CHEMriya - Billions of Molecules for R&D: OTAVA and BioSolveIT Team Up

11 Billion Novel Molecules: CHEMriya - OTAVA's On-Demand Chemical Space

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VAUGHAN, Ontario and SANKT AUGUSTIN, Germany, June 9, 2021 (Newswire.com) - Today, Canadian-based compound specialist OTAVA (aka OTAVAchemicals) and German frontrunner cheminformatics firm BioSolveIT announce the release of a new, multibillion-sized pool of on-demand chemicals, available for therapeutic R&D. "CHEMriya" — alluding to Mriya, the Ukrainian word for "dream" — is a chemical space comprising 11 billion tangible screening compounds that are not present in any other commercial chemical catalog.

This vast pool of opportunities can be explored with BioSolveIT's unique virtual screening platform infiniSee. With utmost precision, infiniSee finds those compounds that are similar to a query molecule, scanning billions of possibilities within seconds. Traditional search technologies, by comparison, are prohibitively slow for such highly relevant applications. "*We are very excited to be at the forefront of this exciting new field — the creation and delivery of compounds mined from huge chemical spaces. BioSolveIT has a globally unique technology that permits our clients, researchers around the globe, to find those precious needles in giga-size haystacks*", Dr. Yaroslav Bilokin, Executive Director of OTAVA says.

The pharma research industry is in desperate need of novel chemical matter. In the past, high-throughput screening (HTS) demanded millions of molecules to be synthesized. Now, the invention of rapid and reliable on-demand synthesis

marks a paradigm shift: Companies favor cherry-picking over mass production and testing; they now explore from billions of compounds — yet they only synthesize hundreds of the most promising candidates. This is a giant leap for pharmaceutical research, accelerating its productivity while reducing costs. Early success stories have reported that a gain of "two times faster" and "ten times cheaper" could be achieved. Dr. Christian Lemmen, CEO of BioSolveIT, explains: "*OTAVA's tangible compound concept and our way of computing are a perfect match: Harnessing the combinatorial explosion, based on their impressive synthetic repertoire in CHEMriya, leads the way to a novel and highly efficient way of early drug discovery.*"
While routinely designing and synthesizing novel molecules at this scale was unthinkable only a few years ago, now, billions of novel molecules have become not only tangible but also affordable.

OTAVA's very distinct building blocks contained within the CHEMriya Chemical Space may now be obtained at www.chemriya.com; infiniSee is available from biosolveit.de/infiniSee.

About BioSolveIT GmbH

BioSolveIT is a globally acting medicinal chemistry informatics and services company. BioSolveIT is highly renowned for its 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, Pfizer, Sanofi, and many others. BioSolveIT's latest portfolio addition, infiniSee™, has rapidly become an industry standard for navigation in molecular chemical spaces of unparalleled sizes. BioSolveIT software helps to predict and visualize the binding of therapeutic molecule candidates with award-winning algorithms. Profiting from radically simple user

interfaces, the company's applications address computationally inexperienced medicinal chemists and experts alike.

BioSolveIT is based in Sankt Augustin, Germany and entertains a support and sales office in Boston, USA, and several distribution partner offices in Japan, China, and India.

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About OTAVA Ltd.
OTAVA Ltd. (aka OTAVAchemicals), founded in 1997, is an international chemicals and drug discovery company.

Specialists in the development and production of featured chemicals, bio-chemicals and bioanalytical reagents for more than 20 years, Otava provides

quality products and services for pharma, biotech, and R&D companies, academic institutions and government agencies.

Beyond on-demand and custom synthesis, the company also offers more than 280,000 compounds for high-throughput screening (HTS), including about 400 target-focused libraries (protein kinases, proteases, GPCRs, ion channels, epigenetic targets and others) as well as libraries of fragments, lead-like, drug-like and CNS-targeting compounds.

OTAVA promptly fulfills orders on over 30,000 chemical building blocks from its inventory and contributes to the available chemical synthon space with more than 5,000,000 new virtual chemical building blocks — ideal for diversity-oriented syntheses and deliverable within 4-12 weeks.

OTAVA's facilities and long-standing experience have enabled a variety of contract research and collaborative research projects. A highly skilled and talented medicinal chemistry team backed by biologists and computational chemists is ready to facilitate hit identification, hit-to-lead optimization, or custom synthesis projects at any level of complexity. Its client list comprises big pharma and academic institutions across Europe, the US, and Canada.

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Tags

Chemical Space, pharmacophore, Chemical Space Navigator, cheminformatics, drug discovery, high-throughput screening, organic synthesis

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