



Int. J. New. Chem., 2021, Vol. 8, Issue 2, pp 131-141.

International Journal of New Chemistry

Published online 2021 in <http://www.ijnc.ir/>.
Open Access



Print ISSN: 2645-7237

Online ISSN: 2383-188x

Original Research Article

Quantum and Statistical Study for Evaluating the Cytotoxicity Ability of Some Pyrazole Derivatives as Potent Anti Hiv-1 Agents Inhibitors

Ahanonu Saviour Ugochukwu*, Gideon Adamu Shallangwa, Adamu Uzairu

Department of Chemistry, Ahmadu Bello University, Zaria- Nigeria.

Received: 2020-08-12

Accepted: 2020-12-06

Published: 2021-06-01

ABSTRACT

A series of 20 compounds isolated from some pyrazole derivatives were subjected to cytotoxicity test against HIV-1. Two statistical approaches namely: Genetic Function Algorithm (GFA) and Multi Linear Regression Analysis (MLRA) were effectively used. Best three descriptors which are: VR2_Dzv, VR1_Dzp and PubchemFP824 were selected for the Quantitative structural and activity relationship (QSAR) using the two aforementioned statistical approaches. The results obtained were as follows: R-squared (R^2) of 0.9698, adjusted squared (R^2_{adj}) of 0.9607, cross validated R-squared (LOO- Q^2_{cv}) value of 0.9299 and external prediction ability (R^2_{pred}) of 0.6827. The result proved that the compounds are attractive platform and clinically viable for developing anti HIV-1 drugs. Multivariate statistics with chemical descriptors molecular shape and polarizability may be useful for the evaluation of cytotoxicity of pyrazole.

Keywords: QSCR, Pyrazole Derivatives, Anti-HIV-1, Validation, Cytotoxicity, MLR