Supplementary material for:

Analysis of Ketoprofen in Fish: Life Cycle Assessment Using Sensors vs. Conventional Methodology

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Table S1: Assumptions made for the elaboration of the life cycle inventory.

Phase	Step	Assumptions	Reference
Sample extraction	1-8	The electric energy consumptions (kWh/analysis) were measured directly in the lab by the authors.	Calculation based on laboratorial measurements and internal records [1]
	1-6	The 50 mL and 15 mL falcon tubes used for sample salting out with QuEChERS salts are assumed to be made of polyethylene.	
	1-4	The weight of a 50 mL falcon tube is 7.6 g.	Calculation based on laboratorial measurements [1]
	5-6	The weight of a 15 mL falcon tube is 3 g.	Calculation based on laboratorial measurements [1]
	4, 6	The spent falcon tubes are sent a landfill under EWC 151001* (“packaging containing residues of or contaminated by hazardous substances”).	[2]
	4, 6	The mass (g) of produced EWC 151001* is obtained considering one 50 mL (7.6 g) and one 15 mL (3 g) flacon tube for each analysis.	Calculation based on laboratorial measurements and internal records [1]
	4, 6	The spent QuEChERS salts dissolved in acetonitrile and dSPE QuEChERS salts with the non-separated salted-out fish samples are assumed to be sent for treatment under EWC 070704* (“the organic solvents, washing liquids, and mother liquors”) as a hazardous liquid solution.	[2]

Phase	Step	Assumptions	Reference
Sample extraction	4	The mass (g) of the salted-out fish sample (1) was calculated considering a solution of 10 mL acetonitrile (0.786 g/mL) and 5 mL ultrapure water (1.0 g/mL) with an average density of 0.86 g/mL. Solutes were neglected.	Calculation based on laboratorial measurements and internal records [1]
Sample extraction	6	As a first approximation, the mass (g) of the salted-out fish sample (2) was calculated considering an average density of 0.86 g/mL, as in Step 4. Solutes were neglected.	
Sample extraction	4, 6	The mass (g) of the EWC 070704* was calculated using a mass balance.	
Sample extraction	7	The amount of emissions in air during evaporation was calculated based on the assumption that the supernatant is composed of 66% v/v acetonitrile (0.786 g/cm^3) and 33% v/v ultrapure water (1.0 g/cm^3), assuming 100% evaporation; therefore, 2.1 $g_{acetonitrile}$ and 1.3 $g_{ultrapurewater}$ were evaporated for each analysis in triplicate. Dissolved salts were neglected.	
Sample extraction	8	Dissolution of the evaporated sample was achieved with 2 mL $acetonitrile_{aq}$ (80% w/w ultrapure water (1.6 g/analysis) and 20% w/w acetonitrile (0.314 g/analysis)).	
Sample extraction	5, 6	For the production process of C18 sorbent, it was assumed that 0.13 g of activated silica is used [1] as a sorbent support material. According to the literature, C18 sorbent is synthesized through the physical sorption of poly (methyloctadecyl siloxane)polymer (PMODS), a source of C18 aliphatic chains, on silica in a ratio of 1.25 g_{PMODS}: $g_{activated\ silica}$ [3] in the presence of n-pentane, followed by thermal immobilization of the PMODS at 120 ℃ for 4 h and final washing with 25 mL of n-hexane and 35mL of methanol per gram of produced C18. The indirect impacts were calculated according to the experimental data obtained in [4].	Calculation based on laboratorial measurements [1], and experiments retrieved from literature [3–5]

Phase	Step	Assumptions	Reference
Sample extraction	5, 6	The following factors were considered: ▪ 4.71×10^{-6} kWh per analysis for thermal treatment calculated as enthalpy change $$\Delta H = (m_i \times cp_i) \times (T_2 - T_1) \quad \text{Eq.1}$$ where m is the total mass (m_i) (g) of activated silica, cp_i is the activated silica-specific heat (1.13 J/g.C) , T_2 is the PMODS immobilization temperature (120 ℃), and T_1 is the initial room temperature (20 ℃). ▪ 1.47×10^{-3} kWh per analysis for the Waters 510 pump (Milford, USA) under 110 VA operation [4,5], assuming a power factor (PF) of 0.8: $$P(kW) = S(VA) \times PF / 1000 \quad \text{Eq.2}$$ where P is the real power in watts (kW). |S|-apparent power is the magnitude of the complex power in Volt·Amps (VA). $$PF = P\ (W) / \|S\ (VA)\| \quad \text{Eq.3}$$	Calculation based on laboratorial measurements [1], and experiments retrieved from literature [3–5]
Electrochemical analysis	9.1	The indirect impacts associated with the production process of CPS made of Toray carbon paper (TGP-H-60, 0.19 mm thickness; Alfa Aesar, Germany) are beyond the scope of this work due to a lack of reliable data. The indirect impacts associated with CPS pretreatment with a solution of 10 mL H_2SO_4 0.5 M for each sensor were included in the scope of this work.	-

Table S2: Methodology used for the economic and profitability analysis.

Step	Description
Capital Investment	Total capital investment (TCI) was calculated based on the value of the purchase cost of delivered equipment (PCDE) reported in Table 6 of the article text. The PCDE is the total cost of acquiring all equipment plus an additional 10% for delivery. Since the equipment is measurement instruments, all the ***direct costs*** (i.e, equipment installation, instrumentation, and electrical system) were assumed to be included in the equipment costs. No additional costs are required for buildings or facilities since existing laboratory conditions are present. Regarding ***indirect costs*****,** 15% of PCDE is assumed for engineering and supervision, and 10% is assumed for contingency for both electrochemical and HPLC analysis**.** In detail: The TCI is calculated according to Eq. 7: $TCI = FCI + WC$ *Eq 7)* where FCI is the fixed capital investment (Eq 8) $F. \quad CI = \sum_{i=1}^{n} Direct\ Costs_i + Indirect\ Costs_i$ *Eq 8)* and WC is working capital, which is calculated according to Eq 9: $\text{PDCE} \times 0.89$ Eq 9) The fraction recommended for fluid processing units is retrieved from [6].

Table S2: *cont.*

Step	Description
Materials, Labor, Utilities, and Waste Disposal	Table S8 reports the calculated values for materials, labor, utilities, and waste disposal. In detail: The number of total annual analyses performed with the electrochemical platform is calculated assuming a duration of 7 min for each analysis, 15 minutes for the sample extraction process (the obtained extract is sufficient for the analysis in triplicate), resulting in 22 minutes per analysis. Thus, 2.73 analyses are expected to be performed per hour (triplicate). Employing one laboratory technician for one shift of 8 h or 1816 h per year or 227 working d/y, the total number of analyses/y is **4950**. The same number of analyses was considered for the HPLC methodology. Regarding materials used, 10.4 mL of acetonitrile *s* used for each analysis (EUR 135/L). For the labor calculation, on one 8 h shift per day on one laboratory technician for 227 d/y was assumed (365 d/y, 104 weekend d/y, 13 d/y for Portuguese public festivities, and 21 days/y of holidays = 227 working d/y). Regarding utilities, the current electric energy price set by the Portuguese electric national energy supplier, EDP, in 2022 [7] was assumed, with a simple tariff and an installed power of 10.35 kW. Regarding waste, the separate disposal of polyethylene packaging (QuEChERS tubes) contaminated by hazardous substances (EWC 150110*) and liquid hazardous solution (EWC 070704*) was considered.
Revenues	For the profitability analysis of the projects, it was assumed that the revenues are derived from the sale price of the analysis, which is assumed to be EUR **23/analysis** for both electrochemical analysis and HPLC.
Inflation Rate	A 7.2 % inflation rate was assumed [8]. The investment is assumed to be made all in the first year (FCI spent at time 0) with the startup of the unit at time 0.
Raw Material	The purchase cost of raw material, which, in this case, corresponds to fish samples, was assumed to equal EUR 0.

Table S2: *cont.*

Step	Description
Annual Cost	For the calculation of the annual cost of the electrochemical analysis, the following variable costs were considered: operating labor, utilities, maintenance and repair (6% of FCI), and operating supplies (15% of maintenance and repair). No additional fixed charges were considered, and 2% operating labor was added for administrative costs as a general expense. For the calculation of the annual costs of HPLC analysis, the following variable costs were considered: operating labor, utilities, maintenance and repair (28% of FCI), and operating supplies (15% of maintenance and repair). No additional fixed charges were considered, and 2% operating labor was added for administrative costs as a general expense. The maintenance and repair percentage was calculated based on the value of the existing maintenance contract.
Depreciation	The depreciation of the investment was calculated considering a 5-year lifetime for both the electrochemical platform and HPLC.
Profitability Analysis	The profitability analysis of the project was developed using the following parameters: (i) the average return-on-investment rate (ROI) (%/ y), (ii) the payback period (PbP) (y), and the net return (NR) on investment (EUR) according to Eqs. 8 to 10: $$ROI\ (average) = \frac{100\ \times\ NP}{lifetime\ \times\ TCI} \qquad Eq. 8$$ where NP is the total net profit (EUR), and TCI is the total capital investment (EUR) assuming an income tax rate of 35 % and a lifetime of 15 years (y) for HPLC and 5 years for the electrochemical platform; $$PbP\ = \frac{FCI\ (inflated)}{\frac{OCF}{life\ time}} \qquad Eq. 9$$ where OCF is the total operating cash flow (EUR), calculated as $NP\ (€) + Total\ Depreciation\ (€)$; $$NR\ = \frac{NP}{life\ time\ (y)} + m_{ar}(\%. y) \times\ TCI(€) \qquad Eq. 10$$ where m_{ar} (%/y) is the minimum acceptable rate of return, which was fixed at 10 %.

Table S3: Depreciation factors used for the development of the profitability analysis.

Year	Depreciation Factors
1	0.200
2	0.320
3	0.192
4	0.115
5	0.115
6	0.058

Table S4: Comparison of the "weighted" total impacts of the novel carbon paper sensor (CPS) with high-performance liquid chromatography (HPLC) calculated according to the ReCiPe endpoint (H) method. The most relevant impact categories are highlighted in gray.

Impact category	Unit	CPS	HPLC
Fine particulate matter formation	mPt	0.3470	0.6980
Global warming, human health	mPt	0.2406	0.6018
Human non-carcinogenic toxicity	mPt	0.2364	0.4949
Human carcinogenic toxicity	mPt	0.0707	0.1488
Fossil resource scarcity	mPt	0.0336	0.0621
Global warming, terrestrial ecosystems	mPt	0.0241	0.0602
Ozone formation, terrestrial ecosystems	mPt	0.0221	0.0260
Terrestrial acidification	mPt	0.0104	0.0216
Water consumption, human health	mPt	0.0062	0.0136
Freshwater ecotoxicity	mPt	0.0036	0.0081
Freshwater eutrophication	mPt	0.0030	0.0055
Terrestrial ecotoxicity	mPt	0.0019	0.0042
Ozone formation, human health	mPt	0.0031	0.0039
Water consumption, terrestrial ecosystem	mPt	0.0018	0.0039
Marine ecotoxicity	mPt	0.0007	0.0015
Mineral resource scarcity	mPt	0.0003	0.0006
Stratospheric ozone depletion	mPt	0.0001	0.0003
Global warming, freshwater ecosystems	mPt	0.0000	0.0000
Marine eutrophication	mPt	0.0000	0.0000
Water consumption, aquatic ecosystems	mPt	0.0000	0.0000
Ionizing radiation	mPt	0.0000	-0.0001
Land use	mPt	0.0008	-0.0009

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