In Silico Profiling of Physicochemical and ADMET Properties of Boron Compounds

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Boron-containing compounds constitute a diverse chemical group with a wide range of structures and properties. While medicinal chemistry has traditionally focused on standard carbon-based compounds, interest in boron-containing compounds has grown in recent decades due to their emerging therapeutic potential [1]. Certain classes of boron containing compounds have been gaining more attention as potential drugs [1, 2]. As persistent health challenges demand broader chemical exploration, diversifying the scope of investigated compounds is essential [1].

In the presented research study, various organoboron derivatives from classes recognized in literature for their medical potential, were compared mutually and with known drugs, based on predicted physicochemical and ADMET properties in order to assess their drug-likeness [2]. Data was collected from the open-access databases DrugBank and PubChem. Molecules were represented by physicochemical descriptors estimated by SimulationsPlus and DataWarrior software and structural fingerprints calculated using RDKit. Descriptor selection was performed through multiple analyses and keeping only features most relevant for characterization of (physico)chemical space of organoborons. Additionally, molecules were analyzed using criteria from Lipinski's Rule of Five and Veber's rule.

Compound comparison was performed using unsupervised machine learning methods, including Principal Component Analysis (PCA), t – distributed Stochastic Neighbor Embedding (t – SNE) and Uniform Manifold Approximation and Projection (UMAP). These methods are useful tools for visualizing high-dimensional spaces. Additionally, other methods of data analysis and visualization were also used in order to illustrate variations in key descriptors across compound classes.

References:

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