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Predicting Compound-Protein Interactions in GPCR Network

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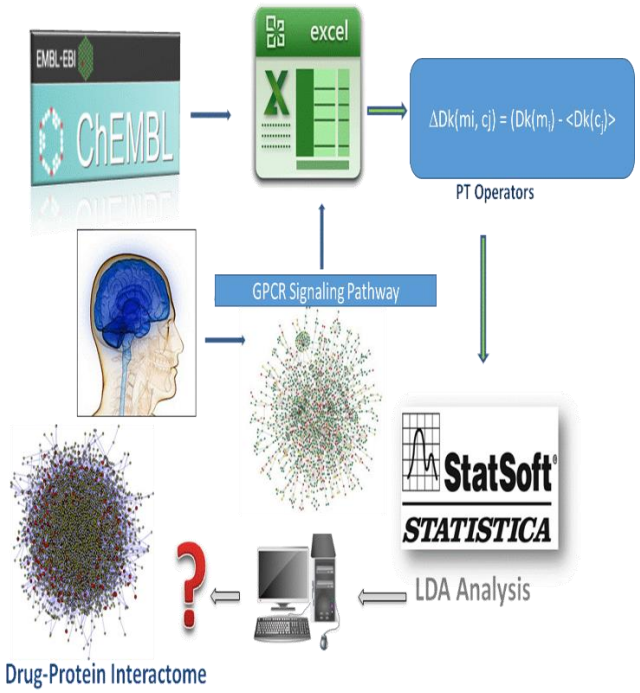
Graphical Abstract



Abstract.

We can combine Perturbation Theory (PT) and Machine Learning (ML) model to seek PTML models useful to explore the effect over drug activity of changes or (perturbations) in multiple parameters or experimental conditions c_j. This include changes in drug chemical structure or assay conditions like c_0 = the biological parameter used (K_i, IC_{50}, *etc*.), c_1 = drug target, c_2 = organism of assay, c_3 = cell line, *etc*. In this work used PTML techniques to explore the Big Data set of >800000 preclinical assays of drugs. These assays reported in CheMBL involved drugs targeting proteins related to G-protein signaling pathways. The data set included 343,738 drugs, 185 experimental parameters, 56 organisms of assay, 52 cellular lines, 592 target proteins. The model predicted correctly 85.4% of control cases (Specificity) and 95.8% of active compounds in training series (Sensitivity). The model also predicted correctly 95.8% and 85.4% cases in external validation series.

References

Martínez-Arzate SG, Tenorio-Borroto E, Barbabosa Pliego A, Díaz-Albiter HM, Vázquez-Chagoyán JC, González-Díaz H. PTML Model for Proteome Mining of B-Cell Epitopes and Theoretical-Experimental Study of Bm86 Protein Sequences from Colima, Mexico. *J Proteome Res*. **2017**; 16(11):4093-4103.