Supporting Information Table ST1. Classification results for combined group D2AB,high, consisting of all D2B,high spectra plus 10 non-outlier D2A,high spectra. The D2A,high spectra, which are uniformly sampled, were first resampled according to D2B,high sampling schedules using the nusCompress utility in NMRPipe.[38] This resampling procedure deletes or sets to zero the subset of data not included in the non-uniform sampling schedule, such that the resampled data can be treated as NUS data, and reprocessed to correspond to the D2B,high data according to the processing protocols used for the interlaboratory study.[2] The outlier detection threshold for this case is $D_{i,k} > 1.27$ at the 95% confidence limit.

Index	Spectrum Study Title	Interactive Score	$D_{i,k}$	Z Score	Outlier, Recursive Method	Notes
211	211-D2B-S-N-800-6211-403-37C	2	4.22	20638.25	YES	
208	208-D2B-S-N-800-2461-103-37C	1	3.42	4817.43	YES	
224	224-D2B-S-N-800-7244-015-37C	2	3.01	2009.95	YES	
212	212-D2B-S-N-800-6211-405-37C	2	1.82	60.48	YES	
219	219-D2B-S-N-800-6272-005-37C	0	1.52	17.43	NO	Above outlier threshold, but not within 15% outlier fraction.
215	215-D2B-S-N-800-6211-409-37C	1	1.36	8.02	NO	Above outlier threshold, but not within 15% outlier fraction.
213	213-D2B-S-N-800-6211-406-37C	0	1.14	2.45	NO	
204	204-D2B-S-N-800-2146-003-37C	0	1.13	2.27	NO	
2	002-D2A-S-U-900-7425-010-37C	0	1.03	1.18	NO	
5	005-D2A-S-U-900-8495-010-37C	0	1.03	1.16	NO	
182	182-D2B-S-N-900-8495-011-37C	0	1.02	1.14	NO	
196	196-D2B-S-N-850-5487-003-37C	0	0.98	0.86	NO	
45	045-D2A-S-U-800-7425-002-37C	0	0.97	0.78	NO	
37	037-D2A-S-U-800-6272-003-37C	0	0.95	0.67	NO	
9	009-D2A-S-U-900-8822-008-37C	0	0.94	0.62	NO	
19	019-D2A-S-U-850-5487-002-37C	0	0.93	0.58	NO	
188	188-D2B-S-N-900-8822-009-37C	0	0.93	0.58	NO	
34	034-D2A-S-U-800-6211-402-37C	0	0.92	0.55	NO	
228	228-D2B-S-N-800-7425-003-37C	0	0.91	0.51	NO	
22	022-D2A-S-U-850-6324-004-37C	0	0.91	0.51	NO	
38	038-D2A-S-U-800-6272-004-37C	0	0.89	0.44	NO	
178	178-D2B-S-N-900-7425-011-37C	0	0.88	0.4	NO	
28	028-D2A-S-U-800-2146-002-37C	0	0.86	0.34	NO	

Supporting Information Table ST2. Classification results for combined group D2CE,mid, with all spectra from group D2E,mid, and all spectra from group D2C,mid that were resampled and reprocessed as described in table ST1 to match the D2E,mid NUS protocol. The outlier detection threshold for this case is $D_{i,k} > 0.88$ at the 95% confidence limit.

| Index	Spectrum Study Title	Interactive Score	$D_{i,k}$	Z Score	Outlier, Recursive Method
78	078-D2C-S-U-700-9516-004-37C	0	0.87	4.96	No
49	049-D2C-S-U-750-2974-004-37C	0	0.86	4.64	No
234	234-D2E-S-N-750-2974-006-37C	0	0.76	2.68	No
68	068-D2C-S-U-700-8473-004-37C	0	0.74	2.41	No
253	253-D2E-S-N-700-4233-106-37C	0	0.67	1.49	No
52	052-D2C-S-U-750-5417-114-37C	0	0.61	1.03	No
268	268-D2E-S-N-700-8473-006-37C	0	0.59	0.89	No
59	059-D2C-S-U-700-4233-104-37C	0	0.57	0.72	No
238	238-D2E-S-N-750-5417-116-37C	0	0.56	0.67	No
73	073-D2C-S-U-700-8495-006-37C	0	0.53	0.53	No
243	243-D2E-S-N-700-9516-006-37C	0	0.5	0.42	No
249	249-D2E-S-N-700-8495-008-37C	0	0.43	0.22	No
75	075-D2C-S-U-700-8543-004-37C	0	0.43	0.21	No

System Suitability Sample Heavy Chain, 232 Residues

EAEAQVTLRE SGPALVKPTQ TLTLTCTFSG FSLSTAGMSV GWIRQPPGKA LEWLADIWWD
DKKHYNPSLK DRLTISKDTS KNQVVLKVTN MDPADTATYY CARDMIFNFY FDVWGQGTTV
TVSSASTKGP SVFPLAPSSK STSGGTAALG CLVKDYFPEP VTVSWNSGAL TSGVHTFPAV
LQSSGLYSLS SVVTVPSSSL GTQTYICNVN HKPSNTKVDK RVEPKSCDKT H

System Suitability Sample Light Chain, 218 residues

EAEADIQMTQ SPSTLSASVG DRVTITCSAS SRVGYMHWYQ QKPGKAPKLL IYDTSKLASG
VPSRFSGSGS GTEFTLTISS LQPDDFATYY CFQGSGYPFT FGGGTKVEIK RTVAAPSVFI
FPPSDEQLKS GTASVVCLLN NFYPREAKVQ WKVDNALQSG NSQESVTEQD SKDSTYSLSS
TLTLSKADYE KHKVYACEVT HQGLSSPVTK SFNRGEC

Supporting Information Figure S1. Amino acid sequences of Fab domain light and heavy chains of the NISTmAb Interlaboratory NMR Study samples. The sequences given here are for the "System Suitability Sample" construct, which is identical to the "NIST-Fab" sequence, but includes four additional amino acids EAEA at the N-terminus of each chain.
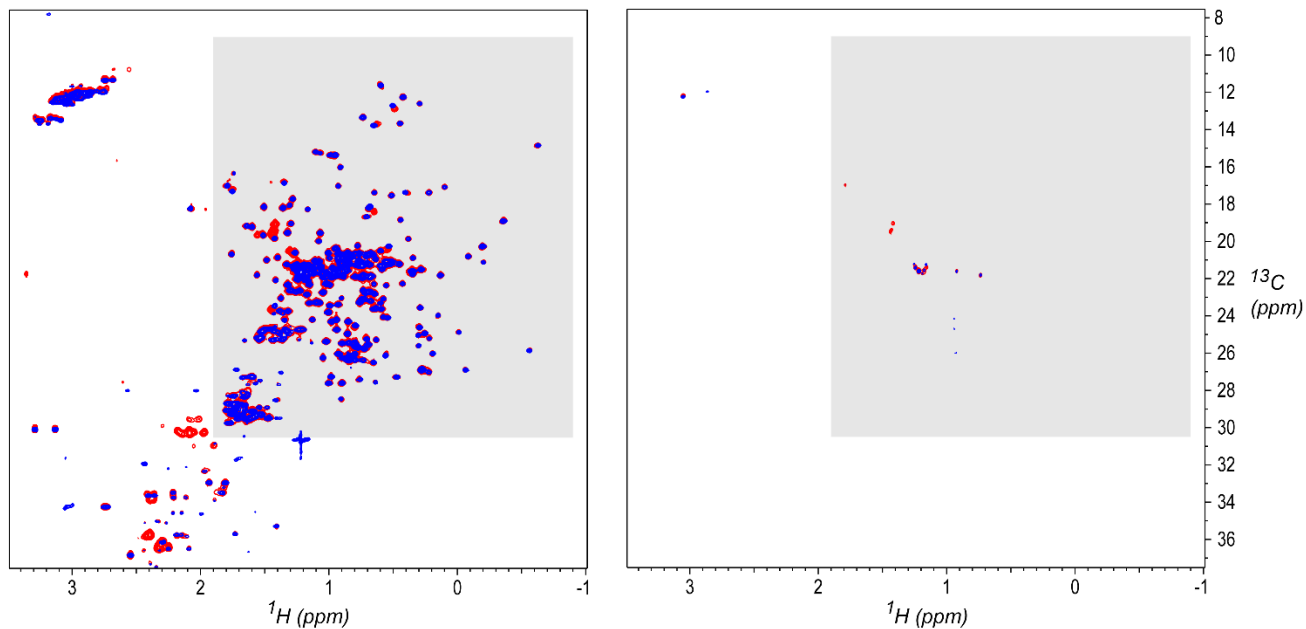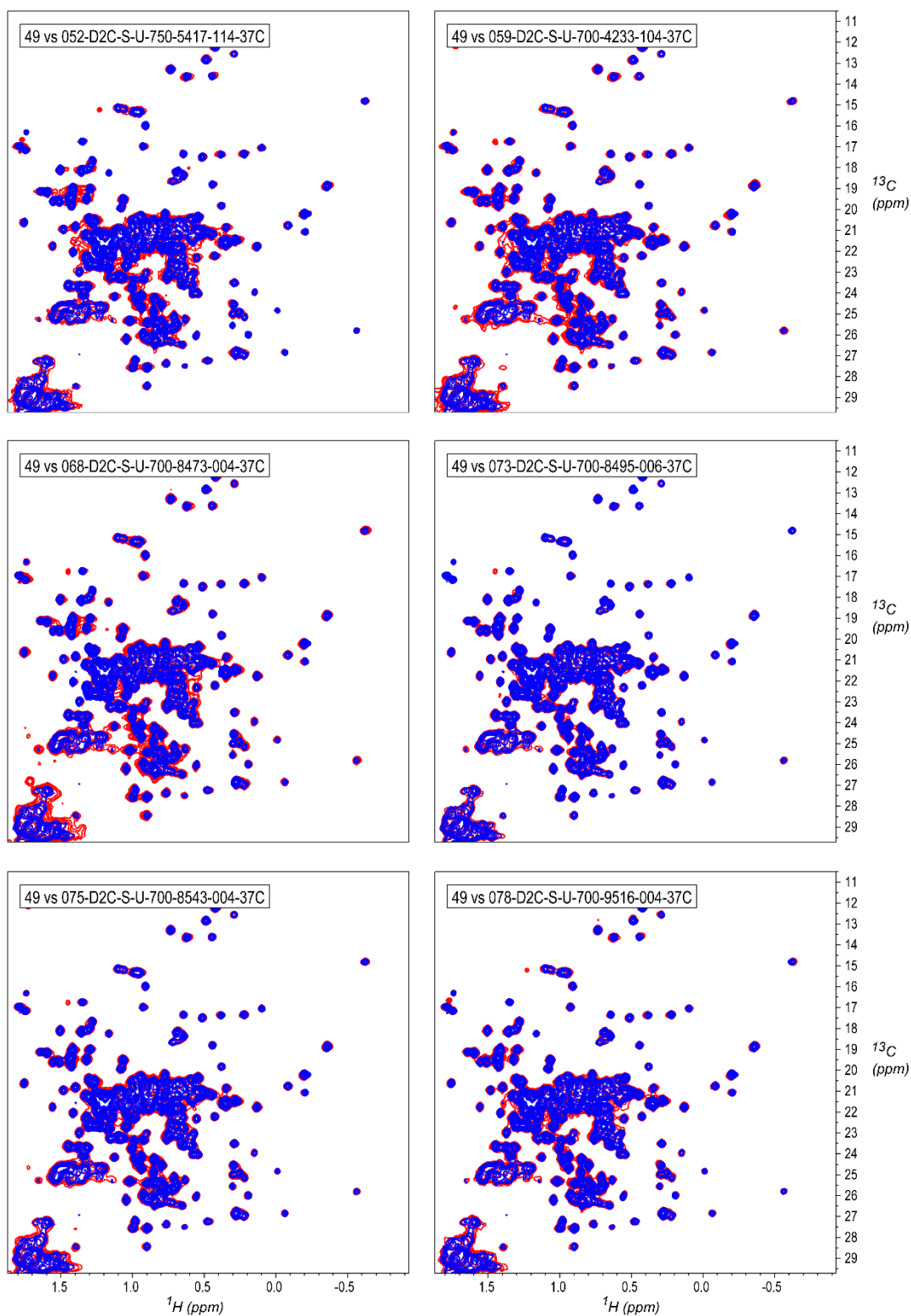
Supporting Information Figure S2. ^{1}H,^{13}C gHSQC[33] spectral overlay for a System Suitability Sample (red, D2C-S-U-900-8822-010-37C) and a NIST-Fab sample (blue, D3A-F-U-900-7425-015-37C).[2] Contour levels start at 2.5% of maximum intensity (left) and 35% of maximum intensity (right). The region shaded in gray was used for the outlier analysis in the present work (^{1}H 1.9 ppm to -0.9 ppm, ^{13}C 30.5 ppm to 9.0 ppm). As seen in the plot on the right, the majority of signals are below the 35% threshold.
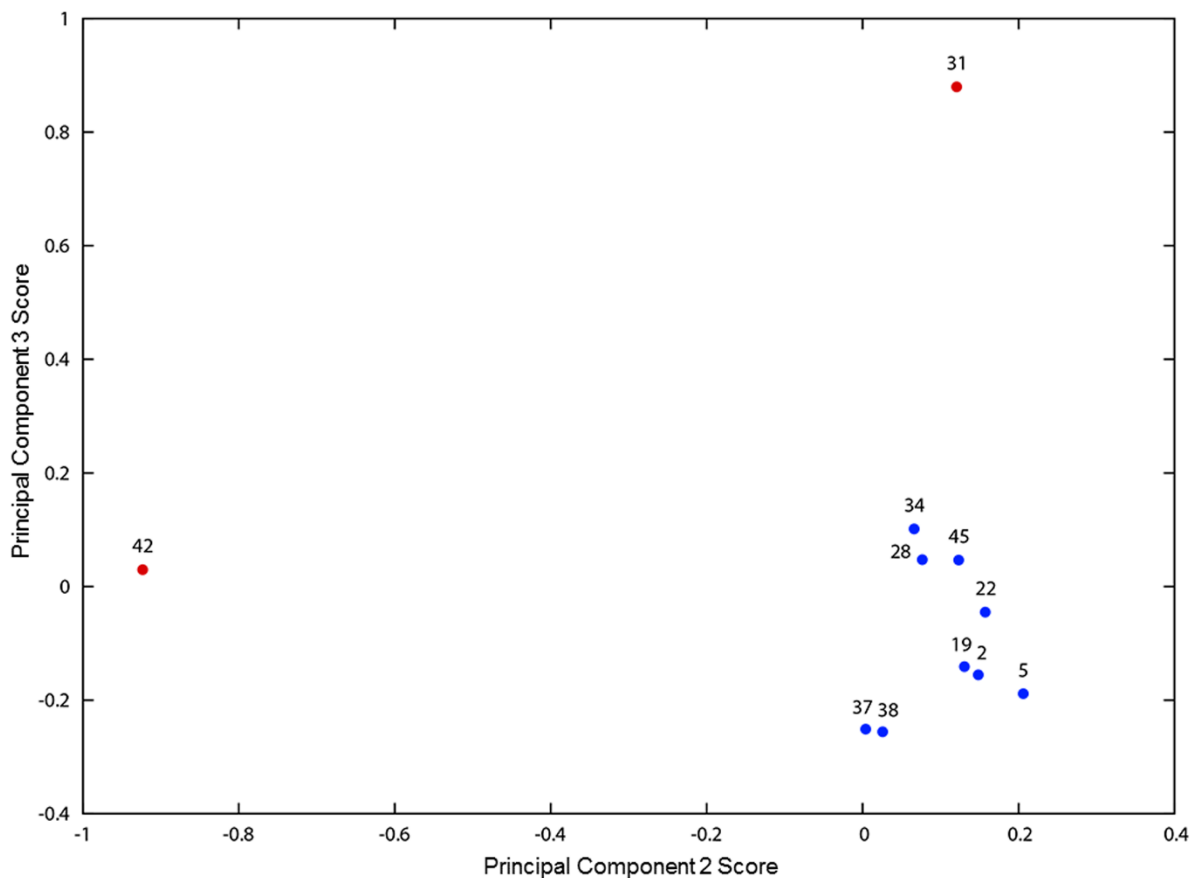
Supporting Information Figure S3. PCA results for the 12 spectra in class D2A,high, with both spectra 42 (D2A-S-U-800-2461-102-37C) and 31 (D2A-S-U-800-2461-102-37C) showing up as outliers having the largest component 2 and 3 scores respectively. PCA results were computed with the specView utility of NMRPipe, using the region of spectral intensities from ^{1}H 1.9 ppm to -0.9 ppm, ^{13}C 30.5 ppm to 9.0 ppm. Regions were scaled to uniform maximum intensity, and used for PCA without binning and without centering (subtraction of the average).
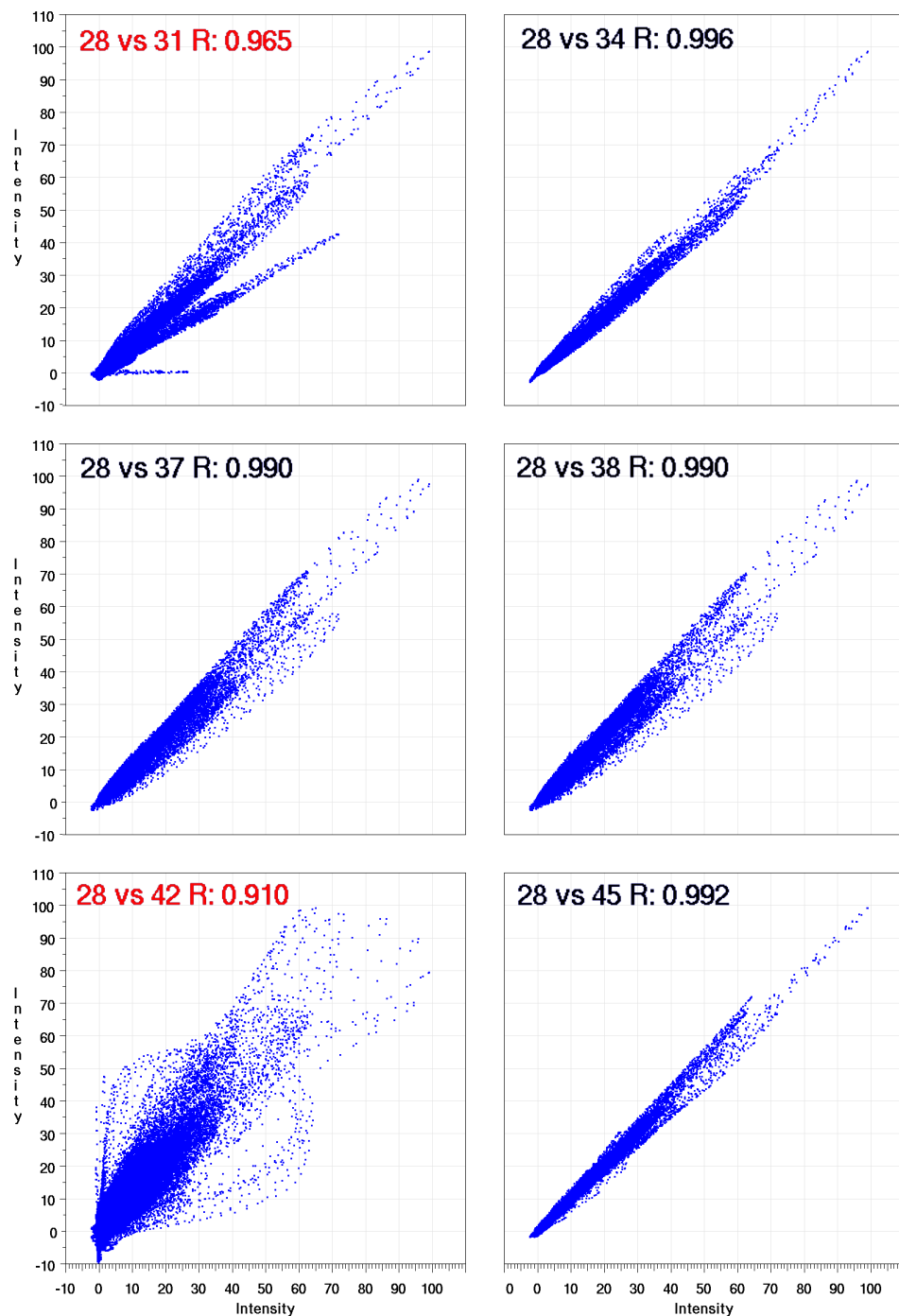
Supporting Information Figure S4. Intensity versus intensity correlation plots for representative spectrum 28 (028-D2A-S-U-800-2146-002-37C) versus the other six 800 MHz spectra in the class. Each plot is labeled with the Pearson's correlation value R. The correlation plot for visually identified outlier spectrum 42 (042-D2A-S-U-800-2461-102-37C) shows extensive systematic deviations, and the lowest correlation coefficient (0.910). Potential outlier spectrum 31 also shows systematic deviations, and the lowest correlation coefficient (0.965) of the remaining pairs of spectra (0.990 to 0.996).

Supporting Information Figure S5. Overlays of false positive outlier spectrum 49 (blue), and the other six spectra in its class D2C,mid (red). As shown, the spectra correspond well, indicating that none of them are true outliers. Contour levels start at 2.5% of maximum intensity.