

CORRECTION

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# Correction to: Optimized SQE atomic charges for peptides accessible via a web application

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## Correction to: *J Cheminform* (2021) 13:45

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It was highlighted that in the original article [1] the heading of Table 2 was misaligned. This Correction article shows the correct Table 2. The original article has been updated.

**Table 2** Comparison of GDMIN and optGM parameterization of SQE with HBO atomic types

DTP_small	R <sup>2</sup>	RMSD	RMSD <sub>at</sub>	Param. time [h:m:s]
GDMIN	0.9941	0.0256	0.0599	19:47:22
optGM	0.9945	0.0249	0.0399	0:40:07
CCD_gen	R <sup>2</sup>	RMSD	RMSD <sub>at</sub>	Param. time [h:m:s]
GDMIN	0.9934	0.0334	0.0884	40:03:11
optGM	0.9950	0.0292	0.0406	10:27:05
PUB_pept	R <sup>2</sup>	RMSD	RMSD <sub>at</sub>	Param. time [h:m:s]
GDMIN	0.9875	0.0519	0.0756	18:37:16
optGM	0.9875	0.0518	0.0746	0:04:58

The original article can be found online at <https://doi.org/10.1186/s13321-021-00528-w>.

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1. Schindler O, Raček T, Maršavelski A, Koča J, Berka K, Svobodová R. Optimized SQE atomic charges for peptides accessible via a web application. *J Cheminform* (2021) 13:45. <https://doi.org/10.1186/s13321-021-00528-w>

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