

## Supporting Information

Profiling of carbohydrate mixtures at unprecedented resolution using high-precision  
 $^1\text{H}$ - $^{13}\text{C}$  chemical shift measurements and a reference library

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**Table S1: Systematic names of oligosaccharides in the reference library of Table 1 and enantiomeric forms of monosaccharides that were used for chemical shift measurements**

glucose (Glc)	D-glucose
2-deoxyglucose (2DG)	2-deoxy-D-glucose
3-deoxyglucose (3DG)	3-deoxy-D-glucose
6 <sup>3</sup> - $\alpha$ -glucosyl-maltotriose (6 <sup>3</sup> GM <sub>3</sub> )	$\alpha$ -D-glucopyranosyl-(1-6)- $\alpha$ -D- glucopyranosyl-(1-4)- $\alpha$ -D- glucopyranosyl-(1-4)-D-glucose
6 <sup>3</sup> - $\alpha$ -maltosyl-maltotriose (6 <sup>3</sup> M <sub>2</sub> M <sub>3</sub> )	$\alpha$ -D-glucopyranosyl-(1-4)- $\alpha$ -D- glucopyranosyl-(1-6)- $\alpha$ -D- glucopyranosyl-(1-4)- $\alpha$ -D- glucopyranosyl-(1-4)-D-glucose
6 <sup>3</sup> - $\alpha$ -maltosyl-maltotetraose (6 <sup>3</sup> M <sub>2</sub> M <sub>4</sub> )	$\alpha$ -D-glucopyranosyl-(1-4)- $\alpha$ -D- glucopyranosyl-(1-6)-[ $\alpha$ -D- glucopyranosyl-(1-4)]- $\alpha$ -D- glucopyranosyl-(1-4)- $\alpha$ -D- glucopyranosyl-(1-4)-D-glucose
allose (All)	L-allose
altrose (Alt)	D-altrose
amylopectin (Amy)	-
arabinose (Ara)	L-arabinose
cellobiose (Cb2)	$\beta$ -D-glucopyranosyl-(1-4)-D- glucose
cellotriose (Cb3)	$\beta$ -D-glucopyranosyl-(1-4)- $\beta$ -D- glucopyranosyl-(1-4)-D-glucose
cellotetraose (Cb4)	$\beta$ -D-glucopyranosyl-(1-4)- $\beta$ -D- glucopyranosyl-(1-4)- $\beta$ -D- glucopyranosyl-(1-4)-D-glucose
$\alpha$ -cyclodextrin ( $\alpha$ CD)	cyclohexaamylose
$\beta$ -cyclodextrin ( $\beta$ CD)	cycloheptaamylose
$\gamma$ -cyclodextrin ( $\gamma$ CD)	cyclooctaamylose
dihydroxyacetone (DHA)	-
erlose (Erl)	$\alpha$ -D-glucopyranosyl-(1-4) $\alpha$ -D- glucopyranosyl-(1-2)- $\beta$ - fructofuranoside
erythrose (Ery)	D-erythrose
fructose (Fru)	D-fructose
fucose (Fuc)	L-fucose
galactosamin (GalN)	2-amino-2-deoxy-galactose
galactose (Gal)	D-galactose
galacturonic acid (Gla)	D-galacturonic acid
galactose-1phosphate (Gal1P)	D-galactose-1phosphate
gentianose (Gen)	$\beta$ -D-glucopyranosyl-(1-6)- $\alpha$ -D-

	glucopyranosyl-(1-2)-β-D-fructofuranoside
gentiobiose (Geb)	β-D-glucopyranosyl-(1-6)-D-glucose
β-glucan (Bgl)	-
glucosamine (GlcN)	2-amino-2-deoxy-glucose
glucose-1-phosphate (Glc1P)	D-glucose-1-phosphate
glucose-6-phosphate (Glc6P)	D-glucose-6-phosphate
glyceraldehyde hydrate (Gad <sub>hyd</sub> )	DL-glyceraldehyde
gulose (Gul)	L-gulose
idose (Ido)	L-idose
inulin (Inu)	-
isomaltose (IM <sub>2</sub> )	α-D-glucopyranosyl-(1-6)-D-glucose
isomaltotriose (IM <sub>3</sub> )	α-D-glucopyranosyl-(1-6)-α-D-glucopyranosyl-(1-6)-D-glucose
isomaltulose (Iml)	α-D-glucopyranosyl-(1-6)-D-fructose
kestose (Kes)	α-D-glucopyranosyl-(1-2)-β-D-fructofuranosyl-(1-2)-β-D-fructofuranose
kojibiose (Koj)	α-D-glucopyranosyl-(1-2)-D-glucose
lactose (Lac)	β-D-galactopyranosyl-(1-4)-D-glucose
lactulose (Lcu)	β-D-galactopyranosyl-(1-4)-D-fructose
laminaribiose (Lam)	β-D-glucopyranosyl-(1-3)-D-glucose
laminarin (Lmn)	-
leucrose (Leu)	α-D-glucopyranosyl-(1-5)-D-fructopyranose
lyxose (Lyx)	D-lyxose
maltose (M2)	α-D-glucopyranosyl-(1-4)-D-glucose
maltotriose (M3)	α-D-glucopyranosyl-(1-4)-α-D-glucopyranosyl-(1-4)-D-glucose
maltotetraose (M4)	α-D-glucopyranosyl-(1-4)-α-D-glucopyranosyl-(1-4)-α-D-glucopyranosyl-(1-4)-D-glucose
maltopentaose (M5)	α-D-glucopyranosyl-(1-4)-α-D-glucopyranosyl-(1-4)-α-D-glucopyranosyl-(1-4)-α-D-glucopyranosyl-(1-4)-D-glucose

maltohexaose (M6)	$\alpha$ -D-Glucopyranosyl-(1-4)- $\alpha$ -D-glucopyranosyl-(1-4)-O- $\alpha$ -D-glucopyranosyl-(1-4)- $\alpha$ -D-glucopyranosyl-(1-4)- $\alpha$ -D-glucopyranosyl-(1-4)-D-glucose
maltoheptaose (M7)	$\alpha$ -D-Glucopyranosyl-(1-4)- $\alpha$ -D-glucopyranosyl-(1-4)- $\alpha$ -D-glucopyranosyl-(1-4)- $\alpha$ -D-glucopyranosyl-(1-4)- $\alpha$ -D-glucopyranosyl-(1-4)-D-glucose
maltooctaose (M8)	$\alpha$ -D-Glucopyranosyl-(1-4)- $\alpha$ -D-glucopyranosyl-(1-4)- $\alpha$ -D-glucopyranosyl-(1-4)- $\alpha$ -D-glucopyranosyl-(1-4)- $\alpha$ -D-glucopyranosyl-(1-4)- $\alpha$ -D-glucopyranosyl-(1-4)-D-glucose
maltulose (Mtu)	$\alpha$ -D-glucopyranosyl-(1-4)-D-fructose
mannose (Man)	-
melezitose (Mez)	$\alpha$ -D-Glucopyranosyl-(1-3)- $\alpha$ -D-fructofuranosyl-(2-1)- $\alpha$ -D-glucopyranoside
melibiose (Mel)	$\alpha$ -D-galactopyranosyl-(1-6)-D-glucose
N-acetyl-glucosamine (GlcNAc)	2-(acetylamino)-2-deoxy-D-glucose
N-acetyl-mannosamine (ManNAc)	2-(acetylamino)-2-deoxy-D-mannose
N-acetyl-lactosamine (LacNAc)	$\beta$ -D-galactopyranosyl-(1-4)-2-acetamido-2-deoxy-D-glucose
neokestose (Nke)	$\beta$ -D-fructofuranosyl-(2-6)- $\beta$ -D-glucopyranosyl-(1-2)- $\beta$ -D-fructofuranoside
nigerose (Nig)	$\alpha$ -D-glucopyranosyl-(1-3)-D-glucose
nystose (Nys)	$\alpha$ -D-glucopyranosyl-(1-2)- $\beta$ -D-fructofuranosyl-(1-2)- $\beta$ -D-fructofuranosyl-(1-2)- $\beta$ -D-fructofuranoside
panose (Pan)	$\alpha$ -D-glucopyranosyl-(1-6)- $\alpha$ -D-glucopyranosyl-(1-4)-D-glucose
pullulan (Pul)	-

raffinose (Raf)	$\alpha$ -D-galactopyranosyl-(1-6)- $\alpha$ -D-glucopyranosyl-(1-2)- $\beta$ -D-fructofuranoside
rhamnose (Rha)	L-rhamnose
ribose (Rib)	D-ribose
rutinose (Rut)	$\alpha$ -L-rhamnosyl-(1-6)-D-glucose
sophorose (Sop)	$\beta$ -D-glucopyranosyl-(1-2)-D-glucose
sorbose (Sor)	D-sorbose
stachyose (Sta)	$\alpha$ -D-galactopyranosyl-(1-6)- $\alpha$ -D-galactopyranosyl-(1-6)- $\alpha$ -D-glucopyranosyl-(1-2)- $\beta$ -D-fructofuranoside
sucrose (Suc)	$\alpha$ -D-glucopyranosyl-(1-2)- $\beta$ -D-fructofuranoside
tagatose (Tag)	D-tagatose
talose (Tal)	D-talose
threose (Thr)	L-threose
$\alpha,\alpha$ -trehalose (Tre <sup>αα</sup> )	$\alpha$ -D-glucopyranosyl-(1-1)- $\alpha$ -D-glucopyranoside
$\alpha,\beta$ -trehalose (Tre <sup>αβ</sup> )	$\alpha$ -D-glucopyranosyl-(1-1)- $\beta$ -D-glucopyranoside
$\beta,\beta$ -trehalose (Tre <sup>ββ</sup> )	$\beta$ -D-glucopyranosyl-(1-1)- $\beta$ -D-glucopyranoside
turanose (Tur)	$\alpha$ -D-glucopyranosyl-(1-3)- $\alpha$ -D-fructose
xylose (Xyl)	D-xylose
xylobiose (Xyl <sub>2</sub> )	$\beta$ -D-xylopyranosyl-(1-4)-D-xylose
xylotriose (Xyl <sub>3</sub> )	$\beta$ -D-xylopyranosyl-(1-4)- $\beta$ -D-xylopyranosyl-(1-4)-D-xylose

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**Figure S2**  $^{13}\text{C}$   $T_2$  measurement at 18.7 T magnetic field (800 MHz proton frequency) for isomatotriose  $\alpha(1-6)$  anomeric signals (reducing end shown in the bottom of the trisaccharide). Relaxation times were measured using  $^1\text{H}$ - $^{13}\text{C}$  correlation through INEPT transfers with sensitivity enhancement and with relaxation delays of 22.4 milliseconds multiplied by loops of 2, 6, 13 and 36, employing ‘chirp’ pulses for adiabatic inversion during relaxation delays. The resultant decay was fit with exponential decay curves in profit 6.2.9 (Quantumsoft, Zurich, CH).

