

KP19

Software tool for chemical structure data mining based on non-terminal vertex graph

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In the preceding work, the authors reported a basic skeletal feature representation of molecules with a graph called Non-Terminal vertex Graph (NTG) that has no vertices of degree of 1. In the present work a software tool for NTG-based structure data mining for chemical compounds was developed, and it was applied to chemical structure data mining of drug molecules that belong to ten different activity classes. The results suggest that the NTG-based structure data analysis would be effective as an approach to chemical data mining and knowledge discovery in structure-activity relations of the drugs.