Electronic Supplementary information

Native mass spectrometry for the design and selection of protein bioreceptors for perfluorinated compounds

Elise Daems, ‡[a,b,c] Giulia Moro, ‡[a,c,d] Herald Berghmans,[e] Ligia M. Moretto,[d] Silvia Dewilde,†[e] Alessandro Angelini,[d,f] Frank Sobott *[b,g,h] and Karolien De Wael *[a,c]

[a.] *AXES Research Group, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerp, Belgium.*
[b.] *BAMS Research Group, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerp, Belgium.*
[c.] *NANOlab Centre of Excellence, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerp, Belgium.*
[d.] *Department of Molecular Science and Nanosystems, Università Ca' Foscari, Via Torino 155, 30172 Mestre, Italy.*
[e.] *PPES Research Group, University of Antwerp, Universiteitsplein 1, 2610 Wilrijk, Belgium*
[f.] *European Centre for Living Technology (ECLT), Ca' Bottacin, Dorsoduro 3911, Calle Crosera, 30123 Venice, Italy*
[g.] *Astbury Centre for Structural Molecular Biology, University of Leeds, Leeds LS2 9JT, UK.*
[h.] *School of Molecular and Cellular Biology, University of Leeds, Leeds LS2 9JT, UK.*
‡ These authors contributed equally to this work.
† Deceased.
* Corresponding authors.

Table S-1. Used parameters for Nanodrop2000 measurements and PDB ID reference used in Figure1.

Protein	*Wavelength (nm)*	*Molecular weight (Da)*	*Extinction coefficient ($mol^{-1}cm^{-1}L$)*	*Protein Data Bank ID*
hSA	280	66531	34445	1BJ5
Hb (oxyhemoglobin)	414	64458	524280	1NQP
NGB	410	17501	12200	1OJ6

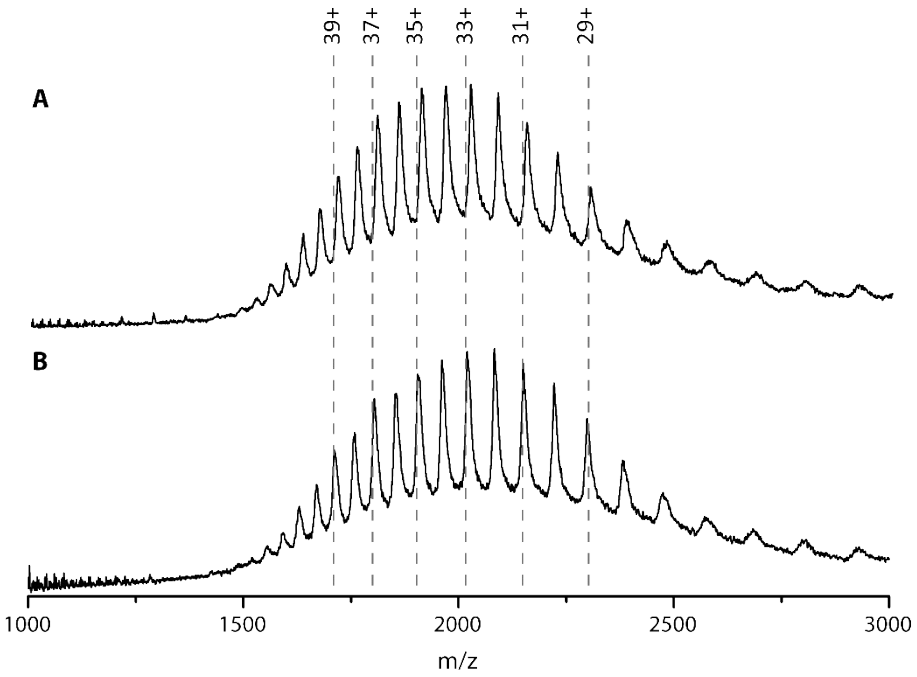

Figure S-1. Denatured MS spectra of untreated (A) and delipidated (B) hSA recorded in 50/50 acetonitrile/MilliQ with 0.1% formic acid. The dashed lines indicate the theoretical m/z-values of hSA calculated from the theoretical mass of 66531 Da.

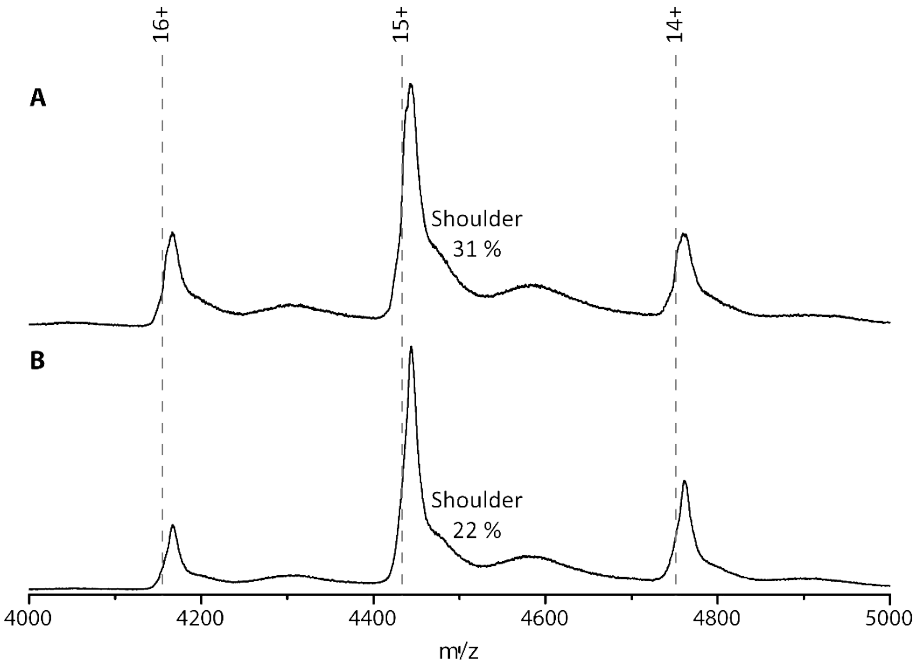

Figure S-2. MS spectra of untreated (A) and delipidated (B) hSA recorded at 100 V trap collision energy. The dashed lines indicate the theoretical m/z-values of hSA.

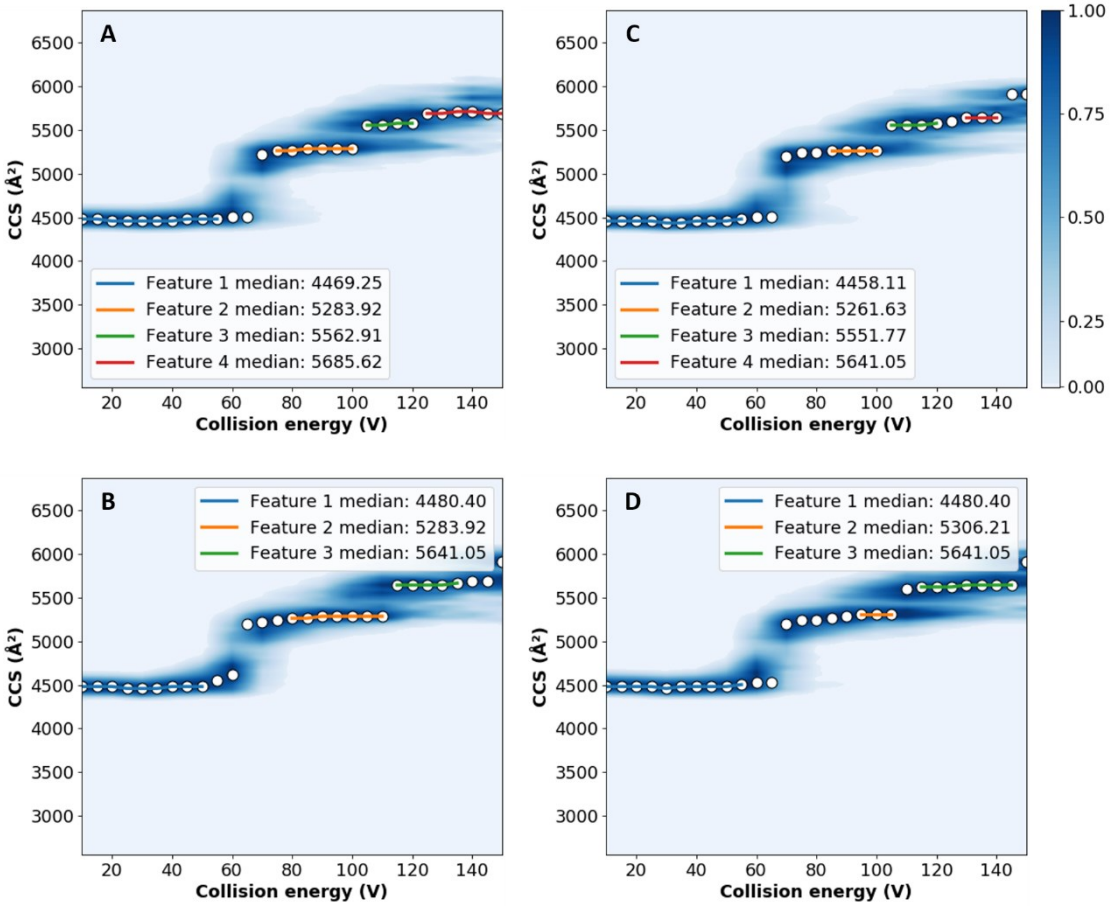

Figure S-3. Feature detection performed using CIUSuite 2 on the CIU plots of untreated (A) and delipidated (B) hSA and of the untreated (C) and delipidated (D) hSA in complex with PFOA (10-fold excess) shown in Figure 3.

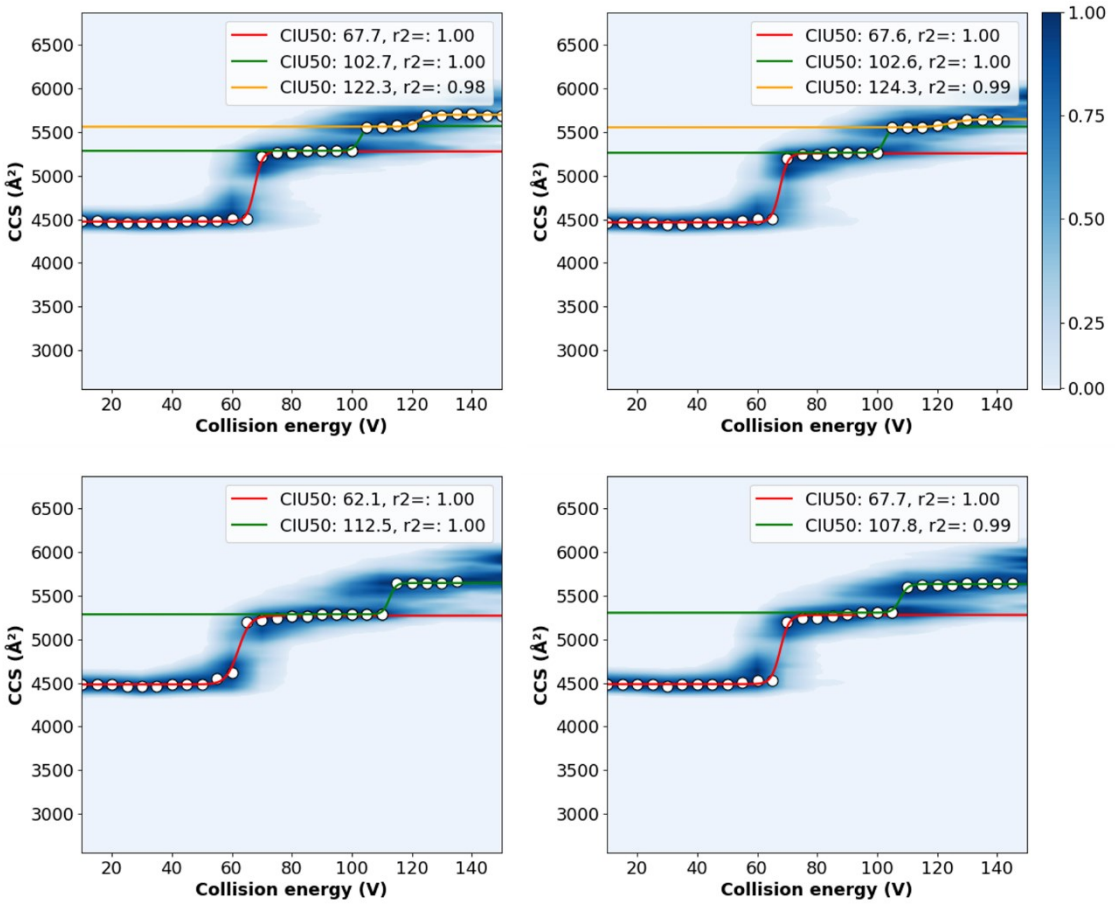

Figure S-4. CIU50 analysis performed using CIUSuite 2 on the CIU plots of untreated (A) and delipidated (B) hSA and of the untreated (C) and delipidated (D) hSA in complex with PFOA (10-fold excess) shown in Figure 3.

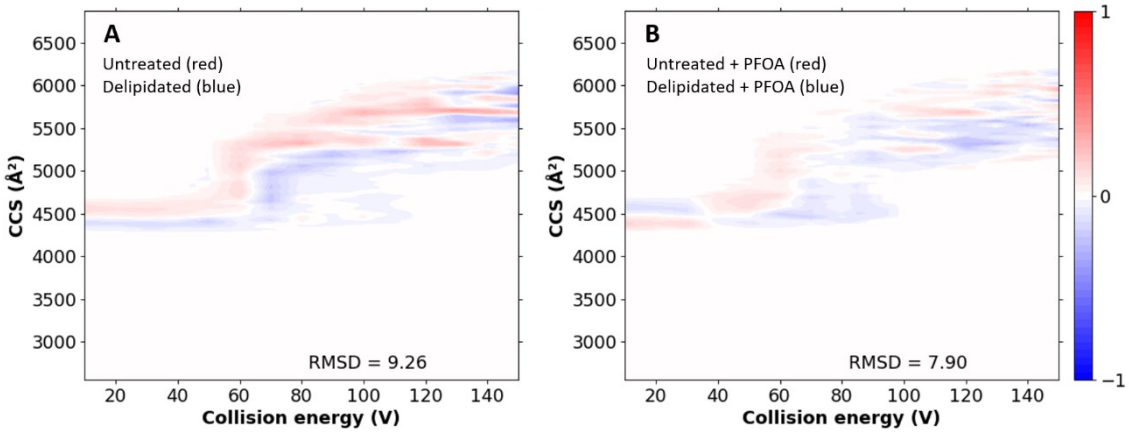

Figure S-5. RMSD values and CIU difference plots, generated with CIUSuite, for comparison of the CIU data shown in Figure 3. The red/blue colour code indicates the intensity differences between the CIU plots. Comparisons are made between untreated and delipidated hSA (A) untreated hSA in complex with PFOA and delipidated hSA in complex with PFOA (B).

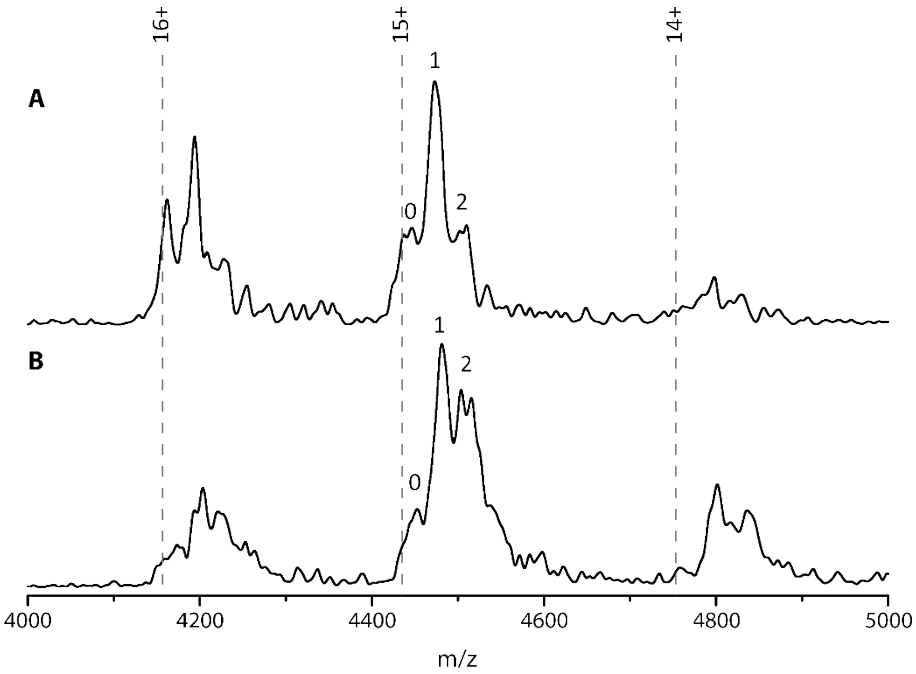

Figure S-6. MS spectra of untreated (A) and delipidated (B) hSA in complex with PFOA at a 1:10 protein:ligand ratio recorded at 150 V trap collision energy on the Synapt G2 instrument. The dashed lines indicate the theoretical m/z-values of hSA.

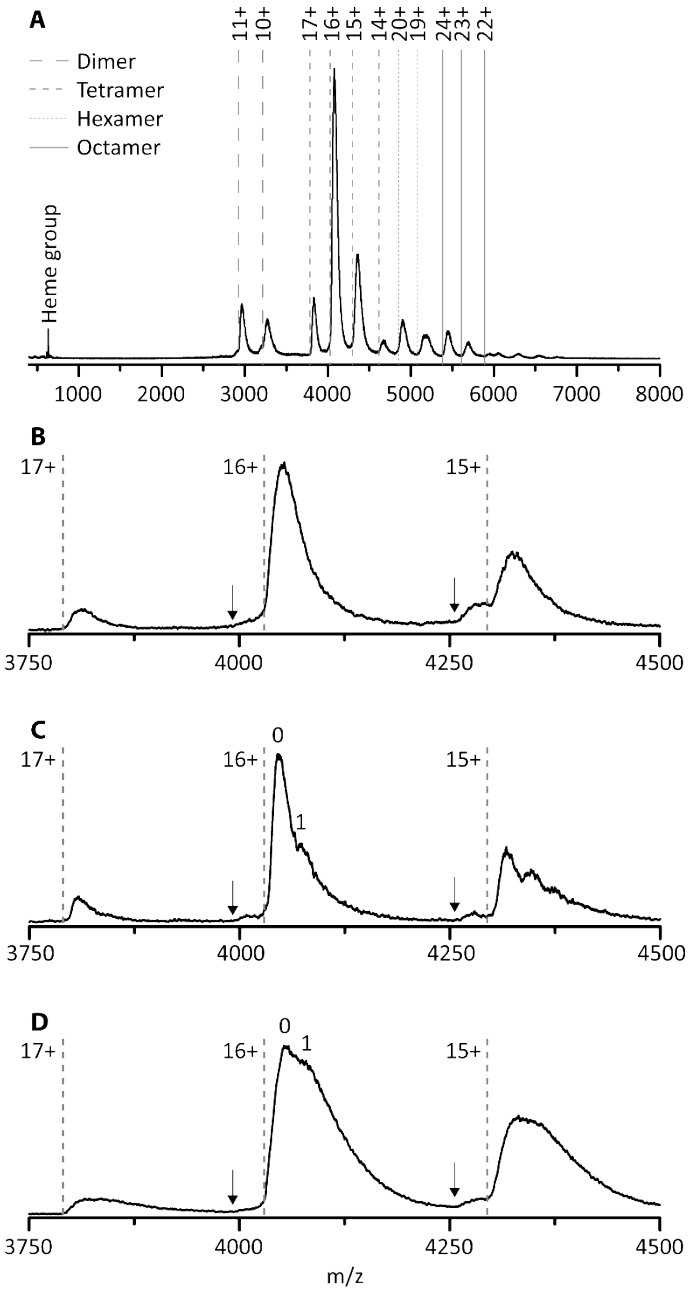

Figure S-7. Native MS spectrum of Hb (A) together with a zoom of the tetramer region (B). Native MS spectrum of Hb in complex with PFOS (C) and PFOA (D) in a 1:10 protein:target ratio. The dashed lines indicate the theoretical m/z-values of Hb. The arrows indicate the theoretical m/z-value of Hb minus one haem group.

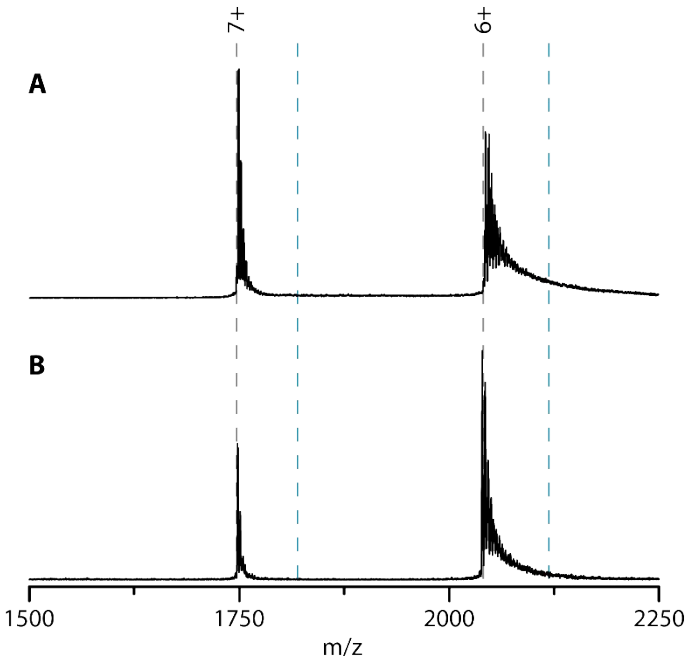

Figure S-8. Native MS spectra of cyt c alone (A), and of cyt c in the presence of PFOS in a 1:10 protein:target ratio (B). The dashed lines indicate the theoretical m/z-values of the protein and 1:1 protein-PFOS complex in grey and blue, respectively

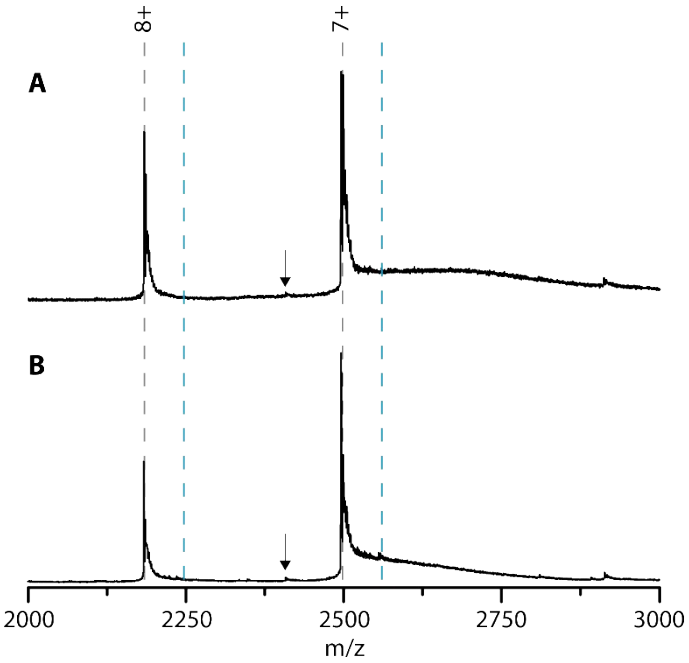

Figure S-9. Native MS spectra of NGB alone (A), and of NGB in the presence of PFOS in a 1:10 protein:target ratio (B). The dashed lines indicate the theoretical m/z-values of the protein and 1:1 protein-PFOS complex in grey and blue, respectively. The arrows indicate the theoretical m/z-value of NGB without haem group.