Chemoinformatics operating in Chemical Space

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With the rise of large make-on-demand chemical fragment spaces the need to directly operate in chemical space rather than in chemical libraries emerged. Due to the shear size, enumerating the spaces to libraries is highly inefficient and energy wasting, in many cases even impossible. Many methods working with chemical spaces are heuristic, i.e. they do not give any optimality guarantee. But this hasn't to be like this. Chemoinformatics standard operations like similarity and substructure search can be done directly in chemical fragment space with little to no approximation loss on standard desktop computers. In this talk, chemical space algorithms, their performance data and some applications will be presented.