Chemography – from Abstract Mathematics to Library Design

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Defining the chemical space is not trivial, and possible definitions need to take into account the many facets of molecular structure – connectivity, geometry, physico-chemical properties, etc. Chemoinformaticians routinely work in chemical spaces defined by molecular descriptor vectors of >1000 dimensions. Chemography – the cartography of chemical space – emerged as a response to the challenge to visualize these high-dimensional spaces as human-readable 2D maps. Here we wish to address the below outlined key aspects of chemography – from the more abstract to the most practical, showing how this approach may be a multivalent "Swiss army knife" in drug discovery. This includes:

- generic introductions to some popular mapping algorithms,
- studying the neighborhood preservation problem upon dimensionality reduction,
- highlighting the multivalency of fuzzy logics-based grid methods which may also serve as QSAR models and library description tools,
- rationalizing and exploring the biologically relevant chemical space, from a global bird's eye view to local neighborhoods of bioactive compounds,
- exploring the ways to explore chemical space maps with Artificial Intelligence algorithms and discover original *de novo* compounds,
- using map-based library encoding tools to compare and design combinatorial libraries for project-specific purposes.