Researchers make new discovery on the molecular structure of natural products

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Researchers from the Institute of Molecular Science (ICMol) of the University of Valencia have managed to synthesize a new porous material that makes it possible to encapsulate a series of active principles of natural substances and determine their chemical structure by using X-ray diffraction. This will allow for the future characterisation of natural products, hitherto unknown, and to reveal their chemical properties. The work has been published in *Nature Communications*.

Natural products—substances produced by living organisms in nature—are frequently used in important and daily fields such as food, medicine, or cosmetics. However, the structure and chemical nature of many of them remain undisclosed, limiting the growth of such applications. This lack of characterisation is due to the fact that the low degree of crystallinity of many natural products prevents the use of X-ray diffraction techniques to solve their structure.

The ICMol team led by the researcher Emilio Pardo has shown that natural products can be analyzed using crystallographic techniques, if it is done using the porous material called MOF (metal-organic framework), whose functionality, control of porosity and high crystallinity enable the encapsulation and arrangement of this type of substances inside its pores. This will help to reveal the structure of many natural products, discover new properties in them and improve their applicability.

The work published in *Nature Communications* focuses on the

encapsulation and structural resolution of a flavonoid present in citrus bergamot—from the Citrus bergamia tree—whose healing, anxiolytic, antipyretic and cholesterol-lowering effects, among others, are used in medicine, in addition to its use as an essence in perfumes. The obtained results have made it possible to confirm its structure and to determine, without ambiguity, its chirality, that is, its absolute configuration.

This work helps open the way to the study of the properties of many other natural products, as well as to establish in a more emphatic and well-founded way their benefits for health and nutrition.

More information: Marta Mon et al. Hydrolase–like catalysis and structural resolution of natural products by a metal–organic framework, *Nature Communications* (2020). DOI: 10.1038/s41467-020-16699-3

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