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1. Dean, P. M. *Br. J. Pharmac.* **74**, 39–46 (1981).
2. Hol, W. G. J., Halie, L. M. & Sander, C. *Nature* **294**, 532–536 (1981).
3. Sheridan, R. P., Levy, R. M. & Salemme, F. R. *Proc. natn. Acad. Sci. U.S.A.* **79**, 4545–4549 (1982).
4. Perutz, M. F. *Science* **201**, 1187–1191 (1978).
5. Hayes, D. M. & Kollman, P. A. *J. Am. chem. Soc.* **98**, 7811–7816 (1976).
6. Sheridan, R. P. & Allen, L. C. *J. Am. chem. Soc.* **103**, 1544–1550 (1981).
7. Warshel, A. & Levitt, M. *J. molec. Biol.* **103**, 227–249 (1976).
8. Blaney, J. M. *et al. J. Am. chem. Soc.* **104**, 6424–6434 (1982).

9. Weiner, P. K., Langridge, R., Blaney, J. M., Schaefer, R. & Kollman, P. A. *Proc. natn. Acad. Sci. U.S.A.* **79**, 3754–3758 (1982).
10. Pullman, B., Lavery, R. & Pullman, A. *Eur. J. Biochem.* **124**, 229–238 (1982).
11. Friend, S. H., March, K. L., Hanania, G. I. H. & Gurd, F. R. N. *Biochemistry* **19**, 3039–3047 (1980).
12. Salin, M. L. & Wilson, W. W. *Molec. cell. Biochem.* **36**, 157–161 (1981).
13. Cudd, A. & Fridovich, I. *J. biol. Chem.* **257**, 11443–11447 (1982).
14. Koppenol, W. H. in *Oxygen and Oxy-Radicals in Chemistry and Biology* (eds Powers, E. L. & Rodgers, M. A. J.) 671–676 (Academic, New York, 1981).
15. Malinowski, D. P. & Fridovich, I. *Biochemistry* **18**, 5905–5917 (1979).
16. Tainer, J. A., Getzoff, E. D., Richardson, J. S. & Richardson, D. C. *Nature* (this issue).
17. Klug, D., Rabani, J. & Fridovich, I. *J. biol. Chem.* **247**, 4839–4842 (1972).
18. Margerum, D. W., Cayley, G. R., Weatherburn, D. C. & Pagenkopf, G. K. in *Coordination Chemistry Vol. 2* (ed. Martell, A. E.) 1–220 (American Chemical Society, Washington DC, 1978).
19. Hopfinger, A. J. in *Conformational Properties of Macromolecules* (eds Horecker, B., Kaplan, N. O., Marmur, J. & Scheraga, H. A.) 39 (Academic, New York, 1973).
20. Gelin, B. R. & Karplus, M. *Biochemistry* **18**, 1256–1268 (1979).
21. Dearing, A., Weiner, P. & Kollman, P. A. *Nucleic Acids Res.* **9**, 1483–1497 (1981).
22. Connolly, M. L. *Science* **221**, 709–713 (1983).
23. Weiner, P. K. & Kollman, P. A. *J. comp. Chem.* **2**, 287–303 (1981).
24. Adams, D. J. *Chem. phys. Lett.* **62**, 329–333 (1979).
25. O'Donnell, T. J. & Olson, A. J. *Computer Graphics* **15**, 133–142 (1981).

Expression of *Klebsiella* nitrogen fixation genes in *Azotobacter*—a caution

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IN 1976 we reported in this journal¹ the correction of structural *nif* mutations of *Azotobacter vinelandii* (strains UW1, 10, 100 and 38) by a plasmid RP41 (now called pRD1) which carries the *nif* cluster of *Klebsiella pneumoniae*.

We are now obliged to report that we cannot repeat this effect. The original *Nif*⁺ transconjugant *Azotobacter* strains were lost and in several attempts to obtain new ones we have used both pRD1 and a derivative, pMF250, which is sometimes more stable in intergeneric transfers. Transconjugants have readily been obtained which retain *nif* according to transfer of the plasmid back to *Escherichia coli* but none shows a *Nif*⁺

phenotype either in growth or acetylene reduction tests, performed in a variety of test conditions.

We have re-examined our paper and our experimental records and are at a loss to explain this discrepancy. Our original controls, which included reversion to the *Nif*⁺ phenotype on eliminating the plasmid and also immunospecific recognition of the peptides of the *Klebsiella* molybdoprotein in the corrected *azotobacters*, seem to eliminate trivial explanations, such as reversion of the *nif* mutants or inadequate separation of donor and recipient organisms. A substantial number of successful transconjugations were performed and human error is therefore unlikely. We are compelled to conclude either that some systematic error, which still eludes us, occurred in our early experiments or that a special nutritional or other condition, favouring *nif* expression, existed fortuitously which we have not been able to reproduce.

We must therefore inform your readers that our evidence for correction of structural *nif* mutations in *A. vinelandii* by *Klebsiella nif* is subject to reasonable doubt. We much regret that our publication will have misled others as much as ourselves. The recent evidence for function of *Klebsiella nifA* in *A. vinelandii*² is, of course, unaffected by these considerations and remains valid.

1. Cannon, F. & Postgate, J. *Nature* **260**, 271–272 (1976).
2. Kennedy, C. & Robson, R. L. *Nature* **301**, 626–628 (1983).