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COMPUTATIONAL NMR OF CARBOHYDRATES: THEORETICAL BACKGROUND, APPLICATIONS, AND PERSPECTIVES

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ВЫЧИСЛИТЕЛЬНЫЙ ЯМР УГЛЕВОДОВ: ТЕОРЕТИЧЕСКИЕ ПРЕДПОСЫЛКИ, ПРИМЕНЕНИЕ И ПЕРСПЕКТИВЫ

Abstract. A review of the main trends and prospects in the field of stereochemical analysis of carbohydrates using computational NMR is carried out

Keywords: computational NMR, ^{1}H and ^{13}C NMR chemical shifts, spin-spin coupling constants, monosaccharides, polysaccharides.

Аннотация. Проведен обзор основных тенденций и перспектив в области стереохимического анализа углеводов с использованием вычислительного ЯМР.

Ключевые слова: вычислительный ЯМР, химические сдвиги ЯМР ^{1}H и ^{13}C, константы спин-спинового взаимодействия, моносахариды, полисахариды.

A major breakthrough the stereochemical studies of carbohydrates by means of computational NMR as compared to experiment has been achieved by Serianni and coworkers who demonstrated that stereochemical analysis of carbohydrates could mostly be performed by using experimental and computational ^{1}H and ^{13}C NMR chemical shifts and spin-spin coupling constants in view of their marked stereochemical dependences.

This review is written amid a marked progress in the calculation of NMR chemical shifts and spin-spin coupling constants of carbohydrates substantiated by a vast amount of experimental data coming from several laboratories. By no means are we trying to cover in the present compilation a huge amount of all available data. The main idea of the present review was to outline the general trends and perspectives in this dynamically developing area on the background of a marked progress in theoretical and computational NMR. The material is arranged in three basic sections: a short theoretical introduction, applications and perspectives in computational NMR of monosaccharides, and computational NMR of di- and polysaccharides.

As an example, $^{3}J_{H,H}$ values, measured experimentally and calculated theoretically, exercised a profound role in the assigning of the preferred conformations of furanose and pyranose rings. This topic is well covered in recent books, book chapters, and numerous reviews from Serianni's group (see most recent reviews by Klepach *et al*. [1] and Hadad *et al*. [2]) and in comprehensive reviews by Toukach and Ananikov [3] and Krivdin [4,5,6]. Those reviews providing a new guide in the fundamental factors controlling molecular recognition and catalysis in biochemical systems. By no means are we trying to cover in the present compilation a huge amount of data coming mostly from Serianni's laboratories. The main idea of the present re-

view was to outline the main trends and perspectives in this field in view of a marked progress of computational NMR [7], applied to the calculation of chemical shifts and spin-spin coupling constants.

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