Electronic Supplementary Information

Isomerization of Glucose to Fructose Catalyzed by Lithium Bromide in Water

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Table S1. Products from glucose isomerization in in LiCl and LiI

	Time [min]	Glucose [%]	Mannose [%]	Fructose [%]	Decomposition products [%]
$LiCl \cdot 3H_2O$	30	79.6	0.7	17.4	2.3
	60	76.4	0.7	16.8	6.1
$LiI \cdot 3H_2O$	15	9.8	3.8	21.4	65.0
	30	11.7	3.4	21.2	63.7

Note: starting glucose concentration was 10 g/L; at 120 °C.

Table S2. Yields of organic acids from glucose at 120 °C in molten salt hydrates

	Glucose [wt%]	Mannose [wt%]	Fructose [wt%]	Lactic acid [wt%]	Formic acid [wt%]	Levulinic acid [wt%]
LiCl_15 min	ND	ND	ND	37.8	10.8	19.6
LiCl_30 min	ND	ND	ND	39.1	10.6	27.1
LiBr_15 min	1.4	0.2	1.7	9.6	12.1	14.6

Note: starting glucose concentration was 10 g/L; NaOH concentrations in $LiCl \cdot 3H_2O$ and $LiBr \cdot 3H_2O$ were 125 and 100 mM, respectively. ND – not detected.

Table S3. Glucose conversion rate (R_G) and fructose formation rate (R_F) in different halide salt hydrates

Halide salt	Residual glucose [%]	Fructose yield [%]	$R_G \times 10^4$ [M/s]*	$R_F \times 10^4$ [M/s]*
LiCl	90.5	7.7	0.06	0.05
LiBr	48.2	30.3	0.32	0.19
LiI	9.8	21.4	0.56	0.13
$CaBr_2$	5.6	22.4	0.59	0.14
$ZnCl_2$	67.1	0	0.20	0.00

Note: starting glucose concentration 10 g/L at 120 °C for 15 min. * Average rate during the first 15 min, mole/second.

Table S4. Glucose conversion rate (R_G) and fructose formation rate (R_F) at different temperatures

	110 °C		120 °C		130 °C		140°C	
t [min]	$R_G \times 10^4$ [M/s]	$R_F \times 10^4$ [M/s]	$R_G \times 10^4$ [M/s]	$R_F \times 10^4$ [M/s]	$R_G \times 10^4$ [M/s]	$R_F \times 10^4$ [M/s]	$R_G \times 10^4$ [M/s]	$R_F \times 10^4$ [M/s]
0								
5	0.49	0.19	0.64	0.45	0.93	0.56	0.99	0.57
15	0.30	0.16	0.34	0.19	0.32	0.17	0.38	0.15
30	0.16	0.09	0.18	0.09	0.19	0.07	0.23	0.03
60	0.09	0.05	0.10	0.04	0.11	0.02	0.12	0.00
120	0.05	0.02	0.06	0.01	0.06	0.00	0.06	0.00

Note: starting glucose concentration 10 g/L in $LiBr \cdot 3H_2O$. Average rate, mole/second.

Table S5. Conversion rate and isomer formation rate of different starting sugars

Starting material	$R_G \times 10^4$ [M/s]	$R_F \times 10^4$ [M/s]	$R_M \times 10^4$ [M/s]
Glucose	0.64	0.45	0.01
Fructose	0.22	0.42	0.08
Mannose	0.05	0.49	0.72

Note: starting sugar concentration 10 g/L in $LiBr \cdot 3H_2O$ at 120 °C for 5 min. Average rate during the first 5 min, mole/second.

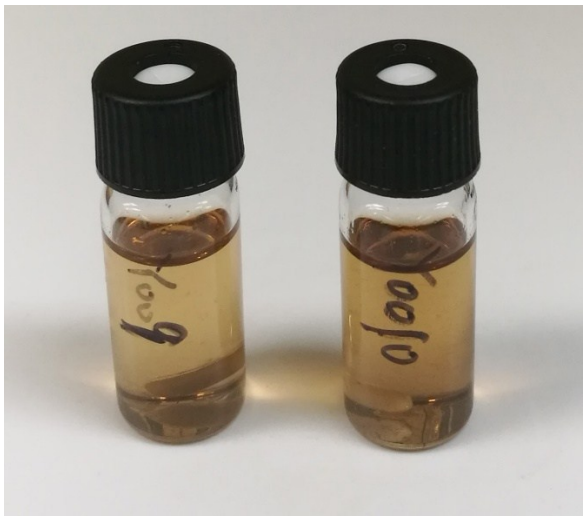

Figure S1. $LiI \cdot 3H_2O$ turned brown after reaction with glucose at 120 °C (Left: 15 min; right: 30 min).

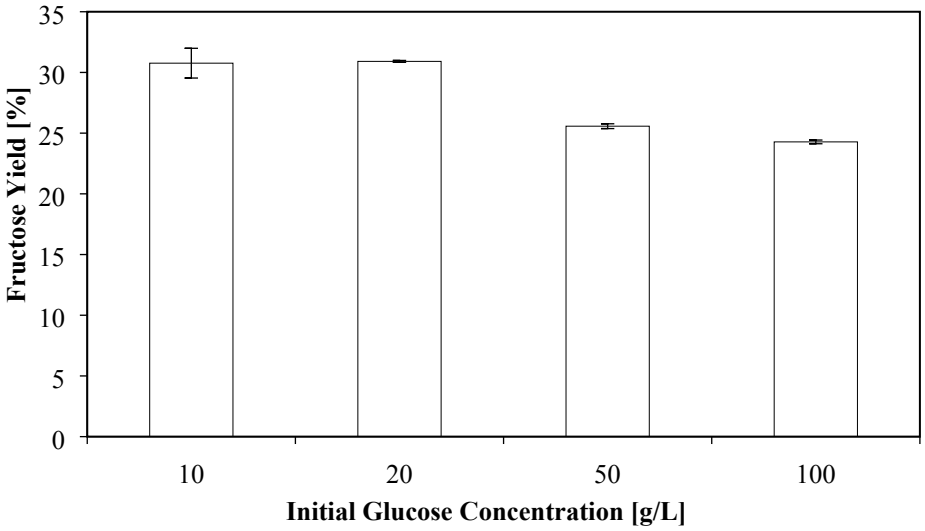

Figure S2. Isomerization of glucose with different starting glucose concentration in $LiBr \cdot 3H_2O$. Reaction conditions: 120 °C and 15 min.

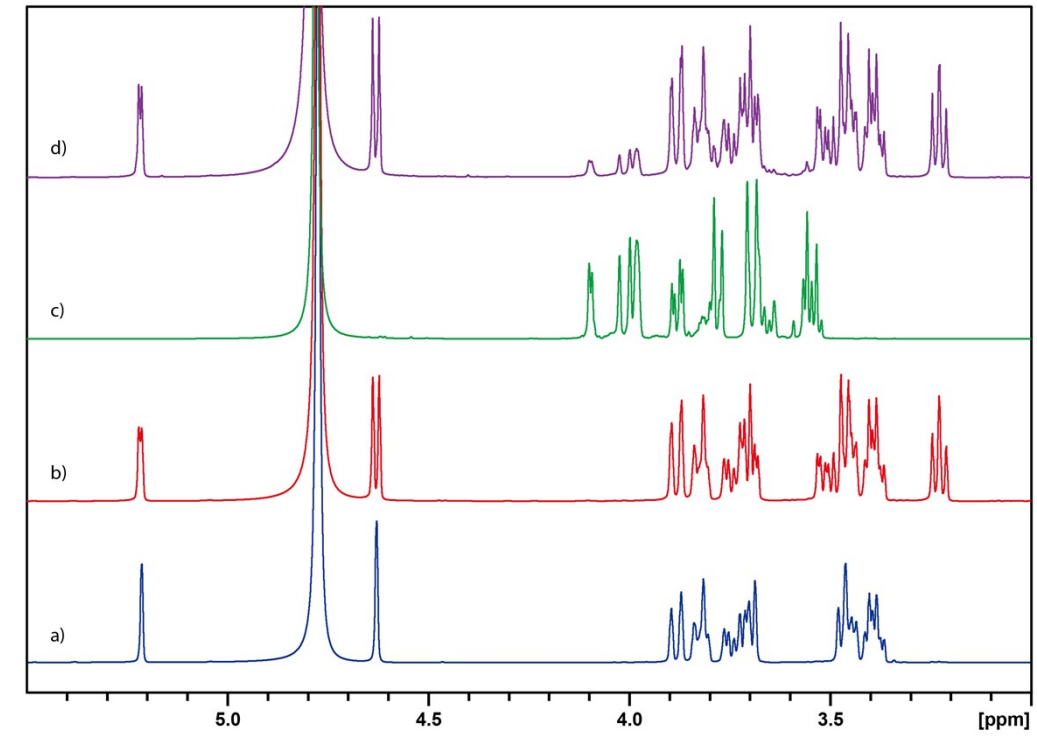

Figure S3. ^{1}H spectra of a) glucose-2-d_1, b) unlabeled glucose, c) unlabeled fructose, and d) mixed sugars (glucose and fructose) from the isomerization of unlabeled glucose in deuterated LiBr trihydrate.

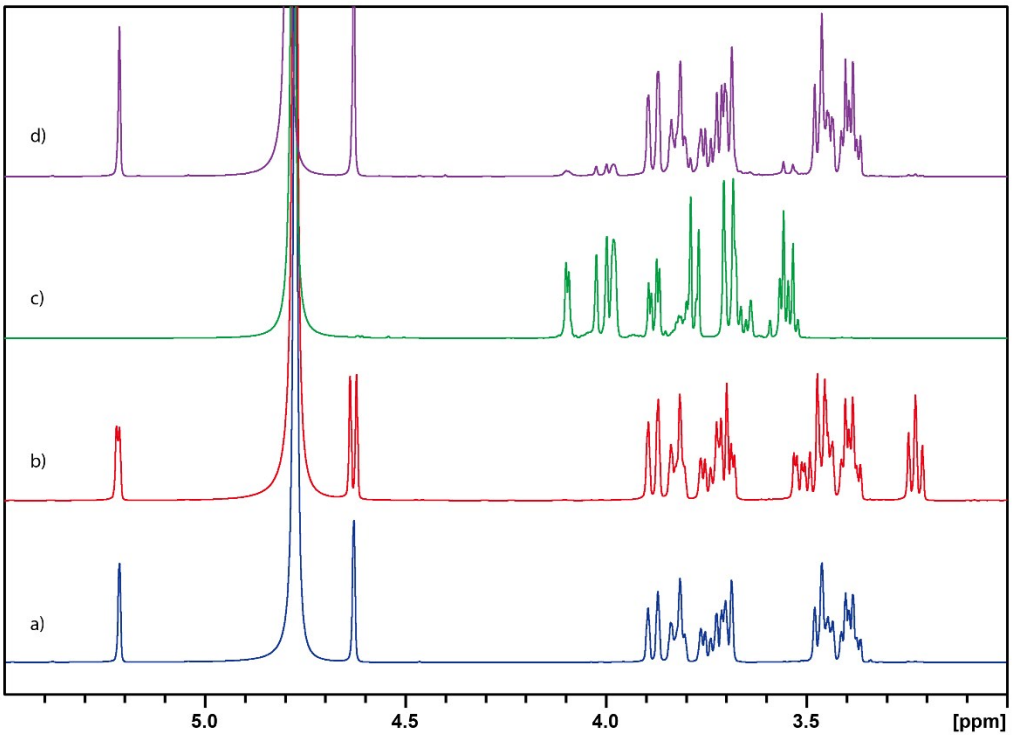

Figure S4. ^{1}H spectra of a) glucose-2-d_1, b) unlabeled glucose, c) unlabeled fructose, and d) mixed sugars (glucose and fructose) from the isomerization of glucose-2-d_1 in LiBr trihydrate.

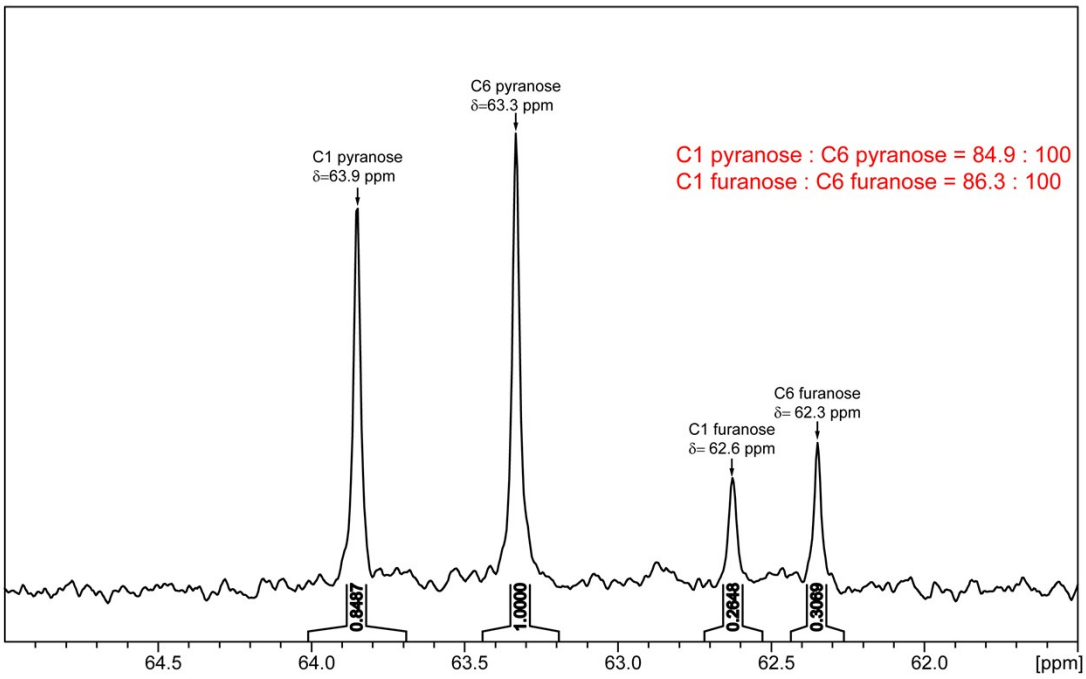

Figure S5. Quantitative ^{13}C NMR spectrum of the mixed sugars (glucose and fructose) from the isomerization of glucose-2-d_1 in LiBr trihydrate.

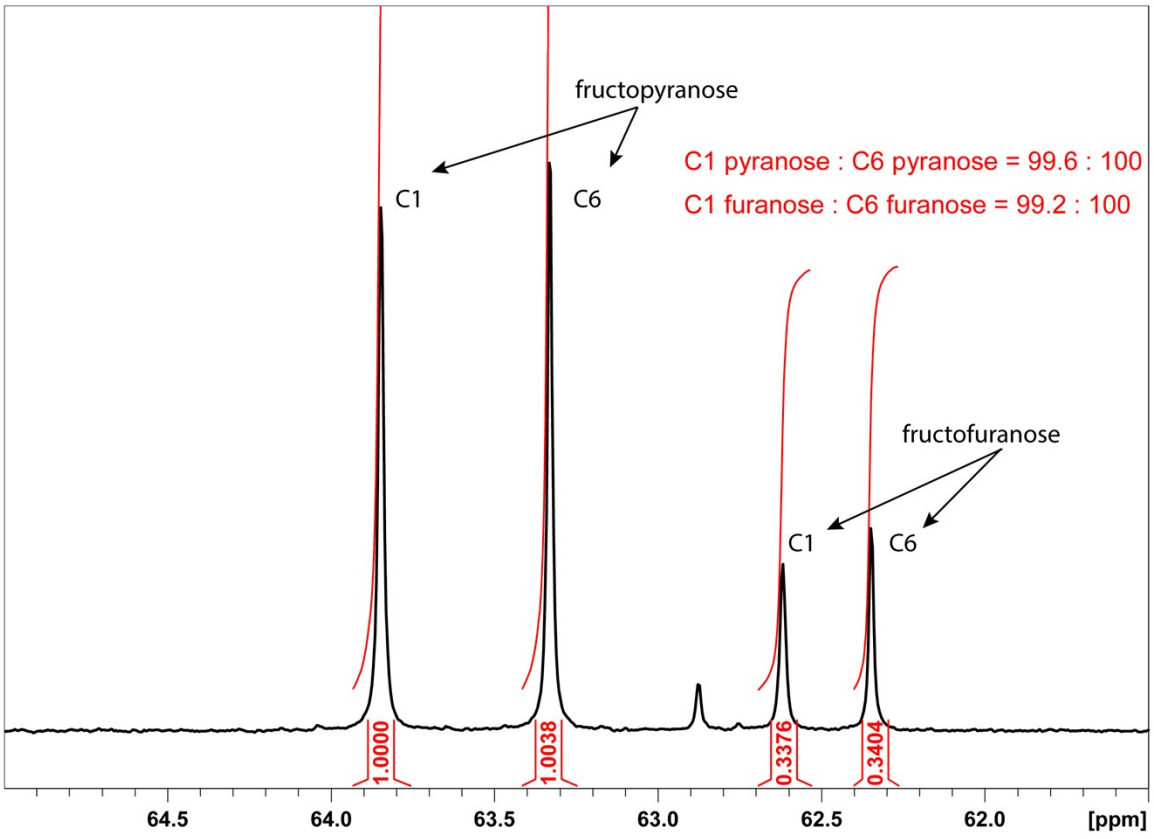

Figure S6. Quantitative ^{13}C NMR spectrum of unlabeled fructose in D_2O.