Supplementary Material

Figure 1: 2D-NOESY spectra recorded at pH 2.8 with mixing time set to 200 ms and 100 points in F1 dimension for both apo- and holo-IFABP. The protein concentration was 1.0mM for holo-form and 0.2mM for apo-form and they were prepared as described in the text.

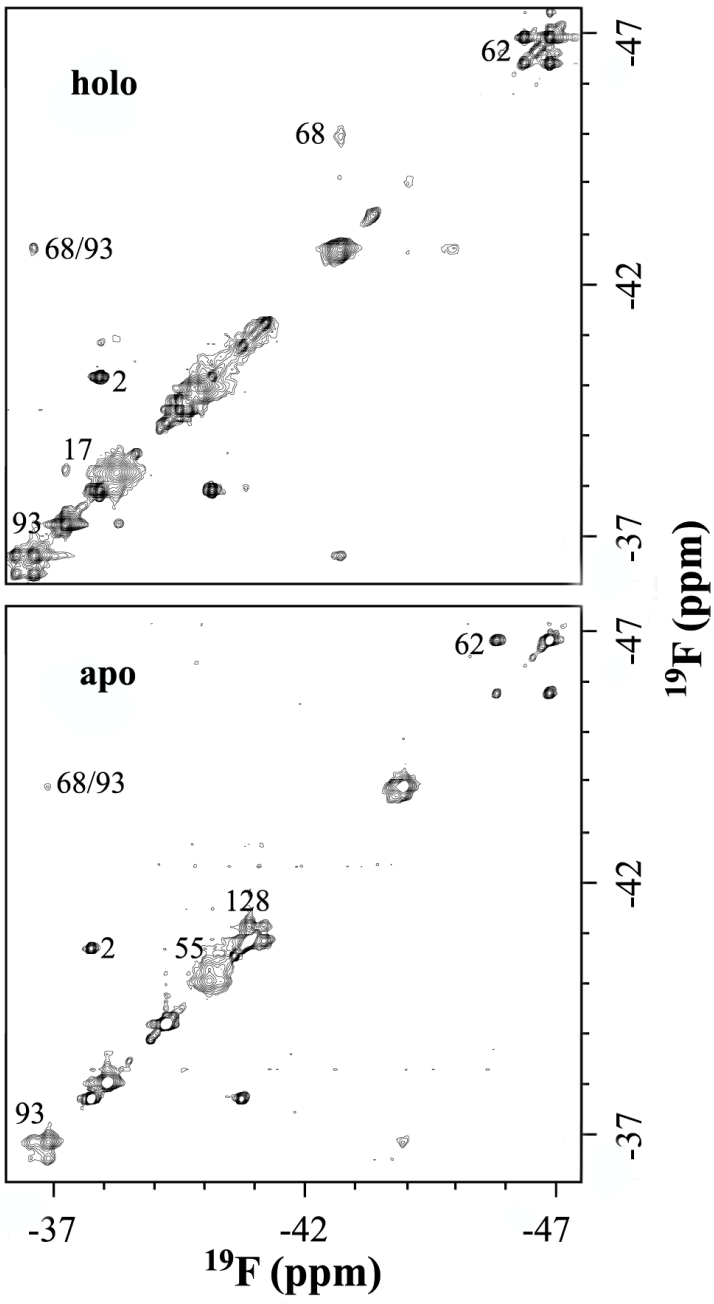
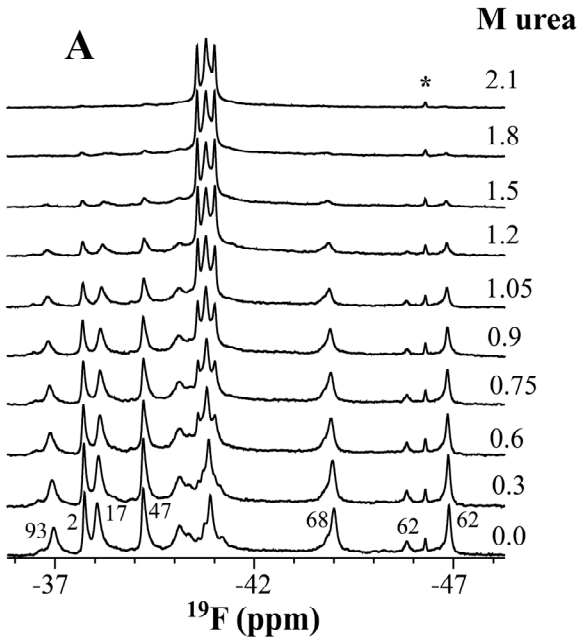

holo
62
68
68/93
2
17
93
apo
62
68/93
128
2
55
93
-47
-42
-37
-37
-42
-47
19F (ppm)
19F (ppm)

Fig.2. ^{19}F-NMR spectra of the acid state at pH 2.8 (A) and chemical shift changes (B) of ^{19}F-Phe-IFABP as a function of urea concentration. The spectra were recorded at 20 °C with100 μM protein. The samples were made by mixing 200 μM protein solution at pH 2.8 with urea stock at the same pH and buffer condition. Each spectrum was acquired with 256 scans and processed with 12 Hz exponential line broadening. The peak marked with star (*) is the reference of 6-fluoro-trytophan.



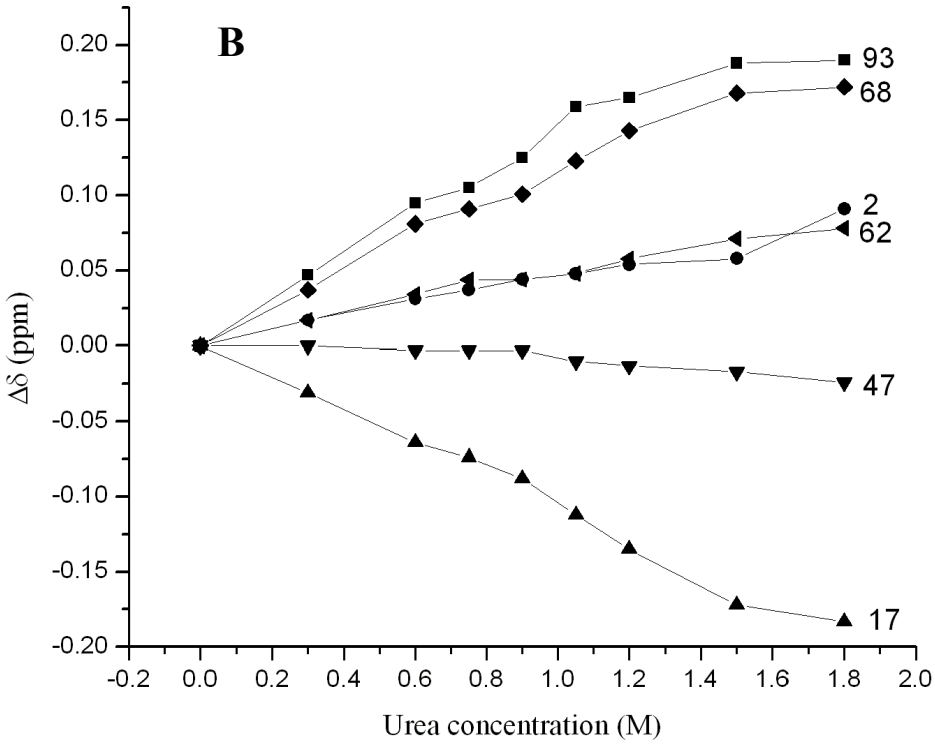
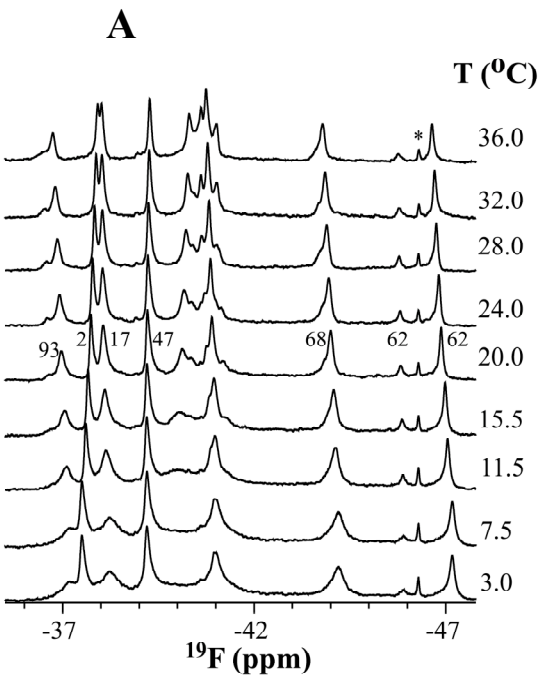

B
0.20
0.15
0.10
0.05
0.00
-0.05
-0.10
-0.15
-0.20
Δδ (ppm)
-0.2
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
Urea concentration (M)
93
68
2
62
47
17

Fig.3. ^{19}F-NMR spectra of IFABP at pH 2.8 (A) and chemical shift change (B) as a function of temperature (temperature coefficient). The protein concentration was 100 μM. Each spectrum was collected with 256 scans and processed with 12 Hz exponential line broadening. The peak marked with star (*) is the reference of 6-fluoro-trytophan. in the text.



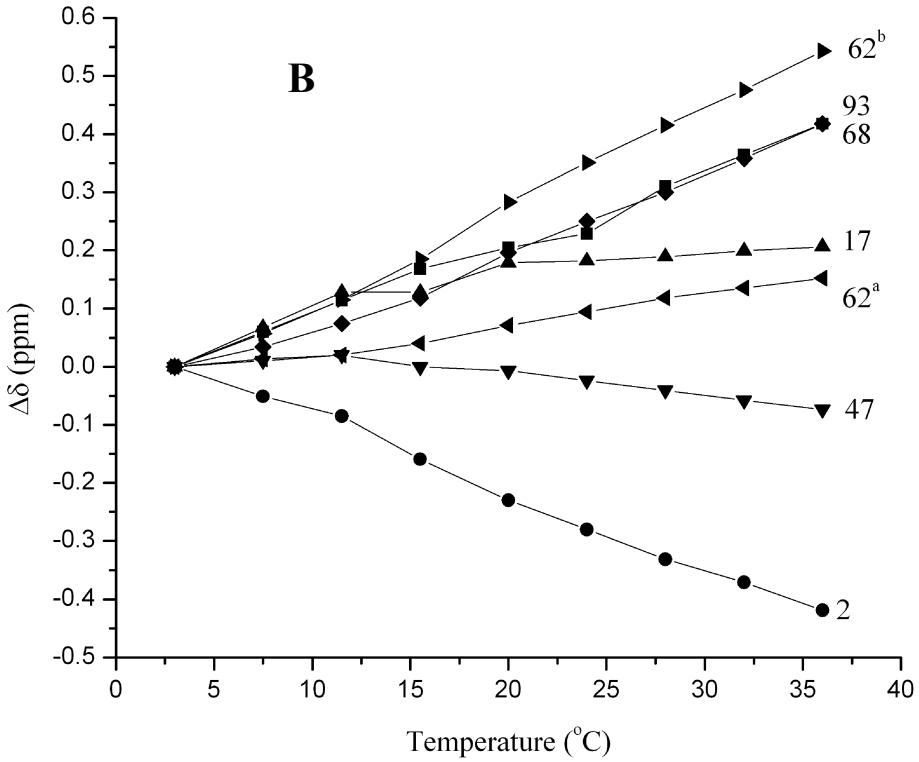

B
62b
93
68
17
62a
47
2
Δδ (ppm)
Temperature (°C)
0.6
0.5
0.4
0.3
0.2
0.1
0.0
-0.1
-0.2
-0.3
-0.4
-0.5
0
5
10
15
20
25
30
35
40

Figure 4: ^{19}F-NMR spectra of holo-IFABP as a function of pH. The spectra were recorded at 20 ºC with 200 μM protein. The sample was prepared as described in the text. Each spectrum was collected with sixty-four scans and processed with 12 Hz exponential line broadening.