

Supplementary information

For

Exploring Anticancer Activity and DNA Binding of Metal(II) Salicylaldehyde Schiff Base Complexes: A Convergence of Experimental and Computational Perspectives

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1.0. Experimental

1.1. Reagents and instruments

The chemical materials and reagents employed in this study were procured from Merck Life Sciences (Pty) Ltd and were utilized without pre-purification. These included salicylaldehyde, 2-amino-5-methylbenzonitrile, palladium acetate, copper(II) acetate, nickel(II) acetate, cobalt(II) chloride hexahydrate, and palladium(II) acetate. To characterize and elucidate the structures of the synthesized compounds, various spectroscopic techniques were employed, including ¹H and ¹³C NMR, FTIR, UV-Vis, single crystal X-ray diffraction, mass spectrometry, and CHN elemental analysis.

1.2. Synthesis of the ligand and its complexes

1.2.1. Synthesis of the ligand (HL)

The ligand was synthesized following established protocols [1]. In brief, a 20 mL methanol solution containing salicylaldehyde (1.00 g, 8.19 mmol, 1 eq) was combined with a 20 mL methanolic solution of 2-amino-5-methylbenzonitrile (1.08 g, 8.19 mmol, 1 eq), with the addition of three drops of formic acid. The

mixture was stirred at room temperature for 3 hours, leading to the formation of a precipitate. The resulting solid was filtered, washed with ether, dried, and subjected to recrystallization in dichloromethane for purification. (**Scheme 1**) [1, 2]. Yield: 1.53 g (76.3 %); m.p. 93 °C; ^1H NMR (500 MHz, $\text{DMSO}-d_6$): δ = 12.46 (s, 1H, OH), 9.10 (s, 1H, HC=N), 7.72 (t, 2H, J = 8.50 Hz, Ar-H), 7.68 (t, 1H, J = 8.0 Hz, Ar-H), 7.61 (d, 1H, J = 8.0 Hz, Ar-H), 7.49-7.45 (m, 1H, J = 8.5 Hz, Ar-H), 7.03-6.99 (m, 2H, J = 7.5 Hz, Ar-H), 2.37 (s, 3H, CH_3); ^{13}C NMR (125 MHz, $\text{DMSO}-d_6$): δ = 164.8, 160.2, 148.2, 137.3, 135.1, 134.1, 133.0, 132.7, 119.3, 119.0, 118.4, 117.0, 116.7, 107.7: (Ar-C), 20.0 (CH_3); IR_{ATR} : $\nu_{\text{max}}/\text{cm}^{-1}$: 3200, 2224, 1645, 1340, 947, 750 cm^{-1} ; UV (DMSO, 10^{-3} M): 215, and 308 nm; CHN Anal. Calc. for $\text{C}_{15}\text{H}_{12}\text{N}_2\text{O}$: C, 76.25; H, 5.12; N, 11.86; Expt.: C, 76.24; H, 5.12; N, 11.85; m/z $[\text{M}+\text{H}]^+$: Calc. for $\text{C}_{15}\text{H}_{12}\text{N}_2\text{O}$ = 237.1023; Found = 237.1149.

1.2.2. Synthesis of the complexes (**C1-C4**)

The solution of HL (0.35 g, 1.5 mmol, 2 eq) in 20 mL of dichloromethane was mixed with one equivalent each of the metal salts: $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ (0.18 g, 0.74 mmol), $\text{Ni}(\text{OAc})_2 \cdot 4\text{H}_2\text{O}$ (0.19 g, 0.74 mmol), $\text{Cu}(\text{OAc})_2$ (0.14 g, 0.74 mmol), and $\text{Pd}(\text{OAc})_2$ (0.17 g, 0.74 mmol) in 20 mL of methanol, respectively. The four solutions were refluxed for six hours. For those that precipitate out, the precipitate was filtered, washed with methanol (10×2 mL) and ether (10×2 mL) and in the absence of precipitate, the solution was concentrated (using rotary evaporator) to obtain the complexes (**C1-C4**). The crude solid products were re-crystallized by slow vapor diffusion of hexane into dichloromethane with **C1**, **C3**, and **C4** providing crystals suitable for single crystal X-ray diffraction analyses. Complex of Co^{2+} yielded micro-crystalline material[1]. The reaction procedure is illustrated in **Scheme 1**.

C1

Greenish solid, Yield: 69%; m.p. 263–266 °C; ^1H NMR (500 MHz, $\text{DMSO}-d_6$): δ = 9.07 (s, 1H, HC=N), 7.70 (d, 2H, J = 8.5 Hz, Ar-H), 7.59 (d, 2H, J = 8.0 Hz, Ar-H), 7.13 (t, 1H, J = 7.5 Hz, Ar-H), 6.68 (d, 2H, J = 6.5 Hz, Ar-H), 2.34 (s, 3H, CH_3); ^{13}C NMR (125 MHz, $\text{DMSO}-d_6$): δ = 164.2 (HC=N), 159.5, 147.6, 136.7, 134.5, 134.3, 133.5, 132.4, 132.1, 118.7, 117.9, 116.1, 107.1 (Ar-C), 20.0 (CH_3); UV-Vis: (DMSO, 10^{-3} M): 270 ($\pi \rightarrow \pi^*$), 348

($n \rightarrow \pi^*$), 436 (d-d); λ_{max}/nm : IR_{ATR}: ν_{max}/cm^{-1} : 2207, 1583, 1446, 1326, 823, 760, 537, 450 cm^{-1} ; CHN Anal. Calculated for $C_{30}H_{22}N_4NiO_2$: C, 68.09; H, 4.19; N, 10.59; Found: C, 68.04; H, 4.14; N, 10.53; MS-ESI m/z $[M+H]^+$, Calculated for $C_{30}H_{22}N_4NiO_2$ = 532.2306; Found = 532.0946.

C2

Red solid; Yield: 65 %; m.p: 187-192 °C; UV-Vis:(DMSO, $10^{-3}M$): λ_{max}/nm : 233 ($\pi \rightarrow \pi^*$), 348 ($n \rightarrow \pi^*$), 524 (d-d); IR_{ATR}: ν_{max}/cm^{-1} : 2215, 1600, 1458, 1389, 1189, 846, 743, 520, 463; CHN Anal. Calculated for $C_{30}H_{22}CoN_4O_2$; C, 68.06; H, 4.19; N, 10.58; Found: C, 68.05; H, 4.16; N, 10.55; HRMS-ESI m/z $[M]^+$: calculated for $C_{30}H_{22}CoN_4O_2$ = 529.1075; Found = 529.1086.

C3

Brown solid; Yield: 70%; m.p: 270-275 °C; UV-Vis:(DMSO, $10^{-3}M$): λ_{max}/nm : 245 ($\pi \rightarrow \pi^*$), 290 ($n \rightarrow \pi^*$), 425 (d-d); IR_{ATR}: ν_{max}/cm^{-1} : 2210, 1600, 1435, 1326, 1189, 846, 743, 510, 453; CHN Anal. Calculated for $C_{30}H_{22}CuN_4O_2$; C, 67.47; H, 4.15; N, 10.49; Found: C, 67.45; H, 4.13; N, 10.45; HRMS-ESI m/z $[M+Na]^+$: calculated for $C_{30}H_{22}CuN_4O_2$ = 557.0570; Found = 557.2946.

C4

Yellow solid, Yield: 66%; m.p. 293–296 °C; ^1H NMR (500 MHz, DMSO- d_6): δ = 8.19 (s, 1H, HC=N), 7.73 (s, 1H, Ar-H), 7.59 (d, 1H, J = 8.0 Hz, Ar-H), 7.45-7.41 (m, 2H, J = 8.0 Hz, Ar-H), 7.23 (t, 1H, J = 7.5 Hz, Ar-H), 6.56 (t, 1H, J = 7.5 Hz, Ar-H), 5.94 (d, 1H, J = 8.5 Hz, Ar-H), 2.42 (s, 3H, CH₃); ^{13}C NMR (125 MHz, DMSO- d_6): δ = 165.2 (HC=N), 164.4, 148.5, 137.1, 136.1, 135.7, 134.1, 131.1, 125.7, 119.8, 117.9, 119.7, 117.1, 115.3, 108.8 (Ar-C), 20.2 (CH₃); UV-Vis:(DMSO, $10^{-3}M$): 232 ($\pi \rightarrow \pi^*$), 291 ($n \rightarrow \pi^*$), 421 (d-d); λ_{max}/nm : IR_{ATR}: ν_{max}/cm^{-1} : 2227, 1566, 1377, 1183, 823, 749, 503, 405 cm^{-1} ; CHN Anal. Calculated for $C_{30}H_{22}N_4O_2Pd$: C, 62.45; H, 3.84; N, 9.71; Found: C, 62.38; H, 3.79; N, 9.68; MS-ESI m/z $[M+H]^+$, Calculated for $C_{30}H_{22}N_4O_2Pd$ = 577.0856; Found = 577.0896.

2.0. Biological evaluation

2.1. Stability study in aqueous buffer

Analysis of the stability of the four transition metal complexes (**C1–C4** and the free ligand **HL**), **C1**, **C3** and **C4** were dissolved in 10% DMF–KH₂PO₄ (50 mM, pH 7.5), while **C2** and **HL** were dissolved in 10% DMF (50 mM, pH 7.5) and their spectra was monitored as a function of time with a spectral acquisition of 250–750 nm. The spectra were recorded using Analytik Jena Specord210 Plus double-beam instrument fitted with an external water circulating thermostatic bath and thermostat cell holders

2.2.Cyto-toxicity study

2.2.1. MTT assay

The effect of the compounds on tumor cell viability was evaluated using MCF-7 breast cancer cells grown in a culture medium supplemented with 10% Fetal Bovine Serum (FBS) and penicillin-streptomycin solution (1%). The cells were first seeded at 7,000 cells/well into 96-well plates. After 24 h incubation at 5% CO₂ and 37°C, the cells were treated with 5 - 80 mM concentration of the compounds in 200 mL final media volume. After 48 hrs incubation with the treatments, the spent media was aspirated before adding 100 µL of 5 g/mL MTT in serum-free media. After 5 hrs incubation at room temperature, the solution in each well was removed, and 100 µL of dimethyl sulfoxide was added to solubilize the cells. Subsequently, the absorbance of the resulting-colored solution was estimated at 540 nm[2].

2.2.2. Lactate dehydrogenase (LDH) release assay

This assay, which measures the concentration of lactate dehydrogenase enzyme released from dead cells, was measured using a Promega (G179A) non-radioactive CytoTox 96® assay kit. The culture medium containing the cell samples treated with the various compounds was aspirated and centrifuged at 4000 r/min for 5 min. Then, 0.1 mL of the supernatant was transferred to a 96-well plate before incubation with 0.1 mL of the restituted mixture supplied with the kit for 25 min in the dark at 25 °C. The absorbance of the coloured solution generated was read at 450 nm in a spectrophotometer[3].

2.2.3. Adenosine triphosphate (ATP) production assay

This assay, which determines the amount of ATP produced from living cells, was done using the CellTiter-Glo[®] ATP reagent kit. Cells were seeded at the initial density and incubated with the treatment for 48 hrs. After removing the spent media, each culture well was washed twice with 1X phosphate buffer saline solution. Then, the detached cells were incubated with 50 μ L of the ATP reagent and incubated in the dark for 30 min at room temperature in an opaque black plate. Subsequently, the ATP luminescence of the live cells was measured in a Modulus Microplate Luminometer (Turner BioSystems, USA)[4].

2.2.4. The cell imaging method

Image analysis of cells in the various experimental groups was done using a Wirsam Olympus inverted light microscope (CKX 41) with an attached Olympus C5060-ADUS digital camera. Before the visualization procedure, cells or media debris in the cell-cultured plates were washed in phenol red-free HBSS. Subsequently, the camera's user interface was accessed on a computer with an installed CellSens imaging analysis software (V1.16), which was employed to capture possible cellular alteration images of the various experimental groups at 400 X magnification. Then, the imaging results were saved to the computer memory in TIFF image format[5,6].

2.3. Biophysical study

2.3.1. Materials and Methods

Materials

All solvents (HPLC grade) and chemical synthons were used as received from Merck Sigma-Aldrich[®] without further purification. All buffer salts were purchased without any further purification from Merck Sigma-Aldrich[®]. Ultrapure water (Type I) was produced using a Merck-Millipore Direct-Q[®] 3 UV Water Purification System.

2.3.2. DNA binding studies

Stock solution of calf thymus DNA (ctDNA) was prepared by dissolving the sodium salt (Sigma-Aldrich) in potassium phosphate buffer (pH 7.5, 50 mM) and slowly agitating it overnight at 140 rpm. The

concentration of the solution was determined spectrophotometrically ($\epsilon=13\,200\text{ M}^{-1}\text{ cm}^{-1}$ at 260 nm). In brief **C2** was prepared in phosphate buffer (10% acetonitrile, 50 mM and pH 7.5) and diluted to a concentration of $\pm 50\text{ }\mu\text{M}$. Increasing concentrations of ctDNA was added to **C2** that was incubated at 37°C and the absorbance spectra was recorded from 200 – 600 nm using a PerkinElmer Lambda 365 double beam spectrometer connected to a Peltier controller and multicell thermostatic cell block. Measurements were carried out in triplicates using 1.0 cm quartz cuvettes. **C2** absorption maxima was monitored at 305 nm, and spectral changes at 305 nm would indicate the interaction of the **C2** with ctDNA.

2.3.3. Linear dichroism

Linear dichroism (LD) measurements were performed on a Jasco-1500 magnetic circular dichroism spectropolarimeter, converted for LD, and equipped with an IBM PC and a Jasco J interface. Linear dichroism was defined as:

$$LD(\lambda) = A_{//}(\lambda) - A_{\perp}(\lambda) \quad (1)$$

$A_{//}$ and $A_{\perp}$ are defined as the absorbances of the sample when polarized light was oriented either parallel or perpendicular to the flow direction. The orientation was produced by a Couette cell that rotated at a shear gradient of $\pm 1000\text{ rpm}$. Each spectrum was accumulated in triplicates from 200 – 600 nm and recorded at 37°C **C2** ranged from 0–300 μM and ctDNA concentration used was at 100 μM .

2.3.4. DNA Circular dichroism

Circular dichroism (CD) measurements were performed on a Jasco-1500 magnetic circular dichroism spectropolarimeter. Measurements were carried out in triplicates using 1.0 cm quartz cuvettes. ctDNA concentration was used at 100 μM and each spectrum was accumulated in triplicates from 200 – 600 nm and recorded at 37 °C **C2** ranged from 0–300 μM .

Molecular docking and dynamics

Molecular dynamic simulations and XP docking were performed in manner similarly described previously [7,8]. Detailed methodologies are described below.

2.3.5. Ligand preparation

The cobalt metal complex used for docking was first optimized with DFT at the CAM-B3LYP/LANL2DZ level of theory to determine the likely coordination geometry at the metal centre and ligand conformation. The optimized DFT structures were then prepared for using the OPLS2005 force field with standard parameters for LigPrep (LigPrep, Schrödinger, LLC, New York, NY, USA, 2021) to generate files associated with Schrödinger. The force field used in this study did not include parameters for the metal chelates under investigation. As a result, zero-order bonds were applied between the metal ion and the organic ligand framework. This approach allows the force field to handle the metal-ligand interactions through parameterized electrostatic forces, disregarding the covalent nature of these bonds. This simplification is necessary for docking metal complexes using Schrödinger software.

2.3.6. DNA preparation

Two DNA structures PDB:425D (2.80 Å)[9] and PDB: 4E1U (0.92 Å)[10] were retrieved for preparation using the Protein Preparation Wizard [11] within the Schrödinger Suite 2022–4. The structures contain co-crystallised water molecules and/or ligands. The DNA was selected, inverted, and all other components of the crystal were deleted, leaving only a single DNA macromolecule. All DNA structures were pre-processed at pH 7.4 using Epik [12] to generate heteroatom ionization states. The missing terminal phosphate backbones were then added in Maestro. Hydrogen-bond assignment was optimized at pH 7.4, followed by restrained minimization using the OPLS2005[13] force field, with heavy atoms converging to a root-mean-square deviation (RMSD) of 0.30 Å. PDB:425D is well-suited for generating groove-binding poses, while PDB:4E1U is ideal for generating intercalated docking poses.

2.3.7. Ligand docking.

The prepared cobalt metal complex was docked into the DNA using Glide[14] to identify potential binding sites for the metal chelate on DNA. The receptor grid was centred on nucleobases near the centre of the

DNA strand, with dimensions of $40 \times 40 \times 40 \text{ \AA}^3$, ensuring that the entire DNA was sampled for potential binding sites. Extra precision (XP) [15] docking was then employed to generate binding poses on the DNA.

2.3.8. Molecular dynamics.

Molecular dynamics (MD) simulations were conducted on the best-docked DNA-ligand complexes using Desmond [16] and the OPLS2005 force field. Prior to simulation, the DNA-ligand complexes were pre-processed, and the System Builder in Desmond was used to solvate the system with TIP3P [17] water molecules. The biomolecular system was placed in an orthorhombic box with a 5 $\text{\AA}$ buffer between the box boundary and the DNA-ligand complex, then neutralized with Na^+ as needed. The simulations were run for 100 ns, with approximately 1000 frames recorded at 100 ps intervals. Before starting the simulation, the system was relaxed and equilibrated under the NPT ensemble[18] at 310 K and 1.01 bar. The resulting trajectories were analyzed using Maestro.

2.4. Density Functional Theory (DFT) Analysis

Simulations were performed to calculate optimized structures, vibrational frequencies, and electronic spectra for **C1–C4**, and free ligand (**HL**) species using Gaussian 16 Rev C.01[19] at the CAM-B3LYP[20]/DEF2-QZVP[21] level of theory using the GD3BJ empirical dispersion correction.[22] Structures were also calculated using the SDD basis set.[23] The default geometry convergence criteria in Gaussian 16 were applied. GaussView 6.0.16[24] was used for preparing input files and data visualization. GaussSum 3.0 was used to visualize electronic spectra and tabulate transition assignments.[25] All geometry-optimized structures were characterized by positive frequency eigenvalues, indicating that true minima were located on the global potential energy surface for each system.

Time-dependent DFT (TD-DFT) simulations were carried out using the above method (CAM-B3LYP) and basis sets in Gaussian 16 for all small molecules. Typically, 60 excited singlet states were computed to cover the full spectral range (150–900 nm).

SEM imaging

SEM imaging was performed by methods previously described [26–28].

2.5. Spectra of the ligand (HL) and its complexes (C1-C4)

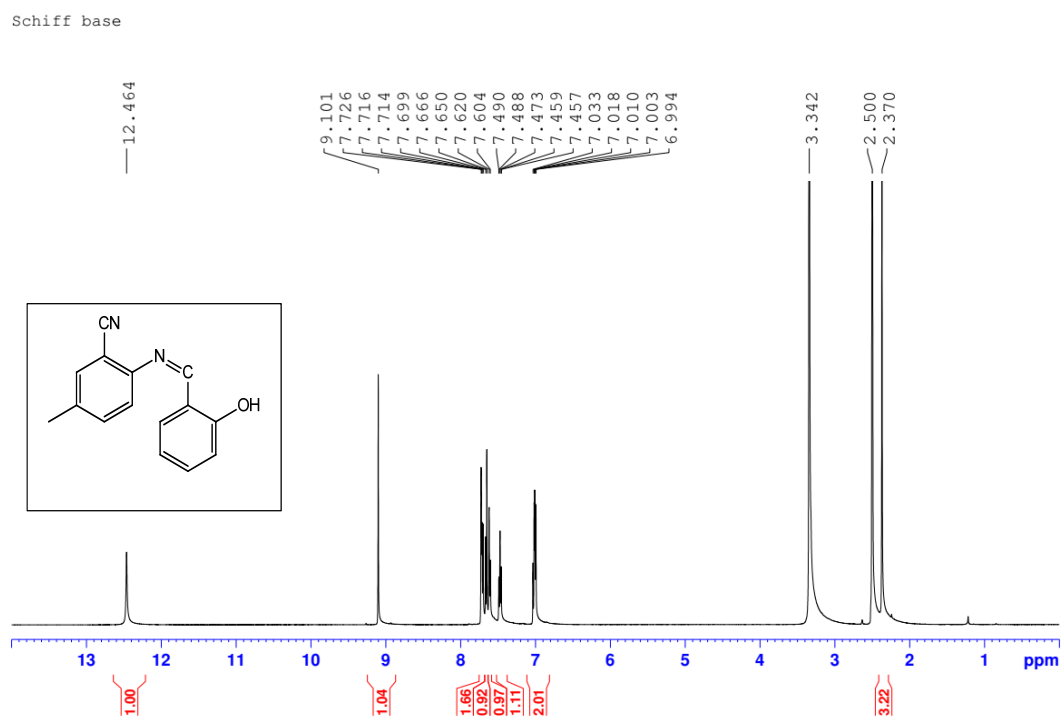


Figure S1: ^1H NMR spectrum of **HL** recorded at room temperature using (500 MHz, $\text{DMSO-}d_6$)

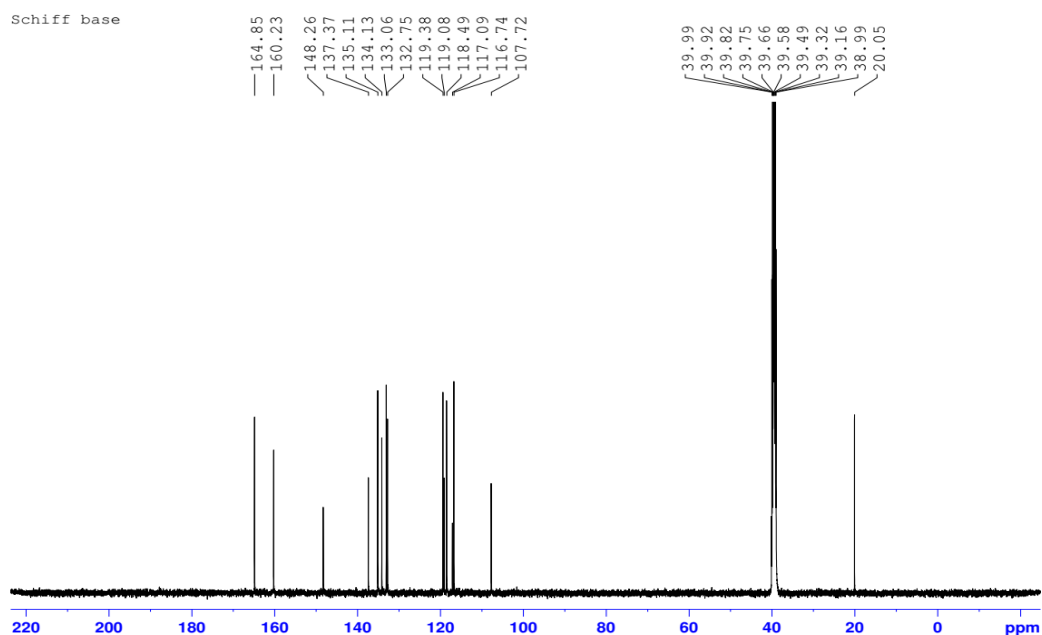


Figure S2: ^{13}C NMR spectrum of **HL** recorded at room temperature using (125 MHz, $\text{DMSO}-d_6$)

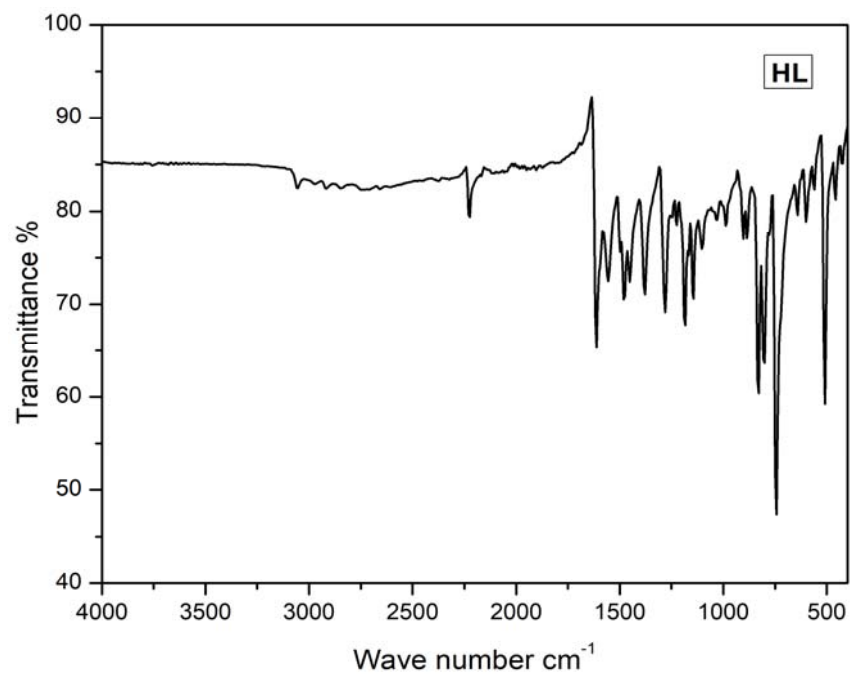


Figure S3: FTIR spectrum of **HL** obtained in solid state at room temperature using ATR method

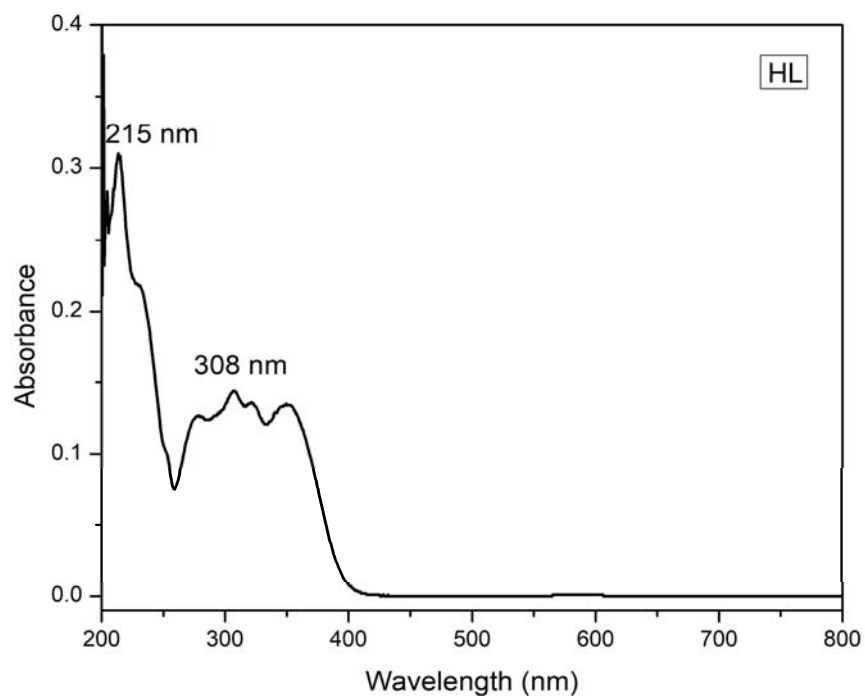


Figure S4: U-Vis spectrum of HL obtained at room temperature using (DMSO, 10^{-3} M)

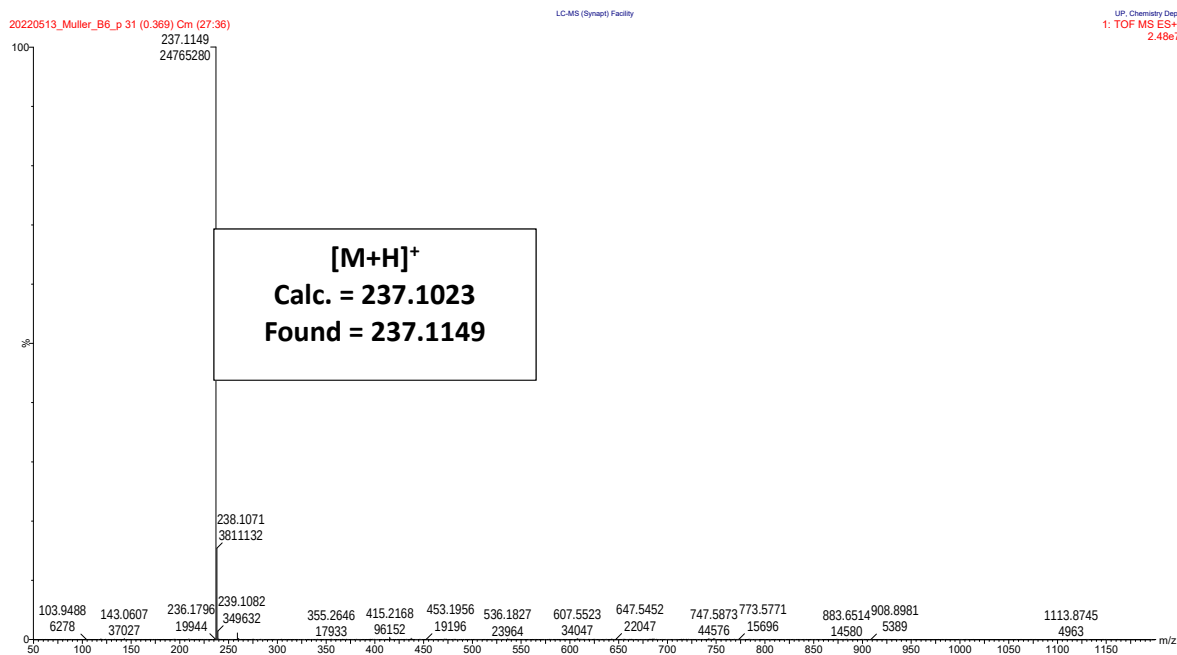


Figure S5: Mass spectrum of HL obtained using high resolution mass spectroscopy (HRMS)

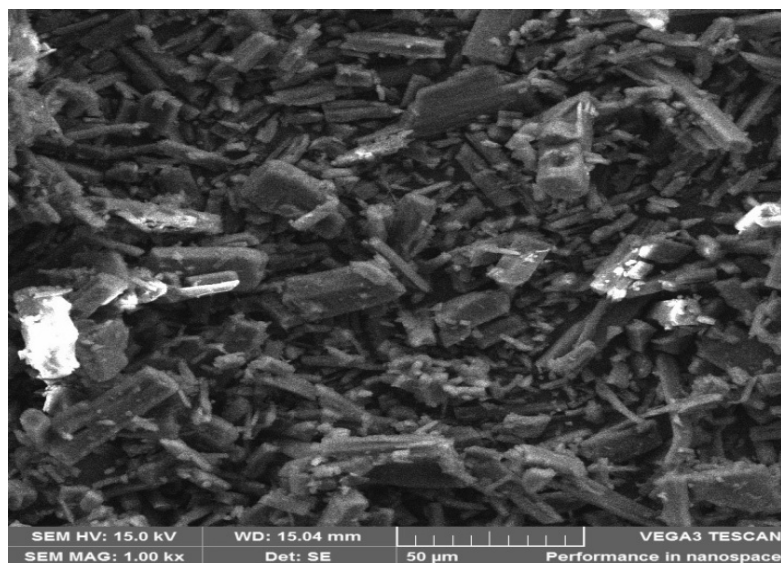


Figure S6: Scanning Electron Microscope (SEM) Image of **HL** shows block-like structures surface morphology in different forms and are well arranged, confirming the crystalline nature of the ligand. This was similar to previously reported structures.

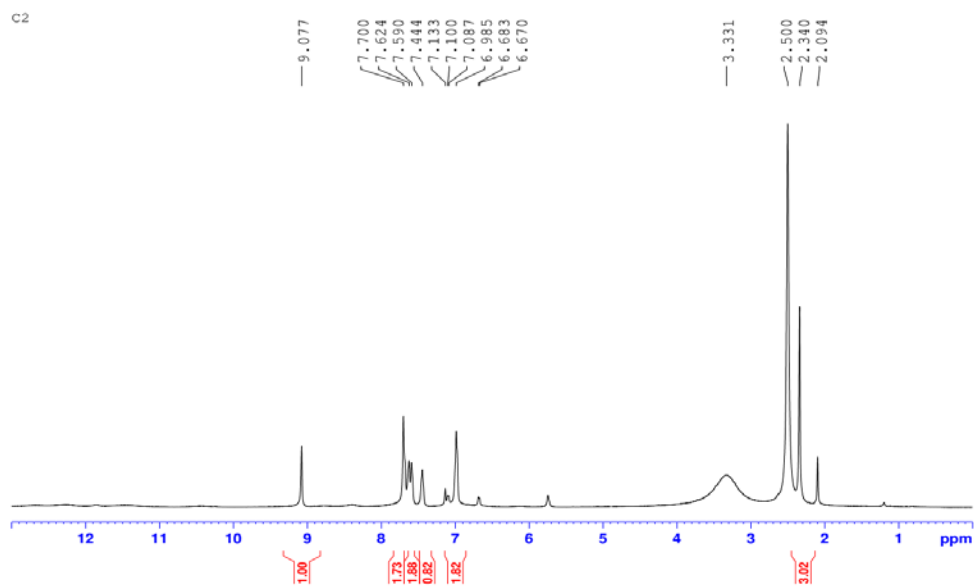


Figure S7: ¹H NMR spectrum of **C1** recorded at room temperature using (500 MHz, DMSO-*d*₆)

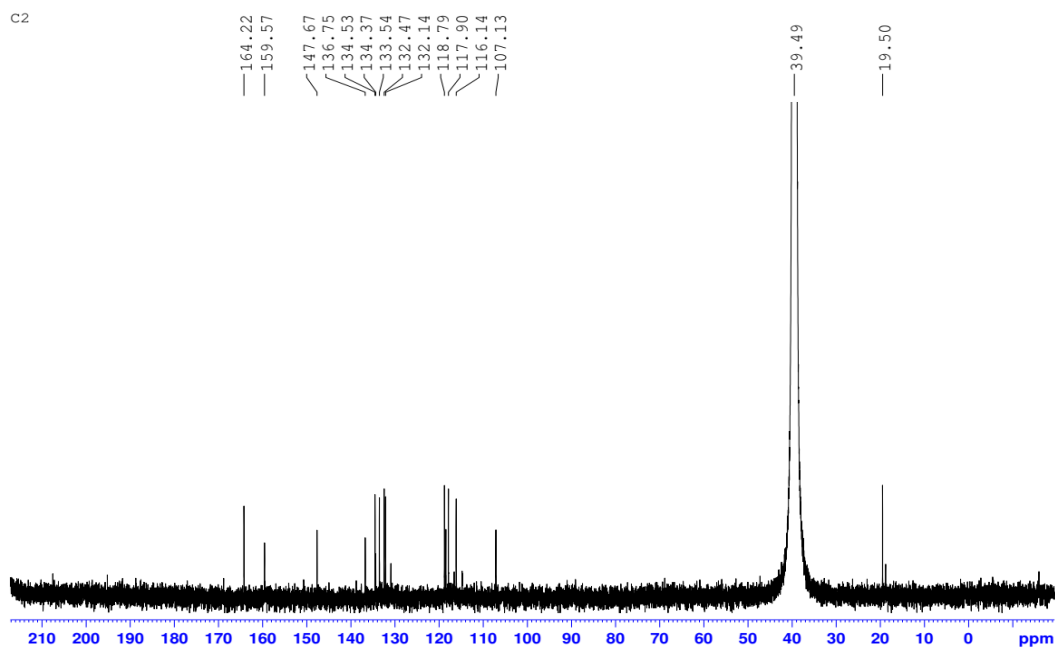


Figure S8: ^{13}C NMR spectrum of **C1** recorded at room temperature using (125 MHz, $\text{DMSO}-d_6$)

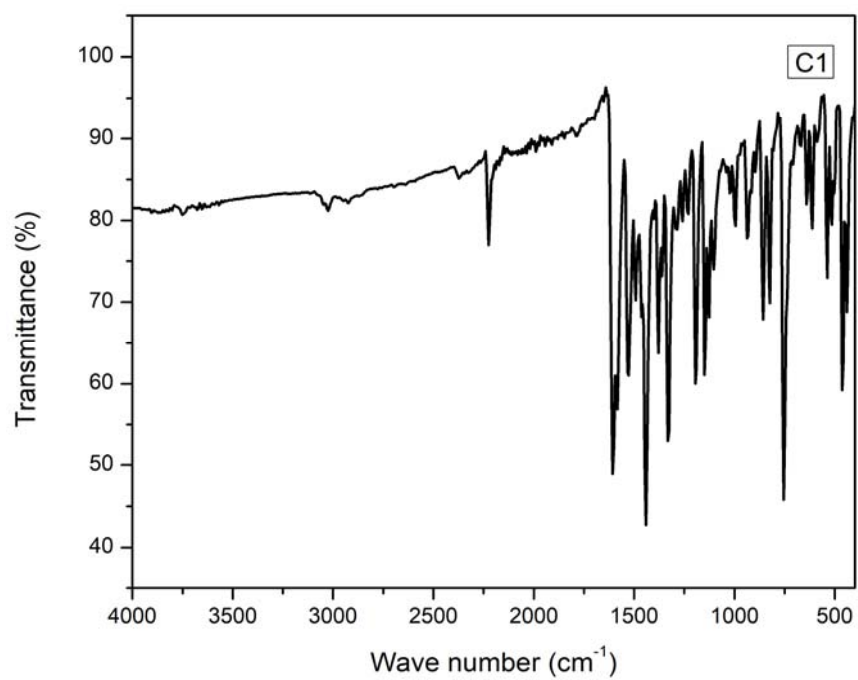


Figure S9: FTIR spectrum of **C1** obtained in solid state at room temperature using ATR method

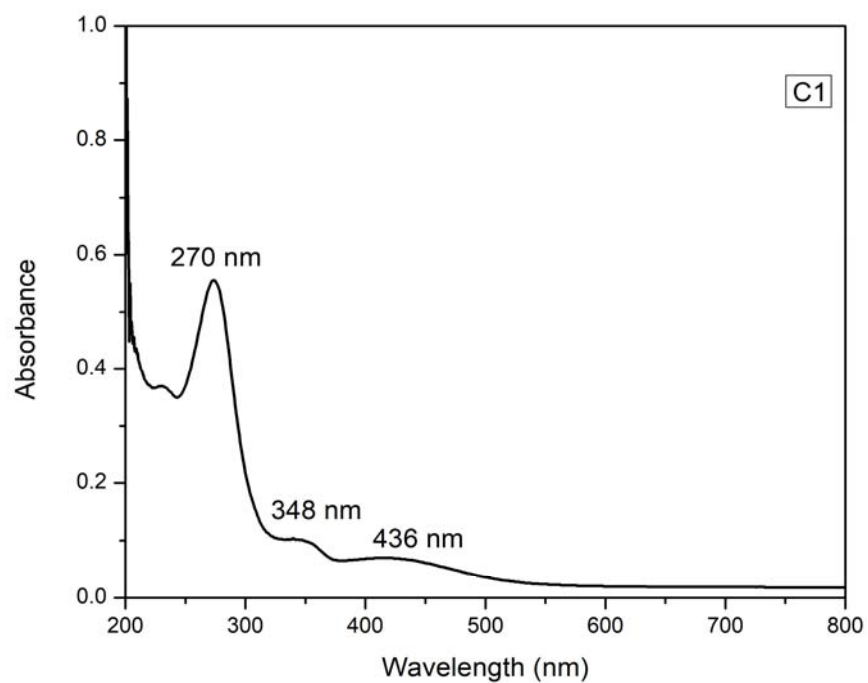


Figure S10: UV-Vis spectrum of **C1** obtained at room temperature using (DMSO, 10^{-3} M).

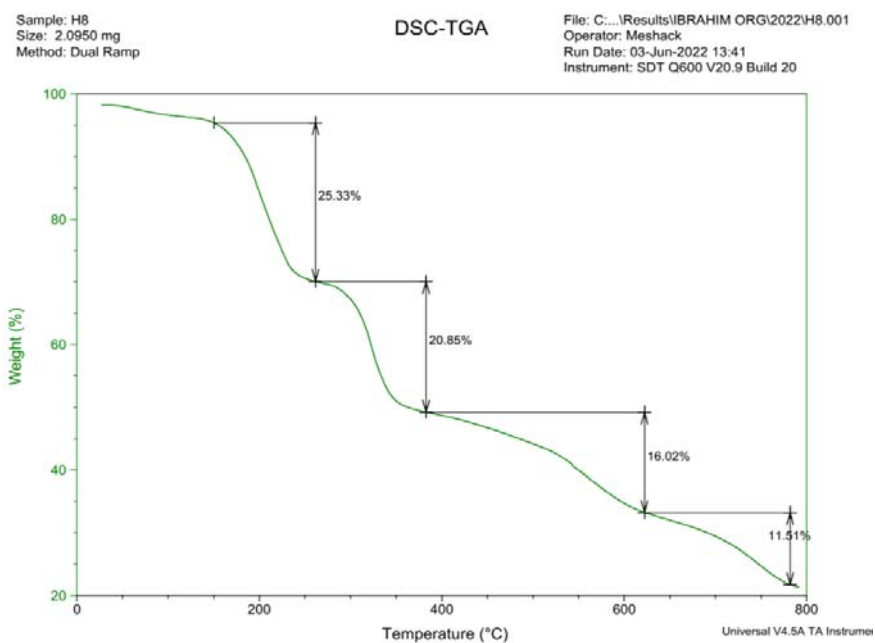


Figure S11: TGA Thermograph of **C1** obtained under inert condition (N_2)

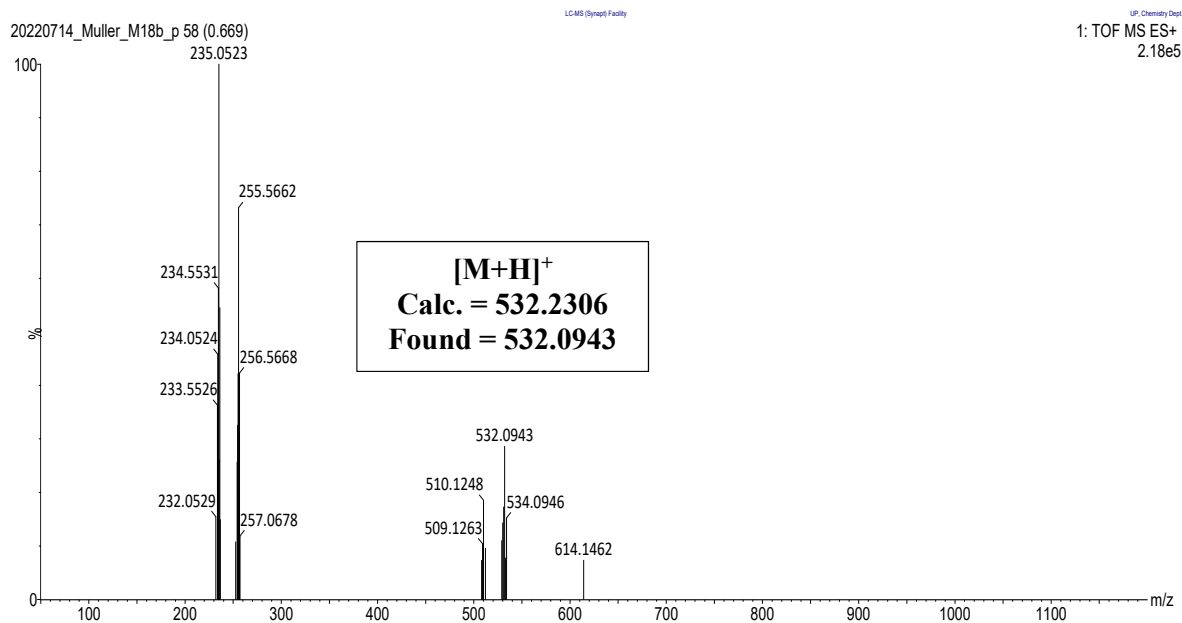


Figure S12: Mass spectrum of **C1** obtained using high resolution mass spectroscopy (HRMS)

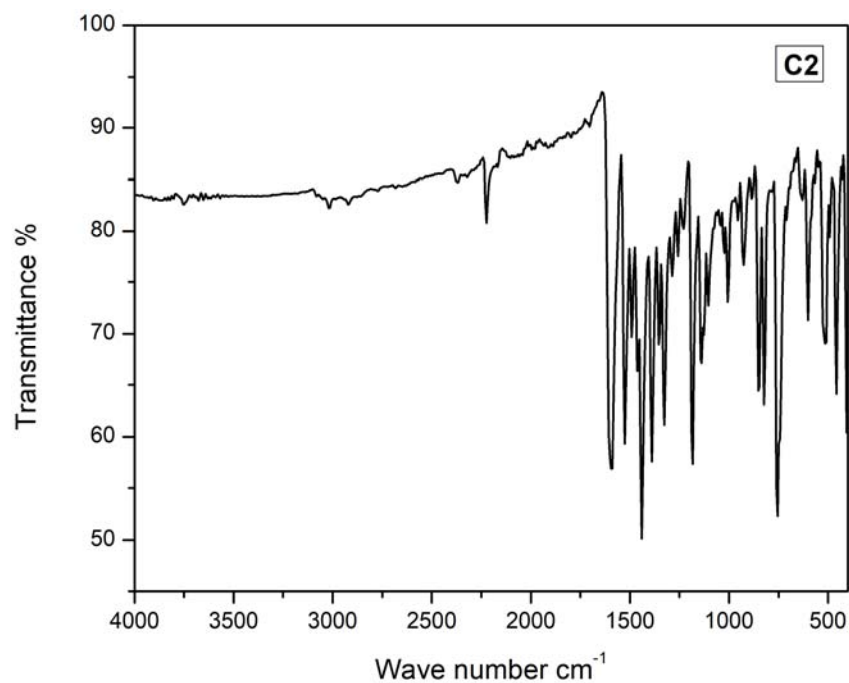


Figure S13: FTIR spectrum of **C2** obtained in solid state at room temperature using ATR method

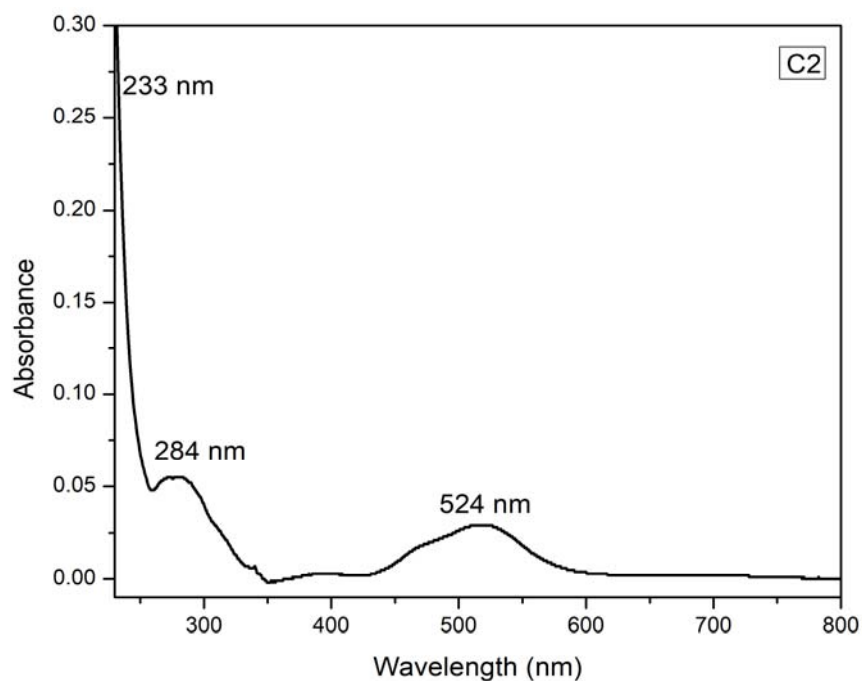


Figure S14: UV-Vis spectrum of **C2** obtained at room temperature using (DMSO, 10^{-3} M)

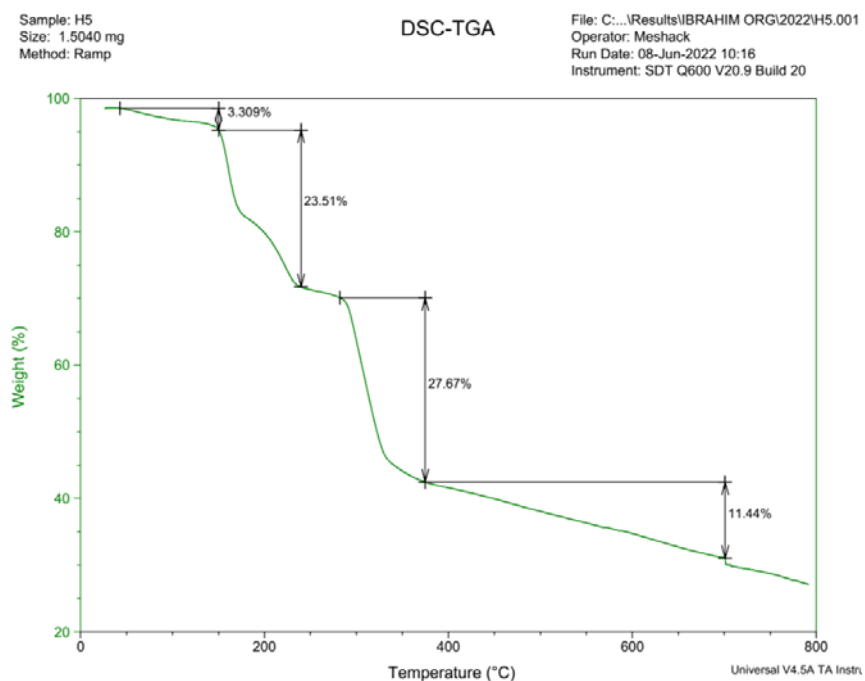


Figure S15: TGA Thermogram of **C2** obtained under inert condition (N_2)

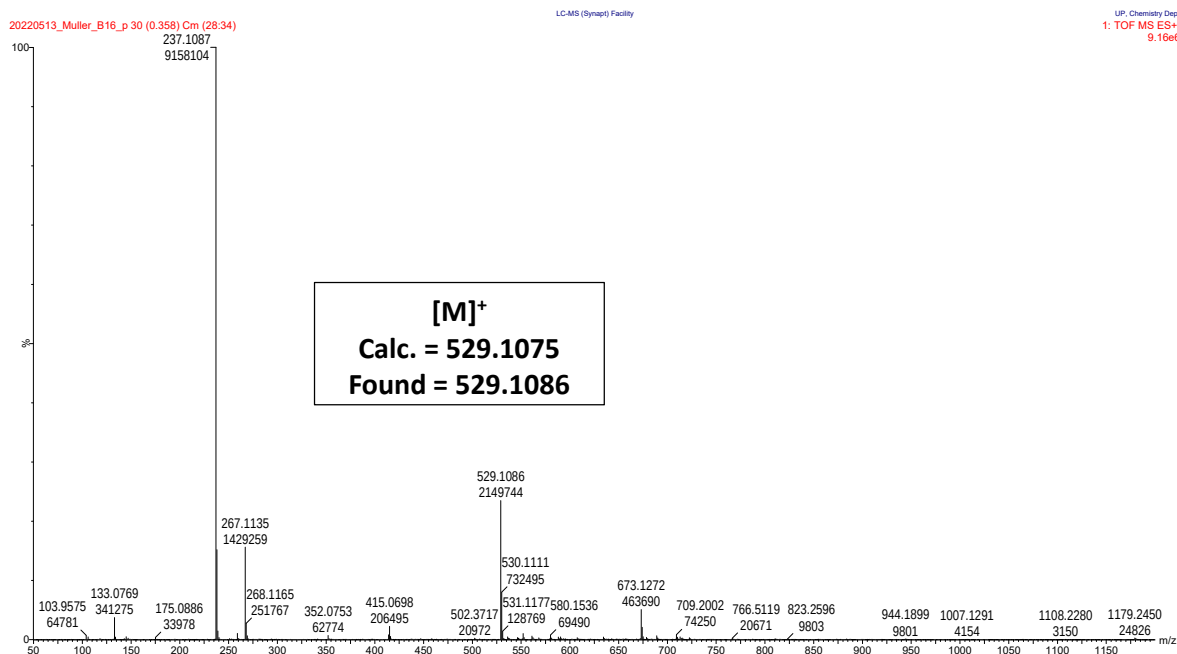


Figure S16: Mass spectrum of **C2** obtained using high resolution mass spectroscopy (HRMS)

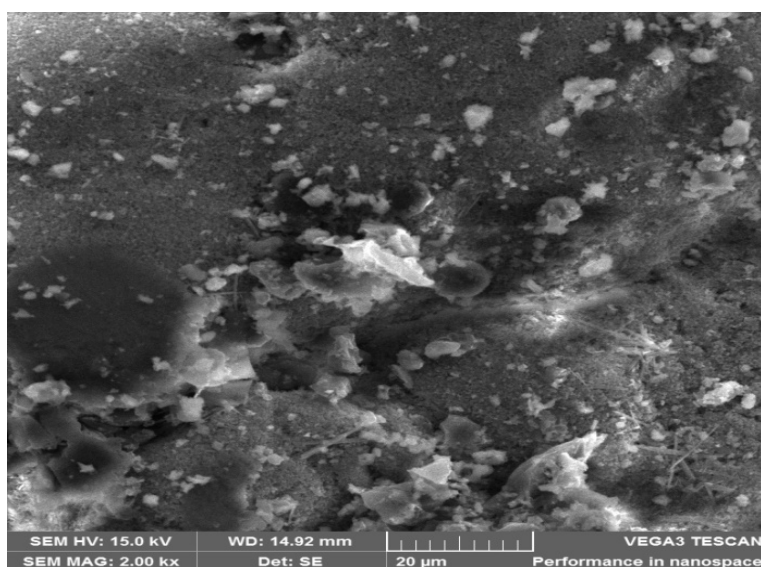


Figure S17: Scanning Electron Microscope (SEM) Image of **C2**. SEM image of the ligand, HL (Figure S6) shows block-like structures surface morphology in different forms and are well arranged, confirming the crystalline nature of the ligand. But the complex's surface morphology here displayed a fine wide surface area with agglomeration of particles of different sizes and shapes scattered over it, indicating the amorphous nature of the complex. This change in the surface morphology of the ligand compared with the C2 herein confirmed the formation of new material (complex).

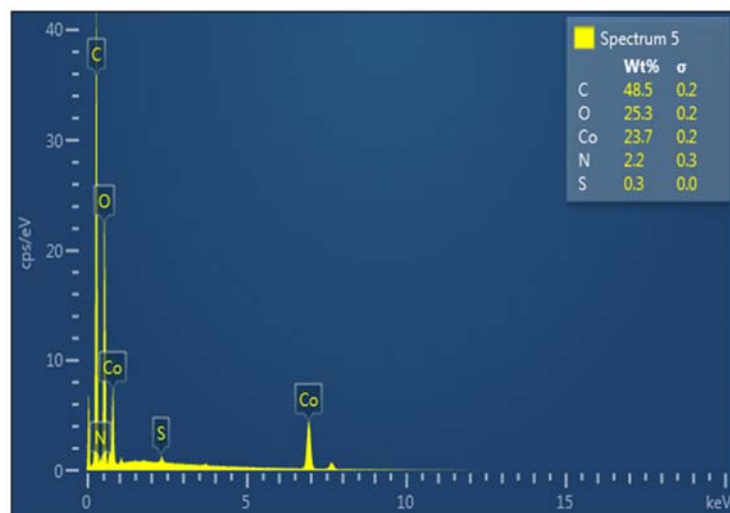


Figure S18: Energy Dispersive X-ray Spectroscopy (EDX) micrograph of **C2** confirming the presence of Co(II) ion in the complex. In addition, carbon, nitrogen and oxygen atoms from the ligand were also confirmed. The presence of these elements within the compound has further affirmed the formation of the complex (**C2**). The trace amount of sulfur (0.3%) could be due to impurity arising from coating of the sample.

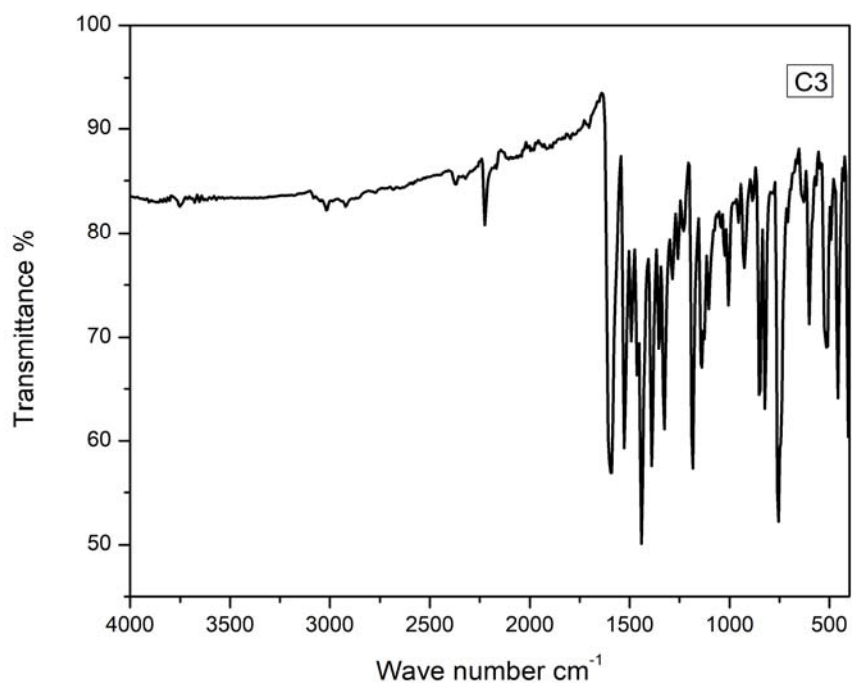


Figure S19: FTIR spectrum of **C3** obtained in solid state at room temperature using ATR method

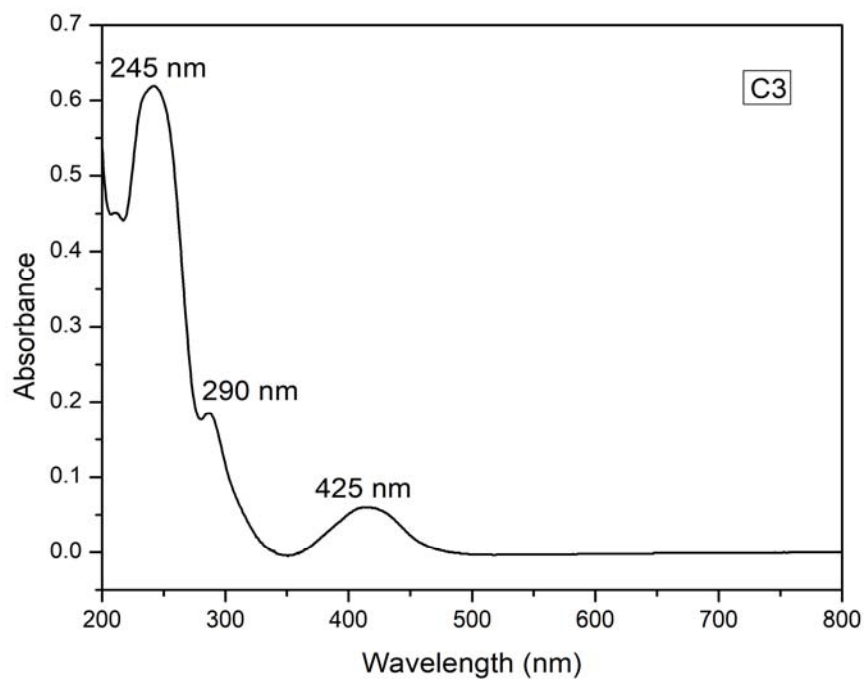


Figure S20: UV-Vis spectrum of **C3** obtained at room temperature using (DMSO, 10^{-3} M)

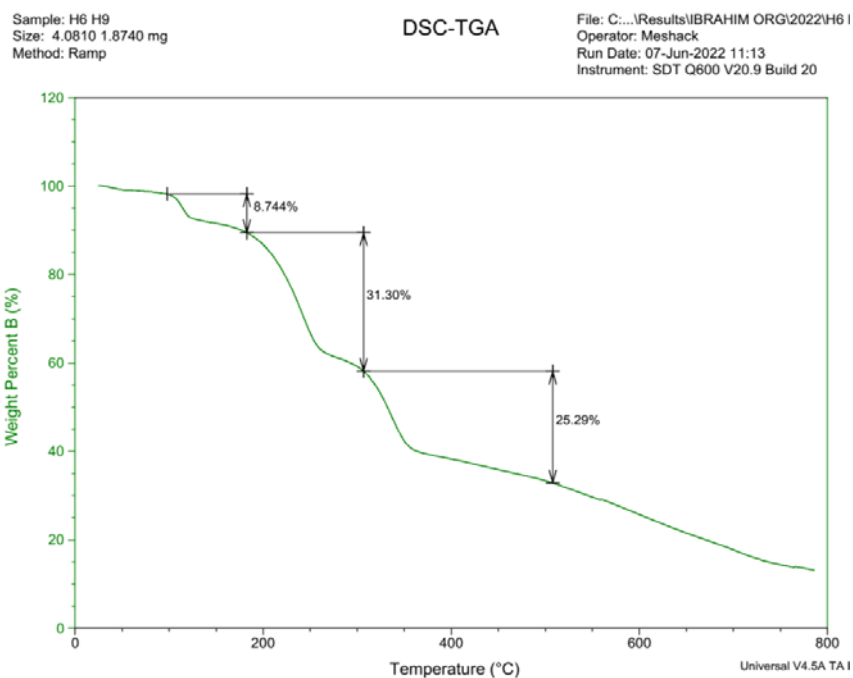


Figure S21: TGA Thermogram of **C3** obtained under inert condition (N_2)

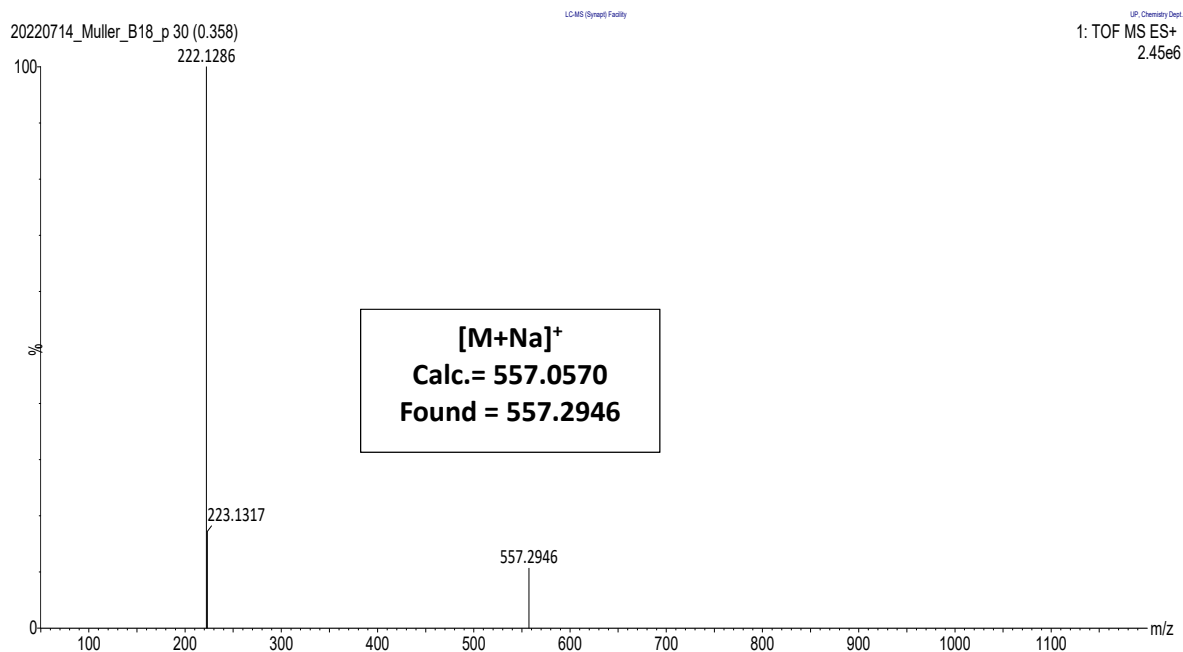


Figure S22: Mass spectrum of **C3** obtained using high resolution mass spectroscopy (HRMS)

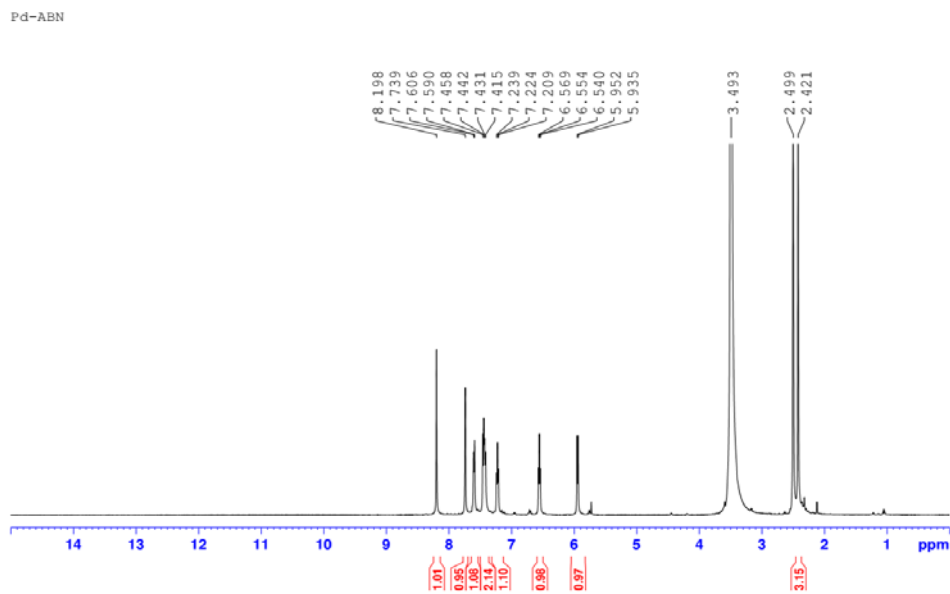


Figure S23: ¹H NMR spectrum of **C4** recorded at room temperature using (500 MHz, DMSO-*d*₆)

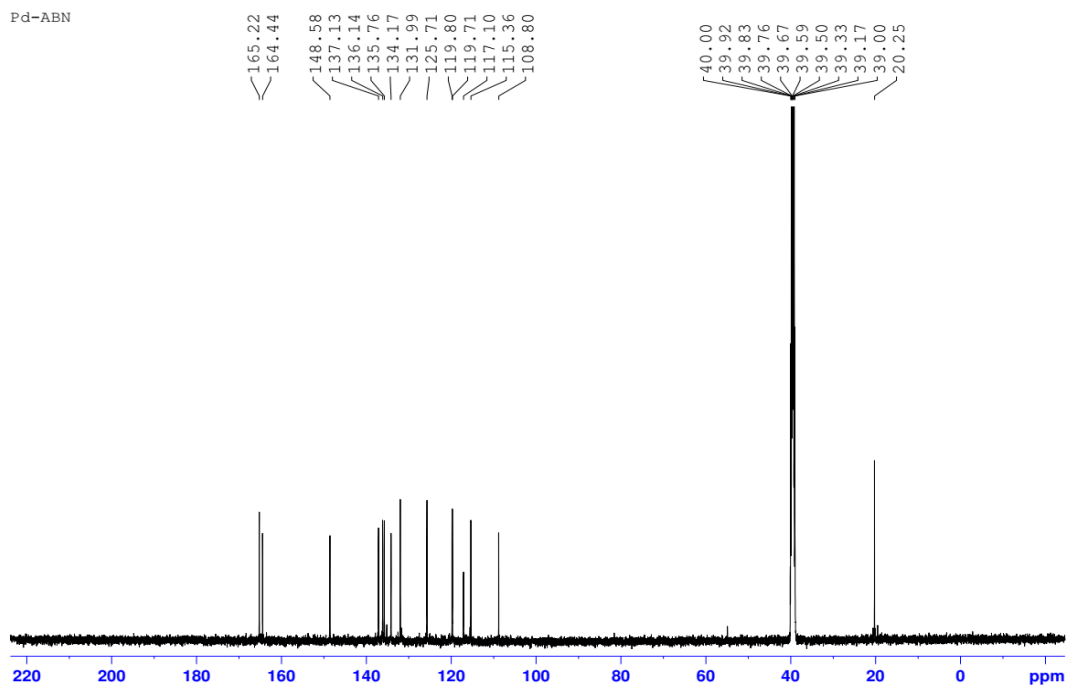


Figure S24: ^1H NMR spectrum of **C4** recorded at room temperature using (125 MHz, $\text{DMSO}-d_6$)

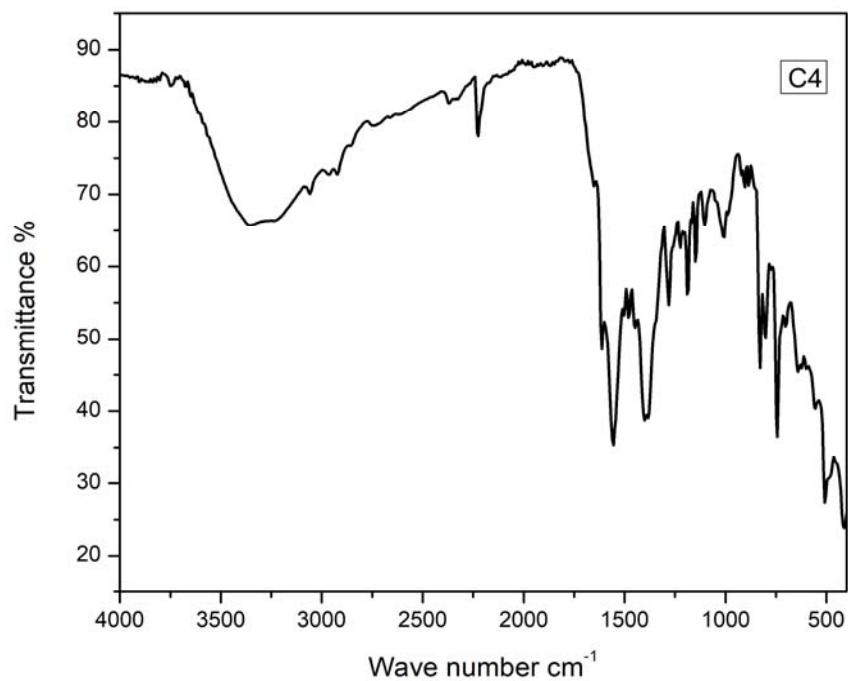


Figure S25: FTIR spectrum of **C4** obtained in solid state at room temperature using ATR method

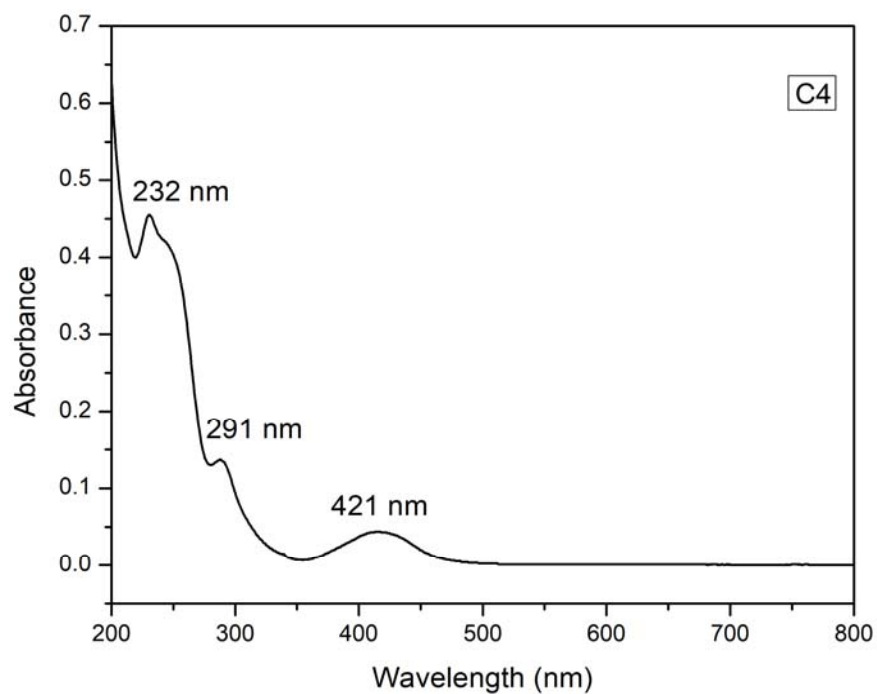


Figure S26: UV-Vis spectrum of **C4** obtained at room temperature using (DMSO, 10^{-3} M)

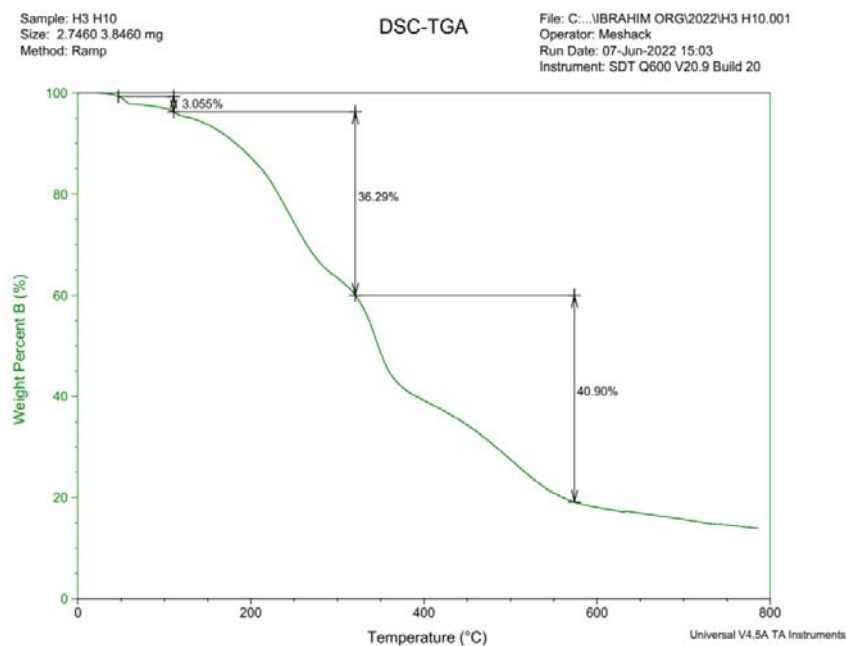


Figure S27: TGA Thermogram of **C4** obtained under inert condition (N_2)

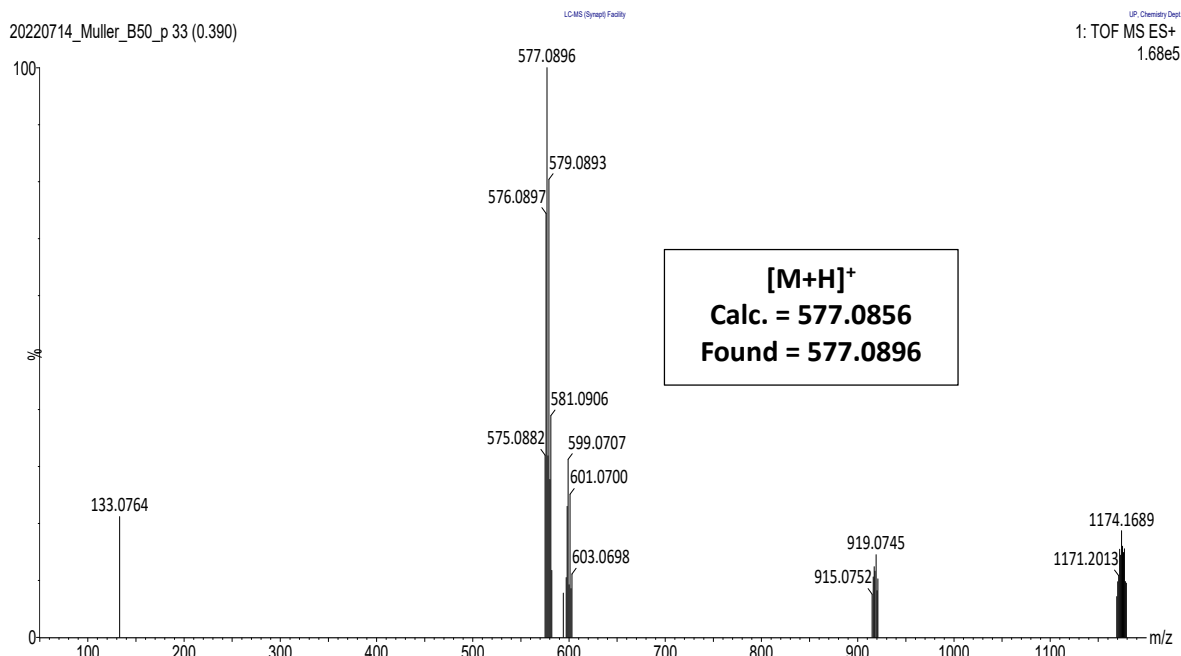


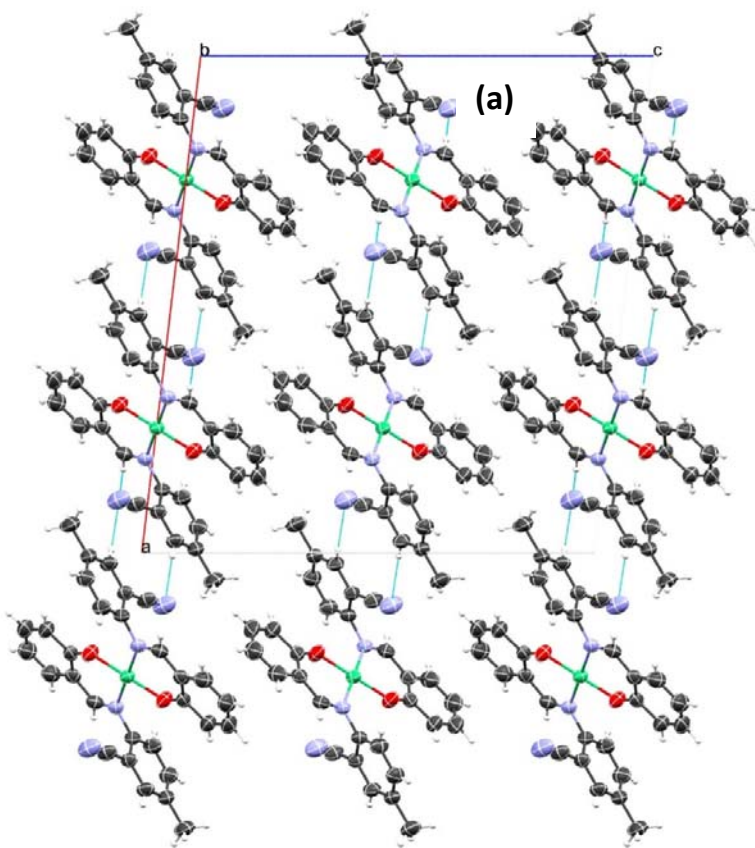
Figure S28: Mass spectrum of **C4** obtained using high resolution mass spectroscopy (HRMS)

Electronic spectroscopy

The electronic spectral analysis of the ligand (**HL**) and its complexes (**C1-C4**) was carried out using DMSO. The individual spectra provided are given alongside with the spectral data for each compound. The ligand exhibited two absorption bands at 215 and 308 nm, which are assignable to $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ transitions, respectively, attributed to the aromatic and azomethine moieties. Similarly, the complexes displayed three absorption bands each, with two in the UV region and one in the visible region. The two bands in the visible region were attributed to the $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ transitions within the ligand system. However, these bands exhibited slight shifts in the complexes due to the perturbation of the ligand's molecular orbitals resulting from metal ion coordination, leading to changes in the absorption bands. The bands in the visible region were observed at 421-524 nm in the spectra of the complexes. These absorption bands are associated with metal-to-ligand charge transfer (MLCT) [29].

Infrared spectroscopy

The FT-IR spectra of **HL**, in comparison to the metal complexes (Figs. S3, 8, 12 and 22), indicated that the vibrational bands either disappeared or shifted. Notably, the C=N bands were observed around 1340-1320 cm^{-1} in the complex spectra, CN bands were found around 2220-2218 cm^{-1} , and C=N bands shifted to 1600-1575 cm^{-1} in the complexes. The shift in azomethine (C=N) vibrational band stretching is attributed to the involvement of the nitrogen atom in coordination, while shifts in other vibrational frequencies result from changes in the ligand's structural orientation due to complexation. The disappearance of the OH band is due to deprotonation, and new bands were observed in the fingerprint region, which are assignable to M-N and M-O bands.



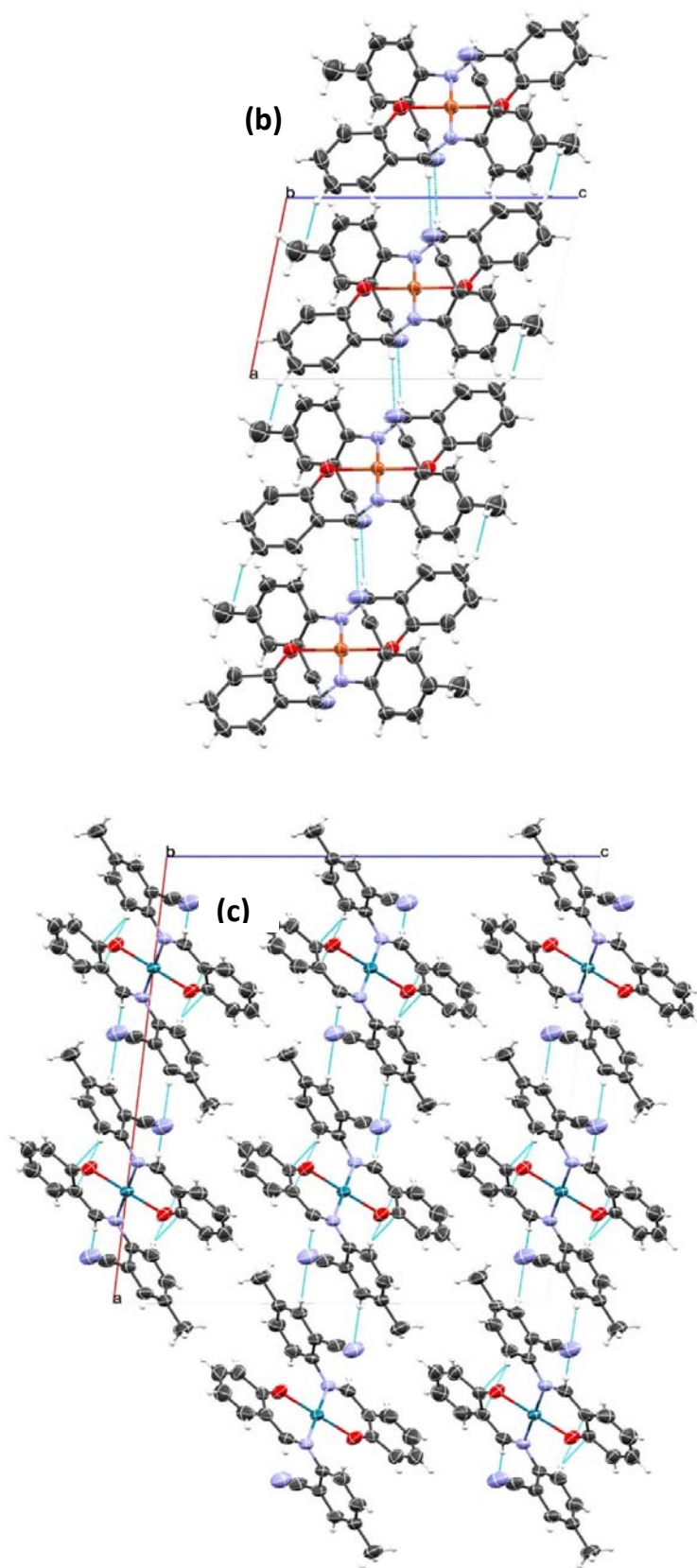


Figure S29: Packing viewed along b axis showing the non-classical hydrogen bonds which contribute to the formation of a three-dimensional supramolecular network; **C1**; (a) **C3**; (b) and **C4**; (c).

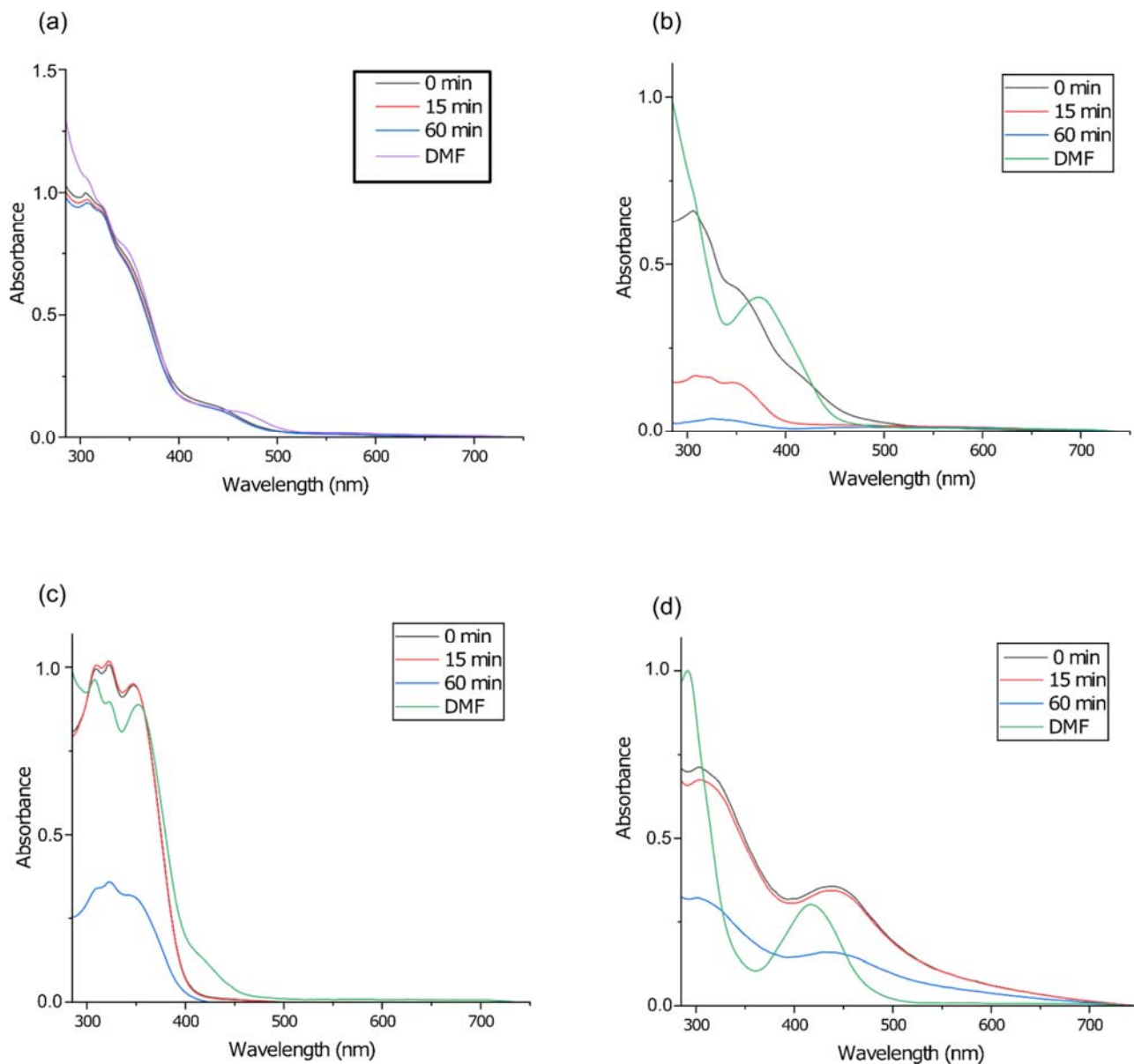
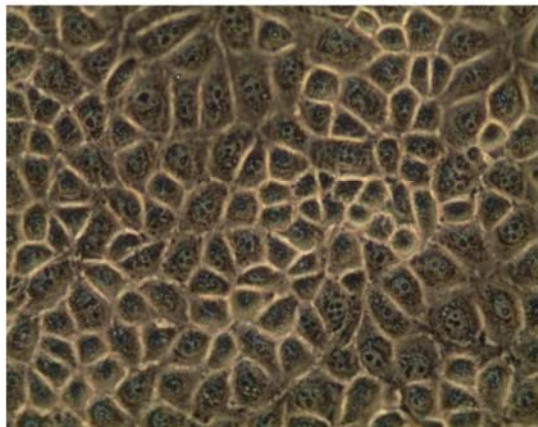
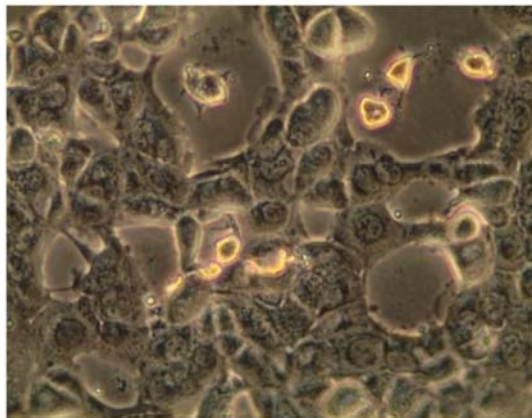


Figure S30: UV-vis spectra of 50 μM solutions of (a) **C2**, (b) **C3**, (c) **C1** and (d) **C4** (bottom) recorded as a function of time in KH_2PO_4 buffer (50 mM pH 7.5). C2 was present with a final concentration of 10% (v/v) acetonitrile, while the other three metal complexes were present with 10% (v/v) DMF. All four metal complexes were dissolved in DMF for a control spectrum to be compared.

(a)



(b)



(c)

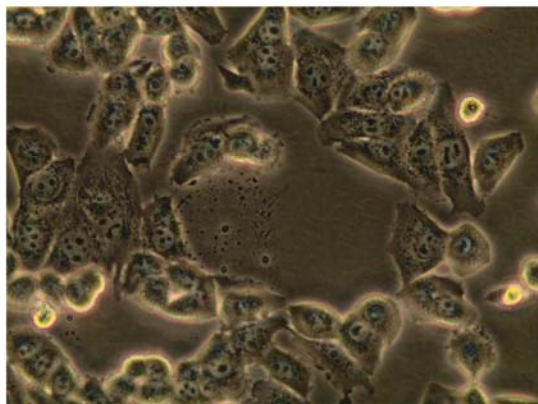


Figure S31:(a) Morphology of MCF-7 cells before treatment of any drug. (b) Morphological changes in MCF-7 cells induced by **HL** (5 μ M). (c) Morphological changes in MCF-7 cells induced by complex **Dox**(5 μ M). Captured using Wirsam Olympus inverted light microscope (CKX 41) equipped with Olympus C5060-ADUS digital camera at $\times 400$ magnification.

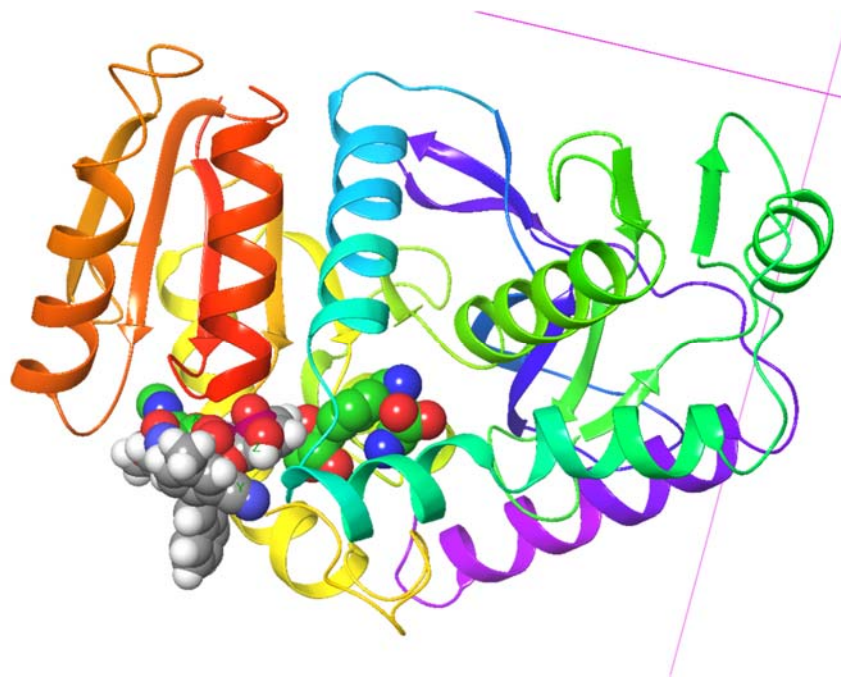


Figure S32: The Highest XP docked pose of **C2** within the active site of LDH (2V7P) [30]. The docked pose indicates the **C2** binds to the NADH binding site and can compete or prevent NADH binding. Therefore, **C2** may interfere with the LDH activity assay.

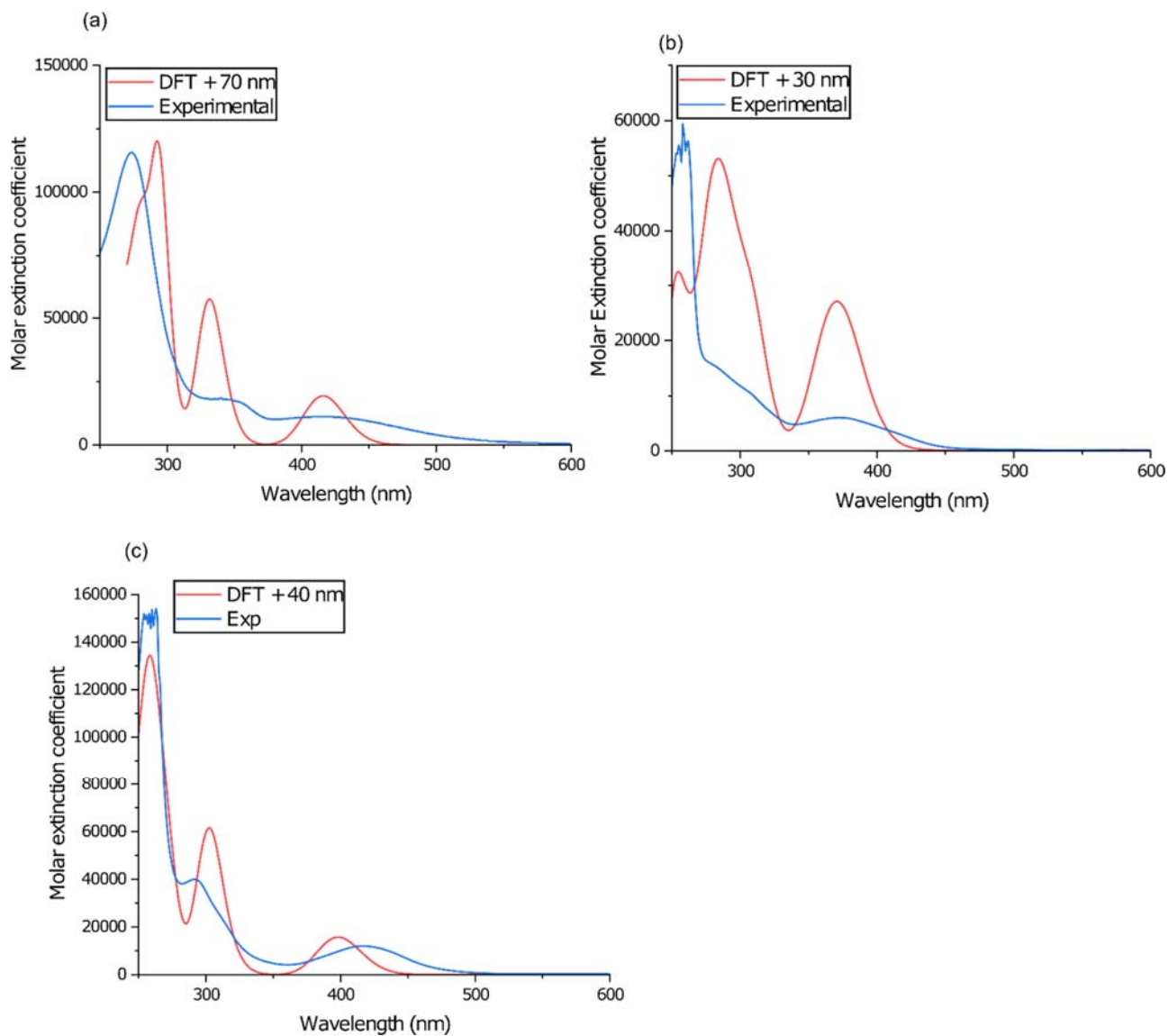


Figure S33: The experimental and DFT calculated UV-Vis spectra of **C1**, **C3**, and **C4** as well as 60 excited singlet state transitions.

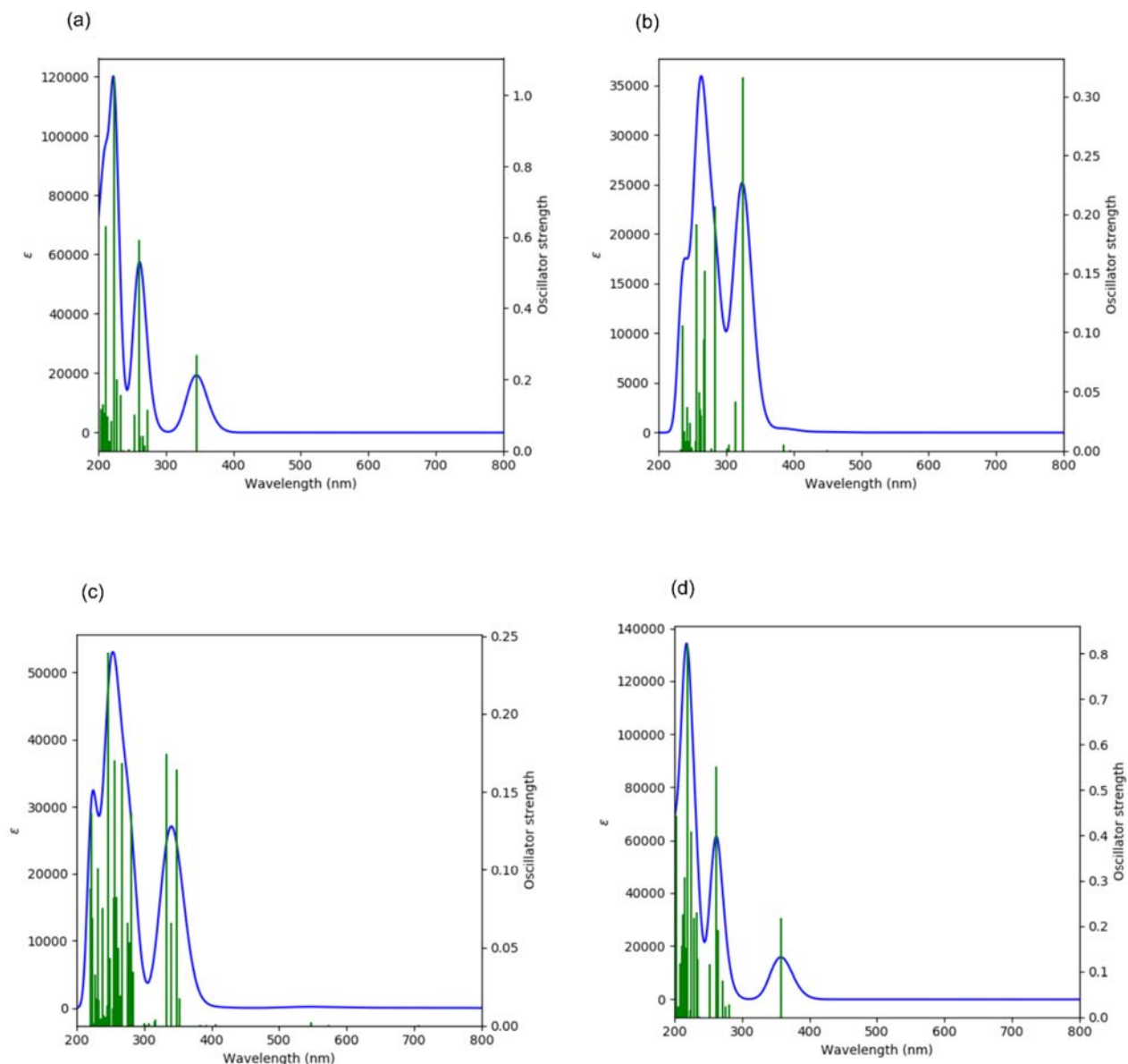
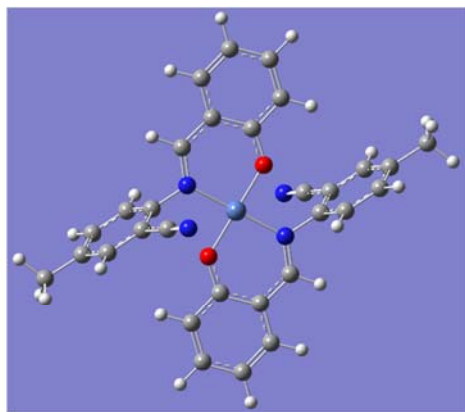


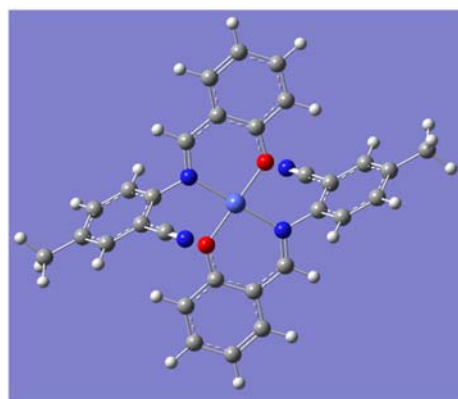
Figure S34: The experimental and DFT calculated UV–Vis spectra of **C1–C4** as well as 60 excited singlet state transitions. Oscillator strength of the 60 transition states is illustrated with the green lines.

Density functional theory (DFT) study: Optimization energy and optimized geometry

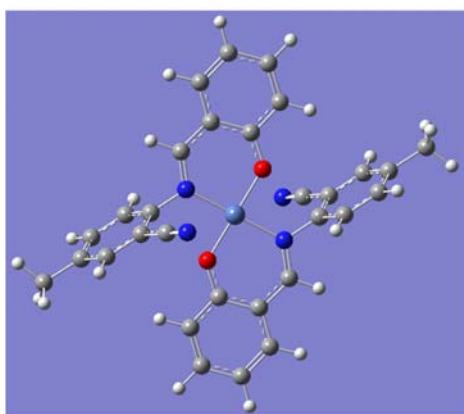
To study the electronic structures and bonding properties of the ligand (**HL**) and its complexes (**C1–C4**), a DFT study was utilized, following the optimization of the compounds. The energies of optimization using different DFT methods are presented in Table S6. The structures were optimized at the CAM-B3LYP/DEF2-QZVP/GD3BJ level of theory and are presented in Fig. S35.



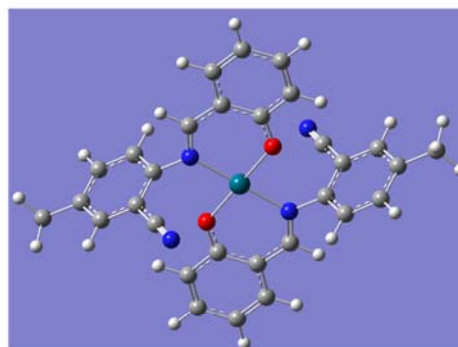
C1



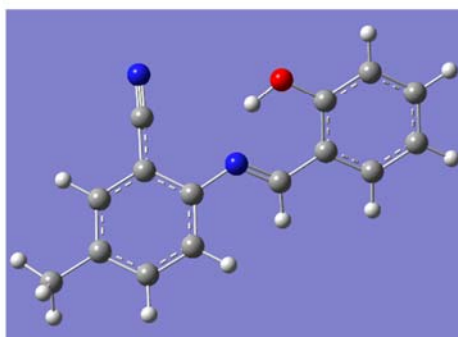
C2



C3



C4



HL

Figure S35: 3D model of the optimized structures for **HL**, and **C1-C4** calculated at M06-2X/3-21G and M06/3-21G level for **HL**, and **C1-C4**, respectively. The colour scheme for different atoms (blue for nitrogen, red for oxygen, grey for carbon, and white for hydrogen)

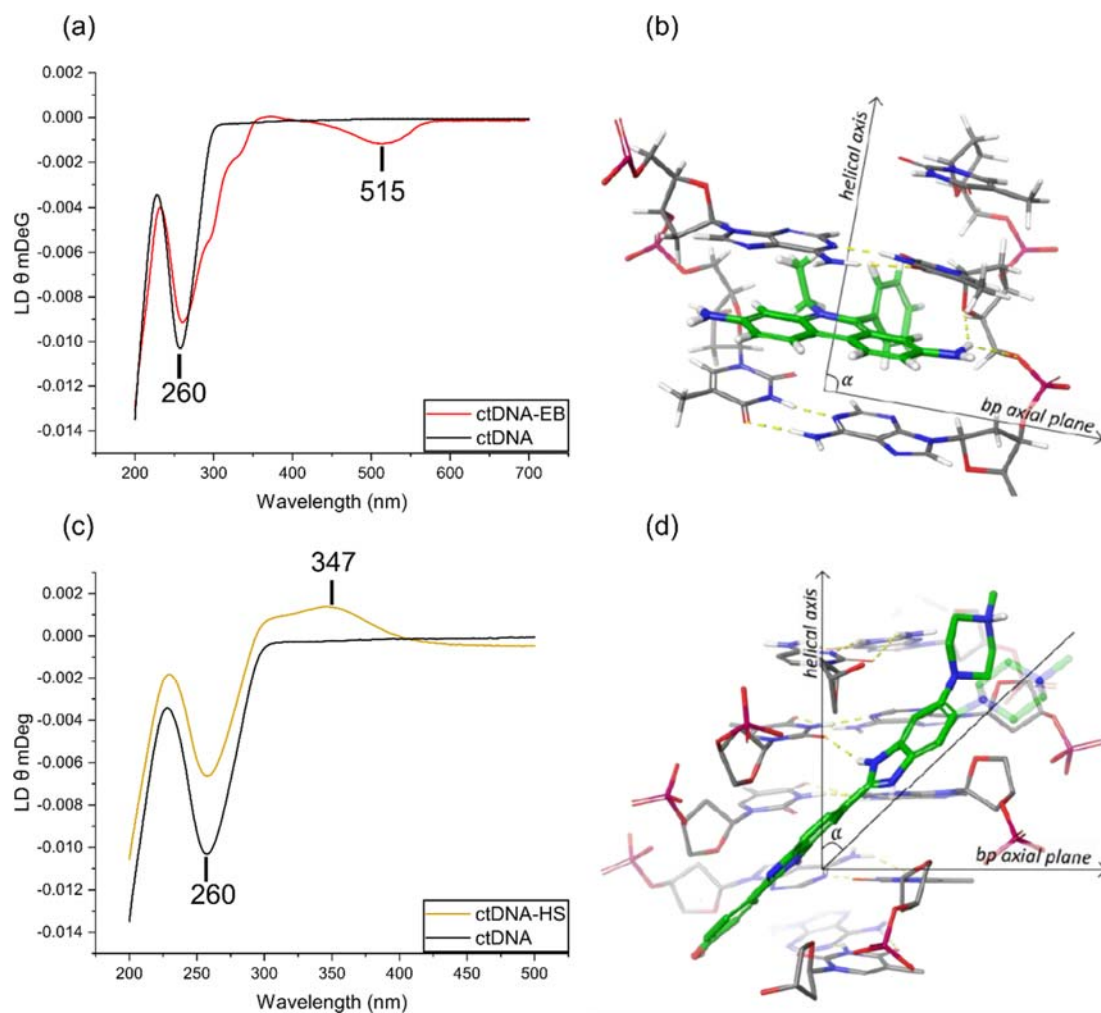


Figure S36:(a) The LD spectrum of EB with ctDNA, with an induced LD at 515 nm indicating binding of EB to ctDNA. (b) The best docking pose generated of EB intercalated with double stranded DNA (PDB: 2O1I).^[31](c) The LD spectrum of HS with ctDNA, with an induced LD at 347 nm indicating binding of HS to ctDNA. (d) An XRD crystal structure of HS in the minor groove of DNA (PDB: 8BNA).^[32]

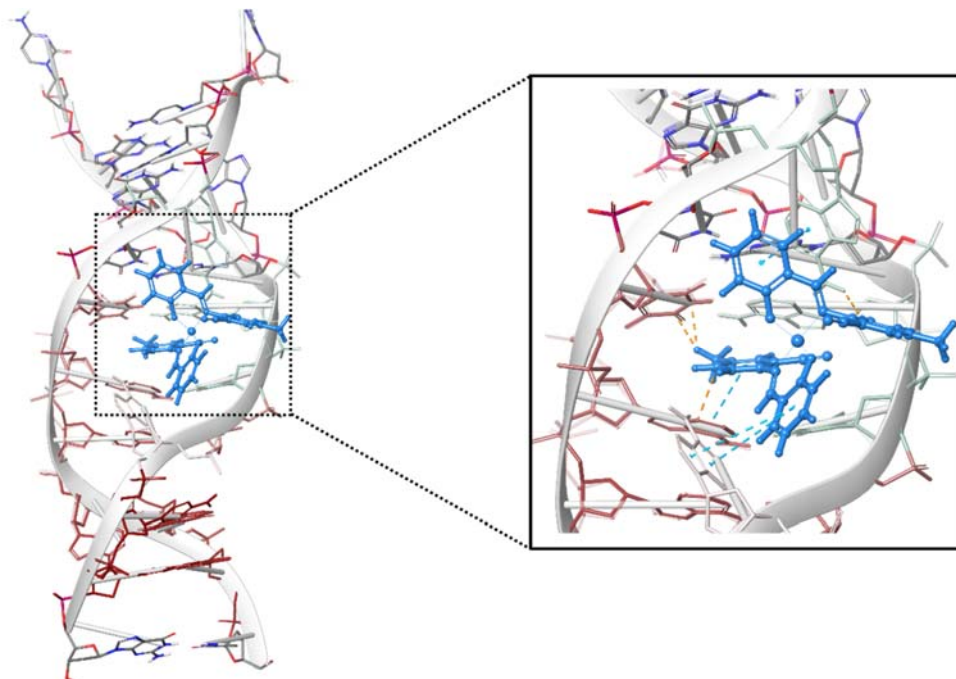


Figure S37: GLIDE XP docking analysis of the binding of complex **C2** to an oligonucleotide of DNA (PDB 4E1U; 5'-D(CGGAATTACCG)-3' bound with a cationic ruthenium complex $[\text{Ru}(\text{bpy})_2(\text{dppz})]^{2+}$ [10] . A large target grid was generated for ligand docking at the $[\text{Ru}(\text{bpy})_2(\text{dppz})]^{2+}$ site close to the centre of the DNA (with $[\text{Ru}(\text{bpy})_2(\text{dppz})]^{2+}$ removed), spanning $40 \times 40 \times 40 \text{ \AA}^3$, thereby facilitating a search of alternative binding packets radiating throughout the oligonucleotide. The structure shown displays the best XP ligand pose (complex **C2** is displayed in blue) within the AT pocket, with the most favourable docking score. The black box is a close-up view of complex **C2** intercalating the AT nucleobase of the 5'-D(CGGAATTACCG)-3' oligonucleotide strand.

Table S1: Crystallographic data

Identification code	HL	C1	C3	C4
Empirical formula	$\text{C}_{15}\text{H}_{12}\text{N}_2\text{O}$	$\text{C}_{30}\text{H}_{22}\text{N}_4\text{O}_2\text{Ni}$	$\text{C}_{30}\text{H}_{22}\text{CuN}_4\text{O}_2$	$\text{C}_{30}\text{H}_{22}\text{N}_4\text{O}_2\text{Pd}$
Formula weight	236.275	529.22	534.080	576.950
Temperature/K	172.99	293.15	273.15	273.15
Crystal system	monoclinic	monoclinic	triclinic	monoclinic
Space group	$P2_1/c$	$C2/c$	$P-1$	$C2/c$
$a/\text{\AA}$	4.653(3)	20.6803(13)	7.4595(6)	20.7112(14)
$b/\text{\AA}$	14.376(8)	6.7679(4)	7.8290(8)	6.8263(4)
$c/\text{\AA}$	17.72(1)	18.6914(11)	10.9833(10)	18.6789(13)
$\alpha/^\circ$	90	90	97.767(4)	90
$\beta/^\circ$	90.804(10)	96.740(2)	99.374(3)	96.368(2)
$\gamma/^\circ$	90	90	97.704(3)	90
Volume/ $\text{\AA}^3$	1185.1(12)	2598.0(3)	619.02(10)	2624.5(3)
Z	4	4	1	4
$\rho_{\text{calc}}/\text{cm}^3$	1.324	1.353	1.433	1.460
μ/mm^{-1}	0.085	0.781	0.918	0.741
F(000)	496.3	1096.0	275.5	1164.7
Crystal size/ mm^3	$0.267 \times 0.086 \times 0.047$	$0.333 \times 0.092 \times 0.088$	$0.123 \times 0.087 \times 0.021$	$0.164 \times 0.089 \times 0.034$

Radiation	Mo K α (λ = 0.71073)	MoK α (λ = 0.71073)	Mo K α (λ = 0.71073)	Mo K α (λ = 0.71073)
2 θ range for data collection/ $^\circ$	3.64 to 54.96	5.56 to 57.012	5.32 to 56.78	3.96 to 56.66
Index ranges	$-6 \leq h \leq 6, -18 \leq k \leq 18, -21 \leq l \leq 23$	$-27 \leq h \leq 27, -9 \leq k \leq 9, -24 \leq l \leq 25$	$-9 \leq h \leq 9, -10 \leq k \leq 10, -14 \leq l \leq 14$	$-27 \leq h \leq 27, -8 \leq k \leq 8, -24 \leq l \leq 24$
Reflections collected	12695	46080	13441	20271
Independent reflections	2704 [$R_{\text{int}} = 0.0875, R_{\text{sigma}} = 0.0732$]	3285 [$R_{\text{int}} = 0.0828, R_{\text{sigma}} = 0.0367$]	3081 [$R_{\text{int}} = 0.0705, R_{\text{sigma}} = 0.0568$]	3046 [$R_{\text{int}} = 0.0379, R_{\text{sigma}} = 0.0316$]
Data/restraints/parameters	2704/0/168	3285/0/170	3081/0/170	3046/0/170
Goodness-of-fit on F^2	0.993	1.021	1.062	1.064
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0580, wR_2 = 0.1240$	$R_1 = 0.0376, wR_2 = 0.0951$	$R_1 = 0.0425, wR_2 = 0.0986$	$R_1 = 0.0261, wR_2 = 0.0625$
Final R indexes [all data]	$R_1 = 0.1264, wR_2 = 0.1548$	$R_1 = 0.0622, wR_2 = 0.1089$	$R_1 = 0.0584, wR_2 = 0.1072$	$R_1 = 0.0359, wR_2 = 0.0704$
Largest diff. peak/hole / e $\text{\AA}^{-3}$	0.35/-0.42	0.24/-0.29	0.46/-0.49	0.30/-0.32

Table S2: Full list of 60 TD-DFT-calculated excited singlet states (CAM-B3LYP/DEF2-QZVP/GD3BJ in a DMSO solvent continuum) for **C1**. State energies are uncorrected. DMSO was chosen as the solvent medium to allow assignment of the UV-vis spectra of **C1**.

No.	Energy (cm ⁻¹)	Wavelength (nm)	Osc. Strength	Symmetry	Major contributions	Minor contributions
1	15346.3111206	651.622394556	0.0	Singlet-A	H-10->L+4 (20%), HOMO->L+2 (12%), HOMO->L+4 (23%)	H-11->L+2 (3%), H-11->L+4 (6%), H-11->L+7 (3%), H-10->L+2 (9%), H-10->L+7 (9%), HOMO->L+7 (9%)
2	16173.0294103	618.31335035	0.0	Singlet-A	H-5->L+2 (17%), H-5->L+4 (36%), H-5->L+7 (16%), H-4->L+4 (13%)	H-4->L+2 (6%), H-4->L+7 (6%)
3	19054.0418307	524.823031714	0.0	Singlet-A	H-11->L+4 (20%), H-2->L+4 (14%)	H-11->L+2 (9%), H-11->L+7 (9%), H-10->L+2 (3%), H-10->L+4 (8%), H-10->L+7 (3%), H-4->L+2 (4%), H-4->L+4 (8%), H-4->L+7 (3%), H-2->L+2 (7%), H-2->L+7 (6%)
4	21234.9650067	470.921425905	0.0	Singlet-A	H-13->L+4 (16%), H-12->L+2 (13%), H-12->L+4 (28%), H-12->L+7 (12%)	H-28->L+4 (2%), H-13->L+2 (7%), H-13->L+7 (8%)
5	28300.3818048	353.352123268	0.0	Singlet-A	H-1->L+1 (14%), HOMO->LUMO (76%)	HOMO->L+2 (5%)
6	28938.3663581	345.562008451	0.2669	Singlet-A	H-1->LUMO (14%), HOMO->L+1 (78%)	H-1->L+2 (2%)
7	35887.6393184	278.647472777	0.0	Singlet-A	H-5->LUMO (51%), H-4->LUMO (25%)	H-5->L+2 (4%), H-2->LUMO (3%), HOMO->L+2 (3%)
8	36195.7431102	276.275582174	0.0	Singlet-A	H-1->L+1 (39%), HOMO->LUMO (13%), HOMO->L+2 (23%)	H-10->LUMO (3%), H-5->LUMO (4%), H-2->LUMO (4%)
9	36663.5446791	272.7504961	0.1135	Singlet-A	H-1->LUMO (52%), HOMO->L+1 (12%), HOMO->L+3 (21%)	H-10->L+1 (5%), H-1->L+4 (3%)
10	37161.9953162	269.092117227	0.0147	Singlet-A	H-5->L+1 (54%), H-4->L+1 (27%)	H-3->LUMO (5%), H-2->L+1 (6%)
11	37668.5114976	265.473723342	0.0423	Singlet-A	H-1->L+2 (47%), H-1->L+4 (30%)	H-2->L+1 (3%), H-1->L+7 (7%)
12	37687.8688039	265.337370283	0.0	Singlet-A	H-1->L+1 (24%), HOMO->L+2 (44%)	H-11->L+4 (3%), H-10->LUMO (5%), H-10->L+4 (5%), H-4->LUMO (2%)
13	38197.611203	261.79647588	0.0398	Singlet-A	H-1->LUMO (11%), HOMO->L+3 (61%)	H-5->L+1 (2%), H-4->L+1 (3%), H-3->L+2 (2%), H-2->L+1 (4%), H-2->L+3 (3%), H-1->L+4 (2%)

14	38351.6630989	260.74488541	0.5903	Singlet-A	H-4->L+1 (11%), H-3->LUMO (12%), H-2->L+1 (44%)	H-6->LUMO (6%), H-5->L+1 (2%), H-4->L+3 (3%), H-1->LUMO (3%), H-1->L+4 (2%)
15	38427.4792153	260.230444573	0.0	Singlet-A	H-3->L+1 (15%), H-2->LUMO (45%)	H-6->L+1 (4%), H-5->LUMO (4%), H-4->L+2 (6%), H-3->L+3 (7%)
16	39493.7441704	253.204658359	0.1021	Singlet-A	H-5->L+1 (12%), H-4->L+1 (13%), H-3->LUMO (17%)	H-10->L+1 (2%), H-8->L+6 (2%), H-7->LUMO (3%), H-7->L+2 (2%), H-6->LUMO (3%), H-4->L+3 (5%), H-3->L+2 (6%), H-2->L+3 (6%), H-1->LUMO (2%), HOMO->L+3 (9%)
17	39778.4578839	251.392349829	0.0	Singlet-A	H-5->LUMO (10%), H-4->LUMO (24%), HOMO->L+4 (12%)	H-6->L+1 (4%), H-3->L+3 (7%), H-2->LUMO (7%), H-2->L+2 (2%), H-2->L+4 (3%)
18	40275.2954121	248.291164538	0.0	Singlet-A	HOMO->L+4 (40%)	H-16->L+4 (2%), H-12->LUMO (5%), H-11->L+2 (2%), H-10->L+2 (4%), H-10->L+4 (2%), H-9->L+1 (8%), H-5->LUMO (2%), H-4->LUMO (8%), H-1->L+1 (2%), HOMO->L+2 (6%), HOMO->L+7 (3%)
19	40655.9891026	245.966220986	0.0052	Singlet-A	H-12->L+1 (20%), H-9->LUMO (37%), H-4->L+1 (11%)	H-9->L+2 (4%), H-5->L+1 (3%), H-3->LUMO (4%), H-2->L+1 (6%)
20	40794.7164644	245.129783136	0.0	Singlet-A	H-12->LUMO (15%), H-9->L+1 (31%), H-3->L+1 (10%)	H-3->L+3 (2%), H-2->LUMO (3%), H-2->L+2 (3%), HOMO->L+4 (7%)
21	41906.1484676	238.628467795	0.0	Singlet-A	H-3->L+1 (38%), H-3->L+3 (15%)	H-8->L+2 (3%), H-7->L+3 (2%), H-5->LUMO (5%), H-4->LUMO (3%), H-4->L+2 (5%), H-2->L+2 (6%), H-1->L+3 (3%)
22	42232.8030113	236.782768061	0.0031	Singlet-A	H-3->LUMO (24%), H-3->L+2 (18%)	H-9->LUMO (4%), H-8->L+3 (3%), H-7->L+2 (4%), H-5->L+1 (8%), H-4->L+1 (4%), H-4->L+3 (6%), H-3->L+4 (3%), H-2->L+3 (5%)
23	42998.2231644	232.567749643	0.157	Singlet-A	H-10->L+1 (16%), H-6->LUMO (10%), HOMO->L+8 (20%)	H-11->L+1 (6%), H-3->L+2 (4%), H-2->L+1 (4%), H-1->LUMO (4%), H-1->L+2 (5%), H-1->L+4 (7%), H-1->L+9 (9%)
24	43269.2254526	231.111139509	0.0	Singlet-A	H-11->LUMO (12%), H-10->LUMO (15%), H-6->L+1 (21%), H-1->L+3 (12%)	H-2->LUMO (3%), H-1->L+1 (4%), H-1->L+8 (4%), HOMO->L+9 (9%)
25	43734.6073581	228.651875576	0.0	Singlet-A	H-1->L+3 (60%)	H-11->LUMO (4%), H-6->L+1 (5%), H-4->L+2 (2%), HOMO->L+5 (8%), HOMO->L+7 (3%)
26	44058.8422386	226.96919601	0.1989	Singlet-A	H-3->L+2 (18%), H-3->L+4 (13%)	H-9->L+2 (5%), H-9->L+4 (5%), H-8->L+1 (3%), H-8->L+3 (5%), H-7->LUMO (7%), H-7->L+2 (5%), H-2->L+3 (3%), H-2->L+6 (3%), H-1->L+2 (4%), H-1->L+4 (5%), HOMO->L+6 (8%)
27	44369.3656937	225.380729331	0.0	Singlet-A	HOMO->L+5 (62%)	H-11->LUMO (4%), H-6->L+1 (6%), H-1->L+3 (3%), HOMO->L+7 (8%), HOMO->L+16 (4%)
28	44758.9314829	223.41909578	0.1563	Singlet-A	H-11->L+1 (15%), H-6->LUMO (13%), H-1->L+2 (23%), H-1->L+4 (21%)	H-6->L+2 (3%), H-4->L+3 (4%), H-1->LUMO (3%), H-1->L+7 (2%)

29	44806.5181942	223.181813785	1.0516	Singlet-A	H-9->L+2 (17%), H-9->L+4 (17%), H-6->LUMO (11%), HOMO->L+8 (14%)	H-11->L+1 (4%), H-10->L+1 (2%), H-9->L+7 (4%), H-8->L+3 (3%), H-3->L+2 (3%), H-1->L+9 (6%), HOMO->L+6 (3%)
30	44857.3311233	222.929000669	0.0	Singlet-A	H-8->LUMO (17%), H-7->L+1 (11%), H-7->L+3 (12%)	H-11->LUMO (3%), H-8->L+2 (8%), H-6->L+3 (3%), H-5->L+2 (4%), H-4->L+2 (3%), H-3->L+3 (6%), H-3->L+6 (6%), H-2->L+2 (9%), HOMO->L+5 (3%)
31	45525.1581905	219.658764461	0.082	Singlet-A	HOMO->L+6 (63%)	H-10->L+1 (3%), H-8->L+1 (3%), H-8->L+3 (3%), H-7->LUMO (4%), HOMO->L+10 (2%)
32	45844.5537444	218.128418389	0.0	Singlet-A	H-11->LUMO (22%), H-10->LUMO (21%)	H-9->L+1 (3%), H-8->LUMO (2%), H-6->L+1 (7%), H-1->L+1 (6%), H-1->L+3 (6%), HOMO->LUMO (4%), HOMO->L+5 (2%), HOMO->L+9 (7%)
33	46229.280207	216.313123527	0.0278	Singlet-A	H-9->LUMO (29%), H-4->L+1 (10%), H-3->LUMO (15%)	H-13->L+1 (2%), H-12->L+1 (4%), H-11->L+1 (3%), H-10->L+1 (2%), H-7->LUMO (2%), H-5->L+1 (8%), H-2->L+1 (8%), HOMO->L+6 (2%)
34	46248.6375133	216.222585955	0.0	Singlet-A	H-9->L+1 (29%), H-3->L+1 (12%)	H-13->LUMO (3%), H-12->LUMO (7%), H-5->LUMO (7%), H-4->LUMO (7%), H-4->L+2 (2%), H-2->LUMO (5%), H-2->L+2 (3%), H-1->L+8 (3%), HOMO->L+9 (9%)
35	46617.2328873	214.512946836	0.0962	Singlet-A	H-11->L+1 (17%), H-10->L+1 (10%), HOMO->L+8 (10%)	H-9->L+2 (5%), H-9->L+4 (3%), H-7->LUMO (6%), H-6->LUMO (3%), H-3->L+4 (5%), H-2->L+3 (6%), H-1->LUMO (2%), H-1->L+2 (7%), H-1->L+4 (3%), H-1->L+9 (2%)
36	47041.480517	212.578343413	0.0	Singlet-A	H-10->LUMO (24%), H-1->L+8 (10%), HOMO->L+9 (22%)	H-12->LUMO (2%), H-9->L+1 (5%), H-6->L+1 (6%), H-2->LUMO (4%), H-1->L+3 (2%), HOMO->L+5 (2%), HOMO->L+7 (3%)
37	47308.450033	211.378728177	0.0371	Singlet-A	H-10->L+1 (25%), H-5->L+3 (12%), HOMO->L+8 (11%)	H-11->L+1 (4%), H-9->L+2 (3%), H-8->L+1 (2%), H-4->L+3 (5%), H-3->LUMO (2%), H-2->L+1 (3%), H-1->L+9 (3%), HOMO->L+6 (7%)
38	47413.3021088	210.911275006	0.6306	Singlet-A	H-8->L+1 (12%), H-7->LUMO (10%), H-5->L+3 (25%), H-3->L+4 (21%)	H-9->L+2 (4%), H-6->LUMO (3%), H-3->L+2 (4%)
39	47658.4946552	209.826182559	0.0	Singlet-A	H-5->L+2 (50%)	H-12->LUMO (2%), H-9->L+3 (3%), H-8->LUMO (2%), H-7->L+1 (2%), H-5->L+4 (9%), H-5->L+7 (3%), H-4->LUMO (3%), H-4->L+2 (7%), H-4->L+4 (4%), H-2->LUMO (2%)
40	47664.1405362	209.801328368	0.1055	Singlet-A	H-5->L+3 (28%), H-4->L+3 (18%)	H-10->L+1 (3%), H-9->L+2 (4%), H-9->L+4 (8%), H-8->L+1 (6%), H-7->LUMO (5%), H-6->LUMO (5%), H-3->L+2 (2%), HOMO->L+8 (7%)
41	47770.6057208	209.333749261	0.0	Singlet-A	HOMO->L+4 (11%), HOMO->L+7 (62%)	HOMO->L+5 (8%), HOMO->L+9 (3%)
42	48074.6767405	208.009719004	0.0	Singlet-A	H-4->L+2 (29%), H-2->L+2 (30%)	H-12->LUMO (2%), H-11->L+4 (3%), H-2->LUMO (5%), H-2->L+4 (4%), H-1->L+3 (5%)
43	48228.7286365	207.345295692	0.1309	Singlet-A	H-4->L+3 (16%), H-2->L+3 (49%)	H-11->L+3 (3%), H-10->L+3 (3%), H-5->L+3 (5%), H-1->L+2 (3%), HOMO->L+8 (3%)
44	48262.6039225	207.199761042	0.0	Singlet-A	H-8->LUMO (20%), H-8->L+2 (10%), H-7->L+1 (28%)	H-7->L+3 (4%), H-5->L+4 (3%), H-4->LUMO (4%), H-4->L+2 (5%), H-2->L+2 (2%), H-2->L+4 (3%), HOMO->L+9 (4%)
45	48419.8820362	206.526731984	0.0	Singlet-A	H-12->LUMO (46%), H-3->L+1 (10%)	H-13->LUMO (5%), H-5->LUMO (3%), H-4->LUMO (5%), H-2->LUMO (5%), H-2->L+2 (8%)

46	48829.6116861	204.793764576	0.076	Singlet-A	H-12->L+1 (36%), H-6->L+2 (10%)	H-13->L+1 (3%), H-8->L+1 (5%), H-8->L+3 (5%), H-7->LUMO (2%), H-7->L+2 (3%), H-5->L+3 (2%), H-4->L+1 (3%), H-3->LUMO (8%), H-3->L+4 (3%), H-2->L+1 (4%)
47	48934.4637619	204.354952139	0.1162	Singlet-A	H-12->L+1 (18%), H-8->L+1 (10%), H-1->L+5 (15%)	H-9->LUMO (3%), H-8->L+3 (8%), H-7->LUMO (3%), H-7->L+2 (8%), H-6->L+2 (4%), H-4->L+3 (3%), H-3->L+4 (2%), H-2->L+1 (2%), HOMO->L+11 (2%), HOMO->L+15 (2%)
48	49114.3253995	203.606583592	0.093	Singlet-A	H-1->L+5 (48%)	H-12->L+1 (4%), H-8->L+1 (3%), H-8->L+3 (3%), H-7->L+2 (3%), H-4->L+3 (3%), H-3->L+4 (3%), H-1->L+16 (2%), HOMO->L+10 (3%), HOMO->L+11 (4%), HOMO->L+13 (4%), HOMO->L+15 (6%)
49	49612.7760366	201.560984868	0.0	Singlet-A	H-8->L+2 (14%), H-7->L+3 (11%), H-2->L+4 (12%)	H-7->L+1 (5%), H-5->L+4 (4%), H-4->LUMO (2%), H-4->L+4 (7%), H-3->L+3 (6%), H-2->L+2 (7%), HOMO->L+14 (3%)
50	49932.1715905	200.271682193	0.2261	Singlet-A	H-7->L+2 (12%), H-6->L+2 (32%), H-6->L+4 (15%)	H-12->L+1 (2%), H-11->L+1 (2%), H-10->L+1 (2%), H-8->L+3 (4%), H-6->LUMO (4%)
51	50472.563058	198.127445767	0.3261	Singlet-A	HOMO->L+10 (23%), HOMO->L+11 (23%)	H-10->L+1 (4%), H-6->LUMO (2%), H-6->L+9 (2%), H-1->L+5 (8%), H-1->L+14 (8%), HOMO->L+6 (4%), HOMO->L+13 (4%)
52	50799.2176017	196.853425547	0.0	Singlet-A	H-2->L+4 (14%), H-1->L+6 (37%)	H-11->L+2 (3%), H-6->L+8 (3%), H-2->L+9 (2%), H-1->L+11 (4%), HOMO->L+14 (6%)
53	51419.4579576	194.478907348	0.0081	Singlet-A	H-8->L+1 (38%), H-7->LUMO (33%)	H-8->LUMO (4%), H-7->L+1 (3%), H-7->L+2 (5%), H-6->LUMO (5%)
54	51419.4579576	194.478907348	0.0009	Singlet-A	H-8->LUMO (40%), H-7->L+1 (32%)	H-8->L+1 (4%), H-8->L+2 (4%), H-7->LUMO (3%), H-6->L+1 (6%)
55	51635.6145446	193.664781337	0.0	Singlet-A	H-11->LUMO (10%), H-6->L+1 (11%)	H-12->L+2 (5%), H-9->L+3 (5%), H-7->L+1 (5%), H-6->L+3 (3%), H-6->L+8 (2%), H-4->LUMO (3%), H-4->L+4 (2%), H-3->L+6 (4%), H-2->L+4 (5%), H-2->L+9 (3%), H-1->L+6 (5%), H-1->L+11 (3%), HOMO->L+14 (5%)
56	52023.5672249	192.220574894	0.0001	Singlet-A	H-11->LUMO (11%), H-6->L+3 (10%)	H-12->L+2 (3%), H-10->LUMO (6%), H-10->L+2 (2%), H-9->L+3 (7%), H-6->L+1 (7%), H-4->L+4 (5%), H-3->L+3 (3%), H-3->L+6 (5%), H-2->LUMO (3%), H-2->L+7 (4%), H-1->L+6 (5%), HOMO->L+14 (4%)
57	52038.0852047	192.16694774	0.1575	Singlet-A	H-11->L+1 (17%), H-6->LUMO (14%), H-6->L+4 (10%)	H-10->L+1 (5%), H-7->LUMO (5%), H-7->L+2 (2%), H-6->L+9 (2%), H-4->L+1 (5%), H-2->L+1 (4%), H-2->L+8 (3%), HOMO->L+10 (8%)
58	52187.297774	191.617508983	0.0	Singlet-A	H-9->L+3 (11%), H-2->L+4 (10%), H-1->L+6 (21%)	H-12->L+2 (5%), H-11->L+2 (7%), H-11->L+4 (2%), H-10->L+2 (5%), H-6->L+1 (5%), H-4->L+2 (2%), H-4->L+4 (3%), H-2->L+7 (4%)
59	52409.100242	190.806557522	0.2831	Singlet-A	H-1->L+7 (13%), HOMO->L+10 (14%)	H-11->L+1 (7%), H-6->LUMO (8%), H-6->L+2 (4%), H-6->L+4 (3%), H-3->L+7 (3%), H-2->L+6 (7%), H-2->L+8 (3%), H-1->L+14 (2%), HOMO->L+15 (4%)
60	52409.9067964	190.803621133	0.0008	Singlet-A	H-12->L+2 (10%), H-9->L+3 (24%), H-4->L+4 (11%)	H-11->L+2 (4%), H-8->L+4 (3%), H-7->L+6 (3%), H-6->L+3 (2%), H-6->L+8 (3%), H-3->L+3 (4%), H-2->L+9 (3%), H-1->L+6 (2%), HOMO->L+14 (4%)

Table S3: Full list of 60 TD-DFT-calculated excited singlet states (CAM-B3LYP/DEF2-QZVP/GD3BJ in a DMSO solvent continuum) for **C2**. State energies are uncorrected. DMSO was chosen as the solvent medium to allow assignment of the UV-vis spectra of **C2**.

No.	Energy (cm ⁻¹)	Wavelength (nm)	Osc. Strength	Symmetry	Major contributions	Minor contributions
1	2745.51127632	3642.3088429	0.0	2.071-A	H-5(B)->L+5(B) (12%), H-3(B)->L+5(B) (40%), H-3(B)->L+6(B) (10%), H-3(B)->L+9(B) (17%)	H-12(B)->L+5(B) (3%), H-5(B)->L+6(B) (3%), H-5(B)->L+9(B) (5%), H-5(B)->L+11(B) (2%), H-3(B)->LUMO(B) (6%), H-3(B)->L+3(B) (2%), H-3(B)->L+11(B) (5%), H-3(B)->L+16(B) (5%), H-2(B)->L+5(B) (5%), H-2(B)->L+9(B) (2%), HOMO(B)->L+5(B) (2%)
2	7692.10958937	1300.03348026	0.0	2.726-A	H-2(B)->L+5(B) (20%), H-2(B)->L+9(B) (13%)	H-11(A)->L+4(A) (2%), H-11(A)->L+9(A) (2%), H-2(A)->L+9(A) (2%), H-10(B)->L+5(B) (8%), H-10(B)->L+9(B) (5%), H-10(B)->L+11(B) (2%), H-10(B)->L+18(B) (2%), H-7(B)->L+5(B) (4%), H-7(B)->L+9(B) (3%), H-2(B)->LUMO(B) (3%), H-2(B)->L+4(B) (2%), H-2(B)->L+11(B) (4%), H-2(B)->L+18(B) (4%), HOMO(B)->L+5(B) (5%), HOMO(B)->L+9(B) (4%)
3	8443.01176277	1184.41147318	0.0	2.976-A	H-2(B)->L+6(B) (10%), H-2(B)->L+11(B) (22%)	H-11(A)->L+4(A) (3%), H-11(A)->L+9(A) (5%), H-4(A)->L+4(A) (2%), H-4(A)->L+9(A) (3%), H-2(A)->L+4(A) (2%), H-2(A)->L+9(A) (3%), H-10(B)->L+5(B) (2%), H-10(B)->L+6(B) (3%), H-10(B)->L+11(B) (7%), H-7(B)->L+11(B) (3%), H-5(B)->L+11(B) (2%), H-2(B)->LUMO(B) (2%), H-2(B)->L+3(B) (3%), H-2(B)->L+5(B) (6%), H-2(B)->L+16(B) (2%), H-2(B)->L+18(B) (2%), HOMO(B)->L+6(B) (2%), HOMO(B)->L+11(B) (3%)
4	11536.147998	866.840474112	0.0	3.232-A	H-5(A)->L+4(A) (10%), H-5(A)->L+9(A) (14%), H-3(B)->L+11(B) (14%)	H-10(A)->L+4(A) (2%), H-10(A)->L+9(A) (3%), H-8(A)->L+4(A) (2%), H-8(A)->L+9(A) (2%), H-5(A)->L+2(A) (3%), H-5(A)->L+5(A) (4%), H-4(A)->L+4(A) (4%), H-4(A)->L+5(A) (2%), H-4(A)->L+9(A) (5%), H-7(B)->L+5(B) (2%), H-5(B)->L+11(B) (4%), H-3(B)->L+6(B) (3%), H-3(B)->L+9(B) (2%), H-3(B)->L+18(B) (3%), H-2(B)->L+11(B) (2%)
5	11968.4611719	835.529301248	0.0	2.345-A	H-7(B)->L+5(B) (24%)	H-11(A)->L+4(A) (3%), H-11(A)->L+9(A) (5%), H-2(A)->L+4(A) (3%), H-2(A)->L+9(A) (4%), H-12(B)->L+5(B) (3%), H-7(B)->LUMO(B) (4%), H-7(B)->L+3(B) (2%), H-7(B)->L+6(B) (7%), H-7(B)->L+9(B) (9%), H-7(B)->L+11(B) (5%), H-7(B)->L+16(B) (3%)
6	13603.3469995	735.113204152	0.0	3.295-A	H-10(A)->L+9(A) (11%), H-7(B)->L+11(B) (16%)	H-13(A)->L+4(A) (3%), H-13(A)->L+9(A) (5%), H-10(A)->L+2(A) (2%), H-10(A)->L+4(A) (8%), H-10(A)->L+5(A) (3%), H-5(A)->L+4(A) (3%), H-5(A)->L+9(A) (4%), H-12(B)->L+11(B) (2%), H-7(B)->L+5(B) (2%), H-7(B)->L+6(B) (2%), H-7(B)->L+9(B) (4%), H-7(B)->L+18(B) (4%), H-2(B)->L+5(B) (3%)
7	21012.3559843	475.910459896	0.0	2.068-A	H-10(A)->L+9(A) (13%), H-7(B)->L+11(B) (19%)	H-13(A)->L+4(A) (3%), H-13(A)->L+9(A) (4%), H-10(A)->L+2(A) (3%), H-10(A)->L+4(A) (9%), H-10(A)->L+5(A) (4%), H-4(A)->L+9(A) (2%), H-7(B)->L+5(B) (3%), H-7(B)->L+6(B) (4%), H-7(B)->L+9(B) (4%), H-7(B)->L+18(B) (5%), H-5(B)->L+11(B) (4%)
8	22122.981433	452.018640899	0.0	2.453-A	H-12(A)->L+4(A) (10%), H-12(A)->L+9(A) (14%)	H-21(A)->L+9(A) (2%), H-12(A)->L+2(A) (3%), H-12(A)->L+5(A) (4%), H-1(A)->LUMO(A) (2%), HOMO(A)->L+1(A) (3%), HOMO(A)->L+2(A) (7%), HOMO(A)->L+4(A) (9%), HOMO(A)->L+5(A) (4%), HOMO(A)->L+8(A) (2%), HOMO(A)->L+9(A) (9%), H-1(B)->L+1(B) (2%), HOMO(B)->LUMO(B) (5%)
9	22156.8567191	451.327556377	0.0	3.172-A	HOMO(A)->L+1(A) (20%), HOMO(B)->LUMO(B) (14%)	H-12(A)->L+4(A) (2%), H-12(A)->L+9(A) (3%), H-6(A)->LUMO(A) (3%), H-2(A)->L+1(A) (3%), H-1(A)->LUMO(A) (8%), HOMO(A)->L+4(A) (3%), HOMO(A)->L+9(A) (4%), H-6(B)->L+1(B) (3%), H-1(B)->L+1(B) (7%), HOMO(B)->L+3(B) (2%)
10	22204.4434304	450.360308798	0.0009	3.482-A	H-1(A)->L+1(A) (10%), HOMO(A)->LUMO(A)	H-6(A)->L+1(A) (3%), H-2(A)->LUMO(A) (3%), H-1(A)->L+2(A) (2%), H-6(B)->LUMO(B) (4%), H-2(B)->L+1(B) (2%)

					(24%), H-1(B)->LUMO(B) (11%), HOMO(B)->L+1(B) (20%)	
11	22442.3769869	445.585599325	0.0	2.064-A	H-5(A)->L+9(A) (10%), H-3(B)->L+11(B) (18%)	H-8(A)->L+9(A) (2%), H-5(A)->L+2(A) (2%), H-5(A)->L+4(A) (8%), H-5(A)->L+5(A) (3%), H-12(B)->L+11(B) (2%), H-5(B)->L+11(B) (3%), H-3(B)->L+3(B) (2%), H-3(B)->L+6(B) (5%), H-3(B)->L+9(B) (3%), H-3(B)->L+18(B) (4%), H-2(B)->L+5(B) (2%), H-2(B)->L+9(B) (2%), H-2(B)->L+11(B) (3%)
12	23081.1680947	433.253635993	0.0	2.124-A	H-2(B)->L+11(B) (11%)	H-11(A)->L+4(A) (5%), H-11(A)->L+5(A) (2%), H-11(A)->L+9(A) (6%), H-4(A)->L+4(A) (3%), H-4(A)->L+9(A) (3%), H-2(A)->L+2(A) (2%), H-2(A)->L+4(A) (4%), H-2(A)->L+5(A) (2%), H-2(A)->L+9(A) (5%), H-10(B)->L+11(B) (4%), H-7(B)->L+5(B) (5%), H-7(B)->L+6(B) (3%), H-7(B)->L+11(B) (4%), H-2(B)->L+6(B) (3%), H-2(B)->L+18(B) (3%), HOMO(B)->L+11(B) (3%)
13	25359.6843566	394.326674551	0.0002	3.535-A		H-8(A)->L+3(A) (5%), H-8(A)->L+6(A) (2%), H-7(A)->L+1(A) (2%), H-7(A)->L+2(A) (4%), H-7(A)->L+4(A) (2%), H-6(A)->L+2(A) (2%), H-5(A)->L+3(A) (3%), H-4(A)->L+3(A) (3%), H-4(A)->L+6(A) (3%), H-3(A)->L+1(A) (4%), H-3(A)->L+2(A) (6%), H-3(A)->L+4(A) (2%), H-3(A)->L+9(A) (2%), H-2(A)->L+3(A) (2%), H-9(B)->L+2(B) (8%), H-8(B)->L+3(B) (5%), H-8(B)->L+6(B) (2%), H-6(B)->L+3(B) (2%), H-5(B)->L+2(B) (4%), H-5(B)->L+7(B) (4%), H-4(B)->LUMO(B) (3%), H-4(B)->L+3(B) (5%), H-4(B)->L+6(B) (3%)
14	25370.9761186	394.151173106	0.0	3.530-A		H-8(A)->L+2(A) (3%), H-8(A)->L+4(A) (2%), H-7(A)->L+3(A) (5%), H-7(A)->L+6(A) (2%), H-6(A)->L+3(A) (2%), H-5(A)->L+2(A) (3%), H-4(A)->L+2(A) (3%), H-3(A)->LUMO(A) (2%), H-3(A)->L+3(A) (5%), H-3(A)->L+6(A) (4%), H-2(A)->L+1(A) (3%), H-9(B)->LUMO(B) (2%), H-9(B)->L+3(B) (6%), H-8(B)->L+2(B) (6%), H-8(B)->L+7(B) (2%), H-6(B)->L+2(B) (2%), H-5(B)->LUMO(B) (2%), H-5(B)->L+3(B) (4%), H-5(B)->L+6(B) (2%), H-4(B)->L+1(B) (2%), H-4(B)->L+2(B) (5%), H-4(B)->L+7(B) (4%)
15	25820.2269356	387.293265274	0.0	3.486-A	H-1(A)->LUMO(A) (10%), H-2(B)->LUMO(B) (14%)	H-6(A)->LUMO(A) (6%), H-4(A)->L+1(A) (3%), H-2(A)->L+1(A) (7%), H-2(A)->L+2(A) (3%), H-1(A)->L+7(A) (2%), HOMO(A)->L+1(A) (8%), HOMO(A)->L+2(A) (2%), HOMO(A)->L+8(A) (2%), H-6(B)->L+1(B) (6%), H-2(B)->L+3(B) (2%), H-2(B)->L+5(B) (2%), H-1(B)->L+1(B) (8%), H-1(B)->L+8(B) (2%)
16	25937.1773278	385.546965023	0.0053	3.494-A	HOMO(A)->LUMO(A) (11%), H-2(B)->L+1(B) (17%)	H-6(A)->L+1(A) (5%), H-4(A)->LUMO(A) (3%), H-2(A)->LUMO(A) (8%), H-1(A)->L+1(A) (7%), H-1(A)->L+2(A) (2%), H-1(A)->L+8(A) (3%), HOMO(A)->L+7(A) (3%), H-10(B)->L+1(B) (2%), H-6(B)->LUMO(B) (6%), H-1(B)->LUMO(B) (3%), H-1(B)->L+5(B) (2%), HOMO(B)->L+8(B) (2%)
17	30298.2171254	330.052423831	0.0	2.247-A	HOMO(A)->L+1(A) (27%), H-1(B)->L+1(B) (18%), HOMO(B)->LUMO(B) (34%)	H-1(A)->LUMO(A) (6%), HOMO(B)->L+3(B) (2%)
18	30763.5990309	325.059496126	0.3164	2.232-A	HOMO(A)->LUMO(A) (28%), H-1(B)->LUMO(B) (23%), HOMO(B)->L+1(B) (30%)	H-1(A)->L+1(A) (6%), H-1(B)->L+3(B) (2%)
19	31537.0847283	317.087013151	0.0	3.438-A	H-2(B)->LUMO(B) (26%)	H-11(A)->L+1(A) (4%), H-2(A)->L+1(A) (4%), H-2(A)->L+8(A) (2%), H-1(A)->L+7(A) (9%), HOMO(A)->L+8(A) (8%), H-10(B)->LUMO(B) (4%), H-2(B)->L+9(B) (5%), H-1(B)->L+8(B) (8%), HOMO(B)->L+5(B) (4%)
20	31896.8080037	313.510994544	0.0415	3.396-A	HOMO(A)->L+7(A) (10%), H-2(B)->L+1(B) (24%)	H-11(A)->LUMO(A) (2%), H-2(A)->LUMO(A) (2%), H-1(A)->L+8(A) (8%), H-10(B)->L+1(B) (3%), H-2(B)->L+8(B) (4%), H-1(B)->LUMO(B) (5%), H-1(B)->L+5(B) (6%), H-1(B)->L+6(B) (2%), H-1(B)->L+9(B) (2%), HOMO(B)->L+1(B) (4%), HOMO(B)->L+8(B) (5%)
21	32199.2659145	310.566086399	0.0	2.911-A	H-3(B)->LUMO(B) (67%)	H-11(B)->L+1(B) (2%), H-5(B)->LUMO(B) (4%), H-3(B)->L+3(B) (2%), H-3(B)->L+9(B) (3%), H-2(B)->LUMO(B) (2%), H-1(B)->L+1(B) (3%)

22	32871.9323083	304.210896585	0.0053	3.118-A	H-3(B)->L+1(B) (49%)	H-8(A)->L+3(A) (2%), H-4(A)->L+3(A) (2%), H-3(A)->L+1(A) (2%), H-3(A)->L+2(A) (2%), H-11(B)->LUMO(B) (2%), H-9(B)->L+2(B) (2%), H-8(B)->L+3(B) (2%), H-5(B)->L+2(B) (3%), H-4(B)->LUMO(B) (2%), H-4(B)->L+3(B) (3%), H-2(B)->L+1(B) (6%)
23	33091.315113	302.194094307	0.0	3.518-A	H-3(A)->L+3(A) (11%), H-4(B)->L+2(B) (10%)	H-8(A)->L+1(A) (2%), H-8(A)->L+2(A) (4%), H-8(A)->L+4(A) (2%), H-7(A)->L+3(A) (6%), H-4(A)->L+1(A) (5%), H-4(A)->L+2(A) (4%), H-3(A)->LUMO(A) (3%), H-2(A)->L+1(A) (2%), H-2(A)->L+2(A) (3%), H-9(B)->L+3(B) (4%), H-8(B)->L+2(B) (6%), H-7(B)->L+3(B) (2%), H-5(B)->LUMO(B) (6%), H-5(B)->L+3(B) (6%), H-4(B)->L+1(B) (2%), H-3(B)->L+3(B) (2%)
24	33167.9377838	301.495982813	0.0019	3.325-A	H-3(B)->L+1(B) (23%)	H-8(A)->L+3(A) (4%), H-7(A)->L+2(A) (2%), H-4(A)->L+3(A) (4%), H-3(A)->L+1(A) (4%), H-3(A)->L+2(A) (5%), H-2(A)->L+3(A) (3%), H-9(B)->L+2(B) (3%), H-8(B)->L+3(B) (3%), H-5(B)->L+1(B) (5%), H-5(B)->L+2(B) (5%), H-4(B)->LUMO(B) (3%), H-4(B)->L+3(B) (6%), H-3(B)->L+2(B) (4%), H-1(B)->LUMO(B) (2%)
25	34998.0097832	285.730533306	0.0	3.205-A		H-11(A)->L+1(A) (3%), H-6(A)->LUMO(A) (8%), H-3(A)->LUMO(A) (2%), H-2(A)->L+1(A) (5%), H-1(A)->L+7(A) (4%), HOMO(A)->L+1(A) (2%), HOMO(A)->L+8(A) (4%), H-10(B)->LUMO(B) (9%), H-6(B)->L+1(B) (5%), H-2(B)->LUMO(B) (8%), H-2(B)->L+5(B) (2%), H-1(B)->L+1(B) (6%), H-1(B)->L+8(B) (6%), HOMO(B)->LUMO(B) (6%), HOMO(B)->L+5(B) (6%), HOMO(B)->L+6(B) (2%), HOMO(B)->L+9(B) (2%)
26	35230.2974587	283.846595724	0.2069	2.901-A	H-2(A)->LUMO(A) (14%), H-2(B)->L+1(B) (24%)	H-6(A)->L+1(A) (7%), H-4(A)->LUMO(A) (4%), H-1(A)->L+8(A) (3%), HOMO(A)->L+7(A) (4%), H-10(B)->L+1(B) (9%), H-5(B)->L+1(B) (2%), H-1(B)->L+5(B) (4%), HOMO(B)->L+8(B) (6%)
27	35979.5865233	277.935378538	0.0018	3.527-A	H-3(A)->L+4(A) (10%)	H-8(A)->L+3(A) (5%), H-8(A)->L+6(A) (2%), H-7(A)->L+1(A) (3%), H-7(A)->L+2(A) (5%), H-4(A)->L+6(A) (6%), H-3(A)->L+9(A) (2%), H-2(A)->L+6(A) (4%), H-9(B)->L+2(B) (6%), H-8(B)->LUMO(B) (3%), H-8(B)->L+3(B) (5%), H-7(B)->L+7(B) (2%), H-5(B)->L+7(B) (9%), H-4(B)->L+5(B) (3%), H-4(B)->L+6(B) (9%), H-3(B)->L+7(B) (2%)
28	35986.8455131	277.87931555	0.0	3.506-A	H-3(A)->L+6(A) (11%), H-4(B)->L+7(B) (11%)	H-8(A)->L+1(A) (2%), H-8(A)->L+2(A) (5%), H-7(A)->LUMO(A) (2%), H-7(A)->L+3(A) (5%), H-7(A)->L+6(A) (2%), H-5(A)->L+1(A) (2%), H-4(A)->L+4(A) (5%), H-2(A)->L+4(A) (3%), H-9(B)->LUMO(B) (2%), H-9(B)->L+3(B) (5%), H-8(B)->L+1(B) (2%), H-8(B)->L+2(B) (5%), H-8(B)->L+7(B) (2%), H-5(B)->L+5(B) (2%), H-5(B)->L+6(B) (7%), H-3(B)->L+6(B) (2%)
29	36594.9875526	273.261467452	0.0	2.897-A	H-5(A)->L+1(A) (29%), H-4(A)->L+1(A) (26%)	H-10(A)->L+1(A) (2%), H-8(A)->L+1(A) (5%), H-5(A)->L+2(A) (3%), H-4(A)->L+2(A) (3%), H-3(A)->LUMO(A) (2%), H-2(A)->L+1(A) (4%), H-1(A)->LUMO(A) (5%), HOMO(A)->L+1(A) (3%)
30	36857.117742	271.318014338	0.0	2.582-A	H-2(A)->L+1(A) (16%), H-1(A)->LUMO(A) (20%), HOMO(A)->L+1(A) (10%)	H-12(A)->L+1(A) (2%), H-11(A)->L+1(A) (4%), H-5(A)->L+1(A) (2%), HOMO(A)->L+2(A) (6%), HOMO(A)->L+8(A) (4%), H-10(B)->LUMO(B) (3%), H-6(B)->L+1(B) (3%), H-4(B)->L+1(B) (2%), H-2(B)->LUMO(B) (4%), H-1(B)->L+1(B) (4%)
31	37116.8282682	269.419572377	0.0	3.092-A	H-7(B)->LUMO(B) (53%), H-5(B)->LUMO(B) (19%)	H-5(A)->L+1(A) (2%), H-11(B)->L+1(B) (4%), H-7(B)->L+3(B) (2%), H-7(B)->L+5(B) (2%), H-7(B)->L+9(B) (4%)
32	37312.8209944	268.004394562	0.1519	2.941-A	H-1(A)->L+1(A) (25%), HOMO(A)->LUMO(A) (11%)	H-12(A)->LUMO(A) (3%), H-11(A)->LUMO(A) (6%), H-4(A)->LUMO(A) (6%), H-2(A)->LUMO(A) (6%), H-1(A)->L+8(A) (2%), HOMO(A)->L+3(A) (5%), HOMO(A)->L+7(A) (4%), H-10(B)->L+1(B) (5%), H-6(B)->LUMO(B) (5%), H-2(B)->L+1(B) (2%)
33	37464.453227	266.919683557	0.0942	2.956-A	H-5(A)->LUMO(A) (19%), H-4(A)->LUMO(A) (17%), H-2(A)->LUMO(A) (20%)	H-11(A)->LUMO(A) (2%), H-10(A)->LUMO(A) (2%), H-9(A)->L+1(A) (2%), H-8(A)->LUMO(A) (2%), H-3(A)->L+1(A) (5%), H-1(A)->L+1(A) (3%), H-10(B)->L+1(B) (2%), H-6(B)->LUMO(B) (2%), H-4(B)->LUMO(B) (2%)
34	38000.0053679	263.157857563	0.0298	3.128-A	H-7(B)->L+1(B) (49%), H-5(B)->L+1(B) (22%)	H-10(A)->LUMO(A) (2%), H-9(A)->L+1(A) (2%), H-4(A)->LUMO(A) (2%), H-1(A)->L+1(A) (2%), H-11(B)->LUMO(B) (5%)

35	38035.4937628	262.912322431	0.0	3.088-A	H-1(A)->LUMO(A) (13%), HOMO(A)->L+1(A) (17%), HOMO(A)->L+2(A) (10%)	H-11(A)->L+1(A) (5%), H-4(A)->L+1(A) (5%), H-2(A)->L+1(A) (5%), H-1(A)->L+7(A) (3%), HOMO(A)->L+8(A) (3%), H-10(B)->LUMO(B) (3%), H-6(B)->L+1(B) (2%), H-1(B)->L+1(B) (5%), HOMO(B)->LUMO(B) (7%), HOMO(B)->L+9(B) (2%)
36	38157.2834816	262.073163694	0.0352	2.845-A	H-4(A)->LUMO(A) (17%), H-1(A)->L+1(A) (13%), HOMO(A)->LUMO(A) (10%), HOMO(A)->L+3(A) (16%)	H-11(A)->LUMO(A) (8%), H-5(A)->LUMO(A) (4%), H-2(A)->LUMO(A) (3%), H-10(B)->L+1(B) (2%), H-7(B)->L+1(B) (4%), H-6(B)->LUMO(B) (2%), H-5(B)->L+1(B) (3%)
37	38537.977172	259.484299224	0.0491	2.507-A	H-1(B)->LUMO(B) (25%), HOMO(B)->L+1(B) (19%)	H-3(A)->L+1(A) (2%), H-1(A)->L+1(A) (2%), H-1(A)->L+8(A) (2%), HOMO(A)->L+7(A) (2%), H-7(B)->L+1(B) (3%), H-4(B)->LUMO(B) (7%), H-3(B)->L+1(B) (6%), H-2(B)->L+1(B) (3%), H-1(B)->L+5(B) (6%)
38	38749.2944324	258.069215104	0.0	2.460-A	H-5(A)->L+1(A) (18%)	H-10(A)->L+1(A) (4%), H-9(A)->LUMO(A) (6%), H-8(A)->L+1(A) (3%), H-4(A)->L+1(A) (2%), H-4(A)->L+2(A) (2%), H-3(A)->LUMO(A) (2%), H-3(A)->L+3(A) (5%), H-2(A)->L+1(A) (4%), H-1(A)->LUMO(A) (2%), H-5(B)->LUMO(B) (7%), H-4(B)->L+1(B) (9%), H-4(B)->L+2(B) (3%), H-3(B)->LUMO(B) (3%), H-1(B)->L+1(B) (4%), HOMO(B)->L+3(B) (2%)
39	39026.749156	256.234511361	0.1913	2.619-A	H-5(A)->LUMO(A) (11%), H-4(B)->LUMO(B) (13%)	H-8(A)->LUMO(A) (2%), H-4(A)->L+3(A) (4%), H-3(A)->L+1(A) (5%), H-3(A)->L+2(A) (5%), H-2(A)->L+3(A) (3%), H-1(A)->L+1(A) (2%), HOMO(A)->L+3(A) (4%), H-7(B)->L+1(B) (3%), H-5(B)->L+1(B) (5%), H-4(B)->L+3(B) (2%), H-3(B)->L+2(B) (2%), H-1(B)->LUMO(B) (6%), HOMO(B)->L+1(B) (7%), HOMO(B)->L+2(B) (5%)
40	39051.7523433	256.070455228	0.0	2.690-A	H-10(A)->L+1(A) (13%), H-9(A)->LUMO(A) (16%), H-1(B)->L+1(B) (11%)	H-5(A)->L+1(A) (6%), H-4(A)->L+1(A) (4%), H-4(A)->L+2(A) (3%), H-3(A)->LUMO(A) (2%), H-2(A)->L+1(A) (2%), H-7(B)->LUMO(B) (3%), H-4(B)->L+1(B) (2%), H-2(B)->LUMO(B) (9%), HOMO(B)->LUMO(B) (5%)
41	39325.9808492	254.284820978	0.0084	2.664-A	H-10(A)->LUMO(A) (20%), H-9(A)->L+1(A) (23%), H-5(A)->LUMO(A) (23%)	H-9(A)->L+2(A) (4%), H-4(A)->LUMO(A) (3%), HOMO(A)->L+3(A) (3%), H-7(B)->L+1(B) (7%)
42	39465.5147654	253.38577387	0.0	2.617-A	HOMO(A)->L+2(A) (15%)	H-11(A)->L+1(A) (2%), H-10(A)->L+1(A) (3%), H-9(A)->LUMO(A) (5%), H-3(A)->L+3(A) (3%), H-2(A)->L+1(A) (3%), H-2(A)->L+2(A) (2%), H-7(B)->LUMO(B) (7%), H-5(B)->LUMO(B) (3%), H-4(B)->L+1(B) (7%), H-2(B)->LUMO(B) (9%), H-1(B)->L+1(B) (9%), HOMO(B)->LUMO(B) (4%)
43	40117.210744	249.269573197	0.0	2.831-A	H-1(A)->LUMO(A) (19%), HOMO(A)->L+2(A) (44%)	H-12(A)->L+9(A) (2%), H-4(A)->L+1(A) (2%), H-1(A)->L+3(A) (2%), H-5(B)->LUMO(B) (3%), H-4(B)->L+1(B) (4%)
44	40218.0300477	248.644699607	0.0028	2.756-A	H-1(A)->L+1(A) (14%), HOMO(A)->L+3(A) (56%)	H-4(A)->L+3(A) (2%), H-1(A)->L+2(A) (6%), HOMO(A)->LUMO(A) (2%), H-4(B)->LUMO(B) (2%)
45	40434.1866346	247.315473175	0.0	3.062-A	H-4(B)->L+1(B) (11%), HOMO(B)->L+3(B) (22%)	H-10(A)->L+1(A) (4%), H-6(A)->LUMO(A) (2%), H-5(A)->L+1(A) (2%), H-3(A)->LUMO(A) (7%), H-5(B)->LUMO(B) (5%), H-5(B)->L+3(B) (3%), H-4(B)->L+2(B) (7%), H-3(B)->L+3(B) (2%), HOMO(B)->LUMO(B) (3%), HOMO(B)->L+5(B) (2%), HOMO(B)->L+6(B) (2%)
46	40599.5302926	246.308268296	0.0231	2.998-A	H-1(A)->L+2(A) (21%), H-1(A)->L+4(A) (10%), H-4(B)->LUMO(B) (10%)	H-3(A)->L+1(A) (2%), H-2(A)->LUMO(A) (2%), H-1(A)->L+5(A) (4%), H-1(A)->L+9(A) (6%), H-7(B)->L+1(B) (2%), H-5(B)->L+1(B) (5%), H-5(B)->L+2(B) (2%), H-4(B)->L+3(B) (7%), H-3(B)->L+2(B) (2%)

47	40926.1848363	244.342345616	0.0083	3.127-A	H-1(A)->L+2(A) (15%), H-1(A)->L+4(A) (10%)	H-10(A)->LUMO(A) (2%), H-5(A)->LUMO(A) (3%), H-3(A)->L+1(A) (6%), H-1(A)->L+5(A) (4%), H-1(A)->L+9(A) (5%), HOMO(A)->L+3(A) (3%), H-5(B)->L+1(B) (4%), H-5(B)->L+2(B) (2%), H-4(B)->LUMO(B) (7%), H-4(B)->L+3(B) (6%), H-3(B)->L+2(B) (2%), H-1(B)->LUMO(B) (2%), H-1(B)->L+3(B) (4%), HOMO(B)->L+2(B) (3%)
48	41047.9745551	243.617379624	0.0	2.881-A	H-3(A)->LUMO(A) (11%), HOMO(B)->L+3(B) (33%)	H-11(A)->L+1(A) (2%), H-5(A)->L+1(A) (2%), H-4(A)->L+1(A) (3%), H-5(B)->L+3(B) (3%), H-4(B)->L+2(B) (2%), H-1(B)->L+2(B) (2%), HOMO(B)->LUMO(B) (2%), HOMO(B)->L+6(B) (3%), HOMO(B)->L+9(B) (2%)
49	41397.2126229	241.562157605	0.037	2.667-A	H-1(B)->L+3(B) (19%), H-1(B)->L+5(B) (10%), HOMO(B)->L+2(B) (38%)	H-11(B)->LUMO(B) (2%), H-5(B)->L+2(B) (2%), H-1(B)->L+6(B) (4%)
50	41767.4211058	239.421054383	0.0081	3.017-A	H-1(B)->L+3(B) (11%), HOMO(B)->L+2(B) (15%)	H-11(A)->LUMO(A) (2%), H-5(A)->LUMO(A) (3%), H-4(A)->LUMO(A) (3%), H-3(A)->L+1(A) (8%), H-3(A)->L+2(A) (3%), H-1(A)->L+4(A) (2%), H-11(B)->LUMO(B) (3%), H-2(B)->L+2(B) (6%), H-1(B)->LUMO(B) (6%), H-1(B)->L+5(B) (2%)
51	41834.3651234	239.037928997	0.0	2.592-A	H-3(A)->LUMO(A) (17%)	H-8(A)->L+2(A) (2%), H-5(A)->L+1(A) (4%), H-4(A)->L+1(A) (2%), H-4(A)->L+2(A) (4%), H-3(A)->L+3(A) (8%), H-2(A)->L+2(A) (2%), H-11(B)->L+1(B) (5%), H-5(B)->LUMO(B) (2%), H-5(B)->L+3(B) (2%), H-4(B)->L+1(B) (3%), H-4(B)->L+2(B) (3%), H-3(B)->L+3(B) (4%), H-1(B)->L+2(B) (7%), HOMO(B)->L+3(B) (2%)
52	41935.184427	238.463241229	0.0165	2.841-A	H-11(B)->LUMO(B) (39%)	H-10(A)->LUMO(A) (2%), H-12(B)->L+1(B) (5%), H-11(B)->L+3(B) (2%), H-11(B)->L+5(B) (3%), H-8(B)->LUMO(B) (4%), H-7(B)->L+1(B) (6%), H-3(B)->L+2(B) (2%), H-2(B)->L+1(B) (2%), H-2(B)->L+2(B) (7%), HOMO(B)->L+2(B) (8%)
53	41944.8630801	238.408216541	0.0	2.938-A	H-3(A)->LUMO(A) (11%), H-11(B)->L+1(B) (13%)	H-11(A)->L+1(A) (2%), H-10(A)->L+1(A) (3%), H-3(A)->L+3(A) (2%), H-1(A)->L+3(A) (2%), H-12(B)->LUMO(B) (3%), H-10(B)->LUMO(B) (6%), H-8(B)->L+1(B) (3%), H-7(B)->LUMO(B) (2%), H-6(B)->L+1(B) (4%), H-4(B)->L+1(B) (2%), H-1(B)->L+2(B) (2%), HOMO(B)->L+5(B) (3%)
54	42412.664649	235.778630811	0.0563	2.597-A	H-3(A)->L+1(A) (17%), H-3(A)->L+2(A) (10%)	H-10(A)->LUMO(A) (2%), H-5(A)->LUMO(A) (7%), H-4(A)->LUMO(A) (2%), H-4(A)->L+3(A) (3%), H-2(A)->L+3(A) (3%), H-1(A)->L+4(A) (2%), H-8(B)->L+3(B) (2%), H-5(B)->L+2(B) (2%), H-4(B)->L+3(B) (3%), H-2(B)->L+2(B) (5%), H-1(B)->L+3(B) (7%)
55	42443.3137173	235.608370888	0.0	2.919-A	H-11(B)->L+1(B) (21%)	H-12(B)->LUMO(B) (3%), H-10(B)->LUMO(B) (2%), H-6(B)->L+1(B) (5%), H-4(B)->L+1(B) (6%), H-3(B)->L+3(B) (2%), H-2(B)->L+3(B) (9%), H-1(B)->L+1(B) (2%), H-1(B)->L+2(B) (6%), HOMO(B)->L+3(B) (6%), HOMO(B)->L+5(B) (8%)
56	42605.4311575	234.711860162	0.1054	2.772-A	H-6(B)->LUMO(B) (15%)	H-11(A)->LUMO(A) (3%), H-6(A)->L+1(A) (4%), H-14(B)->L+1(B) (2%), H-11(B)->LUMO(B) (6%), H-10(B)->L+1(B) (8%), H-4(B)->LUMO(B) (3%), H-3(B)->L+1(B) (3%), H-2(B)->L+1(B) (3%), H-1(B)->LUMO(B) (2%), H-1(B)->L+3(B) (4%), H-1(B)->L+5(B) (4%), HOMO(B)->L+8(B) (4%)
57	42647.3719878	234.481036788	0.0	3.226-A	HOMO(A)->L+4(A) (10%)	H-11(A)->L+1(A) (2%), H-8(A)->L+4(A) (2%), H-7(A)->L+6(A) (3%), H-6(A)->LUMO(A) (2%), H-3(A)->LUMO(A) (2%), H-2(A)->L+1(A) (2%), H-1(A)->L+3(A) (2%), HOMO(A)->L+5(A) (2%), HOMO(A)->L+8(A) (2%), HOMO(A)->L+15(A) (3%), H-11(B)->L+1(B) (4%), H-9(B)->L+6(B) (3%), H-8(B)->L+7(B) (3%), H-3(B)->LUMO(B) (2%), H-1(B)->L+1(B) (3%), HOMO(B)->L+3(B) (3%), HOMO(B)->L+5(B) (5%), HOMO(B)->L+9(B) (3%)
58	42802.2304382	233.632684503	0.0	3.227-A		H-11(A)->L+1(A) (4%), H-8(A)->L+4(A) (5%), H-7(A)->L+6(A) (6%), H-6(A)->LUMO(A) (3%), H-3(A)->L+6(A) (2%), H-1(A)->L+3(A) (8%), HOMO(A)->L+4(A) (2%), HOMO(A)->L+8(A) (2%), H-9(B)->LUMO(B) (2%), H-9(B)->L+5(B) (2%), H-9(B)->L+6(B) (6%), H-8(B)->L+7(B) (7%), H-6(B)->L+1(B) (3%), H-1(B)->L+1(B) (2%), H-1(B)->L+2(B) (2%), HOMO(B)->L+3(B) (2%), HOMO(B)->L+6(B) (2%)

59	42907.8890684	233.057375162	0.0016	3.515-A	H-8(A)->L+6(A) (11%), H-7(A)->L+4(A) (10%), H-9(B)->L+7(B) (14%), H-8(B)->L+6(B) (10%)	H-7(A)->L+9(A) (2%), H-6(A)->L+4(A) (2%), H-5(A)->L+6(A) (4%), H-3(A)->L+4(A) (3%), H-8(B)->L+5(B) (3%), H-6(B)->L+6(B) (2%), H-5(B)->L+7(B) (2%), H-4(B)->L+6(B) (2%), HOMO(B)->L+7(B) (2%)
60	43175.6651388	231.611950108	0.0	2.855-A	H-2(B)->L+3(B) (26%), H-1(B)->L+2(B) (20%)	H-11(A)->L+1(A) (2%), H-6(A)->LUMO(A) (5%), H-11(B)->L+1(B) (4%), H-10(B)->LUMO(B) (2%), H-6(B)->L+1(B) (8%), HOMO(B)->L+9(B) (2%)

Table S4: Full list of 60 TD-DFT-calculated excited singlet states (CAM-B3LYP/DEF2-QZVP/GD3BJ in a DMSO solvent continuum) for **C3**. State energies are uncorrected. DMSO was chosen as the solvent medium to allow assignment of the UV-vis spectra of **C3**.

No.	Energy (cm ⁻¹)	Wavelength (nm)	Osc. Strength	Symmetry	Major contributions	Minor contributions			
1	14155.0302289	706.462638246	0.0002	2.008-A	H-10(B)->L+1(B) (15%), HOMO(B)->L+1(B) (23%)	H-25(B)->L+1(B) (4%), H-24(B)->L+1(B) (3%), H-20(B)->L+1(B) (2%), H-18(B)->L+1(B) (4%), H-10(B)->LUMO(B) (5%), H-10(B)->L+4(B) (2%), H-7(B)->L+1(B) (2%), H-5(B)->L+1(B) (2%), HOMO(B)->LUMO(B) (8%), HOMO(B)->L+4(B) (2%)			
2	17415.9297854	574.186972687	0.0004	2.004-A	H-11(B)->L+1(B) (23%)	H-33(B)->L+1(B) (4%), H-17(B)->L+1(B) (2%), H-13(B)->L+1(B) (4%), H-12(B)->LUMO(B) (3%), H-12(B)->L+1(B) (8%), H-11(B)->LUMO(B) (9%), H-11(B)->L+4(B) (3%), H-9(B)->LUMO(B) (3%), H-9(B)->L+1(B) (9%), H-1(B)->L+1(B) (2%)			
3	18246.6808473	548.044879159	0.0022	2.003-A	H-12(B)->L+1(B) (23%)	H-29(B)->LUMO(B) (2%), H-29(B)->L+1(B) (4%), H-28(B)->LUMO(B) (2%), H-28(B)->L+1(B) (5%), H-21(B)->L+1(B) (2%), H-19(B)->L+1(B) (2%), H-14(B)->L+1(B) (3%), H-12(B)->LUMO(B) (9%), H-12(B)->L+4(B) (3%), H-11(B)->LUMO(B) (2%), H-11(B)->L+1(B) (5%), H-10(B)->LUMO(B) (2%), H-10(B)->L+1(B) (6%), H-4(B)->LUMO(B) (2%), H-4(B)->L+1(B) (4%)			
4	19223.4182608	520.198846237	0.0001	2.004-A	H-33(B)->L+1(B) (11%)	H-34(B)->L+1(B) (2%), H-33(B)->LUMO(B) (4%), H-31(B)->LUMO(B) (4%), H-31(B)->L+1(B) (9%), H-21(B)->L+1(B) (4%), H-19(B)->LUMO(B) (2%), H-19(B)->L+1(B) (6%), H-17(B)->L+1(B) (3%), H-15(B)->LUMO(B) (2%), H-15(B)->L+1(B) (6%), H-12(B)->L+1(B) (2%), H-11(B)->L+1(B) (3%), H-9(B)->LUMO(B) (3%), H-9(B)->L+1(B) (9%), H-1(B)->L+1(B) (2%)			
5	20840.5598909	479.833557848	0.0	3.450-A	H-1(A)->LUMO(A) (13%), HOMO(A)->LUMO(A) (25%), HOMO(B)->LUMO(B) (17%)	H-5(A)->LUMO(A) (2%), H-3(A)->LUMO(A) (2%), HOMO(A)->L+3(A) (2%), H-2(B)->LUMO(B) (2%), H-1(B)->LUMO(B) (8%), H-1(B)->L+1(B) (5%), HOMO(B)->L+1(B) (8%)			
6	21631.7897858	462.282598852	0.0	3.456-A	H-1(A)->L+1(A) (19%), HOMO(A)->L+1(A) (21%), H-1(B)->L+2(B) (16%), HOMO(B)->L+2(B) (24%)	H-4(A)->L+1(A) (6%), H-4(B)->L+2(B) (5%)			
7	24637.0115882	405.893383789	0.0011	3.422-A	H-3(A)->LUMO(A) (11%), H-2(B)->LUMO(B) (17%)	H-8(A)->L+6(A) (2%), H-7(A)->LUMO(A) (2%), H-7(A)->L+3(A) (8%), H-2(A)->LUMO(A) (9%), HOMO(A)->L+3(A) (2%), H-7(B)->L+4(B) (2%), H-6(B)->L+3(B) (2%), H-6(B)->L+4(B) (4%), H-1(B)->L+1(B) (3%), HOMO(B)->L+1(B) (2%)			
8	25491.959283	392.280557528	0.0006	3.433-A	H-6(A)->L+2(A) (17%)	H-6(A)->L+3(A) (2%), H-6(A)->L+5(A) (2%), H-5(A)->L+2(A) (3%), H-5(A)->L+5(A) (2%), H-3(A)->L+2(A) (4%), H-3(A)->L+5(A) (3%), H-2(A)->L+2(A) (5%), H-2(A)->L+5(A) (3%), H-6(B)->L+3(B) (3%), H-5(B)->L+3(B) (8%), H-5(B)->L+4(B) (4%), H-3(B)->LUMO(B) (2%), H-3(B)->L+1(B) (3%), H-3(B)->L+3(B) (7%), H-3(B)->L+4(B) (2%), H-3(B)->L+6(B) (7%), H-3(B)->L+7(B) (2%)			
9	26047.6752846	383.911419762	0.0002	3.430-A		H-8(A)->LUMO(A) (2%), H-7(A)->LUMO(A) (2%), H-7(A)->L+3(A) (2%), H-5(A)->LUMO(A) (5%), H-4(A)->L+1(A) (8%), H-3(A)->LUMO(A) (2%), H-3(A)->L+3(A) (2%), H-1(A)->L+7(A) (3%), HOMO(A)->L+8(A) (3%), H-6(B)->LUMO(B) (5%), H-5(B)->LUMO(B) (2%), H-4(B)->L+2(B) (8%), H-2(B)->L+1(B) (3%), H-2(B)->L+4(B) (2%), H-2(B)->L+7(B) (2%), H-1(B)->L+1(B) (4%), H-1(B)->L+8(B) (4%), HOMO(B)->L+9(B) (4%)			

10	26105.7472034	383.057413453	0.0003	3.448-A	H-4(A)->L+1(A) (15%), H-4(B)->L+2(B) (14%)	H-5(A)->LUMO(A) (3%), H-1(A)->L+1(A) (2%), H-1(A)->L+8(A) (4%), HOMO(A)->L+1(A) (2%), HOMO(A)->L+7(A) (3%), H-6(B)->LUMO(B) (3%), H-2(B)->L+1(B) (2%), H-1(B)->L+2(B) (2%), H-1(B)->L+9(B) (5%), HOMO(B)->L+8(B) (4%)			
11	28397.9748907	352.137785828	0.0178	2.110-A	H-1(B)->LUMO(B) (14%), H-1(B)->L+1(B) (54%)	H-1(A)->LUMO(A) (3%), HOMO(A)->LUMO(A) (5%), H-13(B)->L+1(B) (2%), H-1(B)->L+2(B) (2%), H-1(B)->L+4(B) (2%), HOMO(B)->LUMO(B) (2%)			
12	28706.885237	348.348485649	0.1644	2.052-A	H-1(A)->LUMO(A) (10%), HOMO(A)->LUMO(A) (19%), H-1(B)->LUMO(B) (16%), HOMO(B)->LUMO(B) (35%)	H-8(B)->L+1(B) (2%), H-1(B)->L+4(B) (2%)			
13	29421.4924611	339.887584331	0.0657	2.084-A	HOMO(B)->L+1(B) (33%), HOMO(B)->L+2(B) (11%)	H-1(A)->LUMO(A) (3%), H-1(A)->L+1(A) (2%), HOMO(A)->LUMO(A) (5%), HOMO(A)->L+1(A) (3%), H-18(B)->L+1(B) (3%), H-8(B)->L+1(B) (2%), H-7(B)->L+1(B) (2%), H-5(B)->L+1(B) (2%), H-1(B)->LUMO(B) (4%), H-1(B)->L+2(B) (4%), HOMO(B)->LUMO(B) (2%)			
14	30073.9949941	332.513189616	0.1745	2.052-A	H-1(A)->L+1(A) (20%), HOMO(A)->L+1(A) (20%), H-1(B)->L+2(B) (13%), HOMO(B)->L+1(B) (12%), HOMO(B)->L+2(B) (19%)				
15	31555.6354802	316.900605798	0.0042	2.799-A	H-5(A)->LUMO(A) (10%), H-2(A)->LUMO(A) (42%)	H-9(A)->LUMO(A) (5%), H-8(A)->L+3(A) (2%), H-7(A)->LUMO(A) (4%), H-7(A)->L+3(A) (2%), H-1(A)->LUMO(A) (6%), HOMO(A)->LUMO(A) (2%), H-7(B)->LUMO(B) (2%)			
16	31770.9855127	314.752590724	0.003	2.743-A	H-2(A)->L+1(A) (52%)	H-9(A)->L+1(A) (6%), H-8(A)->L+1(A) (2%), H-3(A)->L+1(A) (9%), H-1(A)->L+1(A) (3%), HOMO(A)->L+1(A) (4%)			
17	32582.3792683	306.914357532	0.0014	3.275-A		H-9(A)->LUMO(A) (3%), H-8(A)->LUMO(A) (3%), H-8(A)->L+3(A) (5%), H-7(A)->L+3(A) (3%), H-5(A)->LUMO(A) (5%), H-3(A)->LUMO(A) (3%), H-3(A)->L+3(A) (3%), H-2(A)->LUMO(A) (3%), H-2(A)->L+3(A) (6%), H-1(A)->LUMO(A) (2%), HOMO(A)->LUMO(A) (4%), HOMO(A)->L+3(A) (3%), H-8(B)->L+3(B) (2%), H-8(B)->L+4(B) (3%), H-7(B)->L+3(B) (2%), H-7(B)->L+4(B) (3%), H-2(B)->LUMO(B) (7%), H-2(B)->L+3(B) (2%), H-2(B)->L+4(B) (4%), HOMO(B)->L+4(B) (2%)			
18	33005.0137891	302.98426972	0.0005	3.347-A	H-2(A)->L+2(A) (13%), H-3(B)->L+3(B) (11%)	H-7(A)->L+2(A) (2%), H-6(A)->L+2(A) (5%), H-5(A)->L+2(A) (3%), H-3(A)->L+2(A) (4%), H-3(A)->L+3(A) (4%), H-2(A)->L+1(A) (3%), HOMO(A)->L+7(A) (2%), H-7(B)->L+3(B) (2%), H-6(B)->L+3(B) (3%), H-3(B)->L+4(B) (4%), H-2(B)->L+4(B) (2%), HOMO(B)->L+8(B) (2%)			
19	33072.7643611	302.363597152	0.0004	3.415-A		H-8(A)->L+3(A) (2%), H-6(A)->L+2(A) (2%), H-5(A)->LUMO(A) (3%), H-3(A)->L+2(A) (4%), H-3(A)->L+3(A) (3%), H-2(A)->L+3(A) (5%), H-1(A)->L+7(A) (5%), HOMO(A)->L+3(A) (2%), HOMO(A)->L+7(A) (6%), HOMO(A)->L+8(A) (2%), H-3(B)->L+3(B) (2%), H-3(B)->L+4(B) (2%), H-2(B)->L+3(B) (3%), H-2(B)->L+4(B) (4%), H-1(B)->L+8(B) (6%), HOMO(B)->L+8(B) (6%), HOMO(B)->L+9(B) (2%)			
20	33289.7275025	300.392966546	0.0016	3.444-A	H-4(A)->L+1(A) (12%), H-1(A)->L+8(A) (11%), H-4(B)->L+2(B) (10%), H-1(B)->L+9(B) (10%), HOMO(B)->L+9(B) (10%)	H-1(A)->L+7(A) (4%), HOMO(A)->L+7(A) (3%), HOMO(A)->L+8(A) (9%), H-1(B)->L+8(B) (4%), HOMO(B)->L+8(B) (3%)			
21	35244.008884	283.736167271	0.0345	3.313-A	H-8(B)->LUMO(B) (10%)	H-8(A)->LUMO(A) (7%), H-8(A)->L+6(A) (2%), H-7(A)->LUMO(A) (2%), H-7(A)->L+3(A) (6%), H-3(A)->L+6(A) (4%), H-2(A)->L+6(A) (3%), HOMO(A)->L+6(A) (2%), H-7(B)->LUMO(B) (4%), H-6(B)->L+4(B) (2%), H-2(B)->LUMO(B) (3%), H-2(B)->L+6(B) (2%), H-2(B)->L+7(B) (5%), H-1(B)->LUMO(B) (3%), HOMO(B)->LUMO(B) (3%), HOMO(B)->L+7(B) (2%)			

22	35649.7057618	280.50722401	0.1372	2.637-A	HOMO(B)->LUMO(B) (10%)	H-6(A)->L+2(A) (3%), H-2(A)->L+5(A) (3%), H-1(A)->LUMO(A) (2%), HOMO(A)->LUMO(A) (2%), H-10(B)->L+1(B) (2%), H-8(B)->L+1(B) (4%), H-7(B)->LUMO(B) (2%), H-7(B)->L+1(B) (2%), H-5(B)->LUMO(B) (3%), H-5(B)->L+1(B) (6%), H-3(B)->LUMO(B) (2%), H-3(B)->L+1(B) (4%), H-3(B)->L+6(B) (4%), H-2(B)->L+1(B) (2%), H-1(B)->LUMO(B) (8%), H-1(B)->L+1(B) (3%)		
23	35826.3411818	279.124232901	0.0281	2.890-A	H-1(B)->LUMO(B) (13%)	H-6(A)->L+2(A) (6%), H-5(A)->L+5(A) (2%), H-3(A)->LUMO(A) (2%), H-3(A)->L+5(A) (4%), H-2(A)->LUMO(A) (2%), H-2(A)->L+5(A) (3%), H-1(A)->LUMO(A) (4%), HOMO(A)->LUMO(A) (2%), H-6(B)->L+3(B) (2%), H-5(B)->L+3(B) (2%), H-3(B)->L+2(B) (2%), H-3(B)->L+6(B) (7%), H-1(B)->L+1(B) (5%), HOMO(B)->LUMO(B) (6%), HOMO(B)->L+1(B) (3%), HOMO(B)->L+4(B) (2%)		
24	35994.9110574	277.817049862	0.0535	2.401-A	H-8(B)->L+1(B) (12%), H-7(B)->L+1(B) (10%)	H-6(A)->L+2(A) (3%), H-3(A)->LUMO(A) (2%), H-2(A)->L+5(A) (2%), H-1(A)->LUMO(A) (4%), H-24(B)->L+1(B) (2%), H-10(B)->L+1(B) (2%), H-8(B)->LUMO(B) (2%), H-7(B)->LUMO(B) (3%), H-5(B)->L+1(B) (6%), H-5(B)->L+3(B) (2%), H-3(B)->L+6(B) (3%), H-2(B)->LUMO(B) (2%), H-1(B)->LUMO(B) (6%), H-1(B)->L+1(B) (2%), HOMO(B)->L+1(B) (2%), HOMO(B)->L+2(B) (2%)		
25	36319.9524923	275.330756617	0.0658	3.222-A	H-1(A)->LUMO(A) (25%), HOMO(A)->LUMO(A) (21%), H-2(B)->LUMO(B) (11%)	H-2(A)->LUMO(A) (8%), HOMO(A)->L+3(A) (3%), H-1(B)->LUMO(B) (8%), H-1(B)->L+1(B) (3%), HOMO(B)->LUMO(B) (5%), HOMO(B)->L+1(B) (2%)		
26	37525.7513637	266.483671522	0.1688	2.459-A	H-3(A)->LUMO(A) (10%), H-1(A)->LUMO(A) (13%), H-2(B)->LUMO(B) (16%)	H-5(A)->LUMO(A) (4%), H-2(A)->L+3(A) (3%), H-1(A)->L+3(A) (3%), HOMO(A)->LUMO(A) (4%), H-7(B)->LUMO(B) (4%), H-5(B)->LUMO(B) (3%), H-2(B)->L+1(B) (5%), H-1(B)->LUMO(B) (2%)		
27	37813.6912948	264.454478195	0.0197	2.772-A	H-1(B)->L+2(B) (38%), HOMO(B)->L+2(B) (27%)	H-2(A)->L+2(A) (2%), H-10(B)->L+2(B) (2%), H-3(B)->L+1(B) (2%), H-3(B)->L+2(B) (7%), HOMO(B)->L+3(B) (3%)		
28	38212.9357372	261.691487636	0.0499	2.612-A	H-2(B)->L+1(B) (31%)	H-8(A)->LUMO(A) (4%), H-5(A)->LUMO(A) (4%), H-2(A)->L+1(A) (2%), H-1(A)->L+1(A) (4%), HOMO(A)->L+1(A) (4%), H-8(B)->L+1(B) (2%), H-3(B)->LUMO(B) (2%), H-3(B)->L+1(B) (2%), H-3(B)->L+2(B) (2%), HOMO(B)->L+3(B) (3%), HOMO(B)->L+4(B) (2%)		
29	38316.9812585	260.980893368	0.001	2.690-A	H-1(A)->L+1(A) (12%), HOMO(A)->L+1(A) (17%), H-2(B)->L+1(B) (15%)	H-2(A)->L+1(A) (5%), HOMO(A)->L+2(A) (3%), H-5(B)->LUMO(B) (2%), H-3(B)->L+2(B) (3%), HOMO(B)->L+3(B) (4%)		
30	38404.8956913	260.383469868	0.0185	2.546-A	H-1(A)->L+1(A) (10%), H-5(B)->LUMO(B) (11%)	H-5(A)->LUMO(A) (3%), H-3(A)->LUMO(A) (3%), H-2(A)->L+1(A) (2%), HOMO(A)->L+1(A) (8%), H-9(B)->LUMO(B) (2%), H-9(B)->L+1(B) (7%), H-8(B)->LUMO(B) (6%), H-7(B)->LUMO(B) (6%), H-7(B)->L+1(B) (2%), H-5(B)->L+1(B) (5%), H-4(B)->LUMO(B) (3%), H-3(B)->LUMO(B) (4%)		
31	38654.1210098	258.70462809	0.0822	2.622-A	H-4(B)->L+2(B) (10%), H-3(B)->L+2(B) (13%)	H-4(A)->L+1(A) (2%), H-1(A)->L+1(A) (8%), HOMO(A)->L+1(A) (6%), H-9(B)->L+2(B) (5%), H-8(B)->LUMO(B) (3%), H-8(B)->L+2(B) (9%), H-7(B)->L+2(B) (6%), H-5(B)->LUMO(B) (2%), H-5(B)->L+2(B) (5%), H-3(B)->L+1(B) (2%), H-1(B)->L+2(B) (3%)		
32	39065.4637686	255.98057812	0.1702	2.321-A	H-2(A)->L+2(A) (11%), HOMO(B)->L+3(B) (17%)	H-6(A)->L+5(A) (2%), H-3(A)->L+2(A) (4%), HOMO(A)->L+2(A) (3%), H-8(B)->L+2(B) (2%), H-5(B)->L+2(B) (3%), H-3(B)->LUMO(B) (2%), H-3(B)->L+1(B) (4%), H-3(B)->L+2(B) (3%), H-3(B)->L+3(B) (7%), H-3(B)->L+4(B) (3%), H-1(B)->L+2(B) (3%), HOMO(B)->L+2(B) (2%), HOMO(B)->L+4(B) (2%)		
33	39177.5748342	255.248060716	0.0816	2.531-A	HOMO(A)->L+3(A) (10%)	H-9(A)->LUMO(A) (2%), H-7(A)->LUMO(A) (3%), H-3(A)->LUMO(A) (8%), H-3(A)->L+3(A) (2%), H-2(A)->L+3(A) (3%), HOMO(A)->L+2(A) (3%), H-8(B)->LUMO(B) (3%), H-8(B)->L+1(B) (2%), H-6(B)->L+1(B) (2%), H-2(B)->LUMO(B) (7%), H-2(B)->L+1(B) (2%), H-2(B)->L+4(B) (5%), HOMO(B)->L+3(B) (4%), HOMO(B)->L+4(B) (4%)		

34	39363.8889073	254.039940605	0.0112	2.889-A	HOMO(B)->L+4(B) (16%)	H-15(A)->LUMO(A) (2%), H-8(A)->L+6(A) (2%), H-4(A)->L+1(A) (2%), HOMO(A)->L+7(A) (2%), H-7(B)->LUMO(B) (2%), H-6(B)->LUMO(B) (6%), H-3(B)->L+3(B) (2%), H-2(B)->LUMO(B) (9%), H-2(B)->L+1(B) (6%), H-2(B)->L+4(B) (2%)			
35	40102.6927643	249.359813785	0.0434	3.027-A	HOMO(A)->L+2(A) (19%), H-3(B)->L+1(B) (12%), HOMO(B)->L+3(B) (24%)	H-3(B)->LUMO(B) (4%), H-2(B)->L+1(B) (2%), HOMO(B)->L+4(B) (7%)			
36	40329.3345589	247.958467686	0.0309	2.910-A	H-3(B)->L+1(B) (11%)	H-14(A)->L+1(A) (4%), H-4(A)->L+1(A) (7%), H-13(B)->L+2(B) (3%), H-4(B)->L+1(B) (2%), H-4(B)->L+2(B) (2%), H-4(B)->L+9(B) (2%), H-3(B)->LUMO(B) (3%), H-3(B)->L+2(B) (4%), H-3(B)->L+3(B) (2%), H-3(B)->L+4(B) (2%), H-1(B)->L+2(B) (3%), H-1(B)->L+3(B) (2%), HOMO(B)->L+2(B) (4%), HOMO(B)->L+9(B) (2%)			
37	40412.409665	247.448743663	0.0222	2.996-A	HOMO(B)->L+3(B) (14%)	H-14(A)->L+1(A) (3%), H-12(A)->L+1(A) (2%), H-4(A)->L+1(A) (3%), H-4(A)->L+8(A) (2%), HOMO(A)->L+1(A) (2%), HOMO(A)->L+2(A) (2%), HOMO(A)->L+8(A) (2%), H-14(B)->L+2(B) (2%), H-13(B)->L+2(B) (2%), H-12(B)->L+2(B) (2%), H-4(B)->L+2(B) (4%), H-3(B)->L+1(B) (3%), H-3(B)->L+2(B) (3%), H-3(B)->L+3(B) (5%), H-3(B)->L+4(B) (3%), HOMO(B)->L+4(B) (3%)			
38	40543.0714825	246.651268252	0.2394	2.289-A	H-4(A)->L+1(A) (16%), H-4(B)->L+2(B) (10%)	H-1(A)->L+1(A) (2%), HOMO(A)->L+2(A) (2%), H-9(B)->LUMO(B) (4%), H-9(B)->L+1(B) (6%), H-5(B)->LUMO(B) (4%), H-5(B)->L+1(B) (2%), H-4(B)->L+1(B) (2%), H-3(B)->L+1(B) (2%), H-3(B)->L+2(B) (9%), H-2(B)->LUMO(B) (2%), HOMO(B)->L+3(B) (2%), HOMO(B)->L+4(B) (2%)			
39	40639.0514596	246.068735387	0.044	2.294-A	HOMO(A)->L+2(A) (51%)	H-3(A)->L+2(A) (3%), H-2(A)->L+2(A) (2%), H-1(A)->L+2(A) (5%), HOMO(A)->L+3(A) (5%), H-3(B)->L+1(B) (2%), H-3(B)->L+3(B) (2%), HOMO(B)->L+3(B) (5%), HOMO(B)->L+4(B) (4%)			
40	40838.2704036	244.86835268	0.0129	3.356-A	HOMO(A)->L+3(A) (24%), HOMO(B)->L+4(B) (17%)	H-1(A)->LUMO(A) (3%), H-8(B)->LUMO(B) (2%), H-2(B)->L+4(B) (3%), H-1(B)->LUMO(B) (3%), HOMO(B)->L+7(B) (2%), HOMO(B)->L+14(B) (2%)			
41	41331.0751597	241.948702311	0.0056	2.642-A	H-1(A)->L+3(A) (13%), HOMO(A)->L+3(A) (18%)	H-7(A)->L+3(A) (2%), H-2(A)->L+3(A) (2%), H-1(A)->L+2(A) (5%), HOMO(A)->L+2(A) (2%), H-8(B)->LUMO(B) (5%), H-7(B)->LUMO(B) (6%), H-6(B)->L+7(B) (2%), H-2(B)->L+4(B) (3%), HOMO(B)->L+3(B) (2%), HOMO(B)->L+4(B) (5%), HOMO(B)->L+7(B) (2%)			
42	41615.7888731	240.293414369	0.0056	3.018-A	H-7(A)->LUMO(A) (10%), H-7(A)->L+6(A) (11%)	H-8(A)->LUMO(A) (3%), H-7(A)->L+5(A) (2%), H-3(A)->LUMO(A) (2%), H-3(A)->L+3(A) (2%), H-3(A)->L+6(A) (2%), H-2(A)->L+3(A) (4%), H-1(A)->L+2(A) (2%), H-1(A)->L+3(A) (2%), HOMO(A)->L+3(A) (6%), HOMO(A)->L+6(A) (2%), H-7(B)->LUMO(B) (2%), H-7(B)->L+4(B) (2%), H-7(B)->L+7(B) (2%), H-6(B)->LUMO(B) (5%), H-6(B)->L+7(B) (2%), H-1(B)->L+3(B) (2%), H-1(B)->L+4(B) (2%)			
43	41815.0078171	239.148586167	0.0071	3.287-A	H-1(B)->L+3(B) (14%)	H-6(A)->L+5(A) (4%), H-1(A)->L+2(A) (5%), H-1(A)->L+3(A) (5%), H-9(B)->L+2(B) (2%), H-8(B)->L+2(B) (2%), H-6(B)->LUMO(B) (3%), H-5(B)->L+2(B) (3%), H-5(B)->L+6(B) (2%), H-3(B)->L+2(B) (4%), H-1(B)->L+4(B) (7%), HOMO(B)->L+3(B) (2%), HOMO(B)->L+4(B) (3%)			
44	41906.955022	238.623875076	0.0025	3.250-A		H-9(A)->L+1(A) (2%), H-6(A)->L+5(A) (4%), H-5(A)->L+1(A) (4%), H-3(A)->L+1(A) (2%), H-1(A)->L+3(A) (5%), H-9(B)->L+2(B) (4%), H-8(B)->L+2(B) (4%), H-7(B)->LUMO(B) (2%), H-7(B)->L+2(B) (2%), H-5(B)->L+2(B) (4%), H-3(B)->L+2(B) (8%), H-3(B)->L+3(B) (2%), H-1(B)->L+3(B) (5%), H-1(B)->L+4(B) (6%), HOMO(B)->L+4(B) (5%)			
45	42039.2299483	237.873053628	0.0755	2.122-A	H-4(B)->LUMO(B) (11%), H-4(B)->L+1(B) (21%)	H-4(A)->L+1(A) (4%), H-9(B)->LUMO(B) (3%), H-9(B)->L+1(B) (5%), H-6(B)->LUMO(B) (2%), H-6(B)->L+1(B) (3%), H-5(B)->LUMO(B) (2%), H-5(B)->L+1(B) (2%), H-4(B)->L+2(B) (7%), H-3(B)->L+1(B) (2%), H-3(B)->L+2(B) (3%)			
46	42417.5039755	235.751731308	0.002	3.005-A	H-1(A)->L+2(A) (26%)	H-6(A)->L+5(A) (3%), H-1(A)->L+3(A) (6%), H-8(B)->L+2(B) (2%), H-7(B)->L+2(B) (2%), H-6(B)->L+1(B) (3%), H-6(B)->L+6(B) (2%), H-5(B)->L+1(B) (2%), H-5(B)->L+6(B) (5%), H-4(B)->L+1(B) (2%), H-3(B)->L+2(B) (3%), H-3(B)->L+6(B) (4%)			

47	42566.7165449	234.925331613	0.0044	2.878-A	H-1(A)->L+2(A) (27%)	H-6(A)->L+1(A) (2%), H-6(A)->L+5(A) (8%), H-5(A)->L+1(A) (2%), H-3(A)->LUMO(A) (2%), H-2(A)->L+5(A) (2%), H-1(A)->L+3(A) (6%), H-9(B)->L+2(B) (2%), H-8(B)->L+2(B) (4%), H-7(B)->L+2(B) (3%), H-6(B)->L+6(B) (2%), H-5(B)->L+6(B) (4%), H-3(B)->L+2(B) (4%)		
48	42671.5686207	234.348075856	0.0028	2.115-A	H-1(A)->L+2(A) (13%), H-1(B)->L+3(B) (19%)	H-8(A)->LUMO(A) (5%), H-5(A)->LUMO(A) (2%), H-3(A)->LUMO(A) (4%), H-1(A)->L+3(A) (5%), H-9(B)->L+1(B) (3%), H-8(B)->LUMO(B) (5%), H-6(B)->LUMO(B) (4%), H-4(B)->LUMO(B) (4%), H-4(B)->L+1(B) (3%)		
49	42846.5909318	233.390796853	0.0162	2.159-A	H-1(A)->L+3(A) (10%), H-4(B)->L+1(B) (12%)	H-8(A)->LUMO(A) (5%), H-5(A)->LUMO(A) (2%), H-5(A)->L+1(A) (2%), H-3(A)->LUMO(A) (3%), H-9(B)->LUMO(B) (4%), H-8(B)->L+1(B) (4%), H-8(B)->L+2(B) (2%), H-6(B)->LUMO(B) (2%), H-6(B)->L+1(B) (3%), H-4(B)->LUMO(B) (2%), H-3(B)->L+2(B) (2%), H-2(B)->LUMO(B) (2%), H-1(B)->L+4(B) (8%)		
50	43022.4197973	232.436949086	0.0037	2.769-A	H-1(B)->L+3(B) (36%), H-1(B)->L+4(B) (15%)	H-9(B)->L+1(B) (4%), H-6(B)->LUMO(B) (2%), H-4(B)->LUMO(B) (5%), H-4(B)->L+1(B) (5%), H-3(B)->L+3(B) (2%), H-1(B)->L+1(B) (2%)		
51	43255.5140273	231.18439868	0.1007	2.377-A	H-7(A)->LUMO(A) (13%), H-1(B)->L+4(B) (19%)	H-9(A)->LUMO(A) (4%), H-9(A)->L+1(A) (2%), H-8(A)->L+3(A) (3%), H-5(A)->L+1(A) (2%), H-1(A)->L+3(A) (3%), HOMO(A)->L+3(A) (2%), H-8(B)->L+4(B) (2%), H-7(B)->LUMO(B) (2%), H-6(B)->LUMO(B) (8%)		
52	43352.3005588	230.668266069	0.0178	2.559-A	H-5(A)->L+1(A) (13%)	H-9(A)->L+1(A) (7%), H-8(A)->L+1(A) (3%), H-7(A)->L+1(A) (2%), H-6(A)->L+5(A) (2%), H-3(A)->LUMO(A) (2%), H-3(A)->L+1(A) (8%), H-2(A)->L+2(A) (2%), H-9(B)->LUMO(B) (2%), H-8(B)->L+1(B) (4%), H-6(B)->L+1(B) (3%), H-4(B)->L+1(B) (4%), H-3(B)->L+1(B) (3%), H-1(B)->L+4(B) (2%)		
53	43465.2181788	230.069016538	0.0093	2.497-A	H-9(A)->LUMO(A) (18%), H-3(A)->LUMO(A) (12%), H-2(A)->LUMO(A) (15%), H-1(A)->L+3(A) (14%)	H-6(A)->LUMO(A) (3%), H-5(A)->LUMO(A) (7%), H-5(A)->L+3(A) (2%), H-2(A)->L+3(A) (5%), H-1(B)->L+4(B) (7%)		
54	43955.6032716	227.50228084	0.0324	3.108-A		H-13(A)->LUMO(A) (3%), H-10(A)->LUMO(A) (3%), H-9(A)->LUMO(A) (5%), H-8(A)->L+3(A) (3%), H-7(A)->LUMO(A) (2%), H-5(A)->LUMO(A) (2%), H-3(A)->LUMO(A) (2%), H-1(A)->L+3(A) (2%), H-12(B)->LUMO(B) (4%), H-9(B)->L+1(B) (5%), H-5(B)->LUMO(B) (2%), H-4(B)->LUMO(B) (2%), H-3(B)->LUMO(B) (6%), H-2(B)->L+4(B) (2%), H-2(B)->L+7(B) (2%), H-1(B)->L+4(B) (2%)		
55	44270.159499	225.885791088	0.0017	3.412-A		H-14(A)->L+1(A) (2%), H-13(A)->L+1(A) (3%), H-1(A)->L+2(A) (2%), H-1(A)->L+5(A) (2%), H-1(A)->L+12(A) (5%), H-1(A)->L+13(A) (5%), HOMO(A)->L+5(A) (2%), HOMO(A)->L+10(A) (2%), HOMO(A)->L+12(A) (5%), HOMO(A)->L+13(A) (3%), H-12(B)->L+2(B) (3%), H-2(B)->L+2(B) (2%), H-1(B)->L+3(B) (3%), H-1(B)->L+4(B) (2%), H-1(B)->L+6(B) (2%), H-1(B)->L+13(B) (5%), H-1(B)->L+14(B) (4%), HOMO(B)->L+6(B) (2%), HOMO(B)->L+11(B) (2%), HOMO(B)->L+12(B) (2%), HOMO(B)->L+13(B) (6%), HOMO(B)->L+14(B) (3%)		
56	44619.3975667	224.117772658	0.0012	3.329-A		H-9(A)->LUMO(A) (2%), H-1(A)->L+3(A) (3%), H-1(A)->L+12(A) (2%), H-1(A)->L+13(A) (2%), HOMO(A)->L+13(A) (4%), H-9(B)->LUMO(B) (2%), H-3(B)->LUMO(B) (6%), H-3(B)->L+1(B) (4%), H-1(B)->L+3(B) (2%), H-1(B)->L+4(B) (5%), H-1(B)->L+13(B) (2%), H-1(B)->L+14(B) (2%), HOMO(B)->L+5(B) (2%), HOMO(B)->L+14(B) (4%)		
57	44825.8755005	223.085436444	0.0688	2.589-A		H-9(A)->LUMO(A) (2%), H-7(A)->L+2(A) (2%), H-6(A)->L+2(A) (9%), H-2(A)->L+2(A) (6%), H-2(A)->L+3(A) (3%), H-2(A)->L+5(A) (2%), H-8(B)->L+1(B) (2%), H-6(B)->L+3(B) (2%), H-5(B)->LUMO(B) (3%), H-5(B)->L+1(B) (7%), H-5(B)->L+3(B) (4%), H-3(B)->L+3(B) (2%), H-3(B)->L+6(B) (2%)		
58	45141.2382823	221.526931483	0.0554	2.811-A	H-2(A)->L+3(A) (10%), HOMO(B)->L+5(B) (28%)	H-9(A)->LUMO(A) (4%), H-8(A)->LUMO(A) (2%), H-2(A)->L+2(A) (2%), H-1(A)->L+3(A) (3%), HOMO(B)->L+7(B) (2%)		

59	45214.6347353	221.167329086	0.1362	2.743-A	HOMO(B)->L+5(B) (19%)	H-9(A)->LUMO(A) (4%), H-8(A)->LUMO(A) (6%), H-7(A)->LUMO(A) (2%), H-2(A)->L+2(A) (2%), H-2(A)->L+3(A) (5%), H-9(B)->L+1(B) (2%), H-6(B)->L+1(B) (4%), HOMO(B)->L+8(B) (2%)
60	45242.8641403	221.029331145	0.088	3.085-A	HOMO(B)->L+5(B) (10%)	H-17(A)->L+9(A) (2%), H-7(A)->L+17(A) (2%), HOMO(A)->L+4(A) (4%), H-20(B)->L+10(B) (2%), H-6(B)->L+1(B) (2%), H-1(B)->L+4(B) (3%)

Table S5: Full list of 60 TD-DFT-calculated excited singlet states (CAM-B3LYP/DEF2-QZVP/GD3BJ in a DMSO solvent continuum) for **C4**. State energies are uncorrected. DMSO was chosen as the solvent medium to allow assignment of the UV-vis spectra of **C4**.

No.	Energy (cm ⁻¹)	Wavelength (nm)	Osc. Strength	Symmetry	Major contributions	Minor contributions			
1	14155.0302289	706.462638246	0.0002	2.008-A	H-10(B)->L+1(B) (15%), HOMO(B)->L+1(B) (23%)	H-25(B)->L+1(B) (4%), H-24(B)->L+1(B) (3%), H-20(B)->L+1(B) (2%), H-18(B)->L+1(B) (4%), H-10(B)->LUMO(B) (5%), H-10(B)->L+4(B) (2%), H-7(B)->L+1(B) (2%), H-5(B)->L+1(B) (2%), HOMO(B)->LUMO(B) (8%), HOMO(B)->L+4(B) (2%)			
2	17415.9297854	574.186972687	0.0004	2.004-A	H-11(B)->L+1(B) (23%)	H-33(B)->L+1(B) (4%), H-17(B)->L+1(B) (2%), H-13(B)->L+1(B) (4%), H-12(B)->LUMO(B) (3%), H-12(B)->L+1(B) (8%), H-11(B)->LUMO(B) (9%), H-11(B)->L+4(B) (3%), H-9(B)->LUMO(B) (3%), H-9(B)->L+1(B) (9%), H-1(B)->L+1(B) (2%)			
3	18246.6808473	548.044879159	0.0022	2.003-A	H-12(B)->L+1(B) (23%)	H-29(B)->LUMO(B) (2%), H-29(B)->L+1(B) (4%), H-28(B)->LUMO(B) (2%), H-28(B)->L+1(B) (5%), H-21(B)->L+1(B) (2%), H-19(B)->L+1(B) (2%), H-14(B)->L+1(B) (3%), H-12(B)->LUMO(B) (9%), H-12(B)->L+4(B) (3%), H-11(B)->LUMO(B) (2%), H-11(B)->L+1(B) (5%), H-10(B)->LUMO(B) (2%), H-10(B)->L+1(B) (6%), H-4(B)->LUMO(B) (2%), H-4(B)->L+1(B) (4%)			
4	19223.4182608	520.198846237	0.0001	2.004-A	H-33(B)->L+1(B) (11%)	H-34(B)->L+1(B) (2%), H-33(B)->LUMO(B) (4%), H-31(B)->LUMO(B) (4%), H-31(B)->L+1(B) (9%), H-21(B)->L+1(B) (4%), H-19(B)->LUMO(B) (2%), H-19(B)->L+1(B) (6%), H-17(B)->L+1(B) (3%), H-15(B)->LUMO(B) (2%), H-15(B)->L+1(B) (6%), H-12(B)->L+1(B) (2%), H-11(B)->L+1(B) (3%), H-9(B)->LUMO(B) (3%), H-9(B)->L+1(B) (9%), H-1(B)->L+1(B) (2%)			
5	20840.5598909	479.833557848	0.0	3.450-A	H-1(A)->LUMO(A) (13%), HOMO(A)->LUMO(A) (25%), HOMO(B)->LUMO(B) (17%)	H-5(A)->LUMO(A) (2%), H-3(A)->LUMO(A) (2%), HOMO(A)->L+3(A) (2%), H-2(B)->LUMO(B) (2%), H-1(B)->LUMO(B) (8%), H-1(B)->L+1(B) (5%), HOMO(B)->L+1(B) (8%)			
6	21631.7897858	462.282598852	0.0	3.456-A	H-1(A)->L+1(A) (19%), HOMO(A)->L+1(A) (21%), H-1(B)->L+2(B) (16%), HOMO(B)->L+2(B) (24%)	H-4(A)->L+1(A) (6%), H-4(B)->L+2(B) (5%)			
7	24637.0115882	405.893383789	0.0011	3.422-A	H-3(A)->LUMO(A) (11%), H-2(B)->LUMO(B) (17%)	H-8(A)->L+6(A) (2%), H-7(A)->LUMO(A) (2%), H-7(A)->L+3(A) (8%), H-2(A)->LUMO(A) (9%), HOMO(A)->L+3(A) (2%), H-7(B)->L+4(B) (2%), H-6(B)->L+3(B) (2%), H-6(B)->L+4(B) (4%), H-1(B)->L+1(B) (3%), HOMO(B)->L+1(B) (2%)			
8	25491.959283	392.280557528	0.0006	3.433-A	H-6(A)->L+2(A) (17%)	H-6(A)->L+3(A) (2%), H-6(A)->L+5(A) (2%), H-5(A)->L+2(A) (3%), H-5(A)->L+5(A) (2%), H-3(A)->L+2(A) (4%), H-3(A)->L+5(A) (3%), H-2(A)->L+2(A) (5%), H-2(A)->L+5(A) (3%), H-6(B)->L+3(B) (3%), H-5(B)->L+3(B) (8%), H-5(B)->L+4(B) (4%), H-3(B)->LUMO(B) (2%), H-3(B)->L+1(B) (3%), H-3(B)->L+3(B) (7%), H-3(B)->L+4(B) (2%), H-3(B)->L+6(B) (7%), H-3(B)->L+7(B) (2%)			

9	26047.6752846	383.911419762	0.0002	3.430-A		H-8(A)->LUMO(A) (2%), H-7(A)->LUMO(A) (2%), H-7(A)->L+3(A) (2%), H-5(A)->LUMO(A) (5%), H-4(A)->L+1(A) (8%), H-3(A)->LUMO(A) (2%), H-3(A)->L+3(A) (2%), H-1(A)->L+7(A) (3%), HOMO(A)->L+8(A) (3%), H-6(B)->LUMO(B) (5%), H-5(B)->LUMO(B) (2%), H-4(B)->L+2(B) (8%), H-2(B)->L+1(B) (3%), H-2(B)->L+4(B) (2%), H-2(B)->L+7(B) (2%), H-1(B)->L+1(B) (4%), H-1(B)->L+8(B) (4%), HOMO(B)->L+9(B) (4%)			
10	26105.7472034	383.057413453	0.0003	3.448-A	H-4(A)->L+1(A) (15%), H-4(B)->L+2(B) (14%)	H-5(A)->LUMO(A) (3%), H-1(A)->L+1(A) (2%), H-1(A)->L+8(A) (4%), HOMO(A)->L+1(A) (2%), HOMO(A)->L+7(A) (3%), H-6(B)->LUMO(B) (3%), H-2(B)->L+1(B) (2%), H-1(B)->L+2(B) (2%), H-1(B)->L+9(B) (5%), HOMO(B)->L+8(B) (4%)			
11	28397.9748907	352.137785828	0.0178	2.110-A	H-1(B)->LUMO(B) (14%), H-1(B)->L+1(B) (54%)	H-1(A)->LUMO(A) (3%), HOMO(A)->LUMO(A) (5%), H-13(B)->L+1(B) (2%), H-1(B)->L+2(B) (2%), H-1(B)->L+4(B) (2%), HOMO(B)->LUMO(B) (2%)			
12	28706.885237	348.348485649	0.1644	2.052-A	H-1(A)->LUMO(A) (10%), HOMO(A)->LUMO(A) (19%), H-1(B)->LUMO(B) (16%), HOMO(B)->LUMO(B) (35%)	H-8(B)->L+1(B) (2%), H-1(B)->L+4(B) (2%)			
13	29421.4924611	339.887584331	0.0657	2.084-A	HOMO(B)->L+1(B) (33%), HOMO(B)->L+2(B) (11%)	H-1(A)->LUMO(A) (3%), H-1(A)->L+1(A) (2%), HOMO(A)->LUMO(A) (5%), HOMO(A)->L+1(A) (3%), H-18(B)->L+1(B) (3%), H-8(B)->L+1(B) (2%), H-7(B)->L+1(B) (2%), H-5(B)->L+1(B) (2%), H-1(B)->LUMO(B) (4%), H-1(B)->L+2(B) (4%), HOMO(B)->LUMO(B) (2%)			
14	30073.9949941	332.513189616	0.1745	2.052-A	H-1(A)->L+1(A) (20%), HOMO(A)->L+1(A) (20%), H-1(B)->L+2(B) (13%), HOMO(B)->L+1(B) (12%), HOMO(B)->L+2(B) (19%)				
15	31555.6354802	316.900605798	0.0042	2.799-A	H-5(A)->LUMO(A) (10%), H-2(A)->LUMO(A) (42%)	H-9(A)->LUMO(A) (5%), H-8(A)->L+3(A) (2%), H-7(A)->LUMO(A) (4%), H-7(A)->L+3(A) (2%), H-1(A)->LUMO(A) (6%), HOMO(A)->LUMO(A) (2%), H-7(B)->LUMO(B) (2%)			
16	31770.9855127	314.752590724	0.003	2.743-A	H-2(A)->L+1(A) (52%)	H-9(A)->L+1(A) (6%), H-8(A)->L+1(A) (2%), H-3(A)->L+1(A) (9%), H-1(A)->L+1(A) (3%), HOMO(A)->L+1(A) (4%)			
17	32582.3792683	306.914357532	0.0014	3.275-A		H-9(A)->LUMO(A) (3%), H-8(A)->LUMO(A) (3%), H-8(A)->L+3(A) (5%), H-7(A)->L+3(A) (3%), H-5(A)->LUMO(A) (5%), H-3(A)->LUMO(A) (3%), H-3(A)->L+3(A) (3%), H-2(A)->LUMO(A) (3%), H-2(A)->L+3(A) (6%), H-1(A)->LUMO(A) (2%), HOMO(A)->LUMO(A) (4%), HOMO(A)->L+3(A) (3%), H-8(B)->L+3(B) (2%), H-8(B)->L+4(B) (3%), H-7(B)->L+3(B) (2%), H-7(B)->L+4(B) (3%), H-2(B)->LUMO(B) (7%), H-2(B)->L+3(B) (2%), H-2(B)->L+4(B) (4%), HOMO(B)->L+4(B) (2%)			
18	33005.0137891	302.98426972	0.0005	3.347-A	H-2(A)->L+2(A) (13%), H-3(B)->L+3(B) (11%)	H-7(A)->L+2(A) (2%), H-6(A)->L+2(A) (5%), H-5(A)->L+2(A) (3%), H-3(A)->L+2(A) (4%), H-3(A)->L+3(A) (4%), H-2(A)->L+1(A) (3%), HOMO(A)->L+7(A) (2%), H-7(B)->L+3(B) (2%), H-6(B)->L+3(B) (3%), H-3(B)->L+4(B) (4%), H-2(B)->L+4(B) (2%), HOMO(B)->L+8(B) (2%)			
19	33072.7643611	302.363597152	0.0004	3.415-A		H-8(A)->L+3(A) (2%), H-6(A)->L+2(A) (2%), H-5(A)->LUMO(A) (3%), H-3(A)->L+2(A) (4%), H-3(A)->L+3(A) (3%), H-2(A)->L+3(A) (5%), H-1(A)->L+7(A) (5%), HOMO(A)->L+3(A) (2%), HOMO(A)->L+7(A) (6%), HOMO(A)->L+8(A) (2%), H-3(B)->L+3(B) (2%), H-3(B)->L+4(B) (2%), H-2(B)->L+3(B) (3%), H-2(B)->L+4(B) (4%), H-1(B)->L+8(B) (6%), HOMO(B)->L+8(B) (6%), HOMO(B)->L+9(B) (2%)			
20	33289.7275025	300.392966546	0.0016	3.444-A	H-4(A)->L+1(A) (12%), H-1(A)->L+8(A) (11%), H-4(B)->L+2(B) (10%), H-1(B)->L+9(B) (10%), HOMO(B)->L+9(B) (10%)	H-1(A)->L+7(A) (4%), HOMO(A)->L+7(A) (3%), HOMO(A)->L+8(A) (9%), H-1(B)->L+8(B) (4%), HOMO(B)->L+8(B) (3%)			

21	35244.008884	283.736167271	0.0345	3.313-A	H-8(B)->LUMO(B) (10%)	H-8(A)->LUMO(A) (7%), H-8(A)->L+6(A) (2%), H-7(A)->LUMO(A) (2%), H-7(A)->L+3(A) (6%), H-3(A)->L+6(A) (4%), H-2(A)->L+6(A) (3%), HOMO(A)->L+6(A) (2%), H-7(B)->LUMO(B) (4%), H-6(B)->L+4(B) (2%), H-2(B)->LUMO(B) (3%), H-2(B)->L+6(B) (2%), H-2(B)->L+7(B) (5%), H-1(B)->LUMO(B) (3%), HOMO(B)->LUMO(B) (3%), HOMO(B)->L+7(B) (2%)		
22	35649.7057618	280.50722401	0.1372	2.637-A	HOMO(B)->LUMO(B) (10%)	H-6(A)->L+2(A) (3%), H-2(A)->L+5(A) (3%), H-1(A)->LUMO(A) (2%), HOMO(A)->LUMO(A) (2%), H-10(B)->L+1(B) (2%), H-8(B)->L+1(B) (4%), H-7(B)->LUMO(B) (2%), H-7(B)->L+1(B) (2%), H-5(B)->LUMO(B) (3%), H-5(B)->L+1(B) (6%), H-3(B)->LUMO(B) (2%), H-3(B)->L+1(B) (4%), H-3(B)->L+6(B) (4%), H-2(B)->L+1(B) (2%), H-1(B)->LUMO(B) (8%), H-1(B)->L+1(B) (3%)		
23	35826.3411818	279.124232901	0.0281	2.890-A	H-1(B)->LUMO(B) (13%)	H-6(A)->L+2(A) (6%), H-5(A)->L+5(A) (2%), H-3(A)->LUMO(A) (2%), H-3(A)->L+5(A) (4%), H-2(A)->LUMO(A) (2%), H-2(A)->L+5(A) (3%), H-1(A)->LUMO(A) (4%), HOMO(A)->LUMO(A) (2%), H-6(B)->L+3(B) (2%), H-5(B)->L+3(B) (2%), H-3(B)->L+2(B) (2%), H-3(B)->L+6(B) (7%), H-1(B)->L+1(B) (5%), HOMO(B)->LUMO(B) (6%), HOMO(B)->L+1(B) (3%), HOMO(B)->L+4(B) (2%)		
24	35994.9110574	277.817049862	0.0535	2.401-A	H-8(B)->L+1(B) (12%), H-7(B)->L+1(B) (10%)	H-6(A)->L+2(A) (3%), H-3(A)->LUMO(A) (2%), H-2(A)->L+5(A) (2%), H-1(A)->LUMO(A) (4%), H-24(B)->L+1(B) (2%), H-10(B)->L+1(B) (2%), H-8(B)->LUMO(B) (2%), H-7(B)->LUMO(B) (3%), H-5(B)->L+1(B) (6%), H-5(B)->L+3(B) (2%), H-3(B)->L+6(B) (3%), H-2(B)->LUMO(B) (2%), H-1(B)->LUMO(B) (6%), H-1(B)->L+1(B) (2%), HOMO(B)->L+1(B) (2%), HOMO(B)->L+2(B) (2%)		
25	36319.9524923	275.330756617	0.0658	3.222-A	H-1(A)->LUMO(A) (25%), HOMO(A)->LUMO(A) (21%), H-2(B)->LUMO(B) (11%)	H-2(A)->LUMO(A) (8%), HOMO(A)->L+3(A) (3%), H-1(B)->LUMO(B) (8%), H-1(B)->L+1(B) (3%), HOMO(B)->LUMO(B) (5%), HOMO(B)->L+1(B) (2%)		
26	37525.7513637	266.483671522	0.1688	2.459-A	H-3(A)->LUMO(A) (10%), H-1(A)->LUMO(A) (13%), H-2(B)->LUMO(B) (16%)	H-5(A)->LUMO(A) (4%), H-2(A)->L+3(A) (3%), H-1(A)->L+3(A) (3%), HOMO(A)->LUMO(A) (4%), H-7(B)->LUMO(B) (4%), H-5(B)->LUMO(B) (3%), H-2(B)->L+1(B) (5%), H-1(B)->LUMO(B) (2%)		
27	37813.6912948	264.454478195	0.0197	2.772-A	H-1(B)->L+2(B) (38%), HOMO(B)->L+2(B) (27%)	H-2(A)->L+2(A) (2%), H-10(B)->L+2(B) (2%), H-3(B)->L+1(B) (2%), H-3(B)->L+2(B) (7%), HOMO(B)->L+3(B) (3%)		
28	38212.9357372	261.691487636	0.0499	2.612-A	H-2(B)->L+1(B) (31%)	H-8(A)->LUMO(A) (4%), H-5(A)->LUMO(A) (4%), H-2(A)->L+1(A) (2%), H-1(A)->L+1(A) (4%), HOMO(A)->L+1(A) (4%), H-8(B)->L+1(B) (2%), H-3(B)->LUMO(B) (2%), H-3(B)->L+1(B) (2%), H-3(B)->L+2(B) (2%), HOMO(B)->L+3(B) (3%), HOMO(B)->L+4(B) (2%)		
29	38316.9812585	260.980893368	0.001	2.690-A	H-1(A)->L+1(A) (12%), HOMO(A)->L+1(A) (17%), H-2(B)->L+1(B) (15%)	H-2(A)->L+1(A) (5%), HOMO(A)->L+2(A) (3%), H-5(B)->LUMO(B) (2%), H-3(B)->L+2(B) (3%), HOMO(B)->L+3(B) (4%)		
30	38404.8956913	260.383469868	0.0185	2.546-A	H-1(A)->L+1(A) (10%), H-5(B)->LUMO(B) (11%)	H-5(A)->LUMO(A) (3%), H-3(A)->LUMO(A) (3%), H-2(A)->L+1(A) (2%), HOMO(A)->L+1(A) (8%), H-9(B)->LUMO(B) (2%), H-9(B)->L+1(B) (7%), H-8(B)->LUMO(B) (6%), H-7(B)->LUMO(B) (6%), H-7(B)->L+1(B) (2%), H-5(B)->L+1(B) (5%), H-4(B)->LUMO(B) (3%), H-3(B)->LUMO(B) (4%)		
31	38654.1210098	258.70462809	0.0822	2.622-A	H-4(B)->L+2(B) (10%), H-3(B)->L+2(B) (13%)	H-4(A)->L+1(A) (2%), H-1(A)->L+1(A) (8%), HOMO(A)->L+1(A) (6%), H-9(B)->L+2(B) (5%), H-8(B)->LUMO(B) (3%), H-8(B)->L+2(B) (9%), H-7(B)->L+2(B) (6%), H-5(B)->LUMO(B) (2%), H-5(B)->L+2(B) (5%), H-3(B)->L+1(B) (2%), H-1(B)->L+2(B) (3%)		
32	39065.4637686	255.98057812	0.1702	2.321-A	H-2(A)->L+2(A) (11%), HOMO(B)->L+3(B) (17%)	H-6(A)->L+5(A) (2%), H-3(A)->L+2(A) (4%), HOMO(A)->L+2(A) (3%), H-8(B)->L+2(B) (2%), H-5(B)->L+2(B) (3%), H-3(B)->LUMO(B) (2%), H-3(B)->L+1(B) (4%), H-3(B)->L+2(B) (3%), H-3(B)->L+3(B) (7%), H-3(B)->L+4(B) (3%), H-1(B)->L+2(B) (3%), HOMO(B)->L+2(B) (2%), HOMO(B)->L+4(B) (2%)		

33	39177.5748342	255.248060716	0.0816	2.531-A	HOMO(A)->L+3(A) (10%)	H-9(A)->LUMO(A) (2%), H-7(A)->LUMO(A) (3%), H-3(A)->LUMO(A) (8%), H-3(A)->L+3(A) (2%), H-2(A)->L+3(A) (3%), HOMO(A)->L+2(A) (3%), H-8(B)->LUMO(B) (3%), H-8(B)->L+1(B) (2%), H-6(B)->L+1(B) (2%), H-2(B)->LUMO(B) (7%), H-2(B)->L+1(B) (2%), H-2(B)->L+4(B) (5%), HOMO(B)->L+3(B) (4%), HOMO(B)->L+4(B) (4%)			
34	39363.8889073	254.039940605	0.0112	2.889-A	HOMO(B)->L+4(B) (16%)	H-15(A)->LUMO(A) (2%), H-8(A)->L+6(A) (2%), H-4(A)->L+1(A) (2%), HOMO(A)->L+7(A) (2%), H-7(B)->LUMO(B) (2%), H-6(B)->LUMO(B) (6%), H-3(B)->L+3(B) (2%), H-2(B)->LUMO(B) (9%), H-2(B)->L+1(B) (6%), H-2(B)->L+4(B) (2%)			
35	40102.6927643	249.359813785	0.0434	3.027-A	HOMO(A)->L+2(A) (19%), H-3(B)->L+1(B) (12%), HOMO(B)->L+3(B) (24%)	H-3(B)->LUMO(B) (4%), H-2(B)->L+1(B) (2%), HOMO(B)->L+4(B) (7%)			
36	40329.3345589	247.958467686	0.0309	2.910-A	H-3(B)->L+1(B) (11%)	H-14(A)->L+1(A) (4%), H-4(A)->L+1(A) (7%), H-13(B)->L+2(B) (3%), H-4(B)->L+1(B) (2%), H-4(B)->L+2(B) (2%), H-4(B)->L+9(B) (2%), H-3(B)->LUMO(B) (3%), H-3(B)->L+2(B) (4%), H-3(B)->L+3(B) (2%), H-3(B)->L+4(B) (2%), H-1(B)->L+2(B) (3%), H-1(B)->L+3(B) (2%), HOMO(B)->L+2(B) (4%), HOMO(B)->L+9(B) (2%)			
37	40412.409665	247.448743663	0.0222	2.996-A	HOMO(B)->L+3(B) (14%)	H-14(A)->L+1(A) (3%), H-12(A)->L+1(A) (2%), H-4(A)->L+1(A) (3%), H-4(A)->L+8(A) (2%), HOMO(A)->L+1(A) (2%), HOMO(A)->L+2(A) (2%), HOMO(A)->L+8(A) (2%), H-14(B)->L+2(B) (2%), H-13(B)->L+2(B) (2%), H-12(B)->L+2(B) (2%), H-4(B)->L+2(B) (4%), H-3(B)->L+1(B) (3%), H-3(B)->L+2(B) (3%), H-3(B)->L+3(B) (5%), H-3(B)->L+4(B) (3%), HOMO(B)->L+4(B) (3%)			
38	40543.0714825	246.651268252	0.2394	2.289-A	H-4(A)->L+1(A) (16%), H-4(B)->L+2(B) (10%)	H-1(A)->L+1(A) (2%), HOMO(A)->L+2(A) (2%), H-9(B)->LUMO(B) (4%), H-9(B)->L+1(B) (6%), H-5(B)->LUMO(B) (4%), H-5(B)->L+1(B) (2%), H-4(B)->L+1(B) (2%), H-3(B)->L+1(B) (2%), H-3(B)->L+2(B) (9%), H-2(B)->LUMO(B) (2%), HOMO(B)->L+3(B) (2%), HOMO(B)->L+4(B) (2%)			
39	40639.0514596	246.068735387	0.044	2.294-A	HOMO(A)->L+2(A) (51%)	H-3(A)->L+2(A) (3%), H-2(A)->L+2(A) (2%), H-1(A)->L+2(A) (5%), HOMO(A)->L+3(A) (5%), H-3(B)->L+1(B) (2%), H-3(B)->L+3(B) (2%), HOMO(B)->L+3(B) (5%), HOMO(B)->L+4(B) (4%)			
40	40838.2704036	244.86835268	0.0129	3.356-A	HOMO(A)->L+3(A) (24%), HOMO(B)->L+4(B) (17%)	H-1(A)->LUMO(A) (3%), H-8(B)->LUMO(B) (2%), H-2(B)->L+4(B) (3%), H-1(B)->LUMO(B) (3%), HOMO(B)->L+7(B) (2%), HOMO(B)->L+14(B) (2%)			
41	41331.0751597	241.948702311	0.0056	2.642-A	H-1(A)->L+3(A) (13%), HOMO(A)->L+3(A) (18%)	H-7(A)->L+3(A) (2%), H-2(A)->L+3(A) (2%), H-1(A)->L+2(A) (5%), HOMO(A)->L+2(A) (2%), H-8(B)->LUMO(B) (5%), H-7(B)->LUMO(B) (6%), H-6(B)->L+7(B) (2%), H-2(B)->L+4(B) (3%), HOMO(B)->L+3(B) (2%), HOMO(B)->L+4(B) (5%), HOMO(B)->L+7(B) (2%)			
42	41615.7888731	240.293414369	0.0056	3.018-A	H-7(A)->LUMO(A) (10%), H-7(A)->L+6(A) (11%)	H-8(A)->LUMO(A) (3%), H-7(A)->L+5(A) (2%), H-3(A)->LUMO(A) (2%), H-3(A)->L+3(A) (2%), H-3(A)->L+6(A) (2%), H-2(A)->L+3(A) (4%), H-1(A)->L+2(A) (2%), H-1(A)->L+3(A) (2%), HOMO(A)->L+3(A) (6%), HOMO(A)->L+6(A) (2%), H-7(B)->LUMO(B) (2%), H-7(B)->L+4(B) (2%), H-7(B)->L+7(B) (2%), H-6(B)->LUMO(B) (5%), H-6(B)->L+7(B) (2%), H-1(B)->L+3(B) (2%), H-1(B)->L+4(B) (2%)			
43	41815.0078171	239.148586167	0.0071	3.287-A	H-1(B)->L+3(B) (14%)	H-6(A)->L+5(A) (4%), H-1(A)->L+2(A) (5%), H-1(A)->L+3(A) (5%), H-9(B)->L+2(B) (2%), H-8(B)->L+2(B) (2%), H-6(B)->LUMO(B) (3%), H-5(B)->L+2(B) (3%), H-5(B)->L+6(B) (2%), H-3(B)->L+2(B) (4%), H-1(B)->L+4(B) (7%), HOMO(B)->L+3(B) (2%), HOMO(B)->L+4(B) (3%)			
44	41906.955022	238.623875076	0.0025	3.250-A		H-9(A)->L+1(A) (2%), H-6(A)->L+5(A) (4%), H-5(A)->L+1(A) (4%), H-3(A)->L+1(A) (2%), H-1(A)->L+3(A) (5%), H-9(B)->L+2(B) (4%), H-8(B)->L+2(B) (4%), H-7(B)->LUMO(B) (2%), H-7(B)->L+2(B) (2%), H-5(B)->L+2(B) (4%), H-3(B)->L+2(B) (8%), H-3(B)->L+3(B) (2%), H-1(B)->L+3(B) (5%), H-1(B)->L+4(B) (6%), HOMO(B)->L+4(B) (5%)			

45	42039.2299483	237.873053628	0.0755	2.122-A	H-4(B)->LUMO(B) (11%), H-4(B)->L+1(B) (21%)	H-4(A)->L+1(A) (4%), H-9(B)->LUMO(B) (3%), H-9(B)->L+1(B) (5%), H-6(B)->LUMO(B) (2%), H-6(B)->L+1(B) (3%), H-5(B)->LUMO(B) (2%), H-5(B)->L+1(B) (2%), H-4(B)->L+2(B) (7%), H-3(B)->L+1(B) (2%), H-3(B)->L+2(B) (3%)
46	42417.5039755	235.751731308	0.002	3.005-A	H-1(A)->L+2(A) (26%)	H-6(A)->L+5(A) (3%), H-1(A)->L+3(A) (6%), H-8(B)->L+2(B) (2%), H-7(B)->L+2(B) (2%), H-6(B)->L+1(B) (3%), H-6(B)->L+6(B) (2%), H-5(B)->L+1(B) (2%), H-5(B)->L+6(B) (5%), H-4(B)->L+1(B) (2%), H-3(B)->L+2(B) (3%), H-3(B)->L+6(B) (4%)
47	42566.7165449	234.925331613	0.0044	2.878-A	H-1(A)->L+2(A) (27%)	H-6(A)->L+1(A) (2%), H-6(A)->L+5(A) (8%), H-5(A)->L+1(A) (2%), H-3(A)->LUMO(A) (2%), H-2(A)->L+5(A) (2%), H-1(A)->L+3(A) (6%), H-9(B)->L+2(B) (2%), H-8(B)->L+2(B) (4%), H-7(B)->L+2(B) (3%), H-6(B)->L+6(B) (2%), H-5(B)->L+6(B) (4%), H-3(B)->L+2(B) (4%)
48	42671.5686207	234.348075856	0.0028	2.115-A	H-1(A)->L+2(A) (13%), H-1(B)->L+3(B) (19%)	H-8(A)->LUMO(A) (5%), H-5(A)->LUMO(A) (2%), H-3(A)->LUMO(A) (4%), H-1(A)->L+3(A) (5%), H-9(B)->L+1(B) (3%), H-8(B)->LUMO(B) (5%), H-6(B)->LUMO(B) (4%), H-4(B)->LUMO(B) (4%), H-4(B)->L+1(B) (3%)
49	42846.5909318	233.390796853	0.0162	2.159-A	H-1(A)->L+3(A) (10%), H-4(B)->L+1(B) (12%)	H-8(A)->LUMO(A) (5%), H-5(A)->LUMO(A) (2%), H-5(A)->L+1(A) (2%), H-3(A)->LUMO(A) (3%), H-9(B)->LUMO(B) (4%), H-8(B)->L+1(B) (4%), H-8(B)->L+2(B) (2%), H-6(B)->LUMO(B) (2%), H-6(B)->L+1(B) (3%), H-4(B)->LUMO(B) (2%), H-3(B)->L+2(B) (2%), H-2(B)->LUMO(B) (2%), H-1(B)->L+4(B) (8%)
50	43022.4197973	232.436949086	0.0037	2.769-A	H-1(B)->L+3(B) (36%), H-1(B)->L+4(B) (15%)	H-9(B)->L+1(B) (4%), H-6(B)->LUMO(B) (2%), H-4(B)->LUMO(B) (5%), H-4(B)->L+1(B) (5%), H-3(B)->L+3(B) (2%), H-1(B)->L+1(B) (2%)
51	43255.5140273	231.18439868	0.1007	2.377-A	H-7(A)->LUMO(A) (13%), H-1(B)->L+4(B) (19%)	H-9(A)->LUMO(A) (4%), H-9(A)->L+1(A) (2%), H-8(A)->L+3(A) (3%), H-5(A)->L+1(A) (2%), H-1(A)->L+3(A) (3%), HOMO(A)->L+3(A) (2%), H-8(B)->L+4(B) (2%), H-7(B)->LUMO(B) (2%), H-6(B)->LUMO(B) (8%)
52	43352.3005588	230.668266069	0.0178	2.559-A	H-5(A)->L+1(A) (13%)	H-9(A)->L+1(A) (7%), H-8(A)->L+1(A) (3%), H-7(A)->L+1(A) (2%), H-6(A)->L+5(A) (2%), H-3(A)->LUMO(A) (2%), H-3(A)->L+1(A) (8%), H-2(A)->L+2(A) (2%), H-9(B)->LUMO(B) (2%), H-8(B)->L+1(B) (4%), H-6(B)->L+1(B) (3%), H-4(B)->L+1(B) (4%), H-3(B)->L+1(B) (3%), H-1(B)->L+4(B) (2%)
53	43465.2181788	230.069016538	0.0093	2.497-A	H-9(A)->LUMO(A) (18%), H-3(A)->LUMO(A) (12%), H-2(A)->LUMO(A) (15%), H-1(A)->L+3(A) (14%)	H-6(A)->LUMO(A) (3%), H-5(A)->LUMO(A) (7%), H-5(A)->L+3(A) (2%), H-2(A)->L+3(A) (5%), H-1(B)->L+4(B) (7%)
54	43955.6032716	227.50228084	0.0324	3.108-A		H-13(A)->LUMO(A) (3%), H-10(A)->LUMO(A) (3%), H-9(A)->LUMO(A) (5%), H-8(A)->L+3(A) (3%), H-7(A)->LUMO(A) (2%), H-5(A)->LUMO(A) (2%), H-3(A)->LUMO(A) (2%), H-1(A)->L+3(A) (2%), H-12(B)->LUMO(B) (4%), H-9(B)->L+1(B) (5%), H-5(B)->LUMO(B) (2%), H-4(B)->LUMO(B) (2%), H-3(B)->LUMO(B) (6%), H-2(B)->L+4(B) (2%), H-2(B)->L+7(B) (2%), H-1(B)->L+4(B) (2%)
55	44270.159499	225.885791088	0.0017	3.412-A		H-14(A)->L+1(A) (2%), H-13(A)->L+1(A) (3%), H-1(A)->L+2(A) (2%), H-1(A)->L+5(A) (2%), H-1(A)->L+12(A) (5%), H-1(A)->L+13(A) (5%), HOMO(A)->L+5(A) (2%), HOMO(A)->L+10(A) (2%), HOMO(A)->L+12(A) (5%), HOMO(A)->L+13(A) (3%), H-12(B)->L+2(B) (3%), H-2(B)->L+2(B) (2%), H-1(B)->L+3(B) (3%), H-1(B)->L+4(B) (2%), H-1(B)->L+6(B) (2%), H-1(B)->L+13(B) (5%), H-1(B)->L+14(B) (4%), HOMO(B)->L+6(B) (2%), HOMO(B)->L+11(B) (2%), HOMO(B)->L+12(B) (2%), HOMO(B)->L+13(B) (6%), HOMO(B)->L+14(B) (3%)
56	44619.3975667	224.117772658	0.0012	3.329-A		H-9(A)->LUMO(A) (2%), H-1(A)->L+3(A) (3%), H-1(A)->L+12(A) (2%), H-1(A)->L+13(A) (2%), HOMO(A)->L+13(A) (4%), H-9(B)->LUMO(B) (2%), H-3(B)->LUMO(B) (6%), H-3(B)->L+1(B) (4%), H-1(B)->L+3(B) (2%), H-1(B)->L+4(B) (5%), H-1(B)->L+13(B) (2%), H-1(B)->L+14(B) (2%), HOMO(B)->L+5(B) (2%), HOMO(B)->L+14(B) (4%)

57	44825.8755005	223.085436444	0.0688	2.589-A		H-9(A)->LUMO(A) (2%), H-7(A)->L+2(A) (2%), H-6(A)->L+2(A) (9%), H-2(A)->L+2(A) (6%), H-2(A)->L+3(A) (3%), H-2(A)->L+5(A) (2%), H-8(B)->L+1(B) (2%), H-6(B)->L+3(B) (2%), H-5(B)->LUMO(B) (3%), H-5(B)->L+1(B) (7%), H-5(B)->L+3(B) (4%), H-3(B)->L+3(B) (2%), H-3(B)->L+6(B) (2%)
58	45141.2382823	221.526931483	0.0554	2.811-A	H-2(A)->L+3(A) (10%), HOMO(B)->L+5(B) (28%)	H-9(A)->LUMO(A) (4%), H-8(A)->LUMO(A) (2%), H-2(A)->L+2(A) (2%), H-1(A)->L+3(A) (3%), HOMO(B)->L+7(B) (2%)
59	45214.6347353	221.167329086	0.1362	2.743-A	HOMO(B)->L+5(B) (19%)	H-9(A)->LUMO(A) (4%), H-8(A)->LUMO(A) (6%), H-7(A)->LUMO(A) (2%), H-2(A)->L+2(A) (2%), H-2(A)->L+3(A) (5%), H-9(B)->L+1(B) (2%), H-6(B)->L+1(B) (4%), HOMO(B)->L+8(B) (2%)
60	45242.8641403	221.029331145	0.088	3.085-A	HOMO(B)->L+5(B) (10%)	H-17(A)->L+9(A) (2%), H-7(A)->L+17(A) (2%), HOMO(A)->L+4(A) (4%), H-20(B)->L+10(B) (2%), H-6(B)->L+1(B) (2%), H-1(B)->L+4(B) (3%)

Table S6: Optimization energies **C1** with various DFT methods

Methods	HF/3- 21G	M06/STO- 2G	M06/3- 21G	M06- LANL2DZ
E_{opt}	-	-2996.74	-	-1693.97
	3007.61		3017.99	

Table S7: Quantum chemical descriptors

	E_{LUMO}	E_{HOMO}	ΔE	I	A	η	δ	χ	C_p	ω	μ_D
HL	-0.37	-7.56	7.18	7.56	0.37	3.59	0.27	3.97	-3.97	2.19	5.02
C1	-1.73	-4.90	3.16	4.90	1.73	1.58	0.63	3.32	-3.32	3.48	8.80
C2	-1.82	-5.34	3.52	5.34	1.82	1.76	0.56	3.58	-3.58	3.64	0.41
C4	-1.79	-5.75	3.95	5.75	1.79	1.97	0.50	3.77	-3.77	3.60	5.23
C4	-1.60	-5.44	3.83	5.44	1.60	1.91	0.52	3.52	-3.52	3.23	0.00

All units are in eV except μ_D (Debye). ΔE : Energy gap A: Electron affinity, I: Ionization potential, η : Global hardness, δ : Global softness, χ : Electronegativity, C_p : Electronic chemical potential, ω : Global electrophilicity, μ_D : Dipole moment.

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