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Correction: Fragment density functional theory calculation of NMR chemical shifts for proteins with implicit solvation

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Correction for 'Fragment density functional theory calculation of NMR chemical shifts for proteins with implicit solvation' by Tong Zhu *et al.*, *Phys. Chem. Chem. Phys.*, 2012, **14**, 7837–7845.

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The last column in Table 2 of the above paper contains typographical errors. The correct correlation functions are given in the following table.

Table 2 Comparison of AF-QM/MM and experimental chemical shifts for the ¹H, ¹³C_α, ¹³C, and ¹⁵N atoms in GB3. (G.: gas phase; S.: in solution. The exchangeable protons were excluded. The chemical shifts of carbonyl carbons are calculated using the B3LYP functional with the mixed (6-311++G**/4-31G*) basis set, while all the other chemical shifts for atoms (excluding the carbonyl carbons) are computed at the B3LYP/6-31G** level.)

		RMSE	MUE	R ²	Correlation function
¹ H	G.	0.86	0.39	0.8558	0.959x – 0.074
	S.	0.56	0.29	0.9687	1.054x – 0.253
¹³ C _α	G.	2.89	2.61	0.7363	0.905x + 4.094
	S.	2.41	2.12	0.7899	0.936x + 2.382
¹³ C	G.	3.35	2.39	0.9970	1.007x – 0.655
	S.	3.33	2.22	0.9978	1.029x – 1.792
¹⁵ N	G.	7.58	5.75	0.5274	1.219x – 23.61
	S.	6.01	4.75	0.7122	1.053x – 12.71

This does not affect the other results presented in the paper.

We are grateful to Professor Jan Jensen for bringing this issue to our attention.

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

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