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Bioactivity-Based Molecular Networking for the comparison of *Calophyllum inophyllum* (tamanu) oil obtained via three ecofriendly extraction processes

Émilie Stienlin¹, Raimana Ho¹, Stéphane Greff², Elnur Garayev², Gaëtan Herbertte³, Sandrine Perino⁴, Farid Chemat⁵, Rémy Le Guével⁶ and Phila Raharivelomanana¹.

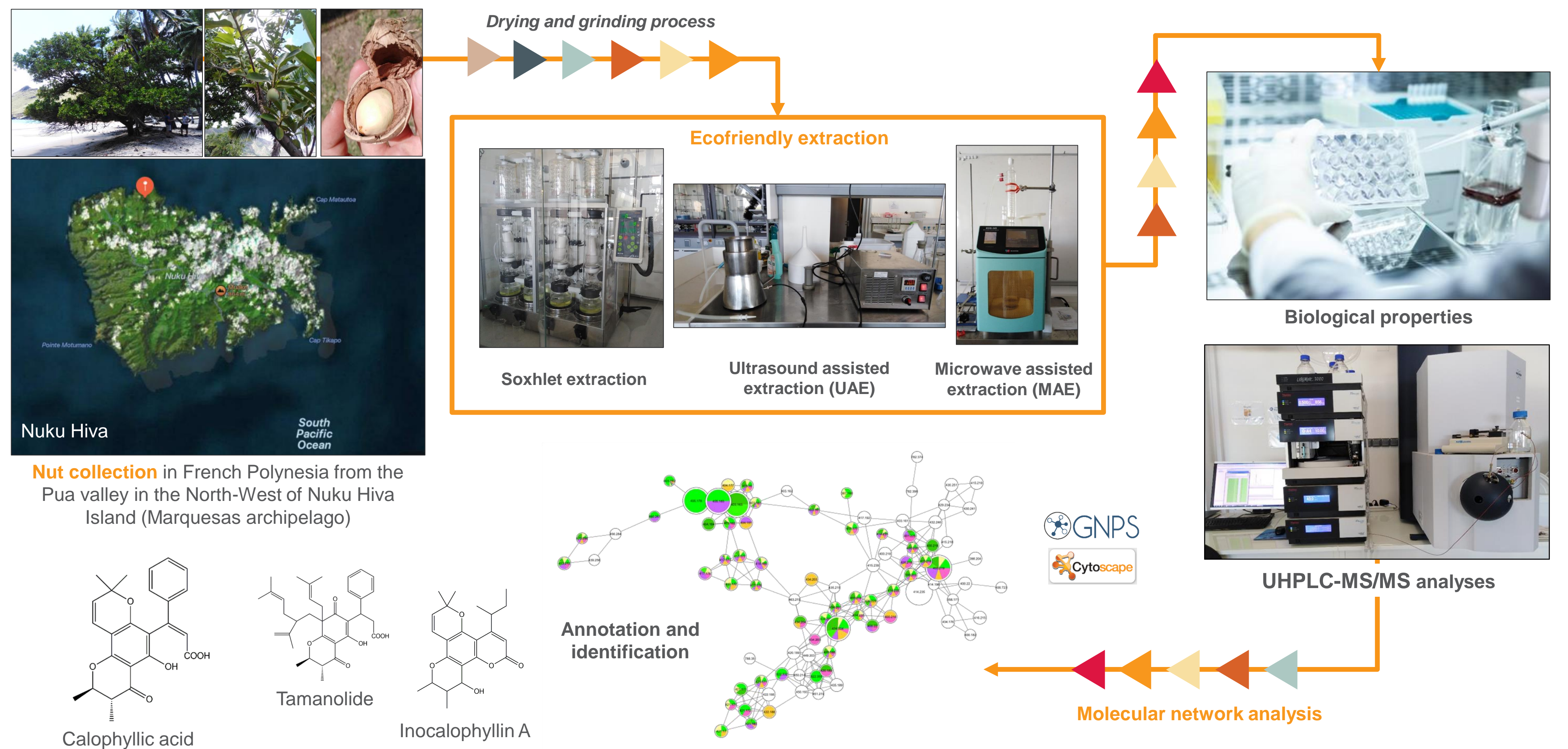
¹SECOPOL, UMR 241, UPF, BP 6570, 98702 Faa'a, French Polynesia, ²IMBE, UMR 7263 CNRS, AMU-AU, rue de la Batterie des Lions, 13007 Marseille, France, ³AMU, CNRS, Centrale Marseille, FSCM, Spectropole, 13013 Marseille, France, ⁴Avignon University, INRAE, UMR 408, GREEN Extraction Team, 84000 Avignon, France, ⁵ImPACcell-BIOSIT, Université de Rennes 1, Campus de Villejean, 35043 Rennes, France.

INTRODUCTION

Tamanu oil, obtained from the seeds of *Calophyllum inophyllum* L. (Calophyllaceae), was traditionally used to cure various skin problems and ailments in French Polynesia. Nuts and especially oil are also used for skin care. It was reported to treat different kinds of skin affections as well as conjunctivitis, and to heal of flat wounds. Aiming to produce high quality tamanu oil from an eco-friendly process, ecological extraction of this oil from nuts had been carried out using different methods such as Soxhlet extraction and microwave-assisted extractions as well Soxhlet extraction using agro-solvent. Bioactivity-Based Molecular Networking was performed in order to compare their eco-extracts chemical composition and cytotoxic properties. Ultrasound assisted extraction seems to be an innovative process to extract tamanu oil because of its richness in compounds (74 features) which can be at the origin responsible of the cytotoxic activity on several cancer cell lines (IC50 < 0.1%V/V): HuH7 (liver), CaCo-2 (colon), MDA-MB-231 (breast), MDA-MB-468 (breast), HCT116 (colon), PC3 (prostate), MCF-7 (breast).

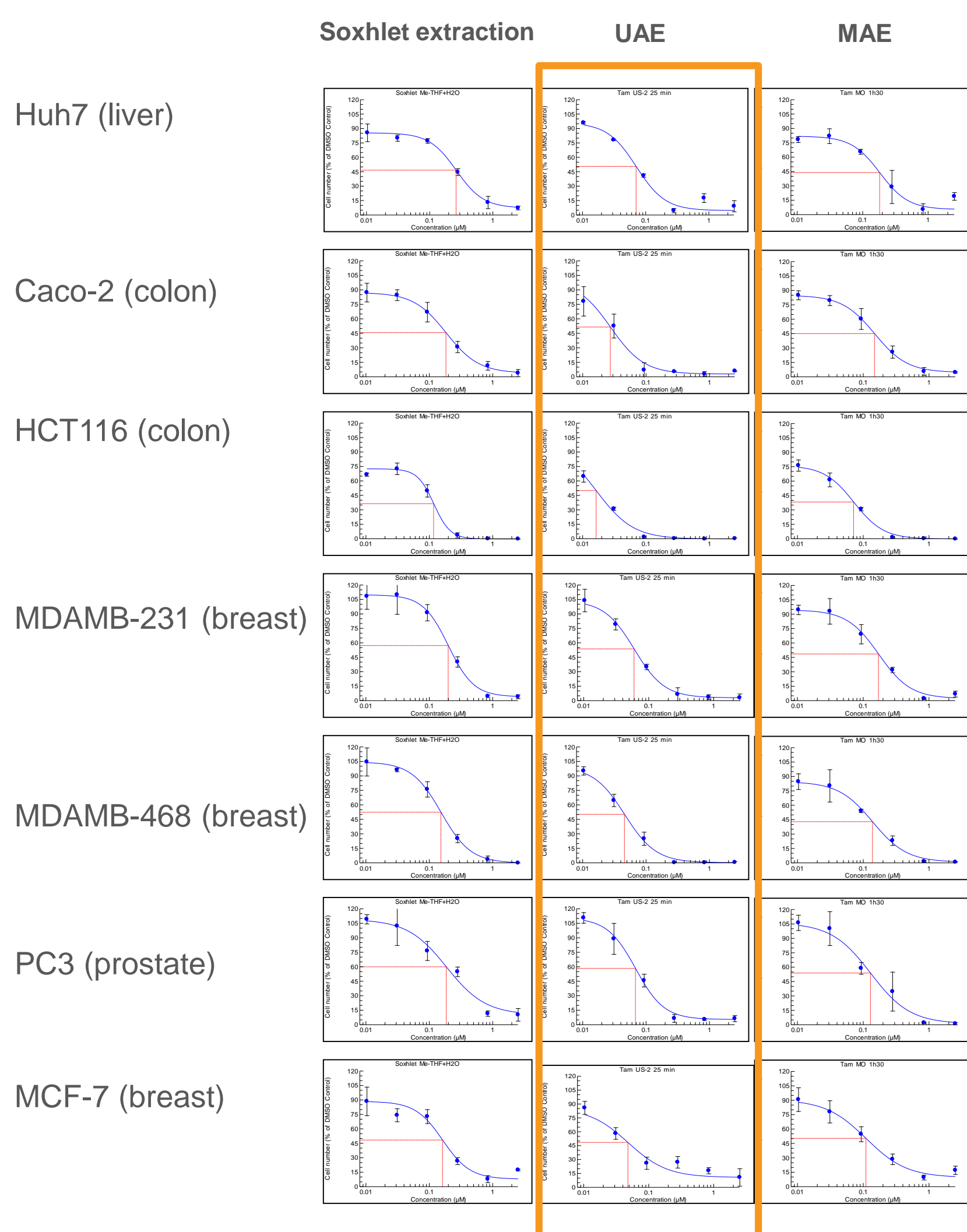
Objective: The aim is to produce high-quality tamanu oil through an eco-friendly extraction process.

MATERIALS AND METHODS



RESULTS

Cytotoxic activities of tamanu oil on HuH7, Caco-2, MDA-MB-231, HCT116, PC3, and MCF7 cancer cell lines

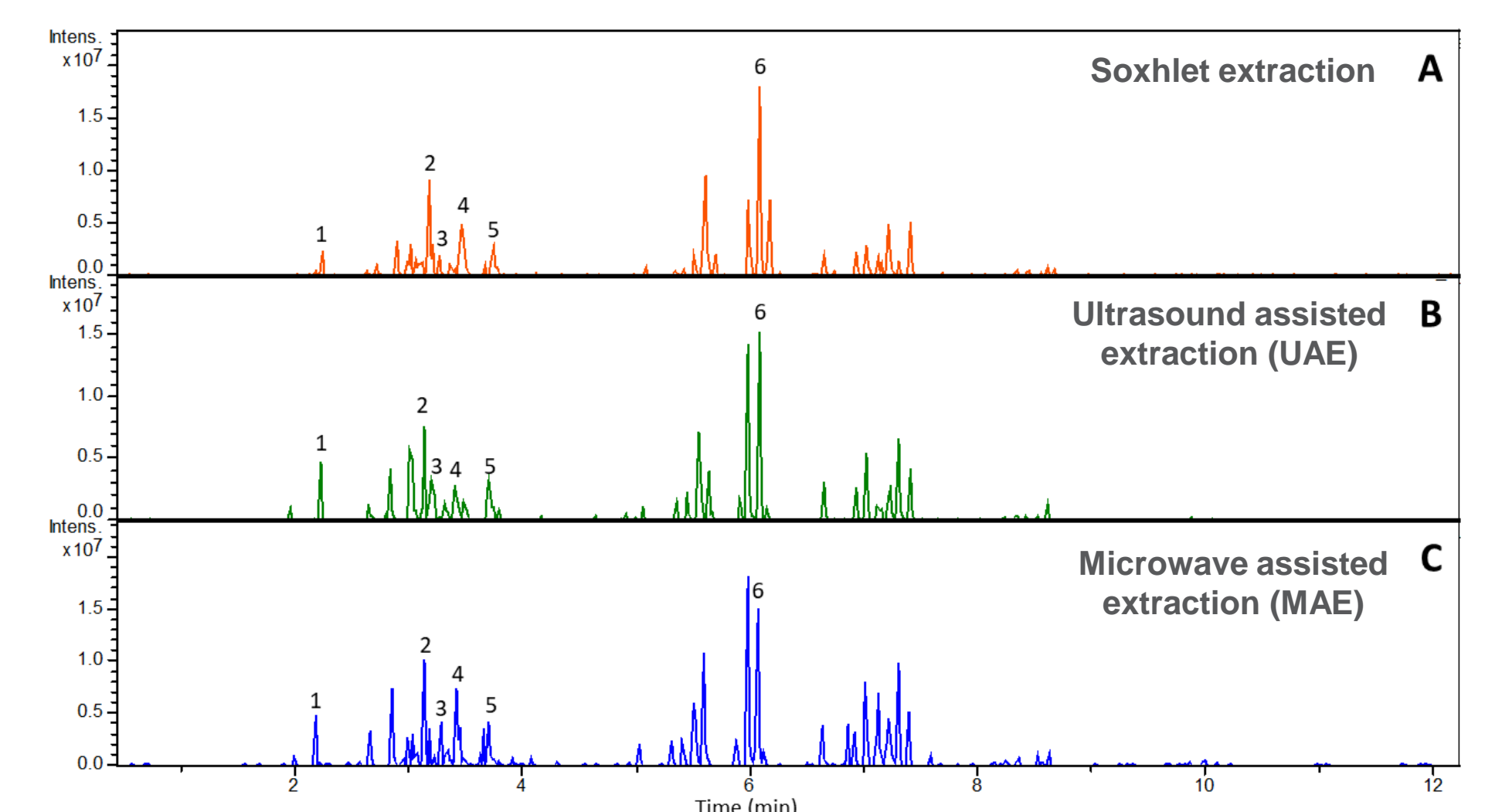


Cytotoxic studies of three eco-extracts of *Calophyllum inophyllum* oil obtained by Soxhlet extraction, UAE or MAE.

IC50 (% V/V)	HuH7	CaCo-2	MDA-MB-231	MDA-MB-468	HCT116	PC3	MCF7
DMSO	>25	>25	>25	>25	>25	>25	>25
ROSCOVITINE	79	58	91	69	98	70	84
DOXORUBICINE	0.03	51	0.03	42	0.01	65	0.030
TAXOL	0.008	48	0.014	64	0.017	61	0.005
Soxhlet	0.3	91	0.2	95	0.2	96	0.2
UAE	0.07	95	0.03	97	0.06	97	0.05
MAE	0.2	93	0.15	94	0.2	97	0.14

- All three eco-extracts showed cytotoxicity on all cancer cell lines studied.
- Only the extract obtained by UAE showed strong cytotoxicity (IC50 range 0.02 to 0.07%V/V) for all cancer cells → cytotoxicity on CaCo-2 (colon), HCT116 (colon) and MCF7 (breast) lines with IC50 less than 0.05 %V/V.

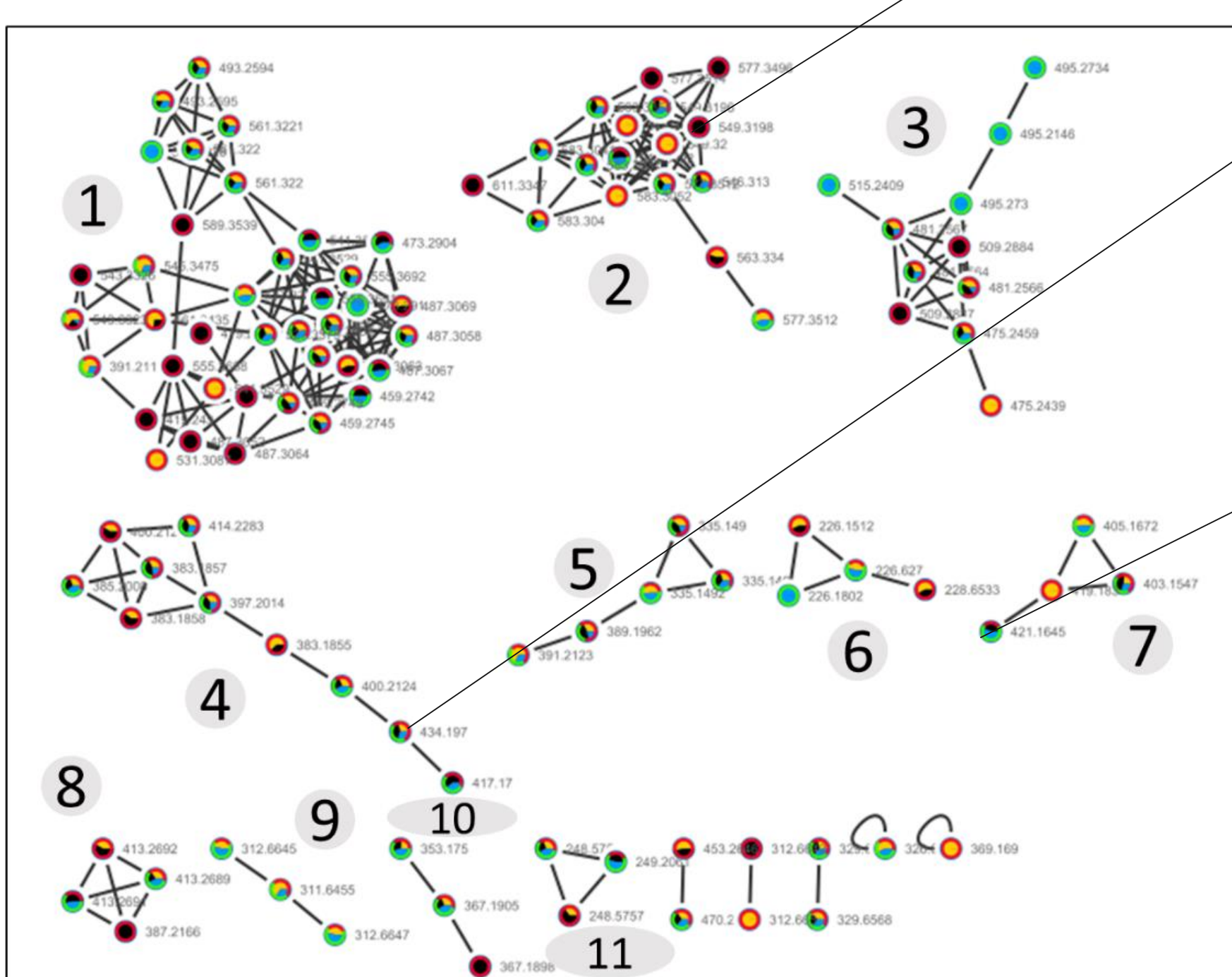
Chemical composition of tamanu oil according to eco-extraction methods



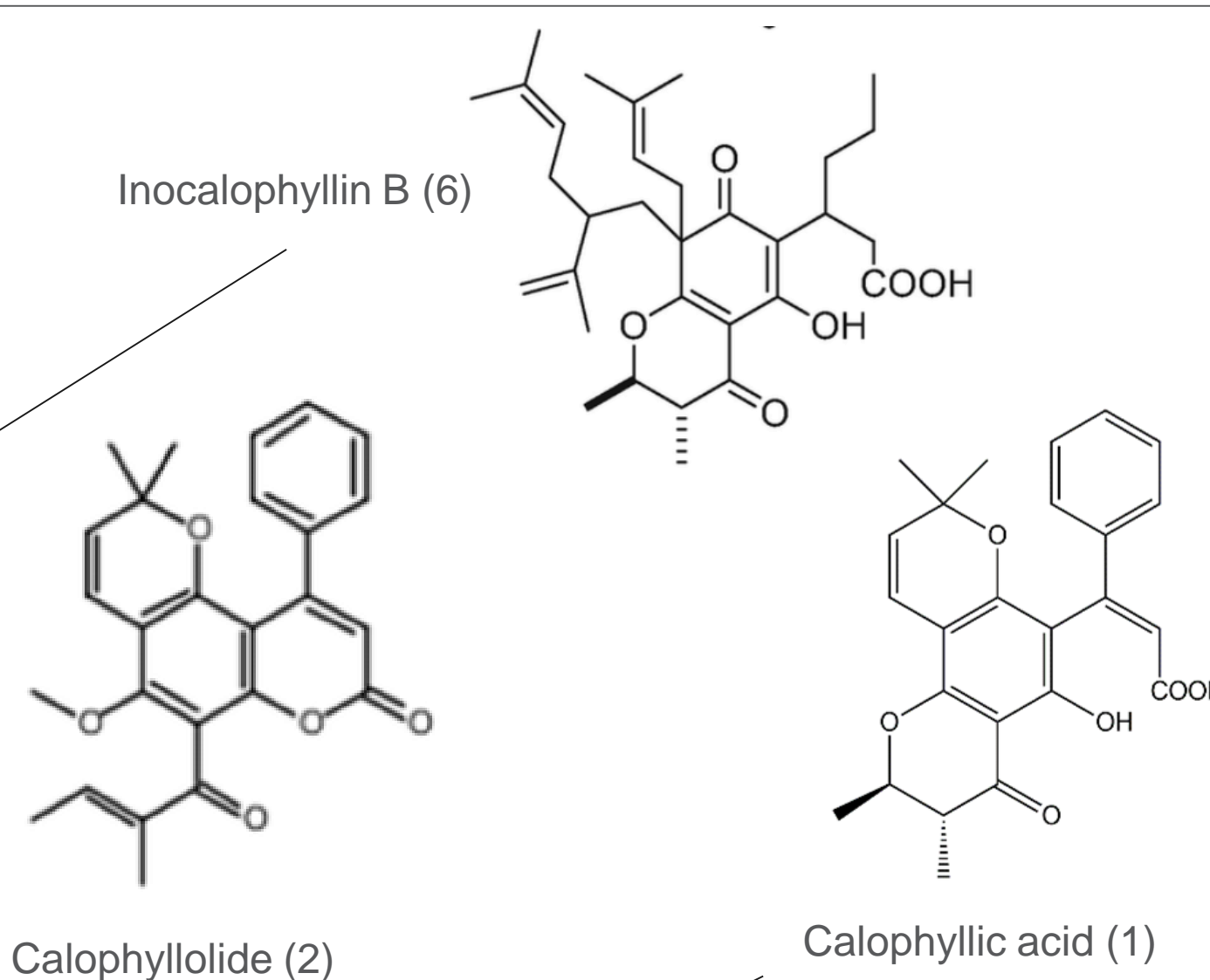
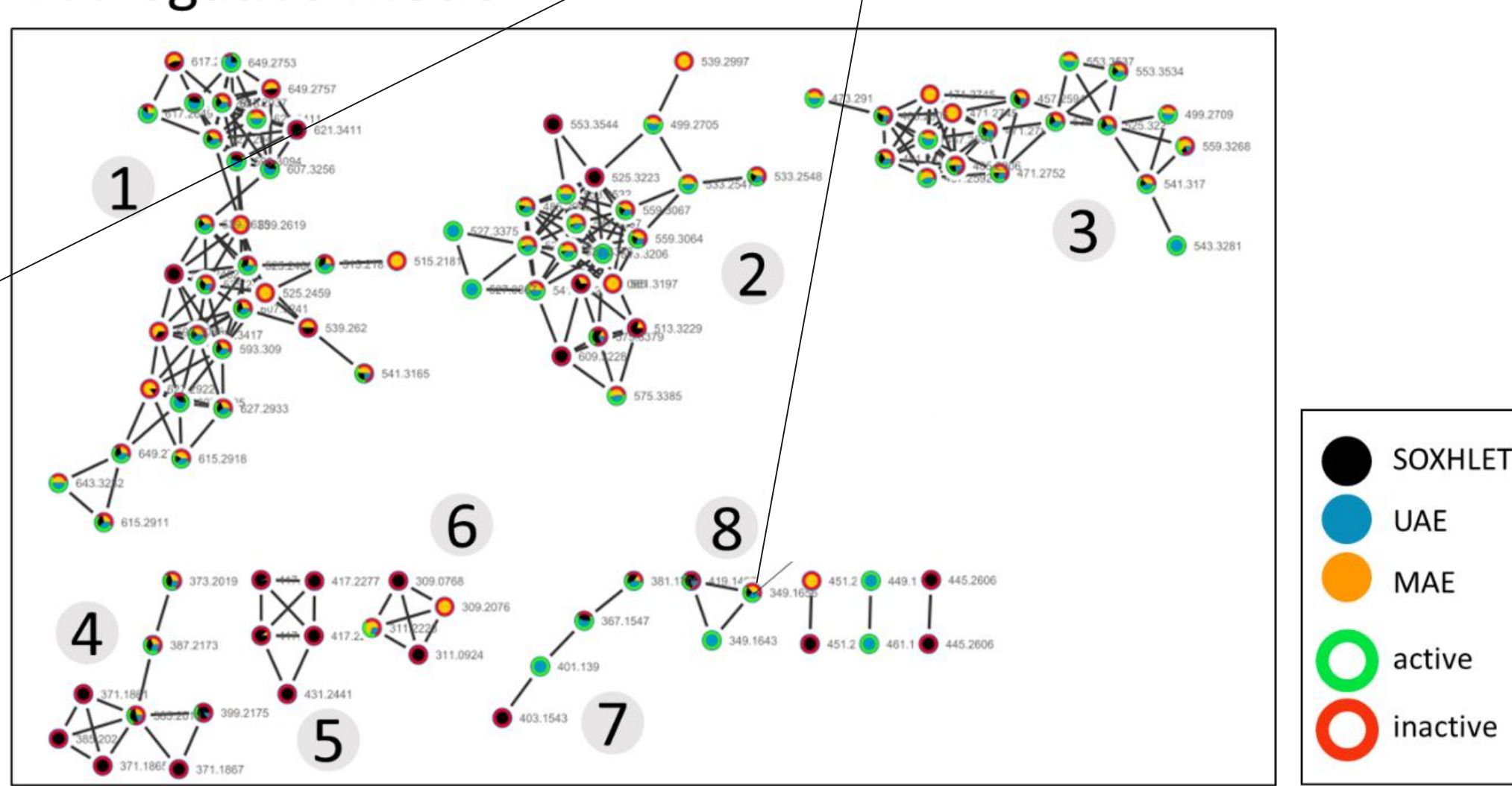
Total ion chromatograms (TIC) in positive ion mode of the three eco-extracts of *Calophyllum inophyllum* obtained on a Dionex Ultimate 3000 UPLC QToF system. The number corresponds to the compounds listed in table 2: 1. Calophyllic acid; 2. Calophylloide; 3. Inophyllum B; 4. Inophyllum C; 5. Tamanolide C; 6. Inocalophyllin B.

Molecular network

A. Positive mode



B. Negative mode



CONCLUSION

The feature-based molecular network associated with the different eco-extraction processes as well as the cytotoxic biological properties allowed us to deepen our knowledge of the bioactive metabolites present in *Calophyllum inophyllum* oil traditionally used against skin diseases in French Polynesia. These eco-extraction methods are defined by an innovative approach by an ecological, economic and competitive extraction of *tamanu* oil.

To date, this study presents for the first-time bioactivity-based Molecular Networking for the comparison of *tamanu* oil obtained via three eco-extraction technologies. It shows that ultrasound assisted extraction could be an interesting eco-extraction method to extract quality *tamanu* oil due to the good extraction yields and the rich composition in bioactive compounds. This ecofriendly extraction could be an excellent tool for cosmetic valorization of *tamanu* oil in French Polynesia.

Acknowledgment

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