



Unravelling the Luminogenic Property of Furan by Molecular Engineering to Develop Multifunctional AIEgens for Applications in TNP Sensing and Cell-imaging

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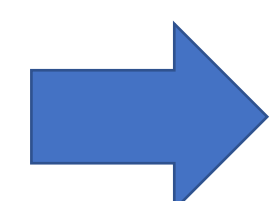
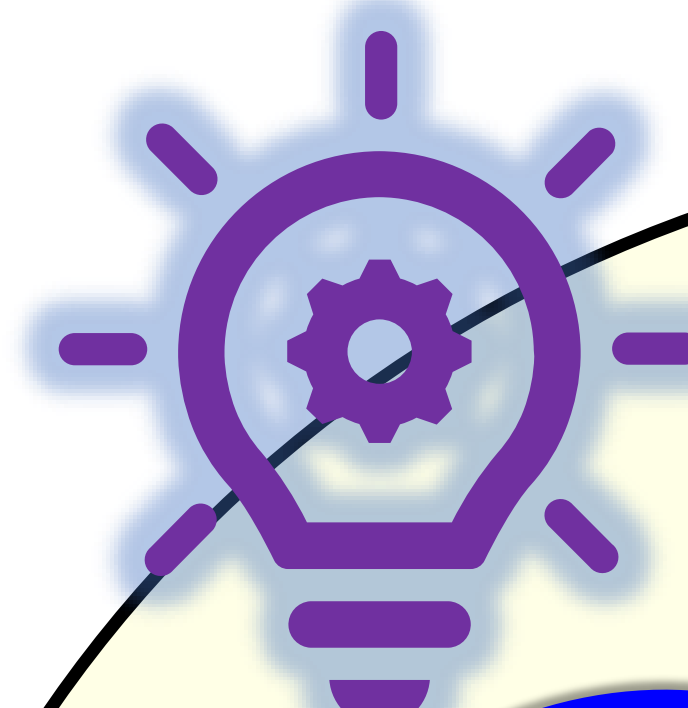
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Molecules exhibiting photoluminescence in the solid, thin-film, or aggregated state is undoubtedly a coveted quality.

However, many planar conjugated organic molecules although strongly emissive in solution becomes non-emissive in the solid or aggregated-state.

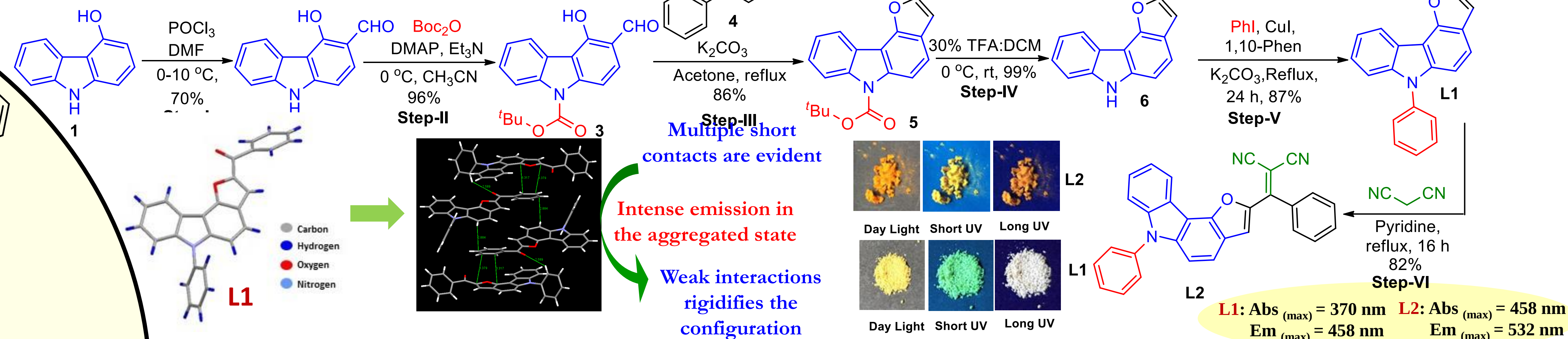
Enhancement in the solid-state emission is achievable by limiting the intermolecular π -stacking of luminogens as well as by restricting molecular motions by precisely controlling the supramolecular interactions

- ✓ Restricted Intramolecular motion (RIM)
- ✓ Restricted Intramolecular Vibration (RIV)
- ✓ Restricted Intramolecular Rotation (RIR)



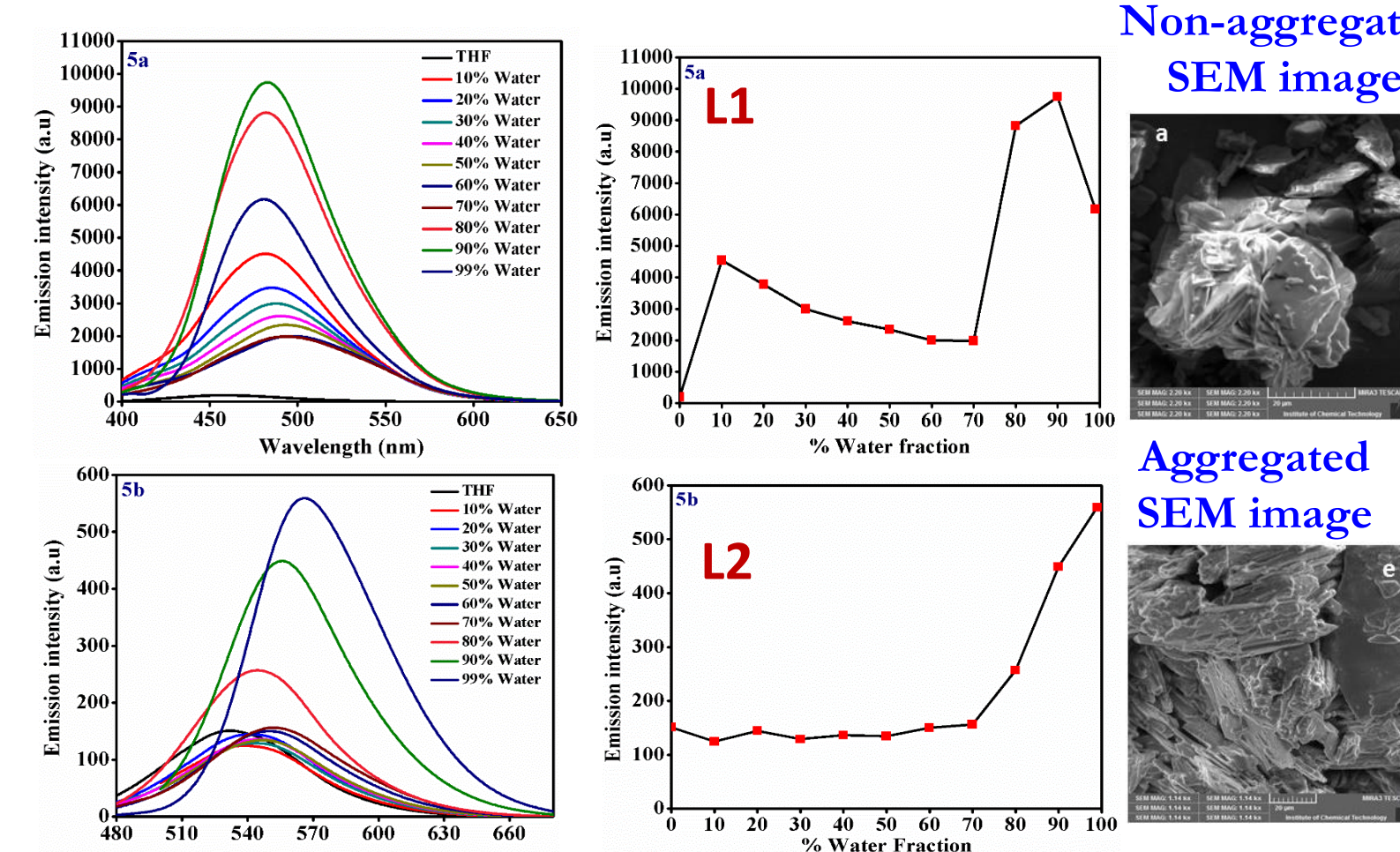
Design strategies

Synthesis of L1 and L2 and Synthesis of S3 and S4



Experimental Details and Results

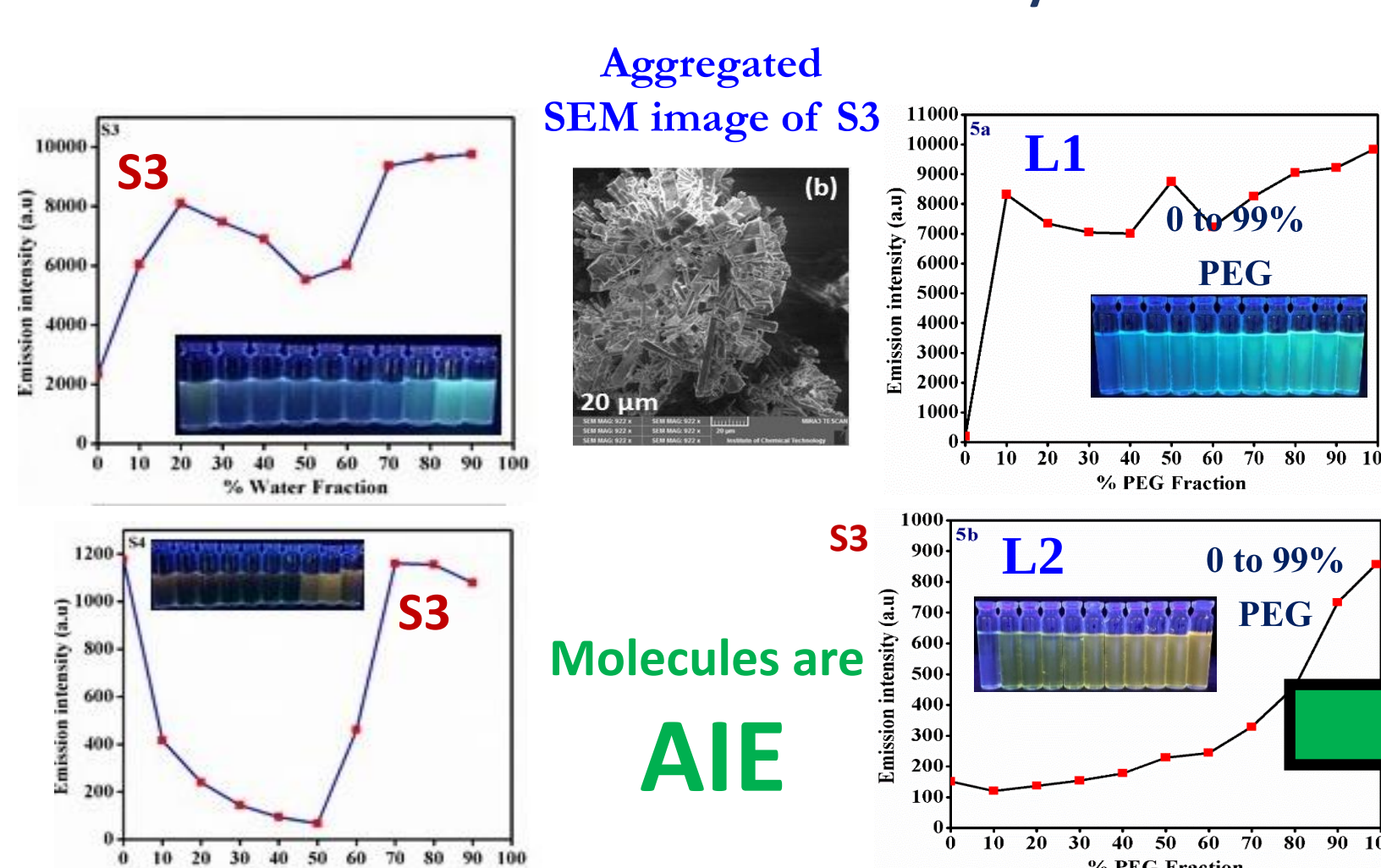
Aggregation Induced Emission of L1-L2 and S3-S4



Non-aggregated SEM image

Aggregated SEM image

Viscosity Induced Emission

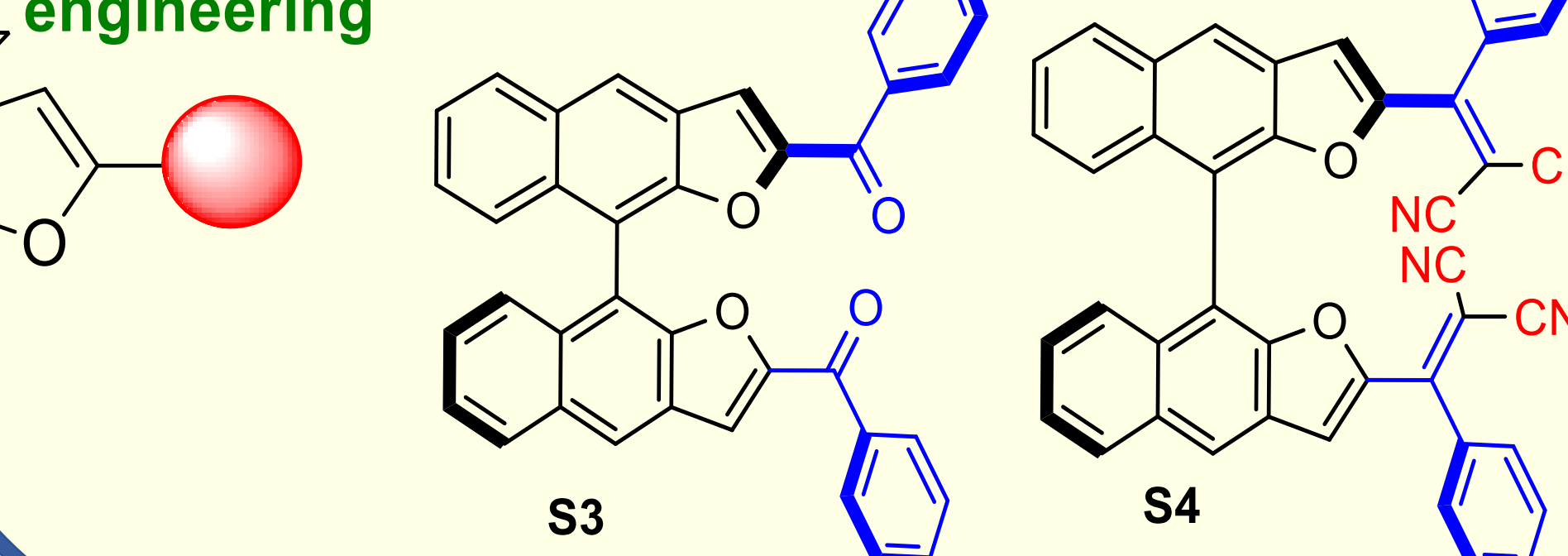
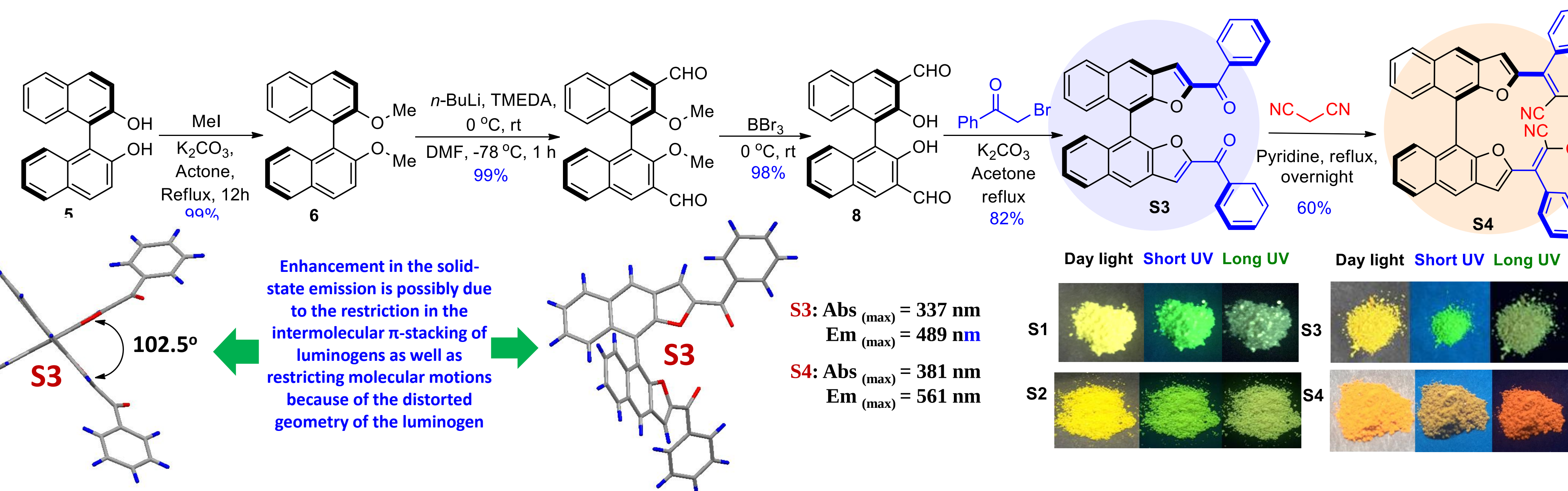


Molecules are AIE

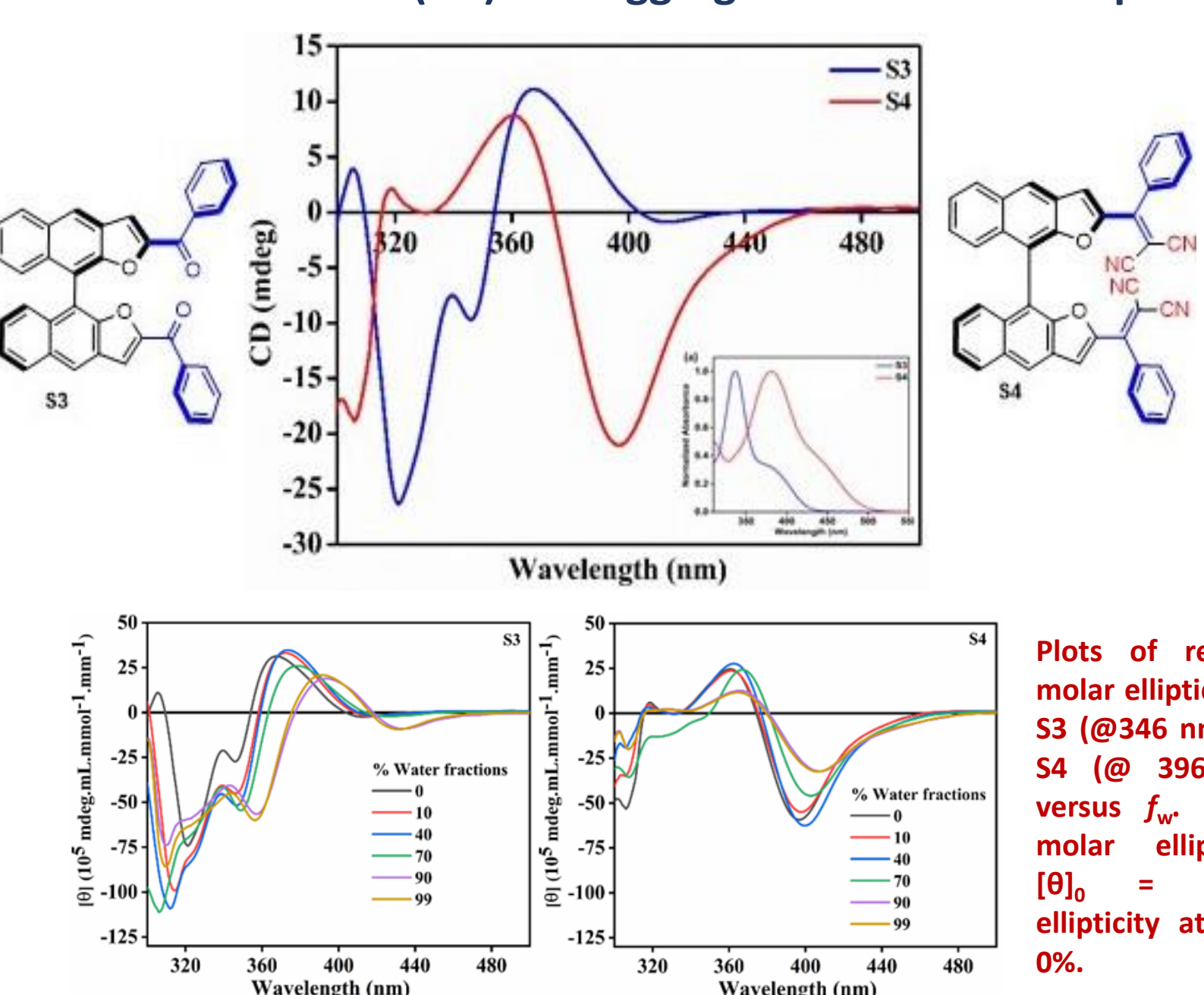
6 to 51% enhancement in emission intensity

Molecules are viscosity sensors

Chiral AIEgens

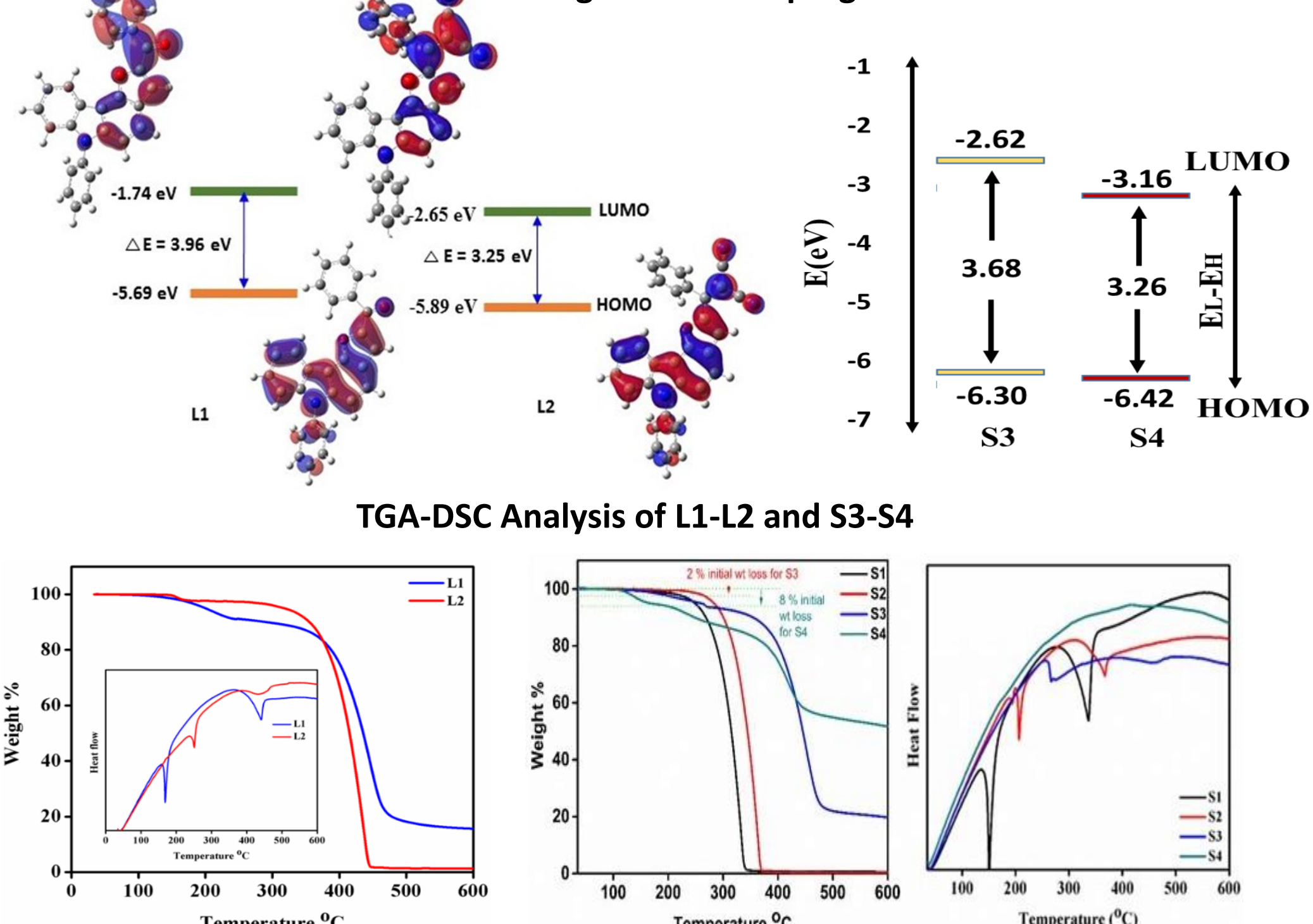


Circular Dichroism (CD) and Aggregation Induced CD Spectra of S3 and S4

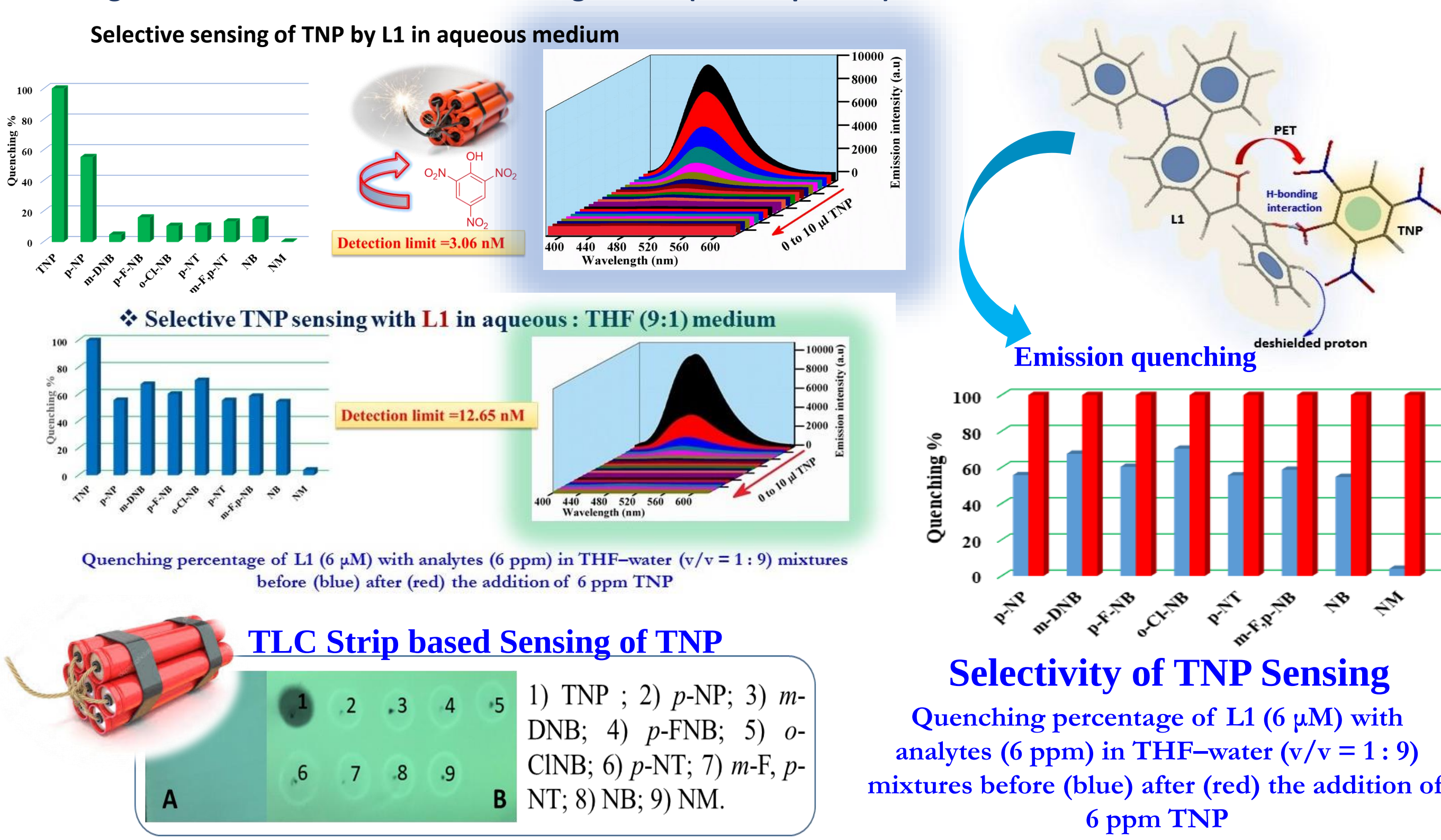
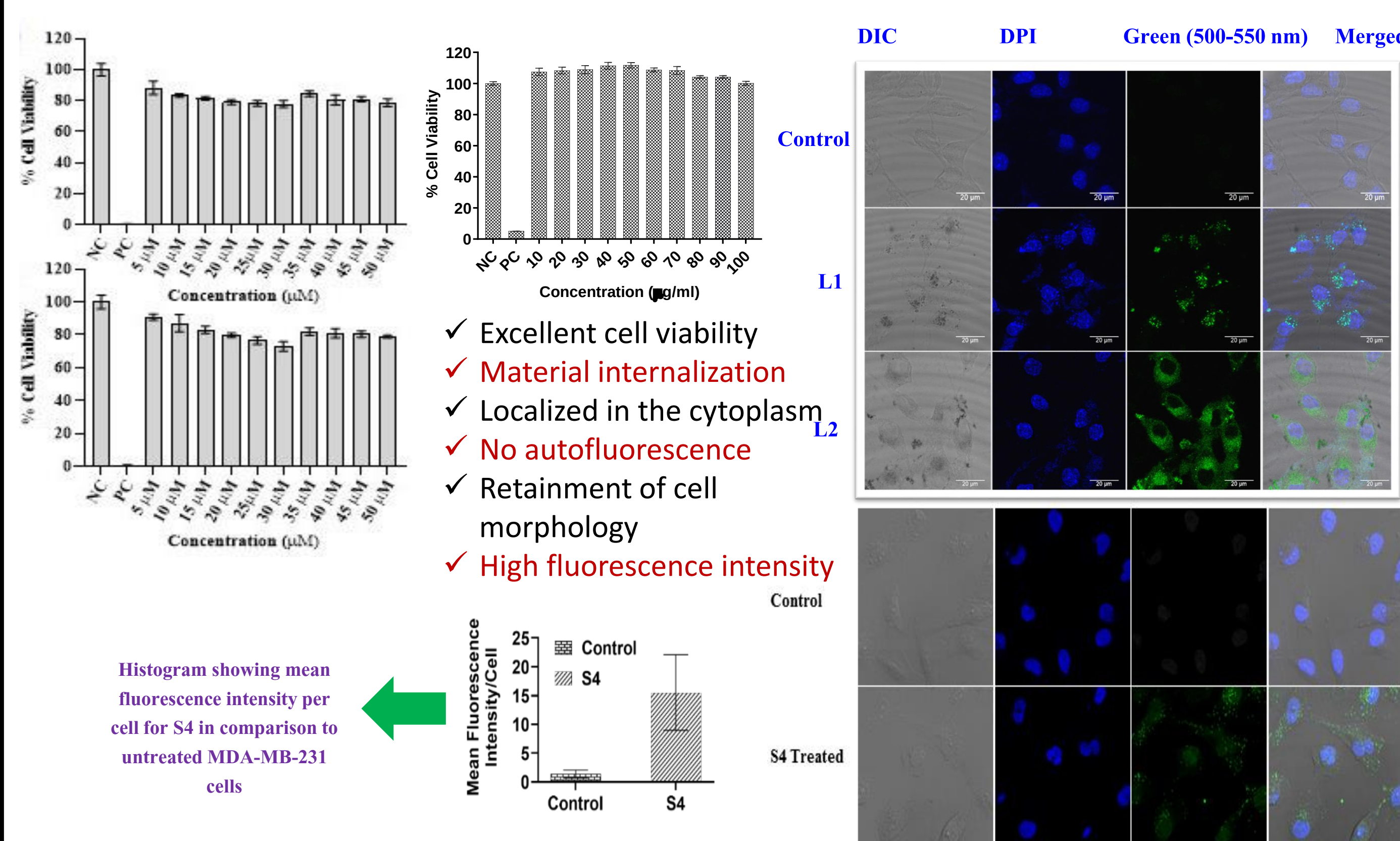


Chirality transfer and retention in the luminogens

Experimental HOMO-LUMO energy gap is in agreement with the Theoretical calculations done at PBE1PBE/6-31G(d,p) level of DFT in vacuum using Gaussian16 programme



Sensing of Nitroaromatics-Selective Sensing of TNP (Nitroexplosive)



- Conclusion:**
1. Furan has been engineered to develop new solid state emissive luminogens
 2. All the AIEgens have high photo and thermal stabilities
 3. Act as nitroaromatic sensor for selectively sensing TNP (nitro explosive) in nano-molar concentration in both organic solvent as well as in water

4. Luminogens have low cytotoxicity and has been used for cancer cell imaging.
5. BINOL based luminogens was first of its kind to be used for cancer cell imaging

References

1. Saha et. al. *ChemPhotoChem* **2020**, 4, 691-703
 2. Saha et. al. *Chem. Eur. J.* **2021**, 27, 5470-5482
- Acknowledgements:** SERB-DST, India, CSIR India, UGC-FRP India, TEQIP-III