Optimization of glycosylation with glycosyl fluoride by using machine learning

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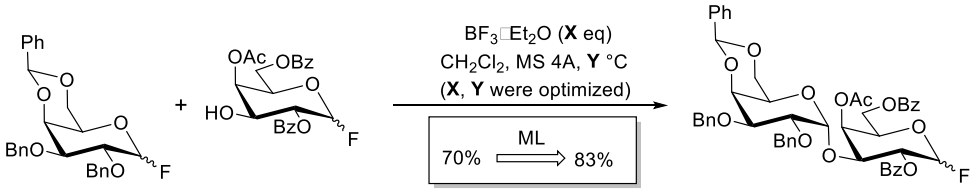
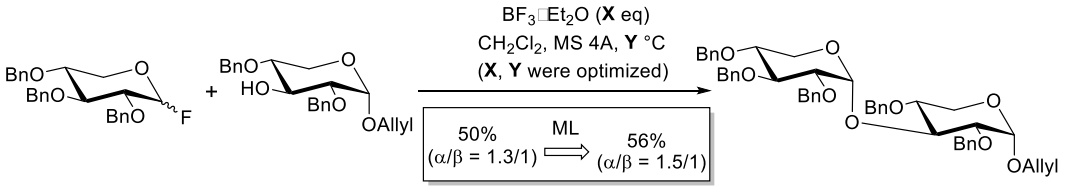
In this study, machine learning was applied to the optimization of glycosylation reactions using glycosyl fluoride. First, we investigated selective activation of armed glycosyl fluoride in the presence of disarmed glycosyl fluoride (Scheme 1). After obtaining XX data set, reaction conditions were optimized by machine learning. Then, the yield was improved from XX% to XX%. We also investigated α-selective xylosylation (Scheme 2). After the reaction condition optimization, the α-selectivity was improved from 1.3/1 to 1.5/1. Further optimization combining machine learning and microflow system is under investigation. These results demonstrate the usefulness of machine learning for the investigation of reaction conditions of glycosylation, which involves complex reaction processes and is difficult to control chemo- and stereo-selectivity.



Scheme 1. Glycosylation between aremed and disarmed glycosyl fluorides.



Scheme 2. α-Selective xylosylation.