A Tool for Molecular Similarity Networks

Chunfei Huang (黄 春飛), Zsolt Lepp, Takashi Okada (岡田 孝)

In this paper, we introduced a tool for molecular similarity networks. With this tool user can create a molecular similarity network from an SDfile, and can view graphical molecule structures on the network and some of chemical properties about molecules. It is implemented in Java using Cytoscape and JChem libraries. It is a useful tool for chemical analysis of molecular similarity networks.