

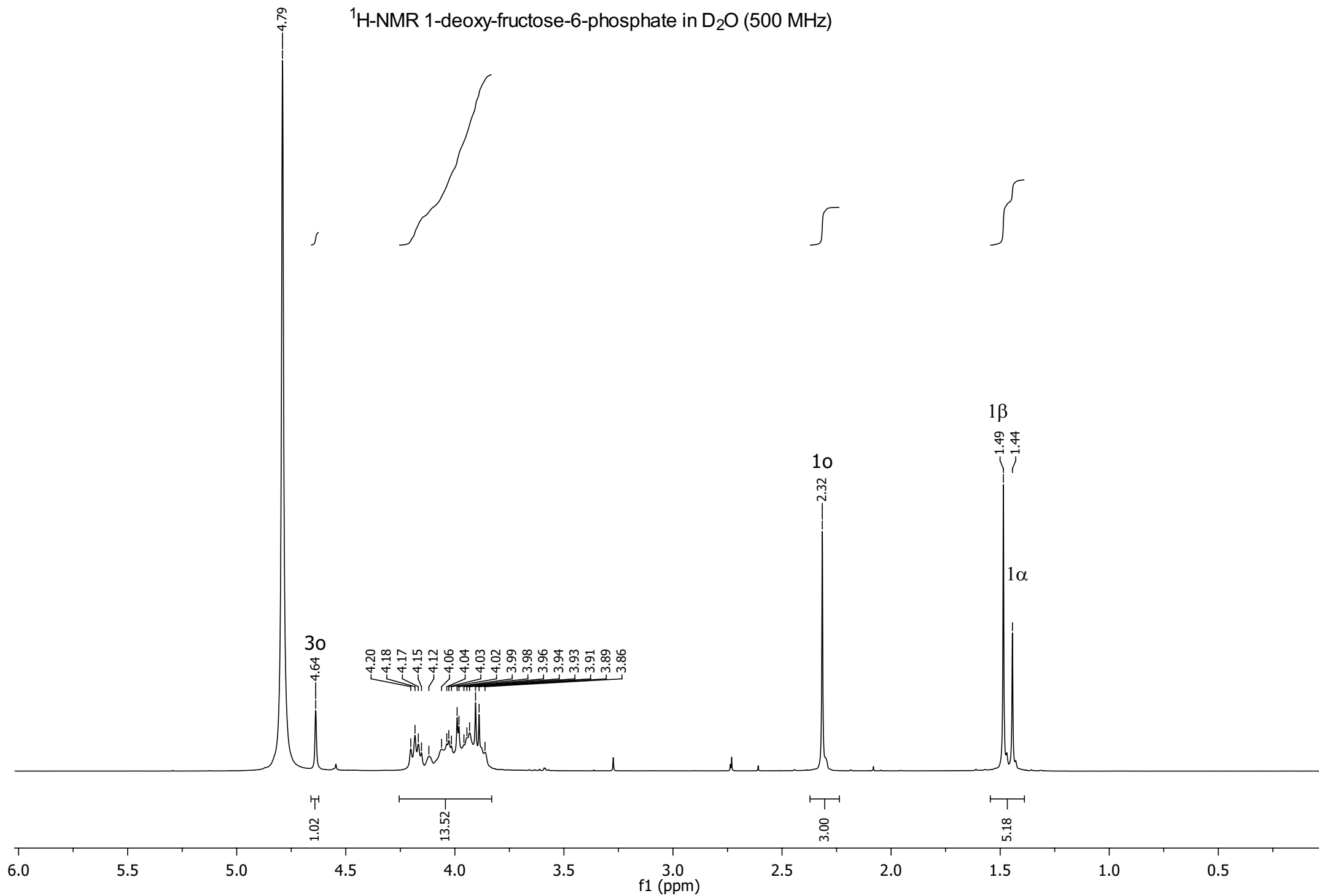
Multi-enzymatic cascade synthesis of D-fructose 6-phosphate and deoxy analogs as substrates for high-throughput aldolase screening

Wolf-Dieter Fessner,^{*a} Dirk Heyl^a and Madhura Rale^a

^a *Technische Universität Darmstadt, Institut für Organische Chemie und Biochemie,
Petersenstr. 22, 64287 Darmstadt, Germany. Fax: +49 6151 166636; Tel: +49 6151 166666;
E-mail: fessner@tu-darmstadt.de*

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



¹³C-NMR spectrum of 1-deoxy-fructose-6-phosphate in D₂O (125 MHz)

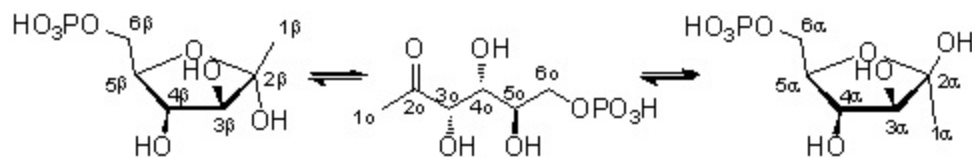
— 213.60

— 105.26

— 101.61

82.15
80.29
79.88
79.26
76.81
76.41
74.58
70.09
69.84
65.60
65.39
64.11

25.66
23.84
21.70



1β

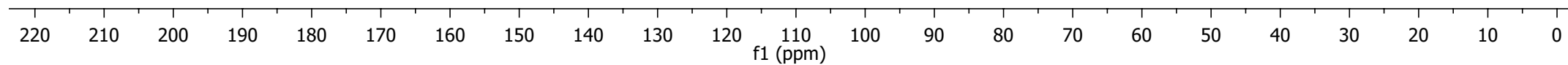
1o

1α

2β

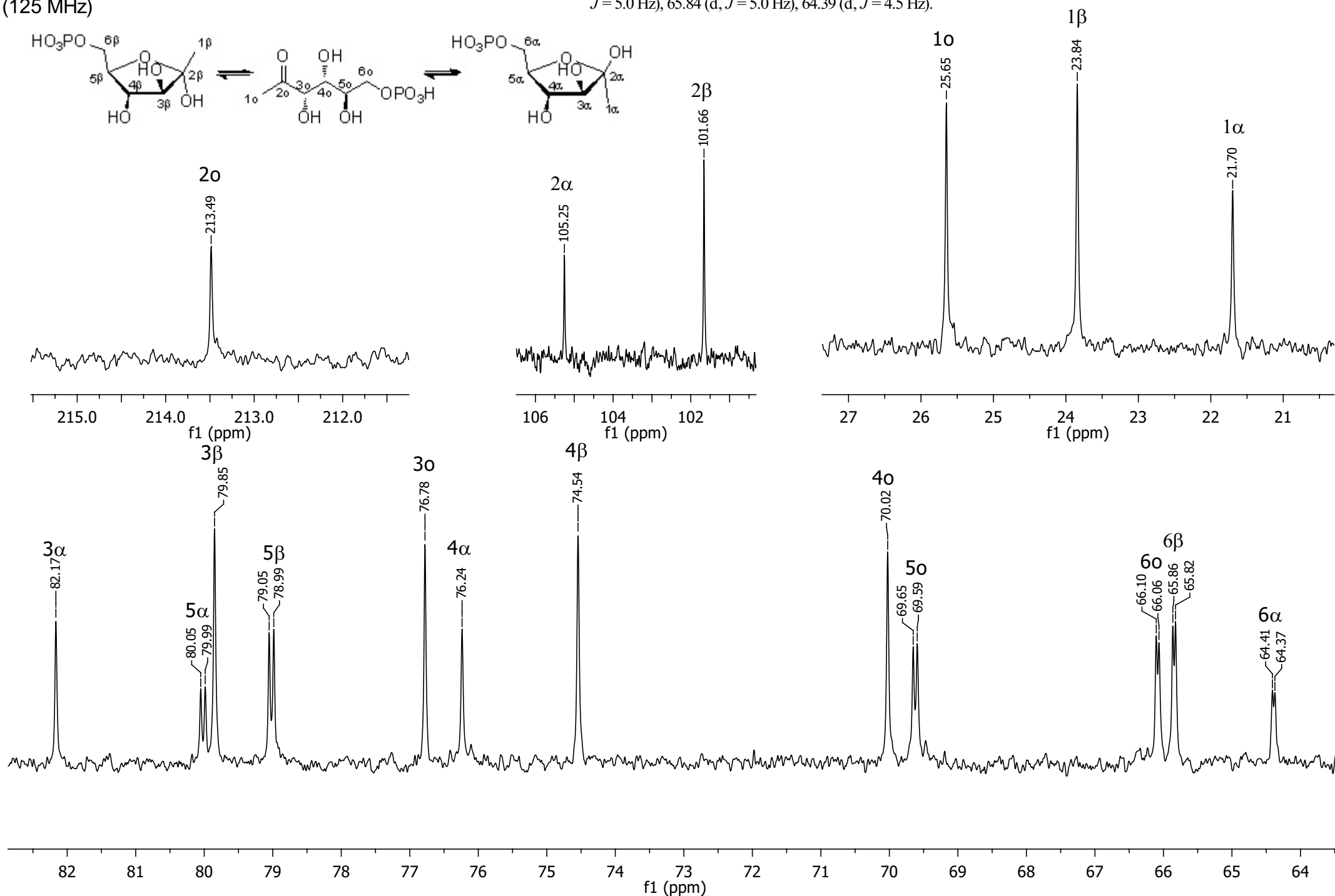
2α

2o



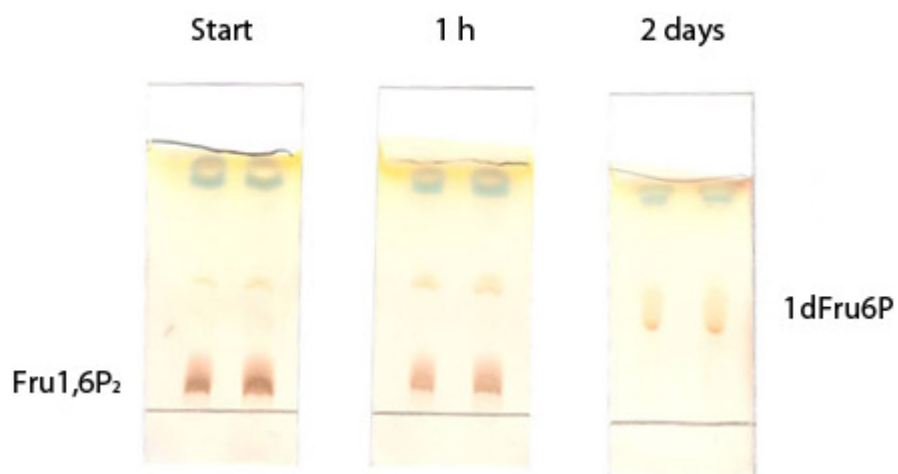
¹³C-NMR spectrum of 1-deoxy-fructose-6-phosphate in D₂O
(125 MHz)

¹³C NMR (126 MHz, D₂O) 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



Route B: aldol-kinase cascade

