Electronic Supplementary Material (ESI) for Analytical Methods.

Electronic Supplementary Information

Imaging the distribution of DMPBD and terpinen-4-ol inclusion complex with 2-hydroxypropyl-β-cyclodextrins by using TOF-SIMS

Auraya Manaprasertsak[1], Per Malmberg[2], Theerachart Leepasert[1] and Thitinun Karpkird[1*]
[1]Department of Chemistry, Faculty of Science, Kasetsart University, 10900 Bangkok, Thailand
[2]Department of Chemistry and Chemical Engineering, Centre for Imaging Mass Spectrometry, Chalmers University of Technology, 412 96 Gothenberg, Sweden

* Corresponding author
E-mail address: fscitnm@ku.ac.th

S1. Plai oil (PO) analysis by GC-MS

The GC-MS chromatogram of Plai oil (Figure S1a) shows three major components of Plai oil at retention time 7.362, 14.173 and 28.390 minutes, they were found to be sabinene (23.46%), terpinen-4-ol (19.53%) and (*E*)-1-(3',4'-dimethoxyphenyl)butadiene (DMPBD) (30.49%), respectively. The amount of terpinen-4-ol and DMPBD (%w/w) in the inclusion complexes were detected by GC-MS. TP4ol and DMPBD were only found in the HPbCD complex (Figure S1b). The loading efficiency of terpinen-4-ol and DMPBD (%w/w) in the inclusion complexes were calculated by percent peak area obtaining 81% and 18%, respectively.

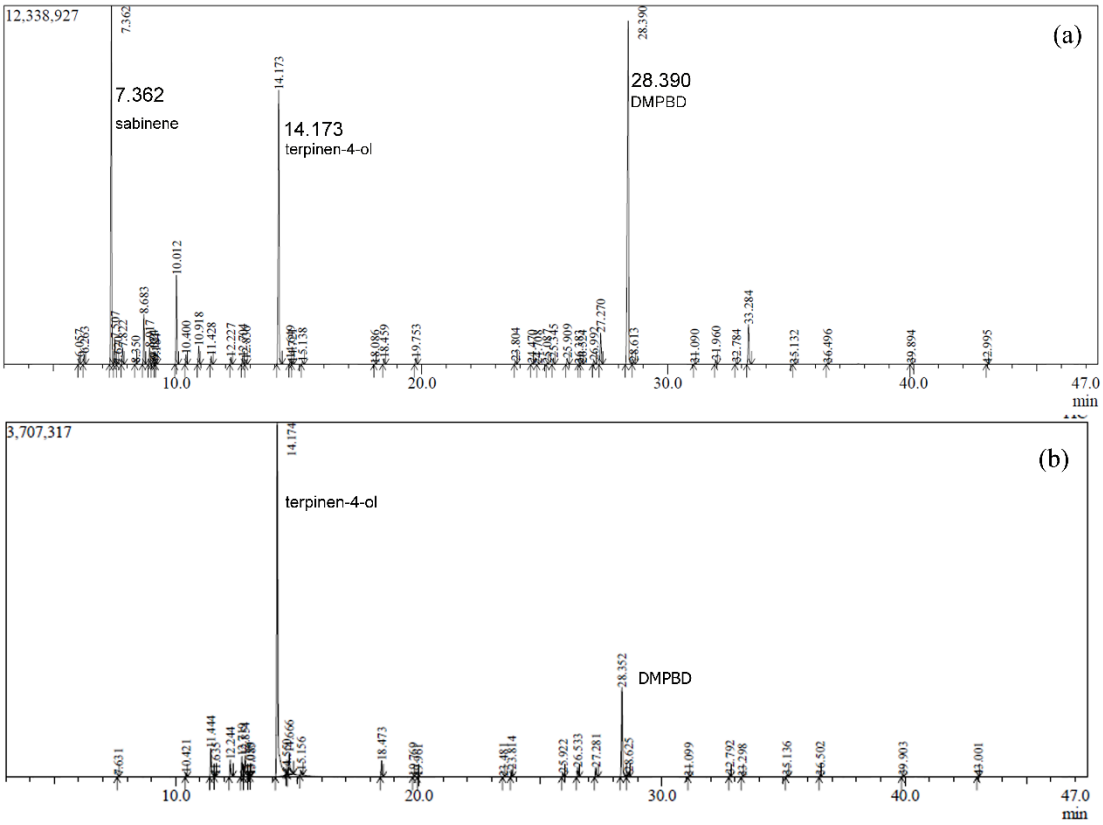

Figure S1 GC-MS chromatogram of Plai oil (PO) (a) and PO-HpbCD inclusion complex (b).

S2. TOF-SIMS study of PO-HpbCD inclusion complex on skin

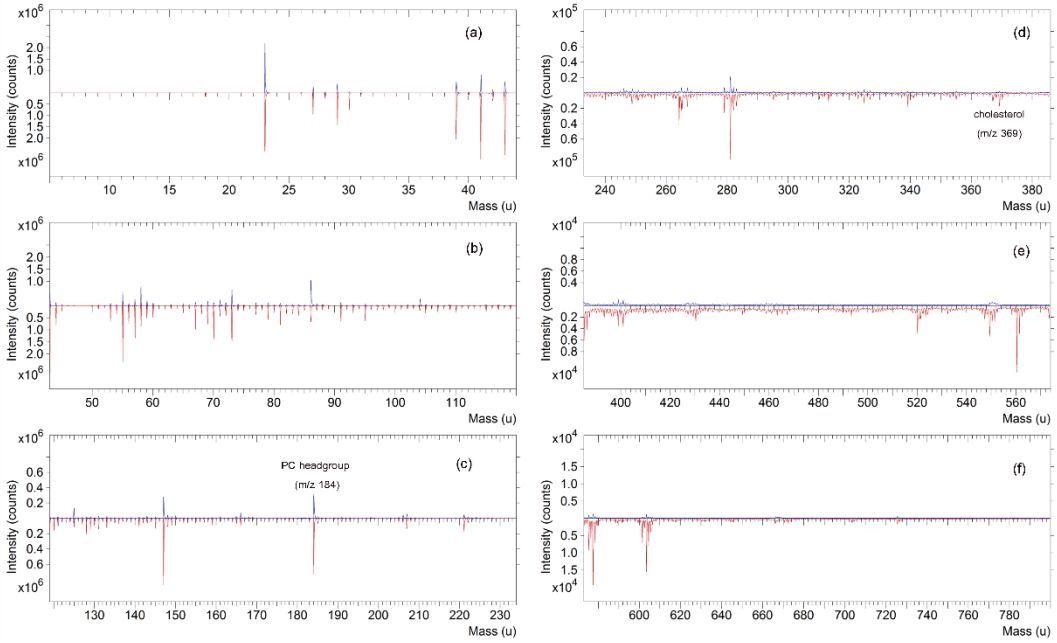

Figure S2 The TOF-SIMS spectra of selected area from control skin (blue) and HPbCD inclusion complex exposed skin (red) in the range of 0-50 (a), 50- 120 (b), 120-240 (c), 240-400 (d), 400-580 (e) and 580-800 (f).

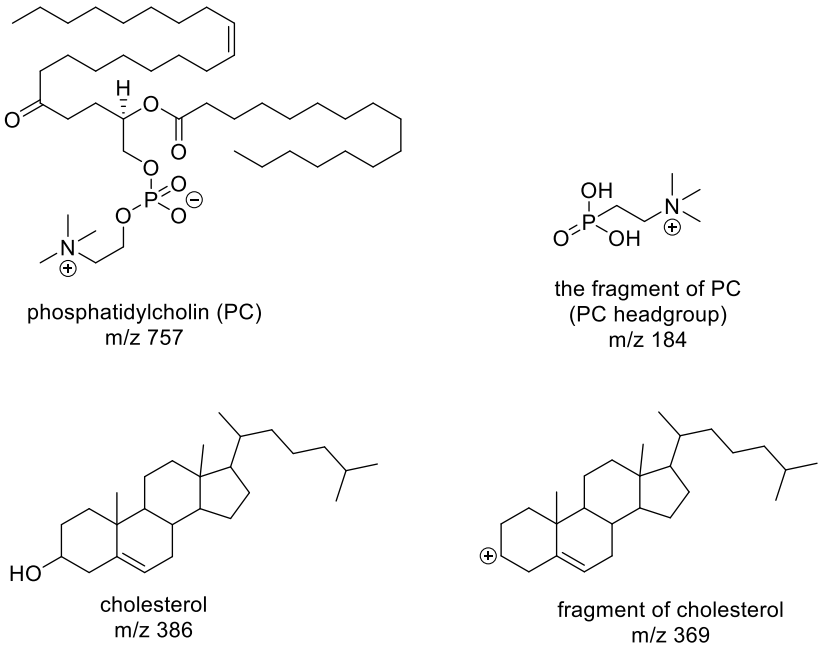

Figure S3 The chemical structure of phosphatidylcholines (PC) at m/z 757, the fragment of PC (PC headgroup) at m/z 184, cholesterol at m/z 386 and the fragment of cholesterol at m/z 369.

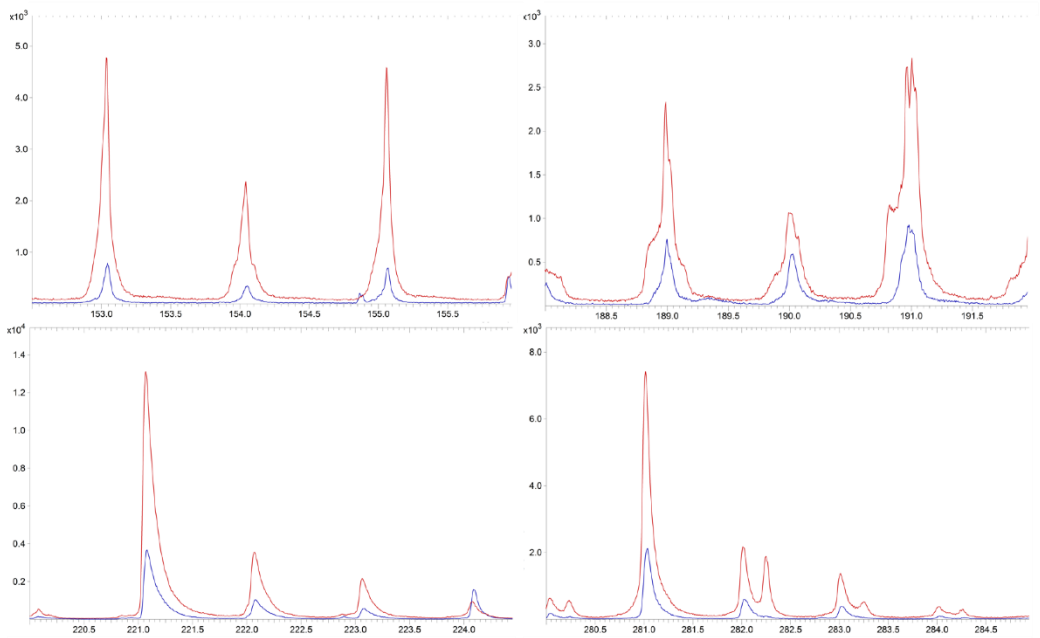

Figure S4. The TOF-SIMS spectra of selected area from control skin (blue) and HPbCD inclusion complex exposed skin (red).

S3. Imaging of TOF-SIMS depth profile study of PO-HPbCD in human skin

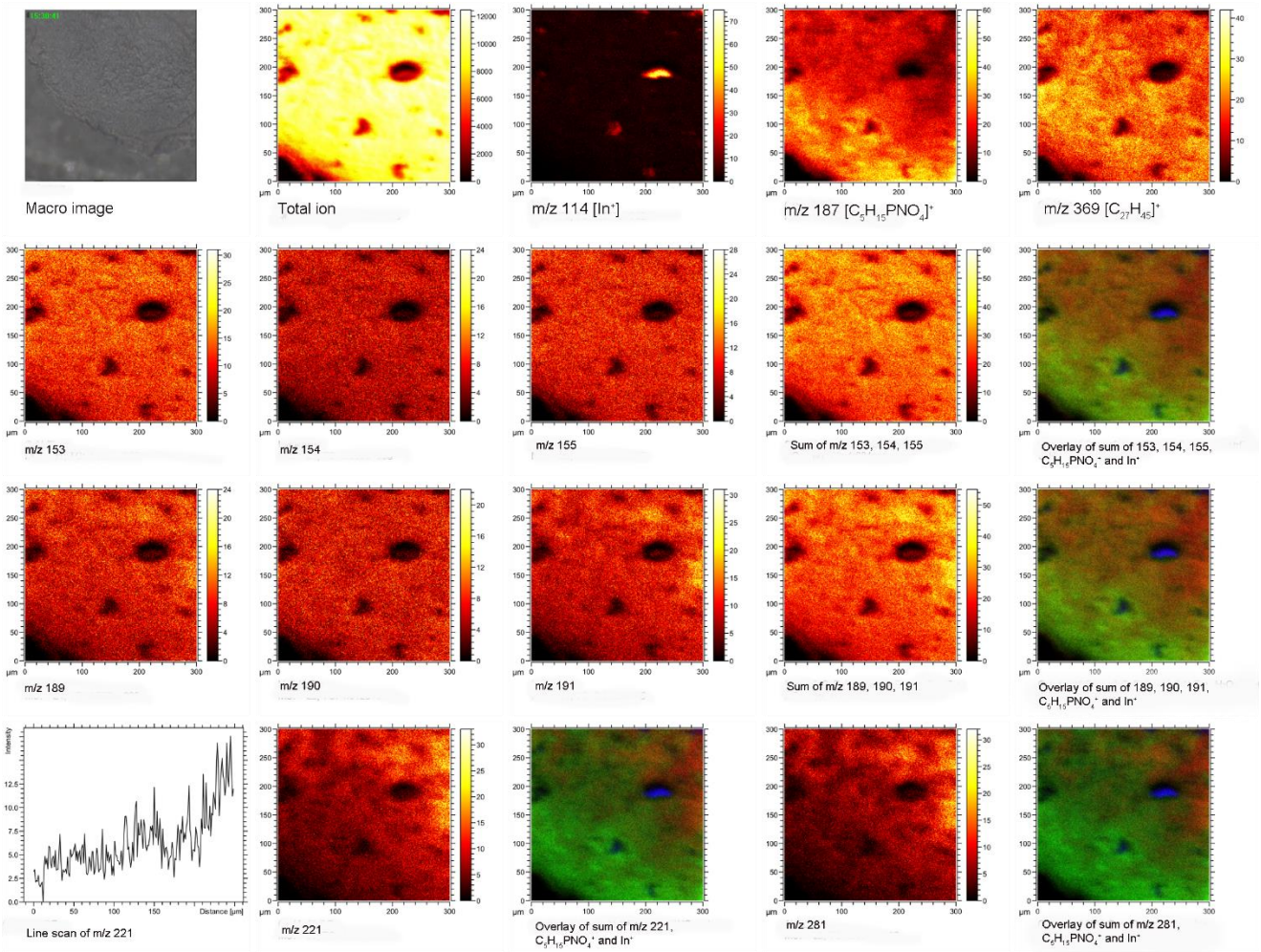

Figure S5. The three dimensional (3D) imaging data from control skin tissue (a) and HPbCD inclusion complex exposed skin tissue (b) obtained by the use of TOF-SIMS depth profiling.