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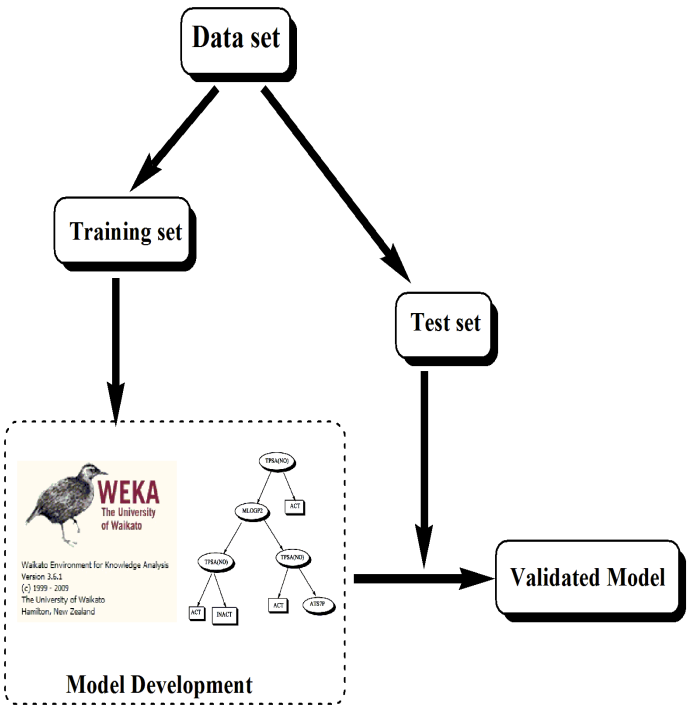
Blood-Brain Barrier Passage Prediction Using Decision Tree

Juan A. Castillo-Garit (jacgarit@yahoo.es)[a], Gerardo M. Casañola-Martin (gmaikelc@gmail.com)[b,c], Huong Le-Thi-Thu (ltthuong1017@gmail.com)[d], Hai Pham-The (hpham.phd@gmail.com)[c] and Stephen J. Barigye (sjbarigye@yahoo.com)[e]

[a]*Unidad de Toxicología Experimental, Universidad de Ciencias Médicas, Santa Clara, 50200, Villa Clara, Cuba.*
[b]*Unidad de Investigación de Diseño de Fármacos y Conectividad Molecular, Departamento de Química Física, Facultad de Farmacia, Universitat de València, Spain.*
[c]*Hanoi University of Pharmacy, 13-15 Le Thanh Tong, Hoan Kiem, Hanoi, Viet-nam.*
[d]*School of Medicine and Pharmacy, Vietnam National University, Hanoi (VNU) 144 Xuan Thuy, Cau Giay, Hanoi, Viet-nam.*
[e]*Department of Chemistry, McGill University, 801 Sherbrooke St. W., Montréal, Québec, Canada H3A*

Graphical Abstract



Abstract.

In this report, the blood brain barrier (BBB) permeability prediction is carried out using a decision tree. A recently published data set of 497 compounds is selected to develop the tree model. The developed model shows an accuracy of 87.66% for training set; 86.09% in the 10-fold cross-validation procedure and 87.93% for the test set. Some structural explanation of how our model describes the passage of molecules through the BBB is given. Moreover, a comparison with other approaches is carried out showing good behaviour of our method. Finally, we can say that, the present results could represent a useful tool available and reproducible by all scientific community in the early stages of neuropharmaceutical drug discovery/development projects. (*Full content can be seen in Ref 9*).

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