

1. Record Nr.	UNINA9910298623103321
Titolo	Noncovalent Forces // edited by Steve Scheiner
Pubbl/distr/stampa	Cham : , : Springer International Publishing : , : Imprint : Springer, , 2015
ISBN	3-319-14163-5
Edizione	[1st ed. 2015.]
Descrizione fisica	1 online resource (528 p.)
Collana	Challenges and Advances in Computational Chemistry and Physics, , 2542-4491 ; ; 19
Disciplina	54 541.2 572 615
Soggetti	Chemistry, Physical and theoretical Pharmacology Biochemistry Theoretical and Computational Chemistry Pharmacology/Toxicology Biochemistry, general
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.
Nota di contenuto	Ionic interactions -- Ionic H-bonds -- Interactions -- Unusual H-bonds -- Charge-inverted HBs -- Dihydrogen bonds -- Cooperativity on Supramolecular Level -- Moderate Strength -- Halogen bonds -- Chalcogen Bonds -- Pnicogen Bonds -- Aromatic -- Attraction -- Radicals -- Weaker Forces -- Aromatic stacking -- Rare gases.
Sommario/riassunto	Computational methods, and in particular quantum chemistry, have taken the lead in our growing understanding of noncovalent forces, as well as in their categorization. This volume describes the current state of the art in terms of what we now know, and the current questions requiring answers in the future. Topics range from very strong (ionic) to very weak (CH--) interactions. In the intermediate regime, forces to be considered are H-bonds, particularly CH--O and OH--metal, halogen, chalcogen, pnicogen and tetrel bonds, aromatic stacking, dihydrogen bonds, and those involving radicals. Applications include

drug development and predictions of crystal structure.
