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Altri autori (Persone)	VarnekAlexandre TropshaAlex
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Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Preface-- 1 -- Fragment Descriptors in SAR/QSAR/QSPR studies, molecular similarity analysis and in virtual screening-- Introduction-- Historical survey-- Main characteristics of Fragment Descriptors-- Types of Fragments-- Simple Fixed Types-- WLN and SMILES Fragments-- Atom-Centered Fragments-- Bond-Centered Fragments-- Maximum Common Substructures-- Atom Pairs and Topological Multiplets-- Substituents and Molecular Frameworks-- Basic Subgraphs-- Mined Subgraphs-- Random Subgraphs-- Library Subgraphs-- Fragments describing supramolecular systems and chemical reactions-- Storage of fragments' information-- Fragment's Connectivity-- Generic Graphs-- Labeling Atoms-- Application in Virtual Screening and In Silico Design-- Filtering-- Similarity Search-- SAR Classification (Probabilistic) Models-- QSAR/QSPR Regression Models-- In Silico Design-- Limitations of Fragment Descriptors-- Conclusion-- 2 -- Topological Pharmacophores-- Introduction-- 3D pharmacophore models and descriptors-- Topological pharmacophores-- Topological pharmacophores from 2D-aligments-- Topological pharmacophores from 2D pharmacophore fingerprints-- Topological index-based 'pharmacophores'?-- Topological pharmacophores from 2D-aligments-- Topological pharmacophores from pharmacophore fingerprints-- Topological pharmacophore pair

fingerprints-- Topological pharmacophore triplets-- Similarity searching with pharmacophore fingerprints -- Technical Issues-- Similarity searching with pharmacophore fingerprints -- Some Examples-- Machine-learning of Topological Pharmacophores from Fingerprints-- Topological index-based 'pharmacophores'?-- Conclusions-- 3 -- Pharmacophore-based Virtual Screening in Drug Discovery-- Introduction-- Virtual Screening Methods-- Chemical Feature-based Pharmacophores-- The Term "3D Pharmacophore"-- Feature Definitions and Pharmacophore Representation-- Hydrogen bonding interactions-- Lipophilic areas-- Aromatic interactions-- Charge-transfer interactions-- Customization and definition of new features-- Current super-positioning techniques for aligning 3D pharmacophores and molecules-- Generation and Use of Pharmacophore Models-- Ligand-based Pharmacophore Modeling-- Structure-based Pharmacophore Modeling-- Inclusion of Shape Information-- Qualitative vs. Quantitative Pharmacophore Models-- Validation of Models for Virtual Screening-- Application of Pharmacophore Models in Virtual Screening-- Pharmacophore Models as Part of a Multi-Step Screening Approach-- Antitarget and ADME(T) Screening Using Pharmacophores-- Pharmacophore Models for Activity Profiling and Parallel Virtual Screening-- Pharmacophore Method Extensions and Comparisons to Other Virtual Screening Methods-- Topological Fingerprints-- Shape-based Virtual Screening-- Docking Methods-- Pharmacophore Constraints Used in Docking-- Further Reading-- Summary and Conclusion-- 4 -- Molecular Similarity Analysis in Virtual Screening-- Ligand-Based Virtual Screening-- Foundations of Molecular Similarity Analysis-- Molecular Similarity and Chemical Spaces-- Similarity Measures-- Activity Landscapes-- Analyzing the Nature of Structure-Activity Relationships-- Relationships between different SARs-- SARs and target-ligand interactions-- Qualitative SAR characterization-- Quantitative SAR characterization-- Implications for molecular similarity analysis and virtual screening-- Strengths and Limitations of Similarity Methods-- Conclusion and Future Perspectives-- 5 -- Molecular Field Topology Analysis in drug design and virtual screening-- Introduction: local molecular parameters in QSAR, drug design and virtual screening-- Supergraph-based QSAR models-- Rationale and history-- Molecular Field Topology Analysis (MFTA)-- General principles-- Local molecular descriptors: facets of ligand-biotarget interaction-- Construction of molecular supergraph-- Formation of descriptor matrix-- Statistical analysis-- Applicability control-- From MFTA model to drug design and virtual screening-- MFTA models in biotarget and drug action analysis-- MFTA models in virtual screening-- MFTA-based virtual screening of compound databases-- MFTA-based virtual screening of generated structure libraries-- Conclusion-- 6 -- Probabilistic approaches in activity prediction-- Introduction-- Biological Activity-- Dose-Effect Relationships-- Experimental Data-- Probabilistic Ligand-Based Virtual Screening Methods-- Preparation of Training Sets-- Creation of Evaluation Sets-- Mathematical Approaches-- Evaluation of Prediction Accuracy-- Single-Targeted vs. Multi-Targeted Virtual Screening-- PASS Approach-- Biological Activities Predicted by PASS-- Chemical Structure Description in PASS-- SAR Base-- Algorithm of Activity Spectrum Estimation-- Interpretation of Prediction Results-- Selection of the Most Prospective Compounds-- Conclusions-- 7 -- Fragment-based de novo design of druglike molecules-- Introduction--From Molecules to Fragments-- From Fragments to Molecules-- Scoring the Design-- Conclusions and Outlook-- 8 -- Early ADME/T predictions: a toy or a tool?-- Introduction-- Which

properties are important for early drug discovery?-- Physico-chemical profiling-- Lipophilicity-- Solubility-- Data availability and accuracy-- Models-- Why models don't work: the challenge of the Applicability Domain-- AD based on similarity in the descriptor space-- AD based on similarity in the property-based space-- How reliable are predictions of physico-chemical properties?-- Available Data for ADME/T biological properties-- Absorption-- Data-- Models-- Distribution-- Data-- Models-- The usefulness of ADME/T models is limited by available data-- Conclusions-- 9 -- Compound Library Design -- Principles and Applications-- Introduction to Compound Library Design-- Methods for Compound Library Design-- Design for Specific Biological Activities-- Similarity Guided Design of Targeted Libraries-- Diversity Based Design of General Screening Libraries-- Pharmacophore Guided Design of Focused Compound Libraries-- QSAR Based Targeted Library Design-- Protein Structure Based Methods for Compound Library Design-- Design for Developability or Drug-likeness-- Rule & Alert Based Approaches-- QSAR Based ADMET Models-- Undesirable Functionality Filters-- Design for Multiple Objectives and Targets Simultaneously-- Concluding Remarks-- 10 -- Integrated Chemo- and Bioinformatics Approaches to Virtual Screening-- Introduction-- Availability of large compound collections for virtual screening-- NIH Molecular Libraries Roadmap Initiative and the PubChem database-- Other chemical databases in public domain-- Structure based virtual screening-- Major methodologies-- Challenges and limitations of current approaches-- The implementation of cheminformatics concepts in structure based virtual screening-- Predictive QSAR models as virtual screening tools-- Critical Importance of model validation-- Applicability domains and QSAR model acceptability criteria-- Predictive QSAR modeling workflow-- Examples of application-- Structure based chemical descriptors of protein ligand interface: the EnTESS method-- Derivation of the EnTESS descriptors-- Validation of the EnTESS descriptors for binding affinity prediction-- Structure based cheminformatics approach to virtual screening: the CoLiBRI method-- The representation of three-dimensional active sites in multidimensional chemistry space-- The mapping between chemistry spaces of active sites and ligands-- Summary and Conclusions.

Sommario/riassunto

Focuses on chemoinformatics approaches applicable to virtual screening of very large available collections of chemical compounds to identify novel biologically active molecules.

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Autore	Schreckenberg Kathrin
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Nota di contenuto	part I Evolving framings and contexts / Kate Schreckenberg -- chapter 1 Seeing the wood for the trees -- Exploring the evolution of frameworks of ecosystem services for human wellbeing / Unai Pascual -- chapter 2 Justice and equity -- Emerging research and policy approaches to address ecosystem service trade-offs / Neil Dawson -- chapter 3 Social-ecological systems approaches -- Revealing and navigating the complex trade-offs of sustainable development / Belinda Reyers -- chapter 4 Limits and thresholds -- Setting global, local and regional safe operating spaces / John Dearing -- part II Ongoing and rapid system changes / Kate Schreckenberg -- chapter 5 Interactions of migration and population dynamics with ecosystem services / W Neil Adger -- chapter 6 Land use intensification -- The promise of sustainability and the reality of trade-offs / Adrian Martin -- chapter 7 Ecosystem services and poverty alleviation in urbanising contexts / Fiona Marshall -- chapter 8 Reciprocal commitments for

addressing forest–water relationships / Lana Whittaker -- chapter 9 Restoration of ecosystems and ecosystem services / Alison Cameron -- part III Improving governance / Kate Schreckenberg -- chapter 10 Governing for ecosystem health and human wellbeing / Fiona Nunan -- chapter 11 Co-generating knowledge on ecosystem services and the role of new technologies / Wouter Buytaert -- chapter 12 PES -- Payments for ecosystem services and poverty alleviation? / Mary Menton -- chapter 13 Scaling-up conditional transfers for environmental protection and poverty alleviation / Ina Porras -- chapter 14 Social impacts of protected areas -- Exploring evidence of trade-offs and synergies / Emily Woodhouse -- part IV Achieving sustainable wellbeing / Kate Schreckenberg -- chapter 15 Multiple dimensions of wellbeing in practice / Sarah Coulthard -- chapter 16 Gender and ecosystem services -- A blind spot / Katrina Brown -- chapter 17 Resilience and wellbeing for sustainability / Lucy Szaboova -- chapter 18 Insights for sustainable small-scale fisheries / Daniela Diz -- part V Concluding thoughts / Kate Schreckenberg -- chapter 19 Ecosystem services for human wellbeing -- Trade-offs and governance / Georgina Mace.

Sommario/riassunto

Understanding how to sustain the services that ecosystems provide in support of human wellbeing is an active and growing research area. This book provides a state-of-the-art review of current thinking on the links between ecosystem services and poverty alleviation. In part it showcases the key findings of the Ecosystem Services for Poverty Alleviation (ESPA) programme, which has funded over 120 research projects in more than 50 countries since 2010. ESPA’s goal is to ensure that ecosystems are being sustainably managed in a way that contributes to poverty alleviation as well as to inclusive and sustainable growth. As governments across the world map how they will achieve the 17 ambitious Sustainable Development Goals, most of which have poverty alleviation, wellbeing and sustainable environmental management at their heart, ESPA’s findings have never been more timely and relevant.