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Analysis of structure-selectivity relationships through single- or dual step selectivity searching using 2D molecular fingerprints

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The identification of small molecules displaying different selectivity patterns against a protein target is a prerequisite to interfere with functions of individual members of protein families [1]. For computational methods it is more difficult to study selectivity than activity because selectivity analysis requires the evaluation of compounds binding to multiple targets [2].

We aim at the development of computational approaches for the study of structure-selectivity relationships and prediction of target-selective ligands. Therefore, we have designed 18 selectivity sets containing target-selective molecules and compounds that are comparably active against related targets (and thus non-selective). This compound collection of a total of 432 compounds focuses on eight targets belonging to four protein families and has enabled us to evaluate different *in silico* approaches to search for target-selective compounds [3].

The results further support previous findings that even low-complexity structure-based 2D fingerprints are capable of identifying compounds having different selectivity against closely related target proteins and revealed a preferred search strategy to enrich database selection sets with target-selective compounds [4][5].

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