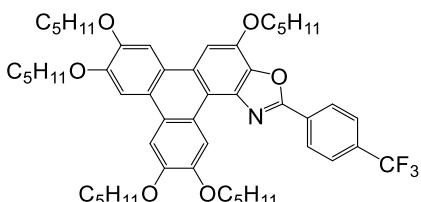


# TpOx-Ph-*p*-CF<sub>3</sub>

TpOx-Ph-*p*-CF<sub>3</sub> 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 (4-trifluoromethyl-phenyl) act as the acceptor group. The push-pull, donor-acceptor, structure facilitates intramolecular charge transfer in the excited state that results in a 255 nm emission Stokes Shift. TpOx-Ph-*p*-CF<sub>3</sub> is also a photo-conducting Discotic Liquid Crystalline (DLC) material with mesophase transition onset temperature of 145°C. TpOx-Ph-*p*-CF<sub>3</sub> is designed for 355 nm and 405 nm excitation with emission at 526 nm with quantum yield of 0.51, high thermal, chemical and photostability. TpOx-Ph-*p*-CF<sub>3</sub> has potential uses in fluorescent dye staining, organic electronics and photonics, and imaging applications.

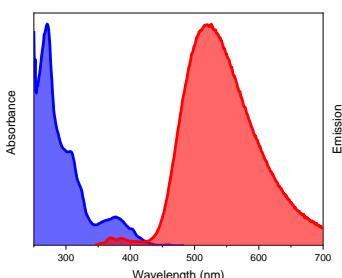
## Chemical Structure



## Chemical Data

- Catalogue Number: 922943
- Other Name: TpOxPh-*p*-CF<sub>3</sub>, CT 526 11 054 01 01
- CAS #: 2377209-48-6
- Molecular Formula: C<sub>51</sub>H<sub>64</sub>F<sub>3</sub>NO<sub>6</sub>
- Molecular Weight: 844.07

## Absorbance and Emission spectra in Ethyl Acetate



## Photophysical Data

- In Solvent: EtOAc
- Abs λ<sub>max</sub> (nm) = 271
- Emis λ<sub>max</sub> (nm) = 526
- pSS (nm) = 255
- ε (M<sup>-1</sup> cm<sup>-1</sup>) at Abs λ<sub>max</sub> = 104,000
- Quantum Yield (Φ) = 0.51
- Fluorescence Lifetime (ns) = 7.31
- Band Gap (Optical, Solution state) = 2.94 eV
- HOMO<sub>CV</sub> = -5.44 eV
- LUMO = -2.5 eV

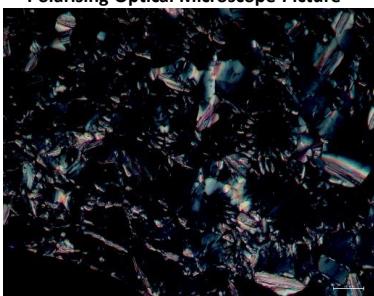
## Fluorescence Emission



## Material Data

- Physical State: Crystal Powder
- Appearance (Colour): Pale yellow
- Polymorph crystalline phase: Solid, Discotic Liquid Crystal, Isotropic
- Solubility: THF > 1 mg/mL, MeCN < 0.23 mg/mL, DMSO < 0.23 mg/mL, DCM > 1 mg /mL

## Polarising Optical Microscope Picture



## Phase Transition Data

Phase transition temperature:

- Heating Crys - Col<sub>h</sub> – 145°C, Col<sub>h</sub> - Iso – 281°C
- Cooling Iso - Col<sub>h</sub> – 276°C, Col<sub>h</sub> - Crys – <74°C