

A fluorescence microscopy image of a cell. The cell's internal structure is visible, with a prominent nucleus. The image shows two different fluorescent signals: a red signal that appears to be distributed throughout the cytoplasm and some organelles, and a green signal that is more localized, possibly highlighting specific organelles or protein expression. The overall appearance is that of a complex, interconnected network of fibers and structures.

Fluorescent organic molecules

Lei Zhu, Florida State University

July 25, 2023







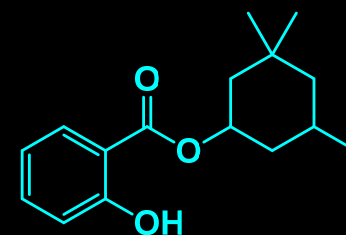


Sunscreen

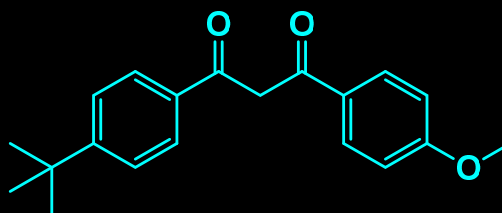
- Ultraviolet (UV): 10 – 400 nm
- UVA: 315 – 400 nm (soft UV)
- UVB: 280 – 315 nm (intermediate UV)
- UVC: 100 – 280 nm (hard UV)
- SPF – “sun protection factor”



oxybenzone (6%)



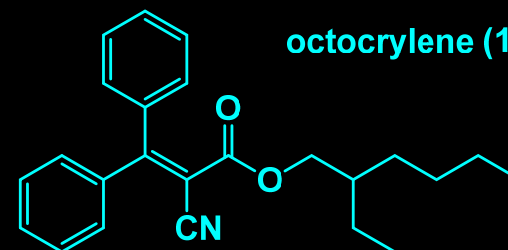
homosalate (15%)



avobenzene (3%)



octisalate (5%)



octocrylene (10%)

“the benefits way outweigh the risks”

[Health](#) | [Sun](#)

Sunscreen: What science says about ingredient safety

Sunscreen is essential for staying protected in the Sun - but recent research suggests some of the ingredients could be improved. BBC Future analyses the evidence.



By Jessica Brown

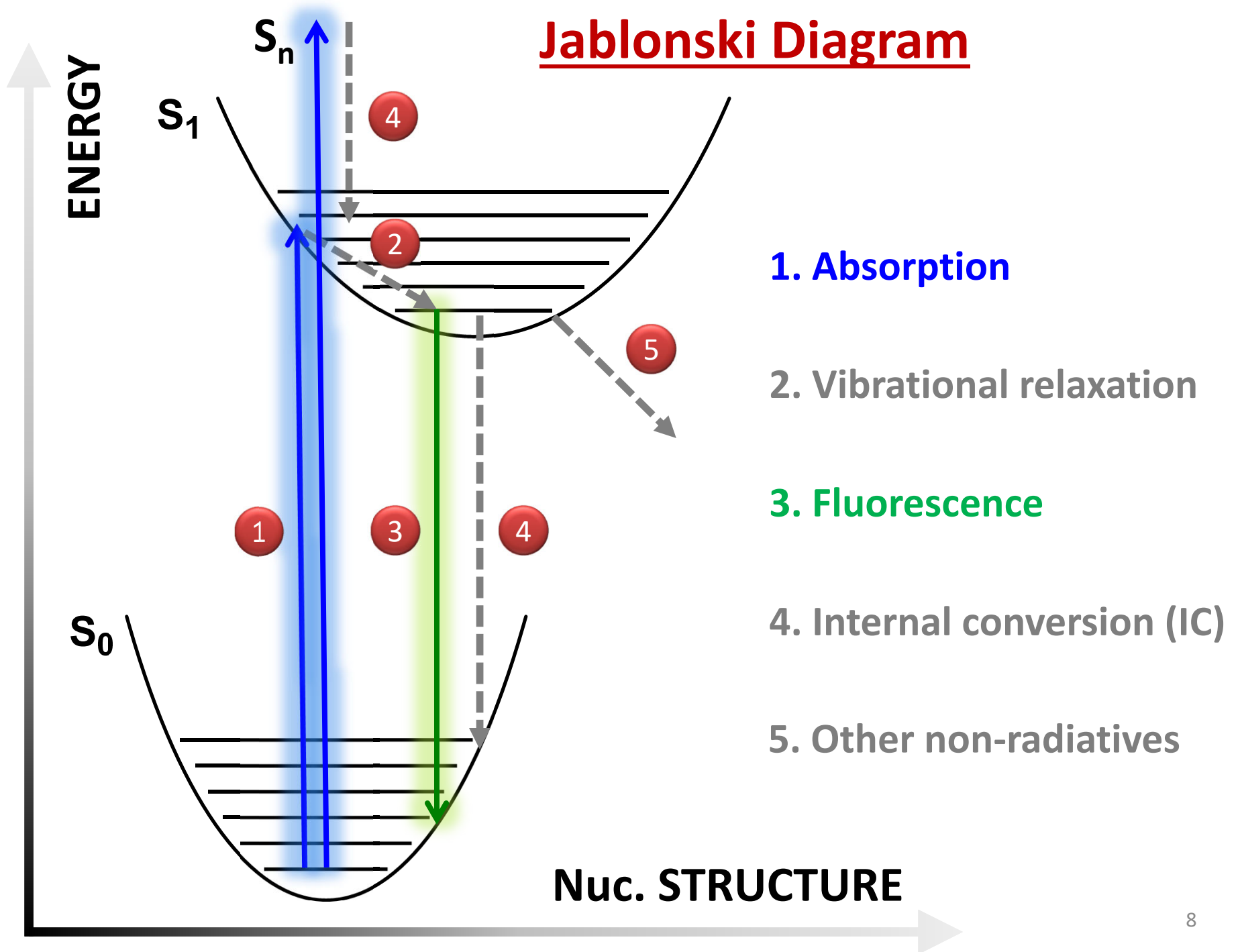
23 July 2019

ONLY TC
CAN WE I
PLANET PI

An exercise of critical thinking

What happens when an organic compound absorbs a photon and how would we quantitatively describe it?

Jablonski Diagram



Born-Oppenheimer Approximation



Max Born

Olivia Newton-John's
grandfather



Robert Oppenheimer

The guy in the movie

“Physics, as we know it, will be
over in six months.”

- Max Born in 1928

Quark?

Neutrino?

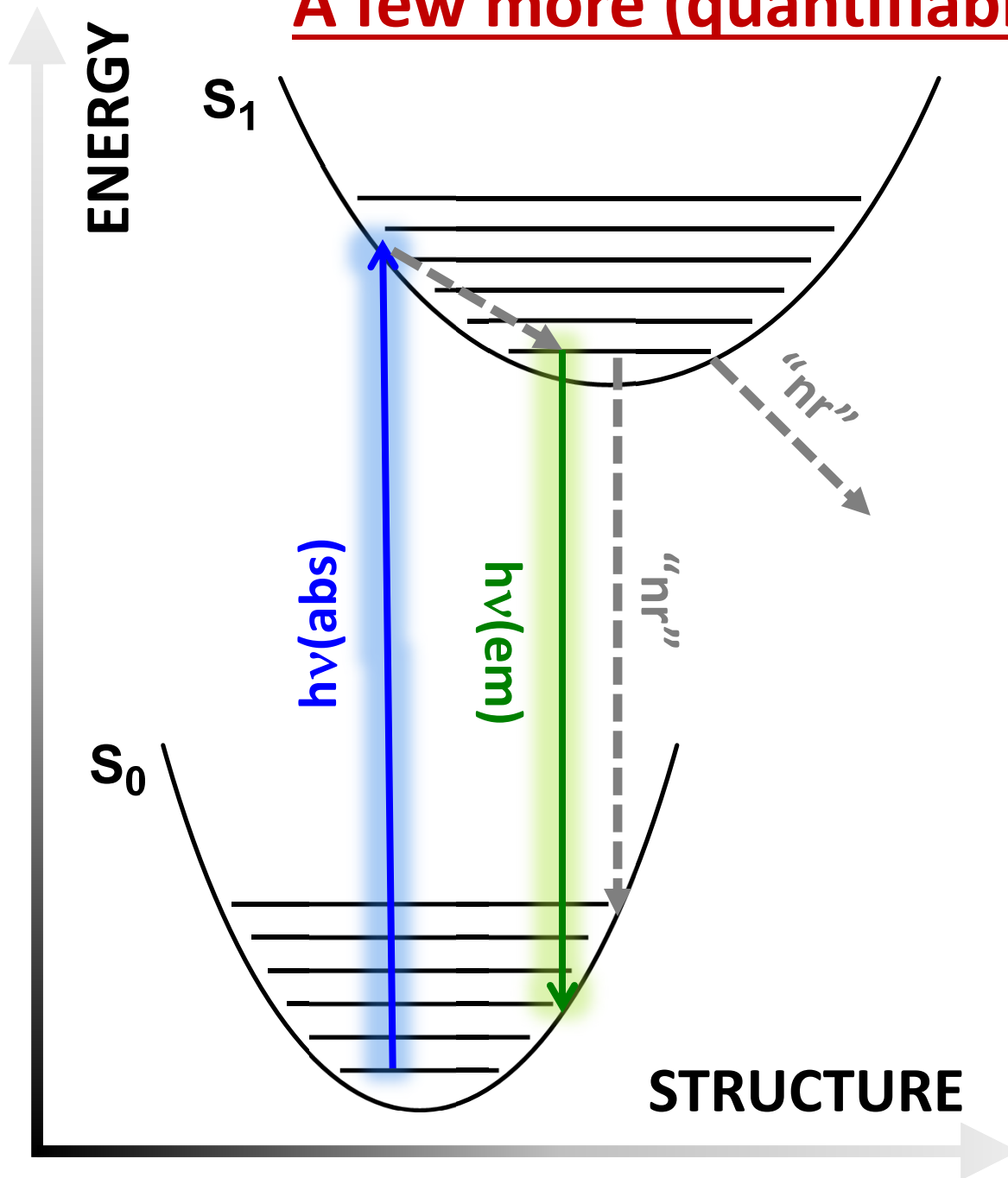
Black hole?

...

...

...

A few more (quantifiable) concepts



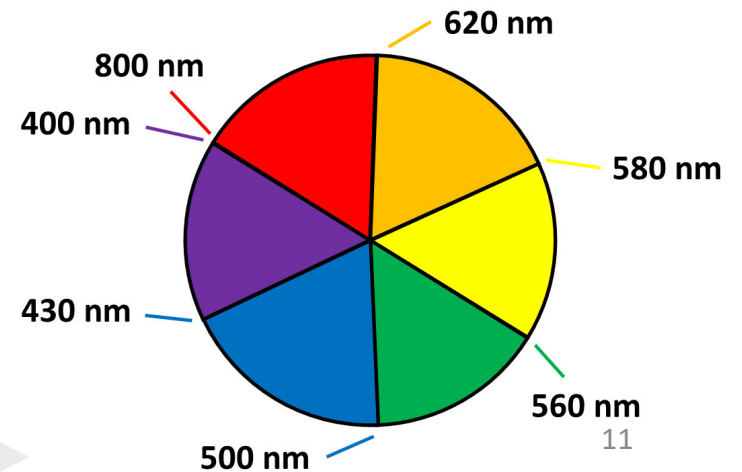
$$E = h\nu = h\frac{c}{\lambda}$$

Vertical radiative transitions

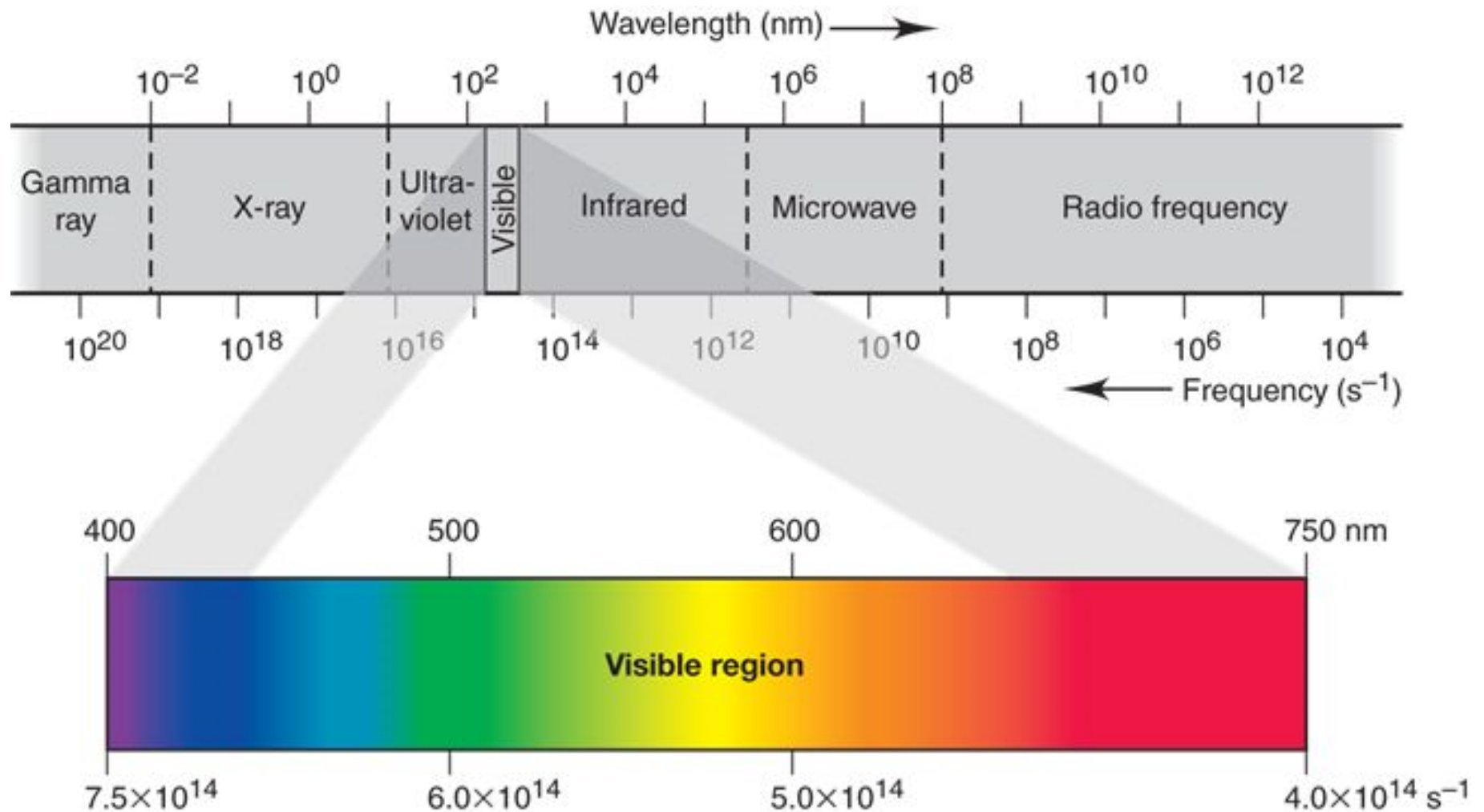
$$h\nu(\text{abs}) > h\nu(\text{em})$$

$$\phi_f = \frac{k_r}{k_r + \sum k_{nr}}$$

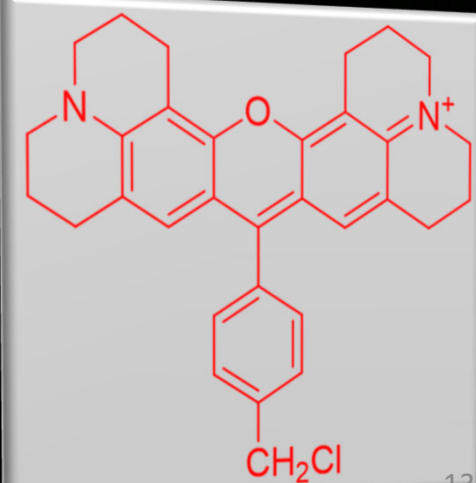
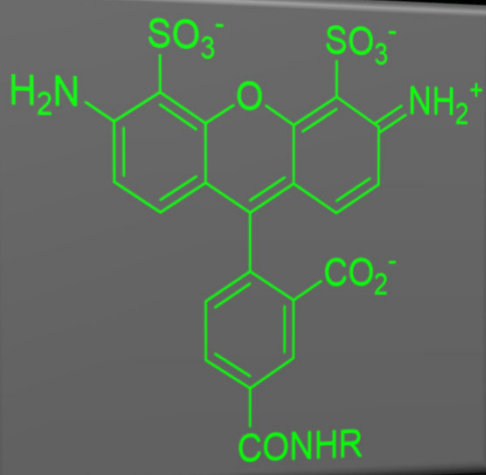
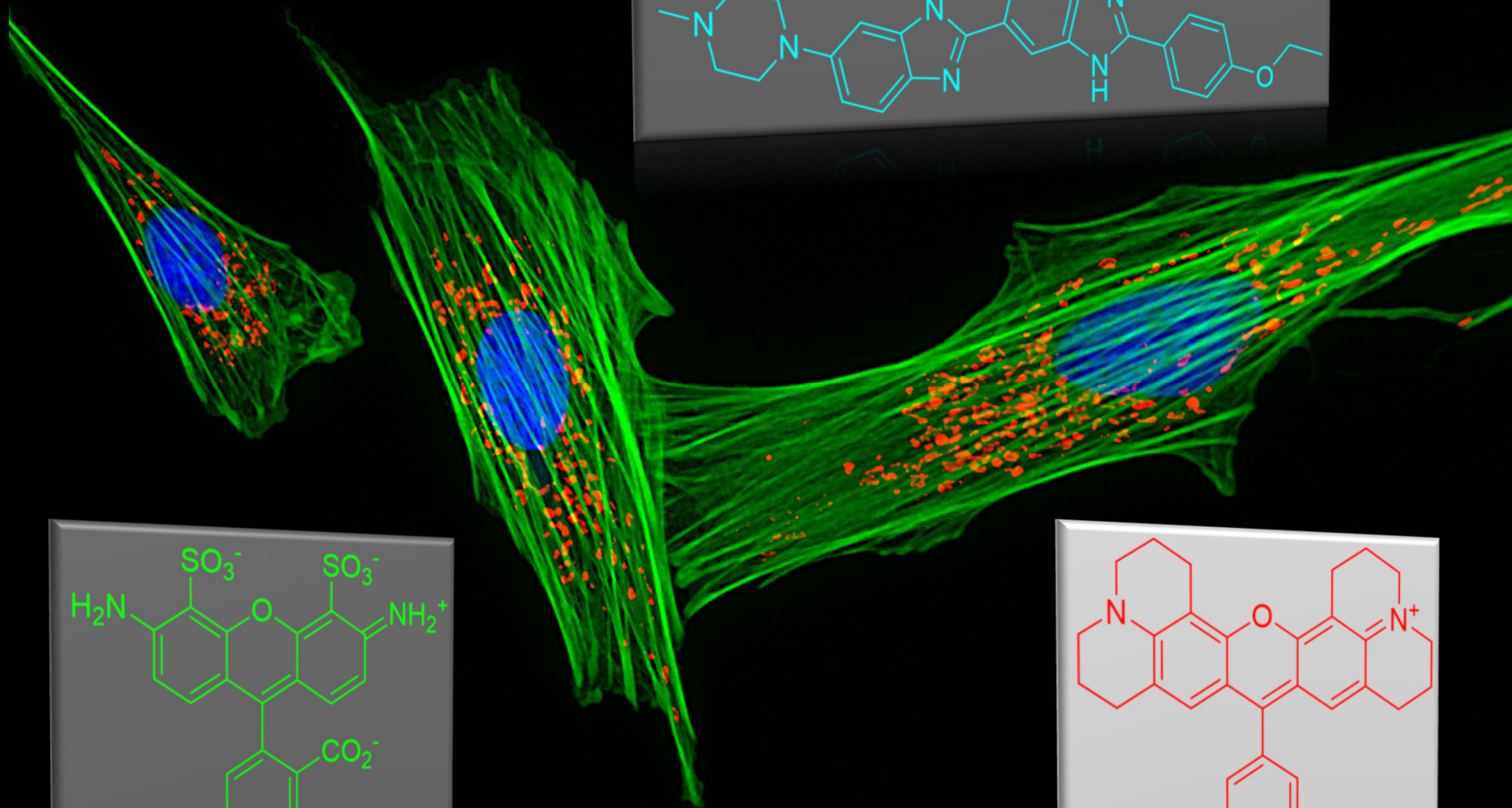
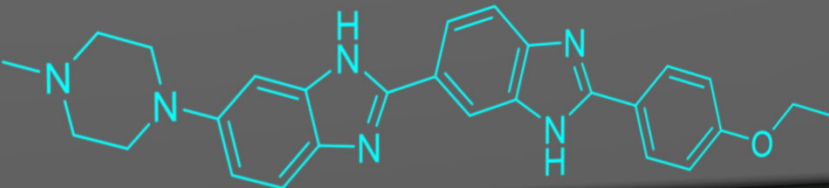
$$\tau = \frac{1}{k_r + \sum k_{nr}}$$



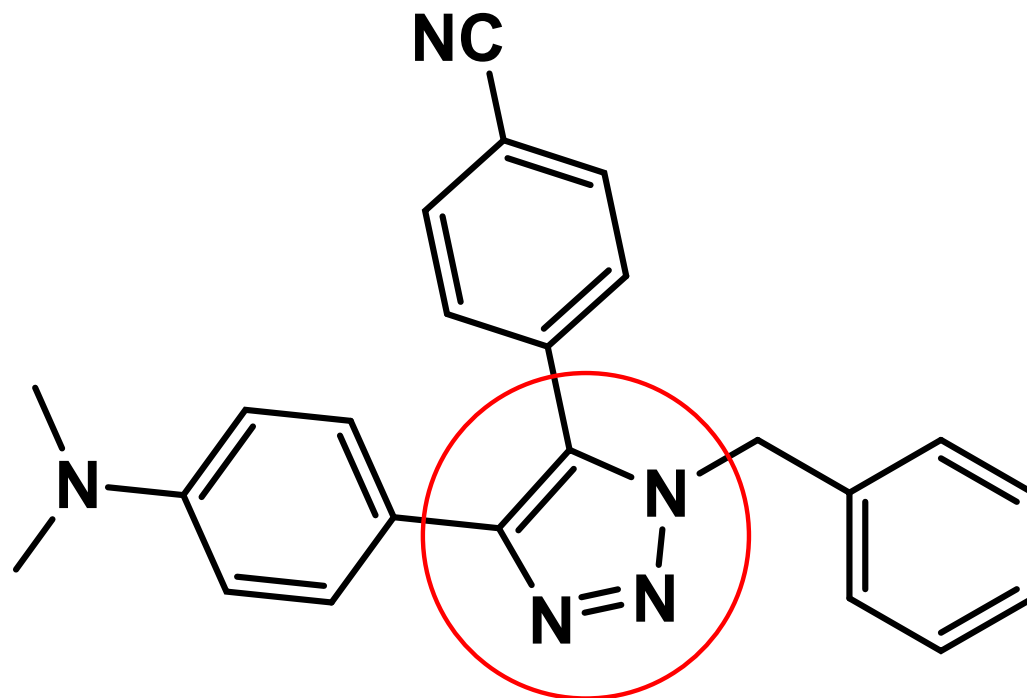
We (visually) perceive a tiny sliver of the physical world



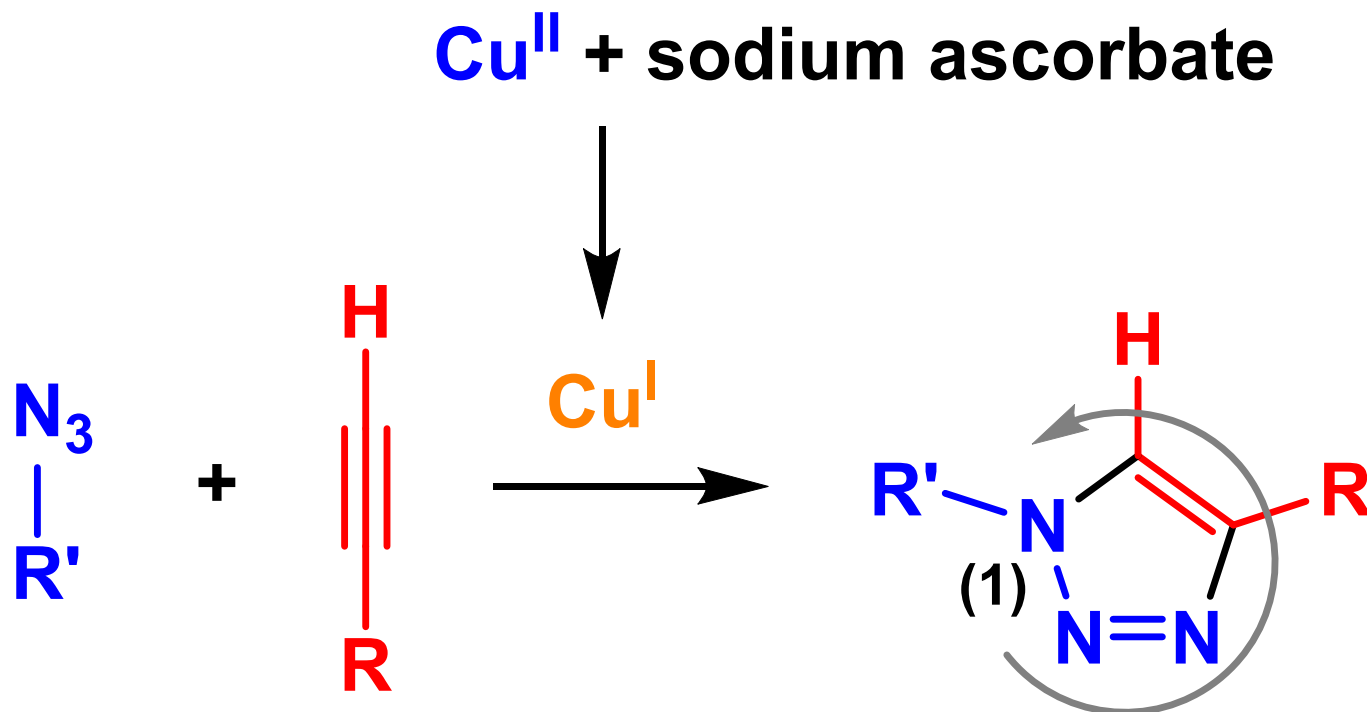
Indian muntjac deer skin fibroblast cells



A Fluorescent Triazole



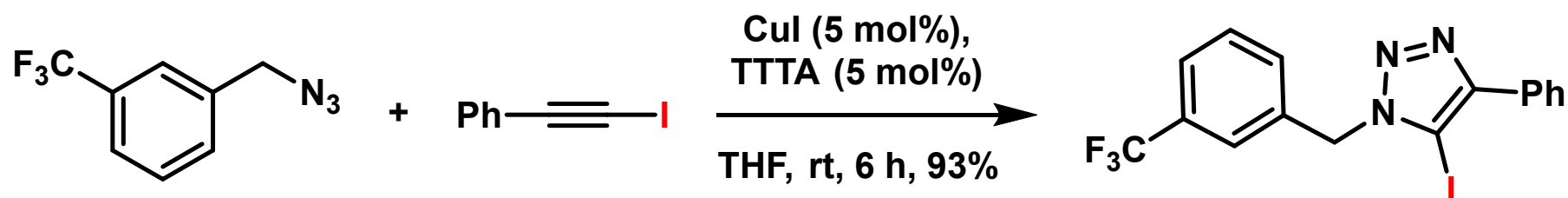
Cu(I)-catalyzed azide-alkyne cycloaddition



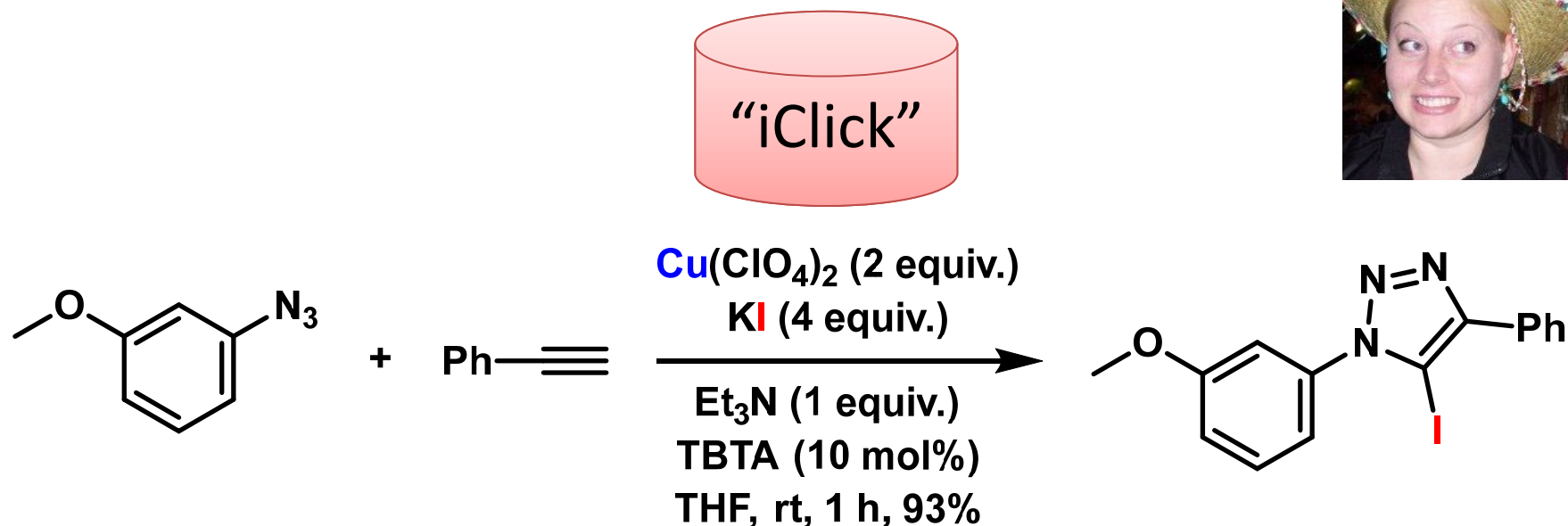
M. Meldal and coworkers, *J. Org. Chem.* **2002**, 67, 3057.

V. V. Fokin, K. B. Sharpless, and coworkers, *Angew. Chem. Int. Ed.* **2002**, 41, 2596.

Reroute CuAAC to make iodotriazole

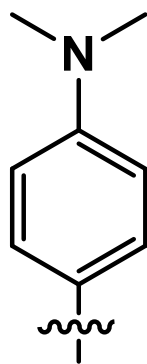
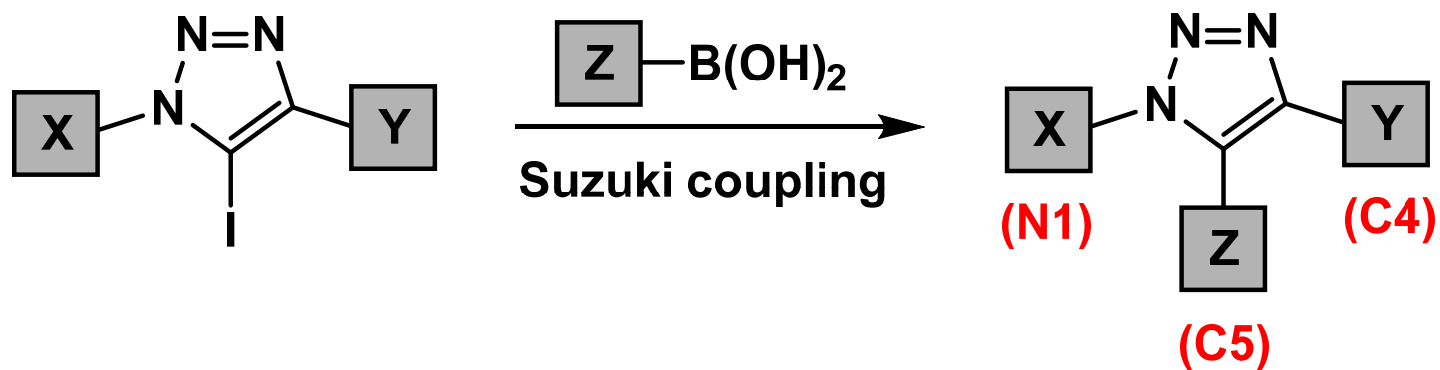


Hein, Fokin, and coworkers, *Angew. Chem. Int. Ed.* **2009**, *48*, 8018.



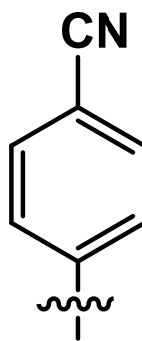
> 50 examples: Brotherton, Clark, and Zhu, *J. Org. Chem.* **2012**, *77*, 6443; Barsoum, Brassard, Deeb, Okashah, Sreenath, Simmons, and Zhu, *Synthesis* **2013**, *45*, 2372.

Aryl-substituted-1,2,3-triazoles



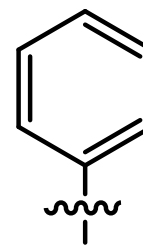
(A)

"aniline"



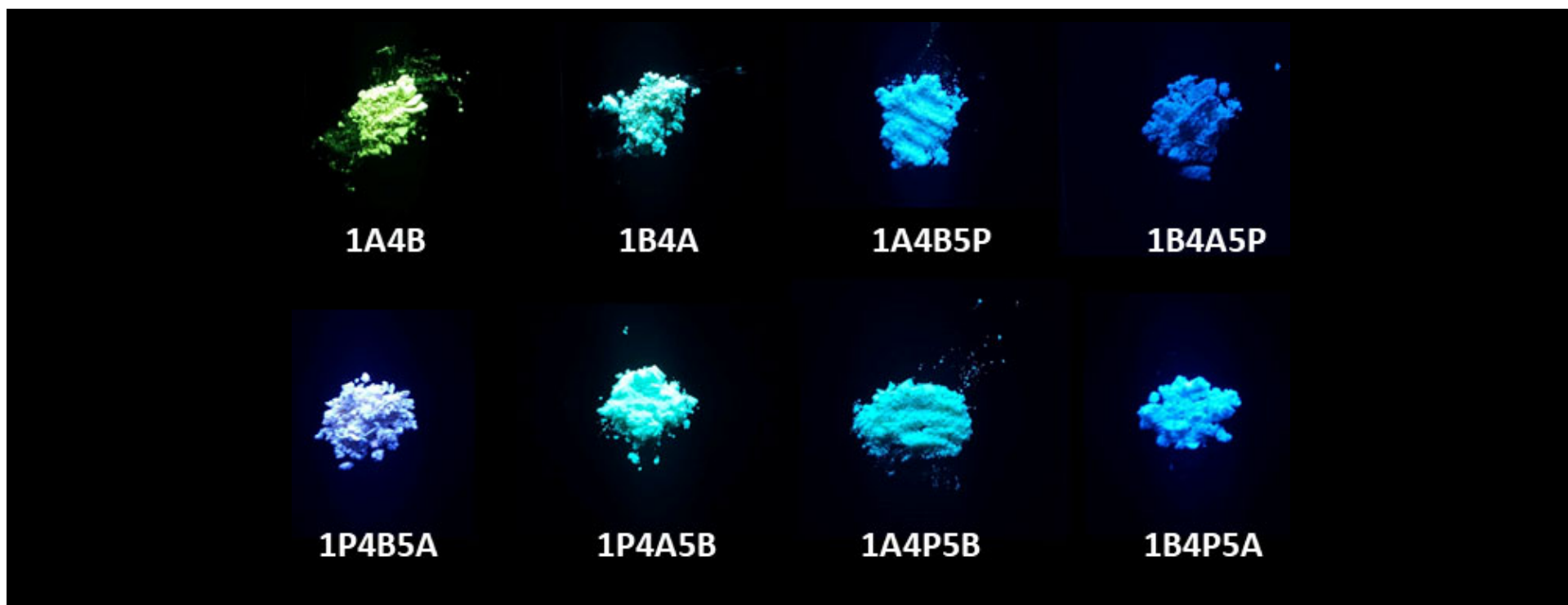
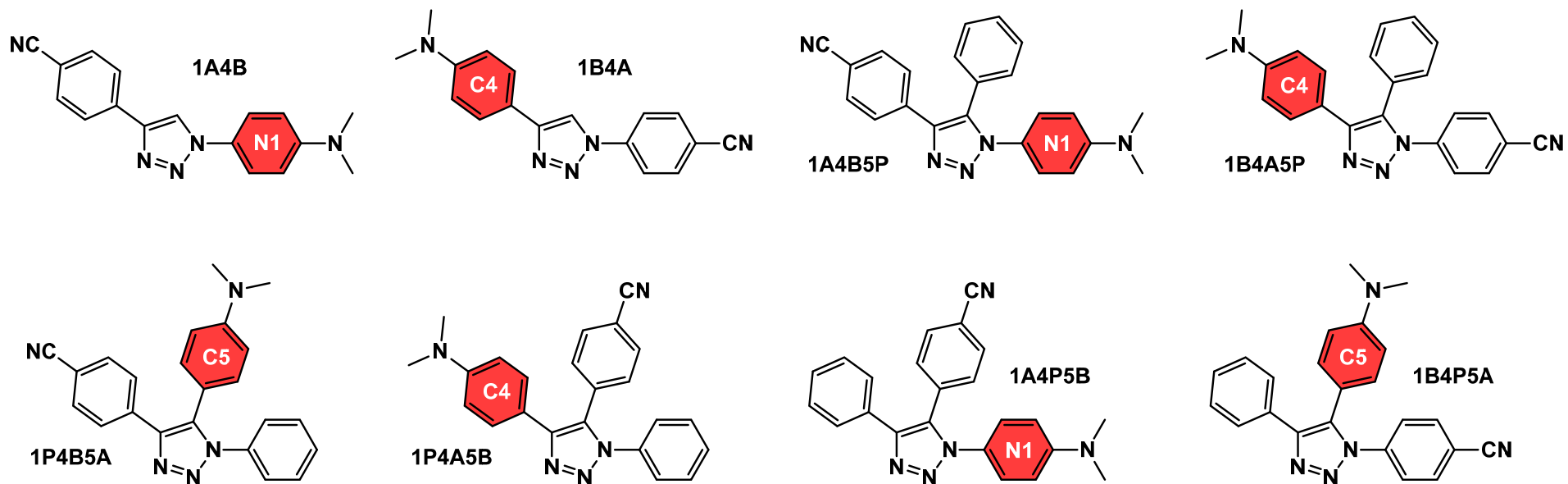
(B)

"benzonitrile"

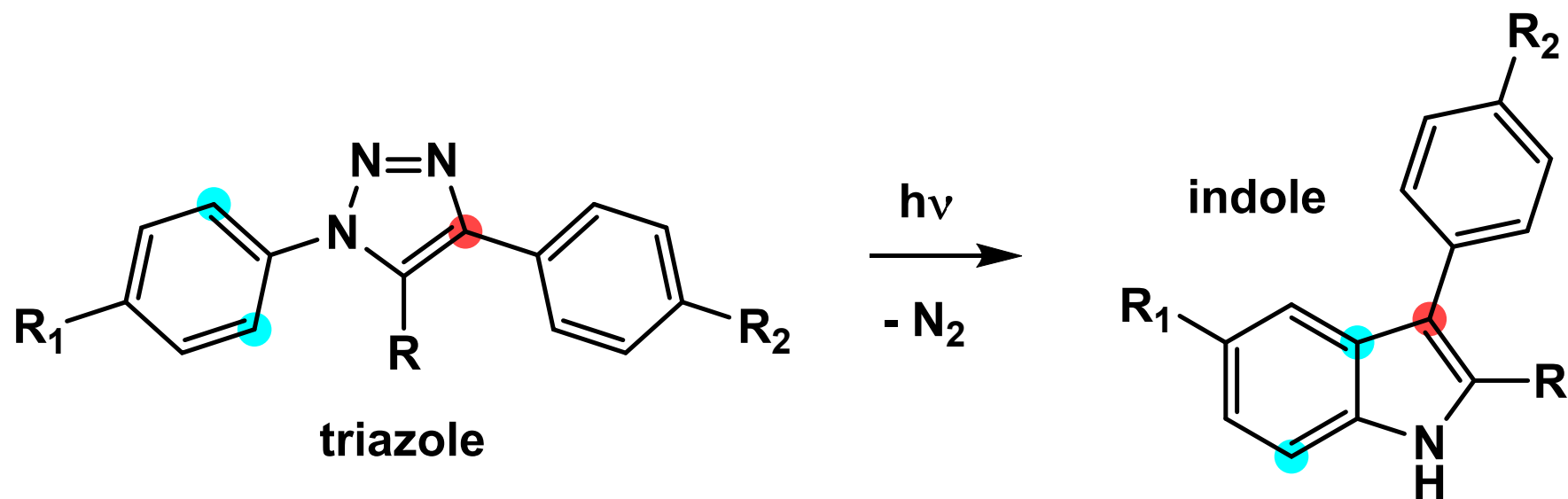


(P)

"phenyl"



Photochemical conversion to indole

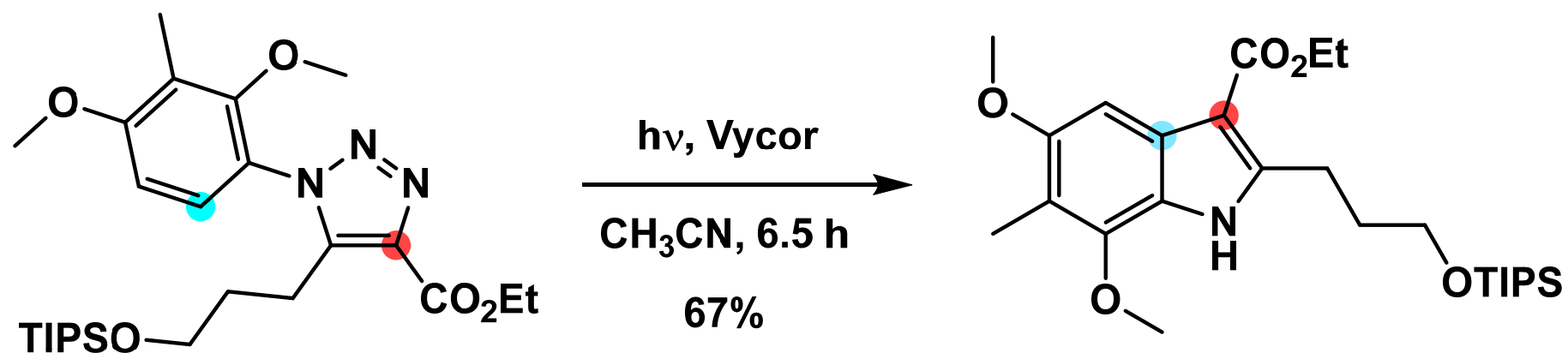


The earliest reference that I can find:

“Photochemical Decomposition of 1H-1,2,3-Triazole Derivatives”

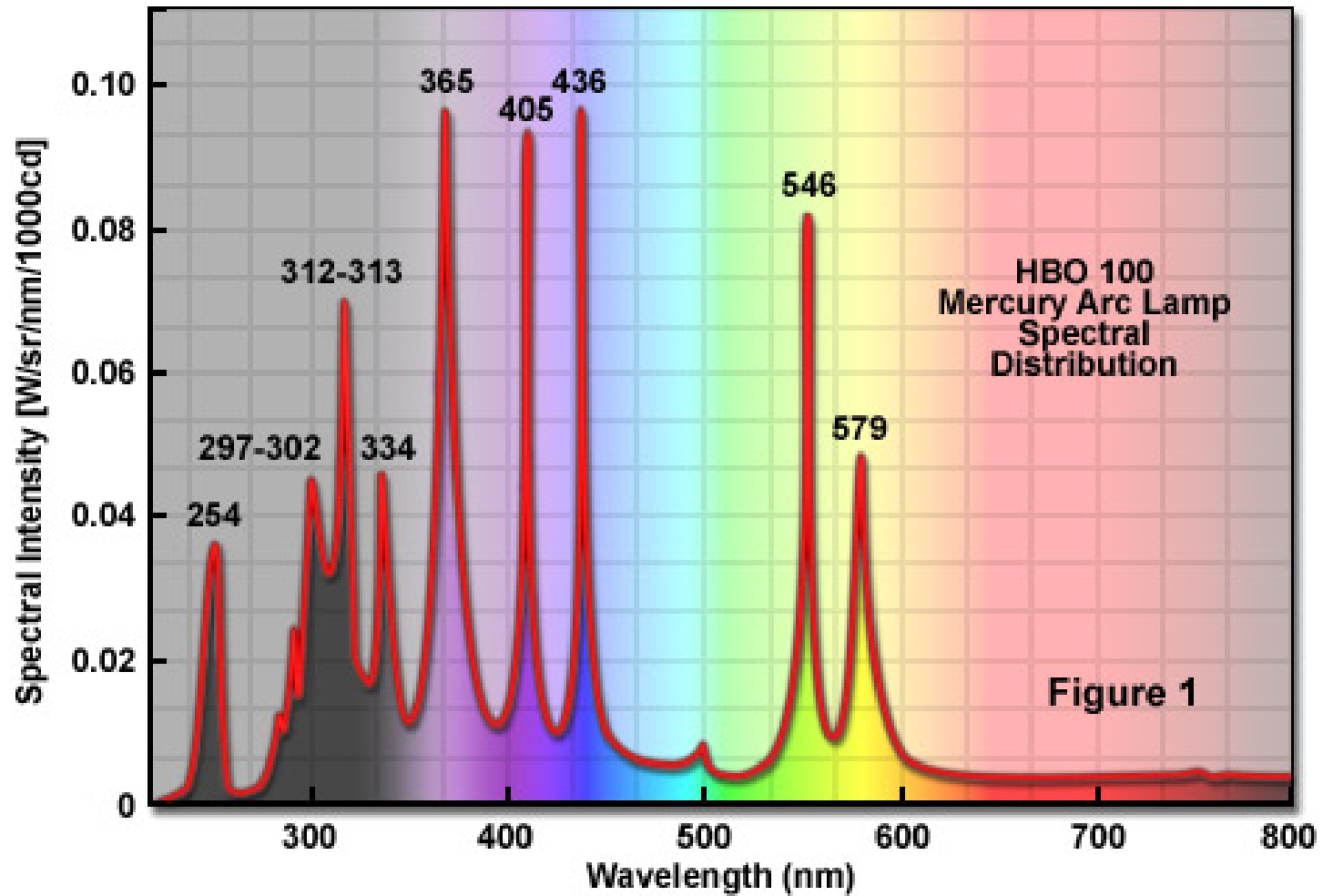
Burgess and coworkers, *J. Am. Chem. Soc.* **1968**, *90*, 1923-1924.

An early example of triazole photoconversion to indole



Wender and Cooper, *Tetrahedron Lett.* **1987**, 28, 6125-6128.

Light Source

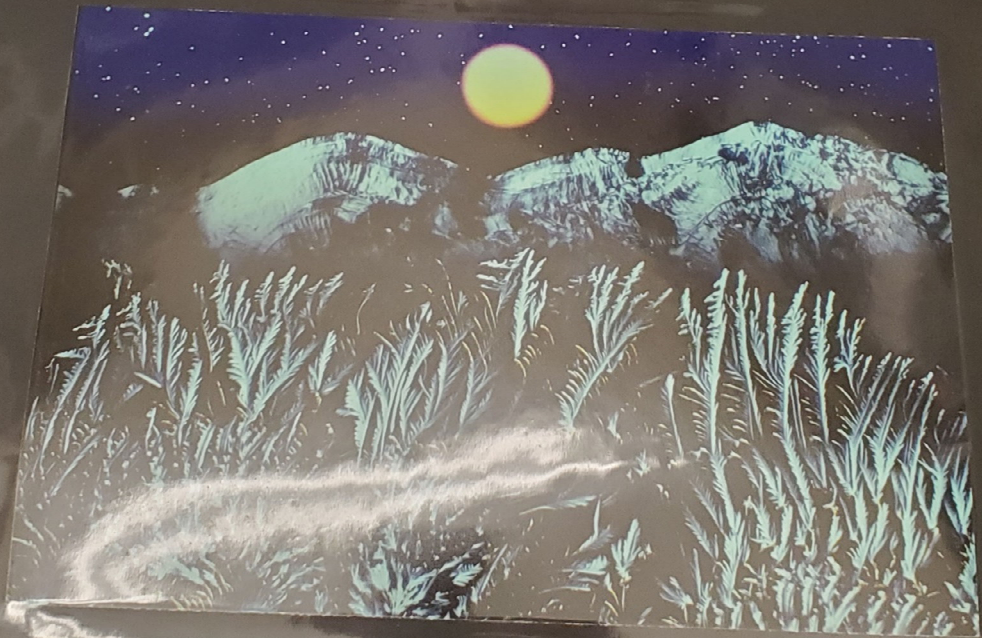




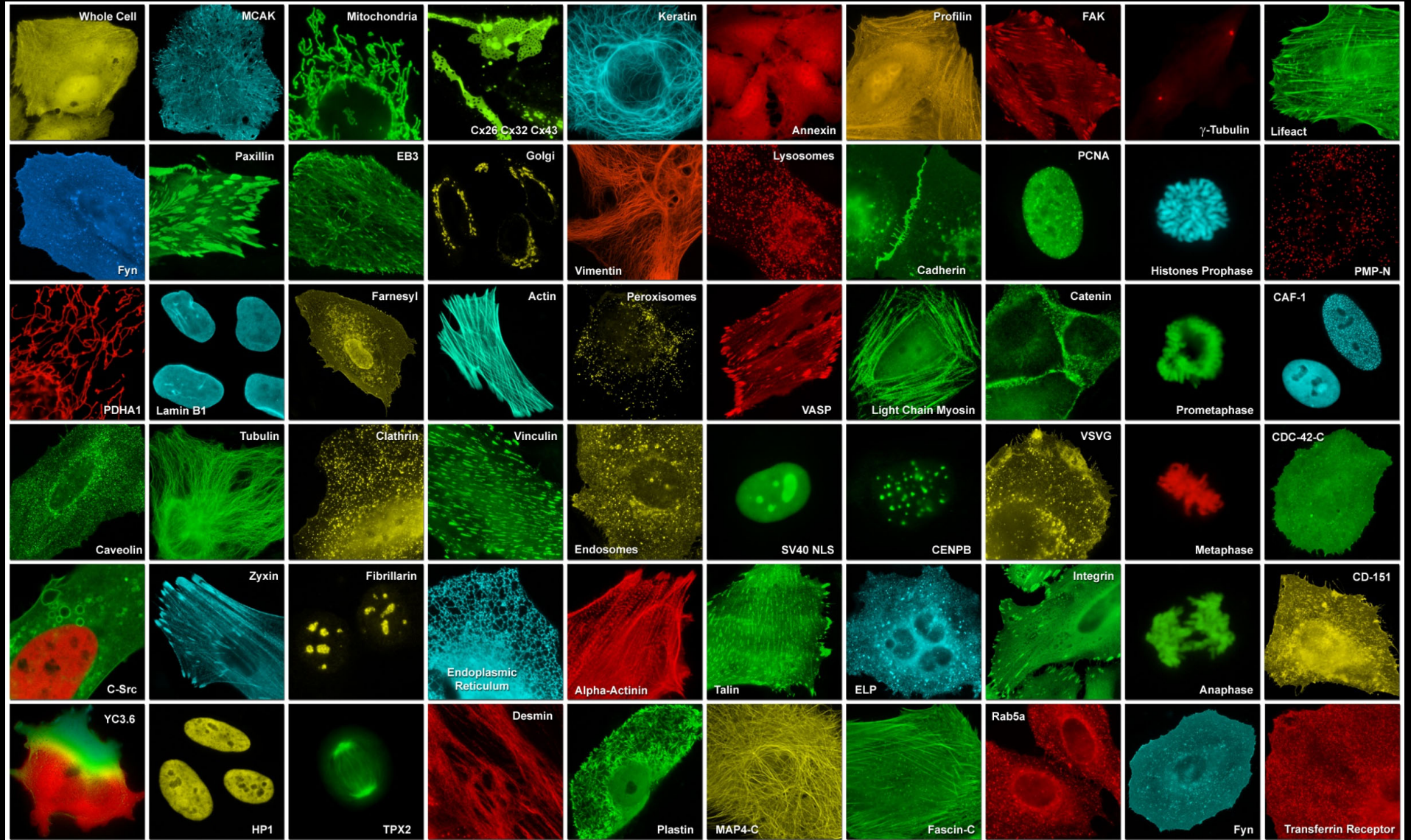
Liquid Crystal Land



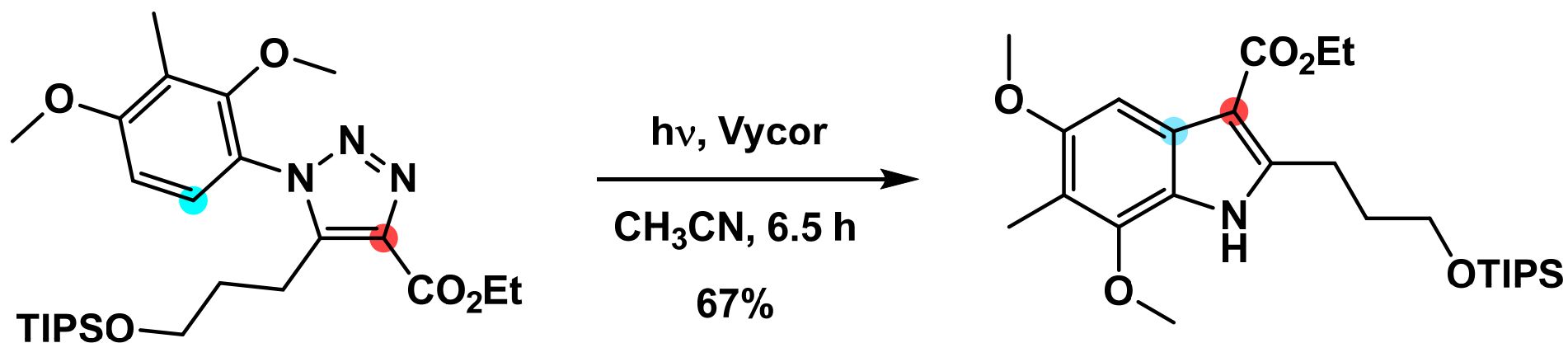
3



Fluorescent Protein Fusions for Live Cell Imaging



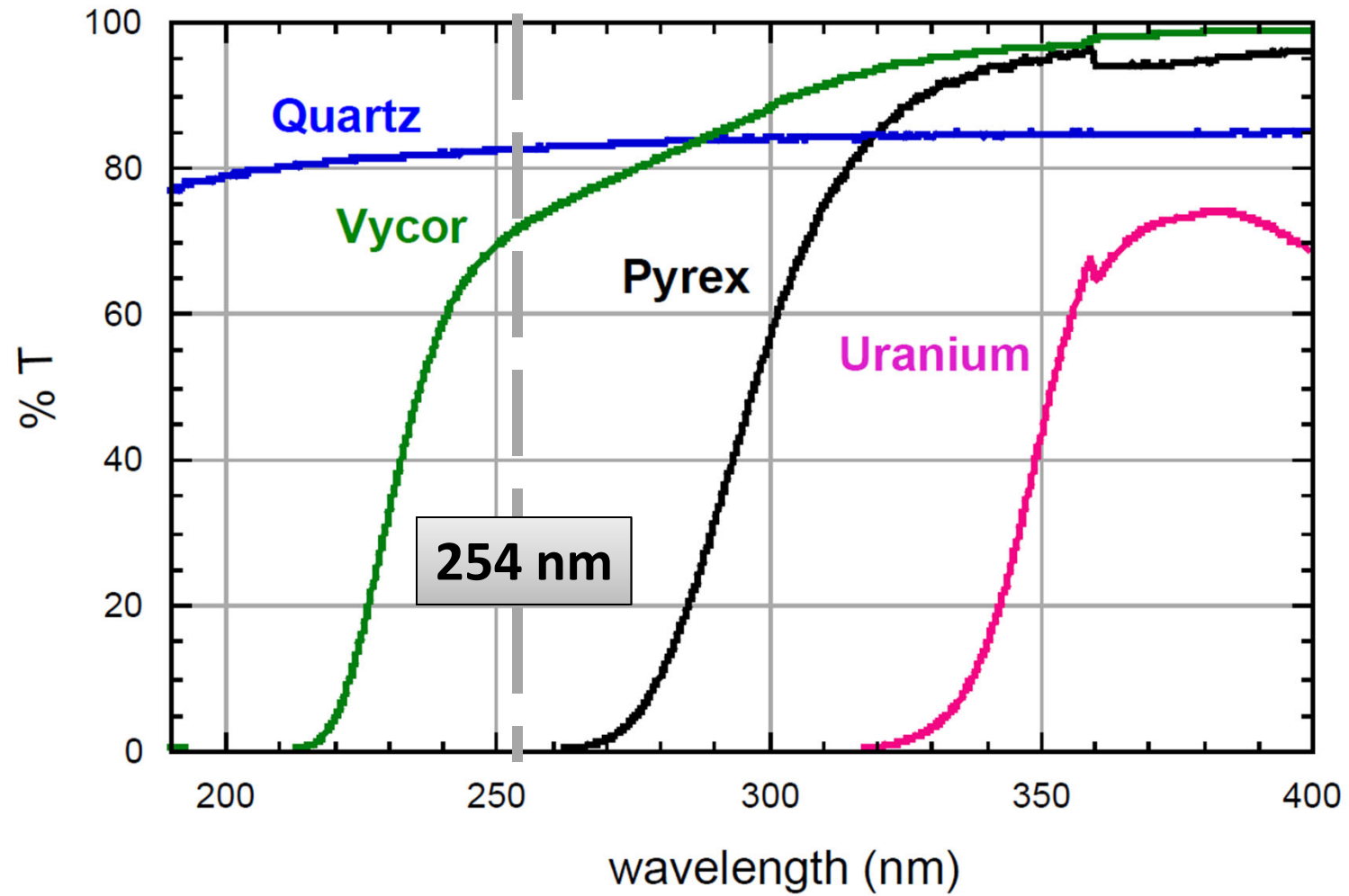
An early example of triazole photoconversion to indole



Wender and Cooper, *Tetrahedron Lett.* **1987**, 28, 6125-6128.

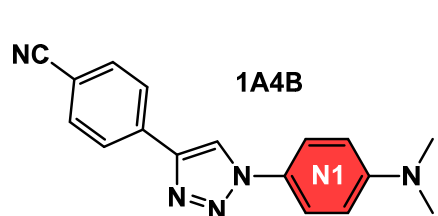
Reaction vessel

Photochemical Cutoff Filters

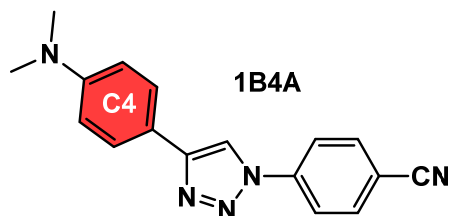


Google found this

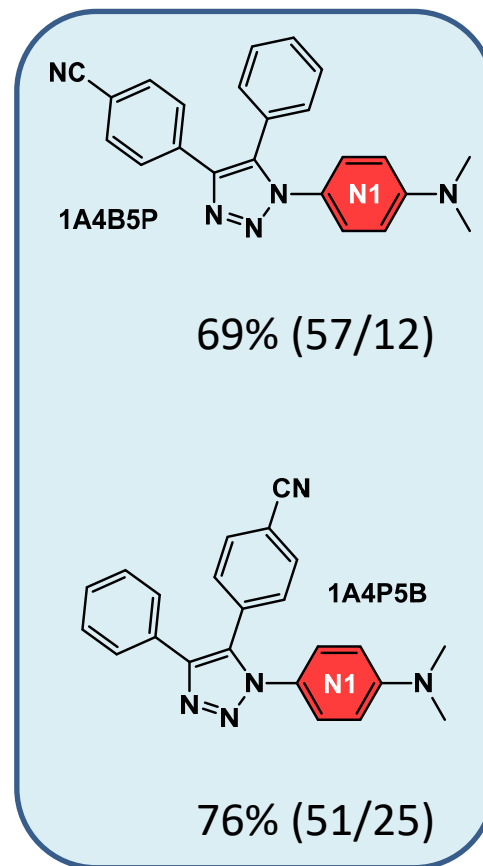
Outcomes of photoconversion



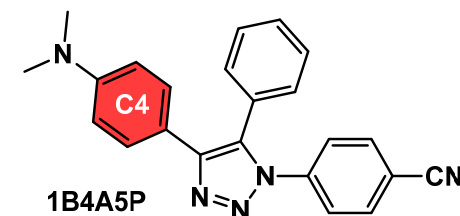
40%



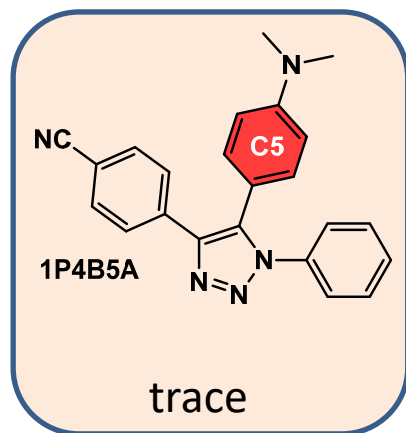
33%



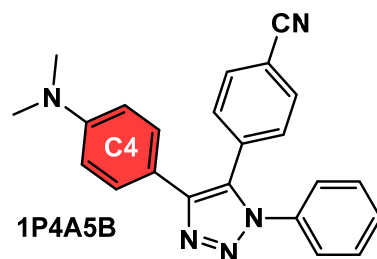
69% (57/12)



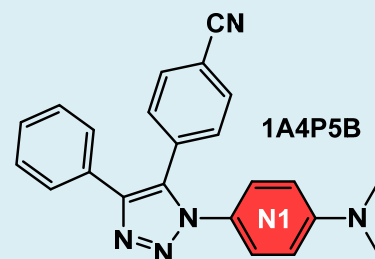
33%



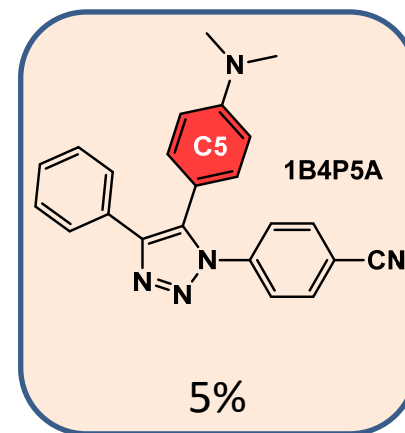
trace



17%



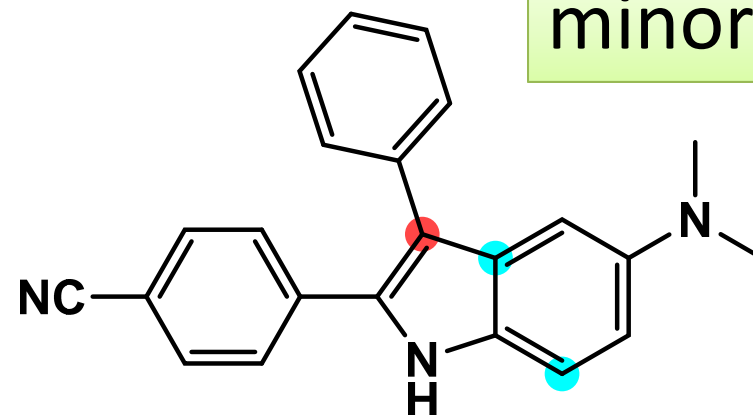
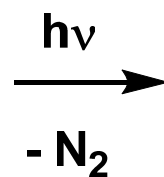
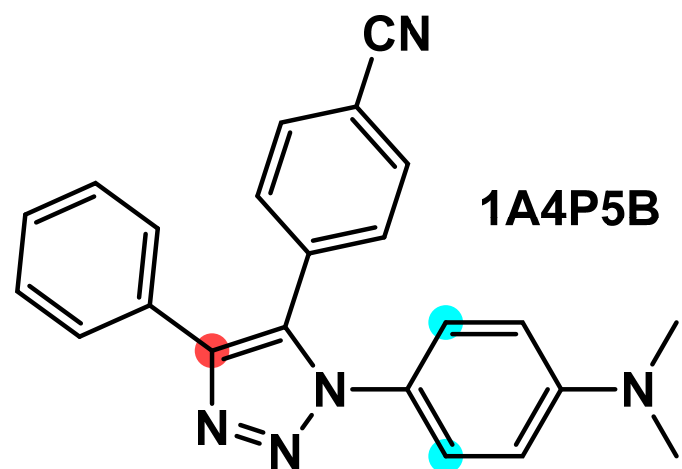
76% (51/25)



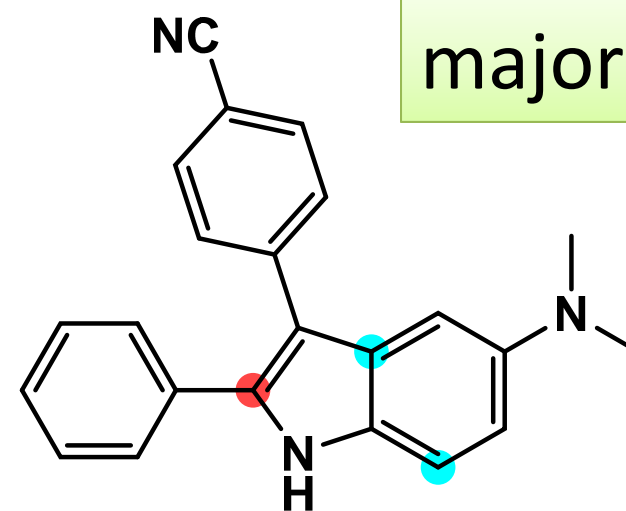
5%

Conditions: irradiation using 390-nm LED for 6 hours. [] = 1.5 mM in acetonitrile.

Two indole isomers



Rearrangement?

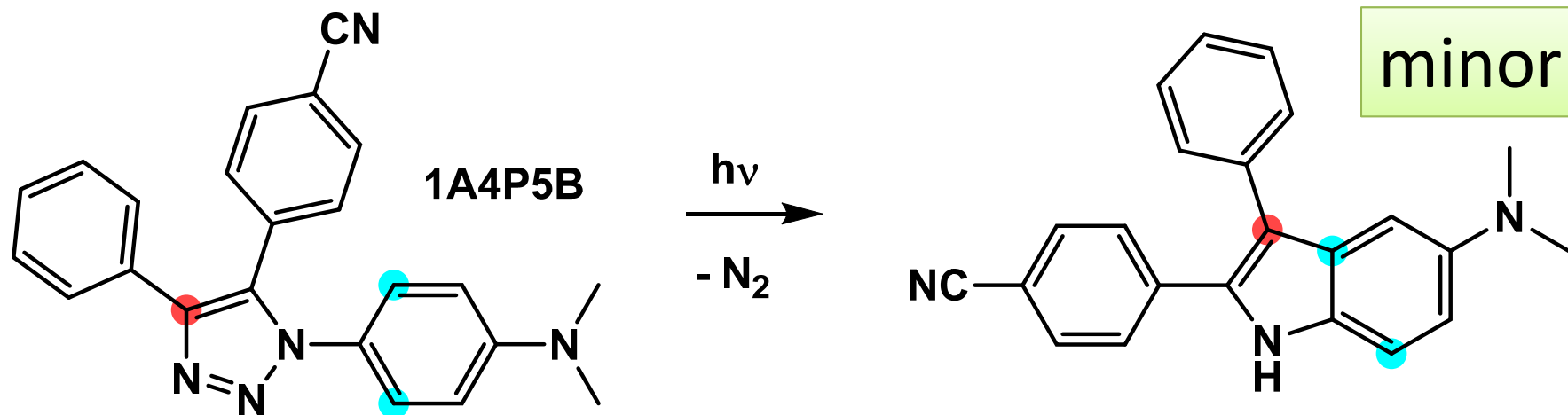


Factors on conversion

Original conditions: irradiation using 390-nm LED for 6 hours. [] = 1.5 mM in acetonitrile.

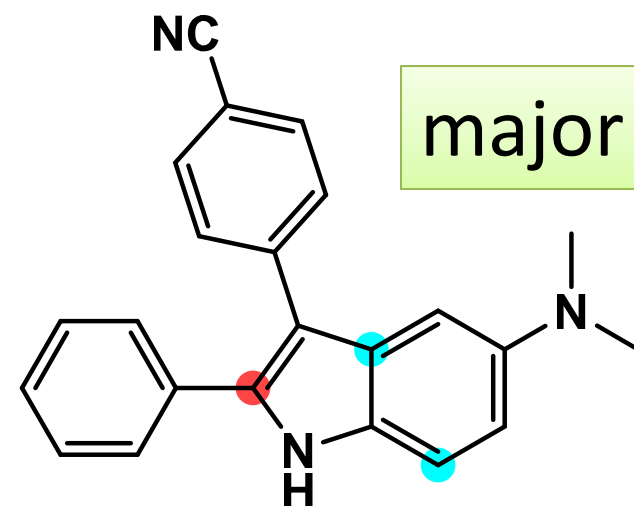
- Solvent
- Irradiation power and wavelength
- Light penetration (pathlength, turbidity)
- Distance from the light source
- Temperature; Additives

Changing solvent from acetonitrile to dichloromethane

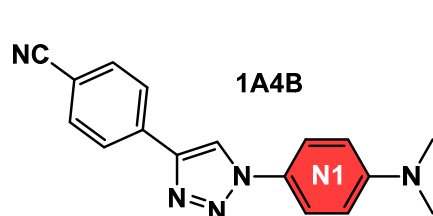


Acetonitrile: 76% in 6 hours

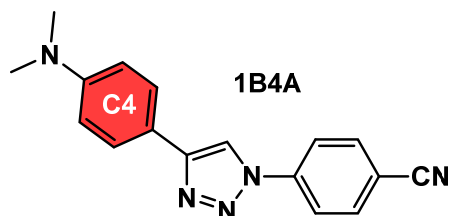
DCM: 100% in 30 minutes



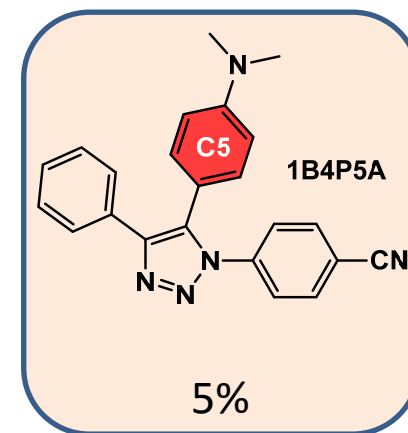
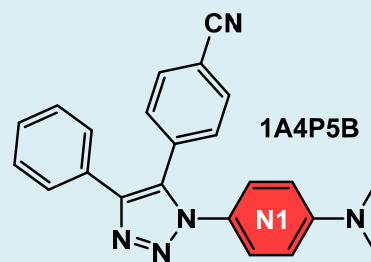
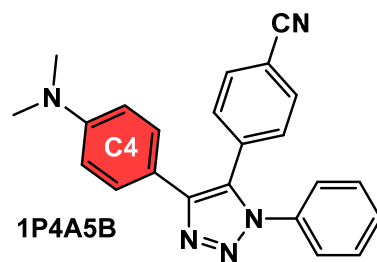
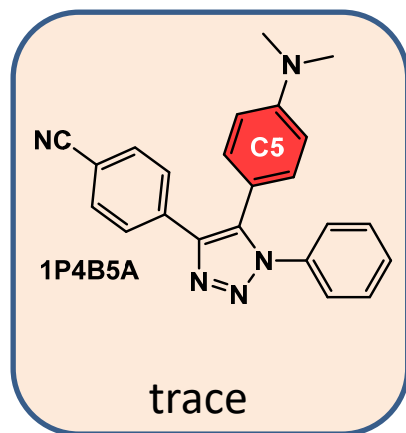
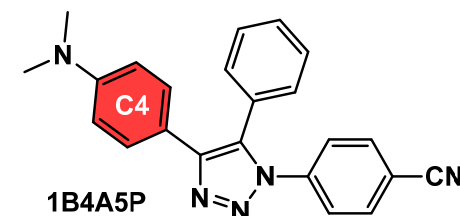
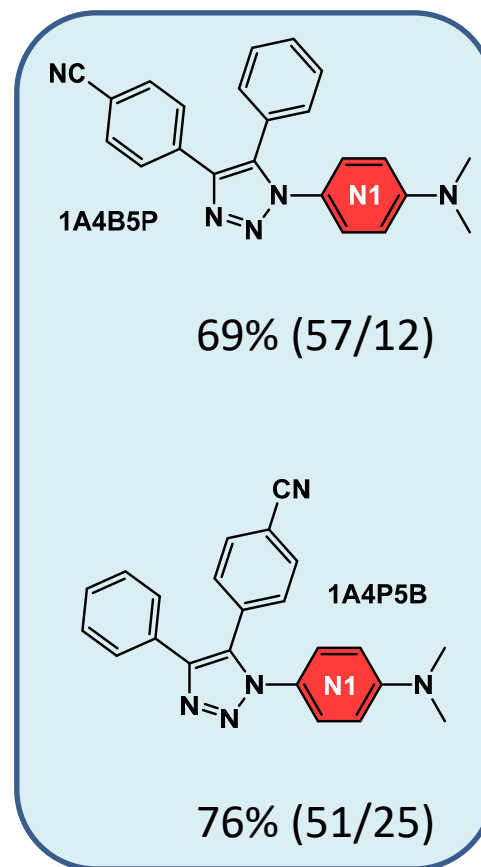
Explain the outcomes of photoconversion



40%

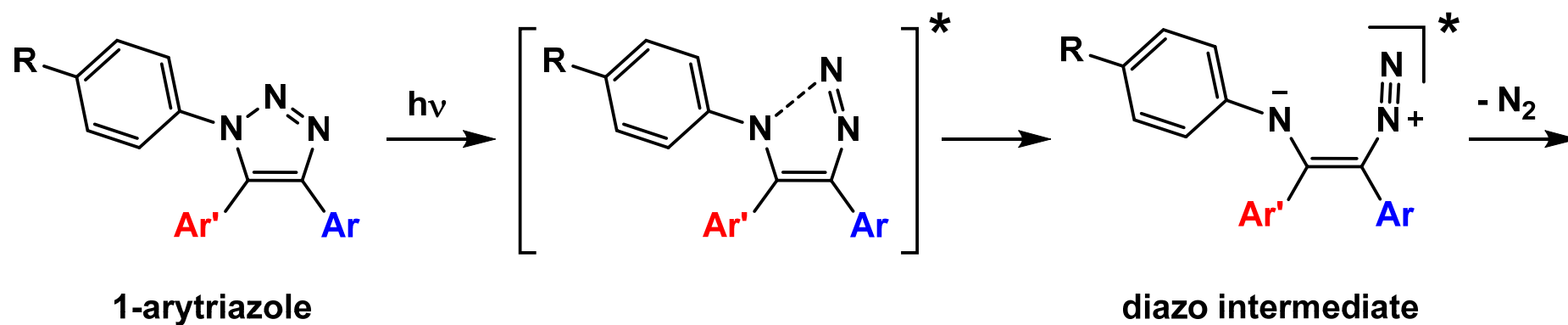


33%



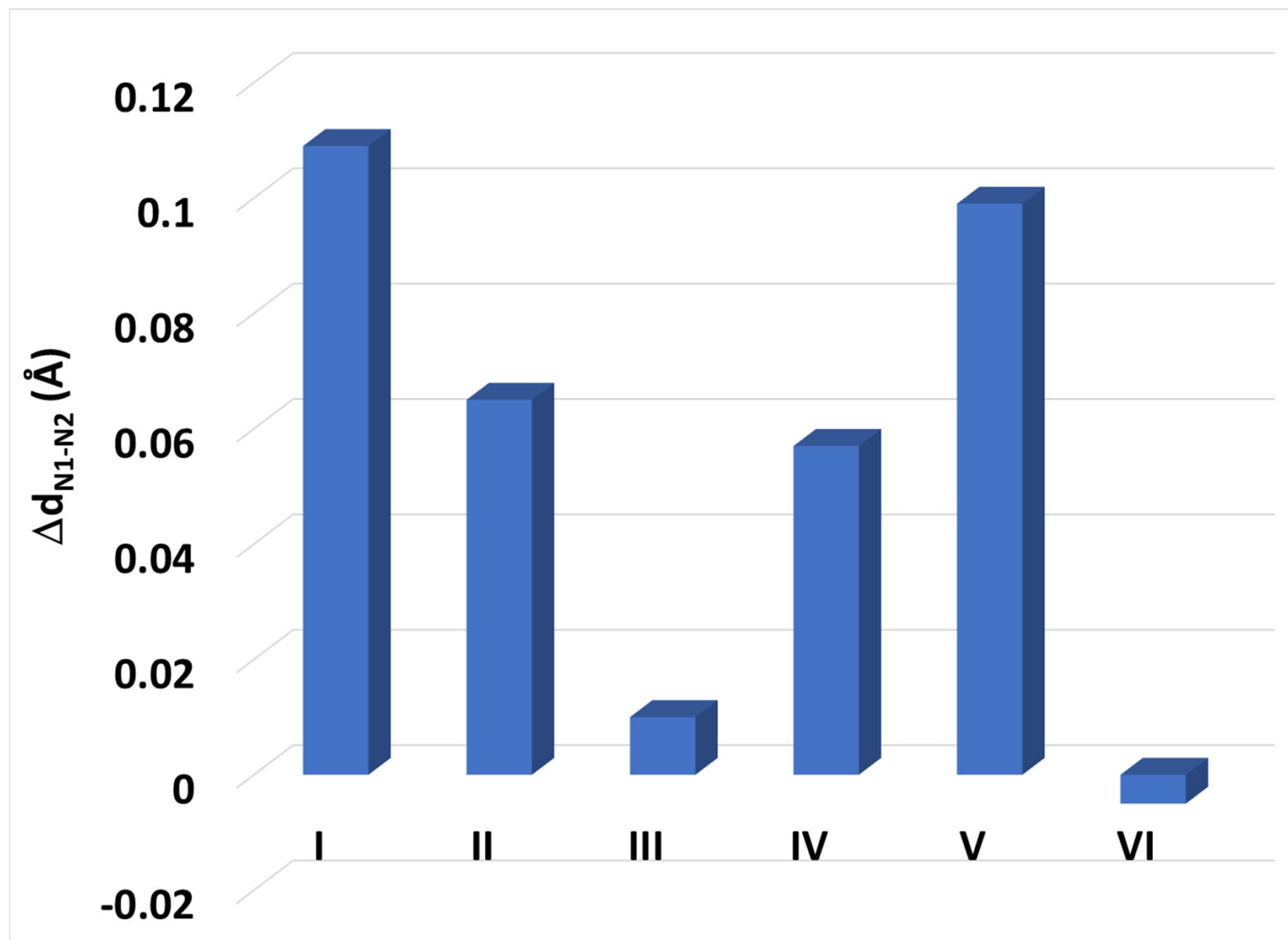
Conditions: irradiation using 390-nm LED for 6 hours. [] = 1.5 mM in acetonitrile.

Reactivity

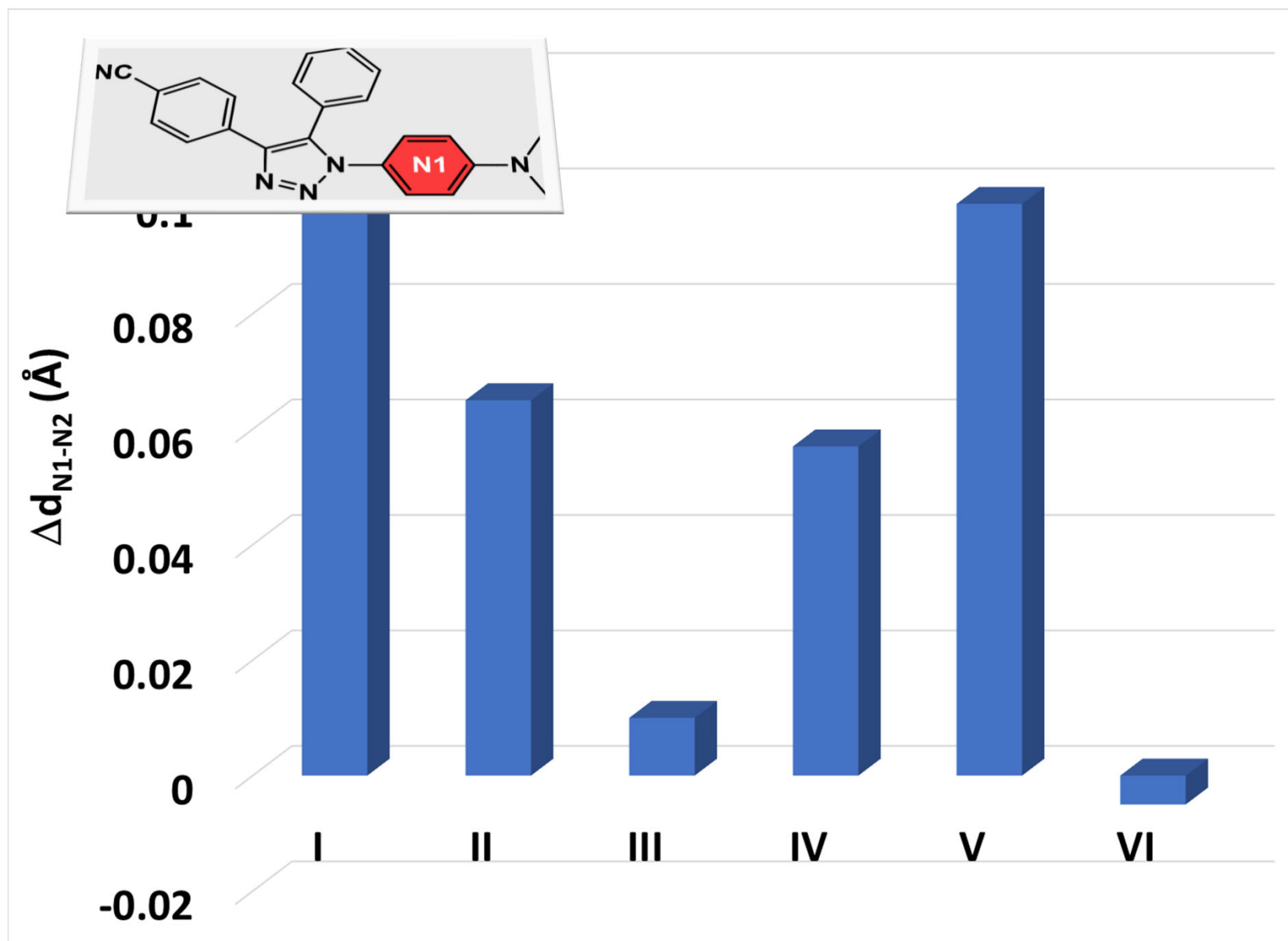


$$\text{Conversion} = F(\Delta d_{N1-N2})$$

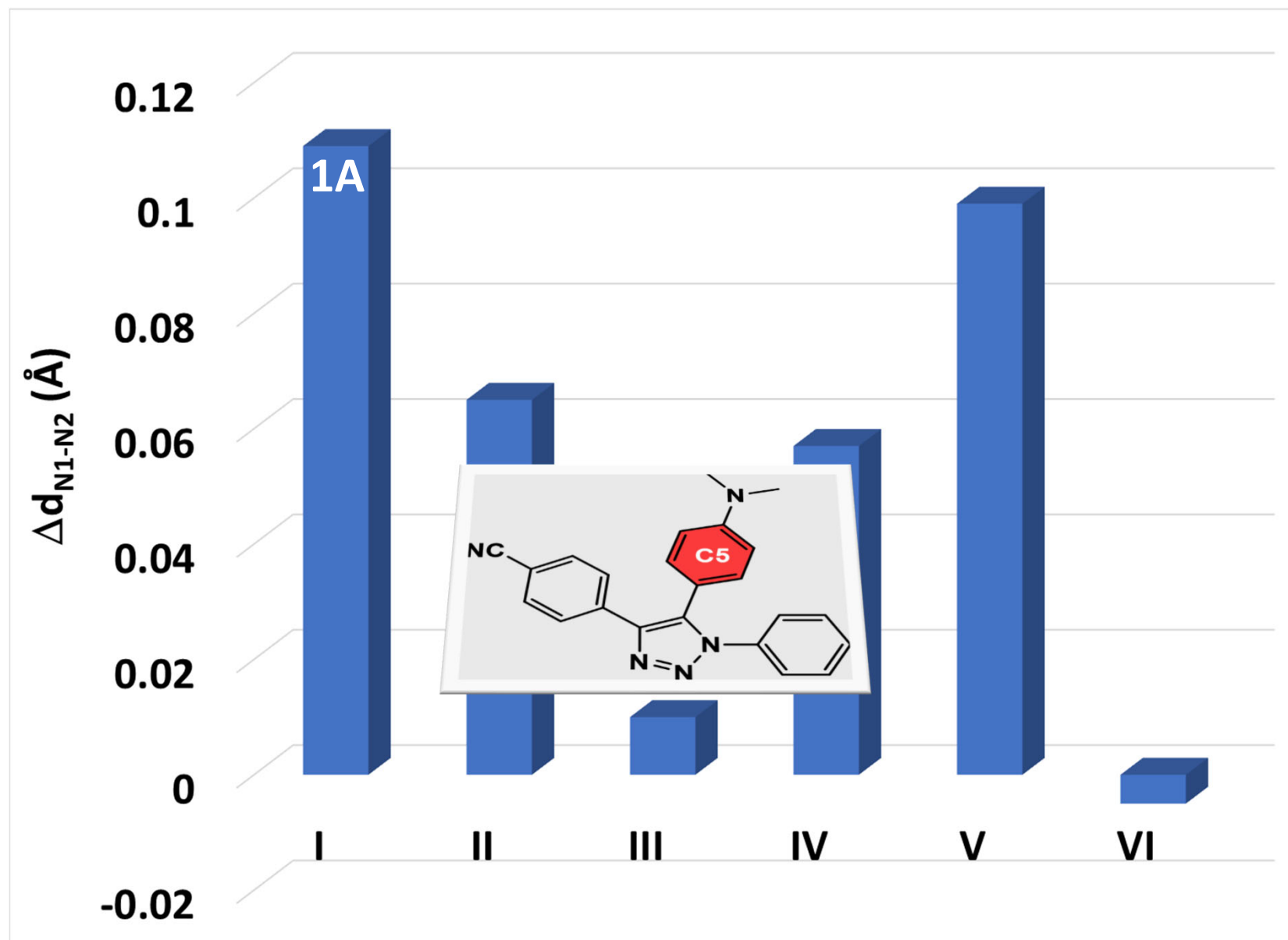
N1-N2 distance change upon excitation



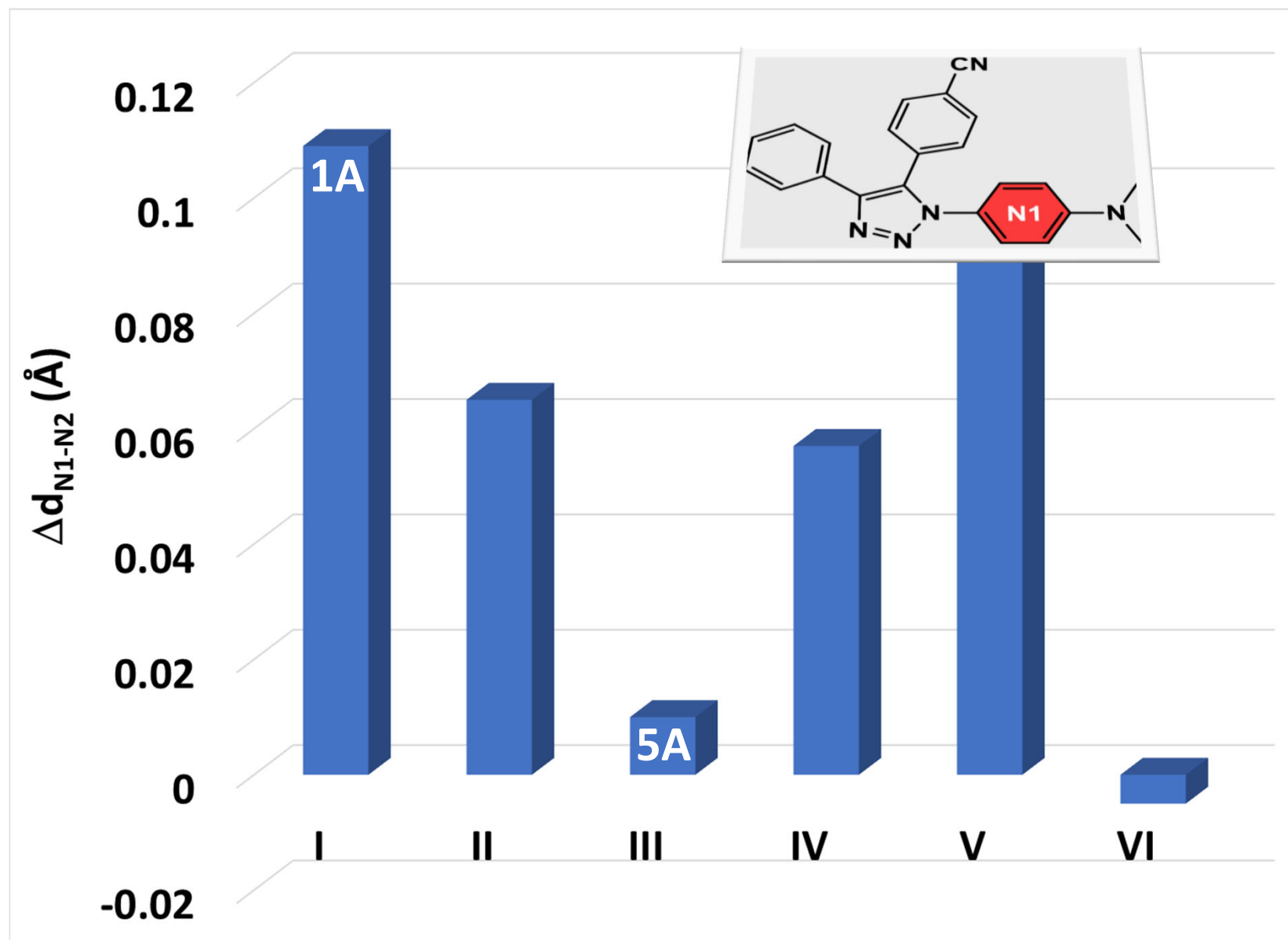
N1-N2 distance change upon excitation



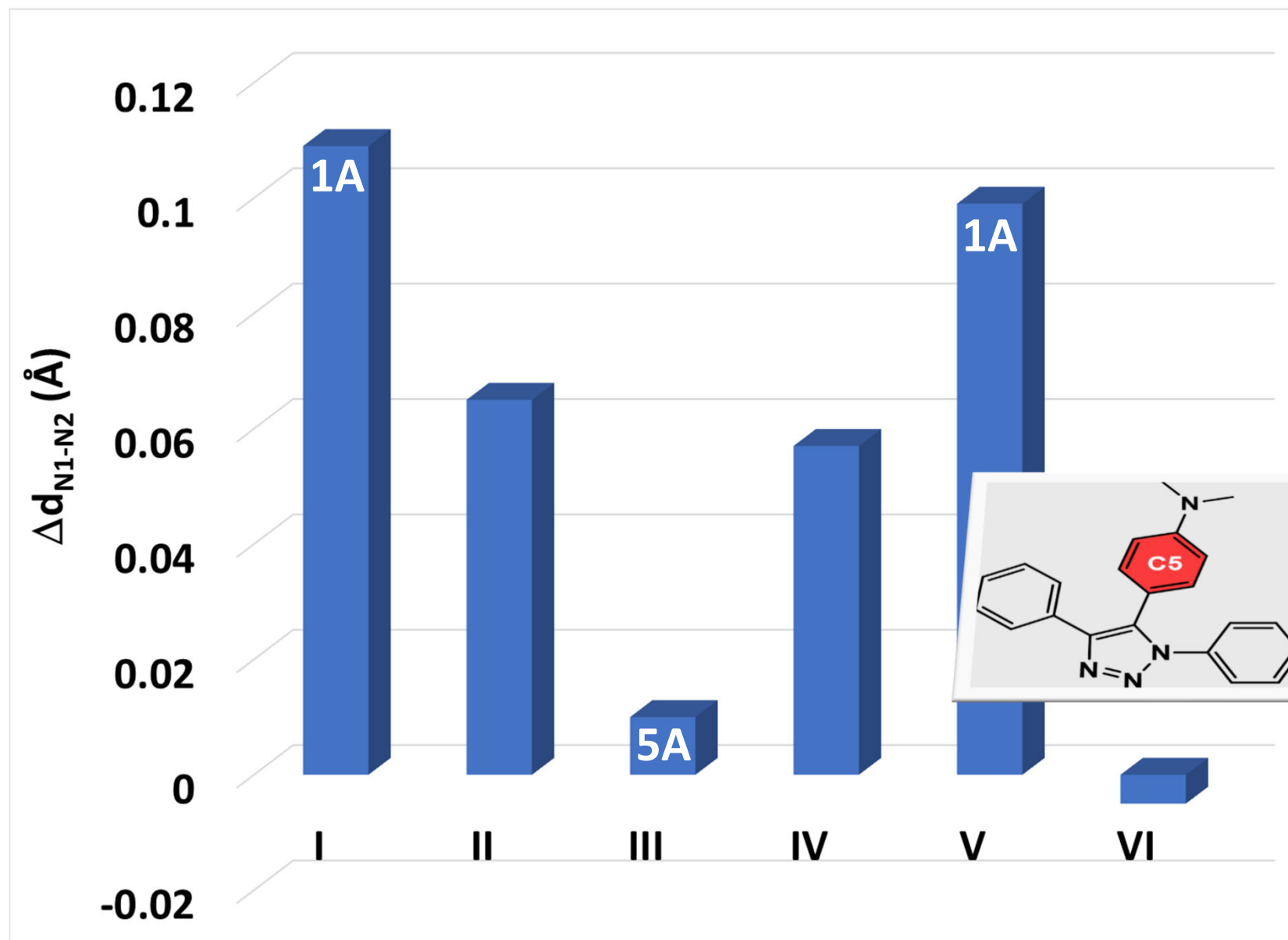
N1-N2 distance change upon excitation



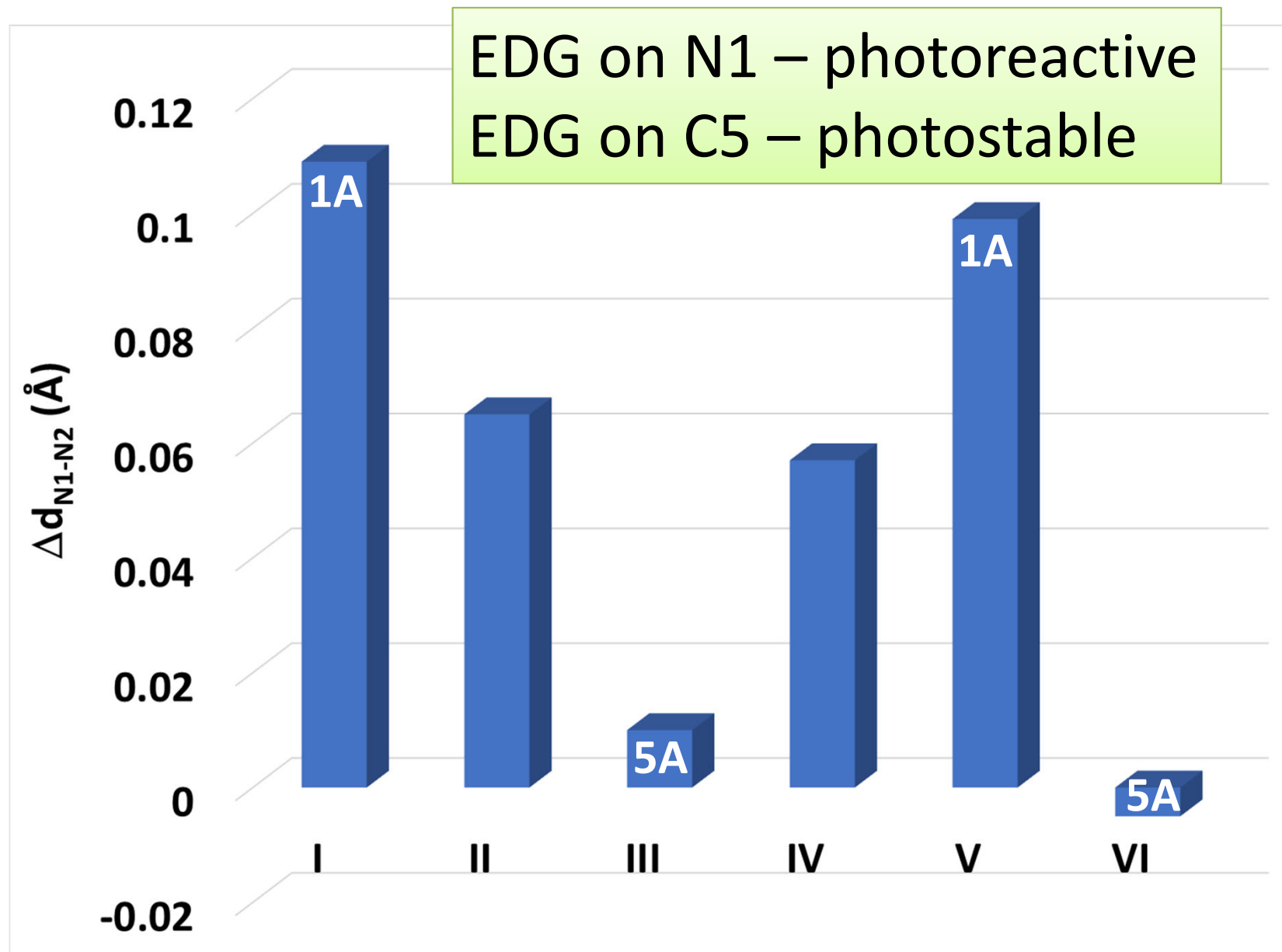
N1-N2 distance change upon excitation



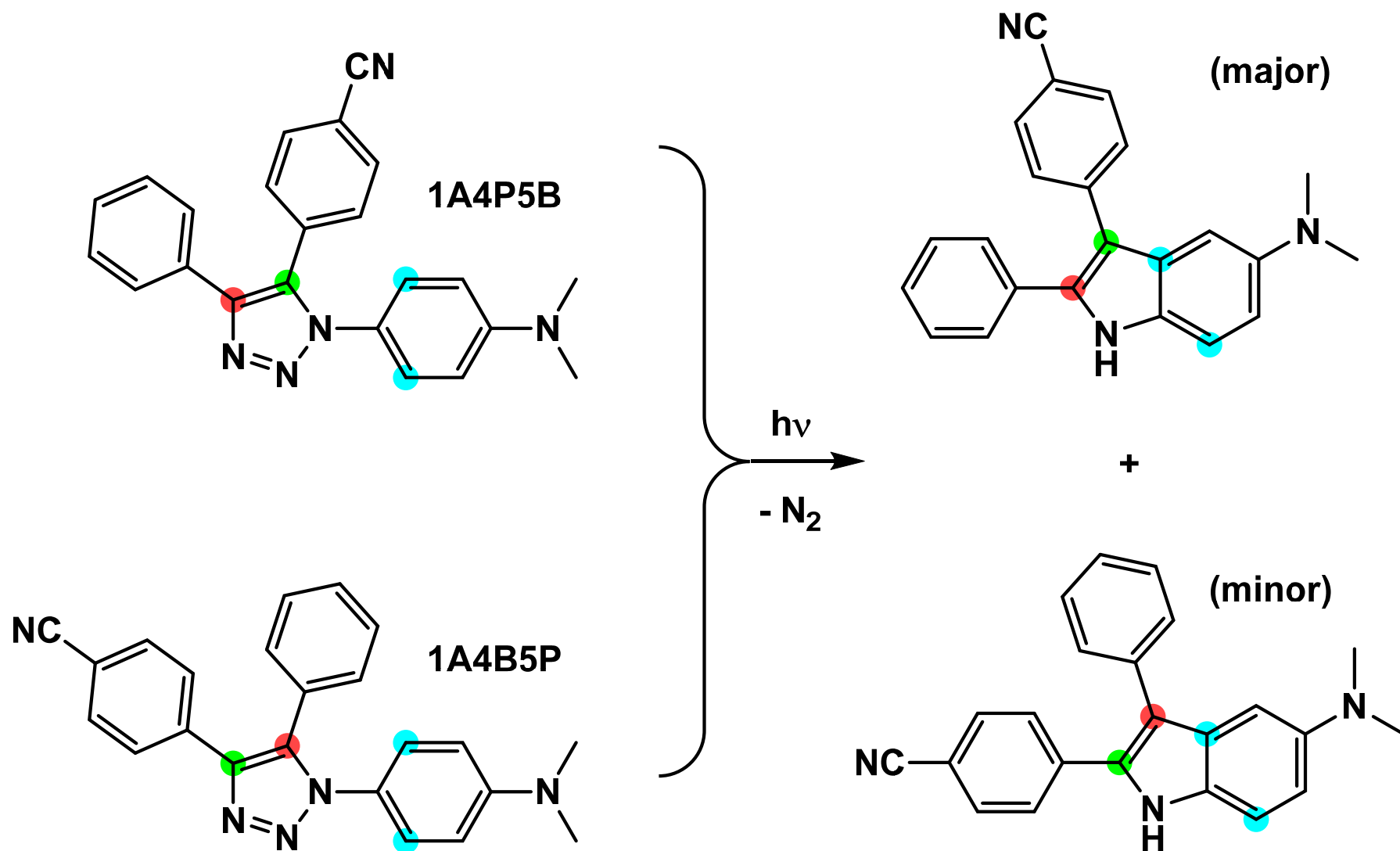
N1-N2 distance change upon excitation



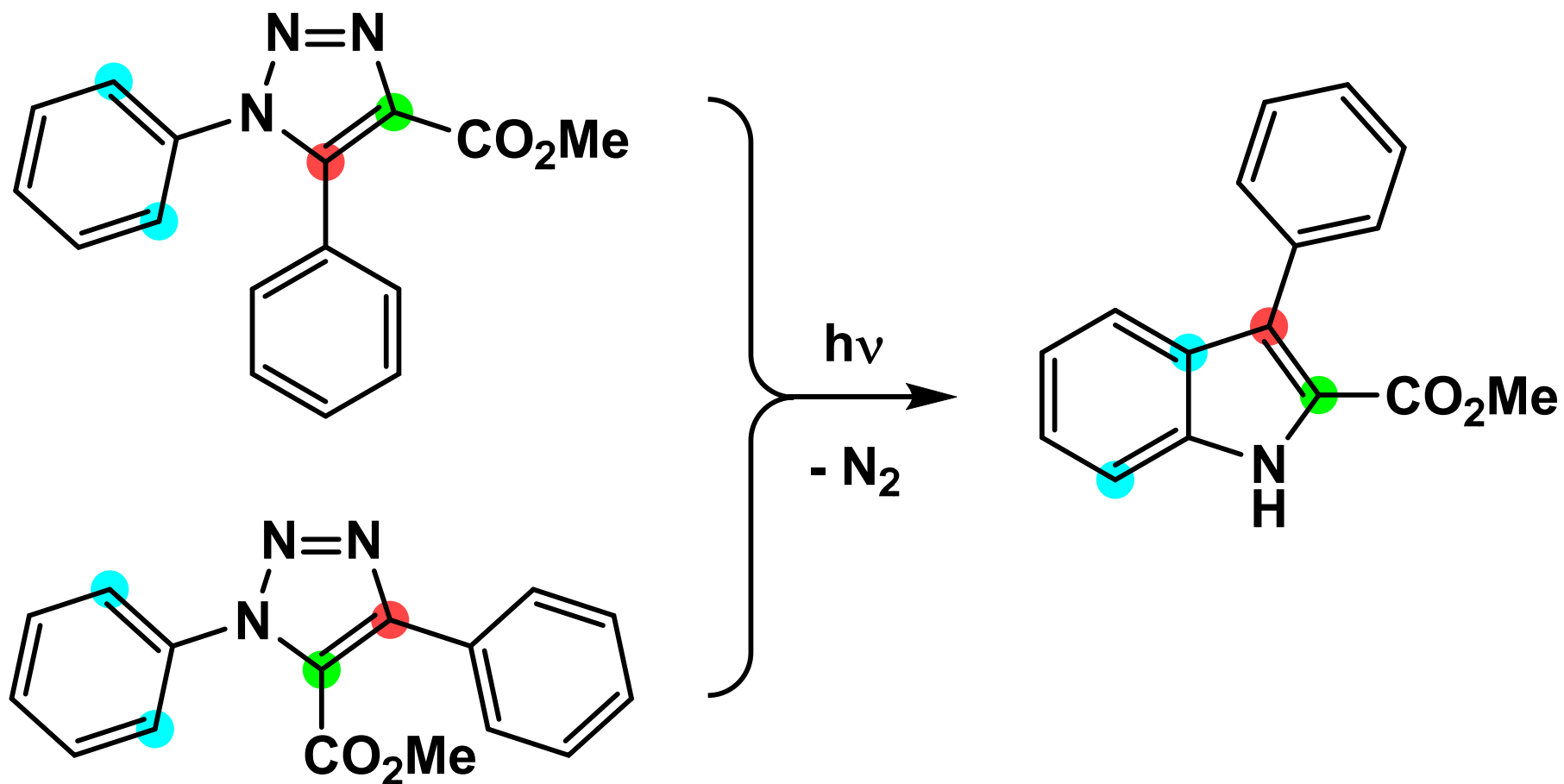
N1-N2 distance change upon excitation



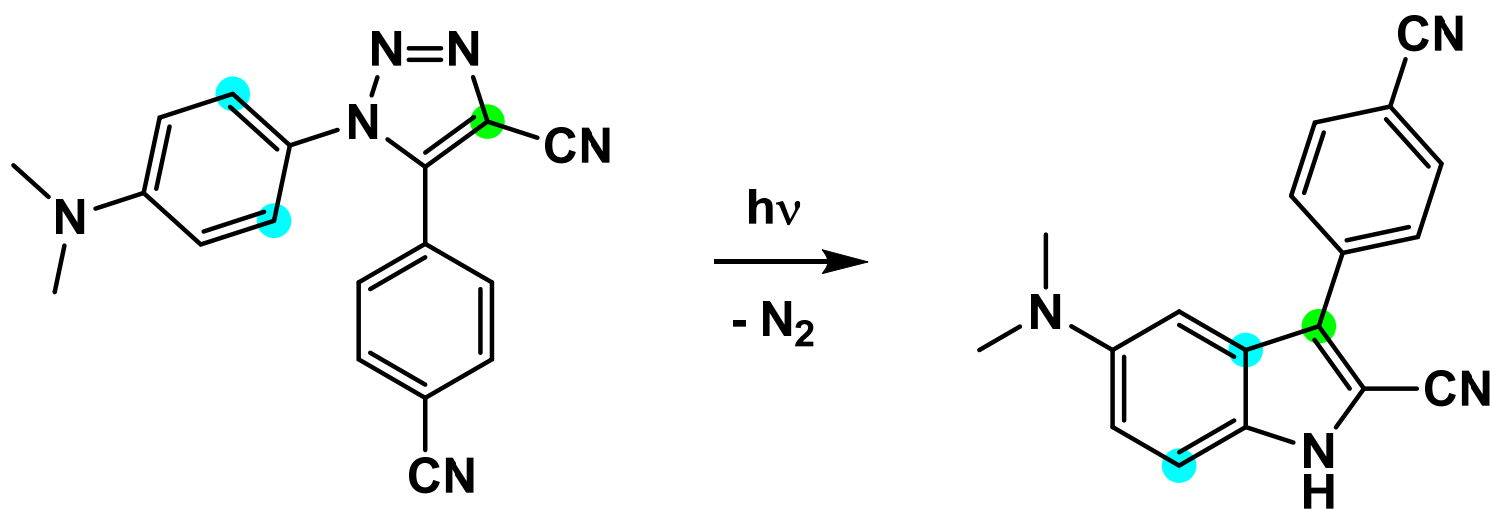
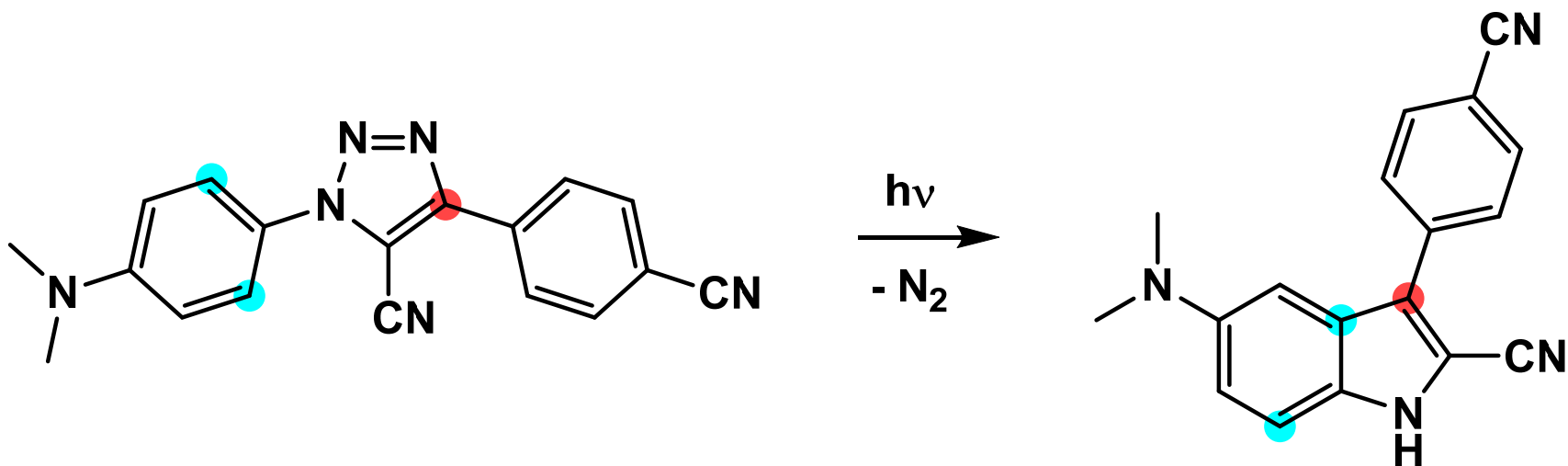
Selectivity – Cat. #1



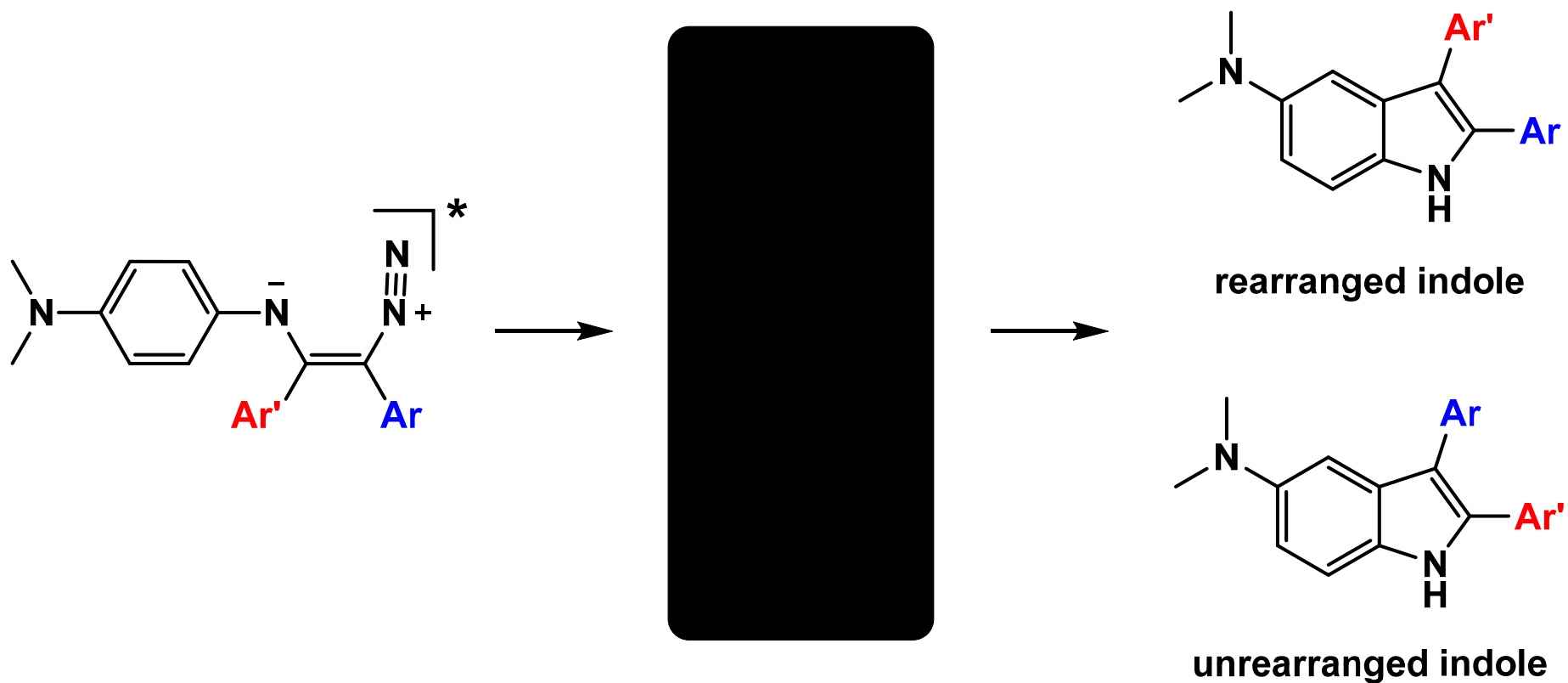
Selectivity – Cat. #2



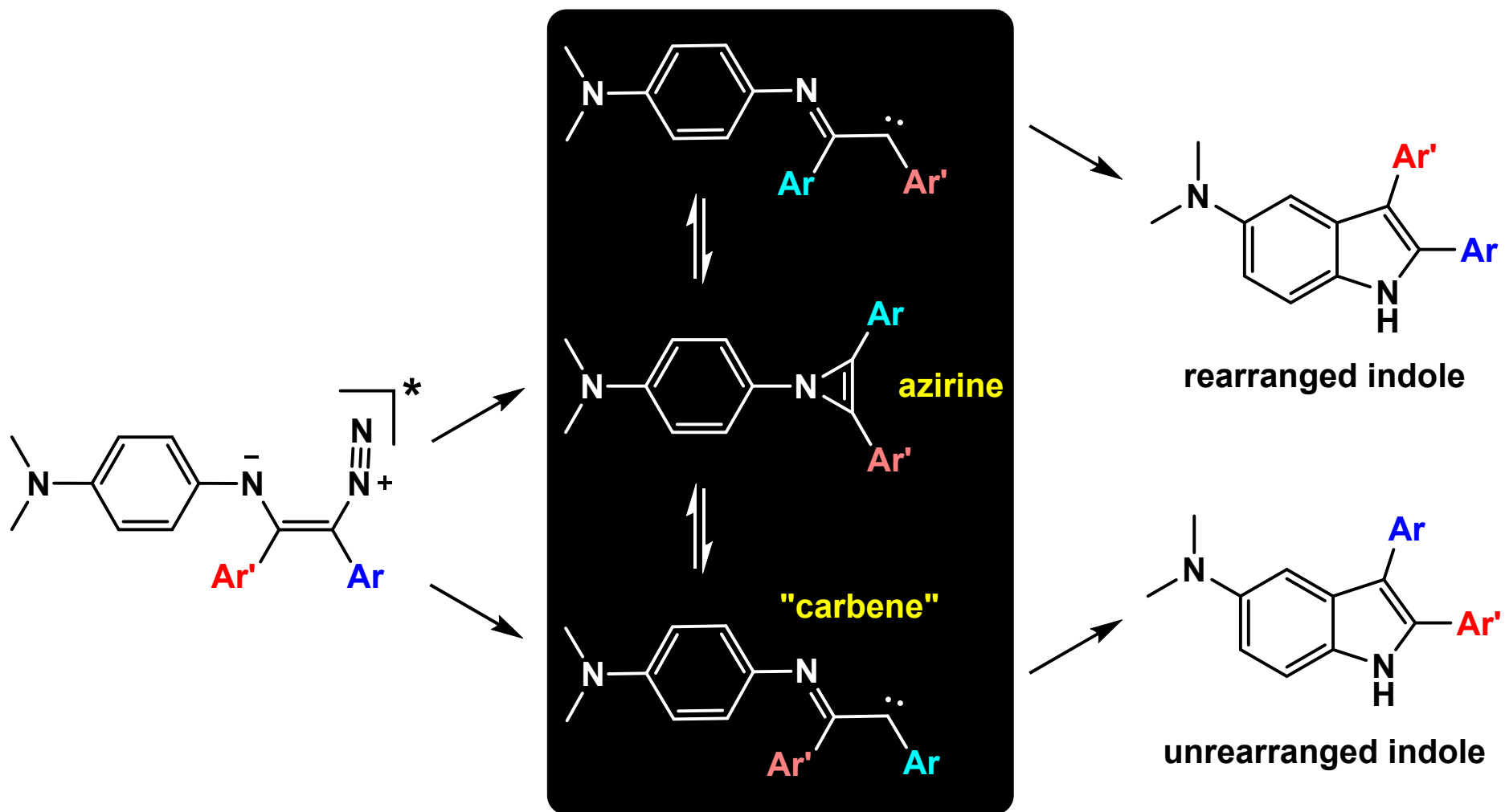
Selectivity – Cat. #3



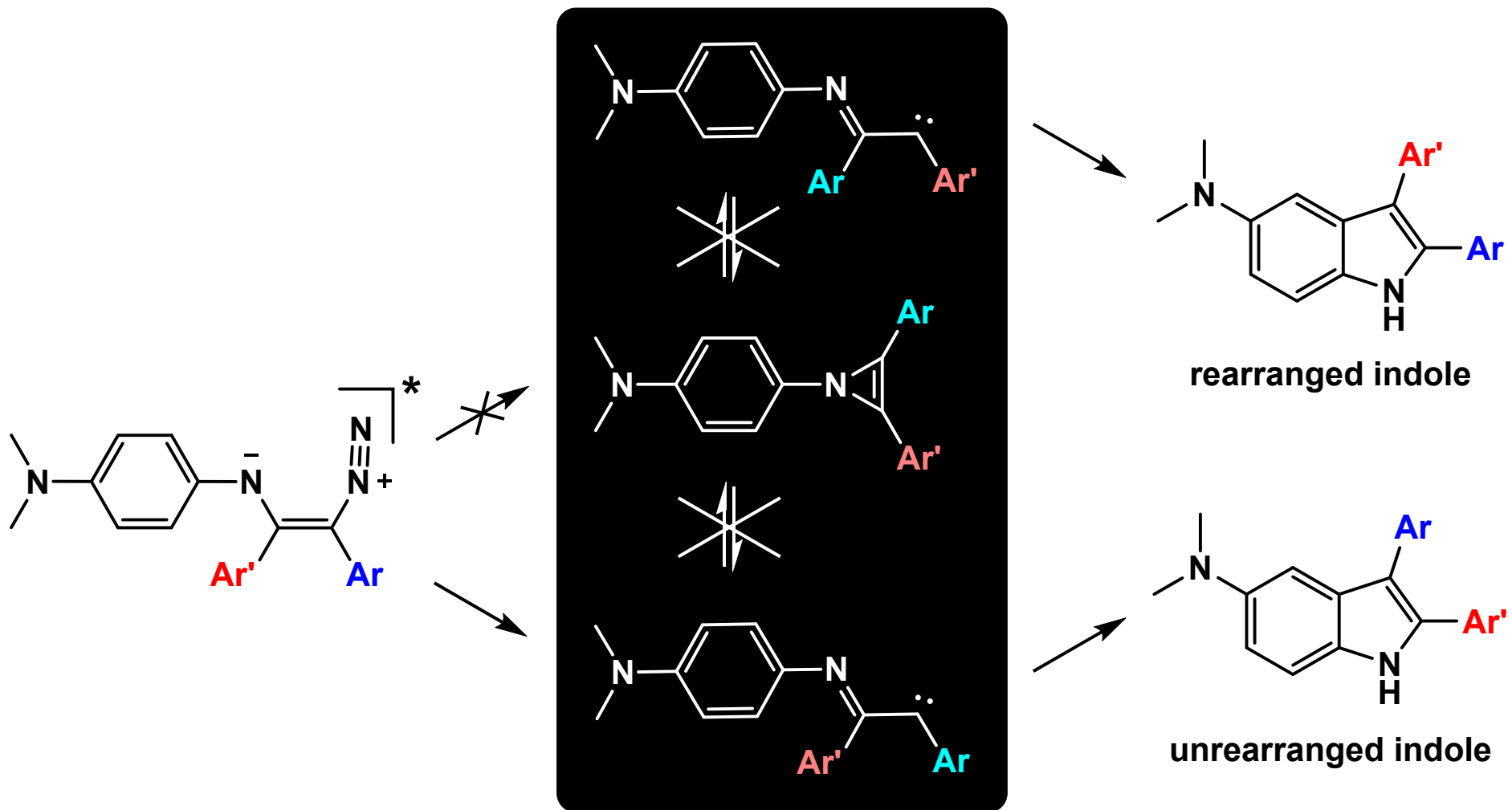
How do We Explain the Selectivity?




Selectivity Cat. #1 and 2



Selectivity Cat. #3



Research Article |  Full Access

Luminescence and Stability of 1,4,5-Triaryl-1,2,3-Triazoles

Brandon D. Nusser, Joseph V. Accardo, Lei Zhu First published: 03 July 2023 | <https://doi.org/10.1002/cphc.202300209>

PDF



TOOLS

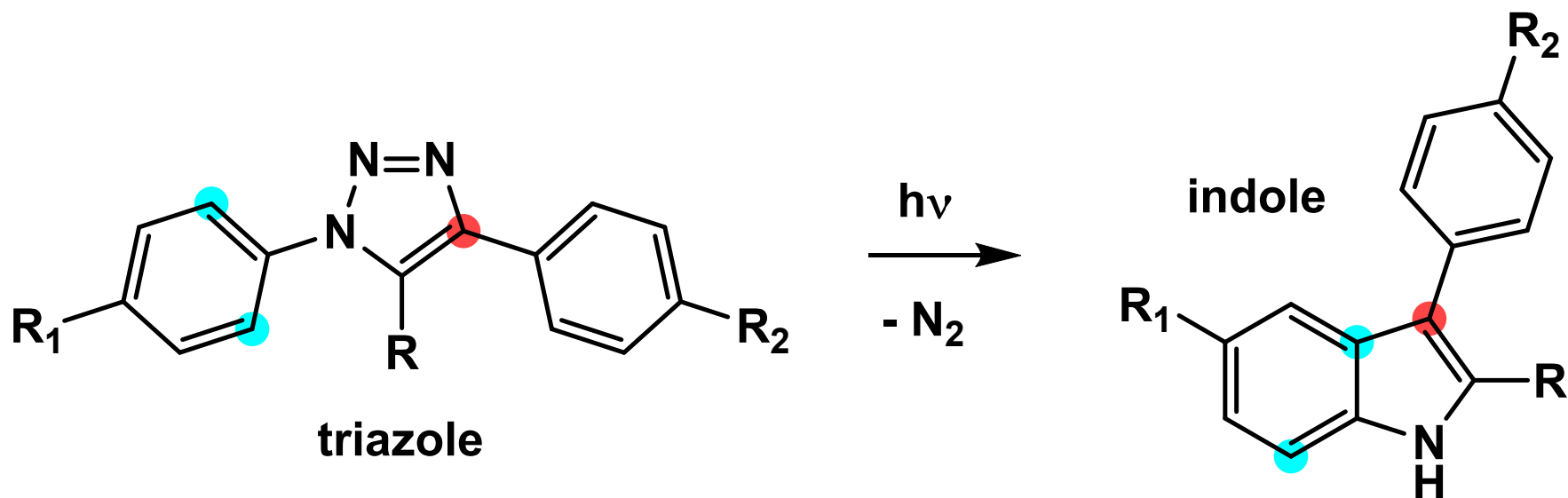


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Abstract

The fluorescence, phosphorescence, and photochemical properties of di- and triaryl-substituted-1,2,3-triazoles are reported in this work. The ease of synthesis of regioisomers of substituted triazoles enables a systematic study on the correlation between regiochemistry and excited state properties, which include the solvent dependence of fluorescence, energy gap between singlet and triplet emitters, and propensity to photon-triggered transformations. The triazoles that carry electron (e)-donor and e-acceptor aryl substituents show high fluorescence quantum yields in weakly

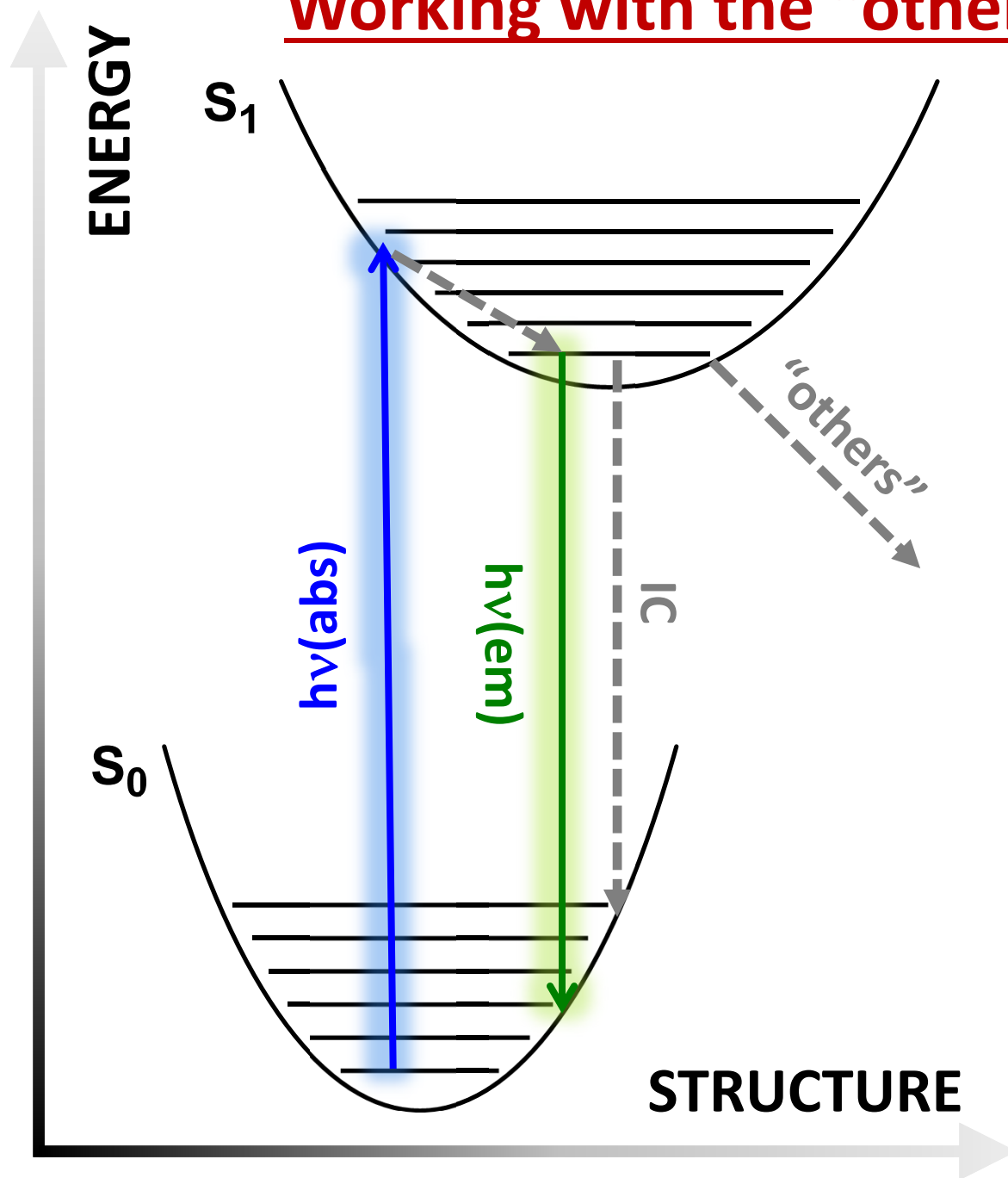
Triazole photoconversion to indole - Summary



Reactivity – the elongation of N1-N2 bond in the S_1

Selectivity – azirine and carbene(s) interconversion in the S_0

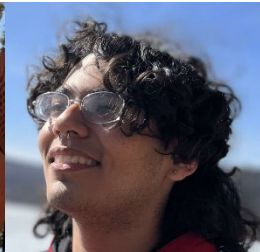
Working with the “other processes”



The “others”

- Photoinduced electron transfer
- Charge transfer
- Energy transfer
- Proton transfer
- ...
- ...

ACKNOWLEDGEMENT



Chris



Joe

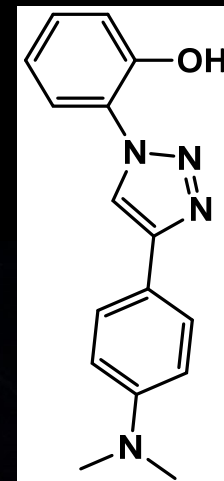
Brandon

Yael



THE FLORIDA STATE UNIVERSITY
CHEMISTRY & BIOCHEMISTRY





ASK THE GROUP
ABOUT CHEMISTRY