Supporting Information for: “Solid-State Nuclear Magnetic Resonance Spectroscopy of Human Immunodeficiency Virus gp41 Protein that Includes the Fusion Peptide: NMR Detection of Recombinant Fgp41 in Inclusion Bodies in Whole Bacterial Cells and Structural Characterization of Purified and Membrane-Associated Fgp41”

Fgp41 amino acid and DNA sequences

Start A V G L G A V F L G F L G A A G S T M G A A S M T L T V Q A R Q L L S G I V Q Q Q S N L L K A I E A Q Q H L L K L T V W G I K Q L Q A R V L A V E R Y L Q D Q Q L L G I W G C S G K L I C T S F V P W N N S W S N K T Y N E I W D N M T W L Q W D K E I S N Y T D T I Y R L L E D S Q N Q Q E K N E Q D L L A L D K L E H H H H H H **Stop**

atggcagttggactaggagctgtcttccttgggttcttgggagcagcagggagcactatgggcgcggcgtcaatgacgctgacg
gtacaggccagacaattattgtctggcatagtgcaacagcaaagcaatttgctgaaggctatagaggctcaacagcatctgttga
aactcacggtctggggtattaaacagctccaggcaagagtcctggctgtggaaagatacctacaggatcaacagctcctgggaa
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acaacatgacctggttgcaatgggataaagaaattagcaattacacagacacaatatacaggctacttgaagactcgcagaacca
gcaggaaaagaatgaacaagacttattggcattagataaactcgagcaccaccaccaccaccactga

HIV-1 Sequences: Fgp41 (black) and HXB2 (blue)

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1
AVGLGAVFLG  FLGAAGSTMG  AASMTLTVQA  RQLLSGIVQQ  QSNLLKAIEA  QQHLLKLTVW
AVGIGALFLG  FLGAAGSTMG  AASMTLTVQA  RQLLSGIVQQ  QNNLLRAIEA  QQHLLQLTVW
61
GIKQLQARVL  AVERYLQDQQ  LLGIWGASGK  LIATSFVPWN  NSWSNKTYNE  IWDNMTWLQW
GIKQLQARIL  AVERYLKDQQ  LLGIWGCSGK  LICTTAVPWN  ASWSNKSLWQ  IWNHTTWMEW
121
DKEISNYTDT  IYRLLEDSQN  QQEKNEQDLL  ALDKLEHHHH  HH
DREINNYTSL  IHSLIEESQN  QQEKNEQELL  ELDK------  --
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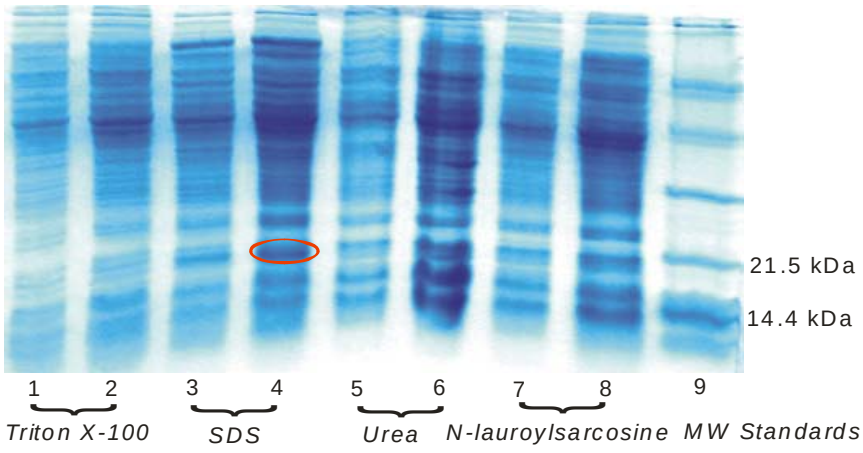
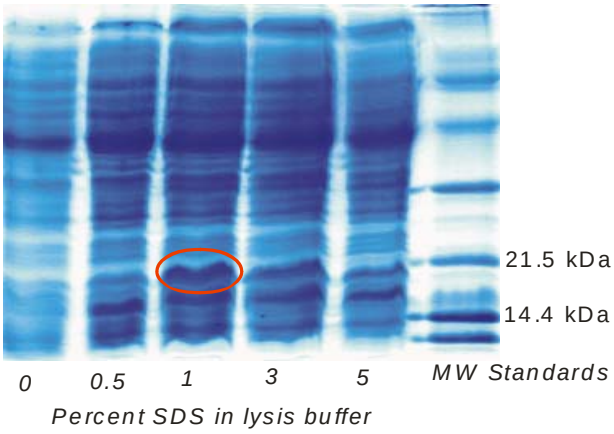
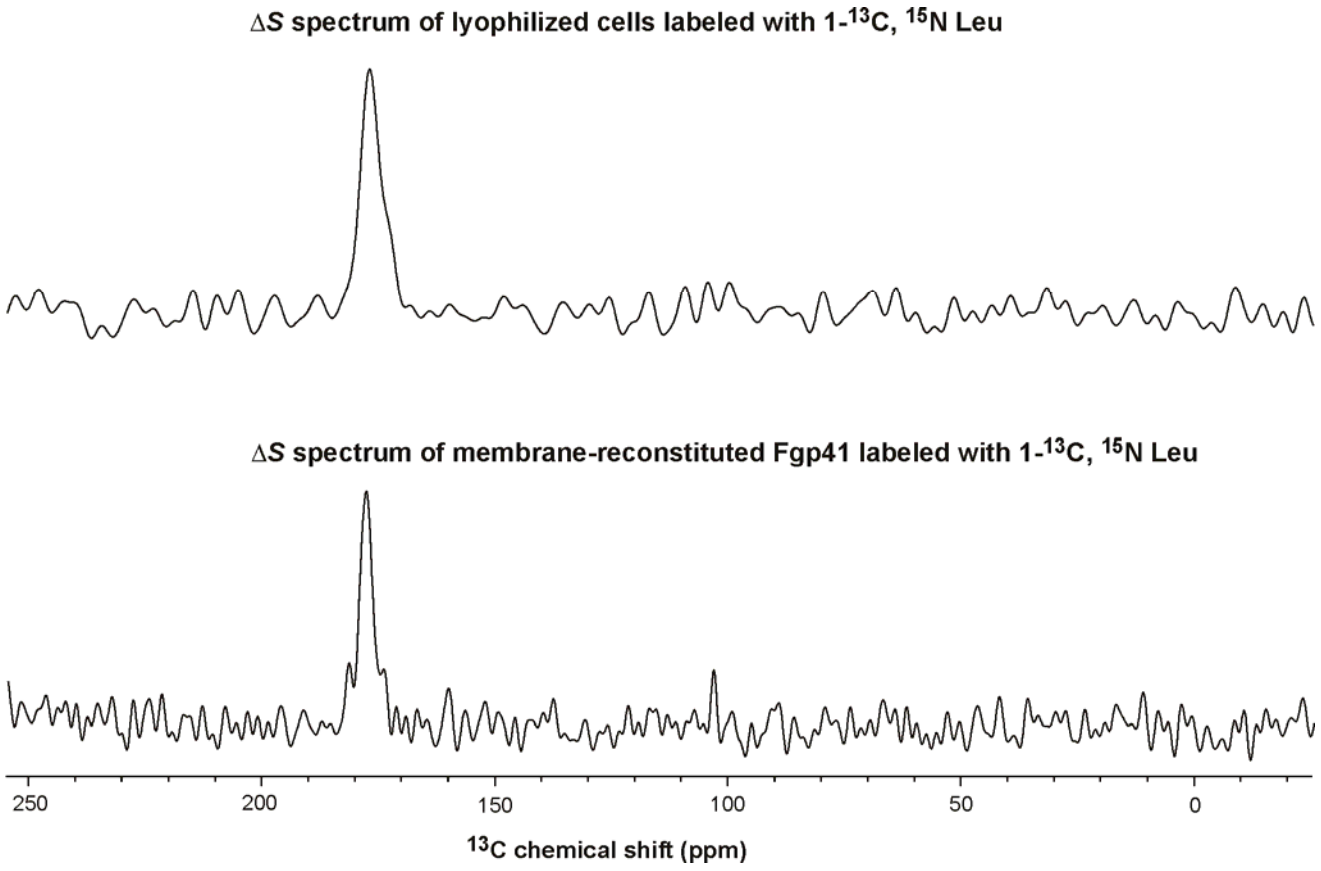
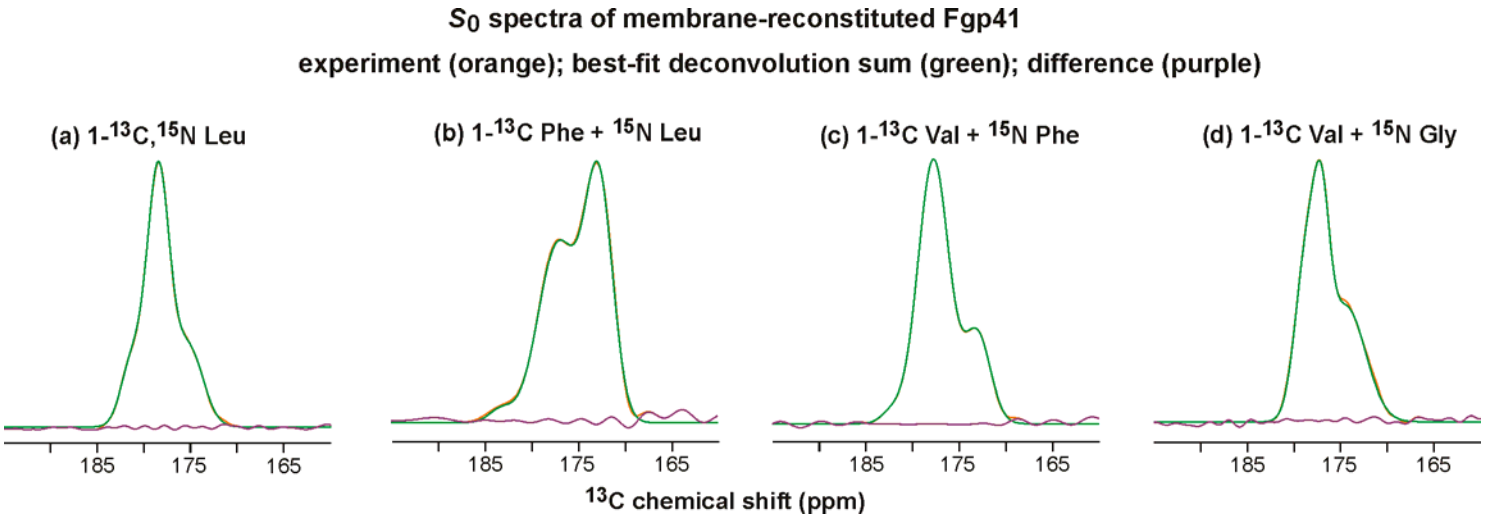
Representative SDS-PAGE of soluble cell lysates produced using buffers with different detergents or urea. For each buffer, the left and right lanes respectively correspond to 2 and 5 μL aliquots of lysate. The ~19 kDa band apparent in some lanes is assigned to Fgp41. One example is circled in red in lane 4 for lysis in SDS. Bands that may be Fgp41 were also apparent for lyses in either urea or *N*-lauroylsarcosine but purifications of these lysates consistently yielded <1 mg Fgp41/L culture whereas purifications of SDS lysates yielded >1 mg Fgp41/L culture. Subsequent lyses were therefore done with SDS.

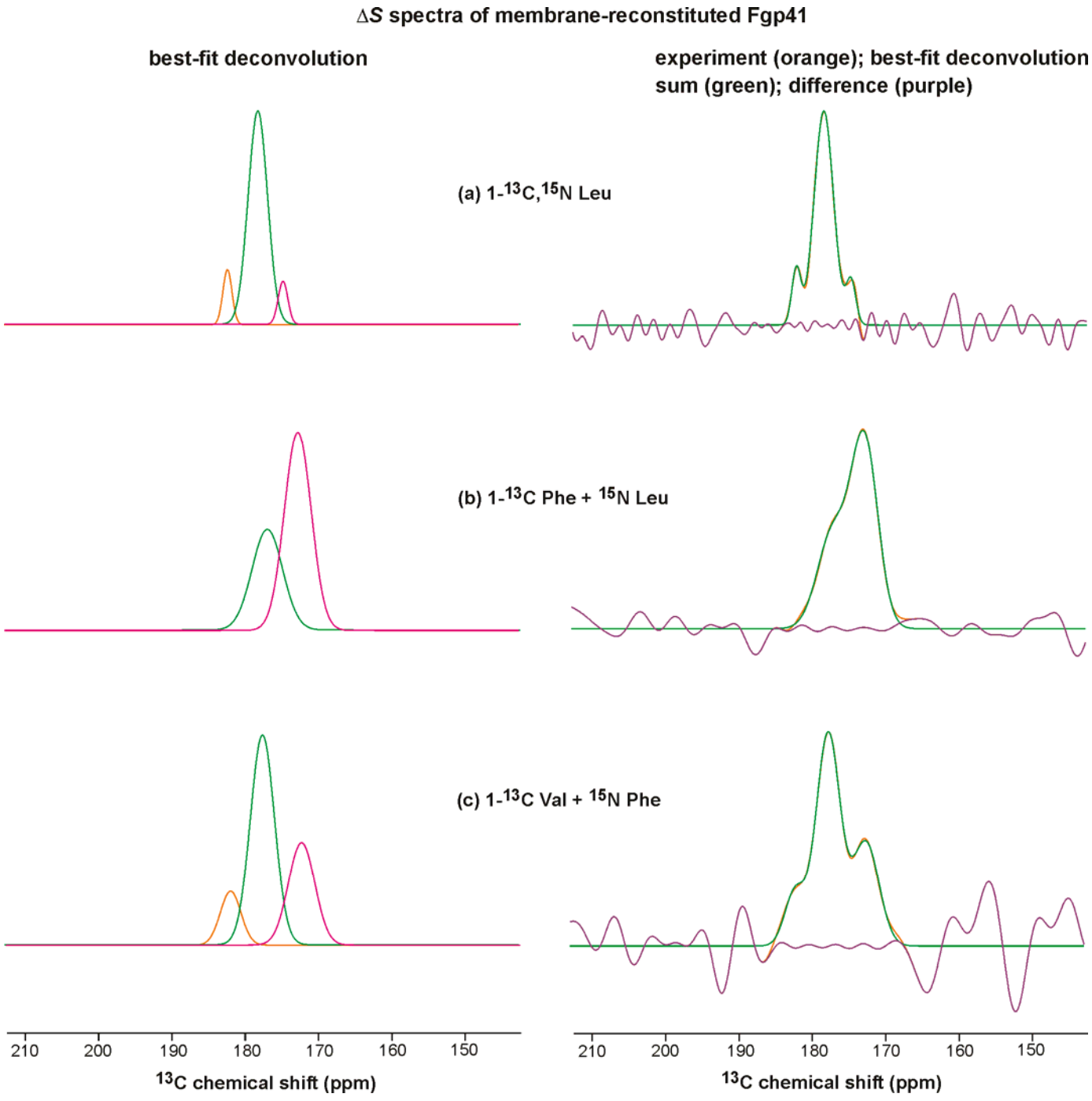


SDS-PAGE of soluble cell lysates produced using buffers with different [SDS].

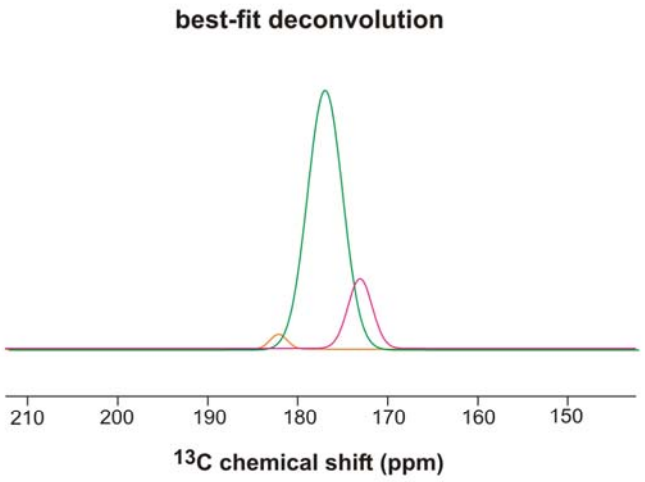


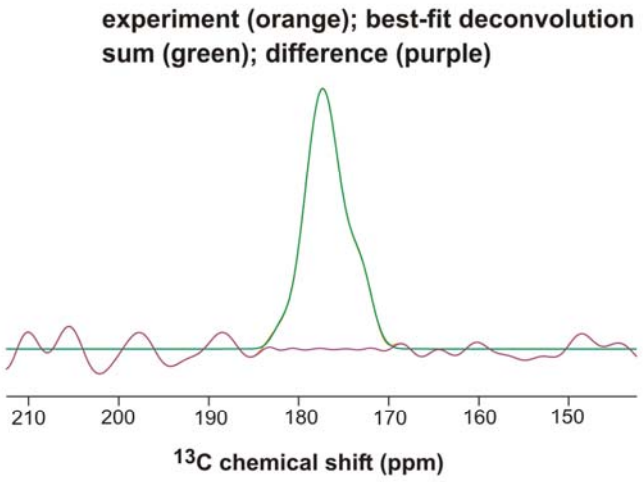

ΔS spectrum of lyophilized cells labeled with 1-13C, 15N Leu
ΔS spectrum of membrane-reconstituted Fgp41 labeled with 1-13C, 15N Leu
250
200
150
100
50
0
13C chemical shift (ppm)


S0 spectra of membrane-reconstituted Fgp41
experiment (orange); best-fit deconvolution sum (green); difference (purple)
(a) 1-13C,15N Leu
(b) 1-13C Phe + 15N Leu
(c) 1-13C Val + 15N Phe
(d) 1-13C Val + 15N Gly
185
175
165
13C chemical shift (ppm)


ΔS spectra of membrane-reconstituted Fgp41
best-fit deconvolution
experiment (orange); best-fit deconvolution sum (green); difference (purple)
(a) 1-13C,15N Leu
(b) 1-13C Phe + 15N Leu
(c) 1-13C Val + 15N Phe
210
200
190
180
170
160
150
13C chemical shift (ppm)

Analysis of ΔS spectrum of lyophilized cells labeled with 1-^{13}C, ^{15}N Leu





Analysis of S_0 spectrum from difference data between lyophilized cells with 1-^{13}C, ^{15}N Leu and cells with unlabeled Leu