

Potential risk resulting from the influence of static magnetic field upon living organisms. Numerically simulated effects of the static magnetic field upon fatty acids and their glycerides

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Abstract

Background: We attempt to recognise the effects of static magnetic field (SMF) of varying flux density on flora and fauna. For this purpose, the influence of static magnetic field is studied for molecules of octadecanoic (stearic), *cis*-octadec-9-enoic (oleic), *cis,cis*-octadec-9,12-dienoic (linoleic), *all cis*-octadec-6,9,12-trienoic (linolenic), *trans*-octadec-9-enoic – (elaidic), *cis*-octadec-11-enoic (vaccenic) and *all trans*-octadec-6,9,12-trienoic (*trans*-linolenic) acids as well as 1- and 2-caproyl monoglycerides, 1,2- and 1,3-caproyl diglycerides and 1,2,3-caproyl triglyceride. In such a manner we attempt to develop an understanding of the interactions of living cells with SMF on a molecular level.

Methods: Computations of the effect of real SMF 0.0, 0.1, 1, 10 and 100 AMFU (Arbitrary Magnetic Field Unit; here 1AMFU \geq 1000 T) flux density were performed *in silico* (computer vacuum), involving advanced computational methods.

Results: SMF polarises molecules depending on applied flux density. It neither ionises nor breaks valence bonds at 0.1 and 1 AMFU. In some molecules under consideration flux density of 10 and 100AMFU some C-H and C-C bonds were broken. Some irregularities were observed in the changes of positive and negative charge densities and bond lengths against increasing flux density. They provide evidence that

molecules slightly change their initially fixed positions with respect to the force lines of the magnetic field. The length of some bonds and bond angles change with an increase in the applied flux density providing, in some cases, polar interactions between atoms through space.

Conclusions: SMF destabilizes lipid acids and caproyl glycerides irregularly against increasing flux density. That irregularity results from the ability of those molecules to twist out of the initially established SMF plain and squeeze molecules around some bonds. In some molecules SMF flux density of 10 AMFU and above breaks some valence bonds and only in case of elaidic acid the *trans-cis* conversion is observed. Depending on the structure and applied flux density SMF either stimulates or inhibits metabolic processes of the lipids under study.

Keywords

di-acyl glycerides, elaidic acid, linoleic acid, linolenic acid, mono-acyl glycerides oleic acid, stearic acid, *trans*-linolenic acid, tri-acyl glycerides, vaccenic acid

Introduction

Environmental pollution with magnetic fields (Hamza et al. 2002; Rankovic and Radulovic 2009; Committee to Assess the Current Status and Future Direction of High Magnetic Field Science in the United States 2013; Bao and Guo 2021; Tang et al. 2021) evokes a concern about its effect upon organisms of flora and fauna (Steiner and Ulrich 1989; Kohno et al. 2000; Woodward 2002; Andreini et al. 2008; Rittie and Perbal 2008; Buchachenko 2009; Buchachenko et al. 2012; Buchachenko 2014; Jaworska et al. 2014; Buchachenko 2016; Jaworska et al. 2016; Jaworska et al. 2017; Letuta and Berdinskiy 2017; Xu 2018; Beretta et al. 2019). This problem was extensively addressed in our former papers. In those papers the effect of static magnetic field (SMF) of 0 to 100T AMFU (Arbitrary Magnetic Field Unit; here 1AMFU > 1000 T) upon simple inorganic molecules (Ciesielski et al. 2021) alkanols (Ciesielski et al. 2022a), carbohydrates (Ciesielski et al. 2022b), porphine (Ciesielski et al. 2022c) and metalloporphyrines (Ciesielski et al. 2022d) was simulated involving *in silico* (computer vacuum) advanced computational methods.

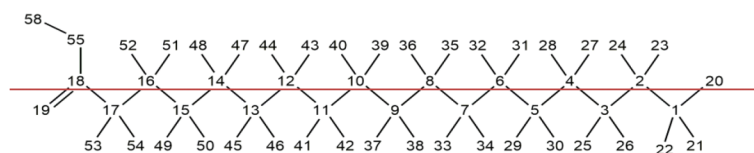
This paper presents results of such computations for selected higher lipid acids belonging to the group of derived lipids and mono-, di- and tri-glycerides constituting a group of simple lipids (Heinz 1996; Berg et al. 2019; Coones et al. 2021). These lipids, in general, co-constitute biological membranes and triglycerides, located in adipose tissue, play a role of a major form of energy storage of animals and plants (Brasaemle 2007; Sul 2017; Berg et al. 2019) and cooperate in elasticity of skin.

Focus on lipids can be rationalized also for their role in the consumption, diet and functional properties of foodstuffs (see, for instance, Sena et al. 2022; Bharti et al. 2023). Recently, the role of static magnetic field (SMF) in building suitable functional properties of foodstuff attracted considerable attention (Arteaga Miñano et al. 2020; Otero and Pozo 2022). Also a specific use of magnetic field in molecular imaging and diagnosis could be mentioned. Magnetic nanomaterial additives are used in this case (Yao and Xu 2014).

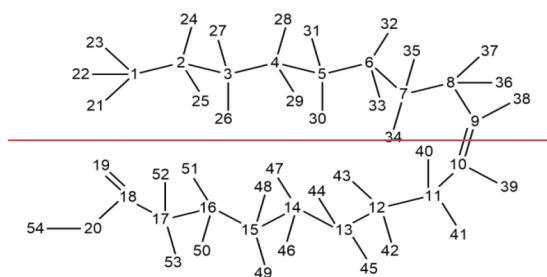
Numerical computations

Computations of the effect of real SMF 0.0, 0.1, 1, 10 and 100 AMFU (Arbitrary Magnetic Field Unit; here $1\text{AMFU} \geq 1000\text{ T}$) flux density were performed in silico (computer vacuum), involving advanced computational methods.

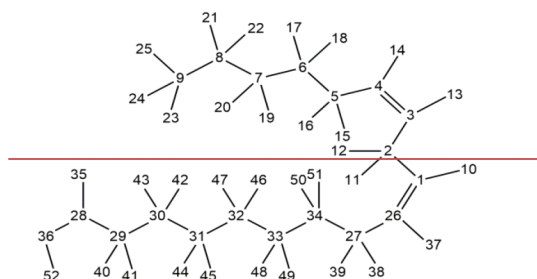
Molecular structures were drawn using the Fujitsu SCIGRESS 2.0 software (Froimowitz 1993; Marchand et al. 2014). Their principal symmetry axes were orientated along the x-axis of the Cartesian system. Molecules were situated inside a three-axial ellipsoid. The longest axis of that ellipsoid was accepted as the x-axis and the shortest quasi-perpendicular axis considered as the z-axis. The magnetic field was fixed in the same direction, along the x-axis with the south pole from the left side, marked in pictures with red line. Orientation of the molecules along the x-axis is presented in Fig. 1.



Octadecanoic (stearic) acid

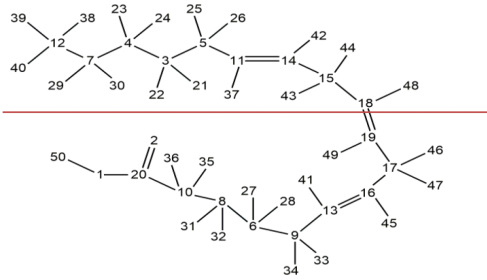


Octadec-9-enoic (oleic) acid

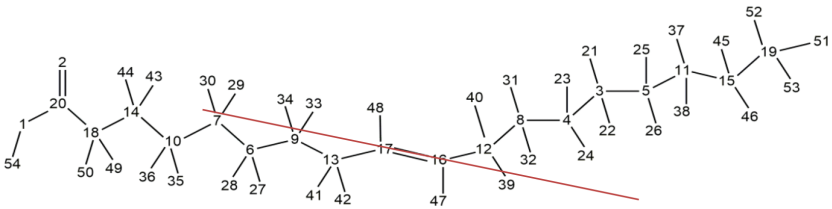


cis,cis-Octadec-9,12-dienoic (linoleic) acid

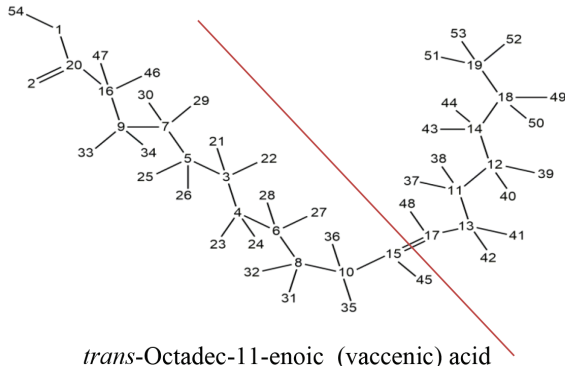
Figure 1. Numbering atoms in the molecules of lipid fatty acid and caproyl glycerides without following the geometry.



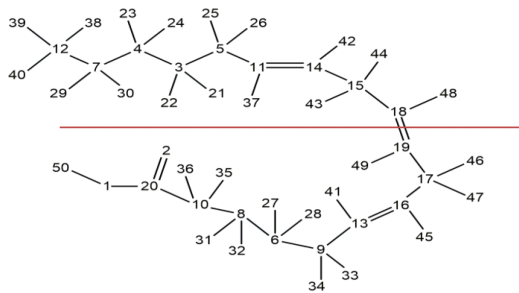
all cis-Octadec-6,9,12-trienoic acid



trans-Octadec-9-enoic – (elaidic) acid

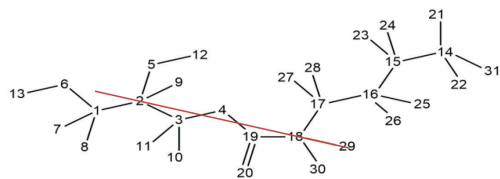


trans-Octadec-11-enoic (vaccenic) acid

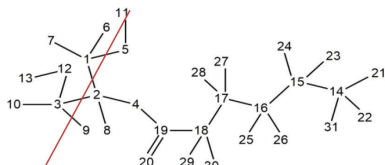


all trans-Octadec-6,9,12-trienoic (*trans*-linolenic) acid

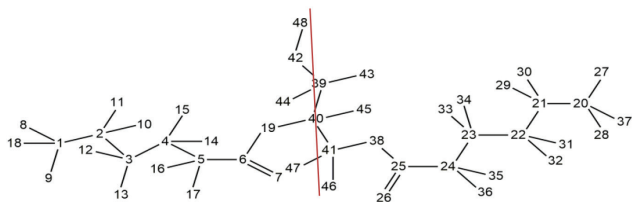
Figure 1. Continued.



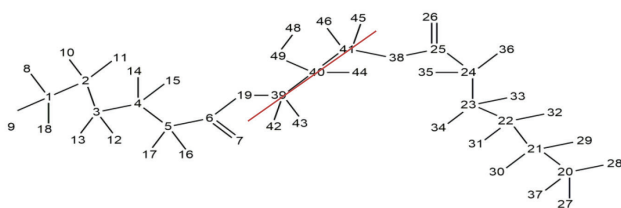
1-Caproyl glyceride



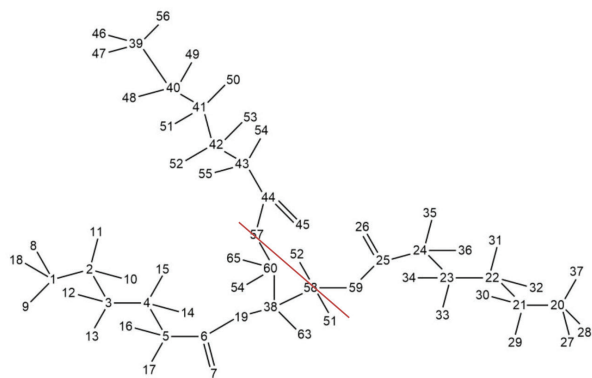
2-Caproyl glyceride



1,2-Dicaproyl glyceride



1,3-Dicaproyl glyceride



1,2,3-Tricaproyl glyceride

Figure 1. Continued.

Subsequently, involving Gaussian 0.9 software equipped with the 6-31G** basis (Frisch et al. 2016), the molecules were optimised and all values of bond length, dipole moment, heat of formation, bond energy and total energy for systems were computed.

In the consecutive steps, the influence of the static magnetic field (SMF) upon optimised molecules was computed with Amsterdam Modelling Suite software (Farberovich and Mazalova 2016; Charistos and Muñoz-Castro 2019) and the NR_LDOTB (non-relativistically orbital momentum L-dot-B) method (Glendening et al. 1987; Carpenter and Weinhold 1988). Following that step, values of bond length, dipole moment, heat of formation equal to the energy of dissociation and charges at the atoms were calculated using Gaussian 0.9 software equipped with the 6-31G** basis (Marchand et al. 2014).

Numbering atoms in particular molecules under consideration are presented in Fig. 1.

Results

Presentation of effect of SMF of flux density from 0 to 100 AMFU upon heat of formation and dipole moment of selected lipid acids (Table 1) and caproyl glycerides (Table 2). Tables 3–6 collect results of SMF effect upon charge density solely on atoms directly participating in biological activity of considered lipids and bond lengths between those atoms. In case of SMF of flux density generating radical scission of the

Table 1. Effect of SMF of increasing flux density upon heat of formation and dipole moment of lipid acids.

| Lipid acids | Heat of formation [kJ·mol ⁻¹] at SMF flux density [AMFU] | | | | | Dipole moment [D] at SMF flux density [AMFU] | | | | |
|-------------------------|----------------------------------------------------------------------|------|------|------|------------------|----------------------------------------------|------|------|------|------------------|
| | 0 | 0.1 | 1.0 | 10 | 100 ^a | 0 | 0.1 | 1.0 | 10 | 100 ^a |
| Stearic | -560 | -531 | -511 | -492 | -416(25.7) | 3.42 | 3.56 | 3.84 | 4.16 | 5.32(35.7) |
| Oleic | -676 | -654 | -621 | -594 | -542(19.8) | 1.88 | 1.92 | 2.06 | 2.63 | 3.01(34.2) |
| Linoleic | -565 | -510 | -457 | -401 | -326(42.3) | 2.39 | 2.45 | 2.63 | 2.95 | 3.06(21.3) |
| Linolenic | -485 | -423 | -404 | -364 | -318(34.5) | 1.76 | 1.86 | 2.18 | 2.63 | 3.28(43.3) |
| Elaidic | -642 | -612 | -586 | -527 | -461(28.2) | 4.51 | 4.68 | 4.77 | 5.16 | 6.24(27.7) |
| Vaccenic | -672 | -653 | -591 | -521 | -423(27.0) | 1.88 | 1.96 | 2.23 | 2.84 | 3.67(48.7) |
| <i>trans</i> -Linolenic | -421 | -401 | -372 | -341 | -216(48.7) | 1.66 | 1.74 | 1.96 | 2.65 | 3.15(47.3) |

^aThe final increase (in %) in the reported value at applied SMF of 100 AMFU is given in parentheses.

Table 2. Effect of SMF of increasing flux density upon heat of formation and dipole moment of caproyl glycerides.

| Caproyl glyceride | Heat of formation [kJ·mol ⁻¹] at SMF flux density [AMFU] | | | | | Dipole moment [D] at SMF flux density [AMFU] | | | | |
|-------------------|----------------------------------------------------------------------|------|------|------|------------------|----------------------------------------------|------|------|------|------------------|
| | 0 | 0.1 | 1.0 | 10 | 100 ^a | 0 | 0.1 | 1.0 | 10 | 100 ^a |
| 1-Caproyl | -192 | -182 | -168 | -136 | -110 (42.7) | 3.43 | 3.53 | 3.98 | 4.65 | 6.52 (90.0) |
| 2-Caproyl | -187 | -172 | -151 | -123 | -96 (48.7) | 1.41 | 1.45 | 1.76 | 3.12 | 4.96 (71.6) |
| 1,2-Dicaproyl | -263 | -252 | -237 | -196 | -118 (55.1) | 4.06 | 4.38 | 4.98 | 5.31 | 7.15 (42.1) |
| 1,3-Dicaproyl | -213 | -207 | -195 | -171 | -138 (35.3) | 1.42 | 1.52 | 1.95 | 2.69 | 3.99 (64.7) |
| 1,2,3-Tricaproyl | -384 | -363 | -335 | -239 | -156 (58.3) | 2.38 | 2.48 | 2.95 | 3.69 | 7.21 (67.0) |

^aThe final increase (in %) in the reported value at applied SMF of 100 AMFU is given in parentheses.

| SMF [AMFU] | | Charge density [a.u.] on particular atoms at SMF flux density | | | | | | | | | | | | | | | | | | | | | | | | | | |
|---------------|--|---------------------------------------------------------------------------|-------|------|-------|-------|------|-------|-------|------|-------|-------|-------|-------|-------|-------|-------|------|-------|------|-------|-------|-------|------|-------|-------|------|------|
| | | Octadecanoic (stearic) acid | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | <i>trans</i> -Octadec-11-enoic (vaccenic) acid | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | H54 | O1 | =C20 | =O2 | C16 | H46 | H47 | C9 | H33 | H34 | =C15 | H35 | =C17 | H45 | C13 | H41 | C12 | H39 | C10 | H35 | C18 | H32 | | | | | |
| 0 | | .242 | -.341 | .324 | -.340 | -.169 | .118 | -.156 | .095 | .095 | -.161 | .122 | -.157 | .121 | | | | | | | | | | | | | | |
| 0.1 | | .255 | -.356 | .325 | -.341 | -.157 | .120 | -.164 | .096 | .097 | -.164 | .124 | -.159 | .121 | | | | | | | | | | | | | | |
| 1 | | .268 | -.371 | .326 | -.341 | -.165 | .122 | -.169 | .098 | .096 | -.166 | .125 | -.171 | .121 | | | | | | | | | | | | | | |
| 10 | | .314 | -.409 | .325 | -.349 | -.150 | .123 | -.178 | .085 | .104 | -.168 | .127 | -.174 | .121 | | | | | | | | | | | | | | |
| 100 | | | | | | | | | | | | | | | -.085 | .038 | -.120 | .085 | -.169 | .134 | -.118 | -.069 | | | | | | |
| | | <i>all trans</i> -Octadec-6,9,12-trienoic (<i>trans</i> -linolenic) acid | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | | H50 | O1 | =C20 | =O2 | C10 | H35 | H36 | C8 | H31 | H32 | =C13 | H41 | =C16 | H45 | C15 | H44 | =C19 | H49 | =C18 | H48 | =C14 | H42 | H37 | C12 | H39 | H40 | |
| 0 | | .239 | -.315 | .311 | -.346 | -.165 | .115 | .113 | -.154 | .094 | .104 | -.165 | .120 | -.160 | .120 | | | | -.150 | .117 | -.162 | .110 | -.166 | .117 | -.163 | .124 | | |
| 0.1 | | .204 | -.418 | .345 | -.252 | -.170 | .126 | .125 | -.174 | .093 | .103 | -.200 | .142 | -.210 | .142 | | | | -.161 | .124 | -.187 | .118 | -.162 | .119 | -.162 | .121 | | |
| 1 | | .240 | -.357 | .313 | -.375 | -.155 | .134 | .133 | -.153 | .101 | .109 | -.191 | .154 | -.177 | .154 | | | | -.139 | .137 | -.172 | .125 | -.157 | .118 | -.159 | .125 | | |
| 10 | | .247 | -.345 | .307 | -.413 | -.152 | .139 | .138 | -.150 | .106 | .112 | -.180 | .149 | -.166 | .149 | | | | -.134 | .137 | -.167 | .123 | -.150 | .117 | -.158 | .126 | | |
| 100 | | | | | | | | | | | | | | | | -.103 | .083 | | | | | | | | | -.101 | .008 | .017 |

| SMF [AMFU] | Atom – atom bond lengths [Å] at SMF flux density | | | | | | | | | | | | | | | | | | | |
|---------------------------------------------------------------------------|--------------------------------------------------|------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| | Octadecanoic (stearic) acid | | | | | | | | | | | | | | | | | | | |
| <i>trans</i> -Octadec-9-enoic – (elaidic) acid | | | | | | | | | | | | | | | | | | | | |
| | H54- O1 | C20- O2 | C18- H49 | C18- H50 | C14- H44 | C14- H43 | C17- O6 | C17- H48 | C17- H47 | | | | | | | | | | | |
| 0 | 0.977 | 1.369 | 1.197 | 1.581 | 1.110 | 1.113 | 1.533 | 1.109 | 1.335 | 1.088 | 1.088 | | | | | | | | | |
| 0.1 | 1.605 | 1.519 | 1.407 | 1.529 | 1.647 | 1.628 | 1.617 | 1.628 | 1.379 | 1.347 | 1.459 | | | | | | | | | |
| 1 | 1.732 | 1.529 | 1.402 | 1.522 | 1.019 | 1.657 | 1.618 | 1.624 | 1.599 | 1.358 | 1.327 | 1.423 | | | | | | | | |
| <i>trans</i> -Octadec-11-enoic (vaccenic) acid | | | | | | | | | | | | | | | | | | | | |
| | H54- O1 | C20= | C18- H49 | C16- H47 | C15- H45 | C15= | C12- H39 | C10- H35 | C9- C7 | C8- H32 | C7- H48 | C7- H30 | C7- H29 | | | | | | | |
| 0 | 0.987 | 1.362 | 1.202 | 1.493 | 1.113 | 1.112 | 1.088 | 1.335 | 1.331 | 1.088 | 1.108 | 1.106 | | | | | | | | |
| 0.1 | 1.062 | 1.374 | 1.206 | 1.488 | 1.152 | 1.110 | 1.113 | 1.361 | 1.520 | 1.076 | 1.195 | 1.122 | | | | | | | | |
| 1 | 1.128 | 1.385 | 1.210 | 1.483 | 1.183 | 1.187 | 1.130 | 1.383 | 1.509 | 1.068 | 1.130 | 1.267 | | | | | | | | |
| 10 | 1.360 | 1.407 | 1.224 | 1.478 | 1.249 | 1.118 | 1.145 | 1.428 | 1.483 | 1.072 | 1.158 | 1.436 | | | | | | | | |
| 100 | | | | 2.487 | | | | | 2.005 | 2.256 | 2.132 | | | | | | | | | |
| <i>all trans</i> -Octadec-6,9,12-trienoic (<i>trans</i> -linolenic) acid | | | | | | | | | | | | | | | | | | | | |
| | H50- O1 | C20= | C10- H36 | C10- H35 | C8- H31 | C8- H32 | C13= | C13- H41 | C16- H45 | C16- H47 | C17- H47 | C18- H48 | C18- H49 | C19- H49 | C19- H38 | C14- H42 | C14- H41 | C11- H37 | C12- H39 | C12- H40 |
| 0 | 0.981 | 1.358 | 1.222 | 1.508 | 1.096 | 1.096 | 1.528 | 1.097 | 1.341 | 1.087 | 1.087 | 1.501 | 1.099 | 1.089 | 1.088 | 1.341 | 1.057 | | | |
| 0.1 | 0.984 | 1.512 | 1.229 | 1.490 | 1.104 | 1.104 | 1.523 | 1.105 | 1.115 | 1.789 | 1.068 | 1.064 | 1.260 | 1.099 | 1.058 | 1.100 | 1.376 | 1.097 | | |
| 1 | 0.970 | 1.477 | 1.345 | 1.405 | 1.104 | 1.104 | 1.526 | 1.117 | 1.108 | 1.632 | 1.037 | 1.064 | 1.494 | 1.051 | 1.102 | 1.337 | 1.097 | | | |
| 10 | 0.939 | 1.481 | 1.441 | 1.382 | 1.110 | 1.109 | 1.519 | 1.110 | 1.119 | 1.577 | 1.121 | 1.132 | 1.417 | 1.112 | 1.106 | 1.105 | 1.353 | 1.100 | | |
| 100 | | | | | | | | | | 2.270 | | | | | | | | | 2.088 | 2.270 |

Table 5. Charge density on selected atoms of mono-, di- and tricaproyl glycerides.

| SMF [AMFU] | Charge density [a.u.] on particular atoms at SMF flux density | | | | | | | | | | | | | | | | | | | | | | | | | |
|----------------------------|---------------------------------------------------------------|------|------|------|------|------|------|------|------|------|-------------------------|-------|------|-------|-------|------|-------|------|-------|------|-------|------|-------|------|------|------|
| | 1-Caproyl glyceride | | | | | | | | | | 1,2-Dicaproyl glyceride | | | | | | | | | | | | | | | |
| | C18 | H29 | H30 | C19 | O20 | O4 | C3 | H11 | H10 | C2 | H9 | H10 | O12 | H13 | C1 | H6 | H7 | H8 | O6 | H13 | | | | | | |
| 0 | -152 | .121 | .121 | .291 | -354 | -248 | -064 | .107 | .098 | .040 | .092 | -319 | .212 | .000 | .075 | .066 | -.323 | .204 | | | | | | | | |
| 0.1 | -157 | .136 | .135 | 200 | -424 | -213 | -071 | .113 | .184 | .045 | .092 | -312 | .214 | -005 | .077 | .056 | -.316 | .205 | | | | | | | | |
| 1 | -258 | .167 | .170 | .337 | -431 | -233 | -057 | .088 | .084 | .046 | .087 | -.323 | .215 | -006 | .077 | .065 | -.316 | .205 | | | | | | | | |
| 10 | -223 | .158 | .189 | .327 | -434 | -252 | -031 | .080 | .089 | .065 | .075 | -.383 | .245 | .023 | .068 | .064 | -.387 | .244 | | | | | | | | |
| 100 | -135 | .145 | .101 | .280 | -390 | -287 | -013 | .070 | .078 | .034 | .063 | -.365 | .272 | .003 | .077 | .072 | -.392 | .262 | | | | | | | | |
| 2-Caproyl glyceride | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | C18 | H29 | H30 | C19 | O20 | O4 | C2 | H8 | H8 | C39 | H9 | H10 | O12 | H13 | C1 | H6 | H7 | O5 | H11 | | | | | | | |
| 0 | -155 | .120 | .118 | .301 | -379 | -226 | .047 | .119 | -041 | .041 | .091 | .350 | .277 | -008 | .058 | .080 | -.319 | .211 | | | | | | | | |
| 0.1 | -147 | .132 | .131 | .290 | -443 | -215 | .056 | .131 | .007 | .083 | .053 | -.328 | .382 | -004 | .048 | .070 | -.312 | .223 | | | | | | | | |
| 1 | -166 | .114 | .110 | .312 | -347 | -242 | .055 | .111 | -082 | .124 | .042 | -.379 | .273 | -006 | .051 | .091 | -.315 | .210 | | | | | | | | |
| 10 | -143 | .139 | .135 | .279 | -482 | -185 | .051 | .131 | -047 | .113 | -012 | -.362 | .309 | -014 | .060 | .086 | -.314 | .212 | | | | | | | | |
| 100 | -179 | .126 | .110 | .331 | -378 | -251 | .012 | .121 | -014 | .158 | .038 | -.380 | .209 | -003 | .052 | .097 | -.320 | .214 | | | | | | | | |
| 1,2-Dicaproyl glyceride | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | C5 | H16 | H17 | C6 | O7 | O19 | C40 | H45 | C39 | H43 | H44 | O42 | H48 | C41 | H46 | H47 | O38 | C25 | O26 | C24 | H35 | H36 | | | | |
| 0 | -152 | .121 | .128 | .289 | -351 | -216 | .029 | .124 | -006 | .085 | .070 | -.332 | .205 | -071 | .150 | .094 | -.243 | .290 | -.353 | -152 | .118 | .121 | | | | |
| 0.1 | -171 | .128 | .128 | .127 | -374 | -236 | .044 | .124 | -007 | .049 | .071 | -.354 | .253 | -065 | .038 | .139 | -.297 | .306 | -.318 | -157 | .123 | .128 | | | | |
| 1 | -168 | .129 | .129 | .130 | -394 | -239 | .048 | .118 | -003 | .033 | .034 | -.370 | .336 | -053 | .0103 | .161 | -.254 | .288 | -.401 | -157 | .129 | .132 | | | | |
| 10 | -182 | .115 | .115 | .121 | -330 | -291 | .060 | .107 | -013 | .033 | .058 | -.386 | .326 | -067 | .092 | .129 | -.278 | .309 | -.337 | -176 | .124 | .119 | | | | |
| 100 | -165 | .132 | .132 | .125 | -387 | -245 | .111 | .056 | -026 | .028 | .079 | -.371 | .299 | -056 | .102 | .144 | -.279 | .295 | -.379 | -170 | .139 | .127 | | | | |
| 1,3-Dicaproyl glyceride | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | C24 | H35 | H36 | C25 | O26 | O30 | C41 | H45 | H46 | C40 | H44 | O49 | H48 | C39 | H42 | H43 | O19 | C6 | O7 | C5 | H16 | H17 | | | | |
| 0 | -152 | .120 | .117 | .288 | -363 | -229 | .013 | .105 | .110 | .034 | .092 | -315 | .207 | -062 | .119 | .088 | -.242 | .289 | -.335 | -152 | .120 | .121 | | | | |
| 0.1 | -155 | .123 | .120 | .303 | -331 | -254 | -034 | .127 | .103 | .045 | .089 | -311 | .213 | -059 | .395 | .088 | -.231 | .285 | -.485 | -158 | .124 | .131 | | | | |
| 1 | -124 | .140 | .128 | .339 | -144 | -342 | -031 | -297 | .136 | .072 | .115 | -.326 | .229 | -040 | .123 | .115 | -.260 | .309 | -.405 | -179 | .124 | .128 | | | | |
| 10 | -134 | .145 | .129 | .337 | -174 | -353 | -001 | -262 | .157 | .067 | .141 | -.344 | .218 | -036 | .139 | .084 | -.281 | .282 | -.488 | -164 | .134 | .153 | | | | |
| 100 | -154 | .150 | .134 | .340 | -230 | -387 | -039 | -043 | .158 | .159 | .154 | -.406 | .055 | -085 | .193 | .158 | -.292 | .226 | -.479 | -199 | .123 | .137 | | | | |
| 1,2,3-Tricaproyl glyceride | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | C5 | H16 | H17 | C6 | O7 | O19 | C38 | H63 | C60 | H64 | H56 | O57 | C44 | O45 | C43 | H54 | H55 | C58 | H51 | H52 | O59 | C25 | C26 | C24 | H35 | H31 |
| 0 | -151 | .121 | .295 | .295 | -359 | -227 | .028 | .122 | -073 | .145 | .112 | -.142 | .285 | -.354 | -153 | .118 | .119 | -023 | .103 | .117 | -.241 | .291 | -.354 | -152 | .120 | .120 |
| 0.1 | -151 | .125 | .291 | .291 | -379 | -222 | .030 | .125 | .000 | .157 | .112 | -.242 | .283 | -365 | -149 | .120 | .120 | -023 | .110 | .122 | -.215 | .283 | -.413 | -157 | .135 | .135 |
| 1 | -216 | .134 | .322 | .322 | -399 | -241 | .041 | .128 | -077 | .152 | .114 | -.249 | .289 | -383 | -157 | .121 | .125 | -022 | .107 | .114 | -.238 | .328 | -411 | -218 | .148 | .158 |
| 10 | -247 | .147 | .338 | .388 | -390 | -269 | .061 | .120 | -073 | .153 | .103 | -.251 | .289 | -377 | -151 | .123 | .118 | -084 | .097 | .108 | -.272 | .346 | -412 | -214 | .145 | .151 |
| 100 | -213 | .116 | .315 | .315 | -412 | -261 | .039 | .125 | -059 | .158 | .105 | -.250 | .290 | -389 | -158 | .125 | .120 | -008 | .110 | .117 | -.283 | .320 | -.426 | -177 | .145 | .155 |

Table 6. SMF flux density dependent bond lengths [\AA] between selected particular atoms in molecules of mono-, di- and tri-caproyl glycerides.

| SMF [AMFU] | Bond length [\AA] between particular atoms at SMF flux density | | | | | | | | | | | | | | | | | | | | | | | |
|------------|---------------------------------------------------------------------------|----------|----------|----------|----------|----------|----------|--------|----------|----------|--------|-------|----------|----------|-------|----------|----------|----------|----------|----------|----------|----------|----------|--------|
| | 1-Caproyl glyceride | | | | | | | | | | | | | | | | | | | | | | | |
| | C18- H29 | C18- H30 | C18- H29 | C19- O20 | C19- O20 | O4- C3 | H11 | C2- H9 | O5- H12 | C2- O5 | C3- H9 | H10 | O12- H13 | C3- H9 | H10 | O12- H13 | C2- O5 | C3- H9 | H10 | O12- H13 | C1- H7 | C1- H8 | O6 | H13 |
| 0 | 1.090 | 1.090 | 1.520 | 1.220 | 1.360 | 1.430 | 1.090 | 1.540 | 0.960 | 1.430 | 0.960 | 1.540 | 0.960 | 1.430 | 0.960 | 1.540 | 0.960 | 1.430 | 0.960 | 1.540 | 1.102 | 1.105 | 1.435 | 0.971 |
| 0.1 | 1.122 | 1.122 | 1.448 | 1.391 | 1.365 | 1.428 | 1.103 | 1.556 | 1.105 | 1.400 | 0.960 | 1.550 | 1.102 | 1.105 | 1.435 | 0.971 | 1.105 | 1.400 | 0.960 | 1.550 | 1.102 | 1.105 | 1.435 | 0.971 |
| 1 | 1.350 | 1.336 | 1.388 | 1.499 | 1.471 | 1.370 | 1.126 | 1.616 | 1.200 | 1.409 | 0.983 | 1.597 | 1.128 | 1.131 | 1.481 | 0.993 | 1.128 | 1.409 | 0.983 | 1.597 | 1.128 | 1.131 | 1.481 | 0.993 |
| 10 | 1.512 | 1.753 | 1.426 | 1.469 | 1.507 | 1.391 | 1.136 | 1.578 | 1.222 | 1.388 | 1.006 | 1.591 | 1.124 | 1.155 | 1.438 | 1.086 | 1.124 | 1.388 | 1.006 | 1.591 | 1.124 | 1.155 | 1.438 | 1.086 |
| 100 | 1.007 | 3.558 | 1.454 | 1.390 | 1.476 | 1.395 | 1.151 | 1.592 | 1.330 | 1.336 | 1.822 | 1.663 | 1.186 | 1.133 | 1.413 | 1.296 | 1.186 | 1.336 | 1.822 | 1.663 | 1.186 | 1.133 | 1.413 | 1.296 |
| | 2-Caproyl glyceride | | | | | | | | | | | | | | | | | | | | | | | |
| | C16- H29 | C16- H30 | C18- C19 | C19- O20 | O4- C2 | C2- C3 | H9 | C3- H9 | H10 | O12- H13 | C3- H9 | H10 | O12- H13 | C3- H9 | H10 | O12- H13 | C3- H9 | H10 | O12- H13 | C1- H7 | C1- H6 | O5 | H11 | |
| 0 | 1.129 | 1.143 | 1.495 | 1.234 | 1.366 | 1.430 | 1.527 | 1.190 | 1.139 | 1.295 | 1.415 | 1.528 | 1.138 | 1.129 | 1.371 | 0.983 | 1.138 | 1.129 | 1.371 | 1.138 | 1.129 | 1.371 | 0.983 | |
| 0.1 | 1.152 | 1.175 | 1.433 | 1.360 | 1.354 | 2.456 | 1.487 | 1.172 | 1.254 | 1.184 | 1.537 | 1.509 | 1.172 | 1.148 | 1.325 | 1.005 | 1.172 | 1.148 | 1.325 | 1.172 | 1.148 | 1.325 | 1.005 | |
| 1 | 1.135 | 1.162 | 1.528 | 1.175 | 1.378 | 1.430 | 1.482 | 1.113 | 1.251 | 1.462 | 1.638 | 1.520 | 1.163 | 1.143 | 1.373 | 0.979 | 1.163 | 1.143 | 1.373 | 1.163 | 1.143 | 1.373 | 0.979 | |
| 10 | 1.145 | 1.150 | 1.433 | 1.424 | 1.334 | 1.434 | 1.549 | 1.160 | 1.267 | 1.281 | 1.823 | 1.524 | 1.169 | 1.144 | 1.356 | 0.983 | 1.169 | 1.144 | 1.356 | 1.169 | 1.144 | 1.356 | 0.983 | |
| 100 | 1.183 | 1.255 | 1.481 | 1.188 | 1.343 | 1.449 | 1.600 | 1.217 | 1.327 | 1.320 | 2.799 | 1.547 | 1.176 | 1.129 | 1.353 | 1.035 | 1.176 | 1.129 | 1.353 | 1.176 | 1.129 | 1.353 | 1.035 | |
| | 1,2-Dicaproyl glyceride | | | | | | | | | | | | | | | | | | | | | | | |
| | C5- H16 | C5- H17 | C6- O7 | O19- C40 | H45 | C40- H45 | C39- H44 | H43 | O42- H48 | C40- H43 | H44 | H43 | O42- H48 | C40- H43 | H44 | H43 | O42- H48 | C40- H43 | H44 | H43 | O42- H48 | C41- H47 | O38 | C23 |
| 0 | 1.090 | 1.090 | 1.220 | 1.360 | 1.430 | 1.090 | 1.540 | 1.090 | 1.430 | 0.950 | 1.540 | 1.090 | 1.430 | 0.950 | 1.540 | 1.090 | 1.430 | 0.950 | 1.540 | 1.090 | 1.430 | 1.360 | 1.220 | 1.520 |
| 0.1 | 1.173 | 1.172 | 1.463 | 1.262 | 1.418 | 1.454 | 1.136 | 1.567 | 1.130 | 1.170 | 1.392 | 1.283 | 1.527 | 1.130 | 1.205 | 1.400 | 1.457 | 1.205 | 1.400 | 1.457 | 1.205 | 1.469 | 1.123 | 1.201 |
| 1 | 1.193 | 1.184 | 1.253 | 1.289 | 1.395 | 1.460 | 1.145 | 1.545 | 1.240 | 1.159 | 1.280 | 1.729 | 1.524 | 1.129 | 1.160 | 1.455 | 1.361 | 1.301 | 1.456 | 1.125 | 1.255 | 1.498 | 1.125 | 1.255 |
| 10 | 1.199 | 1.177 | 1.480 | 1.193 | 1.437 | 1.435 | 1.109 | 1.572 | 1.252 | 1.128 | 1.317 | 2.656 | 1.658 | 1.124 | 1.410 | 1.388 | 1.198 | 1.480 | 1.186 | 1.294 | 1.533 | 1.480 | 1.186 | 1.294 |
| 100 | 1.268 | 1.220 | 1.484 | 1.296 | 1.420 | 1.429 | 1.185 | 1.596 | 1.332 | 1.148 | 1.312 | 3.037 | 1.527 | 1.177 | 1.109 | 1.440 | 1.421 | 1.298 | 1.446 | 1.122 | 1.396 | 1.501 | 1.446 | 1.122 |
| | 1,3-Dicaproyl glyceride | | | | | | | | | | | | | | | | | | | | | | | |
| | C24- H35 | C24- H36 | C25- O26 | O30- C41 | H45 | C41- H45 | C40- H44 | H44 | O47- H48 | C40- H44 | H44 | H43 | O47- H48 | C40- H44 | H44 | H43 | O47- H48 | C40- H44 | H44 | H43 | O47- H48 | C39- H42 | C39- H43 | C5- C4 |
| 0 | 1.090 | 1.090 | 1.520 | 1.220 | 1.360 | 1.430 | 1.090 | 1.540 | 1.090 | 1.420 | 0.960 | 1.540 | 1.090 | 1.420 | 0.960 | 1.540 | 1.090 | 1.420 | 0.960 | 1.540 | 1.090 | 1.420 | 0.960 | 1.540 |
| 0.1 | 1.137 | 1.119 | 1.495 | 1.207 | 1.427 | 1.374 | 1.124 | 1.110 | 1.506 | 1.161 | 1.422 | 1.011 | 1.527 | 1.161 | 1.110 | 1.457 | 1.324 | 1.292 | 1.486 | 1.118 | 1.200 | 1.504 | 1.486 | 1.118 |
| 1 | 1.140 | 1.129 | 1.444 | 1.152 | 1.731 | 1.257 | 1.350 | 1.155 | 1.507 | 1.280 | 1.408 | 1.101 | 1.502 | 1.110 | 1.135 | 1.508 | 1.325 | 1.278 | 1.486 | 1.127 | 1.173 | 1.470 | 1.486 | 1.127 |
| 10 | 1.270 | 1.135 | 1.451 | 1.195 | 1.762 | 1.339 | 2.448 | 1.135 | 1.470 | 1.250 | 1.461 | 1.099 | 1.412 | 1.157 | 1.135 | 1.457 | 1.539 | 1.442 | 1.528 | 1.155 | 1.733 | 1.533 | 1.528 | 1.155 |
| 100 | 1.340 | 1.127 | 1.497 | 1.241 | 1.816 | 1.478 | 2.607 | 1.147 | 1.408 | 1.208 | 1.516 | 1.101 | 1.468 | 1.208 | 1.091 | 1.468 | 1.868 | 1.621 | 1.508 | 1.203 | 1.727 | 1.549 | 1.621 | 1.508 |

| SMF [AMFU] | Bond length [Å] between particular atoms at SMF flux density | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|---------------|--------------------------------------------------------------|------------|-----------|-----------|------------|------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| | 1-Caproyl glyceride | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | C5- H16 | C5- H17 | C6- O7 | C6- O7 | C6- O19 | C6- O19 | C38- H63 | C38- H63 | C60- H54 | C60- H65 | C60- H65 | C60- O57 | C60- O57 | C44- O45 | C44- O45 | C43- H54 | C43- H55 | C43- H55 | C43- H54 | C38- H61 | C38- H62 | C58- H61 | C58- H62 | O59- O26 | O59- O26 | C25- O26 | C25- O26 | C24- H36 | C24- H36 |
| 0 | 1.090 | 1.090 | 1.520 | 1.220 | 1.360 | 1.430 | 1.090 | 1.540 | 1.090 | 1.115 | 1.102 | 1.430 | 1.220 | 1.360 | 1.540 | 1.090 | 1.090 | 1.090 | 1.090 | 1.540 | 1.090 | 1.090 | 1.430 | 1.360 | 1.220 | 1.360 | 1.520 | 1.090 | 1.090 |
| 0.1 | 1.119 | 1.115 | 1.508 | 1.470 | 1.373 | 1.448 | 1.108 | 1.510 | 1.115 | 1.102 | 1.437 | 1.360 | 1.254 | 1.520 | 1.095 | 1.095 | 1.125 | 1.096 | 1.521 | 1.534 | 1.108 | 1.107 | 1.427 | 1.387 | 1.378 | 1.451 | 1.134 | 1.131 | 1.131 |
| 1 | 1.351 | 1.359 | 1.475 | 1.295 | 1.476 | 1.401 | 1.476 | 1.400 | 1.120 | 1.164 | 1.475 | 1.376 | 1.291 | 1.510 | 1.125 | 1.125 | 1.572 | 1.572 | 1.572 | 1.572 | 1.128 | 1.129 | 1.418 | 1.414 | 1.397 | 1.403 | 1.334 | 1.385 | 1.385 |
| 10 | 1.469 | 1.432 | 1.502 | 1.740 | 1.476 | 1.401 | 1.476 | 1.551 | 1.172 | 1.172 | 1.451 | 1.377 | 1.285 | 1.532 | 1.116 | 1.116 | 1.550 | 1.550 | 1.550 | 1.550 | 1.136 | 1.126 | 1.432 | 1.418 | 1.393 | 1.435 | 1.342 | 1.486 | 1.486 |
| 100 | 2.177 | 2.182 | 1.554 | 1.311 | 1.388 | 1.388 | 1.515 | 1.167 | 1.248 | 1.178 | 1.499 | 1.360 | 1.381 | 1.515 | 1.124 | 1.292 | 1.624 | 1.524 | 1.524 | 1.129 | 1.117 | 1.452 | 1.407 | 1.423 | 1.431 | 1.090 | 2.364 | 2.364 | |

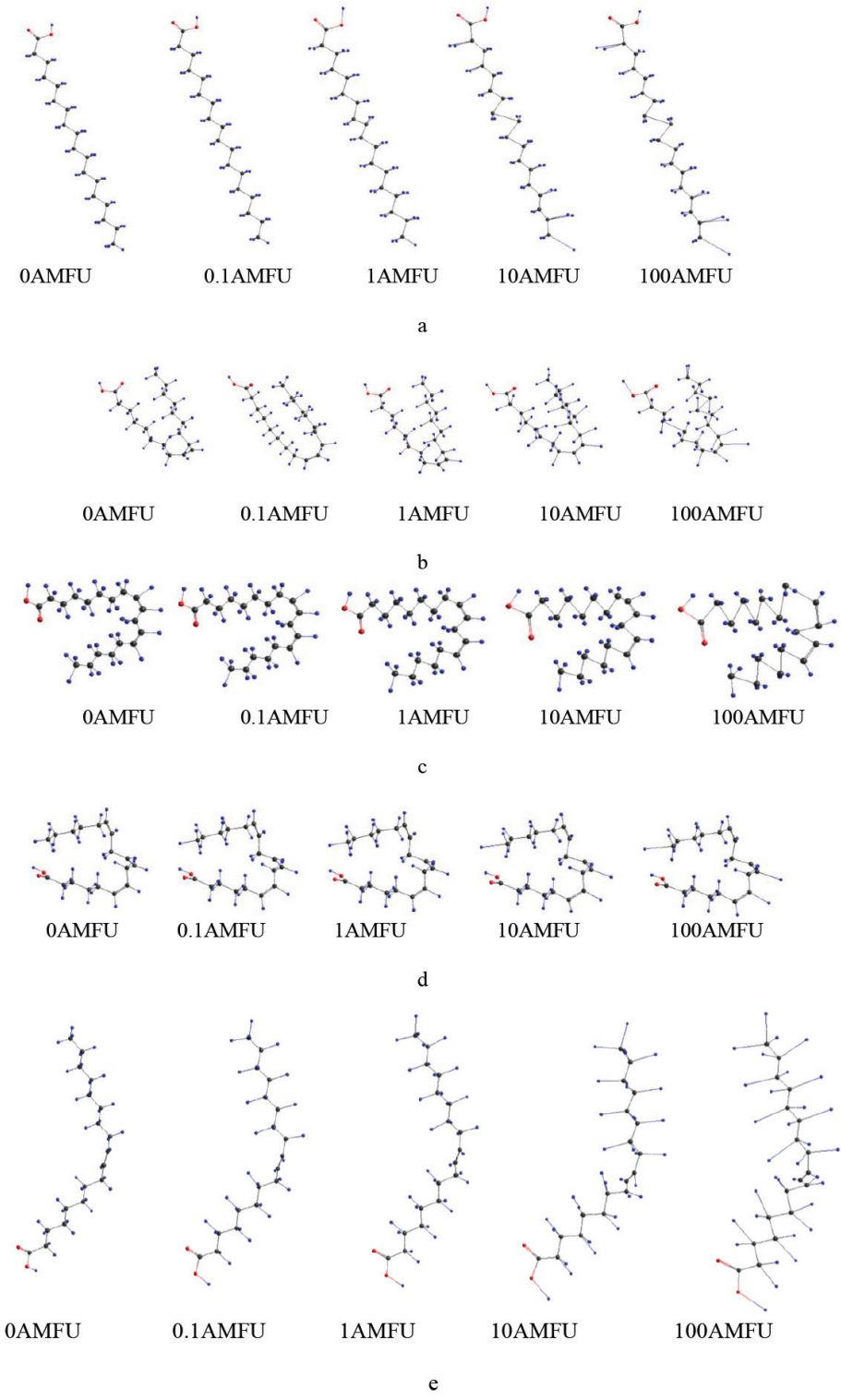
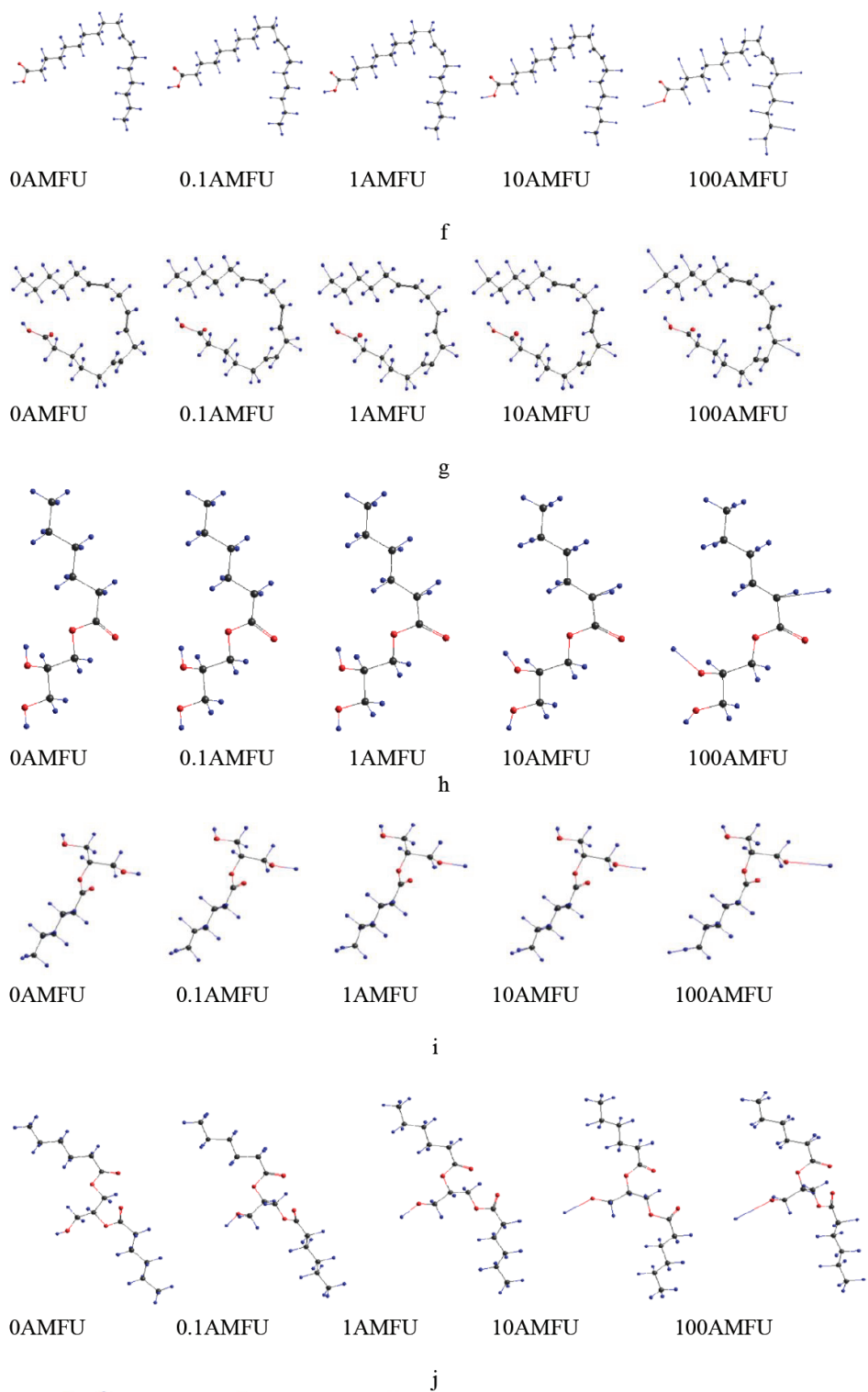


Figure 2. Groups tri-dimensional structures of those molecules affected by increasing SMF flux density.

**Figure 2.** Continued.

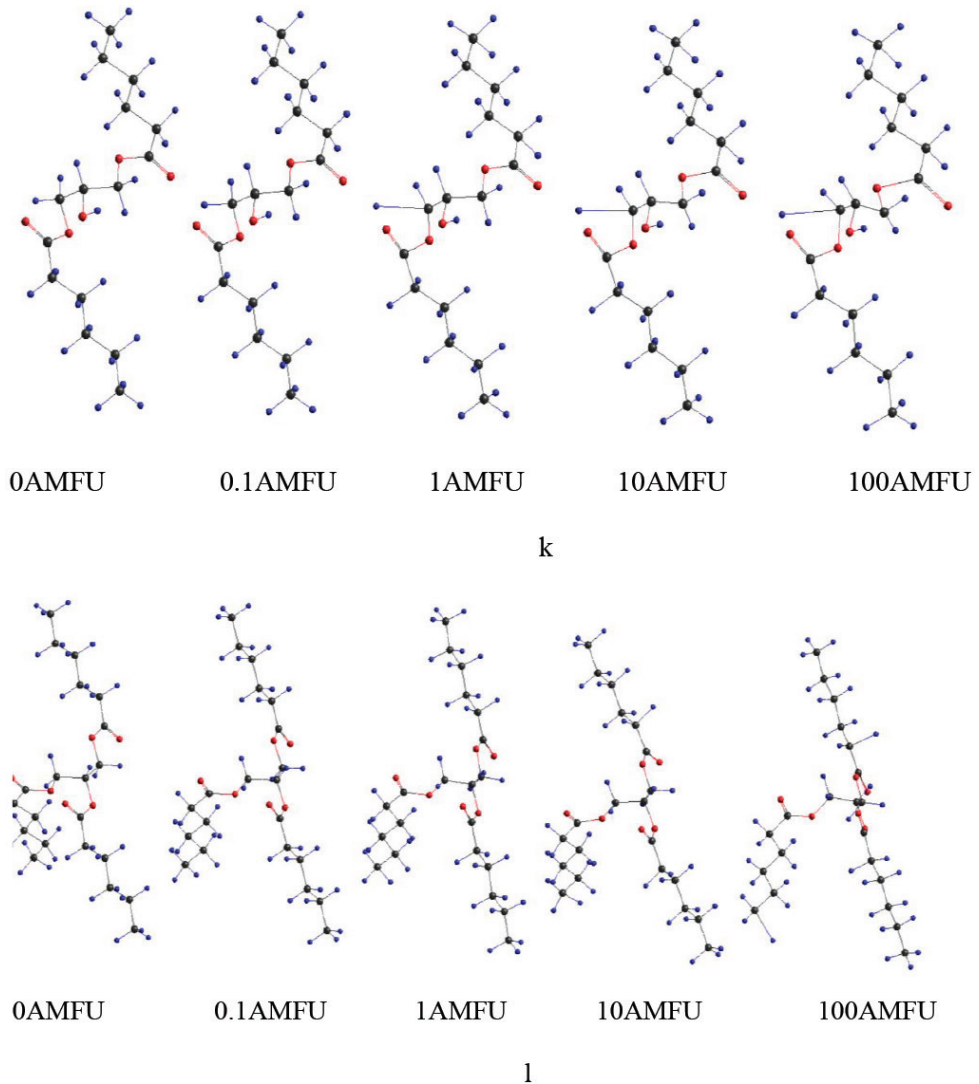


Figure 2. Continued.

bonds, that is, producing radical only data for atoms carrying unpaired electrons are quoted. The data for remained atoms are omitted as they deal with molecules of radical character and, hence, with specific biological activity.

Figure 2 Tri-dimensional structures of the molecules of selected lipid acids and caproyl glycerides affected by increasing SMF flux density [AMFU]. a: octadecanoic acid; b: *cis*-octadec-9-enoic acid c: *cis,cis*-octa-9,12-dienoic acid, d: *all cis*-octa-6,9,12-trienoic acid, e: *trans*-octadec-9-enoic acid, f: *trans*-octadec-11-enoic acid, g: *all trans*-octadec-6,9,12-trienoic acid, h: 1-caproyl glyceride, i: 2-caproyl glyceride, j: 1,2-dicaproyl glyceride, k: 1,3-dicaproyl glyceride, l – 1,2,3, -tricaproyl glyceride. Oxygen atoms are marked red, carbon black and hydrogen atoms are coloured blue, respectively.

Discussion

An increase in heat of formation of lipid acids (Table 1) and caproyl glycerides (Table 2) exposed to increasing flux density provides evidence for destabilization of those molecules by SMF. This effect was accompanied by an increase in their dipole moment.

The structure dependent orders of increasing heat of formation of lipid acids changed in the order:

trans-linolenic > linoleic > linolenic > elaidic > vaccenic > stearic > oleic

and associated dipole moments of those molecules declined in the order:

vaccenic > *trans*-linolenic > linolenic > stearic > oleic > elaidic > linoleic

These orders show that both these parameters are independent of the number of double bonds and chain conformation.

The increase in heat of formation and dipole moment of caproyl glycerides present following orders:

heat of formation: 1,2,3-tricaproyl > 1,2-dicaproyl >
2-monocaproyl > 1-monocaproyl > 1,3-dicaproyl

and

dipole moment: 1-monocaproyl > 2-monocaproyl >
1,2,3-tricaproyl > 1,3-dicaproyl > 1,2-dicaproyl

showing that this sequence of those parameters is independent of the degree and position of the esterification.

An insight in Fig. 2 seems to explain those irregularities. Depending on flux density, SMF induces twisting molecules out of the initially established plain and squeezing molecules around some bonds.

In the living organisms lipids under consideration are utilized in metabolic processes. Fatty acids are beta-oxidized in mitochondria and peroxisomes. The beta oxidation is the major pathway for fatty acid degradation, but certain fatty acids also undergo the alpha oxidation. The mechanism of beta oxidation resembles a reversal process of fatty acid synthesis. Two-carbon fragments are removed sequentially from the carboxyl end of the acid after steps of dehydrogenation, hydration, and oxidation to form a beta-keto acid, which is split by thiolysis which generates acetyl-CoA. The latter may be converted into ATP, CO₂, and H₂O using the citric acid cycle and the electron transport chain. Unsaturated and odd-chain fatty acids require additional enzymatic steps for degradation (Berg et al. 2019). Two auxiliary enzymes enoyl-CoA isomerase and 2,4-dienoyl-CoA reductase are involved into these fatty acids oxidation. The isomerase enzyme converts *cis*-conformer into *trans*. The reductase comes into play during oxidation of

polyunsaturated fatty acids (Mathews et al. 2000). First step of the metabolic process involves bonding of CoA isomerase to the carbonyl group carbon atom repulsing the OH group of the carboxylic group. This step is favoured by a high positive charge density on the carbonyl C- atom and highly polarized C-OH bond. In the consecutive step the abstraction of proton from the chain α -atom generates formation of the $\alpha\text{CH}=\beta\text{CH}$ double bond. This step is favoured by a high positive charge density on the hydrogen atom bound to the α -carbon atom and a high polarization of the $\beta\text{C-H}$ bond.

Metabolism of triacylglycerols, named here as glycerides, usually involves either their partial or complete hydrolysis by lipases yielding lipid acid and glycerol (Winkler et al. 1990). This reaction comes to the hydrolysis of the of the acyl – glycerol ester. This reaction is favoured by a high positive charge density on the carbonyl carbon atom. The lysophosphatidic acid formed by the action on phosphatidic acid of phospholipase A_2 is another metabolic process providing, a main component of cell membranes (Moolenaar 1995). This reaction is favoured by a high negative charge density on the oxygen atom of the glycerol OH group.

Taking into account that information, Table 3 reports solely charge density on the atoms of the carboxylic group and α - and β -methylene groups. Because, SMF can evoke the *cis-trans* transformations also charge density at the H-C=C-H atoms are given. SMF's ability to accelerate the transition of a conformer from *cis* to *trans* can significantly affect the oxidation of unsaturated fatty acids. In molecules of some lipid acids flux density of 10 and 100 AMFU resulted in elongation of certain bonds above 2 Å which is equivalent to ceasing these bonds. Charge densities on involved atoms are also reported in that Table. Table 4 reports bond lengths between all atoms considered in Table 3.

An insight into Tables 3 and 4 reveals that charge density and bond lengths in the molecule of stearic acid change irregularly against increasing SMF flux density. The molecule is linear and retains its linearity even when exposed to SMF of 100 AMFU (Fig. 2a). Thus the observed effect can result from twisting the molecule or its fragments pushing them out of SMF oriented along x -axis. The SMF flux density of 10 and 100 AMFU leads to deterioration of the molecules and that conclusion is drawn from the calculated elongation of the C10-C11, C17-H54, C2-H24 and C1-H20 bonds well above 2Å (Table 4).

The atoms constituting the carboxylic group are the most susceptible to SMF. Apart from atoms of the carboxylic hydroxyl group (atoms H58 and O55) and the β -chain carbon atom (C16), the 0.1 AMFU flux density has negligible effect on the charge densities on remaining atoms under consideration. Generally, flux density raising to 1 AMFU increased the positive charge density on the carbon atom bound hydrogen atoms (H58-51) and O55-bound hydrogen atom H58, indicating the direction of the corresponding bond polarization. Rising SMF flux density to 1 AMFU increases also the negative charge density on the O55 atom. Simultaneously, it decreases negative charge density on the O19, C17 and C16 atoms. Values of the positive charge density on the carbonyl carbon atom (the CDCC criterion) show that SMF of 0.1 AMFU weakly stimulates the first step of the metabolic process of stearic acid and SMF of 1 AMFU inhibits that process. The C=C bond formation (The CCF criterion) is inhibited by SMF of 0.1 AMFU and considerably stimulated by SMF of 1 AMFU,

The bent shape of the molecule of oleic acid (Fig. 2b) offers more ways of its stabilisation when exposed to SMF. They involve not only the twisting of their fragments out of the initial orientation along x-axis but also through space atom – atom van der Waals bonding and dispersion forces. Such circumstances make the molecule more resistant to SMF of higher flux density. Oleic acid molecule survives its exposure to flux density of 10 AMFU. For the vast majority of atoms, the changes of charge density against increasing flux density are more regular than that observed in the case of stearic acid. An increase in the positive charge is observed for H54, H22, H50, H51 and H39, that is, on almost all C and O bonded hydrogen atoms. The decrease in the positive charge is noted for C18, C17, C16, H52 and H38 atoms. The O55, C19, C10 and C9 atoms face decrease in negative charge against increasing flux density. The 100 AMFU flux density breaks the H-54, C18-C17, C15-C14, C10-H39, C9-H38, C8-H36, C8-H37, C4-C5 and C1-H22 bonds. Based on the CDCC and CCF criteria one may state that SMF of 0.1 to 10 AMFU inhibits the first step of the metabolic process and stimulates the formation of the C=C bond, respectively.

The introduction of the subsequent isolated double C=C bond into the 18 carbon chain (linoleic acid) results in further deformation of the chain and, hence, increases efficiency of intramolecular, through space, interaction. An increase in the resistance of the molecule to SMF flux density is noted. Computations reveal that the molecule survives exposure to the flux density of 100 AMFU. In this molecule the positive charge increases against a flux density increase on the H52, H40, H41, H42, H10, H13 and H14 atoms and, simultaneously, the decrease of that charge is observed on the C28, H43 and H37 atoms. An increase in the negative charge against flux density takes place on the O36, O55, C30, C26 and C4 atoms. It is accompanied by a decrease in the negative charge on the C29, C1 and C3. 100 AMFU flux density turns the negative charge on the C1 atom into positive. A relatively weak sensitivity of the bond lengths to an increase in the flux density is observed. Based on the CDCC and CCF criteria SMF of 0.1 to 100 AMFU inhibits the first step of the metabolic process and stimulates its second step.

The third double bond in the 18 carbon atom chain (linolenic acid) offers further possibilities of building resistance to an increase in the flux density (Fig. 2d). However, at 10 AMFU ceases the C19-H49 bond and at 100 AMFU ceases also the C1-H39 bond. Changes in the charge density against increasing flux density is irregular and, generally, fairly subtle. Neither the first nor the second step of the metabolic process are stimulated by SMF of 0.1-to 1 AMFU.

The structure of *trans*-monounsaturated elaidic acid (Fig. 2e) offers very limited possibilities of stabilisation on exposure of SMF. The localisation of the double bond offers most likely a twisting of some fragments out of the x-axis. Computations for the molecule exposed to SMF above 1 AMFU resulted in the transformation of the *trans*-conformation into *cis*-conformation. As a rule, an increase in flux density evokes a sometimes irregular increase in charge density on all hydrogen atoms. Simultaneously, on C atoms, except C18, negative charge increases. On essential for metabolism C18 atom negative charge decreases. SMF of increasing flux density inhibits reaction with CoA but stimulates formation of the C=C bond.

In the molecule of vaccenic acid (*trans*-11-enoic acid) (Fig. 2f), the shift of the double bond modulates the structure of the carbon chain to the extent providing some through space interactions of certain atoms. These circumstances stabilise the molecule to such an extent that it does not suffer the *cis-trans*-transformation even at 100 AMFU. However, above 10 AMFU the molecule deteriorates by splitting the C18-H49, C12-H10, C10-H45 and C8-H35 bonds. An increase in charge density on all hydrogen atoms and the C20 atom follows an increase in flux density. Simultaneously, the negative charge density increases on the O1, O2, C9, C15 and C17 atoms. Solely negative charge density on the C16 atom decreases. The flux density rising up to 10 AMFU has a very subtle effect on the charge density on the carbonyl carbon atom but it stimulates formation of the C=C bond.

No *trans-cis* isomerization takes place in the molecule of *trans*-linolenic acid (Fig. 2g) on its exposure to flux density as high as 100 AMFU. Instead, at 100 AMFU the C17-H44, C12-H39 and C12-H40 bonds split. Changes of the charge density with an increase in flux density are irregular but general tendency of increase in the charge density on all hydrogen and C20 atoms is followed. Simultaneously, negative charge density increases on the O1, O2, C10, C1 and C18 atoms. An decrease in the positive charge takes place on the C8 atom and on the C19, C14 and C11 atoms decreases their negative charge. SMF of 0.1 AMFU strongly stimulates the first step of the metabolic path, whereas SMF of 1 AMFU stimulates it weakly and SMF of 10 AMFU inhibits it. Every value of flux density in the range 0.1 to 10 AMFU stimulates formation of the C=C bond.

In a case of mono-, di- and three-caproyl glycerides the charge density on the carboxylic carbon atom varies irregularly with an increase in applied flux density. Solely in 1,2,3-tricaproyl glyceride the flux density, regardless of its value, always stimulates the hydrolysis (see Table 5). Most frequently, the flux density of 0.1 AMFU inhibits reaction of the hydroxyl groups whereas SMF of higher flux density stimulates their reactivity.

Conclusions

Mainly two factors are responsible for susceptibility of molecules to SMF. The Lorentz force is one of them. It acts on moving electrons, which at high intensity influences the natural geometry of orbitals. This problem is quite difficult to include in the calculations, so the simplified approach does not take it into account. The second reason is the a ceasing of the coherence of the binding electron pair is the second factor. It persists despite electrostatic repulsion by magnetic interactions. A very strong external magnetic field competes with mutual fields evoking splitting the binding electron pairs into two unpaired electrons. The process runs as a gradual weakening of the mutual pairing of electrons. The binding electron pair is the fundamental element of the chemical bond. On growing SMF, such bonds initially expand and in order to disintegrate on exceeding the critical length. It generates a pair of radicals. Such radicals are very chemically active and can bind to ambient molecules, changing their chemical structure and, therefore, also their biological activity.

The distribution of electrical charges in all analyzed lipids resemble one another. Except the carbonyl carbon atom remaining carbon atoms take higher electron density. The exceptional H45 atom in 1,3-dicaproyl glycerol at a field above 1 AMFU faces an electron deficit. The exceptional carbonyl carbon atom carries a clear electron deficit. It results from bonding that atom to the strongly electron withdrawing oxygen atom. The anomaly of the H45 atom is a consequence of the specific conformation of the molecule of this ester.

SMF destabilizes lipid acids and caproyl glycerides irregularly against increasing flux density. The changes in the heat of formation of those compounds are accompanied also by irregular against increasing flux density increase in the dipole moment of those molecules. Observed irregularities result from the ability of those molecules to twist out of the initially established SMF plain, and squeezing fragments of the molecules around some bonds. Such mobility of the molecules in SMF provides a possibility of through space interactions between fragments of the molecules. These interactions involve van der Waals bonding and dispersion forces. These circumstances are responsible for irregular against applied flux density changes of the charge density of the atoms and length of the bonds between them. For these reasons either stimulation or inhibition of the metabolic processes of the lipids under consideration irregularly depends on the flux density.

In some molecules SMF flux density of 10 AMFU and above breaks some C-H valence bonds. In such manner free radicals are generated.

The sole conversion of the *cis-trans* conformations was observed in case of elaidic acid which at 10 AMFU converted into *cis* conformer. Depending on the structure and applied flux density SMF either stimulates or inhibits the metabolic processes of the lipids under study.

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