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Erratum

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Serial Generalized Ensemble Simulations of Biomolecules with Self-Consistent Determination of Weights

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In the proofreading process of the cited paper,[1] we missed an error in the column headers of Table 2 (arrow directions); this table should read as follows:

Table 2. Acceptance Probabilities of Replica Transitions (in Percentage) Calculated in the Whole Simulation Time (12 ns per Replica) for the SGE-1, SGE-8, and RE Simulations[a]

	SGE-1		SGE-8		RE
ensembles	→	←	→	←	⇌
λ_1, λ_2	43.1	40.9	41.3	42.2	24.8
λ_2, λ_3	38.8	38.8	37.7	38.1	22.2
λ_3, λ_4	41.4	41.3	42.3	42.8	25.5
λ_4, λ_5	40.3	38.3	38.7	38.7	22.8
λ_5, λ_6	49.9	47.9	49.5	49.0	33.8
λ_6, λ_7	40.9	38.9	38.7	39.0	23.1
λ_7, λ_8	42.8	41.8	42.6	42.9	27.0

[a]The column "ensembles" reports the ensembles involved in replica transitions, while the arrows indicate the direction of the transitions (the right arrow denotes transitions from λ_n to λ_{n+1}, while the left arrow denotes transitions from λ_{n+1} to λ_n).

Also in proofreading, we missed an error in the Acknowledgments; moreover, there is an additional source of support that was not included. That section should read as reported below.

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REFERENCES

(1) Chelli, R.; Signorini, G. F. Serial Generalized Ensemble Simulations of Biomolecules with Self-Consistent Determination of Weights. *J. Chem. Theory Comput.* **2012**, *8*, 830−842.

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