

Extended Study of the Classification of Dopamine Receptor Agonists and Antagonists using a TFS-based Support Vector machine

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We previously investigated the classification and prediction of dopamine D1 receptor agonists and antagonists using a topological fragment spectra (TFS)-based support vector machine (SVM), in which the dataset contained noise compounds that had no D1 receptor activity. This work extended the dataset to seven activity classes (dopamine D1, D2, and auto-receptor agonists, and D1, D2, D3, and D4 antagonists) and increased the noise ratio to ten times that of active compounds. In total, this study used 16,008 compounds for training and 1,779 compounds for prediction. The TFS-based SVM gave good, stable results for both classification and prediction, even in the case that included ten times the noise data. The resulting model correctly predicted 97.6% of the prediction set of 1,779 compounds.

Keywords Pattern Classification, Topological Fragment Spectra, Support Vector Machine, Dopamine Agonists, Dopamine antagonists.