

Supporting Information for:

Proton Association Constants of His-37 in the Influenza-A M2₁₈₋₆₀ Dimer-of-Dimers

Michael T. Colvin,[†] Loren B. Andreas,[†] James J. Chou[‡], and Robert G. Griffin^{†*}

[†]*Department of Chemistry and Center for Magnetic Resonance, Francis Bitter Magnet Laboratory, Massachusetts Institute of Technology, Cambridge, Massachusetts, 02139 and*

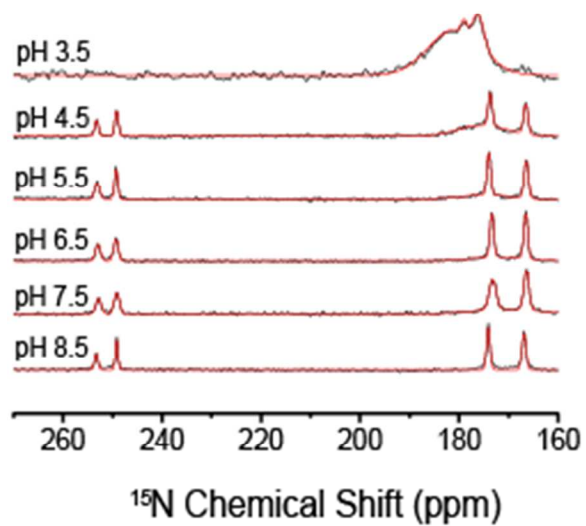
[‡]*Department of Biological Chemistry and Molecular Pharmacology, Harvard Medical School, Boston, Massachusetts 02115*

Email rgg@mit.edu

Table S1. Ratio of protonated nitrogens to unprotonated nitrogen as a function of pH at the temperatures indicated.

pH	$I_{\text{NH}}/I_{\text{N}}(-6^{\circ}\text{C})$	His/His ⁺ (-6°C)	$I_{\text{NH}}/I_{\text{N}}(37^{\circ}\text{C})$	His/His ⁺ (37°C)
3.5	inf	0.00	inf	0.00
4.5	6.33	0.61	29.75	0.10
5.5	3.28	1.40	4.91	0.85
6.5	3.05	1.64	4.10	1.10
7.5	2.15	2.96	3.51	1.43
8.5	1.464	52.2	1.88	5.67

(a) -6°C



(b) 37°C

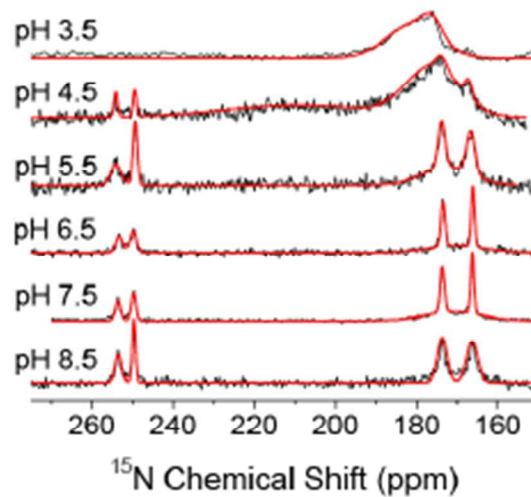


Figure S1. ^{15}N MAS NMR spectra of M2₁₈₋₆₀ H₅₇Y ILFY reverse labeled at pH indicated. (a) at -6°C, and (b) at 37°C.

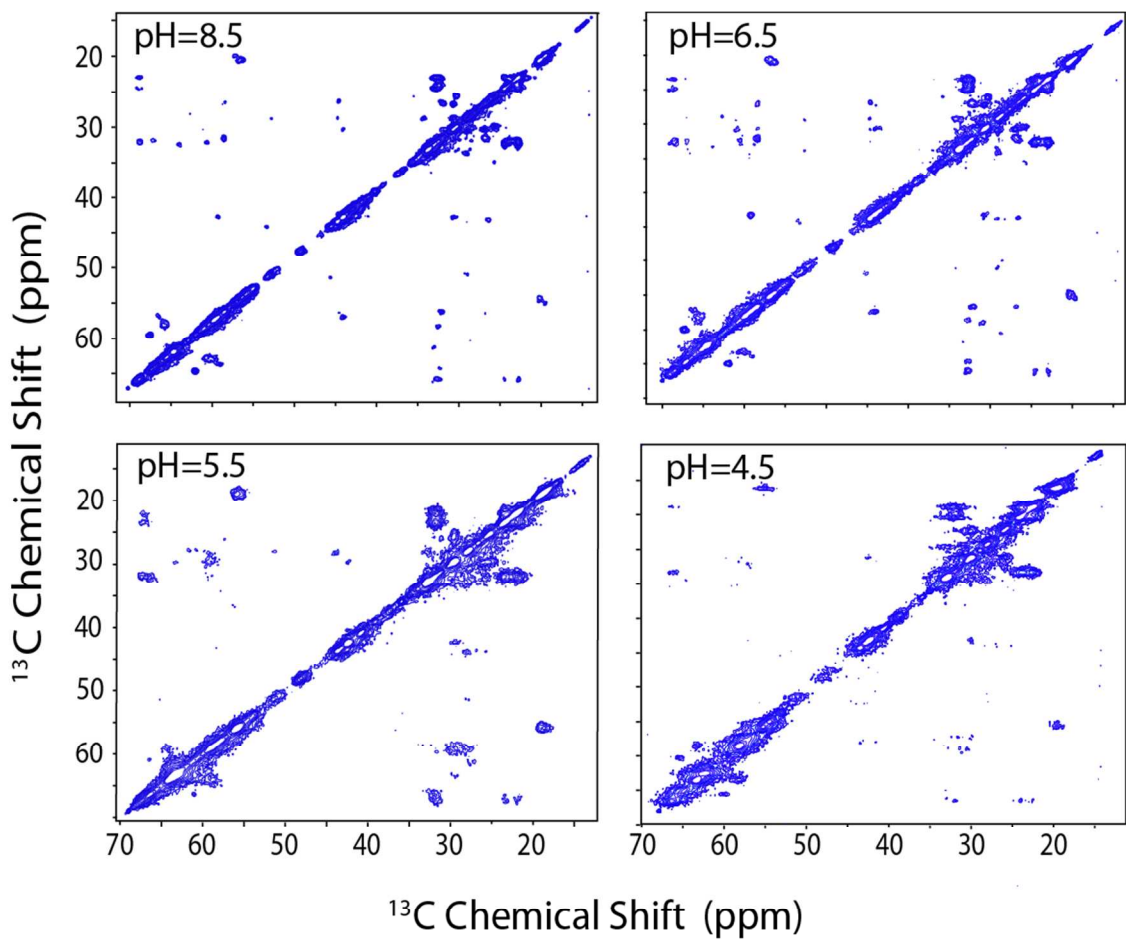


Figure S2. 2D ^{13}C - ^{13}C 20 ms PDS spectra of M2₁₈₋₆₀ -6°C, $\omega_r/2\pi=12.5$ kHz, 700 MHz ^1H frequency at pH indicated.

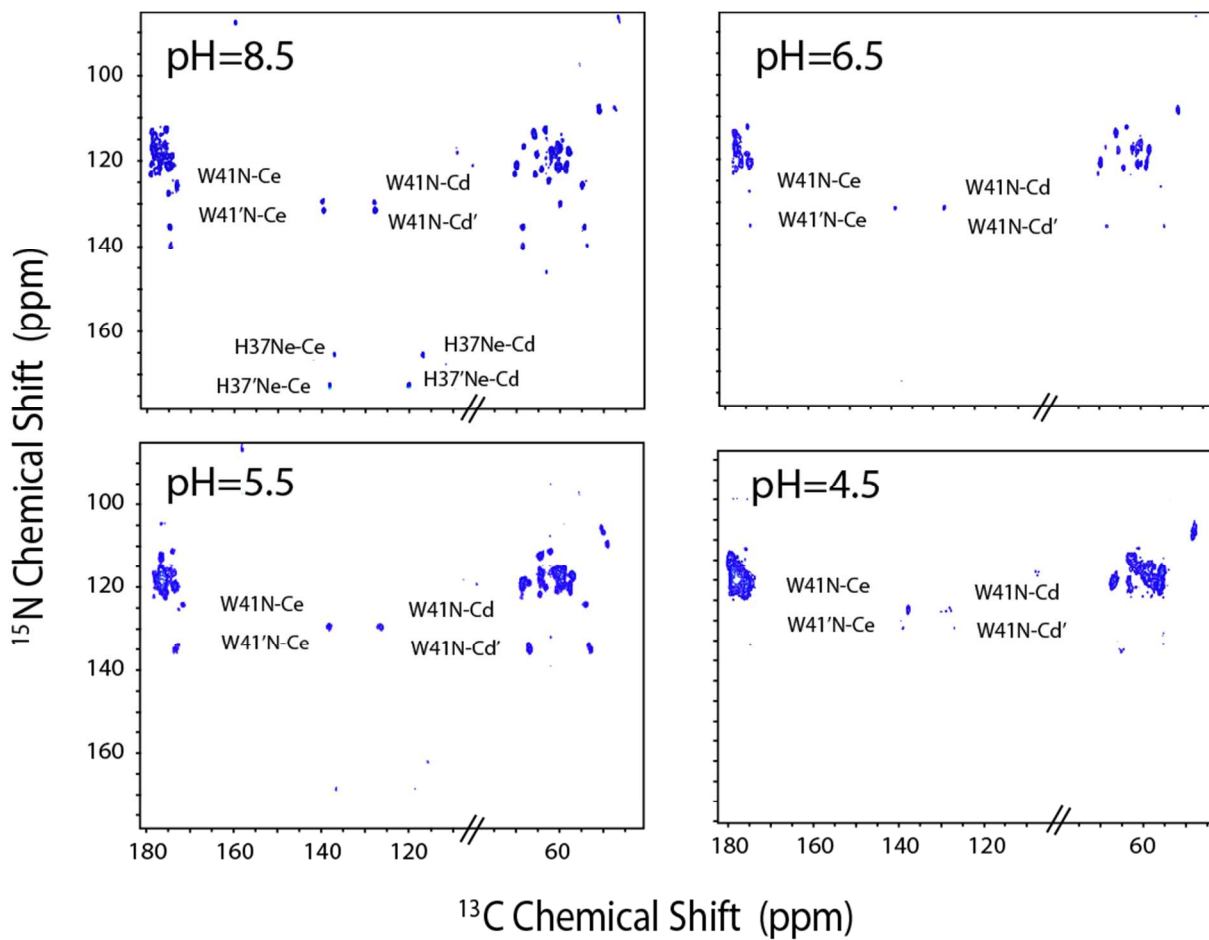


Figure S3. 2D ^{13}C - ^{15}N 3.2 ms zf-TEDOR spectra of M_{218-60} at -6°C , $\omega_r/2\pi = 12.5$ kHz 700 MHz ^1H frequency at pH indicated.

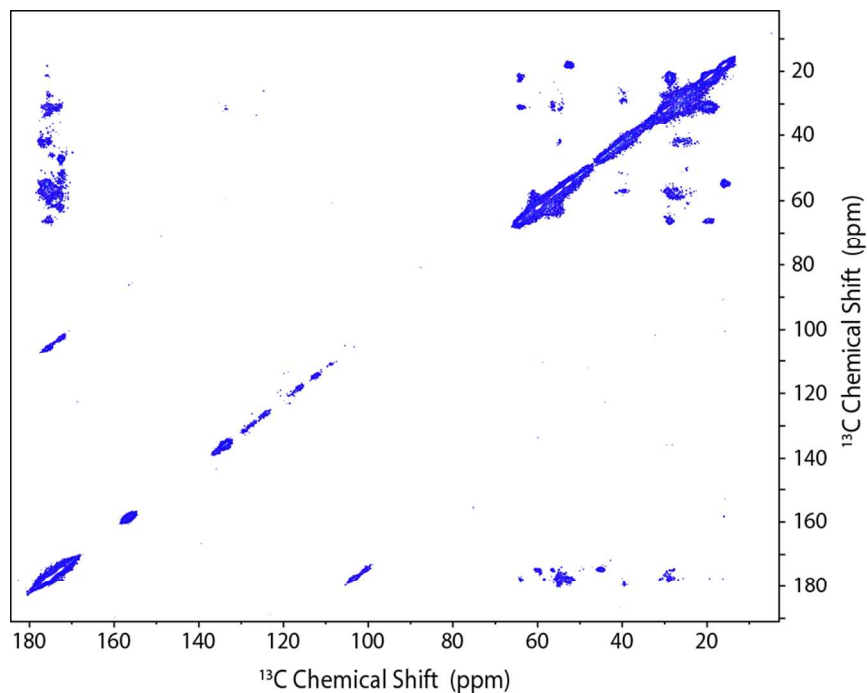


Figure S4. 2D 20 ms ^{13}C - ^{13}C PDS spectrum of M2₁₈₋₆₀ at $\omega_{0\text{H}}/2\pi=700$ MHz, $\omega_r/2\pi=12.5$ kHz, pH =6.5 at T=-45°C.

References:

- (1) Andreas, L. B.; Eddy, M. T.; Chou, J. J.; Griffin, R. G. *J Am Chem Soc* **2012**, *134*, 7215.
- (2) Andreas, L. B.; Eddy, M. T.; Pielak, R. M.; Chou, J.; Griffin, R. G. *J Am Chem Soc* **2010**, *132*, 10958.
- (3) Jaroniec, C. P.; Filip, C.; Griffin, R. G. *J Am Chem Soc* **2002**, *124*, 10728.