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J.A Rothwell, M. Urpi-Sarda, M. Boto-Ordóñez, R. Llorach, D. Kumar, V. Neveu, Claudine Manach, C. Andres-Lacueva, A Scalbert

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Title: EXPLOITING THE PHENOL-EXPLORER 2.0 DATABASE TO ANALYZE AND CHARACTERIZE THE POLYPHENOL METABOLOME

Authors and addresses: J.A. Rothwell¹, M. Urpi-Sarda²³, M. Boto-Ordóñez²³, R. Llorach⁴⁵, D. Kumar¹, V. Neveu¹, C. Manach⁶, C. Andres-Lacueva⁴⁵ and A. Scalbert¹

¹International Agency for Research on Cancer (IARC), Nutrition and Metabolism Section, Biomarkers Group, 150 cours Albert Thomas, F-69372 Lyon Cedex 08, France

²Department of Internal Medicine, Hospital Clinic, Institut d'Investigació Biomèdica August Pi i Sunyer (IDIBAPS), University of Barcelona, Villarroel 170, 08036 Barcelona, Spain

³CIBER 08/08: Fisiopatología de la Obesidad y la Nutrición and RD06/0045/1003 Alimentación Saludable, Instituto de Salud Carlos III, Spain

⁴Nutrition and Food Science Department, Pharmacy Faculty, University of Barcelona, Av. Joan XXIII s/n, 08028 Barcelona, Spain

⁵Ingenio-CONSOLIDER program, FUN-C-FOOD, CSD5009-088, Barcelona, Spain

⁶INRA, UMR1019, Unité Nutrition Humaine, CRNH Auvergne, F-63000 Clermont-Ferrand, France

Presenting author: J.A. Rothwell

Abstract: Phenol-Explorer is an open-access web database on polyphenols, a major group of phytochemicals abundant in plant foods. Version 2.0 of the database was released in late 2011 and includes comprehensive qualitative and quantitative data on the 'polyphenol metabolome' (i.e. all metabolites derived from the over 500 polyphenols known in foods) in humans and experimental animals. Such databases are necessary for the screening of metabolomic profiles and the identification of potential biomarkers of food consumption. The aim of this study was to analyse these new data to characterize and visualize the polyphenol metabolome. The update was implemented by the compilation of data on 383 polyphenol metabolites from 221 original intervention studies. Research articles were first screened for suitability using pre-defined criteria and then entered into a relational database via Microsoft Access. The polyphenol metabolome was then analyzed via a series of database queries and open-source visualization software. Data were mainly obtained in human and rat models, and profiles of metabolites were similar between these species. The highest C_{max} values (maximum plasma concentration) were found in rats, as higher doses of pure polyphenols could be administered, although in both species, administration of pure polyphenols or polyphenol supplements led to much higher plasma concentrations than administration of foods. Conversely, T_{max} (time to reach C_{max}) was species-dependent and always shorter in the rat. Additionally, the ensemble of all studies administering pure compounds to humans and animals allowed an insight into precursor-metabolite specificity. 5-*O*-Caffeoylquinic acid, catechin and epicatechin gave rise to the broadest range of metabolites, while hippuric, ferulic, 4-hydroxybenzoic, dihydrocaffeic and vanillic acids were the metabolites derived from the largest number of precursors. Knowledge of polyphenol metabolism is crucial to understanding their *in vivo* bioactivities and the polyphenol metabolome is an important component of the information-rich food metabolome, which encompasses all metabolites derived from exposure to the diet. We gratefully acknowledge Danone Research, the French National Institute of Cancer and the University of Barcelona for financing the project.