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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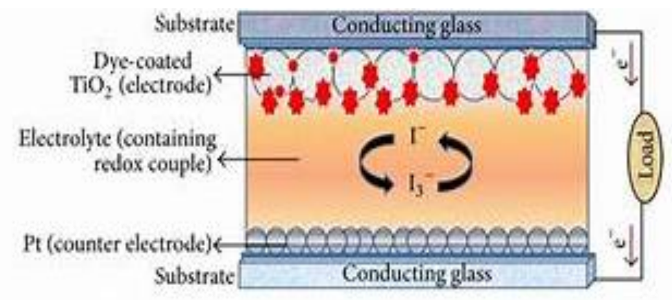
Dye-Sensitized Solar Cells (DSSCs) offer an interesting and sustainable choice for the development of transparent, and even colorless, photovoltaic devices, thanks to their ability to exploit diffuse and low-intensity light as well as their wide versatility in dyes, electrolytes and redox couples. Among 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…

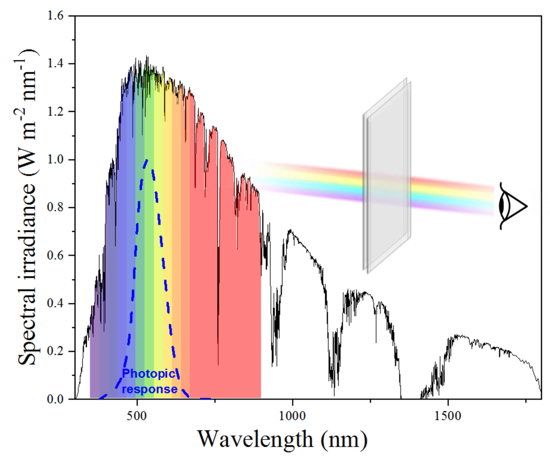


Transparent and sustainable DSSC

efficiency vs aesthetics?

Average **V**isible **T**ransmittance (**AVT**)

Light **U**tilization **E**fficiency
LUE= AVT x PCE



Color **R**enderind **I**ndex

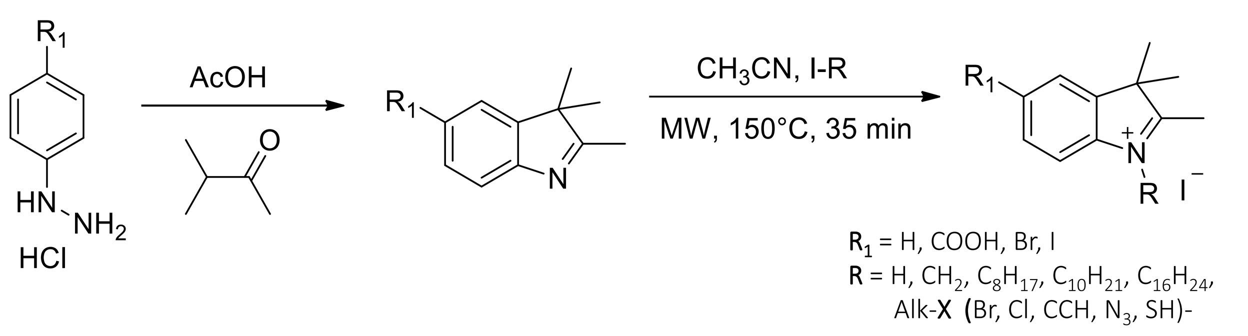
Aesthetic quality: Optical transparency and high CRI

Near-IR Polymethine Dyes

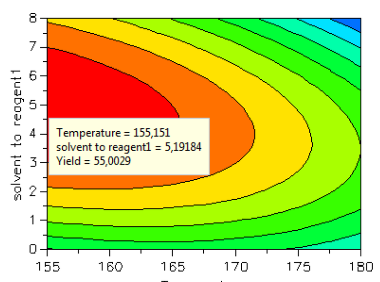
30+ selective NIR dyes developed based on polymethine dyes and derivatives

Selective absorption in Near-IR (negligible in visible)

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

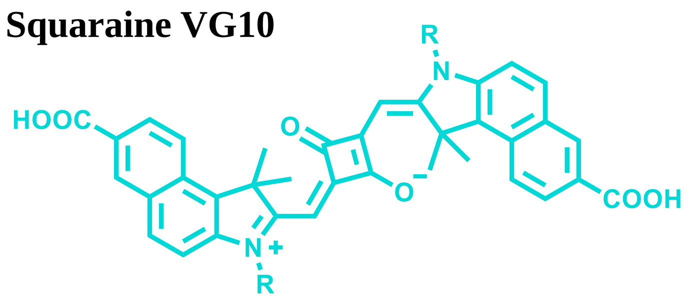


MW synthesis:
-Reduce time and byproducts
-Increase yields
-Avoid anhydrous conditions

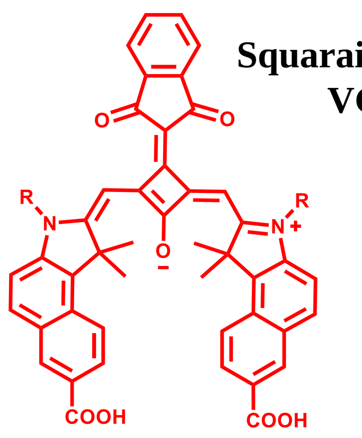


Central core and π–π conjugation

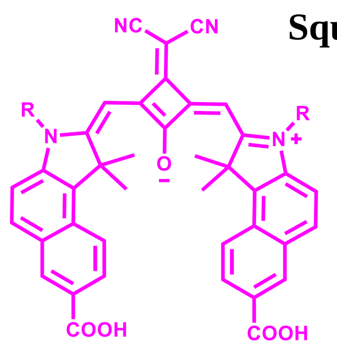
Squaraine VG10



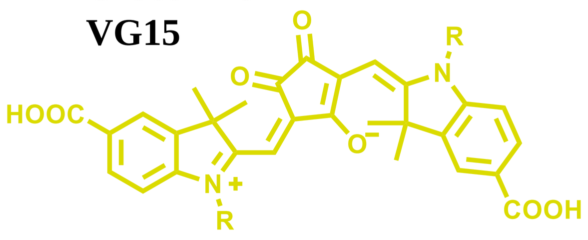
Squaraine VG4

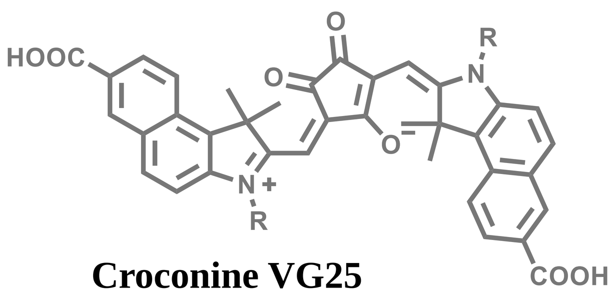


Squaraine VG11



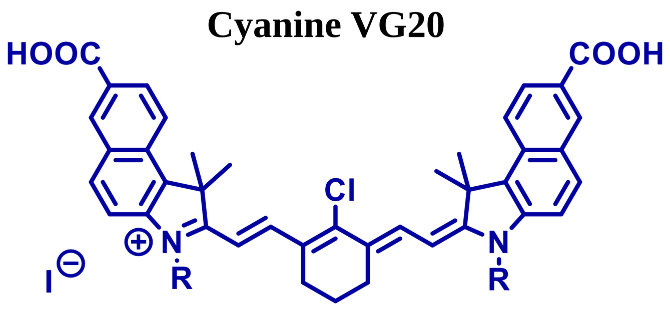
Croconine VG15

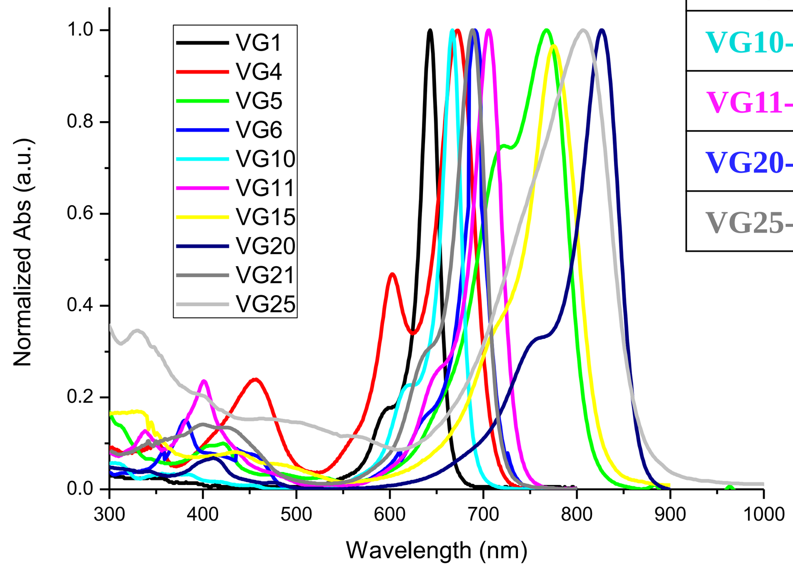




Croconine VG25

Cyanine VG20

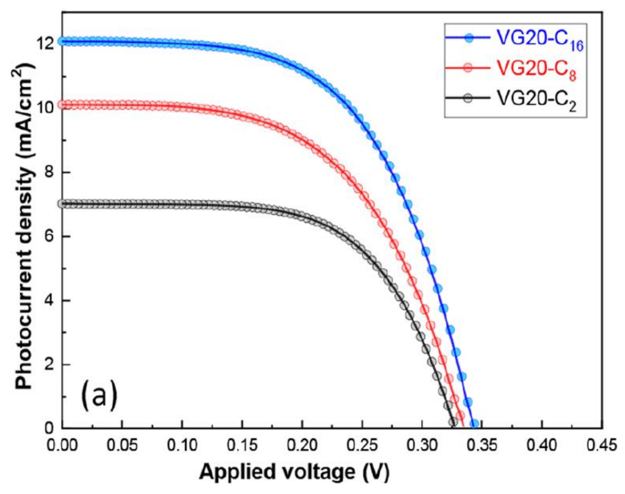




λ_{max} from 643 to 827 nm

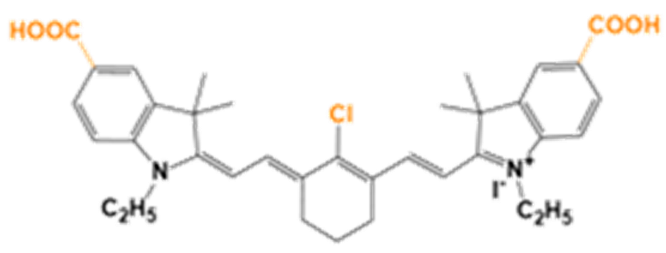
Dye	PCE (%)
VG10-C8	6.1
VG11-C8	2.5
VG20-C8	1.9
VG25-C8	0.3

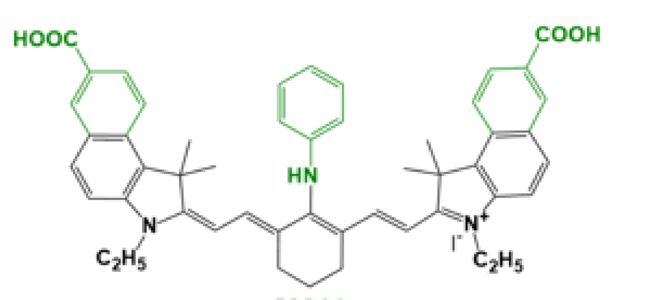
Alkyl chain length

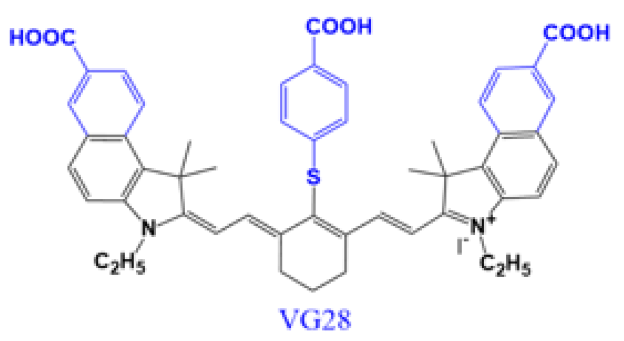


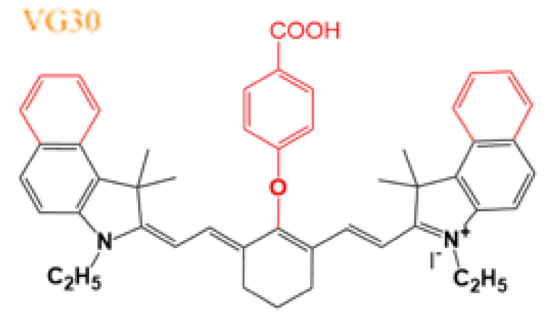
NIR cyanines to improve chemical-physical properties

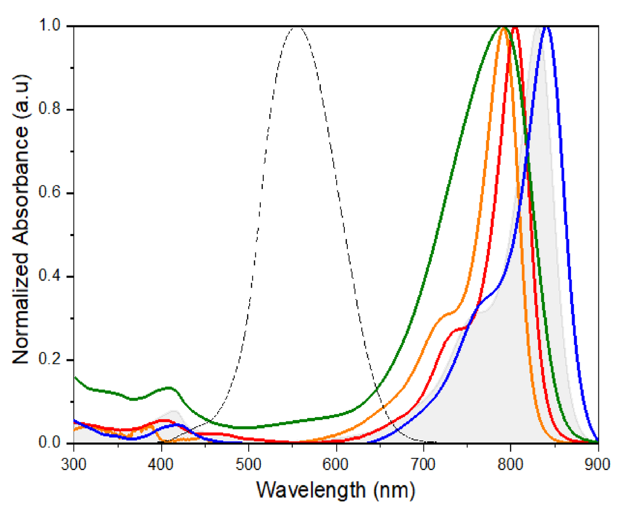
Substitutions on the linker chain between benzo[e]indole moieties


VG30


VG29


VG28

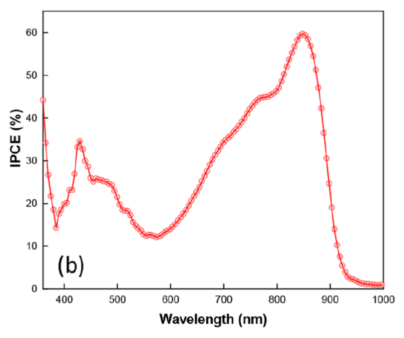

VG47



Dye	J_{SC} (mA/cm²)	V_{OC} (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

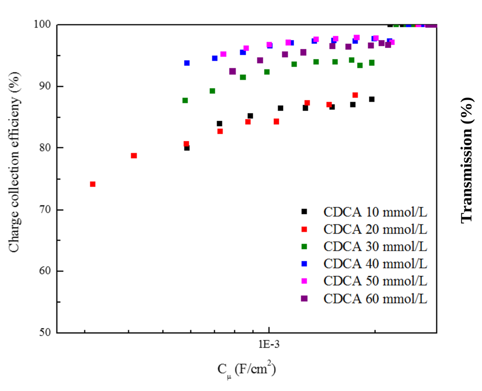
Reaching balance between performance and aesthetics

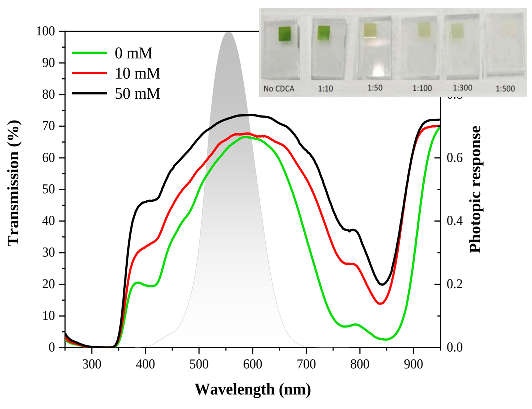


Decreasing in dye loading

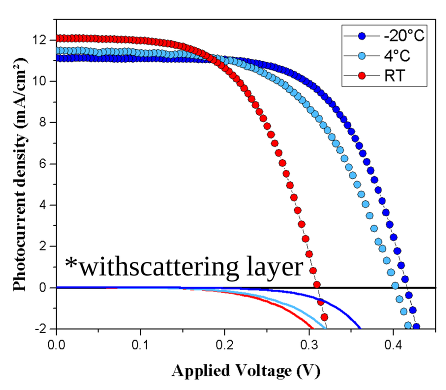
CDCA (mM)	AVT (%)	CRI	PCE* (%)
0	61	90.3	0.5
10	64	93.8	1.8
50	71	95.8	2.6

*PA: 9μm transparent TiO_2 + 5μm scattering layer

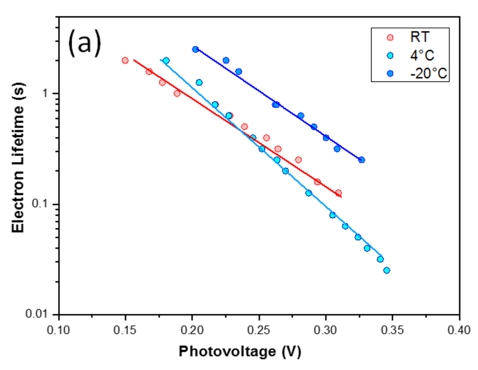




Low-temperature TiO_2 sensitization

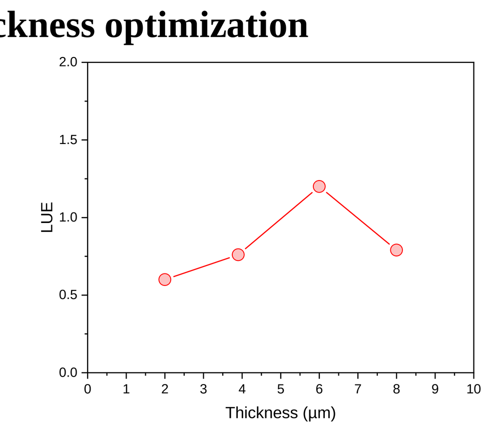


Temp. (°C)	PCE* (%)
RT	2.5
4	2.6
-20	3.1



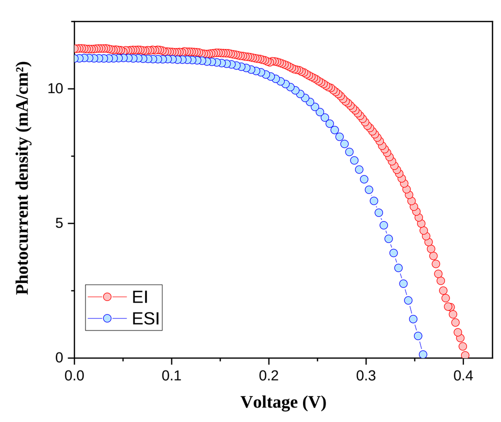
TiO_2 thickness optimization

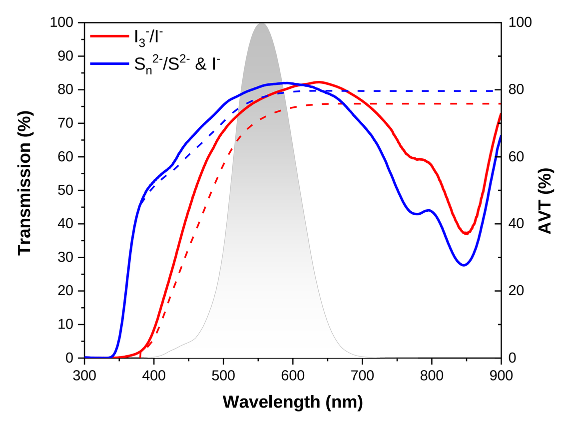
TiO_2 (μm)	AVT (%)
2	80
4	76
6	70
8	65

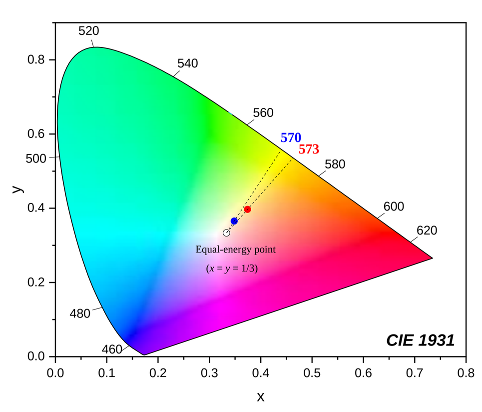


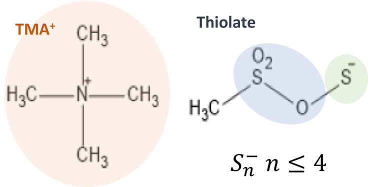
Best LUE with 6 μm TiO_2

Electrolytes for transparent DSSCs

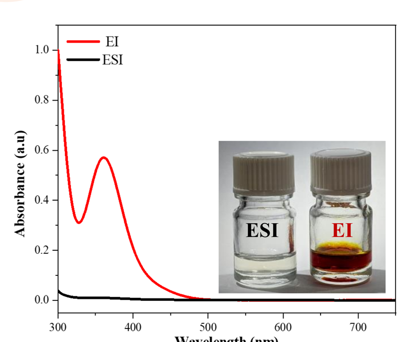


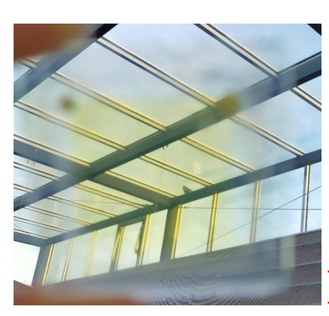


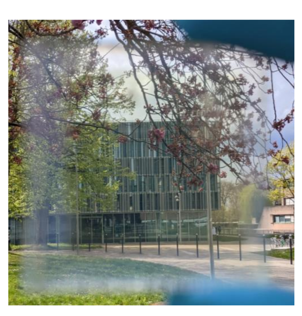




Electrolyte	V_{oc} (mV)	J_{sc} (mA/cm²)	FF (%)	PCE (%)	AVT (%)	CRI	Color purity
Iodine based EI	402	11.5	58	2.6	76	92	31%
Sulphide based ESI	359	11.2	58	2.4	80	96	14%




EI


ESI

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[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., Nikolinakos 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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