Supplementary Information

Analyst

High-sensitivity visualisation of contaminants in heparin samples by spectral filtering of $^1$H NMR spectra

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List of material within:

Figure S1 Illustrative plot of the binned and cut heparin-OSCS [0.25-25%] spectra.

Figure S2. Reconstructed spectra of the OSCS [0.25 - 25 %] contaminant.

Figure S3 Illustrative plot of the binned and cut heparin-OSDxS/OSAS [2-20%] spectra.

Figure S4. Reconstructed spectra of the OSAS [2 - 20 %] contaminant.

Figure S5. Reconstructed spectra of the OSDxS [2 - 20 %] contamination.

Figure S6 2D-COS analysis of unpurified GAG extract (1, 5 and 10 % (w/w)) added to a pharmaceutical heparin sample.

Figure S7 2D-COS analysis of unpurified sulfated GAG extract (1, 5 and 10 % (w/w)) added to a pharmaceutical heparin samples.

Figure S8 The N-acetyl region of the 2D-COS. Difference analysis of (A) unpurified GAG extract (5% w/w) and (B) sulfated GAG extract (5% w/w) added to a pharmaceutical heparin sample.
Figure S1 Illustrative plot of the binned and cut heparin-OSCS [0.25-25%] spectra.
Figure S2. Reconstructed spectra of the OSCS [0.25 - 25 %] contaminant. The above spectra were created by subtracting the heparin 2D-COS power spectrum away from the specific OSCS [0.25 -25 %] plus heparin dataset power spectrum. The power spectrum is the diagonal of the 2D-COS spectrum, or the variance of the covariance matrix.
Figure S3 Illustrative plot of the binned and cut heparin-OSDxS/OSAS [2-20%] spectra.
Figure S4. Reconstructed spectra of the OSAS [2 - 20 %] contaminant. The above spectra were created by subtracting the heparin 2D-COS power spectrum away from the specific OSAS [2 - 20 %] plus heparin dataset power spectrum. The power spectrum is the diagonal of the 2D-COS spectrum, or the variance of the covariance matrix.
Figure S5. Reconstructed spectra of the OSDxS [2 - 20 %] contamination. The above spectra were created by subtracting the heparin 2D-COS power spectrum away from the specific OSDxS [2 - 20 %] plus heparin dataset power spectrum. The power spectrum is the diagonal of the 2D-COS spectrum, or the variance of the covariance matrix.
Figure S6 2D-COS analysis of unpurified GAG extract ¹ (1, 5 5and 10 % (w/w)) added to a pharmaceutical heparin sample. Panels A (1% w/w), C (5% w/w) and E (10 w/w) show the 2D-COS spectra generated when the contaminants were added to the heparin library. Panels B, D and F are the difference 2D-COS spectra, the contaminated heparin added to the heparin library 2D-COS minus the 2D-COS spectra of the heparin
Figure S7 2D-COS analysis of unpurified sulfated GAG extract (1, 5 and 10 % (w/w)) added to a pharmaceutical heparin samples. Panels A (1% w/w), C (5% w/w) and E (10 w/w) show the 2D-COS spectra generated when the contaminants were added to the heparin library. Panels B, D and F are the difference
2D-COS spectra, the contaminated heparin added to the heparin library 2D-COS minus the 2D-COS spectra of the heparin dataset.

![Figure S8](image)

**Figure S8** The N-acetyl region of the 2D-COS. Difference analysis of (A) unpurified GAG extract (5% w/w) and (B) sulfated GAG extract (5% w/w) added to a pharmaceutical heparin sample. The difference spectra were generated by subtracting the 2D-COS spectrum of the heparin reference library from the 2D-COS spectrum of the heparin reference library including the contaminated heparin sample. The multiple cross peak correlations reveal how complicated the pollutant is in this case.