

# BioSolveIT Wins Evotec to Search the Molecular Universe for Better Drug Candidates

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Today, Germany-based Cheminformatics and Virtual Medicinal Chemistry specialists from BioSolveIT announced a strategic partnership with Evotec AG ("Evotec") to create an immeasurably large molecular search space. The database, so-called 'EVOspace' will act as a gigantic "pool" of virtual molecules from which to mine novel, synthetically accessible molecular entities for drug research.



Any current compound collection – virtual or real – irrespective of its size, merely scratches the surface of what *could* in principle be made in the laboratory. Purchasable compound databases as well as in-house molecules typically amount to only a few million compounds, while the "Chemical Universe" appears innumerable. BioSolveIT have a unique technology to search for interesting compounds in chemical libraries that offer around  $10^{16}$  possibilities, so 10 orders of magnitude larger than any traditional molecular compound pool.

The goal of the collaboration is to design *and* tailor the chemistry space - encompassing both Evotec's corporate chemical reactions with their proprietary building blocks and commercially available starting material with literature reactions. This way of cross-linking will boost the size from millions to several thousands of billions, capitalizing on Evotec's intellectual property ("IP"). Once this enormous database is created the search methods from BioSolveIT will be specifically adapted to yield compute times of just a few minutes on a standard PC, thereby enabling all researchers to interactive exploration and visual results feedback.

This project targets an obvious added value: higher quality and more diverse proposals from the computer methods for synthetic Medicinal Chemistry. Indeed, the industry must increase its pecuniary efficiency and speed up the drug discovery process while at the same time ensure a higher likelihood of creating better, yet novel molecular entities that are apt to be patent safe.

As Dr. Christian Lemmen, CEO of BioSolveIT comments: *"Our FTrees-FS™ technology has a pronounced strength in creating molecular proposals that, in the best sense of the word, are 'surprising': Researchers want and need to break out of the known and exploit novel molecules to push boundaries."* The BioSolveIT technology plays out its full potential when it is combined with corporate chemistries. *"We are proud and happy to have the highly renowned Evotec chemists to fill the algorithmic engine with top notch molecules and reactions that you do not find in textbooks; using the EVOspace our client will mine from much deeper than just the tip of the iceberg which is commonly grazed"*, Lemmen continues.

Acknowledging that "bigger is not always better", the proprietary algorithm intelligently disregards the uninteresting parts of the search space and, by design, focuses on synthetically accessible results. Dr. Lemmen summarizes: *"Using the Evotec proprietary reactions our partner Evotec dramatically increases their intellectual property plus ensures good, synthesizable molecules to propel meaningful follow-up with higher success rates!"*

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### About BioSolveIT GmbH

BioSolveIT is a globally acting medicinal chemistry informatics and services company. BioSolveIT is highly renowned for their superior custom software solutions for affinity estimation, structure-based design, docking, flexible molecular alignment, database searching, library design, and analysis. Their visual and fast computational technologies help to innovate pharmaceutical research with a proven track record in almost all big pharma companies, amongst them AstraZeneca, F. A. Hoffmann-LaRoche, BASF, Bayer, Boehringer-Ingelheim, GSK, Novartis, Zealand Pharma, Pfizer, Sanofi, and many others. Their latest portfolio addition, SeeSAR™, roots in co-developments with Bayer, F. A. Hoffmann-LaRoche, and Hamburg University, and helps to predict and visualize binding of therapeutic molecule candidates. Profiting from a radically simple user interface, it addresses computationally inexperienced medicinal chemists and experts alike. BioSolveIT is based in Sankt Augustin, Germany and entertains a support and sales office in Seattle, USA, and several distribution partner offices in Japan, China, and India. For additional information please go to [www.biosolveit.de](http://www.biosolveit.de), [biosolveit.com/linkedin](http://biosolveit.com/linkedin), or [facebook.com/BioSolveIT](https://facebook.com/BioSolveIT).

### About Evotec AG

Evotec is a drug discovery alliance and development partnership company focused on rapidly progressing innovative product approaches with leading pharmaceutical and biotechnology companies, academics, patient advocacy groups and venture capitalists. We operate worldwide providing the highest quality stand-alone and integrated drug discovery solutions, covering all activities from target-to-clinic. The Company has established a unique position by assembling top-class scientific experts and integrating state-of-the-art technologies as well as substantial experience and expertise in key therapeutic areas including neuroscience, pain, metabolic diseases as well as oncology, inflammation and infectious diseases. Evotec has long-term discovery alliances with partners including Bayer, Boehringer Ingelheim, CHDI, Genentech, Janssen Pharmaceuticals, MedImmune/AstraZeneca, Roche and UCB. In addition, the Company has existing development partnerships and product candidates both in clinical and pre-clinical development. These include partnerships with Boehringer Ingelheim and MedImmune in the field of diabetes, with Janssen Pharmaceuticals in the field of depression and with Roche in the field of Alzheimer's disease. For additional information please go to [www.evotec.com](http://www.evotec.com).