

ヘテロ原子に注目したパスフラグメントによる化学構造データマイニング

Chemical Structure Data Mining using Path Fragments with Terminal hetero Atoms

藤島悟志、高橋由雅、岡田孝

Satoshi Fujishima, Yoshimasa Takahashi, and Takashi Okada

In structure data mining of chemicals, many of the method mine and use linear fragments from their chemical structure as knowledge on their structure-activity relationships. However, in most cases, many trivial fragments that are removed in the mining process are mined and examined for the efficiency. Then, the extraction and the synthesis of characteristic feature, which described in the rules derived by a mining method, are performed by the hand of an expert and it took too long to reach the final characteristic structure. In the present work, we propose a new approach to structure data mining of chemicals using path fragments that both of their terminal atoms are hetero atoms. It also allows us to do rational refinement of the seed (a fragment) according to the same restriction when the fragment is extended. The approach has been computerized and tested. The details of the system will be discussed with illustrative examples.