Supporting Information for

J – Based 3D Side-Chain Correlation in Solid-State Proteins

Ye Tian,[1] Lingling Chen,[1] Dimitri Niks,[2] J. Michael Kaiser,[1] Jinfeng Lai,[1] Chad M. Rienstra,[3] Michael F. Dunn,[2] and Leonard J. Mueller*[,1]

[1]*Department of Chemistry, University of California, Riverside, California 92521,*

[2]*Department of Biochemistry, University of California, Riverside, California 92521,*

and [3]*Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801*

* Corresponding Author:

Leonard J. Mueller, Department of Chemistry, University of California, Riverside, CA 92521.

Phone: (951) 827-3565. Fax: (951) 827-4713. E-mail: Leonard.Mueller@ucr.edu

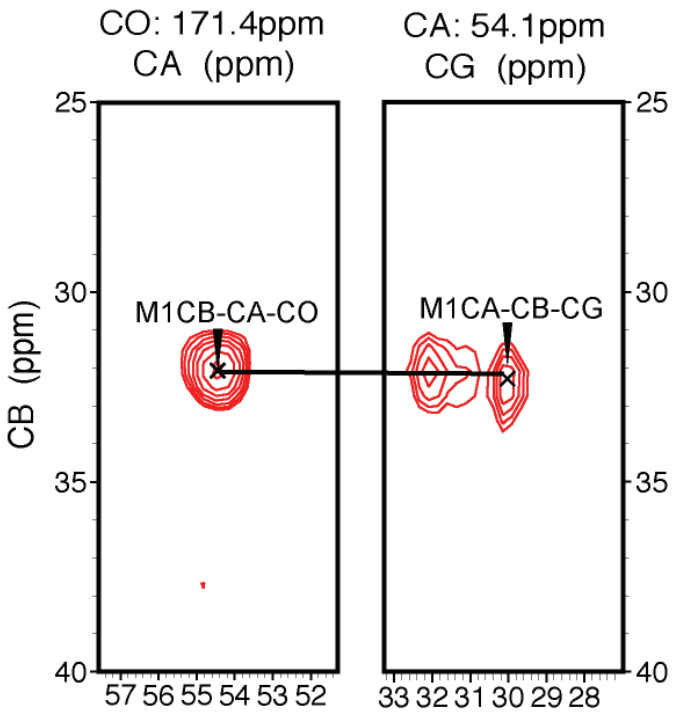
Table of Contents

Table S1: ^{13}C Chemical Shifts of Microcrystalline GB1

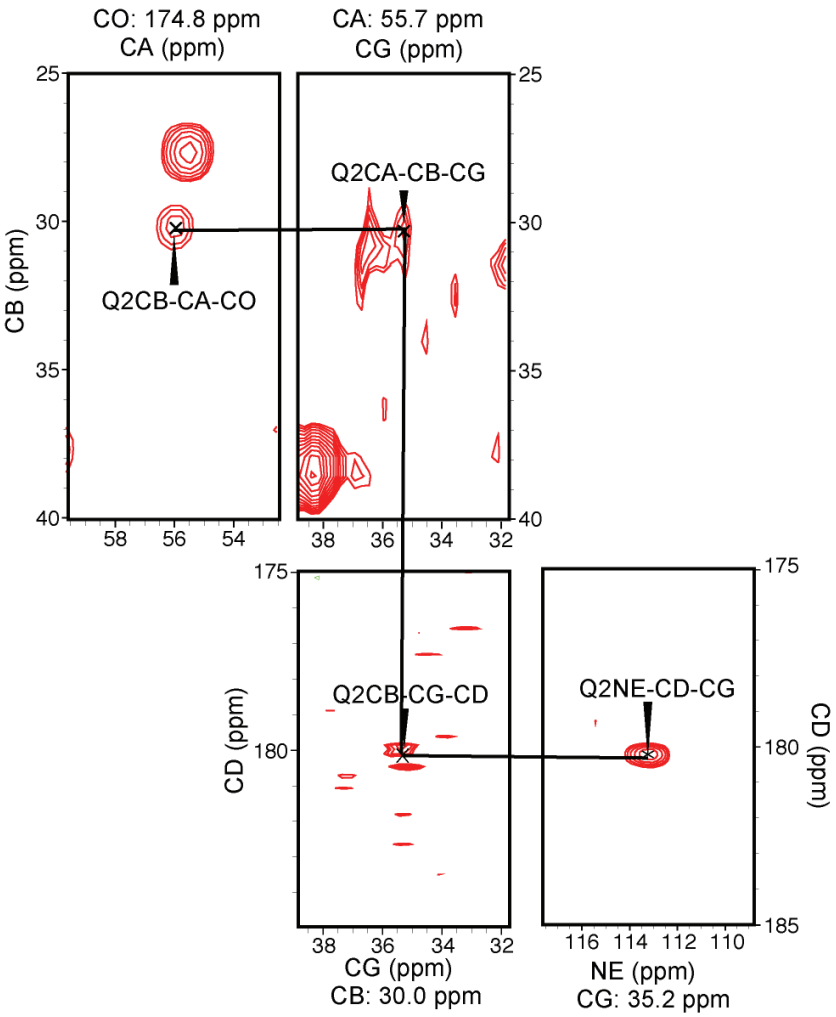
res	C′	C_α	C_β	C_γ	C_δ	C_ε
M1	171.21	54.26	32.22	30.15		----
Q2	174.86	55.88	30.16	35.30	180.26	
Y3	174.89	57.15	----	----	----	----
K4	173.16	54.83	36.17	25.54	29.27	42.30
L5	174.77	53.01	42.47	27.37	25.76	
					25.08	
I6	175.08	59.98	37.86	27.42	12.74	
				17.66		
L7	174.94	54.84	43.20	26.95	26.77	
					25.10	
N8	175.99	50.77	38.47	176.33		
G9	172.88	44.75				
K10	178.73	59.29	32.77	25.96	29.00	42.10
T11	172.99	62.09	69.50	22.44		
L12	173.70	54.58	43.08	27.72	26.10	
					23.00	
K13	175.60	53.47	39.12	25.94	29.46	43.05
G14	170.91	45.09				
E15	173.85	53.97	34.35	35.37	181.70	
T16	172.05	60.28	70.84	19.78		
T17	174.12	60.36	72.90	21.89		
T18	171.03	61.47	70.96	18.74		
E19	175.86	54.50	30.95	35.84	182.40	
A20	177.40	50.88	23.56			
V21	174.84	63.73	31.92	21.63		
				20.31		
D22	175.14	52.58	42.37	179.65		
A23	179.79	54.58	18.46			
A24	181.18	54.48	18.17			
T25	175.51	67.66	67.75	21.49		
A26	177.18	55.18	17.49			
E27	177.68	59.27	29.01	35.57	181.25	
K28	178.50	60.40	32.75	26.58	30.14	42.24
V29	178.10	66.47	31.80	22.27		
				21.22		
F30	178.73	57.49	----	----	----	----
K31	179.56	60.33	31.80	27.19	29.63	41.27
Q32	177.36	58.96	29.13	34.10	179.44	
Y33	178.30	61.71	----	----	----	----
A34	179.64	56.15	17.96			
N35	179.34	57.15	39.56	176.00		
D36	175.69	56.06	38.47	177.37		
N37	174.02	53.71	40.65	176.41		
G38	173.80	46.88				
V39	174.89	61.91	31.80	21.95		
D40	175.21	52.85	41.45	180.80		
G41	172.69	45.26				
E42	177.66	55.37	31.56	36.06	182.30	
W43	176.76	57.62	----	----	----	----
T44	173.69	61.00	72.78	21.19		
Y45	171.85	57.88	----	----	----	----
D46	175.91	51.11	42.95	179.90		
D47	177.11	54.45	43.13	179.40		
A48	179.00	53.96	19.14			
T49	175.33	60.61	69.87	21.65		
K50	175.18	55.50	27.71	24.16	28.12	43.30
T51	174.06	62.56	71.93	21.40		
F52	175.59	56.61	----	----	----	----
T53	171.92	60.38	72.02	21.30		
V54	172.53	58.73	32.59	21.74		
				19.47		
T55	174.20	61.35	72.29	21.33		
E56	180.16	57.64	33.51	38.97	182.98	

Chemical shift assignments

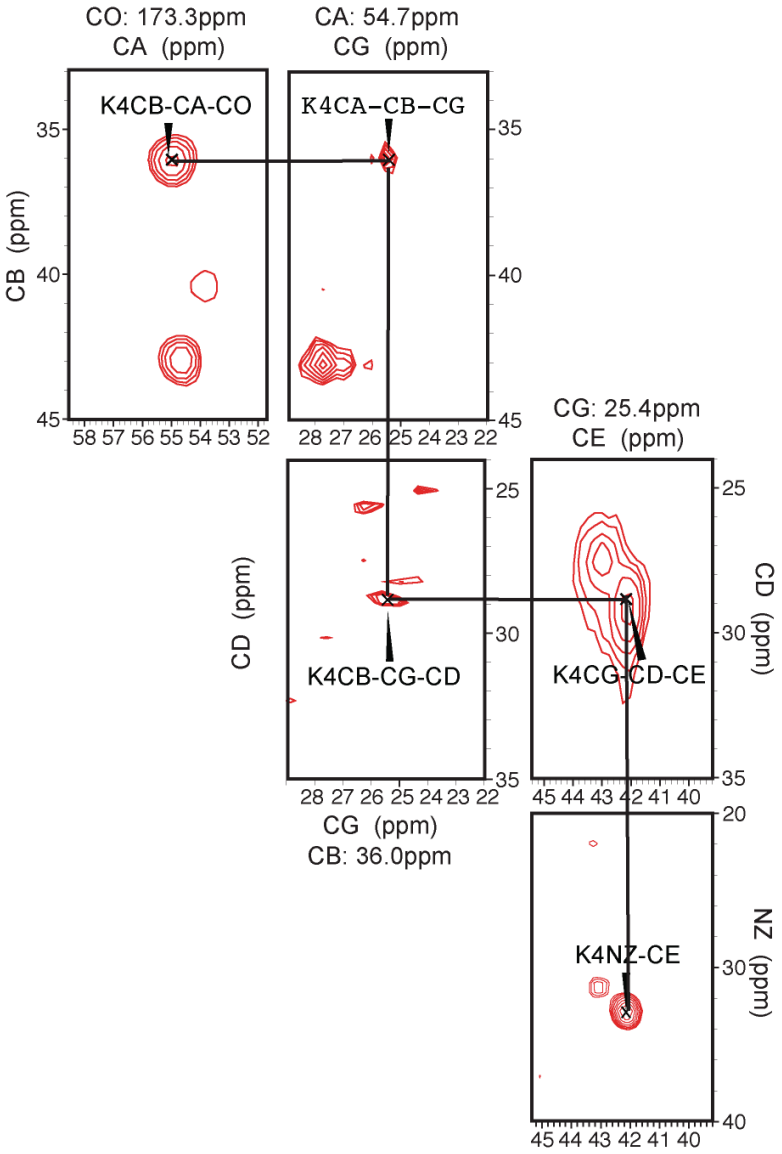
Methionine-1



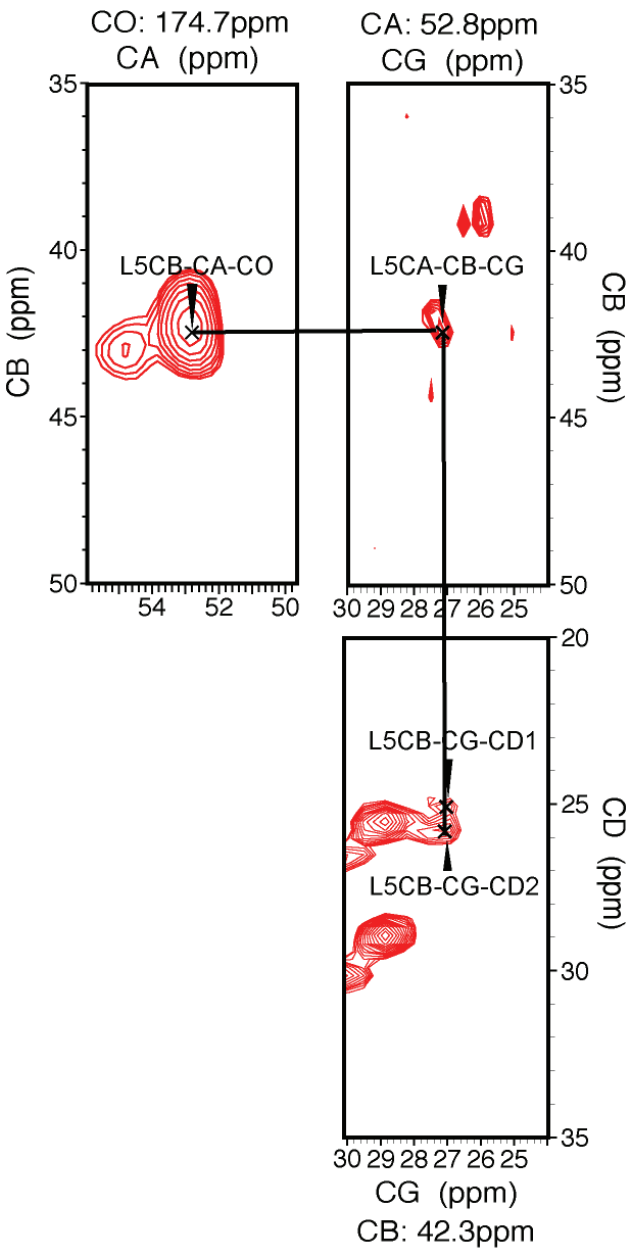
Glutamine-2


CO: 174.8 ppm
CA (ppm)
CA: 55.7 ppm
CG (ppm)
Q2CA-CB-CG
Q2CB-CA-CO
CB (ppm)
Q2CB-CG-CD
Q2NE-CD-CG
CD (ppm)
CG (ppm)
CB: 30.0 ppm
NE (ppm)
CG: 35.2 ppm

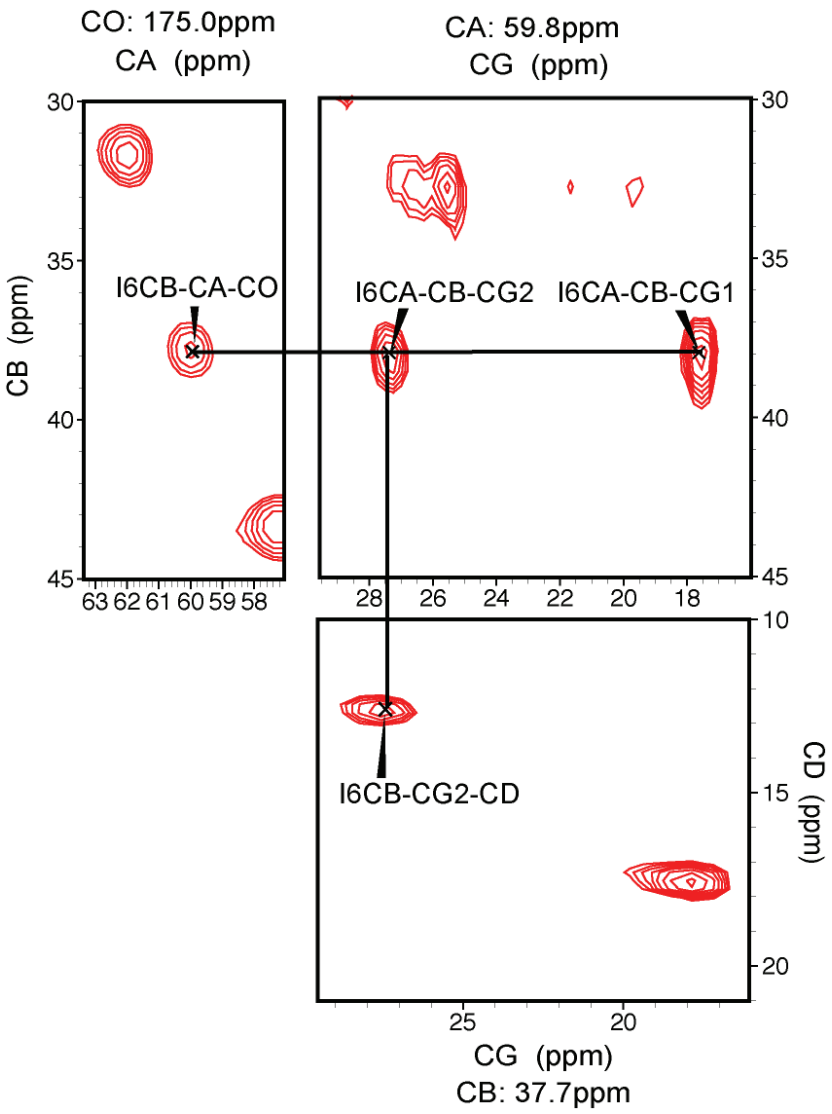
Lysine-4


CO: 173.3ppm
CA (ppm)
CA: 54.7ppm
CG (ppm)
K4CB-CA-CO
K4CA-CB-CG
CB (ppm)
35
40
45
58 57 56 55 54 53 52
28 27 26 25 24 23 22
CG: 25.4ppm
CE (ppm)
CD (ppm)
25
30
35
K4CB-CG-CD
K4CG-CD-CE
45 44 43 42 41 40
CG (ppm)
CB: 36.0ppm
20
NZ (ppm)
K4NZ-CE
40

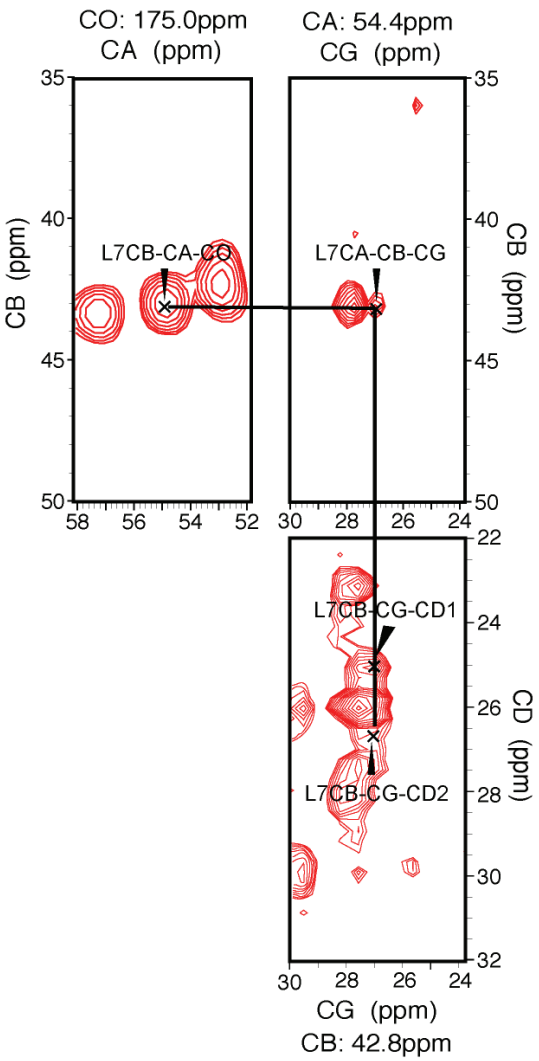
Leucine-5


CO: 174.7ppm
CA (ppm)
CA: 52.8ppm
CG (ppm)
L5CB-CA-CO
L5CA-CB-CG
L5CB-CG-CD1
L5CB-CG-CD2
CB (ppm)
CD (ppm)
CG (ppm)
CB: 42.3ppm

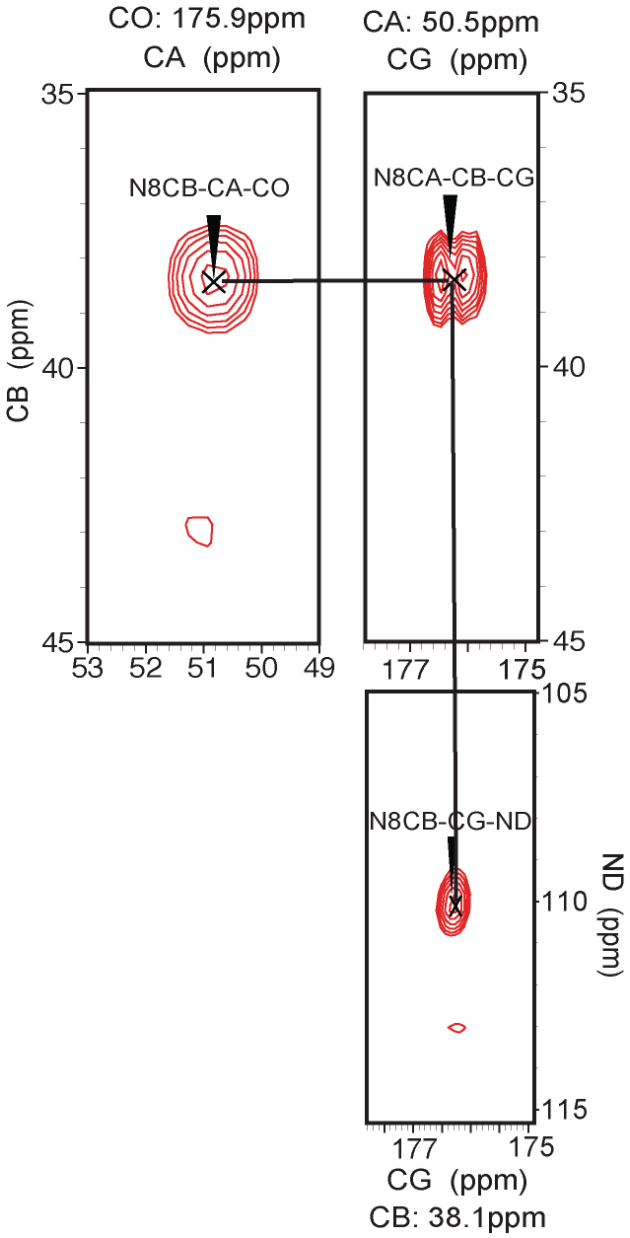
Isoleucine-6



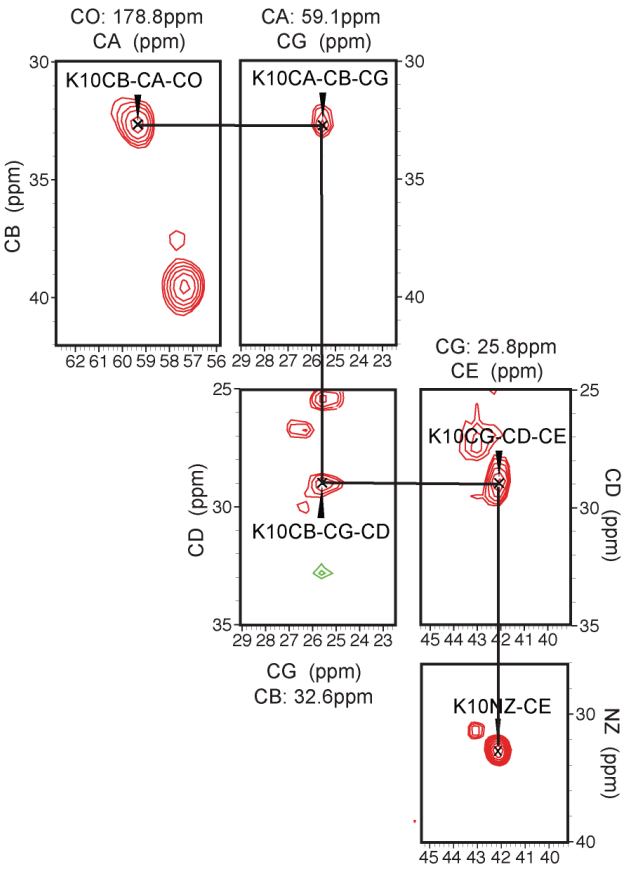
Leucine-7


CO: 175.0ppm
CA (ppm)
CA: 54.4ppm
CG (ppm)
CB (ppm)
L7CB-CA-CG
L7CA-CB-CG
L7CB-CG-CD1
L7CB-CG-CD2
CD (ppm)
CG (ppm)
CB: 42.8ppm

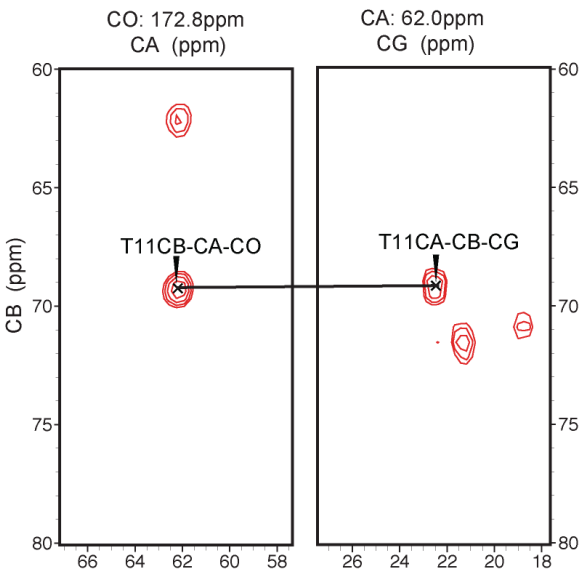
Asparagine-8



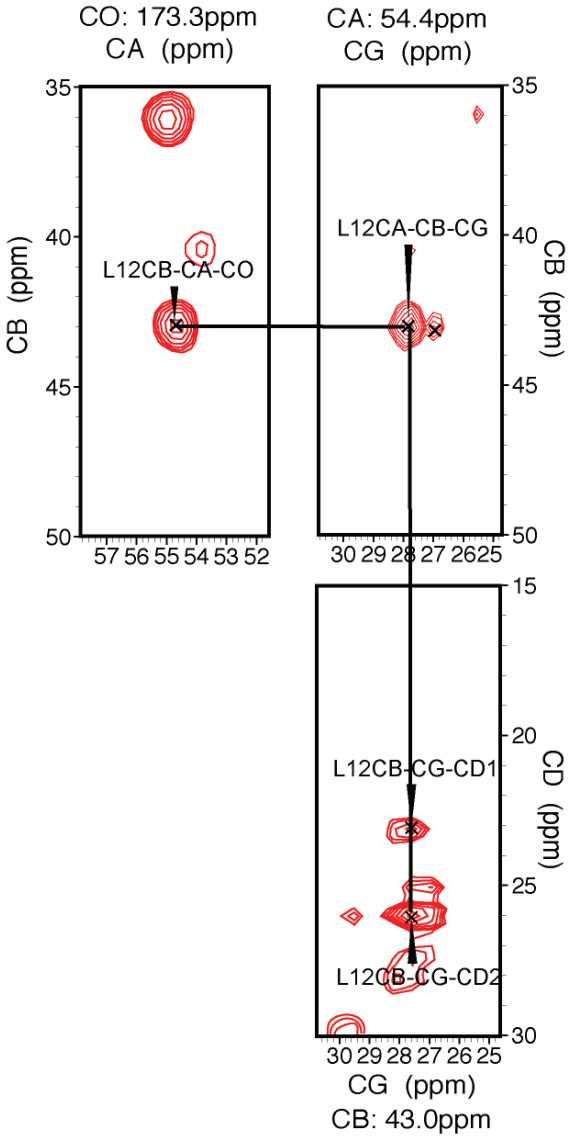
Lysine-10


CO: 178.8ppm
CA (ppm)
CA: 59.1ppm
CG (ppm)
K10CB-CA-CO
K10CA-CB-CG
CB (ppm)
CG: 25.8ppm
CE (ppm)
K10CG-CD-CE
CD (ppm)
K10CB-CG-CD
CG (ppm)
CB: 32.6ppm
K10NZ-CE
NZ (ppm)

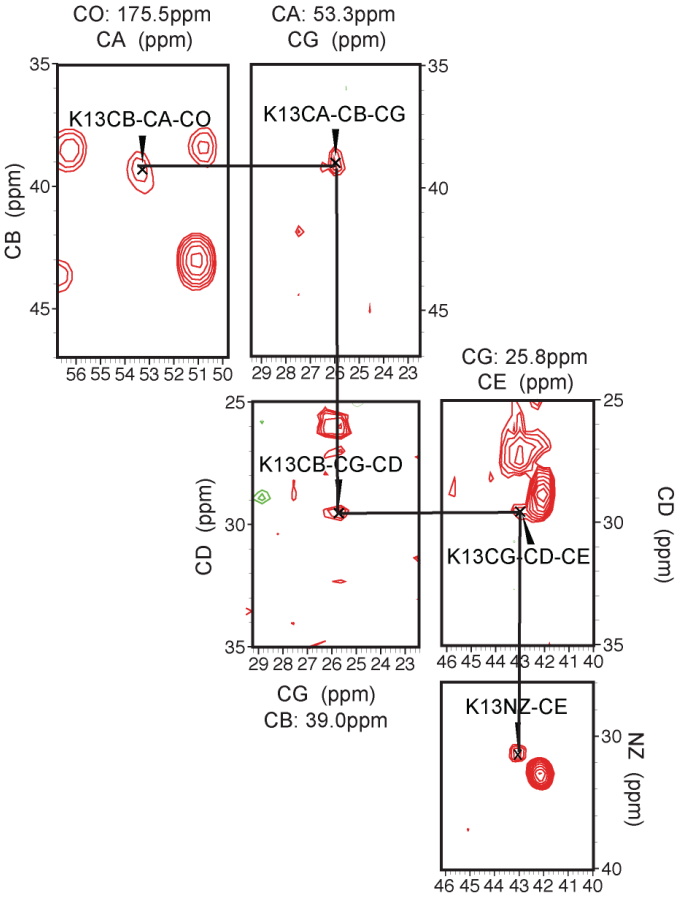
Threonine-11



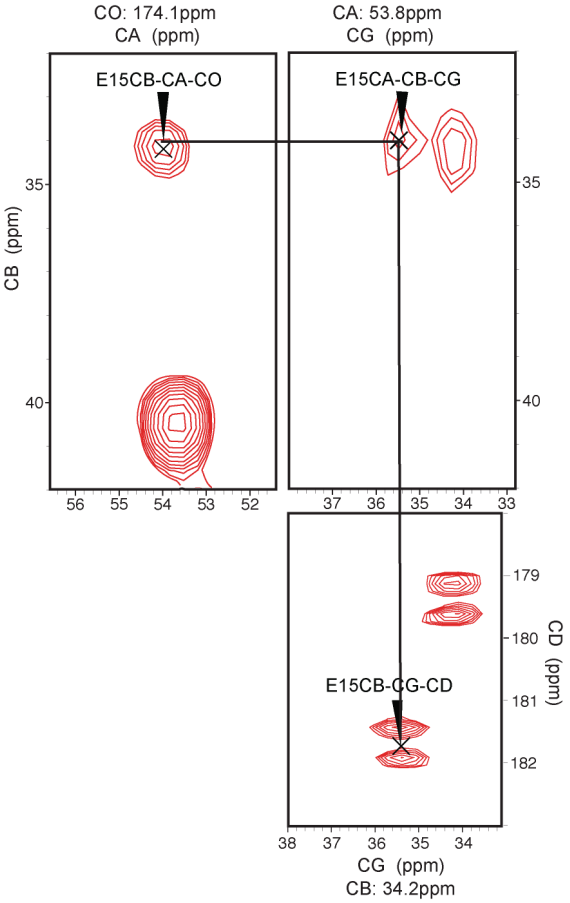
Leucine-12


CO: 173.3ppm
CA (ppm)
CA: 54.4ppm
CG (ppm)
CB (ppm)
L12CB-CA-CO
L12CA-CB-CG
CD (ppm)
L12CB-CG-CD1
L12CB-CG-CD2
CG (ppm)
CB: 43.0ppm

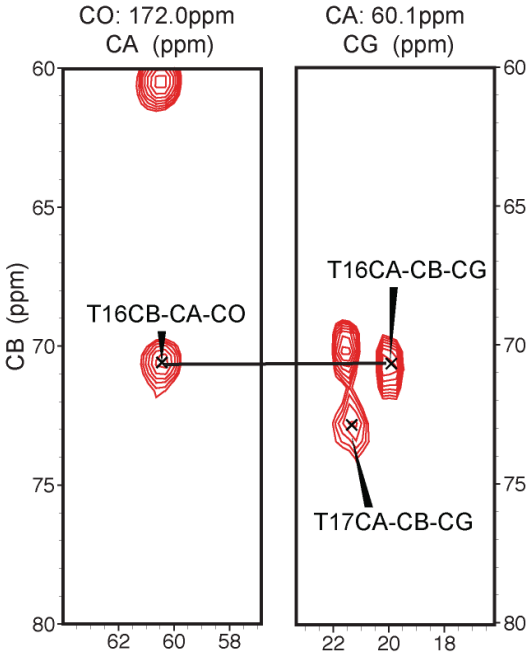
Lysine-13


CO: 175.5ppm
CA (ppm)
CA: 53.3ppm
CG (ppm)
K13CB-CA-CO
K13CA-CB-CG
CB (ppm)
CG: 25.8ppm
CE (ppm)
K13CB-CG-CD
K13CG-CD-CE
CD (ppm)
CG (ppm)
CB: 39.0ppm
K13NZ-CE
NZ (ppm)

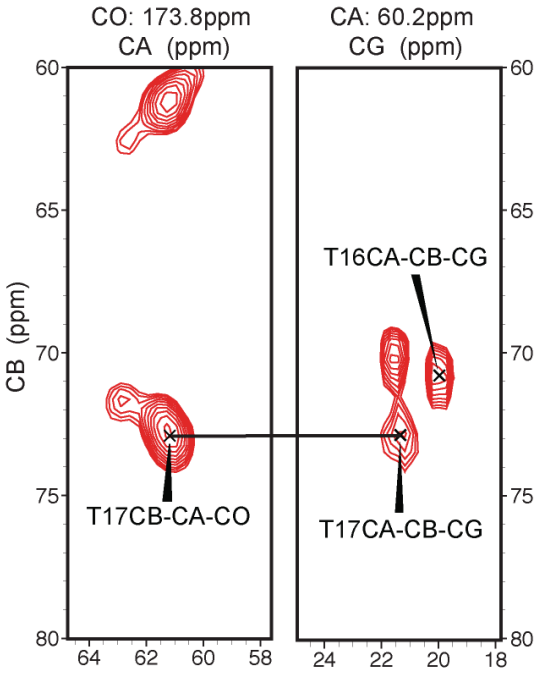
Glutamate-15



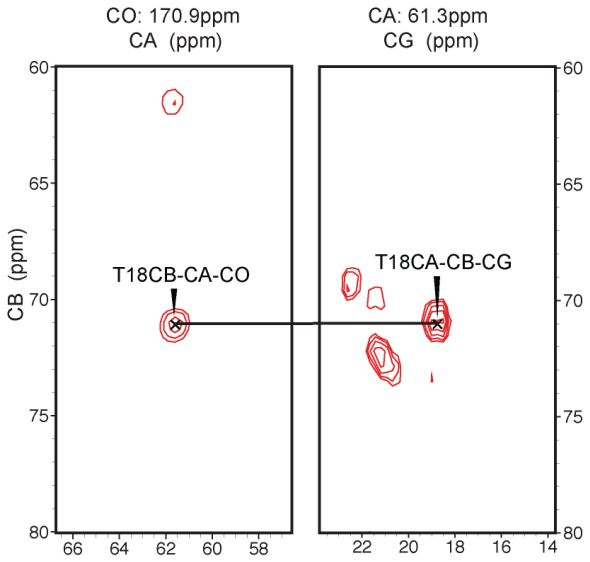
Threonine-16



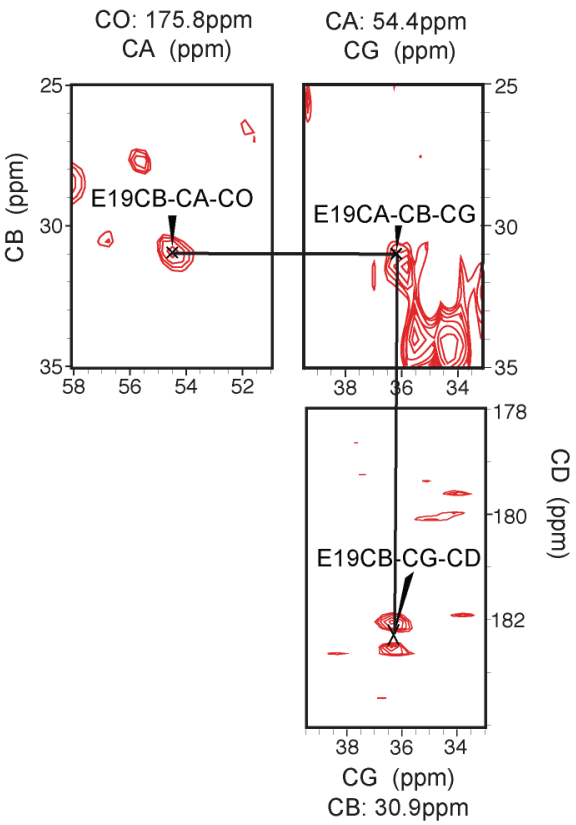
Threonine-17



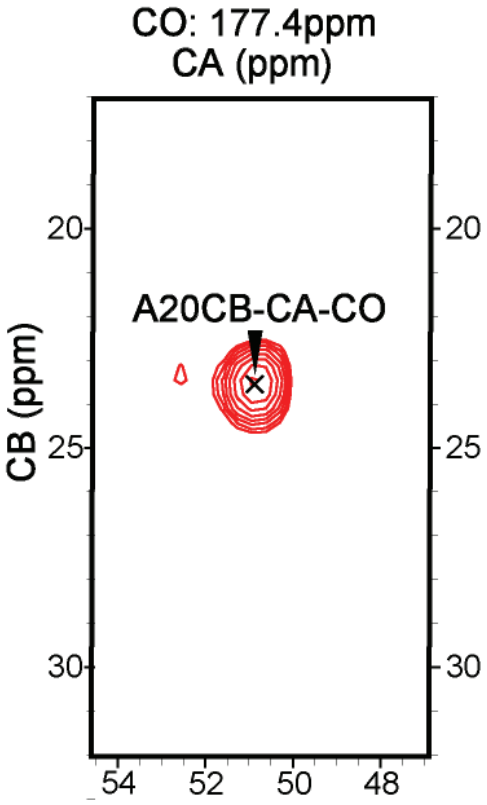
Threonine-18



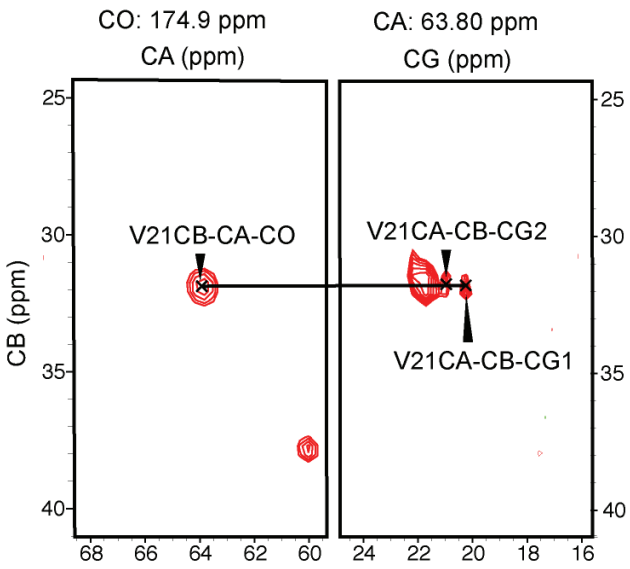
Glutamate-19



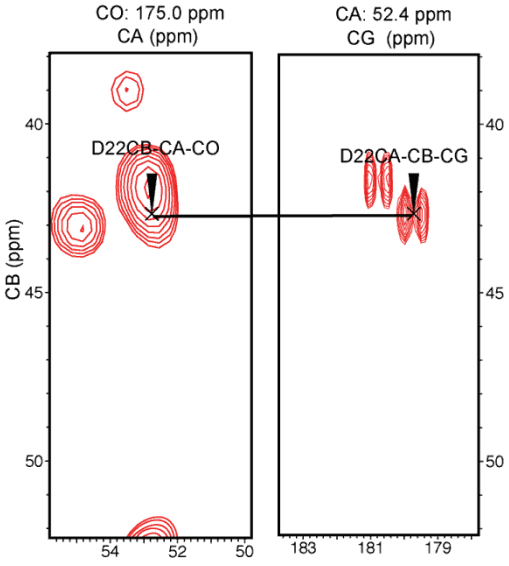
Alanine-20



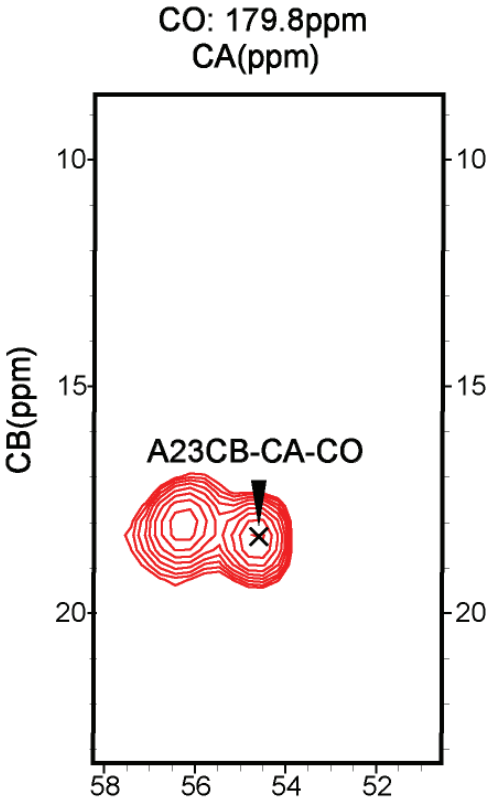
Valine-21


CO: 174.9 ppm
CA (ppm)
CA: 63.80 ppm
CG (ppm)
CB (ppm)
V21CB-CA-CO
V21CA-CB-CG2
V21CA-CB-CG1
25
30
35
40
68
66
64
62
60
24
22
20
18
16

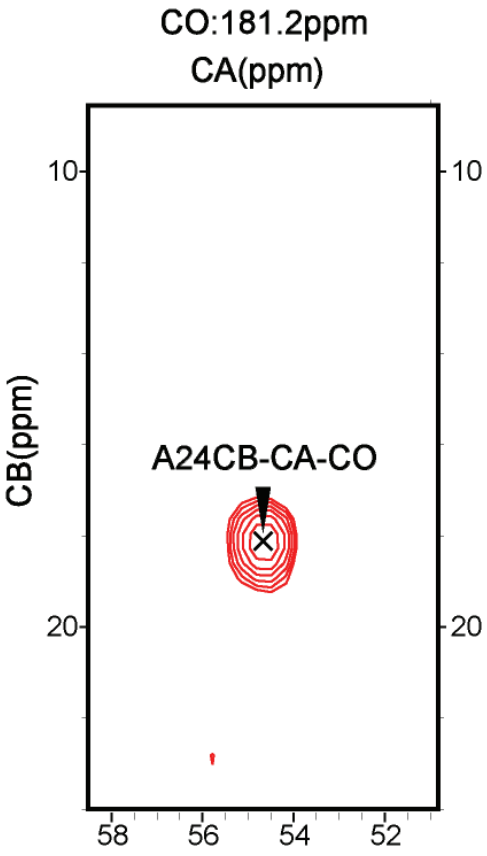
Aspartate-22



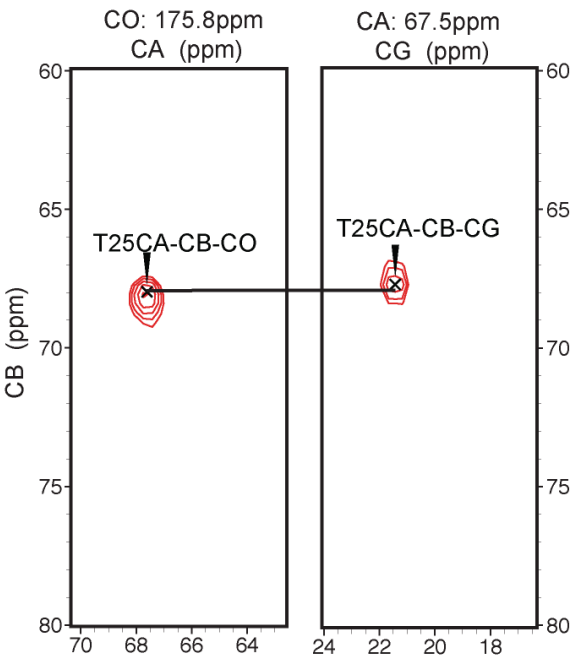
Alanine-23



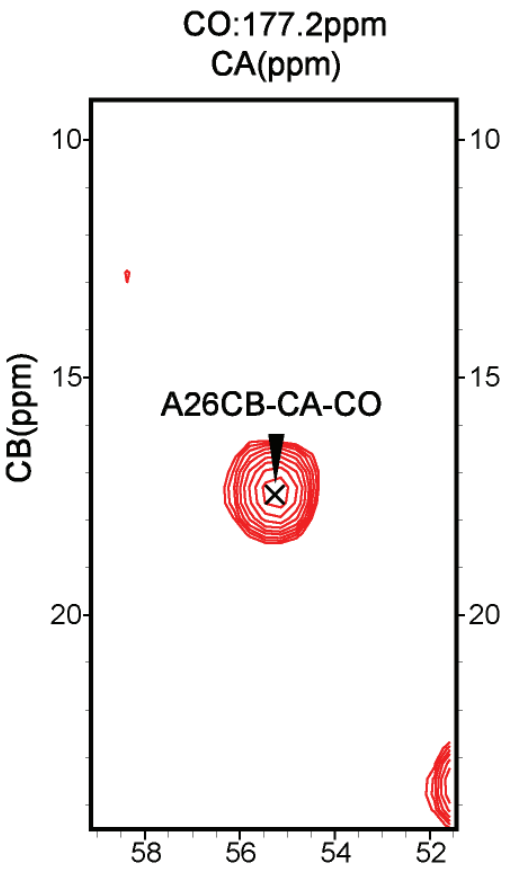
Alanine-24



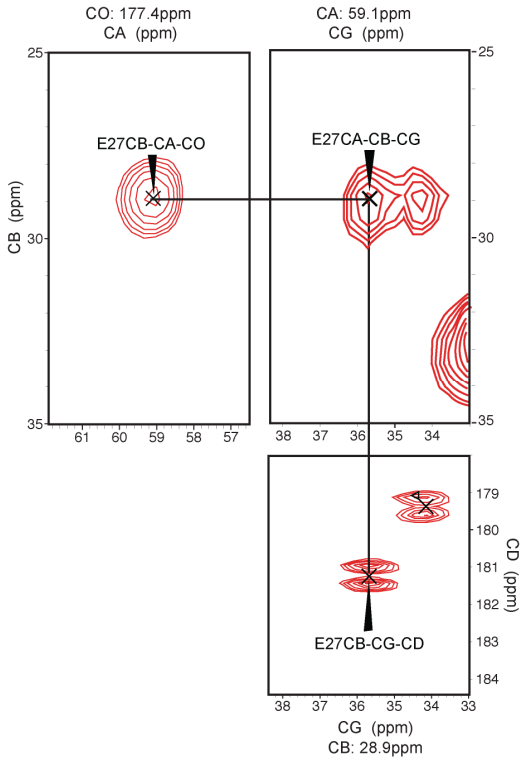
Threonine-25



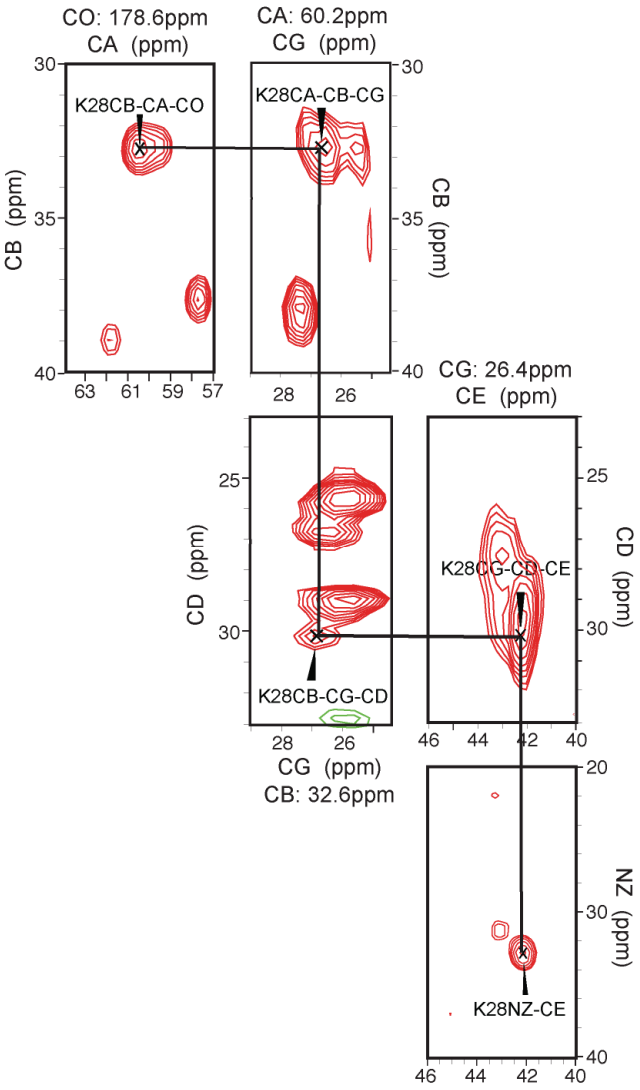
Alanine-26



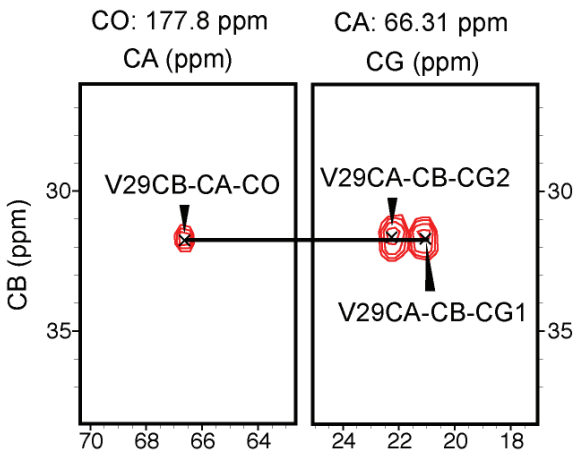
Glutamate-27



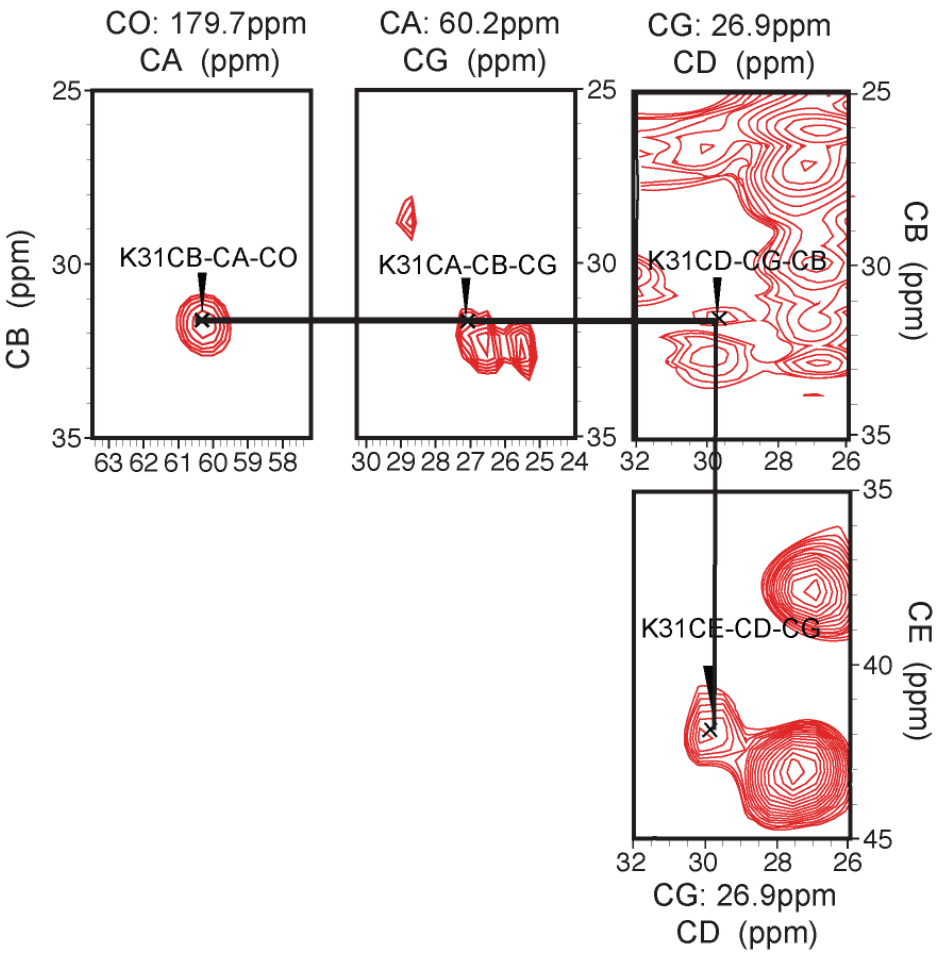
Lysine-28


CO: 178.6ppm
CA (ppm)
CA: 60.2ppm
CG (ppm)
K28CB-CA-CO
K28CA-CB-CG
CB (ppm)
CB (ppm)
CG: 26.4ppm
CE (ppm)
CD (ppm)
CD (ppm)
K28CG-CD-CE
K28CB-CG-CD
CG (ppm)
CB: 32.6ppm
NZ (ppm)
K28NZ-CE

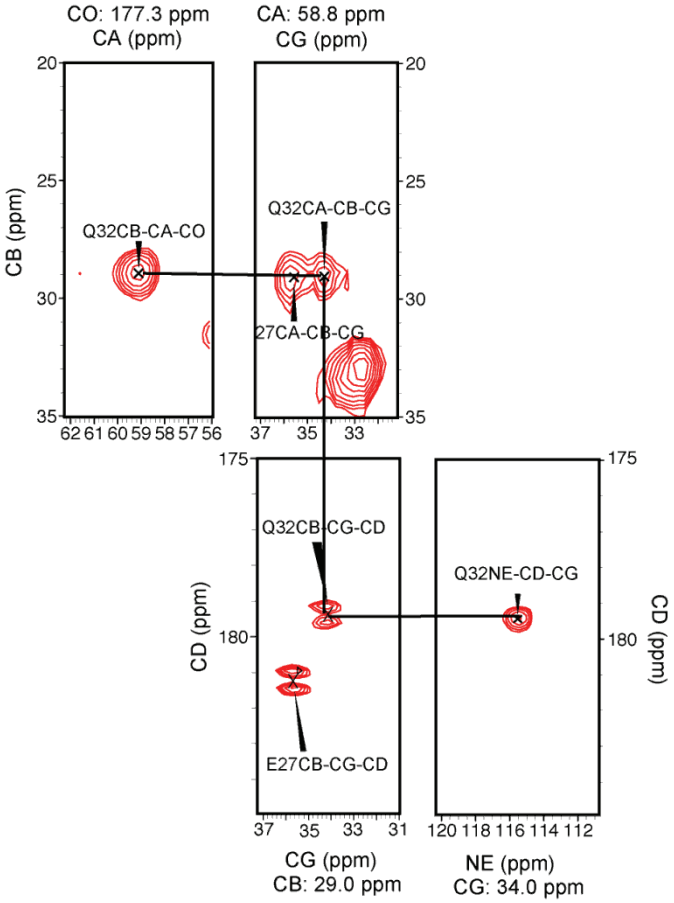
Valine-29


CO: 177.8 ppm
CA (ppm)
CA: 66.31 ppm
CG (ppm)
V29CB-CA-CO
V29CA-CB-CG2
V29CA-CB-CG1
CB (ppm)
30
35
70
68
66
64
24
22
20
18

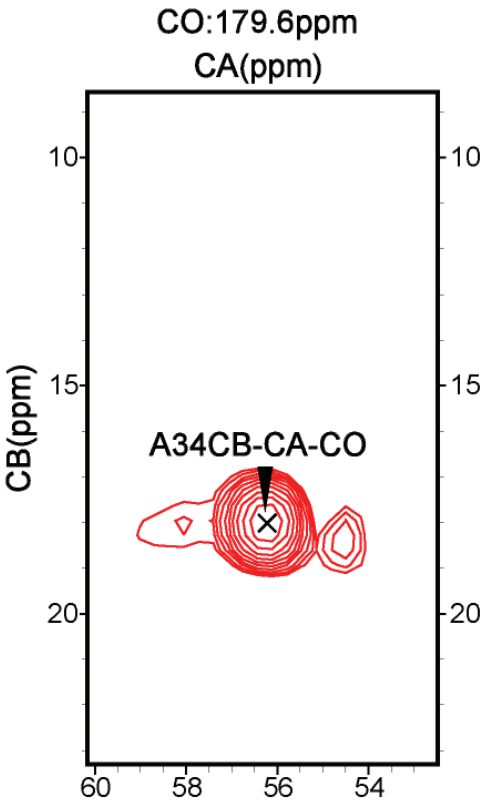
Lysine-31


CO: 179.7ppm
CA (ppm)
CA: 60.2ppm
CG (ppm)
CG: 26.9ppm
CD (ppm)
CB (ppm)
K31CB-CA-CO
K31CA-CB-CG
K31CD-CG-CB
K31CE-CD-CG
CE (ppm)
CG: 26.9ppm
CD (ppm)

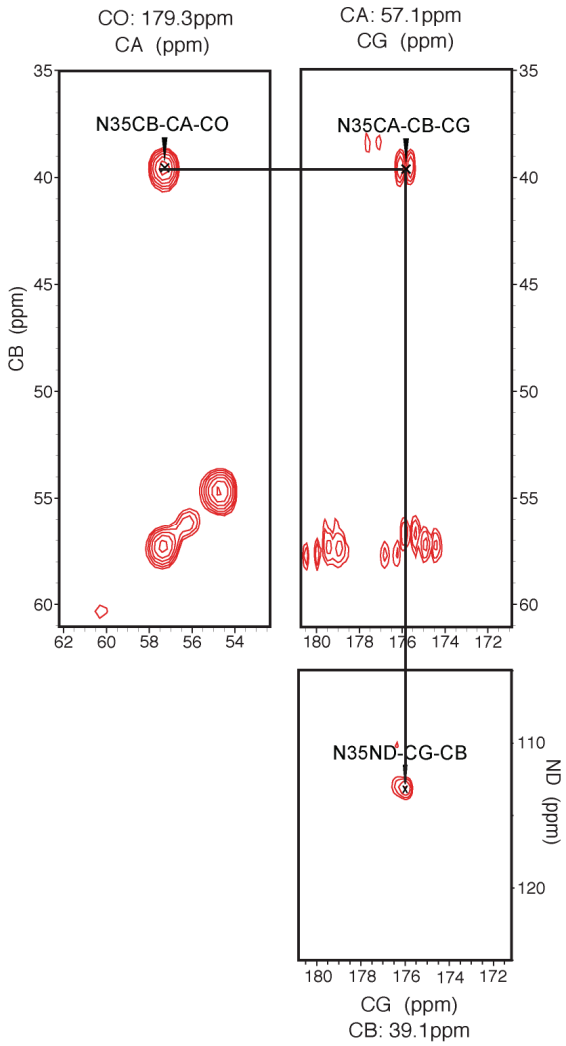
Glutamine-32



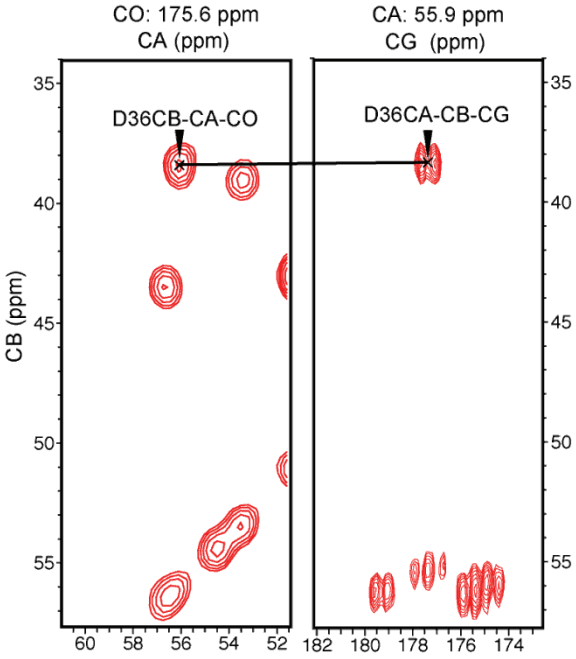
Alanine-34



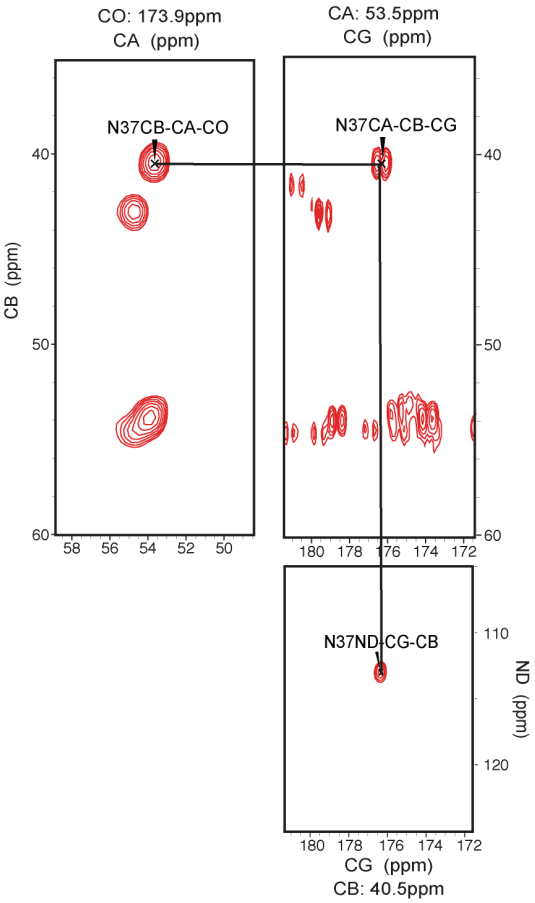
Asparagine-35



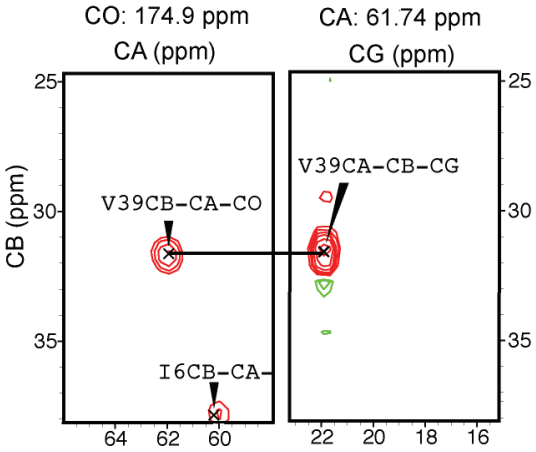
Aspartate-36



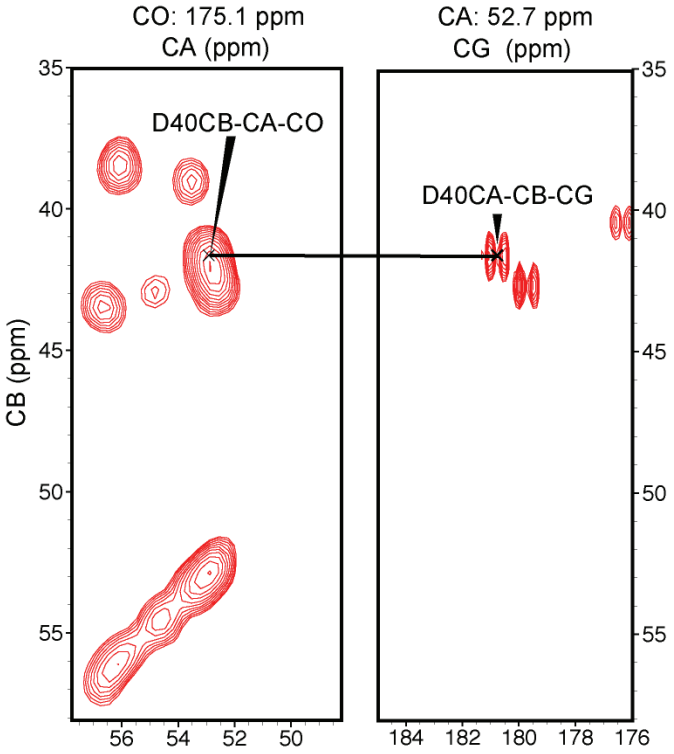
Asparagine-37



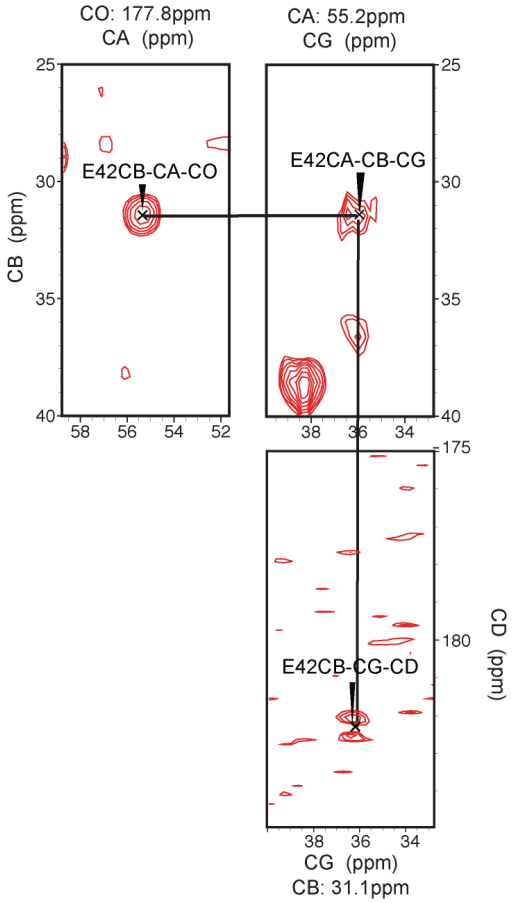
Valine-39


CO: 174.9 ppm
CA (ppm)
CA: 61.74 ppm
CG (ppm)
CB (ppm)
25
30
35
V39CB-CA-CO
V39CA-CB-CG
I6CB-CA-
64
62
60
22
20
18
16

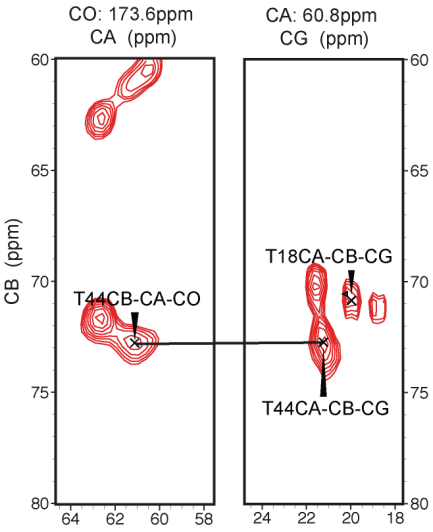
Aspartate-40



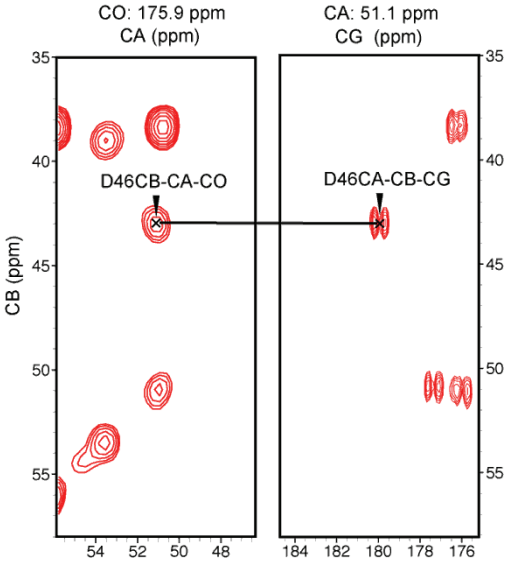
Glutamate-42



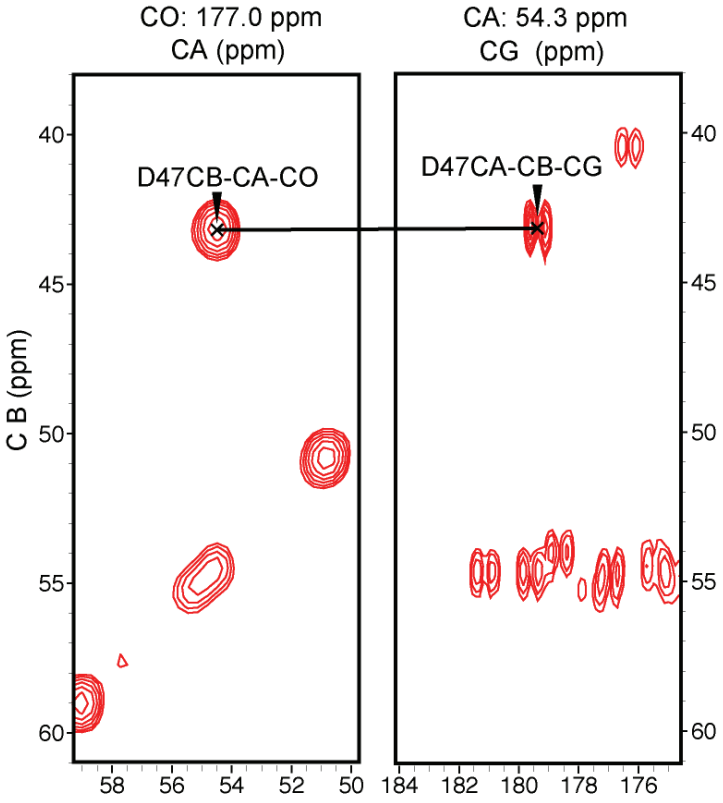
Threonine-44



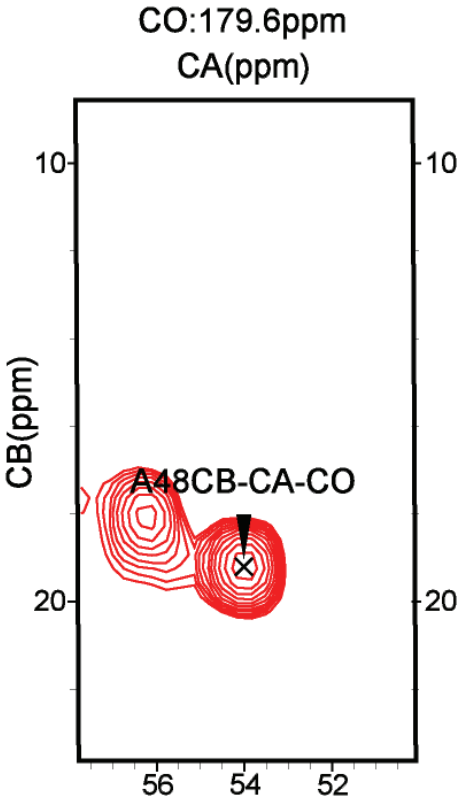
Aspartate-46



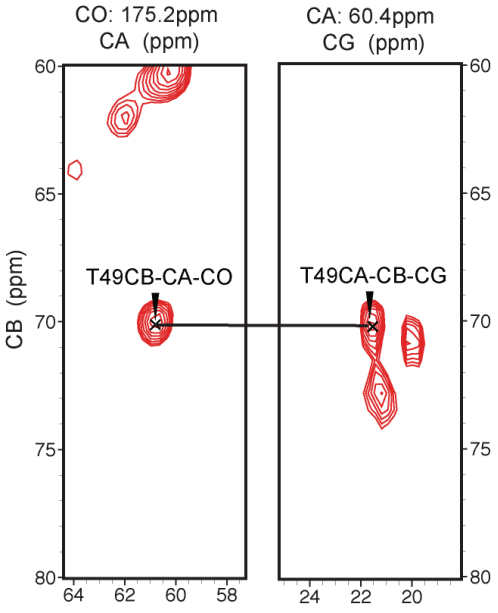
Aspartate-47



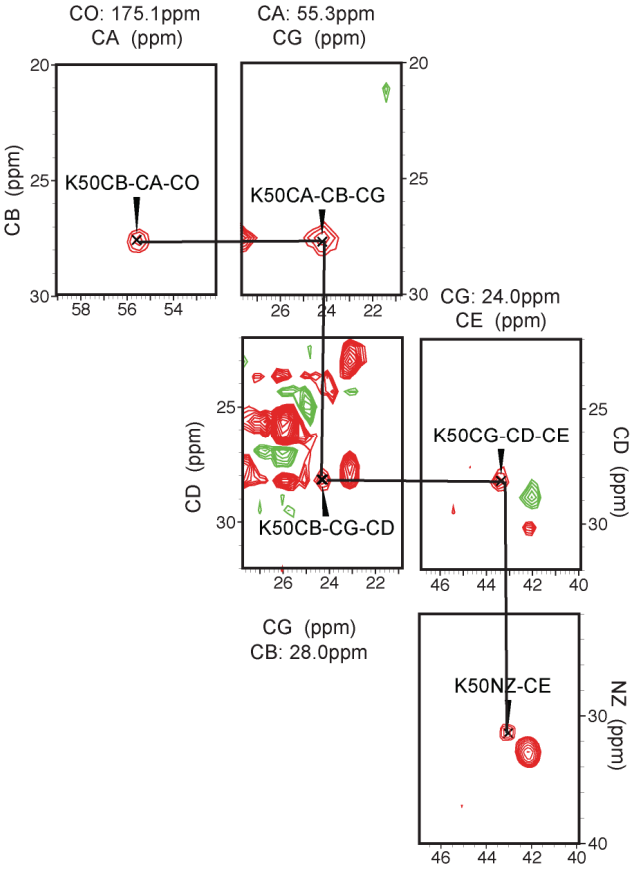
Alanine-48



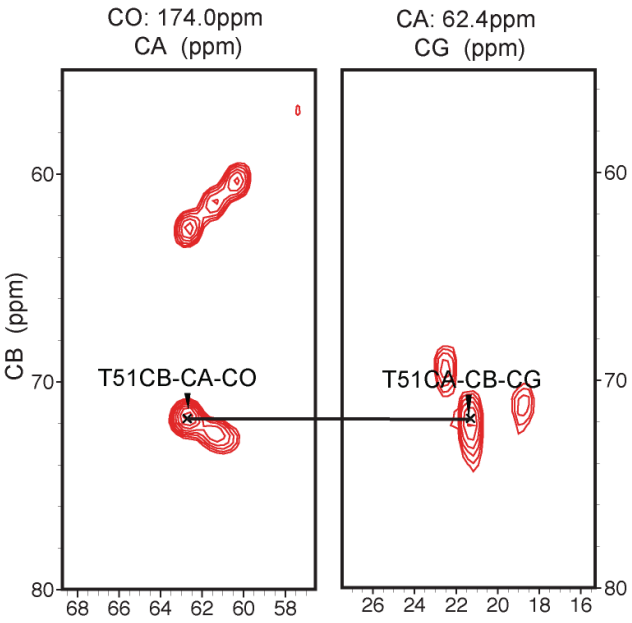
Threonine-49



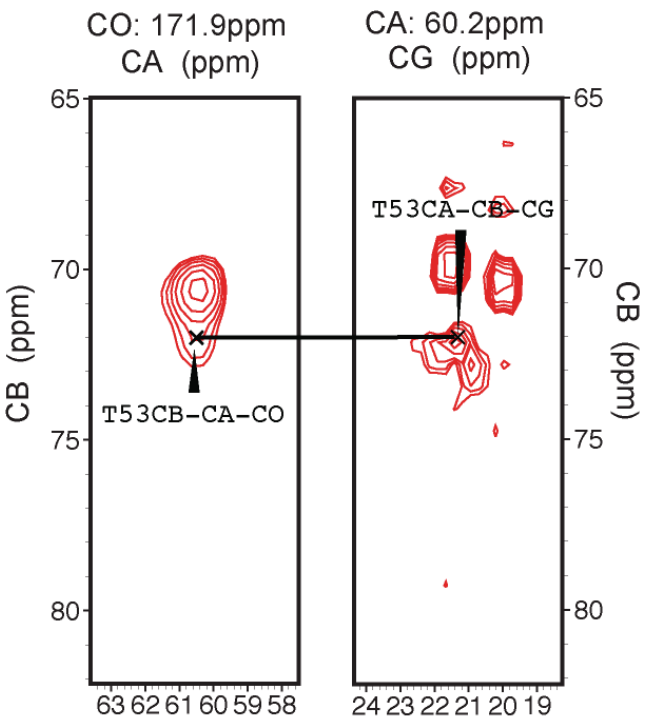
Lysine-50


CO: 175.1ppm
CA (ppm)
CA: 55.3ppm
CG (ppm)
CB (ppm)
K50CB-CA-CO
K50CA-CB-CG
CG: 24.0ppm
CE (ppm)
CD (ppm)
K50CB-CG-CD
K50CG-CD-CE
CG (ppm)
CB: 28.0ppm
K50NZ-CE
NZ (ppm)

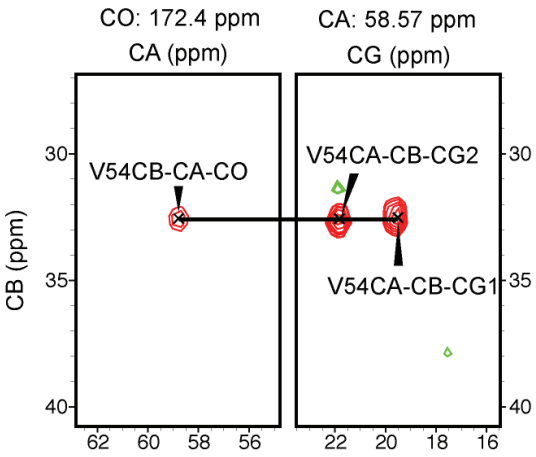
Threonine-51



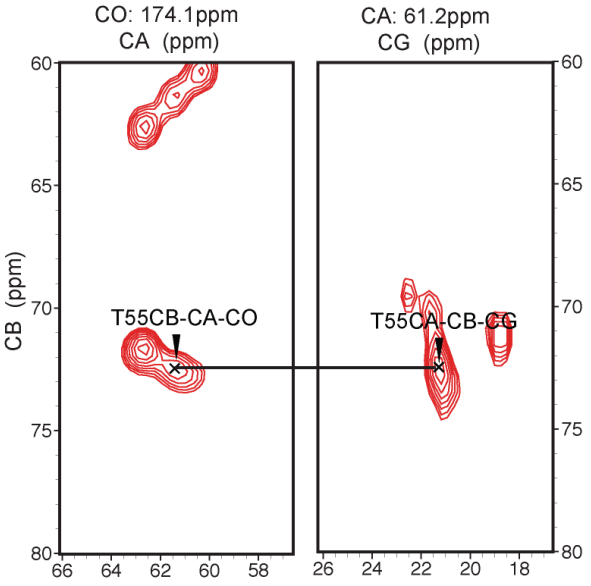
Threonine-53



Valine-54


CO: 172.4 ppm
CA (ppm)
CA: 58.57 ppm
CG (ppm)
V54CB-CA-CO
V54CA-CB-CG2
V54CA-CB-CG1
CB (ppm)
30
35
40
62
60
58
56
22
20
18
16

Threonine-55



Glutamate-56