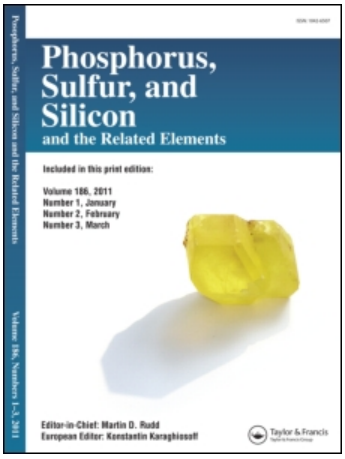

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Bio-Relevant Derivatives of Calixarene Phosphonic Acids

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Bio-Relevant Derivatives of Calixarene Phosphonic Acids

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The calix[4]arenes functionalized at the macrocyclic upper rim with α-hydroxyphosphonic, α-aminophosphonic or methylnebisphosphonic acid groups were synthesized. The complexes formed between the bio-relevent calix[4]arene derivatives and amino acids or dipeptides as well as inhibition effects of calix[4]arene phosphonic acids on alkyline phosphatases acitiy were studied.

Keywords Calixarene; phosphonic acids; enzyme; inhibition; amino acids

Calixarenes endowed with aminoacid or peptide units demonstrate a high bioactivity.[1] Within the project, we have synthesized and investigated a series of the cone-shaped calix[4]arenes functionalyzed at the macrocyclic upper rim with biorelevant α- hydroxyphosphonic or α-aminophosphonic or methylenebisphosphonic acid groups.[2–4]

Complexation of calix[4]arene bis-α-hydroxyphosphonic acids (*Racemic* or *Meso* forms) with a series of natural amino acids and dipeptides was investigated by calorimetry, NMR and molecular modelling methods.[3] The association constants of the host-guest complexes in methanol (up to 45000 M^{-1}) were determined. Hydrophobic, electrostatic, N-H-π, C-H-π interactions in the host-guest complexes are discussed.

Calix[4]arenes grafted with the α-hydroxyphosphonic or α-aminophosphonic or methylene-bis-phosphonic acid groups significantly overcome modelling acyclic phosphonic acids in inhibition of

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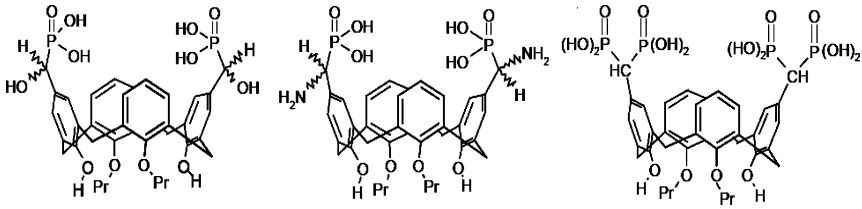

bovine intestinal and porcine kidney alkaline phosphatases.[2,4] In Tris-HCl buffer (pH 9) the (*R*, *R*) diastereomer of calixarene bis-α-aminophosphonic acid demonstrates 50 fold higher potency than the (*S*, *S*) diastereomer.[4]

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