Supporting Information

Absolute Minimal Sampling in High Dimensional NMR Spectroscopy

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Materials and Methods

The absolute minimal sampling (AMS) method was applied to the 8.5 kDa (76 amino-acids) protein ubiquitin and the 42 kDa enzyme arginine kinase (AK) [1-2]. Both proteins were uniformly ^{13}C,^{15}N labeled in 90%/10% H_2O/D_2O solution with final concentrations of ca. 1 mM protein. Standard Bruker pulse sequences were used for the acquisition of the 3D datasets. The ubiquitin data was recorded using the `trhncoetgp3d` sequence on a Bruker Avance III HD 600 MHz spectrometer equipped with a with a 5mm TXI Cryoprobe and the following parameters:

Table S1. Parameters used for Ubiquitin HNCO data acquisition

UBQ HNCO	^{1}H	^{13}C	^{15}N
Carrier	4.77 ppm	175.7 ppm	117.6 ppm
Sweep width	16.0 ppm	16.0 ppm	35.2 ppm
Dwell time	104.0 us	413.4 us	466.8 us
Complex points	1024	40	32

The arginine kinase data was recorded using the `trhncogp2h3d` (HNCO) and `trhncacogp2h3d` (HNCACO) sequences, with only minor modifications. Experiments were carried out on a Bruker Avance II 800 MHz spectrometer equipped with a with a 5mm TCI Cryoprobe and the following parameters:

Table S2. Parameters used for Arginine kinase HNCO and HNCACO data acquisition

AK HNCO/HNCACO	^{1}H	^{13}C	^{15}N
Carrier	4.77 ppm	175.7 ppm	118.1 ppm
Sweep width	20.0 ppm	14.0 ppm	40.0 ppm
Dwell time	104.0 us	308.0 us	354.0 us
Complex points	1024	44	55

The NMR raw data were first processed using the NMRPipe suite of programs [3] and SPARKY [4-5]. Conventional protocols were applied for the processing of the full 3D datasets. For AMS analysis, only the 2nd and 3rd dimensions were Fourier transformed (^{15}N and ^{1}H) leaving the first (^{13}C) dimension in the time-domain. In all datasets, the first complex point was acquired with zero delay in t_1. A peak list was generated from the first 2D plane and used as input for nonlinear least-squares fitting of the remaining 2D planes to extract peak intensities. Peak fitting was accomplished using the NMRPipe functions nlinLS and seriesTab using the same minimally sampled HNCO and HN(CA)CO datasets used for subsequent application of the AMS approach based on the arctan (Eq. (1) of the main text) and the non-linear least squares fitting (Eq. (3) of main text).

^{13}C resonance frequencies were determined from the minimally sampled cosine and sine modulated datasets along the t_1 domain, $C_{exp}(t_1)$ and $S_{exp}(t_1)$, with in-house Matlab programs either using the arctan relationship of Eq. (1) or by a non-linear least squares fit based on Eq. (3) that minimizes the function:

$$\chi^2 = \sum_{n=0}^{N-1} \sum_{k=1}^{M} (A_k \exp(-R_2 n\Delta t_1)\cos(\omega_{C,k} n\Delta t_1) - C_{\exp}(n\Delta t_1))^2 + (A_k \exp(-R_2 n\Delta t_1)\sin(\omega_{C,k} n\Delta t_1) - S_{\exp}(n\Delta t_1))^2 \quad \text{(S1)}$$

where M (= 1, 2, 3, or 4) is the number of resonances with angular frequencies $\omega_{C,k}$ and amplitudes A_k and R_2 was set to a uniform value for all residues in the protein, which was either zero or $R_2 = 20\ s^{-1}$ for ubiquitin and $R_2 = 75\ s^{-1}$ for arginine kinase. The 2M fit parameters are the M frequencies $\omega_{C,k}$ and M amplitudes A_k. The angular frequencies $\omega_{C,k}$ were allowed to vary freely within the spectral range given by the spectral width, i.e. between $-\pi/\Delta t_1$ and $+\pi/\Delta t_1$, and the amplitudes were allowed to take any positive value or zero. Initial frequencies were randomly and uniformly chosen within the above frequency range defined by the spectral width. For each ^{15}N,^{1}H frequency pair, which was defined by the center of the ^{15}N,^{1}H HSQC cross-peak in the ω_2(^{15}N)-ω_3(^{1}H) plane, 25 independent optimizations were performed with randomly selected initial values for the 2M fit parameters and the one with the lowest χ^2 was selected as the best fit.

Residue-by-residue comparison of results from AMS with full-size 3D spectrum

Traces along the carbonyl ^{13}C dimension of individual residues are plotted below in individual panels together with best fitting results. The blue lines refer to the $^{13}C'$ chemical shifts determined using the inverse tangent of a single complex increment (Eq. (1)) and the red lines to the chemical shifts obtained by non-linear least squares fitting to 4 complex increments along the $^{13}C'$ dimension using the expression of Eq. (3). The heights of the red lines reflect the fitted peak amplitudes A_k of Eq. (3). The dashed red lines correspond to minor peaks determined by AMS. Minor peaks with amplitudes smaller than 10% (ubiquitin) or 20% (arginine kinase) of the major peaks are not shown.

References

[1] O. Davulcu, P. F. Flynn, M. S. Chapman, and J. J. Skalicky, *Structure* **2009**, *17*, 1356.
X. Niu, L. Bruschweiler-Li, O. Davulcu, J. J. Skalicky, R. Brüschweiler, and M. S. Chapman, *J. Mol. Biol.* **2011**, *405*, 479.

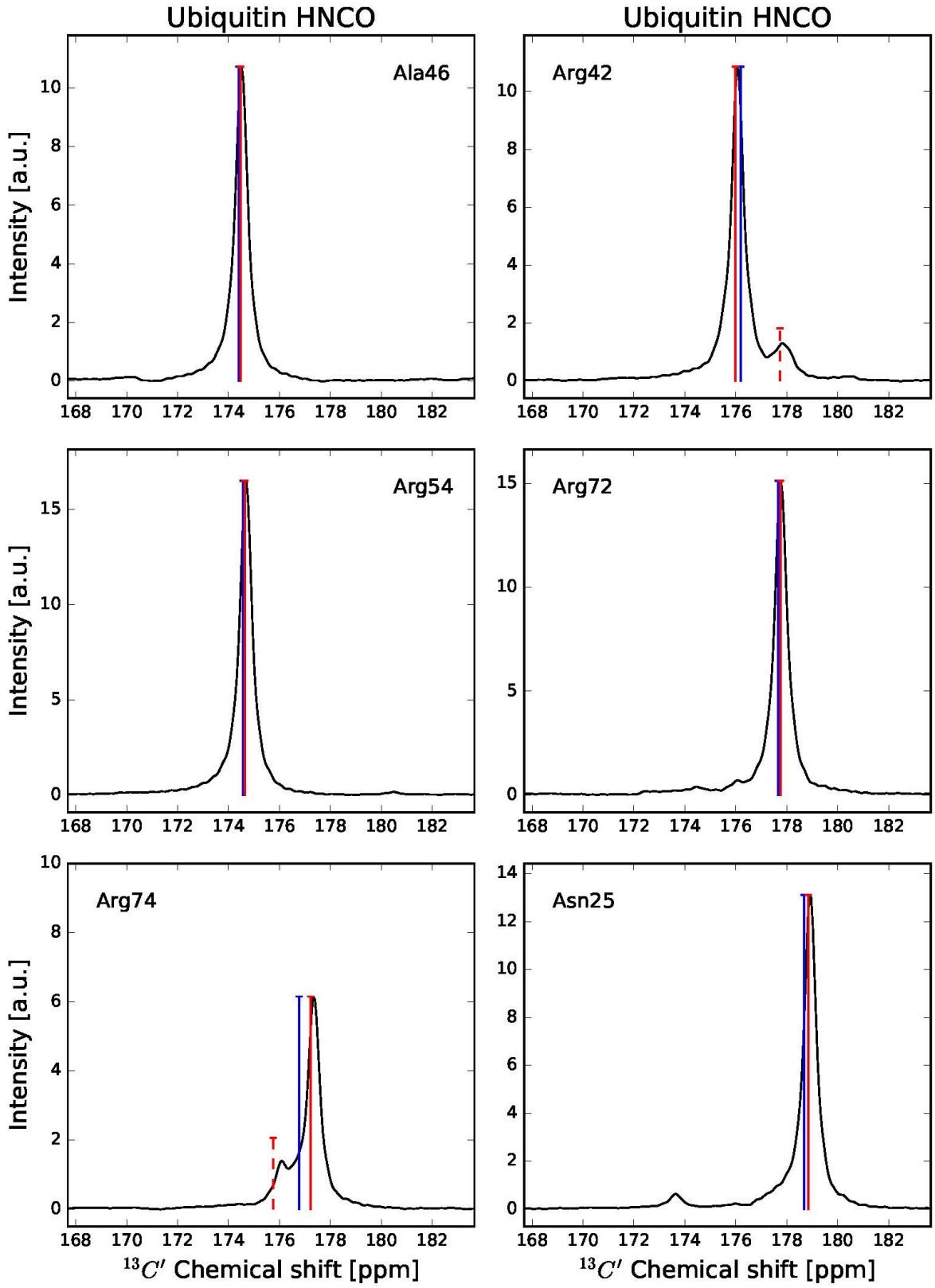
[2] O. Davulcu, X. Niu, L. Bruschweiler-Li, R. Brüschweiler, J. J. Skalicky, and M. S. Chapman *Biomol. NMR Assign.* **2014**, *8*, 335.

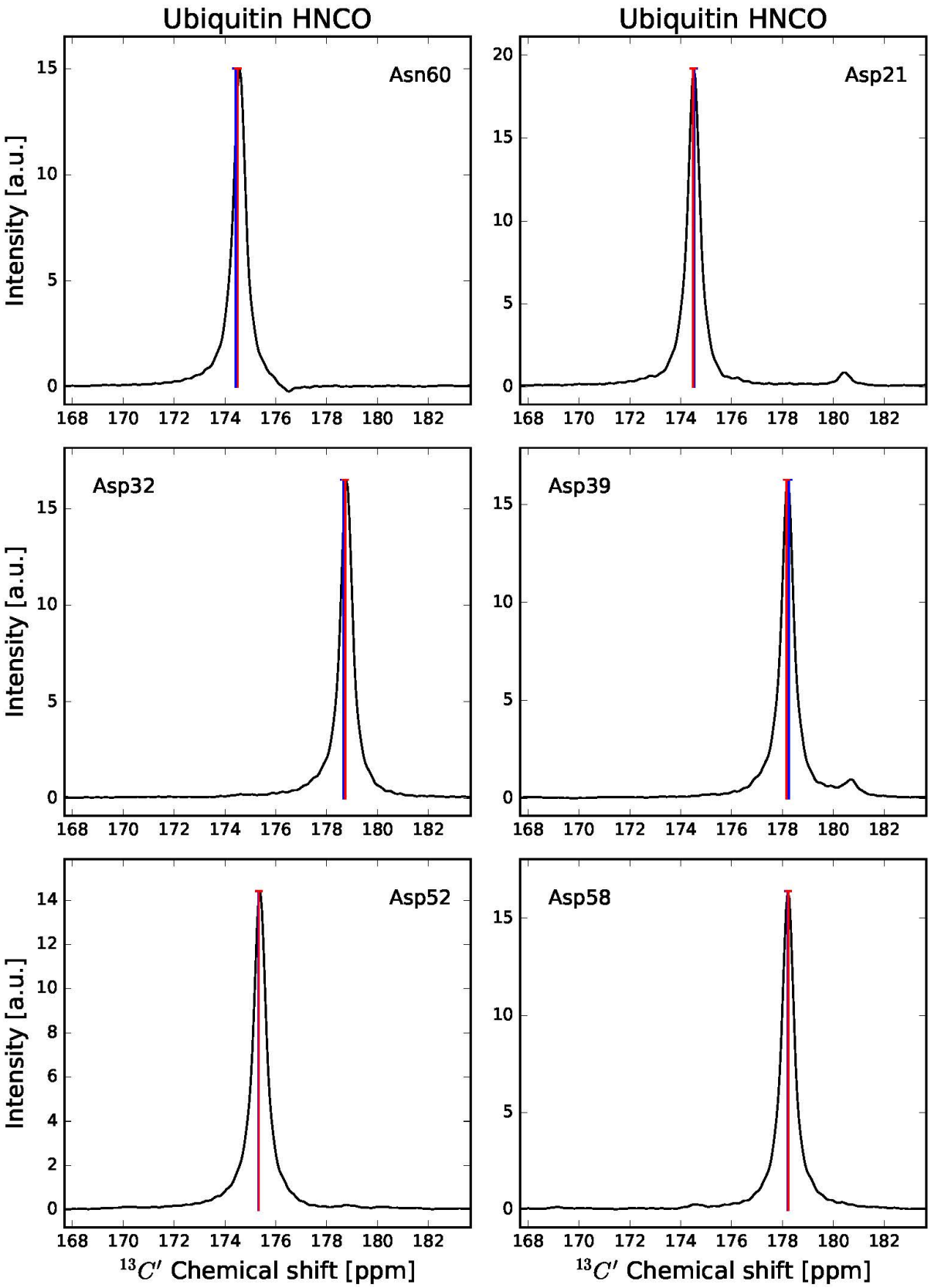
[3] F. Delaglio, S. Grzesiek, G. W. Vuister, G. Zhu, J. Pfeifer, and A. Bax, *J. Biomol. NMR* **1995**, *6*, 277.

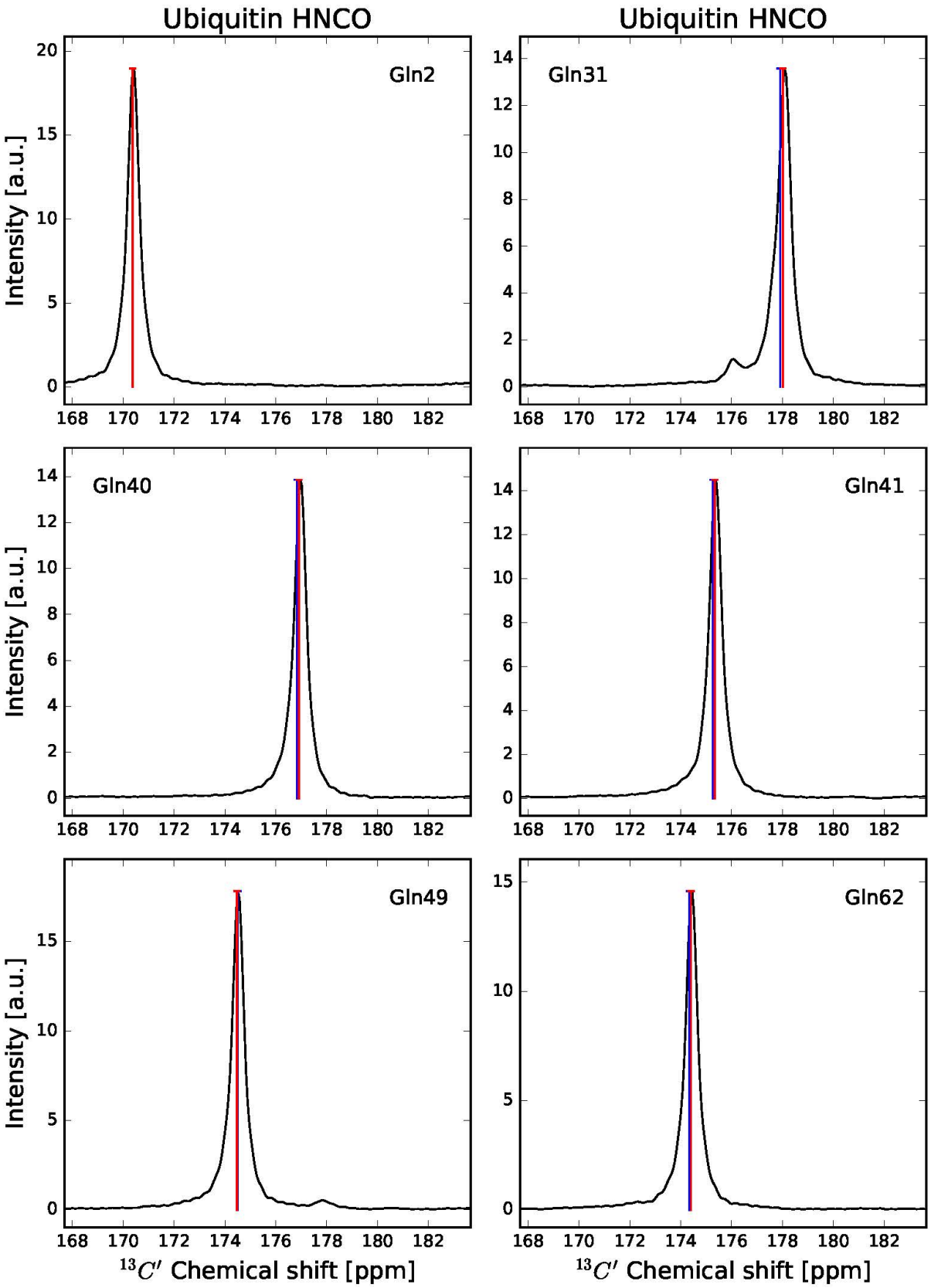
[4] T. D. Goddard and D. G. Kneller, SPARKY 3, University of California, San Francisco

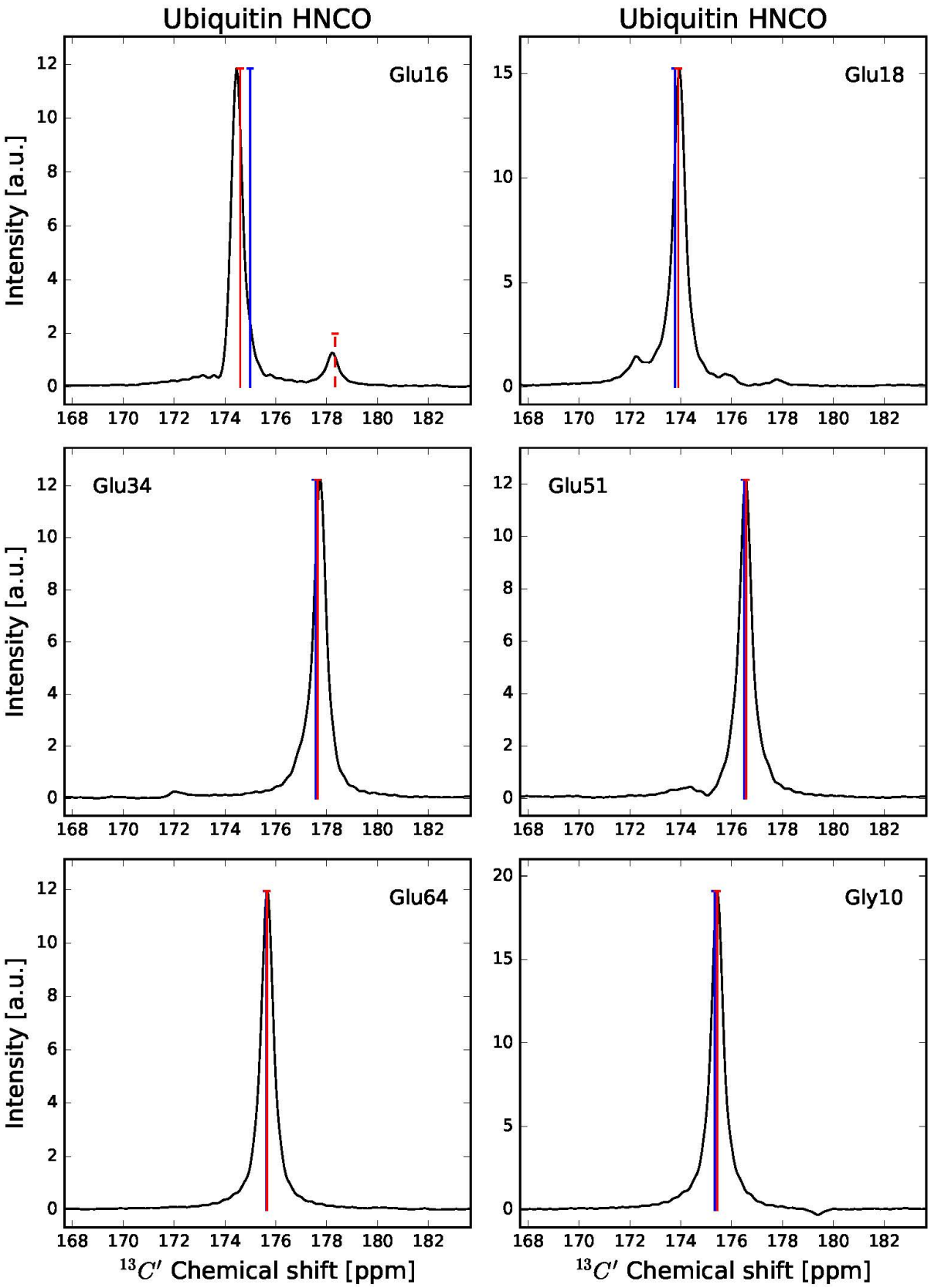
[5] W. Lee, M. Tonelli, and J. L. Markley, *Bioinformatics* **2015**, *31*, 1325.

Figure S1. ^{13}C' traces for ubiquitin HNCO data. FT (black) was performed on 40 complex points, while AMS (red) used 4 points. In blue are the arctan results on the first complex point.




Ubiquitin HNCO
Ubiquitin HNCO
Asn60
Asp21
Asp32
Asp39
Asp52
Asp58
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]


Ubiquitin HNCO
Ubiquitin HNCO
Gln2
Gln31
Gln40
Gln41
Gln49
Gln62
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]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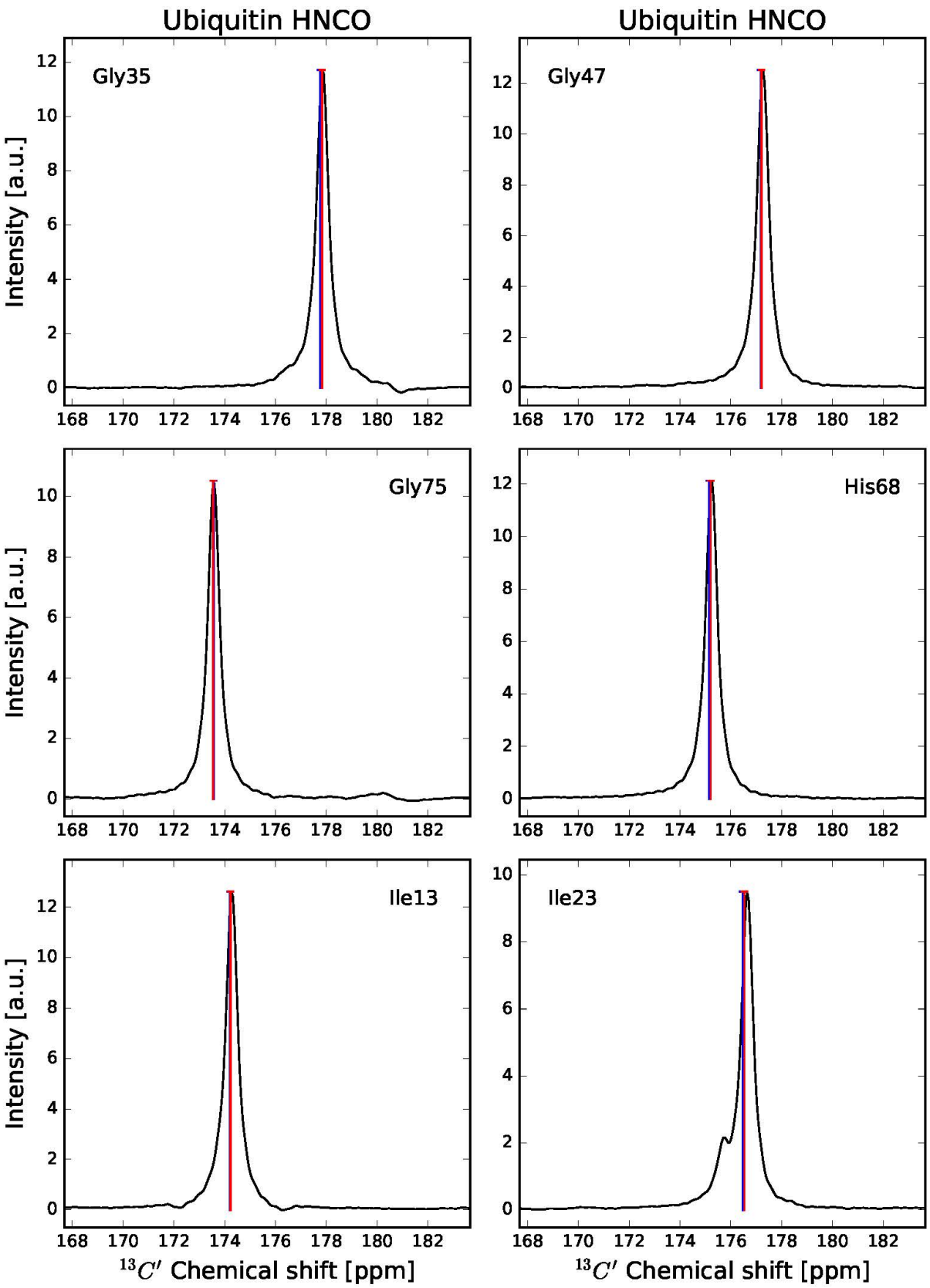
Ubiquitin HNCO
Glu16
Glu18
Glu34
Glu51
Glu64
Gly10
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]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Ubiquitin HNCO
Gly35
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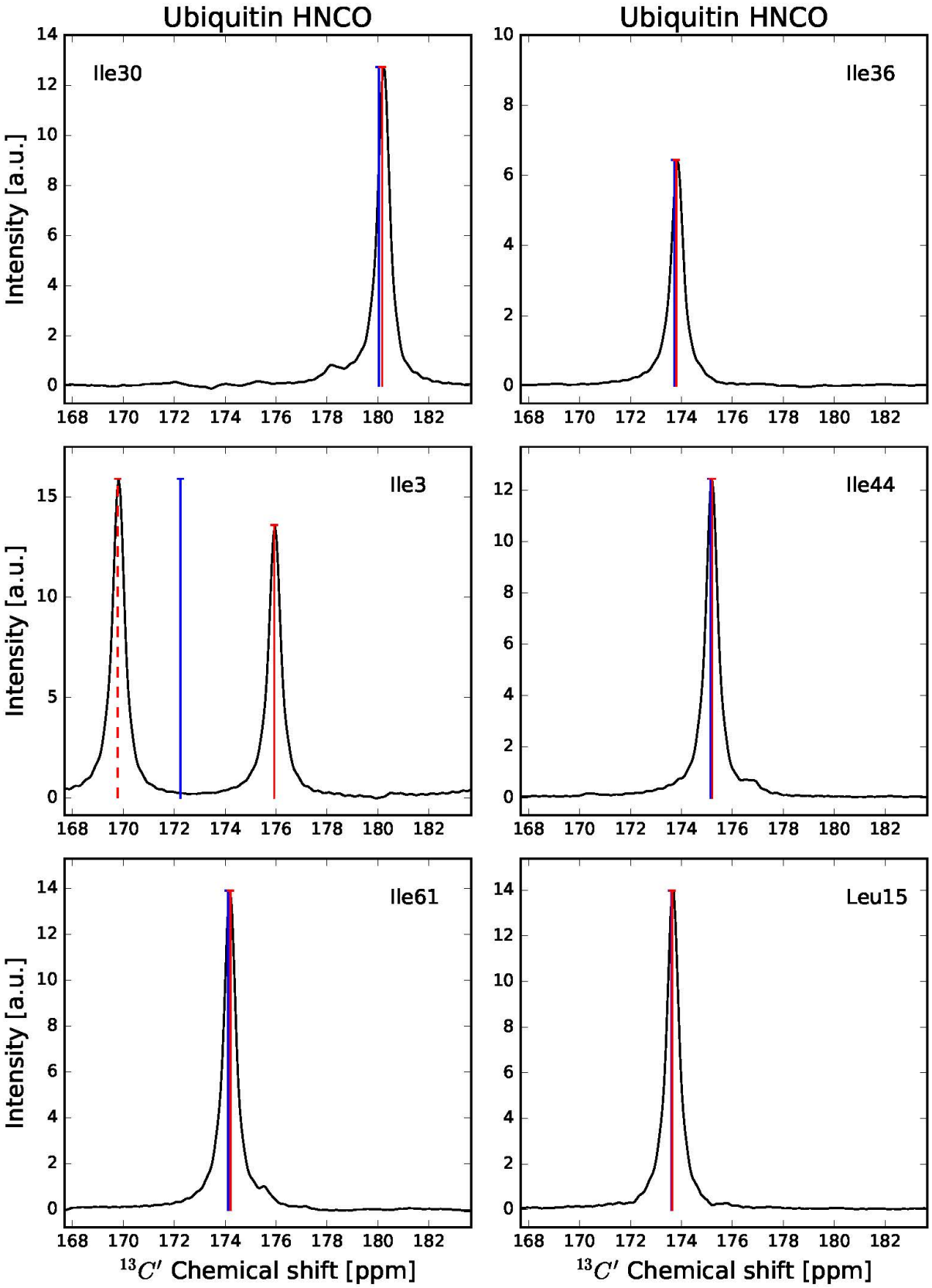
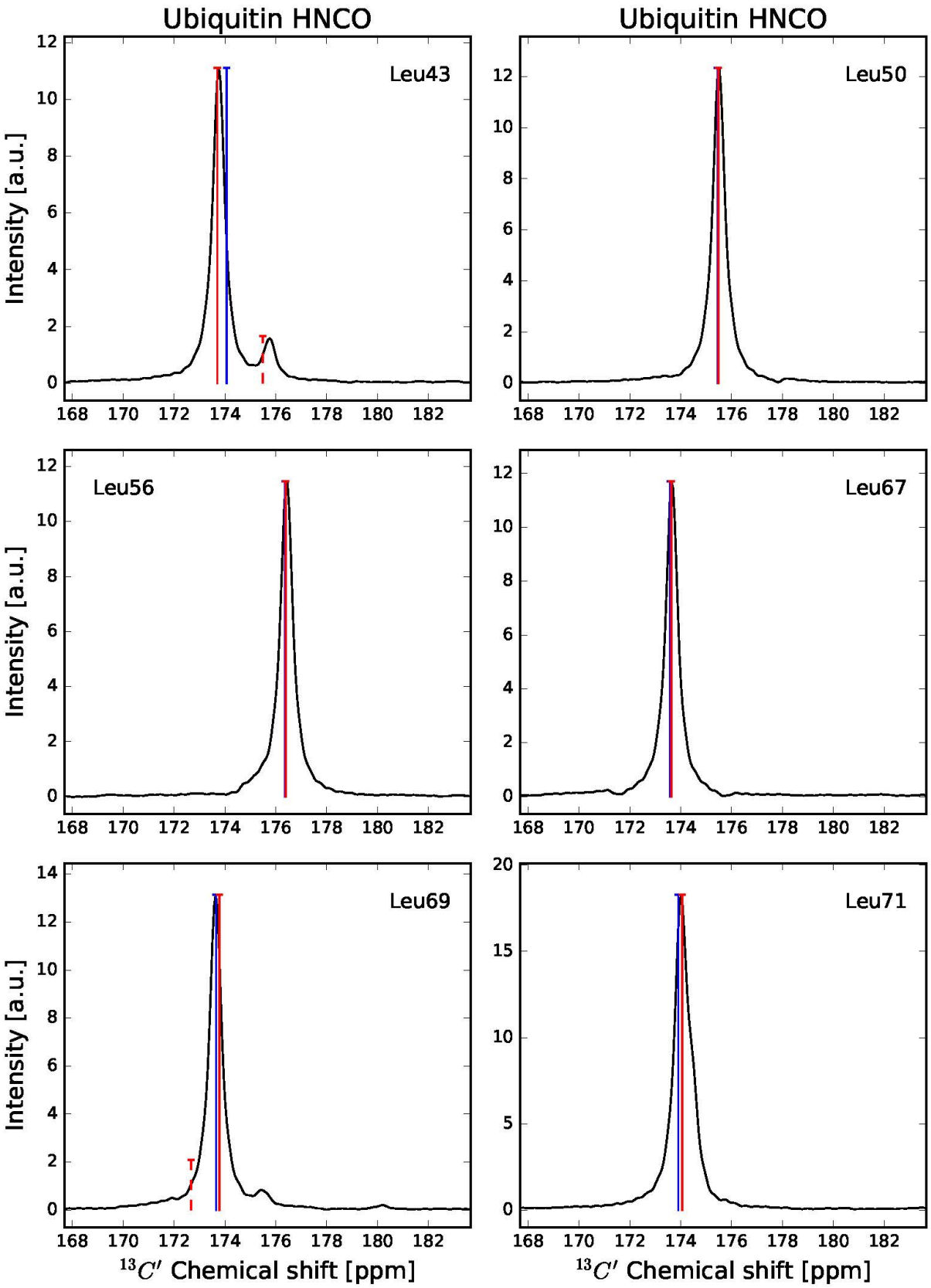
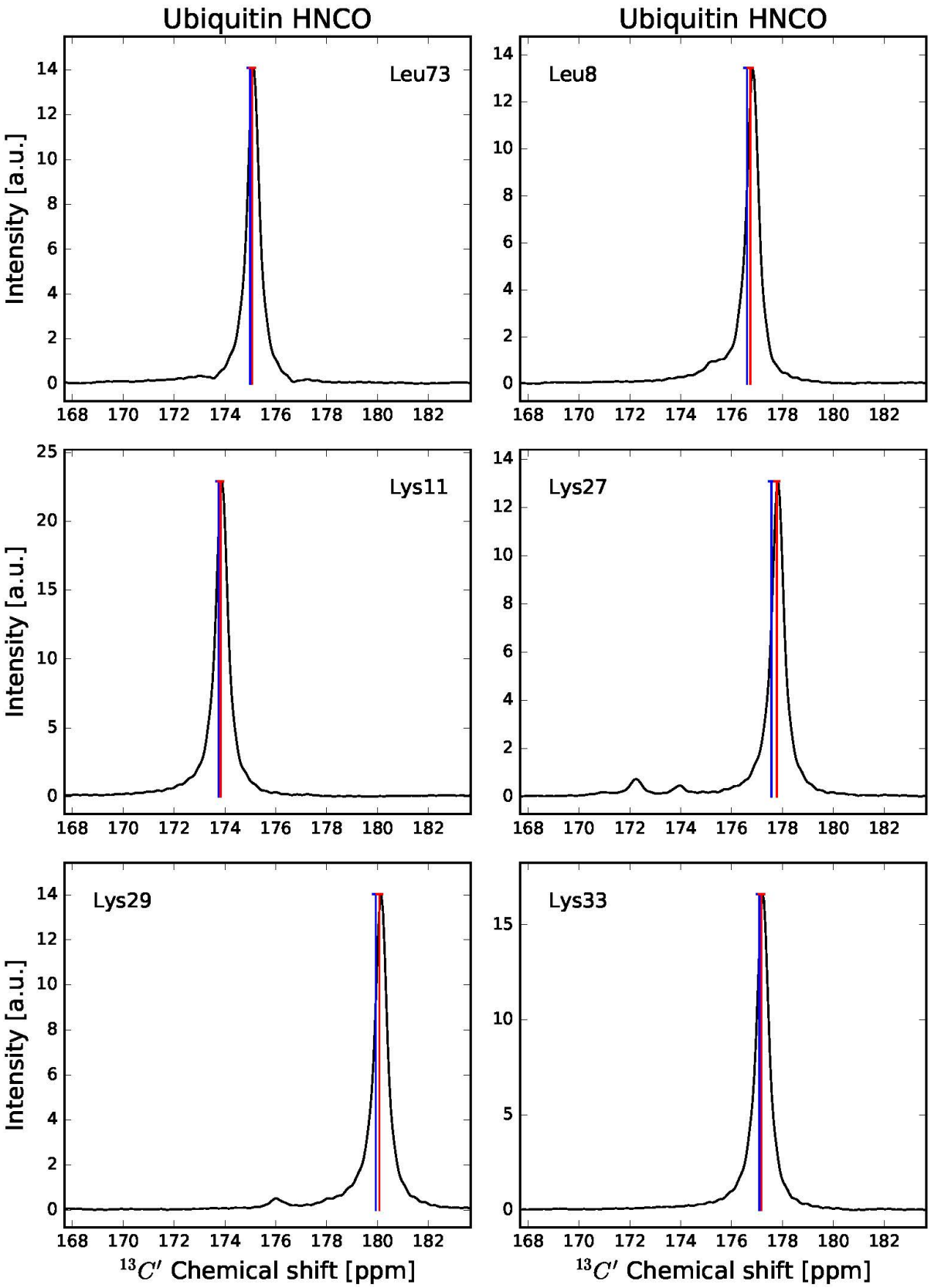
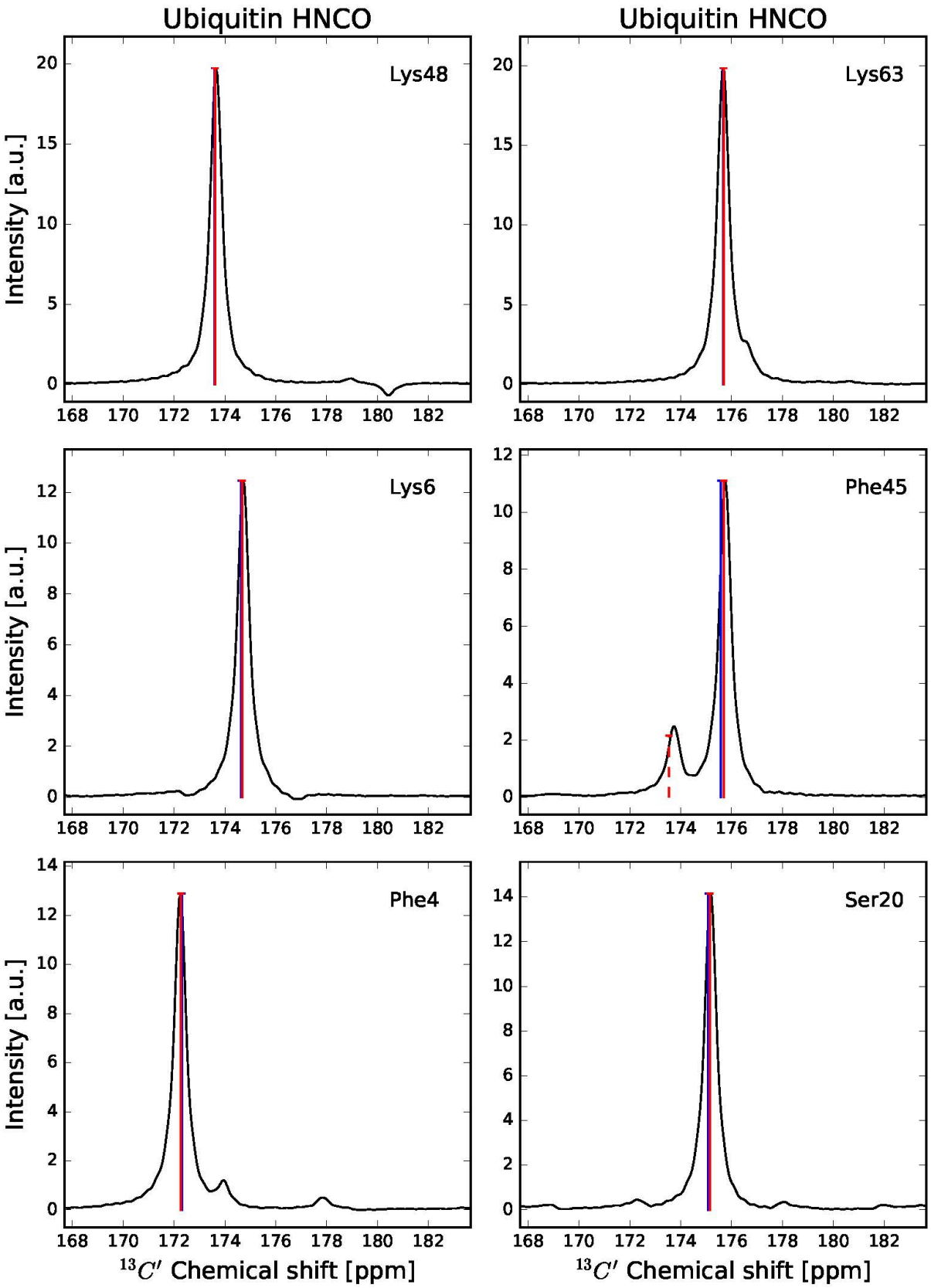
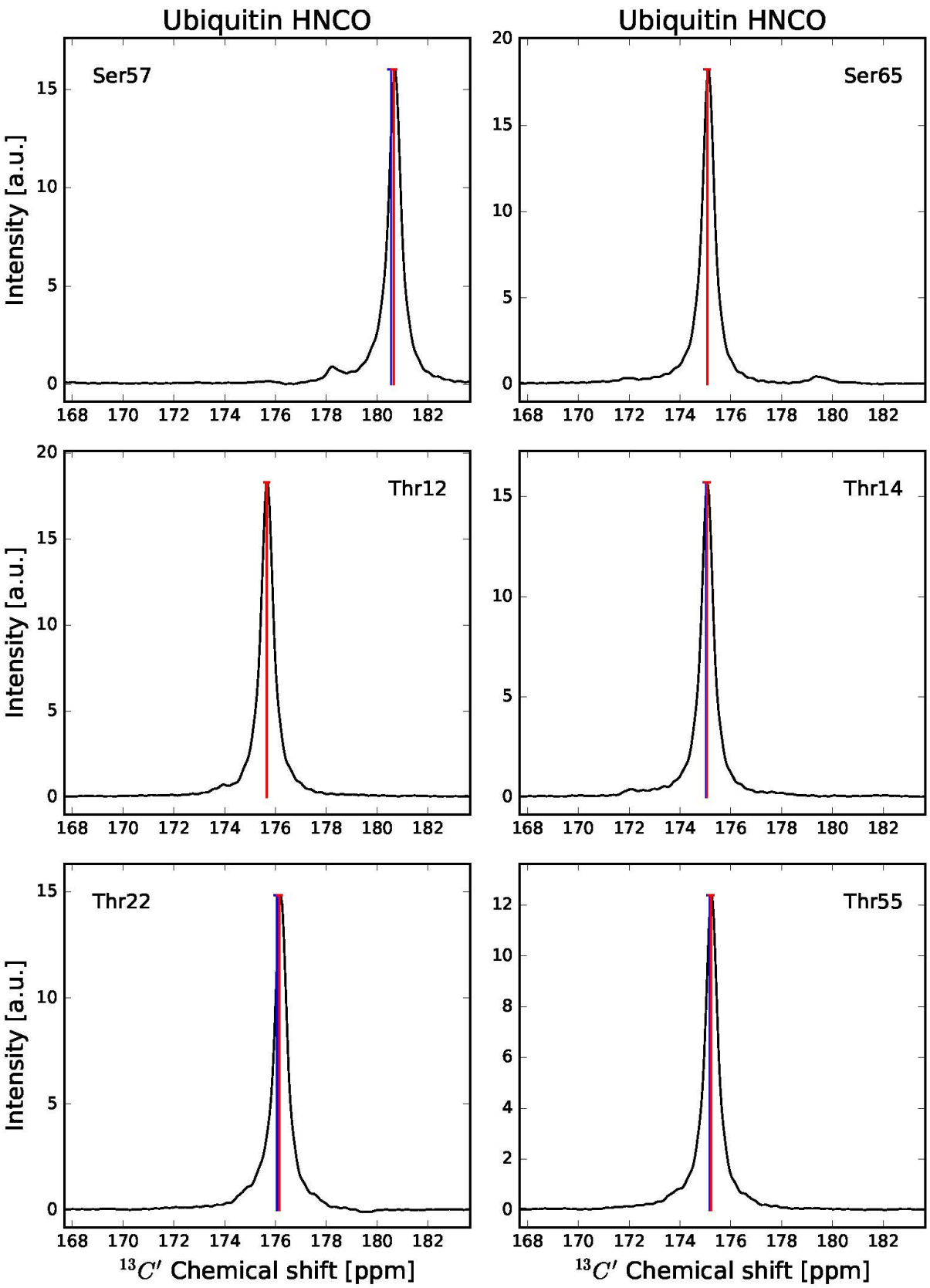
Gly75
His68
Ile13
Ile23
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]

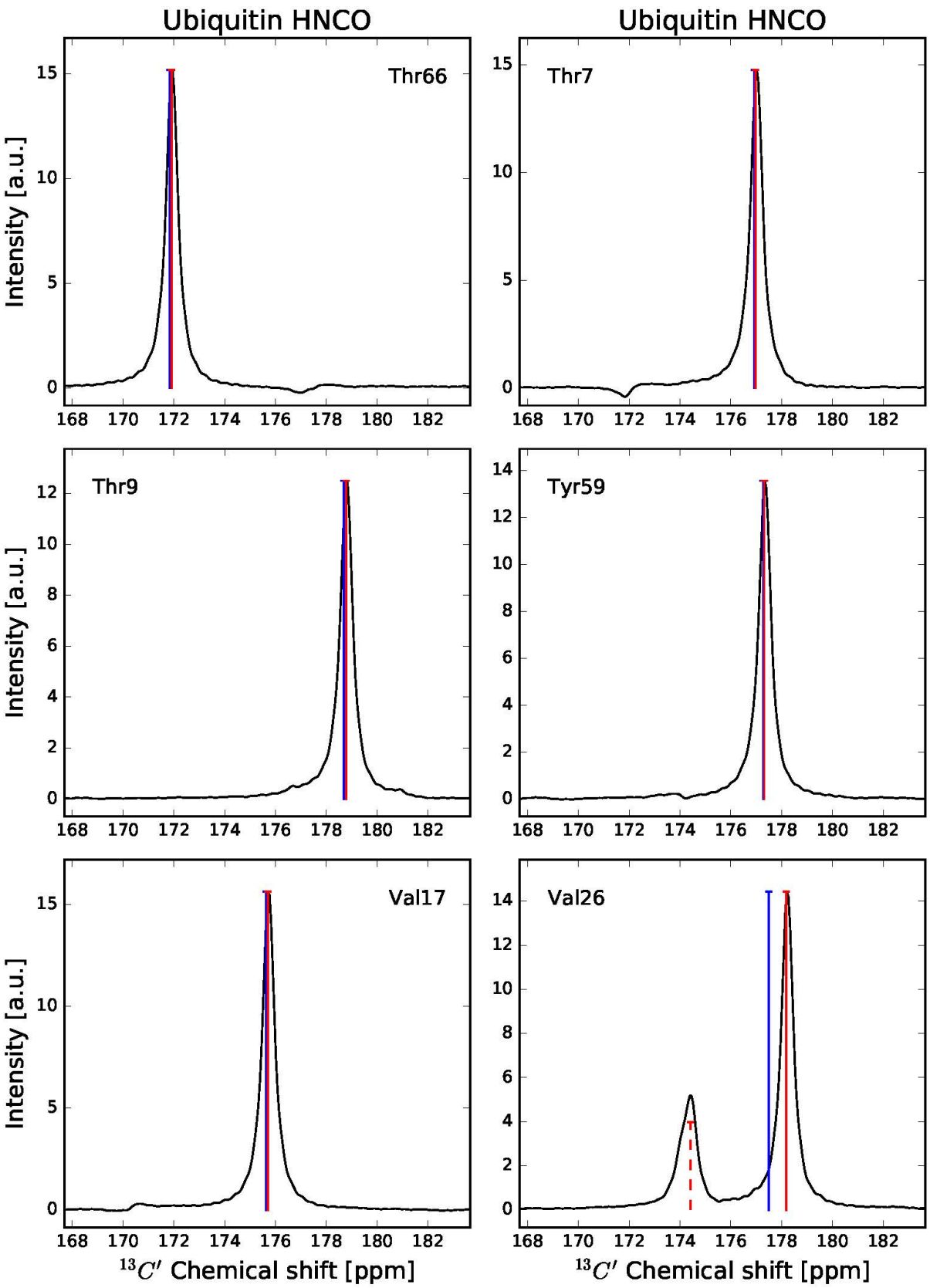

Ubiquitin HNCO
Ile30
Ubiquitin HNCO
Ile36
Ile3
Ile44
Ile61
Leu15
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]


Ubiquitin HNCO
Ubiquitin HNCO
Leu43
Leu50
Leu56
Leu67
Leu69
Leu71
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]


Ubiquitin HNCO
Ubiquitin HNCO
Leu73
Leu8
Lys11
Lys27
Lys29
Lys33
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]


Ubiquitin HNCO
Ubiquitin HNCO
Lys48
Lys63
Lys6
Phe45
Phe4
Ser20
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]


Ubiquitin HNCO
Ubiquitin HNCO
Ser57
Ser65
Thr12
Thr14
Thr22
Thr55
Intensity [a.u.]
Intensity [a.u.]
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]
$^{13}C'$ Chemical shift [ppm]


Ubiquitin HNCO
Ubiquitin HNCO
Thr66
Thr7
Thr9
Tyr59
Val17
Val26
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]

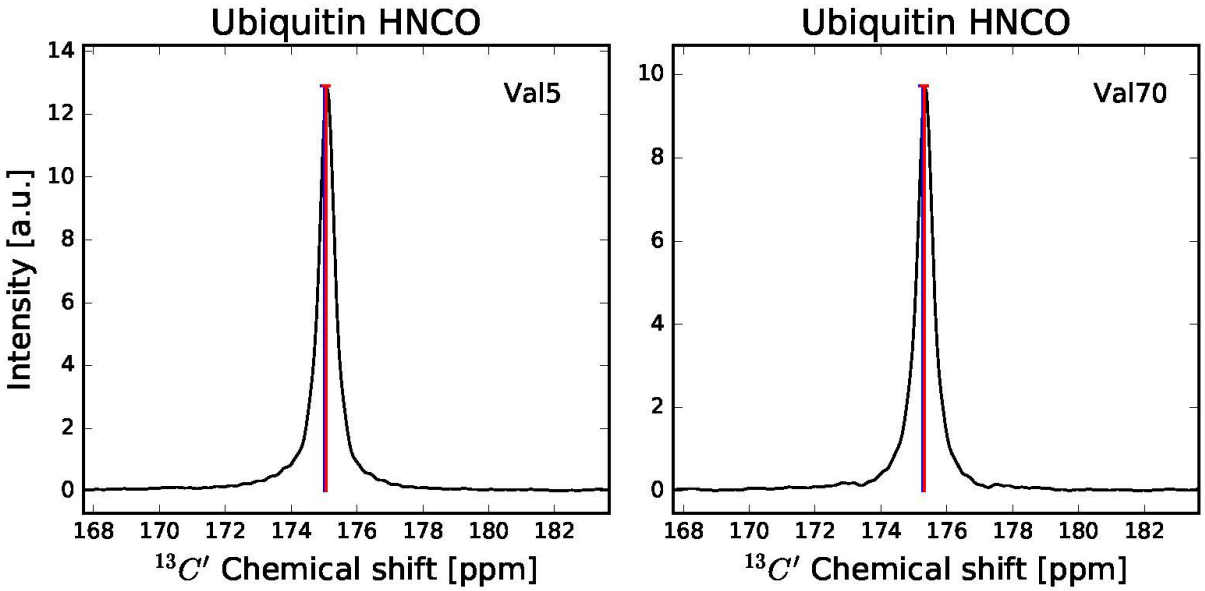
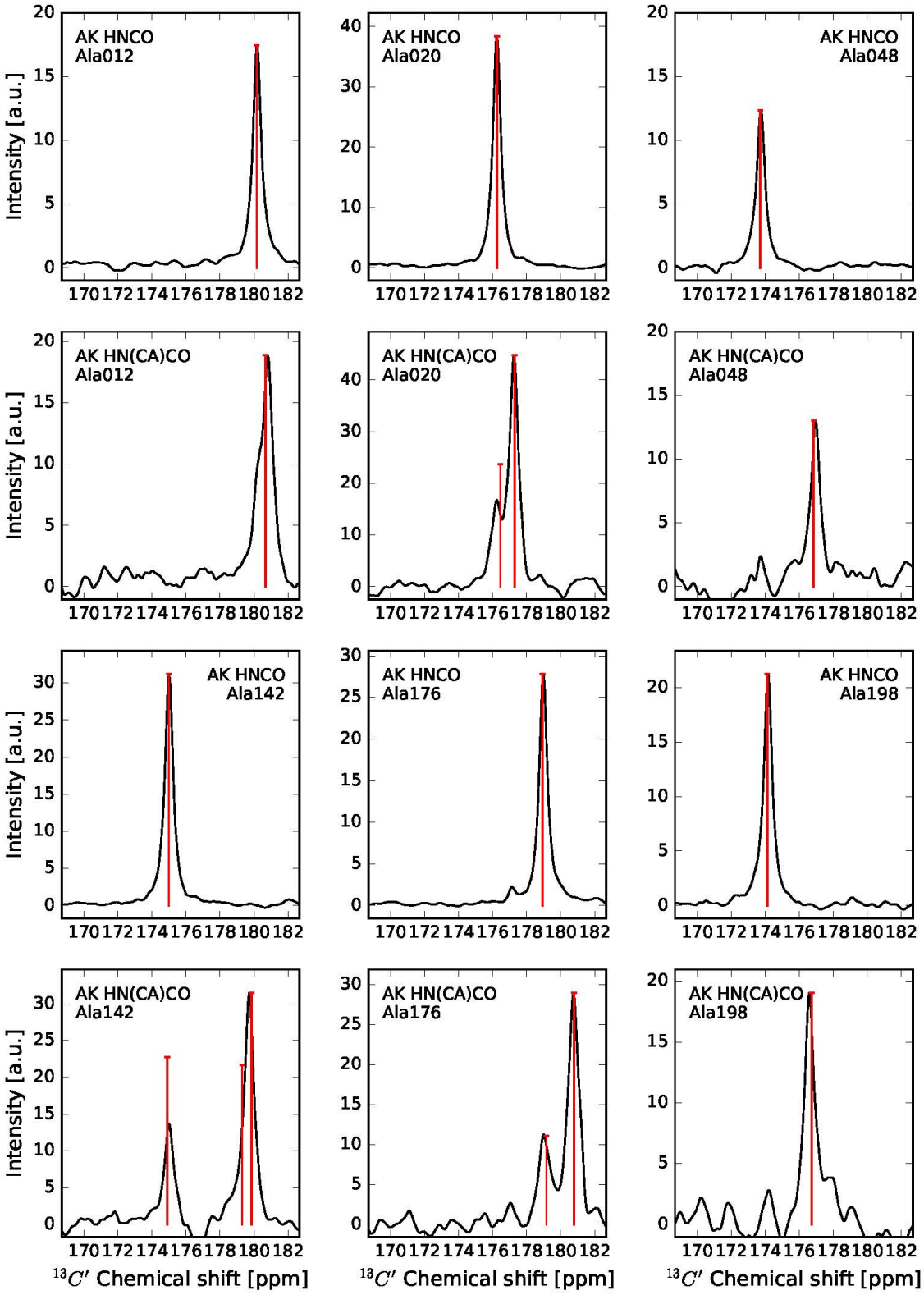
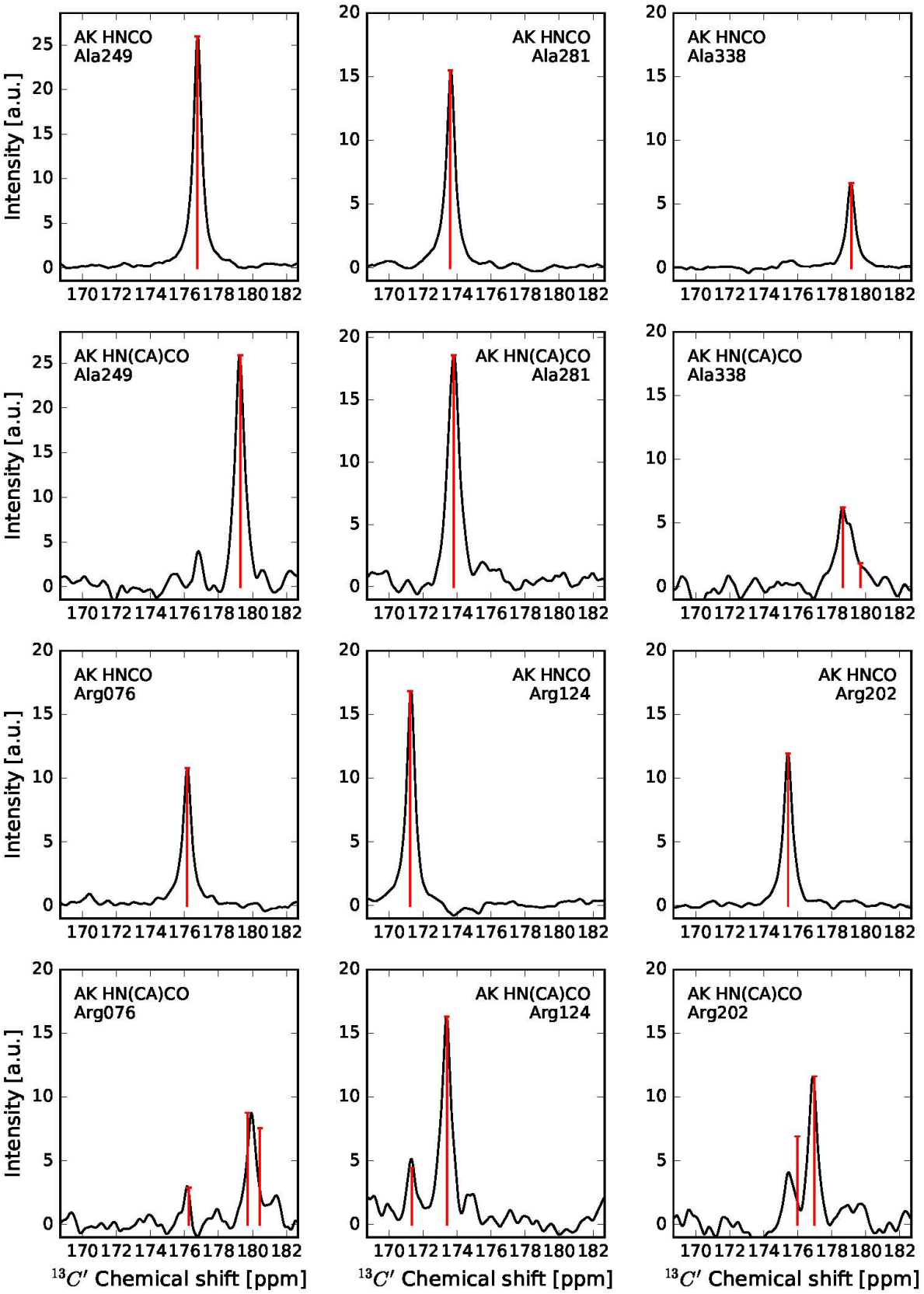

Ubiquitin HNCO
Val5
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]
Ubiquitin HNCO
Val70
$^{13}C'$ Chemical shift [ppm]

Figure S2. ^{13}C' traces for arginine kinase (AK) HNCO & HNCACO data. FT (black) was performed on 40 complex points, while AMS (red) used 4 (6) complex data points for the HNCO (HNCACO).

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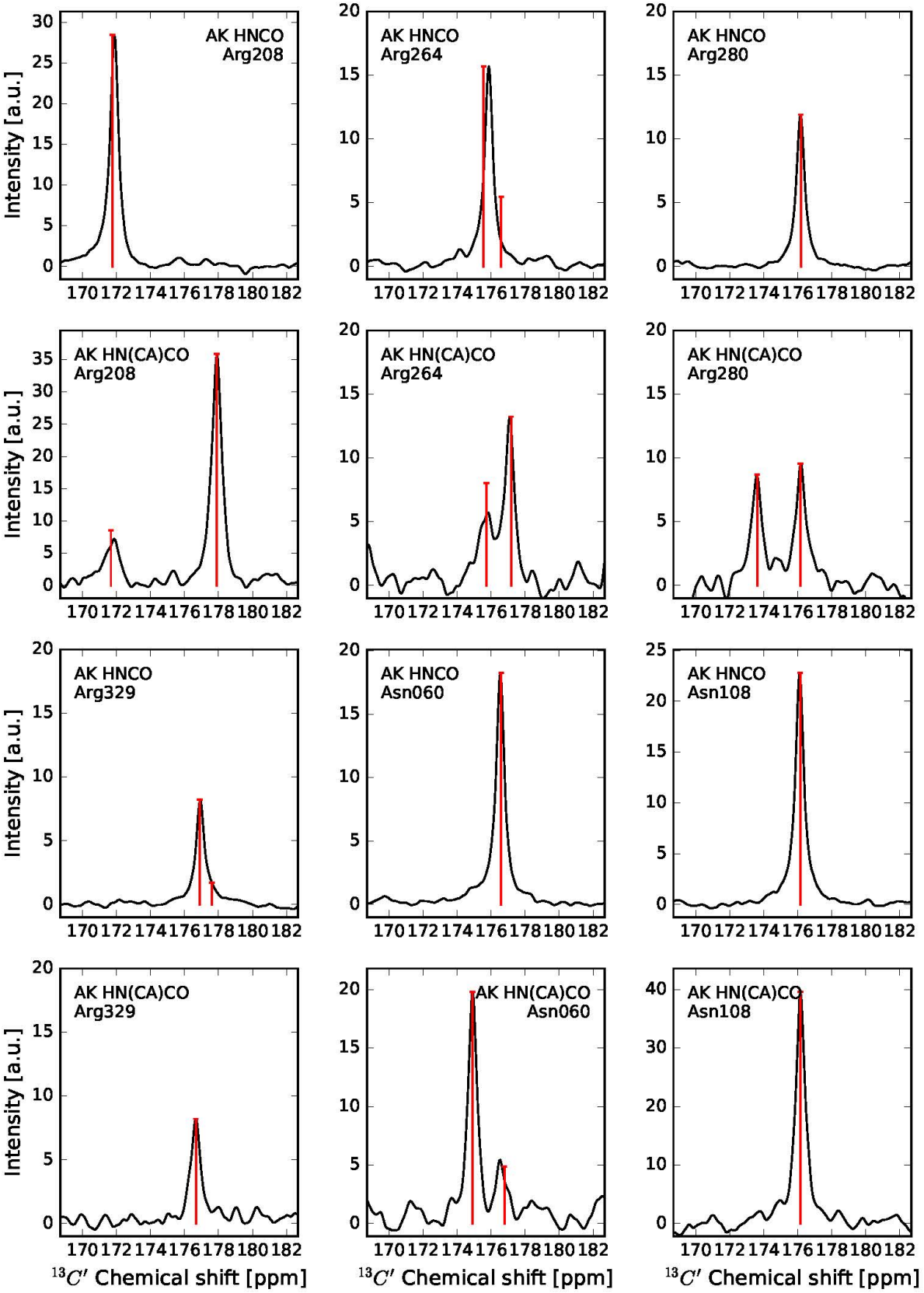
AK HN(CA)CO Arg124
AK HN(CA)CO Arg202
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]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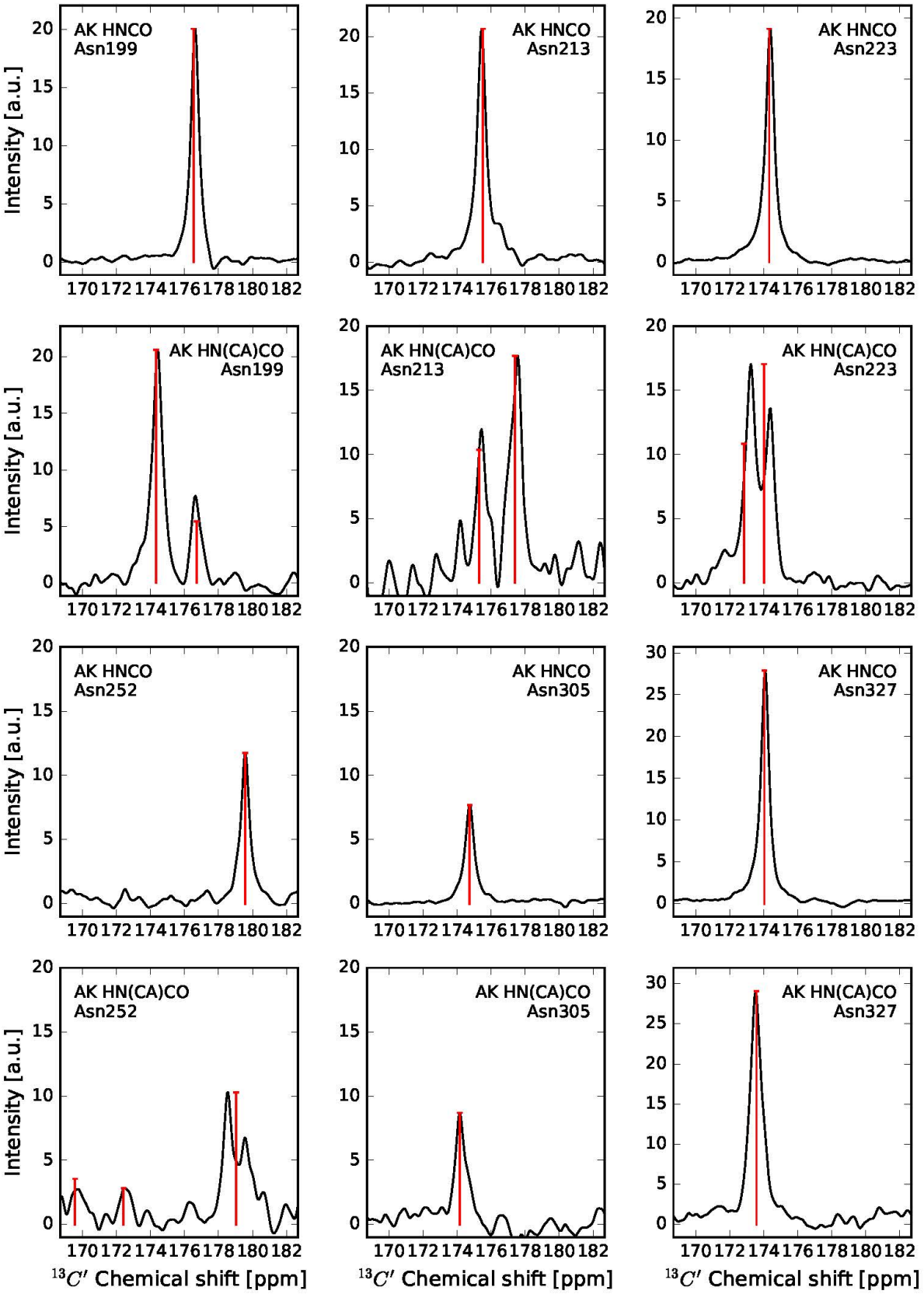
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]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AK HNCO Asn213
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AK HNCO Asn305
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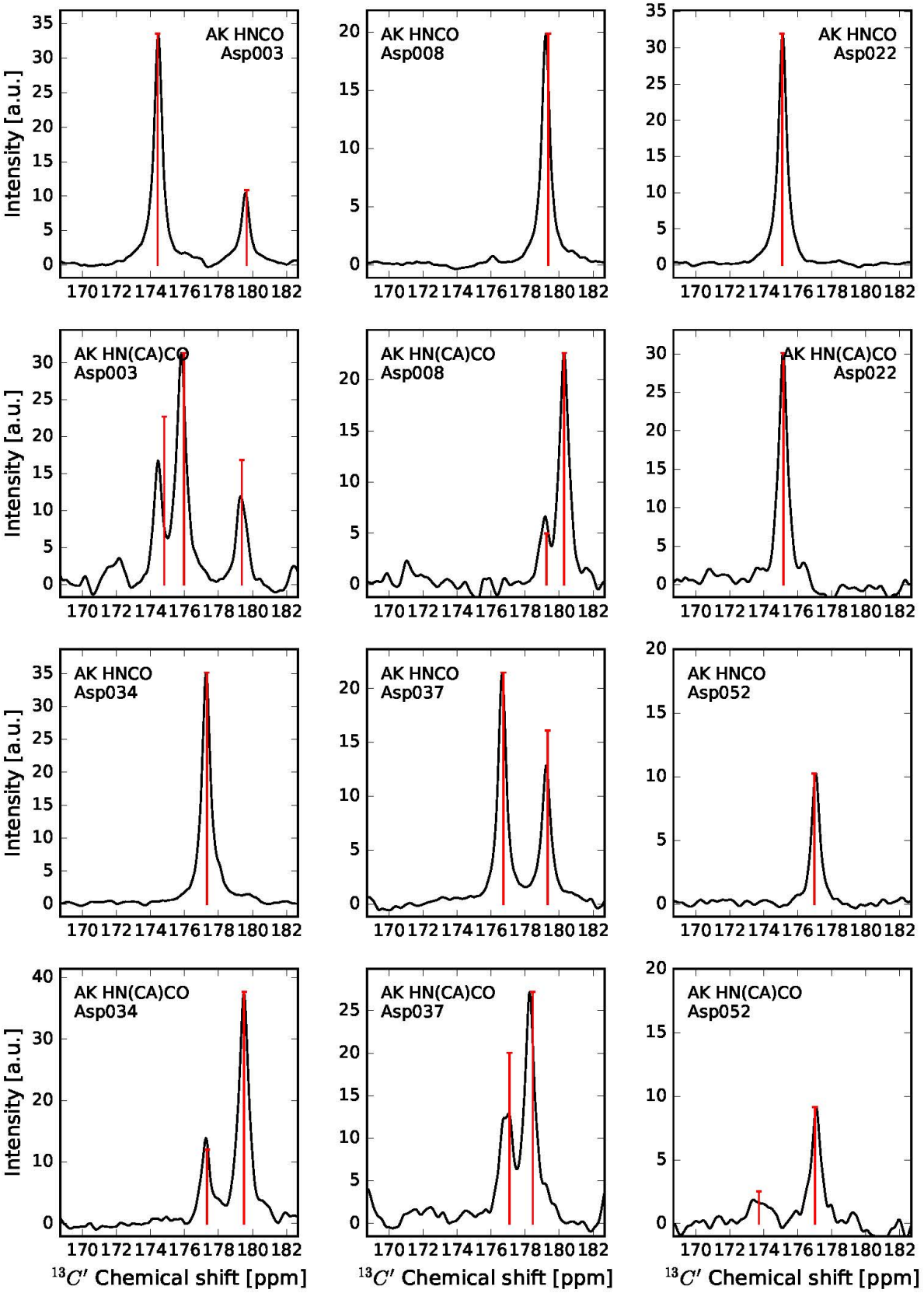
AK HN(CA)CO Asn327
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]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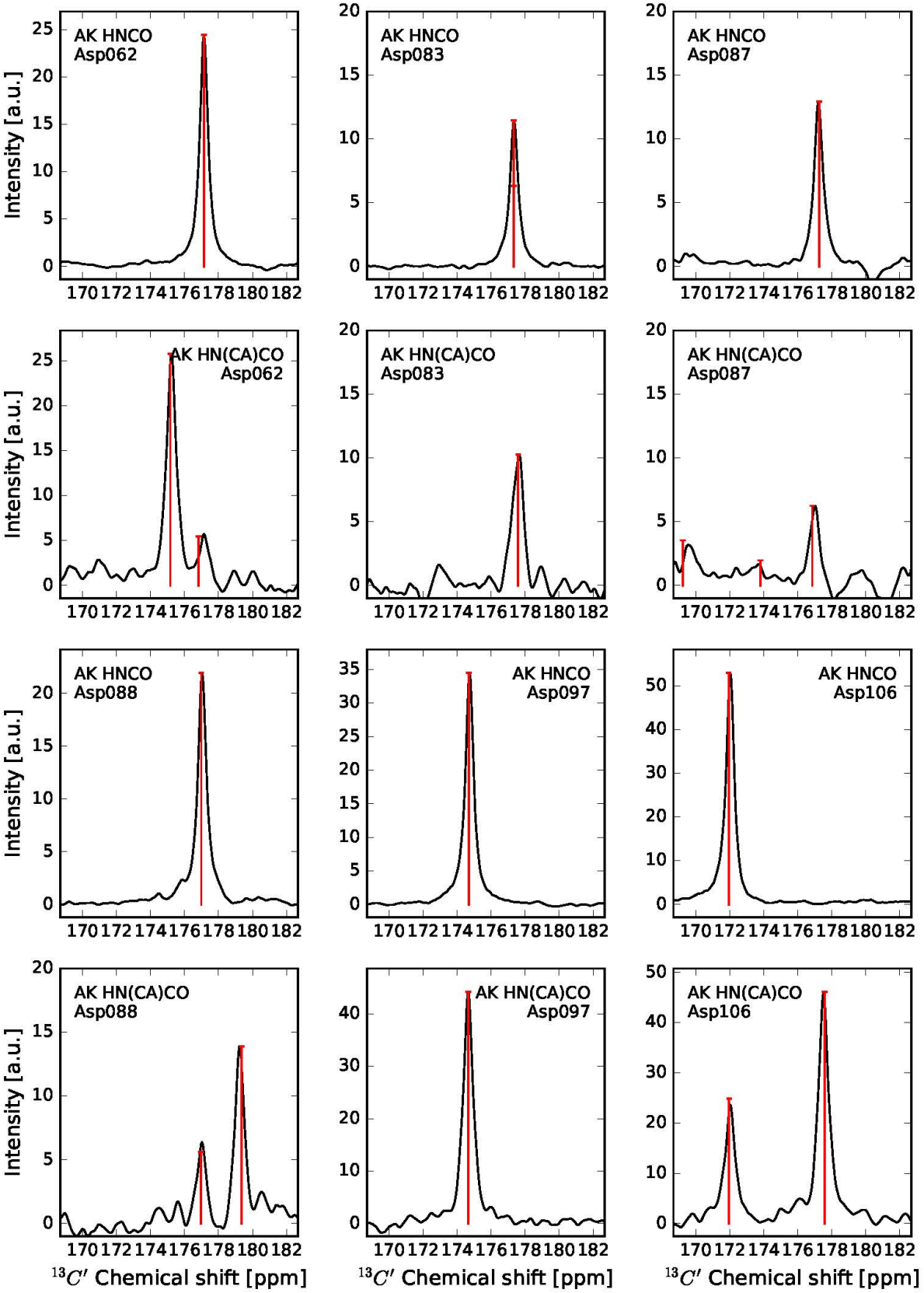
AK HN(CA)CO Asp037
AK HN(CA)CO Asp052
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]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Asp062
AK HNCO
Asp083
AK HNCO
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Asp088
AK HNCO
Asp097
AK HNCO
Asp106
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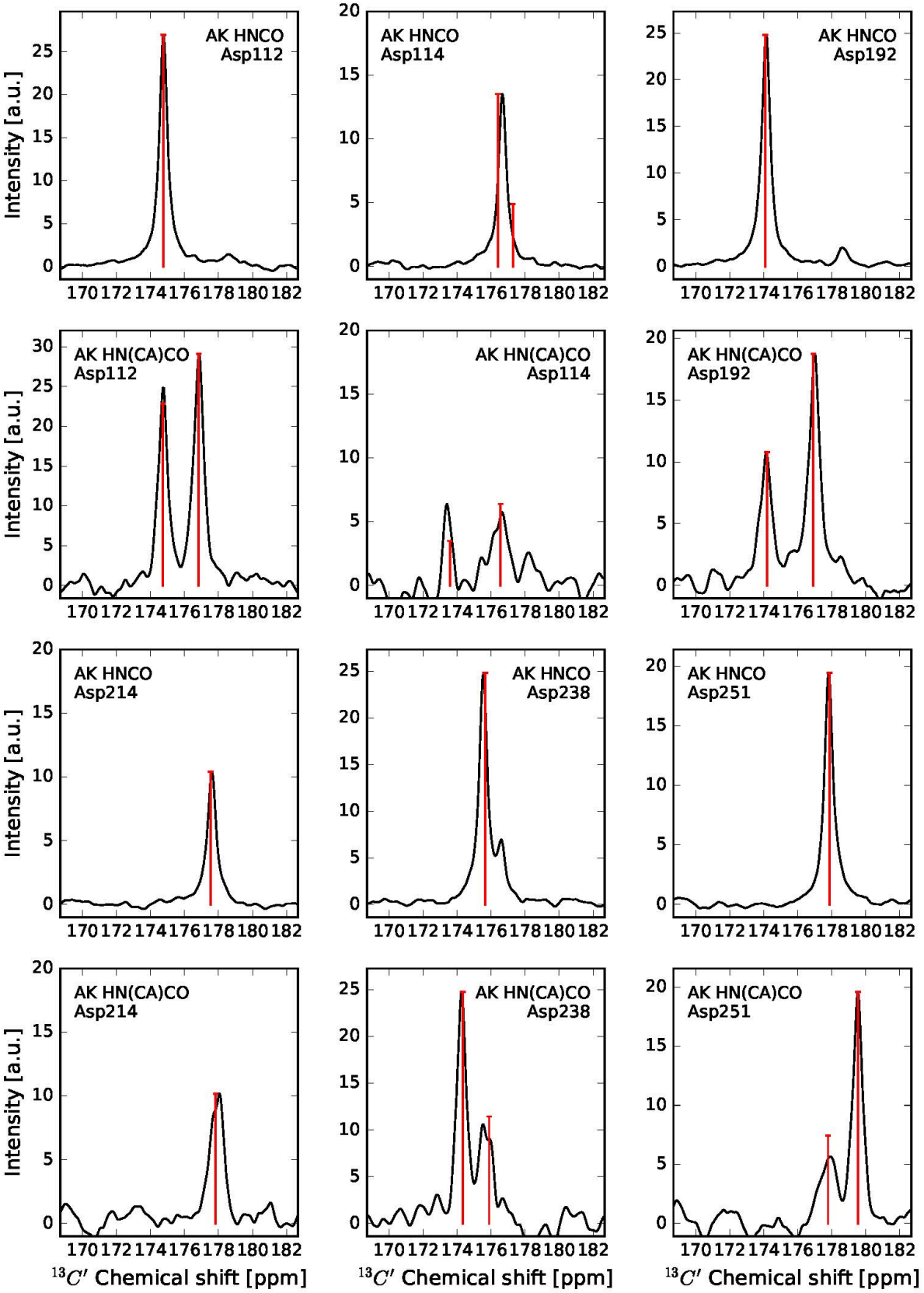
Asp088
AK HN(CA)CO
Asp097
AK HN(CA)CO
Asp106
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]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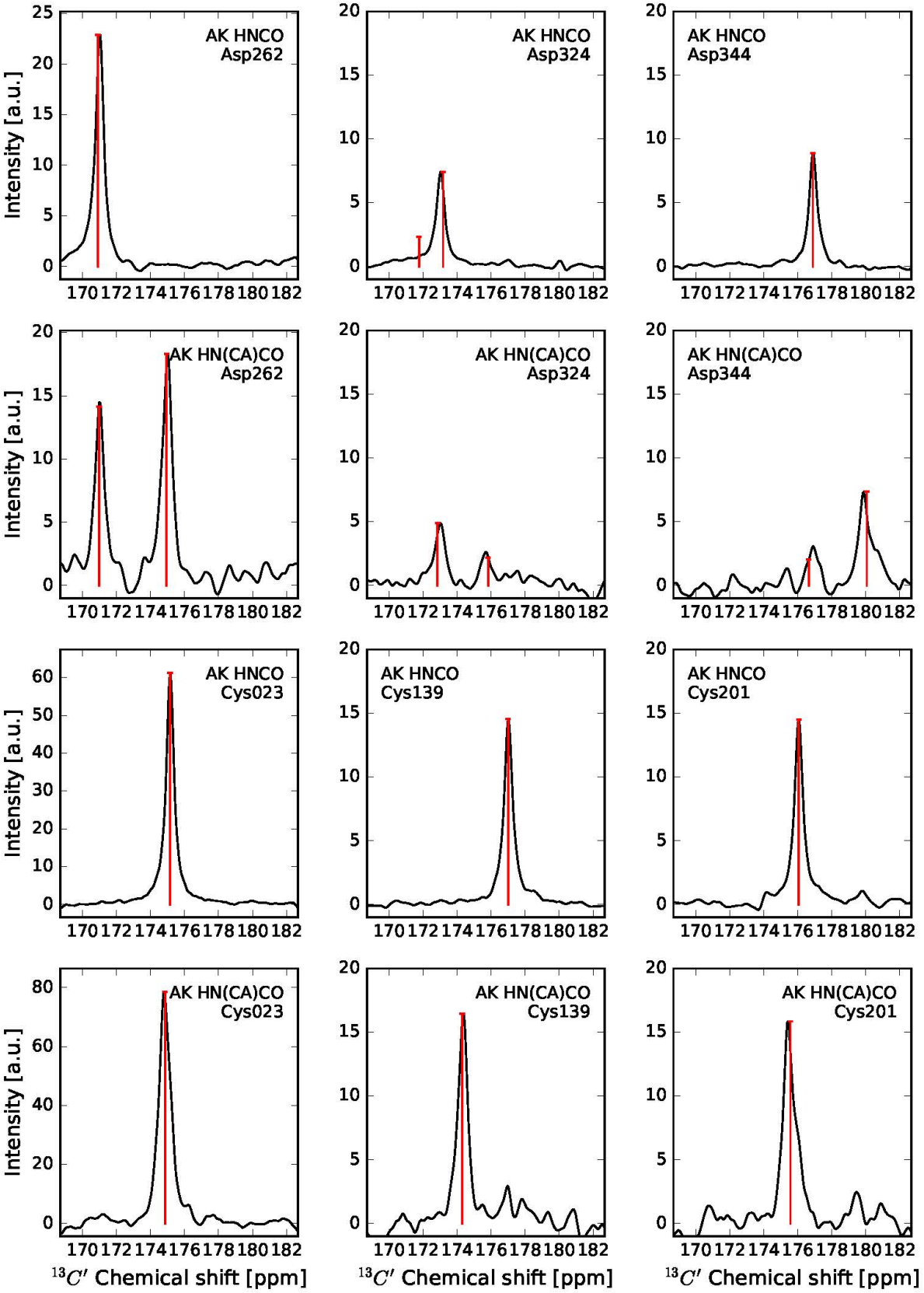
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]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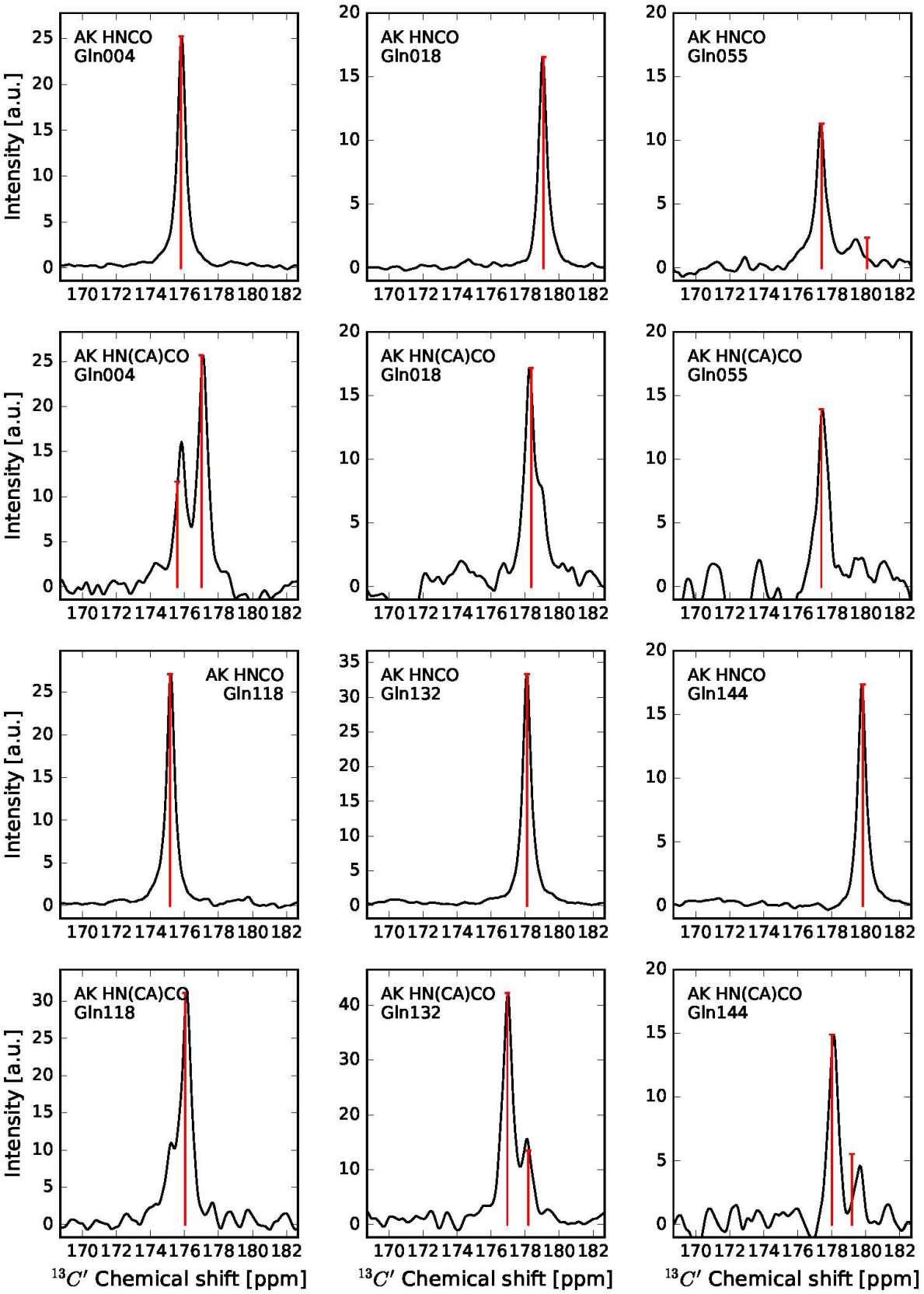
$^{13}C'$ Chemical shift [ppm]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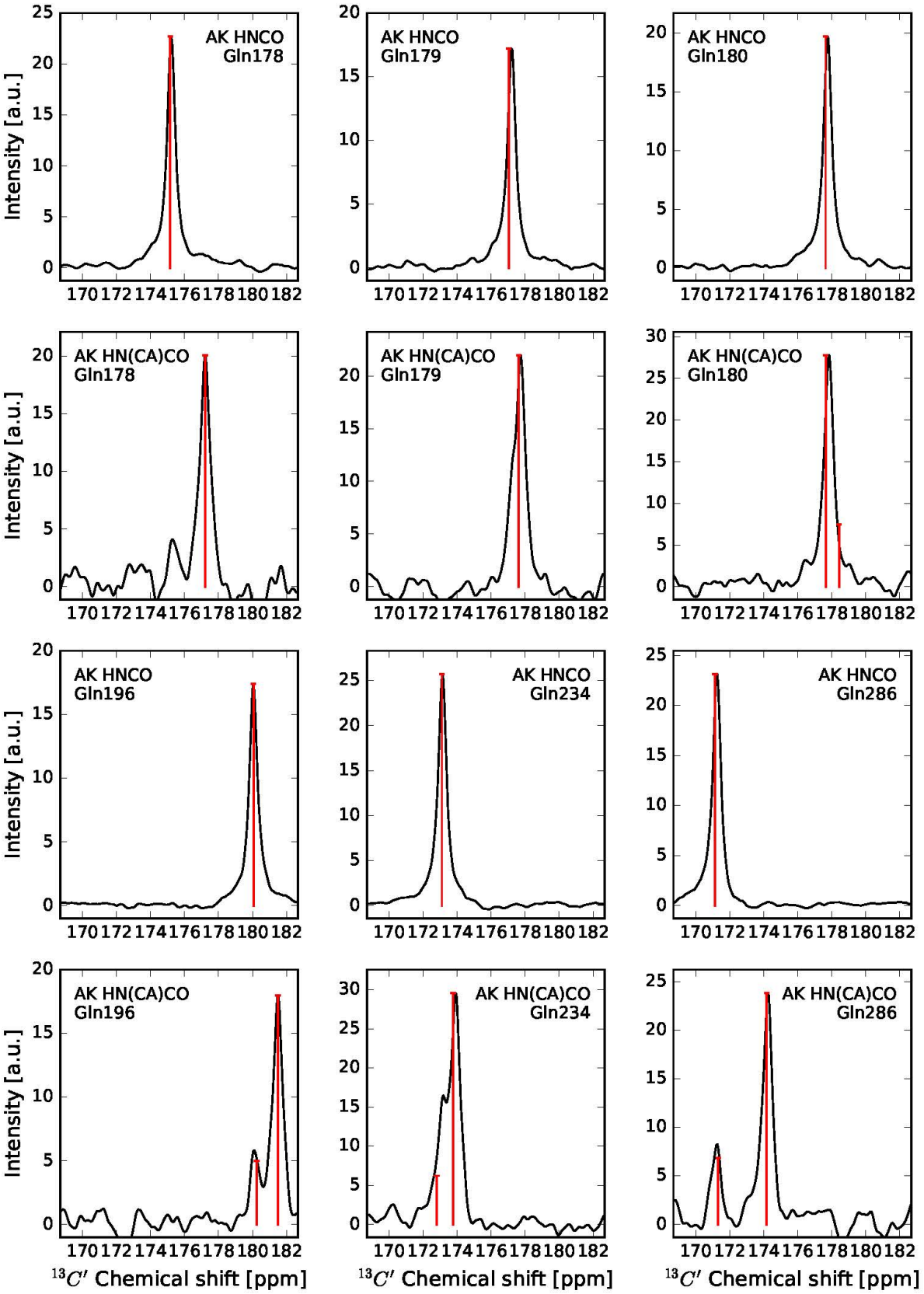
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]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AK HNCO Gln234
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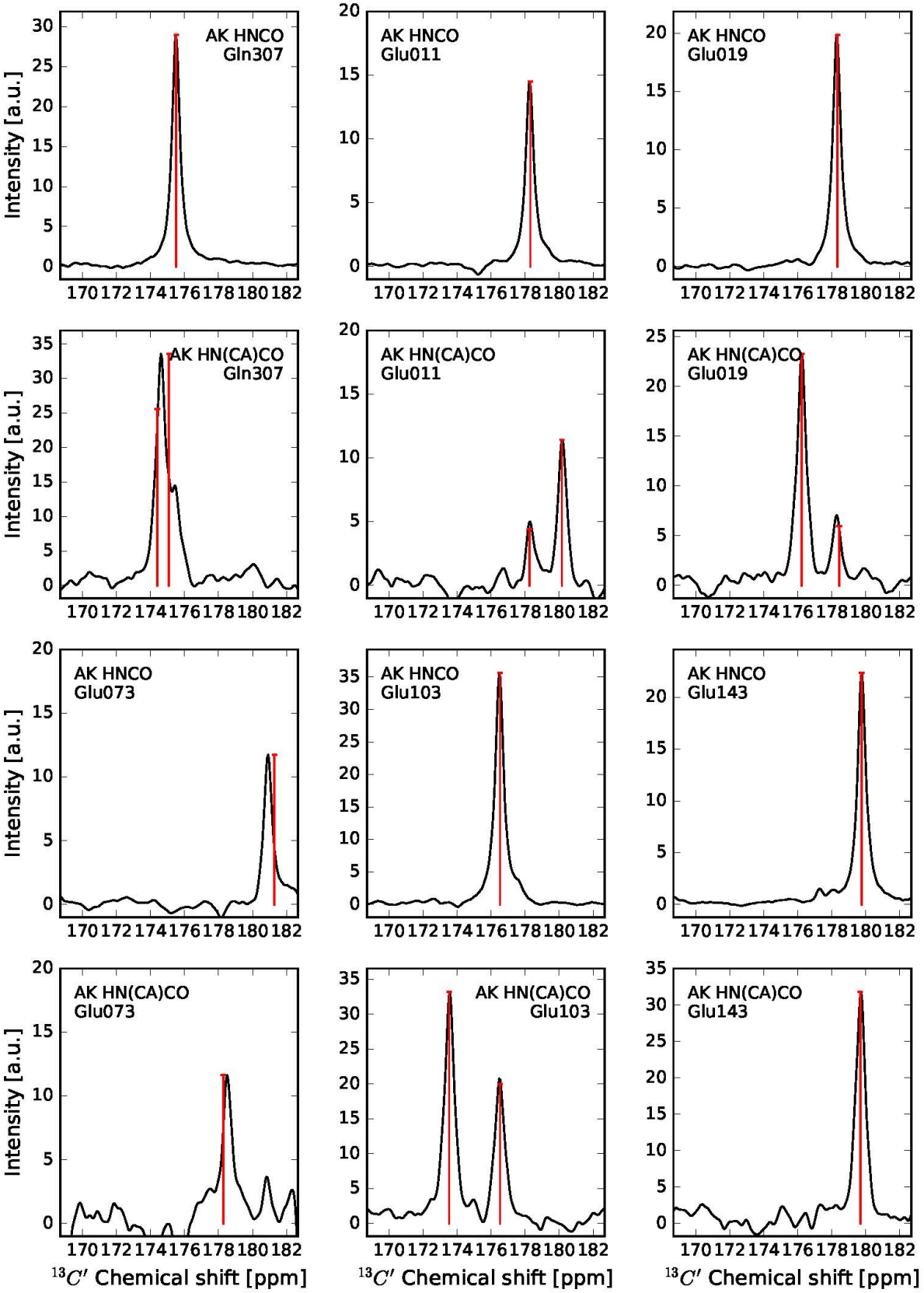
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]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Glu011
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Glu019
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Gln307
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Glu011
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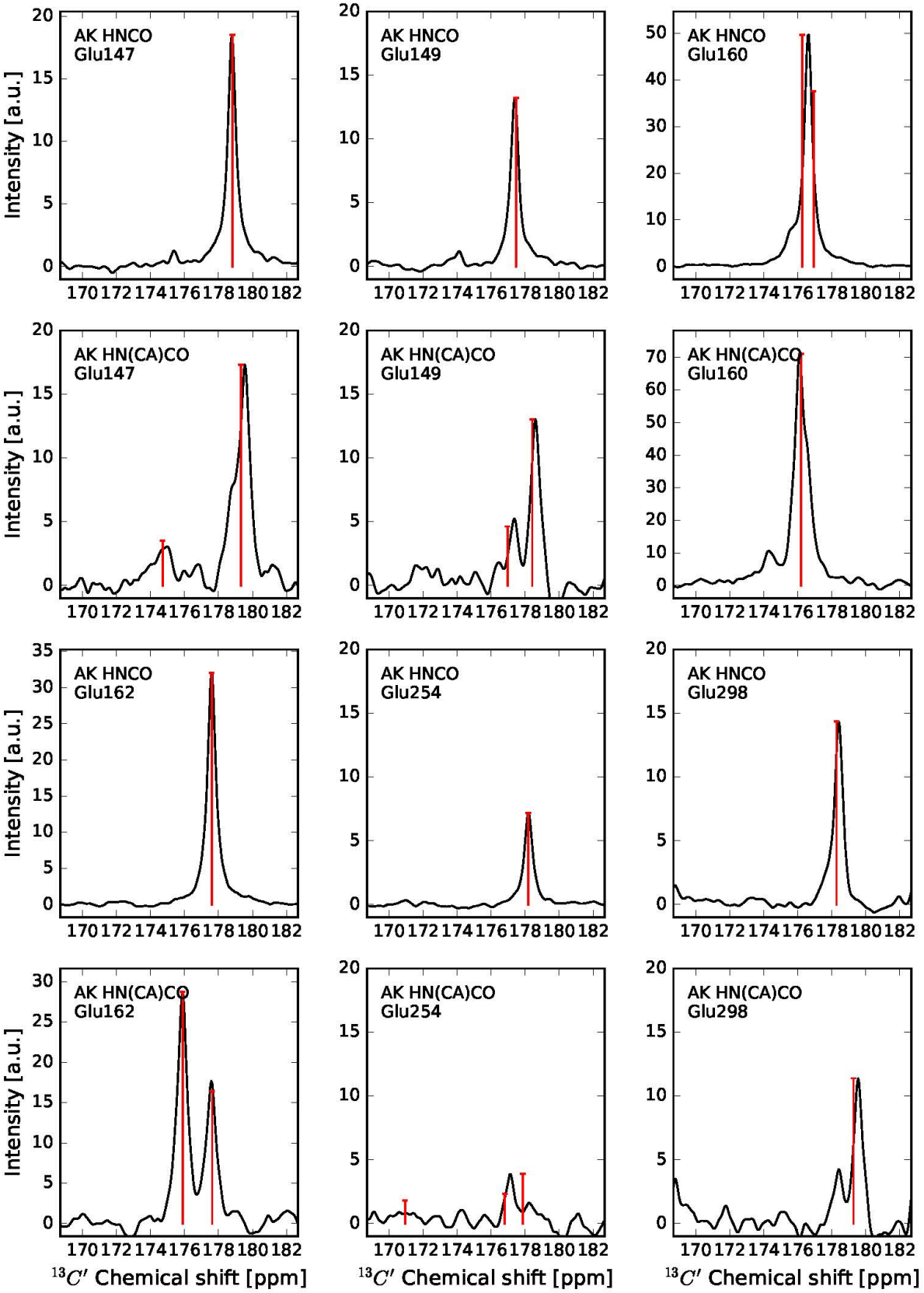
Glu019
AK HNCO
Glu073
AK HNCO
Glu103
AK HNCO
Glu143
AK HN(CA)CO
Glu073
AK HN(CA)CO
Glu103
AK HN(CA)CO
Glu143
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]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AK HNCO Glu254
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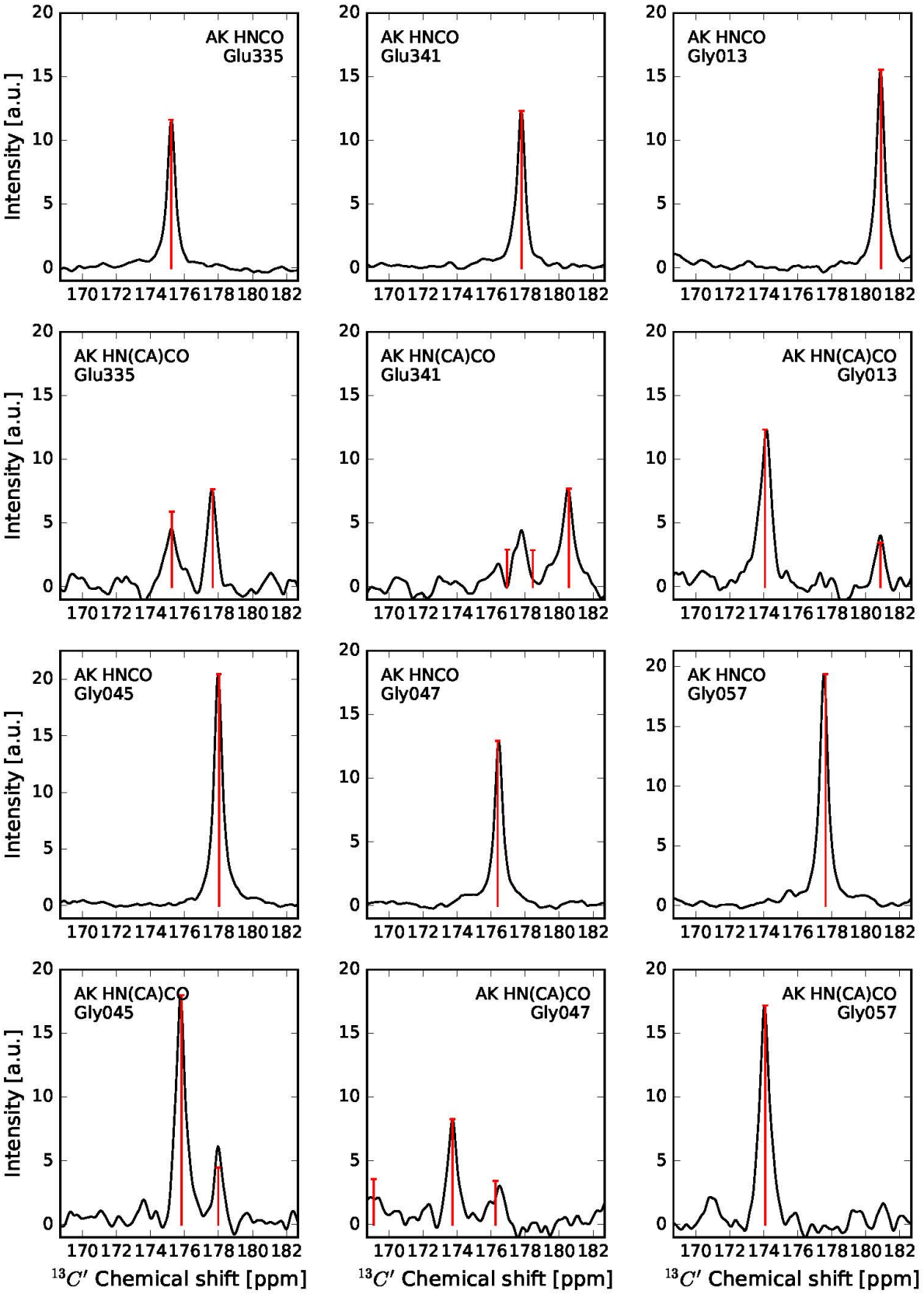
AK HN(CA)CO Glu298
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]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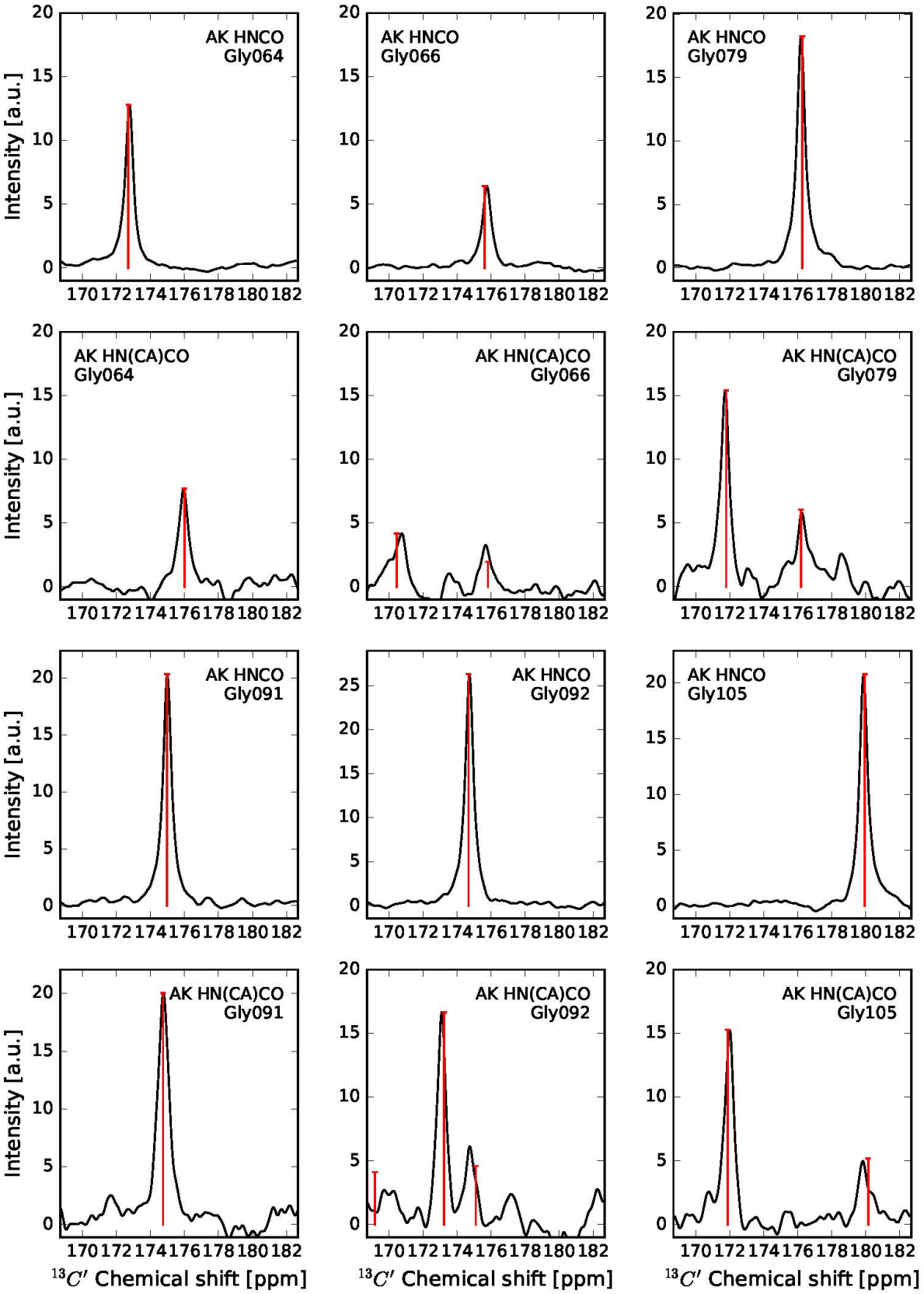
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]
0 5 10 15 20
170 172 174 176 178 180 182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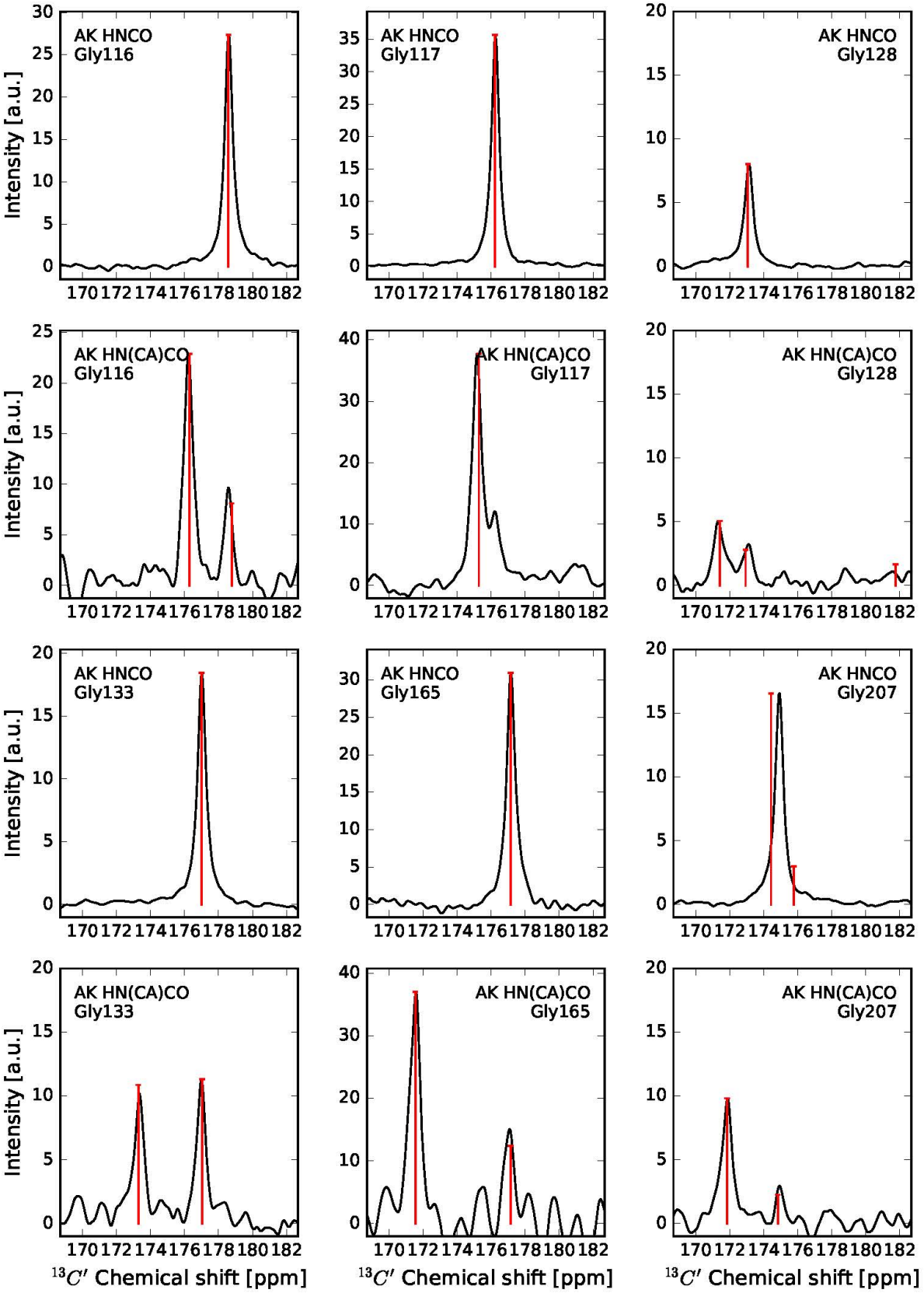
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]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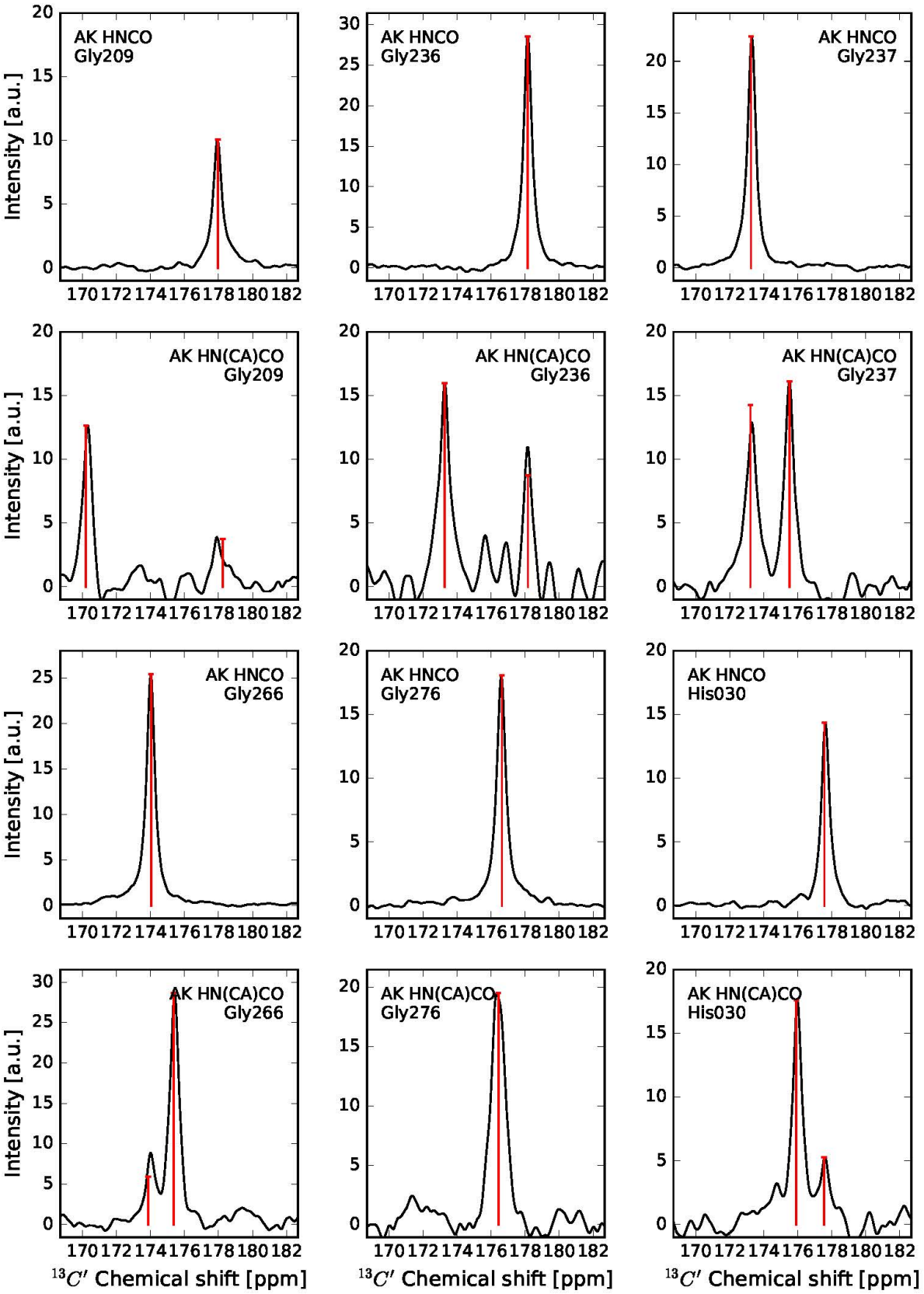
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]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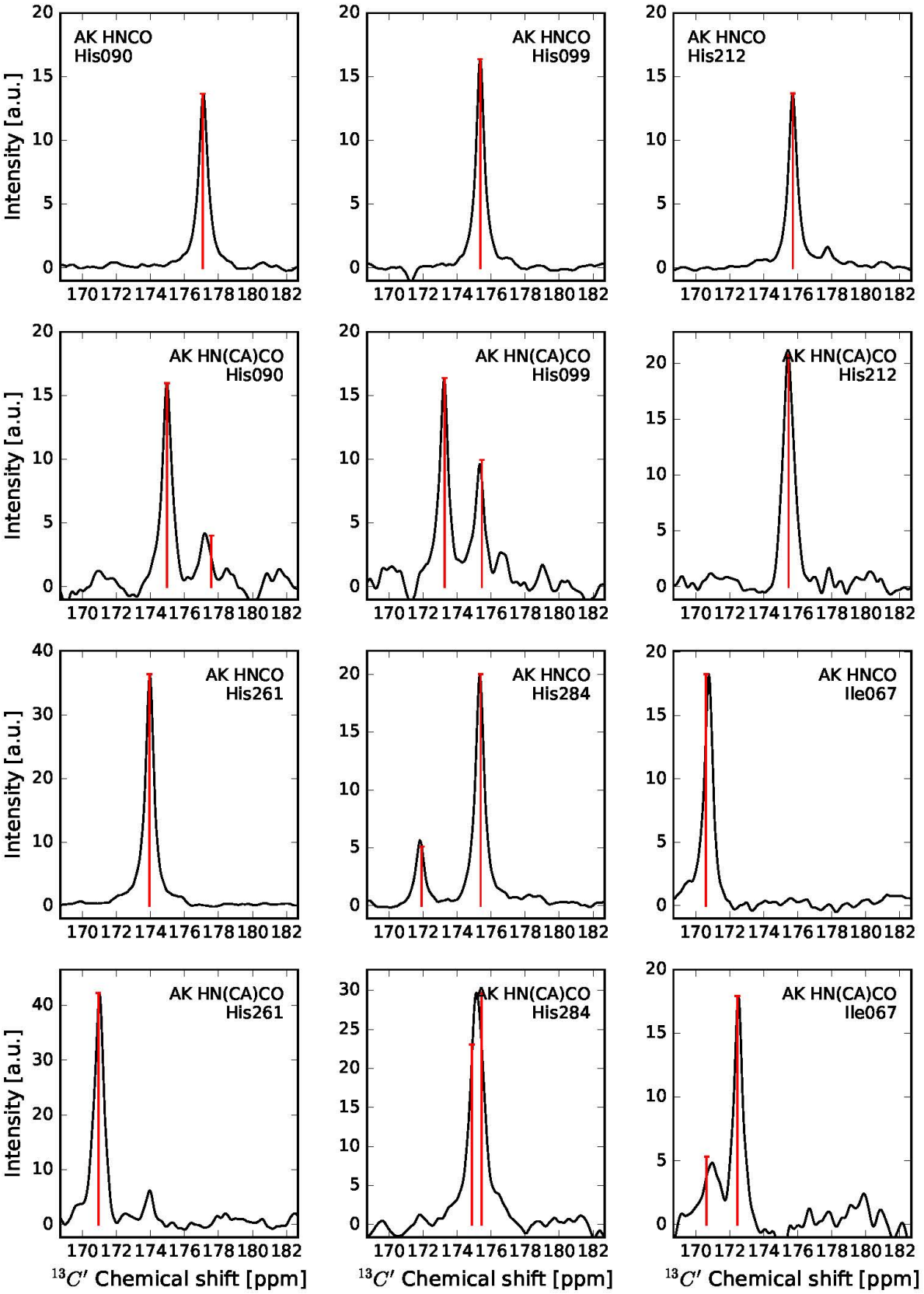
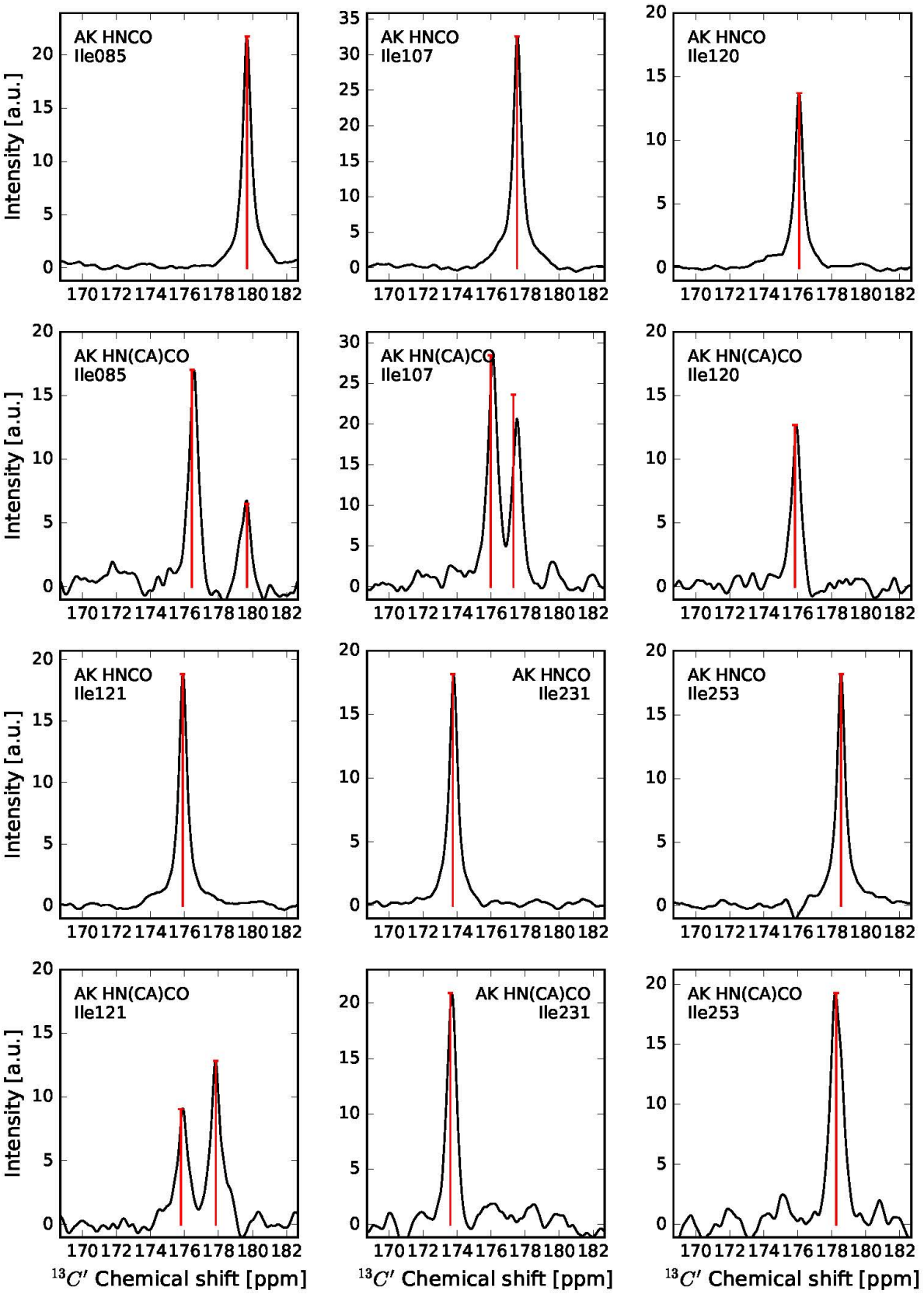
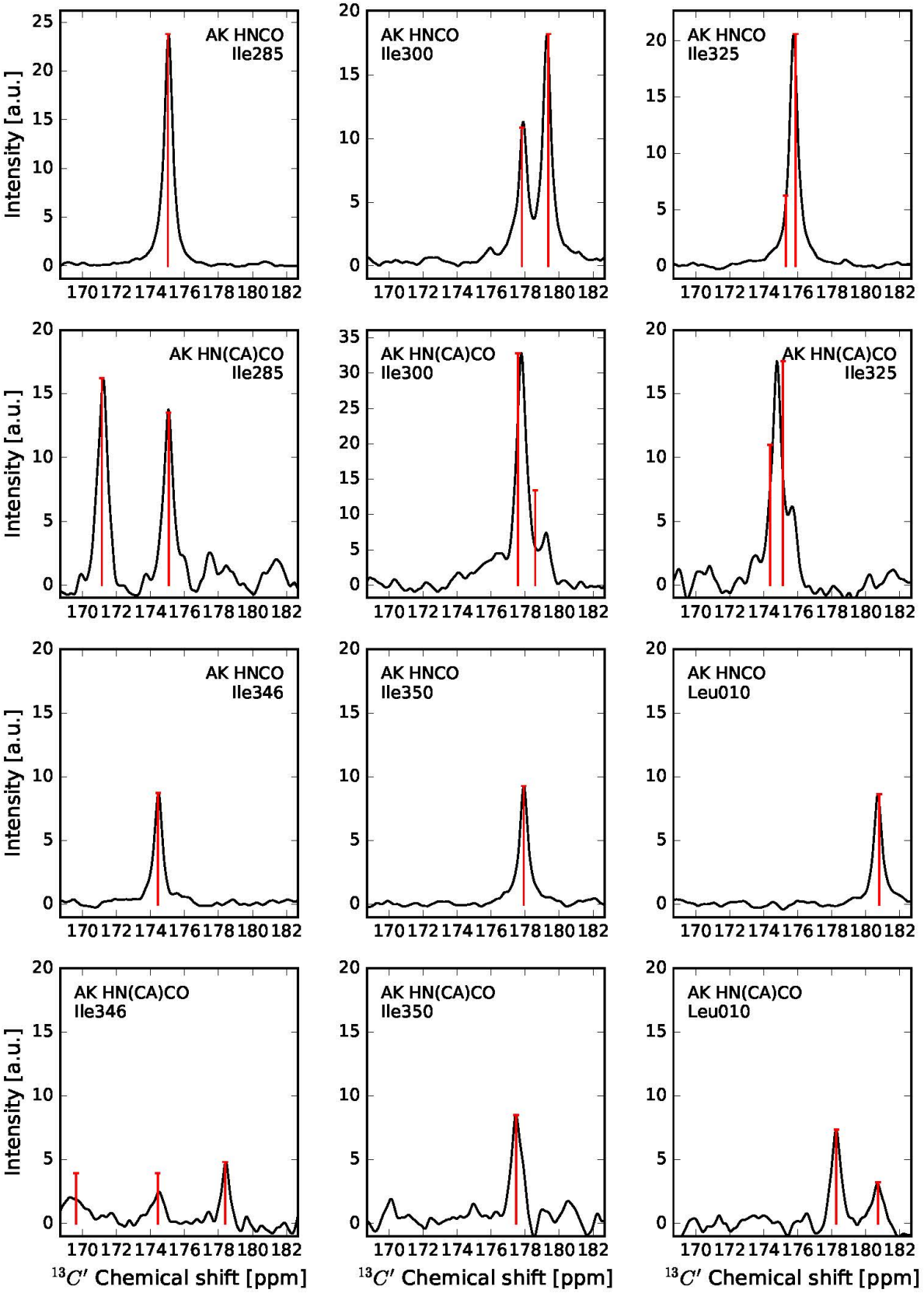
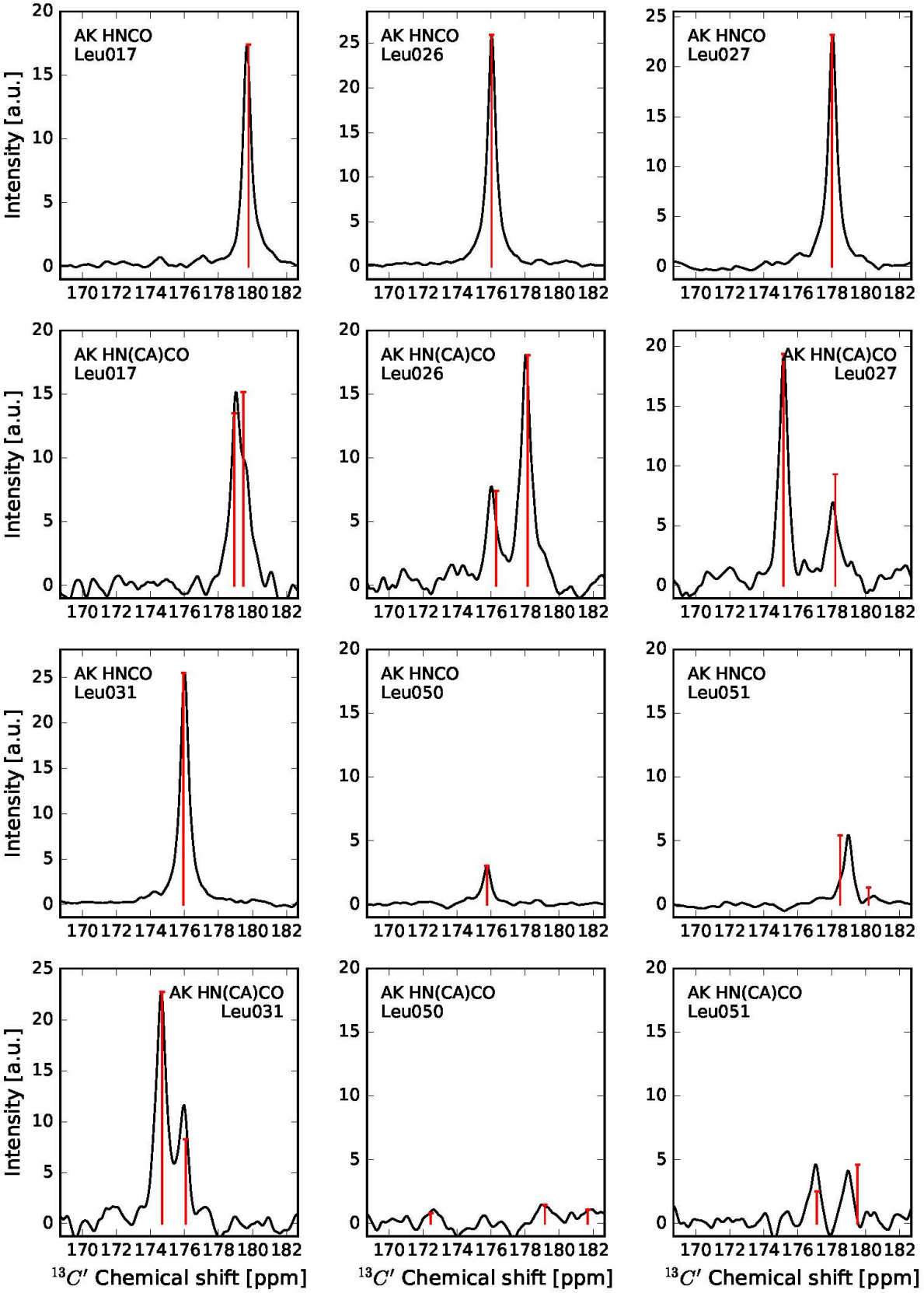
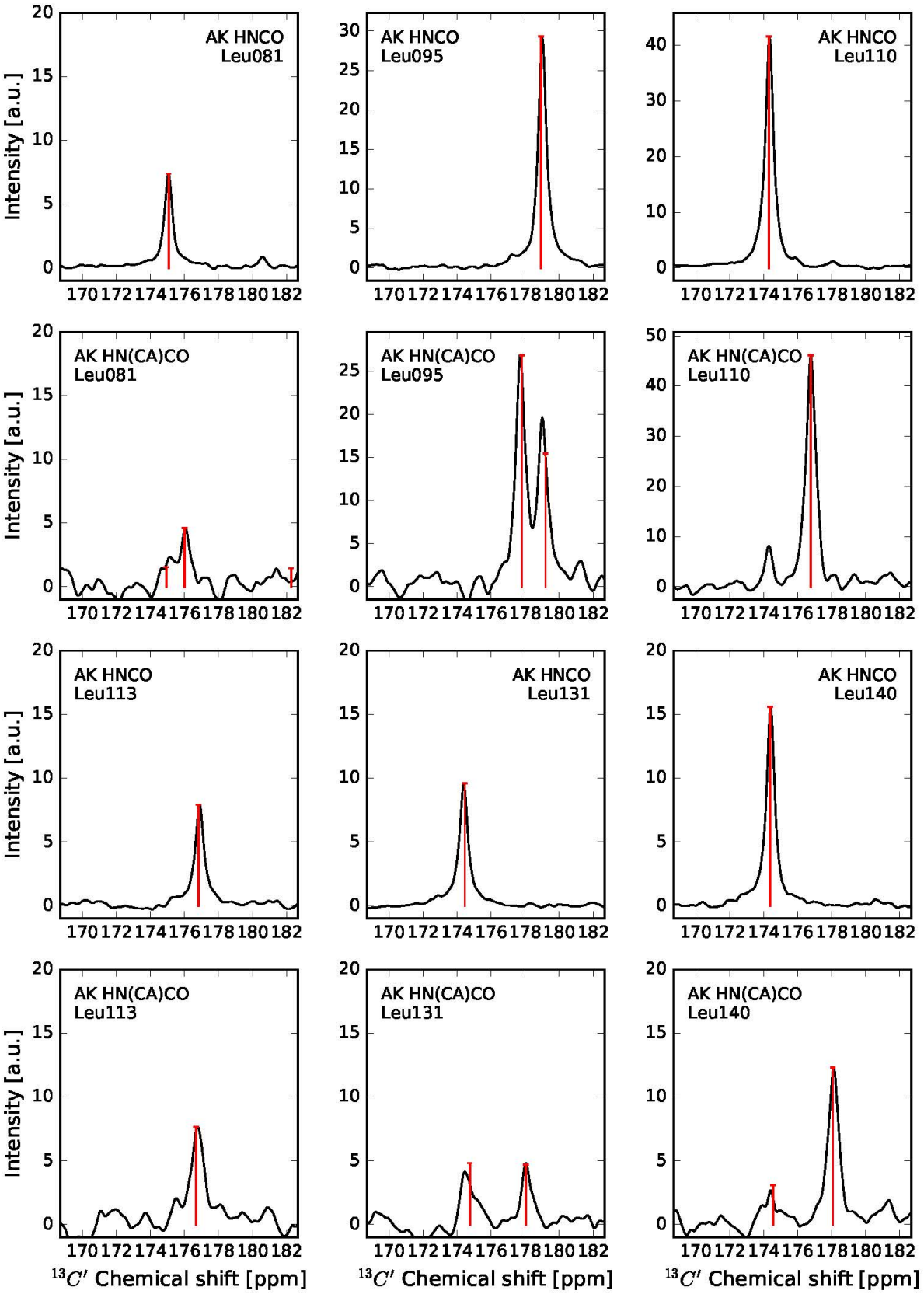
AK HN(CA)CO Gly276
AK HN(CA)CO His030
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]

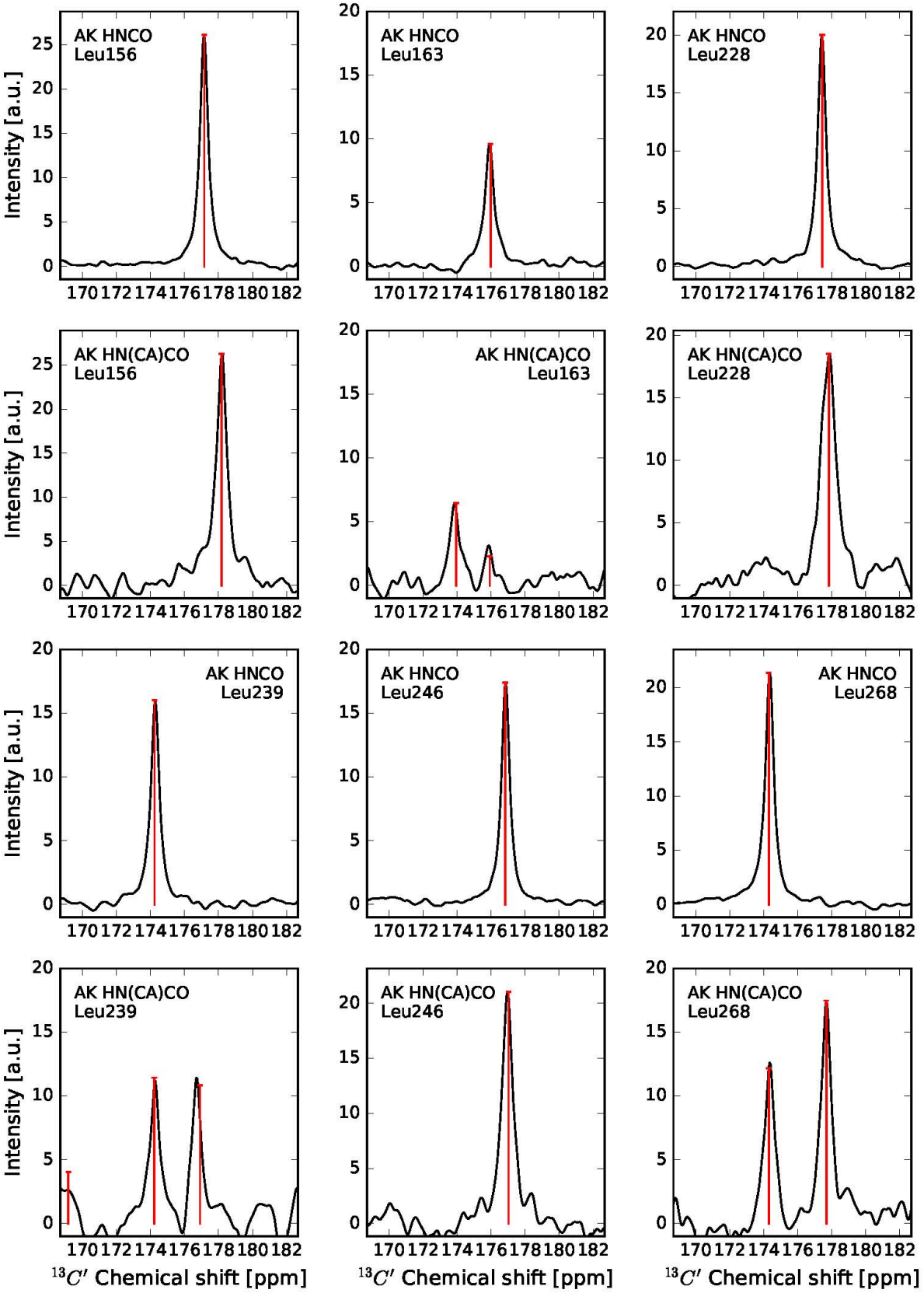

AK HNCO His090
AK HNCO His099
AK HNCO His212
AK HN(CA)CO His090
AK HN(CA)CO His099
AK HN(CA)CO His212
AK HNCO His261
AK HNCO His284
AK HNCO Ile067
AK HN(CA)CO His261
AK HN(CA)CO His284
AK HN(CA)CO Ile067
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]

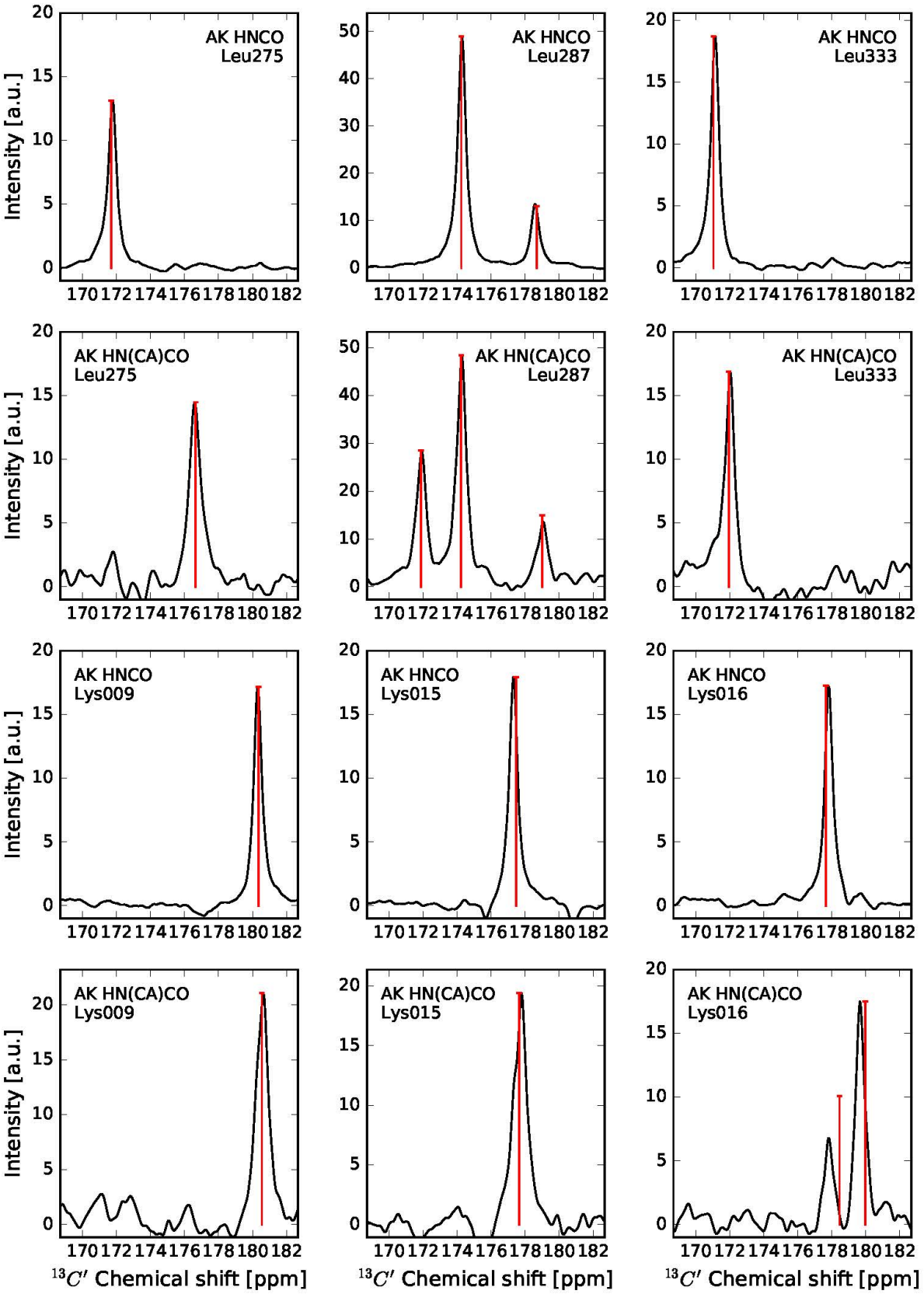

AK HNCO
Ile085
AK HNCO
Ile107
AK HNCO
Ile120
AK HN(CA)CO
Ile085
AK HN(CA)CO
Ile107
AK HN(CA)CO
Ile120
AK HNCO
Ile121
AK HNCO
Ile231
AK HNCO
Ile253
AK HN(CA)CO
Ile121
AK HN(CA)CO
Ile231
AK HN(CA)CO
Ile253
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]

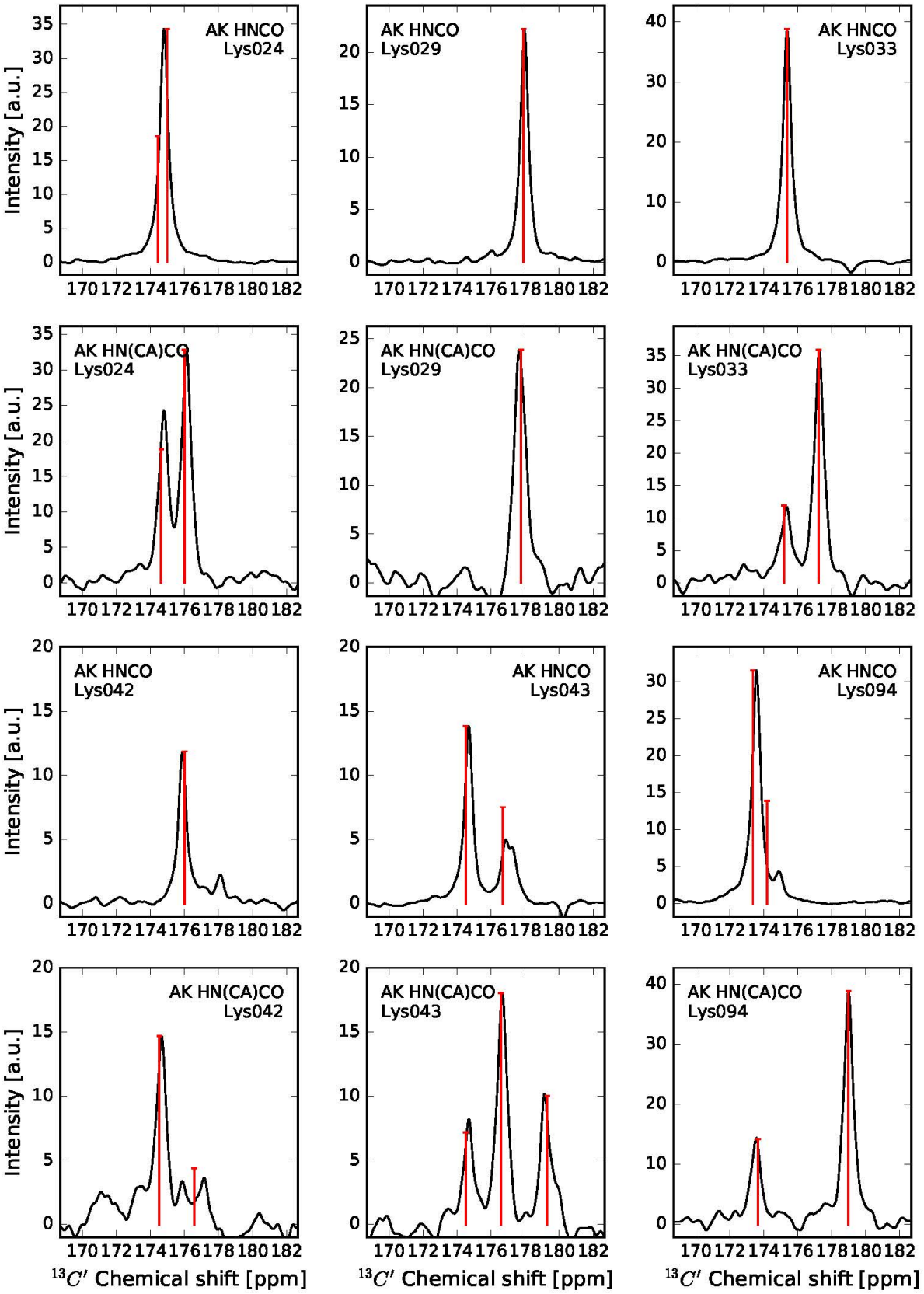

AK HNCO Ile285
AK HNCO Ile300
AK HNCO Ile325
AK HN(CA)CO Ile285
AK HN(CA)CO Ile300
AK HN(CA)CO Ile325
AK HNCO Ile346
AK HNCO Ile350
AK HNCO Leu010
AK HN(CA)CO Ile346
AK HN(CA)CO Ile350
AK HN(CA)CO Leu010
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]

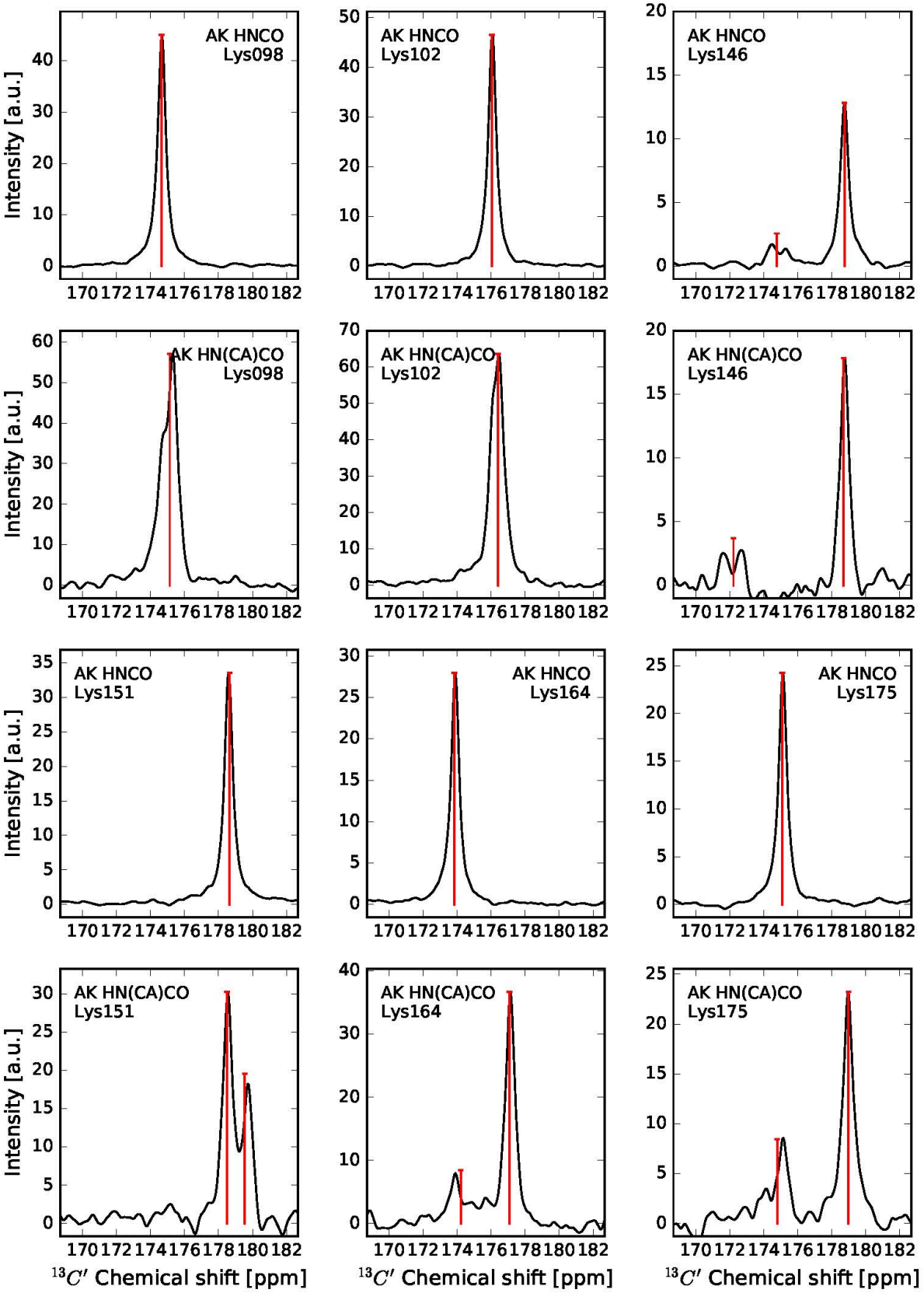

AK HNCO Leu017
AK HNCO Leu026
AK HNCO Leu027
AK HN(CA)CO Leu017
AK HN(CA)CO Leu026
AK HN(CA)CO Leu027
AK HNCO Leu031
AK HNCO Leu050
AK HNCO Leu051
AK HN(CA)CO Leu031
AK HN(CA)CO Leu050
AK HN(CA)CO Leu051
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]

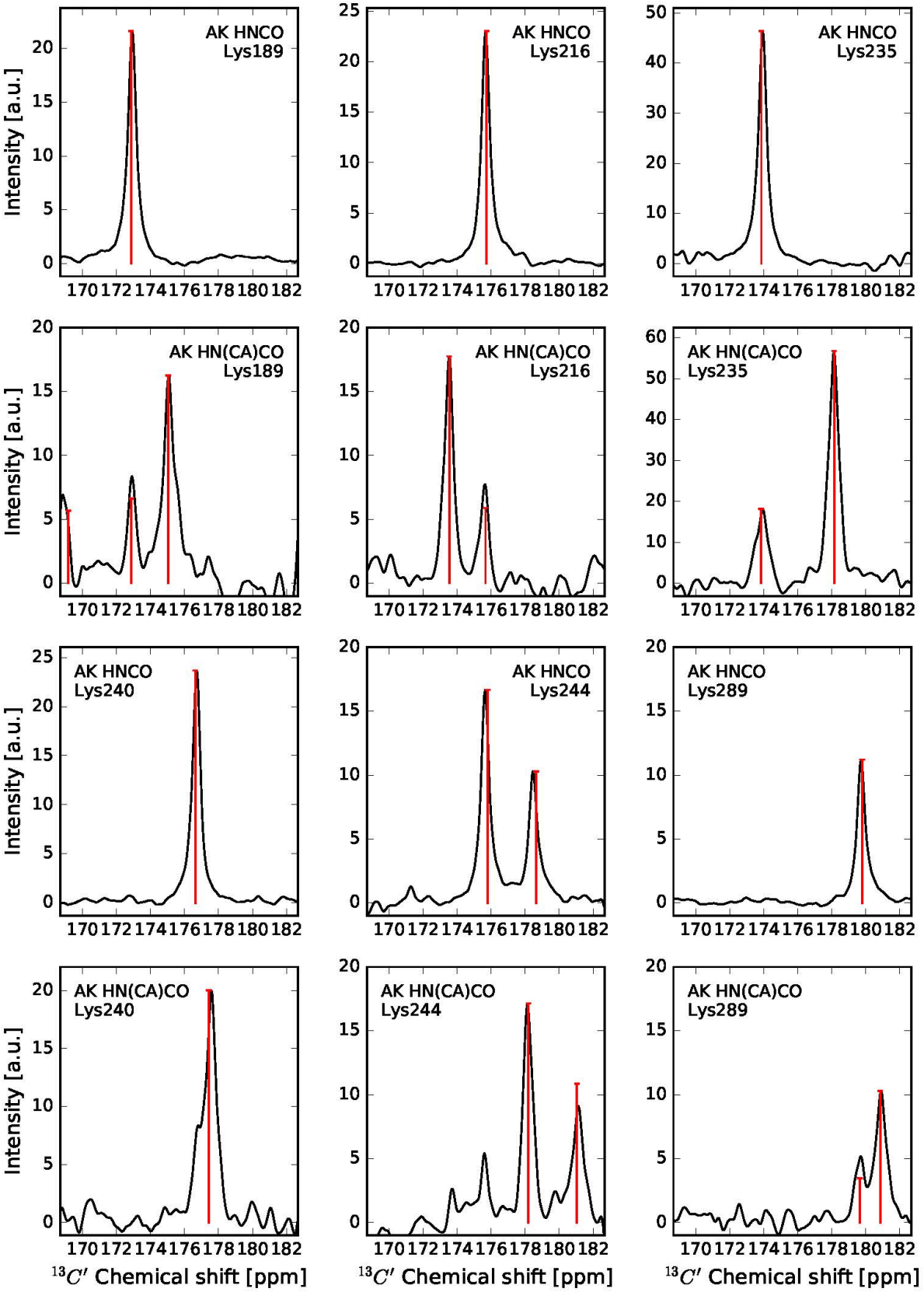

AK HNCO Leu081
AK HNCO Leu095
AK HNCO Leu110
AK HN(CA)CO Leu081
AK HN(CA)CO Leu095
AK HN(CA)CO Leu110
AK HNCO Leu113
AK HNCO Leu131
AK HNCO Leu140
AK HN(CA)CO Leu113
AK HN(CA)CO Leu131
AK HN(CA)CO Leu140
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]

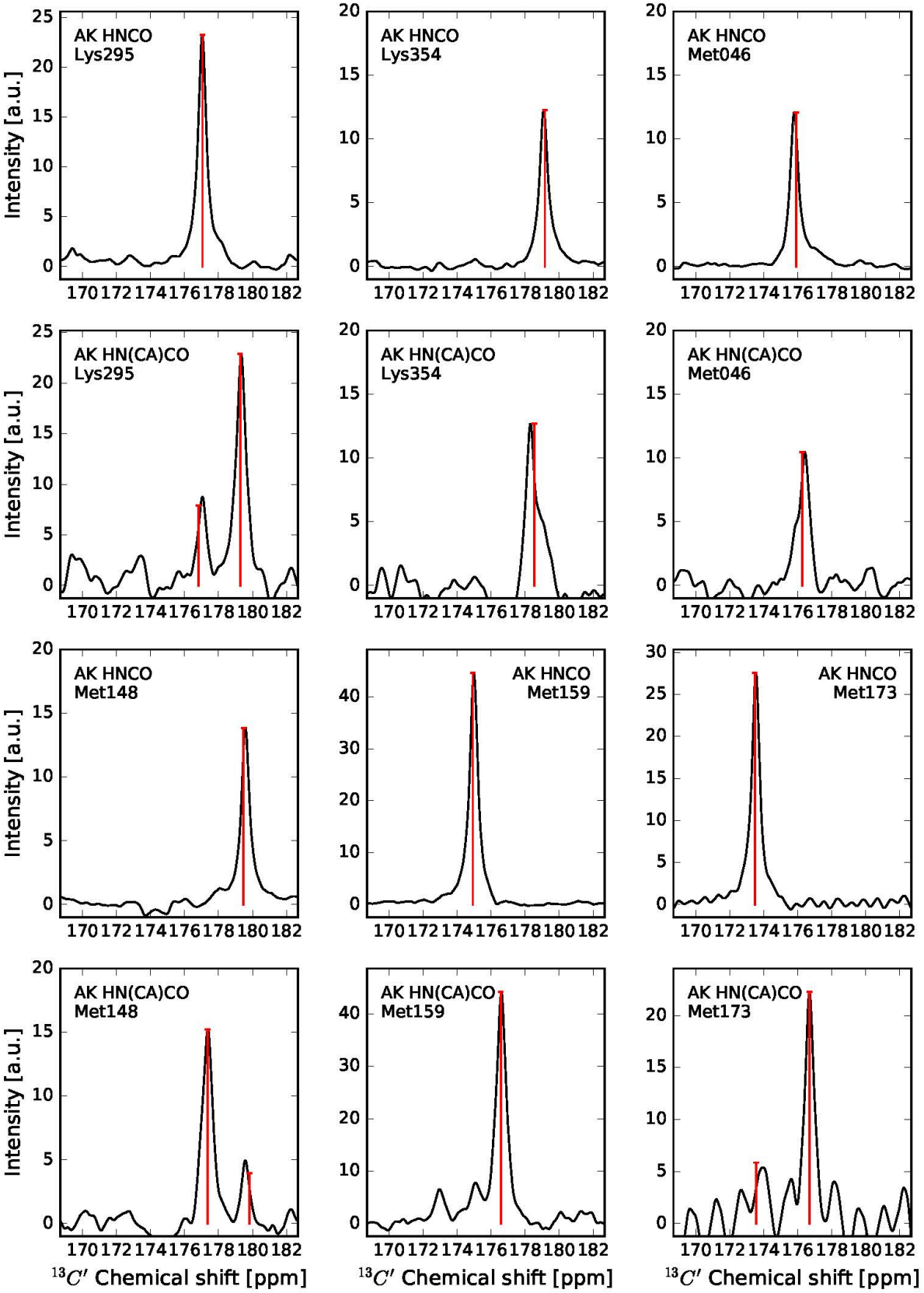

AK HNCO Leu156
AK HNCO Leu163
AK HNCO Leu228
AK HN(CA)CO Leu156
AK HN(CA)CO Leu163
AK HN(CA)CO Leu228
AK HNCO Leu239
AK HNCO Leu246
AK HNCO Leu268
AK HN(CA)CO Leu239
AK HN(CA)CO Leu246
AK HN(CA)CO Leu268
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]
170 172 174 176 178 180 182

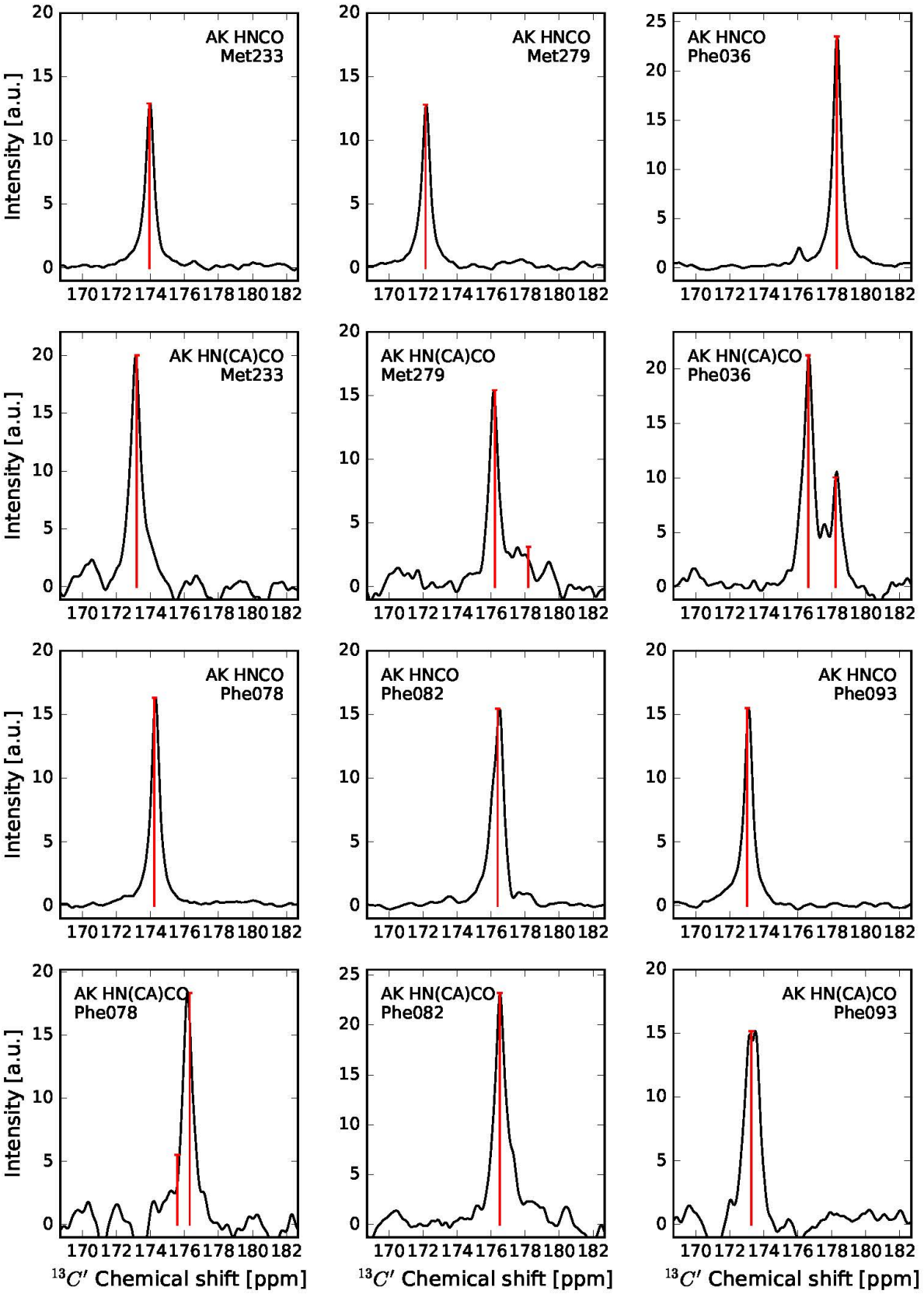

AK HNCO Leu275
AK HNCO Leu287
AK HNCO Leu333
AK HN(CA)CO Leu275
AK HN(CA)CO Leu287
AK HN(CA)CO Leu333
AK HNCO Lys009
AK HNCO Lys015
AK HNCO Lys016
AK HN(CA)CO Lys009
AK HN(CA)CO Lys015
AK HN(CA)CO Lys016
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]

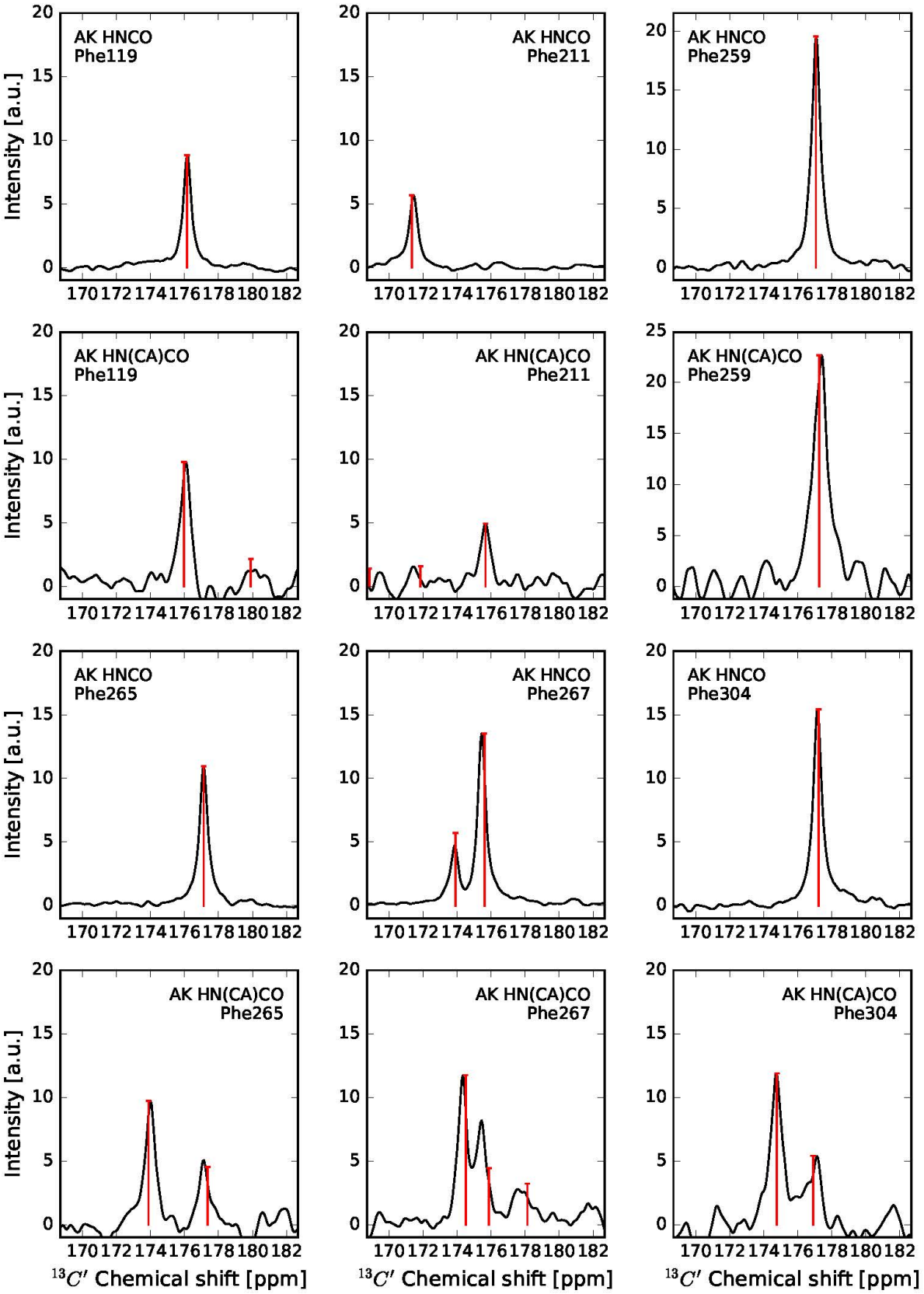

AK HNCO Lys024
AK HNCO Lys029
AK HNCO Lys033
AK HN(CA)CO Lys024
AK HN(CA)CO Lys029
AK HN(CA)CO Lys033
AK HNCO Lys042
AK HNCO Lys043
AK HNCO Lys094
AK HN(CA)CO Lys042
AK HN(CA)CO Lys043
AK HN(CA)CO Lys094
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]

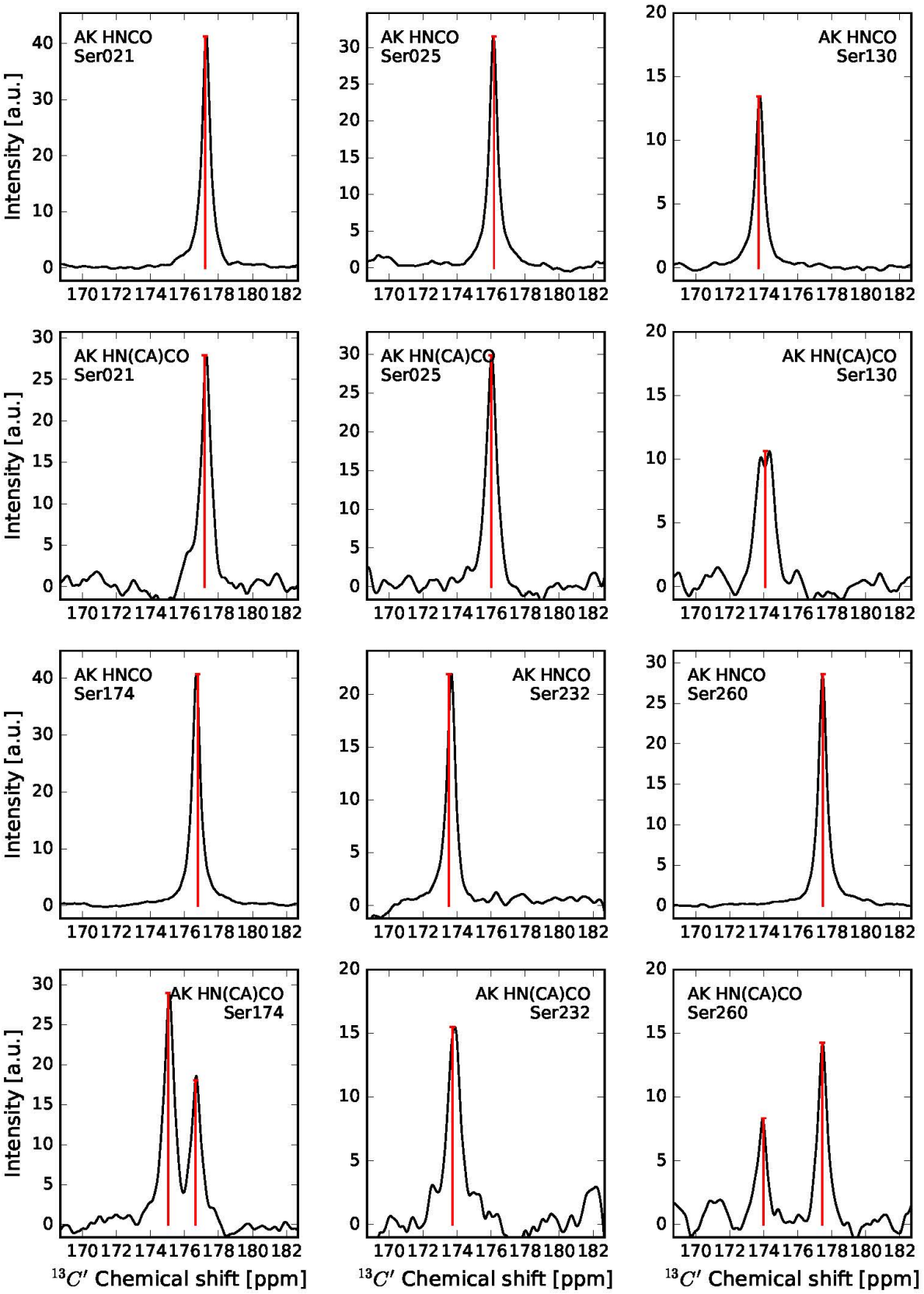

AK HNCO Lys098
AK HNCO Lys102
AK HNCO Lys146
AK HN(CA)CO Lys098
AK HN(CA)CO Lys102
AK HN(CA)CO Lys146
AK HNCO Lys151
AK HNCO Lys164
AK HNCO Lys175
AK HN(CA)CO Lys151
AK HN(CA)CO Lys164
AK HN(CA)CO Lys175
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]

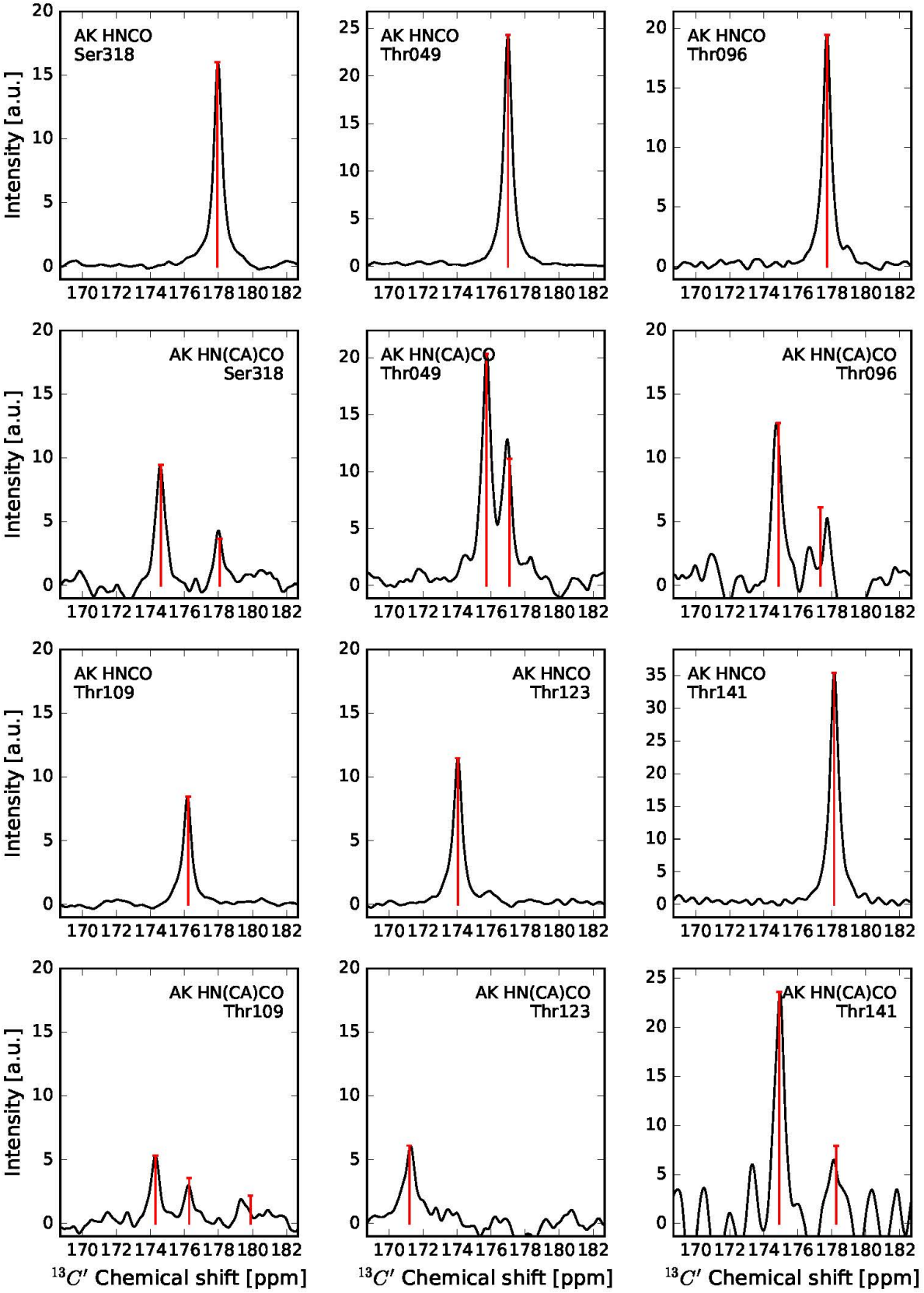

AK HNCO Lys189
AK HNCO Lys216
AK HNCO Lys235
AK HN(CA)CO Lys189
AK HN(CA)CO Lys216
AK HN(CA)CO Lys235
AK HNCO Lys240
AK HNCO Lys244
AK HNCO Lys289
AK HN(CA)CO Lys240
AK HN(CA)CO Lys244
AK HN(CA)CO Lys289
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]

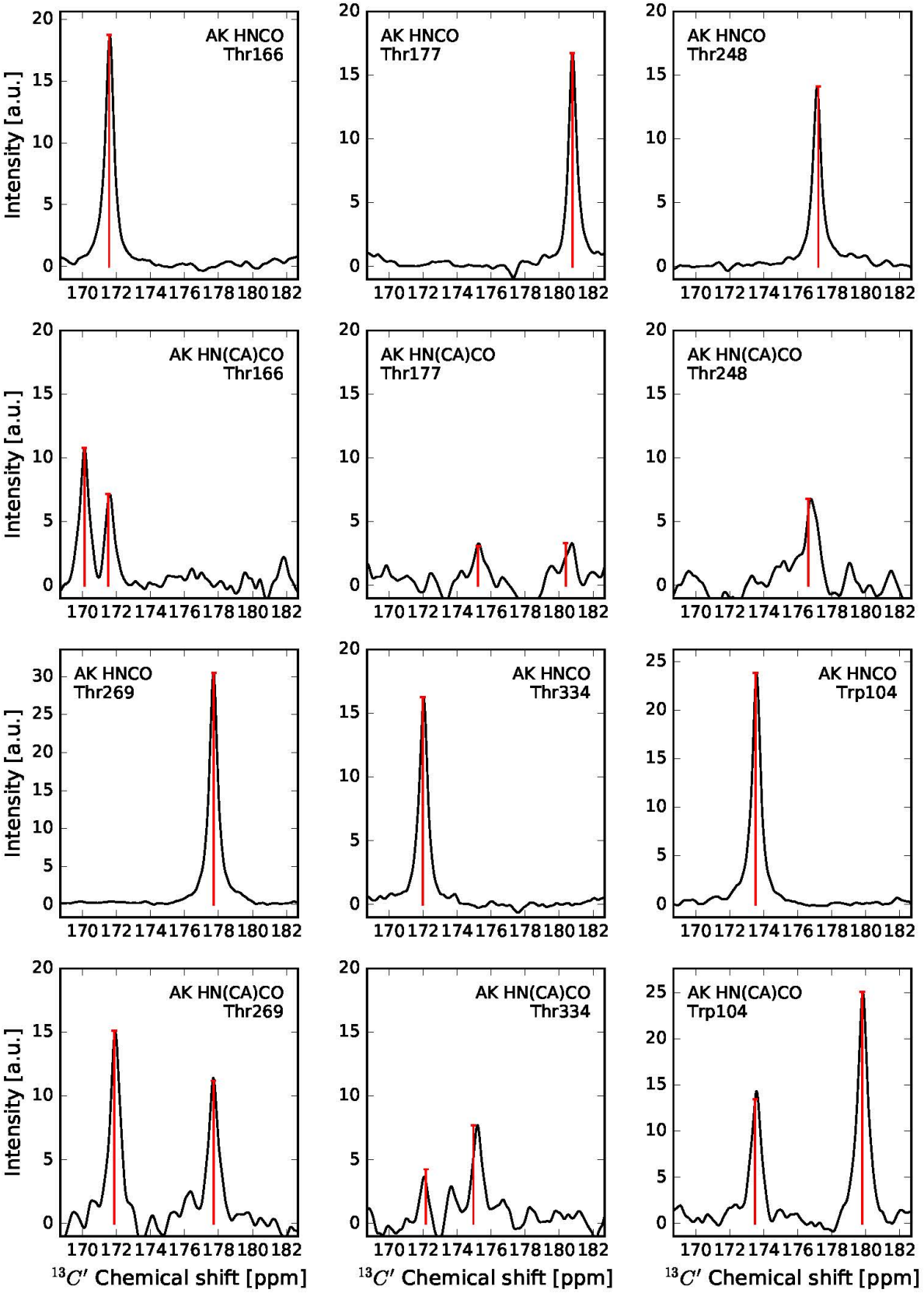

AK HNCO Lys295
AK HNCO Lys354
AK HNCO Met046
AK HN(CA)CO Lys295
AK HN(CA)CO Lys354
AK HN(CA)CO Met046
AK HNCO Met148
AK HNCO Met159
AK HNCO Met173
AK HN(CA)CO Met148
AK HN(CA)CO Met159
AK HN(CA)CO Met173
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]

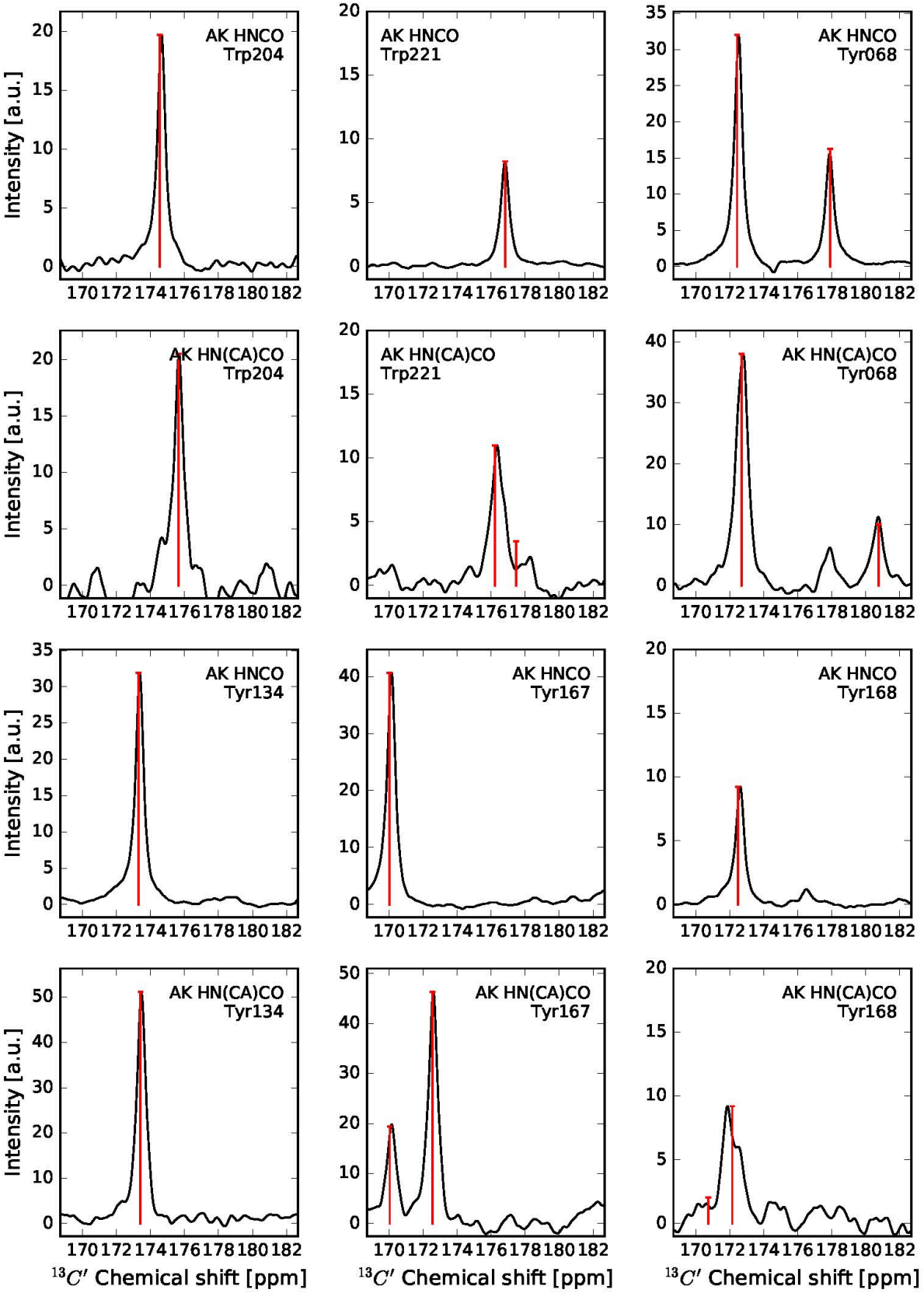

AK HNCO Met233
AK HNCO Met279
AK HNCO Phe036
AK HN(CA)CO Met233
AK HN(CA)CO Met279
AK HN(CA)CO Phe036
AK HNCO Phe078
AK HNCO Phe082
AK HNCO Phe093
AK HN(CA)CO Phe078
AK HN(CA)CO Phe082
AK HN(CA)CO Phe093
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]

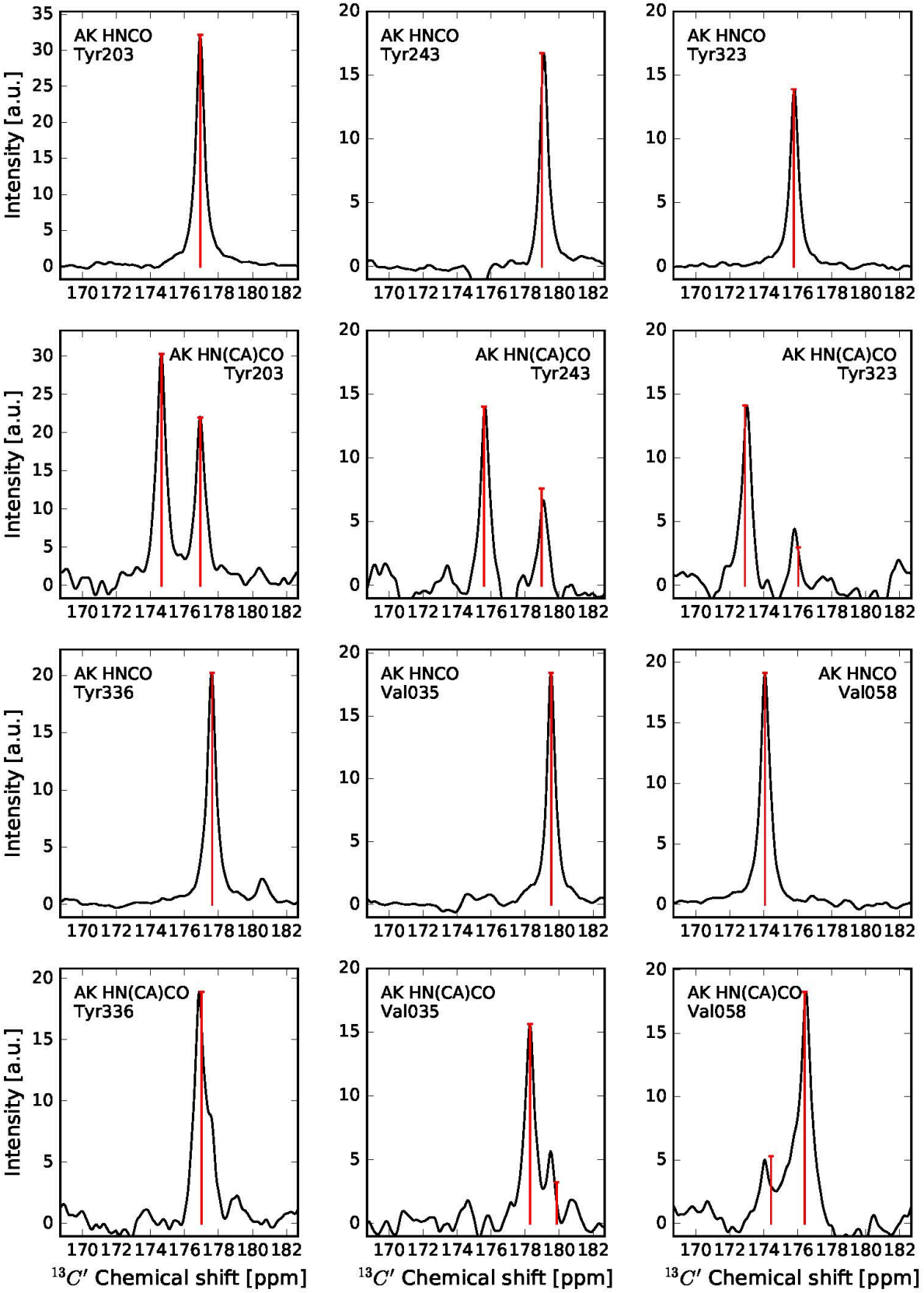

AK HNCO Phe119
AK HNCO Phe211
AK HNCO Phe259
AK HN(CA)CO Phe119
AK HN(CA)CO Phe211
AK HN(CA)CO Phe259
AK HNCO Phe265
AK HNCO Phe267
AK HNCO Phe304
AK HN(CA)CO Phe265
AK HN(CA)CO Phe267
AK HN(CA)CO Phe304
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]

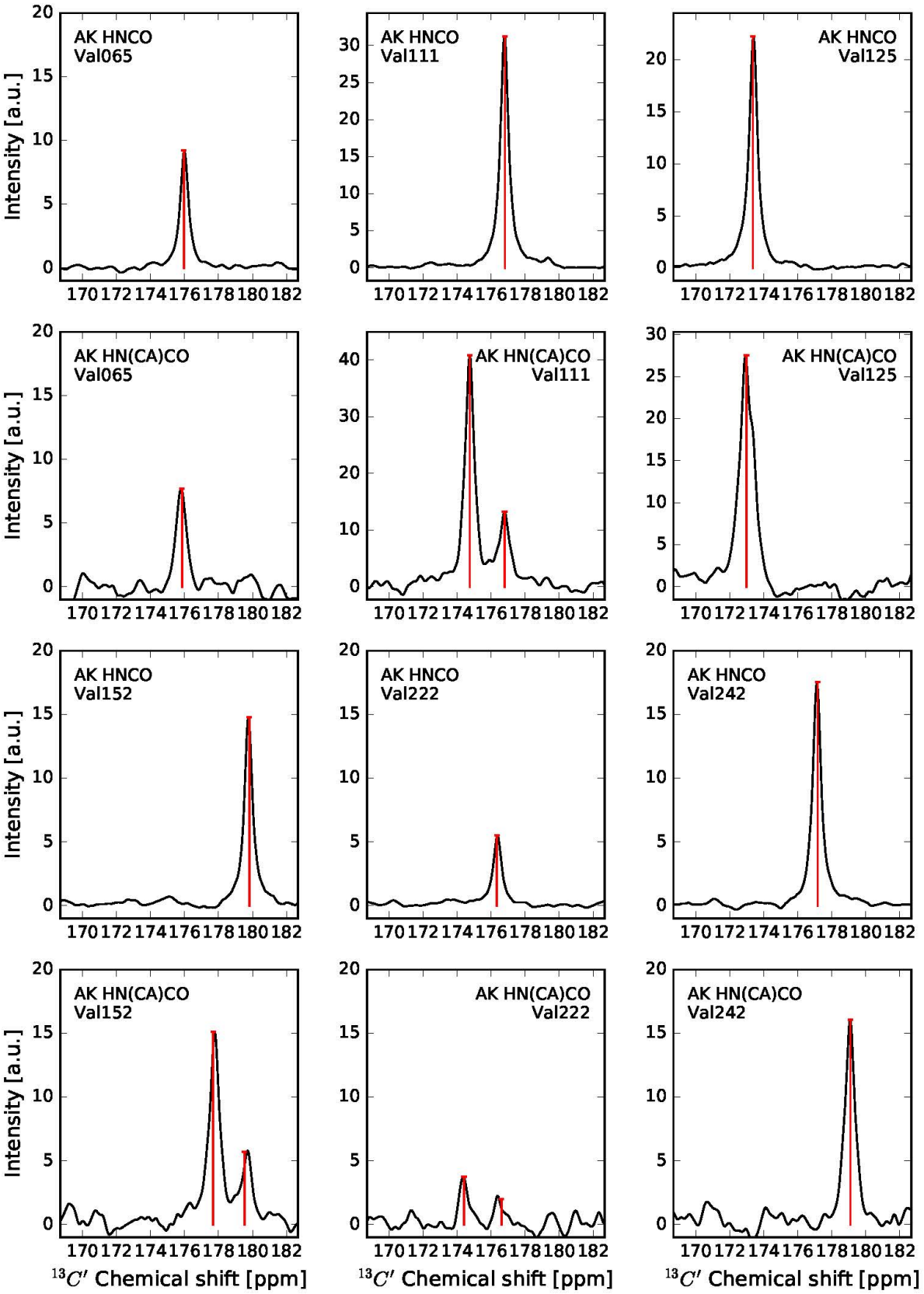

AK HNCO Ser021
AK HNCO Ser025
AK HNCO Ser130
AK HN(CA)CO Ser021
AK HN(CA)CO Ser025
AK HN(CA)CO Ser130
AK HNCO Ser174
AK HNCO Ser232
AK HNCO Ser260
AK HN(CA)CO Ser174
AK HN(CA)CO Ser232
AK HN(CA)CO Ser260
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]

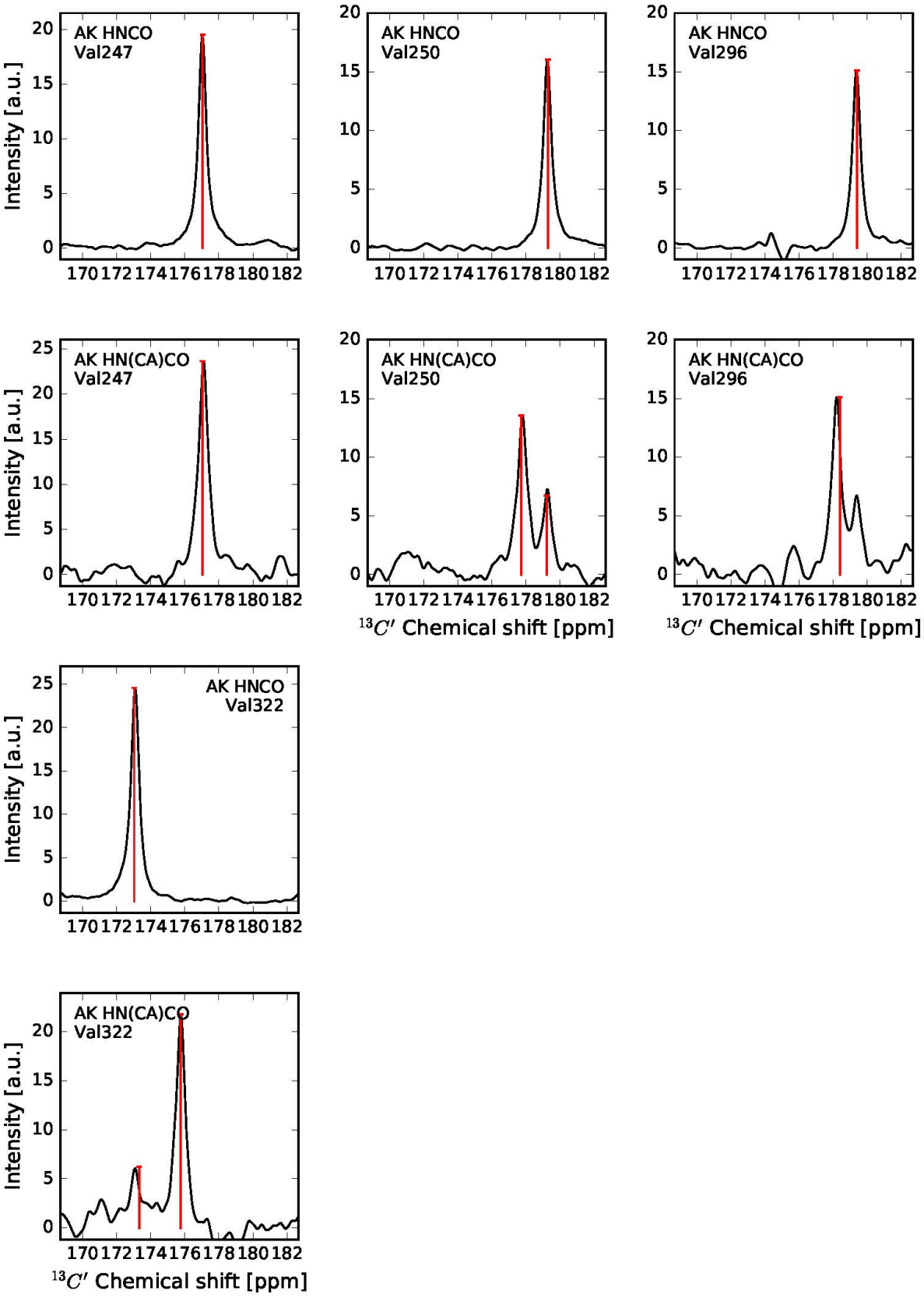

AK HNCO Ser318
AK HNCO Thr049
AK HNCO Thr096
AK HN(CA)CO Ser318
AK HN(CA)CO Thr049
AK HN(CA)CO Thr096
AK HNCO Thr109
AK HNCO Thr123
AK HNCO Thr141
AK HN(CA)CO Thr109
AK HN(CA)CO Thr123
AK HN(CA)CO Thr141
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]


AK HNCO Thr166
AK HNCO Thr177
AK HNCO Thr248
AK HN(CA)CO Thr166
AK HN(CA)CO Thr177
AK HN(CA)CO Thr248
AK HNCO Thr269
AK HNCO Thr334
AK HNCO Trp104
AK HN(CA)CO Thr269
AK HN(CA)CO Thr334
AK HN(CA)CO Trp104
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]


AK HNCO Trp204
AK HNCO Trp221
AK HNCO Tyr068
AK HN(CA)CO Trp204
AK HN(CA)CO Trp221
AK HN(CA)CO Tyr068
AK HNCO Tyr134
AK HNCO Tyr167
AK HNCO Tyr168
AK HN(CA)CO Tyr134
AK HN(CA)CO Tyr167
AK HN(CA)CO Tyr168
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]


AK HNCO Tyr203
AK HNCO Tyr243
AK HNCO Tyr323
AK HN(CA)CO Tyr203
AK HN(CA)CO Tyr243
AK HN(CA)CO Tyr323
AK HNCO Tyr336
AK HNCO Val035
AK HNCO Val058
AK HN(CA)CO Tyr336
AK HN(CA)CO Val035
AK HN(CA)CO Val058
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]


AK HNCO Val065
AK HNCO Val111
AK HNCO Val125
AK HN(CA)CO Val065
AK HN(CA)CO Val111
AK HN(CA)CO Val125
AK HNCO Val152
AK HNCO Val222
AK HNCO Val242
AK HN(CA)CO Val152
AK HN(CA)CO Val222
AK HN(CA)CO Val242
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]


AK HNCO
Val247
AK HNCO
Val250
AK HNCO
Val296
AK HN(CA)CO
Val247
AK HN(CA)CO
Val250
AK HN(CA)CO
Val296
AK HNCO
Val322
AK HN(CA)CO
Val322
Intensity [a.u.]
$^{13}C'$ Chemical shift [ppm]
170 172 174 176 178 180 182