B3Info – An information system for molecular Blood-Brain Barrier penetration data

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This work is aimed to present an ongoing work for building an information system for storage, search and retrieval of chemical molecules as related to their permeation properties to the Blood Brain Barrier (B3Info). The initial molecular information came from the published literature and was curated manually. Either simple information mentioning whether a molecule is known to cross the barrier, as well as quantitative permeation information, expressed as the *LogBB*, is provided when available. The database not only stores the chemical data but also the published references from where the data originated, as well as links to other chemical repositories on the web as the DrugBank, NCBI's PubChem or ChemSpider for each molecule. The system further links to the b3pp model [1] for inferring blood brain barrier penetration for any molecule. Presently this database contains data for over 1900 molecules. B3Into provides full web access to the database, allowing extensive searching capabilities. These include searching molecules according to their common name or their structural representation in the form of SMILES or InChI identifiers. It is further possible to search molecules using similarity queries, thus retrieving molecules that share similar structures, and also allowing for strict sub-structural searches. B3Info further provides an interface for drawing a graphical representation of any molecule and search for similar structures. B3info is open and free to use and the full molecular database can be downloaded.

B3Info web site: http://b3info.lasige.di.fc.ul.pt

[1] I. F. Martins, A. L. Teixeira, L. Pinheiro, A. O. Falcao, *J. Chem. Inf. Model.* **2012**, *52*, 1686-1697.

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