

SUPPLEMENTARY INFORMATION

A dynamic core in human NQO1 controls the functional and stability effects of ligand binding and their communication across the enzyme dimer

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Includes Figures S1-S10 and Tables S1-S2.

Figure S1. Verification of the NQO1 protein by high resolution mass spectrometry. NQO1 was offline desalted on a Protein OptiTrap (Optimize Technologies,). Then 5 μ M sample was directly infused into an ESI source of 15T FT-ICR MS (solariX XR, Bruker Daltonics) and the spectra were recorded in a broad band mode with 2M data points. Spectrum shows the entire charge state envelope (detected charges 19+ to 48+) and inset demonstrates the high resolving power and isotopic pattern for charge state 32+. Spectrum was deconvoluted using the SNAP algorithm (DataAnalysis 5.0). Calculated monoisotopic mass and the experimental deconvoluted values are shown together with the error in ppm. The precise mass exactly fits to the sequence of the construct (shown below the spectrum) without the N-terminal methionine (shown in grey). Grey highlight shows the HisTag sequence. This is also indicated by the negative (non-native) numbering.

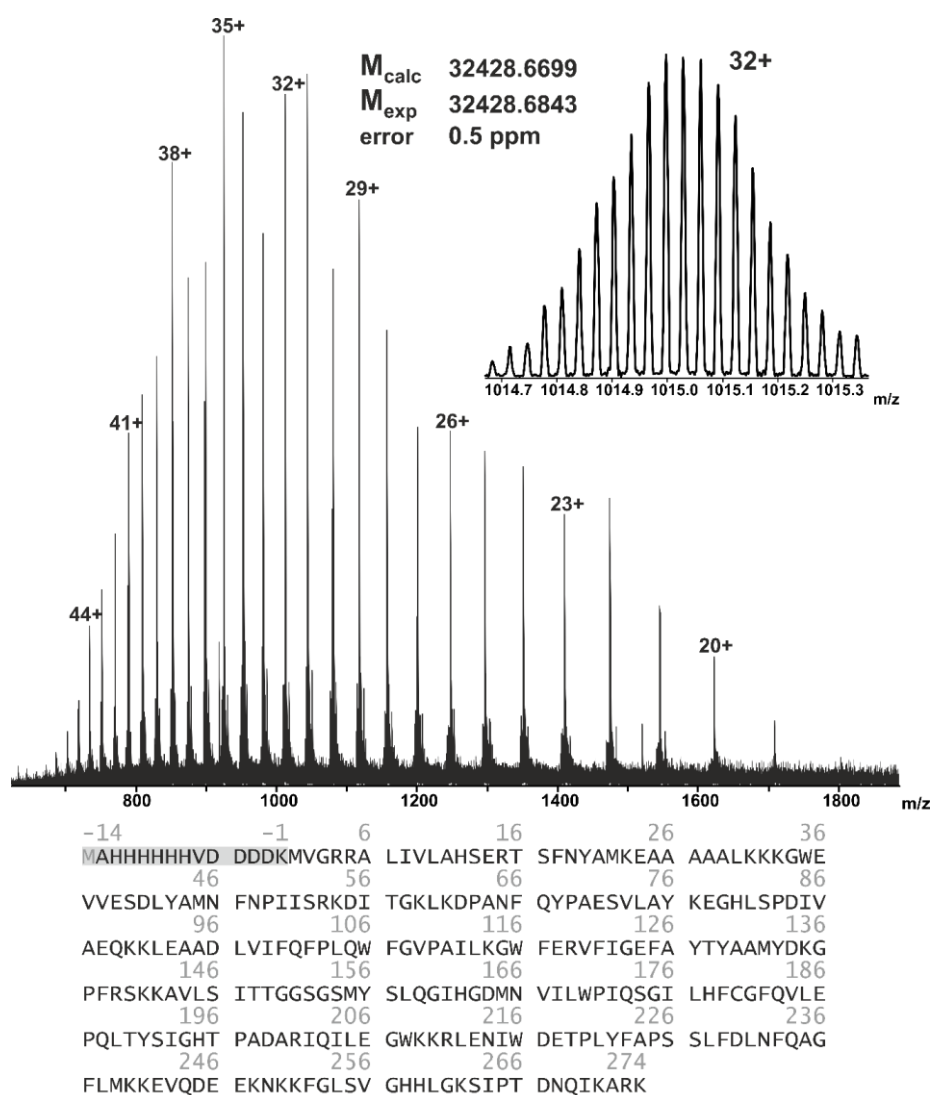


Figure S2. NQO1 dimeric state confirmed by mass spectrometry. NQO1_{apo} (A) and NQO1_{holo} (B) were transferred into 100 mM ammonium acetate pH 7.5 by Zeba spin (Thermo Fisher) desalting columns. Protein solution was transferred into a home-made quartz nESI emitter that was mounted to an nESI source of Synapt G2Si (Waters). Spray voltage was kept at 0.7 kV. Temperature was 20 °C, sampling cone and source offset were 50 V and 20 V, respectively. Trap collisional cooling (CE) of 80 V was required to achieve better S/N and resolution. The analyses proved that NQO1 forms stable dimer in both states. Charge states of individual peaks are shown. Dimeric protein state is indicated by two circles – open for NQO1_{apo} and closed for NQO1_{holo}.

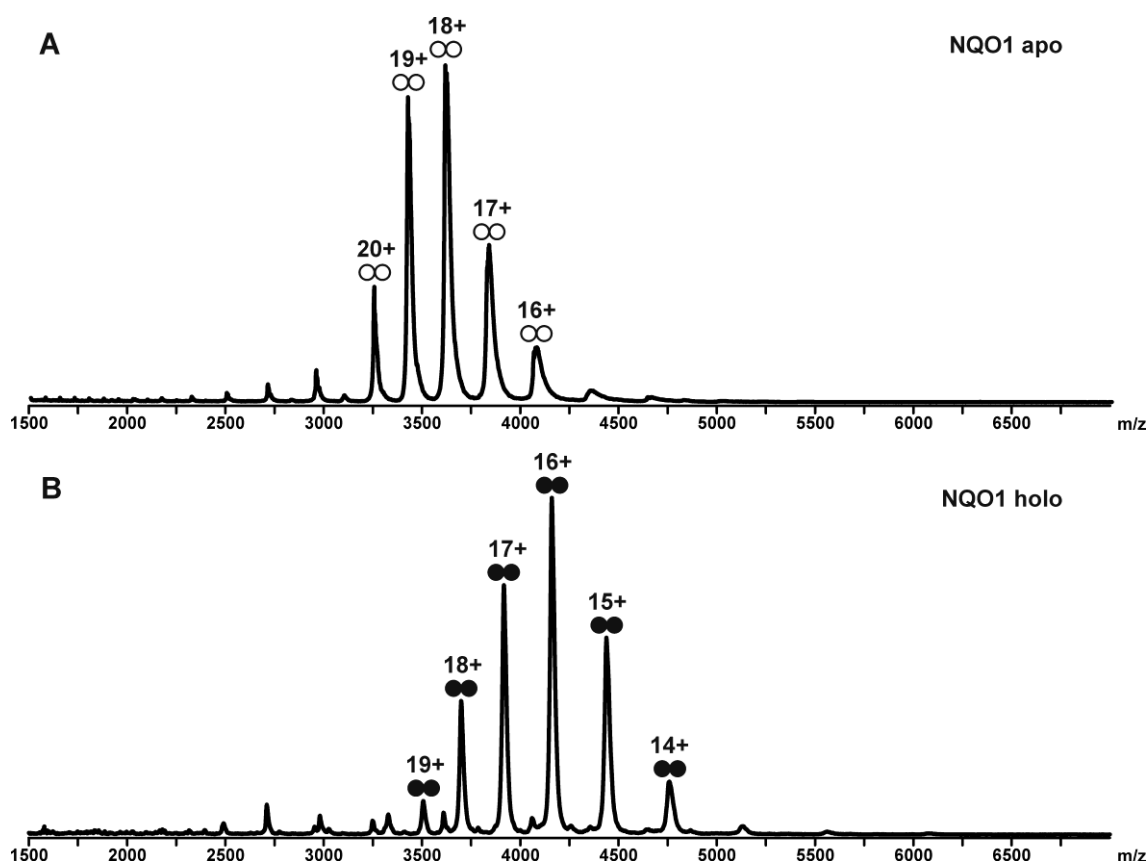


Figure S3. HDX-MS mapping. NQO1 peptide map representing sequence coverage in the HDX-MS study. Protein was digested online by a serial combination of Nepenthesin-2 and Pepsin. This yielded 140 peptides with the average peptide length 8.3 amino acids and redundancy score 4.05 covering nearly 99% of the sequence. Peptides were identified by LC-MS/MS analysis and MASCOT searching as described previously. Coverage is shown on the sequence of the construct with numbering reflecting native one. Secondary structure elements are shown as cylinders (alpha helices) and arrows (beta sheets). Numbering of loops is also indicated (L1-L10) above the sequence. The His-tag is highlighted as a grey box. Map was created using MSTools (<http://peterslab.org/MSTools/DrawMap/DrawMap.php>). [1].

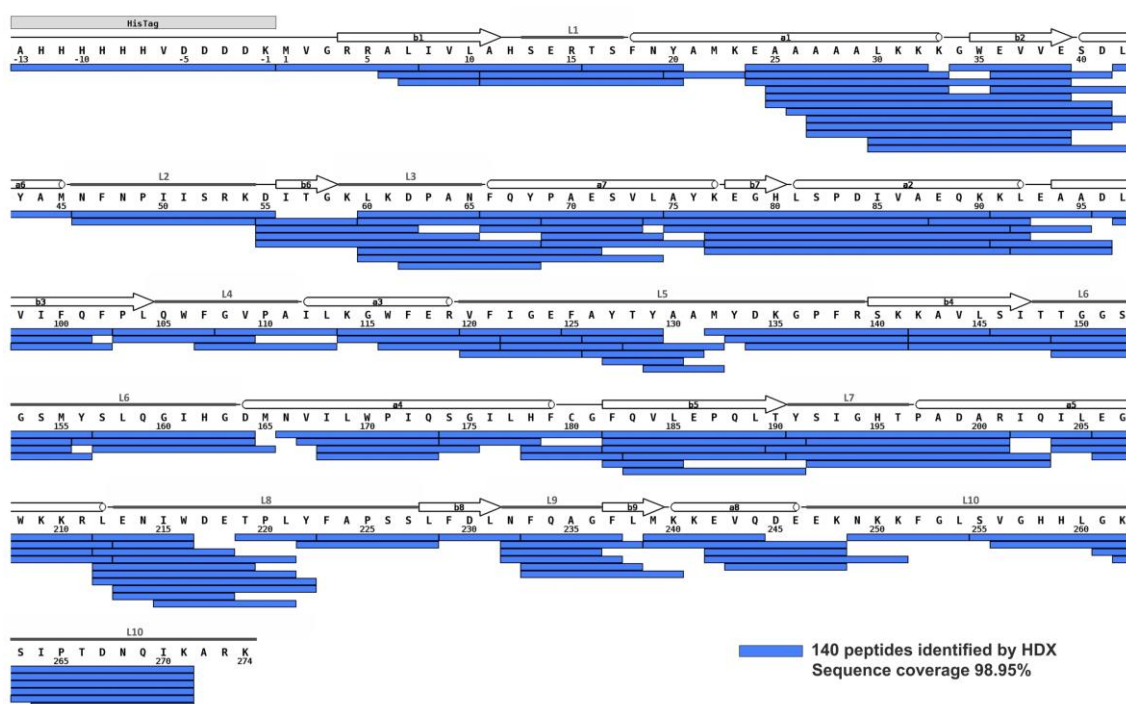
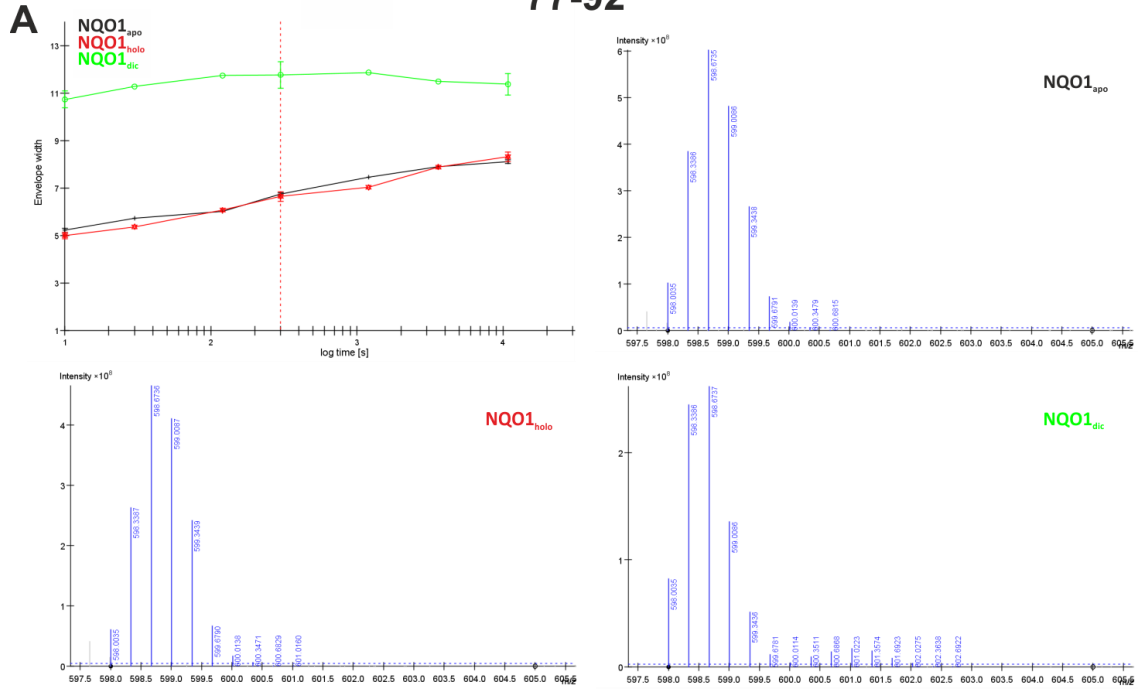


Figure S4. Representative examples of rare EX1/EX2 exchange profiles. The NQO1 protein showed predominantly EX2 exchange behavior in all ligation states as well as in the apo form. Exceptions were two regions covered by peptides 75-90, 77-90, 77-91, 77-92 and 249-254, 255-271, 256-271, 261-271, 262-271, 263-271, 264-271 where very small EX1 signatures were detected for dicoumarol and wild-type states respectively. Two representative examples are shown in this figure. A) peptide 77-92 where top left graph shows peak width detected at 1% of the MS peak intensity as a function of time. Other three panels are showing isotopic envelopes of NQO1_{apo}, NQO1_{holo} and NQO1_{dic} at 300 s of exchange (position in the graph indicate this time point). B) peptide 255-271, peak width is again in top left part of the panel and the other three panels show mass spectra of NQO1_{apo}, NQO1_{holo} and NQO1_{dic} at 10 s of exchange (position in the graph indicate this time point).

77-92



255-271

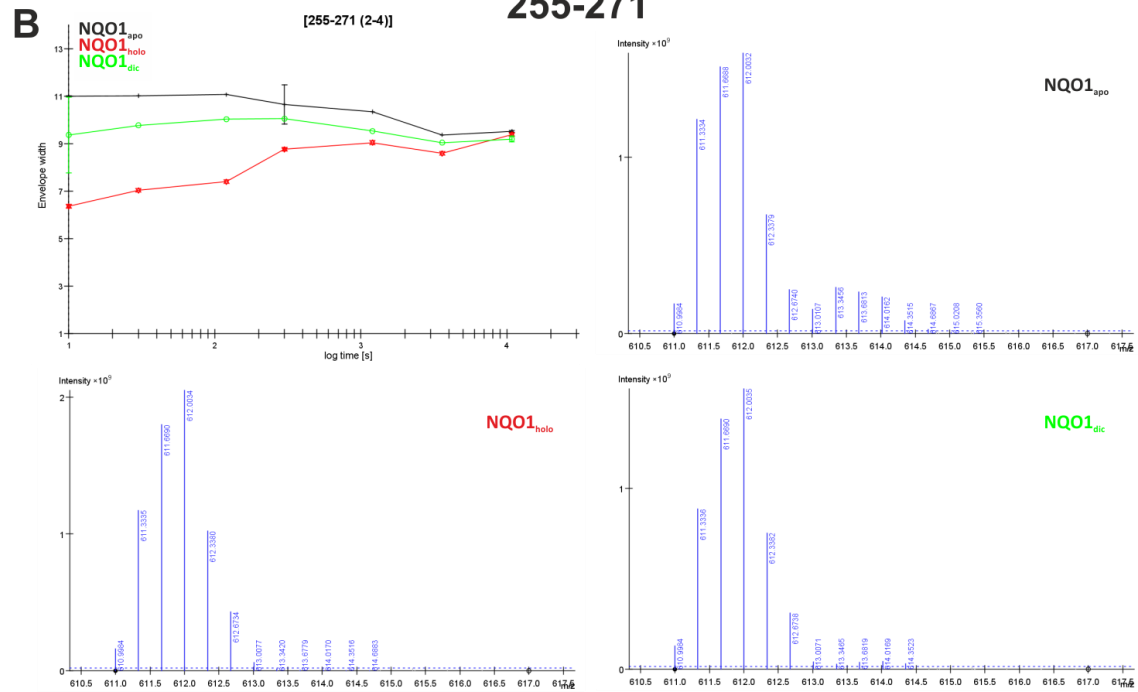


Figure S5 (1 of 3). HDX kinetics for NQO1 segments (spanning residues 1-95) of NQO1 upon FAD and dicoumarol binding. Plots showing percentage of deuteration as a function of time. Segment limits are shown in each graph. Kinetic analysis can be found in Table S1.

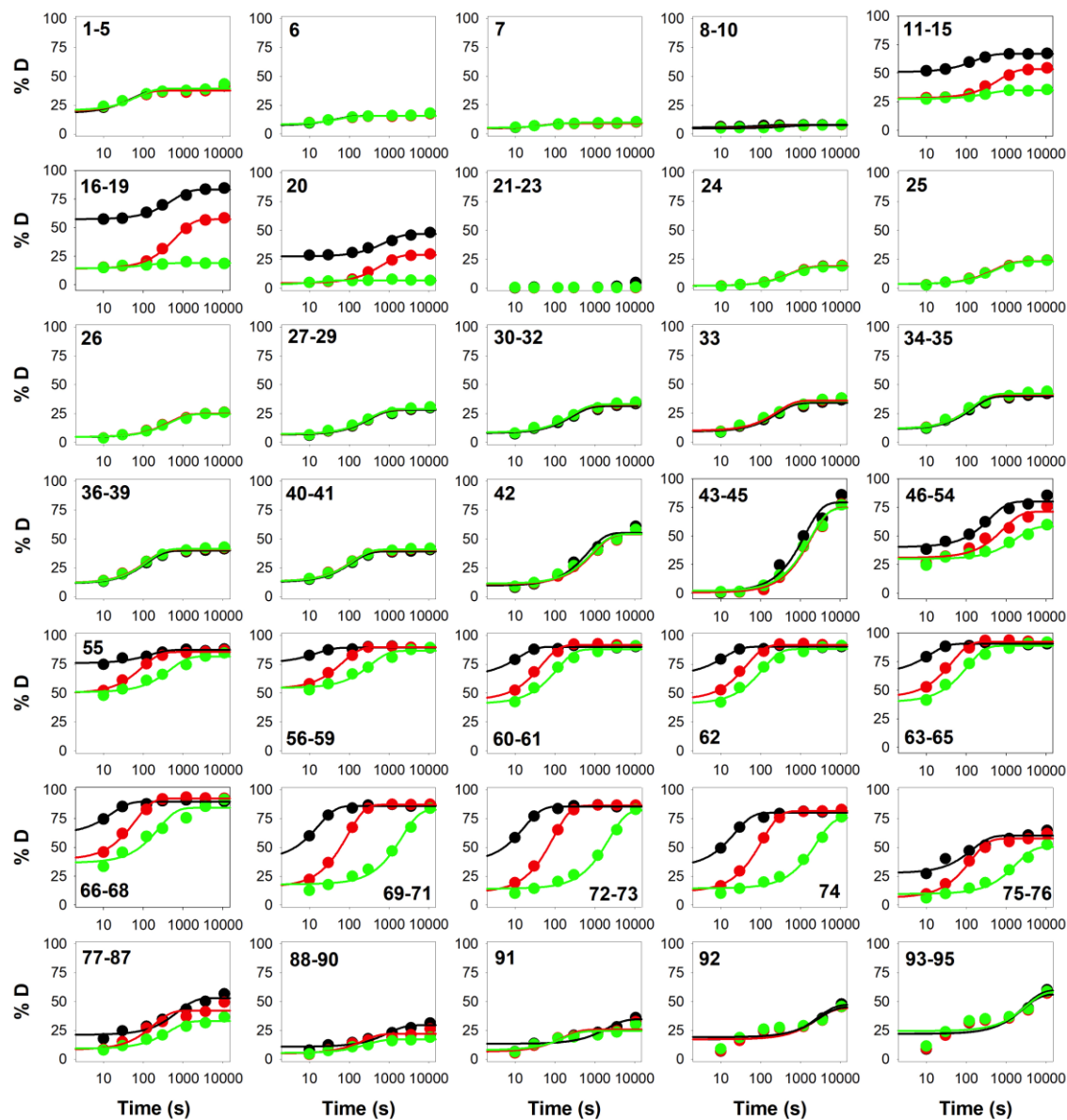


Figure S5 (2 of 3). HDX kinetics for NQO1 segments (spanning residues 96-181) of NQO1 upon FAD and dicoumarol binding. Plots showing percentage of deuteration as a function of time. Segment limits are shown in each graph. Kinetic analysis can be found in Table S1.

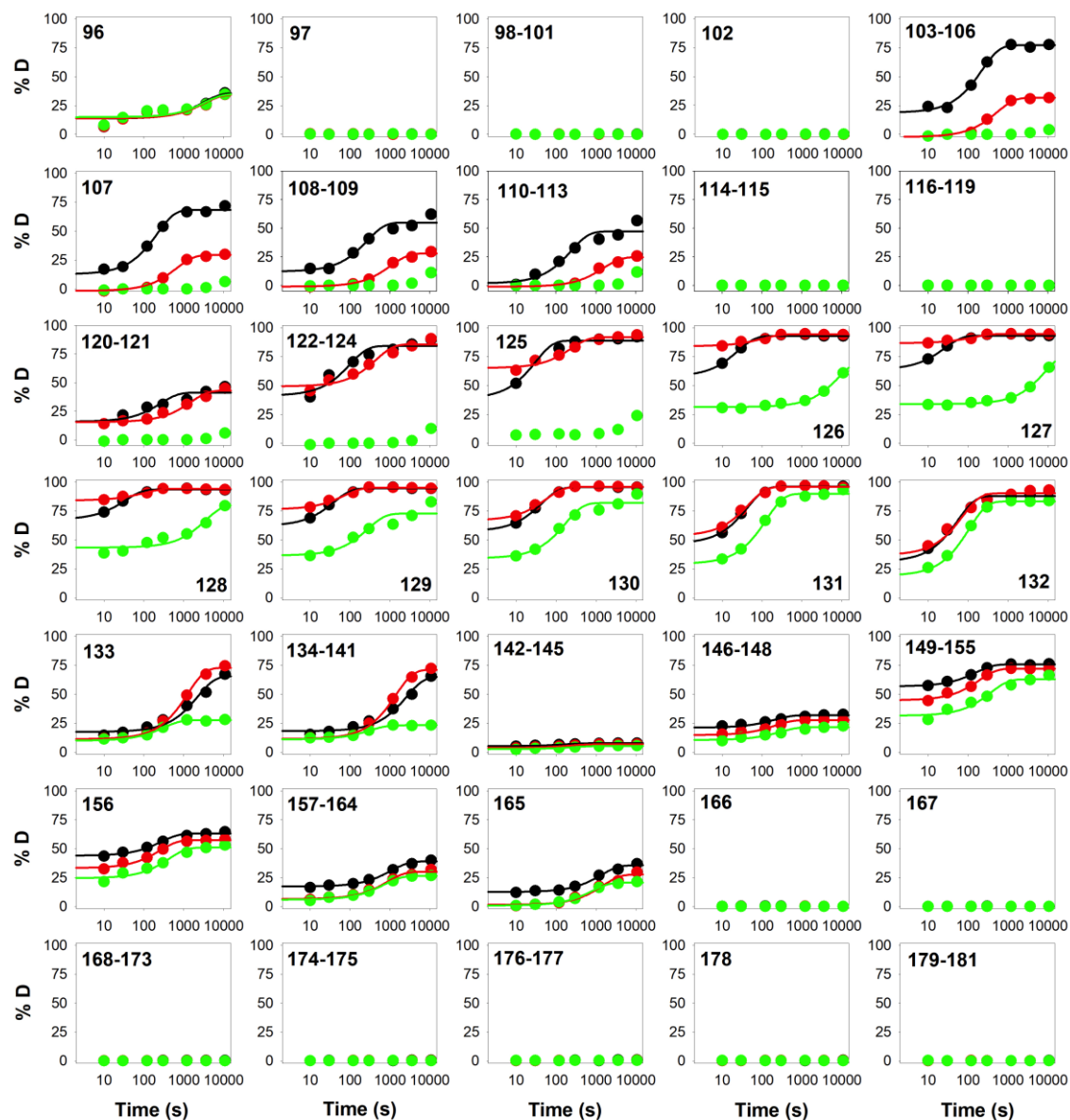


Figure S5 (3 of 3). HDX kinetics for NQO1 segments (spanning residues 182-271) of NQO1 upon FAD and dicoumarol binding. Plots showing percentage of deuteration as a function of time. Segment limits are shown in each graph. Kinetic analysis can be found in Table S1.

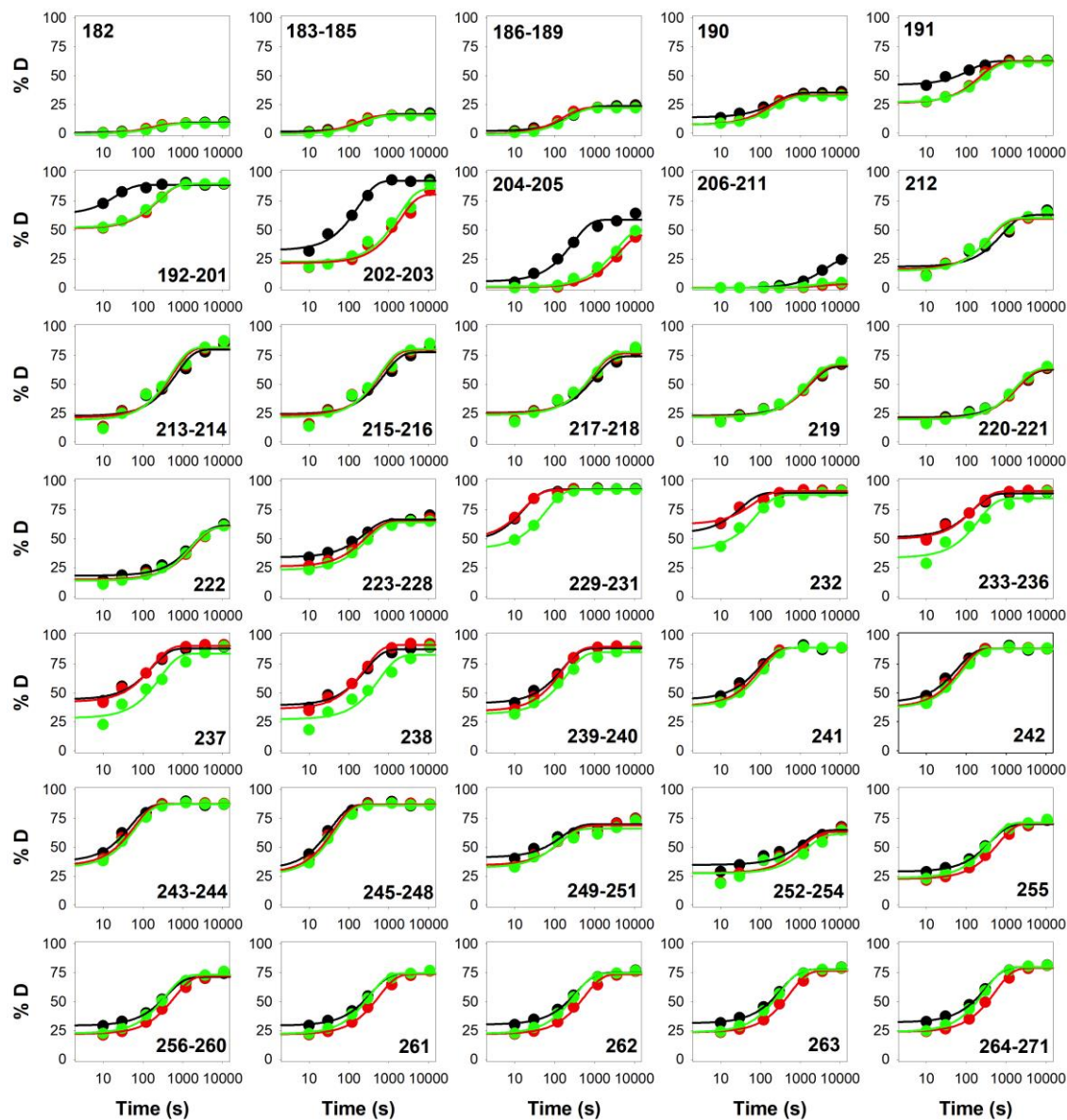


Figure S6. HDX kinetics for 39 non-overlapping and non-redundant peptides of NQO1 upon FAD and dicoumarol binding. Plots showing percentage of deuteration as a function of time. Peptide limits are shown in each graph. These analyses are meant to be compared with those displayed in Figures S7-S9. Kinetic analyses can be found in Table S2.

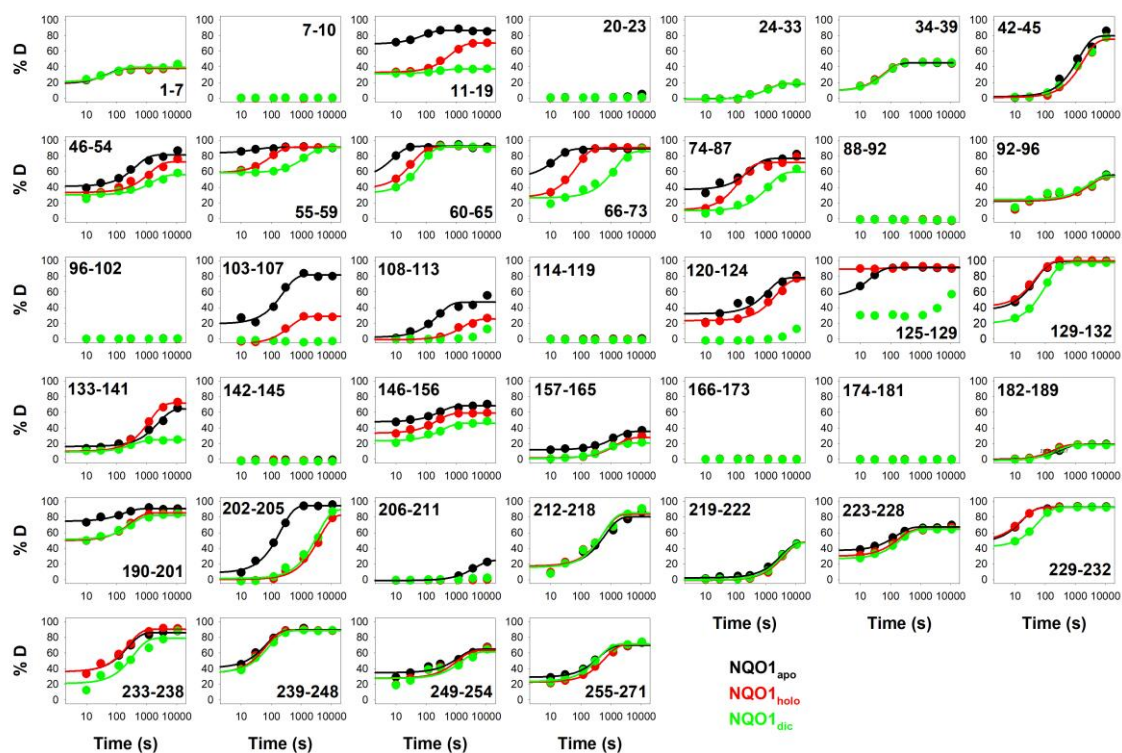


Figure S8. Specific HDX kinetics for 39 peptides of NQO1_{apo}. A) Plots of the amplitudes for the burst- and slow-phase in HDX for peptides (upper panel) and rate constant for the slow phase (lower panel) for peptides with at least 20% D after 3 h. The elements of secondary structure along the protein sequence are also indicated. Note that this analysis for the 39 experimental peptides (Table S2) show little differences when compared with those carried out with NQO1 segments (Table S1 and Figure 3).

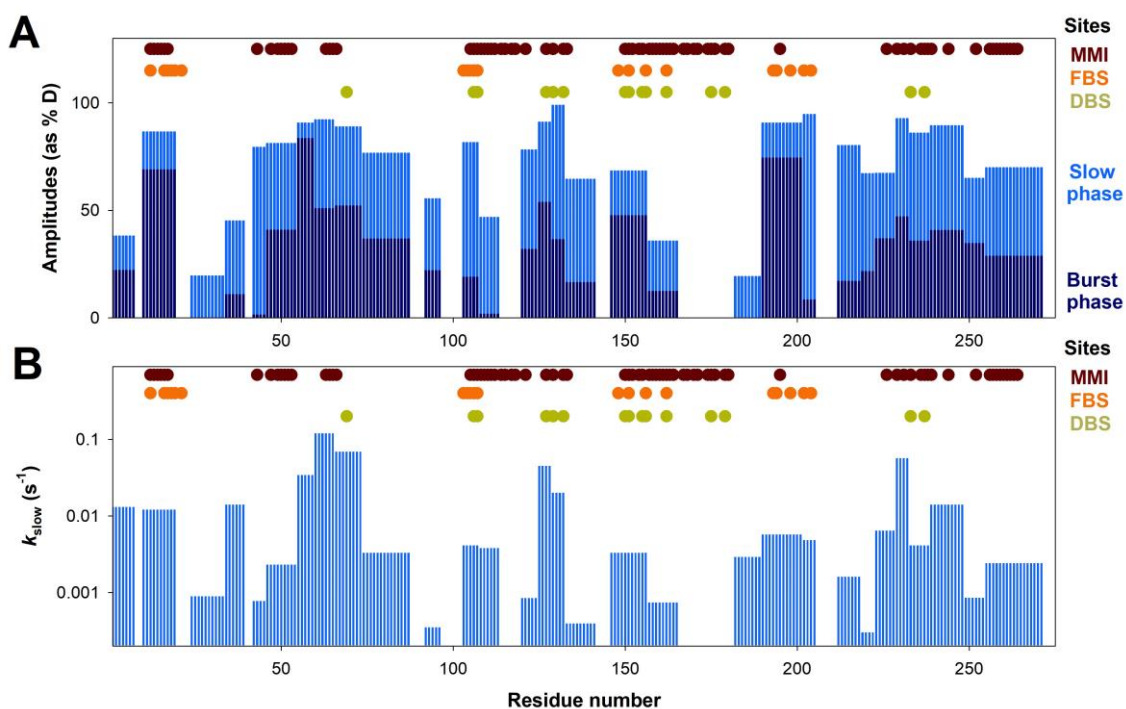


Figure S9. Changes in HDX kinetics for 39 peptides of NQO1 upon binding FAD and dicoumarol as changes in %D_{av} ($\Delta\%D_{av}$). A) $\Delta\%D_{av}$ for the 105 segments upon binding FAD (NQO1_{holo}) and dicoumarol (NQO1_{dic}) using of NQO1_{apo} as a reference (see Figure 6 for details). B) Representation of ($\Delta\%D_{av}$) onto the structure of NQO1 (using PDB code 2F10). The upper row shows the results for $\Delta\%D_{av}$ for NQO1_{holo} and lower row represents NQO1_{dic}. Different panels in each row show results for residues involved in the FBS, DBS or MMI. Note that this analysis for 39 experimental peptides (Table S2) shows little differences with those data carried out with NQO1 segments (Table S1 and Figure 6).

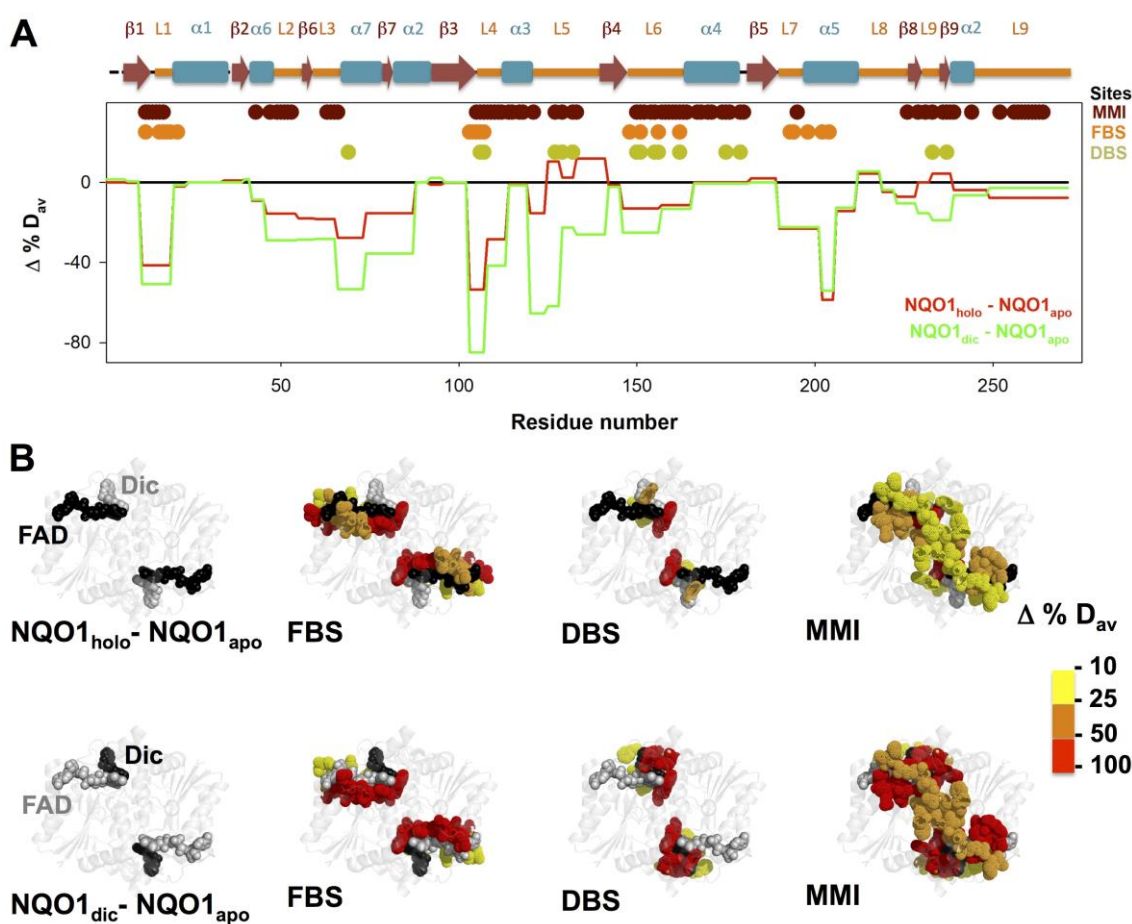
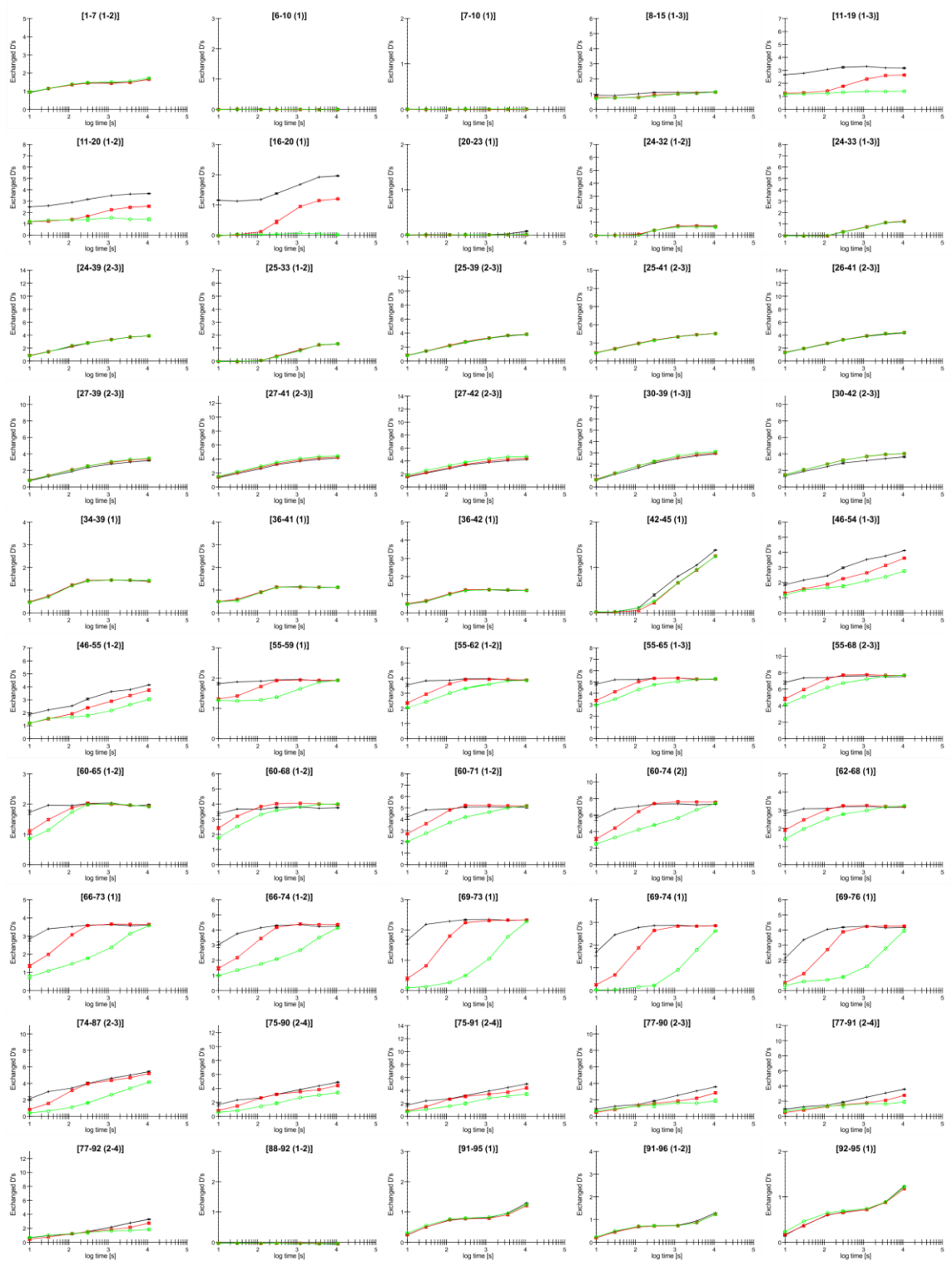
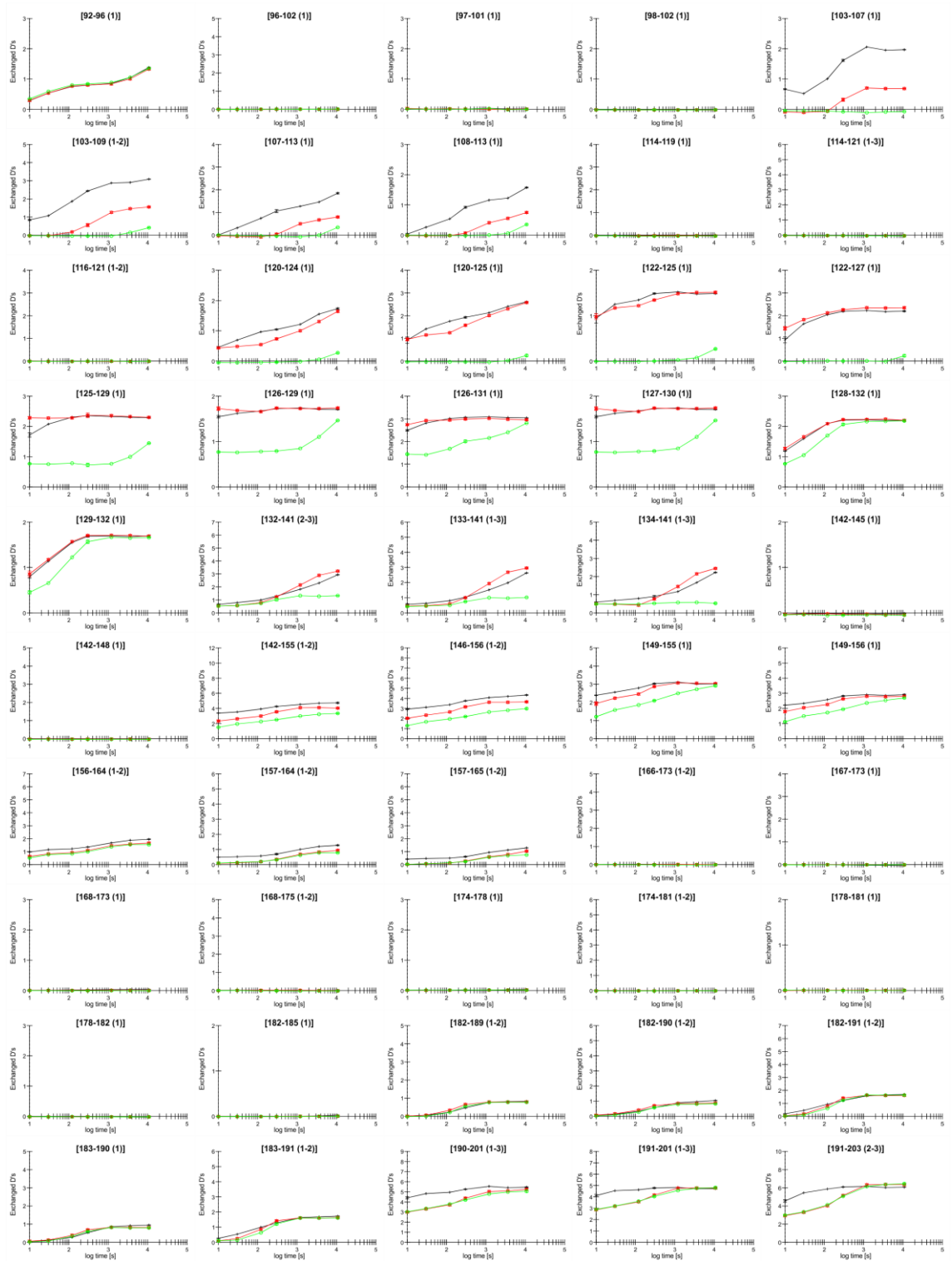


Figure S10 (three pages). HDX kinetics for all peptides detected in HDX-MS experiment. Each peptide is represented by one deuterium uptake plot where number of retained deuterons is plotted as a functions of time. Black stands for NQO1_{apo}, red for NQO1_{holo} and green for NQO1_{dic}. Times points followed during experiment were 10 s, 30 s, 2 min, 5 min, 20 min, 1 h and 3 h. Labeling and analysis at 10 s, 5 min and 3 h was replicated and the data are shown as average values with standard deviation (error bars at these points). Peptide limits are shown at the top of each graph together with the range or charge states that were detected for the peptide.





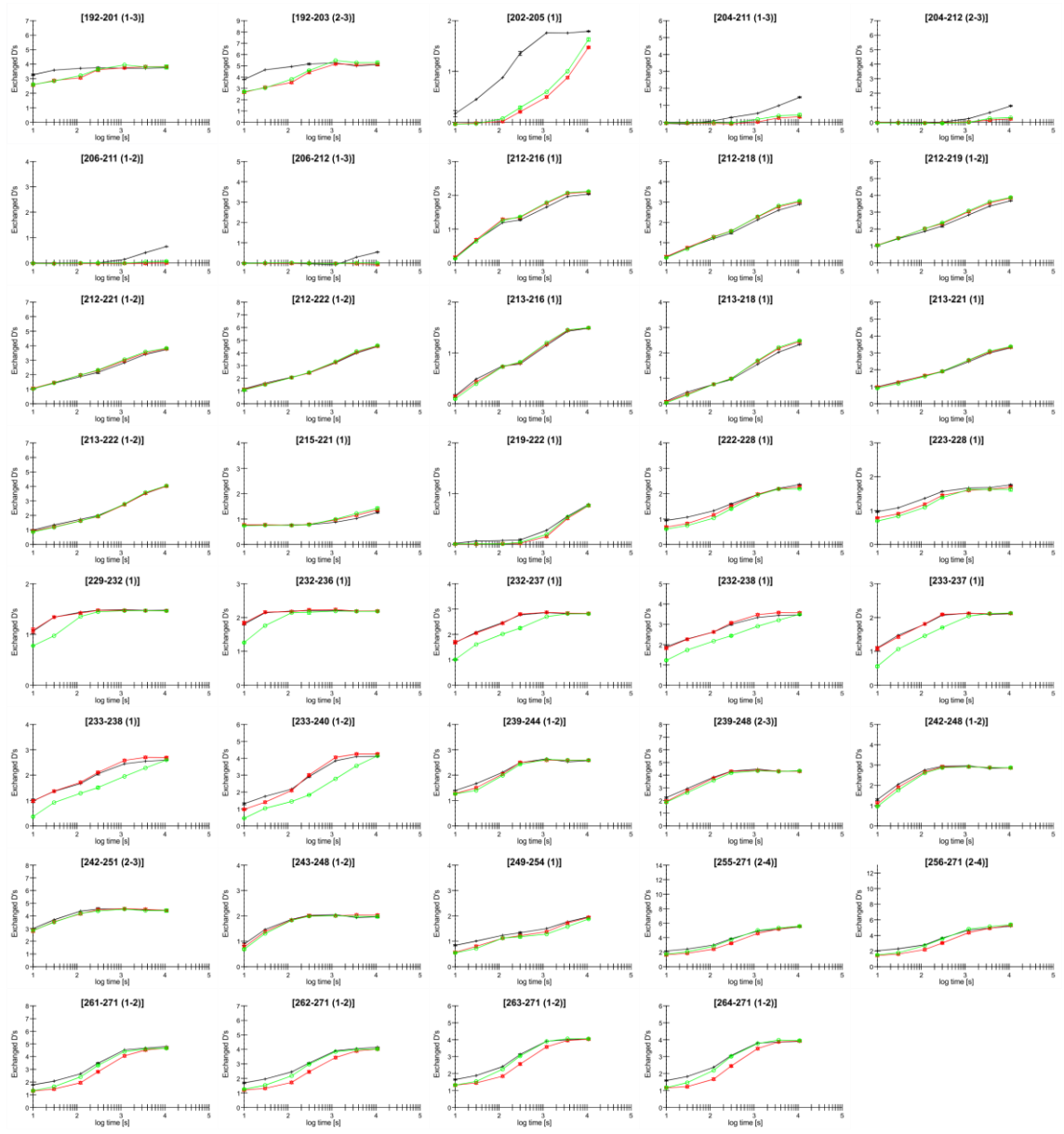


Table S1. Kinetic parameters for fitting of HDX kinetics to a three-parameter exponential function for NQO1 segments. *SLNE* indicates *slow, little or no exchange*.

Segment	NQO1 protein	A _{burst} (%D)	A _{slow} (%D)	k _{slow} (s ⁻¹)	R ²
1-5	NQO1 _{apo}	22.3±2.7	15.8±2.8	1.2±0.6 · 10 ⁻²	0.914
	NQO1 _{holo}	23.0±2.8	15.0±2.8	1.2±0.6 · 10 ⁻²	0.898
	NQO1 _{dic}	23.5±2.6	16.2±2.7	1.0±0.5 · 10 ⁻²	0.912
6	NQO1 _{apo}	8.8±1.3	7.0±1.3	1.5±0.8 · 10 ⁻²	0.916
	NQO1 _{holo}	9.6±1.2	6.3±1.2	1.2±0.7 · 10 ⁻²	0.893
	NQO1 _{dic}	9.5±1.2	7.0±1.2	1.1±0.5 · 10 ⁻²	0.912
7	NQO1 _{apo}	5.2±0.7	4.0±0.7	1.4±0.7 · 10 ⁻²	0.915
	NQO1 _{holo}	5.5±0.7	3.7±0.7	1.2±0.7 · 10 ⁻²	0.893
	NQO1 _{dic}	5.6±0.6	4.1±0.6	1.0±0.4 · 10 ⁻²	0.921
8-10	NQO1 _{apo}	6.1±0.1	1.7±0.1	7.7±1.9 · 10 ⁻³	0.973
	NQO1 _{holo}	5.3±0.2	2.3±0.2	1.9±0.7 · 10 ⁻³	0.957
	NQO1 _{dic}	5.0±0.2	2.7±0.3	1.6±0.5 · 10 ⁻³	0.966
11-15	NQO1 _{apo}	51.0±0.3	15.9±0.4	6.0±0.4 · 10 ⁻³	0.998
	NQO1 _{holo}	28.1±0.7	25.5±1.0	1.5±0.2 · 10 ⁻³	0.994
	NQO1 _{dic}	27.5±0.4	7.6±0.5	2.7±0.6 · 10 ⁻³	0.983
16-19	NQO1 _{apo}	57.4±1.0	26.0±1.3	1.9±0.3 · 10 ⁻³	0.990
	NQO1 _{holo}	14.6±0.8	42.8±1.1	1.5±0.1 · 10 ⁻³	0.997
	NQO1 _{dic}	15.4±0.7	3.6±0.8	5.2±3.2 · 10 ⁻³	0.845
20	NQO1 _{apo}	28.7±0.6	18.5±0.9	1.0±0.2 · 10 ⁻³	0.990
	NQO1 _{holo}	4.5±0.5	24.5±0.6	1.5±0.1 · 10 ⁻³	0.997
	NQO1 _{dic}	5.2±0.6	1.7±0.6	1.0±1.1 · 10 ⁻²	0.695
21-23	NQO1 _{apo}	SLNE			
	NQO1 _{holo}	SNLE			
	NQO1 _{dic}	SNLE			
24	NQO1 _{apo}	1.7±0.7	17.0±0.8	1.7±0.3 · 10 ⁻³	0.990

	NQO1 _{holo}	1.8±0.6	16.9±0.8	1.8±0.3 ·10 ⁻³	0.992
	NQO1 _{dic}	1.7±0.7	16.4±0.8	1.8±0.3 ·10 ⁻³	0.989
25	NQO1 _{apo}	3.7±1.0	19.5±1.3	1.9±0.4 ·10 ⁻³	0.983
	NQO1 _{holo}	3.7±1.0	19.5±1.3	1.9±0.4 ·10 ⁻³	0.984
	NQO1 _{dic}	3.8±1.0	19.2±1.3	1.8±0.4 ·10 ⁻³	0.982
26	NQO1 _{apo}	4.6±1.2	20.0±1.5	2.2±0.5 ·10 ⁻³	0.979
	NQO1 _{holo}	4.7±1.2	20.1±1.4	2.2±0.5 ·10 ⁻³	0.980
	NQO1 _{dic}	4.7±1.2	19.8±1.5	2.1±0.5 ·10 ⁻³	0.977
27-29	NQO1 _{apo}	6.9±1.5	21.2±1.8	2.9±0.5 ·10 ⁻³	0.974
	NQO1 _{holo}	7.3±1.5	21.5±1.8	3.0±0.7 ·10 ⁻³	0.975
	NQO1 _{dic}	7.4±1.5	21.6±1.9	2.9±0.7 ·10 ⁻³	0.973
30-32	NQO1 _{apo}	8.3±1.7	23.1±2.1	3.4±0.9 ·10 ⁻³	0.970
	NQO1 _{holo}	9.0±1.8	23.7±2.1	3.5±0.9 ·10 ⁻³	0.972
	NQO1 _{dic}	9.1±1.8	24.1±2.2	3.5±0.9 ·10 ⁻³	0.971
33	NQO1 _{apo}	9.5±2.0	24.4±2.4	3.5±1.0 ·10 ⁻³	0.965
	NQO1 _{holo}	10.3±2.1	25.7±2.5	3.5±1.0 ·10 ⁻³	0.964
	NQO1 _{dic}	10.4±2.1	25.7±2.3	3.5±1.0 ·10 ⁻³	0.963
34-35	NQO1 _{apo}	12.3±2.1	27.8±2.3	6.4±1.5 ·10 ⁻³	0.975
	NQO1 _{holo}	13.0±2.1	28.6±2.4	6.7±1.5 ·10 ⁻³	0.976
	NQO1 _{dic}	12.9±2.2	29.4±2.5	6.4±1.5 ·10 ⁻³	0.974
36-39	NQO1 _{apo}	12.5±1.5	27.4±1.6	7.5±1.2 ·10 ⁻³	0.988
	NQO1 _{holo}	13.1±1.5	27.9±1.7	7.9±1.3 ·10 ⁻³	0.987
	NQO1 _{dic}	12.9±1.6	28.6±1.7	7.3±1.2 ·10 ⁻³	0.988
40-41	NQO1 _{apo}	12.6 ±1.4	26.7±1.5	8.3±1.3 ·10 ⁻³	0.988
	NQO1 _{holo}	13.3±1.5	27.1±1.6	8.4±1.4 ·10 ⁻³	0.988
	NQO1 _{dic}	13.3±1.4	27.7±1.5	7.9±1.2 ·10 ⁻³	0.989
42	NQO1 _{apo}	9.5±3.4	45.7±4.6	1.4±0.5 ·10 ⁻³	0.961
	NQO1 _{holo}	10.8±2.6	43.3±3.8	1.0±0.3 ·10 ⁻³	0.971
	NQO1 _{dic}	11.3±2.7	42.9±3.9	1.1±0.3 ·10 ⁻³	0.969

43-45	NQO1 _{apo}	1.6±3.6	77.8±6.7	7.7±1.8·10 ⁻⁴	0.987
	NQO1 _{holo}	0.6±2.7	74.4±4.7	5.4±1.1·10 ⁻⁴	0.987
	NQO1 _{dic}	2.0±2.3	72.2±4.2	5.7±1.0·10 ⁻⁴	0.988
46-54	NQO1 _{apo}	40.4±3.1	39.9±3.8	2.5±0.8·10 ⁻³	0.966
	NQO1 _{holo}	31.1±3.6	40.2±5.1	1.1±0.5·10 ⁻³	0.940
	NQO1 _{dic}	30.0±2.1	28.4±3.9	5.4±2.3·10 ⁻⁴	0.939
55	NQO1 _{apo}	75.9±1.5	11.6±1.7	6.7±2.7·10 ⁻³	0.930
	NQO1 _{holo}	50.0±1.7	35.7±1.8	1.0±0.1·10 ⁻²	0.992
	NQO1 _{dic}	50.8±2.7	31.0±3.4	2.1±0.8·10 ⁻³	0.954
56-59	NQO1 _{apo}	76.3±4.9	13.1±4.8	6.5±3.1·10 ⁻²	0.898
	NQO1 _{holo}	53.8±1.2	36.1±1.2	1.4±0.1·10 ⁻²	0.997
	NQO1 _{dic}	54.5±2.7	32.1±3.2	2.8±0.9·10 ⁻³	0.963
60-61	NQO1 _{apo}	65.2±8.8	24.9±8.7	8.1±3.2·10 ⁻²	0.938
	NQO1 _{holo}	44.0±2.8	47.7±2.7	2.2±0.3·10 ⁻²	0.993
	NQO1 _{dic}	40.9±3.6	47.1±3.8	8.7±2.0·10 ⁻³	0.978
62	NQO1 _{apo}	66.0±8.6	24.2±8.5	8.0±3.2·10 ⁻²	0.938
	NQO1 _{holo}	44.4±2.8	47.5±2.8	2.2±0.3·10 ⁻²	0.993
	NQO1 _{dic}	40.9±3.9	47.3±4.1	8.7±2.1·10 ⁻³	0.974
63-65	NQO1 _{apo}	65.2±8.9	25.4±8.8	8.0±3.2·10 ⁻²	0.938
	NQO1 _{holo}	43.9±2.9	48.8±2.9	2.2±0.3·10 ⁻²	0.993
	NQO1 _{dic}	39.8±4.0	49.1±4.2	9.2±2.2·10 ⁻³	0.975
66-68	NQO1 _{apo}	61.8±5.5	27.9±5.5	6.2±1.6·10 ⁻²	0.966
	NQO1 _{holo}	39.5±2.4	53.0±2.4	1.6±0.2·10 ⁻²	0.995
	NQO1 _{dic}	36.6±5.9	47.6±6.9	4.0±1.7·10 ⁻³	0.926
69-71	NQO1 _{apo}	39.5±4.6	46.4±4.6	5.8±0.8·10 ⁻²	0.991
	NQO1 _{holo}	15.7±1.0	71.3±1.0	1.1±0.1·10 ⁻²	0.999
	NQO1 _{dic}	18.0±2.5	64.7±4.9	4.7±1.0·10 ⁻⁴	0.982
72-73	NQO1 _{apo}	37.2±4.6	48.2±4.5	5.8±0.7·10 ⁻²	0.991
	NQO1 _{holo}	11.0±1.5	75.1±1.5	1.1±0.1·10 ⁻²	0.998

	NQO1 _{dic}	14.2±2.2	68.1±4.5	4.3±0.8·10 ⁻⁴	0.968
74	NQO1 _{apo}	33.1±6.7	46.9±6.7	4.3±1.0·10 ⁻²	0.975
	NQO1 _{holo}	11.5±1.2	69.9±1.3	9.1±0.5·10 ⁻³	0.999
	NQO1 _{dic}	14.5±2.0	61.5±4.1	4.0±0.8·10 ⁻⁴	0.986
75-76	NQO1 _{apo}	30.2±4.3	30.3±4.8	5.9±2.6·10 ⁻³	0.914
	NQO1 _{holo}	7.2±3.0	50.4±3.2	7.4±1.3·10 ⁻³	0.985
	NQO1 _{dic}	9.9±2.0	40.7±3.7	5.4±1.5·10 ⁻⁴	0.975
77-87	NQO1 _{apo}	22.2±2.6	31.1±3.7	1.2±0.5·10 ⁻³	0.946
	NQO1 _{holo}	9.0±4.4	33.4±5.0	5.2±2.2·10 ⁻³	0.922
	NQO1 _{dic}	9.8±2.1	23.5±2.7	2.0±0.8·10 ⁻³	0.951
88-90	NQO1 _{apo}	10.9±1.5	18.7±2.3	1.0±0.4·10 ⁻³	0.946
	NQO1 _{holo}	5.0±2.6	17.2±3.0	4.6±2.3·10 ⁻³	0.894
	NQO1 _{dic}	5.4±1.2	11.9±1.4	3.5±1.3·10 ⁻³	0.948
91	NQO1 _{apo}	13.5±2.7	21.2±5.3	4.9±3.6·10 ⁻⁴	0.831
	NQO1 _{holo}	6.6±4.5	19.2±5.0	6.3±4.5·10 ⁻³	0.803
	NQO1 _{dic}	7.9±3.8	16.6±4.3	6.0±4.3·10 ⁻³	0.805
92	NQO1 _{apo}	17.3±3.9	30.0±8.8	3.6±3.0·10 ⁻⁴	0.803
	NQO1 _{holo}	17.4±4.0	27.0±8.6	3.8±3.5·10 ⁻⁴	0.769
	NQO1 _{dic}	19.2±3.8	26.1±8.3	3.3±3.1·10 ⁻⁴	0.763
93-95	NQO1 _{apo}	22.0±5.0	37.8±11.7	3.4±2.9·10 ⁻⁴	0.791
	NQO1 _{holo}	22.2±5.0	34.2±11.1	3.6±3.4·10 ⁻⁴	0.764
	NQO1 _{dic}	24.5±4.8	34.0±11.7	3.2±3.0·10 ⁻⁴	0.764
96	NQO1 _{apo}	14.0±2.8	22.0±6.6	3.2±2.7·10 ⁻⁴	0.803
	NQO1 _{holo}	14.2±2.8	20.4±7.1	3.0±2.8·10 ⁻⁴	0.772
	NQO1 _{dic}	15.3±2.7	19.9±7.1	2.9±2.8·10 ⁻⁴	0.770
97	NQO1 _{apo}	SLNE			
	NQO1 _{holo}	SLNE			
	NQO1 _{dic}	SLNE			
98-101	NQO1 _{apo}	SLNE			

	NQO1 _{holo}	SLNE			
	NQO1 _{dic}	SLNE			
102	NQO1 _{apo}	SLNE			
	NQO1 _{holo}	SLNE			
	NQO1 _{dic}	SLNE			
103-106	NQO1 _{apo}	18.9±2.0	58.3±2.3	4.5±0.5·10 ⁻³	0.994
	NQO1 _{holo}	-3.3±1.1	35.0±1.4	2.0±0.3·10 ⁻³	0.994
	NQO1 _{dic}	SLNE			
107	NQO1 _{apo}	13.8±2.0	54.7±2.3	4.4±0.5·10 ⁻³	0.994
	NQO1 _{holo}	-2.6±0.9	31.8±1.2	1.6±0.2·10 ⁻³	0.995
	NQO1 _{dic}	SLNE			
108-109	NQO1 _{apo}	12.2±3.9	42.8±4.6	3.6±1.2·10 ⁻³	0.958
	NQO1 _{holo}	-1.4±0.9	29.3±1.4	9.7±1.5·10 ⁻⁴	0.991
	NQO1 _{dic}	SLNE			
110-113	NQO1 _{apo}	1.8±5.3	45.4±6.2	4.1±1.6·10 ⁻³	0.934
	NQO1 _{holo}	-1.1±1.1	25.9±1.9	6.4±1.5·10 ⁻³	0.980
	NQO1 _{dic}	SLNE			
114-115	NQO1 _{apo}	SLNE			
	NQO1 _{holo}	SLNE			
	NQO1 _{dic}	SLNE			
116-119	NQO1 _{apo}	SLNE			
	NQO1 _{holo}	SLNE			
	NQO1 _{dic}	SLNE			
120-121	NQO1 _{apo}	17.2±3.9	24.4±4.7	3.2±1.9·10 ⁻³	0.876
	NQO1 _{holo}	16.1±1.4	27.2±2.5	6.3±1.8·10 ⁻⁴	0.972
	NQO1 _{dic}	SLNE			
122-124	NQO1 _{apo}	41.2±6.6	43.1±7.0	9.8±4.5·10 ⁻³	0.919
	NQO1 _{holo}	49.3±3.5	36.4±4.4	2.2±0.9·10 ⁻³	0.946
	NQO1 _{dic}	SLNE			

125	NQO1 _{apo}	38.7±8.9	50.2±8.8	3.2±1.1·10 ⁻²	0.958
	NQO1 _{holo}	65.2±2.4	26.7±2.8	4.1±1.2·10 ⁻³	0.961
	NQO1 _{dic}	SLNE			
126	NQO1 _{apo}	57.6±3.4	35.3±3.4	4.0±0.7·10 ⁻²	0.988
	NQO1 _{holo}	84.1±1.0	10.3±1.1	9.6±2.8·10 ⁻³	0.965
	NQO1 _{dic}	31.4±0.7	41.3±7.3	1.6±0.4·10 ⁻⁴	0.991
127	NQO1 _{apo}	63.8±3.3	29.4±3.3	3.8±0.7·10 ⁻²	0.984
	NQO1 _{holo}	86.7±0.7	8.0±0.8	7.4±2.0·10 ⁻²	0.967
	NQO1 _{dic}	33.9±0.5	45.3±6.0	1.1±0.3·10 ⁻⁴	0.995
128	NQO1 _{apo}	67.7±2.3	26.0±2.3	3.0±0.5·10 ⁻²	0.988
	NQO1 _{holo}	84.3±0.8	10.0±0.8	1.0±0.2·10 ⁻²	0.977
	NQO1 _{dic}	43.4±2.4	37.2±6.5	2.8±1.4·10 ⁻⁴	0.934
129	NQO1 _{apo}	62.1±2.3	32.6±2.3	2.5±0.4·10 ⁻²	0.992
	NQO1 _{holo}	76.5±1.2	18.8±1.2	1.4±0.2·10 ⁻²	0.989
	NQO1 _{dic}	36.6±5.8	36.2±6.9	3.5±2.0·10 ⁻³	0.879
130	NQO1 _{apo}	57.5±2.2	38.2±2.2	2.3±0.3·10 ⁻²	0.994
	NQO1 _{holo}	66.9±1.8	29.0±1.8	1.8±0.3·10 ⁻²	0.991
	NQO1 _{dic}	34.2±4.7	47.9±5.3	5.7±1.7·10 ⁻³	0.957
131	NQO1 _{apo}	46.8±2.4	49.4±2.4	2.3±0.3·10 ⁻²	0.996
	NQO1 _{holo}	53.5±2.6	42.6±2.6	2.2±0.3·10 ⁻²	0.993
	NQO1 _{dic}	29.2±2.2	60.7±2.3	7.8±0.8·10 ⁻³	0.995
132	NQO1 _{apo}	37.4±4.1	51.0±4.2	1.5±0.3·10 ⁻²	0.982
	NQO1 _{holo}	42.2±3.8	48.5±3.9	1.1±0.3·10 ⁻²	0.979
	NQO1 _{dic}	21.3±0.6	62.2±0.6	8.9±0.3·10 ⁻³	0.999
133	NQO1 _{apo}	18.0±2.2	48.0±4.5	4.3±1.2·10 ⁻⁴	0.973
	NQO1 _{holo}	11.6±1.1	61.4±1.7	7.9±0.7·10 ⁻⁴	0.997
	NQO1 _{dic}	10.5±0.6	17.2±0.8	3.0±0.4·10 ⁻³	0.994
134-141	NQO1 _{apo}	18.6±1.8	46.7±3.9	3.7±0.9·10 ⁻⁴	0.980
	NQO1 _{holo}	11.8±1.0	59.6±1.7	7.0±0.6·10 ⁻⁴	0.997

	NQO1 _{dic}	11.6±0.5	11.7±0.6	2.9±0.5·10 ⁻³	0.991
142-145	NQO1 _{apo}	5.1±0.2	2.5±0.3	5.7±1.6·10 ⁻³	0.961
	NQO1 _{holo}	3.6±0.2	3.1±0.2	4.6±0.9·10 ⁻³	0.981
	NQO1 _{dic}	2.6±0.3	2.7±0.4	3.4±1.4·10 ⁻³	0.934
146-148	NQO1 _{apo}	22.6±0.6	9.3±0.6	3.6±0.7·10 ⁻³	0.982
	NQO1 _{holo}	15.5±0.4	12.0±0.5	4.1±0.4·10 ⁻³	0.993
	NQO1 _{dic}	10.8±1.0	10.6±1.2	2.8±1.0·10 ⁻³	0.952
149-155	NQO1 _{apo}	56.9±0.6	19.1±0.6	6.3±0.6·10 ⁻³	0.998
	NQO1 _{holo}	44.8±1.3	27.4±1.5	5.2±0.8·10 ⁻³	0.989
	NQO1 _{dic}	31.5±3.1	31.5±3.7	2.7±1.0·10 ⁻³	0.948
156	NQO1 _{apo}	44.0±1.1	19.2±1.3	3.6±0.7·10 ⁻³	0.982
	NQO1 _{holo}	33.2±1.2	24.1±1.4	3.9±0.7·10 ⁻³	0.987
	NQO1 _{dic}	24.5±2.3	26.5±2.8	2.3±0.8·10 ⁻³	0.959
157-164	NQO1 _{apo}	17.3±0.6	21.7±1.0	9.3±1.4·10 ⁻⁴	0.992
	NQO1 _{holo}	6.6±1.1	23.5±1.6	1.2±0.3·10 ⁻³	0.982
	NQO1 _{dic}	5.9±0.7	20.5±1.0	1.4±0.2·10 ⁻³	0.991
165	NQO1 _{apo}	12.5±0.8	23.2±1.3	7.4±1.3·10 ⁻⁴	0.989
	NQO1 _{holo}	1.5±1.3	26.3±2.2	6.7±1.8·10 ⁻⁴	0.974
	NQO1 _{dic}	0.8±0.4	20.0±0.5	1.2±0.1·10 ⁻³	0.998
166	NQO1 _{apo}	SLNE			
	NQO1 _{holo}	SLNE			
	NQO1 _{dic}	SLNE			
167	NQO1 _{apo}	SLNE			
	NQO1 _{holo}	SLNE			
	NQO1 _{dic}	SLNE			
168-173	NQO1 _{apo}	SLNE			
	NQO1 _{holo}	SLNE			
	NQO1 _{dic}	SLNE			
174-175	NQO1 _{apo}	SLNE			

	NQO1 _{holo}	SLNE			
	NQO1 _{dic}	SLNE			
176-177	NQO1 _{apo}	SLNE			
	NQO1 _{holo}	SLNE			
	NQO1 _{dic}	SLNE			
178	NQO1 _{apo}	SLNE			
	NQO1 _{holo}	SLNE			
	NQO1 _{dic}	SLNE			
179-181	NQO1 _{apo}	SLNE			
	NQO1 _{holo}	SLNE			
	NQO1 _{dic}	SLNE			
182	NQO1 _{apo}	0.6±0.4	8.8±0.5	3.2±0.5 ·10 ⁻³	0.990
	NQO1 _{holo}	-0.3±0.2	9.1±0.2	5.7±0.3 ·10 ⁻³	0.999
	NQO1 _{dic}	-0.5±0.2	9.1±0.2	4.2±0.3 ·10 ⁻³	0.998
183-185	NQO1 _{apo}	1.4±0.6	15.2±0.7	3.4±0.5 ·10 ⁻³	0.992
	NQO1 _{holo}	-0.4±0.2	16.0±0.3	5.8±0.3 ·10 ⁻³	0.999
	NQO1 _{dic}	-0.7±0.3	16.0±0.3	4.4±0.2 ·10 ⁻³	0.999
186-189	NQO1 _{apo}	1.9±0.7	21.7±0.9	3.6±0.4 ·10 ⁻³	0.994
	NQO1 _{holo}	-0.5±0.3	22.9±0.4	5.9±0.3 ·10 ⁻³	0.999
	NQO1 _{dic}	-0.9±0.7	22.9±0.5	4.4±0.2 ·10 ⁻³	0.998
190	NQO1 _{apo}	13.9±0.9	21.4±1.1	4.0±0.6 ·10 ⁻³	0.991
	NQO1 _{holo}	7.5±0.3	25.5±0.3	5.4±0.2 ·10 ⁻³	0.999
	NQO1 _{dic}	7.5±0.2	24.9±0.2	4.3±0.1 ·10 ⁻³	0.999
191	NQO1 _{apo}	42.4±1.9	20.6±2.1	7.8±2.2 ·10 ⁻³	0.965
	NQO1 _{holo}	26.3±0.5	35.9±0.5	4.5±0.2 ·10 ⁻³	0.999
	NQO1 _{dic}	27.0±0.8	34.5±0.9	3.8±0.3 ·10 ⁻³	0.997
192-201	NQO1 _{apo}	63.5±5.1	25.7±5.1	4.6±1.4 ·10 ⁻²	0.955
	NQO1 _{holo}	51.3±1.2	38.6±1.4	3.9±0.4 ·10 ⁻³	0.995
	NQO1 _{dic}	52.1±1.0	37.9±1.2	4.1±0.4 ·10 ⁻³	0.997

202-203	NQO1 _{apo}	32.4±3.0	60.3±3.4	5.7±0.9 ·10 ⁻³	0.988
	NQO1 _{holo}	21.4±3.4	59.5±6.4	5.2±1.7 ·10 ⁻⁴	0.962
	NQO1 _{dic}	22.4±3.9	63.5±7.1	5.5±1.9 ·10 ⁻⁴	0.958
204-205	NQO1 _{apo}	5.3±3.3	53.5±4.0	3.4±0.8 ·10 ⁻³	0.979
	NQO1 _{holo}	0.4±0.9	46.1±2.6	2.5±0.4 ·10 ⁻⁴	0.994
	NQO1 _{dic}	1.0±1.2	49.7±3.1	2.9±0.5 ·10 ⁻⁴	0.991
206-211	NQO1 _{apo}	-0.2±0.2	26.9±0.6	2.2±0.1 ·10 ⁻⁴	0.999
	NQO1 _{holo}	-0.1±0.2	3.3±0.6	2.3±1.0 ·10 ⁻⁴	0.955
	NQO1 _{dic}	-0.2±0.2	5.0±0.5	3.4±1.0 ·10 ⁻⁴	0.973
212	NQO1 _{apo}	18.3±4.3	44.8±6.0	1.2±0.6 ·10 ⁻³	0.933
	NQO1 _{holo}	16.0±4.8	43.6±5.8	2.4±1.1 ·10 ⁻³	0.935
	NQO1 _{dic}	14.8±4.9	45.7±5.9	2.5±1.1 ·10 ⁻³	0.939
213-214	NQO1 _{apo}	22.6±5.4	57.5±7.3	1.4±0.6 ·10 ⁻³	0.939
	NQO1 _{holo}	21.2±5.7	60.5±7.4	1.7±0.7 ·10 ⁻³	0.944
	NQO1 _{dic}	19.1±6.0	63±7.5	1.9±0.8 ·10 ⁻³	0.946
215-216	NQO1 _{apo}	24.2±4.9	53.5±6.8	1.3±0.6 ·10 ⁻³	0.940
	NQO1 _{holo}	23.2±5.1	56.6±6.8	1.5±0.6 ·10 ⁻³	0.946
	NQO1 _{dic}	21.4±5.3	59.2±6.9	1.7±0.7 ·10 ⁻³	0.948
217-218	NQO1 _{apo}	25.2±3.5	49.0±5.3	9.6±3.4 ·10 ⁻⁴	0.957
	NQO1 _{holo}	24.7±3.6	52.2±5.2	1.1±0.4 ·10 ⁻³	0.962
	NQO1 _{dic}	23.5±3.7	54.6±5.3	1.1±0.4 ·10 ⁻³	0.964
219	NQO1 _{apo}	22.9±2.1	42.6±3.8	5.6±1.6 ·10 ⁻⁴	0.973
	NQO1 _{holo}	22.2±2.0	44.6±3.6	5.6±1.4 ·10 ⁻⁴	0.978
	NQO1 _{dic}	21.5±2.1	46.0±3.6	6.3±1.6 ·10 ⁻⁴	0.978
220-221	NQO1 _{apo}	21.2±1.7	41.4±3.3	4.9±1.2 ·10 ⁻⁴	0.979
	NQO1 _{holo}	20.1±4.5	43.5±2.9	4.9±1.0 ·10 ⁻⁴	0.985
	NQO1 _{dic}	19.5±1.6	44.8±3.0	5.4±1.1 ·10 ⁻⁴	0.985
222	NQO1 _{apo}	17.9±1.8	43.3±3.4	5.4±1.3 ·10 ⁻⁴	0.980
	NQO1 _{holo}	14.7±1.7	45.6±3.2	5.4±1.1 ·10 ⁻⁴	0.984

	NQO1 _{dic}	13.6±1.7	46.2±2.9	6.1±1.2 · 10 ⁻⁴	0.986
223-228	NQO1 _{apo}	33.8±2.3	32.9±2.7	3.8±0.9 · 10 ⁻³	0.975
	NQO1 _{holo}	25.9±1.8	39.0±2.2	3.8±0.6 · 10 ⁻³	0.989
	NQO1 _{dic}	23.0±1.3	41.1±1.5	3.4±0.4 · 10 ⁻³	0.995
229-231	NQO1 _{apo}	47.2±4.5	45.5±4.4	5.7±0.8 · 10 ⁻²	0.991
	NQO1 _{holo}	49.7±5.6	42.5±5.5	5.7±1.0 · 10 ⁻²	0.984
	NQO1 _{dic}	41.2±0.6	51.0±0.6	1.7±0.4 · 10 ⁻²	0.999
232	NQO1 _{apo}	54.6±6.6	35.2±6.6	3.0±1.1 · 10 ⁻²	0.950
	NQO1 _{holo}	62.5±4.2	28.8±4.2	1.4±0.6 · 10 ⁻²	0.943
	NQO1 _{dic}	40.5±5.1	47.5±5.2	1.2±0.4 · 10 ⁻²	0.964
233-236	NQO1 _{apo}	51.1±3.1	38.0±3.5	6.6±1.7 · 10 ⁻³	0.970
	NQO1 _{holo}	49.8±2.8	41.4±3.1	6.3±1.3 · 10 ⁻³	0.979
	NQO1 _{dic}	33.4±6.3	51.5±7.2	4.8±1.9 · 10 ⁻³	0.995
237	NQO1 _{apo}	44.4±2.9	44.2±3.2	5.8±1.2 · 10 ⁻³	0.980
	NQO1 _{holo}	42.2±2.6	48.6±2.9	5.8±1.0 · 10 ⁻³	0.987
	NQO1 _{dic}	28.4±6.2	55.7±7.3	3.6±1.4 · 10 ⁻³	0.938
238	NQO1 _{apo}	39.3±2.6	48.4±3.1	3.7±0.7 · 10 ⁻³	0.984
	NQO1 _{holo}	36.2±2.6	55.2±3.0	3.9±0.6 · 10 ⁻³	0.989
	NQO1 _{dic}	27.2±6.0	55.6±7.8	1.7±0.8 · 10 ⁻³	0.927
239-240	NQO1 _{apo}	41.1±2.0	47.7±2.3	6.2±0.8 · 10 ⁻³	0.992
	NQO1 _{holo}	34.7±1.7	55.6±1.9	6.4±0.6 · 10 ⁻³	0.996
	NQO1 _{dic}	31.8±3.6	53.4±4.2	5.0±1.0 · 10 ⁻³	0.978
241	NQO1 _{apo}	44.0±2.3	44.8±2.4	1.0±0.2 · 10 ⁻²	0.991
	NQO1 _{holo}	38.7±1.4	50.5±1.4	1.0±0.1 · 10 ⁻²	0.997
	NQO1 _{dic}	38.1±0.7	51.1±0.8	8.4±0.4 · 10 ⁻³	0.999
242	NQO1 _{apo}	41.9±3.2	46.5±3.2	1.6±0.3 · 10 ⁻²	0.988
	NQO1 _{holo}	37.5±2.8	51.0±2.8	1.4±0.2 · 10 ⁻²	0.992
	NQO1 _{dic}	36.7±2.1	51.6±2.2	1.2±0.1 · 10 ⁻²	0.995
243-244	NQO1 _{apo}	37.7±4.2	49.6±4.2	2.0±0.4 · 10 ⁻²	0.985

	NQ01 _{holo}	34.1±3.6	53.7±3.6	$1.6 \pm 0.3 \cdot 10^{-2}$	0.989
	NQ01 _{dic}	32.5±3.0	54.7±3.0	$1.5 \pm 0.2 \cdot 10^{-2}$	0.996
245-248	NQ01 _{apo}	31.1±4.9	55.8±4.8	$2.8 \pm 0.5 \cdot 10^{-2}$	0.988
	NQ01 _{holo}	26.7±4.9	59.5±4.8	$2.4 \pm 0.4 \cdot 10^{-2}$	0.988
	NQ01 _{dic}	26.4±4.3	60.2±4.2	$2.1 \pm 0.4 \cdot 10^{-2}$	0.990
249-251	NQ01 _{apo}	41.2±4.1	28.8±4.5	$6.4 \pm 2.8 \cdot 10^{-3}$	0.917
	NQ01 _{holo}	34.5±4.8	34.4±5.4	$6.1 \pm 2.7 \cdot 10^{-3}$	0.916
	NQ01 _{dic}	32.6±5.3	33.7±5.8	$7.7 \pm 3.7 \cdot 10^{-3}$	0.905
252-254	NQ01 _{apo}	34.8±3.1	30.2±4.9	$8.5 \pm 4.5 \cdot 10^{-4}$	0.910
	NQ01 _{holo}	27.7±4.4	35.7±6.7	$9.0 \pm 5.6 \cdot 10^{-4}$	0.882
	NQ01 _{dic}	27.4±4.7	34.1±7.9	$6.8 \pm 5.1 \cdot 10^{-4}$	0.837
255	NQ01 _{apo}	28.9±1.8	41.0±2.2	$2.4 \pm 0.4 \cdot 10^{-3}$	0.989
	NQ01 _{holo}	22.5±1.8	48.3±2.4	$1.6 \pm 0.3 \cdot 10^{-3}$	0.990
	NQ01 _{dic}	23.3±1.9	48.0±2.3	$2.6 \pm 0.4 \cdot 10^{-3}$	0.991
256-260	NQ01 _{apo}	29.2±1.7	42.1±2.1	$2.4 \pm 0.4 \cdot 10^{-3}$	0.991
	NQ01 _{holo}	21.9±1.9	50.3±2.5	$1.6 \pm 0.3 \cdot 10^{-3}$	0.990
	NQ01 _{dic}	22.5±1.9	50.8±2.3	$2.7 \pm 0.4 \cdot 10^{-3}$	0.992
261	NQ01 _{apo}	29.3±1.4	45.0±1.7	$2.7 \pm 0.3 \cdot 10^{-3}$	0.994
	NQ01 _{holo}	21.6±1.7	52.2±2.2	$1.7 \pm 0.2 \cdot 10^{-3}$	0.993
	NQ01 _{dic}	22.0±1.6	52.6±1.9	$3.0 \pm 0.3 \cdot 10^{-3}$	0.995
262	NQ01 _{apo}	30.2±1.3	44.8±1.6	$2.7 \pm 0.3 \cdot 10^{-3}$	0.995
	NQ01 _{holo}	21.9±1.6	51.9±2.1	$1.8 \pm 0.2 \cdot 10^{-3}$	0.993
	NQ01 _{dic}	22.3±1.4	52.3±1.7	$3.1 \pm 0.3 \cdot 10^{-3}$	0.996
263	NQ01 _{apo}	31.3±1.2	46.6±1.5	$2.9 \pm 0.3 \cdot 10^{-3}$	0.996
	NQ01 _{holo}	23.5±1.6	53.3±2.0	$1.8 \pm 0.2 \cdot 10^{-3}$	0.993
	NQ01 _{dic}	23.5±1.3	54.2±1.5	$3.2 \pm 0.3 \cdot 10^{-3}$	0.997
264-271	NQ01 _{apo}	32.1±1.1	47.9±1.3	$3.1 \pm 0.3 \cdot 10^{-3}$	0.997
	NQ01 _{holo}	23.8±1.5	55.3±1.9	$1.9 \pm 0.2 \cdot 10^{-3}$	0.995
	NQ01 _{dic}	23.9±1.3	56.2±1.6	$3.4 \pm 0.3 \cdot 10^{-3}$	0.997

Table S2. Kinetic parameters for fitting of HDX kinetics to a three-parameter exponential function for 39 experimental peptides covering almost the entire NQO1 sequence. *SLNE* indicates *slow, little or no exchange*. *PF* indicates *poor fitting*.

Peptide	NQO1 protein	A _{burst} (%D)	A _{slow} (%D)	k _{slow} (s ⁻¹)	R ²
1-7	NQO1 _{apo}	22.3±2.7	15.8±2.8	1.3±0.6·10 ⁻²	0.914
	NQO1 _{holo}	23.0±2.8	15.0±2.8	1.2±0.6·10 ⁻²	0.898
	NQO1 _{dic}	23.5±2.6	16.1±2.7	1.0±0.5·10 ⁻²	0.912
7-10	NQO1 _{apo}	SLNE			
	NQO1 _{holo}	SLNE			
	NQO1 _{dic}	SLNE			
11-19	NQO1 _{apo}	69.1±1.7	17.4±1.7	1.2±0.3·10 ⁻²	0.971
	NQO1 _{holo}	32.8±0.8	37.4±1.1	1.4±0.1·10 ⁻³	0.997
	NQO1 _{dic}	31.2±0.2	6.0±0.2	3.4±0.4·10 ⁻³	0.995
20-23	NQO1 _{apo}	SLNE			
	NQO1 _{holo}	SLNE			
	NQO1 _{dic}	SLNE			
24-33	NQO1 _{apo}	-1.3±0.6	19.5±0.9	8.9±1.4·10 ⁻⁴	0.992
	NQO1 _{holo}	-1.6±0.8	20.3±1.2	9.0±1.8·10 ⁻⁴	0.987
	NQO1 _{dic}	-1.5±0.6	19.8±0.9	8.8±1.3·10 ⁻⁴	0.993
34-39	NQO1 _{apo}	11.0±1.1	34.1±1.1	1.4±0.1·10 ⁻²	0.997
	NQO1 _{holo}	10.9±0.9	34.7±0.9	1.4±0.1·10 ⁻²	0.998
	NQO1 _{dic}	10.4±0.3	35.1±0.3	1.3±0.1·10 ⁻²	1.000
42-45	NQO1 _{apo}	1.6±4.2	77.8±6.7	7.7±2.2·10 ⁻⁴	0.973
	NQO1 _{holo}	0.6±2.6	74.4±4.7	5.4±1.1·10 ⁻⁴	0.986
	NQO1 _{dic}	2.0±2.3	72.4±4.2	5.7±1.0·10 ⁻⁴	0.988
46-54	NQO1 _{apo}	41.0±3.2	40.2±3.9	2.3±0.7·10 ⁻³	0.964
	NQO1 _{holo}	33.1±3.3	39.2±5.2	7.9±3.4·10 ⁻⁴	0.939
	NQO1 _{dic}	30.1±2.3	25.7±3.9	6.5±3.1·10 ⁻⁴	0.923
55-59	NQO1 _{apo}	83.6±2.6	7.1±2.6	3.4±2.3·10 ⁻²	0.845

	NQO1 _{holo}	58.2±0.7	32.9±0.7	1.0±0.1·10 ⁻²	0.998
	NQO1 _{dic}	58.4±0.5	32.1±0.7	7.2±0.5·10 ⁻⁴	0.998
60-65	NQO1 _{apo}	51.0±42.8	41.2±42.5	1.2±1.0·10 ⁻¹	0.892
	NQO1 _{holo}	38.1±4.1	53.0±4.1	2.8±0.5·10 ⁻²	0.991
	NQO1 _{dic}	32.0±2.3	59.6±2.3	1.4±0.2·10 ⁻²	0.996
66-73	NQO1 _{apo}	52.3±5.3	36.6±5.2	6.9±1.2·10 ⁻²	0.985
	NQO1 _{holo}	26.9±1.5	63.5±1.5	1.3±0.1·10 ⁻²	0.998
	NQO1 _{dic}	26.3±3.8	59.4±6.2	7.3±2.5·10 ⁻⁴	0.961
74-87	NQO1 _{apo}	36.9±4.6	39.7±5.5	3.3±1.4·10 ⁻³	0.931
	NQO1 _{holo}	10.7±5.1	60.9±5.6	7.0±1.8·10 ⁻³	0.970
	NQO1 _{dic}	9.8±2.8	49.4±4.4	8.1±2.4·10 ⁻⁴	0.971
88-92	NQO1 _{apo}	SLNE			
	NQO1 _{holo}	SLNE			
	NQO1 _{dic}	SLNE			
92-96	NQO1 _{apo}	22.5±4.1	33.2±9.6	3.3±2.7·10 ⁻⁴	0.814
	NQO1 _{holo}	22.9±4.1	30.6±9.9	3.2±2.9·10 ⁻⁴	0.783
	NQO1 _{dic}	24.5±4.0	29.6±9.0	3.5±3.1·10 ⁻⁴	0.790
96-102	NQO1 _{apo}	SLNE			
	NQO1 _{holo}	SLNE			
	NQO1 _{dic}	SLNE			
103-107	NQO1 _{apo}	19.1±3.8	62.5±4.5	4.1±0.8·10 ⁻³	0.981
	NQO1 _{holo}	-6.8±2.3	35.5±2.8	2.4±0.6·10 ⁻³	0.977
	NQO1 _{dic}	SLNE			
108-113	NQO1 _{apo}	1.9±4.8	44.9±5.7	3.8±1.4·10 ⁻³	0.943
	NQO1 _{holo}	-1.2±1.1	26.4±2.0	5.9±1.4·10 ⁻⁴	0.981
	NQO1 _{dic}	SLNE			
114-119	NQO1 _{apo}	---	---	---	---
	NQO1 _{holo}	---	---	---	---
	NQO1 _{dic}	---	---	---	---

120-124	NQ01 _{apo}	32.0±5.2	46.1±8.2	8.4±4.9·10 ⁻⁴	0.893
	NQ01 _{holo}	23.2±2.1	52.8±4.2	4.4±1.0·10 ⁻⁴	0.980
	NQ01 _{dic}	SLNE			
125-129	NQ01 _{apo}	54.0±3.2	37.1±3.2	4.5±0.6·10 ⁻²	0.991
	NQ01 _{holo}	PF			
	NQ01 _{dic}	PF			
129-132	NQ01 _{apo}	36.6±2.9	62.3±2.9	2.0±0.2·10 ⁻²	0.995
	NQ01 _{holo}	40.9±2.6	58.9±2.6	2.0±0.2·10 ⁻²	0.996
	NQ01 _{dic}	19.7±0.5	77.7±0.5	9.2±0.2·10 ⁻³	1.000
133-141	NQ01 _{apo}	16.7±2.0	47.8±4.2	3.9±1.0·10 ⁻⁴	0.977
	NQ01 _{holo}	10.4±0.9	61.5±1.5	8.0±0.6·10 ⁻⁴	0.998
	NQ01 _{dic}	9.6±0.7	15.2±0.9	2.6±0.5·10 ⁻³	0.987
142-145	NQ01 _{apo}	SLNE			
	NQ01 _{holo}	SLNE			
	NQ01 _{dic}	SLNE			
146-156	NQ01 _{apo}	47.8±1.2	20.6±1.4	3.3±0.7·10 ⁻³	0.982
	NQ01 _{holo}	33.2±0.9	25.7±1.1	4.1±0.5·10 ⁻³	0.993
	NQ01 _{dic}	23.3±2.1	22.8±2.6	2.9±1.0·10 ⁻³	0.954
157-165	NQ01 _{apo}	12.5±0.8	23.2±1.3	7.4±1.3·10 ⁻⁴	0.989
	NQ01 _{holo}	1.5±1.3	26.2±2.2	6.7±1.8·10 ⁻⁴	0.975
	NQ01 _{dic}	0.8±0.4	20.0±0.5	1.2±0.1·10 ⁻³	0.998
166-173	NQ01 _{apo}	SLNE			
	NQ01 _{holo}	SLNE			
	NQ01 _{dic}	SLNE			
174-181	NQ01 _{apo}	SLNE			
	NQ01 _{holo}	SLNE			
	NQ01 _{dic}	SLNE			
182-189	NQ01 _{apo}	-0.2±0.2	19.2±0.3	2.9±0.1·10 ⁻³	0.999

	NQO1 _{holo}	-1.1±0.4	19.8±0.5	5.4±0.4·10 ⁻³	0.998
	NQO1 _{dic}	-1.8±0.6	19.9±0.7	4.1±0.4·10 ⁻³	0.996
190-201	NQO1 _{apo}	74.6±1.9	16.1±2.1	5.7±2.1·10 ⁻³	0.939
	NQO1 _{holo}	49.8±1.3	35.4±1.5	3.4±0.4·10 ⁻³	0.993
	NQO1 _{dic}	51.2±1.7	31.1±2.0	3.2±0.6·10 ⁻³	0.984
202-205	NQO1 _{apo}	8.6±2.5	86.0±2.9	4.8±0.5·10 ⁻³	0.996
	NQO1 _{holo}	0.2±2.1	82.7±6.1	2.7±0.5·10 ⁻⁴	0.989
	NQO1 _{dic}	1.3±2.9	88.2±7.6	2.9±0.7·10 ⁻⁴	0.982
206-211	NQO1 _{apo}	-1.3±0.3	25.9±0.8	2.4±0.2·10 ⁻⁴	0.998
	NQO1 _{holo}	SLNE			
	NQO1 _{dic}	SLNE			
212-218	NQO1 _{apo}	17.2±5.5	63.0±7.3	1.6±0.6·10 ⁻³	0.949
	NQO1 _{holo}	17.1±5.9	66.7±7.6	1.8±0.7·10 ⁻³	0.950
	NQO1 _{dic}	15.6±6.1	69.5±7.8	1.8±0.7·10 ⁻³	0.952
219-222	NQO1 _{apo}	21.8±0.6	45.4±1.4	3.0±0.3·10 ⁻⁴	0.998
	NQO1 _{holo}	-1.0±1.0	49.3±3.1	2.4±0.4·10 ⁻⁴	0.993
	NQO1 _{dic}	-0.6±0.7	48.0±2.0	2.8±0.3·10 ⁻⁴	0.996
223-228	NQO1 _{apo}	37.1±1.5	30.2±1.6	6.4±1.0·10 ⁻³	0.989
	NQO1 _{holo}	29.9±1.2	34.9±1.4	5.4±0.6·10 ⁻³	0.994
	NQO1 _{dic}	26.6±0.8	37.6±0.9	4.8±0.3·10 ⁻³	0.998
229-232	NQO1 _{apo}	47.2±4.5	45.5±4.5	5.7±0.8·10 ⁻²	0.991
	NQO1 _{holo}	49.7±5.9	42.5±5.5	5.7±1.0·10 ⁻²	0.983
	NQO1 _{dic}	41.2±0.7	51.0±0.6	1.7±0.1·10 ⁻²	1.000
233-238	NQO1 _{apo}	35.9±3.1	50.1±3.7	4.1±0.9·10 ⁻³	0.980
	NQO1 _{holo}	35.9±3.2	54.5±3.8	4.0±0.8·10 ⁻³	0.982
	NQO1 _{dic}	20.8±7.7	58.0±9.3	2.7±1.4·10 ⁻³	0.910
239-248	NQO1 _{apo}	40.9±3.0	48.6±3.0	1.4±0.2·10 ⁻²	0.989
	NQO1 _{holo}	34.0±3.1	54.8±3.1	1.5±0.2·10 ⁻²	0.991
	NQO1 _{dic}	34.7±2.7	53.9±2.7	1.2±0.2·10 ⁻²	0.992

249-254	NQO1 _{apo}	34.8±3.1	30.2±4.9	8.5±4.5·10 ⁻⁴	0.911
	NQO1 _{holo}	27.7±4.4	35.7±6.7	9.0±5.6·10 ⁻⁴	0.882
	NQO1 _{dic}	27.4±4.7	34.1±7.9	6.8±5.1·10 ⁻⁴	0.837
255-271	NQO1 _{apo}	28.9±1.8	41.0±2.2	2.4±0.4·10 ⁻³	0.989
	NQO1 _{holo}	22.5±1.8	48.3±2.4	1.6±0.3·10 ⁻³	0.990
	NQO1 _{dic}	23.3±1.9	48.0±2.3	2.6±0.4·10 ⁻³	0.991

Supplementary references

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