Big data, machine learning and artificial intelligence are becoming increasingly more central in the chemical sciences. It is important to consider how data drives new discoveries in chemistry at present and how data-driven discovery may develop in the future.

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- Discovering chemical structure
- Discovering structure–property correlations
- Discovering trends in big data
- Discovering synthesis targets

Front cover image: Large property models convert design constraints (depicted by letters - left) directly into molecules (emerging from the model - right). © Image reproduced with permission of Brett Savoie from B. Savoie *et al.*, *Faraday Discuss.*, 2025, **256**, DOI: 10.1039/D4FD00113C.

Faraday Discussions

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