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Molecular properties and bioactivity score of hydroxy-substituted hydrazones

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Hydrazones are compounds possessing diverse biological activities such as analgesic, anti-inflammatory, anticancer, antimicrobial, antibacterial, *etc.* Especially active are the aroylhydrazones of the type R'-CH = N-NH-CO-R obtained by the condensation of aromatic aldehydes and various hydrazides. Different substituents in the molecules of the compounds could improve their pharmacological effect. The presence of a hydroxy group in the molecules of different hydrazones strongly influences the biological activity of the compounds. Novel hydroxy-substituted hydrazone derivatives were designed by inserting the OH-group in both the aldehyde and hydrazide moieties and by varying the position of the substituents. The molecular properties of the compounds, important for drug pharmacokinetics in the human body, were assessed by a method based on group contribution. *In silico* evaluation of the value of logP and the remaining parameters of drug similarity, as well as the topological polar surface area and absorption percentage, were used to find the lead candidates with encouraging properties for further elaboration.

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