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QSAR Study on Thiosemicarbazone Derivatives as Ribonucleotide Reductase Inhibitors

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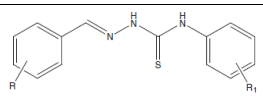
Abstract: QSAR analysis on thiosemicarbazone derivatives exposing RNR inhibitory activities [1] were performed. In this series of 21 compounds, 13 of them were reported with inhibitory concentration (IC50) in the l M range. The inhibitory concentration of those compounds were converted into -logIC50 before being correlated with the structural features.

The quantum chemical calculations have been carried out at the B3LYP level of theory using Gaussian-09 series of program package. The density functional theory (DFT), with the Becke's three parameter exchange functional along with the Lee– Yang–Parr correlation functional (B3LYP) were performed in order to calculate the quantum chemical descriptors such as HOMO, LUMO, Energy gap, Hardness, Softness, Chemical potential and Dipole moment of the investigated molecules. Calculated descriptors for some thiosemicarbazone derivatives were given in Table 1.

Tablo 1: Some descriptor calculations of thiosemicarbazone derivatives

		HOMO	LUMO	Energy gap	Hardness	Softness	chemical potential	Dipole moment
2-OH	H	-0.218	-0.079	0.139	0.070	14.380	0.063	6.536
2-OH	4-Cl	-0.260	-0.083	0.177	0.088	11.305	0.092	7.953
4-OH	H	-0.217	-0.074	0.143	0.071	14.020	0.075	6.122
4-OH	4-Cl	-0.221	-0.078	0.143	0.072	13.983	0.066	7.725
3-OCH3-4-OH	H	-0.250	-0.072	0.178	0.089	11.265	0.089	6.171
3-OCH3-4-OH	4-Cl	-0.217	-0.076	0.140	0.070	14.244	0.073	8.088
2-Furyl	H	-0.220	-0.080	0.140	0.070	14.264	0.071	6.171

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References:

[1] Moorthy N. S. H. N., Cerqueira N. M. F. S. A., Ramos M. J., Fernandes P. A., Med. Chem. Res. 21 (2012) 739–746.
