Supporting Information

The Quest for Highly Fluorescent Chromophores: An Evaluation of 1*H*,3*H*-Isochromeno[6,5,4-*mna*]xanthene-1,3-dione (CXD)

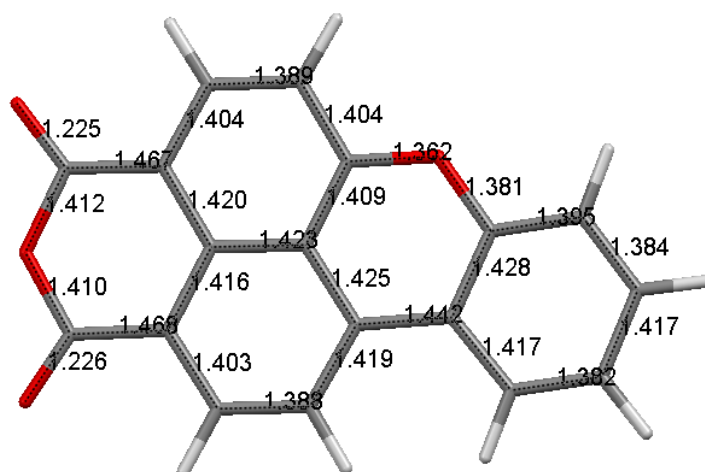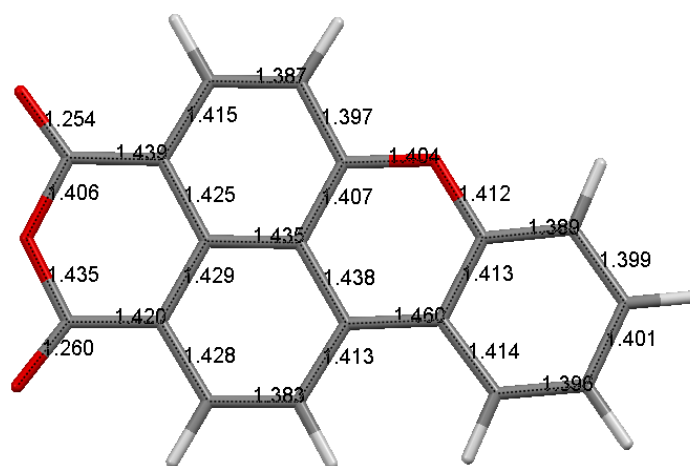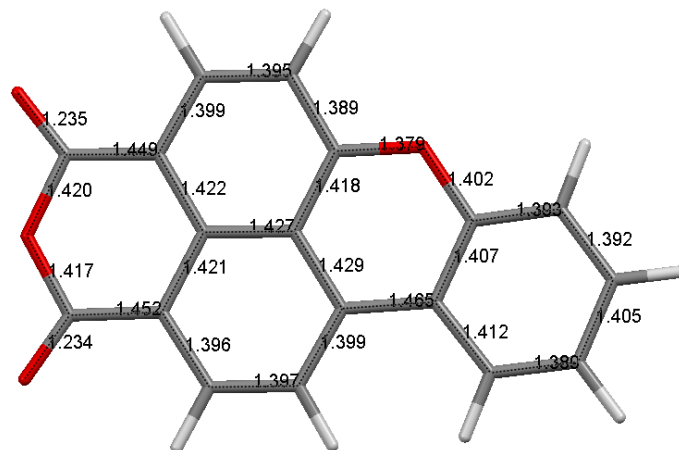Roza Al-Aqar, Daniel Avis, Andrew C. Benniston and Anthony Harriman

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S1. Calculated bond lengths for **CXD** (top) and **CXD⁻·** (middle) and **CXD⁺·** (bottom).

S2. Comparison of recorded absorption spectrum for **CXD** in THF (black) and calculated (blue) using TD-DFT (B3LYP, 6-31G(d)) in a THF solvent continuum. Bars depict calculated electronic transitions with selected molecular orbitals shown for (a) to (e). The number of the molecular orbital is shown and the square of the coefficient multiplied by two is given above the arrow.

S3. Absorption spectrum (black) and fluorescence spectrum (red) for **CXD** in toluene.

S4. Absorption spectrum (black) and fluorescence spectrum (red) for **CXD** in MeCN.

S5. Absorption spectrum (black) and fluorescence spectrum (red) for **CXD** in Et_2O.

S6. Absorption spectrum (black) and fluorescence spectrum (red) for **CXD** in propylene carbonate.

S7. Absorption spectra for **JBD** prepared in a thin film of PMMA (black) and for the dye after uptake into a PMMA polymer disc (red).
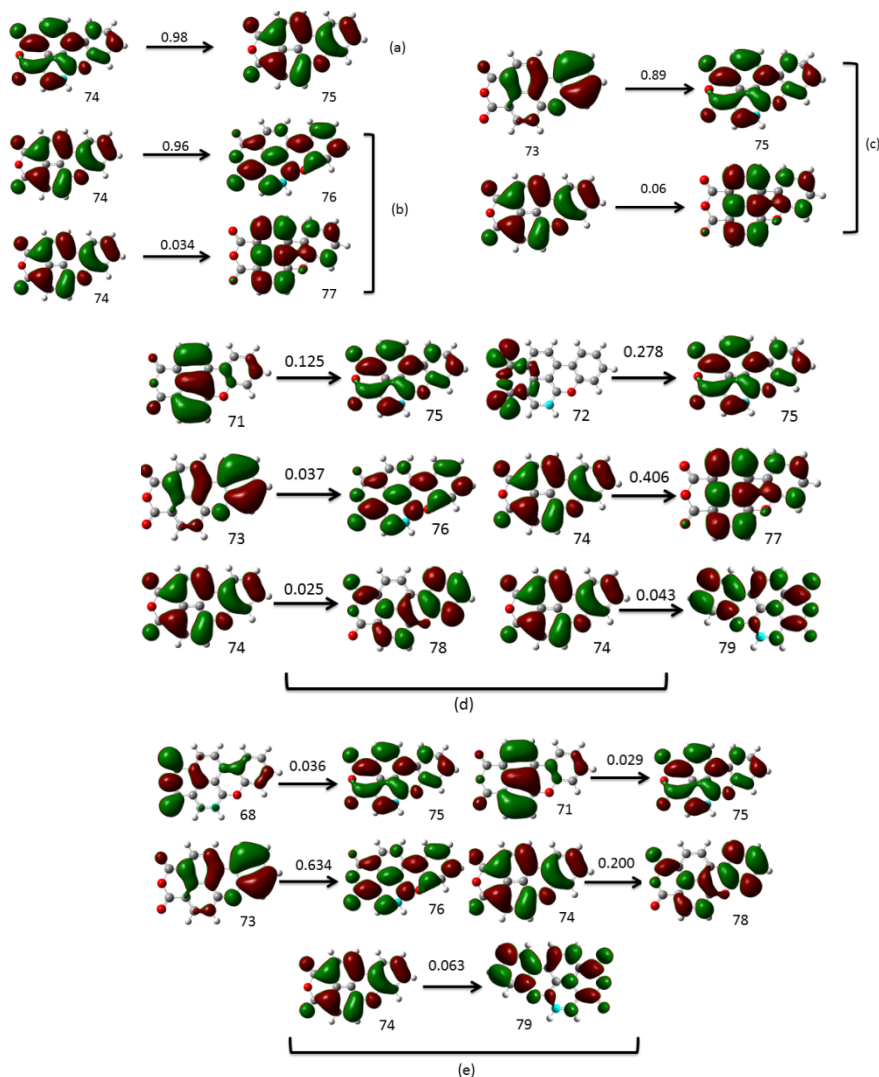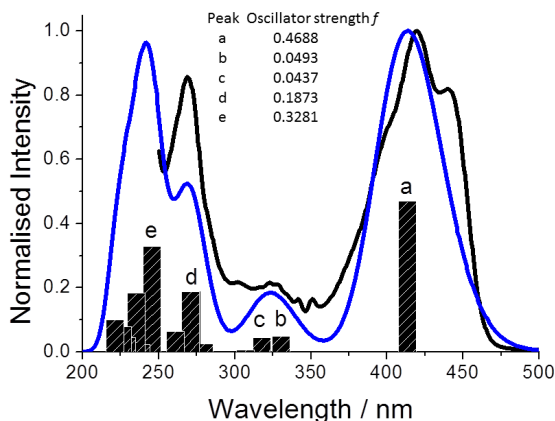
Strickler-Berg Expression

$$k_{RAD} = 2.88 \times 10^{-9} n^2 \frac{\int F(v)dv}{\int \frac{F(v)dv}{v^3}} \int \frac{\varepsilon(v)dv}{v}$$
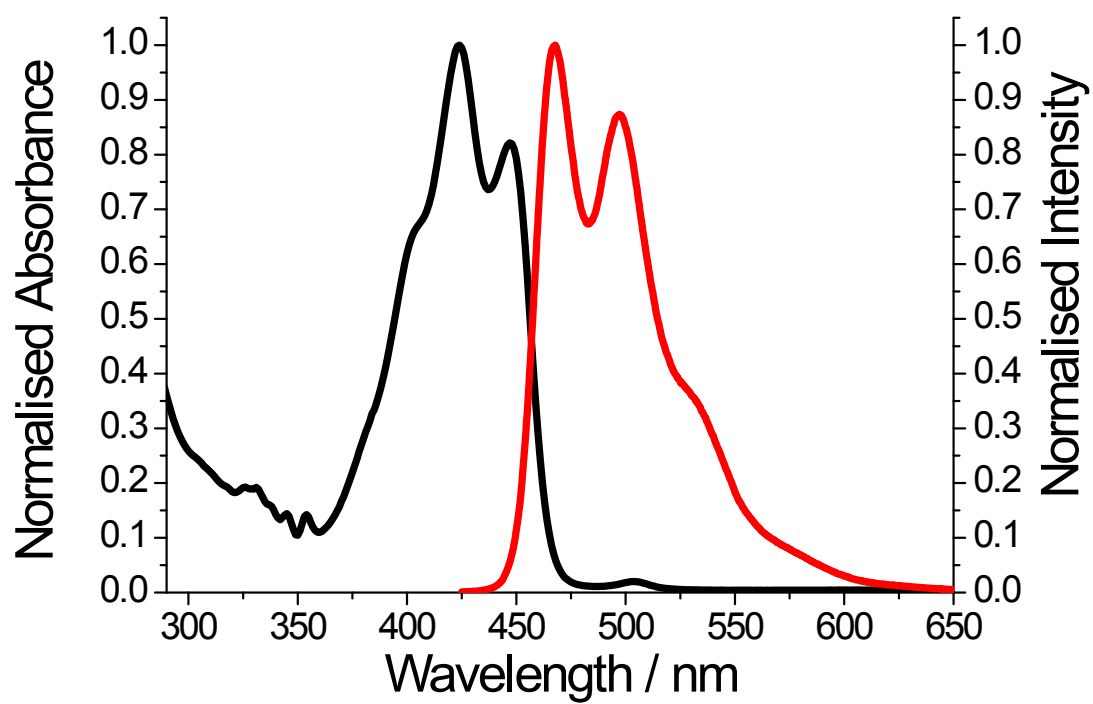
(Eq. 1)

where F = fluorescence intensity at wavenumber v, ε = molar absorption coefficient and n = refractive index of the solvent.
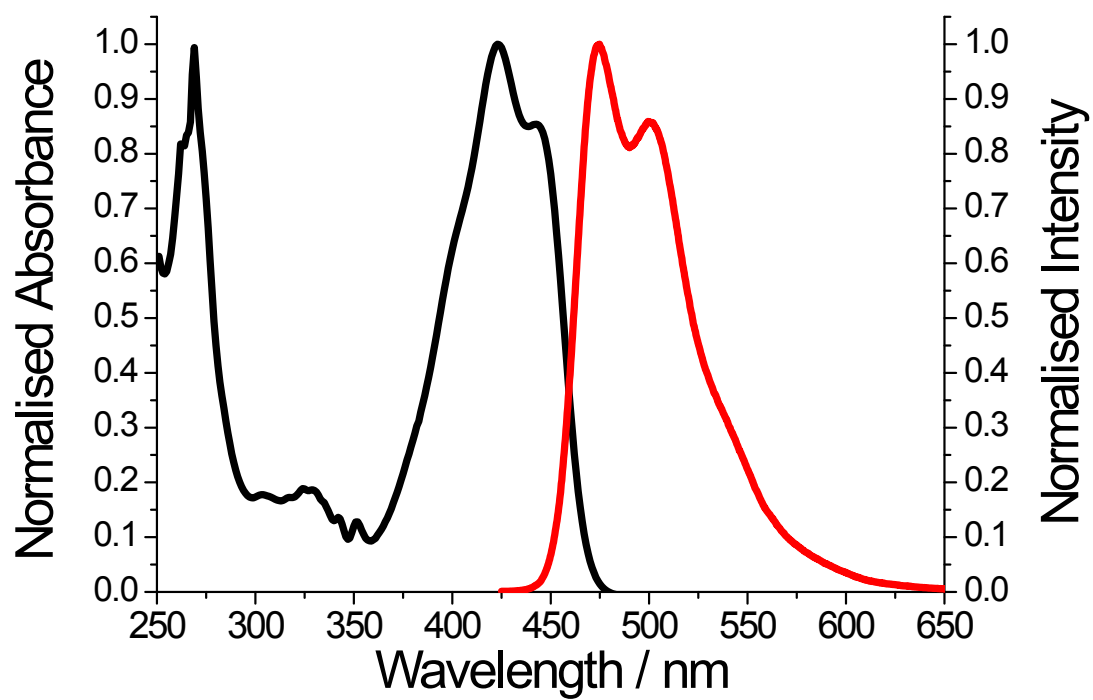
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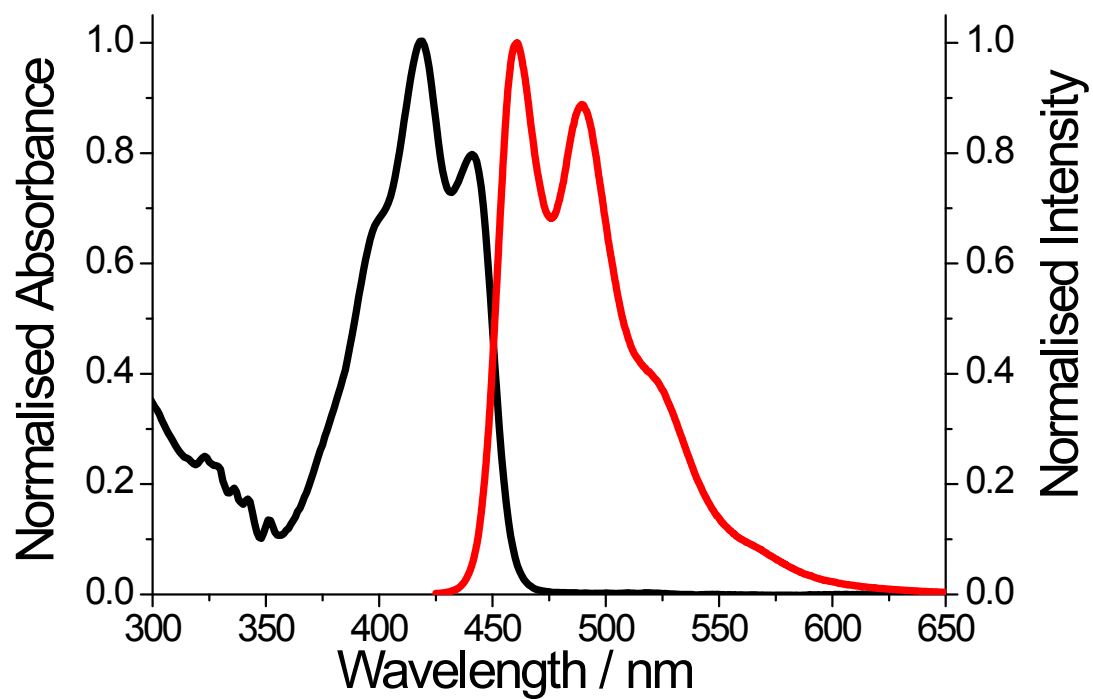
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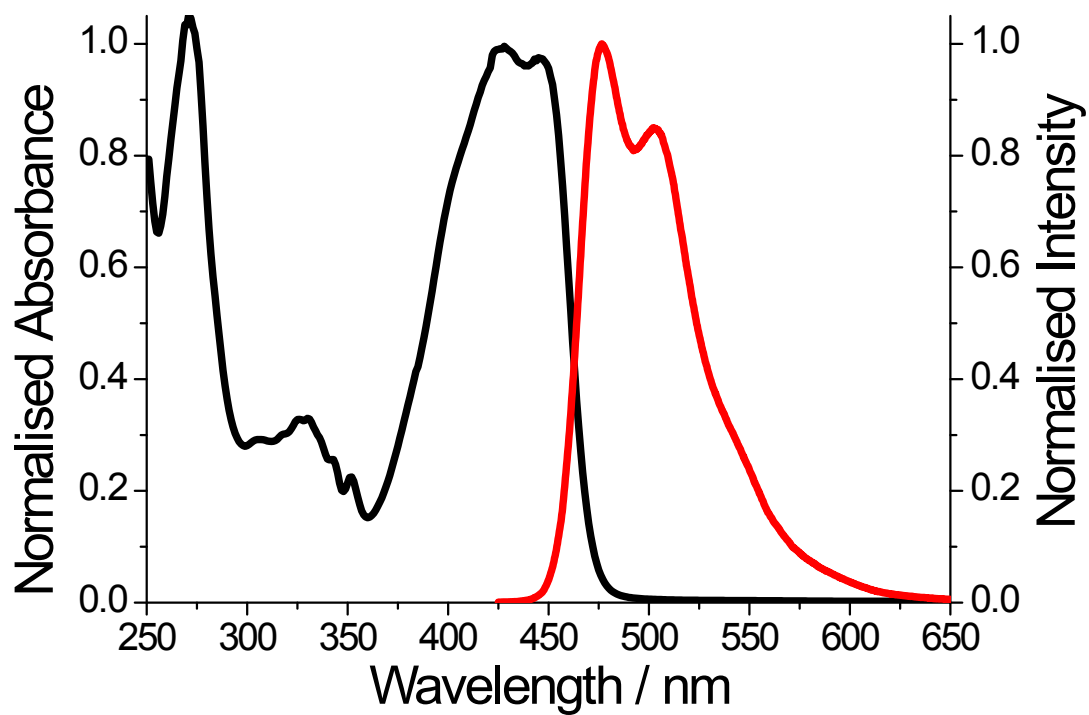
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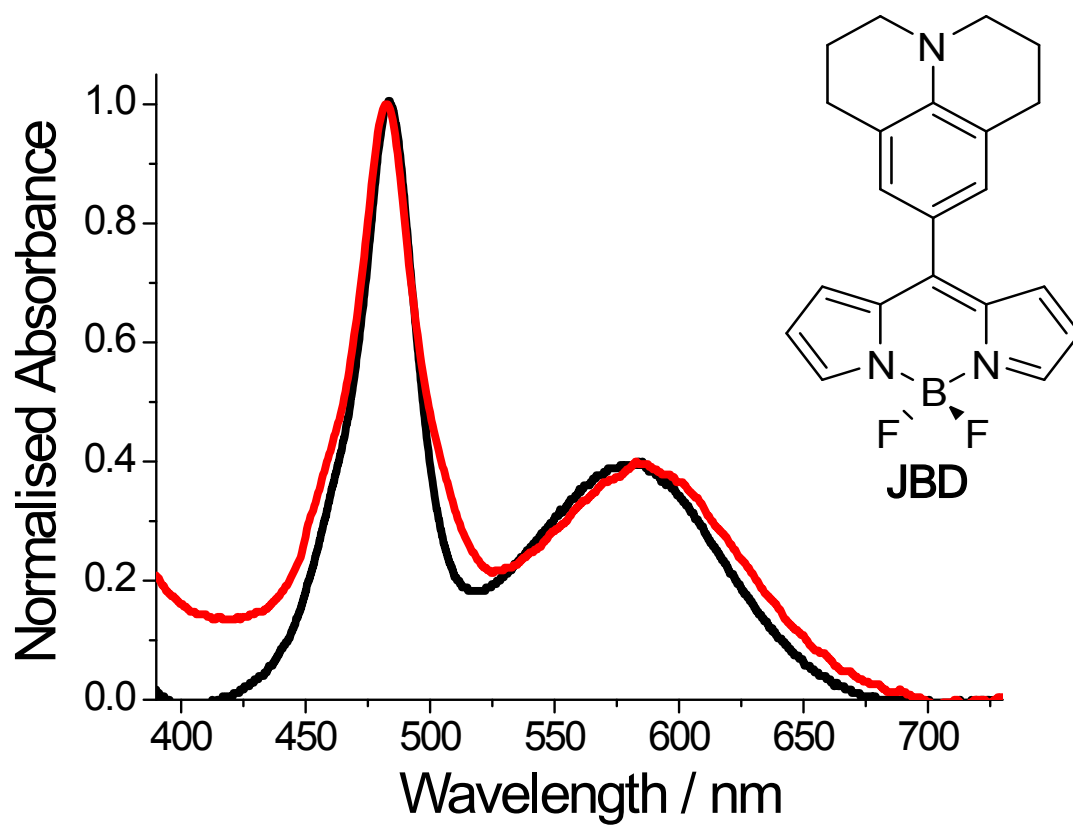
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