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Adaptation of formal concept analysis for the systematic exploration of structure-activity and structure-selectivity relationships

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Formal Concept Analysis (FCA) is a data mining and visualization approach originating from information science. It operates on binary relationships between objects and attributes, which are reported in a formal context. Formal concepts are sets of objects that share a defined subset of attributes. FCA organizes these concepts in lattices that reflect their relationship in terms of shared objects and/or attributes and allows the identification of objects with defined sets of attributes [1].

Two adaptations of FCA that allow the systematic analysis of structure-activity and-selectivity relationships are presented. Fragment Formal Concept Analysis (FragFCA) assesses the distribution of molecular fragment combinations among ligands with closely related biological targets. This allows the identification of fragment signatures that exclusively occur in compounds with a defined activity profile. FragFCA also identifies fragment combinations that are characteristic of highly potent compounds against defined targets. Fragment signatures usually represent combinations of two or three fragments and can be used to differentiate active compounds of closely related targets for different target families [2,3].

Molecular Formal Concept Analysis (MolFCA) is introduced for the systematic comparison of the selectivity of a compound against multiple targets and the extraction of compounds with complex selectivity profiles from biologically annotated databases. Selectivity is assessed based on pair-wise compound potency ratios. This allows the definition multiple selectivity queries involving the comparison of an arbitrary number of targets and compound potency values or ratios. The individual queries are applied in a sequential manner to retrieve compounds with desired selectivity against targets of interest. MolFCA operates on activity space representations of compounds and thus allows the identification of structurally diverse compounds matching a given selectivity profile [4].

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References

1. Priss U: *Ann Rev Inf Sci Technol* 2006, **40**:521.
2. Lounkine E, Auer J, Bajorath J: *J Med Chem* 2008, **51**:5342.
3. Krüger F, Lounkine E, Bajorath J: *Chem Med Chem* 2009, **4**:1174.
4. Lounkine E, Stumpfe D, Bajorath J: *J Chem Inf Model* 2009, **49**:1359.

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