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The salt bridge - systematic QM and database search study

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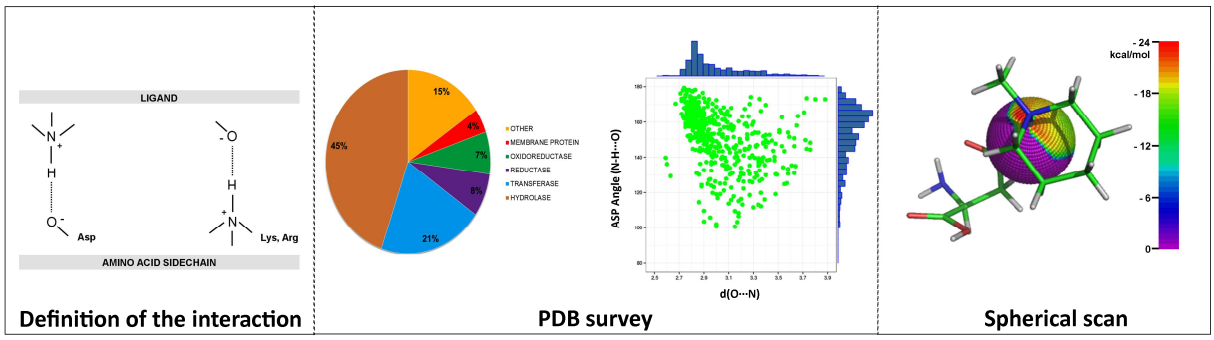
Salt bridges occur frequently in proteins, providing conformational specificity and contributing to molecular recognition [1]. It can be defined as an interaction between two groups of opposite charge in which at least one pair of heavy atoms is within hydrogen bonding distance, moreover, it was also classified as an double charge-assisted hydrogen bond (+/-CAHB) by Gilli et al. [2]. Among all known non-covalent ligand-protein interaction salt bridge is the strongest one [3], however, no comprehensive study of their role and significance in drug design have been performed so far.



Herein we report on a systematic study of the role and nature of salt bridge in biological systems including: comprehensive geometrical and target occurrence analysis of Protein Data Bank survey and quantum mechanical-based study of the geometrical preferences of several model salt bridges. The results indicated that salt bridge is a key interaction in many different drug targets and shows larger hydrogen bond contribution than ionic.

[1] Donald JE. et al., *Proteins*, 79(3) (2011) 898-915,
[2] Gilli P. et al. *J. Mol. Struct*. 552 (2000) 1-15,
[3] Xie NZ. et al. *PLOS One* 10(9) (2015) 1-19,

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