

Computational chemistry in the life sciences industriesA. Feldman-Salit¹

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Computational chemistry is not only a tool to crack a scientific drug-design riddle but also an essential contributor to productive manufacturing for life sciences industries.

In our talk we want to address the advantages of computational chemistry field for drug or chemical production processes as the ultimate future vision of digitalized and automated manufacturing era. We will also walk you through known challenges and corresponding technical or administrative solutions, which we witnessed during our 20-year-old collaborative work with various pharmaceutical, chemical, and biotechnological companies.

It will be shown, how e.g., good project management or technical advisory and support may facilitate more efficient use of the computational predictive tool to reduce workload in the wet labs, to accelerate generated data analysis and transfer, thereby improving a production performance, also increasing patient safety and compliance of final products.

We will demonstrate how essential and valuable a contribution of computational predictions in the life sciences industry is, and not only due to its scientific mystery.