



生物信息学研究中心

Center of Bioinformatics

学术报告

题目： Application of Self-Organizing Map to Structure-Odour Relationships

报告人： Prof. Shin-ya Takane

Department of Information Systems Engineering
Osaka Sangyo University, Japan

时间： 8月11日（星期六）上午10:30

地点： 思源楼1013室

摘要： We have previously studied structure-odour relationship analyses using hierarchical clustering on a diverse dataset of 47 molecules. These molecules were divided into seven odour categories: ambergris, bitter almond, camphoraceous, rose, jasmine, muguet, and musk. We used the alignment-independent QSAR descriptor EVA and compared with those of another kind of descriptor, UNITY 2D fingerprint. The dendrograms produced by EVA consistently outperformed those from UNITY 2D in reproducing the experimental odour classifications of these 47 molecules. In this study, we used the Kohonen's self-organizing map (SOM) neural network to classify the same dataset. It is also unsupervised learning method. Unlike hierarchical clustering techniques, however, SOM can find useful clusters / segmentations intuitively, remaking visually understandable maps. The result of the classification of the dataset (47 molecules) is in good agreement with the previous hierarchical clustering study. We also carried out other dataset composed of only nitro and / or macro musks.