

Universal Chemical Programming Language for Robotic Synthesis Reproducibility

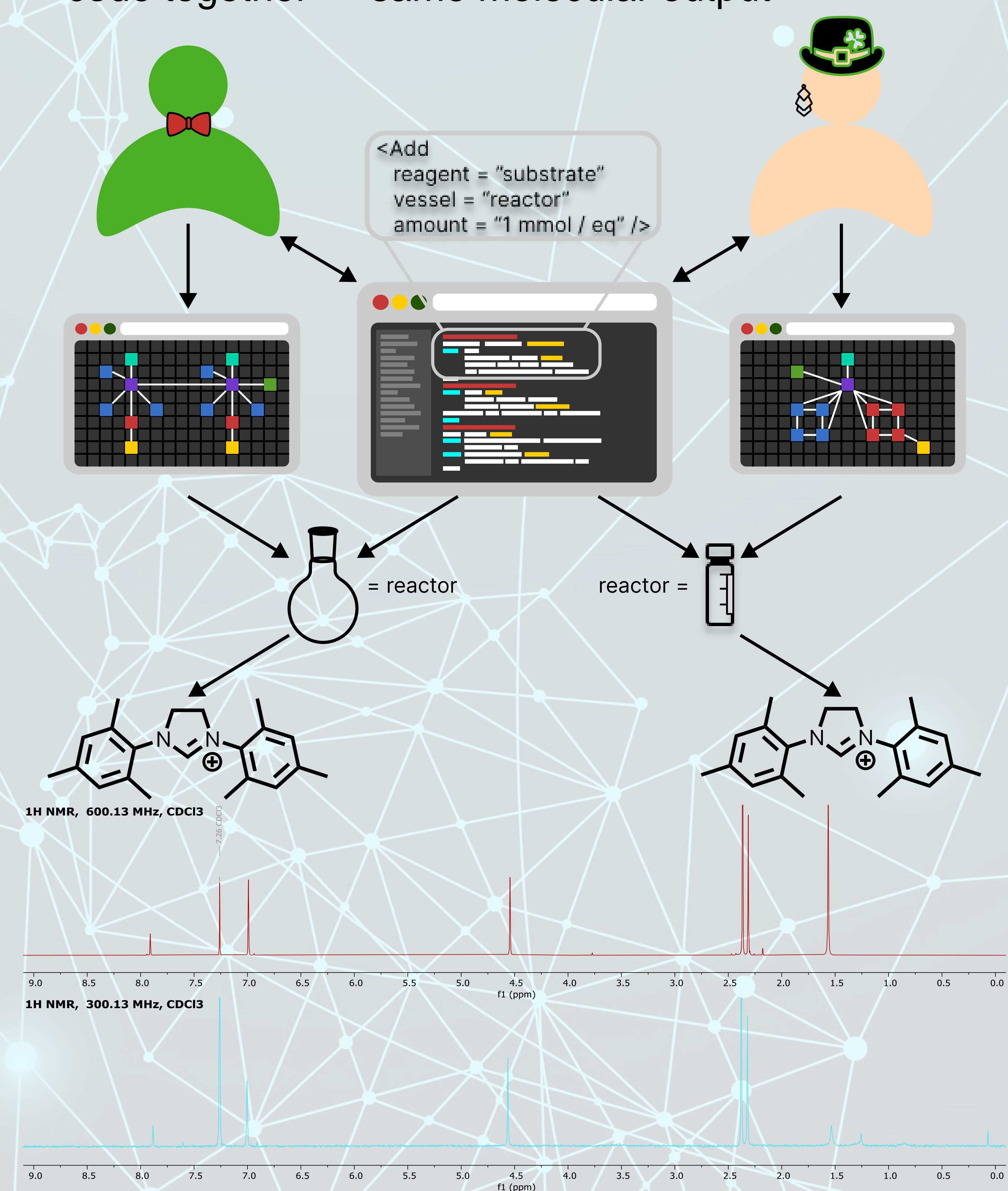
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1 Rationale

- Reproducibility and falsifiability are foundational for modern research
- chemical literature grows exponentially
- Need for new methods to disseminate and validate synthesis protocols

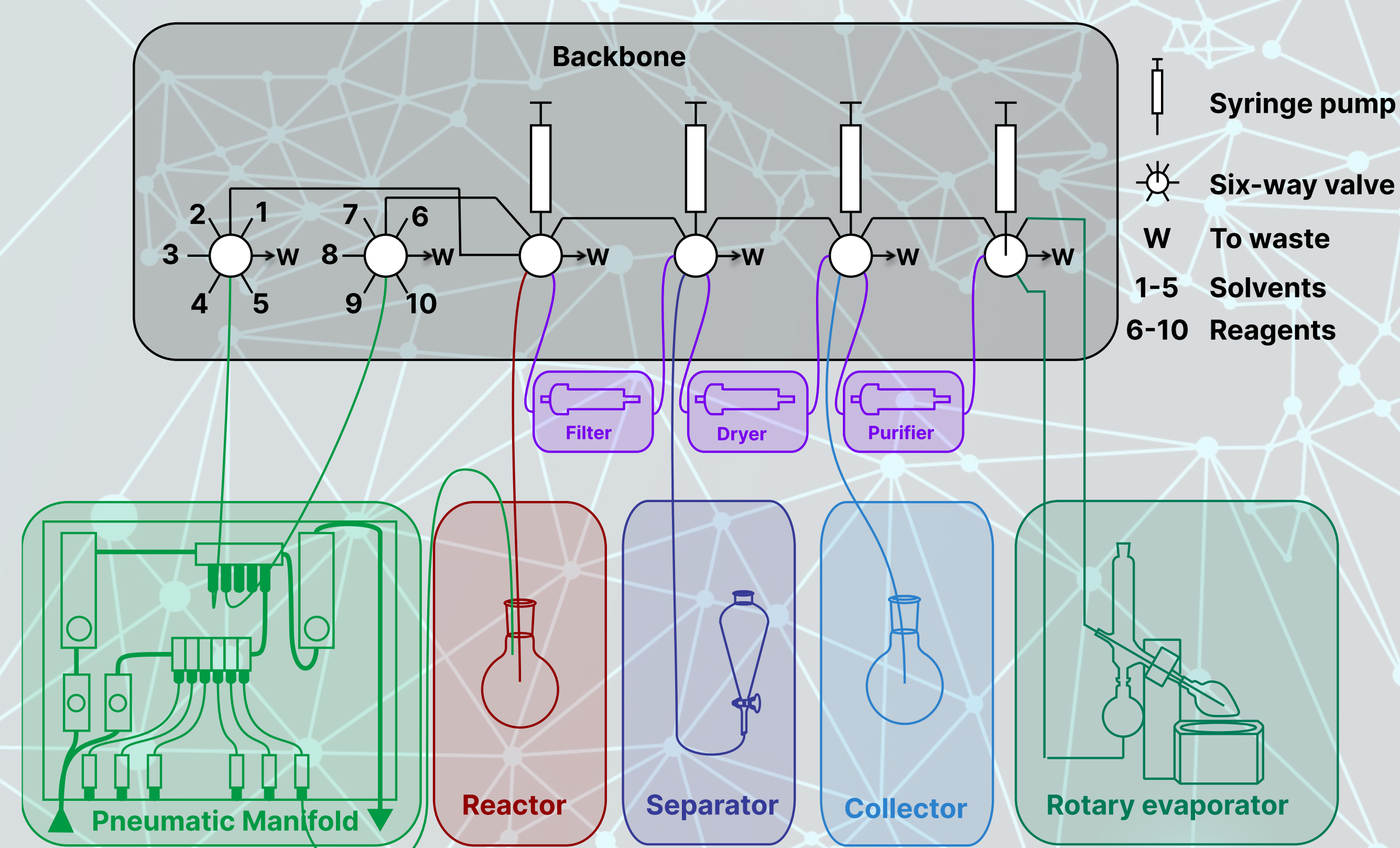
3 Universality of χ DL

- Labs with different hardware capabilities develop χ DL code together → same molecular output



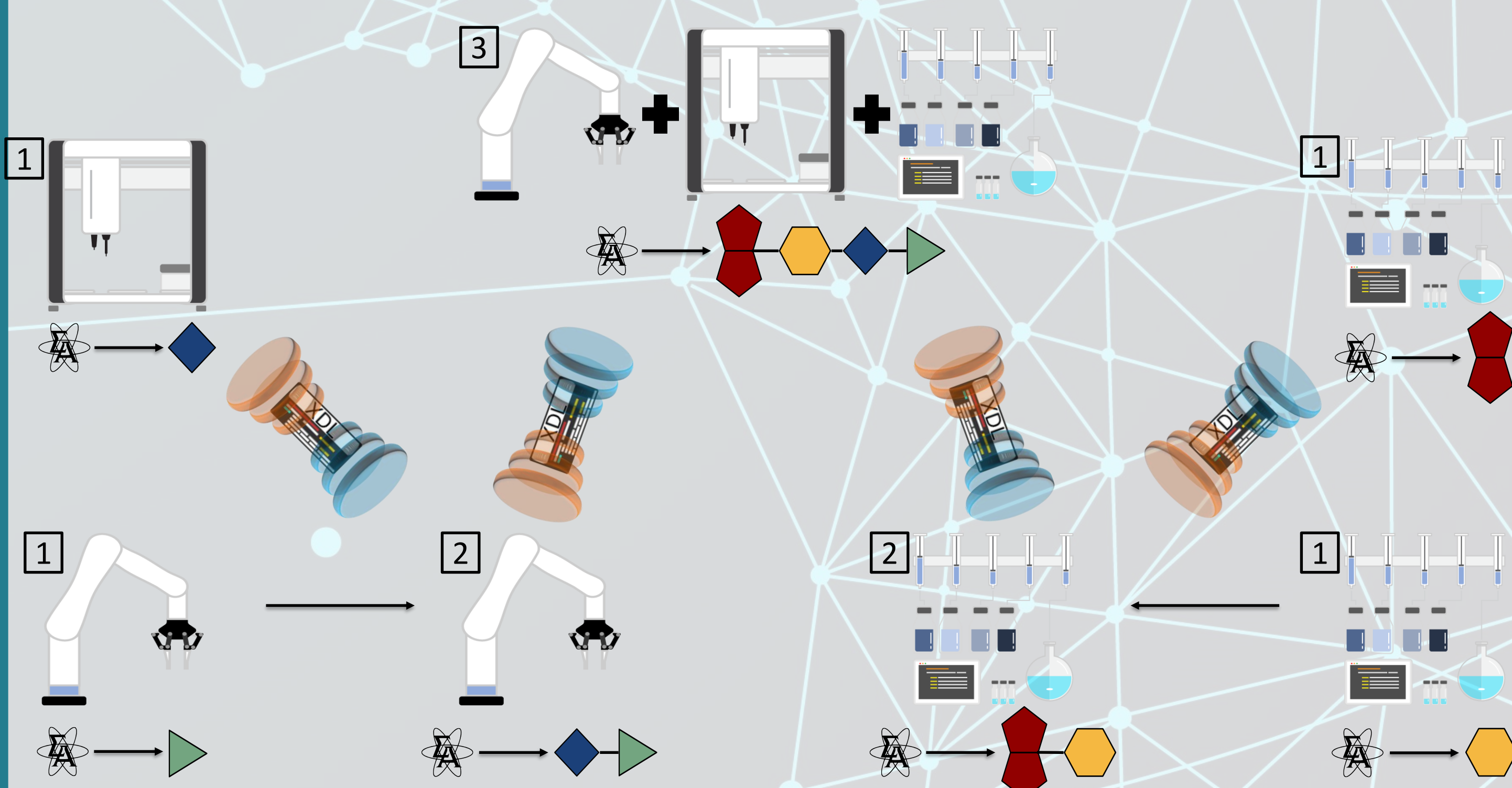
2 The concept of Chemputation

- χ DL (Chemical Description Language) captures chemical knowledge in universally readable format
- Together with a hardware graph chemical unit operations for synthesis can be inferred

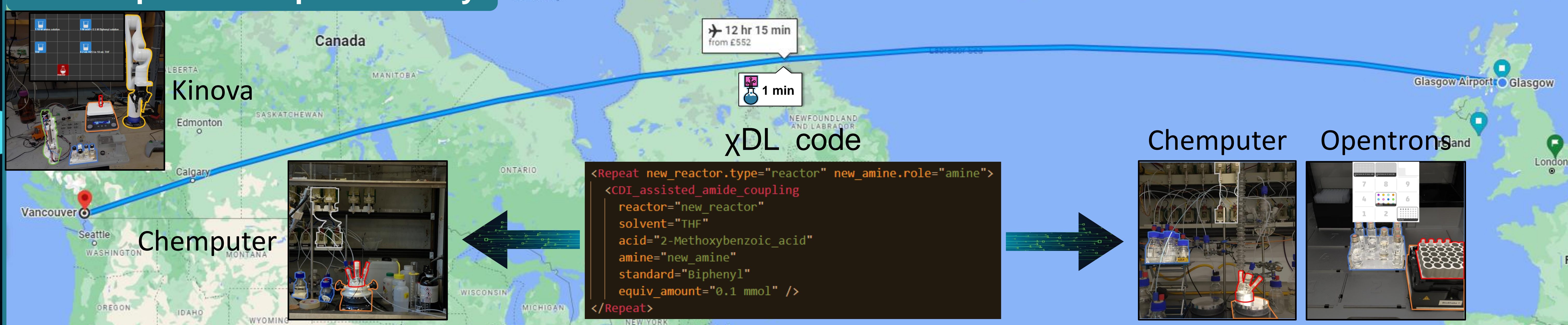


4 Convergent synthesis with ChemTorrents

- Seamless transfers of chemical knowledge with χ DL in collaborative workflows



5 Cross-platform reproducibility



6 Key References

- 1) Mehr et al., *Science*, **2020**, 370, 101–108.
- 2) Malig et al., *ACS Catalysis*, **2020**, 10, 22, 13236–13244.

7 Acknowledgements

