Supplementary Information

Rhodamine-Based Turn-On Fluorescent and Colorimetric Chemosensor for Selective Pb^{2+} Detection: Insights from Crystal Structure, Molecular Docking, Real Sample Analysis, and Logic Gate Applications

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Figure Caption

Figure S1. FTIR spectrum of **L**.

Figure S2. ^{1}H NMR of compound **L** in (DMSO-d_6, 400 MHz).

Figure S3. ^{13}C NMR of compound **L** in (DMSO-d_6, 100 MHz).

Figure S4. Gliding plane passing through the centroid of the molecule for the confirmation of planar structure.

Figure S5. 3D packing arrangement of cell axis passing through the molecule.

Figure S6. Double-decker π-stacked arrangement of two phenolic rings colored by symmetry equivalence and hydrogen bonding between adjacent molecules.

Figure S7. 1D arrangement of **L** *via* intra- and intermolecular hydrogen bonding and noncovalent interactions between adjacent molecules.

Figure S8. Simulated absorption spectrum of the complex.

Figure S9. 2D-interaction of **L** with human DNA (PDB ID: 5vbn).

Figure S10. The hydrogen bonding interactions between **L** and the 5VBN protein are depicted, with pink areas denoting hydrogen bond donors and green areas signifying hydrogen bond acceptors.

Figure S11. The hydrophobicity surface representation of compound **L** binding to the 5VBN protein indicates that blue regions denote areas where the protein or ligand possesses polar functional groups that can form hydrogen bonds or electrostatic interactions with adjacent water molecules or other polar groups within the binding pocket.

Table S1. Crystal data and structure refinement for ligand **L**.

Table S2. Summary of 20 lowest TDDFT excitations: singlet Alda **L**.

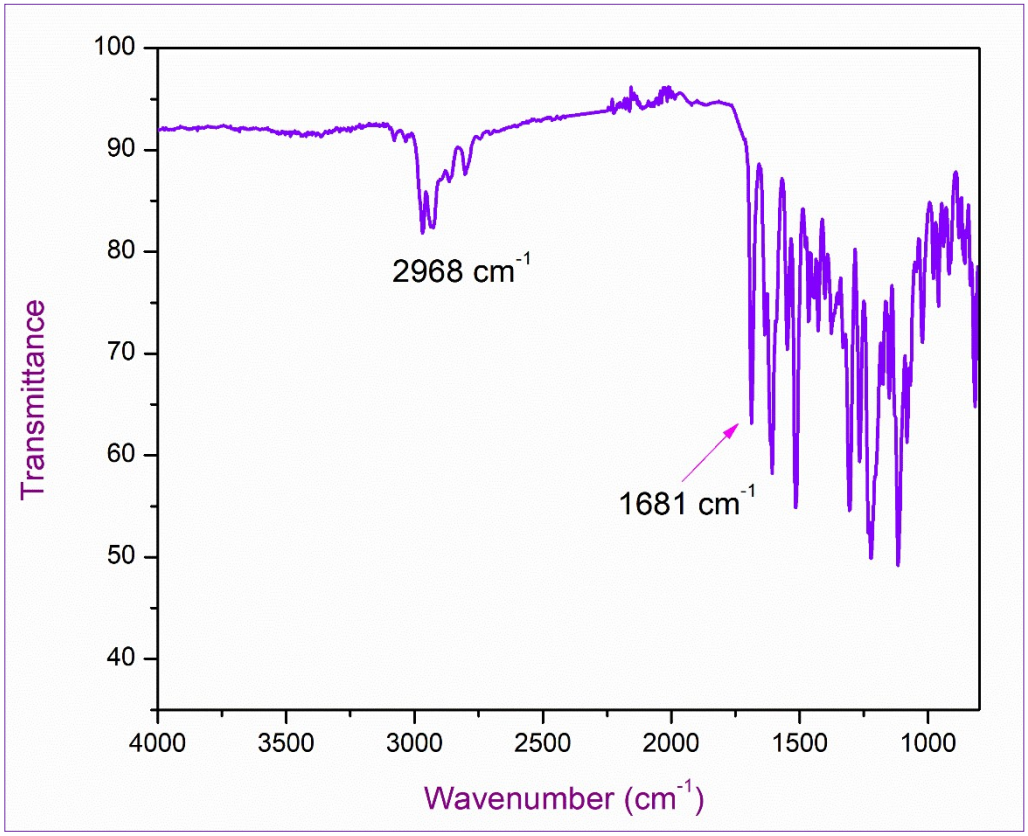
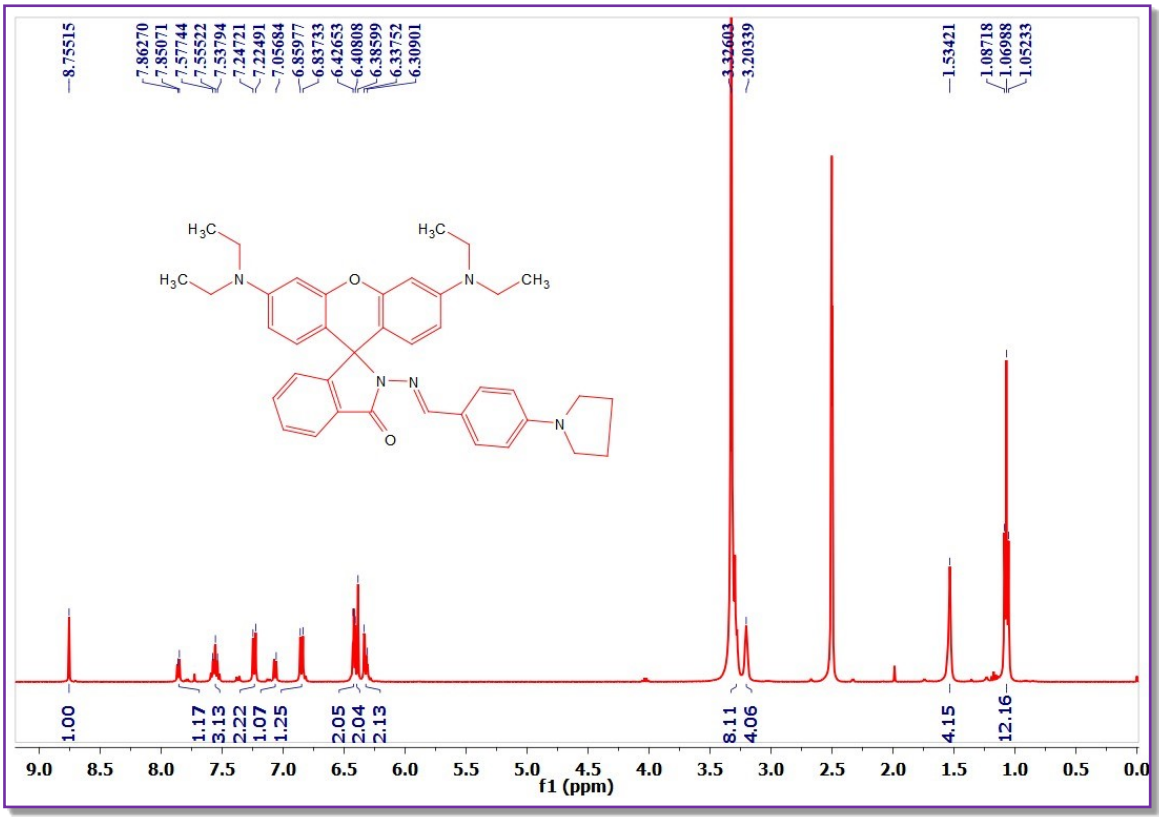


Figure S1. FTIR spectrum of **L**.



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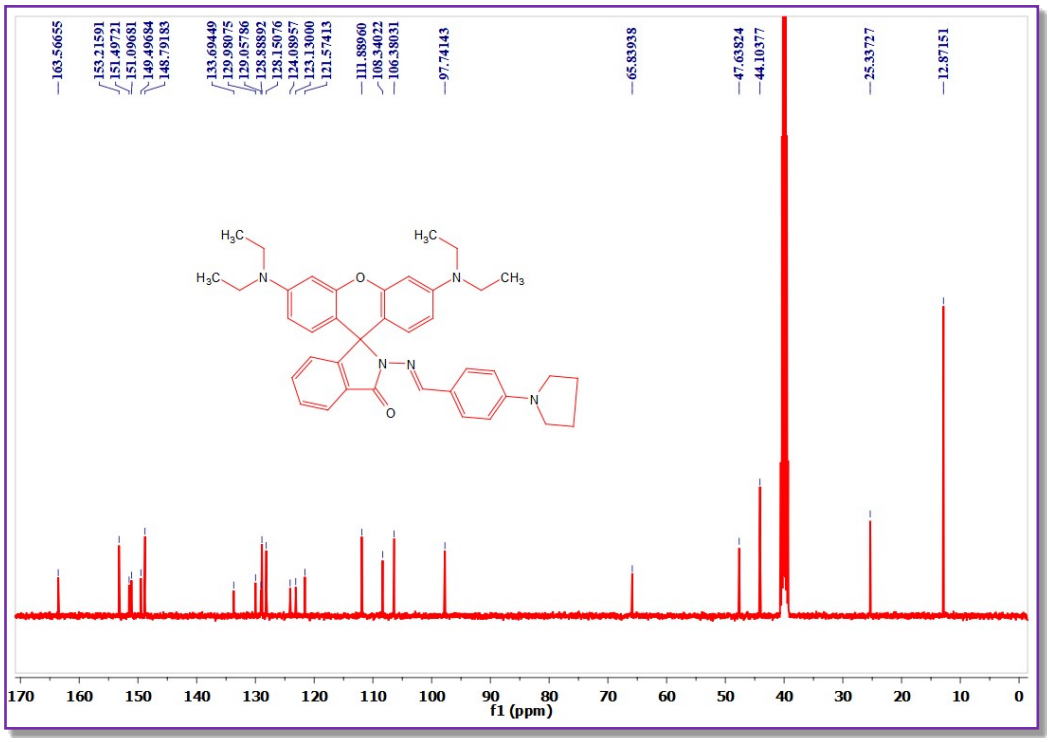


Figure S3. [13]C NMR of compound **L** in (DMSO-d_6, 100 MHz).

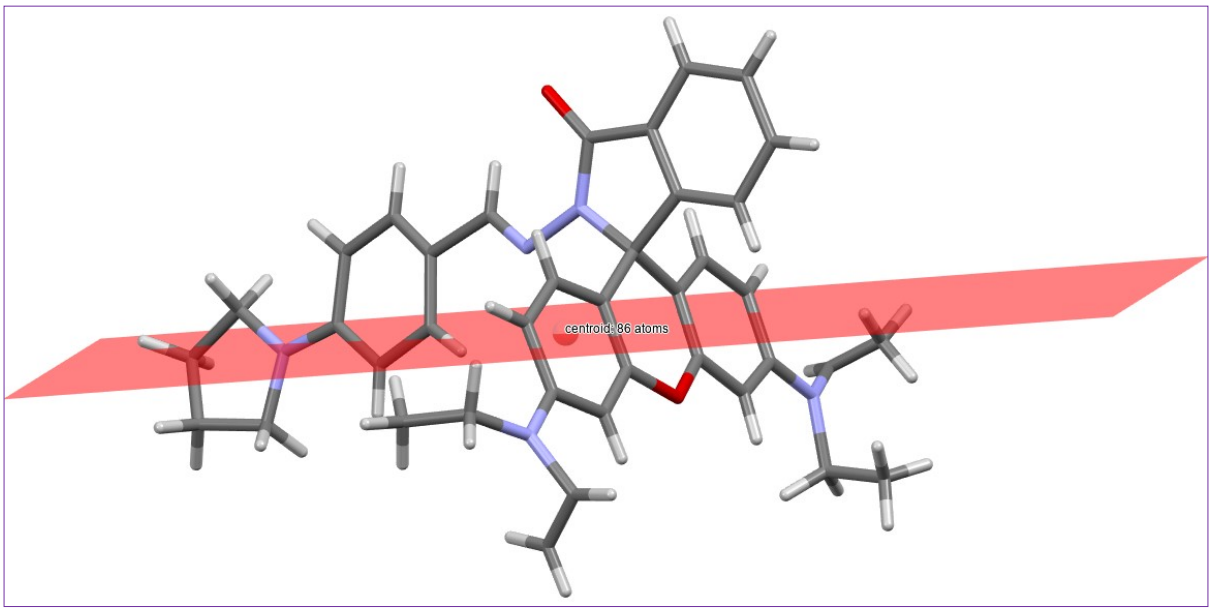


Figure S4. Gliding plane passing through the centroid of the molecule for the confirmation of planar structure.

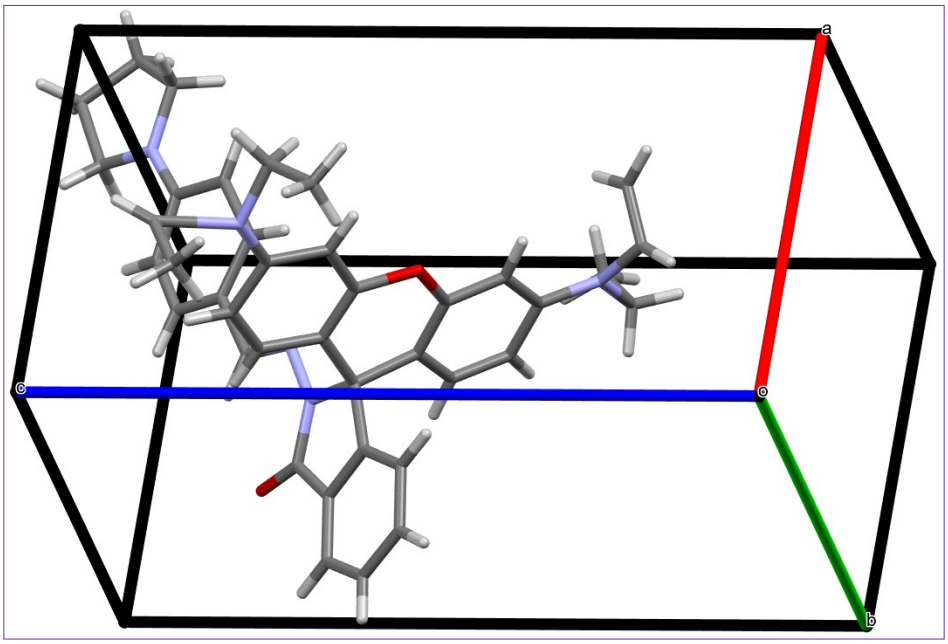


Figure S5. 3D packing arrangement of cell axis passing through the molecule.

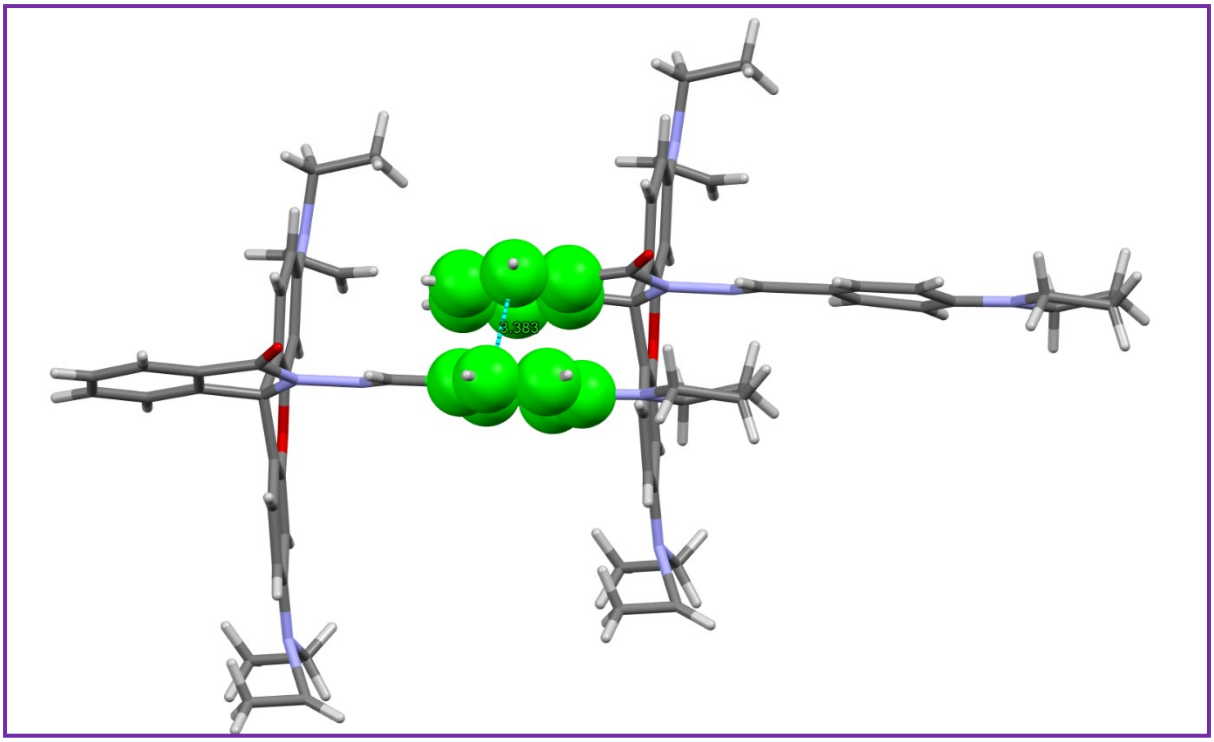


Figure S6. Double-decker π-stacked arrangement of two phenolic rings colored by symmetry equivalence and hydrogen bonding between adjacent molecules.

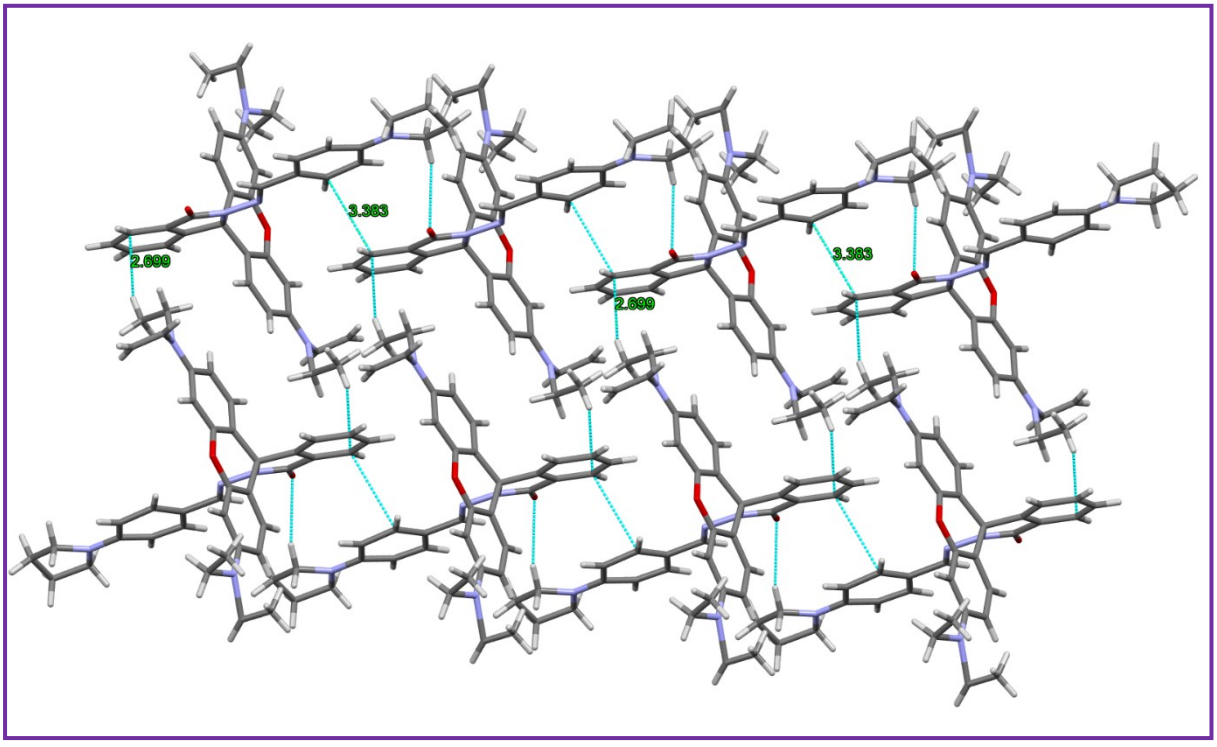


Figure S7. 1D arrangement of **L** *via* intra- and intermolecular hydrogen bonding and noncovalent interactions between adjacent molecules.

Table S1. Crystal data and structure refinement for ligand	
Identification code	**L**
Empirical formula	$C_{40}H_{41}N_5O_3$
Temperature/K	293(2)
Crystal system	Triclinic
Space group	P -1
a/Å	9.3013(4)
b/Å	12.0691(5)
c/Å	16.7261(8)
α/°	78.387(4)
β/°	83.319(3)
γ/°	76.114(3)
Volume/Å^3	1780.88(14)
Z	33
ρ_{calc}g/cm^3	1.193
μ/mm^{-1}	0.076
F(000)	680.4
Radiation	Mo/K_α (λ = 0.71073)
2Θ range for data collection/°	3.03 to 30.93
Index ranges	$11 \leq h \leq -12$, $16 \leq k \leq -16$, $23 \leq l \leq -22$
No of Reflections measured	8872
Independent reflections	4599
Goodness-of-fit on F^2	1.572
R [$F^2 > 2\sigma(F^2)$], *wR*(all data)	0.1304, 0.4577

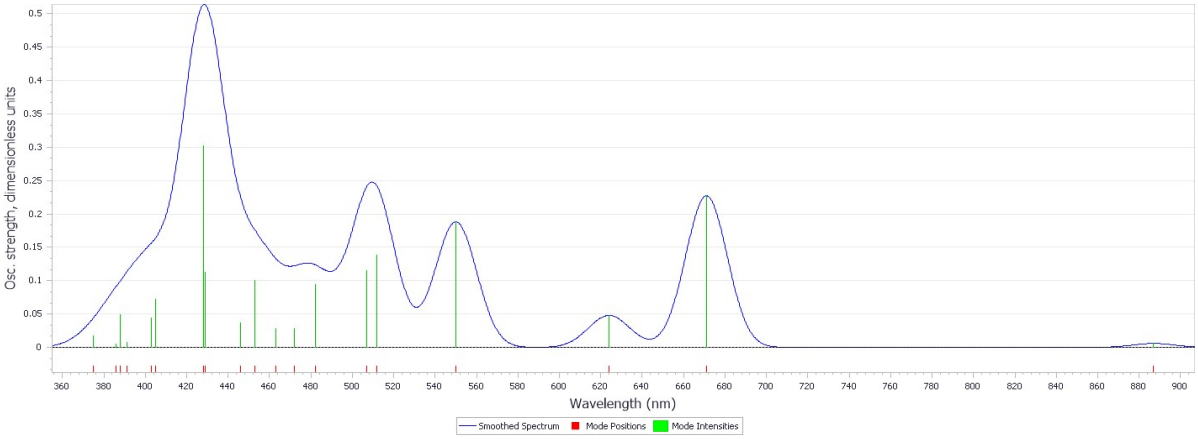


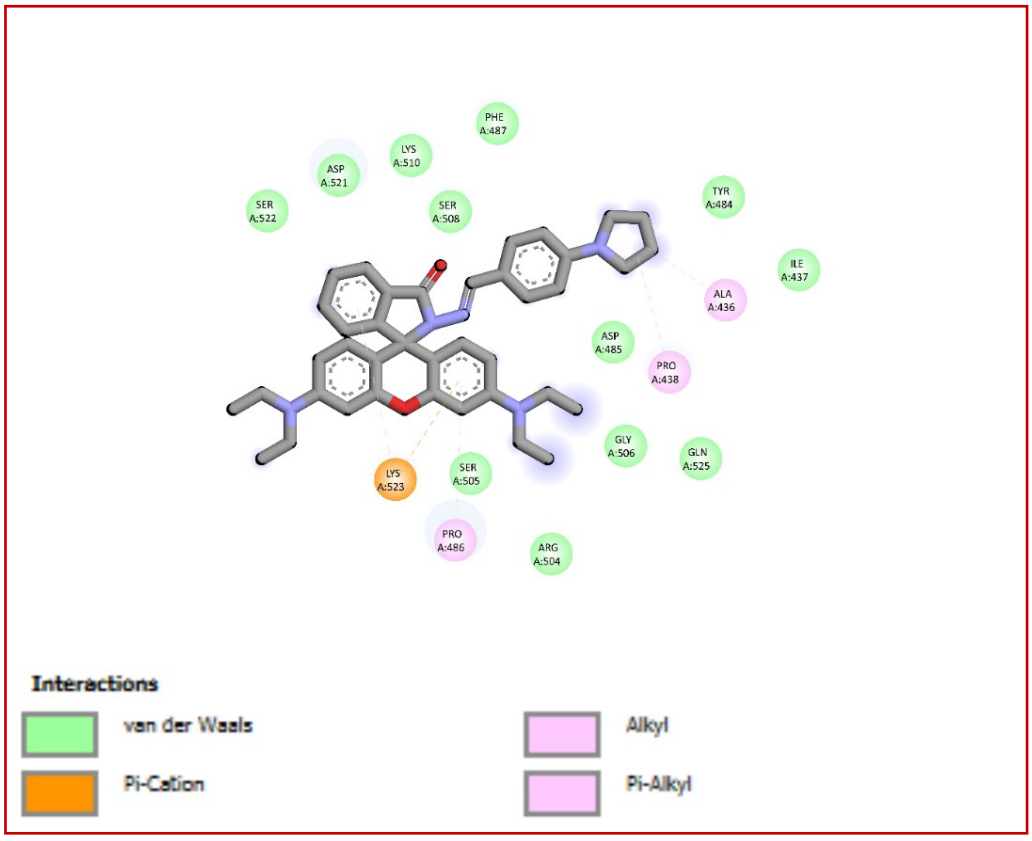
Figure S8. Simulated absorption spectrum of the complex.

Table S2. Summary of 20 lowest TDDFT excitations: singlet Alda.

From*	**To**	**Δ*E* [eV]**	**λ [nm]**	**f_osc**	**Overlap**
174	176	1.51	821	0.002408	0.21
173	175	1.58	785	0.068232	0.28
174	175	1.80	688	0.207851	0.57
172	175	2.19	567	0.012761	0.24
173	**176**	**2.36**	**524**	**0.480735**	**0.68**
171	175	2.53	491	0.039463	0.53
171	176	2.55	486	0.013491	0.34
173	177	2.60	476	0.123166	0.24
172	176	2.64	470	0.024011	0.65
170	175	2.68	463	0.011599	0.34
174	178	2.71	457	0.085480	0.40
173	178	2.87	432	0.126623	0.19
173	178	2.89	429	0.136312	0.19
170	176	2.92	424	0.042294	0.71
169	176	2.96	418	0.172185	0.37
168	175	3.06	405	0.004033	0.23

From*	To	Δ*E* [eV]	λ [nm]	f_osc	Overlap
170	176	3.10	400	0.073734	0.71
167	175	3.17	392	0.021176	0.32
172	177	3.19	389	0.000485	0.21
174	180	3.25	382	0.067889	0.41

* HOMO is orbital number 174; LUMO is orbital number 175



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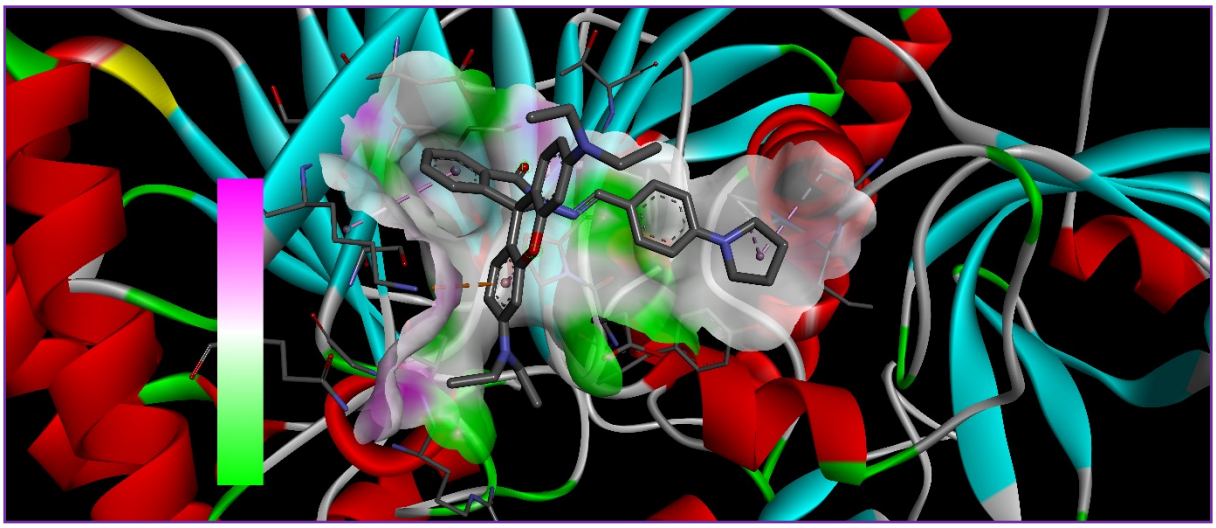

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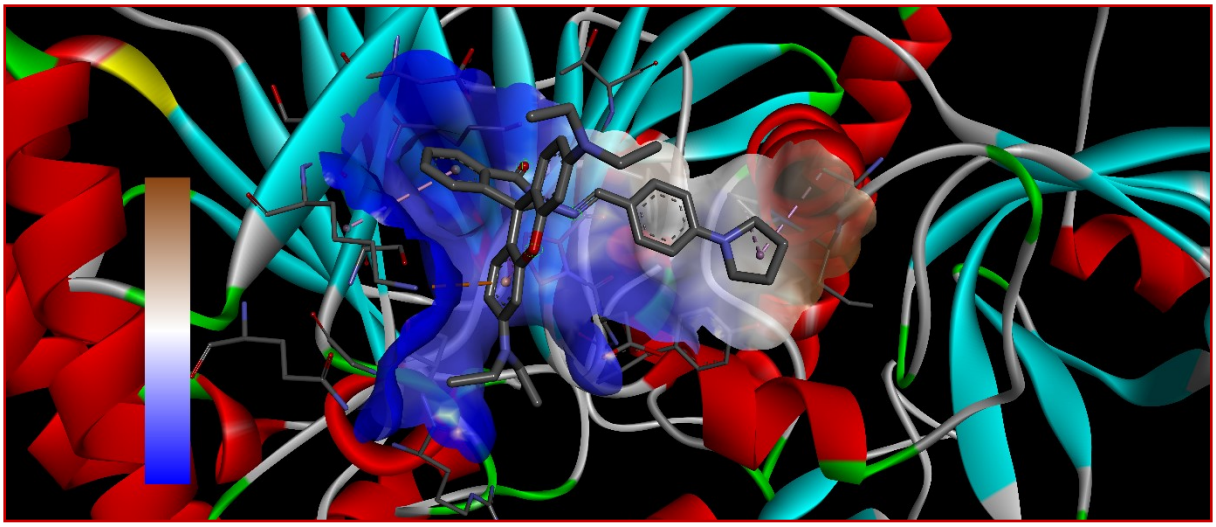

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