

CORRECTION

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Correction: AI molecular catalysis: where are we now?Zhenzhi Tan,^a Qi Yang^{*a,b} and Sanzhong Luo^{*a}DOI: 10.1039/d5qo90021b
rsc.li/frontiers-organicCorrection for 'AI molecular catalysis: where are we now?' by Zhenzhi Tan et al., *Org. Chem. Front.*, 2025, <https://doi.org/10.1039/d4qo02363c>.

The authors regret that references 10, 11, 18, 27, 31, 35, 36 and 107 were incorrect in the original article. The corrected references are shown below as ref. 1–8.

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

References

- 1 H. Mayr, CC Bond Formation by Addition of Carbenium Ions to Alkenes: Kinetics and Mechanism, *Angew. Chem., Int. Ed. Engl.*, 1990, **29**, 1371–1384.
- 2 H. Mayr and M. Patz, Scales of Nucleophilicity and Electrophilicity: A System for Ordering Polar Organic and Organometallic Reactions, *Angew. Chem., Int. Ed. Engl.*, 1994, **33**, 938–957.
- 3 S. Q. Zhang, L. C. Xu, S. W. Li, J. C. A. Oliveira, X. Li, L. Ackermann and X. Hong, Bridging Chemical Knowledge and Machine Learning for Performance Prediction of Organic Synthesis, *Chem. – Eur. J.*, 2023, **29**, e202202834.
- 4 S.-W. Seo, Y. Y. Song, J. Y. Yang, S. Bae, H. Lee, J. Shin, S. J. Hwang and E. Yang, GTA: Graph Truncated Attention for Retrosynthesis, Proceedings of the AAAI Conference on Artificial Intelligence, 2021, vol. 35, pp. 531–539.
- 5 E. J. Corey, W. T. Wipke, R. D. Cramer and W. J. Howe, Computer-assisted synthetic analysis. Facile man-machine communication of chemical structure by interactive computer graphics, *J. Am. Chem. Soc.*, 1972, **94**, 421–430.
- 6 J. B. Hendrickson and A. G. Toczko, SYNGEN program for synthesis design: basic computing techniques, *J. Chem. Inf. Comput. Sci.*, 1989, **29**, 137–145.
- 7 I. Ugi, J. Bauer, K. Bley, A. Dengler, A. Dietz, E. Fontain, B. Gruber, R. Herges, M. Knauer, K. Reitsam and N. Stein, Computer-Assisted Solution of Chemical Problems—The Historical Development and the Present State of the Art of a New Discipline of Chemistry, *Angew. Chem., Int. Ed. Engl.*, 1993, **32**, 201–227.
- 8 G. P. Hicks, A. A. Eggert and E. C. Toren, Application of an on-line computer to the automation of analytical experiments, *Anal. Chem.*, 1970, **42**, 729–737.

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