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Automated drug design of kinase inhibitors to treat chronic myeloid leukemia

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Medicinal chemistry has in the past been dominated by learned insights from experienced organic chemists. However, with the advent of computer based methods, computer aided drug design has become prominent. We have compared here the ability of expert chemists to purely automated methods and found that the automated method produces a better potential candidate drug than the expert input. The example chosen is based on inhibitors to Abl-kinase and the successful anti-leukaemic drug imatinib. The proposed molecule is a simple modification of nilotinib which has a docking energy of 4.2 kJ/mol better than the best intuitive molecule.

Biography

Aramice Y S Malkhasian completed PhD at Concordia University 1985. He was a Research Scientist at McGill. with M. A. Whitehead at 1995, at 2003 and 2004 work with Prof Michael Sevillaand Prof. Ferman Chaves at Oakland university. Currently professor at King Abdulaziz University

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