

PRESS RELEASE  
08 February 2018



## Enamine and BioSolveIT Launch the World's Largest Searchable Chemical Space for Novel Compound Sourcing

*REAL Space Navigator offers access to over 640 million pharma-oriented compounds*

**Kiev, Ukraine, and Sankt Augustin, Germany, 08 February 2018.** Enamine Ltd., a leading chemical research organization and producer of the world's largest collections of novel building blocks (150,000) and screening compound libraries (2,400,000), and BioSolveIT GmbH, premium provider of medicinal chemistry software, today announced the launch of the 'REAL Space Navigator'. Jointly developed, the new software tool capitalizes on Enamine's REAL (readily accessible) virtual compound concept and provides efficient 'search & find' access to more than 640 million pharma-oriented molecules, to date the world's largest chemical space of commercially accessible compounds.

Searching databases of commercially available compounds is a standard approach to advance hit compounds. However, the global stock of screening compounds has already been largely explored, making the identification of new and promising lead molecules difficult and the need for fast access to novel compounds increasingly necessary.

Enamine can quickly and efficiently assemble new compounds through appropriate single step combinations of the 150,000 building blocks available in its stock. By selecting the most characterized of these and proving their utility in parallel synthesis using 106 reaction protocols developed at Enamine, the Company confidently ensures a minimum synthesis rate of 80% and delivery time of 3-4 weeks. BioSolveIT's unique software capabilities have allowed for the searchability of a huge virtual chemical space that would be a challenge to navigate using traditional search technologies. REAL Space Navigator can be easily deployed on a standard computer, allowing for convenient, ultra-fast similarity searches and scaffold hopping without the need to connect to the internet and potentially disclose confidential queries.

**Michael Bossert, Head of Strategic Alliances at Enamine, commented:** *"The drug discovery industry has an enormous interest in new chemical compounds. Our REAL concept provides an efficient solution for virtual screening initiatives and analog searches to our clients, who appreciate going beyond the availability bias. BioSolveIT's fantastic team and its exceptional software platforms have already expanded the borders of Enamine's REAL database. We will continue to evolve this and hope to put billions of our future tangible molecules at researchers' fingertips."*

**Dr. Christian Lemmen, CEO of BioSolveIT, explained:** *"Our technology is based on extremely fast tree-based algorithms that avoid visiting every virtual molecule while traversing vast chemistry spaces for interesting hits. With Enamine's outstanding experience in chemical syntheses and quality-driven selection of building blocks, that space is not only impressively large but also packed with unique chemical matter. We are proud to be Enamine's partner in this exciting endeavor and thus offer users of the REAL Space Navigator a considerable competitive advantage."*

Both Companies continue to collaborate with plans to grow the database beyond 1 billion compounds by Q2 2018.

For further information on the REAL Space Navigator:

[http://www.enamine.net/index.php?option=com\\_content&id=259](http://www.enamine.net/index.php?option=com_content&id=259)

**ENDS**

### Notes to Editors



For high-resolution images, please contact [sarah.jeffery@zymecommunications.com](mailto:sarah.jeffery@zymecommunications.com)

### Contacts

#### Enamine

Michael Bossert

Head of Strategic Alliances

Email: [m.bossert@enamine.net](mailto:m.bossert@enamine.net)

Phone: +38 044 537 32 18

#### BioSolveIT

Dr. Marcus Gastreich

Director Application Science

Email: [contact@biosolveit.com](mailto:contact@biosolveit.com),

Phone: +49 2241 25 25 0

#### Media enquiries

Sarah Jeffery

Zyme Communications

Email: [sarah.jeffery@zymecommunications.com](mailto:sarah.jeffery@zymecommunications.com)

Phone: +44 7771 730919

#### About Enamine Ltd. <http://www.enamine.net>

Established in Kiev, Ukraine in 1991, Enamine is a chemical company producing building blocks and screening libraries of world reputation. The major asset of the company is the world's largest collection of building blocks: 150,000 in stock with 2,000 additions synthesized each month. These research functionalized compounds provide a significant competitive advantage to the company in supplying custom compound libraries particularly in the frame of medicinal chemistry collaborations or compound collection enhancement programs. Enamine's REAL (readily accessible) concept is based on the careful and knowledge-guided enumeration and selection of compounds that can be confidently produced from the stock building blocks using over 106 validated reactions.

#### About BioSolveIT GmbH [www.biosolveit.com](http://www.biosolveit.com)

BioSolveIT is a global medicinal chemistry, informatics and services company. The Company 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. BioSolveIT's

visual and fast computational technologies hold several world records and have a proven track record in helping to innovate pharmaceutical research in almost all the big pharma, amongst them AstraZeneca, F. A. Hoffmann-LaRoche, BASF, Bayer, Boehringer-Ingelheim, GSK, Novartis, Zealand Pharma, Pfizer, Sanofi, and many others.

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