

Pushing the boundaries of molecular replacement with maximum likelihood. Erratum

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In the calculations testing maximum-likelihood molecular-replacement methods reported in the paper by Read [(2001). *Acta Cryst. D* **57**, 1373–1382] simulated data constructed to test isomorphous replacement methods in the presence of known errors were used inadvertently. The test calculations have been repeated using the measured data, and the results are given.

In the reported calculations testing maximum-likelihood molecular-replacement methods (Read, 2001) on the structure of *Streptomyces griseus* trypsin (SGT), I inadvertently used simulated data computed from the final refined structure of SGT (Read & James, 1986). The simulated data had been constructed to test isomorphous replacement methods in the presence of known errors. The test calculations have been repeated using the measured data, and the results are given in new Tables 1 and 2. The original conclusions are upheld, except that in a translation search with an orientation in error by 6.9°, the correct translation no longer has the highest likelihood score. However, when this translation search is repeated, increasing the assumed r.m.s. error of the molecular-replacement model from the

Table 1
Rotation function results for *S. griseus* trypsin.

Algorithm	Resolution range (Å)	Correct peak†	Orientation error‡ (°)
Crowther	10.0–2.8	5.32	6.9
Crowther	10.0–3.5	5.62	3.4
Likelihood	14.7–2.8	7.39	0.6

† Peak height expressed in terms of r.m.s. deviations from the mean. ‡ Compared with final orientation from molecular replacement after rigid-body refinement.

Table 2
Translation function results for *S. griseus* trypsin.

Orientation error (°)	Correct peak†	Highest noise peak†	Mean of search†	R.m.s. from mean†
6.9	–11.3	–5.3	–54.7	10.5
6.9‡	15.3	14.5	–5.1	4.3
3.4	77.3	30.7	–35.9	11.5
0.6	117.9	50.5	–27.0	11.6

† Scores are expressed in terms of log-likelihood gain. ‡ Results from run in which r.m.s. error of 2 Å was assumed instead of default of 1.4 Å, to compensate for effect of orientation error.

default value of 1.4 to 2.0 Å to compensate for the effect of orientation error, the correct translation again has the highest likelihood score. As before, the discrimination from incorrect translations is poor with the most inaccurate orientation.

References

- Read, R. J. (2001). *Acta Cryst. D* **57**, 1373–1382.
Read, R. J. & James, M. N. G. (1988). *J. Mol. Biol.* **200**, 523–551.