Electronic Supplementary Information (ESI)

Design and application of a water-soluble phosphorescent Ru(II) complex as turn-on sensing material for Hg^{2+}

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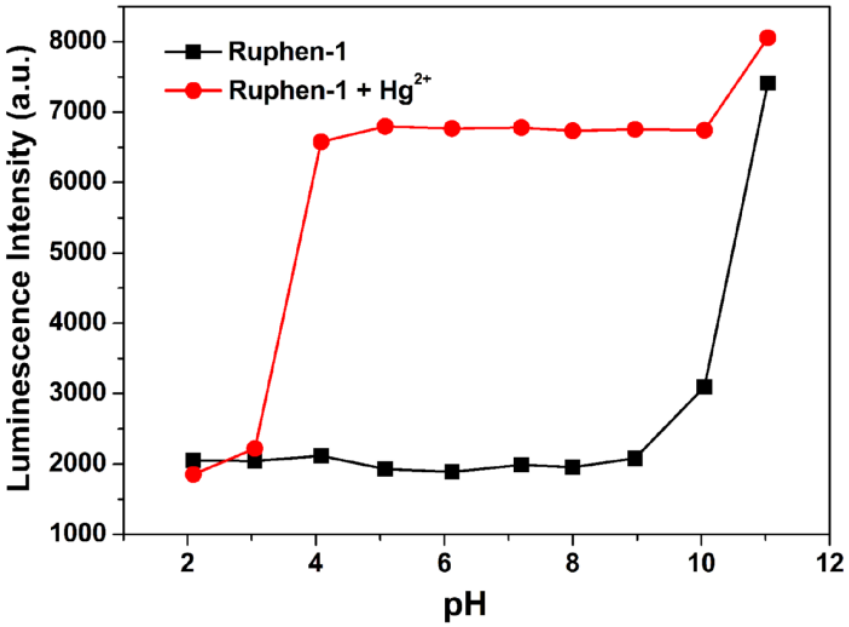


Fig. S1 Luminescence intensity of **Ruphen-1** (10 μM) at 598 nm in the absence and presence of 10 equiv of Hg^{2+} as a function of pH in water solutions. λ_{ex} = 467 nm.

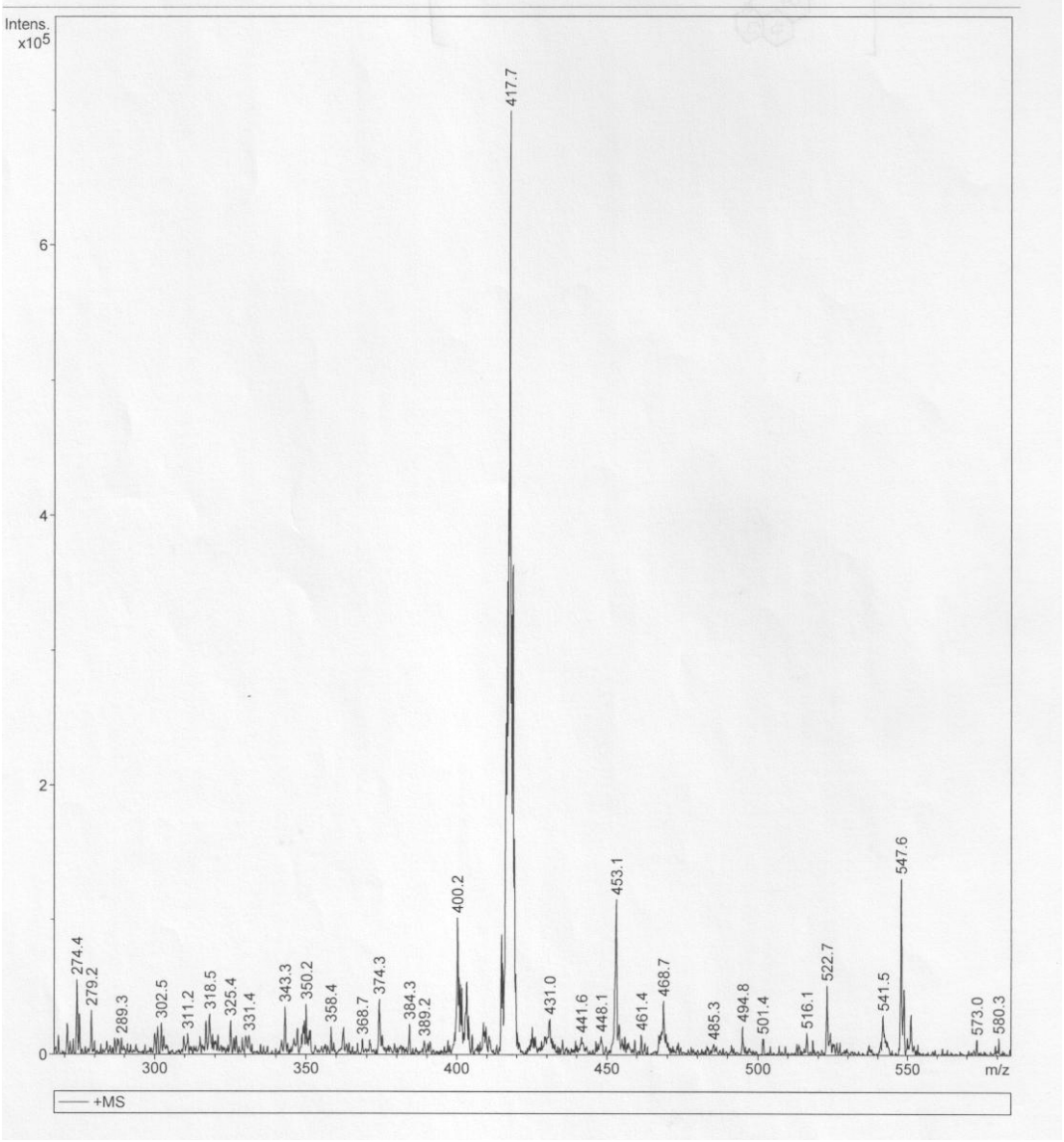


Fig. S2 ESI mass spectrum of **Ruphen-1** (*m/z* 417.7).

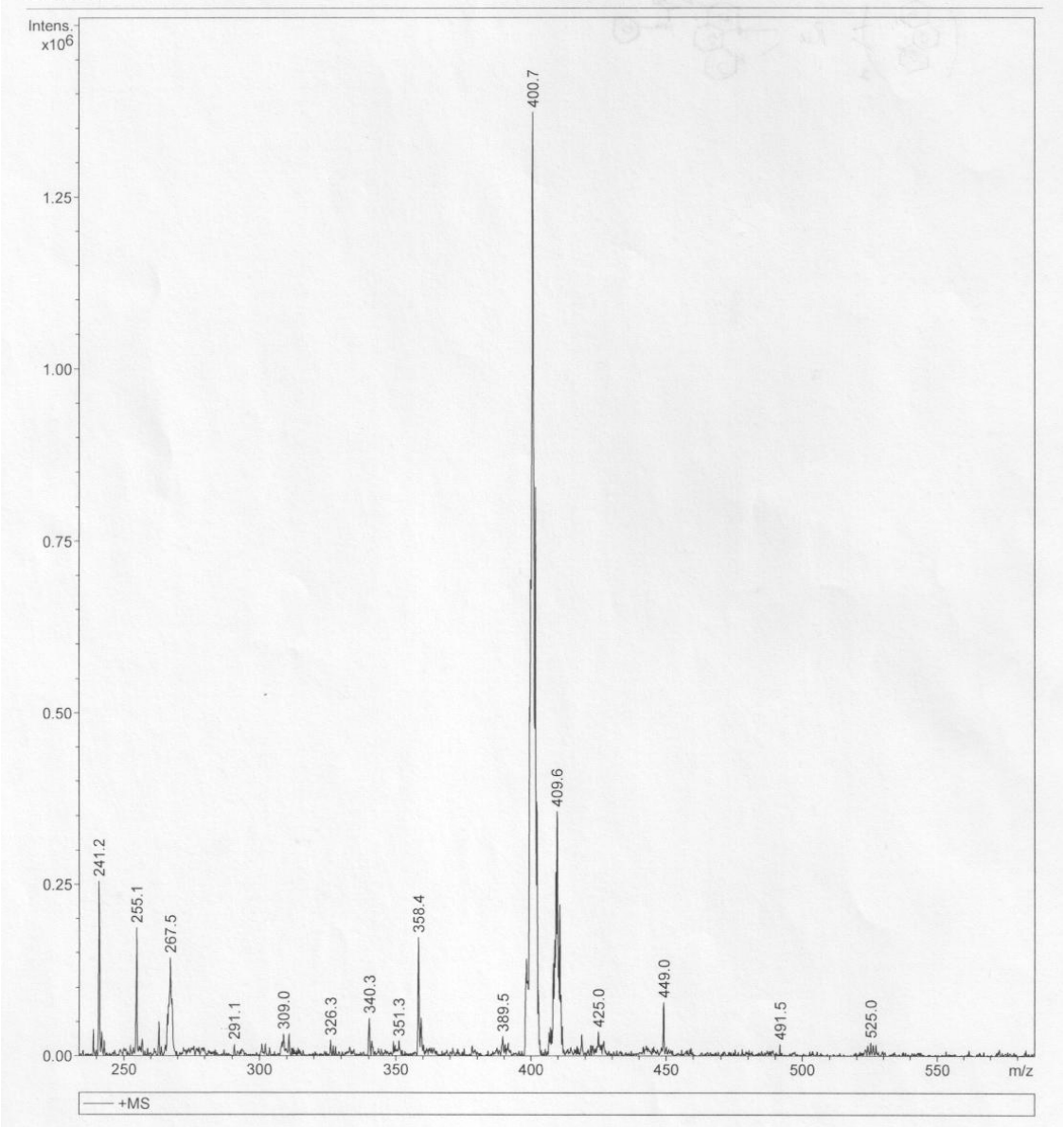


Fig. S3 ESI mass spectrum of **Ruphen-2** (*m/z* 400.7).

Theoretical calculations

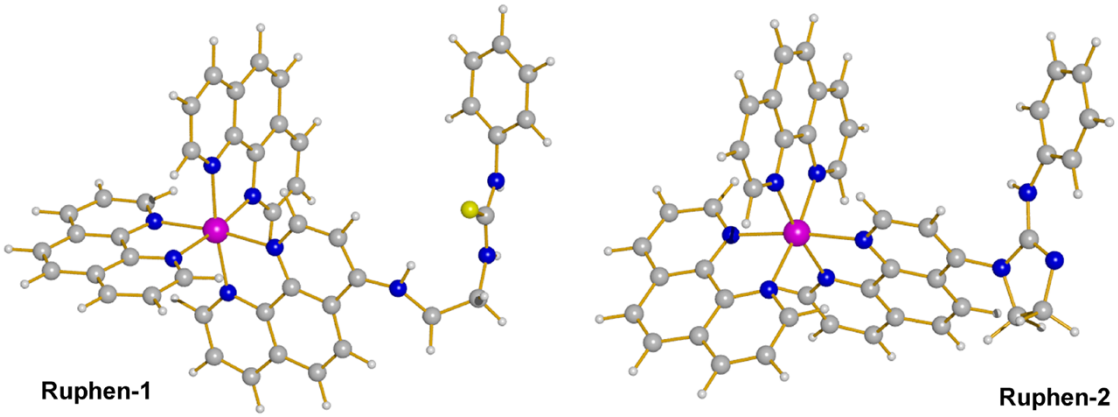


Fig. S4 The calculated ground-state geometries of **Ruphen-1** and **Ruphen-2**.

Table S1 DFT optimized coordinates for **Ruphen-1** in the ground state.

Number	Atom	Coordinates		
		X	Y	Z
1	Ru	2.009712	0.102352	0.127188
2	C	1.132852	-3.8325	1.675416
3	C	2.258305	-4.21921	2.440481
4	C	3.323377	-3.34762	2.56225
5	C	3.270781	-2.09843	1.918019
6	N	2.224196	-1.70722	1.187573
7	C	1.15516	-2.55624	1.065397
8	C	0.042621	-2.09981	0.276964
9	N	0.192998	-0.88359	-0.32489
10	C	-0.80867	-0.45823	-1.11019
11	C	-1.98833	-1.16186	-1.28715
12	C	-2.21233	-2.38876	-0.62634
13	C	-1.11276	-2.9154	0.144619
14	C	-1.08204	-4.22297	0.741001
15	C	-0.01309	-4.66433	1.47063
16	C	3.511776	-2.02854	-3.45731
17	C	4.853397	-1.69195	-3.45468
18	C	5.352548	-0.85204	-2.43313
19	C	4.436163	-0.39808	-1.4544
20	C	4.883063	0.454902	-0.39339
21	C	6.241509	0.847042	-0.3252
22	C	6.624832	1.689021	0.743549
23	C	5.672904	2.087586	1.664409
24	C	4.344248	1.648786	1.523484

25	N	3.950269	0.852773	0.526188
26	C	0.756912	0.739497	2.914669
27	C	0.069234	1.535569	3.847871
28	C	-0.36091	2.798515	3.482777
29	C	-0.10239	3.263561	2.173304
30	C	0.591794	2.395771	1.296442
31	C	0.879481	2.811127	-0.04412
32	C	0.474359	4.091593	-0.49161
33	C	0.783416	4.444876	-1.82494
34	C	1.455176	3.538687	-2.62528
35	C	1.818489	2.285514	-2.10114
36	N	1.542555	1.922208	-0.84609
37	N	-3.42169	-2.99494	-0.78638
38	C	-4.10783	-3.90145	0.138999
39	C	-5.62522	-3.67901	0.094531
40	N	-6.04587	-2.36948	0.583001
41	C	-6.35591	-1.28528	-0.16886
42	S	-6.23376	-1.27787	-1.87205
43	N	-6.75235	-0.19901	0.551907
44	C	-7.14326	1.082524	0.054796
45	C	-6.43998	2.212974	0.488255
46	C	-6.84208	3.486203	0.071897
47	C	-7.93787	3.631548	-0.78448
48	C	-8.63995	2.498017	-1.21184
49	C	-8.25326	1.224651	-0.78709
50	H	2.273941	-5.19273	2.922042
51	H	4.203021	-3.60634	3.141885
52	H	4.094276	-1.39824	1.996735
53	H	-0.66521	0.497299	-1.60214
54	H	-2.76687	-0.73518	-1.91154
55	H	-1.9117	-4.89865	0.589277
56	H	-0.01928	-5.66198	1.899623
57	H	3.093248	-2.67053	-4.22493
58	H	5.523865	-2.06294	-4.22454
59	H	7.657705	2.01308	0.831829
60	H	5.929629	2.733127	2.497431
61	H	3.583237	1.945822	2.236097
62	H	1.107756	-0.25083	3.181291
63	H	-0.11121	1.144351	4.84335
64	H	-0.89101	3.433448	4.186747
65	H	0.490922	5.4182	-2.20815
66	H	1.707908	3.773686	-3.65362
67	H	2.339881	1.558368	-2.71275
68	H	-4.06158	-2.48413	-1.39451

69	H	-3.74543	-3.73559	1.158935
70	H	-3.92495	-4.95161	-0.12279
71	H	-6.09599	-4.43657	0.728196
72	H	-6.00494	-3.80759	-0.92133
73	H	-6.1549	-2.29477	1.58929
74	H	-6.6482	-0.25052	1.560876
75	H	-5.58232	2.093594	1.144993
76	H	-6.29339	4.359973	0.412729
77	H	-8.24723	4.620272	-1.11222
78	H	-9.49987	2.604464	-1.86766
79	H	-8.80703	0.34652	-1.10118
80	C	2.668739	-1.53015	-2.44807
81	H	1.613336	-1.77594	-2.43139
82	N	3.10988	-0.7346	-1.47058
83	N	1.017731	1.15019	1.670962
84	C	6.726471	-0.44029	-2.34156
85	H	7.42299	-0.79184	-3.09723
86	C	7.152159	0.375323	-1.33214
87	H	8.192431	0.682271	-1.27256
88	C	-0.50353	4.558308	1.695496
89	H	-1.03501	5.218319	2.375141
90	C	-0.22501	4.956159	0.419014
91	H	-0.5315	5.93752	0.068559

Table S2 DFT optimized coordinates for **Ruphen-2** in the ground state.

Number	Atom	Coordinates		
		X	Y	Z
1	Ru	1.639009	0.093979	0.149847
2	C	0.204848	-3.27524	2.440697
3	C	1.3058	-3.75297	3.188775
4	C	2.530244	-3.12432	3.062702
5	C	2.656224	-2.02007	2.200519
6	N	1.635594	-1.54525	1.483009
7	C	0.419461	-2.16653	1.588899
8	C	-0.65706	-1.63854	0.800241
9	N	-0.37045	-0.54806	0.026039
10	C	-1.36342	-0.02253	-0.6966
11	C	-2.65572	-0.55154	-0.72073
12	C	-2.97179	-1.68188	0.03757
13	C	-1.93811	-2.23924	0.85851
14	C	-2.13569	-3.34016	1.759073
15	C	-1.11108	-3.83931	2.513047
16	C	2.293224	-2.81154	-3.13837
17	C	3.666731	-2.76681	-3.2946

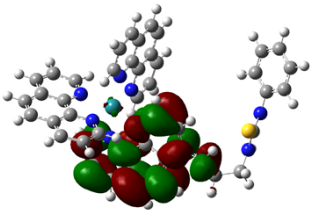
18	C	4.427846	-1.90614	-2.47123
19	C	3.72928	-1.12851	-1.51677
20	C	4.446917	-0.23574	-0.65611
21	C	5.85427	-0.12742	-0.76234
22	C	6.507536	0.771359	0.111436
23	C	5.757693	1.494713	1.021081
24	C	4.362691	1.322651	1.062966
25	N	3.716274	0.481976	0.251496
26	C	0.906354	1.393551	2.89389
27	C	0.515555	2.449308	3.736654
28	C	0.285086	3.7027	3.199093
29	C	0.448307	3.898094	1.808555
30	C	0.842717	2.781288	1.033615
31	C	1.028242	2.918867	-0.3803
32	C	0.81715	4.171765	-1.00404
33	C	1.01646	4.246723	-2.40153
34	C	1.402501	3.111401	-3.0908
35	C	1.588361	1.904901	-2.39268
36	N	1.406482	1.801495	-1.0739
37	N	-4.24211	-2.26518	0.010588
38	C	-4.4566	-3.6851	-0.38517
39	C	-5.58589	-3.54903	-1.43137
40	N	-6.23066	-2.25488	-1.15063
41	C	-5.41776	-1.58132	-0.41231
42	N	-5.59219	-0.31308	0.074608
43	C	-6.55057	0.65742	-0.27441
44	C	-6.48173	1.892732	0.398512
45	C	-7.38857	2.908924	0.102268
46	C	-8.37767	2.716327	-0.87058
47	C	-8.44271	1.49001	-1.53763
48	C	-7.54296	0.457902	-1.24893
49	H	1.179203	-4.60338	3.85242
50	H	3.398468	-3.46132	3.618636
51	H	3.60412	-1.50567	2.093263
52	H	-1.11703	0.83722	-1.30922
53	H	-3.39112	-0.08965	-1.36822
54	H	-3.12477	-3.77037	1.854936
55	H	-1.28501	-4.66936	3.191453
56	H	1.676794	-3.45886	-3.75273
57	H	4.163728	-3.38094	-4.03995
58	H	7.586574	0.884755	0.0621
59	H	6.223864	2.193369	1.707391
60	H	3.75615	1.873178	1.772692
61	H	1.096083	0.404473	3.294383

62	H	0.401555	2.261463	4.798813
63	H	-0.01684	4.533856	3.829866
64	H	0.865523	5.189659	-2.91915
65	H	1.56527	3.130613	-4.16298
66	H	1.887322	1.002331	-2.91283
67	H	-4.78642	-4.27171	0.478486
68	H	-3.53633	-4.11567	-0.78318
69	H	-6.31331	-4.36098	-1.34591
70	H	-5.19477	-3.55596	-2.45802
71	H	-4.95366	-0.03949	0.810733
72	H	-5.71396	2.053363	1.152524
73	H	-7.31922	3.85445	0.633741
74	H	-9.08463	3.508356	-1.10108
75	H	-9.20567	1.322881	-2.29397
76	H	-7.60654	-0.49281	-1.76108
77	C	1.678448	-2.00262	-2.16623
78	H	0.603446	-2.01814	-2.02975
79	N	2.369309	-1.17982	-1.37315
80	N	1.069182	1.54604	1.57735
81	C	5.857062	-1.78154	-2.55686
82	H	6.385544	-2.38266	-3.29105
83	C	6.540574	-0.92725	-1.73944
84	H	7.620553	-0.83886	-1.81429
85	C	0.238055	5.159002	1.151788
86	H	-0.06513	6.010977	1.753364
87	C	0.416005	5.290483	-0.19597
88	H	0.255835	6.248424	-0.68207

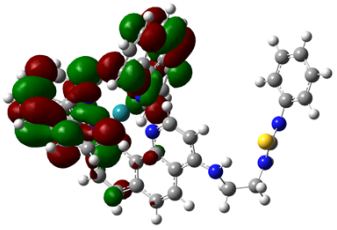
Table S3 TD-DFT calculated singlet absorption data for **Ruphen-1** (Selected absorption wavelength > 350 nm)

state (*E*/nm, o.s.)	transition	coefficient	state (*E*/nm, o.s.)	transition	coefficient
S1	198 -> 200	0.19741	**S10**	197 -> 201	-0.22389
(483.87, 0.0018)	198 -> 201	-0.12186	(418.69, 0.0179)	197 -> 202	-0.22233
	199 -> 200	0.52409		197 -> 203	-0.27196
	199 -> 201	-0.37169		198 -> 202	-0.27609
S2	198 -> 200	0.19487		198 -> 203	0.37835
(479.89, 0.0092)	198 -> 201	0.27538		199 -> 202	0.11837
	199 -> 200	0.34544		199 -> 203	-0.22587
	199 -> 201	0.49704	**S11**	197 -> 200	-0.10011
S3	198 -> 200	0.4308	(411.55, 0.1019)	197 -> 201	0.16744
(458.06, 0.0204)	198 -> 202	0.15343		197 -> 202	0.24891
	198 -> 203	0.21275		197 -> 203	0.40764
	199 -> 200	-0.24674		198 -> 202	-0.21467
	199 -> 202	0.27397		198 -> 203	0.37619
	199 -> 203	0.29199	**S12**	197 -> 202	-0.23603
S4	198 -> 200	-0.293	(405.61, 0.0314)	198 -> 204	0.63402
(455.87, 0.0050)	198 -> 201	0.48237		199 -> 204	-0.12045
	199 -> 201	-0.16127	**S13**	197 -> 202	0.52402
	199 -> 202	0.25371	(398.92, 0.0289)	197 -> 203	-0.39057
	199 -> 203	0.21923		198 -> 204	0.20172
S5	197 -> 200	0.1428	**S14**	197 -> 201	-0.27461
(451.98, 0.0042)	197 -> 201	0.16031	(389.29, 0.1075)	197 -> 203	0.17869
	198 -> 200	0.34832		197 -> 204	0.2379
	198 -> 201	0.35208		198 -> 202	0.22994
	198 -> 202	-0.13572		198 -> 205	0.11964
	199 -> 200	-0.11466		199 -> 203	-0.13341
	199 -> 201	-0.1963		199 -> 205	0.46345
	199 -> 202	-0.3063	**S15**	197 -> 201	0.11532
	199 -> 203	-0.14647	(388.69, 0.0540)	197 -> 204	0.64313
S6	197 -> 200	0.27778		199 -> 205	-0.15498
(439.20, 0.0022)	197 -> 201	0.20809	**S16**	194 -> 200	0.1249
	198 -> 203	-0.17043	(376.09, 0.0309)	197 -> 201	0.30348
	199 -> 202	0.40945		197 -> 203	-0.15656
	199 -> 203	-0.40127		198 -> 202	-0.25906
S7	197 -> 200	0.49875		198 -> 205	0.14153
(433.52, 0.0581)	198 -> 201	-0.11672		199 -> 203	0.14555
	198 -> 204	-0.16214		199 -> 205	0.44729
	199 -> 202	-0.17423	**S17**	198 -> 205	0.66114
	199 -> 203	0.13668	(367.41, 0.0357)	199 -> 205	-0.1894
	199 -> 204	-0.36664	**S18**	196 -> 200	0.65889

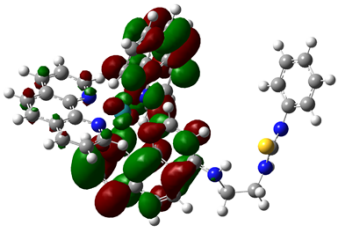
S8	197 -> 200	-0.16524
(427.83, 0.0593)	197 -> 201	0.34234
	197 -> 202	-0.1409
	197 -> 203	-0.12404
	198 -> 202	0.39703
	198 -> 203	0.19335
	199 -> 202	-0.14223
	199 -> 203	-0.1768
	199 -> 204	-0.21545
S9	197 -> 200	0.28617
(426.76, 0.0641)	198 -> 202	0.13378
	198 -> 203	0.24504
	199 -> 202	-0.10008
	199 -> 204	0.52258
(362.93, 0.0003)	196 -> 201	0.23786
S19 (356.96, 0.0034)	197 -> 205	0.67873
S20	196 -> 200	-0.20295
(352.15, 0.0001)	196 -> 201	0.63369
	196 -> 202	0.10796
	196 -> 203	0.15097
S21	196 -> 200	0.13287
(350.22, 0.0002)	196 -> 201	-0.15388
	196 -> 202	0.47125
	196 -> 203	0.43942
	196 -> 204	-0.11446



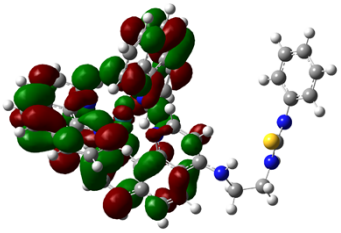
LUMO+5 (205)



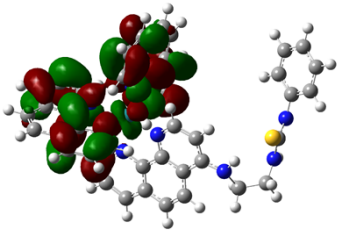
LUMO+4 (204)



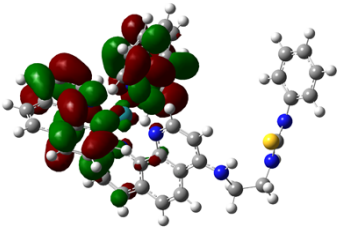
LUMO+3 (203)



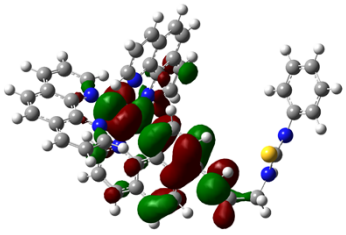
LUMO+2 (202)



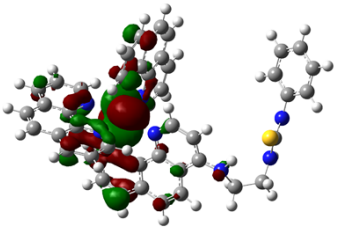
LUMO+1 (201)



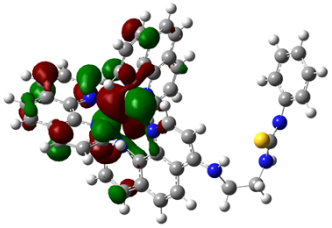
LUMO (200)



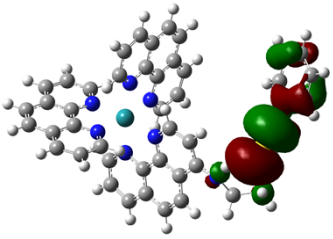
HOMO (199)



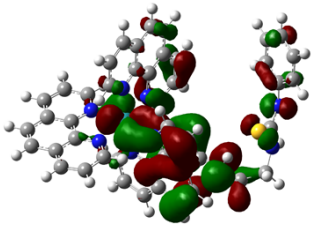
HOMO–1 (198)



HOMO–2 (197)



HOMO–3 (196)



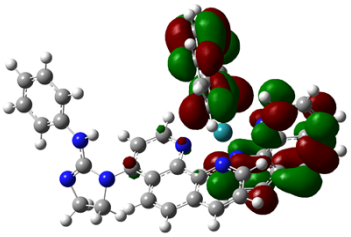
HOMO–5 (194)

Table S4 TD-DFT calculated singlet absorption data for **Ruphen-2** (Selected absorption wavelength > 350 nm)

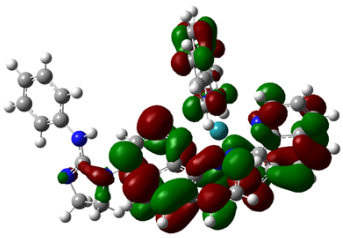
state (*E*/nm, o.s.)	transition	coefficient	state (*E*/nm, o.s.)	transition	coefficient
S1	188 -> 191	0.28093	**S12**	187 -> 191	0.12467
(462.15, 0.0043)	188 -> 193	-0.13097	(404.16, 0.1119)	188 -> 194	0.42589
	190 -> 191	0.56096		188 -> 196	0.15005
	190 -> 192	-0.16406		190 -> 194	-0.24625
	190 -> 193	-0.21246		190 -> 196	0.41255
S2	188 -> 191	0.10646	**S13**	188 -> 195	-0.10231
(461.04, 0.0015)	188 -> 192	0.33149	(400.26, 0.0101)	189 -> 191	0.53192
	190 -> 191	0.18203		189 -> 193	0.32086
	190 -> 192	0.56793		189 -> 194	0.24837
S3	188 -> 192	-0.11351		189 -> 195	-0.15046
(454.20, 0.0091)	188 -> 193	0.34222	**S14**	187 -> 193	-0.12617
	190 -> 191	0.22316	(397.17, 0.0454)	187 -> 194	0.62433
	190 -> 193	0.54129		188 -> 195	0.14912
S4	188 -> 191	0.5125		188 -> 196	-0.18478
(440.55, 0.0133)	188 -> 192	-0.31132	**S15**	187 -> 192	0.10202
	188 -> 193	-0.14738	(394.20, 0.0094)	187 -> 195	-0.18835
	190 -> 191	-0.22207		188 -> 193	0.11832
	190 -> 192	0.12834		188 -> 194	-0.10069
S5	187 -> 191	0.18694		188 -> 195	0.37249
(438.74, 0.0160)	187 -> 192	0.20972		188 -> 196	0.45726
	187 -> 193	-0.21183		190 -> 195	-0.11169
	188 -> 191	0.30979		190 -> 196	-0.12287
	188 -> 192	0.40643	**S16**	187 -> 194	-0.25784
	190 -> 191	-0.1559	(390.92, 0.0439)	188 -> 195	0.43295
	190 -> 192	-0.22936		188 -> 196	-0.35959
S6	187 -> 191	0.51643		189 -> 195	-0.14804
(429.01, 0.0239)	187 -> 192	0.12102		190 -> 195	-0.14954
	187 -> 193	0.26008		190 -> 196	0.15133
	188 -> 193	-0.28297	**S17**	189 -> 191	0.37641
	188 -> 194	-0.10113	(387.06, 0.0043)	189 -> 192	0.35128
	190 -> 193	0.16911		189 -> 193	-0.28119
S7	187 -> 191	0.29048		189 -> 194	-0.31589
(426.25, 0.0184)	188 -> 192	-0.16681		189 -> 195	0.19254
	188 -> 193	0.21256	**S18**	187 -> 192	-0.10849
	188 -> 194	0.21825	(385.17, 0.0030)	187 -> 195	0.58249
	190 -> 192	0.10598		187 -> 196	-0.25588
	190 -> 193	-0.20911		188 -> 195	0.11871
	190 -> 194	0.44972		188 -> 196	0.18013
S8	187 -> 191	-0.27728	**S19**	187 -> 196	-0.16508

(422.29, 0.1239)	187 -> 192	0.43555
	188 -> 193	-0.24077
	188 -> 194	0.14059
	188 -> 195	0.11734
	190 -> 193	0.10913
	190 -> 194	0.28625
	190 -> 195	0.12086
S9	187 -> 192	-0.16645
(419.63, 0.0705)	187 -> 193	0.53498
	187 -> 194	0.13547
	188 -> 192	0.19859
	188 -> 193	0.11993
	188 -> 194	0.15154
	190 -> 192	-0.11814
	190 -> 194	0.13242
	190 -> 196	0.13276
S10	187 -> 192	-0.10061
(408.91, 0.0423)	188 -> 194	-0.22824
	188 -> 195	0.12699
	190 -> 195	0.53743
	190 -> 196	0.30385
S11	188 -> 194	-0.32604
(407.44, 0.1071)	188 -> 195	-0.18451
	188 -> 196	0.14495
	190 -> 194	0.21732
	190 -> 195	-0.35072
	190 -> 196	0.37278

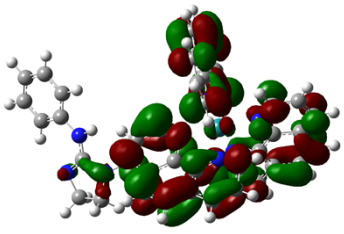
(382.63, 0.0095)	188 -> 195	0.11494
	189 -> 192	-0.10656
	189 -> 193	0.46818
	189 -> 194	-0.36953
	189 -> 195	0.25544
S20	187 -> 195	0.28402
(381.43, 0.0444)	187 -> 196	0.60233
	188 -> 195	0.10611
S21	189 -> 191	-0.23034
(377.26, 0.0002)	189 -> 192	0.59196
	189 -> 193	0.25472
	189 -> 194	0.10747
S22	187 -> 192	0.39228
(371.57, 0.0030)	187 -> 193	0.18056
	187 -> 195	0.17413
	188 -> 192	-0.11182
	188 -> 193	0.28648
	188 -> 194	-0.12551
	188 -> 195	-0.10605
	188 -> 196	-0.1008
	190 -> 193	-0.17343
	190 -> 194	-0.2221
S23	189 -> 194	0.34212
(368.53, 0.0012)	189 -> 195	0.44736
	189 -> 196	-0.39247



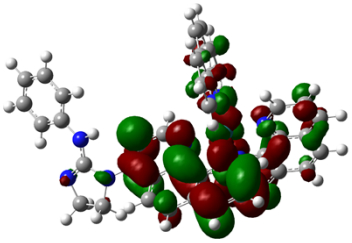
LUMO+5 (196)



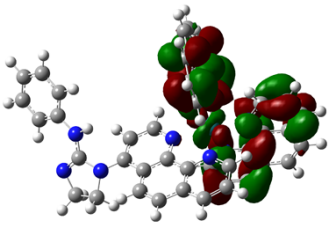
LUMO+4 (195)



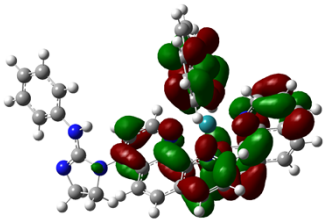
LUMO+3 (194)



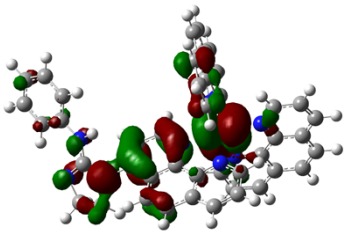
LUMO+2 (193)



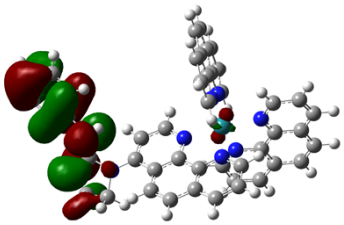
LUMO+1 (192)



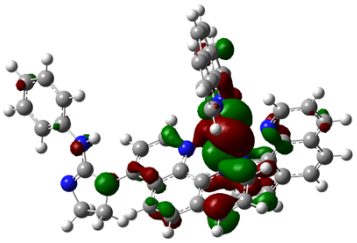
LUMO (191)



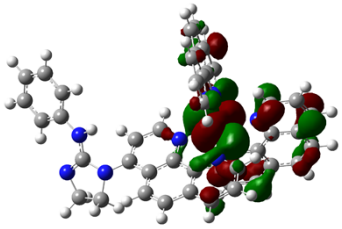
HOMO (190)



HOMO–1 (189)



HOMO–2 (188)



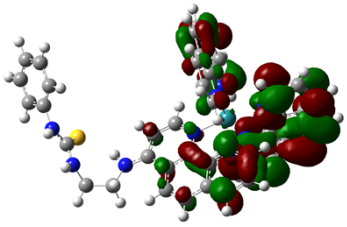
HOMO–3 (187)

Table S5 Molecular orbital compositions of **Ruphen-1** under TD-DFT triplet excitation calculation (Emission transition study)

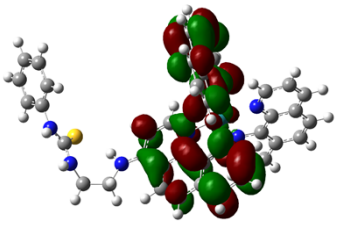
Orbital	Energy (eV)	MO contribution (%)			
		Ru	L		2phen
			1,10-phen	substituent group	
LUMO+6	– 1.32138	2.28	12.77	0.51	84.44
LUMO+5	– 1.99840	1.27	88.92	8.10	1.71
LUMO+4	– 2.34997	1.23	17.72	0.11	80.94
LUMO+3	– 2.37447	3.90	50.33	0.41	45.36
LUMO+2	– 2.43243	2.98	24.67	0.11	72.24
LUMO+1	– 2.51188	5.29	1.28	0.02	93.41
LUMO	– 2.81066	6.51	2.31	0.13	91.05
HOMO	– 5.64827	46.33	30.34	12.68	10.66
HOMO–1	– 6.15630	76.35	8.99	0.92	13.74
HOMO–2	– 6.19875	70.63	6.94	0.22	22.21
HOMO–3	– 6.36365	0.15	0.49	99.31	0.04
HOMO–4	– 6.58107	3.33	2.96	92.10	1.60
HOMO–5	– 6.69999	24.23	37.95	22.47	15.34
HOMO–6	– 6.95224	0.01	0.26	99.73	0.00

Table S6 TD-DFT excitation calculation for emission of **Ruphen-1**.

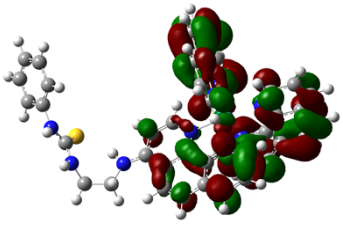
State	Transition	Contribution(%)	*E*,nm(eV)	o.s.	Assignment
T1	HOMO→LUMO	93.3	688 (1.80)		^{3}MLCT/^{3}LLCT
S1	HOMO→LUMO	91.2	581 (2.13)	0.0323	^{1}MLCT/^{1}LLCT
S2	HOMO→LUMO+1	97.8	516 (2.41)	0.0017	^{1}MLCT/^{1}LLCT
S3	HOMO–1→LUMO	73.3	505 (2.46)	0.0104	^{1}MLCT
S4	HOMO→LUMO+2	72.1	487 (2.55)	0.0284	^{1}MLCT/^{1}ILCT/^{1}LLCT
S5	HOMO–2→LUMO	53.6	482 (2.57)	0.0361	^{1}MLCT/^{1}ILCT
S6	HOMO→LUMO+4	57.3	464 (2.67)	0.0207	^{1}MLCT/^{1}ILCT/^{1}LLCT
S7	HOMO→LUMO+3	39.7	459 (2.70)	0.0488	^{1}MLCT/^{1}ILCT/^{1}LLCT
	HOMO→LUMO+4	41.9			^{1}MLCT/^{1}ILCT/^{1}LLCT
S8	HOMO–1→LUMO+1	100	442 (2.81)	0.0045	^{1}MLCT



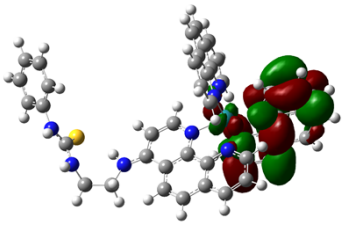
LUMO+4



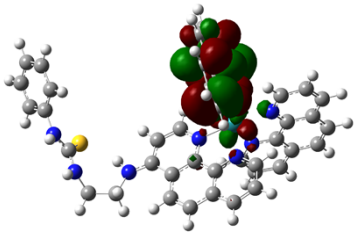
LUMO+3



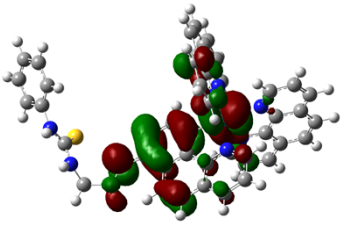
LUMO+2



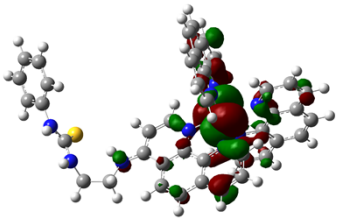
LUMO+1



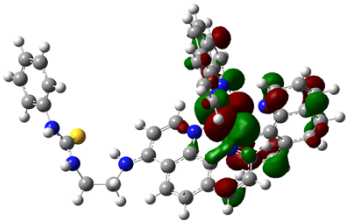
LUMO



HOMO



HOMO–1



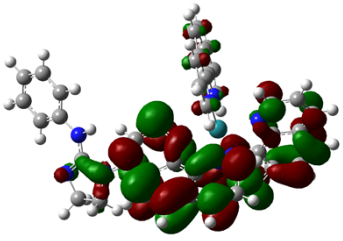
HOMO–2

Table S7 Molecular orbital compositions of **Ruphen-2** under TD-DFT triplet excitation calculation (Emission transition study)

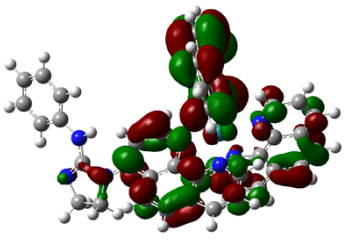
Orbital	Energy (eV)	MO contribution (%)			
		Ru	L		2phen
			1,10-phen	substituent group	
LUMO+6	– 1.39241	2.20	32.98	1.22	63.61
LUMO+5	– 2.38317	1.00	10.17	1.27	87.55
LUMO+4	– 2.39460	0.91	61.98	4.70	32.42
LUMO+3	– 2.44821	2.80	23.62	2.46	71.12
LUMO+2	– 2.52331	5.92	63.55	1.30	29.23
LUMO+1	– 2.55678	4.69	20.52	0.88	73.91
LUMO	– 2.85937	6.09	3.05	0.26	90.61
HOMO	– 5.92092	56.03	18.17	12.51	13.29
HOMO–1	– 6.14351	1.06	0.85	97.88	0.22
HOMO–2	– 6.26297	72.46	9.86	3.95	13.73
HOMO–3	– 6.29562	69.50	6.30	0.31	23.89
HOMO–4	– 6.76557	19.08	26.23	41.65	13.03
HOMO–5	– 7.20829	0.11	2.53	95.94	1.42
HOMO–6	– 7.25319	4.97	2.45	1.00	91.59

Table S8 TD-DFT excitation calculation for emission of **Ruphen-2**.

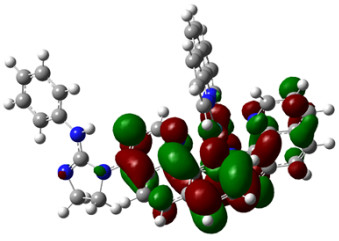
State	Transition	Contribution	*E*,nm(eV)	o.s.	Assignment
T1	HOMO→LUMO	90.0	638 (1.94)		^{3}MLCT/^{3}LLCT
S1	HOMO→LUMO	85.1	543 (2.29)	0.0199	^{1}MLCT/^{1}LLCT
S2	HOMO–2→LUMO	57.1	489 (2.53)	0.0096	^{1}MLCT
S3	HOMO→LUMO+1	68.1	478 (2.59)	0.0031	^{1}MLCT/^{1}ILCT/^{1}LLCT
S4	HOMO→LUMO+2	49.2	472 (2.62)	0.0552	^{1}MLCT/^{1}ILCT/^{1}LLCT
S5	HOMO–3→LUMO	38.0	463 (2.68)	0.0408	^{1}MLCT/^{1}ILCT
	HOMO–2→LUMO	23.0			^{1}MLCT
S6	HOMO→LUMO+3	66.6	435 (2.85)	0.0563	^{1}MLCT/^{1}ILCT/^{1}LLCT
S7	HOMO–2→LUMO+1	54.7	430 (2.88)	0.0011	^{1}MLCT
S8	HOMO→LUMO+4	74.5	428 (2.90)	0.0390	^{1}MLCT/^{1}ILCT/^{1}LLCT



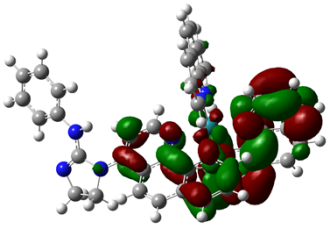
LUMO+4



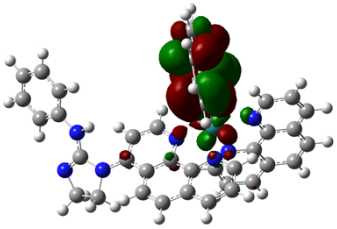
LUMO+3



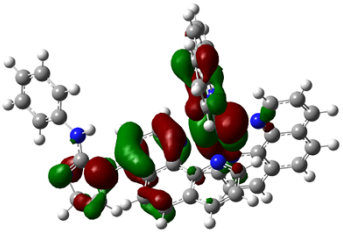
LUMO+2



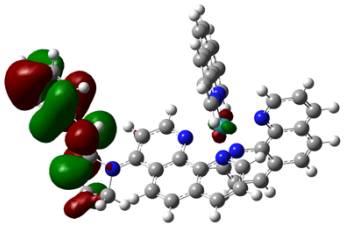
LUMO+1



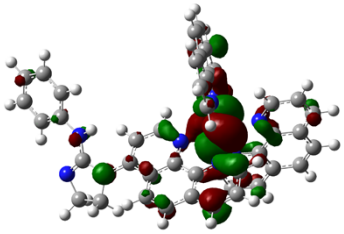
LUMO



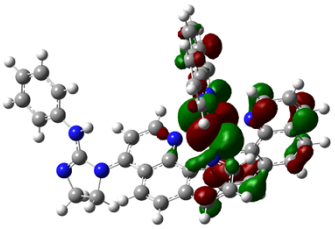
HOMO



HOMO–1



HOMO–2



HOMO–3