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addenda and errata

AMPLE: a cluster-and-truncate approach to solve the crystal structures of small proteins using rapidly computed *ab initio* models. Corrigendum

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The article by Bibby *et al.* [(2012), *Acta Cryst.* D**68**, 1622–1631] is corrected.

In the article by Bibby *et al.* (2012), owing to an oversight, the results given in the text and the figures refer to different runs of *AMPLE* for some test cases. Although the results are very similar, the following corrections to the text are necessary for consistency with the figures. The authors sincerely apologise for any confusion.

On p. 1625, in §2.3 the last sentence of the first paragraph should read as follows: 'Default parameters were used for these methods; the inputs comprise the number of molecules in the asymmetric unit predicted by *MrBUMP*, the resulting estimated molecular weight of the asymmetric unit and estimated error values of 0.1 Å (*Phaser*) or SIM = 1 (*MOLREP*)'.

On p. 1626, in §3.1 the fourth, fifth and sixth sentences of paragraph 2 should read 'In 43% of cases the top cluster contained a model better than the 99th percentile, *i.e.* one of the best ten models in the population. The equivalent figures for the second and third largest clusters were 32 and 26%, respectively. More importantly, in 98% of cases the top cluster contained a model better than the 70th percentile'.

On p. 1627, in §3.2 from the fourth sentence of paragraph 3 onwards should read 'Indeed, search models derived from the largest *SPICKER* cluster were able to solve 116 cases. Search models from the second largest cluster solved 102 cases, but only 12 of these were uniquely solved by this cluster, giving a total of 128 solved cases. For 114 cases the third largest cluster was also sampled. Although there were 28 successful cases, all were also solved using search models from clusters 1 or 2; thus, sampling beyond the two largest clusters is unnecessary'. The first sentence of paragraph 4 should read as follows 'Using the *SHELXE* CC score as an indicator, we achieved 128 successes from the 295 cases (43%)'.

On p. 1627, in §3.3 the sixth sentence of paragraph 2 should read 'A high proportion of all-α cases (81%) were successful, but only two all-β proteins (5%) were successfully solved'.

On p. 1628, in §3.4 the second sentence of paragraph 1 should read 'However, a sizeable proportion came from clusters of less accurately modelled decoys; the best decoy in the parent cluster had a GDT total score of <40 in 42% of cases (Supplementary Fig. S10)'.

On p. 1629, in §3.4 the second sentence of paragraph 5 should read 'The success rate of ensembles derived from each class of subcluster is similar: 29% for 1 Å subcluster ensembles, 36% for 2 Å subcluster ensembles and 35% for 3 Å subcluster ensembles'. Sentences 4, 5 and 6 of paragraph 6 should read 'For subclusters with a 1 Å radius that gave rise to successful search models, only 55% had the maximum of 30 models. Furthermore, successes were achieved with search models deriving from 1 Å radius subclusters containing from two to 30 decoys. In contrast, for successful subclusters with a 2 Å radius 79% have 30 decoys; for those with a radius of 3 Å this rises to 91%'. The last sentence of paragraph 7 should read '35% of these were successful, while the figures for polyalanine and all-side-chain search models were 31 and 34%, respectively'. The third sentence of paragraph 8 should read 'On the other hand, 14 of the 128 successful cases were solved by only one search model'.

On p. 1630, in §4 the fifth sentence should read 'All-α proteins are particularly favourable (81% success) and mixed α/β targets were solved in 37% of cases'.

References

Bibby, J., Keegan, R. M., Mayans, O., Winn, M. D. & Rigden, D. J. (2012). *Acta Cryst.* D**68**, 1622–1631.

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