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Sustainability Spotlight Statement

This study advances sustainable food systems by demonstrating that lycopene extraction from tomato residues can be significantly optimized through the combined use of green solvents and ultrasound-assisted technologies. By integrating Life Cycle Assessment (LCA) with functional efficiency metrics, the work highlights extraction routes that substantially reduce energy demand, solvent use, and environmental burdens while increasing the added value of agro-industrial byproducts. These findings directly support SDG 12 (Responsible Consumption and Production) by promoting circular resource use, SDG 9 (Industry, Innovation and Infrastructure) through the development of cleaner and more efficient processing technologies, and SDG 13 (Climate Action) by identifying lower-impact production pathways. These results support the transition toward low-impact, circular processing strategies that promote waste valorization, resource efficiency, and more sustainable food production chains.

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SUSTAINABLE VALORIZATION OF TOMATO WASTE THROUGH LIFE BOORS OR A CONTROL OF TOMATO WASTE THROUGH LIFE BOORS OF TOWATO WASTE BOORS OF

CYCLE ASSESSMENT OF LYCOPENE EXTRACTION METHODS

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15 Abstract

Tomato processing produces substantial quantities of residues that constitute both an environmental 99A challenge and a potential resource for recovery. This study assessed the environmental performance of four lycopene extraction strategies from tomato discards through a Life Cycle Assessment approach. Conventional and ultrasound-assisted extractions were compared with either a hexane:acetone:ethanol (50:25:25, v/v) mixture or ethyl acetate as solvent, defining four scenarios: Scenario 1 (C-HAE, conventional extraction with hexane:acetone:ethanol); Scenario 2 (C-EA, conventional extraction with ethyl acetate); Scenario 3 (U-HAE, ultrasound-assisted extraction with hexane:acetone:ethanol); Scenario 4 (U-EA, ultrasound-assisted extraction with ethyl acetate). The functional unit was defined as 1 kg of lycopene-equivalent extract. Environmental impacts were calculated with the ReCiPe 2016 Midpoint (H) method, considering eighteen impact categories. Scenario 4 exhibited the lowest environmental impact (117.3±27.6 mg/100g of lycopene yield; 1187.9±103.5 µg Txeq/g_{ww}) whereas Scenario 2 the highest, with the lowest lycopene yield (18.6±18.5 mg/100g) but the highest antioxidant capacity per unit of lycopene. A sensitivity analysis based on the antioxidant activity-to-lycopene ratio confirmed *Scenario 4* as the most favorable option. Beyond energy efficiency and solvent selection, the extraction process also affected lycopene isomerization: ultrasound-assisted methods promoted Z-isomers formation over E- ones, with increases of 41% for the hexane:acetone:ethanol solvent mixture and 140% for ethyl acetate. Since Z-isomers are more bioaccessible and display comparable or higher antioxidant activity than Eisomers, this shift may further enhance the functional value of the recovered pigment. Overall, combining green solvents with ultrasound technologies can reduce the environmental burdens and

Keywords: Valorization of residues; Green solvent extraction; Natural colorant; Life Cycle Assessment

support sustainable valorization of tomato waste.

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1. Introduction

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Tomatoes represent one of the most important agricultural commodities worldwide and and a some of the most important agricultural commodities worldwide and a some of the most important agricultural commodities worldwide and a some of the most important agricultural commodities worldwide and a some of the most important agricultural commodities worldwide and a some of the most important agricultural commodities worldwide and a some of the most important agricultural commodities worldwide and a some of the most important agricultural commodities worldwide and a some of the most important agricultural commodities worldwide and a some of the most important agricultural commodities worldwide and a some of the most important agricultural commodities worldwide and a some of the most important agricultural commodities worldwide and a some of the some of 2023, ranked as the leading vegetable crop, with a global production of approximately 192 million tons [1]. They are particularly valued for their rich composition of antioxidants, including ascorbic acid (vitamin C), tocopherol (vitamin E), carotenoids (lycopene and β-carotene), and various phenolic compounds, including quercetin, kaempferol, naringenin, lutein, and chlorogenic acids [2]. Beyond their health-promoting properties, these compounds also contribute to the sensory attributes of tomatoes, influencing aroma, taste, and texture [3].

Despite their remarkable nutritional and sensory qualities, postharvest losses in tomatoes remain a major global concern, estimated between 25 % and 42 % annually [4]. Food loss and waste not only generate significant socio-economic costs but also account for about 8 % of global greenhouse gas emissions and lead to the depletion of natural resources (e.g., water, soil, energy) used to produce food that is never consumed, which ultimately occupies 21 % of landfill capacity [5]. To mitigate these challenges, international organizations have established initiatives aimed at reducing food loss and waste. The 2030 Agenda for Sustainable Development Goals (SDGs) includes Target 12.3, which seeks to halve per capita global food waste at the retail and consumer levels by 2030 while also reducing food losses along production and supply chains, including postharvest stages [6]. The European Commission has aligned its policies with this objective through the "Farm to Fork Strategy", a central component of the European Green Deal [7].

Accordingly, the valorization of tomato discards (losses, wastes) represents a promising approach. Recovering bioactive compounds from agro-industrial residues not only adds value through the extraction of nutrients and functional ingredients but also reduces the environmental impacts associated with waste disposal [8]. Likewise, the valorization strategy can be extended to surplus tomatoes, which are often discarded during periods of high production due to their seasonal nature and high perishability. The reuse of these derivatives can simultaneously provide additional income sources, reduce disposal costs, and enhance the nutritional value of functional foods [9].

The use of synthetic dyes has raised increasing health and regulatory concerns. Some artificial colorants, such as Erythrosine (Red No. 3), have been associated with potential adverse effects, including genotoxicity [10] thyroid dysfunction, and hyperactivity in children [11,12]. Due to such evidence, the Food and Drug Administration (FDA) banned the use of Red No. 3 in cosmetics and topical drugs and is moving towards restricting its use in food products [13,14]. Several studies have further linked synthetic dyes to allergic reactions and behavioral effects, prompting stricter regulations and a growing consumer preference for safer, natural alternatives [15]. Within this framework, natural pigments offer innovative opportunities for replacement. Their use has expanded across multiple industries, including food, pharmaceutical, textile, dairy, and seafood sectors. In this

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context, lycopene, a key carotenoid predominantly found in tomatoes, is increasingly valued in the food industry as a natural and safe coloring agent, owing to both its vivid red hue and its /strongs99A antioxidant capacity [16]. Because tomatoes account for 80-90% of dietary lycopene intake, with levels ranging from 0.72 to 4.2 mg per 100 g depending on ripeness, temperature, and soil conditions, they constitute a major and reliable source for natural pigment-based applications [17].

The growing consumer preference for natural, health-promoting, and sustainable products further drives the demand for functional foods enriched with natural antioxidants such as lycopene [16, 18-21]. The global carotenoids market reflects this trend, being valued at USD 2 billion in 2023 and projected to reach USD 2.9 billion by 2029, at a compound annual growth rate (CAGR) of 6.7 % [17].

Despite increasing interest in lycopene extraction from tomato residues, the environmental implications of these processes remain largely underexplored. The available research typically focuses on extraction yields, antioxidant properties, or process optimization [22], but few works integrate these metrics within a comprehensive environmental quantification [23, 24]. Moreover, no study to date has jointly evaluated the combined effect of extraction conditions and lycopene isomerization on both environmental performance and functional efficiency.

Given this context, the aim of this study is to compare the environmental impact of different extraction techniques used for the recovery of bioactive compounds from tomato discards. Specifically, the study evaluates conventional extraction methods employing petrochemical solvents against sustainable alternatives such as ultrasound-assisted extraction (UAE) and the use of lowtoxicity, biodegradable solvents like ethyl acetate. A life cycle assessment (LCA) approach was applied to quantify the environmental performance of each extraction process in terms of energy consumption, greenhouse gas emissions, and solvent use. The outcomes aimed to identify the most sustainable strategies for the valorization of tomato residues, contributing to the development of greener extraction technologies aligned with sustainable food processing.

2. Materials and methods

2.1 Materials

Analytical-grade hexane, acetone, ethanol, and ethyl acetate, together with HPLC-grade hexane, tetrahydrofuran, acetonitrile, and methanol, were obtained from ANEDRA (Research, ARG) and CICCARELLI (Reagents S.A., ARG). The HPLC calibration curve was prepared using a lycopene standard (HPLC grade, 98% purity, from tomato; Sigma-Aldrich Chemie GmbH, Germany).

2.2. Methods

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2.2.1. Tomato pre-processing. Mature tomatoes (Solanum lycopersicum cv. 'Platense') were donated by Quinta Flores, located in Arana (35.00° S, 57.90° W) (La Plata, Argentina). The fruits were washed 99A with running tap water to remove surface impurities. Seeds were manually separated, while the pulp and peel were homogenized using an 800 W hand mixer until a uniform purée was obtained. The homogenate was then concentrated by centrifugation at 7,000 rpm for 15 minutes. The resulting concentrate was divided into regenerated cellulose bags and stored at -20 °C until processing (maximum storage time until processing: four weeks). To minimize exposure to light and avoid lycopene degradation, the tomato stock was covered with aluminum foil.

2.2.2. Lycopene extraction. The lycopene extracts were obtained using two solvent mixtures [hexane:acetone:ethanol (50:25:25) and ethyl acetate] and two methods (conventional and ultrasound-assisted extraction). For each extraction, 1 g of concentrated tomato waste was used in triplicate, maintaining a sample-to-solvent ratio of 1:16 in 15 mL Falcon tubes. The conventional method, modified according to [25], consisted of mixing 1 g of the homogenized sample with the solvent mixture [hexane:acetone:ethanol (50:25:25) or ethyl acetate] for 1 minute in a vortex, and then incubating it at 40 °C for 1 minute. Ultrasound-assisted extraction was carried out using a Branson 2510 ultrasonic cleaner (tank capacity: 1/2 gallon) operating at a maximum power of 300 W and a frequency of 40 kHz for 29 minutes at 60 °C, according to [26] with modifications. Ten milliliters of distilled water were added to the lycopene extracts to remove any interfering watersoluble compounds [27]. The mixture was then centrifuged at 4000 rpm for one minute in a centrifuge 5430 (Eppendorf AG, Hamburg, Germany). Finally, the organic phase was collected and filtered through 0.45 µm nylon filters prior to lycopene analysis. All extraction procedures were performed in the dark to minimize carotenoid degradation.

2.2.3. Lycopene analysis. The lycopene concentration in the samples was determined using a UVvis spectrophotometer (UVmini-1240, Shimadzu) and high-performance liquid chromatography (HPLC). For the former, the absorbance at the maximum wavelength (λ_{max}) of 472 nm was used for the calculations.

For the HPLC analysis, the samples were evaporated and resuspended in a mixture of tetrahydrofuran, acetonitrile and methanol (15:30:55 v/v/v) via ultrasonication for 15 minutes to ensure the solubilization of the extracts. Chromatographic analyses were performed using a Waters Spherisorb C18 column (250 mm × 4.6 mm, 5 µm particle size) maintained at 35 °C under isocratic conditions. The mobile phase consisted of acetonitrile and water (90:10, v/v) containing 9 µM triethylamine (TEA), with a flow rate of 1 mL/min. The system was equipped with a Waters 1525 binary HPLC pump and a Waters 2998 photodiode array detector, set at $\lambda_{max} = 472$ nm. The mobile

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phase was freshly prepared prior to each run.

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2.2.4. LCA methodology

2.2.4.1 Study design and goal definition. The goal of this study was to compare the environmental performance of conventional and ultrasound-assisted extraction techniques for the recovery of bioactive compounds -particularly carotenoids, predominantly lycopene- from tomato discards. The assessment focused on four extraction strategies, referred to as *scenarios* (Table 1), which describe the different scenarios based on the solvents and extraction methodologies employed in this study.

Scenario 1 (C-HAE): Conventional solvent extraction using a mixture of hexane, acetone, and ethanol (50:25:25, v/v) with a solid-to-solvent ratio of 1:16 (w/v). The mixture was vortexed for 1 min and maintained in a water bath at 40 °C for 1 min.

Scenario 2 (C-EA): Conventional solvent extraction with ethyl acetate and a solid-to-solvent ratio of 1:16 (w/v). The mixture was vortexed for 1 min and maintained in a water bath at 40 °C for 1 min.

Scenario 3 (U-HAE): Ultrasound-assisted extraction using a mixture of hexane, acetone, and ethanol (50:25:25, v/v) with a solid-to-solvent ratio of 1:16 (w/v). The extraction was performed in an ultrasonic bath for 29 min at 60 °C, 40 kHz, 300 W.

Scenario 4 (U-EA): Ultrasound-assisted extraction with ethyl acetate at a solid-to-solvent ratio of 1:16 (w/v). The extraction was carried out in an ultrasonic bath for 29 min at 60 °C, 40 kHz, 300 W.

A LCA framework was applied in accordance with ISO 14040 and ISO 14044 standards (International Organization for Standardization [ISO] [28].

2.2.4.2. Functional unit and system boundaries. The functional unit was defined as 1 kg of lycopene-equivalent extract obtained from tomato discards. This unit allows for the comparison of extraction methods based on the same quantity of target compound produced, independent of yield variations.

The system boundaries considered a gate-to-gate approach, encompassing all processes from tomato pulp preparation (tomato discards collection, washing, removal of peel and seeds, mixing and centrifugation) through lycopene extraction (Scenarios 1 to 4) and solvent recovery (Figure 1). Upstream agricultural production, downstream product formulation (*e.g.*, encapsulation or food incorporation) and waste management were excluded to isolate the environmental impact of the extraction stage.

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2.2.4.3. Life cycle inventory (LCI): Inventory data collection. The LCI involved the systematic collection of input and output data related to each stage of the process for the four scenarios. The

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inventory considered the consumption of electricity, tomatoes, solvents (hexane, acetone, ethanol, and ethyl acetate), and water (tap and deionized), as well as the generation of liquid organic standard and ethyl acetate). chemical wastes, solvent losses, and the production of dried lycopene. Detailed data corresponding to the four evaluated scenarios are presented in Table 2.

Energy data were obtained from direct laboratory measurements, and emission factors for electricity and solvents were sourced from the ELCD 3.2 database (Greendelta v2.18 correction20220908).

Environmental impacts were evaluated using the ReCiPe 2016 Midpoint method, adopting the hierarchist perspective and World (2010) (H) normalization approach [29,30]. The impact categories selected for this analysis (Table 3) included global warming (GW, kg CO₂-eq), stratospheric ozone depletion (SOD, kg CFC-11 eq), ionizing radiation (IR, kBq Co-60 eq), ozone formation (human health) (OHh, kg NOx eq), ozone formation (terrestrial ecosystems) (OTe, kg NOx eq), fine particulate matter formation (FPMF, kg PM2.5 eq), terrestrial acidification (TA, kg SO₂ eq), freshwater eutrophication (FE, kg P eq), marine eutrophication (ME, kg N eq), terrestrial ecotoxicity (TE, kg 1,4-DCB eq), freshwater ecotoxicity (FEco, kg 1,4-DCB eq), marine ecotoxicity (MEco, kg 1,4-DCB eq), human carcinogenic toxicity (HCT, kg 1,4-DCB eq), human non-carcinogenic toxicity (HNCT, kg 1,4-DCB eq), land use (L, m² year crop eq), mineral resource scarcity (MRS, kg Cu eq), fossil resource scarcity (FRS, kg oil eq), and water consumption (WC, m³).

Electrical consumption (MJ) was calculated according to Eq. 1 [31], where P is the power of the equipment (kW) (bath, mixer, ultrasonic bath, rotavapor system) and t is the duration of use (hour).

$$Electrical \ consumption = P \times t \tag{1}$$

- 2.2.4.4. Life cycle assessment. Calculations were performed using Open LCA software. Impact categories were normalized and weighted to facilitate comparison among the four scenarios (section 2.2.4.1). Sensitivity analyses were conducted to evaluate the impact of solvent recovery on antioxidant efficiency and the total environmental impact. To achieve this, the inputs and outputs were adjusted according to the ratio of extracted lycopene to antioxidant activity, as well as to the functional unit.
- 2.2.4.5. Data quality and assumptions. Primary data were collected from controlled laboratory-scale experiments, complemented by literature data where necessary. Assumptions included a 90% solvent recovery rate for ethyl acetate, and 80% for hexane, consistent with prior studies [32,33].
- **2.2.5.** Antioxidant activity. Antioxidant activity of lycopene extracts was measured as Trolox

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Equivalent Antioxidant Capacity (TEAC) using ABTS (2,2-azinobis-3-ethylbenzothiazoline-6sulfonate) method according to [34]. ABTS was dissolved in water to a 7 mM concentration of the fitness of the state of th radical cation (ABTS^{•+}) was produced by reacting that ABTS solution with 2.45 mM potassium persulfate (final concentration), and the mixture was kept in the dark at 20 °C for 12-16 h before use. From this concentrated solution, an ethanolic ABTS^{•+} solution was prepared adjusting the absorbance to 0.70±0.02 at 734 nm (UVmini-1240 spectrophotometer, Shimadzu). The addition of antioxidants led to a decrease in absorbance at 734 nm, and the resulting decolorization, expressed as the percentage inhibition of the radical cation, was evaluated as a function of concentration and time. A 10-point calibration curve was constructed using a Trolox standard solution (2.22 mM; Sigma-Aldrich) within the concentration range of 0.0125-0.08 mM. The curve was obtained by plotting Trolox concentration (mM) on the x-axis against the percentage of radical inhibition on the y-axis. Sample absorbance values were expressed as Trolox equivalents (umol Trolox/g sample, dry basis). One milliliter of each extract was evaporated to dryness and re-dissolved in 1 mL of dimethyl sulfoxide (DMSO), followed by sonication in an ultrasonic bath for 15 min. A reaction mixture was then prepared by combining 1 mL of ethanolic ABTS^{•+} solution with 50 µL of sample, blank (DMSO), or Trolox standard. The mixture was vortexed for 5 s and allowed to react for 6 min, after which the absorbance was measured at 734 nm. The percentage inhibition of absorbance was used to calculate the Trolox equivalent antioxidant capacity (TEAC) from the calibration curve, according to equation 2:

$$y = 22.069x - 14.311 \tag{2}$$

where y represents the percentage of inhibition, calculated as % inhibition = $[(A_{734} \text{ control} - A_{734})]$ sample) / A_{734} control] \times 100, and x corresponds to the Trolox Equivalent Antioxidant Capacity (TEAC) expressed in µM.

2.2.6 Reproducibility of results. All experiments were performed on triplicate samples. The relative differences were reproducible irrespective the synthesis used. Analysis of variance (ANOVA) was used to analyze the results obtained using the statistical program Infostat v2009 software (Córdoba, Argentina). Comparison of means by Tukey mean were tested, and if p<0.05 the difference was considered statistically significant.

3. Results and discussion

3.1. Lycopene content and antioxidant activity

The lycopene content of the tomato concentrate showed significant differences in the four

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extraction strategies (Table 4). Unexpectedly, Scenario 2 (conventional extraction with ethyl acetate) yielded the lowest lycopene concentration, as determined by both UV-vis and HPLC analyses, 500 per 1899A values of 18.6 ± 0.3 and 18.6 ± 18.5 mg/100 g ww (wet weight), respectively. Scenario 4 followed, showing 186.3 ± 3.0 mg/100 g ww by UV-vis and 117.3 ± 27.6 mg/100 g ww by HPLC. Scenarios 1 and 3 exhibited the highest lycopene contents, with 207.6 ± 4.5 and 168.4 ± 18.5 mg/100 g ww, and 208.2 ± 6.0 and 147.0 ± 39.3 mg/100 g ww, respectively. These values are consistent with the higher extraction efficiencies generally reported for ultrasound-assisted and mixed-solvent systems, as shown in Table 5 [35-37].

Interestingly, while the UV-vis results revealed statistically significant differences for *Scenario* 4 compared with Scenarios 1 and 3, the HPLC data did not confirm these differences (Table 4). This discrepancy may be attributed to the presence of co-extracted compounds (β-carotenes, lutein) with overlapping absorbance in the visible range, which could affect the UV-vis quantification but are more effectively resolved by HPLC analysis [38].

Despite these differences, Scenario 4 exhibited the highest antioxidant activity (1187.9 µg Tx eq/g ww), indicating that antioxidant compounds other than lycopene may contribute to the overall activity [38]. The ratio between antioxidant activity and lycopene content was markedly higher in Scenario 2 (approximately 3.4-fold greater) than in the other scenarios, suggesting that the extraction solvent and processing conditions may differentially influence both lycopene yield and antioxidant potential. In fact, the extraction conditions in Scenario 2 could favor the co-extraction of other highly active compounds, despite its poor lycopene recovery. In contrast, the lower ratios observed for Scenarios 1 and 3 reflect a weaker functional contribution per unit of lycopene extracted. Scenario 4 showed an intermediate behavior, supporting the idea that ultrasound combined with ethyl acetate enhances the extraction of a more functionally efficient antioxidant profile than in the other scenarios. These results underscore the importance of considering functional efficiency -not only compound yield- when evaluating extraction performance.

3.2. Environmental profile

Figures 2 and 3 show the relative contribution of each environmental impact category across the different scenarios for obtaining 1 kg of lycopene-equivalent extract from tomato discards. Scenario 2 exhibited the highest impact in all categories, followed by Scenarios 3 and 1, whereas Scenario 4 was the most favorable overall (Figure 2). The lycopene extraction stage represented the main hotspot in all scenarios (data not shown), exceeding the impacts associated with tomato pulp preparation. This predominance is particularly evident in Scenario 2, where the lower lycopene yield led to a greater amount of tomato and solvent required to achieve the functional unit of 1 kg of lycopene, thereby amplifying the overall environmental burden.

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Figures 3 shows that the categories *Ozone formation-Terrestrial ecosystems (OTe)*, *Ozone formation-Human health (OHh)*, *Marine ecotoxicity (MEco)*, *Terrestrial ecotoxicity (TE)*, *Fossil* Polarice online *resource scarcity (FRS)*, and *Human non-carcinogenic toxicity (HNCT)* were the main contributors to the overall environmental impact. Regarding *OTe* and *OHh*, ozone is not directly emitted into the atmosphere but is formed through photochemical reactions involving nitrogen oxides (NOx) and non-methane volatile organic compounds (NMVOCs). In the atmosphere, NOx and NMVOCs are transformed into ozone, which can subsequently be inhaled by humans or absorbed by plants [29]. The energy consumption associated with lycopene extraction processes, together with solvent use, had a significant impact on both ecosystems and human health, with *Scenario 2* contributing up to 643.1 kg NOx eq (Table 6).

In turn, the results for MEco and TE categories were expressed in kg 1,4-dichlorobenzene equivalents (1,4-DCB eq) to characterize pollutant emissions. *Scenario 2* contributed 274.5 and 1.2 \times 10⁵ kg 1,4-DCB eq/FU (functional unit), respectively, whereas *Scenarios 1* and 3 showed corresponding values of 7.6 and 7.6 \times 10³, and 14.5 and 1.6 \times 10⁴ kg 1,4-DCB eq/FU, respectively.

For the *FRS* category, as mentioned previously, the lycopene extraction process was identified as the main environmental hotspot, where most of the energy consumption is concentrated. In La Plata (Buenos Aires, Argentina), natural gas and oil are the primary fuels used for thermal electricity generation, thereby contributing to fossil resource scarcity. *Scenario 2* consumed 3.7×10^4 kg oil eq/FU, whereas *Scenarios 3* and 4 showed values of 6.9×10^3 and 7.9×10^3 kg oil eq/FU, respectively (Table 6).

For the category *HNCT*, expressed in kg 1,4-dichlorobenzene equivalents (kg 1,4-DCB eq), *Scenarios 1* and 3 showed comparable values of 7.0×10^3 and 8.4×10^3 kg 1,4-DCB eq, respectively, while *Scenario 2* contributed 2.1×10^4 kg 1,4-DCB eq. The use of toxic solvents and the fuel consumption associated with electricity production generated industrial process emissions that have been linked to adverse effects on human health [39,40].

Finally, Freshwater ecotoxicity (FEco), Human carcinogenic toxicity (HCT), Ionizing radiation (IR) and Terrestrial acidification (TA) contributed to the environmental impact to a minor degree. However, Scenario 2 showed the highest values compared to the other scenarios. FEco and HCT contributed 20.2 and 77.9 kg 1,4-DCB eq, respectively, Ionizing radiation (IR), with 1.2×10^4 kBq Co-60 eq, and Terrestrial acidification (TA), with 606.4 kg SO2 eq. All of these are related to the emission of gases generated during industrial processes that contribute to the toxicity and acidification of the terrestrial ecosystem, with direct impacts on human health and environmental toxicity.

3.3. Sensitivity analysis

Lycopene in fresh tomatoes occurs predominantly in the all-E form (more than 90%) [41].

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However, in the human body, the *Z*-isomers of lycopene are more soluble than *E*- ones, and form micelles, thereby facilitating intestinal absorption [42]. Furthermore, studies indicate of that file 99A intestinal absorption and antioxidant activity of *Z*-isomers, particularly 5-*Z*-lycopene, are superior. Isomerization occurs not only during digestion, but also as a result of temperature, for example, during extraction processes [41]. Nevertheless, many studies have reported that the *Z*-isomers of carotenoids exhibit equal or even higher antioxidant capacity compared with their all-*E* counterparts [43], and display similar functionality, such as anti-obesity activity [44]. The increased formation of *Z*-isomers may enhance lycopene bioaccessibility and antioxidant potential, as these isomeric forms are generally more stable than *E*- isomers against heat and light and more readily incorporated into biological membranes.

In this work, the isomerization analysis demonstrated that, within each solvent system (*Scenarios 1* vs. 3 and *Scenarios 2* vs. 4), the introduction of ultrasound shifted the carotenoid profile toward a greater proportion of *Z*-isomers, whereas the conventional extractions consistently favored the formation of *E*-isomers (Table 4). In other words, *Scenarios 3* and 4 showed higher proportions of *Z*-isomers compared with their counterparts obtained without ultrasound-assisted extraction (*Scenarios 1* and 2, respectively). This shift in lycopene isomerization can be attributed to the temperature increase during the ultrasound-assisted extraction process [42].

When comparing the effect of the solvents on the functionality of the extracts, it is worth noting that the use of ethyl acetate led to a higher proportion of E-isomers than the mixture of hexane, acetone, and ethanol (50:25:25, v/v), because E-isomers are less soluble than Z-isomers in non-polar solvents such as hexane [43]. This finding is consistent with the higher antioxidant activity-to-lycopene ratio observed under these conditions (*Scenario 2* vs. I and *Scenario 4* vs. I) (Table 4).

As shown in section 3.1, *Scenario 2* resulted in the lowest lycopene yield, considerably lower than that obtained in the other three scenarios (Table 4). However, it exhibited the highest antioxidant capacity relative to the amount of lycopene extracted. Therefore, the functional unit of the baseline LCA was adjusted to account for this relationship, and a sensitivity analysis was performed by adjusting the inputs and outputs according to the ratio between extracted lycopene content and antioxidant activity (Table 7).

After this adjustment, *Scenario 4* represented the most favorable situation, and *Scenario 2* shifted from the least sustainable state to an intermediate level of sustainability (Figure 4). *Scenarios 1* and 3, however, exerted negative effects on most environmental impact categories. In *Scenario 4*, ozone formation in terrestrial ecosystems (OTe), ozone formation in human health (OHh) and marine ecotoxicity (MEco) presented negative values, which could reflect environmental benefits mainly resulting from 'avoided' emissions, either by directly reducing NOx and VOC concentrations or by indirectly avoiding electricity consumption [45,46]. The main contributing categories remained

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consistent with the baseline LCA (OHh, OTe, MEco, TE, FRS, HNCT). Nevertheless, *Human* carcinogenic toxicity (HCT) appeared in *Scenarios 1* and 3 (Figure 5), likely associated with 99A secondary emissions from industrial processes, such as those arising from energy production, metals, or combustion by-products, rather than from the use of solvents (*e.g.*, hexane or ethanol) [47,48]. Additionally, *Scenario 4* required the smallest amount of tomato discards to achieve the same level of antioxidant activity relative to the amount of lycopene extracted (Table 7) [49]. Therefore, its potential application at the pilot scale appears highly promising, given the proven scalability of ultrasound-assisted extraction, its efficiency, and its well-documented and widespread implementation at the industrial level [50-52].

4. Conclusions

This study demonstrates that the valorization of tomato discards through lycopene recovery can contribute to waste reduction and resource efficiency within sustainable food systems. The comparative LCA revealed that ultrasound-assisted extraction with ethyl acetate (*Scenario 4*) achieved the best environmental performance, primarily due to its lower energy requirements and reduced fossil resource consumption. Conversely, conventional extraction with ethyl acetate (*Scenario 2*) initially appeared as the least sustainable; however, when lycopene yield and antioxidant capacity were jointly considered, its relative performance improved substantially.

The sensitivity analysis, performed by adjusting the inputs and outputs of the four scenarios according to the antioxidant activity-to-lycopene ratio, revealed markedly different results, shifting the least favorable scenario (*Scenario 2*) to an intermediate position. This analysis proved essential for refining the interpretation of results and highlighted the importance of considering LCA as a dynamic process that incorporates feedback among different stages of analysis to improve accuracy and avoid misinterpretation. Integrating functional efficiency metrics, such as antioxidant activity, into environmental assessments enables a comprehensive evaluation of sustainability outcomes. In addition, since energy consumption represents the primary hotspot in the lycopene extraction stage, its influence was particularly evident in impact categories such as ozone formation, human non-carcinogenic toxicity, terrestrial ecotoxicity, and fossil resource scarcity, which are directly associated with electricity use and energy origin. Therefore, future improvements should prioritize substituting conventional energy sources with cleaner alternatives, such as wind power, in order to further enhance the environmental performance and overall sustainability of the lycopene recovery process.

Finally, the results of this work indicate that solvent selection and energy optimization are key levers for reducing environmental impacts in bioactive compound extraction, and that adopting green solvents together with ultrasound-assisted technologies provides a viable route toward low-impact,

circular processes that increase the added value of tomato residues while supporting sustainable food production and waste valorization.

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Authors contributions: NDC conducted the experimental work, methodology design, data interpretation and curation, and formal analysis. E.G. contributed to the conceptualization, methodology design, supervision of the experimental procedures, and data interpretation. A.G.Z. conceived the study, coordinated the research, contributed to the writing, review, and editing of the manuscript, and funding acquisition. All authors read and approved the final version of the manuscript.

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Captions to figures

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Figure 1. System boundaries, inputs, and outputs of the evaluated scenarios: Scenario 1: C-HAE: conventional extraction using hexane:acetone:ethanol (50:25:25, v/v); Scenario 2: C-EA: conventional extraction using ethyl acetate; Scenario 3: U-HAE: ultrasound-assisted extraction using hexane:acetone:ethanol (50:25:25, v/v); Scenario 4: U-EA: ultrasound-assisted extraction using ethyl acetate.

- Figure 2. Relative comparative environmental profiles of the four different scenarios. FPMF: Fine particulate matter formation; FRS: Fossil resource scarcity; FEco: Freshwater ecotoxicity; FE: Freshwater eutrophication; GW: Global warming; HCT: Human carcinogenic toxicity; HNCT: Human non-carcinogenic toxicity; IR: Ionizing radiation; L: Land use; MEco: Marine ecotoxicity; ME: Marine eutrophication; MRS: Mineral resource scarcity; OHh: Ozone formation, Human health; OTe: Ozone formation, Terrestrial ecosystems; SOD: Stratospheric ozone depletion; TA: Terrestrial acidification; TE: Terrestrial ecotoxicity; WC: Water consumption.
- Figure 3. Percentage environmental contribution of each extraction scenario based on normalized results. FPMF: Fine particulate matter formation; FRS: Fossil resource scarcity; FEco: Freshwater ecotoxicity; FE: Freshwater eutrophication; GW: Global warming; HCT: Human carcinogenic toxicity; HNCT: Human non-carcinogenic toxicity; IR: Ionizing radiation; L: Land use; MEco: Marine ecotoxicity; ME: Marine eutrophication; MRS: Mineral resource scarcity; OHh: Ozone formation, Human health; OTe: Ozone formation, Terrestrial ecosystems; SOD: Stratospheric ozone depletion; TA: Terrestrial acidification; TE: Terrestrial ecotoxicity; WC: Water consumption.
- **Figure 4.** Sensitivity analysis illustrating the relative environmental performance of the four extraction scenarios after adjusting the functional unit based on the antioxidant activity.
- Figure 5. Percentage contribution of each extraction scenario to the overall environmental impact, as determined following the sensitivity analysis. FPMF: Fine particulate matter formation; FRS: Fossil resource scarcity; FEco: Freshwater ecotoxicity; FE: Freshwater eutrophication; GW: Global warming; HCT: Human carcinogenic toxicity; HNCT: Human non-carcinogenic toxicity; IR: Ionizing radiation; L: Land use; MEco: Marine ecotoxicity; ME: Marine eutrophication; MRS: Mineral resource scarcity; OHh: Ozone formation, Human health; OTe: Ozone formation, Terrestrial ecosystems; SOD: Stratospheric ozone depletion; TA: Terrestrial acidification; TE: Terrestrial ecotoxicity; WC: Water consumption.

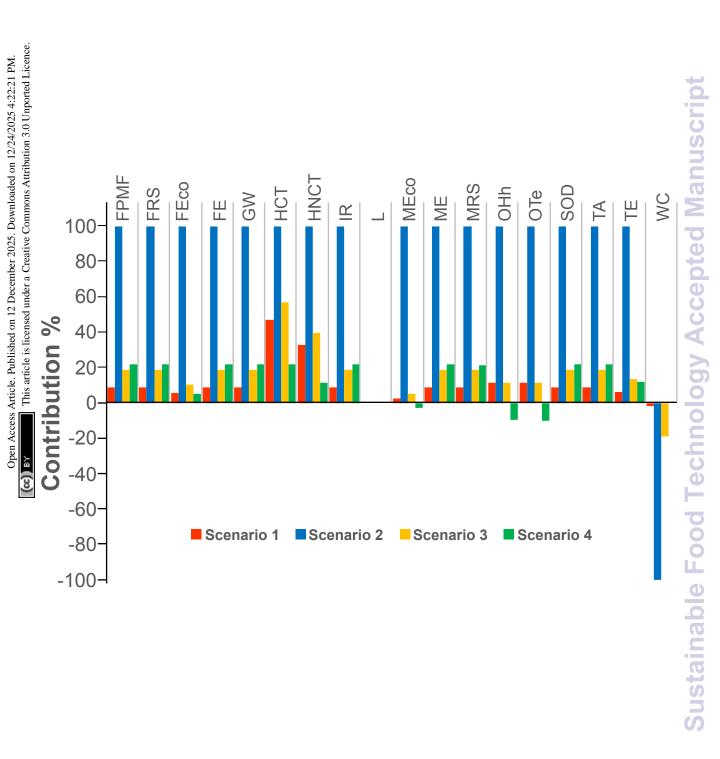


Figure 2

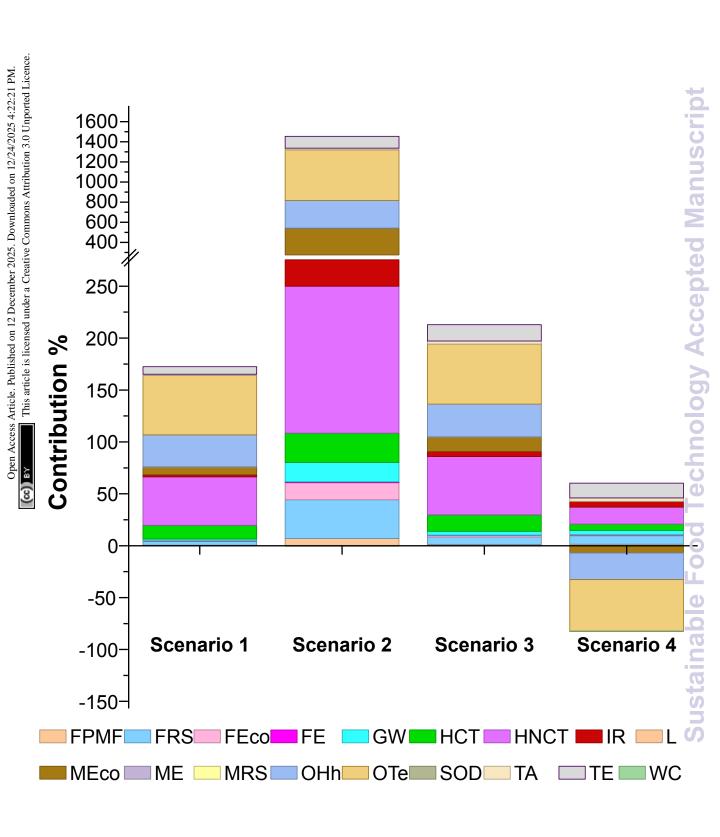
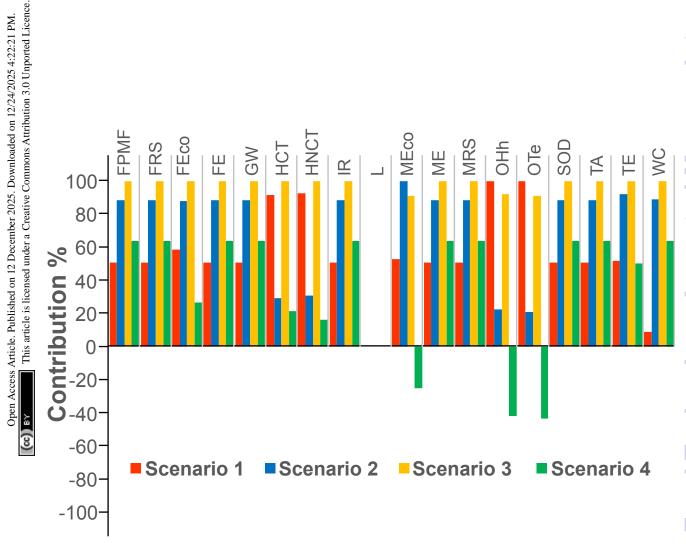


Figure 3





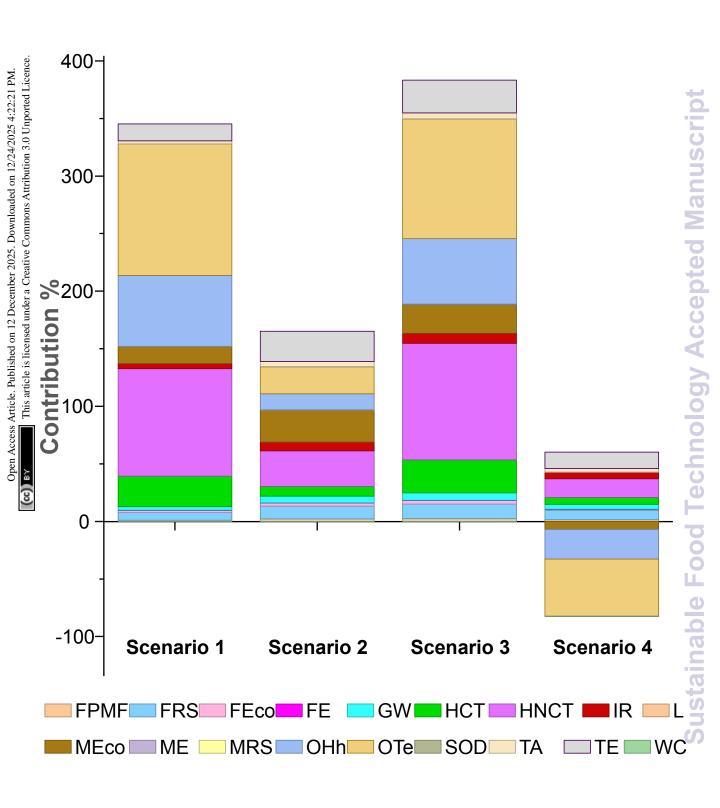


Figure 5

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Table 1. Description of different scenarios analyzed in this study.

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Scenario	Method	Solvent
1	Convectional	Hexane:Acetone:Ethanol
2	Convectional	Ethyl acetate
3	Ultrasonic	Hexane:Acetone:Ethanol
4	Ultrasonic	Ethyl acetate

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Table 2. Life cycle inventory of material and energy flows (inputs and outputs) per functional unit (1 kg of lycopene-equivalent extract) for the four process scenarios.

	Unit	Scenario 1	Scenario 2	Scenario 3	Scenario 4
Inputs					
Tomatoes pulp preparation					
Tomatoes	Kg	5214	58841	5196	5889
Electricity	MJ	6100	68844	6079	6890
Tap water	L	10428	117682	10391	11779
Lycopene extraction					
Solvent	L				
Hexane		4406		4390	
Acetone		2203		2195	
Ethanol		2203		2195	
Ethyl acetate			99441		9953
Deionized water	L	5507	62151	5488	6221
Electricity	MJ	13658	154133	37455	42455
Solvent recovery					
Lycopene in extract	Kg	2533	78933	2495	8350
Electricity	MJ	242	8200	241	821
Outputs					
Tomatoes pulp preparation					
Liquid waste	L	12158	137209	12116	13733
Organic waste	Kg	2933	33098	2923	3313
Lycopene extraction					
Organic waste	Kg	550	6214	548	621
Chemical waste	Kg	8972	62151	8941	6221
Lost Solvent	Kg				
Hexane		378		406	
Acetone					
Ethanol					
Ethyl acetate			10763		628
Solvent recovery					
Solvent	Kg	2532	78932	2494	8349
Dried lycopene	Kg	1	1	1	1

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Table 3. ReCiPe 2016 Midpoint indicators.

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Impact categories	Abbreviation	Unit
Fine particulate matter formation	FPMF	kg PM2.5 eq
Fossil resource scarcity	FRS	kg oil eq
Freshwater ecotoxicity	FEco	kg 1,4-DCB
Freshwater eutrophication	FE	kg P eq
Global warming	GW	kg CO ₂ eq
Human carcinogenic toxicity	НСТ	kg 1,4-DCB
Human non-carcinogenic toxicity	HNCT	kg 1,4-DCB
Ionizing radiation	IR	kBq Co-60 eq
Land use	L	m ² a crop eq
Marine ecotoxicity	MEco	kg 1,4-DCB
Marine eutrophication	ME	kg N eq
Mineral resource scarcity	MRS	kg Cu eq
Ozone formation, Human health	OHh	kg NOx eq
Ozone formation, Terrestrial ecosystems	OTe	kg NOx eq
Stratospheric ozone depletion	SOD	kg CFC11 eq
Terrestrial acidification	TA	kg SO ₂ eq
Terrestrial ecotoxicity	TE	kg 1,4-DCB
Water consumption	WC	m^3

Table 4. Lycopene content and antioxidant activity of tomato extracts obtained under different extraction conditions.

Scenario	Method	Solvent ^a	Concentration (UV-vis, 472nm) (mg/100g _{ww}) ^b	Concentration (HPLC) (mg/100g _{ww}) ^b	Antioxidant activity (μg Tx eq/ g _{ww})	Lycopene (μg/g _{ww})	Antioxidant activity: Lycopene	% E- isomers	% Z- isomers	E/Z
1	Convectional	H:A:E	208.2 ± 6.0 (a)	147.0 ± 39.3 (a)	734.7 ± 97.0 (c)	1470.4 ± 392.7 (a)	0.5	82.4	17.6	5.6
2	Convectional	EA	18.6 ± 0.3 (c)	18.6 ± 18.5 (b)	$630.1 \pm 49.1^{(c)}$	186.3 ± 23.3 (b)	3.4	93.6	6.4	15.4
3	Ultrasonic	H:A:E	$207.6 \pm 4.5 \ ^{\rm (a)}$	168.4 ± 18.5 (a)	$934.8 \pm 26.9 \ ^{\text{(b)}}$	1683.6 ± 185.5 (a)	0.6	75.2	24.8	3.1
4	Ultrasonic	EA	186.3 ± 3.0 (b)	117.3 ± 27.6 (a)	1187.9 ± 103.5 ^(a)	1173.3 ± 275.5 (a)	1.0	84.6	15.4	5.5

^a H:A:E: Hexane:Acetone:Ethanol; EA: Ethyl acetate

^b ww: wet weight of concentrated tomato; different letters in columns indicate significant differences (p<0.05)

Table 5. Literature review for lycopene extraction ^a

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Extraction	Sample	Solvent	Yield	Parameters	Reference
method					
UAE	Freeze-dried	Ethyl lactate/Ethyl	133 mg/100 g dw	100 mL/g S:S	[35]
	tomato pomace	acetate (7:3)		63.4°C; 20 min	
UAE	Freeze-dried	hexane/acetone/ethanol	511 mg/100 g dw	74.4:1 mL/g S:S	[36]
	tomato pulp	(50:25:25 v/v/v)		47.6°C; 45.6 min	
Non-UAE	Tomato puree	hexane/ethanol/acetone	15.8 mg/100 g w/w	25:1 S:S	[37]
(shaking)		(50:25:25 v/v/v)			

^a UAE: ultrasound-assisted extraction; v/w: volume-to-weight ratio; S:S solvent-to-sample ratio

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Table 6. Total impacts obtained with ReCiPe 2016 Midpoint from the hierarchist perspective for 1 kg of lycopene-equivalent extract obtained from tomato discards.^a DOI: 10.1039/D5FB00899A

Impact categories ^b	Unit	Scenario 1	Scenario 2	Scenario 3	Scenario 4
FPMF	kg PM2.5 eq	15.2	176.1	33.3	38.2
FRS	kg oil eq	3.2×10^3	3.7×10^4	6.9×10^3	7.9×10^3
FEco	kg 1.4-DCB	1.1	20.2	2.1	1.0
FE	kg P eq	0	1	0	0
GW	kg CO ₂ eq	1.3×10^4	1.5×10^5	2.8×10^4	3.3×10^4
HCT	kg 1.4-DCB	36.4	77.9	44.1	16.9
HNCT	kg 1.4-DCB	7.0×10^{3}	2.1×10^4	8.4×10^3	2.4×10^3
IR	kBq Co ⁻⁶⁰ eq	1.1×10^{3}	1.2×10^4	2.3×10^{3}	2.7×10^{3}
L	m ² a crop eq	0	0	0	0
MEco	kg 1.4-DCB	7.6	274.5	14.5	-7.2
ME	kg N eq	0.2	2.8	0.5	0.6
MRS	kg Cu eq	2.2	25.1	4.8	5.4
OHh	kg NOx eq	634.9	5643.1	649.6	-530.9
OTe	kg NOx eq	1.0×10^{3}	9.0×10^{3}	1.0×10^3	-8.8×10^{2}
SOD	kg CFC11 eq	2.5×10^{-3}	2.9×10^{-2}	5.5×10^{-3}	6.4×10^{-3}
TA	kg SO ₂ eq	52.5	606.4	114.8	131.5
TE	kg 1.4-DCB	7.6×10^{3}	1.2×10^5	1.6×10^4	1.5×10^4
WC	m^3	-2.3×10^{0}	-1.5×10^{2}	-2.8×10^{1}	-3.2×10^{1}

^a Bold rows indicate the most impactful categories

^b FPMF: Fine particulate matter formation; FRS: Fossil resource scarcity; FEco: Freshwater ecotoxicity; FE: Freshwater eutrophication; GW: Global warming; HCT: Human carcinogenic toxicity; HNCT: Human non-carcinogenic toxicity; IR: Ionizing radiation; L: Land use; MEco: Marine ecotoxicity; ME: Marine; eutrophication; MRS: Mineral resource scarcity; OHh: Ozone formation, Human health; OTe: Ozone formation, Terrestrial ecosystems; SOD: Stratospheric ozone depletion; TA: Terrestrial acidification; TE: Terrestrial ecotoxicity; WC: Water consumption

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Table 7. Inputs and outputs used in the sensitivity analysis after adjusting the functional unit according to the antioxidant activity-to-lycopene ratio.

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	Unit	Scenario 1	Scenario 2	Scenario 3	Scenario 4
Inputs					
Tomatoes pulp preparation					
Tomatoes	Kg	10428	17652	9352	5889
Electricity	MJ	12200	20653	10942	6890
Tap water	L	20855	35304	18704	11779
Lycopene extraction					
Solvent	L				
Hexane		8811		7903	
Acetone		4406		3951	
Ethanol		4406		3951	
Ethyl acetate			29832		9953
Deionized water	L	11014	18645	9878	6221
Electricity	MJ	27315	46240	67419	42455
Solvent recovery					
Lycopene in extract	Kg	5066	23680	4491	8350
Electricity	MJ	484	2460	434	821
Outputs					
Tomatoes pulp preparation					
Liquid waste	L	24316	41163	21808	13733
Organic waste	Kg	5866	9929	5261	3313
Lycopene extraction					
Organic waste	Kg	1099	1864	986	621
Chemical waste	Kg	17944	18645	16094	6221
Lost Solvent	Kg				
Hexane		757		731	
Acetone					
Ethanol					
Ethyl acetate			3229		628
Solvent recovery					
Solvent	Kg	5064	23680	4490	8349
Dried lycopene	Kg	2	0.3	1.8	1

Data availability: The data supporting the findings of this study are included within the article. Additional datasets related to the analytical determinations and LCA calculations are available from the corresponding author upon reasonable request.

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