

化合物の線形フラグメントに基づいた特徴的リード構造抽出システムの開発

Development of Characteristics Lead Structure Extraction System based on Linear Fragment of Compounds

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Rules derived by the cascade model could give useful insights for characteristic features affecting the pharmaceutical activity. But the extraction and the synthesis of characteristic feature were performed by the hand of an expert and it took too long to reach the final characteristic structure. The characteristics lead structure extraction system based on linear fragments of compounds has been developed to solve this problem. The system has shown its usefulness in the refinement from the seeds found in the rule to the expert level knowledge. The details of the system will be discussed with illustrative examples.