Nature of Supramolecular Interactions - Legami deboli

Week interactions are relatively weak compared to normal chemical bonds, but play a fundamental role in fields as diverse as supramolecular chemistry, structural biology, polymer science, nanotechnology, surface science, and condensed matter physics.

Van der Waals forces define the chemical character of many organic compounds.
They also define the solubility of organic substances in polar and non-polar media.
In low molecular weight alcohols, the properties of the polar hydroxyl group dominate the weak intermolecular forces of van der Waals. In higher molecular weight alcohols, the properties of the nonpolar hydrocarbon chain(s) dominate and define the solubility. Van der Waals-London forces grow with the length of the non polar part of the substance.

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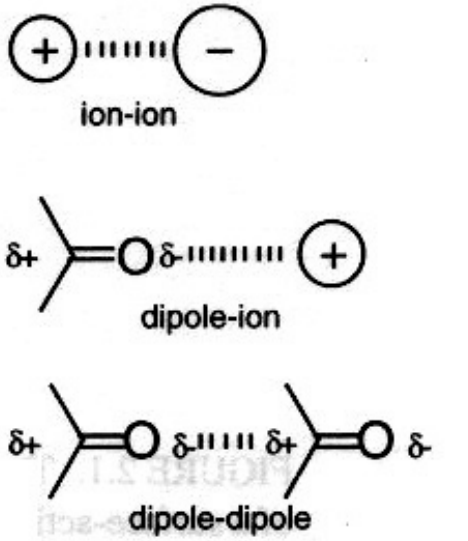
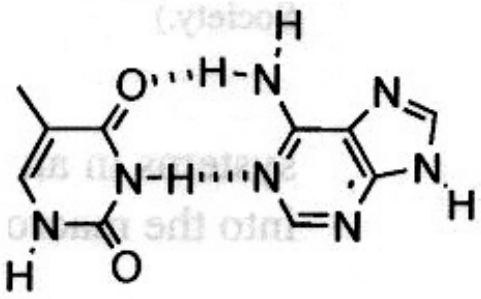
TABLE 2.1. Intermolecular interactions

Interaction	Interaction Strength[a] (kJ mol^{-1})	Description	Example
Electrostatics	>190 (ion-ion) 40–120 (ion-dipole) 5–40 (dipole-dipole)	coulombic interactions between opposite charges	
Hydrogen bonding	15–40 (strong) 5–15 (moderate <5(weak)	donor-acceptor interactions specifically involving hydrogen as the proton donor and a base as the proton acceptor	

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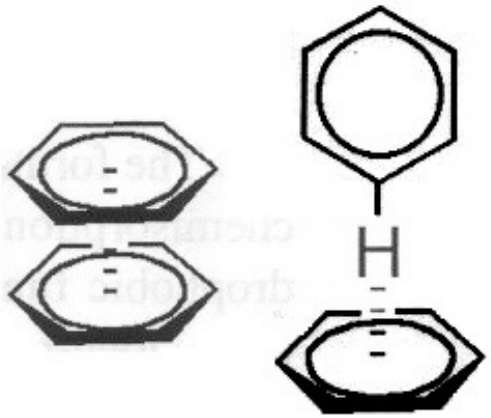
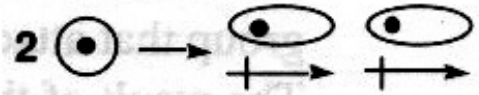
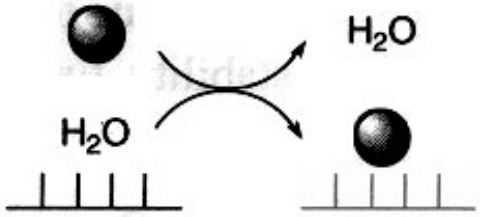
Interaction	Interaction Strength[a] (kJ mol^{-1})	Description	Example
π-π Interactions	10–15 (face to face) 15–20 (edge to face)	attractive forces between electron-rich interior of an aromatic ring with the electron-poor exterior of an aromatic ring	
Dispersion forces Van der Waals	<5	momentary induced dipole-dipole interactions (also called London forces)	
Hydrophobic effects	varied 5–40	association of non-polar binding partners in an aqueous medium or vice versa	

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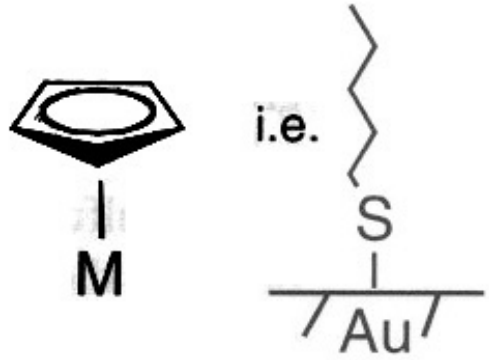
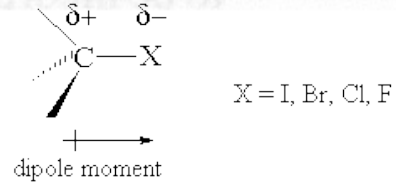
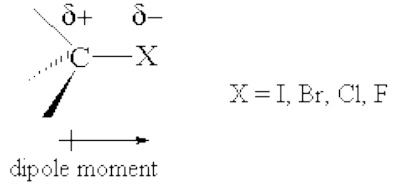
Interaction	Interaction Strength[a] (kJ mol^{-1})	Description	Example
Dative bonding	varied 20–380	coordination of a metal by a ligand donating two electrons	

[a] Association constants are for systems in chloroform.



Halogen Bond (def. *Pure Appl. Chem.* **2013**, *85*, 1711)

A halogen bond R−X···Y−Z occurs when there is evidence of a net attractive interaction between an electrophilic region on a halogen atom X belonging to a molecule or a molecular fragment R–X (where R can be another atom, including X, or a group of atoms) and a nucleophilic region of a molecule, or molecular fragment, Y−Z.

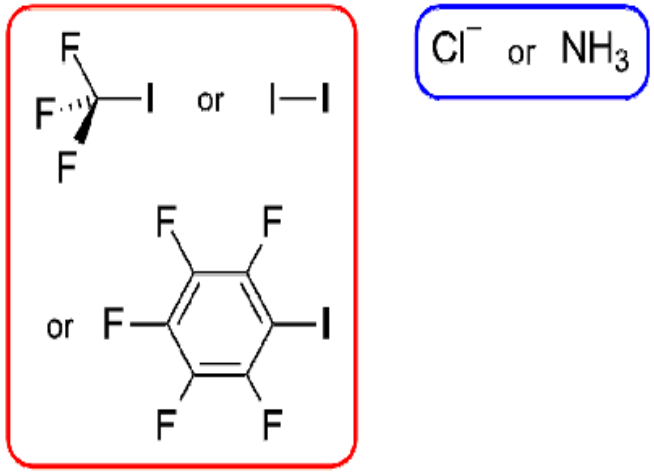


2.9 – 7.0 kJ mol^{-1} 0.7 – 1.7 kcal/mol

Halogen Bond Adducts

R–X -------- :LB

Halogen Bond Donor (Lewis Acid) *Halogen Bond Acceptor (Lewis Base)*



Legami deboli

1 cal = 4.16 Joule

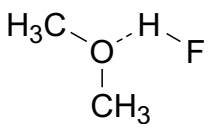
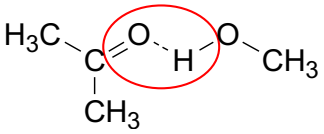
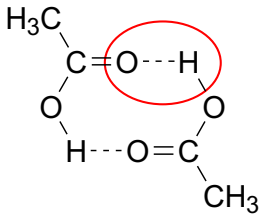
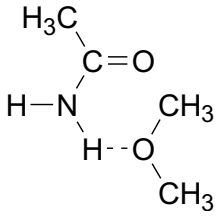
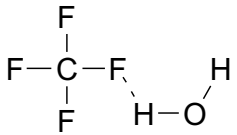
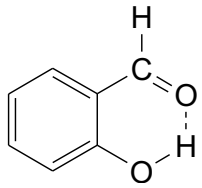
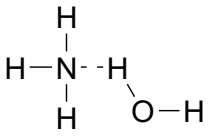
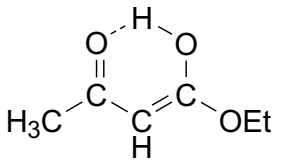
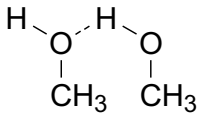
legami covalenti: 50÷100 kcal/mol

interazioni di van der Waals: alcuni decimi di kcal/mol
(attrazione elettrostatica dipolo-dipolo)

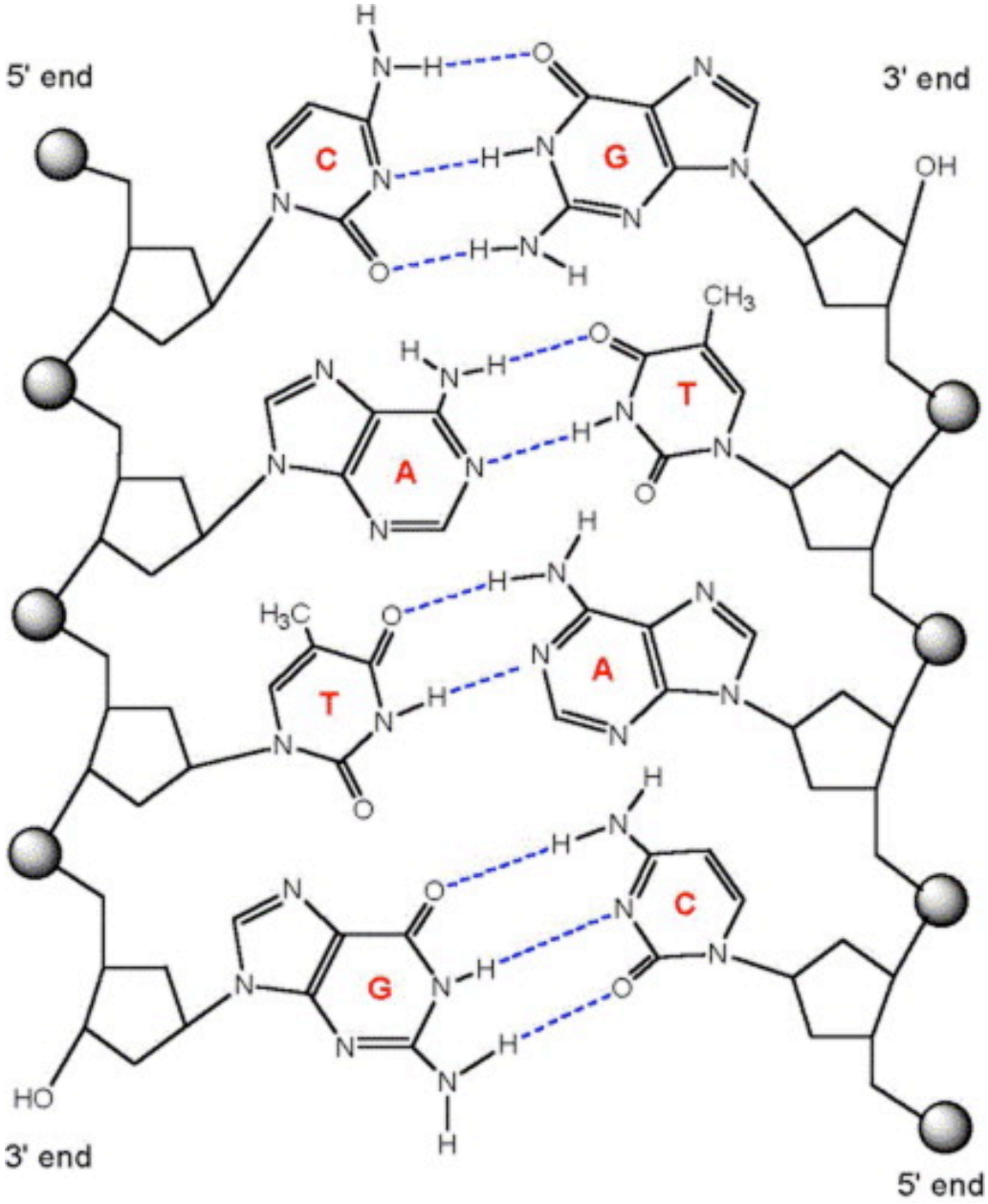
legami deboli: 2÷10 kcal/mol

H-F 568 kJ/mol
C-C 348 kJ/mol

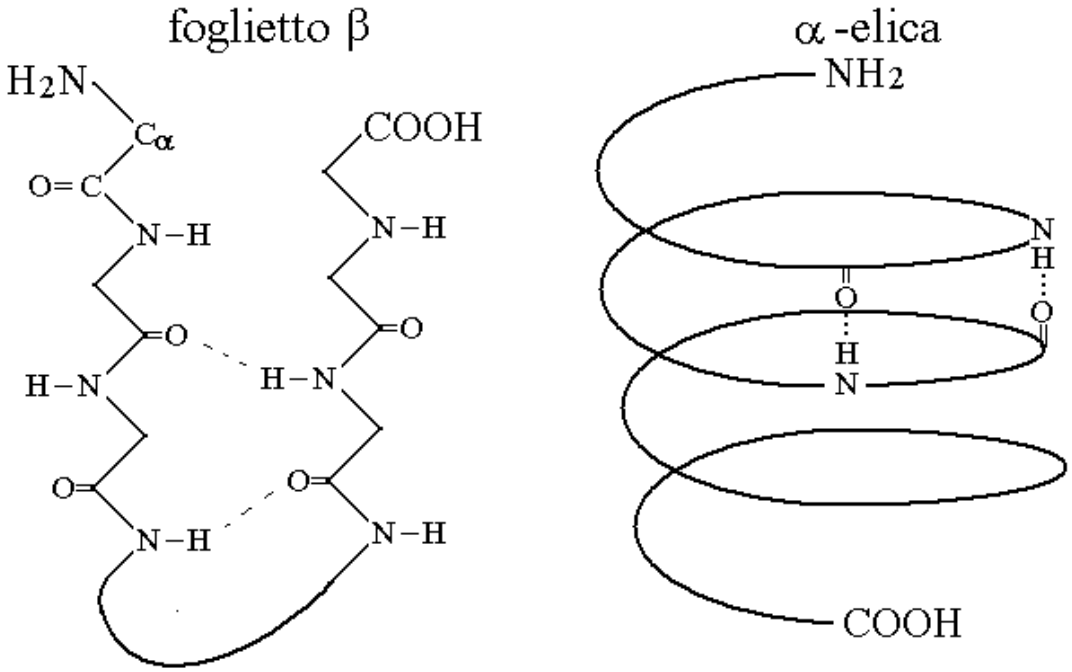
legami ad idrogeno

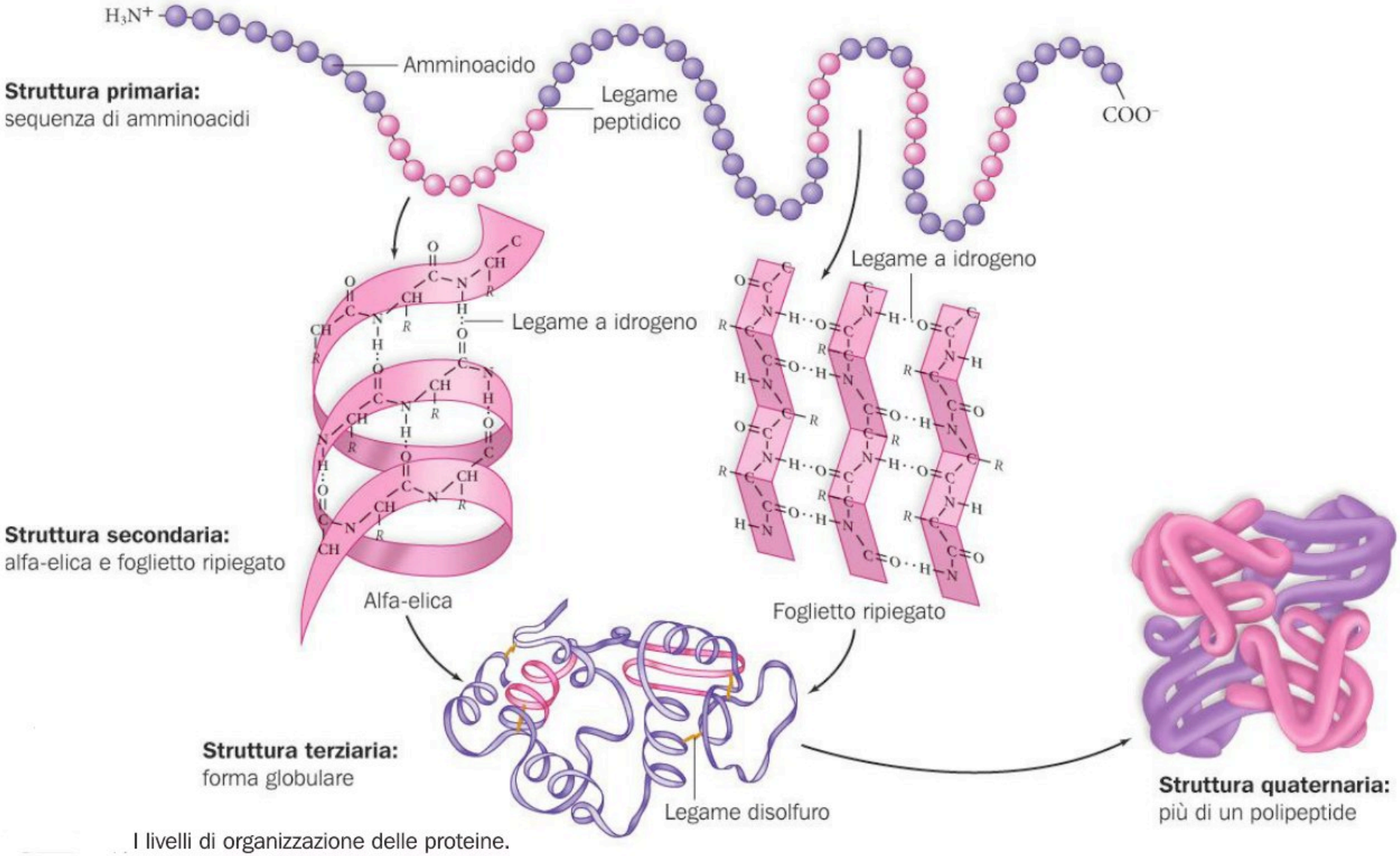
H-bond tra basi azotate in doppio strand DNA



In sequenze peptidiche:

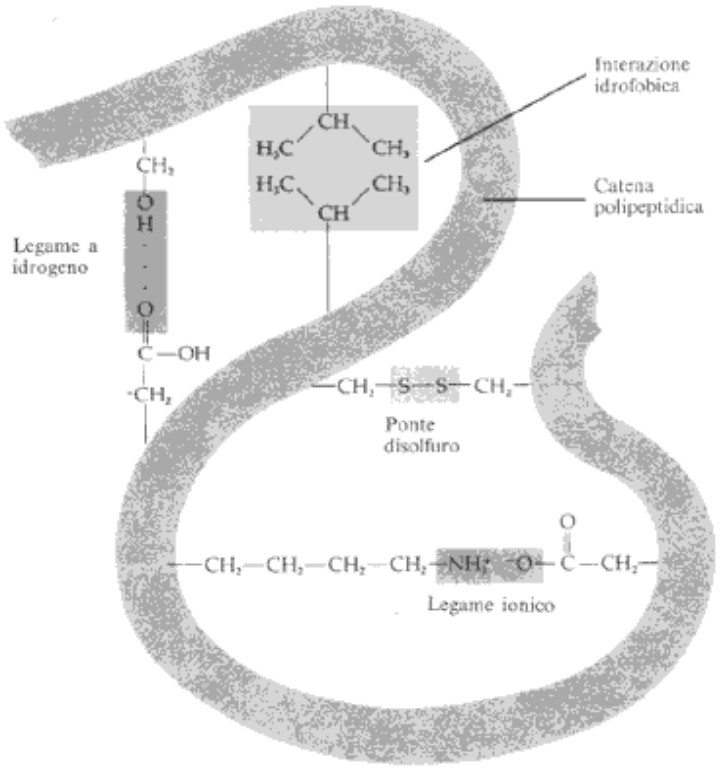


Interazioni deboli in proteine



I livelli di organizzazione delle proteine.

Interazioni deboli in proteine



LEGAMI COVALENTI

legame	energia, kcal mol^{-1}
H-F	135
H-H	104
C-H	99
C-C	79
O-H	110
C=C	141
S-H	88