

Closing and Coupling: Metal Linked Biliazine Dimers

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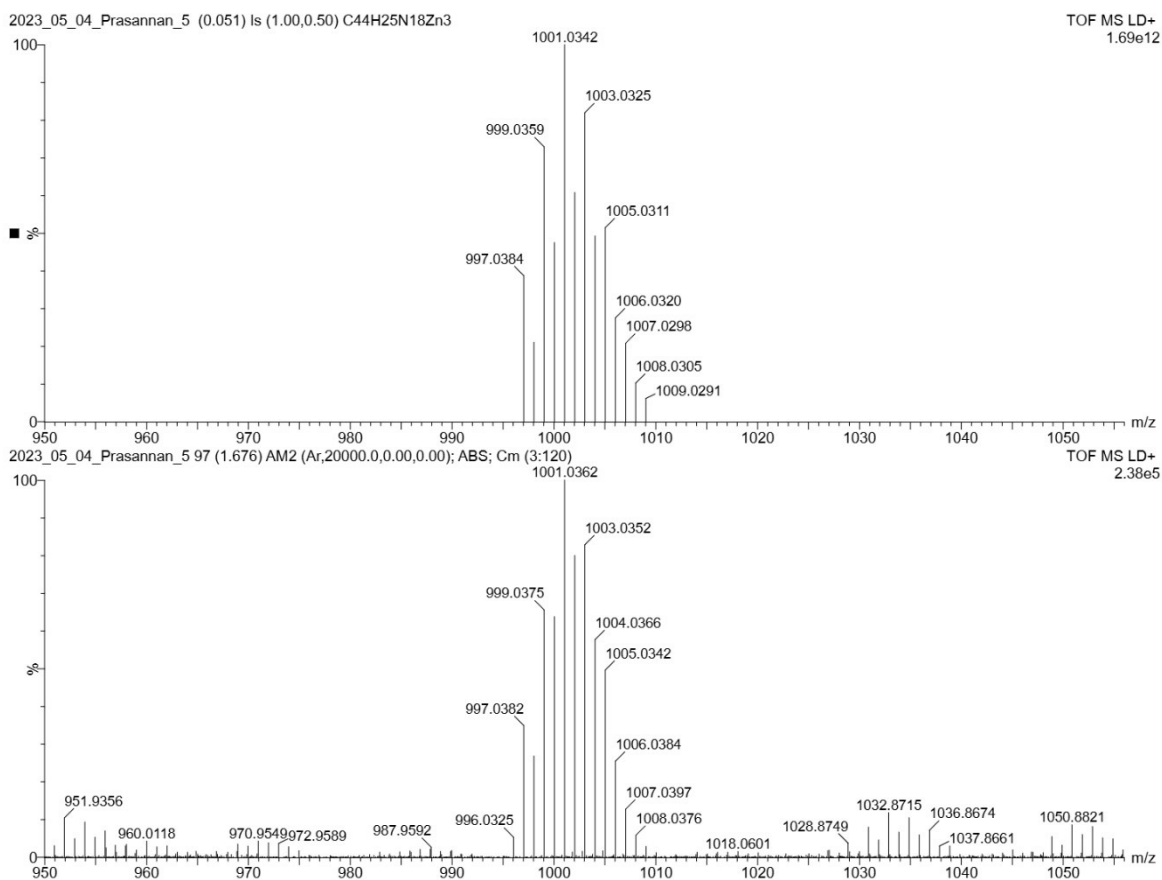


Figure S1: Mass spectra of **1**. Top: calculated spectrum. Bottom: experimental spectrum.

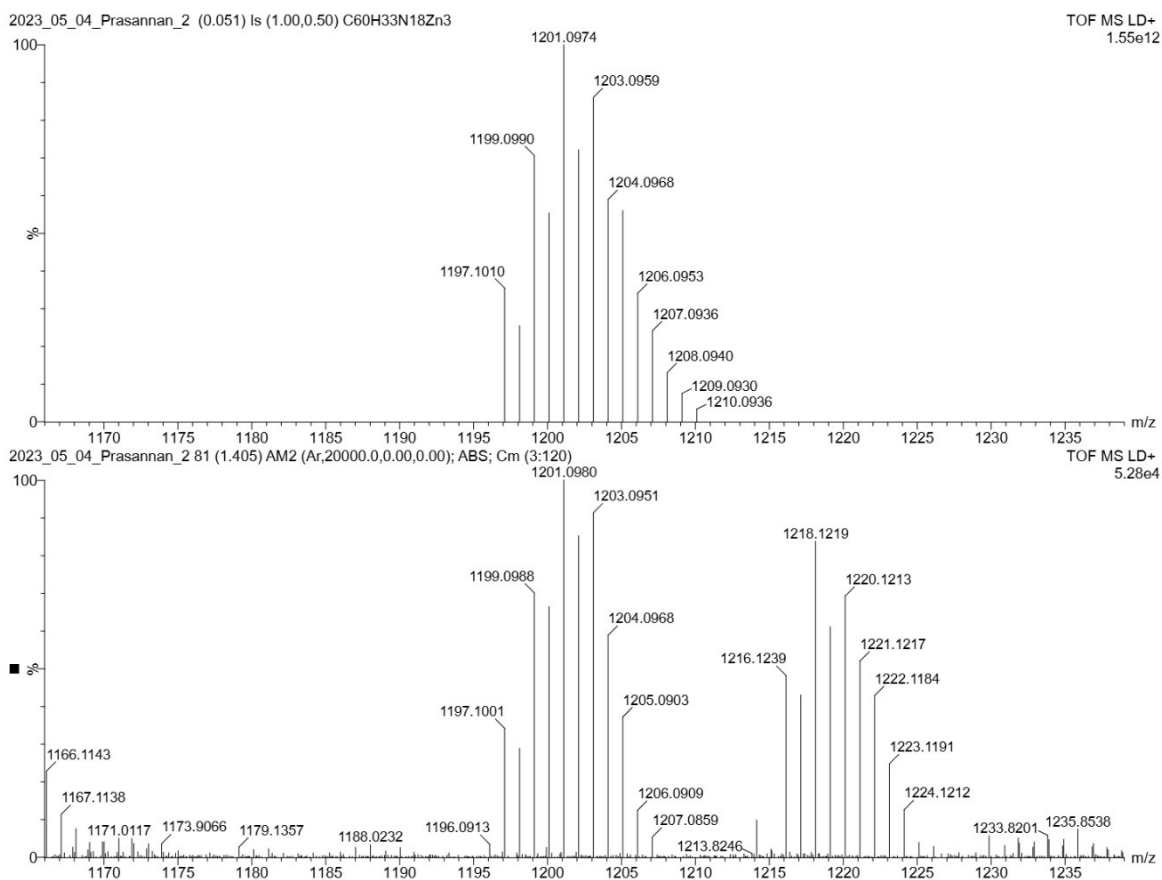


Figure S2: Mass spectra of **2**. Top: calculated spectrum. Bottom: experimental spectrum.

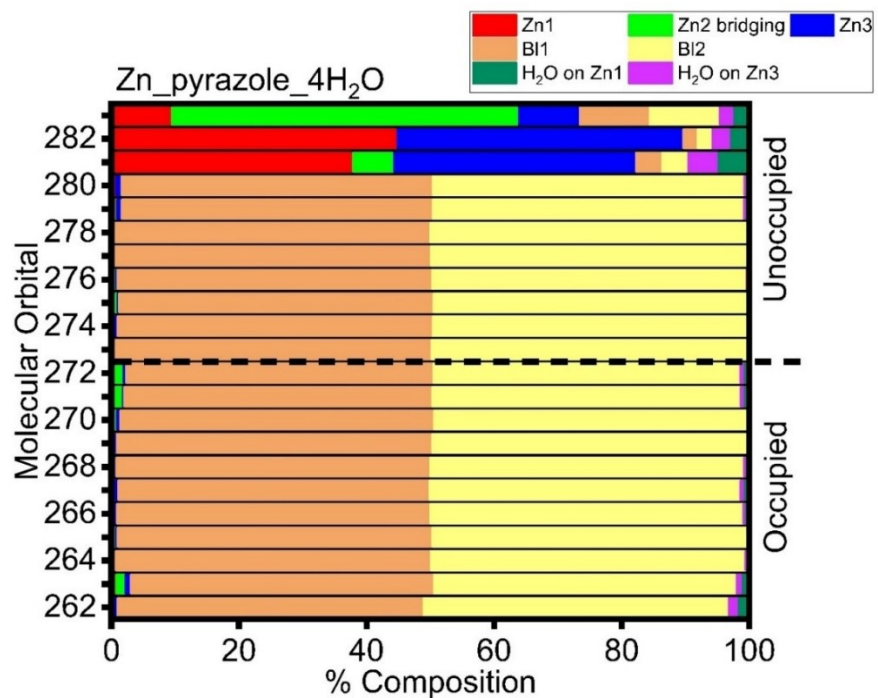


Figure S3: Orbital composition chart for compound 1.

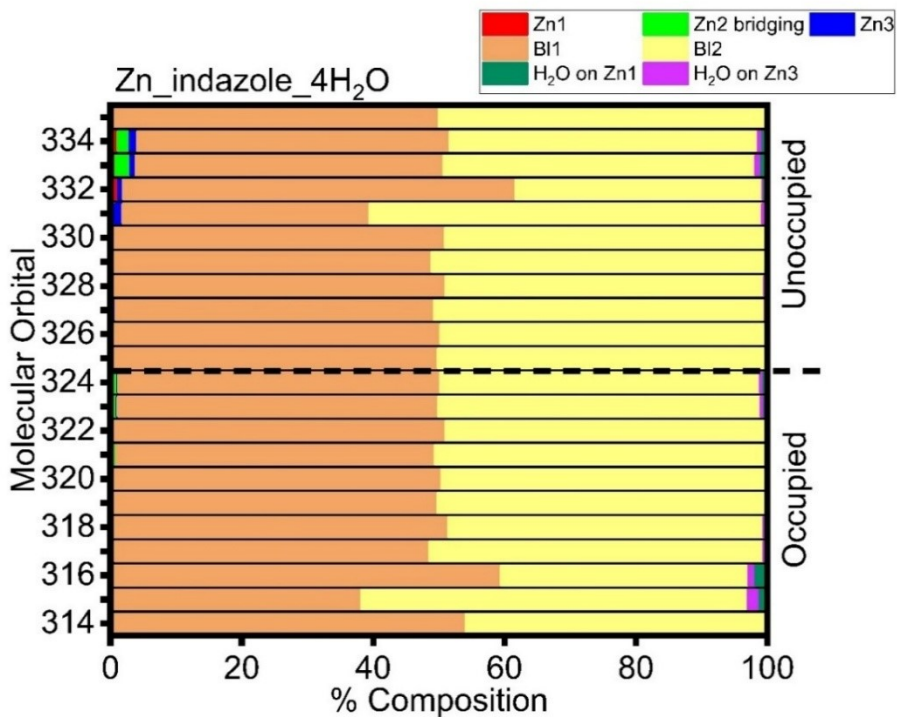


Figure S4: Orbital composition chart for compound 2.

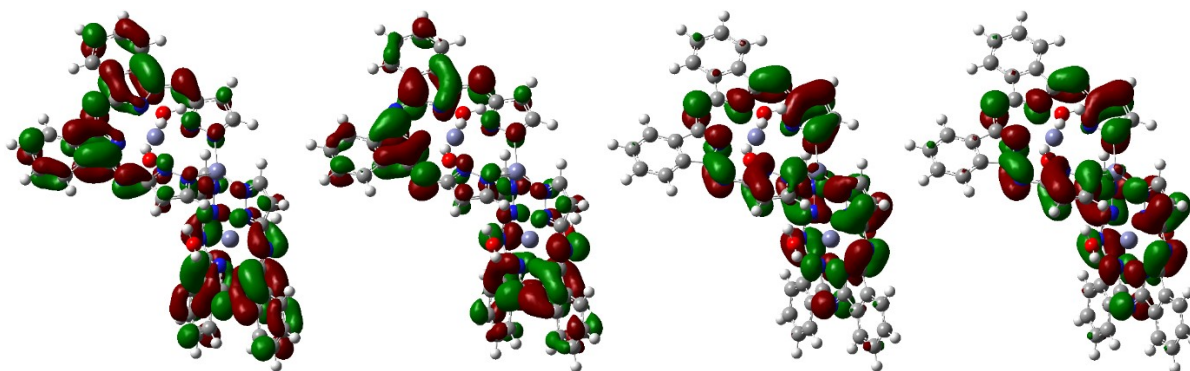


Figure S5: Frontier orbital structures for compound 1. From left to right: LUMO+1, LUMO, HOMO, HOMO-1.

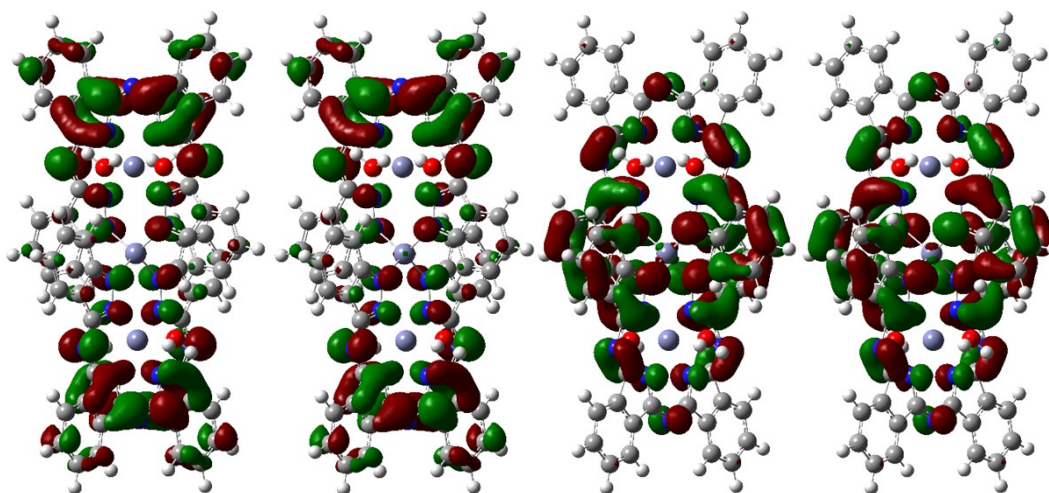


Figure S6: Frontier orbital structures for compound 2. From left to right: LUMO+1, LUMO, HOMO, HOMO-1.

Compound	1a	1b	2
CCDC number	2531176	2531175	2531177
Empirical formula	C53 H47 N21 O4 Zn3	C56 H52 N22 O4 Zn3	C72 H64 N22 O6 Zn3
Formula weight	1238.22	1293.30	1529.56
Temperature (K)	100(2)	100(2)	100(2)
Wavelength (Å)	0.71073	0.71073	1.54178
Crystal system	Triclinic	Monoclinic	Monoclinic
Space group	P-1	C2/c	C2/c
a/ Å	11.064(2)	29.964(4)	25.5950(13)
b/ Å	13.595(3)	11.8314(15)	17.0614(8)
c/ Å	17.394(4)	16.308(2)	20.0999(10)
α(°)	91.281(8)	90	90
β(°)	92.138(7)	102.336(6)	124.932(2)
γ(°)	92.972(7)	90	90
Volume (Å³)	2610.1(10)	5648.0(13)	7196.0(6)
Z	2	4	4
Dc (mg/m³)	1.575	1.521	1.412
Abs. Coef. (mm⁻¹)	1.438	1.333	1.724
F(000)	1268	2656	3152
Reflns collected	116814	54145	88274
Indep. reflns	13280 [R(int) = 0.0872]	5050 [R(int) = 0.1283]	6383 [R(int) = 0.1461]
Data/restraints/parameters	13280 / 0 / 737	5050 / 0 / 388	6383 / 147 / 504
GOF on F²	1.029	1.101	1.084
Final R1 (I>2σ(I))	0.0387	0.0737	0.0808
Final wR2 (I>2σ(I))	0.0982	0.1587	0.1803
R1 (all data)	0.0506	0.0952	0.1013
wR2 (all data)	0.1079	0.1665	0.1918

Table S1: X-ray data collection and structure parameters.

Table S2: B3LYP TDDFT-predicted energies and expansion coefficients for compound **1**.

Index	Energy.cm ⁻¹	Wavelength h	Osc.Strength	Contributions Zn_pyrazole_4H ₂ O/B3LYP/ 6-311+G for Zn, 6-311G(d) for C, N, O, H
0	18799.171	531.938	1.95E-01	53.7% HOMO => LUMO, 45.6% H-1 => L+1
1	18920.96	528.514	3.81E-01	54.6% H-1 => LUMO, 44.8% HOMO => L+1
2	19919.475	502.021	2.00E-04	53.9% H-1 => L+1, 45.6% HOMO => LUMO
3	19921.088	501.981	1.48E-02	54.6% HOMO => L+1, 44.8% H-1 => LUMO
4	22303.65	448.357	1.06E+00	62.1% H-2 => LUMO, 36.4% H-3 => L+1
5	22549.649	443.466	4.01E-01	55.1% H-2 => L+1, 42.6% H-3 => LUMO
6	23201.345	431.01	1.60E-03	56.0% H-3 => LUMO, 43.4% H-2 => L+1
7	23217.476	430.71	2.52E-02	62.7% H-3 => L+1, 36.7% H-2 => LUMO
8	26534.834	376.863	1.33E-02	21.8% H-5 => L+1, 12.7% H-4 => LUMO, 10.8% H-8 => LUMO, 9.91% H-6 => LUMO, 8.11% H-16 => LUMO, 7.37% H-10 => L+1, 6.26% H-12 => L+1, 5.45% H-11 => LUMO, 4.64% H-7 => L+1, 3.11% H-17 => L+1, 2.65% H-14 => L+1, 2.05% H-18 => L+1
9	26536.447	376.84	2.36E-02	23.8% H-5 => LUMO, 11.6% H-4 => L+1, 10.4% H-6 => L+1, 10.1% H-8 => L+1, 7.74% H-16 => L+1, 7.72% H-10 => LUMO, 6.35% H-12 => LUMO, 5.25% H-11 => L+1, 4.11% H-7 => LUMO, 3.19% H-17 => LUMO, 2.66% H-14 => LUMO, 2.04% H-18 => LUMO
10	26657.43	375.13	6.71E-02	35.7% H-7 => L+1, 30.5% H-6 => LUMO, 9.79% H-8 => LUMO, 7.00% H-4 => LUMO, 3.66% H-5 => L+1, 3.20% H-15 => LUMO, 2.94% H-17 => L+1
11	26664.689	375.028	3.50E-03	38.7% H-7 => LUMO, 28.3% H-6 => L+1, 9.97% H-8 => L+1, 7.05% H-4 => L+1, 3.75% H-5 => LUMO, 2.64% H-15 => L+1, 2.53% H-17 => LUMO
12	26927.626	371.366	1.40E-03	42.6% H-15 => LUMO, 35.3% H-17 => L+1, 5.06% H-5 => L+1, 4.76% H-6 => LUMO, 3.73% H-13 => LUMO
13	26930.852	371.321	9.00E-04	42.0% H-15 => L+1, 36.8% H-17 => LUMO, 5.26% H-5 => LUMO, 3.97% H-6 => L+1, 3.73% H-13 => L+1
14	27111.521	368.847	9.00E-03	26.2% H-16 => L+1, 13.0% H-12 => LUMO, 12.9% H-14 => LUMO, 9.52% H-8 => L+1, 8.87% H-5 => LUMO, 7.58% H-9 => LUMO, 7.43% H-18 => LUMO, 5.41% H-11 => L+1, 2.07% H-6 => L+1
15	27113.94	368.814	1.17E-02	27.0% H-16 => LUMO, 12.6% H-12 => L+1, 12.5% H-14 => L+1, 9.81% H-8 => LUMO, 8.62% H-5 => L+1, 7.27% H-18 => L+1, 7.20% H-9 => L+1, 5.56%

				H-11 => LUMO, 2.45% H-6 => LUMO
16	27589.807	362.453	3.00E-04	46.0% H-4 => LUMO, 20.6% H-8 => LUMO, 12.0% H-9 => L+1, 8.37% H-10 => L+1, 7.63% H-5 => L+1
17	27613.197	362.146	6.30E-03	42.8% H-4 => L+1, 19.9% H-8 => L+1, 12.9% H-9 => LUMO, 9.91% H-10 => LUMO, 9.06% H-5 => LUMO
18	28190.69	354.727	1.70E-03	26.7% H-10 => LUMO, 14.7% H-5 => LUMO, 10.5% H-19 => L+1, 10.2% H-9 => LUMO, 7.35% H-18 => LUMO, 6.84% H-14 => LUMO, 5.41% H-12 => LUMO, 4.51% H-4 => L+1, 4.42% H-16 => L+1, 2.53% H-11 => L+1
19	28207.628	354.514	2.52E-02	24.6% H-10 => L+1, 14.7% H-5 => L+1, 12.7% H-19 => LUMO, 9.01% H-18 => L+1, 7.92% H-9 => L+1, 6.85% H-14 => L+1, 5.49% H-12 => L+1, 4.08% H-16 => LUMO, 3.32% H-4 => LUMO, 2.27% H-11 => LUMO
20	28437.496	351.648	1.31E-01	25.0% H-18 => L+1, 19.4% H-19 => LUMO, 12.0% H-11 => LUMO, 8.41% H-10 => L+1, 8.18% H-5 => L+1, 5.43% H-1 => L+3, 5.03% H-9 => L+1, 3.39% H-4 => LUMO, 3.14% HOMO => L+2
21	28452.014	351.469	5.40E-03	30.6% H-18 => LUMO, 23.0% H-19 => L+1, 10.4% H-11 => L+1, 6.58% H-10 => LUMO, 6.23% H-5 => LUMO, 4.31% H-9 => LUMO, 3.45% H-4 => L+1, 3.01% H-12 => LUMO, 2.71% H-1 => L+2
22	28932.72	345.629	2.00E-04	46.2% H-9 => LUMO, 24.2% H-4 => L+1, 15.0% H-7 => LUMO, 9.28% H-5 => LUMO, 2.07% H-11 => L+1
23	28948.045	345.446	3.06E-01	39.9% H-9 => L+1, 19.2% H-4 => LUMO, 11.0% H-7 => L+1, 7.78% H-5 => L+1, 7.17% H-1 => L+3, 7.05% HOMO => L+2, 2.92% H-11 => LUMO, 2.22% H-14 => L+1
24	28994.825	344.889	4.56E-01	40.6% H-13 => LUMO, 26.2% H-12 => L+1, 18.6% H-14 => L+1, 5.00% H-15 => LUMO
25	28994.825	344.889	2.92E-01	40.0% H-13 => L+1, 26.3% H-12 => LUMO, 21.3% H-14 => LUMO, 4.89% H-15 => L+1
26	29048.058	344.257	9.98E-01	38.6% HOMO => L+2, 30.3% H-1 => L+3, 8.09% H-9 => L+1, 5.37% H-18 => L+1, 5.29% H-7 => L+1, 4.19% H-19 => LUMO, 2.15% H-5 => L+1, 2.10% H-4 => LUMO
27	29259.375	341.771	6.30E-03	32.7% H-6 => LUMO, 29.1% H-11 => LUMO, 18.3% H-5 => L+1, 4.21% H-16 => LUMO, 3.32% H-10 => L+1, 2.49% H-8 => LUMO, 2.38% H-7 => L+1, 2.17% H-4 => LUMO
28	29279.539	341.535	5.56E-02	33.1% H-6 => L+1, 27.8% H-11 => L+1, 16.3% H-5 => LUMO, 4.18% H-16 =>

				L+1, 3.95% H-1 => L+2, 3.49% H-10 => LUMO, 2.90% HOMO => L+3
29	29331.965	340.925	4.92E-01	42.0% H-1 => L+2, 40.4% HOMO => L+3, 2.87% H-18 => LUMO, 2.33% H-19 => L+1, 2.07% H-6 => L+1
30	29940.107	334	4.10E-03	51.6% H-1 => L+3, 46.5% HOMO => L+2
31	29950.592	333.883	1.00E-04	51.5% HOMO => L+3, 46.7% H-1 => L+2
32	30153.037	331.642	0.00E+00	34.3% H-7 => L+1, 31.4% H-8 => LUMO, 12.8% H-9 => L+1, 10.2% H-6 => LUMO, 6.07% H-11 => LUMO, 2.12% H-10 => L+1
33	30155.457	331.615	0.00E+00	33.3% H-8 => L+1, 32.7% H-7 => LUMO, 12.2% H-9 => LUMO, 10.3% H-6 => L+1, 6.44% H-11 => L+1
34	30551.475	327.316	0.00E+00	36.7% H-10 => L+1, 31.7% H-11 => LUMO, 12.4% H-8 => LUMO, 4.93% H-6 => LUMO, 4.61% H-14 => L+1, 3.24% H-9 => L+1, 2.91% H-12 => L+1
35	30554.701	327.282	3.00E-04	34.9% H-10 => LUMO, 34.0% H-11 => L+1, 12.2% H-8 => L+1, 5.04% H-6 => L+1, 4.56% H-14 => LUMO, 3.06% H-9 => LUMO, 2.90% H-12 => LUMO
36	31263.663	319.86	2.00E-04	47.9% H-16 => LUMO, 18.9% H-12 => L+1, 17.0% H-14 => L+1, 7.29% H-19 => LUMO, 3.38% H-10 => L+1
37	31277.374	319.72	1.00E-04	49.2% H-16 => L+1, 18.0% H-12 => LUMO, 16.7% H-14 => LUMO, 7.17% H-19 => L+1, 3.28% H-10 => LUMO
38	31629.838	316.157	7.65E-02	51.5% H-2 => L+2, 40.1% H-3 => L+3
39	31661.294	315.843	1.46E-01	48.4% H-2 => L+3, 41.8% H-3 => L+2
40	31870.998	313.765	1.43E-02	29.7% H-17 => L+1, 24.4% H-13 => LUMO, 20.3% H-15 => LUMO, 10.8% H-14 => L+1, 6.91% H-12 => L+1
41	31872.611	313.749	4.00E-03	30.1% H-17 => LUMO, 25.1% H-13 => L+1, 21.5% H-15 => L+1, 10.2% H-14 => LUMO, 6.55% H-12 => LUMO
42	31991.981	312.578	2.70E-03	25.7% H-13 => L+1, 21.9% H-15 => L+1, 16.3% H-14 => LUMO, 16.2% H-17 => LUMO, 15.5% H-12 => LUMO
43	31993.595	312.563	4.50E-03	24.2% H-13 => LUMO, 21.1% H-15 => LUMO, 17.0% H-14 => L+1, 16.7% H-17 => L+1, 16.1% H-12 => L+1
44	32519.468	307.508	3.43E-02	48.7% H-20 => LUMO, 41.6% H-21 => L+1, 2.31% H-18 => L+1
45	32566.248	307.066	1.42E-02	44.3% H-20 => L+1, 42.5% H-21 => LUMO, 3.67% H-18 => LUMO
46	32706.589	305.749	1.39E-02	47.4% H-19 => LUMO, 43.1% H-18 => L+1, 3.25% H-16 => LUMO
47	32713.848	305.681	1.38E-02	48.0% H-19 => L+1, 40.4% H-18 => LUMO, 3.21% H-16 => L+1, 2.97% H-21 => LUMO

48	33164.712	301.525	1.27E-02	27.9% H-25 => L+1, 20.4% H-22 => LUMO, 20.1% H-24 => LUMO, 8.78% H-3 => L+2, 5.70% H-2 => L+3, 4.69% H-17 => L+1, 3.09% H-23 => L+1, 2.37% H-18 => L+2, 2.10% H-19 => L+3
49	33165.518	301.518	1.70E-03	26.6% H-25 => LUMO, 18.6% H-22 => L+1, 18.3% H-24 => L+1, 12.5% H-3 => L+3, 7.73% H-2 => L+2, 4.21% H-17 => LUMO, 2.99% H-23 => LUMO, 2.20% H-18 => L+3
50	33238.108	300.859	6.00E-03	44.5% H-3 => L+2, 40.3% H-2 => L+3, 4.58% H-25 => L+1, 3.54% H-22 => LUMO, 3.32% H-24 => LUMO
51	33242.947	300.816	4.00E-04	43.2% H-3 => L+3, 35.8% H-2 => L+2, 6.52% H-25 => LUMO, 4.96% H-22 => L+1, 4.40% H-24 => L+1

Table S3: B3LYP TDDFT-predicted energies and expansion coefficients for compound **2**.

Index	Energy.cm ⁻¹	Wavelength h	Osc.Strength	Contributions Zn_indazole_4H₂O /B3LYP/ 6-311+G for Zn, 6-311G(d) for C, N, O, H
0	15060.791	663.976	2.31E-01	82.8% HOMO => LUMO, 17.0% H-1 => L+1
1	15180.161	658.755	3.02E-01	62.1% H-1 => LUMO, 37.7% HOMO => L+1
2	15799.595	632.928	5.90E-03	62.1% HOMO => L+1, 37.7% H-1 => LUMO
3	15893.155	629.202	4.05E-02	82.8% H-1 => L+1, 17.0% HOMO => LUMO
4	17436.094	573.523	1.39E+00	82.0% H-2 => LUMO, 17.3% H-3 => L+1
5	17644.991	566.733	0.00E+00	95.2% H-3 => LUMO, 3.71% H-2 => L+1
6	17902.282	558.588	1.44E-01	82.2% H-3 => L+1, 17.5% H-2 => LUMO
7	17938.577	557.458	0.00E+00	95.2% H-2 => L+1, 4.01% H-3 => LUMO
8	24410.37	409.662	1.95E+00	64.5% HOMO => L+2, 30.3% H-1 => L+3
9	24791.063	403.371	0.00E+00	58.8% HOMO => L+3, 29.4% H-1 => L+2, 4.62% H-5 => LUMO, 4.53% H-4 => L+1
10	25109.652	398.253	5.35E-02	61.5% H-1 => L+3, 31.7% HOMO => L+2, 3.41% H-1 => L+2
11	25114.492	398.176	2.80E-03	59.6% H-1 => L+2, 33.9% HOMO => L+3, 3.59% H-1 => L+3
12	25361.297	394.302	5.42E-02	49.1% H-6 => LUMO, 31.5% H-7 => L+1, 4.35% H-8 => LUMO, 3.62% H-9 => L+1, 3.26% H-2 => L+2, 2.91% H-3 => L+3
13	25365.33	394.239	6.22E-02	47.8% H-7 => LUMO, 32.7% H-6 => L+1, 4.21% H-9 => LUMO, 3.82% H-8 => L+1, 3.19% H-3 => L+2, 3.01% H-2 => L+3
14	25630.687	390.157	5.80E-03	68.6% H-4 => LUMO, 24.1% H-5 => L+1, 3.21% H-1 => L+3
15	25714.568	388.885	0.00E+00	50.6% H-5 => LUMO, 35.6% H-4 => L+1, 5.97% H-1 => L+2, 4.02% HOMO => L+3
16	26317.064	379.982	3.78E-02	37.7% H-2 => L+2, 28.7% H-3 => L+3, 15.4% H-6 => LUMO, 9.42% H-8 => LUMO, 6.29% H-9 => L+1
17	26330.776	379.784	5.68E-02	35.0% H-3 => L+2, 33.0% H-2 => L+3, 13.4% H-7 => LUMO, 9.28% H-9 => LUMO, 6.10% H-8 => L+1
18	26463.857	377.874	0.00E+00	56.2% H-4 => L+1, 43.0% H-5 => LUMO
19	26492.893	377.46	3.80E-03	56.8% H-5 => L+1, 27.9% H-4 => LUMO, 8.30% H-10 => LUMO, 5.56% H-11 => L+1
20	26616.296	375.71	2.92E-02	39.8% H-7 => L+1, 31.0% H-6 => LUMO, 6.34% H-2 => L+2, 6.29% H-8 =>

				LUMO, 5.21% H-3 => L+3, 3.13% H-13 => LUMO, 2.65% H-6 => L+1
21	26620.329	375.653	0.00E+00	48.8% H-11 => LUMO, 40.2% H-10 => L+1, 2.70% H-4 => L+1, 2.56% H-14 => L+1, 2.34% H-15 => LUMO
22	26620.329	375.653	2.33E-02	45.9% H-6 => L+1, 35.3% H-7 => LUMO, 3.95% H-9 => LUMO, 3.54% H-3 => L+2, 3.09% H-2 => L+3, 2.31% H-7 => L+1, 2.02% H-12 => LUMO
23	26638.073	375.403	1.10E-02	40.8% H-10 => LUMO, 35.3% H-11 => L+1, 16.7% H-5 => L+1, 2.40% H-14 => LUMO
24	26685.66	374.733	0.00E+00	57.0% H-18 => LUMO, 39.1% H-21 => L+1
25	26716.309	374.303	8.21E-02	27.0% H-9 => LUMO, 22.0% H-8 => L+1, 15.8% H-6 => L+1, 8.84% H-3 => L+2, 8.69% H-13 => L+1, 8.66% H-12 => LUMO, 5.91% H-2 => L+3
26	26722.761	374.213	0.00E+00	51.7% H-18 => L+1, 44.5% H-21 => LUMO
27	26733.247	374.066	4.60E-02	24.1% H-7 => L+1, 23.8% H-8 => LUMO, 21.3% H-9 => L+1, 8.21% H-12 => L+1, 7.24% H-13 => LUMO, 5.89% H-2 => L+2, 5.28% H-3 => L+3
28	27165.56	368.113	1.00E-04	44.2% H-2 => L+3, 40.1% H-3 => L+2, 7.65% H-3 => L+3, 7.30% H-2 => L+2
29	27167.979	368.08	0.00E+00	47.8% H-3 => L+3, 36.7% H-2 => L+2, 7.80% H-2 => L+3, 7.10% H-3 => L+2
30	27667.237	361.438	5.40E-03	36.8% H-20 => LUMO, 33.4% H-19 => L+1, 8.93% H-22 => LUMO, 7.55% H-23 => L+1, 4.62% H-19 => LUMO, 3.38% H-20 => L+1
31	27668.85	361.417	3.20E-03	37.6% H-19 => LUMO, 33.0% H-20 => L+1, 9.35% H-23 => LUMO, 7.04% H-22 => L+1, 4.65% H-20 => LUMO, 3.30% H-19 => L+1
32	28030.993	356.748	3.74E-01	37.8% H-12 => LUMO, 26.9% H-13 => L+1, 17.3% H-9 => LUMO, 4.72% H-17 => L+1, 4.57% H-16 => LUMO
33	28033.412	356.717	2.90E-01	37.8% H-13 => LUMO, 27.0% H-12 => L+1, 16.5% H-8 => LUMO, 5.01% H-16 => L+1, 4.36% H-17 => LUMO
34	28368.132	352.508	3.06E-02	48.1% H-8 => L+1, 21.2% H-9 => LUMO, 13.1% H-8 => LUMO, 10.6% H-9 => L+1, 2.08% H-13 => L+1
35	28370.552	352.478	2.87E-02	48.7% H-9 => L+1, 21.0% H-8 => LUMO, 13.0% H-9 => LUMO, 10.6% H-8 => L+1, 2.02% H-12 => L+1
36	28461.693	351.349	1.74E-02	39.8% H-23 => LUMO, 34.5% H-22 => L+1, 9.46% H-19 => LUMO, 7.11% H-20 => L+1
37	28464.919	351.31	3.70E-03	40.8% H-22 => LUMO, 34.3% H-23 => L+1, 8.62% H-20 => LUMO, 8.23% H-19 => L+1
38	28744.793	347.889	2.85E-01	58.3% H-14 => LUMO, 32.9% H-15 => L+1, 4.63% H-10 => LUMO

39	28791.573	347.324	0.00E+00	51.4% H-15 => LUMO, 40.3% H-14 => L+1, 2.62% H-11 => LUMO, 2.09% H-10 => L+1
40	29048.864	344.248	1.00E-01	46.2% H-17 => LUMO, 35.2% H-16 => L+1, 3.77% H-13 => LUMO, 3.61% H-9 => L+1, 3.07% H-12 => L+1, 3.04% H-17 => L+1
41	29050.477	344.228	1.26E-01	44.9% H-16 => LUMO, 35.9% H-17 => L+1, 3.77% H-12 => LUMO, 3.45% H-8 => L+1, 3.13% H-16 => L+1, 3.09% H-13 => L+1
42	29721.531	336.456	0.00E+00	47.7% H-10 => L+1, 38.0% H-11 => LUMO, 7.46% H-14 => L+1, 5.83% H-15 => LUMO
43	29736.049	336.292	3.20E-03	48.8% H-11 => L+1, 37.1% H-10 => LUMO, 10.5% H-15 => L+1, 2.42% H-14 => LUMO
44	30392.584	329.028	0.00E+00	47.2% H-14 => L+1, 37.7% H-15 => LUMO, 6.87% H-10 => L+1, 6.72% H-11 => LUMO
45	30403.876	328.905	4.00E-04	51.4% H-15 => L+1, 34.3% H-14 => LUMO, 6.73% H-11 => L+1, 5.88% H-10 => LUMO
46	30604.708	326.747	1.00E-04	47.4% H-12 => L+1, 37.3% H-13 => LUMO, 5.96% H-12 => LUMO, 5.53% H-13 => L+1
47	30607.127	326.721	4.00E-04	47.9% H-13 => L+1, 36.9% H-12 => LUMO, 5.83% H-13 => LUMO, 5.63% H-12 => L+1
48	30778.924	324.898	1.22E-01	60.7% HOMO => L+4, 34.0% H-1 => L+5
49	30795.055	324.727	8.62E-02	50.3% HOMO => L+5, 44.5% H-1 => L+4
50	31538.698	317.071	1.49E-02	44.5% H-19 => L+1, 39.2% H-20 => LUMO, 7.09% H-19 => LUMO, 6.96% H-20 => L+1
51	31542.731	317.03	1.57E-02	46.1% H-20 => L+1, 38.1% H-19 => LUMO, 7.08% H-20 => LUMO, 6.87% H-19 => L+1
52	31629.032	316.165	0.00E+00	47.9% H-21 => LUMO, 44.9% H-18 => L+1, 4.81% H-26 => L+1
53	31644.356	316.012	0.00E+00	51.5% H-21 => L+1, 39.2% H-18 => LUMO, 6.48% H-26 => LUMO
54	31781.471	314.649	4.00E-04	33.8% H-16 => LUMO, 33.7% H-17 => L+1, 18.9% H-16 => L+1, 10.2% H-17 => LUMO
55	31783.89	314.625	3.00E-04	33.2% H-17 => LUMO, 33.0% H-16 => L+1, 19.5% H-17 => L+1, 10.1% H-16 => LUMO
56	31804.861	314.417	4.00E-04	47.2% H-1 => L+4, 42.2% HOMO => L+5, 4.56% H-1 => L+10, 3.04% HOMO => L+11

57	31822.605	314.242	6.00E-04	58.4% H-1 => L+5, 31.9% HOMO => L+4, 5.10% HOMO => L+10, 2.79% H-1 => L+11
58	32227.495	310.294	6.79E-02	39.6% HOMO => L+6, 31.9% H-1 => L+7, 12.2% H-3 => L+4, 11.4% H-2 => L+5
59	32262.984	309.953	0.00E+00	41.4% HOMO => L+7, 33.5% H-1 => L+6, 11.8% H-2 => L+4, 9.62% H-3 => L+5
60	32768.693	305.169	3.00E-03	45.7% HOMO => L+9, 36.9% H-1 => L+8, 3.46% H-3 => L+10, 3.05% H-2 => L+11
61	32779.179	305.072	0.00E+00	58.3% HOMO => L+8, 27.0% H-1 => L+9, 3.58% H-2 => L+10, 2.38% H-3 => L+11
62	33072.764	302.364	2.20E-03	33.1% H-22 => L+1, 23.8% H-22 => LUMO, 21.5% H-23 => LUMO, 17.1% H-23 => L+1
63	33075.184	302.341	1.70E-03	26.8% H-23 => L+1, 19.0% H-23 => LUMO, 17.1% H-22 => LUMO, 13.9% H-22 => L+1, 9.40% H-26 => LUMO, 6.74% H-27 => L+1
64	33075.184	302.341	4.00E-04	38.8% H-26 => LUMO, 27.8% H-27 => L+1, 6.61% H-23 => L+1, 5.28% H-21 => L+1, 4.51% H-23 => LUMO, 4.24% H-22 => LUMO, 3.25% H-22 => L+1
65	33096.154	302.15	0.00E+00	44.7% H-26 => L+1, 39.8% H-27 => LUMO, 4.91% H-21 => LUMO, 2.48% H-22 => L+3, 2.48% H-23 => L+2
66	33185.682	301.335	3.34E-02	46.6% HOMO => L+10, 31.4% H-1 => L+11, 5.11% H-2 => L+8, 4.19% H-3 => L+9
67	33196.167	301.24	2.69E-02	42.3% HOMO => L+11, 36.0% H-1 => L+10, 4.82% H-2 => L+9, 4.69% H-3 => L+8
68	33222.783	300.998	2.64E-02	39.5% H-3 => L+4, 32.7% H-2 => L+5, 13.6% HOMO => L+6, 7.15% H-1 => L+7, 4.30% HOMO => L+9
69	33228.429	300.947	0.00E+00	44.8% H-2 => L+4, 29.5% H-3 => L+5, 12.5% HOMO => L+7, 7.24% H-1 => L+6, 2.88% HOMO => L+8