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ERRATUM

Erratum to: Computing translational diffusion and sedimentation coefficients: an evaluation of experimental data and programs

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In the original publication of the article, the minus sign is omitted in the last two entries of the last column "BEST Heur" in Table 2. Similar error is also found in Table 3, in the fifth entry under Column 7. The correct version of both Tables 2 and 3 are given for your reading:

The online version of the original article can be found under doi:10.1007/s00249-015-1042-9.

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Table 2 Proteins used for the comparison, with their PDB code, molecular weight (mol. wt.), partial specific volume ($\bar{\nu}_{(20,w)}$), experimental sedimentation coefficient (±SD) ($s^0_{(20,w)}$ expt.) taken from the literature (Ref.), and percent difference between the computed and experimental $s^0_{(20,w)}$ values (Δ % $s^0_{(20,w)}$ comp.) for each of the different methods used. The horizontal line between entries 13 and 14 separates monomeric from multimeric solution forms

#	Protein[a]	PDB	Mol. wt.	$\bar{\nu}_{(20,w)}$ [b] cm^3/g	$s^0_{(20,w)}$ expt.[c] S	Ref.[d]	Δ % $s^0_{(20,w)}$ comp.							
							SoMo SMI	SoMo Zeno	SoMo ov Zeno	AtoB G5 SMI	AtoB G2 SMI	HP auto	BEST man	BEST heur
1	Cytochrome *c*	1HRC	12,357.5	0.724	2.00 ± 0.04*	2,3	−21.0	−14.2	−16.3	−23.5	−23.0	−17.5	−18.1	−17.8
2	Ribonuclease A	8RAT	13,683.8	0.709	2.00 ± 0.03	2[e]	−3.0	−4.0	−6.5	−5.0	−4.0	−10.0	−10.4	−10.4
3	α-Lactalbumin	1A4V[f]	15,784.7	(0.718)	1.76 ± n.a.*	3[e]	+13.6	+12.6	+9.4	+10.8	+10.8	0.0	+5.7	+5.6
4	Lysozyme	1AKI	14,306.7	(0.716)	1.88 ± 0.02	2[e]	+5.9	+5.1	+2.4	+3.2	+4.3	−2.7	−1.8	−1.6
5	Myoglobin apo	2V1 K	17,568.3	0.743	2.05 ± n.a.	3[e]	−1.0	−1.9	−4.6	−3.9	−3.4	−6.3	−6.7	−6.8
6	Soybean trypsin inh.	1AVU	19,962.8	(0.735)	2.29 ± n.a.	4	−2.6	−3.8	−5.7	−4.4	−3.9	−4.4	−8.7	−8.8
7	β-Trypsin	1TPO	23,335.9	(0.724)	2.54 ± 0.02	5	+6.3	+5.6	+2.4	+3.5	+3.9	−1.2	−0.5	−0.5
8	Trypsinogen	1TGN	23,182.7	0.73	2.48 ± 0.01	5	+7.7	+5.1	+2.0	+4.8	+5.6	−1.6	−0.9	−0.9
9	α-Chymotrypsin (mon)	4CHA	25,236.5	(0.733)	2.59 ± 0.02	6	+3.1	+3.0	+0.8	+1.5	+1.5	−3.5	−2.8	−2.7
10	Chymotrypsinogen A	2CGA	25,659.0	(0.732)	2.56 ± 0.03	3[e]	+6.6	+6.3	+4.1	+4.7	+5.5	−0.8	+0.4	+0.2
11	Carbonic anhydrase B	2CAB	28,820.5	0.73	3.01 ± 0.19	7–10	+1.0	−1.5	−3.9	−1.7	−1.0	−6.3	−6.0	−6.0
12	Pepsin	4PEP	34,588.6	(0.723)	3.19 ± 0.08	11	+6.3	+5.5	+3.6	+4.4	+5.0	−0.3	+0.5	+0.4
13	H. serum albumin	1AO6	66,428.6	(0.734)	4.28 ± 0.04	12	+5.1	+5.5	+4.3	+5.1	+5.4	+0.9	+2.8	+2.5
14	Superoxide dismutase	2SOD	31,442.2	(0.718)	3.03 ± 0.05	13	+1.7	+1.6	−0.4	+1.0	+1.0	−3.0	−2.1	−1.9
15	β-Lactoglobulin	1BEB	35,224.7	(0.745)	2.87 ± 0.06	3[e]	+4.9	+1.8	+0.3	+4.2	+4.2	−2.1	−1.4	−1.4
16	α-Chymotrypsin (dim)	4CHA	50,473.5	(0.733)	3.5 ± 0.02*	14	+18.0	+18.7	+16.8	+16.9	+16.9	+12.3	+13.7	+13.3
17	Triosephosphate isom.	8TIM	52,971.4	(0.742)	3.75 ± 0.05	15	+7.5	+6.7	+5.4	+6.1	+6.4	+2.9	+3.7	+3.4
18	Hemoglobin CO	1HCO	64,559.7	0.749	4.5 ± n.a.	3[e]	+4.4	+3.2	+1.9	+3.1	+3.3	−0.7	+2.5	+2.2
19	Citrate synthase	1CTS	97,845.5	0.733	6.1 ± 0.1	2[e]	+1.1	+3.3	+3.7	+0.2	+0.5	−1.6	+0.6	+0.1
20	Inorganic pyrophosph.	1FAJ	117,339.0	(0.743)	7.01 ± 0.04	16	−4.6	−4.2	−5.3	−5.1	−5.1	−8.0	−6.5	−5.8
21	G3PD apo	2GD1	143,787.8	(0.742)	7.6 ± 0.15	3[e]	+2.2	+2.5	+1.1	+0.9	+1.2	−0.8	0.0	−0.4
22	G3PD holo	1GD1	146,437.7	(0.741)	8.1 ± 0.16	3[e]	−1.5	−1.3	−2.7	−2.6	−2.3	−5.2	−3.5	−3.8
23	LDH pig H + NAD	5LDH	148,942.6	(0.746)	7.80 ± 0.08	3[e]	+2.8	+2.8	+1.8	+1.7	+1.9	0.0	−0.2	+0.4
24	LDH pig M + NAD	9LDH	149,063.5	(0.745)	7.79 ± 0.08	3[e]	+5.6	+5.9	+4.4	+4.1	+4.2	+1.2	+2.6	+2.4
25	Aldolase	1ADO	157,131.2	0.742	7.85 ± 0.05	3[e]	+2.5	+1.2	−0.5	+1.9	+2.0	−2.5	−2.7	−2.5
26	Catalase	4BLC	235,775.1	0.73	11.4 ± 0.15	3[e]	+2.1	+1.3	+0.2	+1.2	+1.5	−5.3	–	–
27	β-Galactosidase	1BGL	465,257.6	(0.725)	16.23 ± 0.13	17	+6.0	+6.6	+5.9	+5.4	+3.3	+2.8	–	–

Table 2 continued

#	Protein[a]	PDB	Mol. wt.	$\bar{\nu}_{(20,w)}$ [b] cm^3/g	$s^0_{(20,w)}$ expt.[c] S	Ref.[d]	Δ % $s^0_{(20,w)}$ comp.							
							SoMo SMI	SoMo Zeno	SoMo ov Zeno	AtoB G5 SMI	AtoB G2 SMI	HP auto	BEST man	BEST heur
			Mean Δ % monomeric (without * values)				+3.2 ± 4.0	+2.3 ± 4.2	−0.1 ± 4.2	+1.1 ± 4.1	+1.7 ± 4.0	−3.3 ± 3.2	−3.1 ± 4.2	−3.1 ± 4.2
			Mean Δ % all (without * values)				+2.9 ± 3.5	+2.3 ± 3.5	+0.6 ± 3.7	+1.4 ± 3.5	+1.7 ± 3.4	−2.4 ± 3.2	−1.9 ± 3.8	−1.9 ± 3.7

SoMo SoMo models without overlaps, *SoMo ov* SoMo models with overlaps, *AtoB G5* AtoB models generated with a 5 Å grid, *AtoB G2* AtoB models generated with a 2 Å grid, *SMI* hydrodynamic computations with the supermatrix inversion procedure, *Zeno* hydrodynamic computations using the Zeno method, *HP auto* HYDROPRO shell models generation and hydrodynamic computations via the SMI method, with the automatic determination of the number of beads in each shell model with a maximum of 2000 beads, *BEST man* BEST models and hydrodynamic computations, with the manual setting for the determination of minimum and maximum number of plates, *BEST heur* BEST models and hydrodynamic computations, with the heuristic approach for the determination of minimum and maximum number of plates

[a] For the species of origin of the protein considered, see the PDB headers and the literature cited (Ref.). *Mon* monomer, *dim* dimer

[b] The values in parentheses were calculated by US-SOMO, the other are experimental, taken from the literature

[c] The values marked with "*" were not considered when taking the reported mean values

[d] See the correspondence between the numbers listed and the references at the end of these table footnotes

[e] See references cited within this paper

[f] Carbohydrate not present in the PDB structure, manually modelled

[1] Stellwagen (1968); [2]Rai et al. (2005); [3]Brookes et al. (2010b); [4]Rackis et al. (1962); [5]Cunningham (1954); [6]Ghirlando (2011); [7]Armstrong et al. (1966); [8]Coleman (1965); [9]Nyman (1961); [10]Rickli et al. (1964); [11]Edelhoch (1957); [12]Charlwood (1952); [13]Wood et al. (1971); [14]Schwert (1949); [15]McVittie et al. (1977); [16]Wong et al. (1970); [17]Sund and Weber (1963)

Table 3 Characteristics and performances of the main hydrodynamic modelling/computational methods discussed in this work

Program (conditions)	Structure check?	NMR?[a]	Modelling method	Computational method	$D^0_{t\,(20,w)}$ average Δ %[b]	$s^0_{(20,w)}$ average Δ %[c]	Computing time (minutes) for selected structures[d]		
							1AKI (14 kDa)	1AO6 (66 kDa)	1ADO (160 kDa)
SoMo (with overlaps) in US-SOMO	Yes[e]	Yes	BM, residue to bead	Zeno	-0.2 ± 2.4	-0.6 ± 3.7	0.5	7.8	20.3
AtoB (5 Å grid) in US-SOMO	Yes[e]	Yes	BM, grid	SMI	$+0.3 \pm 2.4$	$+1.4 \pm 3.5$	0.03	1	9
SoMo (no overlaps) in US-SOMO	Yes[e]	Yes	BM, residue to bead	SMI	$+1.9 \pm 2.5$	$+2.9 \pm 3.5$	0.02	0.2	0.5
BEST (manual) in US-SOMO	Yes[f]	No	BE (2000–6000 plates)	SI	-2.7 ± 2.1	-1.9 ± 3.8	356	100	93
BEST (heuristic) in US-SOMO	Yes[f]	No	BE (variable # of plates)	SI	-2.8 ± 2.2	-1.9 ± 3.7	170	261	1072
HYDROPRO (WinHydropro)	No	No	Shell BM ($\leq$2000 beads)	SMI	-3.6 ± 3.0	-2.4 ± 3.2	0.3	0.3	0.3

BM bead modelling, *BE* boundary elements, *SMI* supermatrix inversion, *SI* surface integrals

[a] Automatic computation and averaging of hydrodynamic parameters possible for multiple structures in NMR-type files

[b] For all test proteins listed in Table 1, outliers excluded ($\pm$SD)

[c] For all test proteins listed in Table 2, outliers excluded ($\pm$SD)

[d] For the Zeno and SMI methods within US-SOMO (Windows version) and HYDROPRO (WinHydropro), computations were run on an Intel Core i5-3470 3.2 GHz PC with 6 GB RAM, operating under the Windows 7 Professional OS; for BEST within US-SOMO, they were run on the TACC Stampede cluster, and do not include waiting times in the queue (see "Materials and methods")

[e] Approximate methods available for non-coded or incomplete residues

[f] Checks performed but no influence on program execution