Documents

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A QSAR study for 2-(4-aminophenyl)benzothiazoles: Using DFT optimisation of geometry of molecules

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Abstract
Quantitative structure-activity relationships (QSARs) have been established for two sets of antitumour drugs 2-(4-aminophenyl) benzothiazoles (APBT). Constitutional, geometrical, topological, electronic descriptors (computed at the B3LYP/6-31G** level) and some empirical descriptors related to the hypophilicity were computed and analysed. Multiple regression analysis led to a set of equations that reflected the weight of each of the studied descriptors. The most relevant of these descriptors were grouped, and a new multiple regressions analysis was carried out and we arrived at the final QSAR models. A validation set of 11 APBT were selected, and their activities were computed using the proposed QSAR model. The correlation between the predicted and observed activities was excellent. The resulting best models exhibited good q2 and r2 values up to 0.867 and 0.954. © 2011 Taylor & Francis.

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2-(4-aminophenyl)benzothiazole (APBT); DFT; EHOMO- ELUMO; MlogP; QSAR

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