Update on the REDIAL project, 6 October 2025 (funded by Kidney Research UK)
Visit our webpage: https://suspromgroup.eng.ed.ac.uk/redial

The REDIAL project uses computational techniques, specifically an AI method called Machine Learning, to screen materials which could remove urea, from the dialysate stream, paving the way to a device called the **wearable artificial kidney.**

- **Selection of Materials**: After an initial evaluation, we narrowed the selection to **1,034** suitable Covalent Organic Framework (COFs) materials.
- **Data Preparation for Machine Learning**: To harness machine learning effectively, we needed precise details about each COF's properties. We computed these characteristics using advanced software.
- **Evaluating Material Performance**: Using computer models, we assessed how tightly each COF can bind urea - the tighter the binding, the more effective the material would be for dialysis. These data served as training for our machine learning models, allowing them to predict which COFs are likely to perform best. Figure 1 shows the model performance: the closer are the data points to the dashed line, the better the model performs. The performance was satisfactory.

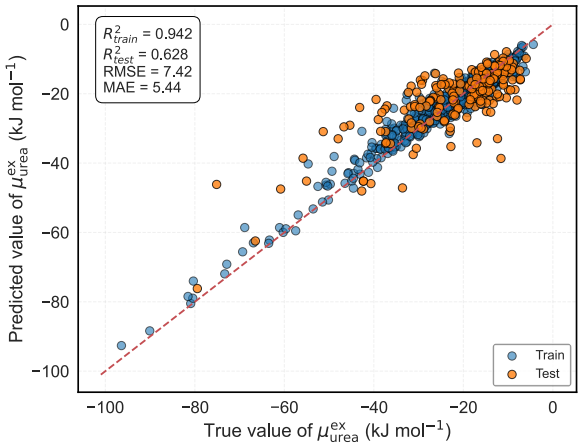


Figure 1: the performance of the Machine Learning model to predict the urea removal performance of 1034 COFs.

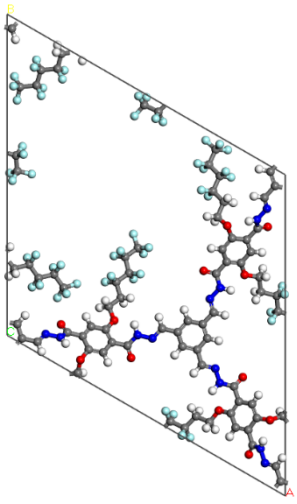


Figure 1: molecular structure of one of the best performing COF materials. See how urea interacts with COF at this video.

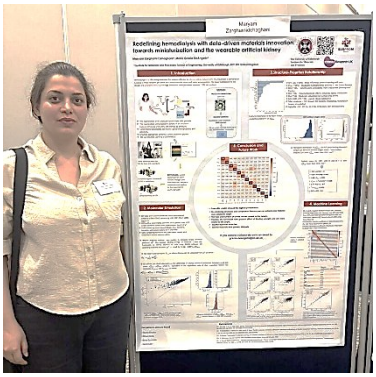
- **Identifying the Most Promising Materials**: The models identified which COFs have the strongest potential for urea capture, to help prioritise which materials should be synthesised and tested. Figure 2 shows one of the candidate materials, which we will start fabricating and testing them in the new project.
- **Establishing Guidelines for New Materials**: One of our main accomplishments this year was determining the specific features that make some COFs more effective at capturing urea. To do that, we have expanded our analysis to a data containing 58,000 hypothetical materials. The best candidates include features such as those identified by the labels linker110 and linker99.
- **Experimental testing**. Thanks to the involvement of **Ievgen Nykytiuk,** a research

assistant specifically hired on this project, and collaboration with the group of dr. Sam Lau that fabricated some COFS, we were able to tests some COF materials and validate our model.

- **Future Directions**: Our next steps involve manufacturing the most promising COFs and validating their effectiveness in practical dialysis scenarios.

Publications and dissemination events

1. *M. Zarghamidehaghani, M.G. De Angelis – "Machine learning-driven computational screening of covalent organic frameworks for gas separation applications," Separation and Purification Journal (2025).* Read the paper here.
2. **In preparation** *"Benchmarking Machine Learning Models for Predicting Urea Adsorption in Covalent Organic Frameworks"* is almost ready for submission.
3. **Annual Report:** The 2nd year report has been submitted on the Kidney Research UK portal.
4. **Edinburgh Kidney PPIE event,** 16 September 2025.



5. **Driving Discoveries conference**, 24-25 September 2025, Bristol, UK. Maryam and Grazia attended with a poster.

Contacts: Grazia De Angelis,
Grazia.deangelis@ed.ac.uk