Digital Total - Computing & Data Science an der Universität Hamburg und in der Wissenschaftsmetropole Hamburg



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Calculating More Property Distributions of Chemical Fragment Spaces

In the early stages of drug discovery projects, it is a common task to search digital molecule collections to find promising lead structures that serve as a starting point for developing new drugs. Recently developed combinatorial compound catalogs are orders of magnitude larger than traditional databases, promising higher potential for finding relevant lead structures. Many cheminformatics tasks require new algorithms dealing with these chemical fragment spaces as traditional methods are incompatible. Here, we address the problem of calculating property distributions in the form of histograms for entire catalogs.

For this purpose, Bellmann et al. developed the SpaceProp algorithm. We introduce SpaceProp2, an extension of SpaceProp that supports further molecular properties, namely the TPSA, rotatable bond counts, and SMARTS patterns.

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Autor: LÜBBERS, Justin

Co-Autoren: Dr. BELLMANN, Louis; Prof. RAREY, Matthias; Dr. LESSEL, Uta