Multi-enzymatic cascade synthesis of D-fructose 6-phosphate and deoxy analogs as substrates for high-throughput aldolase screening

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Electronic Supplementary Information

1) ¹H NMR spectrum of 1-deoxy-D-fructose 6-phosphate (500 MHz, D₂O)

2) ¹³C NMR spectrum of 1-deoxy-D-fructose 6-phosphate (125 MHz, D₂O) overview

3) ¹³C NMR spectrum of 1-deoxy-D-fructose 6-phosphate (125 MHz, D₂O), expanded signals

4) Reaction control by t.l.c. for routes A and B
$^1$H-NMR 1-deoxy-fructose-6-phosphate in D$_2$O (500 MHz)
$^{13}$C-NMR spectrum of 1-deoxy-fructose-6-phosphate in D$_2$O (125 MHz)
$^{13}$C-NMR spectrum of 1-deoxy-fructose-6-phosphate in D$_2$O (125 MHz)

$^{13}$C NMR (126 MHz, D$_2$O) δ 80.02 (d, $J = 8.2$ Hz), 79.02 (d, $J = 8.4$ Hz), 69.62 (d, $J = 7.5$ Hz), 66.08 (d, $J = 5.0$ Hz), 65.84 (d, $J = 5.0$ Hz), 64.39 (d, $J = 4.5$ Hz).
Documentation of reaction control by t.l.c. for routes A and B

Route A: aldol-aldol cascade

Start | 1 h | 2 days
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Fru1,6P₂ | | 1dFru6P

Route B: aldol-kinase cascade

Start | 12 h | 24 h | 4 days
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1dFru | | | 1dFru6P
ATP | ADP | ATP