Quantitatively structure-activity relationships on cyclin-dependent kinase 2 inhibitors

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Cyclin-dependent kinase 2 (CDK2) plays an important role in cell cycle arrest. CDK2 inhibitors function as a ligand of the apoptosis induction by cell cycle arrest. To search CDK2 inhibitors efficiently, quantitively structure-activity relationships (QSAR) are available. 41 ligand compounds were used for training set and the activity data were obtained from the binding assay[1)]. The QSAR equation of the results was obtained with the molecular field analysis (MFA). In order to find candidates showing high CDK2 binding affinity, 13 peptides were tested. We calculated their predicted activities by MFA equation. The predicted activity data were compared with experimental data tested as apoptotic inducer in the cancer cells.

Reference

1. H. Neal Bramson, John Corona, Oxindole-Based Inhibitors of Cyclin-Dependent Kinase 2 (CDK2): Design, Synthesis, Enzymatic Activities, and X-ray Crystallographic Analysis (2001). J. Med. Chem. 44(25), 4339-4358.