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

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Background: Chemical compounds affecting a bioactivity can usually be classified into several groups, each of which shares a characteristic substructure. We call these substructures “basic active structure” 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.

Results: This paper presents a BAS knowledge base, BASiC, which currently covers 46 activities and is available on the Internet. We use the dopamine agonists D1, D2, and Dauto as examples and illustrate the process of BAS extraction. The resulting BASs were reasonably interpreted after proposing a few template structures.

Conclusions: The knowledge base is useful for drug design. Proposed BASs and their supporting structures in the knowledge base will facilitate the development of new template structures for other activities, and will be useful in the design of new lead compounds via reasonable interpretations of active structures.