**Showcasing research from Bayer Pharmaceuticals in collaboration with the Proppe Group (TU Braunschweig, Germany). Artwork by Kerrin Janssen.**

"When machine learning models learn chemistry I: quantifying explainability with matched molecular pairs" and "When machine learning models learn chemistry II: applying WISP to real-world examples"

Explainability is increasingly used in machine-learning-driven chemistry, yet its reliability remains difficult to assess. WISP, a model-agnostic Python workflow based on matched molecular pairs, enables quantitative evaluation of explainability methods across regression and classification tasks. Applied to diverse datasets WISP reveals when explanations truly reflect chemical principles and when models rely on spurious correlations, making explainability performance a diagnostic for model quality.

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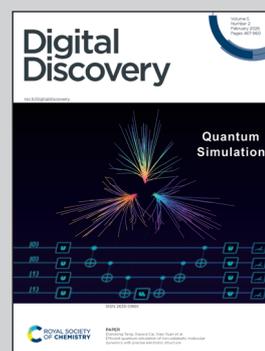
See Kerrin Janssen, Jonny Proppe, Andreas H. Göller *et al.*, *Digital Discovery*, 2026, **5**, 571–591.

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