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Article

Sustainable Synthesis of Omega-3 Fatty Acid Ethyl Esters from Monkfish Liver Oil

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Citation: Aguilera-Oviedo, J.; Yara-Varón, E.; Torres, M.; Canela-Garayoa, R.; Balcells, M. Sustainable Synthesis of Omega-3 Fatty Acid Ethyl Esters from Monkfish Liver Oil. *Catalysts* **2021**, *11*, x. https://doi.org/10.3390/catal11010100

Received: 28 November 2020
Accepted: 7 January 2021
Published: 13 January 2021

1. Contents

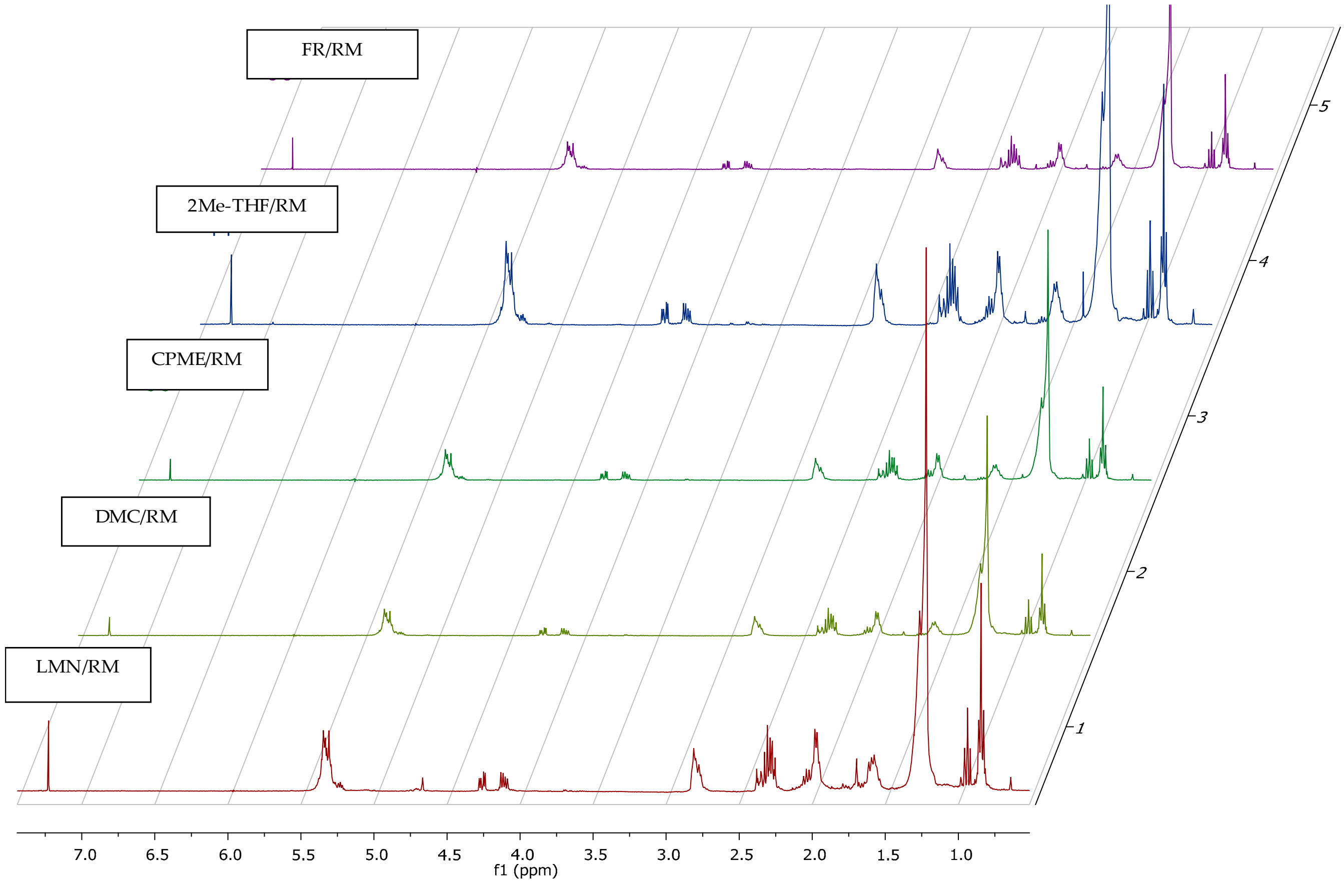

Figure S1. [1]H-NMR spectrum of monkfish liver oil (MLO) extracted with Roller mixer (RM) and different solvents. Lines colour: red: LMN, limonene; light green: DMC, dimethyl carbonate; green: CPME, cyclopentyl methyl ether; blue: 2-MeTHF, 2-methyltetrahydrofuran, and purple: FR, Folch Reagent.

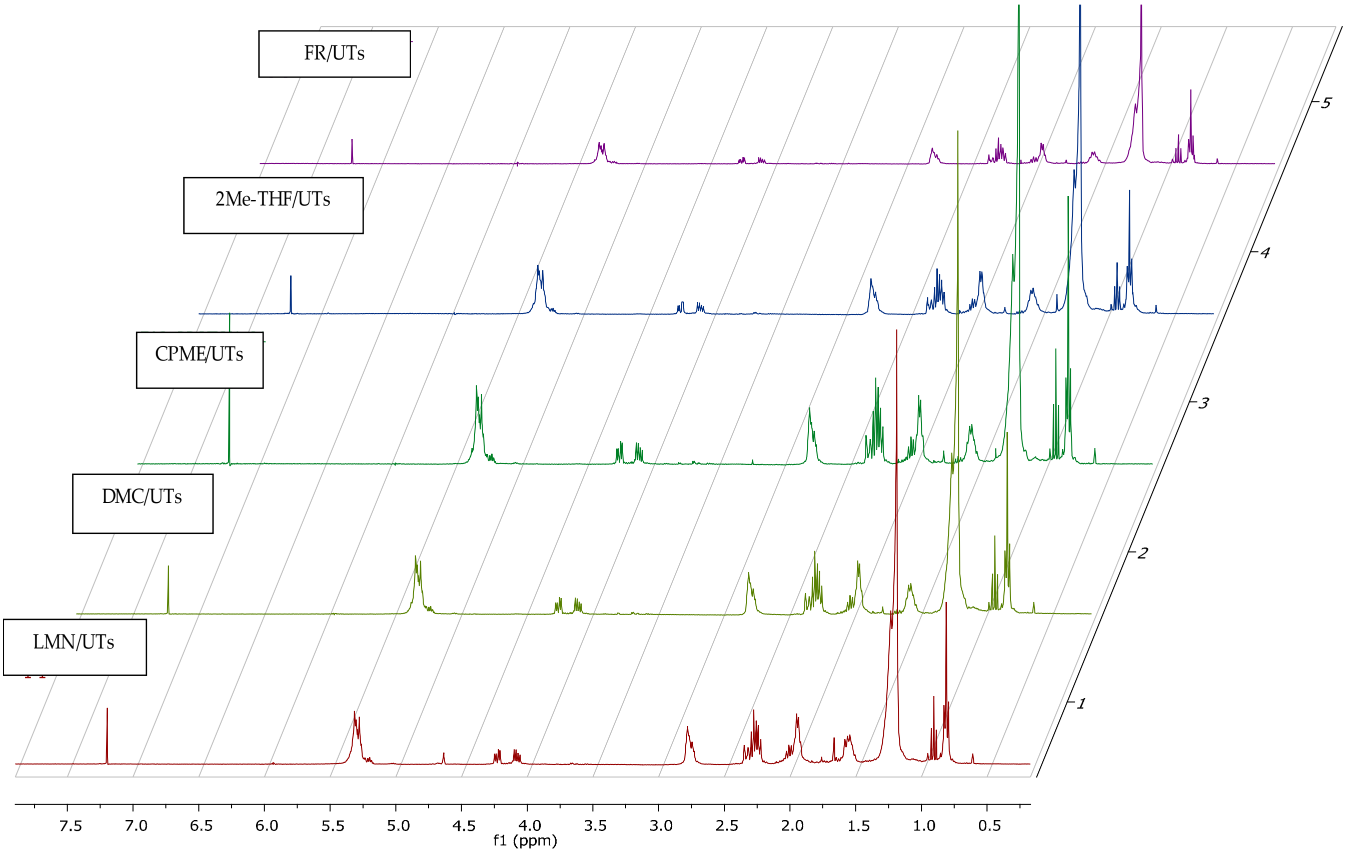

Figure S2. [1]H-NMR spectrum of hydrolysed monkfish liver oil (HMLO) extracted with ULTRA-TURRAX® (UT) and different solvents. Lines colour: red: LMN, limonene; light green: DMC, dimethyl carbonate; green: CPME, cyclopentyl methyl ether; blue: 2-MeTHF, 2-methyltetrahydrofuran, and purple: FR, Folch Reagent.

Table S1. Green solvent properties, extraction yields (MLO), substance information and cost analysis.

Solvent *(CAS)*	**Extraction Yield (%)**		**Boiling point (°C)**	**Vapour pressure to 20 °C (KPa)**	**Substance Information (Solvent guides) ****						**Cost. €/L**	**Resource**
	RM	**UTs**			**Use**		**Environment**			**Life cycle**		
					Safety	**Health**	**Air**	**Water**	**Waste**			
CFM* *(67663)*	100.0	100.0	62.0	212.0	2	9	7	7	6	5	22.6	Chemical synthesis
Methanol* *(67561)*	100.0	100.0	64.7	12.9	3	5	6	3	6	2	5.0	Chemical synthesis
2-MeTHF *(96479)*	100.0	87.0	80.0	10.0	5	6	8	6	4	7	60.8	Cereal crop/Chemical synthesis
CPME *(5614379)*	100.0	100.0	106.0	6.0	6	4	6	6	3	7	74.0	Chemical synthesis
DMC *(616386)*	99.0	75.0	90.0	7.4	1	3	5	3	5	3	66.3	Chemical synthesis
LMN *(5989275)*	89.0	29.1	178.0	0.2	5	4	3	3	7	8	23.4	Citric fruits

CFM, Chloroform; *Folch reagent (FR): (chloroform/methanol (2:1, v/v)); 2-MeTHF, 2-methyltetrahydrofuran; CPME, cyclopentyl methyl ether; DMC, dimethyl carbonate; LMN, limonene; RM, Roller mixer; UTs, ULTRA-TURRAX®; ** Date from solvent guides [1,2,3,4], Cost., prices taken from Sigma Aldrich in october (https://www.sigmaaldrich.com/spain.html).

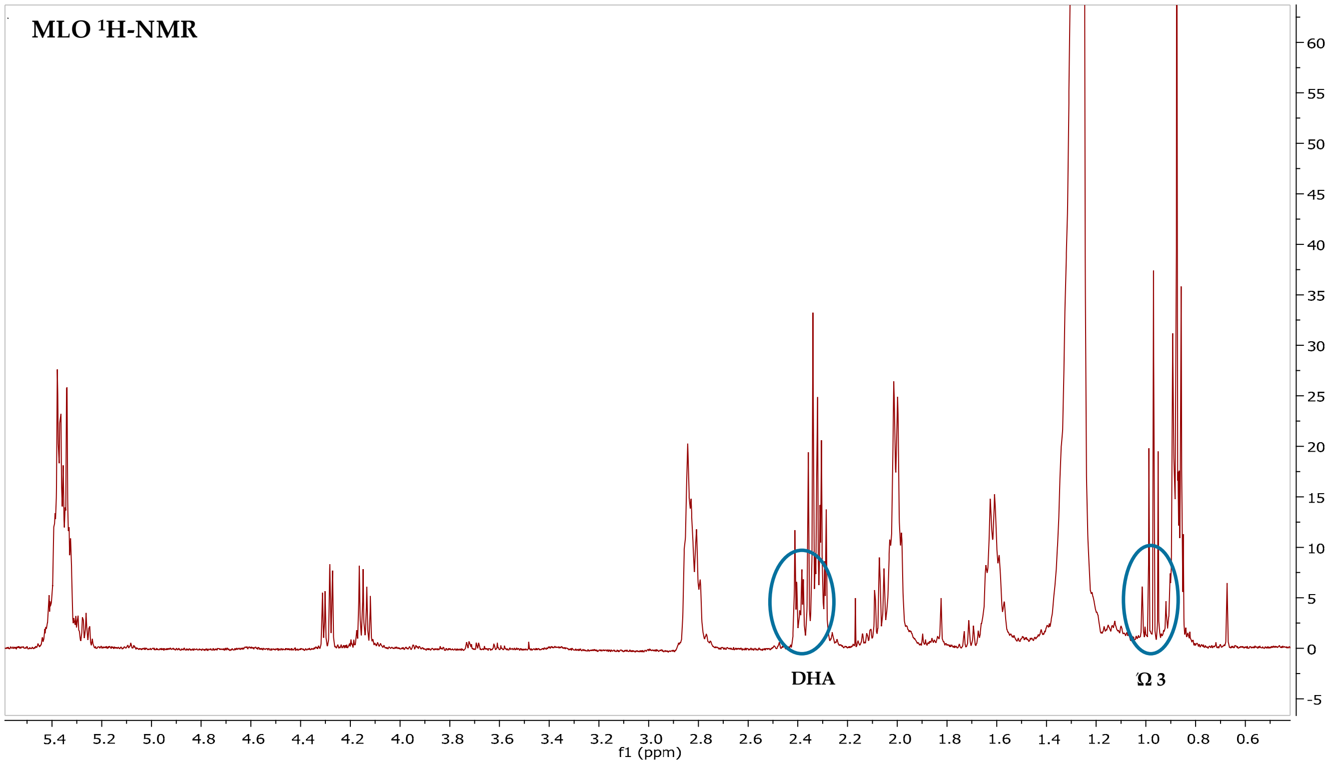

Figure S3. ¹H-NMR spectrum of MLO extracted by Folch method (FM) and with RM agitation. (DHA and Ω3 according to Nestor et al. [5].)**.**

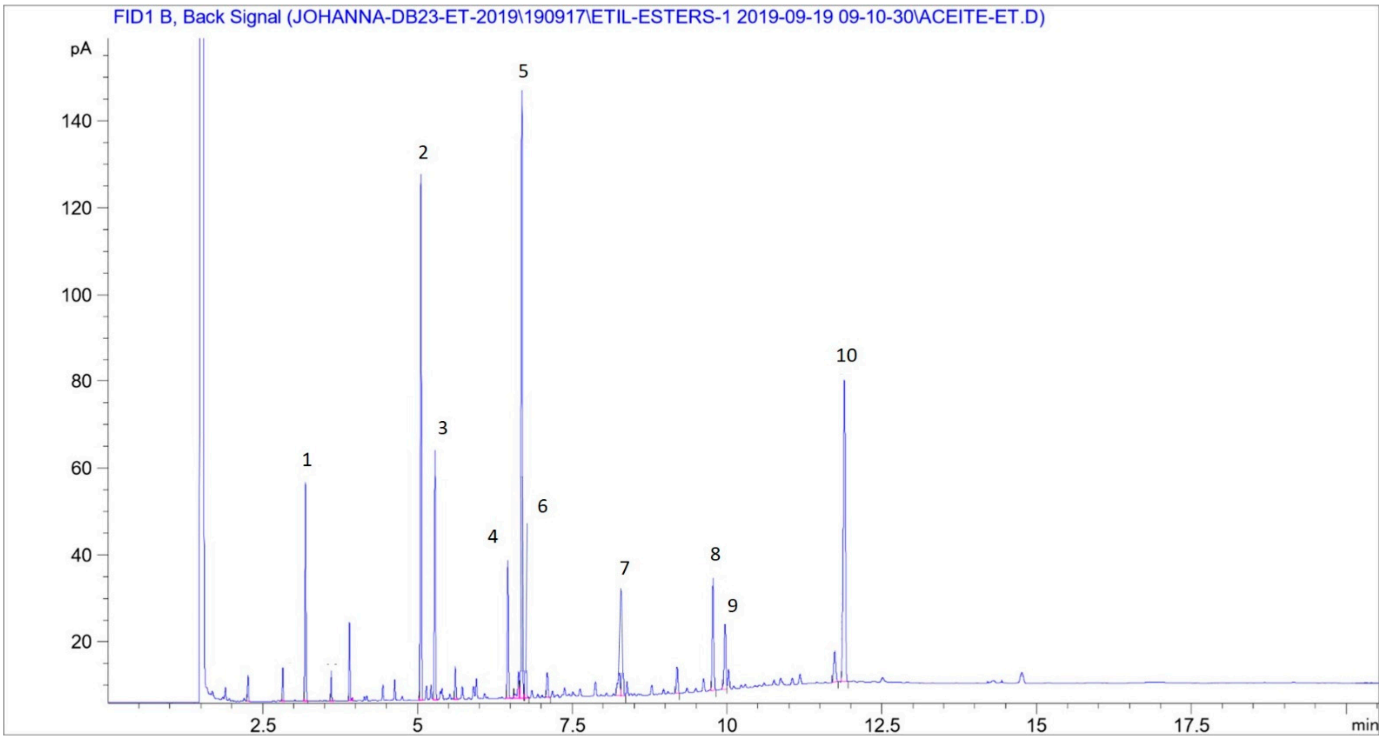

Figure S4. Chromatogram (GC-FID on DB-23, 30 m) chemically esterified monkfish liver oil. The assignment and identification of the peaks corresponds to fatty acid ethyl esters (FAEEs) 1: miristic, 2: palmitic, 3: palmitoleic, 4: stearic, 5: oleic, 6: vacenic, 7: gadoleic, 8: EPA, 9: behemic, 10: DHA. The standards used were the esters of palmitic, stearic and oleic acid. The data processing was done under the FAAES method.

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