

SUPPLEMENTARY TABLES

Table S1. Characteristic constants of phenyl-3,5-di-tert-butyl-2-hydroxibenzoate* and **B1**.

| Compound | Molecular formula | MW (g mol ⁻¹) | Melting point (°C) | Solid color | TLC R _f |
|---|---|---------------------------|--------------------|-------------|--------------------|
| B2 | C ₂₀ H ₂₅ N ₃ O | 323,4320 | 311-312 | Light brown | 0.38 |
| phenyl-3,5-di-tert-butyl-2-hydroxibenzoate* | C ₂₁ H ₂₆ N ₃ O ₃ | 365,4256 | ND | White | 0.80 |

MW: Molecular weight

TLC: Thin layer chromatography, using ethyl acetate as solvent

ND: not determined

* Precursor for **B2** synthesis

Table S2. UV-Vis absorption spectra of **B2** in different organic solvents at room temperature.

| Compound | Chloroform | | Acetonitrile | | DMSO | |
|-----------|---------------|------------|---------------|------------|---------------|------------|
| | λ exp | ϵ | λ exp | ϵ | λ exp | ϵ |
| B2 | 332 | 13.32 | 327 | 12.91 | 332 | 11.30 |
| | 294 | 19.09 | 292 | 18.67 | 294 | 15.44 |
| | 284 | 15.51 | 282 | 14.88 | 284 | 12.23 |

λ is in nm

ϵ is in mol⁻¹ dm³ cm⁻¹

Table S3. Scan-rate study for determining diffusional control of described electrochemical processes at **B2**.

| Process | Scan-rate vs current- density peak | (Scan- rate) ^{1/2} vs current- density peak | Diff. control? | Process | Scan-rate vs current- density peak | (Scan- rate) ^{1/2} vs current- density peak | Diff. control? |
|---|--|--|----------------------|----------------------|--|--|----------------------|
| | m | n | R² | | m | n | R² |
| Red ^I _(rev) | -5.3×10 ⁵ | -2.2×10 ² | 0.833 | -2.1×10 ⁴ | -3.2 | 0.921 | yes |
| O _X ^I _(irr) | 9.5×10 ⁵ | 3.6×10 ² | 0.989 | 3.5×10 ⁴ | -7.5 | 0.999 | yes |
| O _X ^{II} _(irr) | 2.4×10 ⁵ | 1.1×10 ² | 0.961 | 8.9×10 ³ | 1.5 | 0.996 | yes |

“m”, “n” and “R²” are the slope, intercept and linear regression coefficient, respectively.

The scan-rate study provides a fast determination of the nature of electrochemical processes, allowing a differentiation between processes controlled by mass-transport (diffusion) from others. For each identified process for **B2**, several cyclic voltammetry runs must be recorded at different scan rates. Thus, two plots must be constructed, an “Scan-rate vs current-density peak” and a “(Scan-rate)^{1/2} vs current density peak” for each reduction an oxidation identified in the system (see **Table S3**).

Table S4. Results for the geometry optimization of the ground (S_0) and first excited singlet (S_1) state.

| Compound | d(N-H) | d(O-H) |
|-----------------|---------------|---------------|
| S_0 | 1.731 | 0.989 |
| S_1 | 1.673 | 1.006 |

Table S5. The most important absorption and emission bands for **B2** in DMSO.

| | λ (nm) | f^* | Assignment |
|-------------------|----------------|----------------------|---|
| Absorption | 271.8 | 1.1×10^{-2} | HOMO-2 \rightarrow LUMO+1 (n \rightarrow π^*) |
| | 293.4 | 1.2×10^{-2} | HOMO-1 \rightarrow LUMO ($\pi \rightarrow \pi^*$) |
| | | 1.4×10^{-1} | HOMO \rightarrow LUMO ($\pi \rightarrow \pi^*$) |
| Emission | 514.8 | 6.5×10^{-3} | LUMO \rightarrow HOMO ($\pi^* \rightarrow \pi$) |

*The oscillator strength was obtained using COSMO for DMSO as solvent.