

Séminaire

Jeudi 7 mai 2026 à 10h00
Amphithéâtre Henri Benoît

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PolyENU: A Program for Enumerating Polymer Constitutional Isomers and Applications to LCST-type Thermoresponsive Polymer Design

Polymer informatics is an emerging field that aims to accelerate the discovery of new functional polymers. However, existing polymer databases (DBs) are largely limited to structures accessible by known polymerization reactions, making the identification of novel polymer structures challenging. In this presentation, we propose a new methodology to construct a virtual polymer DB by enumerating all polymer constitutional isomers for a given molecular formula and set of functional groups in a repeating unit (PolyENU)¹. This approach enables visualization of broad polymer chemical spaces and systematic exploration of new polymers to uncover structure–function correlations. We further apply the PolyENU DB to explore novel LCST-type thermoresponsive polymers in water. Guided by PNIPAM, a representative LCST-type thermoresponsive polymer, the PolyENU DB was constrained using a C₆H₁₁NO unit per amide group to screen for matching constitutional isomers. Among 387 candidates generated by the PolyENU DB, only 34 corresponded to known polymers, leaving a large unexplored chemical space. From this unexplored space, we synthesized 10 novel polymers, five of which exhibited LCST-type thermoresponsive behavior.

1) Usuki, *et al.*, *ChemRxiv*. **2024**, doi:10.26434/chemrxiv-2024-f5fz2 (preprint).

Les personnes souhaitant rencontrer l'orateur sont priées de prendre contact avec Emilie Moulin.