A BODIPY-luminol chemiluminescent resonance energy-transfer (CRET) cassette for imaging of cellular superoxide

Electronic Supplementary Information

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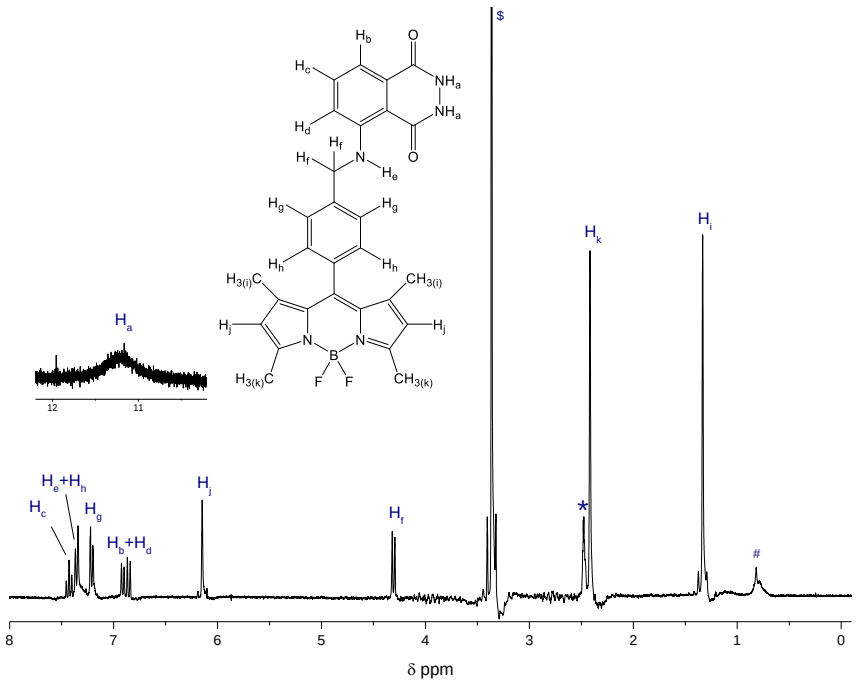

Figure ESI-1. ^{1}H NMR spectrum of BODIPY-luminol recorded in d_6-DMSO (* = residual DMSO signal; $ = H_2O; # = silicone grease).

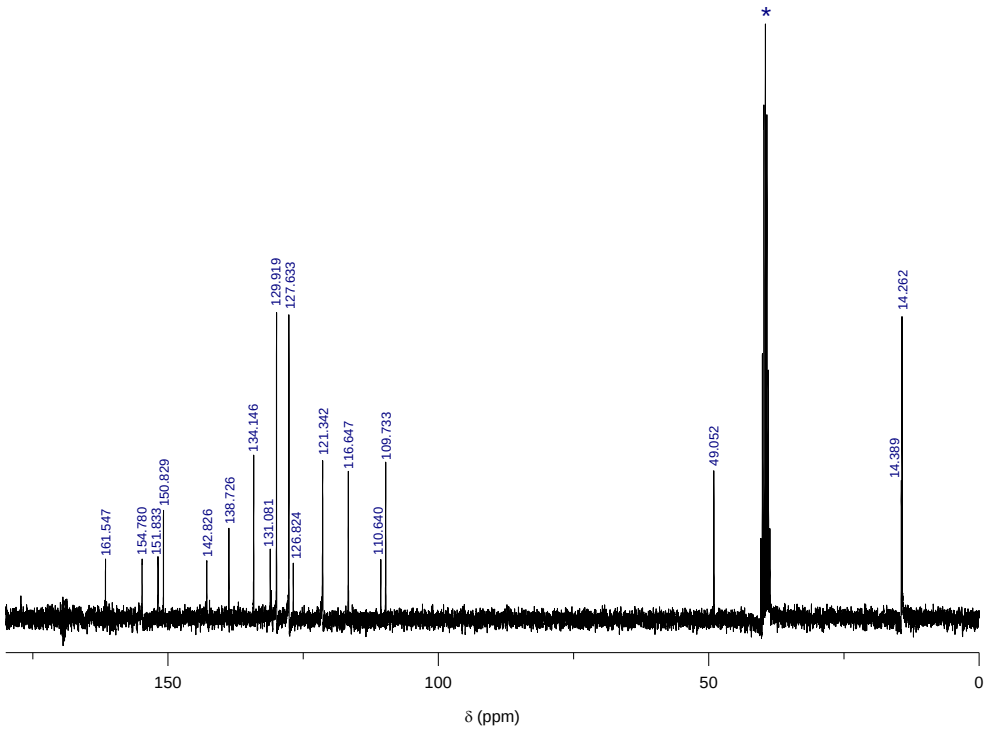

Figure ESI-2. ^{13}C NMR spectrum of BODIPY-luminol recorded in d_6-DMSO (* = residual DMSO signal).

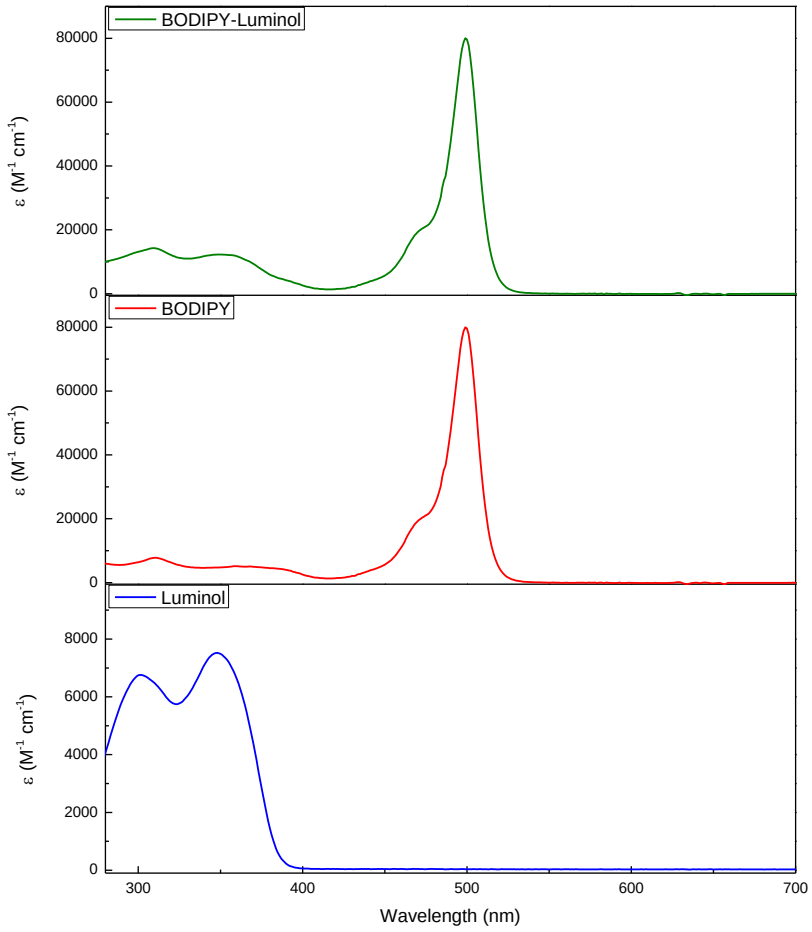

Figure ESI-3. UV/Vis spectra of luminol, BODIPY-COOH and BODIPY-luminol cassette recorded in pH 10 Na_2CO_3:$NaHCO_3$ buffer.

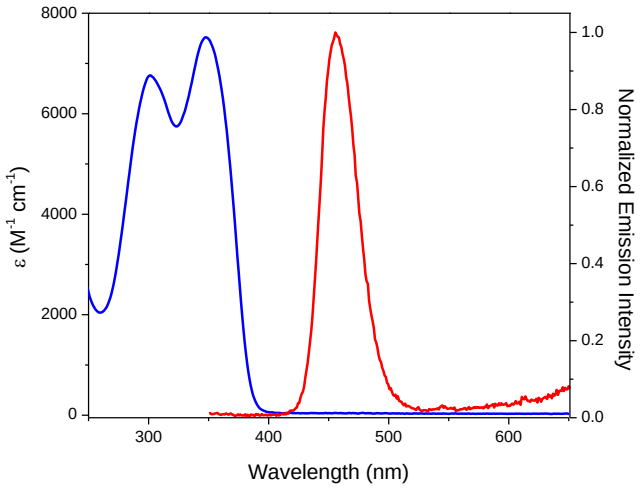

Figure ESI-4. Overlay of electronic absorption and chemiluminescence spectra of Luminol recorded in pH 10 Na_2CO_3:$NaHCO_3$ buffer.

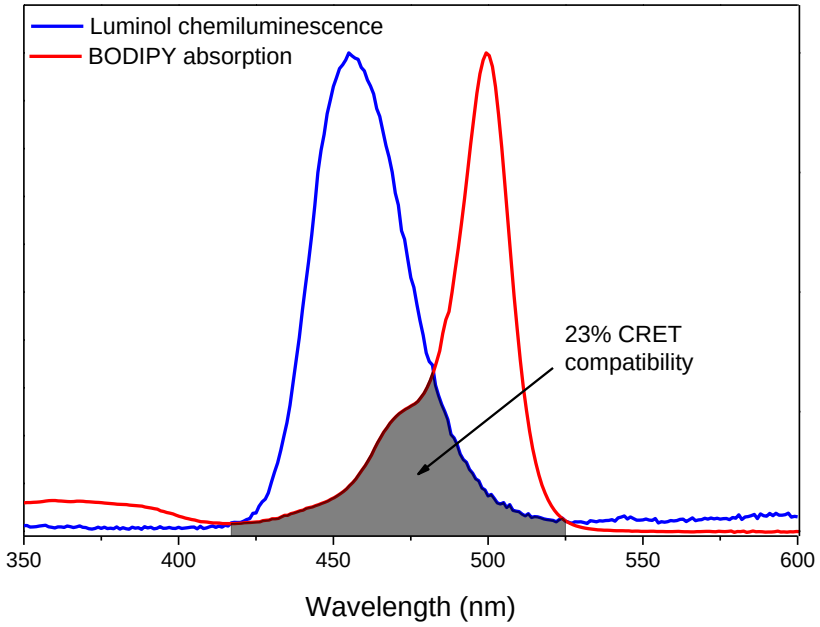

Figure ESI-5. Overlay of normalized luminol chemiluminescence and BODIPY absorption recorded in pH 10 Na_2CO_3:$NaHCO_3$ buffer. Integration of spectral overlap indicates a 23% chemiluminescent resonance energy transfer (CRET) compatibility.

Computational analysis

Computational experiments were carried out using density functional theory (DFT) with the B3LYP functional as implemented in the Spartan '14 program package.[2] The 6-31g* basis set was used for all C, H, N, O, B and F elements.[3, 4] A vibrational frequency analysis was carried out in order to confirm the minimum-energy geometry.

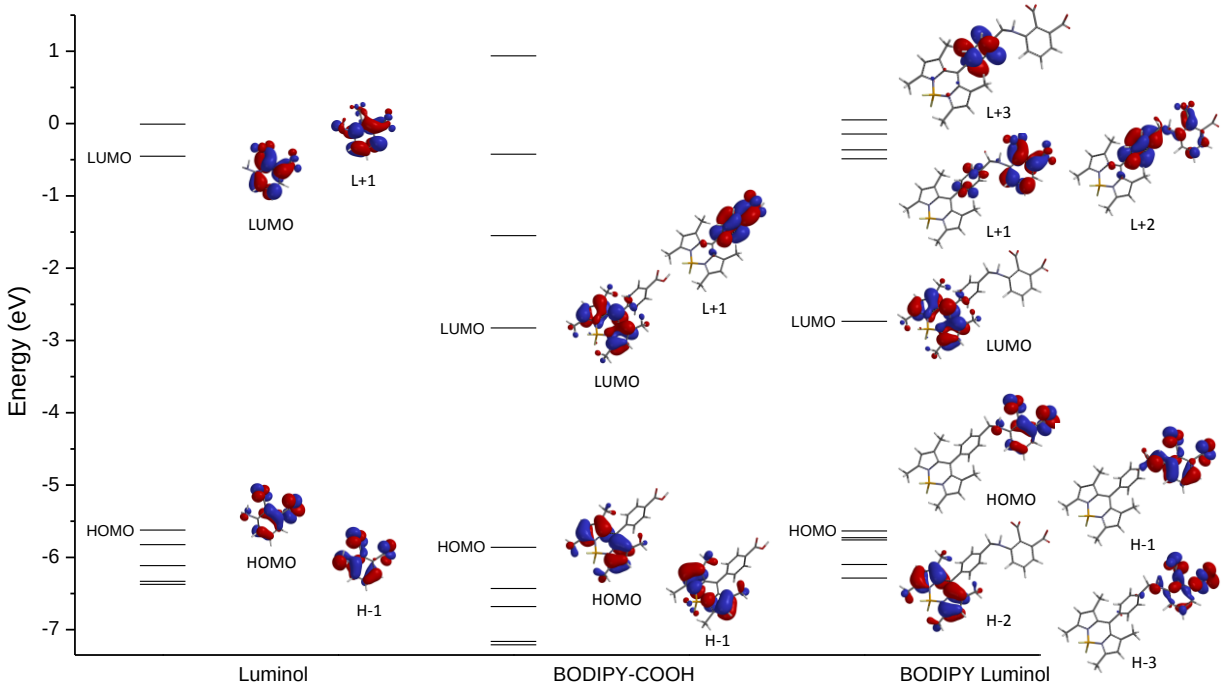

Figure ESI-6. Energy level alignment of luminol (chemiluminescent dicarboxy reactive intermediate), *meso*-(4-carboxyphenyl)BODIPY and the BODIPY-luminol dyad calculated by DFT (B3LYP/6-31g*) using Spartan '09 Wavefunction software.

References

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