Tamsin Mansley gave this presentation at the ACS National Spring Meeting 2018 in New Orleans.

Abstract

The pharma sector has generated a wealth of experience in cheminformatics methods that are used in the optimisation of small, ‘drug like’ molecules. While there are differences in the chemistries used to develop flavors and fragrances and the optimisation objectives of these projects, many computational methods can be translated from pharma to guide the design and selection of compounds in this context and improve efficiency and productivity. The properties that describe molecules in these fields are typically different, but both disciplines have the goal of quickly targeting compounds with a balance of properties for the project’s objectives.

In the presentation Tamsin discusses approaches to compound selection and design, including chemical space analysis, property prediction and multi-parameter optimisation, comparing and contrasting datasets and models from pharma with those in flavors and fragrances. This is illustrated by case studies to build and apply robust QSAR models predicting relevant properties, design and prioritisation of new compound ideas and analysis of chemical spaces for selection of compounds, using fragrances and flavors datasets.

A copy of Tamsin's slides are available to download here