P25 - Predictive Modeling of Natural Medicinal Compounds for Alzheimer's Disease Using Cheminformatics

2. MT vetenskap
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Abstract text*: Alzheimer's Disease (AD) is a neurodegenerative disorder with limited therapeutic options that are often accompanied by severe side effects. In the pursuit of safer and more accessible alternatives, this study aims to identify natural compounds with potential anti-Alzheimer's activity using cheminformatics based study. The purpose of this study is to develop a predictive model that can efficiently screen natural compounds for their therapeutic relevance to AD.

To achieve this, over 7000 compounds were collected from public natural compound databases including ChEBI, SynSysNet, and INDOFINE. Molecular descriptors for these compounds were calculated using Dragon software and pre-processed with Open Babel. A Random Forest classification model was developed in Statistica to distinguish active vs. inactive compounds based on existing FDA-approved treatments. The model was trained and validated using a dataset of known active and inactive compounds.

Our model predicted 73 compounds with potential therapeutic relevance to AD, showing notable structural similarities and high classification confidence scores. The most important molecular descriptors included atomic polarizability, bond multiplicity, and non-H bond counts. Precision and recall metrics ranged from 59–70% and 65–90%, respectively, indicating robust model performance. The main results demonstrate that the model can effectively identify compounds with potential anti-Alzheimer's activity, providing a valuable tool for early-stage drug discovery.

In conclusion, this study presents a promising cheminformatics-based workflow for the identification of natural compounds with potential therapeutic effects against AD. The findings highlight the potential of using cheminformatics in drug discovery, offering a safer and more accessible approach to developing treatments for Alzheimer's Disease.