

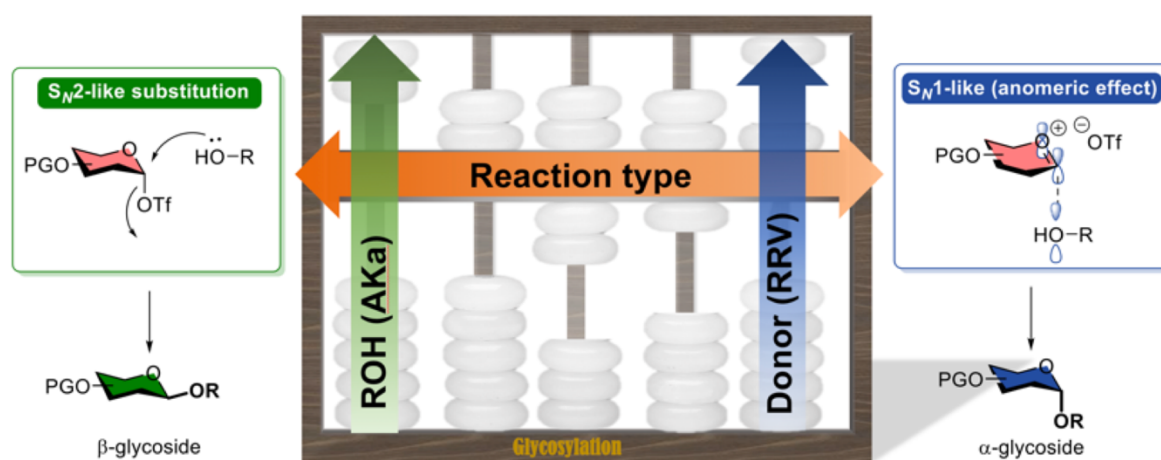
Statistical Analysis: A New Perspective on Stereoselective Glycosylation Reactions

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Carbohydrates are ubiquitous biomolecules that mediate numerous biological processes and exhibit important pathogenic effects. However, chemical synthesis of glycoconjugates has been hampered by challenges in glycosylation reaction, of which the stereoselectivity and yield are paramount but unpredictable. We develop a database composed of relative reactivity value (RRV) [1-5] and acceptor nucleophilic constant (AKa) [6] to quantify the reactivity of glycosyl donors and nucleophilicity of hydroxyl groups in glycosylation influenced by the steric, electronic and structural effects, providing a connection between experiments and computer algorithm. A diverse range of glycosylation donors and acceptors with well-defined reactivity and promoters were organized and processed by the designed program "GlycoComputer" for prediction of glycosylation reaction without involving sophisticated computational processing. The applicability of this system was further tested by the synthesis of a Lewis A skeleton to show that the stereoselectivity and yield can be accurately estimated.[6]



A predictive platform for stereoselective glycosylation reactions using RRV and Aka

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