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

Phosphorescent Cyclometalated Iridium(III) Complexes: Synthesis, Photophysics, DNA Interaction, Cellular Internalization, and Cytotoxic Activity

Satish S. Bhat,*[a] Vidyanand K. Revankar,*[a] Rahul V. Pinjari,[b] Naveen S.,[c] N. K. Lokhanath,[d] Vijay Kumbhar,[e] Kishore Bhat,[e] Doolesh G. Kokare [a]

Method and Instrumentation

^{1}H and ^{13}C NMR spectra of ligand and iridium complexes **1** and **2** were recorded on a Joel 400 MHz spectrometer using DMSO-d6 at room temperature. The FT-IR spectra of the ligand and iridium complexes **1** and **2** were recorded on a NICOLET, USA model-NICOLET 6700, IR spectrometer. Elemental analysis (C, H, and N) of ligand and complexes were performed with a Thermo Quest microanalysis instrument capable of carrying out C, H, N (carbon, hydrogen, nitrogen) analysis. The electro-spray ionization mass spectra of iridium complexes 1 and 2 were recorded on a waters UPLC-TQD triple quadrupole mass spectrometer in methanol.

UV-Visible spectra were recorded on a Jasco V670 spectrophotometer. Emission spectra were measured on a Hitachi F-7000 spectrometer. The fluorescence microscopy images of HeLa cells were taken on a high resolution optical microscope, Axio Imager 2, Carl Zeiss, Germany.

Emission quantum yields (ϕ) were calculated by integrating the area under the fluorescence spectra of complexes and by using equation 1[1]

$$\phi_{Sample} = \{OD_{Standard} \times A_{Sample}\} / \{OD_{Sample} \times A_{Standard}\} \times \phi_{Standard} \quad \text{--(1)}$$

where, OD is the optical density of the compound at the excitation wavelength of iridium complexes 1 and 2 (370 nm) and A is the area under the emission curve of complexes. The relative quantum yield calculated were compared to the $[Ru(bpy)_3]^{2+}$ ϕ=0.028 in aerated aqueous solution.[2] The quantum yield of iridium complexes calculated was corrected for the refractive index of the solvent according to the reference.[3]

X-ray Crystallography

Single crystal data of complex 2 was recorded at 155 K on a Bruker X8 Proteum diffractometer equipped with an X-ray generator operating at 45 kV and 10 mA, using

Cu-Kα radiation (λ=1.54178 Å). The complete collected data sets were processed using SAINT PLUS.[4] The structure of the complex 2 was solved on Olex2[5] using SHELXT program and refined (full matrix least-squares refinement on F2) using SHELXL program.[6] All non-hydrogen atoms of complex 2 were refined anisotropically. CCDC 1819244 contains the supplementary crystallographic data for this paper.

Computational methodology

The quantum chemical calculations were performed by using the Gaussian 09 program package.[7] The singlet and triplet state geometries of complexes 1 and 2 were optimized in the gas phase using density functional theory employing the B3LYP functional.[8, 9] Different conformations of these complexes with cis- and trans- arrangement of Ir-N(BenzoPyridine) bonds are considered, where the trans- form is turned out to be lower energy, which is used for the further calculations. The triplet states were destabilized atleast by 55 kcal $mole^{-1}$ compared to the lowest energy singlet state of all the aforementioned conformers. The mixed basis set was used in all calculations; for Ir, the Stuttgart/Dresden (SDD) energy-consistent pseudopotentials basis[10-12] and for C, H, O and N the 6-31G(d) basis sets were used.[13] These ground-state geometries of 1 and 2 were further optimized in dichloromethane as a solvent by using the conductive polarizable continuum model (CPCM).[14, 15] The optimized ground-state geometries of complexes 1 and 2 were confirmed to be local minima from the real value of the lowest vibrational frequency. The electronic orbitals were visualized by using VMD software.[16] The first 100 excited singlet states were calculated using time-dependent density functional theory (TD-DFT) framework. The UV–Vis absorption spectra were simulated using fwhm 3000 cm^{-1} and convoluted with Gaussian curves by employing GabEdit.[17] The analyses of the UV-Visible transitions were performed using QmFordge.[18]

DNA Binding Studies

The Interaction of complexes with DNA was carried out as per our earlier report.[19-22] Briefly, in UV-Vis titration experiments, to an iridium complex solution (10 μM taken from 2mM stock solution prepared in 10% dimethyl formamide) increasing concentration of CT-DNA (0–80 μM) was added in the pH 7.2 phosphate buffer . After each addition of

CT-DNA, the solution was allowed to equilibrate at 25 °C for 10 min, after which absorption spectra was recorded. The data was then fit in equation 2[23] to obtain intrinsic binding constant K_b.

$$[DNA]/[\varepsilon_a-\varepsilon_f] = [DNA]/[\varepsilon_b-\varepsilon_f] + 1/K_b\,[\varepsilon_b-\varepsilon_f] \text{ ----------(2)}$$

where, [DNA] is the concentration of DNA in base pairs, εa is the extinction coefficient observed for the MLCT absorption band at the given DNA concentration, ε_f is the extinction coefficient of the complex free in solution and ε_b is the extinction coefficient of the complex when fully bound to DNA. A plot of $[DNA]/[\varepsilon_a-\varepsilon_f]$ versus [DNA] gave a slope $1/[\varepsilon_a-\varepsilon_f]$ and Y intercept equal to $1/K_b\,[\varepsilon_b-\varepsilon_f]$, respectively. The intrinsic binding constant K_b is the ratio of the slope to the intercept.[23]

For emission titration experiments increasing the concentration of DNA was added to the 10 μM of the metal complex(10 μMtaken from 2mM stock solution prepared in 10% dimethyl formamide) in buffer. Before recording the emission spectra, the DNA-complex solution was allowed to react for 10 min.

Electrophoretic mobility shift assay

The electrophoretic mobility shift assay was carried out as per our earlier report.[20, 22, 24] The plasmid pBR322 DNA (200 ng in nucleotides) in TAE buffer (40 mM Tris-Acetate, 1 mM EDTA) was reacted with the 5-80 μM of complexes for 30 minutes at 37 °C in dark. Then the reaction was quenched by addition of 2μL of gel loading dye (0.25% bromophenol blue, 0.25% xylene cyanol, 40% glycerol and 2 mM EDTA). Then the reaction mixture was subjected to electrophoresis at 60V on a 1% agarose gel in TBE (Tris acetic acid-EDTA) buffer (pH 8.2). The gel was stained with ethidium bromide and visualized and photographed for analysis using a Gel documentation system (Major Science).

Cytotoxicity: Cell viability assay

Cytotoxicity of complexes against HeLa cell line was determined as per our earlier report.[19, 20, 24] The number of viable cells left behind after appropriate treatment was determined by 3-(4,5-dimethylthiazol-2-yl)- 2,5-diphenyltetrazolium bromide (MTT; Sigma Chemical Co.) assay.[25]

Fluorescence microscopic images

For fluorescence microscopy experiments, Hela Cells were grown on sterile glass cover slips in a 35 mm tissue culture dish and incubated at 37 °C under a 5% CO_2 atmosphere for 48 h. The cell culture medium was replaced with medium containing a 10 μM of iridium complexes **1** and **2**. After incubation of cell with iridium complexes for 1 h, the culture medium was removed and the cell layer was washed gently with PBS (2 mL x 3 times). After washing with PBS, the cover slips were mounted on the slides for measurements. Imaging was performed using high resolution optical microscope Axio Imager M2, Carl Zeiss, Germany.

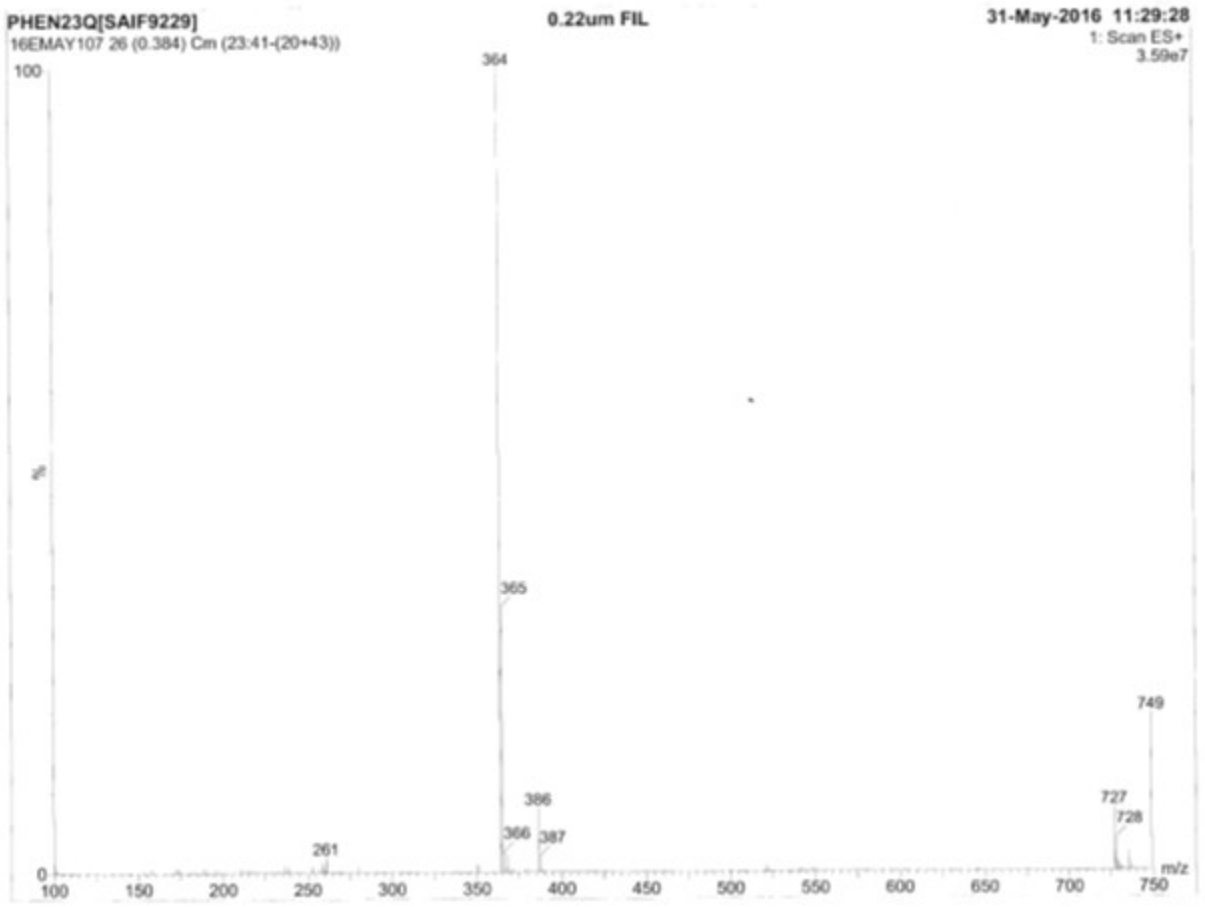


Figure S1. ESI-MS spectra of qip.

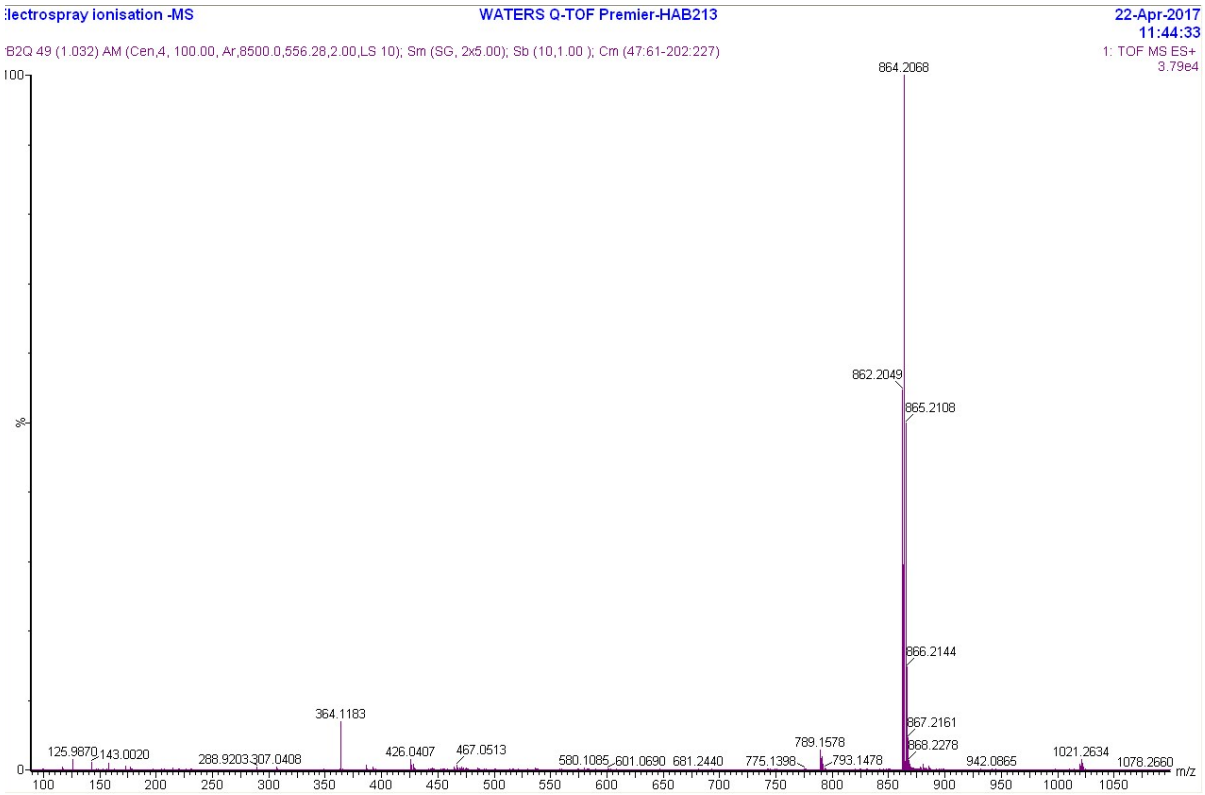


Figure S2. ESI-MS spectra of complex **1**.

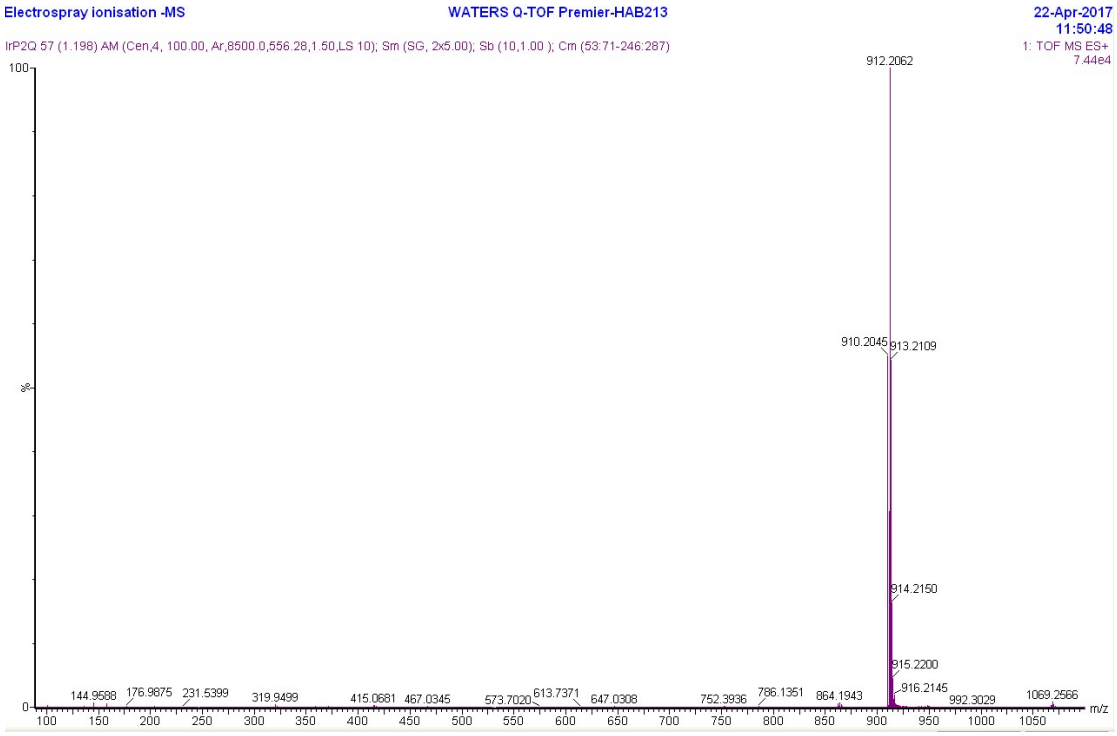


Figure S3. ESI-MS spectra of complex **2**.

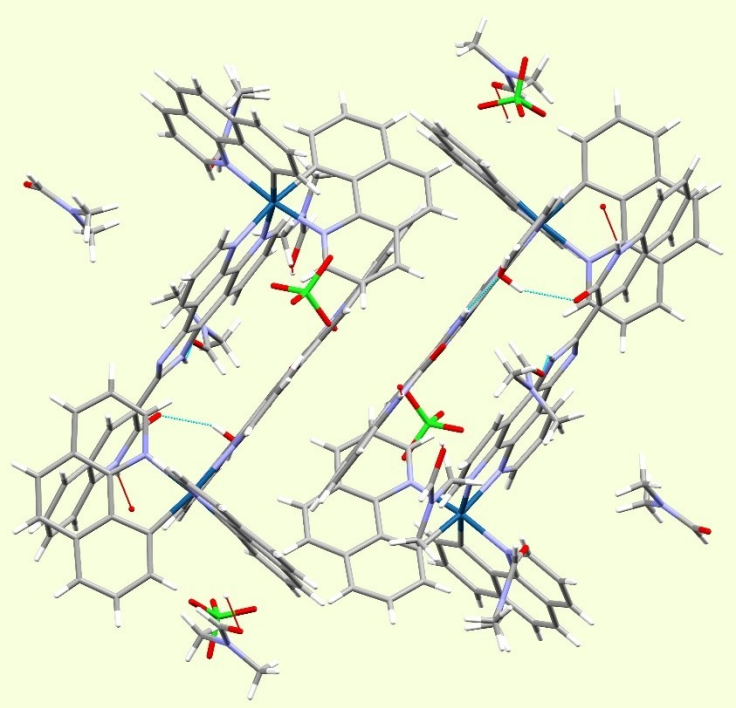


Figure S4. Packing Diagram of **2**.

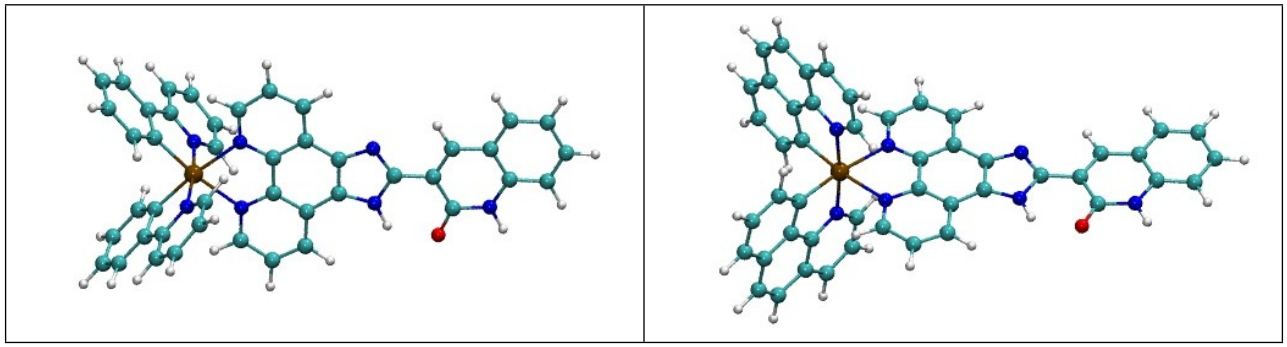
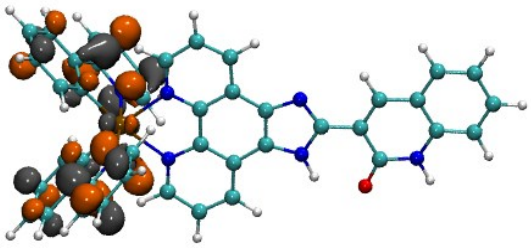
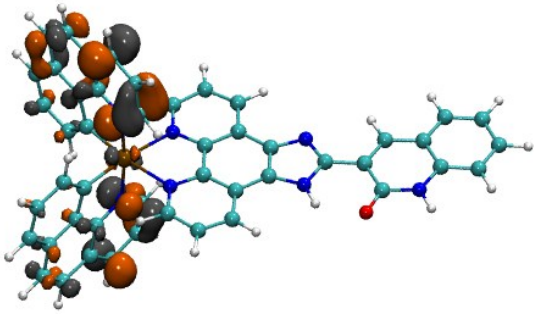
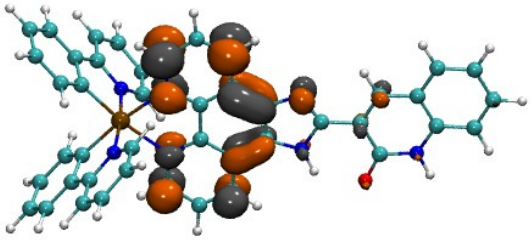
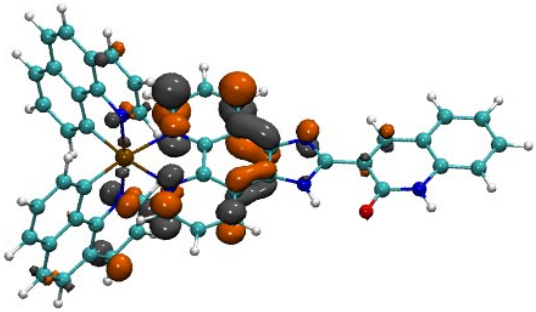
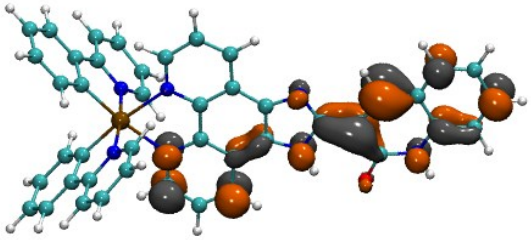
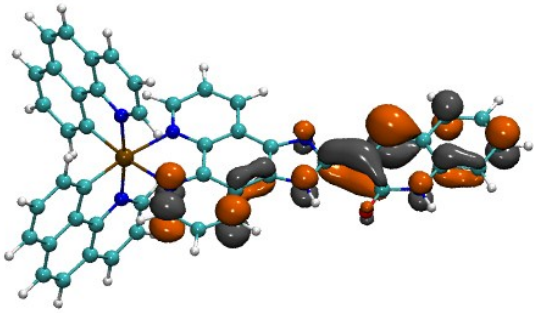
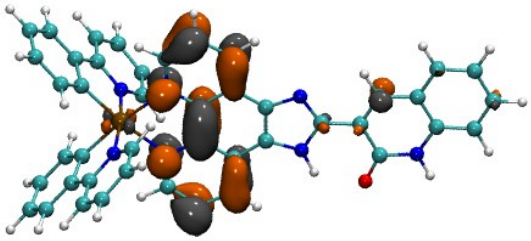
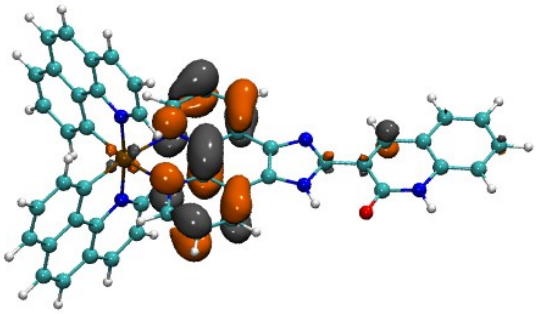


Figure S5. DFT optimised structure of complexes (a) **1** and (b) **2**.

Orbital	Complex 1	Complex 2
LUMO+3	 [187] -0.0701 a.u. (-1.91 eV)	 [199] -0.0766 a.u. (-2.08 eV)
LUMO+2	 [186] -0.0776 a.u. (-2.11 eV)	 [198] -0.0784 a.u. (-2.13 eV)
LUMO+1	 [185] -0.0878 a.u. (-2.39 eV)	 [197] -0.0878 a.u. (-2.39 eV)
LUMO	 [184] -0.0952 a.u. (-2.59 eV)	 [196] -0.0954 a.u. (-2.59 eV)

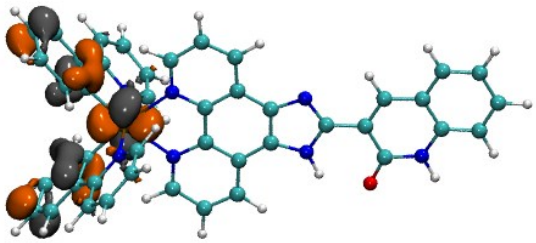
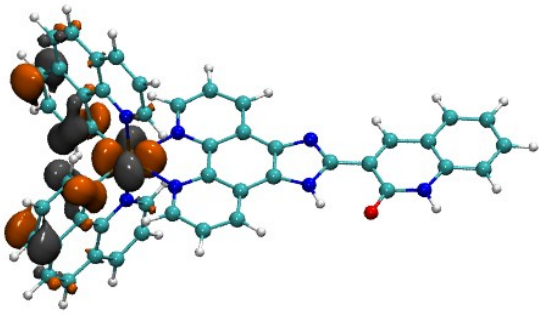
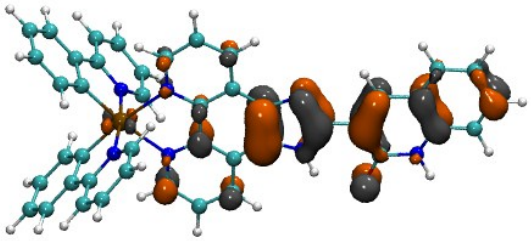
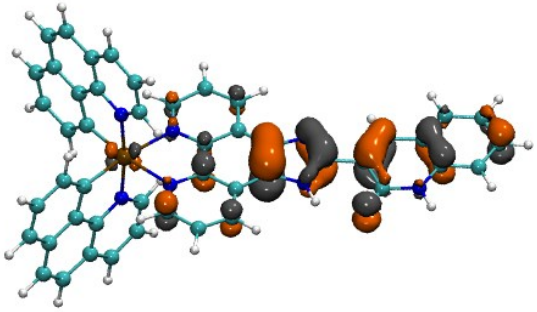
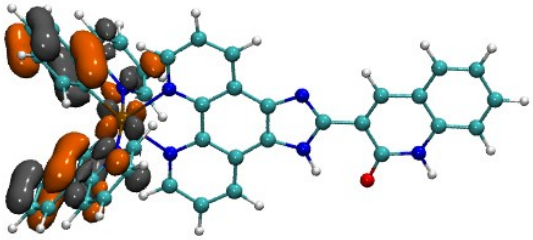
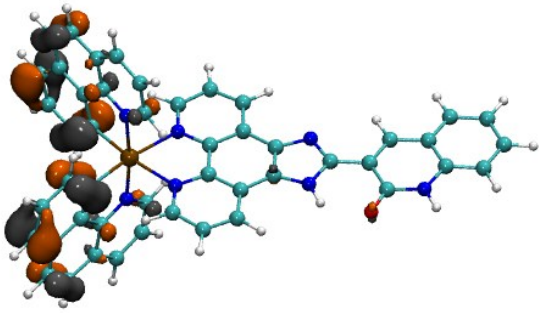
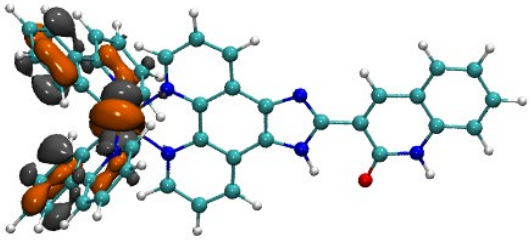
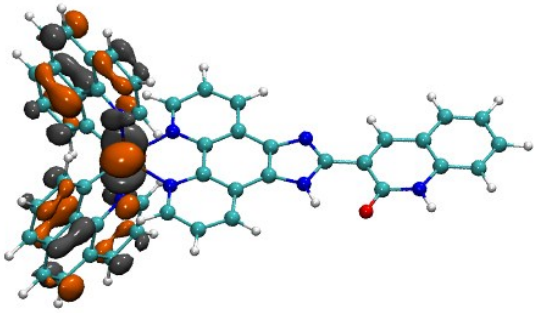
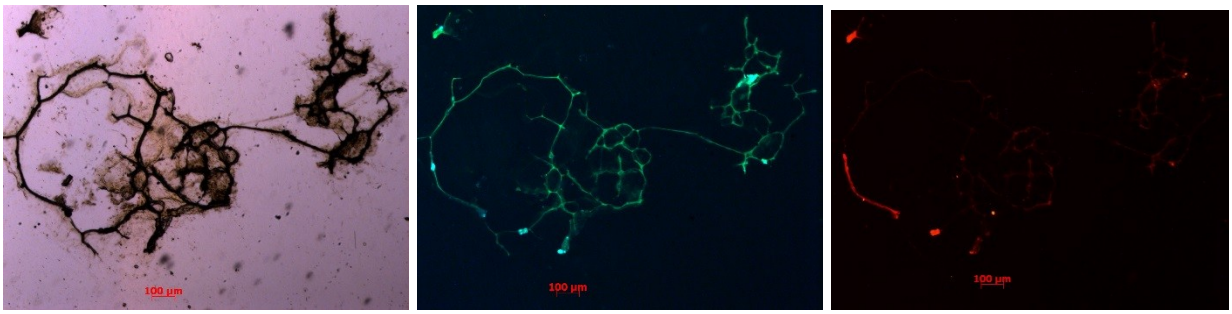
Orbital	Complex 1	Complex 2
HOMO	 [183] -0.2131 a.u. (-5.80 eV)	 [195] -0.2104 a.u. (-5.73 eV)
HOMO-1	 [182] -0.2252 a.u. (-6.13 eV)	 [194] -0.2249 a.u. (-6.12 eV)
HOMO-2	 [181] -0.2364 a.u. (-6.43 eV)	 [193] -0.2279 a.u. (-6.20 eV)
HOMO-3	 [180] -0.2417 a.u. (-6.58 eV)	 [192] -0.2385 a.u. (-6.49 eV)

Figure S6. Molecular orbital energy diagrams of complexes **1** and **2**.



Bright field green emission red emission

Figure S7. Fluorescence microscopy images of CT_DNA condensates induced by complex **2**.

Table S1. Bond angle and bond length table of complex **2.**

Bond length			
Ir1—N1	2.145 (4)	C62—C63	1.369 (8)
Ir1—C23	2.076 (5)	C81—C80	1.379 (9)
Ir1—N2	2.105 (4)	C52—C51	1.415 (7)
Ir1—N6	2.031 (5)	N16—C102	1.327 (8)
Ir1—N7	2.061 (4)	N16—C101	1.487 (9)
Ir1—C36	2.018 (5)	N16—C100	1.454 (10)
Ir2—N8	2.127 (5)	C64—C63	1.422 (7)
Ir2—N13	2.065 (5)	C64—C69	1.401 (8)
Ir2—N9	2.109 (4)	C64—C65	1.405 (8)
Ir2—N14	2.068 (5)	C90—C89	1.391 (8)
Ir2—C71	2.028 (6)	C90—C91	1.384 (8)
Ir2—C90	2.041 (5)	C15—C16	1.418 (8)
Cl2—O9	1.412 (8)	C15—C14	1.353 (9)
Cl2—O10	1.401 (6)	C36—C37	1.396 (8)
Cl2—O8	1.422 (7)	C21—C20	1.410 (9)
Cl2—O7	1.390 (8)	C21—C22	1.383 (9)
Cl1—O5	1.372 (9)	O15—C105	1.212 (10)
Cl1—O4	1.383 (8)	C89—C88	1.429 (8)
Cl1—O2	1.304 (11)	C89—C94	1.429 (8)
Cl1—O3	1.305 (11)	C46—C45	1.402 (8)
O6—C70	1.237 (7)	C77—C76	1.425 (9)
N8—C53	1.369 (7)	C77—C78	1.381 (8)

N8—C49	1.338 (7)	C88—C87	1.400 (8)
N1—C1	1.325 (7)	C7—C12	1.435 (8)
N1—C5	1.366 (7)	C7—C8	1.391 (8)
O1—C18	1.228 (8)	C26—C25	1.374 (10)
N4—C13	1.374 (8)	C26—C27	1.403 (9)
N4—C11	1.379 (7)	C45—C44	1.359 (9)
O14—C102	1.192 (8)	C16—C17	1.389 (8)
N11—C60	1.376 (7)	C16—C19	1.424 (9)
N11—C61	1.359 (7)	C40—C39	1.397 (8)
C23—C24	1.326 (8)	C43—C44	1.406 (8)
C23—C28	1.380 (7)	C43—C47	1.429 (8)
N3—C13	1.319 (8)	C51—C50	1.366 (8)
N3—C12	1.366 (7)	C31—C30	1.414 (9)
N2—C6	1.383 (7)	C31—C32	1.363 (10)
N2—C10	1.332 (7)	C49—C50	1.378 (8)
N6—C29	1.415 (8)	C58—C57	1.387 (8)
N6—C33	1.393 (8)	C55—C56	1.402 (8)
N13—C81	1.333 (8)	C76—C75	1.404 (9)
N13—C77	1.383 (8)	C57—C56	1.364 (8)
N12—C70	1.359 (7)	C69—C68	1.408 (8)
N12—C69	1.381 (7)	C91—C92	1.410 (9)
N7—C42	1.368 (7)	C20—C19	1.373 (9)
N7—C46	1.330 (7)	C17—C22	1.408 (8)
N10—C59	1.366 (7)	C95—C94	1.441 (10)
N10—C61	1.329 (7)	C95—C96	1.353 (11)
N9—C54	1.387 (7)	C37—C38	1.380 (9)
N9—C58	1.345 (7)	C14—C18	1.457 (8)
C24—C25	1.390 (9)	C3—C2	1.367 (9)
C53—C54	1.453 (7)	C10—C9	1.379 (8)
C53—C52	1.395 (7)	O16—C99	1.159 (11)
N5—C17	1.370 (8)	O12—C111	1.239 (13)
N5—C18	1.368 (8)	C93—C94	1.382 (10)
C13—C14	1.477 (8)	C93—C92	1.357 (10)
C70—C62	1.468 (7)	N17—C105	1.327 (10)
N14—C88	1.371 (8)	N17—C104	1.461 (12)
N14—C84	1.336 (8)	N17—C103	1.445 (13)
C4—C5	1.427 (7)	C72—C73	1.402 (9)

C4—C11	1.444 (8)	C84—C85	1.392 (9)
C4—C3	1.391 (8)	C8—C9	1.373 (8)
C1—C2	1.414 (8)	C27—C35	1.453 (9)
C5—C6	1.434 (8)	C30—C34	1.406 (9)
C41—C42	1.426 (7)	C65—C66	1.378 (8)
C41—C36	1.396 (8)	C87—C86	1.409 (10)
C41—C40	1.409 (8)	C87—C96	1.427 (10)
C29—C28	1.429 (8)	C39—C38	1.380 (9)
C29—C30	1.411 (8)	O13—C106	1.237 (11)
C11—C12	1.378 (8)	C86—C85	1.368 (10)
C59—C60	1.376 (7)	C78—C79	1.407 (10)
C59—C55	1.440 (7)	C78—C82	1.428 (10)
C6—C7	1.392 (8)	C80—C79	1.368 (10)
C33—C32	1.408 (8)	C35—C34	1.371 (10)
C71—C76	1.410 (8)	C75—C83	1.426 (10)
C71—C72	1.391 (8)	C75—C74	1.424 (10)
C42—C43	1.413 (8)	C68—C67	1.378 (10)
N18—C107	1.393 (11)	C66—C67	1.392 (10)
N18—C106	1.349 (12)	C73—C74	1.347 (10)
N18—C108	1.431 (12)	C82—C83	1.362 (11)
C48—C40	1.434 (8)	N15—C99	1.373 (12)
C48—C47	1.359 (9)	N15—C97	1.430 (12)
C28—C27	1.393 (8)	N15—C98	1.457 (12)
C60—C52	1.433 (7)	N19—C111	1.346 (12)
C54—C55	1.389 (7)	N19—C110	1.422 (18)
C62—C61	1.465 (7)	N19—C109	1.493 (16)
Bond angle			
C23—Ir1—N1	93.96 (17)	C100—N16—C101	117.2 (6)
C23—Ir1—N2	91.89 (17)	C69—C64—C63	118.3 (5)
N2—Ir1—N1	77.90 (17)	C69—C64—C65	118.6 (5)
N6—Ir1—N1	170.69 (18)	C65—C64—C63	123.0 (5)
N6—Ir1—C23	81.3 (2)	C89—C90—Ir2	112.3 (4)
N6—Ir1—N2	94.17 (18)	C91—C90—Ir2	130.4 (4)
N6—Ir1—N7	93.11 (19)	C91—C90—C89	117.2 (5)
N7—Ir1—N1	92.18 (16)	C14—C15—C16	121.5 (6)
N7—Ir1—C23	172.81 (17)	C41—C36—Ir1	113.3 (4)
N7—Ir1—N2	93.04 (17)	C37—C36—Ir1	131.7 (4)

C36—Ir1—N1	99.12 (19)	C37—C36—C41	114.9 (5)
C36—Ir1—C23	94.23 (19)	C22—C21—C20	121.2 (6)
C36—Ir1—N2	173.37 (19)	C90—C89—C88	117.6 (5)
C36—Ir1—N6	89.3 (2)	C90—C89—C94	122.9 (6)
C36—Ir1—N7	81.10 (19)	C94—C89—C88	119.4 (5)
N13—Ir2—N8	93.60 (18)	N11—C61—C62	125.1 (5)
N13—Ir2—N9	91.03 (17)	N10—C61—N11	112.8 (4)
N13—Ir2—N14	171.72 (18)	N10—C61—C62	122.1 (4)
N9—Ir2—N8	78.31 (16)	N7—C46—C45	121.6 (5)
N14—Ir2—N8	93.73 (17)	N13—C77—C76	115.2 (5)
N14—Ir2—N9	94.23 (18)	C78—C77—N13	122.5 (6)
C71—Ir2—N8	169.87 (19)	C78—C77—C76	122.4 (6)
C71—Ir2—N13	81.0 (2)	N14—C88—C89	115.7 (5)
C71—Ir2—N9	93.16 (19)	N14—C88—C87	122.4 (6)
C71—Ir2—N14	92.3 (2)	C87—C88—C89	122.0 (5)
C71—Ir2—C90	93.6 (2)	C62—C63—C64	121.7 (5)
C90—Ir2—N8	95.39 (19)	C6—C7—C12	116.6 (5)
C90—Ir2—N13	94.5 (2)	C8—C7—C6	118.9 (5)
C90—Ir2—N9	171.89 (19)	C8—C7—C12	124.4 (5)
C90—Ir2—N14	81.0 (2)	C25—C26—C27	119.4 (6)
O9—Cl2—O8	110.5 (5)	C44—C45—C46	120.5 (5)
O10—Cl2—O9	108.6 (5)	C15—C16—C19	123.2 (5)
O10—Cl2—O8	109.3 (5)	C17—C16—C15	118.0 (6)
O7—Cl2—O9	110.0 (6)	C17—C16—C19	118.8 (5)
O7—Cl2—O10	108.3 (5)	N3—C12—C11	111.4 (5)
O7—Cl2—O8	110.1 (5)	N3—C12—C7	126.9 (5)
O5—Cl1—O4	111.7 (6)	C11—C12—C7	121.7 (5)
O2—Cl1—O5	110.8 (7)	C41—C40—C48	118.9 (5)
O2—Cl1—O4	115.2 (7)	C39—C40—C41	117.2 (5)
O2—Cl1—O3	106.7 (10)	C39—C40—C48	123.9 (5)
O3—Cl1—O5	111.7 (10)	C42—C43—C47	117.1 (5)
O3—Cl1—O4	100.1 (9)	C44—C43—C42	117.8 (5)
C53—N8—Ir2	114.4 (3)	C44—C43—C47	125.0 (5)
C49—N8—Ir2	127.0 (4)	C45—C44—C43	119.2 (5)
C49—N8—C53	118.4 (5)	C50—C51—C52	118.9 (5)
C1—N1—Ir1	126.6 (4)	C32—C31—C30	119.4 (5)
C1—N1—C5	119.9 (5)	N8—C49—C50	122.3 (5)

C5—N1—Ir1	113.5 (3)	N9—C58—C57	122.2 (5)
C13—N4—C11	106.0 (5)	C54—C55—C59	116.5 (5)
C61—N11—C60	106.8 (4)	C54—C55—C56	118.7 (5)
C24—C23—Ir1	128.5 (4)	C56—C55—C59	124.8 (5)
C24—C23—C28	118.6 (5)	C71—C76—C77	117.2 (5)
C28—C23—Ir1	112.9 (4)	C75—C76—C71	123.8 (6)
C13—N3—C12	104.5 (5)	C75—C76—C77	118.9 (5)
C6—N2—Ir1	115.0 (4)	C56—C57—C58	120.6 (5)
C10—N2—Ir1	128.0 (4)	N12—C69—C64	118.8 (5)
C10—N2—C6	116.9 (5)	N12—C69—C68	120.2 (5)
C29—N6—Ir1	112.4 (4)	C64—C69—C68	121.0 (5)
C33—N6—Ir1	131.4 (4)	C90—C91—C92	120.3 (6)
C33—N6—C29	116.1 (5)	C19—C20—C21	119.6 (6)
C81—N13—Ir2	128.2 (4)	N5—C17—C16	119.4 (5)
C81—N13—C77	118.2 (5)	N5—C17—C22	119.5 (6)
C77—N13—Ir2	113.7 (4)	C16—C17—C22	121.1 (6)
C70—N12—C69	125.5 (5)	C96—C95—C94	122.2 (6)
C42—N7—Ir1	112.9 (3)	C38—C37—C36	122.1 (6)
C46—N7—Ir1	127.8 (4)	C15—C14—C13	119.4 (5)
C46—N7—C42	119.1 (5)	C15—C14—C18	121.0 (5)
C61—N10—C59	103.7 (4)	C18—C14—C13	119.6 (6)
C54—N9—Ir2	114.7 (3)	C2—C3—C4	120.0 (5)
C58—N9—Ir2	127.8 (3)	N2—C10—C9	123.9 (5)
C58—N9—C54	117.6 (4)	C48—C47—C43	121.7 (5)
C23—C24—C25	122.2 (6)	C92—C93—C94	120.6 (6)
N8—C53—C54	116.7 (4)	C105—N17—C104	119.1 (8)
N8—C53—C52	122.3 (5)	C105—N17—C103	122.9 (8)
C52—C53—C54	121.1 (4)	C103—N17—C104	118.0 (7)
C18—N5—C17	125.4 (5)	C71—C72—C73	120.6 (6)
N4—C13—C14	124.9 (6)	N14—C84—C85	121.6 (6)
N3—C13—N4	112.7 (5)	C51—C50—C49	120.5 (5)
N3—C13—C14	122.4 (6)	C21—C22—C17	118.8 (6)
O6—C70—N12	121.2 (5)	C57—C56—C55	118.8 (5)
O6—C70—C62	123.0 (5)	C26—C25—C24	119.9 (6)
N12—C70—C62	115.8 (5)	C89—C94—C95	117.0 (6)
C88—N14—Ir2	113.2 (4)	C93—C94—C89	117.3 (6)
C84—N14—Ir2	128.0 (4)	C93—C94—C95	125.7 (6)

C84—N14—C88	118.8 (5)	C9—C8—C7	118.8 (5)
C5—C4—C11	114.8 (5)	C28—C27—C26	117.8 (6)
C3—C4—C5	118.0 (5)	C28—C27—C35	117.1 (6)
C3—C4—C11	127.2 (5)	C26—C27—C35	125.0 (6)
N1—C1—C2	121.5 (5)	O1—C18—N5	121.0 (6)
N1—C5—C4	120.9 (5)	O1—C18—C14	124.3 (5)
N1—C5—C6	117.6 (5)	N5—C18—C14	114.7 (5)
C4—C5—C6	121.5 (5)	C29—C30—C31	117.2 (6)
C36—C41—C42	116.3 (5)	C34—C30—C29	119.7 (6)
C36—C41—C40	124.7 (5)	C34—C30—C31	123.1 (5)
C40—C41—C42	118.9 (5)	C66—C65—C64	120.8 (6)
N6—C29—C28	117.1 (5)	C88—C87—C86	117.5 (6)
C30—C29—N6	124.1 (5)	C88—C87—C96	117.5 (6)
C30—C29—C28	118.8 (5)	C86—C87—C96	125.1 (6)
N4—C11—C4	131.4 (5)	C38—C39—C40	119.5 (5)
C12—C11—N4	105.4 (5)	C31—C32—C33	122.7 (6)
C12—C11—C4	123.2 (5)	C8—C9—C10	119.4 (6)
N10—C59—C60	112.0 (4)	C20—C19—C16	120.5 (6)
N10—C59—C55	126.8 (4)	C85—C86—C87	119.3 (6)
C60—C59—C55	121.2 (4)	C77—C78—C79	117.9 (6)
N2—C6—C5	115.8 (5)	C77—C78—C82	117.7 (6)
N2—C6—C7	122.0 (5)	C79—C78—C82	124.4 (6)
C7—C6—C5	122.2 (5)	C79—C80—C81	120.9 (6)
N6—C33—C32	120.5 (6)	C95—C96—C87	121.7 (6)
C76—C71—Ir2	112.7 (4)	C34—C35—C27	121.0 (6)
C72—C71—Ir2	130.6 (4)	C86—C85—C84	120.4 (6)
C72—C71—C76	116.3 (5)	C93—C92—C91	121.7 (6)
N7—C42—C41	116.3 (5)	C76—C75—C83	118.4 (6)
N7—C42—C43	121.7 (5)	C76—C75—C74	116.9 (6)
C43—C42—C41	121.9 (5)	C74—C75—C83	124.7 (6)
C107—N18—C108	119.6 (9)	O14—C102—N16	125.5 (6)
C106—N18—C107	119.5 (8)	C67—C68—C69	118.2 (6)
C106—N18—C108	120.9 (8)	C80—C79—C78	118.8 (6)
C47—C48—C40	121.3 (5)	C65—C66—C67	119.4 (6)
C23—C28—C29	115.9 (5)	C74—C73—C72	122.6 (6)
C23—C28—C27	122.1 (6)	C83—C82—C78	120.9 (6)
C27—C28—C29	122.0 (5)	C37—C38—C39	121.5 (6)

N11—C60—C52	132.0 (5)	C68—C67—C66	122.0 (6)
C59—C60—N11	104.7 (4)	C99—N15—C97	121.7 (8)
C59—C60—C52	123.3 (5)	C99—N15—C98	122.1 (8)
N9—C54—C53	116.0 (4)	C97—N15—C98	116.2 (9)
N9—C54—C55	122.0 (5)	C3—C2—C1	119.5 (5)
C55—C54—C53	122.0 (5)	O16—C99—N15	121.7 (10)
C61—C62—C70	120.5 (5)	C82—C83—C75	121.7 (6)
C63—C62—C70	119.8 (5)	C73—C74—C75	119.8 (6)
C63—C62—C61	119.7 (5)	O15—C105—N17	124.6 (9)
N13—C81—C80	121.8 (6)	C35—C34—C30	121.3 (6)
C53—C52—C60	116.0 (5)	O13—C106—N18	124.1 (9)
C53—C52—C51	117.7 (5)	C111—N19—C110	127.0 (15)
C51—C52—C60	126.4 (5)	C111—N19—C109	121.9 (11)
C102—N16—C101	121.0 (6)	C110—N19—C109	110.3 (14)
C102—N16—C100	121.4 (6)	O12—C111—N19	123.8 (11)

Table S2. Molecular orbital composition analysis of complexes **1** and **2** using Hirshfeld method.

	Energy (in a.u.)	Molecular orbital composition (in %)			
		Fragment 1 (Ru)	Fragment 2 (ppy)	Fragment 3 (ppy′)	Fragment 4 (qip)
Pop-1-NNtrans					
HOMO-4	-0.2449	26.34	15.59	14.40	43.68
HOMO-3	-0.2417	39.78	27.42	28.50	4.31
HOMO-2	-0.2364	6.56	45.55	45.64	2.26
HOMO-1	-0.2252	2.06	0.45	0.43	97.04
HOMO	-0.2131	35.88	30.54	30.42	3.16
LUMO	-0.0952	2.46	0.73	0.71	96.10
LUMO+1	-0.0878	0.73	0.29	0.41	98.56
LUMO+2	-0.0776	1.09	1.41	1.12	96.36
LUMO+3	-0.0701	4.16	46.81	47.36	1.67
LUMO+4	-0.0670	4.28	46.41	46.10	3.21
Pop-2-NNtrans		Fragment 1 (Ru)	Fragment 2 (bhq)	Fragment 3 (bhq′)	Fragment 4 (qip)
HOMO-4	-0.2420	27.16	27.86	30.24	14.77
HOMO-3	-0.2385	31.92	33.49	31.54	3.07
HOMO-2	-0.2279	1.47	43.48	43.94	11.15
HOMO-1	-0.2249	2.30	5.21	5.08	87.46
HOMO	-0.2104	27.55	35.09	34.70	2.70
LUMO	-0.0954	2.50	0.65	0.68	96.21
LUMO+1	-0.0878	0.69	0.73	0.24	98.38

LUMO+2	-0.0784	1.96	8.97	20.84	68.27
LUMO+3	-0.0766	3.05	57.02	38.14	1.84
LUMO+4	-0.0755	1.49	30.27	37.71	30.57

Table S3. Analysis of transitions in complex **1** by TD-DFT.

Index	Energy.cm^-1	Wavelength	Osc.Strength	Contributions
0	20550.200	486.613	3.000e-04	92.4% HOMO => LUMO, 6.47% HOMO => L+1
1	24065.971	415.524	3.360e-02	50.9% HOMO => L+1, 29.8% HOMO => L+2, 14.5% H-1 => LUMO, 2.98% HOMO => LUMO
2	24145.013	414.164	2.676e-01	80.4% H-1 => LUMO, 9.30% HOMO => L+1, 5.20% HOMO => L+2
3	25311.291	395.081	6.140e-02	97.2% HOMO => L+3
4	25524.221	391.785	1.100e-03	58.1% HOMO => L+2, 31.0% HOMO => L+1, 5.57% HOMO => L+4, 3.24% HOMO => LUMO
5	26254.153	380.892	1.180e-02	70.7% H-3 => LUMO, 15.8% H-6 => LUMO, 5.44% H-3 => L+1, 3.87% HOMO => L+4
6	26304.160	380.168	7.300e-03	83.3% HOMO => L+4, 5.12% HOMO => L+2, 3.91% H-3 => LUMO
7	26645.332	375.300	7.625e-01	67.9% H-1 => L+1, 21.0% H-2 => LUMO, 3.27% HOMO => L+4
8	26770.348	373.548	1.814e-01	69.0% H-2 => LUMO, 23.5% H-1 => L+1, 2.72% H-2 => L+1
9	28106.002	355.796	4.940e-02	48.4% H-4 => LUMO, 26.3% H-1 => L+2, 7.80% H-5 => LUMO, 5.39% H-7 => LUMO, 2.87% H-2 => LUMO
10	28398.781	352.128	2.160e-02	62.9% H-1 => L+2, 20.9% H-4 => LUMO, 5.89% H-8 => LUMO, 3.51% H-5 => LUMO
11	29252.923	341.846	5.000e-04	73.4% H-6 => LUMO, 18.2% H-3 => LUMO, 4.43% H-6 => L+1
12	29636.036	337.427	9.000e-03	61.1% H-2 => L+1, 15.0% H-2 => L+2, 7.72% H-4 => L+1, 3.75% H-5 => LUMO, 2.78% H-2 => LUMO
13	29945.753	333.937	3.150e-02	51.7% H-5 => LUMO, 14.9% H-4 => L+1, 7.37% H-2 => L+1, 7.00% H-5 => L+1, 6.89% H-4 => LUMO, 3.71% H-2 => L+2
14	30119.162	332.015	1.400e-02	37.1% H-3 => L+1, 24.3% H-3 => L+2, 13.8% H-7 => LUMO, 3.34% H-5 => L+1, 3.17% H-4 => LUMO, 3.15% H-6 => L+2, 2.57% H-6 => L+1, 2.30% H-4 => L+1
15	30178.041	331.367	1.750e-02	92.2% HOMO => L+5, 2.67% HOMO => L+7
16	30452.269	328.383	1.130e-02	44.0% H-7 => LUMO, 21.9% H-1 => L+3, 6.31% H-3 => L+1, 4.44% H-5 => LUMO, 4.19% H-2 => L+3, 3.25% H-4 => L+3, 2.21% H-4 => L+1, 2.04% H-5 => L+1
17	30641.003	326.360	7.000e-04	48.4% H-1 => L+3, 14.5% H-7 => LUMO, 13.6%

				H-3 => L+1, 5.12% H-2 => L+3, 3.59% H-4 => L+3
18	30809.573	324.574	4.000e-03	16.1% H-1 => L+4, 14.0% H-2 => L+2, 12.8% H-2 => L+1, 10.2% H-4 => L+2, 9.80% H-4 => L+1, 9.66% H-3 => L+3, 3.97% H-4 => L+4, 3.93% H-2 => L+4, 3.01% H-7 => L+2, 2.88% H-5 => L+2, 2.15% H-6 => L+3
19	31037.828	322.187	4.800e-03	32.9% H-4 => L+1, 16.1% H-5 => LUMO, 11.1% H-1 => L+4, 8.54% H-7 => LUMO, 5.50% H-3 => L+3, 5.49% H-5 => L+1, 4.66% H-4 => LUMO, 2.93% H-2 => L+4, 2.25% H-4 => L+4, 2.06% H-8 => LUMO
20	31135.421	321.178	4.100e-03	38.8% H-2 => L+2, 13.0% H-1 => L+4, 12.0% H-3 => L+3, 8.55% H-2 => L+1, 4.02% H-5 => L+1, 3.14% H-5 => LUMO, 2.89% H-4 => L+4, 2.80% H-6 => L+3
21	31224.948	320.257	3.000e-04	87.9% HOMO => L+6
22	31389.485	318.578	5.160e-02	39.5% H-5 => L+1, 16.6% H-2 => L+2, 13.0% H-4 => L+2, 5.41% H-1 => L+4, 5.17% H-7 => L+1, 3.59% H-4 => LUMO, 3.00% H-2 => L+4, 2.46% H-3 => L+3, 2.08% H-4 => L+1
23	31474.980	317.713	6.730e-02	48.6% H-3 => L+3, 28.4% H-1 => L+4, 7.96% H-6 => L+3, 3.44% H-5 => L+1, 3.35% H-2 => L+2
24	31666.940	315.787	3.210e-02	29.4% H-2 => L+3, 24.8% H-3 => L+2, 16.0% H-3 => L+1, 14.5% H-1 => L+3, 4.10% H-6 => L+2
25	31758.081	314.880	2.000e-04	46.9% H-2 => L+3, 24.1% H-3 => L+2, 13.0% H-3 => L+1, 4.50% H-6 => L+2, 3.68% H-1 => L+3
26	32157.325	310.971	2.590e-02	59.6% H-3 => L+4, 11.9% H-6 => L+4, 8.41% H-4 => L+3, 4.98% H-2 => L+3, 3.36% H-5 => L+3, 2.95% H-1 => L+3
27	32311.377	309.489	4.900e-03	66.7% H-6 => L+1, 9.20% H-6 => L+2, 7.76% H-3 => L+2, 3.73% H-6 => LUMO
28	32344.446	309.172	4.280e-02	74.2% H-2 => L+4, 15.0% H-1 => L+4, 2.43% H-7 => L+4
29	32621.094	306.550	3.580e-02	37.5% H-4 => L+2, 16.7% H-5 => L+1, 15.8% H-4 => L+1, 5.45% H-7 => L+2, 5.22% H-5 => L+2, 3.20% H-8 => LUMO, 2.09% H-6 => L+1, 2.05% H-2 => L+2
30	33257.465	300.684	2.220e-02	33.9% H-7 => L+1, 20.9% H-4 => L+3, 7.22% H-5 => L+3, 5.02% H-5 => L+2, 4.66% H-3 => L+4, 4.36% H-5 => L+1, 4.25% H-7 => L+2, 2.64% H-6 => L+1, 2.24% H-7 => LUMO
31	33343.767	299.906	1.460e-02	21.4% H-4 => L+3, 19.3% H-7 => L+1, 10.1% HOMO => L+7, 7.25% H-5 => L+3, 6.65% H-3 => L+4, 5.50% H-5 => L+2, 3.57% H-6 => L+2, 3.36% H-7 => L+2, 2.95% H-4 => L+4, 2.39% H-3 => L+2

32	33521.209	298.319	1.640e-02	55.8% HOMO => L+7, 9.48% H-6 => L+2, 9.17% H-7 => L+1, 2.96% H-4 => L+4, 2.70% H-8 => LUMO, 2.32% H-4 => L+3, 2.06% HOMO => L+8
33	33542.986	298.125	8.950e-02	43.9% H-4 => L+4, 15.0% H-5 => L+4, 7.92% H-7 => L+1, 5.96% H-1 => L+4, 4.66% H-8 => LUMO, 3.38% H-2 => L+4, 2.90% H-3 => L+3, 2.86% H-4 => L+2, 2.80% H-7 => L+4
34	33719.621	296.563	1.380e-02	46.5% H-6 => L+2, 20.7% HOMO => L+7, 8.90% H-6 => L+1, 5.40% H-3 => L+2, 3.79% H-5 => L+2, 2.89% H-8 => LUMO
35	33837.378	295.531	4.370e-02	45.3% H-5 => L+2, 12.0% H-8 => LUMO, 9.04% H-6 => L+2, 4.99% H-4 => L+2, 3.60% H-7 => L+2, 2.97% H-1 => L+2, 2.55% H-4 => L+4, 2.14% H-6 => L+1
36	34268.885	291.810	8.480e-02	64.0% H-6 => L+3, 10.6% H-3 => L+3, 6.64% H-3 => L+5, 6.24% H-2 => L+6
37	34341.474	291.193	1.020e-02	42.2% H-1 => L+5, 12.2% H-6 => L+4, 10.8% H-2 => L+5, 9.35% H-7 => L+3, 4.13% H-3 => L+4, 2.66% H-5 => L+3, 2.37% H-4 => L+5, 2.35% H-8 => L+2
38	34564.890	289.311	5.710e-02	20.6% H-8 => LUMO, 13.5% H-1 => L+5, 11.9% H-7 => L+2, 10.1% H-4 => L+2, 7.69% H-6 => L+4, 5.80% H-8 => L+2, 2.97% H-7 => L+3, 2.66% H-9 => LUMO, 2.57% H-2 => L+5, 2.20% H-3 => L+4
39	34648.772	288.611	7.150e-02	20.6% H-7 => L+2, 15.9% H-1 => L+5, 10.2% H-6 => L+4, 7.65% H-7 => L+3, 7.11% H-4 => L+2, 6.70% H-8 => LUMO, 6.17% H-2 => L+5, 3.23% H-1 => L+7, 2.34% H-7 => L+1, 2.29% H-3 => L+4
40	34796.371	287.386	9.950e-02	34.3% H-7 => L+2, 21.4% H-8 => LUMO, 16.7% H-5 => L+2, 7.84% H-7 => L+1, 3.42% H-8 => L+1
41	35029.465	285.474	3.500e-03	44.8% H-7 => L+3, 31.9% H-6 => L+4, 9.33% H-5 => L+3, 8.65% H-3 => L+4, 2.02% H-2 => L+3
42	35219.006	283.938	1.145e-01	49.1% H-8 => L+1, 23.4% H-9 => LUMO, 7.72% H-1 => L+5, 3.77% H-8 => L+2, 2.49% H-5 => L+2
43	35427.903	282.263	6.600e-03	54.9% H-7 => L+4, 13.7% H-5 => L+4, 9.69% H-3 => L+5, 5.23% H-6 => L+3, 4.32% H-7 => L+2, 2.20% H-2 => L+6
44	35969.908	278.010	4.800e-03	78.4% H-1 => L+6, 8.58% H-3 => L+5, 4.64% H-4 => L+6, 2.82% H-2 => L+6
45	36052.176	277.376	1.190e-02	34.5% H-1 => L+7, 30.6% H-9 => LUMO, 7.51% H-8 => L+1, 6.24% H-9 => L+1, 5.93% H-1 => L+5, 2.15% H-4 => L+5

46	36235.264	275.974	2.020e-02	25.1% H-8 => L+1, 20.4% H-1 => L+7, 17.1% H-9 => LUMO, 13.4% H-8 => L+2, 4.87% H-9 => L+1, 3.73% H-11 => LUMO, 2.12% H-1 => L+6, 2.09% H-1 => L+5
47	36421.578	274.563	1.000e-04	65.7% H-10 => L+1, 26.6% H-10 => LUMO, 3.81% H-10 => L+2
48	36510.299	273.895	9.610e-02	48.7% H-3 => L+5, 9.16% H-6 => L+5, 8.65% H-1 => L+6, 7.52% H-2 => L+6, 7.25% H-7 => L+4
49	36569.178	273.454	2.970e-02	58.3% H-2 => L+5, 12.0% H-3 => L+6, 5.95% H-6 => L+4, 3.14% H-5 => L+3, 2.96% H-7 => L+3, 2.52% H-1 => L+5, 2.32% H-1 => L+7
50	36735.328	272.218	8.100e-03	81.7% H-11 => LUMO, 5.97% H-11 => L+1, 2.65% H-8 => L+2
51	36892.606	271.057	0.000e+00	54.5% H-5 => L+3, 29.9% H-4 => L+3, 7.69% H-7 => L+3, 3.39% H-3 => L+6
52	37234.585	268.568	3.950e-02	59.5% H-9 => L+1, 12.9% H-8 => L+2, 5.75% H-9 => LUMO, 2.84% H-4 => L+5, 2.27% H-5 => L+5
53	37398.316	267.392	2.620e-02	36.2% H-4 => L+5, 12.9% H-3 => L+6, 10.8% H-5 => L+5, 5.34% H-2 => L+5, 3.74% HOMO => L+14, 3.30% H-9 => L+1, 3.27% H-7 => L+3, 2.95% H-6 => L+6, 2.93% H-1 => L+5, 2.68% H-1 => L+7, 2.65% H-8 => L+2
54	37491.070	266.730	9.480e-02	41.0% H-5 => L+4, 24.2% H-2 => L+6, 22.6% H-4 => L+4, 3.62% HOMO => L+11
55	37665.285	265.496	2.409e-01	37.2% H-2 => L+6, 18.2% H-5 => L+4, 13.0% H-7 => L+4, 10.9% HOMO => L+11, 7.06% H-4 => L+4, 2.72% H-6 => L+3
56	37720.938	265.105	2.520e-02	44.9% H-3 => L+6, 18.5% H-4 => L+5, 6.41% H-6 => L+6, 5.79% H-5 => L+5, 5.11% H-6 => L+4, 5.09% H-7 => L+3, 2.52% H-2 => L+5
57	37802.400	264.533	3.700e-02	35.3% HOMO => L+14, 16.2% HOMO => L+10, 16.0% HOMO => L+13, 6.54% HOMO => L+9, 5.22% H-4 => L+5, 2.97% H-3 => L+6, 2.51% H-6 => L+14, 2.15% H-5 => L+5
58	37865.311	264.094	2.000e-03	81.5% H-12 => LUMO, 5.28% H-12 => L+1, 4.07% H-13 => LUMO, 3.24% H-10 => LUMO
59	38439.578	260.149	1.520e-02	44.2% H-4 => L+6, 17.1% H-5 => L+6, 12.4% HOMO => L+11, 9.52% H-2 => L+6, 6.01% H-6 => L+5, 2.50% H-1 => L+6
60	38642.829	258.780	4.176e-01	33.1% H-8 => L+2, 20.1% H-1 => L+7, 8.84% H-9 => L+1, 5.53% H-1 => L+8, 4.96% H-9 => LUMO, 3.37% H-5 => L+8, 2.55% H-4 => L+6, 2.41% H-6 => L+5, 2.02% HOMO => L+11
61	38750.908	258.058	1.518e-01	35.2% H-6 => L+5, 16.2% HOMO => L+11, 16.0% H-4 => L+6, 5.10% H-5 => L+6, 3.26% H-8 => L+2, 2.44% HOMO => L+16, 2.26% H-1 =>

				L+7
62	38929.963	256.872	1.625e-01	39.3% H-6 => L+5, 22.5% HOMO => L+11, 11.5% H-3 => L+5, 3.85% HOMO => L+16, 3.75% HOMO => L+18, 3.12% H-7 => L+4, 2.65% HOMO => L+21
63	39030.782	256.208	1.600e-03	47.4% HOMO => L+8, 38.2% HOMO => L+9, 5.80% H-2 => L+7
64	39256.617	254.734	6.000e-04	66.9% H-10 => LUMO, 24.9% H-10 => L+1, 4.71% H-12 => LUMO
65	39287.266	254.535	3.350e-02	70.5% H-2 => L+7, 10.5% HOMO => L+8, 3.15% H-7 => L+5
66	39326.787	254.280	3.410e-02	51.6% H-9 => L+2, 20.3% H-3 => L+7, 3.86% H-6 => L+7, 3.58% H-1 => L+8, 2.42% H-5 => L+5, 2.38% H-2 => L+7
67	39502.616	253.148	3.500e-03	51.9% H-13 => LUMO, 15.0% HOMO => L+9, 9.41% H-7 => L+5, 3.87% HOMO => L+8, 3.49% H-13 => L+1, 2.46% H-5 => L+5, 2.02% H-12 => LUMO
68	39544.557	252.879	4.100e-03	40.7% H-7 => L+5, 26.9% H-8 => L+3, 8.24% H-5 => L+5, 6.76% H-13 => LUMO, 3.02% H-6 => L+6, 2.38% H-9 => L+2, 2.23% H-2 => L+7
69	39590.531	252.586	5.800e-03	55.3% H-8 => L+3, 14.3% H-13 => LUMO, 8.77% H-7 => L+5, 6.10% HOMO => L+8, 2.87% HOMO => L+9, 2.50% H-5 => L+5, 2.15% H-9 => L+3
70	39626.826	252.354	6.600e-03	33.8% HOMO => L+9, 26.5% HOMO => L+8, 7.51% H-7 => L+5, 7.24% H-13 => LUMO, 6.51% H-2 => L+7, 6.26% H-8 => L+3, 2.75% H-5 => L+5
71	39742.163	251.622	4.750e-02	55.2% H-3 => L+7, 19.5% H-9 => L+2, 4.37% H-6 => L+7, 2.25% H-8 => L+3, 2.18% H-1 => L+8, 2.03% H-3 => L+8
72	39838.143	251.016	2.300e-03	81.4% H-6 => L+6, 11.2% H-3 => L+6
73	39975.257	250.155	5.000e-04	68.2% H-15 => LUMO, 24.1% H-15 => L+1, 3.60% H-12 => L+1
74	40203.512	248.734	8.800e-03	79.8% H-8 => L+4, 2.82% H-9 => L+4, 2.06% H-3 => L+14
75	40309.171	248.083	7.400e-03	27.1% H-3 => L+14, 18.0% HOMO => L+10, 12.3% H-6 => L+14, 8.94% H-3 => L+13, 5.17% H-8 => L+4, 4.87% H-3 => L+10, 4.10% H-6 => L+13, 2.02% H-6 => L+10
76	40373.695	247.686	2.000e-03	43.3% H-11 => L+2, 40.9% H-11 => L+1, 2.21% H-11 => LUMO
77	40390.633	247.582	1.900e-03	14.7% H-4 => L+14, 9.52% H-7 => L+6, 8.99% H-7 => L+14, 7.66% H-4 => L+13, 6.09% H-2 => L+14, 5.01% H-7 => L+13, 4.57% H-8 => L+4, 3.76% H-5 => L+14, 3.12% H-4 => L+10, 3.08%

				H-1 => L+14, 2.63% H-2 => L+13
78	40595.498	246.333	5.700e-03	67.3% H-7 => L+6, 13.5% H-5 => L+6, 2.00% H-4 => L+14
79	40636.632	246.083	9.380e-02	41.1% H-5 => L+5, 23.8% H-4 => L+5, 12.8% H-7 => L+5, 11.1% H-4 => L+7, 4.27% H-9 => L+2
80	40698.736	245.708	3.120e-02	43.5% HOMO => L+10, 15.5% HOMO => L+13, 10.5% H-4 => L+7, 6.83% HOMO => L+14, 5.04% H-3 => L+14, 3.41% H-5 => L+7, 2.05% H-5 => L+5
81	40818.913	244.984	1.420e-02	40.3% H-4 => L+7, 13.0% H-5 => L+7, 10.4% HOMO => L+10, 9.14% H-5 => L+5, 6.14% HOMO => L+14, 3.63% H-7 => L+7, 2.83% H-1 => L+8
82	41037.489	243.680	8.200e-02	68.0% H-1 => L+8, 4.43% H-9 => L+2, 3.65% H-8 => L+2, 2.66% H-4 => L+7
83	41331.075	241.949	4.300e-03	30.6% H-12 => L+1, 20.6% H-12 => L+2, 12.4% H-15 => L+1, 11.3% H-15 => LUMO, 5.43% H-11 => L+3, 4.33% H-10 => L+2, 2.28% H-11 => L+2, 2.20% H-1 => L+8
84	41524.648	240.821	7.000e-04	46.5% H-15 => L+1, 15.6% H-15 => LUMO, 14.0% H-11 => L+3, 8.49% H-12 => L+2, 3.12% H-12 => L+4, 2.13% H-15 => L+2
85	41677.087	239.940	2.900e-03	50.1% H-11 => L+3, 7.80% H-12 => L+4, 6.56% H-9 => L+3, 5.94% H-12 => L+1, 5.64% H-15 => L+1, 5.21% H-12 => L+2, 4.40% H-10 => L+2, 3.05% H-11 => L+2, 2.00% H-14 => LUMO
86	41804.523	239.209	2.500e-03	45.0% H-14 => LUMO, 21.7% H-6 => L+7, 9.03% H-12 => L+3, 5.48% H-11 => L+4, 3.02% H-1 => L+9, 2.85% H-3 => L+7
87	41841.624	238.996	2.800e-03	29.2% H-11 => L+4, 26.2% H-12 => L+3, 10.7% H-14 => LUMO, 10.5% H-11 => L+1, 3.41% H-11 => L+2, 2.95% H-10 => L+2, 2.84% H-6 => L+7
88	41856.949	238.909	1.340e-02	56.4% H-6 => L+7, 18.6% H-14 => LUMO, 9.21% H-1 => L+9, 6.72% H-3 => L+7
89	41944.863	238.408	3.000e-04	72.8% H-10 => L+2, 6.03% H-12 => L+2, 4.13% H-12 => L+1, 3.67% H-10 => L+1, 2.27% H-10 => L+7
90	42070.686	237.695	3.320e-02	52.1% H-1 => L+9, 17.2% H-17 => LUMO, 14.1% H-14 => LUMO, 3.10% H-17 => L+1
91	42133.597	237.340	9.300e-03	31.9% H-11 => L+2, 31.1% H-11 => L+1, 8.32% H-12 => L+3, 5.64% H-11 => L+4, 5.28% H-12 => L+1, 3.22% H-11 => LUMO, 2.03% H-15 => L+1
92	42164.246	237.168	3.000e-03	57.1% H-5 => L+6, 27.7% H-4 => L+6, 11.8% H-7 => L+6
93	42224.737	236.828	2.520e-02	81.4% H-16 => LUMO, 3.81% H-16 => L+1,

				3.69% HOMO => L+13, 3.09% HOMO => L+14
94	42297.327	236.422	1.080e-02	76.8% H-9 => L+3, 5.19% H-11 => L+3, 2.90% H-16 => LUMO, 2.64% H-8 => L+3, 2.14% HOMO => L+13
95	42441.701	235.617	6.740e-02	33.6% HOMO => L+13, 22.5% HOMO => L+14, 7.22% H-16 => LUMO, 6.91% H-9 => L+3, 4.97% H-7 => L+7, 3.93% H-4 => L+7
96	42487.674	235.362	1.155e-01	41.2% H-5 => L+7, 28.5% H-17 => LUMO, 6.38% H-4 => L+7, 3.56% H-1 => L+9, 2.04% H-11 => L+4
97	42594.139	234.774	7.940e-02	30.0% H-17 => LUMO, 29.0% H-5 => L+7, 9.29% H-1 => L+9, 6.11% H-4 => L+7, 3.83% H-11 => L+4, 3.83% H-12 => L+3
98	42823.201	233.518	1.820e-02	25.7% H-7 => L+7, 21.0% H-13 => L+1, 14.9% H-9 => L+4, 13.9% H-13 => L+2, 3.98% HOMO => L+16, 2.56% H-4 => L+7, 2.27% H-12 => L+3
99	42849.011	233.378	7.000e-02	27.2% HOMO => L+16, 14.9% H-9 => L+4, 10.5% HOMO => L+11, 7.56% H-7 => L+7, 5.60% H-13 => L+1, 5.00% HOMO => L+18, 4.13% H-13 => L+2, 3.59% HOMO => L+21, 3.00% H-12 => L+3, 2.50% HOMO => L+15, 2.21% H-11 => L+4

Table S3. Analysis of transitions in complex **2** by TD-DFT.

Index	Energy.cm^-1	Wavelength	Osc.Strength	Contributions
0	20260.647	493.568	2.000e-04	92.8% HOMO => LUMO, 5.46% HOMO => L+1
1	23607.042	423.602	1.100e-03	54.4% HOMO => L+1, 39.1% HOMO => L+2, 2.56% HOMO => LUMO
2	24051.453	415.775	2.687e-01	90.7% H-1 => LUMO, 2.66% HOMO => L+4
3	24095.814	415.010	5.470e-02	83.7% HOMO => L+3, 8.90% HOMO => L+2
4	24401.498	409.811	3.290e-02	49.8% HOMO => L+4, 17.4% HOMO => L+2, 16.9% HOMO => L+1, 8.68% HOMO => L+3, 2.61% H-1 => LUMO
5	25108.846	398.266	8.800e-03	67.0% H-2 => LUMO, 10.3% HOMO => L+4, 9.16% HOMO => L+1, 7.93% HOMO => L+2, 2.71% H-2 => L+1
6	25341.940	394.603	8.000e-04	32.4% HOMO => L+4, 27.0% H-2 => LUMO, 23.5% HOMO => L+2, 11.6% HOMO => L+1
7	25969.440	385.068	3.300e-03	81.7% H-3 => LUMO, 10.4% H-6 => LUMO, 5.08% H-3 => L+1
8	26641.299	375.357	9.720e-01	89.2% H-1 => L+1, 3.79% H-2 => L+1
9	27513.185	363.462	1.000e-02	81.9% H-4 => LUMO, 4.24% H-7 => LUMO, 3.08% H-4 => L+1, 2.27% H-1 => L+2
10	27985.826	357.324	2.840e-02	63.9% H-2 => L+1, 13.9% H-2 => L+2, 12.8% H-1 => L+2, 2.32% H-2 => LUMO
11	28243.923	354.058	3.990e-02	66.4% H-1 => L+2, 8.94% H-2 => L+1, 5.91% H-

				1 => L+4, 5.58% H-9 => LUMO, 2.34% H-2 => L+4, 2.31% H-2 => L+2
12	28562.512	350.109	1.140e-02	55.3% H-2 => L+3, 15.3% H-2 => L+2, 14.9% H-1 => L+3, 2.73% H-2 => L+4, 2.60% H-1 => L+4
13	28723.823	348.143	5.010e-02	28.8% H-2 => L+4, 21.4% H-2 => L+2, 13.4% H-2 => L+3, 10.2% H-1 => L+4, 9.07% H-2 => L+1, 5.13% HOMO => L+5, 3.19% H-1 => L+3
14	29169.847	342.820	4.100e-03	46.8% HOMO => L+6, 26.2% H-1 => L+3, 9.51% H-4 => L+3, 3.28% H-3 => L+2, 2.87% HOMO => L+5, 2.63% H-2 => L+3, 2.60% H-3 => L+4
15	29193.238	342.545	2.380e-02	63.4% HOMO => L+5, 13.4% H-1 => L+4, 5.89% H-3 => L+3, 2.39% H-4 => L+4, 2.35% H-4 => L+2, 2.07% HOMO => L+6
16	29414.233	339.971	1.210e-02	24.8% H-1 => L+4, 15.5% H-1 => L+3, 11.3% H-3 => L+2, 8.96% HOMO => L+6, 8.65% H-2 => L+2, 5.51% H-2 => L+3, 4.33% H-3 => L+1, 3.41% HOMO => L+5, 2.45% H-1 => L+2, 2.11% H-3 => L+4
17	29456.174	339.487	1.630e-02	23.4% H-1 => L+4, 15.0% H-1 => L+3, 8.97% H-2 => L+3, 7.52% H-2 => L+2, 6.55% HOMO => L+6, 6.36% H-3 => L+1, 6.33% H-3 => L+2, 5.76% H-3 => L+3, 4.22% HOMO => L+5
18	29618.292	337.629	4.100e-03	48.4% H-2 => L+4, 24.0% H-2 => L+2, 7.32% H-6 => LUMO, 6.50% H-2 => L+1, 2.55% H-1 => L+2
19	29769.924	335.909	4.600e-03	32.7% H-3 => L+1, 11.0% H-6 => LUMO, 8.55% H-3 => L+4, 7.78% H-1 => L+3, 7.24% HOMO => L+6, 7.20% H-3 => LUMO, 4.27% H-5 => LUMO, 4.16% H-3 => L+2, 3.63% H-2 => L+4, 3.07% H-6 => L+1, 2.30% H-2 => L+3, 2.02% H-7 => LUMO
20	29852.999	334.975	3.230e-02	49.5% H-5 => LUMO, 15.6% H-5 => L+1, 14.5% H-4 => L+1, 7.21% H-6 => LUMO
21	29928.815	334.126	5.500e-03	53.3% H-6 => LUMO, 14.0% H-3 => L+1, 3.97% H-3 => L+2, 3.78% H-3 => LUMO, 3.36% H-2 => L+4, 2.60% H-5 => L+1, 2.54% H-3 => L+4
22	30191.752	331.216	9.280e-02	53.4% H-3 => L+3, 8.01% HOMO => L+5, 5.83% H-1 => L+4, 5.66% H-3 => L+2, 5.26% H-6 => L+3, 5.19% H-4 => L+2, 3.68% H-4 => L+1, 2.14% H-5 => LUMO, 2.08% H-1 => L+2
23	30458.721	328.313	8.720e-02	35.8% H-4 => L+1, 14.3% H-5 => LUMO, 13.7% H-4 => L+2, 12.5% H-3 => L+3, 2.97% H-4 => L+4, 2.95% H-7 => LUMO, 2.62% HOMO => L+5, 2.28% H-7 => L+1, 2.14% H-3 => L+4, 2.05% H-3 => L+1
24	30628.904	326.489	7.000e-04	27.6% H-3 => L+4, 15.7% H-4 => L+3, 15.2% H-

				3 => L+2, 7.29% H-1 => L+3, 5.93% HOMO => L+6, 4.85% H-3 => L+1, 3.84% H-7 => LUMO, 3.46% H-4 => L+1, 3.40% H-6 => L+4, 2.01% H-7 => L+3
25	30916.844	323.448	9.000e-03	29.0% H-5 => L+1, 26.9% H-7 => LUMO, 13.5% H-4 => L+2, 5.68% H-3 => L+4, 5.49% H-3 => L+1, 5.09% H-5 => LUMO, 3.75% H-4 => L+3
26	31216.076	320.348	5.100e-03	29.9% H-5 => L+1, 24.9% H-7 => LUMO, 15.8% H-5 => LUMO, 4.30% H-3 => L+4, 4.13% H-4 => L+3, 3.99% H-4 => LUMO, 3.45% H-3 => L+2, 2.97% H-3 => L+1, 2.59% H-7 => L+1
27	31287.859	319.613	4.110e-02	29.7% H-3 => L+4, 19.7% H-3 => L+2, 16.1% H-3 => L+1, 11.7% H-7 => LUMO, 6.46% H-4 => L+3
28	31372.548	318.750	1.319e-01	40.0% H-4 => L+4, 18.3% H-4 => L+2, 7.56% H-4 => L+1, 6.87% H-5 => L+1, 3.50% HOMO => L+5, 3.08% H-1 => L+4, 2.87% H-3 => L+3, 2.19% H-7 => LUMO
29	31859.706	313.876	1.160e-02	21.4% H-4 => L+3, 13.1% H-3 => L+2, 12.5% H-4 => L+4, 10.7% H-7 => LUMO, 9.62% HOMO => L+6, 8.77% H-4 => L+2, 5.69% H-2 => L+5, 3.19% H-4 => L+1
30	32137.968	311.158	8.000e-03	20.3% H-4 => L+4, 18.6% H-4 => L+1, 15.2% H-4 => L+2, 12.3% H-4 => L+3, 5.60% H-5 => L+1, 3.89% H-2 => L+5, 3.33% HOMO => L+6, 2.92% H-6 => L+2, 2.23% H-3 => L+2, 2.15% H-7 => L+2, 2.15% H-9 => LUMO
31	32416.229	308.487	4.000e-04	80.7% H-8 => LUMO, 9.14% HOMO => L+7, 4.78% H-8 => L+1
32	32853.382	304.383	5.000e-04	80.8% HOMO => L+7, 9.31% H-8 => LUMO, 2.44% HOMO => L+8
33	32942.909	303.555	2.290e-02	34.5% H-6 => L+3, 16.9% H-2 => L+6, 10.1% H-7 => L+4, 6.70% H-6 => L+1, 6.00% H-1 => L+6, 5.46% H-7 => L+2, 5.41% H-3 => L+5, 2.87% H-4 => L+4
34	33088.089	302.224	7.000e-04	22.2% H-6 => L+4, 21.0% H-6 => L+2, 14.7% H-7 => L+3, 7.15% H-4 => L+3, 6.14% H-3 => L+6, 4.72% H-2 => L+5, 3.96% H-6 => L+1, 3.88% H-1 => L+5, 3.23% H-4 => L+5
35	33167.131	301.503	5.600e-02	50.7% H-6 => L+1, 6.45% H-6 => L+2, 5.46% H-6 => L+4, 4.59% H-7 => L+1, 3.83% H-2 => L+5, 3.16% H-7 => L+3, 2.75% H-6 => LUMO, 2.64% H-9 => LUMO, 2.26% H-5 => L+2
36	33553.471	298.032	4.010e-02	34.0% H-5 => L+2, 19.7% H-9 => LUMO, 6.92% H-7 => L+1, 5.95% H-5 => L+4, 4.81% H-6 => L+2, 4.18% H-6 => L+3, 3.60% H-7 => L+2, 3.57% H-6 => L+1, 2.06% H-1 => L+2

37	33809.149	295.778	2.710e-02	34.7% H-6 => L+3, 9.11% H-1 => L+6, 8.96% H-2 => L+6, 7.38% H-8 => L+3, 4.27% H-5 => L+2, 3.57% H-6 => L+2, 3.47% H-5 => L+4, 3.33% H-3 => L+3, 2.99% H-4 => L+6, 2.99% H-7 => L+2, 2.60% H-7 => L+4, 2.46% HOMO => L+9
38	33966.427	294.408	2.150e-02	18.4% H-6 => L+4, 14.7% H-6 => L+2, 14.1% H-1 => L+5, 10.6% H-2 => L+5, 7.37% H-6 => L+1, 6.16% H-6 => L+3, 4.97% H-7 => L+3, 3.15% H-8 => L+4, 2.89% H-3 => L+4, 2.36% H-8 => L+2
39	34052.728	293.662	2.470e-02	55.3% H-7 => L+1, 8.40% H-7 => L+2, 8.37% H-5 => L+2, 3.78% H-9 => LUMO, 2.91% H-4 => L+2, 2.20% H-7 => LUMO
40	34359.219	291.043	5.710e-02	22.4% H-9 => LUMO, 16.7% H-5 => L+2, 12.1% H-6 => L+4, 10.3% H-6 => L+2, 6.39% H-1 => L+5, 3.28% H-6 => L+1, 3.12% H-10 => LUMO, 2.58% H-7 => L+2, 2.50% H-9 => L+2, 2.42% H-4 => L+2
41	34630.221	288.765	1.360e-02	26.8% H-1 => L+5, 13.0% H-7 => L+3, 9.08% H-7 => L+4, 6.91% H-7 => L+2, 6.10% H-1 => L+6, 5.73% H-2 => L+6, 5.12% H-5 => L+2, 3.88% H-9 => LUMO, 3.73% H-5 => L+3, 2.90% H-3 => L+5, 2.14% H-5 => L+4, 2.12% H-6 => L+4
42	34677.808	288.369	5.920e-02	19.2% H-1 => L+5, 16.4% H-2 => L+6, 10.8% H-7 => L+2, 8.21% H-7 => L+4, 6.04% H-2 => L+5, 5.36% H-1 => L+6, 5.08% H-3 => L+5, 4.37% H-5 => L+4, 4.05% H-7 => L+3, 3.07% H-7 => L+1, 2.91% H-1 => L+7
43	34704.424	288.148	4.860e-02	40.5% H-2 => L+5, 21.7% H-7 => L+3, 7.50% H-5 => L+3, 4.07% H-4 => L+3, 2.06% H-6 => L+4
44	34857.669	286.881	6.490e-02	16.1% H-3 => L+5, 15.3% H-2 => L+6, 6.96% H-8 => L+3, 6.72% H-6 => L+4, 6.58% H-6 => L+2, 4.96% H-9 => LUMO, 4.91% H-4 => L+6, 4.90% H-1 => L+6, 4.75% H-5 => L+2, 3.46% H-6 => L+1, 3.41% H-7 => L+4, 3.18% HOMO => L+9, 3.15% H-7 => L+2
45	34877.027	286.722	2.270e-02	14.9% H-6 => L+2, 14.8% H-6 => L+4, 12.9% H-3 => L+5, 8.78% H-9 => LUMO, 7.60% H-7 => L+2, 5.35% H-6 => L+1, 5.05% H-8 => L+3, 3.77% H-2 => L+5, 2.91% H-9 => L+1, 2.09% HOMO => L+9
46	34918.161	286.384	3.000e-03	44.3% H-1 => L+6, 20.7% H-2 => L+6, 8.08% H-3 => L+5, 4.81% H-4 => L+6, 2.57% H-3 => L+6, 2.13% H-7 => L+6
47	35038.338	285.402	1.400e-03	44.3% H-3 => L+6, 8.95% H-8 => L+2, 7.06% H-5 => L+3, 5.56% H-8 => L+4, 5.38% H-7 => L+3, 4.66% H-2 => L+5, 2.58% H-6 => L+6, 2.18% H-8 => L+1

48	35239.976	283.769	3.810e-02	36.3% H-9 => L+1, 18.5% H-1 => L+7, 8.16% H-10 => LUMO, 8.04% H-9 => L+2, 5.73% H-1 => L+5, 4.24% H-2 => L+5, 2.83% H-9 => L+4, 2.26% H-7 => L+1
49	35471.457	281.917	1.014e-01	20.8% H-7 => L+4, 18.2% H-7 => L+2, 14.2% H-1 => L+7, 11.7% H-5 => L+4, 9.17% H-9 => L+1, 6.06% H-10 => L+1, 3.49% H-9 =>LUMO, 2.33% H-10 => LUMO, 2.24% H-7 => L+1
50	35505.333	281.648	5.000e-04	62.5% H-5 => L+3, 9.29% H-7 => L+3, 5.12% H-4 => L+3, 4.43% H-5 => L+4, 2.83% H-7 => L+2, 2.38% H-1 => L+7, 2.06% H-5 => L+2
51	35635.188	280.622	3.500e-03	48.4% H-5 => L+4, 9.12% H-7 => L+4, 9.10% H-5 => L+2, 7.02% H-5 => L+3, 4.57% H-4 => L+4, 3.93% H-1 => L+7, 3.43% H-10 => LUMO
52	35709.391	280.038	1.030e-02	60.7% H-8 => L+1, 12.8% H-8 => L+2, 5.48% H-8 => L+4, 4.97% H-3 => L+6, 2.84% H-11 => LUMO, 2.71% H-8 => LUMO
53	35798.918	279.338	3.300e-03	25.6% H-10 => LUMO, 17.8% H-1 => L+7, 14.9% H-7 => L+4, 9.78% H-7 => L+1, 7.50% H-7 => L+2, 5.94% H-5 => L+4, 2.78% H-7 => L+3
54	36112.668	276.911	1.300e-02	26.1% H-4 => L+6, 19.3% H-3 => L+5, 11.0% H-6 => L+5, 9.96% HOMO => L+9, 9.14% H-1 => L+6, 5.74% H-8 => L+3, 2.88% H-11 => LUMO, 2.04% H-6 => L+3
55	36158.642	276.559	1.910e-02	43.0% H-11 => LUMO, 21.3% H-13 => LUMO, 5.99% H-9 => L+1, 4.55% H-8 => L+1, 2.98% H-10 => LUMO, 2.97% H-4 => L+6, 2.39% H-11 => L+1
56	36321.566	275.319	2.910e-02	23.9% H-4 => L+5, 15.1% H-9 => L+1, 12.0% H-10 => LUMO, 6.42% H-3 => L+6, 5.65% H-9 => L+2, 5.25% H-1 => L+5, 3.49% H-8 => L+4, 2.94% H-1 => L+7, 2.82% H-6 => L+6, 2.43% H-8 => L+2, 2.11% H-8 => L+1
57	36356.247	275.056	3.000e-02	18.7% H-4 => L+5, 16.2% H-10 => LUMO, 15.7% H-9 => L+1, 10.5% H-11 => LUMO, 6.30% H-3 => L+6, 4.90% H-8 => L+4, 3.40% H-13 => LUMO, 3.25% H-1 => L+5, 2.97% H-9 => L+2, 2.23% H-6 => L+6, 2.19% H-8 => L+2
58	36408.673	274.660	4.000e-04	65.9% H-12 => L+1, 25.7% H-12 => LUMO, 3.19% H-12 => L+2
59	36560.306	273.521	3.400e-03	44.4% HOMO => L+9, 19.4% H-8 => L+3, 7.75% HOMO => L+8, 7.55% H-4 => L+6, 4.14% H-7 => L+6, 3.12% H-6 => L+5, 2.34% H-1 => L+6
60	36995.039	270.307	1.360e-02	28.3% HOMO => L+14, 25.3% H-8 => L+2, 16.4% HOMO => L+10, 5.97% H-8 => L+1, 4.00% HOMO => L+12, 2.74% H-3 => L+14,

				2.73% H-7 => L+3
61	37111.989	269.455	2.680e-02	26.8% H-8 => L+2, 15.3% HOMO => L+14, 9.13% H-8 => L+1, 8.19% H-8 => L+4, 7.91% HOMO => L+10, 6.42% H-4 => L+5, 2.66% H-4 => L+6, 2.57% H-10 => L+1, 2.52% HOMO => L+12
62	37209.582	268.748	8.000e-04	70.4% H-2 => L+7, 8.67% H-10 => L+1, 5.44% H-1 => L+7, 3.69% H-8 => L+2
63	37253.943	268.428	3.940e-02	37.0% H-10 => L+1, 10.9% H-9 => L+2, 10.6% H-2 => L+7, 8.36% H-8 => L+3, 4.85% H-4 => L+6, 4.77% H-8 => L+4, 2.69% H-10 => LUMO, 2.65% H-8 => L+2, 2.02% H-8 => L+1
64	37345.890	267.767	1.195e-01	26.5% H-8 => L+3, 17.0% H-4 => L+6, 15.1% H-10 => L+1, 6.67% H-7 => L+6, 5.45% H-6 => L+5, 2.14% H-9 => L+2, 2.12% H-7 => L+4, 2.10% H-3 => L+5
65	37529.784	266.455	5.520e-02	42.4% H-8 => L+4, 15.2% H-4 => L+5, 9.66% H-6 => L+6, 7.27% H-7 => L+5, 4.70% H-2 => L+7, 2.04% H-10 => L+1
66	37902.412	263.835	1.000e-04	83.9% H-14 => LUMO, 5.01% H-14 => L+1, 3.11% H-12 => LUMO, 2.68% H-13 => LUMO
67	38102.438	262.450	9.700e-03	19.1% H-6 => L+6, 16.0% HOMO => L+10, 11.4% HOMO => L+14, 8.57% H-7 => L+5, 7.94% H-8 => L+4, 6.04% HOMO => L+12, 3.23% H-13 => LUMO, 2.91% H-2 => L+9, 2.72% H-11 => LUMO, 2.37% H-3 => L+14, 2.32% H-9 => L+4, 2.16% HOMO => L+11, 2.02% H-2 => L+7
68	38179.867	261.918	1.800e-03	55.5% H-13 => LUMO, 28.2% H-11 => LUMO, 3.27% H-13 => L+1, 2.24% HOMO => L+10, 2.05% H-14 => LUMO
69	38280.686	261.228	5.270e-02	29.6% H-9 => L+2, 27.6% H-9 => L+3, 27.0% H-9 => L+4, 3.29% H-1 => L+7, 2.64% H-10 => L+1
70	38296.817	261.118	2.120e-02	64.6% H-9 => L+3, 14.5% H-9 => L+2, 6.36% H-9 => L+4, 2.37% H-10 => L+3
71	38617.020	258.953	1.210e-02	51.0% HOMO => L+8, 16.3% HOMO => L+11, 7.31% HOMO => L+9, 7.00% H-3 => L+7, 4.26% H-9 => L+4, 4.20% HOMO => L+10
72	38733.970	258.171	1.451e-01	35.9% H-3 => L+7, 19.0% H-9 => L+4, 10.0% HOMO => L+8, 4.54% H-10 => L+2, 4.30% H-1 => L+7, 3.77% HOMO => L+11, 3.13% H-10 => L+1, 2.20% H-9 => L+2, 2.13% H-6 => L+7
73	38845.274	257.432	2.743e-01	36.2% H-3 => L+7, 20.6% H-9 => L+4, 7.52% H-1 => L+7, 4.85% H-1 => L+8, 4.24% H-10 => LUMO, 3.81% H-9 => L+2, 2.75% H-10 => L+1, 2.29% H-5 => L+8

74	39113.857	255.664	9.650e-02	23.6% H-6 => L+5, 16.2% HOMO => L+11, 14.0% HOMO => L+10, 13.1% HOMO => L+8, 5.91% H-6 => L+6, 2.86% H-3 => L+5, 2.26% HOMO => L+12, 2.14% H-2 => L+10, 2.07% HOMO => L+14
75	39163.863	255.337	1.281e-01	33.0% H-6 => L+5, 8.94% HOMO => L+10, 8.15% HOMO => L+9, 7.85% HOMO => L+11, 6.48% HOMO => L+8, 5.28% H-6 => L+6, 5.00% H-3 => L+5, 3.31% H-2 => L+10, 3.10% HOMO => L+15, 2.28% H-8 => L+3
76	39194.512	255.138	8.000e-04	68.7% H-12 => LUMO, 24.4% H-12 => L+1, 4.04% H-14 => LUMO
77	39383.246	253.915	2.170e-02	28.9% H-10 => L+2, 11.9% H-4 => L+7, 7.73% H-3 => L+14, 5.70% H-6 => L+6, 5.16% H-6 => L+14, 4.15% H-10 => L+4, 3.60% H-1 => L+8, 3.13% H-11 => L+2, 3.12% H-11 => L+1, 3.10% H-3 => L+7, 2.59% H-7 => L+5
78	39423.574	253.655	1.160e-02	32.5% HOMO => L+11, 25.0% H-6 => L+6, 5.61% H-10 => L+2, 5.49% H-7 => L+5, 3.43% H-3 => L+6, 3.31% HOMO => L+10, 2.36% H-11 => L+3, 2.22% HOMO => L+8, 2.11% H-2 => L+9
79	39442.125	253.536	2.080e-02	17.2% H-10 => L+2, 15.0% H-3 => L+14, 10.8% H-6 => L+14, 9.45% HOMO => L+11, 7.17% HOMO => L+12, 2.92% HOMO => L+14, 2.88% H-3 => L+10, 2.78% H-11 => L+2, 2.31% H-10 => L+4
80	39563.914	252.756	2.770e-02	21.0% H-7 => L+6, 12.8% H-11 => L+2, 8.38% H-11 => L+1, 6.78% H-6 => L+5, 5.54% HOMO => L+15, 5.40% H-4 => L+14, 4.18% H-10 => L+2, 3.93% H-5 => L+6, 3.45% H-7 => L+14, 3.17% H-4 => L+6, 2.98% H-13 => L+2
81	39711.514	251.816	2.040e-02	29.8% H-4 => L+7, 13.7% H-11 => L+1, 9.17% H-7 => L+5, 4.69% H-11 => L+2, 4.48% H-7 => L+6, 3.45% H-6 => L+6, 3.30% H-5 => L+5, 3.23% H-13 => L+2, 2.98% HOMO => L+15, 2.01% H-13 => L+1
82	39743.776	251.612	3.930e-02	27.9% H-4 => L+7, 16.1% H-11 => L+1, 7.31% H-10 => L+2, 5.20% H-11 => L+2, 3.84% H-7 => L+5, 3.67% H-7 => L+6, 3.51% H-13 => L+2, 2.86% HOMO => L+15, 2.31% H-13 => L+1, 2.29% H-6 => L+6
83	39855.081	250.909	2.900e-03	21.6% H-7 => L+5, 12.6% H-3 => L+14, 12.1% H-4 => L+7, 8.74% H-2 => L+9, 8.05% H-6 => L+14, 6.97% H-5 => L+5, 5.62% HOMO => L+10, 3.44% HOMO => L+11, 2.28% H-11 => L+3

84	39969.611	250.190	5.000e-04	70.1% H-15 => LUMO, 23.6% H-15 => L+1, 2.40% H-14 => L+1
85	40125.276	249.219	2.330e-02	21.6% H-7 => L+6, 20.4% H-4 => L+14, 11.9% H-7 => L+14, 7.94% H-5 => L+6, 5.10% H-4 => L+10, 4.12% H-1 => L+14
86	40146.247	249.089	1.100e-03	65.7% HOMO => L+12, 23.1% HOMO => L+14, 2.80% HOMO => L+10
87	40265.617	248.351	3.880e-02	37.0% H-11 => L+3, 16.5% H-13 => L+3, 6.14% H-11 => L+2, 4.52% H-10 => L+3, 3.94% H-13 => L+2, 3.10% H-14 => L+2, 3.02% H-11 => L+4, 2.55% H-14 => L+4, 2.36% H-11 => L+1, 2.11% HOMO => L+15
88	40414.023	247.439	1.330e-02	23.2% HOMO => L+15, 16.7% H-11 => L+4, 10.8% H-11 => L+3, 7.05% H-11 => L+1, 5.27% H-13 => L+4, 4.82% H-14 => L+3, 3.30% H-13 => L+3, 3.18% HOMO => L+18, 2.70% HOMO => L+21, 2.65% HOMO => L+9, 2.52% H-11 => L+2
89	40556.783	246.568	9.060e-02	22.6% HOMO => L+15, 8.13% H-11 => L+4, 5.40% H-8 => L+5, 5.04% HOMO => L+9, 4.52% H-4 => L+14, 4.52% H-13 => L+4, 4.27% H-10 => L+4, 4.06% H-11 => L+1, 3.74% H-7 => L+6, 3.69% H-13 => L+2, 3.11% H-11 => L+2, 2.64% H-4 => L+6, 2.45% H-7 => L+14, 2.14% HOMO => L+18, 2.01% HOMO => L+21
90	40655.183	245.971	3.630e-02	73.3% H-5 => L+5, 8.09% H-7 => L+5, 4.38% H-4 => L+5, 2.71% H-5 => L+7
91	40858.434	244.748	5.350e-02	60.2% H-1 => L+8, 9.56% H-10 => L+2, 3.46% H-9 => L+4, 2.98% H-10 => L+4, 2.96% H-2 => L+8
92	40907.634	244.453	2.300e-03	76.6% H-10 => L+3, 3.09% H-10 => L+4, 2.76% H-1 => L+8, 2.58% H-11 => L+3, 2.22% H-9 => L+3
93	40964.899	244.111	4.500e-03	72.5% H-5 => L+6, 11.2% H-7 => L+6, 5.75% H-4 => L+6, 2.04% H-10 => L+4
94	41018.132	243.795	7.000e-03	24.3% H-10 => L+4, 21.7% H-11 => L+1, 10.6% H-13 => L+2, 8.26% H-13 => L+1, 5.66% H-11 => L+4, 5.13% H-10 => L+3, 4.16% H-11 => L+2, 3.90% H-13 => L+4, 3.87% H-1 => L+8, 2.19% H-10 => L+2
95	41083.463	243.407	2.050e-02	39.6% H-10 => L+4, 10.4% H-11 => L+4, 7.65% H-11 => L+1, 6.27% H-13 => L+1, 5.46% H-5 => L+6, 4.95% H-10 => L+2, 4.90% H-13 => L+4, 4.70% H-13 => L+2, 2.36% H-1 => L+8
96	41326.236	241.977	1.610e-02	26.6% H-14 => L+1, 23.5% H-14 => L+2, 11.2% H-15 => L+1, 8.94% H-15 => LUMO, 5.84% H-11 => L+3, 3.94% H-12 => L+2, 2.61% H-8 =>

				L+6, 2.39% H-14 => L+3, 2.10% H-1 => L+9
97	41428.668	241.379	8.050e-02	37.4% H-8 => L+6, 14.9% H-2 => L+9, 11.1% H-1 => L+9, 9.58% H-7 => L+5, 6.09% H-15 => L+1, 5.78% H-2 => L+8, 2.85% H-15 => LUMO
98	41485.127	241.050	1.530e-02	29.7% H-11 => L+2, 14.5% H-14 => L+3, 12.6% H-13 => L+1, 8.98% H-13 => L+2, 8.90% H-15 => L+1, 5.98% H-13 => L+4, 3.42% H-15 => LUMO, 2.65% H-3 => L+9
99	41507.711	240.919	1.700e-03	36.3% H-15 => L+1, 17.5% H-14 => L+2, 11.3% H-15 => LUMO, 5.48% H-11 => L+3, 4.31% H-13 => L+2, 3.50% H-13 => L+3, 2.54% H-11 => L+2, 2.31% H-12 => L+2

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