

Identification of Dopamine D1 Receptor Agonists and Antagonists under Existing Noise Compounds by TFS-based ANN and SVM

Yoshimasa Takahashi, Satoshi Fujishima, Katsumi Nishikoori, Hiroaki Kato, and
Takashi Okada

Abstract: This paper describes classification and prediction for pharmacologically active classes of drugs under the presence of noise chemical compounds. Dopamine D1 receptor agonists (63 compounds), antagonists (169 compounds) and other drugs (696 compounds) were used for the works. Each drugs molecule was characterized with Topological Fragment Spectra (TFS) reported by the authors. TFS-based artificial neural network (TFS/ANN) and support vector machine (TFS/SVM) were employed and evaluated for their classification and prediction abilities. It was concluded that the TFS/SVM works better than TFS/ANN in both the training and the prediction.