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Synthesis and CD anomeric assignment of novel disubstituted 2-(β-L-erythrofuranosyl)benzimidazole C-nucleoside analogs

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A series of 2-(β-L-erythrofuranosyl) benzimidazole C-nucleoside analogs having 5,6 dichloro and 5,6-dimethyl substituents at the base moiety as well as naphthbenzimidazole have been prepared by dehydrative cyclization of the corresponding acyclic 2-(L-arabino-tetritol-1-yl) benzimidazole analogs. The ECD (electronic circular dichroism) spectra of the prepared C-nucleoside analogs were studied. The anomeric configuration was obtained from their ^{1}H NMR spectra and confirmed by ECD spectra. "In addition to the experimental work we performed *ab initio* calculations (MP2/6-311++G**) on the structures as well as calculations at the time-dependent level of density functional theory (TD/B3LYP/6-311++(3df,3pd)) including 30 states on the CD (circular dichroism) spectra of some of the compounds under consideration. The solvents were included by means of the CPCM model. Comparison of the calculated with the experimental CD spectra allow a detailed analysis of the involved states and might provide a theoretical foundation for the extension of a recently derived empirical rule for the anomeric configuration of 1,2,3-triazole C-nucleoside to benzimidazole C-nucleoside analogs.

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