HUN-REN cloud alkalmazása a szerves kémiában

Eredmények, tapasztalatok, előnyök és kihívások

HUN-REN Cloud Meetup

Mucsi Zoltán

Miskolci egyetem, Anyag és vegyészmérnöki kar, Kémiai intézet

2025. november 13.

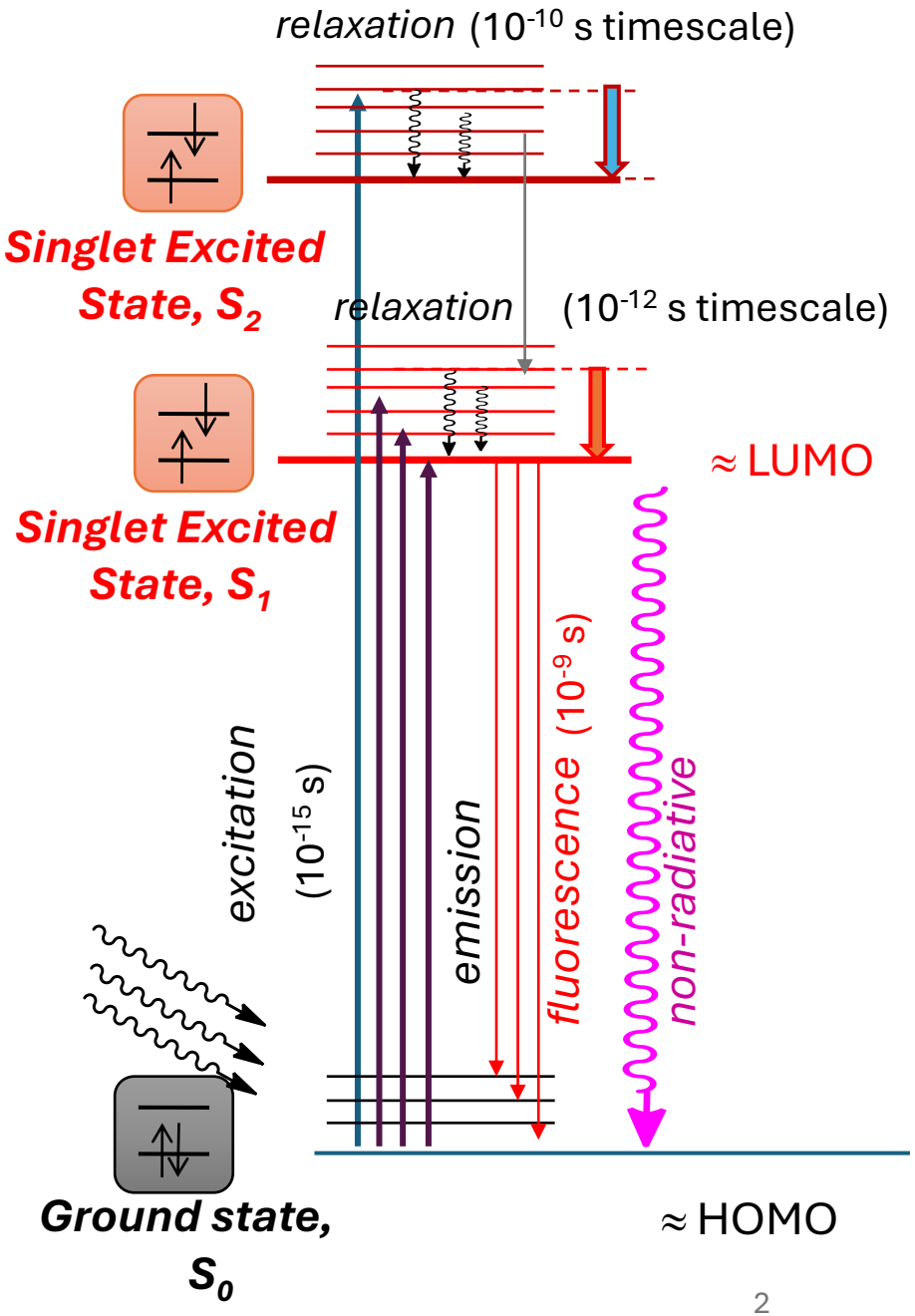
Célok és Tudományos háttér:

- Szerves fotokémiai molekulák szerkezetváltozásainak vizsgálata
- Szerves fotokémiai átalakulásokban a **π–π*** és **n–π*** állapotok kölcsönhatása
- S_1 és T_1 felületek metszése → metszéspontok (ISC)
- Kísérleti megfigyelések értelmezése elméleti úton

- **Cél**: gerjesztett állapotú (S_1, T_1) reakciómechanizmusok feltárása
- Kémiai interpretáció: TICT, PET, Dewar-benzol típusú folyamatok

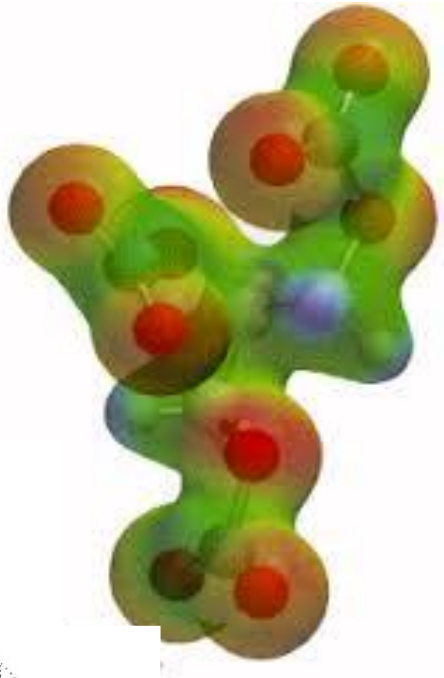
Célunk, hogy a gerjesztett állapotú reakciókat a kvantumkémiai szinten értelmezzük, és ezzel segítsük a fotoaktív molekulák tervezését.

A fotokémia ma már nem csak spektroszkópiai kérdés: a kvantumkémia nélkülözhetetlen az S_0–S_1 átmenetek dinamikájának értelmezésében.



Kvantumkémiai számításos módszerek

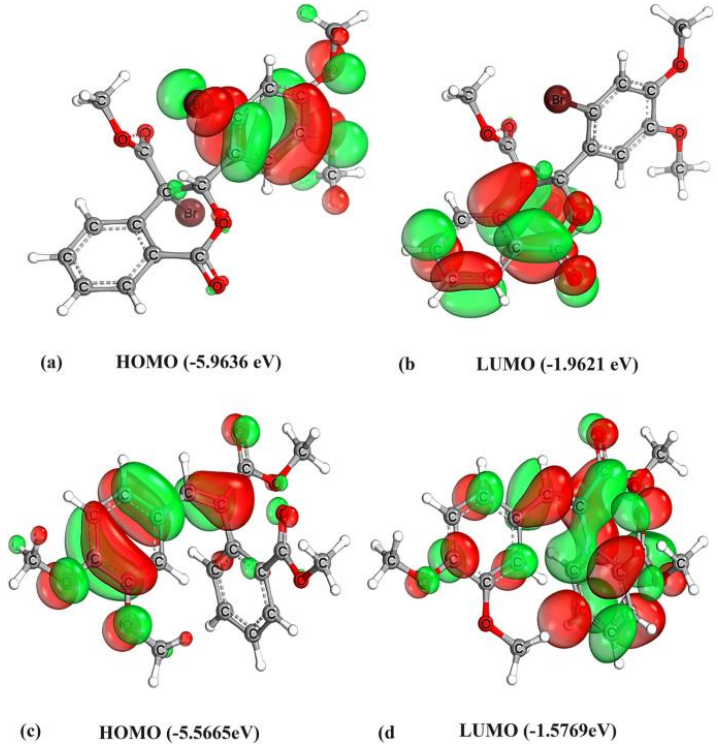
Molekulák geometriája



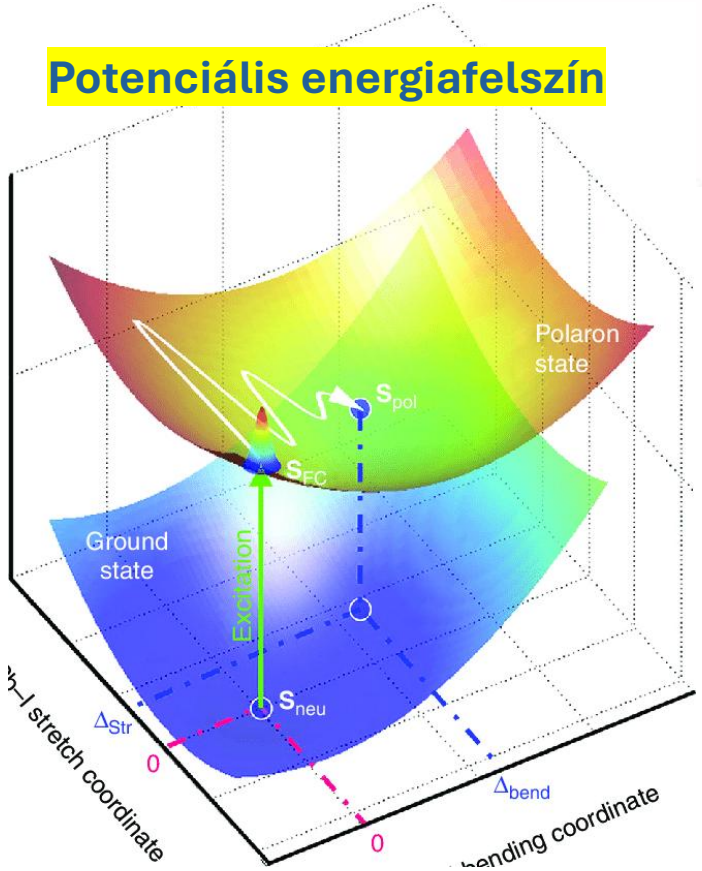
- DFT, TD-DFT, CAS-SCF, M06-2X / def2-TZVP
- Geometriaoptimalizálások, PES (potential energy surface) profilok
- TICT és PET folyamatok energetikai elemzése

A számításokat jellemzően TD-DFT módszerrel végezzük, különböző konformációk energetikai és fotofizikai jellemzésével.

Molekulapályák számítása



Potenciális energiafelszín



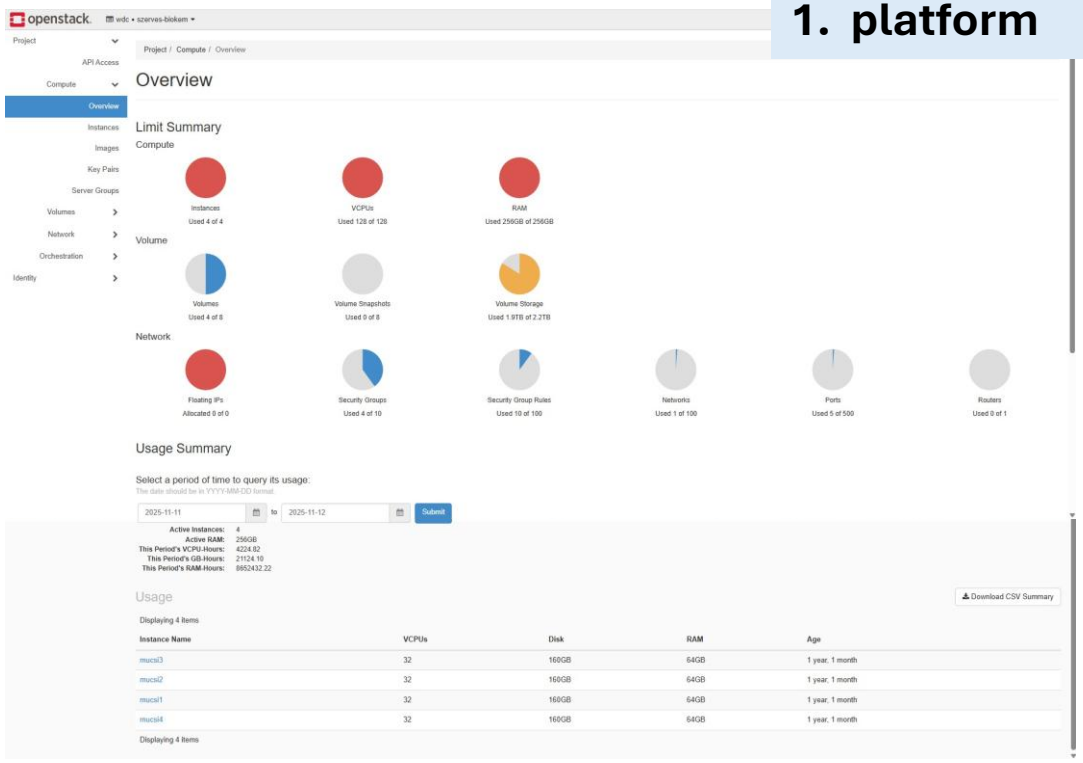
HUN-REN Cloud infrastruktúra

• Két fő erőforrásigénylő platform

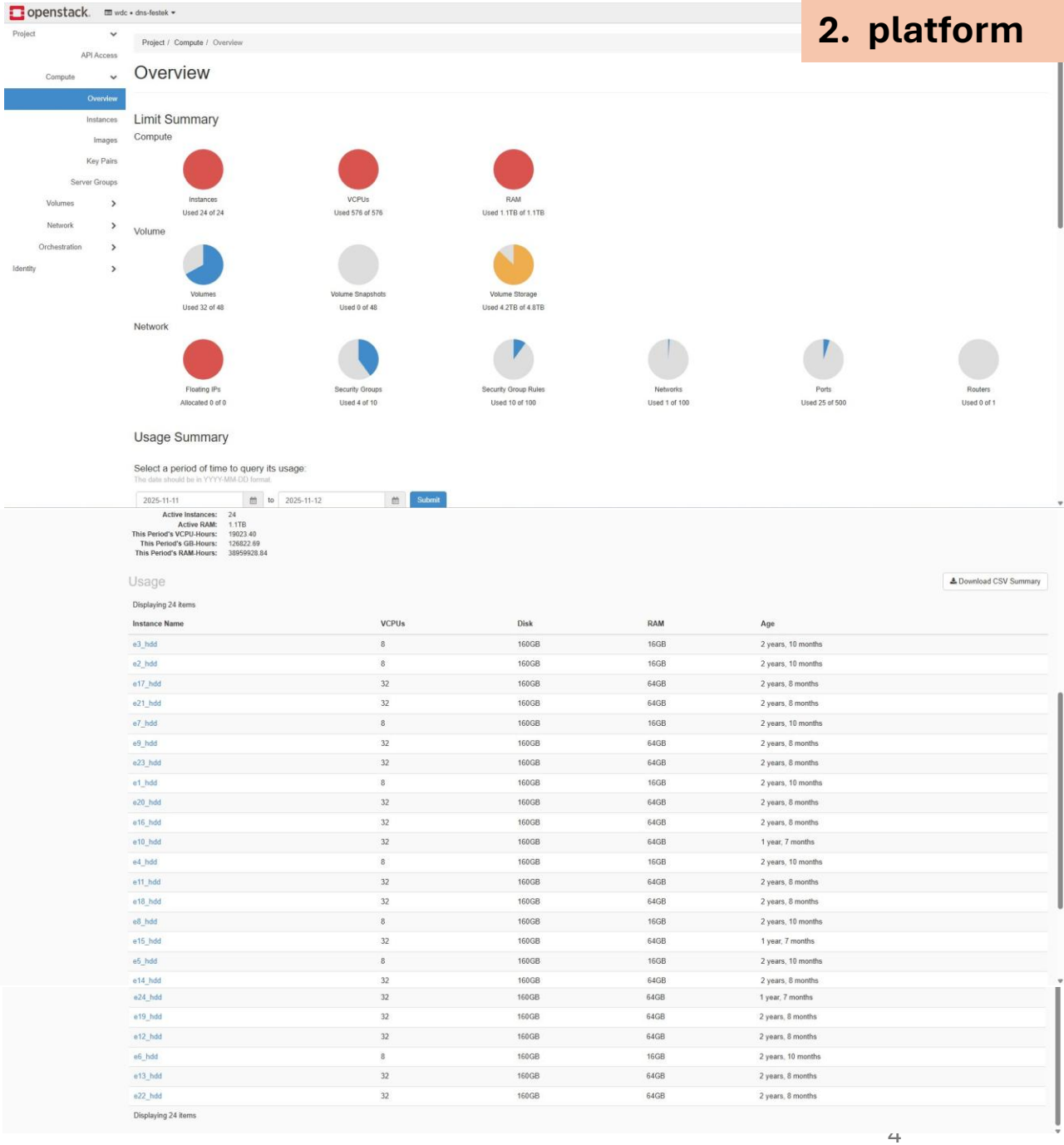
- **1. platform (szerves mechanizmusok számolása)**: 4 kisebb teljesítményű gép (referencia = 1×) (1 + 1 + 1 + 1)
- **2. platform (KE, DNS szenzorok fotokémiai számítása)**: 24 nagyobb számítási kapacitású gép 6 csoportba foglalva rugalmas, moduláris felhős környezet

A HUN-REN Cloud számítási környezetének kialakításakor a cél az volt, hogy párhuzamosan 6 + 4 futtatható, automatizált munkafolyamatokat építsünk fel.

1. platform



2. platform



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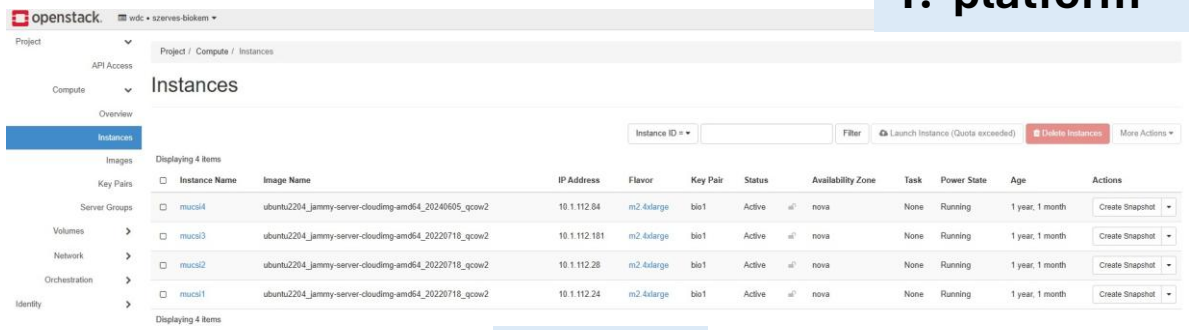
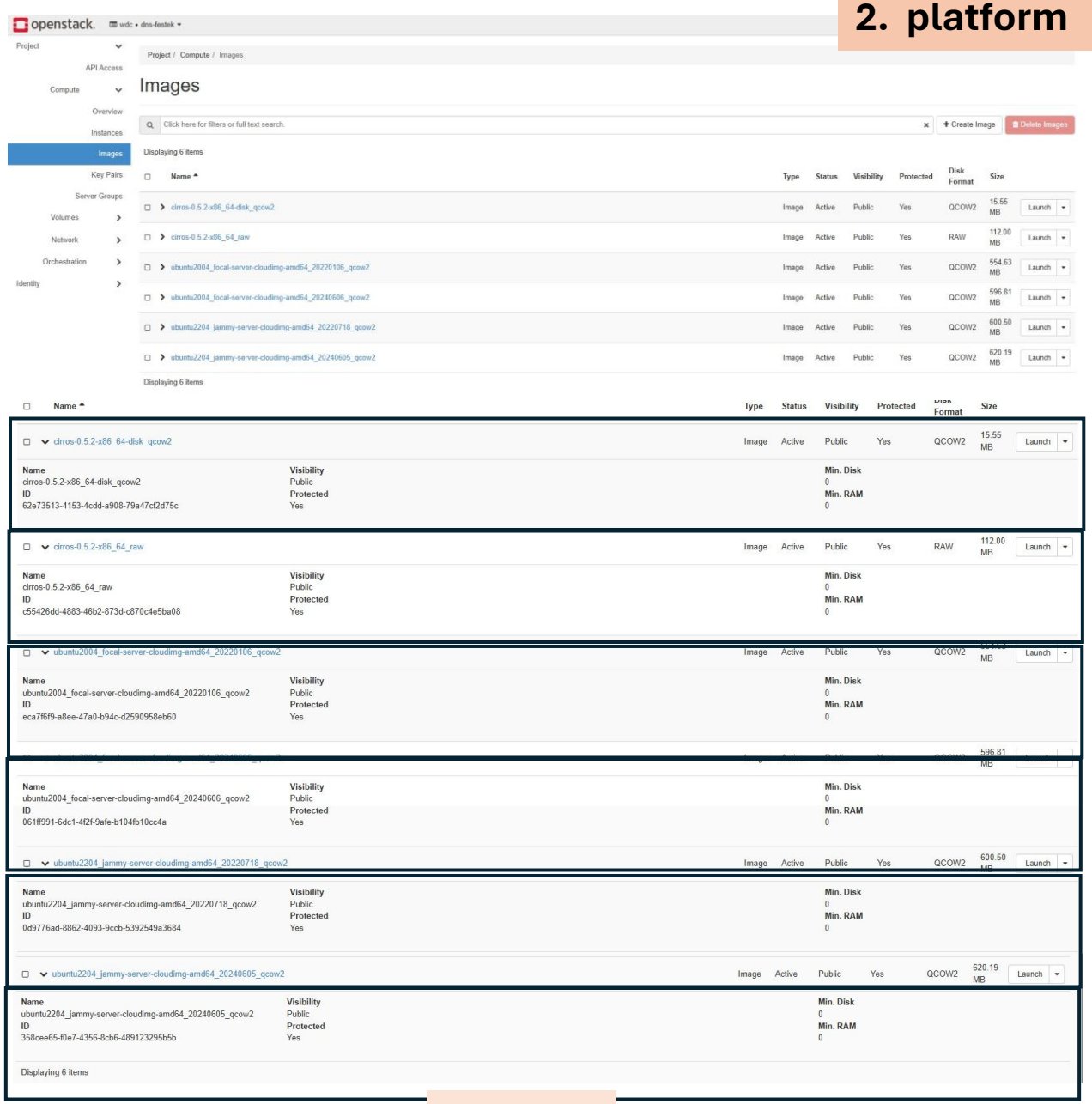


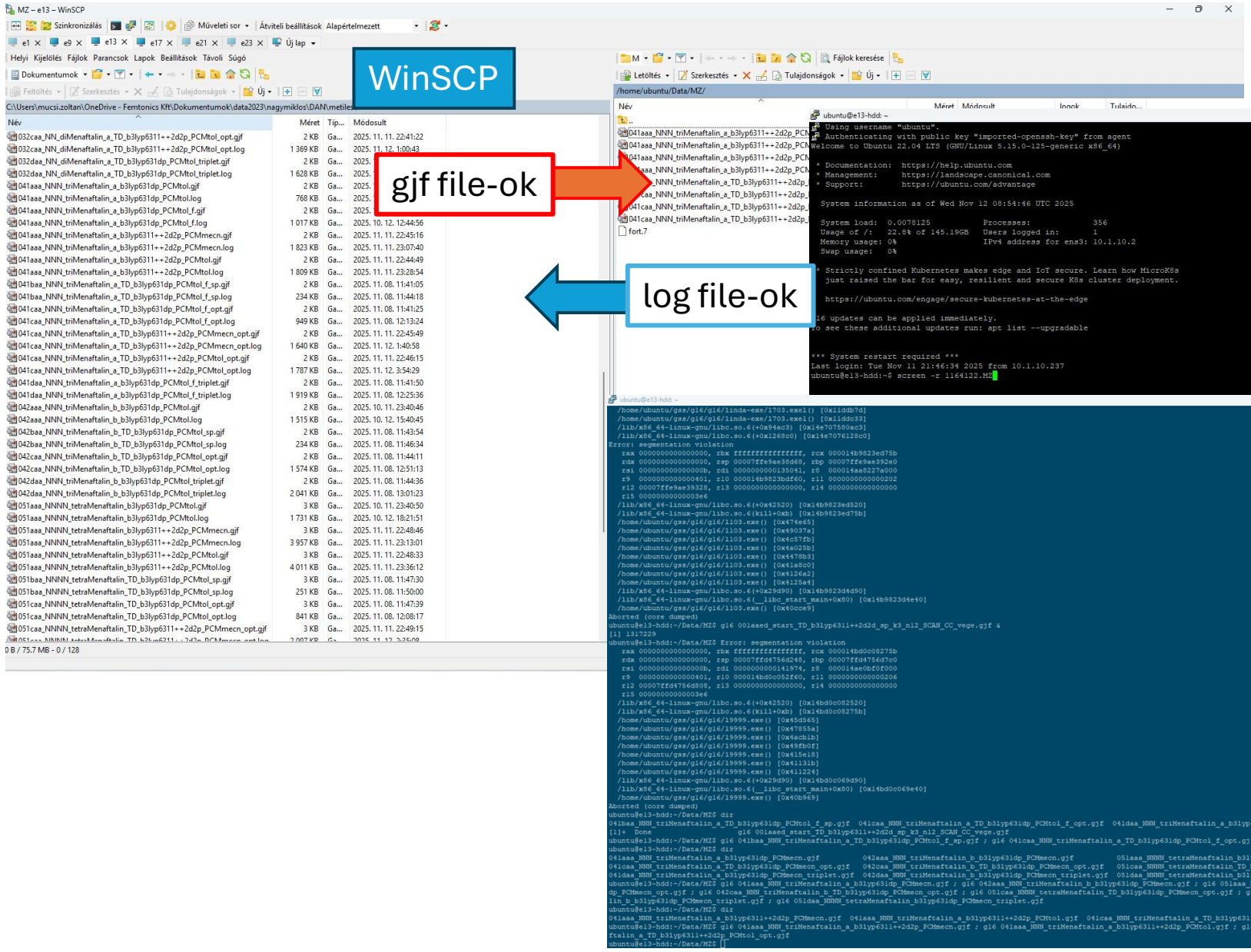
4 db gép

2. platform



6 db gép

Adatkezelés



ubuntu-@e13-hdd:~$ screen –r MZ

```
ubuntu@e13-hdd:~/Data/MZ$ g16 041aaa_NNN_triMenaftalin_a_b3lyp6311++2d2p_PCMmecn.gjf ; g16 041aaa_NNN_triMenaftalin_a_b3lyp6311++2d2p_PCMtol.gjf ; g16 041caa_NNN_triMenaftalin_a_TD_b3lyp6311++2d2p_PCMmecn_opt.gjf ; g16 041caa_NNN_triMenaftalin_a_TD_b3lyp6311++2d2p_PCMtol_opt.gjf
```

ubuntu-@e13-hdd:~/Data/MZ/$ g16 xyz1.gjf; g16 xyz2.gjf; g16 xyz4.gjf

Team members and fellow researchers

Senior Researchers

Zoltán Mucsi
Head of chemistry

MSc 1999 (ELTE)
PhD 2002 (ELTE)
Post-doc 2005 (Sanofi)
14 years in pharma
8 years in R&D

Levente Cseri
Senior researcher

BSc 2016 (BME)
PhD 2021 (Manchester)
2 years in pharma
4 years in R&D

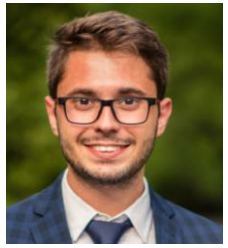
Ervin Kovács
Senior researcher

MSc 2008 (BME)
PhD 2014 (BME)
Post-doc 2015-2019 (incl. Manchester)
4 years in R&D

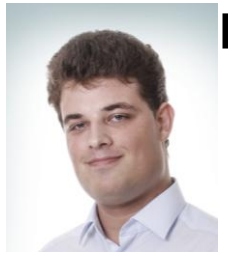
Junior researchers

Farkas Domahidy
PhD candidate

Attila Csomos PhD candidate



Ph.D. students



Bence Kontra
PhD student

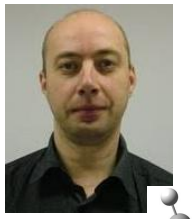
Etelka Kiss
PhD student

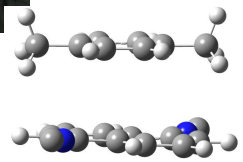
1 MSc students
5 BSc students

Miklós Nagy
Miskolci egyetem
Kémia intézet

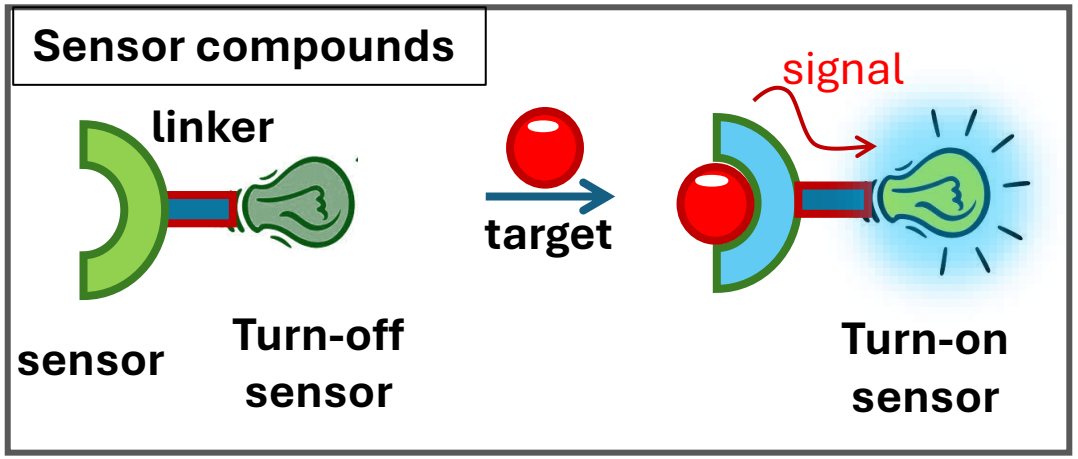
Béla Viskolcz
Miskolci egyetem
Kémia intézet

Research Directions

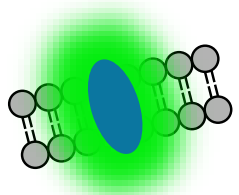




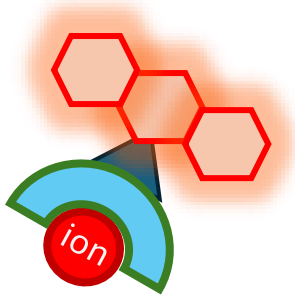
1) Small molecular sensors for BTX fractions



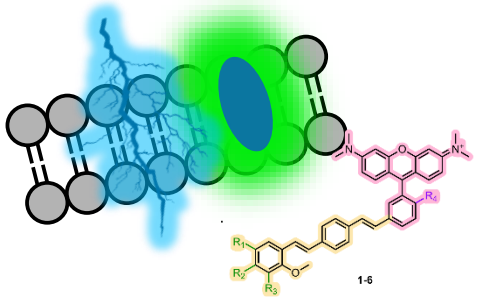
6) FL-Antibody for tumor diagnostic



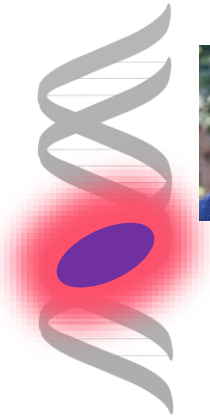
5) Membrane sensors



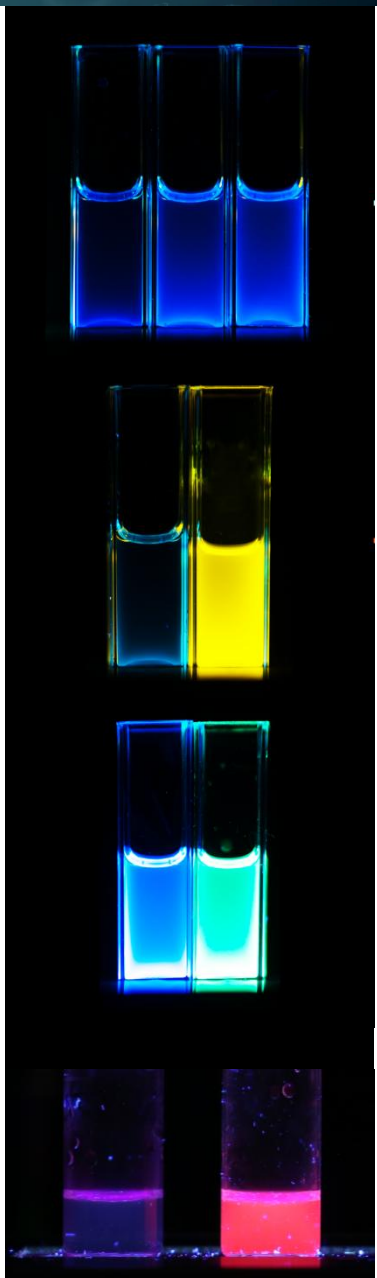
2) Human dye project Ion sensors for human diagnostic purpose
incl.: Ca^{2+}, Mg^{2+}, Zn^{2+}



3) Human dye project for voltage sensitive dyes



4) DNA sensors

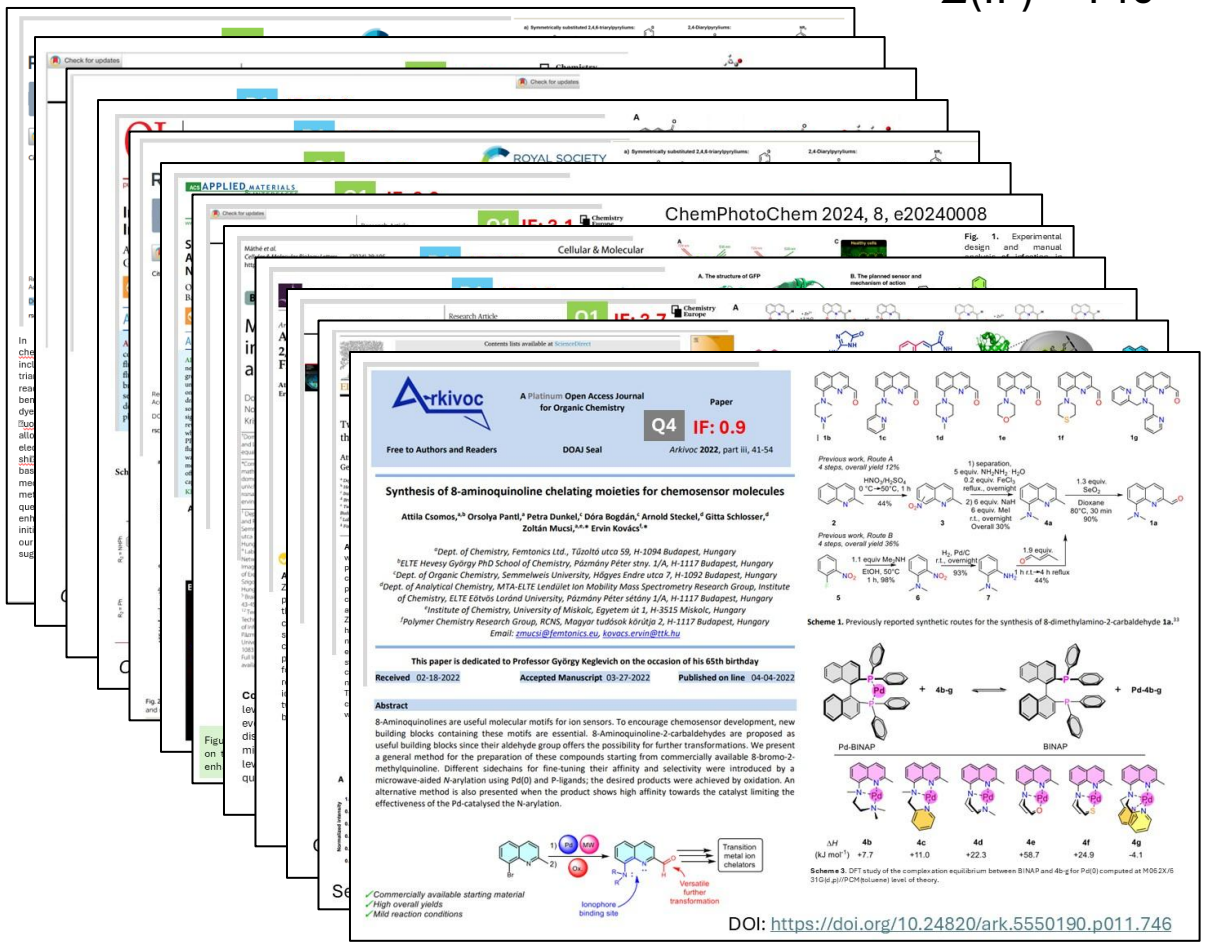


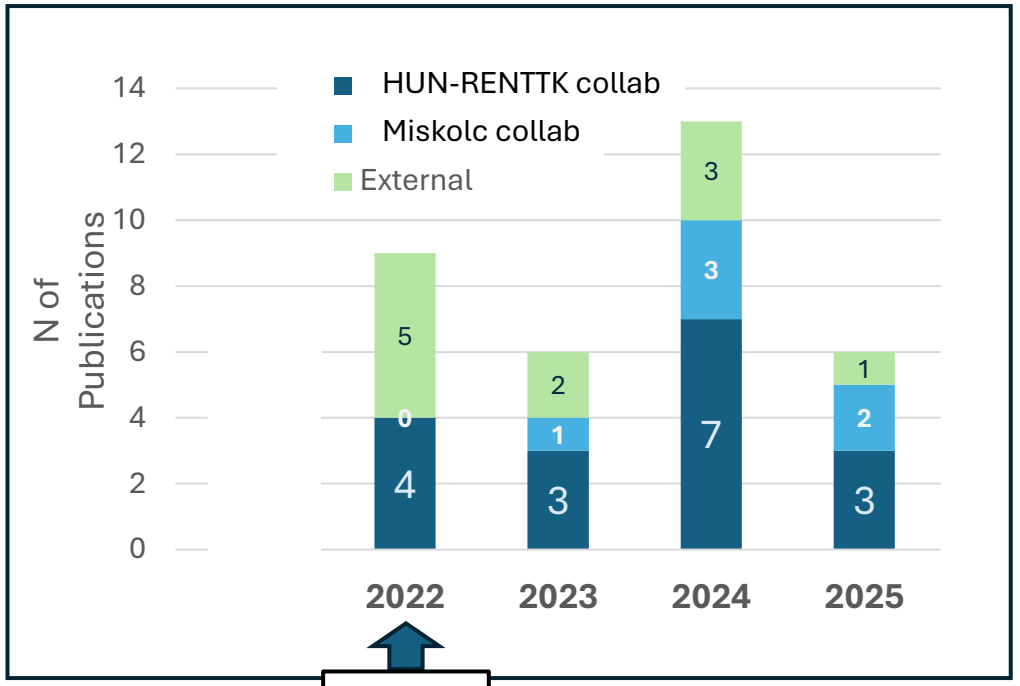
Scientific output: Publications

Several relevant exapmles from the period of 2022-2025

7 Q1 publications
7 D1 publications

Σ(IF) > 140

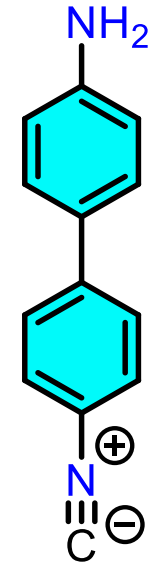




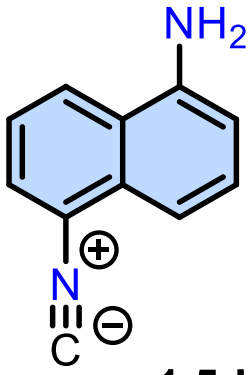
Cloud

From 2022	N of publication	
$\Sigma_{only\ BVC}$	17	HUN-REN research
Σ_{collab}	6	Miskolc research
Σ_{ext}	11	BME, SE,
Σ_{total}	**34**	

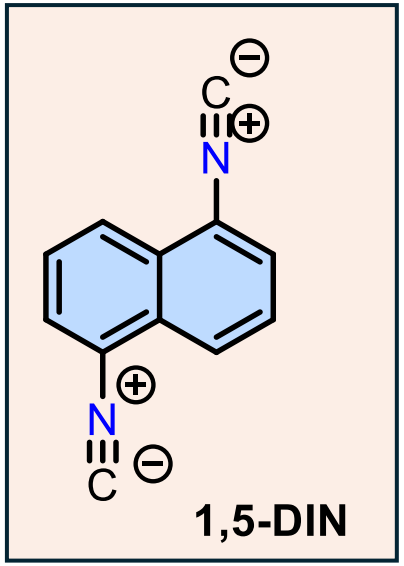
Sensing of aromatic compounds



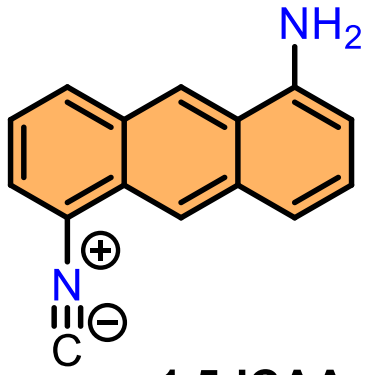
1,5-ICABP



1,5-ICAN



1,5-DIN

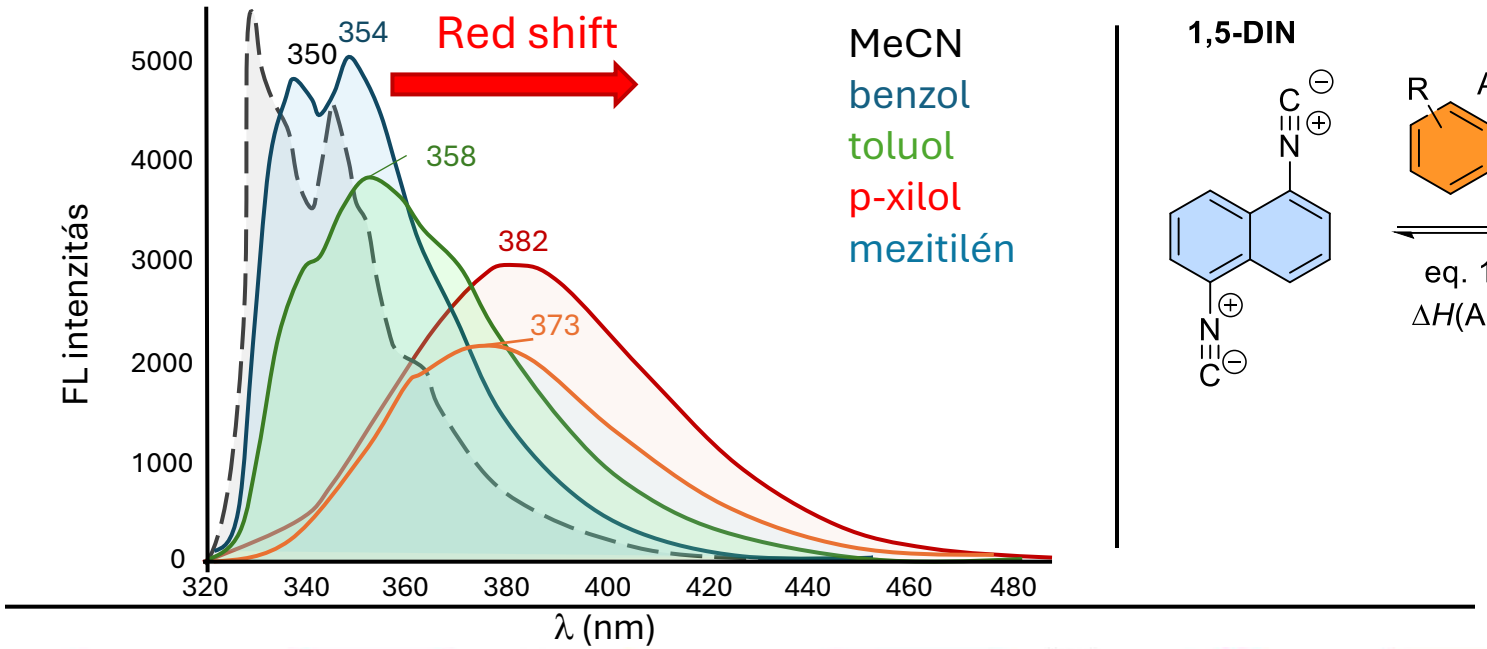


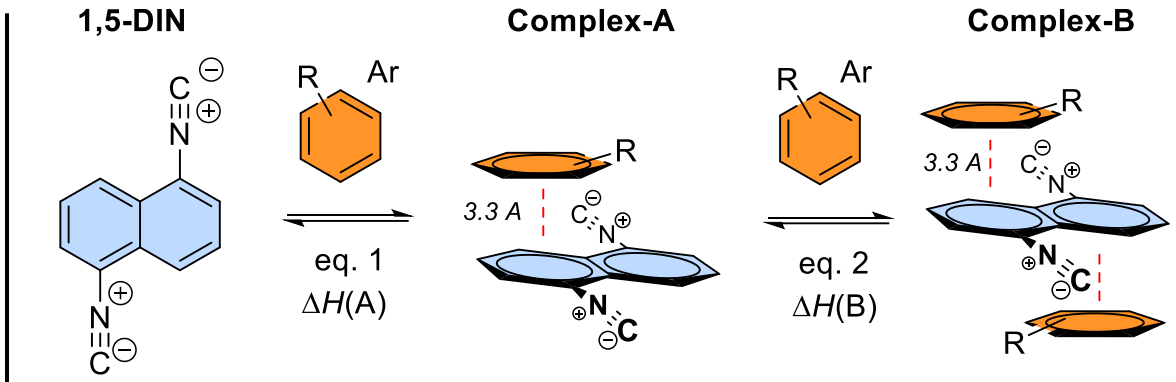
1,5-ICAA

Nagy Miklós
Miskolci egyetem
Kémia intézet

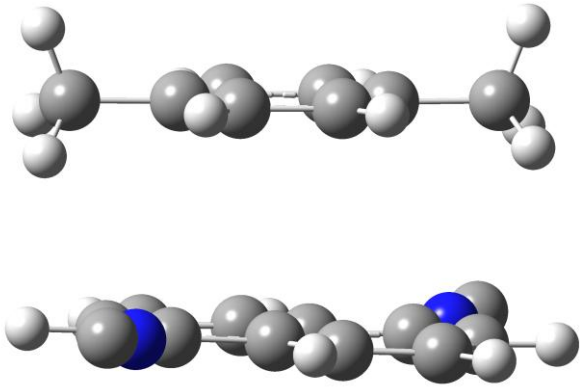
1) Detecting of Hg^{2+}
2) Detecting of aromatic compounds
3) Detection of Hydrogen Bond

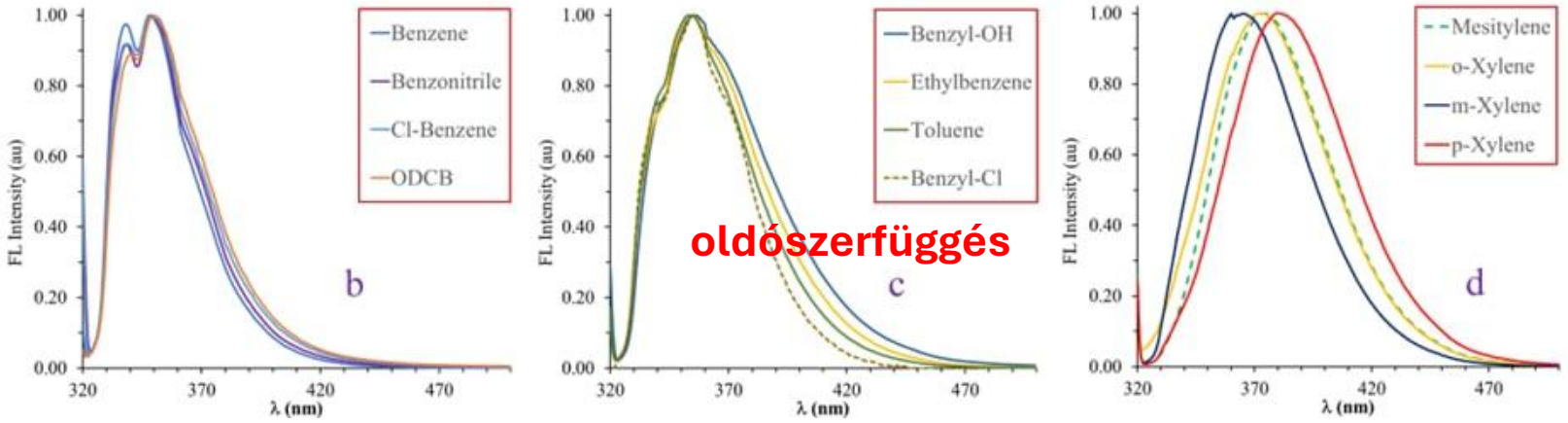
New xylene sensor- DIN





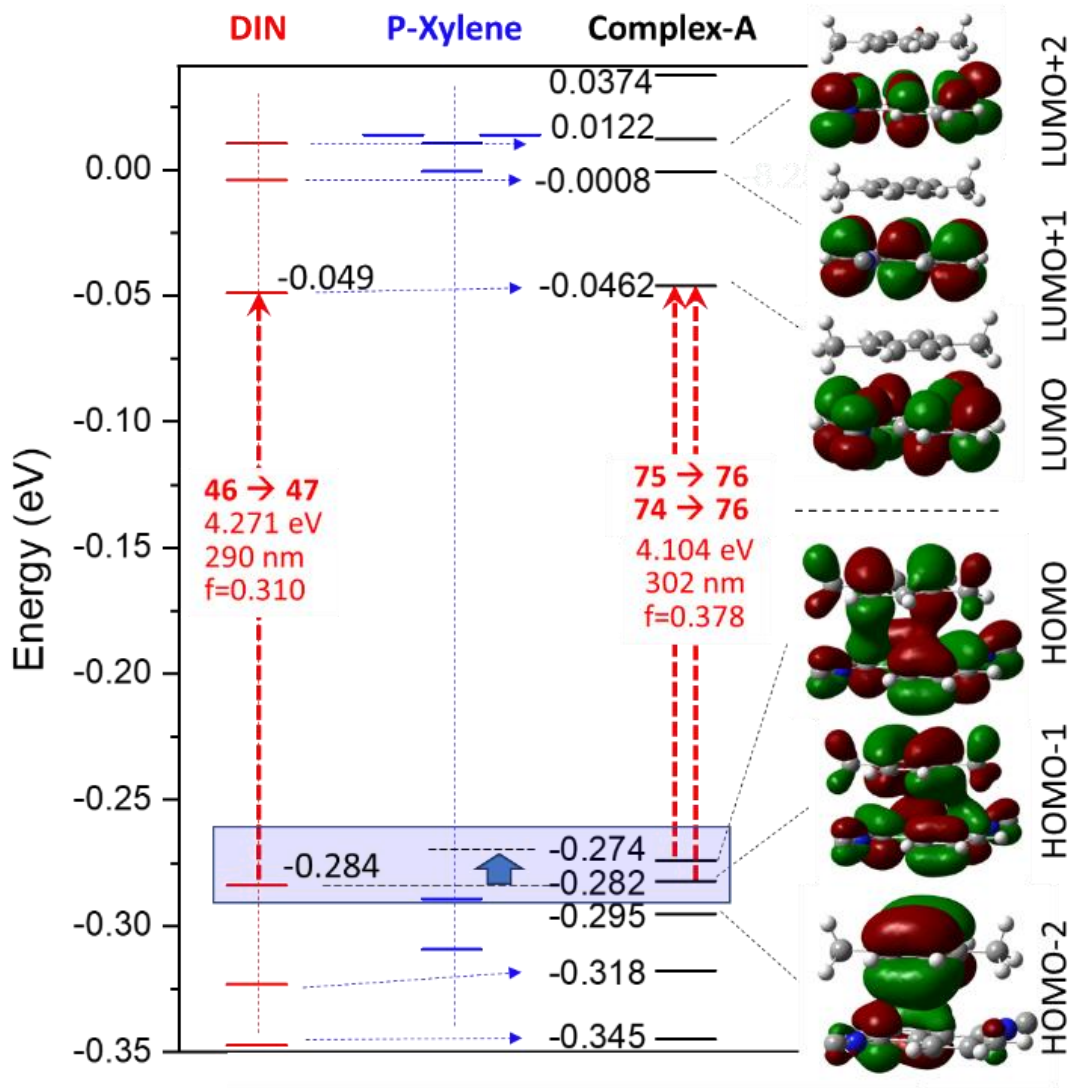
π - π comlpex formation





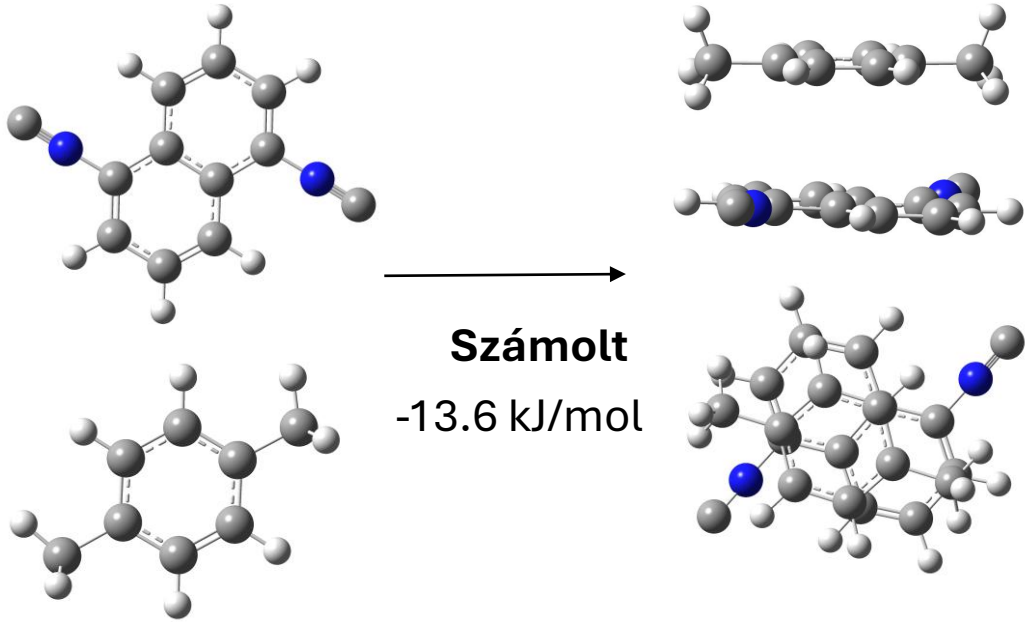
oldószerfüggés

New xylene sensor- DIN



π - π komlpex

Computed Abs: 298 nm → 305 nm
experimental (300 nm) (350 nm)
Computed Fl: 364 nm → 396 nm
experimental (382 nm)



Számolt
-13.6 kJ/mol

B3LYP/6-31G(d,p)[PCM(MCN)]

scientific reports

OPEN

Aromatic pi-complexation of 1,5-diisocyanonaphthalene with benzene derivatives

Erika Kopcsik[1], Zoltán Mucsi[1,2]✉, Rajmond Schiwert[1], László Vanyorek[1], Béla Viskolcz[1] & Miklós Nagy[1]✉

Aromatic π-complexes play a significant role in various chemical and biological systems, significantly influencing their physico-chemical and spectroscopic properties. The identification of new compounds capable of π-complex formation is therefore of great interest. The paper investigates the fluorescent properties of 1,5-diisocyanonaphthalene (1,5-DIN) in different aromatic solvents, demonstrating its potential for distinguishing between aromatics based on emission spectra. The resulting spectra can be classified as benzene-, toluene-, and xylene-like types and may be used for the fingerprint identification of benzenes with different electron donating/withdrawing substituents. Comparative studies with related compounds revealed that lower electron density in the naphthalene core favors π-complex formation. The study also found that electron-donating groups in solvents caused more significant redshifts, while electron-withdrawing groups had minimal impact. High-level DFT calculations supported these observations, showing that stronger π-π interactions lead to greater redshifts, particularly in solvents, such as toluene and xylenes. The research suggests that 1,5-DIN's distinct emission behaviors can be leveraged for compositional analysis of benzene-toluene-xylene (BTX) mixtures, with specific emphasis on the influence of electron density and solvent interactions on the emission properties.

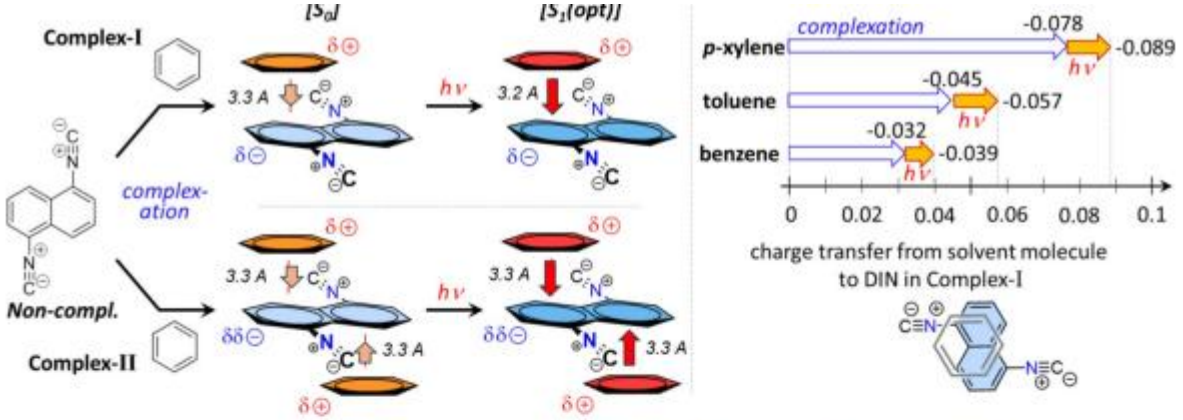
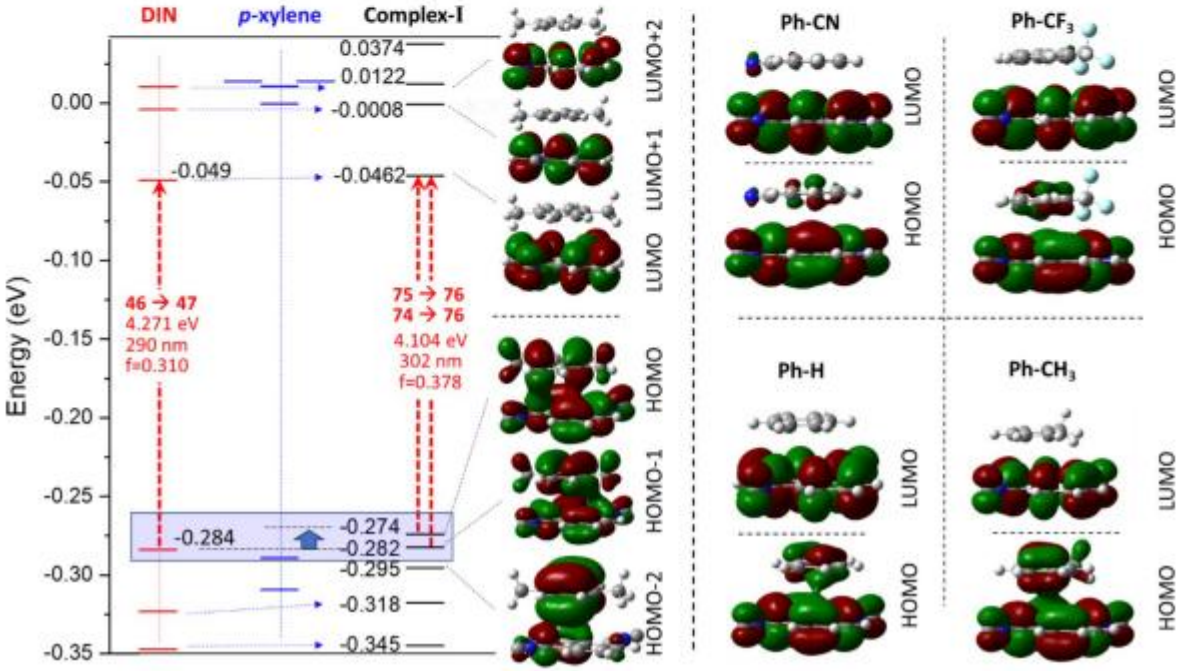


Fig. 4. Photochemical processes of Complex-I as well as II of 1,5-DIN and aromatic at M06-2X/6-311G++(2d,2p)[PCM(MeCN)] level of theory.



Issue 8, 2024

Previous Article | Next Article

From the journal:
Chemical Communications

Excited state iminium form can explain the unexpected solvatochromic behavior of symmetric 1,5- and 1,8-diaminonaphthalenes†

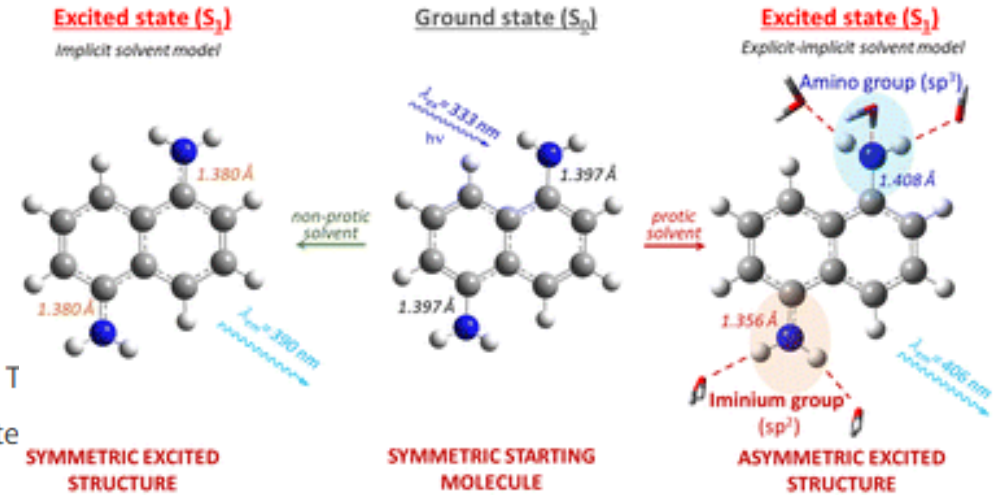
Check for updates

Erika Kopcsik,[a] Zoltán Mucsi,[*a] Bence Kontra,[c] László Vanyorek,[a] Rajmond Gál,[a] Béla Viskolcz[ab] and Miklós Nagy[*a]

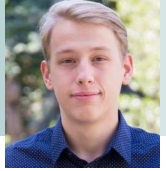
Author affiliations

Abstract

A new model, based on the presence of the excited state iminium ion (Ar = NH_2^+), is proposed to interpret the solvatochromic behavior of symmetric 1,5- and 1,8-diaminonaphtahelenes (DANs) in aprotic to protic media. T importance of using explicit solvent models during DFT calculations in protic solvents to find the proper excite structure for symmetric molecules is also highlighted.

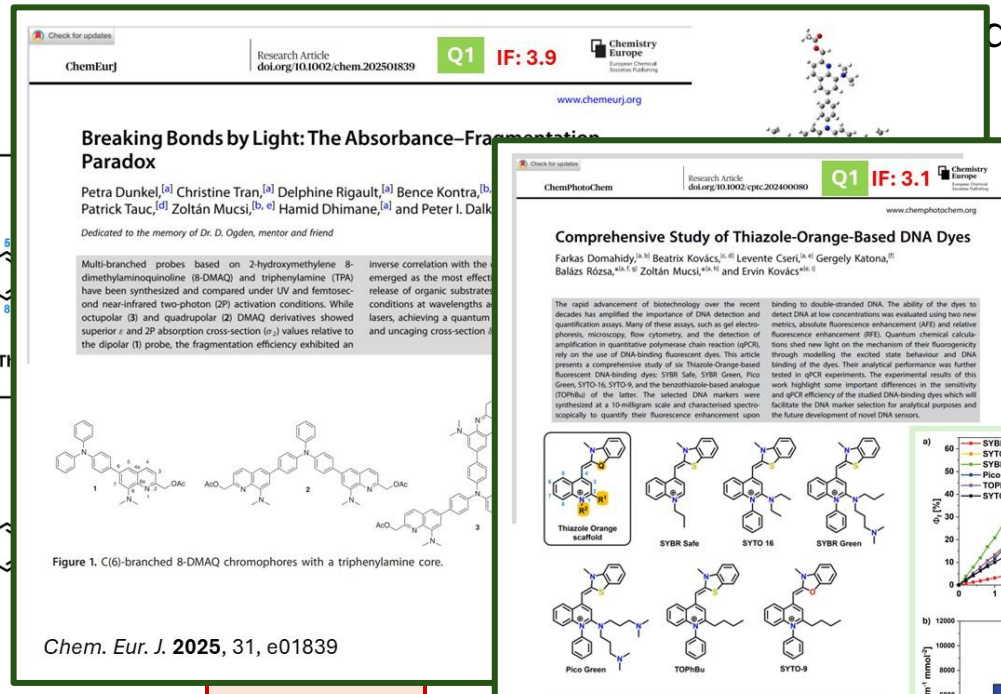


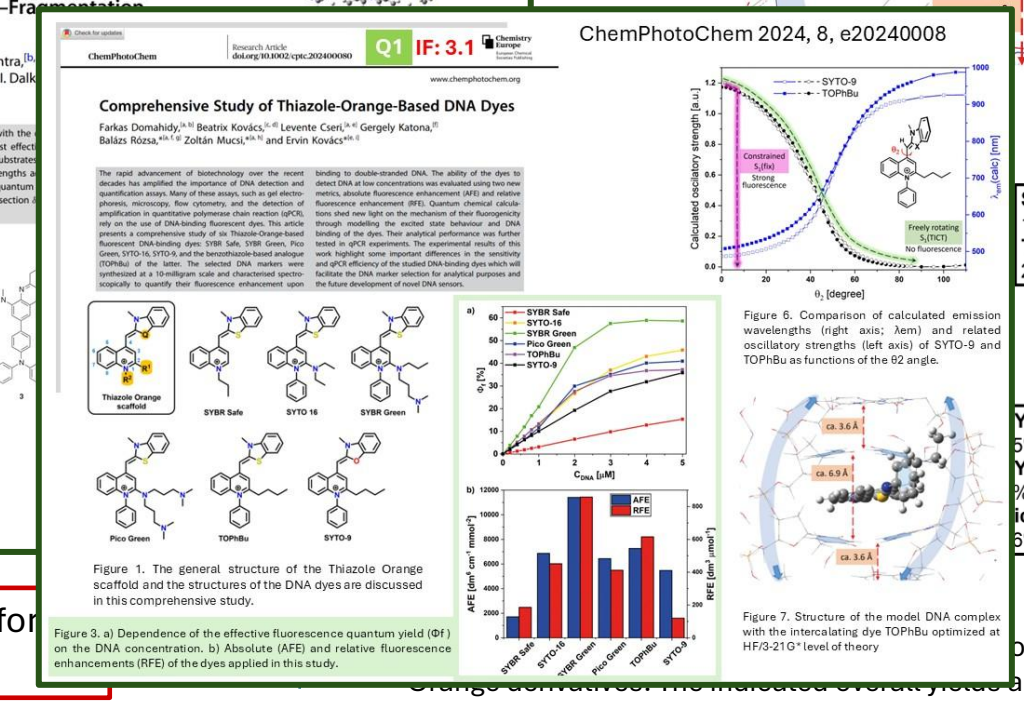
1) From the COVID period



Objective: Finding the Optimal DNA Dye for LAMP (Commercial Use)
Product Development

Excellence collaboration with
the **Molecular biology lab**

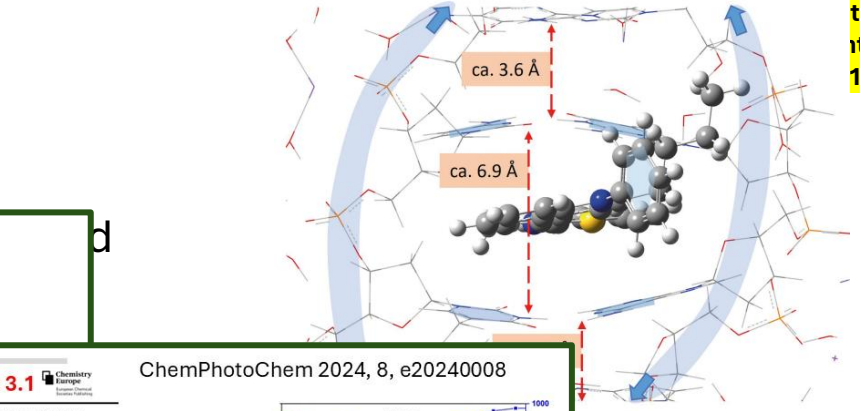




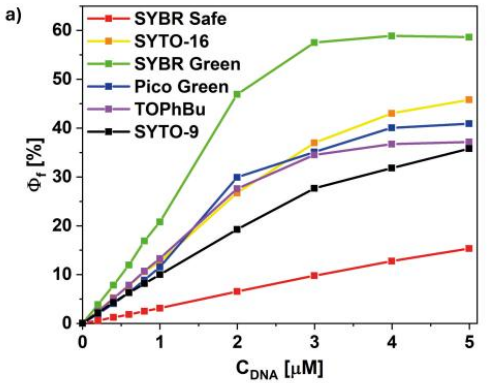
ChemPhotoChem 2024, 8, e20240008

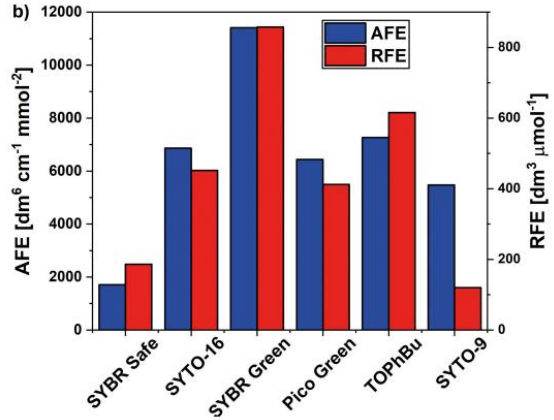
Figure 6. Comparison of calculated emission wavelengths (right axis; λem) and related oscillatory strengths (left axis) of SYTO-9 and TOPhBu as functions of the θ2 angle.

Figure 7. Structure of the model DNA complex with the intercalating dye TOPhBu optimized at HF/3-21G* level of theory



tructure of the model DNA complex with the ntercalating dye TOPhBu optimized at HF/3-1G* level of theory





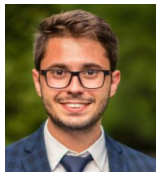
SYTO-9
10%
TOPhBu
20%

YTO-16
5%
YBR Green
%
ico Green
6%

TOPhBu: Novel dye for
PCR/LAMP test

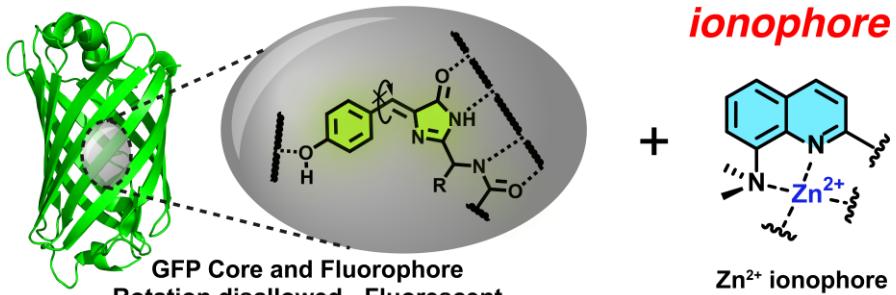
on of Thiazole
are calculated
from the 4- methyl-1-phenylquinolin-2-one intermediate.

ZN^{2+} SENSORS – CLASS 1A

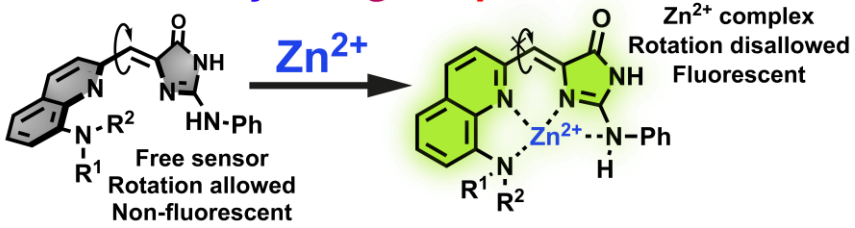


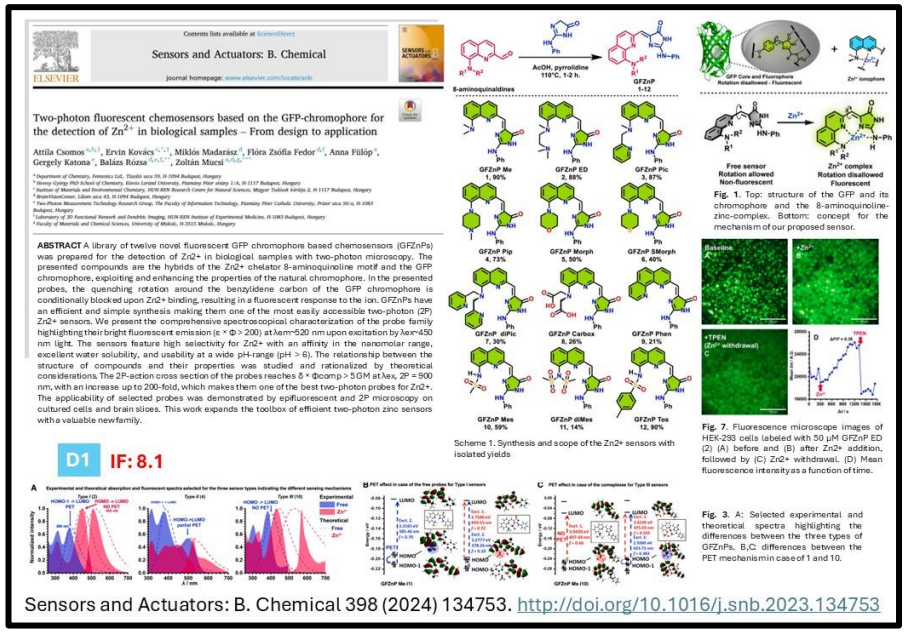
Bioinspiration

Artificial ionophore

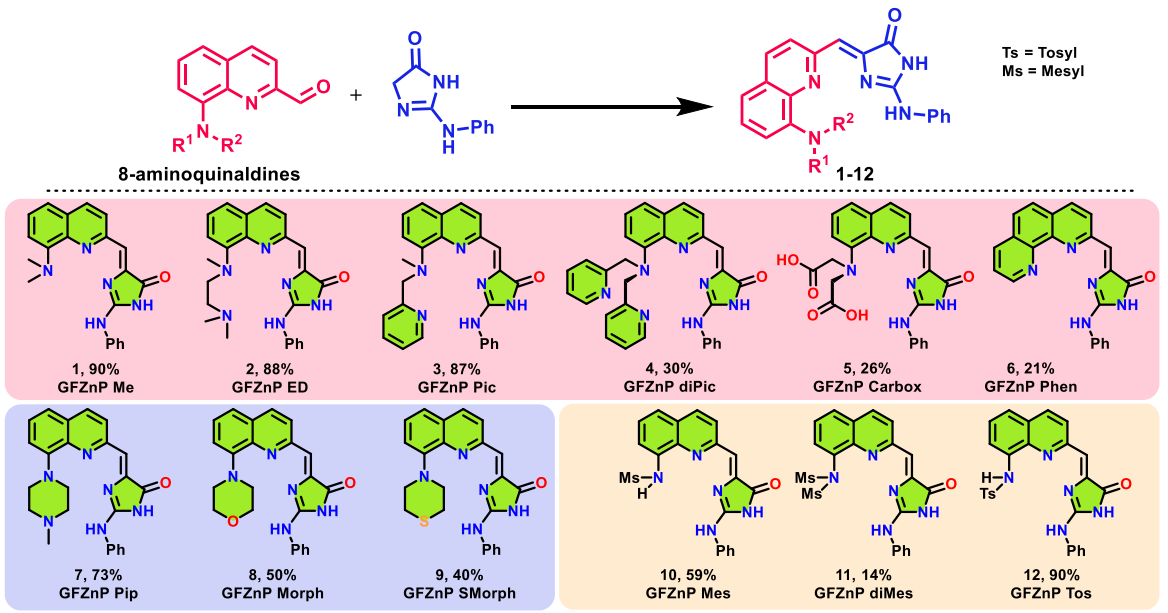


Rationally designed probe

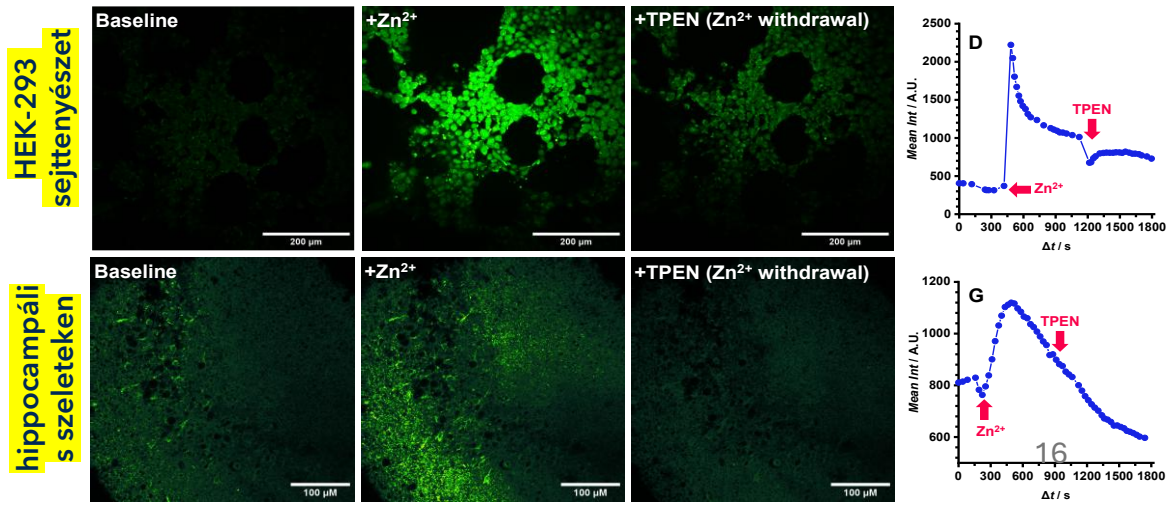




Sensors and Actuators: B. Chemical 398 (2024) 134753. http://doi.org/10.1016/j.snb.2023.134753



Kétfoton mérések HEK-293 sejttenyészeten (felül) és egér hippocampális szeleteken (alul) GFZnP ED (2) jelenlétében. Alapvonal; +Zn^{2+}, +kelátképző (TPEN):

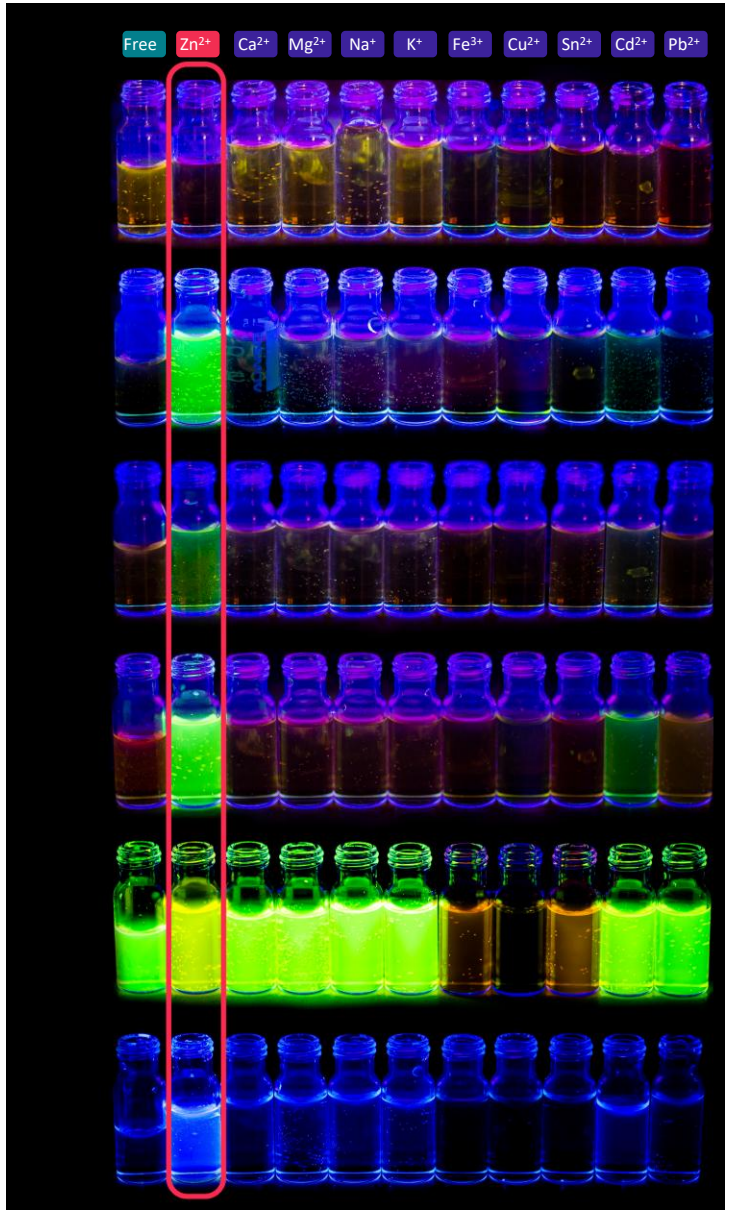


ZN^{2+} SENSORS – CLASS 1A

Two-photon imaging techniques

Attila Csomos

~ 0.05 mg compound in 1 ml solution
200 µl 10 mM metal ion solution



GFPHQ1 (11)

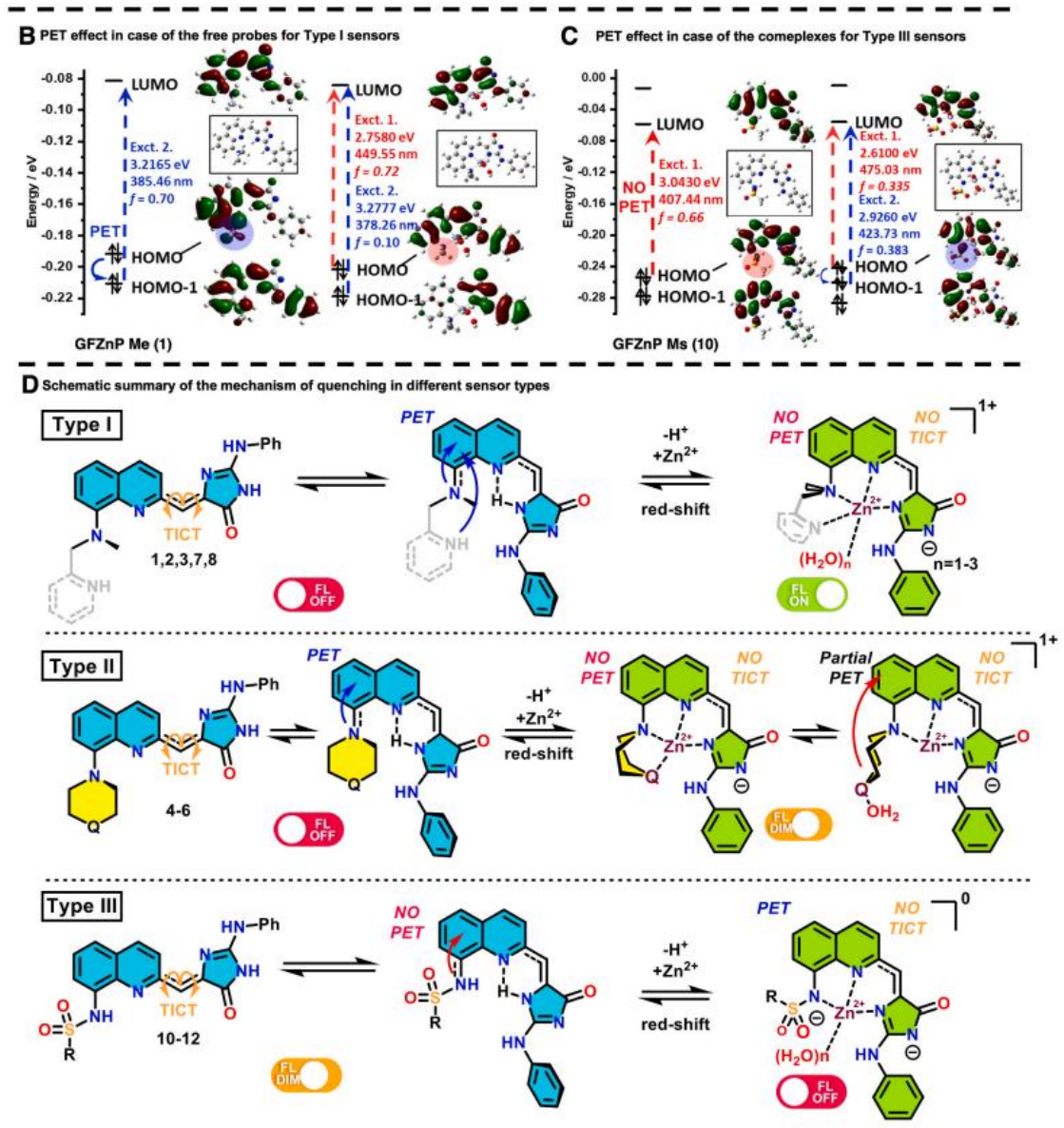
GFPAQ1 (12)

GFPAQ2 (13)

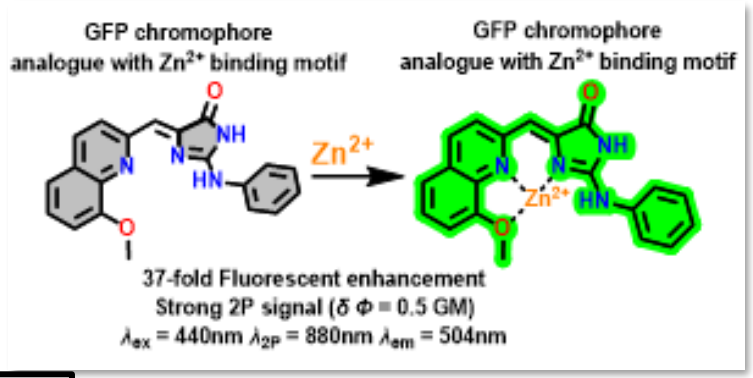
GFPAQ3 (14)

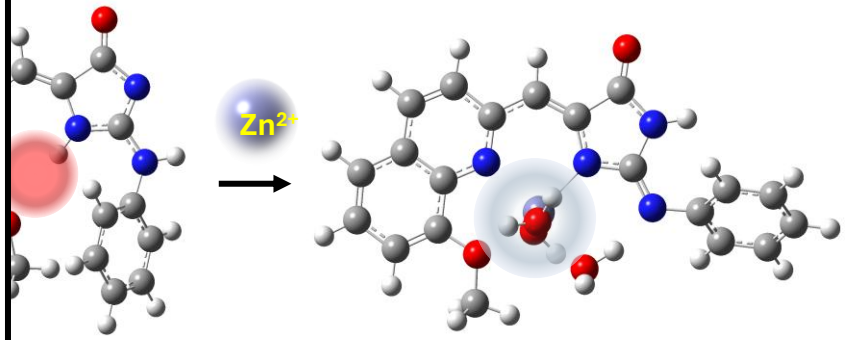
GFPDPA1 (15)

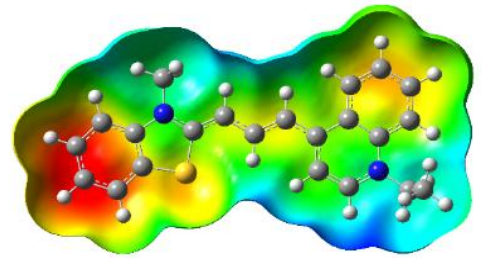
GFPDPA2 (16)



ZN^{2+} SENSORS –CLASS 1B







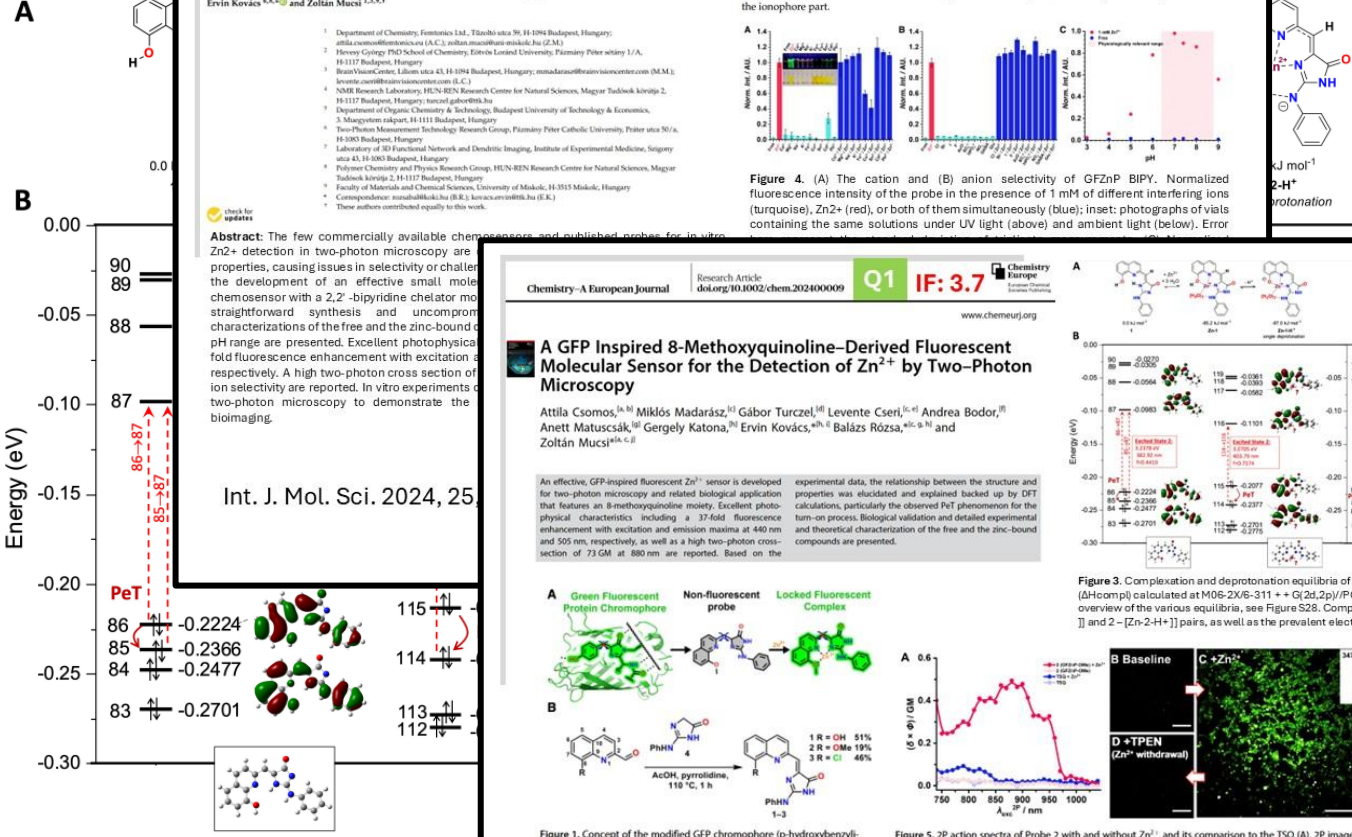


Figure 1. (A) Illustrative structure of the Green Fluorescent Protein (GFP), where its chromophore is highlighted in red [32]. (B) The planned sensor and its mechanism of action. The rings filled with green show the parts of the sensors resembling the GFP chromophore; the dark green lines represent the ionophore part.

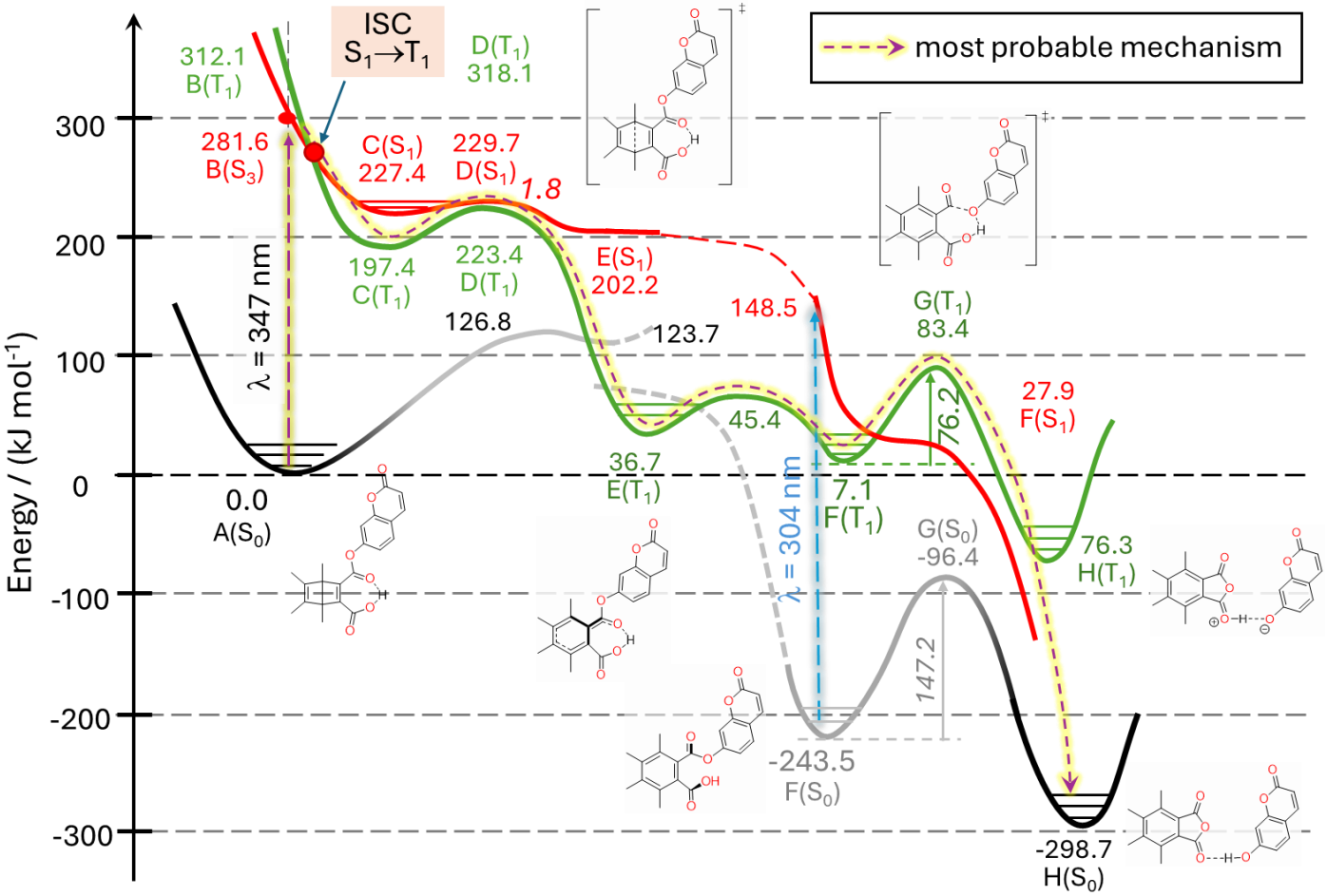
Figure 4. (A) The cation and (B) anion selectivity of GFZnP BIPY. Normalized fluorescence intensity of the probe in the presence of 1 mM of different interfering ions (turquoise), Zn2+ (red), or both of them simultaneously (blue); inset: photographs of vials containing the same solutions under UV light (above) and ambient light (below). Error

Figure 3. Complexation and deprotonation equilibria of 1 and 2 with the complexation enthalpies (ΔHcompl) calculated at M06-2X/6-311 + + G(2d,2p)//PCM(water) level of theory (A). For a complete overview of the various equilibria, see Figure S28. Computed molecular orbitals (MOs) of 1 – [Zn-1-H+]] and 2 – [Zn-2-H+]] pairs, as well as the prevalent electronic excitations (red boxes), computed by TD

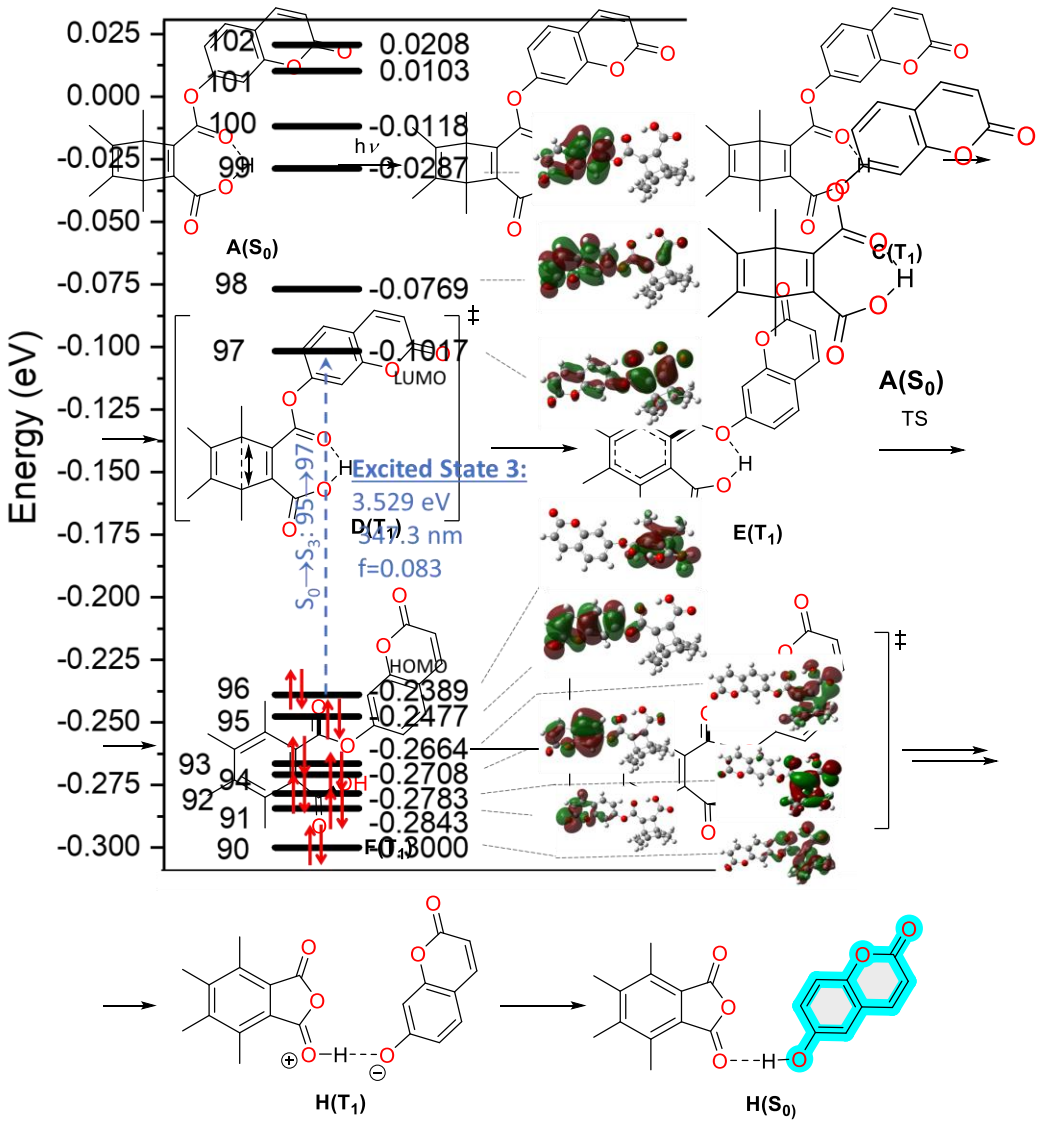
Figure 1. Concept of the modified GFP chromophore (p-hydroxybenzylidene-dimethylimidazolidinone) for Zn^{2+} sensing (A). Preparation of the quinoline-based probes (1–3) using Knoevenagel condensation (B).

Figure 5. 2P action spectra of Probe 2 with and without Zn^{2+} and its comparison to the TSQ (A). 2P image of HEK-293 cell cultures stained with 2 without Zn^{2+} addition (B), the same field of view after Zn^{2+} addition (C) and after Zn^{2+} withdrawal with TPEN (D). Scale bars represent 200 μm. Mean image intensity against the time from the start of the measurement (E).

One example for a complex photochemical processes

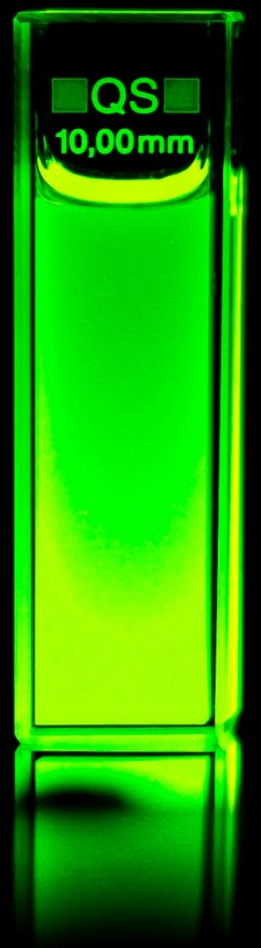


B3LYP/6-311++G(2d2p)



Összefoglalás

- Alkalmazható modellek fotokémiai folyamatok értelmezésére
- Xilol szenzor fejlesztése
- Új DNS festék fejlesztése
- Négy új Zn-ion szenzorcsalád sikeres fejlesztése
- Komplex fotokémiai folyamatok felderítése



Jövőbeli tervek, folytatjuk a tudományos munkát

új igények nincsenek!!! ☺

Köszönöm a figyelmet

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Nemzeti Kutatási, Fejlesztési és Innovációs Hivatal

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