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: 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)

B:

C:

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

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