Interactive Knowledge-Based Solvent Selection Tool

Hewan Zewdu, University of Nottingham
pcyhz@nottingham.ac.uk
Supervisors: Jonathan Hirst*, Christopher Handley, Samuel Boobier, Joe Davies, Ivan Derbenev

Skills 4 Scientists

Sponsored by: optibrium, dotmatics knowledge solutions

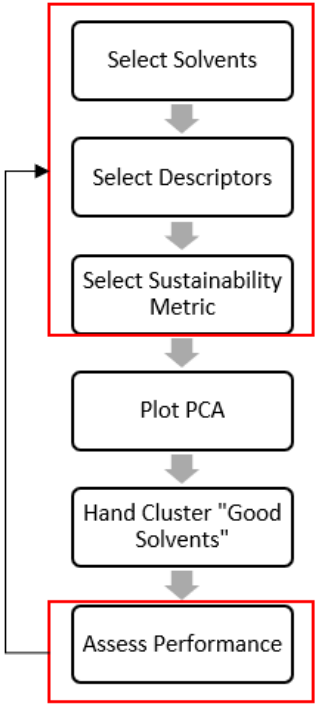
I. Introduction

Solvents are heavily relied upon in chemical processes (~80% of the total volume of chemicals used in several manufacturing processes[1], 70% of pharmaceutical waste[2]), however traditionally used solvents have negative safety, health and environmental (SHE) complications and greener solvents are sought after.

We are developing a solvent selection tool for replacement of such solvents with greener alternatives through similarities in solvent properties and SHE considerations using interactive Principal Component Analysis (PCA).

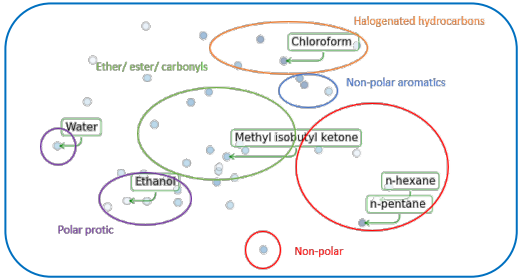
II. Methods

- Compile solvent database, map onto PCA
- PCA: Data analysis method reducing dimensionality while maintaining data variance for eased interpretation of the large solvent database
- Solvents in proximity to one another have similar properties and can act as a suitable replacement

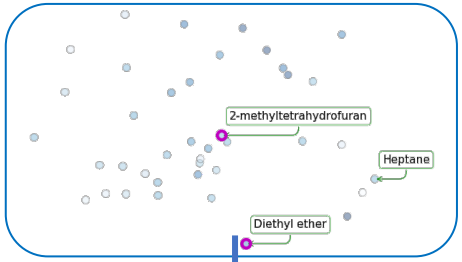


III. Results

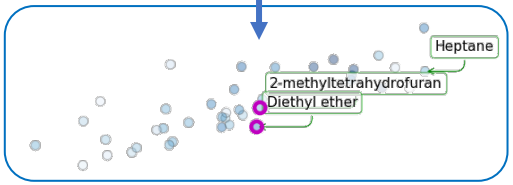
A:



B:



C:



Highlighted points 2Me-THF and diethyl ether moved together from panel B to C, as exchangeable solvents. Other points move relative, altering distribution of PCA map (note change in shape and movement of heptane)

IV. Conclusions

- Accurate description of solvent types on map
- Improve interactive feature
- Repackage to other operating systems
- More modern interface

V. References

1. K. Häckl and W. Kunz, *Comptes Rendus Chimie*, 2018, **21**, 572–580
2. Welton T, *Solvents and Sustainable Chemistry*. Proc. R. Soc. A, 2015 **471**: 20150502

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