Special Report

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Innovative computer-aided methods for the discovery of new kinase ligands

Recent evidence points to significant roles played by protein kinases in cell signaling and cellular proliferation. Faulty protein kinases are involved in cancer, diabetes and chronic inflammation. Efforts are continuously carried out to discover new inhibitors for selected protein kinases. In this review, we discuss two new computer-aided methodologies we developed to mine virtual databases for new bioactive compounds. One method is ligand-based exploration of the pharmacophoric space of inhibitors of any particular biotarget followed by quantitative structure–activity relationship based selection of the best pharmacophore(s). The second approach is structure-based assuming that potent ligands come into contact with binding site spots distinct from those contacted by weakly potent ligands. Both approaches yield pharmacophores useful as 3D search queries for the discovery of new bioactive (kinase) inhibitors.

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