NMR Isotope Tracking Reveals Cascade Steps in Carbohydrate Conversion by Sn-Beta - DTU Orbit (19/08/2019)

Quantitative isotope tracking studies were used to investigate the reaction pathways occurring for Sn-Beta catalyzed carbohydrate conversion to various alpha-hydroxy esters. Experimental insight into the conversion of pentoses was sought (i) by identifying pathways based on isotope patterns in the reaction products and (ii) through probing asymmetric isotope incorporation into products. The results indicate that reaction intermediates remain coordinated to the active site throughout the reaction cascades, regardless of the reaction pathway. A predominant transformation of the C1 carbohydrate position to the C3 position of methyl lactate resembles enzymatic glycolysis. Likewise, the majority of retro-aldol cleavage occurs from the carbohydrate in the ketose form, again resembling biological glycolysis. In addition, various side-activities are detected in Sn-Beta catalyzed carbohydrate conversion, including 5,1-hydride and 1,2-carbon shift reaction of the carbohydrates.

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