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Determination of 3 monochloropropane-1,2-diol (3-MCPD) and 1,3-Dichloropropan-2-ol (1,3-DCP) levels in edible vegetable oils: A health risk assessment for Iranian consumers



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ABSTRACT

As food toxicants, 3-monochloropropane-1,2-diol (3-MCPD) and 1,3-Dichloropropan-2-ol (1,3-DCP) are potentially carcinogenic and/or genotoxic chemicals formed during high-temperature refining of vegetable oils. We examined 45 edible vegetable oil samples (i.e. sunflower, rapeseed, corn, olive, and sesame oils) randomly collected from Iran market (3 batches \times 3 brands \times 5 types of vegetable oils = 45 samples) for the presence of 3-MCPD and 1,3-DCP by chromatography-mass spectrometry (GC–MS). Our results showed statistically significant associations between the mean concentration of 3-MCPD and 1,3-DCP and the type of vegetable oils, while no significant differences in either chloropropanol mean level among the brands were found. Sesame and corn oils had respectively the highest and lowest mean concentration of 3-MCPD and 1,3-DCP. Based on the probabilistic scenario, Hazard Index (HI) values calculated for 3-MCPD and 1,3-DCP levels indicated no major risk (HI < 1.0) to Iranian consumers. Nonetheless, to protect the consumers, understanding the dynamics of processes that contribute to contaminants' formation, providing online real-time methods for monitoring reactions that lead to their production, developing new technologies to mitigate the occurrence of such chemicals while maintaining food safety and sensory properties, seem necessary.

1. Introduction

The compounds 3-monochloropropane-1,2-diol (3-MCPD, $C_3H_7ClO_2$) and 1,3-Dichloropropan-2-ol (1,3-DCP, $C_3H_6Cl_2O$) are found in acid-hydrolyzed vegetable proteins. The colorless liquid 3-MCPD with pleasant odor is soluble in various solvents including alcohol, diethyl ether, water, and acetone and 1,3-DCP is highly soluble in water. Free 3-MCPD was discovered in foods with low water activity that had been heat-treated in the presence of fat such as glycerol, allyl alcohol, lipids, hydrochloric acid, and carbohydrates. 1,3-DCP is formed during the production and treatment of foodstuffs like oil, bakery, toasted, roasted, and meat products, soy sauce, and acid-hydrolyzed vegetable proteins

[18].

In terms of carcinogenicity, as per the International Agency for Research on Cancer (IARC), free 3-MCPD and 1,3-DCP are classified as Group 2B (possibly carcinogenic to humans) [18]. The presence of these compounds in human diet is a concern due to their toxicological properties. Although scarce data is available on their toxicity in humans, their untoward effects have been observed *in vitro* and *in vivo*; several studies indicated that free 3-MCPD and 1,3-DCP produce neurotoxicity, reproductive toxicity, renal toxicity, cardiotoxicity, genotoxicity, and carcinogenicity [18,22,27,41]. In this regard, the Joint World Health Organization/Food and Agriculture Organization (FAO/WHO) Expert Committee on Food Additives (JECFA) suggested a tolerable daily intake

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Fig. 1. Diagram of sample collection (A, B and C are randomly chosen to represent the brand names).

(TDI) or provisional maximum tolerable daily intake (PMTDI) of 0.004 mg/kg body weight (bw)/day for 3-MCPD and 1,3-DCP [37,39], while the European Food Safety Agency (EFSA) suggests a TDI of < 0.002 mg/ kg bw/day [6,19]. According to the findings, short-term exposure to 3-MCPD at levels greater than 1 mg/kg bw/day can result in decreased sperm motility and male fecundity in rats. Higher doses were associated with longer treatment durations and a decrease in sperm count as well as histopathological changes in the testis and epididymis [6]. BMD analysis using model averaging revealed a BMDL₁₀ of 0.20 mg/kg bw/day in male rats, which was chosen as the new reference point for renal effects in relation to the increased incidence of kidney tubular hyperplasia [5,9]. A BMDL₀₅ of 0.44 mg/kg bw/day was calculated for the effects on male fertility with decreased sperm motility chosen as the most sensitive relevant endpoint [6]. The reference point was thought to protect against effects on male fertility and to derive an updated group TDI of 0.002 mg/kg bw/ day for these chemicals and its fatty acid esters. In the adult population, the TDI of 0.002 mg/kg bw/ day is not exceeded [19].

New developments in food processing designed to produce safe foods while maintaining their nutritional and sensory qualities, are originated from the growing consumer demand for food that is healthy, varied, nutritious, and convenient. New processing methods include food irradiation, pulsed electric field, ohmic heating, and biotechnology. High hydrostatic pressure treatment, also known as high pressure pasteurization or high-pressure processing, has also been evaluated within the European Union (EU). One of the primary goals of food processing is to improve chemical and microbiological food safety, such as by removing toxic components. Other desired effects include longer storage times, improved texture and flavor, and lessening negative nutritional effects like inactivating digestive enzyme inhibitors [10,31,34].

The undesired substances 3-MCPD and 1,3-DCP can be produced during industrial processes performed on edible oils [3]. Such compounds are specially produced during the deodorization step which includes application of super-heated water steam into vegetable oil [11,28]. In this regard, a positive correlation between the temperature applied in the deodorization step and the concentration of 3-MCPD content was reported [13].

Because of its inherent natural variability, the probabilistic method can be a useful predictive tool for getting an indirect estimate of dietary exposure or risk assessment. Due to its robustness, a Monte Carlo Simulation (MCS) method which can examine the uncertainties associated with various health risks for probabilistic estimation, has received increasing attention [17,30].

3-MCPD was found to induce nephrotoxic effects (e.g. renal tubular hyperplasia) and reproductive toxicity (i.e. male antifertility effects), as well as carcinogenic effects. In food industry, several strategies have been introduced to mitigate the occurrence of these chemicals including controlling the deodorization temperature, adding chelating agents, changing the processing conditions, etc. However, these potential mitigation strategies often do not yield favorable results when used in full-scale refining. Physical refining strategies were most successful in mitigating glycidyl esters, but has been less effective on 3-MCPD [23]. Over the past decades, numerous studies and investigations have been conducted on the occurrence and exposure to free 3-MCPD. Nevertheless, few studies similar to the present work, have determined and compared 3-MCPD and 1,3-DCP levels in different oil types and conducted probabilistic risk assessment of oral exposure to these compounds. Of note, we found no comprehensive study on the occurrence of these chemicals in different vegetable oils (i.e. sunflower, rapeseed, corn, olive, and sesame oils) from various brands names marketed in Iran.

The objectives of this study were determination of the concentration of 3-MCPD and 1,3-DCP in 45 vegetable oils (i.e. sunflower, rapeseed, corn, olive, and sesame oils) available in Iran market, a preliminary dietary exposure assessment and MCS identification of the potential health risks associated with chloropropanol exposure through oral exposure to the vegetable oils.

2. Materials and methods

2.1. Chemicals and reagents

The standards of 3-MCPD (CAS Number 96–24-2) (98%) and 1,3-DCP (CAS Number 96–23-1) (97%) were purchased from Sigma– Aldrich (Steinheim, Germany). Trimethylsilyl trifluoromethanesulfonate (TMSOTf), hexamethyldisilazane (HMDS), 1,5pentanediol, ethyl acetate, and dichloromethane were supplied from Sigma–Aldrich. Their purity was not<99%. All the reagents were of high-performance liquid chromatography (HPLC) grade.

2.2. Sampling

A total of 45 vegetable oil (five types i.e. sunflower, rapeseed, corn, olive, and sesame oils) samples (from three brand names) were randomly collected from Iran retail market and analyzed. (5 types of vegetable oils \times 3 brands \times 3 batches = 45 samples) (Fig. 1). The vegetable oils were stored at room temperature (25 °C) until analyzed by chromatography-mass spectrometry (GC–MS).

Table 1

Recoveries (%), relative standard deviation (RSD, %), correlation coefficients (R²), limit of detection (LOD) and limit of quantification (LOQ) (mg/kg) of 3-MCPD and 1,3-DCP (mg/kg) level determination.

Sample	Spiked concentration (mg/kg) 3-MCPD		RSD%	R ² Spiked concentration (mg/kg)		RSD%	\mathbb{R}^2	LOD	LOQ	
					1,3-DCP					
	0.5	1			0.5	1				
Sunflower oil	93.2	99.1	(2.1)	0.994	92.5	99.4	(2.0)	0.995	0.001	0.003
Rapeseed oil	90.5	95.3	(4.3)	0.962	90.3	94.5	(3.5)	0.960	0.001	0.003
Corn oil	92.4	97.0	(3.5)	0.965	93.0	98.4	(2.5)	0.983	0.001	0.003
Olive oil	91.3	96.5	(3.1)	0.973	92.4	97.2	(3.2)	0.980	0.001	0.003
Sesame oil	90.0	94.5	(4.2)	0.963	93.1	98.0	(4.0)	0.995	0.001	0.003

2.3. Sample preparation

Using trimethylsilyl (TMS) derivatization with TMSOTf as the catalyst and hexamethyldisilazane as the derivatizing agent, 3-MCPD and 1,3-DCP in vegetable oils were analyzed [20,39]. In brief, the sample (2.0 g) was weighed and added to an aluminum oxide (8.0 g)-filled centrifuge tube (50.0 mL). The surrogate standard (1.00 mg/L of 1,5pentanediol) was added to the mixture after the sample was homogenized. The samples were repeatedly spiked with 0.5 and 1.0 mg/kg of each of the chloropropanols to assess recovery. After some gentle mixing, the sample was put into a glass chromatography column (diameter 2 cm and length 40.0 cm) and a sintered disc with zero porosity. Before addition of the sample, 1.0 g of anhydrous sodium sulfate and 1.0 g of cotton wool that had been dichloromethane-soaked, were loaded into the column. At a flow rate of 8.0 mL/min, dichloromethane was eluted from the glass chromatography column. Purified nitrogen gas was then used to concentrate the collected eluent until it was nearly dry. The extract was then immediately mixed with 1.0 mL of ethyl acetate. For derivatization, TMSOTf (10.0 µL) and hexamethyldisilazane (50.0 µL) were added to the ethyl acetate mixture. A vortex shaker was used to seal the mixture-filled sample vial and shake it for 30 sec. For 10 min, the derivatization process was carried out at room temperature (25 $^\circ\text{C}).$ Water (1.0 mL) was then added to the vial and vortexed for 30 sec to conclude derivatization. Before performing quantitative gas chromatography-mass spectrometry (GC-MS) measurements, the organic layer was moved to a GC vial and a small amount of sodium sulfate was added to dry it out [20,39].

2.4. GC-MS analysis

An Agilent, Santa Clara, USA quadrupole GC–MS instrument with a DB-5MS capillary column (30 m length, 0.23 mm diameter, and 0.25 μ m film thickness) was used. In split-less mode, the derivatized sample (1.0 μ L) was injected into the oven. The GC oven was monitored as follows: the inlet temperature was set to 270 °C, kept at 60 °C for 2 min, increased to 120 °C at a rate of 5 °C/min, increased to 300 °C for 2 min, increased to 120 °C at a rate of 5 °C/min, increased to 300 °C dat a rate of 30 °C/min, and then kept at 300 °C for 8 min. At a flow rate of 1.0 mL/min, purified nitrogen was selected as the carrier gas. The total temperature program took about 12 min to complete. Additionally, the *m*/z values of the characteristic ions chosen for the qualification of 3-MCPD-TMS were 116, 119, and 147, while the *m*/z values of the characteristic ions chosen for 1,3-DCP-TMS were 93, 151, and 154. The characteristic ions chosen for the quantification of 3-MCPD-TMS was carried out in the single-ion monitoring (SIM) mode for peak confirmation [31].

2.5. Method validation

The method's limits of detection and quantification (LOD and LOQ, respectively) were estimated using EURACHEM guidelines [8]. Blanks were used to calculate the LOD and LOQ with a signal-to-noise ratio of 3.0 and 10.0 (S/N = 3 and 10), respectively. The spiked calibration curves were used to calculate the method's recovery. Samples were

spiked with 0.5 and 1.0 mg/kg of both 3-MCPD and 1,3-DCP and triplicate to determine the recovery.

2.6. Estimation of dietary exposure and risk assessment

The estimated daily intake (EDI, mg/kg bw) exposure to 3-MCPD and 1,3-DCP. The Eq. (1) was used to determine the EDI of 3-MCPD and 1,3-DCP via consumption of the analyzed vegetable oils:

$$EDIi = \frac{F \times C}{BW} \tag{1}$$

In this equation, concentration (C) is the level of 3-MCPD and 1,3-DCP (mg of 3-MCPD or 1,3-DCP/ kg vegetable oil), and F is the daily consumption of vegetable oils (0.04 kg/day) [14,33]. The average bw for the Iranian adult population was considered 70 kg [32].

The ratio of EDI to the exposure dose at which adverse health effects are expected is known as the target hazard quotient (THQ). The TDI of 0.002 mg/kg bw/day, as recommended by EFSA [6], and the estimated daily intakes of 3-MCPD and 1,3-DCP to determine the potential risk to human health. The THQ calculated for 3-MCPD and 1,3-DCP was used to calculate the Hazard Index (HI) (Eq. (2) [29].

$$HI = \sum_{i=1}^{n} THQ_i \tag{2}$$

A THQ < 1 represents no adverse health effects following exposure while a THQ greater than 1, indicates adverse health effects [7].

2.7. Probabilistic risk assessment approach

The third parameters from the preliminary results were fitted with a suitable distribution prior to the MCS, and a Kolmogorov–Smirnov (K-S) test using JMP 8 software (Campus Drive, Cary, NC 27513) was used to evaluate the goodness of fit. The log-normal distribution served for the statistical distributions of the parameters that were taken into consideration. These individual exposure variable distributions were used as input parameters in the MCS technique to calculate Equation's probability functions for human daily exposures. In this study, the MCS was run for 10,000 iterations. The MCS, which provides a comprehensive description of the probabilities of various risk levels, was used to determine the process of determining the mean as well as the various percentiles of the exposure distributions [21].

According to the EFSA framework for non-detected results, when values are below the LOD, they are considered either (I) the LOD (upper bound), (II) zero (lower bound), or (III) LOD/2 (medium bound) [4]. In this study, we used the middle bound.

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2.8. Statistical analysis

GraphPad Prism 9.0 (GraphPad Software, San Diego, CA, USA) was used to statistically analyze the mean concentration of 3-MCPD and 1,3-DCP in collected vegetable oil samples. Means were compared by posttest for parametric data. The statistical significance was determined



Fig. 2. Comparison of the mean concentration of 3-MCPD in the vegetable oil samples of different brands. * Shows a significant difference at P < 0.05.



1,3-DCP

Fig. 3. Comparison of the mean concentration of 1,3-DCP in the vegetable oil samples of different brands.* Shows a significant difference at P < 0.05.

with a *p*-value of < 0.05.

3. Results and discussion

3.1. Method validation

Table 1 shows that 3-MCPD and 1,3-DCP were added to each of the matrices at two concentrations of 0.5 and 1.0 mg/kg. With a relative standard deviation (RSDs %) of <4.3%, the average recovery of 3-MCPD was 90.5–99.1%. Using the calibration plot, we calculated 3-MCPD and 1,3-DCP coefficients of determination (R^2) which was 96.0–99.5%. Based on signal-to-noise ratios of 3.0 and 10.0, the LOD and LOQ were respectively 0.001 and 0.003 mg/kg (Table 1).

3.2. Mean concentration of 3-MCPD and 1,3-DCP in the vegetable oil samples

To the best of our knowledge, this study is the first to assess the risk of oral exposure to 3-MCPD and 1,3-DCP through consumption of edible vegetable oils (collected from Iranian markets) for Iranian consumers. Along with the mean levels of 3-MCPD and 1,3-DCP are mentioned in Figs. 2 and 3. There was a statistically significant difference in the mean concentration of 3-MCPD and 1,3-DCP among the different types of vegetable oils, while no significant associations between the brands and the levels of these chemicals were observed (P = 0.43 and 0.169 for 3-MCPD and 1,3-DCP, respectively). The mean level of 3-MCPD in vegetable oil samples ranged from the LOD (0.001 mg/kg) to 0.60 \pm 0.0.05 mg/kg (Fig. 2). Also, mean levels of 1,3-DCP in oil samples were in the



Fig. 4. Correlation between 3-MCPD and 1,3-DCP levels in samples in which both analytes were at levels above LOQ.

range of LOD to $0.043 \pm 0.0.01 \text{ mg/kg}$ (Fig. 3). Sesame and corn oils had respectively the highest and lowest mean concentration of 3-MCPD and 1,3-DCP. The spectra of 3-MCPD and 1,3-DCP compounds in the oil samples are presented in Figs S1-S15.

The relationship between the concentrations of 3-MCPD and 1,3-DCP in samples where they were both at levels above LOQ was assessed by Spearman correlation coefficient. We found a correlation coefficient between the concentrations of 3-MCPD and 1,3-DCP of 0.819 (Fig. 4).

For co-occurrence of 3-MCPD and 1,3-DCP in glycerol, correlation coefficients of 0.72 by[2] and 0.52 by[41] have been reported. In the present study, this co-occurrence had a correlation coefficient of 0.819 (Fig. 4).

3-MCPD and 1,3- DCP have been detected in acid-hydrolyzed vegetable proteins. 3-MCPD which is found in heat-processed food, refined oil, and the environment. Occurrence of 1,3- DCP in processed food (e.g. products of baking, toasting and roasting) as well as the water samples from plants that employ epichlorohydrin-linked cationic polymer resin, have been reported. Considering the untoward effects of these chemicals, a maximum level of 0.02–1.0 mg/kg in acid-hydrolyzed vegetable proteins and soy sauce has been regulated by the USA, European Union, China, and Korea [41].

The toxicological effects of 3-MCPD have been the subject of extensive research. The kidney is the primary target of toxicity in rats and mice, with effects on male fertility also observed [15]. In terms of reproductive toxicity, it was demonstrated that 3-MCPD inhibits male fertility [1].

Chloropropanols level is strongly influenced by temperature, lipid, glycerol, and water content. It was reported that high concentrations of 3-MCPD found in some canned vegetable products may be due to differences in the composition of the analyzed matrices and the high temperature of the production process [12]. The characteristics of the substrate, such as the composition of the lipids and the hydrolytic activity and selectivity (including substrate specificity) of the enzymes, as

well as the use of glycerol as a precursor, are found to affect the quantity of chloropropanols produced. However, more research is required to clarify the precise mechanisms and key intermediates involved in the formation of 3-MCPD and 1,3-DCP [40]. A report from Germany stated mean 3-MCPD concentrations of 1000 and 1400 ng/g in refined oils and margarine, respectively [35]. The concentration of these chemicals was higher in our study. 3-MCPD in vegetable oils is formed by the hydrolysis of triglycerides during the refining process. The hydrolysis is caused by high temperatures and strong acids or bases, which can break down the triglyceride molecules into their component fatty acids and glycerol [25,36].

3.3. Health risk assessment

The deterministic values of THQ are presented in Table 2. The total HI values for oral exposure to 3-MCPD and 1,3-DCP via consumption of the analyzed samples, were lower than 1 (i.e. 3.03×10^{-2} and 7.98×10^{-3} , respectively), indicating no risk to consumers' health (Table 2). Under probabilistic scenario, the MCS model results showed that exposure to 3-MCPD and 1,3-DCP at three centiles (50th, 80th, and 95th) were below one. The HI values for exposure to 3-MCPD were 3.94×10^{-2} , 8.44×10^{-2} , and 1.76×10^{-1} , respectively at the 50th, 80th, and 95th centiles. Considering 1,3-DCP mean concentration in vegetable oils, at the 50th, 80th, and 95th centiles, HIs were 9.72×10^{-3} , 1.85×10^{-2} , and 2.44×10^{-2} , respectively (Table 3).

These methods that are implemented in different steps of the production include gumming, neutralization of the oil, bleaching with synthetic magnesium silicate, addition of various antioxidants, doubledeodorization, implementation of a longer deodorization time, use of enzymes, absorbents, and rebleaching of the oil and treatment with calcinated zeolite [24].

To diminish the levels of chloropropanols in food, and thus, reduce the level of human exposure, various methods including adding rosemary extract, despite leaving a strong scent in the oil [42], use of a shortpath distillation, using a vacuum to reduce the boiling point of these chloropropanols, and use of contaminant adsorbents such as activated carbon or bleaching clays have been developed. However, much efforts need to be made to decrease chloropropanols occurrence while maintaining the desired quality of the food [26].

The following uncertainties should be noted regarding the current work: (a): ingestion rate data used in this study was from the Institute of Standards and Industrial Research of Iran [14] and in real life, it may have evolved over time; and (b): undetected values of 3-MCPD and 1,3-DCP may have influenced our overall calculations (see Figs. 5 and 6).

Nonetheless, to protect the consumers, understanding the dynamics of major processing that produce contaminants, providing online realtime methods for monitoring reactions that lead to contaminant formation, developing new processing technologies to mitigate contaminants while maintaining the food's safety and sensory properties are all necessary.

Table 2

Deterministic THQ values for 3-MCPD and 1,3-DCP in vegetable oil samples.

Sample	3-MCPD			HI (3-MCPD)	1,3-DCP			HI (1,3-DCP)
	Brand A	Brand B	Brand C		Brand A	Brand B	Brand C	
Sunflower oil Rapeseed oil Corn oil Olive oil Sesame oil HI (Total)	$\begin{array}{c} 3.47\times 10^{-3}\\ 1.38\times 10^{-2}\\ 1.58\times 10^{-3}\\ 3.86\times 10^{-3}\\ 1.70\times 10^{-1} \end{array}$	$\begin{array}{c} 3.45 \times 10^{\cdot3} \\ 2.10 \times 10^{\cdot2} \\ 9.53 \times 10^{\cdot3} \\ 2.50 \times 10^{\cdot3} \\ 2.56 \times 10^{\cdot2} \end{array}$	$\begin{array}{c} 1.27\times10^{-2}\\ 1.71\times10^{-2}\\ 1.80\times10^{-3}\\ 1.43\times10^{-2}\\ 1.52\times10^{-1} \end{array}$	$\begin{array}{c} 6.56\times 10^{-3}\\ 1.73\times 10^{-2}\\ 4.31\times 10^{-3}\\ 6.91\times 10^{-3}\\ 1.16\times 10^{-1}\\ \textbf{3.03}\times \textbf{10^{-2}}\end{array}$	$\begin{array}{c} 2.85 \times 10^{\cdot3} \\ 7.14 \times 10^{\cdot3} \\ 1.42 \times 10^{\cdot3} \\ 1.42 \times 10^{\cdot3} \\ 1.22 \times 10^{\cdot2} \end{array}$	$\begin{array}{c} 3.14 \times 10^{-3} \\ 1.71 \times 10^{-2} \\ 8.57 \times 10^{-3} \\ 1.42 \times 10^{-3} \\ 1.42 \times 10^{-2} \end{array}$	$\begin{array}{c} 8.57 \times 10^{\cdot 3} \\ 1.57 \times 10^{\cdot 2} \\ 1.42 \times 10^{\cdot 3} \\ 1.17 \times 10^{\cdot 2} \\ 1.14 \times 10^{\cdot 2} \end{array}$	$\begin{array}{c} 4.85\times10^{-3}\\ 1.33\times10^{-2}\\ 3.80\times10^{-3}\\ 4.85\times10^{-3}\\ 1.26\times10^{-2}\\ \textbf{7.98}\times10^{-3}\end{array}$

HI: Hazard index.

Table 3

Probabilistic THQ values at the 50th, 80th, and 95th centile for 3–3-MCPD and 1,3-DCP in vegetable oil samples.

Sample	3-MCPD			HI (3-MCPD)	1,3-DCP			HI (1,3-DCP)
	Brand A	Brand B	Brand C		Brand A	Brand B	Brand C	
Sunflower oil								
50th	$4.51\times10^{\text{-}3}$	$4.50 imes10^{-3}$	$1.66 imes 10^{-2}$	$8.53\times10^{\text{-}3}$	$3.51\times 10^{\text{-}3}$	$3.86\times 10^{\text{-}3}$	$1.05 imes10^{-2}$	$5.97\times10^{\text{-}3}$
80th	$9.67 imes10^{-3}$	$9.62 imes10^{-3}$	$3.56 imes 10^{-2}$	$1.83 imes10^{-2}$	$6.70 imes10^{-3}$	$7.36 imes10^{-3}$	$2.00 imes10^{-2}$	$1.13 imes10^{-2}$
95th	$2.01 imes10^{-2}$	$2.00 imes10^{-2}$	$7.42 imes 10^{-2}$	$3.81 imes 10^{-2}$	$8.83 imes10^{-3}$	$9.71 imes10^{-3}$	$2.65 imes 10^{-2}$	$1.50 imes 10^{-2}$
Rapeseed oil								
50th	$1.80 imes10^{-2}$	$2.73 imes10^{-2}$	$2.23 imes10^{-2}$	$2.25 imes10^{-2}$	$8.78\times10^{\text{-}3}$	$2.10 imes10^{-2}$	$1.93 imes10^{-2}$	$1.64 imes 10^{-2}$
80th	$3.86 imes 10^{-2}$	$5.85 imes10^{-2}$	$4.80 imes 10^{-2}$	$4.83 imes10^{-2}$	$1.67 imes10^{-2}$	$4.01 imes 10^{-2}$	$3.68 imes 10^{-2}$	$3.12 imes10^{-2}$
95th	$8.05 imes 10^{-2}$	$1.22 imes10^{-1}$	$1.00 imes10^{-1}$	$1.00 imes10^{-1}$	$2.20 imes10^{-2}$	$5.30 imes10^{-2}$	$4.85 imes 10^{-2}$	$4.12 imes10^{-2}$
Corn oil								
50th	$2.06 imes10^{-3}$	$1.23 imes10^{-2}$	$2.35 imes10^{-3}$	$5.60 imes 10^{-3}$	$1.75 imes10^{-3}$	$1.05 imes10^{-2}$	$1.75 imes10^{-3}$	$4.68 imes 10^{-3}$
80th	$4.42 imes10^{-3}$	$2.65 imes 10^{-2}$	$5.04 imes10^{-3}$	$1.20 imes10^{-2}$	$3.34 imes10^{-3}$	$2.00 imes10^{-2}$	$3.34 imes10^{-3}$	$8.92 imes10^{-3}$
95th	$9.22 imes 10^{-3}$	$5.54 imes10^{-2}$	$1.05 imes 10^{-2}$	$2.50 imes10^{-2}$	$4.41 imes 10^{-3}$	$2.65 imes10^{-2}$	$4.41 imes 10^{-3}$	$1.17 imes10^{-2}$
Olive oil								
50th	$5.02 imes10^{-3}$	$3.25 imes10^{-3}$	$1.86 imes 10^{-2}$	$9.00 imes10^{-3}$	$1.75 imes10^{-3}$	$1.75 imes10^{-3}$	$1.44 imes10^{-2}$	$5.97 imes10^{-3}$
80th	$1.07 imes10^{-2}$	$6.96 imes10^{-3}$	$4.00 imes 10^{-2}$	$1.92 imes 10^{-2}$	$3.34 imes10^{-3}$	$3.34 imes10^{-3}$	$2.74 imes10^{-2}$	$1.13 imes10^{-2}$
95th	$2.24 imes10^{-2}$	$1.45 imes 10^{-2}$	$8.35 imes 10^{-2}$	$4.01 imes 10^{-2}$	$4.41 imes 10^{-3}$	$4.41 imes10^{-3}$	$3.62 imes 10^{-2}$	$1.50 imes10^{-2}$
Sesame oil								
50th	$2.22 imes10^{-1}$	$3.33 imes10^{-2}$	$1.98 imes10^{-1}$	$1.51 imes10^{-3}$	$1.51 imes10^{-2}$	$1.75 imes10^{-2}$	$1.40 imes10^{-2}$	$1.55 imes10^{-2}$
80th	$4.76 imes 10^{-1}$	$7.14 imes10^{-2}$	$4.25 imes 10^{-1}$	$3.24 imes10^{-1}$	$2.87 imes10^{-2}$	$3.34 imes10^{-2}$	$2.67 imes10^{-2}$	$2.96 imes10^{-2}$
95th	$9.92 imes10^{-1}$	$1.48 imes10^{-1}$	$8.87\times10^{\text{-}1}$	$6.76 imes10^{-1}$	$3.80 imes10^{-2}$	$4.41 imes 10^{-2}$	$3.53 imes10^{-2}$	$3.91 imes10^{-2}$
HI 50th (Total)				$3.94 imes10^{-2}$				$9.72 imes10^{-3}$
HI 80th (Total)				$8.44 imes10^{-2}$				$1.85 imes10^{-2}$
HI 95th (Total)				$1.76 imes10^{-1}$				$2.44 imes 10^{-2}$

HI: Hazard index.



Fig. 5. Parameters (%) influencing THQ calculated for 3-MCPD. (C) Mean concentration of 3-MCPD in vegetable oils, (F) Daily consumption of vegetable oils and (bw) body weight.

4. Conclusions

In this work, we assessed the health risk associated with oral exposure to 3-MCPD and 1,3-DCP via consumption of vegetable oils by Iranian consumers was assessed. The mean levels of 3-MCPD and 1,3-DCP showed statistically significant variations among different types of vegetable oils, while no significant associations between the brands and the levels of these chemicals were observed. Sesame and corn oils had the highest and lowest mean concentration of 3-MCPD and 1,3-DCP, respectively. The risks reflected as total HI values of 3-MCPD and 1,3-DCP, respectively. The risks reflected as total HI values of 3-MCPD and 1,3-DCP were < 1.0 in both deterministic and probabilistic mathematical methods. Therefore, we found that increased daily consumption of these matrices can directly enhance the risk. The growing concern associated with the toxicity of chloropropanols, necessitates periodical monitoring of food stuff prone to occurrence of these chemicals. In parallel, policy measures should be adopted to minimize the intake of 3-MCPD and 1,3-DCP.

1,3-DCP



Fig. 6. Parameters (%) influencing THQ calculated for1,3-DCP. (C) Mean concentration of 1,3-DCP in vegetable oils, (F) Daily consumption of vegetable oils and (bw) body weight.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.microc.2023.108946.

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