Tom Blundell is the chair of the School of Biological Sciences and Sir William Dunn Professor of Biochemistry, University of Cambridge, UK. He is the co-founder of two drug discovery companies, Astex Technology Ltd. and Biofabrika Ltd. He has received numerous awards and honors. His research interests include the elucidation of macromolecular structure using methods from biochemistry, protein crystallography, bioinformatics and structure-based drug design. His group has also written several bioinformatics programs.

John Irwin received his Ph.D. for work with Jack Dunitz in chemical crystallography in 1991 at ETH Zurich. He worked at a startup molecular modeling company in Strasbourg, France before joining Gerard Bricogne's group at the Medical Research Council's Laboratory of Molecular Biology in Cambridge UK, where he helped develop software for macromolecular crystallographic structure solution and refinement methods (BUSTER and SHARP). He spent a year and a half as a staff scientist at EMBL-EBI also in Cambridge working in the macromolecular structure database group before moving to Northwestern University Medical School to join Brian Shoichet in 2000 where he began work on DOCK, ZINC, and SEA. John is an adjunct associate professor in the Department of Pharmaceutical Chemistry at the University of California San Francisco. He works together with Brian Shoichet on methods to discover new chemistry for biological targets using docking and ligand-based methods. Most recently, John released “DOCK Blaster”, a public access molecular docking service.

Weiliang Zhu is the head of Drug Discovery and Design Centre in Shanghai Institute of Materia Medica. He received his Ph.D. in 1998 in computer aided drug design from Shanghai Institute of Materia Medica, Chinese Academy of Sciences, China. He then moved to Singapore and worked in School of Life Sciences, Singapore Polytechnic as a Visiting Lecturer (1998-2002) and later as a lecturer (2002-2004), and as a researcher at the Technology Centre for Life Sciences, Singapore Polytechnic as well. In 2004, he joined the Drug Discovery and Design Centre, Shanghai Institute of Materia Medica, as a “100-Talent Program” principal investigator of Chinese Academy of Sciences. Currently, he works on drug design, molecular modeling, molecular dynamics simulation, computational chemistry and biology. He has published more than 100 research papers in various journals including *J. Am. Chem. Soc., J. Virol., J. Med. Chem., Biophys. J., J. Phys. Chem. (A, B).* He is also the visiting professors of Singapore Polytechnic, East China University of Science and Technology, and Dalin University of Science and Technology.

Michael Keiser received his B.Sc. in Computer Science from Stanford University in 2004, along with a B.A. in Slavic Languages & Literature, and a M.A. in Russian, Eastern European and Eurasian Studies. He completed his Bioinformatics Ph.D. as a National Science Foundation Fellow in Brian Shoichet's laboratory at UC San Francisco, where he developed techniques to relate proteins based on the statistical similarity of their ligands. This research has since expanded to investigating drug polypharmacology and the prediction of drug off-target activities. Micahel is now a cofounder of SeaChange Pharmaceuticals Inc, a company applying this work to drug repositioning.

Irwin Kuntz is the Founder of the University of California, San Francisco Molecular Design Institute and Emeritus Professor of Pharmaceutical Chemistry. He received his Ph.D. in Chemistry from the University of California at Berkeley and taught at Princeton University before joining the Department of Pharmaceutical Chemistry at the University of California San Francisco. His work has been focused on structure-based ligand design and docking algorithms. His group also developed the DOCK software program (DOCK 4.0: search strategies for automated molecular docking of flexible molecule databases. J. Comput-Aided Molec. Design. 15: 411, 2001). It uses database and graph theoretic techniques to suggest molecules which have good steric and chemical complementary to proteins of known structures. The program has been proven to be useful at UCSF and in other academic and industrial laboratories around the world for finding lead compounds in the search for new drugs against viruses, bacteria and parasites.

Arthur Olson is the director of the Molecular Graphics Laboratory at the Scripps Research Institute. His group leads the development of a popular docking program, AUTODOCK, for automated docking of flexible ligands to protein targets. One of his current research interest focuses on the use of computation methodology on the design of HIV protease inhibitors. His group also hosts the popular distributed computing project "FightAIDS@Home" for the discovery of novel inhibitor against HIV protease.

Stefano Forli graduated in Medicinal Chemistry at the "Universita' degli Studi di Siena" in Italy, under the supervision of Prof. Maurizio Botta in the European Research Training Network for Microtubule Stabilizing Agents.
In 2004 he was visiting student to the University Luis Pasteur of Strasburg at Charles Mioskowski's synthetic lab. During his Ph.D. he got an industrial fellowship from SienaBiotech SpA, where eventually joined the Alessandro Padova's Drug Design Unit with an industrial stage fellowship. He's now Research Assistant in the Molecular Graphics Lab of Prof. Artur Olson, where he works on high-throughput virtual screening techniques applied to the design of new HIV protease and integrase inhibitors with the distributed computation on FightAIDS@Home. He's also involved in the development of AUTODOCK and the automation of docking procedures for virtual screening.

Seong Eon Ryu was awarded his Ph.D at Columbia University in 1991 with the work of structure determination of HIV receptor CD4. After postdoctoral studies regarding CD4 and gp120 at Harvard University, he returned to Korea in 1994 to establish a laboratory in Korea Research Institute of Bioscience and Biotechnology (KRIBB). His laboratory has been engaged in structural proteomics and structure-based drug design of protein tyrosine phosphatases. He was awarded with various scientific prizes from Korea government and scientific associations such as Scientist of the year (2001), Best Bioscientist (2001), and Academic Award of Korea Biophysics Association (2006).

Brian Shoichet received his Ph.D. for the work with Irwin (Tach) Kuntz on molecular docking in 1991 from UCSF. After a postdoctoral training with Brian Matthews at the Institute of Molecular Biology in Eugene, Oregon, he joined the faculty at Northwestern University as an Assistant Professor in 1996. In 2002, he was recruited back to UCSF, where he is now a professor in the Department of Pharmaceutical Chemistry. Brian’s Laboratory is interested in how enzyme structure determines function, with a focus on novel inhibitor discovery. A major emphasis is the inhibition and evolution of ß-lactamase. The research combines computational modeling with enzymology, protein stability, and x-ray crystallography. He has been instrumental in the further development of the DOCK program, the construction of the ZINC chemical database (ZINC – a free database of commercially available compounds for virtual screening. J. Chem. Inf. Model 45: 177, 2005) and the SEA chemoinformatics tool for relating proteins that interact with similar ligands (Relating protein pharmacology by ligand chemistry. Nat. Biotech. 25: 197, 2007).

Dr. Cheng Yang is a senior scientist and director of Asian market of Rigaku Americas corporation. Dr. Yang has joined Rigaku Americas Corporation since 1998. His research focuses on structure based drug design including designing new herbicidal inhibitors and improving specificity of diabetes- related drug candidates. Dr. Yang also spent substantial time on development of X-ray apparatus and software including multilayer confocal optics, CCD detectors and high throughput automation. Dr. Yang also studied on new in-house phasing approach and developed a new procedure of using long wavelength X-ray to collect sulphur anomalous scattering and phase protein data. In recent years, Dr. Yang also worked with his colleagues to develop fragment based screening, its related libraries and techniques.