

# Phosphocholines and chlorophyll derived molecules from the diatom *Cylindrotheca closterium* with anti-inflammatory activity

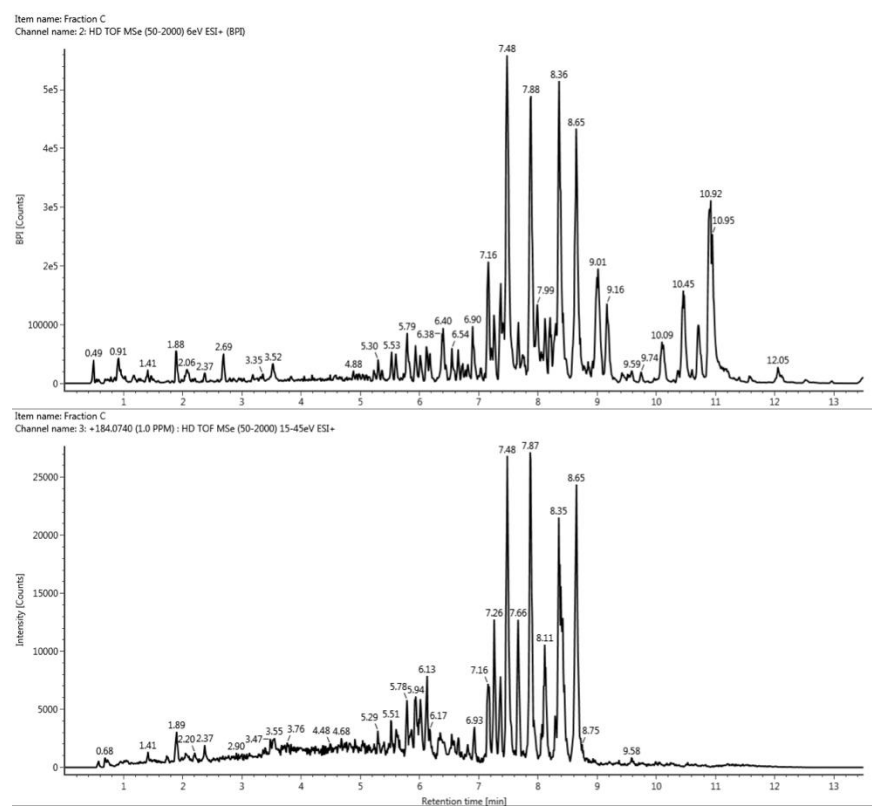
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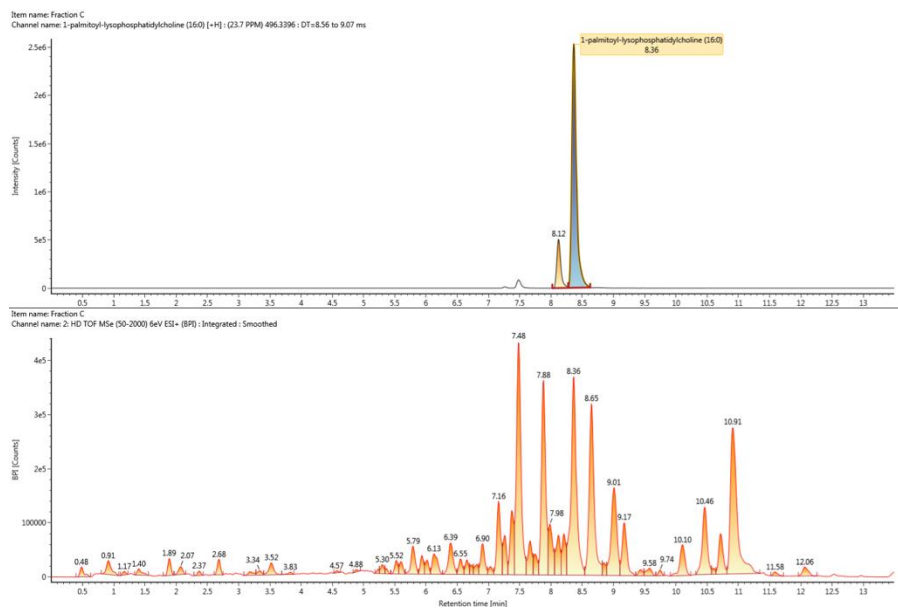
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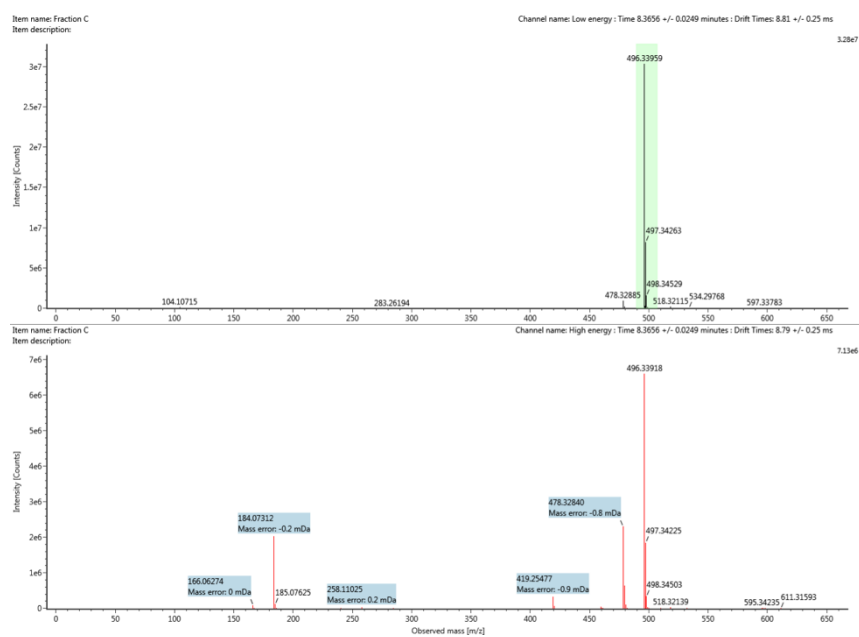
## Supplementary information



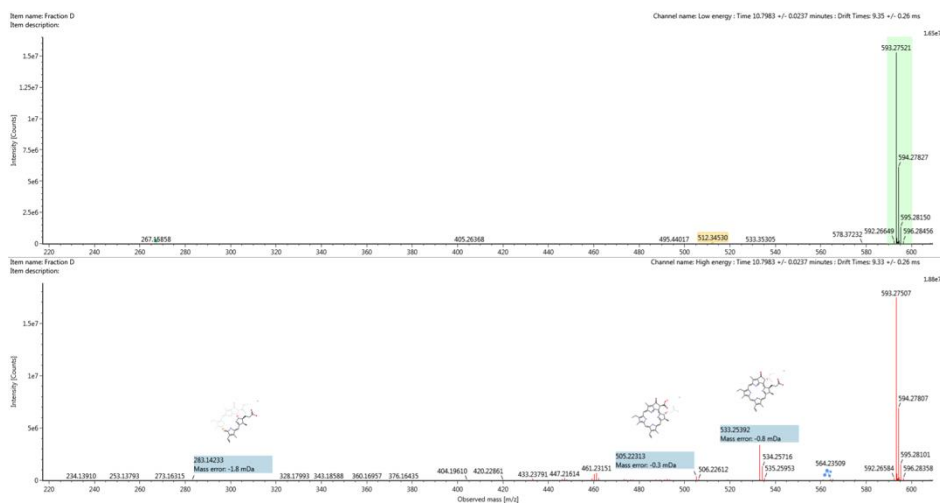
**Figure S1.** Top: Base peak intensity chromatogram from the UHPLC-HR-MS/MS analysis of fraction C using positive electrospray. Bottom: Ion chromatogram of  $m/z$  184. 0740 from fraction C indicating the presence of phosphocholines.



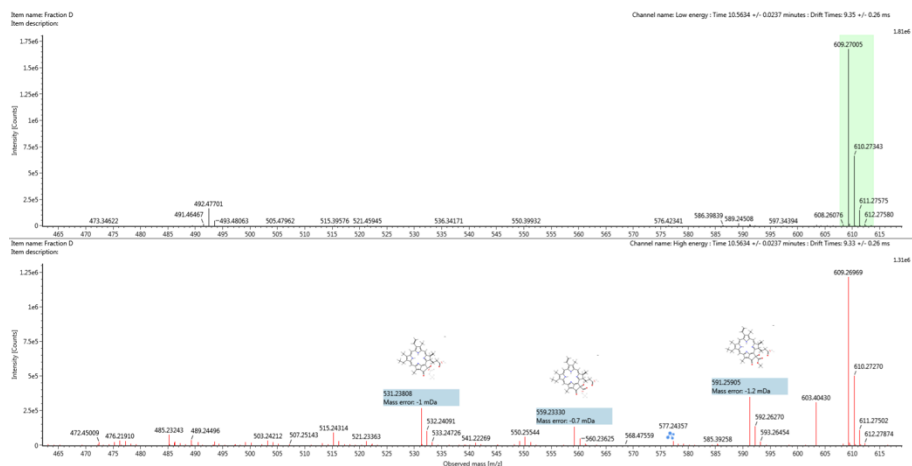
**Figure S2.** Top: Ion chromatogram of  $m/z$  496.3396 from fraction C showing the presence of LysoPC. . Bottom: Base peak intensity chromatogram from the UHPLC-HR-MS/MS analysis of fraction C using positive electrospray.



**Figure S3.** Top: Low energy mass spectrum of 1-Palmitoyl-sn-glycero-3-phosphocholine from fraction C. Bottom: High energy mass spectrum of 1-Palmitoyl-sn-glycero-3-phosphocholine showing fragments and mass deviations corresponding with the commercial standard.



**Figure S4.** Top: Low energy mass spectrum of pheophorbide A from fraction D. Bottom: High energy mass spectrum of pheophorbide A showing fragments and mass deviations corresponding with the theoretical fragmentation of the database hit.



**Figure S5.** Top: Low energy mass spectrum of hydroxypheophorbide A from fraction D. Bottom: High energy mass spectrum of hydroxypheophorbide A showing fragments and mass deviations corresponding with the theoretical fragmentation of the database hit.

**Table S1.** The most abundant lysophosphatidylcholines in fraction C. The type indicates number of carbons and double bonds in the fatty acid moiety of the respective LysoPCs, and the retention times are given in minutes.

<b>Number</b>	<b>Type</b>	<b>Observed mass (<i>m/z</i>)</b>	<b>Elemental composition</b>	<b>Retention time</b>
1	14:0	468	C <sub>22</sub> H <sub>47</sub> NO <sub>7</sub> P	7.16
2	18:3	518	C <sub>26</sub> H <sub>49</sub> NO <sub>7</sub> P	7.36
3	16:1	494	C <sub>24</sub> H <sub>49</sub> NO <sub>7</sub> P	7.48
4	18:2	520	C <sub>26</sub> H <sub>51</sub> NO <sub>7</sub> P	7.88
5	16:0	496	C <sub>24</sub> H <sub>51</sub> NO <sub>7</sub> P	8.36
6	18:1	522	C <sub>26</sub> H <sub>53</sub> NO <sub>7</sub> P	8.65