Electronic Supplementary Material (ESI) for RSC Advances.

Computational Design of A Two-Photon Excited FRET-Based Ratiometric Fluorescent Cu^{2+} Probe for Living Cell Imaging

Dan Wang,[a] Ai-Min Ren,[*,a] Jing-Fu Guo,[b] Lu-Yi Zou,[a] Shuang Huang [c]

[a] Institute of Theoretical Chemistry, Jilin University, Changchun 130023, People's Republic of China

[b] School of Physics, Northeast Normal University, Changchun 130021, People's Republic of China

[c] School of Mathematics and Physics, Changzhou University, Changzhou 213164, People's Republic of China

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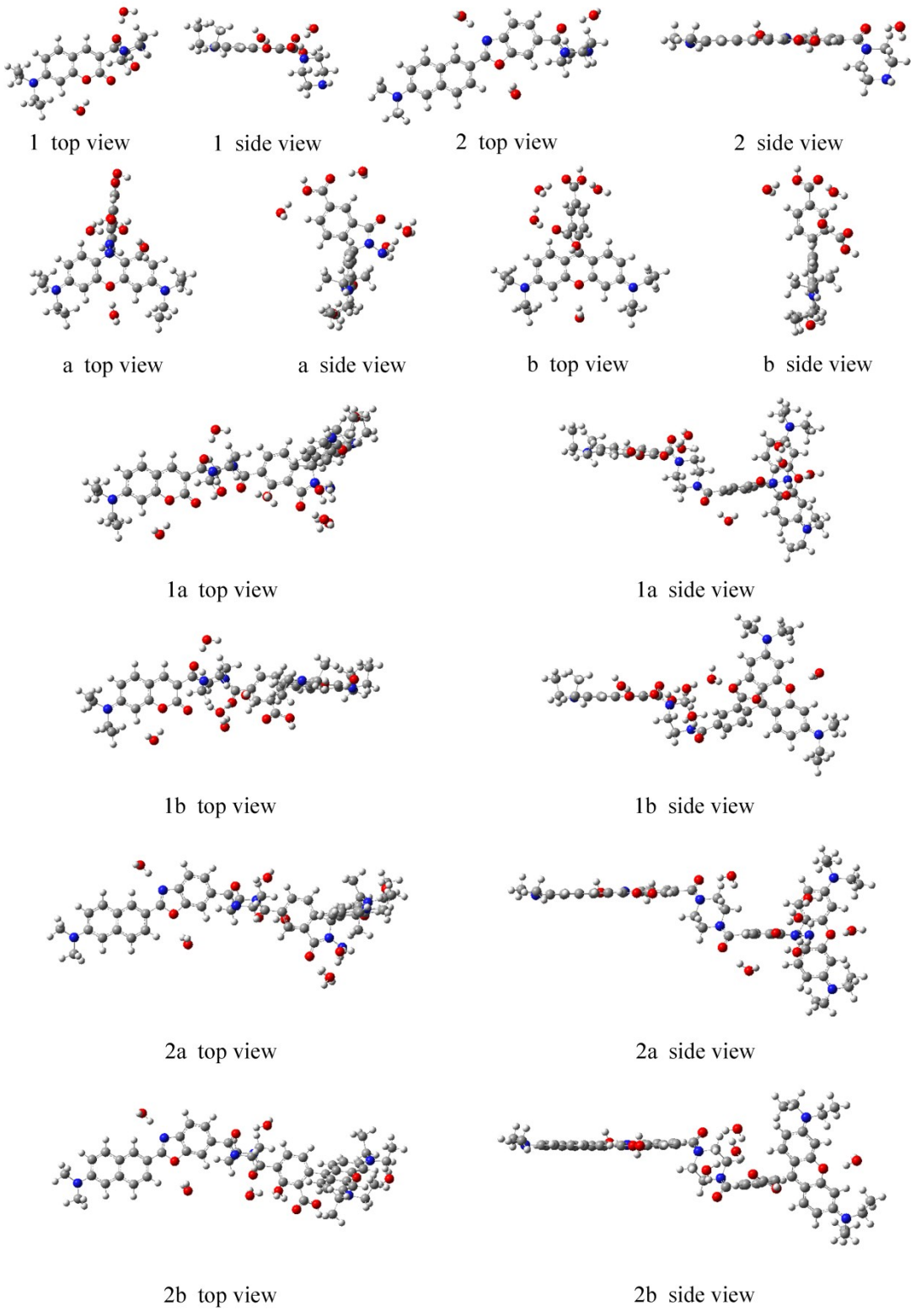

Figure S1. Optimized ground-state geometries of the studied molecules.

Table S1. OPA properties of studied molecules calculated by TDDFT method

Molecules	λ^{O}_{max}/nm	f^{O}	Transition nature		EXP/nm
1	421.90	0.4870	$S_0 \rightarrow S_2$	H→L (56.6%), H-1→L (39.2%)	410
2	448.85	0.7131	$S_0 \rightarrow S_2$	H→L (61.4%), H-1→L (36.8%)	
a	348.77	0.2110	$S_0 \rightarrow S_7$	H→L+2 (95.8%)	
b	541.84	0.6741	$S_0 \rightarrow S_2$	H→L (96.6%)	560
1a	428.15	0.7401	$S_0 \rightarrow S_5$	H-2→L (92.9%)	410
1b	534.00	0.7508	$S_0 \rightarrow S_2$	H-1→L (98.0%)	560
	428.74	0.6649	$S_0 \rightarrow S_6$	H→L+1 (84.7%), H→L+2 (7.5%)	410
2a	449.39	0.9293	$S_0 \rightarrow S_3$	H-2→L (98.2%)	
2b	538.54	0.7340	$S_0 \rightarrow S_2$	H-2→L (57.0%), H-1→L (41.9%)	
	449.99	0.9300	$S_0 \rightarrow S_5$	H→L+1 (96.7%)	

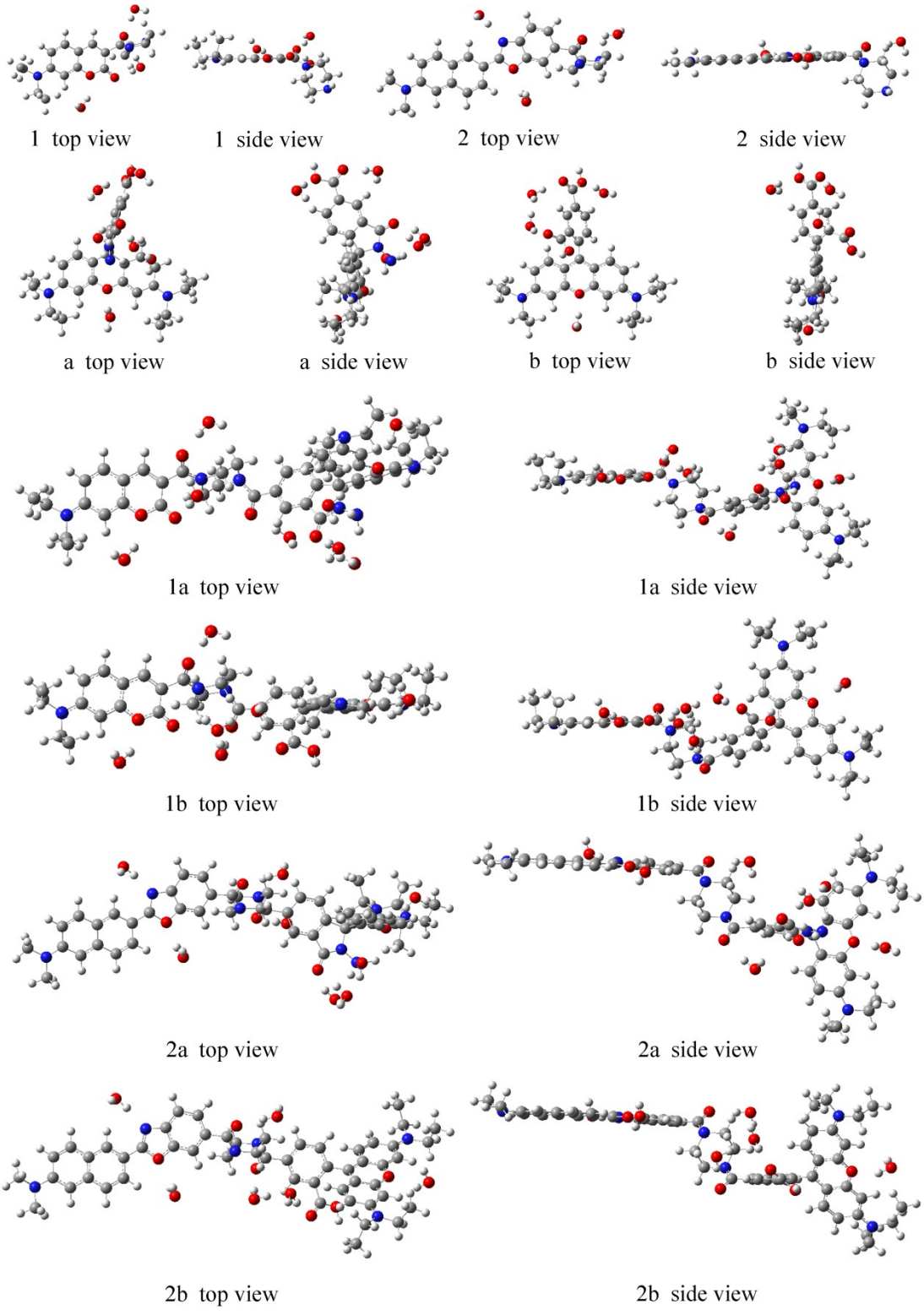

Figure S2. Optimized geometries in the first excited state of the studied molecules.

Table S2. Fluorescence properties of studied molecules calculated by TDDFT method

Molecules	λ^{flu}_{max}/nm	f^F	Transition nature	Γ/ns	EXP/nm
1	465.60	1.0946	H→L (97.9%)	2.97	470
2	501.08	1.8031	H→L (96.3%)	2.09	
a	471.94	0.0105	H→L (95.8%)	---	
b	630.12	1.1998	H→L (97.9%)	4.96	583
1a	465.94	1.1241	H-1→L (97.8%)	2.90	473
1b	612.64	1.2679	H-1→L (98.3%)	4.44	583
2a	502.58	1.8142	H→L (96.0%)	2.09	
2b	613.82	1.2648	H-1→L (98.2%)	4.47	

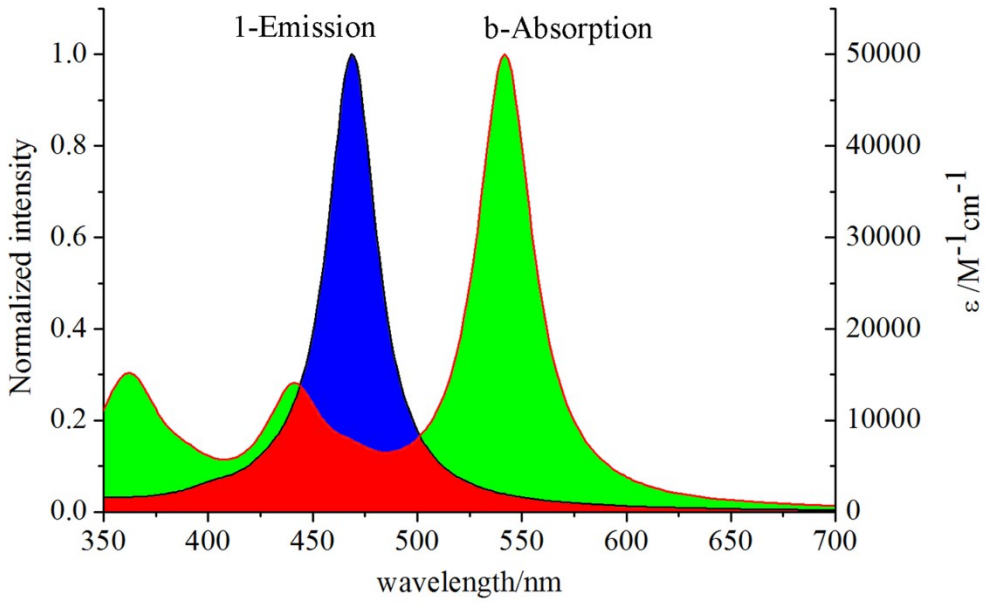

Figure S3. The spectral overlap between the emission of **1** and the absorption of **b**

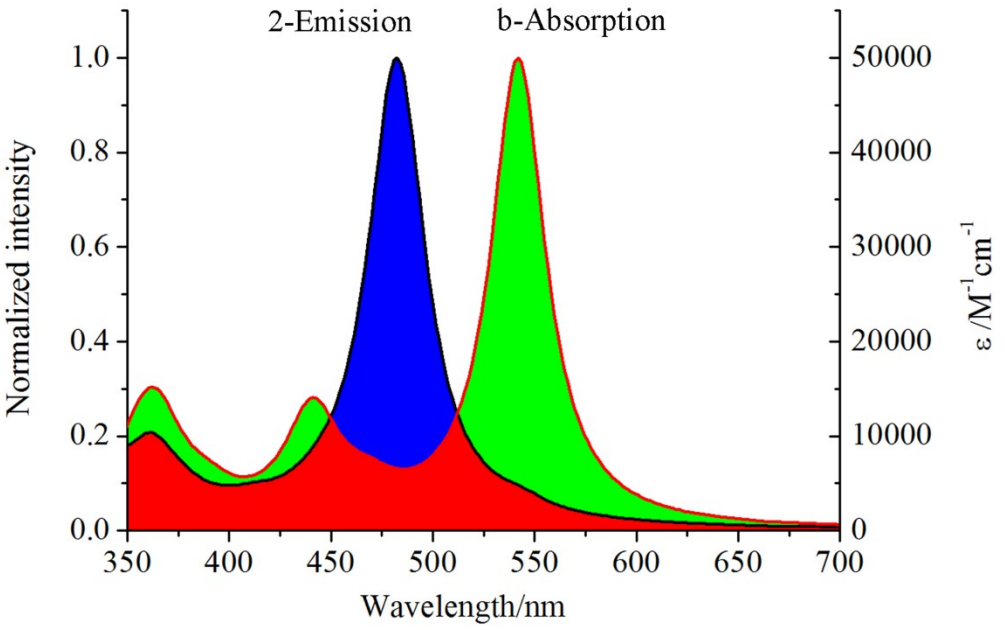

Figure S4. The spectral overlap between the emission of **2** and the absorption of **b**

Table S3. The detail data of TPA properties of studied molecules

	1			**2**			**a**			**b**		
State	*E*/eV	λ^T/nm	δ/GM	*E*/eV	λ^T/nm	δ/GM	*E*/eV	λ^T/nm	δ/GM	*E*/eV	λ^T/nm	δ/GM
1	3.41	727.2	0.9	**3.41**	**727.2**	**144.5**	3.35	740.2	37.7	2.75	901.7	10.0
					780[a]	**150**[a]						
2	**3.55**	**698.5**	**12.5**	3.78	656.0	75.4	3.39	731.5	12.9	**3.17**	**782.2**	**63.4**
3	3.93	630.9	50.5	3.85	644.1	38.9	3.78	656.0	4.9	3.63	683.1	8.3
	1a			**1b**			**2a**			**2b**		
State	*E*/eV	λ^T/nm	δ/GM	*E*/eV	λ^T/nm	δ/GM	*E*/eV	λ^T/nm	δ/GM	*E*/eV	λ^T/nm	δ/GM
1	3.03	818.4	3.8	1.08	2296.0	3.3	3.34	742.4	0.6	0.58	4275.3	20.3
2	3.16	784.7	0.8	1.96	1265.2	9.2	**3.37**	**735.8**	**227.5**	1.59	1559.6	0.4
3	**3.53**	**702.5**	**15.2**	2.25	1102.1	12.3	3.46	716.7	0.3	1.76	1408.9	11.6
4				2.37	1046.3	0.6				1.99	1246.1	8.3
5				2.47	1003.9	9.2				2.05	1209.6	19.4
6				2.75	901.7	3.7				2.3	1078.1	0.0
7				2.77	895.2	7.9				2.54	976.3	16.5
8				2.88	861.0	4.1				2.59	957.4	0.2
9				3.03	818.4	8.6				2.74	905.0	13.5
10				3.13	792.2	0.1				2.74	905.0	13.8
11				**3.19**	**777.3**	**48.3**				2.89	858.0	27.7
12				3.20	774.9	15.3				3.00	826.6	0.0
13				3.24	765.3	4.2				3.06	810.4	1.6
14				3.26	760.6	11.2				3.06	810.4	0.4
15				**3.49**	**710.5**	**38.0**				3.15	787.2	1.3
16										3.16	784.7	9.0
17										**3.17**	**782.2**	**59.9**
18										**3. 25**	**763.0**	**359.9**
19										3.26	760.6	37.0
20										3.26	760.6	0.2

a is from Ref. 62.