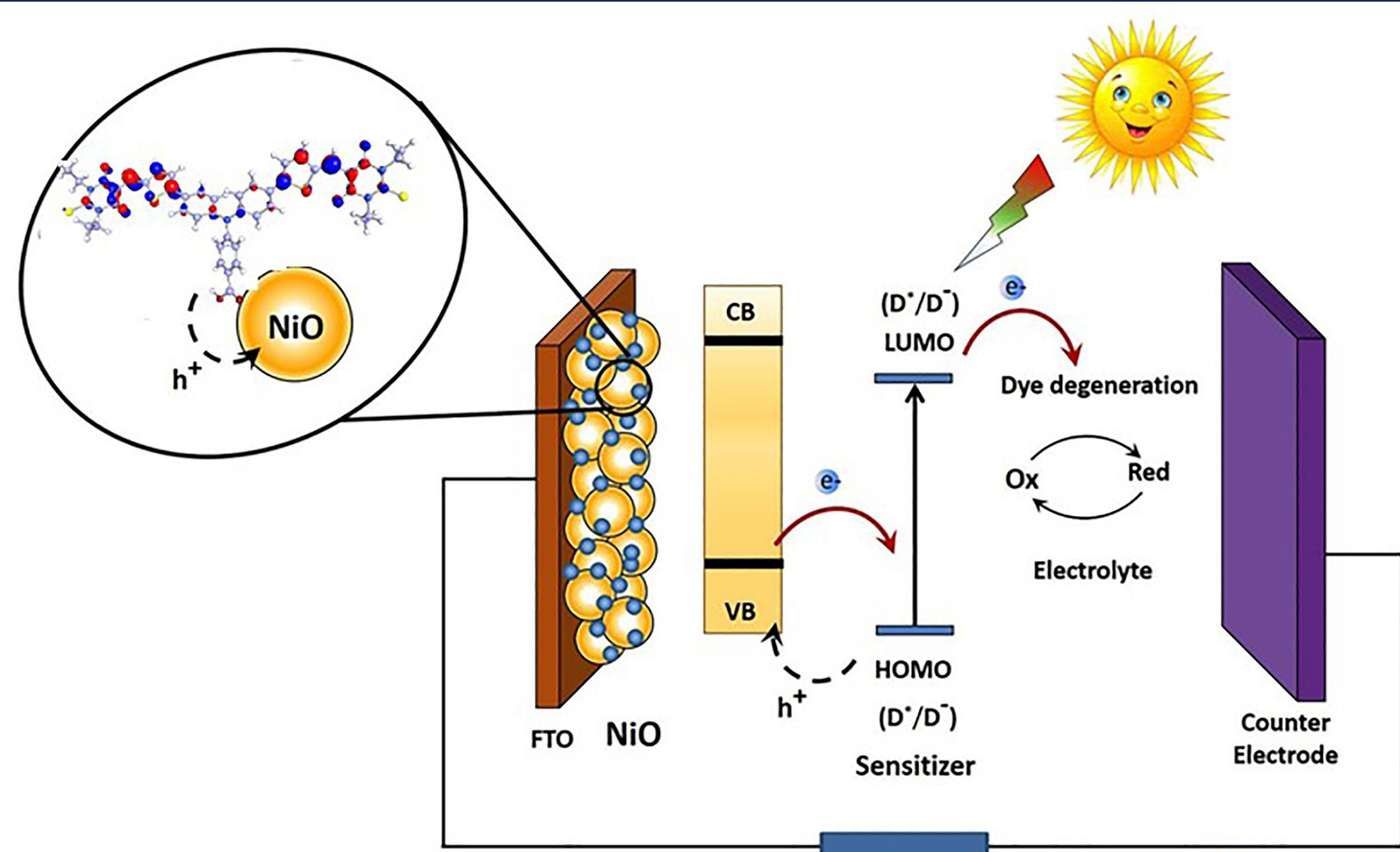


**Praveen Naik,**

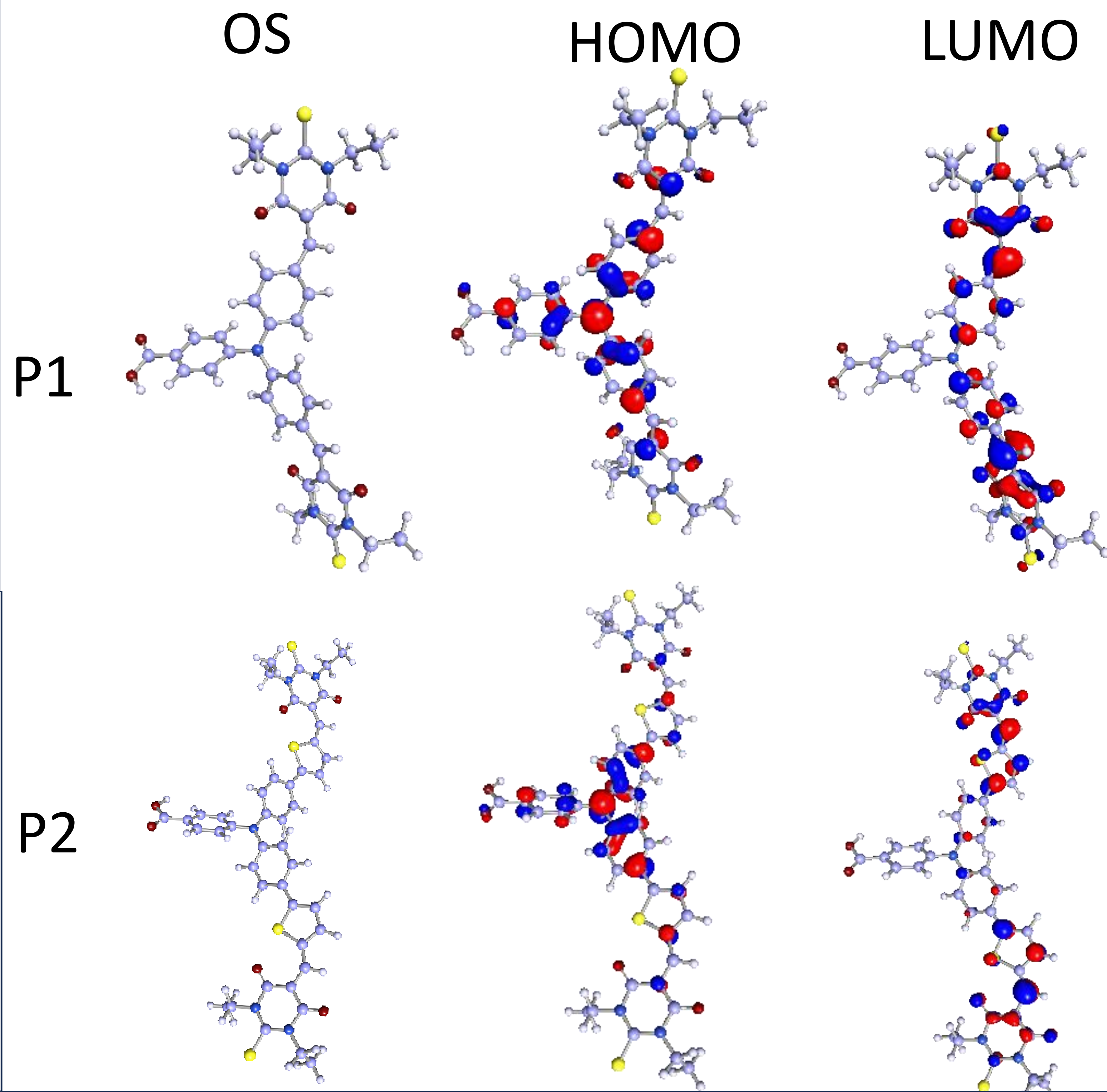
Department of Chemistry, Nitte Meenakshi Institute of Technology Bengaluru, India.

**Introduction:** Triphenylamine-based organic dyes are promising sensitizers for dye-sensitized solar cells due to their excellent electron-donating ability and tunable structures. This study employs DFT and TD-DFT to investigate their electronic and optical properties, providing insights for designing efficient light-harvesting materials.

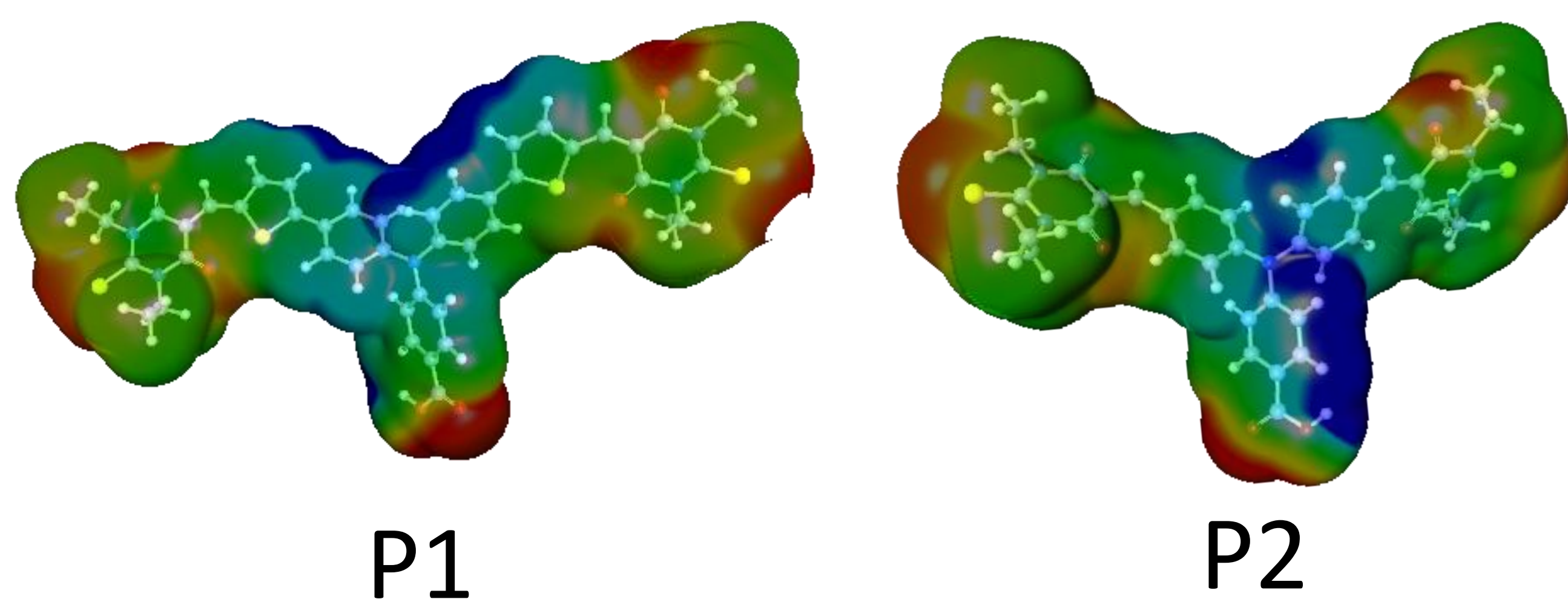
## Working Principle



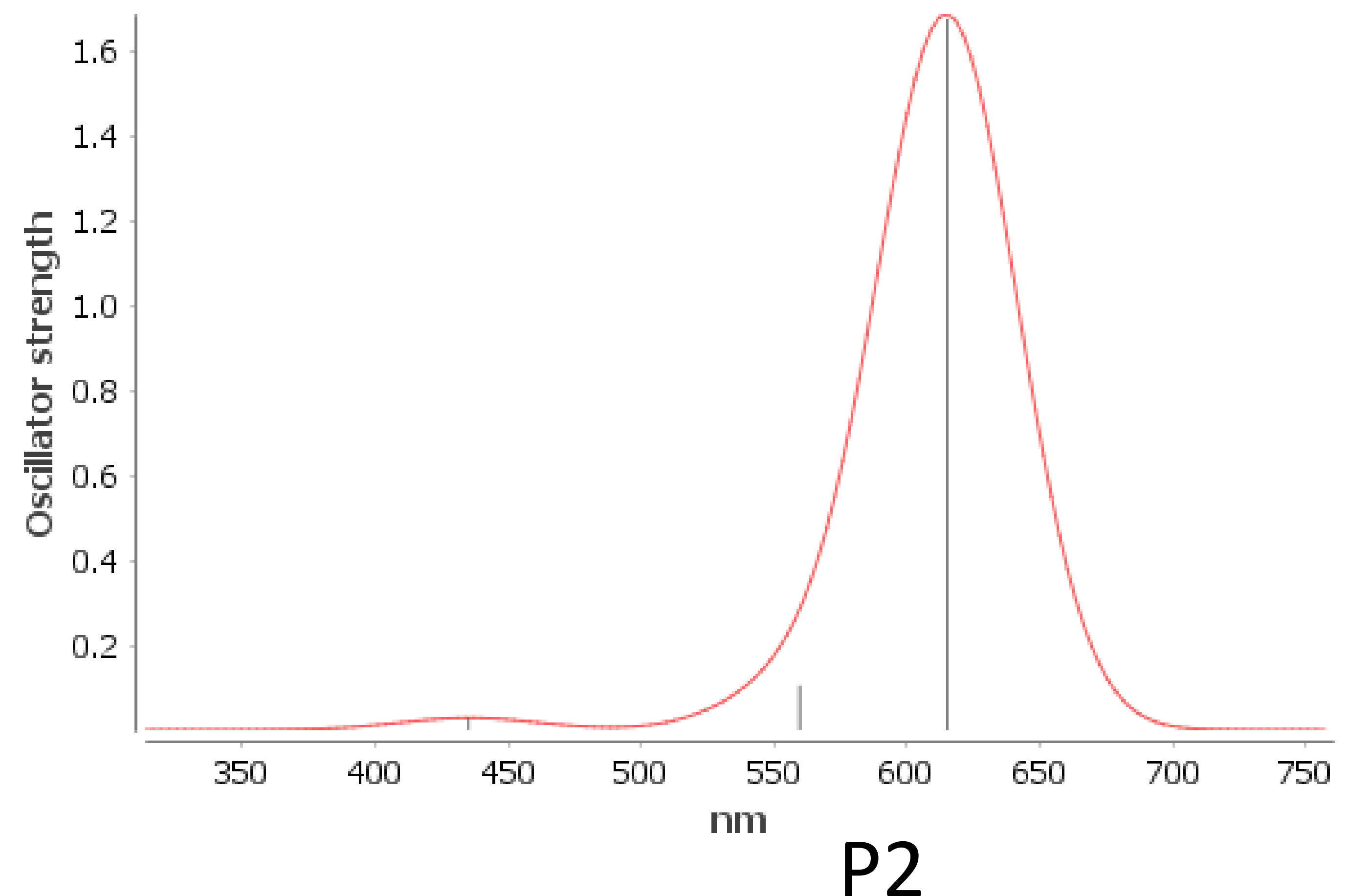
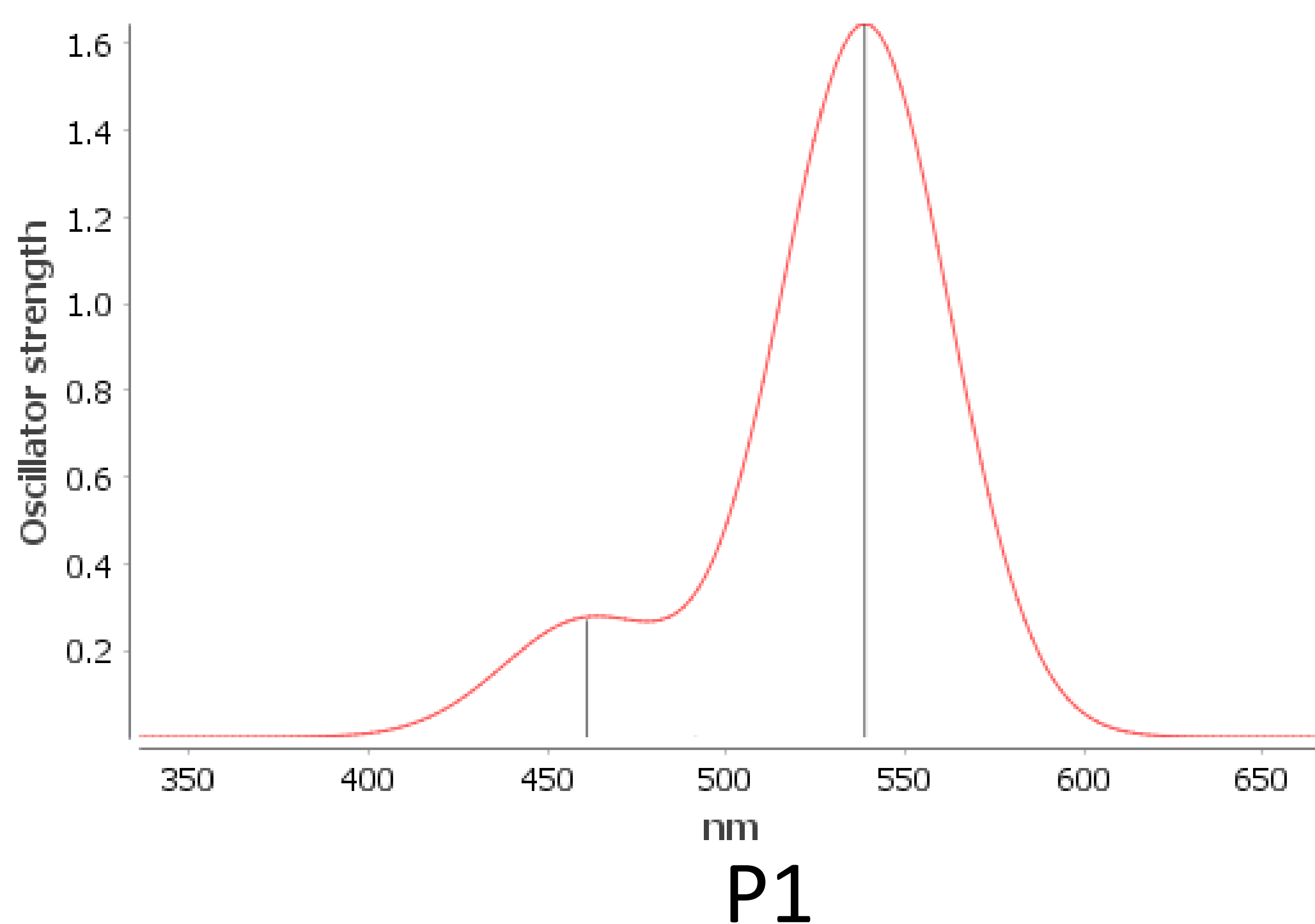
## Designed P2 dye along with Standard P1



## Electrostatic potential map



## Simulated Absorption Spectra



## Conclusion

- Triphenylamine-based dyes exhibit suitable electronic properties, with HOMO–LUMO alignment facilitating efficient charge transfer and electron injection in DSSCs.
- Structural modifications, particularly increased  $\pi$ -conjugation and molecular planarity, reduce energy gaps and enhance intramolecular charge transfer.
- TD-DFT results indicate red-shifted absorption with higher oscillator strength, improving overlap with the solar spectrum and light-harvesting efficiency.
- Molecular electrostatic potential analysis reveals effective donor–acceptor interactions, providing guidance for designing high-performance organic sensitizers.

## References

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