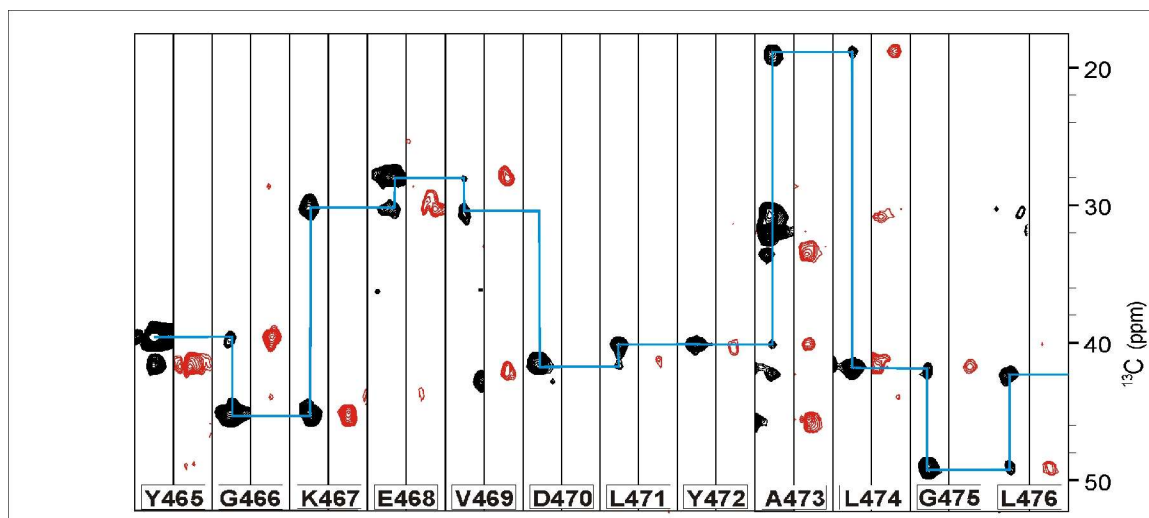
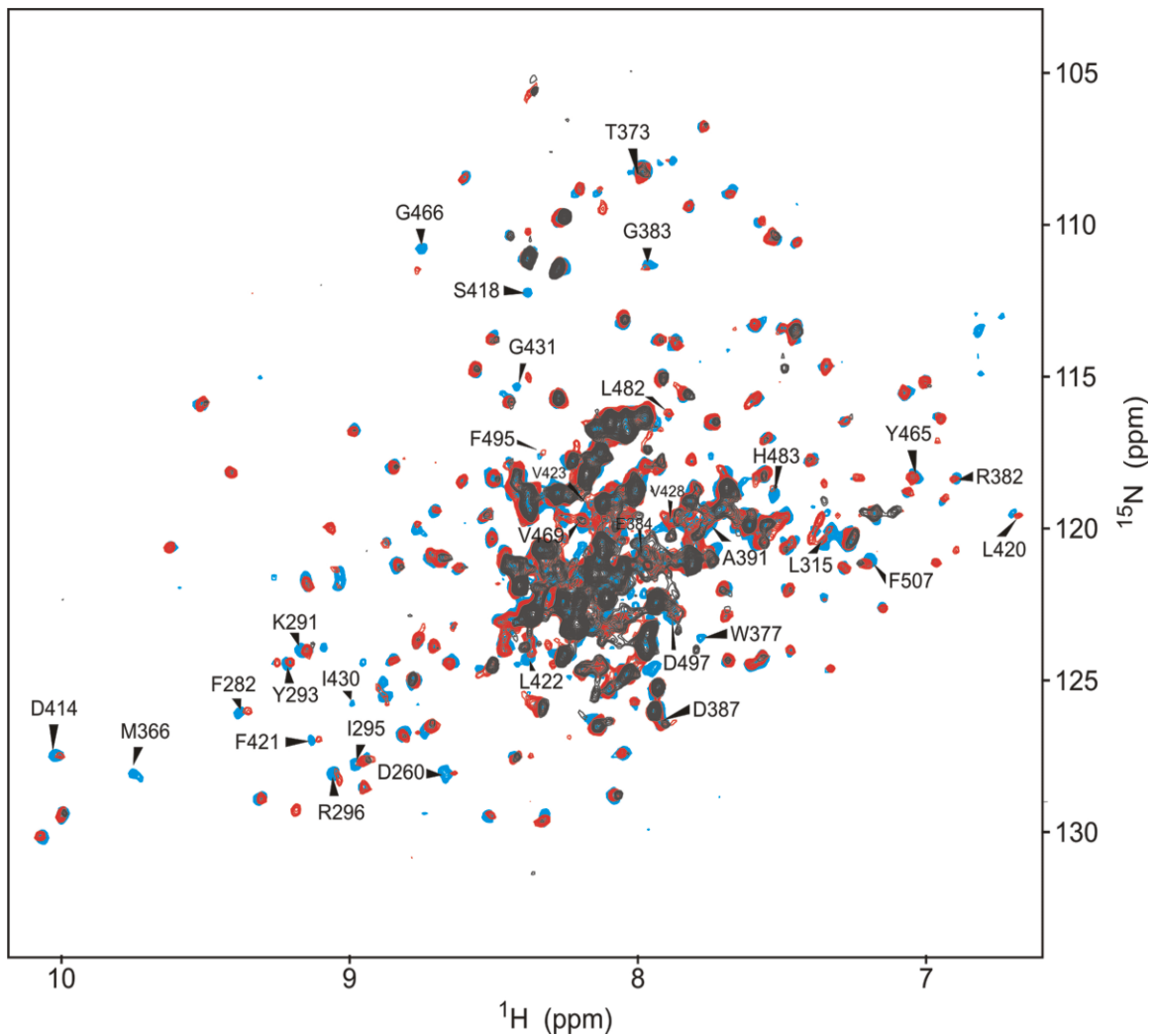


**Supporting Information for**  
**Mapping of the Auto-Inhibitory Interactions of Protein Kinase R by Nuclear Magnetic**  
**Resonance**

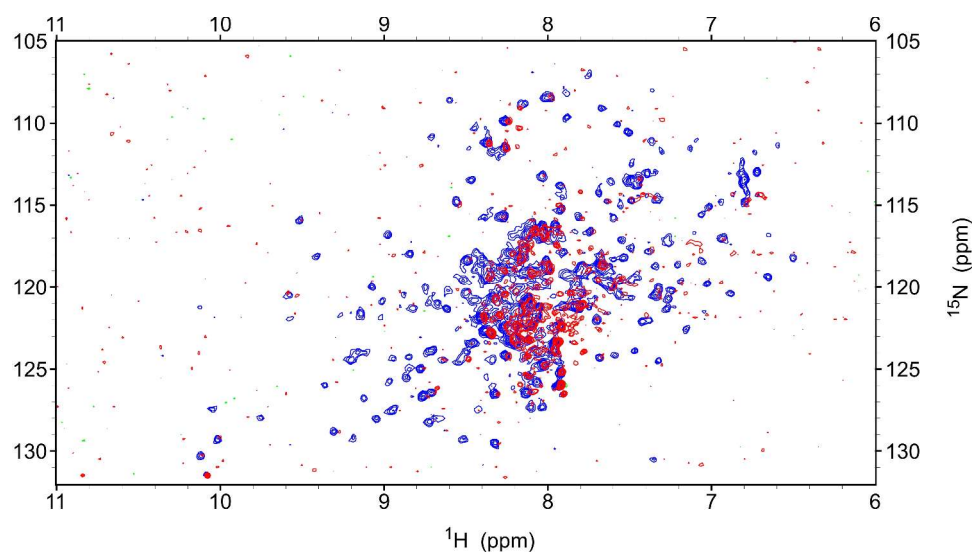
by  
Vladimir Gelev<sup>1†</sup>, Husseyin Aktas<sup>2</sup>, Assen Marintchev<sup>1</sup>, Takuhiro Ito<sup>1</sup>, Dominique Frueh<sup>1</sup>,  
Michael Hemond<sup>1</sup>, David Rovnyak<sup>4</sup>, Miriam Debus<sup>2</sup>, Sven Hyberts<sup>1</sup>, Anny Usheva<sup>3</sup>, Jose  
Halperin<sup>2</sup> and Gerhard Wagner<sup>1\*</sup>



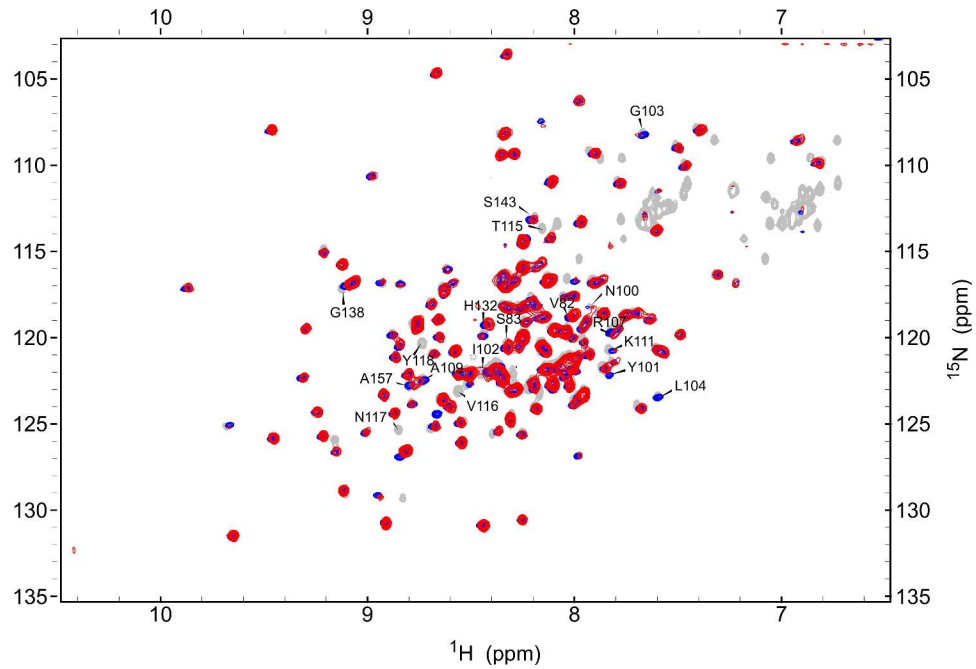
**Figure 1\_SI.** 2D strips from the non-linear Trosy-HNCACB (black) and Trosy-HNCOCACB (red) spectra of the K296R kinase domain (residues 252-551, 250 $\mu$ M in 50 mM sodium phosphate, 25 mM ammonium sulfate, pH 6.70). Sequential connectivities are shown in blue.



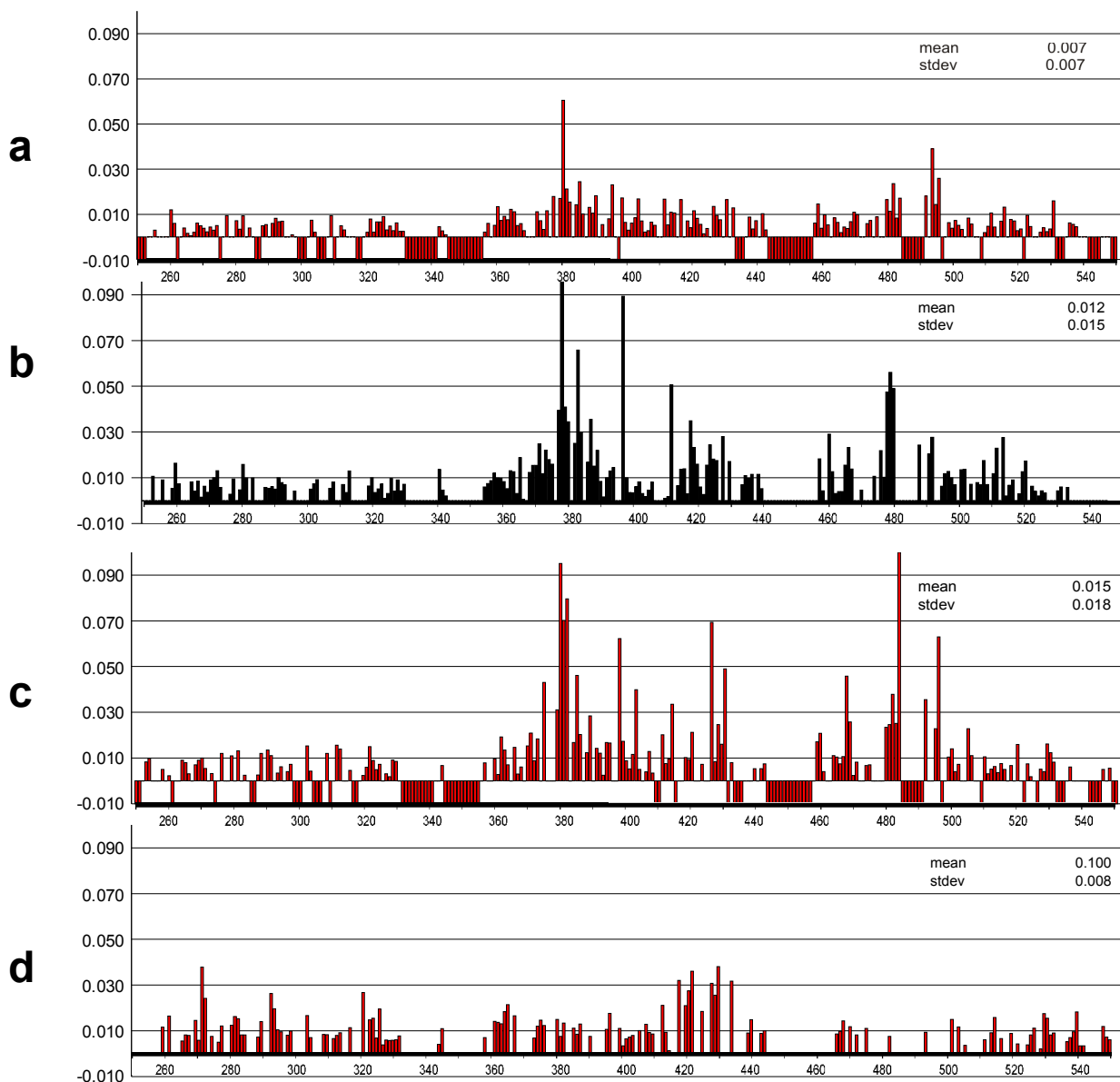
**Figure 2\_SI.**  $^{15}\text{N}$ -HSQC spectrum of the kinase domain (K296R) alone (50  $\mu\text{M}$ , blue trace) and in the presence of 0.2 mM (red) and 0.6 mM (black) RBD (1-178). Amide residues that display the most significant changes are labeled;



**Figure 3\_SI.**  $^{15}\text{N}$ -HSQC spectrum of the H483D/K296R kinase alone (blue) and in the presence of 5-fold excess RBD (1-178) (red).



**Figure 4\_SI.** <sup>15</sup>N-HSQC spectrum of the mutant N117R full-length dsRNA binding domain, RBD (1-178) alone (blue trace) and in the presence of two-fold excess KD (K296R 252-551, red). The spectrum of the wild-type RBD is shown in gray.



**Figure 5\_SI.** Chemical shift perturbation data for the PKR kinase domain (251-551). Peaks that have been assigned but whose shift can not be determined due to overlap are omitted. Unassigned residues are shown as negative values in a) and c); a) Changes in 0.1 mM K296R KD upon addition of 2-fold excess RBD2 (97-178); b) changes in K296R KD upon addition of 7-fold excess RBD2 (97-178); c) changes in the K296R KD upon addition of 3-fold excess RBD1+2 (1-178); d) changes in the K296R/F495A mutant KD upon addition of 5-fold excess RBD1+2 (1-178).

**Table 1\_SI.** NMR assignments of the PKR kinase domain (M252-C551, K296R) backbone. The data was collected in 20 mM Na phosphate buffer, pH 6.70 at 25° C and referenced to DSS. The amide chemical shifts are from TROSY data and uncorrected. CO chemical shifts are from HNC0 spectra and are shown as the 'CO-1' resonance for the n+1 amino acid.

Group	Atom	Nuc	Shift	SDev	Assignments
T4	CA	13C	61.525	0.000	1
T4	CA-1	13C	56.647	0.000	1
T4	CB	13C	69.675	0.000	1
T4	CB-1	13C	29.596	0.000	1
T4	CO-1	13C	177.249	0.000	1
T4	H	1H	7.463	0.007	10
T4	N	15N	113.497	0.050	8
K5	CA	13C	56.722	0.000	1
K5	CA-1	13C	61.434	0.000	1
K5	CB	13C	32.412	0.000	1
K5	CB-1	13C	69.686	0.000	1
K5	CO-1	13C	174.460	0.000	1
K5	H	1H	8.097	0.005	10
K5	N	15N	125.008	0.087	8
Y6	CA	13C	59.221	0.000	1
Y6	CA-1	13C	56.689	0.000	1
Y6	CB	13C	40.056	0.000	1
Y6	CB-1	13C	32.379	0.000	1
Y6	CO-1	13C	177.130	0.000	1
Y6	H	1H	8.454	0.008	12
Y6	N	15N	118.018	0.070	9
T7	CA	13C	59.031	0.000	1
T7	CA-1	13C	59.192	0.000	1
T7	CB	13C	69.988	0.000	1
T7	CB-1	13C	40.079	0.000	1
T7	CO-1	13C	176.064	0.000	1
T7	H	1H	7.440	0.015	8
T7	N	15N	113.695	0.125	7
V8	CB	13C	31.444	0.000	1
V8	CB-1	13C	69.996	0.000	1
V8	CO-1	13C	172.600	0.000	1
V8	H	1H	9.167	0.009	10
V8	N	15N	122.097	0.053	7
D9	CA	13C	55.493	0.000	1
D9	CB	13C	44.231	0.000	1
D9	CB-1	13C	31.319	0.000	1
D9	CO-1	13C	177.048	0.000	1
D9	H	1H	8.669	0.009	9
D9	N	15N	128.099	0.073	7
K10	CA	13C	59.247	0.000	1
K10	CA-1	13C	55.505	0.000	1
K10	CB	13C	31.883	0.000	1
K10	CB-1	13C	44.224	0.000	1
K10	CO-1	13C	178.612	0.000	1
K10	H	1H	8.342	0.015	13
K10	N	15N	129.615	0.094	9
R11	CA	13C	59.131	0.000	1
R11	CA-1	13C	59.330	0.000	1
R11	CB	13C	28.152	0.000	1
R11	CB-1	13C	31.814	0.000	1
R11	CO-1	13C	178.354	0.000	1

R11	H	1H	7.953	0.014	15
R11	N	15N	121.228	0.141	10
F12	CA	13C	57.420	0.000	1
F12	CA-1	13C	59.358	0.000	1
F12	CB	13C	37.524	0.000	1
F12	CB-1	13C	28.243	0.000	1
F12	CO-1	13C	178.522	0.000	1
F12	H	1H	9.286	0.006	18
F12	N	15N	121.682	0.120	12
G13	CA	13C	46.106	0.007	2
G13	CA-1	13C	57.247	0.000	1
G13	H	1H	7.352	0.006	13
G13	N	15N	98.572	0.117	6
M14	CA	13C	57.102	0.000	1
M14	CA-1	13C	46.116	0.000	1
M14	CB	13C	32.897	0.000	1
M14	CB-1	13C	45.961	0.000	1
M14	CO-1	13C	178.350	0.000	1
M14	H	1H	7.685	0.007	14
M14	N	15N	118.867	0.045	10
D15	CA	13C	55.294	0.000	1
D15	CA-1	13C	56.872	0.000	1
D15	CB	13C	41.533	0.000	1
D15	CB-1	13C	32.979	0.000	1
D15	CO-1	13C	178.779	0.000	1
D15	H	1H	8.036	0.008	14
D15	N	15N	118.442	0.054	10
F16	C	13C	175.642	0.000	0
F16	CA	13C	56.854	0.009	2
F16	CA-1	13C	55.326	0.000	1
F16	CB	13C	41.245	0.094	2
F16	CB-1	13C	41.406	0.000	1
F16	CO-1	13C	175.642	0.000	1
F16	H	1H	7.563	0.014	11
F16	N	15N	117.046	0.052	9
K17	C	13C	173.800	0.000	0
K17	CA	13C	53.523	0.050	2
K17	CB	13C	35.668	0.018	2
K17	CO-1	13C	173.800	0.000	1
K17	H	1H	9.429	0.005	10
K17	N	15N	118.250	0.076	8
E18	C	13C	174.024	0.000	0
E18	CA	13C	56.743	0.060	2
E18	CB	13C	26.435	0.050	2
E18	CO-1	13C	174.024	0.000	1
E18	H	1H	8.844	0.005	10
E18	N	15N	118.021	0.119	8
I19	C	13C	175.364	0.000	0
I19	CA	13C	63.046	0.061	2
I19	CB	13C	38.024	0.130	2
I19	CO-1	13C	175.364	0.000	1
I19	H	1H	7.801	0.009	10
I19	N	15N	118.769	0.043	8
E20	C	13C	177.598	0.000	0
E20	CA	13C	54.609	0.003	2
E20	CB	13C	33.456	0.014	2
E20	CO-1	13C	177.598	0.000	1
E20	H	1H	9.331	0.014	10
E20	N	15N	128.979	0.116	8
L21	C	13C	175.402	0.000	0
L21	CA	13C	55.560	0.000	1
L21	CB	13C	41.604	0.000	1
L21	CO-1	13C	175.402	0.000	1
L21	H	1H	8.048	0.013	8

L21	N	15N	127.333	0.104	7
I22	CA	13C	61.361	0.000	1
I22	CA-1	13C	55.658	0.000	1
I22	CB	13C	38.942	0.000	1
I22	CB-1	13C	41.701	0.000	1
I22	CO-1	13C	177.129	0.000	1
I22	H	1H	8.955	0.006	11
I22	N	15N	124.528	0.103	8
G23	CA	13C	45.873	0.068	4
G23	CA-1	13C	61.465	0.000	1
G23	CB-1	13C	38.798	0.000	1
G23	CO-1	13C	176.851	0.000	1
G23	H	1H	7.591	0.008	12
G23	N	15N	109.958	0.093	9
S24	C	13C	171.794	0.000	0
S24	CA	13C	57.328	0.035	2
S24	CB	13C	64.469	0.046	2
S24	CO-1	13C	171.794	0.000	1
S24	H	1H	8.270	0.007	8
S24	N	15N	115.709	0.028	7
S24	ca	13C	57.230	0.000	0
G25	C	13C	173.997	0.000	0
G25	CA	13C	45.381	0.112	2
G25	CO-1	13C	173.997	0.000	1
G25	H	1H	8.064	0.013	12
G25	N	15N	113.093	0.081	9
G26	CA	13C	46.602	0.000	1
F27	C	13C	174.341	0.000	0
F27	CA	13C	55.945	0.051	2
F27	CA-1	13C	46.666	0.000	1
F27	CB	13C	38.400	0.025	2
F27	CO-1	13C	174.341	0.000	1
F27	H	1H	7.719	0.009	10
F27	N	15N	118.245	0.129	8
G28	C	13C	175.411	0.000	0
G28	CA	13C	44.977	0.046	4
G28	CO-1	13C	175.411	0.000	1
G28	H	1H	7.553	0.014	13
G28	N	15N	110.527	0.091	10
Q29	C	13C	174.828	0.000	0
Q29	CA	13C	55.816	0.011	2
Q29	CB	13C	33.518	0.000	1
Q29	CO-1	13C	173.281	0.000	1
Q29	H	1H	8.082	0.005	8
Q29	N	15N	119.183	0.099	7
V30	C	13C	174.541	0.000	0
V30	CA	13C	61.451	0.049	2
V30	CB	13C	33.424	0.027	2
V30	CO-1	13C	174.541	0.000	1
V30	H	1H	8.319	0.005	7
V30	N	15N	121.795	0.086	6
V30?	H	1H	8.319	0.002	3
V30?	N	15N	121.751	0.055	2
F31	C	13C	173.911	0.000	0
F31	CA	13C	56.079	0.012	2
F31	CB	13C	42.680	0.055	2
F31	CO-1	13C	173.911	0.000	1
F31	H	1H	9.377	0.008	11
F31	N	15N	125.919	0.097	9
K32	C	13C	175.534	0.000	0
K32	CA	13C	54.688	0.082	2
K32	CB	13C	35.266	0.095	2
K32	CO-1	13C	175.534	0.000	1
K32	H	1H	9.159	0.007	10



K32	N	15N	121.648	0.105	8
A33	C	13C	175.043	0.000	0
A33	CA	13C	51.559	0.011	2
A33	CB	13C	24.099	0.082	2
A33	CO-1	13C	175.043	0.000	1
A33	H	1H	8.724	0.006	8
A33	N	15N	123.899	0.100	7
K34	CA	13C	54.527	0.077	2
K34	CB	13C	34.410	0.139	2
K34	CO-1	13C	174.977	0.000	1
K34	H	1H	8.688	0.009	13
K34	N	15N	121.013	0.101	9
H35	CA	13C	58.468	0.000	1
H35	CB	13C	31.880	0.000	1
H35	CO-1	13C	176.603	0.000	1
H35	H	1H	9.202	0.008	12
H35	N	15N	129.255	0.128	9
H35	C	13C	176.603	0.000	0
H35	CA	13C	58.468	0.000	0
H35	CB	13C	31.880	0.000	0
H35	H	1H	9.203	0.000	0
H35	N	15N	129.255	0.000	0
R36	CA	13C	59.587	0.000	1
R36	CA-1	13C	58.515	0.000	1
R36	CB	13C	29.715	0.000	1
R36	CB-1	13C	31.908	0.000	1
R36	CO-1	13C	178.784	0.000	1
R36	H	1H	8.148	0.004	13
R36	N	15N	126.404	0.098	10
G39	CA	13C	46.426	0.051	2
G39	CA-1	13C	54.138	0.000	1
G39	CB-1	13C	40.549	0.000	1
G39	CO-1	13C	178.985	0.000	1
G39	H	1H	7.690	0.003	11
G39	N	15N	109.019	0.119	9
K40	CA	13C	56.189	0.066	2
K40	CA-1	13C	46.364	0.152	2
K40	CB	13C	32.153	0.000	1
K40	CO-1	13C	174.685	0.000	1
K40	H	1H	9.181	0.016	11
K40	N	15N	124.008	0.103	9
T41	CA	13C	62.570	0.031	2
T41	CB	13C	69.238	0.046	2
T41	CB-1	13C	32.087	0.000	1
T41	CO-1	13C	175.604	0.000	1
T41	H	1H	8.149	0.006	8
T41	N	15N	118.092	0.099	7
Y42	CA	13C	57.829	0.012	2
Y42	CB	13C	42.773	0.037	2
Y42	CO-1	13C	173.193	0.000	1
Y42	H	1H	9.224	0.006	10
Y42	N	15N	124.447	0.088	9
V43	CA	13C	61.120	0.019	2
V43	CB	13C	33.194	0.068	2
V43	CO-1	13C	174.574	0.000	1
V43	H	1H	8.771	0.005	10
V43	N	15N	120.078	0.101	8
I44	CA	13C	58.114	0.000	1
I44	CB	13C	40.044	0.000	1
I44	CO-1	13C	175.770	0.000	1
I44	H	1H	8.987	0.005	10
I44	N	15N	127.655	0.095	8
R45	CA	13C	54.061	0.000	1
R45	CA-1	13C	58.336	0.000	1

R45	CB	13C	32.421	0.000	1
R45	CB-1	13C	40.031	0.000	1
R45	CO-1	13C	176.041	0.000	1
R45	H	1H	9.058	0.005	8
R45	N	15N	128.078	0.069	7
R46	CA	13C	54.427	0.000	1
R46	CA-1	13C	54.148	0.000	1
R46	CB	13C	33.227	0.000	1
R46	CB-1	13C	32.568	0.000	1
R46	CO-1	13C	174.388	0.000	1
R46	H	1H	8.945	0.008	9
R46	N	15N	127.534	0.092	8
V47	CA	13C	58.030	0.000	1
V47	CA-1	13C	54.669	0.000	1
V47	CB	13C	35.138	0.000	1
V47	CB-1	13C	33.065	0.000	1
V47	CO-1	13C	174.580	0.000	1
V47	H	1H	8.467	0.005	10
V47	N	15N	120.918	0.126	8
K48	CA	13C	57.814	0.027	2
K48	CA-1	13C	58.265	0.000	1
K48	CB	13C	32.906	0.020	2
K48	CB-1	13C	35.106	0.000	1
K48	CO-1	13C	175.353	0.000	1
K48	H	1H	8.866	0.011	10
K48	N	15N	125.378	0.183	8
Y49	CA	13C	58.547	0.000	1
Y49	CB	13C	38.729	0.000	1
Y49	CO-1	13C	176.059	0.000	1
Y49	H	1H	8.436	0.012	10
Y49	N	15N	127.450	0.140	8
K53	CA	13C	59.581	0.000	1
K53	CA-1	13C	58.822	0.000	1
K53	CB	13C	31.482	0.000	1
K53	CB-1	13C	29.128	0.000	1
K53	CO-1	13C	178.092	0.000	1
K53	H	1H	8.202	0.004	12
K53	N	15N	121.581	0.094	9
A54	CA	13C	54.912	0.049	2
A54	CA-1	13C	59.585	0.000	1
A54	CB	13C	18.025	0.167	2
A54	CB-1	13C	31.556	0.000	1
A54	CO-1	13C	179.127	0.000	1
A54	H	1H	7.712	0.010	12
A54	N	15N	122.023	0.093	9
E55	CA	13C	59.087	0.000	1
E55	CB	13C	29.100	0.000	1
E55	CO-1	13C	179.773	0.000	1
E55	H	1H	7.407	0.009	12
E55	N	15N	117.853	0.087	9
K59	CA	13C	59.967	0.000	1
K59	CA-1	13C	66.449	0.000	1
K59	CB	13C	31.836	0.000	1
K59	CB-1	13C	30.842	0.000	1
K59	CO-1	13C	178.454	0.000	1
K59	H	1H	8.086	0.006	10
K59	N	15N	119.965	0.037	8
A60	CA	13C	54.654	0.000	1
A60	CA-1	13C	59.932	0.000	1
A60	CB	13C	17.701	0.000	1
A60	CB-1	13C	31.820	0.000	1
A60	CO-1	13C	179.762	0.000	1
A60	H	1H	7.294	0.008	12
A60	N	15N	121.262	0.140	10

A62	C	13C	179.762	0.000	0
A62	CA	13C	53.394	0.000	1
A62	CB	13C	17.672	0.000	1
A62	H	1H	7.713	0.010	9
A62	N	15N	120.547	0.209	6
K63	CA	13C	56.017	0.000	1
K63	CA-1	13C	53.279	0.000	1
K63	CB	13C	32.236	0.000	1
K63	CB-1	13C	17.813	0.000	1
K63	CO-1	13C	178.122	0.000	1
K63	H	1H	7.081	0.006	12
K63	N	15N	115.582	0.097	9
L64	CA	13C	55.295	0.000	1
L64	CA-1	13C	55.926	0.000	1
L64	CB	13C	41.140	0.000	1
L64	CB-1	13C	32.070	0.000	1
L64	CO-1	13C	177.945	0.000	1
L64	H	1H	7.364	0.007	12
L64	N	15N	120.522	0.132	9
D65	CA	13C	53.878	0.000	1
D65	CA-1	13C	55.414	0.000	1
D65	CB	13C	42.224	0.000	1
D65	CB-1	13C	41.103	0.000	1
D65	CO-1	13C	177.407	0.000	1
D65	H	1H	8.290	0.006	8
D65	N	15N	121.627	0.151	7
H66	CA	13C	57.561	0.000	1
H66	CA-1	13C	54.111	0.000	1
H66	CB	13C	34.085	0.000	1
H66	CB-1	13C	42.649	0.000	1
H66	CO-1	13C	173.015	0.000	1
H66	H	1H	8.716	0.004	9
H66	N	15N	126.548	0.132	7
V67	CA	13C	64.398	0.000	1
V67	CA-1	13C	57.466	0.000	1
V67	CB	13C	31.272	0.000	1
V67	CB-1	13C	34.094	0.000	1
V67	CO-1	13C	176.347	0.000	1
V67	H	1H	7.337	0.005	12
V67	N	15N	124.619	0.094	10
V70	C	13C	176.181	0.000	0
V70	CA	13C	63.662	0.031	2
V70	CA-1	13C	60.284	0.000	1
V70	CB	13C	32.742	0.129	2
V70	CB-1	13C	40.243	0.000	1
V70	CO-1	13C	176.181	0.000	1
V70	H	1H	8.674	0.009	8
V70	N	15N	127.961	0.104	7
H71	C	13C	174.779	0.000	0
H71	CA	13C	56.954	0.006	2
H71	CB	13C	29.161	0.031	2
H71	CO-1	13C	174.779	0.000	1
H71	H	1H	9.101	0.010	10
H71	N	15N	123.906	0.101	8
Y72	C	13C	174.908	0.000	0
Y72	CA	13C	57.866	0.000	1
Y72	CB	13C	38.947	0.000	1
Y72	CO-1	13C	174.908	0.000	1
Y72	H	1H	8.750	0.013	8
Y72	N	15N	126.696	0.115	7
N73	CA	13C	55.602	0.000	1
N73	CA-1	13C	58.000	0.000	1
N73	CB	13C	40.969	0.000	1
N73	CB-1	13C	38.920	0.000	1

N73	CO-1	13C	175.122	0.000	1
N73	H	1H	8.881	0.007	12
N73	N	15N	120.455	0.070	9
G74	CA	13C	45.239	0.105	2
G74	CA-1	13C	55.550	0.000	1
G74	CB-1	13C	40.691	0.000	1
G74	CO-1	13C	175.934	0.000	1
G74	H	1H	7.515	0.005	12
G74	N	15N	103.685	0.096	9
C75	CA	13C	55.693	0.001	2
C75	CA-1	13C	45.133	0.053	2
C75	CB	13C	32.228	0.101	2
C75	CO-1	13C	171.115	0.000	1
C75	H	1H	8.564	0.007	8
C75	N	15N	114.869	0.068	7
W76	CA	13C	57.761	0.038	2
W76	CB	13C	31.294	0.003	2
W76	CO-1	13C	173.445	0.000	1
W76	H	1H	8.741	0.008	10
W76	N	15N	120.948	0.118	8
W76	H*	1H	9.717	0.005	8
W76	N*	15N	135.424	0.060	4
D77	C	13C	172.673	0.000	0
D77	CA	13C	51.980	0.027	2
D77	CB	13C	44.352	0.035	2
D77	CO-1	13C	172.673	0.000	1
D77	H	1H	8.417	0.009	8
D77	N	15N	118.330	0.069	7
G78	CA	13C	45.436	0.055	4
G78	CO-1	13C	175.849	0.000	1
G78	H	1H	8.613	0.009	8
G78	N	15N	108.546	0.065	7
F79	CA	13C	58.216	0.005	2
F79	CB	13C	40.566	0.006	2
F79	CO-1	13C	173.210	0.000	1
F79	H	1H	8.794	0.010	9
F79	N	15N	125.092	0.125	8
D80	CA	13C	51.674	0.006	2
D80	CB	13C	46.007	0.002	2
D80	CO-1	13C	174.925	0.000	1
D80	H	1H	8.658	0.007	15
D80	N	15N	124.460	0.162	10
Y81	CA	13C	57.669	0.007	2
Y81	CB	13C	38.380	0.072	2
Y81	CO-1	13C	174.736	0.000	1
Y81	H	1H	8.525	0.005	13
Y81	N	15N	119.555	0.096	10
D82	CA	13C	51.626	0.000	1
D82	CB	13C	42.136	0.000	1
D82	CO-1	13C	174.628	0.000	1
D82	H	1H	7.838	0.010	14
D82	N	15N	119.245	0.107	10
S93	CA	13C	58.961	0.000	1
S93	CA-1	13C	58.536	0.000	1
S93	CB	13C	63.680	0.000	1
S93	CB-1	13C	63.764	0.000	1
S93	CO-1	13C	175.397	0.000	1
S93	H	1H	8.292	0.005	8
S93	N	15N	119.036	0.071	7
D94	CA	13C	54.434	0.000	1
D94	CA-1	13C	58.978	0.000	1
D94	CB	13C	41.069	0.000	1
D94	CB-1	13C	63.583	0.000	1
D94	CO-1	13C	174.770	0.000	1

D94	H	1H	8.115	0.002	6
D94	N	15N	122.369	0.064	6
Y95	CA	13C	58.046	0.000	1
Y95	CA-1	13C	54.476	0.000	1
Y95	CB	13C	38.358	0.000	1
Y95	CB-1	13C	41.100	0.000	1
Y95	H	1H	7.815	0.007	5
Y95	N	15N	121.257	0.074	5
S106	CA	13C	58.689	0.000	0
S106	CB	13C	63.940	0.000	0
K107	CA	13C	55.401	0.013	2
K107	CA-1	13C	58.807	0.000	1
K107	CB	13C	35.108	0.003	2
K107	CB-1	13C	63.940	0.000	1
K107	CO-1	13C	174.299	0.000	1
K107	H	1H	8.256	0.006	14
K107	N	15N	122.766	0.076	10
T108	CA	13C	60.602	0.056	2
T108	CB	13C	71.094	0.021	2
T108	CO-1	13C	176.004	0.000	1
T108	H	1H	8.981	0.007	14
T108	N	15N	116.770	0.064	10
K109	CA	13C	58.066	0.000	1
K109	CB	13C	32.236	0.000	1
K109	CO-1	13C	172.946	0.000	1
K109	H	1H	8.131	0.011	8
K109	N	15N	126.530	0.133	7
C110	CA	13C	59.010	0.000	1
C110	CA-1	13C	58.152	0.000	1
C110	CB	13C	31.825	0.000	1
C110	CB-1	13C	32.158	0.000	1
C110	CO-1	13C	176.731	0.000	1
C110	H	1H	8.721	0.010	6
C110	N	15N	126.409	0.059	6
L111	C	13C	172.507	0.000	0
L111	CA	13C	53.306	0.014	2
L111	CA-1	13C	59.013	0.000	1
L111	CB	13C	44.849	0.022	2
L111	CB-1	13C	31.847	0.000	1
L111	CO-1	13C	172.507	0.000	1
L111	H	1H	8.859	0.006	10
L111	N	15N	124.322	0.069	8
F112	CA	13C	55.862	0.063	2
F112	CB	13C	38.201	0.130	2
F112	CO-1	13C	173.296	0.000	1
F112	H	1H	8.557	0.004	10
F112	N	15N	124.629	0.110	8
I113	C	13C	175.448	0.000	0
I113	CA	13C	60.778	0.041	2
I113	CB	13C	41.091	0.009	2
I113	CO-1	13C	175.448	0.000	1
I113	H	1H	8.632	0.007	8
I113	N	15N	121.388	0.086	7
Q114	C	13C	174.289	0.000	0
Q114	CA	13C	54.352	0.000	1
Q114	CB	13C	29.736	0.005	2
Q114	CO-1	13C	174.289	0.000	1
Q114	H	1H	8.533	0.009	12
Q114	N	15N	129.352	0.057	9
M115	C	13C	174.892	0.000	0
M115	CA	13C	54.567	0.092	2
M115	CB	13C	37.285	0.000	2
M115	CO-1	13C	174.892	0.000	1
M115	H	1H	9.755	0.007	9

M115	N	15N	128.009	0.101	7
E116	C	13C	177.707	0.000	0
E116	CA	13C	56.319	0.122	2
E116	CB	13C	31.332	0.014	2
E116	CO-1	13C	174.232	0.000	1
E116	H	1H	8.097	0.008	10
E116	N	15N	121.719	0.100	8
F117	CA	13C	55.907	0.000	1
F117	CB	13C	40.370	0.000	1
F117	CO-1	13C	174.516	0.000	1
F117	H	1H	8.124	0.005	8
F117	N	15N	123.227	0.141	7
C118	CA	13C	57.858	0.000	1
C118	CA-1	13C	55.864	0.000	1
C118	CB	13C	28.042	0.000	1
C118	CB-1	13C	40.437	0.000	1
C118	CO-1	13C	175.019	0.000	1
C118	H	1H	7.963	0.003	6
C118	N	15N	129.921	0.089	6
D119	CA	13C	53.868	0.000	1
D119	CA-1	13C	57.961	0.000	1
D119	CB	13C	41.184	0.000	1
D119	CB-1	13C	27.944	0.000	1
D119	CO-1	13C	174.057	0.000	1
D119	H	1H	7.942	0.007	9
D119	N	15N	124.500	0.146	8
K120	CA	13C	54.417	0.000	1
K120	CA-1	13C	54.130	0.000	1
K120	CB	13C	32.443	0.000	1
K120	CB-1	13C	41.161	0.000	1
K120	CO-1	13C	173.072	0.000	1
K120	H	1H	7.646	0.017	11
K120	N	15N	119.649	0.078	8
G121	CA	13C	44.851	0.121	4
G121	CA-1	13C	54.472	0.000	1
G121	CB-1	13C	32.424	0.000	1
G121	CO-1	13C	176.828	0.000	1
G121	H	1H	7.987	0.009	11
G121	N	15N	108.411	0.148	9
T122	C	13C	174.344	0.000	0
T122	CA	13C	59.783	0.077	2
T122	CB	13C	73.229	0.011	2
T122	CO-1	13C	174.344	0.000	1
T122	H	1H	8.007	0.014	14
T122	N	15N	108.364	0.154	10
L123	CA	13C	56.473	0.038	2
L123	CB	13C	41.147	0.006	2
L123	CO-1	13C	178.056	0.000	1
L123	H	1H	9.276	0.009	15
L123	N	15N	124.421	0.081	11
E124	C	13C	177.985	0.000	0
E124	CA	13C	58.996	0.060	2
E124	CB	13C	29.151	0.000	2
E124	CO-1	13C	177.985	0.000	1
E124	H	1H	6.907	0.005	17
E124	N	15N	120.726	0.092	11
Q125	C	13C	178.359	0.000	0
Q125	CA	13C	58.700	0.019	2
Q125	CB	13C	28.070	0.030	2
Q125	CO-1	13C	178.359	0.000	1
Q125	H	1H	7.513	0.008	17
Q125	N	15N	119.774	0.082	11
W126	C	13C	178.446	0.000	0
W126	CA	13C	62.263	0.000	1

W126	CB	13C	29.774	0.000	1
W126	CO-1	13C	178.446	0.000	1
W126	H	1H	7.790	0.007	15
W126	N	15N	123.513	0.133	11
I127	CA	13C	54.288	0.000	1
I127	CA-1	13C	62.242	0.000	1
I127	CB	13C	37.930	0.000	1
I127	CB-1	13C	29.711	0.000	1
I127	CO-1	13C	179.055	0.000	1
I127	H	1H	8.689	0.008	13
I127	N	15N	120.956	0.093	10
E128	CA	13C	59.322	0.000	1
E128	CA-1	13C	54.448	0.000	1
E128	CB	13C	29.131	0.000	1
E128	CB-1	13C	37.986	0.000	1
E128	CO-1	13C	179.504	0.000	1
E128	H	1H	7.802	0.008	6
E128	N	15N	120.730	0.044	6
K129	CA	13C	57.906	0.000	1
K129	CA-1	13C	59.325	0.000	1
K129	CB	13C	31.826	0.000	1
K129	CB-1	13C	29.073	0.000	1
K129	H	1H	7.722	0.009	12
K129	N	15N	119.382	0.091	9
R130	CA	13C	55.628	0.000	1
R130	CA-1	13C	57.927	0.000	1
R130	CB	13C	29.665	0.000	1
R130	CB-1	13C	31.865	0.000	1
R130	CO-1	13C	177.253	0.000	1
R130	H	1H	7.072	0.004	13
R130	N	15N	118.839	0.149	10
R131	CA	13C	59.075	0.000	1
R131	CA-1	13C	55.765	0.000	1
R131	CB	13C	29.322	0.000	1
R131	CB-1	13C	29.732	0.000	1
R131	CO-1	13C	175.766	0.000	1
R131	H	1H	6.903	0.006	14
R131	N	15N	118.403	0.117	10
G132	CA	13C	45.382	0.083	2
G132	CA-1	13C	58.960	0.000	1
G132	CB-1	13C	29.523	0.000	1
G132	CO-1	13C	177.847	0.000	1
G132	H	1H	7.984	0.007	10
G132	N	15N	111.380	0.070	8
E133	CA	13C	54.441	0.000	1
E133	CA-1	13C	45.454	0.006	2
E133	CB	13C	30.819	0.000	1
E133	CO-1	13C	174.640	0.000	1
E133	H	1H	7.984	0.011	8
E133	N	15N	121.013	0.070	7
K134	CA	13C	55.895	0.000	1
K134	CA-1	13C	54.484	0.000	1
K134	CB	13C	32.375	0.000	1
K134	CB-1	13C	30.775	0.000	1
K134	H	1H	8.134	0.003	5
K134	N	15N	120.487	0.048	5
L135	CA	13C	55.741	0.000	1
L135	CA-1	13C	55.882	0.000	1
L135	CB	13C	42.169	0.000	1
L135	CB-1	13C	32.314	0.000	1
L135	CO-1	13C	177.143	0.000	1
L135	H	1H	8.346	0.011	8
L135	N	15N	125.945	0.084	7
D136	CA	13C	52.585	0.000	1

D136	CA-1	13C	56.034	0.000	1
D136	CB	13C	40.641	0.000	1
D136	CB-1	13C	42.054	0.000	1
D136	CO-1	13C	176.466	0.000	1
D136	H	1H	7.923	0.009	6
D136	N	15N	126.443	0.077	6
K137	CA	13C	60.344	0.000	1
K137	CA-1	13C	52.606	0.000	1
K137	CB	13C	32.421	0.000	1
K137	CB-1	13C	41.067	0.000	1
K137	CO-1	13C	177.329	0.000	1
K137	H	1H	8.959	0.014	11
K137	N	15N	128.556	0.163	9
V138	CA	13C	66.421	0.000	1
V138	CA-1	13C	60.391	0.000	1
V138	CB	13C	31.316	0.000	1
V138	CB-1	13C	32.387	0.000	1
V138	H	1H	7.717	0.005	9
V138	N	15N	119.439	0.136	7
L139	CA	13C	57.286	0.000	1
L139	CA-1	13C	66.199	0.000	1
L139	CB	13C	41.689	0.000	1
L139	CB-1	13C	30.850	0.000	1
L139	CO-1	13C	179.736	0.000	1
L139	H	1H	7.492	0.012	13
L139	N	15N	122.007	0.122	10
A140	CA	13C	55.811	0.028	2
A140	CA-1	13C	57.176	0.000	1
A140	CB	13C	18.586	0.201	2
A140	CB-1	13C	41.668	0.000	1
A140	CO-1	13C	178.987	0.000	1
A140	H	1H	7.766	0.005	13
A140	N	15N	119.874	0.113	9
L141	CA	13C	57.404	0.000	1
L141	CB	13C	41.061	0.000	1
L141	CO-1	13C	180.042	0.000	1
L141	H	1H	8.285	0.006	13
L141	N	15N	115.848	0.113	10
E142	CA	13C	59.605	0.000	1
E142	CA-1	13C	57.534	0.000	1
E142	CB	13C	29.099	0.000	1
E142	CO-1	13C	180.527	0.000	1
E142	H	1H	8.110	0.004	10
E142	N	15N	125.346	0.075	8
L143	CA	13C	57.735	0.000	1
L143	CA-1	13C	59.485	0.000	1
L143	CB	13C	40.375	0.000	1
L143	CB-1	13C	29.099	0.000	1
L143	CO-1	13C	180.419	0.000	1
L143	H	1H	8.039	0.009	10
L143	N	15N	119.433	0.093	8
F144	CA	13C	62.126	0.000	1
F144	CA-1	13C	57.719	0.000	1
F144	CB	13C	39.018	0.000	1
F144	CB-1	13C	39.852	0.000	1
F144	CO-1	13C	179.752	0.000	1
F144	H	1H	8.428	0.006	12
F144	N	15N	118.617	0.135	9
E145	CA	13C	60.185	0.000	1
E145	CA-1	13C	61.977	0.000	1
E145	CB	13C	29.226	0.000	1
E145	CB-1	13C	39.055	0.000	1
E145	CO-1	13C	178.375	0.000	1
E145	H	1H	8.771	0.006	14



E145	N	15N	123.648	0.112	11
Q146	CA	13C	59.591	0.000	1
Q146	CA-1	13C	60.120	0.000	1
Q146	CB	13C	29.820	0.000	1
Q146	CB-1	13C	29.041	0.000	1
Q146	CO-1	13C	177.806	0.000	1
Q146	H	1H	7.246	0.010	12
Q146	N	15N	118.343	0.087	9
I147	CA	13C	65.056	0.000	1
I147	CA-1	13C	59.747	0.000	1
I147	CB	13C	38.387	0.000	1
I147	CO-1	13C	178.444	0.000	1
I147	H	1H	7.600	0.008	11
I147	N	15N	118.433	0.089	8
T148	CB	13C	67.266	0.000	0
K149	C	13C	176.807	0.000	0
K149	CA	13C	60.547	0.089	2
K149	CA-1	13C	68.063	0.000	1
K149	CB	13C	32.104	0.177	2
K149	CB-1	13C	67.266	0.000	1
K149	CO-1	13C	176.807	0.000	1
K149	H	1H	8.469	0.008	10
K149	N	15N	124.022	0.118	8
G150	C	13C	180.166	0.000	0
G150	CA	13C	46.931	0.160	4
G150	CO-1	13C	180.166	0.000	1
G150	H	1H	7.906	0.016	14
G150	N	15N	107.965	0.074	10
V151	CA	13C	66.469	0.023	2
V151	CB	13C	29.959	0.241	2
V151	CO-1	13C	175.033	0.000	1
V151	H	1H	8.061	0.006	13
V151	N	15N	123.019	0.108	10
D152	CA	13C	57.433	0.023	2
D152	CB	13C	43.370	0.005	2
D152	CO-1	13C	176.236	0.000	1
D152	H	1H	8.844	0.007	14
D152	N	15N	121.194	0.084	10
Y153	CA	13C	61.186	0.049	2
Y153	CB	13C	37.622	0.022	2
Y153	CO-1	13C	178.692	0.000	1
Y153	H	1H	7.499	0.008	15
Y153	N	15N	120.654	0.079	10
I154	CA	13C	66.648	0.163	2
I154	CB	13C	37.667	0.132	2
I154	CO-1	13C	179.041	0.000	1
I154	H	1H	7.952	0.008	12
I154	N	15N	122.262	0.159	9
H155	C	13C	178.916	0.000	0
H155	CA	13C	57.630	0.000	1
H155	CB	13C	30.853	0.000	1
H155	CO-1	13C	178.916	0.000	1
H155	H	1H	9.083	0.008	15
H155	N	15N	119.897	0.133	11
S156	C	13C	181.657	0.000	0
S156	CA	13C	61.600	0.144	2
S156	CO-1	13C	181.657	0.000	1
S156	H	1H	8.440	0.005	12
S156	N	15N	121.889	0.097	8
K157	C	13C	175.727	0.000	0
K157	CA	13C	53.852	0.026	2
K157	CB	13C	30.218	0.017	2
K157	CO-1	13C	175.727	0.000	1
K157	H	1H	7.165	0.008	14

K157	N	15N	122.591	0.095	9
K158	CA	13C	57.043	0.000	1
K158	CB	13C	27.762	0.214	2
K158	CO-1	13C	175.375	0.000	1
K158	H	1H	7.944	0.008	14
K158	N	15N	113.882	0.084	10
L159	C	13C	175.681	0.000	0
L159	CA	13C	53.129	0.000	1
L159	CA-1	13C	57.177	0.000	1
L159	CB	13C	44.975	0.000	1
L159	CO-1	13C	175.681	0.000	1
L159	H	1H	7.342	0.006	13
L159	N	15N	120.051	0.059	9
I160	CA	13C	60.333	0.000	0
I160	CB	13C	39.459	0.000	0
R162	CA	13C	60.200	0.000	1
R162	CA-1	13C	61.568	0.000	1
R162	CB	13C	30.221	0.000	1
R162	CO-1	13C	178.376	0.000	1
R162	H	1H	9.390	0.005	12
R162	N	15N	110.619	0.104	9
D163	CA	13C	52.785	0.000	1
D163	CA-1	13C	60.168	0.000	1
D163	CB	13C	42.161	0.000	1
D163	CO-1	13C	175.856	0.000	1
D163	H	1H	10.039	0.008	13
D163	N	15N	127.458	0.071	9
L164	CA	13C	55.978	0.000	1
L164	CA-1	13C	52.800	0.000	1
L164	CB	13C	41.060	0.000	1
L164	CB-1	13C	42.200	0.000	1
L164	CO-1	13C	175.450	0.000	1
L164	H	1H	8.898	0.008	11
L164	N	15N	125.119	0.103	9
K165	CA	13C	53.777	0.000	1
K165	CA-1	13C	56.090	0.000	1
K165	CB	13C	30.288	0.000	1
K165	CB-1	13C	41.100	0.000	1
K165	CO-1	13C	175.103	0.000	1
K165	H	1H	6.610	0.007	8
K165	N	15N	116.626	0.149	7
S167	CA	13C	60.168	0.000	1
S167	CA-1	13C	66.167	0.000	1
S167	CB	13C	62.331	0.000	1
S167	CB-1	13C	31.274	0.000	1
S167	CO-1	13C	177.411	0.000	1
S167	H	1H	8.409	0.022	12
S167	N	15N	112.209	0.089	9
N168	CA	13C	51.476	0.000	1
N168	CA-1	13C	60.195	0.000	1
N168	CB	13C	39.922	0.000	1
N168	CO-1	13C	176.634	0.000	1
N168	H	1H	7.636	0.008	11
N168	N	15N	119.596	0.053	8
I169	CA	13C	60.368	0.000	1
I169	CA-1	13C	51.600	0.000	1
I169	CB	13C	39.465	0.000	1
I169	CB-1	13C	39.818	0.000	1
I169	CO-1	13C	172.679	0.000	1
I169	H	1H	6.709	0.009	15
I169	N	15N	119.539	0.084	10
F170	CA	13C	57.431	0.039	2
F170	CA-1	13C	60.333	0.000	1
F170	CB	13C	41.108	0.062	2

F170	CB-1	13C	39.459	0.000	1
F170	CO-1	13C	173.949	0.000	1
F170	H	1H	9.133	0.006	9
F170	N	15N	127.001	0.060	8
L171	CA	13C	53.968	0.106	2
L171	CB	13C	41.719	0.007	2
L171	CO-1	13C	175.369	0.000	1
L171	H	1H	8.388	0.006	8
L171	N	15N	124.284	0.089	7
V172	CA	13C	61.849	0.075	2
V172	CB	13C	32.333	0.029	2
V172	CO-1	13C	176.708	0.000	1
V172	H	1H	8.185	0.001	8
V172	N	15N	119.279	0.160	7
D173	CA	13C	53.761	0.020	2
D173	CB	13C	41.657	0.023	2
D173	CO-1	13C	175.514	0.000	1
D173	H	1H	8.313	0.007	11
D173	N	15N	121.302	0.062	8
T174	CA	13C	65.168	0.010	2
T174	CB	13C	69.078	0.021	2
T174	CO-1	13C	176.006	0.000	1
T174	H	1H	8.499	0.004	13
T174	N	15N	113.593	0.100	10
K175	CA	13C	54.936	0.054	2
K175	CB	13C	32.940	0.039	2
K175	CO-1	13C	174.799	0.000	1
K175	H	1H	8.136	0.007	12
K175	N	15N	116.735	0.083	9
Q176	CA	13C	55.037	0.089	2
Q176	CB	13C	31.279	0.027	2
Q176	CO-1	13C	175.197	0.000	1
Q176	H	1H	7.289	0.007	14
Q176	N	15N	120.221	0.112	10
V177	C	13C	175.172	0.000	0
V177	CA	13C	59.201	0.030	2
V177	CB	13C	34.578	0.017	2
V177	CO-1	13C	175.172	0.000	1
V177	H	1H	7.888	0.004	9
V177	N	15N	119.934	0.050	8
K178	CA	13C	55.118	0.057	2
K178	CB	13C	37.028	0.184	2
K178	CO-1	13C	176.335	0.000	1
K178	H	1H	9.039	0.006	8
K178	N	15N	121.532	0.067	7
I179	CA	13C	63.295	0.022	2
I179	CB	13C	38.953	0.007	2
I179	CO-1	13C	175.484	0.000	1
I179	H	1H	8.992	0.004	8
I179	N	15N	125.715	0.088	7
G180	CA	13C	44.683	0.091	2
G180	CO-1	13C	175.592	0.000	1
G180	H	1H	8.433	0.011	8
G180	N	15N	115.336	0.054	7
D181	CA	13C	55.521	0.000	1
D181	CB	13C	41.577	0.000	1
D181	CO-1	13C	172.824	0.000	1
D181	H	1H	8.316	0.005	9
D181	N	15N	119.069	0.182	8
D181	h	1H	8.298	0.000	0
G181	CA-1	13C	44.866	0.000	1
G183	CA	13C	46.551	0.013	2
G183	CA-1	13C	58.471	0.000	1
G183	CB-1	13C	38.936	0.000	1

G183	CO-1	13C	177.349	0.000	1
G183	H	1H	8.149	0.008	11
G183	N	15N	108.947	0.081	9
T186	CA	13C	61.531	0.000	0
T186	CB	13C	69.954	0.000	0
S187	C	13C	175.004	0.000	0
S187	CA	13C	58.580	0.000	1
S187	CA-1	13C	61.531	0.000	1
S187	CB	13C	63.943	0.000	1
S187	CB-1	13C	69.954	0.000	1
S187	CO-1	13C	175.004	0.000	1
S187	H	1H	8.018	0.005	8
S187	N	15N	119.000	0.049	7
L188	CA	13C	55.403	0.000	1
L188	CA-1	13C	58.494	0.000	1
L188	CB	13C	41.727	0.000	1
L188	CB-1	13C	64.114	0.000	1
L188	CO-1	13C	174.718	0.000	1
L188	H	1H	8.048	0.015	8
L188	N	15N	124.840	0.115	7
K189	CA	13C	56.419	0.000	1
K189	CA-1	13C	55.517	0.000	1
K189	CB	13C	32.527	0.000	1
K189	CB-1	13C	41.744	0.000	1
K189	CO-1	13C	177.707	0.000	1
K189	H	1H	8.077	0.007	8
K189	N	15N	121.833	0.112	7
N190	CA	13C	53.256	0.000	1
N190	CA-1	13C	56.352	0.000	1
N190	CB	13C	38.880	0.000	1
N190	CB-1	13C	32.504	0.000	1
N190	CO-1	13C	176.732	0.000	1
N190	H	1H	8.349	0.006	6
N190	N	15N	120.767	0.088	6
D191	CA	13C	54.371	0.000	1
D191	CA-1	13C	53.413	0.000	1
D191	CB	13C	41.048	0.000	1
D191	CB-1	13C	38.935	0.000	1
D191	CO-1	13C	175.360	0.000	1
D191	H	1H	8.121	0.004	8
D191	N	15N	121.464	0.177	7
G192	CA	13C	45.864	0.064	2
G192	CA-1	13C	54.318	0.000	1
G192	CB-1	13C	41.170	0.000	1
G192	CO-1	13C	177.359	0.000	1
G192	H	1H	8.273	0.012	8
G192	N	15N	109.845	0.106	7
K193	CA	13C	56.515	0.000	1
K193	CA-1	13C	45.924	0.028	2
K193	CB	13C	32.432	0.000	1
K193	CO-1	13C	175.019	0.000	1
K193	H	1H	8.063	0.008	8
K193	N	15N	121.336	0.094	7
Q208	C	13C	177.515	0.000	0
Q208	CA	13C	57.224	0.099	2
Q208	CA-1	13C	58.679	0.000	1
Q208	CB	13C	29.770	0.087	2
Q208	CB-1	13C	26.955	0.000	1
Q208	CO-1	13C	177.515	0.000	1
Q208	H	1H	7.176	0.006	12
Q208	N	15N	120.635	0.088	9
I209	C	13C	178.286	0.000	0
I209	CA	13C	63.588	0.030	2
I209	CB	13C	37.825	0.024	2

I209	CO-1	13C	178.286	0.000	1
I209	H	1H	7.384	0.011	13
I209	N	15N	119.316	0.121	9
S210	CA	13C	59.028	0.035	2
S210	CB	13C	63.965	0.088	2
S210	CO-1	13C	178.055	0.000	1
S210	H	1H	7.600	0.006	14
S210	N	15N	113.289	0.118	10
S211	CA	13C	58.335	0.127	2
S211	CB	13C	63.780	0.173	2
S211	CO-1	13C	174.395	0.000	1
S211	H	1H	7.750	0.006	13
S211	N	15N	116.455	0.081	10
Q212	CA	13C	55.088	0.094	2
Q212	CB	13C	29.744	0.049	2
Q212	CO-1	13C	173.950	0.000	1
Q212	H	1H	8.248	0.010	10
Q212	N	15N	118.941	0.117	8
D213	C	13C	176.040	0.000	0
D213	CA	13C	54.127	0.004	2
D213	CB	13C	41.070	0.021	2
D213	CO-1	13C	176.040	0.000	1
D213	H	1H	8.160	0.009	9
D213	N	15N	121.281	0.038	8
Y214	CA	13C	56.114	0.032	2
Y214	CB	13C	39.011	0.004	2
Y214	CO-1	13C	174.858	0.000	1
Y214	H	1H	7.040	0.011	11
Y214	N	15N	118.351	0.106	8
G215	CA	13C	44.547	0.127	4
G215	CO-1	13C	174.785	0.000	1
G215	H	1H	8.746	0.010	15
G215	N	15N	110.780	0.096	10
K216	CA	13C	58.318	0.020	2
K216	CB	13C	29.639	0.070	2
K216	CO-1	13C	175.351	0.000	1
K216	H	1H	8.511	0.007	12
K216	N	15N	120.337	0.116	9
E217	CA	13C	59.587	0.023	2
E217	CB	13C	27.458	0.009	2
E217	CO-1	13C	176.988	0.000	1
E217	H	1H	9.630	0.009	14
E217	N	15N	120.676	0.106	10
V218	CA	13C	64.923	0.000	1
V218	CB	13C	29.865	0.000	1
V218	CO	13C	180.556	0.000	0
V218	CO-1	13C	180.556	0.000	1
V218	H	1H	8.199	0.004	16
V218	N	15N	119.772	0.074	12
D219	C	13C	178.583	0.000	0
D219	CA	13C	56.167	0.000	2
D219	CB	13C	41.012	0.016	2
D219	CO-1	13C	178.583	0.000	1
D219	H	1H	7.479	0.007	13
D219	N	15N	123.991	0.074	9
L220	CA	13C	57.243	0.059	2
L220	CB	13C	39.488	0.000	1
L220	CO-1	13C	178.168	0.000	1
L220	H	1H	6.954	0.006	15
L220	N	15N	116.961	0.115	10
Y221	CA	13C	60.773	0.043	2
Y221	CB	13C	39.514	0.050	2
Y221	CO-1	13C	177.442	0.000	1
Y221	H	1H	7.186	0.007	13

Y221	N	15N	119.531	0.062	9
A222	CA	13C	55.926	0.047	2
A222	CB	13C	18.320	0.000	2
A222	CO-1	13C	177.761	0.000	1
A222	H	1H	7.275	0.012	11
A222	N	15N	120.461	0.047	9
L223	CA	13C	58.037	0.015	2
L223	CB	13C	41.233	0.093	2
L223	CO-1	13C	180.790	0.000	1
L223	H	1H	8.018	0.008	11
L223	N	15N	116.281	0.069	9
G224	C	13C	179.441	0.000	0
G224	CA	13C	48.397	0.154	4
G224	CO-1	13C	179.441	0.000	1
G224	H	1H	7.785	0.007	15
G224	N	15N	106.776	0.127	12
L225	CA	13C	57.719	0.000	1
L225	CB	13C	41.697	0.000	1
L225	CO-1	13C	174.082	0.000	1
L225	H	1H	7.364	0.004	12
L225	N	15N	122.307	0.102	9
I226	CA	13C	65.530	0.000	1
I226	CA-1	13C	57.629	0.000	1
I226	CB	13C	38.373	0.000	1
I226	CB-1	13C	41.696	0.000	1
I226	CO-1	13C	179.060	0.000	1
I226	H	1H	8.399	0.010	11
I226	N	15N	118.854	0.086	8
L227	CA	13C	57.841	0.000	1
L227	CA-1	13C	65.524	0.000	1
L227	CB	13C	38.976	0.000	1
L227	CO-1	13C	177.938	0.000	1
L227	H	1H	8.462	0.006	9
L227	N	15N	121.079	0.136	7
A228	CA	13C	55.399	0.000	1
A228	CA-1	13C	57.729	0.000	1
A228	CB	13C	18.760	0.000	1
A228	CB-1	13C	38.757	0.000	1
A228	CO-1	13C	177.916	0.000	1
A228	H	1H	7.756	0.008	10
A228	N	15N	119.463	0.069	8
E229	CA	13C	59.094	0.000	1
E229	CA-1	13C	55.345	0.000	1
E229	CB	13C	30.252	0.000	1
E229	CB-1	13C	18.695	0.000	1
E229	CO-1	13C	179.240	0.000	1
E229	H	1H	8.086	0.006	11
E229	N	15N	116.993	0.100	8
L230	CA	13C	57.567	0.000	1
L230	CA-1	13C	59.311	0.000	1
L230	CB	13C	41.674	0.000	1
L230	CB-1	13C	30.319	0.000	1
L230	CO-1	13C	179.763	0.000	1
L230	H	1H	8.624	0.012	14
L230	N	15N	118.505	0.057	10
L231	CA	13C	55.120	0.000	1
L231	CA-1	13C	57.564	0.000	1
L231	CB	13C	42.714	0.000	1
L231	CB-1	13C	41.194	0.000	1
L231	CO-1	13C	178.964	0.000	1
L231	H	1H	7.896	0.005	13
L231	N	15N	116.241	0.118	10
H232	CA	13C	55.505	0.000	1
H232	CA-1	13C	55.233	0.000	1

H232	CB	13C	30.388	0.000	1
H232	CB-1	13C	42.370	0.000	1
H232	CO-1	13C	176.372	0.000	1
H232	H	1H	7.532	0.011	12
H232	N	15N	118.867	0.104	9
V233	CB	13C	31.578	0.000	1
V233	CB-1	13C	30.315	0.000	1
V233	CO-1	13C	172.275	0.000	1
V233	H	1H	7.855	0.012	4
V233	N	15N	126.507	0.028	4
C234	CA	13C	57.986	0.000	1
C234	CA-1	13C	62.815	0.000	1
C234	CB	13C	29.159	0.000	1
C234	CO-1	13C	176.028	0.000	1
C234	H	1H	8.007	0.006	7
C234	N	15N	125.660	0.106	6
K242	C	13C	177.457	0.000	0
K242	CA	13C	59.060	0.000	1
K242	CA-1	13C	62.094	0.000	1
K242	CB	13C	31.823	0.000	1
K242	CO-1	13C	177.457	0.000	1
K242	H	1H	7.627	0.005	13
K242	N	15N	124.550	0.113	9
F243	CA	13C	59.696	0.000	1
F243	CA-1	13C	58.859	0.000	1
F243	CB	13C	39.541	0.076	2
F243	CB-1	13C	31.983	0.000	1
F243	CO-1	13C	176.563	0.000	1
F243	H	1H	8.162	0.015	10
F243	N	15N	121.639	0.150	8
F244	C	13C	177.710	0.000	0
F244	CA	13C	62.427	0.186	2
F244	CB	13C	38.924	0.028	2
F244	CO-1	13C	177.710	0.000	1
F244	H	1H	8.338	0.009	14
F244	N	15N	117.478	0.190	10
T245	C	13C	178.656	0.000	0
T245	CA	13C	66.665	0.000	1
T245	CB	13C	68.484	0.000	1
T245	CO-1	13C	178.656	0.000	1
T245	H	1H	7.982	0.007	10
T245	N	15N	118.003	0.064	8
D246	CA	13C	57.932	0.000	1
D246	CA-1	13C	67.136	0.000	1
D246	CB	13C	38.430	0.000	1
D246	CB-1	13C	68.646	0.000	1
D246	CO-1	13C	176.723	0.000	1
D246	H	1H	7.879	0.017	9
D246	N	15N	122.846	0.272	8
R248	CA	13C	58.626	0.000	1
R248	CA-1	13C	58.009	0.000	1
R248	CB	13C	29.560	0.000	1
R248	CO-1	13C	181.479	0.000	1
R248	H	1H	7.997	0.005	10
R248	N	15N	118.547	0.132	8
D249	CA	13C	54.323	0.000	1
D249	CA-1	13C	58.776	0.000	1
D249	CB	13C	41.666	0.000	1
D249	CB-1	13C	29.581	0.000	1
D249	CO-1	13C	178.068	0.000	1
D249	H	1H	7.571	0.004	13
D249	N	15N	120.049	0.090	10
G250	CA	13C	45.692	0.086	2
G250	CA-1	13C	54.245	0.000	1

G250	CB-1	13C	41.535	0.000	1
G250	CO-1	13C	176.961	0.000	1
G250	H	1H	7.833	0.007	12
G250	N	15N	109.440	0.072	8
I251	CA	13C	60.774	0.000	1
I251	CA-1	13C	45.922	0.065	2
I251	CB	13C	36.971	0.000	1
I251	CO-1	13C	174.202	0.000	1
I251	H	1H	8.198	0.006	12
I251	N	15N	124.669	0.097	9
I252	CA	13C	59.535	0.000	1
I252	CA-1	13C	60.779	0.000	1
I252	CB	13C	37.028	0.000	1
I252	CB-1	13C	36.866	0.000	1
I252	CO-1	13C	174.279	0.000	1
I252	H	1H	8.091	0.012	11
I252	N	15N	128.693	0.103	9
S253	CA	13C	58.536	0.000	1
S253	CA-1	13C	59.379	0.000	1
S253	CB	13C	63.979	0.000	1
S253	CB-1	13C	36.817	0.000	1
S253	CO-1	13C	176.096	0.000	1
S253	H	1H	8.464	0.022	10
S253	N	15N	122.978	0.062	8
D254	CA	13C	55.740	0.000	1
D254	CA-1	13C	58.637	0.000	1
D254	CB	13C	39.978	0.000	1
D254	CB-1	13C	63.974	0.000	1
D254	H	1H	8.132	0.006	10
D254	N	15N	120.468	0.074	7
I255	CA	13C	62.610	0.000	1
I255	CA-1	13C	55.778	0.000	1
I255	CB	13C	37.171	0.000	1
I255	CB-1	13C	39.996	0.000	1
I255	CO-1	13C	176.558	0.000	1
I255	H	1H	7.291	0.011	12
I255	N	15N	116.515	0.137	9
F256	CA	13C	57.291	0.000	1
F256	CA-1	13C	62.672	0.000	1
F256	CB	13C	39.526	0.000	1
F256	CB-1	13C	37.070	0.000	1
F256	CO-1	13C	176.728	0.000	1
F256	H	1H	7.203	0.005	12
F256	N	15N	121.089	0.116	10
D257	CA	13C	53.252	0.000	1
D257	CA-1	13C	57.429	0.000	1
D257	CB	13C	41.183	0.000	1
D257	CB-1	13C	39.496	0.000	1
D257	CO-1	13C	175.630	0.000	1
D257	H	1H	8.429	0.003	8
D257	N	15N	123.071	0.132	7
K258	CA	13C	60.690	0.000	1
K258	CA-1	13C	53.196	0.000	1
K258	CB	13C	31.836	0.000	1
K258	CB-1	13C	41.106	0.000	1
K258	CO-1	13C	176.883	0.000	1
K258	H	1H	8.271	0.009	6
K258	N	15N	121.340	0.036	6
K259	CA	13C	59.237	0.000	0
K259	CB	13C	30.247	0.000	0
K259	H	1H	8.185	0.000	0
K259	N	15N	121.225	0.000	0
E260	CA	13C	58.903	0.052	2
E260	CA-1	13C	59.237	0.000	1



E260	CB	13C	28.566	0.000	2
E260	CB-1	13C	30.247	0.000	1
E260	CO-1	13C	179.546	0.000	1
E260	H	1H	7.708	0.020	11
E260	N	15N	122.917	0.226	9
K261	CA	13C	60.266	0.043	2
K261	CB	13C	32.345	0.005	2
K261	CO-1	13C	178.533	0.000	1
K261	H	1H	8.716	0.014	13
K261	N	15N	119.418	0.095	10
T262	CA	13C	66.468	0.116	2
T262	CB	13C	68.929	0.038	2
T262	CO-1	13C	178.328	0.000	1
T262	H	1H	7.861	0.008	14
T262	N	15N	113.894	0.105	10
L263	C	13C	176.335	0.000	0
L263	CA	13C	57.900	0.030	2
L263	CB	13C	41.379	0.000	1
L263	CO-1	13C	176.335	0.000	1
L263	H	1H	6.973	0.005	13
L263	N	15N	121.143	0.099	10
L264	CA	13C	58.549	0.084	2
L264	CB	13C	42.194	0.000	1
L264	CB-1	13C	41.439	0.000	1
L264	CO-1	13C	178.936	0.000	1
L264	H	1H	8.391	0.010	14
L264	N	15N	119.567	0.139	10
Q265	CA	13C	58.708	0.002	2
Q265	CB	13C	28.537	0.016	2
Q265	CB-1	13C	42.138	0.000	1
Q265	CO-1	13C	178.253	0.000	1
Q265	H	1H	8.456	0.006	14
Q265	N	15N	115.810	0.091	10
K266	CA	13C	58.413	0.075	2
K266	CB	13C	32.360	0.031	2
K266	CO-1	13C	178.726	0.000	1
K266	H	1H	6.954	0.005	12
K266	N	15N	116.424	0.122	9
L267	CA	13C	58.611	0.015	2
L267	CB	13C	42.270	0.077	2
L267	CO-1	13C	179.450	0.000	1
L267	H	1H	8.144	0.007	16
L267	N	15N	119.801	0.054	11
L268	CA	13C	52.927	0.124	2
L268	CB	13C	38.980	0.035	2
L268	CO-1	13C	176.046	0.000	1
L268	H	1H	7.450	0.007	13
L268	N	15N	110.532	0.088	10
S269	C	13C	177.571	0.000	0
S269	CA	13C	58.773	0.000	1
S269	CB	13C	64.007	0.000	1
S269	CO-1	13C	177.571	0.000	1
S269	H	1H	7.009	0.005	12
S269	N	15N	115.222	0.114	9
K270	C	13C	176.779	0.000	0
K270	CA	13C	58.530	0.000	1
K270	CA-1	13C	58.848	0.000	1
K270	CB	13C	31.928	0.000	1
K270	CB-1	13C	63.986	0.000	1
K270	CO-1	13C	176.779	0.000	1
K270	H	1H	8.816	0.008	10
K270	N	15N	126.746	0.122	8
K271	C	13C	176.894	0.000	0
K271	CA	13C	53.294	0.000	1

K271	CA-1	13C	58.598	0.000	1
K271	CB	13C	31.123	0.000	1
K271	CB-1	13C	31.951	0.000	1
K271	CO-1	13C	176.894	0.000	1
K271	H	1H	8.349	0.006	12
K271	N	15N	122.310	0.104	9
E273	CA	13C	58.380	0.000	1
E273	CA-1	13C	65.400	0.000	1
E273	CB	13C	27.876	0.000	1
E273	CB-1	13C	31.836	0.000	1
E273	CO-1	13C	178.855	0.000	1
E273	H	1H	9.519	0.010	12
E273	N	15N	115.911	0.043	9
D274	CA	13C	54.966	0.000	1
D274	CA-1	13C	58.498	0.000	1
D274	CB	13C	41.619	0.000	1
D274	CB-1	13C	28.000	0.000	1
D274	CO-1	13C	177.283	0.000	1
D274	H	1H	7.592	0.006	12
D274	N	15N	120.545	0.108	9
R275	CA	13C	54.136	0.000	1
R275	CA-1	13C	55.004	0.000	1
R275	CB	13C	30.048	0.000	1
R275	CB-1	13C	41.671	0.000	1
R275	CO-1	13C	177.208	0.000	1
R275	H	1H	7.280	0.007	12
R275	N	15N	120.552	0.087	9
N277	CA	13C	51.900	0.000	1
N277	CA-1	13C	62.293	0.000	1
N277	CB	13C	38.354	0.000	1
N277	CB-1	13C	31.389	0.000	1
N277	CO-1	13C	174.216	0.000	1
N277	H	1H	7.914	0.006	9
N277	N	15N	115.044	0.066	8
T278	CA-1	13C	51.752	0.000	1
T278	CB-1	13C	38.285	0.000	1
T278	CO-1	13C	176.646	0.000	1
T278	H	1H	8.223	0.010	10
T278	N	15N	108.844	0.111	7
S279	CA	13C	62.010	0.093	2
S279	CO-1	13C	177.382	0.000	1
S279	H	1H	7.931	0.005	11
S279	N	15N	117.887	0.075	8
E280	CA	13C	58.503	0.000	1
E280	CA-1	13C	61.977	0.000	1
E280	CB	13C	28.605	0.008	2
E280	CB-1	13C	62.001	0.000	1
E280	CO-1	13C	177.678	0.000	1
E280	H	1H	7.699	0.008	14
E280	N	15N	124.333	0.076	10
I281	CA	13C	66.247	0.000	1
I281	CA-1	13C	58.586	0.000	1
I281	CB	13C	38.097	0.000	1
I281	CO-1	13C	180.348	0.000	1
I281	H	1H	8.474	0.009	11
I281	N	15N	123.499	0.156	8
L285	CA	13C	57.658	0.000	1
L285	CA-1	13C	67.050	0.000	1
L285	CB	13C	40.580	0.000	1
L285	CB-1	13C	68.427	0.000	1
L285	CO-1	13C	174.851	0.000	1
L285	H	1H	8.086	0.010	9
L285	N	15N	119.457	0.088	7
T286	CA	13C	67.112	0.000	2

T286	CA-1	13C	57.418	0.000	1
T286	CB	13C	68.643	0.145	2
T286	CB-1	13C	40.612	0.000	1
T286	CO-1	13C	180.477	0.000	1
T286	H	1H	7.594	0.003	13
T286	N	15N	115.687	0.166	10
V287	CA	13C	66.288	0.000	1
V287	CB	13C	30.811	0.000	1
V287	CO-1	13C	176.878	0.000	1
V287	H	1H	7.582	0.006	13
V287	N	15N	124.267	0.138	11
W288	CA	13C	57.870	0.000	1
W288	CA-1	13C	66.462	0.000	1
W288	CB	13C	29.067	0.000	1
W288	CB-1	13C	30.937	0.000	1
W288	CO-1	13C	180.054	0.000	1
W288	H	1H	8.384	0.008	13
W288	N	15N	121.159	0.117	8
K289	C	13C	175.103	0.000	0
K289	CA	13C	57.964	0.000	1
K289	CA-1	13C	57.829	0.000	1
K289	CB	13C	32.798	0.000	1
K289	CB-1	13C	29.089	0.000	1
K289	CO-1	13C	178.819	0.000	1
K289	H	1H	7.557	0.009	10
K289	N	15N	118.227	0.052	8
K290	CA	13C	56.567	0.000	1
K290	CA-1	13C	57.927	0.000	1
K290	CB	13C	32.453	0.000	1
K290	CB-1	13C	32.623	0.000	1
K290	CO-1	13C	177.710	0.000	1
K290	H	1H	7.630	0.008	11
K290	N	15N	120.010	0.123	9
S291	CA-1	13C	56.587	0.000	1
S291	CB	13C	63.216	0.000	1
S291	CB-1	13C	32.381	0.000	1
S291	CO-1	13C	177.008	0.000	1
S291	H	1H	8.029	0.009	7
S291	N	15N	118.691	0.141	6
E296	CA	13C	56.575	0.000	1
E296	CA-1	13C	53.211	0.000	1
E296	CB	13C	30.135	0.000	1
E296	CB-1	13C	38.957	0.000	1
E296	CO-1	13C	175.484	0.000	1
E296	H	1H	8.277	0.006	6
E296	N	15N	122.489	0.081	6
R297	CA	13C	56.290	0.000	1
R297	CA-1	13C	56.735	0.000	1
R297	CO-1	13C	177.111	0.000	1
R297	H	1H	8.216	0.003	4
R297	N	15N	122.988	0.070	4
H298	CA	13C	55.938	0.000	1
H298	CA-1	13C	56.481	0.000	1
H298	CB	13C	30.237	0.000	1
H298	CB-1	13C	29.879	0.000	1
H298	CO-1	13C	176.644	0.000	1
H298	H	1H	8.209	0.002	6
H298	N	15N	122.410	0.054	6