1. Record Nr. UNINA990000341270403321

Autore	Han, Chang Dae
Titolo	Multiphase flow in polymer processing / Chang Dae Han.
Pubbl/distr/stampa	New York : Academic Press, 1981
ISBN	0-12-322460-8
Descrizione fisica	XV,459 p., ill., 24 cm
Disciplina	668
Locazione	DINCH DINMP
Collocazione	04 206-24 14 P.014.048
Lingua di pubblicazione	Italiano
Formato	Materiale a stampa
Livello bibliografico	Monografia

2.

Record Nr.	UNINA9910780074703321
Autore	Neeley Kathryn A (Kathryn Angelyn), <1954->
Titolo	Mary Somerville : science, illumination, and the female mind / / Kathryn A. Neeley [[electronic resource]]
Pubbl/distr/stampa	Cambridge : , : Cambridge University Press, , 2001
ISBN	0-511-15652-9 0-511-61332-6 0-511-01965-3
Descrizione fisica	1 online resource (xvi, 263 pages) : digital, PDF file(s)
Collana	Cambridge science biographies
Altri autori (Persone)	SomervilleMary <1780-1872.>
Disciplina	500.2/092
Soggetti	Women scientists - Great Britain
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Title from publisher's bibliographic system (viewed on 05 Oct 2015).
Nota di bibliografia	Includes bibliographical references (p. 241-251) and index.
Sommario/riassunto	In an era when science was perceived as a male domain, Mary Somerville (1780-1872) became both the leading woman scientist of her day and an integral part of the British scientific community. She achieved this status through careful management of her gender identity and by creating rich, readable, and authoritative accounts of science that were rhetorically compelling, aesthetically satisfying, and valuable to the scientific community in the UK and abroad. This biography offers detailed analysis of the underlying patterns, themes, and rhetorical strategies of her major works and argues that Somerville employed a transcendent feminine style that retained the advantages but transcended the limitations usually associated with women's ways of knowing. The book advocates a new narrative for women's participation in science and demonstrates the many ways that gender relates to science and science functions in culture.

3. Record Nr. UNINA9910585940503321

Autore	Ribaudo Giovanni
Titolo	From a Molecule to a Drug: Chemical Features Enhancing Pharmacological Potential
Pubbl/distr/stampa	Basel, : MDPI - Multidisciplinary Digital Publishing Institute, 2022
Descrizione fisica	1 online resource (234 p.)
Soggetti	Medicine and Nursing Pharmacology
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Sommario/riassunto	This book collects contributions published in the Special Issue "From a Molecule to a Drug: Chemical Features Enhancing Pharmacological Potential" and dealing with successful stories of drug improvement or design using classic protocols, quantum mechanical mechanistic investigation, or hybrid approaches such as QM/MM or QM/ML (machine learning). In the last two decades, computer-aided modeling has strongly supported scientists' intuition to design functional molecules. High-throughput screening protocols, mainly based on classical mechanics' atomistic potentials, are largely employed in biology and medicinal chemistry studies with the aim of simulating drug-likeness and bioactivity in terms of efficient binding to the target receptors. The advantages of this approach are quick outcomes, the possibility of repurposing commercially available drugs, consolidated protocols, and the availability of large databases. On the other hand, these studies do not intrinsically provide reactivity information, which requires quantum mechanical methodologies that are only applicable to significantly smaller and simplified systems at present. These latter studies focus on the drug itself, considering the chemical properties related to its structural features and motifs. Overall, such simulations provide necessary insights for a better understanding of the chemistry principles that rule the diseases at the molecular level, as well as

possible mechanisms for restoring the physiological equilibrium.