Supplementary information for:

Optimized ‘Detectors’ for dynamics analysis in solid-state NMR

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I. Glossary of terms

Name	Symbol	Units	Description
Distribution of motion	$(1-S^2)\theta(z)$	unitless	Describes how motion is distributed as a function of correlation time, where $z = \log_{10}(\tau_c/1\text{ s})$. $(1-S^2)$ gives the total amplitude of motion, so that $\theta(z)$ always integrates to one.
Relaxation rate constant	$R_\zeta^{(\theta,S)}$	s^{-1}	The relaxation-rate constant obtained under experimental conditions denoted by ζ, for a distribution of motion $(1-S^2)\theta(z)$. May be obtained by integrating the product of the sensitivity of that rate constant, $R_\zeta(z)$, times the distribution of motion, $(1-S^2)\theta(z)$.
Sensitivity	$R_\zeta(z)$	s^{-1}	The relaxation rate constant obtained under experimental conditions denoted by ζ, for a mono-exponential correlation function, having correlation time $\tau_c = 10^z$ s, and amplitude $1-S^2 = 1$.
Detector	–	–	A mathematical tool used to quantify the amount of motion for a range of correlation times.
Detector sensitivity	$\rho_n(z)$	unitless	Defines how a detector responds to a particular correlation time, $\tau_c = 10^z$ s. Its value as a function of z is obtained by taking a linear combination of rate constant sensitivities (using the same linear combination as is used to obtain the detector responses).
Detector response	$\rho_n^{(\theta,S)}$	unitless	A quantity, describing the amount of motion for a particular range of correlation times, rigorously defined as the integral of the product of the detector sensitivity, $\rho_n(z)$, and the distribution of motion, $(1-S^2)\theta(z)$. Obtained by taking an appropriate linear combination of experimental rate constants (strictly speaking, by fitting a vector of the rate constants to the detection vectors, $\vec{r}_n$).
Normalized rate constant	$\Re_\zeta^{(\theta,S)}$	unitless	The relaxation rate constant divided by some normalization constant, c_ζ, to yield a dimensionless relaxation rate constant. Here, $c_\zeta = \max(R_\zeta(z))$.
Allowed region	–	–	For a given set of experiments, the allowed region is all sets of rate constants ($R_\zeta^{(\theta,S)}$) that can be obtained for any arbitrary distribution of motion, given by $(1-S^2)\theta(z)$.
Detection vector	$\vec{r}_n$	s^{-1}	A vector containing carefully chosen values of the $R_\zeta^{(\theta,S)}$, so that a vector containing the full set of experimentally determined relaxation rate constants is assumed to be a linear combination of all detection vectors, given by $\rho_1^{(\theta,S)}\vec{r}_1 + \rho_2^{(\theta,S)}\vec{r}_2 + \ldots$.

Sum of normalized rate constants	$\Sigma_\zeta \Re_\zeta^{(\theta,S)}$	unitless	Sum of all normalized rate constants for an experimental data set, used for calculating the ratio of rates.
Ratio of rates	κ_ζ	unitless	For experimental conditions denoted by ζ, this is the ratio of the normalized rate constants, $\Re_\zeta^{(\theta,S)}$, divided by the sum of normalized rate constants, $\Sigma\Re^{(\theta,S)}$, which is used for defining positions in the reduced space.
Reduced space	–	–	For a set of experiments, the reduced space is defined by the ratios of rates, κ_ζ, for that set of experiments. The dimensionality of this space is one less than the number of experiments- achieved by omitting one of the experiments when calculating the κ_ζ.
Reduced vector	$\vec{\kappa}$	unitless	Vector of ratios of rates, κ_ζ, defining a position in the reduced space. These positions can be used to define detection vectors, although note that the reduced vector only defines the direction of the detection vector, but not the length.
Effective width	Δz_n	unitless (vs. 1 s)	The effective width of a detector is defined as the detector integral divided by its maximum, given on a base-10 log scale. $\Delta z = \int \rho_n(z)dz \Big/ \max(\rho_n(z))$
Detector center	z_n^0	unitless (vs. 1 s)	This gives the center of the detector sensitivity, on a logarithmic scale (unitless, with reference to 1 s using a base-10 log). Defined as follows: $z_n^0 = \int z\rho_n(z)dz \Big/ \int \rho_n(z)dz$

II. Detector analysis results for Ubiquitin

Table I: Detector analysis results for Ubiquitin. $\rho_n^{(\theta,S)}$ gives the best fit value, and the + and – columns 95% confidence interval as deviations from the best fit value (see text Fig. 12). Original experimental data is found in references [1,2].

Residue	$\rho_0^{(\theta,S)}$	+	–	$\rho_1^{(\theta,S)}$	+	–	$\rho_2^{(\theta,S)}$	+	–
2	0.1209	0.0242	0.0231	0.0220	0.0106	0.0142	0.0228	0.0150	0.0120
3	0.1269	0.0199	0.0192	0.0073	0.0032	0.0034	0.0054	0.0032	0.0038
4	0.9836	0.0164	1.5421	0.0002	0.0032	0.0002	0.0137	0.0014	0.0057
6	0.9960	0.0039	1.5546	0.0000	1.0000	0.0000	0.0000	1.0000	0.0000
7	0.1189	0.0220	0.6774	0.0000	0.0172	0.0000	0.0451	0.0056	0.0259
9	0.9635	0.0364	1.5221	0.0000	1.0000	0.0000	0.0000	1.0000	0.0000
10	0.1102	0.0529	0.0495	0.0847	0.0092	0.0355	0.0000	0.0293	0.0000
11	0.0764	0.0677	0.1086	0.2952	0.0471	0.2155	0.0000	0.2544	0.0000
12	0.1111	0.0302	0.0323	0.0075	0.0434	0.0075	0.0417	0.0144	0.0417
13	0.9946	0.0053	1.5532	0.0000	1.0000	0.0000	0.0000	1.0000	0.0000
14	0.9959	0.0041	1.5544	0.0000	1.0000	0.0000	0.0000	1.0000	0.0000
15	0.1127	0.0155	0.0192	0.0149	0.0033	0.0031	0.0077	0.0027	0.0030
16	0.1621	0.0222	0.0244	0.0324	0.0047	0.0065	0.0041	0.0060	0.0041
17	0.9698	0.0302	1.5283	0.0169	0.0056	0.0071	0.0088	0.0083	0.0079
18	0.9964	0.0035	1.5550	0.0000	1.0000	0.0000	0.0000	1.0000	0.0000
20	0.1406	0.0407	0.0374	0.0271	0.0019	0.0083	0.0010	0.0067	0.0010
21	0.1203	0.0192	0.0247	0.0086	0.0030	0.0029	0.0059	0.0035	0.0035
22	0.1378	0.0454	0.0444	0.0081	0.0026	0.0050	0.0016	0.0048	0.0016
23	0.1104	0.0227	0.0223	0.0108	0.0052	0.0098	0.0037	0.0074	0.0037
24	0.9767	0.0233	1.5352	0.0000	1.0000	0.0000	0.0000	1.0000	0.0000
25	0.9878	0.0122	1.5463	0.0000	1.0000	0.0000	0.0000	1.0000	0.0000
26	0.1052	0.0323	0.0319	0.0015	0.0033	0.0015	0.0121	0.0022	0.0036
27	0.1025	0.0473	0.0560	0.0010	0.0069	0.0010	0.0123	0.0037	0.0085
29	0.9747	0.0253	1.5332	0.0000	0.0120	0.0000	0.0231	0.0034	0.0231
30	0.1146	0.0417	0.0335	0.0000	0.0039	0.0000	0.0175	0.0018	0.0064
31	0.1105	0.0938	0.0931	0.0000	0.0046	0.0000	0.0107	0.0012	0.0045
32	0.1090	0.0389	0.0402	0.0000	0.0022	0.0000	0.0099	0.0013	0.0040
33	0.1246	0.0422	0.0492	0.0166	0.0048	0.0060	0.0041	0.0053	0.0041
34	0.0969	0.0441	0.0442	0.0059	0.0037	0.0041	0.0185	0.0051	0.0059
35	0.0720	0.0389	0.0416	0.0000	0.0057	0.0000	0.0252	0.0022	0.0109
36	0.2406	0.0275	0.0327	0.0262	0.0036	0.0040	0.0058	0.0046	0.0047
39	0.1281	0.0275	0.0327	0.0131	0.0191	0.0131	0.0310	0.0184	0.0249
40	0.1227	0.0405	0.0461	0.0185	0.0059	0.0051	0.0122	0.0064	0.0074
41	0.1455	0.0362	0.0401	0.0201	0.0063	0.0064	0.0059	0.0063	0.0059
42	0.1119	0.0281	0.0323	0.0000	0.0072	0.0000	0.0229	0.0026	0.0129
43	0.1055	0.0272	0.0264	0.0195	0.0025	0.0175	0.0000	0.0136	0.0000
44	0.1034	0.0182	0.0151	0.0064	0.0034	0.0037	0.0086	0.0047	0.0041

45	0.1118	0.0206	0.0235	0.0010	0.0063	0.0010	0.0112	0.0039	0.0112
46	0.0952	0.0358	0.0441	0.0125	0.0029	0.0048	0.0027	0.0057	0.0027
47	0.1269	0.0343	0.0348	0.0227	0.0043	0.0059	0.0058	0.0054	0.0050
48	0.1499	0.0364	0.0361	0.0305	0.0058	0.0052	0.0075	0.0074	0.0075
49	0.1379	0.0280	0.0328	0.0202	0.0038	0.0045	0.0069	0.0050	0.0049
51	0.0988	0.0318	0.0367	0.0022	0.0123	0.0022	0.0389	0.0051	0.0162
52	0.1730	0.0256	0.0295	0.0284	0.0060	0.0060	0.0190	0.0075	0.0077
54	0.1769	0.0330	0.0304	0.0235	0.0072	0.0076	0.0104	0.0070	0.0079
55	0.1419	0.0228	0.0235	0.0130	0.0037	0.0049	0.0033	0.0036	0.0033
56	0.1233	0.0246	0.0210	0.0000	0.0066	0.0000	0.0108	0.0021	0.0108
57	0.9957	0.0043	1.5542	0.0000	1.0000	0.0000	0.0000	1.0000	0.0000
58	0.1093	0.0436	0.0412	0.0054	0.0030	0.0026	0.0087	0.0025	0.0031
59	0.1412	0.0287	0.0292	0.0068	0.0039	0.0040	0.0108	0.0043	0.0049
60	0.1154	0.0380	0.0449	0.0102	0.0041	0.0042	0.0140	0.0055	0.0066
61	0.1483	0.0300	0.0292	0.0182	0.0020	0.0093	0.0004	0.0074	0.0004
62	-0.1044	0.2602	0.4541	0.0049	0.0032	0.0036	0.0198	0.0042	0.0038
63	0.1571	0.0194	0.0263	0.0111	0.0039	0.0058	0.0058	0.0093	0.0058
64	0.1048	0.0208	0.6633	0.0000	0.0059	0.0000	0.0292	0.0008	0.0064
65	0.1756	0.0287	0.0407	0.0036	0.0024	0.0023	0.0089	0.0034	0.0042
66	0.9978	0.0022	1.5563	0.0000	1.0000	0.0000	0.0000	1.0000	0.0000
67	0.9977	0.0023	1.5562	0.0000	1.0000	0.0000	0.0000	1.0000	0.0000
68	0.1281	0.0453	0.0454	0.0062	0.0029	0.0047	0.0031	0.0075	0.0031
69	0.9973	0.0027	1.5558	0.0000	1.0000	0.0000	0.0000	1.0000	0.0000
70	0.0999	0.0174	0.0157	0.0158	0.0045	0.0053	0.0046	0.0058	0.0046
71	0.9863	0.0137	1.5448	0.0000	1.0000	0.0000	0.0000	1.0000	0.0000

Table 1 cont.

Residue	$\rho_3^{(\theta,S)}$	+	–	$\rho_4^{(\theta,S)}$	+	–
2	0.0042	0.0004	0.0004	0.0020	0.0003	0.0003
3	0.0029	0.0002	0.0002	0.0014	0.0002	0.0002
4	0.0015	0.0001	0.0001	0.0010	0.0002	0.0001
6	0.0026	0.0001	0.0001	0.0014	0.0001	0.0002
7	0.0000	0.6970	0.0000	0.0000	0.6978	0.0000
9	0.0111	0.0160	0.0111	0.0254	0.0120	0.0177
10	0.0165	0.0030	0.0050	0.0116	0.0048	0.0042
11	0.0230	0.0044	0.0047	0.0054	0.0036	0.0031
12	0.0066	0.0015	0.0017	0.0030	0.0015	0.0020
13	0.0040	0.0003	0.0003	0.0014	0.0003	0.0003
14	0.0027	0.0001	0.0002	0.0014	0.0001	0.0001
15	0.0018	0.0001	0.0001	0.0009	0.0001	0.0001
16	0.0023	0.0002	0.0001	0.0011	0.0001	0.0002
17	0.0029	0.0007	0.0006	0.0017	0.0013	0.0016
18	0.0027	0.0002	0.0002	0.0009	0.0003	0.0002
20	0.0042	0.0005	0.0004	0.0041	0.0007	0.0008

21	0.0021	0.0001	0.0001	0.0021	0.0002	0.0001
22	0.0017	0.0002	0.0002	0.0018	0.0002	0.0002
23	0.0016	0.0002	0.0003	0.0014	0.0002	0.0002
24	0.0139	0.0077	0.0075	0.0094	0.0060	0.0067
25	0.0077	0.0025	0.0031	0.0045	0.0043	0.0042
26	0.0010	0.0001	0.0001	0.0012	0.0001	0.0001
27	0.0010	0.0001	0.0001	0.0012	0.0001	0.0001
29	0.0014	0.0001	0.0001	0.0009	0.0001	0.0001
30	0.0011	0.0001	0.0001	0.0008	0.0001	0.0001
31	0.0017	0.0001	0.0010	0.0000	0.0020	0.0000
32	0.0010	0.0001	0.0002	0.0011	0.0001	0.0001
33	0.0016	0.0002	0.0002	0.0011	0.0002	0.0002
34	0.0023	0.0002	0.0001	0.0013	0.0001	0.0001
35	0.0024	0.0002	0.0002	0.0014	0.0001	0.0002
36	0.0036	0.0005	0.0004	0.0018	0.0005	0.0006
39	0.0030	0.0003	0.0003	0.0018	0.0003	0.0003
40	0.0051	0.0009	0.0007	0.0055	0.0009	0.0012
41	0.0052	0.0006	0.0006	0.0044	0.0004	0.0005
42	0.0028	0.0001	0.0001	0.0014	0.0001	0.0001
43	0.0025	0.0001	0.0001	0.0015	0.0001	0.0001
44	0.0013	0.0001	0.0001	0.0013	0.0001	0.0001
45	0.0011	0.0001	0.0001	0.0009	0.0001	0.0001
46	0.0015	0.0001	0.0001	0.0011	0.0001	0.0001
47	0.0025	0.0001	0.0001	0.0011	0.0001	0.0001
48	0.0019	0.0002	0.0002	0.0012	0.0002	0.0002
49	0.0028	0.0001	0.0001	0.0012	0.0002	0.0002
51	0.0037	0.0004	0.0003	0.0025	0.0003	0.0004
52	0.0052	0.0004	0.0004	0.0035	0.0004	0.0005
54	0.0021	0.0001	0.0001	0.0022	0.0001	0.0001
55	0.0021	0.0004	0.0003	0.0017	0.0003	0.0004
56	0.0010	0.0001	0.0001	0.0009	0.0001	0.0001
57	0.0025	0.0003	0.0003	0.0018	0.0004	0.0002
58	0.0014	0.0001	0.0001	0.0012	0.0002	0.0002
59	0.0016	0.0002	0.0002	0.0016	0.0002	0.0002
60	0.0023	0.0001	0.0001	0.0011	0.0001	0.0001
61	0.0019	0.0001	0.0001	0.0012	0.0001	0.0001
62	0.0000	0.7187	0.0000	0.2447	0.4746	0.2447
63	0.0029	0.0009	0.0009	0.0010	0.0008	0.0009
64	0.0000	0.6875	0.0000	0.0000	0.6874	0.0000
65	0.0019	0.0001	0.0001	0.0010	0.0001	0.0001
66	0.0015	0.0001	0.0001	0.0008	0.0001	0.0001
67	0.0013	0.0001	0.0000	0.0010	0.0001	0.0001
68	0.0022	0.0005	0.0005	0.0014	0.0006	0.0006
69	0.0016	0.0001	0.0001	0.0012	0.0001	0.0001
70	0.0043	0.0003	0.0003	0.0014	0.0003	0.0003

71	0.0089	0.0021	0.0021	0.0048	0.0022	0.0023

Table II. Detectors calculated from explicit models (text Fig. 13). Original analyses are found in references [1,2].

Residue	$\rho_0^{(\theta,S)}$	$\rho_1^{(\theta,S)}$	$\rho_2^{(\theta,S)}$	$\rho_3^{(\theta,S)}$	$\rho_4^{(\theta,S)}$
2	0.1188	0.0224	0.0223	0.0048	0.0020
3	0.1257	0.0082	0.0062	0.0034	0.0014
5	0.1227	0.0121	0.0005	0.0019	0.0010
7	0.1142	0.0005	0.0457	0.0029	0.0014
10	0.1309	0.0698	0.0148	0.0182	0.0114
11	0.0630	0.2617	0.0399	0.0247	0.0040
12	0.1180	0.0067	0.0438	0.0074	0.0030
14	0.1235	0.0066	0.1006	0.0045	0.0013
15	0.1107	0.0153	0.0070	0.0040	0.0017
16	0.1637	0.0328	0.0041	0.0017	0.0008
18	0.1390	0.0152	0.0005	0.0024	0.0010
20	0.1337	0.0266	0.0015	0.0046	0.0044
21	0.1161	0.0083	0.0058	0.0021	0.0019
22	0.1333	0.0084	0.0010	0.0020	0.0019
23	0.1095	0.0108	0.0037	0.0017	0.0014
26	0.0992	0.0014	0.0119	0.0167	0.0095
27	0.0990	0.0009	0.0129	0.0091	0.0052
28	0.0912	0.0106	0.0120	0.0013	0.0014
30	0.1081	0.0005	0.0155	0.0014	0.0013
31	0.1109	0.0003	0.0101	0.0019	0.0010
32	0.1057	0.0003	0.0085	0.0014	0.0009
33	0.1231	0.0163	0.0042	0.0015	0.0012
34	0.0889	0.0054	0.0175	0.0016	0.0010
35	0.0689	0.0003	0.0253	0.0026	0.0012
36	0.2377	0.0266	0.0053	0.0026	0.0013
39	0.1238	0.0118	0.0318	0.0041	0.0018
40	0.1223	0.0186	0.0120	0.0032	0.0017
41	0.1448	0.0200	0.0061	0.0058	0.0058
42	0.1090	0.0004	0.0221	0.0057	0.0044
43	0.1102	0.0191	0.0007	0.0031	0.0015
44	0.1040	0.0005	0.0082	0.0026	0.0012
45	0.1105	0.0006	0.0124	0.0014	0.0013
46	0.0909	0.0124	0.0022	0.0016	0.0011
47	0.1227	0.0226	0.0054	0.0017	0.0010
48	0.1515	0.0316	0.0071	0.0025	0.0010
49	0.1327	0.0197	0.0065	0.0023	0.0013
51	0.0966	0.0011	0.0425	0.0033	0.0014
52	0.1684	0.0283	0.0184	0.0040	0.0023
53	0.2009	0.0204	0.0021	0.0058	0.0035
54	0.1729	0.0245	0.0100	0.0025	0.0024

55	0.1424	0.0133	0.0032	0.0023	0.0015
56	0.1219	0.0003	0.0104	0.0015	0.0011
58	0.1080	0.0051	0.0097	0.0036	0.0023
59	0.1419	0.0072	0.0102	0.0016	0.0011
60	0.1768	0.0216	0.0017	0.0020	0.0019
61	0.1463	0.0178	0.0006	0.0025	0.0011
62	0.1298	0.0286	0.0015	0.0024	0.0012
63	0.1423	0.0105	0.0059	0.0024	0.0012
64	0.1064	0.0004	0.0243	0.0020	0.0009
65	0.1747	0.0035	0.0092	0.0018	0.0012
67	0.1135	0.0100	0.0003	0.0026	0.0013
68	0.1239	0.0077	0.0002	0.0018	0.0012
69	0.1088	0.0012	0.0119	0.0048	0.0011
70	0.1036	0.0191	0.0010	0.0140	0.0063

III. References

[1] J. D. Haller and P. Schanda, J. Biomol. NMR **57** (3), 263 (2013).

[2] N. A. Lakomek, S. Penzel, A. Lends, R. Cadalbert, M. Ernst, and B. H. Meier, Chemistry **23** (39), 9425 (2017).