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Dependence of the anticancer activity of 1,3-oxazole derivatives on the donor/acceptor nature of his substitues

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Abstract

A series of new 1,3-oxazole derivatives, containing in position 5 both donor and acceptor substituents were synthesized. These substances were considered as potentially active anticancer pharmacophores in the human tumor cell line panel derived from nine cancer types, including lung, colon, melanoma, renal, ovarian, brain, leukemia, breast, and prostate. Primary in vitro one-dose anticancer screening was shown that compounds with acceptor substituents (such as –C(O)OMe, –CN) in the position 5 inhibit the growth of most cell lines, and compounds with donor substituents (such as –NHR, –SR) in the position 5 do not practically inhibit the growth of cancer cell lines. It can be assumed that the pharmacological activity of 1,3-oxazole derivatives depends on donor/acceptor nature of the substituents in position 5. It was proposed to evaluate the donor/acceptor ability of 1,3-oxazole derivatives using the special parameter φ_0, which takes into account the relative position of the boundary levels (HOMO end LUMO). The quantum-chemical modeling was performed; the special parameter φ_0 for 1,3-oxazole derivatives correlates with the experimental results. Quantum-chemical calculations of the special parameter φ_0 allow modeling the pharmacological activity of 1,3-oxazole derivatives by introducing donor or acceptor substituents at position 2 or 5. This work may be useful for chemists to develop a target synthesis of potential biologically active compounds.