[P6] Perception of 3D-Molecular Shape and Pharmacophores from 2D-Structures Using Atom Pair Fingerprints

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3D-molecular shape and pharmacophores are important determinants of the biological activity of organic molecules, however a precise computation of 3D-shape is generally too slow for virtual screening of very large databases. A reinvestigation of the concept of atom pairs initially reported by Carhart et al[1]. And extended by Schneider et al[2]. showed that a simple atom pair fingerprint (APfp) counting atom pairs at increasing topological distances in 2D-structures without atom property assignment correlates with various representations of molecular shape extracted from the 3D-structures. A related 55-dimensional atom pair fingerprint extended with atom properties (Xfp) provided an efficient pharmacophore fingerprint with good performance for ligand-based virtual screening and overlap with the 3D-pharmacophore scoring function ROCS. The Xfp data is compact and enables preorganization of large databases for web-based extremely fast searching as enabled for ZINC and GDB-17 (free access at www.gdb.unibe.ch).

[1] Carhart, R. E.; Smith, D. H.; Venkataraghavan, R. 25 (1985) 64-73.
[2] Schneider, G.; Neidhart, W.; Giller, T.; Schmid, G. 38 (1999) 2894-2896.
[3] Ruddigkeit, L.; Blum, L. C.; Reymond, J. L. 53 (2013), 56-65.