Title: Titration_DB: Storage and Analysis of NMR-monitored Protein pH Titration Curves

Supplementary Material

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Table 1: List of all extracted 'primary' pKa values from the titration database for ^{1}H data.

H^{β}* and H^{γ}* in Asp/Glu denote undifferentiated $H^{\beta 2}$/ $H^{\beta 3}$ and $H^{\gamma 2}$/ $H^{\gamma 3}$ assignments.

protein	res type	res num	atom	Δδ	Δδ error	pKa	pKa error
Amicyanin (Paracoccus Versutus) - Met99Gln	HIS	96	HE1	1.01	0.01	7.08	0.02
Apomyoglobin (Horse)	HIS	1	HD2	0.29	0.01	6.62	0.05
Apomyoglobin (Horse)	HIS	4	HE1	0.92	0.02	5.68	0.03
Apomyoglobin (Horse)	HIS	36	HD2	0.52	0.01	7.61	0.04
Apomyoglobin (Horse)	HIS	48	HE1	0.69	0.03	5.41	0.04
Apomyoglobin (Whale)	HIS	119	HD2	0.18	0.01	5.8	0.12
Apomyoglobin (Whale) (Paper 2)	HIS	12	HE1	0.78	0.02	6.2	0.05
Apomyoglobin (Whale) (Paper 2)	HIS	12	HD2	0.29	0.02	6.24	0.09
Apomyoglobin (Whale) (Paper 2)	HIS	48	HE1	0.61	0.01	5.58	0.03
Apomyoglobin (Whale) (Paper 2)	HIS	48	HD2	0.31	0.01	5.55	0.05
Apomyoglobin (Whale) (Paper 2)	HIS	81	HD2	0.22	0.02	6.07	0.13
Apomyoglobin (Whale) (Paper 2)	HIS	116	HD2	0.23	0.06	6.09	0.18
Apomyoglobin (Whale) (Paper 2)	HIS	116	HE1	0.6	0.24	6.11	0.18
ATP Synthase	GLU	2	HG*	0.16	0.01	5.6	0.17
ATP Synthase	GLU	37	HG*	0.24	0.03	5.53	0.16
ATP Synthase	ASP	44	HA	0.11	0.01	5.62	0.1
ATP Synthase - D24D61	ASP	44	HB*	0.23	0.01	5.62	0.08
ATP Synthase - D24D61	ASP	61	HB*	0.22	0.01	6.94	0.07

ATP Synthase - D24N61	ASP	7	HB*	0.34	0.01	6.3	0.04
ATP Synthase - D24N61	ASP	24	HB*	0.25	0.01	6.84	0.08
ATP Synthase - D24N61	ASP	44	HB*	0.23	0.01	5.59	0.07
Barnase	ASP	22	HB*	0.23	0.03	3.27	0.14
Barnase	GLU	29	HG*	0.14	0.01	3.79	0.12
Barnase	ASP	44	HB*	0.21	0.01	3.31	0.1
Barnase	ASP	86	HB*	0.31	0.01	3.66	0.04
Bovine Beta-Lactoglobulin	LYS	101	H	0.58	0.12	2.65	0.11
Bovine Beta-Lactoglobulin	GLU	112	H	0.13	0.01	5.73	0.08
Bovine Beta-Lactoglobulin	GLU	114	H	0.33	0.01	3.71	0.05
Bovine Beta-Lactoglobulin	LYS	135	H	0.07	0.01	4.77	0.29
Calbindin D9k - P43G	LYS	1	H	0.4	0.01	10.65	0.03
Calbindin D9k - P43G	LYS	7	H	0.42	0.01	11.41	0.04
Calbindin D9k - P43G	LYS	16	H	0.38	0.01	10.16	0.03
Calbindin D9k - P43G	LYS	25	H	0.33	0.04	11.92	0.08
Calbindin D9k - P43G	LYS	29	H	0.28	0.01	11.06	0.05
Calbindin D9k - P43G	LYS	41	H	0.33	0.01	10.97	0.06
Calbindin D9k - P43G	LYS	55	H	0.44	0.01	11.44	0.04
Calbindin D9k - P43G	LYS	71	H	0.37	0.01	10.72	0.04
Calbindin D9k - P43G	LYS	72	H	0.23	0.01	11.01	0.07
Cardiotoxin V (Cobra)	GLU	17	HG*	0.24	0.01	3.89	0.1
Chymotrypsin inhibitor 2	GLU	4	H	0.18	0.01	2.86	0.13
Chymotrypsin inhibitor 2	GLU	4	H	0.2	0.01	3.2	0.07
Chymotrypsin inhibitor 2	GLU	7	H	1.93	0.01	3.18	0.03

Chymotrypsin inhibitor 2	GLU	7	H	1.79	0.03	2.88	0.03
Chymotrypsin inhibitor 2	GLU	14	H	0.22	0.01	3.43	0.11
Chymotrypsin inhibitor 2	GLU	15	H	0.25	0.01	2.75	0.08
Chymotrypsin inhibitor 2	GLU	26	H	1.23	0.01	3.59	0.03
Chymotrypsin inhibitor 2	GLU	26	H	1.16	0.01	3.84	0.03
Chymotrypsin inhibitor 2	GLU	41	H	0.74	0.01	3.44	0.02
Chymotrypsin inhibitor 2	GLU	41	H	0.79	0.01	3.1	0.03
Chymotrypsin inhibitor 2	ASP	45	H	0.23	0.01	3.73	0.08
Chymotrypsin inhibitor 2	ASP	52	H	0.28	0.01	2.82	0.05
Chymotrypsin inhibitor 2	ASP	52	H	0.47	0.03	2.35	0.07
Chymotrypsin inhibitor 2	ASP	55	H	0.28	0.01	4.9	0.08
Chymotrypsin inhibitor 2	ASP	55	H	0.25	0.01	4.81	0.07
Cytotoxic Ribonuclease alpha-Sarcin	LYS	11	H	0.79	0.01	4.06	0.03
Cytotoxic Ribonuclease alpha-Sarcin	HIS	35	HE1	1.02	0.01	6.24	0.02
Cytotoxic Ribonuclease alpha-Sarcin	ASP	59	HB*	0.37	0.01	4.05	0.05
Cytotoxic Ribonuclease alpha-Sarcin	ASP	59	H	0.44	0.01	3.88	0.05
Cytotoxic Ribonuclease alpha-Sarcin	LYS	61	H	0.76	0.02	3.87	0.03
Cytotoxic Ribonuclease alpha-Sarcin	HIS	92	HE1	0.96	0.01	7.09	0.02
Cytotoxic Ribonuclease alpha-Sarcin	HIS	137	HE1	1.23	0.01	5.83	0.02
Cytotoxic Ribonuclease alpha-Sarcin	HIS	137	HE1	1.16	0.01	6.82	0.02
Cytotoxic Ribonuclease alpha-Sarcin	HIS	137	HB*	0.5	0.01	5.73	0.03
Cytotoxic Ribonuclease alpha-Sarcin	HIS	150	HE1	0.7	0.01	7.59	0.04
Flavodoxin (Desulfovibrio vulgaris) - N14H	HIS	14	HD2	0.32	0.01	6.93	0.05
Flavodoxin (Desulfovibrio vulgaris) - N14H	HIS	14	HE1	0.79	0.01	6.82	0.03

Flavodoxin (Desulfovibrio vulgaris) - N14H	HIS	142	HE1	0.94	0.01	6.93	0.02
Flavodoxin (Desulfovibrio vulgaris) - N14H	HIS	142	HD2	0.28	0.01	7.04	0.04
Flavodoxin (Desulfovibrio vulgaris) - T12H	HIS	12	HE1	1.05	0.01	6.7	0.02
Flavodoxin (Desulfovibrio vulgaris) - T12H	HIS	12	HD2	0.35	0.01	6.74	0.04
Flavodoxin (Desulfovibrio vulgaris) - T12H	HIS	142	HD2	0.29	0.01	7.1	0.05
Flavodoxin (Desulfovibrio vulgaris) - T12H	HIS	142	HE1	0.94	0	7.09	0.02
GDP-Mannose Mannosyl Hydrolase	HIS	124	HE1	0.87	0.01	6.96	0.02
GDP-Mannose Mannosyl Hydrolase - E70Q	HIS	124	H	0.78	0.01	7.08	0.03
Glucocorticoid Receptor DNA-Binding Domain (Rat)	HIS	472	H	0.89	0.04	6.32	0.05
Glucocorticoid Receptor DNA-Binding Domain (Rat)	HIS	472	H	1.09	0.13	6.27	0.08
Glucose 6-phosphate dehydrogenase (Leuconostoc mesenteroides)	HIS	240	HE1	0.27	0.01	6.43	0.05
HasA SM hemophore (Serratia marcescens)	HIS	83	H	0.96	0.01	5.61	0.04
Heterodimeric Leucine Zipper	GLU	1	HG*	0.17	0	4.22	0.09
Heterodimeric Leucine Zipper	GLU	1	HG*	0.26	0.01	4.13	0.04
Heterodimeric Leucine Zipper	GLU	8	HG*	0.29	0.01	4.52	0.05
Heterodimeric Leucine Zipper	GLU	13	HG*	0.26	0.01	4.33	0.05
Heterodimeric Leucine Zipper	GLU	29	HG*	0.24	0.01	4.62	0.05
HEWL	ASP	101	H	0.1	0.01	3.83	0.21
HEWL	ASP	119	H	0.08	0.01	3.9	0.14
Hirudin	ASP	33	HB*	0.3	0.01	4.36	0.04
Hirudin	GLU	35	H	0.27	0.01	4	0.05
Hirudin	GLU	35	HG*	0.3	0.01	4.84	0.05
Hirudin	GLU	43	HG*	0.23	0.01	4.24	0.06

Hirudin (Hirudo medicinalis) - D33N	GLU	35	H	0.14	0.01	4.33	0.15
Kinase ArcB	HIS	717	HD2	0.38	0	6.76	0.02
Kinase ArcB	HIS	717	HE1	0.98	0	6.76	0.01
Kinase ArcB	HIS	730	HD2	0.15	0.01	5.87	0.09
Kinase ArcB	HIS	763	HE1	0.94	0.01	7.08	0.02
Kinase ArcB	HIS	763	HD2	0.36	0.01	7.17	0.04
Leucine Zippers	GLU	15	HG*	0.21	0.01	4.3	0.06
Leucine Zippers	GLU	15	HG*	0.23	0.01	4.08	0.04
Leucine Zippers	GLU	22	HG*	0.23	0.01	4.64	0.14
Lysozyme (Hen)	GLU	7	HA	0.07	0.01	2.83	0.38
Lysozyme (Hen)	HIS	15	HB*	0.35	0.01	5.36	0.05
Lysozyme (Hen)	ASP	18	HB*	0.27	0.01	2.66	0.04
Lysozyme (Hen)	ASP	52	HB*	0.27	0	3.68	0.06
Lysozyme (Hen)	ASP	87	HB*	0.18	0.02	2.13	0.12
Lysozyme (Hen)	ASP	87	HA	0.14	0.01	2.08	0.11
Lysozyme (Hen)	ASP	119	HB*	0.21	0.01	3.2	0.07
Lysozyme (Hen)	ASP	119	HA	0.11	0.01	3.28	0.12
Lysozyme (Turkey)	GLU	7	HB*	0.24	0.01	2.68	0.07
Lysozyme (Turkey)	GLU	7	HA	0.08	0.01	2.67	0.28
Lysozyme (Turkey)	ASP	18	HB*	0.28	0.01	2.68	0.07
Lysozyme (Turkey)	ASP	18	HB*	0.14	0.01	2.57	0.14
Lysozyme (Turkey)	HIS	41	HB*	0.43	0.01	5.53	0.04
Lysozyme (Turkey)	ASP	66	HB*	0.27	0.07	1.48	0.2
Lysozyme (Turkey)	ASP	66	H	0.12	0.01	3.69	0.08

Lysozyme (Turkey)	ASP	87	H	0.08	0.01	2.18	0.21
Lysozyme (Turkey)	ASP	87	HA	0.15	0.01	2.14	0.13
Lysozyme (Turkey)	ASP	87	HB*	0.1	0.01	2.85	0.21
Lysozyme (Turkey)	ASP	87	H	0.08	0.01	2.18	0.15
Lysozyme (Turkey)	ASP	119	HA	0.09	0.01	3.09	0.12
Lysozyme (Turkey)	ASP	119	H	0.12	0.01	3.13	0.11
Lysozyme (Turkey)	HIS		HD2	0.27	0.01	5.28	0.05
Lysozyme (Turkey)	HIS		HD1	0.29	0.01	4.98	0.04
Lysozyme (Turkey)	ASP		HB*	0.13	0.01	2.48	0.14
Metaquomyoglobin (Whale)	HIS	24	HE1	0.22	0.01	6.1	0.06
Metaquomyoglobin (Whale)	HIS	119	HD2	0.21	0.01	6.17	0.06
N-Terminal Domain of L9	ASP	8	HB*	0.37	0.01	3.16	0.03
N-Terminal Domain of L9	ASP	8	HB*	0.36	0.01	2.99	0.03
N-Terminal Domain of L9	GLU	17	HG*	0.25	0.01	3.57	0.05
N-Terminal Domain of L9	GLU	17	HG*	0.27	0.01	3.75	0.05
N-Terminal Domain of L9	ASP	23	HB*	0.3	0.01	3.07	0.06
N-Terminal Domain of L9	ASP	23	HB*	0.35	0.01	3.21	0.05
N-Terminal Domain of L9	GLU	38	HG*	0.18	0.01	4.09	0.1
N-Terminal Domain of L9	GLU	38	HG*	0.22	0.01	4.04	0.07
N-Terminal Domain of L9	GLU	48	HG*	0.32	0.01	4.17	0.05
N-Terminal Domain of L9	GLU	48	HG*	0.28	0.01	4.34	0.05
N-Terminal Domain of L9	GLU	54	HG*	0.3	0.01	4.24	0.05
N-Terminal Domain of L9	GLU	54	HG*	0.18	0.01	4.16	0.08
Nucleocapsid Protein (HIV-1)	HIS	44	HD2	0.88	0.01	6.47	0.02

Nucleocapsid Protein (HIV-1)	HIS	44	HE1	0.32	0.01	6.43	0.06
Ovomucoid Third Domain(Turkey)	ASP	7	HB*	0.25	0.01	2.68	0.06
Ovomucoid Third Domain(Turkey)	GLU	10	HG*	0.25	0	4.08	0.05
Ovomucoid Third Domain(Turkey)	GLU	10	H	0.2	0	4.1	0.05
Ovomucoid Third Domain(Turkey)	GLU	10	H	0.21	0	4.05	0.04
Ovomucoid Third Domain(Turkey)	GLU	10	H	0.2	0	4.13	0.05
Ovomucoid Third Domain(Turkey)	GLU	19	H	0.62	0.01	3.2	0.02
Ovomucoid Third Domain(Turkey)	GLU	19	H	0.46	0.01	3.97	0.03
Ovomucoid Third Domain(Turkey)	GLU	19	H	0.63	0	3.17	0.02
Ovomucoid Third Domain(Turkey)	ASP	27	H	0.88	0.01	2.8	0.02
Ovomucoid Third Domain(Turkey)	ASP	27	H	0.92	0.01	2.27	0.03
Ovomucoid Third Domain(Turkey)	ASP	27	H	0.48	0.03	2.33	0.06
Ovomucoid Third Domain(Turkey)	GLU	43	HG*	0.19	0.01	4.79	0.07
Plastocyanin (Anabaena variabilis)	HIS	39	HD1	0.32	0.01	5.19	0.05
Plastocyanin (Anabaena variabilis)	HIS	39	H	0.27	0.01	5.1	0.05
Plastocyanin (Phormidium)	ASP	10	H	0.63	0.06	4.36	0.06
Plastocyanin (Phormidium)	HIS	39	H	0.33	0.01	5.16	0.04
Plastocyanin (Phormidium)	GLU	70	H	0.11	0.07	8.08	0.25
Prolactin	HIS	27	HE1	0.71	0.01	6.48	0.03
Prolactin	HIS	46	HE1	0.83	0.01	6.54	0.02
Prolactin	HIS	59	HE1	0.84	0.01	6.26	0.02
Prolactin	HIS	138	HE1	0.88	0.01	5.84	0.02
Prolactin	HIS	195	HE1	0.91	0.01	5.87	0.02
Prolactin (H180A)	HIS	46	HE1	0.82	0.01	6.51	0.04

Prolactin (H180A)	HIS	59	HE1	0.87	0.01	6.17	0.03
Prolactin (H180A)	HIS	97	HE1	0.86	0.01	6.24	0.03
Prolactin (H180A)	HIS	138	HE1	0.92	0.01	5.8	0.04
Prolactin (H180A)	HIS	173	HE1	0.85	0.02	4.98	0.03
Prolactin (H180A)	HIS	195	HE1	0.94	0.01	5.88	0.03
Prolactin (H27A)	HIS	30	HE1	0.57	0.1	5.95	0.12
Prolactin (H27A)	HIS	97	HE1	0.79	0.02	6.21	0.06
Prolactin (H27A)	HIS	138	HE1	0.9	0.01	5.72	0.02
Prolactin (H27A)	HIS	195	HE1	0.94	0.01	5.81	0.03
Prolactin (H30A)	HIS	46	HE1	0.82	0.01	6.66	0.04
Prolactin (H30A)	HIS	59	HE1	0.86	0.01	6.28	0.03
Prolactin (H30A)	HIS	97	HE1	0.82	0.02	6.33	0.06
Prolactin (H30A)	HIS	180	HE1	0.91	0.01	6.14	0.04
Prolactin (H30A)	HIS	195	HE1	0.91	0.01	6.04	0.03
Protein Tyrosine Phosphatase	HIS	66	HD2	0.48	0.01	7	0.03
Protein Tyrosine Phosphatase	HIS	66	HD2	0.43	0.01	8.34	0.04
Protein Tyrosine Phosphatase	HIS	66	HE1	1.03	0	7	0.03
Protein Tyrosine Phosphatase	HIS	66	HD2	0.39	0	8.18	0.06
Protein Tyrosine Phosphatase	HIS	72	HE1	1.02	0.01	7.46	0.02
Protein Tyrosine Phosphatase	HIS	72	HD2	0.12	0.02	5.42	0.19
Protein Tyrosine Phosphatase	HIS	72	HE1	1.03	0.01	9.19	0.03
Protein Tyrosine Phosphatase	HIS	72	HE1	0.97	0.01	9.18	0.02
Pseudoazurin (Achromobacter cycloclastes)	HIS	6	H	1.01	0.01	7.29	0.02
Pseudoazurin (Achromobacter cycloclastes)	HIS	6	H	1.09	0.01	6.61	0.02

Ribonuclease HI (Escherichia coli)	GLU	32	HG*	0.44	0.01	3.39	0.05
Ribonuclease HI (Escherichia coli)	GLU	48	HG*	0.24	0.01	3.85	0.1
Ribonuclease HI (Escherichia coli)	GLU	61	HB*	0.21	0.01	4.23	0.08
Ribonuclease HI (Escherichia coli)	GLU	64	HG*	0.25	0.01	4.6	0.05
Ribonuclease HI (Escherichia coli)	ASP	70	HB*	0.18	0.01	6.07	0.07
Ribonuclease HI (Escherichia coli)	ASP	94	HB*	0.14	0.01	2.99	0.18
Ribonuclease HI (Escherichia coli)	ASP	108	HD2	0.09	0.01	3.59	0.16
Ribonuclease HI (Escherichia coli)	GLU	135	HG*	0.3	0.01	4.6	0.06
Ribonuclease HI (Escherichia coli)	GLU	147	HG*	0.23	0.01	4.18	0.07
Ribonuclease HI (Escherichia coli)	GLU	147	HB*	0.21	0.01	4.04	0.06
Ribonuclease HI (Escherichia coli) (Paper 2)	HIS	83	H	1.02	0.01	5.39	0.02
Ribonuclease HI (Escherichia coli) (Paper 2)	HIS	114	H	0.31	0.02	4.64	0.09
Ribonuclease S (Bovine)	HIS	12	H	1.05	0.01	6.7	0.02
Ribonuclease S (Bovine)	HIS	105	H	0.99	0.01	6.75	0.02
Ribonuclease S (Bovine)	HIS	105	HE1	1.04	0.01	6.74	0.02
Sso7d	GLU	11	H	0.24	0	3.5	0.04
Sso7d	ASP	34	H	0.21	0.01	2.21	0.07
Sso7d	GLU	35	H	0.12	0	5.29	0.05
Sso7d	ASP	49	H	0.18	0.01	3.08	0.04
Sso7d	ASP	49	H	0.17	0.01	3.06	0.06
Sso7d	GLU	53	H	0.07	0	8.01	0.24
Staphylococcal Nuclease	HIS	8	HE1	1.01	0.01	6.52	0.02
Staphylococcal Nuclease	HIS	8	HE1	1.02	0.01	7.01	0.02
Staphylococcal Nuclease	HIS	46	HE1	0.8	0	5.86	0.02

Staphylococcal Nuclease	HIS	124	HE1	1.03	0	6.25	0.02
Staphylococcal Nuclease	HIS	124	HE1	0.96	0.01	5.72	0.02
Staphylococcal Nuclease (Paper 2)	HIS	8	HB*	0.37	0.01	6.81	0.03
Staphylococcal Nuclease (Paper 2)	HIS	46	HE1	0.78	0.02	5.82	0.04
Subtilisin BPN	HIS	64	HE1	0.81	0	7.47	0.02
Subtilisin BPN	HIS	238	HD2	0.32	0.01	7.27	0.06
Subtilisin BPN	HIS	238	HE1	1.1	0.01	7.31	0.02
T4 Lysozyme	HIS	31	HB*	1.07	0.01	9.04	0.01
T4 Lysozyme - D70N	HIS	31	HB*	1.23	0.01	6.96	0.02
Ubiquitin	GLU	18	H	1.33	0.01	2.9	0.02
Ubiquitin	ASP	32	HB*	0.29	0.01	3.74	0.04
Ubiquitin	ASP	32	H	0.29	0.01	3.82	0.05
Ubiquitin	GLU	34	H	0.24	0.01	4.46	0.04
Ubiquitin	GLU	34	HG*	0.24	0.01	4.47	0.06
Ubiquitin	ASP	39	H	0.37	0.01	3.53	0.05
Ubiquitin	GLU	51	H	0.27	0.01	3.76	0.05
Ubiquitin	ASP	52	H	0.35	0.01	3.32	0.06
Ubiquitin	GLU	64	H	0.11	0.01	4.57	0.14
Ubiquitin - K11T	GLU	34	HG*	0.24	0.01	5.36	0.11
Ubiquitin - K33Q	ASP	32	HB*	0.3	0.01	3.89	0.04
Ubiquitin - K33Q	GLU	34	HG*	0.23	0.01	4.16	0.05
Ubiquitin - K33T	GLU	34	HG*	0.15	0.01	3.64	0.12
Urokinase Kringle Domain (Human)	HIS	37	HD2	0.37	0	6.47	0.02

Table 2: List of all extracted 'primary' pKa values for ^{15}N data.

protein	res type	res num	atom	Δδ	Δδ error	pKa	pKa error
Apomyoglobin (Whale) (Paper 2)	HIS	36	NE2	2	0.13	6.43	0.07
Apomyoglobin (Whale) (Paper 2)	HIS	48	NE2	2.25	0.04	6.05	0.02
Apomyoglobin (Whale) (Paper 2)	HIS	24	ND1	2.06	0.02	6.42	0.03
Bovine Beta-Lactoglobulin	ASP	11	N	1.81	0.11	2.89	0.07
Bovine Beta-Lactoglobulin	ASP	33	N	0.16	0.04	7.85	0.82
Bovine Beta-Lactoglobulin	GLU	65	N	1.08	0.02	5.25	0.07
Bovine Beta-Lactoglobulin	GLU	108	N	0.94	0.03	6.37	0.04
Bovine Beta-Lactoglobulin	GLU	89	N	0.3	0.04	6.8	0.15
Bovine Beta-Lactoglobulin	LYS	75	N	0.85	0.05	3.73	0.11
Bovine Beta-Lactoglobulin	LYS	8	N	0.61	0.04	4.08	0.21
Bovine Beta-Lactoglobulin	LYS	91	N	0.21	0.01	4.9	0.33
Bovine Beta-Lactoglobulin	LYS	135	N	0.37	0.03	4.76	0.14
Cryptogein	ASP	30	N	2.43	0.03	2.64	0.03
Cryptogein	ASP	21	N	2.12	0.05	2.46	0.04
HEWL	HIS	15	N	2.76	0.02	5.52	0.03
HEWL	LYS	13	N	1.22	0.03	5.65	0.03
Kinase ArcB	HIS	730	NE2	4.08	0.02	5.61	0.03
N-Terminal Domain of Rat CD2	GLU	41	N	0.35	0.02	4.45	0.11
Plastocyanin (Anabaena variabilis)	HIS	92	N	4.32	0.05	5.09	0.02
Plastocyanin (Anabaena variabilis)	LYS	57	N	0.35	0.03	7.17	0.13
Plastocyanin (Phormidium)	ASP	10	N	1.28	0.45	4.26	0.15
Plastocyanin (Phormidium)	ASP	44	N	0.12	0.03	5.82	0.4
Plastocyanin (Phormidium)	HIS	92	N	4.31	0.07	5.11	0.03
Plastocyanin (Phormidium)	HIS	24	N	1.88	0.14	8.01	0.06

Plastocyanin (Phormidium)	HIS	39	N	1.05	0.04	4.95	0.04
Plastocyanin (Phormidium)	LYS	35	N	0.96	0.04	5.04	0.05

Table 3: List of all extracted 'primary' pKa for ^{13}C data.

protein	res type	res num	atom	Δδ	Δδ error	pKa	pKa error
Apolipoprotein E (Human)	LYS	22	CE	1.08	0.07	10.27	0.11
Apolipoprotein E (Human)	LYS	22	CE	1.11	0.06	9.5	0.1
Apolipoprotein E (Human)	LYS	22	CE	1.07	0.12	11.04	0.14
BPTI	ASP	3	CG	2.81	0.04	3.21	0.04
BPTI	ASP	3	CB	3.19	0.05	3.03	0.04
BPTI	GLU	49	CD	3.5	0.04	3.82	0.03
BPTI	ASP	50	CG	2.85	0.05	3.52	0.03
BPTI	ASP	50	CB	2.59	0.05	3.27	0.04
Calbindin D9k - P43G	LYS	7	CE	1.13	0.08	11.35	0.1
Calbindin D9k - P43G	LYS	12	CE	1.38	0.07	11.1	0.11
Calbindin D9k - P43G	LYS	16	CE	1.65	0.04	10.13	0.07
Calbindin D9k - P43G	LYS	25	CE	1.48	0.19	11.74	0.13
Calbindin D9k - P43G	LYS	29	CE	1.6	0.07	10.92	0.08
Calbindin D9k - P43G	LYS	41	CE	0.9	0.04	10.83	0.09
Calbindin D9k - P43G	LYS	71	CE	1.09	0.03	10.73	0.08
Calbindin D9k - P43G	LYS	72	CE	1.46	0.06	10.93	0.07
FNfn10 (Human)	ASP	3	CG	3.92	0.04	3.4	0.04
FNfn10 (Human)	ASP	3	CG	3.29	0.04	3.65	0.04

FNfn10 (Human)	ASP	80	CG	3.5	0.06	3.41	0.04
FNfn10 (Human) - D7K	ASP	3	CG	3.38	0.03	3.7	0.03
FNfn10 (Human) - D7K	GLU	9	CD	3.95	0.04	4.55	0.03
FNfn10 (Human) - D7K	GLU	38	CD	3.74	0.04	3.86	0.04
FNfn10 (Human) - D7K	GLU	47	CD	4.43	0.04	3.96	0.03
FNfn10 (Human) - D7K	ASP	67	CG	3.95	0.05	4.1	0.02
FNfn10 (Human) - D7K	ASP	80	CG	3.48	0.04	3.48	0.04
FNfn10 (Human) - D7N	ASP	3	CG	3.34	0.06	3.72	0.02
FNfn10 (Human) - D7N	GLU	38	CD	3.77	0.04	3.86	0.03
FNfn10 (Human) - D7N	GLU	47	CD	4.37	0.04	3.97	0.03
FNfn10 (Human) - D7N	ASP	80	CG	3.52	0.1	3.49	0.04
HEWL	ASP	52	CG	2.22	0.04	3.58	0.03
HEWL	ASP	52	CG	2.23	0.04	3.58	0.04
HIV-1 Protease	ASP	60	CG	3.07	0.24	2.98	0.09
N-Terminal Domain of Rat CD2	GLU	56	CD	3.76	0.04	3.97	0.02
N-Terminal Domain of Rat CD2	ASP	62	CG	2.31	0.03	4.13	0.03
Prolactin	HIS	27	CE1	2.05	0.03	6.42	0.05
Prolactin	HIS	46	CE1	2.26	0.04	6.55	0.04
Prolactin	HIS	138	CE1	2.37	0.04	5.83	0.03
Prolactin	HIS	195	CE1	2.49	0.04	5.89	0.02
Prolactin (H180A)	HIS	46	CE1	2.18	0.07	6.47	0.06

Prolactin (H180A)	HIS	138	CE1	2.37	0.05	5.77	0.05
Prolactin (H180A)	HIS	173	CE1	1.63	0.09	4.89	0.09
Prolactin (H180A)	HIS	195	CE1	2.61	0.06	5.87	0.05
Prolactin (H27A)	HIS	30	CE1	1.2	0.13	6.12	0.16
Prolactin (H27A)	HIS	46	CE1	2.37	0.06	6.56	0.06
Prolactin (H27A)	HIS	59	CE1	1.66	0.13	6	0.11
Prolactin (H27A)	HIS	138	CE1	2.5	0.06	5.69	0.04
Prolactin (H27A)	HIS	195	CE1	2.6	0.06	5.89	0.05
Prolactin (H30A)	HIS	46	CE1	2.23	0.07	6.64	0.09
Prolactin (H30A)	HIS	138	CE1	2.3	0.07	5.92	0.06
Prolactin (H30A)	HIS	173	CE1	1.23	0.19	5.21	0.15
Prolactin (H30A)	HIS	195	CE1	2.42	0.08	6.09	0.06
Ribonuclease HI (Escherichia coli)	GLU	6	CD	4.34	0.06	4.5	0.04
Ribonuclease HI (Escherichia coli)	GLU	6	CD	3.98	0.04	4.5	0.03
Ribonuclease HI (Escherichia coli)	ASP	10	CG	2.81	0.06	4.52	0.03
Ribonuclease HI (Escherichia coli)	GLU	48	CD	3.56	0.08	4.49	0.04
Ribonuclease HI (Escherichia coli)	GLU	57	CD	4.33	0.09	3.44	0.04
Ribonuclease HI (Escherichia coli)	GLU	61	CD	4.05	0.19	3.93	0.05
Ribonuclease HI (Escherichia coli)	GLU	61	CD	4.97	0.05	4	0.03

Ribonuclease HI (Escherichia coli)	GLU	64	CD	4.31	0.04	4.39	0.02
Ribonuclease HI (Escherichia coli)	GLU	64	CD	4.41	0.05	4.38	0.03
Ribonuclease HI (Escherichia coli)	ASP	94	CG	3.32	0.08	3.5	0.04
Ribonuclease HI (Escherichia coli)	ASP	108	CG	3.26	0.1	3.42	0.06
Ribonuclease HI (Escherichia coli)	ASP	108	CG	3.23	0.06	3.17	0.04
Ribonuclease HI (Escherichia coli)	GLU	119	CD	4.36	0.06	4.3	0.03
Ribonuclease HI (Escherichia coli)	ASP	134	CG	3.82	0.05	4.42	0.04
Ribonuclease HI (Escherichia coli)	GLU	135	CD	3.87	0.06	4.28	0.03
Ribonuclease HI (Escherichia coli)	GLU	147	CD	4.3	0.05	4.17	0.03
Ribonuclease HI (Escherichia coli)	GLU	147	CD	4.63	0.06	4.15	0.03
Ribonuclease HI (Escherichia coli)	GLU	154	CD	4.75	0.03	4.31	0.03
Ribonuclease HI (Escherichia coli)	GLU	154	CD	4.43	0.03	4.3	0.02
Ribonuclease Sa	ASP	1	CA	1.42	0.06	9.17	0.09
Ribonuclease Sa	GLU	54	CD	3.11	0.5	2.13	0.75
Ribonuclease Sa	GLU	78	CD	3.35	0.07	2.81	0.04
Ribonuclease Sa	ASP	79	CA	1.43	0.05	7.83	0.06

Ribonuclease Sa	ASP	79	CB	1.13	0.03	6.17	0.05
Xylanase (Bacillus agaradhaerens)	ASP	5	CG	3.88	0.12	3.85	0.03
Xylanase (Bacillus agaradhaerens)	HIS	11	CG	1.12	0.08	3.7	0.08
Xylanase (Bacillus agaradhaerens)	GLU	17	CD	0.72	0.13	3.93	0.18
Xylanase (Bacillus agaradhaerens)	HIS	32	CE1	2.19	0.02	6.7	0.05
Xylanase (Bacillus agaradhaerens)	HIS	60	CD2	2.16	0.05	4.14	0.04
Xylanase (Bacillus agaradhaerens)	HIS	60	CG	4.08	0.08	3.97	0.03
Xylanase (Bacillus agaradhaerens)	GLU	126	CD	3.72	0.03	4.54	0.03
Xylanase (Bacillus agaradhaerens)	GLU	167	CD	1.82	0.09	3.88	0.06
Xylanase (Bacillus agaradhaerens)	GLU	184	CD	0.57	0.03	5.56	0.08
Xylanase (Bacillus circulans)	ASP	4	CG	3.11	0.09	2.91	0.03
Xylanase (Bacillus circulans)	ASP	106	CG	2.21	0.09	2.66	0.04
Xylanase (Bacillus circulans)	ASP	121	CG	3.15	0.05	3.56	0.03

Xylanase (Bacillus circulans) - N35D (Paper 2)	ASP	106	CG	2.3	0.11	2.65	0.05

Figures

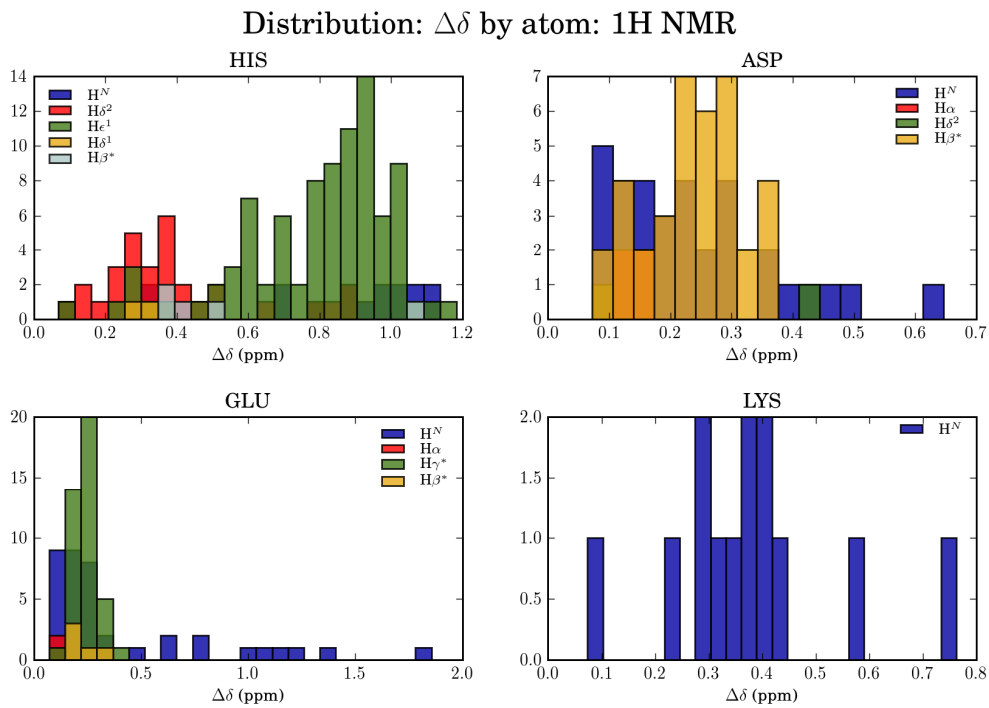

Figure 1: Δδ distributions associated with extracted pKas for all ^{1}H data

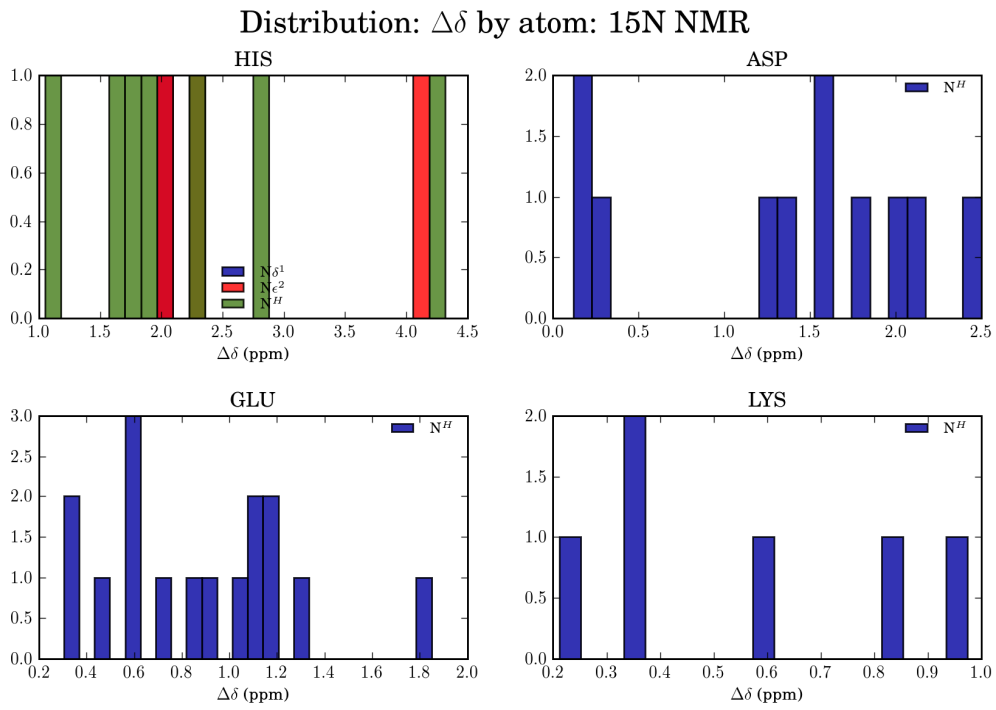

Figure 2: Δδ distributions associated with significant pKas for all ^{15}N data

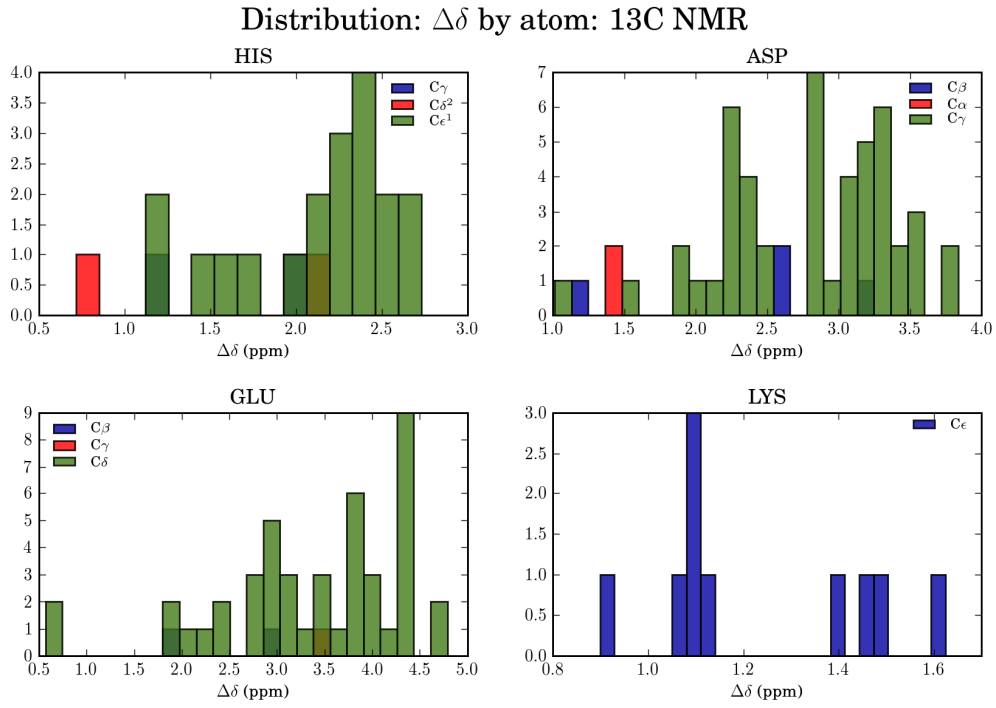

Figure 3: Δδ distributions associated with significant pKas for all ^{13}C data

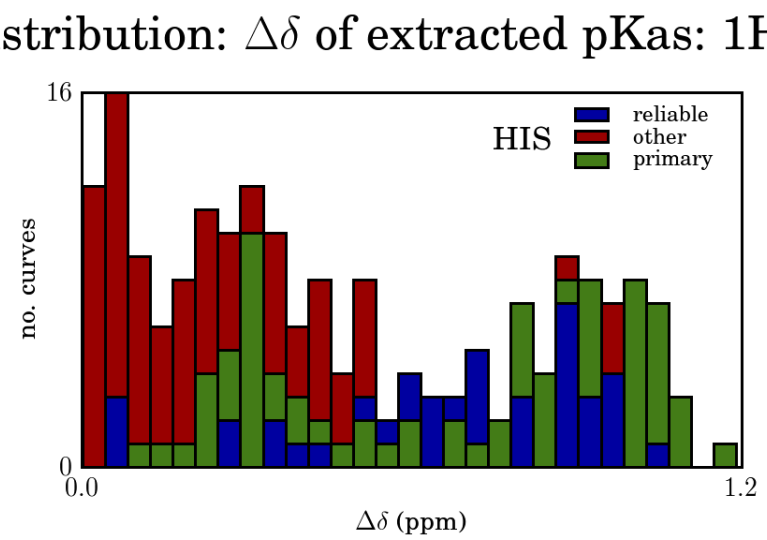

Figure 4: Sample breakdown of Δδ associated with pKas for 1H Histidine residues by our reliability criteria, Primary values are the subset of reliable pKas with a model of only 1 pKa. Other are the fitted pKa values that do not meet the reliability criteria.