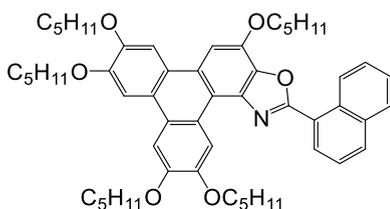


# TpOx-1-Nap

TpOx-1-Nap is a UV excitable fluorescent material with a polycyclic aromatic donor-acceptor structure where the triphenoxazole core acts as a donor and the aromatic group on the two position of the oxazole (1-naphthalene) act as the acceptor group. The push-pull, donor-acceptor, structure facilitates intramolecular charge transfer in the excited state that results in a 235 nm emission Stokes Shift. TpOx-1-Nap is also a photo-conducting Discotic Liquid Crystalline (DLC) material with mesophase transition onset temperature of 96°C. TpOx-1-Nap is designed for 355 nm and 405 nm excitation with emission at 510 nm with quantum yield of 0.48, high thermal, chemical and photostability. TpOx-1-Nap has potential uses in fluorescent dye staining, organic electronics and photonics, and imaging applications.

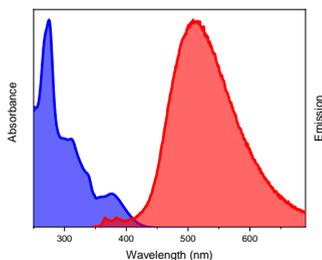
## Chemical Structure



## Chemical Data

- Catalogue Number: **922986**
- Other Name: TpOx-1-Nap, CT 510 11 100 01 01
- CAS #: 2377209-30-6
- Molecular Formula: C<sub>54</sub>H<sub>67</sub>NO<sub>6</sub>
- Molecular Weight: 826.13

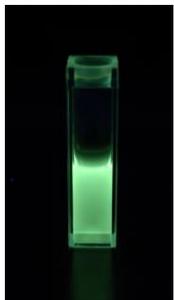
## Absorbance and Emission spectra in Ethyl Acetate



## Photophysical Data

- In Solvent: EtOAc
- Abs  $\lambda_{max}$  (nm) = 275,
- Emis  $\lambda_{max}$  (nm) = 510
- pSS (nm) = 235
- $\epsilon$  (M<sup>-1</sup> cm<sup>-1</sup>) at Abs  $\lambda_{max}$  = 117,000
- Quantum Yield ( $\Phi$ ) = 0.48
- Fluorescence Lifetime (ns) = 6.01
- Band Gap (Optical, Solution state) = 2.94 eV
- HOMO<sub>CV</sub> = -5.45 eV
- LUMO = -2.51 eV
- Thermal degradation onset = ~380°C

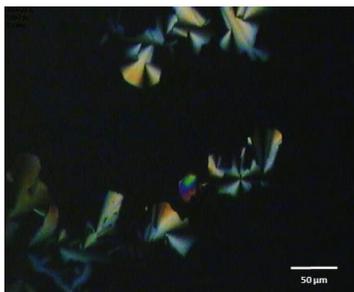
## Fluorescence Emission



## Material Data

- Physical State: Crystal Powder
- Appearance (Colour): Pale yellow
- Polymorph crystalline phase: Solid, Discotic Liquid Crystal, Isotropic
- Solubility: THF > 1 mg/mL, MeCN < 0.24 mg/mL, DCM > 1 mg/mL

## Polarising Optical Microscope Picture



## Phase Transition Data

Phase transition temperature:

- Heating Crys - Col<sub>h</sub> - 86°C, Col<sub>h</sub> - Iso - 168°C
- Cooling Iso - Col<sub>h</sub> - 161°C, Col<sub>h</sub> - Crys - 43°C