Dynamic Networks Observed in the Nucleosome Core Particles Couple the Histone Globular Domains with DNA

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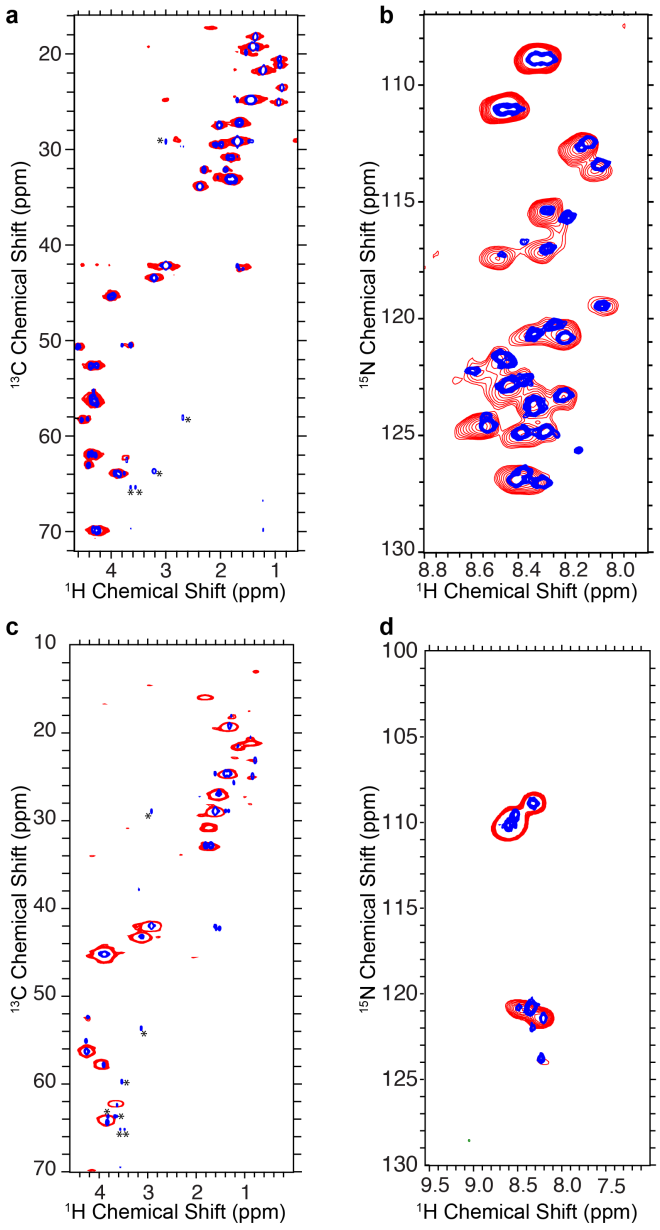
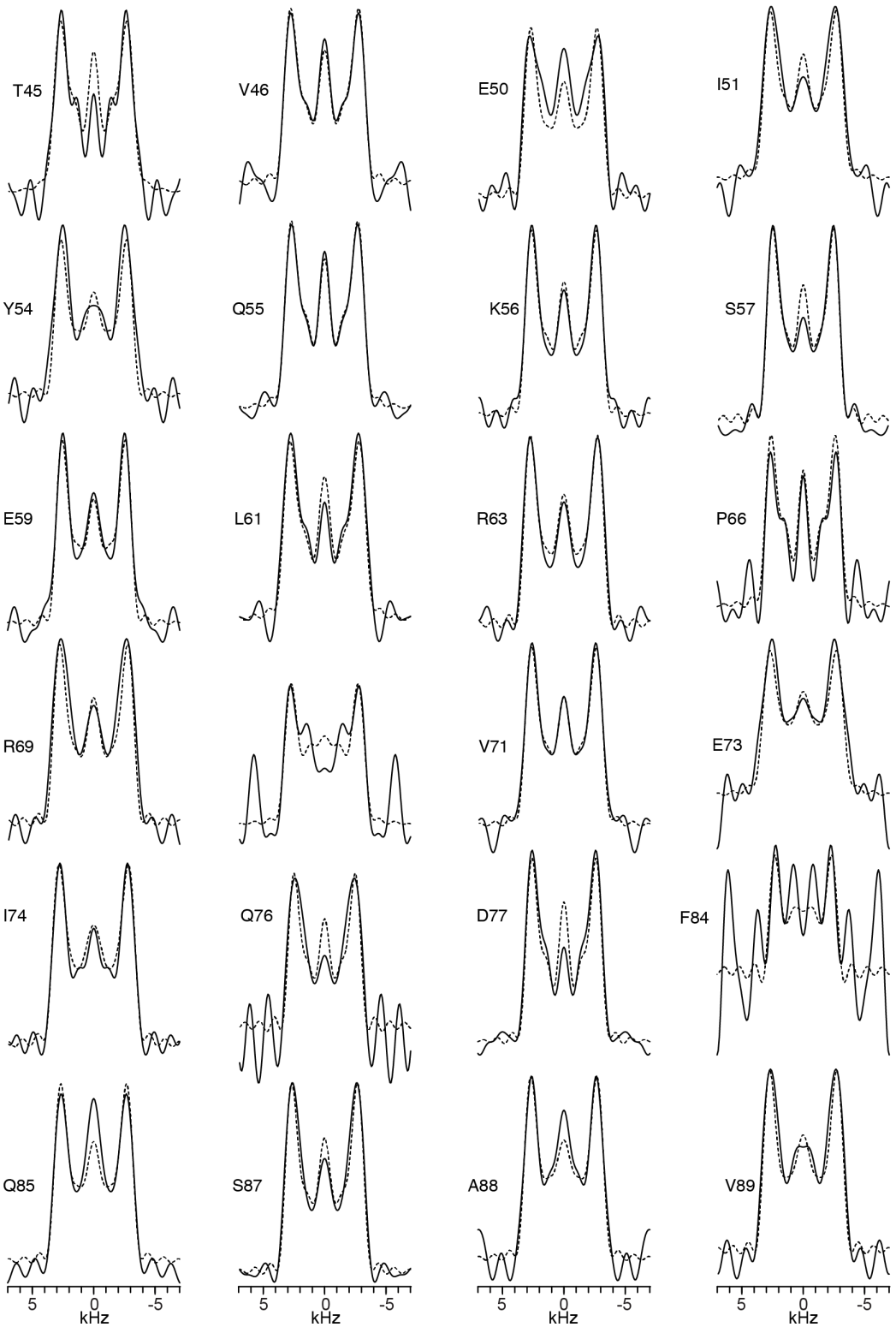
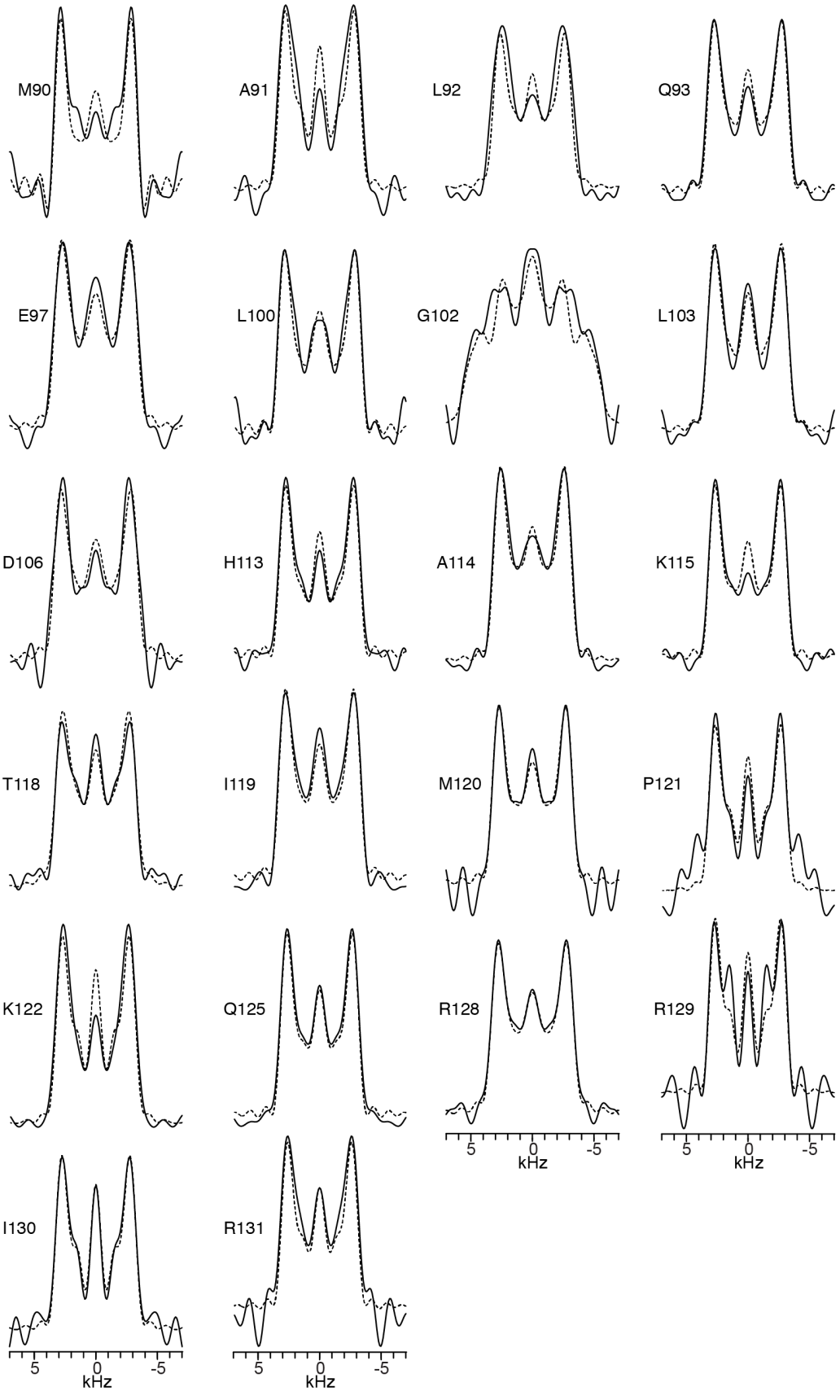


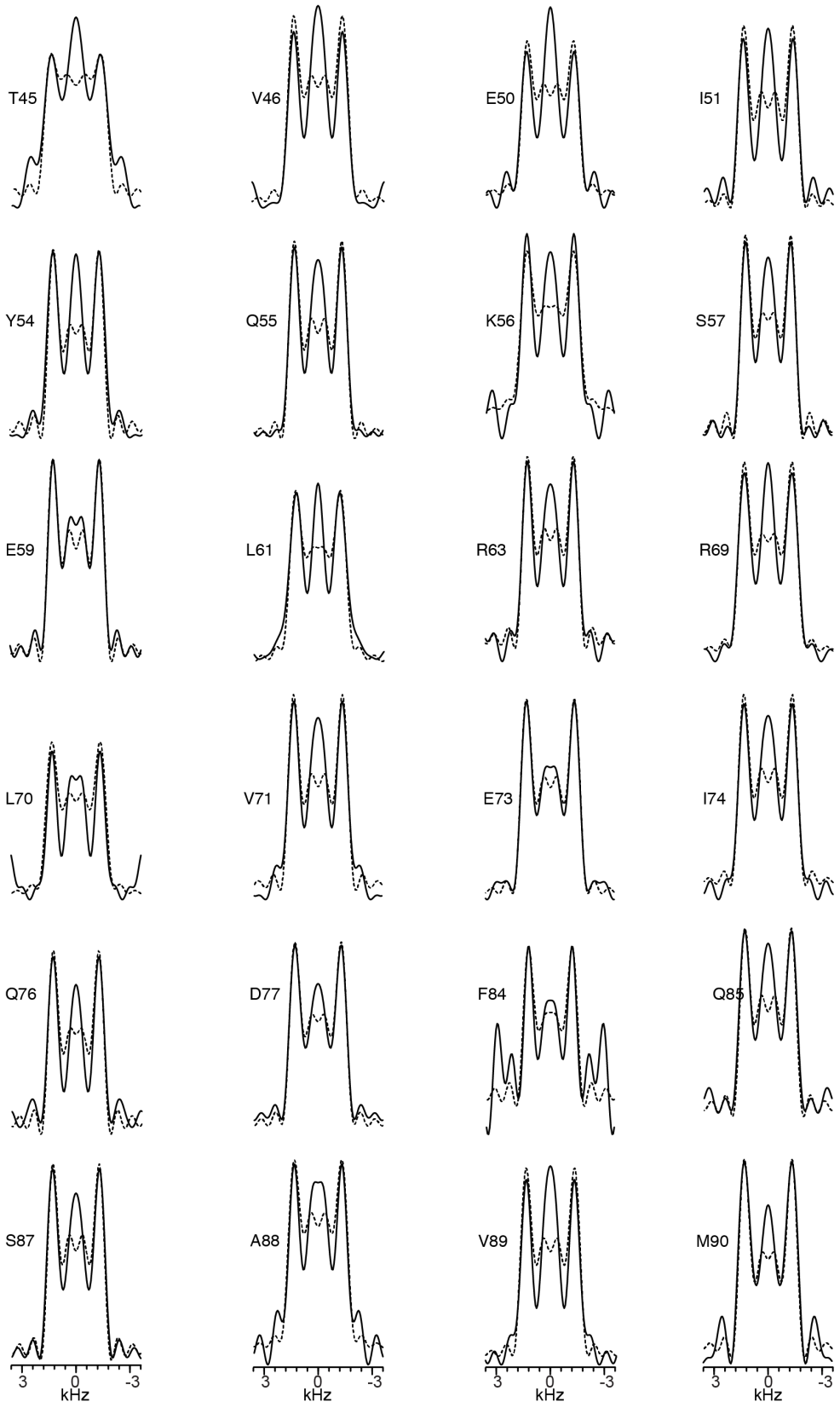
Supplementary Fig. 1 a Overlaid SSNMR ^{1}H-^{13}C correlation spectrum of the precipitated Widom 601 NCP (red) and liquid-state HSQC NMR spectrum of the solubilized NCP (blue) contained uniformly ^{13}C, ^{15}N labelled hH3. **b** Overlaid SSNMR ^{1}H-^{15}N correlation spectrum of the precipitated Widom 601 NCP (red) and liquid-state HSQC NMR spectrum of the solubilized NCP (blue) contained uniformly ^{13}C, ^{15}N labelled hH3. **c** Overlaid SSNMR ^{1}H-^{13}C correlation spectrum of the precipitated Widom 601 NCP (red) and liquid-state HSQC NMR spectrum of the solubilized NCP (blue) contained uniformly ^{13}C, ^{15}N labelled hH4. **d** Overlaid SSNMR ^{1}H-^{15}N correlation spectrum of the precipitated Widom 601 NCP (red) and liquid-state HSQC NMR spectrum of the solubilized NCP (blue) contained uniformly ^{13}C, ^{15}N labelled hH4. Asterisks mark the peaks do not belong to the NCPs.



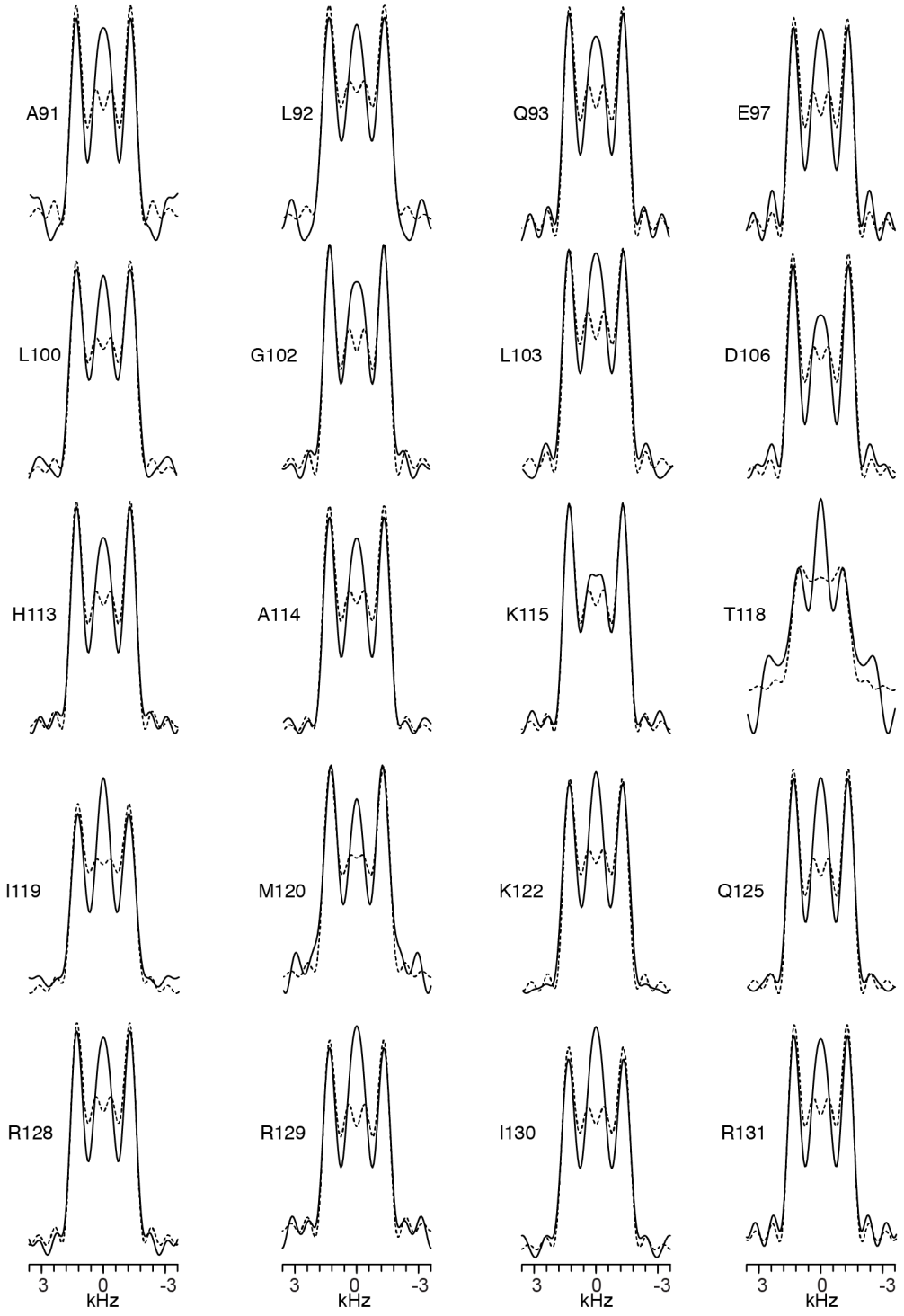
Supplementary Fig. 2 Site-resolved experimental (solid) and simulated (dotted) ^{1}H-^{13}Cα dipolar line shapes for hH3 in the Widom 601 NCP. The experimental line shapes are extracted from a 3D DIPSHIFT with $R12_1^4$ symmetry dipolar recoupling pulses. The SIMPSON output values of the root-mean-square (rms) deviation between experimental and simulated line shapes are provided.



Supplementary Fig. 2 (Continued)



Supplementary Fig. 3 Site-resolved experimental (solid) and simulated (dotted) ^{1}H-^{15}N dipolar line shapes for hH3 in the Widom 601 NCP. The experimental line shapes are extracted from a 3D DIPSHIFT with $R12_1^4$ symmetry dipolar recoupling pulses. The SIMPSON output values of the root-mean-square (rms) deviation between experimental and simulated line shapes are provided.



Supplementary Fig. 3 (Continued)

Supplementary Table 1 SSNMR parameters of experiments performed for the Widom 601 and telomeric NCPs.

Field (T)	18.8						
Sample	Widom 601 NCP (^{13}C, ^{15}N hH3)				Telomeric NCP (^{13}C, ^{15}N hH3)		
weight	55.2 mg				11.7 mg		
hydration level	65% (by wt)				66% (by wt)		
Experiment	CC	NCA	NCO	CANCO	CC	NCA	NCO
MAS rate (kHz)	15.151	15.151	15.151	15.151	15.151	15.151	15.151
Probe	3.2 mm HCN EFree MAS probe				1.9 mm HCN MAS probe		
transfer 1	HC CP	HN CP	HN CP	HC CP	HC CP	HN CP	HN CP
rf field (kHz), ^{1}H shape	70.4 ramp	52.2 ramp	52.2 ramp	70.0 ramp	67.4 ramp	64.9 ramp	64.9 ramp
rf field (kHz), ^{15}N/^{13}C	53.0	37.9	37.9	53.0	53.0	53.0	53.0
transfer time	1.0	1.0	1.0	0.8	1.0	1.2	1.2
carrier (ppm)	103.0	–	–	55.0	–	–	–
^{13}C, ^{15}N	–	115.4	115.4	–	102.7	120.1	120.1
transfer 2	DARR	NCA SPECIFIC	NCO SPECIFIC	CAN SPECIFIC	DARR	NCA SPECIFIC	NCO SPECIFIC
rf field (kHz), ^{13}C shape	–	28.5 tangent	45.1 tangent	28.9 tangent	–	27.2 tangent	43.9 tangent
rf field (kHz), ^{15}N	–	37.9	22.7	37.9	–	37.9	22.7
rf field (kHz), ^{1}H cw	14.1	89.4	89.4	89.4	15.1	93.6	91.8
transfer time	20	4.0	4.0	3.0	20	3.0	3.5
carrier (ppm)	103.0	58.0	178.0	55.0	102.7	54.7	177.8
^{13}C, ^{15}N	–	115.4	115.4	115.4	–	120.1	120.1
transfer 3	–	–	–	NCO SPECIFIC	–	–	–
rf field (kHz), ^{13}C shape	–	–	–	45.0	–	–	–
rf field (kHz), ^{15}N	–	–	–	22.7	–	–	–
rf field (kHz), ^{1}H cw	–	–	–	89.4	–	–	–
transfer time	–	–	–	3.0	–	–	–
carrier (ppm)	–	–	–	178.0	–	–	–
^{13}C, ^{15}N	–	–	–	115.4	–	–	–
digitalization, F1	C	N	N	CA	C	N	N
t1 increments	768	192	192	84	768	76	76
sweep width (kHz)	45453	7575.5	7575.5	7575.5	45453	3030.2	3030.2
acquisition time (ms)	8.4	12.7	12.7	5.5	8.4	12.5	12.5
digitalization, F2	C	C	C	N	C	C	C
t2 increments	1536	832	832	48	1536	448	448
sweep width (kHz)	53571.43	29761.904	29761.904	3030.2	53571.43	15151.516	15151.516
acquisition time (ms)	14.4	14.0	14.0	7.9	14.4	14.8	14.8
digitalization, F3	–	–	–	CO	–	–	–
t3 increments	–	–	–	1088	–	–	–
sweep width (kHz)	–	–	–	45454.547	–	–	–
acquisition time (ms)	–	–	–	11.9	–	–	–
^{1}H decoupling rf filed (kHz) shape	73.5 SPINAL 64	73.5 SPINAL 64	73.5 SPINAL 64	73.5 SPINAL 64	81.4 SPINAL 64	81.4 SPINAL 64	81.4 SPINAL 64
number of scans	96	192	196	56	512	4224	5832
pulse delay (s)	1.5	1.5	1.5	1.5	1.5	1.5	1.5

Supplementary Table 1 (Continued)

Field (T)	18.8					
Sample	Widom 601 NCP (^{13}C, ^{15}N hH4)			Telomeric NCP (^{13}C, ^{15}N hH4)		
weight	46 mg			13.7 mg		
hydration level	57% (by wt)			63% (by wt)		
Experiment	CC	NCA	NCO	CC	NCA	NCO
MAS rate (kHz)	15.151	15.151	15.151	17.857	17.857	17.857
Probe	3.2 mm HCN EFree MAS probe			1.9 mm HCN MAS probe		
transfer 1	HC CP	HN CP	HN CP	HC CP	HN CP	HN CP
rf field (kHz), ^{1}H	82.2	63.7	63.7	81.5	76.9	76.9
shape	ramp	ramp	ramp	ramp	ramp	ramp
rf field (kHz), ^{15}N/^{13}C	56.9	44.6	44.6	62.5	44.6	44.6
transfer time	1.4	1.4	1.4	1.2	1.0	1.0
carrier (ppm)	103.5	–	–	–	–	–
^{13}C, ^{15}N	–	115.8	115.8	102.6	115.0	115.0
transfer 2	DARR	NCA SPECIFIC	NCO SPECIFIC	DARR	NCA SPECIFIC	NCO SPECIFIC
rf field (kHz), ^{13}C	–	30.8,	48.8,	–	31.7	51.8
shape		tangent	tangent		tangent	tangent
rf field (kHz), ^{15}N	–	44.6	26.8	–	44.6	26.8
rf field (kHz), ^{1}H cw	15.5	88.6	90.6	16.1	93.6	91.8
transfer time	20	3.5	4.5	20	3.5	4.0
carrier (ppm)	103.5	55.5	178.5	102.6	54.6	177.6
^{13}C, ^{15}N	–	115.8	115.8	–	115.0	118
transfer 3	–	–	–	–	–	–
rf field (kHz), ^{13}C	–	–	–	–	–	–
shape						
rf field (kHz), ^{15}N	–	–	–	–	–	–
rf field (kHz), ^{1}H cw	–	–	–	–	–	–
transfer time	–	–	–	–	–	–
carrier (ppm)	–	–	–	–	–	–
^{13}C, ^{15}N	–	–	–	–	–	–
digitalization, F1	C	N	N	C	N	N
t1 increments	896	112	112	896	88	72
sweep width (kHz)	53571	4464.25	4464.25	53571	3571.4	2976.167
acquisition time (ms)	8.4	12.5	12.5	8.4	12.3	12.1
digitalization, F2	C	C	C	C	C	C
t2 increments	1664	512	512	1664	1536	512
sweep width (kHz)	53571.43	17857.143	17857.143	53571.43	53571.43	17857.143
acquisition time (ms)	15.5	14.3	14.3	15.5	14.3	14.3
digitalization, F3	–	–	–	–	–	–
t3 increments	–	–	–	–	–	–
sweep width (kHz)	–	–	–	–	–	–
acquisition time (ms)	–	–	–	–	–	–
^{1}H decoupling rf filed (kHz) shape	80.6 SPINAL 64	80.6 SPINAL 64	80.6 SPINAL 64	78.5 SPINAL 64	78.5 SPINAL 64	78.5 SPINAL 64
number of scans	48	196	196	168	1728	1408
pulse delay (s)	1.5	1.5	1.5	1.5	1.5	1.5