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MINISTRY
OF EDUCATION
AND SCIENCE

Organic Functional Materials

Part of the project №BG-RRP-2.004-0002, "BiOrgaMCT"



University of Chemical
Technology and
Metallurgy

15-17 December 2024, Separeva Banya
Laboratory of Organic Functional Materials

WP 1 Synthesis of Organic Materials

- *Design of new molecules*
- *Synthesis and purification*
- *Structure elucidation*

WP 2 Investigation of the Photophysical Properties

- *Steady-state and transient spectroscopy measurements*
- *Dynamic spectral measurements upon external stimuli*
- *Preparation of 1D and 2D solid-state materials*

WP 3 Study and Evaluation their Working Functions as Molecular Devices

- *Solid-state performance of organic materials (thin films, bulk material, deposition of various substrates)*
- *Investigation microscopic characteristics by TEM, SEM, XRD*
- *Structure-properties relationship evaluation*

Maria Atanasova

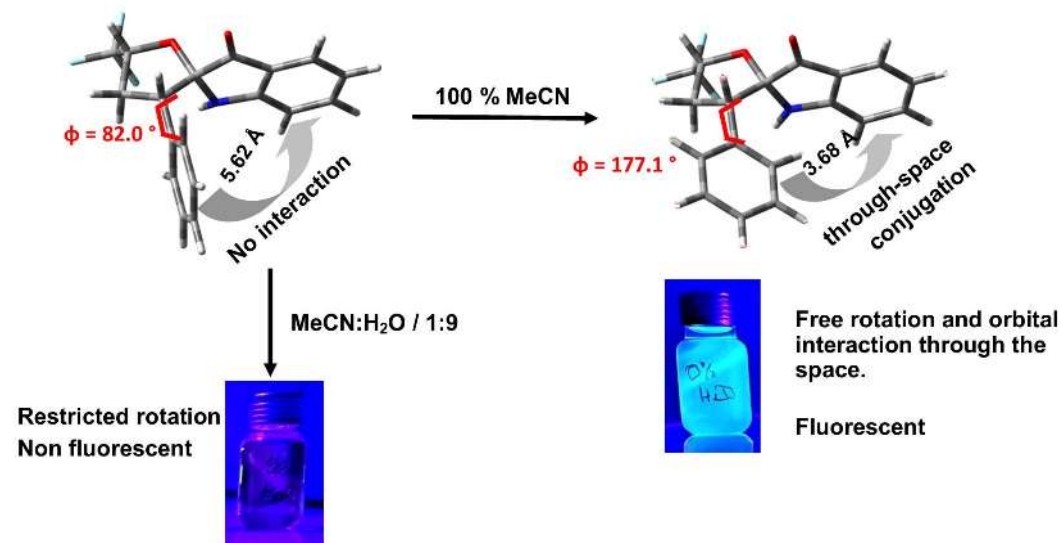
1. Maria Atanasova, Rositsa Kukeva, Vanya Kurteva, „*Chemical and mechanistic modelling of green solvent extraction of metallic species with 4-acylpyrazolones*“, **Journal of Molecular Liquids (Elsevier)** 415 (2024) 126332 <https://doi.org/10.1016/j.molliq.2024.126332> Q1 (Web of Science)

Desislava Grabcheva (Staneva) collaboration with 3.1.3 group (Bioactive compounds)

1. Staneva, D.; Todorov, P.; Georgieva, S.; Peneva, P.; Grabchev, I. „*Novel Peptide Analogues of Valorphin-Conjugated 1,8-Naphthalimide as Photodynamic Antimicrobial Agent in Solution and on Cotton Fabric*“, **Molecules (MDPI)** 2024, 29, 5421. <https://doi.org/10.3390/molecules29225421> IF = 4.1, Q2 (Web of Science)

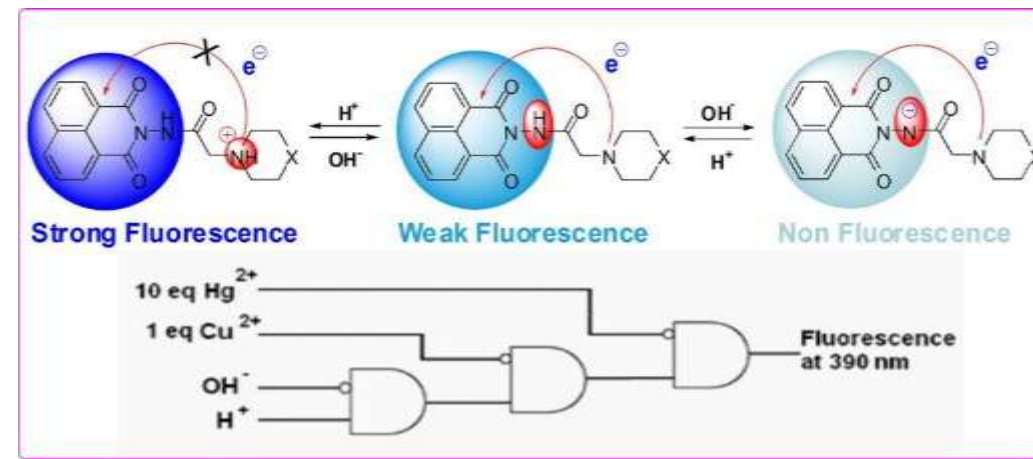
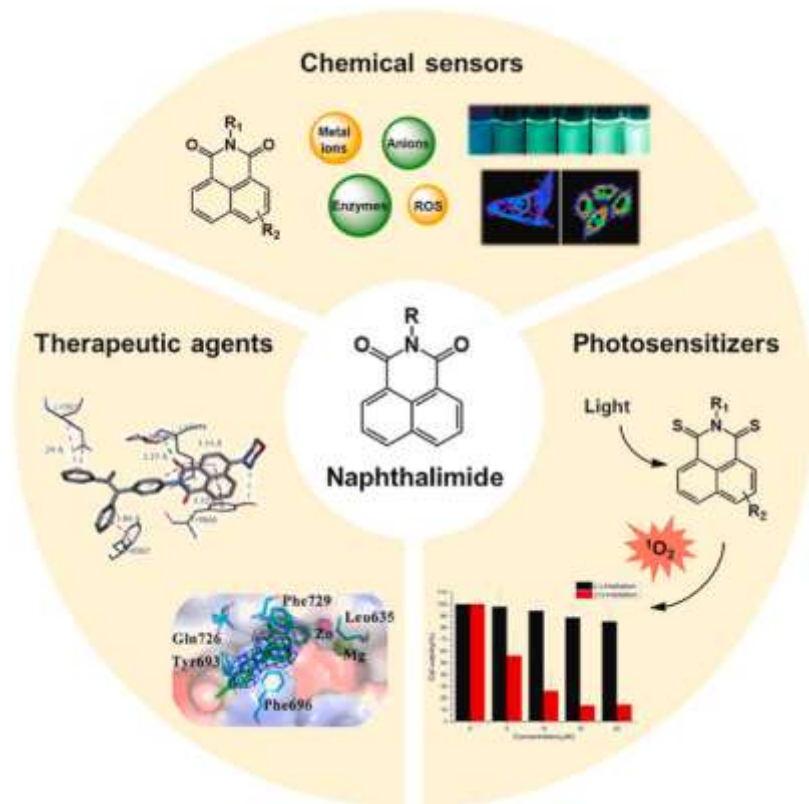
Anton Georgiev

1. Kosuke Nakashima, Aoi Imamura, Yasuyuki Matsushima, Shin-ichi Hirashima, Dancho Yordanov, Tsuyoshi Miura, Anton Georgiev, „*Intramolecular through-space conjugation of chiral C2-spirooxindole*“, Submitted to the journal (Under Review) 2024



Planned activities in 2025 y:

- ✓ Design and synthesis of novel naphthalimide based architecture as molecular sensors and logic gates;
- ✓ Application and testing in real conditions;
- ✓ At least two published papers are expected.

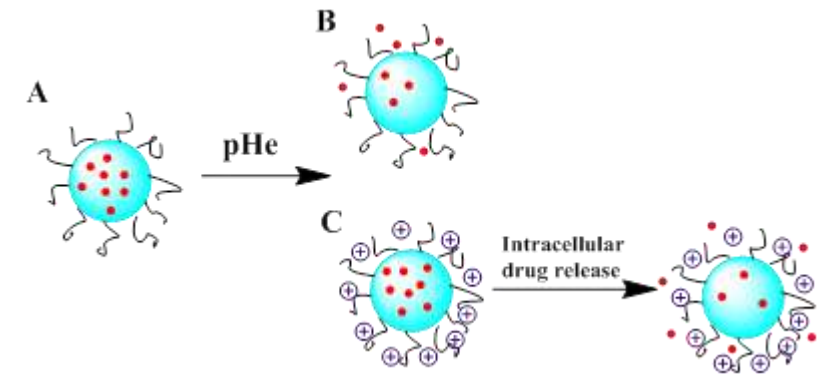
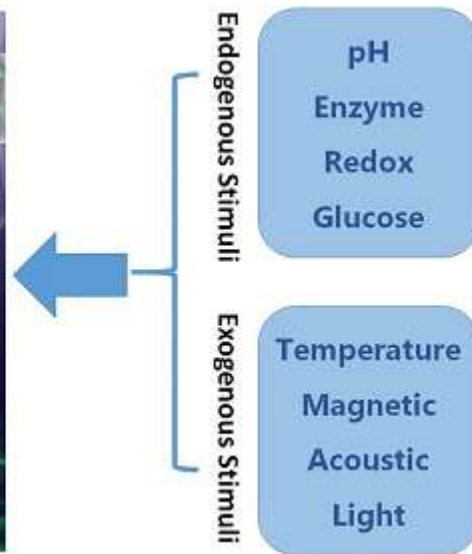


Planned activities in 2025 y:

- ✓ Design and synthesis of polymer systems for drug delivery;
- ✓ Synthesis of nanoparticles;
- ✓ Biological evaluation and two published papers.

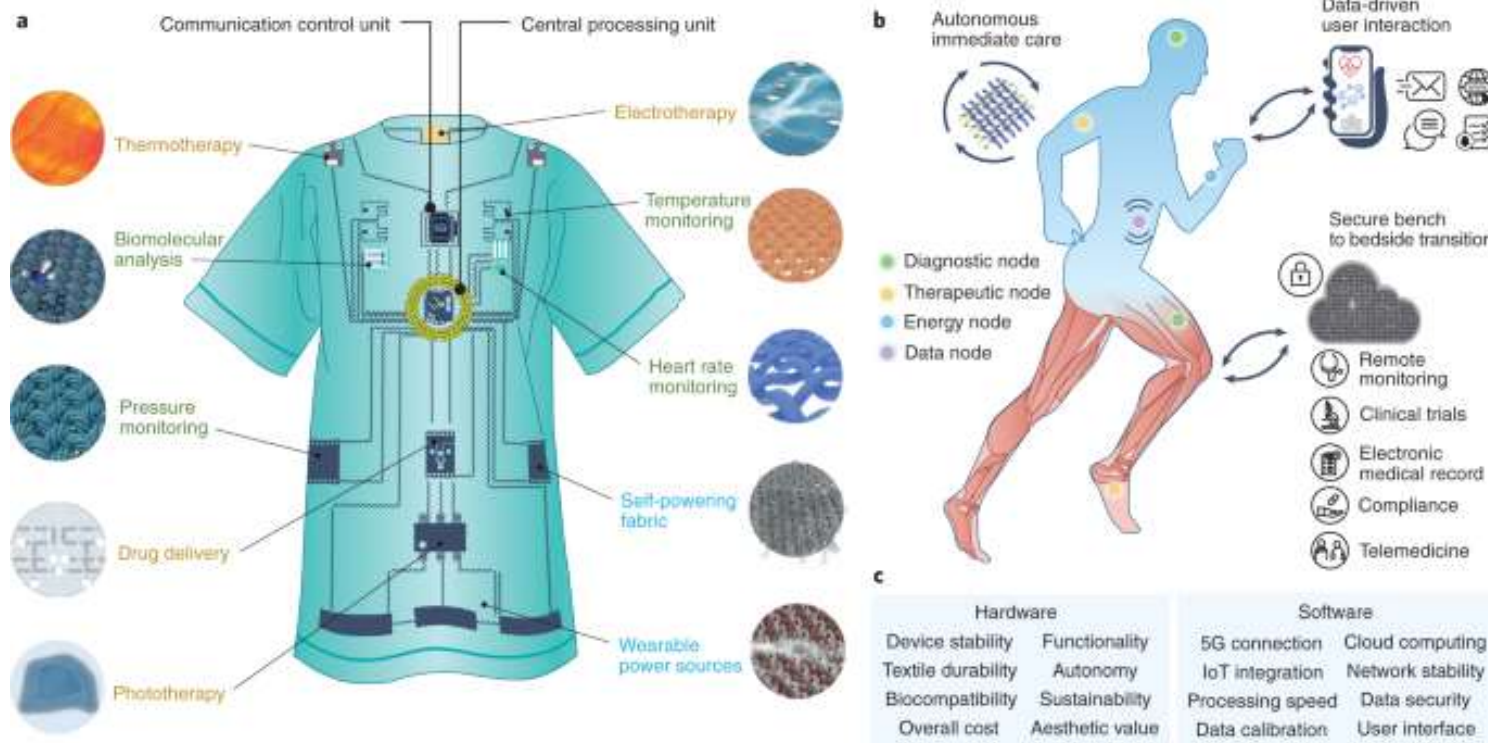


Theranostics 2016; 6(9):1306-1323

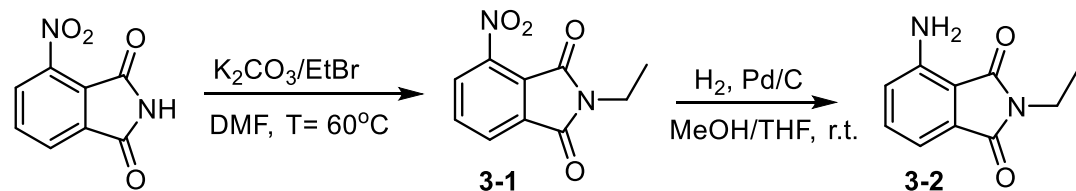


Planned activities in 2025 y:

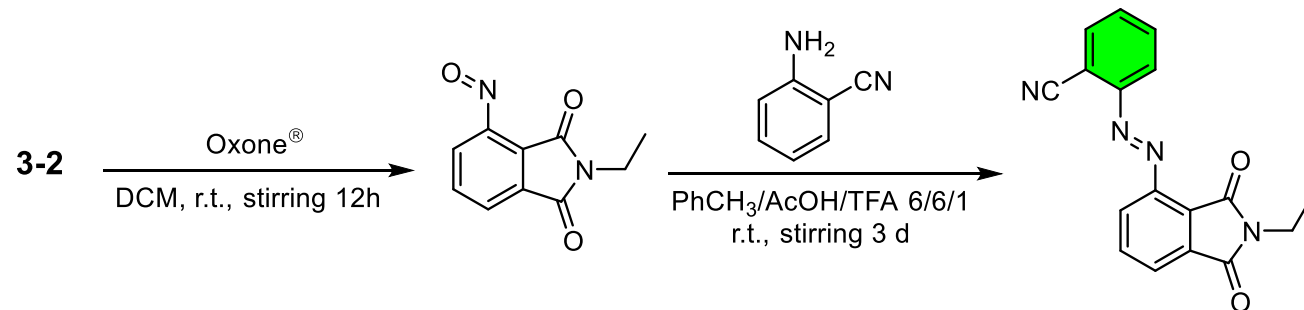
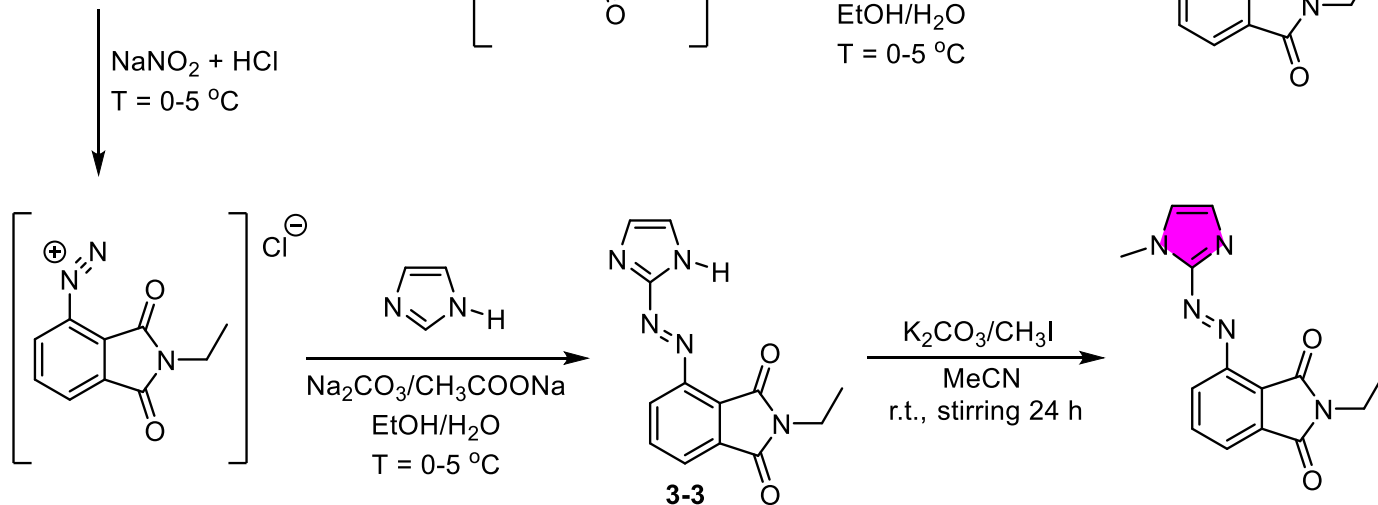
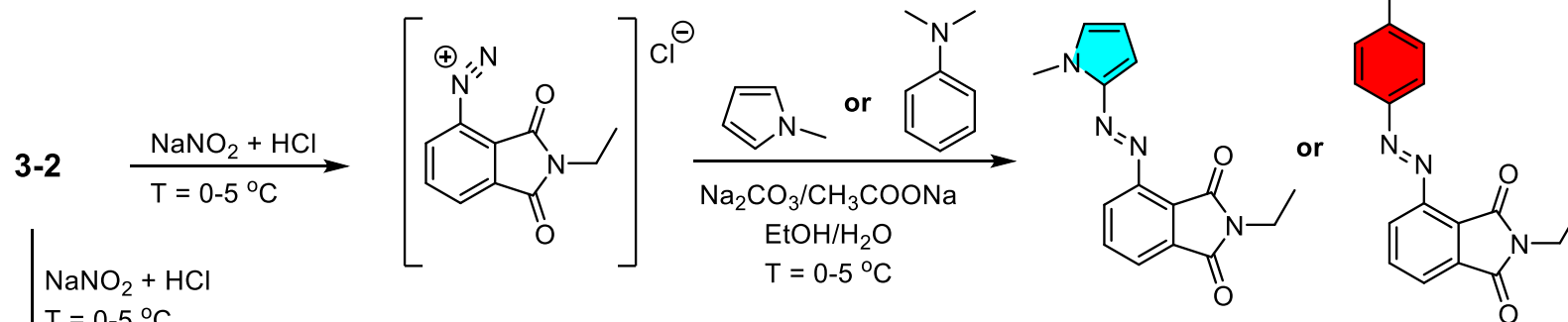
- ✓ Design of novel textile materials for smart performance;
- ✓ Antibacterial and biocompatibility;
- ✓ At least two published papers are expected.

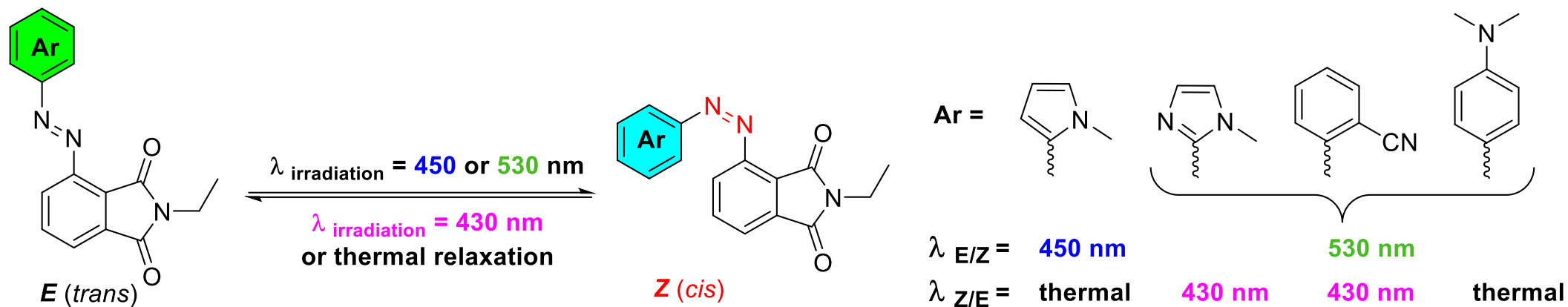


3-Azo Phthalimides by Anton Georgiev

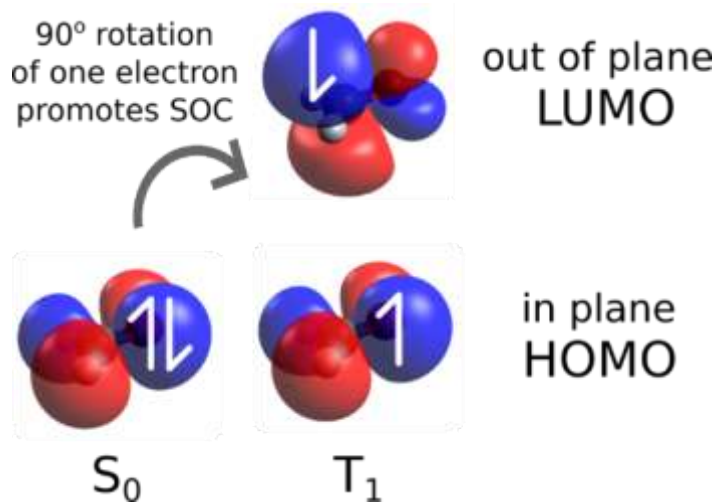


3-nitrophthalimide



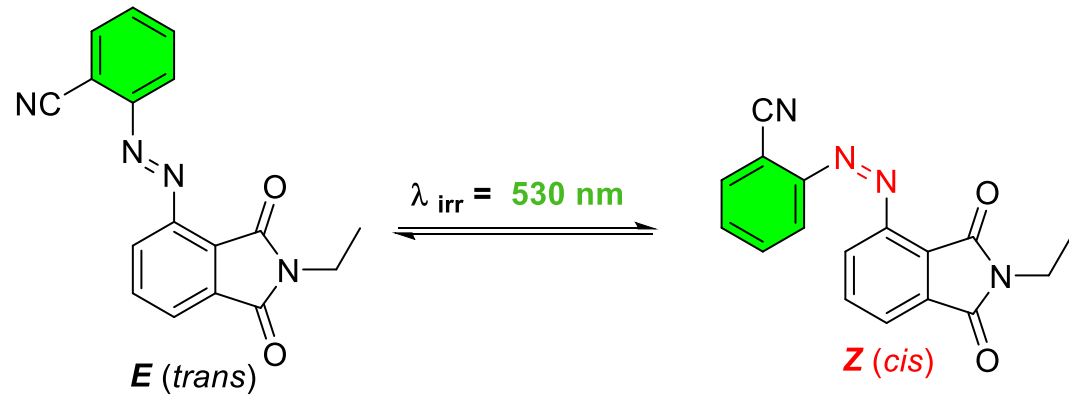
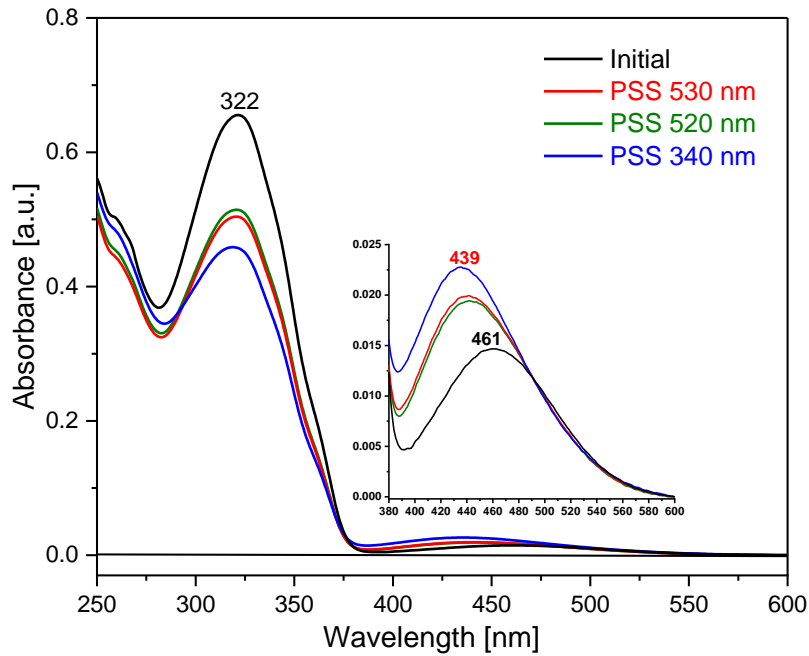
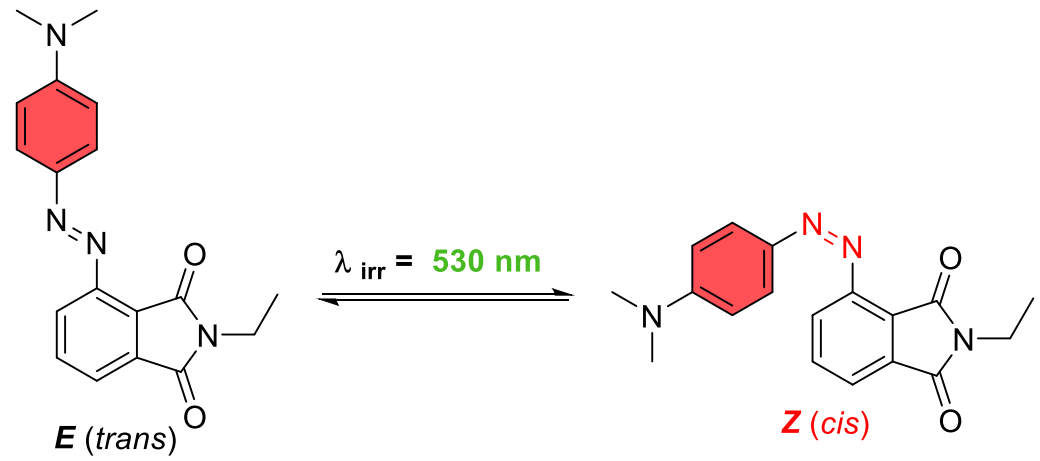
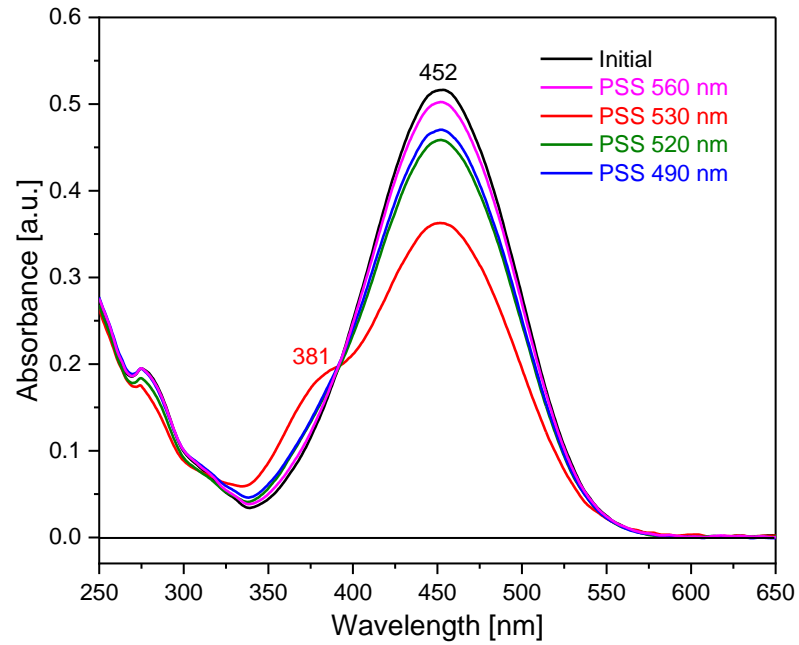


Ortho-functionalized phthalimide azo switches

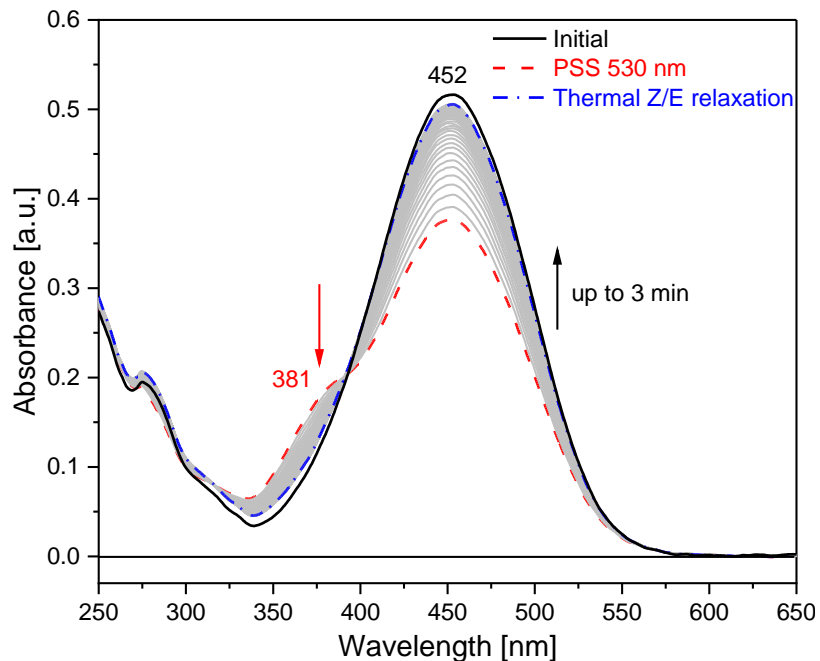


- ✓ Spin-orbit coupling occurs with ortho-functionalization by σ or π EA.
- ✓ Enhances the n - π^* bands separation between two switched states.
- ✓ Visible light E/Z activated < 500 nm irradiation.

3-Azo Phthalimides by Anton Georgiev



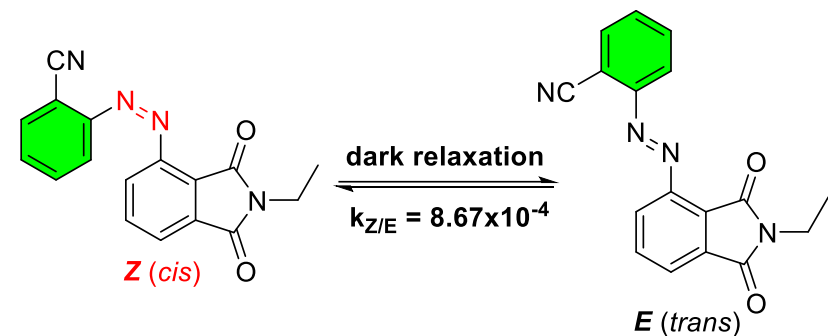
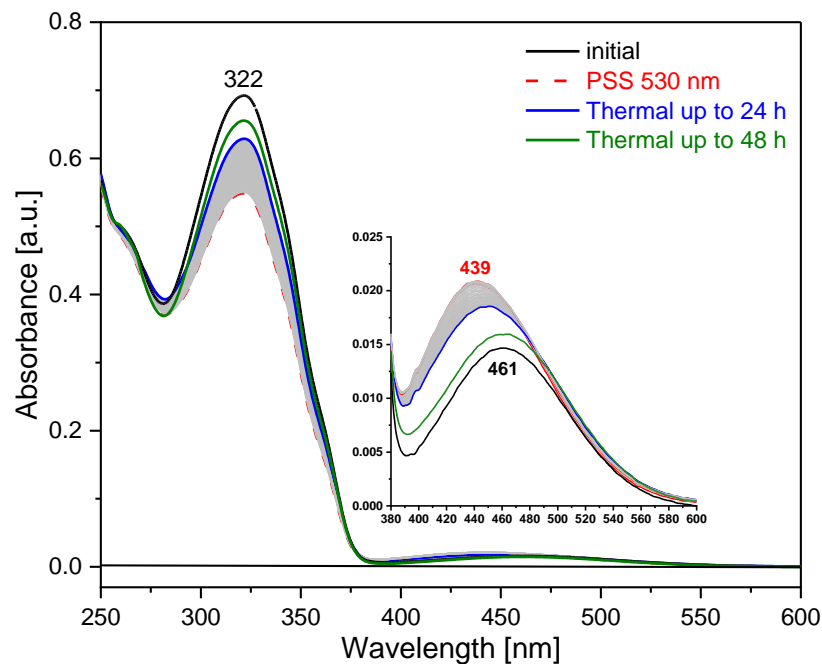
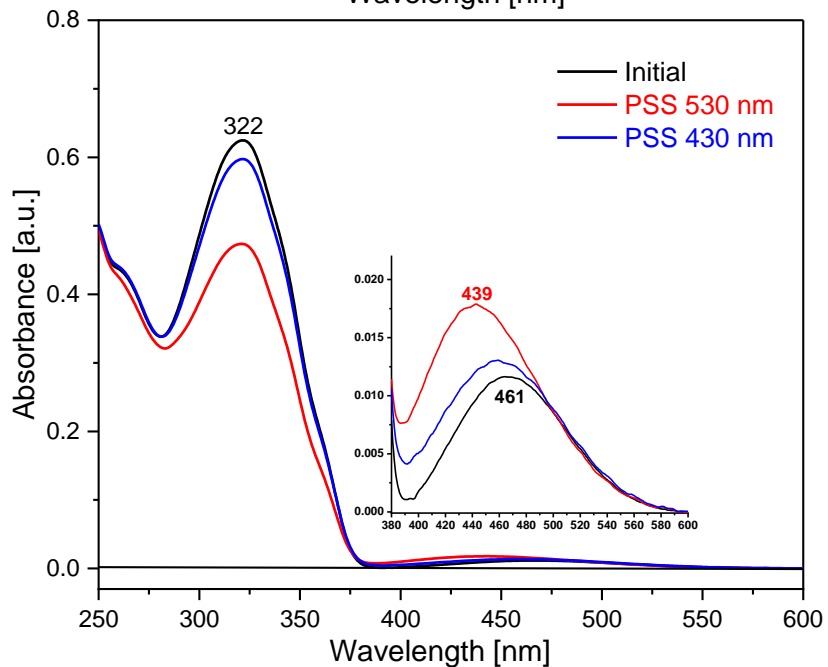
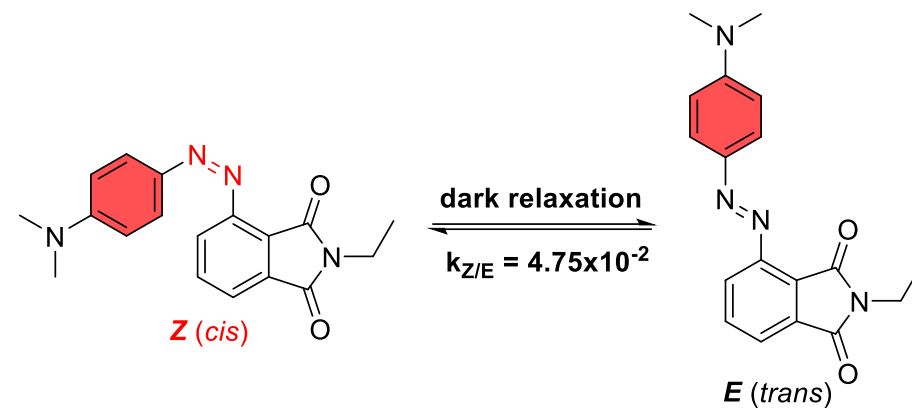
3-Azo Phthalimides by Anton Georgiev



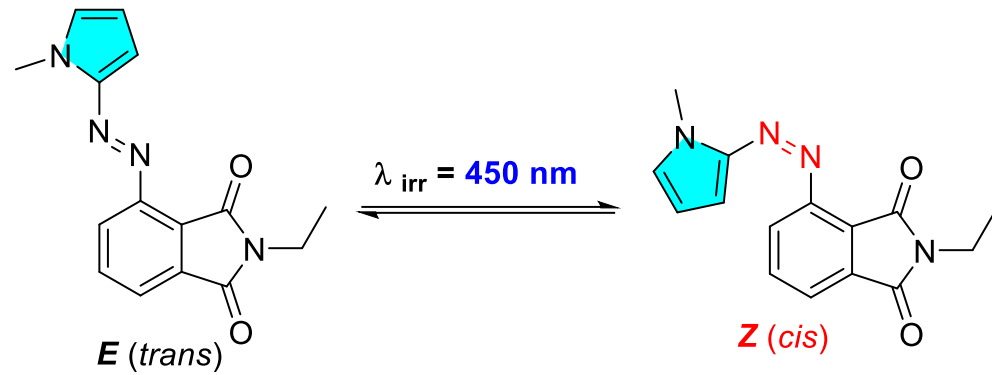
$$\ln\left(\frac{A_0 - A_\infty}{A_t - A_\infty}\right) = k \cdot t \quad \text{E/Z conversion}$$

$$\ln\left(\frac{A_\infty - A_0}{A_\infty - A_t}\right) = k \cdot t \quad \text{Z/E conversion}$$

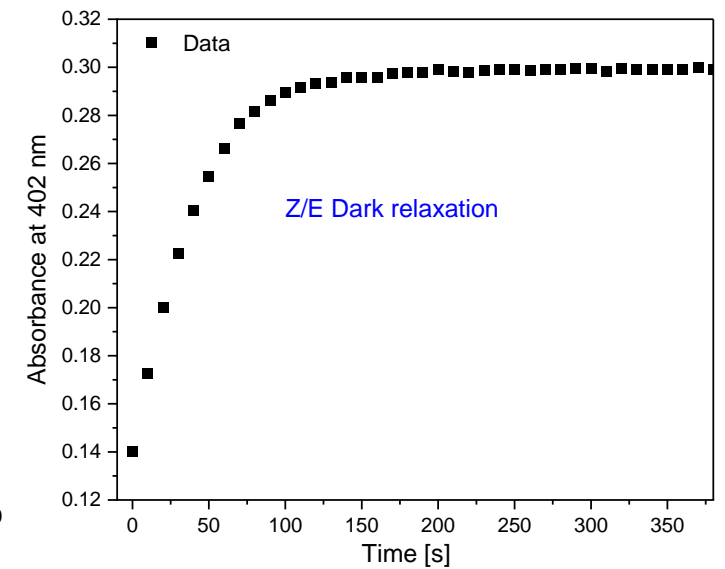
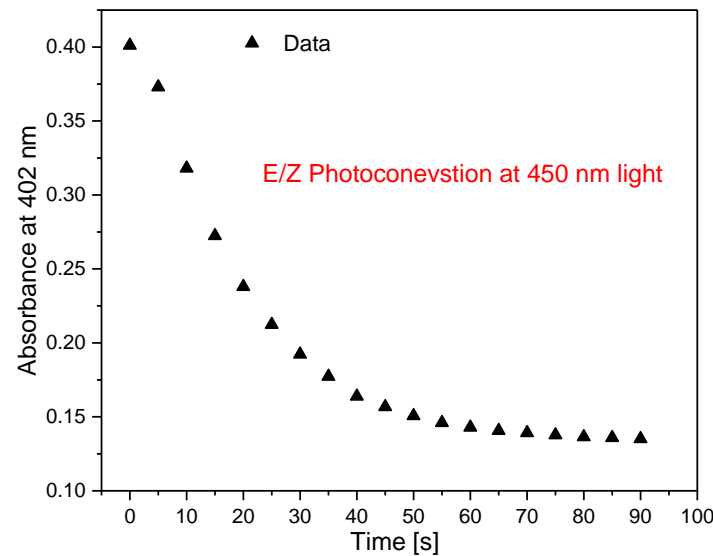
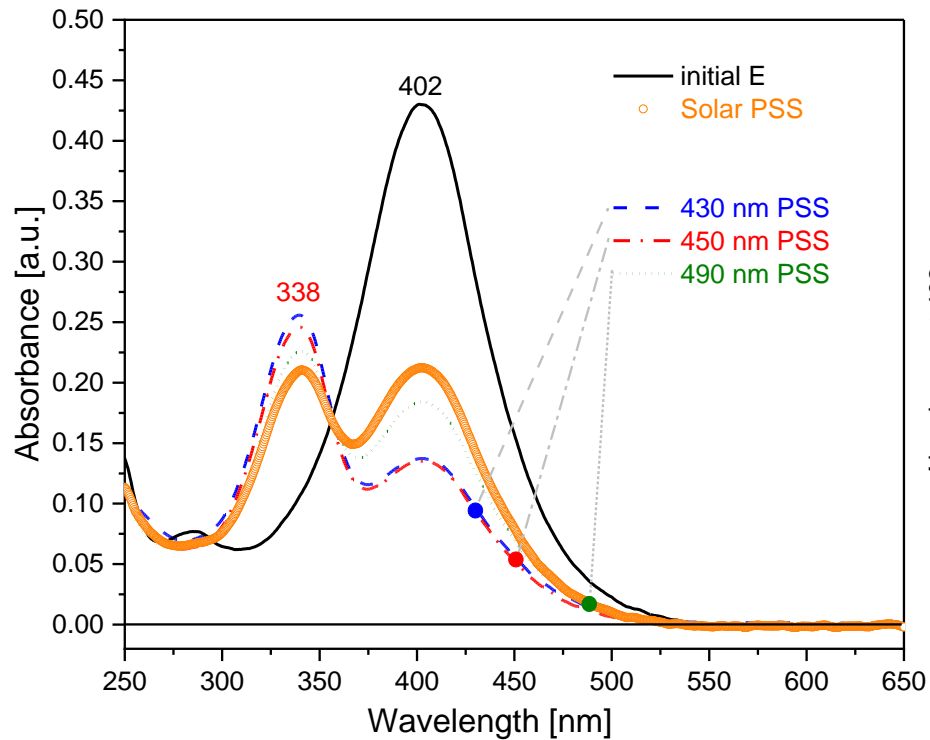
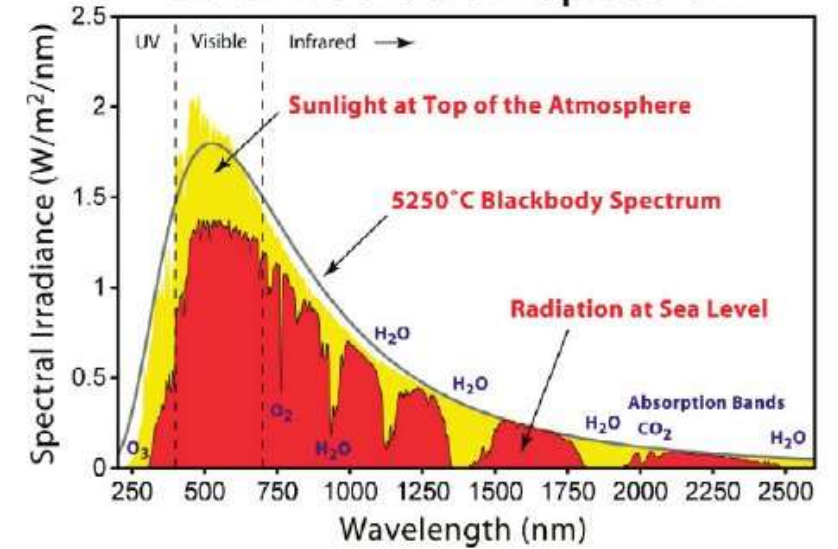
$$\frac{\ln 2}{k} = t_{1/2} \quad \text{half-life of the reaction}$$



Ortho-functionalized azo switches covered visible spectral solar region

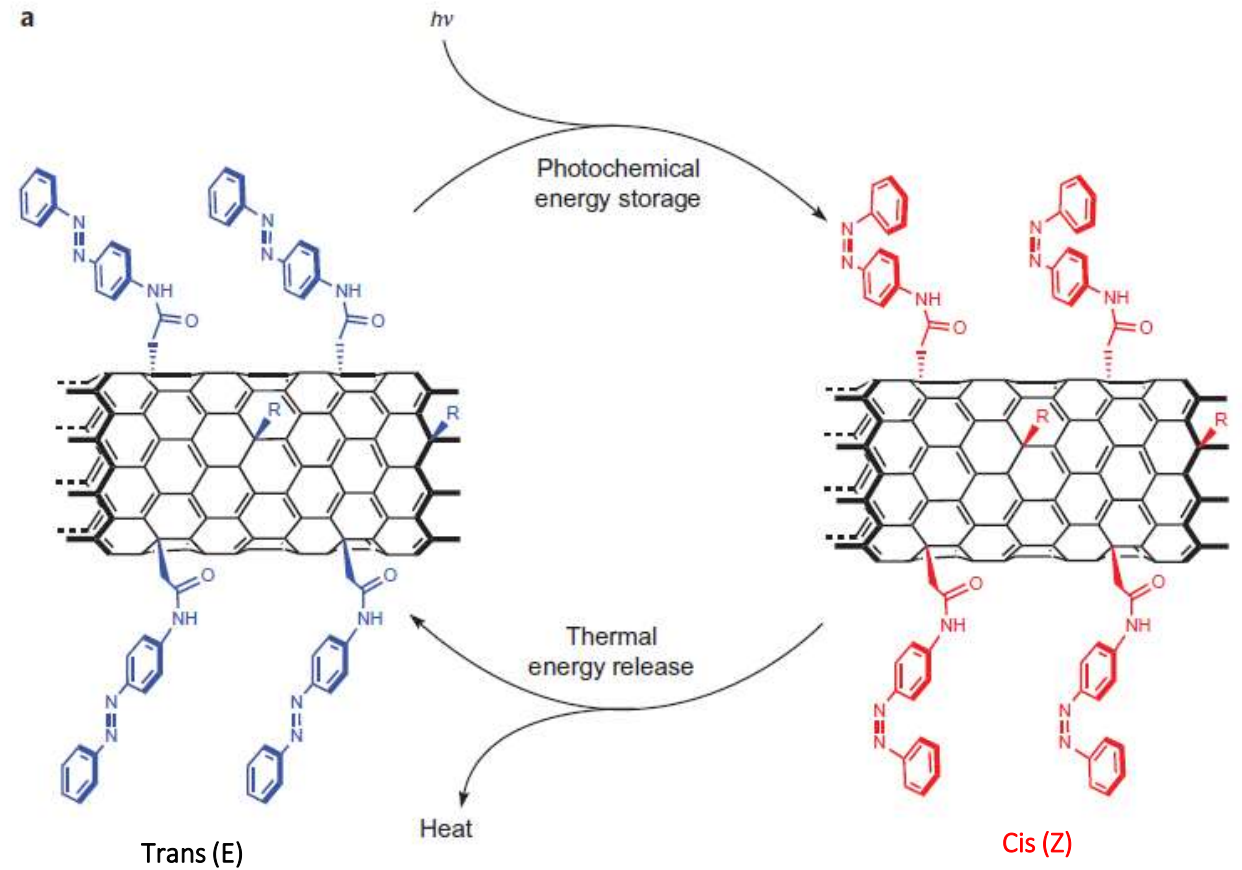


Solar Radiation Spectrum



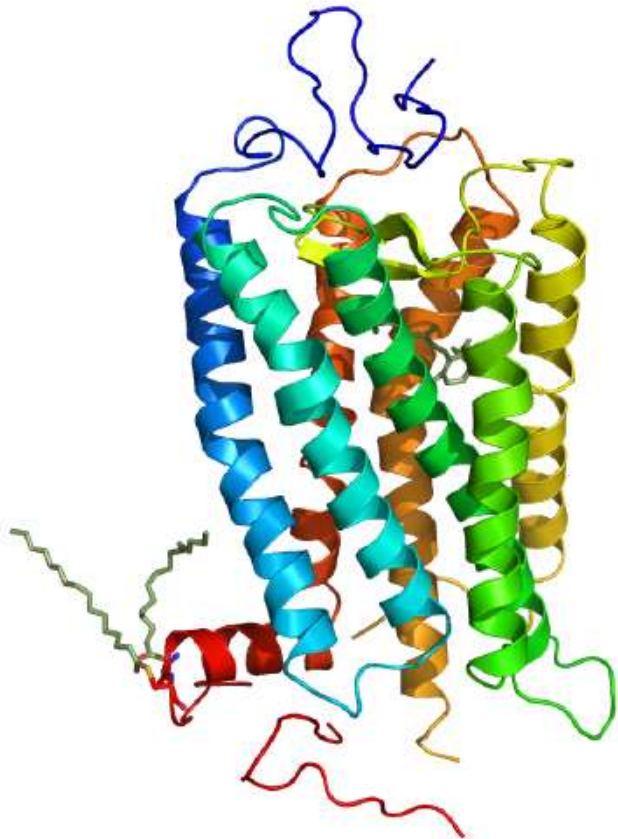
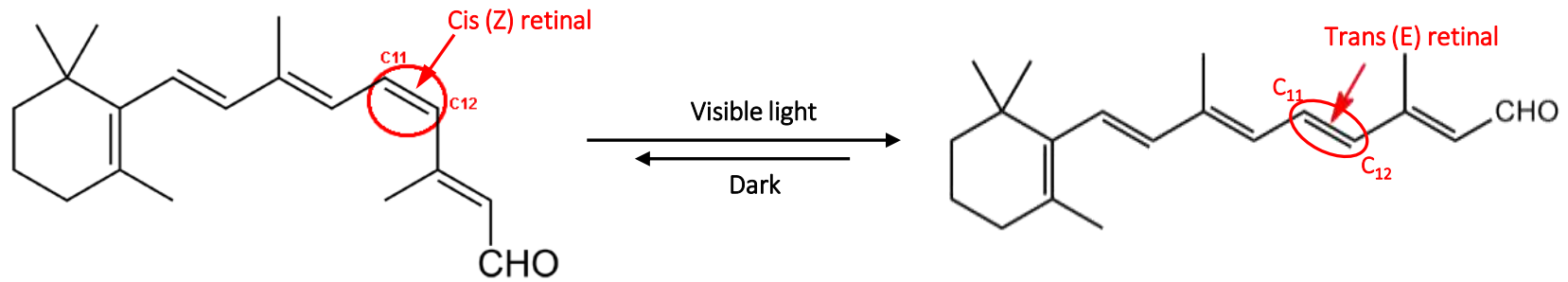


ACS Appl. Mater. Interfaces 2022, 14, 31, 35623–35634

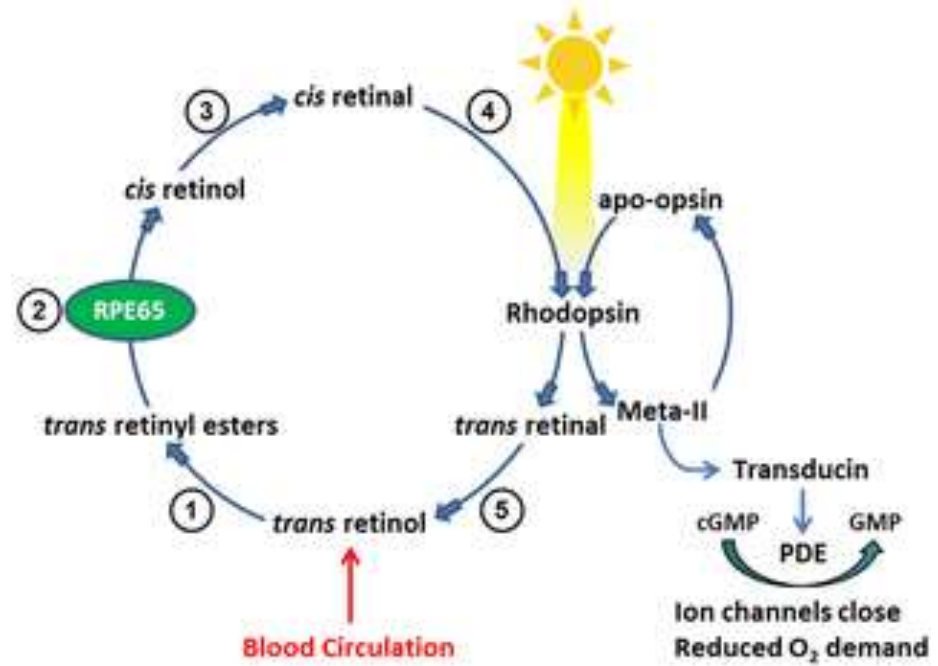


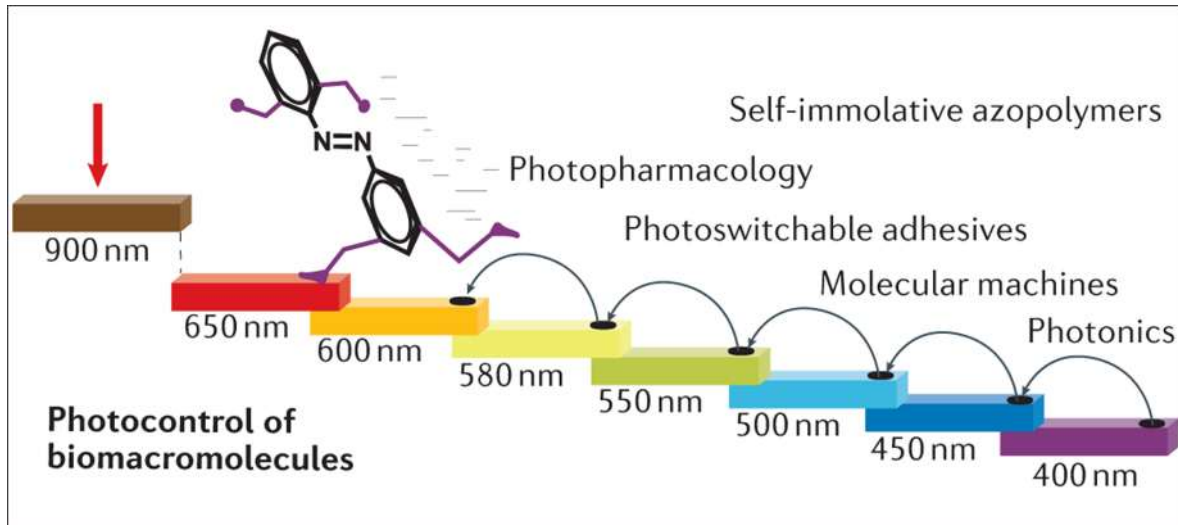
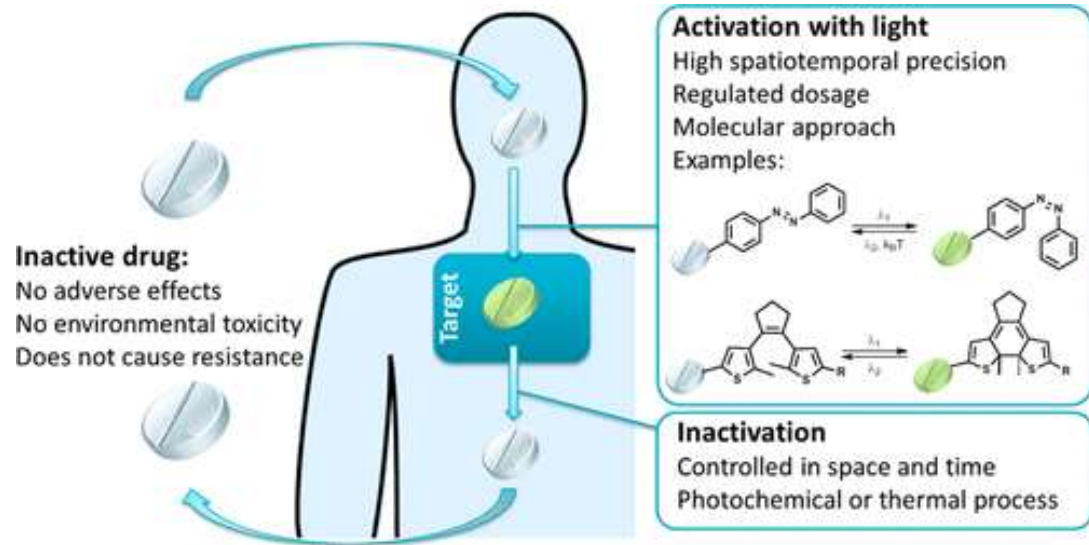
T.J. Kucharski et al., Nature Chemistry 6, 441-447 (2014)

Artificial Molecular Photoswitches: vision cycle and restoration



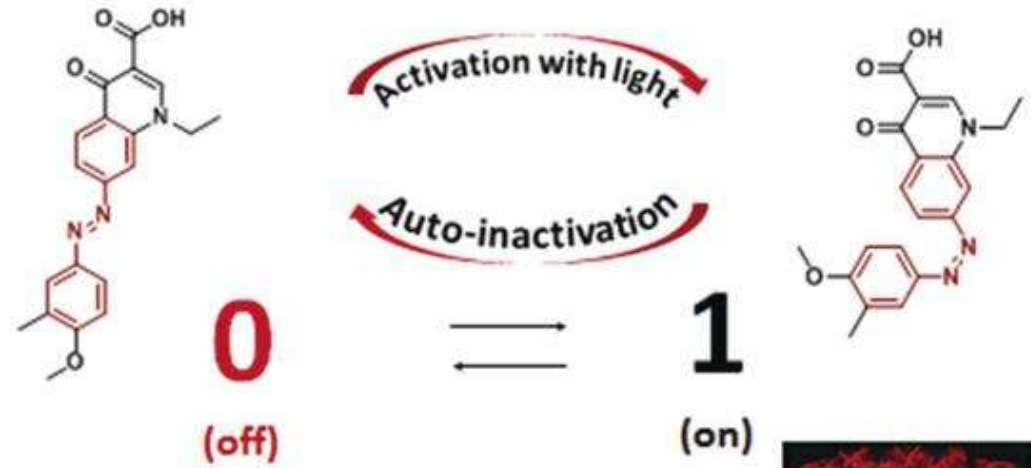
The Visual Cycle



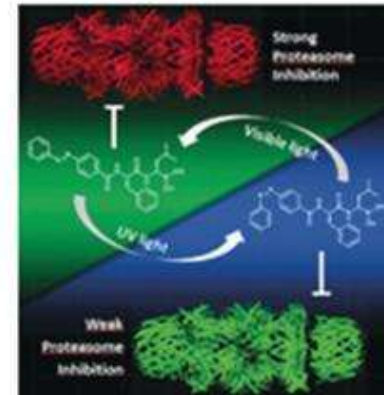
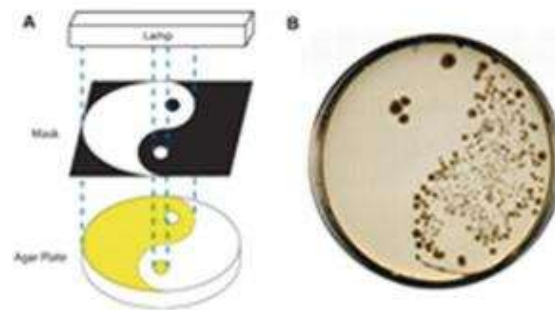


b)

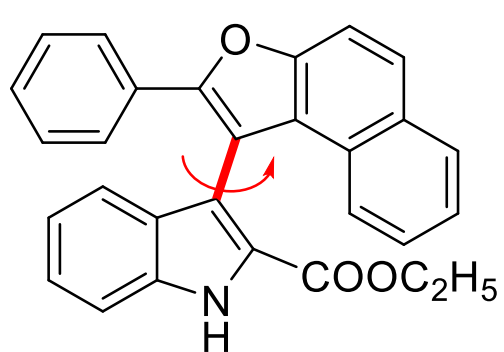
Photocontrolled Antibiotic



c)

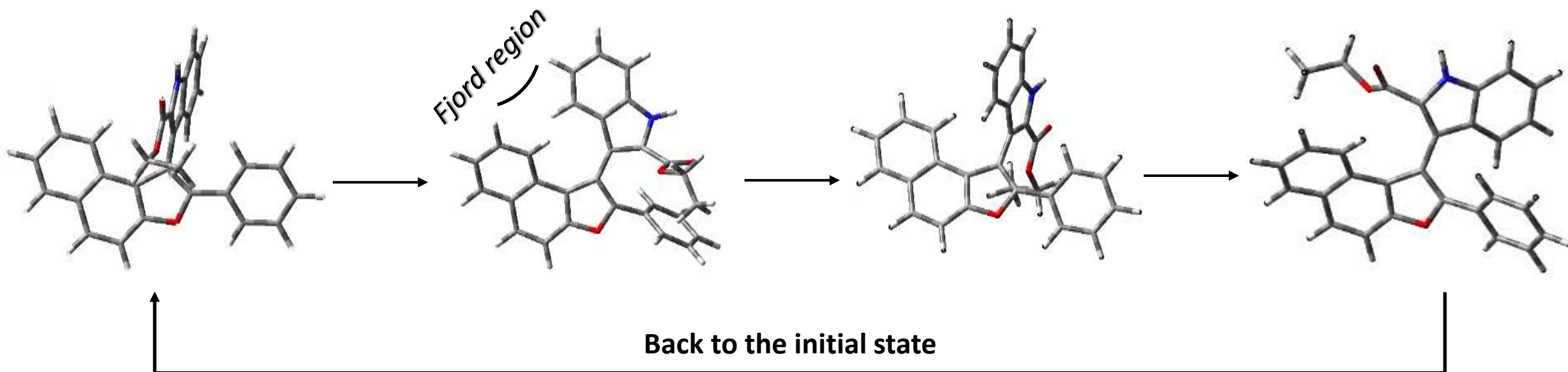


C3-indole Rotary switches

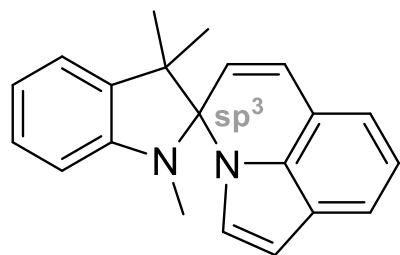
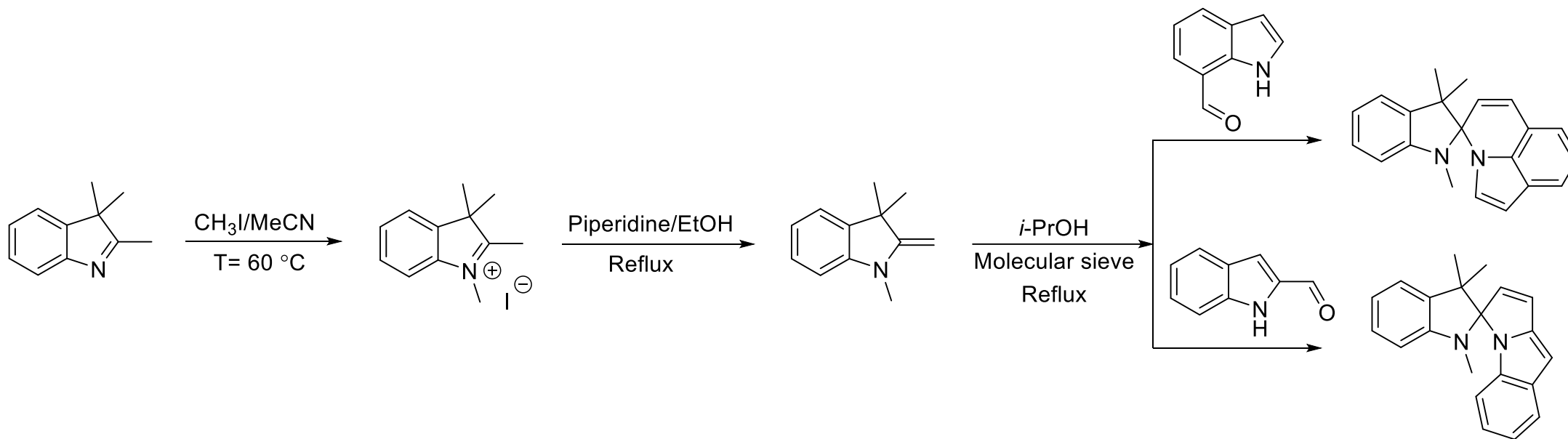


From **Blue** to **White** light controlled fluorescence

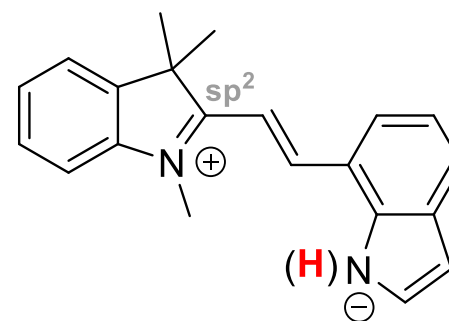
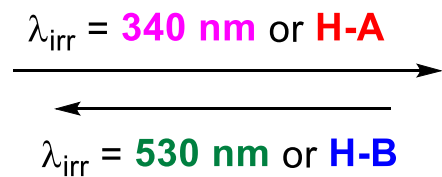
Atropisomers (axial chirality) – optically active



Indolo-spiroindolizine switches by Anton Georgiev



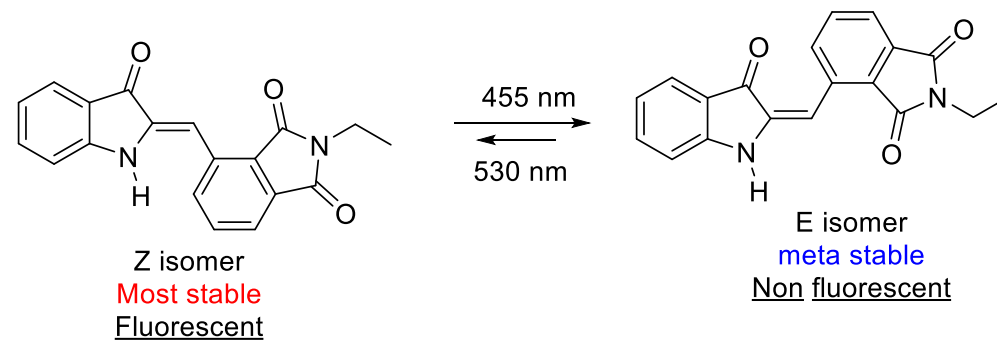
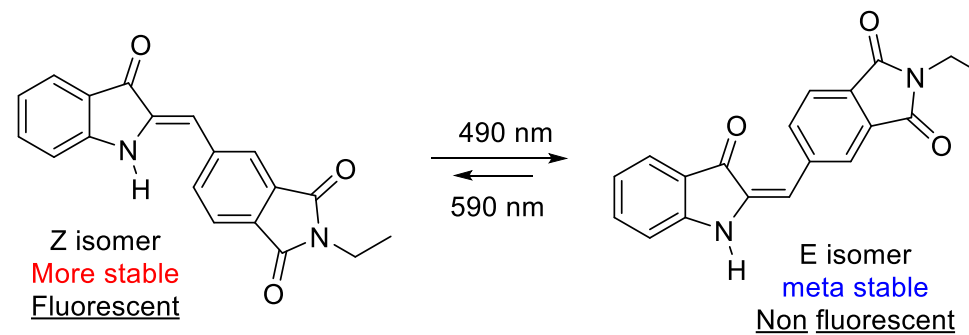
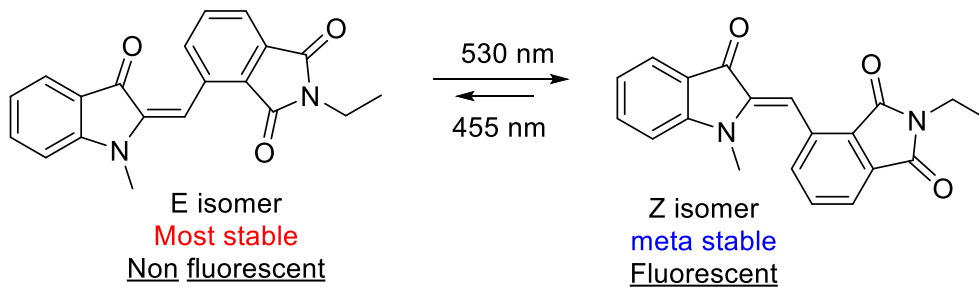
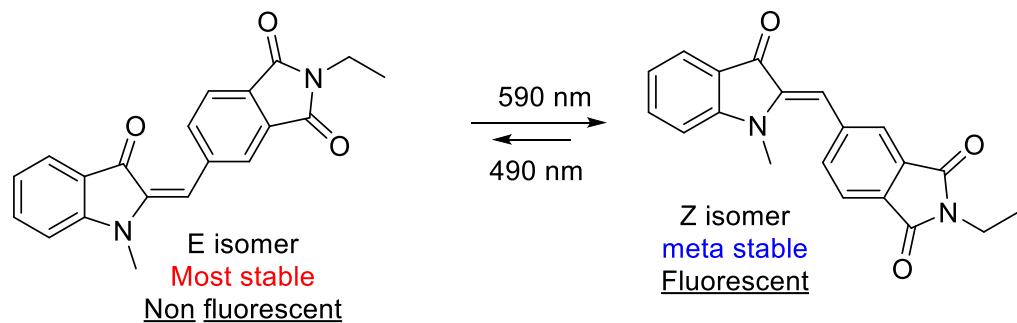
closed
colourless



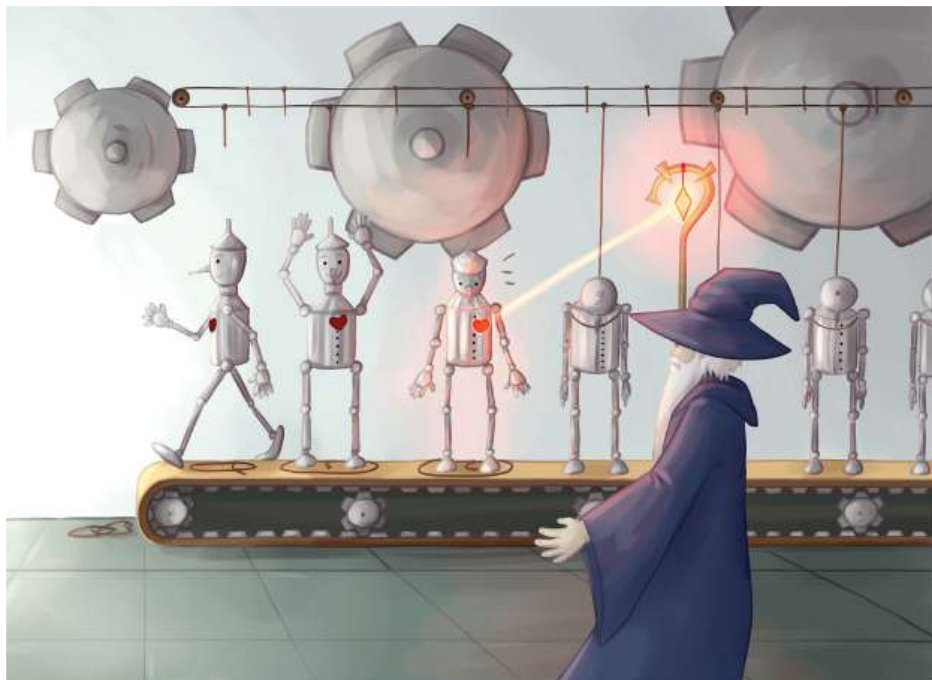
open
coloured (merocyanine)



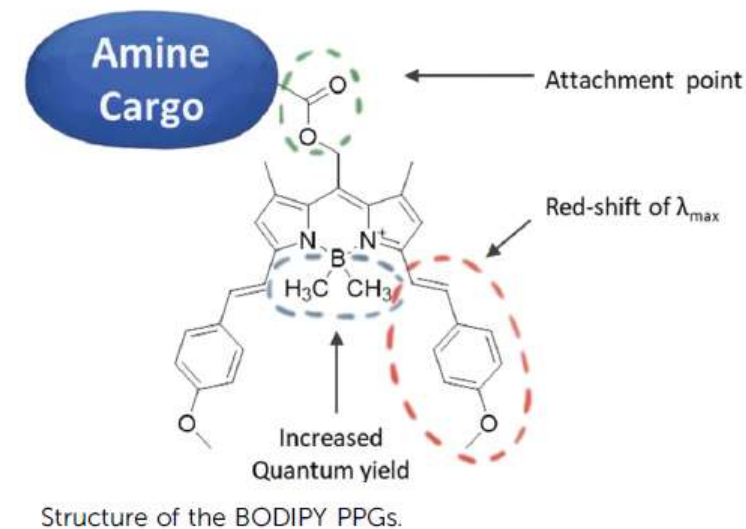
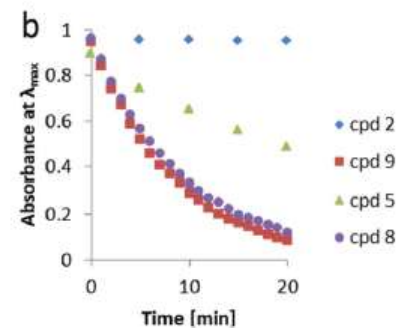
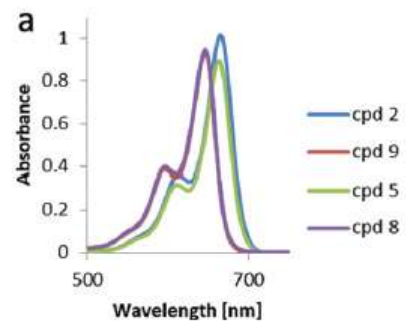
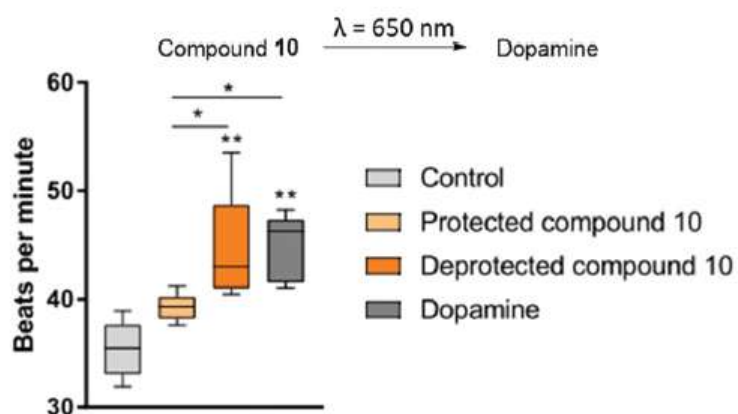
Oxindole fluorescent switches by Anton Georgiev



BODIPY cargo transport : biological application in controlling heart rhythm



Photoremovable protecting groups



Anton Georgiev

1. Kosuke Nakashima, Dancho Yordanov, Yasuyuki Matsushima, Shin-ichi Hirashima, Tsuyoshi Miura, Anton Georgiev, “*Rearrangement of C2-Spirooxindoles: Conversion to the 2-Hydroxyhemi-Indigo and Chromenoindole*”, **The Journal of Organic Chemistry (American Chemical Society)** 2024 89 (17), 12401-12409, <https://doi.org/10.1021/acs.joc.4c01362> Q1 (Web of Science)
2. Dancho Yordanov, Rastislav Smolka, Kosuke Nakashima, Shin-ichi Hirashima, Yasuyuki Matsushima, Martin Vala, Jozef Krajčovič, Martin Weiter, Tsuyoshi Miura, and Anton Georgiev, “*Fluorescent Rotary Switches: 4- vs 3-Substituted Phthalimide Boron Difluoride Schiff Base Complexes*”, **The Journal of Organic Chemistry (American Chemical Society)** 2023, 88, 24, 17206–17214, <https://doi.org/10.1021/acs.joc.3c02056> Q1 (Web of Science)
3. Dancho Yordanov, Rastislav Smolka, Martin Vala, Martin Weiter, Anton Georgiev, “*Versatile photoluminescence behavior of polycyclic hydroxybenzimidazoles driven by intermolecular hydrogen bonding*”, **Optical Materials (Elsevier)** 2024 157 (2) , 116274. <https://doi.org/10.1016/j.optmat.2024.116274> Q1 (Web of Science)
4. Tatiana Munteanu, Dancho Yordanov, Gabriel Canard, Olivier Siri, Denis Jacquemin, Anton Georgiev and Simon Pascal, “*Feasibility of multiple excited-state proton transfer processes in hydroxyquinoline-containing benzobisimidazole dyes*”, **New Journal of Chemistry (Royal Society of Chemistry)**, 2024, 48, 13289-13295, <https://doi.org/10.1039/D4NJ01787K> Q2 (Web of Science)
5. Dominik Veselý, Dancho Yordanov, Martin Vala, Martin Weiter, Jozef Krajčovič, Anton Georgiev, “*Acid-base fluorescence switching and aggregation induced emission (AIE) of phenylene-thienyl chalcones*”, **Journal of Molecular Liquids (Elsevier)** 397 (2024) 124119, <https://doi.org/10.1016/j.molliq.2024.124119> Q1 (Web of Science)
6. Rastislav Smolka, Dancho Yordanov, Kosuke Nakashima, Martin Vala, Jozef Krajčovič, Martin Weiter, Anton Georgiev, „*Control over rotary motion and multicolour switching in 3-hydroxyphthalimide fluorophores: An interplay between AIE and ESIPT*”, **Dyes and Pigments (Elsevier)** 215 (2023) 111279, <https://doi.org/10.1016/j.dyepig.2023.111279> Q1 (Web of Science)

Nikolay Georgiev, Rayna Bryaskova and Vecislav Bakov

7. Awad I. Said, Nikolai I. Georgiev, Vladimir B. Bojinov, “Simple excited state intramolecular proton transfer (ESIPT) based probe for pH and selective detection of copper(II) ion in aqueous alkaline environment: Sensitivity, selectivity and logic behavior”, **Journal of Photochemistry and Photobiology A: Chemistry (Elsevier)** 446, (2024), 115176, <https://doi.org/10.1016/j.jphotochem.2023.115176> Q2 (Web of Science)
8. Georgiev, N.I.; Bakov, V.V.; Anichina, K.K.; Bojinov, V.B. „Fluorescent Probes as a Tool in Diagnostic and Drug Delivery Systems“, **Pharmaceuticals (MDPI)** 2023, 16, 381. <https://doi.org/10.3390/ph16030381> Q2 (Web of Science)
9. Bryaskova, R.; Georgiev, N.; Philipova, N.; Bakov, V.; Anichina, K.; Argirova, M.; Apostolova, S.; Georgieva, I.; Tzoneva, R., “Novel Fluorescent Benzimidazole-Hydrazone-Loaded Micellar Carriers for Controlled Release: Impact on Cell Toxicity, Nuclear and Microtubule Alterations in Breast Cancer Cells”, **Pharmaceutics (MDPI)** 2023, 15, 1753. <https://doi.org/10.3390/pharmaceutics15061753> Q1 (Web of Science)
10. Georgiev, N.I.; Bakov, V.V.; Bojinov, V.B. “A Tutorial Review on the Fluorescent Probes as a Molecular Logic Circuit—Digital Comparator”, **Molecules (MDPI)** 2023, 28, 6327. <https://doi.org/10.3390/molecules28176327> Q2 (Web of Science)
11. Bakov, V.V., Georgiev, N.I. & Bojinov, V.B., “Unusually Sensitive Solid State Emissive 1,8-naphthalimide for Detection of Acid Vapors in Turn-off Mode and Base Vapors in Turn-on Mode”, **Journal of Fluorescence (Springer Nature)** (2024). <https://doi.org/10.1007/s10895-024-03755-0> Q2 (Web of Science)

Maria Atanassova

12. Atanassova, M.; Kurteva, V., “*Mutual Solubilities between Ethylene Glycol and Organic Diluents: Gas Chromatography and NMR*”, **Molecules (MDPI)** 2023, 28, 5121. <https://doi.org/10.3390/molecules28135121> Q2 (Web of Science)
13. Atanassova, M.; Kukeva, R., “*Improvement of Gd(III) Solvent Extraction by 4-Benzoyl-3-methyl-1-phenyl-2-pyrazolin-5-one: Non-Aqueous Systems*”, **Separations (MDPI)** 2023, 10, 286, <https://doi.org/10.3390/separations10050286> Q3 (Web of Science)
14. Atanassova, M.; Kukeva, R.; Kurteva, V., “*New Sustainable Solvent Extraction Pathways for Rare Earth Metals via Oximes Molecules*”, **Molecules (MDPI)** 2023, 28, 7467, <https://doi.org/10.3390/molecules28227467> Q2 (Web of Science)
15. Atanassova, M.; Petkova, Z.; Kurteva, V., “*Aliquat 336 in Solvent Extraction Chemistry of Metallic ReO_4^- Anions*”, **Molecules (MDPI)** 2024, 29, 2257. <https://doi.org/10.3390/molecules29102257> Q2 (Web of Science)

Desislava Staneva Grabcheva

16. Staneva, D.; Atanasova, D.; Grabchev, I. „*Fluorescent Composite Cotton Fabric Modified with Crosslinked Chitosan for Theranostic Applications*“ **Applied Science (MDPI)** 2023, 13, 12660. <https://doi.org/10.3390/app132312660> Q1 (Web of Science)
17. Said, A.I.; Staneva, D.; Vasileva-Tonkova, E.; Grozdanov, P.; Nikolova, I.; Stoyanova, R.; Jordanova, A.; Grabchev, I., „*Synthesis, Spectral Characteristics, Sensing Properties and Microbiological Activity of New Water-Soluble 4-Sulfo-1,8-naphthalimides*“, **Chemosensors (MDPI)** 2024, 12, 79. <https://doi.org/10.3390/chemosensors12050079> Q2 (Web of Science)

Daniela Angelova

18. Stratiev, D.; Shishkova, I.; Ivanov, M.; Dinkov, R.; Toteva, V.; Angelova, D.; Kolev, I.; Tavlieva, M.; Yordanov, D. “*Alternative Options for Ebullated Bed Vacuum Residue Hydrocracker Naphtha Utilization*”, **Processes (MDPI)** 2023, 11, 3410. <https://doi.org/10.3390/pr11123410> Q2 (Web of Science)

The results are developed as part of contract №: BG-RRP-2.004-0002-C01, **Laboratory of Organic Functional Materials** (Project BiOrgaMCT), Procedure BG-RRP-2.004 “Establishing of a network of research higher education institutions in Bulgaria”, funded by BULGARIAN NATIONAL RECOVERY AND RESILIENCE PLAN