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Keywords: Electronic structure calculation, Ligand docking, Protein modeling

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[1] Alon, U. *An Introduction to Systems Biology: Design Principles of Biological Circuits*, CRC Press, 2006.

[2] Altschul, S. F.; Gish, W.; Miller, W.; Myers, E. W.; Lipman, D. J. Basic local alignment search tool, *Journal of Molecular Biology*, **1990**, *215*, 403–410.

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[4] Smith, T. F.; Waterman, M.S. Identification of common molecular subsequences, *Journal of Molecular Biology*, **1981**, *147*, 195–197.

[5] Venter, J. C.; *et al.*, The sequence of the human genome, *Science*, **2001**, *291*, 1304–1351.

[6] <https://cbi-society.org/taikai/taikai21/index.html>