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E-man Part 3[#]: Tutorial on gravitational algorithm in Structure activity relationships (SXR)

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(Dedicated with reverence to Prof (Dr.) Antonio Braibanti, Section of Applied Physical Chemistry, Pharmaceutical Department, University of Parma, Italy, on his eighty fifth-birth anniversary)

ABSTRACT

The challenges for the twenty-first century chemist are nano-, molecular- level processes in biology, interfaces of environment and industry. The on-line acquisition of terabytes of multi-dimensional data from hyphenated instruments, knowledge extraction and intelligent planning require interdisciplinary tools. The current research-tutorial on application of gravitational algorithm, Nature's algorithms mimics Evolution (Name), in rational drug design throws light on prospects of multi-disciplinary tools in chemical science. The applications of gravitational algorithm in chemical industry and engineering and recent advances along with its hybridization with PSO, etc. are briefed. The mapping of nature's way into mathematical space and futuristic focus in core methodology are covered. The indispensable rationalization of experiential and computational output with the state-of-the-art optimization and feature selection algorithms is illustrated with QSAR dataset. The tools used are computational quantum chemistry for optimization of 3D-geometry of molecules, molecular descriptors as explanatory feature variables, neural networks in data driven QSAR, gravitational algorithm in selecting optimum number of features from a pool of more than one thousand topological, electrostatic, quantum-chemical, WHIM descriptors of 2D- and 3D- category.

Keywords: Gravitational algorithm, Research-tutorial, E-man, Neural network, QSAR, Feature selection, Name, Chemicalindustry, Hybrid-Gravalg.

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