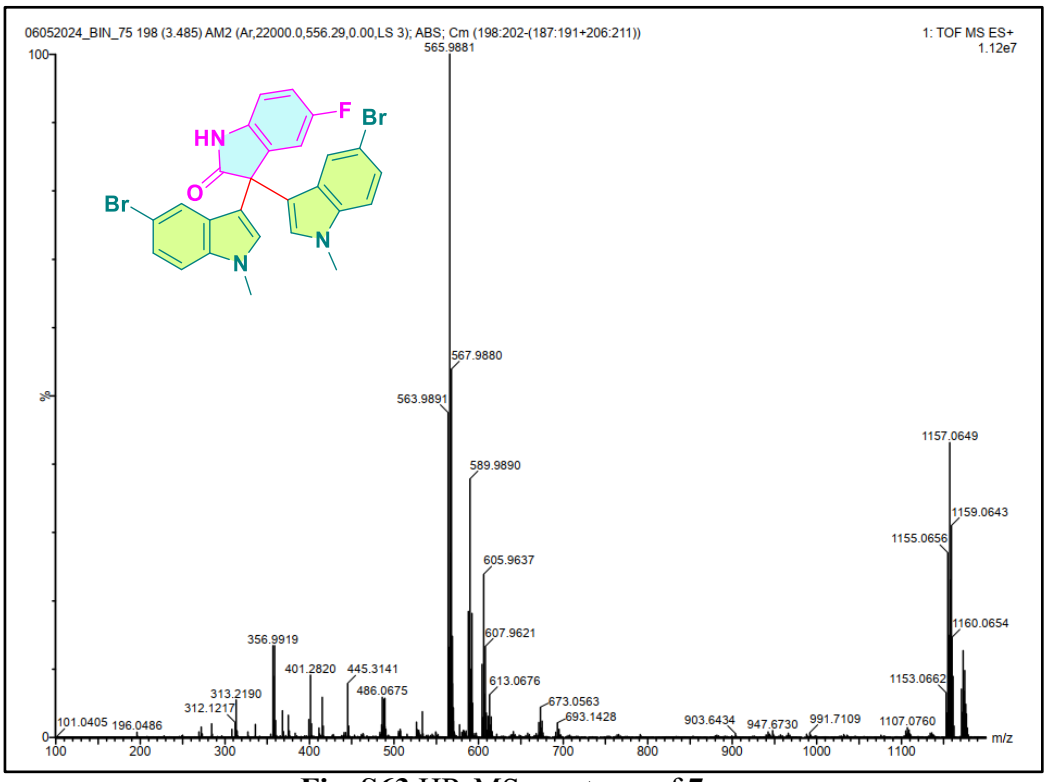


Fig. S63 HR-MS spectrum of **7gc**.

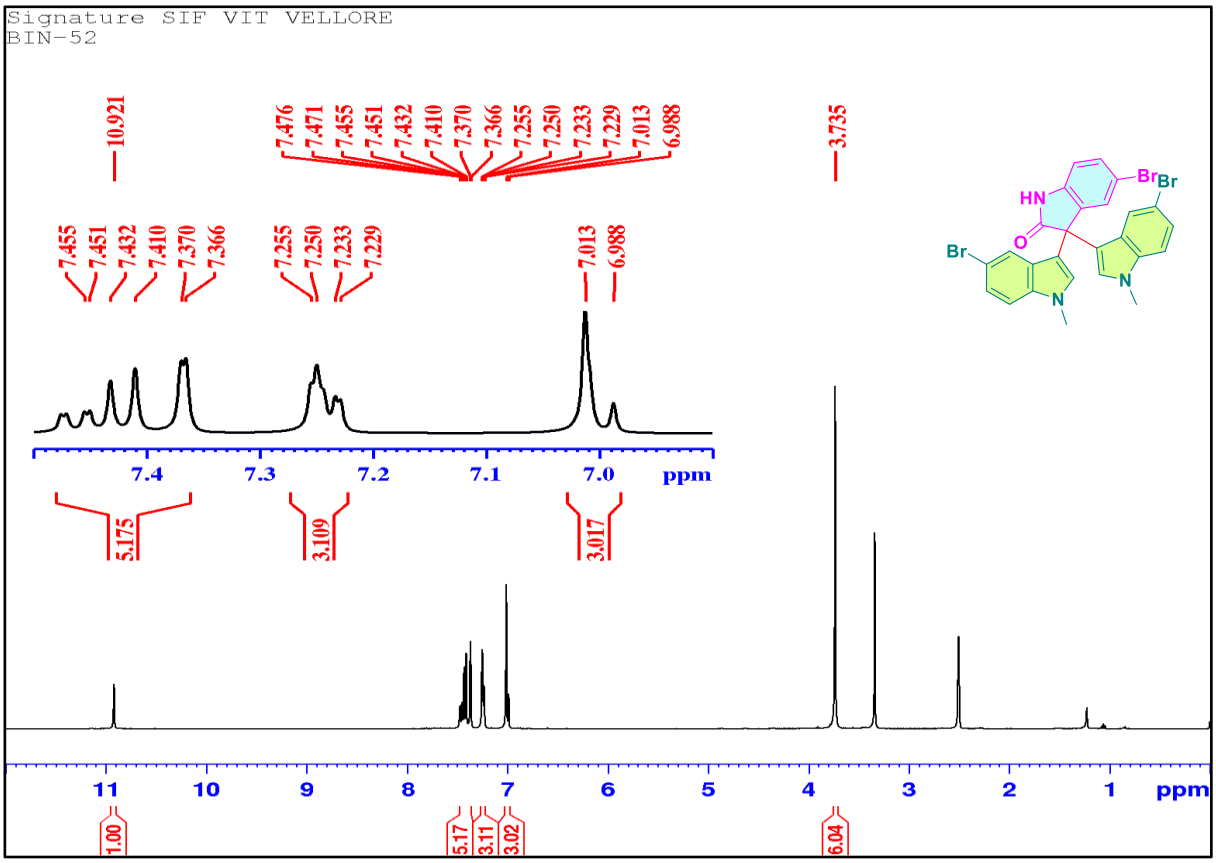


Fig. S64 ^{1}H NMR spectrum (400 MHz) of **7gd** in DMSO-d_6.

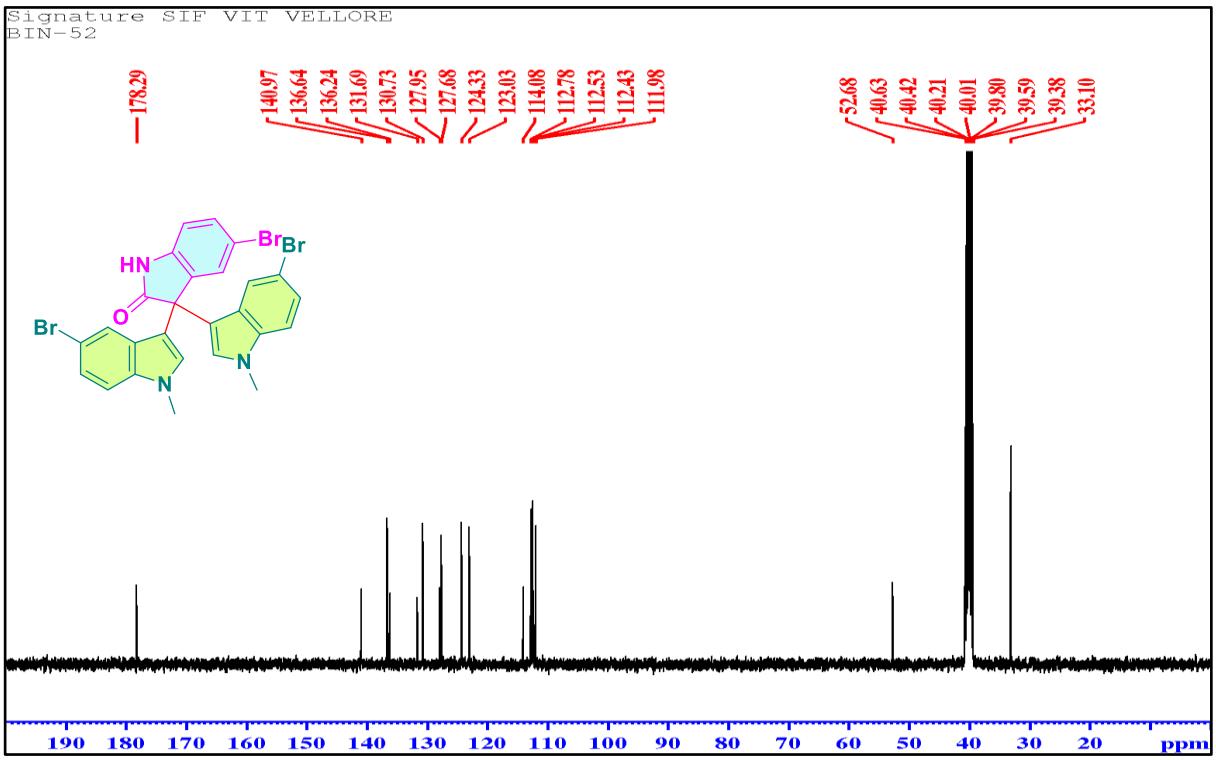


Fig. S65 ^{13}C NMR spectrum (100 MHz) of **7gd** in DMSO-d_6.

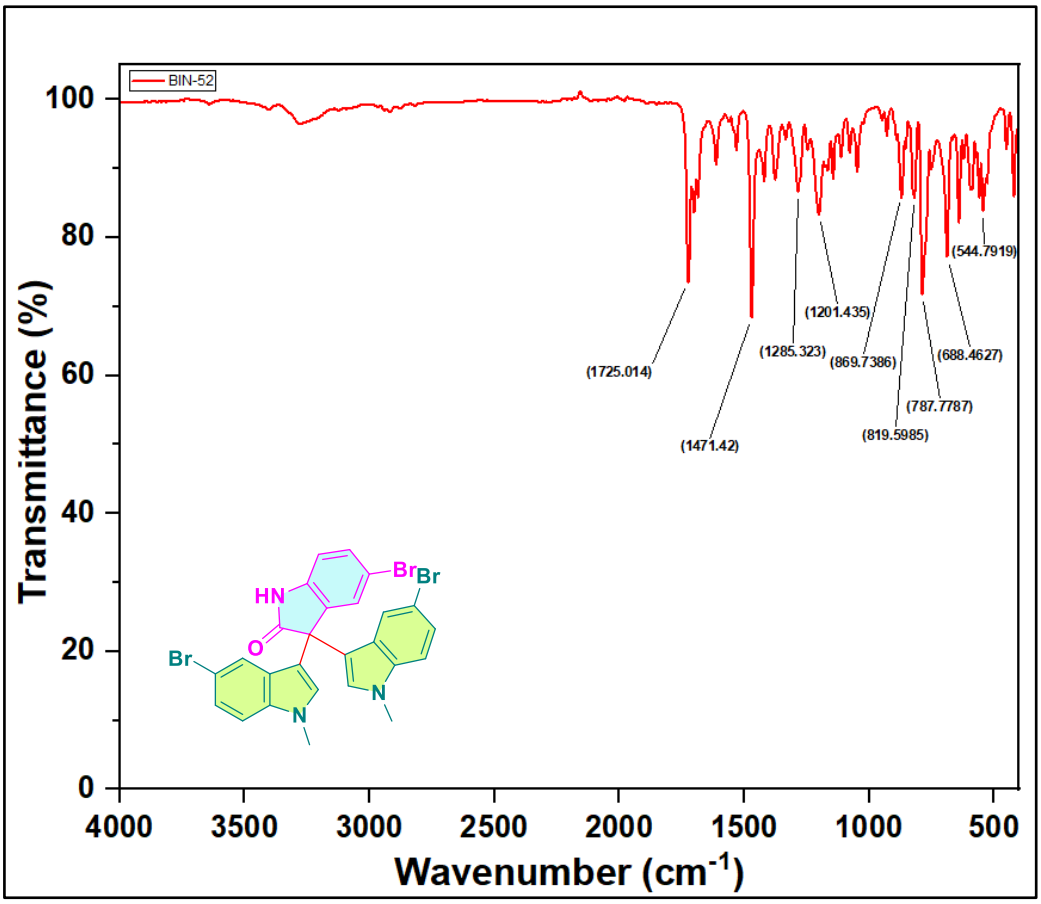


Fig. S66 FT-IR spectrum of **7gd**.

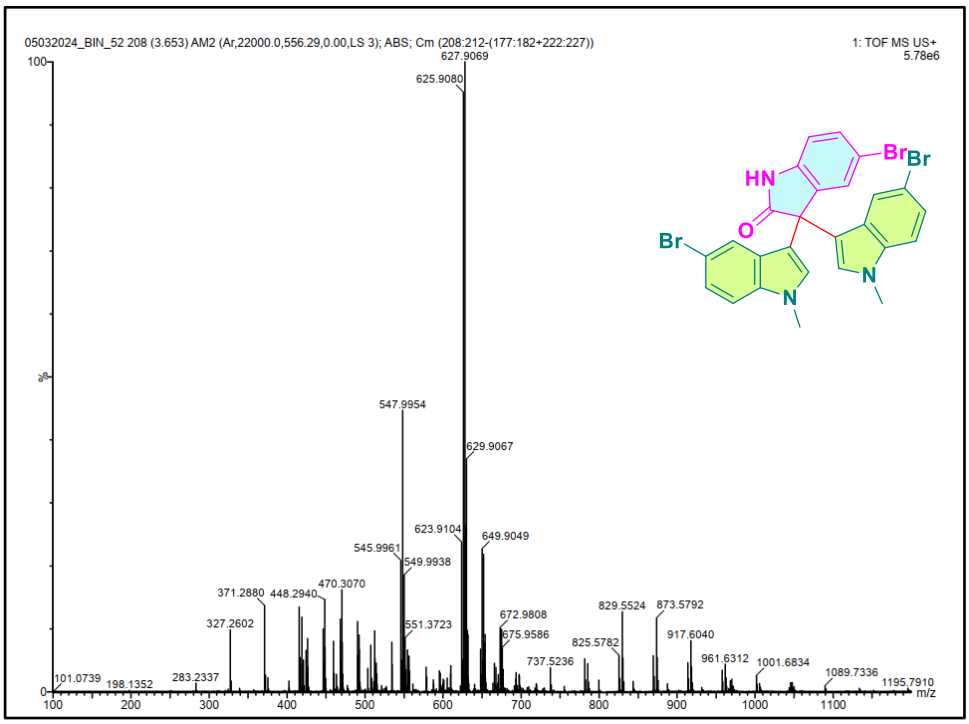


Fig. S67 HR-MS spectrum of **7gd**.

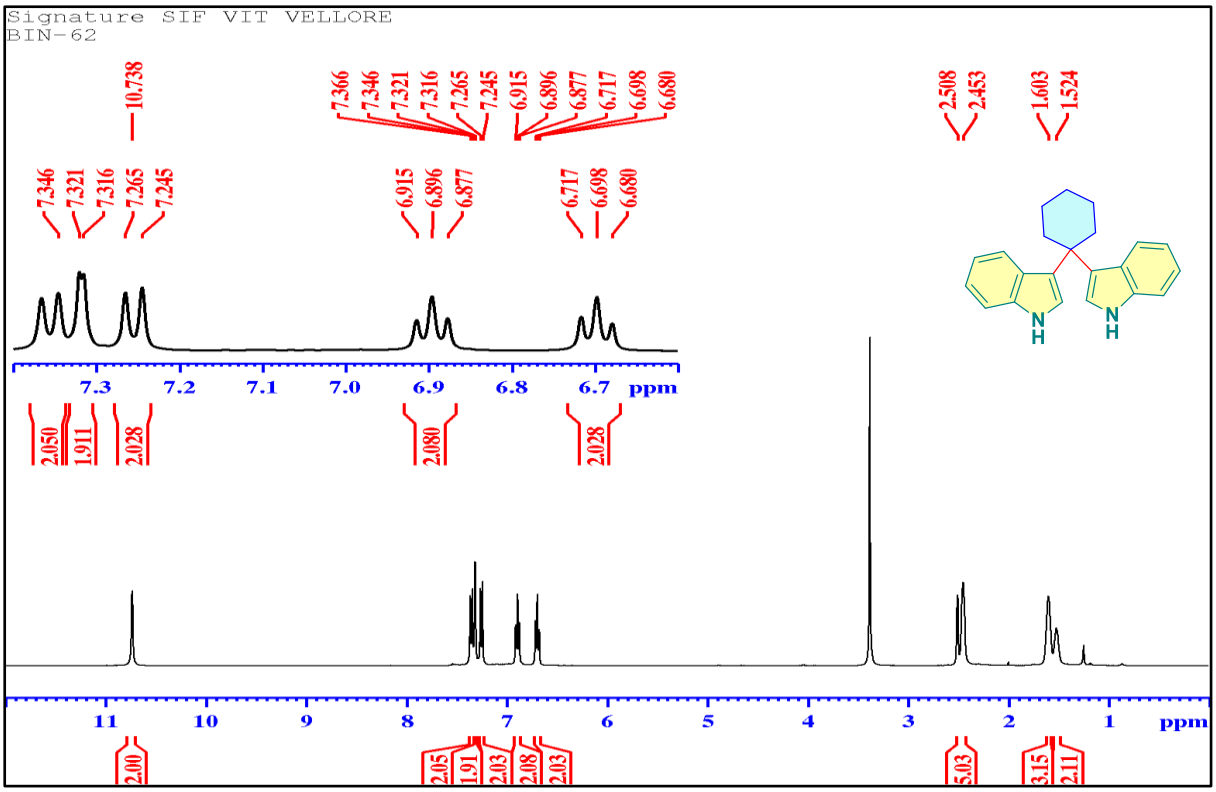


Fig. S68 ^{1}H NMR spectrum (400 MHz) of **7ai** in DMSO-d_6.

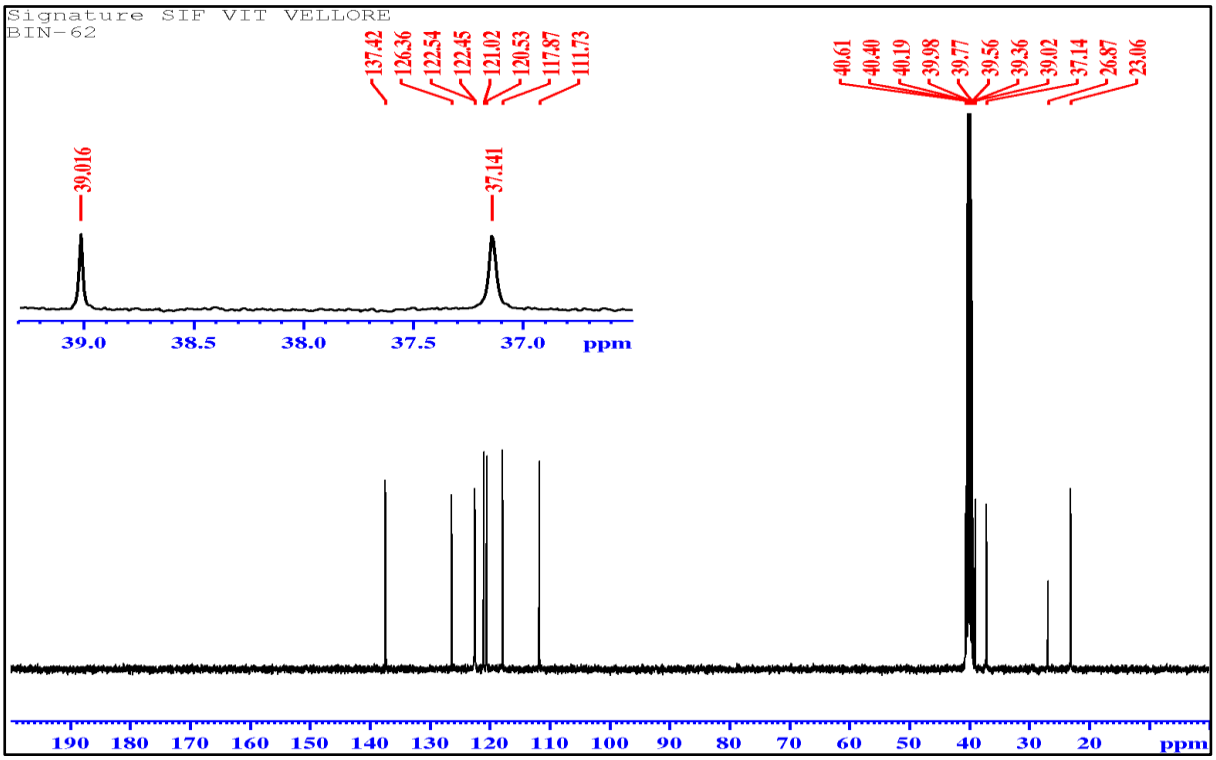


Fig. S69 ^{13}C NMR spectrum (100 MHz) of **7ai** in DMSO-d_6.

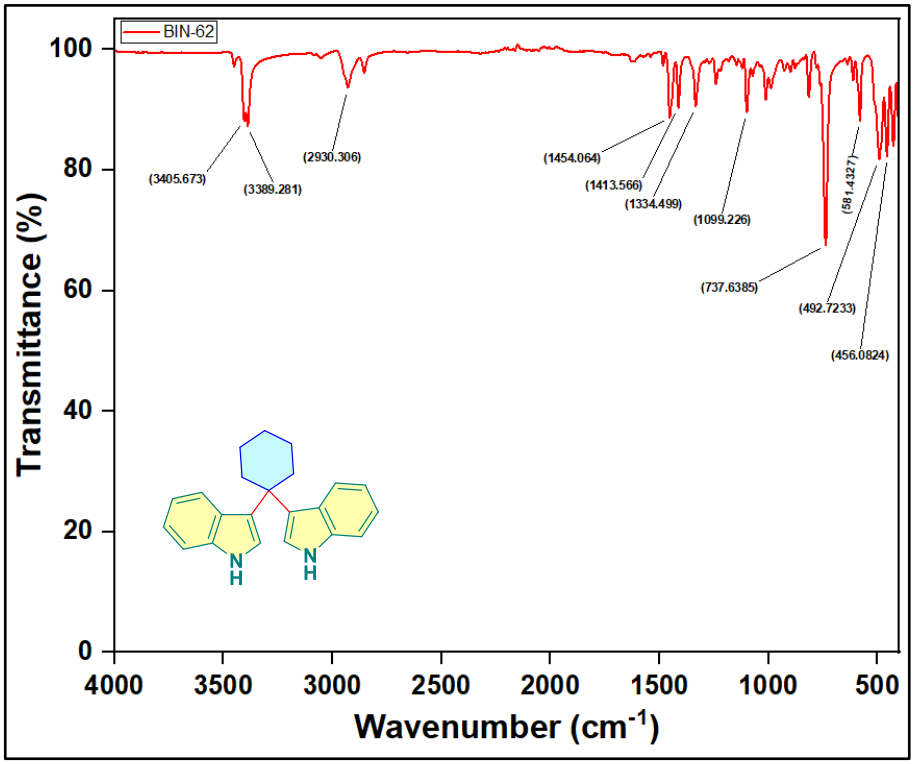


Fig. S70 FT-IR spectrum of **7ai**.

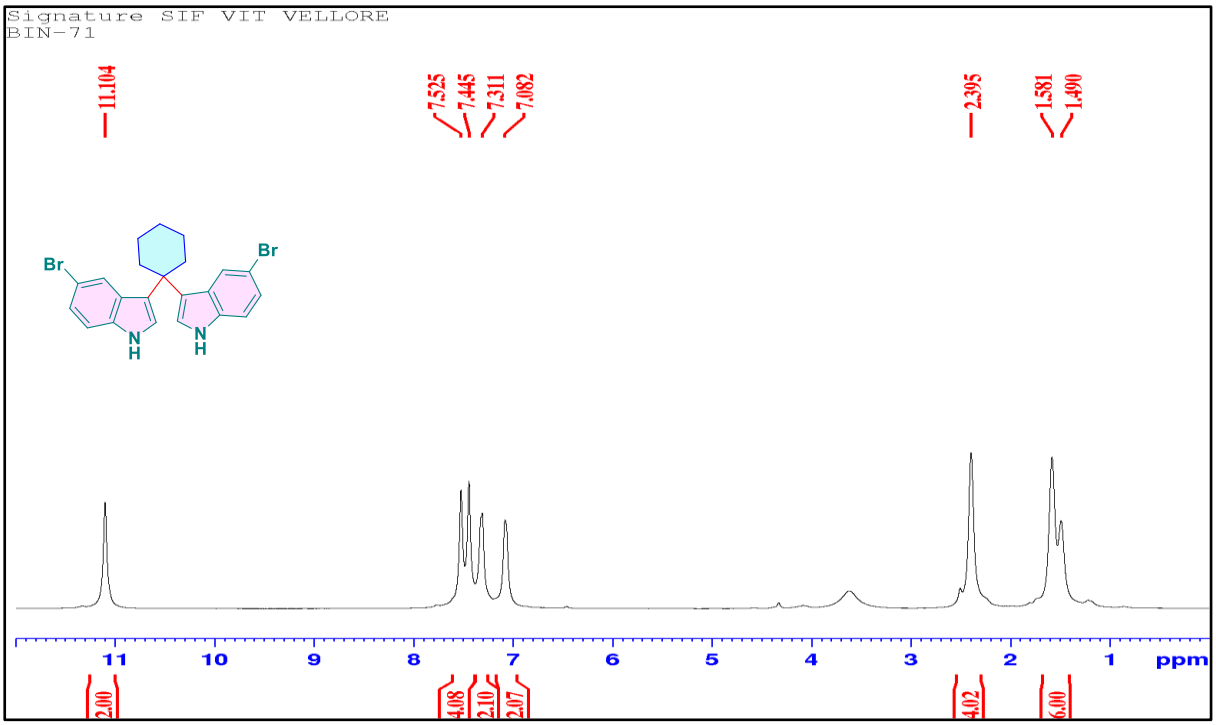


Fig. S71 ^{1}H NMR spectrum (400 MHz) of **7ei** in DMSO-d_6.

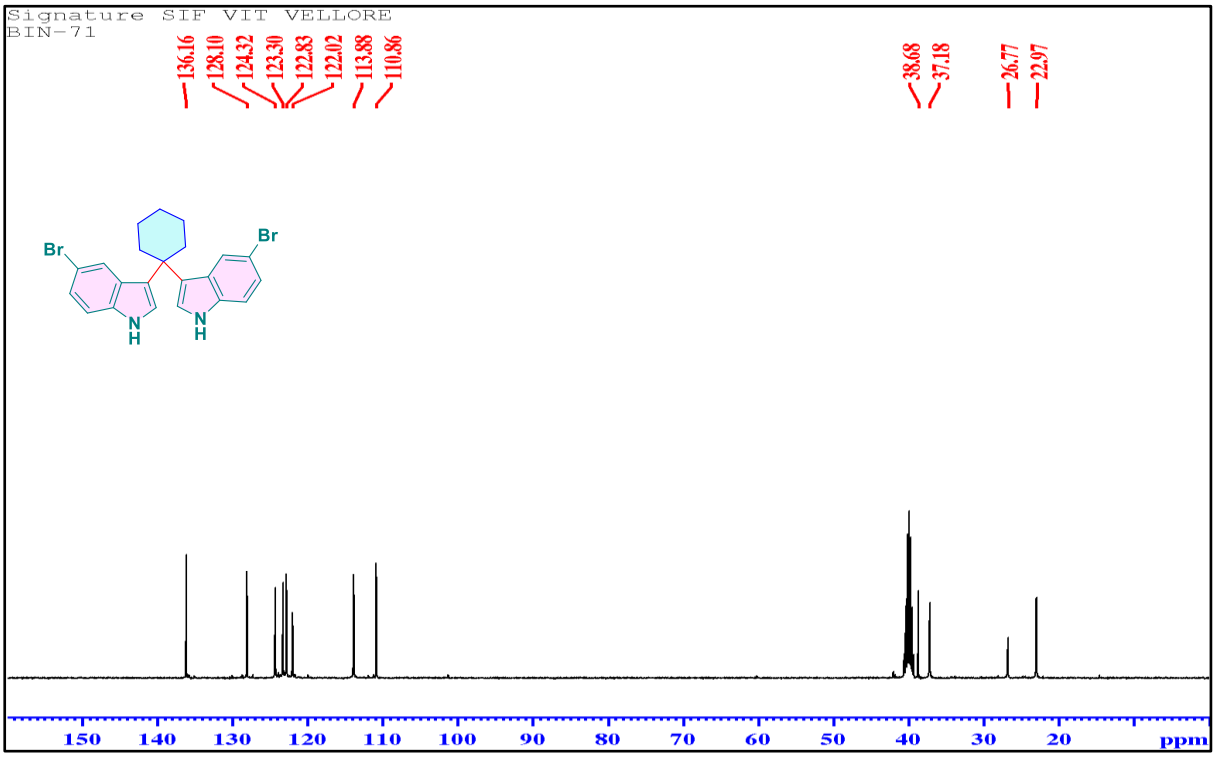


Fig. S72 ^{13}C NMR spectrum (100 MHz) of **7ei** in DMSO-d_6.

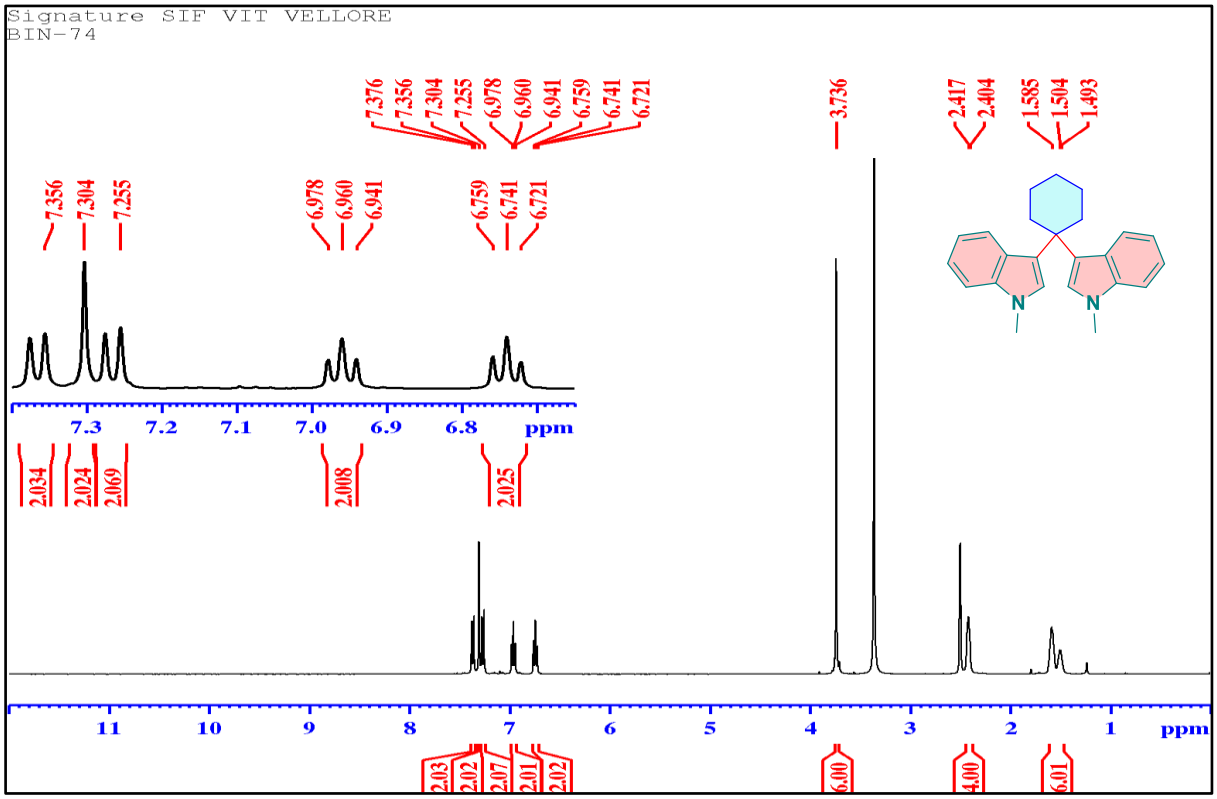


Fig. S73 ^{1}H NMR spectrum (400 MHz) of **7fi** in DMSO-d$_6$.

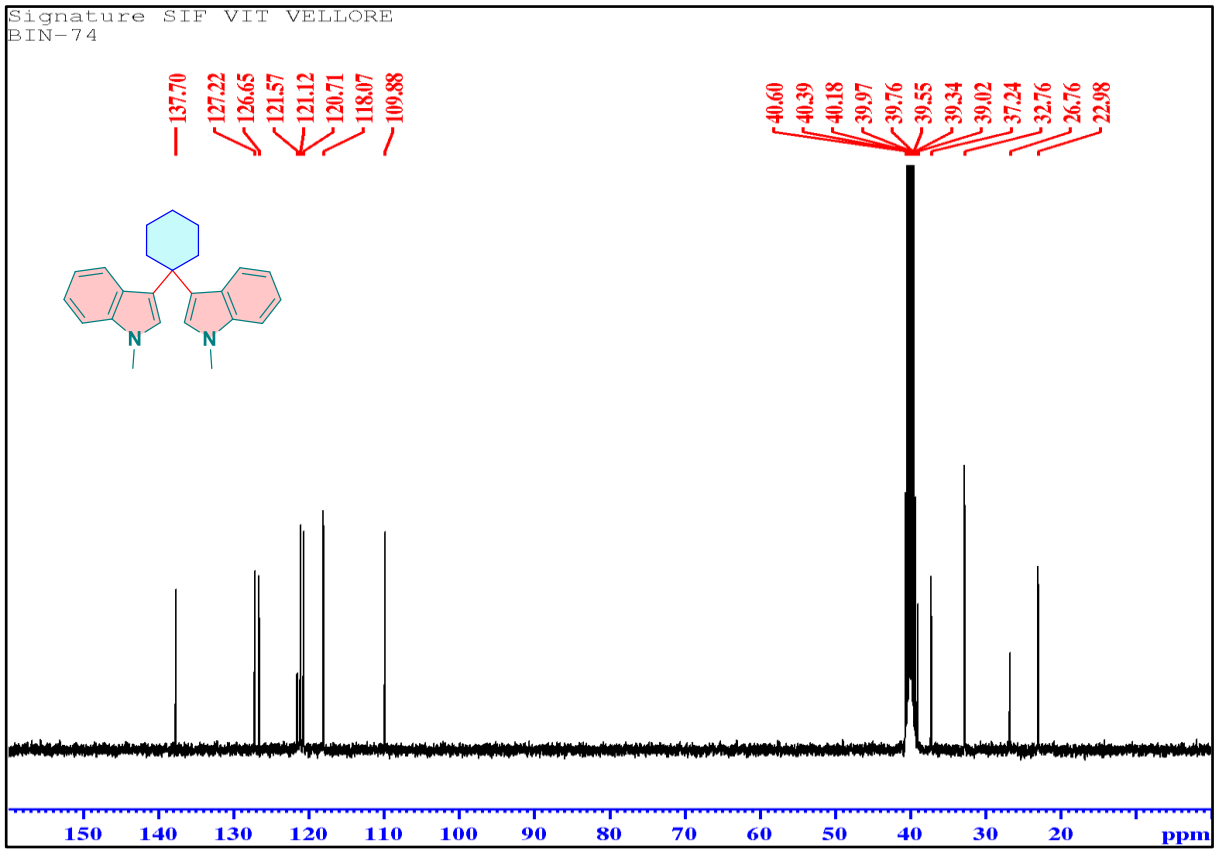


Fig. S74 ^{13}C NMR spectrum (100 MHz) of **7fi** in DMSO-d$_6$.

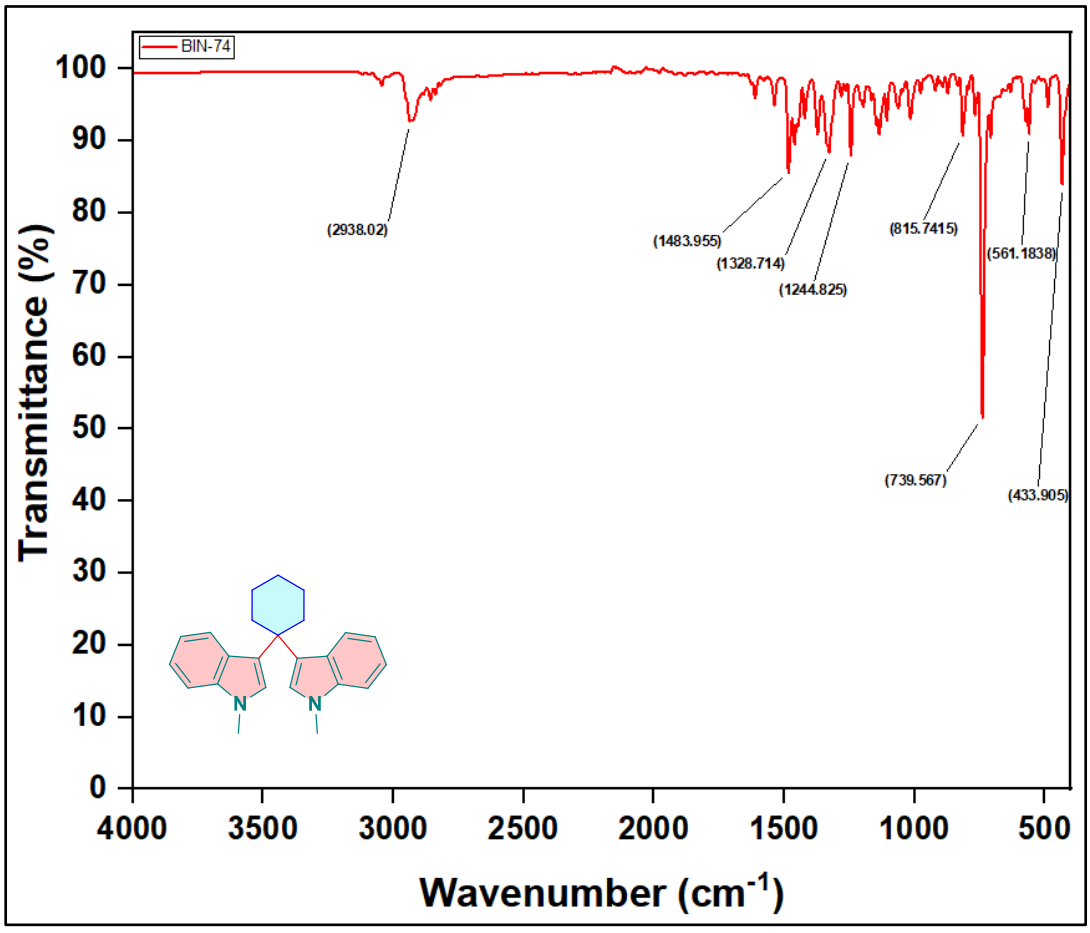


Fig. S75 FT-IR spectrum of **7fi**.

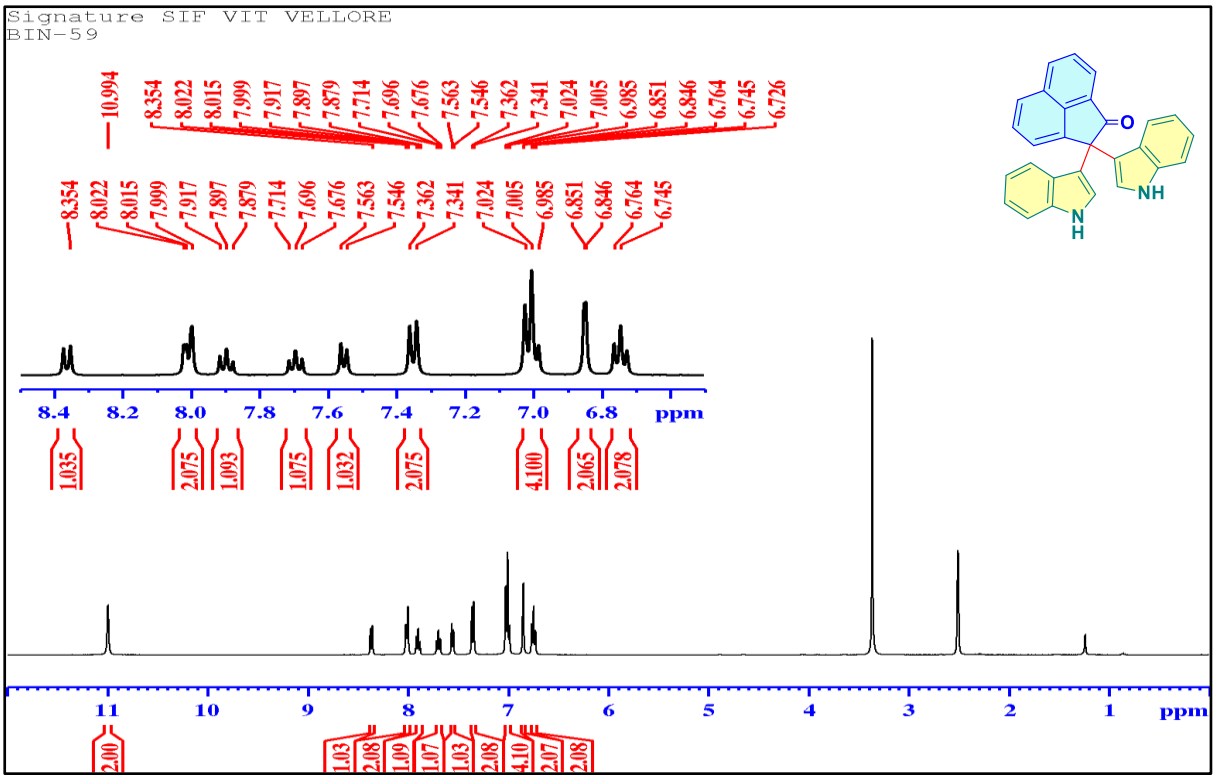


Fig. S76 ^{1}H NMR spectrum (400 MHz) of **7aj** in DMSO-d_6.

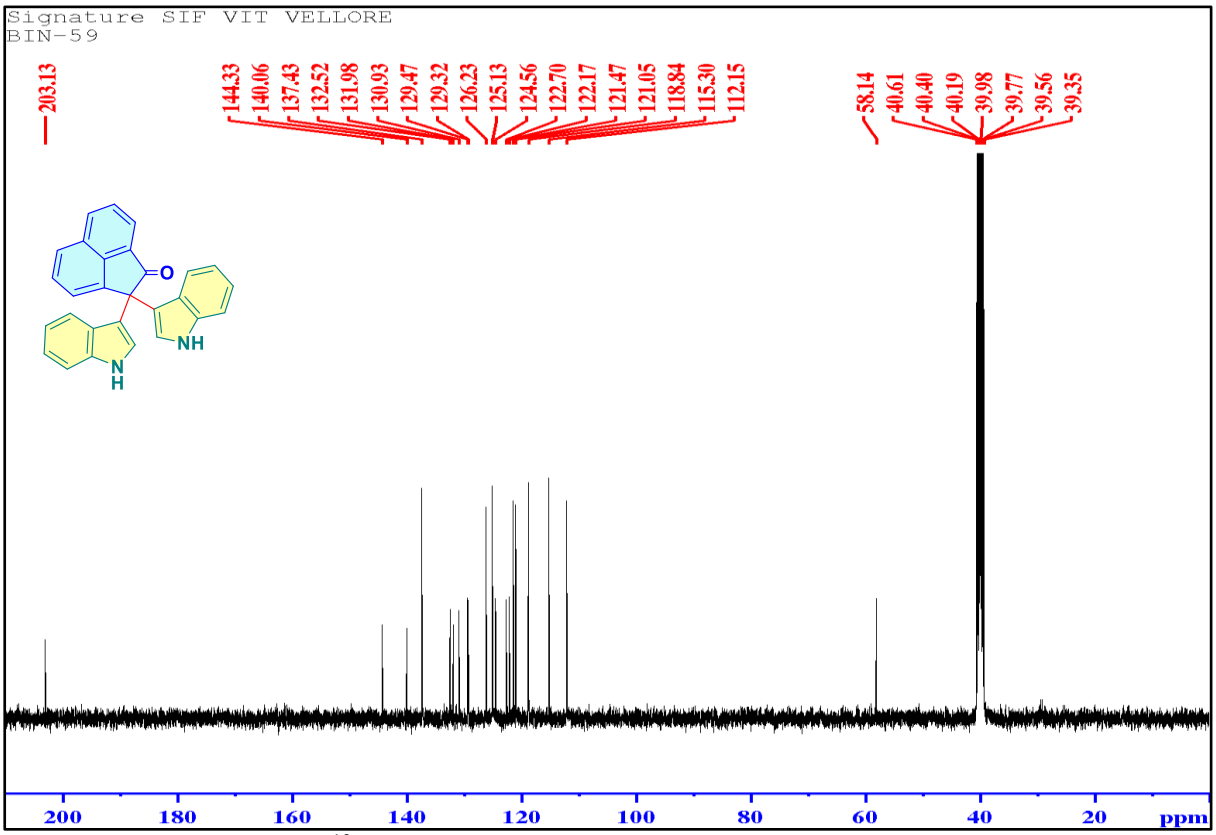


Fig. S77 ^{13}C NMR spectrum (100 MHz) of **7aj** in DMSO-d_6.

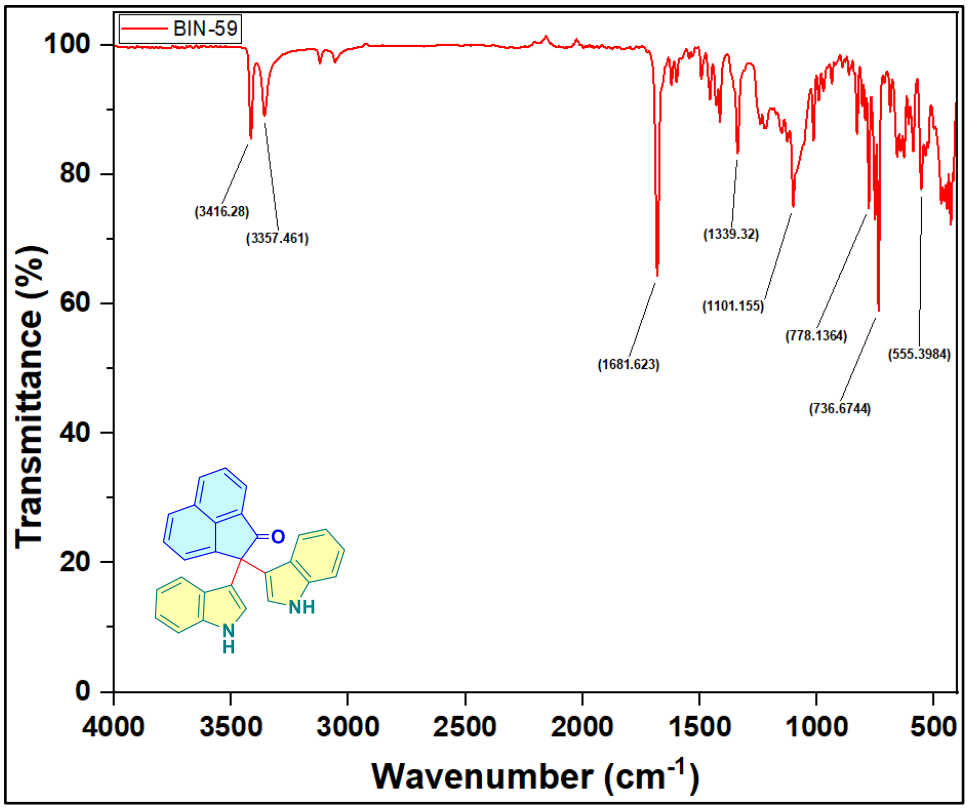


Fig. S78 FT-IR spectrum of **7aj**.

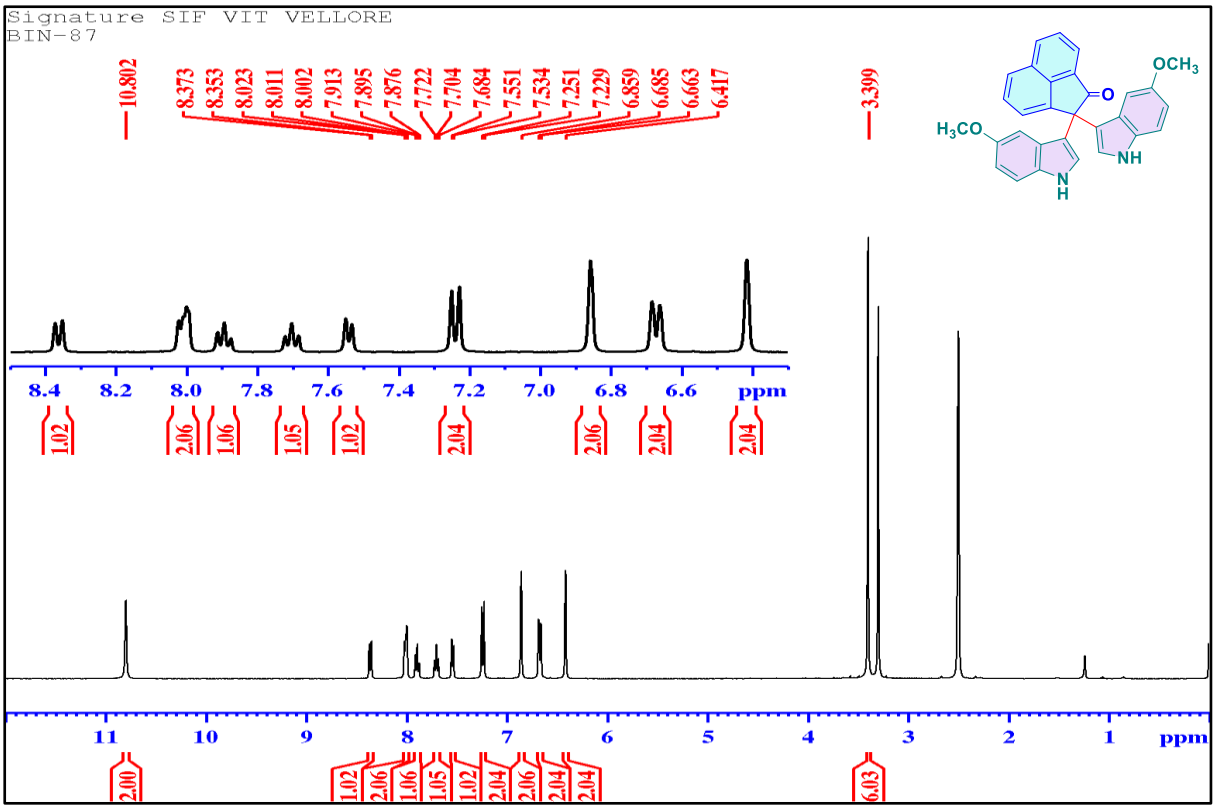


Fig. S79 ^{1}H NMR spectrum (400 MHz) of **7cj** in DMSO-d_6.

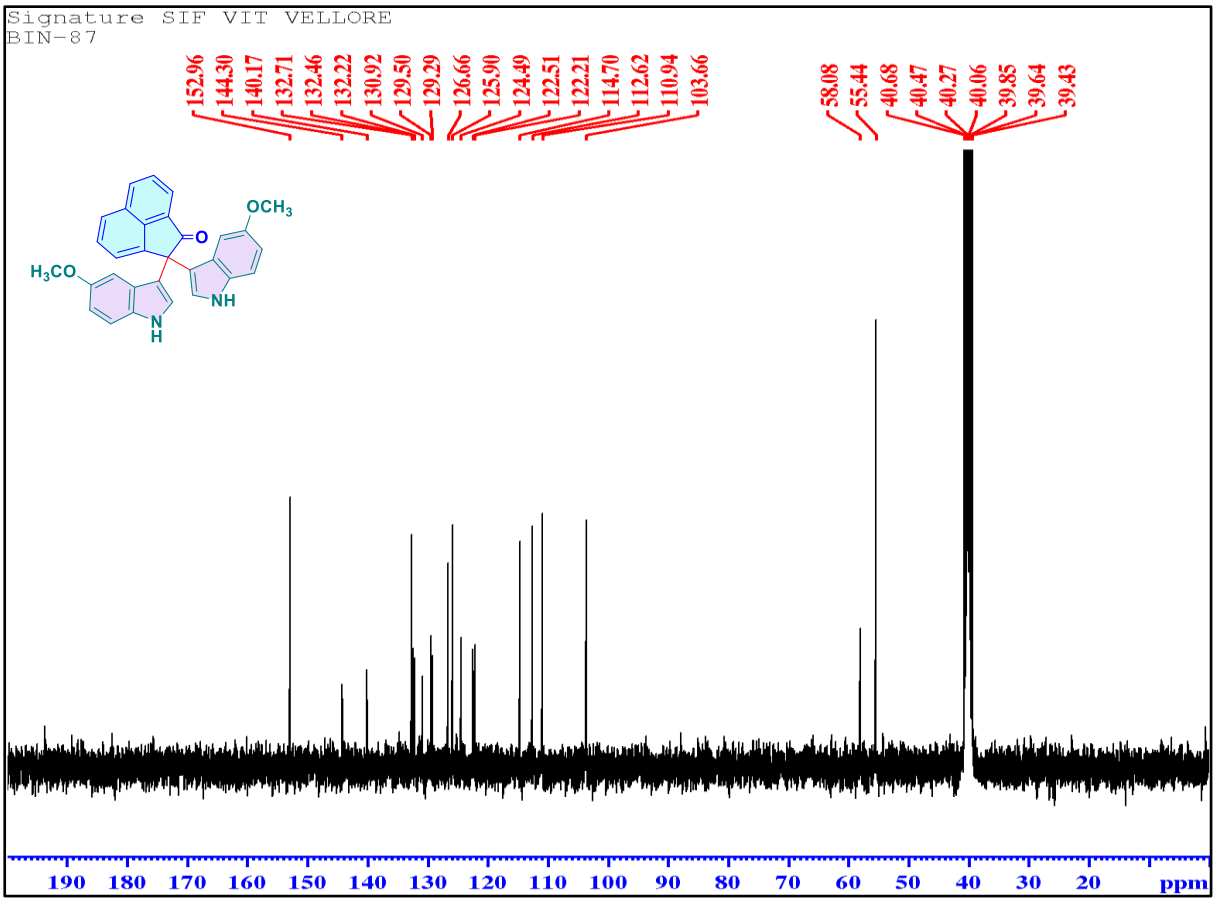


Fig. S80 ^{13}C NMR spectrum (100 MHz) of **7cj** in DMSO-d_6.

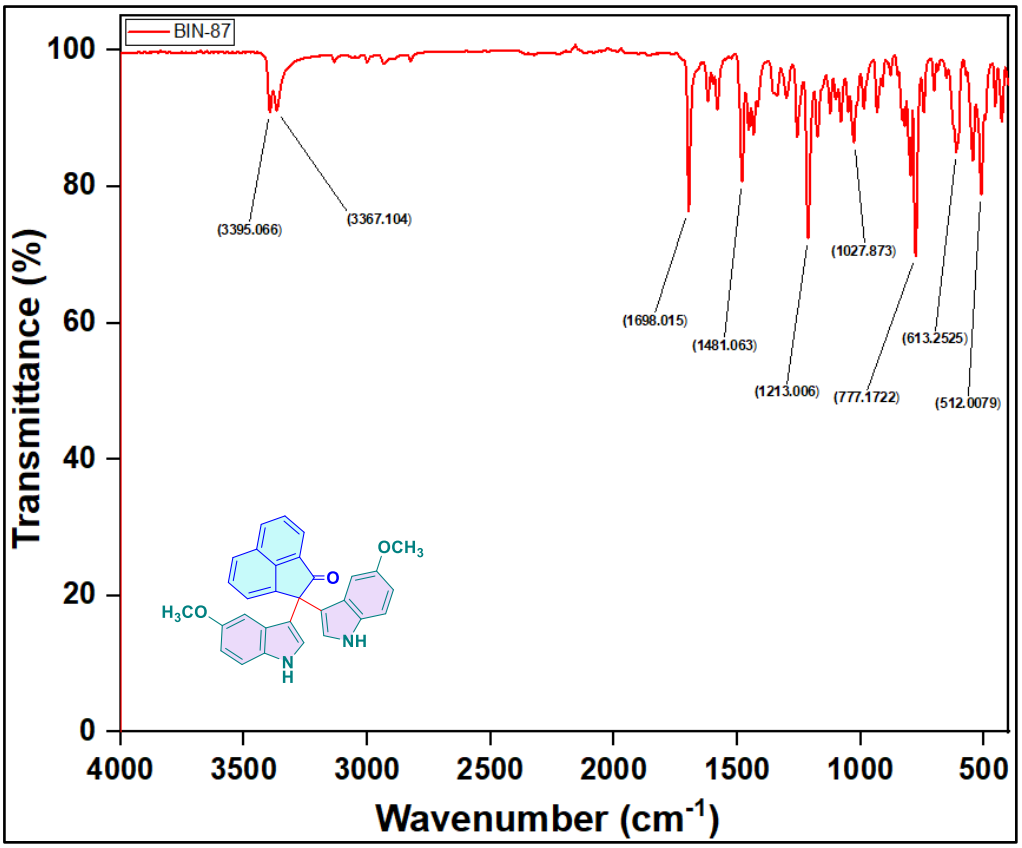


Fig. S81 FT-IR spectrum of **7cj**.

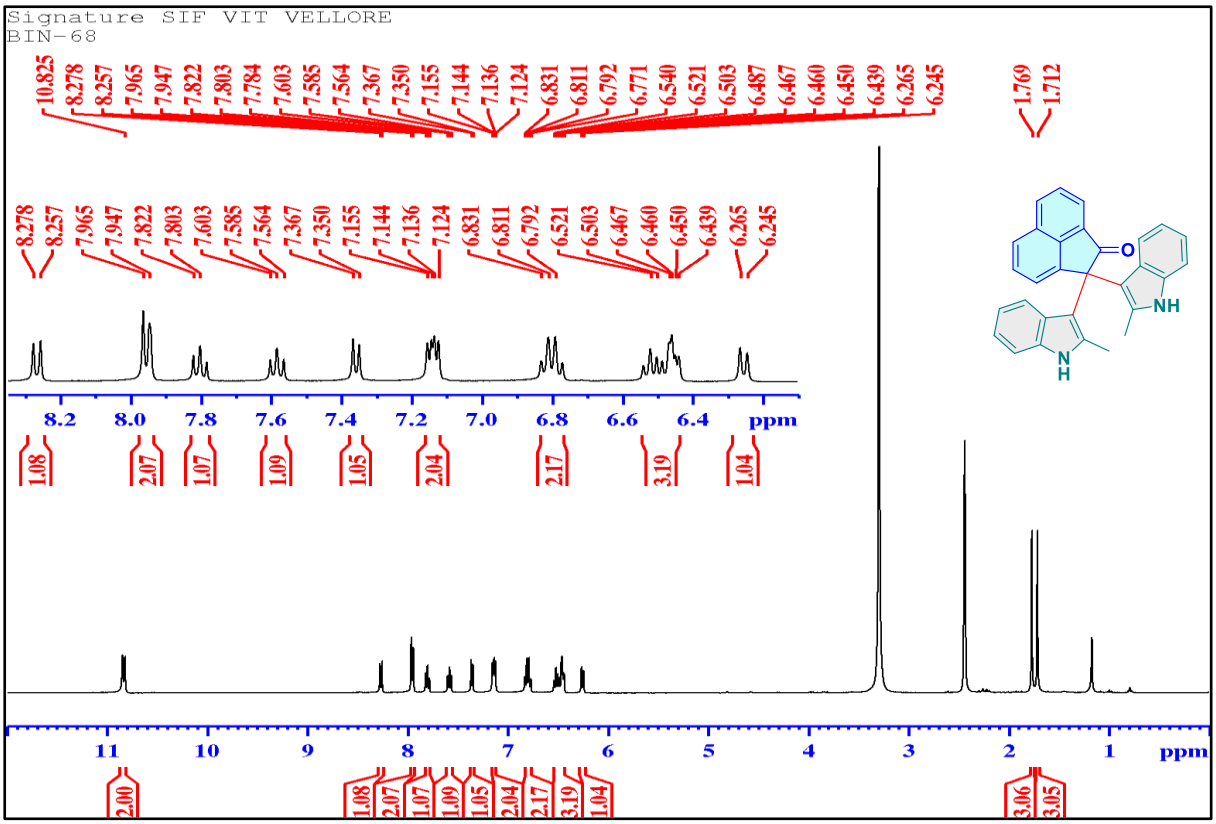


Fig. S82 ^{1}H NMR spectrum (400 MHz) of **7dj** in DMSO-d$_6$.

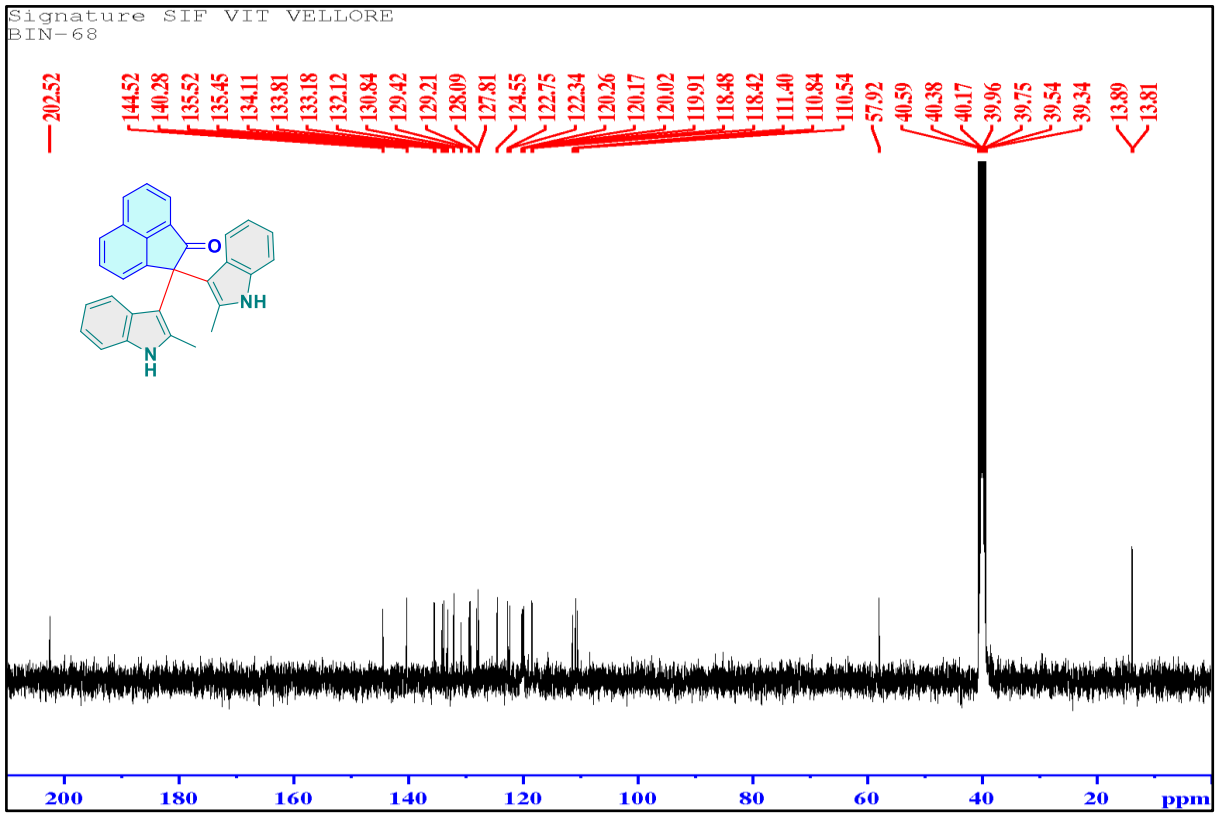


Fig. S83 ^{13}C NMR spectrum (100 MHz) of **7dj** in DMSO-d$_6$.

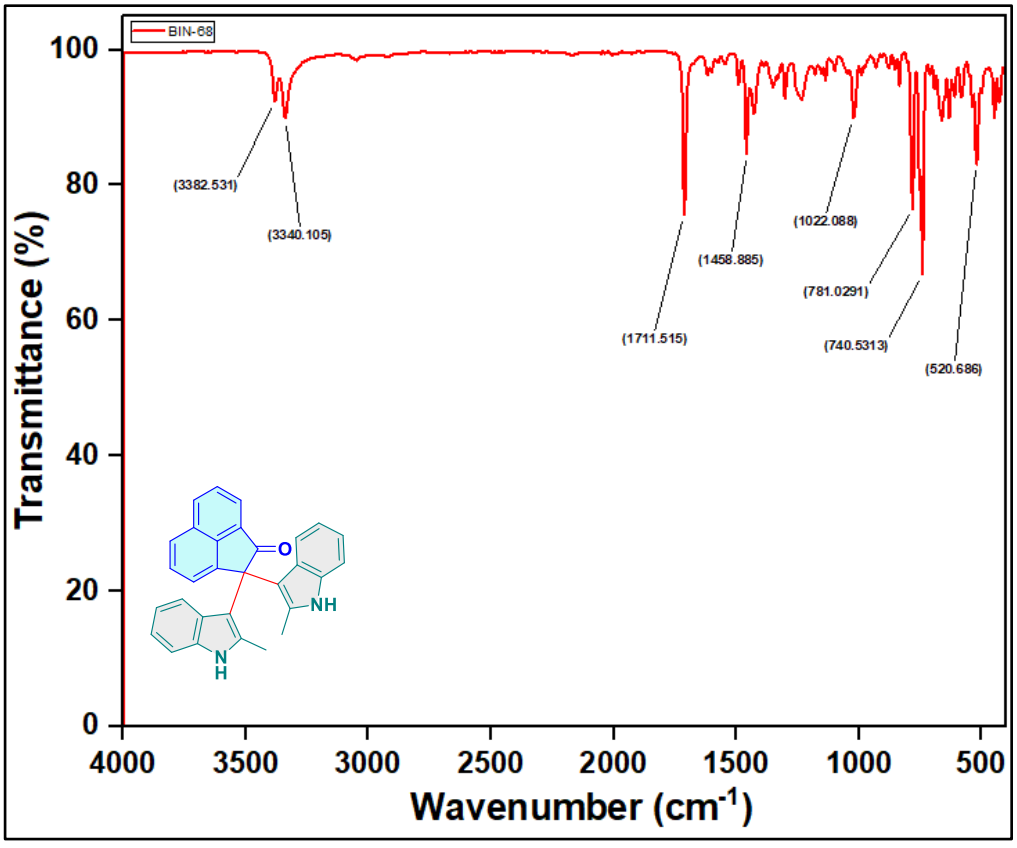


Fig. S84 FT-IR spectrum of **7dj**.

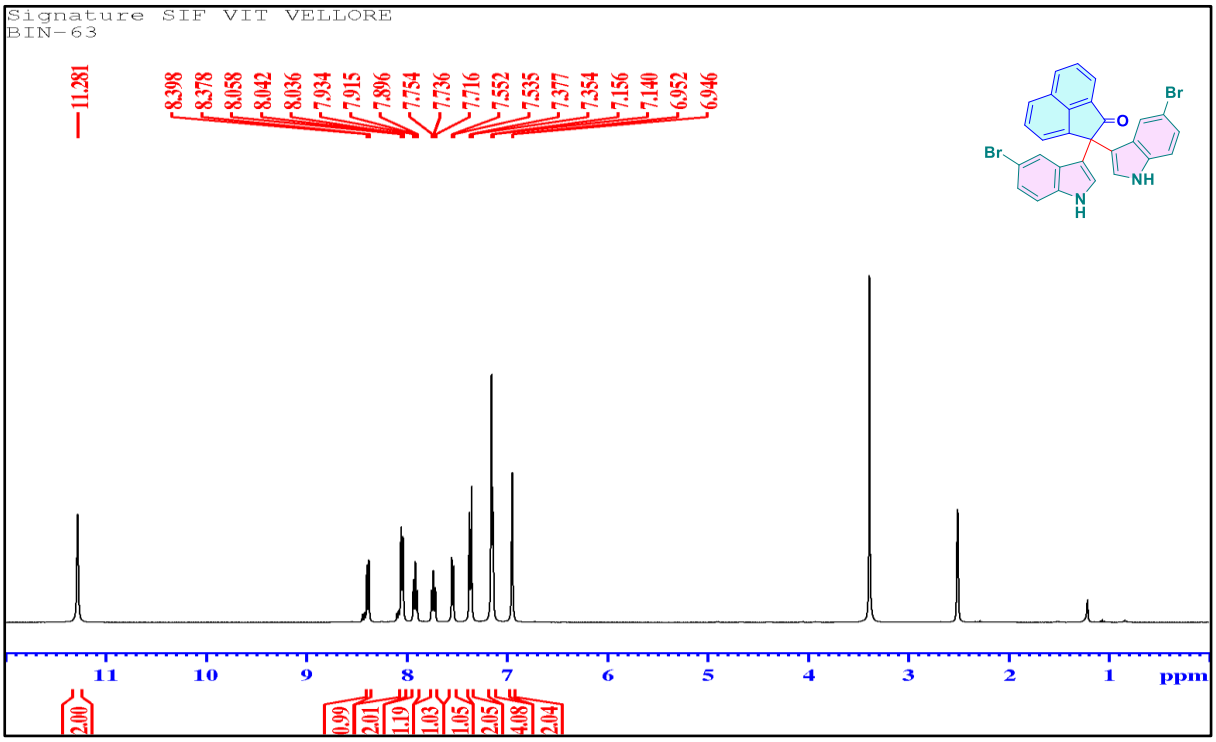


Fig. S85 ^{1}H NMR spectrum (400 MHz) of **7ej** in DMSO-d_6.

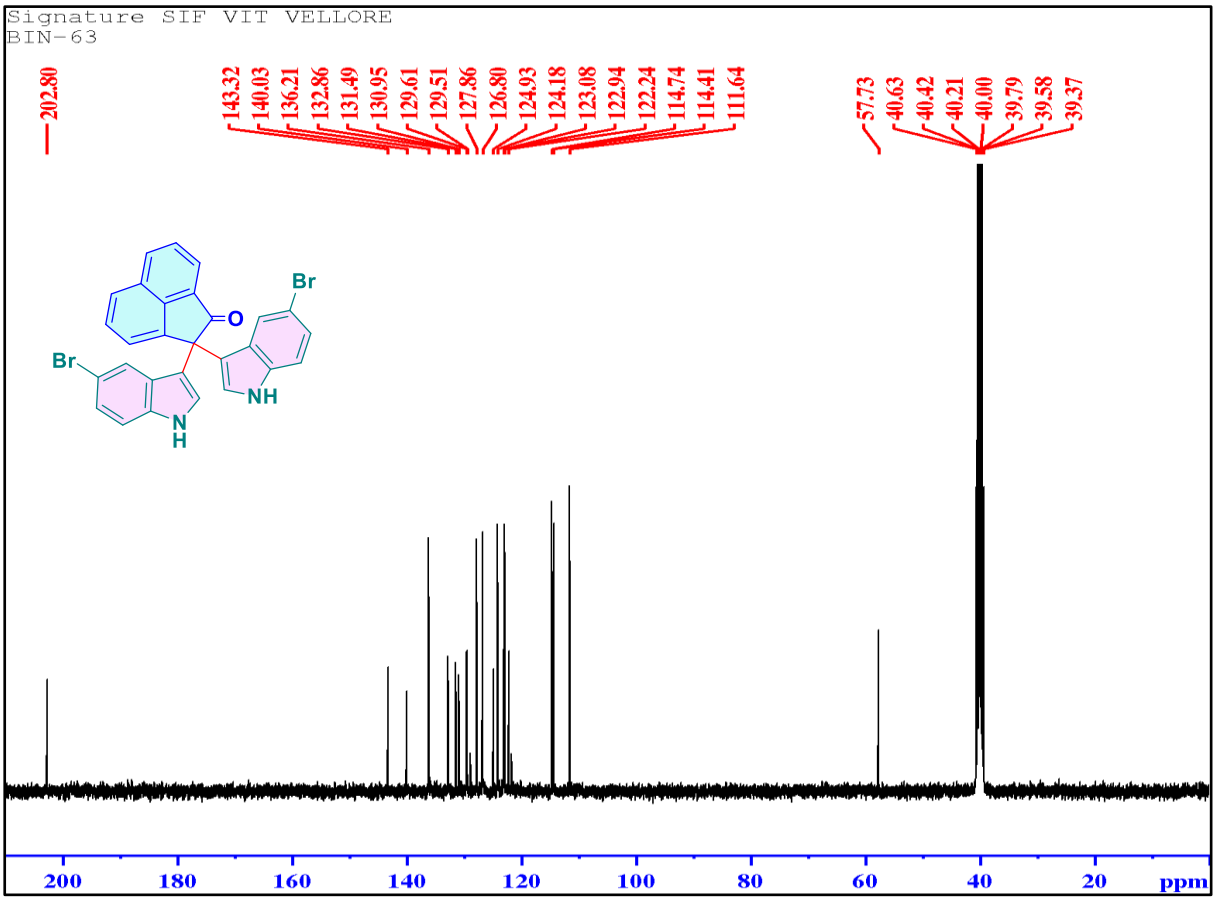


Fig. S86 ^{13}C NMR spectrum (100 MHz) of **7ej** in DMSO-d_6.

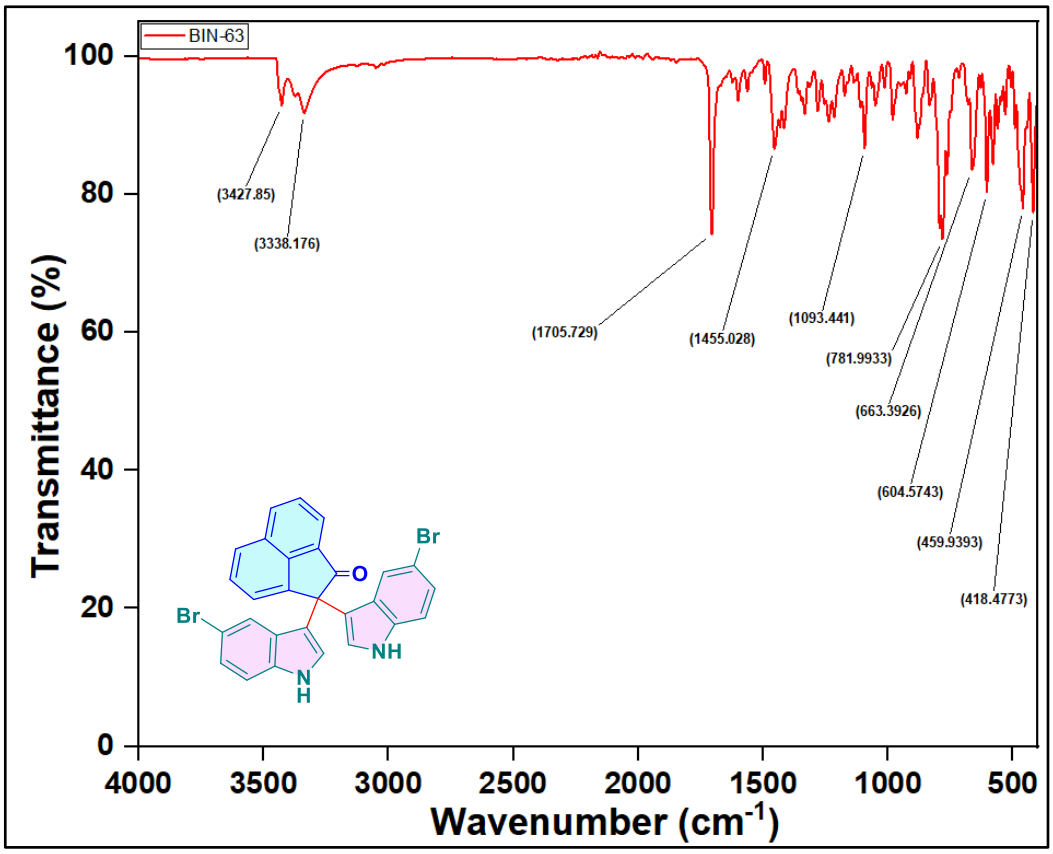


Fig. S87 FT-IR spectrum of **7ej**.

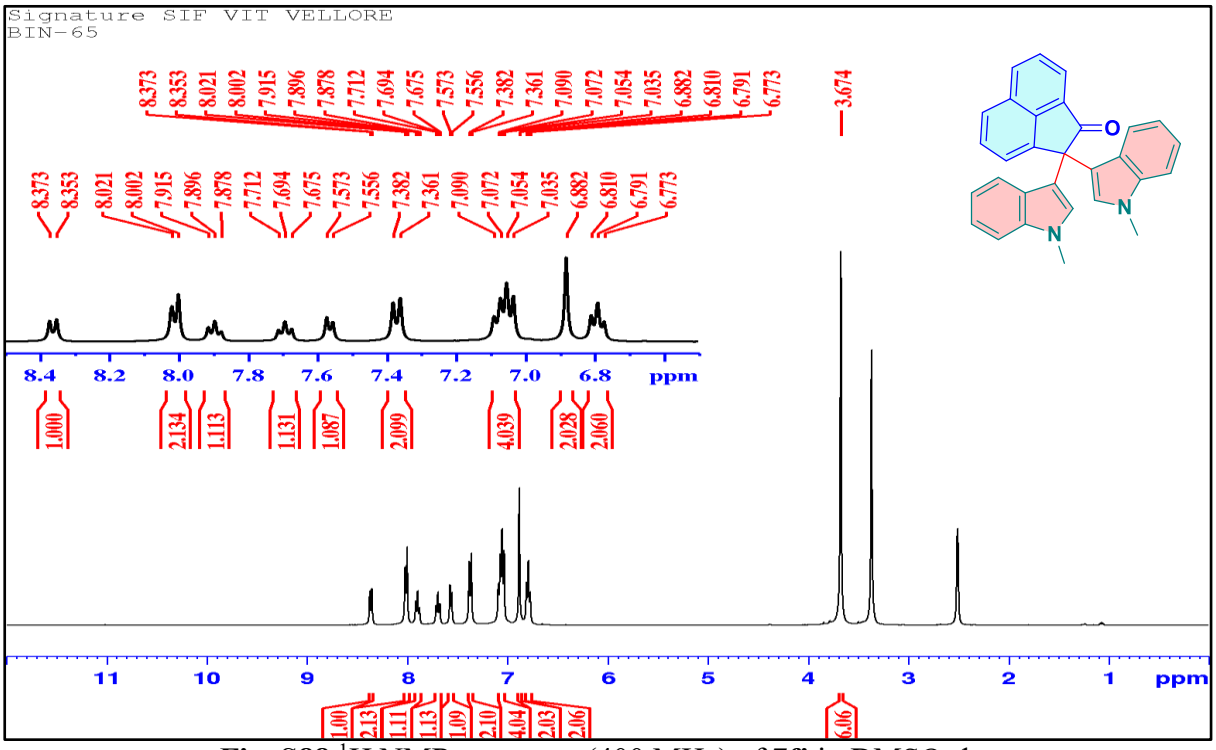


Fig. S88 ^{1}H NMR spectrum (400 MHz) of **7fj** in DMSO-d_6.

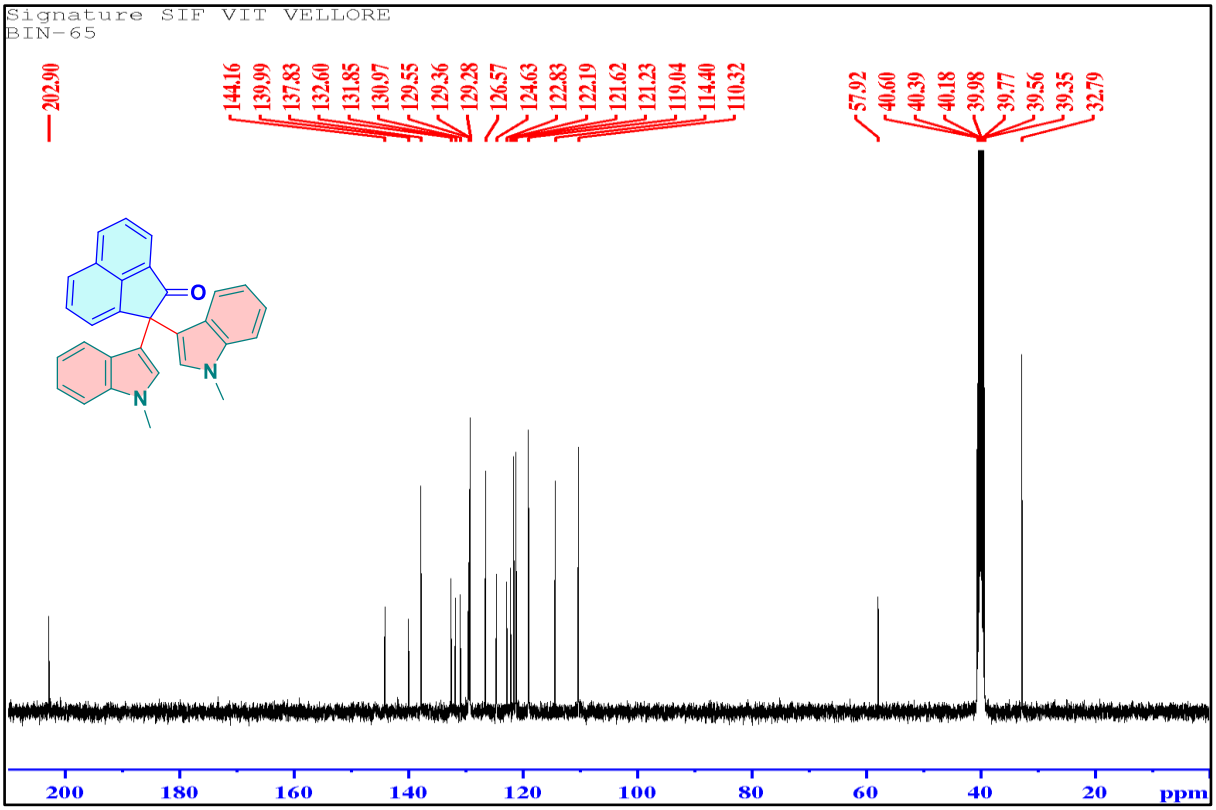


Fig. S89 ^{13}C NMR spectrum (100 MHz) of **7fj** in DMSO-d_6.

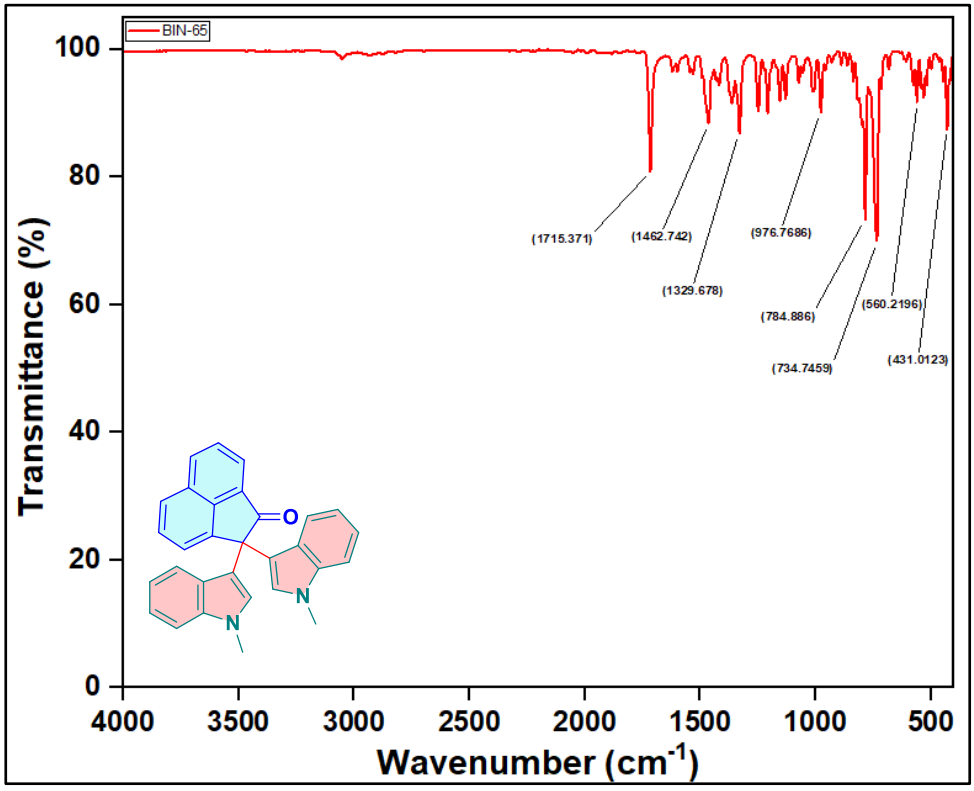


Fig. S90 FT-IR spectrum of **7fj**.

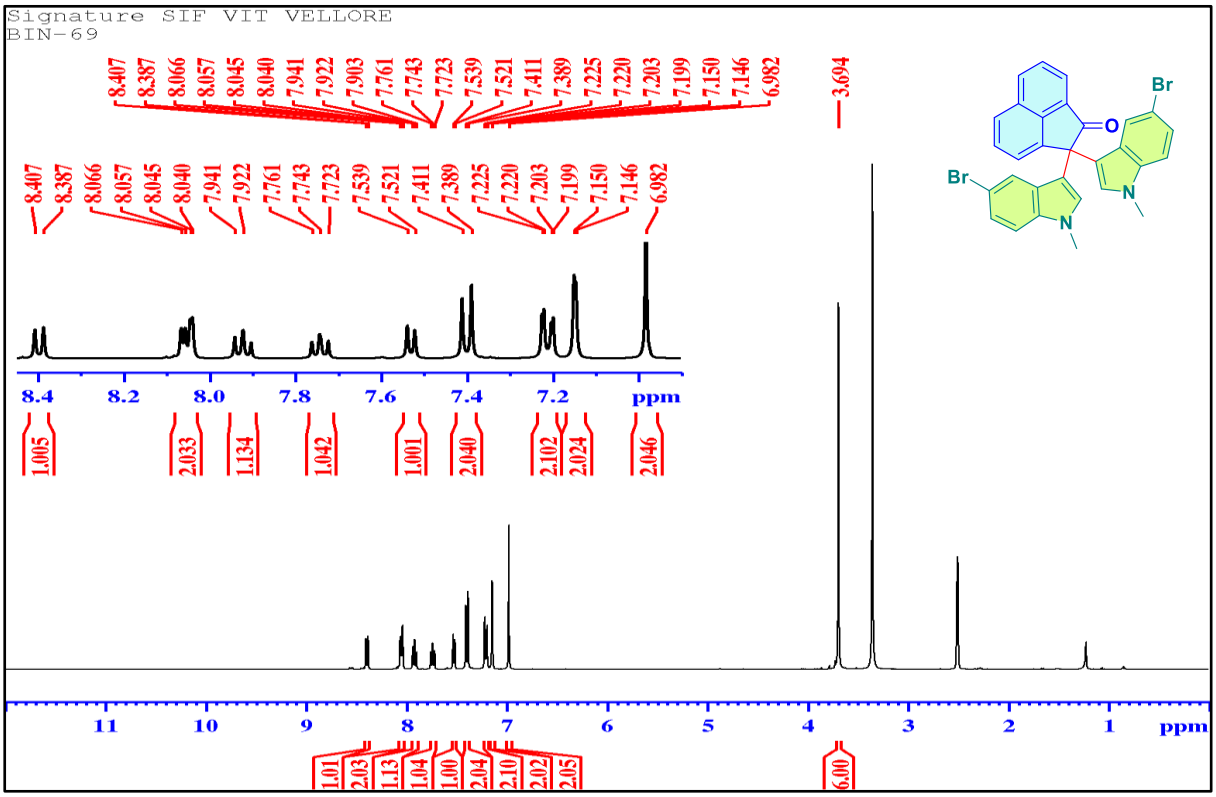


Fig. S91 ^{1}H NMR spectrum (400 MHz) of **7gj** in DMSO-d_6.

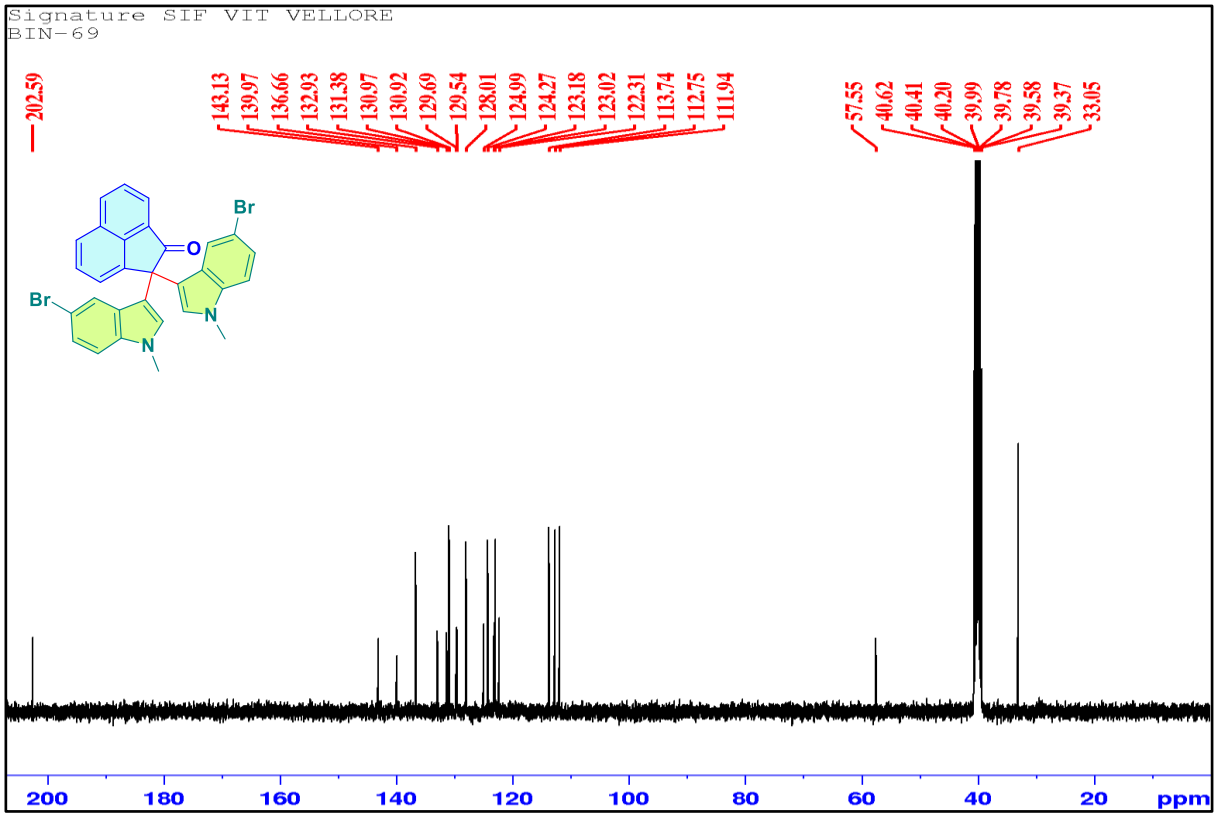


Fig. S92 ^{13}C NMR spectrum (100 MHz) of **7gj** in DMSO-d_6.

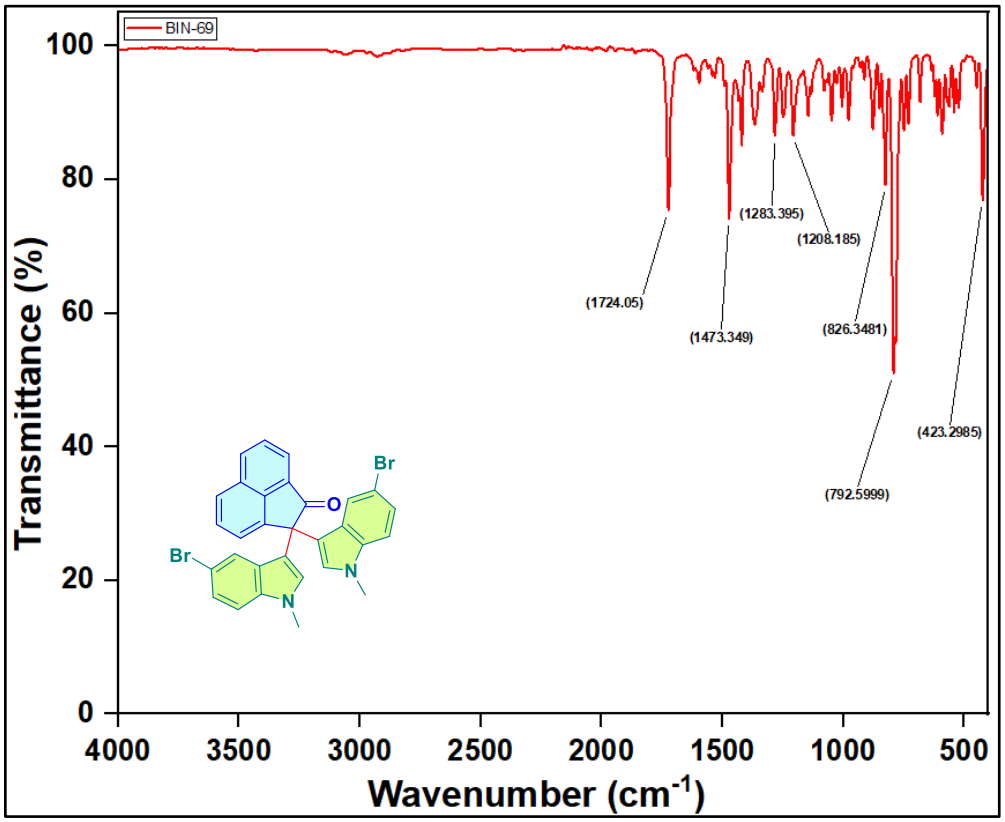


Fig. S93 FT-IR spectrum of **7gj**.

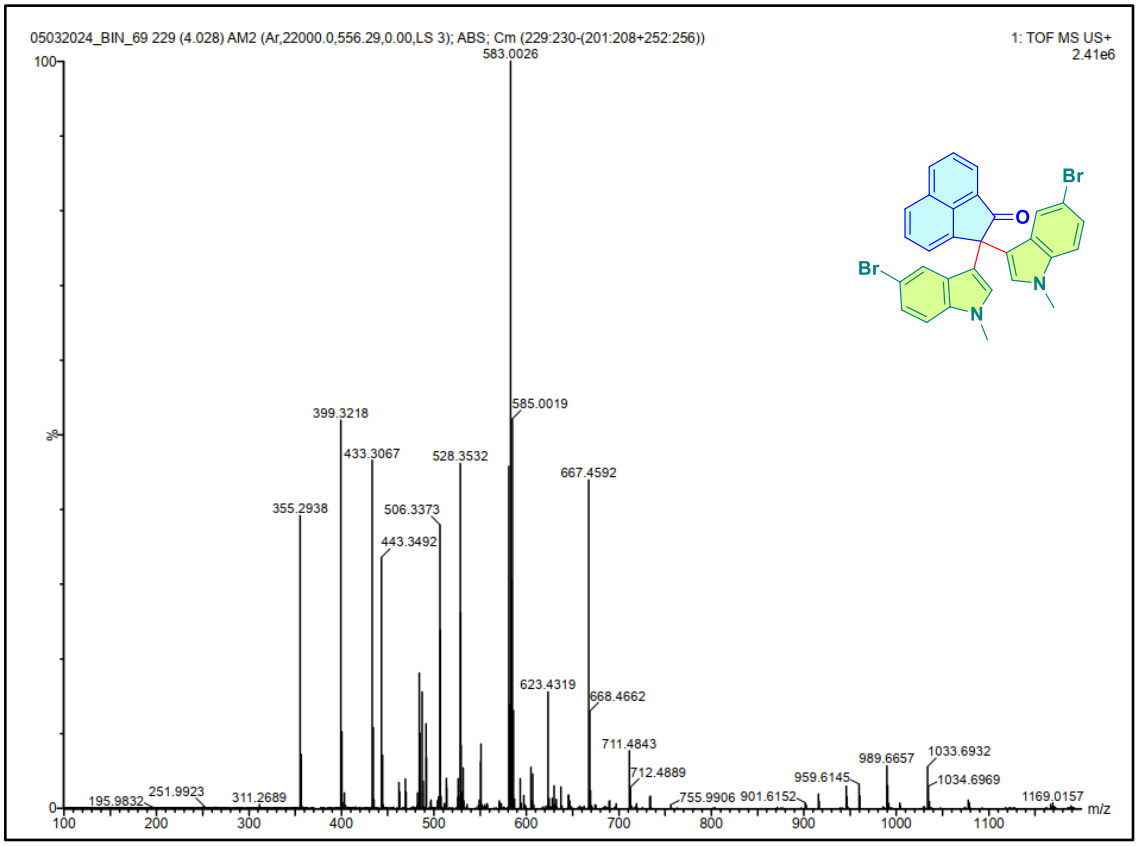


Fig. S94 HR-MS spectrum of **7gj**.

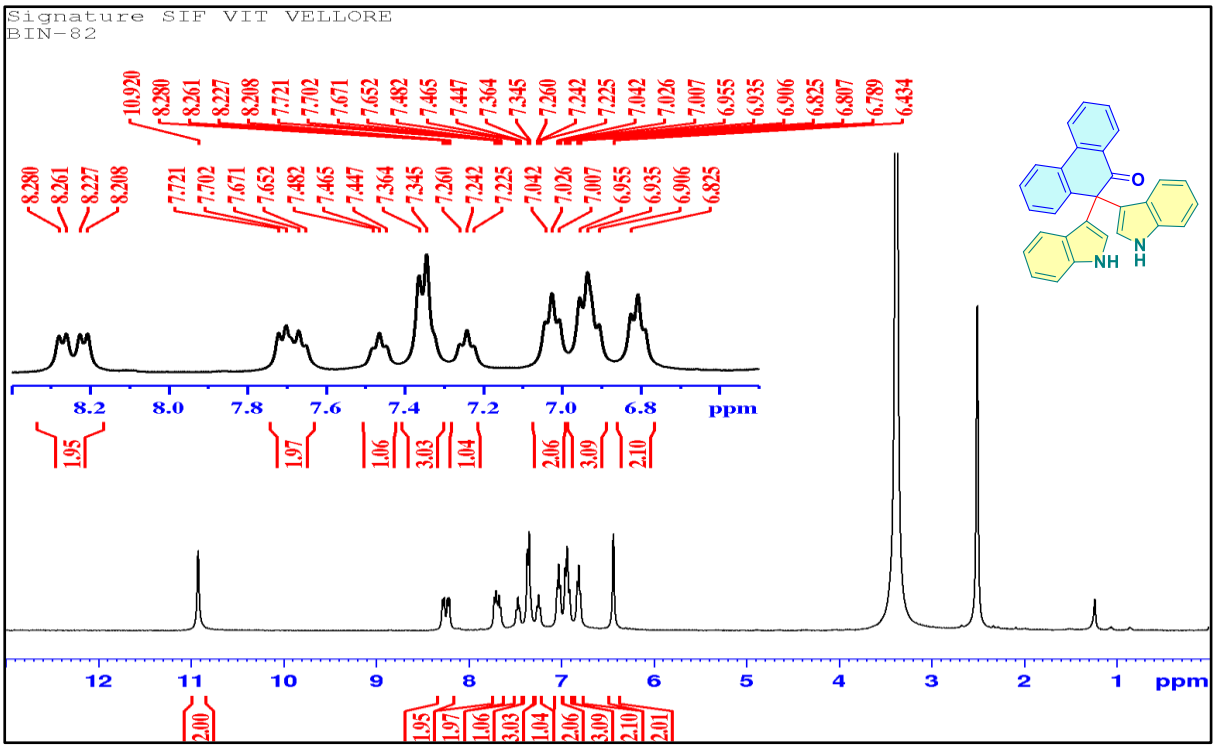


Fig. S95 ^{1}H NMR spectrum (400 MHz) of **7gk** in DMSO-d_6.

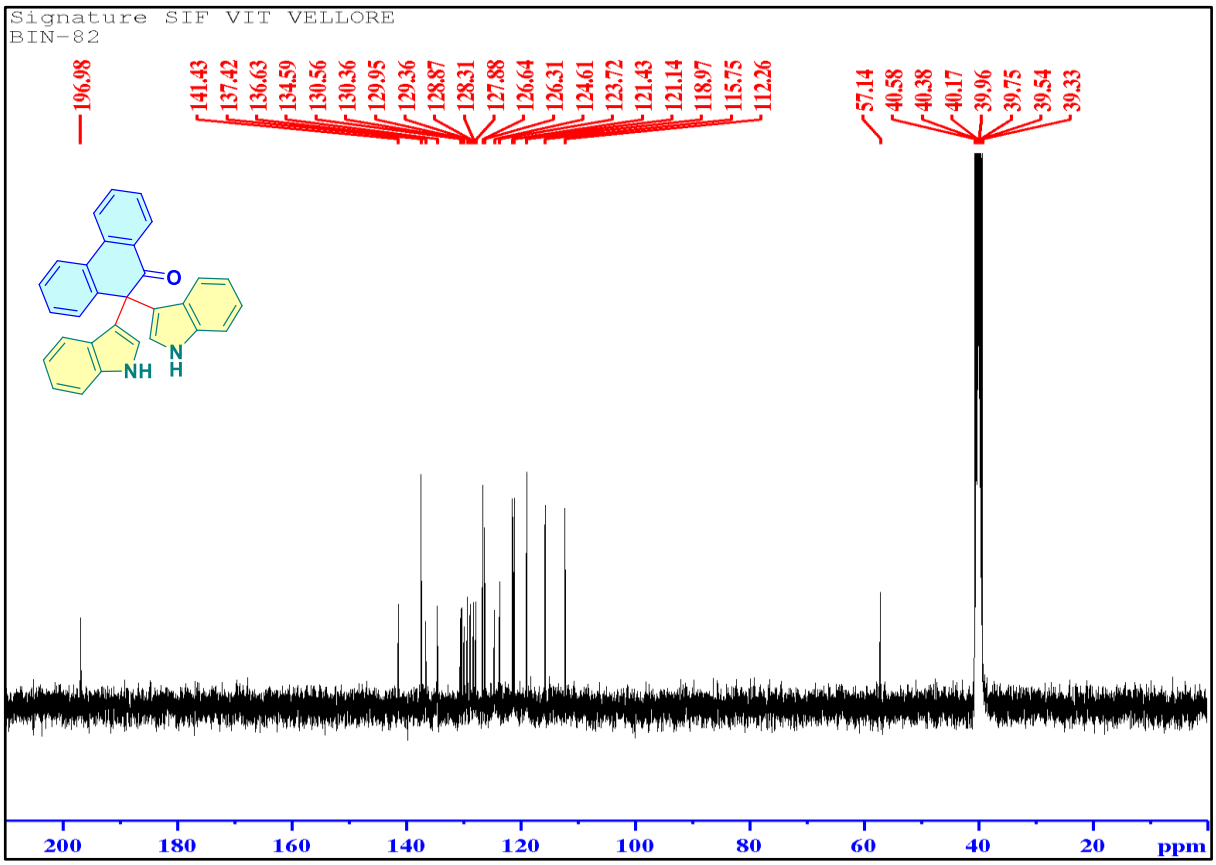


Fig. S96 ^{13}C NMR spectrum (100 MHz) of **7gk** in DMSO-d_6.

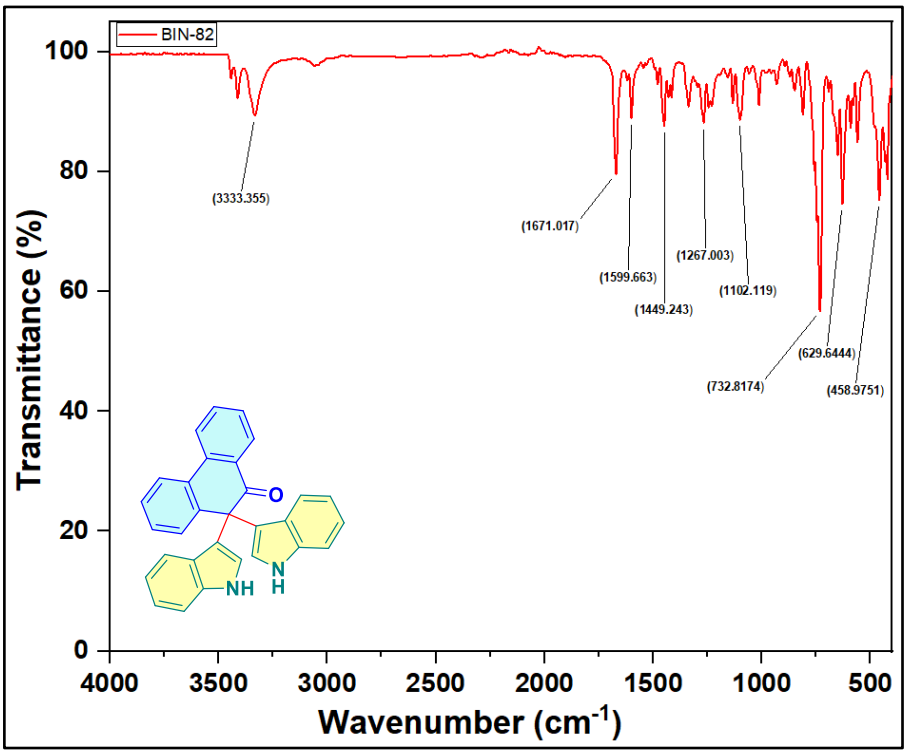


Fig. S97 FT-IR spectrum of **7gk**.

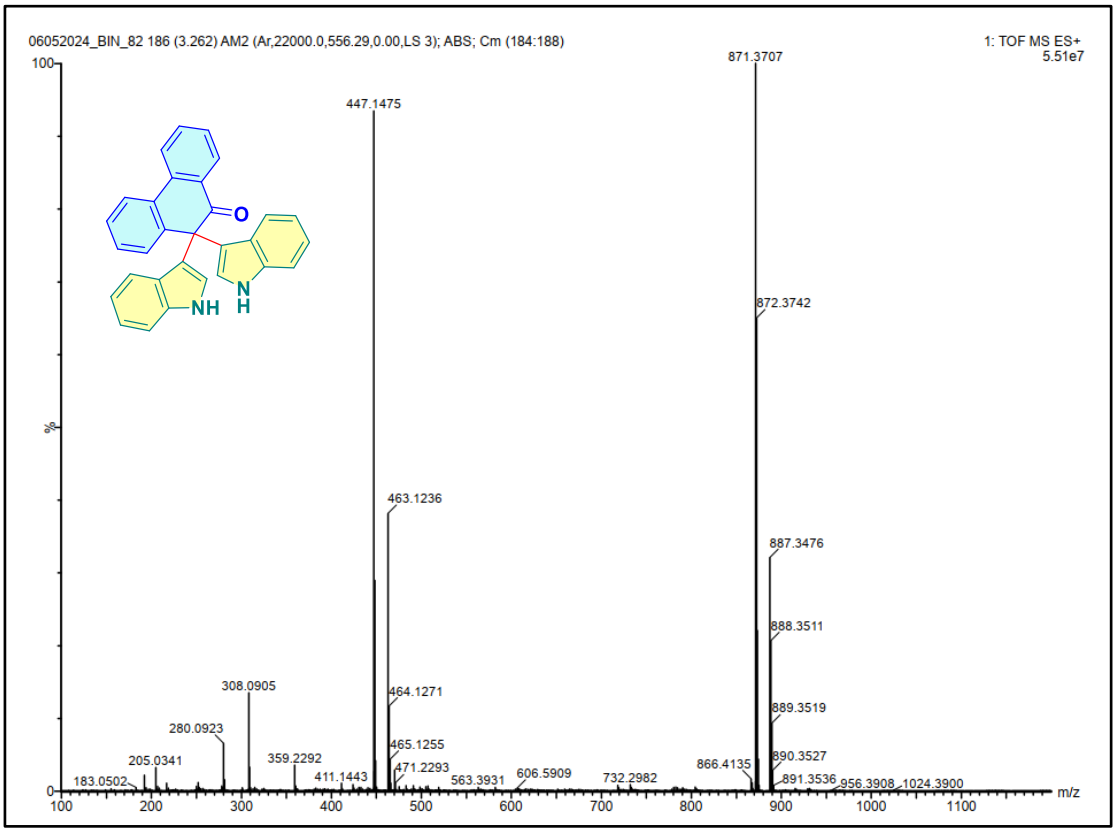


Fig. S98 HR-MS spectrum of **7gk**.

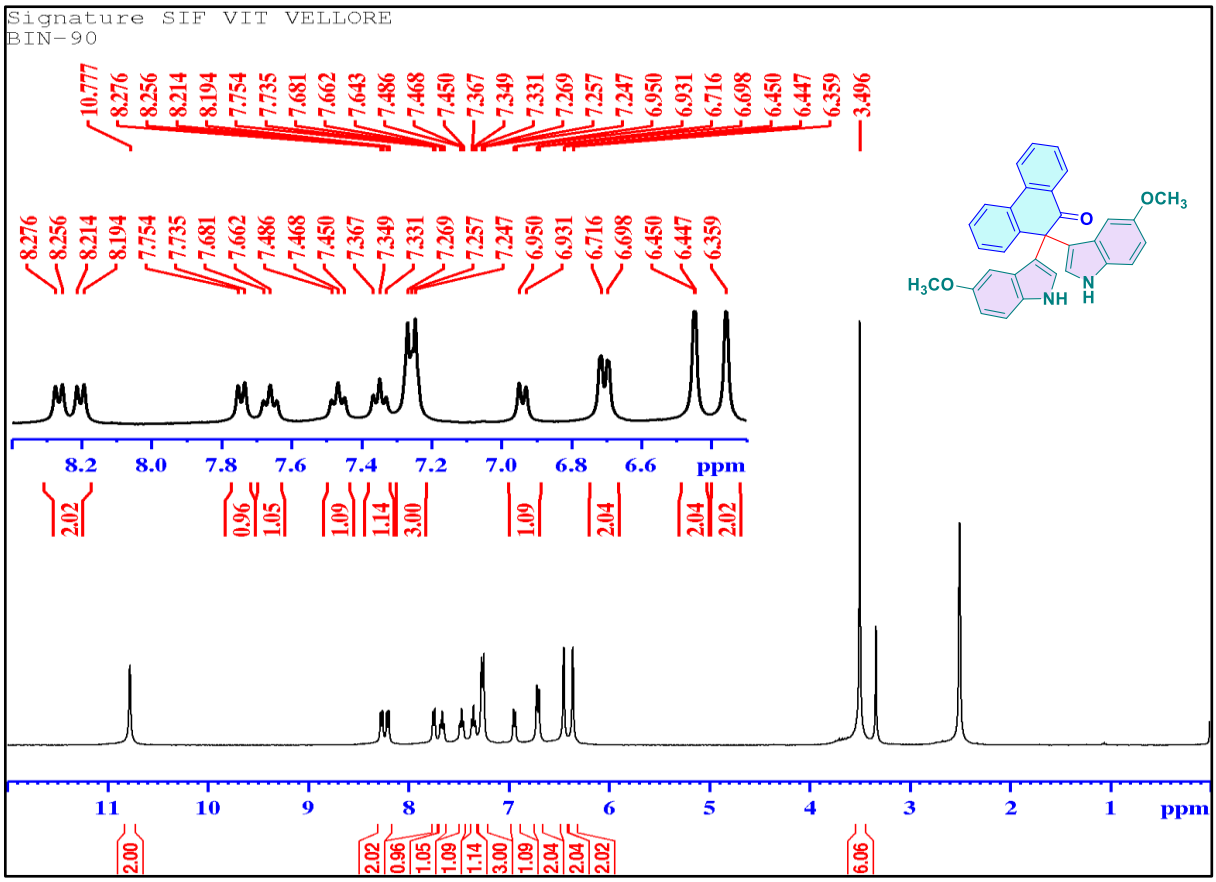


Fig. S99 ^{1}H NMR spectrum (400 MHz) of **7ck** in DMSO-d_6.

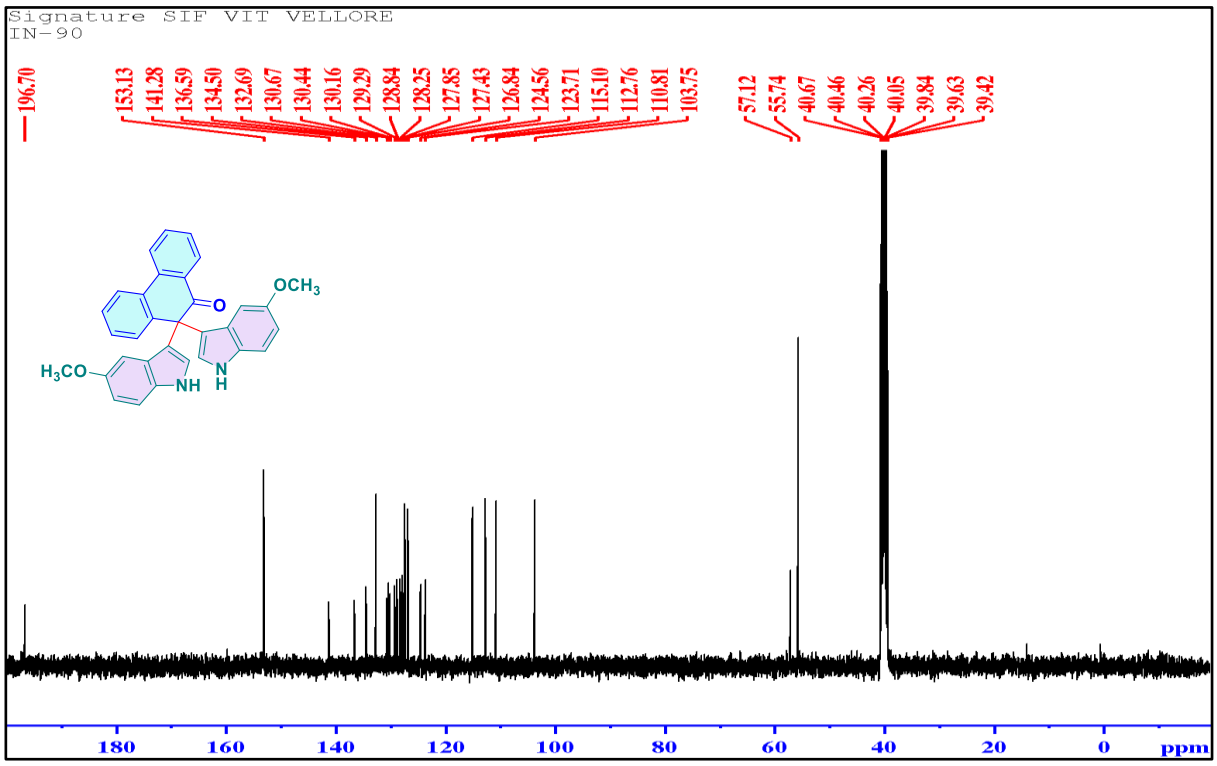


Fig. S100 ^{13}C NMR spectrum (100 MHz) of **7ck** in DMSO-d_6.

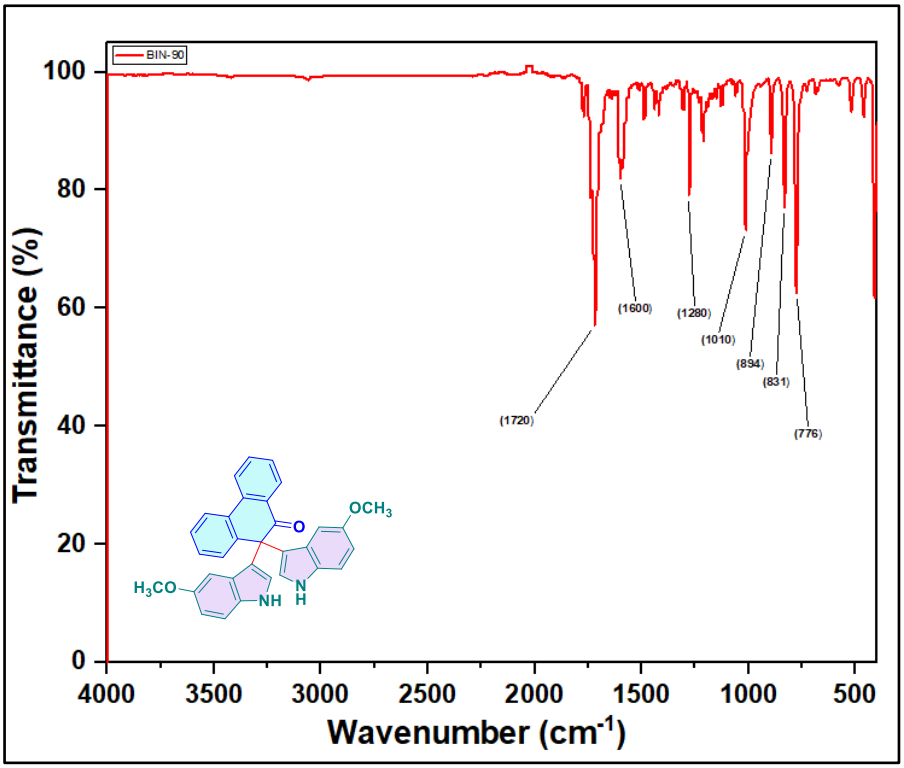


Fig. S101 FT-IR spectrum of **7ck**.

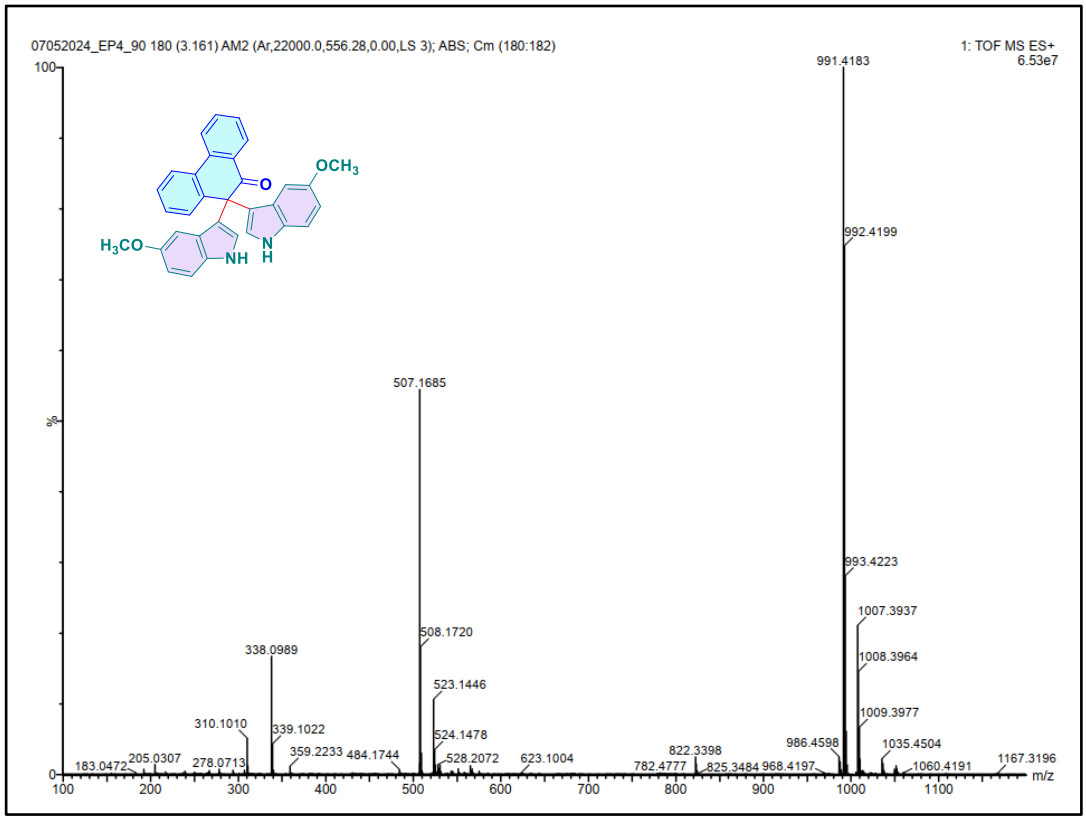


Fig. S102 HR-MS spectrum of **7ck**.

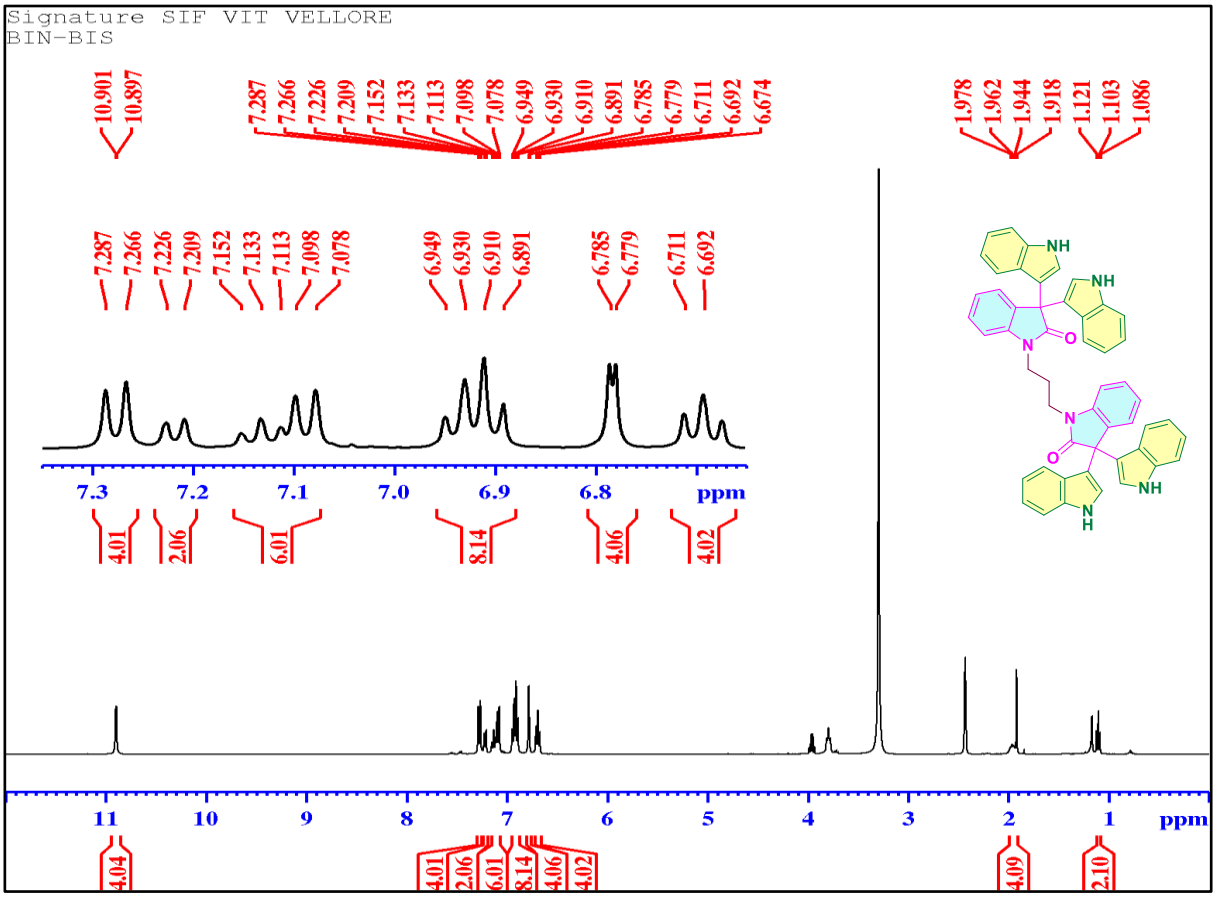


Fig. S103 ^{1}H NMR spectrum (400 MHz) of **10aa** in DMSO-d_6.

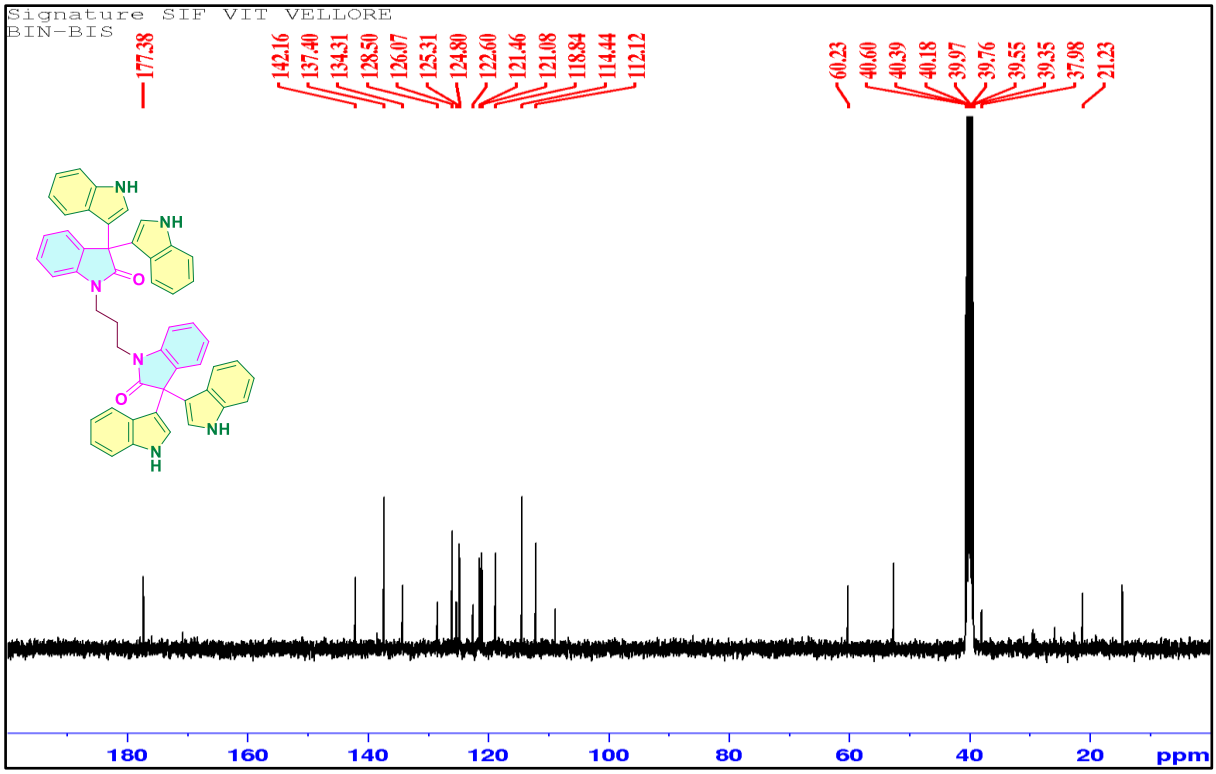


Fig. S104 ^{13}C NMR spectrum (100 MHz) of **10aa** in DMSO-d_6.

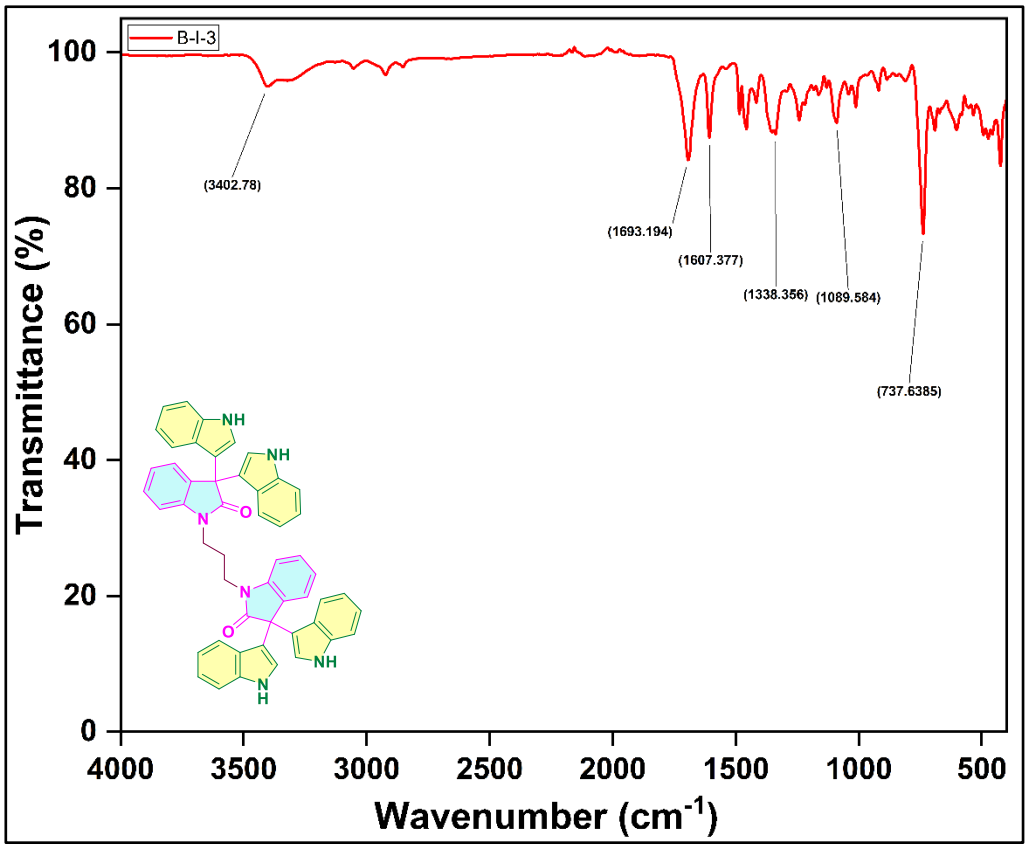


Fig. S105 FT-IR spectrum of **10aa**.

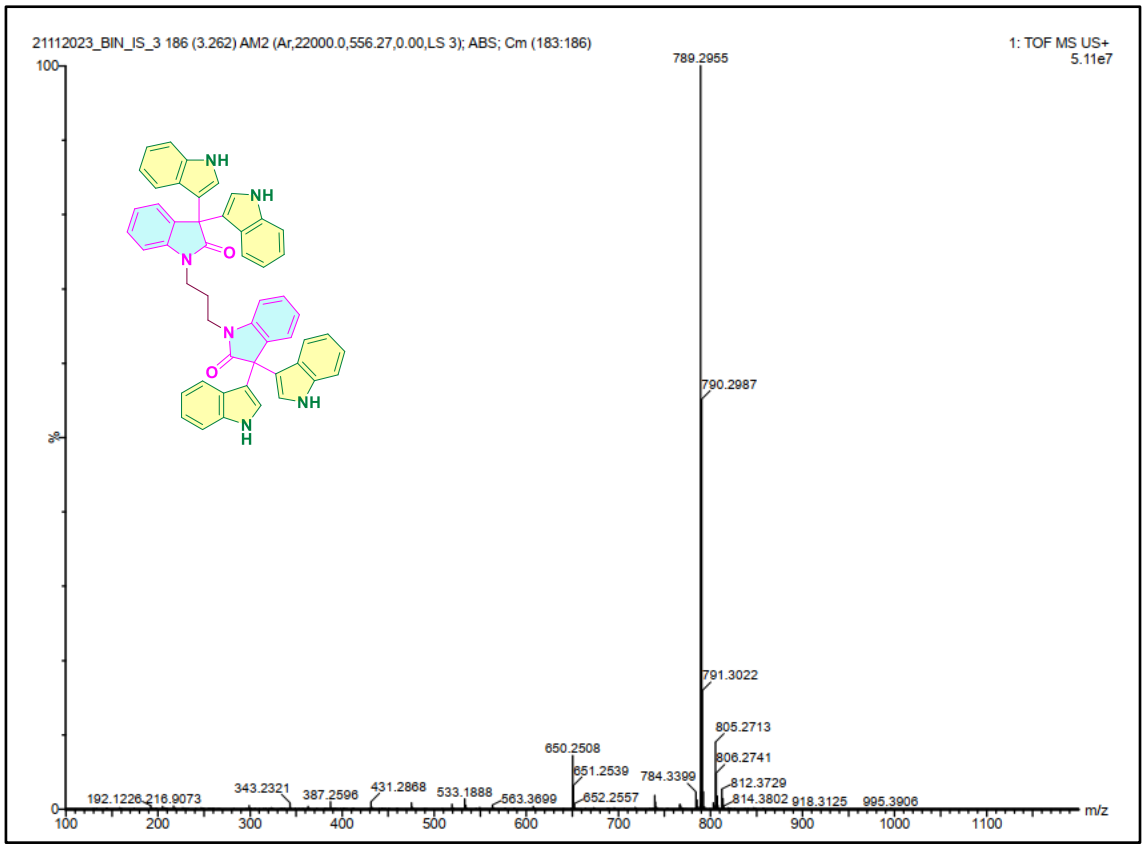


Fig. S106 HR-MS spectrum of **10aa**.

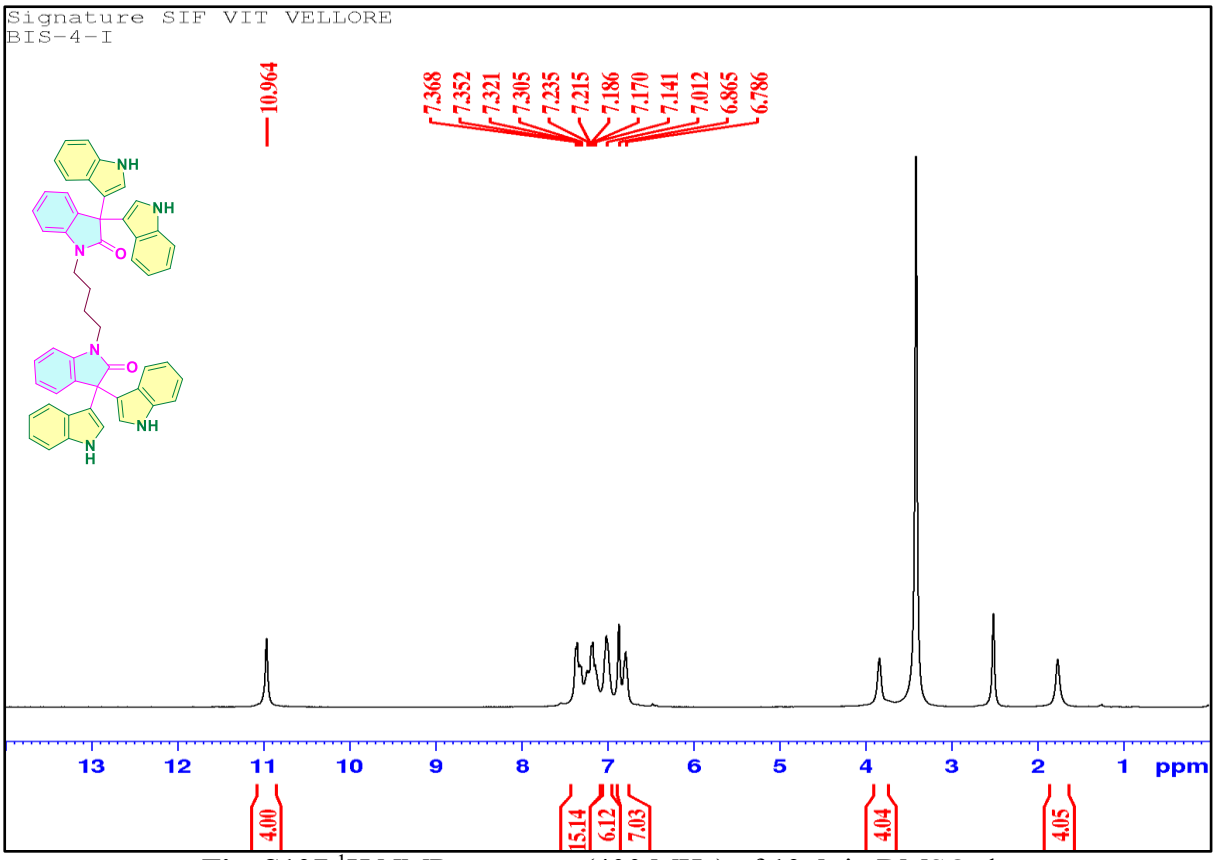


Fig. S107 ^{1}H NMR spectrum (400 MHz) of **10ab** in DMSO-d_6

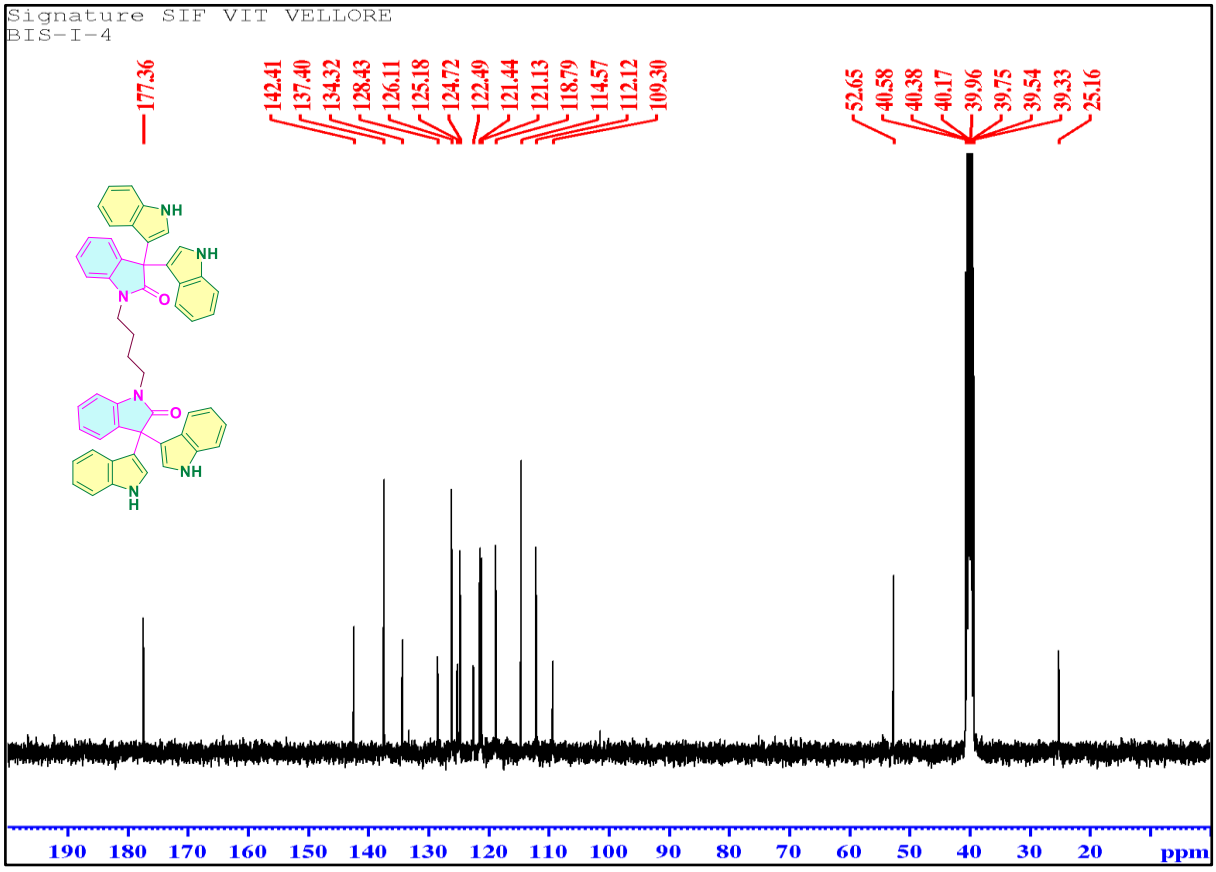


Fig. S108 ^{13}C NMR spectrum (100 MHz) of **10ab** in DMSO-d_6.

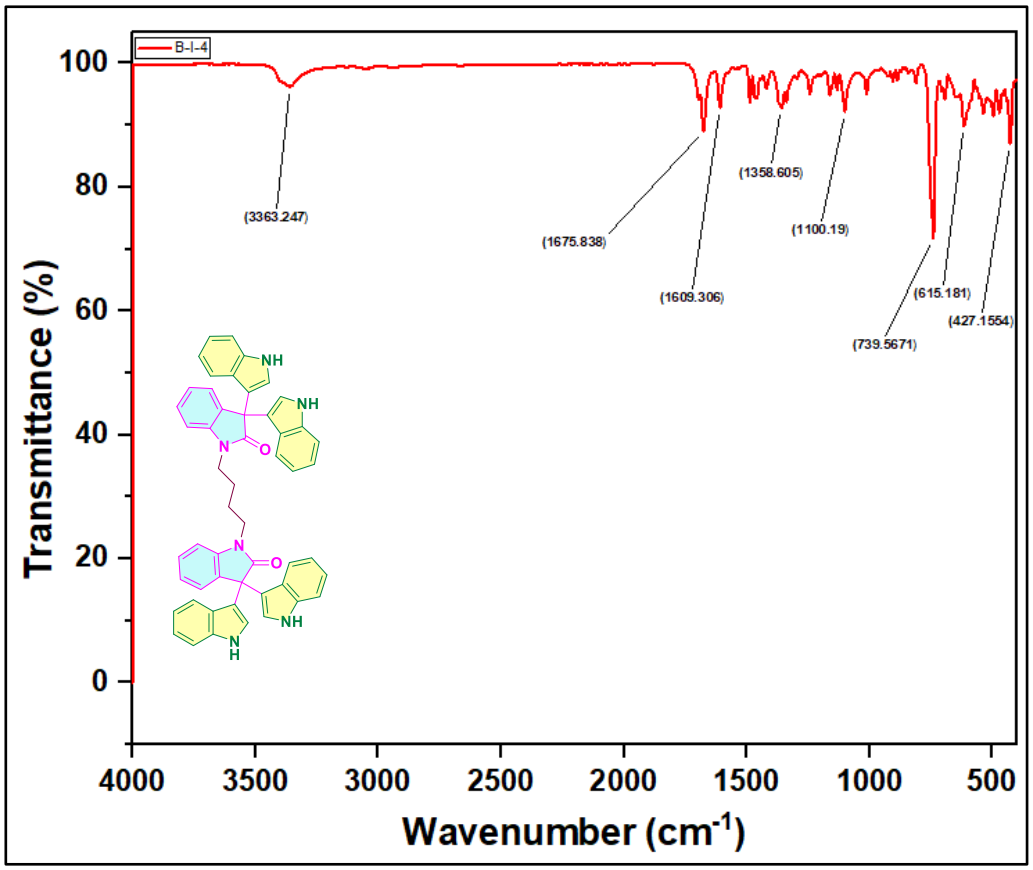


Fig. S109 FT-IR spectrum of **10ab**.

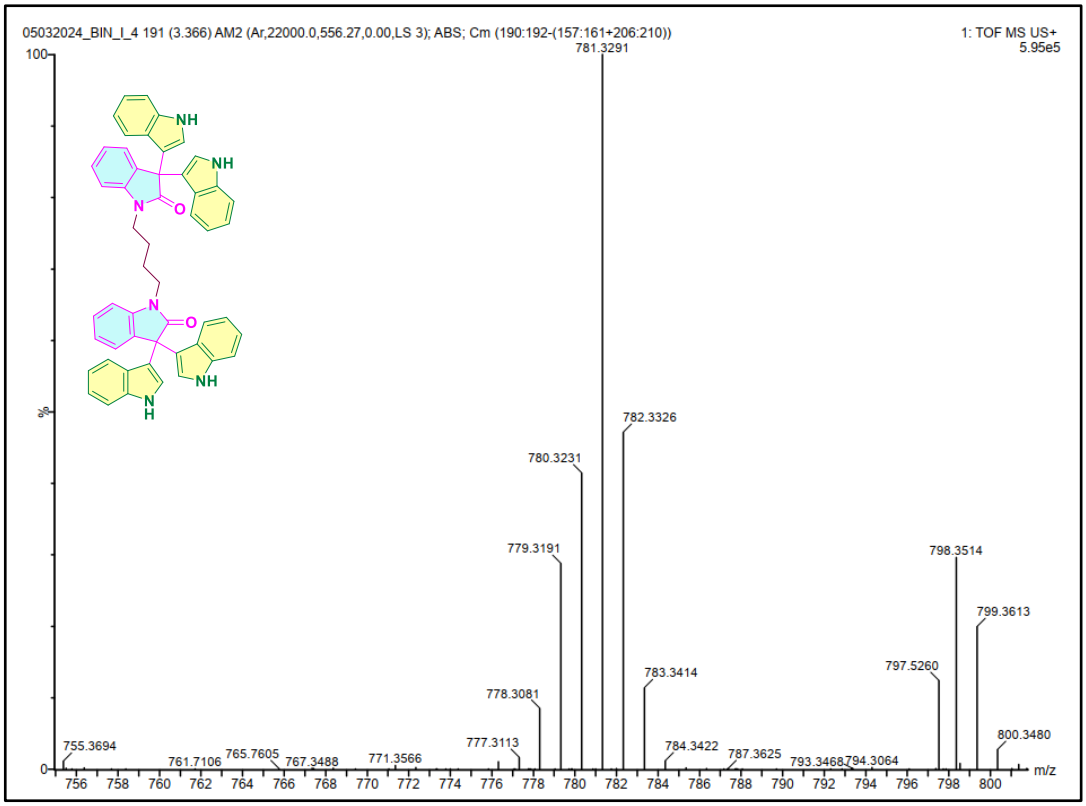


Fig. S110 HR-MS spectrum of **10ab**.

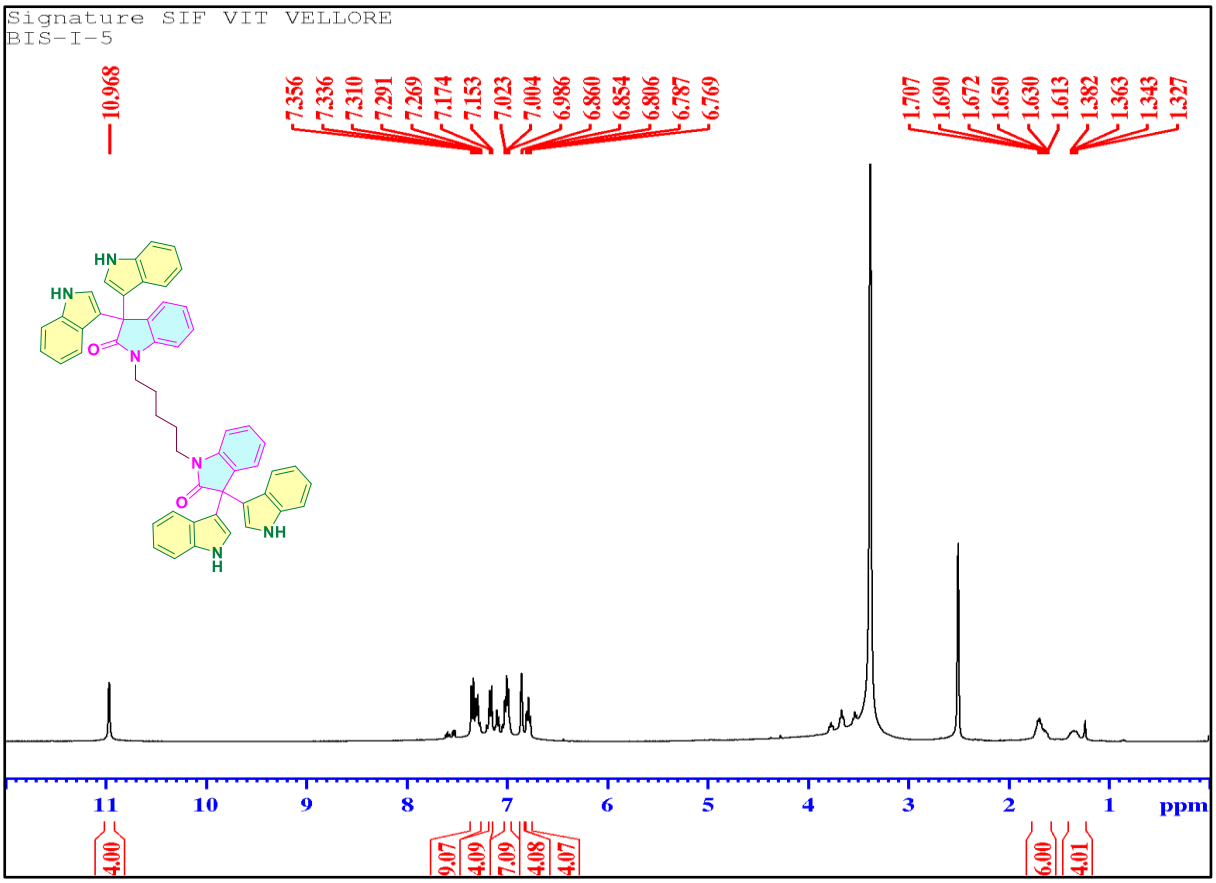


Fig. S111 ^{1}H NMR spectrum (400 MHz) of **10ac** in DMSO-d_6

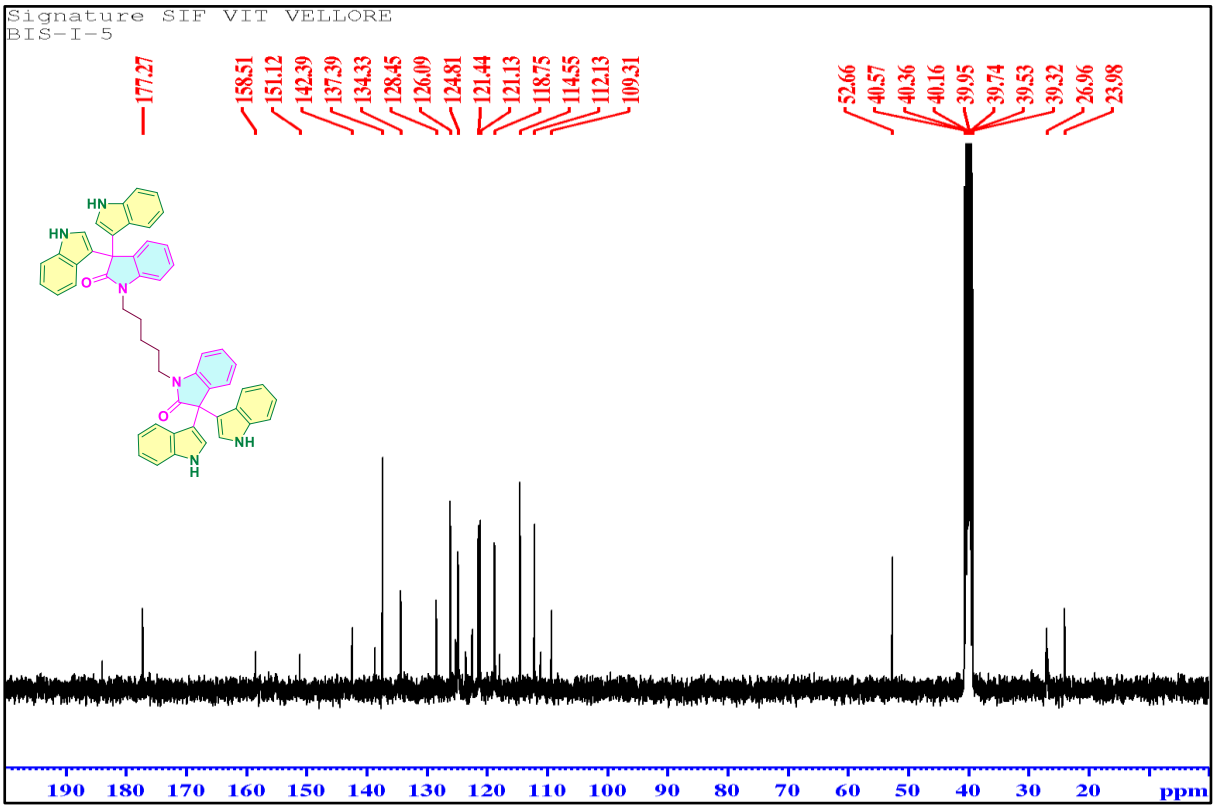


Fig. S112 ^{13}C NMR spectrum (100 MHz) of **10ac** in DMSO-d_6.

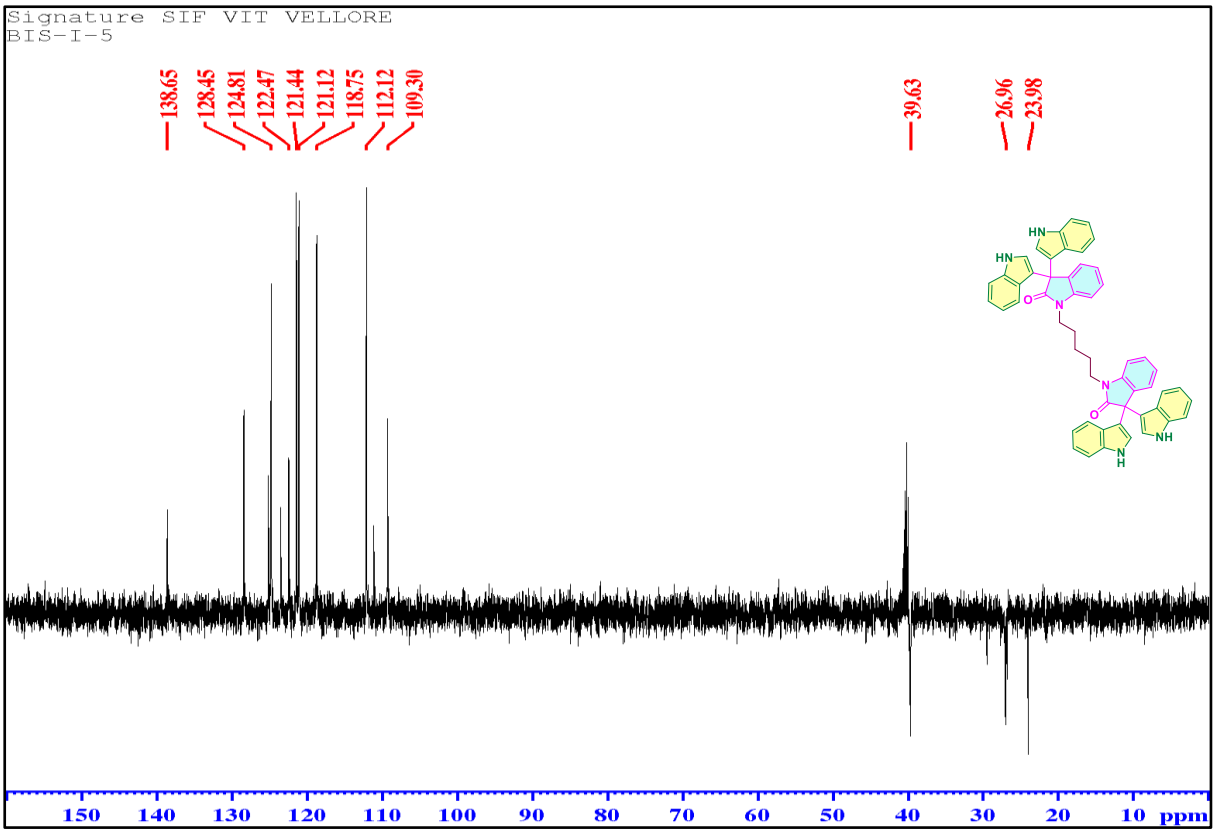


Fig. S113 DEPT-135 NMR spectrum (400 MHz) of **10ac** in DMSO-d_6

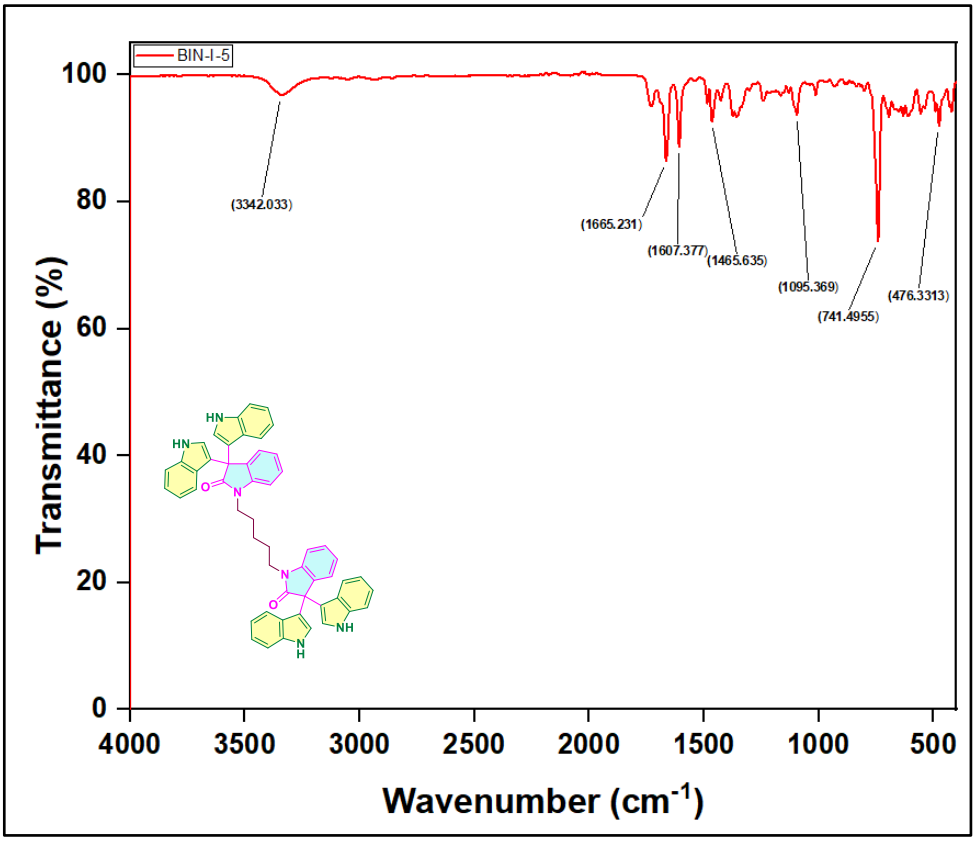


Fig. S114 FT-IR spectrum of **10ac**.

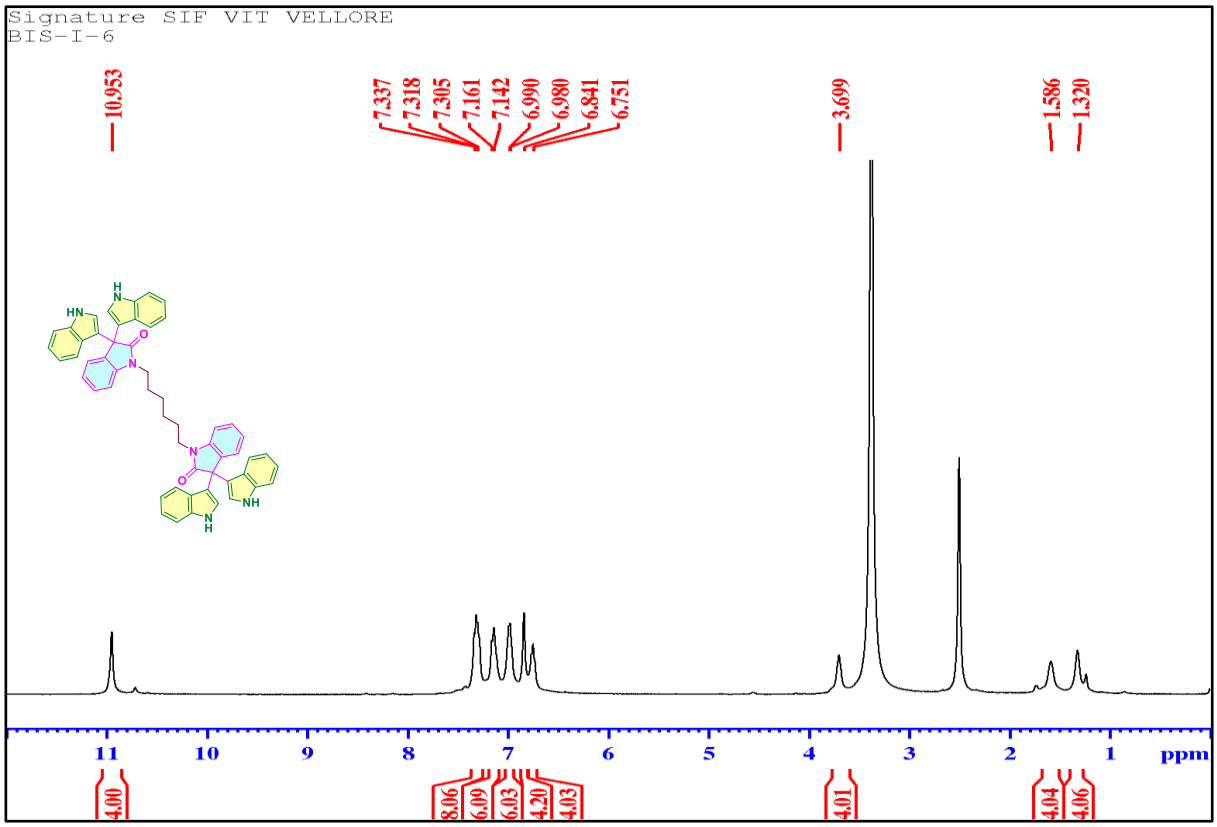


Fig. S115 ^{1}H NMR spectrum (400 MHz) of **10ad** in DMSO-d_6.

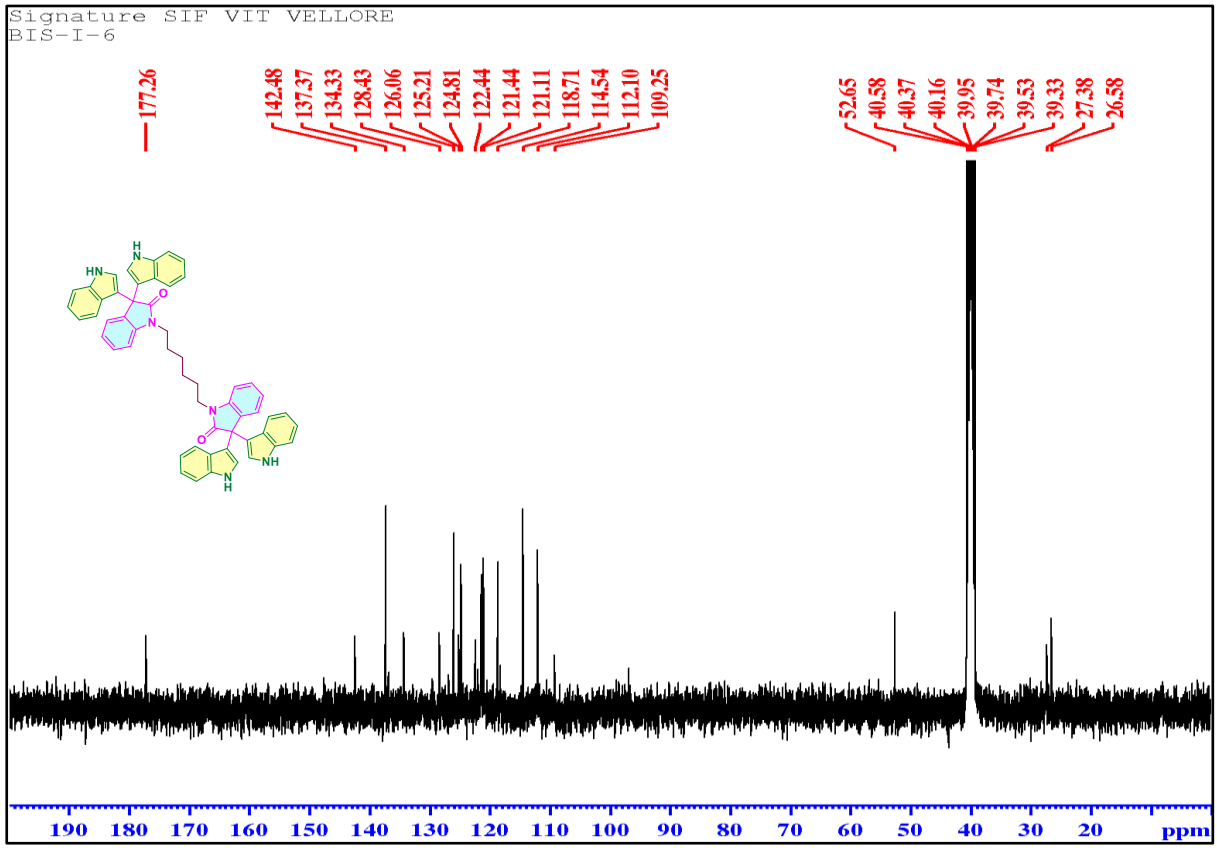


Fig. S116 ^{13}C NMR spectrum (100 MHz) of **10ad** in DMSO-d_6.

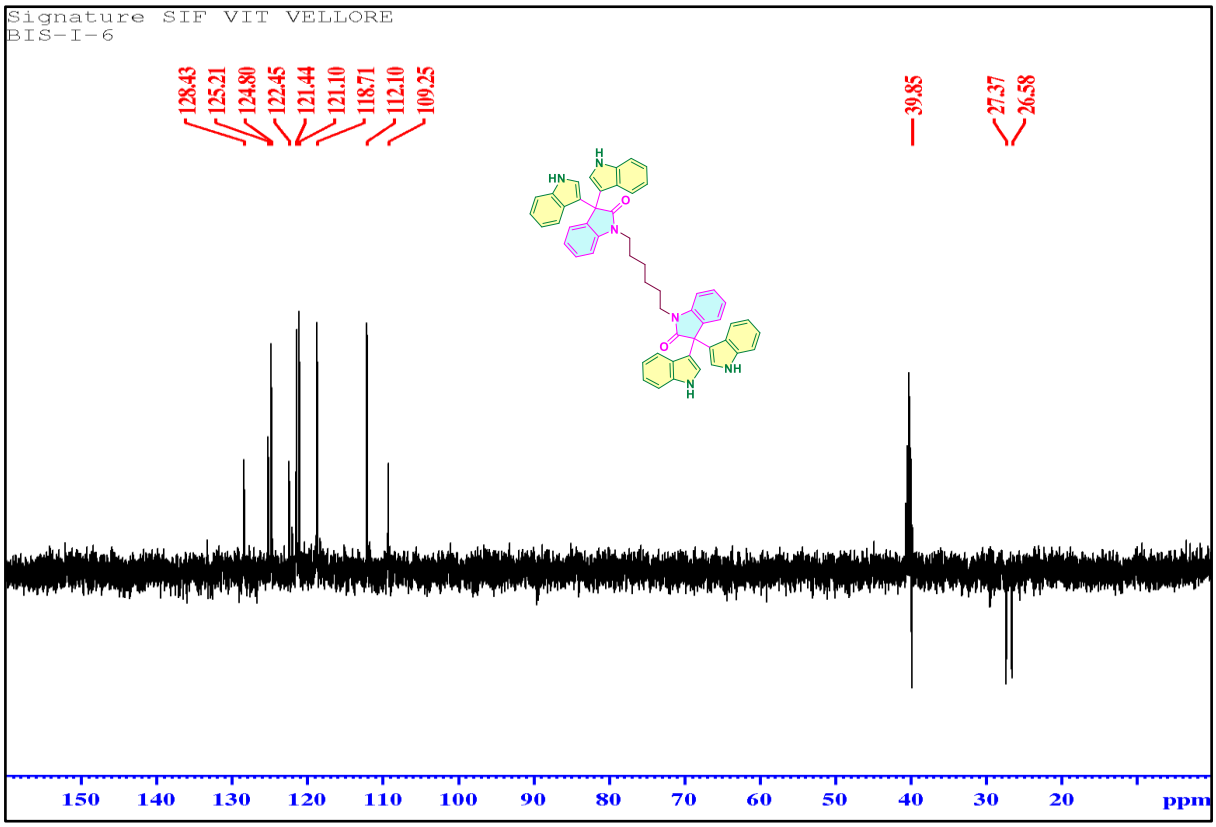


Fig. S117 DEPT-135 NMR spectrum (400 MHz) of **10ad** in DMSO-d_6.

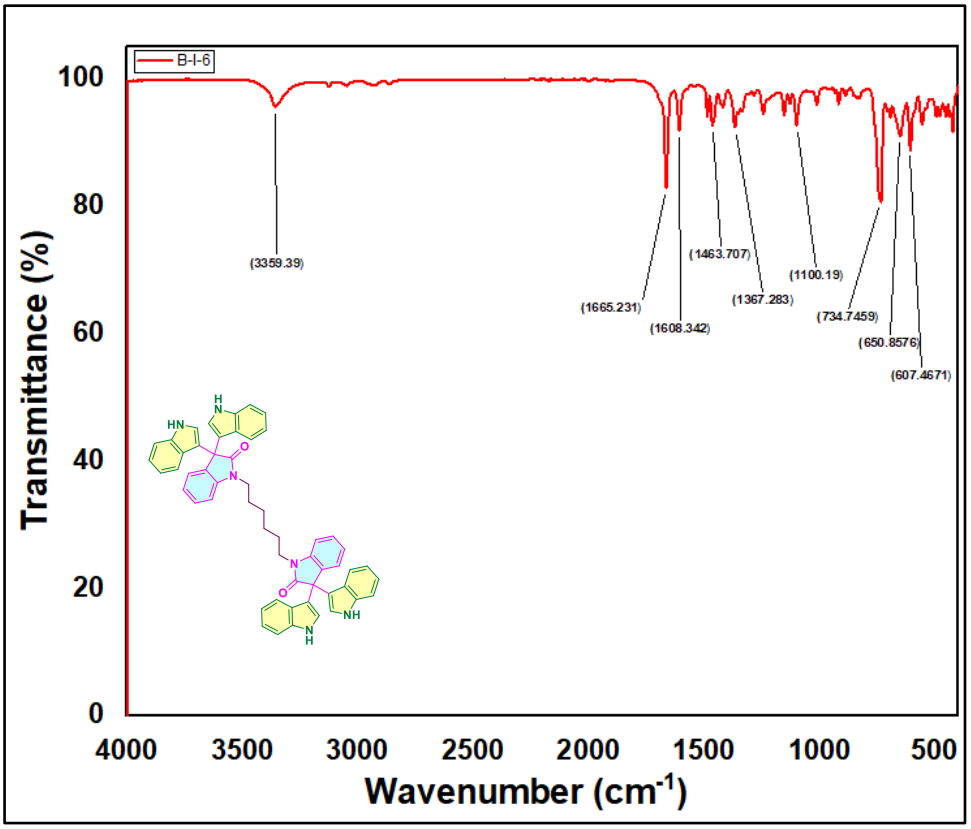


Fig. S118 FT-IR spectrum of **10ad**.

Crystal Structure Report for 7gj

A specimen of $C_{30}H_{20}Br_2N_2O$, approximate dimensions 0.190 mm x 0.241 mm x 0.274 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured (λ = 0.71073 Å). The integration of the data using a triclinic unit cell yielded a total of 55571 reflections to a maximum θ angle of 28.35° (0.75 Å resolution), of which 6063 were independent (average redundancy 9.166, completeness = 99.5%, R_{int} = 5.16%, R_{sig} = 3.84%) and 3605 (59.46%) were greater than $2\sigma(F^2)$. The final cell constants of a = 8.9565(7) Å, b = 12.0727(9) Å, c = 12.5432(10) Å, α = 107.005(3)°, β = 105.112(3)°, γ = 97.415(3)°, volume = 1220.78(17) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 $\sigma(I)$. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.4610 and 0.5690. The final anisotropic full-matrix least-squares refinement on F^2 with 318 variables converged at R1 = 5.35%, for the observed data and wR2 = 15.77% for all data. The goodness-of-fit was 1.029. The largest peak in the final difference electron density synthesis was 0.695 $e^-/Å^3$ and the largest hole was -1.084 $e^-/Å^3$ with an RMS deviation of 0.083 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.590 g/cm^3 and F (000), 584 e^-.

Table S1a Sample and crystal data for **7gj**

CCDC No	**2360038**	
Identification code	**7gj**	
Chemical formula	$C_{30}H_{20}Br_2N_2O$	
Formula weight	584.30 g/mol	
Temperature	300(2) K	
Wavelength	0.71073 Å	
Crystal size	0.190 x 0.241 x 0.274 mm	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.9565(7) Å	α = 107.005(3)°
	b = 12.0727(9) Å	β = 105.112(3)°
	c = 12.5432(10) Å	γ = 97.415(3)°
Volume	1220.78(17) $Å^3$	
Z	2	
Density (calculated)	1.590 g/cm^3	
Absorption coefficient	3.347 mm^{-1}	
F(000)	584	

Table S1b Data collection and structure refinement for **7gj**

Theta range for data collection	1.79 to 28.35°
Index ranges	-11<=h<=11, -16<=k<=16, -16<=l<=16
Reflections collected	55571
Independent reflections	6063 [R(int) = 0.0516]
Max. and min. transmission	0.5690 and 0.4610
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2019/1 (Sheldrick, 2019)
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	6063 / 0 / 318
Goodness-of-fit on F^2	1.029
Final R indices	3605 data; $I>2\sigma(I)$ R1 = 0.0535, wR2 = 0.1355
	all data R1 = 0.1015, wR2 = 0.1577
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0645P)^2+1.2110P]$
	where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	0.695 and -1.084 $eÅ^{-3}$
R.M.S. deviation from mean	0.083 $eÅ^{-3}$

Table S1c Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for **7gj**

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
Br1	0.90861(6)	0.13612(4)	0.94322(4)	0.0835(2)
Br2	0.59175(11)	0.90378(5)	0.09954(7)	0.1374(4)
O1	0.0938(3)	0.5957(2)	0.1614(3)	0.0636(7)
N1	0.1285(3)	0.3962(3)	0.4613(3)	0.0503(7)
N2	0.5814(4)	0.4431(4)	0.1880(3)	0.0664(9)
C1	0.1233(4)	0.3826(3)	0.2767(3)	0.0430(7)
C2	0.0687(4)	0.3224(3)	0.3460(3)	0.0478(8)
C3	0.9735(4)	0.2091(3)	0.2975(4)	0.0583(10)
C4	0.9312(5)	0.1549(3)	0.1776(4)	0.0633(10)
C5	0.9800(4)	0.2143(3)	0.1087(3)	0.0556(9)
C6	0.0748(4)	0.3268(3)	0.1553(3)	0.0486(8)
C7	0.2229(4)	0.4952(3)	0.3573(3)	0.0420(7)
C8	0.2204(4)	0.4988(3)	0.4663(3)	0.0469(8)
C9	0.3106(4)	0.5932(3)	0.3283(3)	0.0408(7)
C10	0.1803(4)	0.6463(3)	0.2607(3)	0.0465(8)
C11	0.1855(4)	0.7650(3)	0.3405(3)	0.0504(9)
C12	0.3154(4)	0.7918(3)	0.4419(3)	0.0458(8)
C13	0.3972(4)	0.6990(3)	0.4394(3)	0.0444(8)
C14	0.4192(4)	0.5497(3)	0.2593(3)	0.0459(8)
C15	0.5004(4)	0.6140(3)	0.2037(3)	0.0503(8)
C16	0.6006(4)	0.5439(4)	0.1604(3)	0.0607(11)
C17	0.4730(4)	0.4480(4)	0.2483(3)	0.0561(9)
C18	0.1120(5)	0.3640(4)	0.5615(4)	0.0681(11)
C19	0.0944(5)	0.8472(4)	0.3321(4)	0.0617(10)
C20	0.3616(5)	0.9000(3)	0.5364(4)	0.0600(10)
C21	0.2656(6)	0.9824(4)	0.5239(5)	0.0752(13)
C22	0.1381(6)	0.9554(4)	0.4262(5)	0.0785(13)
C23	0.5290(4)	0.7160(3)	0.5313(3)	0.0549(9)

C24	0.4976(6)	0.9132(4)	0.6294(4)	0.0699(11)
C25	0.5782(5)	0.8247(4)	0.6263(4)	0.0660(11)
C26	0.4972(5)	0.7225(4)	0.1861(3)	0.0618(10)
C27	0.5949(6)	0.7568(4)	0.1274(4)	0.0819(15)
C28	0.6944(6)	0.6878(6)	0.0866(4)	0.0965(19)
C29	0.6980(5)	0.5813(6)	0.1016(4)	0.0827(16)
C30	0.6674(6)	0.3483(5)	0.1648(5)	0.0989(19)

Table S1d Bond lengths (Å) for **7gj**

Br1-C5	1.901(4)	Br2-C27	1.908(5)
O1-C10	1.206(4)	N1-C8	1.371(4)
N1-C2	1.375(5)	N1-C18	1.455(4)
N2-C16	1.362(6)	N2-C17	1.375(5)
N2-C30	1.462(5)	C1-C6	1.393(5)
C1-C2	1.422(5)	C1-C7	1.441(5)
C2-C3	1.383(5)	C3-C4	1.376(6)
C3-H3	0.930000	C4-C5	1.389(6)
C4-H4	0.930000	C5-C6	1.374(5)
C6-H6	0.930000	C7-C8	1.362(5)
C7-C9	1.520(4)	C8-H8	0.930000
C9-C14	1.509(4)	C9-C13	1.522(5)
C9-C10	1.576(5)	C10-C11	1.476(5)
C11-C19	1.374(5)	C11-C12	1.402(5)
C12-C20	1.408(5)	C12-C13	1.413(5)
C13-C23	1.361(5)	C14-C17	1.359(5)
C14-C15	1.434(5)	C15-C26	1.392(6)
C15-C16	1.414(5)	C16-C29	1.391(6)
C17-H17	0.930000	C18-H18A	0.960000
C18-H18	0.960000	C18-H18C	0.960000
C19-C22	1.405(7)	C19-H19	0.930000
C20-C24	1.403(6)	C20-C21	1.413(6)
C21-C22	1.361(7)	C21-H21	0.930000
C22-H22	0.930000	C23-C25	1.414(5)
C23-H23	0.930000	C24-C25	1.361(6)
C24-H24	0.930000	C25-H25	0.930000
C26-C27	1.379(5)	C26-H26	0.930000
C27-C28	1.389(8)	C28-C29	1.357(8)
C28-H28	0.930000	C29-H29	0.930000
C30-H30	0.960000	C30-H30	0.960000
C30-H30	0.960000		

Table S1e Bond angles (°) for **7gj**

C8-N1-C2	108.4(3)	C8-N1-C18	126.1(3)
C2-N1-C18	125.2(3)	C16-N2-C17	108.4(3)
C16-N2-C30	126.5(4)	C17-N2-C30	124.9(4)
C6-C1-C2	118.8(3)	C6-C1-C7	134.8(3)
C2-C1-C7	106.4(3)	N1-C2-C3	129.9(3)
N1-C2-C1	107.9(3)	C3-C2-C1	122.2(4)
C4-C3-C2	117.6(4)	C4-C3-H3	121.200000
C2-C3-H3	121.200000	C3-C4-C5	120.6(4)
C3-C4-H4	119.700000	C5-C4-H4	119.700000
C6-C5-C4	122.7(4)	C6-C5-Br1	119.3(3)
C4-C5-Br1	118.0(3)	C5-C6-C1	118.0(3)
C5-C6-H6	121.000000	C1-C6-H6	121.000000
C8-C7-C1	106.4(3)	C8-C7-C9	125.9(3)
C1-C7-C9	127.7(3)	C7-C8-N1	111.0(3)
C7-C8-H8	124.500000	N1-C8-H8	124.500000
C14-C9-C7	112.4(3)	C14-C9-C13	112.3(3)
C7-C9-C13	110.5(3)	C14-C9-C10	112.6(3)
C7-C9-C10	106.7(2)	C13-C9-C10	101.8(3)
O1-C10-C11	127.9(3)	O1-C10-C9	124.4(3)
C11-C10-C9	107.8(3)	C19-C11-C12	119.0(4)
C19-C11-C10	133.4(4)	C12-C11-C10	107.6(3)
C11-C12-C20	124.0(3)	C11-C12-C13	113.0(3)
C20-C12-C13	123.0(3)	C23-C13-C12	118.6(3)
C23-C13-C9	132.3(3)	C12-C13-C9	109.2(3)
C17-C14-C15	106.3(3)	C17-C14-C9	126.9(3)
C15-C14-C9	126.5(3)	C26-C15-C16	119.5(4)
C26-C15-C1	133.9(3)	C16-C15-C14	106.6(4)
N2-C16-C29	130.4(4)	N2-C16-C15	108.0(3)
C29-C16-C15	121.6(5)	C14-C17-N2	110.6(4)
C14-C17-H17	124.700000	N2-C17-H17	124.700000
N1-C18-H18	109.500000	N1-C18-H18	109.500000
H18-C18-H18	109.500000	N1-C18-H18	109.500000

H18-C18-H18	109.500000	H18-C18-H18	109.500000
C11-C19-C22	117.8(4)	C11-C19-H19	121.100000
C22-C19-H19	121.100000	C24-C20-C12	116.4(3)
C24-C20-C21	128.4(4)	C12-C20-C21	115.2(4)
C22-C21-C20	120.7(4)	C22-C21-H21	119.700000
C20-C21-H21	119.700000	C21-C22-C19	123.4(4)
C21-C22-H22	118.300000	C19-C22-H22	118.300000
C13-C23-C25	119.2(4)	C13-C23-H23	120.400000
C25-C23-H23	120.400000	C25-C24-C20	120.7(4)
C25-C24-H24	119.600000	C20-C24-H24	119.700000
C24-C25-C23	122.2(4)	C24-C25-H25	118.900000
C23-C25-H25	118.900000	C27-C26-C15	117.5(4)
C27-C26-H26	121.200000	C15-C26-H26	121.200000
C26-C27-C28	122.5(5)	C26-C27-Br2	118.8(4)
C28-C27-Br2	118.7(4)	C29-C28-C27	120.9(4)
C29-C28-H28	119.500000	C27-C28-H28	119.500000
C28-C29-C1	118.0(5)	C28-C29-H29	121.000000
C16-C29-H2	121.000000	N2-C30-H30A	109.500000
N2-C30-H30	109.500000	H30-C30-H30	109.500000
N2-C30-H30	109.500000	H30-C30-H30	109.500000
H30-C30-H30	109.500000		

Table S1f Torsion angles (°) for **7gj**

C8-N1-C2-C3	178.4(3)	C18-N1-C2-C3	5.2(6)
C8-N1-C2-C1	-1.1(4)	C18-N1-C2-C1	-174.3(3)
C6-C1-C2-N1	-178.3(3)	C7-C1-C2-N1	1.6(4)
C6-C1-C2-C3	2.2(5)	C7-C1-C2-C3	-177.9(3)
N1-C2-C3-C4	-179.8(3)	C1-C2-C3-C4	-0.4(5)
C2-C3-C4-C5	-1.5(6)	C3-C4-C5-C6	1.7(6)
C3-C4-C5-Br1	-177.2(3)	C4-C5-C6-C1	0.1(5)
Br1-C5-C6-C1	179.0(2)	C2-C1-C6-C5	-2.0(5)
C7-C1-C6-C5	178.1(3)	C6-C1-C7-C8	178.4(4)
C2-C1-C7-C8	-1.5(3)	C6-C1-C7-C9	0.0(6)
C2-C1-C7-C9	-179.9(3)	C1-C7-C8-N1	0.9(4)
C9-C7-C8-N1	179.3(3)	C2-N1-C8-C7	0.1(4)
C18-N1-C8-C7	173.2(3)	C8-C7-C9-C14	126.1(3)
C1-C7-C9-C14	-55.8(4)	C8-C7-C9-C13	-0.2(4)
C1-C7-C9-C13	177.9(3)	C8-C7-C9-C10	-110.0(4)
C1-C7-C9-C10	68.1(4)	C14-C9-C10-O1	51.7(4)
C7-C9-C10-O1	-72.0(4)	C13-C9-C10-O1	172.2(3)
C14-C9-C10-C11	-128.4(3)	C7-C9-C10-C11	107.8(3)
C13-C9-C10-C11	-8.0(3)	O1-C10-C11-C19	4.9(6)
C9-C10-C11-C19	-174.9(4)	O1-C10-C11-C12	-173.9(3)
C9-C10-C11-C12	6.2(3)	C19-C11-C12-C20	-1.4(5)
C10-C11-C12-C20	177.7(3)	C19-C11-C12-C13	179.2(3)
C10-C11-C12-C13	-1.7(4)	C11-C12-C13-C23	177.7(3)
C20-C12-C13-C23	-1.7(5)	C11-C12-C13-C9	-3.7(4)
C20-C12-C13-C9	176.9(3)	C14-C9-C13-C23	-54.1(5)
C7-C9-C13-C23	72.3(4)	C10-C9-C13-C23	-174.7(4)
C14-C9-C13-C12	127.7(3)	C7-C9-C13-C12	-106.0(3)
C10-C9-C13-C12	7.0(3)	C7-C9-C14-C17	-17.5(5)
C13-C9-C14-C17	107.8(4)	C10-C9-C14-C17	-138.0(4)
C7-C9-C14-C15	170.2(3)	C13-C9-C14-C15	-64.5(4)
C10-C9-C14-C15	49.7(4)	C17-C14-C15-C26	-179.9(4)
C9-C14-C15-C26	-6.3(6)	C17-C14-C15-C16	0.4(4)

C9-C14-C15-C16	174.0(3)	C17-N2-C16-C29	179.0(4)
C30-N2-C16-C29	2.5(7)	C17-N2-C16-C15	-0.5(4)
C30-N2-C16-C15	-177.0(4)	C26-C15-C16-N2	-179.7(3)
C14-C15-C16-N2	0.0(4)	C26-C15-C16-C29	0.8(5)
C14-C15-C16-C29	-179.5(3)	C15-C14-C17-N2	-0.8(4)
C9-C14-C17-N2	-174.3(3)	C16-N2-C17-C14	0.8(4)
C30-N2-C17-C14	177.4(4)	C12-C11-C19-C22	0.7(5)
C10-C11-C19-C22	-178.0(4)	C11-C12-C20-C24	-178.0(3)
C13-C12-C20-C24	1.3(5)	C11-C12-C20-C21	0.8(5)
C13-C12-C20-C21	-179.9(3)	C24-C20-C21-C22	179.0(4)
C12-C20-C21-C22	0.3(6)	C20-C21-C22-C19	-0.9(7)
C11-C19-C22-C21	0.3(7)	C12-C13-C23-C25	0.8(5)
C9-C13-C23-C25	-177.3(3)	C12-C20-C24-C25	-0.1(6)
C21-C20-C24-C25	-178.8(4)	C20-C24-C25-C23	-0.7(7)
C13-C23-C25-C24	0.3(6)	C16-C1-C26-C27	-0.6(5)
C14-C15-C26-C27	179.8(4)	C15-C26-C27-C28	-0.2(6)
C15-C26-C27-Br2	179.1(3)	C26-C27-C28-C29	1.0(7)
Br2-C27-C28-C29	-178.4(4)	C27-C28-C29-C16	-0.8(7)
N2-C16-C29-C28	-179.5(4)	C15-C16-C29-C28	-0.1(6)

Table S1g Anisotropic atomic displacement parameters (Å^2) for **7gj**

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Br1	0.0895(4)	0.0714(3)	0.0699(3)	0.0049(2)	0.0237(3)	-0.0010(2)
Br2	0.2022(8)	0.0786(4)	0.1319(6)	0.0224(4)	0.1031(6)	-0.0398(4)
O1	0.0586(16)	0.0683(17)	0.0631(18)	0.0296(14)	0.0094(14)	0.0148(13)
N1	0.0447(16)	0.0634(18)	0.0564(18)	0.0345(15)	0.0212(14)	0.0145(14)
N2	0.0491(18)	0.094(3)	0.058(2)	0.0164(19)	0.0206(16)	0.0378(18)
C1	0.0407(17)	0.0462(17)	0.055(2)	0.0261(16)	0.0221(15)	0.0160(14)
C2	0.0381(17)	0.054(2)	0.064(2)	0.0315(18)	0.0214(16)	0.0164(15)
C3	0.050(2)	0.057(2)	0.082(3)	0.040(2)	0.024(2)	0.0115(17)
C4	0.055(2)	0.046(2)	0.087(3)	0.024(2)	0.021(2)	0.0050(17)
C5	0.054(2)	0.049(2)	0.064(2)	0.0162(18)	0.0218(18)	0.0123(17)
C6	0.0478(19)	0.0456(18)	0.060(2)	0.0208(16)	0.0252(17)	0.0135(15)
C7	0.0375(16)	0.0466(17)	0.0520(19)	0.0227(15)	0.0208(15)	0.0163(14)
C8	0.0398(18)	0.055(2)	0.054(2)	0.0241(16)	0.0191(15)	0.0147(15)
C9	0.0375(16)	0.0454(17)	0.0490(18)	0.0212(15)	0.0214(14)	0.0130(13)
C10	0.0413(18)	0.0531(19)	0.057(2)	0.0279(17)	0.0240(17)	0.0107(15)
C11	0.050(2)	0.058(2)	0.065(2)	0.0344(18)	0.0333(18)	0.0202(17)
C12	0.0465(19)	0.0475(18)	0.056(2)	0.0238(16)	0.0284(17)	0.0148(15)
C13	0.0456(19)	0.0459(18)	0.0518(19)	0.0207(15)	0.0259(16)	0.0132(15)
C14	0.0365(17)	0.056(2)	0.0481(19)	0.0164(16)	0.0176(15)	0.0128(15)
C15	0.0326(16)	0.069(2)	0.0411(18)	0.0110(16)	0.0131(14)	0.0004(15)
C16	0.0340(18)	0.095(3)	0.0422(19)	0.008(2)	0.0140(15)	0.0094(19)
C17	0.045(2)	0.071(2)	0.057(2)	0.0213(19)	0.0180(17)	0.0244(18)
C18	0.064(3)	0.095(3)	0.068(3)	0.052(2)	0.030(2)	0.018(2)
C19	0.065(2)	0.071(3)	0.078(3)	0.046(2)	0.038(2)	0.034(2)
C20	0.069(3)	0.052(2)	0.069(3)	0.0199(19)	0.036(2)	0.0181(19)
C21	0.097(4)	0.054(2)	0.088(3)	0.022(2)	0.046(3)	0.031(2)
C22	0.096(4)	0.069(3)	0.102(4)	0.042(3)	0.052(3)	0.048(3)
C23	0.046(2)	0.059(2)	0.062(2)	0.0195(18)	0.0203(18)	0.0149(17)
C24	0.079(3)	0.055(2)	0.065(3)	0.0059(19)	0.026(2)	0.007(2)

C25	0.060(2)	0.065(3)	0.061(2)	0.013(2)	0.014(2)	0.005(2)
C26	0.063(2)	0.060(2)	0.054(2)	0.0081(18)	0.0288(19)	-0.0107(18)
C27	0.080(3)	0.083(3)	0.063(3)	0.003(2)	0.038(2)	-0.029(2)
C28	0.066(3)	0.131(5)	0.063(3)	0.000(3)	0.037(2)	-0.038(3)
C29	0.044(2)	0.127(5)	0.055(3)	0.000(3)	0.0245(19)	0.000(3)
C30	0.074(3)	0.131(5)	0.086(3)	0.009(3)	0.027(3)	0.064(3)

Table S1h Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for **7gj**

	x/a	y/b	z/c	U(eq)
H3	-0.0606	0.1708	0.3441	0.070000
H4	-0.1307	0.0780	0.1425	0.076000
H6	0.1057	0.3646	0.1072	0.058000
H8	0.2739	0.5624	0.5350	0.056000
H17	0.4409	0.3897	0.2776	0.067000
H18	0.1182	0.4343	0.6246	0.102000
H18	0.1957	0.3260	0.5867	0.102000
H18	0.0113	0.3105	0.5392	0.102000
H19	0.0068	0.8318	0.2665	0.074000
H21	0.2898	1.0559	0.5829	0.090000
H22	0.0767	1.0113	0.4214	0.094000
H23	0.5860	0.6569	0.5315	0.066000
H24	0.5331	0.9832	0.6938	0.084000
H25	0.6686	0.8362	0.6887	0.079000
H26	0.4317	0.7700	0.2131	0.074000
H28	0.7594	0.7151	0.0484	0.116000
H29	0.7637	0.5346	0.0735	0.099000
H30	0.6163	0.2805	0.1776	0.148000
H30	0.7746	0.3757	0.2167	0.148000
H30	0.6677	0.3263	0.0849	0.148000

Table S1i Hydrogen bond distances (Å) and angles (°) for **7gj**

	Donor-H	Acceptor-H	Donor-Acceptor	Angle
C4-H4...Br2	0.93	2.86	3.705(4)	151.6

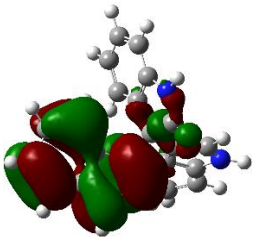
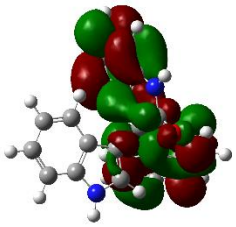
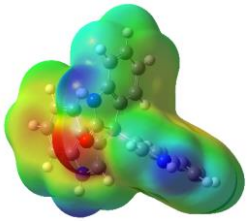
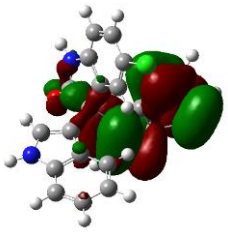
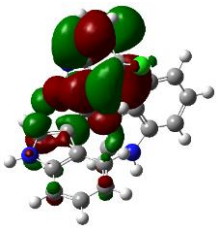
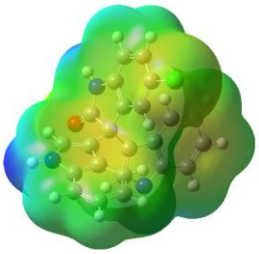
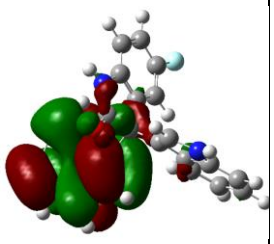
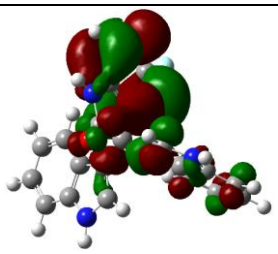
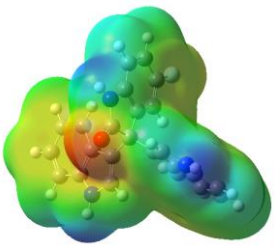
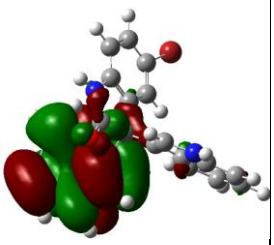
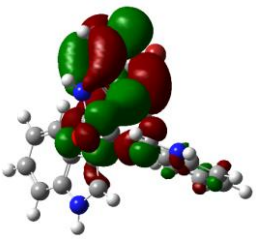
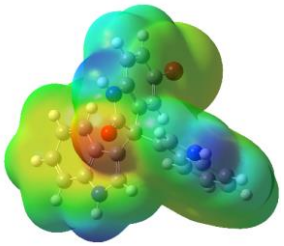
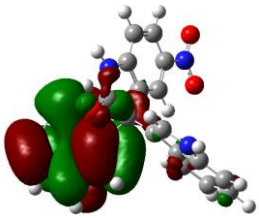
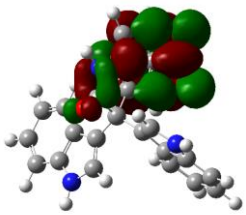
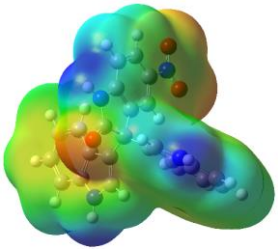
Symmetry transformations used to generate equivalent atoms: x-1, y-1, z

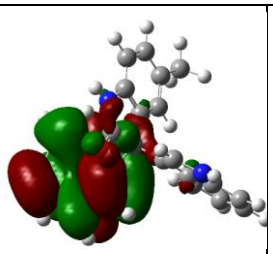
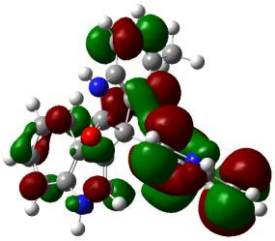
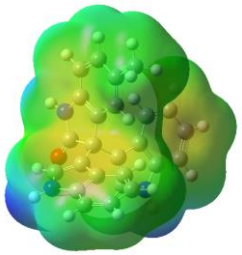
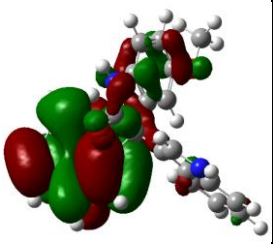
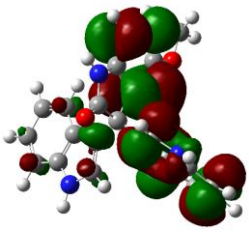
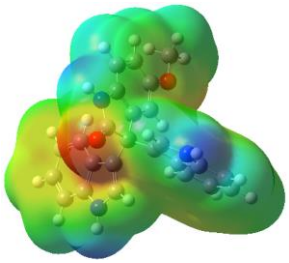
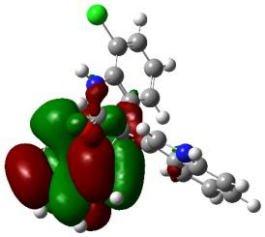
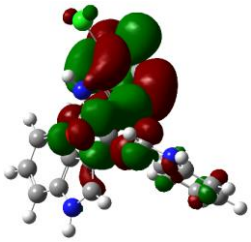
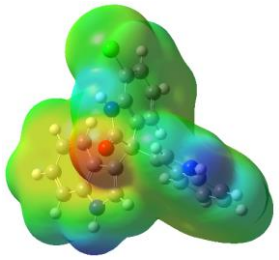
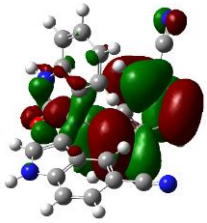
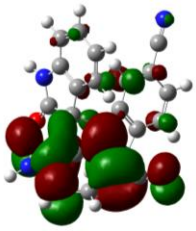
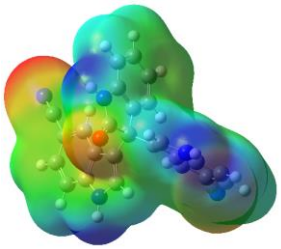
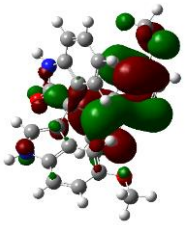
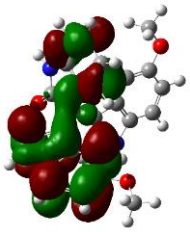
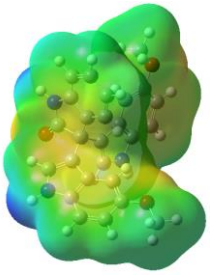
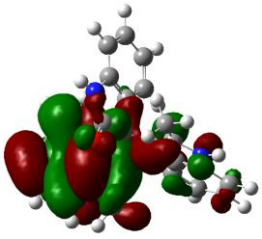
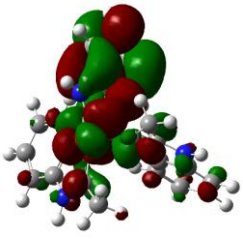
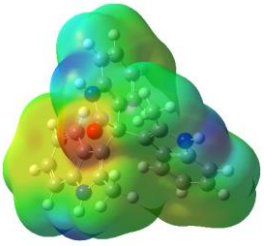
Table S2 Interactions of Hirshfeld Surface in percentages for **7gj**

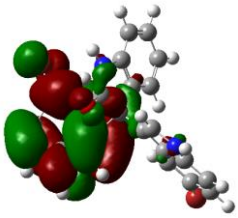
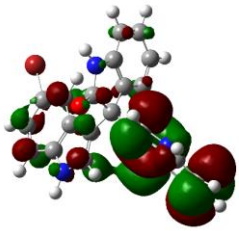
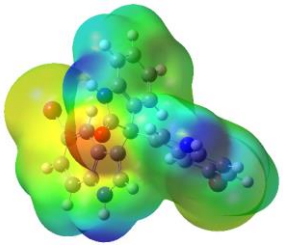
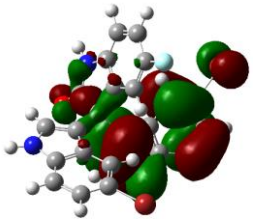
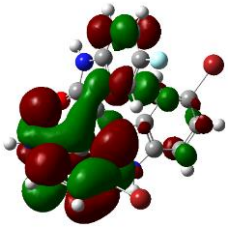
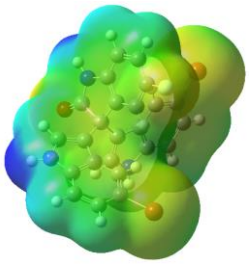
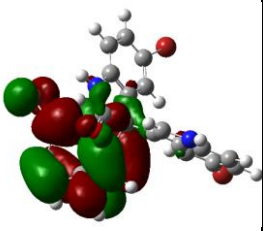
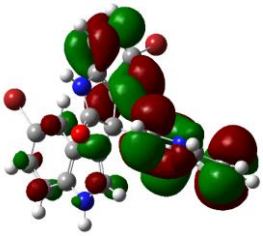
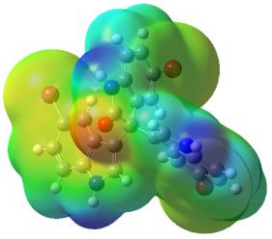
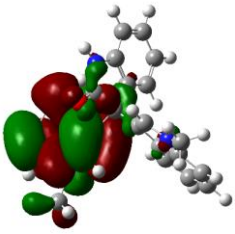
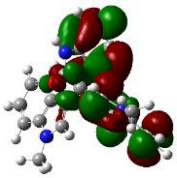
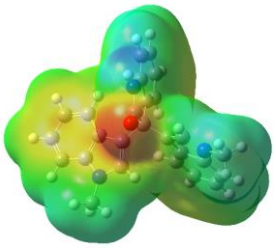
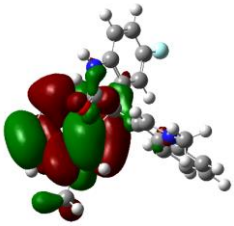
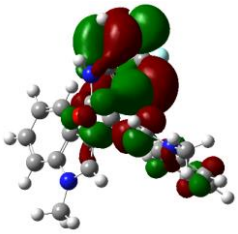
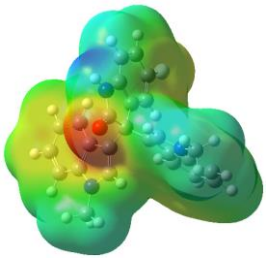
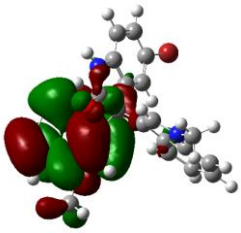
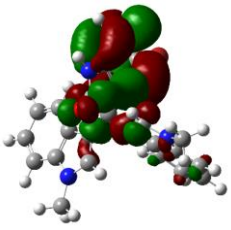
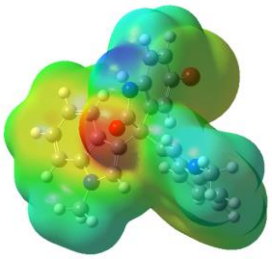
S. No	Inside atom	Outside atom	Percentage	S. No	Inside atom	Outside atom	Percentage
1	All	All	100	37	All	All	100
2	All	Br	10.3	38	Br	All	16.0
3	All	O	2.9	39	O	All	3.3
4	All	N	1.3	40	N	All	1.4
5	All	C	16.3	41	C	All	19.3
6	All	H	69.1	42	H	All	59.9
7	Br	All	16.0	43	All	Br	10.3
8	Br	Br	1.6	44	Br	Br	1.6
9	Br	O	0.4	45	O	Br	0.3
10	Br	N	0.0	46	N	Br	0.0
11	Br	C	0.4	47	C	Br	0.3
12	Br	H	13.7	48	H	Br	8.1
13	O	All	3.3	49	All	O	2.9
14	O	Br	0.3	50	Br	O	0.4
15	O	O	0.2	51	O	O	0.2
16	O	N	0.0	52	N	O	0.0
17	O	C	0.0	53	C	O	0.0
18	O	H	0.0	54	H	O	2.4
19	N	All	1.4	55	All	N	1.3
20	N	Br	0.0	56	Br	N	0.0
21	N	O	0.0	57	O	N	0.0
22	N	N	0.1	58	N	N	0.1
23	N	C	0.3	59	C	N	0.3
24	N	H	1.0	60	H	N	1.0
25	C	All	19.3	61	All	C	16.3
26	C	Br	0.3	62	Br	C	0.4
27	C	O	0.0	63	O	C	0.0
28	C	N	0.3	64	N	C	0.3
29	C	C	2.3	65	C	C	2.3

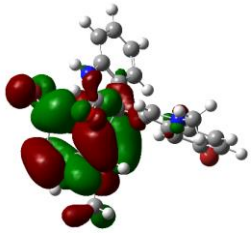
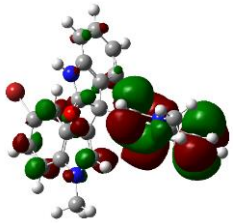
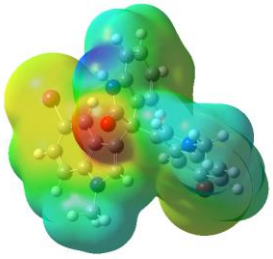
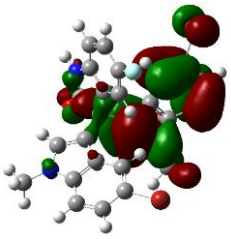
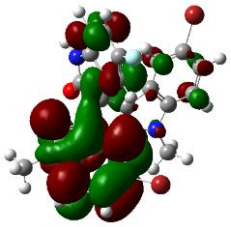
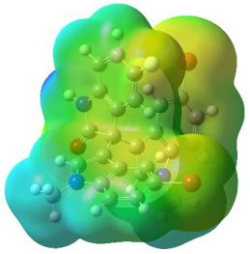
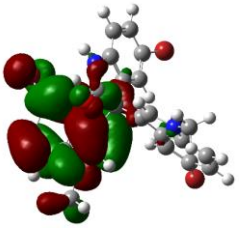
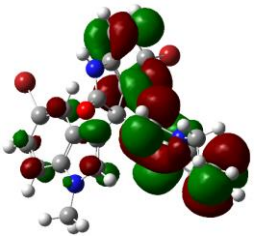
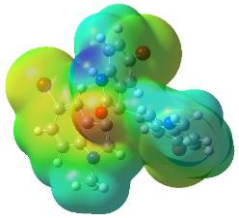
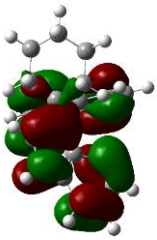
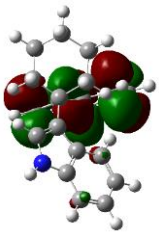
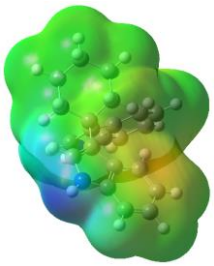
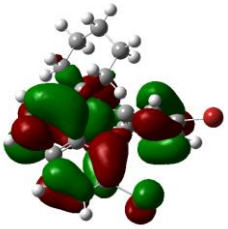
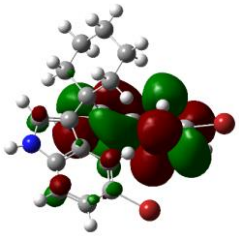
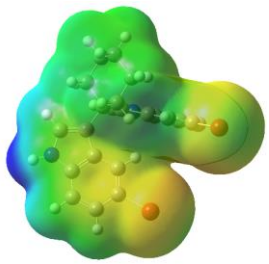
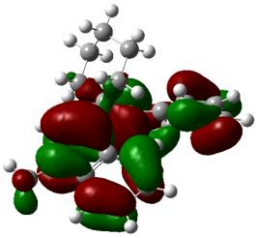
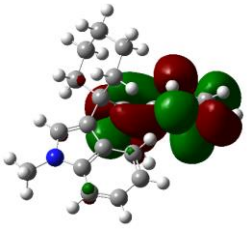
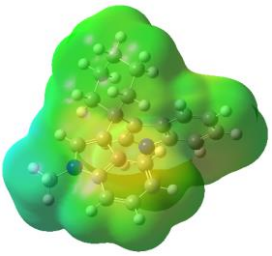
30	C	H	16.4	66	H	C	13.4
31	H	All	59.9	67	All	H	69.1
32	H	Br	8.1	68	Br	H	13.7
33	H	O	2.4	69	O	H	2.8
34	H	N	1.0	70	N	H	1.0
35	H	C	13.4	71	C	H	16.4
36	H	H	35.1	72	H	H	35.1

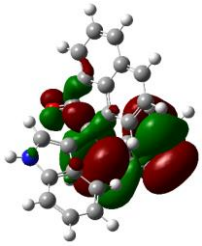
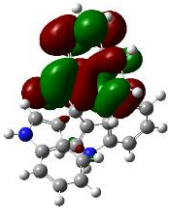
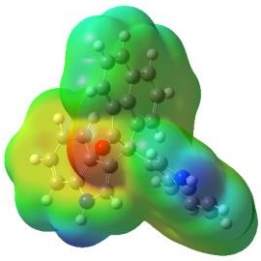
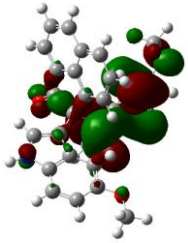
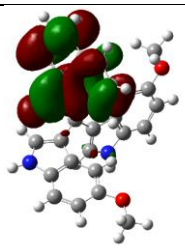
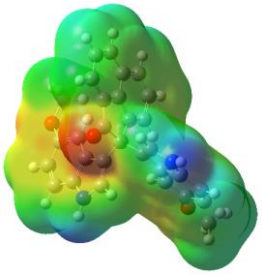
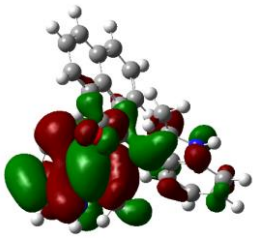
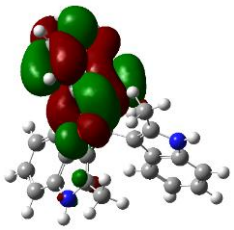
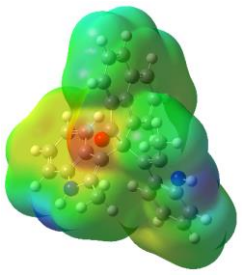
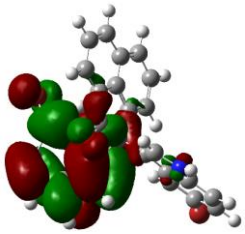
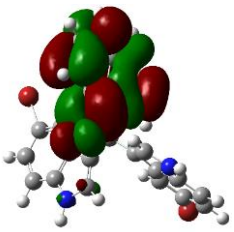
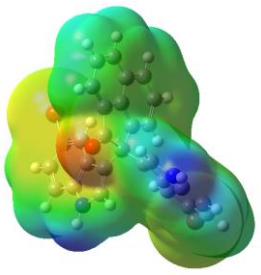
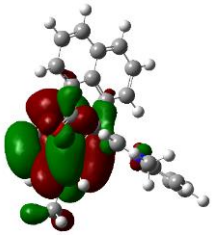
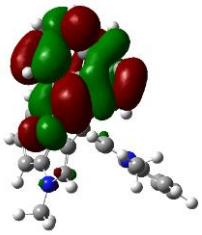
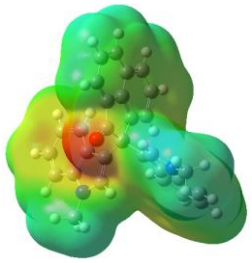
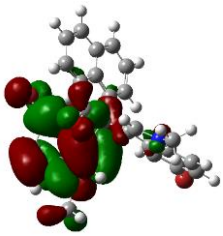
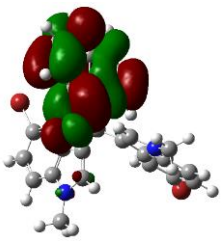
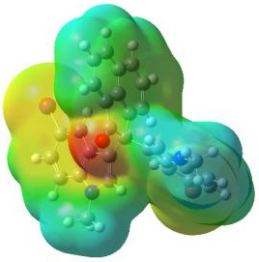
Table S3 The charge densities in HOMO, LUMO and electrostatic potential energy surface of the synthesized derivatives **7** and **10**

	HOMO	**LUMO**	**Band gap (eV)**	**ESP**
7aa	 -5.2425	 -0.2519	4.9906	
7ab	 -5.3514	 -0.5418	4.8096	
7ac	 -5.3163	 0.4612	4.8551	
7ad	 -5.3495	 -0.5434	4.8061	
7ae	 -5.5098	 -2.1263	3.3835	

7af	 -5.2265	 -0.2288	4.9977	
7ag	 -5.1919	 -0.2174	4.9745	
7ah	 -5.3522	 -0.5151	4.8371	
7ba	 -5.9756	 -1.7951	3.4116	
7ca	 -5.0559	 -0.2520	4.8039	
7da	 -5.0186	 -0.3059	4.6600	

7ea	 -5.5786	 -0.6493	4.9293	
7ec	 -5.6491	 -0.7219	4.9272	
7ed	 -5.6774	 -0.7472	4.9302	
7fa	 -5.1106	 -0.2106	4.8999	
7fb	 -5.1827	 -0.4188	4.7639	
7fd	 -5.2159	 -0.5009	4.7149	

7ga	 -5.4300	 -0.6038	4.8262	
7gc	 -5.4981	 -0.6732	4.8249	
7gd	 -5.5266	 -0.6991	4.8276	
7ai	 -5.0238	 -0.1211	4.9027	
7ei	 -5.3642	 -0.5099	4.8543	
7fi	 -4.8923	 -0.0879	4.8044	

7aj	 -5.1919	 -1.8074	3.3845	
7cj	 -5.9756	 -1.1946	4.7810	
7dj	 -4.9876	 -1.8188	3.1688	
7ej	 -5.5149	 -1.9666	3.5483	
7fj	 -5.0638	 -1.7717	3.2921	
7gj	 -5.3707	 -1.9263	5.1781	

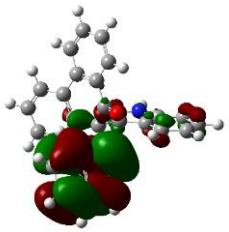
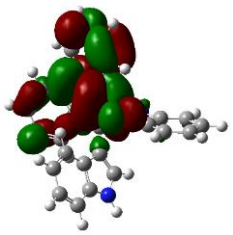
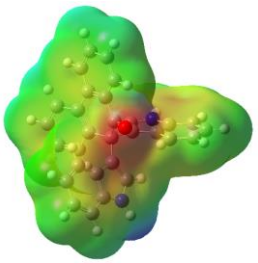
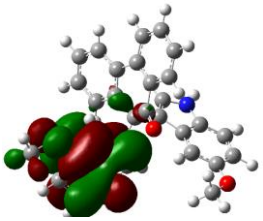
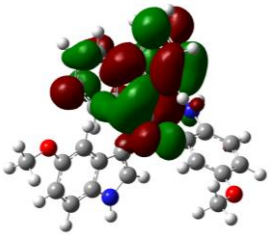
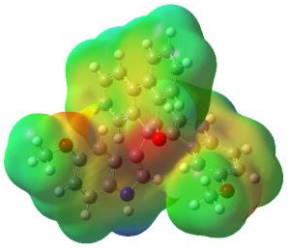
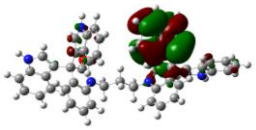
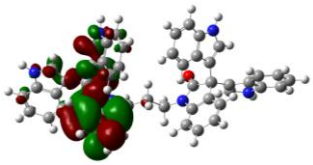
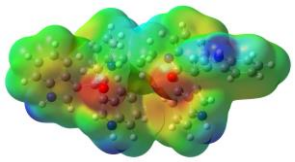
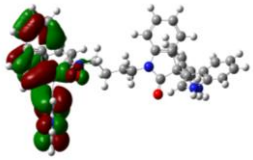
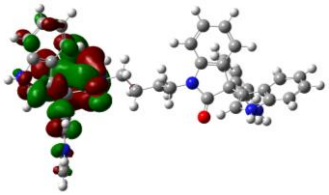
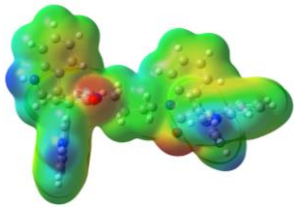
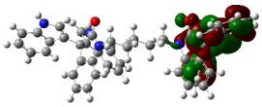
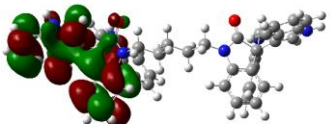
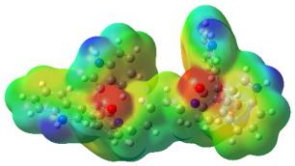
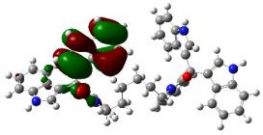
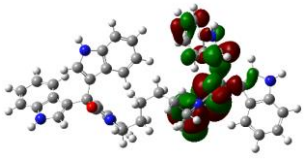
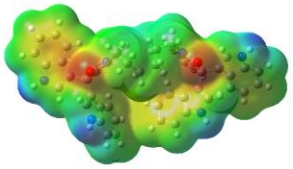
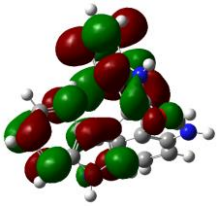
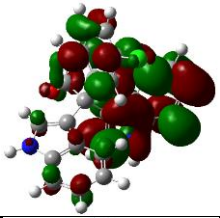
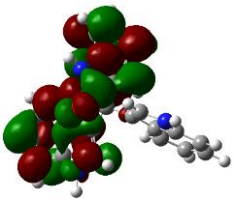
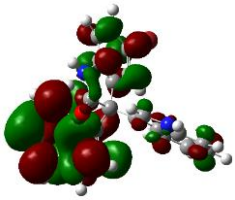
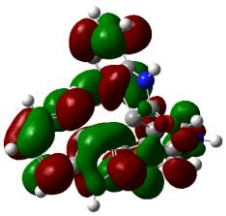
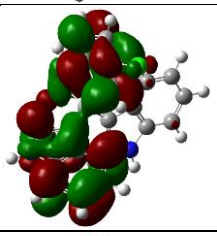
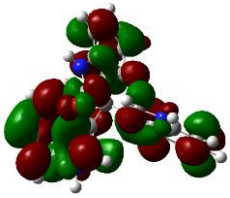
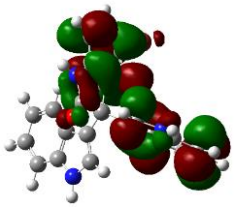
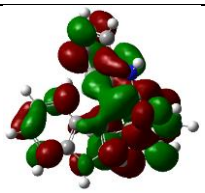
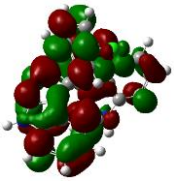
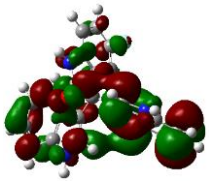
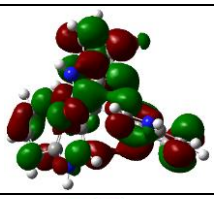
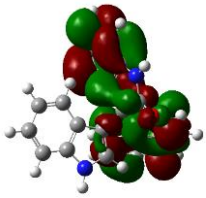
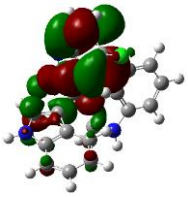
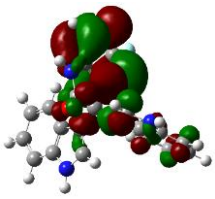
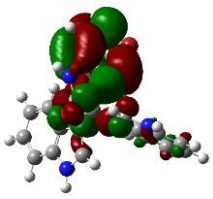
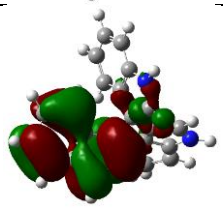
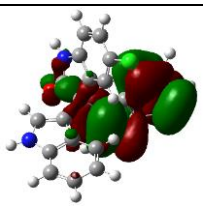
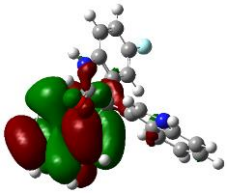
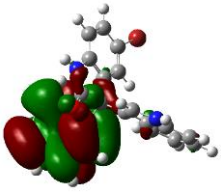
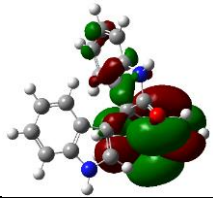
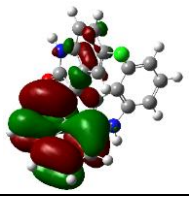
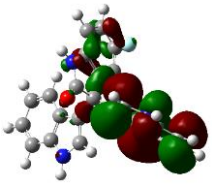
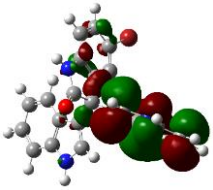
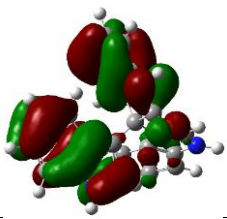
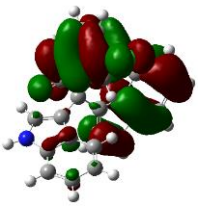
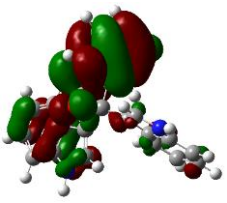
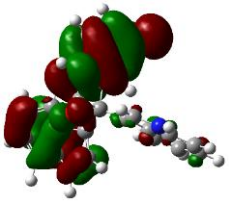
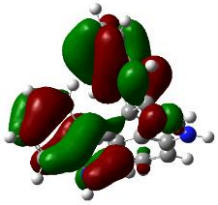
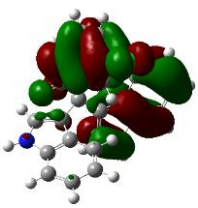
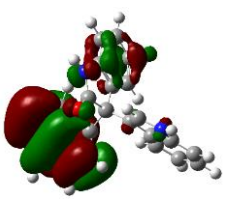
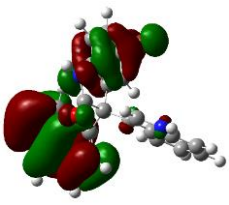
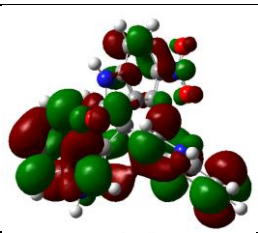
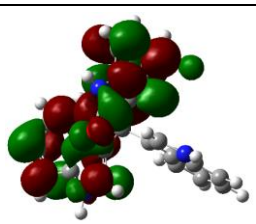
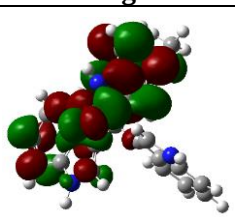
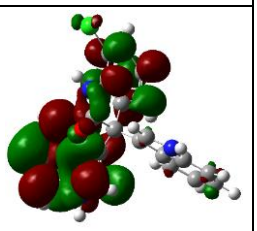
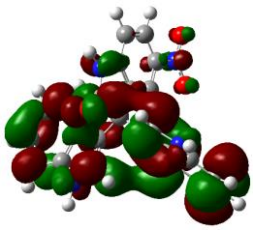
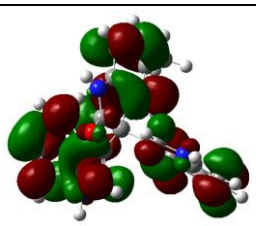
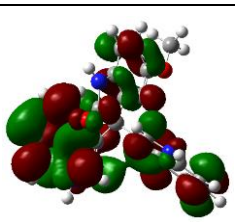
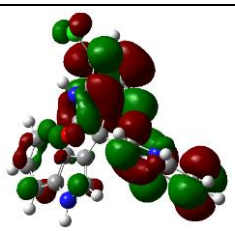
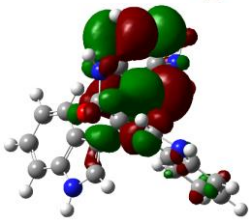
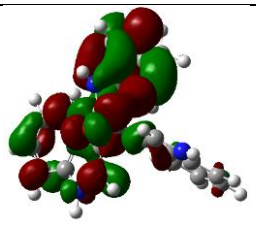
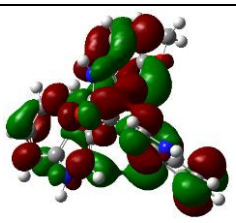
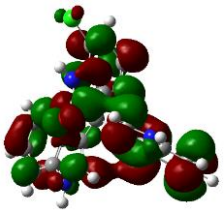
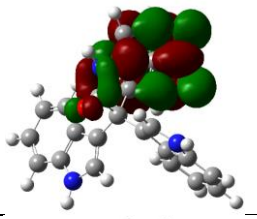
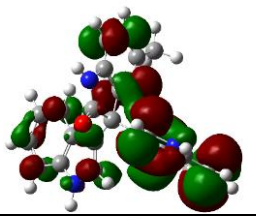
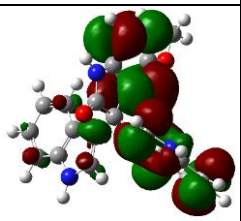
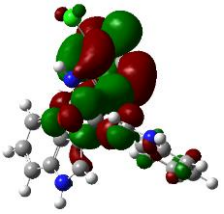
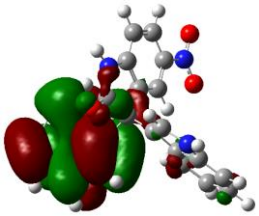
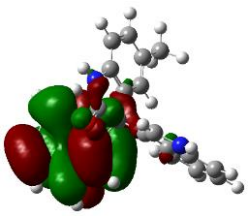
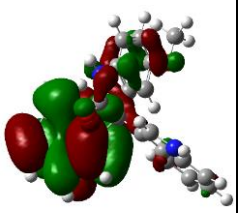
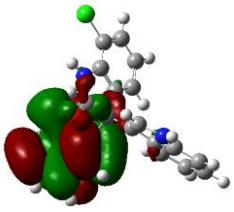
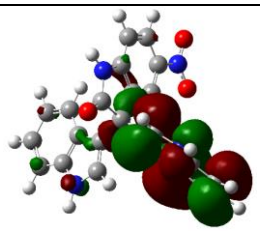
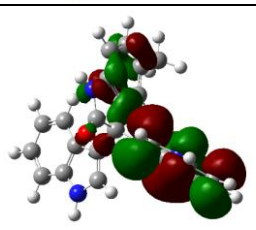
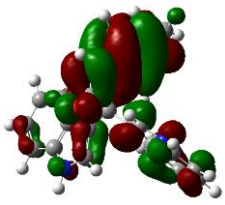
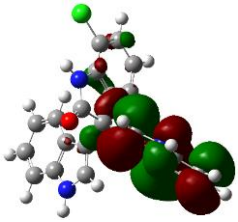
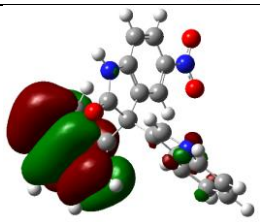
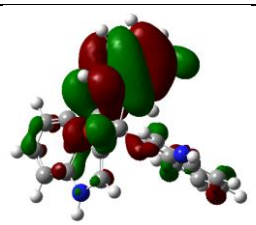
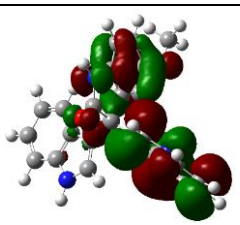
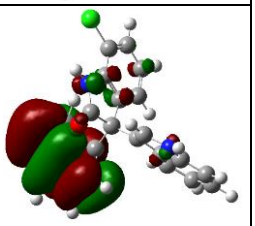
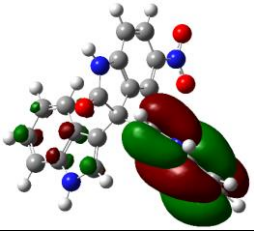
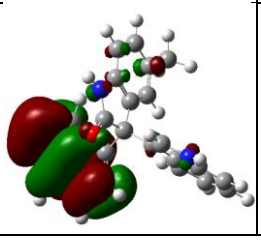
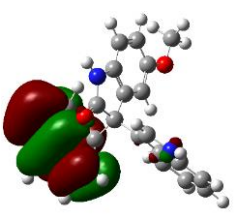
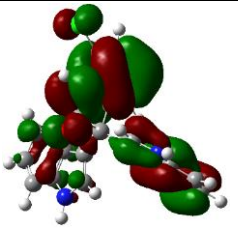
7gk	 -5.2382	 -1.5364	3.7018	
7ck	 -4.9843	 -1.4879	3.4964	
10aa	 -5.1522	 -0.2757	4.8765	
10ab	 -5.2053	 -0.2800	4.9253	
10ac	 -5.1296	 -0.2310	4.8986	
10ad	 -5.1596	 -0.2906	4.8690	

Table S4 Frontier molecular orbitals of HOMO and LUMO of all the synthesized derivatives **7** and **10** obtained at B3LYP/6-31G (d,p) level of theory in gas phase

Orbitals	7aa	7ab	7ac	7ad
LUMO+3				
LUMO+2				
LUMO+1				
LUMO				
HOMO				
HOMO-1				
HOMO-2				
HOMO-3				

Orbitals	7ae	7af	7ag	7ah
LUMO+3				
LUMO+2				
LUMO+1				
LUMO				
HOMO				
HOMO-1				
HOMO-2				
HOMO-3				

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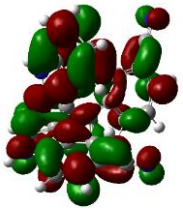
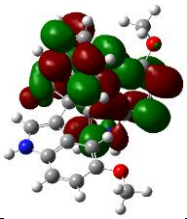
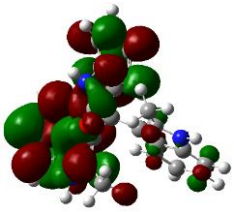
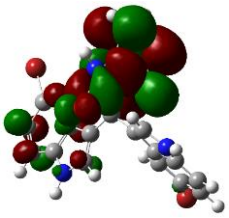
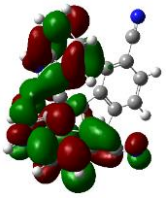
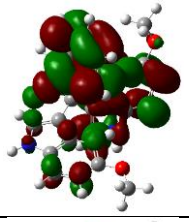
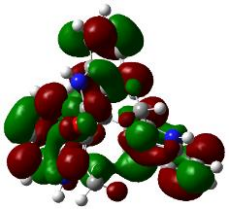
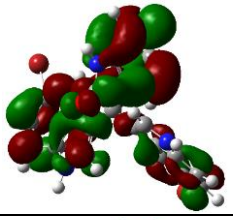
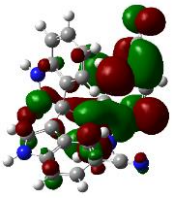
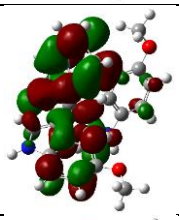
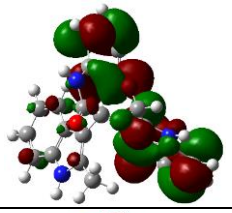
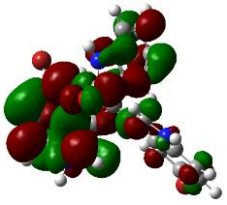
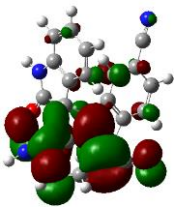
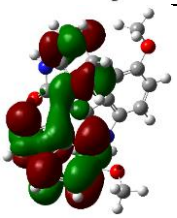
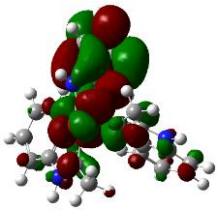
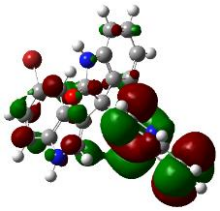
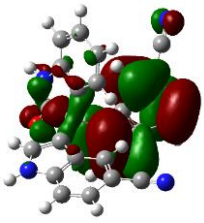
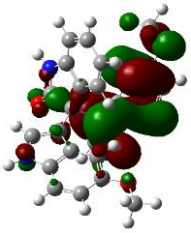
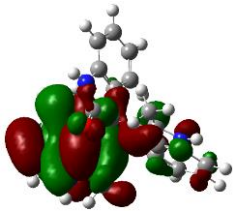
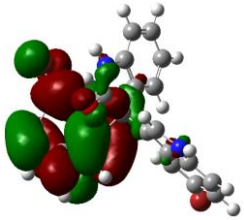
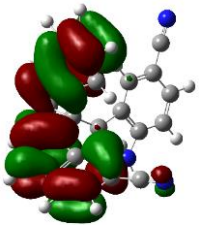
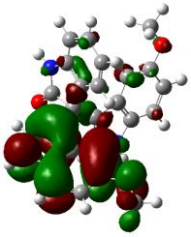
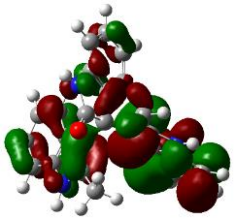
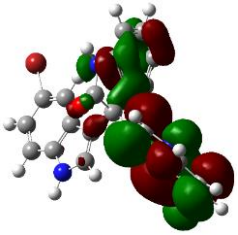
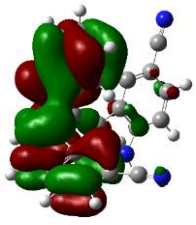
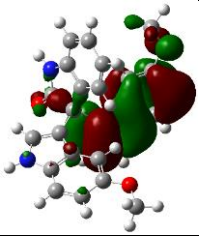
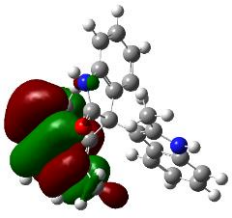
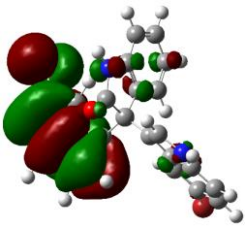
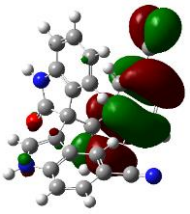
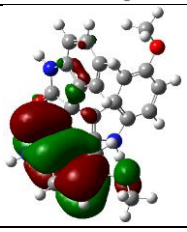
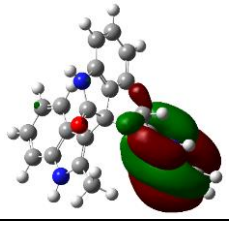
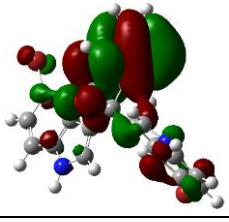
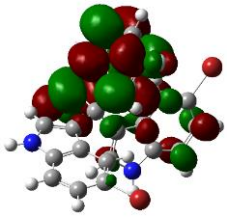
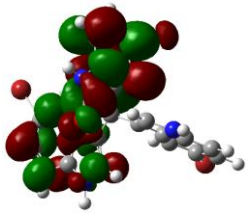
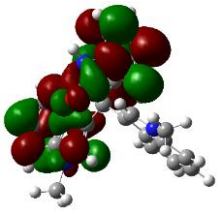
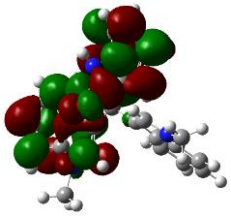
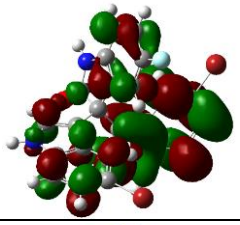
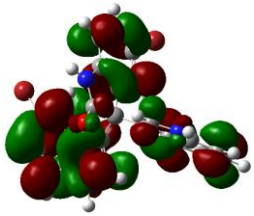
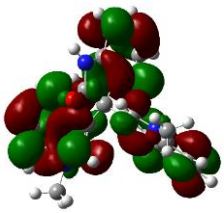
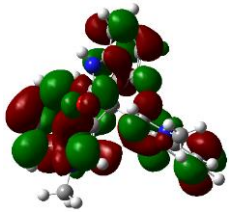
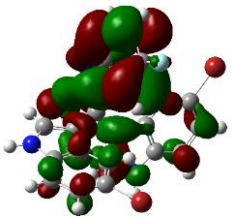
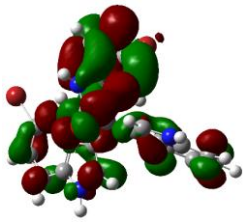
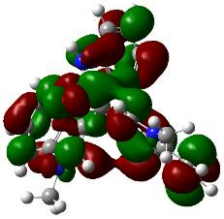
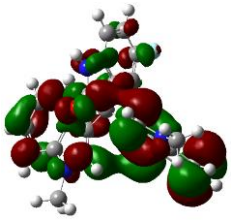
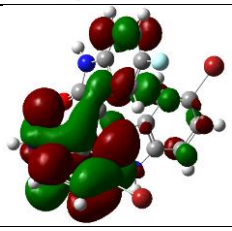
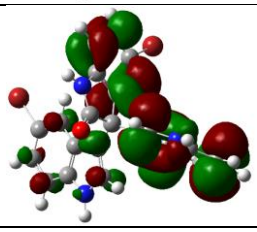
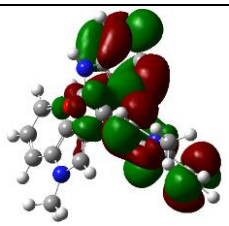
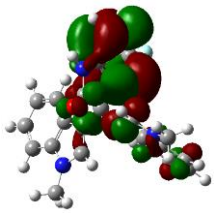
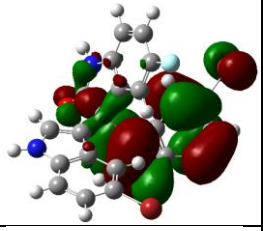
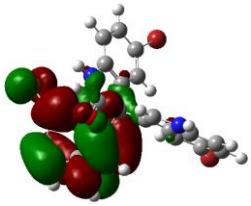
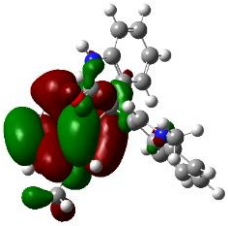
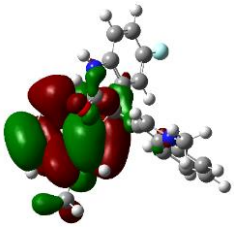
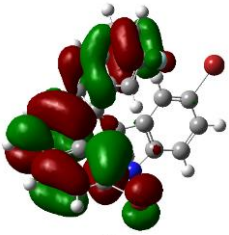
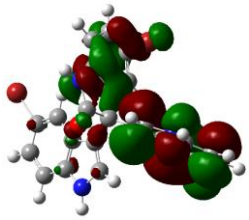
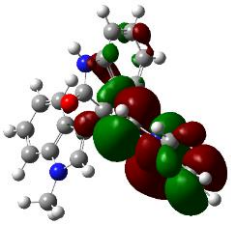
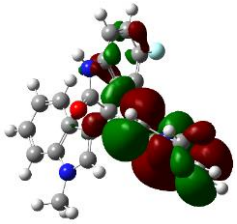
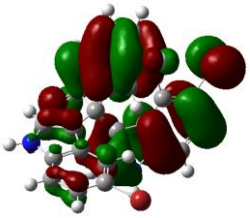
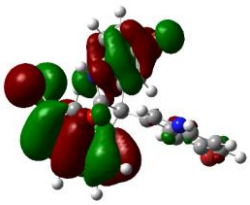
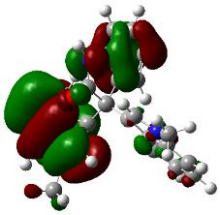
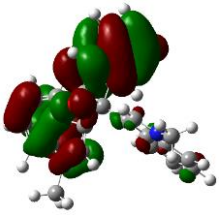
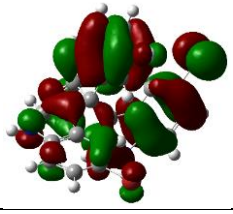
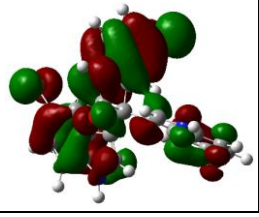
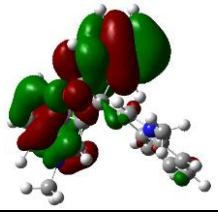
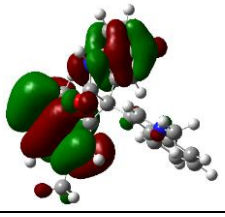
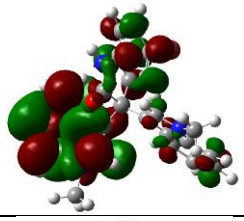
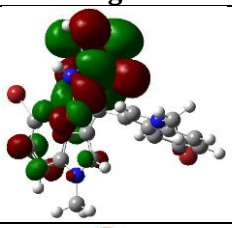
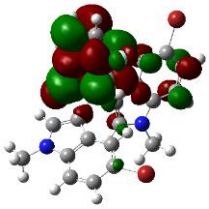
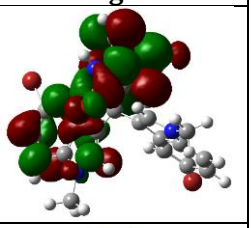
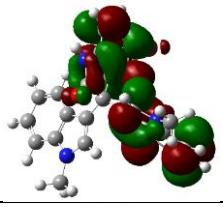
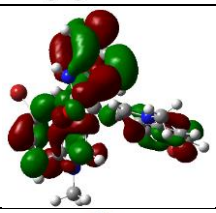
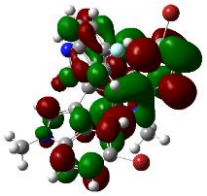
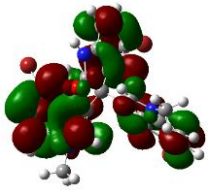
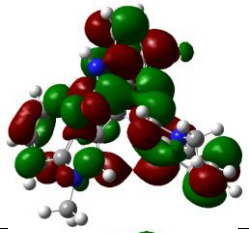
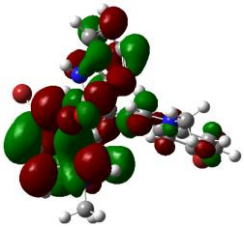
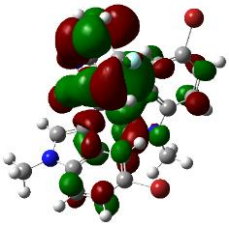
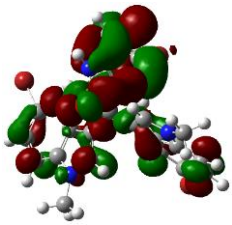
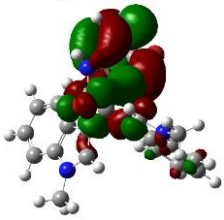
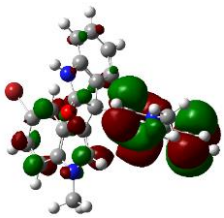
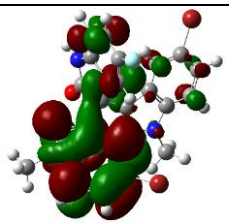
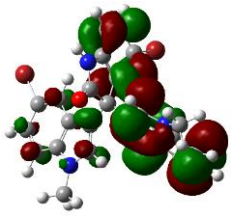
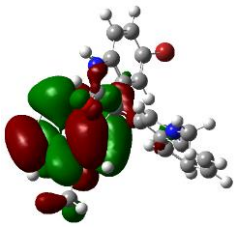
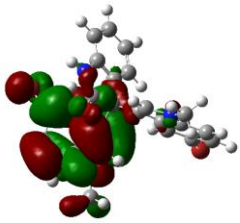
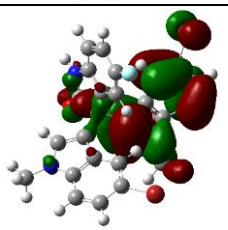
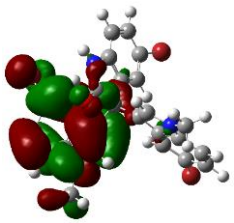
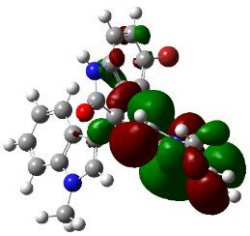
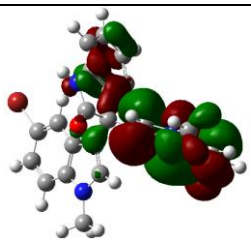
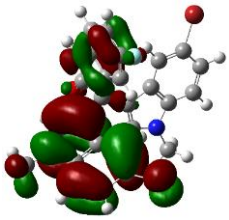
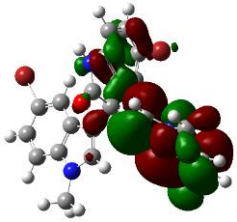
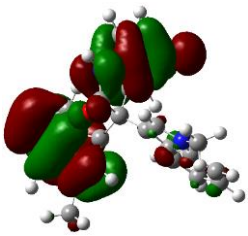
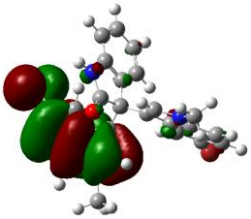
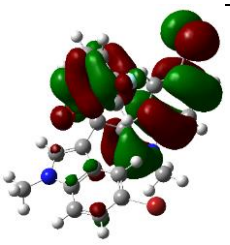
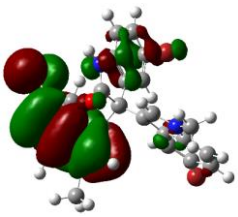
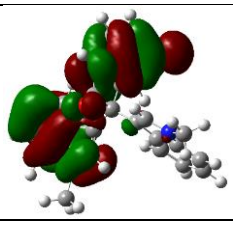
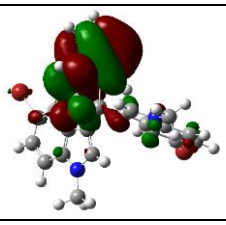
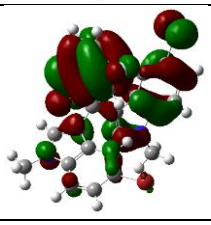
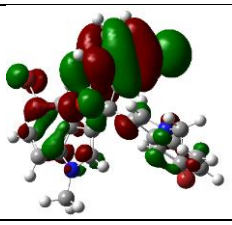
LUMO+3				
LUMO+2				
LUMO+1				
LUMO				
HOMO				
HOMO-1				
HOMO-2				
HOMO-3				

Orbitals	7ec	7ed	7fa	7fb
LUMO+3				
LUMO+2				
LUMO+1				
LUMO				
HOMO				
HOMO-1				
HOMO-2				
HOMO-3				

Orbitals	7fd	7ga	7gc	7gd
LUMO+3				
LUMO+2				
LUMO+1				
LUMO				
HOMO				
HOMO-1				
HOMO-2				
HOMO-3				

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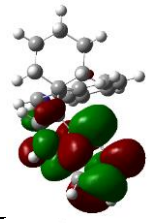
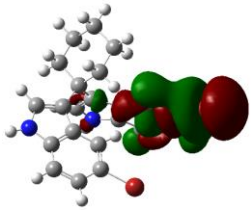
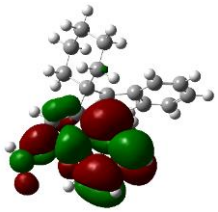
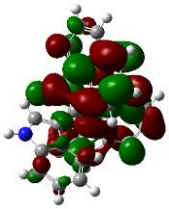
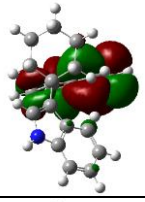
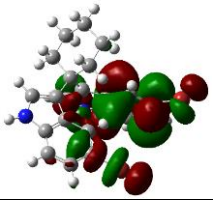
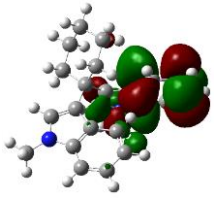
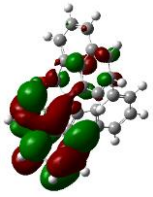
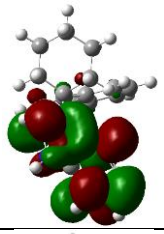
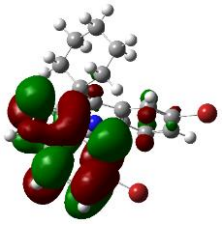
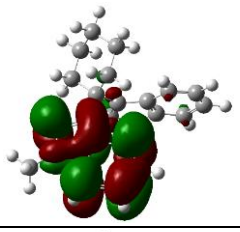
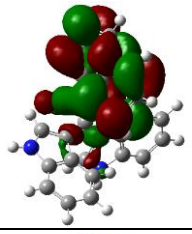
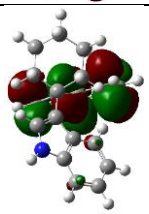
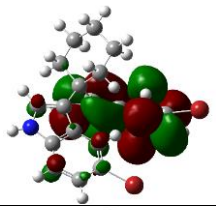
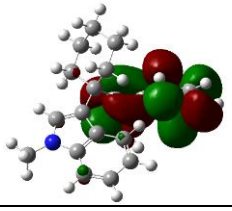
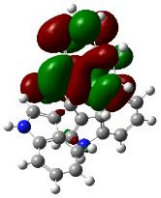
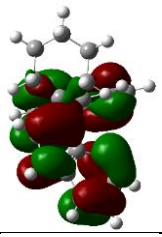
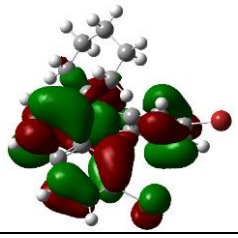
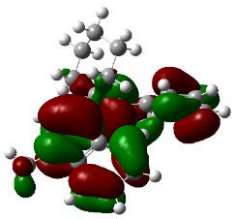
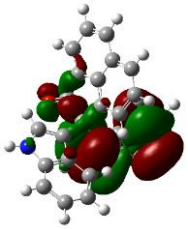
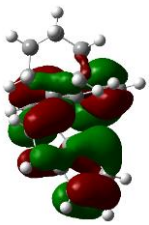
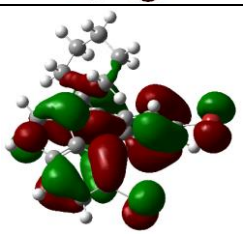
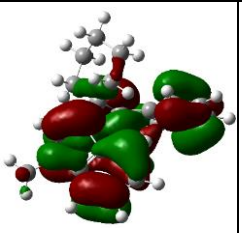
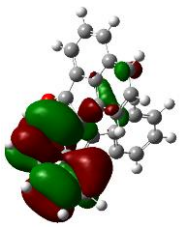
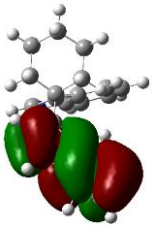
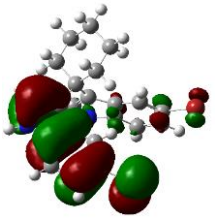
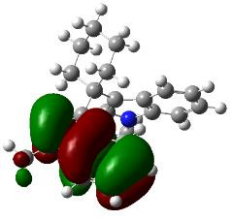
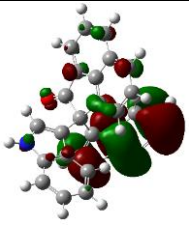
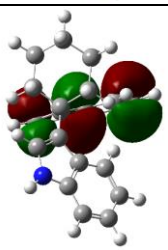
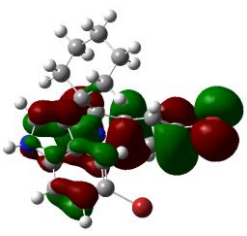
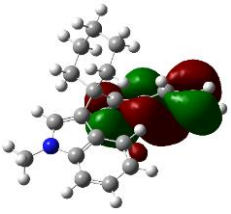
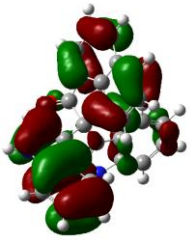
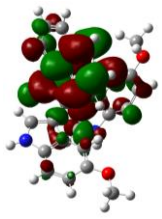
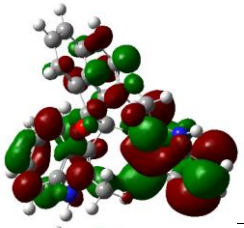
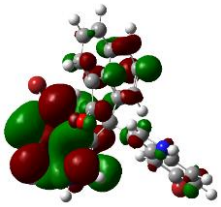
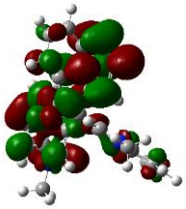
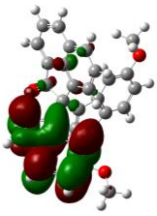
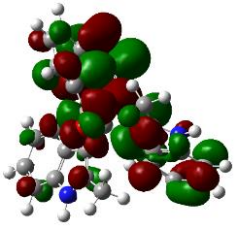
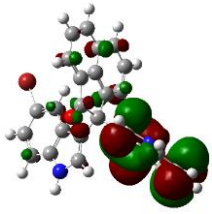
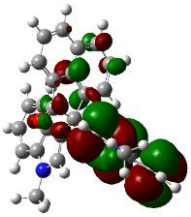
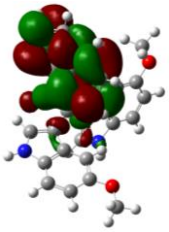
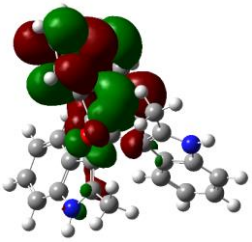
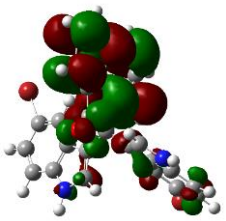
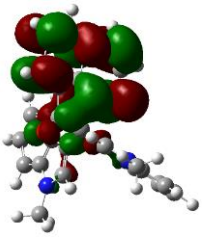
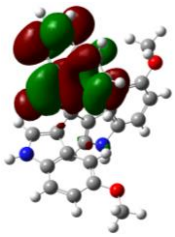
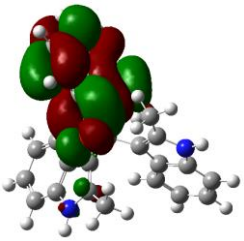
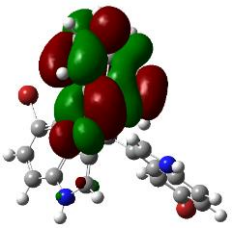
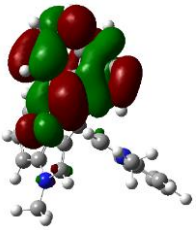
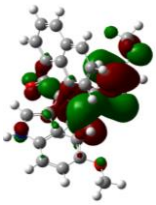
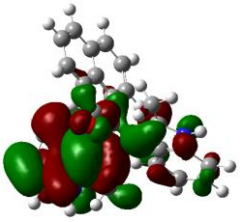
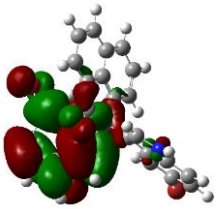
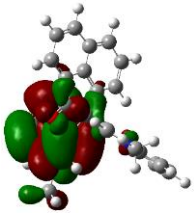
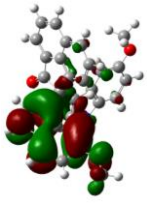
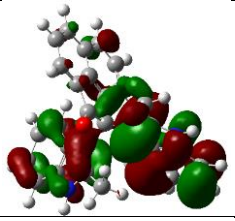
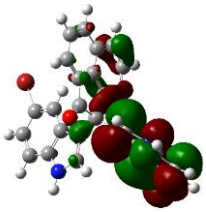
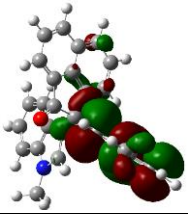
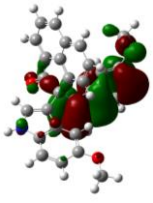
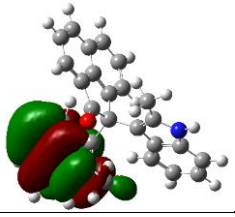
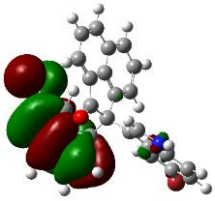
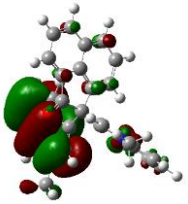
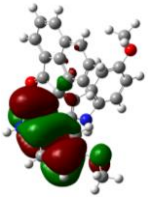
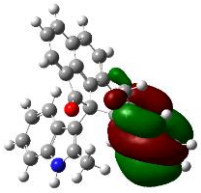
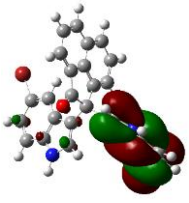
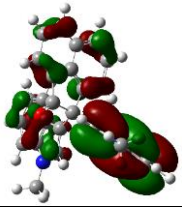
LUMO+3				
LUMO+2				
LUMO+1				
LUMO				
HOMO				
HOMO-1				
HOMO-2				
HOMO-3				

Orbitals	7cj	7dj	7ej	7fj
LUMO+3				
LUMO+2				
LUMO+1				
LUMO				
HOMO				
HOMO-1				
HOMO-2				
HOMO-3				

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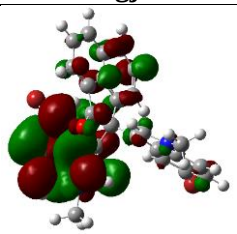
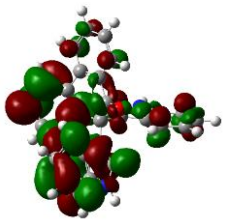
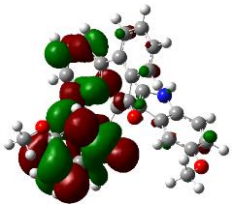
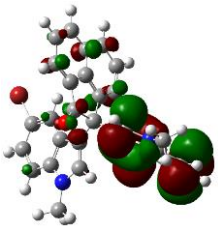
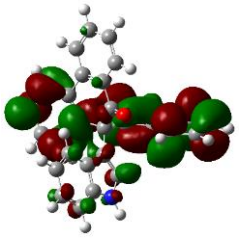
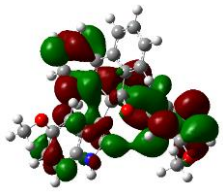
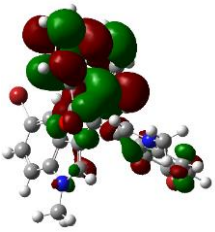
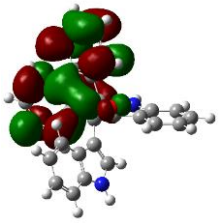
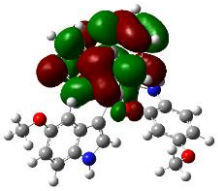
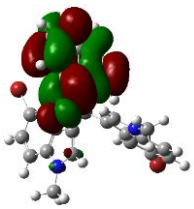
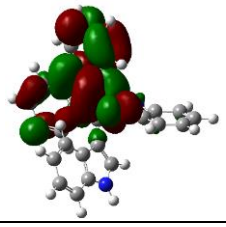
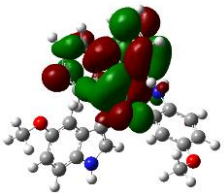
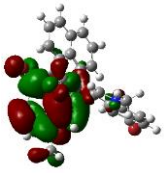
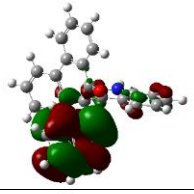
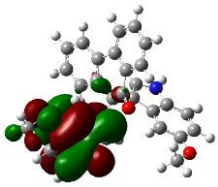
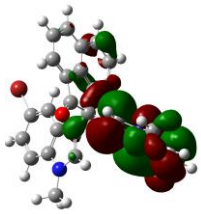
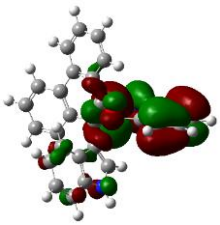
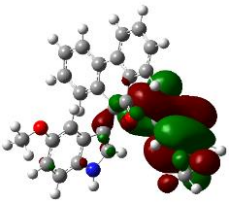
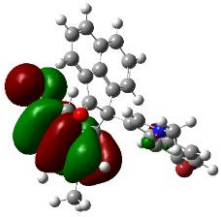
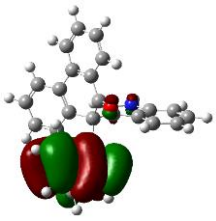
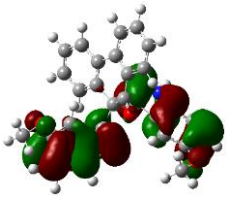
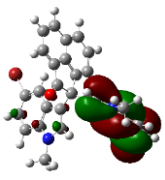
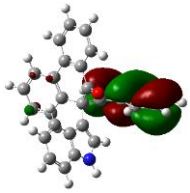
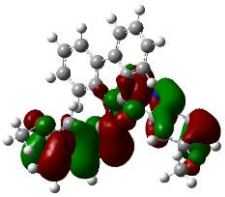
LUMO+3				
LUMO+2				
LUMO+1				
LUMO				
HOMO				
HOMO-1				
HOMO-2				
HOMO-3				

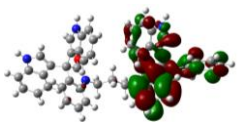
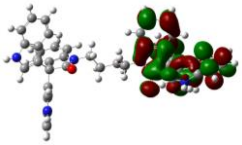
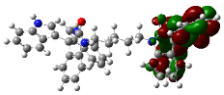
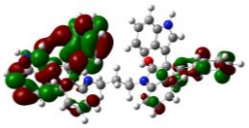
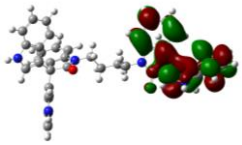
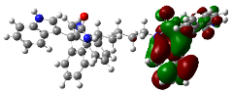
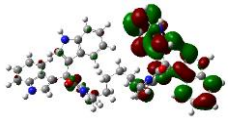
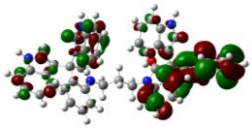
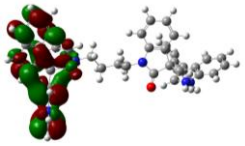
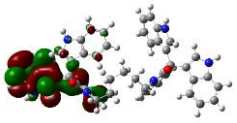
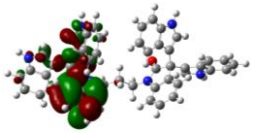
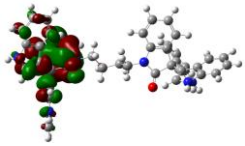
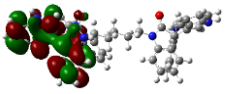
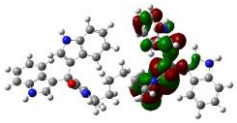
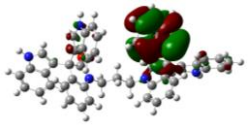
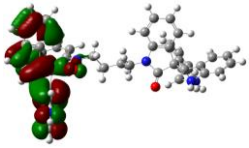
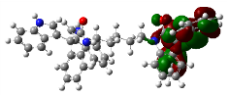
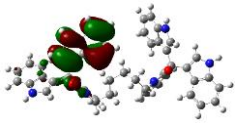
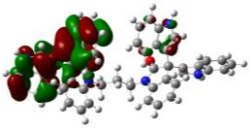
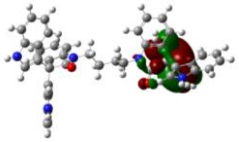
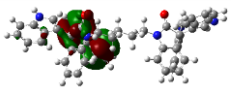
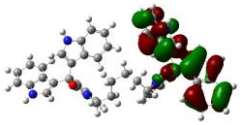
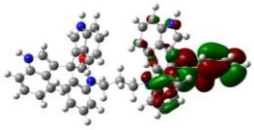
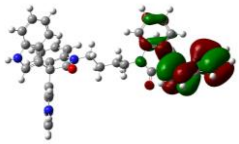
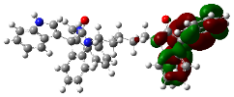
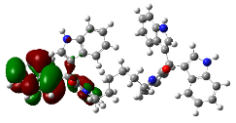
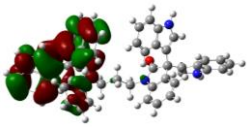
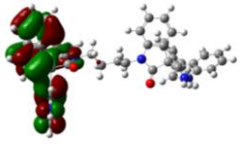
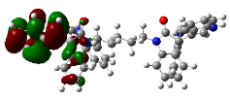
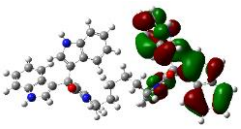
Orbitals	10aa	10ab	10ac	10ad
LUMO+3				
LUMO+2				
LUMO+1				
LUMO				
HOMO				
HOMO-1				
HOMO-2				
HOMO-3				

Table S5 Theoretical UV-Vis Characteristics of synthesized derivatives

S. No	Code	Excitation energy/ Theoretical λ_{abs} (nm)	Oscillator strength	Key transitions*
1	**7aa**	266.76	0.0598	H-1→L (51.19%) H-1→ L+1 (29.09%)
2	**7ab**	261.85	0.0501	H-1→L+2 (65.13%)
3	**7ac**	270.36	0.0399	H→ L+2 (51.10%)
4	**7ad**	262.09	0.0485	H-1→L+2 (65.97%)
5	**7ae**	307.91	0.1608	H-4→ L (70.64%) H→ L+1 (25.82%)
6	**7af**	267.85	0.0549	H-1→L (72.30%)
7	**7ag**	266.77	0.0504	H→ L+2 (75.68%)
8	**7ah**	261.22	0.0501	H-1→ L+2 (59.96%)
9	**7ba**	284.57	0.0478	H-1→L (89.45%)
10	**7ca**	282.39	0.0473	H-2→L+1 (32.59%) H-1→ L (37.36%)
11	**7da**	266.20	0.0546	H→L+3 (50.71%)
12	**7ea**	267.20	0.0501	H-1→ L+1 (72.76%)
13	**7ec**	273.87	0.0674	H-1→L (30.10%) H-1→ L+1 (62.49%)
14	**7ed**	273.77	0.0569	H-1→ L (59.04%)
15	**7fa**	273.17	0.0775	H-1 →L (62.75%) H-1 →L+1 (25.65%)
16	**7fb**	288.70	0.0408	H-1→ L (90.31%)
17	**7fd**	268.17	0.0615	H-2→ L (22.52%) H→ L+3 (35.29%)
18	**7ga**	272.69	0.0488	H-1→ L+1 (75.17%)
19	**7gc**	279.67	0.0790	H-1→ L (77.15%)
20	**7gd**	279.69	0.0785	H-1→ L+1 (86.01%)
21	**7ai**	224.59	0.0634	H-1→ L+2 (26.06%) H→ L+2 (63.58%)
22	**7ei**	262.62	0.0226	H-2→ L+1 (26.51%) H→ L+1 (38.07%)
23	**7fi**	229.89	0.0569	H-1→ L+2 (28.45%) H→ L+2 (57.29%)
24	**7aj**	331.73	0.0691	H-4→ L (91.11%)
25	**7cj**	334.37	0.0901	H-4→ L (92.91%)
26	**7dj**	333.84	0.0773	H-4→ L (87.66%)

27	**7ej**	333.68	0.0801	H-4 → L (93.48%)
28	**7fj**	332.47	0.0805	H-4 → L (93.12%)
29	**7gj**	334.00	0.0844	H-4 → L (93.45%)
30	**7gk**	314.77	0.0485	H-4 → L (38.46%) H-1 → L+1 (36.33%)
31	**7ck**	310.90	0.0481	H-5 → L (22.02%) H-4 → L (40.01%) H-1 → L+1 (21.71%)
32	**10aa**	268.95	0.0237	H → L+5 (53.77%)
33	**10ab**	268.08	0.0532	H-2 → L+2 (53.54%)
34	**10ac**	268.10	0.0471	H-1 → L+4 (60.99%)
35	**10ad**	269.45	0.0212	H → L+5 (67.95%)

Table S6 Binding affinity of BSA-ligand **7** calculated from Molecular docking studies (kcal mol^{-1}) using AutoDock Vina

S. No	Ligand	BSA Binding affinity ($\Delta G_{binding}$)	S. No	Ligand	BSA Binding affinity ($\Delta G_{binding}$)
1	**7aa**	-8.7	17	**7fd**	-8.7
2	**7ab**	-8.2	18	**7ga**	-8.0
3	**7ac**	-8.2	19	**7gc**	-8.0
4	**7ad**	-8.4	20	**7gd**	-7.9
5	**7ae**	-8.5	21	**7ai**	-9.4
6	**7af**	-9.2	22	**7ei**	-8.8
7	**7ag**	-8.7	23	**7fi**	-8.2
8	**7ah**	-8.2	24	**7aj**	-10.2
9	**7ba**	-8.9	25	**7cj**	-9.1
10	**7ca**	-8.4	26	**7dj**	-9.5
11	**7da**	-9.0	27	**7ej**	-9.2
12	**7ea**	-8.3	28	**7fj**	-9.1
13	**7ec**	-9.0	29	**7gj**	-9.4
14	**7ed**	-9.0	30	**7gk**	-9.3
15	**7fa**	-9.7	31	**7ck**	-8.6
16	**7fb**	-9.0			

Table S7 Binding affinity of DNA with ligand **7** calculated from Molecular docking studies (kcal mol^{-1}) using AutoDock Vina

S. No	Ligand	BSA Binding affinity ($\Delta G_{binding}$)	S. No	Ligand	BSA Binding affinity ($\Delta G_{binding}$)
1	**7aa**	-8.2	17	**7fd**	-7.7
2	**7ab**	-8.9	18	**7ga**	-7.3
3	**7ac**	-8.9	19	**7gc**	-7.3
4	**7ad**	-8.9	20	**7gd**	-7.3
5	**7ae**	-8.6	21	**7ai**	-8.3
6	**7af**	-8.7	22	**7ei**	-8.3
7	**7ag**	-8.2	23	**7fi**	-7.0
8	**7ah**	-8.6	24	**7aj**	-8.7
9	**7ba**	-8.8	25	**7cj**	-7.9
10	**7ca**	-8.6	26	**7dj**	-7.5
11	**7da**	-8.2	27	**7ej**	-9.0
12	**7ea**	-8.8	28	**7fj**	-7.8
13	**7ec**	-8.8	29	**7gj**	-8.0
14	**7ed**	-8.8	30	**7gk**	-8.6
15	**7fa**	-7.7	31	**7ck**	-8.1
16	**7fb**	-7.7			

Table S8 The binding site residues of BSA with derivatives **7** as determined from Autodock Vina

	Conventional Hydrogen Bonding	**Pi-Donor Hydrogen Bonding**	**Carbon Hydrogen Bond**	**Pi-cation**	**Pi-anion**	**Pi-Pi T-shaped/ Pi-Pi stacked**	**Pi-Sigma**	**Alkyl/ Pi-Alkyl**	**Amide-Pi Stacked**
7aa	LYS116, GLU140	-	-	-	-	PHE133	-	LEU122	-
7ab	-	-	-	-	-	-	LEU397, GLU540	LYS396 ALA405, VAL408, LYS544	-
7ac	GLU540	-	-	-	-	-	LEU397	LYS396 ALA405, VAL408, LYS544	-
7ae	ARG217, LYS221, LYS294, PRO446	-	-	-	-	-	-	ALA341	-
7af	SER109, LEU112, ARG144	-	-	GLU424, ARG458	ARG185, GLU424, ARG458	-	-	LYS114, LEU115	-
7ag	THR52	-	GLU45, PHE49	-	ASP72, GLU73	-	-	LEU46	-
7ah	PRO420	-	ASP111	-	GLU424	-	ILE522	LYS114, VAL423, LEU462	-
7ba	GLU45, THR52, LYS64	-	GLY61	GLU73	ASP72, GLU73, LYS76	PHE49	-	-	-
7ca	-	-	GLU16	LYS20	-	-	VAL40	LEU24, VAL43, LYS131	-
7da	SER428		-	GLU424, LYS431	GLU424, ARG427	-	-	LEU189, ILE522	VAL423
7fa	ARG458	-	-	LYS431	-	-	LEU189, ALA193	ARG196	-

	Conventional Hydrogen Bonding	Pi-Donor Hydrogen Bonding	Carbon Hydrogen Bond	Pi-cation	Pi-anion	Pi-Pi T-shaped/ Pi-Pi stacked	Pi-Sigma	Alkyl/ Pi-Alkyl	Amide-Pi Stacked
7fb	LYS131	-	-	LYS20	-	-	VAL40	LEU24, LYS132	-
7ai	-	PHE133	-	-	GLU125	TYR137	LEU115	PRO117, LEU122, LYS136	-
7fi	-	-	-	-	ASP72, GLU73	PHE49	-	LEU46, PHE49, HIS59, LYS64, LEU69	-
7aj	-	-	-	LYS116	GLU125	TYR160	LEU115	PRO117, LEU122, LYS136	-
7cj	SER109, LEU112	-	PRO110, GLU519	GLU424	HIS145, GLU424, ARG458	-	ARG144	LYS114, LEU115, LEU189, ILE522	-
7dj	-	-	-	-	GLU45, ASP72, GLU73	PHE49	-	LEU46	
7fj	-	-	-	-	GLU45, ASP72, GLU73	PHE49	-	LEU46, LEU69	-
7gk	-	GLU339	TYR340	-	-	TYR340	VAL380, SER442	MET445, PRO446	-
7ck	-	GLU339	TYR340, GLN384, SER442	-	-	-	VAL380	MET445, PRO446	-

Table S9 The interacting nucleobases of DNA with derivatives **7** as determined from Autodock Vina

	Conventional Hydrogen Bonding	**Van der Waals**	**Pi-Donor Hydrogen Bonding**	**Carbon Hydrogen Bond**	**Pi-Pi T-shaped/ Pi-Pi stacked**	**Pi-Sigma**	**Alkyl/ Pi-Alkyl**
7aa	Gua4, Cyt23	Gua2, Cyt3, Ade5, Ade6, Gua22, Gua24	-	-	-	-	-
7ab	Gua4, Gua22, Cyt23, Gua24	Gua2, Cyt3, Ade5, Ade6	Gua4, Gua22	-	-	-	-
7ac	Gua4, Gua22, Cyt23, Gua24	Gua2, Cyt3, Ade5, Ade6	Gua4, Gua22	-	-	-	-
7ae	Gua4, Gua22, Cyt23, Gua24	Gua2, Cyt3, Ade5, Ade6	Gua4, Gua22	-	-	-	-
7af	Gua4, Gua22, Cyt23, Gua24	Gua2, Cyt3, Ade5, Ade6	Gua22	-	-	-	-
7ag	Ade5, Ade6, Cyt23	Thy7	Gua4, Gua22	Cyt21, Thy20,	-	-	Ade5, Ade6
7ah	Gua4, Cyt23	Gua2, Cyt3, Ade5, Ade6	Gua22	-	-	-	-
7ba	Gua4, Ade5, Ade6, Cyt23	Thy7, Thy20, Cyt21	-	Ade5, Gau22	-	-	-
7ca	Gua4, Gua22, Cyt23, Gua24	Gua2, Cyt3, Ade5	-	Gua2, Cyt3, Ade6	-	-	-
7da	Gua4, Gua24	Gau2, Cyt3, Ade5, Gua22, Cyt23	-	-	-	-	-

	Conventional Hydrogen Bonding	Van der Waals	Pi-Donor Hydrogen Bonding	Carbon Hydrogen Bond	Pi-Pi T-shaped/ Pi-Pi stacked	Pi-Sigma	Alkyl/ Pi-Alkyl
7fa	Gua2, Cyt3	Cyt1, Gua4	Cyt3, Cyt21	Thy20, Gau22	Gua2	Thy20	Cyt21, Gua22
7fb	Gua2, Cyt4	Cyt1, Gua4	Cyt3	Thy20, Gua22	Gua2, Thy20, Cyt21	-	Cyt21, Gua22
7ai	Cyt3, Gua4, Gua22	Gua2, Ade5, Ade6, Cyt21, Gua24	-	Cyt23	-	-	-
7fi	-	Gua4, Thy7, Gua22, Cyt23	-	Ade6, Thy20, Cyt21	-	-	Ade5
7aj	Gua4, Ade5, Ade6, Cyt23	-	Gua22	Gua22	Gua4	-	-
7cj	Gua4, Gua22	Gua2, Ade5, Cyt23	-	Cyt3, Ade5	-	-	-
7dj	Ade4, Ade5	Cyt3, Ade6, Gua22, Cyt23, Gua24	-	-	-	-	-
7fj	-	Cyt3, Ade5, Gua4, Gua24	Gua22	Ade6, Cyt23	-	-	-
7gk	Gua4	Gua2, Cyt3, Ade5, Ade6, Cyt21, Gua22, Gua24	-	Cyt23	-	-	-
7ck	Ade5, Ade6, Gua16, Ade17, Ade18	Thy7, Thy19	Ade18	Thy8	-	-	Gua4, Gua16

Table S10 Cartesian Coordinates of the optimized structures obtained at B3LYP 631-G (d,p) level of theory

Code	Cartesian Coordinates					
	Center number	Atomic number	Atom type	Coordinates (Angstroms)		
				X	Y	Z
	1	6	C	-0.882828	2.632954	0.301305
	2	6	C	-0.301890	1.533980	-0.352121
	3	6	C	-0.134179	1.577119	-1.728968
	4	6	C	-0.553141	2.711697	-2.438574
	5	6	C	-1.133810	3.790496	-1.771076
	6	6	C	-1.306602	3.766712	-0.381956
	7	6	C	-0.405949	1.153808	2.015767
	8	6	C	0.049541	0.457712	0.682273
	9	1	H	0.319295	0.745425	-2.255662
	10	1	H	-0.425121	2.748025	-3.515802
	11	1	H	-1.456255	4.663150	-2.331280
	12	1	H	-1.755648	4.605354	0.141649
	13	1	H	-1.326216	2.999300	2.372261
	14	8	O	-0.303690	0.718660	3.145887
	15	6	C	1.550039	0.207529	0.744913
	16	6	C	2.408019	0.665980	1.715295
	17	6	C	2.368484	-0.491560	-0.224774
	18	1	H	2.185501	1.199347	2.626670
	19	1	H	4.509812	0.511296	1.976924
	20	6	C	-0.742556	-0.832155	0.535000
	21	6	C	-0.314452	-2.052454	0.998561
7aa	22	6	C	-2.091884	-1.029723	0.043728
	23	1	H	0.629795	-2.312516	1.451459
	24	6	C	-2.398012	-2.408431	0.231129
	25	1	H	-1.213279	-3.974063	1.050794
	26	7	N	-0.946094	2.375558	1.675555
	27	7	N	-1.297081	-2.999143	0.815092
	28	7	N	3.705385	0.316400	1.404299
	29	6	C	3.715627	-0.397218	0.224380
	30	6	C	2.110482	-1.208844	-1.408577
	31	6	C	3.169442	-1.777192	-2.105012
	32	6	C	4.495960	-1.654802	-1.645322
	33	6	C	4.785339	-0.967740	-0.473099
	34	1	H	2.972701	-2.332050	-3.017582
	35	1	H	5.303253	-2.109836	-2.211350
	36	1	H	5.805209	-0.879039	-0.109275
	37	6	C	-3.079435	-0.205027	-0.530300
	38	6	C	-4.300211	-0.758258	-0.894874
	39	6	C	-4.572333	-2.127340	-0.704155
	40	6	C	-3.623899	-2.969906	-0.138996
	41	1	H	-2.892912	0.849970	-0.693051
	42	1	H	-5.061535	-0.122922	-1.337947
	43	1	H	-5.536230	-2.529450	-1.001662
	44	1	H	-3.827167	-4.026161	0.014252
	45	1	H	1.092329	-1.338850	-1.759398
	Center number	Atomic number	Atom type	Coordinates (Angstroms)		
				X	Y	Z
	1	6	C	-0.922840	1.746385	1.748207
	2	6	C	-0.327514	1.141241	0.629301
	3	6	C	-0.205277	1.856623	-0.552399
	4	6	C	-0.689533	3.170004	-0.590031
	5	6	C	-1.284786	3.766252	0.519325
	6	6	C	-1.406229	3.048551	1.714443
	7	6	C	-0.336726	-0.361389	2.499415
7ab	8	6	C	0.100018	-0.286557	0.991291
	9	1	H	0.256281	1.424144	-1.430692
	10	1	H	-1.650557	4.784544	0.454120
	11	1	H	-1.866408	3.505014	2.585145
	12	1	H	-1.309315	1.023764	3.733567
	13	8	O	-0.183342	-1.291793	3.264489
	14	6	C	1.610820	-0.453978	0.907291
	15	6	C	2.481787	-0.488114	1.969830
	16	6	C	2.423420	-0.536745	-0.289335
	17	1	H	2.269151	-0.486982	3.027874

	18	1	H	4.595487	-0.636436	2.100750
	19	6	C	-0.645481	-1.372144	0.231970
	20	6	C	-0.146695	-2.632549	0.007601
	21	6	C	-2.008798	-1.375377	-0.259913
	22	1	H	0.828537	-3.028405	0.245282
	23	6	C	-2.250511	-2.676980	-0.785605
	24	1	H	-0.965463	-4.369357	-0.894384
	25	7	N	-0.930386	0.843771	2.815381
	26	7	N	-1.099286	-3.414812	-0.604344
	27	7	N	3.780288	-0.567820	1.514346
	28	6	C	3.779825	-0.603301	0.135541
	29	6	C	2.155436	-0.587344	-1.670836
	30	6	C	3.213095	-0.677600	-2.566506
	31	6	C	4.548121	-0.726668	-2.118174
	32	6	C	4.848281	-0.695011	-0.762289
	33	1	H	3.008838	-0.716724	-3.632252
	34	1	H	5.354021	-0.796648	-2.842491
	35	1	H	5.875337	-0.742173	-0.411336
	36	6	C	-3.055354	-0.434103	-0.316900
	37	6	C	-4.269961	-0.800210	-0.882204
	38	6	C	-4.477844	-2.093300	-1.401134
	39	6	C	-3.470189	-3.048055	-1.359639
	40	1	H	-2.920177	0.569161	0.070026
	41	1	H	-5.076486	-0.074393	-0.927650
	42	1	H	-5.438532	-2.347548	-1.838808
	43	1	H	-3.623789	-4.048196	-1.755190
	44	1	H	1.132696	-0.583184	-2.032376
	45	17	Cl	-0.543270	4.091294	-2.084745
7ac	**Center number**	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
	1	6	C	-0.894491	2.318498	1.055804
	2	6	C	-0.306531	1.418019	0.152040
	3	6	C	-0.148216	1.786286	-1.176245
	4	6	C	-0.590783	3.052450	-1.561848
	5	6	C	-1.178211	3.945536	-0.675196
	6	6	C	-1.335579	3.577328	0.666592
	7	6	C	-0.385631	0.473348	2.357000
	8	6	C	0.068044	0.128386	0.891498
	9	1	H	0.306659	1.133258	-1.910176
	10	1	H	-1.504365	4.915121	-1.034277
	11	1	H	-1.790091	4.261630	1.376048
	12	1	H	-1.324142	2.163661	3.157237
	13	8	O	-0.268216	-0.223716	3.345314
	14	6	C	1.572721	-0.102478	0.882500
	15	6	C	2.431534	0.116920	1.932627
	16	6	C	2.393585	-0.523334	-0.234603
	17	1	H	2.208141	0.403065	2.948904
	18	1	H	4.537429	-0.058901	2.137703
	19	6	C	-0.707208	-1.097188	0.435416
	20	6	C	-0.250734	-2.386664	0.563335
	21	6	C	-2.064821	-1.189076	-0.063561
	22	1	H	0.707586	-2.735122	0.916145
	23	6	C	-2.346786	-2.575468	-0.229304
	24	1	H	-1.120959	-4.274858	0.140118
	25	7	N	-0.942604	1.733380	2.327761
	26	7	N	-1.224014	-3.273863	0.163092
	27	7	N	3.731039	-0.120917	1.538552
	28	6	C	3.742752	-0.518453	0.217950
	29	6	C	2.137373	-0.928022	-1.558753
	30	6	C	3.199696	-1.284694	-2.379394
	31	6	C	4.527846	-1.255801	-1.909348
	32	6	C	4.815830	-0.877215	-0.604199
	33	1	H	3.004399	-1.597625	-3.400720
	34	1	H	5.337701	-1.539878	-2.574543
	35	1	H	5.837177	-0.862692	-0.234166
	36	6	C	-3.077149	-0.264658	-0.387826
	37	6	C	-4.298228	-0.729890	-0.858496
	38	6	C	-4.546146	-2.107298	-1.019629
	39	6	C	-3.572996	-3.047587	-0.707234
	40	1	H	-2.910322	0.800522	-0.277685
	41	1	H	-5.078663	-0.017595	-1.109512

	42	1	H	-5.510851	-2.438745	-1.392003
	43	1	H	-3.757717	-4.111628	-0.825877
	44	1	H	1.118749	-0.987201	-1.927079
	45	9	F	-0.442351	3.421428	-2.854801
7ad	**Center number**	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
	1	6	C	1.225834	-0.089842	2.232728
	2	6	C	0.587160	-0.244304	0.991248
	3	6	C	1.167033	-1.044922	0.018632
	4	6	C	2.383216	-1.673126	0.310282
	5	6	C	3.017627	-1.514368	1.539382
	6	6	C	2.434213	-0.710480	2.525269
	7	6	C	-0.705905	1.165986	2.437822
	8	6	C	-0.718417	0.560505	0.987445
	9	1	H	0.697725	-1.193332	-0.945024
	10	1	H	3.960028	-2.013874	1.731345
	11	1	H	2.919177	-0.581699	3.487871
	12	1	H	0.697749	1.030908	3.986981
	13	8	O	-1.555661	1.865450	2.950707
	14	6	C	-1.931764	-0.347555	0.842952
	15	6	C	-2.787061	-0.722646	1.851161
	16	6	C	-2.376383	-1.041165	-0.348761
	17	1	H	-2.815422	-0.396842	2.879615
	18	1	H	-4.472999	-2.011505	1.910230
	19	6	C	-0.737309	1.713085	-0.003407
	20	6	C	-1.884535	2.246255	-0.539422
	21	6	C	0.356452	2.547759	-0.458997
	22	1	H	-2.905081	1.916015	-0.422447
	23	6	C	-0.216195	3.556813	-1.285292
	24	1	H	-2.245915	3.891673	-1.828815
	25	7	N	0.460289	0.748840	3.047230
	26	7	N	-1.578945	3.344863	-1.309839
	27	7	N	-3.720971	-1.615518	1.370997
	28	6	C	-3.500078	-1.829394	0.026421
	29	6	C	-1.966415	-1.065136	-1.695699
	30	6	C	-2.650816	-1.865400	-2.601317
	31	6	C	-3.751522	-2.647816	-2.198808
	32	6	C	-4.192985	-2.636317	-0.881805
	33	1	H	-2.336393	-1.885534	-3.640452
	34	1	H	-4.266331	-3.264041	-2.929729
	35	1	H	-5.046865	-3.230451	-0.568546
	36	6	C	1.751735	2.564135	-0.265564
	37	6	C	2.513076	3.547272	-0.884180
	38	6	C	1.919725	4.528645	-1.702363
	39	6	C	0.547208	4.545432	-1.913520
	40	1	H	2.234266	1.817354	0.354153
	41	1	H	3.588912	3.559280	-0.736586
	42	1	H	2.543148	5.282422	-2.173839
	43	1	H	0.081964	5.300623	-2.540872
	44	1	H	-1.141260	-0.445265	-2.029753
	45	35	Br	3.197903	-2.780204	-1.022964
7ae	**Center number**	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
	1	6	C	-0.963116	1.365545	1.978070
	2	6	C	-0.357783	0.910132	0.789964
	3	6	C	-0.291214	1.753122	-0.303196
	4	6	C	-0.836054	3.038812	-0.180190
	5	6	C	-1.436168	3.490266	0.995026
	6	6	C	-1.504780	2.644282	2.100001
	7	6	C	-0.289295	-0.788665	2.477487
	8	6	C	0.139746	-0.526635	0.991065
	9	1	H	0.165220	1.460849	-1.238543
	10	1	H	-1.839766	4.494065	1.026781
	11	1	H	-1.967983	2.975439	3.023625
	12	1	H	-1.303166	0.418797	3.866690
	13	8	O	-0.107400	-1.789382	3.136522
	14	6	C	1.658512	-0.602315	0.901606
	15	6	C	2.526430	-0.731410	1.959926
	16	6	C	2.477919	-0.483375	-0.287603
	17	1	H	2.311772	-0.880156	3.007085
	18	1	H	4.643801	-0.786205	2.091591

	19	6	C	-0.548432	-1.552698	0.106884
	20	6	C	0.029880	-2.728540	-0.306467
	21	6	C	-1.923786	-1.587068	-0.348262
	22	1	H	1.038343	-3.080017	-0.152777
	23	6	C	-2.091511	-2.815861	-1.048080
	24	1	H	-0.694447	-4.374816	-1.430114
	25	7	N	-0.921880	0.358637	2.933350
	26	7	N	-0.885903	-3.484758	-1.000563
	27	7	N	3.827880	-0.684115	1.510966
	28	6	C	3.833990	-0.536220	0.139315
	29	6	C	2.218138	-0.362832	-1.666457
	30	6	C	3.282611	-0.278033	-2.554154
	31	6	C	4.616541	-0.318202	-2.101748
	32	6	C	4.909546	-0.452749	-0.750809
	33	1	H	3.084520	-0.182194	-3.617267
	34	1	H	5.427625	-0.248521	-2.820164
	35	1	H	5.936145	-0.493524	-0.397932
	36	6	C	-3.034577	-0.727089	-0.245367
	37	6	C	-4.239302	-1.098324	-0.827998
	38	6	C	-4.373584	-2.317411	-1.520972
	39	6	C	-3.301082	-3.191547	-1.639987
	40	1	H	-2.957808	0.219798	0.276766
	41	1	H	-5.095491	-0.434879	-0.750813
	42	1	H	-5.328273	-2.577510	-1.967964
	43	1	H	-3.398000	-4.134389	-2.170819
	44	1	H	1.198829	-0.361588	-2.037137
	45	7	N	-0.777472	3.942143	-1.331197
	46	8	O	-1.254690	5.072012	-1.201911
	47	8	O	-0.254843	3.522670	-2.365264
7af	**Center number**	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
	1	6	C	-0.909287	2.271310	1.165086
	2	6	C	-0.318427	1.412383	0.224111
	3	6	C	-0.175683	1.837519	-1.086615
	4	6	C	-0.623205	3.115925	-1.474105
	5	6	C	-1.211625	3.942521	-0.512021
	6	6	C	-1.363124	3.536053	0.820167
	7	6	C	-0.373630	0.385285	2.394037
	8	6	C	0.071683	0.098822	0.913479
	9	1	H	0.286066	1.189331	-1.824062
	10	1	H	-1.560779	4.929707	-0.802915
	11	1	H	-1.820228	4.193099	1.554033
	12	1	H	-1.322023	2.035313	3.262299
	13	8	O	-0.241787	-0.345910	3.356227
	14	6	C	1.577319	-0.125348	0.887057
	15	6	C	2.442636	0.064858	1.937255
	16	6	C	2.392676	-0.509255	-0.247346
	17	1	H	2.225112	0.318838	2.963297
	18	1	H	4.550940	-0.109891	2.123446
	19	6	C	-0.699269	-1.116177	0.421454
	20	6	C	-0.240987	-2.407563	0.519042
	21	6	C	-2.053549	-1.198610	-0.088618
	22	1	H	0.715760	-2.762863	0.869382
	23	6	C	-2.331376	-2.581112	-0.291624
	24	1	H	-1.104431	-4.286785	0.042742
	25	7	N	-0.943426	1.639362	2.414522
	26	7	N	-1.209625	-3.286903	0.089704
	27	7	N	3.741111	-0.155064	1.527525
	28	6	C	3.745148	-0.513047	0.195902
	29	6	C	2.128886	-0.875439	-1.581074
	30	6	C	3.186657	-1.204485	-2.419150
	31	6	C	4.518014	-1.184880	-1.957663
	32	6	C	4.813681	-0.843510	-0.643907
	33	1	H	2.985304	-1.488861	-3.447737
	34	1	H	5.324248	-1.447045	-2.636232
	35	1	H	5.837549	-0.836473	-0.280532
	36	6	C	-3.066223	-0.268400	-0.395364
	37	6	C	-4.283348	-0.724490	-0.885197
	38	6	C	-4.527129	-2.097856	-1.083313
	39	6	C	-3.553515	-3.043607	-0.789167
	40	1	H	-2.901780	0.793673	-0.256490

	41	1	H	-5.064331	-0.007756	-1.121833
	42	1	H	-5.488942	-2.421952	-1.469584
	43	1	H	-3.734967	-4.104762	-0.935898
	44	1	H	1.107728	-0.925607	-1.943437
	45	6	C	-0.468995	3.571104	-2.906932
	46	1	H	0.579566	3.545265	-3.224998
	47	1	H	-1.028503	2.926618	-3.595093
	48	1	H	-0.832378	4.593671	-3.041418
	Center number	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
	1	6	C	-1.069557	1.581118	1.760394
	2	6	C	-0.417560	1.059378	0.628697
	3	6	C	-0.388145	1.793421	-0.541701
	4	6	C	-1.016144	3.053459	-0.584153
	5	6	C	-1.665942	3.559196	0.545114
	6	6	C	-1.694212	2.816369	1.736497
	7	6	C	-0.243601	-0.456953	2.483933
	8	6	C	0.167358	-0.316714	0.971834
	9	1	H	0.108057	1.435223	-1.435083
	10	1	H	-2.153183	4.526045	0.519896
	11	1	H	-2.197842	3.212367	2.613169
	12	1	H	-1.351082	0.790681	3.742552
	13	8	O	0.023774	-1.375634	3.234643
	14	6	C	1.686414	-0.323211	0.872332
	15	6	C	2.566190	-0.287613	1.927157
	16	6	C	2.492826	-0.302826	-0.331238
	17	1	H	2.363330	-0.327917	2.986284
	18	1	H	4.685786	-0.223804	2.040143
	19	6	C	-0.464545	-1.469026	0.207268
	20	6	C	0.163329	-2.666342	-0.035991
	21	6	C	-1.824502	-1.613662	-0.272497
	22	1	H	1.177576	-2.958091	0.188613
	23	6	C	-1.931643	-2.928402	-0.810403
7ag	24	1	H	-0.474431	-4.472280	-0.950144
	25	7	N	-0.963916	0.666539	2.818850
	26	7	N	-0.706581	-3.540642	-0.648220
	27	7	N	3.862664	-0.226202	1.460999
	28	6	C	3.853174	-0.238835	0.082026
	29	6	C	2.218758	-0.357214	-1.711201
	30	6	C	3.271790	-0.326341	-2.616446
	31	6	C	4.609156	-0.247860	-2.179418
	32	6	C	4.917037	-0.207504	-0.825368
	33	1	H	3.062486	-0.368550	-3.681191
	34	1	H	5.411391	-0.224949	-2.910936
	35	1	H	5.946900	-0.156514	-0.483003
	36	6	C	-2.965896	-0.788840	-0.308781
	37	6	C	-4.140695	-1.277121	-0.866179
	38	6	C	-4.215284	-2.579713	-1.397621
	39	6	C	-3.110981	-3.421740	-1.376768
	40	1	H	-2.932531	0.218978	0.088263
	41	1	H	-5.020946	-0.641528	-0.894941
	42	1	H	-5.148242	-2.930947	-1.828401
	43	1	H	-3.161376	-4.428656	-1.781845
	44	1	H	1.197129	-0.447402	-2.064174
	45	8	O	-0.932700	3.702008	-1.787384
	46	6	C	-1.545244	4.973751	-1.904394
	47	1	H	-1.361502	5.305089	-2.927575
	48	1	H	-2.628651	4.921327	-1.732620
	49	1	H	-1.109110	5.701439	-1.207039
	Center number	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
	1	6	C	1.667613	-1.658748	0.155133
	2	6	C	0.639247	-0.916497	-0.448900
	3	6	C	0.469795	-0.973235	-1.824287
7ah	4	6	C	1.333244	-1.769129	-2.590333
	5	6	C	2.355155	-2.502571	-1.988413
	6	6	C	2.523142	-2.448527	-0.602634
	7	6	C	0.634214	-0.624623	1.936565
	8	6	C	-0.131084	-0.162878	0.643406
	9	1	H	-0.322709	-0.413621	-2.306318
	10	1	H	1.208885	-1.817624	-3.667176

	11	1	H	3.022996	-3.117927	-2.580876
	12	1	H	2.307282	-1.880765	2.181211
	13	8	O	0.385041	-0.323477	3.085580
	14	6	C	-1.574186	-0.640595	0.731135
	15	6	C	-2.090508	-1.486751	1.683050
	16	6	C	-2.652459	-0.362727	-0.195635
	17	1	H	-1.618064	-1.894729	2.563445
	18	1	H	-4.013658	-2.339429	1.967761
	19	6	C	-0.028516	1.350650	0.548920
	20	6	C	-0.960395	2.215942	1.069184
	21	6	C	1.063834	2.167799	0.059475
	22	1	H	-1.905844	1.992393	1.538738
	23	6	C	0.702568	3.523433	0.306285
	24	1	H	-1.048941	4.331257	1.204641
	25	7	N	1.656361	-1.461482	1.533014
	26	7	N	-0.531497	3.515323	0.922358
	27	7	N	-3.410166	-1.767442	1.400486
	28	6	C	-3.786869	-1.092013	0.258609
	29	6	C	-2.793390	0.440193	-1.343728
	30	6	C	-4.015874	0.478140	-2.002039
	31	6	C	-5.118865	-0.266466	-1.538527
	32	6	C	-5.019984	-1.056832	-0.400465
	33	1	H	-4.127615	1.097911	-2.886727
	34	1	H	-6.062004	-0.216620	-2.074305
	35	1	H	-5.870186	-1.624967	-0.033567
	36	6	C	2.305796	1.915788	-0.555876
	37	6	C	3.122868	2.984059	-0.902450
	38	6	C	2.735672	4.315402	-0.652884
	39	6	C	1.520035	4.601803	-0.045541
	40	1	H	2.625597	0.901436	-0.763738
	41	1	H	4.080523	2.790002	-1.376379
	42	1	H	3.396659	5.128583	-0.937457
	43	1	H	1.215932	5.625667	0.153402
	44	1	H	-1.963976	1.044504	-1.695281
	45	17	Cl	3.799153	-3.365456	0.190392
7ba	**Center number**	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
	1	6	C	-1.155520	-2.646570	0.431467
	2	6	C	-0.387131	-1.492776	0.653740
	3	6	C	-0.199313	-1.043086	1.953606
	4	6	C	-0.784504	-1.746587	3.015462
	5	6	C	-1.549860	-2.887785	2.772442
	6	6	C	-1.746284	-3.358028	1.468773
	7	6	C	-0.490283	-2.009458	-1.690860
	8	6	C	0.102912	-0.947184	-0.692669
	9	1	H	0.391119	-0.156430	2.154756
	10	1	H	-0.644426	-1.395926	4.032708
	11	1	H	-2.003394	-3.420666	3.602413
	12	1	H	-2.342539	-4.244679	1.276808
	13	1	H	-1.705900	-3.680722	-1.371809
	14	8	O	-0.340738	-2.041393	-2.896406
	15	6	C	1.620595	-0.969551	-0.799094
	16	6	C	2.370636	-1.879743	-1.502125
	17	6	C	2.566395	-0.092464	-0.139794
	18	1	H	2.043754	-2.674840	-2.154300
	19	1	H	4.464073	-2.160657	-1.735638
	20	6	C	-0.477460	0.409148	-1.060597
	21	6	C	0.112514	1.295820	-1.927156
	22	6	C	-1.768917	0.972459	-0.720342
	23	1	H	1.070405	1.229620	-2.419452
	24	6	C	-1.871709	2.215538	-1.412356
	25	1	H	-0.491169	3.176639	-2.707364
	26	7	N	-1.210103	-2.912639	-0.943152
	27	7	N	-0.714890	2.378508	-2.135272
	28	7	N	3.716288	-1.638827	-1.308143
	29	6	C	3.871557	-0.551508	-0.483543
	30	6	C	2.451904	1.042306	0.674984
	31	6	C	3.614036	1.669215	1.137743
	32	6	C	4.900377	1.179603	0.793527
	33	6	C	5.037897	0.069483	-0.021793
	34	1	H	5.777675	1.691298	1.172899

	35	1	H	6.020662	-0.302313	-0.294909
	36	6	C	-2.846349	0.567832	0.081459
	37	6	C	-3.971198	1.393984	0.176673
	38	6	C	-4.040979	2.629841	-0.516024
	39	6	C	-2.991368	3.049314	-1.314152
	40	1	H	-2.822907	-0.365193	0.629624
	41	1	H	-4.929199	3.242969	-0.413270
	42	1	H	-3.039607	3.993093	-1.848502
	43	1	H	1.482132	1.452333	0.930584
	44	6	C	3.507347	2.834227	1.965822
	45	6	C	-5.078284	0.984347	0.989961
	46	7	N	3.425120	3.781356	2.637495
	47	7	N	-5.977392	0.651081	1.649897
7ca	**Center number**	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
	1	6	C	-1.397230	-2.562740	0.486402
	2	6	C	-0.540229	-1.460785	0.642837
	3	6	C	-0.283958	-0.979043	1.918752
	4	6	C	-0.889110	-1.597285	3.022850
	5	6	C	-1.741745	-2.687564	2.845601
	6	6	C	-2.008654	-3.189785	1.565971
	7	6	C	-0.740245	-2.055217	-1.673638
	8	6	C	-0.043038	-1.005759	-0.734956
	9	1	H	0.378556	-0.134073	2.066196
	10	1	H	-0.690763	-1.222771	4.022167
	11	1	H	-2.204517	-3.158428	3.707967
	12	1	H	-2.668741	-4.040303	1.423821
	13	1	H	-2.065778	-3.621959	-1.260002
	14	8	O	-0.632742	-2.152069	-2.880243
	15	6	C	1.466338	-1.156681	-0.865725
	16	6	C	2.125063	-2.154057	-1.545475
	17	6	C	2.491539	-0.337553	-0.251021
	18	1	H	1.717618	-2.940501	-2.162201
	19	1	H	4.179500	-2.612070	-1.813920
	20	6	C	-0.521498	0.379486	-1.141858
	21	6	C	0.122739	1.174863	-2.061746
	22	6	C	-1.746382	1.066806	-0.790520
	23	1	H	1.059757	1.001650	-2.568022
	24	6	C	-1.758528	2.280354	-1.527762
	25	1	H	-0.331085	3.068683	-2.898655
	26	7	N	-1.507743	-2.875166	-0.872882
	27	7	N	-0.609949	2.313229	-2.295198
	28	7	N	3.486104	-2.026470	-1.379620
	29	6	C	3.745106	-0.917917	-0.595109
	30	6	C	2.481744	0.830161	0.527441
	31	6	C	3.690405	1.375049	0.958542
	32	6	C	4.922327	0.776091	0.617698
	33	6	C	4.954431	-0.374114	-0.166525
	34	1	H	5.856378	1.206849	0.956216
	35	1	H	5.904191	-0.828019	-0.434877
	36	6	C	-2.830826	0.782137	0.068514
	37	6	C	-3.865626	1.705430	0.169074
	38	6	C	-3.851392	2.910677	-0.571395
	39	6	C	-2.801684	3.206909	-1.423341
	40	1	H	-2.844732	-0.134143	0.641111
	41	1	H	-4.685912	3.592872	-0.451071
	42	1	H	-2.793899	4.131967	-1.992854
	43	1	H	1.560280	1.339974	0.782506
	44	8	O	-4.967881	1.545928	0.972934
	45	8	O	3.584156	2.517413	1.715354
	46	6	C	4.771887	3.129124	2.181513
	47	6	C	-5.047971	0.370764	1.758506
	48	1	H	5.419192	3.452700	1.355086
	49	1	H	4.457015	4.006055	2.749937
	50	1	H	5.345452	2.463593	2.840794
	51	1	H	-4.203676	0.286662	2.455344
	52	1	H	-5.977372	0.447749	2.325787
	53	1	H	-5.079384	-0.533910	1.136455
7da	**Center number**	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
	1	6	C	-0.976077	2.722726	0.106684

	2	6	C	-0.421361	1.596420	-0.518739
	3	6	C	-0.339708	1.554703	-1.903179
	4	6	C	-0.849863	2.625548	-2.650796
	5	6	C	-1.424100	3.725982	-2.011579
	6	6	C	-1.489535	3.794392	-0.614393
	7	6	C	-0.223851	1.412592	1.860695
	8	6	C	0.056076	0.605261	0.545898
	9	1	H	0.107908	0.700333	-2.400065
	10	1	H	-0.798418	2.596974	-3.734651
	11	1	H	-1.819120	4.547730	-2.601523
	12	1	H	-1.920995	4.656771	-0.115163
	13	1	H	-1.208301	3.230993	2.184907
	14	8	O	0.042732	1.094323	3.005955
	15	6	C	1.532936	0.286928	0.342044
	16	6	C	2.623254	0.963353	0.858479
	17	6	C	2.053852	-0.724318	-0.555249
	18	1	H	4.710596	0.705773	0.582169
	19	6	C	-0.817097	-0.653247	0.662229
	20	6	C	-0.499463	-1.745660	1.453169
	21	6	C	-2.122737	-0.916727	0.082105
	22	6	C	-2.518907	-2.206916	0.539073
	23	1	H	-1.522666	-3.556331	1.843043
	24	7	N	-0.883183	2.568102	1.496508
	25	7	N	-1.515975	-2.674078	1.357049
	26	7	N	3.780457	0.400203	0.346274
	27	6	C	3.471790	-0.625978	-0.517292
	28	6	C	1.479296	-1.696560	-1.398750
	29	6	C	2.308915	-2.521449	-2.149199
	30	6	C	3.711405	-2.407106	-2.083526
	31	6	C	4.310671	-1.456300	-1.266189
	32	1	H	1.867274	-3.270471	-2.799983
	33	1	H	4.332697	-3.067537	-2.681070
	34	1	H	5.391517	-1.357938	-1.214198
	35	6	C	-3.022506	-0.223452	-0.755409
	36	6	C	-4.229117	-0.816421	-1.106924
	37	6	C	-4.583575	-2.098589	-0.646981
	38	6	C	-3.729346	-2.809033	0.186150
	39	1	H	-2.788636	0.765295	-1.126542
	40	1	H	-4.915525	-0.275368	-1.751906
	41	1	H	-5.533506	-2.534387	-0.941807
	42	1	H	-3.991539	-3.796650	0.555809
	43	1	H	0.402059	-1.802789	-1.459967
	44	6	C	0.686677	-2.051836	2.314174
	45	6	C	2.742854	2.122849	1.802549
	46	1	H	1.050955	-1.144174	2.793716
	47	1	H	0.410346	-2.762924	3.100732
	48	1	H	1.503622	-2.491857	1.730967
	49	1	H	3.771310	2.496964	1.820094
	50	1	H	2.100983	2.954569	1.497668
	51	1	H	2.455575	1.847880	2.821066
	Center number	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
	1	6	C	1.248654	2.695508	1.054387
	2	6	C	0.377181	1.604332	0.908309
	3	6	C	0.109126	0.799847	2.007179
	4	6	C	0.716462	1.090616	3.236852
	5	6	C	1.583671	2.176686	3.359459
	6	6	C	1.862951	3.000847	2.262965
	7	6	C	0.596467	2.800256	-1.163156
	8	6	C	-0.118719	1.545001	-0.541546
7ea	9	1	H	-0.562559	-0.046790	1.923609
	10	1	H	0.512156	0.461852	4.097430
	11	1	H	2.051712	2.389280	4.315833
	12	1	H	2.537572	3.846583	2.354685
	13	1	H	1.943478	4.174429	-0.342806
	14	8	O	0.491402	3.215205	-2.300634
	15	6	C	-1.624884	1.742763	-0.634478
	16	6	C	-2.269867	2.892573	-1.023653
	17	6	C	-2.663004	0.800859	-0.273277
	18	1	H	-1.852415	3.813274	-1.401277
	19	1	H	-4.319864	3.427165	-1.162412

	20	6	C	0.346797	0.316919	-1.307667
	21	6	C	-0.301906	-0.203034	-2.402176
	22	6	C	1.571740	-0.441984	-1.162261
	23	1	H	-1.239094	0.101133	-2.842092
	24	6	C	1.577711	-1.416923	-2.200621
	25	1	H	0.143000	-1.802873	-3.722625
	26	7	N	1.369245	3.361943	-0.171531
	27	7	N	0.425903	-1.241375	-2.936415
	28	7	N	-3.634402	2.734587	-0.909809
	29	6	C	-3.909422	1.462742	-0.456833
	30	6	C	-2.670159	-0.538745	0.159256
	31	6	C	-3.892218	-1.142980	0.406657
	32	6	C	-5.119015	-0.476527	0.237249
	33	6	C	-5.135101	0.840346	-0.203012
	34	1	H	-6.045888	-0.997215	0.446128
	35	1	H	-6.075785	1.363758	-0.346249
	36	6	C	2.664253	-0.403513	-0.273828
	37	6	C	3.687149	-1.320308	-0.452709
	38	6	C	3.680551	-2.284713	-1.475745
	39	6	C	2.614914	-2.339250	-2.363638
	40	1	H	2.713125	0.314381	0.533827
	41	1	H	4.507701	-2.978628	-1.565634
	42	1	H	2.595717	-3.076314	-3.160959
	43	1	H	-1.749631	-1.096928	0.274185
	44	35	Br	-3.924147	-2.969606	0.994759
	45	35	Br	5.186557	-1.282073	0.746425
	Center number	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
	1	6	C	1.247513	2.692341	0.817012
	2	6	C	0.366385	1.603508	0.714974
	3	6	C	0.076482	0.847821	1.842256
	4	6	C	0.684591	1.208447	3.045687
	5	6	C	1.561269	2.280691	3.152282
	6	6	C	1.853380	3.045155	2.016608
	7	6	C	0.611446	2.699244	-1.408161
	8	6	C	-0.122182	1.481827	-0.733234
	9	1	H	-0.598819	0.001798	1.820640
	10	1	H	2.006938	2.509401	4.113656
	11	1	H	2.536089	3.886492	2.079583
	12	1	H	1.967114	4.096872	-0.644692
	13	8	O	0.517630	3.059365	-2.564876
	14	6	C	-1.625339	1.694058	-0.839701
	15	6	C	-2.253088	2.832338	-1.287181
	16	6	C	-2.677092	0.785456	-0.434824
	17	1	H	-1.821818	3.727106	-1.709023
	18	1	H	-4.294551	3.387713	-1.458001
	19	6	C	0.332680	0.212828	-1.435064
	20	6	C	-0.331919	-0.373574	-2.485570
7ec	21	6	C	1.564227	-0.530103	-1.266698
	22	1	H	-1.278158	-0.100552	-2.926417
	23	6	C	1.557802	-1.564810	-2.245080
	24	1	H	0.098360	-2.047532	-3.715294
	25	7	N	1.382833	3.299788	-0.439076
	26	7	N	0.392423	-1.438313	-2.969709
	27	7	N	-3.619394	2.698732	-1.170082
	28	6	C	-3.913395	1.454893	-0.655038
	29	6	C	-2.704444	-0.530871	0.063669
	30	6	C	-3.935542	-1.105296	0.336414
	31	6	C	-5.152111	-0.430325	0.130189
	32	6	C	-5.148392	0.863139	-0.374650
	33	1	H	-6.086842	-0.926870	0.361521
	34	1	H	-6.081195	1.391943	-0.546610
	35	6	C	2.671849	-0.432281	-0.402367
	36	6	C	3.697771	-1.352240	-0.544103
	37	6	C	3.678642	-2.376236	-1.507377
	38	6	C	2.597876	-2.489647	-2.371119
	39	1	H	2.731559	0.333513	0.359378
	40	1	H	4.508358	-3.070008	-1.570539
	41	1	H	2.569673	-3.273307	-3.122370
	42	1	H	-1.792729	-1.096682	0.208380
	43	35	Br	-3.994952	-2.899937	1.011749

	44	35	Br	5.217559	-1.232630	0.622425
	45	9	F	0.409139	0.480602	4.150138
7ed	**Center number**	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
	1	6	C	-1.237674	0.559479	2.646998
	2	6	C	-0.352499	0.398158	1.568754
	3	6	C	-0.076521	1.477013	0.741879
	4	6	C	-0.698450	2.701262	1.013042
	5	6	C	-1.580494	2.856848	2.079319
	6	6	C	-1.860397	1.771782	2.917263
	7	6	C	-0.568879	-1.649333	2.802707
	8	6	C	0.159049	-1.047729	1.544819
	9	1	H	0.604462	1.391414	-0.094898
	10	1	H	-2.048866	3.817494	2.258466
	11	1	H	-2.546541	1.883332	3.750849
	12	1	H	-1.941152	-0.811586	4.143854
	13	8	O	-0.462055	-2.776469	3.241631
	14	6	C	1.662825	-1.115758	1.768367
	15	6	C	2.292582	-1.472265	2.937366
	16	6	C	2.711998	-0.758742	0.836774
	17	1	H	1.864538	-1.836601	3.858579
	18	1	H	4.333870	-1.571236	3.509797
	19	6	C	-0.280903	-1.840956	0.325456
	20	6	C	0.406011	-2.913239	-0.191968
	21	6	C	-1.516581	-1.748556	-0.424035
	22	1	H	1.361940	-3.314500	0.107054
	23	6	C	-1.489737	-2.792793	-1.391763
	24	1	H	0.001164	-4.259522	-1.780076
	25	7	N	-1.357421	-0.651747	3.335743
	26	7	N	-0.308505	-3.481885	-1.220663
	27	7	N	3.657191	-1.343206	2.800174
	28	6	C	3.948475	-0.912219	1.524070
	29	6	C	2.737622	-0.353418	-0.511306
	30	6	C	3.967041	-0.103810	-1.099661
	31	6	C	5.183538	-0.243527	-0.407678
	32	6	C	5.181771	-0.655474	0.918202
	33	1	H	6.116853	-0.033731	-0.916291
	34	1	H	6.114628	-0.775312	1.461060
	35	6	C	-2.643001	-0.904347	-0.380685
	36	6	C	-3.667075	-1.129626	-1.285958
	37	6	C	-3.627603	-2.157872	-2.244068
	38	6	C	-2.527846	-3.002770	-2.303429
	39	1	H	-2.718922	-0.094321	0.332324
	40	1	H	-4.456692	-2.285264	-2.929707
	41	1	H	-2.483699	-3.803268	-3.035896
	42	1	H	1.826535	-0.261419	-1.088976
	43	35	Br	4.024560	0.442759	-2.937294
	44	35	Br	-5.212850	0.007052	-1.238408
	45	35	Br	-0.326282	4.199660	-0.116377
7fa	**Center number**	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
	1	6	C	0.678557	2.865786	-0.441465
	2	6	C	0.279817	1.763847	0.332386
	3	6	C	0.203704	1.897962	1.711424
	4	6	C	0.532125	3.126136	2.303149
	5	6	C	0.932276	4.206945	1.516825
	6	6	C	1.010078	4.091581	0.123698
	7	6	C	0.262203	1.209116	-2.002616
	8	6	C	-0.010962	0.574628	-0.591132
	9	1	H	-0.109753	1.064702	2.329737
	10	1	H	0.475457	3.234055	3.381728
	11	1	H	1.186271	5.152739	1.986221
	12	1	H	1.318493	4.931183	-0.492044
	13	1	H	0.929710	3.112541	-2.561774
	14	8	O	0.133046	0.676737	-3.087651
	15	6	C	-1.470475	0.148380	-0.516384
	16	6	C	-2.446416	0.428347	-1.442541
	17	6	C	-2.129353	-0.561703	0.558161
	18	1	H	-2.355065	0.912599	-2.403393
	19	6	C	0.940924	-0.598166	-0.414571
	20	6	C	0.637078	-1.892449	-0.761693

	21	6	C	2.332623	-0.602128	-0.016311
	22	1	H	-0.297485	-2.294009	-1.123815
	23	6	C	2.785268	-1.948515	-0.136190
	24	7	N	0.676282	2.507610	-1.794468
	25	7	N	1.731111	-2.713959	-0.595488
	26	7	N	-3.674049	-0.040737	-1.018957
	27	6	C	-3.506225	-0.654309	0.206716
	28	6	C	-1.707845	-1.151015	1.764533
	29	6	C	-2.642084	-1.780438	2.578124
	30	6	C	-4.001509	-1.845235	2.214349
	31	6	C	-4.450308	-1.288005	1.022772
	32	1	H	-2.318884	-2.236859	3.509100
	33	1	H	-4.708466	-2.343858	2.870785
	34	1	H	-5.496074	-1.346352	0.736480
	35	6	C	3.251532	0.369316	0.424887
	36	6	C	4.551618	-0.013193	0.731739
	37	6	C	4.970139	-1.352579	0.612623
	38	6	C	4.091881	-2.337780	0.178099
	39	1	H	2.952756	1.405578	0.531341
	40	1	H	5.260389	0.735878	1.072691
	41	1	H	5.992601	-1.619567	0.863079
	42	1	H	4.411109	-3.371313	0.083573
	43	1	H	-0.659815	-1.136564	2.044257
	44	6	C	1.766559	-4.142361	-0.828640
	45	6	C	-4.919868	0.054888	-1.750438
	46	1	H	0.800985	-4.461793	-1.223628
	47	1	H	2.542320	-4.399590	-1.558118
	48	1	H	1.963273	-4.692266	0.098995
	49	1	H	-5.674556	0.599236	-1.171857
	50	1	H	-4.743899	0.593487	-2.682862
	51	1	H	-5.315163	-0.938449	-1.991935
7fb	**Center number**	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
	1	6	C	0.708645	2.567740	-1.088448
	2	6	C	0.298377	1.638041	-0.118562
	3	6	C	0.237151	2.020099	1.213790
	4	6	C	0.595630	3.329729	1.536439
	5	6	C	1.007915	4.252480	0.583870
	6	6	C	1.066656	3.870007	-0.761943
	7	6	C	0.247499	0.654696	-2.306970
	8	6	C	-0.024967	0.302908	-0.799075
	9	1	H	-0.081110	1.344611	1.997715
	10	1	H	1.276138	5.255581	0.895758
	11	1	H	1.383970	4.576901	-1.522116
	12	1	H	0.943954	2.404394	-3.219748
	13	8	O	0.099015	-0.071851	-3.269757
	14	6	C	-1.492809	-0.065484	-0.635612
	15	6	C	-2.470504	0.052734	-1.594432
	16	6	C	-2.157436	-0.536911	0.559797
	17	1	H	-2.376784	0.338600	-2.631523
	18	6	C	0.903960	-0.834431	-0.406178
	19	6	C	0.564406	-2.164014	-0.477215
	20	6	C	2.304179	-0.792800	-0.042010
	21	1	H	-0.386724	-2.606715	-0.732355
	22	6	C	2.725152	-2.146398	0.106025
	23	7	N	0.685464	1.960742	-2.350805
	24	7	N	1.644317	-2.961973	-0.168060
	25	7	N	-3.703840	-0.295939	-1.082290
	26	6	C	-3.538989	-0.662901	0.238964
	27	6	C	-1.738806	-0.890107	1.856166
	28	6	C	-2.680055	-1.325634	2.780858
	29	6	C	-4.043724	-1.426973	2.442361
	30	6	C	-4.490123	-1.102287	1.166854
	31	1	H	-2.359221	-1.598864	3.781718
	32	1	H	-4.756111	-1.770226	3.186595
	33	1	H	-5.539429	-1.189766	0.901867
	34	6	C	3.253433	0.224271	0.174454
	35	6	C	4.552023	-0.120544	0.528352
	36	6	C	4.939046	-1.466443	0.676599
	37	6	C	4.030326	-2.496740	0.468242
	38	1	H	2.979873	1.268051	0.072507

	39	1	H	5.284218	0.663805	0.696475
	40	1	H	5.961164	-1.702840	0.957148
	41	1	H	4.325480	-3.535630	0.580154
	42	1	H	-0.688273	-0.848561	2.123709
	43	9	F	0.540700	3.712882	2.832800
	44	6	C	1.644206	-4.408636	-0.106666
	45	6	C	-4.954303	-0.313570	-1.812348
	46	1	H	0.662294	-4.776760	-0.407745
	47	1	H	2.395317	-4.827978	-0.784875
	48	1	H	1.853507	-4.763379	0.909080
	49	1	H	-5.688845	0.355028	-1.349823
	50	1	H	-4.773895	0.023901	-2.834095
	51	1	H	-5.376851	-1.324088	-1.849360
	Center number	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
	1	6	C	1.336027	-0.589849	2.247820
	2	6	C	0.759550	-0.515631	0.969085
	3	6	C	1.331954	-1.217480	-0.081106
	4	6	C	2.478509	-1.978949	0.172531
	5	6	C	3.051908	-2.046960	1.439401
	6	6	C	2.475356	-1.343378	2.503011
	7	6	C	-0.504561	0.780108	2.542283
	8	6	C	-0.478964	0.387580	1.020735
	9	1	H	0.908355	-1.189846	-1.076488
	10	1	H	3.941406	-2.644771	1.600287
	11	1	H	2.912914	-1.391276	3.495325
	12	1	H	0.795142	0.315548	4.118583
	13	8	O	-1.326927	1.468763	3.111766
	14	6	C	-1.747409	-0.386292	0.689953
	15	6	C	-2.685914	-0.829470	1.591275
	16	6	C	-2.176818	-0.865467	-0.605853
	17	1	H	-2.747284	-0.651650	2.654626
	18	6	C	-0.350949	1.664993	0.207161
	19	6	C	-1.419827	2.365566	-0.297953
	20	6	C	0.824374	2.462822	-0.070338
	21	1	H	-2.468136	2.108006	-0.277681
	22	6	C	0.372323	3.622364	-0.764760
	23	7	N	0.590166	0.186769	3.138558
	24	7	N	-1.001189	3.538116	-0.887550
7fd	25	7	N	-3.665746	-1.564936	0.956284
	26	6	C	-3.377072	-1.601513	-0.393925
	27	6	C	-1.697426	-0.735851	-1.922717
	28	6	C	-2.391284	-1.342034	-2.962679
	29	6	C	-3.568960	-2.077290	-2.724104
	30	6	C	-4.079796	-2.212448	-1.438740
	31	1	H	-2.022927	-1.243685	-3.979459
	32	1	H	-4.089179	-2.540205	-3.557312
	33	1	H	-4.992752	-2.770674	-1.254981
	34	6	C	2.203260	2.338635	0.185674
	35	6	C	3.068703	3.335294	-0.247925
	36	6	C	2.595972	4.467141	-0.939741
	37	6	C	1.241796	4.624823	-1.207990
	38	1	H	2.594108	1.474490	0.710314
	39	1	H	4.132577	3.238944	-0.052058
	40	1	H	3.298710	5.227084	-1.268236
	41	1	H	0.873573	5.496712	-1.740096
	42	1	H	-0.809732	-0.147164	-2.128385
	43	9	F	-1.847759	4.505825	-1.553734
	44	6	C	-4.822356	-2.165755	1.587569
	45	6	C	-2.888073	4.190034	-1.462486
	46	1	H	-1.743694	5.495623	-1.096103
	47	1	H	-1.599048	4.584890	-2.618243
	48	1	H	-4.835537	-3.250261	1.432320
	49	1	H	-4.783579	-1.969861	2.660196
	50	1	H	-5.753081	-1.744903	1.190540
	51	35	Br	3.282434	-2.952500	-1.267583
	Center number	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
7ga	1	6	C	-1.176297	2.847636	-0.964977
	2	6	C	-0.401381	1.677282	-0.930910
	3	6	C	-0.226328	0.946636	-2.097891

	4	6	C	-0.829336	1.389520	-3.283581
	5	6	C	-1.599961	2.552580	-3.294917
	6	6	C	-1.784498	3.303935	-2.128271
	7	6	C	-0.473278	2.711306	1.235400
	8	6	C	0.115539	1.454895	0.495579
	9	1	H	0.369940	0.041351	-2.100313
	10	1	H	-0.697795	0.819057	-4.197368
	11	1	H	-2.065931	2.883206	-4.218234
	12	1	H	-2.383867	4.209247	-2.133413
	13	1	H	-1.711974	4.258750	0.566021
	14	8	O	-0.310141	3.020833	2.399484
	15	6	C	1.634746	1.512307	0.564016
	16	6	C	2.388844	2.566242	1.023433
	17	6	C	2.579121	0.519328	0.104451
	18	1	H	2.061305	3.487165	1.482335
	19	6	C	-0.443358	0.212260	1.170003
	20	6	C	0.173526	-0.451299	2.204095
	21	6	C	-1.731284	-0.422827	0.998288
	22	1	H	1.142526	-0.266490	2.643040
	23	6	C	-1.799553	-1.473432	1.958944
	24	7	N	-1.213296	3.418051	0.313610
	25	7	N	-0.624731	-1.466391	2.683027
	26	7	N	3.736439	2.312306	0.869590
	27	6	C	3.880645	1.060273	0.308454
	28	6	C	2.464084	-0.776463	-0.431486
	29	6	C	3.625912	-1.458910	-0.756193
	30	6	C	4.907615	-0.913142	-0.566279
	31	6	C	5.044102	0.358790	-0.024437
	32	1	H	5.782649	-1.491037	-0.838776
	33	1	H	6.029579	0.785174	0.134228
	34	6	C	-2.833413	-0.220286	0.145939
	35	6	C	-3.928835	-1.058229	0.280394
	36	6	C	-3.985340	-2.098650	1.223665
	37	6	C	-2.910088	-2.315210	2.075517
	38	1	H	-2.835926	0.561257	-0.602003
	39	1	H	-4.867464	-2.725111	1.280730
	40	1	H	-2.941793	-3.114922	2.808671
	41	1	H	1.497253	-1.244592	-0.566977
	42	6	C	-0.277949	-2.399365	3.736104
	43	6	C	4.819338	3.191263	1.262477
	44	1	H	0.689893	-2.118705	4.153794
	45	1	H	-1.022958	-2.373837	4.538359
	46	1	H	-0.209029	-3.423379	3.352184
	47	1	H	5.440904	3.457671	0.400655
	48	1	H	4.398745	4.106013	1.682398
	49	1	H	5.454598	2.720284	2.020845
	50	35	Br	-5.443095	-0.795899	-0.871597
	51	35	Br	3.490700	-3.229363	-1.485905
	Center number	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
	1	6	C	1.185183	2.856201	0.620687
	2	6	C	0.396177	1.695851	0.678476
	3	6	C	0.203200	1.057440	1.895402
	4	6	C	0.813109	1.604858	3.025136
	5	6	C	1.599372	2.748872	2.974130
	6	6	C	1.793458	3.395258	1.747657
	7	6	C	0.485568	2.549823	-1.564115
	8	6	C	-0.121650	1.364841	-0.726166
	9	1	H	-0.399081	0.163317	1.996468
7gc	10	1	H	2.051737	3.124060	3.885067
	11	1	H	2.404635	4.290120	1.687277
	12	1	H	1.742262	4.130994	-1.019903
	13	8	O	0.328287	2.763451	-2.750106
	14	6	C	-1.639724	1.438643	-0.798623
	15	6	C	-2.377773	2.462501	-1.344594
	16	6	C	-2.598522	0.502165	-0.257358
	17	1	H	-2.036295	3.336457	-1.878976
	18	6	C	0.421357	0.063412	-1.292697
	19	6	C	-0.215288	-0.693316	-2.247849
	20	6	C	1.712726	-0.553959	-1.087275
	21	1	H	-1.192607	-0.549294	-2.683494

	22	6	C	1.762863	-1.690302	-1.945619
	23	7	N	1.231915	3.320471	-0.701235
	24	7	N	0.573879	-1.749973	-2.644035
	25	7	N	-3.728345	2.242927	-1.170753
	26	6	C	-3.891419	1.044462	-0.506632
	27	6	C	-2.503550	-0.746066	0.385208
	28	6	C	-3.675682	-1.381104	0.764734
	29	6	C	-4.948626	-0.832550	0.529006
	30	6	C	-5.065531	0.391651	-0.117056
	31	1	H	-5.832475	-1.371797	0.848223
	32	1	H	-6.044227	0.818826	-0.311341
	33	6	C	2.831446	-0.272082	-0.280748
	34	6	C	3.925445	-1.119149	-0.357042
	35	6	C	3.963758	-2.244348	-1.198408
	36	6	C	2.871910	-2.540004	-2.004150
	37	1	H	2.849259	0.577475	0.388805
	38	1	H	4.845281	-2.874036	-1.213658
	39	1	H	2.890083	-3.405527	-2.658764
	40	1	H	-1.544493	-1.217551	0.559470
	41	6	C	0.207677	-2.776792	-3.598928
	42	6	C	-4.798312	3.102784	-1.635572
	43	1	H	-0.770913	-2.538460	-4.017807
	44	1	H	0.934050	-2.823030	-4.417161
	45	1	H	0.152605	-3.761065	-3.120679
	46	1	H	-5.414121	3.449678	-0.798698
	47	1	H	-4.364346	3.972542	-2.130710
	48	1	H	-5.441718	2.579634	-2.351596
	49	35	Br	5.462036	-0.747984	0.732778
	50	35	Br	-3.567890	-3.086623	1.637547
	51	9	F	0.631529	0.992532	4.215940
	Center number	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
	1	6	C	-1.173300	1.062174	2.580170
	2	6	C	-0.376547	0.771387	1.460917
	3	6	C	-0.216752	1.725795	0.467298
	4	6	C	-0.863999	2.957875	0.615998
	5	6	C	-1.658540	3.241488	1.723879
	6	6	C	-1.820983	2.282316	2.729671
	7	6	C	-0.400747	-1.079755	2.988076
	8	6	C	0.191418	-0.646979	1.596931
	9	1	H	0.394049	1.538623	-0.406355
	10	1	H	-2.149798	4.203950	1.805432
	11	1	H	-2.438267	2.494149	3.597001
	12	1	H	-1.691211	-0.097482	4.312807
	13	8	O	-0.210564	-2.127253	3.572478
	14	6	C	1.710204	-0.637800	1.690683
	15	6	C	2.453726	-0.797727	2.836524
	16	6	C	2.661490	-0.392999	0.630125
	17	1	H	2.120302	-1.033206	3.836214
	18	6	C	-0.318406	-1.620249	0.547247
7gd	19	6	C	0.362836	-2.738500	0.127751
	20	6	C	-1.614382	-1.676830	-0.091732
	21	1	H	1.357382	-3.063753	0.393675
	22	6	C	-1.621622	-2.853219	-0.895597
	23	7	N	-1.182608	-0.038634	3.442666
	24	7	N	-0.403071	-3.482907	-0.741110
	25	7	N	3.799978	-0.655844	2.573453
	26	6	C	3.955186	-0.408050	1.224900
	27	6	C	2.560431	-0.190692	-0.758789
	28	6	C	3.726988	0.004472	-1.481454
	29	6	C	5.000215	0.003367	-0.884922
	30	6	C	5.123613	-0.208470	0.482321
	31	1	H	5.879494	0.162546	-1.497611
	32	1	H	6.102891	-0.219638	0.950231
	33	6	C	-2.768424	-0.871155	-0.070402
	34	6	C	-3.854532	-1.259998	-0.838167
	35	6	C	-3.850626	-2.416499	-1.636906
	36	6	C	-2.723141	-3.226572	-1.671880
	37	1	H	-2.819471	0.033245	0.521143
	38	1	H	-4.727812	-2.669228	-2.220412
	39	1	H	-2.708645	-4.122543	-2.284248

	40	1	H	1.602095	-0.210688	-1.262353
	41	6	C	0.009148	-4.698138	-1.414784
	42	6	C	4.874516	-0.779892	3.538047
	43	1	H	1.003800	-4.977538	-1.064828
	44	1	H	-0.680957	-5.518710	-1.192037
	45	1	H	0.048125	-4.555363	-2.500389
	46	1	H	5.457136	0.145800	3.596935
	47	1	H	4.447041	-0.983787	4.520714
	48	1	H	5.548163	-1.602532	3.273997
	49	35	Br	-0.651476	4.286381	-0.744296
	50	35	Br	-5.439146	-0.176707	-0.817252
	51	35	Br	3.611579	0.275006	-3.377316
7ai	**Center number**	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
	1	6	C	-1.475318	0.914115	-0.240970
	2	6	C	-2.453259	1.663154	-0.851167
	3	6	C	-2.118502	-0.323320	0.161000
	4	1	H	-2.396980	2.644982	-1.295941
	5	1	H	-4.518749	1.322198	-1.240595
	6	6	C	0.906182	0.279876	-0.653951
	7	6	C	1.021010	0.138797	-2.018099
	8	6	C	1.747640	-0.760667	-0.083998
	9	1	H	0.532822	0.695882	-2.804347
	10	6	C	2.335754	-1.469376	-1.175241
	11	1	H	2.106687	-1.192648	-3.268857
	12	7	N	1.873093	-0.895290	-2.336219
	13	7	N	-3.655624	0.979244	-0.853653
	14	6	C	-3.482768	-0.239959	-0.236544
	15	6	C	-1.688313	-1.497486	0.808209
	16	6	C	-2.599878	-2.518589	1.045173
	17	6	C	-3.946550	-2.404982	0.646956
	18	6	C	-4.404837	-1.265226	-0.001264
	19	1	H	-2.268059	-3.424797	1.543398
	20	1	H	-4.635468	-3.220657	0.846212
	21	1	H	-5.441078	-1.172868	-0.315072
	22	6	C	2.076960	-1.203414	1.216792
	23	6	C	2.942859	-2.275941	1.386853
	24	6	C	3.511302	-2.943744	0.285248
	25	6	C	3.212428	-2.546088	-1.010226
	26	1	H	1.662857	-0.719663	2.092362
	27	1	H	3.186905	-2.605910	2.392360
	28	1	H	4.186179	-3.778158	0.450300
	29	1	H	3.639842	-3.055137	-1.869839
	30	1	H	-0.653644	-1.617145	1.108152
	31	6	C	0.207730	1.517566	1.516955
	32	6	C	-0.021545	1.328756	-0.013450
	33	6	C	0.234222	2.720598	-0.668051
	34	6	C	1.616476	3.303096	-0.348195
	35	6	C	1.809616	3.460615	1.165397
	36	6	C	1.571488	2.126535	1.884602
	37	1	H	-0.584553	2.190637	1.869138
	38	1	H	0.087365	2.661976	-1.752135
	39	1	H	2.394866	2.644377	-0.752739
	40	1	H	2.814606	3.839020	1.387440
	41	1	H	1.621647	2.267356	2.971647
	42	1	H	-0.526308	3.416287	-0.289227
	43	1	H	1.729829	4.271837	-0.850189
	44	1	H	1.100914	4.211823	1.543066
	45	1	H	2.377995	1.432910	1.623223
	46	1	H	0.043868	0.574108	2.044564
7ei	**Center number**	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
	1	6	C	-2.477864	-1.128242	-0.145513
	2	6	C	-3.802480	-1.486317	-0.054389
	3	6	C	-2.461396	0.321825	-0.117954
	4	1	H	-4.253704	-2.466543	-0.037297
	5	1	H	-5.608676	-0.369726	0.094415
	6	6	C	-0.291778	-1.790217	0.861959
	7	6	C	-0.571904	-2.097280	2.174593
	8	6	C	1.008313	-1.141355	0.887204
	9	1	H	-1.453869	-2.561118	2.591482

	10	6	C	1.437814	-1.111109	2.248316
	11	1	H	0.470435	-1.813363	4.003813
	12	7	N	0.453011	-1.701999	3.003606
	13	7	N	-4.604775	-0.363461	0.025264
	14	6	C	-3.811599	0.760471	-0.015148
	15	6	C	-1.443612	1.293684	-0.162419
	16	6	C	-1.807455	2.629817	-0.115381
	17	6	C	-3.145013	3.053226	-0.020964
	18	6	C	-4.164347	2.112428	0.032594
	19	1	H	-3.371577	4.112286	0.011703
	20	1	H	-5.201931	2.424337	0.109151
	21	1	H	1.867341	-0.565113	-0.074873
	22	6	C	3.069636	-0.017507	0.342110
	23	6	C	3.479760	-0.005641	1.686010
	24	6	C	2.655137	-0.558273	2.654830
	25	6	C	1.615007	-0.538694	-1.125179
	26	1	H	4.431229	0.436187	1.956150
	27	1	H	2.949965	-0.555294	3.700171
	28	1	H	-0.398286	1.019573	-0.218392
	29	6	C	-0.671978	-1.907191	-1.702335
	30	6	C	-1.285437	-2.075356	-0.278660
	31	6	C	-1.778360	-3.551641	-0.184736
	32	6	C	-0.682735	-4.583425	-0.479627
	33	6	C	-0.100198	-4.378769	-1.883754
	34	6	C	0.410038	-2.942257	-2.054948
	35	1	H	-1.502293	-2.011318	-2.412353
	36	1	H	-2.225082	-3.739837	0.797860
	37	1	H	0.115666	-4.496427	0.267756
	38	1	H	0.708543	-5.094477	-2.072534
	39	1	H	0.741655	-2.776758	-3.087308
	40	1	H	-2.581031	-3.686529	-0.921759
	41	1	H	-1.097990	-5.593820	-0.381653
	42	1	H	-0.880478	-4.582395	-2.631196
	43	1	H	1.291613	-2.801685	-1.420172
	44	1	H	-0.299599	-0.888108	-1.838977
	45	35	Br	4.235380	0.757319	-0.970454
	46	35	Br	-0.434767	3.969863	-0.177239
	Center number	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
	1	6	C	1.473021	0.687495	0.081978
	2	6	C	2.543294	1.233133	0.750351
	3	6	C	1.930249	-0.601626	-0.398107
	4	1	H	2.629215	2.180093	1.262599
	5	6	C	-0.985940	0.395812	0.424697
	6	6	C	-1.150220	0.174432	1.773091
	7	6	C	-1.962089	-0.461363	-0.224911
	8	1	H	-0.599363	0.593495	2.603394
	9	6	C	-2.668796	-1.146949	0.810533
	10	7	N	-2.151828	-0.740368	2.020930
	11	7	N	3.636968	0.383294	0.722422
	12	6	C	3.284101	-0.749218	0.018718
	13	6	C	1.342630	-1.651387	-1.128088
	14	6	C	2.096211	-2.780550	-1.425566
7fi	15	6	C	3.436041	-2.897335	-1.007411
	16	6	C	4.047141	-1.884694	-0.277772
	17	1	H	1.642569	-3.591409	-1.988042
	18	1	H	3.999201	-3.792365	-1.255508
	19	1	H	5.078786	-1.973880	0.049479
	20	6	C	-2.330111	-0.756979	-1.555822
	21	6	C	-3.345095	-1.671413	-1.809128
	22	6	C	-4.027665	-2.319752	-0.762820
	23	6	C	-3.695734	-2.063890	0.560876
	24	1	H	-1.831440	-0.281916	-2.391261
	25	1	H	-3.617402	-1.889556	-2.837646
	26	1	H	-4.818140	-3.027972	-0.992290
	27	1	H	-4.213514	-2.562362	1.374863
	28	1	H	0.307856	-1.593447	-1.445607
	29	6	C	-0.064787	1.664086	-1.641429
	30	6	C	0.103312	1.333479	-0.127120
	31	6	C	0.048096	2.697538	0.626008
	32	6	C	-1.223756	3.504918	0.338218

	33	6	C	-1.361046	3.798114	-1.161218
	34	6	C	-1.313262	2.498343	-1.974983
	35	1	H	0.827032	2.231831	-1.936677
	36	1	H	0.162836	2.539570	1.704092
	37	1	H	-2.100413	2.944549	0.685948
	38	1	H	-2.292631	4.340201	-1.363388
	39	1	H	-1.320256	2.722760	-3.049077
	40	1	H	0.912327	3.294952	0.306342
	41	1	H	-1.199669	4.441168	0.909449
	42	1	H	-0.539502	4.457738	-1.476244
	43	1	H	-2.220236	1.918482	-1.772289
	44	1	H	-0.035655	0.746477	-2.235263
	45	6	C	-2.586884	-1.200774	3.322084
	46	6	C	4.929501	0.636016	1.319868
	47	1	H	-3.638212	-0.947884	3.501651
	48	1	H	-2.468982	-2.286202	3.415182
	49	1	H	-1.979332	-0.720378	4.090798
	50	1	H	4.909691	1.608394	1.815349
	51	1	H	5.178166	-0.127647	2.066192
	52	1	H	5.721821	0.650213	0.562201
	Center number	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
	1	6	C	-1.649137	-1.672157	0.241290
	2	6	C	-0.569564	-0.870696	0.680261
	3	6	C	-0.311620	-0.818664	2.031353
	4	6	C	-1.135529	-1.559649	2.926703
	5	6	C	-2.192656	-2.336957	2.494508
	6	6	C	-2.484622	-2.417663	1.105087
	7	6	C	-0.756830	-0.804097	-1.735600
	8	6	C	0.110614	-0.219859	-0.536109
	9	1	H	0.507113	-0.230639	2.430181
	10	1	H	-0.918702	-1.505728	3.989770
	11	1	H	-2.799341	-2.886071	3.209278
	12	8	O	-0.549065	-0.584080	-2.911578
	13	6	C	1.549713	-0.695158	-0.677605
	14	6	C	2.013704	-1.632012	-1.569520
	15	6	C	2.685300	-0.316902	0.139396
	16	1	H	1.489861	-2.139825	-2.364662
	17	1	H	3.926130	-2.496691	-1.896301
	18	6	C	0.001141	1.294758	-0.577720
	19	6	C	0.874215	2.106913	-1.260951
	20	6	C	-1.052375	2.156628	-0.077522
	21	1	H	1.778057	1.839795	-1.786400
	22	6	C	-0.727711	3.482143	-0.487072
	23	1	H	0.931187	4.199863	-1.608774
7aj	24	7	N	0.446674	3.414722	-1.206469
	25	7	N	3.354469	-1.872988	-1.351171
	26	6	C	3.797465	-1.080308	-0.313649
	27	6	C	2.889329	0.598212	1.189765
	28	6	C	4.151936	0.712501	1.757550
	29	6	C	5.233077	-0.065662	1.297492
	30	6	C	5.070913	-0.968293	0.253960
	31	1	H	4.312539	1.418845	2.566691
	32	1	H	6.208823	0.045901	1.760835
	33	1	H	5.903358	-1.564264	-0.109714
	34	6	C	-2.233212	1.966413	0.666997
	35	6	C	-3.026415	3.063040	0.978899
	36	6	C	-2.675257	4.363822	0.567347
	37	6	C	-1.520965	4.589439	-0.171143
	38	1	H	-2.525671	0.976958	0.997612
	39	1	H	-3.937022	2.915642	1.552153
	40	1	H	-3.315933	5.200770	0.828780
	41	1	H	-1.245045	5.588940	-0.495766
	42	1	H	2.074612	1.225826	1.534831
	43	6	C	-1.820365	-1.658664	-1.156478
	44	6	C	-3.522846	-3.160421	0.481111
	45	6	C	-3.686844	-3.141846	-0.897358
	46	6	C	-2.834920	-2.389886	-1.742292
	47	1	H	-4.198304	-3.751061	1.094796
	48	1	H	-4.491695	-3.720930	-1.340592
	49	1	H	-2.974686	-2.386702	-2.818812

	Center number	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
7cj	1	6	C	-1.663766	-1.884468	0.471359
	2	6	C	-0.562236	-1.011238	0.630524
	3	6	C	-0.208371	-0.645121	1.909558
	4	6	C	-0.957797	-1.150531	3.010866
	5	6	C	-2.035564	-2.000449	2.851106
	6	6	C	-2.427148	-2.401457	1.543999
	7	6	C	-0.930812	-1.501269	-1.714070
	8	6	C	0.018765	-0.663923	-0.751124
	9	1	H	0.629503	0.015956	2.098985
	10	1	H	-0.664262	-0.851475	4.013145
	11	1	H	-2.581939	-2.364197	3.717036
	12	8	O	-0.816616	-1.560915	-2.921527
	13	6	C	1.446581	-1.173824	-0.887690
	14	6	C	1.847933	-2.294354	-1.576692
	15	6	C	2.638346	-0.634894	-0.262742
	16	1	H	1.266259	-2.960297	-2.195482
	17	1	H	3.731634	-3.233483	-1.848388
	18	6	C	-0.107396	0.802474	-1.127281
	19	6	C	0.716510	1.438887	-2.027922
	20	6	C	-1.135870	1.757302	-0.768504
	21	1	H	1.590416	1.057023	-2.532658
	22	6	C	-0.849729	2.952837	-1.479378
	23	1	H	0.738321	3.402920	-2.825744
	24	7	N	0.280046	2.724262	-2.240911
	25	7	N	3.199565	-2.500717	-1.409900
	26	6	C	3.716127	-1.496277	-0.613021
	27	6	C	2.906693	0.489238	0.533546
	28	6	C	4.209256	0.720721	0.973339
	29	6	C	5.262109	-0.152260	0.623984
	30	6	C	5.019267	-1.265612	-0.176401
	31	1	H	6.271100	0.035978	0.969129
	32	1	H	5.832692	-1.931645	-0.449997
	33	6	C	-2.266569	1.724549	0.077354
	34	6	C	-3.052111	2.866173	0.191268
	35	6	C	-2.740536	4.047842	-0.521174
	36	6	C	-1.641140	4.100461	-1.360172
	37	1	H	-2.509847	0.826395	0.626363
	38	1	H	-3.389041	4.907416	-0.391387
	39	1	H	-1.405741	5.007704	-1.909403
	40	1	H	2.133442	1.201463	0.796081
	41	6	C	-1.939659	-2.192116	-0.874878
	42	6	C	-3.501905	-3.260234	1.187911
	43	6	C	-3.767878	-3.559857	-0.141340
	44	6	C	-2.988478	-3.030044	-1.198434
	45	1	H	-4.124214	-3.687638	1.970146
	46	1	H	-4.597832	-4.219473	-0.377439
	47	1	H	-3.208719	-3.273638	-2.233142
	48	8	O	-4.171290	2.958544	0.982196
	49	8	O	4.378125	1.843699	1.747786
	50	6	C	-4.552198	1.814667	1.724395
	51	6	C	5.676989	2.146814	2.220161
	52	1	H	-3.770207	1.507336	2.431522
	53	1	H	-5.447962	2.098060	2.280138
	54	1	H	-4.787408	0.964360	1.070343
	55	1	H	6.384363	2.316918	1.397131
	56	1	H	5.580450	3.066042	2.800709
	57	1	H	6.073491	1.354617	2.869666
	Center number	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
7dj	1	6	C	-2.116191	-1.245871	0.354204
	2	6	C	-0.889770	-0.707178	0.802631
	3	6	C	-0.671947	-0.625478	2.159364
	4	6	C	-1.699412	-1.047104	3.050920
	5	6	C	-2.911530	-1.544981	2.609004
	6	6	C	-3.155979	-1.669202	1.213588
	7	6	C	-0.894453	-0.899565	-1.607890
	8	6	C	-0.013252	-0.351794	-0.407075

	9	1	H	0.259969	-0.239006	2.558673
	10	1	H	-1.519728	-0.966973	4.119291
	11	1	H	-3.672332	-1.849651	3.322345
	12	8	O	-0.555369	-0.938214	-2.775968
	13	6	C	1.341070	-1.038516	-0.282434
	14	6	C	1.696736	-2.297615	-0.731751
	15	6	C	2.475048	-0.524455	0.459267
	16	1	H	3.490062	-3.415955	-0.542808
	17	6	C	0.100873	1.157109	-0.664781
	18	6	C	0.957184	1.721361	-1.597858
	19	6	C	-0.676395	2.245759	-0.095784
	20	6	C	-0.210275	3.444944	-0.708063
	21	1	H	1.277838	3.725030	-2.198009
	22	7	N	0.773596	3.089071	-1.601413
	23	7	N	2.995659	-2.564886	-0.329682
	24	6	C	3.497482	-1.510632	0.398715
	25	6	C	2.734903	0.656356	1.183643
	26	6	C	3.970644	0.818449	1.799210
	27	6	C	4.968291	-0.172321	1.713616
	28	6	C	4.743281	-1.350890	1.012245
	29	1	H	4.172103	1.727805	2.357894
	30	1	H	5.924314	-0.015611	2.204267
	31	1	H	5.505557	-2.122446	0.946907
	32	6	C	-1.720478	2.366536	0.845874
	33	6	C	-2.236110	3.622116	1.143846
	34	6	C	-1.743369	4.787732	0.527931
	35	6	C	-0.722337	4.710285	-0.410133
	36	1	H	-2.129857	1.495734	1.339557
	37	1	H	-3.040364	3.704417	1.869282
	38	1	H	-2.166806	5.754226	0.784360
	39	1	H	-0.335322	5.599752	-0.899870
	40	1	H	1.980821	1.431890	1.257708
	41	6	C	-2.195269	-1.346450	-1.048550
	42	6	C	-4.318504	-2.181602	0.576407
	43	6	C	-4.397203	-2.265038	-0.807211
	44	6	C	-3.330534	-1.857545	-1.645887
	45	1	H	-5.155216	-2.518193	1.183275
	46	1	H	-5.300187	-2.663669	-1.260340
	47	1	H	-3.401271	-1.948635	-2.725281
	48	6	C	1.979944	1.124453	-2.514374
	49	6	C	0.961577	-3.339845	-1.520481
	50	1	H	2.946093	1.001385	-2.011604
	51	1	H	1.648285	0.150547	-2.871364
	52	1	H	2.131326	1.771134	-3.385984
	53	1	H	1.465281	-4.308133	-1.434931
	54	1	H	-0.060449	-3.473172	-1.156310
	55	1	H	0.893896	-3.078175	-2.580802
7ej	**Center number**	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
	1	6	C	-1.476926	2.283277	-0.720060
	2	6	C	-0.430620	1.332220	-0.691297
	3	6	C	-0.090025	0.709095	-1.870477
	4	6	C	-0.799447	1.037437	-3.061600
	5	6	C	-1.824280	1.963249	-3.084762
	6	6	C	-2.199608	2.628679	-1.885357
	7	6	C	-0.783632	2.288705	1.510067
	8	6	C	0.116299	1.222032	0.741949
	9	1	H	0.706139	-0.025337	-1.917366
	10	1	H	-0.520051	0.533605	-3.982252
	11	1	H	-2.344541	2.183314	-4.012682
	12	8	O	-0.665230	2.570655	2.685224
	13	6	C	1.573914	1.652865	0.811939
	14	6	C	2.047503	2.857027	1.276388
	15	6	C	2.731458	0.922007	0.340440
	16	1	H	1.509773	3.672559	1.734851
	17	1	H	3.992463	3.700953	1.397277
	18	6	C	-0.110167	-0.131064	1.393682
	19	6	C	0.644067	-0.620063	2.434179
	20	6	C	-1.186173	-1.080455	1.192737
	21	1	H	1.524079	-0.194286	2.891026
	22	6	C	-0.996484	-2.126295	2.141258

	23	1	H	0.518604	-2.380837	3.611572
	24	7	N	0.122057	-1.812183	2.881637
	25	7	N	3.414451	2.928581	1.109830
	26	6	C	3.865708	1.757221	0.542244
	27	6	C	2.927603	-0.358384	-0.210481
	28	6	C	4.216731	-0.737593	-0.548295
	29	6	C	5.331066	0.098948	-0.357117
	30	6	C	5.161133	1.360701	0.197439
	31	1	H	6.317621	-0.248558	-0.639582
	32	1	H	6.014228	2.013546	0.356922
	33	6	C	-2.288379	-1.162875	0.319368
	34	6	C	-3.127508	-2.260132	0.422455
	35	6	C	-2.926914	-3.291887	1.356253
	36	6	C	-1.849566	-3.229755	2.229252
	37	1	H	-2.485581	-0.397798	-0.418999
	38	1	H	-3.615130	-4.127943	1.389809
	39	1	H	-1.681995	-4.016714	2.958648
	40	1	H	2.100279	-1.043224	-0.347684
	41	6	C	-1.741395	2.861066	0.537090
	42	6	C	-3.222767	3.600461	-1.719716
	43	6	C	-3.478916	4.165605	-0.477691
	44	6	C	-2.739580	3.805869	0.674853
	45	1	H	-3.814297	3.902885	-2.579971
	46	1	H	-4.269951	4.904115	-0.387295
	47	1	H	-2.951373	4.257127	1.639138
	48	35	Br	4.506885	-2.479931	-1.299787
	49	35	Br	-4.635243	-2.388675	-0.759754
7fj	**Center number**	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
	1	6	C	-1.526324	-2.053328	0.188046
	2	6	C	-0.644849	-1.092927	0.736742
	3	6	C	-0.504391	-1.053057	2.105466
	4	6	C	-1.247804	-1.964975	2.908680
	5	6	C	-2.112402	-2.897809	2.369224
	6	6	C	-2.278200	-2.970255	0.958737
	7	6	C	-0.653535	-0.959848	-1.683133
	8	6	C	-0.002586	-0.280255	-0.400280
	9	1	H	0.162656	-0.346688	2.586439
	10	1	H	-1.125997	-1.918483	3.987147
	11	1	H	-2.663616	-3.574902	3.015929
	12	8	O	-0.397390	-0.660165	-2.831830
	13	6	C	1.505686	-0.480941	-0.433638
	14	6	C	2.202934	-1.282218	-1.305958
	15	6	C	2.487305	0.061070	0.481188
	16	1	H	1.843209	-1.844934	-2.154441
	17	6	C	-0.385985	1.189738	-0.408502
	18	6	C	0.369681	2.175794	-0.996621
	19	6	C	-1.612919	1.826547	0.023496
	20	1	H	1.345055	2.098383	-1.453220
	21	6	C	-1.501964	3.203973	-0.326834
	22	7	N	-0.283865	3.388630	-0.950983
	23	7	N	3.548924	-1.292725	-0.995957
	24	6	C	3.749811	-0.473937	0.097485
	25	6	C	2.443245	0.953762	1.568088
	26	6	C	3.618848	1.268654	2.238850
	27	6	C	4.853924	0.715979	1.846557
	28	6	C	4.936509	-0.158084	0.769007
	29	1	H	3.587848	1.958446	3.077174
	30	1	H	5.756105	0.981282	2.389732
	31	1	H	5.889305	-0.577524	0.460328
	32	6	C	-2.792644	1.399481	0.662633
	33	6	C	-3.793585	2.323865	0.934929
	34	6	C	-3.653316	3.681122	0.586461
	35	6	C	-2.505233	4.138663	-0.048512
	36	1	H	-2.925260	0.361525	0.943816
	37	1	H	-4.703590	1.993512	1.427298
	38	1	H	-4.452989	4.379362	0.815399
	39	1	H	-2.394056	5.183865	-0.320980
	40	1	H	1.504558	1.410509	1.863358
	41	6	C	-1.589303	-2.011542	-1.218200
	42	6	C	-3.115745	-3.857528	0.230521

	43	6	C	-3.174287	-3.810146	-1.155736
	44	6	C	-2.408447	-2.884999	-1.906037
	45	1	H	-3.719508	-4.583279	0.769496
	46	1	H	-3.826114	-4.502864	-1.680047
	47	1	H	-2.463502	-2.861449	-2.989957
	48	6	C	0.228739	4.651016	-1.440175
	49	6	C	4.582426	-2.006268	-1.716245
	50	1	H	1.195982	4.481247	-1.915577
	51	1	H	-0.450283	5.087535	-2.180806
	52	1	H	0.362868	5.369544	-0.623251
	53	1	H	5.108781	-2.706007	-1.057521
	54	1	H	4.123281	-2.573702	-2.527229
	55	1	H	5.315430	-1.314699	-2.147300
	Center number	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
	1	6	C	-1.421986	2.428491	-0.705596
	2	6	C	-0.471009	1.383320	-0.762155
	3	6	C	-0.227147	0.795828	-1.982861
	4	6	C	-0.937165	1.253714	-3.130013
	5	6	C	-1.868930	2.271752	-3.069962
	6	6	C	-2.142862	2.903278	-1.825645
	7	6	C	-0.663163	2.247519	1.495883
	8	6	C	0.105883	1.144157	0.643323
	9	1	H	0.493402	-0.006601	-2.094636
	10	1	H	-0.735043	0.776676	-4.084562
	11	1	H	-2.393206	2.589840	-3.966694
	12	8	O	-0.482646	2.454419	2.678924
	13	6	C	1.599617	1.430089	0.683938
	14	6	C	2.203268	2.556993	1.190492
	15	6	C	2.666990	0.622626	0.137334
	16	1	H	1.759906	3.394549	1.707951
	17	6	C	-0.231690	-0.215344	1.230377
	18	6	C	0.500776	-0.832689	2.217213
	19	6	C	-1.399061	-1.044652	1.022766
	20	1	H	1.432723	-0.518626	2.662927
	21	6	C	-1.277793	-2.152056	1.912135
	22	7	N	-0.110690	-1.995621	2.631226
	23	7	N	3.568396	2.519915	0.988241
	24	6	C	3.879306	1.340275	0.344367
	25	6	C	2.726658	-0.637868	-0.484625
	26	6	C	3.965077	-1.114995	-0.884388
7 gj	27	6	C	5.157382	-0.396218	-0.687752
	28	6	C	5.122099	0.844414	-0.063378
	29	1	H	6.098710	-0.817205	-1.020317
	30	1	H	6.038251	1.403213	0.099749
	31	6	C	-2.531529	-0.976509	0.189032
	32	6	C	-3.468578	-1.994143	0.269433
	33	6	C	-3.337053	-3.088057	1.142035
	34	6	C	-2.229826	-3.174330	1.975809
	35	1	H	-2.678450	-0.158429	-0.502923
	36	1	H	-4.100506	-3.856600	1.159503
	37	1	H	-2.117134	-4.013299	2.655185
	38	1	H	1.835145	-1.235135	-0.629350
	39	6	C	-1.591840	2.959159	0.588154
	40	6	C	-3.062817	3.956522	-1.574462
	41	6	C	-3.226144	4.474659	-0.296798
	42	6	C	-2.490302	3.984719	0.809141
	43	1	H	-3.648321	4.359673	-2.396716
	44	1	H	-3.939792	5.278245	-0.140842
	45	1	H	-2.628830	4.400773	1.802161
	46	6	C	0.399101	-2.921154	3.622609
	47	6	C	4.520271	3.526526	1.412487
	48	1	H	1.319076	-2.515733	4.045983
	49	1	H	-0.324316	-3.060798	4.432975
	50	1	H	0.620616	-3.897260	3.176670
	51	1	H	5.076246	3.925244	0.556976
	52	1	H	3.980641	4.347117	1.887349
	53	1	H	5.234934	3.115895	2.134543
	54	35	Br	-5.019956	-1.916874	-0.860048
	55	35	Br	4.069327	-2.833786	-1.733294

	Center number	Atomic number	Atom type	Coordinates (Angstroms)		
				X	Y	Z
7gk	1	6	C	-1.683440	1.892900	-2.576139
	2	6	C	-2.384927	3.074975	-2.776997
	3	6	C	-2.350311	4.064503	-1.789605
	4	6	C	-1.609505	3.877701	-0.626086
	5	6	C	-0.884850	2.693217	-0.408282
	6	6	C	-0.954921	1.689629	-1.397080
	7	6	C	-0.038824	2.482137	0.788190
	8	6	C	0.463981	1.196325	1.090678
	9	6	C	0.115891	-0.032140	0.226695
	10	6	C	-0.246494	0.394166	-1.224056
	11	6	C	0.303819	3.555078	1.631579
	12	6	C	1.087033	3.368883	2.764915
	13	6	C	1.554958	2.092472	3.076350
	14	6	C	1.244964	1.023637	2.238720
	15	8	O	-0.041630	-0.345806	-2.172158
	16	6	C	1.268272	-1.020002	0.193785
	17	6	C	2.580575	-0.790340	-0.369600
	18	6	C	3.343411	-1.968840	-0.147447
	19	7	N	2.531632	-2.859398	0.525528
	20	6	C	1.290916	-2.285524	0.723310
	21	6	C	3.189189	0.289177	-1.032713
	22	6	C	4.507751	0.170215	-1.452303
	23	6	C	5.241786	-1.011019	-1.224201
	24	6	C	4.670854	-2.095304	-0.568775
	25	1	H	2.637771	1.205769	-1.217780
	26	1	H	4.983244	0.999577	-1.967401
	27	1	H	6.270582	-1.075502	-1.566053
	28	1	H	5.234889	-3.006733	-0.390947
	29	1	H	2.782179	-3.798962	0.784590
	30	1	H	1.337478	4.217451	3.394654
	31	1	H	-0.029150	4.557534	1.386948
	32	1	H	2.169836	1.930345	3.956696
	33	1	H	-1.610330	4.660989	0.123456
	34	1	H	-2.904864	4.988572	-1.926210
	35	1	H	-2.960647	3.224908	-3.685113
	36	1	H	-1.686714	1.097265	-3.313386
	37	6	C	-1.174625	-0.668741	0.760786
	38	6	C	-1.910078	-1.793921	0.211209
	39	6	C	-1.885259	-0.244175	1.859528
	40	6	C	-3.046982	-1.989831	1.043278
	41	1	H	-1.674715	0.568096	2.537877
	42	1	H	-3.678593	-0.919358	2.771459
	43	7	N	-3.001821	-1.031017	2.034759
	44	1	H	1.622009	0.032638	2.465144
	45	1	H	0.505058	-2.832318	1.221151
	46	6	C	-1.724998	-2.659471	-0.885032
	47	6	C	-3.983750	-3.003861	0.817806
	48	6	C	-2.654745	-3.665991	-1.112457
	49	6	C	-3.772575	-3.839226	-0.271482
	50	1	H	-0.873438	-2.527774	-1.541430
	51	1	H	-2.519819	-4.333779	-1.958252
	52	1	H	-4.480177	-4.636843	-0.477900
	53	1	H	-4.842919	-3.132292	1.470305
	Center number	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
7ck	1	6	C	0.801850	2.121179	2.832861
	2	6	C	0.940194	3.405791	3.342820
	3	6	C	0.537295	4.495205	2.564268
	4	6	C	-0.011125	4.297388	1.300422
	5	6	C	-0.168899	3.005152	0.770448
	6	6	C	0.271677	1.916829	1.552446
	7	6	C	-0.800550	2.752274	-0.544305
	8	6	C	-0.713596	1.476387	-1.145737
	9	6	C	0.074356	0.324667	-0.490807
	10	6	C	0.173023	0.522248	1.047828
	11	6	C	-1.519726	3.762757	-1.208848
	12	6	C	-2.106896	3.542813	-2.449485
	13	6	C	-1.991884	2.290879	-3.053291
	14	6	C	-1.303985	1.272538	-2.397753

	15	6	C	0.262190	-0.431147	1.805268
	16	6	C	-0.568692	-1.016862	-0.792048
	17	6	C	-1.880805	-1.455931	-0.368719
	18	6	C	-2.077302	-2.758300	-0.904778
	19	7	N	-0.940517	-3.082485	-1.624199
	20	6	C	-0.044799	-2.036240	-1.547724
	21	6	C	-2.899679	-0.875529	0.397856
	22	6	C	-4.074896	-1.591053	0.620684
	23	6	C	-4.250894	-2.885345	0.085399
	24	6	C	-3.250414	-3.476478	-0.683003
	25	1	H	-2.804564	0.115056	0.828417
	26	1	H	-5.166844	-3.434439	0.265087
	27	1	H	-3.391581	-4.472039	-1.094261
	28	1	H	-0.769596	-3.958547	-2.088175
	29	1	H	-2.658671	4.341729	-2.935958
	30	1	H	-1.641900	4.732250	-0.739026
	31	1	H	-2.446788	2.101792	-4.021142
	32	1	H	-0.305528	5.163774	0.719041
	33	1	H	0.651624	5.506655	2.943750
	34	1	H	1.364618	3.562752	4.329666
	35	1	H	1.105919	1.248334	3.400441
	36	6	C	1.533175	0.384880	-0.964973
	37	6	C	2.642521	-0.449235	-0.543372
	38	6	C	2.050734	1.287635	-1.868691
	39	6	C	3.788619	0.005500	-1.243675
	40	1	H	1.551082	2.078516	-2.406361
	41	1	H	3.996585	1.590791	-2.653420
	42	7	N	3.395756	1.063830	-2.041784
	43	1	H	-1.227779	0.291552	-2.853134
	44	1	H	0.917257	-2.098394	-2.032786
	45	6	C	2.766718	-1.535311	0.349579
	46	6	C	5.045317	-0.589048	-1.079793
	47	6	C	4.018406	-2.117994	0.514998
	48	6	C	5.148969	-1.650410	-0.197440
	49	1	H	1.898253	-1.877578	0.894028
	50	1	H	6.098500	-2.146676	-0.028229
	51	1	H	5.915310	-0.232576	-1.623995
	52	8	O	-5.021771	-0.948263	1.382445
	53	8	O	4.272565	-3.170237	1.357313
	54	6	C	-6.232412	-1.623864	1.661718
	55	6	C	3.193540	-3.668220	2.131265
	56	1	H	-6.823863	-0.942976	2.276641
	57	1	H	-6.794265	-1.857089	0.746809
	58	1	H	-6.064426	-2.554619	2.220534
	59	1	H	2.393337	-4.074378	1.498629
	60	1	H	3.607089	-4.469217	2.746534
	61	1	H	2.766635	-2.892743	2.779673
10aa	**Center number**	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
	1	6	C	-2.816373	-1.489906	-1.313550
	2	6	C	-3.998311	-0.749130	-1.148010
	3	6	C	-4.685631	-0.305893	-2.267941
	4	6	C	-4.191204	-0.606997	-3.545421
	5	6	C	-3.018574	-1.346347	-3.691983
	6	6	C	-2.310820	-1.800860	-2.572226
	7	6	C	-3.093401	-1.387519	0.971540
	8	6	C	-4.292929	-0.596124	0.347690
	9	1	H	-5.601889	0.263123	-2.162890
	10	1	H	-4.726227	-0.259934	-4.423746
	11	1	H	-2.643039	-1.574594	-4.685106
	12	1	H	-1.398854	-2.376553	-2.689966
	13	8	O	-2.884755	-1.588148	2.154333
	14	6	C	-5.596248	-1.280942	0.736161
	15	6	C	-5.709303	-2.480257	1.397114
	16	6	C	-6.948077	-0.854458	0.434689
	17	1	H	-4.934725	-3.099037	1.823282
	18	1	H	-7.376341	-3.659328	1.980244
	19	6	C	-4.211934	0.835474	0.853829
	20	6	C	-4.957866	1.343799	1.889006
	21	6	C	-3.263275	1.867651	0.485806
	22	1	H	-5.753019	0.875471	2.447942

	23	6	C	-3.513447	2.979043	1.339473
	24	1	H	-4.957238	3.218123	2.884887
	25	7	N	-2.287790	-1.837251	-0.059722
	26	7	N	-4.552290	2.628396	2.177036
	27	7	N	-7.036474	-2.837347	1.509262
	28	6	C	-7.821931	-1.861218	0.934016
	29	6	C	-7.520792	0.277761	-0.176385
	30	6	C	-8.902275	0.365442	-0.291422
	31	6	C	-9.742551	-0.654639	0.197522
	32	6	C	-9.213465	-1.777933	0.820370
	33	1	H	-9.345039	1.238765	-0.761166
	34	1	H	-10.819111	-0.558398	0.092947
	35	1	H	-9.857071	-2.562376	1.208730
	36	6	C	-2.220559	1.975045	-0.455109
	37	6	C	-1.474912	3.145382	-0.515814
	38	6	C	-1.749431	4.231216	0.338707
	39	6	C	-2.774319	4.164288	1.274030
	40	1	H	-1.999165	1.157246	-1.131278
	41	1	H	-0.659614	3.226540	-1.228070
	42	1	H	-1.145250	5.130536	0.266399
	43	1	H	-2.989199	4.997599	1.937568
	44	1	H	-6.890860	1.087298	-0.528870
	45	6	C	-1.020583	-2.510173	0.176847
	46	6	C	0.187198	-1.588452	-0.048499
	47	6	C	1.516189	-2.302162	0.237812
	48	6	C	3.366264	-0.780323	0.928102
	49	6	C	4.432362	0.124833	0.218319
	50	6	C	4.292753	-0.337750	-1.227415
	51	6	C	3.223149	-1.240460	-1.327530
	52	1	H	-0.962547	-3.394828	-0.470315
	53	1	H	-1.051690	-2.852737	1.214699
	54	1	H	0.100253	-0.716749	0.607845
	55	1	H	0.184406	-1.214615	-1.078360
	56	1	H	1.597042	-3.229299	-0.343745
	57	1	H	1.589129	-2.562109	1.297251
	58	7	N	2.668694	-1.465831	-0.056731
	59	8	O	3.142973	-0.855091	2.120657
	60	6	C	3.965675	1.561460	0.467910
	61	6	C	3.963938	2.115277	1.728418
	62	6	C	3.362222	2.546410	-0.411353
	63	6	C	3.048404	3.677572	0.400010
	64	1	H	3.288931	3.974967	2.491331
	65	6	C	5.829338	-0.137108	0.751684
	66	6	C	6.466180	-1.424920	0.926758
	67	6	C	6.773010	0.807322	1.073274
	68	6	C	7.794574	-1.177069	1.369422
	69	6	C	5.059217	-0.046216	-2.343853
	70	6	C	4.721394	-0.623129	-3.576785
	71	6	C	3.633102	-1.491727	-3.670168
	72	6	C	2.869733	-1.820837	-2.542556
	73	1	H	2.039029	-2.514398	-2.620532
	74	1	H	3.376357	-1.932581	-4.628953
	75	1	H	5.309554	-0.394792	-4.459985
	76	1	H	5.907751	0.626216	-2.259819
	77	7	N	3.431258	3.382010	1.690354
	78	6	C	3.031221	2.617461	-1.780892
	79	6	C	2.455737	4.839599	-0.103351
	80	6	C	2.436279	3.767601	-2.283725
	81	6	C	2.152652	4.873506	-1.457773
	82	1	H	3.232086	1.785580	-2.442755
	83	1	H	2.185498	3.816034	-3.339408
	84	1	H	1.692211	5.759864	-1.883915
	85	1	H	2.237922	5.682889	0.546205
	86	1	H	4.281276	1.669817	2.658647
	87	7	N	7.952085	0.191458	1.442688
	88	1	H	8.783318	0.668665	1.749385
	89	1	H	6.691186	1.883102	1.066349
	90	6	C	8.699569	-2.205728	1.649309
	91	6	C	6.055272	-2.759247	0.756963
	92	6	C	6.950402	-3.784862	1.031471
	93	6	C	8.259920	-3.512037	1.474715

	94	1	H	5.051782	-2.989987	0.415160
	95	1	H	8.936752	-4.335481	1.682353
	96	1	H	9.708986	-1.991555	1.989248
	97	1	H	6.638019	-4.816927	0.903024
	Center number	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
	1	6	C	3.274553	-1.358898	0.670027
	2	6	C	4.670576	-1.212513	0.611539
	3	6	C	5.475372	-2.034581	1.386115
	4	6	C	4.881442	-2.993574	2.219619
	5	6	C	3.493899	-3.121482	2.270764
	6	6	C	2.666238	-2.302221	1.492654
	7	6	C	3.592325	0.316809	-0.876259
	8	6	C	5.018634	-0.100303	-0.380661
	9	1	H	6.554777	-1.943673	1.347420
	10	1	H	5.507739	-3.637691	2.828722
	11	1	H	3.042826	-3.865571	2.920652
	12	1	H	1.587110	-2.405974	1.534106
	13	8	O	3.327014	1.159256	-1.715490
	14	6	C	5.818525	-0.629898	-1.562840
	15	6	C	5.330870	-0.878241	-2.823108
	16	6	C	7.208996	-1.036137	-1.576998
	17	1	H	4.350457	-0.677731	-3.227108
	18	1	H	6.213132	-1.671865	-4.584248
	19	6	C	5.667710	1.121241	0.252416
	20	6	C	6.461275	2.009539	-0.431742
	21	6	C	5.488658	1.670317	1.581810
	22	1	H	6.807214	1.962299	-1.452741
	23	6	C	6.225023	2.889391	1.624189
	24	1	H	7.397351	3.832564	0.120142
	25	7	N	2.658760	-0.445628	-0.200631
	26	7	N	6.801350	3.065573	0.383873
	27	7	N	6.318103	-1.428864	-3.613213
	28	6	C	7.482076	-1.535322	-2.881598
	29	6	C	8.260517	-1.010339	-0.640993
	30	6	C	9.512104	-1.487248	-1.009236
	31	6	C	9.750476	-1.990326	-2.303806
10ab	32	6	C	8.740417	-2.016629	-3.257240
	33	1	H	10.324918	-1.467140	-0.289291
	34	1	H	10.739434	-2.356676	-2.562562
	35	1	H	8.921659	-2.394645	-4.259562
	36	6	C	4.791927	1.278020	2.741919
	37	6	C	4.849678	2.080215	3.874461
	38	6	C	5.591632	3.277732	3.889196
	39	6	C	6.289441	3.696859	2.763877
	40	1	H	4.220729	0.357257	2.758768
	41	1	H	4.313805	1.777408	4.769358
	42	1	H	5.618403	3.881507	4.791452
	43	1	H	6.861947	4.620298	2.766444
	44	1	H	8.101885	-0.598451	0.349896
	45	6	C	1.225797	-0.275090	-0.391383
	46	6	C	0.588130	0.624485	0.680202
	47	6	C	-1.764122	-0.409618	0.750348
	48	6	C	-3.909777	-0.591692	-0.502787
	49	6	C	-5.384483	-0.083372	-0.343000
	50	6	C	-5.341635	0.501019	1.064597
	51	6	C	-4.028455	0.442228	1.555054
	52	1	H	0.762890	-1.267314	-0.415778
	53	1	H	1.098795	0.178596	-1.378028
	54	1	H	1.101686	1.591272	0.652832
	55	1	H	0.776102	0.201108	1.675706
	56	1	H	-1.568373	-0.790681	1.761079
	57	1	H	-1.526064	-1.203642	0.038463
	58	7	N	-3.192474	-0.173822	0.608348
	59	8	O	-3.445015	-1.211345	-1.440679
	60	6	C	-5.580153	0.950980	-1.452713
	61	6	C	-5.626607	0.595633	-2.781892
	62	6	C	-5.620481	2.401523	-1.416096
	63	6	C	-5.717022	2.840387	-2.770141
	64	1	H	-5.755860	1.719015	-4.576759
	65	6	C	-6.377797	-1.229428	-0.431111

	66	6	C	-6.304609	-2.501915	0.254899
	67	6	C	-7.578347	-1.219201	-1.098193
	68	6	C	-7.495203	-3.213945	-0.057945
	69	6	C	-6.359929	0.985731	1.869176
	70	6	C	-6.052570	1.456095	3.154049
	71	6	C	-4.736862	1.420588	3.618392
	72	6	C	-3.702416	0.904955	2.826920
	73	1	H	-2.685719	0.863672	3.203161
	74	1	H	-4.506825	1.787948	4.614185
	75	1	H	-6.840925	1.846510	3.789823
	76	1	H	-7.381744	1.002454	1.501944
	77	7	N	-5.718994	1.718282	-3.570802
	78	6	C	-5.575929	3.392066	-0.412550
	79	6	C	-5.786725	4.188777	-3.133708
	80	6	C	-5.639333	4.732303	-0.770431
	81	6	C	-5.747201	5.132359	-2.116649
	82	1	H	-5.489600	3.119186	0.630866
	83	1	H	-5.603071	5.490246	0.006637
	84	1	H	-5.795372	6.189039	-2.362131
	85	1	H	-5.862675	4.484317	-4.176539
	86	1	H	-5.567642	-0.389792	-3.217591
	87	7	N	-8.252332	-2.403752	-0.878324
	88	1	H	-9.141707	-2.647535	-1.281239
	89	1	H	-8.006972	-0.447966	-1.719076
	90	6	C	-7.756687	-4.497455	0.431721
	91	6	C	-5.361548	-3.115079	1.099389
	92	6	C	-5.616917	-4.388614	1.590588
	93	6	C	-6.802136	-5.075101	1.259437
	94	1	H	-4.443893	-2.602861	1.368354
	95	1	H	-6.973065	-6.070549	1.658322
	96	1	H	-8.672794	-5.022474	0.175901
	97	1	H	-4.891634	-4.866418	2.242444
	98	6	C	-0.918739	0.845632	0.479643
	99	1	H	-1.252765	1.650143	1.144410
	100	1	H	-1.116681	1.188037	-0.543355

	Center number	**Atomic number**	**Atom type**	**Coordinates (Angstroms)**		
				X	**Y**	**Z**
10ac	1	6	C	4.077401	-1.663192	1.511218
	2	6	C	5.109574	-0.749155	1.241594
	3	6	C	5.837401	-0.212495	2.293146
	4	6	C	5.527983	-0.588808	3.608332
	5	6	C	4.499400	-1.496109	3.859035
	6	6	C	3.756035	-2.049890	2.809040
	7	6	C	4.113675	-1.529597	-0.786553
	8	6	C	5.219892	-0.547135	-0.271490
	9	1	H	6.644007	0.486577	2.104761
	10	1	H	6.093906	-0.169533	4.434218
	11	1	H	4.266951	-1.781497	4.880810
	12	1	H	2.958232	-2.757410	3.007997
	13	8	O	3.838851	-1.775270	-1.947803
	14	6	C	6.573427	-0.995274	-0.804125
	15	6	C	6.831390	-2.165539	-1.476178
	16	6	C	7.848096	-0.323728	-0.652129
	17	1	H	6.141910	-2.922795	-1.816275
	18	1	H	8.613284	-3.029478	-2.243292
	19	6	C	4.849578	0.851251	-0.743343
	20	6	C	5.294869	1.409097	-1.917063
	21	6	C	3.887482	1.781091	-0.185931
	22	1	H	6.004657	1.015730	-2.628238
	23	6	C	3.821752	2.888080	-1.080534
	24	1	H	4.867374	3.241054	-2.899395
	25	7	N	3.484970	-2.088429	0.310883
	26	7	N	4.689111	2.628641	-2.120788
	27	7	N	8.181705	-2.276162	-1.734130
	28	6	C	8.832388	-1.162411	-1.246626
	29	6	C	8.264186	0.904318	-0.103113
	30	6	C	9.610200	1.245494	-0.139430
	31	6	C	10.565806	0.388544	-0.721083
	32	6	C	10.188778	-0.823470	-1.285680
	33	1	H	9.933140	2.192789	0.282127
	34	1	H	11.611132	0.682303	-0.734537

	35	1	H	10.920336	-1.483191	-1.743912
	36	6	C	3.070666	1.809449	0.962444
	37	6	C	2.240014	2.901716	1.180152
	38	6	C	2.199877	3.984476	0.279936
	39	6	C	2.992192	3.991874	-0.860754
	40	1	H	3.093064	0.995222	1.677285
	41	1	H	1.609858	2.924058	2.064331
	42	1	H	1.539901	4.823305	0.479380
	43	1	H	2.965320	4.822400	-1.560736
	44	1	H	7.537431	1.588992	0.320843
	45	6	C	2.384113	-3.034644	0.190870
	46	6	C	1.005983	-2.439633	0.524803
	47	6	C	-1.978581	-1.624659	-0.294596
	48	6	C	-4.119114	-0.550498	-0.993606
	49	6	C	-5.348173	0.131205	-0.296359
	50	6	C	-5.067723	-0.189552	1.167263
	51	6	C	-3.820866	-0.824514	1.274450
	52	1	H	2.593464	-3.892494	0.841080
	53	1	H	2.403337	-3.383504	-0.845209
	54	1	H	0.287152	-3.268449	0.492719
	55	1	H	1.006605	-2.070840	1.559071
	56	1	H	-1.891620	-2.530338	0.316806
	57	1	H	-2.024921	-1.930264	-1.343511
	58	7	N	-3.260855	-0.998729	-0.001437
	59	8	O	-3.917915	-0.648144	-2.189375
	60	6	C	-5.247149	1.615828	-0.655732
	61	6	C	-5.380375	2.055952	-1.953391
	62	6	C	-4.922609	2.785216	0.140702
	63	6	C	-4.902450	3.895283	-0.755892
	64	1	H	-5.211398	3.966680	-2.858737
	65	6	C	-6.657209	-0.488507	-0.754720
	66	6	C	-6.980621	-1.898109	-0.813647
	67	6	C	-7.800392	0.184792	-1.108798
	68	6	C	-8.338488	-1.998292	-1.224093
	69	6	C	-5.852007	-0.010460	2.295240
	70	6	C	-5.362346	-0.422142	3.543338
	71	6	C	-4.104887	-1.019751	3.640951
	72	6	C	-3.315884	-1.237952	2.504407
	73	1	H	-2.347925	-1.720722	2.586150
	74	1	H	-3.731678	-1.333797	4.611394
	75	1	H	-5.964652	-0.278123	4.434796
	76	1	H	-6.832765	0.447655	2.208091
	77	7	N	-5.186463	3.415866	-2.016567
	78	6	C	-4.632698	3.041073	1.497442
	79	6	C	-4.629814	5.204245	-0.346873
	80	6	C	-4.356919	4.339212	1.906392
	81	6	C	-4.357389	5.415253	0.997617
	82	1	H	-4.617503	2.236720	2.220742
	83	1	H	-4.133156	4.528492	2.952267
	84	1	H	-4.138343	6.418614	1.350536
	85	1	H	-4.626741	6.024138	-1.059964
	86	1	H	-5.569719	1.475234	-2.842960
	87	7	N	-8.811147	-0.712967	-1.389463
	88	1	H	-9.736346	-0.465496	-1.698402
	89	1	H	-7.970459	1.247636	-1.182458
	90	6	C	-8.984766	-3.226299	-1.396720
	91	6	C	-6.267859	-3.084710	-0.564441
	92	6	C	-6.905136	-4.307127	-0.732415
	93	6	C	-8.250346	-4.378677	-1.145823
	94	1	H	-5.232130	-3.050770	-0.243474
	95	1	H	-8.721126	-5.349457	-1.269435
	96	1	H	-10.022628	-3.277382	-1.713955
	97	1	H	-6.358982	-5.226271	-0.542191
	98	6	C	0.572588	-1.309776	-0.420562
	99	1	H	-0.786216	-0.681298	-0.073520
	100	1	H	1.328669	-0.517700	-0.398447
	101	1	H	0.555261	-1.683299	-1.453036
	102	1	H	-0.778909	-0.332369	0.967179
	103	1	H	-0.941089	0.207090	-0.695396
10ad			**Atom type**	**Coordinates (Angstroms)**		

	Center number	Atomic number		X	Y	Z
	1	6	C	0.000001421	0.000014646	0.000011074
	2	6	C	-0.000005819	-0.000008415	-0.000003728
	3	6	C	0.000001051	0.000002341	-0.000003366
	4	6	C	-0.000001418	0.000005315	0.000000864
	5	6	C	0.000004403	0.000003253	0.000004516
	6	6	C	-0.000003968	-0.000005393	-0.000006265
	7	6	C	-0.000005876	-0.000006741	-0.000009344
	8	6	C	0.000012337	0.000023986	-0.000009763
	9	1	H	0.000000853	-0.000002666	0.000001183
	10	1	H	-0.000001036	-0.000002383	-0.000000008
	11	1	H	0.000000261	-0.000000464	0.000000139
	12	1	H	0.000000639	-0.000000341	0.000000303
	13	8	O	0.000004085	0.000004828	0.000006546
	14	6	C	-0.000000944	-0.000013693	0.000018815
	15	6	C	0.000002331	0.000001791	-0.000004861
	16	6	C	-0.000010263	0.000000092	-0.000005646
	17	1	H	-0.000001821	-0.000001435	-0.000002707
	18	1	H	-0.000000723	0.000003599	0.000003719
	19	6	C	-0.000011201	-0.000001712	-0.000015361
	20	6	C	0.000003014	0.000000539	0.000012814
	21	6	C	0.000007652	0.000000476	0.000006380
	22	1	H	0.000000695	-0.000001015	0.000000456
	23	6	C	-0.000005294	0.000002363	-0.000002545
	24	1	H	-0.000002128	0.000001677	-0.000006128
	25	7	N	-0.000000941	-0.000015074	0.000001031
	26	7	N	-0.000001823	-0.000003516	0.000002395
	27	7	N	-0.000001184	-0.000000838	-0.000002194
	28	6	C	0.000005945	-0.000000903	0.000001764
	29	6	C	0.000004686	-0.000001915	-0.000006157
	30	6	C	0.000002593	0.000005940	0.000001881
	31	6	C	-0.000001433	-0.000000564	0.000006588
	32	6	C	-0.000002158	0.000000497	-0.000004588
	33	1	H	-0.000000503	-0.000000457	0.000000072
	34	1	H	-0.000000047	-0.000001572	-0.000001196
	35	1	H	-0.000000842	0.000001422	-0.000000855
	36	6	C	0.000004706	-0.000000503	-0.000003523
	37	6	C	-0.000002683	-0.000011565	-0.000003768
	38	6	C	-0.000010166	0.000007369	0.000006592
	39	6	C	0.000012625	0.000001167	0.000005072
	40	1	H	-0.000000786	-0.000000690	0.000001043
	41	1	H	0.000000492	0.000003044	0.000002081
	42	1	H	-0.000000129	0.000000846	-0.000003023
	43	1	H	0.000000023	0.000000002	-0.000002437
	44	1	H	-0.000000639	0.000000728	0.000001907
	45	6	C	0.000017986	0.000014953	0.000000427
	46	6	C	-0.000013184	-0.000017208	-0.000008583
	47	6	C	0.000006211	-0.000001039	-0.000001807
	48	6	C	0.000002973	-0.000005759	0.000004789
	49	6	C	-0.000010376	-0.000004824	0.000010470
	50	6	C	0.000000075	0.000005301	0.000009101
	51	6	C	0.000009230	0.000003778	-0.000004990
	52	1	H	-0.000004391	-0.000002808	-0.000002035
	53	1	H	-0.000001937	0.000000080	0.000002068
	54	1	H	0.000006116	0.000003600	0.000004015
	55	1	H	-0.000003020	0.000004147	0.000007210
	56	1	H	0.000003996	-0.000000484	-0.000006842
	57	1	H	0.000003205	0.000011671	-0.000002453
	58	7	N	-0.000015047	-0.000015345	0.000007802
	59	8	O	0.000004908	-0.000000675	-0.000002979
	60	6	C	-0.000011989	0.000003716	-0.000028309
	61	6	C	0.000011753	-0.000000529	0.000004767
	62	6	C	-0.000004537	-0.000006313	0.000009552
	63	6	C	0.000008258	0.000003028	-0.000001048
	64	1	H	-0.000004409	-0.000002484	0.000001736
	65	6	C	0.000001167	0.000008044	-0.000002253
	66	6	C	0.000007594	-0.000003485	-0.000000394
	67	6	C	0.000010959	-0.000000083	0.000002518
	68	6	C	-0.000001399	0.000005195	0.000004130
	69	6	C	-0.000010117	0.000009114	-0.000003070

	70	6	C	0.000004760	-0.000003459	0.000001748
	71	6	C	0.000005812	-0.000008899	0.000003913
	72	6	C	-0.000007542	0.000000595	-0.000008915
	73	1	H	0.000000444	0.000003797	0.000001558
	74	1	H	-0.000002252	0.000003153	-0.000000292
	75	1	H	-0.000000625	0.000001182	0.000000539
	76	1	H	-0.000000175	-0.000000722	-0.000000485
	77	7	N	-0.000000048	0.000005450	0.000000496
	78	6	C	0.000004996	-0.000004226	0.000002539
	79	6	C	-0.000000688	0.000003388	-0.000004073
	80	6	C	-0.000002006	-0.000002759	-0.000003791
	81	6	C	0.000001869	0.000004049	0.000008203
	82	1	H	0.000000774	-0.000004616	-0.000000956
	83	1	H	0.000002261	-0.000002005	-0.000000875
	84	1	H	-0.000000598	-0.000000525	-0.000000119
	85	1	H	0.000001238	-0.000000019	-0.000000235
	86	1	H	-0.000004196	-0.000002529	0.000001059
	87	7	N	-0.000007043	0.000000854	-0.000008696
	88	1	H	0.000001291	-0.000001202	0.000002764
	89	1	H	0.000000149	-0.000002162	0.000000691
	90	6	C	0.000001477	-0.000006335	0.000000214
	91	6	C	-0.000003575	-0.000005558	0.000001490
	92	6	C	-0.000006071	-0.000000524	0.000001125
	93	6	C	0.000003698	0.000004854	-0.000001292
	94	1	H	0.000002980	0.000001080	-0.000001621
	95	1	H	0.000000494	0.000000087	-0.000000270
	96	1	H	0.000000076	-0.000001364	-0.000000216
	97	1	H	0.000000754	0.000000063	0.000000285
	98	6	C	-0.000006934	0.000003831	-0.000005642
	99	6	C	-0.000002148	0.000004014	0.000004226
	100	1	H	0.000001088	-0.000003452	0.000002628
	101	1	H	-0.000000723	-0.000002173	-0.000001383
	102	1	H	-0.000000822	-0.000004439	-0.000003999
	103	1	H	0.000000898	0.000001751	0.000001092
	104	6	C	0.000000206	0.000005935	0.000004694
	105	1	H	-0.000000281	-0.000000703	-0.000001645
	106	1	H	0.000000451	-0.000002065	0.000001650

Table S11 Z matrix of the optimized structures obtained at B3LYP 631-G (d,p) level of theory

7aa	7ab	7ac	7ad	7ae
1 2 2.0 6 1.0 26 1.0	1 2 2.0 6 1.0 25 1.0	1 2 2.0 6 1.0 25 1.0	1 2 2.0 6 1.0 25 1.0	1 2 2.0 6 1.0 25 1.0
2 3 1.0 8 1.0	2 3 1.0 8 1.0	2 3 1.0 8 1.0	2 3 1.0 8 1.0	2 3 1.0 8 1.0
3 4 2.0 9 1.0	3 4 2.0 9 1.0	3 4 2.0 9 1.0	3 4 2.0 9 1.0	3 4 2.0 9 1.0
4 5 1.0 10 1.0	4 5 1.0 45 1.0	4 5 1.0 45 1.0	4 5 1.0 45 1.0	4 5 1.0 45 1.0
5 6 2.0 11 1.0	5 6 2.0 10 1.0	5 6 2.0 10 1.0	5 6 2.0 10 1.0	5 6 2.0 10 1.0
6 12 1.0	6 11 1.0	6 11 1.0	6 11 1.0	6 11 1.0
7 8 1.0 14 2.0 26 1.0	7 8 1.0 13 2.0 25 1.0	7 8 1.0 13 2.0 25 1.0	7 8 1.0 13 2.0 25 1.0	7 8 1.0 13 2.0 25 1.0
8 15 1.0 20 1.0	8 14 1.0 19 1.0	8 14 1.0 19 1.0	8 14 1.0 19 1.0	8 14 1.0 19 1.0
9	9	9	9	9
10	10	10	10	10
11	11	11	11	11
12	12 25 1.0	12 25 1.0	12 25 1.0	12 25 1.0
13 26 1.0	13	13	13	13
14	14 15 2.0 16 1.0	14 15 2.0 16 1.0	14 15 2.0 16 1.0	14 15 2.0 16 1.0
15 16 2.0 17 1.0	15 17 1.0 27 1.0	15 17 1.0 27 1.0	15 17 1.0 27 1.0	15 17 1.0 27 1.0
16 18 1.0 28 1.0	16 28 2.0 29 1.0	16 28 2.0 29 1.0	16 28 2.0 29 1.0	16 28 2.0 29 1.0
17 29 2.0 30 1.0	17	17	17	17
18	18 27 1.0	18 27 1.0	18 27 1.0	18 27 1.0
19 28 1.0	19 20 2.0 21 1.0	19 20 2.0 21 1.0	19 20 2.0 21 1.0	19 20 2.0 21 1.0
20 21 2.0 22 1.0	20 22 1.0 26 1.0	20 22 1.0 26 1.0	20 22 1.0 26 1.0	20 22 1.0 26 1.0
21 23 1.0 27 1.0	21 23 2.0 36 1.0	21 23 2.0 36 1.0	21 23 2.0 36 1.0	21 23 2.0 36 1.0
22 24 2.0 37 1.0	22	22	22	22
23	23 26 1.0 39 1.0	23 26 1.0 39 1.0	23 26 1.0 39 1.0	23 26 1.0 39 1.0
24 27 1.0 40 1.0	24 26 1.0	24 26 1.0	24 26 1.0	24 26 1.0
25 27 1.0	25	25	25	25
26	26	26	26	26
27	27 28 1.0	27 28 1.0	27 28 1.0	27 28 1.0
28 29 1.0	28 32 1.0	28 32 1.0	28 32 1.0	28 32 1.0
29 33 1.0	29 30 2.0 44 1.0	29 30 2.0 44 1.0	29 30 2.0 44 1.0	29 30 2.0 44 1.0
30 31 2.0 45 1.0	30 31 1.0 33 1.0	30 31 1.0 33 1.0	30 31 1.0 33 1.0	30 31 1.0 33 1.0
31 32 1.0 34 1.0	31 32 2.0 34 1.0	31 32 2.0 34 1.0	31 32 2.0 34 1.0	31 32 2.0 34 1.0
32 33 2.0 35 1.0	32 35 1.0	32 35 1.0	32 35 1.0	32 35 1.0
33 36 1.0	33	33	33	33
34	34	34	34	34
35	35	35	35	35
36	36 37 2.0 40 1.0	36 37 2.0 40 1.0	36 37 2.0 40 1.0	36 37 2.0 40 1.0
37 38 2.0 41 1.0	37 38 1.0 41 1.0	37 38 1.0 41 1.0	37 38 1.0 41 1.0	37 38 1.0 41 1.0
38 39 1.0 42 1.0	38 39 2.0 42 1.0	38 39 2.0 42 1.0	38 39 2.0 42 1.0	38 39 2.0 42 1.0
39 40 2.0 43 1.0	39 43 1.0	39 43 1.0	39 43 1.0	39 43 1.0
40 44 1.0	40	40	40	40
41	41	41	41	41
42	42	42	42	42
43	43	43	43	43
44	44	44	44	44
45	45	45	45	45 46 1.5 47 1.5
				46
				47

7af	7ag	7ah	7ba	7ca
1 2 2.0 6 1.0 25 1.0	1 2 2.0 6 1.0 25 1.0	1 2 2.0 6 1.0 25 1.0	1 2 2.0 6 1.0 26 1.0	1 2 2.0 6 1.0 26 1.0
2 3 1.0 8 1.0	2 3 1.0 8 1.0	2 3 1.0 8 1.0	2 3 1.0 8 1.0	2 3 1.0 8 1.0
3 4 2.0 9 1.0	3 4 2.0 9 1.0	3 4 2.0 9 1.0	3 4 2.0 9 1.0	3 4 2.0 9 1.0
4 5 1.0 45 1.0	4 5 1.0 45 1.0	4 5 1.0 10 1.0	4 5 1.0 10 1.0	4 5 1.0 10 1.0
5 6 2.0 10 1.0	5 6 2.0 10 1.0	5 6 2.0 11 1.0	5 6 2.0 11 1.0	5 6 2.0 11 1.0
6 11 1.0	6 11 1.0	6 45 1.0	6 12 1.0	6 12 1.0
7 8 1.0 13 2.0 25 1.0	7 8 1.0 13 2.0 25 1.0	7 8 1.0 13 2.0 25 1.0	7 8 1.0 14 2.0 26 1.0	7 8 1.0 14 2.0 26 1.0
8 14 1.0 19 1.0	8 14 1.0 19 1.0	8 14 1.0 19 1.0	8 15 1.0 20 1.0	8 15 1.0 20 1.0
9	9	9	9	9
10	10	10	10	10
11	11	11	11	11
12 25 1.0	12 25 1.0	12 25 1.0	12	12
13	13	13	13 26 1.0	13 26 1.0
14 15 2.0 16 1.0	14 15 2.0 16 1.0	14 15 2.0 16 1.0	14	14
15 17 1.0 27 1.0	15 17 1.0 27 1.0	15 17 1.0 27 1.0	15 16 2.0 17 1.0	15 16 2.0 17 1.0
16 28 2.0 29 1.0	16 28 2.0 29 1.0	16 28 2.0 29 1.0	16 18 1.0 28 1.0	16 18 1.0 28 1.0
17	17	17	17 29 2.0 30 1.0	17 29 2.0 30 1.0
18 27 1.0	18 27 1.0	18 27 1.0	18	18
19 20 2.0 21 1.0	19 20 2.0 21 1.0	19 20 2.0 21 1.0	19 28 1.0	19 28 1.0
20 22 1.0 26 1.0	20 22 1.0 26 1.0	20 22 1.0 26 1.0	20 21 2.0 22 1.0	20 21 2.0 22 1.0
21 23 2.0 36 1.0	21 23 2.0 36 1.0	21 23 2.0 36 1.0 22	21 23 1.0 27 1.0	21 23 1.0 27 1.0
22	22	23 26 1.0 39 1.0	22 24 2.0 36 1.0	22 24 2.0 36 1.0
23 26 1.0 39 1.0	23 26 1.0 39 1.0	24 26 1.0	23	23
24 26 1.0	24 26 1.0	25	24 27 1.0 39 1.0	24 27 1.0 39 1.0

25 26 27 28 1.0 28 32 1.0 29 30 2.0 44 1.0 30 31 1.0 33 1.0 31 32 2.0 34 1.0 32 35 1.0 33 34 35 36 37 2.0 40 1.0 37 38 1.0 41 1.0 38 39 2.0 42 1.0 39 43 1.0 40 41 42 43 44 45 46 1.0 47 1.0 48 1.0 46 47 48	25 26 27 28 1.0 28 32 1.0 29 30 2.0 44 1.0 30 31 1.0 33 1.0 31 32 2.0 34 1.0 32 35 1.0 33 34 35 36 37 2.0 40 1.0 37 38 1.0 41 1.0 38 39 2.0 42 1.0 39 43 1.0 40 41 42 43 44 45 46 1.0 46 47 1.0 48 1.0 49 1.0 47 48 49	26 27 28 1.0 28 32 1.0 29 30 2.0 44 1.0 30 31 1.0 33 1.0 31 32 2.0 34 1.0 32 35 1.0 33 34 35 36 37 2.0 40 1.0 37 38 1.0 41 1.0 38 39 2.0 42 1.0 39 43 1.0 40 41 42 43 44 45	25 27 1.0 26 27 28 29 1.0 29 33 1.0 30 31 2.0 43 1.0 31 32 1.0 44 1.0 32 33 2.0 34 1.0 33 35 1.0 34 35 36 37 2.0 40 1.0 37 38 1.0 45 1.0 38 39 2.0 41 1.0 39 42 1.0 40 41 42 43 44 46 3.0 45 47 3.0 46 47	25 27 1.0 26 27 28 29 1.0 29 33 1.0 30 31 2.0 43 1.0 31 32 1.0 45 1.0 32 33 2.0 34 1.0 33 35 1.0 34 35 36 37 2.0 40 1.0 37 38 1.0 44 1.0 38 39 2.0 41 1.0 39 42 1.0 40 41 42 43 44 47 1.0 45 46 1.0 46 48 1.0 49 1.0 50 1.0 47 51 1.0 52 1.0 53 1.0 48 49 50 51 52 53
7da	**7ea**	**7ec**	**7ed**	**7fa**
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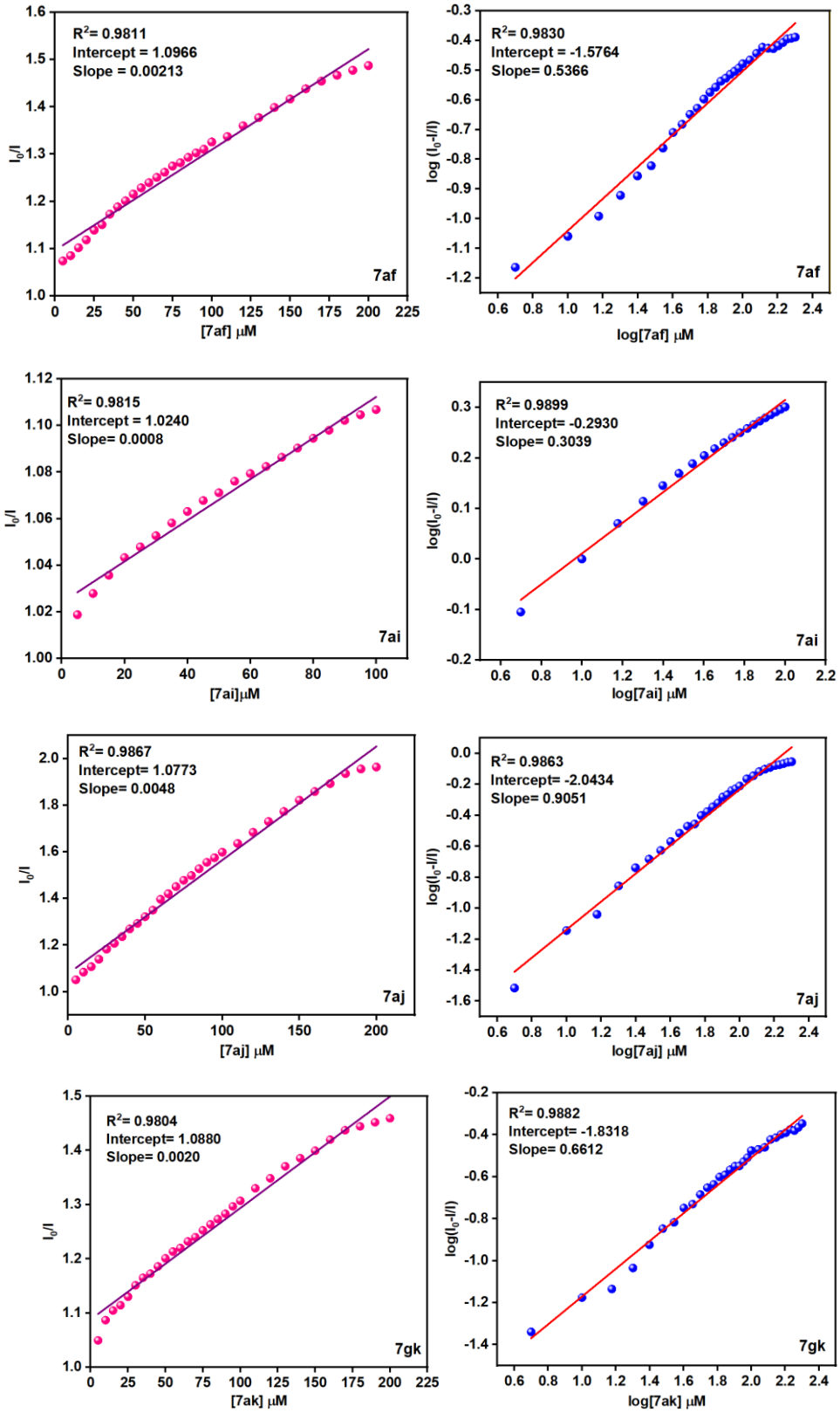

Fig. S119 Plot of I_0/I vs. concentrations of compounds; Scatchard plot of log ($[I_0-I]/I$) vs. log [compound] for BSA in the presence of selected ligands.

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