

[P3] Cluster Analysis of the NRLiSt BDB using ACPC

Francois BERENGER^{1,2}

¹*Antique team, INRIA/ENS/CNRS/PSL*, 45 rue d'Ulm, 75230, Paris, France.*

²*Laboratoire GBA, CNAM, 292 rue St Martin, 75003, Paris, France.*

In this poster, we will show clustering analysis results of the Manually Curated Nuclear Receptors Ligands and Structures Benchmarking Database (NRLiSt BDB in short).

The novelty of this work is that we will use the AutoCorrelation of Partial Charges molecular descriptor (and corresponding open source software ACPC) in order to encode and compare molecules.

Bibliography:

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