

Zwitterionic phosphorylated quinines as chiral solvating agents for NMR spectroscopy.

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Streszczenie

Because of their unique 3D arrangement, naturally occurring *Cinchona* alkaloids and their synthetic derivatives have found wide-ranging applications in chiral recognition. Recently, we determined the enantioselective properties of C-9-phosphate mixed triesters of quinine as versatile chiral solvating agents in nuclear magnetic resonance (NMR) spectroscopy. In the current study, we introduce new zwitterionic members of this class of molecules containing a negatively charged phosphate moiety (i.e., ethyl, *n*-butyl and phenyl hydrogen quininyll phosphate). An efficient approach for synthesizing these compounds is elaborated, and full characterization, including conformational and autoaggregation phenomena studies, was performed. Therefore, their ability to induce NMR anisochrony of selected enantiomeric substrates (i.e., primarily *N*-DNB-protected amino acids and their methyl esters) was analyzed compared to uncharged diphenyl quininyll phosphate and its positively charged quaternary ammonium hydrochloride salt. In addition, ^1H and ^{13}C NMR experiments revealed their enantiodiscrimination potential toward novel analytes, such as secondary amines and nonprotected amino acids.

Słowa kluczowe

phosphorylated quinine, enantiodiscrimination, Amino acids, nuclear magnetic resonance spectroscopy

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