

# Balancing Molecular Twist & Conformational Rigidity In Imidazo[1,2-a]pyridines To Achieve Dual-state Emissive Luminogens For Applications In Oleds & Cell-imaging

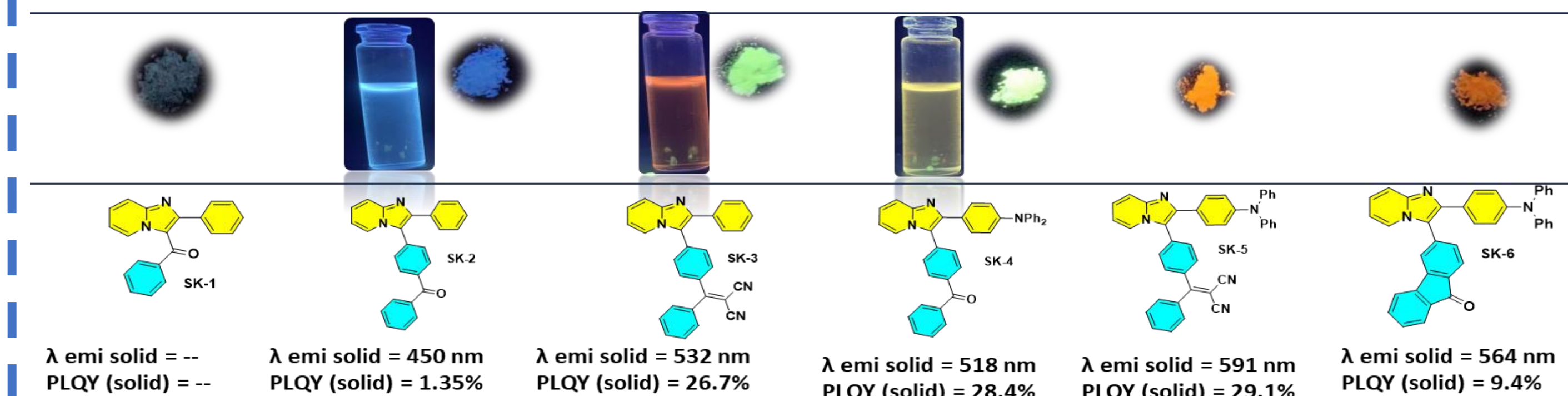
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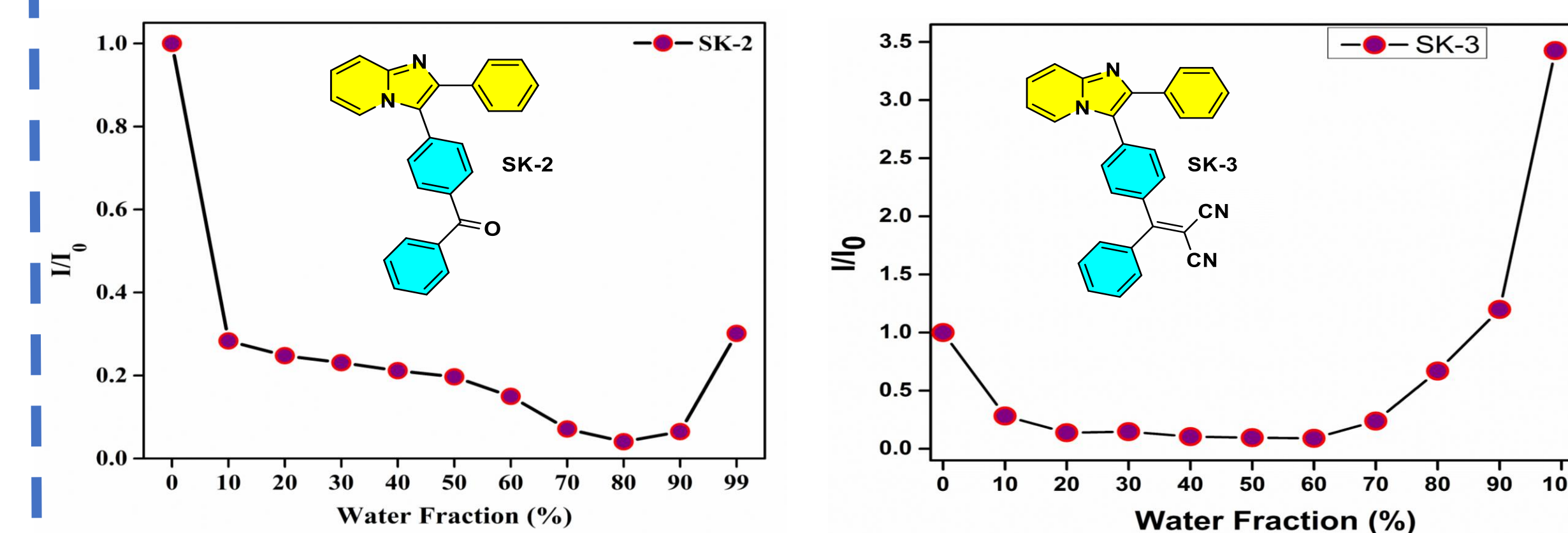
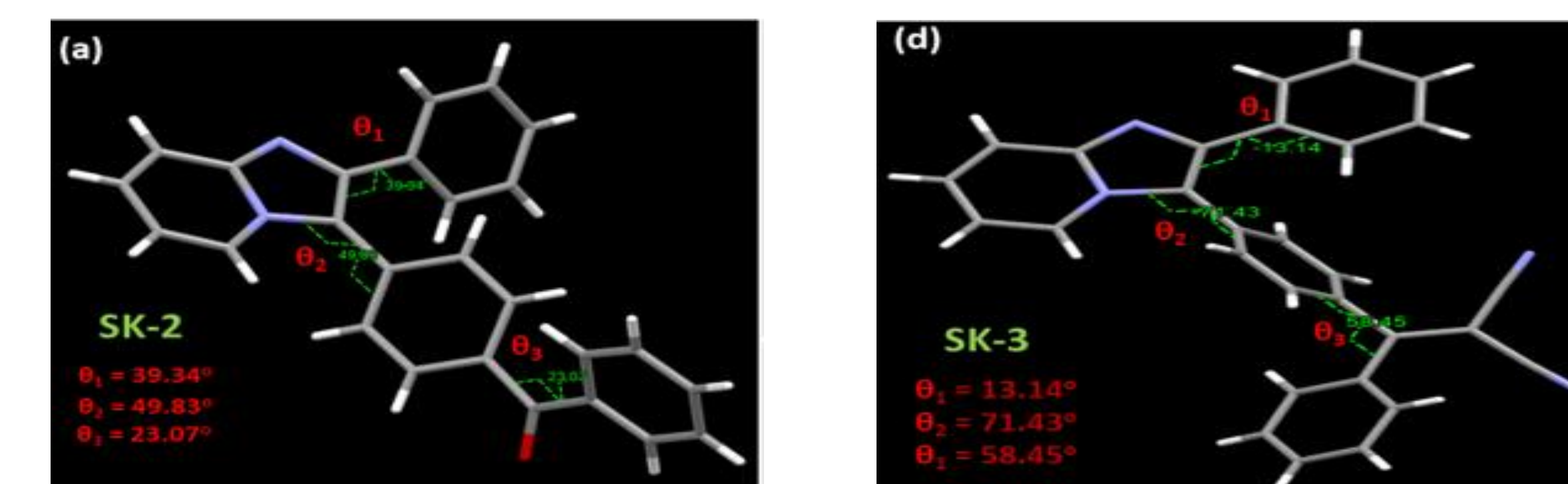


## Photophysical Properties of all the Luminogens



## Single Crystal Analysis and Aggregation Induced Emission of SK-2 and SK-3

Dihedral angles between the imidazo[1,2-a]pyridine ring and the phenyl rings of -COPh of SK-2 = **49.83°** and -C(CN)<sub>2</sub>Ph in SK-3 = **71.43°** which accounts for their differences in their emissive properties.



## Luminescence

## Introduction

Luminescent molecules have become indispensable in our daily life. Particularly, photoluminescence has created a revolution in many scientific innovations and technological advancements

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

Many chromophores are fluorescent in solutions but become less or even non-emissive when fabricated into thin solid films

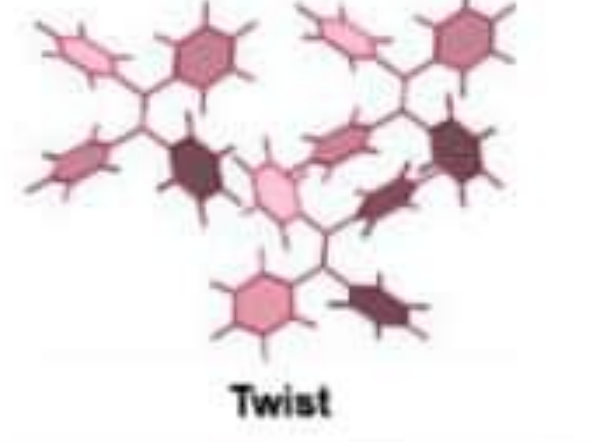
## Aggregation Caused Quenching



## Rigidity



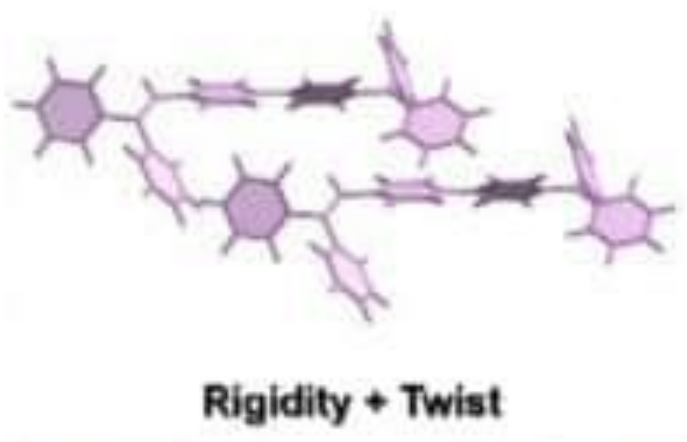
Aggregation-caused quenching  
Only emissive in solution



## Twist



Aggregation-induced emission  
Only emissive in aggregates



## Rigidity + Twist



Dual-state emission  
Both emissive in solution and aggregates

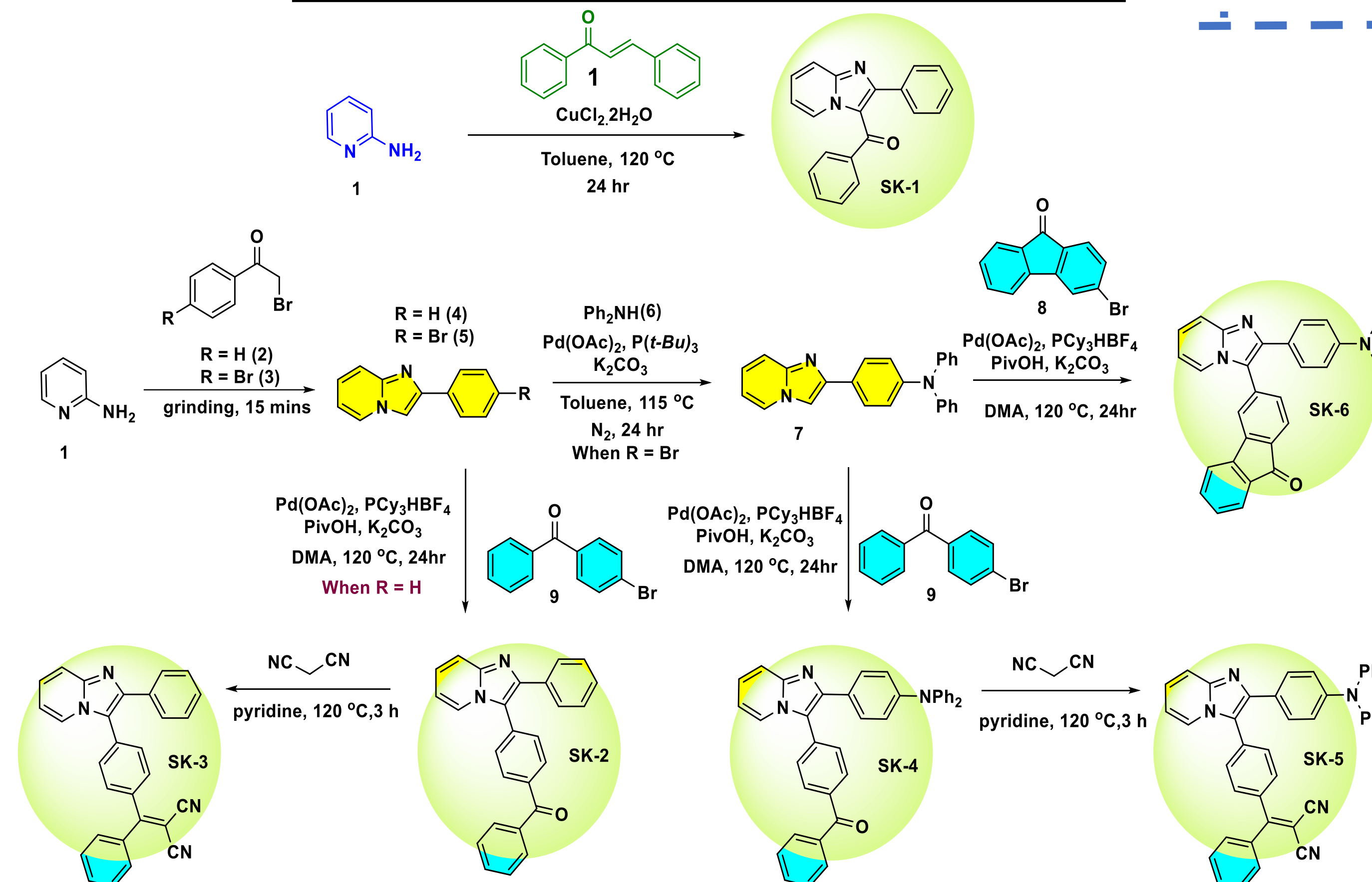
## Dual State Emissive Luminogens (DSEgens)



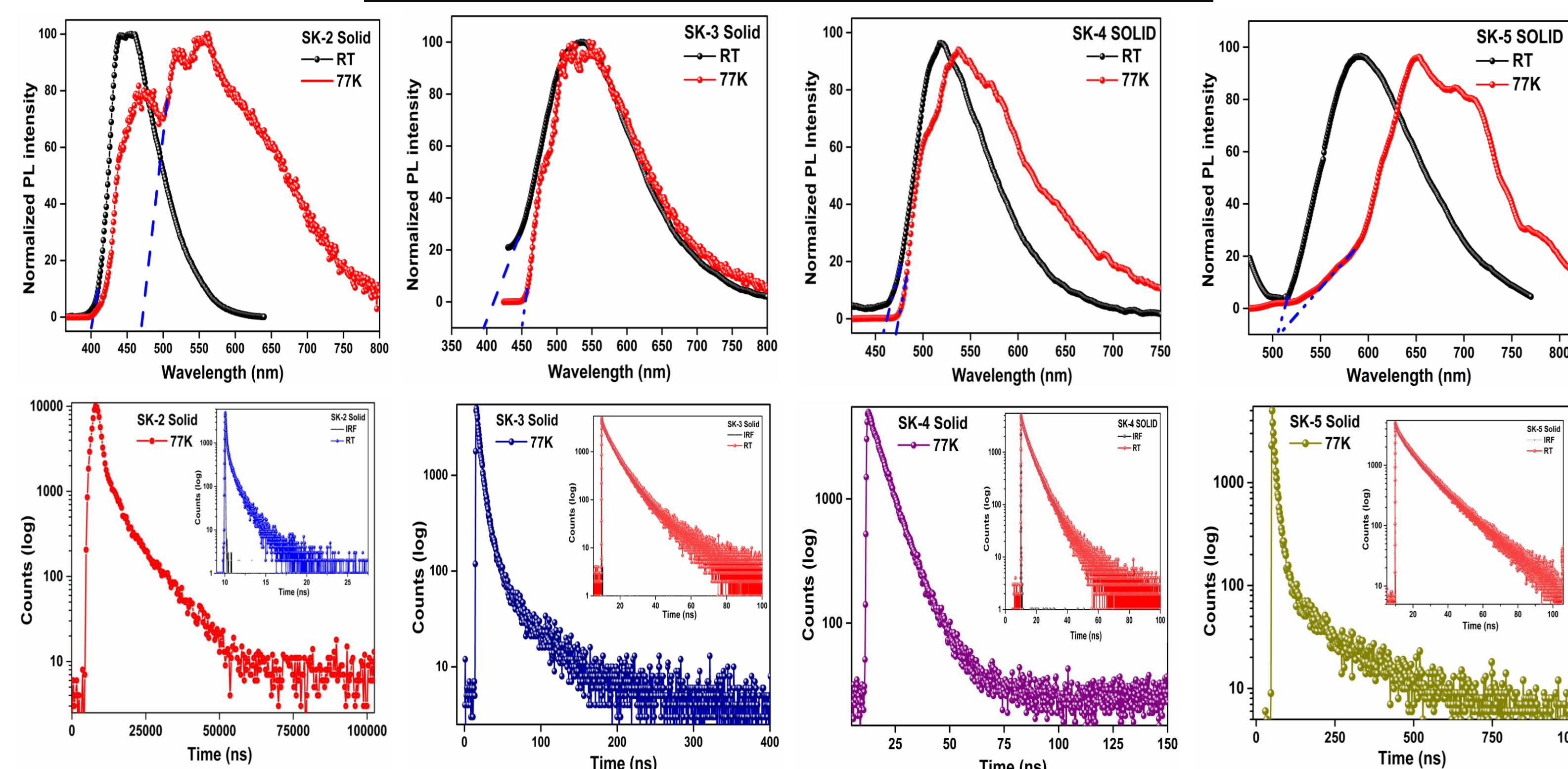
## Existing Strategies to Create DSEgens

- The use of highly conjugated and twisted structures
- The inclusion of aliphatic chains or voluminous substituents in the periphery of the molecules
- The inclusion of heteroatoms to achieve donor-acceptor (D-A) architectures

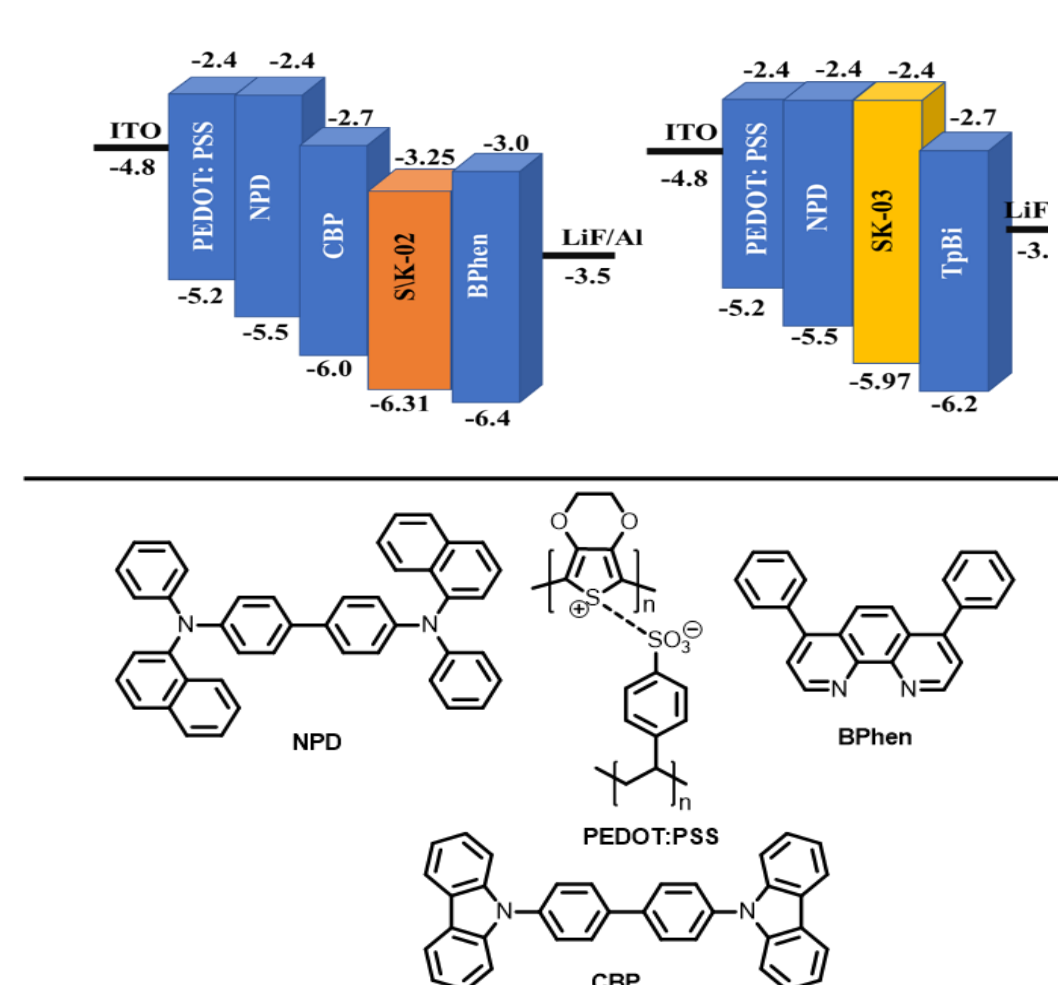
## Synthesis of SK-1 to SK-6



## Thermally Activated Delayed Fluorescence Analysis



| Compound | $\lambda_{abs}$ (nm) liquid | $\lambda_{em}$ (nm) liquid | $\lambda_{em}$ (nm) solid | FWHM (nm) | $\phi_{PL}$ (%) thin film | $\Delta_{ST}$ (eV) Calculated | $\Delta_{ST}$ (eV) Experimental | $\tau_p$ (ns) Solid | $\tau_d$ (ns) Solid |
|----------|-----------------------------|----------------------------|---------------------------|-----------|---------------------------|-------------------------------|---------------------------------|---------------------|---------------------|
| SK-2     | 252, 338                    | 473                        | 450                       | 74        | 1.35                      | 0.4554                        | 0.4604                          | 0.115               | 4879                |
| SK-3     | 312, 405                    | 566                        | 534                       | 121       | 26.7                      | 2.59                          | 0.3908                          | 4.74                | 13.89               |
| SK-4     | 244, 346                    | 535                        | 518                       | 90        | 28.45                     | 0.110                         | 0.1014                          | 4.23                | 8.321               |
| SK-5     | 304, 450                    | 505                        | 558                       | 117       | 29.1                      | 0.058                         | 0.0246                          | 9.17                | 60.3                |
| SK-6     | 257, 350                    | 535                        | 560                       | 69        | 9.4                       | 0.090                         | 0.068                           | 1.76                | 24                  |

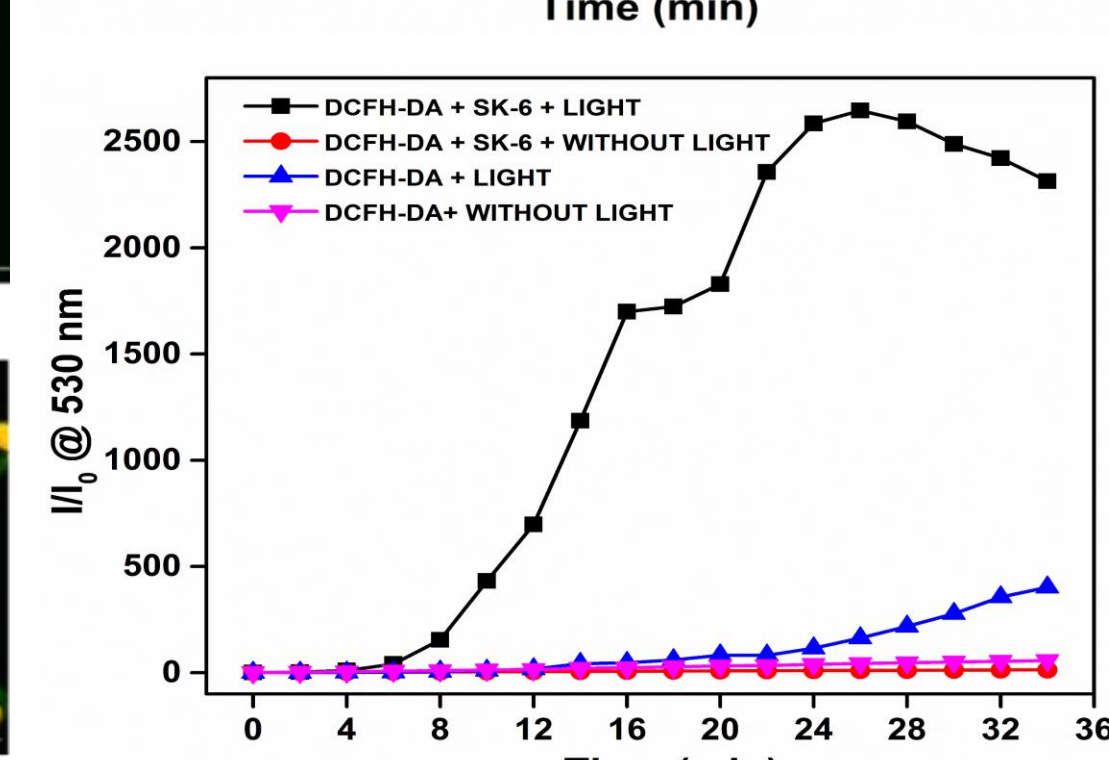
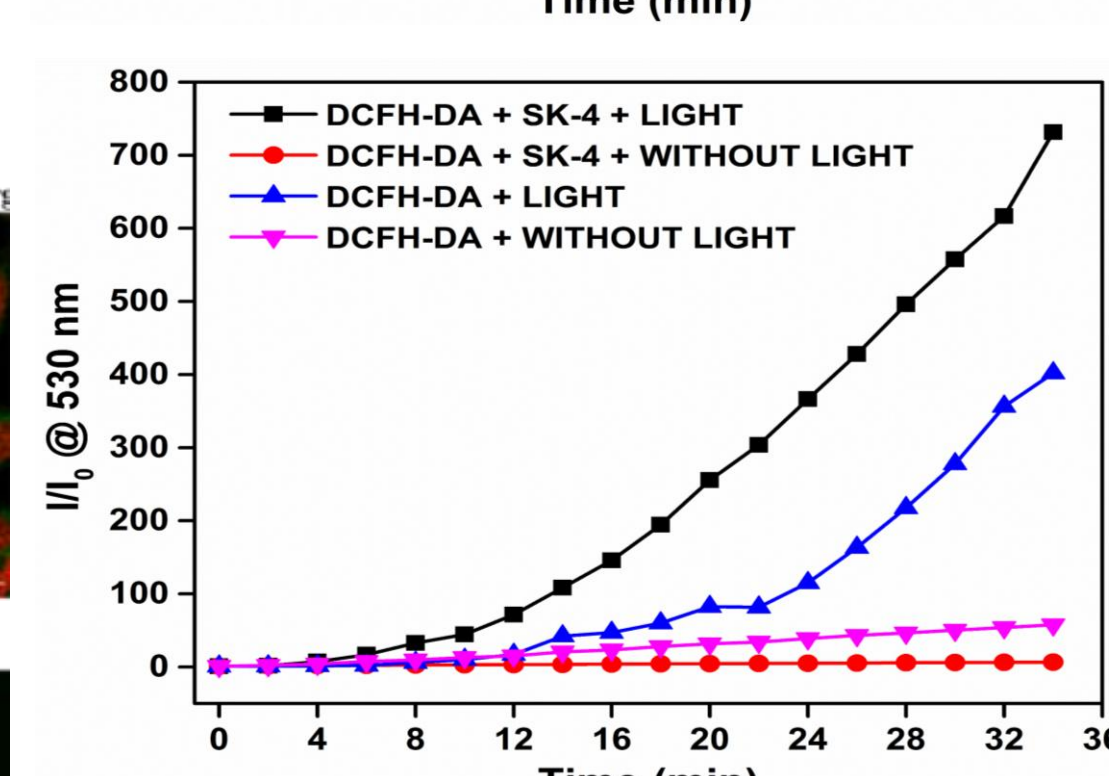
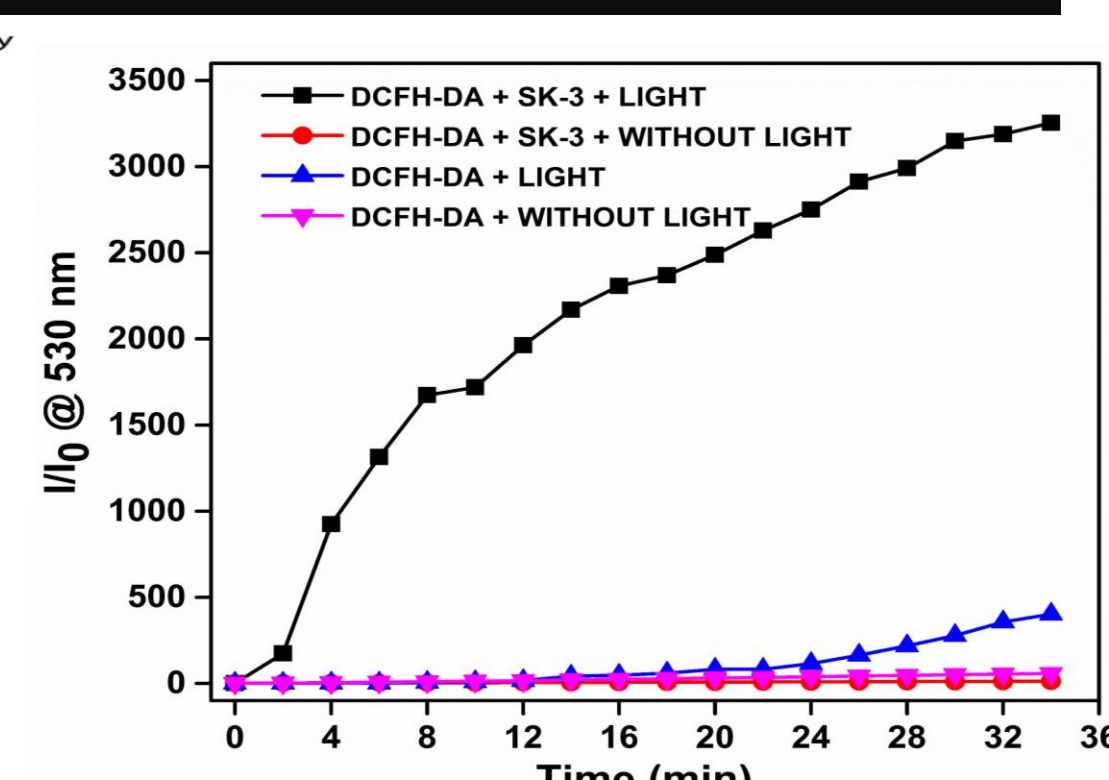
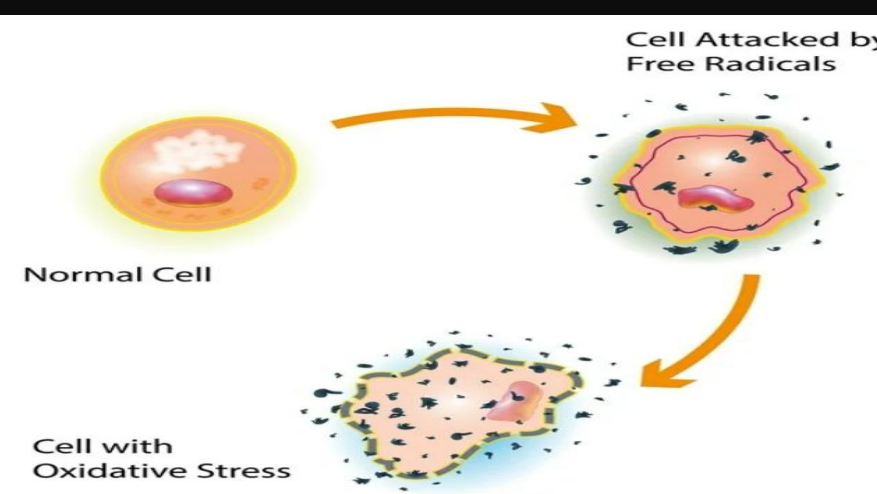


| Device | EML  | $V_{on}$ (@ $L = 1$ Cd/m <sup>2</sup> ) in V | $\lambda_{peak}$ (nm) | CIE (x,y)    | EQE <sub>max</sub> |
|--------|------|----------------------------------------------|-----------------------|--------------|--------------------|
| 4      | SK-2 | 5.0                                          | 583                   | (0.50, 0.45) | 6.4%               |
| 5      | SK-3 | 4.5                                          | 538                   | (0.33, 0.44) | 10.0%              |

**Conclusions:** ➤ Engineered imidazo[1,2-a]pyridines to solid state and dual state emissive luminogens  
➤ Potential molecules for simultaneous cancer cell imaging on (SiHa cells) with extremely low IC<sub>50</sub> values  
➤ Molecules show TADF properties and used for OLED application with EQE as high as **10.2%**

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**References:** 1) J. Mater. Chem. C., 2025, 13, 10576-10591.

## Bio-Imaging and ROS study of SK-3, SK-4, SK-6



- Luminogens are highly bio-compatible on SiHa cells (cervical cancer cells) – **10 µg/ml**
- Luminogens could pass through the cell wall and were emissive even in the nucleus of the cells
- ROS study revealed combined effect of imidazopyridine core and ROS generation capacity of the compounds

