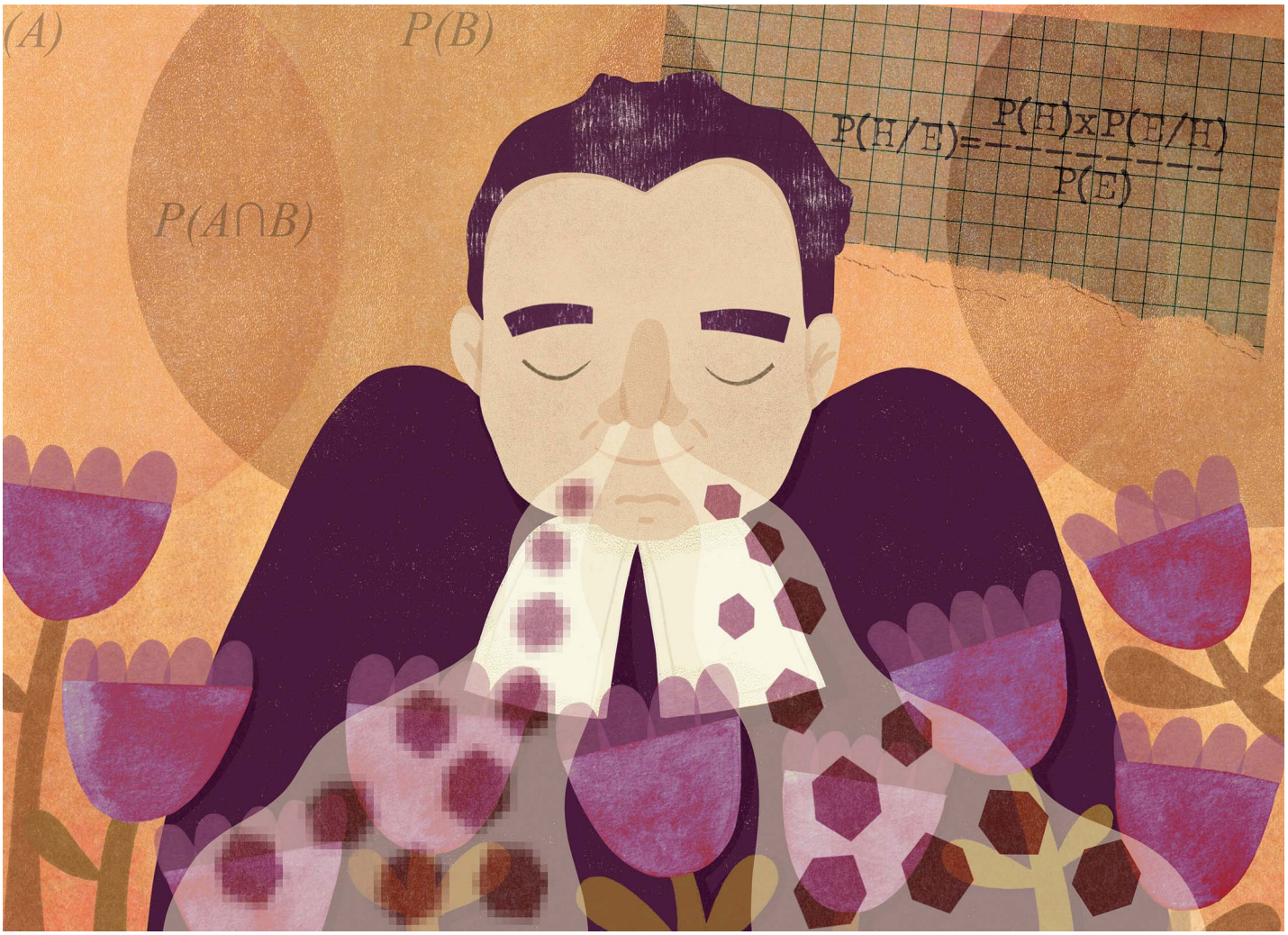

Showcasing research collaboration from Dr Emma Gibson and Dr Laia Vilà-Nadal's groups, School of Chemistry, University of Glasgow, Scotland, United Kingdom.

DFT meets Bayesian inference: creating a framework for the assignment of calculated vibrational frequencies

Computational chemistry can take hours to generate an IR spectrum of a molecule, while experiments take only minutes, yet the two often fail to align. This persistent mismatch motivated our work. We combine Density Functional Theory (DFT) with Bayesian inference to bridge theory and experiment in a statistically rigorous way. For each calculated DFT frequency, probability modelling is performed and the likelihood of every possible experimental band assignment is evaluated. These likelihoods are then used to iteratively update assignment probabilities across all hypotheses. Our approach improves the consistency, transparency, and reliability of spectral interpretation. The resulting framework is robust and transferable, offering a general strategy for analysing complex vibrational data across organic and molecular chemistry.

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See Emma Gibson, Laia Vilà-Nadal *et al.*, *Digital Discovery*, 2026, **5**, 592.

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