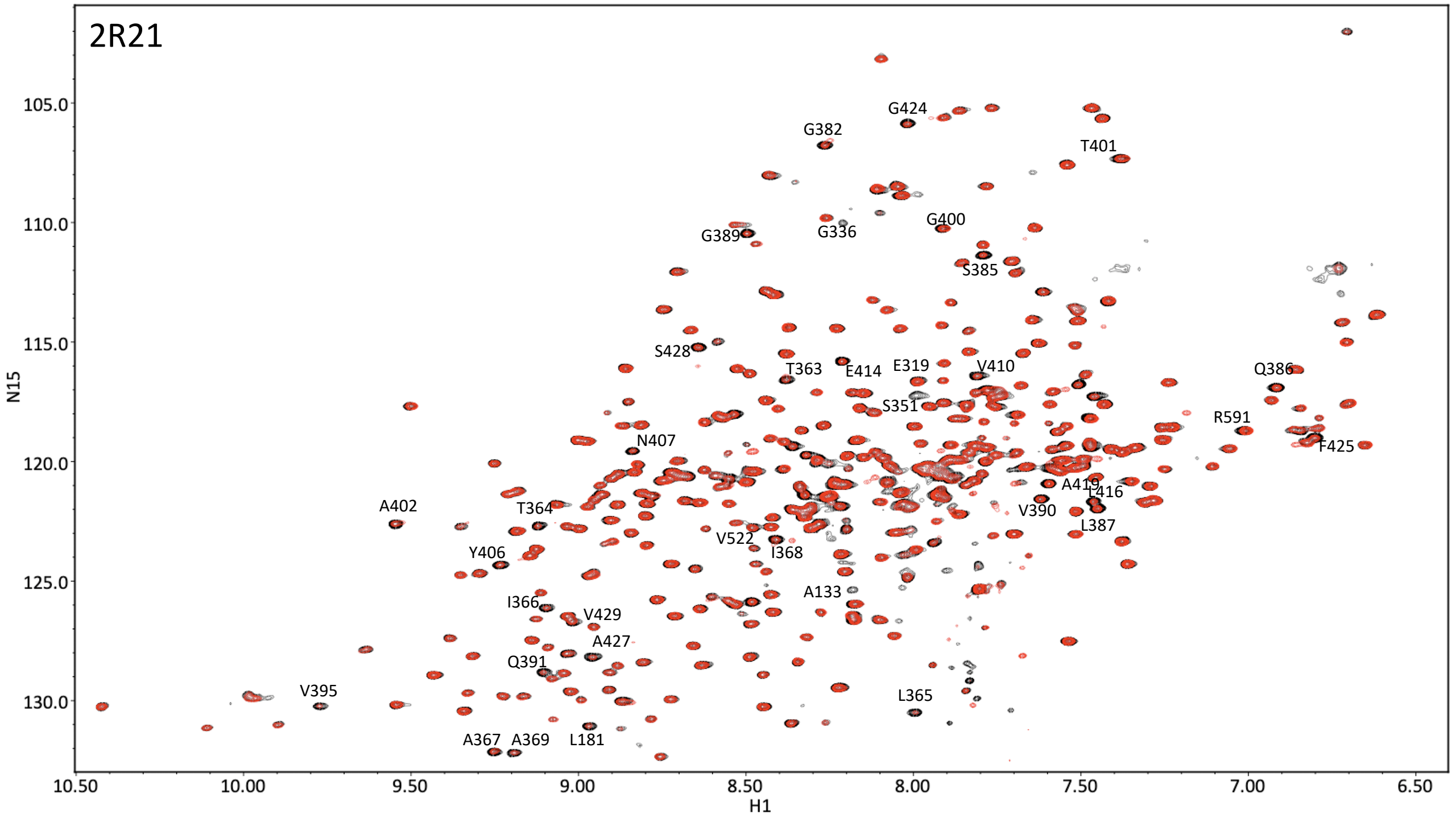
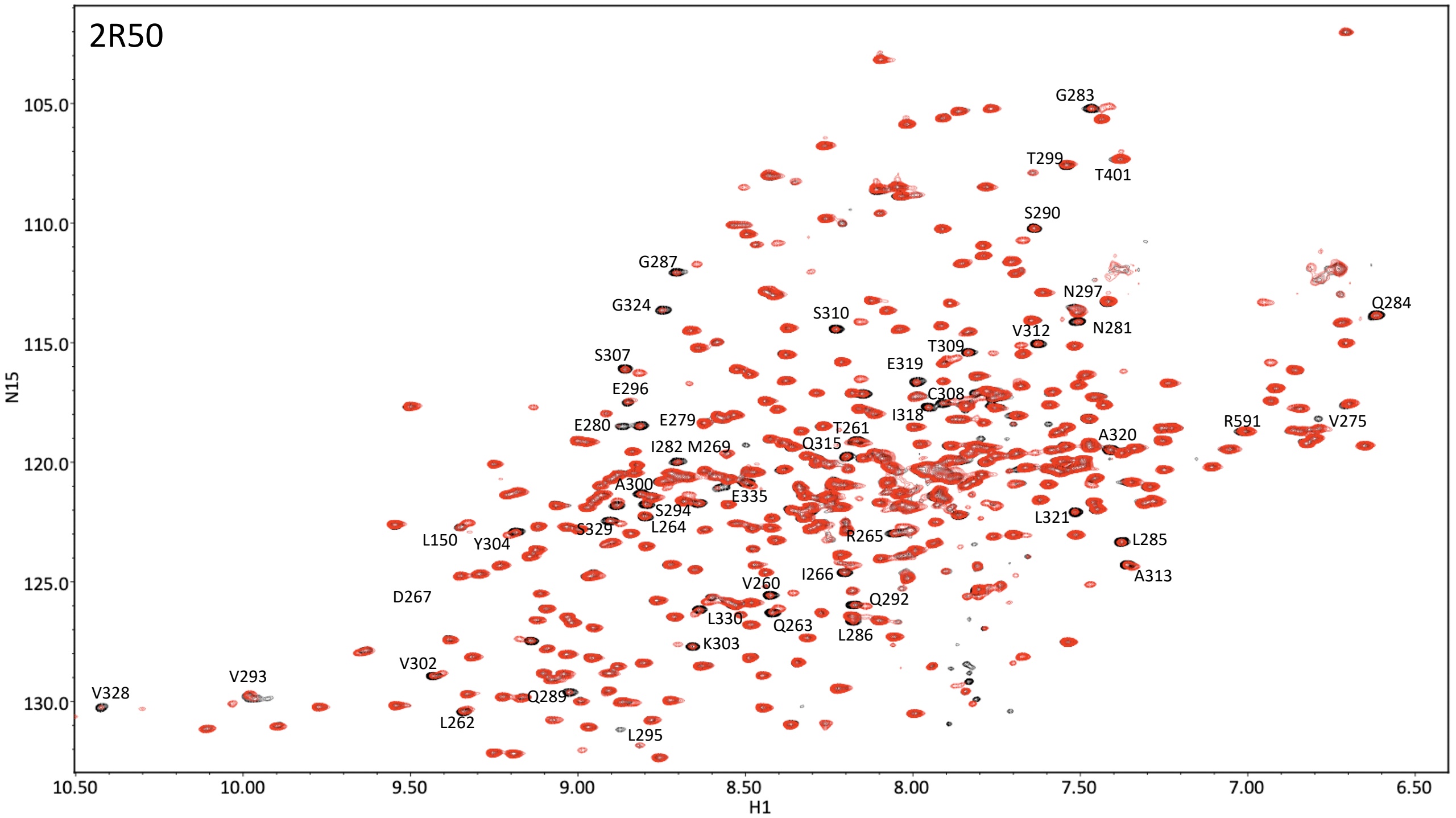
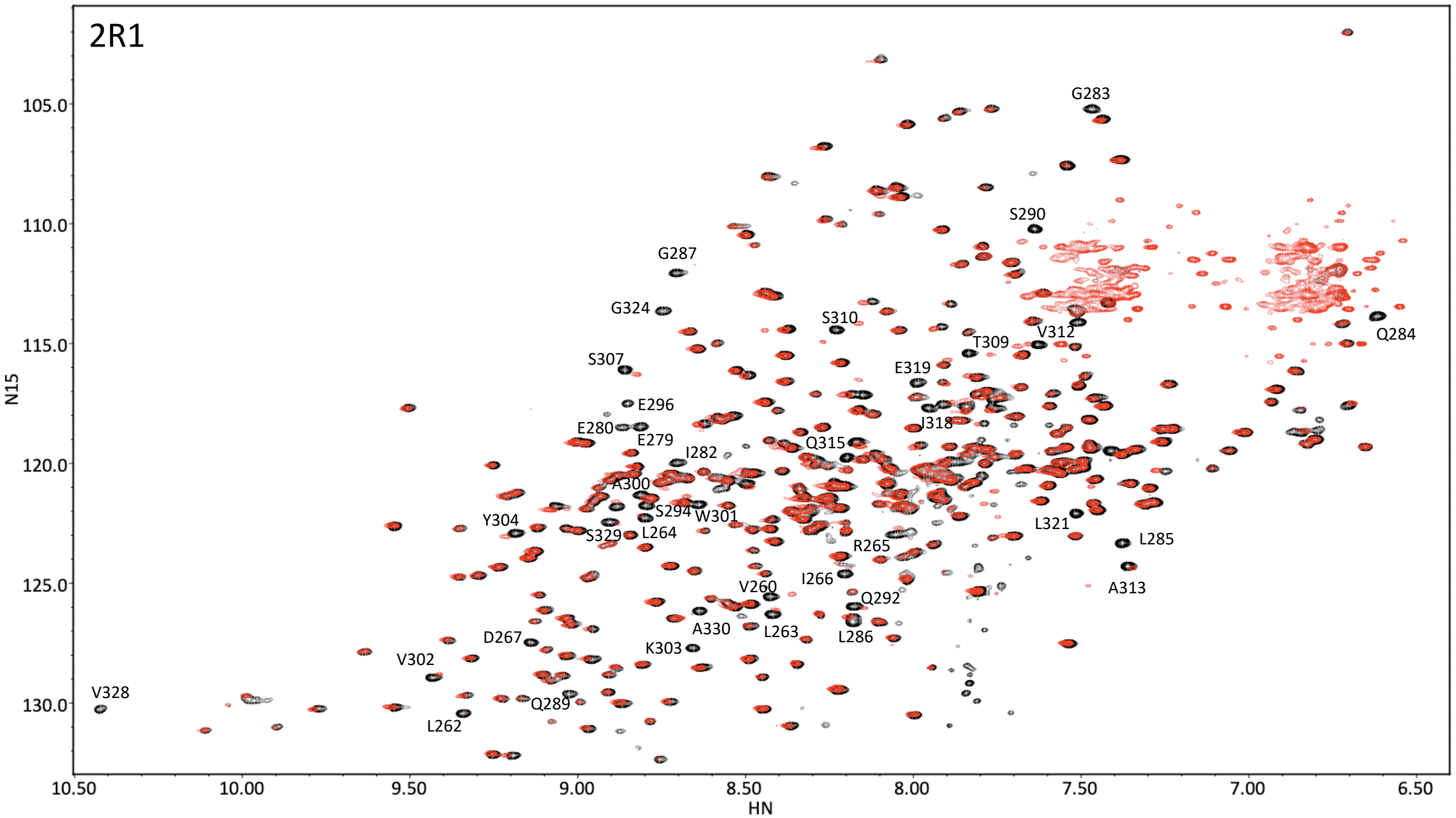
Electronic Supplementary Material (ESI) for Metallomics.
This journal is © The Royal Society of Chemistry 2020

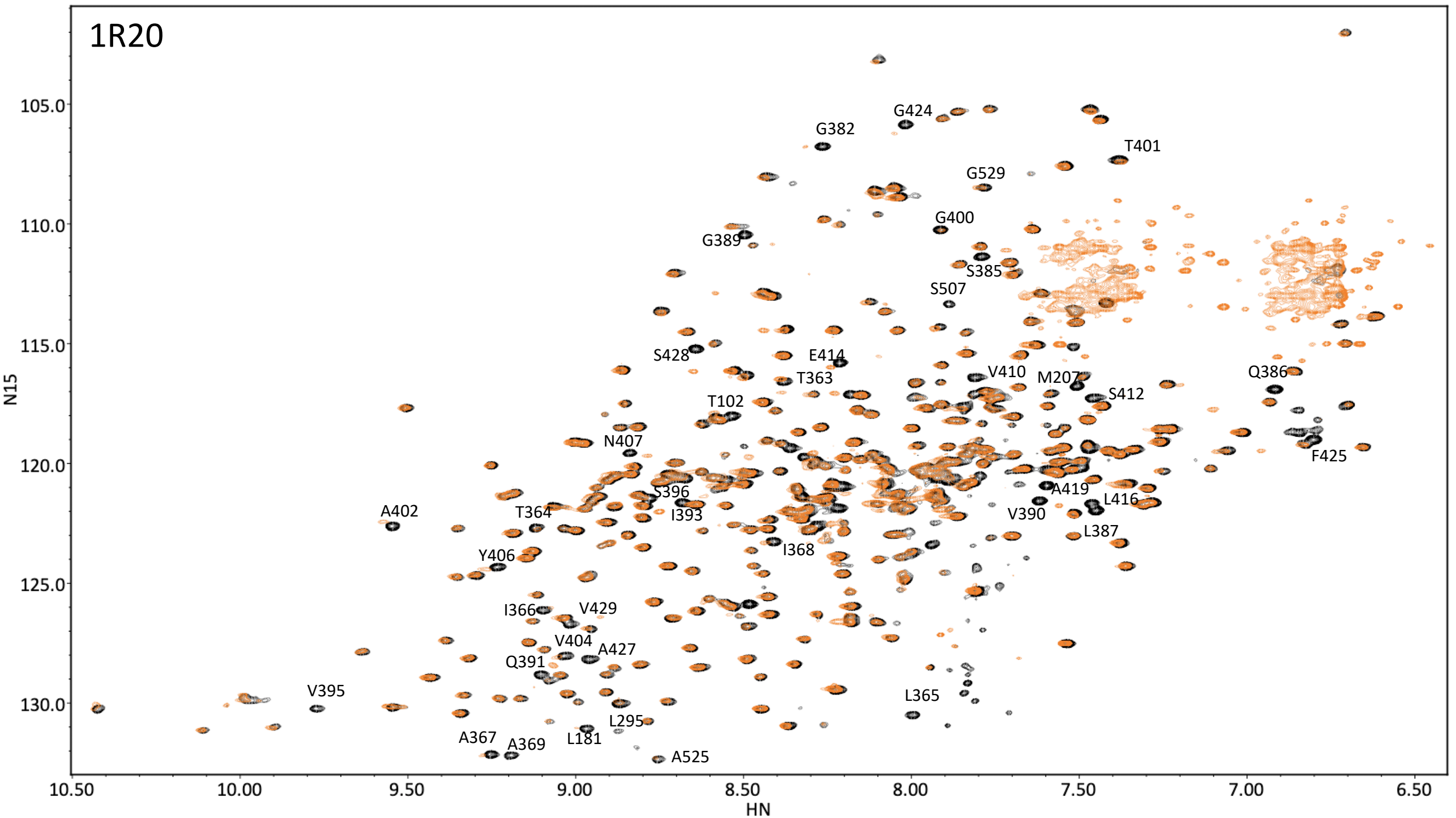
Mapping of the Nanobody Binding Sites by NMR

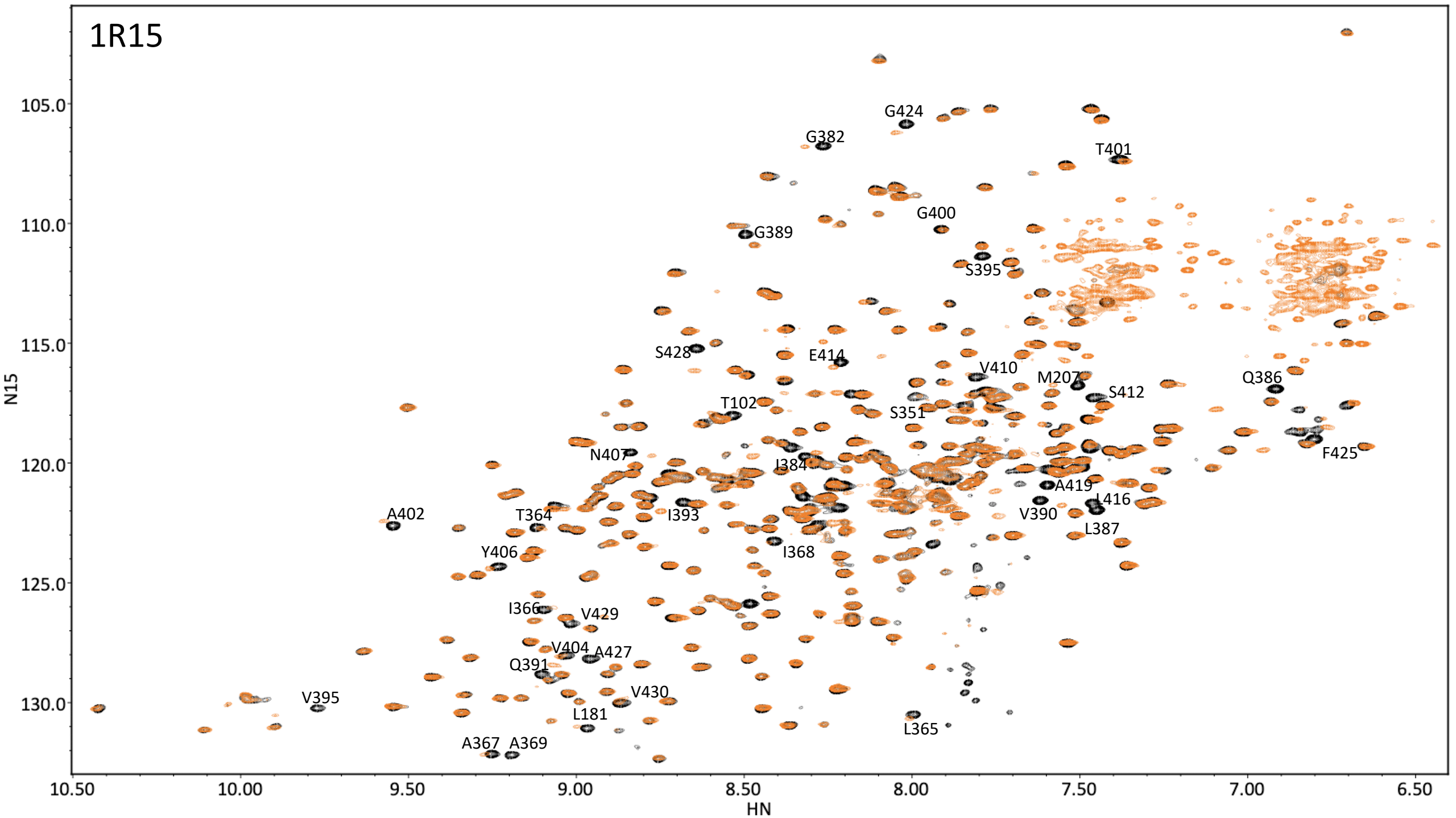
Overlays of the $^{1}H,^{15}N$-TROSY spectra of MBD1-6 recorded with (color) and without the Nanobody (black) are shown. Nanobody ID is in the upper left corner. Signals of the amino acid residues showing chemical shift change or intensity loss are labeled. Residue numbering corresponds to the MBD1-6 construct used in the experiments, including the N-terminal AGH sequence retained from the purification tag, and is shifted by +3 relative to the wild type ATP7B sequence.

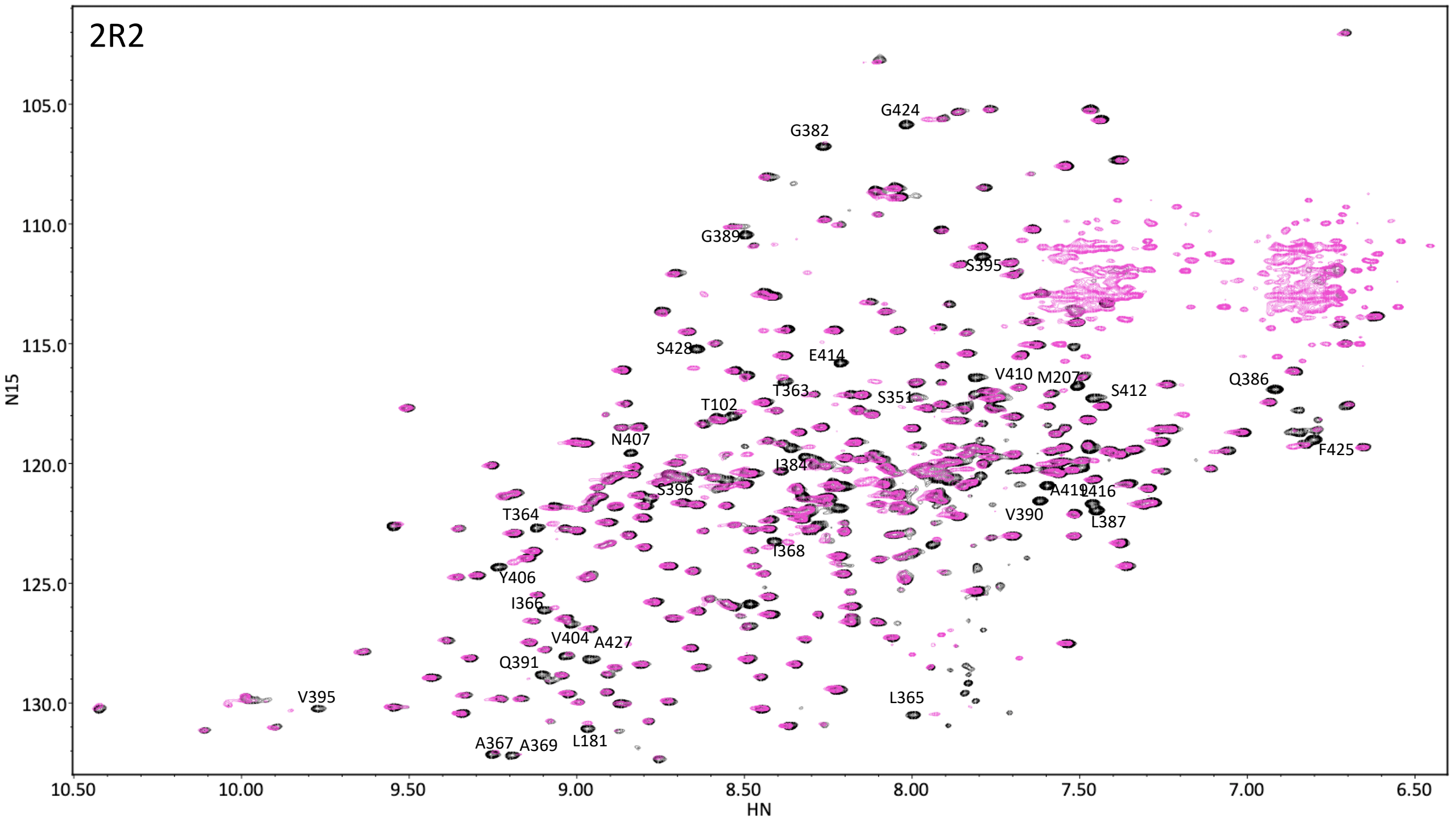

2R21
G424
G382
T401
G400
G389
G336
S385
S428
T363
E414
E319
V410
Q386
S351
R591
N407
F425
A419
L416
A402
T364
V390
L387
V522
I368
Y406
A133
I366
V429
A427
Q391
V395
L365
A367
A369
L181
105.0
110.0
115.0
120.0
125.0
130.0
N15
10.50
10.00
9.50
9.00
8.50
8.00
7.50
7.00
6.50
H1

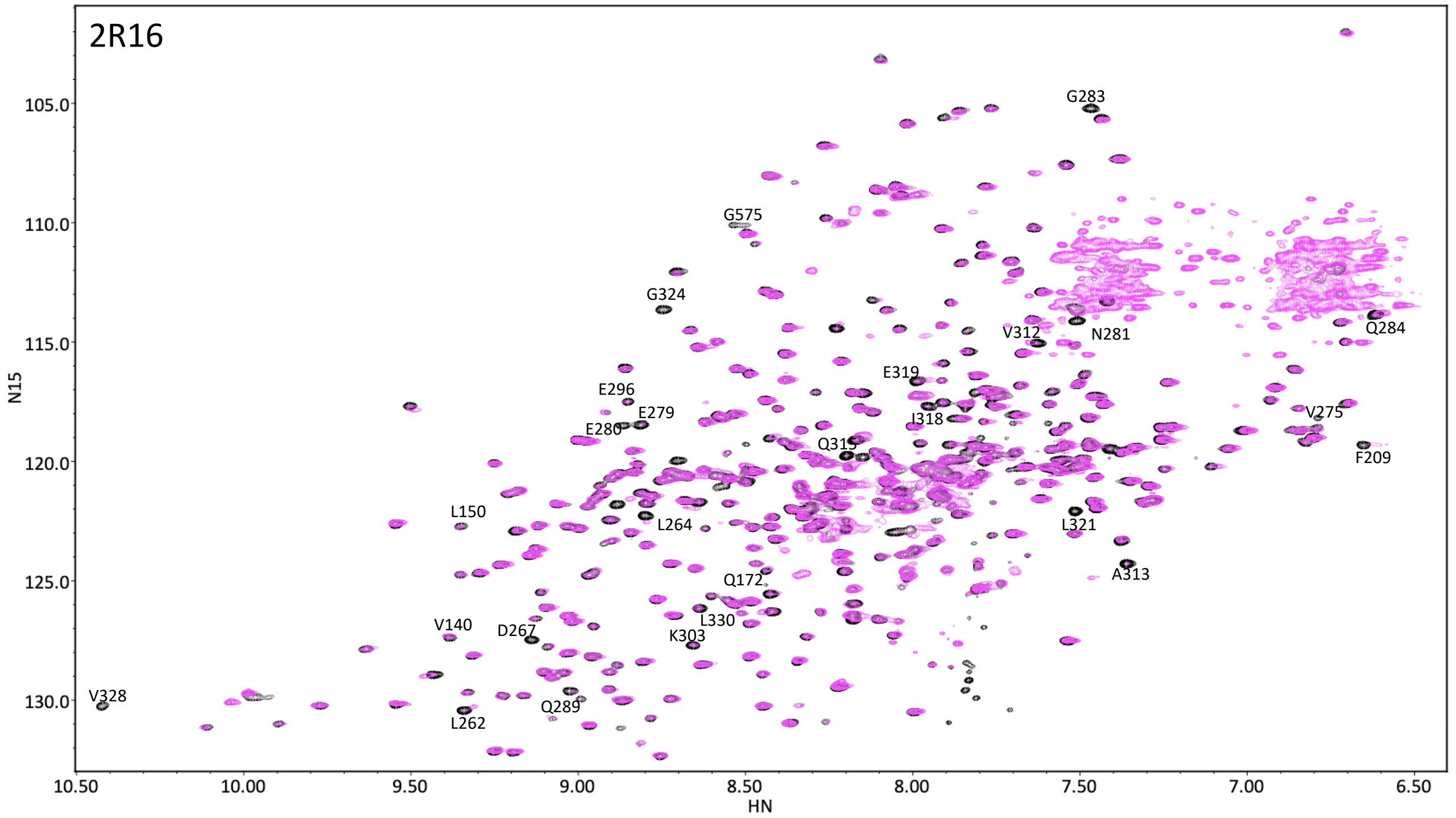

2R50
G283
T299
T401
S290
G287
N297
Q284
G324
S310
V312
N281
T309
S307
E319
E296
C308
I318
E280
E279
T261
R591
V275
A320
Q315
I282 M269
A300
E335
S294
L321
S329
L264
L150
Y304
R265
L285
I266
A313
V260
D267
Q292
L330
Q263
L286
K303
V302
V293
V328
Q289
L262
L295
105.0
110.0
115.0
120.0
125.0
130.0
N15
10.50
10.00
9.50
9.00
8.50
8.00
7.50
7.00
6.50
H1

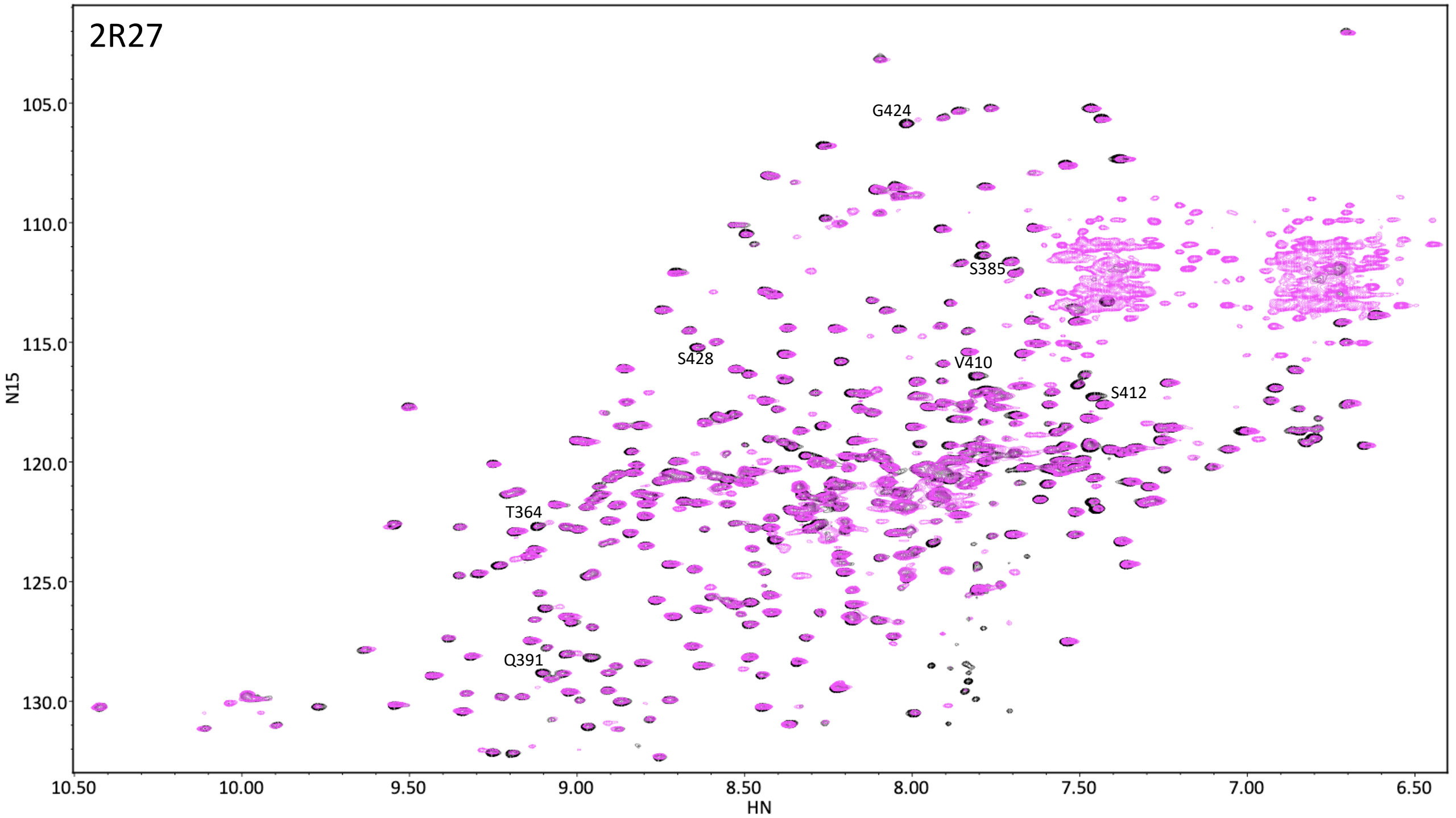

2R1
G283
S290
G287
G324
S310
V312
T309
Q284
S307
E319
E296
I318
E280
E279
Q315
I282
A300
S294
W301
Y304
S329
L264
L321
L285
R265
I266
V260
A313
Q292
A330
L263
L286
D267
K303
V302
V328
Q289
L262
105.0
110.0
115.0
120.0
125.0
130.0
N15
10.50
10.00
9.50
9.00
8.50
8.00
7.50
7.00
6.50
HN

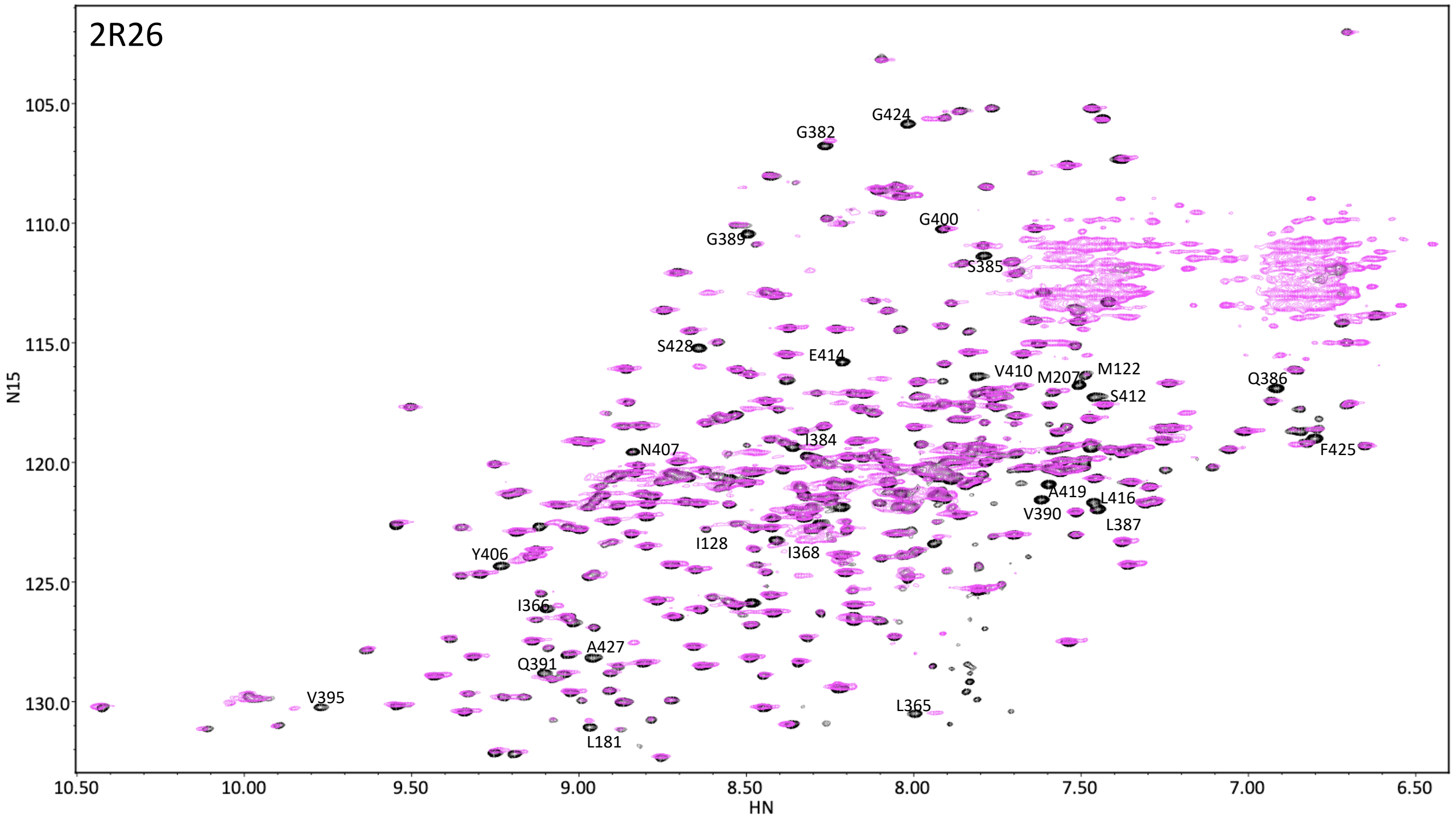

1R20
G424
G382
T401
G529
G400
G389
S385
S507
S428
E414
T363
V410
M207
S412
Q386
T102
N407
F425
S396
A419
L416
A402
T364
I393
V390
L387
I368
Y406
I366
V429
V404
A427
Q391
V395
L365
L295
A367
A369
L181
A525
105.0
110.0
115.0
120.0
125.0
130.0
N15
10.50
10.00
9.50
9.00
8.50
8.00
7.50
7.00
6.50
HN

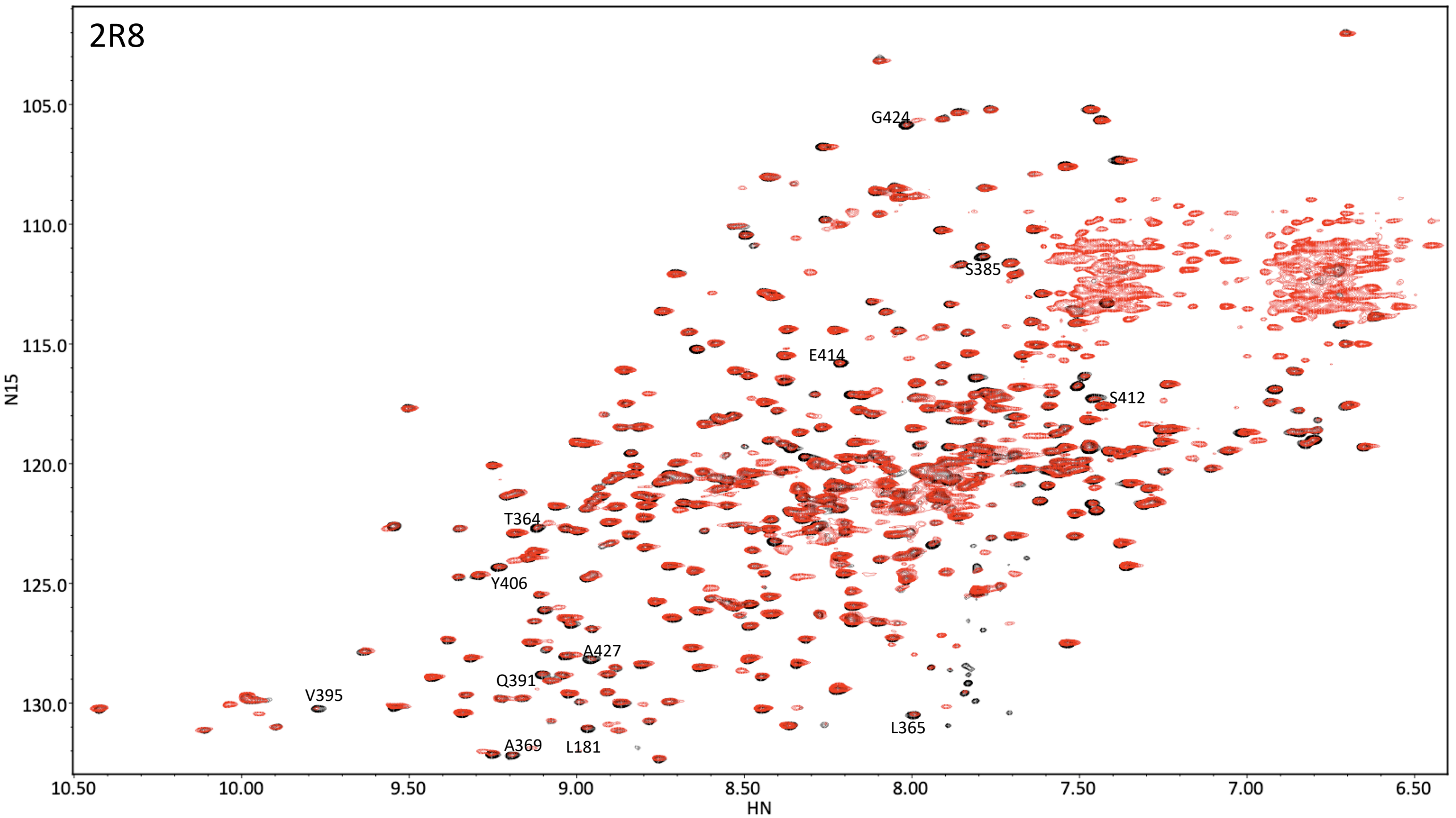

1R15
N15
HN
105.0
110.0
115.0
120.0
125.0
130.0
10.50
10.00
9.50
9.00
8.50
8.00
7.50
7.00
6.50
G424
G382
T401
G400
G389
S395
S428
E414
V410
M207
S412
Q386
T102
S351
F425
N407
I384
A419
L416
A402
T364
I393
V390
L387
Y406
I368
I366
V429
V404
A427
Q391
V395
V430
L181
L365
A367
A369

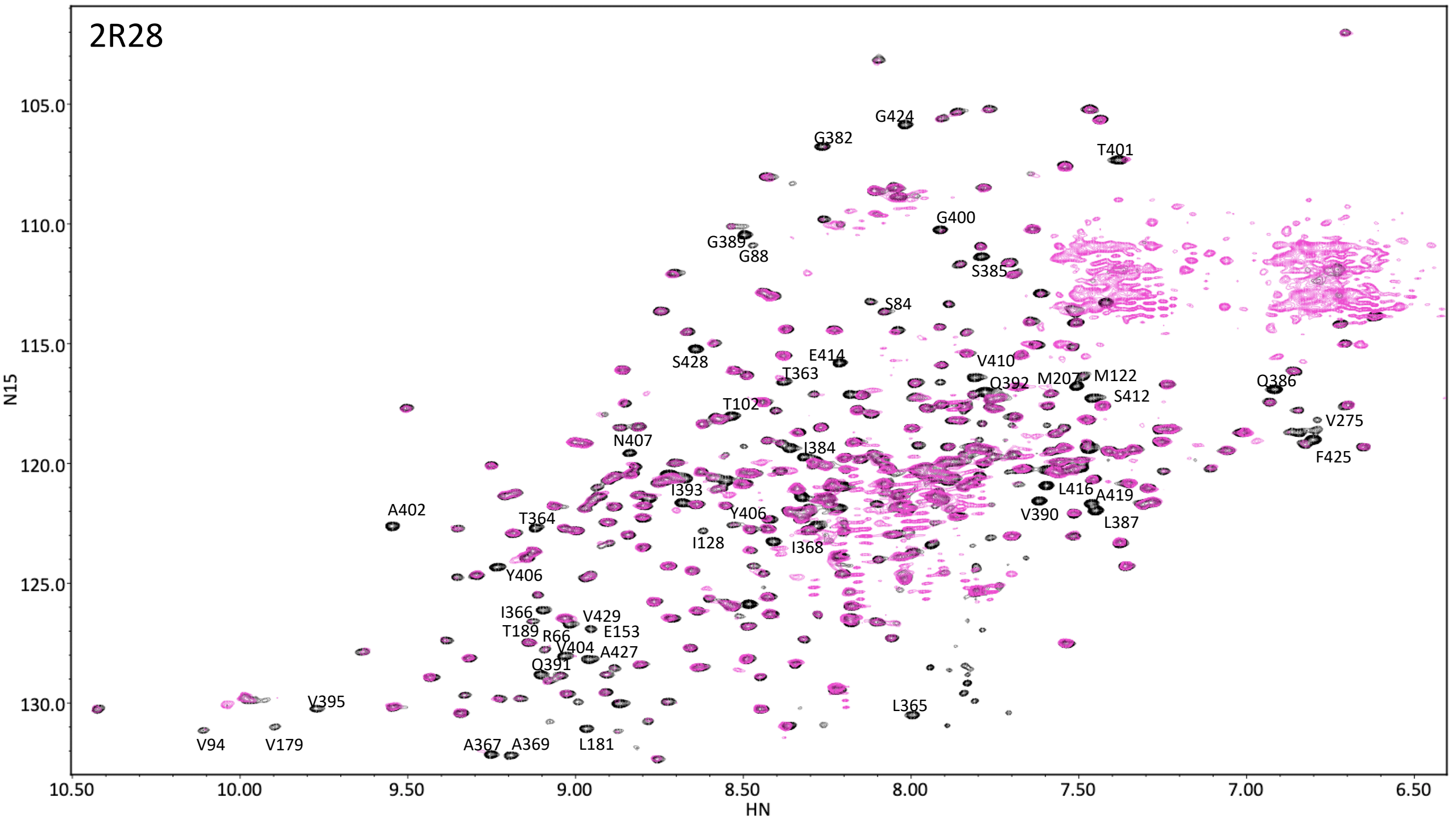

2R2
G424
G382
G389
S395
S428
E414
V410
M207
S412
Q386
T363
S351
T102
N407
F425
I384
S396
A419
I416
T364
V390
L387
I368
Y406
I366
V404
A427
Q391
V395
L365
A367
A369
L181
105.0
110.0
115.0
120.0
125.0
130.0
N15
10.50
10.00
9.50
9.00
8.50
8.00
7.50
7.00
6.50
HN

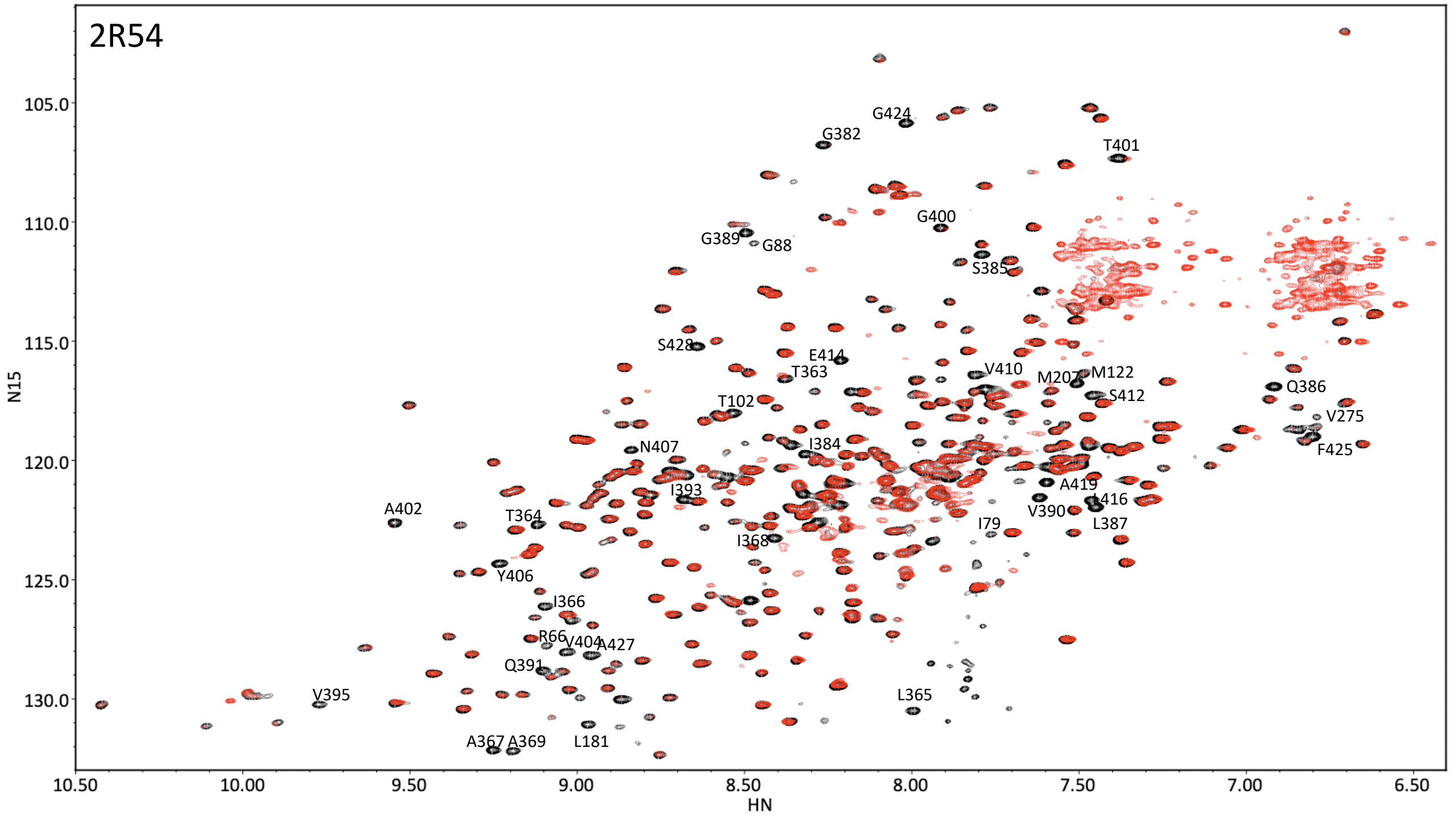

2R16
G283
G575
G324
V312
N281
Q284
E319
E296
E279
E280
I318
V275
Q315
F209
L150
L264
L321
A313
Q172
L330
V140
D267
K303
V328
Q289
L262
105.0
110.0
115.0
120.0
125.0
130.0
N15
10.50
10.00
9.50
9.00
8.50
8.00
7.50
7.00
6.50
HN

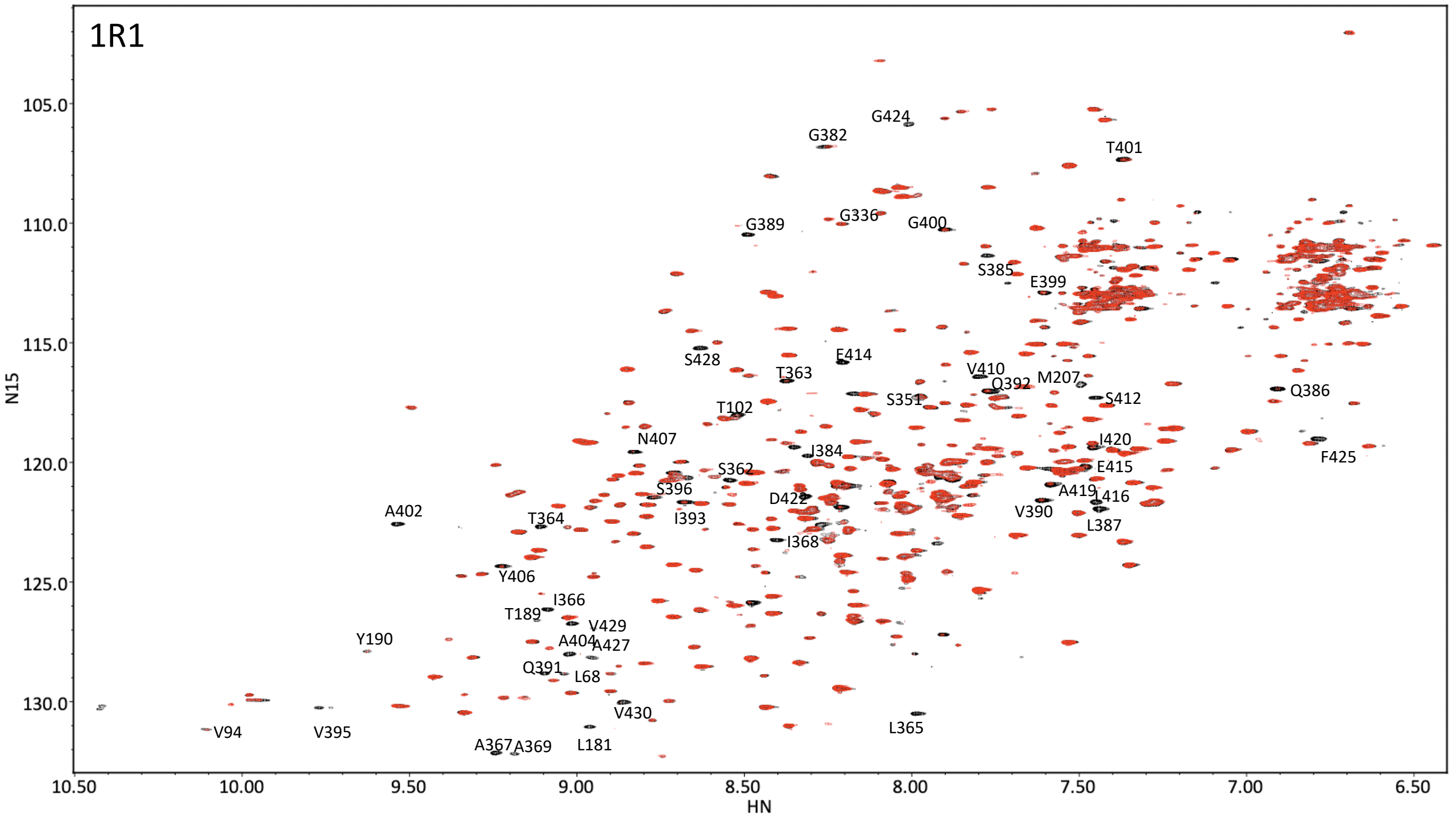

2R27
G424
S385
S428
V410
S412
T364
Q391
105.0
110.0
115.0
120.0
125.0
130.0
N15
10.50
10.00
9.50
9.00
8.50
8.00
7.50
7.00
6.50
HN

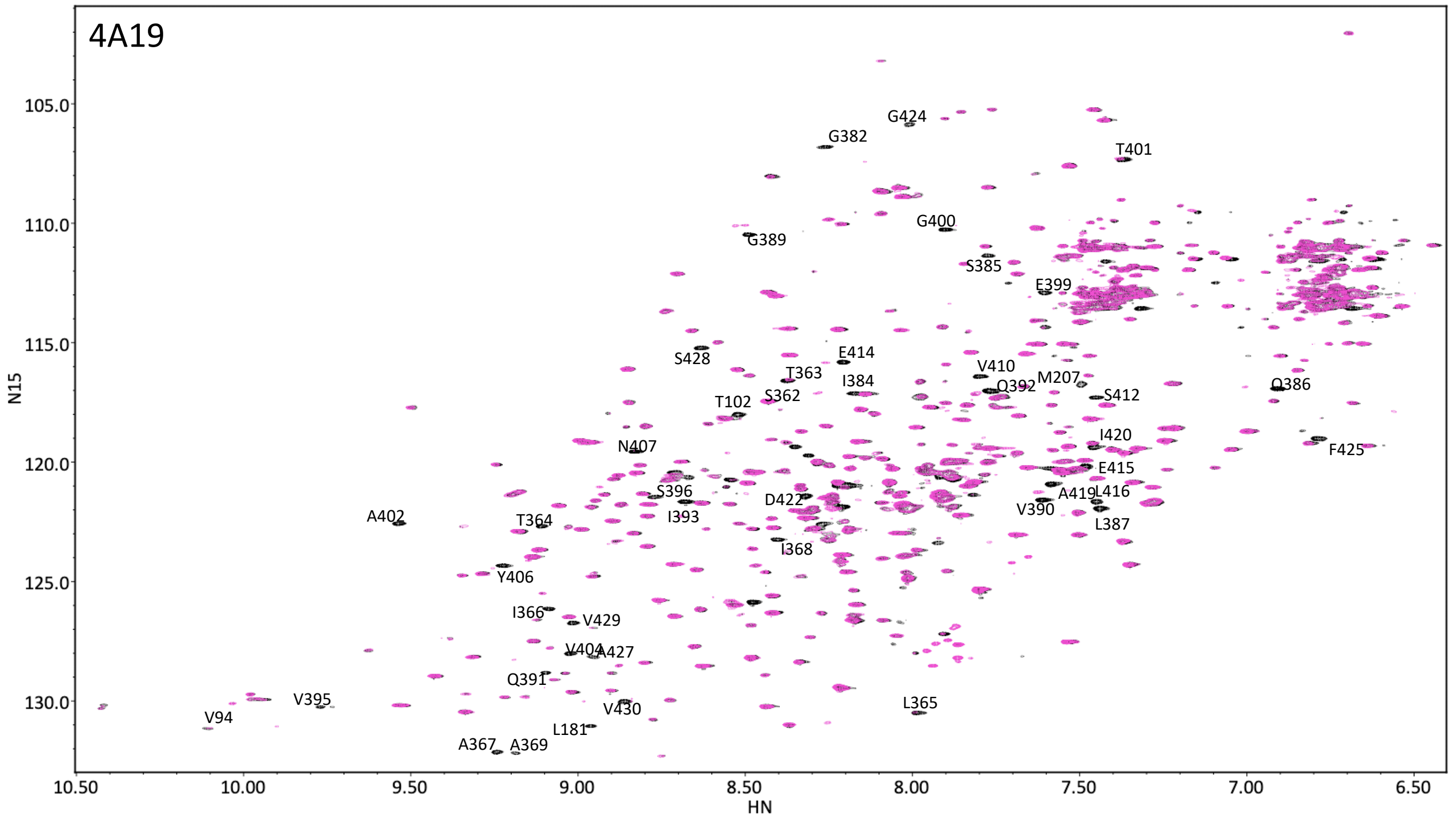

2R26
G424
G382
G400
G389
S385
S428
E414
V410
M207
M122
S412
Q386
I384
N407
F425
A419
L416
V390
L387
I128
I368
Y406
I366
A427
Q391
V395
L365
L181
105.0
110.0
115.0
120.0
125.0
130.0
N15
10.50
10.00
9.50
9.00
8.50
8.00
7.50
7.00
6.50
HN

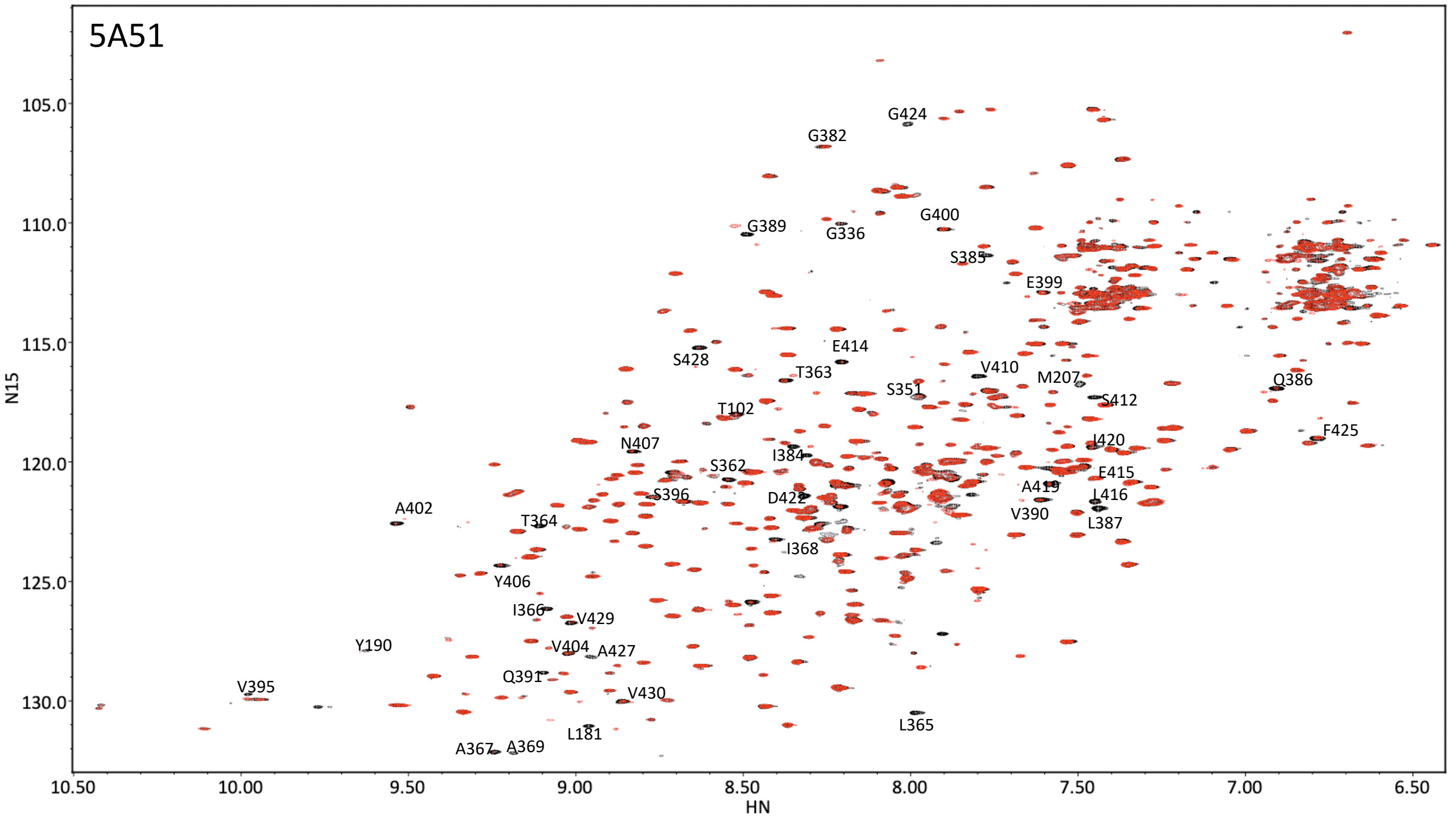

2R8
G424
S385
E414
S412
T364
Y406
A427
Q391
V395
L365
A369
L181
105.0
110.0
115.0
120.0
125.0
130.0
N15
10.50
10.00
9.50
9.00
8.50
8.00
7.50
7.00
6.50
HN

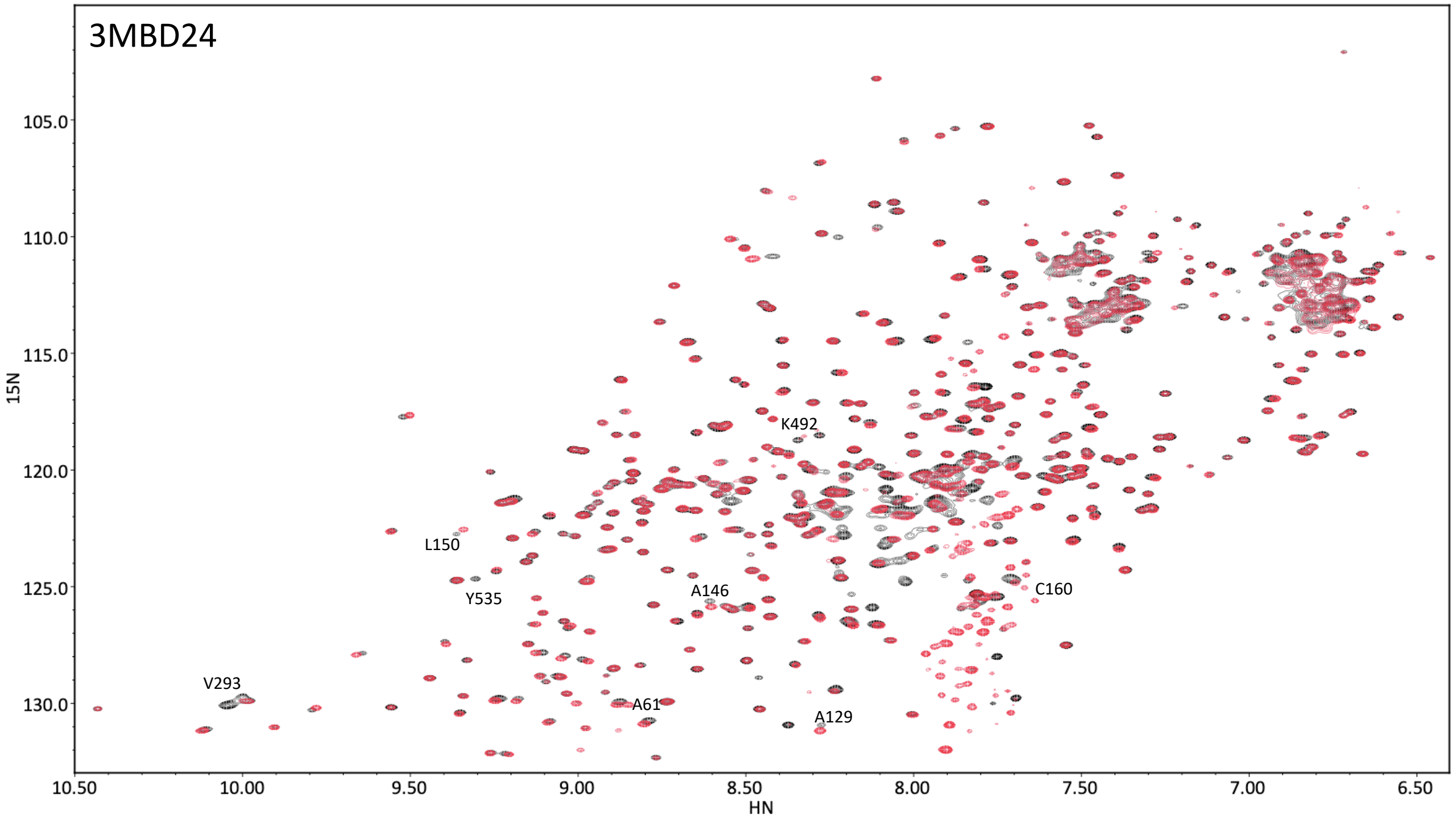

2R28
N15
HN
105.0
110.0
115.0
120.0
125.0
130.0
10.50
10.00
9.50
9.00
8.50
8.00
7.50
7.00
6.50
G424
G382
T401
G400
G389
G88
S385
S84
S428
E414
T363
V410
Q392
M207
M122
S412
Q386
T102
V275
N407
I384
F425
I393
L416
A419
A402
T364
Y406
V390
L387
I128
I368
Y406
I366
V429
T189
R66
E153
V404
A427
Q391
V395
L365
V94
V179
A367
A369
L181

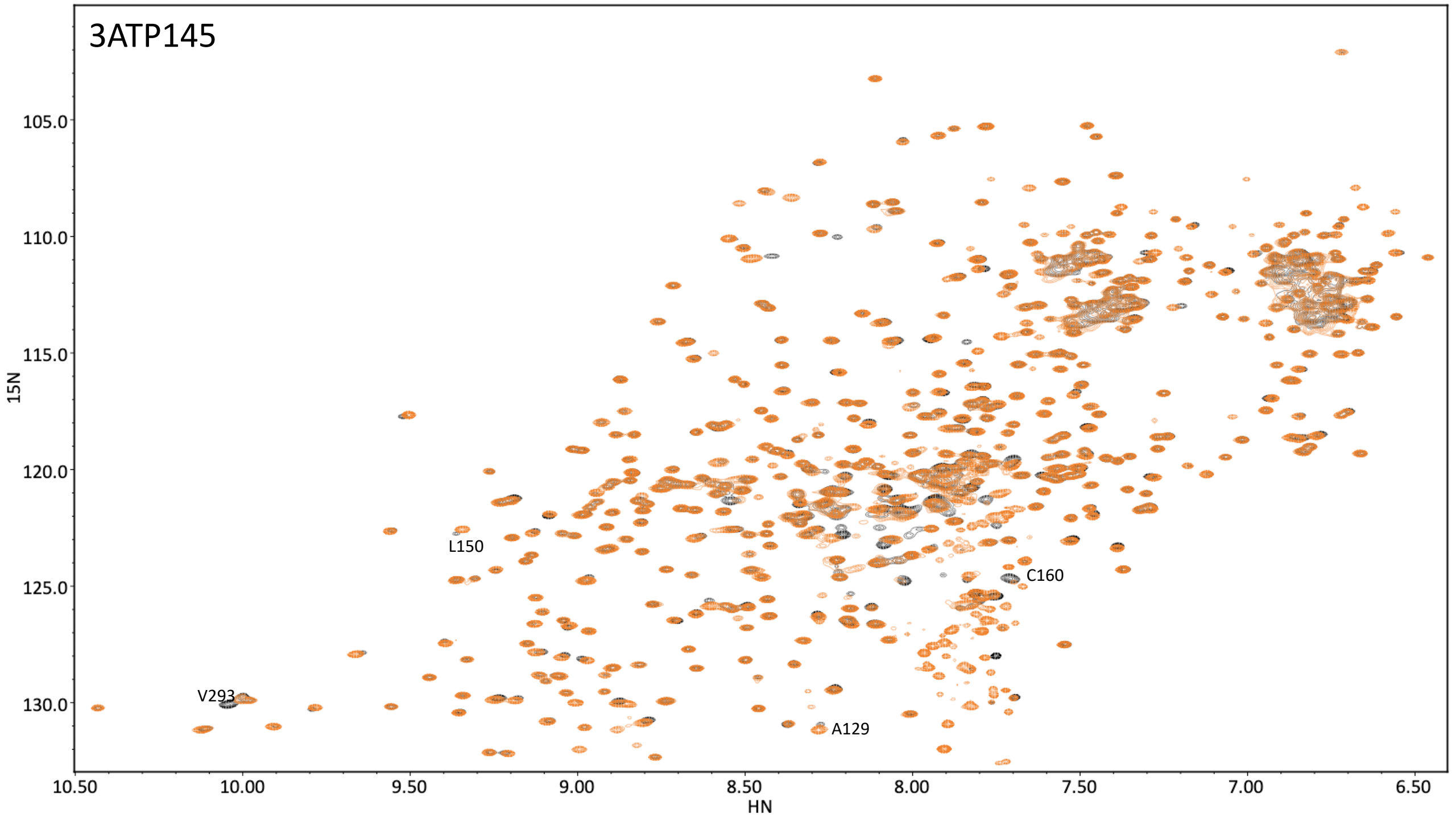

2R54
N15
HN
105.0
110.0
115.0
120.0
125.0
130.0
10.50
10.00
9.50
9.00
8.50
8.00
7.50
7.00
6.50
G424
G382
T401
G400
G389
G88
S385
S428
E414
T363
V410
M207
M122
S412
Q386
V275
F425
T102
N407
I384
I393
A419
L416
V390
L387
A402
T364
I79
I368
Y406
I366
R66
V404
A427
Q391
V395
L365
A367
A369
L181


1R1
N15
HN
105.0
110.0
115.0
120.0
125.0
130.0
10.50
10.00
9.50
9.00
8.50
8.00
7.50
7.00
6.50
G424
G382
T401
G389
G336
G400
S385
E399
S428
E414
T363
V410
Q392
M207
S351
S412
Q386
T102
N407
I384
I420
F425
S362
E415
S396
A419
L416
D422
A402
T364
I393
V390
L387
I368
Y406
I366
T189
V429
Y190
A404
A427
Q391
L68
V430
V94
V395
L365
A367
A369
L181


4A19
N15
HN
105.0
110.0
115.0
120.0
125.0
130.0
10.50
10.00
9.50
9.00
8.50
8.00
7.50
7.00
6.50
G424
G382
T401
G400
G389
S385
E399
S428
E414
T363
V410
I384
M207
Q392
Q386
S412
T102
S362
I420
N407
F425
E415
S396
D422
A419
L416
V390
A402
T364
I393
L387
I368
Y406
I366
V429
V404
A427
Q391
V395
V430
L365
V94
L181
A367
A369


5A51
N15
HN
105.0
110.0
115.0
120.0
125.0
130.0
10.50
10.00
9.50
9.00
8.50
8.00
7.50
7.00
6.50
G424
G382
G400
G389
G336
S385
E399
E414
S428
T363
V410
M207
Q386
S351
S412
T102
F425
N407
I420
I384
S362
F415
A419
S396
D422
L416
A402
V390
T364
L387
I368
Y406
I366
V429
Y190
V404
A427
Q391
V395
V430
L365
L181
A367
A369


3MBD24
105.0
110.0
115.0
120.0
125.0
130.0
15N
10.50
10.00
9.50
9.00
8.50
8.00
7.50
7.00
6.50
HN
K492
L150
Y535
A146
C160
V293
A61
A129


3ATP145
105.0
110.0
115.0
120.0
125.0
130.0
15N
L150
C160
V293
A129
10.50
10.00
9.50
9.00
8.50
8.00
7.50
7.00
6.50
HN