ERRATA

On Evaluating Molecular-Docking Methods for Pose Prediction and Enrichment Factors. [*J. Chem. Inf. Model*. *46*, 401−415 (2006)] by Timothy Lovell, Hongming Chen,* Paul D. Lyne, Fabrizio Giordanetto, and Jin Li. DECS Global Compound Sciences, Computational Chemistry, AstraZeneca R&D, Pepparedsleden 1, 43183 Mölndal, Sweden, Cancer Discovery, AstraZeneca R&D, 35 Gatehouse Drive, Waltham, Massachusetts 02451, and Lead Generation Computational Chemistry, AstraZeneca R&D, Pepparedsleden 1, 43183 Mölndal, Sweden.

Pages 401−415. In a previous article[1] we examined several docking programs for their ability to reproduce the binding modes of ligands in proteins. Recently Perola et al. published a paper[2] indicating their inability to repeat our results using ICM. They reported ICM docking accuracy for binding mode prediction significantly lower than ours (61% correct predictions versus our reported 91%). Following their observation we have now revisited previous calculations leading us to retract the ICM results published previously[1] and report here a set of corrected results.

We repeated the calculations following two different procedures. The first one is a fully automated process similar to the one reported by Perola et al.,[2,3] whereby a cleaned pdb file is taken as input, a grid box is automatically generated to include residues within 8 Å of the crystallographic ligand, and the probe is placed at the default position. The grid maps are then generated based on the grid box and probe location. The second procedure uses manually generated grid boxes and probe placements to get an optimal docking performance, mimicking a computational chemist's daily usage. Starting conformations of the ligands are created from SMILES using three different programs Corina, Omega, and the ICM conversion module. The converted 3D conformations are manually checked to make sure they have correct tautomeric forms, protonation states, ring conformations, etc.

Table 1. ICM Docking Results

test no.	ligand source	% correct[c]
1[a]	Corina 3D	54−57
2[a]	Omega 3D	52−55
3[a]	ICM 3D conversion	55−57
4[b]	Corina 3D	63−66
5[b]	Omega 3D	59−63
6[b]	ICM 3D conversion	63−67

[a] Fully automated procedure. [b] Manual procedure. [c] Percentage of docking solutions with rmsd to crystal conformations less than 2 Å.

For each protein structure, the ICM docking version 3.4.9c is run five times to check the consistency of the docking results. The final results for the 164 complexes previously analyzed[1,2] are listed in Table 1.

Our renewed investigation shows that in five ICM docking runs the percent of correct predictions for each single run is between 59 and 67%. Therefore we retract our previous results concerning ICM docking accuracy.[1] Having carried out the above reproducible study procedures, we can only conclude that the data reported previously were due to some errors in the manual preparation and processing of the enormous amount of data.

REFERENCES AND NOTES

(1) Chen, H.; Lyne, P. D.; Giordanetto, F.; Lovell, T.; Li, J. On Evaluating Molecular-Docking Methods for Pose Prediction and Enrichment Factors. *J. Chem. Inf. Model.* **2006**, *46*, 401−415.
(2) Perola, E.; Walters, W. P.; Charifson, P. Comments on the Article "On Evaluating Molecular-Docking Methods for Pose Prediction and Enrichment Factors". **2007**, *47*, 251−253.
(3) Perola, E.; Walters, W. P.; Charifson, P. S. A Detailed Comparison of Current Docking and Scoring Methods on Systems of Pharmaceutical Relevance. *Proteins* **2004**, *56*, 235−249.

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