Optibrium acquires BioPharmics LLC, expanding its 3D drug design and visualisation offering

BioPharmics' Drs Ajay Jain (CEO) and Ann Cleves (Director of Applied Science) join the Optibrium team as Vice Presidents in the newly-created BioPharmics Division

CAMBRIDGE, UK, 31 August 2023 – Optibrium, a leading developer of software and AI solutions for drug discovery, today announced the acquisition of BioPharmics LLC, expanding its 3D drug design and modelling offering. Bringing decades of experience in computational chemistry and biology, BioPharmics' CEO, Dr Ajay Jain, and Director of Applied Science, Dr Ann Cleves, join the Optibrium team, respectively focusing on R&D and Application Science in the newly-created BioPharmics Division.

BioPharmics has developed a series of industry-leading algorithms and software for 3D ligand-based and structure-based computational drug design, including software for 2D to 3D ligand conversion and conformer generation (ForceGen), molecular docking (Surflex-Dock), molecular similarity (eSim), and binding affinity prediction (QuanSA). These highly performant products have all been rigorously researched and their results demonstrated in numerous peer-reviewed papers, many published jointly with key pharmaceutical industry partners.

The strategic acquisition brings powerful technology for 3D ligand- and structure-based design into Optibrium's comprehensive StarDrop™ platform for small molecule design, optimisation and data analysis, complementing its existing range of artificial intelligence, de novo design, and in silico modelling software. The deal follows a long-standing collaboration between the two companies, including partnering on the development of the Surflex eSim3D StarDrop module.

"After years of close collaboration, we are delighted that Optibrium was chosen to support BioPharmics' continued scientific innovation and expanding customer base." **Dr Matthew Segall, CEO, Optibrium said.** *"We are delighted to welcome Ajay and Ann to the team. Their extensive experience in computational chemistry and biology, alongside BioPharmics' world-leading software for 3D ligand- and structure-based design, will bring Optibrium to the forefront of these essential technologies for small molecule discovery and design."*

In their new roles, Ajay and Ann will continue the research and application of novel methods to extend the application of 3D modelling to traditional small molecules, as well as to *beyond Rule-of-Five* compounds that are becoming increasingly prevalent in drug discovery.

Ajay has over 30 years of experience working in the field of computer-aided drug design (CADD). Prior to founding BioPharmics, he held a series of senior scientific roles in multiple small biopharma companies, including Arris Pharmaceuticals, MetaXen, and Iconix Pharmaceuticals. He was also faculty at the University of California, San Francisco (UCSF) for over two decades, with a broad research program encompassing genomics and cancer genetics, in addition to CADD. Ajay holds a PhD in Computer Science from Carnegie Mellon University.

Ann brings extensive expertise in applied research in computational chemistry and biology, and in the relationship between molecular structure and pharmacology, gained through her long tenure both within academic and biopharmaceutical settings. Ann and Ajay began their collaboration at MetaXen, which then continued at UCSF, and she has been an integral part of BioPharmics for many years. Ann holds a PhD in Microbiology and Cell Biology from the University of Illinois.

Dr Ajay Jain, Founder and CEO of BioPharmics, commented: *"We have always been impressed by Optibrium's focus on scientific rigour, and we firmly believe that there is no better team to continue the powerful software developments that BioPharmics has introduced over the years. I look forward to working as part of the Optibrium team to expand their internal expertise in 3D drug design, as well as on future drug discovery innovations."*

Dr Ann Cleves, Director of Applied Science at BioPharmics, added: *"We have enjoyed working with Optibrium over the years, and the high levels of mutual respect for the scientific expertise from each side of the partnership has enabled this next step. I am excited to see the new products and ground-breaking science that we will deliver together."*

For further information on Optibrium, please visit www.optibrium.com, contact info@optibrium.com or call +44 1223 815900.

ENDS

Notes to Editors:

Dr Matthew Segall, CEO, Optibrium

Dr Ajay Jain, Founder and CEO, BioPharmics

Dr Ann Cleves, Director of Applied Science, BioPharmics

For high-resolution images, please email Zyme Communications.

To opt-out from receiving press releases from Zyme Communications, please email info@zymecommunications.com.
To view our privacy policy, please click here.

Media contact
Esmé Walters
Zyme Communications
Email: esme.walters@zymecommunications.com
Phone: +44 (0)7377 543244

Optibrium
Michelle Harrison
Head of Marketing
Email: michelle@optibrium.com
Phone: +44 (0)1223 815903

About Optibrium

Optibrium provides innovative software solutions for small molecule design, optimisation and data analysis. Optibrium's lead product, StarDrop™, is a comprehensive suite of integrated software with a highly visual and user-friendly interface. StarDrop enables a seamless flow from the latest data through to predictive modelling and decision-making regarding the next round of synthesis and research, improving the speed, efficiency, and productivity of the discovery process. The company's Augmented Chemistry® products and services, including Cerella™ deliver proven artificial intelligence technologies that continuously learn from all available data to supplement researchers' experience and skills.

Optibrium was founded in 2009 and is headquartered in Cambridge, UK, with a US subsidiary, Optibrium Inc., based in Cambridge MA. The company works closely with over 180 customers and collaborators worldwide, including leading global pharma, biotech, agrochemical and flavouring companies and not-for-profit and academic groups.

For further information, visit www.optibrium.com.

About BioPharmics

BioPharmics LLC was founded in 1998 to develop algorithms and software for computational drug design. They have leading solutions in the areas of 2D to 3D ligand conversion and conformer generation (FGen3D and ForceGen), molecular docking (Surflex-Dock), molecular similarity (eSim), binding affinity prediction (QuanSA), and real-space modelling of ligand ensembles in X-ray density maps (xGen). All methods within the BioPharmics computational platform couple physical realism in modelling protein-ligand interactions with algorithms for rapid optimisation of conformation and alignment of small molecules.

For further information, visit https://www.biopharmics.com/.