



BioTools announces a collaboration with Schrödinger aimed at accelerating the discovery and development of chiral small molecule therapeutics

Florida, USA – [January 2022] – BioTools, the pioneer in vibrational circular dichroism (VCD) technology and provider of proprietary instrumentation and analytical services for structure elucidation of chiral molecules, announces a collaboration with Schrödinger, Inc., whose physics-based software platform is transforming the way therapeutics and materials are discovered, to help chemists expedite the determination of the critical three-dimensional stereo structure.

A molecule with a chiral center exists in one of two mirror-image forms (stereo-configurations) which can exhibit different biological properties. Identification of the molecule's stereo-configuration, or handedness, is known as the determination of the absolute configuration. It can be achieved via VCD technology, which includes both experimental measurements and theoretically predicted results.

BioTools revolutionized the determination of the absolute configuration through commercialization of VCD instrumentation. For over 21 years, the VCD method has been proven to be a highly reliable, easier, quicker alternative or replacement to traditional X-Ray crystallography. The VCD technology does not require a single crystal, unlike crystallography, and only needs a very low quantity of material (2-10 mg) that can be easily recovered. VCD has been published as a standard method in the US Pharmacopeia, Chapters <782> and <1782>, and approximately 10,000 absolute configurations have now been determined with VCD. Currently, VCD is being used by virtually all major pharmaceutical companies worldwide.

Schrödinger recognizes the importance of the VCD technology for the determination of chirality and remains dedicated to delivering and periodically improving its seamless VCD computational workflow. Combining BioTools experimental results with those of calculations through Schrödinger's workflow based on the fast quantum chemistry engine Jaguar will allow chemists to determine the absolute configuration rapidly and effortlessly.

"BioTools is known worldwide for their knowledge and expertise in the field of VCD. We are very pleased to have had an opportunity to work with their scientists to deliver this refined

capability in our digital chemistry platform.” – Mathew D. Halls, Senior Vice President, Materials Science, Schrödinger Inc.

“Schrödinger’s drug discovery platform and its user base are an ideal match for our instrumentation and vision of bringing VCD to every pharmaceutical company and academic institution. We have seen a significant increase in Schrödinger’s customers requesting experimental spectra. The VCD implementation in Jaguar is a great step forward for the field.” – BioTools, President & Co-Founder, Dr. Rina Dukor

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About BioTools

BioTools is a life sciences tools company that revolutionized characterization technology for the most important therapeutics of our time - chiral small molecules and biologics. The breakthrough analytical techniques developed by the company provide molecular structure information which governs safety and efficacy – analyzed in a fraction of a time compared to traditional methodology.

BioTools product offerings include instrumentation, specialized CRO services, and unique software and accessories. The products are used globally by most of the world’s top 100 pharmaceutical companies, renowned academic institutions, and government laboratories, including the US Food & Drug Administration (FDA).

Founded in 2000, BioTools has R&D, sales, customer support, contract research lab and manufacturing facilities in Jupiter, Florida, and two international divisions, BioTools Europe, headquartered in the United Kingdom, and BioTools China, headquartered in Dalian. BioTools’ co-founders and products have been recognized by numerous International Awards, including the R&D 100 Top Innovation Award.

For more information, visit <https://biotools.us/> or contact us at info@biotools.us.

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