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Random molecular substructures as fragment-type descriptors

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A novel approach for analysis of structure-activity relationships for sets of active compounds is reported. Molecular similarity relationships are analyzed among compounds with related biological activity based on the evaluation of randomly generated fragment populations. Fragments are randomly generated by iterative bond deletion in molecular graphs and hence depart from those obtained by well-defined fragmentation schemes [1]. A major finding has been that for any given activity class, dependency relationships of fragment co-occurrence exists within random fragment populations. Through the analysis of these relationships the chemical information content of generated substructures can be quantified [2]. This has lead to the identification of small numbers (10- 40) of so-called activity class characteristic substructures (ACCS) that have been successfully utilized in virtual screening applications [3,4].

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