[P27] Visualization of multi-property landscapes for compound selection and optimization

Antonio de la Vega de Leon[1], Shilva Kayastha[1], Dilyana Dimova[1], Thomas Schultz[2], Jürgen Bajorath[1]

[1]Department of Life Science Informatics, B-IT, LIMES Program Unit Chemical Biology and Medicinal Chemistry, Rheinische Friedrich-Wilhelms-Universität, Dahlmannstr. 2, 53113 Bonn, Germany
[2]Institute of Computer Science II, Computer Graphics, Rheinische Friedrich-Wilhelms-Universität, Friedrich-Ebert-Allee 144, 53113 Bonn, Germany

Compound optimization methods depend on multiple parameters and therefore it is important to try and achieve a balance between more than one property. Computational multi-objective optimization techniques are usually applied to solve multi-property compound optimization problems to provide a numerical solution [1-3]. However, such methods could give rise to a number of reasonably optimal solutions and prioritizing the best multi-property solution is not straightforward. Star [4] and parallel coordinates [5] are visualization methods used in computer graphics that were adapted herein to visualize multi-property landscapes. We show that the visualization methods aid in comparing numerically equivalent optimal solutions arising from multi-property optimization algorithms and prioritize a subset. In our analysis, the goal was to get descriptor weight settings that could distinguish drugs from bioactive compounds. As such bioactive compounds that are in the vicinity of drug-like subspaces could be selected from multi-dimensional property space for further optimization. Furthermore, we have demonstrated that similar settings of descriptor weights could give rise to similar or different projections of compounds in multi-property space [6].

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