ELETRONIC SUPPLEMENTARY INFORMATION (ESI)

Phase behavior of cholesterol in mixtures with hipo- and hipercholesterolemic lipids

Eduardo de S. Esperança[1]; Mariane S. Bonatto[1]; Gustavo G. Shimamoto[2]; Matthieu Tubino[2]; Mariana C. Costa[3]; Antonio J. A. Meirelles[1], Guilherme J. Maximo[1]

[1]School of Food Engineering, University of Campinas, Campinas, Brazil. [2] Chemical Institute, University of Campinas, Campinas, Brazil. [3] School of Chemical Engineering, University of Campinas, Campinas, Brazil

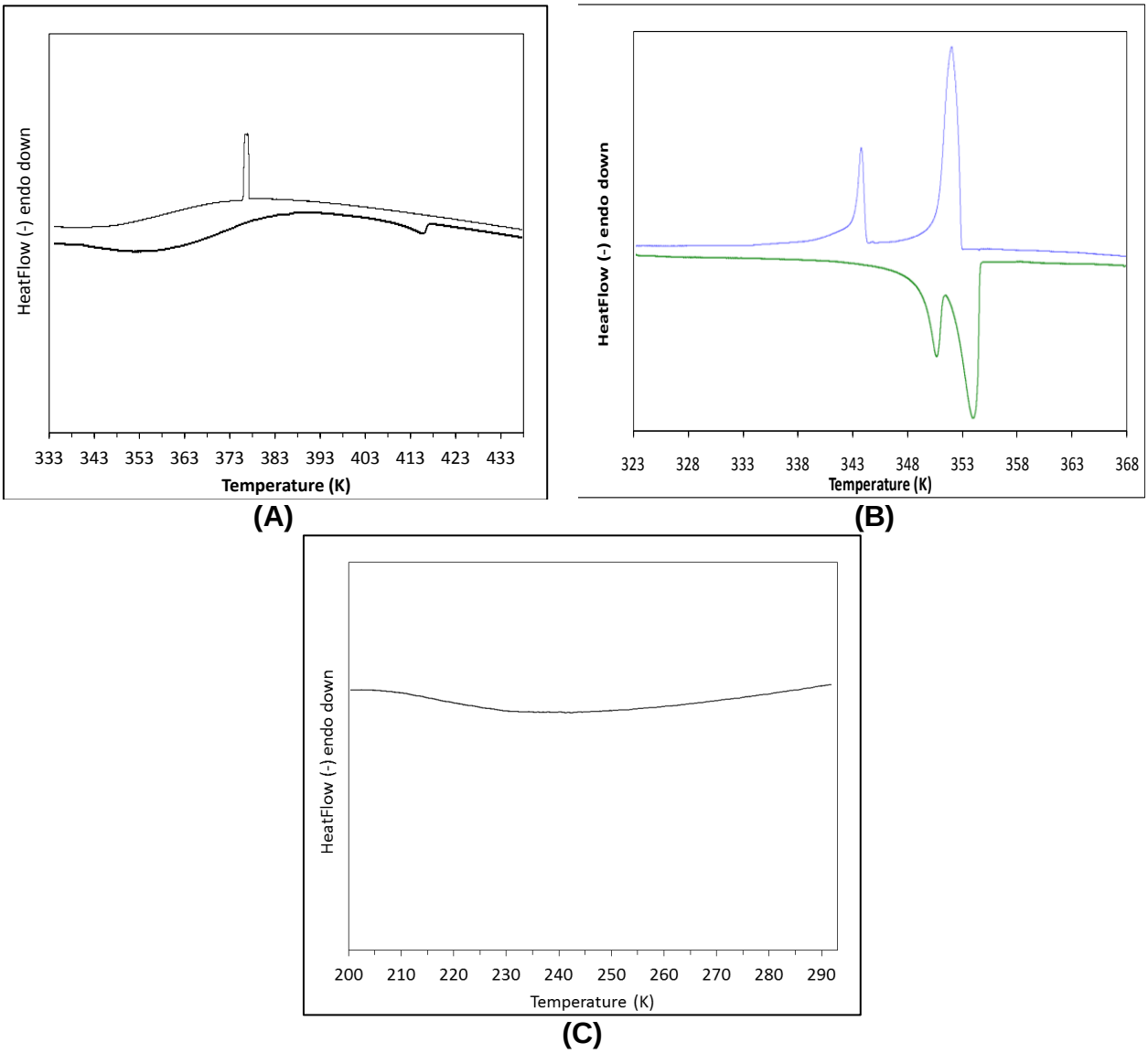

Figure S1. DSC thermograms for cholesterol (A), octacosanol (B) and α-tocopherol (C)

Equation S1 shows the Margules 3-suffixes equation for the calculation of the activity coefficient γ of the compounds in a binary system *i* + *j* with molar fraction x_i and x_j. A_{ij} and B_{ij} are the adjustable parameters (REID *et al.*, 1987).

$$\begin{cases} \gamma_i = \exp\left[\dfrac{\left(A_{ij} + 3B_{ij}\right)x_j^2 - 4B_{ij}x_j^3}{RT}\right] \\ \gamma_j = \exp\left[\dfrac{\left(A_{ij} + 3B_{ij}\right)x_i^2 - 4B_{ij}x_i^3}{RT}\right] \end{cases}$$

Equation S1

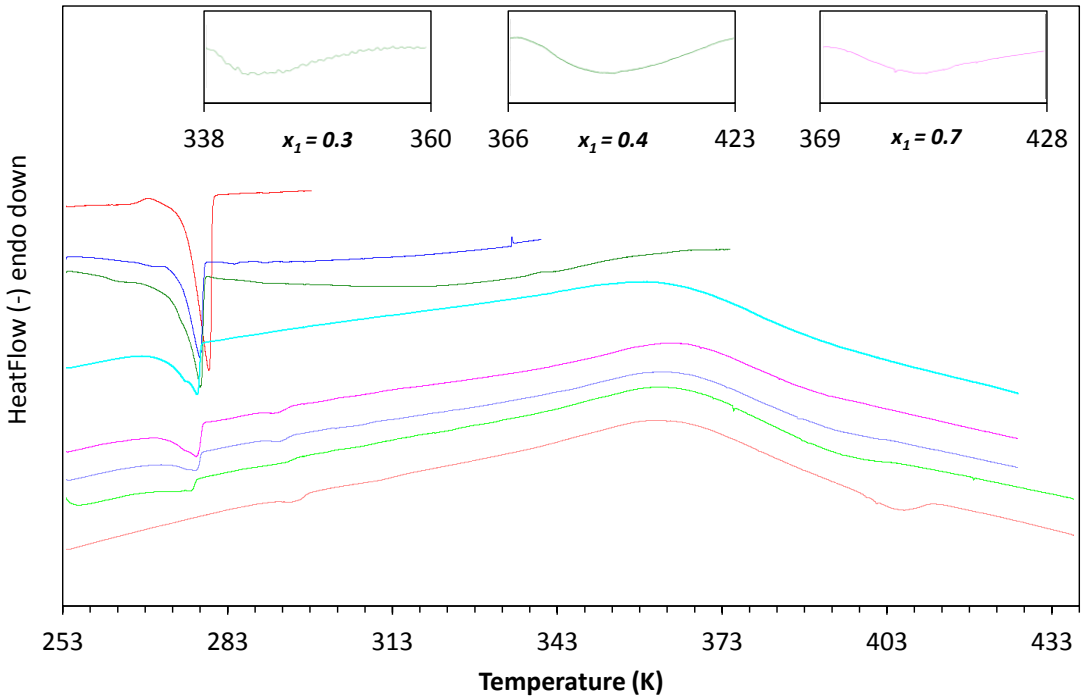

Figure S2. DSC thermograms (heating) for cholesterol (1) + oleic acid (2). From top to bottom x_1 = 0.1; 0.2; 0.3; 0.4; 0.6; 0.7; 0.8; 0.9. Magnification of the higher thermal transition (melting temperature) for some mixtures.

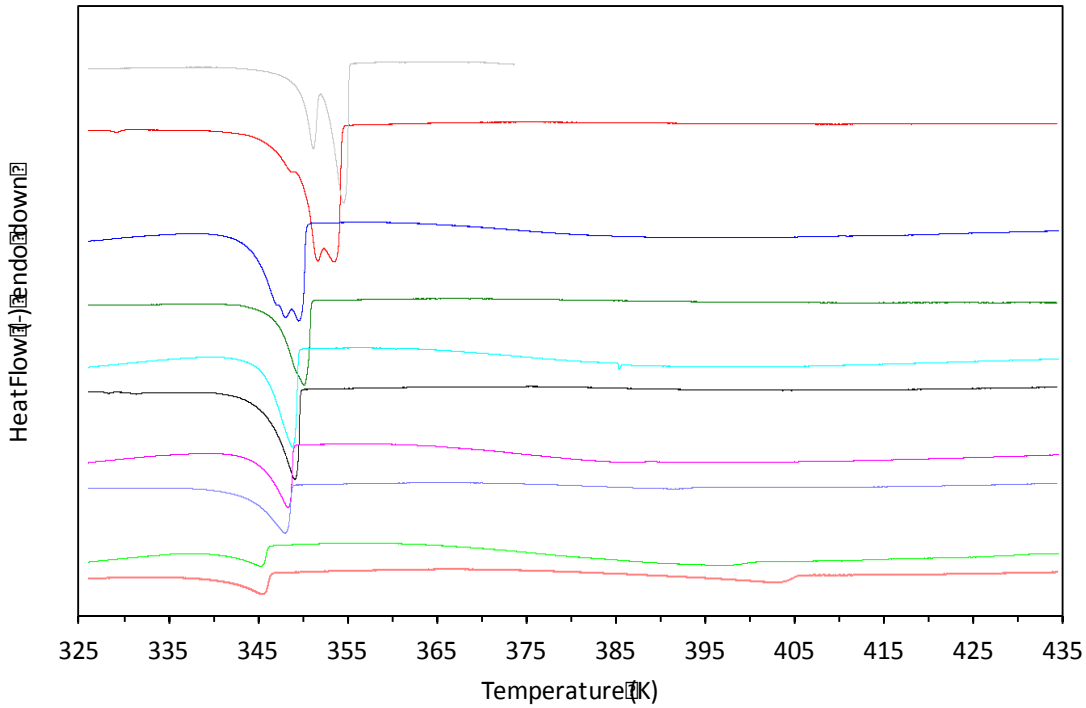

Figure S3. DSC thermograms (heating) for cholesterol (1) + octacosanol (2) mixtures. From top to bottom x_1 = 0.0; 0.1; 0.2; 0.3; 0.4; 0.5; 0.6; 0.7; 0.8; 0.9.

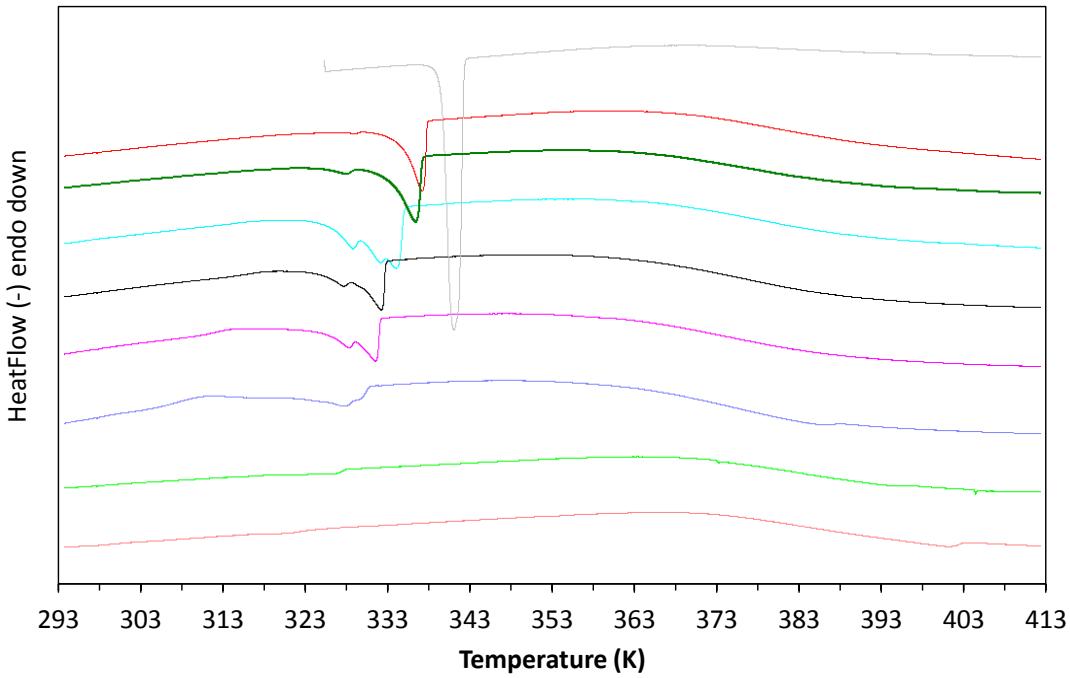

Figure S4. DSC thermograms (heating) for cholesterol (1) + stearic acid (2). From top to bottom x_1 = 0.0; 0.1; 0.2; 0.3; 0.4; 0.5; 0.7; 0.8; 0.9

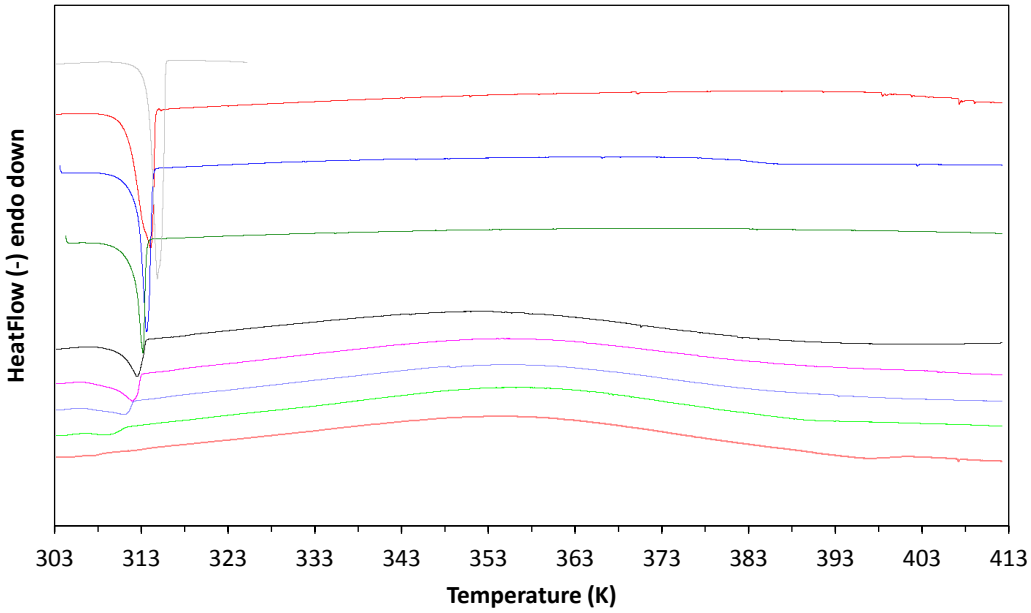

Figure S5. DSC thermograms (heating) for cholesterol (1) + elaidic acid (2). From top to bottom x_1 = 0.0; 0.1; 0.2; 0.3; 0.5; 0.6; 0.7; 0.8; 0.9

Table S1. Melting temperatures T_{fus} and enthalpies ΔH_{fus} for pure cholesterol and fatty acids.

Compound	**T_{fus} (K)**	**ΔH_{fus} (J/mol)**	**Reference**
Cholesterol	421.7	28500	(CHEN *et al.*, 2009)
	422.3	28400	(MILTENBURG *et al.*, 1998)
	420.2	27410	(DOMALSKI e HEARING, 1996)
	421.15	-	(DOMAŃSKA *et al.*, 1994)
Oleic Acid	289.45	-	(MOD *et al.*, 1960)
	286.5	39600	(DOMALSKI e HEARING, 1996)
Stearic Acid	342.75	61300	(SATO *et al.*, 1990)
	338.3	60400	(MOORE *et al.*, 2007)
	342.8	63200	(MORENO *et al.*, 2007)
	344.1	57800	(TEIXEIRA *et al.*, 2006)
Elaidic Acid	317.6	61550	(DOMALSKI e HEARING, 1996)
	317.2	-	(ALVIK *et al.*, 1972)

Table S2. Solid-liquid equilibrium data for cholesterol (1) + oleic acid (2).

x	**T_{eut}**	**T_{fus}**
0.101	280.19	-
0.200	278.57	341.45
0.299	278.66	359.00
0.398	278.10	379.65
0.497	278.72	393.85
0.597	277.89	404.55
0.695	277.78	408.55
0.799	277.03	412.05
0.896	-	412.00

Table S3. Solid-liquid equilibrium data for cholesterol (1) + octacosanol (2).

x	T_{eut}	T_{fus}
0.099	329.10	355.00
0.181	343.36	353.00
0.304	349.82	364.50
0.382	348.53	384.62
0.466	348.83	390.00
0.612	348.09	396.00
0.687	347.74	402.00
0.787	345.32	411.00
0.886	345.04	413.00

Table S4. Solid-liquid equilibrium data for cholesterol (1) + α-tocopherol (2).

x	T_{fus}
0.10	281.80
0.30	355.00
0.50	386.00
0.70	397.76
0.80	407.12
0.90	409.54

Table S5. Solid-liquid equilibrium data for cholesterol (1) + stearic acid (2)

x	T_{eut}	T_{fus}
0.102	337.43	343.85
0.199	336.61	343.45
0.297	334.22	340.45
0.405	332.36	372.95
0.499	331.65	388.00
0.604	-	392.05
0.702	327.94	398.65
0.801	326.60	407.75
0.902	320.53	410.65

Table S6. Solid-liquid equilibrium data for cholesterol (1) + elaidic acid (2)

x	T_{eut}	T_{fus}
0.100	312.75	315.75
0.200	312.95	334.75
0.300	311.75	363.25
0.400	308.59	370.05
0.500	311.04	388.45
0.600	310.05	389.73
0.699	309.66	404.85
0.800	307.49	407.95
0.899	-	410.36

REFERENCES

ALVIK, T.; BORGEN, G.; DALE, J. Conformational studies of normal, medium and large ring diametric cycloalkanediones and their ethylene ketal derivatives. **Acta Chem Scand,** v. 26, p. 1805-16, 1972.

CHEN, W.; SU, B.; XING, H.; YANG, Y.; REN, Q. Solubilities of cholesterol and desmosterol in binary solvent mixtures of n-hexane+ethanol. **Fluid Phase Equilibria,** v. 287, n. 1, p. 1-6, 2009.

DOMALSKI, E. S.; HEARING, E. D. Heat capacities and entropies of organic compounds in the condensed phase, vol 3. **Journal of Physical and Chemical Reference Data,** v. 25, n. 1, p. 1-525, 1996.

DOMAŃSKA, U.; KLOFUTAR, C.; PALJK, Š. Solubility of cholesterol in selected organic solvents. **Fluid Phase Equilibria,** v. 97, p. 191-200, 1994.

MILTENBURG, J. C. V.; GENDEREN, A. C. G. V.; DEN BERG, G. J. K. V. Design improvements in adiabatic calorimetry: The heat capacity of cholesterol between 10 and 425 K. **Thermochimica Acta,** v. 319, n. 1, p. 151-162, 1998.

MOD, R.; MAGNE, F.; SKAU, E. Pure Acid-Free Amides of C18 Fatty Acids. **Journal of Chemical and Engineering Data,** v. 5, n. 4, p. 478-479, 1960.

MOORE, D. J.; KOELMEL, D.; LAURA, D.; BEDFORD, E. Infrared spectroscopy and differential scanning calorimetry studies of binary combinations of cis-6-octadecenoic acid and octadecanoic acid. **Chemistry and Physics of Lipids,** v. 150, n. 1, p. 109-115, 2007.

MORENO, E.; CORDOBILLA, R.; CALVET, T.; CUEVAS-DIARTE, M. A.; GBABODE, G.; NEGRIER, P.; MONDIEIG, D.; OONK, H. A. J. Polymorphism of even saturated carboxylic acids from n-decanoic to n-eicosanoic acid. **New Journal of Chemistry,** v. 31, n. 6, p. 947-957, 2007.

REID, R. C.; PRAUSNITZ, J. M.; POULING, B. E. **The properties of gases and liquids**. 4th. New York: McGraw-Hill, 1987.

SATO, K.; YOSHIMOTO, N.; SUZUKI, M.; KOBAYASHI, M.; KANEKO, F. Structure and transformation in polymorphism of petroselinic acid (cis-.omega.-12-octadecenoic acid). **The Journal of Physical Chemistry,** v. 94, n. 7, p. 3180-3185, 1990.

TEIXEIRA, A. C. T.; GONÇALVES DA SILVA, A. M. P. S.; FERNANDES, A. C. Phase behaviour of stearic acid–stearonitrile mixtures: A thermodynamic study in bulk and at the air–water interface. **Chemistry and Physics of Lipids,** v. 144, n. 2, p. 160-171, 2006.