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Estimation of biological affinity of nitrogen-containing conjugated heterocyclic pharmacophores

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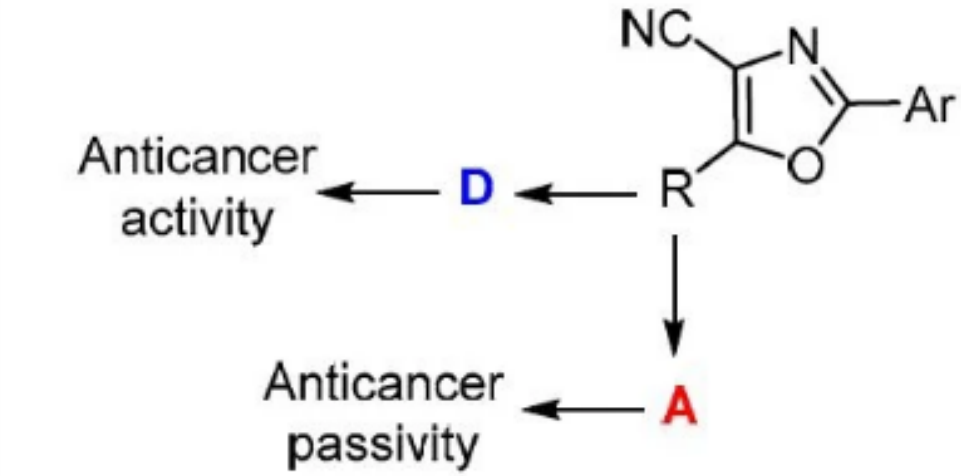

For the estimation of donor/acceptor character of conjugated heterocyclic compounds, the φ_o index is used. This parameter is determined by the relative positions of the frontier molecular orbital energy levels. It is shown that φ_o value of 0.5 means that the donor and acceptor properties in the conjugated molecule are balanced, while an increase of the index ($\varphi_o > 0.5$) corresponds to increasing of the donor strength, and, conversely, its lowered value ($\varphi_o < 0.5$) points to increased acceptor strength. In this work, a series of widely known heterocyclic compounds, as well as derivatives of oxazole and nucleobases are analyzed in detail. It is shown that change in φ_o index is connected to the biological activity. As an example, the influence of the conjugated substituents is studied and it is found that the oxazole derivatives with acceptor substituents inhibit cancer cells.