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Quantitative Structure Activity Relationship Model for Predicting the Aromatase Inhibition Activity of 1,2,3-Triazole Derivatives

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Abstract : Aromatase is an estrogen biosynthetic enzyme belonging to the cytochrome P450 family, which catalyzes the limiting step in the conversion of androgens to estrogens. As it is relevant for the promotion of tumor cell growth. A set of thirty 1,2,3-triazole derivatives was used in the quantitative structure activity relationship (QSAR) study using regression multiple linear (MLR), We divided the data into two training and testing groups. The results showed a good predictive ability of the MLR model, the models were statistically robust internally (R^2 = 0.982) and the predictability of the model was tested by several parameters. including external criteria (R^2pred = 0.851, CCC = 0.946). The knowledge gained in this study should provide relevant information that contributes to the origins of aromatase inhibitory activity and, therefore, facilitates our ongoing quest for aromatase inhibitors with robust properties.

Keywords : aromatase inhibitors, QSAR, MLR, 1,2,3-triazole
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