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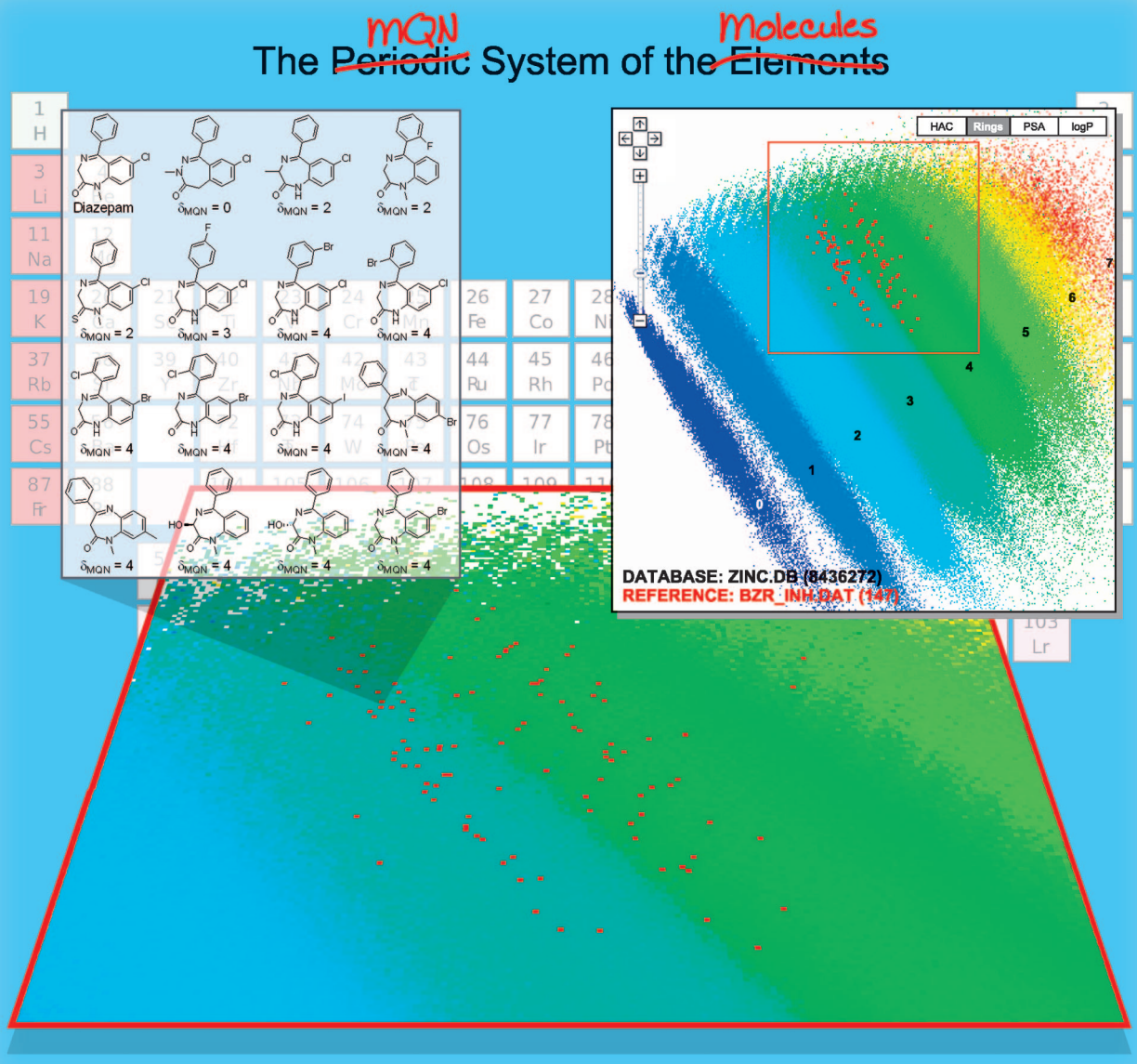
CHEMMEDCHEM

CHEMISTRY ENABLING DRUG DISCOVERY



11/2009

A Journal of

ChemPubSoc Europe

Cluster: Computational Medicinal Chemistry
Minireview: Aryloxy Phosphoramidate Triesters (C. McGuigan)
Highlight: Repurposing Sulindac (J. R. Simard and D. Rauh)

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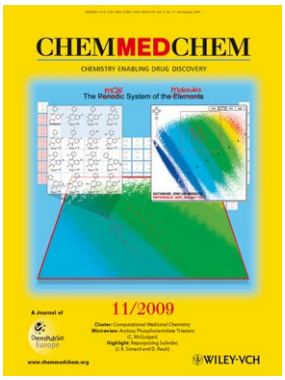
Cover Picture

Kong T. Nguyen, Lorenz C. Blum, Ruud van Deursen, and Jean-Louis Reymond*



The cover picture shows the classification, using the MQN system, of 8.4 million molecules in the public database of drug-like molecules ZINC. In analogy to the Periodic System of the Elements, in which atoms are classified by their atomic and main quantum numbers, the MQN system classifies molecules according to 42 molecular quantum numbers (MQN), defined as counts for structural features such as atoms, bonds, polar groups, and ring types. The 42-dimensional MQN space is represented as a projection in two dimensions along the first two principal components, the surface of which is color-coded by the number of cycles per molecule (blue to orange, 0 to 7 cycles). The red dots represent a family of known benzodiazepine receptor ligands. Related molecules are grouped closely in MQN space, as illustrated for diazepam and its nearest neighbors (structural formulae, MQN distance is indicated below each molecule). The MQN system provides a general and unifying concept for classifying large databases of organic molecules. For more details, see the Communication by J.-L. Reymond et al. on p. 1803 ff.