

Supporting Information for “Solid-State Nuclear Magnetic Resonance Measurements of HIV Fusion Peptide ^{13}C to Lipid ^{31}P Proximities Support Similar Partially Inserted Membrane Locations of the α Helical and β Sheet Peptide Structures”

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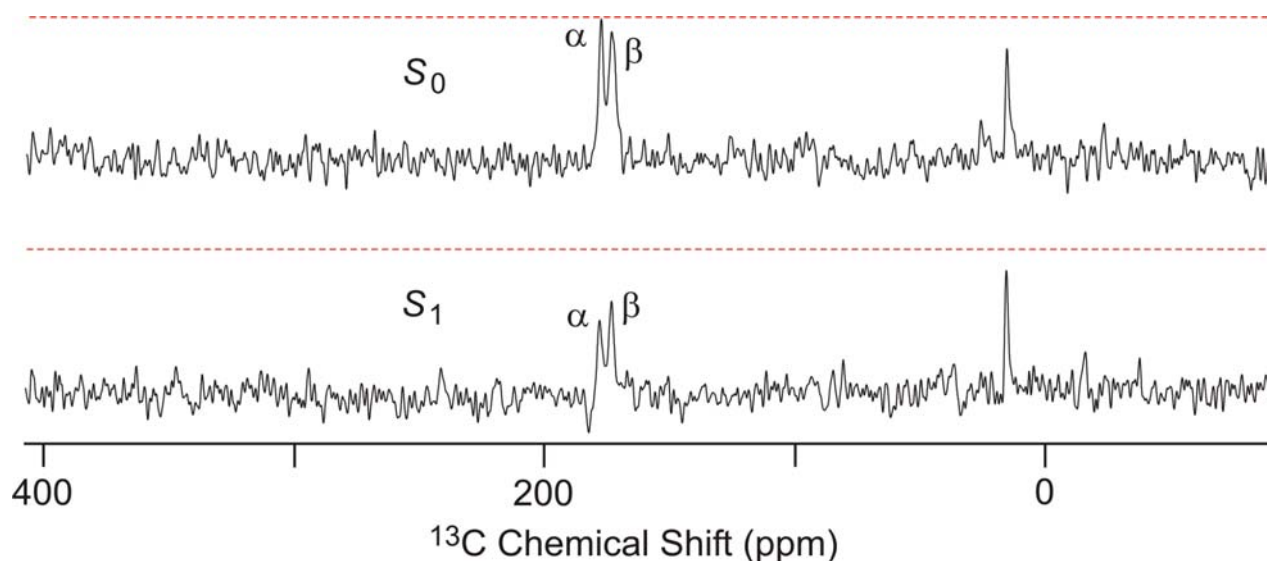


Figure S1. ^{13}C - ^{31}P REDOR S_0 and S_1 spectra at 24 ms dephasing time of the sample containing HFPmn that was ^{13}C labeled at L9. The α and β signals are respectively due to the HFPmn populations with either α helical or β sheet structure at L9. The dashed red lines are at the peak intensity of the S_0 α signal. The signals at 15 ppm are due to natural abundance $^{13}\text{CH}_3$ nuclei of the lipid molecules. Both the S_0 and S_1 spectra were processed with 100 Hz Gaussian line broadening and baseline correction and are the sum of 24704 scans.

Table S1. Full peak $(\Delta S/S_0)^{exp} \times 100$ ^a

Construct	Labeling	Dephasing time (ms)				
		2 ms	8 ms	16 ms	24 ms	32 ms
HFPmn_V2E	A1	5 (9)	−11 (16)	−12 (13)	73 (24)	
	I4	16 (10)	−9 (8)	20 (5)	27 (6)	41 (5)
	A6	1 (5)	15 (6)	46 (6)	52 (5)	
	L9	2 (4)	11 (4)	14 (5)	22 (4)	27 (7)
	L12	−5 (7)	10 (4)	23 (4)	43 (2)	51 (3)
	A14	−7 (11)	12 (7)	20 (7)	21 (7)	
HFPmn	A1	11 (7)	49 (6)	63 (7)	81 (7)	
	A6	3 (5)	15 (5)	27 (7)	18 (5)	28 (6)
	L9	3 (6)	12 (4)	28 (4)	42 (4)	
	L12	12 (6)	21 (5)	47 (6)	77 (6)	
	A14	7 (7)	21 (5)	46 (4)	67 (4)	74 (5)
HFPtr	A1	−15 (7)	21 (7)	42 (10)	43 (5)	
	I4	4 (12)	10 (11)	40 (7)	52 (3)	
	A6	4 (5)	10 (4)	1 (4)	7 (3)	2 (4)
	L9	8 (5)	5 (6)	19 (4)	37 (4)	
	L12	−1 (10)	8 (7)	22 (9)	37 (6)	
	A14	7 (6)	18 (6)	39 (8)	54 (5)	

^a Each number in parentheses is one standard deviation based on measurement of spectral noise.

Table S2. α and β peak $(\Delta S/S_0)^{exp} \times 100$ ^{a,b}

Construct	Labeling	Peak	Dephasing time (ms)				
			2 ms	8 ms	16 ms	24 ms	32 ms
HFPmn_V2E	L9	α	4 (4)	1 (5)	12 (6)	17 (4)	24 (7)
		β	6 (9)	20 (12)	24 (17)	39 (12)	
	L12	α	-2 (11)	16 (7)	18 (7)	35 (3)	44 (4)
		β	-1 (11)	4 (8)	26 (8)	47 (4)	53 (5)
HFPmn	A6	α	7 (12)	29 (10)	44 (15)	10 (10)	52 (11)
		β	2 (6)	3 (7)	16 (9)	26 (5)	13 (8)
	L9	α	7 (11)	15 (8)	37 (8)	45 (7)	
		β	1 (9)	9 (7)	20 (6)	35 (7)	
	L12	α	1 (13)	25 (11)	56 (12)	68 (10)	
		β	11 (8)	25 (7)	36 (11)	77 (10)	
	A6	α	2 (9)	5 (6)	0 (7)	10 (5)	9 (7)
		β	11 (8)	10 (6)	2 (7)	3 (5)	-2 (7)
HFPtr	L9	α	7 (9)	2 (10)	19 (5)	32 (5)	
		β	7 (8)	11 (9)	17 (6)	38 (7)	
	L12	α	14 (13)	11 (11)	28 (16)	25 (13)	
		β	-22 (22)	2 (13)	20 (13)	42 (9)	

^a Integration was done using a 2 ppm window centered at the peak shift.^b Each number in parentheses is one standard deviation based on measurement of spectral noise.