Supporting information

Sulfonyl hydrazine-functionalized polymer as a specific capturer of reducing glycans from complex samples for high-throughput analysis by electrospray ionization mass spectrometry

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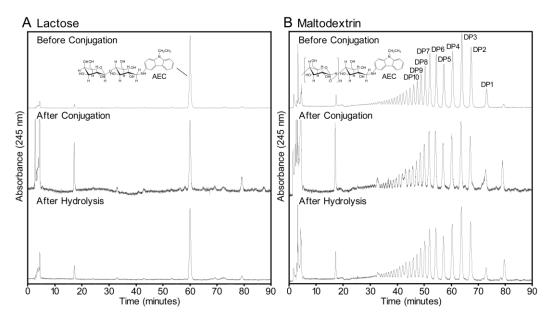


Fig. S1 RP-HPLC chromatograms of AEC derivatives of lactose (A) and maltodextrin (B) obtained using the SHPS-based glycan capturing procedure. Each sample was analyzed before and after the conjugation reaction as well as after the hydrolytic release reaction.

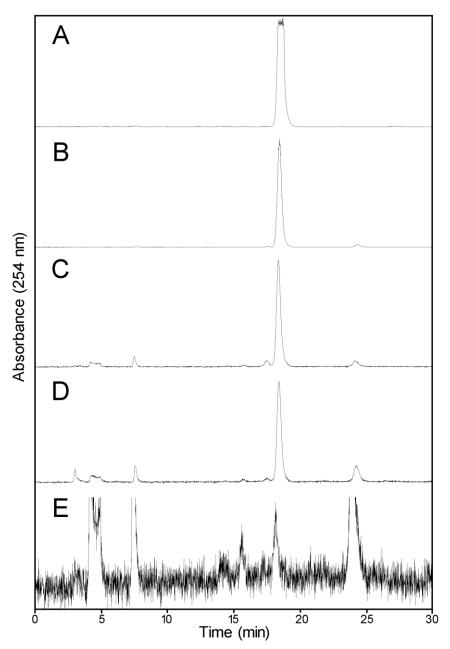


Fig. S2 RP-HPLC chromatograms of AEC derivatives of lactose obtained using different functional materials, including SHPS beads (B), hydrazide resin (C), hydrazide magnetic beads (D) and aminoethyl resin (E), under the reaction conditions developed merely on the basis of SHPS beads. (A) is the RP-HPLC chromatogram of the AEC derivative of lactose before the conjugation reaction.

10-

1000

1100

1200

1300

1400

A Ribonuclease B N-glycans before SHPS-capture SHPS recovery RiboB_130612162702 #100-255 RT: 0.38-0.96 AV: 156 NL: 7.63E3 T: ITMS + p ESI Full ms [50.00-2000.00] 1419.50 100-1157.42 1257.50 90 80 70-Relative Abundance 60 1743.58 50 40 1581.50 30-20-1905.67 1173.33 1435.33 1759.42 2000 1100 1900 1300 1400 1500 1600 1700 1800 B Ribonuclease B N-glycans after SHPS-capture 100-90 80 70-Relative Abundance 1419.50 60 1257 50 50 40 1743.58 30 1581.50 20-1905.67 1435.33

Fig. S3 Recovery of the SHPS-based glycan capturing procedure tested on ribonuclease B N-glycans. (A) ESI-MS profile of the ribonuclease B N-glycans purified using graphitized carbon SPE columns used as a control. (B) ESI-MS profile of ribonuclease B N-glycans purified using graphitized carbon SPE columns and continuously processed by the SHPS-based procedure. The mass peak with an m/z value of 1157.42 is assigned to β -cyclodextrin, which is used as an internal standard for the calculation of glycan recovery. The other mass peaks are assigned to the typical N-glycans of ribonuclease B.

1500

1598.42

1700

1800

1900

2000

1600

Table S1 The reproducibility of the SHPS-based glycan capturing procedure investigated by the analysis of maltodextrin (n=3)

Glycan ^a	Sample1	Sample2	Sample3	Average	SD value	CV (%)
DP1	1289273	1401622	1301895	1330930	61545.5	4.6
DP2	4003057	3925321	4014050	3980809.3	48367.6	1.2
DP3	4838611	4877151	4930139	4881967	45953.7	0.9
DP4	3721440	3729419	3844194	3765017.7	68684.7	1.8
DP5	2985179	2993152	2954829	2977720	20221.0	0.7
DP6	3556423	3649201	3592938	3599520.7	46738.0	1.3
DP7	3325155	3444840	3329744	3366579.7	67814.3	2.0
DP8	2268926	2417842	2317561	2334776.3	75936.0	3.3
DP9	1675735	1772021	1705758	1717838	49266.6	2.9
DP10	1258954	1284186	1308901	1284013.7	24973.9	1.9

^a DP, degree of polymerization.