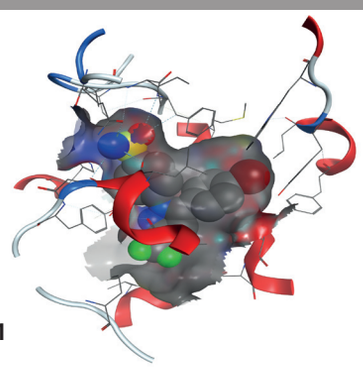
Fraunhofer
IME

FRAUNHOFER INSTITUTE FOR MOLECULAR BIOLOGY AND APPLIED ECOLOGY IME



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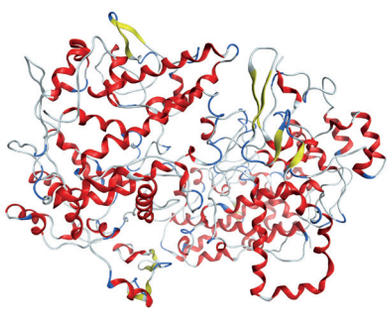

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1 *Crystal structure of celecoxib inside the binding pocket of COX-2.*
2 *Crystal structure of celecoxib.*

MEDICINAL CHEMISTRY AND DRUG DESIGN

Research within the IME-TMP is conducted on drug synthesis, in silico drug design, virtual screening and fragment-based screening methods, combined with the pharmacological characterization of these lead compounds at the molecular and cellular level.

Medicinal chemistry
- histamine and dopamine receptor ligands
- cyclooxygenase inhibitors
- 5-lipoxygenase inhibitors
- dual 5-lipoxygenase/soluble epoxide hydrolase inhibitors
- PPAR and FXR ligands
- secretase inhibitors

In silico drug design
- ligand-based virtual screening (pharmacophores, shape-based, 2D methods)
- structure-based virtual screening (structure-based pharmacophores, molecular docking)
- QSAR analysis of activity data
- computer-aided design of focused libraries

Analytical characterization
- NMR, LC-MS
- MALDI-MS

Drug target identification
- proteomics and SNP analysis
- reporter gene assays
- signal transduction research
- enzyme assays

Fraunhofer Institute for Molecular Biology and Applied Ecology IME
Project Group for Translational Medicine and Pharmacology TMP

Theodor-Stern-Kai 7
60596 Frankfurt am Main

Contact

Prof. Dr. Michael Parnham
Phone +49 69 6301-84234
michael.parnham@ime.fraunhofer.de

www.ime.fraunhofer.de