

Schrödinger Contributes to RDKit

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NOTE: This contains archival information which should not be considered current.

Schrödinger integrates cheminformatics toolkit across drug discovery platform and contributes to the latest release of RDKit

New York, NY - June 19, 2018 - Schrödinger, Inc., a privately-held company dedicated to revolutionizing drug discovery through advanced computational methods, has announced their contribution, a 2D coordinate generation tool, to the latest release of RDKit, an open source cheminformatics toolkit.

“We’ve been very pleased with the results of integrating RDKit into various aspects of our drug discovery platform,” said Schrödinger Senior Vice President & Chief Technology Officer, Patrick Lorton. “Pairing Schrödinger’s commitment for scientific breakthrough with the scientific power and performance of RDKit has accelerated our drug discovery efforts and helped us to continue providing users with industry-leading solutions.” Dr. Greg Landrum, creator of RDKit adds “It’s been a pleasure to work with the Schrödinger team. The new 2D Coordinate Generation library brings some important new functionality to the scientists using RDKit and software built on top of it; we’re excited for future projects with Schrödinger and look forward to their further contributions to the RDKit platform.”

In addition to developing the 2D coordinate generation tool, Schrödinger has also utilized RDKit to develop an open source GPU-enabled similarity search tool, and will continue to support and improve both of these currently available tools. Schrödinger’s open source product, PyMOL, now contains RDKit-based plugins, with plans for further integration. Schrödinger is also proud to contribute to the open source Python library toolchain DeepChem, a project developed through academic and industrial collaborators, which heavily uses RDKit.

Further instances of Schrödinger's use of RDKit include LiveDesign, a collaborative drug design platform, as well as several aspects of machine learning applications such as pKa prediction, synthetic feasibility monitoring, experimental prioritization, and hERG modeling. Product functionality in which Schrödinger extensively utilizes RDKit include processing input data for quantum mechanical rate calculations, reaction-based enumerations, bioisostere replacement, hit expansion, and quantitative structure-activity relationships identification. The toolkit has also proven valuable in tools developed for Schrödinger's drug discovery collaborators.

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About Schrödinger

Schrödinger is a leading provider of advanced molecular simulations and enterprise software solutions and services to accelerate and increase the efficiency of drug discovery for its clients, which include all major pharmaceutical and biotechnology companies worldwide, as well as leading materials science researchers. Schrödinger also establishes deep partnerships and collaborations with companies in such fields as biotechnology, pharmaceuticals, chemicals, and electronics, and was a cofounder of leading biotech companies including Nimbus Therapeutics, Morphic Therapeutic, and others. Schrödinger's investors include David E. Shaw and Bill Gates. Through significant long-term investments in basic research, Schrödinger has made scientific breakthroughs across many areas of drug discovery and materials science. Hundreds of peer-reviewed scientific publications by Schrödinger scientists are frequently among the most heavily cited in their fields. Founded in 1990, Schrödinger has nearly 400 employees and operations in the United States, Europe, Japan, and India, as well as business partners in China and Korea. For more information, please visit www.schrodinger.com.

About RDKit

RDKit is a widely used open source cheminformatics toolkit that covers both 2D (e.g., fingerprints and chemical reactions) and 3D (e.g., conformation generation) tools, and is usable from C++, Python, Java, and C#. It has been tightly integrated with other open source projects such as PostgreSQL and KNIME Analytics Platform. RDKit has been broadly adopted across academia and industry, benefits from a highly active open source community, and has been integrated into multiple commercial software tools. Commercial support for RDKit is available from T5 Informatics GmbH. For more information, please visit www.rdkit.org.