

Slovenian NMR Centre

@ National Institute of Chemistry

vabi na SEMINAR:

Dieter Buyst

NMR & structural analysis unit

Department of Organic and Macromolecular Chemistry, Ghent University

Krijgslaan 281 S4, B-9000 Gent

Belgium

z naslovom:

Identification of a pKa-regulating motif stabilizing imidazole modified double stranded DNA

v četrtek, 12. februarja 2015 ob 15:00

v Veliki predavalnici na Kemijskem inštitutu, Hajdrihova 19, Ljubljana

Kratek povzetek:

Inspired by nature, the de novo design of artificial enzymes using physico-chemical principles, intuition and computational methods is rapidly coming of age. Using a 14-mer DNA duplex as a rigid scaffold for the precise and predictable positioning of catalytic functionalities, our systems of interest can be classified as first generation hydrolase-like DNAzymes equipped with one histidine mimicking functionality based on a modified thymine nucleotide building block (TIm). The mutual interactions between the imidazole and the duplex and its influence on the imidazolium pKa_H are investigated by placing a single modified thymine at four different positions in the center of the 14-mer double helix. Using NMR and unrestrained MD simulations, a structural motif involving the formation of H-bond between the imidazole and the Hoogsteen side of the guanine bases of two neighboring GC base pairs is established. The motif contributes to stabilization against thermal melting of 6 °C and is key inmodulating the pKa_H of the imidazolium group.

prof. dr. Janez Plavec e-pošta: janez.plavec@ki.si tel: 01-47-60-353