

The Lipid Activation Mechanism of a Transmembrane Potassium Channel

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Supporting Text:

To fully understand the time dependent evolution of ^1H - ^1H spin diffusion, we found a single R_1 value was insufficient to describe the relaxation rate associated with the buildup of protein polarization from water as a function of ^1H - ^1H spin diffusion times. ^1H - ^1H cross relaxational rates were investigated by Najbauer *et al.* who proposed a cross relaxation model that fits these $^1\text{H}_{\text{water}}\text{-}^1\text{H}_{\text{protein}}$ spin diffusion buildup curves to high precision assuming fast spinning and extensive deuteration attenuate intra-protein spin diffusion. Additionally, the different rates of polarization buildup and relaxation between the SM and the TQ spectra suggest physiologically relevant interpretation of dynamic relaxation. The ^1H - ^{13}C HETCOR experiment shows the SM lipid resonances are completely filtered out through the implementation of the T_2 filter, but the TQ lipid ^1H resonances do correlate to NA- ^{13}C -lipid signals without the appearance of any discernable protein peaks (Figure S1). We are confident that there is no magnetization that comes to KirBac1.1 via lipid ^1H s as there are no resonances that correspond to lipid associated transmembrane residues in the T_2 filtered ^{13}C - ^{13}C 2D. Therefore, we can assert that all polarization is transferring from the water species, and that intra-protein polarization transfer does severely impact data analysis in the regime of moderate spinning and fully protonated proteins. Our interpretation follows below.

REDOR simulations: For all the simulation, three carbon atoms and a phosphorus atom were considered. Dipolar couplings were calculated to represent the distance between atoms. All simulation were run considering a 600MHz field strength, and 25kHz spinning rate. For each simulation, 18 gamma angles were considered. Rep320 crystal file was used and each simulation used 1024 points.

Distance	Dipole coupling
8.0 Å between ^{31}P - ^{13}C	23.90 Hz
7.4 Å between ^{31}P - ^{13}C	30.20 Hz
7.3 Å between ^{31}P - ^{13}C	31.46 Hz
6.5 Å between ^{31}P - ^{13}C	44.57 Hz
6.3 Å between ^{31}P - ^{13}C	48.95 Hz
5.0 Å between ^{31}P - ^{13}C	97.92 Hz
4.9 Å between ^{31}P - ^{13}C	104.00 Hz
4.6 Å between ^{31}P - ^{13}C	125.75 Hz

Supporting Information:

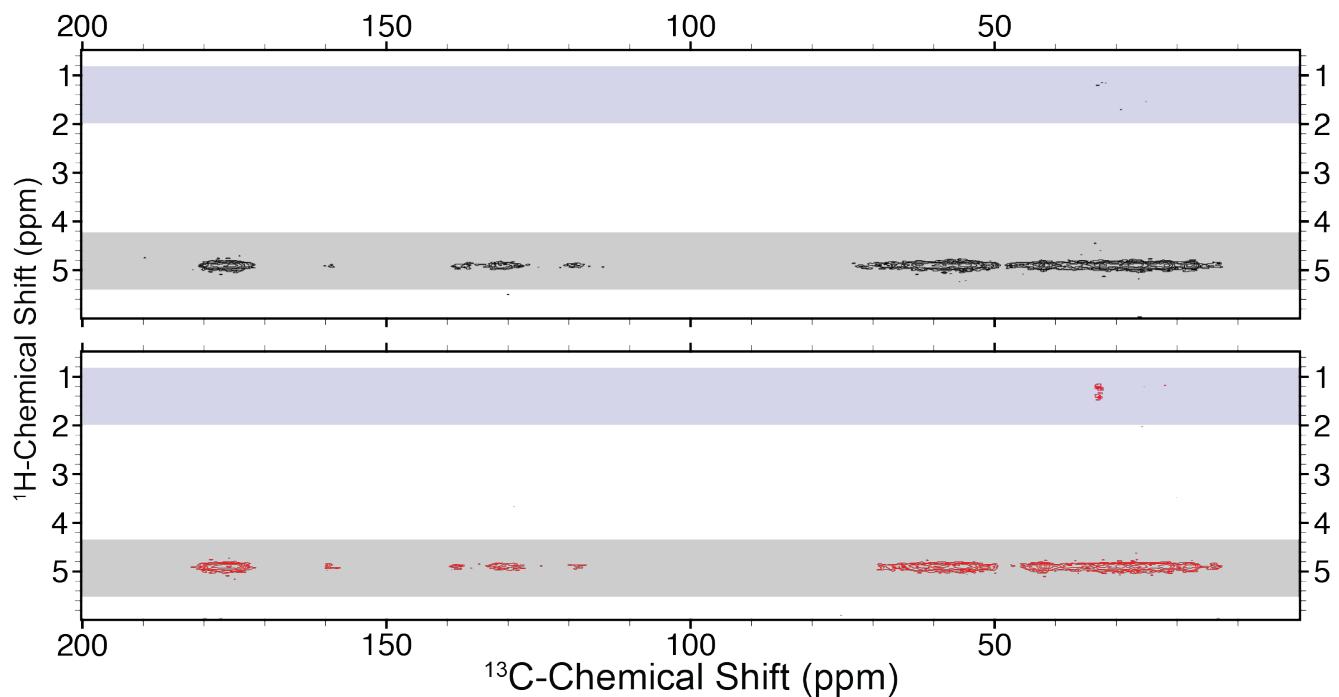


Figure S1: Water-edited ^1H - ^{13}C HETCOR spectra of SM (black) and TQ (red) in PE:PG:CL lipids. Region in blue correspond to lipid acyl chain ^1H - ^{13}C correlations. Grey region corresponds to protein ^1H - ^{13}C correlations that originated from solvent

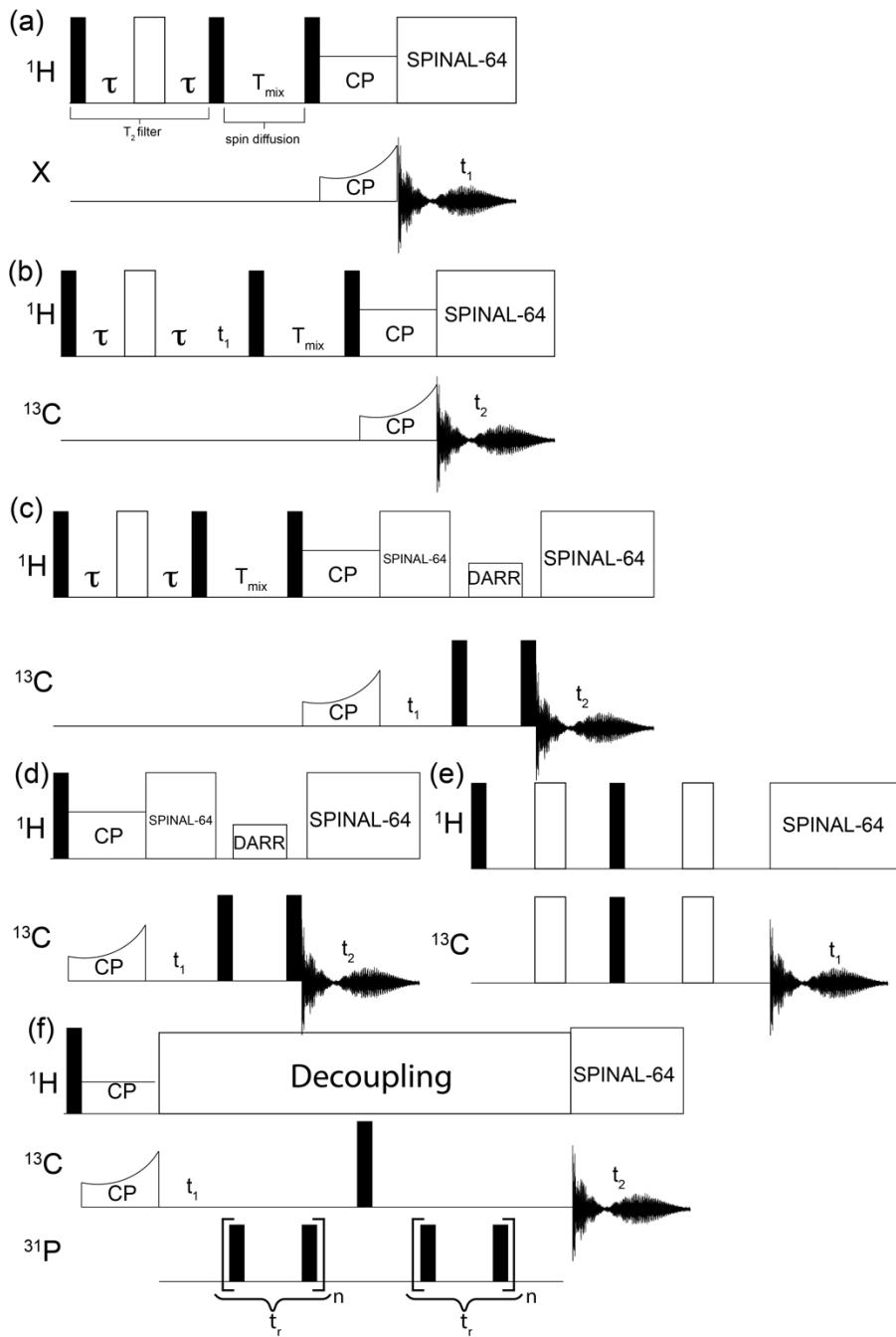


Figure S2: Pulse sequences used. (a) 1D H_2O -edited ^1H -buildup for transfer to variable nuclei, (b) 2D H_2O -edited ^1H - ^{13}C HETCOR, (c) 2D H_2O -edited ^{13}C - ^{13}C DARR, (d) ^{13}C - ^{13}C DARR, (e) ^1H - ^{13}C rINEPT, and (f) ^{13}C - ^{31}P REDOR.

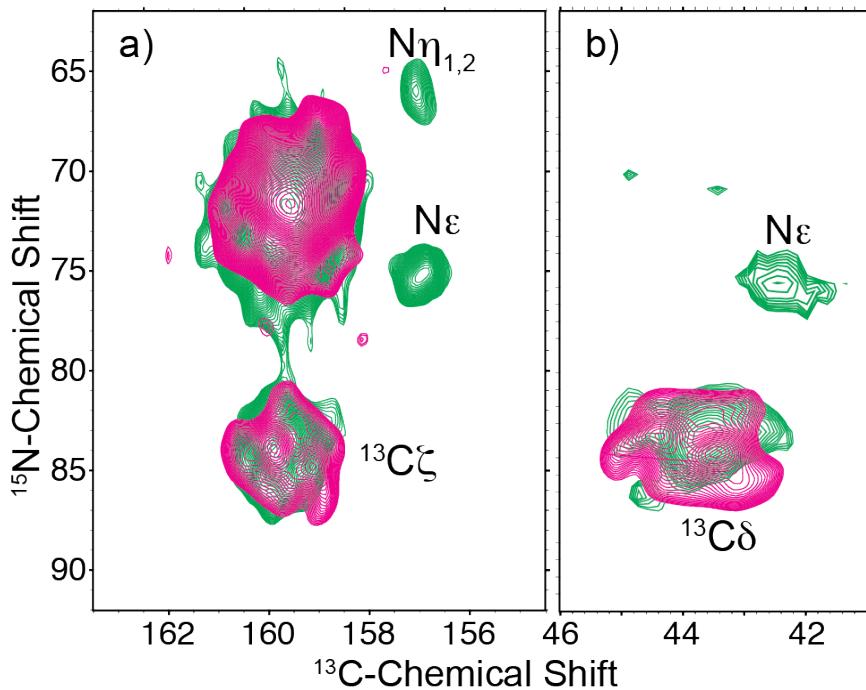


Figure S3: Spectral identification of arginines bound to anionic lipids. a) NcoCX 2D of KirBac1.1 in 3:1 POPE:POPG (w/w) lipid bilayer (green) and POPE bilayer (magenta) allowing for identification of $\text{N}\eta_{1,2}$ and $\text{N}\epsilon$ outlier peaks. b) NcaCX 2D showing isolated $\text{N}\epsilon$ peak.

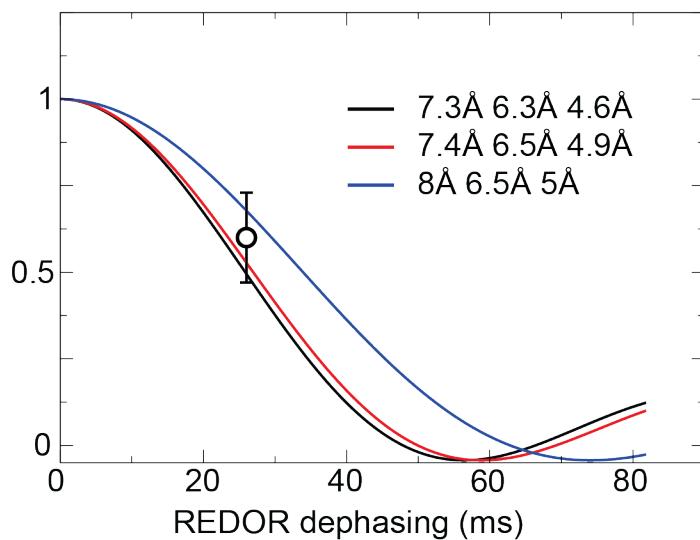


Figure S4: Simulated REDOR dephasing curve via SIMPSON. For all the simulation three carbons and one phosphorus atom has been considered. Longer distance than crystal structure (blue line), distance in crystal structure (red line), and a lower distance than the crystal structure (black line) has been simulated.

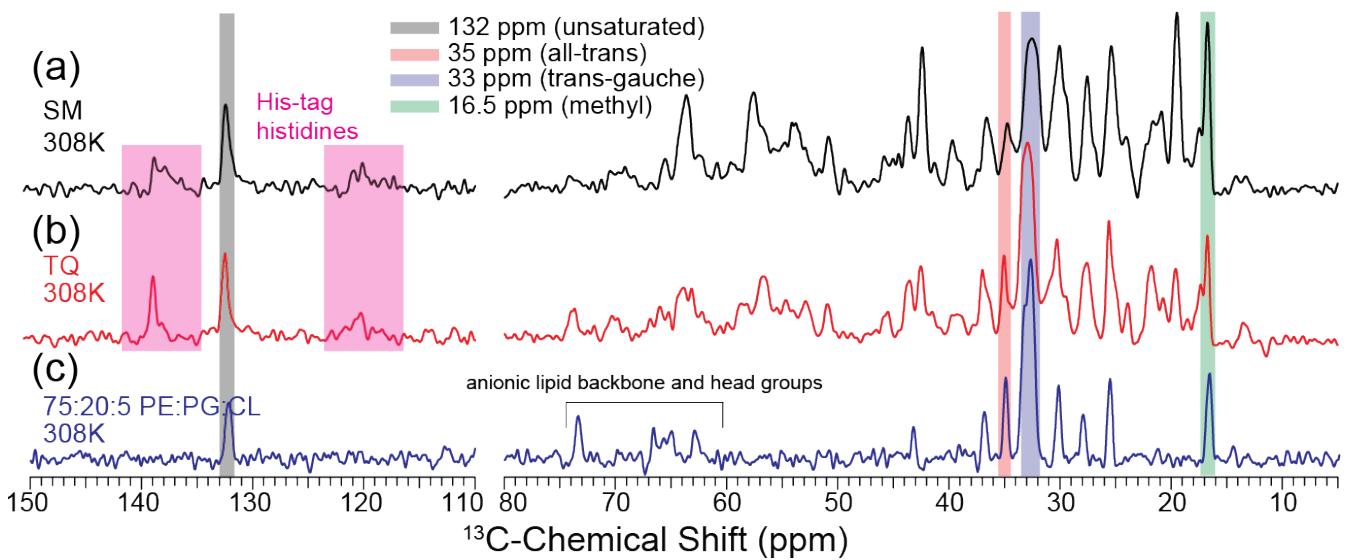


Figure S5: 1D rINEPT spectra of ^{13}C - ^{15}N KirBac1.1 in proteoliposomes (a) Stability mutant(SM)-KirBac1.1 proteoliposome in natural abundance 75:20:5 PE:PG:CL. (b) Triple Q(TQ)-KirBac1.1 proteoliposome in natural abundance 75:20:5 PE:PG:CL. (c) Natural abundance 75:20:5 PE: PG:CL liposomes without protein. Note: rINEPT polarization filters out the majority of the protein resonances sufficiently enough for 1% natural abundance lipids to be identified. Resonances corresponding to highly mobile His-tag are identified in magenta.

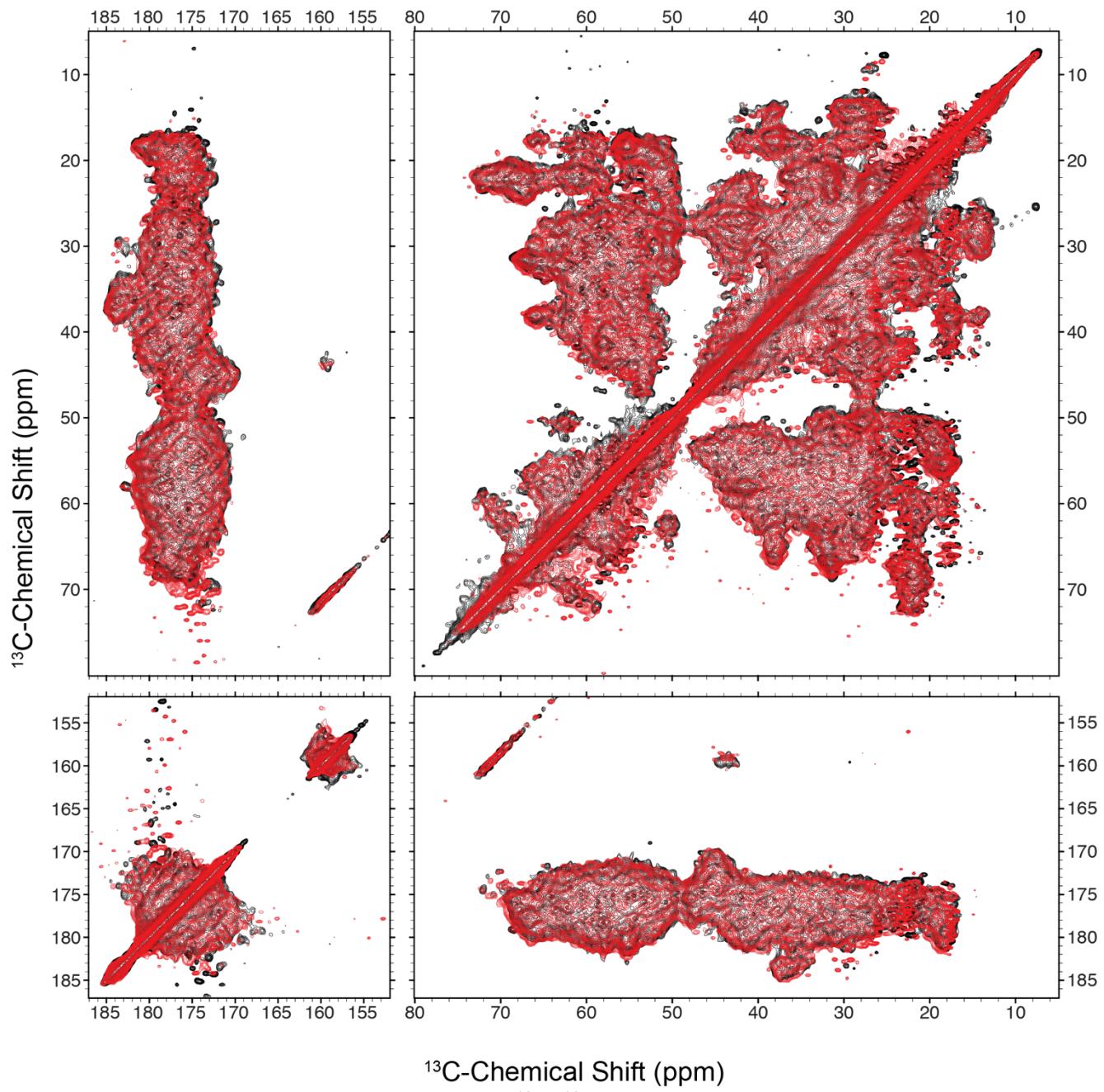


Figure S6: Standard (not water edited) 2D ^{13}C - ^{13}C DARR spectra of SM and TQ proteins. The spectrum of the TQ sample (red) is overlaid onto the spectrum of the SM sample (black). Both samples are reconstituted into the same activating PE:PG:CL lipid mixture.

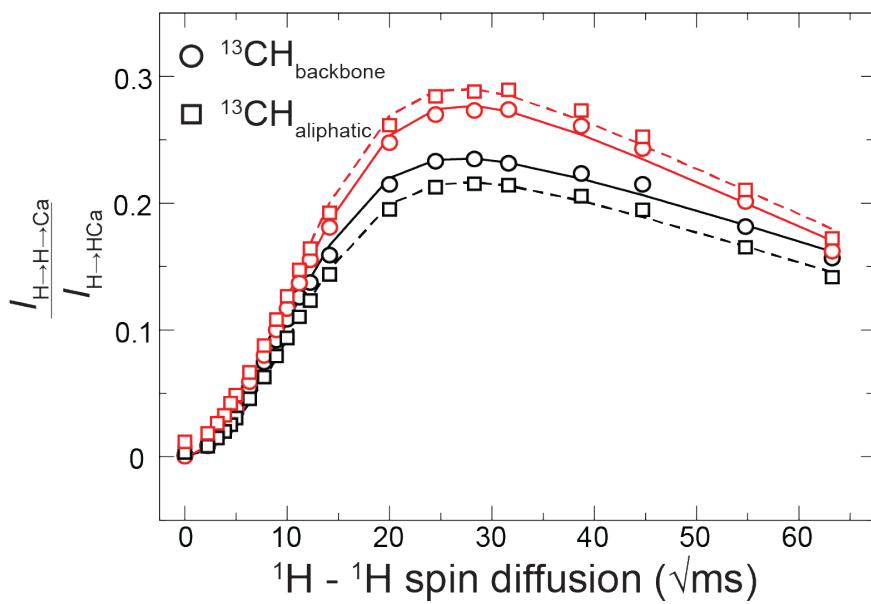


Figure S7: ${}^1\text{H}_2\text{O}-{}^1\text{H}_{\text{protein}}$ spin diffusion buildup curves of the bracketed $\text{C}\alpha$ and aliphatic spin systems of SM (black) and TQ(red) proteins. Error bars are within the size of the icons on each point.

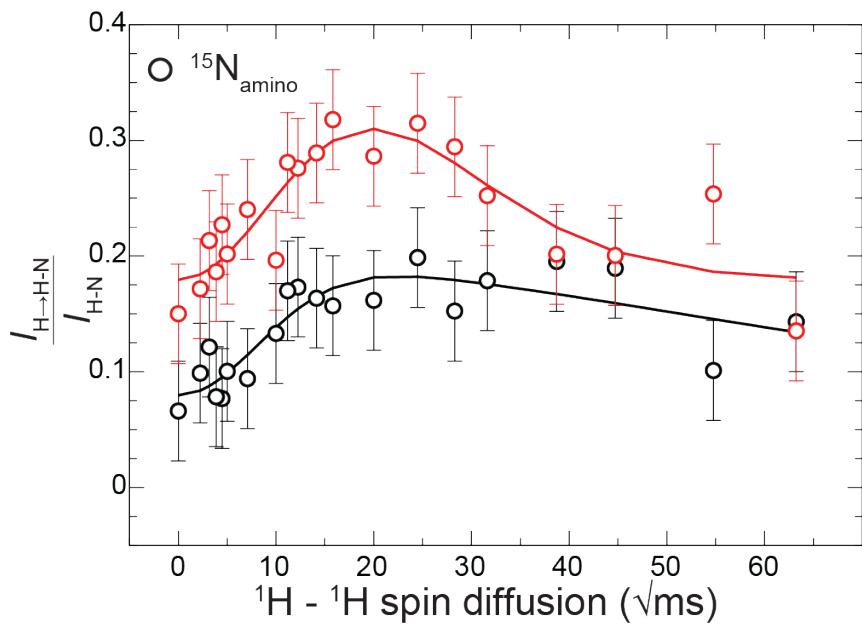


Figure S8: ${}^1\text{H}_2\text{O}-{}^1\text{H}_{\text{protein}}$ spin diffusion buildup curves of the bracketed lysine sidechain amino group spin systems for SM (black) and TQ(red) samples. Fitted values of the lysine amino group buildup are closely representative of equation (3) with the addition of a corrective term $M_p(0)$ to the end of the equation to represent polarization that survived the T_2 filter on the terminal amino group.

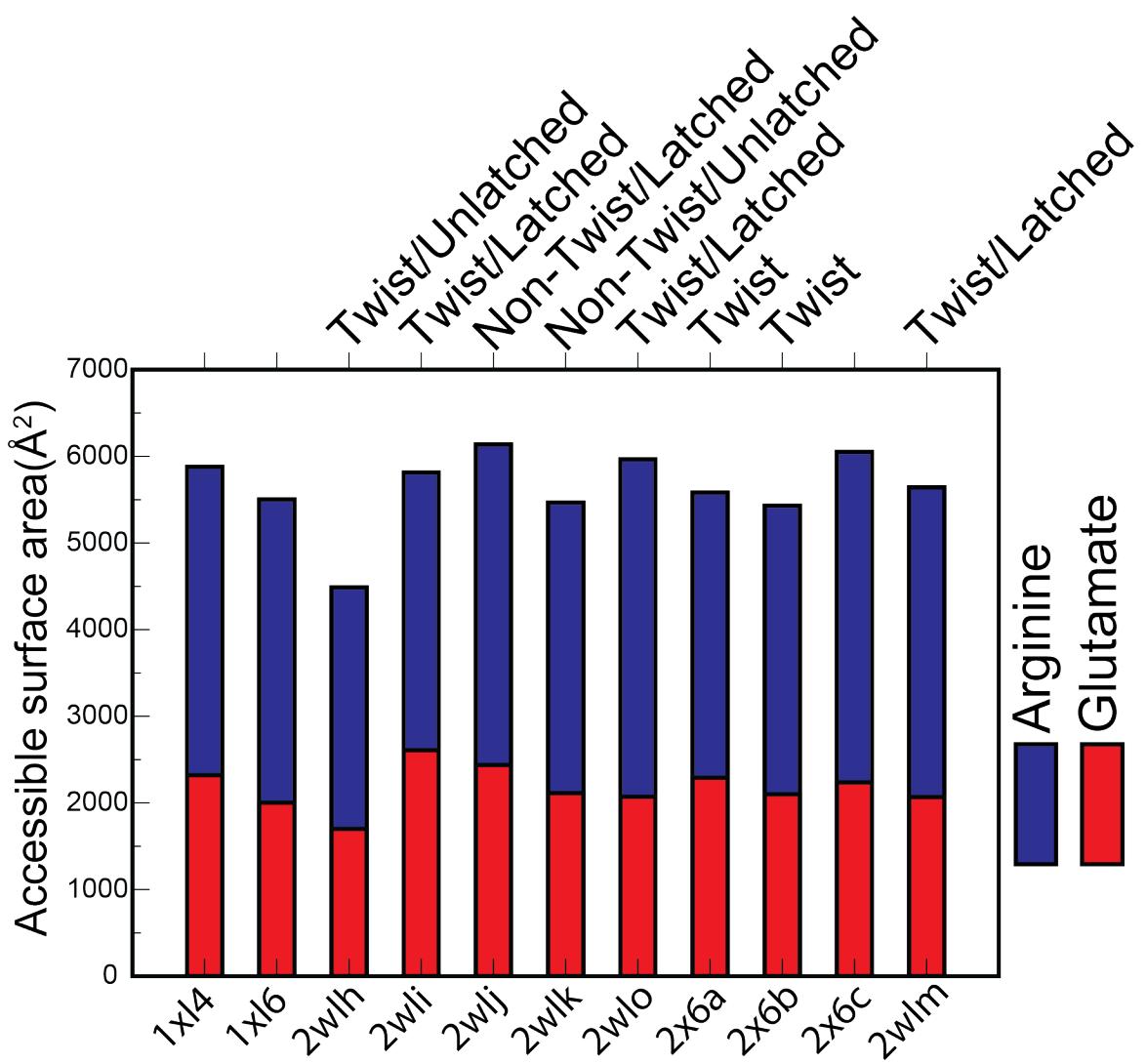


Figure S9: Exposed surface area calculations for arginine and glutamate residues in several KirBac3.1 crystal structures. The observed trend indicates the active “twist/unlatched” state (2wlh) has less exposure for these residues than the inactive “non-twist/latched” structures and their variations. While the activation gate is closed for all these structures, it is possible the conformation of the c-terminus of the 2wlh structure is similar to the open-activated conformation observed in activating lipid bilayers.

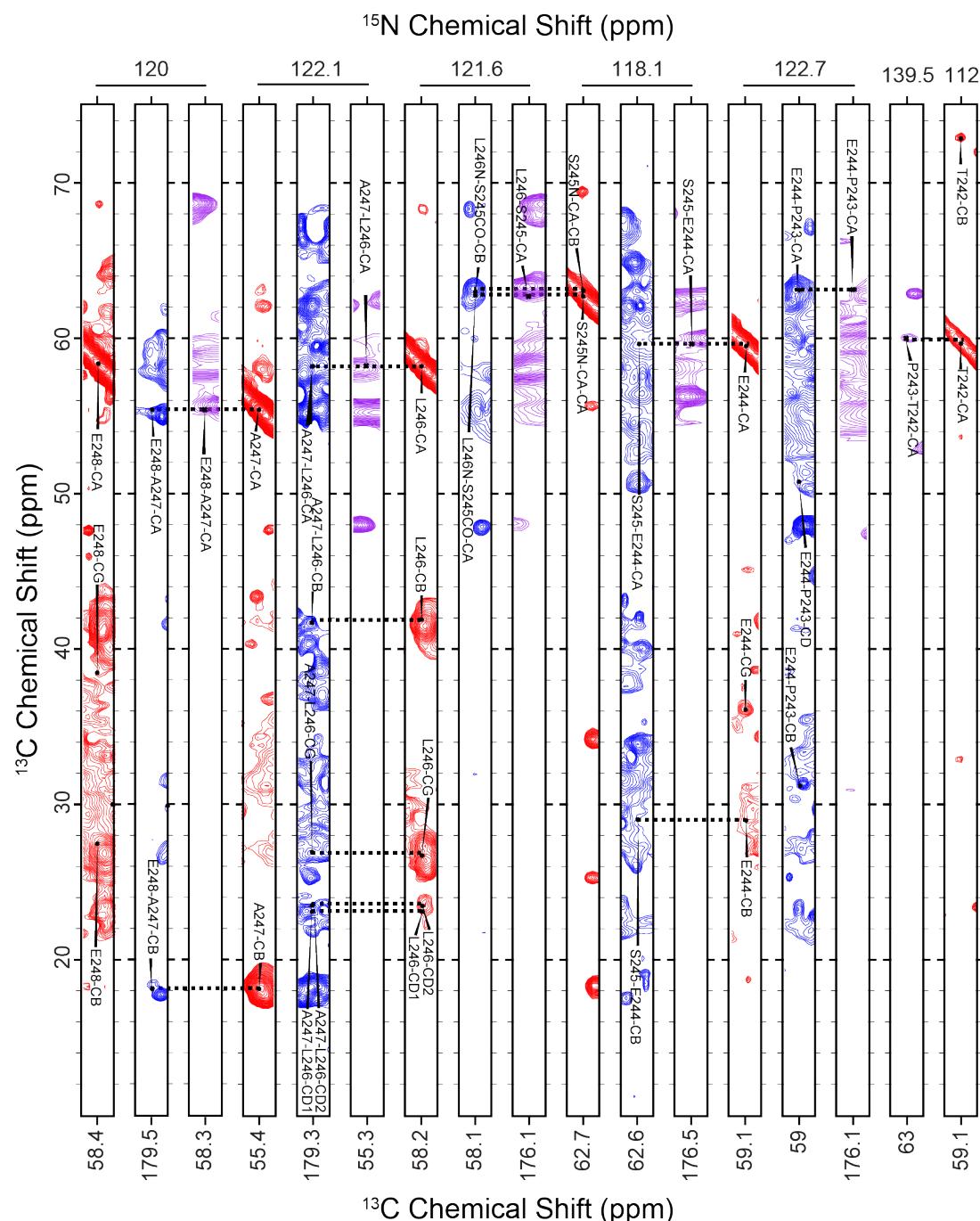


Fig. S10: Strip plot of 3D assignments for residues T242 to E248 of SM KirBac1.1 in POPC lipid bilayers. NCACX (red), CANcoCA (purple), and NCOCX (blue) spectra were used.

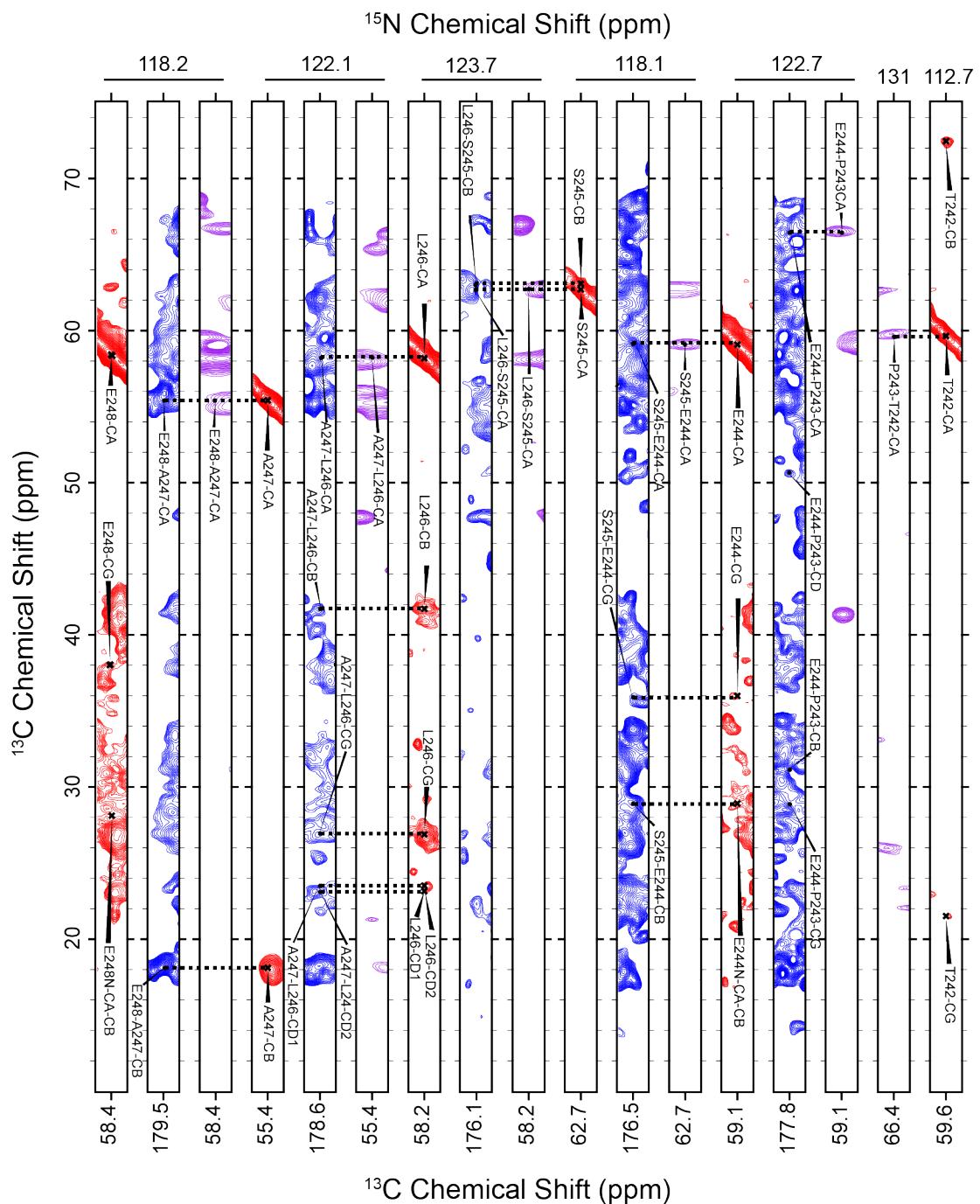


Fig. S11: Strip plot of 3D assignments for residues T242 to E248 of SM KirBac1.1 in POPC:POPG (3:2) w/w lipid bilayers. NCACX (red), CANcoCA (purple), and NCOCX (blue) spectra were used.

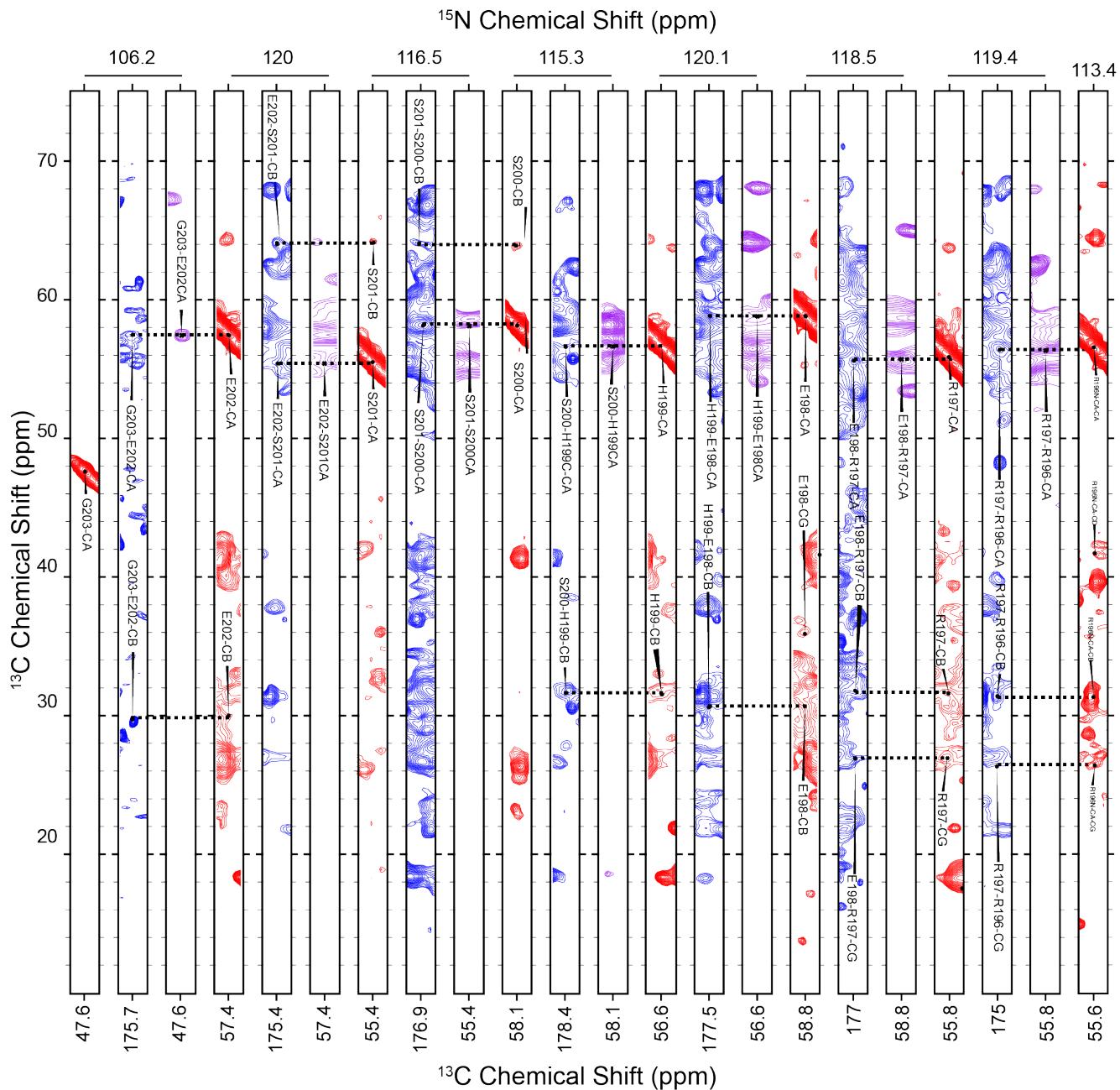


Fig. S12: Strip plot of 3D assignments for residues R196 to G203 of SM KirBac1.1 in POPC lipid bilayers. NCACX (red), CANcoCA (purple), and NCOCX (blue) spectra were used.

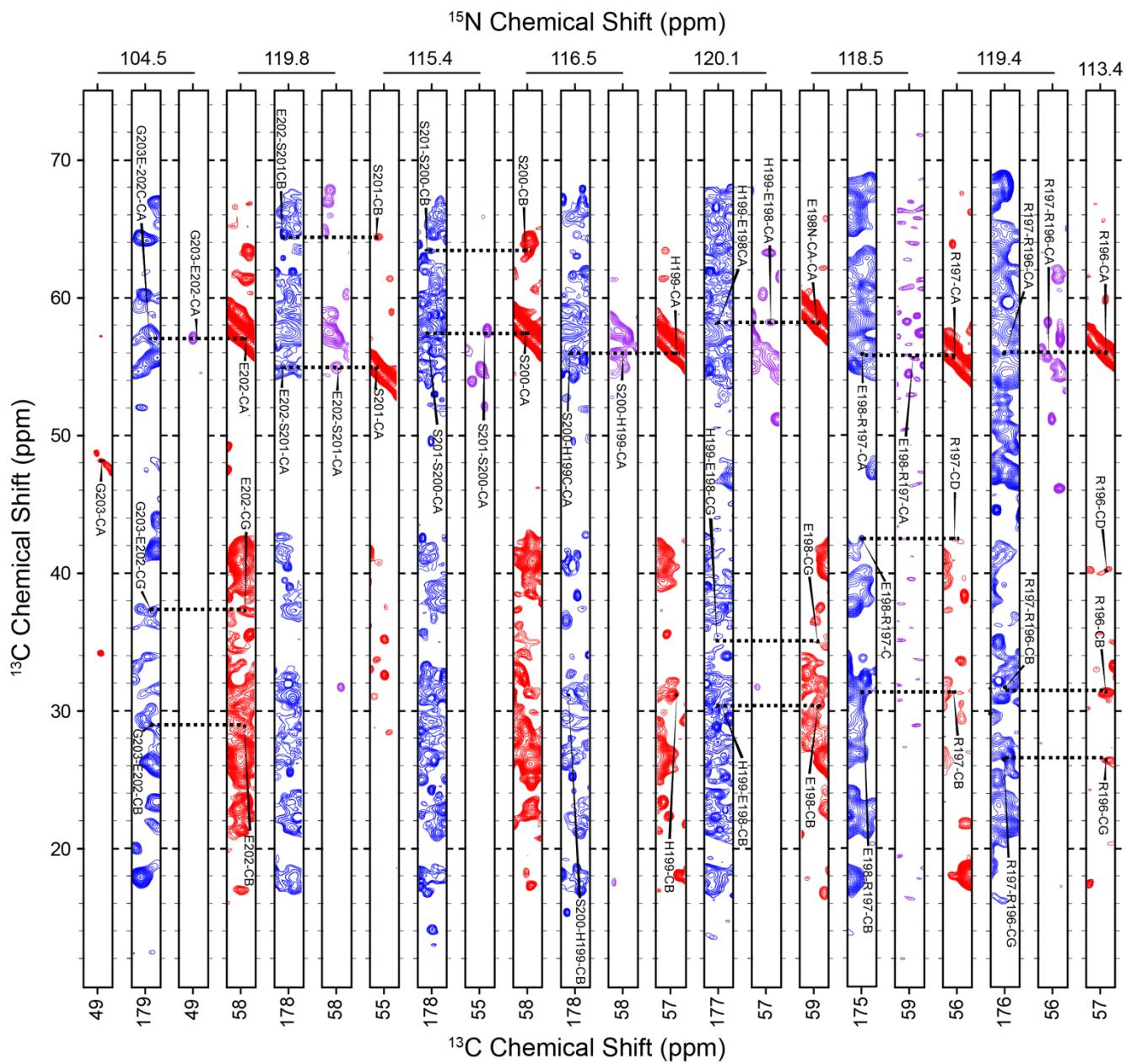


Fig. S13: Strip plot of 3D assignments for residues R196 to G203 of SM KirBac1.1 a in POPC:POPG (3:2) w/w lipid bilayer. NCACX (red), CANcoCA (purple), and NOCOX (blue) spectra were used.

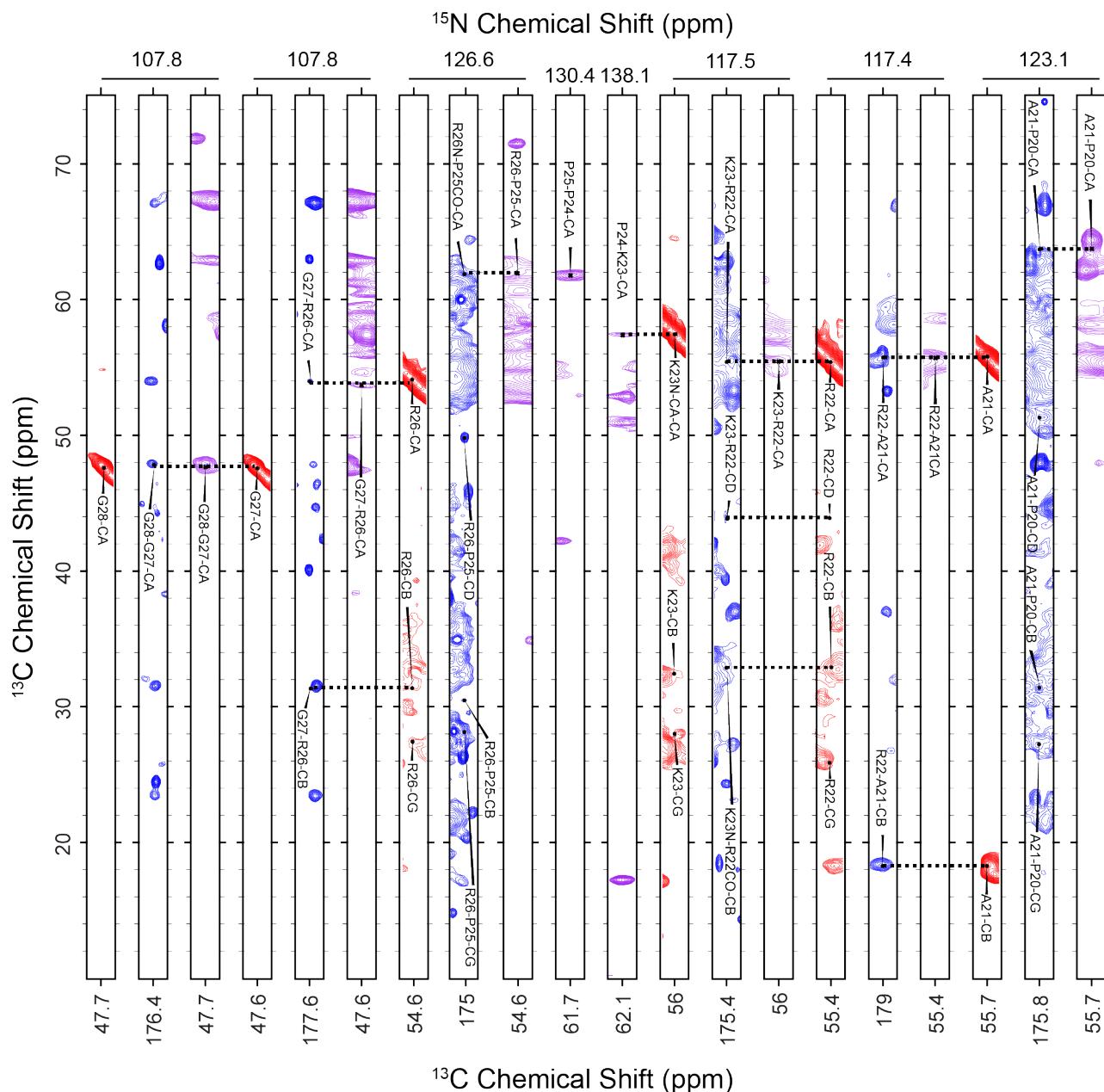


Fig. S14: Strip plot of 3D assignments for residues P20 to R28 of SM KirBac1.1 in POPC lipid bilayers. NCACX (red), CANcoCA (purple), and NCOCX (blue) spectra were used.

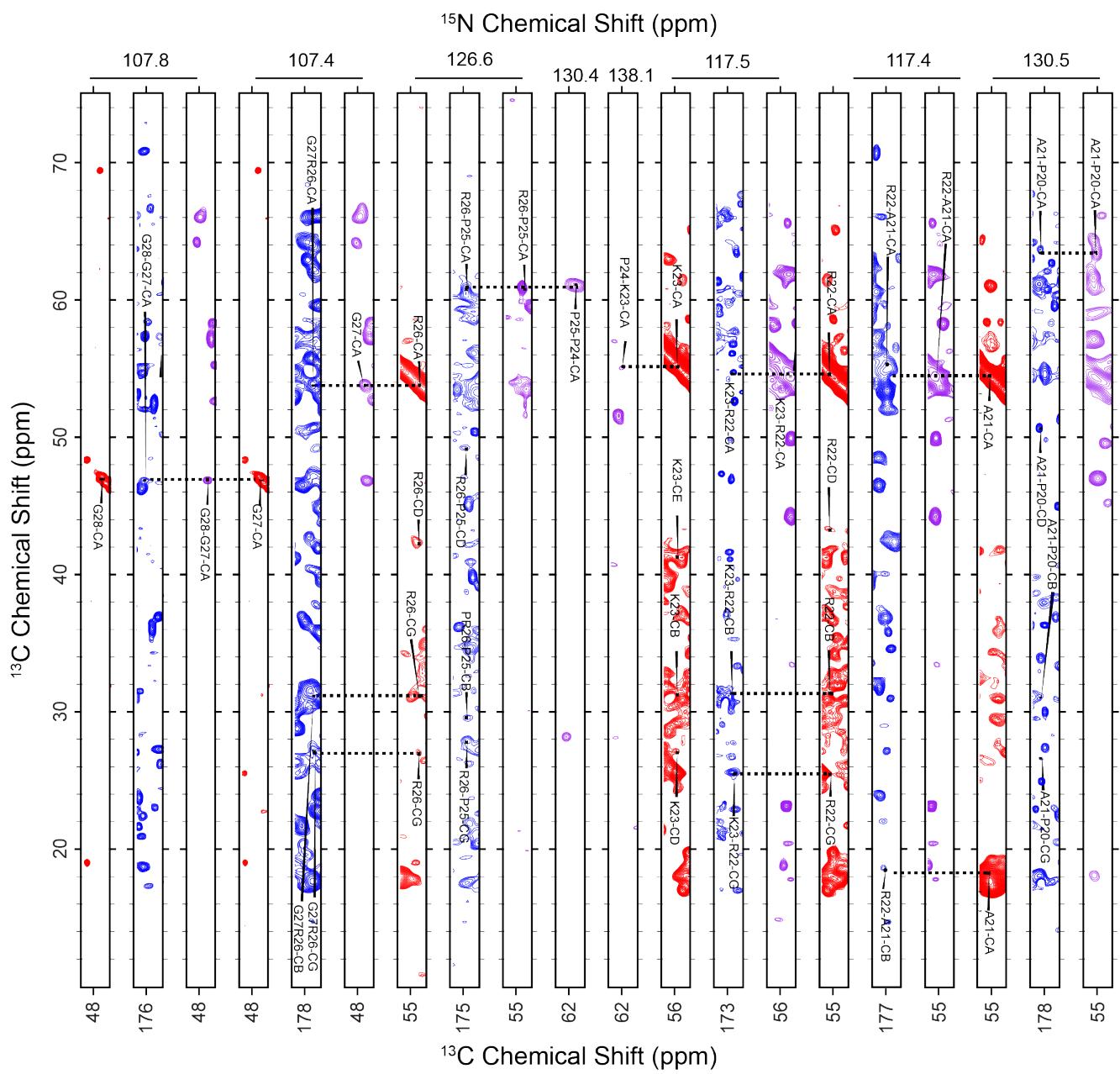


Fig. S15: Strip plot of 3D assignments for residues R28 to P20 of SM KirBac1.1 in 3:2 POPC:POPG (w/w) lipid bilayers. NCACX (red), CANcoCA (purple), and NCOCX (blue) spectra were used.

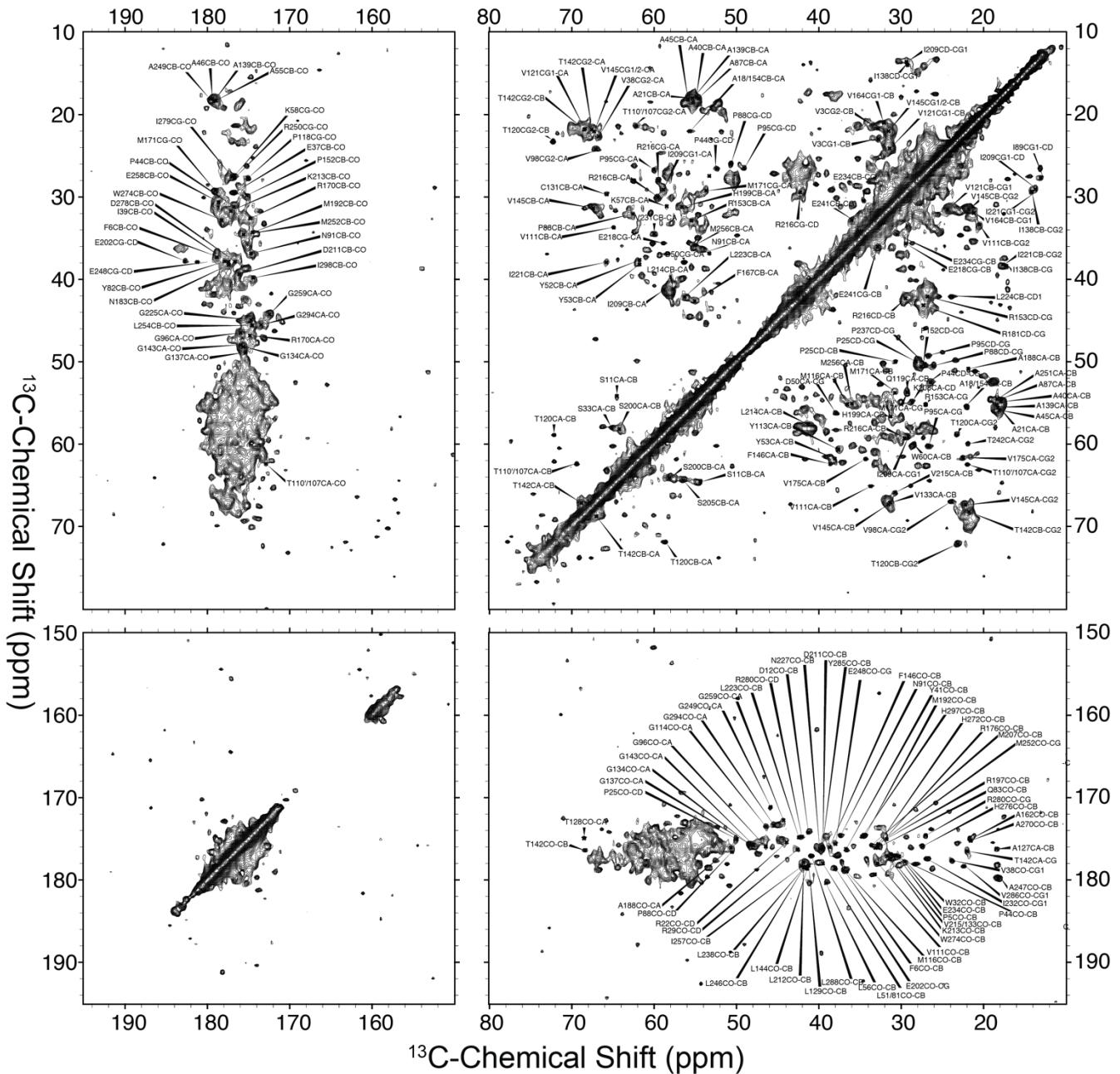


Figure S16: Assigned water-edited ^{13}C - ^{13}C correlation spectrum of U- ^{13}C , ^{15}N KirBac1.1 (SM) in the PE:PG:CL lipid mixture with 5 ms of $^1\text{H}_{\text{mix}}$.

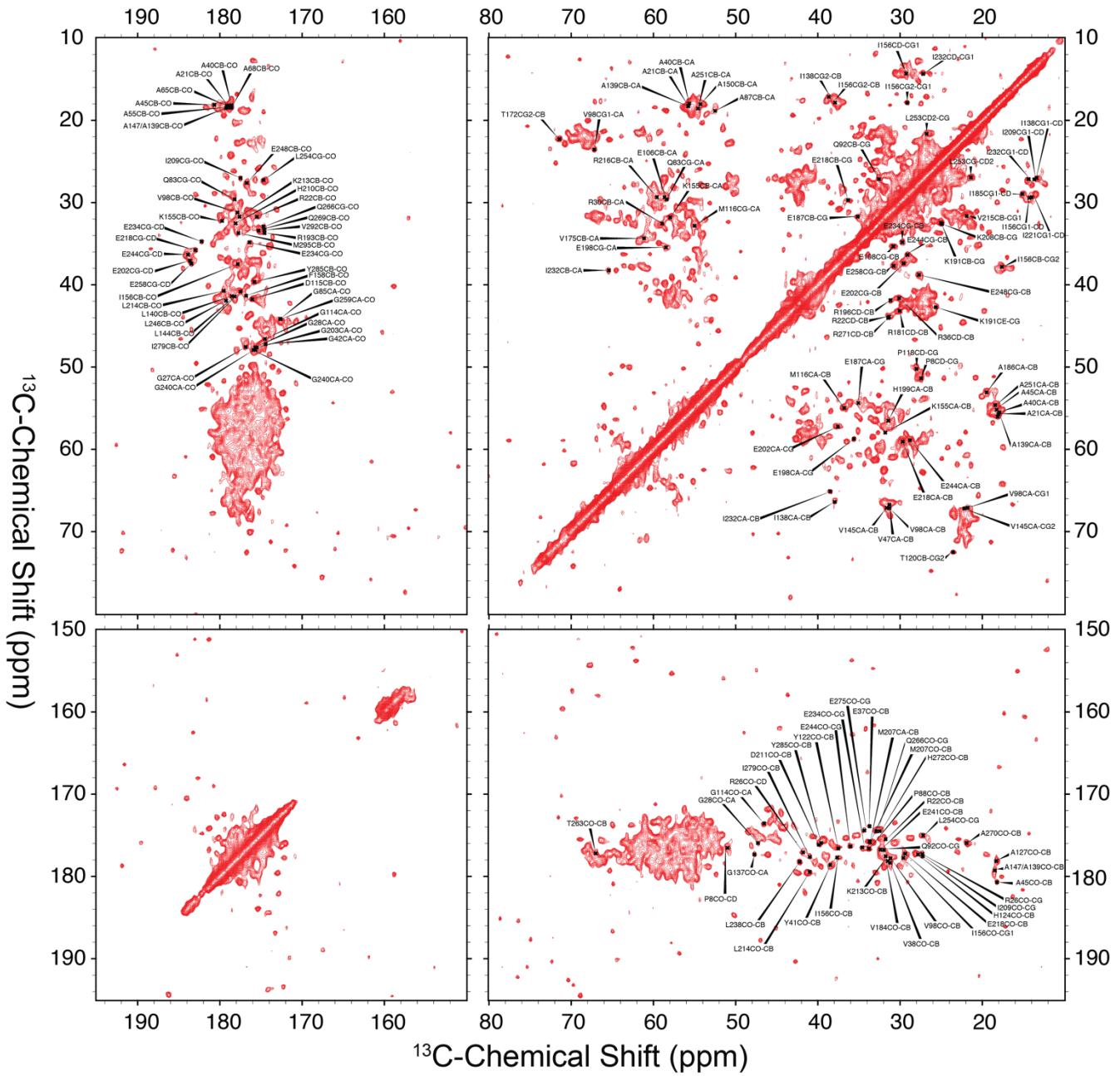


Figure S17: Assigned water-edited ^{13}C - ^{13}C correlation spectrum of U- ^{13}C , ^{15}N KirBac1.1 (R49/151/153Q) in the PE:PG:CL lipid mixture using 5 ms of $^1\text{H}_{\text{mix}}$.

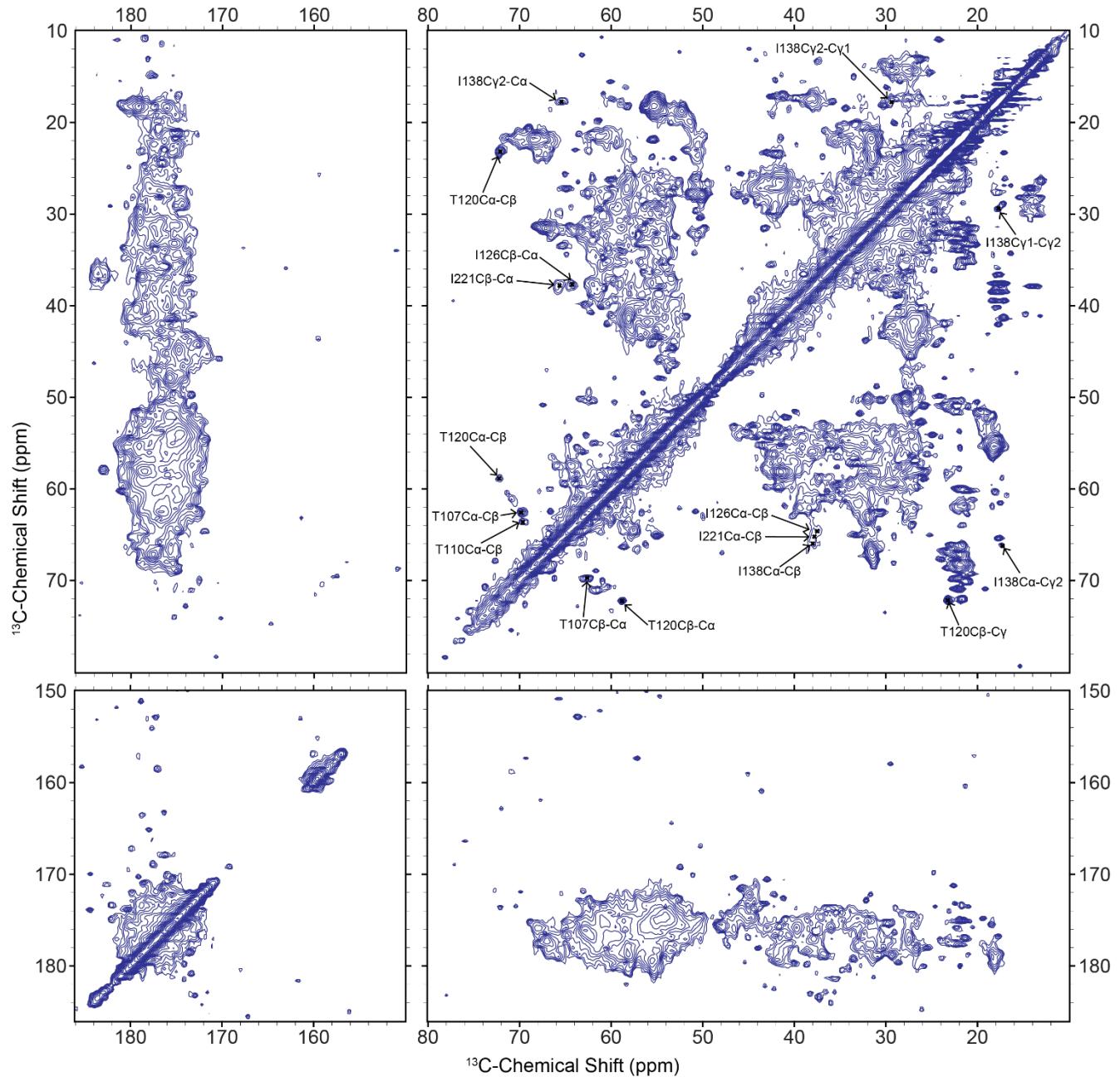


Figure S18: Water-edited 2D ^{13}C - ^{13}C DARR experiment on the SM PE:PG:CL sample implementing 12 ms of $^1\text{H}_{\text{mix}}$. Residues further from the proposed water-protein interface are observed, namely I126.

Table S1: List of chemical shifts for the water-edited ^{13}C - ^{13}C 2D spectrum assignments of SM KirBac1.1 in PE:PG:CL bilayers. Residues in blue were more exposed than in TQ.

Residue	C	CA	CB	CG1	CG2	CD1
V3			32.7	22.9	21.6	
P5	177.1		30.6			
F6	177.1		37.2			
S11		54.3	64.5			
D12	174.217		41.266			
Q16			29.0	34.2		
A18/154		55.6	22.0			
S19		64.5	57.8			
A21		55.2	18.4			
R22	175.4	43.9				
P25	175.1	50.0	30.7	28.2		
R29	176.2				42.5	
W32	177.8		29.5			
S33		58.0	65.2			
E37	176.8		29.5			
V38		66.7		23.8	22.6	
I39	177.5		37.8			
A40		54.9	17.8			
Y41	176.2		36.7			
P44	176.8			26.5		52.4
A45		55.9	18.2			
A46	179.4		18.1			
D50		56.3	37.9			
L51/81	178.0		39.5			
Y52		61.8	37.7			
Y53		61.8	38.1			
A55	179.0		18.3			
L56	180.4		39.1			
K57	176.7	58.5	31.1	27.4		
W60		60.1	28.4			
Y82	177.9		37.8			
Q83	176.1		32.8			
A87		54.6	17.9			
P88		62.6	32.1	50.6		26.0
I89				27.7		13.1

N91	174.6	53.9	36.5			
P95		60.2		26.7	49.1	
G96	175.9	46.5				
V98		67.0			24.0	
T110'/T107	172.9	62.3	69.4		21.7	
V111	179.3	65.0	33.5		20.5	
G112	175.6	48.1				
Y113	178.0	60.7	37.6			
G114	173.4	46.4				
M116	179.0	55.2	36.6			
Q119		53.7	29.3		23.2	
P118	175.1			27.7		
Q119		53.7	29.3			
T120		58.8	72.1		23.2	
V121		68.4	31.5	23.4		
A127	176.2		18.4			
T128	174.9		68.5			
L129	178.3		41.3			
C131		65.7	29.7			
V133		67.1	31.4			
G134	175.8	48.2				
G137	175.5	48.5			17.4	
I138			38.4	29.3	17.3	14.1
A139	179.2	55.4	18.2		21.8	
T142	176.5	67.2	68.5		21.9	
G143	175.9	47.9				
L144	178.6		41.4			
V145		67.3	31.5		22.0	
F146	176.0	62.4	38.7			
P152	175.2		29.8	27.6		
R153		55.3	32.9	26.9		42.1
A154		55.6	22.0	26.9		
A162	174.9		21.7			
V164			32.0	21.1		
F167		55.1	42.6			
M171	179.0	53.7	30.8	29.2		43.2
N183	177.4		38.2			
A188	176.1	50.8	21.9			
M192	174.5		34.3			

R197	175.0		31.8			
H199		56.6	31.3			
S200		58.2	64.2			
E202	178.6			37.9	178.6	
S205		56.5	64.4			
M207	175.8		33.6			
K208		54.9			28.7	
I209		58.9	41.3	29.1		13.6
D211	176.2		39.5			
L212	177.8		41.8			
K213	177.1		31.7			
L214		57.6	41.3			
V215	177.3	65.9	30.7			
R216		59.4	29.7	28.7		42.3
E218		58.9	29.4	35.6		
I221		65.8	38.1	29.4	17.6	14.2
L223	174.8	56.3	42.1			
L224			42.0			23.9
G225	174.7	44.9				
N227	176.2		39.9			
V231		60.0	34.5			
I232	177.4			26.9		
E234	177.1		30.4	34.6		
P237				27.1		50.2
L238	178.4		41.6			
E241			32.8	36.0		
T242		59.9			21.9	
E248	175.6			37.9		181.2
G249	171.1	45.8				
R250	176.7			27.7		
A251		54.6	18.3			44.0
M252	175.6		34.6	32.8		
L254	174.6		45.6			
M256		55.1	35.9			
I257	178.3		42.1			
E258	178.6		30.6			
G259	172.6	44.3				
A270	175.2		21.6			
H272	176.1		33.1			

W274	178.1		32.8			
H276	175.9		27.3			
D278	176.6		37.8			
I279	177.0			27.5		
R280	174.7			27.0		42.0
Y285	175.9		39.6			
V286	178.3			22.4		
L288	177.1		41.0			
G294	173.4	45.5				
H297	174.7		34.7			
I298	174.5		39.8			

Table S2: List of chemical shifts for the water-edited ^{13}C - ^{13}C 2D spectrum of TQ (R49/151/153Q) KirBac1.1 in PE:PG:CL bilayers. Residues with greater water exposure than SM are in red.

Residue	C	CA	CB	CG1	CG2	CD1	CD2	CE
P8	176.5			27.4		51.2		
A21	179.0	55.7	18.2					
R22	175.5		31.6			43.9		
R26	177.2			27.3		41.8		
G27	176.9	47.6						
G28	175.8	47.4						
R30		58.9	32.5					
R36			30.1			41.6		
E37	173.9		33.7					
V38	178.3		31.2					
A40	178.6	55.6	18.0					
Y41	178.6		38.5					
G42	174.4	47.2						
A45	180.7	55.2	18.2					
V47		66.7	31.3					
A55	179.0		18.4					
A65	179.2		18.2					
A68	178.6		18.5					
Q83	178.2	58.4		29.6				
G85	172.7	44.1						
A87		52.5	18.9					
P88	176.6		33.8					
Q92	176.8		27.1	32.3				
V98	177.8	67.2	31.2	22.7				
E106		58.6	29.3					
D115	176.1	41.7						
G114	174.0	46.6						
M116		55.0	36.8	32.8				
P118				28.0		50.2		
T120			72.5		23.6			
Y122	176.6		37.5					
H124	177.3		27.8					
A127	178.1		18.3					
G137	177.3	47.7						

I138		66.4	38.3	27.0	17.1	13.4		
A139		55.9	18.2					
L140	178.6		41.3					
L144	178.2		41.4					
V145		67.2	31.6	22.2				
A147/A139	179.3		18.5					
A150		179.3	18.5					
K155	179.7	57.9	31.9					
I156	177.8		37.7	29.4	17.8	14.3		
M157		56.3		30.4				42.7
F158	176.8		41.3					
T172			71.4		22.3			
V175		61.1	34.4					
R181			30.1			43.1		
V184	178.1		31.5					
I185				29.0		15.1		
A186		53.0	19.5					
E187		54.4	31.7	35.1				
K191			32.5	25.3				42.7
R193	174.6		33.7					
R196			31.2		41.9			
E198		58.6	30.8	35.5				
H199		56.5	31.4					
E202		57.2	29.5	37.3		183.6		
G203	175.5	47.6						
M207	175.8		33.7					
K208			32.6	24.9				
I209	177.5			27.1		13.5		
H210	178.1		32.5					
D211	176.2		39.9					
K213	177.6		31.7					
L214	179.5		40.9					
V215			31.6	21.9				
R216		59.6	29.3					
E218	177.2	59.1	29.6	36.0		183.0		
H219		55.9	29.9			183.0		
I221				29.3		14.0		
I232		65.3	38.4	27.2		14.4		
E234	176.4		29.7	34.7		182.2		

L238	178.2		42.2					
G240	175.8	47.9						
E241	176.7		32.4					
E244	176.3	58.9	28.9	36.2		183.9		
L246	179.3		41.9					
E248	176.7		27.7	38.8		183.6		
A251		54.6	18.5					
L253				26.9		21.5		
L254	174.8			27.2				
E258			30.8	37.6		183.5		
G259	172.6	44.2						
T263	177.2		67.0					
Q266	175.3			32.9				
Q269	175.3		33.4					
A270	175.9		21.9					
R271			31.4			44.1		
H272	174.5		32.5					
E275	174.4		34.3					
I279	177.6			27.2				
Y285	175.9		39.6					
V292	174.6		33.3					
M295	177.7		33.7					

Table S3: List of chemical shift assignments from 3D spectra of SM KirBac1.1 in 3:2 POPC:POPG (w/w) bilayers.

Residue	¹³ C'	¹⁵ N	¹³ C α	¹³ C β	¹³ C γ 1	¹³ C γ 2	¹³ C δ 1	¹³ C δ 2	¹³ C ϵ
1M	178.1		57.7	32	30.6				17.9
2'G	175.7	107.1	44.8						
2N	178.3	117.2	55.6	37.6	175.5				
3V	177.1	115.6	65.8	32.6	22.3	21.3			
4D	174.3	116.5	55.1	37.3					
5P	176.9	130	66.8	30.4	28		52.6		
6F	178.8	119.1	59	37	138.6				
7S	175.8	123	62.2	62.9					
8P	176	130.3	62.6	31.8	27.6		51.8		
9H	176	122.9	55.6	31.9	135.1				
10S	175.6	123.4	54.1	63					
11S	175.8	125.2	54.3	64.7					
12D	174.2	121.5	54.2	41.3	179.5				
13S	175.9	124.7	60.3	61					
14F	174.6	119.9	60.1	41	139				
15A	173.6	122.5	54.7	17.4					
16Q	174	117.9	59.3	28	35.5		176.8		
17A	179.5	127	51.8	19					
18A	180.4	120.3	55.5	22.2					
19S	178.5	115.6	63	63.5					
20P	178.5	130.5	64.4	31.5	27		51.4		
21A	174.5	122.4	55.3	18.5					
22R	175.4	117.4	55.4	31.8	25.8		43.9		
23K		117.5	56	31.7	27.4				
24P		138.1	62						
25P	175	130.4	61.7	30	28.2		49.9		
26R	177.6	126.6	54.6	31.6	27.3		42.9		
27G	176.4	107.4	47.5						
28G	175.9	107.8	47.6						
29R	176.2	124.3	58.8	32.7	27.2		42.3		
30R	176.1	117.6	58.4	32.2	27.5		41.3		
31I	178.8	125.7	58.9	40.3	27.5	17.4	14.1		
32W	178.8	120.7	57	31.8	112.8				
33S	175.6	116.9	58	65					
34G	171.5	111.4	44.5						
35T	177.3	121.2	57.5	65.6	22.3				
36R	175.9	120.5	58.5	29.8	26.5		41.4		
37E	176.5	120	58.5	29.7	33.4		182.3		

38V	177.9	120	66.4	31.1	23.8	22.2			
39I	177.5	119	67.1	37.7		17.8	13.6		
40A	179	122.2	54.9	17.8					
41Y	176.2	122.2	58.3	36.7	131				
42G	174.4	106.6	47.4						
43M		122.2	55	34.8	29.9				17.36
44P	176.8	137.2	63.4	31.2	27		52.1		
45A	179.4	123.1	55.9	18.1					
46S	177.9	119.1	62	62.3					
47V	177.4	122.8	67.3	31.4	23.5	21.3			
48W	180.2	121.4	61.7	27.9	111.6				
49R	177.7	117.8	58.8	29	28.2		43.1		
50D	175.2	118.9	56.3	37.6	178.1				
51L	178	117.9	58	39.4	26.5		24.1	23.3	
52Y	175.7	120.3	61.7	37.8					
53Y	179	120.8	61.7	38	128.3				
54W	173.8	119.9	61.3	27.9	107.7				
55A	179	127.3	55.6	18.3					
56L	180.2	118.1	58	39.3	26.9		24.2	22.9	
57K	176.7	120.8	58.4	31.1	27.4				
58V	177.3	121.9	65.7	31.2	23	21.6			
59S	175.7	115.2	63	63.6					
60W		120.4	59.9	28.3	112.2				
61P	177.1	130.8	65.7	31.6	28		50.4		
62V	177.3	120.4	68.2	31.1	22.5	21.5			
63F	176	120	62.7	38.6					
64F	175.9	116.7	62.5	38.8					
65A	178.9	117.2	55.6	17.35					
66S	176.1	115.7	62.7	63.1					
67L	175.4	122.4	58	41.5	25.8		23.3	22.2	
68A	178.1	123.1	55.7	18					
69A	180	123.2	55.8	18.6					
70L	174.9	120.8	57.8	41	26.3		23.5	22.5	
71F	176.2	119.7	62.5	38.6					
72V	178	118.9	67.4	31.4	23.5	21.8			
73V	175.9	118.8	67.7	31.4	23.5	22			
74N	177.9	120.3	58.3	39.4	176.4				
75N	179.3	121.1	55.7	36.7	177.7				
76T	175.9	118.8	67.1	68.3		21			
77L	178.6	119.5	58	41.4	26.4		23.1	21.5	
78F	178.7	115.7	60	38.1					

79A	180.8	122.8	55.6	18.1					
80L	176.2	119.1	57.7	41.5	26.2		24.1	23	
81L	177.9	118.7	57.7	39.5	25.7		24.2	22.9	
82Y	177.9	119.6	61	37.8	129.3				
83Q	176.1	120	57.1	31.5	32.8		179.5		
84L	179.1	122.2	57.2	41.6	26.2				
85G	174.3	107.4	46.2						
86D	175	123.1	54.4	40	180.7				
87A	172	120.9	54.3	17.9					
88P	176.6	134.4	62.2	31.1	25.9		50.6		
89I	175.5	117.4	58.33	41	27.7	17.1	13.1		
90A	175.9	130.7	52.18	18.4					
91N	174.6	113.5	53.4	36.8	178.5				
92Q	176.7	117.9	58.8	26.7	33.8		179.8		
93S	175.6	118.5	58.4	66.5					
94P	175.3	131.4	64.6						
95P	179.1	131.1	60	33.1	26.7				
96G	175.9	102.2	46.5						
97F	178.7	125	58.7	41.8					
98V	177.5	118	67.2	31.8	24	21.8			
99G	175.3	109	48.2						
100A	177.2	123	55.1	18.34					
101F	178.2	119.9	61.5	37.7			131.9		
102F	176.7	122	61.6	38.2			130.6		
103F	176.5	121.2	61.8	39.2			129.1		
104S	177.1	119	61.6	62					
105V	177.7	117.6	65.5	30.6	22	21.5			
106E	174.1	119.1	58.5	29.2	38		182.2		
107T	176.4	109.8	62.4	69.3	20.7				
108L	175.5	122.6	58.2	40.9	26.6		24.4	22.2	
109A	176.2	130.9	52	18					
110T	172.5	109.3	63.5	69.5	21				
111V	179.3	120.8	65.4	33.3	21.1	20.5			
112G	175.1	102.2	48.2						
113Y	179.4	118.1	60.5	37.5					
114G	173.7	102.5	46.6						
115D	178.9	119.2	55.7	40	176.9				
116M	179	120.8	55.2	36.6	32.7			18.1	
117H	176	120.7	54.6	31.6					
118P	175.3	137.1	63.5	32.2	27.5		50.4		
119Q	173.9	116	53.6	29	30.6		180.8		

120T	174.5	110.5	58.7	72		23.1			
121V	177.5	124.1	68.4	31.1	24.2	22			
122Y	176.1	120	62.6	38	134.6				
123A	177.2	117.4	54.9	17.9					
124H	174.9	118	58.6	27.2	131.8				
125A	174.9	124.7	54.4	17.9					
126I	177.6	121.1	64	37.5	28.6	17.3	13.5		
127A	176.1	120.6	56.6	18.4					
128T	175.2	118.2	68.6	67.9	21.2				
129L	178.3	120.5	58.4	41.3	27.8		23.1	22.75	
130E	177	118.5	60.7	28.5	36.6		179.9		
131C	176.9	118.7	65.7	29.6					
132F	177.2	119.5	61.6	38.9					
133V	177.1	122.5	67.1	31.4	23.3	23			
134G	175.7	107.1	48.2						
135M	178.6	122.2	58.3	32.3	35.6				17.5
136S	175.9	114.7	63.6	64					
137G	175.4	109.5	48.9						
138I	177.3	121.4	66.1	38.1	29.3	17.2	14		
139A	179.2	121	55.6	18.3					
140L	178.5	118.7	58.4	41	27		23.3	22.1	
141S	175.5	114.4	63.3	63					
142T	176.5	118.9	67.6	68.34	21.9				
143G	175.8	106.6	47.9						
144L	178.6	122	58	41.4	28.5		23.4	22.1	
145V	176	119.5	67.3	31.5	23.5	22.1			
146F	176	123.8	62.4	38.7					
147A	179.7	120.5	55.5	19.2					
148R	178	120.5	58	29.5	26.6		42.3		
149F	174.8	120.3	60.6	39.4					
150A	174.1	125.4	54.3	18					
151R	172	125.5	54.5	33.3	26.3		42.9		
152P	175.2	134.4	61.9	29.8	27.5		50.5		
153R	175.1	121.8	55.5	32.8	26.8		42.1		
154A	177.6	120.2	55.4	22.2					
155K	179.2	120.7	57.9	32.2	24.1		28.5		41.5
156I	177.4	121.8	64.6	37.9	29.5	17.1	14.1		
157M	175.2	117.6	58.3	32.3	35.7				16.9
158F	175.9	124.3	55.4	41.3	139.6				
159A	175.3	118.3	54.7	19.2					
160R	174.7	122.7	54.3	34.6	27.6		44		

161H	174.2	120.6	53.8	32.8					
162A	174.7	122.3	53.4	21.7					
163I	177.5	117.6	57.8	42.6	28.3	18.5	14.2		
164V	175	118.6	59.9	31.9	21.03	21.4			
165R		122.6	56.1	31.2	26.9		42.2		
166P	175.5	133.8	64.7	32.1	27.3		51.8		
167F	177.8	121.6	55.1	42.6	138.2				
168N	173	121	55.3	36.6	177.9				
169G	174.2	105.7	46.7						
170R	174.8	121.2	53.6	32.6	26.7		46.8		
171M	179	115.8	53.7	30.7	29.2				18.8
172T	174.7	109.8	58.9	71.9	21.9				
173L	175.8	116.8	54.8	44.5	25.5		22.6	22.1	
174M	178	121.1	55.5	36.6	31.6				18.1
175V	176.2	122.3	61.3	34.2	22.7	21.3			
176R	176	121	55.1	32.7	27.1		41.8		
177A	174.6	124.8	52.6	20.2					
178A	178.5	120.4	52.2	20.9					
179N	176.4	113.2	53.2	37.1	178.5				
180A	174.8	121.2	53.8	18.5					
181R	174.2	117.8	56.4	29	27.42		43.1		
182Q	176.2	121.8	54.4	29.8	31.5		180.6		
183N	177.4	120.4	55.3	38.2	180				
184V	177.6	117	67.1	31.2	23.5	21.8			
185I	177.4	119.4	59.8	42.6	28.5	18.8	15.3		
186A	176.1	118.5	53.1	19.1					
187E	174.1	125.8	54.1	31.6	35.5		182.1		
188A	176.1	126.8	50.7	21.7					
189R	177	118	55.2	32.6	26.3		43.9		
190A	176.8	113.3	52.1	20.6					
191K	174.7	116.8	54.4	32.4	25.2		29		42.8
192M	174.5	124	54	34.3	33				17.9
193R	174.6	123.3	53.1	33.7	26.6		45.8		
194L	174.8	124.1	54.6	40.6	27.5		23.3	23.6	
195M	175.6	115.4	55	35.9	33				17
196R	176	113.4	56.6	31.7	26.7		40.6		
197R	175.1	119.4	56.3	31.7	26.9		43		
198E	176.6	118.5	58.8	30.6	35.4		182.4		
199H	177.3	120.1	56.6	31.5	131.9				
200S	176.7	116.5	58.1	64.2					
201S	178.4	115.4	55.5	65.1					

202E	178.7	119.8	57.7	29.2	37.7		182.8		
203G	174.4	104.5	48.7						
204Y	176.7	121.4	58.8	38.2	133.2				
205S	175.7	119.2	56.3	64.7					
206L	175.7	121.9	54.6	42.3	28.3		25.6	26.8	
207M	175.7	121.2	54.4	33.7	31.9				18
208K	178.8	117.1	54.9	32.4	25.6		28.8		40.4
209I	176.8	120.4	58.9	41.5	29.1	19.2	13.3		
210H	178.1	121.3	55	32.8	130.7				
211D	176.1	122.8	54	39.4	178.9				
212L	177.8	117.8	55.6	41.8	25.9		22.6	23.3	
213K	177.3	117.5	57.8	31.7	25.5		28.4		41.6
214L	179.5	116	57.6	41.3	26.3		23.5	23.4	
215V	177.4	120.4	65.6	31.2	21.5	22.9			
216R	179.2	119.4	59.3	29.6	28.1		42.25		
217N	178.5	117.8	53.4	42	176.1				
218E	177.1	117.3	58.8	29.4	35.6		181		
219H		120.4	55.9	30.8	130.6				
220P	179.2	133.7	65.2	32.3	26.8		50.6		
221I	178.1	118.9	66	38.4	29.4	17.3	14.1		
222F	176.5	115.4	57.8	41	138.3		132.1		
223L	174.8	122.3	56.2	42.4	27.2		25.5	25.9	
224L	178.3	117.7	56.4	42.1	26.1		23.7	23.3	
225G	174.7	104.8	44.9						
226W	178.3	117.1	55.4	29.5	108.2				
227N	176.2	125	52.8	39.9	174.7				
228M	176.2	116.2	55.6	32.3	31.3				17.8
229M	176.4	119.3	55.8	34	31.6				18.3
230H	177.6	117.3	55.3	30.5	133.9			125.5	
231V	178	122.7	59.6	34.3	21.7	20.9			
232I	177.6	119.4	65.2	38.7	26.9	17.6	14.2		
233D	177.8	121.4	57.6	39.2	178.9				
234E	177	115.7	57.6	30.2	34.7		182.8		
235S	175.2	119.6	55.6	68.3					
236S	174.3	124.2	55.2	63.1					
237P	178.2	129.9	66.5	29.6	26.8		50.2		
238L	178.4	116.2	55.6	41.6	27		23.7	23.5	
239F	178	116.3	63.1	38.3			130.5		
240G	175	109.7	47.9						
241E	176.8	121.9	57.8	32.4	35.9		180.8		
242T	173.6	112.7	59.6	72.4		21.5			

243P	177.8	131	66.4	31.1	28.9		50.8		
244E	176.5	122.7	59.1	28.8	36		180.7		
245S	176.1	118.1	62.7	63					
246L	178.6	123.7	58.2	41.7	26.9		23.5	23.1	
247A	179.5	122.1	55.4	18.1					
248E	175.6	119	58.4	28.1	38		181.9		
249G	171.4	109.9	45.9						
250R	176.7	123.5	54.4	27.6	25.6		41.9		
251A	175	121.3	54.6	18.2					
252M	175.6	120.4	54	34.6	32.8			17.5	
253L	178.8	120.5	54.5	43.3	27.4		22.8	21.6	
254L	174.6	119.7	54.5	45.6	27.2		23.1	21.7	
255V	178.2	118	60.3	34.3	22.2	21.2			
256M	174.7	117.6	55	35.8	34.7				18.2
257I	178.4	117.6	59	42	27.4	20.7	13.6		
258E	178.6	118	56.4	30.6	37.3		182.2		
259G	172.5	105	44.2						
260S	175.1	121.1	55.1	65.1					
261D	177.7	120.1	55.7	42.7	179.3				
262E	175.7	117.9	58.1	31.7	35.7		182.6		
263T	175.9	118.6	60.1	67.7		21.2			
264T	173.3	123.6	60.5	69.6		21.4			
265A	175.4	129.7	50.4	20.3					
266Q	174.5	122.1	54.7	31.3	32.6		180.4		
267V	176.4	123.4	61.1	34.9	20.4	20.1			
268M	176.6	126	54.2	35.4	33.4				17.6
269Q	174.9	117.2	55.2	33.2	34.7		177.7		
270A	175	125	52.2	21.7					
271R	174.8	126.2	54.4	31.6	26.8		44.2		
272H	176.1	121.4	54.1	33.1	131.3				
273A	175.4	127.7	52.7	19.1					
274W	178.2	123.7	58.7	32.8	113.5				
275E	174.5	115.8	55.4	31.3	34.1		182.9		
276H	175.7	122.3	59.9	27.2	133.8				
277D	178.6	122.5	55.9	39.4	176				
278D	176.6	117.9	55.6	37.8	178.6				
279I	176.9	120.2	57.9	41.2	27.5	17.1	14.3		
280R	174.6	122.3	55.1	34.8	26.9		42.1		
281W	178.2	124.6	55.7	33.3	113.4				
282H	178.9	115.7	59.5	25.7				122.6	
283H	179.8	119.8	58.2	27	135.7				

284R	179.1	124.1	55.2	32.3	27.7		41		
285Y	176	121.3	61.7	39.6	132.2				
286V	178.6	124.4	61.7	32.5	22.5	21.3			
287D	174.6	121.1	55.6	44.2	176.7				
288L	176.9	116.2	57.8	41	26.5		23.5	22.7	
289M	178.4	119.2	55.6	34	31.6				17.7
290S	176.9	121.3	56.8	63.5					
291D	174.7	124.2	54.8	40.7	176.1				
292V	174.6	122.7	60.8	33.3	21.3	21.6			
293D	177.8	125.86	54.7	43.1	174.8				
294G	173.5	106.9	45.5						
295M	177	121.2	54.5	33.7	31.7				18
296T	176.1	119	60.9	70.2		21.5			
297H	174.5	126	55.2	34.7	130.3				
298I	174.5	126.3	60.4	39.8	27.2	18.5	14.5		
299D	177.2	125.8	54.4	41.6	175.9				
300Y	176	118.2	55	39.3	131.1			136.7	
301T	176	119.9	61.7	68.4		22.2			

Table S4: List of chemical shifts from 3D spectra of SM KirBac1.1 in POPC bilayers.

Residue	$^{13}\text{C}'$	^{15}N	$^{13}\text{C}\alpha$	$^{13}\text{C}\beta$	$^{13}\text{C}\gamma 1$	$^{13}\text{C}\gamma 2$	$^{13}\text{C}\delta 1$	$^{13}\text{C}\delta 2$	$^{13}\text{C}\varepsilon$
1M	177.8		57.7	32.1	31.1				19.1
2'G	177.2	107.1	46.5						
2N	177.5	114.6	55.4	37.5	179.5				
3V	177.4	116.1	65.7	31.3	23.9				
4D		120.4	55.4	37.7					
5P	175.8	135.6	62.1	30.5	27.1		51.3		
6F	176.5	119.5	59	37	138.8				
7S	178.6	120.5	62.2	62.9					
8P	176	130.9	63.5	31.4	27.3		51.3		
9H	177.3	120	55.7	31.6	132.7				
10S	177.3	118.2	54.1	62.7					
11S	174.7	125.1	55	64.6					
12D	175.4	121.5	54.2	41.9	178.4				
13S	175.5	123.6	61.6	61.1					
14F	175.6	123.7	59.9	37.6	140.3				
15A	179	124	55	17.7					
16Q	174.7	120	59	29.2	30.1		180.4		
17A	176.6	128	51.4	22.5					
18A	180.4	120.4	55.7	22					
19S		115.5	63.4	62.3					
20P	175.8	130.8	63.7	31.4	27.2		51.3		
21A	179	123.1	55.7	18.2					
22R	175.4	117.4	55.4	31.8	25.8		43.9		
23K		117.5	57.4	32.4	28				
24P	173.2	138.1	61.8				50.9		
25P	173.8	133.9	61.9	30.4	28.1		49.8		
26R	177.3	126.7	54.1	31.6	27.3		41.7		
27G	177	106.5	47.6						
28G	175.7	107.8	47.6						
29R	176.2	125	58.8	32.8	27.3		42.7		
30R	176.1	117.6	58.4	32.3	27.2		43.5		
31I	176.6	125.3	58.9	40.7	27.6	17.3	14.7		
32W	177.7	119.8	56.7	29.5	111.4				
33S	176.2	121.4	57.7	67.4					
34G	172.7	110.2	43.9						
35T	174.5	120.7	62.2	71.4	21.6				
36R	178.4	116	59.4	29.9	28.5		41.6		
37E	173.8	120	55.4	33.6	37.7		183.8		
38V	178.2	120	66.5	31.1	23.6	21.7			

39I	177.8	119.2	66.6	38.4	29.5	18.2	14.2		
40A	178.6	118	55.5	18.3					
41Y	178.5	122.6	58.7	38.6	134.8				
42G	174.4	107	47.2						
43M	176.9	120.8	55.3	34.2	31.3				17.3
44P	175.4	138.9	64.2	28.1	26.6		50.4		
45A	181	122.6	55.2	18.2					
46S	176.5	120.6	62.2	63.2					
47V	178.1	123	66.7	31.5	23.2	21.5			
48W	178	119.6	59.5	30	110.7				
49R	178.1	120.7	58.1	27.2	28.3		41.1		
50D	177.3	120.2	56.4	37.6	179				
51L	178	116	58	41.5	26.4		23.3	22.8	
52Y	175.1	120	61.5	37.5	131.5				
53Y	178.1	120.2	62.2	37.5	132.2				
54W	177	121.2	61.8	29	111.3				
55A	179	121	55.7	18.3					
56L	178	118.5	57.8	41.6	27		24.2	22.8	
57K	176.6	120	57.8	31.6	26.8		29.6		
58V	177.4	120.2	67.4	31.5	23.4	22			
59S	178.6	117.1	61.5	62.5					
60W	176.9	123.6	59.3		105.8				
61P	175.7	138.7	64	32.2	27		50.2		
62V	177.3	120	68.2	31.3					
63F	176.3	120.1	62.7						
64F	176.3	123.6	62.7	39.8					
65A	179.1	118	55.7	18.3					
66S	176.3	115.4	63.1	62.5					
67L	179.4	122.4	58	42	27.2		24	22.1	
68A	178.6	123.1	55.7	18.4					
69A	177.3	123.2	55.8	18.2					
70L	177.9	120.8	57.8	41.7	27.2		23.7	21.5	
71F	178.4	120	62.3	37.5	139.7		131.4		
72V	177.5	123.4	67.8	31.45	24	22			
73V	177.4	120.4	67.8	31.3	23.7	21.7			
74N	176.4	121	58.4	37.6					
75N	178.7	119.5	55.7	37					
76T	175.5	117.3	66.6	68.9	21.6				
77L	178	124.1	58.3	41.6	26.6		23.6	22.5	
78F	176.2	119.3	60.1	39.9	137.6				
79A	179.4	121.4	55.5	18.3					

80L	178.2	118.3	57.8	42.3	26.8		23.7	21.7	
81L	178	118.7	58	41.6	27		23.7	21.7	
82Y	177	119.9	61.3	39.1	139.3		130.3		
83Q	178.2	119.6	58.3	29.6	32.1		180.8		
84L	177.6	117.7	56.3	41.8					
85G	172.7	105	44.1						
86D	175.5	121.7	54.3	42					
87A	175.4	127.8	52.4	19					
88P	176.6	132	64.9	33.9	25.9		50.6		
89I	176	117.9	58.5	41.3	26.1	17.2	13.1		
90A	176	131.7	52.3	18.5					
91N	174.8	113	53.4	37	178.7				
92Q	175.8	117.7	58.2	27.1	32.35		178.8		
93S	176.1	114.1	56.4	64.5					
94P		137	63.7	32	27.2		50.1		
95P	177.5	129.3	61.45	31.4	26.6		50.8		
96G	176.1	108.3	46.8						
97F	178.4	125	58.6	39.4					
98V	177.8	118.6	67.2	31.2	24	21.4			
99G	175.9	111.3	48						
100A	179	122.6	55.2	17.7					
101F	176.9	120.6	62	37.6			131.9		
102F	178.4	119	61.7	37.6			130.9		
103F	176.8	122.6	61.8	38.1	137.9		130.6		
104S	176.2	115	62.3	63.1					
105V	177.4	123.6	67.6	31.4	21.5	23.6			
106E	178.2	118	58.2	27.3	36.1		182.8		
107T	175.8	117.6	61.6	70.8	21.8				
108L	178.3	118.4	58.1	40.8	27				
109A	179	112.8	51.5	20.5					
110T	172.2	110.7	62.6	70.1	20.9				
111V	179.1	120.8	65.6	33.5	22.45	20.4			
112G	175.1	103.8	48.5						
113Y	177.3	116.2	61	39.8	130				
114G	174.5	106.6	46.6						
115D	176.1	121	54.5	41.7	178.9				
116M	175.4	116.3	55.1	32.9	36.1			18.1	
117H	169.5	114.8	52.9	26	128.4				
118P	176.6	137.4	62.6	30.9	27.9		50.3		
119Q	174.4	115.8	53.8	29.2	30.9				
120T	174.3	111.3	58.5	72	23.3				

121V	177.4	124.2	68.3	31.4	24.2	22.1			
122Y	176.8	120.5	62.2	37.5	130.3				
123A	177.2	119.5	54.8	17.5					
124H	177.4	118.2	58.1	27.8					
125A	177.7	122	55.7	18.2					
126I	177.1	119	64.1	37.8	26.9	17.3	13.8		
127A	178.2	120.7	56.5	18.4					
128T	175.6	119	68.6	68	21.8				
129L	178.3	120.9	58.5	41.4	26.7		23.8	21.7	
130E	176.4	119.1	59.9	28	36.8		180.1		
131C	177.1	119.6	65.1	29.6					
132F	178.7	120.2	62.1	39					
133V	177	122.8	67.1	31.5	23.8	23.2			
134G	175.8	106.8	48						
135M	175.3	122.4	58.3	32.8	35.2				17.1
136S	175.7	114.7	63.2	64.3					
137G	177.4	110.5	47.5						
138I	179.1	126.5	66.3	38.5	27	17	13.6		
139A	179.4	125.8	56.3	18.4					
140L	178.5	118.7	58.1	41.3	26.8		23.3	22.5	
141S	177.1	114.7	63.3	62.6					
142T	176.2	120	67.9	67.4	21.7				
143G	175.8	110.2	48.1						
144L	178.2	122.6	58	41.4	27.3		23.7	21.6	
145V	178.9	120.2	67.1	31.6	24.3	22.1			
146F	176.3	124	62.5	39.8	137.7				
147A	179.2	120.8	55.6	18.3					
148R	177.5	118.2	58.3	29.7	26.6		44.8		
149F	174.4	120.1	60.6	37.3	136.5				
150A	174.7	125.4	54.3	18					
151R	171.9	125.5	54.6	33.3	26.3		42.9		
152P	175.2	135.5	61.5	29.8	27.5		50.5		
153R	175.1	121.8	55.5	32.8	26.8		42.1		
154A	177.3	120.2	55.4	22.2					
155K	179.7	120.7	57.9	32.2	25.1		28.7		40.7
156I	177.8	121.8	64.6	37.9	29.7	17.8	14.1		
157M	174.8	117.6	58.3	32.3	35.7				16.9
158F	176.8	124.3	55.4	41.3	139.6				
159A	175.3	118.3	54.7	19.2					
160R	174.7	122.7	54.3	34.6	27.6		44		
161H	176.1	120.6	53.8	32.8	128.3				

162A	175.2	123.3	53.4	21.7					
163I	177.5	117.7	57.8	42.6	28.3	18.1	13.2		
164V	175	118.6	59.9	32.5	21.3	22			
165R	175.7	122.6	56	31.2	26.9		42.2		
166P	176.2	132	62.8	32.1	27		51.5		
167F	177.8	120.7	55.1	41.5	140				
168N	177	121	55.2	35.3	176				
169G	174.2	107.7	45.1						
170R	175.3	120.5	53.6	33	26.6		47		
171M	174.5	115.8	53.7	30.7	29.2			17.5	
172T	174.5	111.7	58.9	71.9	21.9				
173L	176.3	116.8	54.8	44.5	25.8		22.6	22.1	
174M	178	121.1	55.5	36.6	31.6			18.1	
175V	176.5	121.8	61.3	34.1	22.7	21.3			
176R	175.9	121	55.1	32.7	27.5		41.8		
177A	176.4	124.4	52.6	19.6					
178A	178	120.4	52.2	19.9					
179N	176.4	113.2	53.2	37.1	178.5				
180A	174.6	121.2	53.8	18.2					
181R	174.5	118.3	56.4	29.5	27.42		43.1		
182Q	176.2	121.8	54.4	29.8	31.5		180.6		
183N	177.4	120.4	55.6	37.8	180				
184V	178	117	66.6	31.6	23.4	21.9			
185I	177.9	120	59.8	42.3	28.5	17.8	15.1		
186A	175.1	118.8	53.2	19.4					
187E	174.1	125.8	53.8	31.6	35.5		182.3		
188A	175.3	126.8	51.1	20.7					
189R	175.2	121.5	54.3	32.6	26.6		43.9		
190A	176	127.8	52.6	19.1					
191K	174.7	116.8	54.4	32.4	25.2		29		42.8
192M	174.5	124	54	34.3	33			17.9	
193R	174.6	123.3	53.1	33.7	26.6		45.8		
194L	174.4	124.1	54.6	41	27.8		23.3	23.6	
195M	175.6	115.4	55	36.2	32.8			18.8	
196R	176	113.4	56.6	31.3	26.3		41.6		
197R	175.1	119.4	56.3	31.7	26.9		43		
198E	177	118.5	58.8	30.6	35.9		182.4		
199H	177.5	120.1	56.6	31.5	131.7				
200S	177.9	115.3	58.1	63.9					
201S	177	116.5	55.4	64.2					
202E	175.4	120	57.4	29.7	37.4		182.8		

203G	175.7	106.2	47.6						
204Y	176.5	120.2	59.4	37	131.3				
205S	176.2	119.9	55.8	63.7					
206L	176.3	121.9	54.6	42.3	28.3		25.6	26.8	
207M	175.7	121.2	54.4	33.7	31.9				18
208K	176.5	117.1	54.9	32.6	24.8		29.5		40.8
209I	177.5	118.7	58.9	42	27.2	18.1	13.7		
210H	178.1	124	55.3	32.5	130.7				
211D	176.1	122.8	54	39.9	178.9				
212L	177.8	117.8	55.6	41.6	25.9		21.8	23.3	
213K	177.6	118	58.1	31.7	26.5		27.8		41.6
214L	179.5	116	58	40.8	27.6		22.8	22.1	
215V	176.7	120	65.3	31.8	22.9	21.8			
216R	179.7	117.9	59.6	29.8	28.4		42		
217N	178.6	118.6	53.4	42.4	175.1				
218E	177.1	117.3	58.8	29.4	36		181		
219H	177.2	120.6	55.7	31	130.6				
220P	179.2	142.4	64.1	32.3	26.8		50.6		
221I	178	118.9	66	38.4	29.4	17.3	14.1		
222F	176.5	117	57.3	41.3	137.7		132.1		
223L	176.4	121.6	56.4	41.8	26		24.2	23.7	
224L	177.5	118	56.4	41.9	26.2		23.7	23.3	
225G	174	105.2	45.1						
226W	176.6	118.3	55.4	29.4					
227N	176.2	125.9	52.8	40.3	174.7				
228M	176.2	116.2	55.6	32.3	31.3			17.8	
229M	176.4	119.3	55.8	34	31.6			18.3	
230H	177.1	118.3	55.6	30.4	133.9				
231V	178.5	119.5	59.9	33.9	22.1	21.2			
232I	177.4	119.4	65.2	37.8	26.9	16.9	14.2		
233D	177.8	121.4	54.4	40.9	178.9				
234E	176.7	115.7	57.6	30.2	34.4		182.8		
235S	177.2	121.6	55.7	68.3					
236S		123.8	58.4	64					
237P	176.8	134.6	65.4	29.6	26.6		50.4		
238L	178	115.7	56	42.1	26.2		22.5	21.9	
239F	177.4	114.8	63.1	37.8			132.3		
240G	175.7	110	47.9						
241E	176.8	121.2	58.2	32.4	36.1		180.1		
242T	173.7	112	59.7	72.9		21.7			
243P	176.1	139.5	63.1	31.2	29.2		50.7		

244E	176.5	122.7	59.1	28.8	36		180.7		
245S	176.1	118.1	62.7	63					
246L	179.3	121.6	58.2	41.9	26.7		23.5	23.1	
247A	179.5	122.1	55.4	18.1					
248E	176.7	120	58.4	27.6	38.4		181.9		
249G	174.8	107.4	45.5						
250R	176.7	123.5	54.4	27.6	25.6		41.9		
251A	175	121.3	54.6	18.2					
252M	175.6	120.4	54	34.4	32.6			17.5	
253L	178.5	120.5	54.5	43.3	27.3		22.8	21.6	
254L	174.9	120.3	54.5	45.5	27.2		22.6	21.8	
255V	178.2	119.1	60.3	34	22.2	21.3			
256M	174.6	117.6	55	36.1	34.5			18	
257I	176	117.6	59	41.3	27.6	17.1	13		
258E	175.5	118	56.3	30.5	37.6		182.6		
259G	172.7	104.8	44.1						
260S	176	122	55.1	63.1					
261D	177.7	120.1	55.7	42.7	179.3				
262E	175.5	117.9	58.1	31.7	35.4		183		
263T	177.2	117.2	60.1	67		21.5			
264T	174.9	121	60.4	70.1		21.2			
265A	175.4	129.4	50.4	20.3					
266Q	174.5	122.1	54.9	31.3	32.9		180.4		
267V	175.2	123.4	61.1	34.4	21.1	20.4			
268M	176.2	126	54.2	35.4	33.4			17.6	
269Q	175.3	118.3	55.3	33.4	34.6		179.4		
270A	175.9	126	52.4	21.9					
271R	175	125.9	54.3	31.6	26.8		44.5		
272H	174.5	124	55.7	32.5	130.1				
273A	176.9	127.4	52.8	20.4					
274W	178.8	122.7	58.7	34.5	111.1				
275E	174.5	115.8	55.4	31.3	34.1		182.2		
276H	175.8	123.1	59.9	27.3	133.4				
277D	178.6	122.5	55.9	39.3	176				
278D	177	117.8	55.6	37.5	178.6				
279I	177.5	120.4	57.9	41.2	27	18.2	14.1		
280R	174.6	124.2	55.1	34.8	27		42.1		
281W	178.2	124.6	55.7	33					
282H	178.9	115.7	59.5	26					
283H	178.7	119.8	58.2	27					
284R	179.1	123.9	55.2	32.3	27.5		41.2		

285Y	176	121.3	61.7	39.6	132.2				
286V	178.6	123.1	61.6	32.9	22.5	21.3			
287D	174.6	121.1	55.6	44.6	176.7				
288L	176.9	116.2	57.8	41	26.5		23.5	22.7	
289M	178.6	119.2	55.6	34.2	31.6				17.7
290S	176.9	121.5	56.8	63.7					
291D	174.7	124.2	54.8	41.1	176.1				
292V	174.6	122.7	60.8	33.3	21.3	21.6			
293D	176.4	125.8	54.7	42.8	174.5				
294G	173.9	107	45.7						
295M	177	121.5	54.5	33.7	31.7				18
296T	172.6	117.9	61.3	70.8		21.2			
297H	174.3	125.8	55.1	33.6	130.3				
298I	174.8	126.7	60.5	42.5	27.4	17.4	14.4		
299D	176.3	127.4	54.3	43	174.6				
300Y	176	119.6	55	39.5	131.1		136.7		
301T		117.7	61.7	70.8		23.9			