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Computer analysis of structure-activity relationships of the compounds of diterpenoid nature

Davronov R R
National University of Uzbekistan, Uzbekistan

Diterpenoid alkaloids (DA) of different structural types, isolated from plant of the genus *Aconitum, Delphinium* and *Consolida*, - the most suitable candidates to find among them substance with antispasmodic action. We investigated spasmogenic activity of 82 compounds. C_{19} and C_{18} diterpenoid alkaloids have been investigated including types of aconitine, likoktonin, lappaconitin, lactone-containing alkaloids geteratizin type, C_{20} diterpenoid alkaloids napellin and denudatin types with their derivatives. Antispasmodic or spasmogenic effect of compounds studied *in vitro* experiments on isolated segments of the small intestine of rats and rabbits. The effect of DA on the smooth muscles of the small intestine of rats and rabbits can be divided into three groups:1) alkaloids, not significantly affecting the intestinal smooth muscle at concentrations up to 200mcM; 2) compounds having spazmogenic action, increase the tone, the frequency and amplitude of spontaneous contractions, and in high concentrations cause spasm of smooth muscle; 3) alkaloids having myotropic antispasmodic effect, and lowering the tone, reducing the amplitude and preventing and relieving spasms caused by barium chloride, acetylcholine, and the compounds of mezakonitin, aconitine types. We designed optimal predictive models for diterpenoid alkaloids of different structural types. We proved the positive effect of pre-clustering the original data set, although not all of the classes show a valid statistics. The work confirms two well-known position of the correct design of QSAR models: the linearity of the equation gives a better interpretability, and the high value of the standard statistics provides the predictive efficiency of the model.

rifqat@rambler.ru

Advances in targeted cancer therapy

S C Mehta
G R Medical College, India

Cancer is a disease of cells characterized by a defect in the normal control mechanisms that govern cell survival, proliferation and differentiation. It is the second most common cause of death in the United States. As our understanding of tumor biology and the molecules that make tumors grow and spread is expanding, new drugs that target these changes have emerged for the treatment of many different types of cancer. Targeted therapy is designed to target molecules in or on the tissue surrounding a tumor. Unlike standard chemotherapy drugs, targeted therapy drugs produce less severe side effects. Recently FDA approved Olaparib for the treatment of advanced ovarian cancer and Palbociclib for the treatment of advanced breast cancer. These drugs act by blocking a specific molecules responsible for the growth of cancer. Using the genetic makeup of different cancers new uses of existing drugs were also discovered. For example, the targeted therapy drug Ibrutinib, previously approved for chronic lymphocytic leukemia was found to be effective for the treatment of another type of blood cancer sharing the same genetic mutation,Waldestrom's macrogloulinaemia (WM). Similarly, Sorafenib is a drug used to treat liver, kidney and thyroid cancer is effective against acute myeloid leukemia (AML) and Cabozantinib was found effective in advanced kidney cancer and non-small cell lung cancer (NSCLC). The present paper will discuss the different ways the targeted therapy can work and the types and common adverse effects of targeted therapy drugs.

drscmehta@yahoo.co.in