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Prediction of the melting points of fatty acids from computed molecular descriptors: A quantitative structure–property relationship study

Abdelkrim Guendouzi^{a,*}, Sidi Mohamed Mekelleche^b

^a Laboratory of Applied Thermodynamics and Molecular Modeling, Department of Chemistry, Faculty of Science and Technology, University of Saida, PB 138, Saida, 20000, Algeria ^b Laboratory of Applied Thermodynamics and Molecular Modeling, Department of Chemistry, Faculty of Science, University of Tlemcen, PB 119, Tlemcen, 13000, Algeria

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ABSTRACT

The aim of these works present in this paper consisted in the development and evaluation of quantitative structure property models (QSPR) for the prediction of the melting points of a series constituted by 62 fatty acids. The best multilinear regressions method (MLR) is used to develop models for the prediction of the melting points. The descriptors of the model are selected among an extended set of more than 500 descriptors (constitutional, topological, geometric, quantum chemical and thermodynamic descriptors). Applicability domains were defined and the predictive power was determined using a set of validations The QSPR models are established using the BMLR method implemented in CODESSA software, It turns out that the best QSPR model ($R^2 = 0.948$, $R^2_{adj} = 0.936$, SD = 0.940 and *F*-test = 190.90) is obtained with five molecular descriptors.

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1. Introduction

The economic importance of the distinctive melting and solidification behavior of fatty acids and their esters was well described by Bailey (1950). Fatty acids and their derivatives constitute an almost infinite variety of long-chain compounds differing in carbon chain length, unsaturation, and isomerism, resulting in a complex and fascinating gamut of physical properties. The transformation from the liquid to the solid state is accompanied by release of heat (latent heat of crystallization signifying an exothermic reaction); the reverse, transformation from solid to liquid, is accompanied by a negative heat effect (endothermic reaction). This forms the basis for the widely used technique of differential scanning calorimetry. Another important phenomenon is melting expansion. Conversion from the solid state to the liquid state results in a melting expansion that is added to the normal thermal expansion. This phenomenon constitutes the basis for the determination of the solid fat index by dilatometry. Protons in the solid state of a fat behave differently from those in the liquid state when subjected to radiofrequency energy when the sample is contained in a magnetic field. This serves as the basis for the determination of the solid fat content in a product by wide-line or pulsed-nuclear magnetic resonance (Harold et al., 2002).

* Corresponding author. Tel.: +213662623590.

E-mail addresses: guendouzzi@yahoo.fr (A. Guendouzi), sidi_mekelleche@yahoo.fr (S.M. Mekelleche). Melting of a fat is an instantaneous reaction, whereas crystallization is usually a slow process. The driving force in crystallization is the degree of supercooling phases: nucleation and crystal growth. A high degree of supercooling will be conducive to nucleation, and many small crystals will be formed. At temperatures closer to the crystallization point, crystal growth will be favored and large crystals will be formed. Another result of a high degree of supercooling is the formation of mixed crystals, also known as solid solutions. Molecules with a range of melting points may crystallize together. As a result, rapidly cooled fats may have higher solid fat content than the same fats that cooled more gradually. These mixed crystals will partially melt when the fat is subjected to temperature variations below its melting point, a phenomenon known as tempering (Moziar et al., 1989).

Svenstrup et al. (2005) have shown that the number of melting points and the melting temperature are correlated with the cooling rate for pork fat, lard, and leaf fat in three different products: extracted fat, raw fat, and fat as an ingredient in liver pate, a rapid cooling leads to lowering of the melting point, assigned to the presence of unstable β' crystals, and that the melting points vary with the treatment of the fat. The findings suggest that the fraction of unsaturated fatty acids present in the fat is important for both crystallization rate and melting points of α and β crystals in extracted lard, and is less pronounced in liver pate because of the presence of diverse components such as proteins. The identification of the various levels of structure present in fat crystal networks, and the development of analytical techniques to quantify these levels have

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Table 1

Experimental and calculated values of Mp of fatty acids A, B, and C correspond to the subsets used in cross validation procedure.

1A3-7-11-15-Termentylivexadecanic acid-5-85-6-506.533CC: cit-cit-cit-S-8-11-4 Enconstruction acid-46.8-45.0-23.24AC: cit-cit-cit-S-8-11-4 Enconstruction acid-46.8-45.0-3.86CD: Methylthunion acid-46.0-45.0-3.87AC: Cit-cit-cit-S-12-12-15-12-12-12-12-12-12-12-12-12-12-12-12-12-			Structure names	Cal. Mp	Exp. Mp	Residual
2 B cls-cis-cis-cis-9-12-15-Octafacastratemic aid -9.05 -9.00 22.0 4 A Cls-cis-cis-5-14-11-15-19-Doctafacastratemic aid -48.05 -48.00 -3.03 5 Cls-cis-cis-5-14-11-15-19-Doctafacastratemic aid -48.05 -48.00 -3.03 7 C Cls-cis-cis-cis-14-11-15-000000000000000000000000000000	1	А	3-7-11-15-Tetramethylhexadecanoic acid	-58.5	-65.0	6.5
3 C circls-to-fo-5-8-11-14-Eirostattacenic add -46.8 -45.0 -3.8 3 8 Pentancic add 19.10 19.00 stonshearenic add -2132 -330 98 4 C 34Minifhandias curdi -2132 -230 -330 98 6 C 34Minifhandias curdi -213 -70 98 7 A C 19.00 classicatedia curdi -75 -70 98 9 C Hopanola cadd -23 -70 98 10 A Butanoic add -23 -70 98 11 C C Floridoccina cird 213 -70 98 12 C C Floridoccina cird 213 -70 132 13 C C Floridoccina cird 177 50 127 14 B C C Floridoccina cird 170 130 40 15 C C C C C <td>2</td> <td>В</td> <td>cis-cis-cis-cis-6-9-12-15-Octadecatetraenoic acid</td> <td>-30.6</td> <td>-57.0</td> <td>26.4</td>	2	В	cis-cis-cis-cis-6-9-12-15-Octadecatetraenoic acid	-30.6	-57.0	26.4
4 A ciscic-trictic-tri-trict-tri-tri-trictic-tri-tri-trictic-tricti-tri-trictic-trict	3	С	cis-cis-cis-5-8-11-14-Eicosatetraenoic acid	-46.8	-49.0	2.2
58Pertanic add-232-230-3307Acis cisc (s. 9.12) 5-0 ctadecatinolic add-276-110-1658CHeptanole add153-708.839CHeptanole add23-708.9310ABC-9-10 ctadecatinole add23-708.9311BC-9-10 ctadecatinole add231-40-71312CCC-9-10 ctadecatinole add1320013213ABC-9-10 ctadecatinole add1320013214BC-9-10 ctadecatinole add1361103615CC12-10 ctadecatinole add1361003616CC-10 ctadecatinole add13200-18017SCC12-10 ctadecatinole add114230-1018Ctrans-sin 10-2-0 ctadecatinole add114230-10-2019AO ctanole add210220200-18021Ctrans-sin 10-2-0 ctadecatinole add13123020-1023Bcis-9-Eloconne add233220-10-2024Ctrans-sin -10-2-0 ctadecatinole add233230-2125Bcis-9-Eloconne add233230-10-3226ADecnole add233230-21-2125BUndecanole add <td< td=""><td>4</td><td>А</td><td>cis-cis-cis-cis-cis-cis-4-7-10-13-16-19-Docosahexaenoic acid</td><td>-48.6</td><td>-45.0</td><td>-3.6</td></td<>	4	А	cis-cis-cis-cis-cis-cis-4-7-10-13-16-19-Docosahexaenoic acid	-48.6	-45.0	-3.6
6C3-Methylburanic acid-12.9-12.9-2.90-3.87AC: Cics-P1-2: Ortadecatinetic acid-7.5-7.0-8.58CHeptania caid-15.5-7.0-8.59CHeptania caid-7.3-4.0-1.110AC: Cics-P1-2: Ortadecatinetic acid-7.3-4.0-1.111AHexanoic acid-7.3-4.0-1.3-1.012CCics-P1-2: Ortadecanic acid13.20.0-1.3213AHexanoic acid13.20.0-1.3214BC12.4 Mexanoic acid13.613.0-1.215C12.4 Mexanoic acid13.613.0-3.0-3.016ANanaoic acid13.613.0-3.0-3.017ACCics-P1-Alcandecalinia caid13.6-3.0-3.018CCCics-P1-Alcandecalinia caid2.302.00-1.019ACCics-P1-Alcandecalinia caid2.302.00-1.020BCics-P1-Alcandecalinia caid2.302.00-1.021CCics-P1-Alcandecalinia caid2.302.00-1.022ACics-P1-Alcandecalinia caid2.302.00-1.023ACics-P1-Alcandecalinia caid2.313.00-1.024CCics-P1-Alcandecalinia caid2.313.00-1.025ACics	5	В	Pentanoic acid	-23.2	-33.0	9.8
7Acick-ic-f-2-12-13-Contradecational carid27.611.016.89CHeptanola carid-2.87.0-8.859CHeptanola carid-2.8-7.0-8.9510ABatanola carid-2.310.0-0.9111Bcick-9-Ternadecenoia carid1.310.0-1.3112Ccick-9-Ternadecenoia carid1.32-0.00-1.3213Ccick-9-Heradecenoia carid1.320.00-1.3214Bcick-9-Heradecenoia carid1.961.20-7.6315Ccick-19-Octadecenoia carid1.961.20-7.6316ANonanoia carid1.861.503.8417Bcick-19-Octadecenoia carid1.861.503.8418Ccick-19-Octadecenoia carid1.142.30-1.1618Ccick-19-Octadecenoia carid1.142.30-1.1618cick-9-Eicosenoia carid2.812.80-2.7324Ctrans-tick-19-Octadecenoia carid2.812.80-2.7325Acick-9-Eicosenoia carid2.812.80-2.7326Acick-9-Eicosenoia carid2.813.90-2.7327Ctrans-tick-19-19-Octadecenoic carid2.813.90-3.6428Acick-9-Eicosenoia carid3.333.20-2.7327Ctrans-tick-9-I1-19-Octadecenoic carid3.14	6	C	3-Methylbutanoic acid	-32.9	-29.0	-3.9
886:is-1-2-betadecadenoic acid-15.5-7.0-8.510AButanoic acid-5.9-5.0-0.911BC.8-5-1-2-betadecanic acid-3.9-5.0-0.912CC.1-5-5-1-2-betadecanic acid23.1-4.027.113AHeinanic acid12.1-4.027.114AHeinanic acid12.1-0.012.215C12-1-1-2-betadecanic acid12.0-7.616AHonanoit acid17.013.040.017BC.5-0-Ctadecanic acid17.013.040.018CC-1-1-Octadecanic acid12.0-7.67.619AOctanoic acid12.014.020.0-6.820BCtanos Et 10-Octadecaniencia acid12.420.0-11.621CHonanic acid22.024.0-2.022ACP-Deconic acid23.224.0-2.023ADecanoic acid23.224.0-2.124CP-Deconic acid23.224.0-2.125ADecanoic acid23.224.0-2.126BUndecanoic acid23.224.0-2.127CHofacanic acid23.224.0-2.128ADecanoic acid23.224.0-2.129CHofacanic acid23.33.0-3.220	7	A	cis-cis-9-12-15-Octadecatrienoic acid	-27.6	-11.0	-16.6
0 C Heptanoc add 2.8 -7.0 98 11 A Butanoc add -33 -4.0 113 12 C cis-9-Terrafacenoic add 31 -4.0 17.1 13 A Hexaneconic add -33 -3.0 -63 13 A Hexaneconic add 17.0 50 12.2 14 R cis-9-Terrafacenoic add 17.0 50 12.2 15 C 12-1/y/100y (cis-9-octadecenoic add 18.6 15.0 -6.8 15 C 12-1/y/100y (cis-9-octadecenoic add 18.6 15.0 -6.8 20 B C cis-11-Octadecadienci add 2.0 2.0 -1.16 21 C Taras-51-10-2 todadecadienci add 2.0 2.0 -1.2 22 A C 9-boccnoic add 2.0 2.0 -2.2 23 C 9-boccnoic add 2.0 2.0 -2.2 24 C 9-boccnoi	8	В	cis-cis-9-12-Octadecadienoic acid	-15.5	-7.0	-8.5
10AKuranoc acid-5.9-5.00.0811B0.5-9-Etradecenoic acid23.1-4.011.312C0.5-9-Etradecenoic acid23.1-4.027.113AB0.5-9-Etradecenoic acid13.20.013.214B0.5-9-Etradecenoic acid13.20.013.215C0.2-1/1/dtox/-5-9-Etradecenoic acid13.014.013.016ANonanoc acid13.014.014.014.017B0.5-0-Ctradecenoic acid13.014.014.014.018C0.5-1/1/Ctradecalienoic acid11.423.0-11.619A0.5-0-Cenoic acid24.024.0-10.021Ctrans-ts-10-12-Octadecalienoic acid14.123.0-10.723B0.5-9-Econoic acid25.727.01.724Cets-5-Econoic acid25.320.0-3.125Aets-5-Econoic acid23.320.0-10.726B0.0-Conoic acid25.320.0-1.627Cets-6-Ottadecatienoic acid25.320.0-1.628B0.0-Conoic acid25.320.0-1.629ADoctanoic acid25.320.0-1.620Cets-6-Ottadecatienoic acid25.320.0-1.629B0.0-Conoic acid25.320.0-1.620C </td <td>9</td> <td>C</td> <td>Hentanoic acid</td> <td>2.8</td> <td>-7.0</td> <td>9.8</td>	9	C	Hentanoic acid	2.8	-7.0	9.8
11 0 cis-9-Fordacemic add 7.3 -4.0 17.3 12 C cis-tis-51-30-costalemica add -3.3 -3.0 -6.3 13 A Hexanoic add -9.3 -9.3 -0.3 15 C 12-hydroxy-cis-9-octadecemic add 17.7 5.0 12.2 16 A Monanic add 13.6 12.0 7.8 17 B cis-9-octadecemic add 10.0 4.0 4.0 18 A Monanic add 12.0 7.8 6.0 -6.8 20 B cis-rans-9-1-Octadecadiencia add 2.0 2.00 -11.6 21 C tis-rans-9-1-Octadecadiencia add 2.30 2.40 -2.0 23 B cis-rans-raid 2.30 2.40 -2.0 24 C 9-Decemic add 2.10 2.10 1.2 25 A cis-rais-rais-rais-rais-rais-rais-rais-ra	10	A	Butanoic acid	-59	-5.0	-0.9
12 C cs-cts-513-Docosadiencic acid 2.1, 1 -4.0 2.7, 1 13 A Hexanoic acid -3.3 -3.0 -6.3 14 B cis-9-Hexadecenoic acid 13,2 0.0 13,2 15 C C1-lydioxyci-9-octadecenoic acid 15,6 12.0 7,6 17 B cis-9-Octadecenoic acid 18,6 15,0 3,6 18 C cis-11-ottadecenoic acid 18,8 15,0 3,6 19 B cis-11-0ttadecenoic acid 14,4 20,0 -11,6 21 C cis-11-ficosenoic acid 20,0 -20,0 -24,0 -20,0 24 C 9-Decenoic acid 23,0 24,0 -0,0 -33,0 25 A cis-5-Eicosenoic acid 23,0 24,0 -10,0 -32,0 24 C p-Decenoic acid 23,0 -6,1,0 -22,0 -23,0 -23,0 -24,0 -20,0 25 A cis-5-Eicosen	11	B	cis-9-Tetradecenoic acid	73	-40	11.3
13 A Hexanor and Hexanor and	12	C	cis-cis-5-13-Docosadienoic acid	23.1	-4.0	27.1
14Bcis-9-tradecenoic acid12,20.013.215C1.21/dtoxy,cis-9-octadecenoic acid18,612,07,616ANonanoic acid18,613,04,018Ccis-11-ottadecenoic acid18,615,03,619AOctanoic acid2,020,0-6,820Bcis-trans-91-1-Octadecadinoic acid2,020,0-11,621Ctrans-sis-10-12-Ottadecadinoic acid2,024,0-10,023Bcis-11-60senoic acid2,102,00-2,1324C9-Decenoic acid-13,32,00-10,725Acis-11-60senoic acid2,132,00-10,726NOne-6Octadecentrino acid2,132,00-10,727BOne-6Octadecentrino acid2,132,00-10,728ADecennoic acid2,132,00-10,729Bcis-12-50senoic acid2,533,20-6,530Ctrans-trans-eis-9-11-3-Octadecatrinoic acid2,533,20-6,531Acis-12-50senoic acid2,513,10-3,2232Bcis-13-50senoic acid2,513,10-3,2233Ctrans-trans-eis-9-10-2-Octadecatrinoic acid2,513,10-3,2134Atrans-trans-eis-9-10-2-Octadecatrinoic acid3,134,00-5,935Bcis-13-50senoic acid3,13 <td< td=""><td>13</td><td>A</td><td>Hexanoic acid</td><td>-9.3</td><td>-3.0</td><td>-6.3</td></td<>	13	A	Hexanoic acid	-9.3	-3.0	-6.3
15C12-Hydroxy-cis-9-octadecenoic acid17,95012.716ANonanoic acid17,912.07,617Bcis-9-Octadecenoic acid17,013.04,018Ccis-1-Octadecenoic acid200,00-16,019AOctanoic acid2020,00-16,020Bcis-trans-51-10-Ctadecadienoic acid11,423,00-11,621Ctrans-cis-10-12-Octadecadienoic acid20,024,00-10,023Bcis-9-Eicosenoic acid20,024,00-2,024Acis-9-Eicosenoic acid20,024,00-2,025Acis-9-Eicosenoic acid28,324,00-2,026BUnderanic acid28,228,00-10,727Ccis-9-Ctadecenoic acid28,332,00-10,728ADecanoic acid27,531,00-3,230Ctrans-trans-cis-9-11-13-Octadecatrinonic acid28,134,00-5,931Acis-13-Decosenoic acid28,134,00-5,932Bcis-13-Decosenoic acid28,134,00-6,833Ctrans-trans-cis-9-11-3-Octadecatrinonic acid28,134,00-6,834ATridecanoic acid28,134,00-6,935Ctrans-trans-cis-9-11-3-Octadecatrinonic acid31,345,0-3,134ATridecanoic acid31,3 <td>14</td> <td>В</td> <td>cis-9-Hexadecenoic acid</td> <td>13.2</td> <td>0.0</td> <td>13.2</td>	14	В	cis-9-Hexadecenoic acid	13.2	0.0	13.2
i6 A Nonanoic acid 196 12.0 7.6 17 B cis-9-Octadecenoic acid 17.0 13.0 4.0 18 C cis-9-Octadecenoic acid 18.6 15.0 3.6 19 A Octanoic acid 20 20.0 -18.0 20 B cis-trans-9-11-Octadecatienoic acid 21.0 20.0 -18.0 21 C trans-ets-10-12-Octadecatienoic acid 23.0 24.0 -1.0 22 A cis-11-5icosenoic acid 28.0 24.0 -2.0 23 B cis-5-Eicosenoic acid 28.7 27.0 1.7 24 C 9-Decenoic acid 28.7 27.0 1.7 25 A cis-5-Eicosenoic acid 28.7 27.0 1.7 26 C Undecenoic acid 28.7 27.0 1.7 26 C Social Cacial 28.0 28.0 21.0 -6.2 27 B Cis-13-Doccenoic	15	C	12-Hvdroxy-cis-9-octadecenoic acid	17.7	5.0	12.7
17 B cis-9-Octadecenoia aid 17.0 13.0 40 18 C cis-11-Octadecenoia aid 9.2 16.0 -6.8 19 A Octanica aid 9.2 16.0 -6.8 21 C ttrans-61-10-20ctadecallenoica cid 21.0 20.0 -18.0 21 C ttrans-61-10-20ctadecallenoica cid 21.0 24.0 -1.0 23 B cis-9-Eticosenoica cid 23.0 24.0 -1.0 23 B cis-9-Eticosenoica cid 23.1 26.0 -27.3 24 C 9-Deccnoica cid 28.7 27.0 1.7 25 A cis-Eticosenoica cid 27.8 31.0 -3.2 26 B Undecanoic acid 27.8 31.0 -3.2 27 C cis-Eticosenoic acid 27.8 31.0 -3.2 28 A Decanoica cid 23.3 32.0 21.3 39 C trans-tin-9-Citadecentrinocica cid 33.3 32.0 -1.3 30 C trans-t	16	A	Nonanoic acid	19.6	12.0	7.6
18 C cis-11-Octadecennoi acid 18 15.0 36 20 B cis-trans-9-11-Octadecalienoir acid 2.0 2.00 -18.0 21 C trans-61-10-Octadecalienoir acid 11.4 23.0 -11.6 22 A cis-11-Bicosenoir acid 2.0 2.00 -1.0 23 B cis-9-Eirosenoir acid 2.0 2.0 2.0 24 C 9-Decenoir acid 2.8.7 2.7.0 1.7 26 B Undecenoir acid 2.8.7 2.7.0 1.7 27 C cis-6-Octadecenoir acid 2.8.3 3.1.0 -3.2 27 C cis-6-Octadecenoir acid 2.5.3 3.0 -6.5 30 C trans-trans-cis-9-11-13-Octadecatrienoir acid 3.3 3.0 -6.8 31 A cis-13-Docesenoir acid 2.5.4 3.0 -6.8 32 B cis-13-Docesenoir acid 3.1 4.0 -0.9 34 A	17	В	cis-9-Octadecenoic acid	17.0	13.0	4.0
19AOctanicard0.216.0-6.820Bcistrans-91-10-cotadecadienoic acid2.020.0-18.021Ctrans-01-10-Cotadecadienoic acid2.3024.0-1.023Bcis-9-Econoic acid2.3024.0-2.024C9-Decenoic acid2.302.40-2.025Acis-9-Econoic acid2.812.70-7.7326BUndecanoic acid2.822.804.227Ccis-6-Cotadecenoic acid2.822.80-6.328ADecanoic acid2.7831.0-3.229Bcis-12-Econoic acid2.7831.0-3.229Bcis-12-Econoic acid2.8134.0-5.931Acis-13-Docconoic acid2.8134.0-5.932Bcis-13-Docconoic acid3.1140.01.1134Atrafectonic acid3.1140.0-6.335Bcis-13-Docconoic acid3.1140.0-6.336CDodecanoic acid3.1140.0-6.337Atrans-trans-cis-11-3-Octadecatrienoic acid3.1140.0-6.336CDodecanoic acid3.1140.0-6.337Atrans-trans-cis-11-3-Octadecatrienoic acid3.1140.0-1.938Bcis-trans-trans-11-3-Octadecatrienoic acid3.1140.0-1.340A <t< td=""><td>18</td><td>C</td><td>cis-11-Octadecenoic acid</td><td>18.6</td><td>15.0</td><td>3.6</td></t<>	18	C	cis-11-Octadecenoic acid	18.6	15.0	3.6
no no cits trans-9:11-Octadecadienoic acid 2.0 2.00 -180 21 C trans-sit:01-Octadecadienoic acid 11.4 230 -11.6 22 A cis-11-Ecosenoic acid 260 240 -2.0 24 C 9-Decenoic acid 260 240 2.0 24 C 9-Decenoic acid 287 270 1.7 26 B Undecanoic acid 283 280 -42 27 C cis-5-Eicosenoic acid 255 320 -653 30 C trans-trans-cis-9-11-3-Octadecarinenoic acid 253 32.0 -213 31 A cis-13-Doccsenoic acid 262 330 -68 32 B cis-13-Doccsenoic acid 344 430 -86 33 C trans-trans-8-10-12-Octadecarinenoic acid 31.1 400 -109 34 A trians-trans-8-10-12-Octadecarinenoic acid 31.1 450 -139 34	19	Ā	Octanoic acid	9.2	16.0	-6.8
11Ctrans-tics-10-12-Octadecadiencia caid11423.0-11.623Acis-11-Eicosenoic acid23.024.02.023Bcis-PEicosenoic acid-1.326.02.7.324CP-Decenoic acid32.228.04.225Acis-FEicosenoic acid32.228.04.226BUndecanoic acid32.228.0-10.727Ccis-Octadecenoic acid27.831.0-3.228ADecanoic acid27.831.0-3.229Bcis-12-JEpoxy-cis-Portadecenoic acid25.532.0-6.531Acis-12-Docosenoic acid28.134.0-5.932Bcis-12-Docosenoic acid28.134.0-6.833Ctrans-trans-cis-Pi-11-3-Octadecatrienoic acid35.140.0-1.134Atrafecanoic acid36.641.0-4.535Bcis-13-Docosenoic acid36.641.0-6.836CDodecanoic acid36.643.0-6.837Atrafes-anoic acid36.641.0-1.938Bcis-trans-cis-Pi-11-3-Octadecatrienoic acid51.345.0-1.939Ctrafes-anoic acid55.352.04.541BPetradecanoic acid51.345.0-1.942Ctraff-secanoic acid51.345.0-1.943A	20	В	cis-trans-9-11-Octadecadienoic acid	2.0	20.0	-18.0
22Acis-Hicosenoic acid23.024.0-1.023Bcis-Selicosenoic acid26.024.02.024C9-Decenoic acid28.727.01.1726BUndecanoic acid28.727.01.1727CCis-Selicosenoic acid18.329.0-4.228ADecanoic acid28.727.831.0-3.229BCis-12-13-Papxy-cis-9-citadecenoic acid25.532.0-6.530Ctrans-trans-cis-9-11-13-Octadecatrienoic acid26.233.0-6.831ADecanoic acid26.233.0-6.832Bcis-11-Obcosenoic acid26.233.0-6.833Ctrans-trans-cis-9-11-3-Octadecatrienoic acid36.641.0-6.934ATidecanoic acid36.641.0-6.835Bcis-15-Teratosenoic acid36.643.0-8.636CDodecanoic acid36.643.0-6.937Atrans-11-0-Ctadecatrienoic acid36.643.0-1.938Bcis-trans-tras-9-11-13-Octadecatrienoic acid51.345.0-1.240Acis-tras-tras-9-11-13-Octadecatrienoic acid52.761.0-2.741Btrans-9-11-13-Octadecatrienoic acid58.961.0-2.743AHeptadcanoic acid58.961.0-2.144Btrans-13-Doccadecatrieno	21	С	trans-cis-10-12-Octadecadienoic acid	11.4	23.0	-11.6
23Bcis-0-Elcosenoic acid26.024.02.024C9-Decenoic acid28.727.01.725Acis-5-Elcosenoic acid28.727.01.726BUndecanoic acid28.727.01.727Ccis-6-Ottadecenoic acid18.329.0-0.728ADecanoic acid25.532.0-6.530Ctrans-trans-cis-9-1-13-Octadecarinoic acid25.532.021.331Acis-11-10-Scotenoic acid28.134.0-5.932Bcis-13-Docsenoic acid28.134.0-5.933Ctrans-trans-cis-8-10-12-Octadecarinoic acid51.140.011.134ATrans-trans-cis-8-10-12-Octadecarinoic acid31.44.0-9.938Bcis-15-Terras-cis-9-11-13-Octadecarinoic acid31.145.06.339Ctrans-cis-9-11-13-Octadecarinoic acid51.145.0-1.940Acis-15-Terras-cis-9-11-13-Octadecarinoic acid51.154.0-2.939Ctrans-9-10-tadecarinoic acid51.154.0-2.941Btrans-13-Doctadecarinoic acid58.961.0-2.742CTeras-cis-9-11-13-Octadecarinoic acid67.869.0-1.144Btrans-trans-fis-9-11-13-Octadecarinoic acid67.869.0-1.144Btrans-trans-fis-9-11-13-Octadecarinoic acid67.86	22	A	cis-11-Eicosenoic acid	23.0	24.0	-1.0
24C9-Decenoic acid-1.326.0-27.325Acis-5-Eicosonic acid21.228.04.226Cis-6-Ottadecenoic acid18.322.228.04.227Ccis-6-Ottadecenoic acid21.228.0-10.728ADecanoic acid27.831.0-3.229Bcis-12-13-Foxy-cis-9-ottadecenoic acid25.332.021.331Acis-11-Doctadecatrienoic acid28.134.0-6.832Bcis-11-Doctadecatrienoic acid28.134.0-6.833Ctrans-trans-cis-8-10-12-Ottadecatrienoic acid45.641.045.634ATrdecanoic acid31.643.0-8.835Bcis-15-Fortacosonic acid39.643.0-0.936Bcis-tars-tis-9-11-3-Ottadecatrienoic acid51.346.0-0.937Atrans-1-1-Ottadecatrienoic acid51.345.0-6.339Ctrans-1-1-Ottadecatrienoic acid51.345.0-6.339Ctrans-1-1-Ottadecatrienoic acid51.345.0-6.339Ctrans-1-1-Ottadecatrienoic acid51.345.0-7.341Btrans-1-1-Ottadecatrienoic acid51.345.0-7.342Ctrans-tis-9-1-1-3-Ottadecatrienoic acid51.345.0-7.343AHeptadecanoic acid51.345.0-7.344B<	23	В	cis-9-Eicosenoic acid	26.0	24.0	2.0
25Acis-5-Eicosenoic acid28.727.01.726BUndecanoic acid22.842.027Ccis-6-Ottadecenoic acid18.329.0-10.728ADecanoic acid27.532.0-6.529Bcis-12-13-Epoxy-cis-9-ottadecencic acid25.532.0-6.530Ctrans-trans-cis-9-11-13-Octadecatrienoic acid26.233.0-6.831Acis-11-Docosenoic acid26.233.0-6.832Bcis-13-Docosenoic acid26.134.0-5.933Ctrans-trans-cis-8-10-12-Octadecatrienoic acid51.140.0-11.134ATrans-trans-cis-8-10-12-Octadecatrienoic acid31.140.0-8.635Bcis-15-Terns-cis-9-11-13-Octadecatrienoic acid31.145.0-7.938Bcis-15-Terns-cis-9-11-13-Octadecatrienoic acid41.140.0-9.939Ctrans-oft-9-11-13-Octadecatrienoic acid41.145.0-1.940Acis-trans-cis-9-11-13-Octadecatrienoic acid51.154.0-2.941Btrans-trans-9-11-13-Octadecatrienoic acid51.154.0-2.742CTeradecanoic acid57.762.0-4.343AHeptadecanoic acid57.762.0-4.344Btrans-trans-trans-9-11-13-Octadecatrienoic acid77.181.0-3.943AHeptadecanoic acid77.	24	С	9-Decenoic acid	-1.3	26.0	-27.3
26BUndecanoic acid2228.04.227Ccis-6-Ordeleconic acid27.831.0-3.228ADecanoic acid27.831.0-3.229Bcis-12-13-Epoxy-cis-9-ortadecencic acid25.532.021.331ACtrans-trans-tis-9-11-13-Octadecatrienoic acid26.233.0-6.832BCtrans-trans-tis-9-10-12-Octadecatrienoic acid26.134.0-5.933Ctrans-trans-tis-8-10-12-Octadecatrienoic acid51.140.0-7.334ATridecanoic acid34.443.0-8.635BCDodecanoic acid34.443.0-8.636CDodecanoic acid43.145.0-0.937Atrans-11-Octadecenoic acid43.145.0-1.938BCcis-trans-cis-9-11-3-Octadecentrienoic acid43.145.0-1.940Atrans-13-Octadecenoic acid51.154.0-2.941BPentadecanoic acid55.152.0-4.542CTertadecanoic acid55.150.0-1.243AHeptadecanoic acid57.762.0-4.344Btrans-trans-trans-9-11-13-Octadecatrienoic acid67.869.0-1.245CHeptadecanoic acid57.762.0-4.546ANonadecanoic acid77.181.0-3.950 <td< td=""><td>25</td><td>А</td><td>cis-5-Eicosenoic acid</td><td>28.7</td><td>27.0</td><td>1.7</td></td<>	25	А	cis-5-Eicosenoic acid	28.7	27.0	1.7
27Cccis-0ctadecenoic acid18.329.0-10.728ADecanoic acid25.531.0-3.229Bcis-12-13-Epoxycic-9-octadecenoic acid25.532.0-6530Ctrans-trans-cis-9-11-13-Octadecatrienoic acid53.332.021.331ACis-11-Docesnoic acid26.233.0-68.932Bcis-13-Docesnoic acid28.134.0-5.933Ctrans-trans-cis-8-10-12-Octadecatrienoic acid31.440.011.134ATridecanoic acid34.443.0-8.635Bcis-15-Tetraosenoic acid39.643.0-3.436CDoceanoic acid31.440.0-0.937Atrans-trans-of-acid41.140.0-1.938Bcis-trans-cis-9-11-13-Octadecatrienoic acid51.345.0-1.940Acis-trans-trans-9-11-13-Octadecatrienoic acid51.154.0-2.941BPentadecanoic acid51.154.0-2.742CTetradecenoic acid57.762.0-4.343AHeptadecanoic acid57.762.0-4.344Btrans-trans-9-11-13-Octadecatrienoic acid63.369.0-1.245CHeradecanoic acid57.762.0-4.346ANonadecanoic acid57.762.0-5.350BPentacoanoic acid <td>26</td> <td>В</td> <td>Undecanoic acid</td> <td>32.2</td> <td>28.0</td> <td>4.2</td>	26	В	Undecanoic acid	32.2	28.0	4.2
28ADecanoic acid27.831.0-32298cis-12-15-Popy-cis-9-otadecenoic acid25.532.021.330Ctrans-trans-cis-9-11-13-Octadecatrienoic acid53.332.021.331Acis-11-Docosenoic acid26.233.0-6.832Bcis-13-Docosenoic acid28.134.0-5.933Ctrans-trans-cis-8-10-12-Octadecatrienoic acid34.443.0-6.635Bcis-15-Tetracosenoic acid34.443.0-8.636CDodcanoic acid39.643.0-3.437Atrans-11-Octadecenoic acid43.144.0-0.938Bcis-trans-5-11-31-Octadecatrienoic acid43.145.0-1.940Acis-trans-5-11-3-Octadecatrienoic acid43.145.0-1.941BPentadecanoic acid56.552.04.542CTetrads-noic acid57.761.0-2.743AHeptadecanoic acid63.761.0-2.744Btrans-trans-9-11-13-Octadecatrienoic acid63.761.0-2.745CTetrads-noic acid67.860.0-1.146ANonadecanoic acid67.762.0-4.347BOctadecanoic acid69.971.0-1.148Pentacosanoic acid73.370.00.350BPentacosanoic acid73.880.0 <t< td=""><td>27</td><td>С</td><td>cis-6-Octadecenoic acid</td><td>18.3</td><td>29.0</td><td>-10.7</td></t<>	27	С	cis-6-Octadecenoic acid	18.3	29.0	-10.7
29Bcirl-13-Epory.cirs-0-ottadecentrienoic acid25.532.0-65.30Ctrans-trans-cirs-9-11-13-Ottadecatrienoic acid26.233.0-6.831Acis-13-Docosenoic acid26.134.0-5.932Bcis-13-Docosenoic acid28.134.0-5.933Ctrans-trans-cis-8-10-12-Ottadecatrienoic acid35.140.041.134ATrifecanoic acid35.643.0-8.636CDodecanoic acid39.643.0-8.636CDodecanoic acid39.643.0-3.437Atrans-trans-cis-9-11-13-Ottadecatrienoic acid51.345.0-6.339Ctrans-trans-9-11-13-Ottadecatrienoic acid41.249.0-7.840Atrans-trans-9-11-13-Ottadecatrienoic acid41.249.0-7.841BPentadecanoic acid51.154.0-2.943AHeptadecanoic acid51.154.0-2.944Btrans-trans-9-11-13-Ottadecatrienoic acid57.762.0-4.345CTeradecanoic acid57.762.0-4.346ANonadecanoic acid70.776.0-5.347BDocosonic acid70.379.00.348Ctrans-trans-9-11-13-Ottadecatrienoic acid71.181.0-3.949Atrans-trans-di-1-11-15-Ottadecatrienoic acid73.379.00.3 </td <td>28</td> <td>Α</td> <td>Decanoic acid</td> <td>27.8</td> <td>31.0</td> <td>-3.2</td>	28	Α	Decanoic acid	27.8	31.0	-3.2
10Ctrans-trans-cis-9-11-13-Octadecatrienoic acid53.322.021.331Acis-11-Docosenoic acid26.233.0-6.832Bcis-13-Docosenoic acid26.134.0-5.933Ctrans-trans-cis-8-10-12-Octadecatrienoic acid51.140.011.134ATridecanoic acid34.443.0-8.635Bcis-15-Tetracosenoic acid34.443.0-8.636CDodecanoic acid31.144.0-0.937Atrans-11-Octadecatrienoic acid51.345.06.339Ctrans-of-Doctadecatrienoic acid43.145.0-7.840Acis-trans-of-Doctadecatrienoic acid51.350.0-7.841BPentadecanoic acid51.154.0-2.943AHeptadecanoic acid51.154.0-2.944Btrans-13-Docosenoic acid57.762.0-4.345CHexadecanoic acid63.961.0-2.744Btrans-13-Docosenoic acid64.369.0-1.147BOctadecanoic acid77.762.0-4.347BOctadecanoic acid79.379.00.350BPentacosonic acid79.379.0-3.951CHexadosonic acid77.181.0-3.952ADocosonic acid77.181.0-3.953 </td <td>29</td> <td>В</td> <td>cis-12-13-Epoxy-cis-9-octadecenoic acid</td> <td>25.5</td> <td>32.0</td> <td>-6.5</td>	29	В	cis-12-13-Epoxy-cis-9-octadecenoic acid	25.5	32.0	-6.5
11Acis-11-Decosenoic acid26.233.0-6.832Bcis-1-Decosenoic acid28.134.0-5.933Ctrans-trans-cis-8-10-12-Octadecatrienoic acid51.140.011.134ATridecanoic acid34.443.0-8.635Bcis-15-Tetracosenoic acid34.443.0-8.636CDodecanoic acid39.643.0-3.437Atrans-trans-cis-9-11-13-Octadecatrienoic acid41.145.0-1.940Acis-trans-trans-9-11-13-Octadecatrienoic acid41.249.0-7.841BPentadecanoic acid51.154.0-2.943AHeptadecanoic acid51.154.0-2.944Btrans-13-Doctadecatrienoic acid58.961.0-2.145CHeptadecanoic acid57.762.0-4.346ANonadecanoic acid67.869.0-1.247BCatcanoic acid70.776.0-5.350BPentacosnoic acid77.181.0-3.951Ctrans-trans-1-13-Octadecatrienoic acid77.18.0-2.148Ctrans-trans-trans-9-11-13-Octadecatrienoic acid77.16.0-5.350BPentacosnoic acid77.76.0-5.351Ctrans-trans-trans-9-11-13-Octadecatrienoic acid78.58.0-8.252ANonadecanoic ac	30	С	trans-trans-cis-9-11-13-Octadecatrienoic acid	53.3	32.0	21.3
128c:13-Decosencia cid28.134.0-5.933Ctrans-trans-cis-7-10-20cataciatrienoia caid51.140.011.134ATridecanoic acid34.443.0-8.635Bc:15-Tetracosencia caid34.443.0-8.636CDodecanoic acid31.144.0-0.937ATans-11-Octadecentienoic acid51.345.06.339Ctrans-trans-91-12-Octadecatrienoic acid43.144.0-7.841Bcis-trans-10-Catadecatrienoic acid41.249.0-7.842CTetradecanoic acid51.154.0-2.943AHeptadecanoic acid63.761.02.744Btrans-13-Docosenoic acid58.961.02.745CHeptadecanoic acid63.761.02.746ANonadecanoic acid63.361.02.747BOctadecanoic acid64.369.0-1.148CIrans-13-Doctadecatrienoic acid64.369.0-1.749BOctadecanoic acid70.776.0-3.350BPentacosanoic acid73.882.0-8.254CLicosanoic acid73.882.0-8.255AHepeicosanoic acid73.882.0-1.156AHoricosanoic acid73.68.0-2.357CHeseicosa	31	Α	cis-11-Docosenoic acid	26.2	33.0	-6.8
33Ctrans-trans-sis-10-12-Octadecatrienoic acid51.140.011.134ATridecanoic acid36.641.046.635Bcis-15-Tetracosenoic acid34.443.0-8.636CDodecanoic acid39.643.0-3.437Atrans-ti-10-Ctadeccenoic acid43.144.0-0.938Bcis-trans-cis-911-13-Octadecatrienoic acid41.145.0-1.940Acis-trans-trans-91-13-Octadecatrienoic acid41.249.0-7.841BPentadecanoic acid56.552.04.542CTetradecanoic acid58.961.0-2.743AHeptadecanoic acid57.762.0-4.344Btrans-trans-9-11-3-Octadecatrienoic acid58.961.0-2.145CHexadecanoic acid57.762.0-4.346ANonadecanoic acid64.369.0-1.147BOctadecanoic acid70.776.0-5.350BPentacosanoic acid73.882.0-4.351CTrans-trans-1-3-Octadecatrienoic acid73.882.0-4.353BHeneicosanoic acid73.882.0-5.354CTrans-trans-6-1-3-Octadecateraenoic acid73.882.0-6.055ADocosanoic acid73.882.0-6.054CCis-trans-trans-6-9-11-13-Octadecateraenoi	32	В	cis-13-Docosenoic acid	28.1	34.0	-5.9
34ATridecanoic acid45.641.04.635Bcis-15-tertarcosenoic acid39.643.0-8.636CDodecanoic acid39.643.0-8.437Atrans-11-Octadecenoic acid43.144.0-0.938Bcis-trans-cis-9-11-13-Octadecatrienoic acid43.145.06.339Ctrans-9-Octadecenoic acid41.145.0-1.940Acis-trans-trans-9-11-13-Octadecatrienoic acid41.249.0-7.841BPentadecanoic acid56.552.04.542CTetradecanoic acid63.761.0-2.143AHeptadecanoic acid57.762.0-4.344Btrans-13-Docosenoic acid57.762.0-4.345CHexadecanoic acid67.869.0-1.246ANonadecanoic acid67.869.0-1.247BOctadecanoic acid69.971.0-1.148Ctrans-trans-trans-9-11-13-Octadecatrienoic acid70.776.0-5.350BPentacosanoic acid77.181.0-3.951Ctrans-trans-fi-9-11-13-Octadecatrienoic acid77.186.0-1.149AEicosanoic acid73.882.0-8.251Ctrans-trans-fi-9-11-13-Octadecatrienoic acid73.882.0-8.252ADocosanoic acid73.8	33	С	trans-trans-cis-8-10-12-Octadecatrienoic acid	51.1	40.0	11.1
35Bcis-15-Tetracosenoic acid34.443.08.636CDode canoic acid39.643.0-3.437Atrans-11-Octadecancia caid43.144.0-0.938Bcis-trans-cis-9-11-13-Octadecatrienoic acid43.145.06.339Ctrans-9-0-Octadecencic acid41.249.0-7.840Acis-trans-trans-9-11-13-Octadecatrienoic acid41.249.0-7.841BPentadecanoic acid56.552.04.542CTetradecanoic acid51.154.0-2.943AHeptadecanoic acid58.961.0-2.144Btrans-13-Docosenoic acid57.762.0-4.345CHexadecanoic acid67.865.0-1.246ANonadecanoic acid70.776.0-5.347BOctadecanoic acid70.776.0-5.348Pentacosanoic acid77.181.0-3.950BHeneicosanoic acid77.181.0-3.951Ctrans-trans-9-11-13-Octadecatrienoic acid74.186.0-11.953BHeneicosanoic acid73.882.0-8.254Ccis-trans-trans-9-11-13-15-Octadecateriaenoic acid74.186.0-11.955AHeptacosanoic acid73.882.0-8.254Ccis-trans-trans-9-11-13-15-Octadecateriaenoic acid74.	34	Α	Tridecanoic acid	45.6	41.0	4.6
36CDodecanoic acid39.643.0-3.437Atrans-11-Octadecenoic acid31.144.0-0.938Bcis-trans-cis-9-11-13-Octadecatrienoic acid51.345.06.339Ctrans-s-octadecenoic acid43.145.0-1.940Acis-trans-trans-9-11-13-Octadecatrienoic acid43.145.0-7.841BPentadecanoic acid56.552.04.542CTetradecanoic acid63.761.0-2.743AHeptadecanoic acid57.762.0-4.345CHexadecanoic acid67.869.0-1.246ANonadecanoic acid67.869.0-4.747BOctadecanoic acid69.971.0-1.148Ctrans-trans-fans-9-11-13-Octadecatrienoic acid69.971.0-1.149AEicosanoic acid70.776.0-5.350BPentacosanoic acid73.882.0-8.251CTricosanoic acid73.882.0-8.253BHeneicosanoic acid73.882.0-8.254Ccis-trans-trans-cis-9-11-3-15-Octadecateraenoic acid74.186.0-11.955AHentacosanoic acid73.882.0-8.254Ccis-trans-trans-cis-9-11-3-Octadecateraenoic acid74.186.0-11.955AHentacosanoic acid73.8	35	В	cis-15-Tetracosenoic acid	34.4	43.0	-8.6
37Atrans-11-Octadecenoic acid43.144.0-0.938Bcis-trans-cis-9-11-13-Octadecatrienoic acid51.345.06.339Ctrans-9-Octadecenoic acid43.145.0-1.940Acis-trans-trans-9-11-13-Octadecatrienoic acid41.249.0-7.841BPentadecanoic acid56.552.04.542CTetradecanoic acid63.761.0-2.143AHeptadecanoic acid57.762.0-4.344Btrans-13-Docosenoic acid57.762.0-4.345CHexadecanoic acid67.869.0-1.246ANonadecanoic acid64.369.0-4.747BOctadecanoic acid69.971.0-1.148Ctrans-trans-9-11-13-Octadecatrienoic acid69.971.0-1.149AEicosnoic acid79.379.00.350BPentacosanoic acid71.181.0-3.951CTricosanoic acid73.882.0-8.254Ceis-trans-trans-9-11-13-Doctadecateraenoic acid74.186.0-11.955AHeptacosanoic acid73.882.0-8.254Ceis-trans-trans-9-11-13-Doctadecateraenoic acid73.882.0-8.255AHeptacosanoic acid73.09.03.09.056BTetracosanoic acid81.0<	36	С	Dodecanoic acid	39.6	43.0	-3.4
38 B cis-trans-cis-9-11-13-Octadecatrienoic acid 51.3 45.0 6.3 39 C trans-9-Octadeconic acid 43.1 45.0 -1.9 40 A cis-trans-trans-9-11-13-Octadecatrienoic acid 41.2 49.0 -7.8 41 B Pentadecanoic acid 56.5 52.0 4.5 42 C Tetradecanoic acid 63.7 61.0 -2.7 43 A Heptadecanoic acid 57.7 62.0 -4.3 44 B trans-13-Docosenoic acid 67.8 69.0 -1.2 45 C Hexadecanoic acid 67.8 69.0 -1.2 46 A Nonadecanoic acid 67.8 69.0 -4.3 47 B Octadecanoic acid 67.8 69.0 -4.7 48 C trans-trans-trans-9-11-13-Octadecatrienoic acid 69.9 71.0 -1.1 49 A Eicosanoic acid 70.7 76.0 -5.3 50 B Pentcosanoic acid 73.8 82.0 -8.2 51	37	A	trans-11-Octadecenoic acid	43.1	44.0	-0.9
39 C trans-9-Octadecenoic acid 43.1 45.0 -1.9 40 A cistnas-trans-9-11-13-Octadecatrienoic acid 41.2 49.00 -7.8 41 B Pentadecanoic acid 56.5 52.0 4.5 42 C Tetradecanoic acid 51.1 54.0 -2.9 43 A Heptadecanoic acid 63.7 61.0 -2.7 44 B trans-13-Docosenoic acid 58.9 61.0 -2.1 45 C Hexadecanoic acid 67.8 69.0 -1.2 46 A Nonadecanoic acid 67.8 69.0 -1.1 47 B Octadecanoic acid 67.8 69.0 -1.2 47 B Octadecanoic acid 67.8 69.0 -1.1 48 C trans-trans-trans-9-11-13-Octadecatrienoic acid 70.7 76.0 -5.3 50 B Pentacosanoic acid 70.7 76.0 -5.3 51 C Ticosanoic acid 77.1 81.0 -3.9 52 A	38	В	cis-trans-cis-9-11-13-Octadecatrienoic acid	51.3	45.0	6.3
40 A cis-trans-9-11-3-Octadecatrienoic acid 41.2 49.0 -7.8 41 B Pentadecanoic acid 56.5 52.0 45 42 C Tetradecanoic acid 51.1 54.0 -2.9 43 A Heptadecanoic acid 58.9 61.0 -2.7 44 B trans-13-Docosenoic acid 58.9 61.0 -2.1 45 C Hexadecanoic acid 57.7 62.0 -4.3 46 A Nonadecanoic acid 67.8 69.0 -1.2 47 B Octadecanoic acid 69.9 71.0 -1.1 48 C trans-trans-trans-9-11-13-Octadecatrienoic acid 69.9 71.0 -1.1 49 A Eicosanoic acid 70.7 76.0 -5.3 50 B Petracosanoic acid 79.3 79.0 0.3 51 C Ticosanoic acid 77.1 81.0 -3.9 53 B Hencicosanoic acid 74.1 86.0 -11.9 54 C cistrans-tra	39	С	trans-9-Octadecenoic acid	43.1	45.0	-1.9
41BPentadecanoic acid56.552.04.742CTetradecanoic acid51.154.0-2.943AHeptadecanoic acid63.761.02.744Btrans-13-Docosenoic acid58.961.0-2.145CHexadecanoic acid57.762.0-4.346ANonadecanoic acid67.869.0-1.247BOctadecanoic acid69.971.0-1.148Ctrans-trans-rans-9-11-13-Octadecatrienoic acid69.977.06.950BPentacosanoic acid70.776.0-5.351CTricosanoic acid79.379.00.352ADocosanoic acid77.181.0-3.953BHeneicosanoic acid74.186.0-11.954Cctaras-trans-cis-9-11-13-15-Octadecatetraenoic acid74.186.0-11.955AHeptacosanoic acid74.186.0-1.156BTetracosanoic acid88.587.01.556BTetracosanoic acid81.087.0-2.357CHexacosanoic acid93.090.03.058ANonacosanoic acid93.090.03.059BOctacosanoic acid97.693.04.661ATriacotanoic acid94.893.01.862BDotriacotanoic acid102.8 <td< td=""><td>40</td><td>A</td><td>cis-trans-trans-9-11-13-Octadecatrienoic acid</td><td>41.2</td><td>49.0</td><td>-7.8</td></td<>	40	A	cis-trans-trans-9-11-13-Octadecatrienoic acid	41.2	49.0	-7.8
42CTetradecanoic acid51.154.0-2.943AHeptadecanoic acid63.761.02.744Btrans-13-Docosenoic acid58.961.0-2.145CHexadecanoic acid57.762.0-4.346ANonadecanoic acid64.369.0-1.247BOctadecanoic acid64.369.0-4.748Ctrans-trans-trans-911-13-Octadecatrienoic acid69.971.0-1.149AEicosanoic acid70.776.0-5.350BPentacosanoic acid79.379.00.351CTricosanoic acid77.181.0-3.953BHeneicosanoic acid73.882.0-8.254Ccis-trans-trans-cis-9-11-13-15-Octadecateraenoic acid74.186.0-11.955AHeptacosanoic acid88.587.01.556BTetracosanoic acid88.587.0-6.057CHexacosanoic acid93.090.03.058ANonacosanoic acid93.090.03.059BOctacosanoic acid94.893.01.861ATriacontanoic acid94.893.01.862BDotriacontanoic acid94.896.03.163BTetracosanoic acid94.896.0-64ATriacontanoic acid94.8 <td< td=""><td>41</td><td>В</td><td>Pentadecanoic acid</td><td>56.5</td><td>52.0</td><td>4.5</td></td<>	41	В	Pentadecanoic acid	56.5	52.0	4.5
43 A Heptadecanoic acid 63.7 61.0 2.1 44 B trans-13-Docosenoic acid 58.9 61.0 -2.1 45 C Hexadecanoic acid 57.7 62.0 -4.3 46 A Nonadecanoic acid 67.8 69.0 -1.2 47 B Octadecanoic acid 64.3 69.0 -1.1 48 C trans-trans-9-11-13-Octadecatrienoic acid 69.9 71.0 -1.1 49 A Eicosanoic acid 70.7 76.0 -5.3 50 B Pentacosanoic acid 79.3 79.0 0.3 51 C Tricosanoic acid 77.1 81.0 -3.9 52 A Docosanoic acid 73.8 82.0 -8.2 54 C cis-trans-trans-9-11-13-15-Octadecatetraenoic acid 74.1 86.0 -11.9 55 A Heptacosanoic acid 81.0 87.7 6.60 -11.9 55 A Heptacosanoic acid 93.0 90.0 3.0 0.0 56<	42	C	letradecanoic acid	51.1	54.0	-2.9
44Btrans-13-Decension acid38.961.0-2.145CHexadecanoic acid57.762.0-4.346ANonadecanoic acid67.869.0-1.247BOctadecanoic acid64.369.0-4.748Ctrans-trans-9-11-13-Octadecatrienoic acid69.971.0-1.149AEicosanoic acid70.776.0-5.350BPentacosanoic acid79.379.06.951CTricosanoic acid77.181.0-3.952ADocosanoic acid73.882.0-8.254Ccistrans-trans-of-9-11-13-15-Octadecateraenoic acid73.882.0-8.255AHeneicosanoic acid73.882.0-1.956BTetracosanoic acid81.087.0-1.957CHexacosanoic acid93.090.03.058ANonacosanoic acid93.090.03.059BOctacosanoic acid97.693.04.661ATriacontanoic acid97.693.04.662BDotriacontanoic acid97.693.04.661ATriacontanoic acid97.693.04.662BDotriacontanoic acid97.693.04.663ANonacosanoic acid96.03.11.864ATriacontanoic acid94.893.0	43	A	Heptadecanoic acid	63.7	61.0	2.7
45 C HexadeCanoic acid 57.7 62.0 4.3 46 A Nonadecanoic acid 67.8 69.0 -1.2 47 B Octadecanoic acid 64.3 69.0 -4.7 48 C trans-trans-trans-9-11-13-Octadecatrienoic acid 69.9 71.0 -1.1 49 A Eicosanoic acid 70.7 76.0 -5.3 50 B Pentacosanoic acid 79.3 79.0 6.9 51 C Tricosanoic acid 77.1 81.0 -3.9 53 B Heneicosanoic acid 77.1 81.0 -3.9 54 C cis-trans-trans-cis-9-11-13-15-Octadecatetraenoic acid 74.1 86.0 -11.9 55 A Heptacosanoic acid 74.1 86.0 -11.9 55 A Heptacosanoic acid 81.0 87.0 -6.0 57 C Hexacosanoic acid 93.0 90.0 3.0 58 A Nonacosanoic acid 91.0 90.0 3.0 59 B O	44	В	trans-13-Docosenoic acid	58.9	61.0	-2.1
40 A Nonadecanoic acid 67.8 69.0 -1.2 47 B Octadecanoic acid 64.3 69.0 -4.7 48 C trans-trans-9-11-13-Octadecatrienoic acid 69.9 71.0 -1.1 49 A Eicosanoic acid 70.7 76.0 -5.3 50 B Pentacosanoic acid 83.9 77.0 6.9 51 C Tricosanoic acid 79.3 79.0 0.3 52 A Docosanoic acid 73.8 82.0 -8.2 54 C cis-trans-trans-cis-9-11-13-15-Octadecatetraenoic acid 74.1 86.0 -11.9 55 A Heptacosanoic acid 74.1 86.0 -11.9 55 A Heptacosanoic acid 88.5 87.0 1.5 56 B Tetracosanoic acid 88.5 87.0 -2.3 57 C Hexacosanoic acid 93.0 90.0 3.0 58 A Nonacosanoic acid 93.0 90.0 3.0 59 B Octacosanoic	45	C	Hexadecanoic acid	57.7	62.0	-4.3
47 B OctadeCation card 64.3 69.0 -4.7 48 C trans-trans-9-11-13-Octadecatrienoic acid 69.9 71.0 -1.1 49 A Eicosanoic acid 70.7 76.0 -5.3 50 B Pentacosanoic acid 83.9 77.0 6.9 51 C Tricosanoic acid 79.3 79.0 0.3 52 A Docosanoic acid 73.8 82.0 -8.2 53 B Heneicosanoic acid 74.1 86.0 -11.9 55 A Heptacosanoic acid 74.1 86.0 -11.9 55 A Heptacosanoic acid 88.5 87.0 1.5 56 B Tetracosanoic acid 81.0 87.0 -6.0 57 C Hexacosanoic acid 93.0 90.0 3.0 58 A Nonacosanoic acid 90.4 90.0 0.4 60 C Hentriacontanoic acid 94.8 93.0 1.8 62 B Dotriacontanoic acid 102.8 <td>46</td> <td>A</td> <td>Nonadecanoic acid</td> <td>67.8</td> <td>69.0</td> <td>-1.2</td>	46	A	Nonadecanoic acid	67.8	69.0	-1.2
48 C trains-trains-9-11-13-Octade catinenoic acid 69.9 71.0 1.1 49 A Eicosanoic acid 70.7 76.0 -53 50 B Pentacosanoic acid 83.9 77.0 6.9 51 C Tricosanoic acid 79.3 79.0 0.3 52 A Docosanoic acid 77.1 81.0 -3.9 53 B Heneicosanoic acid 74.1 86.0 -11.9 54 C cis-trans-trans-cis-9-11-3-15-Octadecatetraenoic acid 74.1 86.0 -11.9 55 A Heptacosanoic acid 88.5 87.0 1.5 56 B Tetracosanoic acid 88.5 87.0 -6.0 57 C Hexacosanoic acid 81.0 87.0 -2.3 58 A Nonacosanoic acid 90.4 90.0 0.4 60 C Hentriacontanoic acid 97.6 93.0 0.46 61 A Triacontanoic acid 94.8 93.0 1.8 62 B Dotri	47	В	Octadecanoic acid	64.3	69.0 71.0	-4./
AsElcosanoic acid70.776.0-3.350BPentacosanoic acid83.977.06.951CTricosanoic acid79.379.00.352ADocosanoic acid77.181.0-3.953BHeneicosanoic acid73.882.0-8.254Ccis-trans-trans-cis-9-11-13-15-Octadecatetraenoic acid74.186.0-11.955AHeptacosanoic acid81.087.01.556BTetracosanoic acid81.087.0-6.057CHexacosanoic acid85.788.0-2.358ANonacosanoic acid93.090.03.059BOctacosanoic acid97.693.04.661ATriacontanoic acid94.893.01.862BDotriacontanoic acid102.896.03.1Maximum-58.5-65.0Maximum102.896.0Mean34.934.80.0-Median33.333.5-0.9-0.9	48	C A	Trans-trans-trans-9-11-13-Octadecathenoic acid	69.9	71.0	-1.1
50BPentacosanoic acid83.977.06.951CTricosanoic acid79.379.00.352ADocosanoic acid77.181.0-3.953BHeneicosanoic acid73.882.0-8.254Ccis-trans-trans-cis-9-11-13-15-Octadecatetraenoic acid74.186.0-11.955AHeptacosanoic acid88.587.01.556BTetracosanoic acid81.087.0-6.057CHexacosanoic acid93.090.03.059BOctacosanoic acid90.490.00.460CHentriacontanoic acid97.693.04.661ATriacontanoic acid94.893.01.862BDotriacontanoic acid102.896.03.162BDotriacontanoic acid102.896.0-Maimum102.896.0Mean34.934.80.0Median33.333.5-0.9	49	A	Elcosaliole acid	/0./	76.0	-5.3
51 C Introballol actual 79.3 79.0 0.3 52 A Docosanoic acid 77.1 81.0 -3.9 53 B Hencicosanoic acid 73.8 82.0 -8.2 54 C cis-trans-trans-cis-9-11-13-15-Octadecatetraenoic acid 74.1 86.0 -11.9 55 A Heptacosanoic acid 88.5 87.0 1.5 56 B Tetracosanoic acid 81.0 87.0 -6.0 57 C Hexacosanoic acid 81.0 87.0 -2.3 58 A Nonacosanoic acid 93.0 90.0 3.0 59 B Octacosanoic acid 90.4 90.0 0.4 60 C Hentriacontanoic acid 97.6 93.0 4.6 61 A Triacontanoic acid 97.6 93.0 4.6 62 B Dotriacontanoic acid 94.8 93.0 1.8 62 B Dotriacontanoic acid 102.8 96.0 3.1 Maimum -58.5 -65.0	50	В		83.9	77.0	0.9
52 A Docosanio acid 77.1 81.0 -3.9 53 B Heneicosanoic acid 73.8 82.0 -8.2 54 C cis-trans-trans-cis-9-11-13-15-Octadecatetraenoic acid 74.1 86.0 -11.9 55 A Heptacosanoic acid 88.5 87.0 1.5 56 B Tetracosanoic acid 81.0 87.0 -6.0 57 C Hexacosanoic acid 85.7 88.0 -2.3 58 A Nonacosanoic acid 93.0 90.0 0.0 59 B Octacosanoic acid 90.4 90.0 0.4 60 C Hentriacontanoic acid 97.6 93.0 4.6 61 A Triacontanoic acid 97.6 93.0 4.6 62 B Dotriacontanoic acid 91.8 93.0 1.8 62 B Dotriacontanoic acid 92.8 96.0 3.1 Maimum -58.5 -65.0 - - Mean 34.9 34.8 0.0 - </td <td>51</td> <td>C A</td> <td>Decementa acid</td> <td>79.3</td> <td>/9.0</td> <td>0.3</td>	51	C A	Decementa acid	79.3	/9.0	0.3
53 B Henerosanoic acid 75.8 82.0 6.2 54 C cis-trans-trans-cis-9-11-13-15-Octadecatetraenoic acid 74.1 86.0 11.9 55 A Heptacosanoic acid 88.5 87.0 1.5 56 B Tetracosanoic acid 81.0 87.0 -6.0 57 C Hexacosanoic acid 85.7 88.0 -2.3 58 A Nonacosanoic acid 93.0 90.0 3.0 59 B Octacosanoic acid 97.6 93.0 4.6 61 A Triacontanoic acid 97.6 93.0 4.6 62 B Dotriacontanoic acid 94.8 93.0 1.8 62 B Dotriacontanoic acid 94.8 93.0 1.8 62 B Dotriacontanoic acid 96.0 3.1 Minimum -58.5 -65.0 - - Maximum 102.8 96.0 - - Median 33.3 33.5 -0.9	52	R	Docosanoic acid	77.0	01.0	-5.9
54 C Clastitatiscurates for 155 for cladecate fraction action 74.1 30.0 -11.5 55 A Heptacosanoic acid 88.5 87.0 1.5 56 B Tetracosanoic acid 81.0 87.0 -6.0 57 C Hexacosanoic acid 85.7 88.0 -2.3 58 A Nonacosanoic acid 93.0 90.0 3.0 59 B Octacosanoic acid 97.6 93.0 4.6 61 A Triacontanoic acid 94.8 93.0 1.8 62 B Dotriacontanoic acid 94.8 93.0 1.8 62 B Dotriacontanoic acid 94.8 93.0 1.8 62 B Dotriacontanoic acid 96.0 3.1 Minimum -58.5 -65.0 - Maximum 102.8 96.0 - Mean 34.9 34.8 0.0 Median 33.3 33.5 -0.9	55	Б	cis trans trans sis 0 11 12 15 Octadocatotraonois acid	75.0	82.0	-0.2
55 A Ineptacosanoic acid 86.5 87.0 1.7 56 B Tetracosanoic acid 81.0 87.0 -6.0 57 C Hexacosanoic acid 85.7 88.0 -2.3 58 A Nonacosanoic acid 93.0 90.0 3.0 59 B Octacosanoic acid 97.6 93.0 0.4 60 C Hentriacontanoic acid 97.6 93.0 4.6 61 A Triacontanoic acid 94.8 93.0 1.8 62 B Dotriacontanoic acid 94.8 96.0 3.1 62 B Dotriacontanoic acid 94.8 96.0 3.1 62 B Dotriacontanoic acid 94.8 96.0 - Maximum -58.5 -66.0 - - Maximum 102.8 96.0 - Meain 34.9 34.8 0.0 33.3 33.5 -0.9	55 55	Δ	Hoptacosapoic acid	74.1	80.0	-11.9
57 C Hexacosanoic acid 81.0 67.0 67.0 57 C Hexacosanoic acid 85.7 88.0 -2.3 58 A Nonacosanoic acid 93.0 90.0 3.0 59 B Octacosanoic acid 90.4 90.0 0.4 60 C Hentriacontanoic acid 97.6 93.0 4.6 61 A Triacontanoic acid 94.8 93.0 1.8 62 B Dotriacontanoic acid 102.8 96.0 3.1 62 B Minimum -58.5 -65.0 - Maximum 102.8 96.0 - - Maximum 34.9 34.8 0.0 Mean 33.3 33.5 -0.9	56	B	Tetracosanoic acid	81.0	87.0	6.0
57 C Incatositatic acid 50.7 50.6 72.5 58 A Noncosanoic acid 90.0 3.0 59 B Octacosanoic acid 90.4 90.0 0.4 60 C Hentriacontanoic acid 97.6 93.0 4.6 61 A Triacontanoic acid 94.8 93.0 1.8 62 B Dotriacontanoic acid 102.8 96.0 3.1 62 B Minimum -58.5 -65.0 - Maximum 102.8 96.0 - - Mean 34.9 34.8 0.0 Median 33.3 33.5 -0.9	57	C	Heracosanoic acid	85.7	88.0	-0.0
59 B Octosanoic acid 90.4 90.0 0.4 60 C Hentriacontanoic acid 97.6 93.0 4.6 61 A Triacontanoic acid 94.8 93.0 1.8 62 B Dotriacontanoic acid 102.8 96.0 3.1 62 B Dotriacontanoic acid 102.8 96.0 - Maximum -58.5 -65.0 - Mean 34.9 34.8 0.0 Median 33.3 33.5 -0.9	58	A	Nonacosanoic acid	93.0	90.0	-2.5
50 B Octational actual 50.4 50.4 50.4 60 C Hentriacontanoic acid 97.6 93.0 4.6 61 A Triacontanoic acid 94.8 93.0 1.8 62 B Dotriacontanoic acid 102.8 96.0 3.1 Minimum -58.5 -65.0 - Maximum 102.8 96.0 - Mean 34.9 34.8 0.0 Median 33.3 33.5 -0.9	50	B	Octacosanoic acid	90.4	90.0	0.4
61 A Triacontanoic acid 94.8 93.0 1.8 62 B Dotriacontanoic acid 102.8 96.0 3.1 Minimum -58.5 -65.0 - Maximum 102.8 96.0 - Mean 34.9 34.8 0.0 Median 33.3 33.5 -0.9	60	C	Hentriacontanoic acid	97.6	93.0	4.6
62 B Dotriacontanoic acid 102.8 96.0 3.1 Minimum -58.5 -65.0 - Maximum 102.8 96.0 - Mean 34.9 34.8 0.0 Median 33.3 33.5 -0.9	61	Ă	Triacontanoic acid	94.8	93.0	1.8
Minimum -58.5 -65.0 - Maximum 102.8 96.0 - Mean 34.9 34.8 0.0 Median 33.3 33.5 -0.9	62	В	Dotriacontanoic acid	102.8	96.0	3.1
Maximum 102.8 96.0 - Mean 34.9 34.8 0.0 Median 33.3 33.5 -0.9		2	Minimum	-58.5	-65.0	-
Mean34.934.80.0Median33.333.5-0.9			Maximum	102.8	96.0	-
Median 33.3 33.5 -0.9			Mean	34.9	34.8	0.0
			Median	33.3	33.5	-0.9

been reviewed by Narine and Marangoni (1999, 2002). The types, formulations, functionality, and processing required for the production of lipid-shortening systems, as well as their crystallization, structural elucidation, and mechanical modeling of fat crystal networks have been reviewed by Ghotra et al. (2002). Also, Humphrey et al. (2004) have compared the lipid-shortening functionality as a function of molecular ensemble and shear: crystallization and melting.

Alternatively, the quantitative structure–property relationship (QSPR) provides a promising method for estimating the melting point of fatty acids based on descriptors derived solely from the molecular structure to fit experimental data. The QSPR is based Download English Version:

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