



Protein Crystallography in Drug Discovery, Volume 20 (Methods and Principles in Medicinal Chemistry)

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The rational, structure-based approach has become standard in present-day drug design. As a consequence, the availability of high-resolution structures of target proteins is more often than not the basis for an entire drug development program. Protein structures suited for rational drug design are almost exclusively derived from crystallographic studies, and drug developers are relying heavily on the power of this method. Here, researchers from leading pharmaceutical companies present valuable first-hand information, much of it published for the first time. They discuss strategies to derive high-resolution structures for such important target protein classes as kinases or proteases, as well as selected examples of successful protein crystallographic studies. A special section on recent methodological developments, such as for high-throughput crystallography and microcrystallization, is also included. A valuable companion for crystallographers involved in protein structure determination as well as drug developers pursuing the structure-based approach for use in their daily work.

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Editorial Review

Review

"Medicinal chemists will find the book invaluable whether they are working in an area of one of the chapters or wish to apply the methods described to other projects. Structural and computational biologists should also find it useful and thought-provoking."

ChemBioChem August

Lars-Oliver Essen, Fachbereich Chemie, Philipps-Universität Marburg, Angewandte Chemie, 3.
Dezemberheft 2004-116/47 und Angewandte Chemie International Edition, 3rd December Issue 2004-43/47

"The quality of the individual chapters of this volume is high, and each of the contributors is to be commended for their efforts."

Steven W. Muchmore, Department of Structural Biology, Global Pharmaceutical Research Division, Abbott Laboratories, Abbott Park, Illinois, Journal of Medicinal Chemistry, Vol. 47, No. 26, 2004

"... an important contribution to pharmaceutical research and development."

American Journal of Therapeutics

From the Back Cover

The rational, structure-based approach has become standard in present-day drug design. As a consequence, the availability of high-resolution structures of target proteins often forms the basis for an entire drug development program. Protein structures suited for rational drug design are almost exclusively derived from crystallographic studies, and drug developers are relying heavily on the power of this method.

Here, researchers from academia and from leading pharmaceutical companies present valuable first-hand information on how to obtain the desired protein structures and how to exploit crystallographic data for the drug discovery process.

From the contents:

- * Crystallography of important target classes such as kinases and proteases
- * Structure-based design of protease inhibitors
- * Structure-based design of kinase inhibitors
- * The ribosome and the proteasome as drug targets
- * Recent methodological advances in high-throughput crystallography and microcrystallization

An indispensable companion for crystallographers involved in protein structure determination as well as drug developers following the structure-based approach.

About the Author

Robert E. Babine has diverse drug discovery experience over the past 20 years and is presently the Director of Structural & Computational Chemistry at SPRL in Cambridge, Massachusetts. After receiving his Ph.D. in synthetic organic chemistry at Brown University he joined the medicinal chemistry group at Lederle Laboratories. During his 10 years at Lederle his research evolved into structure-based drug design, culminating in a project that discovered hydroxylaminepentanamide HIV protease inhibitors. Thereafter, he

was in the medicinal chemistry group at Agouron Pharmaceuticals where he was involved in the early phase discovery of rhinovirus 3C protease inhibitors. After a 2-year stay at Eli Lilly he joined the new startup company SPRL in 2000.

Sherin S. Abdel-Meguid is Chief Scientific Officer and Founder of Suntory Pharmaceutical Research Laboratories (SPRL), a structure-based drug discovery company located in Cambridge, Massachusetts. He joined SPRL from SmithKline Beecham (SB) where he was Director of Macromolecular Sciences and Structural Biology, and director of the IL18, Herpes virus protease and CD28 programs. Prior to his work for SB, he was Head of Biophysical Sciences and Protein Engineering at Monsanto. At Monsanto, he built one of the first macromolecular crystallography groups in the pharmaceutical industry. He holds a Ph.D. in Physical Chemistry and M.S. and B.S. degrees in Biochemistry.

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