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## Structure-activity relationship in NIR photosensitizers for transparent Dye-Sensitized Solar Cells

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# Structure-activity relationship in NIR photosensitizers for transparent Dye-Sensitized Solar Cells

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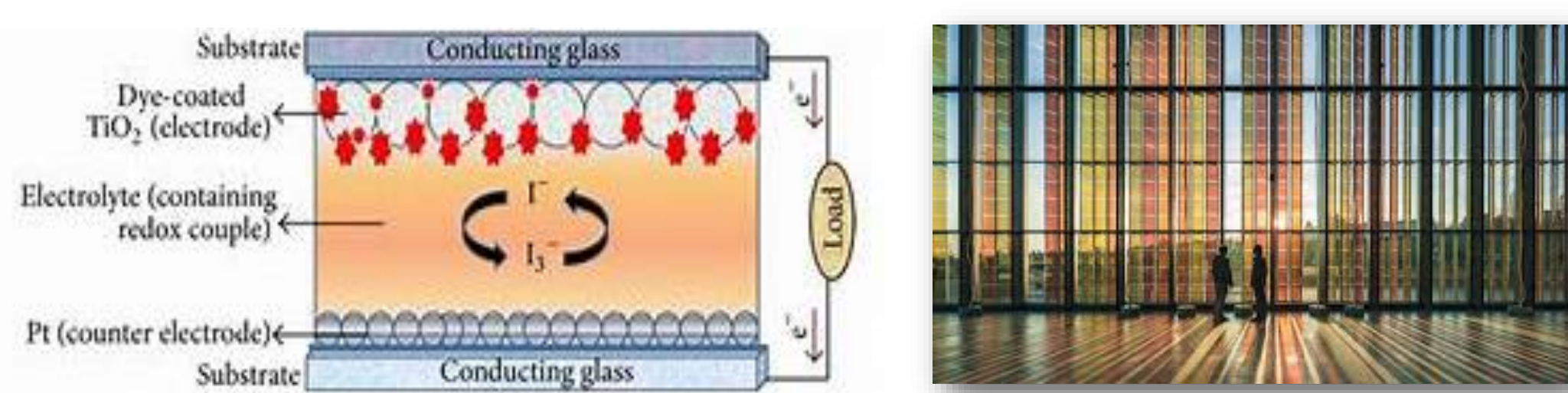
Dye-Sensitized Solar Cells (DSSCs) offer an interesting and sustainable choice for the development of transparent, and even colorless, photovoltaic devices, thanks to their ability to exploit diffuse and low-intensity light as well as their wide versatility in dyes, electrolytes and redox couples. Among them, the photosensitizer plays a crucial role in obtaining transparent wavelength-selective NIR-DSSC system [1]. Until now, different families of NIR chromophores have been investigated with relatively low success in terms of transparency to visible light and power conversion efficiency. In this work, thanks to the joint efforts of different research groups within the European IMPRESSIVE project, we proposed fully transparent DSSCs based on organic polymethine dyes that show intense absorption in NIR region close to 900 nm, while negligible in visible region. Power conversion efficiency up to 3% and average visible transmittance (AVT) up to 76% have been obtained, while reaching a color rendering index (CRI) of 92 [2]. Starting from these results and their structure-activity relationship, innovative strategies on synthesis approach and device optimization should be applied to outperform the obtained values and to design stable and low-cost materials for the implementation in real devices [3].

## BUILDING INTEGRATED PHOTOVOLTAICS

### Dye-sensitized solar cells in BIPV

- ✓ Architectural compatibility
- ✓ Environmental compatibility
- ✓ Weak / diffuse light
- ✓ Indoor / IoT
- ✓ Tunable colours

...from highly coloured to transparent non intrusive PV...

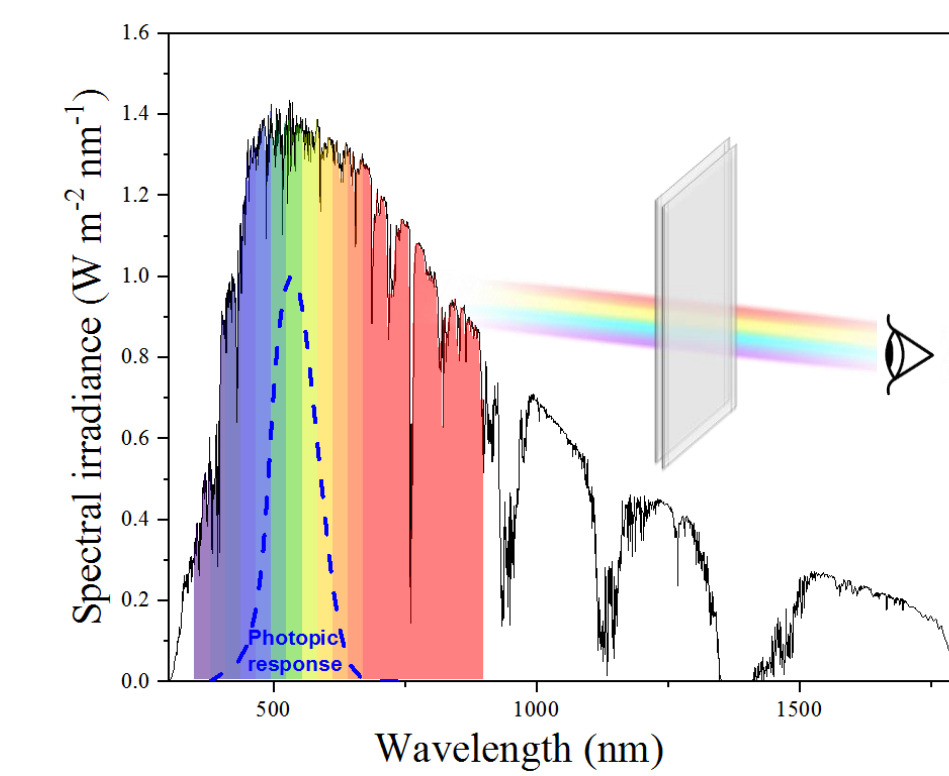


### Transparent and sustainable DSSC

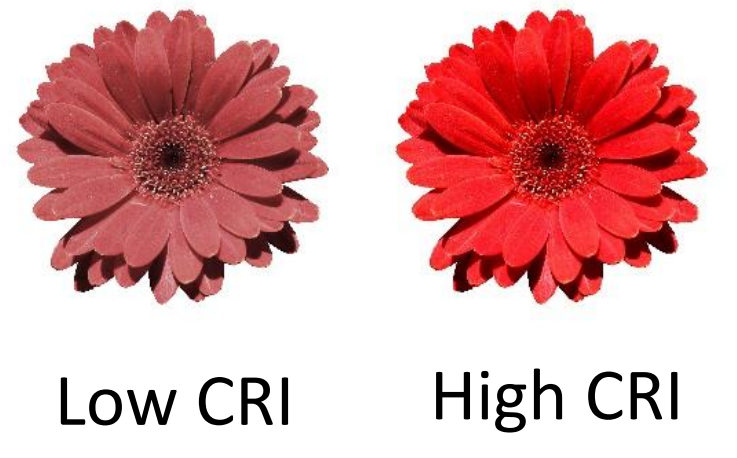
efficiency vs aesthetics?

Average Visible Transmittance (AVT)

Light Utilization Efficiency  
LUE = AVT x PCE



### Color Rendering Index

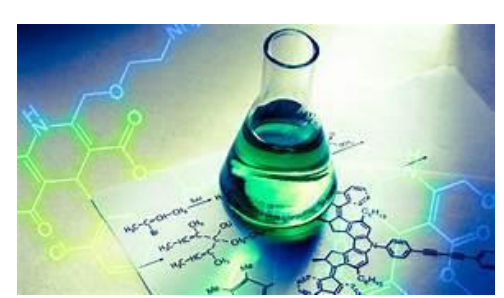


Aesthetic quality: Optical transparency and high CRI

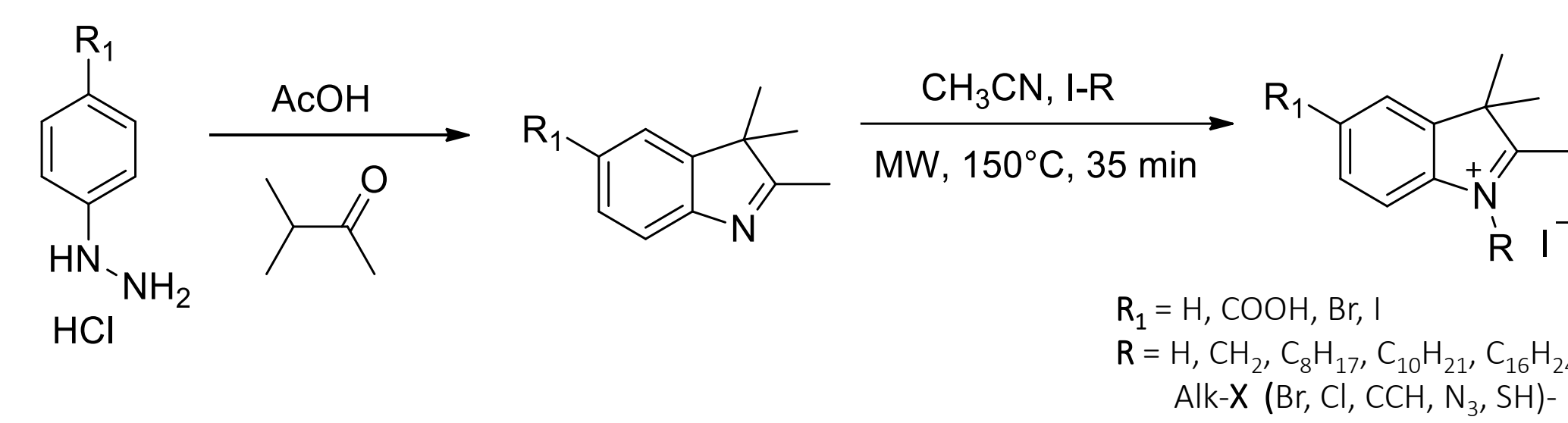
## NEAR-IR POLYMETHINE DYES

30+ selective NIR dyes developed based on polymethine dyes and derivatives

Selective absorption in Near-IR (negligible in visible)

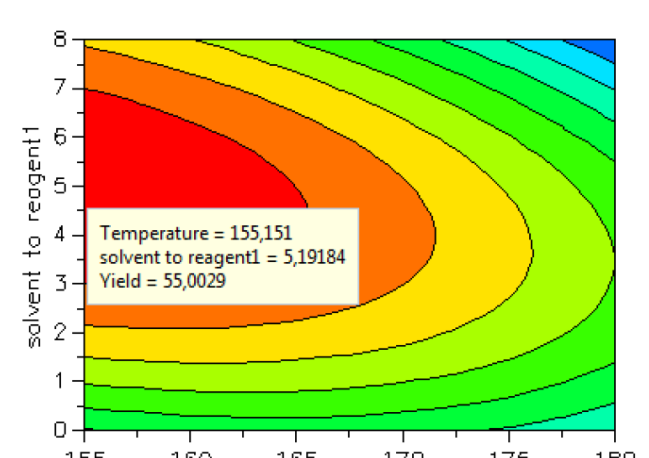


Quaternization reactions in order to increase the acidity of the methyl group



MW synthesis:

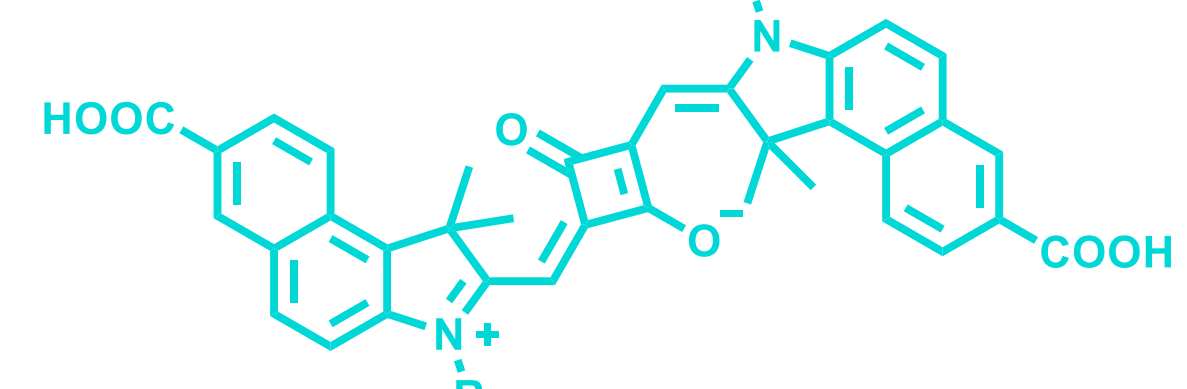
- Reduce time and byproducts
- Increase yields
- Avoid anhydrous conditions



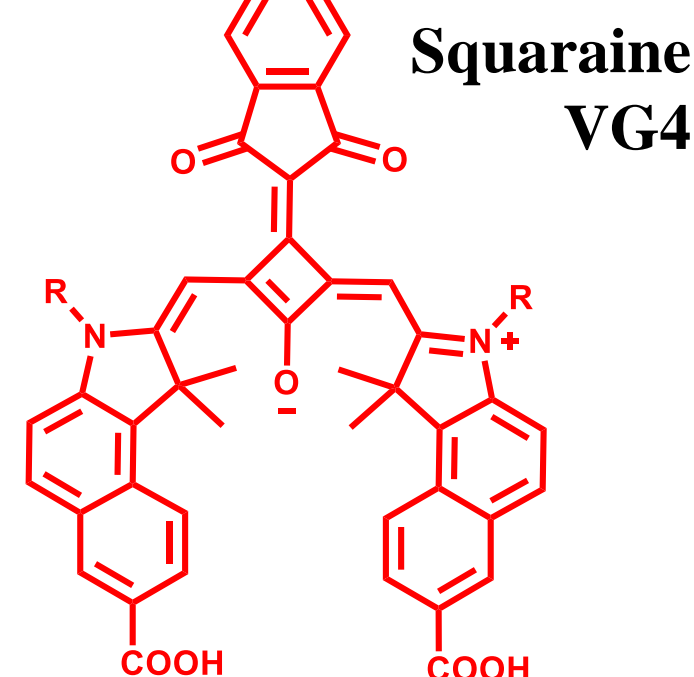
Design of Experiment

### Central core and π-π conjugation

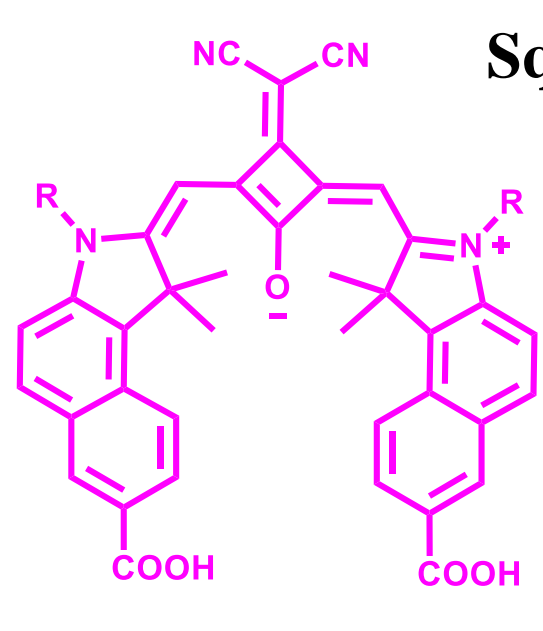
#### Squaraine VG10



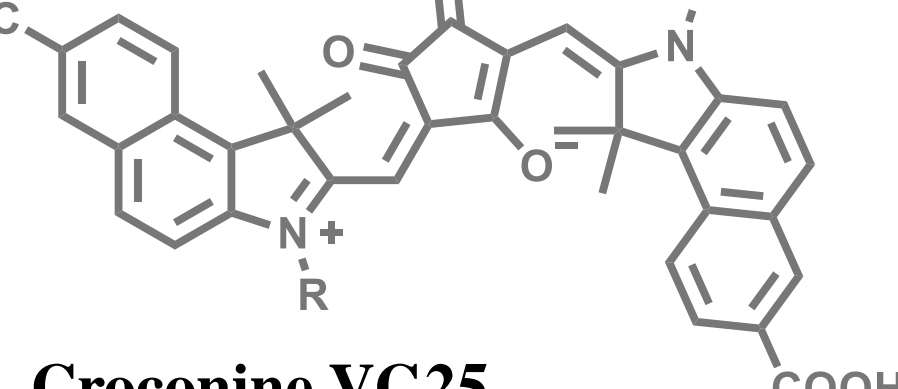
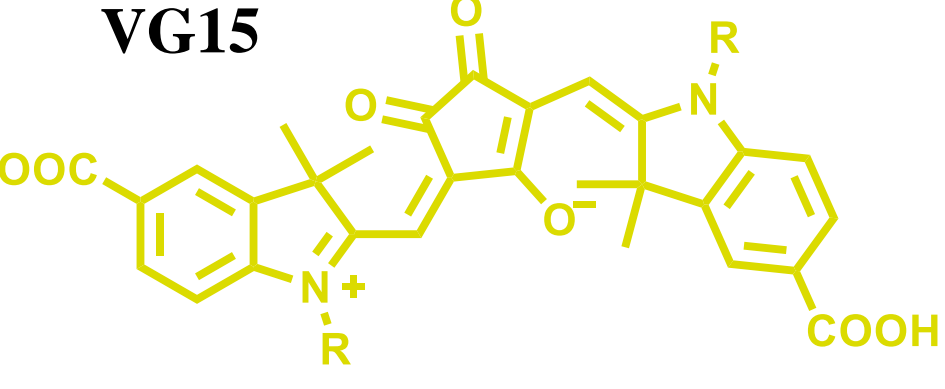
#### Squaraine VG4



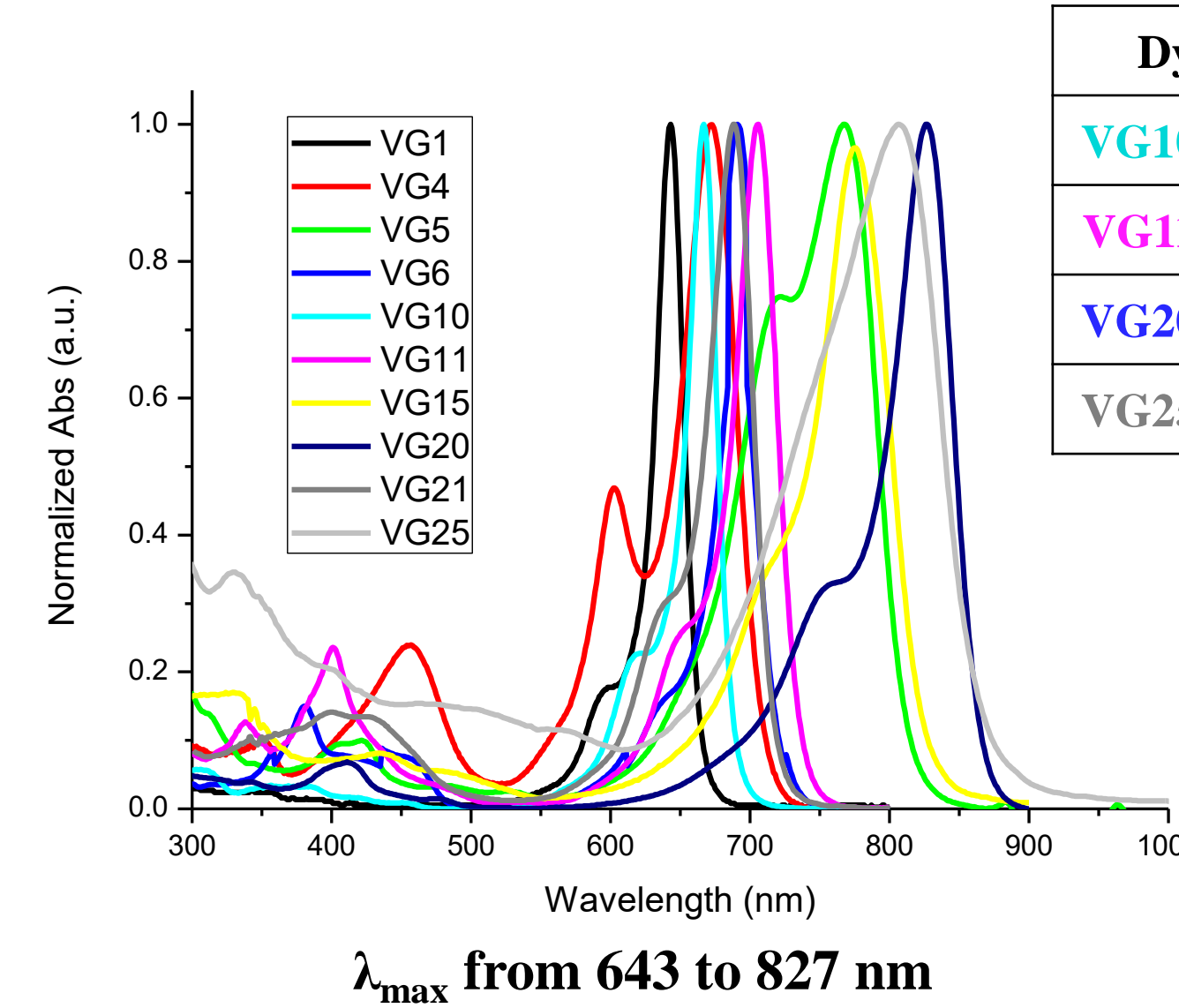
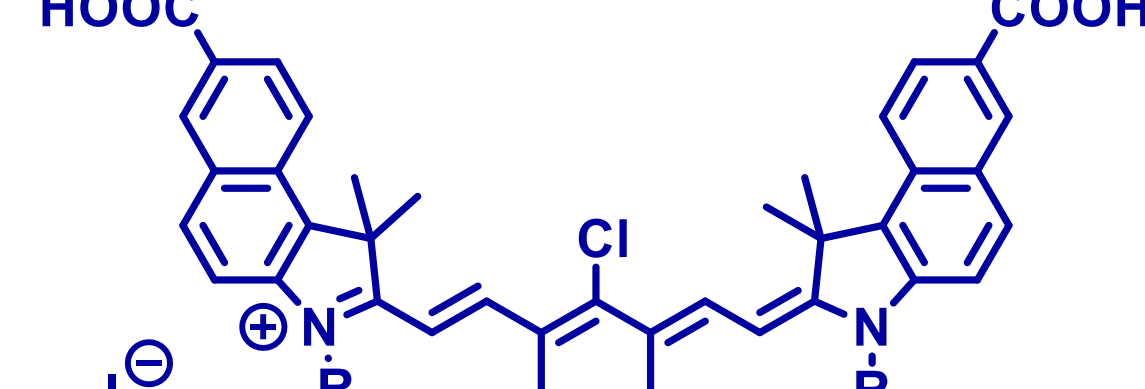
#### Squaraine VG11



#### Croconine VG15

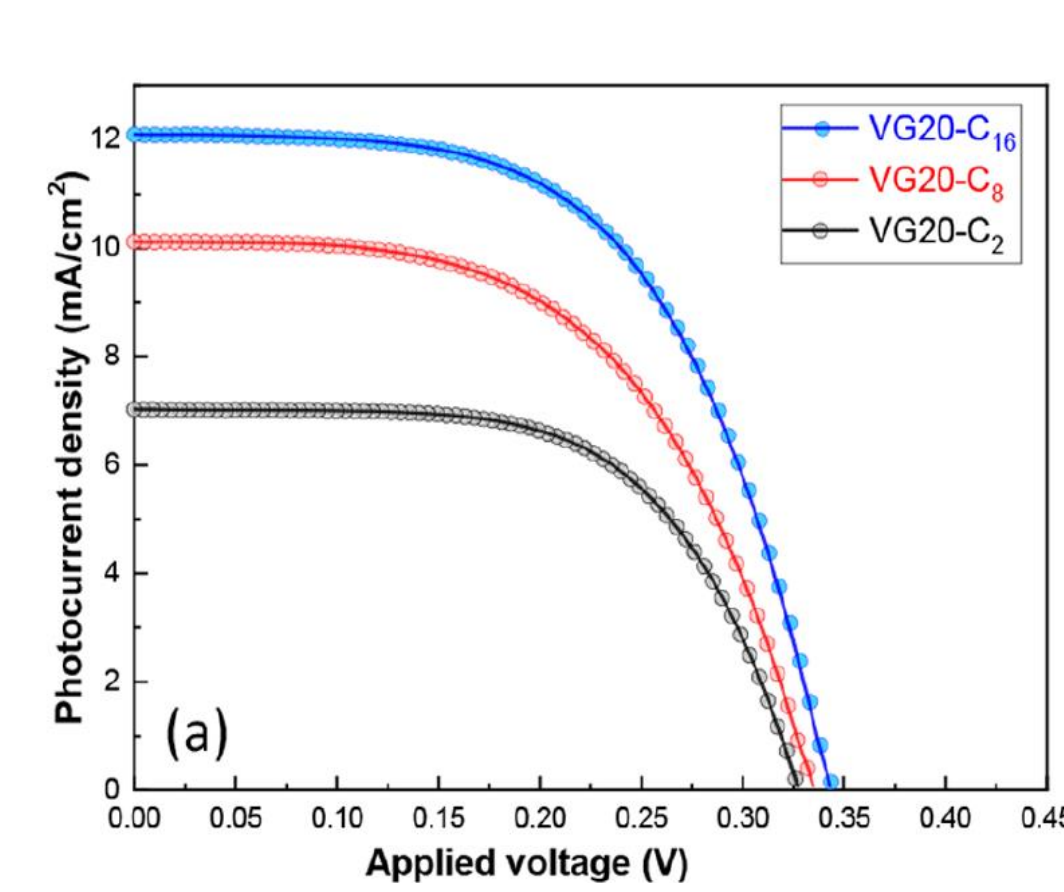


#### Cyanine VG20



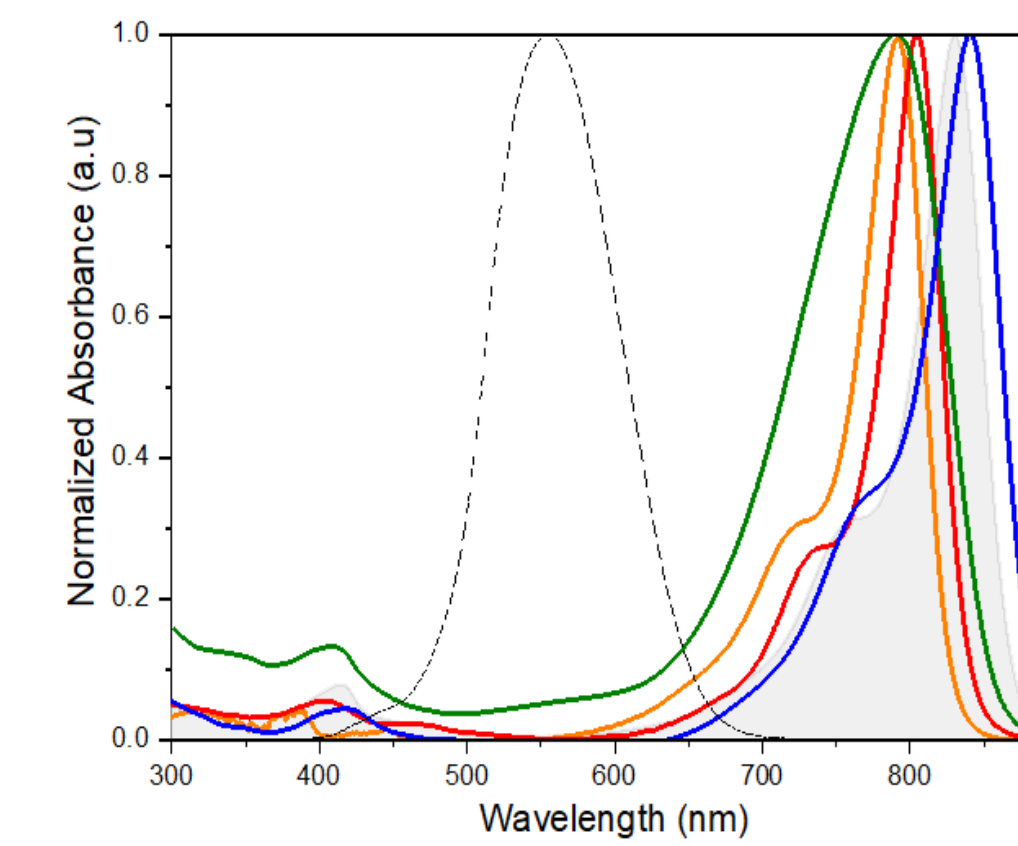
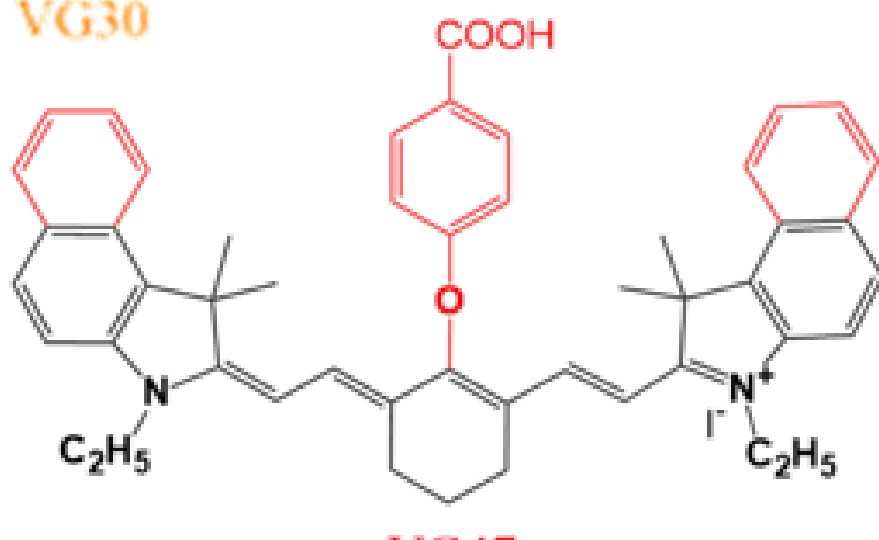
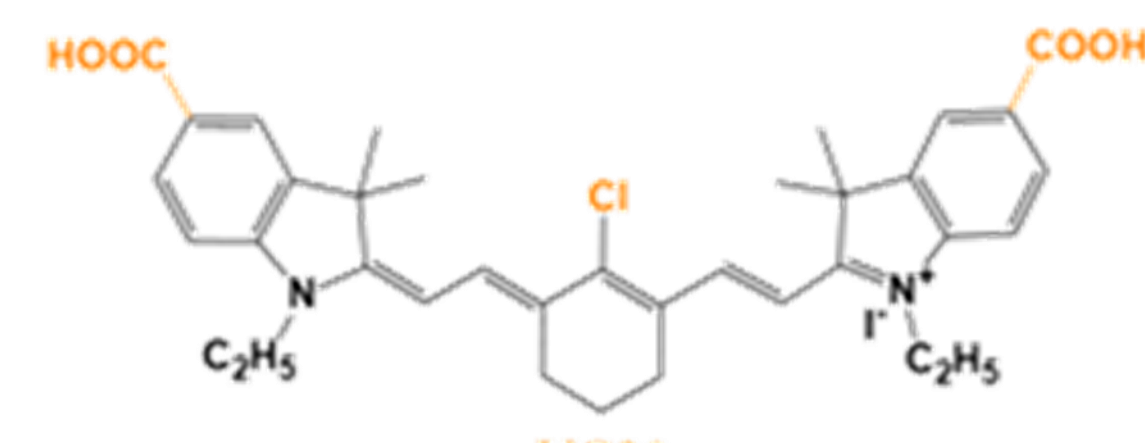
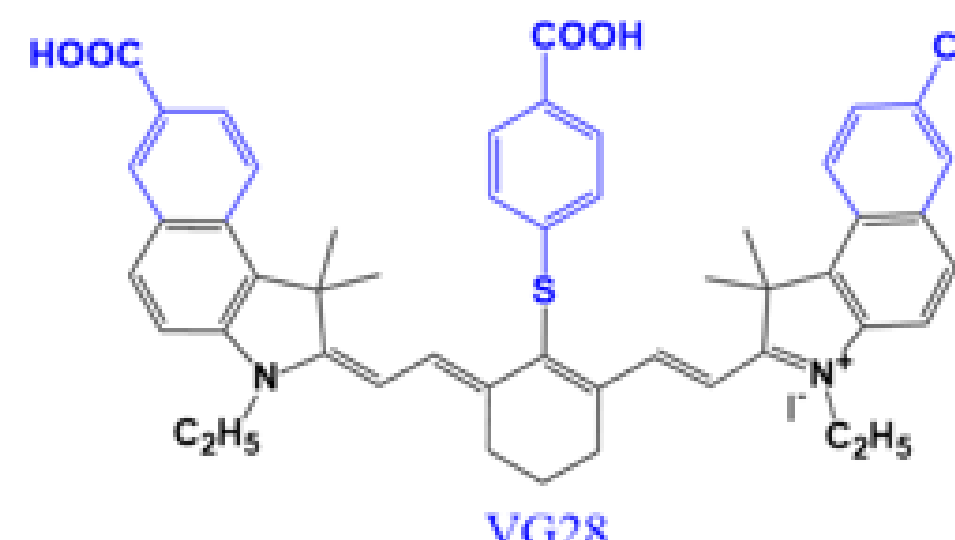
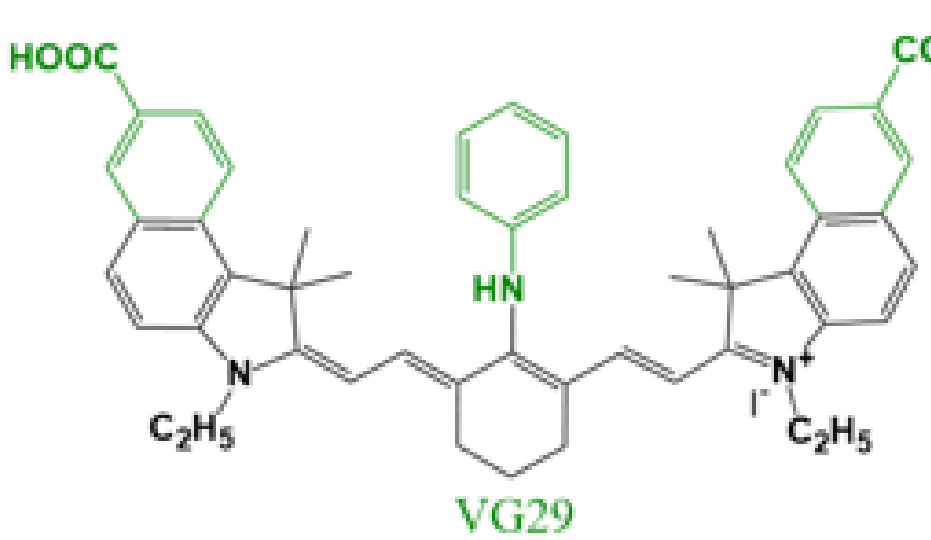
Dye	PCE (%)
VG10-C8	6.1
VG11-C8	2.5
VG20-C8	1.9
VG25-C8	0.3

### Alkyl chain length



## NIR cyanines to improve chemical-physical properties

Substitutions on the linker chain between benzo[e]indole moieties



Dye	J <sub>sc</sub> (mA/cm <sup>2</sup> )	V <sub>oc</sub> (mV)	PCE (%)
VG20-C16	13.0	375	3.1
VG20-C2	7.8	415	2.2
VG28-C2	8.1	275	1.4
VG29-C2	9.1	422	2.4
VG30-C2	7.2	340	1.9
VG47-C2	1.3	328	0.32

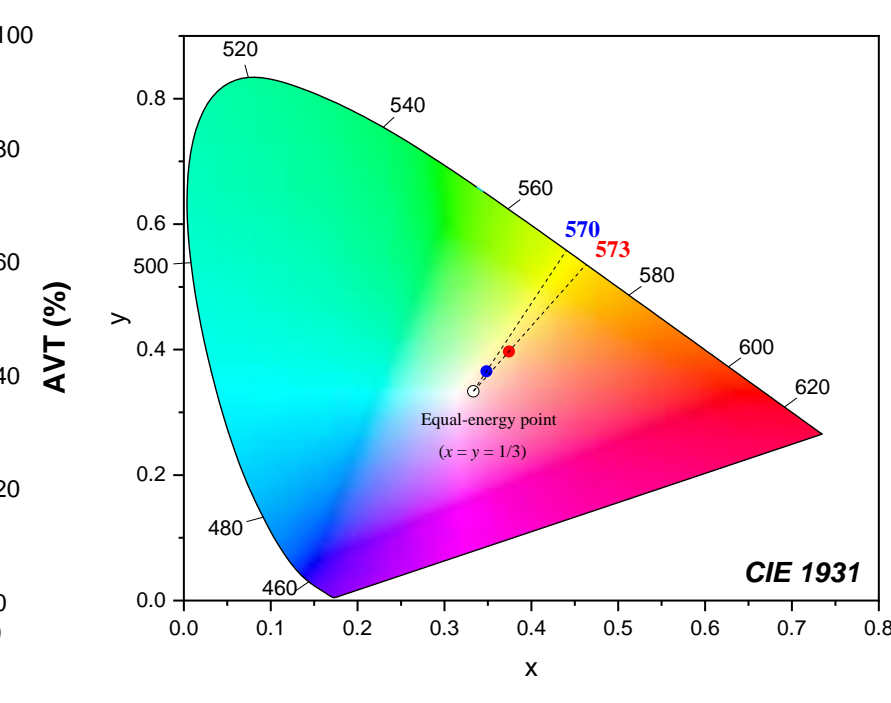
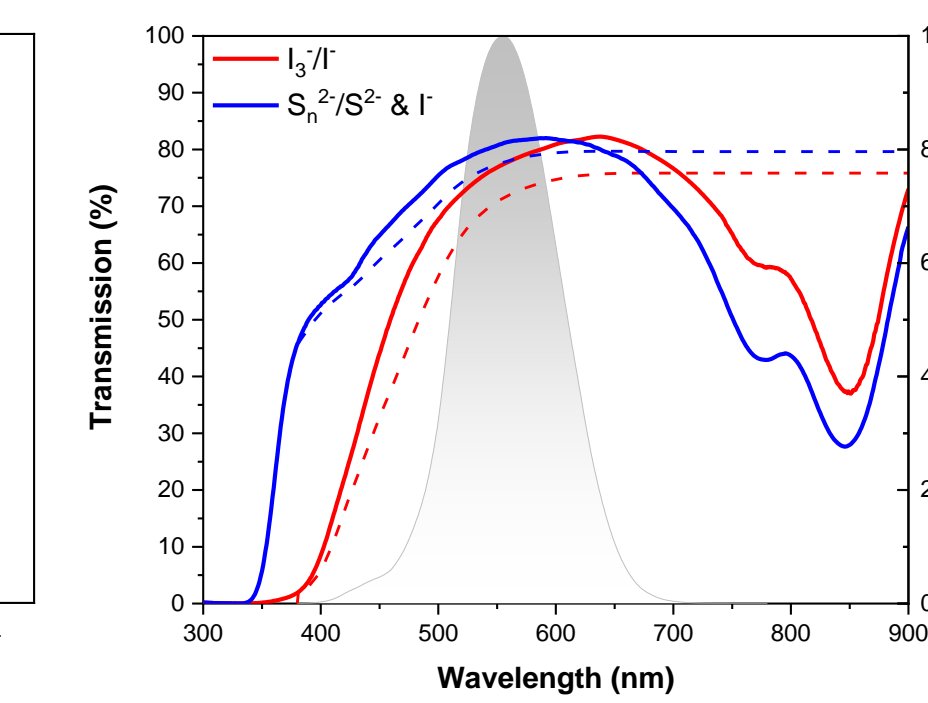
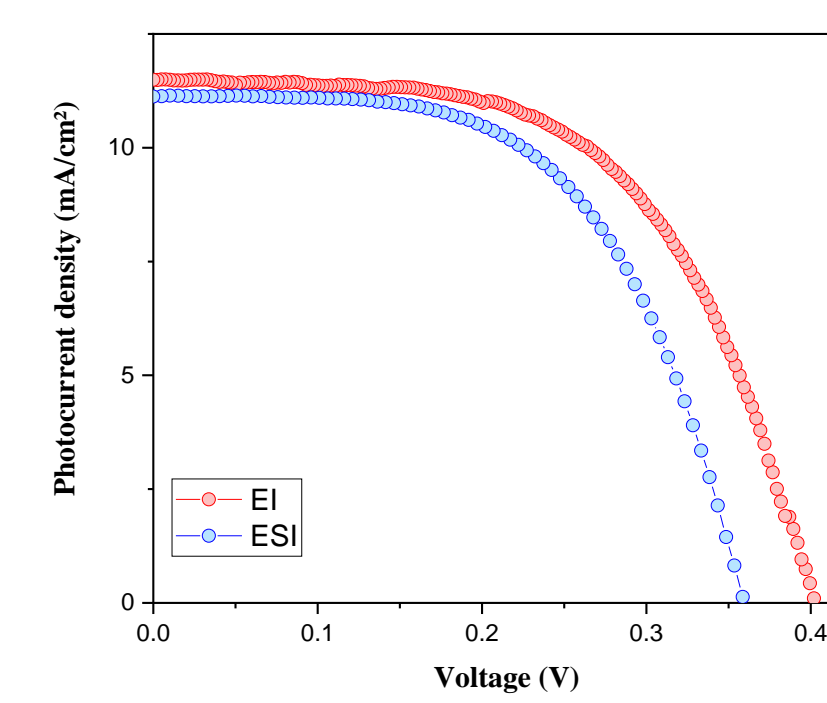
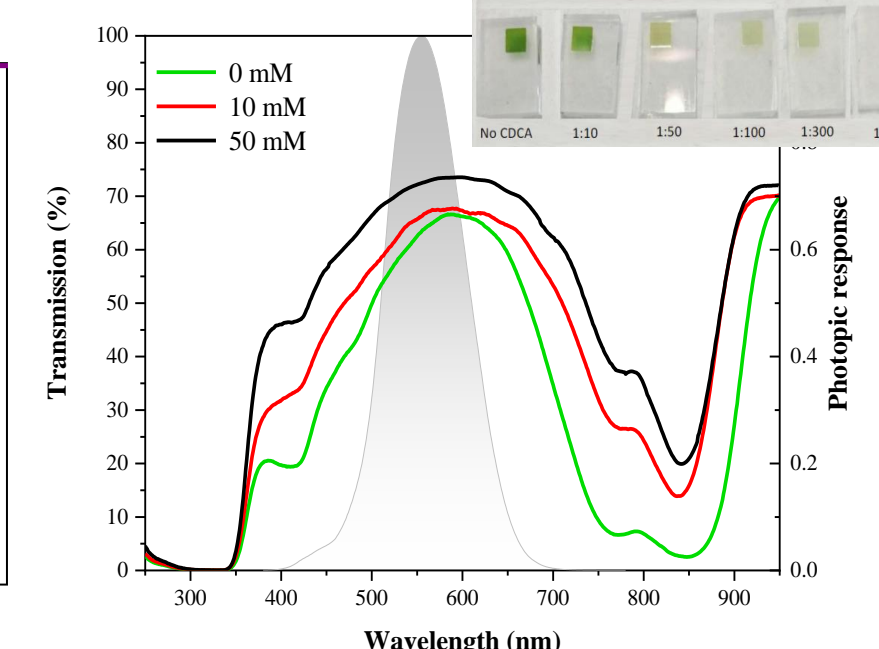
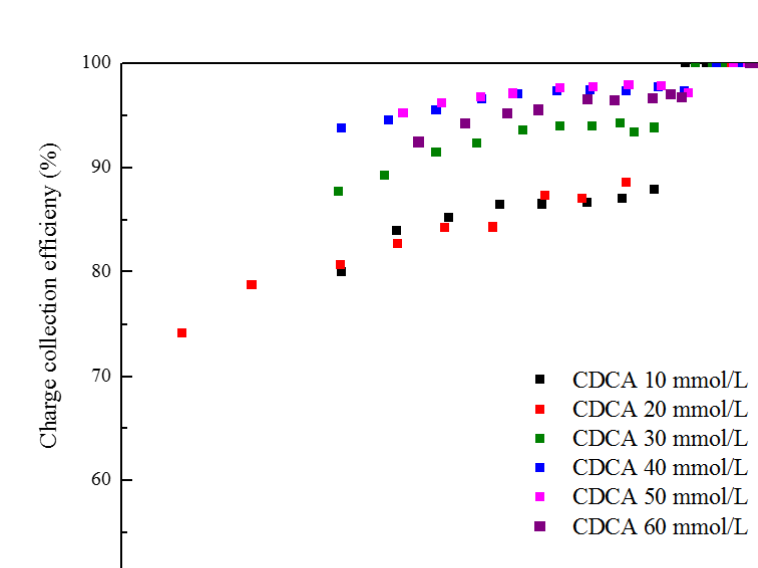
## TRANSPARENT DSSCs WITH VG20-C16

Reaching balance between performance and aesthetics

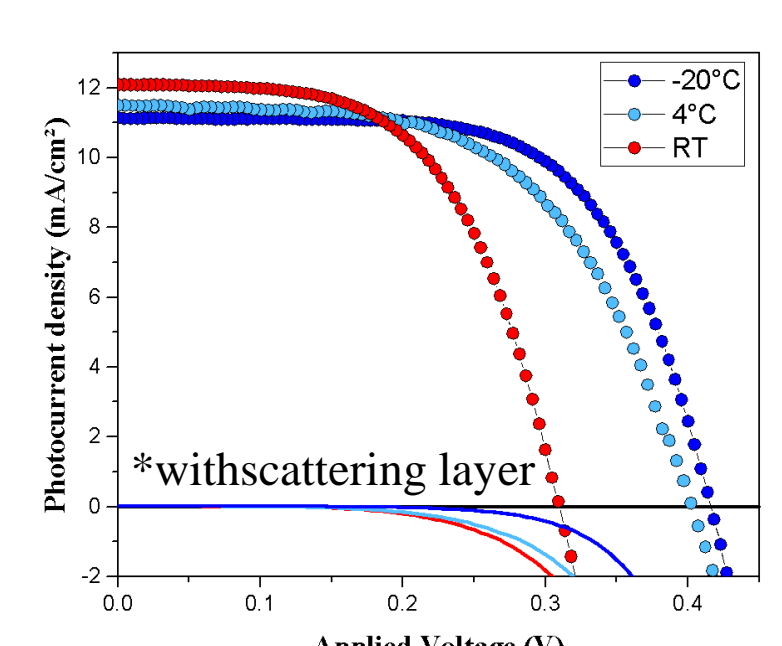
Decreasing in dye loading

CDCA (mM)	AVT (%)	CRI	PCE <sup>a</sup> (%)
0	61	90.3	0.5
10	64	93.8	1.8
50	71	95.8	2.6

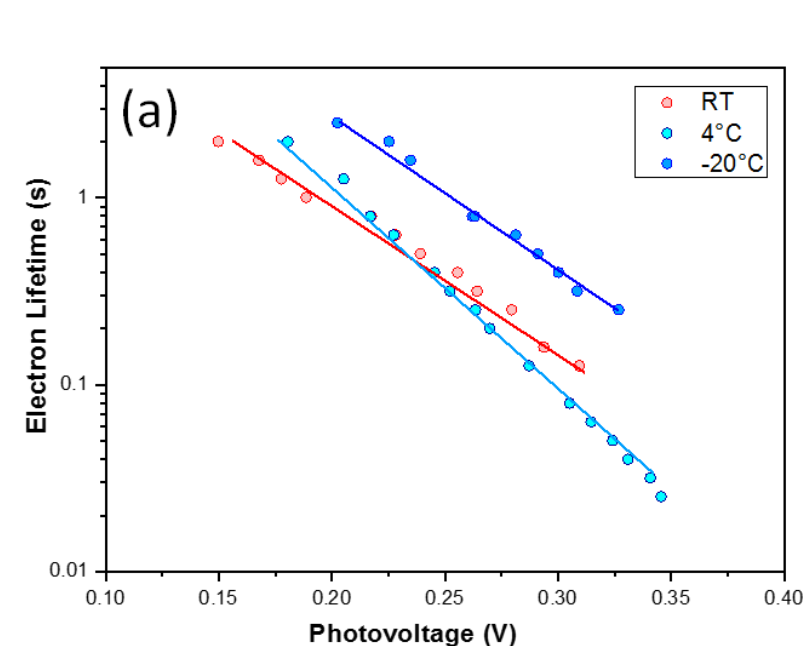
<sup>a</sup> PA: 9µm transparent TiO<sub>2</sub> + 5µm scattering layer



### Low-temperature TiO<sub>2</sub> sensitization

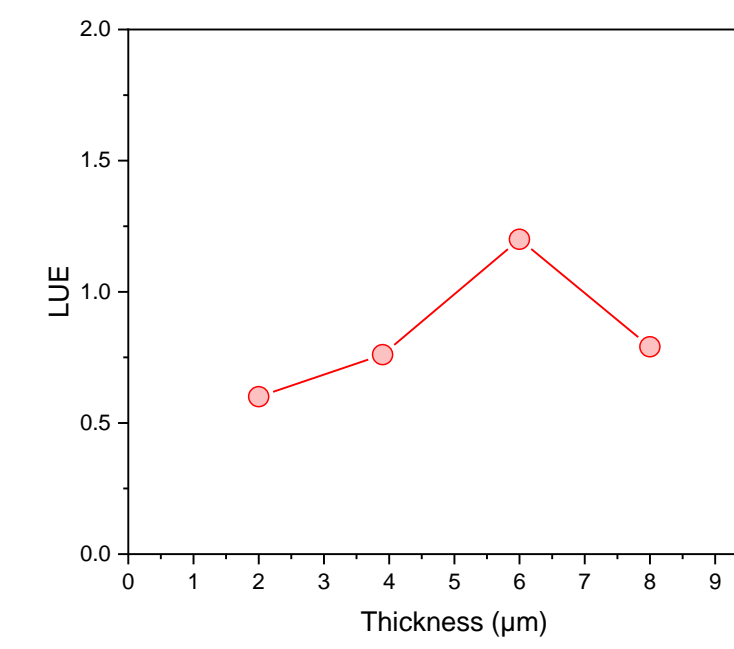


Temp. (°C)	PCE <sup>a</sup> (%)
RT	2.5
4	2.6
-20	3.1



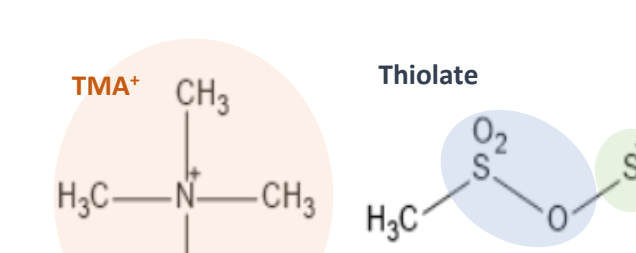
### TiO<sub>2</sub> thickness optimization

TiO <sub>2</sub> (µm)	AVT (%)
2	80
4	76
6	70
8	65

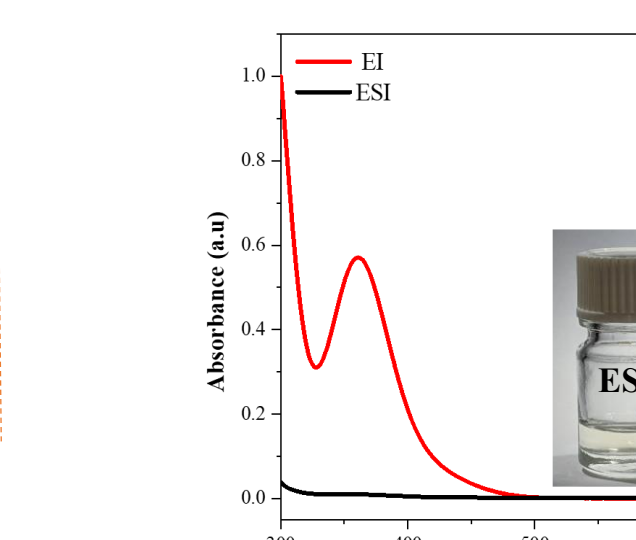


Best LUE with 6 µm TiO<sub>2</sub>

## Electrolytes for transparent DSSCs



Electrolyte	V <sub>oc</sub> (mV)	J <sub>sc</sub> (mA/cm <sup>2</sup> )	FF (%)	PCE (%)	AVT (%)	CRI	Color purity
Iodine based EI	402	11.5	58	2.6	76	92	31%
Sulphide based ESI	359	11.2	58	2.4	80	96	14%



## REFERENCES

[1] Grifoni F., Bonomo M., Naim W., Barbero N., Alnasser T., Dzeba I., Giordano M., Tsaturyan A., Urbani M., Torres T., Barolo C., Sauvage, F., *Adv. Energy Mater.* **2021**, 11 (43), 2101598. [2] Naim W., Novelli V., Nikolinos I., Barbero N., Dzeba I., Grifoni F., Ren Y., Alnasser T., Velardo A., Borrelli R., Haacke S., Zakeeruddin S.M., Graetzel M., Barolo C., Sauvage F., *JACS Au* **2021**, 1 (4), 409-426. [3] Naim W., Grifoni F., Challuri V., Mathiron D., Ceurstemont S., Chotard P., Alnasser T., Dzeba I., Barbero N., Pilard S., Barolo C., Sauvage F., *Cell Reports Physical Science* **2023**, 4, 101455.

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