ratory [2] we established that calcium ion can be bound tigtly in the molecule and this binding increases the affinity of the protein to N-acetylglucosamine and N-acetylgalactosamine. The positions of binding sites has been suggested by molecular modeling and proved by site-directed mutagenesis.

These data allowed us to find potential high affinity ligands among branched oligosaccharides terminated with N-acetylglucosamine units. We isolated these molecules by deglycosylation of ovomucoid and characterized them by mass spectrometry. From results of our binding studies we can conclude that pentaantenary structure is the ligand with the highest known affinity for CD69 molecule. It has been published [3, 4] that similar structures are expressed on the surface of some tumor cells. This finding indicates that one role of CD69 molecule on the cells of the immune system may be to attract killer lymphocytes to the tumor sites.

Acknowledgement: *This work was supported by Institutional Research Concept No. AV0Z5020903 (for Institut of Microbiology) and by grants MSM 113100001, GACR 203/01/1018 and A7020006.*

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A DFT INVESTIGATION OF STRUCTURE-CHEMICAL SHIFT RELATIONSHIPS FOR 13C AND 15N IN DNA

Jana Přecechtělová, Markéta L. Munzarová and Vladimír Sklenář

National Centre for Biomolecular Research, Faculty of Science, Masaryk University, Kotlárská 2, CZ-611 37 Brno, Czech Republic

Density functional theory has been applied to explore the dependence of ^{13}C and ^{15}N chemical shifts in deoxyribonucleosides on various structural features such as the orientation about the glycosidic bond, the CH2OH group conformation, the sugar pucker, and the hydrogen bonding. Geometry optimizations have been performed with sugar-phosphate backbone dihedral angles frozen to their average experimental values in BI-DNA. Results obtained in NMR parameter calculations have been compared to available experimental data for C1`, C2` and N9.

The effect of the glycosidic torsion angle has already been studied [1] but we wished to involve the relaxation of the geometry after changing , which has not been considered in the previous work [1]. C1`, C2` and N1/N9 chemical shifts appeared to be influenced most by the base orientation. The trends uncovered in chemical shifts are significantly different from those reported previously [1] and the absolute chemical shift values are in the case of C2` approximately the same for all deoxyribonucleosides, except for the anti orientation of the base. On the contrary, for C1` and N1/N9 the trends for purine nucleosides differ from those for pyrimidine nucleosides and the absolute N1 chemical shifts in deoxycytidine are found upfield relative to deoxythymidine.

Besides the influence of varying the glycosidic torsion angle, we wanted to assess the effect of the sugar puckering and the hydroxymethyl rotation, both of which were studied on deoxyguanosine. N9 experienced the largest changes, namely 10 or 8 ppm difference between the south and north conformation in both the syn and anti region, respectively. The N9 chemical shift for deoxyguanosine (*S, anti, gg*) differed significantly from the other two CH_2OH-rotamers.

The comparison with the experiment has been carried out using the data from BMRB database [2] (C1`, C2`) and the data for the $[d(G_4T_4G_4)]_2$ quadruplex (C1`, N9) [3], on which changes upon the hydrogen bonding have also been studied.

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NATURE OF STACKING INTERACTIONS BETWEEN INTERCALATORS AND DNA BASE PAIRS. AB INITIO QUANTUM-CHEMICAL, DENSITY FUNCTIONAL THEORY AND EMPIRICAL POTENTIAL STUDY.

David Řeha, Martin Kabeláč, Filip Ryjáček, Jiří Šponer and Pavel Hobza

J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, and Center for Complex Molecular Systems and Biomolecules, 182 23 Prague 8, Czech Republic

Properties of isolated intercalators (ethidium (E), daunomycin (D), ellipticine (EL) and 4,6'-diaminido-2-phenylidone (DAPI)) and their stacking interactions with adenine…thymine (AT) and guanine…cytosine (GC) nucleic acid base pairs were investigated by means of a nonempirical correlated *ab initio* method [1]. All intercalators exhibit large charge delocalization and neither of them (including dicationic DAPI) exhibit a site with dominant charge. All intercalators have large polarizability and are good electron acceptors while base pairs are good electron donors. MP2/6-31G*(0.25) stabilization energies of complexes intercalator…base pair are large (E…AT : 22.4 kcal/mol; D…GC :17.8 kcal/mol; EL…GC :18.2 kcal/mol; DAPI…GC :21.1 kcal/mol) and are well reproduced by modified AMBER potential (vdW radii of intercalator atoms are enlarged and their vdW energy depths are increased). Standard AMBER potential give less satisfactory results especially for DAPI containing complexes. Because DAPI is the best electron acceptor (among all