1. Record Nr. UNISA990000794750203316

Titolo	L'educazione dei figli
Pubbl/distr/stampa	Scandicci : La nuova Italia
Descrizione fisica	v. ; 24 cm
Collana	Biblioteca di scienze dell'educazione
Disciplina	649.109
Soggetti	Famiglie -- Educazione -- Storia
Collocazione	II.4. Coll.23/ 1/(VI B Coll. 77/24)L.M.
Lingua di pubblicazione	Italiano
Formato	Materiale a stampa
Livello bibliografico	Monografia

2. Record Nr. UNINA990004241910403321

Autore	Byron, George Gordon
Titolo	Alas! The love of women! : 1813-1814 / edited by Leslie A. Marchand
Pubbl/distr/stampa	London : Murray, 1974
ISBN	0-7195-2989-1
Descrizione fisica	XIV, 285 p. ; 23 cm
Locazione	FLFBC
Collocazione	P.3 BR.C.1332(3)
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia

3. Record Nr. UNINA9910830195903321

Titolo	Computational modeling for homogeneous and enzymatic catalysis [[electronic resource]] : a knowledge-base for designing efficient catalysts / / edited by Keiji Morokuma and Djamaladdin G. Musaev
Pubbl/distr/stampa	Weinheim, : Wiley-VCH Chichester, : John Wiley [distributor], 2008
ISBN	1-282-37223-8 9786612372230 3-527-62196-2 3-527-62197-0
Descrizione fisica	1 online resource (400 p.)
Altri autori (Persone)	MorokumaK <1934-> (Keiji) MusaevDjamaladdin G
Disciplina	660.2995
Soggetti	Catalysis - Computer simulation Catalysts
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Computational Modeling for Homogeneous and Enzymatic Catalysis; Contents; Preface; List of Contributors; 1 Computational Insights into the Structural Properties and Catalytic Functions of Selenoprotein Glutathione Peroxidase (GPx); 1.1 Introduction; 1.2 Catalytic Functions; 1.2.1 Peroxidase Activity; 1.2.2 Reductase Activity; 1.3 Computational Details; 1.3.1 Computational Methods; 1.3.2 Computational Models; 1.4 Results and Discussion; 1.4.1 Refinement of the Active Site; 1.4.2 Catalytic Functions: Peroxidase Activity 1.4.3 Catalytic Functions: Effect of the Surrounding Protein on the Peroxidase Activity1.4.3.1 Hydrogen Peroxide Coordination; 1.4.3.2 Formation of Selenenic Acid [E-Se-OH]; 1.4.4 Catalytic Functions: Reductase Activity; 1.4.4.1 Peroxynitrite/Peroxynitrous Acid (ONOO /ONOOH) Coordination; 1.4.4.2 Oxidation Pathway; 1.4.4.3 Nitration Pathways; 1.5 Summary; References; 2 A Comparison of Tetrapyrrole Cofactors in Nature and their Tuning by Axial Ligands; 2.1 Introduction; 2.2 Methodology; 2.3 Comparison of the Intrinsic Chemical Properties

Sommario/riassunto

Here, the world's most active and productive computational scientists from academia and industry present established, effective and powerful tools for understanding catalysts. With its broad scope -- nitrogen fixation, polymerization, C-H bond activation, oxidations, biocatalysis and much more -- this book represents an extensive knowledge base for designing efficient catalysts, allowing readers to improve the performance of their own catalysts.