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# Theoretical p$K_a$ prediction of the α-phosphate moiety of uridine 5'-diphosphate-GlcNAc

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**Abstract**

The p$K_a$ value of the α-phosphate moiety of uridine 5'-diphosphate-GlcNAc (UDP-GlcNAc) has been successfully calculated using density functional theory methods in conjunction with the Polarizable Continuum Models. Theoretical methods were benchmarked over a dataset comprising of alkyl phosphates. B3LYP/6-31+G(d,p) calculations using SMD solvation model provide excellent agreement with the experimental data. The predicted p$K_a$ for UDP-GlcNAc is consistent with most recent NMR studies but much higher than what it has long been thought to be. The importance of this study is evident that the predicted p$K_a$ for UDP-GlcNAc supports its potential role as a catalytic base in the substrate-assisted biocatalysis.

**Keywords**

UDP-GlcNAc; OGT; Gaussian; p$K_a$; Density functional theory; SMD

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