

Visualising Structured Compound Data in an Unstructured Way

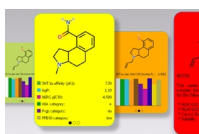
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Abstract

When we view compound data sets, we almost always find ourselves looking at a 'chemical spreadsheet' or a 'form view' of compounds and data in a long list. However, compounds have much more complex relationships that can't be captured in a single, sequential order. We present an alternative view, implemented in the StarDrop™ software [1], in which compound structure and associated data are presented on cards that can be moved and organised freely. This allows chemists to explore their data in a flexible and interactive way and to organise their data based on their perspective and thought processes. Algorithms, such as clustering or matched pair algorithms, can also be applied to organise compounds to draw out interesting patterns or features.



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