Predicting Extreme pKa Shifts in Staphylococcal Nuclease Mutants with Constant pH Molecular Dynamics

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Content

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Notes on Computational Methods and Output

Every pKa calculation used in these simulaitons used all-residue titration simulations with one exception, to compare single-residue to all-residue titration. Although only pKa values for ASP and GLU appear in the manuscript, these were among 39 residues in total for Δ+PHS, and 40 residues for its similar variants. The information on the following pages is a list of tables containing and the results of all titration calculations for aspartic acid, glutamic acid, arginine, and lysine. Titrations of other residues, such as histidine, were not included in this study. Additionally, the calculations were biased towards acidities near the pKa of target residues. Predicted pKa values for lysine, for example, are not accurate if only acidic pH environments were explored.

Part A is a list of figures containing correlation data from the experiment. These are present simply to show that there is either little or no correlation between large structural phenomena and error in pKa value prediction. This is a testament to the robustness of CPHMD calculations of pKa values. The tables at the end of part A list direct comparisons to work by Wallace et al.

Part B includes the tables of pKa values calculated from PDB coordinates. There is some variation between the tables, such as the addition or omission of residues at the terminating ends. 3BDC, for instance, omits titrating residues at both ends of the chain due to their coordinates being unsolved in the crystal structure.

Part C includes tables of pKa values calculated from modeled structures based on the coordinates of 3BDC.

The Hill Coefficient and correlation integrity that appear next to each pKa prediction are provided to give a relative concept of the quality of fit for each titration curve. For any protein, a relatively low Hill Coefficient and a relatively high correlation value indicate a good fit, such as for aspartic and glutamic acids. The opposite indicates a poor fit, such as for many of the lysines and arginines.

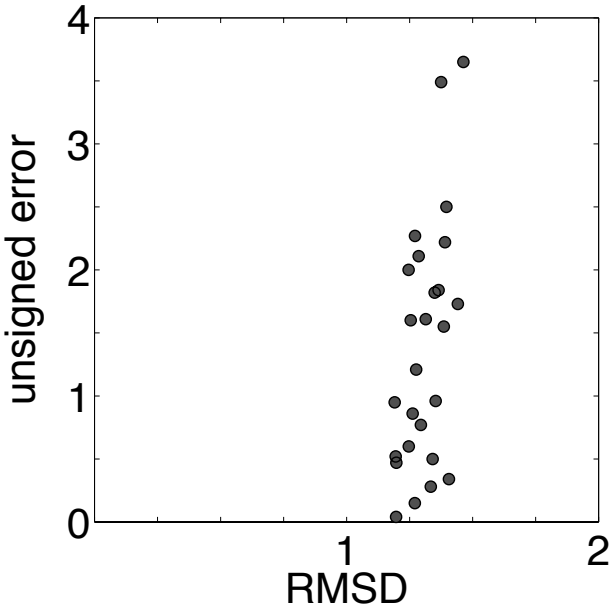

Figure SI 1: The effect of conformational changes due to protein relaxation vs. error of pKa prediction. This graph shows the RMSD between the initial structure and the average structure of each simulation. This set of data points shows a weak correlation (R^2 value of 0.29) between RMSD and error of pKa prediction. This indicates the protein's conformation changed relatively little during the 4 ns trajectory of the simulation, and that the minor fluctuations inherent with the simulation have little effect on pKa predictions.

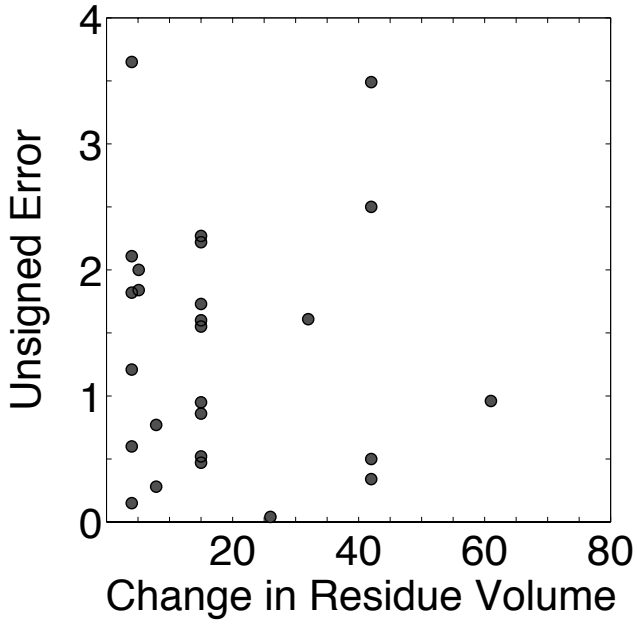

Figure SI 2: Change in residue volume from mutation vs. error of pKa prediction. The difference in volume between the initial residue and its mutation had little correlation to error of pKa prediction (R^2 value of 0.002). This indicates that the conformational changes associated with the mutation have virtually no effect on pKa prediction over the trajectory of this simulation.

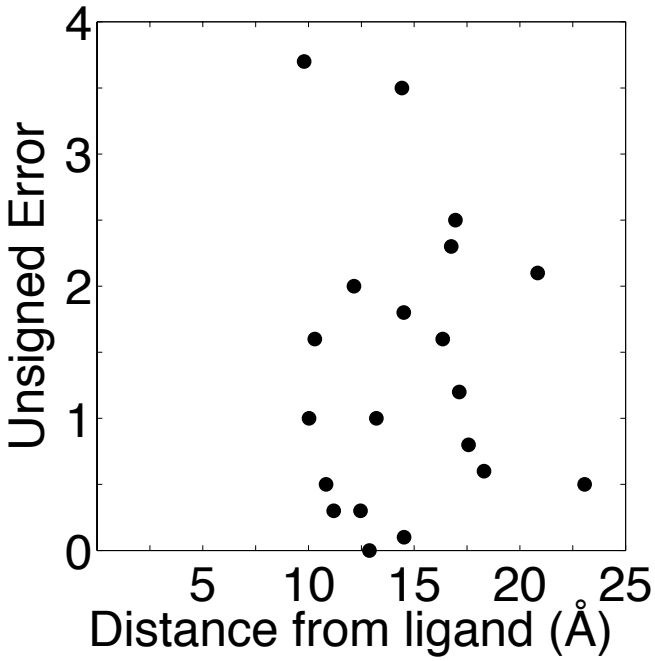

Figure SI 3: Proximity between target residue and the bound ligand thymidine-3',5'-diphosphate vs. error of pKa prediction. The bound ligand thymidine-3',5'-diphosphate was in the PDB structures of all proteins used in this experiment to enable proper crystallization. There was virtually no correlation between distance to the ligand and error of pKa prediction (R^2 value of 0.001). This suggests that the conformational adjustments required by the protein to accommodate this ligand have no observable effect on pKa predictions.

Table SI1: Calculated pKa values from a single pH, and its comparison to values by Wallace et al. The "calc. pKa (HH-fit)" are the values that appear in Tables 2 and 3 of the main manuscript. The "calc. pKa (single pH, HH-centered)" were each calculated from single values of S^{unprot} at the closest pH to "calc. pKa (HH-fit)". The "calc. pKa (single pH, Wallace et al.-centered)" were each calculated from single values of S^{unprot} at the closest pH to "calc. pKa (Wallace et al.)".

PDB	mutation	exp. pKa	calc. pKa (HH fit)	calc. pKa (single pH, HH-centered)	calc. pKa (single pH, Wallace et al.-centered)	calc. pKa (Wallace et al.)
1U9R	V66E	8.9	8.2	8.1	8.7	8.4
2OXP	V66D	8.8	7.5	7.8	7.2	6.8
2OEO	I92D	7.5	7.5	7.2	7.2	6.8
3H6M	V104E	9.4	7.6	7.8		
1TR5	I92E	9.0	6.8	7.4		
1TQO	I92E	9.0	7.3	6.2	6.2	6.9
3EVQ	L25E	7.5	8.4	8.3	8.3	8.4
3ERO	I72E	7.3	6.8	6.8	6.8	6.7
3D4D	Y91E	7.1	5.5	5.8	5.2	4.9
	L125E	9.1	6.8	7.2	7.6	7.9
	L103E	8.9	7.4	7.5	7.9	7.8
	L36E	8.7	7.1	7.3	7.3	7.1
	V66E	8.5	6.4	6.6		
	V99E	8.4	7.2	7.3	7.5	7.6
	V39E	8.2	4.6	4.6	8.7	8.9
	A109E	7.9	4.4	4.7	7.0	7.4
	V74E	7.8	8.4	8.1	9.3	9.8
	A58E	7.7	5.2	5.1	5.2	5.2
	T62E	7.7	6.9	7.1	6.8	7.3
	N100E	7.6	5.8	5.9	4.6	4.6
	F34E	7.3	7.3	7.6	7.6	7.5
	V23E	7.1	7.0	6.8	7.4	7.5
	A132E	7.0	6.5	5.9	6.6	6.8
	L38E	6.8	6.3	6.3		
	T41E	6.8	6.5	6.7	6.7	6.3
	A90E	6.4	6.7	6.3	8.5	9.1
	L37E	5.2	6.2	5.7	5.7	6.1
	G20E	4.5	5.5	5.3	4.5	4.2
	N118E	4.5	2.5	2.2	5.1	5.4

3BDC (Δ+PHS)			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 9	12.73	0.23	0.00
GLU 10	3.32	0.19	0.50
LYS 16	12.73	0.23	0.00
ASP 19	3.76	0.34	0.54
ASP 21	5.43	0.38	0.56
LYS 24	12.73	0.23	0.00
LYS 28	12.73	0.23	0.00
ARG 35	12.73	0.23	0.00
ASP 40	2.03	0.19	0.48
GLU 43	3.76	0.24	0.51
GLU 52	4.90	0.77	0.65
LYS 53	12.73	0.23	0.00
GLU 57	4.42	0.71	0.62
LYS 63	12.73	0.23	0.00
LYS 64	12.73	0.23	0.00
GLU 67	3.62	0.98	0.61
LYS 70	12.73	0.23	0.00
LYS 71	12.73	0.23	0.00
GLU 73	2.14	0.19	0.48
GLU 75	4.89	0.65	0.62
ASP 77	0.79	0.15	0.44
LYS 78	12.73	0.23	0.00
ARG 81	12.73	0.23	0.00
ASP 83	3.83	1.12	0.61
LYS 84	12.73	0.23	0.00
ARG 87	12.73	0.23	0.00
ASP 95	3.44	0.43	0.54
LYS 97	12.73	0.23	0.00
GLU 101	3.51	0.48	0.55
ARG 105	12.73	0.23	0.00
LYS 110	12.73	0.23	0.00
LYS 116	12.73	0.23	0.00
GLU 122	4.69	1.21	0.66
ARG 126	12.73	0.23	0.00
LYS 127	12.73	0.23	0.00
GLU 129	4.43	0.47	0.60
LYS 133	12.73	0.23	0.00
LYS 134	12.73	0.23	0.00
GLU 135	4.44	0.97	0.64
LYS 136	12.73	0.23	0.00

3ERO (Δ+PHS I72E)			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 9	13.24	1.96	1.00
GLU 10	3.62	0.56	0.99
LYS 16	10.68	1.82	0.82
ASP 19	3.80	1.45	0.99
ASP 21	5.64	0.57	0.97
LYS 24	10.49	1.80	0.80
LYS 28	13.01	0.24	0.06
ARG 35	13.21	1.96	0.00
ASP 40	2.43	0.66	1.00
GLU 43	4.28	0.68	0.99
GLU 52	4.52	1.01	1.00
LYS 53	12.86	1.62	0.58
GLU 57	3.97	0.87	0.99
LYS 63	11.08	0.48	0.96
LYS 64	11.00	0.72	1.00
GLU 67	3.46	0.62	0.99
LYS 70	12.02	1.90	0.09
LYS 71	12.95	0.31	0.08
GLU 72	6.78	0.80	0.97
GLU 73	3.23	1.73	1.00
GLU 75	4.33	0.57	0.98
ASP 77	1.68	1.32	0.99
LYS 78	11.21	1.86	0.69
ARG 81	13.21	1.96	0.00
ASP 83	4.47	1.45	1.00
LYS 84	13.00	0.24	0.07
ARG 87	13.22	1.96	1.00
ASP 95	3.28	1.02	1.00
LYS 97	12.33	1.92	0.06
GLU 101	3.67	0.63	0.98
ARG 105	13.21	1.96	0.00
LYS 110	13.62	0.37	0.91
LYS 116	10.52	1.56	0.72
GLU 122	4.64	0.94	1.00
ARG 126	13.21	1.96	0.00
LYS 127	10.11	1.28	0.99
GLU 129	3.98	0.83	1.00
LYS 133	10.53	0.57	0.98
LYS 134	10.31	0.62	0.99
GLU 135	4.38	1.28	1.00
LYS 136	9.88	1.87	0.64

1TQO (Δ+PHS I92E)			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 9	11.95	1.32	0.99
GLU 10	3.88	0.88	0.99
LYS 16	10.71	1.83	0.98
ASP 19	3.58	1.86	1.00
ASP 21	5.64	1.01	1.00
LYS 24	9.91	1.82	0.98
LYS 28	11.29	1.55	1.00
ARG 35	13.16	0.17	0.70
ASP 40	2.48	0.81	1.00
GLU 43	3.60	1.64	1.00
GLU 52	5.09	0.91	1.00
LYS 53	11.25	1.51	0.99
GLU 57	4.59	0.85	1.00
LYS 63	11.15	1.69	0.96
LYS 64	10.39	1.80	0.96
GLU 67	3.76	1.08	1.00
LYS 70	10.94	1.81	0.98
LYS 71	10.85	1.83	0.97
GLU 73	3.20	0.88	1.00
GLU 75	4.53	0.53	0.99
ASP 77	0.52	1.21	1.00
LYS 78	11.31	0.94	1.00
ARG 81	13.10	0.23	0.82
ASP 83	3.63	1.46	1.00
LYS 84	11.14	1.60	0.96
ARG 87	12.41	1.87	0.86
GLU 92	7.27	0.70	1.00
ASP 95	3.83	0.91	1.00
LYS 97	10.85	1.83	0.98
GLU 101	3.29	1.07	1.00
ARG 105	12.84	1.76	0.87
LYS 110	12.01	1.54	0.95
LYS 116	9.98	1.80	0.97
GLU 122	4.94	1.16	1.00
ARG 126	13.16	0.18	0.73
LYS 127	10.44	0.34	0.99
GLU 129	4.24	1.26	1.00
LYS 133	10.82	1.74	0.97
LYS 134	10.81	1.82	0.97
GLU 135	4.56	0.80	1.00
LYS 136	10.93	1.80	0.98
GLU 142	4.41	0.56	1.00
ASP 143	3.74	0.90	1.00

1TR5 (Δ+PHS I92E)			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 6	10.83	1.04	0.98
LYS 9	12.81	0.41	0.10
GLU 10	4.55	0.77	1.00
LYS 16	10.53	1.70	0.88
ASP 19	1.55	0.36	0.93
ASP 21	5.63	0.91	1.00
LYS 24	9.75	1.86	0.94
LYS 28	12.68	1.75	0.65
ARG 35	12.86	0.31	0.59
ASP 40	2.54	1.36	0.99
GLU 43	3.40	1.64	1.00
GLU 52	4.81	0.96	1.00
LYS 53	10.93	1.79	0.75
GLU 57	4.50	1.85	1.00
LYS 63	10.63	1.60	0.87
LYS 64	10.65	1.36	0.97
GLU 67	3.87	1.00	0.99
LYS 70	10.76	1.19	0.95
LYS 71	10.83	0.90	0.98
GLU 73	3.21	0.85	1.00
GLU 75	4.69	0.79	0.99
ASP 77	1.25	1.17	1.00
LYS 78	10.87	1.42	0.94
ARG 81	12.86	0.31	0.59
ASP 83	4.30	0.64	1.00
LYS 84	12.34	1.91	0.63
ARG 87	12.86	0.31	0.73
GLU 92	6.78	0.64	0.99
ASP 95	3.42	1.28	1.00
LYS 97	10.67	1.54	0.97
GLU 101	3.38	0.55	0.97
ARG 105	12.85	0.32	0.72
LYS 110	11.98	1.88	0.76
LYS 116	10.67	1.05	0.99
GLU 122	5.16	0.96	1.00
ARG 126	12.86	0.31	0.59
LYS 127	10.35	1.55	0.96
GLU 129	4.14	0.89	1.00
LYS 133	10.84	0.65	0.95
LYS 134	10.36	1.78	0.89
GLU 135	4.54	0.64	1.00
LYS 136	10.82	1.60	0.96

3D4D (Δ+PHS Y91E)			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 9	13.53	1.92	0.79
GLU 10	3.51	1.27	0.99
LYS 16	10.56	0.63	0.92
ASP 19	3.52	0.60	0.94
ASP 21	5.34	0.50	0.92
LYS 24	10.48	1.75	0.78
LYS 28	13.51	1.81	0.98
ARG 35	13.53	1.96	0.00
ASP 40	2.81	1.03	1.00
GLU 43	3.99	1.18	1.00
GLU 52	4.80	0.83	0.98
LYS 53	12.44	1.84	0.30
GLU 57	4.39	0.77	0.96
LYS 63	11.00	0.43	0.99
LYS 64	10.49	0.76	0.98
GLU 67	3.79	0.69	0.99
LYS 70	12.65	1.80	0.39
LYS 71	12.43	1.83	0.31
GLU 73	3.45	0.94	1.00
GLU 75	4.88	1.19	0.98
ASP 77	3.69	0.62	0.89
LYS 78	11.82	1.85	0.07
ARG 81	13.53	1.96	0.00
ASP 83	4.85	1.76	0.97
LYS 84	12.95	0.25	0.05
ARG 87	13.53	1.95	1.00
GLU 91	5.49	1.30	0.95
ASP 95	3.51	0.88	1.00
LYS 97	12.74	1.43	0.64
GLU 101	3.38	1.01	0.99
ARG 105	13.53	1.96	1.00
LYS 110	13.07	0.22	0.05
LYS 116	10.36	1.10	0.97
GLU 122	4.38	0.61	0.98
ARG 126	13.53	1.96	0.00
LYS 127	10.18	1.23	0.98
GLU 129	4.11	0.72	0.98
LYS 133	12.77	0.82	0.22
LYS 134	10.86	1.60	0.95
GLU 135	4.50	0.97	0.99
LYS 136	10.21	1.84	0.66

3EVQ (Δ+PHS L25E)			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 9	13.53	0.42	0.93
GLU 10	4.36	1.10	1.00
LYS 16	10.65	1.76	0.77
ASP 19	3.91	0.68	0.99
ASP 21	5.51	0.55	0.97
LYS 24	9.86	0.37	0.93
GLU 25	8.36	1.78	0.92
LYS 28	13.48	0.20	0.79
ARG 35	13.23	1.96	0.00
ASP 40	2.42	1.08	0.98
GLU 43	4.15	0.97	1.00
GLU 52	4.43	0.87	1.00
LYS 53	12.77	1.71	0.61
GLU 57	4.20	1.08	1.00
LYS 63	10.48	0.73	0.88
LYS 64	10.02	1.84	0.65
GLU 67	4.47	0.93	1.00
LYS 70	12.38	1.89	0.25
LYS 71	12.28	1.90	0.12
GLU 73	3.22	0.89	1.00
GLU 75	4.51	1.06	0.99
ASP 77	0.61	0.66	0.98
LYS 78	12.73	1.85	0.46
ARG 81	13.23	1.96	0.00
ASP 83	3.89	1.07	1.00
LYS 84	12.79	1.82	0.63
ARG 87	13.23	1.96	0.00
ASP 95	3.51	0.80	1.00
LYS 97	12.59	1.90	0.29
GLU 101	3.72	1.12	0.99
ARG 105	13.23	1.96	0.00
LYS 110	12.75	1.74	0.58
LYS 116	11.34	0.23	0.82
GLU 122	4.82	0.89	0.99
ARG 126	13.23	1.96	0.00
LYS 127	9.90	1.82	0.97
GLU 129	4.09	0.84	1.00
LYS 133	12.76	1.73	0.60
LYS 134	10.76	1.46	0.94
GLU 135	4.73	1.40	1.00
LYS 136	10.75	1.86	0.68

3H6M (Δ+PHS V104E)			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 9	12.60	1.87	0.71
GLU 10	4.10	0.68	0.95
LYS 16	10.30	1.80	0.91
ASP 19	3.72	1.87	0.99
ASP 21	4.97	0.35	0.96
LYS 24	9.56	1.84	0.95
LYS 28	11.98	1.91	0.70
ARG 35	12.99	0.21	0.00
ASP 40	2.72	1.08	1.00
GLU 43	4.40	1.78	1.00
GLU 52	4.53	0.81	1.00
LYS 53	10.84	0.91	0.96
GLU 57	4.61	0.50	0.99
LYS 63	11.13	0.76	0.98
LYS 64	10.86	1.58	0.89
GLU 67	3.80	0.66	0.99
LYS 70	10.79	1.01	0.97
LYS 71	10.89	0.78	0.98
GLU 73	3.16	0.95	1.00
GLU 75	4.48	1.15	1.00
ASP 77	1.47	0.75	0.95
LYS 78	10.76	0.51	0.95
ARG 81	12.98	0.22	0.59
ASP 83	3.88	0.86	1.00
LYS 84	11.06	1.51	0.98
ARG 87	12.92	0.42	0.82
ASP 95	3.82	1.11	1.00
LYS 97	10.83	1.43	0.97
GLU 101	3.70	1.08	1.00
GLU 104	7.58	0.90	0.98
ARG 105	12.95	0.28	0.73
LYS 110	11.69	1.85	0.74
LYS 116	10.49	1.08	0.98
GLU 122	4.61	1.01	1.00
ARG 126	12.99	0.21	0.50
LYS 127	10.74	1.61	0.88
GLU 129	4.32	1.86	1.00
LYS 133	10.98	1.54	0.96
LYS 134	10.55	1.58	0.89
GLU 135	4.54	0.71	1.00
LYS 136	10.84	1.14	0.97

1U9R (Δ 44-49, V66E, P117G, H124L, S128A)			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 9	11.31	1.40	1.00
GLU 10	3.73	0.80	1.00
LYS 16	10.33	1.80	0.97
ASP 19	3.45	0.55	1.00
ASP 21	4.73	0.66	1.00
LYS 24	9.86	1.81	0.99
LYS 28	11.60	0.81	1.00
ARG 35	13.10	0.22	0.84
ASP 40	3.41	1.74	0.99
GLU 43	3.78	0.64	0.99
GLU 52	4.89	1.48	1.00
LYS 53	10.78	1.84	0.97
GLU 57	4.64	1.78	1.00
LYS 63	10.81	1.70	0.98
LYS 64	10.65	1.80	0.98
GLU 66	8.15	1.65	0.98
GLU 67	4.04	0.65	1.00
LYS 70	11.01	1.77	0.97
LYS 71	10.93	1.79	0.97
GLU 73	3.23	0.75	1.00
GLU 75	4.47	0.57	0.98
ASP 77	1.24	0.33	0.92
LYS 78	11.48	1.12	1.00
ARG 81	13.14	0.19	0.78
ASP 83	3.86	0.94	1.00
LYS 84	10.95	1.76	0.96
ARG 87	12.84	1.78	0.94
ASP 95	3.36	0.86	1.00
LYS 97	11.04	1.69	0.97
GLU 101	3.77	0.71	1.00
ARG 105	12.81	1.75	0.84
LYS 110	11.01	1.66	0.96
LYS 116	9.63	1.81	0.97
GLU 122	4.52	1.45	1.00
ARG 126	13.45	1.60	0.98
LYS 127	10.33	1.80	0.97
GLU 129	4.17	0.97	1.00
LYS 133	10.86	1.80	0.98
LYS 134	10.15	1.80	0.98
GLU 135	4.47	0.59	1.00
LYS 136	10.66	1.84	0.98

2OXP (Δ 44-49, V66D, P117G, H124L, S128A)			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 9	11.62	0.73	1.00
GLU 10	3.62	1.51	1.00
LYS 16	9.91	1.82	0.98
ASP 19	1.96	0.81	1.00
ASP 21	5.47	0.58	1.00
LYS 24	9.02	1.78	0.98
LYS 28	11.46	1.11	1.00
ARG 35	13.19	0.15	0.74
ASP 40	3.15	1.34	1.00
GLU 43	4.21	0.84	1.00
GLU 52	4.61	0.61	0.99
LYS 53	10.77	1.84	0.98
GLU 57	4.47	1.28	1.00
LYS 63	11.01	1.69	0.98
LYS 64	10.65	1.84	0.97
ASP 66	7.47	0.70	1.00
GLU 67	3.82	1.35	1.00
LYS 70	11.12	1.70	0.96
LYS 71	10.88	1.81	0.98
GLU 73	3.13	0.81	0.99
GLU 75	4.32	1.31	1.00
ASP 77	0.69	0.60	0.98
LYS 78	10.86	1.80	0.97
ARG 81	13.16	0.18	0.73
ASP 83	3.53	1.46	1.00
LYS 84	10.97	1.70	0.96
ARG 87	13.62	1.84	0.98
ASP 95	3.24	0.97	1.00
LYS 97	10.67	1.84	0.99
GLU 101	3.70	1.02	1.00
ARG 105	12.78	1.77	0.82
LYS 110	11.00	1.44	0.97
LYS 116	10.03	1.81	0.99
GLU 122	4.84	1.45	1.00
ARG 126	13.62	1.83	0.98
LYS 127	10.93	1.82	0.98
GLU 129	4.34	0.88	1.00
LYS 133	10.82	1.83	0.98
LYS 134	10.35	1.80	0.97
GLU 135	3.80	1.14	1.00
LYS 136	10.80	0.30	0.98

2OEO (Δ+PHS, I92D, K64A, K97A, K110A, K116S, K127A)			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 6	10.44	1.80	0.98
LYS 9	11.84	1.03	1.00
GLU 10	4.24	1.11	1.00
LYS 16	9.97	1.82	0.98
ASP 19	3.76	1.38	1.00
ASP 21	5.74	0.48	0.99
LYS 24	9.12	1.79	0.98
LYS 28	11.36	0.70	1.00
ARG 35	13.15	0.17	0.82
ASP 40	2.92	0.96	1.00
GLU 43	3.88	0.80	1.00
GLU 52	4.86	1.14	1.00
LYS 53	10.86	1.78	0.96
GLU 57	4.67	1.11	1.00
LYS 63	10.86	1.74	0.97
GLU 67	4.36	1.04	1.00
LYS 70	10.93	1.63	0.96
LYS 71	10.97	1.72	0.98
GLU 73	3.24	1.22	1.00
GLU 75	4.74	0.42	0.98
ASP 77	1.88	1.11	1.00
LYS 78	11.00	1.64	0.96
ARG 81	13.11	0.21	0.80
ASP 83	3.54	1.92	1.00
LYS 84	11.39	0.84	1.00
ARG 87	13.32	1.19	1.00
ASP 92	7.50	0.62	1.00
ASP 95	3.57	0.90	1.00
GLU 101	4.37	1.28	1.00
ARG 105	12.84	1.75	0.85
GLU 122	4.73	1.18	1.00
ARG 126	13.13	0.19	0.77
GLU 129	3.83	1.36	1.00
LYS 133	10.87	1.59	0.96
LYS 134	10.75	1.84	0.98
GLU 135	4.54	1.14	1.00
LYS 136	10.35	1.80	0.97

pKa calculations of titrating residues from modeled structures

Δ+PHS A58E			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 9	12.05	1.84	0.80
GLU 10	3.82	0.74	0.97
LYS 16	10.35	1.63	0.95
ASP 19	3.29	0.45	0.91
ASP 21	5.12	0.49	0.90
LYS 24	9.92	1.78	0.97
LYS 28	11.49	1.74	0.86
ARG 35	13.14	0.18	0.79
ASP 40	2.84	0.54	0.92
GLU 43	3.76	0.65	0.99
GLU 52	4.56	0.97	0.98
LYS 53	10.98	1.54	0.99
GLU 57	4.84	0.96	0.98
GLU 58	5.20	0.87	0.97
LYS 63	11.05	0.88	0.99
LYS 64	10.35	1.68	0.94
GLU 67	3.97	0.91	0.96
LYS 70	11.17	1.43	0.98
LYS 71	11.01	0.70	1.00
GLU 73	3.05	1.71	0.99
GLU 75	4.84	0.76	0.97
ASP 77	1.30	0.77	0.94
LYS 78	10.97	1.07	1.00
ARG 81	13.15	0.18	0.74
ASP 83	4.43	1.02	0.99
LYS 84	11.15	1.55	0.99
ARG 87	13.11	0.20	0.77
ASP 95	3.28	1.27	1.00
LYS 97	10.95	0.95	1.00
GLU 101	3.66	1.21	1.00
ARG 105	13.11	1.67	0.94
LYS 110	11.61	1.77	0.86
LYS 116	10.93	0.83	1.00
GLU 122	4.81	1.07	0.98
ARG 126	13.13	0.18	0.67
LYS 127	10.22	1.83	0.94
GLU 129	4.28	1.01	1.00
LYS 133	10.86	1.42	1.00
LYS 134	10.28	1.79	0.94
GLU 135	4.40	1.16	0.99
LYS 136	10.76	0.78	0.99

pKa calculations of titrating residues from modeled structures

Δ+PHS A90E			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 9	11.89	1.87	0.76
GLU 10	3.95	0.64	0.97
LYS 16	10.28	1.82	0.95
ASP 19	3.75	0.72	0.97
ASP 21	5.51	0.67	0.99
LYS 24	10.18	1.79	0.95
LYS 28	11.22	1.82	0.90
ARG 35	13.08	0.20	0.69
ASP 40	2.66	0.70	0.99
GLU 43	3.94	0.74	0.99
GLU 52	4.88	0.99	0.99
LYS 53	10.99	1.04	1.00
GLU 57	4.39	0.86	0.99
LYS 63	10.95	1.37	0.97
LYS 64	10.59	0.92	1.00
GLU 67	3.57	0.72	0.98
LYS 70	10.79	0.89	1.00
LYS 71	10.85	1.35	0.97
GLU 73	2.72	0.77	1.00
GLU 75	5.15	1.56	1.00
ASP 77	1.24	0.31	0.71
LYS 78	10.83	1.22	1.00
ARG 81	13.09	0.19	0.69
ASP 83	3.98	0.76	0.98
LYS 84	11.81	1.86	0.78
ARG 87	13.07	0.21	0.73
GLU 90	6.74	0.72	0.93
ASP 95	3.49	0.84	1.00
LYS 97	10.88	0.79	1.00
GLU 101	3.25	0.62	0.94
ARG 105	13.40	1.93	0.99
LYS 110	10.96	1.55	0.93
LYS 116	10.42	1.60	0.95
GLU 122	4.83	0.80	0.99
ARG 126	13.08	0.20	0.69
LYS 127	10.32	1.82	0.93
GLU 129	4.10	1.67	1.00
LYS 133	10.97	1.67	0.84
LYS 134	10.26	1.82	0.93
GLU 135	4.53	0.97	1.00
LYS 136	10.79	0.49	0.99

Δ+PHS A109E			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 9	11.68	1.58	0.97
GLU 10	3.67	0.83	1.00
LYS 16	10.88	1.80	0.96
ASP 19	3.87	0.88	0.99
ASP 21	5.36	0.67	0.96
LYS 24	9.80	1.79	0.94
LYS 28	11.49	0.85	1.00
ARG 35	13.22	0.19	0.68
ASP 40	3.66	0.76	0.99
GLU 43	3.73	0.59	0.98
GLU 52	5.08	1.11	0.99
LYS 53	11.21	1.10	1.00
GLU 57	3.98	1.27	0.98
LYS 63	10.54	1.72	0.97
LYS 64	10.73	1.80	0.94
GLU 67	3.46	0.84	1.00
LYS 70	11.14	1.49	0.97
LYS 71	10.69	1.80	0.94
GLU 73	2.60	1.16	0.97
GLU 75	4.76	1.39	0.99
ASP 77	0.50	0.75	0.00
LYS 78	10.72	1.80	0.94
ARG 81	13.19	0.22	0.70
ASP 83	4.14	0.72	0.99
LYS 84	11.62	1.34	0.99
ARG 87	13.05	1.78	0.99
ASP 95	3.41	1.08	0.99
LYS 97	10.72	1.80	0.94
GLU 101	3.44	0.92	0.98
ARG 105	12.38	1.56	0.99
GLU 109	4.41	0.55	0.97
LYS 110	11.41	1.36	1.00
LYS 116	10.98	1.78	0.95
GLU 122	4.76	1.35	0.98
ARG 126	13.17	0.25	0.87
LYS 127	10.49	1.75	0.94
GLU 129	4.08	0.63	0.97
LYS 133	10.57	1.79	0.97
LYS 134	10.38	1.74	0.92
GLU 135	4.40	1.53	0.98
LYS 136	10.56	1.79	0.94

Δ+PHS A132E			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 9	12.00	1.73	0.86
GLU 10	3.67	0.81	0.99
LYS 16	10.41	1.79	0.94
ASP 19	3.36	0.87	0.99
ASP 21	5.89	0.63	0.95
LYS 24	9.91	1.80	0.95
LYS 28	11.61	1.42	0.99
ARG 35	13.19	0.22	0.75
ASP 40	3.01	0.67	0.98
GLU 43	4.28	0.95	0.99
GLU 52	4.67	0.99	0.98
LYS 53	11.14	1.53	0.96
GLU 57	3.91	0.92	0.99
LYS 63	10.53	1.78	0.93
LYS 64	10.88	1.78	0.94
GLU 67	4.26	0.90	0.97
LYS 70	11.13	0.83	0.99
LYS 71	10.87	1.80	0.94
GLU 73	3.37	1.05	1.00
GLU 75	4.85	0.71	0.96
ASP 77	1.64	0.79	0.97
LYS 78	10.86	1.79	0.94
ARG 81	13.21	0.20	0.71
ASP 83	3.71	0.61	0.99
LYS 84	11.29	1.66	1.00
ARG 87	13.55	1.88	0.96
ASP 95	3.16	1.17	0.99
LYS 97	10.85	1.79	0.95
GLU 101	3.65	0.79	0.99
ARG 105	13.52	1.92	0.96
LYS 110	11.31	1.64	0.99
LYS 116	10.78	1.79	0.94
GLU 122	4.68	0.79	0.96
ARG 126	13.21	0.20	0.72
LYS 127	10.60	1.80	0.97
GLU 129	3.87	0.71	1.00
GLU 132	6.50	0.74	0.96
LYS 133	10.74	1.80	0.94
LYS 134	10.66	1.80	0.94
GLU 135	4.50	1.26	0.99
LYS 136	10.74	1.79	0.93

Δ+PHS F34E			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 9	11.61	1.85	0.79
GLU 10	3.64	0.62	0.98
LYS 16	10.44	0.48	0.99
ASP 19	3.74	0.69	0.99
ASP 21	5.17	0.48	0.93
LYS 24	9.96	1.84	0.97
LYS 28	11.56	1.85	0.79
GLU 34	7.26	0.81	0.98
ARG 35	13.14	0.18	0.81
ASP 40	2.78	1.13	0.98
GLU 43	3.82	0.75	0.99
GLU 52	4.56	0.75	0.99
LYS 53	10.91	1.55	0.90
GLU 57	4.09	0.84	0.96
LYS 63	10.79	1.20	0.99
LYS 64	10.60	0.94	1.00
GLU 67	3.70	1.14	0.99
LYS 70	10.92	1.55	0.95
LYS 71	10.85	1.43	0.98
GLU 73	2.89	0.97	0.99
GLU 75	4.62	0.76	0.98
ASP 77	0.92	0.38	0.87
LYS 78	10.84	1.37	0.98
ARG 81	13.14	0.19	0.66
ASP 83	4.02	0.64	0.95
LYS 84	11.47	1.81	0.82
ARG 87	13.62	1.97	1.00
ASP 95	3.44	1.37	1.00
LYS 97	10.77	0.98	1.00
GLU 101	3.70	1.09	0.98
ARG 105	13.63	1.96	1.00
LYS 110	11.65	1.83	0.82
LYS 116	10.92	0.78	0.99
GLU 122	4.89	0.87	0.98
ARG 126	13.13	0.19	0.73
LYS 127	10.38	0.61	0.99
GLU 129	4.17	0.83	0.98
LYS 133	10.84	0.80	1.00
LYS 134	10.57	0.92	1.00
GLU 135	4.26	0.72	0.96
LYS 136	10.82	0.90	1.00

Δ+PHS G20E			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 9	13.17	1.60	0.44
GLU 10	3.75	0.79	0.97
LYS 16	12.15	0.24	0.99
ASP 19	3.61	0.66	0.97
GLU 20	5.46	0.50	0.95
ASP 21	4.11	0.64	0.95
LYS 24	9.68	0.72	0.99
LYS 28	13.15	0.37	0.91
ARG 35	13.19	1.58	0.00
ASP 40	2.90	0.83	0.97
GLU 43	3.98	0.77	0.98
GLU 52	4.62	1.35	1.00
LYS 53	13.37	0.29	0.84
GLU 57	4.48	0.61	0.98
LYS 63	11.96	0.32	0.32
LYS 64	12.91	0.34	0.97
GLU 67	3.92	0.99	1.00
LYS 70	10.72	1.63	0.71
LYS 71	12.38	0.21	0.97
GLU 73	3.04	0.76	0.99
GLU 75	4.93	0.98	1.00
ASP 77	1.42	0.53	0.96
LYS 78	12.42	0.20	1.00
ARG 81	13.19	1.58	0.00
ASP 83	3.76	0.74	0.98
LYS 84	13.10	1.71	0.96
ARG 87	13.18	1.60	1.00
ASP 95	3.49	0.89	0.98
LYS 97	13.35	0.24	0.93
GLU 101	3.48	0.81	0.98
ARG 105	13.19	1.58	0.00
LYS 110	12.25	0.25	0.29
LYS 116	11.64	0.58	0.23
GLU 122	4.75	0.85	0.99
ARG 126	13.19	1.58	0.00
LYS 127	12.00	0.33	0.29
GLU 129	4.13	0.75	0.98
LYS 133	11.51	0.76	0.21
LYS 134	10.33	0.33	0.88
GLU 135	4.52	1.02	0.99
LYS 136	10.65	1.69	0.67

Δ+PHS L36E			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 9	12.62	1.86	0.67
GLU 10	3.41	1.35	1.00
LYS 16	10.47	1.46	0.95
ASP 19	3.84	1.25	1.00
ASP 21	5.47	0.69	0.98
LYS 24	9.83	1.71	0.89
LYS 28	12.18	1.93	0.67
ARG 35	13.01	1.89	1.00
GLU 36	7.10	0.78	0.97
ASP 40	2.95	1.16	1.00
GLU 43	3.81	0.83	1.00
GLU 52	4.86	0.67	1.00
LYS 53	10.69	1.58	0.89
GLU 57	4.62	0.80	0.99
LYS 63	10.90	0.58	0.94
LYS 64	10.74	0.94	0.98
GLU 67	3.48	0.83	1.00
LYS 70	11.42	1.87	0.74
LYS 71	10.75	0.89	0.98
GLU 73	2.74	0.53	1.00
GLU 75	4.57	0.65	0.98
ASP 77	2.20	0.67	0.98
LYS 78	11.05	1.75	0.80
ARG 81	13.01	1.89	1.00
ASP 83	4.31	0.68	0.99
LYS 84	12.26	1.92	0.71
ARG 87	12.96	1.92	0.99
ASP 95	3.14	1.03	1.00
LYS 97	11.10	1.47	0.90
GLU 101	3.43	1.52	1.00
ARG 105	13.06	1.87	0.96
LYS 110	11.85	1.91	0.72
LYS 116	10.74	1.07	0.99
GLU 122	5.03	1.36	1.00
ARG 126	13.01	1.88	0.90
LYS 127	10.53	1.72	0.87
GLU 129	4.10	0.84	1.00
LYS 133	10.76	1.67	0.98
LYS 134	10.28	0.76	0.98
GLU 135	4.26	0.59	0.98
LYS 136	10.75	0.98	0.98

Δ+PHS L37E			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 9	13.53	1.60	1.00
GLU 10	3.86	1.02	0.99
LYS 16	10.33	0.60	0.99
ASP 19	3.52	0.80	0.97
ASP 21	5.35	0.67	0.98
LYS 24	9.94	0.74	1.00
LYS 28	13.21	1.82	1.00
ARG 35	13.31	1.79	0.00
GLU 37	6.15	0.43	0.96
ASP 40	2.71	0.88	0.99
GLU 43	4.10	0.64	0.96
GLU 52	4.78	0.83	0.99
LYS 53	12.81	0.66	0.99
GLU 57	4.44	0.78	0.92
LYS 63	11.10	1.76	0.64
LYS 64	10.61	1.77	0.77
GLU 67	3.99	0.75	0.98
LYS 70	10.19	1.62	0.95
LYS 71	10.98	1.71	0.73
GLU 73	3.00	0.71	0.96
GLU 75	4.56	0.98	0.99
ASP 77	0.78	0.39	0.91
LYS 78	11.17	1.75	0.65
ARG 81	13.31	1.79	0.00
ASP 83	4.06	0.61	0.95
LYS 84	11.54	1.71	1.00
ARG 87	13.30	1.79	1.00
ASP 95	3.55	0.65	0.99
LYS 97	11.14	1.71	0.71
GLU 101	3.72	0.82	0.98
ARG 105	13.30	1.79	1.00
LYS 110	11.95	0.74	0.23
LYS 116	9.88	0.96	0.99
GLU 122	4.58	0.90	0.99
ARG 126	13.31	1.79	0.00
LYS 127	10.13	1.50	0.97
GLU 129	4.03	1.18	0.99
LYS 133	10.73	0.30	0.89
LYS 134	10.36	0.42	0.96
GLU 135	4.40	1.69	0.99
LYS 136	11.52	0.35	0.96

Δ+PHS L38E			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 9	12.14	1.74	0.83
GLU 10	3.77	1.07	0.99
LYS 16	10.42	0.79	0.99
ASP 19	3.51	0.63	0.95
ASP 21	5.37	0.99	0.96
LYS 24	9.64	1.74	0.99
LYS 28	11.89	1.83	0.83
ARG 35	13.15	0.18	0.67
GLU 38	6.33	0.85	0.98
ASP 40	3.44	1.04	0.98
GLU 43	3.97	0.75	0.97
GLU 52	4.83	0.95	0.99
LYS 53	11.06	1.66	0.86
GLU 57	4.04	0.89	0.99
LYS 63	10.75	0.57	0.98
LYS 64	10.65	0.81	1.00
GLU 67	3.90	1.03	0.98
LYS 70	11.37	1.81	0.82
LYS 71	10.44	0.98	1.00
GLU 73	3.04	0.86	0.99
GLU 75	4.51	0.70	0.96
ASP 77	0.58	0.42	0.99
LYS 78	11.01	1.63	0.86
ARG 81	13.14	0.18	0.80
ASP 83	3.90	0.64	0.94
LYS 84	11.43	1.83	0.80
ARG 87	13.59	1.97	0.85
ASP 95	3.42	0.91	0.99
LYS 97	10.87	1.27	0.98
GLU 101	3.90	0.77	0.98
ARG 105	13.61	1.81	1.00
LYS 110	11.93	1.80	0.78
LYS 116	10.68	1.03	1.00
GLU 122	4.64	0.79	0.99
ARG 126	13.14	0.18	0.77
LYS 127	10.76	1.44	1.00
GLU 129	4.28	0.83	0.97
LYS 133	10.92	0.67	0.99
LYS 134	10.49	0.86	1.00
GLU 135	4.32	1.07	0.99
LYS 136	10.73	1.38	0.99

Δ+PHS L103E			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 9	12.21	1.90	0.70
GLU 10	3.93	0.79	0.99
LYS 16	10.43	1.79	0.90
ASP 19	4.18	0.99	0.96
ASP 21	5.43	0.60	0.98
LYS 24	9.97	1.83	0.92
LYS 28	12.30	1.91	0.63
ARG 35	12.92	0.30	0.62
ASP 40	2.47	1.36	0.99
GLU 43	3.81	0.42	0.98
GLU 52	4.35	1.03	1.00
LYS 53	11.44	1.85	0.74
GLU 57	4.39	1.30	1.00
LYS 63	10.84	0.34	0.87
LYS 64	10.72	1.71	0.84
GLU 67	3.64	0.90	0.99
LYS 70	10.93	0.95	0.99
LYS 71	11.04	0.80	0.99
GLU 73	3.00	1.27	1.00
GLU 75	4.94	0.66	1.00
ASP 77	0.53	0.57	1.00
LYS 78	10.91	1.55	0.97
ARG 81	12.91	0.31	0.75
ASP 83	4.26	0.79	1.00
LYS 84	11.21	1.81	0.76
ARG 87	12.92	0.30	0.75
ASP 95	3.57	1.82	1.00
LYS 97	10.92	0.90	0.99
GLU 101	3.67	1.81	1.00
GLU 103	7.35	0.47	0.91
ARG 105	12.89	0.42	0.79
LYS 110	11.37	1.81	0.77
LYS 116	10.66	1.36	0.94
GLU 122	5.07	1.20	1.00
ARG 126	12.92	0.29	0.09
LYS 127	10.54	1.62	0.86
GLU 129	4.04	0.70	0.98
LYS 133	10.65	0.99	0.97
LYS 134	10.42	1.41	0.98
GLU 135	4.60	1.85	1.00
LYS 136	10.66	0.72	0.99

Δ+PHS L125E			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 9	12.17	1.89	0.81
GLU 10	4.14	0.87	0.99
LYS 16	10.47	1.69	0.91
ASP 19	3.55	0.70	1.00
ASP 21	5.42	0.59	0.99
LYS 24	9.99	1.86	0.96
LYS 28	12.06	1.86	0.82
ARG 35	13.09	1.95	0.99
ASP 40	3.13	0.76	0.99
GLU 43	3.70	1.02	0.99
GLU 52	4.56	0.53	0.98
LYS 53	11.08	1.52	0.93
GLU 57	4.21	1.00	1.00
LYS 63	10.91	1.70	0.92
LYS 64	10.61	1.63	0.94
GLU 67	3.82	1.21	0.99
LYS 70	11.06	1.51	0.97
LYS 71	10.60	1.75	0.96
GLU 73	2.70	1.20	1.00
GLU 75	4.73	0.92	1.00
ASP 77	0.61	0.31	0.95
LYS 78	10.91	1.79	0.92
ARG 81	13.10	1.95	0.97
ASP 83	3.58	1.69	0.98
LYS 84	11.22	1.36	0.99
ARG 87	13.04	1.56	0.99
ASP 95	3.34	1.10	1.00
LYS 97	10.79	1.85	0.90
GLU 101	3.79	0.69	0.99
ARG 105	12.84	1.90	0.77
LYS 110	11.43	0.70	1.00
LYS 116	10.55	1.44	0.99
GLU 122	4.59	0.76	0.99
GLU 125	6.83	0.71	0.96
ARG 126	13.10	1.95	0.99
LYS 127	10.59	1.63	0.94
GLU 129	4.35	0.99	1.00
LYS 133	10.84	1.81	0.93
LYS 134	10.68	1.77	0.92
GLU 135	3.98	1.49	1.00
LYS 136	10.86	1.83	0.94

Δ+PHS N100E			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 9	11.75	1.81	0.84
GLU 10	3.96	0.83	0.97
LYS 16	10.39	1.72	0.95
ASP 19	3.79	0.82	0.99
ASP 21	5.17	0.50	0.95
LYS 24	9.70	1.77	0.94
LYS 28	11.52	1.81	0.82
ARG 35	13.13	0.18	0.67
ASP 40	3.36	1.19	0.99
GLU 43	4.07	0.99	0.99
GLU 52	4.91	0.72	0.99
LYS 53	10.94	0.75	1.00
GLU 57	4.65	0.77	0.98
LYS 63	10.77	0.88	1.00
LYS 64	10.80	0.70	1.00
GLU 67	4.08	1.91	1.00
LYS 70	10.81	0.79	0.98
LYS 71	10.99	1.39	0.98
GLU 73	2.58	0.86	1.00
GLU 75	4.71	1.79	0.99
ASP 77	1.06	0.36	0.74
LYS 78	10.64	0.73	1.00
ARG 81	13.13	0.19	0.73
ASP 83	4.11	1.12	0.99
LYS 84	11.36	1.70	0.86
ARG 87	13.10	0.21	0.81
ASP 95	3.69	1.54	1.00
LYS 97	11.02	1.41	0.99
GLU 100	5.76	0.95	0.99
GLU 101	3.71	0.55	0.97
ARG 105	13.43	1.59	0.85
LYS 110	11.50	1.76	0.84
LYS 116	10.68	0.92	0.99
GLU 122	4.98	0.78	0.97
ARG 126	13.12	0.19	0.74
LYS 127	10.29	1.78	0.95
GLU 129	4.39	0.96	1.00
LYS 133	11.10	0.79	1.00
LYS 134	10.29	1.80	0.95
GLU 135	4.27	1.14	0.99
LYS 136	10.73	1.18	1.00

Δ+PHS N118E			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 9	13.46	0.44	0.96
GLU 10	3.76	0.80	0.97
LYS 16	9.91	1.74	0.71
ASP 19	3.38	0.90	0.98
ASP 21	5.44	0.98	0.98
LYS 24	9.62	0.79	1.00
LYS 28	13.10	1.68	0.90
ARG 35	13.19	1.58	0.00
ASP 40	2.81	1.06	1.00
GLU 43	4.07	0.76	0.98
GLU 52	4.76	0.84	0.99
LYS 53	11.81	0.43	0.25
GLU 57	4.23	0.77	0.99
LYS 63	12.37	0.21	0.99
LYS 64	10.45	1.70	0.73
GLU 67	3.76	0.94	0.99
LYS 70	13.15	0.31	0.96
LYS 71	13.35	0.27	0.94
GLU 73	2.82	0.99	0.98
GLU 75	4.24	0.76	0.96
ASP 77	5.35	0.40	0.92
LYS 78	12.23	0.24	0.75
ARG 81	13.19	1.58	0.00
ASP 83	4.23	0.99	0.96
LYS 84	13.15	1.59	0.18
ARG 87	13.19	1.58	0.00
ASP 95	3.51	1.18	0.98
LYS 97	12.14	0.27	0.35
GLU 101	3.84	0.91	0.98
ARG 105	13.18	1.60	1.00
LYS 110	12.84	0.43	0.99
LYS 116	10.55	1.69	0.69
GLU 118	2.50	0.44	0.88
GLU 122	4.66	0.85	0.99
ARG 126	13.19	1.58	0.00
LYS 127	10.70	1.46	0.80
GLU 129	4.23	0.81	0.98
LYS 133	11.82	0.39	0.29
LYS 134	12.33	0.22	0.96
GLU 135	4.40	1.02	0.99
LYS 136	12.04	0.29	0.36

Δ+PHS T41E			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 9	11.90	1.80	0.78
GLU 10	3.81	0.88	0.97
LYS 16	10.51	0.88	0.99
ASP 19	4.32	0.61	0.94
ASP 21	5.95	0.45	0.95
LYS 24	9.71	1.74	0.93
LYS 28	11.91	1.79	0.80
ARG 35	13.15	0.18	0.71
ASP 40	2.53	1.09	1.00
GLU 41	6.52	0.42	0.91
GLU 43	4.02	0.70	0.98
GLU 52	4.65	0.82	0.99
LYS 53	10.92	1.63	0.90
GLU 57	4.19	1.63	0.98
LYS 63	10.74	1.41	1.00
LYS 64	10.89	0.86	1.00
GLU 67	4.08	1.34	0.99
LYS 70	11.28	1.79	0.82
LYS 71	10.61	1.14	0.99
GLU 73	2.37	0.62	0.97
GLU 75	4.78	1.02	0.99
ASP 77	1.76	0.78	0.98
LYS 78	11.09	1.69	0.86
ARG 81	13.15	0.18	0.75
ASP 83	4.08	1.04	0.99
LYS 84	11.11	1.67	0.82
ARG 87	13.62	1.97	1.00
ASP 95	3.34	0.76	0.98
LYS 97	10.35	1.02	0.99
GLU 101	3.90	0.97	0.99
ARG 105	13.63	1.81	0.98
LYS 110	11.87	1.81	0.75
LYS 116	10.66	1.42	1.00
GLU 122	4.92	0.93	0.99
ARG 126	13.15	0.18	0.65
LYS 127	9.94	1.77	0.93
GLU 129	4.22	0.78	0.99
LYS 133	10.48	0.98	0.99
LYS 134	10.45	1.22	1.00
GLU 135	4.61	0.87	0.99
LYS 136	10.70	0.86	1.00

Δ+PHS T62E			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 9	11.52	0.76	0.99
GLU 10	3.41	0.82	0.98
LYS 16	10.23	1.78	0.95
ASP 19	2.93	0.65	0.99
ASP 21	5.11	0.47	0.96
LYS 24	9.70	1.77	0.94
LYS 28	11.76	1.69	1.00
ARG 35	13.25	0.16	0.74
ASP 40	2.75	0.59	0.95
GLU 43	4.13	0.75	0.99
GLU 52	4.84	0.95	0.98
LYS 53	10.67	1.78	0.93
GLU 57	4.34	1.15	0.98
GLU 62	6.93	1.17	0.97
LYS 63	10.68	1.81	0.95
LYS 64	10.67	1.78	0.95
GLU 67	3.90	1.08	0.99
LYS 70	11.26	0.94	1.00
LYS 71	10.72	1.80	0.95
GLU 73	3.05	0.79	0.98
GLU 75	5.04	0.70	0.97
ASP 77	1.17	0.47	0.90
LYS 78	10.97	1.72	0.94
ARG 81	13.24	0.17	0.77
ASP 83	3.58	1.01	0.99
LYS 84	11.35	1.36	0.99
ARG 87	13.20	0.19	0.82
ASP 95	3.32	0.78	0.98
LYS 97	11.02	1.74	0.95
GLU 101	3.77	1.91	0.99
ARG 105	13.59	1.77	0.93
LYS 110	11.55	0.82	1.00
LYS 116	10.80	1.81	0.95
GLU 122	4.80	0.74	0.98
ARG 126	13.22	0.17	0.67
LYS 127	10.27	1.79	0.95
GLU 129	4.13	0.96	0.99
LYS 133	10.61	1.81	0.94
LYS 134	10.39	1.78	0.94
GLU 135	4.15	1.03	0.99
LYS 136	11.17	1.64	0.95

Δ+PHS V23E			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 9	11.35	1.79	0.83
GLU 10	3.87	0.98	0.98
LYS 16	10.54	1.59	0.94
ASP 19	3.47	0.78	0.99
ASP 21	5.20	0.44	0.92
GLU 23	6.95	0.71	0.97
LYS 24	10.16	1.82	0.96
LYS 28	12.15	1.06	0.98
ARG 35	13.14	0.18	0.88
ASP 40	2.95	0.75	0.99
GLU 43	4.02	0.64	0.98
GLU 52	4.53	0.81	0.97
LYS 53	10.92	1.61	0.87
GLU 57	4.48	0.78	0.97
LYS 63	10.49	0.89	1.00
LYS 64	10.54	1.08	1.00
GLU 67	3.71	0.67	0.98
LYS 70	10.92	1.58	0.93
LYS 71	10.74	0.88	1.00
GLU 73	2.80	0.98	0.99
GLU 75	4.63	0.65	0.96
ASP 77	0.75	0.39	0.86
LYS 78	10.90	1.40	0.99
ARG 81	13.13	0.19	0.71
ASP 83	4.05	1.05	0.98
LYS 84	11.39	1.77	0.84
ARG 87	13.12	0.20	0.75
ASP 95	3.17	1.07	0.98
LYS 97	11.00	0.84	0.99
GLU 101	3.43	0.59	0.97
ARG 105	13.12	0.20	0.82
LYS 110	10.82	1.26	1.00
LYS 116	10.34	0.88	0.99
GLU 122	4.92	0.94	0.98
ARG 126	13.13	0.19	0.73
LYS 127	10.69	1.56	1.00
GLU 129	4.37	1.15	0.99
LYS 133	10.82	0.67	0.99
LYS 134	10.54	1.47	0.95
GLU 135	4.43	1.36	0.99
LYS 136	10.58	0.81	1.00

Δ+PHS V39E			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 9	11.48	1.70	0.88
GLU 10	3.32	0.62	0.99
LYS 16	10.23	1.66	0.90
ASP 19	3.61	0.77	0.99
ASP 21	5.34	0.39	0.94
LYS 24	9.85	1.69	0.92
LYS 28	11.36	0.72	1.00
ARG 35	13.21	0.21	0.70
GLU 39	4.55	0.50	0.94
ASP 40	2.95	0.43	0.95
GLU 43	3.88	0.79	0.99
GLU 52	5.23	0.91	0.99
LYS 53	10.98	0.86	0.99
GLU 57	4.42	0.71	0.99
LYS 63	10.61	1.84	0.91
LYS 64	10.63	1.78	0.90
GLU 67	4.15	1.56	1.00
LYS 70	11.13	1.32	0.98
LYS 71	10.80	1.75	0.92
GLU 73	2.22	0.64	1.00
GLU 75	4.76	0.92	0.97
ASP 77	0.94	0.77	1.00
LYS 78	10.56	1.45	0.98
ARG 81	13.19	0.24	0.70
ASP 83	4.37	1.71	0.99
LYS 84	11.40	0.91	0.99
ARG 87	13.53	1.88	0.86
ASP 95	3.59	1.86	0.99
LYS 97	10.67	1.82	0.93
GLU 101	3.75	0.86	0.99
ARG 105	13.31	1.61	0.92
LYS 110	11.29	0.87	1.00
LYS 116	10.49	1.69	0.87
GLU 122	4.89	1.00	0.98
ARG 126	13.17	0.28	0.84
LYS 127	10.84	1.81	0.94
GLU 129	3.82	0.99	0.99
LYS 133	10.78	1.79	0.94
LYS 134	10.45	1.45	0.97
GLU 135	4.21	0.76	0.99
LYS 136	10.48	1.68	0.91

Δ+PHS V66E			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 9	13.23	1.89	0.27
GLU 10	3.62	1.11	0.99
LYS 16	10.30	0.87	0.99
ASP 19	3.52	0.71	0.99
ASP 21	5.34	0.67	0.99
LYS 24	9.81	1.80	0.91
LYS 28	13.53	1.82	0.90
ARG 35	13.32	1.90	0.99
ASP 40	2.27	0.72	1.00
GLU 43	3.57	0.94	1.00
GLU 52	4.62	0.58	0.99
LYS 53	12.03	1.84	0.14
GLU 57	4.19	0.67	0.97
LYS 63	11.08	0.44	0.93
LYS 64	10.88	1.75	0.94
GLU 66	6.39	0.37	0.92
GLU 67	4.00	0.67	1.00
LYS 70	11.86	0.30	0.70
LYS 71	12.12	1.70	0.53
GLU 73	2.77	0.69	0.99
GLU 75	4.68	0.68	0.99
ASP 77	0.51	0.56	0.80
LYS 78	10.82	1.72	0.88
ARG 81	12.95	0.30	0.00
ASP 83	3.78	1.31	1.00
LYS 84	13.53	1.82	0.84
ARG 87	13.32	1.90	0.93
ASP 95	3.69	0.96	1.00
LYS 97	12.16	1.80	0.35
GLU 101	3.53	0.82	0.99
ARG 105	12.95	0.30	0.42
LYS 110	12.61	0.42	0.16
LYS 116	10.59	1.85	0.68
GLU 122	4.57	0.83	0.99
ARG 126	12.95	0.30	0.58
LYS 127	10.37	1.06	0.98
GLU 129	3.93	0.84	1.00
LYS 133	11.74	0.32	0.83
LYS 134	11.17	0.38	0.93
GLU 135	4.37	0.79	0.98
LYS 136	10.71	0.31	0.87

Δ+PHS V74E			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 9	11.61	1.69	0.87
GLU 10	3.94	0.73	0.99
LYS 16	10.60	1.83	0.94
ASP 19	2.99	1.09	0.99
ASP 21	5.35	0.67	0.99
LYS 24	9.74	0.35	0.96
LYS 28	11.84	1.83	0.80
ARG 35	13.11	1.85	1.00
ASP 40	2.81	0.80	1.00
GLU 43	4.29	0.76	0.99
GLU 52	4.30	0.98	0.99
LYS 53	11.01	1.63	0.92
GLU 57	4.39	0.67	0.99
LYS 63	10.24	1.93	0.82
LYS 64	10.63	1.88	0.94
GLU 67	3.96	1.11	1.00
LYS 70	10.87	1.83	0.90
LYS 71	10.74	1.88	0.94
GLU 73	3.07	0.95	1.00
GLU 74	8.40	0.74	0.94
GLU 75	5.02	0.86	0.99
ASP 77	0.52	0.75	0.08
LYS 78	11.29	1.92	0.80
ARG 81	13.11	1.85	1.00
ASP 83	4.34	1.69	1.00
LYS 84	11.35	0.69	1.00
ARG 87	13.15	1.93	0.89
ASP 95	3.53	0.69	1.00
LYS 97	10.53	1.93	0.82
GLU 101	3.21	0.55	0.98
ARG 105	12.99	1.66	0.89
LYS 110	11.37	0.71	1.00
LYS 116	10.45	1.93	0.82
GLU 122	5.09	0.84	0.98
ARG 126	13.17	1.92	1.00
LYS 127	10.01	1.91	0.84
GLU 129	4.15	1.13	1.00
LYS 133	10.69	1.90	0.97
LYS 134	10.38	1.92	0.84
GLU 135	4.34	0.99	1.00
LYS 136	10.65	1.88	0.97

Δ+PHS V99E			
Residue	Calculated pKa	Hill Coefficient	Correlation
LYS 9	12.38	1.98	0.76
GLU 10	3.35	0.61	0.97
LYS 16	12.83	0.14	0.13
ASP 19	0.42	0.28	0.60
ASP 21	5.69	1.52	0.93
LYS 24	11.02	0.17	0.91
LYS 28	12.30	1.98	0.79
ARG 35	13.82	0.17	0.00
ASP 40	3.25	0.69	1.00
GLU 43	4.06	0.86	0.99
GLU 52	4.75	1.05	1.00
LYS 53	12.92	1.98	0.80
GLU 57	4.82	0.98	0.99
LYS 63	13.20	0.13	0.78
LYS 64	13.26	0.19	0.91
GLU 67	3.56	0.78	0.99
LYS 70	12.85	1.98	0.77
LYS 71	10.23	1.98	0.80
GLU 73	3.39	1.45	1.00
GLU 75	4.53	1.12	0.97
ASP 77	0.93	0.52	0.24
LYS 78	13.29	0.17	0.87
ARG 81	13.83	0.13	0.54
ASP 83	4.47	1.81	1.00
LYS 84	12.92	1.98	0.76
ARG 87	13.82	0.15	0.54
ASP 95	3.49	0.76	1.00
LYS 97	13.27	0.16	0.87
GLU 99	7.19	1.88	0.85
GLU 101	3.70	0.94	1.00
ARG 105	13.87	1.99	0.95
LYS 110	12.32	1.98	0.76
LYS 116	13.17	0.13	0.87
GLU 122	4.68	1.24	1.00
ARG 126	13.83	0.13	0.58
LYS 127	12.91	0.15	0.12
GLU 129	4.58	1.02	1.00
LYS 133	13.16	0.13	0.83
LYS 134	13.10	0.13	0.87
GLU 135	4.47	0.81	0.98
LYS 136	10.32	1.98	0.73