Calculations of one-, two- and three-bond nuclear spin-spin couplings in a model peptide and correlations with experimental data

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In Table 2 on page 527, the coefficient for ${}^3J_{H^NH\alpha}$ multiplying sin (ϕ) should be -1.0475 instead of 1.0475. The correct coefficient was used in all computations and figures reported in the paper. The authors thank Harald Schwalbe for bringing this error to their attention.

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¹H, ¹³C and ¹⁵N random coil NMR chemical shifts of the common amino acids.

I. Investigations of nearest-neighbor effects

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In Tables 3 and 6 (on pages 76 and 78, respectively), the values given for the 15 N chemical shift of lysine ϵ NH₃ should be 32.7 ppm instead of 125.9 ppm.

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