

Theoretical Fingerprinting of the Photophysical Properties of Four Firefly Bioluminophores

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Supplementary Data:

Table S1. Cartesian geometries of firefly oxyluciferin, obtained at the PBE0/cc-pVDZ level of theory.

Table S2. Cartesian geometries of BtOxyLH₂, obtained at the PBE0/cc-pVDZ level of theory.

Table S3. Cartesian geometries of AminoSeOxyLH₂, obtained at the PBE0/cc-pVDZ level of theory.

Table S4. Cartesian geometries of CALOxyLH₂, obtained at the PBE0/cc-pVDZ level of theory.

Table S1. Cartesian geometries of firefly oxyluciferin, obtained at the PBE0/cc-pVDZ level of theory.

O	-5.54538	-0.54778	0.00002
C	-4.35505	-0.18775	0.00000
C	-3.24556	-1.12324	0.00003
C	-1.95169	-0.66382	0.00001
C	-1.62761	0.74139	-0.00003
C	-2.69992	1.67924	-0.00006
C	-3.98864	1.23617	-0.00004
N	-0.32788	1.05299	-0.00004
C	0.43583	-0.02830	0.00002
S	-0.45081	-1.56686	0.00003
C	1.84716	0.01652	0.00004
S	2.62134	1.63226	-0.00002
C	4.22621	0.80956	0.00016
C	3.96107	-0.71207	-0.00002
N	2.62544	-1.03725	0.00007
O	4.88525	-1.50252	-0.00022
H	-3.48959	-2.18721	0.00006
H	-2.45200	2.74393	-0.00009
H	-4.82920	1.93524	-0.00007
H	4.81451	1.07369	0.89170
H	4.81493	1.07391	-0.89102

Table S2. Cartesian geometries of BtOxyLH₂, obtained at the PBE0/cc-pVDZ level of theory.

O	-5.56441	-0.72588	0.00000
C	-4.40211	-0.28344	-0.00001
C	-3.22818	-1.13573	-0.00002
C	-1.96711	-0.59210	-0.00002
C	-1.73771	0.82866	0.00000
C	-2.87709	1.68713	0.00003
C	-4.13414	1.16160	0.00002
C	-0.38395	1.15518	0.00000
C	0.47704	0.05599	0.00003
S	-0.43746	-1.46113	-0.00001
C	1.88012	0.04553	0.00008
S	2.76481	1.62248	-0.00010
C	4.31916	0.71495	0.00011
C	3.96349	-0.79106	0.00002
N	2.61807	-1.04136	0.00008
O	4.85052	-1.62479	-0.00009
H	-3.39553	-2.21482	-0.00003
H	-2.72200	2.77096	0.00004
H	-5.01912	1.80366	0.00003
H	4.91963	0.94507	0.89265
H	4.91996	0.94515	-0.89217
H	-0.01316	2.18284	0.00002

N	5.94429	0.42013	-0.05827
C	4.60754	0.08513	-0.00190
C	3.62001	1.07700	-0.00348
C	2.28345	0.68551	-0.00639
C	1.90189	-0.68110	-0.00427
C	2.90548	-1.66549	-0.00175
C	4.22903	-1.28413	-0.00187
N	0.55648	-0.91546	-0.00224
C	-0.10222	0.20589	-0.00291
S	0.85888	1.68012	-0.00632
C	-1.54856	0.27621	-0.00052
Se	-2.51538	-1.36966	0.00100
C	-4.07276	-0.21361	0.00399
C	-3.58103	1.24312	0.00359
N	-2.18512	1.39426	0.00082
O	-4.35108	2.16901	0.00574
H	3.89887	2.13226	-0.00583
H	2.61892	-2.71792	0.00109
H	5.01324	-2.04465	-0.00596
H	-4.68957	-0.38813	0.89637
H	-4.69172	-0.38702	-0.88761
H	6.18262	1.35522	0.24820
H	6.59067	-0.27906	0.28571

C	2.03558	-0.04555	0.00152
S	2.63711	-1.68400	0.42325
C	4.30987	-1.11985	0.08291
C	4.21044	0.36729	-0.30400
N	2.89712	0.85328	-0.31873
O	5.18432	1.01936	-0.57587
H	4.76371	-1.68313	-0.74499
H	4.94584	-1.22757	0.97259
C	0.59301	0.17388	0.04366
C	-0.28162	-0.87420	-0.06782
C	-1.68588	-0.68698	-0.07059
C	0.07917	1.54300	0.20552
O	-1.31593	1.67014	0.17713
O	0.70181	2.54739	0.37916
C	-2.16578	0.63351	0.04687
C	-2.63214	-1.72447	-0.19962
C	-3.98190	-1.46021	-0.20813
C	-4.45045	-0.12618	-0.08978
C	-3.52305	0.91805	0.03717
N	-5.79048	0.13534	-0.14592
H	0.10856	-1.88961	-0.18611
H	-2.27695	-2.75313	-0.29228
H	-4.70269	-2.27372	-0.31109
H	-3.84352	1.95667	0.12869
H	-6.42876	-0.62880	0.02777
H	-6.11148	1.03806	0.17641