

Supporting Information for Skrynnikov et al., "The Relative Orientation of Peptide Planes in Proteins is Reflected in Carbonyl-Carbonyl Chemical Shift Anisotropy Cross-Correlated Spin Relaxation"

Figure 1. Percent occurrence vs. signal-to-noise (S/N) for zero-quantum (ZQ) and double-quantum (DQ) correlations measured at 600 MHz on a sample of the spectrin SH3 domain.

Table S1. $R_{DQ} - R_{ZQ}$ rates for sequential ^{13}CO spins measured at 500 and 600 MHz

Correlation	$R_{DQ} - R_{ZQ}$ (500 MHz)		$R_{DQ} - R_{ZQ}$ (600 MHz)	
	Rate (s ⁻¹) (a)	error (s ⁻¹) (b)	Rate (s ⁻¹) (a)	error (s ⁻¹) (b)
D2M1	-1.920	- (c)	-2.839	0.150
E3D2	-3.783	0.358	-5.399	0.221
T4E3	-3.689	0.161	-5.229	0.507
G5T4	-4.592	0.153	-7.588	0.708
K6G5	-5.055	0.166	-6.705	0.173
E7K6	-8.187	0.314	-12.680	0.144
L8E7	-2.519	0.298	-3.876	0.636
V9L8	0.514	0.124	0.578	0.765
L10V9	-10.069	0.078	-15.636	1.524
A11L10	-15.688	0.739	-23.966	1.404
L12A11	-17.220	0.085	-24.927	0.186
Y13L12	9.230	0.665	14.210	0.292
D14Y13	-12.610	0.148	-16.417	0.102

2

Y15D14	-5.509	0.450	-7.367	0.327
Q16Y15	-12.766	0.316	-19.187	0.313
E17Q16	-9.809	0.586	-13.972	0.544
K18E17	-7.861	-	-11.072	-
S19K18	9.794	0.509	13.117	0.871
R21P20	-12.237	-	-18.344	-
E22R21	-3.248	0.051	-4.107	0.459
V23E22	-0.940	0.855	-1.266	0.467
T24V23	-13.326	0.709	-20.812	0.339
M25T24	4.168	-	6.200	0.009
K26M25	-6.860	0.091	-9.621	0.218
G28K27	-12.192	0.104	-16.945	0.155
D29G28	-8.768	-	-10.444	-
I30D29	-16.382	0.424	-24.547	0.522
L31I30	1.206	0.008	2.416	-
T32L31	-15.482	0.840	-22.862	0.728
L33T32	-12.620	0.816	-19.263	0.047
L34L33	-11.777	0.305	-18.626	-
N35L34	-0.292	0.365	0.476	-
T37S36	-17.395	0.058	-25.974	0.151
N38T37	-10.441	0.155	-16.348	0.307
K39N38	-15.577	0.286	-23.040	0.224
D40K39	-12.255	-	-17.641	-
W41D40	-4.944	0.067	-8.232	1.295
K43W42	-16.210	0.128	-23.764	1.065
V44K43	7.481	0.289	11.807	0.067
E45V44	-7.258	-	-10.558	0.548

V46E45	-5.363	-	-7.191	-
N47V46	-14.938	0.395	-21.434	0.144
D48N47	-11.370	-	-15.779	-
Q50R49	-3.680	0.432	-5.467	0.322
G51Q50	18.002	-	27.006	1.340
F52G51	-3.972	-	-6.665	1.215
V53F52	5.236	-	7.069	0.578
A55P54	-17.895	0.458	-24.855	0.901
A56A55	-12.841	-	-18.714	-
V58Y57	3.027	-	6.278	0.537
K59V58	-6.425	0.197	-9.969	1.014
K60K59	-12.391	-	-17.487	0.982
L61K60	-12.412	-	-17.957	0.782
D62L61	2.067	0.062	3.069	0.695

(a) Average of two measurements.

(b) Absolute differences between the two measurements.

(c) Only a single value could be measured at 500 or 600 MHz; therefore errors are not reported. Note that axial peaks were suppressed using the scheme described in the Appendix for only one data set recorded at 500 and one data set at 600 MHz. Therefore errors are not listed for residues that fall within approximately ± 0.4 ppm of the ^{13}CO carrier.