Journal of Computer-Aided Molecular Design manuscript No.
(will be inserted by the editor)

Supporting Information: Blind prediction of solvation free energies from the SAMPL4 challenge

David L. Mobley, Karisa L. Wymer, Nathan M. Lim, and J. Peter Guthrie

Received: date / Accepted: date

Abstract Here, we provide Supporting Information associated with our main article – specifically, we provide full submission data for all submissions for which participants were willing to share the data; this includes predicted values, as well as method descriptions. We also provide the SAMPL challenge inputs, and error/analysis statistics for the "blind" and "supplementary" components separately. We also give SMILES strings and IUPAC names for the compounds, provide the mean error by compound, and give tables showing results of our *t*-test experiments.

Keywords hydration free energy · transfer free energy · SAMPL · free energy calculation

1 Supporting Materials

Statistics for the blind and supplementary subsets are shown in Tables 1 and 2, respectively.

D. Mobley · K. Wymer · N. Lim
Department of Pharmaceutical Sciences
and Department of Chemistry
147 Bison Modular
University of California, Irvine
Irvine, CA 92697
Tel.: 949-824-6383
Fax: 949-824-2949
E-mail: dmobley@mobleylab.org

D. Mobley
Department of Chemistry
University of New Orleans
2000 Lakeshore Drive
New Orleans, LA 70148

J. P. Guthrie
Department of Chemistry
University of Western Ontario
London, ON, Canada

Experimental values and uncertainties, as used for the analysis here, are shown in Table 3.

Results from applying Student's paired *t*-test to assess whether differences between methods are significant are shown in Table 4 for comparison to one of the top methods, submission 145, and in Tables 5 and 6 for control submissions 014 and 015, respectively.

Additional supporting information, in the form of input files provided to participants, and participant submissions (predictions and method descriptions, at least from those participants who gave us permission to share this information) are provided as a supporting archive file.

ID	avg. err.	RMS	AUE	tau	R
004	0.37 ± 0.34	1.55 ± 0.35	1.15 ± 0.23	0.62 ± 0.07	0.94 ± 0.02
005	-0.38 ± 0.28	1.30 ± 0.22	1.02 ± 0.18	0.68 ± 0.06	0.96 ± 0.02
014	0.58 ± 0.55	2.50 ± 0.38	1.90 ± 0.35	0.31 ± 0.11	0.87 ± 0.22
015	0.61 ± 0.51	2.47 ± 0.42	1.93 ± 0.33	0.42 ± 0.10	0.84 ± 0.21
137	2.59 ± 0.46	3.32 ± 0.49	2.84 ± 0.38	0.65 ± 0.06	0.88 ± 0.03
138	0.87 ± 0.44	2.14 ± 0.33	1.74 ± 0.28	0.50 ± 0.07	0.91 ± 0.05
141	-0.30 ± 0.39	1.85 ± 0.43	1.34 ± 0.28	0.70 ± 0.06	0.93 ± 0.02
145	-0.63 ± 0.29	1.47 ± 0.35	1.05 ± 0.22	0.73 ± 0.05	0.98 ± 0.02
149	0.43 ± 0.35	1.54 ± 0.19	1.28 ± 0.19	0.74 ± 0.06	0.97 ± 0.05
152	-3.11 ± 0.39	3.57 ± 0.37	3.17 ± 0.36	0.68 ± 0.10	0.94 ± 0.18
153	-2.23 ± 0.61	3.55 ± 0.56	2.57 ± 0.53	0.66 ± 0.06	0.89 ± 0.12
158	-2.74 ± 2.67	12.88 ± 2.59	9.58 ± 1.83	0.76 ± 0.05	0.56 ± 0.09
166	-0.42 ± 0.36	1.68 ± 0.24	1.38 ± 0.21	0.62 ± 0.07	0.93 ± 0.04
167	1.04 ± 0.36	1.92 ± 0.35	1.36 ± 0.29	0.46 ± 0.10	0.93 ± 0.17
168	1.00 ± 0.41	2.06 ± 0.33	1.55 ± 0.29	0.42 ± 0.10	0.91 ± 0.18
169	-0.45 ± 0.49	2.30 ± 0.26	1.91 ± 0.27	0.31 ± 0.09	0.86 ± 0.09
178	0.47 ± 0.28	1.34 ± 0.21	1.10 ± 0.17	0.70 ± 0.07	0.96 ± 0.02
179	0.46 ± 0.33	1.54 ± 0.29	1.17 ± 0.22	0.70 ± 0.07	0.94 ± 0.03
180	-0.84 ± 0.35	1.77 ± 0.32	1.29 ± 0.27	0.68 ± 0.07	0.96 ± 0.03
181	-0.53 ± 0.28	1.35 ± 0.25	1.00 ± 0.20	0.69 ± 0.08	0.96 ± 0.03
189	1.01 ± 0.59	2.89 ± 0.74	1.92 ± 0.47	0.41 ± 0.10	0.83 ± 0.14
196	-2.14 ± 2.72	12.46 ± 2.62	9.45 ± 1.82	0.74 ± 0.05	0.51 ± 0.09
197	-2.19 ± 2.85	13.63 ± 2.44	10.47 ± 1.85	0.70 ± 0.05	0.41 ± 0.08
529	0.61 ± 0.58	2.77 ± 0.53	1.98 ± 0.42	0.46 ± 0.08	0.81 ± 0.06
530	-0.09 ± 0.53	2.32 ± 0.45	1.72 ± 0.34	0.45 ± 0.13	0.85 ± 0.13
531	0.41 ± 0.64	2.82 ± 0.45	2.25 ± 0.40	0.43 ± 0.14	0.80 ± 0.18
532	-0.34 ± 0.42	1.91 ± 0.30	1.57 ± 0.25	0.50 ± 0.14	0.90 ± 0.24
533	-0.60 ± 0.33	1.60 ± 0.22	1.33 ± 0.21	0.62 ± 0.11	0.95 ± 0.13
534	0.84 ± 0.63	3.01 ± 1.01	1.70 ± 0.53	0.44 ± 0.16	0.85 ± 0.21
542	0.15 ± 0.42	1.86 ± 0.38	1.30 ± 0.29	0.64 ± 0.08	0.94 ± 0.07
543	0.55 ± 0.40	1.82 ± 0.39	1.30 ± 0.27	0.57 ± 0.08	0.93 ± 0.07
544	0.59 ± 0.30	1.43 ± 0.28	1.07 ± 0.21	0.70 ± 0.06	0.96 ± 0.02
545	1.67 ± 0.54	3.07 ± 0.51	2.49 ± 0.40	0.41 ± 0.10	0.81 ± 0.11
548	2.44 ± 0.54	3.43 ± 0.68	2.47 ± 0.53	0.36 ± 0.10	0.84 ± 0.08
561	0.06 ± 0.23	1.00 ± 0.17	0.78 ± 0.14	0.79 ± 0.05	0.98 ± 0.04
562	0.62 ± 0.39	1.80 ± 0.23	1.46 ± 0.23	0.67 ± 0.06	0.92 ± 0.03
563	0.17 ± 0.54	2.51 ± 0.51	1.89 ± 0.36	0.40 ± 0.08	0.82 ± 0.07
564	0.92 ± 0.62	2.94 ± 0.64	2.11 ± 0.46	0.28 ± 0.11	0.79 ± 0.11
565	0.66 ± 0.30	1.49 ± 0.33	1.01 ± 0.24	0.79 ± 0.05	0.96 ± 0.02
566	0.53 ± 0.30	1.40 ± 0.32	0.96 ± 0.23	0.74 ± 0.05	0.96 ± 0.02
567	-0.62 ± 0.63	2.99 ± 0.69	2.12 ± 0.44	0.58 ± 0.08	0.75 ± 0.05
568	-0.86 ± 0.32	1.65 ± 0.26	1.25 ± 0.24	0.72 ± 0.05	0.95 ± 0.02
569	-3.03 ± 0.61	4.14 ± 0.52	3.42 ± 0.50	0.60 ± 0.08	0.80 ± 0.06
570	-2.57 ± 0.43	3.23 ± 0.52	2.59 ± 0.41	0.76 ± 0.06	0.91 ± 0.05
572	-0.65 ± 0.65	2.84 ± 0.68	1.99 ± 0.45	0.59 ± 0.08	0.78 ± 0.04
573	-0.89 ± 0.28	1.49 ± 0.22	1.20 ± 0.20	0.72 ± 0.06	0.96 ± 0.02
575	-0.27 ± 0.31	1.45 ± 0.21	1.20 ± 0.19	0.63 ± 0.07	0.95 ± 0.04
581	0.37 ± 0.39	1.77 ± 0.56	1.14 ± 0.30	0.71 ± 0.10	0.93 ± 0.04
582	1.40 ± 0.77	3.73 ± 0.65	2.79 ± 0.54	0.50 ± 0.08	0.83 ± 0.05

Table 1 Statistics for SAMPL4 hydration prediction. Shown are statistics for each submission, by submission ID. We report average error, RMS error, average unsigned error, Kendall tau, and Pearson R. Units, when applicable, are kcal/mol. Submission 575 was apparently affected with a propagation bug when running the molecular dynamics simulations, introducing errors.

ID	avg. err.	RMS	AUE	tau	R
004	-0.06 ± 0.27	1.26 ± 0.14	1.07 ± 0.14	0.68 ± 0.07	0.95 ± 0.02
005	-0.46 ± 0.22	1.14 ± 0.16	0.92 ± 0.14	0.83 ± 0.06	0.98 ± 0.02
014	1.53 ± 0.62	3.46 ± 0.77	1.90 ± 0.57	0.43 ± 0.11	0.41 ± 0.22
015	1.35 ± 0.64	3.52 ± 0.75	2.10 ± 0.54	0.31 ± 0.10	0.31 ± 0.21
137	1.95 ± 0.31	2.49 ± 0.26	2.18 ± 0.24	0.65 ± 0.06	0.91 ± 0.03
138	0.23 ± 0.38	1.87 ± 0.18	1.60 ± 0.19	0.65 ± 0.07	0.90 ± 0.05
141	0.12 ± 0.22	1.04 ± 0.16	0.85 ± 0.13	0.80 ± 0.06	0.97 ± 0.02
145	-0.29 ± 0.20	1.00 ± 0.17	0.73 ± 0.14	0.83 ± 0.05	0.98 ± 0.02
149	-0.30 ± 0.29	1.39 ± 0.31	0.99 ± 0.20	0.75 ± 0.06	0.92 ± 0.05
152	-3.78 ± 1.13	6.68 ± 1.31	4.75 ± 0.97	0.23 ± 0.10	0.21 ± 0.18
153	-2.45 ± 0.71	4.25 ± 0.52	3.47 ± 0.50	0.44 ± 0.06	0.55 ± 0.12
158	3.21 ± 1.24	7.19 ± 1.78	5.33 ± 0.97	0.58 ± 0.05	0.35 ± 0.09
166	-0.36 ± 0.29	1.49 ± 0.21	1.12 ± 0.19	0.78 ± 0.07	0.91 ± 0.04
167	-1.58 ± 1.08	5.77 ± 1.79	2.80 ± 0.97	0.51 ± 0.10	0.45 ± 0.17
168	-1.57 ± 1.09	5.80 ± 1.78	2.76 ± 0.97	0.52 ± 0.10	0.44 ± 0.18
169	-0.60 ± 0.44	2.33 ± 0.44	1.62 ± 0.33	0.62 ± 0.09	0.83 ± 0.09
178	0.07 ± 0.33	1.65 ± 0.17	1.42 ± 0.17	0.66 ± 0.07	0.94 ± 0.02
179	0.07 ± 0.30	1.55 ± 0.19	1.27 ± 0.18	0.64 ± 0.07	0.92 ± 0.03
180	-0.64 ± 0.38	2.10 ± 0.22	1.74 ± 0.22	0.68 ± 0.07	0.94 ± 0.03
181	-0.46 ± 0.32	1.70 ± 0.17	1.43 ± 0.18	0.67 ± 0.08	0.93 ± 0.03
189	-0.31 ± 0.51	2.61 ± 0.45	1.97 ± 0.35	0.58 ± 0.10	0.69 ± 0.14
196	3.14 ± 1.29	7.15 ± 1.80	5.34 ± 0.94	0.60 ± 0.05	0.32 ± 0.09
197	3.35 ± 1.32	7.30 ± 1.76	5.53 ± 0.94	0.58 ± 0.05	0.31 ± 0.08
529	-0.02 ± 0.39	2.04 ± 0.24	1.69 ± 0.24	0.73 ± 0.08	0.90 ± 0.06
542	-0.30 ± 0.39	1.92 ± 0.43	1.29 ± 0.29	0.69 ± 0.08	0.86 ± 0.07
543	0.20 ± 0.35	1.79 ± 0.30	1.40 ± 0.22	0.72 ± 0.08	0.86 ± 0.07
544	0.20 ± 0.23	1.11 ± 0.13	0.94 ± 0.12	0.73 ± 0.06	0.96 ± 0.02
545	0.53 ± 0.56	2.87 ± 0.52	2.17 ± 0.37	0.51 ± 0.10	0.70 ± 0.11
548	0.36 ± 0.44	2.15 ± 0.27	1.77 ± 0.25	0.67 ± 0.10	0.90 ± 0.08
561	-0.44 ± 0.36	1.93 ± 0.46	1.32 ± 0.27	0.74 ± 0.05	0.91 ± 0.04
562	0.72 ± 0.30	1.57 ± 0.13	1.44 ± 0.14	0.70 ± 0.06	0.92 ± 0.03
563	-0.43 ± 0.48	2.47 ± 0.36	1.85 ± 0.31	0.51 ± 0.08	0.78 ± 0.07
564	-0.28 ± 0.53	2.71 ± 0.38	2.28 ± 0.30	0.54 ± 0.11	0.80 ± 0.11
565	0.33 ± 0.22	1.13 ± 0.13	0.95 ± 0.13	0.78 ± 0.05	0.96 ± 0.02
566	0.19 ± 0.22	1.08 ± 0.12	0.93 ± 0.12	0.78 ± 0.05	0.96 ± 0.02
567	-0.75 ± 0.28	1.64 ± 0.16	1.41 ± 0.16	0.56 ± 0.08	0.93 ± 0.05
568	-0.87 ± 0.25	1.48 ± 0.21	1.17 ± 0.19	0.75 ± 0.05	0.95 ± 0.02
569	-2.93 ± 0.67	4.49 ± 0.87	3.11 ± 0.63	0.50 ± 0.08	0.77 ± 0.06
570	-2.40 ± 0.46	3.30 ± 0.63	2.48 ± 0.44	0.69 ± 0.06	0.85 ± 0.05
572	-0.71 ± 0.29	1.60 ± 0.16	1.35 ± 0.17	0.57 ± 0.08	0.93 ± 0.04
573	-0.81 ± 0.24	1.43 ± 0.20	1.12 ± 0.18	0.75 ± 0.06	0.95 ± 0.02
575	-1.25 ± 0.44	2.51 ± 0.43	1.90 ± 0.33	0.65 ± 0.07	0.88 ± 0.04
582	-0.65 ± 0.99	5.04 ± 0.98	3.62 ± 0.71	0.78 ± 0.08	0.93 ± 0.05

Table 2 Statistics for SAMPL4 hydration prediction. Shown are statistics for each submission, by submission ID. We report average error, RMS error, average unsigned error, Kendall tau, and Pearson R. Units, when applicable, are kcal/mol. Submission 575 was apparently affected with a propagation bug when running the molecular dynamics simulations, introducing errors.

ID	SMILES	name	MW	ΔG_{hyd}	uncertainty
SAMPL4_047	O=C1c2c(cccc2NCCO)C(=O)c2c1cccc2	1-(2-hydroxyethylamino)-9,10-anthraquinone	267.28	-14.21	1.1
SAMPL4_020	C=C(c1ccccc1)c2ccccc2	1,1-diphenylethene	180.245	-2.78	0.1
SAMPL4_005	O(C)c1ccccc1OC	1,2-dimethoxybenzene	138.17	-5.33	0.1
SAMPL4_028	O(N(=O)=O)C(CCON(=O)=O)C	1,3-bis-(nitrooxy)butane	180.12	-4.29	0.39
SAMPL4_027	O(N(=O)=O)C(CCON(=O)=O)	1,3-bis-(nitrooxy)propane	166.09	-4.8	0.39
SAMPL4_048	O=C1c2c(C(=O)c3c1cccc3)c(N)ccc2N	1,4-diamino-9,10-anthraquinone	238.25	-11.85	0.35
SAMPL4_044	O1CCOCC1	1,4-dioxane	88.11	-5.08	0.1
SAMPL4_051	Nc1c2c(c(cc1)O)C(=O)c3c(cccc3)C2=O	1-amino-4-hydroxy-9,10-anthraquinone	239.23	-9.53	0.28
SAMPL4_046	Nc1c2c(ccc1)C(=O)c3c(cccc3)C2=O	1-amino-9,10-anthraquinone	223.23	-9.44	0.74
SAMPL4_021	c1(ccccc1)Cn2cncc2	1-benzylimidazole	159.214	-7.63	0.12
SAMPL4_025	O(CC(O)C)CCCC	1-butoxy-2-propanol	132.2	-5.73	0.15
SAMPL4_039	c1cccc(C)c1CC	1-ethyl-2-methylbenzene	120.2	-0.85	0.1
SAMPL4_009	Clc1c(C=O)c(Cl)c(OC)c(O)c1OC	2,6-dichlorosyringaldehyde	251.06	-8.24	0.76
SAMPL4_033	O(C)c1cccc(OC)c1O	2,6-dimethoxyphenol	154.16	-6.96	0.1
SAMPL4_045	O=C1c2c(ccc(N)c2)C(=O)c2c1cccc2	2-amino-9,10-anthraquinone	223.23	-11.53	0.29
SAMPL4_011	Clc1c(OC)c(O)c(OC)cc1C=O	2-chlorosyringaldehyde	216.62	-7.78	0.77
SAMPL4_026	C(C)OCCOC(=O)C	2-ethoxyethyl acetate	132.16	-5.31	0.1
SAMPL4_036	Oc1ccccc1CC	2-ethylphenol	122.17	-5.66	0.1
SAMPL4_035	Oc1ccccc1C=O	2-hydroxybenzaldehyde	122.12	-4.68	0.1
SAMPL4_037	COc1c(cccc1)O	2-methoxyphenol	124.14	-5.94	0.1
SAMPL4_038	O=Cc1ccccc1C	2-methylbenzaldehyde	120.15	-3.93	0.1
SAMPL4_032	Clc1cc(O)ccc1Cl	3,4-dichlorophenol	163	-7.29	0.1
SAMPL4_010	Clc1cc(Cl)c(OC)c(O)c1OC	3,5-dichlorosyringol	223.05	-6.24	0.38
SAMPL4_034	Cc1cc(c(cc1)O)OC	4-methyl-2-methoxyphenol	138.17	-5.8	0.1
SAMPL4_006	Oc1ccc(cc1OC)CCC	4-propylguaiacol	166.217	-5.26	0.18
SAMPL4_019	C1c2c(Cc3c1cccc3)cccc2	9,10-dihydroanthracene	180.25	-3.78	0.1
SAMPL4_024	CN(C)CCC=C1c2ccccc2CCc3c1cccc3	amitriptyline	277.41	-7.43	0.6
SAMPL4_050	c12c(cc3c(c1)cccc3)cccc2	anthracene	178.23	-4.14	0.1
SAMPL4_049	O1c2c(Oc3c1cccc3)cccc2	dibenzo-p-dioxin	184.19	-3.16	0.1
SAMPL4_013	OC1CC(CC=C1C)C(C)=C	carveol	152.24	-4.44	0.43
SAMPL4_043	C1CCC=CC1	cyclohexene	82.15	0.14	0.1
SAMPL4_012	CC1C(=O)CC(CC1)C(=C)C	dihydrocarvone	152.238	-3.75	0.21
SAMPL4_023	c1ccccc1C(c2ccccc2)OCCN(C)C	diphenhydramine	255.363	-9.34	0.62
SAMPL4_052	O(c1ccccc1)c1ccccc1	diphenyl ether	170.21	-2.87	0.69
SAMPL4_004	OC\C=C(\CCC=C(C)C)/C	geraniol	154.25	-4.45	0.24
SAMPL4_030	O(C(=O)C)CCCCCC	hexyl acetate	144.21	-2.29	0.12
SAMPL4_029	O([N+](=O)[O-])CCCCCC	hexyl nitrate	147.17	-1.66	0.1
SAMPL4_002	CC(=CCCC(C)(C=C)OC(=O)C)C	linalyl acetate	196.292	-2.49	0.85
SAMPL4_001	C(C(C(C(C(CO)O)O)O)O)O	mannitol	182.178	-23.62	0.32
SAMPL4_016	OC1CC(CCC1C(C)C)C	menthol	156.27	-3.2	0.27
SAMPL4_017	CC1CCC(C(=O)C1)C(C)C	menthone	154.25	-2.53	0.25
SAMPL4_022	Cc1c(cccc1Nc2ccccc2C(=O)O)C	mefenamic acid	241.29	-6.78	0.1
SAMPL4_003	CC(=CCCC(=CCO)C)C	nerol	154.254	-4.78	0.25
SAMPL4_014	O=C\C1=C\CC(\C(=C)C)CC1	l-perillaldehyde	150.22	-4.09	0.17
SAMPL4_041	N1CCCCC1	piperidine	85.15	-5.05	0.1
SAMPL4_015	CC1=CC(=O)C(CC1)C(C)C	piperitone	152.238	-4.51	0.1
SAMPL4_042	O1CCCCC1	tetrahydropyran	86.13	-3.13	0.1

Table 3 Compound identifiers, SMILES strings, molecular weights, hydration free energies, and uncertainties, as provided by J. Peter Guthrie for analysis of the SAMPL challenge. This data was provided after the submission deadline, with updates as described in the main text. Units of free energy are kcal/mol.

SID	t	p
168	-0.03	0.98
167	-0.04	0.96
005	-0.07	0.94
181	0.18	0.85
166	-0.20	0.84
169	0.25	0.81
158	-0.66	0.51
567	0.67	0.51
572	0.67	0.5
563	-0.69	0.49
561	-0.78	0.44
196	-0.84	0.41
197	-0.84	0.41
180	0.91	0.37
582	-1.04	0.3
542	-1.04	0.3
575	1.11	0.27
141	-1.36	0.18
564	-1.57	0.12
189	-1.66	0.1
573	1.67	0.1
568	1.67	0.1
149	-1.71	0.094
529	-1.80	0.079
004	-2.16	0.036
179	-2.42	0.019
178	-2.48	0.017
543	-2.55	0.014
138	-2.89	0.0059
015	-3.16	0.0028
566	-3.23	0.0023
544	-3.31	0.0018
545	-3.34	0.0016
014	-3.40	0.0014
565	-3.74	0.00049
153	3.84	0.00036
562	-3.94	0.00027
548	-4.30	8.6e-05
152	4.65	2.7e-05
569	5.10	5.9e-06
570	5.70	7.6e-07
137	-8.41	6.3e-11

Table 4 Student's *t*-test results comparing errors for submission 145 to that from other submissions. Shown are the *t*-statistic and p-value.

SID	t	p
545	0.11	0.91
015	0.14	0.89
197	0.14	0.89
196	0.21	0.83
548	-0.33	0.74
158	0.36	0.72
562	0.90	0.37
582	1.07	0.29
138	1.16	0.25
565	1.37	0.18
189	1.42	0.16
564	1.43	0.16
543	1.52	0.14
529	1.54	0.13
544	1.60	0.12
566	1.67	0.1
178	1.80	0.078
179	1.81	0.077
168	1.94	0.059
167	1.94	0.058
004	2.07	0.044
137	-2.26	0.029
563	2.27	0.028
149	2.28	0.027
542	2.38	0.021
141	2.48	0.017
561	2.75	0.0084
169	3.05	0.0038
166	3.11	0.0031
567	3.35	0.0016
181	3.36	0.0015
005	3.37	0.0015
572	3.39	0.0014
145	3.40	0.0014
180	3.67	0.00062
575	3.75	0.00048
568	4.26	9.7e-05
573	4.27	9.4e-05
153	5.49	1.6e-06
152	6.04	2.3e-07
569	6.48	5e-08
570	6.80	1.6e-08

Table 5 Student's *t*-test results comparing errors for control submission 014 to that from other submissions. Shown are the *t*-statistic and p-value.

SID	t	p
545	-0.03	0.97
197	0.09	0.93
014	-0.14	0.89
196	0.16	0.88
158	0.30	0.77
548	-0.48	0.63
562	0.71	0.48
582	0.95	0.35
138	0.98	0.33
565	1.16	0.25
189	1.25	0.22
564	1.27	0.21
543	1.32	0.19
529	1.37	0.18
544	1.39	0.17
566	1.45	0.15
178	1.59	0.12
179	1.60	0.12
168	1.82	0.076
167	1.82	0.075
004	1.86	0.069
149	2.06	0.045
563	2.09	0.042
542	2.18	0.034
141	2.26	0.028
137	-2.40	0.021
561	2.53	0.015
169	2.85	0.0064
166	2.89	0.0058
005	3.12	0.0031
181	3.13	0.003
567	3.15	0.0028
145	3.16	0.0028
572	3.19	0.0025
180	3.44	0.0012
575	3.54	0.00093
568	4.01	0.00022
573	4.01	0.00021
153	5.30	3e-06
152	5.89	4e-07
569	6.29	9.8e-08
570	6.56	3.9e-08

Table 6 Student's *t*-test results comparing errors for control submission 015 to that from other submissions. Shown are the *t*-statistic and p-value.