Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

Discrimination between sialic acid linkage modes using sialyllactose-imprinted polymers

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^{1}NMR titration study

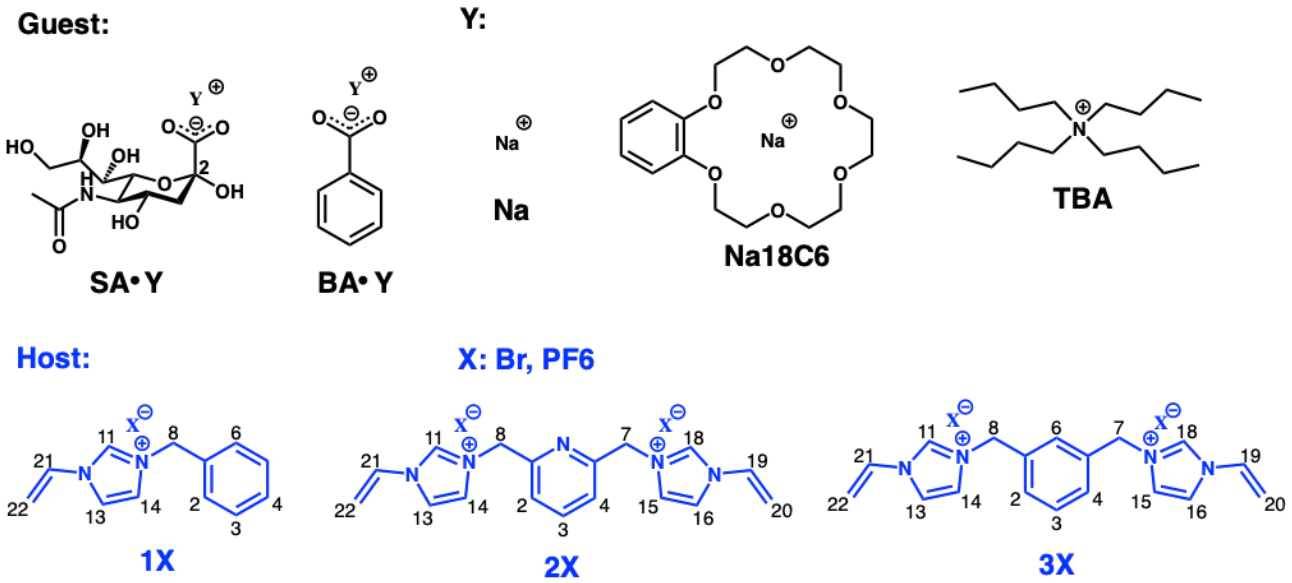

Figure S1. Structures of guest and host molecules with their corresponding counterions used in ^{1}H NMR titration studies.

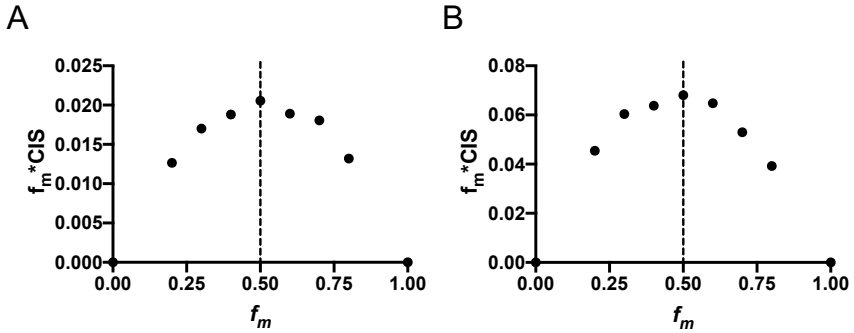

Figure S2. Job's plot of **1Br** (A) and **2Br** (B) with BA-TBA for the protons CH(11,18) in DMSO-d_6.

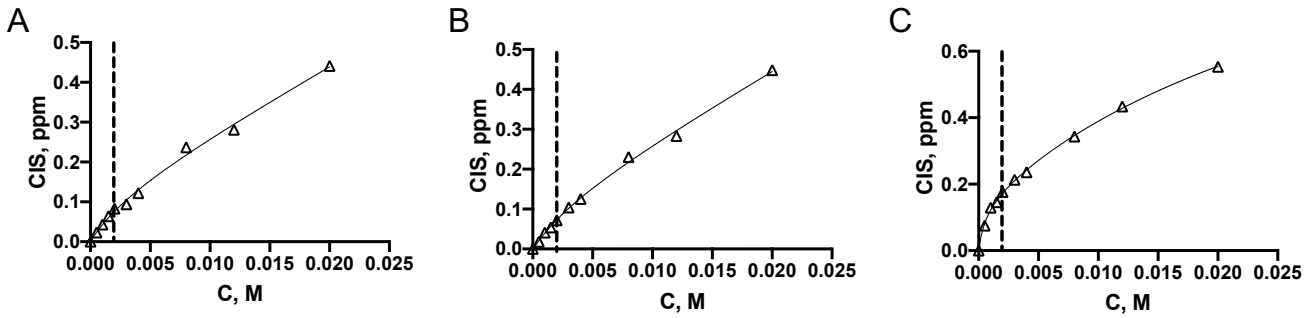

Figure S3. Complexation induced shifts (CIS) of the CH(11,18) protons upon titration of monomers **1Br** (A), **3Br** (B) and **2Br** (C) with BA-TBA in DMSO-d_6, fitted with mono-Langmuir (A, B) and bi-Langmuir (C) binding models. Vertical dashed line represents 1:1 equivalents of H:G.

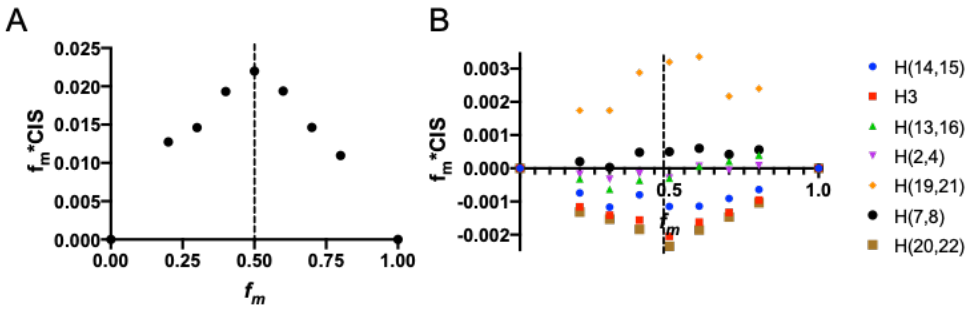

Figure S4 Job's plot of **2Br** with SA-Na for the protons CH(11,18) (A) and other protons (B) in DMSO-d_6.

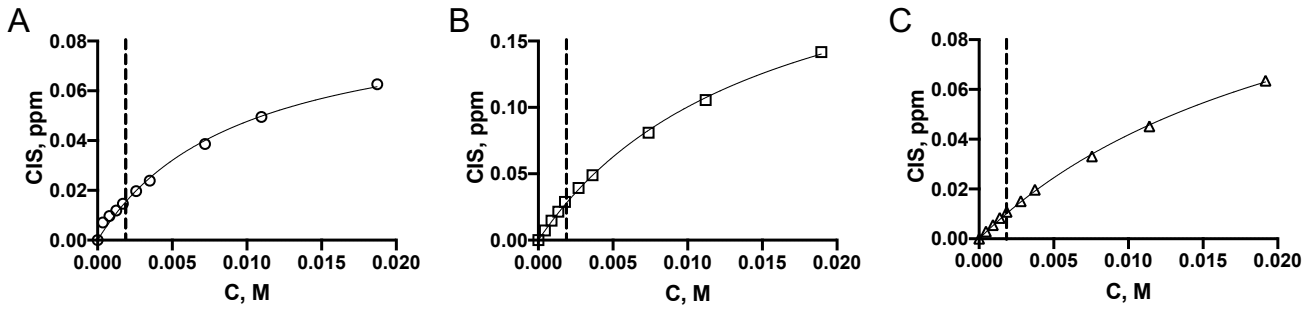

Figure S5. Complexation induced shifts (CIS) of the H(11,18) protons upon titration of monomer **2Br** with Na (A), Na-18C6 (B) and TBA (C) salts of SA in DMSO-d_6. Curves were fitted with Langmuir binding model. Vertical dashed line represents 1:1 equivalents of H:G.

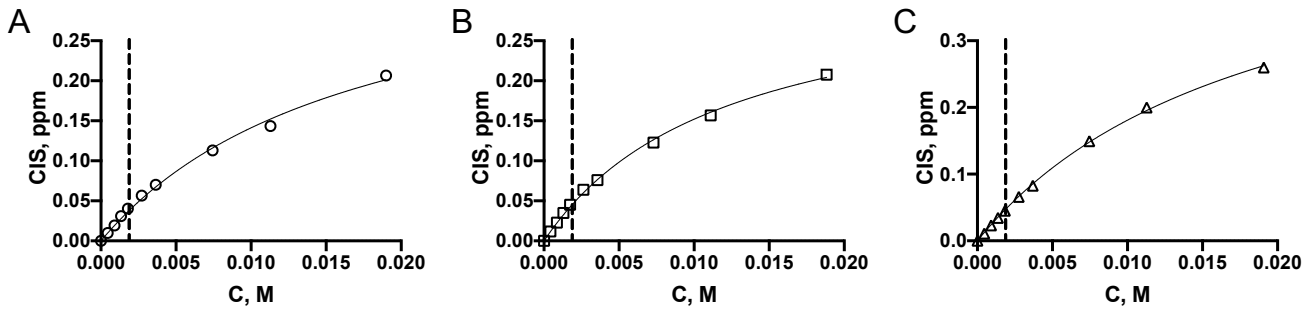

Figure S6. Complexation induced shifts (CIS) of the H(11,18) protons upon titration of monomer **2PF6** with Na (A), Na-18C6 (B) and TBA (C) salts of SA in DMSO-d_6. Curves were fitted with Langmuir binding model. Vertical dashed line represents 1:1 equivalents of H:G.

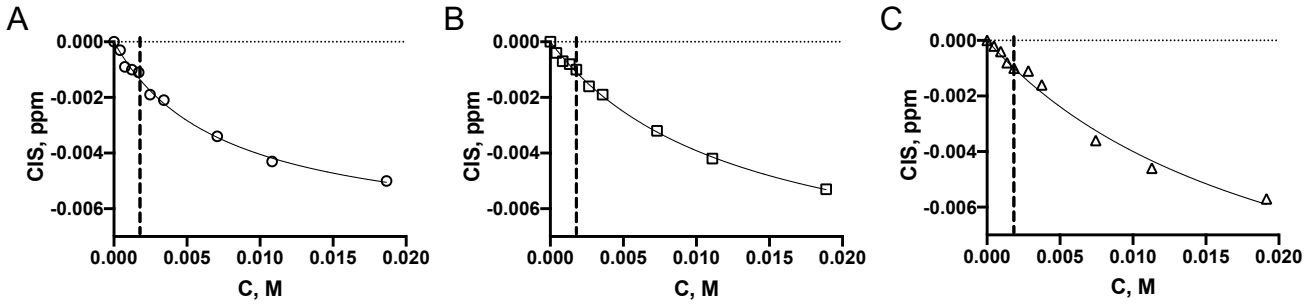

Figure S7. Complexation induced shifts (CIS) of the H(14,15) protons upon titration of monomer **2Br** with Na (A), Na-18C6 (B) and TBA (C) salts of SA in CD_3OD. Curves were fitted with Langmuir binding model. Vertical dashed line represents 1:1 equivalents of H:G.

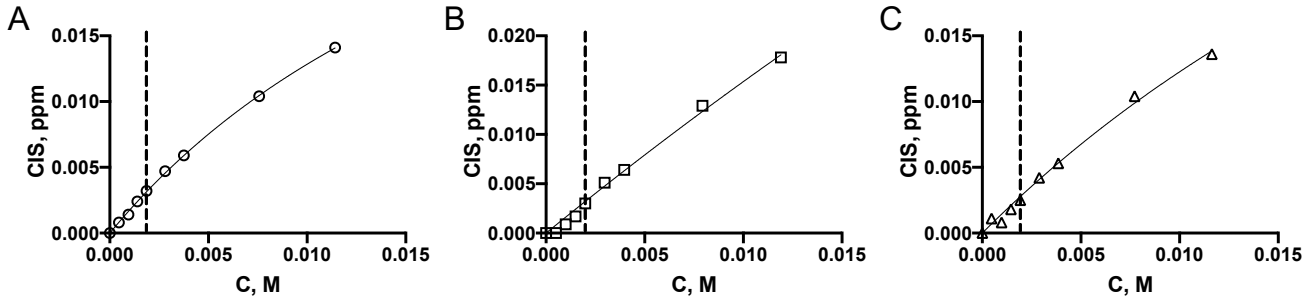

Figure S8. Complexation induced shifts (CIS) of the H(7,8) protons upon titration of monomer **2PF6** with Na (A), Na-18C6 (B) and TBA (C) salts of SA in CD_3OD. Curves were fitted with Langmuir binding model. Vertical dashed line represents 1:1 equivalents of H:G.

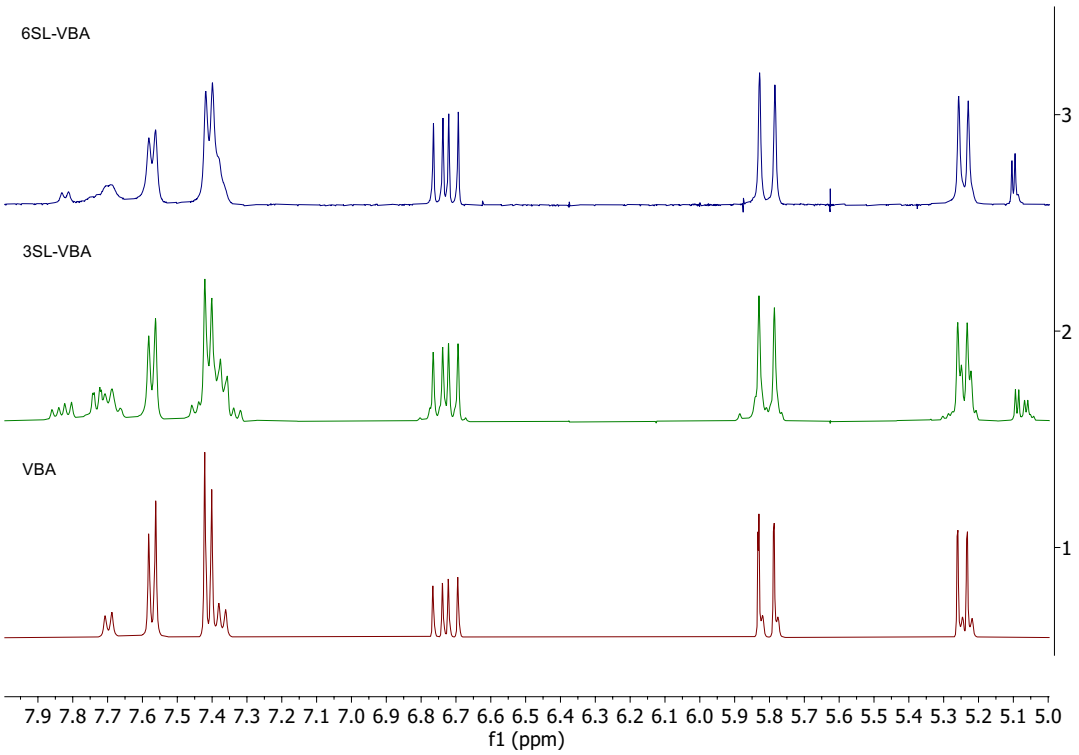

Figure S9. ^{1}H NMR spectra of VBA-6SL, VBA-3SL and VBA in CD_3OD. Ratio of boronate-diol was 2:1 with 20mM VBA and 10mM SL.

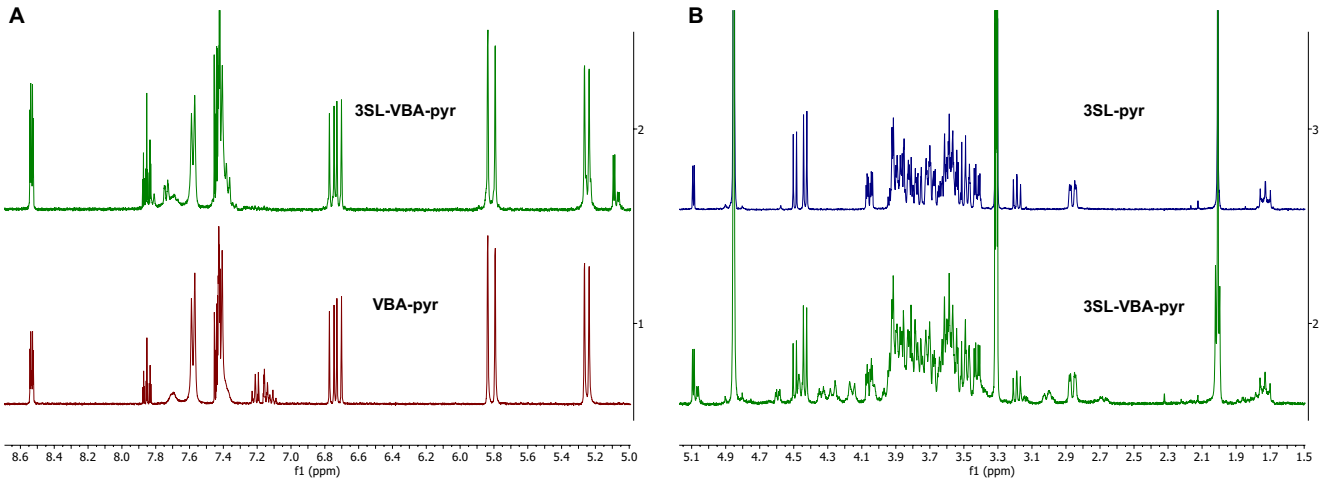

Figure S10. ^{1}H NMR of 3SL and VBA aromatic region (A) and 3SL and 3SL-VBA aliphatic (B) regions in CD_3OD prepared with esterification in pyridine.

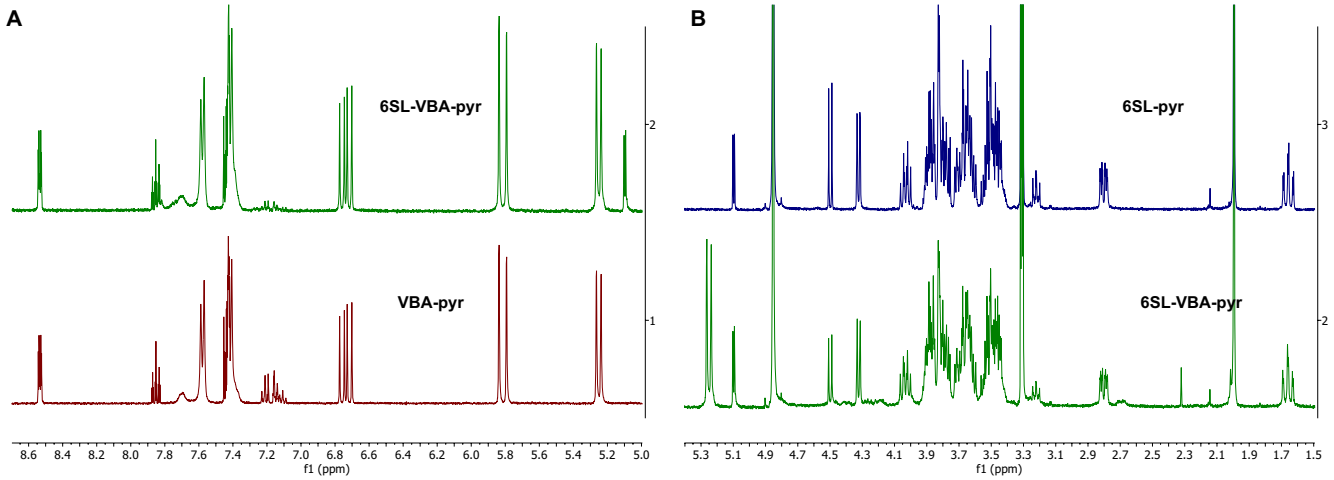

Figure S11. ^{1}H NMR of 6SL and VBA aromatic region (A) and 6SL and 6SL-VBA aliphatic (B) regions in CD_3OD prepared with esterification in pyridine.

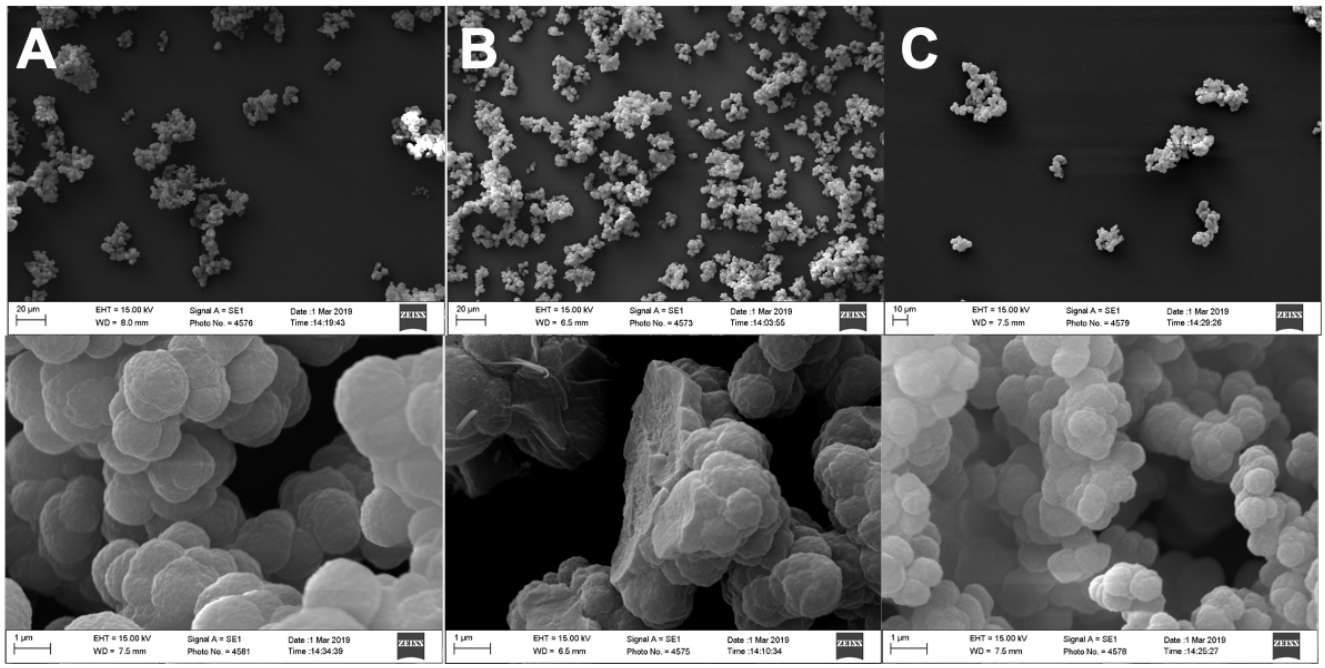

Figure S12. SEM images of polymers 6SL-MIP (A), 3SL-MIP (B) and NIP (C).

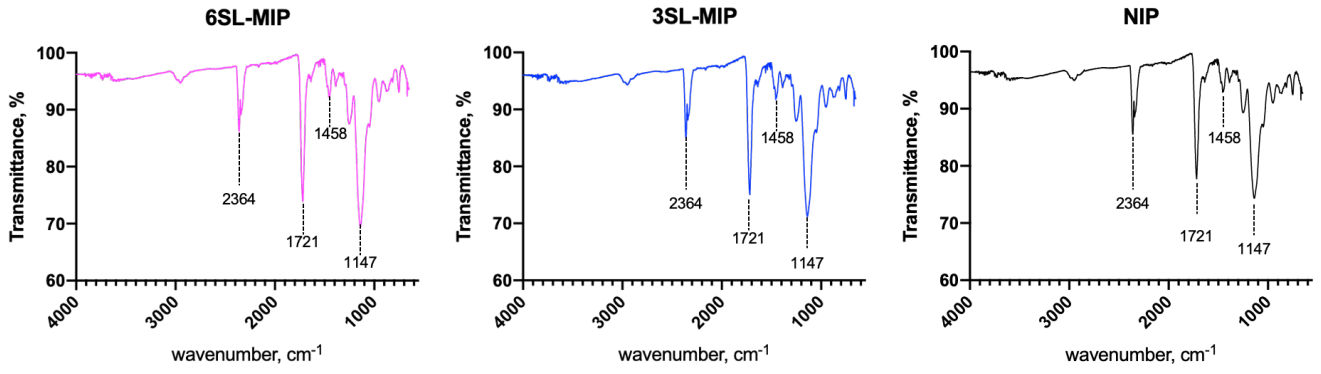

Figure S13. FT-IR spectra of polymers 6SL-MIP, 3SL-MIP and NIP.

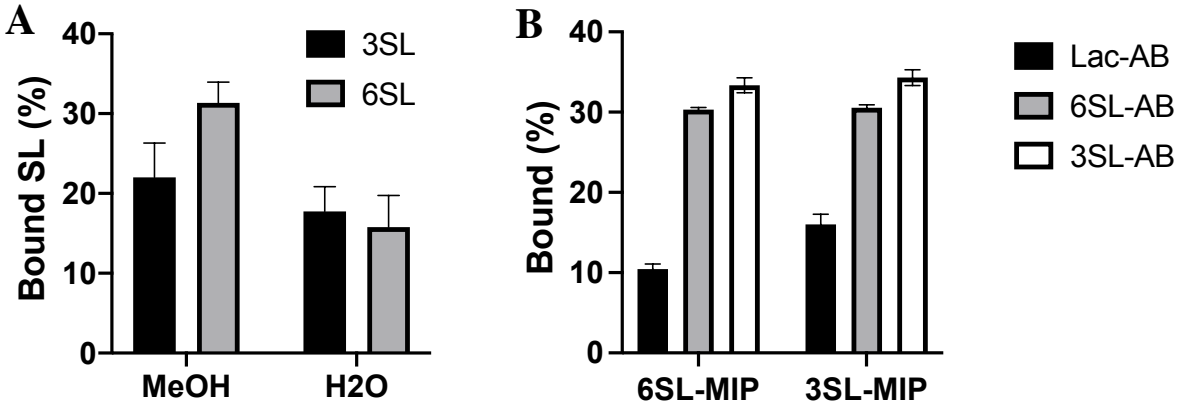

Figure S14. Binding 0.125 mM equimolar mixture of 6SL/3SL in 100% MeOH and 100% H2O by NIP (A) and binding of 2AB labelled lactose (Lac-AB), 2,6'-sialyllactose (6SL-AB) and 2,3'-sialyllactose (3SL-AB) sodium salts in 80-20 MeOH-H_2O (B).

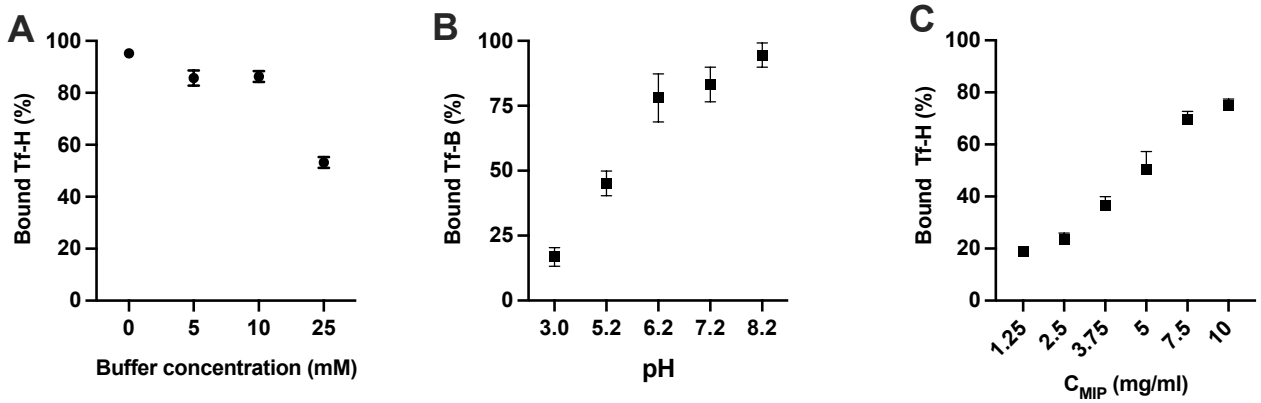

Figure S15. Effect of buffer strength (pH 7.4) (A), pH (B) and amount of polymer on the uptake of transferrin human by 6SL-MIP.

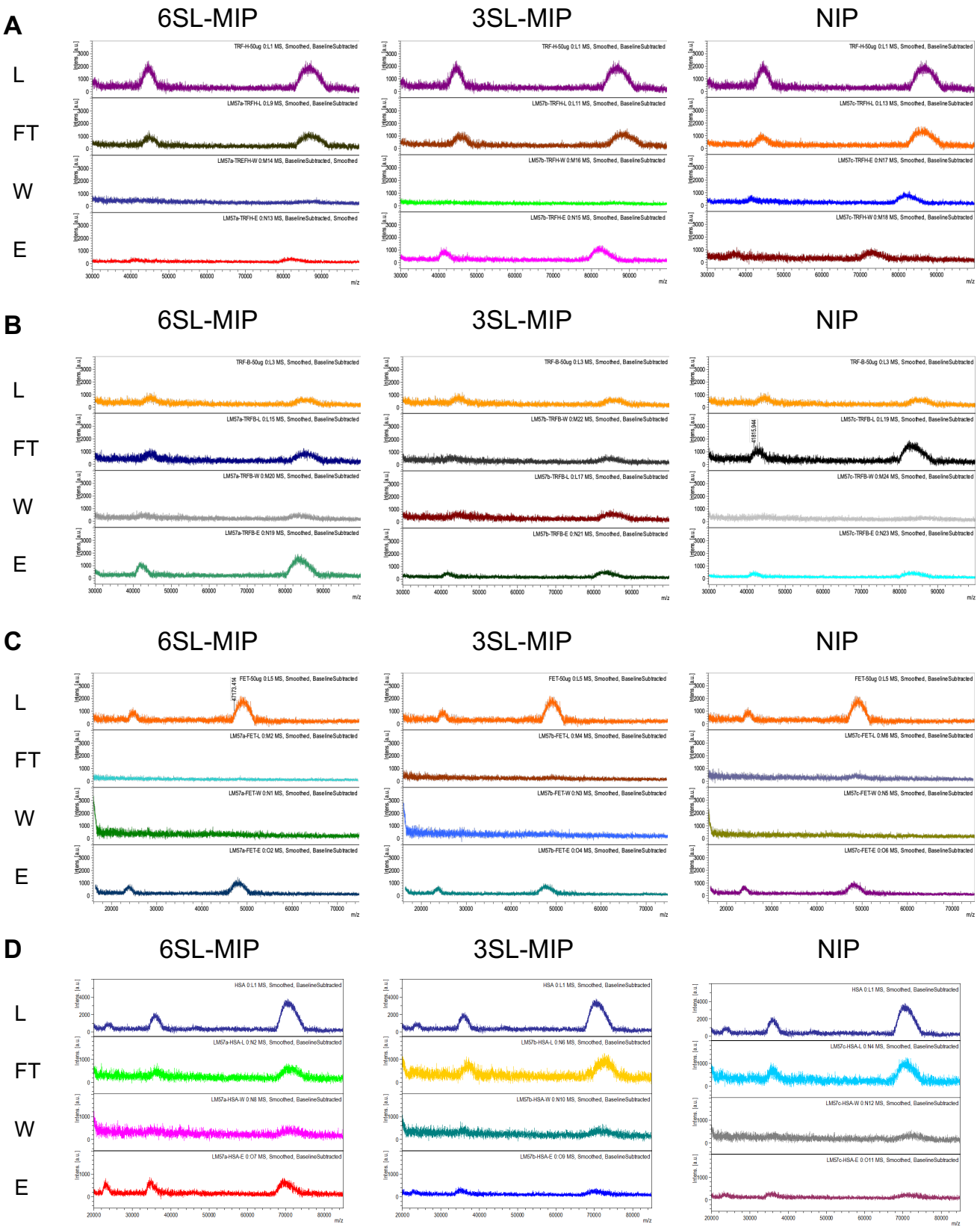

Figure S16. MALDI mass spectra for proteins loading (L), flowthrough (FT), washing (W) and elution (E) steps of transferrin human (A), transferrin bovine (B), fetuin (C) and HSA (D) and for polymers: 6SL-MIP, 3SL-MIP and NIP.

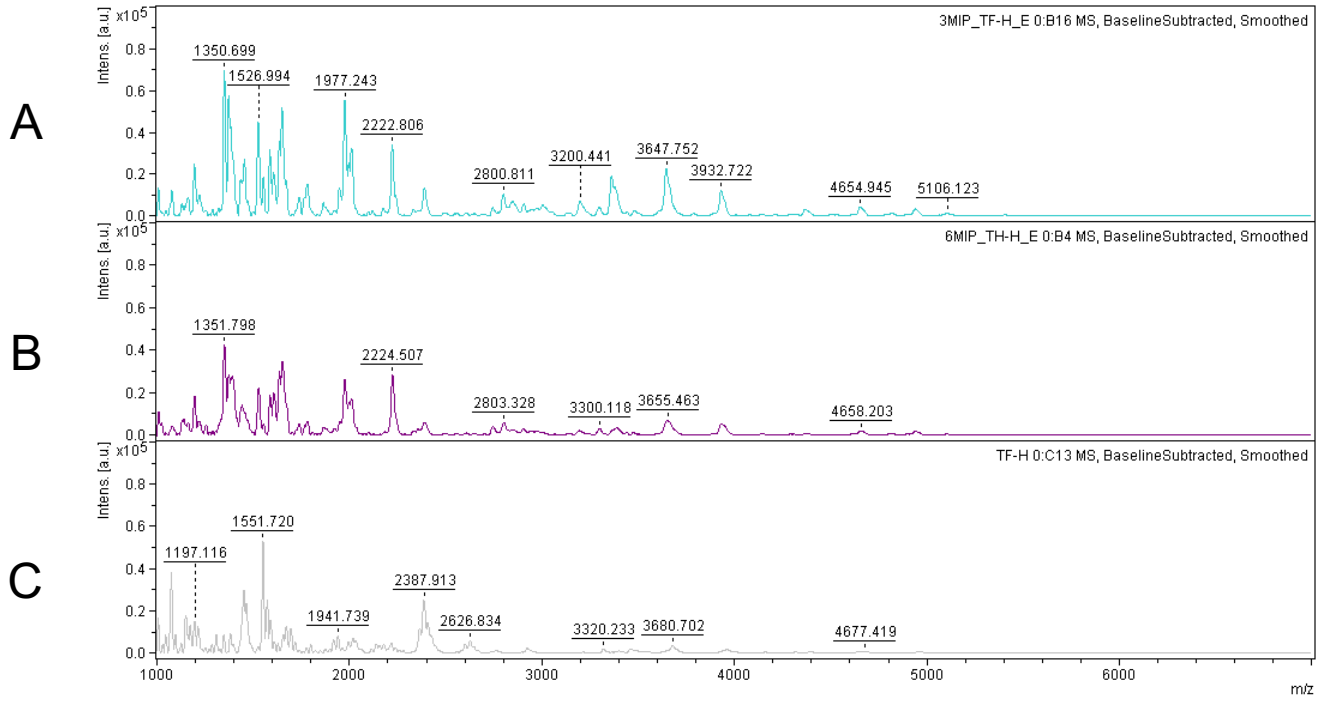

Figure S17. MALDI profile of elution fractions from 3SL-MIP (A), 6SL-MIP (B) and loading fractions (C) of transferrin human.

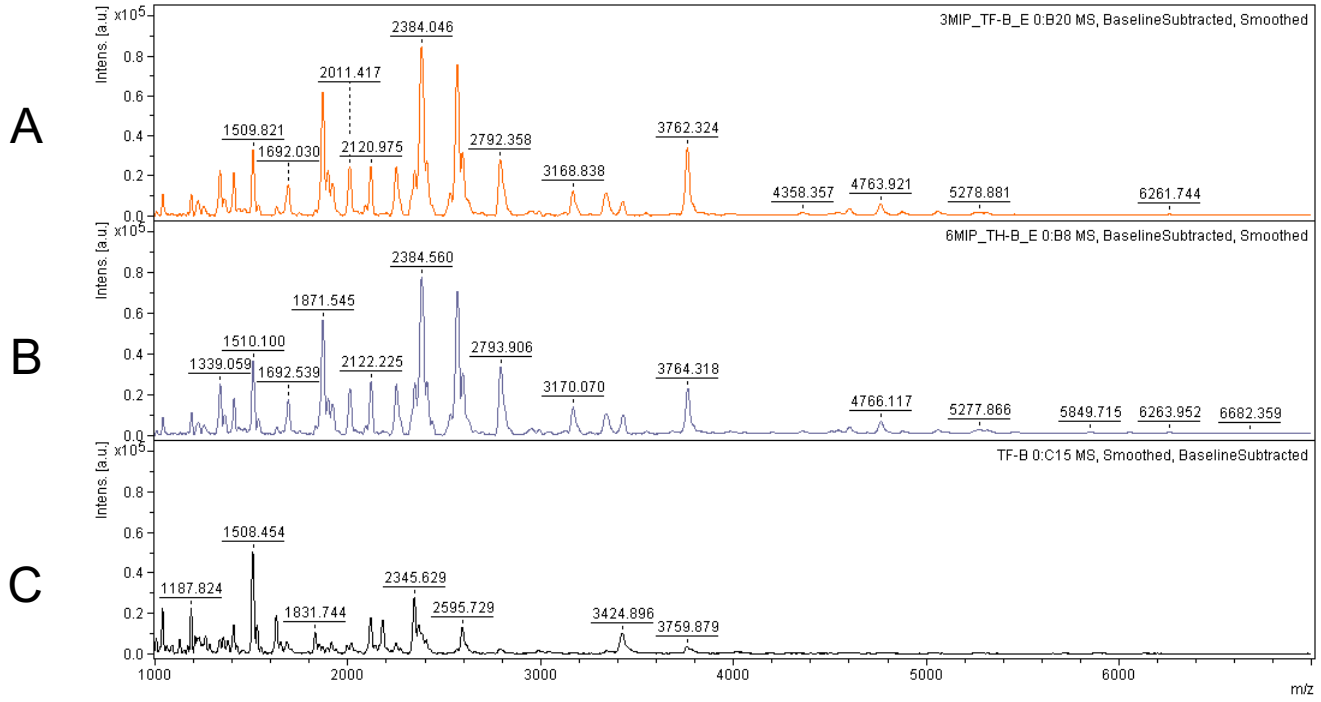

Figure S18. MALDI profile of elution fractions from 3SL-MIP (A), 6SL-MIP (B) and loading fractions (C) of transferrin bovine.

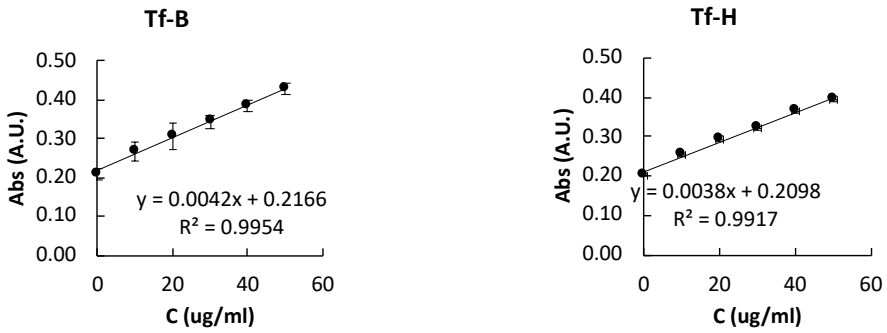

Figure S19. Calibration curves for BCA assay of transferrins bovine (Tf-B) and human (Tf-H) (B).

Table S1. Elemental analysis of polymers

	N [%]	C [%]	H [%]	N/C
6SL-MIP	0.69	59.17	6.86	0.0117
3SL-MIP	0.66	59.46	6.69	0.0110
NIP	0.67	59.30	6.91	0.0113

Table S2. Physical properties of SL-MIP and NIP: the BET specific surface area (S), specific pore volume (V_p), average pore diameter (D_p), polymer swelling (SW) in MeOH and Zeta potential (ζ) in PB (10 mM, pH 7.4)

	S [m^2/g]	V_p [ml/g]	D_p [nm]	SW [ml/ml]	ζ [mV]
6SL-MIP	13	0.07	22.5	1.1	+27.4
3SL-MIP	11	0.05	18.3	1.1	+24.6
NIP	195	0.90	17.1	1.1	+25.1