Supporting Information for:

Comparison of Nine Programs Predicting pK_a Values of Pharmaceutical Substances

Chenzhong Liao, and Marc C. Nicklaus*

Chemical Biology Laboratory, Center for Cancer Research, National Cancer Institute, National Institutes of Health, DHHS, NCI-Frederick, 376 Boyles St., Frederick, MD 21702, USA

* Corresponding author. Tel.: +1 301 846 5903; fax: +1 301 846 6033; e-mail: mn1@helix.nih.gov.

Table S1. Experimental and Calculated pK_a Values of the Protonation Sites in the Data Set Used in This Study

Cpds	pK_a value(s)	Ionization type	Data quality	ACD/pK_a		ADME Boxes		ADMET Predictor		Epik		Jaguar		Marvin		Pallas		Pipeline Pilot		SPARC	
				Cal	Dev[a]	Cal	Dev	Cal	Dev	Cal	Dev	Cal	Dev	Cal	Dev	Cal	Dev	Cal	Dev	Cal	Dev
1	9.63	-H	A	9.86	0.23	9.8	0.2	10.02	0.39	10.12	0.49	10.0	0.4	9.46	-0.17	9.48	-0.15	9.50	-0.13	9.49	-0.14
2	4.756	-H	R	4.79	0.03	4.7	-0.1	4.00	-0.76	4.76	0.00	4.0	-0.8	4.54	-0.22	4.66	-0.10	4.76	0.00	4.77	0.01
3	3.742	-H	R	3.74	-0.00	3.6	-0.1	3.86	0.12	3.71	-0.03	3.3	-0.4	4.27	0.53	4.66	0.92	[b]	-	3.75	0.01
4	4.874	-H	R	4.79	-0.08	4.9	0.0	4.33	-0.54	4.76	-0.11	4.4	-0.5	4.75	-0.12	4.81	-0.06	4.87	0.00	4.75	-0.12
5	12.35[c]	-H	A	13.6	1.25	12.9	0.6	12.16	-0.19	12.87	0.52	12.2	-0.2	13.17	0.82	14.88	2.53	[b]	-	12.50	0.15
6	3.28	+H	A	4.67	1.39	3.3	0.0	1.96	-1.32	3.73	0.45	5.0	1.7	3.58	0.30	5.69	2.41	[b]	-	3.18	-0.10
	9.93	-H	A	17.00	7.07	9.8	-0.1	11.59	1.66	11.33	1.40	[b]	-	11.13	1.20	13.25	3.32	[b]	-	8.41	-1.52
7	10.58	+H	A	10.76	0.18	10.4	-0.2	10.08	-0.50	12.06	1.48	10.2	-0.4	10.71	0.13	10.72	0.14	10.63	0.05	10.40	-0.18
8	2.501	+H	R	2.51	0.01	2.1	-0.4	2.53	0.03	2.84	0.34	[d]	0.4	2.69	0.19	2.04	-0.46	2.19	-0.31	2.36	-0.14
	4.874	-H	R	4.86	-0.01	5.0	0.1	4.72	-0.15	4.49	-0.38	[d]	-1.0	4.77	-0.10	5.17	0.30	3.16	-1.71	4.76	-0.11
9	2.3	-H	A	2.42	0.12	3.6	1.3	2.42	0.12	2.56	0.26	7.4	5.1	2.92	0.62	2.25	-0.05	6.50	4.20	3.18	0.88
	4.9	+H	A	5.69	0.79	6.7	1.8	6.61	1.71	7.79	2.89	5.3	0.4	7.40	2.50	6.93	2.03	2.97	-1.93	7.17	2.27
10	5.06	+H	A	4.50	-0.56	4.7	-0.4	4.05	-1.01	6.75	1.69	[b]	-	0.98	-4.08	4.70	-0.36	5.00	-0.06	4.23	-0.83
11	9.94	+H	A	9.94	0.00	9.9	-0.0	9.86	-0.08	10.04	0.10	9.1	-0.8	10.01	0.07	9.81	-0.13	9.91	-0.03	9.96	0.02
12	9.7	+H	A	10.53	0.83	8.9	-0.8	9.41	-0.29	10.04	0.34	[d]	-	9.80	0.10	10.37	0.67	9.73	0.03	9.57	-0.13
13	9.86	+H	A	10.00	0.14	9.5	-0.4	9.70	-0.16	10.04	0.18	8.8	-1.1	9.99	0.13	9.45	-0.41	10.66	0.80	10.08	0.22
14	9.99	+H	A	10.00	0.01	9.6	-0.4	9.71	-0.28	10.04	0.05	9.2	-0.8	10.04	0.05	9.45	-0.54	9.52	-0.47	10.32	0.33
15	2.735	-H	A	2.44	-0.30	2.8	0.1	3.09	0.36	2.70	-0.04	3.1	0.4	2.89	0.16	2.54	-0.20	3.00	0.27	3.56	0.83
16	2.62	-H	A	2.45	-0.17	2.6	-0.0	2.92	0.30	2.73	0.11	7.1	4.5	2.80	0.18	2.55	-0.07	3.00	0.38	3.49	0.87
17	2.65	-H	A	2.44	-0.21	2.6	-0.0	2.91	0.26	2.66	0.01	8.3	5.7	2.74	0.09	2.54	-0.11	3.00	0.35	3.51	0.86

	7.25	+H	A	6.81	-0.44	7.2	-0.0	7.00	-0.25	7.27	0.02	4.4	-2.9	7.44	0.19	7.10	-0.15	7.02	-0.23	6.82	-0.43
18	2.72	-H	A	2.45	-0.27	2.8	0.1	3.14	0.42	2.67	-0.05	3.4	0.7	3.03	0.31	2.55	-0.17	3.00	0.28	3.57	0.85
19	2.68	-H	A	2.45	-0.23	2.6	-0.1	2.98	0.30	2.68	0.00	9.0	6.3	2.80	0.12	2.56	-0.12	3.00	0.32	3.49	0.81
20	2.73	-H	A	2.44	-0.29	2.8	0.1	3.13	0.40	2.70	-0.03	3.6	0.9	2.97	0.24	2.54	-0.19	3.00	0.27	3.52	0.79
21	9.07	+H	A	8.44	-0.63	9.1	0.0	8.84	-0.23	10.88	1.81	8.7	-0.4	8.61	-0.46	9.15	0.08	8.89	-0.18	9.70	0.63
22	7.64	+H	A	7.84	0.20	7.1	-0.5	7.61	-0.03	7.23	-0.41	8.6	1.0	7.73	0.09	6.92	-0.72	7.80	0.16	8.18	0.54
23	4.13	-H	A	4.09	-0.04	5.1	1.0	5.51	1.38	3.35	-0.78	4.4	0.3	3.52	-0.61	3.94	-0.19	11.56	7.43	3.96	-0.17
	11.39	-H	A	11.08	-0.31	[b]	-	10.32	-1.07	11.13	-0.26	15.9	4.5	8.32	-3.07	12.78	1.39	4.17	-7.22	11.00	-0.39
24	3.47	-H	A	3.48	0.01	3.6	-0.3	4.29	0.82	4.57	1.10	3.9	0.4	3.41	-0.06	3.83	0.36	3.48	0.01	3.62	0.15
25	9.58	+H	A	9.43	-0.15	9.3	0.7	9.35	-0.23	9.09	-0.49	9.1	-0.5	9.67	0.09	10.08	0.50	9.60	0.02	9.05	-0.53
26	3.19	-H	A	3.71	0.52	2.7	-0.1	3.20	0.01	4.43	1.24	5.7	2.5	8.53	5.34	3.25	0.06	3.63	0.44	3.09	-0.10
	7.87	+H	A	7.55	-0.32	7.8	0.1	7.80	-0.07	8.24	0.37	11.5	3.6	14.80	6.93	8.12	0.25	8.92	1.05	7.27	-0.60
27	7.905	-H	A	8.29	0.38	8.6	-0.4	7.64	-0.27	8.17	0.27	[b]	-	8.65	0.75	8.07	0.17	[b]	-	9.10	1.20
28	5.68	-H	A	5.38	-0.30	5.3	-0.3	6.41	0.73	3.96	-1.72	4.1	-1.6	3.35	-2.33	5.72	0.04	4.00	-1.68	3.74	-1.94
29	5.55	-H	A	5.38	-0.17	5.3	-0.3	5.90	0.35	3.99	-1.56	3.6	-2.0	3.25	-2.30	5.78	0.23	4.00	-1.55	3.77	-1.78
30	8.505	-H	A	7.90	-0.61	8.7	0.2	8.11	-0.40	7.40	-1.11	7.5	-1.0	6.99	-1.52	7.90	-0.61	3.89	-4.62	7.30	-1.21
31	8.28	-H	A	7.91	-0.37	8.5	0.2	8.16	-0.12	7.40	-0.88	7.4	-0.9	6.99	-1.29	7.95	-0.33	7.26	-1.02	7.30	-0.98
32	8.45	-H	A	7.92	-0.53	8.7	0.3	8.19	-0.26	7.53	-0.92	7.6	-0.9	6.98	-1.47	7.99	-0.46	7.83	-0.62	7.08	-1.37
33	7.9798	-H	VR	7.92	-0.06	8.1	0.1	8.24	0.26	7.53	-0.45	7.3	-0.7	6.98	-1.00	7.99	0.01	7.83	-0.15	7.08	-0.90
34	8.14	-H	A	7.93	-0.21	8.4	0.3	8.29	0.15	7.67	-0.47	7.5	-0.6	6.98	-1.16	8.03	-0.11	8.01	-0.13	7.08	-1.06
35	8.13	-H	A	7.93	-0.20	7.9	-0.2	8.33	0.20	7.99	-0.14	7.5	-0.6	6.98	-1.15	7.97	-0.16	7.97	-0.16	7.08	-1.05
36	7.95	-H	A	7.92	-0.03	7.9	-0.0	8.27	0.32	7.88	-0.07	6.8	-1.2	6.98	-0.97	7.96	0.01	7.96	0.01	7.08	-0.87
37	8.14	-H	A	7.93	-0.21	8.0	-0.1	8.41	0.27	8.01	-0.13	8.1	0.0	6.98	-1.16	7.96	-0.18	8.37	0.23	7.30	-0.84
38	7.89	-H	A	7.80	-0.09	8.0	0.1	7.98	0.09	7.38	-0.51	7.2	-0.7	6.98	-0.91	7.95	0.06	7.40	-0.49	6.85	-1.04

39	8.01	-H	A	7.81	-0.20	8.1	0.1	8.06	0.05	7.52	-0.49	7.2	-0.8	6.98	-1.03	7.99	-0.02	7.99	-0.02	6.85	-1.16
40	7.81	-H	A	7.67	-0.14	7.9	0.1	7.75	-0.06	7.37	-0.44	7.2	-0.6	6.98	-0.83	7.90	0.09	7.79	-0.02	6.62	-1.19
41	8.39	-H	A	7.85	-0.54	8.5	0.1	7.73	-0.66	7.48	-0.91	7.9	-0.5	6.98	-1.41	7.87	-0.52	6.84	-1.55	7.31	-1.08
42	8.06	-H	A	7.86	-0.20	8.0	-0.1	7.88	-0.18	7.48	-0.58	7.9	-0.2	6.98	-1.08	7.91	-0.15	7.40	-0.66	7.31	-0.75
43	8.19	-H	A	7.87	-0.32	8.2	0.0	8.01	-0.18	7.62	-0.57	7.7	-0.5	6.98	-1.21	7.95	-0.24	7.99	-0.20	7.31	-0.88
44	8.39	-H	A	7.88	-0.51	7.9	-0.5	8.14	-0.25	7.68	-0.71	8.0	-0.4	6.98	-1.41	8.00	-0.39	8.55	0.16	7.31	-1.08
45	8.13	-H	A	7.80	-0.33	7.9	-0.2	7.61	-0.52	7.56	-0.57	9.0	0.9	6.98	-1.15	7.83	-0.3	7.79	-0.34	7.53	-0.60
46	7.78	-H	A	7.72	-0.06	8.4	0.6	7.72	-0.06	7.74	-0.04	7.0	-0.8	6.64	-1.14	7.66	-0.12	7.39	-0.39	6.95	-0.83
47	7.48	-H	A	7.72	0.24	7.9	0.4	7.89	0.41	7.80	0.32	7.0	-0.5	6.64	-0.84	7.71	0.23	7.96	0.48	6.95	-0.53
48	7.78	-H	A	7.58	-0.20	7.7	-0.1	7.07	-0.71	6.51	-1.27	7.0	-0.8	6.64	-1.14	7.56	-0.22	7.73	-0.05	6.87	-0.91
49	7.48	-H	A	7.58	0.10	8.0	0.5	7.22	-0.26	6.64	-0.84	6.8	-0.7	6.64	-0.84	7.61	0.13	7.30	-0.18	6.87	-0.61
50	7.015	-H	A	7.37	0.36	7.5	0.5	5.79	-1.23	6.64	-0.38	6.2	-0.8	6.64	-0.38	7.40	0.39	7.30	0.29	6.35	-0.67
51	6.94	-H	A	7.29	0.35	7.5	0.6	5.70	-1.24	6.64	-0.3	6.2	-0.7	6.64	-0.30	7.38	0.44	7.30	0.36	6.30	-0.64
52	7.3	-H	A	7.23	-0.07	8.8	1.5	6.18	-1.12	6.44	-0.86	6.7	-0.6	6.29	-1.01	7.23	-0.07	2.34	-4.96	6.94	-0.36
53	8.73	-H	A	9.31	0.58	8.9	0.2	7.69	-1.04	7.40	-1.33	7.6	-1.1	6.98	-1.75	7.90	-0.83	6.73	-2.00	7.30	-1.43
54	8.82	-H	A	9.30	0.48	8.9	0.1	7.84	-0.98	7.27	-1.55	7.9	-0.9	6.98	-1.84	7.90	-0.92	6.73	-2.09	7.30	-1.52
55	8.83	-H	A	9.30	0.47	9.0	0.2	8.04	-0.79	7.47	-1.36	7.8	-1.0	6.98	-1.85	7.90	-0.93	8.88	0.05	7.30	-1.53
56	8.88	-H	A	9.31	0.43	9.0	0.1	8.05	-0.83	7.39	-1.49	8.0	-0.9	6.98	-1.9	8.00	-0.88	8.88	0.00	7.30	-1.58
57	2.515	+H	A	2.51	-0.01	2.6	0.1	2.67	0.16	2.03	-0.49	2.7	0.2	2.78	0.27	2.51	-0.01	3.46	0.95	2.39	-0.13
58	4.207	-H	R	4.20	-0.01	3.9	0.3	4.05	-0.16	4.20	-0.01	3.4	-0.8	4.08	-0.13	4.20	-0.01	3.53	-0.68	4.02	-0.19
59	8.7	+H	A	8.97	0.27	8.5	-0.2	7.88	-0.82	7.81	-0.89	6.9	-1.8	7.65	-1.05	7.29	-1.41	8.65	-0.05	7.56	-1.14
60	9.234	-H	VR	8.91	-0.32	[b]	-	1.37	-7.86	[b]	-	[b]	-	8.70	-0.53	[b]	-	8.97	-0.26	[b]	-
61	8.28	+H	A	8.31	0.03	8.1	-0.2	7.34	-0.94	9.81	1.53	9.9	1.6	7.95	-0.33	7.65	-0.63	5.13	-3.15	9.04	0.76
62	6.352	-H	R	4.36	-1.99	2.9	-3.5	1.59	-4.76	2.66	-3.69	4.4[e]	-2.0	6.05	-0.30	2.19	-4.16	3.43	-2.92	3.24	-3.11

	10.39	-H	R	10.30	-0.09	8.9	-1.5	8.25	-2.14	6.59	-3.80	1.6	-8.8	10.64	0.25	9.46	-0.93	6.37	-4.02	[b]	-
63	5.03	-H	A	4.76	-0.27	5.4	0.4	5.15	0.12	5.12	0.09	7.2	2.2	4.60	-0.43	4.82	-0.21	5.70	0.67	4.74	-0.29
64	5.04	-H	A	4.76	-0.28	5.4	0.4	5.15	0.11	5.13	0.09	7.0	2.0	4.60	-0.44	4.82	-0.22	5.70	0.66	4.74	-0.30
65	2.12	+H	A	2.24	0.12	2.7	0.6	2.55	0.43	2.70	0.58	2.3	0.2	2.17	0.05	-1.76	-3.88	2.04	-0.08	3.32	1.20
	7.65	+H	A	7.47	-0.18	8.1	0.4	8.28	0.63	7.50	-0.15	9.2	1.6	8.00	0.35	5.89	-1.76	8.30	0.65	8.31	0.66
66	2.16	+H	A	2.47	0.31	2.8	0.6	2.74	0.58	2.70	0.54	2.8	0.6	2.81	0.65	-1.76	-3.92	2.50	0.34	3.64	1.48
	8.05	+H	A	7.50	-0.55	8.2	0.1	8.42	0.37	7.51	-0.54	9.3	1.3	8.51	0.46	7.20	-0.85	8.30	0.25	8.39	0.34
67	5.32	+H	A	8.06	2.74	5.5	0.2	7.61	2.29	9.22	3.90	[d]	-	6.64	1.32	5.68	0.36	4.77	-0.55	6.33	1.01
68	5.29	+H	A	8.05	2.76	5.5	0.2	7.63	2.34	9.21	3.92	[d]	-	6.89	1.60	5.65	0.36	4.77	-0.52	6.36	1.07
69	5.3	+H	A	8.07	2.77	5.6	0.3	7.71	2.41	9.22	3.92	[d]	-	6.89	1.59	5.65	0.35	4.77	-0.53	6.40	1.10
70	10.95	+H	A	11.19	0.24	11.0	0.1	10.51	-0.44	8.31	-2.64	10.6	-0.4	7.07	-3.88	13.69	2.74	9.77	-1.18	9.52	-1.43
71	11.01	+H	A	11.19	0.18	11.1	0.1	10.85	-0.16	8.58	-2.43	10.3	-0.7	7.10	-3.91	12.53	1.52	9.77	-1.24	9.52	-1.49
72	11.02	+H	A	11.17	0.15	11.1	0.1	10.88	-0.14	8.63	-2.39	10.3	-0.7	7.15	-3.87	12.58	1.56	9.77	-1.25	9.52	-1.50
73	10.83	+H	A	11.20	0.37	11.1	0.3	11.07	0.24	8.97	-1.86	10.3	-0.5	7.17	-3.66	12.02	1.19	9.77	-1.06	9.52	-1.30
74	3.285	-H	A	4.5	1.22	3.3	0.0	6.70	3.42	4.61	1.33	[d]	-	4.12	0.84	8.87	5.59	3.05	-0.24	[b]	-
	7.435	+H	A	11.01	3.58	9.3	1.9	3.15	-4.29	10.42	2.99	[d]	-	8.36	0.93	8.92	1.49	9.48	2.05	[b]	-
	9.3	-H	A	8.03	-1.27	11.4	2.1	8.53	-0.77	7.55	-1.75	[d]	-	10.97	1.67	7.56	-1.74	7.33	-1.97	[b]	-
75	3.27	-H	A	4.5	1.23	3.2	-0.1	7.67	4.40	[g]	-	[d]	-	4.31	1.04	10.70	7.43	3.50	0.23	[b]	-
	7.32	+H	A	10.80	3.48	9.0	1.7	3.80	-3.52	8.39	1.07	[d]	-	7.87	0.55	6.52	-0.80	9.25	1.93	[b]	-
	9.11	-H	A	8.48	-0.63	12.5	3.4	8.87	-0.24	7.43	-1.68	[d]	-	11.43	2.32	8.04	-1.07	7.79	-1.32	[b]	-
76	3.3	-H	A	4.50	1.20	3.3	0.0	7.46	4.16	4.62	1.32	[d]	-	4.41	1.11	8.87	5.57	3.05	-0.25	[b]	-
	7.68	+H	A	11.02	3.34	9.4	1.7	3.32	-4.36	10.43	2.75	[d]	-	8.36	0.68	8.92	1.24	9.48	1.80	[b]	-
	9.69	-H	A	8.50	-1.19	12.0	2.3	8.90	-0.79	8.49	-1.20	[d]	-	11.44	1.75	8.06	-1.63	7.81	-1.88	[b]	-
77	4.45	-H	A	4.34	-0.11	4.7	0.3	4.46	0.01	4.45	0.00	4.5	0.0	4.51	0.06	4.45	0.00	4.16	-0.29	4.10	-0.35

78	9.355	-H	A	9.57	0.22	9.0	-0.4	8.49	-0.87	9.46	0.11	9.3	-0.1	9.20	-0.16	9.29	-0.07	9.40	0.04	8.70	-0.66
79	3.128	-H	VR	2.93	-0.20	2.8	-0.3	2.97	-0.16	3.48	0.35	[d]	-	3.05	-0.08	2.84	-0.29	2.25	-0.88	2.84	-0.29
	4.761	-H	VR	4.23	-0.53	4.2	-0.6	4.40	-0.36	5.28	0.52	[d]	-	4.67	-0.09	4.01	-0.75	6.50	1.74	4.41	-0.35
	6.396	-H	VR	5.09	-1.31	5.4	-1.0	6.20	-0.20	6.20	-0.20	[d]	-	5.39	-1.01	4.90	-1.50	8.51	2.11	5.19	-1.21
80	7.72	+H	A	8.74	1.02	7.6	-0.1	7.15	-0.57	9.25	1.53	9.4	1.7	7.55	-0.17	7.96	0.24	7.66	-0.06	7.96	0.24
81	8.16	-H	A	7.23	-0.93	7.9	-0.3	7.91	-0.25	6.15	-2.01	8.3	0.1	7.34	-0.82	3.83	-4.33	7.90	-0.26	7.80	-0.36
82	8.12	+H	A	8.02	-0.10	7.9	-0.2	7.94	-0.18	7.12	-1.00	9.9	1.8	9.34	1.22	8.37	0.25	8.05	-0.07	10.20	2.08
83	9.7	+H	A	9.84	0.14	9.7	0.0	9.66	-0.04	10.19	0.49	11.3	1.6	9.64	-0.06	9.95	0.25	9.52	-0.18	9.89	0.19
84	8.39	+H	A	8.50	0.11	8.6	0.2	8.60	0.21	8.46	0.07	9.6	1.2	8.80	0.41	8.36	-0.03	8.66	0.27	8.51	0.12
85	3.443	+H	A	3.40	-0.04	4.2	0.8	3.43	-0.01	4.62	1.18	3.1	-0.3	2.92	-0.52	3.66	0.22	4.78	1.34	3.83	0.39
	6.14	+H	A	7.03	0.89	8.2	2.1	8.04	1.90	7.84	1.70	8.2	2.1	8.43	2.29	7.78	1.64	7.17	1.03	8.29	2.15
86	8.22	+H	A	8.23	0.01	8.4	0.2	8.29	0.07	9.42	1.20	9.0	0.8	9.19	0.97	8.80	0.58	8.10	-0.12	9.67	1.45
87	9.23	+H	A	9.28	0.05	8.8	-0.4	8.79	-0.44	9.93	0.70	9.1	-0.1	10.07	0.84	9.12	-0.11	9.23	0.00	10.54	1.31
88	5.68	+H	A	6.65	0.97	5.6	-0.1	5.99	0.31	7.73	2.05	6.4	0.7	7.18	1.50	5.69	0.01	5.68	0.00	7.14	1.46
89	3.6	-H	A	3.56	-0.04	3.7	0.1	3.61	0.01	3.37	-0.23	6.9	3.3	4.09	0.49	3.56	-0.04	3.58	-0.02	3.42	-0.18
90	3.56	-H	A	3.39	-0.17	3.7	0.1	3.79	0.23	3.38	-0.18	7.8	4.2	4.27	0.71	3.60	0.04	3.58	0.02	3.42	-0.14
91	3.6	-H	A	3.39	-0.21	3.8	0.2	4.04	0.44	3.39	-0.21	9.3	5.7	4.22	0.62	3.60	0.00	3.58	-0.02	3.42	-0.18
92	3.65	-H	A	3.39	-0.26	3.8	0.2	4.13	0.48	3.39	-0.26	8.0	4.4	4.22	0.57	3.60	-0.05	3.58	-0.07	3.42	-0.23
93	3.451	+H	A	-0.60	-4.05	[b]	-	1.04	-2.41	0.06	-3.39	[b]	-	-6.43	-9.88	-1.12	-4.57	3.20	-0.25	[b]	-
	8.275	+H	A	8.78	0.50	8.2	-0.1	8.10	-0.18	8.48	0.21	7.9	-0.4	8.23	-0.04	8.47	0.20	7.04	-1.24	8.90	0.63
94	3.99	-H	A	4.18	0.19	4.2	0.2	3.83	-0.16	4.40	0.41	4.6	0.6	4.00	0.01	4.46	0.47	3.80	-0.19	4.12	0.13
95	8.75	+H	A	8.43	-0.32	8.5	-0.3	8.57	-0.18	9.92	1.17	9.3	0.6	9.33	0.58	8.80	0.05	8.35	-0.40	9.69	0.94
96	9.35	+H	A	8.44	-0.91	8.3	-1.1	8.47	-0.88	9.88	0.53	[d]	-	9.24	-0.11	8.90	-0.45	8.79	-0.56	9.44	0.09
97	10.29	-H	A	10.15	-0.14	10.5	0.2	10.24	-0.05	11.01	0.72	10.8	0.5	9.41	-0.88	10.28	-0.01	11.12	0.83	10.40	0.11

98	9.77	-H	A	10.15	0.38	10.5	0.7	10.24	0.47	11.01	1.24	10.7	0.9	9.41	-0.36	10.28	0.51	11.12	1.35	10.40	0.63
99	7.55	+H	A	8.02	0.47	9.1	1.6	9.15	1.60	9.77	2.22	[d]		9.25	1.70	9.03	1.48	10.12	2.57	9.78	2.23
100	3.2	-H	A	3.41	0.21	3.1	-0.1	3.45	0.25	3.60	0.40	6.1	2.9	3.28	0.08	3.44	0.24	3.20	0.00	3.29	0.09
	7.18	+H	A	7.43	0.25	7.4	0.2	7.74	0.56	8.29	1.11	7.8	0.6	8.01	0.83	7.70	0.52	7.11	-0.07	7.54	0.36
101	3.37	-H	A	3.49	0.12	3.1	-0.3	3.91	0.54	3.72	0.35	6.3	2.9	3.16	-0.21	3.44	0.07	3.37	0.00	3.54	0.17
	7.04	+H	A	6.91	-0.13	7.3	0.3	7.52	0.48	8.09	1.05	7.3	0.3	7.71	0.67	7.70	0.66	7.11	0.07	7.00	-0.04
102	5.24	-H	A	1.85	-3.39	8.3	3.1	6.71	1.47	[g]	-	[d]	-	8.22	2.98	9.54	4.30	8.78	3.54	5.25	0.01
103	2.975	-H	A	3.15	0.18	3.0	0.0	3.24	0.27	2.89	-0.09	[d]	-	3.18	0.21	1.80	-1.18	2.94	-0.04	3.82	0.85
	5.36	+H	A	5.43	0.07	5.5	0.1	5.97	0.61	7.37	2.01	[d]	-	5.19	-0.17	1.39	-3.97	5.50	0.14	5.55	0.19
104	3.68	-H	A	3.23	-0.45	3.1	-0.6	3.95	0.27	3.41	-0.27	6.6	2.9	3.11	-0.57	3.50	-0.18	3.21	-0.47	3.77	0.09
	7.77	+H	A	7.21	-0.56	7.4	-0.4	7.69	-0.08	8.14	0.37	[d]	-	7.73	-0.04	7.43	-0.34	7.69	-0.08	7.34	-0.43
	9.89	-H	A	9.97	0.08	9.8	-0.1	9.94	0.05	10.15	0.26	[d]	-	9.51	-0.38	9.71	-0.18	8.53	-1.36	10.00	0.11
105	9.61	+H	A	9.38	-0.23	9.3	-0.3	9.43	-0.18	8.64	-0.97	9.5	-0.1	9.52	-0.09	9.86	0.25	9.50	-0.11	9.70	0.09
106	10.71	-H	A	10.27	-0.44	10.5	-0.2	10.41	-0.30	11.42	0.71	10.9	0.2	10.33	-0.38	10.37	-0.34	13.18	2.47	10.54	-0.17
107	10.34	-H	A	10.25	-0.09	10.4	0.1	10.30	-0.04	11.19	0.85	10.7	0.4	10.33	-0.01	10.37	0.03	13.18	2.84	10.48	0.14
108	10.4	-H	A	10.24	-0.16	10.4	0.0	10.41	0.01	11.41	1.01	10.8	0.4	10.33	-0.07	10.37	-0.03	13.18	2.78	10.51	0.11
109	6.38	-H	A	5.70	-0.68	6.1	-0.3	4.99	-1.39	3.53	-2.85	4.0	-2.4	6.00	-0.38	6.25	-0.13	6.67	0.29	5.58	-0.80
110	3.65	-H	A	3.04	-0.61	3.5	-0.2	3.79	0.14	4.59	0.94	3.7	0.1	4.25	0.60	4.06	0.41	3.90	0.25	3.20	-0.45
	10.4	-H	A	9.79	-0.61	8.7	-1.7	9.48	-0.92	10.18	-0.22	8.4	-2.0	9.91	-0.49	9.84	-0.56	11.57	1.17	[b]	-
111	4.21	-H	A	4.33	0.12	4.3	0.1	3.25	-0.96	4.40	0.19	3.7	-0.5	3.94	-0.27	4.32	0.11	4.33	0.12	3.99	-0.22
112	3.62	-H	A	3.35	-0.27	3.7	0.1	4.26	0.64	3.41	-0.21	2.9	-0.7	3.39	-0.23	3.20	-0.42	4.43	0.81	3.07	-0.55
113	6.1	-H	A	6.36	0.26	6.1	0.0	6.82	0.72	6.27	0.17	[b]	-	6.24	0.14	6.13	0.03	4.55	-1.55	6.52	0.42
	8.14	+H	A	8.42	0.28	7.5	-0.6	7.96	-0.18	7.68	-0.46	[d]	-	8.23	0.09	7.69	-0.45	8.23	0.09	7.74	-0.40
114	11.4	+H	A	11.24	-0.16	10.6	-0.8	10.20	-1.20	10.16	-1.24	11.5	0.1	10.25	-1.15	11.28	-0.12	11.40	0.00	10.10	-1.30

115	10.55	+H	A	10.55	0.00	10.4	-0.2	9.06	-1.49	9.96	-0.59	10.9	0.4	8.46	-2.09	11.28	0.73	10.55	0.00	9.81	-0.74
116	4.52	+H	A	4.93	0.41	5.4	0.9	5.36	0.84	5.88	1.36	7.5	3.0	5.67	1.15	5.55	1.03	5.08	0.56	5.78	1.26
	8.47	+H	A	8.21	-0.26	8.5	0.0	8.81	0.34	8.88	0.41	7.0[f]	-1.5	9.66	1.19	8.56	0.09	8.71	0.24	8.70	0.23
117	5.784	+H	R	5.45	-0.33	6.0	0.2	5.85	0.07	5.40	-0.38	7.2	1.4	6.24	0.46	6.14	0.36	6.04	0.26	5.30	-0.48
	9.756	+H	R	9.26	-0.50	9.7	-0.1	9.54	-0.22	10.21	0.45	9.0	-0.8	9.58	-0.18	8.77	-0.99	9.77	0.01	10.40	0.64
118	4.06	+H	A	3.21	-0.85	4.1	0.0	4.84	0.78	4.69	0.63	4.2	0.1	5.28	1.22	4.23	0.17	4.64	0.58	3.33	-0.73
	9.2	+H	A	8.94	-0.26	8.9	-0.3	9.69	0.49	10.21	1.01	9.2	0.0	9.51	0.31	8.16	-1.04	9.77	0.57	9.96	0.76
	11.88	-H	A	11.98	0.10	[b]	-	12.12	0.24	12.89	1.01	[b]	-	12.48	0.60	12.12	0.24	[b]	-	11.73	-0.15
119	2.31	+H	A	1.07	-1.24	1.6	-0.7	1.75	-0.56	4.22	1.91	2.0	-0.3	3.19	0.88	2.14	-0.17	4.10	1.79	[b]	-
	8.2	+H	A	8.20	0.00	8.6	0.4	8.97	0.77	10.18	1.98	[d]	-	9.44	1.24	7.55	-0.65	9.52	1.32	8.47	0.27
	10.11	-H	A	9.55	-0.56	[b]	-	10.56	0.45	9.45	-0.66	[d]	-	10.41	0.30	8.90	-1.21	[b]	-	11.08	0.97
120	1.975	+H	A	2.10	0.13	2.7	0.7	2.61	0.64	2.69	0.72	[d]	-	2.09	0.12	1.79	-0.19	5.84	3.87	2.93	0.96
121	8.78	-H	A	8.95	0.17	8.7	-0.1	9.60	0.82	8.42	-0.36	[d]	-	9.96	1.18	8.70	-0.08	10.04	1.26	10.41	1.63
	10.13	-H	U	9.57	-0.56	9.9	-0.2	8.35	-1.78	9.90	-0.23	[d]	-	9.24	-0.89	9.03	-1.10	9.39	-0.74	9.52	-0.61
122	4.44	-H	A	4.41	-0.03	4.6	0.2	4.53	0.09	4.36	-0.08	4.8	0.4	4.85	0.41	4.08	-0.36	4.55	0.11	4.53	0.09
123	8.65	+H	A	9.26	0.61	8.5	-0.2	8.72	0.07	8.82	0.17	[d]	-	8.96	0.31	10.85	2.20	9.67	1.02	8.52	-0.13
	10.07	-H	A	9.60	-0.47	9.5	-0.6	9.81	-1.30	9.75	-0.32	[d]	-	9.81	-0.26	9.38	-0.69	10.01	-0.06	10.49	0.42
124	3.861[h]	-H	R	3.91	0.05	3.7	-0.2	3.89	0.03	3.54	-0.32	3.5	-0.4	3.78	-0.08	3.70	-0.16	3.86	0.00	3.86	-0.00
125	3.861[h]	-H	R	3.91	0.05	3.7	-0.2	3.89	0.03	3.54	-0.32	3.5	-0.4	3.78	-0.08	3.70	-0.16	3.86	0.00	3.86	-0.00
126	7.928	+H	A	7.96	0.03	7.9	-0.0	7.62	-0.31	8.63	0.70	8.4	0.5	7.75	-0.18	8.63	0.70	7.89	-0.04	8.21	0.28
127	3.459	-H	A	3.61	0.15	3.5	0.0	3.41	-0.05	4.14	0.68	[d]	-	3.20	-0.26	3.08	-0.38	3.52	0.06	3.32	-0.14
	5.097	-H	A	4.82	-0.28	5.0	-0.1	5.22	0.12	5.88	0.78	[d]	-	5.13	0.03	4.59	-0.51	5.02	-0.08	5.12	0.02
128	1.93	-H	A	2.39	0.46	2.2	0.3	2.94	1.01	2.71	0.78	1.5[e]	-0.4	3.05	1.12	4.09	2.16	2.52	0.59	3.17	1.24
	6.225	-H	A	5.34	-0.89	4.0	-2.2	4.81	-1.42	4.46	-1.77	5.2	-1.0	5.91	-0.32	5.32	-0.90	5.41	-0.82	4.22	-2.01

129	7.41	-H	A	8.21	0.80	7.7	0.3	9.28	1.87	8.20	0.79	[d]	-	8.05	0.64	8.04	0.63	8.54	1.13	9.98	2.57
	9.36	+H	A	9.30	-0.06	9.1	-0.3	8.06	-0.08	9.32	-0.04	[d]	-	9.80	0.44	10.05	0.69	8.60	-0.76	8.87	-0.49
130	2.85	-H	A	2.92	0.07	2.8	-0.1	3.02	0.17	3.60	0.75	2.9[e]	0.0	2.43	-0.42	2.77	-0.08	4.12	1.27	2.66	-0.19
	5.66	-H	A	5.61	-0.05	5.0	-0.7	5.00	-0.66	6.93	1.27	4.9	-0.8	5.92	0.26	5.38	-0.28	5.69	0.03	5.26	-0.40
131	10.37	+H	A	10.38	0.01	10.3	-0.1	10.28	-0.09	9.70	-0.67	10.3	-0.1	10.30	-0.07	10.16	-0.21	10.17	-0.20	10.23	-0.14
132	9.99	+H	A	10.38	0.39	10.1	0.1	10.18	0.19	9.70	-0.29	9.8	-0.2	10.21	0.22	10.16	0.17	10.25	0.26	10.28	0.29
133	9.62	+H	A	9.82	0.2	9.3	-0.3	10.56	0.94	9.70	0.08	[d]	-	10.58	0.96	10.74	1.12	10.25	0.63	9.63	0.01
134	7.77[i]	-H	A	8.71	0.94	7.6	-0.2	10.10	2.33	[b]	-	3.0	-4.8	7.51	-0.26	10.43	2.66	4.64	-3.13	7.10[j]	-0.67
135	9.32	+H	A	8.29	-1.03	9.1	-0.2	8.71	-0.61	8.47	-0.85	9.1	-0.2	9.28	-0.04	8.79	-0.53	9.50	0.18	9.18	-0.14
136	10.45	+H	A	10.36	-0.09	10.0	-0.4	9.94	-0.51	9.70	-0.75	9.8	-0.6	10.04	-0.41	9.78	-0.67	10.40	-0.05	9.90	-0.55
137	3.13	+H	A	3.21	0.08	3.5	0.4	3.39	0.26	4.79	1.66	4.0	0.9	2.70	-0.43	2.96	-0.17	3.09	-0.04	3.20	0.07
138	2.218	-H	A	2.28	0.06	2.3	0.1	2.21	-0.01	2.41	0.19	6.0	3.8	1.73	-0.49	2.13	-0.09	2.72	0.50	2.32	0.10
139	6.65	+H	A	7.14	0.49	6.9	0.3	7.16	0.51	7.94	1.29	8.2	1.6	8.63	1.98	6.64	-0.01	6.69	0.04	9.09	2.44
140	6.62	+H	A	7.15	0.53	6.9	0.3	6.92	0.30	7.94	1.32	8.5	1.9	8.55	1.93	6.64	0.02	6.62	0.00	9.09	2.47
141	9.555	+H	A	9.43	-0.13	9.4	-0.2	9.39	-0.16	9.09	-0.47	9.3	-0.3	9.67	0.12	10.08	0.53	9.60	0.04	9.08	-0.48
142	9.14	+H	A	8.58	-0.56	9.2	0.1	8.96	-0.18	9.32	0.18	7.9	-1.2	9.52	0.38	9.06	-0.08	9.19	0.05	8.86	-0.28
143	8.18	+H	A	8.25	0.07	8.0	-0.2	8.21	0.03	9.37	1.19	[d]	-	9.12	0.94	7.97	-0.21	8.19	0.01	9.28	1.10
	9.4	-H	A	9.48	0.08	9.4	0.0	9.71	0.31	11.22	1.82	[d]	-	10.26	0.86	10.38	0.98	8.16	-1.24	10.34	0.94
144	8.66	-H	A	9.17	0.51	8.3	-0.4	9.79	1.13	11.75	3.09	[d]	-	10.47	1.81	10.65	1.99	9.8	1.14	9.53	0.87
	9.8	+H	A	9.54	-0.26	9.7	-0.1	8.54	-1.26	9.89	0.09	[d]	-	9.77	-0.03	9.22	-0.58	9.67	-0.13	10.96	1.16
145	4.44	+H	A	4.71	0.27	4.8	0.4	1.96	-2.48	5.76	1.32	[d]	-	5.76	1.32	6.87	2.43	-1.20	-5.64	4.77	0.33
146	2.87	-H	A	2.77	-0.10	2.8	-0.1	3.77	0.90	2.97	0.10	5.9	3.0	2.67	-0.20	2.50	-0.37	2.86	-0.01	3.33	0.46
	8.21	+H	A	8.23	0.02	8.4	0.2	8.02	-0.19	9.42	1.21	7.7	-0.5	9.17	0.96	8.25	0.04	8.19	-0.02	9.62	1.41
147	2.89	-H	A	2.79	-0.10	2.8	-0.1	3.88	0.99	3.09	0.20	9.3	6.4	2.87	-0.02	2.60	-0.29	2.77	-0.12	[b]	-

	8.14	+H	A	8.09	-0.05	8.3	0.2	7.85	-0.29	9.42	1.28	[d]	-	9.12	0.98	7.97	-0.17	8.19	0.05	[b]	-
	9.36	-H	A	9.43	0.07	9.6	0.2	9.70	0.34	11.19	1.83	[d]	-	10.25	0.89	10.43	1.07	8.16	-1.20	[b]	-
148	2.05	-H	A	2.20	0.15	2.1	0.1	1.14	0.15	2.20	0.15	4.7	2.7	2.79	0.74	2.20	0.15	0.74	-1.31	1.86	-0.19
	4.83	+H	A	4.80	-0.03	4.7	-0.1	5.15	0.32	5.31	0.48	2.1	-2.7	4.19	-0.64	4.74	-0.09	3.70	-1.13	4.91	0.08
149	1.77	-H	A	1.95	0.18	2.1	0.3	2.08	0.31	0.14	-1.63	3.9	2.1	3.73	1.96	0.14	-1.63	-0.48	-2.25	2.03	0.26
	4.87	+H	A	4.58	-0.29	4.8	-0.1	4.78	-0.09	5.32	0.45	3.7	-1.2	2.35	-2.52	5.78	0.91	4.53	-0.34	4.89	0.02
150	6.51	-H	A	5.93	-0.58	5.6	-0.9	6.39	-0.12	7.01	0.50	4.1	-2.4	6.86	0.35	8.17	1.66	5.90	-0.61	4.92	-1.59
151	2.92	+H	A	2.55	-0.37	2.8	-0.1	2.53	-0.39	5.62	2.70	1.8	-1.1	2.61	-0.31	3.47	0.55	2.88	-0.04	3.18	0.26
	10.525	-H	A	11.35	0.82	10.7	0.2	10.10	-0.43	10.29	-0.24	[b]	-	11.90	1.38	14.57	4.05	[b]	-	9.70	-0.83
152	9.05	+H	A	8.47	-0.58	8.9	-0.2	9.06	0.01	8.47	-0.58	9.0	-0.1	9.37	0.32	9.52	0.47	9.55	0.50	9.43	0.38
153	9.19	+H	A	8.47	-0.72	8.9	-0.3	9.06	-0.13	8.47	-0.72	9.3	0.1	9.37	0.18	9.52	0.33	9.55	0.36	9.43	0.24
154	6.43	+H	A	6.32	-0.11	5.3	-1.1	6.08	-0.35	5.80	-0.63	7.1	0.7	6.28	-0.15	6.12	-0.31	5.90	-0.53	7.17	0.74
155	7.83	+H	A	9.14	1.31	8.3	0.5	10.30	2.47	9.78	1.95	10.3	2.5	9.09	1.26	8.30	0.47	7.90	0.07	8.38	0.55
156	1.67	+H	A	0.71	-0.96	3.2	1.5	1.63	-0.04	5.04	3.37	3.2	1.5	2.97	1.30	1.90	0.23	8.24	6.57	2.42	0.75
	5.5	+H	A	8.08	2.58	6.2	0.7	7.06	1.56	6.65	1.15	1.9	-3.6	8.33	2.83	7.18	1.68	4.05	-1.45	8.60	3.10
157	4.53	-H	A	4.64	0.11	4.6	0.1	5.17	0.64	10.79	6.26	[b]	-	5.13	0.60	5.59	1.06	4.80	0.27	3.20	-1.33
158	10.07	+H	A	10.35	0.28	10.1	0.0	9.99	-0.08	9.59	-0.48	9.4	-0.7	10.25	0.18	10.02	-0.05	9.88	-0.19	10.33	0.26
159	6.488	+H	A	6.32	-0.17	6.8	0.3	5.97	-0.52	7.18	0.69	5.1	-1.4	0.61	-5.88	8.28	1.79	5.85	-0.64	5.58	-0.91
160	2.95	-H	R	2.95	0.00	2.8	-0.2	3.07	0.12	3.90	0.95	2.7[e]	-0.3	2.94	-0.01	2.95	0.00	2.95	0.00	3.05	0.10
	5.408	-H	R	5.40	-0.01	5.0	-0.4	4.89	-0.52	5.41	0.00	4.2	-1.2	5.49	0.18	5.41	0.00	5.41	0.00	5.57	0.16
161	8.17	+H	A	8.32	0.15	8.1	-0.1	7.95	-0.22	9.15	0.98	8.5	0.3	6.59	-1.58	8.46	0.29	8.08	-0.09	8.26	0.09
162	0.99	-H	A	1.00	0.01	1.3	0.3	0.35	-0.64	-0.51	-1.50	3.5	2.5	0.99	0.00	0.99	0.00	1.48	0.49	1.23	0.24
	5.39	+H	A	4.71	-0.68	5.5	0.1	4.67	-0.72	5.31	-0.08	4.9	-0.5	5.53	0.14	5.25	-0.14	3.74	-1.65	5.03	-0.36
163	7.03	+H	A	7.02	-0.01	7.1	0.1	6.76	-0.27	7.10	0.07	7.9	0.9	6.61	-0.42	6.66	-0.37	7.07	0.04	6.83	-0.20

164	5.333	+H	R	5.30	-0.03	5.8	0.5	5.37	0.04	5.74	0.41	6.3	1.0	5.18	-0.15	5.38	0.05	5.33	0.00	5.53	0.20
	9.731	+H	R	9.55	-0.18	9.7	-0.0	10.11	0.38	10.11	0.38	10.8[f]	0.5	9.56	-0.17	9.71	-0.02	9.73	0.00	9.99	0.26
165	11.123	+H	R	10.45	-0.67	10.9	-0.2	10.72	-0.40	10.27	-0.85	11.0	-0.1	10.40	-0.72	10.59	-0.53	10.39	-0.73	10.90	-0.22
166	5.07	-H	A	4.50	-0.57	5.0	-0.1	5.53	0.46	5.30	0.23	10.1	5.0	1.79	-3.28	[b]	-	5.07	0.00	7.83	2.76
167	2.29	+H	A	2.12	-0.17	2.4	0.1	2.63	0.34	1.94	-0.35	1.1	-1.2	2.70	0.41	3.23	0.94	3.46	1.17	2.22	-0.07
	9.04	+H	A	9.24	0.20	8.9	-0.1	8.85	-0.19	8.39	-0.65	9.1	0.1	8.96	-0.08	9.60	0.56	8.57	-0.47	8.80	-0.24
168	9.5	+H	A	9.50	0.00	9.2	-0.3	9.25	-0.25	9.09	-0.41	9.6	0.1	9.67	0.17	10.08	0.58	9.20	-0.30	8.98	-0.52
169	9.7	+H	A	11.43	1.73	10.5	0.8	9.50	-0.20	10.14	0.44	9.6	-0.1	8.49	-1.21	9.39	-0.31	8.98	-0.72	9.47	-0.23
170	8.15	+H	A	9.57	1.42	8.7	0.5	8.44	0.29	8.41	0.26	8.1	-0.1	7.70	-0.45	7.80	-0.35	9.16	1.01	8.12	-0.03
171	10.06	+H	A	10.80	0.74	10.8	0.7	9.77	-0.29	9.70	-0.36	10.3	0.2	8.50	-1.56	9.08	-0.98	10.33	0.27	9.59	-0.47
172	10.33	+H	A	10.80	0.47	10.8	0.5	9.77	-0.56	9.70	-0.63	10.3	0.0	8.50	-1.83	9.08	-1.25	10.33	0.00	9.59	-0.74
173	9.73	+H	A	9.38	-0.35	9.3	-0.4	9.43	-0.30	8.64	-1.09	9.6	-0.1	9.52	-0.21	9.86	0.13	9.50	-0.23	9.70	-0.03
174	4.215	+H	A	3.69	-0.53	4.2	-0.0	3.70	-0.52	2.97	-1.25	2.6	-1.6	4.11	-0.11	-0.65	-4.87	4.09	-0.13	4.16	-0.05
	8.68	-H	A	8.23	-0.45	8.2	-0.5	8.37	-0.31	7.24	-1.44	5.0	-3.7	7.77	-0.91	7.45	-1.23	8.66	-0.02	8.13	-0.55
175	4.14	+H	A	3.57	-0.57	4.5	0.4	1.70	-2.44	2.85	-1.29	-0.1	-4.2	4.11	-0.03	-0.83	-4.97	4.09	-0.05	4.14	0.00
	6.2	-H	A	6.13	-0.07	7.0	0.8	6.55	0.35	6.25	0.05	[b]	-	6.68	0.48	6.42	0.22	7.90	1.70	6.31	0.11
	8.69	-H	A	8.22	-0.47	9.0	0.3	8.32	-0.37	7.30	-1.39	[d]	-	7.81	-0.88	7.21	-1.48	10.12	1.43	8.02	-0.67
176	3.455	+H	A	3.74	0.29	2.2	-1.3	4.17	0.72	3.69	0.24	4.5	1.0	4.57	1.12	3.48	0.02	2.26	-1.20	4.02	0.57
	8.11	+H	A	7.02	-1.09	7.9	-0.2	7.84	-0.27	9.74	1.63	[d]	-	8.02	-0.09	9.41	1.30	6.74	-1.37	8.20	0.09
	10.38	-H	A	9.98	-0.40	10.1	-0.3	10.35	-0.03	7.70	-2.68	[d]	-	9.01	-1.37	8.10	-2.28	10.13	-0.25	10.97	0.59
177	8.96	-H	A	9.63	0.67	8.9	-0.1	10.07	1.11	7.51	-1.45	8.9	-0.1	8.60	-0.36	8.67	-0.29	8.96	0.00	9.48	0.52
178	4.33	+H	A	4.77	0.44	5.0	0.7	4.20	-0.13	5.14	0.81	4.7	0.4	4.02	-0.31	4.00	-0.33	4.36	0.03	4.74	0.41
	8.56	+H	A	9.28	0.72	8.4	-0.2	7.62	-0.94	10.48	1.92	9.2	0.6	9.05	0.49	10.50	1.94	8.05	-0.51	9.09	0.53
179	9.69	-H	A	9.89	0.20	10.2	0.5	9.66	-0.03	9.69	0.00	9.9	0.2	6.97	-2.72	7.29	-2.40	9.69	0.00	[b]	-

180	2.78	-H	A	3.01	0.23	3.0	0.2	3.00	0.22	3.06	0.28	3.1	0.3	2.79	0.01	2.66	-0.12	2.98	0.20	3.06	0.28
181	4.5	-H	A	4.60	0.10	4.8	0.3	4.48	-0.02	4.35	-0.15	3.8	-0.7	5.01	0.51	4.39	-0.11	4.65	0.15	4.30	-0.20
182	8.29	-H	A	8.28	-0.01	8.3	0.0	9.73	1.44	8.03	-0.26	[d]	-	10.07	1.78	9.12	0.83	9.98	1.69	9.51	1.22
	9.72	+H	A	9.31	-0.41	9.7	-0.0	8.56	-1.16	9.14	-0.58	[d]	-	9.43	-0.29	10.56	0.84	9.50	-0.22	10.54	0.82
183	8.26	+H	A	8.37	0.11	8.1	-0.2	7.45	-0.81	9.80	1.54	8.8	0.5	8.37	0.11	7.88	-0.38	5.60	-2.66	8.39	0.13
184	4.207	-H	R	4.24	0.03	3.8	-0.4	3.75	-0.46	4.63	0.42	2.7[e]	-1.5	3.55	-0.66	3.86	-0.35	4.20	-0.01	3.97	-0.24
	5.638	-H	R	5.52	-0.12	5.3	-0.3	5.45	-0.19	6.55	0.91	[d]	-	5.69	0.05	5.44	-0.20	5.60	-0.04	5.57	-0.07
185	1.76	+H	A	0.93	-0.83	1.9	0.1	1.81	0.05	1.51	-0.25	1.8	0.0	2.14	0.38	1.87	0.11	4.16	2.40	1.64	-0.12
	5.26	-H	A	5.43	0.17	5.3	0.0	4.76	-0.50	5.07	-0.19	6.7	1.4	4.30	-0.96	5.01	-0.25	5.40	0.14	6.86	1.60
186	9.6	+H	A	9.37	-0.23	8.8	-0.8	9.03	-0.57	8.33	-1.27	[d]	-	9.15	-0.45	10.47	0.87	9.31	-0.29	10.63	1.03
187	3.033	-H	R	3.07	0.04	3.1	0.1	3.17	0.14	3.51	0.48	2.9	-0.1	2.72	-0.31	2.62	-0.41	3.04	0.01	2.87	-0.16
	4.366	-H	R	4.35	-0.02	4.6	0.2	4.72	0.35	5.43	1.06	[d]	-	4.79	0.42	3.93	-0.44	4.37	0.00	4.53	0.16
188	8.65	+H	A	9.65	1.00	10.0	1.4	8.56	-0.09	9.42	0.77	[d]	-	9.75	1.10	12.01	3.36	10.59	1.94	10.22	1.57
189	8.65	+H	A	9.41	0.76	9.0	0.4	8.92	0.27	9.82	1.17	[d]	-	9.41	0.76	9.48	0.83	10.35	1.70	9.35	0.70
190	8.55	-H	A	8.60	0.05	8.9	0.4	10.63	2.08	12.42	3.87	[b]	-	11.34	2.79	10.96	2.41	[b]	-	10.78	2.23
191	8.08	+H	R	7.78	-0.30	8.1	0.0	8.22	0.14	7.50	-0.58	9.4	1.3	8.95	0.87	7.81	-0.27	8.08	0.00	8.15	0.07
192	2.36	-H	A	2.30	-0.06	2.1	-0.3	2.27	-0.09	2.05	-0.31	7.4	5.0	2.54	0.18	2.29	-0.07	2.29	-0.07	2.47	0.11
	9.42	+H	A	9.71	0.29	9.4	-0.0	8.89	-0.53	9.31	-0.11	8.0	-1.4	9.40	-0.02	9.58	0.16	9.30	-0.12	9.90	0.48
193	2.06	-H	A	2.25	0.19	2.1	0.0	2.29	0.23	2.45	0.39	6.7	4.6	2.00	-0.06	2.16	0.10	2.18	0.12	2.31	0.25
	9.145	+H	A	9.09	-0.05	9.0	-0.1	8.84	-0.31	9.21	0.07	[d]	-	9.19	0.04	9.71	0.57	9.21	0.07	9.30	0.16
	10.265	-H	A	10.01	-0.26	10.2	-0.1	10.02	-0.25	10.38	0.12	[d]	-	9.79	-0.48	9.43	-0.84	10.47	0.21	10.47	0.21
194	7.396	-H	R	7.78	0.38	7.6	0.2	8.91	1.51	7.62	0.22	7.6	0.2	7.81	0.41	7.59	0.19	7.25	-0.15	7.79	0.39
195	8.889	-H	A	9.25	0.36	8.7	-0.2	9.53	0.64	9.12	0.23	9.2	0.3	9.39	0.50	8.98	0.09	8.89	0.00	9.18	0.29
196	7.912	-H	A	8.18	0.27	7.9	-0.0	7.98	0.07	8.25	0.34	7.7	-0.2	8.74	0.83	8.17	0.26	7.91	0.00	7.58	-0.33

197	5.02	-H	A	4.50	-0.52	5.0	-0.0	5.86	0.84	5.92	0.90	4.2	-0.8	3.83	-1.19	4.54	-0.48	5.00	-0.02	5.69	0.67

[a] Dev = calculated pK_a value (Cal) – experimental pK_a value. [b] Program failed to predict the value. [c] Average of results for ionization of the 2' and 3' –OH groups of the ribose. [d] Site was not calculated because of complexity. [e] Correction factor (-0.60) was applied. [f] Correction factor (+0.60) was applied. [g] The enol group was tautomerized to a carbonyl group by the program when calculating. [h] Value is for the mesomer. [i] Value was measured at 20 °C. [j] Value was calculated for 20 °C (the value calculated for 25 °C is 7.00)