

Thematic course: Studying “structure – property” interrelation among organic compounds with the pronounced antitumoral activity. Part 2.

Revealing of structural signs of medicinal preparations for treating ductal invasive carcinoma of a mammary gland of series MCF-7

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Abstract

With the use of computer system SARD-21 (Structure Activity Relationship and Design) structural signs, characteristic for compounds with high, moderate and low antitumoral activity are revealed; the degree of their influence on tumoral cells of invasive adenocarcinoma of ducts of mammary gland is estimated. On the basis of the received data, the forecasting model of interval levels of antitumoral activity in the series of sulphur – nitrogen – and oxygen-containing heterogeneous compounds with the level of the authentic forecast of 80% by two recognition methods of is constructed. The identified structural patterns can be used for designing new antitumoral drugs.