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CORRECTION

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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.

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 ^{1}H, $^{13}C_{\alpha}$, ^{13}C, and ^{15}N 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	$1.054x - 0.253$
$^{13}C_{\alpha}$	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.

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

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