Supporting Information

Signaling-Related Mobility Changes in Bacterial Chemotaxis Receptors Revealed by Solid-State NMR

Maryam Kashefi and Lynmarie K. Thompson*

Department of Chemistry, University of Massachusetts Amherst, 710 N Pleasant St, Amherst, Massachusetts, 01003, USA

*Department of Chemistry, 122 LGRT, 710 North Pleasant St, University of Massachusetts Amherst, Amherst, MA, 01003, USA. E-mail: Thompson@chem.umass.edu, Telephone: (413) 545-0827

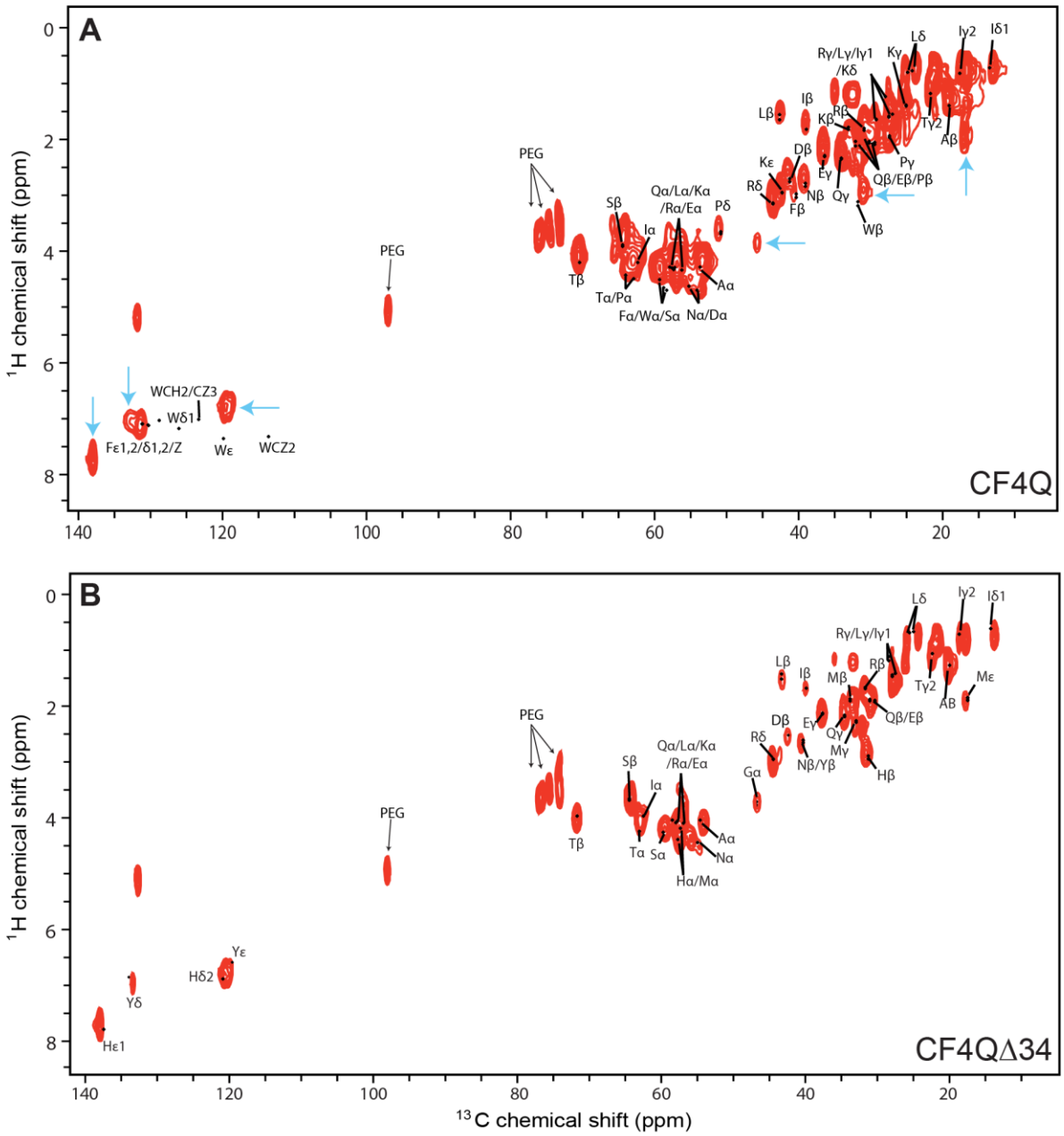

Figure S1. ^{1}H-^{13}C INEPT spectra of (A) U-^{13}C,^{15}N-CF4Q and (B) U-^{13}C,^{15}N-CF4QΔ34 in PEG-mediated functional arrays with Che A and CheW. Spectra are shown at comparable contour levels. CF4Q spectrum has more intensity for most of the peaks except for residues which are not found in the tail (cyan arrows, His, Tyr, Gly, and Met). same NMR condition as Figure 6.

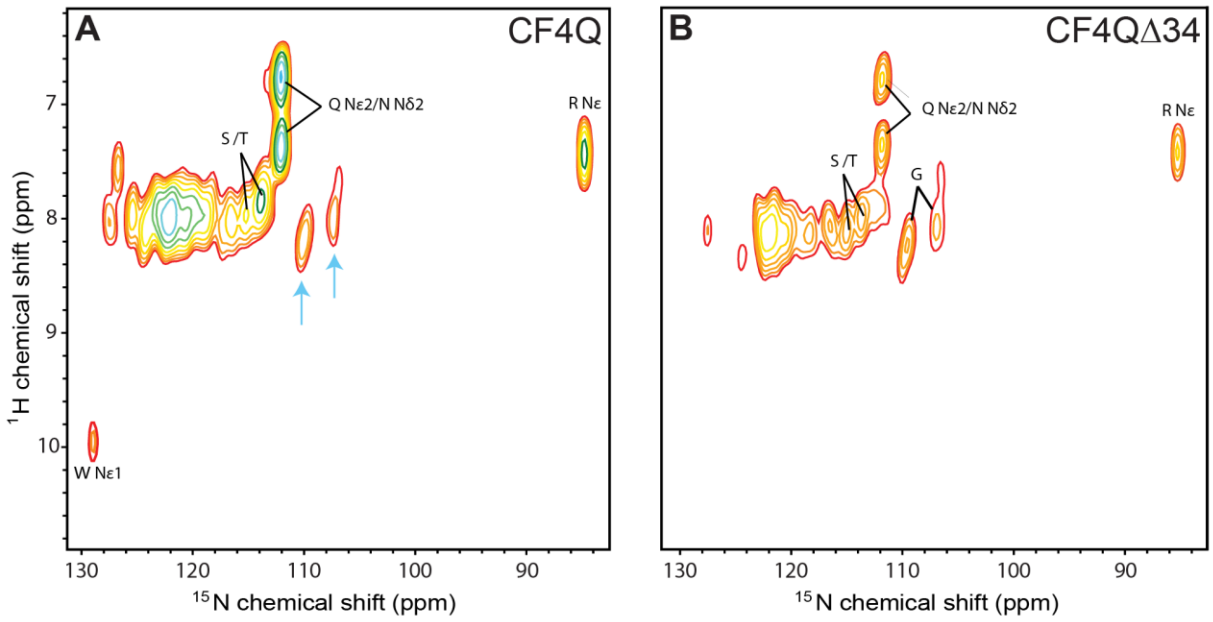

Figure S2. ^{1}H-^{15}N INEPT spectra of (A) U-^{13}C,^{15}N-CF4Q and (B) U-^{13}C,^{15}N-CF4QΔ34 in PEG-mediated functional arrays with Che A and CheW. Assigned residue types are based on average chemical shifts tabulated in the BMRB. (A) CF4Q spectra contain the expected resonances for the mobile of C-terminal tail, but also contain resonances for Gly which is not in the tail. (B) CF4QΔ34 spectra demonstrate there is another mobile region besides the tail. Same NMR conditions as Figure S1.

Table S1. PCR Primers used for plasmid construction.

Construct	PCR Primers
HisTev-CheY	F:5'CATCATCACCACCATCACGAAAACCTGTATTTTCAGGGAGCGGA TAAAGAACTTAAATTTTTGG 3' R:5'GTGGCGGCCGCTCTATTACATGCCCAGTTTCTCAAAGAT 3'
His-Tev-CheA	F:5' CATCATCACCACCATCACGAAAACCTGTATTTTCAGGGAAGCATGGATATA AGCG 3' R:5' GGCCGCTCTATTAGGCGGCGGTGTTCGCCATACG 3'
His-Tev-CheW	F:5'CATCATCACCACCATCACGAAAACCTGTATTTTCAGGGAACCGGT ATG ACGAATGTAAC 3' R:5'GGCGGCCGCTCTATTACGCCACTTCTGACG C 3'
CF4QΔ34	F: 5'-TGACGAGTATTTACTAACGCG -3' R: 5'- GTTAGTAAATACTCGTCATGGGCTGGCTGCCAGACG -3'
CF4Q.A411V	F: 5'- GTCGCAGCGCCCAGGTGGCAAAAG -3' R: 5'- CTTTGATCTCTTTTGCCACCTGGGCGC -3'

Table S2. Peak volumes in 2D ^{1}H-^{13}C INEPT of $^{13}C^{15}N$CF4Q and $^{13}C^{15}N$CF4QΔ34 assembled with CheA and CheW into functional native-like arrays with PEG.[a]

Residue/s	$\omega_1/^{1}H$	$\omega_2/^{13}C$	CF4Q volume[b]	**CF4QΔ34 volume[b]**	**Mobile region residues**	***CF4Q – CF4QΔ34 = Δ34 volume***	***Δ34 residues***
Total Cα			86.1	**53.9**	**51**	*32.2*	*34*
Arg Nε	7.3	84.9	6.3	**3.1**	**3**	*3.2*	*3*
Asn Cβ + Tyr Cβ	2.6	39.1	3.9	**2**	**1 Asn, 1 Tyr**	*1.9*	*2 Asn*
Glu Cγ	2.2	36.3	8.1	**4.3**	**5**	*3.7*	*3*
Gly Cα	4.0	45.4	2.5	**2.8**	**3**	*-0.3*	*0*
Gly N	8.6, 8.3	110.4, 107.8	3.5	**3.5**	**3**	*0*	*0*
His Cβ	3.1	29.7	5.6	**5.4**	**1**	*0.2*	*0*
His Cε1	7.8	138.4	4.8	**4.6**	**1**	*0.2*	*0*
Ile Cβ	1.8	38.7	3	**1.7**	**2**	*1.3*	*1*
Ile Cδ1	0.8	13.0	3.7	**3.0**	**2**	*0.7*	*1*
Leu Cβ	1.6	42.2	3.6	**1.7**	**3**	*1.9*	*2*
Met Cβ	2.0	17.1	1.6	**2.2**	**1**	*-0.6*	*0*
Phe*	7.2	131.8	1.3	**0**	**0**	*1.3*	*1*
Pro Cδ	3.7	50.7	1.6	**0**	**0**	*1.6*	*7*
Thr Cβ	4.2	69.8	8.2	**4.5**	**6**	*3.7*	*3*
Trp Nε	10.0	129.1	1.0	**0**	**0**	*1.0*	*1.0*
Tyr Cδ*	7.1	133.4	1.2	**1.0**	**1**	*0.2*	*0*

[a]Bold columns compare peak volumes to residues of the most probable 50-residue mobile region; italicized columns compare difference volumes to residues of the deleted 34-residue tail.

[b]All peak volumes are corrected for differences in nmol of CF in the sample. HC peak volumes are then calibrated based on Tyr Cδ = 2 in the CF4QΔ34 PEG sample, and then normalized to the number of unresolved correlations contributing to the peak (5 for Phe and 2 for Tyr Cδ) so that the reported volume should correspond to the number of residues. HN peak volumes are calibrated based on Trp Nε = 1 in the CF4Q PEG sample.