Record Nr. UNINA9910437613403321 Autore Strasser Andrea Titolo Modelling of GPCRs: a practical handbook / / Andrea Strasser, Hans-Joachim Wittmann New York, : Springer, 2013 Pubbl/distr/stampa **ISBN** 1-283-63384-1 9786613946294 94-007-4596-6 Edizione [1st ed.] Descrizione fisica 1 online resource (218 p.) Altri autori (Persone) WittmannHans-Joachim Disciplina 572.696 Soggetti G proteins - Receptors Lingua di pubblicazione Inglese **Formato** Materiale a stampa Livello bibliografico Monografia Note generali Description based upon print version of record. Includes bibliographical references and index. Nota di bibliografia Nota di contenuto Preface -- 1. Introduction -- 2. G Protein Coupled Receptors --3. Sequence alignment and homology modelling -- 4. Construction of ligands -- 5. Lipids -- 6. Minimization and molecular dynamics. - 7. Calculation of Gibbs energy of salvation -- 8. Special topics in GPCR research -- 9. Force fields -- 10. Thermodynamics of ligandreceptor interaction -- 11. Important LINUX commands -- Literature --Appendix -- Index. G protein coupled receptors (GPCRs) comprise an important protein Sommario/riassunto family, which is involved in signal transduction in the cell. Besides that a large number of drugs, available on market, address GPCRs. For an efficient and improved development of appropriate drugs, molecular modelling of GPCRs is - in order to understand the ligand-receptor interactions and functionality of GPCRs on molecular level - an important tool. The book "Modelling of GPCRs – a practical handbook" is focussed onto a practical introduction into molecular modelling of GPCRs. This book is very useful for beginners in GPCR modelling, but also addresses the advanced GPCR modeller: On the one hand, the book introduces principles of GPCR modelling, including extensive examples. On the other hand, detailed outlooks onto advanced GPCR modelling techniques are presented. Furthermore, the book includes important data, like information about crystal structures in a

summarized manner or amino acid sequences, which are essential for

GPCR modelling in general. Due to an increase in efficacy and data handling most modellers use LINUX as operating system. To address this, a summary of most important LINUX commands with examples is presented within the book.