The Development of a Knowledge Base for Basic Active Structures: An Example Case of Dopamine Agonists

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Chemical compounds affecting a bioactivity can usually be classified into several groups, each of which shares characteristic substructure. We call these substructures “basic active structures”or BASs. The extraction of BASs is challenging when the database of compounds contains a variety of skeletons. Data mining technology, associated with the work of chemists, has enabled the systematic elaboration of BASs. This paper presents a BAS knowledge base, BASiC, which currently covers about 35 activities and is useful for drug design and the recognition of adverse effects. We use dopamine agonists (D1, D2 and Dauto) as an example, and illustrate the process of BAS extraction. The resulting BASs are interpreted after proposing a few template structures.