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Research Article

Potential risk resulting from the influence of static magnetic field upon living organisms. Numerically simulated effects of the static magnetic field upon model complex lipids

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Abstract

Background: Recognising effects of static magnetic field (SMF) of varying flux density on flora and fauna is attempted. For this purpose, the influence of static magnetic field is studied for molecules of five complex lipids i.e. such as β-carotene, sphingosine, ceramide, cholesterol and phosphatidylcholine.

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

Results: SMF polarises molecules depending on applied flux density. Only β-carotene survives exposure to SMF of 10 and 100 AMFU without radical splitting of some valence bonds. Molecules of remaining lipids suffered radical cleavage of some bonds on exposure to SMF of 10 and 100 AMFU. Manipulation with applied flux density provides either inhibition or stimulation of biological functions of the lipids under study.

Conclusions: SMF destabilises complex lipids to the extent depending applied flux density. Biological functions of β-carotene are fairly sensitive to SMF, whereas only slight response to the effect of SMF is observed in case of sphingosine, ceramide and cholesterol. Enzymatic hydrolysis of phosphatidylcholine is stimulated by SMF regardless of the catalysed enzyme employed.

Key words: β-carotene, ceramide, cholesterol, phosphatidylcholine, sphingosine

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Introduction

Lipids play a diverse role in animal and plant organisms. They co-constitute biological membranes and triglycerides, located in adipose tissue, play a role in a major form of energy storage of animals and plants (Wang 2004; Dinasarapu et al. 2011; Berg at al. 2019).

Other functions involve transporting fat-soluble vitamins, oligosaccharides across cell membranes, participation in polysaccharide biosynthesis, activation of certain enzymes and formation of the basis for steroid hormones (Gohil and Greenberg 2009). Such role of lipids prompted us to extend this study. For that purpose, in our studies on the effect of Static Magnetic Field (SFM) upon biologically important components of plant and animal cells, we focused, amongst others, on lipids. In our former paper (Ciesielski et al. 2022), attention was paid to lipid acids and acyl glycerides. This paper is devoted to recognising the effect of SMF upon some model complex lipids, that is, β-carotene (carotenoids), cholesterol (sterols), sphingosine and ceramide (sphingolipids) and phosphatidylcholine (phospholipids) which are the most essential components of that group of compounds.

β-Carotene, a hydrocarbon with 11 conjugated double C=C bond systems is known as a lipid antioxidant (Anguelova and Warthesen 2008) and the precursor of A-vitamin. One molecule of β-carotene can be cleaved by the intestinal enzymes β,β-carotene-9',10'-mono-oxygenase into two molecules of vitamin A (Biesalski et al. 2007), whereas β,β-carotene 15,15'-mono-oxygenase does it eccentrically (Eroglu and Harrison 2013).

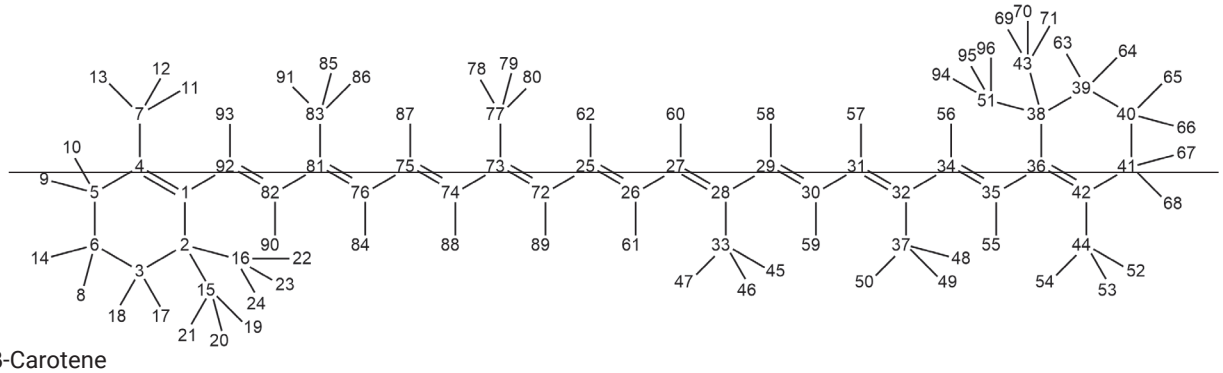
Sphingosine (2-amino-4-octadecene-1,3-diol) forms a primary part of cell membrane sphingolipids. Involving two type kinases, it is phosphorylated into sphingosine-1-phosphtate accounting for signalling lipids (Kataoka et al. 2005; Gergely et al. 2012; Huwiler and Zangemeister-Wittke 2017).

Ceramide (Fig. 3) is the sphingosine with a long fatty acids acylated amino group. It occupies cell membranes. Further modification with the phosphatidylcholine group leads to sphingomyelin constituting a lipid bilayer (Eder et al. 2022). Additionally, it participates in the differentiation, proliferation and programmed cell death mechanism (Siskind et al. 2002, 2006; Stiban et al. 2006). In this work as a simple model for calculation, except for long fatty acid amides, the formamide was accepted.

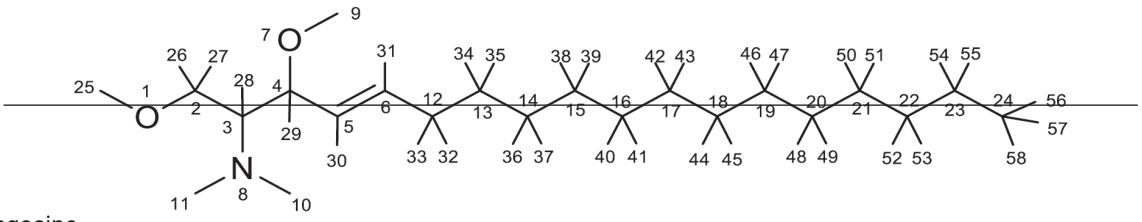
Cholesterol (Fig. 1) a specific unsaturated alcohol includes a cyclopentaphenanthrene (CPP) moiety. The C=C bond and the secondary hydroxyl group determine its chemical reactivity. Amongst others, cholesterol acts as a lipid antioxidant. The CPP moiety is common for steroids. Hence, apart from several physiological functions, it is a precursor of steroids – important biocatalysts formed enzymatically through steroidogenesis (Häggström and Richfield 2014).

Phosphatidylcholine, a phospholipid, is a major component of cell membranes and pulmonary surfactant. It is also a membrane-mediated cell signalling factor (Kanno et al. 2007). In this work, for simplification of calculations, a shorter 1,2-dibutyryl ester was taken.

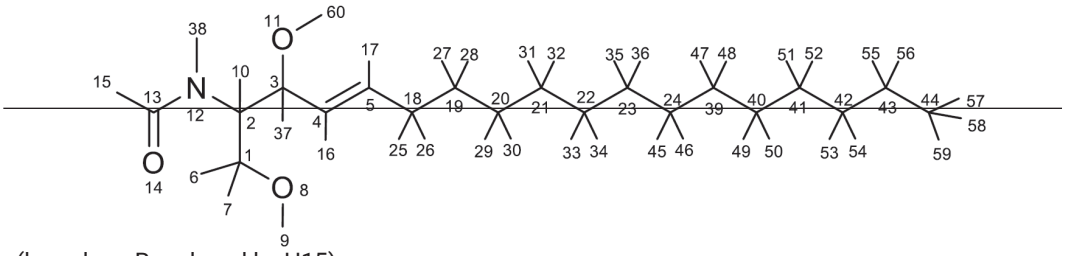
The biological role of those molecules in living organisms of flora and fauna rationalises including them in our systematic studies on the influence of Static Magnetic Field (SMF) on biologically important elements of living cells. Thus, this report is devoted to advanced numerical simulations of SFM of 0, 0.1, 1, 10 and 100 AMFU (Arbitrary Field Density) arbitrary units performed for those molecules. The results could also be interesting for developing and functioning novel materials (Ramburrun et al. 2022) and systems (Smułek et al. 2023) of biomedical and food applications. Potentially, application of SMF of various field densities could offer either stimulation or inhibition of some processes as well as changing of the pathways.



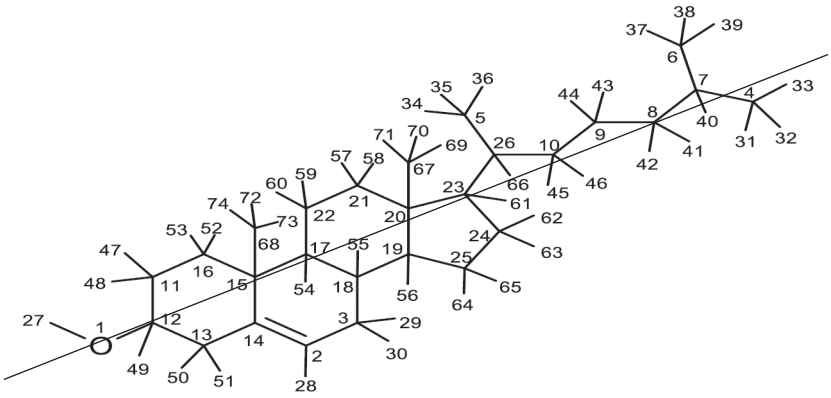
β-Carotene



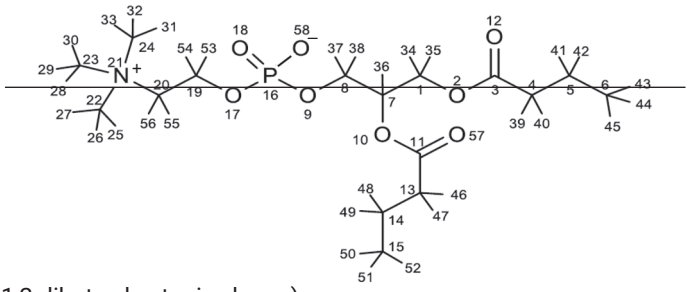
Sphingosine



Ceramide (here: long R replaced by H15).



Cholesterol



Phosphatidylcholine (here: 1,2-dibutyryl ester is shown).

Figure 1. Numbering atoms in the molecules of complex lipids. Orientation of molecules against x-axis is marked with red lines.

Materials and methods

Numerical computations

Computations of the effect of real SMF 0.0, 0.1, 1, 10 and 100 AMFU (Arbitrary Magnetic Field Units; here 1AFU > 1000 T) flux density were performed in silico (computer vacuum), involving advanced computational methods. The procedures follow those described in our former paper (Ciesielski et al. 2022).

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

Results and discussion

The effect of SMF of flux density from 0 to 100 AMFU upon heat of formation and dipole moment of five complex lipids is demonstrated in Table 1. Tables 2–8 present the effect of SMF in terms of charge density on selected atoms directly participating in biological activity of those lipids and bond lengths between those atoms. When the SMF of flux density generated the radical through extremely expanding some C-H bonds, only data for electron atoms carrying unpaired electrons are quoted. The data for the remaining atoms are omitted as they deal with molecules of radical character and, hence, with specific biological activity.

Table 1. Heat of formation (HF) [kJ.mole^{-1}] and dipole moment (DM) [D] of complex lipid molecules at flux density varying from 0 to 100 AMFU.

Molecule	HF [kJ.mole^{-1}] at flux density [AMFU]						DM [D] at flux density [AMFU]					
	0	0.1	1	10	100	HF_0 –HF_{100}	0	0.1	1	10	100	DM_{100}-DM_0
β-Carotene	-158	-151	-142	-106	-81	-77	0.25	0.31	0.71	0.93	1.53	1.28
Sphingosine	-1364	-1302	-1211	-1023	-817	-547	5.84	6.23	8.17	10.36	13.52	7.68
Ceramide	-1659	-1621	-1584	-1428	-985	-674	5.94	6.18	9.68	11.41	13.85	7.91
Cholesterol	-531	-501	-464	-403	-306	-225	1.62	1.78	2.06	3.57	6.51	5.89
Phosphatidylcholine	-1254	-1174	-1086	-964	-721	-533	2.48	2.94	3.85	5.13	12.15	9.67

Table 2. Charge density [a.u] on the C atoms of the conjugated double bond chain of β-carotene.

SMF [AMFU]	Charge density [a.u.] at SMF flux density [AMFU]																					
	C4	C1	C92	C82	C81	C76	C75	C74	C73	C72	C25	C26	C27	C28	C29	C30	C31	C32	C34	C35	C36	C42
0	-.065	-.282	.221	-.676	.351	-.416	-.202	-.245	.384	-.345	-.031	-.209	-.115	.198	-.171	-.310	-.205	.212	-.549	.199	-.262	-.095
0.1	-.115	-.249	.213	-.593	.321	-.388	-.225	-.221	.329	-.337	.002	-.191	-.108	.143	-.154	-.317	-.185	.170	-.568	.191	-.231	-.149
1	-.132	-.212	.209	-.763	.232	-.316	-.286	-.158	.166	-.338	.149	-.096	-.107	-.003	-.114	-.343	-.139	.083	-.725	.196	-.193	-.178
10	-.134	-.198	.207	-.781	.204	-.298	-.307	-.144	.126	-.416	.204	-.002	-.124	-.037	-.102	-.353	-.130	.061	-.743	.201	-.179	-.178
100	-.208	-.058	.200	-.488	.158	-.050	-.509	.005	-.371	-.161	-115	-.163	-.279	-.388	-.004	-.564	-.158	.001	-.396	.204	-.061	-.207

Table 3. Flux density dependent lengths [Å] of the double bonds potentially involved in oxidative reactions of β-carotene.

SMF [AMFU]	Bond length [Å] at flux density [AMFU]										
	C4=C1	C92=C82	C81=C76	C75=C74	C73=C72	C25=C26	C27=C28	C29=C30	C31=C32	C34=C35	C36=C42
0	.825	.825	.825	.825	.825	.825	.825.	.825	.825	.825	.825
0.1	.811	.841	.837	.840	.841	.784	.842	.842	.838	.842	.845
1	.888	.892	.878	.888	.889	.715	.899	.901	.887	.900	.899
10	.905	.911	.895	.909	.911	.674	.915	.923	.984	.920	.915
100	1.033	1.098	1.085	1.128	1.027	.782	1.023	1.117	1.076	1.091	1.026

Table 4. Flux density depende nt charge density [a.u.] on particular atoms in sphingosine.[a]

SMF [AMFU]	Charge density [a.u] on particular atoms at flux density [AMFU]																	
	H25	O1	C2	H26	H27	C3	H28	N8	H10	H11	C4	H29	O7	H9	=C5	H30	=C6	H
0	.205	-.350	-.006	.080	.072	-.018	.080	-.349	.140	.165	.069	.094	-.335	.208	-.209	.138	-.150	.120
0.1	.195	-.350	-.018	.085	.093	-.042	.092	-.339	.137	.151	.053	.107	-.340	.195	-.288	.134	-.162	.126
1	.305	-.326	-.001	.020	.062	-.062	.065	-.327	.123	.147	.020	.109	-.345	.224	-.181	.129	-.153	.109
10	*.204*	*-.090*																
100[b]	*.175*	*-.514*	*.140*	*.125*	*.119*	*.117*					*.114*	*.054*	*-.409*	*.208*				

[a]Values in italics relate to radical generated at given flux density.

[b]Also the following atoms carry free electrons: C18, H45, C19, H46, H47, C20, H48, H49, C21, H50, H51, C22, H52, H53, C23, H54, H55, C24, H56, H57, H58.

Table 5. Flux density dependent bond lengths [Å] between particular atoms in sphingosine.[a]

SMF [AMFU]	Bond lengths [Å] at flux density [AMFU]																
	H25-O1	O1-C2	C2-H26	C2-H27	C2-C3	C3-H28	C3-N8	N8-H10	N8-H11	C3-C4	C4-O7	O7-H9	C4-H29	C4-C5	C5-H30	C5-C6	C6-H31
0	0.950	1.430	1.090	1.090	1.510	1.090	1.470	1.010	1.010	1.540	1.430	0.960	1.090	1.520	1.080	1.340	1.080
0.1	0.952	1.502	1.095	1.092	1.573	1.092	1.520	1.084	1.085	1.567	1.514	0.952	1.093	1.517	1.074	1.365	1.084
1	1.993	1.278	1.513	1.467	1.591	1.208	1.558	1.028	1.035	1.016	1.640	1.430	1.297	1.421	1.208	1.388	1.164
10	*2.245*																
100	*2.509*		*2.727*	*2.506*		*2.040*							*2.180*				

[a]Values in italics relate to radical generated at given flux density.

Table 6. Effect of SMF flux density on the reaction site charge density of ceramide and selected bond atoms in that molecule.[a]

SMF [AMFU]	Charge density [a.u.] on the atoms of reacting hydroxyl group				
	O8	H9			
0	-.358	.212			
0.1	-.348	.199			
1	-.361	.320			
10	*-.392*	*.348*			
100	*-.398*	*.190*			
	Length of bonds [Å]				
	C8-H9	C1-H6	O11-H60	C44-H57	C44-H58
0	.950				
0.1	.962				
1	1.729				
10	*2.142*				
100	*2.508*	*2.161*	*2.037*	*2.351*	*2.301*

[a]Values in italics relate to radical generated at given flux density.

Discussion

A decrease in the negative value of heat of formation (Table 1) provides clear evidence for the destabilising effect of SMF upon the molecules of the lipids under consideration. That effect increased with an increase of the applied flux density. Accompanying increase in dipole moment of those molecules points to elongation of bonds and facility of polarisation of the molecules as the reason of destabilisation.

Table 7. Effect of SMF flux density on the reaction sites charge density of cholesterol and selected bond atoms in that molecule.[a]

SMF [AMFU]	Charge density [a.u.] on the reacting site atom										
	O1	H27	C2	H28	C14						
0	-0.333	0.251	-0.169	-0.131	-0.193						
0.1	-0.343	0.251	-0.170	-0.148	-0.194						
1	-0.389	0.382	-0.178	-0.142	-0.132						
	Bond length [Å]										
	C1-O27	C2-C14	C2-H28	O1-H27	C4-H33	C8-H39	C10-H46	C12-H49	C12-C13	C8-H41	C67-H69
0	1.430	1.336	1.000	0.960							
0.1	1.330	1.531	1.123	1.143							
1	1.199	1.385	1.142	1.518							
10	*2.162*				*2.496*	*2.138*	*2.059*				
100	*3.032*				*3.413*	*2.844*	*2.780*	*2.347*	*2.048*	*2.780*	*2.981*

[a]Values in italics relate to radical generated at given flux density.

Table 8. Effect of SMF flux density on the reaction sites charge density of phosphatidylcholine and selected bond atoms in that molecule.[a]

SMF [AMFU]	Charge density [a.u.] on the reacting site atom						
	O17	P16	O9	C3			
0	-0.556	1.731	-0.547	0.261			
0.1	-0.583	1.787	-0.578	0.271			
1	-0.636	1.891	-0.640	0.278			
	Bond length [Å]						
	P16-O17	P16-O9	C3-O2	P16-O18	C15-H51	C13-H47	C6-H45
0	1.790	1.790	1.360				
0.1	1.777	1.767	1.357				
1	1.795	1.717	1.360				
10	*1.932*	*1.777*	*1.369*	*2.064*	*2.597*		
100	*1.890*	*1.848*	*1.408*	*2.067*	*3.965*	*2.084*	*4.282*

[a]Values in italics relate to radical generated at given flux density.

The effect of SMF upon the stability of considered molecules increases in the order:

β-carotene < cholesterol < phosphatidylcholine < sphingosine < ceramide,

whereas the accompanying increase in the values of the dipole moment arranges in the order:

β-carotene < cholesterol <sphingosine < ceramide <phosphatidylcholine,

suggesting that the polarisation of the bonds is not the sole effect involved.

Amongst the five molecules under consideration (Fig. 1), β-carotene is the sole molecule surviving the effect of 100 AMFU flux density without generating radical split bonds. The remaining molecules already generated radicals on exposure to 10 AMFU (Tables 2–8).

The role of β-carotene as an antioxidant involves the whole conjugated double C=C bond system of the molecule. The process is due to trapping molecules of triplet oxygen following the radical mechanism. Such a process is stimu-

lated by a low polarisation of bonds accepting oxygen. The length of the double bonds in the β-carotene molecule increases with an increase of flux density (Table 3). It is accompanied by either an increase or decrease in the charge density on the atoms of the bonds depending on their positions in the chain.

This is surprising because it only applies to bonds located in the middle of the conjugated chain, in which, from a chemical point of view, all bonds are almost identical.

Review of Table 2 shows that, in such manner, some bonds turn more polar and some lose their original polarity in respect to that maintained in the molecule situated out of SMF. It suggests only a small effect of SMF upon a functioning β-carotene as an antioxidant and, depending on the applied flux density, varies the position of the reaction of that molecule with triplet oxygen. The enzymatically catalysed conversion of β-carotene into A vitamin involves a rupture of the C25=C26 double bond with the addition of the oxygen atom. Since that reaction follows an ionic mechanism, this reaction is stimulated by an increase in the polarity of that bond. At 0.1, 1 and 10 AMFU, the polarity of that bond increased in order to decrease dramatically at 100 AMFU. Another enzyme - β,β-carotene 15,15'-monooxygenase splits the C31=C32 bond, producing β-apo-10'-carotenal and β-ionone. SMF of 0.1, 10 and 100 AMFU decreased the polarity of that bond, whereas SMF of 1 AMFU increased its polarity (Table 2).

Biological function of sphingosine requires its introductory enzymatic phosphorylation at the O1 atom to convert the phosphorylated product into sphingomyelin (Fig. 2: (1)):

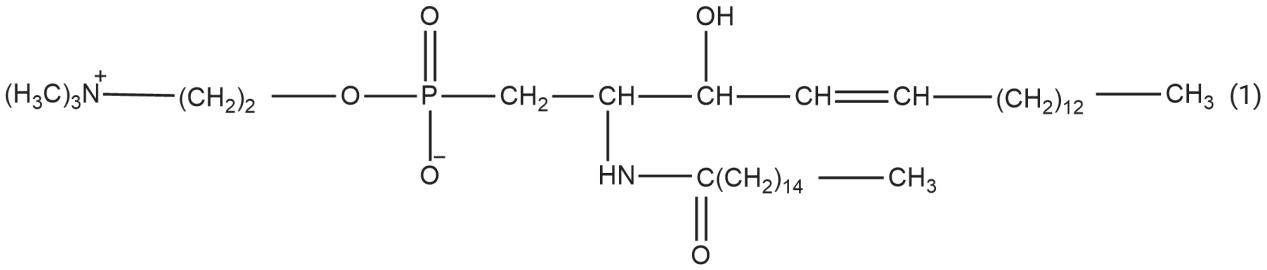


Figure 2. Structure of sphingomyelin.

The phosphorylation is stimulated by a high negative charge at the O1 atom. As shown in Table 4, SMF of 0.1 AMFU has no effect on that reaction and exposure to 1 AMHU slightly inhibits it. Exposure of sphingosine to 10 and 100 AMFU turns it to radicals. The positions of homolytic cleavage are marked in Tables 4 and 5.

The negative charge on the O8 atom in ceramide is slightly modulated by SMF. At 0.1 AMFU, it slightly decreases in order to slightly increase at 1 AMFU. Higher flux density produces radicals as shown in Table 6.

SMF of 0.1 AMFU subtly decreases the polarity of the C2=C14 bond stimulating in this manner the role of cholesterol as antioxidant, but at 1 AMFU, the polarity of that bond increases, inhibiting that role of cholesterol. Simultaneously, the negative charge density on the O8 atom increases, stimulating reactivity of the OH group. SMF of 10 and 100 AMFU generates radical cleavage of certain bonds (Table 7).

There are three reaction sites in phosphatidylcholine, each employed by another enzyme (Fig. 3)

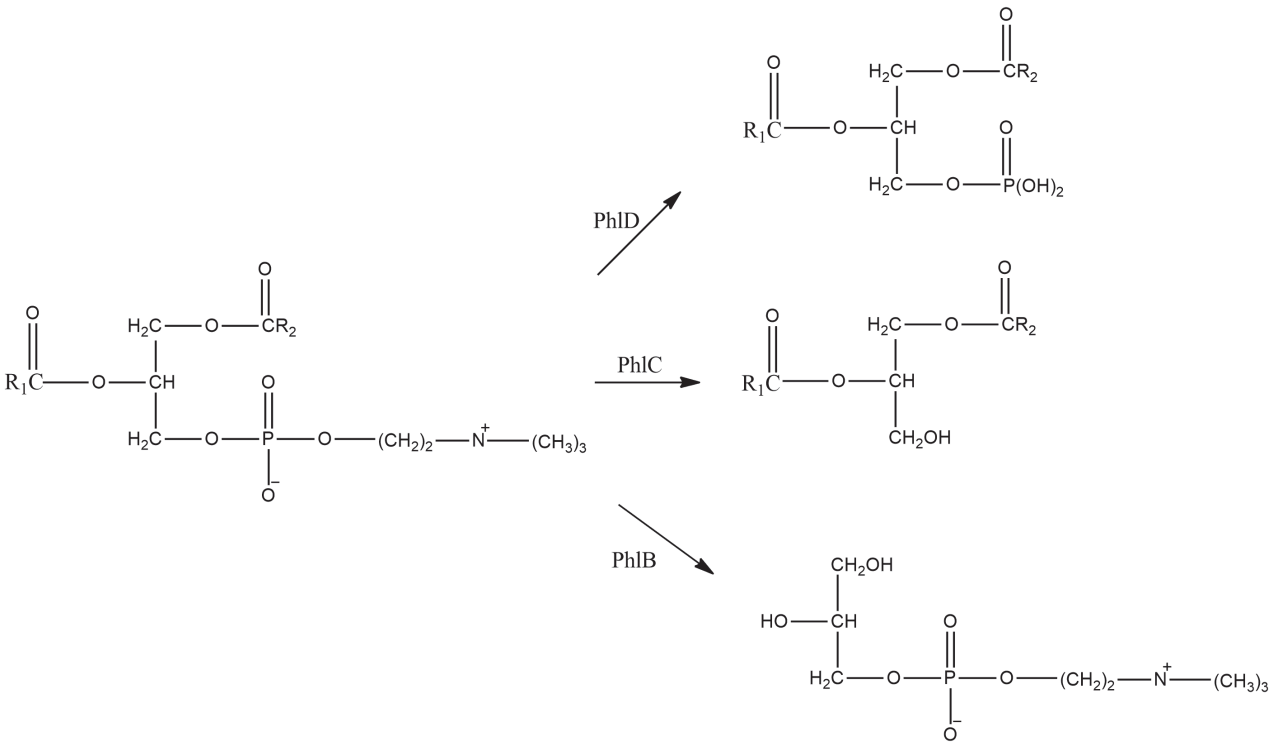


Figure 3. Hydrolysis of phosphatidylcholine with B, C and D phospholipases (Phl).

B, D and C phospholipases belong to the group of hydrolases. Their action should be stimulated by a high positive charge density on the P16 atom, whereas the hydrolysis with B phospholipase should be stimulated by a high positive charge density on the C3 atom. Data in Table 8 identify that SMF of 0.1 and 1 stimulated all three enzymatic hydrolyses. SMF of 10 and 100 AMFU generates radicals by splitting bonds shown in that Table.

Conclusions

In terms of heat of formation, SMF destabilises molecules of the lipids under study. An increase in the polarity of the molecules is the main reason of observed effect. Amongst five complex lipids under consideration, only β-carotene survives exposure to 10 and 100 AMFU without radical cleavage of some bonds. SMF has a diverse effect upon a functioning β-carotene as antioxidant. Depending on the applied flux density, there is a variation in the position of the reaction of that molecule with triplet oxygen. The enzymatically catalysed conversion of β-carotene into A vitamin is stimulated by an increase in the polarity of that bond. At 0.1, 1 and 10 AMFU, the polarity of that bond increased in order to decrease dramatically at 100 AMFU. The reaction catalysed by β,β-carotene 15,15'-monooxygenase leading to β-apo-10'-carotenal and β-ionone is inhibited by SMF of 0.1, 10 and 100 AMFU and stimulated by SMF of 1 AMFU.

The phosphorylation of sphingosine, which is responsible for biological function of that lipid, remains unaffected by SMF of 0.1 AMFU and slightly inhibited by SMF of 1 AMFU. The biological function of ceramide is only slightly modulated by SMF. Flux density of 0.1 AMFU slightly inhibits it, whereas a weak stimulation takes place at 1 AMFU.

SMF of 0.1 AMFU subtly stimulates the role of cholesterol as antioxidant, but at 1 AMFU, inhibition of that role is observed. Simultaneously, the reactivity of the primary hydroxyl group is stimulated at SMF of 0.1 and 1 AMFU. SMF of 0.1 and 1 AMFU stimulates hydrolysis of phosphatidylcholine with B, C and D phospholipases.

The presented results concern only changes caused by SMF in selected substrates, but all bioprocesses also involve enzymes. They are also exposed to SMF. We shall address that problem in our subsequent works.

Additional information

Conflict of interest

The authors have declared that no competing interests exist.

Ethical statement

No ethical statement was reported.

Funding

No funding was reported.

Author contributions

Conceptualization: WC, PT. Formal analysis: JAS, HK, WC. Investigation: WC, ZO. Methodology: WC. Writing - original draft: WC. Writing - review and editing: PT.

Data availability

All of the data that support the findings of this study are available in the main text.

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