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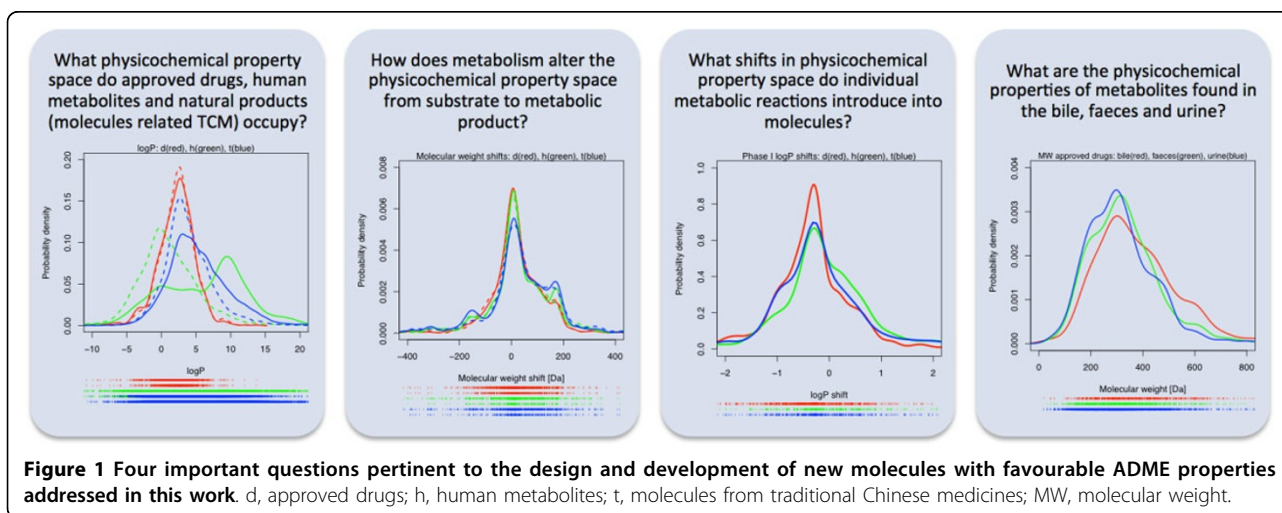
Quantifying the shifts in physicochemical property space introduced by the metabolism of small organic molecules

Johannes Kirchmair¹, Andrew Howlett¹, Julio Peironcely^{2,3,4}, Daniel S Murrell¹, Mark Williamson¹, Samuel E Adams¹, Thomas Hankemeier^{3,4}, Leo van Buren⁵, Guus Duchateau⁵, Werner Klaffke⁵, Robert C Glen^{1*}

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Understanding the metabolic fate of small organic molecules is of fundamental importance to the successful design and development of drugs, nutritional supplements, cosmetics and agrochemicals [1,2]. In the current study we investigated how the products of metabolism differ from their parent molecules by analysing a large dataset of experimentally determined metabolic transformations (Figure 1). This dataset was split into three specific chemical domains representing approved drug

molecules, human metabolites and molecules from traditional Chinese medicines to allow individual analysis. We also quantified the impact of individual Phase I and Phase II metabolic reactions on calculated chemical descriptors using MetaPrint2D [3] and suggest new approaches to utilise metabolism for the design of drugs and cosmetics. The last section of this study investigates the properties of metabolites found in the bile, faeces and urine and analyses their commonalities and differences.



* Correspondence: rcg28@cam.ac.uk

¹Unilever Centre for Molecular Sciences Informatics, Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge, CB2 1EW, UK
Full list of author information is available at the end of the article

Author details

¹Unilever Centre for Molecular Sciences Informatics, Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge, CB2 1EW, UK. ²TNO Research Group Quality & Safety, P.O. Box 360, 3700 AJ Zeist, The Netherlands. ³Leiden/Amsterdam Center for Drug Research, Leiden University, 2333 CC Leiden, The Netherlands. ⁴Netherlands Metabolomics Centre, 2333 CC Leiden, The Netherlands. ⁵Unilever R&D, 3133 AT Vlaardingen, The Netherlands.

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