

Firefly Luciferin as a Multifunctional Chemiluminescence Molecule

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Supplementary Data:

Table S1. Cartesian coordinates of firefly luciferin, at the CAM-B3LYP/6-31+G(d,p) level of theory.

Table S2. Cartesian coordinates of firefly luciferin radical, at the CAM-B3LYP/6-31+G(d,p) level of theory.

Figure S1. Representation of firefly luciferin dianion (a) and luciferin radical (b).

Table S1. Cartesian coordinates of firefly luciferin, at the CAM-B3LYP/6-31+G(d,p) level of theory.			
C	4.68847	0.92750	0.22243
C	4.86962	-0.50363	0.10562
C	3.68229	-1.28386	-0.03746
C	2.44512	-0.65947	-0.05977
C	2.29631	0.74231	0.05546
C	3.45413	1.53009	0.19886
O	6.03864	-1.02906	0.13040
N	1.00184	1.20482	0.01961
C	0.15253	0.23615	-0.11816
S	0.85692	-1.37868	-0.22283
C	-1.28984	0.42909	-0.20454
S	-1.94177	2.08782	-0.15712
C	-3.61835	1.37599	-0.01324
C	-3.49919	-0.07850	-0.49501
N	-2.11475	-0.53084	-0.34179
C	-4.44138	-1.05784	0.25959
O	-4.60907	-0.85717	1.48817
O	-4.93284	-1.98704	-0.43012
H	-3.73845	-0.15490	-1.56187
H	5.58671	1.52838	0.33298
H	3.77606	-2.36158	-0.12737
H	3.35682	2.60841	0.28957
H	-4.31534	1.95368	-0.62018
H	-3.92998	1.40123	1.03116

Table S2. Cartesian coordinates of firefly luciferin radical, at the CAM-B3LYP/6-31+G(d,p) level of theory.			
C	4.67967	0.94537	0.22180
C	4.82856	-0.50330	0.11523
C	3.63335	-1.31132	-0.02841
C	2.41233	-0.68472	-0.05932
C	2.29654	0.73046	0.04696
C	3.45714	1.53952	0.18882
O	5.96047	-1.03769	0.14678
N	1.02181	1.21023	0.00402
C	0.16301	0.23841	-0.13134
S	0.81825	-1.37942	-0.22290
C	-1.28226	0.45619	-0.21701
S	-1.93181	2.10387	-0.13361
C	-3.60950	1.38155	-0.02773
C	-3.48040	-0.07391	-0.50775
N	-2.09054	-0.51195	-0.37768
C	-4.39368	-1.07125	0.26694
O	-4.59977	-0.82816	1.48048
O	-4.81604	-2.04841	-0.39856
H	-3.73265	-0.16391	-1.57017
H	5.59032	1.52400	0.32872
H	3.74905	-2.38607	-0.10665
H	3.34104	2.61474	0.26787
H	-4.29347	1.95914	-0.64875
H	-3.94198	1.40490	1.01001

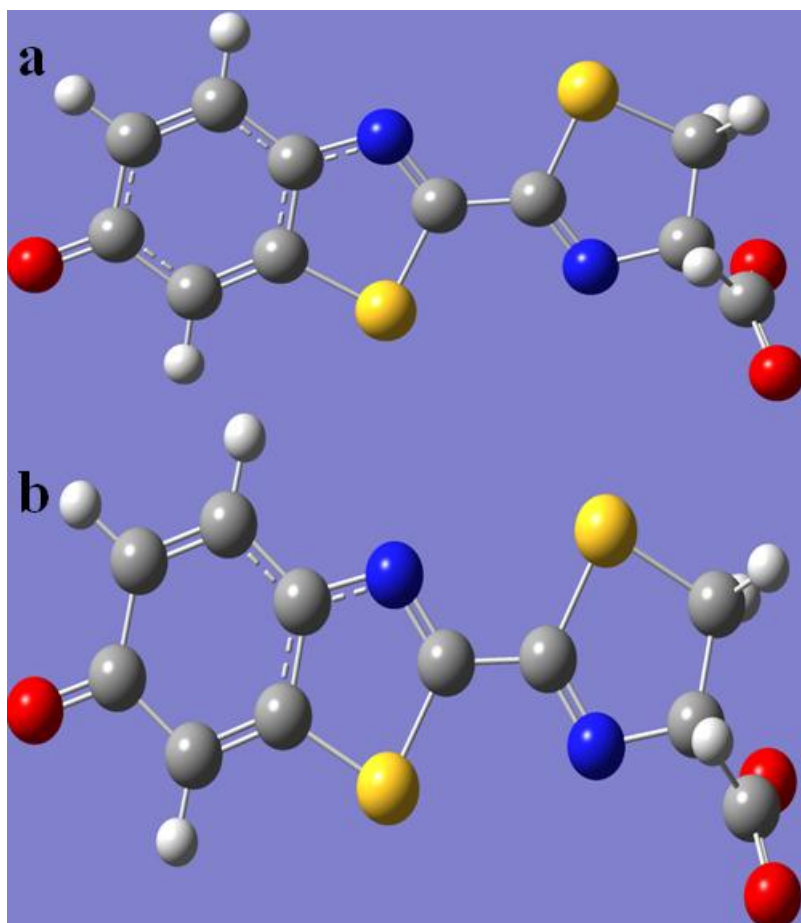


Figure S1. Representation of firefly luciferin dianion (a) and luciferin radical (b).