Supplementary Information

Practical Use of Chemical Shift Databases for Protein Solid-State NMR: 2D Chemical Shift Maps and Amino-Acid Assignment with Secondary-Structure Information

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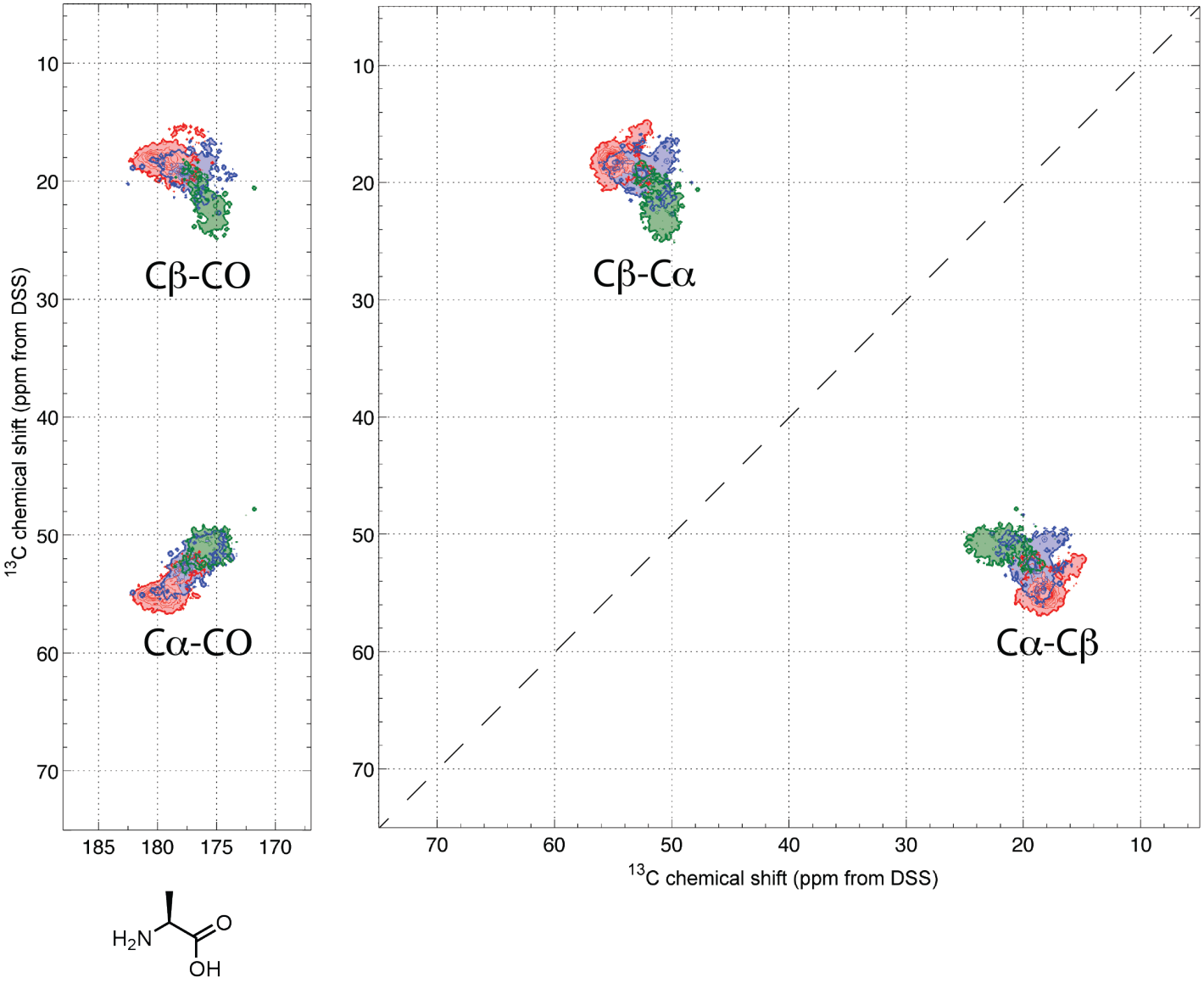
Figures S1-20. Full 2D ^{13}C-^{13}C chemical shift correlation maps for the 20 amino acids, organized in alphabetical order for the one-letter amino acid code. In each figure the chemical shifts are color-coded as red for helix, green for sheet, and blue for coil. Each figure is annotated with peak assignments. On the top of each figure the numbers of residues in the PACSY database for each secondary structure are shown (the same information in Table 1). At the bottom of each figure the contour-level ranges are given.

Supplemental Figure S1

Ala Helix: 8,462 Sheet: 3,064 Coil: 7,123 Total:18,649

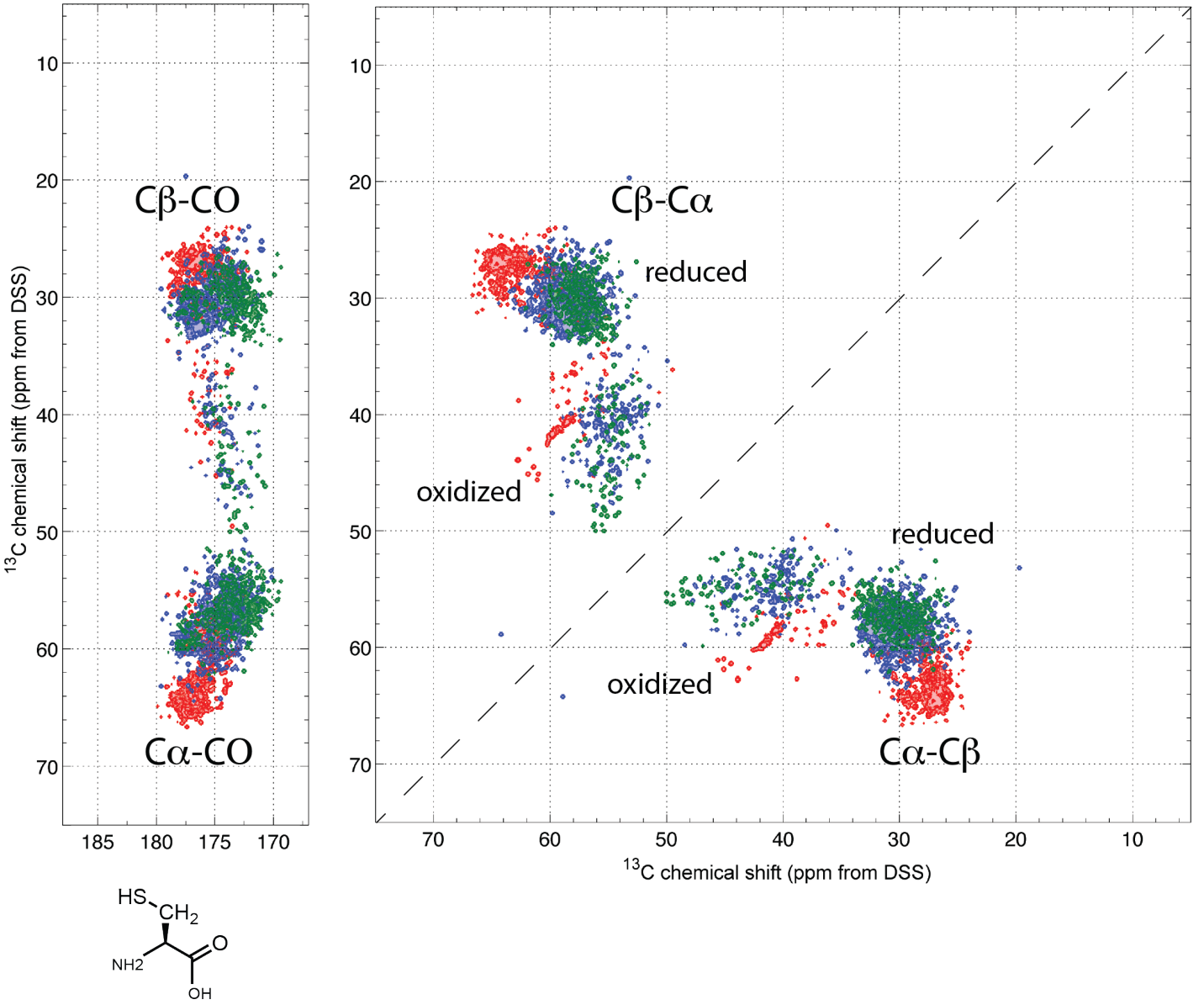
A



2% -- 50% Contour Levels

Supplemental Figure S2

Cys Helix: 1,224 Sheet: 1,297 Coil: 2,187 Total:4,708

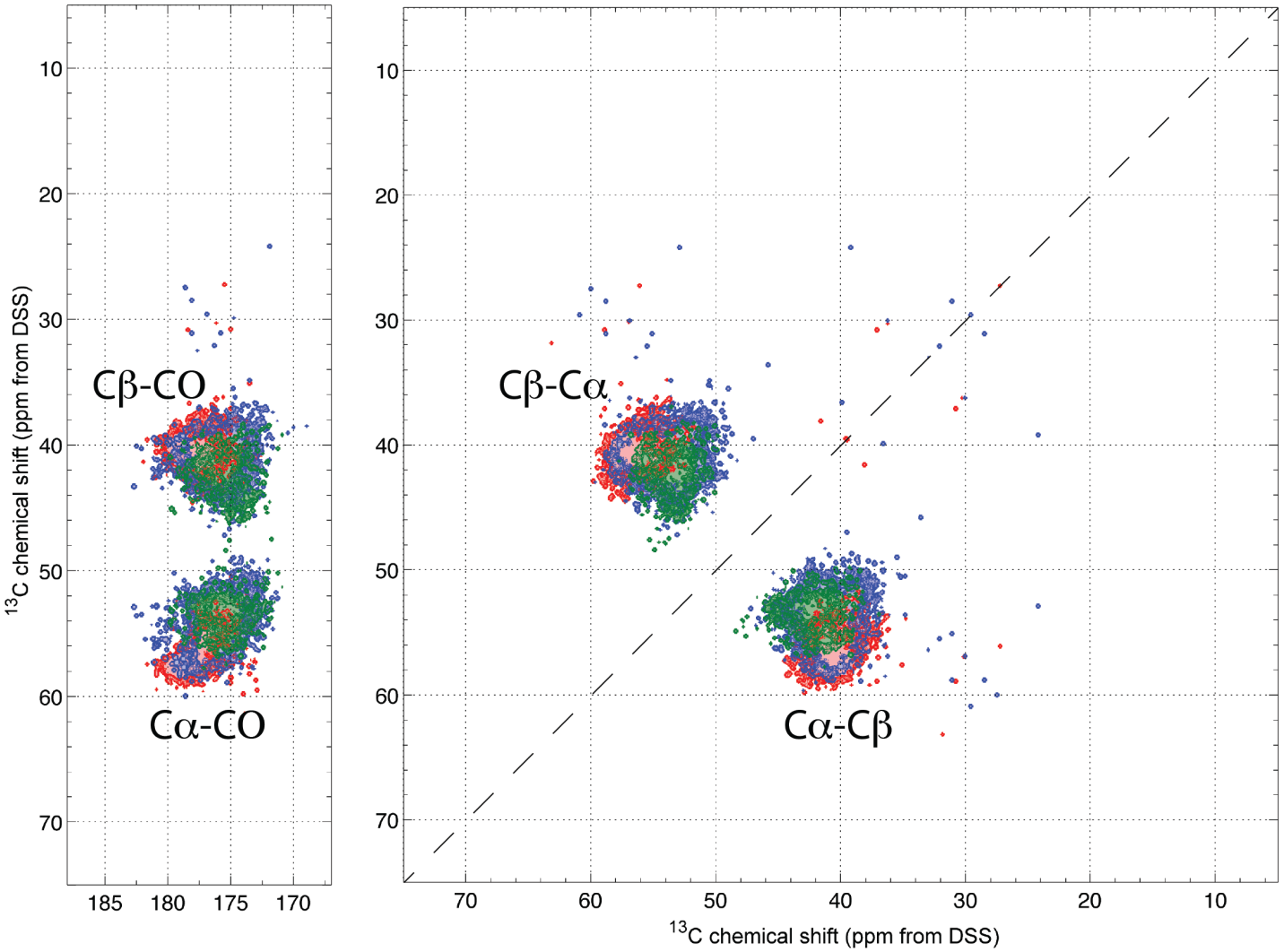


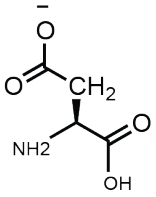
10% -- 50% Contour Levels

Supplemental Figure S3

Asp Helix: 4,441 Sheet: 1,893 Coil: 9,005 Total:15,339

D



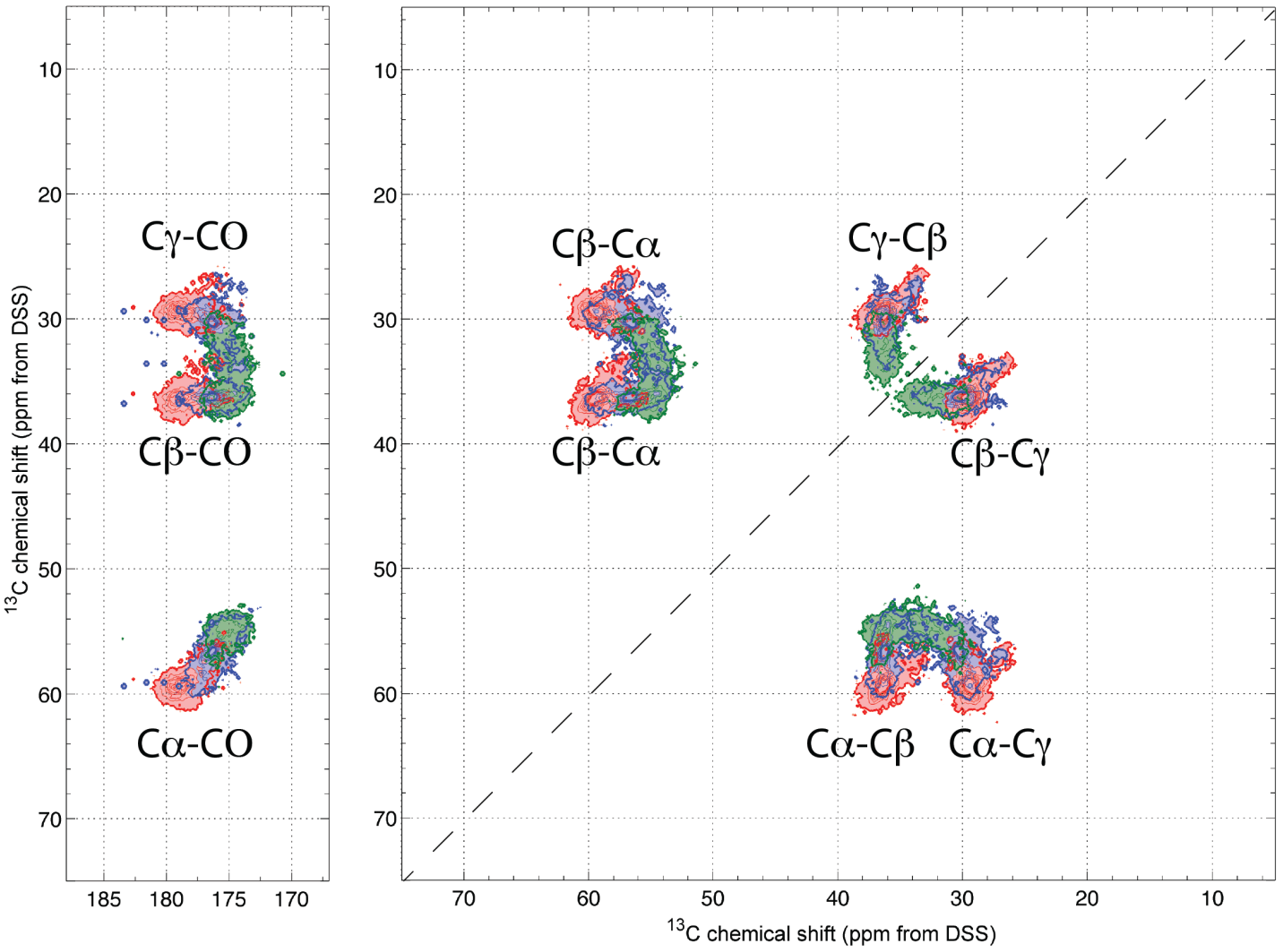


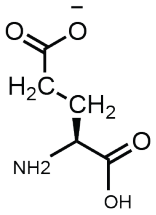
7.5% -- 50% Contour Levels

Supplemental Figure S4

Glu Helix: 8,862 Sheet: 3,590 Coil: 7,824 Total: 20,276

E



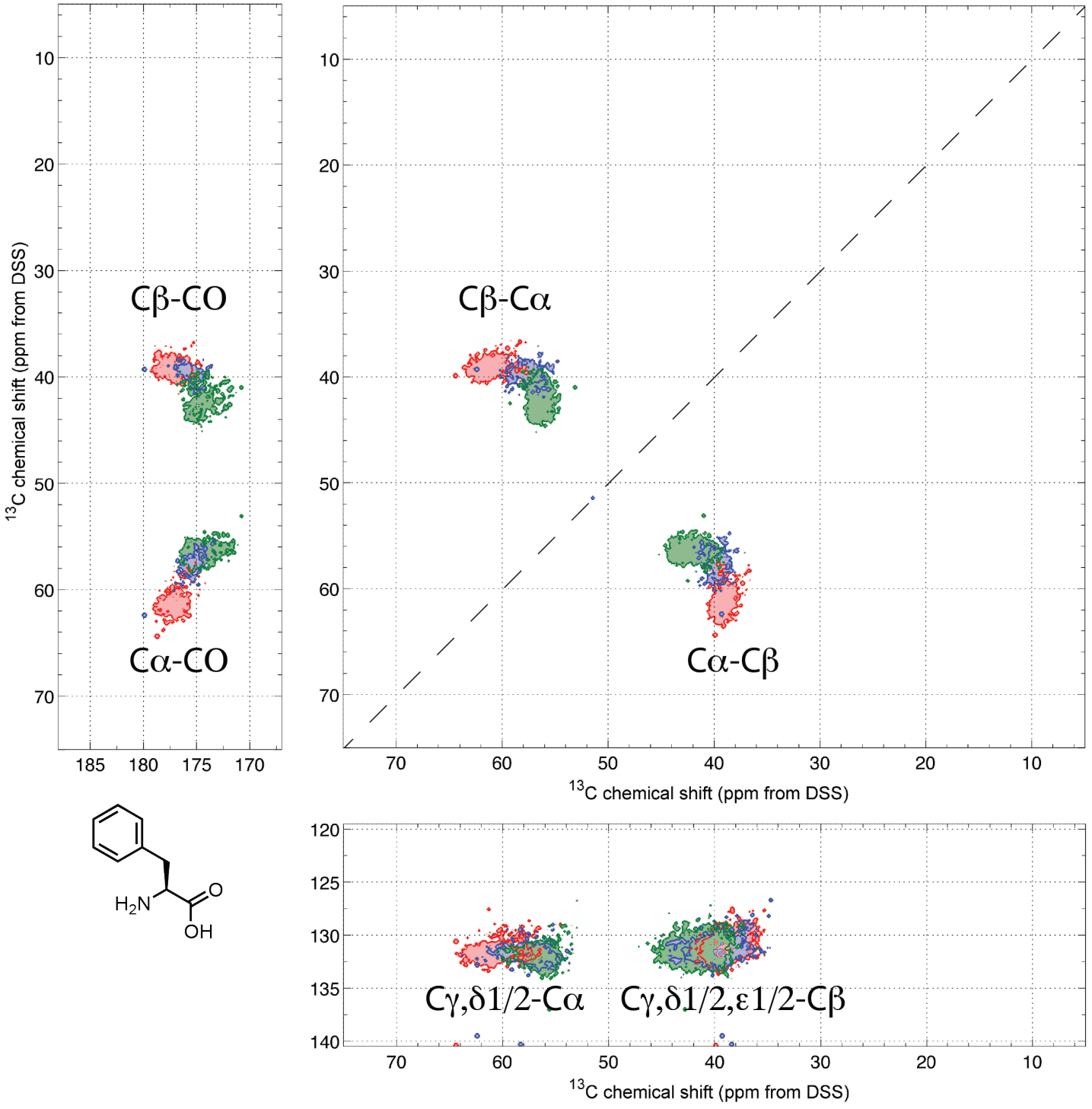


2% -- 50% Contour Levels

Supplemental Figure S5

Phe Helix: 3,358 Sheet: 3,387 Coil: 2,879 Total: 9624

F

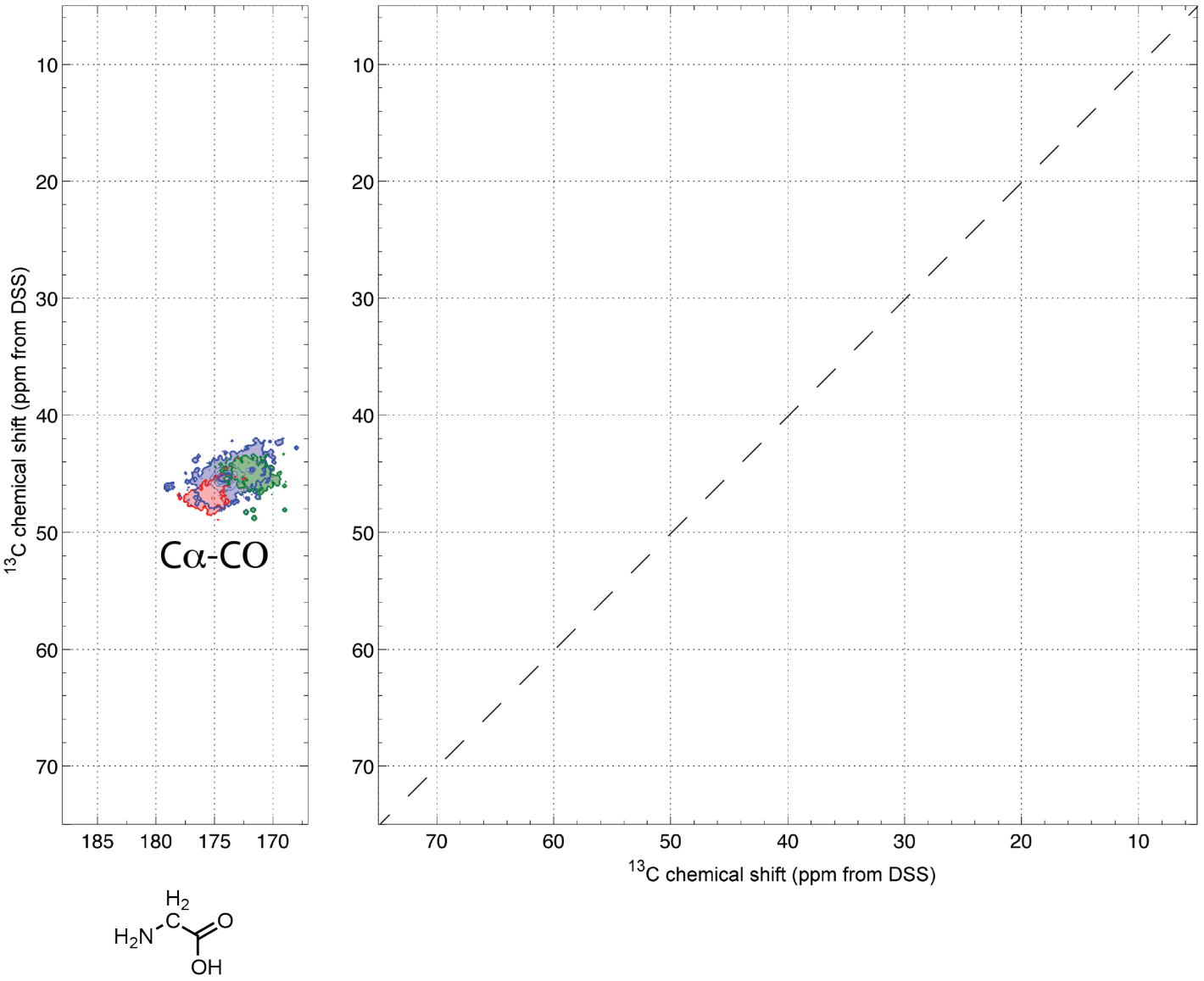


0.5% -- 50% Contour Levels

Supplemental Figure S6

Gly Helix: 2,209 Sheet: 2,314 Coil: 14,470 Total:18,993

G

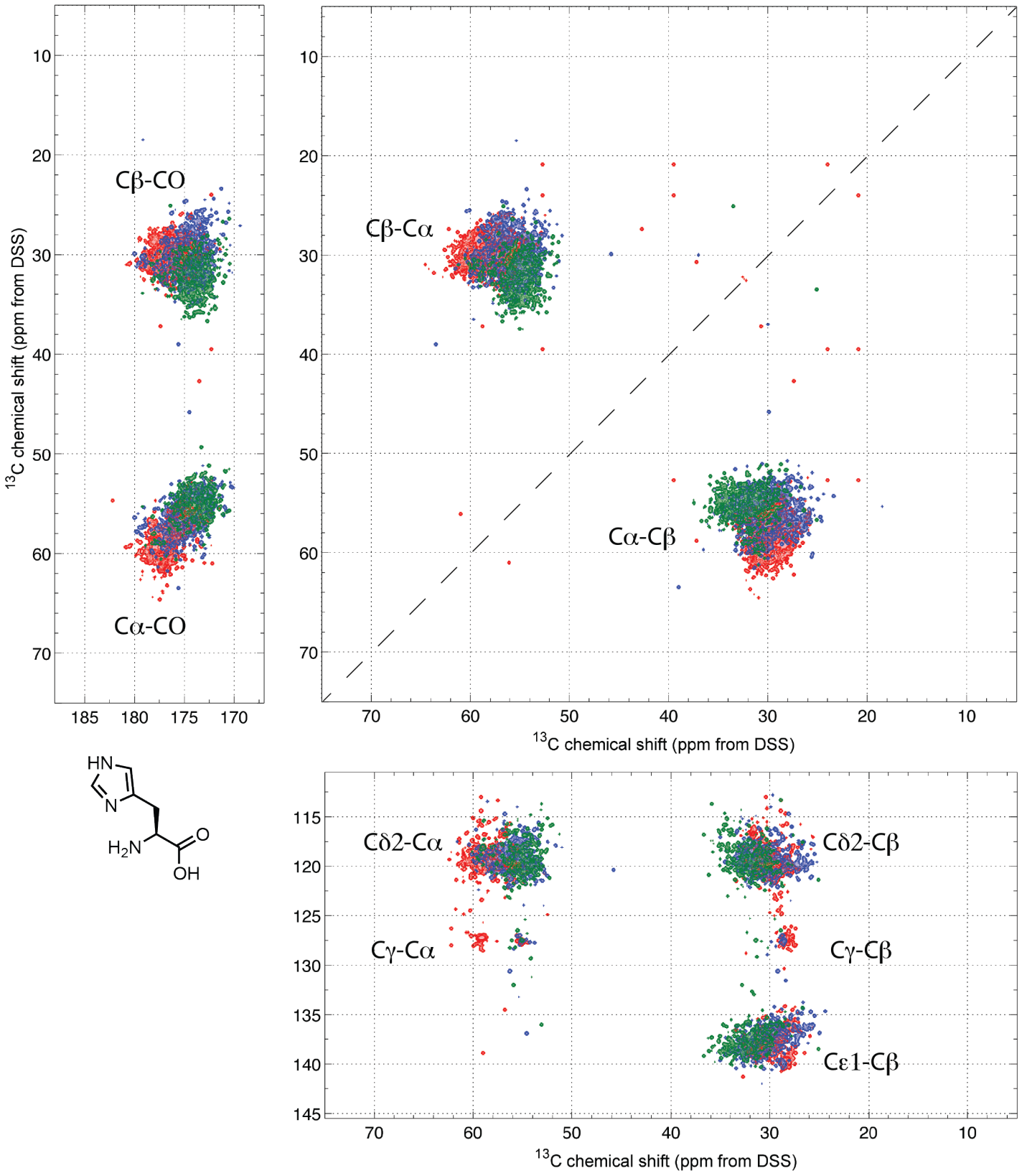


6% -- 50% Contour Levels

Supplemental Figure S7

His Helix: 1,844 Sheet: 1,253 Coil: 2,915 Total: 6,012

H

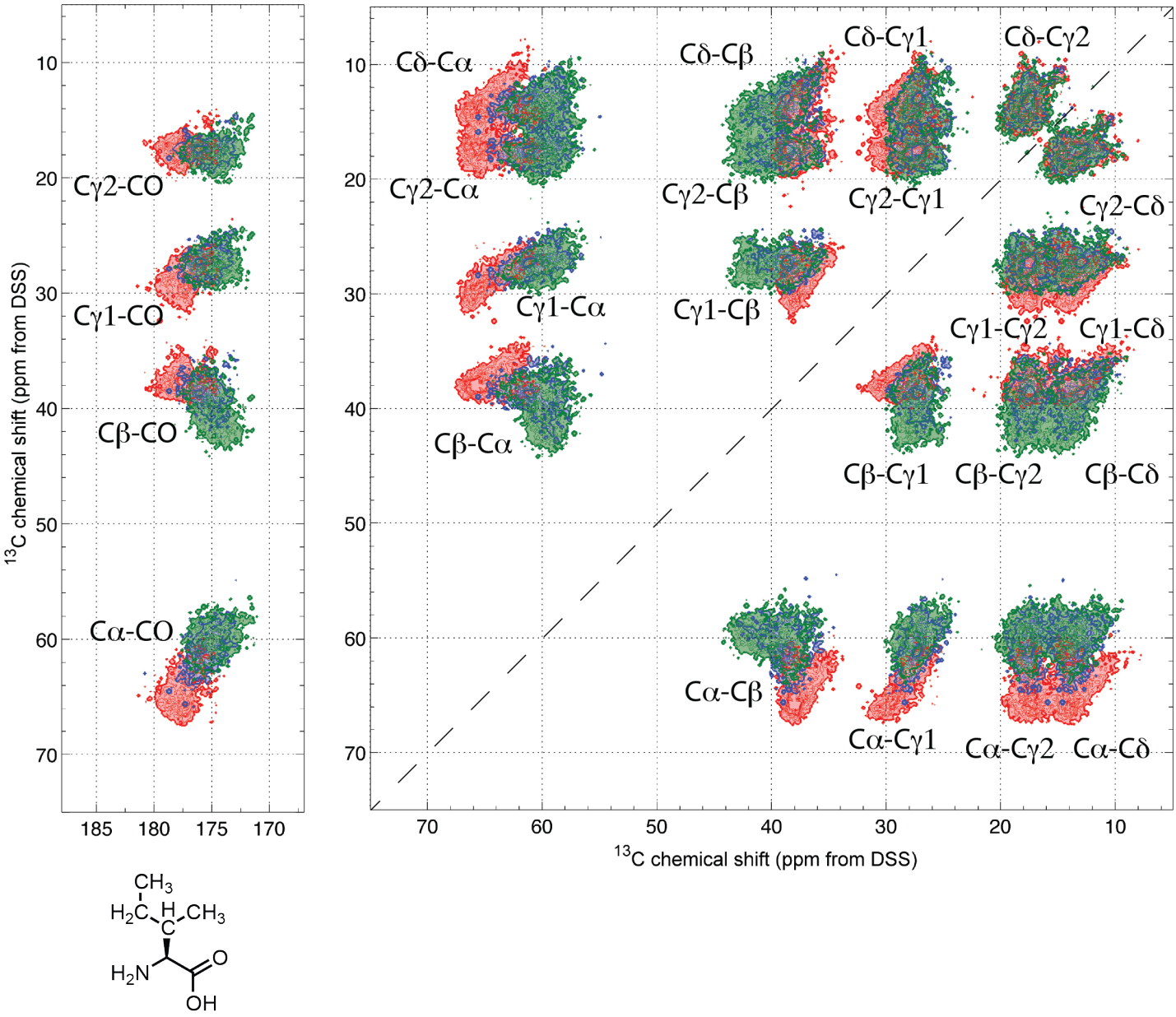


6% -- 50% Contour Levels

Supplemental Figure S8

Ile

Helix: 4,914 Sheet: 5,323 Coil: 3,712 Total: 13,949

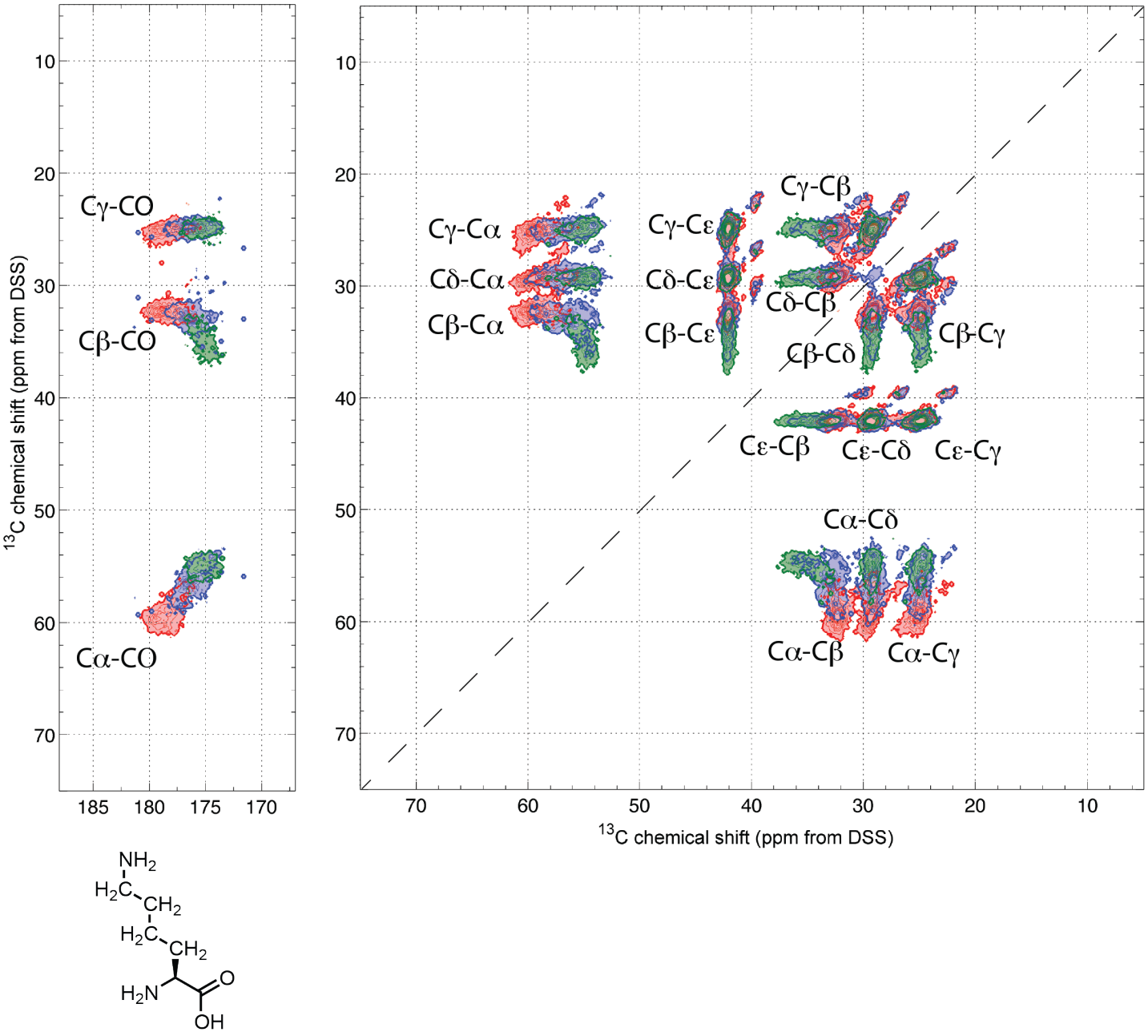


2% -- 50% Contour Levels

Supplemental Figure S9

Lys Helix: 6,992 Sheet: 3,607 Coil: 8,119 Total: 18,718

K

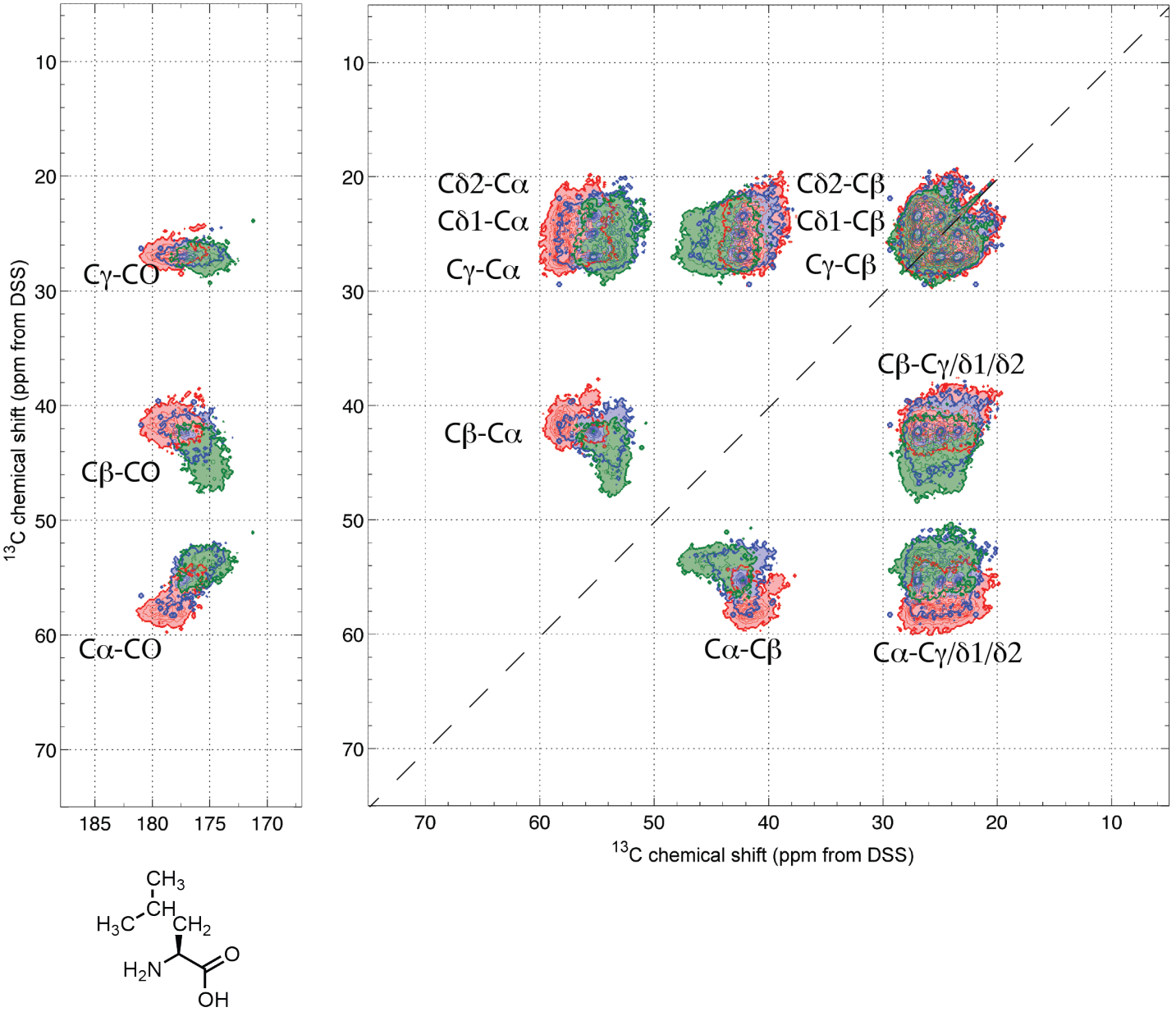


4% -- 50% Contour Levels

Supplemental Figure S10

Leu Helix: 9,832 Sheet: 5,765 Coil: 7,150 Total: 22,747

L

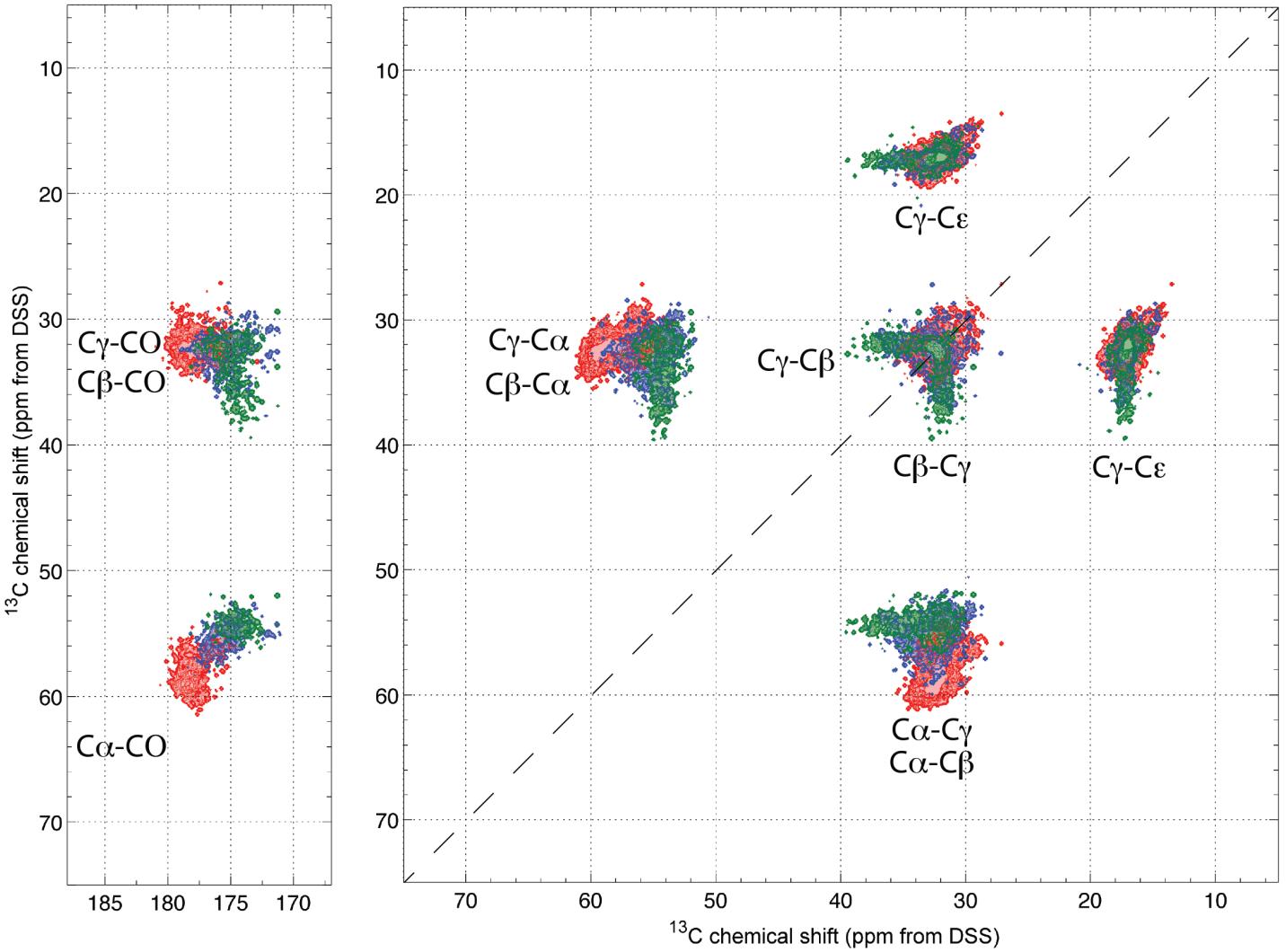


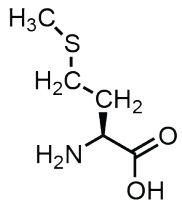
2% -- 50% Contour Levels

Supplemental Figure S11

Met Helix: 2,293 Sheet: 1,136 Coil: 2,307 Total: 5,736

M





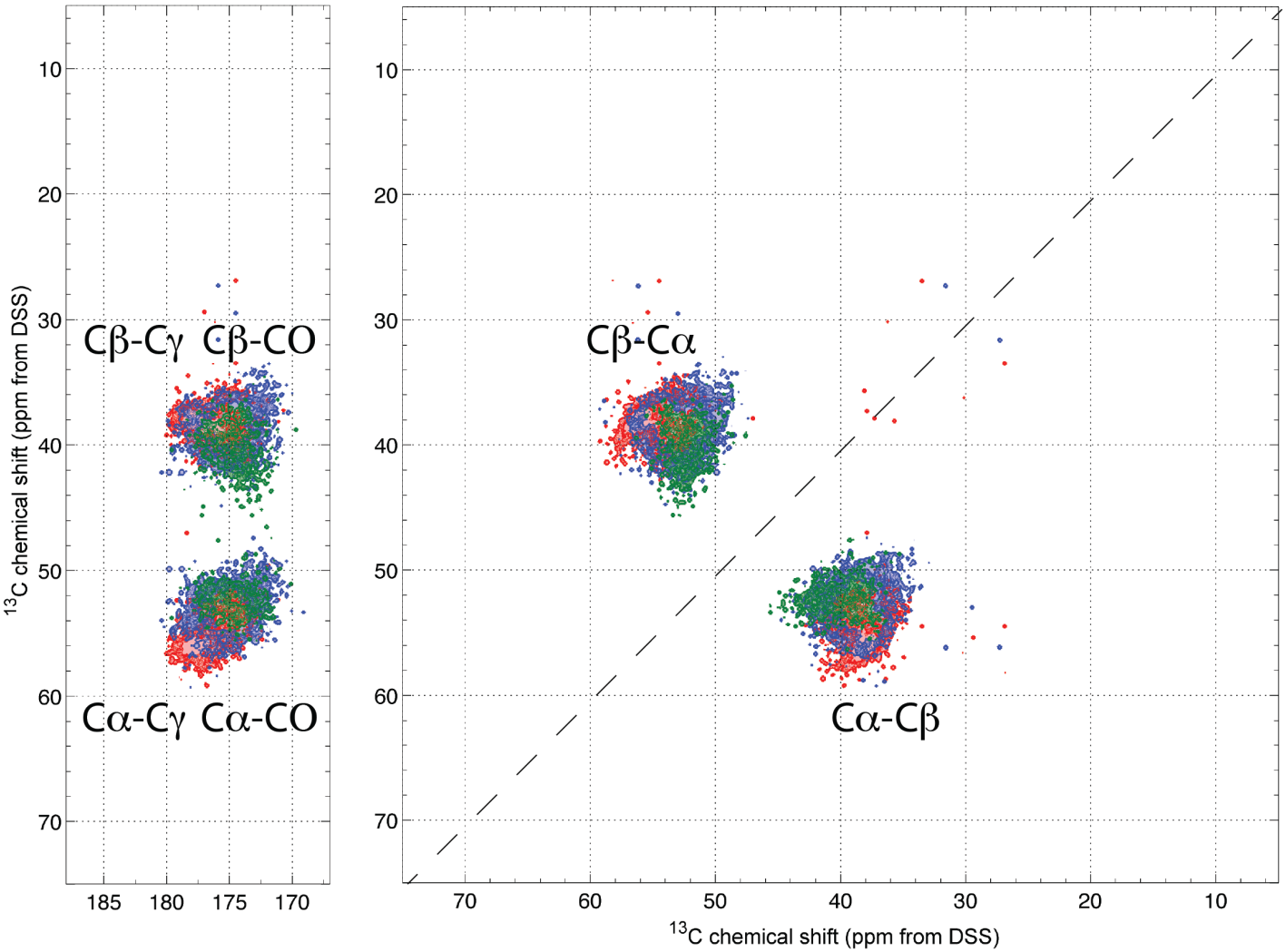
7.5% -- 50% Contour Levels

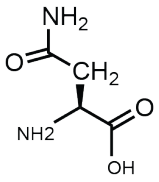
Supplemental Figure S12

Asn

Helix: 2,913 Sheet: 1,353 Coil: 6,452 Total: 10,718

N





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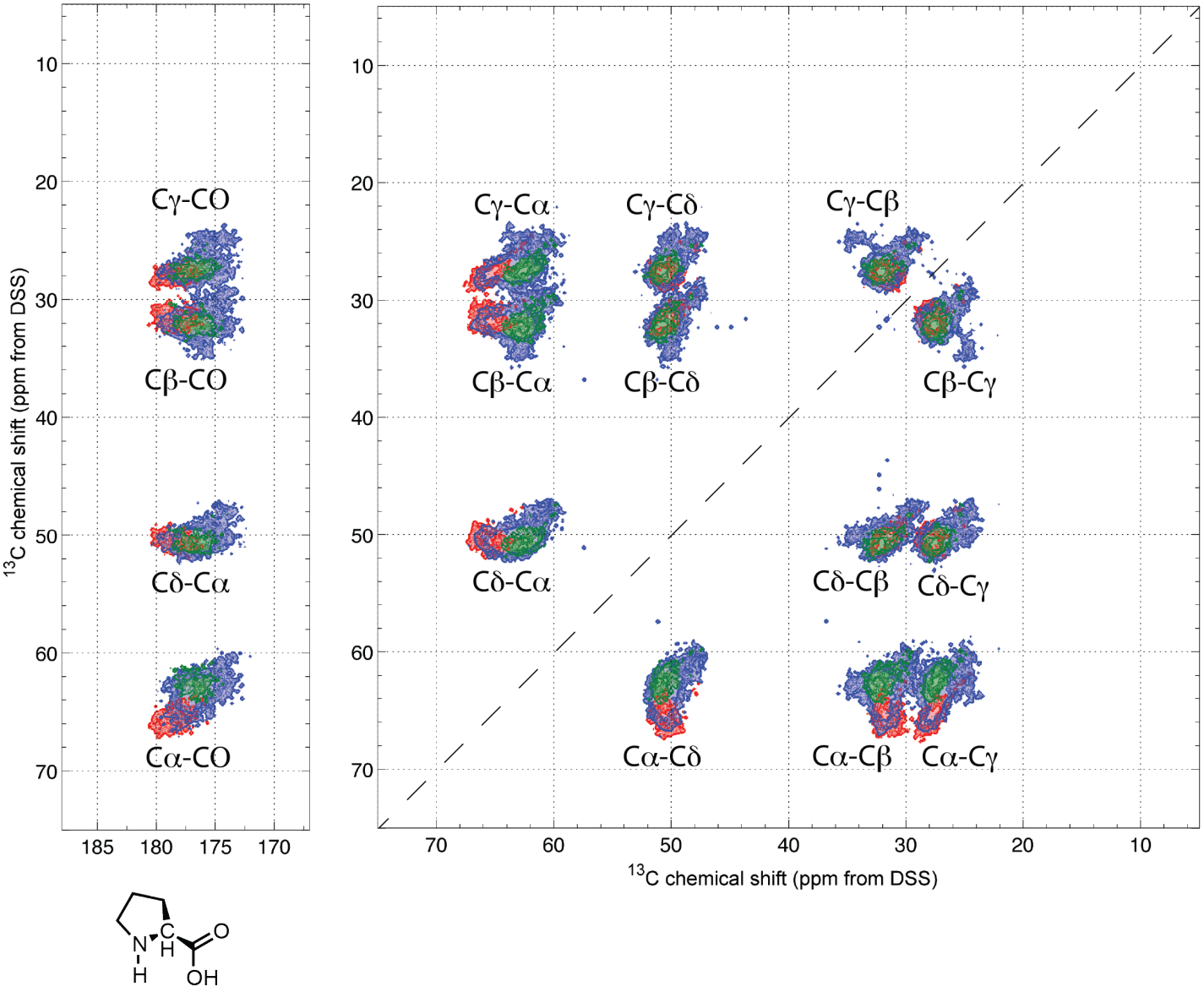
Supplemental Figure S13

Pro Helix: 1,366 Sheet: 1,011 Coil: 8,795 Total: 11,172

P

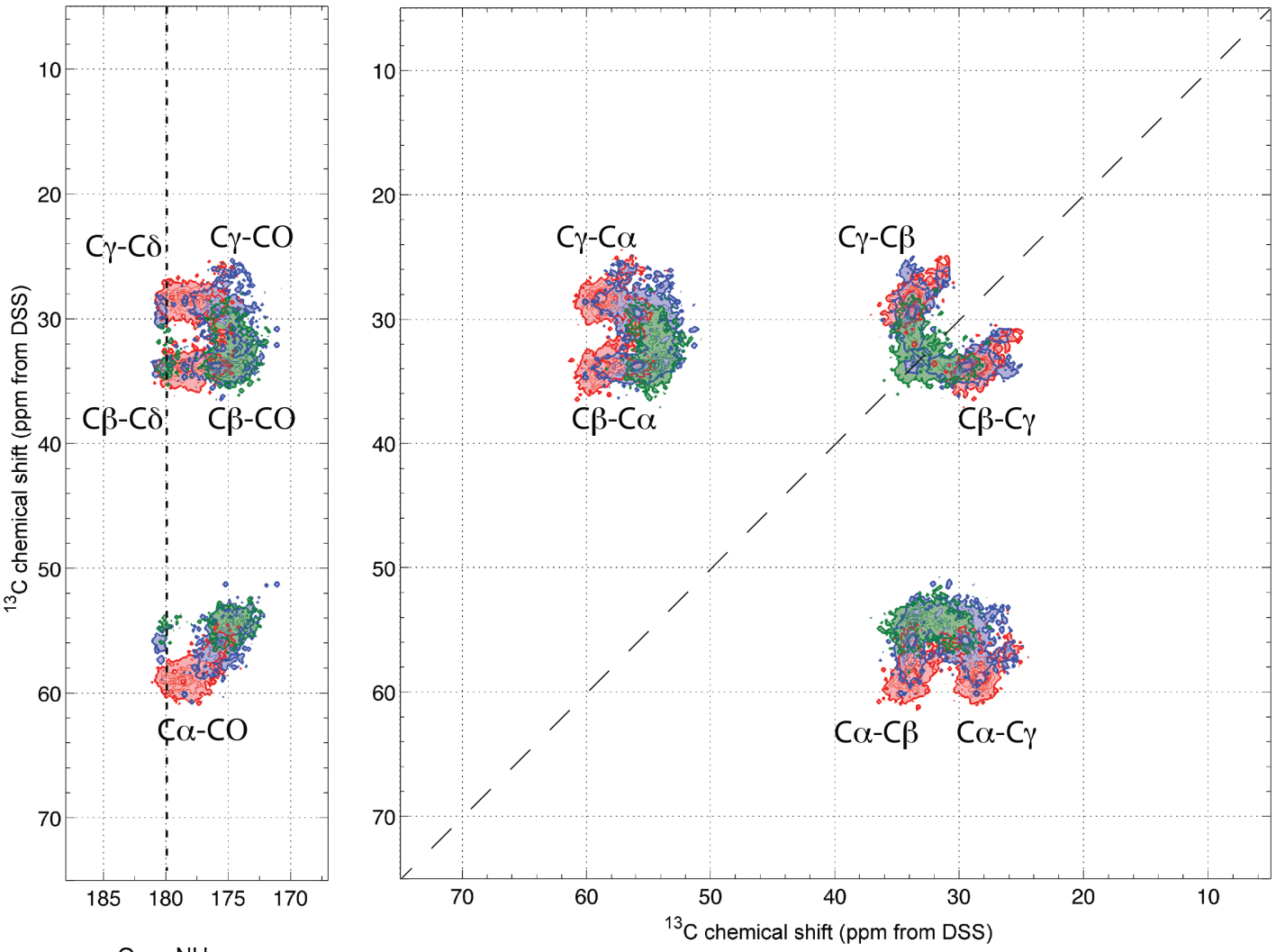


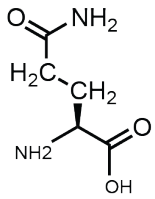
7.5% -- 50% Contour Levels

Supplemental Figure S14

Gln Helix: 4,765 Sheet: 1,984 Coil: 4,283 Total: 11,032

Q





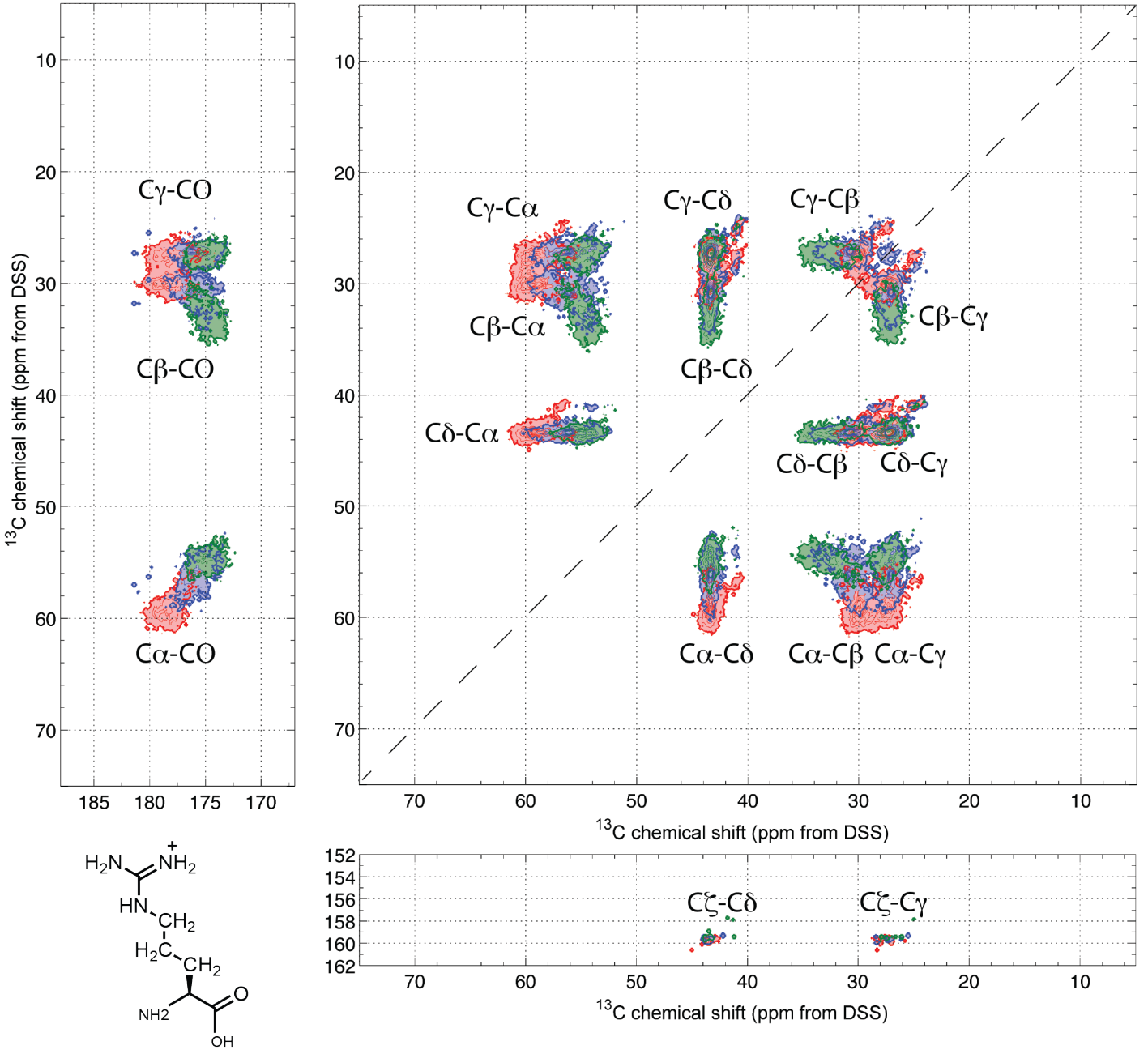
2% -- 50% Contour Levels

Supplemental Figure S15

Arg

Helix: 4,987 Sheet: 2,900 Coil: 5,323 Total:13,210

R

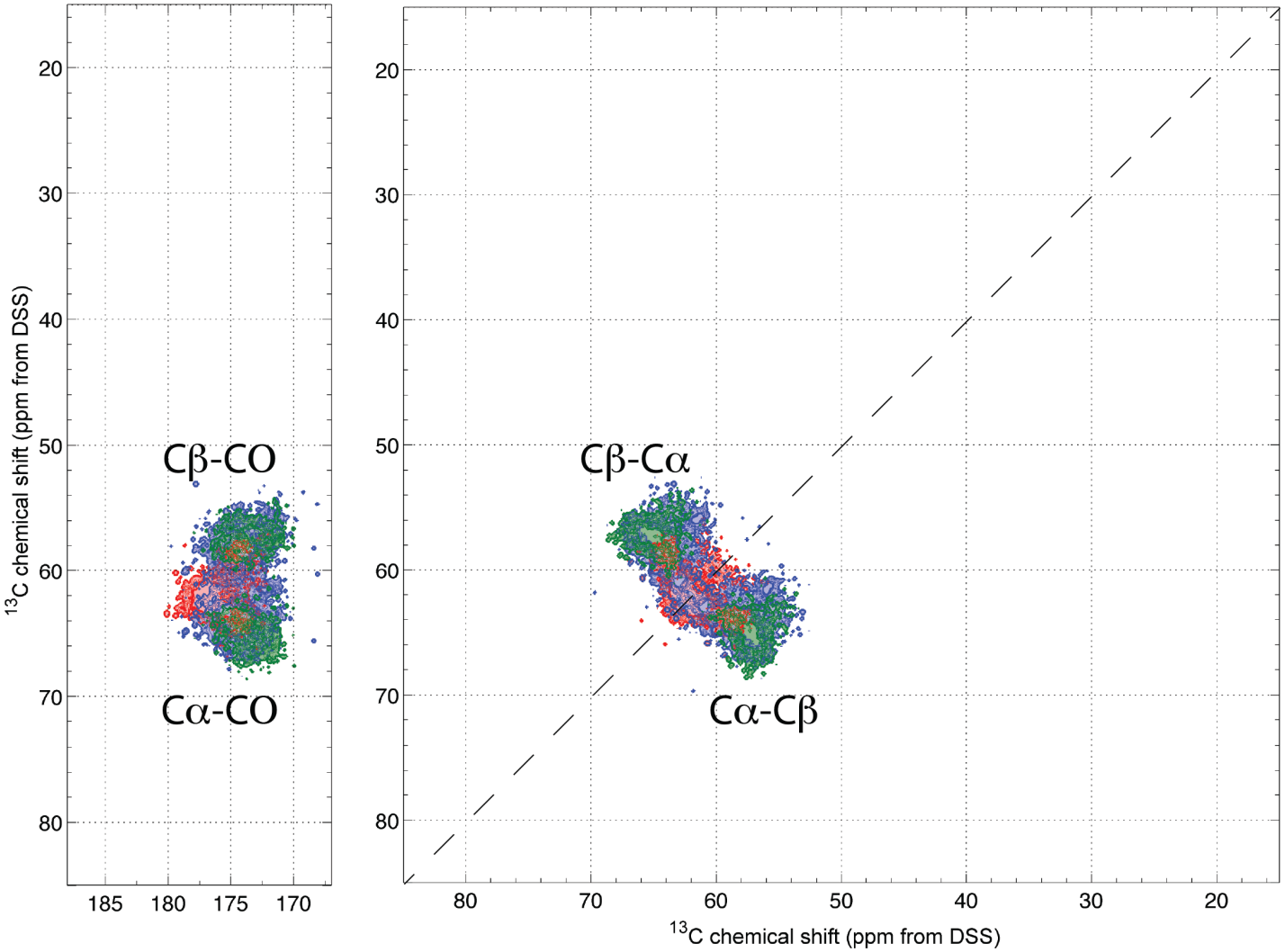


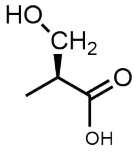
2% -- 50% Contour Levels

Supplemental Figure S16

Ser Helix: 4,246 Sheet: 3,000 Coil: 10,085 Total: 17,331

S



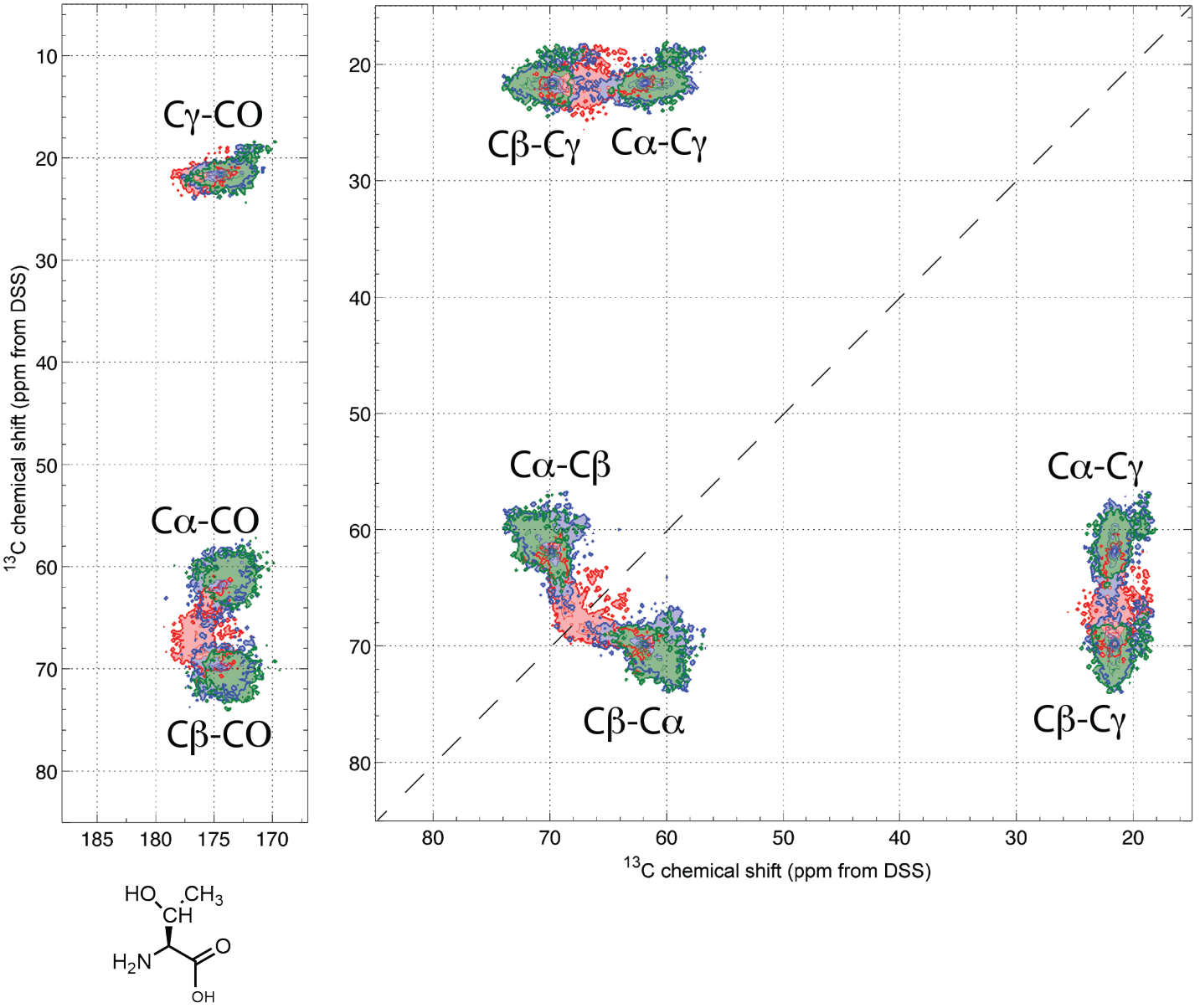


6% -- 50% Contour Levels

Supplemental Figure S17

Thr Helix: 3,367 Sheet: 4,084 Coil: 6,709 Total: 14.160

T



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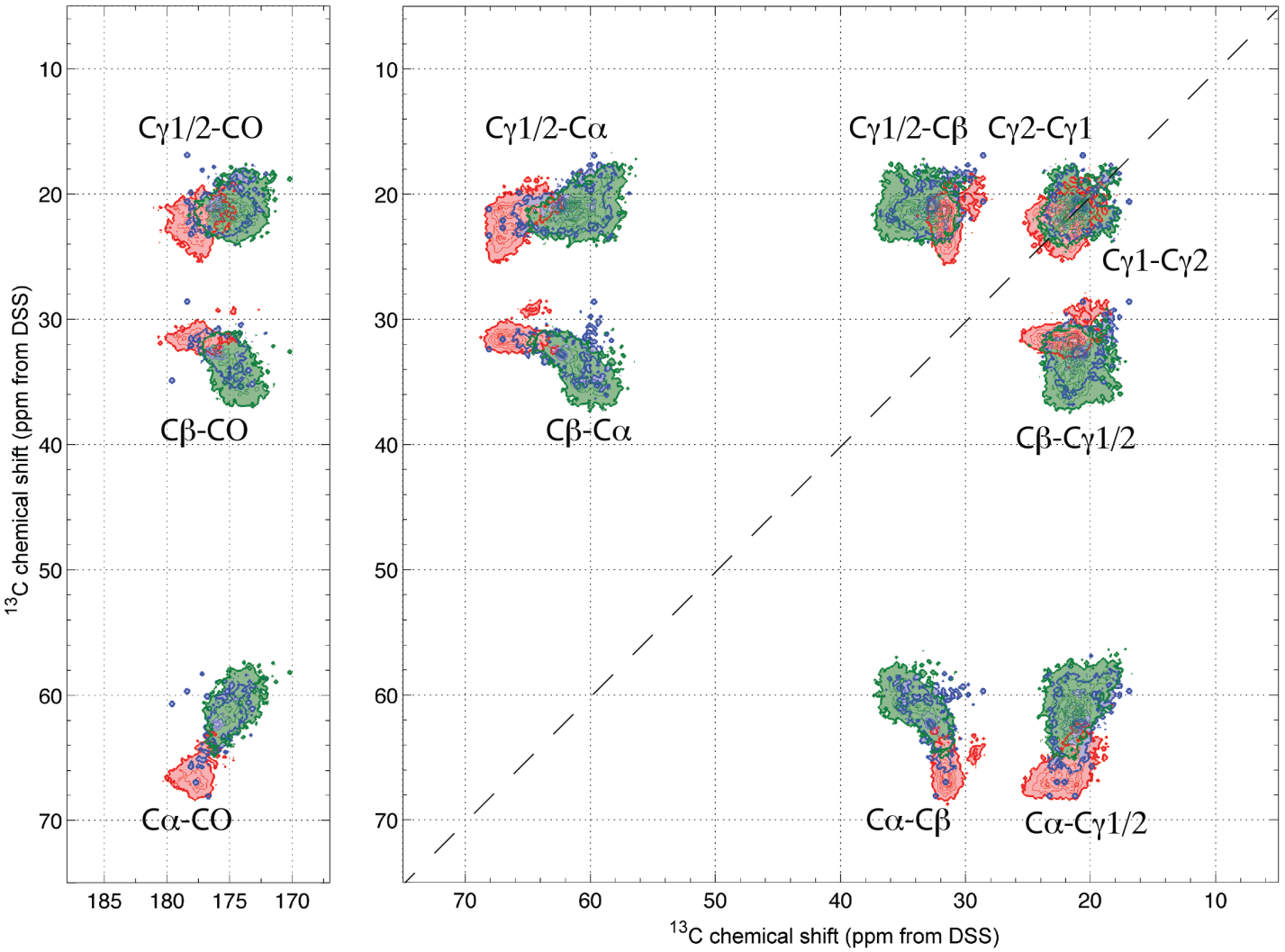
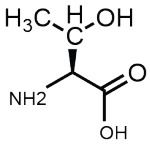
Supplemental Figure S18

Val Helix: 5,287 Sheet: 7,668 Coil: 5,367 Total: 18,322

V





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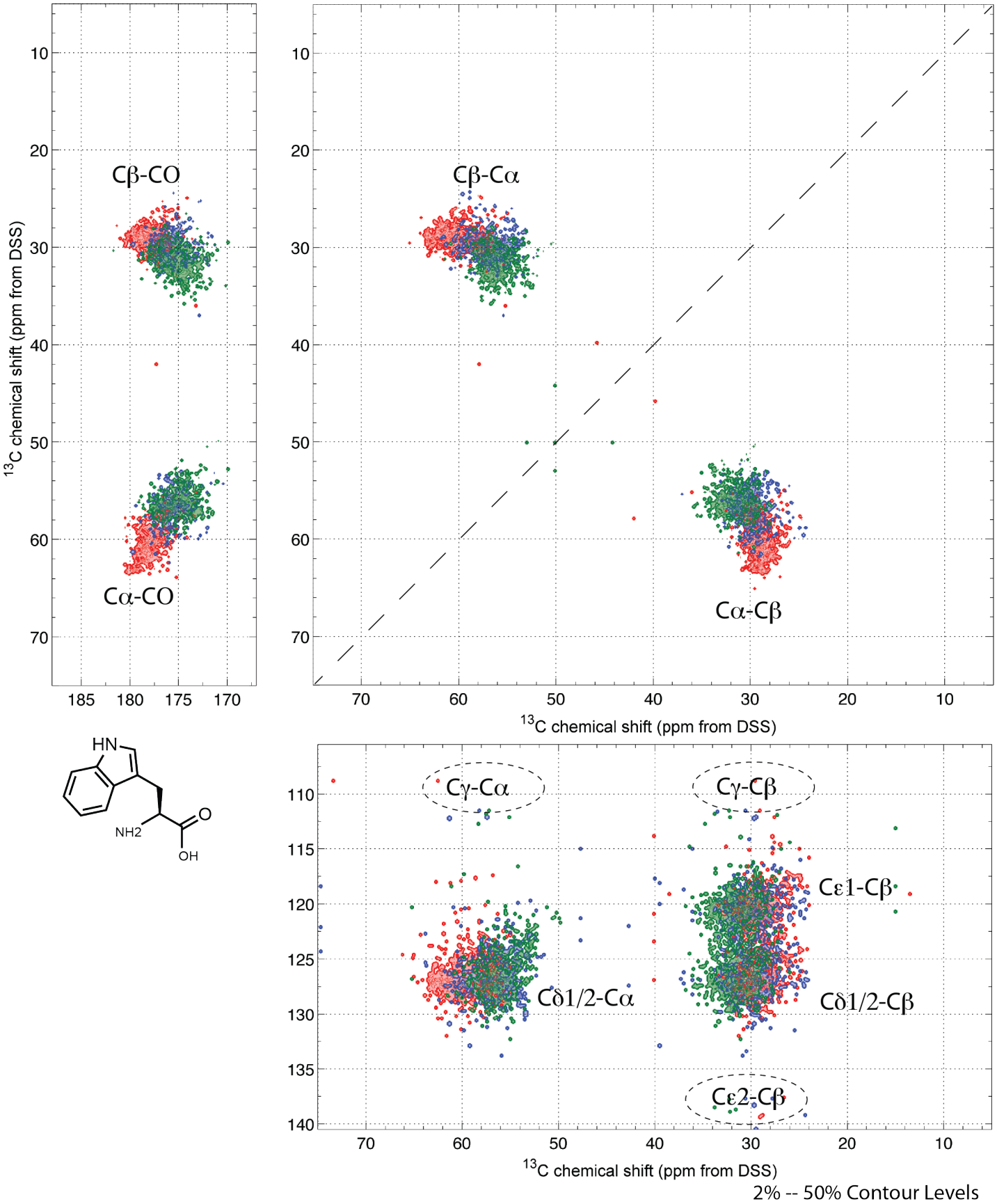
Supplemental Figure S19

Trp

Helix: 1,077 Sheet: 1,112 Coil: 1,023 Total: 3,212

W



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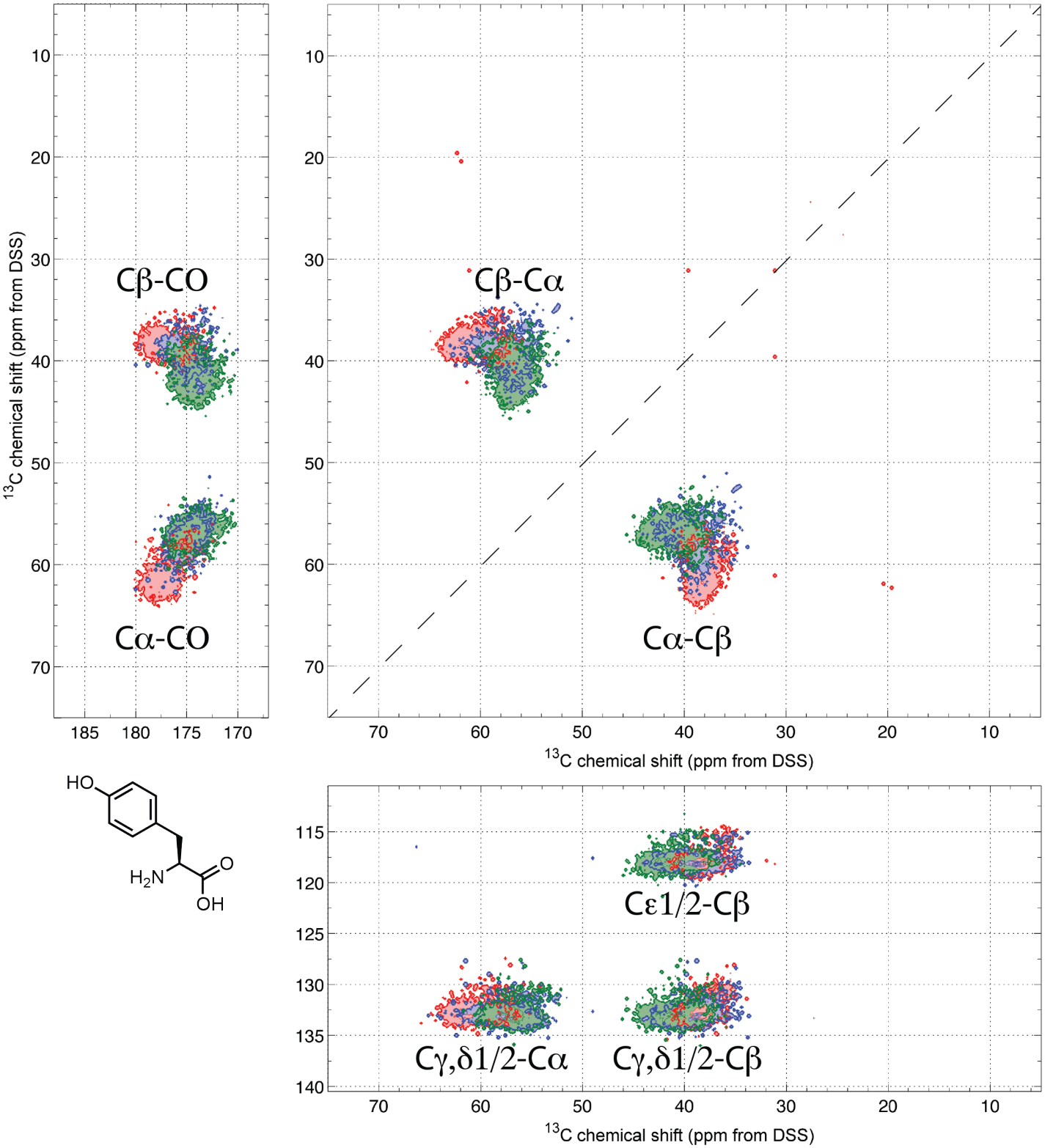
Supplemental Figure S20

Tyr Helix: 2,590 Sheet: 2,925 Coil: 2,786 Total: 8,301

Y



0.5% -- 50% Contour Levels

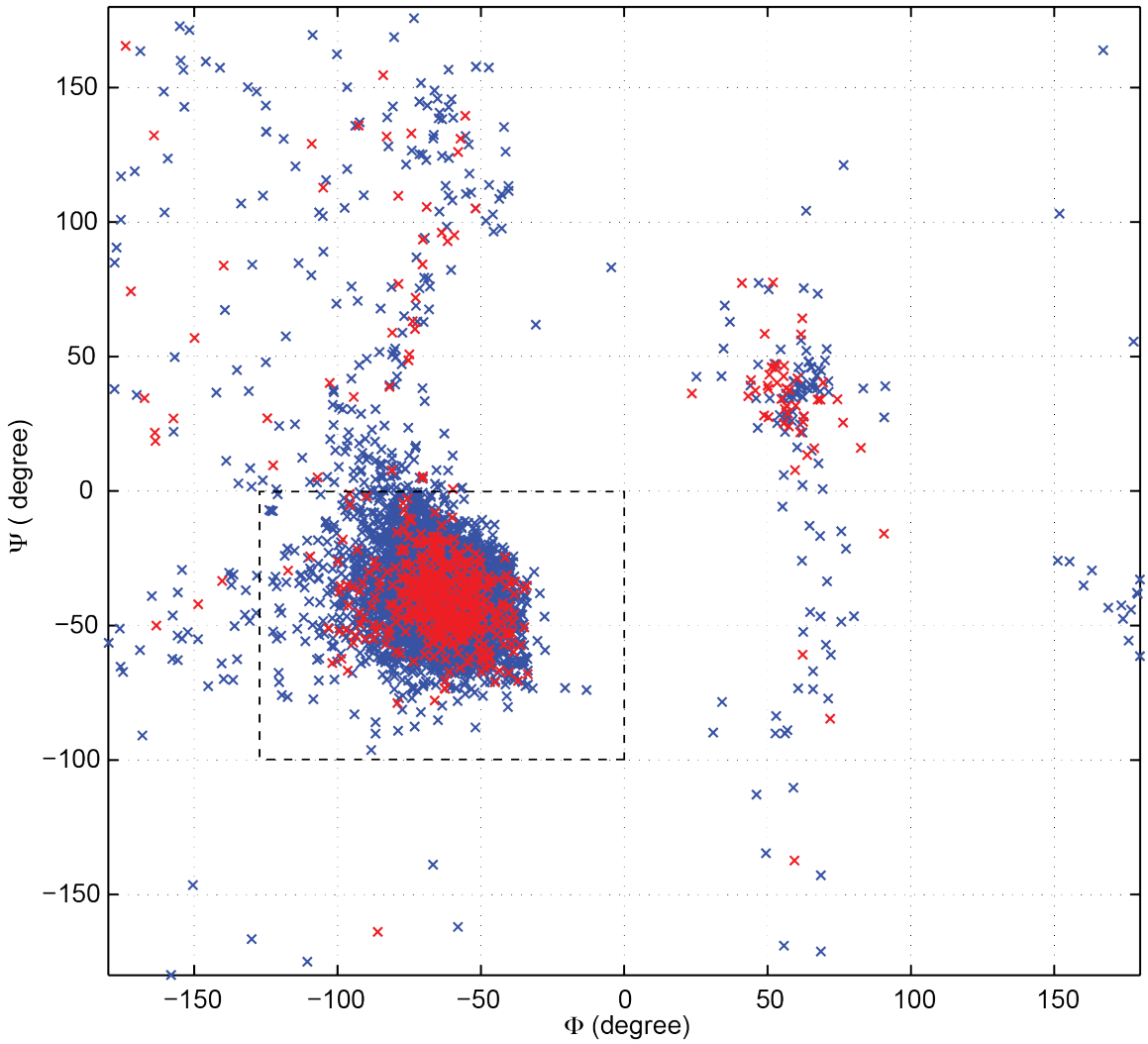


Figure S21. Ramachandran diagram of the Ala residues with different α-helical chemical shift ranges as shown in Figure 1a. Torsion angles from the main (Cα, Cβ) chemical shift range of (54.0-57.0 ppm, 16.4-20.4 ppm) are plotted in blue. Torsion angles from the second (Cα, Cβ) chemical shifts of (51.6-54.0 ppm, 14.8-16.8 ppm) are shown in red. Dashed box indicates the range of (ϕ, ψ) torsion angles that were included in the calculation of the average torsion angles and their standard deviations reported in the main text.

AA	Strc	C′	Cα	Cβ	Cγ/Cγ1	Cγ2	Cδ/Cδ1	Cδ2	Cε/Cε1	Cε2	Cε3	Cζ	Cζ2	Cζ3	Cη2
A	Helix	179.02	54.66	18.36	-	-	-	-	-	-	-	-	-	-	-
	Coil	177.02	52.46	19.32	-	-	-	-	-	-	-	-	-	-	-
	Sheet	175.67	50.92	21.72	-	-	-	-	-	-	-	-	-	-	-
C	Helix	176.16	61.40	30.93	-	-	-	-	-	-	-	-	-	-	-
	Coil	175.07	57.59	33.05	-	-	-	-	-	-	-	-	-	-	-
	Sheet	173.75	56.45	34.18	-	-	-	-	-	-	-	-	-	-	-
D	Helix	177.70	56.75	40.34	157.08	-	-	-	-	-	-	-	-	-	-
	Coil	175.94	54.08	40.95	165.85	-	-	-	-	-	-	-	-	-	-
	Sheet	175.41	53.57	42.31	162.25	-	-	-	-	-	-	-	-	-	-
E	Helix	177.97	58.89	29.35	36.12	-	158.17	-	-	-	-	-	-	-	-
	Coil	176.07	56.66	30.18	36.06	-	174.49	-	-	-	-	-	-	-	-
	Sheet	175.08	55.04	32.37	36.24	-	180.68	-	-	-	-	-	-	-	-
F	Helix	176.52	60.51	38.86	139.63	-	130.98	130.83	130.63	130.62	-	129.02	-	-	-
	Coil	174.86	57.47	39.68	138.45	-	131.12	131.17	130.64	130.60	-	129.07	-	-	-
	Sheet	174.18	56.40	41.78	139.63	-	131.54	131.64	130.42	130.51	-	128.94	-	-	-
G	Helix	175.30	46.72	-	-	-	-	-	-	-	-	-	-	-	-
	Coil	173.81	45.33	-	-	-	-	-	-	-	-	-	-	-	-
	Sheet	172.08	45.17	-	-	-	-	-	-	-	-	-	-	-	-
H	Helix	176.62	58.57	29.85	128.00	-	-	120.48	137.99	-	-	-	-	-	-
	Coil	174.73	55.95	30.17	133.23	-	-	119.23	137.22	-	-	-	-	-	-
	Sheet	173.96	55.17	32.26	132.86	-	-	119.48	137.09	-	-	-	-	-	-
I	Helix	176.84	64.26	37.51	28.67	17.42	13.46	-	-	-	-	-	-	-	-
	Coil	175.47	60.71	38.67	27.17	17.60	13.36	-	-	-	-	-	-	-	-
	Sheet	174.77	59.83	39.95	27.38	17.72	13.71	-	-	-	-	-	-	-	-
K	Helix	177.46	58.82	32.20	25.09	-	29.01	-	41.79	-	-	-	-	-	-
	Coil	175.82	56.23	32.82	24.82	-	28.93	-	41.96	-	-	-	-	-	-
	Sheet	175.09	55.05	34.82	24.93	-	29.20	-	41.94	-	-	-	-	-	-
L	Helix	178.12	57.34	41.46	26.84	-	24.74	24.06	-	-	-	-	-	-	-
	Coil	176.42	54.78	42.31	26.79	-	24.83	23.97	-	-	-	-	-	-	-
	Sheet	175.43	53.83	44.24	27.10	-	25.07	24.70	-	-	-	-	-	-	-
M	Helix	177.73	57.99	32.20	32.15	-	-	-	17.11	-	-	-	-	-	-
	Coil	175.43	55.26	33.16	31.96	-	-	-	17.14	-	-	-	-	-	-
	Sheet	174.52	54.27	35.28	32.02	-	-	-	17.28	-	-	-	-	-	-
N	Helix	176.35	55.27	38.23	169.18	-	-	-	-	-	-	-	-	-	-
	Coil	174.68	53.12	38.66	171.79	-	-	-	-	-	-	-	-	-	-
	Sheet	174.37	52.26	40.28	171.76	-	-	-	-	-	-	-	-	-	-
P	Helix	177.52	65.27	31.54	27.74	-	50.17	-	-	-	-	-	-	-	-
	Coil	176.21	63.06	32.04	27.21	-	50.26	-	-	-	-	-	-	-	-
	Sheet	175.97	62.71	32.15	27.34	-	50.47	-	-	-	-	-	-	-	-
Q	Helix	177.56	58.30	28.57	33.84	-	177.25	-	-	-	-	-	-	-	-
	Coil	175.48	55.73	29.46	33.71	-	175.48	-	-	-	-	-	-	-	-
	Sheet	174.66	54.49	31.47	33.81	-	178.00	-	-	-	-	-	-	-	-
R	Helix	177.83	58.79	29.99	27.42	-	43.14	-	-	-	-	160.80	-	-	-
	Coil	175.78	55.96	30.75	27.07	-	43.17	-	-	-	-	159.95	-	-	-

	Sheet	174.82	54.77	32.80	27.29	-	43.32	-	-	-	-	159.99	-	-	-
Q	**Helix**	175.83	60.94	62.56	-	-	-	-	-	-	-	-	-	-	-
	Coil	174.35	58.22	63.67	-	-	-	-	-	-	-	-	-	-	-
	Sheet	173.43	57.17	64.96	-	-	-	-	-	-	-	-	-	-	-
T	**Helix**	175.95	65.42	68.20	-	21.67	-	-	-	-	-	-	-	-	-
	Coil	174.48	61.46	69.44	-	21.61	-	-	-	-	-	-	-	-	-
	Sheet	173.58	61.08	70.39	-	21.55	-	-	-	-	-	-	-	-	-
V	**Helix**	177.34	65.82	31.54	21.94	22.11	-	-	-	-	-	-	-	-	-
	Coil	175.49	61.78	32.76	21.21	20.89	-	-	-	-	-	-	-	-	-
	Sheet	174.60	60.68	34.00	21.46	21.13	-	-	-	-	-	-	-	-	-
W	**Helix**	177.64	60.02	29.07	111.47	-	126.23	128.50	-	147.78	120.14	-	114.01	121.19	123.75
	Coil	175.76	57.09	30.02	112.14	-	126.31	130.64	-	138.49	120.17	-	114.12	121.24	123.43
	Sheet	175.06	56.11	31.54	112.66	-	126.03	122.84	-	132.99	120.02	-	114.07	121.05	123.57
Y	**Helix**	177.00	60.61	38.08	130.13	-	132.04	131.81	117.76	117.74	-	157.84	-	-	-
	Coil	175.08	57.56	38.98	127.65	-	132.63	132.33	117.88	117.73	-	158.10	-	-	-
	Sheet	174.31	56.63	41.07	129.54	-	132.65	132.68	117.78	117.75	-	155.87	-	-	-

Supplementary Table S1. Average ^{13}C chemical shifts of different amino acids and secondary structures obtained from PACSYlite. The shifts are referenced to DSS.