Recommendations for Oil Extraction and Refining Process to Prevent the Formation of Monochloropropane-diol Esters in Sunflower Oil

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Table S1: Phosphatidylcholine levels at various stages of the refining process of a solvent extracted cake oil

Type of Oil	dipalmitoyl-PC	palmitoyl-oleoyl-PC	dioleoyl-PC	palmitoyl-linoleoyl-PC (PA ratio)	oleoyl-linoleoyl-PC	dilinoleoyl-PC	Sum of PC
SE cake oil	0.07	2.31	13.32	6.25	7.21	17.95	47.11
Deg. SE cake oil	0.00	0.00	0.02	0.00	0.01	0.01	0.04
1-week cooling SE cake oil	0.03	1.23	7.15	3.37	4.07	10.34	26.19
1-week cooling Deg. SE cake oil	0.00	0.00	0.07	0.03	0.04	0.08	0.23

SUPPLEMENTAL FIGURE CAPTIONS

Figure S1: Relative abundance of reported discovered chlorine carrying substances (see Table 1, ion $[M-H]^-$) and levels of sunflower major MCPD diesters formed during the in-vitro heat treatment of crude sunflower oil.

Figure S2: Distribution of chlorine-carrying substances identified in negative ionization mode (A) in various bio sunflower oil fractions.

(peak areas were all normalized to OLL peak area)

Figure S3: Distribution of major MCPDEs (LL, OL, PL, OO) in various bio sunflower oil fractions.

(peak areas were all normalized to their deuterated ISTD peak area)

Figure S4: Relative distribution of chlorine carriers class A (A); class B (B); class C (C) and class D (D) along the sunflower refining process. The sum of each carrier class was taken into account and normalized to their internal standard nicarbazin.

Process step identity: A (Crude); B (Degummed); C (Degummed short cooling); D (Degummed short cooling bleached); E (Degummed bleached short cooling); F (Degummed bleached)

Figure S5: Total 2-MCPD (A) and glycidol content (B) along the sunflower refining process.

Process step identity: A (Crude); B (Degummed); C (Degummed short cooling); D (Degummed short cooling bleached); E (Degummed bleached short cooling); F (Degummed bleached)

SUPPLEMENTAL FIGURES

Figure S1

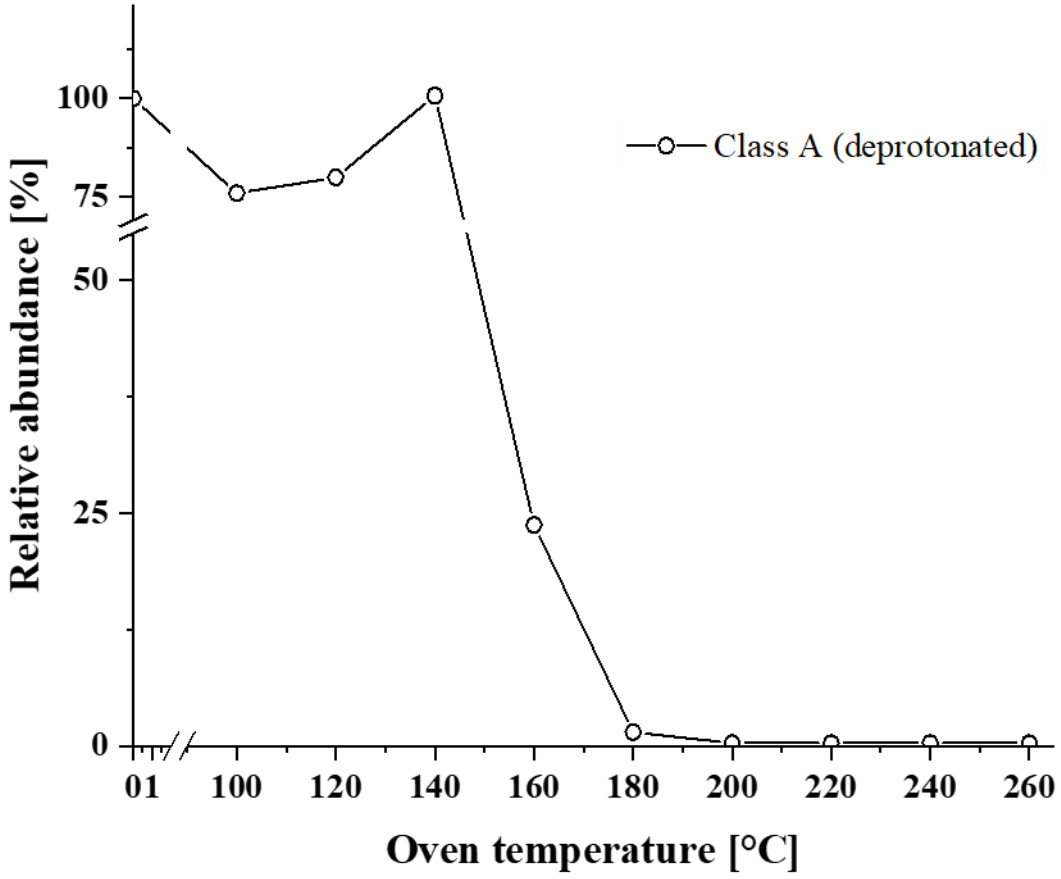


Figure S2

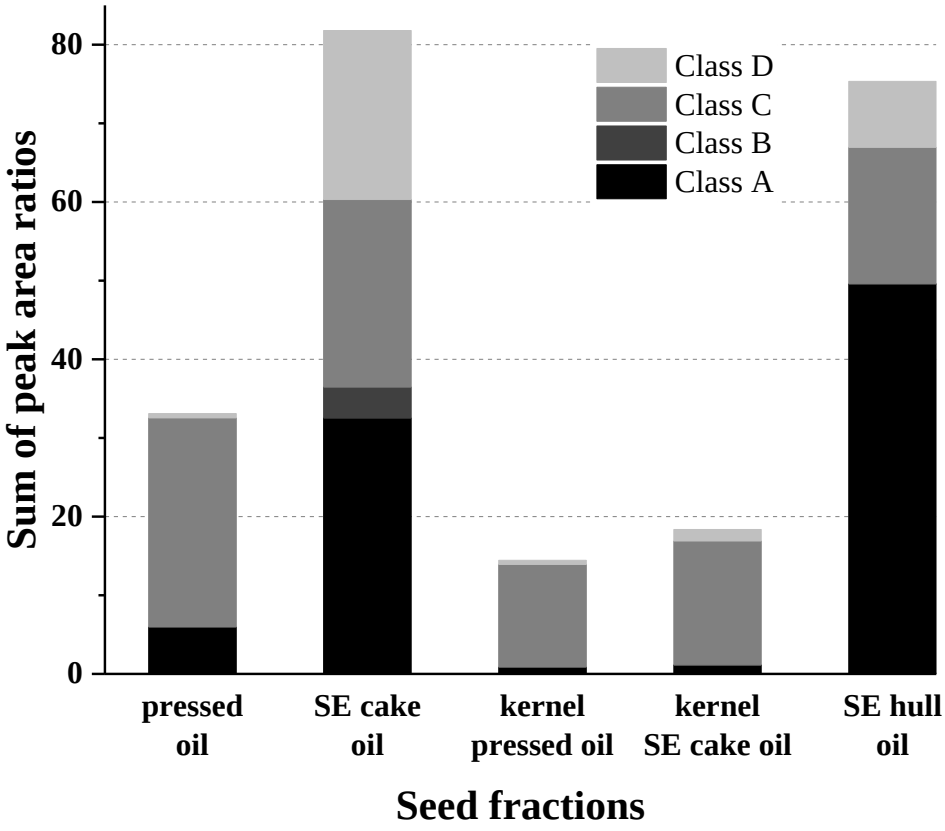

Sum of peak area ratios
80
60
40
20
0
Class D
Class C
Class B
Class A
pressed oil
SE cake oil
kernel pressed oil
kernel SE cake oil
SE hull oil
Seed fractions

Figure S3

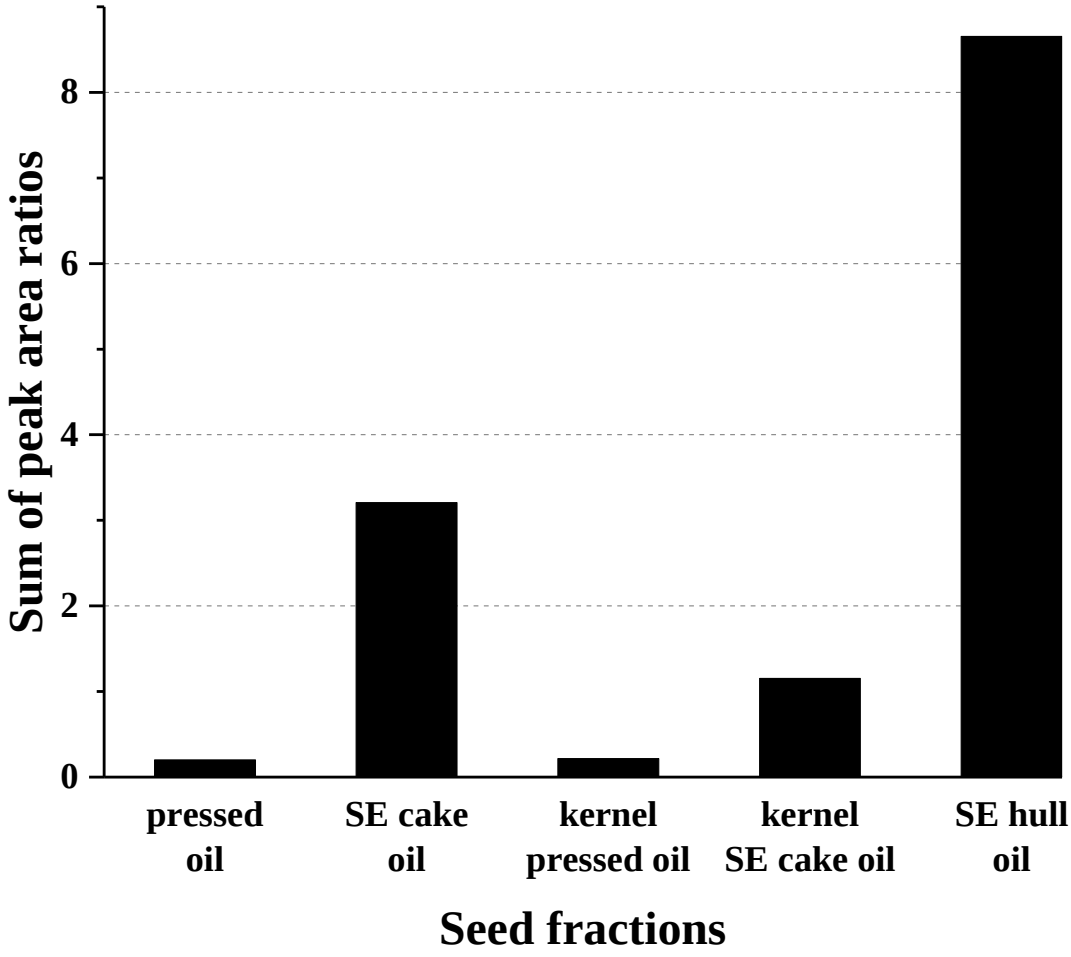

Sum of peak area ratios
0
2
4
6
8
pressed oil
SE cake oil
kernel pressed oil
kernel SE cake oil
SE hull oil
Seed fractions

Figure S4

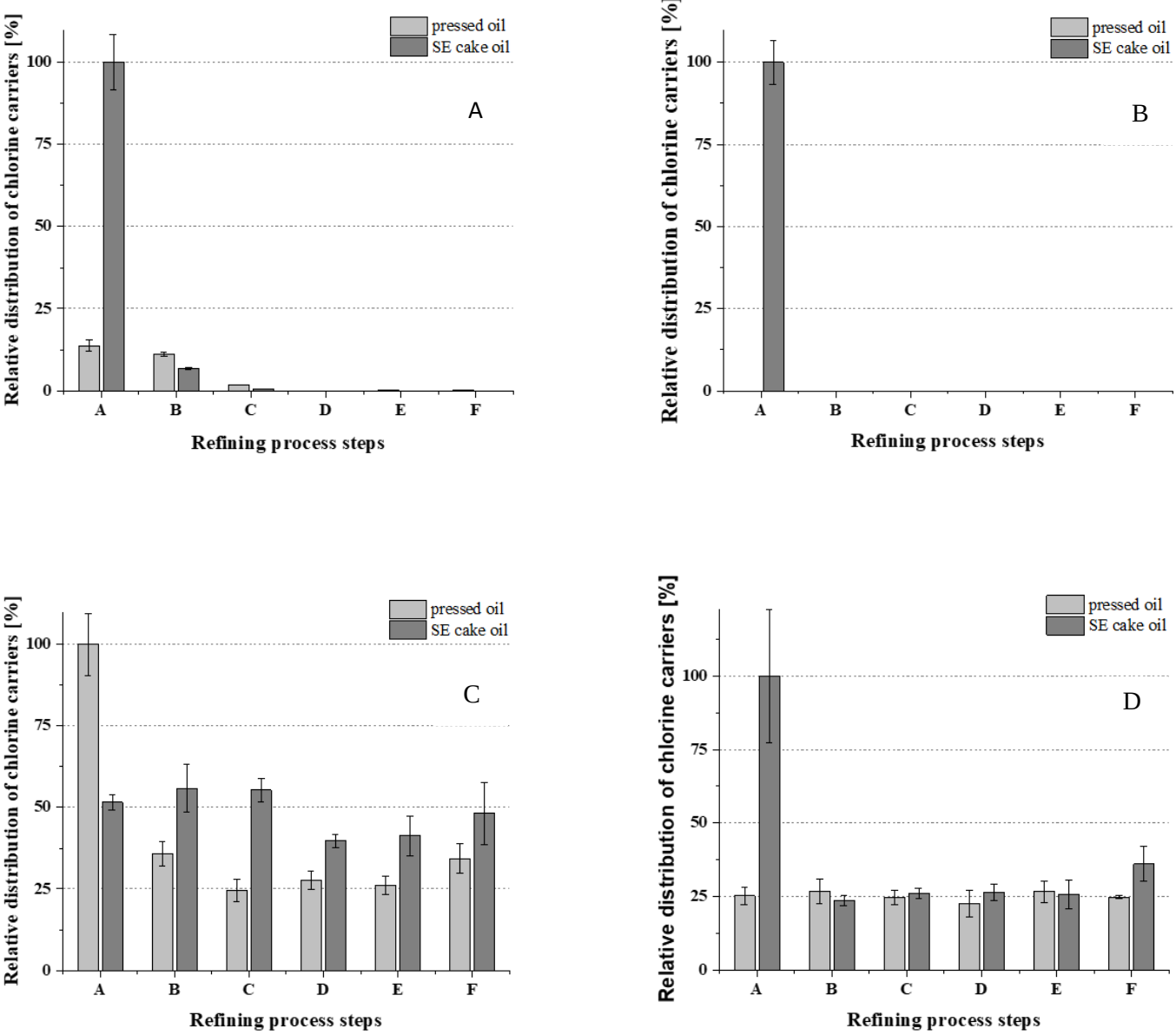
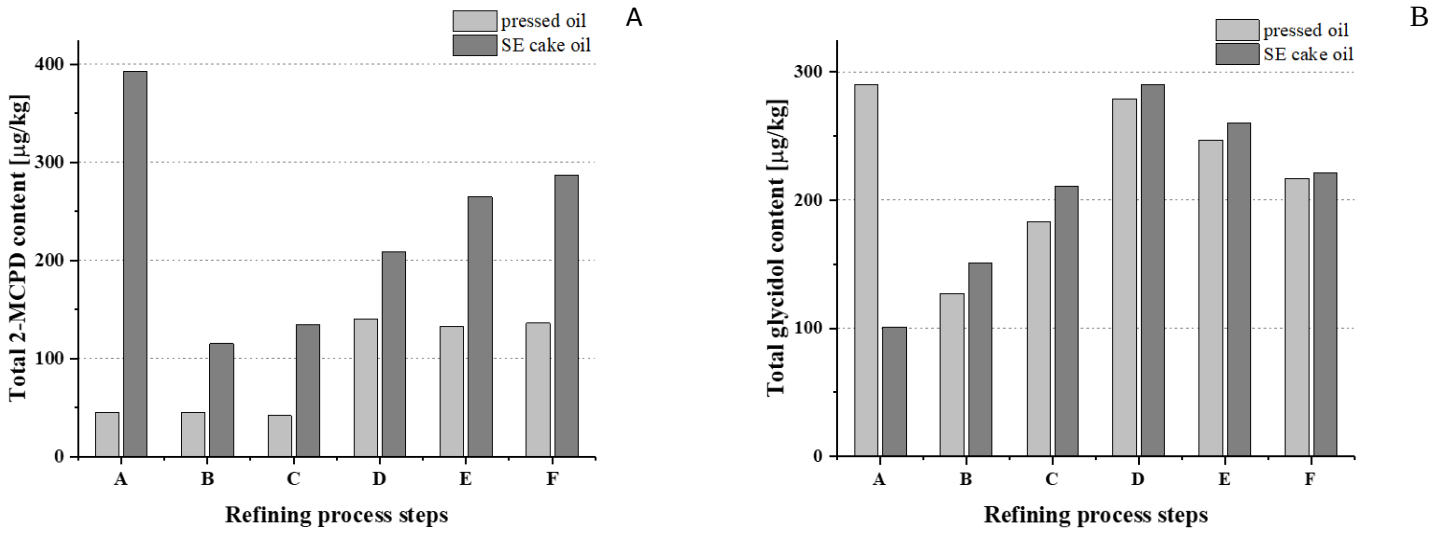

pressed oil
SE cake oil
A
B
C
D
Relative distribution of chlorine carriers [%]
Refining process steps
0
25
50
75
100
A
B
C
D
E
F

Figure S5


A
pressed oil
SE cake oil
Total 2-MCPD content [µg/kg]
0
100
200
300
400
A
B
C
D
E
F
Refining process steps
B
pressed oil
SE cake oil
Total glycidol content [µg/kg]
0
100
200
300
A
B
C
D
E
F
Refining process steps