Supplemental Material belonging to
Insights into Protein Dynamics from ^{15}N-^{1}H HSQC

Erik R.P. Zuiderweg

Department of Biological Chemistry, The University of Michigan, Ann Arbor, MI 41109, USA

Institute for Molecules and Materials, Faculty of Science, Radboud University Nijmegen, The Netherlands.

Correspondence to: Erik R.P. Zuiderweg (zuiderwe@umich.edu)

Table S1
Integration data 600 MHz ^{15}N-^{1}H HSQC for GB1, 3 ^{0}C, pH6.5,
processed with a cos^2 and 1 Hz EM window in t_1 and t_2, respectively.

Assignment	wN	wH	Volume	Height	S/N	lw-N	lw-H
	ppm	ppm	a.u.	a.u.	a.u.	Hz	Hz
K4N-H	122.543	9.124	4.02E+08	2683135	253	31	19.9
L5N-H	126.506	8.579	4.00E+08	2852088	269	30.3	19.7
I6N-H	126.374	9.13	4.30E+08	2997682	282	29	21.3
L7N-H	125.607	8.709	4.24E+08	3337335	314	27.3	19.6
N8N-H	126.627	8.94	4.58E+08	3264575	308	27.6	19.8
G9N-H	110.054	7.96	4.50E+08	3950550	372	30.7	17.2
K10N-H	121.3	9.559	4.89E+08	5615360	529	28.5	14.1
T11N-H	108.622	8.87	5.24E+08	3283542	309	30	20.5
L12N-H	126.031	7.422	5.96E+08	4800404	452	30.3	16.8
K13N-H	124.171	8.209	5.10E+08	3638287	343	28.3	18.7
G14N-H	109.56	8.469	4.62E+08	5452903	514	29	13.5
E15N-H	118.928	8.507	5.47E+08	4030626	380	31.8	16.6
T16N-H	115.767	8.731	4.42E+08	4283450	404	29.8	15
T17N-H	111.628	8.065	5.45E+08	4118756	388	30.7	17.7
T18N-H	114.821	8.992	4.09E+08	3817011	360	30.3	15.7
E19N-H	126.297	7.99	4.96E+08	3496489	329	30	18.5
A20N-H	128.072	9.401	4.70E+08	4166918	393	29.2	16.6
V21N-H	115.724	8.523	4.93E+08	6144372	579	28	13.6
D22N-H	115.268	7.297	5.65E+08	5474399	516	31.8	14
A23N-H	121.502	8.32	4.63E+08	5339469	503	30.6	13.4
T25N-H	116.51	8.267	5.36E+08	5347722	504	30.3	14.9
A26N-H	124.003	7.135	4.61E+08	5400432	509	29	13.6
E27N-H	116.899	8.399	3.95E+08	4980832	469	28.8	13
K28N-H	116.542	6.891	4.60E+08	5238552	494	28.9	14.3
V29N-H	120.985	7.236	4.62E+08	4913756	463	29.1	14.7
F30N-H	120.932	8.519	3.69E+08	4139830	390	29.2	14.2
K31N-H	123.162	9.1	3.66E+08	4559574	430	28.4	13

Q32N-H	119.762	7.394	4.65E+08	5292754	499	28.9	13.8
Y33N-H	121.209	8.275	3.78E+08	4484484	422	29.5	13.4
A34N-H	122.811	9.22	4.20E+08	4901862	462	29.1	13.9
N35N-H	117.744	8.186	4.33E+08	5550734	523	29.1	12.4
D36N-H	121.555	8.987	3.35E+08	4376426	412	29.2	11.8
N37N-H	115.692	7.386	3.88E+08	2510190	236	30.7	19.5
G38N-H	108.215	7.784	3.07E+08	2697680	254	33.1	15.9
V39N-H	121.086	8.1	5.45E+08	2802336	264	46.2	17.8
D40N-H	128.119	8.674	4.88E+08	4171258	393	28	17.6
G41N-H	107.362	7.774	5.06E+08	6007708	566	29.5	13.1
W43N-H	128.897	9.456	4.07E+08	3299148	311	29.4	18
T44N-H	114.956	9.357	4.46E+08	3233455	305	29.5	18.5
Y45N-H	120.293	8.633	4.31E+08	3231193	304	30.1	17.9
D46N-H	128.452	7.581	4.30E+08	2868318	270	29.9	20.3
D47N-H	125.133	8.66	3.94E+08	4836374	456	29.2	12.9
A48N-H	120.082	8.417	5.19E+08	6899136	650	28.5	12.2
T49N-H	103.387	6.988	4.99E+08	3080205	290	30.4	20.2
K50N-H	123.666	7.848	4.29E+08	3575756	337	32.2	16.2
T51N-H	111.068	7.359	5.42E+08	3316018	312	30.9	20.5
F52N-H	131.406	10.404	3.48E+08	2343456	221	30	21
T53N-H	117.437	9.153	4.11E+08	2908778	274	29.7	19.5
V54N-H	123.443	8.155	4.92E+08	3419361	322	29.5	20.2
T55N-H	124.032	8.363	5.02E+08	3577118	337	28.1	20.4
E56N-H	134.436	7.823	4.83E+08	3815238	359	29.5	17.8

Table S2
Results of 600 MHz T_{1rho}-HSQC for GB1, 3 ^{0}C, pH6.5.
The single exponential fits were calculated with Microsoft Excel, with the R^2 of fit indicated.

Residue	nr integrated cross peaks	R_{1rhO}	R^2
		Rad/s	
K4N-H	3	29.56	0.9217
L5N-H	4	24.02	0.9926
I6N-H	3	31.12	0.9434
L7N-H	3	32.06	0.9908
N8N-H	3	36.07	0.9952
G9N-H	4	24.14	0.9824
K10N-H	4	3.42	0.9927
L12N-H	4	24.71	0.9937
K13N-H	4	22.19	0.9956
G14N-H	4	20.53	0.99789
E15N-H	4	19.88	0.99263
T16N-H	4	21.76	0.968
T17N-H	4	18.86	0.99626
T18N-H	3	32.04	0.9594
E19N-H	4	24.53	0.9855
A20N-H	4	24.34	0.9982
V21N-H	4	26.64	0.9999
D22N-H	4	20.69	0.9964
A23N-H	4	23.5	0.9984
T25N-H	3	34.15	0.9986
A26N-H	4	21.84	0.9995
E27N-H	4	32.19	1
V29N-H	4	23.64	0.9955
F30N-H	4	32.41	0.9995
K31N-H	4	23.33	0.9416
Q32N-H	4	25.76	0.9864
Y33N-H	4	25.87	0.998
A34N-H	3	36.5	0.96
N35N-H	4	21.22	0.9983
D36N-H	4	27.96	0.9858
N37N-H	4	28.13	0.995
G38N-H	4	22.15	0.9462

V39N-H	4	19.12	0.9964
D40N-H	4	22.55	0.9939
G41N-H	4	19.25	0.9829
W43N-H	4	29.41	0.9961
T44N-H	4	22.41	0.994
Y45N-H	4	26.73	0.9995
D46N-H	4	22.99	0.9546
D47N-H	4	28.3	0.9912
A48N-H	4	19.89	0.9985
T49N-H	4	27.15	0.9995
K50N-H	3	41.38	0.996
T51N-H	4	24.87	0.9969
F52N-H	4	24.83	0.9941
T53N-H	4	24.52	0.9764
V54N-H	4	23.41	0.9997
T55N-H	3	39.7	0.9999
E56N-H	4	28.3	0.9744

Radius (A)	<LW> (Hz)
3	4.69
4	5.37
5	5.72
6	5.85
7	5.9
8	5.93
9	5.95
10	5.95

Table S3. Average calculated ^{1}HN linewidths as a function of the radius of the sphere of surrounding protons in GB1.

Table S4
Integration data 500 MHz ^{15}N-^{1}H HSQC for BPTI, 30 ^{0}C, pH6.5, processed with a 1 Hz and 1 Hz EM window in t_1 and t_2, respectively.

Assignment	wN	wH	Volume	Height	S/N	lw-N	lw-H
	ppm	ppm	a.u.	a.u.	a.u.	Hz	Hz
D3N-H	123.688	8.704	8.97E+08	273614	13	34.6	83.7
F4N-H	116.929	7.889	4.87E+08	1370283	63	16.6	15.7
C5N-H	121.442	7.502	1.59E+09	5818645	268	15.6	13
L6N-H	114.198	7.613	1.88E+09	5242934	242	15.2	16.6
E7N-H	120.733	7.566	2.00E+09	6417062	296	15.9	14
Y10N-H	123.532	7.858	1.21E+09	2848075	131	14.6	20.7
T11N-H	128.474	8.945	2.08E+08	258682	12	24.7	34.7
G12N-H	107.496	7.207	1.58E+09	4083052	188	17.3	16.6
C14N-H	120.238	8.747	8.26E+08	1674421	77	16.6	21.5
K15N-H	115.797	8.02	4.90E+08	696466	32	20	27.3
A16N-H	123.774	8.247	1.51E+09	3807130	175	16.2	17.7
R17N-H	118.75	8.251	1.40E+09	3603935	166	15.2	18.3
I18N-H	125.924	8.166	1.65E+09	4148872	191	14.7	19.9
I19N-H	128.52	8.749	1.88E+09	6501855	300	14.7	14
R20N-H	130.147	8.431	1.82E+09	4248952	196	16.1	18.1
Y21N-H	115.608	9.226	1.89E+09	4128798	190	15.9	19.8
F22N-H	120.143	9.814	1.54E+09	3986008	184	15.2	17.5
Y23N-H	125.078	10.596	1.39E+09	4344250	200	14.4	15.9
N24N-H	125.557	7.794	1.54E+09	3984908	184	14.5	18.7
A25N-H	126.538	8.847	1.66E+09	6652706	307	15	12.2
K26N-H	117.282	7.96	1.09E+09	3420886	158	16.6	14.3
A27N-H	118.772	6.852	1.91E+09	5346197	246	15.3	16.3
G28N-H	107.257	8.173	1.65E+09	4343654	200	16.6	16.9
L29N-H	114.905	6.857	1.81E+09	5303712	244	16.2	14.7
C30N-H	118.668	8.458	1.44E+09	4577096	211	13.9	15.5
Q31N-H	123.141	8.805	1.87E+09	4236566	195	15.7	18.6
T32N-H	108.692	8.081	2.11E+09	6233404	287	15.5	15.4
F33N-H	119.32	9.408	1.41E+09	4293664	198	15.4	15.4
V34N-H	118.988	8.42	1.86E+09	5492192	253	14.6	17
Y35N-H	129.868	9.444	1.26E+09	3568274	164	13.8	17.7
G36N-H	114.457	8.66	1.07E+09	2722916	126	15	19.4
G37N-H	98.523	4.35	1.10E+09	2477053	114	16.5	18.9
C38N-H	115.245	7.791	8.73E+08	1915624	88	18.8	18.1

R39N-H	105.064	3.41	1.15E+09	3110502	143	15.5	17.1
A40N-H	118.314	7.444	7.69E+08	2320110	107	17.2	14.4
K41N-H	121.331	8.365	1.07E+09	2671406	123	15.2	18.4
R42N-H	116.071	8.422	1.31E+09	4589204	212	15	14.2
N43N-H	116.402	7.257	1.68E+09	4815814	222	15.3	15.8
N44N-H	121.03	6.809	1.64E+09	5175156	239	14.5	15.2
F45N-H	122.819	9.978	1.69E+09	3365330	155	16.3	19.5
K46N-H	120.637	9.979	3.22E+08	475529	22	22.5	27.8
S47N-H	109.078	7.499	1.74E+09	4678566	216	16.3	16.2
A48N-H	125.585	8.195	1.16E+09	5126964	236	14.6	11.6
E49N-H	117.874	8.66	7.79E+08	2817970	130	16.1	13
D50N-H	120.573	7.906	1.39E+09	5209340	240	15.1	12.8
C51N-H	119.89	7.028	1.51E+09	6121373	282	14.3	12.6
M52N-H	121.06	8.633	1.20E+09	5092582	235	14.1	12.2
R53N-H	121.524	8.307	1.80E+09	7351498	339	14.8	12.2
T54N-H	113.491	7.438	1.49E+09	4934337	227	14.8	14.3
C55N-H	115.157	8.286	1.50E+09	3985704	184	14.4	17.3
G56N-H	107.988	8.003	3.24E+09	7406184	341	21.8	14.2
G57N-H	109.398	8.248	7.50E+08	1995830	92	17.2	16.6
A58N-H	129.518	7.996	1.70E+09	6669430	307	14.8	12.3

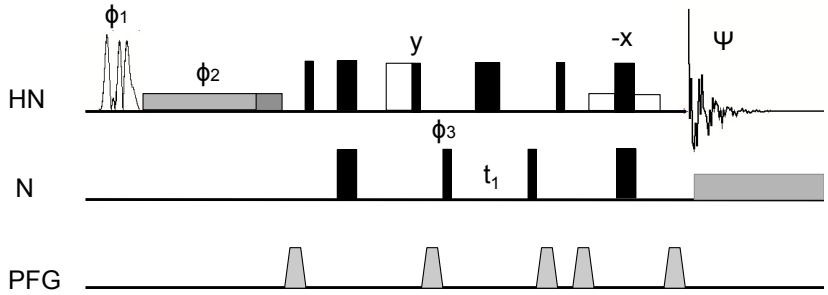
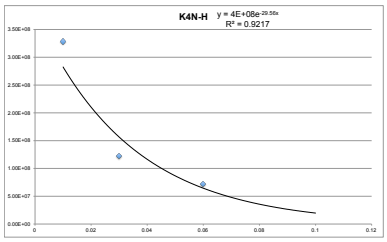
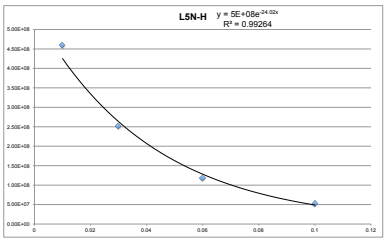
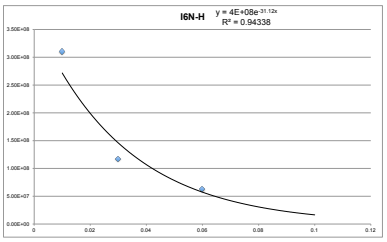


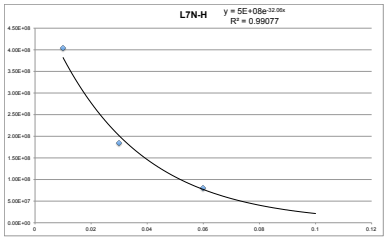
Figure S1. Pulse scheme for the T_{1rho}-HSQC experiment.
We used a G5 excitation pulse (phase ϕ1) centered at 8.5 ppm, covering from 7 – 10 ppm. The spinlock (phase ϕ2) was 5.2 kHz, also at 8.5 ppm. The lock times were 10, 30, 60 and 100 ms. The flip-back pulse following the spinlock (dark grey) was at the same power as the spinlock. After the gradient, the carrier was switched to 4.8 ppm, and full proton power was used in the HSQC. The solvent suppression was carried out with Watergate, and with an additional 1 ms spin-lock in the first INEPT. All phases were <x> unless indicated differently.
ϕ1=x,x,-x,-x; ϕ2=4(y),4(-y), ϕ3=x,-x and ψ=x,-x,-x,x

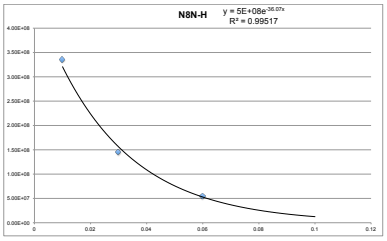
Figures S2 (below)
Sample T_{1rho} decay curves for GB1 at 3 ^{0}C.
The single-exponential trendlines were computed in Excel.

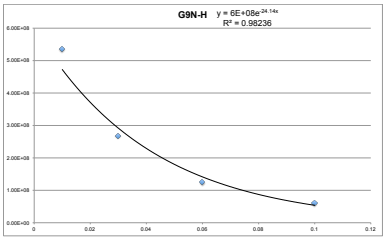

K4N-H
y = 4E+08e-29.59x
R² = 0.9217

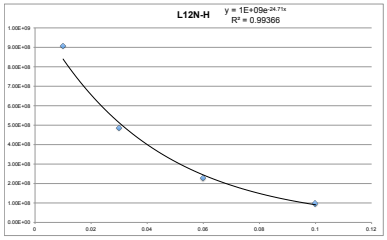

L5N-H
y = 5E+08e-24.02x
R² = 0.99264

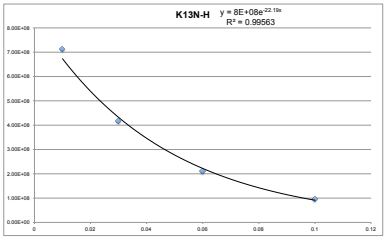

I6N-H
y = 4E+08e-31.12x
R² = 0.94338

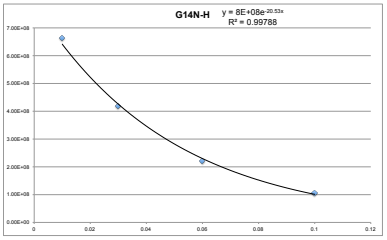

L7N-H
y = 5E+08e-32.06x
R² = 0.99077

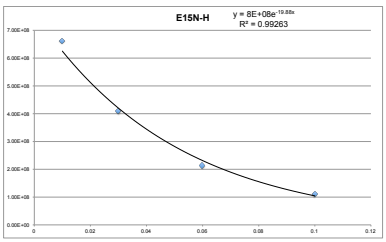

N8N-H
y = 5E+08e-36.07x
R² = 0.99517

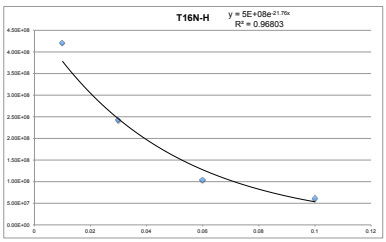

G9N-H
y = 6E+08e-24.14x
R² = 0.98236

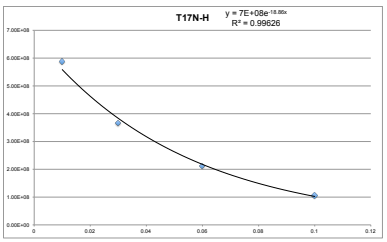

L12N-H
y = 1E+09e-24.71x
R² = 0.99366

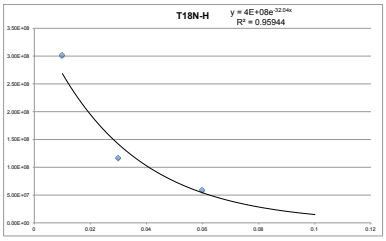

K13N-H
y = 8E+08e-22.19x
R² = 0.99563

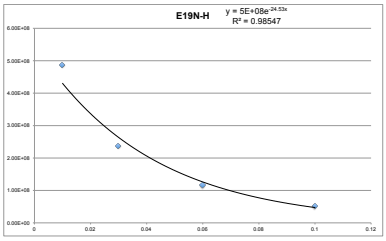

G14N-H
y = 8E+08e-20.53x
R² = 0.99788

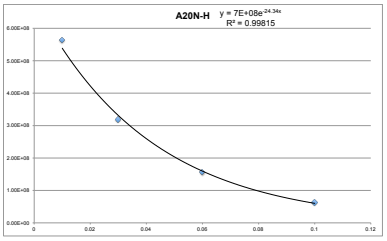

E15N-H
y = 8E+08e-19.88x
R² = 0.99263

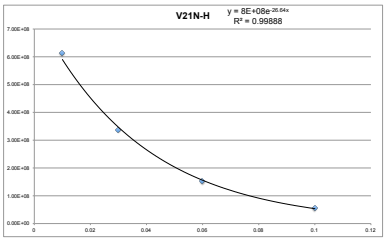

T16N-H
y = 5E+08e-21.76x
R² = 0.96803

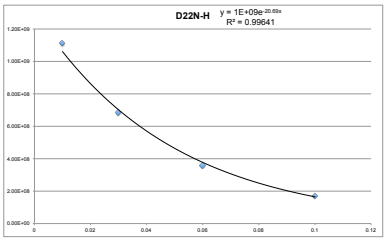

T17N-H
y = 7E+08e-18.86x
R² = 0.99626

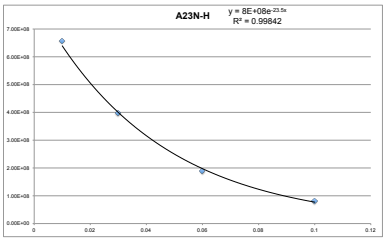

T18N-H
y = 4E+08e-32.04x
R² = 0.95944

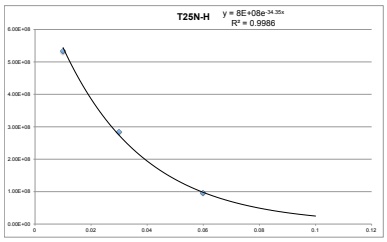

E19N-H
y = 5E+08e-24.53x
R² = 0.98547

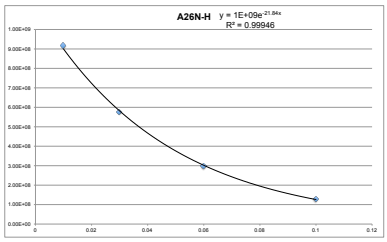

A20N-H
y = 7E+08e-24.34x
R² = 0.99815

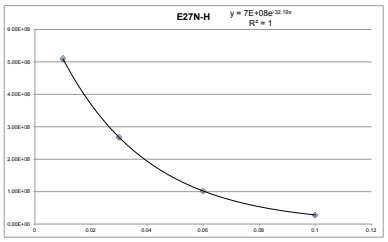

V21N-H
y = 8E+08e-26.64x
R² = 0.99888

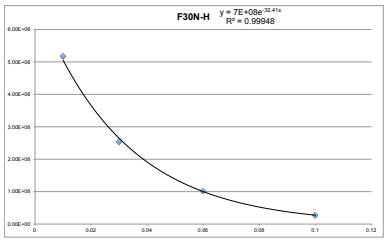

D22N-H
y = 1E+09e-20.69x
R² = 0.99641

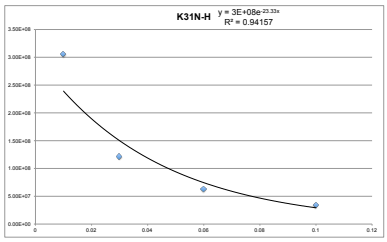

A23N-H
y = 8E+08e-23.5x
R² = 0.99842

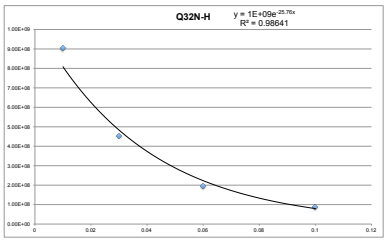

T25N-H
y = 8E+08e-34.35x
R² = 0.9986

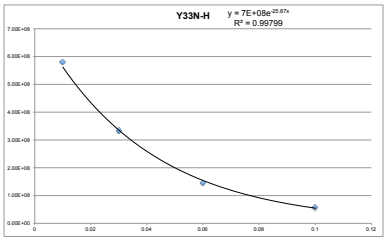

A26N-H
y = 1E+09e-21.84x
R² = 0.99946

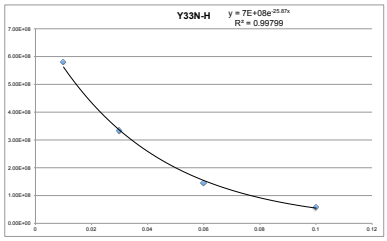

E27N-H
y = 7E+08e-32.19x
R² = 1

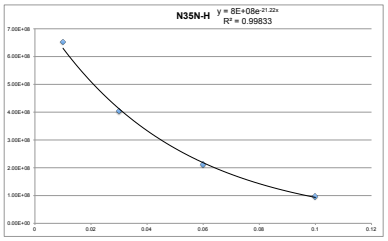

F30N-H
y = 7E+08e-32.41x
R² = 0.99948

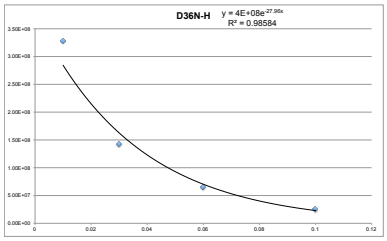

K31N-H
y = 3E+08e-23.33x
R² = 0.94157

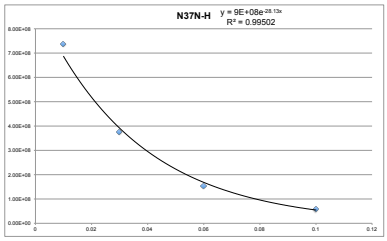

Q32N-H
y = 1E+09e-25.76x
R² = 0.98641

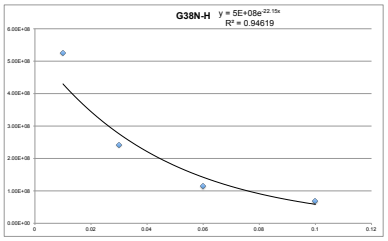

Y33N-H
y = 7E+08e-25.87x
R² = 0.99799

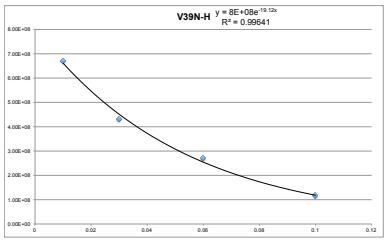

Y33N-H
y = 7E+08e-25.87x
R² = 0.99799

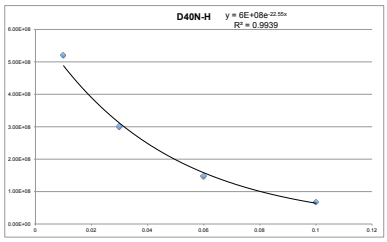

N35N-H
y = 8E+08e-21.22x
R² = 0.99833

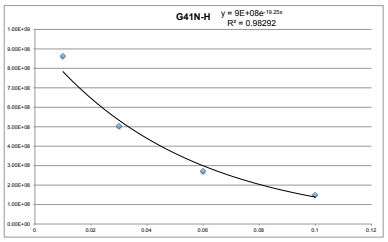

D36N-H
y = 4E+08e-27.96x
R² = 0.98584

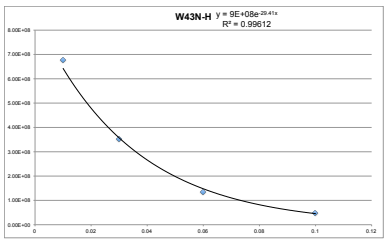

N37N-H
y = 9E+08e-28.13x
R² = 0.99502

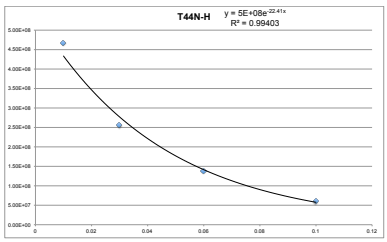

G38N-H
y = 5E+08e-22.15x
R² = 0.94619

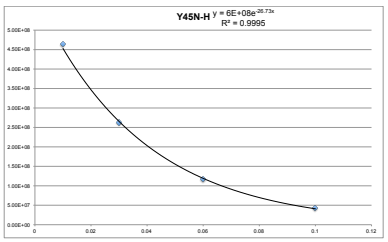

V39N-H
y = 8E+08e-19.12x
R² = 0.99641

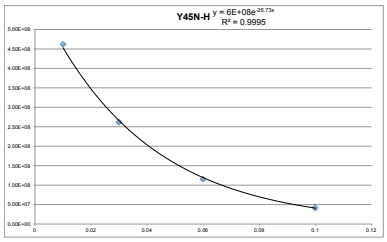

D40N-H
y = 6E+08e-22.55x
R² = 0.9939

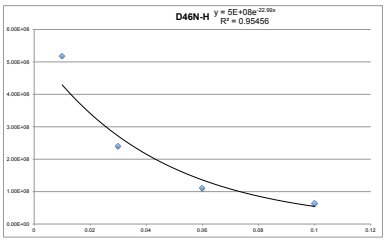

G41N-H
y = 9E+08e-19.25x
R² = 0.98292

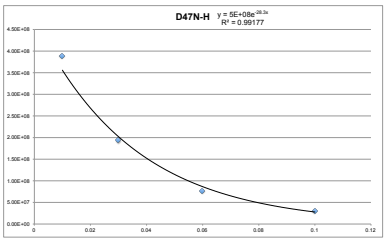

W43N-H
y = 9E+08e-29.41x
R² = 0.99612

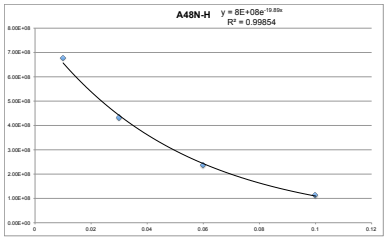

T44N-H
y = 5E+08e-22.41x
R² = 0.99403

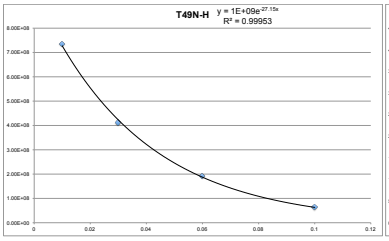

Y45N-H
y = 8E+08e-26.73x
R² = 0.9995

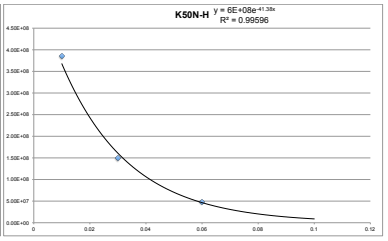

Y45N-H
y = 6E+08e-26.73x
R² = 0.9995

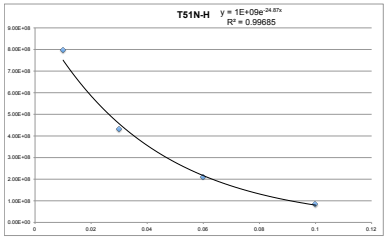

D46N-H
y = 5E+08e-22.99x
R² = 0.95456

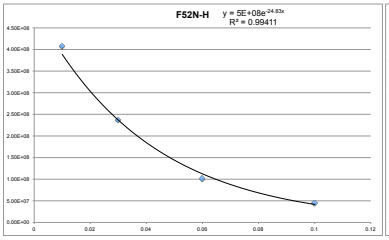

D47N-H
y = 5E+08e-28.3x
R² = 0.99177

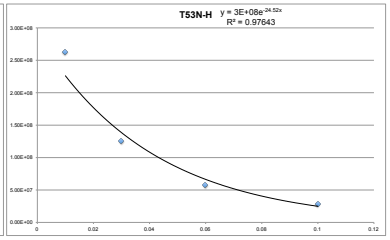

A48N-H
y = 8E+08e-19.89x
R² = 0.99854

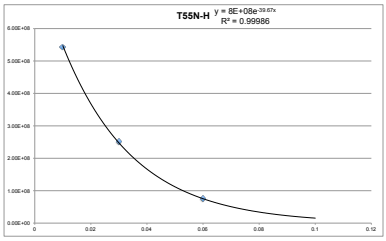

T49N-H
y = 1E+09e-27.15x
R² = 0.99953

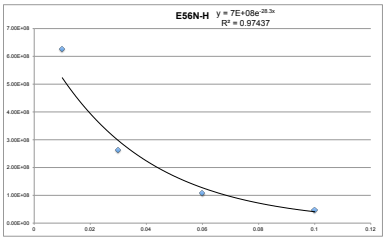

K50N-H
y = 6E+08e-41.38x
R² = 0.99596


T51N-H
y = 1E+09e-24.87x
R² = 0.99685


F52N-H
y = 5E+08e-24.83x
R² = 0.99411


T53N-H
y = 3E+08e-24.52x
R² = 0.97643


T55N-H
y = 8E+08e-39.67x
R² = 0.99986


E56N-H
y = 7E+08e-28.3x
R² = 0.97437