

Taste Active Components in Plants Identified by Data-Mining of Chinese Historical Manuscripts

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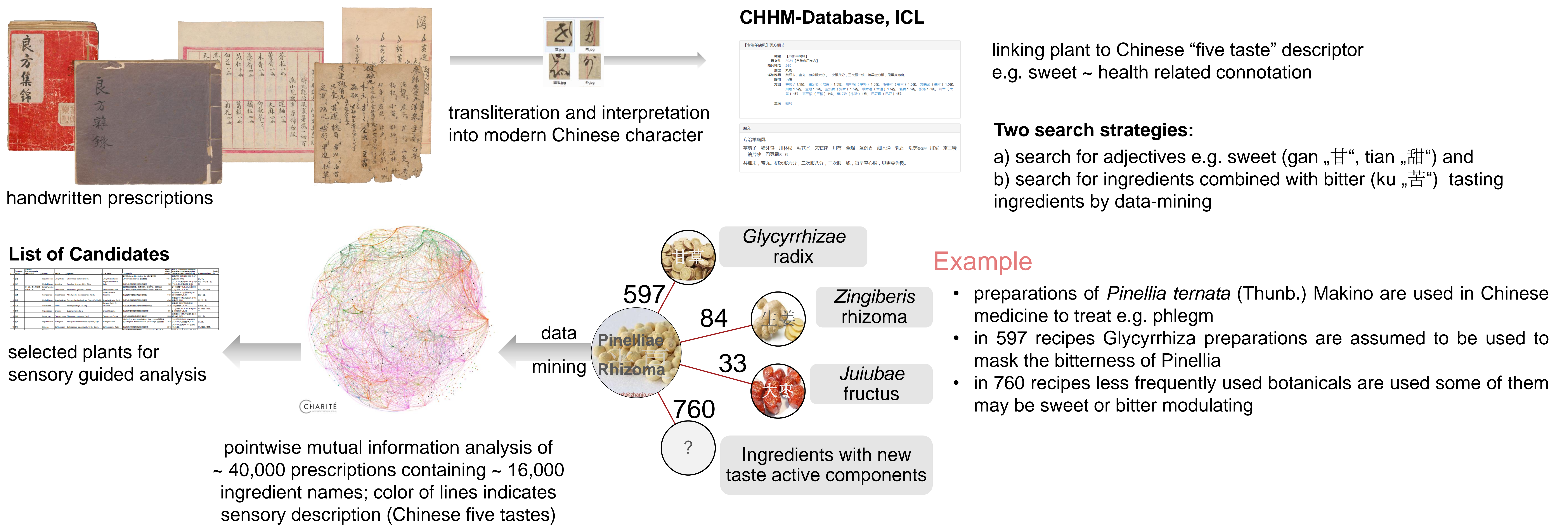
Background

- The development of ingredients to improve taste perception of low caloric food is important to meet the consumer demand for healthier products.
- Manuscripts on Chinese historical healthcare provide access to such ingredients and substances used in China's history.
- The SimLeap (abbreviation for "Sweet and Bitter Modulating Compounds: Leveraging Ancient Prescriptions") consortium combines knowledge in Chinese historical healthcare practice, data-mining, natural product chemistry and sensory guided analysis.

Approach

- The digitized Unschuld Collection¹ with over 40,000 historical recipes was used for data-mining to reveal frequent combinations of ingredients („Chinese Historical Healthcare Database“, CHHM).
- Botanical materials were identified, extracts and fractions had then undergone a decision tree-based safety assessment before tasting.
- Relevant materials were further fractionated by LC Taste® according to Reichelt et al.²

Workflow for determining botanicals with potential sweet and bitter modulating property by data-mining



Occurrence of botanicals and their TCM flavor

- Prior to data mining, recipes data were consolidated by exclusion of animal, mineral and metal materials. Botanical names were assigned and synonyms eliminated.
- Analysis of the frequency of plant based ingredients revealed that the most frequently prescribed botanicals in the manuscripts were Glycyrrhiza (Gan Cao, 8,709 times), Angelica sinensis (Dang Gui, 7,272 times), Ligusticum ssp. (Chuan Xiong, 4,056 times), Wolfiporia cocos (Fu Ling, 3,360 times), Rheum ssp. (Da Huang, 3,083 times), Saposhnikovia divaricata (Fang Feng, 3,016 times) and Rehmannia glutinosa (Sheng Di Huang, 2,890 times).
- Modern literature on Chinese medicinal plants uses flavor expressions, so called "Five Tastes" to characterize a potential impact on patient's body functions which differs from human sensory language and has developed over centuries. The tasting of decocts from 51 randomly selected botanicals showed that 'sweet' herbs did not have off-notes such as bitter or astringent taste in 80% percent of cases, but were lacking a sweet taste compared to a 5% sucrose solution. On the other side, 'bitter and acrid' herbs showed off-notes in 72% of the cases.
- Data-mining for deconvolution of said prescriptions is necessary to combine the taste-related "Five Tastes" descriptor and the co-occurrence of bitter-tasting active ingredients. Digitized prescriptions were studied using PMI (pointwise mutual information) and ARL (association-rule-learning) for quantitative assessment by employing with finally 3.100 ingredients in 27.000 of the recipes.

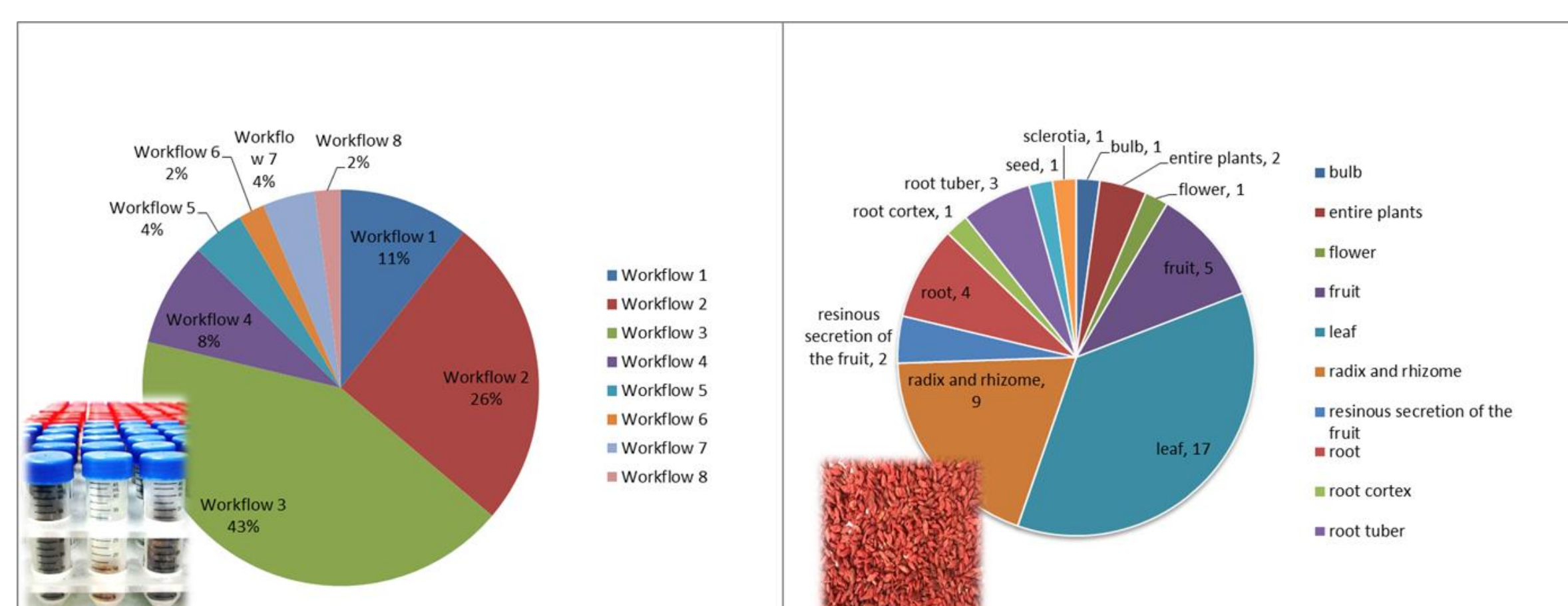


Figure 1:

Application of 8 different extraction workflows (left) of 10 different plant materials (right) reproducing the described historical preparation, best

LC Taste® fractionation of Ilex pubescens

- LC Taste® fractionation**
- Chromatographic fractionation using high temperature liquid chromatography on a polymer-based PRP-1 column
 - Semipreparative scale (250 mm × 10 mm; 10 µm particle size)
 - Elevated temperature (80 ° C isotherm) using food grade solvents

Herbal leaf tea, locally known as "Shan-lu-cha" which originates from species of the genus Ilex like *I. hainanensis*, *I. stewardii*, *I. pubescens*, *I. triflora* and *I. angulata* is reported to be edible.³ Leaves have been sourced, extracted with 95 vol% ethanol and fractionated.

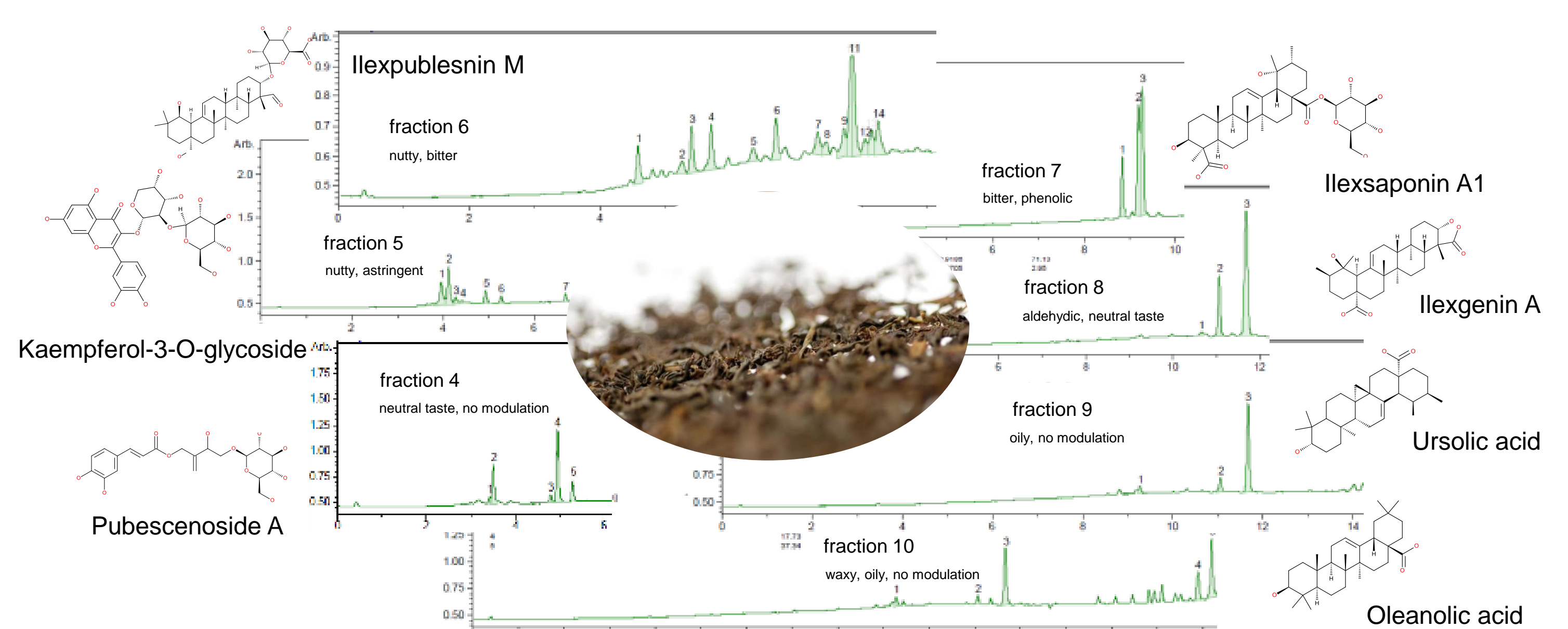


Figure 2: Tentative Identification of non volatiles components by liquid chromatography (Kinetex, 1.7 µm, 100 mm × 2.1 mm; Phenomenex) high resolution mass spectrometry (Bruker microTOFQII). Mass formula are compared with those reported in literature, for example, Chen et al., report the quantitation of ursolic, ilexgenin A, ilexsaponin A1 and ilexhainanoside D in ethanolic extracts of *Ilex hainanensis*, *Ilex stewardii* and *Ilex pubescens* leaves.³

Conclusions

- Digitization of Chinese historical prescriptions and data consolidation have finally resulted in a data matrix of 27,000 recipes x 3,100 ingredients.
- The sensory-guided analysis of taste-active molecules proved to be useful for identification sweet and bitter modulating compounds.

Literature

- Unschuld, P.U.; Zheng, J.: Chinese Traditional Healing: The Berlin Collections of Manuscript Volumes from the 16th through the Early 20th Century, Sir Henry Wellcome Asian Series. Leiden, Brill, **2014**.
- Reichelt, K.V. et al. Characterization of Flavor Modulating Effects in Complex Mixtures via High Temperature Liquid Chromatography, *Journal of Agricultural and Food Chemistry* **2010**, 58(1), 458-464.
- Chen et al., Quantitative analysis of triterpenoids in different parts of *Ilex hainanensis*, *Ilex stewardii* and *Ilex pubescens* using HPLC-ELSD and HPLC-MSn and antibacterial activity, *Food Chemistry* **2011**, 126, 1454-1459.