Homonuclear decoupling for enhancing resolution and sensitivity in NOE and RDC measurements of peptides and proteins

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Supplementary Material

Table S1. Isotropic $^{1}J_{C\alpha H\alpha}$ couplings in ubiquitin, and $^{1}D_{C\alpha H\alpha}$ RDCs measured at 600 MHz ^{1}H frequency, from a $^{1}H^{\alpha}$-coupled HN(CO)CA experiment, recorded with band-selective $^{13}C^{\beta}$ decoupling during $^{13}C^{\alpha}$ evolution (causing Gly values to be missing).

Residue	$^{1}DH\alpha C\alpha$ (with BASH) (Hz)	Downfield component (with BASH) S/N	Upfield component (with BASH) S/N	$^{1}DH\alpha C\alpha$ (no BASH) (Hz)	Downfield component (no BASH) S/N	Upfield component (no BASH) S/N	$^{1}JH\alpha C\alpha$ (isotropic) (Hz)
M1	-55.1	73	63	-55.0	46	38	147.5
Q2	19.3	33	24	26.3	10	9	145.8
I3	17.5	40	22	18.7	23	27	142.3
F4	48.3	42	31	43.8	33	27	145.3
K6	-38.6	37	30	-36.5	43	34	143.4
T9	67.7	18	10	75.7	10	7	142.0
K11	-69.4	19	11	-70.8	54	38	144.0
I13	-43.8	68	52	-42.1	79	57	141.9
T14	33.1	13	12	38.8	6	3	144.2
L15	37.2	73	55	36.7	52	43	141.8
E16	26.0	31	19	22.0	16	6	144.2
V17	32.5	49	15	25.7	22	12	141.7
T22	8.2	15	11	9.9	4	3	140.7
E24	15.8	24	20	14.3	27	28	147.7
N25	40.9	35	30	34.0	18	12	150.1
K27	-1.2	18	19	-0.3	11	5	151.6
A28	-20.4	27	22	-23.7	27	26	148.6
K29	87.5	33	26	83.3	12	9	147.0
I30	-78.8	16	12	-68.7	9	9	146.2
Q31	30.8	36	32	26.5	26	25	149.5
D32	16.8	31	26	15.7	37	35	151.2
K33	30.9	28	22	27.9	11	8	147.4
E34	-93.6	56	45	-87.2	35	29	143.8
P38	-31.5	28	27	-27.0	28	21	149.1
D39	-45.8	22	20	-44.4	11	10	145.9
Q40	14.1	44	35	15.7	42	36	142.2
Q41	-29.6	45	35	-30.5	18	11	143.0
R42	-43.5	25	17	-41.7	28	20	141.7
F45	2.8	42	33	2.1	25	22	143.7
A46	-20.4	17	14	-23.0	34	26	135.5
K48	18.3	42	29	18.9	69	54	142.1
Q49	-69.0	17	13	-56.9	7	3	143.4
L50	-28.4	32	25	-27.5	18	15	142.0
E51	-15.3	37	27	-21.9	13	11	141.9
R54	-44.0	29	24	-30.0	10	10	141.4
Y59	20.0	39	29	18.2	30	23	142.1
I61	61.0	20	16	57.0	6	9	142.2
E62	48.2	59	45	49.0	32	27	140.2
S65	69.6	27	21	71.0	42	34	145.8
T66	54.2	26	19	73.5	12	8	144.1
L67	17.2	28	17	17.0	13	11	142.4
H68	-87.0	24	13	-72.5	13	7	143.3
L69	-82.2	32	24	-74.9	14	10	143.5
V70	-67.8	86	68	-69.9	65	53	139.6
L71	44.6	25	19	52.2	14	11	144.1

R72	57.4	67	53	56.8	118	101	142.7
L73	34.3	19	18	35,9	106	96	142.6