



FÉLAG ÍSLENSKRA
NÁTTÚRUFRAEÐINGA

EFNAFRÆÐI Á ÍSLANDI

Kennsla, rannsóknir og atvinnulíf

10. ráðstefna EFNÍS



Efnafræðifélag Íslands
The Icelandic Chemical Society

25. OKTÓBER 2024
REYKJAVÍK

LÉTTARI HEIMUR

MEÐ ÍSLENSKU ÁLI

Í 25 ár hefur Norðurál framleitt hreint ál úr íslenskri orku, endurvinnanlegan málm sem er allt í kringum okkur í öllu sem við gerum. Við hlökkum til að halda áfram að gera heiminn léttari.

DAGSKRÁ

Föstudagur — 25. október 2024

Gullfoss A salur, Fosshótel Reykjavík, Þórunnartún 1, 105, Reykjavík

08:30 - 09:00 Húsið opnar / Venue opens

09:00-10:30 Fyrirlestrar / Presentations 1

09:00-09:30	O-01	DTE - Kristján Leósson
09:30-09:50	O-02	Norðurál - Gæðaeftirlit í framleiðslu Guðlaugur Bjarki Lúðvíksson
09:50-10:10	O-03	Efnafræði vökva úr ofurheitu IDDP-borholunum í Kröflu, á Reykjanesi og Nesjavöllum Finnbogi Óskarsson
10:10-10:30	O-04	From analytical chemistry to biological insights: an introduction to analytical facilities in the Faculty of Pharmaceutical Sciences, University of Iceland Maonian Xu

10:30-10:50 Kaffipása / Coffee break

10:50-12:00 Fyrirlestrar / Presentations 2

10:50-11:20	O-05	"Can we really make bread from air?" Egill Skúlason
11:20-11:40	O-06	Advanced perturbation scheme for efficient polarizability computations Anoop Ajaya Kumar Nair
11:40-12:00	O-07	Dynamic Nuclear Polarization: The Next Frontier in NMR Satyaki Chatterjee

12:00-13:00 Hádegismatur / Lunch break

13:00-14:30 Fyrirlestrar / Presentations 3

13:00-13:30	O-08 / O-09	Notkun gervigreindar í efnafræðikennslu: Reynsla og framtíðarþróun / Tvíþætt gildi opins námsefnis í efnafræði á íslensku: Áhrif á menntun og þróun mállíkana Sigurður E. Vilhelmsson
13:30-13:50	O-10	DNA and nucleosome binding redistribute activation domain ensemble and accessibility in reprogramming factor Sox2 Sveinn Bjarnason
13:50-14:10	O-11	Electrostatic Regulation of Intramolecular Interactions in Pioneer Factor PU.1 Sigríður Stefanía Hlynsdóttir
14:10-14:30	O-12	Auðna tækniorg Einar Mantyla

14:30-14:45 Kaffipása / Coffee break

14:45-16:10 Fyrirlestrar / Presentations 4

14:45-15:15	O-13	Mass Spectrometry Network in Iceland and Protein Characterization Guðrún Rútsdóttir
15:15-15:30	O-14	High-Resolution Mass Spectrometry for Monitoring New Psychoactive Substances in Wastewater: Addressing False Positives and Emerging Trends Adam Bauer
15:30-16:50	O-15	Selective adsorption of DMF using porous materials based on Zinc metal and mercaptobenzoic acid Baldur Kristinsson
15:50-16:10	O-16	Orka í Iðnaðarferlum í 22 ár Guðrún Arinbjörg Sævarsdóttir

16:10-17:00 Veggspjöld / Poster session

19:00-22:00 Ráðstefnukvöldverður / Conference dinner - Gullfoss A

Einkaleyfi

Vörumerki

Höfundaréttur

Hönnunarvernd

Hugverkaréttur

Nýsköpun

Lén

Guðríðarstíg 2-4 · 113 Reykjavík

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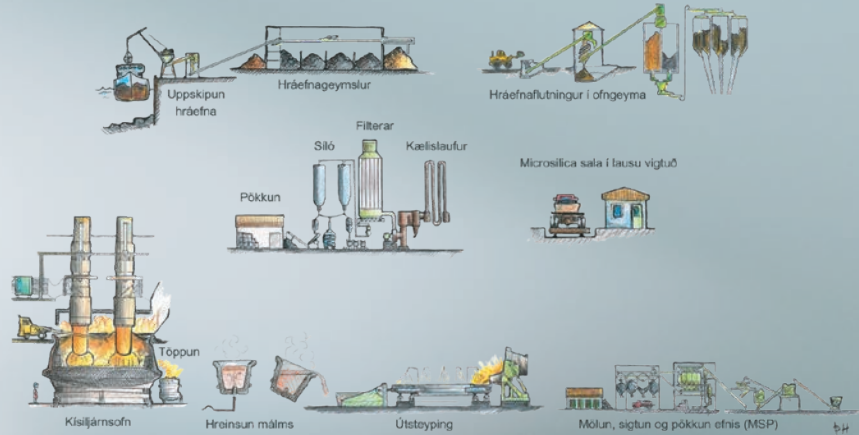
Rafmagnsstál
Kísill eykur segulmagn stáls og þar með nýtni í rafmagnsmóturum, rafölum og spennum

Sérstál & ryðfrítt stál
Kísill getur m.a. aukið styrk, hörku, viðnám stáls og dregur úr tæringu

Elkem Microsilica
Eykur styrk og endingartíma steypu og eldþol gífsplatna

Hjá Elkem Ísland umbreytum við kvasi og járni í hágæða kísilmálm með hjálp íslenskrar raforku. Kísilmálmur er notaður til þess að hreinsa stál og sem íblöndunarefni til þess að ná fram ákveðnum eiginleikum í stáli sem bætir stálframleiðslu og gæði.

Elkem á Íslandi sérhæfir sig í framleiðslu á kísilmálmi fyrir rafmagnsstál. Rafmagnsstál er grundvöllur orkuskipta í heiminum og kísill er forsenda framleiðslu hans. Í hverjum rafmagnsbíl sem fer á götuna eru um 4kg af hágæða kísilmálmi.



RÁÐSTEFNUNEFND

Adam Erik Bauer
Anna Bergljót Gunnarsdóttir
Benjamín Ragnar Sveinbjörnsson
Steinar Birgisson
Vilhjálmur Ásgeirsson

VEGGSPJÖLD

No.	Titill / Title	Kynnir / Presenting author
P-01	Tæknisetur: Iceland's Hub for Technical Innovation and R&D Collaboration	Andrés Castro Ruiz
P-02	MS eining Rannsóknakjarna Landspítala	Baldur Bragi Sigurðsson
P-03	DINUCLEAR MOLYBDENUM COMPLEXES AS CATALYSTS FOR SYNTHESIS OF BIOBASED FURANIC POLYESTER MATERIALS (PEF) AND THEIR CHEMICAL RECYCLING	Dmitrii Razinkov
P-04	Efnagreiningar á Hafrannsóknastofnun	Egill Antonsson
P-05	Supramolecular Gels Based on C3-Symmetric Amide for Dye Removal from Water	Geethanjali Kuppadakkath
P-06	Identification of human enzyme inhibitors against cancer glycolysis	Jens G. Hjörleifsson
P-07	DINUCLEAR MOLYBDENUM COMPLEXES AS CATALYSTS FOR SYNTHESIS OF BIOBASED FURANIC POLYESTER MATERIALS (PEF) AND THEIR CHEMICAL RECYCLING	Dmitrii Razinkov
P-08	Stimuli-Responsive Supramolecular Gels Based on Multi-functional ligands	Sreejith S Jayabhavan
P-09	CO2 reduction to fuel through surface engineering	Sebastian Francis
P-10	Stimuli-Responsive Supramolecular Gels Based on Multi-functional ligands	Sreejith S Jayabhavan
P-11	Non-covalent spin-labeling of RNA through helical stacking	Iram M. Ahmad

Ráðstefnunefnd EFNÍS vill þakka styrktaraðilum kærlega fyrir samstarfið.



FÉLAG ÍSLENSKRA
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O-04

From analytical chemistry to biological insights: an introduction to analytical facilities in the Faculty of Pharmaceutical Sciences, University of Iceland

Maonian Xu¹

¹Faculty of Pharmaceutical Sciences, University of Iceland, Hofsvallagata 53, 107 Reykjavik

ABSTRACT

The Faculty of Pharmaceutical Sciences, University of Iceland hosts a broad array of analytical instruments, including sample preparation (e.g. TubeMiller, SpeedMiller) chromatographic systems (analytical to preparative scale for both small and macro-molecules), gel electrophoresis, calorimetric devices (e.g. differential scanning calorimetry), particle size measurements (e.g. Nanoparticle analyzer) and viscometer, etc. This presentation aims to introduce analytical facilities in the Faculty of Pharmaceutical Sciences, University of Iceland, and a few example studies resulting from our facilities will also be presented. The scheme for future collaboration with research institutes and commercial partners will be discussed. Plans for future instrumental trainings and courses are also proposed to facilitate and promote the use the valuable devices.

O-05

“Can we really make bread from air?”

Egill Skúlason

Professor of Chemical Engineering at the University of Iceland

Chief Scientific Officer and co-founder of Atmonia ehf.

ABSTRACT

Artificial nitrogen fixation is essential to provide food security. Today ammonia is produced through the Haber-Bosch process from nitrogen and hydrogen gases whereas nitrates are produced through the Ostwald process from ammonia and oxygen. From these, various nitrogen containing fertilizers are produced depending on the application of use. The Haber-Bosch process is, however, not sustainable since it relies on natural gas resources for hydrogen generation, and at the same time highly polluting of CO₂ emission. It is therefore necessary to develop alternative routes for ammonia and nitrate synthesis. One of the most attractive solution would be to have a heterogenous electrolytic cell with an aqueous electrolyte that works at ambient conditions, where a nitrogen fertilizer can be produced on-site. There are, however, several factors that make it difficult to accomplish this, mainly because the N₂ molecule is inert and difficult to reduce and because of the side reaction, the hydrogen evolution reaction (HER), which usually takes place more easily than the nitrogen reduction reaction (NRR). It has been predicted that all the transition metals will much more easily catalyze HER than NRR.

Over the last few years we have been searching, using density functional theory (DFT) calculations, for alternative materials that can catalyze NRR while suppressing HER. The class of materials we have investigated are transition metal ceramics of e.g. nitrides, oxides, sulfides, carbides, oxynitrides and carbonitrides. Several promising candidates are predicted within each class of materials and we have tested several of them experimentally. There, we grow the catalysts in thin-films using magnetron sputtering, which are then tested in a micro reactor for electrocatalytic performance. The electrochemical micro reactor is connected in-line with the ammonia detection unit, preventing any possible contamination which makes the results reliable and robust. Experiments are done both in N₂ saturated electrolyte and in Ar saturated electrolyte and isotope labelled ¹⁵N₂ is used to proof catalysis. In this presentation, I will discuss both the theoretical predictions and the experimental performance of several candidates for NRR.

O-06

Advanced perturbation scheme for efficient polarizability computations

Anoop Ajaya Kumar Nair¹, Julian Bessner², Timo Jacob², Elvar Örn Jónsson¹

¹ Science Institute and Faculty of Physical Sciences, University of Iceland, Reykjavík, Iceland² Institute of Electrochemistry, Ulm University, Albert-Einstein-Allee 47, 89081 Ulm, Germany

ABSTRACT

We present an efficient moment based perturbation scheme to evaluate polarizability tensors of small molecules and at the fraction of the computational cost compared to conventional energy based perturbation schemes¹. Furthermore, the simplicity of the scheme allows for the seamless integration into modern quantum chemistry codes. We apply the method to systems where the wavefunctions are described on a real-space grid and are therefore not subject to finite size basis set errors. In the grid-based scheme errors can be attributed to the resolution and the size of the grid-space. The applicability and generality of the method is exhibited by calculating polarizability tensors including the dipole-dipole and up to the quadrupole-quadrupole for a series of small molecules, representing the most common symmetry groups. By a direct comparison with standard techniques based on energy perturbation we show that the method reduces the number of explicit computations by a factor of ~ 30 . Numerical errors introduced due to the arrangement of the explicit point charges are eliminated with an extrapolation scheme to the effective zero-perturbation limit.

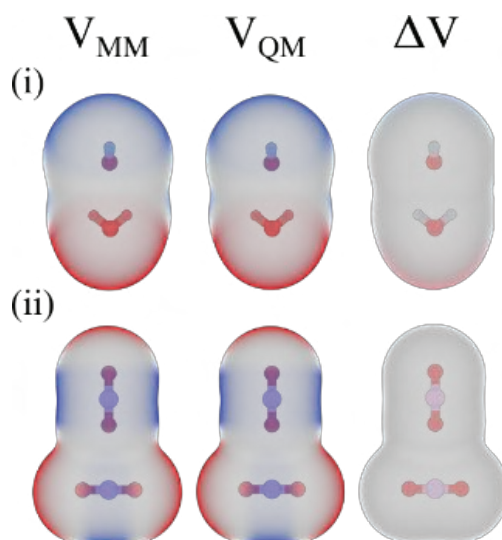


FIGURE 1: The potential energy (e/a_0) mapped on to a fixed iso-surface. It consists of the potential calculated from the Buckingham expansion (V_{MM}), QM potential calculated via GPAW (V_{QM}) and the difference between the surfaces ($\Delta V = V_{QM} - V_{MM}$).

REFERENCES

1. [Advanced perturbation scheme for efficient polarizability computations AAK Nair, J Bessner, T Jacob, EÖ Jónsson - arXiv preprint arXiv:2409.10184, 2024](https://arxiv.org/abs/2409.10184)

O-07

Dynamic Nuclear Polarization: The Next Frontier in NMR

Satyaki Chatterjee¹ and Snorri Th. Sigurdsson¹

¹University of Iceland, Department of Chemistry, Science Institute, Dunhaga 3, 107-Reykjavik, Iceland

ABSTRACT

Nuclear Magnetic Resonance (NMR) spectroscopy is a well-established technique and extensively applied for elucidating molecular structures and dynamics in a wide range of applications, from drug discovery to material science.¹ Traditional solution-state NMR spectroscopy is limited to the study of large, insoluble, or complex biological samples and materials, but solid-state NMR (ssNMR) has emerged as a powerful companion, enabling the study of such systems. A disadvantage of ssNMR is line-broadening, which limits spectral resolution, but magic angle spinning (MAS) sharpens the peaks and thereby increases the resolution. However, a major limitation of NMR spectroscopy is its lack of sensitivity, particularly for low-abundance nuclei. Dynamic nuclear polarization (DNP) has emerged as a transformative technique that significantly enhances the sensitivity of both solution-state and ssNMR. DNP facilitates the transfer of spin polarization from unpaired electrons in so-called polarizing agents, that are typically persistent biradicals, to nuclei of interest. This results in signal enhancements of up to 10000-fold.² In this presentation, I will begin by giving an overview of NMR spectroscopy and DNP, followed by describing my contribution to the field through designing and synthesizing polarizing agents for DNP-NMR in the solid state. This work paves the way for more efficient structural analysis of previously inaccessible systems, significantly broadening the scope and impact of NMR technologies.

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2. Thankamony A. S; Wittmann, J. J; Kaushik, M; Corzilius, B. Dynamic nuclear polarization for sensitivity enhancement in modern solid-state NMR, *Prog. Nucl. Magn. Reson. Spectrosc.*, **2017**, 102-103, 120-195.

Tvíþætt gildi opins námsefnis í efnafræði á íslensku: Áhrif á menntun og þróun mállíkana

Sigurður E. Vilhelmsson¹ (sigurdurev@kvenno.is)

¹Kvennaskólinn í Reykjavík, Fríkirkjuvegi 9, 101-Reykjavík

Hér er fjallað um tvíþætt gildi opins námsefnis í efnafræði á íslensku: (1) möguleg áhrif þess á gæði náms og kennslu, og (2) hlutverk þess í þróun íslenskra mállíkana fyrir raungreinar. Markmið er að meta hugsanleg áhrif aukins aðgengis að opnu, íslensku námsefni í efnafræði og kynna áætlanir um þróun slíks efnis.

Fræðilegur bakgrunnur: Erindið byggir á alþjóðlegri reynslu af notkun opins námsefnis í háskólanámi. Rannsóknir benda til þess að opið námsefni geti haft jákvæð áhrif á námsárangur, sérstaklega meðal nemenda í viðkvæmri stöðu. Þá hefur verið sýnt fram á verulegan sparnað fyrir nemendur og menntastofnanir með notkun opins námsefnis. Einnig er stuðst við nýlegar rannsóknir á þróun mállíkana og mikilvægi fjölbreyttra þjálfunargagna fyrir nákvæmni þeirra í sérhæfðum fræðigreinum.

Væntanlegur ávinningur:

1. Aukið aðgengi nemenda að gæðaeefni og stuðningur við sjálfsnám.
2. Lækkun kostnaðar við námsgögn, sem gæti aukið jafnrétti til náms.
3. Aukin sveigjanleiki kennara við aðlögun námsefnis.
4. Bætt frammistaða íslenskra mállíkana í meðhöndlun efnafræðihugtaka.
5. Stuðningur við varðveislu og þróun íslensks fagmáls í raungreinum.
6. Möguleg jákvæð áhrif á námsárangur og þátttöku nemenda í námi.

Framtíðarþróun: Kynnt verða áform um þýðingu og aðlögun opins námsefnis í efnafræði, með áherslu á OpenStax Chemistry 2e. Verkefnið felur í sér:

1. Þróun verkferla fyrir þýðingar með aðstoð gervigreindar.
2. Eiginlega þýðingarvinnu og gæðaeftirlit.
3. Undirbúningur fyrir útgáfu og dreifingu þýddra kafla.
4. Reglulegt notendasamráð við kennara og nemendur.
5. Sérstaka áherslu á að skilgreina og útskýra helstu hugtök í efnafræði á íslensku.

Samhliða þessu verður unnið að þróun matsviðmiða fyrir mállíkön sem meta getu þeirra til að þýða efnafræðitexta frá ensku yfir á íslensku og útbúin sérstök efnafræðipróf á íslensku til að meta getu mállíkana í efnafræði.

Erindið miðar að því að kynna þessar hugmyndir og leita eftir samstarfi við efnafræðinga og efnafræðikennara um verkefnið. Markmiðið er að skapa umræðu um mikilvægi opins námsefnis á íslensku í efnafræði og hvernig við getum í sameiningu stuðlað að þróun þess til hagsbóta fyrir nemendur, kennara og íslenskt menntakerfi í heild.

Electrostatic Regulation of Intramolecular Interactions in Pioneer Factor PU.1

Sigríður St. Hlynsdóttir¹, Mariya P. Monoba¹, Kinga S. Demény¹ and Pétur O. Heiðarsson¹

¹Department of Biochemistry, The Science Institute, University of Iceland, Address for affiliation institution

ABSTRACT

PU.1, a pioneer transcription factor (pTF) within the hematopoietic lineage, plays a crucial role in numerous blood disorders and diseases. As a pTF, PU.1 selectively targets and binds to compacted chromatin and initiates cell fate changes. The N-terminal domain of PU.1 is an intrinsically disordered region (IDR) that includes the transactivation domain. Despite the recognized significance of the IDR in PU.1's pioneering activity, the underlying mechanisms remain poorly understood. It is thought that the region may be important for recruiting other transcription factors (TFs) or interacting with nucleosomes. While PU.1 has been identified as a potential therapeutic target, comprehensive insights into the biochemical and biophysical properties of this protein are currently lacking.

We employed **single-molecule spectroscopy coupled with Förster resonance energy transfer (smFRET)** to investigate the conformational dynamics of PU.1's IDRs. Our findings demonstrate that PU.1 binds with high-affinity to short DNA sequences containing its recognition motif, and binding induces distal conformational changes in the disordered N-terminal tail. Analysis of transfer efficiency histograms revealed two distinct PU.1 populations, each displaying unique and varying sensitivity to denaturants, ionic strength, and DNA binding. These two conformational states are the result of intramolecular interdomain interactions.

Characterizing the physical principles governing PU.1's function provides valuable knowledge that aids in the research of PU.1 as a therapeutic target. Furthermore, our findings contribute to the broader understanding of the role of IDRs in pioneer function, thereby facilitating advancements in stem cell research.

O-13

Mass Spectrometry Network in Iceland and Protein Characterization

Guðrún Rútsdóttir^{1,2}

¹ Faculty of biochemistry, Sturlugata 7

² Faculty of pharmaceutical science, Hofsvallagata 53

ABSTRACT

Mass spectrometry (MS) is an invaluable tool for the characterization and quantification of a wide range of molecules, from small compounds to large proteins. Despite its versatility, MS is a complex technique requiring highly specialized expertise and significant resources to operate effectively. The instruments are not only costly but also demand meticulous maintenance, making them difficult to sustain, especially in smaller countries like Iceland.

To address these challenges, we have formed a dedicated mass spectrometry society under the umbrella of the Icelandic Chemical Society. Our goal is to foster collaboration among specialists in MS, facilitating knowledge-sharing and mutual support. In doing so, we also aim to create a visible platform for collaboration with others who may benefit from MS expertise.

Iceland is home to experts in various MS applications, including lipidomics, metabolomics, and proteomics. As a specialist in protein characterization through MS, I would like to highlight the extensive potential of mass spectrometry in advancing protein research. By leveraging MS, we can unlock deeper insights into the structure, function, and dynamics of proteins, offering powerful solutions for a broad range of scientific inquiries.

High-Resolution Mass Spectrometry for Monitoring New Psychoactive Substances in Wastewater: Addressing False Positives and Emerging Trends

Adam E. Bauer¹, Oddný Ragnarsdóttir¹, Arndís Sue Ching Löve², and Kristín Ólafsdóttir¹

¹Department of pharmacology and toxicology, University of Iceland, Reykjavik, Iceland

²Department of Pharmaceutical Sciences, University of Iceland, Reykjavik, Iceland

ABSTRACT

The rise of new psychoactive substances (NPSs) has created significant public health challenges, with traditional monitoring methods often falling short in detecting these rapidly evolving compounds. To address this, wastewater-based epidemiology (WBE) has emerged as a valuable alternative.¹⁻⁴ This study employs high-resolution mass spectrometry (HRMS)-based suspect screening to profile NPSs, illicit drugs, and drug-related compounds in wastewater samples from Reykjavik, Iceland from January to August 2024. The screening involved approximately 2000 substances from the commercial Waters Toxicology Library. While common pharmaceuticals and illicit drugs were identified, the consistent detection of 4¹⁴C₁-alpha-PPP, a synthetic cathinone, in all tested wastewater samples was unexpected. Although the retention time and fragment match criteria were strong, the absence of this cathinone in seized drug samples and other forensic cases submitted for analysis at the Department of pharmacology and toxicology at the University of Iceland raised doubts about its authenticity. Further analysis revealed the result to be a false positive, caused by in-source fragmentation of hydroxybupropion, a metabolite of the commonly prescribed drug bupropion. This was confirmed through the analysis of a hydroxybupropion reference standard. These findings underscore the utility of HRMS for monitoring drug trends, while also emphasizing the need for careful validation of surprising results to avoid reporting false positives.

REFERENCES

1. United Nations Office on Drugs and Crime. *World Drug Report 2022*; United Nations Office on Drugs and Crime: New York, NY, USA, 2023.
2. Simão, A. Y.; Antunes, M.; Cabral, E.; Oliveira, P.; Rosendo, L. M.; Brinca, A. T.; Alves, E.; Marques, H.; Rosado, T.; Passarinha, L. A. An Update on the Implications of New Psychoactive Substances in Public Health. *Int. J. Environ. Res. Public Health* 2022, 19, 4869.
3. Huizer, M.; Ter Laak, T. L.; de Voogt, P.; van Wezel, A. P. Wastewater-Based Epidemiology for Illicit Drugs: A Critical Review on Global Data. *Water Res.* 2021, 207, 117789. <https://doi.org/10.1016/j.watres.2021.117789>.
4. Van Wel, J.; Gracia-Lor, E.; Van Nuijs, A.; Kinyua, J.; Salvatore, S.; Castiglioni, S.; Bramness, J. G.; Covaci, A.; Van Hal, G. Investigation of Agreement Between Wastewater-Based Epidemiology and Survey Data on Alcohol and Nicotine Use in a community. *Drug Alcohol Depend.* 2016, 162, 170–175. <https://doi.org/10.1016/j.drugalcdep.2016.02.012>.

Selective adsorption of DMF using porous materials based on Zinc metal and mercaptobenzoic acid

Baldur Kristinsson¹, and Krishna K. Damodaran¹

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ABSTRACT

Porous coordination polymers (PCPs)¹ are an excellent class materials constructed from metal ions or clusters as nodes and organic ligands as linkers and one of the main advantages of PCPs over traditional porous materials is the tunable structural properties. The nature of the ligand plays a vital role in the generation of the porous architecture in PCPs, which can be anionic, cationic, or neutral.¹ In this work, we have selected a disulfide-based dicarboxylate ligand, namely, 4,4'-dithiodibenzoic acid (DTBA), because the disulfide bonds could induce a bent structure arising from the 90.0° twist of the disulfide bonds with the adjacent atoms. We have synthesized and characterized a PCP based on zinc nitrate and a 4,4'-dithiodibenzoic acid ligand and the structural analysis revealed the presence of two molecules of DMF in the porous network (HI-103).² The stability of the porous network was analyzed by heating the compound at 60.0 °C for two days, and the structural analysis revealed a new PCP (HI-104) was formed with one of the DMF molecules, indicating a single-crystal to single-crystal (SCSC) transformation. The reversibility of SCSC transformation was confirmed by treating HI-103-dry with DMF molecules, resulting in HI-103 after five days. The adsorption studies of HI-103-dry with other solvents revealed that SCSC transformation was not observed for DMA and DEA, but some structural changes were observed in the presence of DMSO. The presence of disulfide bond in the MOF prompted us to evaluate the sensing properties towards heavy metals and experiments were repeated with DTBA and heavy metals such as Cd and Hg. We are also analysing the post synthetic modification of HI-103 in the presence of mercury ions and analysing the adsorption properties arising from the structural changes in the presence of heavy metal ions.

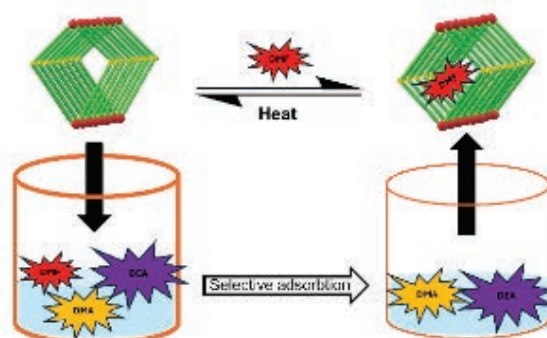


FIGURE 1: Selective adsorption of HI-103.

REFERENCES

1. J.-S. M. Lee, K.-I. Otake, S. Kitagawa, *Coord. Chem. Rev.* 2020, 421, 213447.
2. B. Kristinsson, M. Janiw, K. K. Damodaran, *ChemPlusChem* 2024, e202400351. <https://doi.org/10.1002/cplu.202400351>.

O-16

Orka í lðnaðarferlum í 22 ár

Guðrún Arnbjörg Sævarsdóttir, Prófessor, Háskólinn í Reykjavík

Orka í lðnaðarferlum er námskeið sem kennt hefur verið við Háskólann í Reykjavík frá því ég hóf störf þar árið 2008, og fyrir þann tíma kenndi ég Orkufrek Framleiðsluferli við Háskóla Íslands, sem á þeim tíma var sambærilegt námskeið. Í þessum námskeiðum fá nemendur nokkuð traustan grunn í efnafræðinni sem liggur að baki kísilframleiðsluferlinu, sem og rafefnafræðinni sem er grunnurinn að álframleiðslu ásamt mögulegri rafeldsneytisframleiðslu í framtíðinni. Eitt aðal hæfniviðmið námskeiðsins er að nemendur geti reiknað orkubalans og efnabalans fyrir framleiðsluferli, hvort sem þau hafa séð þau áður eða ekki.

Öll þessi ár hafa nemendurnir mínir fengið að heimsækja málmframleiðslufyrirtækin, og höfum við fengið frábærar móttökur hjá sérfræðingum þeirra.



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Framleiðsla á iðnaðarskala frá 2012

Metanólverksmiðja CRI í Svartsengi var fyrsta sinnar gerðar
í heiminum til að framleiða og selja vottað rafeldsneyti



**CRI þróar og hannar
efnaverksmiðjur sem
framleiða raf-metanól**

ETL tæknin hefur þegar sannað sig í
nýtingu endurnýjanlegrar orku og
dregur úr losun gróðurhúsalofttegunda

P-01

Tæknisetur: Iceland's Hub for Technical Innovation and R&D Collaboration

Andrés Castro Ruiz

Abstract:

Tæknisetur serves as a central hub for technical infrastructure and R&D collaboration in Iceland, offering shared facilities co-owned with Icelandic universities. This partnership ensures our state-of-the-art facilities are accessible to a broad audience, including startups, entrepreneurs, academic researchers, and established enterprises throughout the country. Our comprehensive platform includes advanced laboratories, workshops, and testing environments, featuring tools like electron microscopes, Raman spectrometer, and diverse surface analysis equipment.

Our offerings span key areas such as materials science, life sciences, biomedical technology, and green solutions, making Tæknisetur an adaptable partner for projects of all sizes. We support prototyping, testing, and analysis through specialized facilities, including electrical, wood, and metal workshops, as well as cutting-edge capabilities in 3D printing and biotechnological processes. Notably, our biomedical research focuses on developing innovative medical devices and biomaterials, contributing to significant advancements in healthcare technology.

Through partnerships with over 60 international and domestic companies, universities, and institutions, Tæknisetur plays an important role in advancing Iceland's technological landscape. Our expertise promotes sustainable and efficient outcomes across sectors, from pioneering carbon-neutral solutions for the aluminum and geothermal industry to enhancing biomaterial properties for medical applications. This poster highlights Tæknisetur's facilities, services, and collaborative projects, showcasing our commitment to promoting innovation and technological growth in Iceland.

P-02

MS eining Rannsóknakjarna Landspítala

Baldur Bragi Sigurðsson¹, Íris Thelma Halldórsdóttir¹, Pitsiree Praphanwittaya¹, Guðmundur Sigbórsson¹ og Ísleifur Ólafsson¹

¹Klínísk lífefnafræðideild, Rannsóknakjarna Landspítala

ABSTRACT

Rannsóknakjarni Landspítala hýsir bæði klíníska lífefnafræðideild og blóðmeinafræðideild. Saman framkvæma þessar deildir yfir 2.600.000 rannsóknir á ári. Stór hluti þessara rannsókna er framkvæmdur á sjálfvirkum efnagreinum. Sjálfvirku efnagreinarnir ráða þó ekki við allar mælingar, og því eru minni einingar innan Rannsóknakjarna sem sinna þeim með sérhæfðum tækjabúnaði.

Innan klínískrar lífefnafræðideildar er starfrækt massagreiningareining (MS-eining), sem hefur vaxið ört á undanförunum árum. Einingin er búin góðum tækjabúnaði, þar á meðal tveimur mjög næmum UPLC-MS/MS tækjum, einu UPLC-UV tæki, einu GC-FID tæki, og nýjasta viðbótin, óuppsett ICP-MS tæki. LC-MS/MS tæknin er í mörgum tilfellum gullstaðall fyrir ákveðnar mælingar eins og sterahormón. MS-einingin framkvæmir fjölbreyttar mælingar á lífsýnum, eins og plasma, sermi, heilblóði og þvagi. Meðal mælinga eru sterahormón eins og 17-hýdroxýprógéstérón og andróstendíón, lífræn amín eins og metanefrín og adrenalín, og joðhexól til að meta gaukulsíunarhraða. Einnig sinnir einingin lyfjameðferðareftirliti fyrir krampalyf eins og lamótrigín og 10-hýdroxýkarbazepín, sveppalyf eins og vorikonazól og ítrakonazól, og geðrofslyf eins og klózapín. Auk þess framkvæmir einingin mælingar vegna gruns um metanóleitrun.

Mikilvægur þáttur í starfi einingarinnar er sýnameðhöndlun lífsýna til undirbúnings fyrir mælingar með fyrrnefndum tækjabúnaði. Meðhöndlun sýna felur meðal annars í sér aðferðir eins og þynningu, próteinfellingu, vökva-vökvaútdrátt eða fastfasaútdrátt, allt eftir því hvaða greiningu á að framkvæma. Hingað til hefur sýnameðhöndlun verið framkvæmd handvirk, en nýlega var keyptur opinn vökvaþjarkur til að auðvelda sýnameðhöndlun og auka rekjanleika sýna.

MS-einingin er í stöðugri þróun og bætir reglulega við nýjum mæliaðferðum. Nýjasta viðbótin, ICP-MS/MS tæki, verður notað til nákvæmra mælinga á snefilefnum í lífsýnum. Auk þess að veita þjónustu fyrir Landspítalann, heilsugæslur og landsbyggðarsjúkrahús, tekur einingin reglulega þátt í rannsóknaverkefnum, bæði innan og utan spítalans.

English summary.

Rannsóknakjarni of Landspítali (National University Hospital of Iceland) hosts both the Clinical Biochemistry and Hematology departments, conducting over 2.6 million tests annually. Most tests are performed using automated analyzers, though specialized equipment is required for certain analyses.

The Clinical Biochemistry department houses a Mass Spectrometry (MS) unit, which has grown significantly in recent years and includes advanced equipment such as UPLC-MS/MS, GC-FID, and ICP-MS. The unit performs a wide range of analyses on biological samples like plasma, serum, blood, and urine, focusing on hormones (e.g., 17-hydroxyprogesterone), organic amines (e.g., adrenaline), and drug monitoring for antiepileptics, antifungals, and antipsychotics. It also handles cases involving suspected methanol poisoning.

Sample preparation, previously done manually, now includes automation with the introduction of a liquid handler. The MS unit continues to implement new methods and participates in research projects both within and outside the hospital.

DINUCLER MOLYBDENUM COMPLEXES AS CATALYSTS FOR SYNTHESIS OF BIOBASED FURANIC POLYESTER MATERIALS (PEF) AND THEIR CHEMICAL RECYCLING

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ABSTRACT

In the last decades, a burgeoning search for sustainable chemicals, polymers, and materials has witnessed the interest in furan-based monomers and polymers due to their potential to replace fossil-based counterparts [1]. Among the most promising bio-based polymers is indisputably poly(ethylene-2,5-furandicarboxylate) (PEF) derived from biomass. However, the use of sustainable approaches for their synthesis is often overlooked, i.e., mild temperatures, negligible use of solvents, safe catalysts, etc. On the other hand, biodegradation of plant-based PEF is slow, and it can lead to environmental accumulation if not adequately managed [2,3]. The presented molybdenum complexes are promising candidates for safe and effective synthesis and chemical recycling of biobased furanic polyester materials.

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P-04

Efnagreiningar á Hafrannsóknastofnun

Egill Antonsson, Ester Inga Eyjólfsdóttir og Kristmann Gíslason

Hafrannsóknastofnun – Rannsókn- og ráðgjafarstofnun hafs og vatna,

Fornubúðum 5, 220 Hafnarfirði

ABSTRACT

Á Hafrannsóknastofnun starfar efnagreiningardeild sem stundar margskonar rannsóknir í efnagreiningum. Í brennidepli starfseminnar standa efnagreiningar, þróun efnagreiningaraðferða og sýnatökur tengdar umhverfinu og atvinnulífi. Meðal efnagreiningaaðferða sem er beitt eru magngreiningar frumefna á borð við þungmálma ýmis konar, flúor, kolefni og köfnunarefni. Jafnframt jónagreiningaraðferðir með “flow injection” uppstillingu og greining blandna með skiljuaðferðum. Sýni sem greind eru koma að miklu leyti úr umhverfinu eða úr atvinnulífinu (frá orkufrekum iðnaði, lagareldi, nýsköpunarfyrirtækjum, landbúnaði og fleira). Í tengslum við umhverfisvaktanir víðs vegar um Ísland eru sýni úr umhverfismiðlunum lofti, ferskvatni, sjó, gróðri og dýrum greind.

Til viðbótar við þjónusturannsóknir fyrir aðila í einka- og opinberum geirum tekur efnagreiningadeild Hafrannsóknastofnunar þátt í grunnrannsóknnum á sviði umhverfis- og iðnaðarefnafræði í samstarfi við innlenda og erlenda háskóla, rannsóknarstofnanir og fyrirtæki. Á veggspjaldinu verða kynntar niðurstöður tveggja nýlegra rannsóknarverkefna. (i) Rannsókn á flúor í beinum grasbíta á Íslandi og (ii) magngreining á örplasti í ferskvatni og hafi á Íslandi.

Supramolecular Gels Based on C_3 -Symmetric Amide for Dye Removal from Water

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ABSTRACT

Supramolecular gels based on low-molecular-weight gelators (LMWGs) are promising candidates for adsorption studies, owing to their porous network structures, high surface area, and stimuli-responsive properties.¹ Several reports on LMWGs with tunable properties rely on amide moieties.² Amide-based compounds generate a 1-D fibril structure by the complementary N–H···O=C interactions, arising from the donor (N–H) and acceptor (C=O) of the amide moieties and these 1-D chains self-assemble to 3-D porous architecture within which the solvent molecules are entrapped.² Supramolecular gels based on C_3 -symmetric amides exhibit versatile gelation properties in a wide range of solvents due to their hydrogen-bonded helical columnar structures that are stabilized by hydrogen bonding and π - π stacking. However, C_3 -symmetric amides have not been widely used for dye removal, presumably due to the lack of suitable porous architectures and poor substrate selectivity.³

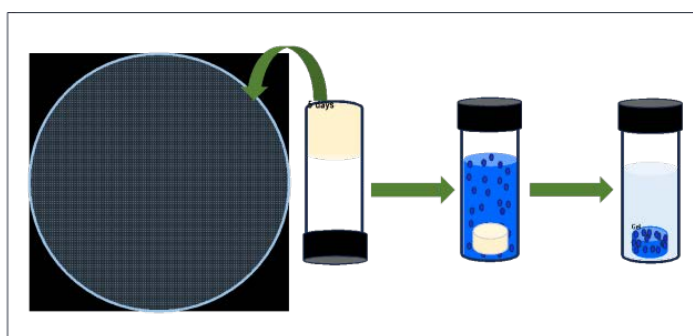


FIGURE 1: Dye adsorption by N-BTA gel

Supramolecular gels based on C_3 -symmetric benzene-1,3,5-*tris*-amide (BTA) can be classified as either C=O centered or N-centered BTA molecules based on their connection to the aromatic platform. In this work, we have modified the C_3 -symmetric N-centered BTA (N-BTA) by introducing flexible linkers (methylene group) between the aromatic core and the amine to explore its ability to act as an adsorbent of hazardous cationic and anionic dyes in water.⁴ We reported that the ethanolic gels of N-BTA successfully adsorbed methylene blue and methyl orange dyes from water (Figure 1).⁴ Adsorption studies using other dyes are currently in progress. This study offers an easy synthetic route for synthesizing N-centered BTA molecules by altering functional groups and evaluates their potential for dye removal from wastewater.

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P-06

Identification of human enzyme inhibitors against cancer glycolysis

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ABSTRACT

Glycolysis is an essential pathway involved in tumor development and progression. In this study, we look for compounds that inhibit the activity of two human glycolytic enzymes: glucose-6-phosphate isomerase (GPI) and triosephosphate isomerase (TPI), both of which are potential targets for cancer glycolysis inhibition. The therapeutic potential of these two enzymes is largely unexplored and warrants further attention. Screening of metabolites, using a combination of activity and binding assays, revealed few novel modulators that weakly inhibit the enzymes' activities via binding to their active sites. Despite being weak, the identified target-ligand interactions might provide new structural insights for the design of human GPI and TPI inhibitors with improved target selectivity.

P-07

DINUCLEAR MOLYBDENUM COMPLEXES AS CATALYSTS FOR SYNTHESIS OF BIOBASED FURANIC POLYESTER MATERIALS (PEF) AND THEIR CHEMICAL RECYCLING

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²CICECO - Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal.

³Centre for Mechanical Engineering, Materials and Processes, Department of Chemical Engineering, University of Coimbra Rua Sílvio Lima – Polo II, 3030-790 Coimbra, Portugal

ABSTRACT

In the last decades, a burgeoning search for sustainable chemicals, polymers, and materials has witnessed the interest in furan-based monomers and polymers due to their potential to replace fossil-based counterparts [1]. Among the most promising bio-based polymers is indisputably poly(ethylene-2,5-furandicarboxylate) (PEF) derived from biomass. However, the use of sustainable approaches for their synthesis is often overlooked, i.e., mild temperatures, negligible use of solvents, safe catalysts, etc. On the other hand, biodegradation of plant-based PEF is slow, and it can lead to environmental accumulation if not adequately managed [2,3]. The presented molybdenum complexes are promising candidates for safe and effective synthesis and chemical recycling of biobased furanic polyester materials.

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Stimuli-Responsive Supramolecular Gels Based on Multi-functional ligands

Sreejith S Jayabhavan, Krishna K Damodaran*

*Department of Chemistry, University of Iceland, Dunhagi 3, Reykjavik, 107, Iceland.***ABSTRACT**

Stimuli-responsive low molecular weight gelators (LMWGs)¹ are excellent class of soft materials where the gelation properties can be switched on/off by an external stimulus such as light, redox, pH and salts/ions.^{2, 3} We have synthesized and characterized metronidazole based carbamates with 3-pyridyl functionality and their corresponding *N*-oxides. Metronidazole, a nitroimidazole antibiotic, is used to treat periodontal disease and shows activity against anaerobic protozoa and bacteria.⁴ Here, we have observed the functional group modification induced hydrogelation by introducing an *N*-oxide functionality in 3-pyridyl carbamate. The addition of salts/ions disrupts the self-assembly of the gelator by altering the non-bonding interactions, which can result constructively by triggering gelation or destructively by gel dissolution.² The analysis of stimuli responsive properties of 3-PCMNox hydrogel with salts revealed that the gel was stable in the presence of various halide salts of potassium, however the gel was broken in presence of potassium cyanide (Figure 1). Cyanide is a highly toxic compound that can cause serious health issues or be lethal even at low concentrations.⁵ We will be performing photophysical studies to understand the mechanism behind breaking of the self-assembly in 3-PCMNox hydrogel.

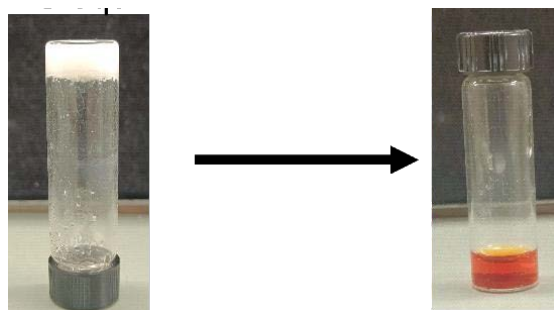


FIGURE 1: Breaking of 3-PCMNox hydrogel in the presence of 1.0 equiv. of potassium cyanide.

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P-09

CO₂ reduction to fuel through surface engineering

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ABSTRACT

Amidst the pressing global challenges of climate change and environmental degradation, the imperative for CO₂ reduction has become more relevant than ever. Developing an efficient catalyst for reducing CO₂ to economically relevant products such as methanol offers environmental benefits and significant economic incentives, as they are essential in various industries, serving roles from chemical synthesis to energy production. In light of these promising opportunities, we are currently screening for a heterogeneous catalyst composed of transition metal dioxide (TMO) that demonstrates the capability to efficiently convert CO₂ into either methanol or formic acid. Building upon insights gleaned from prior publications, 1-5 we have devised a workflow. Our model systems are based on stable bi-metallic transition metal oxides (TMOs) characterized by a stable tetragonal crystal structure (P42/mnm). We particularly focus on the 110 facets as the primary reaction surface. Following the screening process a handful of promising candidates emerge. Leveraging the insights gained from this initial screening, we try to broaden the search space by, for instance, exploring variations in ratios and incorporating additional metals into the mixture. The end goal is to postulate an efficient, stable and cost-effective catalyst. The most promising candidates for our screening are synthesized and tested in collaboration with experimental groups at Grein Research and Johnson Matthey. Their results are integrated into our screening process to reassess our search criteria. Therefore, we aim to present the preliminary results of our joint computational-experimental endeavour.

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P-10

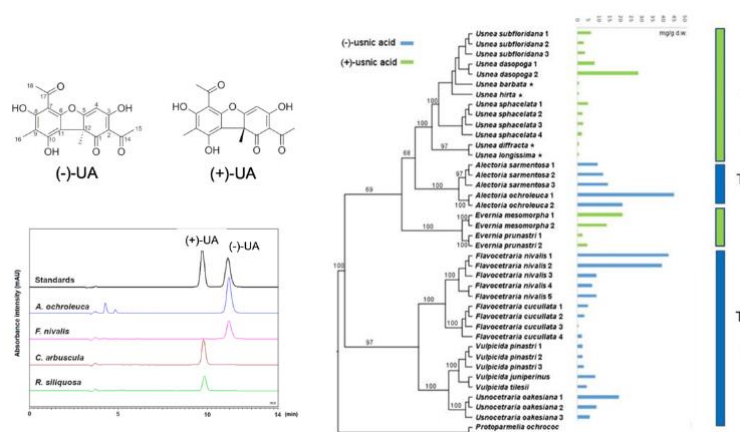
Biochirality of usnic acid enantiomers in lichens

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ABSTRACT

Chiral compounds of natural origins usually occur in one major enantiomeric form. Enantiomers may have drastically different bioactivity and toxicological profiles. Usnic acid (UA) enantiomers in lichens are potentially excellent candidates to study enantiomer biosynthesis [1]. This study aims to characterize the biosynthesis of usnic acid enantiomers in the lichen-forming fungal family Parmeliaceae. Determination of usnic acid enantiomers is performed by a chiral high performance liquid chromatography (HPLC) method [2]. Fungal phylogenetic tree is constructed by concatenating three fungal loci, i.e. nrITS, MCM7 and RPB1. Purified enantiomers are used for antimicrobial assay tests against bacterial and fungal pathogens. Polyketide synthase genes are annotated and their phylogenetic relationship is analyzed. A chiral HPLC method has been developed and validated for quantitative analysis of usnic acid enantiomers. There is a strong phylogenetic pattern for enantiomeric biosynthesis: the cetrarioid clade is producing the (-)-usnic acid, while the parmelioid clade the (+)-usnic acid. Phylogenetic analysis of biosynthetic genes also revealed the same pattern. (+)-usnic acid has stronger antibacterial activity than the (-)-usnic acid, which may explain the herbal selection of (+)-usnic acid-containing lichens. The study revealed the biosynthetic divergence of usnic acid enantiomers in the family Parmeliaceae, and key variations in the biosynthetic genes have been identified. Stronger antibacterial activity of (+)-usnic acid may explain the herbal selection of (+)-usnic acid-containing lichens.



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Non-covalent spin-labeling of RNA through helical stacking

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ABSTRACT

Small double stranded RNAs have been shown by electron paramagnetic resonance (EPR) spectroscopy to exhibit end-to-end helical stacking, due to π - π interactions between the base pairs at the end of the strands, forming a pseudo-continuous helix.^{1,2} Such helical stacking of spin-labeled RNAs may cause complications in the structural analysis of RNA by EPR spectroscopy, since additional distances can be observed.² Here we show how helical stacking can be utilized for non-covalent spin labeling. This involved preparation of a small hairpin RNA into which the rigid nitroxide spin label ζm ³ was incorporated by automated chemical synthesis (**Figure 1A, B**).⁴ The presence of helical stacking between the spin-labeled hairpins was observed by continuous wave (cw) EPR. We will show how this strategy can be used to measure medium to long-range distances in nucleic acids, using RNA duplexes for proof-of-principle experiments (**Figure 1C**). This labeling strategy should also be applicable to more complex RNA molecules that contain blunt-ended duplexes, to study their structure and dynamics by EPR spectroscopy.

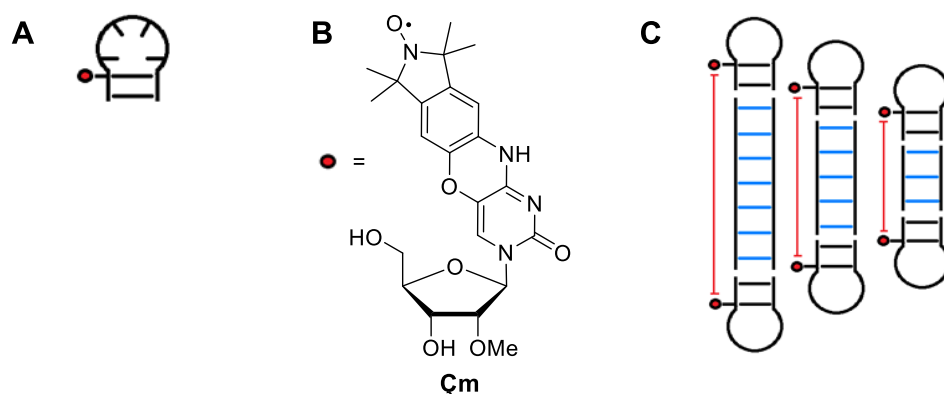


Figure 1. A. Schematic representation of a small RNA hairpin containing the spin label ζm . **B.** Structure of the spin label ζm .³ **C.** Helical stacking of the spin-labeled hairpin on RNA duplexes of different lengths.

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O-10

DNA and nucleosome binding redistribute activation domain ensemble and accessibility in reprogramming factor Sox2

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ABSTRACT

Through their interaction with chromatin, pioneer transcription factors not only initiate gene expression changes essential for development but also serve as key regulators in cellular reprogramming and disease processes. The process by which the pioneer transcription factor Sox2 remodels nucleosomes and its capacity to displace histone H1 remains poorly understood. Similarly, the structural configuration of Sox2's intrinsically disordered regions (IDRs) when engaged with nucleosomes, and the subsequent effects on nucleosome conformation, are not well defined. In an attempt to address these gaps, we employed single molecule Förster Resonance Energy Transfer (smFRET) and Nuclear Magnetic Resonance (NMR) spectroscopy to elucidate the conformations of Sox2 in complex with nucleosomes. We explore its binding modes, the location dependent affinity of binding sites and the resulting structural impacts on the nucleosome itself. Our findings reveal that Sox2's IDR extends significantly upon interaction with the nucleosome, and we identify a specific interaction site within the IDR. Interestingly, Sox2's binding affinity remains consistent, irrespective of the location of the binding site. Moreover, our data not only confirms Sox2's capability to displace linker histone H1, highlighting a critical mechanism in chromatin remodeling, but also positions this activity within the wider context of pioneer transcription factors strategies for chromatin engagement. Identifying an interaction site within Sox2's IDRs marks a step forward in our grasp of pioneer transcription factor mechanism, offering promising leads for development strategies aimed at fine-tuning Sox2's function in cellular reprogramming and oncogenesis.

Notkun gervigreindar í efnafræðikennslu: Reynsla og framtíðarþróun

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Hér er kynnt reynsla af notkun gervigreindar (GG) í efnafræðikennslu og settar fram áætlanir um framtíðarþróun þessara aðferða. Markmið er að meta árangur af notkun GG-studdra kennsluaðferða og leggja grunn að frekari rannsóknum og þróun á þessu sviði.

Aðferðafræði: Yfir rúmlega eins árs tímabil voru prófaðar þrjár megin aðferðir GG-studdrar kennslu: (1) Notkun spjallmenna sem aðstoðarkennara, (2) sjálfvirk endurgjöf á verkefni, og (3) GG-studd hönnun og endurbætur á námsefni. Athuganir byggja á eigin reynslu, óformlegum viðtölum við nemendur og samkennara, og mati á áhrifum á námsferli.

Niðurstöður: Bráðabirgðaniðurstöður benda til aukinnar einstaklingsmiðunar í námi og bættrar endurgjafar til nemenda. Aukinn sveigjanleiki í verkefnagerð og bætt aðlögun að þörfum nemenda með sérþarfir hafa einnig komið fram. Þó hafa einnig komið upp áskoranir, sérstaklega varðandi áreiðanleika mállíkana og íslenskukunnáttu þeirra þegar kemur að sérhæfðu efni á borð við efnafræði. Einnig hefur reynst krefjandi að viðhalda persónulegum tengslum, bæði milli kennara og nemenda og nemenda innbyrðis.

Ályktanir: Þessar athuganir benda til þess að GG geti haft jákvæð áhrif á gæði efnafræðikennslu. Þó er ljóst að þörf er á ítarlegri rannsóknum til að meta langtímaáhrif á námsárangur og gagnrýna hugsun nemenda.

Framtíðarþróun: Byggt á þessari reynslu er ætlunin að þróa sérhæfðar GG-lausnir fyrir efnafræðikennslu, t.d. greiningar- og endurgjafakerfi fyrir verklegar æfingar. Jafnframt verður lögð áhersla á að rannsaka áhrif GG-notkunar á vellíðan nemenda og félagslega þætti námsins. Stefnt er að samstarfi við efnafræðikennara og aðra sérfræðinga til að tryggja sem bestan árangur. Mikilvægir þættir til frekari skoðunar:

1. Námsmat: Nauðsynlegt er að endurhugsa námsmat í ljósi aukinnar notkunar nemenda á GG við úrlausn verkefna. Þróa þarf nýjar aðferðir til að meta raunverulegan skilning og hæfni nemenda í efnafræði.
2. Skipulag kennslu: Endurskoða þarf skipulag kennslu til að tryggja að nemendur séu að tileinka sér grundvallarþekkingu á hugtökum, aðferðafræði og hagnýtingu efnafræði, fremur en að reiða sig eingöngu á GG til að finna lausnir.
3. Undirliggjandi þekking: Áhersla verður lögð á mikilvægi þess að nemendur öðlist djúpan skilning á fræðasviðinu. Slík þekking er forsenda þess að nemendur geti nýtt sér GG á gagnrýninn og uppbyggilegan hátt, frekar en að treysta blindandi á niðurstöður hennar.
4. Þessi þróunarvinna miðar að því að nýta kosti GG í efnafræðikennslu á ábyrgan og árangursríkan hátt, um leið og gætt er að grunnstöðum gagnrýninnar hugsunar og vísindalegrar aðferðafræði.