

Computational Chemistry Labs – Spring 2011

Alkaline and Alkaline-Earth Metal Cation Hydration: Computational Chemistry Investigations. Reference: J. Chem. Ed. 2009, Vol. 86, Issue 12, p. 1403.

Identification of unknown proteins using structural bioinformatics

Conformational analysis of glutathione in the gas phase and aqueous solution

Differences in covalency between trivalent lanthanides (Gd^{3+}) and actinides (Cm^{3+}) with oxygen and sulfur donor ligands