according to the Sauerbray equation, the density of coatings was assumed to be equal 1.3 g/cm^3 [4].

Table. Properties of PAH-PEG/DexScoatings

PAH-PEG	m(PEG)/m(PAH), mg/mg	Grafting degree (g)	Bilayer thick-ness*, nm	Mass of adsorbed FBS proteins**, μg/cm^2
PAH	–	–	0.7	1.6
1	0.2	58	1.0	1.0
2	2.7	18	1.1	0.7
3	5.5	9.6	0.9	0.6
4	11.0	5.3	0.9	0.2

* ± 15 %; ** ± 0.2 μg/cm^2

Thus, replacing PAH in a $(PAH/DexS)_{3.5}$ coating by PEG-grafted copolymer allowed us to reduce FBS proteins adsorption on the films surface by 38–88 %.

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Aggregation of kanamycin A. Quantum chemical calculations

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Kanamycin is an aminoglycoside antibiotic. The study of the structure of kanamycin provides valuable information for the investigation of other antibiotics, which can facilitate an understanding of their biological activity, and is also useful for molecular modeling calculations. The absolute configuration of kanamycin A was determined by X-ray diffraction study of kanamycin monosulfate [1]. Kanamycin can form stable dimers and higher aggregates in solutions. However, in literature there are a few data on the aggregation of kanamycin. Theoretical determination of the structure of kanamycin dimer is a difficult task, because kanamycin is a flexible molecule and a lot of conformations should be considered.

In this work, the structure of kanamycin A dimer has been investigated. The semi-empirical GFN-xTB method has been used for the conformational search to obtain the initial structures for global minimum searching. The resulting

structures were ranked by energy and the geometry of the ten lowest energy structures has been optimized using PBEh-3c method, which is more accurate than the widely used B3LYP/6-31G(d). Obtained global minimum dimer structure (Fig.) is more than 150 kJ/mol lower in energy than the kanamycin A monomer in the gas phase. For this lowest energy structure electronic properties, NMR and IR spectra have been calculated.

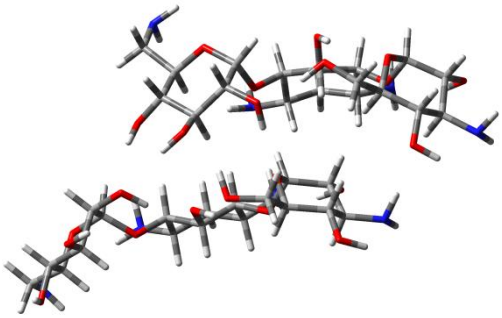

Fig. The calculated lowest energy structure of kanamycin A dimer

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Formation enthalpies of five-membered nitrogen-containing aromatic heterocycles. Quantum chemical calculations

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Five-membered nitrogen-containing aromatic heterocycles are important due to their wide application in various fields of technology, medicine, agriculture. In addition, tetrazoles and nitrotriazoles have a sufficiently high thermal stability along with considerable energetics and high nitrogen content, therefore they are effective components of composite propellants, explosive and gas-generating compositions. So, it is especially important to have information on the enthalpy of formation of these substances. Thermodynamic properties are also useful for developing methods of selective azole ring functionalization or introduction of azole fragment into more complex molecules. However, in literature there are a few data on the formation enthalpies of these compounds.