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Article

Comparison of ThreeÃƒÂ¢Ã‚€Ã‚•Dimensional LigandÃƒÂ¢Ã‚€Ã‚•based Pharmacophores among 11 Phosphodiesterases (PDE 1 to PDE 11) Pharmacophores

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Abstract

Phosphodiesterases (PDEs) are major regulators of cyclic nucleotide signaling with a variety of pharmacological functions. Currently, more than 30 drugs targeting PDEs are on the market, and many drug candidates are under development. In this study, we generated threeÃƒÂ¢Ã‚Â€Ã‚Â•dimensional ligandÃƒÂ¢Ã‚Â€Ã‚Â•based pharmacophores (3DÃƒÂ¢Ã‚Â€Ã‚Â•LBPs) of PDE1 to PDE11 using the ligands of each PDE obtained from BindingDB to identify critical chemical features of novel potential PDE inhibitors and the accuracy of each model was evaluated by cost difference, test set prediction, and Fischer's randomization test. Among 10 generated pharmacophore hypotheses, Hypo1 was selected as the best hypothesis. Hypo1 hypothesis with the highest predictability of each PDE, have correlation coefficients larger than 0.9 and cost differences larger than 40. Since the generated pharmacophores were validated with four ways, cost analysis, Fischer randomization test, the test set prediction, and ligand profiling and got high predictability for all the 11 PDEs; the results in this study will be used to develop novel inhibitors of 11 PDEs that are highly selective for its subtypes.

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