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Quantitative Structure-Activity Relationship Modeling of Detoxication Properties of Some 1,2-Dithiole-3-Thione Derivatives

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Abstract : Quantitative Structure-Activity Relationship (QSAR) studies have been performed on nineteen molecules of 1,2-dithiole-3-thione analogues. The compounds used are the potent inducers of enzymes involved in the maintenance of reduced glutathione pools as well as phase-2 enzymes important to electrophile detoxication. A multiple linear regression (MLR) procedure was used to design the relationships between molecular descriptor and detoxication properties of the 1,2-dithiole-3-thione derivatives. The predictivity of the model was estimated by cross-validation with the leave-one-out method. Our results suggest a QSAR model based of the following descriptors: qS2, qC3, qC5, qS6, DM, Pol, log P, MV, SAG, HE and EHOMO for the specific activity of quinone reductase; qS1, qS2, qC3, qC4, qC5, qS6, DM, Pol, logP, MV, SAG, HE and EHOMO for the production of growth hormone. To confirm the predictive power of the models, an external set of molecules was used. High correlation between experimental and predicted activity values was observed, indicating the validation and the good quality of the derived QSAR models.

Keywords : QSAR, quinone reductase activity, production of growth hormone, MLR
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