## Effects of Ortho Substituent Groups of Protocatechualdehyde Derivatives

## on Binding to the C1 Domain of Novel Protein Kinase C

Narsimha Mamidi, Rituparna Borah, Narayan Sinha, Chandramohan Jana, and Debasis

Manna\*

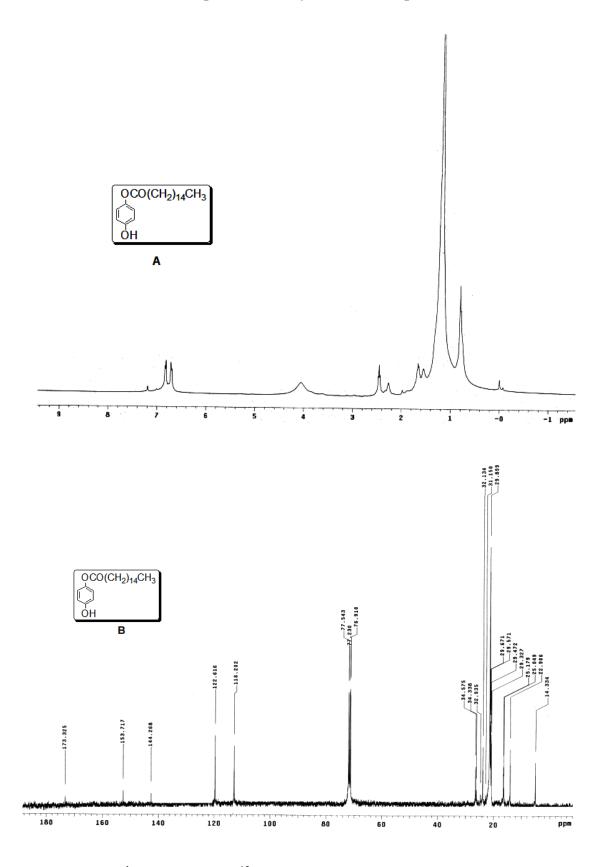
Department of Chemistry, Indian Institute of Technology Guwahati, Assam 781039, India

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## NMR spectra of the synthesized compounds



**Figure S1:** <sup>1</sup>H NMR (**A**) and <sup>13</sup>C NMR (**B**) of 4-hydroxylphenyl palmitate (**1a**).

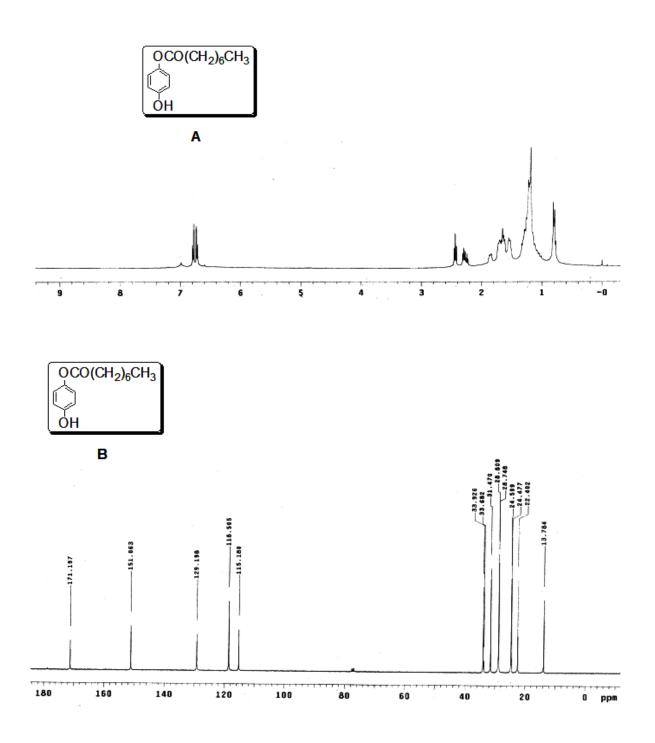
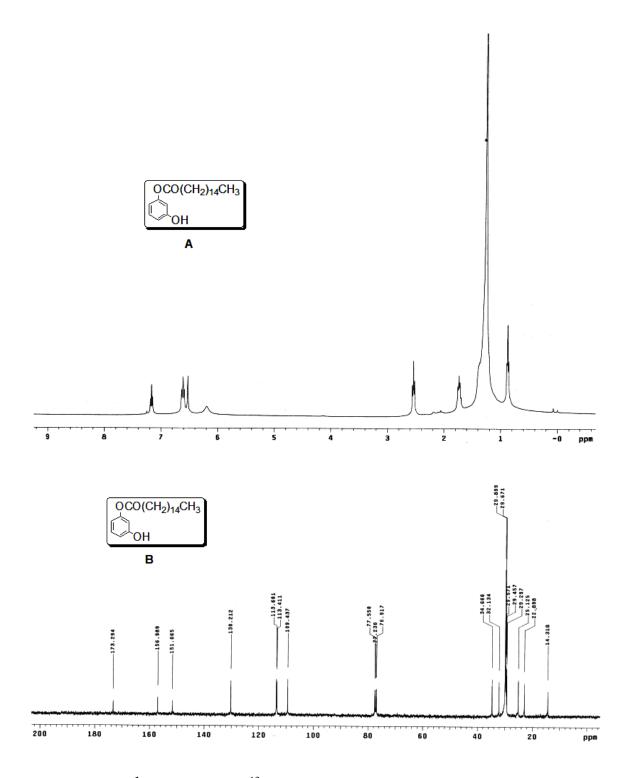
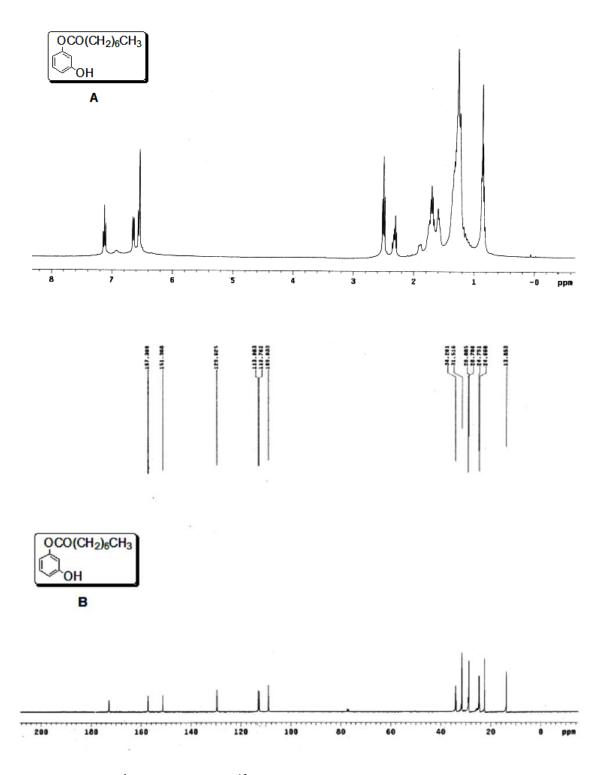


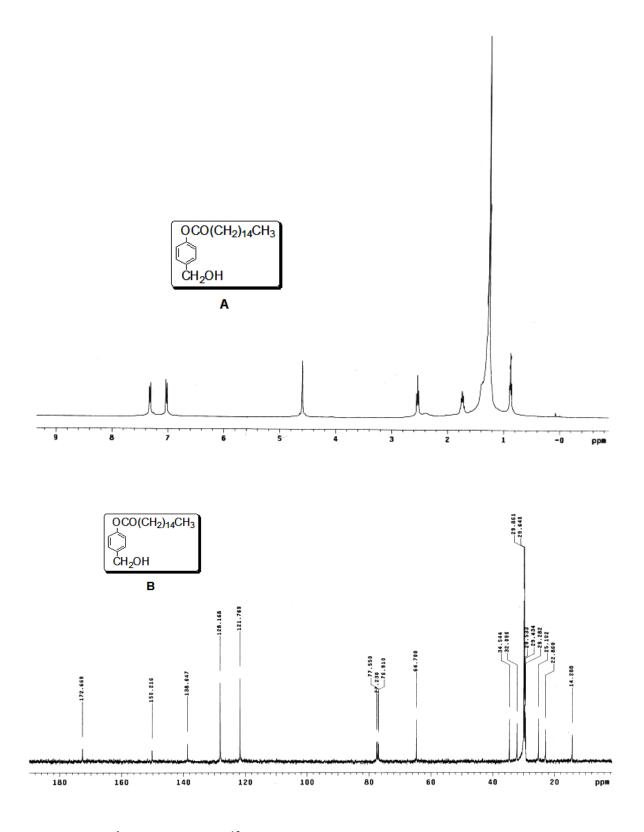
Figure S2: <sup>1</sup>H NMR (A) and <sup>13</sup>C NMR (B) of 4-hydroxylphenyl octanoate (1b).



**Figure S3:** <sup>1</sup>H NMR (**A**) and <sup>13</sup>C NMR (**B**) of 3-hydroxylphenyl palmitate (**2a**).



**Figure S4:** <sup>1</sup>H NMR (**A**) and <sup>13</sup>C NMR (**B**) of 3-hydroxylphenyl octanoate (**2b**).



**Figure S5:** <sup>1</sup>H NMR (**A**) and <sup>13</sup>C NMR (**B**) of 4-(hydroxymethyl)phenyl palmitate (**3a**).

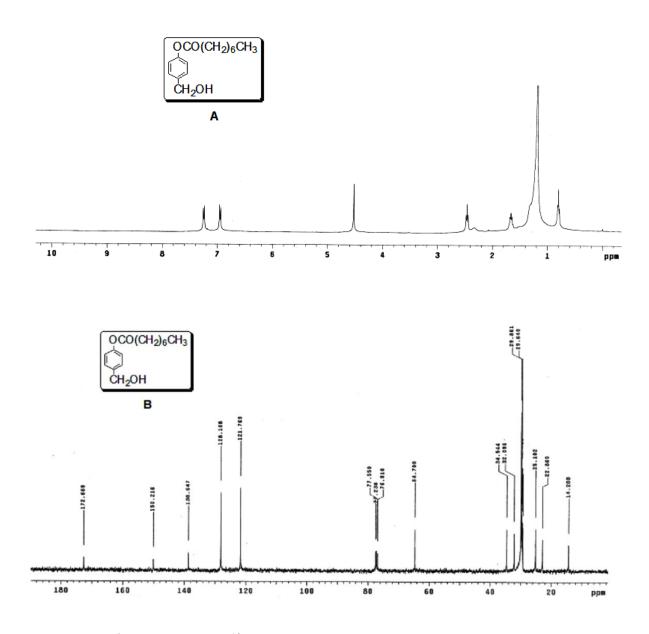


Figure S6: <sup>1</sup>H NMR (A) and <sup>13</sup>C NMR (B) of 4-(hydroxymethyl)phenyl octanoate (3b).

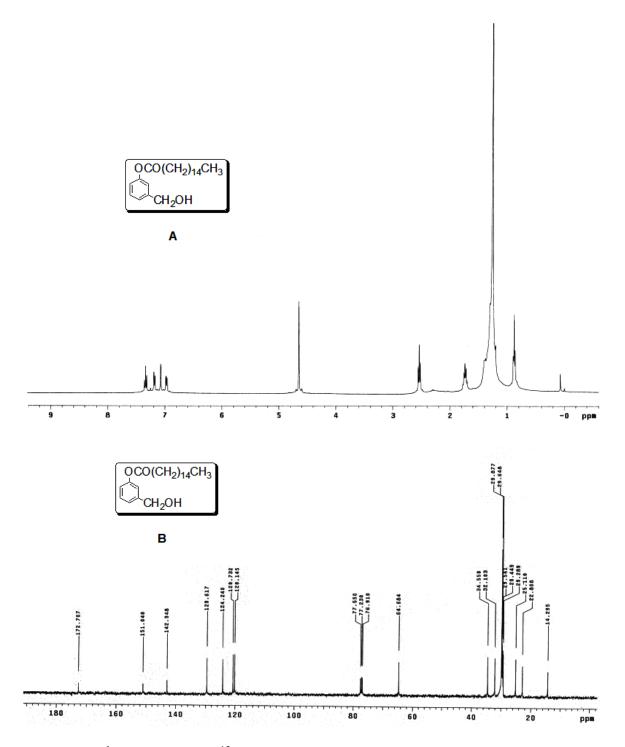


Figure S7: <sup>1</sup>H NMR (A) and <sup>13</sup>C NMR (B) of 3-(hydroxymethyl)phenyl palmitate (4a).

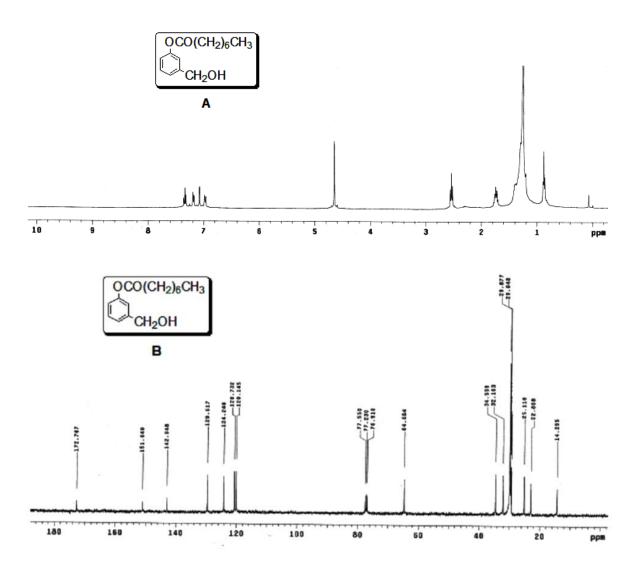


Figure S8: <sup>1</sup>H NMR (A) and <sup>13</sup>C NMR (B) of 3-(hydroxymethyl)phenyl octanoate (4b).

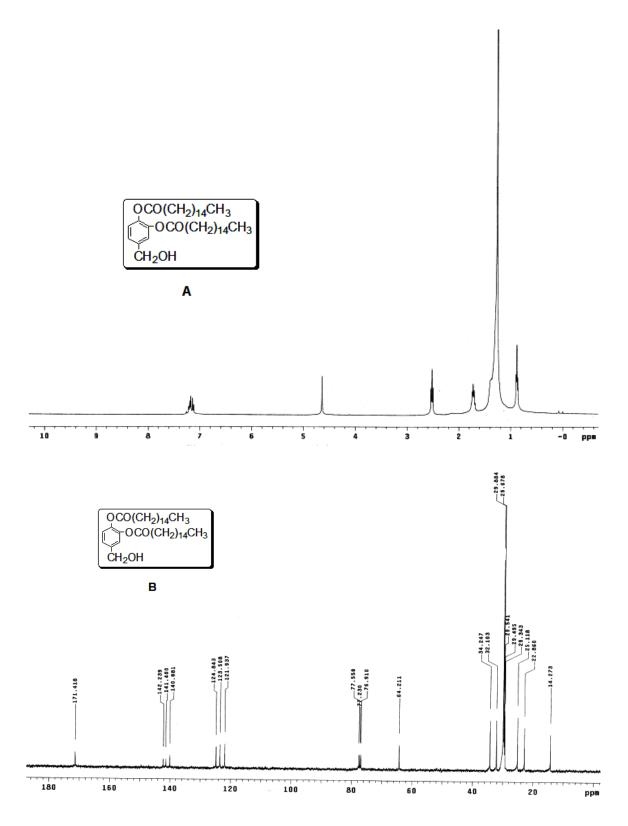
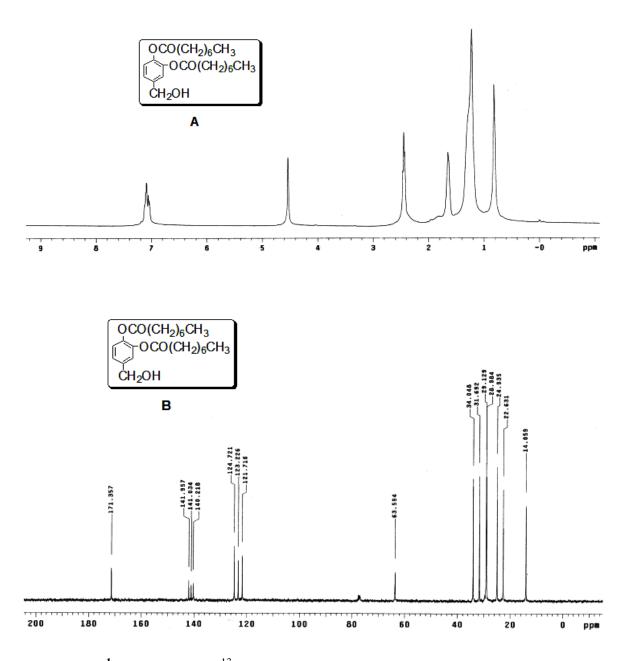
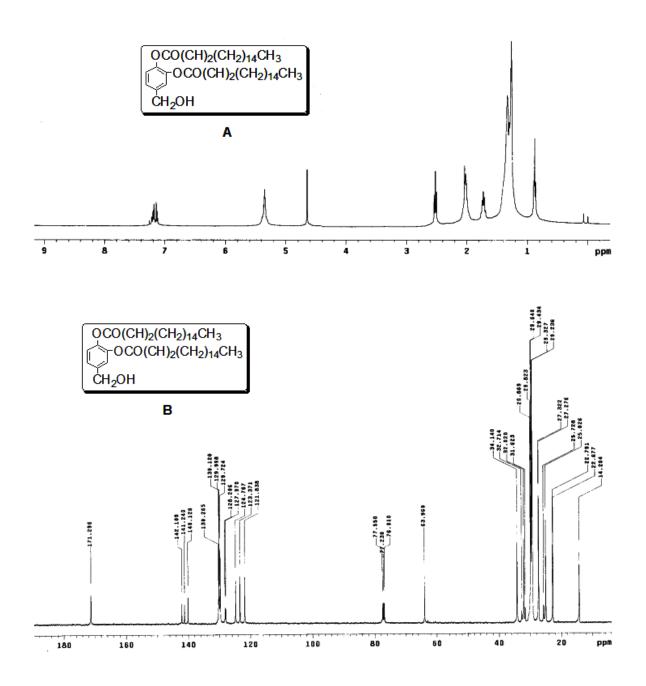


Figure S9: <sup>1</sup>H NMR (A) and <sup>13</sup>C NMR (B) of 4-(hydroxymethyl)-2-

(hexadecanoyloxy)phenyl palmitate (5a).



**Figure S10:** <sup>1</sup>H NMR (**A**) and <sup>13</sup>C NMR (**B**) of 4-(hydroxymethyl)-2-(octanoyloxy)phenyl octanoate (**5b**).



**Figure S11:** <sup>1</sup>H NMR (**A**) and <sup>13</sup>C NMR (**B**) of **2**-(Z)-(octadec-9-enoyloxy)-4-(hydroxymethyl)phenyl oleate (**6**).

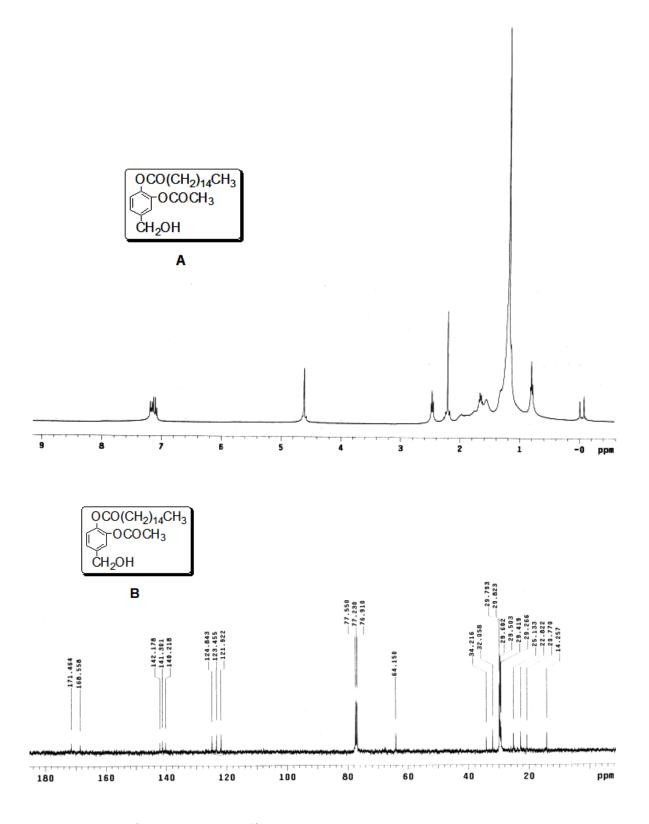
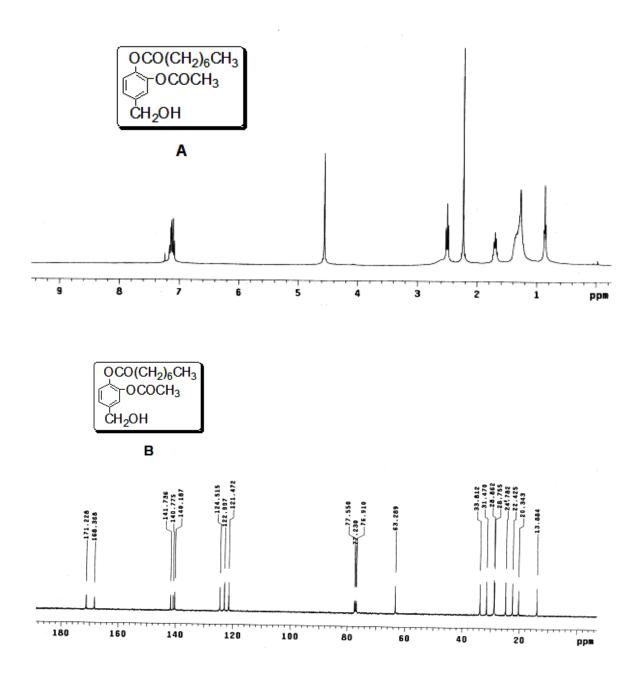


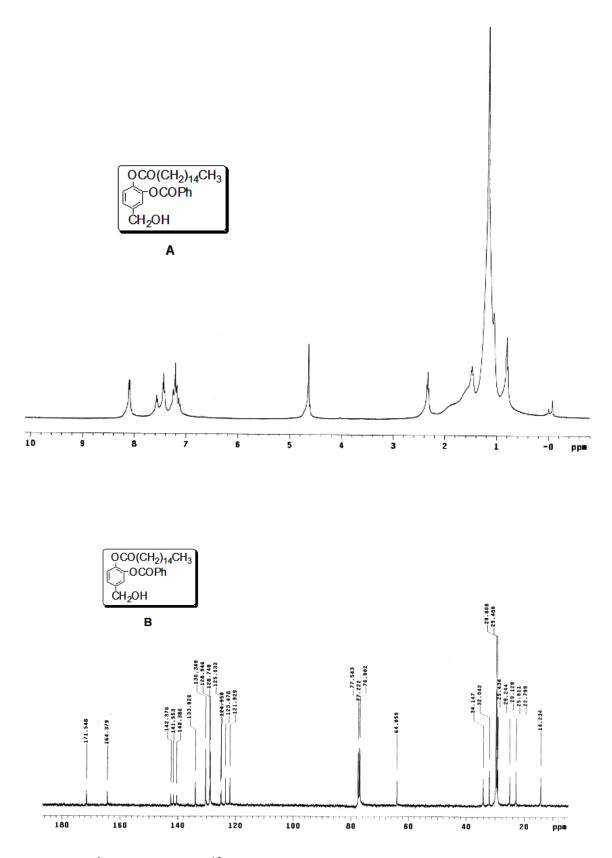
Figure S12: <sup>1</sup>H NMR (A) and <sup>13</sup>C NMR (B) of 2-acetoxy-4-(hydroxylmethyl)phenyl

palmitate (7a).



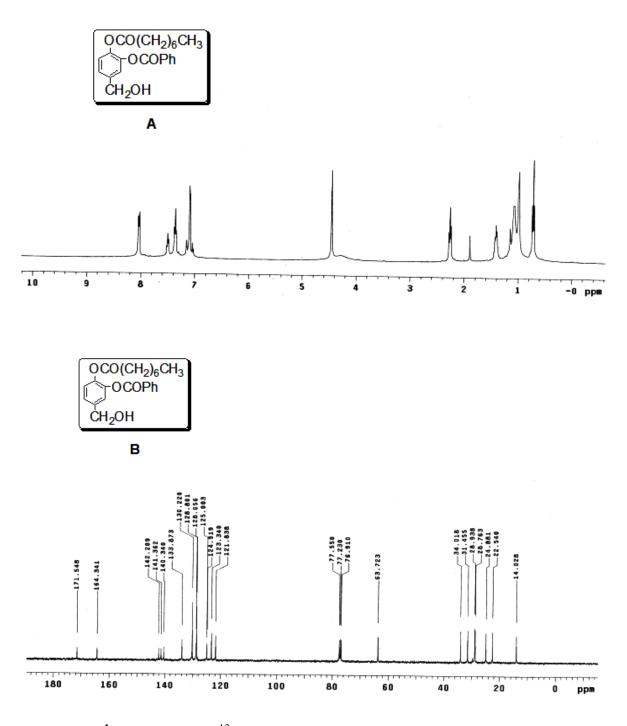
**Figure S13:** <sup>1</sup>H NMR (**A**) and <sup>13</sup>C NMR (**B**) of 2-acetoxy-4-(hydroxylmethyl)phenyl

octanoate (7b).



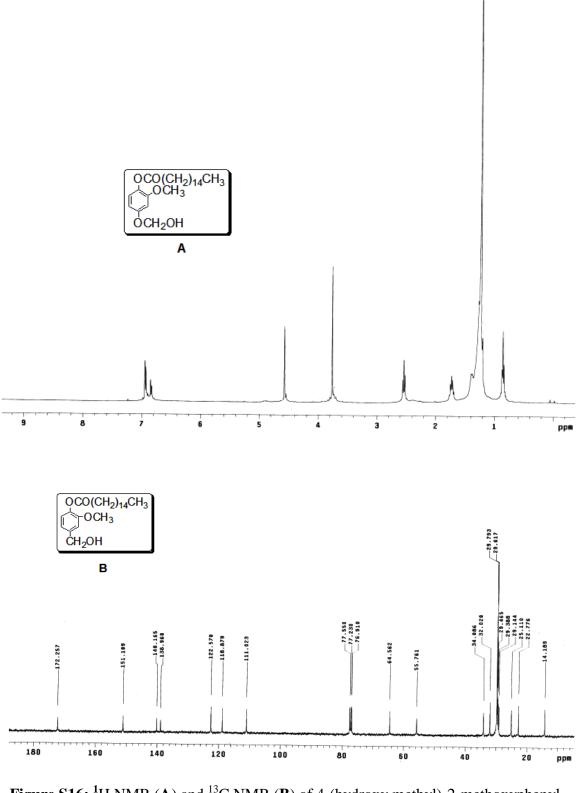
**Figure S14:** <sup>1</sup>H NMR (**A**) and <sup>13</sup>C NMR (**B**) of 5-(hydroxymethyl)-2-(palmitoyloxy)phenyl

benzoate (8a).

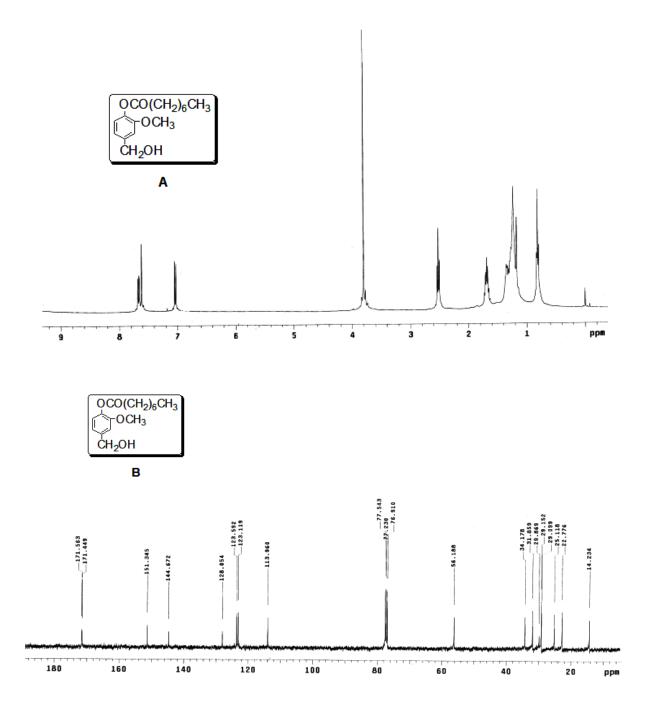


**Figure S15:** <sup>1</sup>H NMR (**A**) and <sup>13</sup>C NMR (**B**) of 5-(hydroxymethyl)-2-(octanoyloxy)phenyl

benzoate (8b).



**Figure S16:** <sup>1</sup>H NMR (**A**) and <sup>13</sup>C NMR (**B**) of 4-(hydroxy methyl)-2-methoxyphenyl palmitate (**9a**).



**Figure S17:** <sup>1</sup>H NMR (**A**) and <sup>13</sup>C NMR (**B**) of 4-(hydroxy methyl)-2-methoxyphenyl

octanoate (9b).

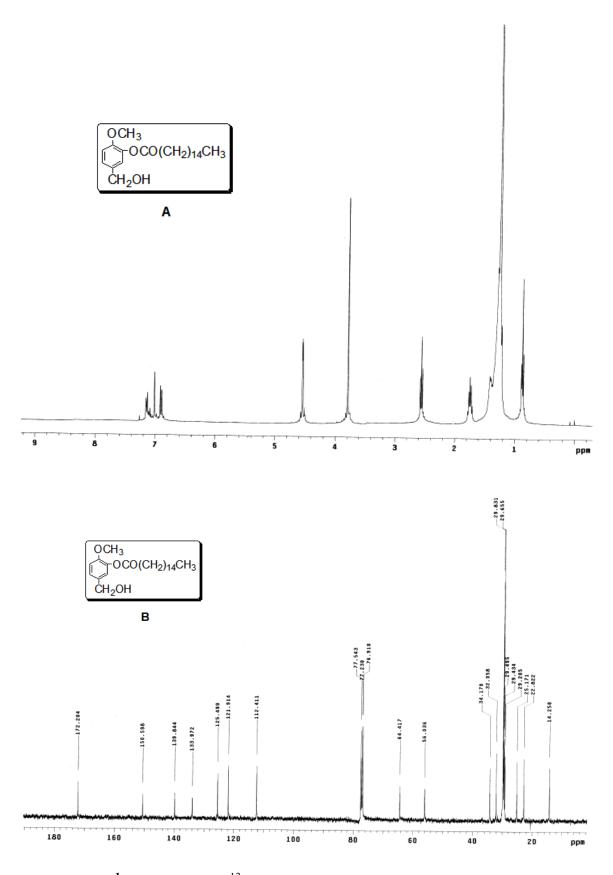


Figure S18: <sup>1</sup>H NMR (A) and <sup>13</sup>C NMR (B) of 5-(hydroxymethyl)-2-methoxyphenyl palmitate (10a).

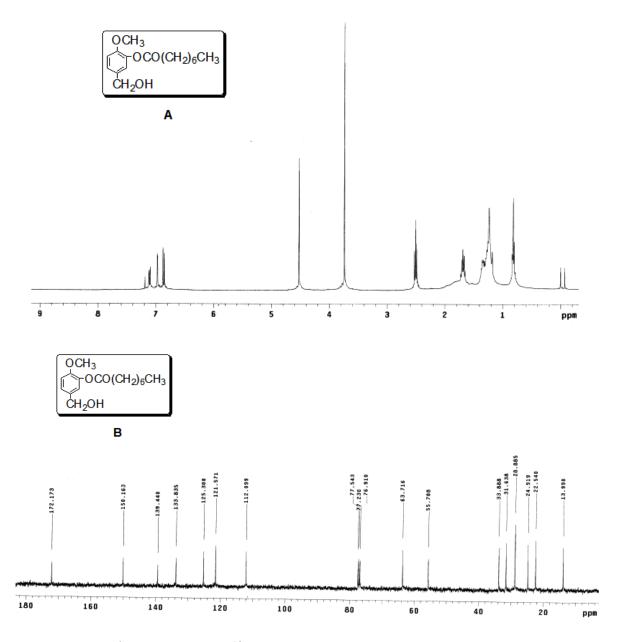
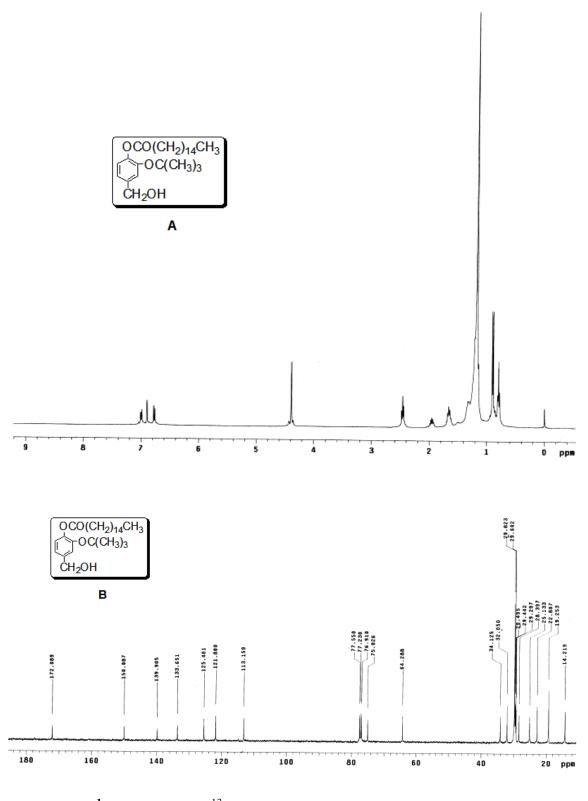
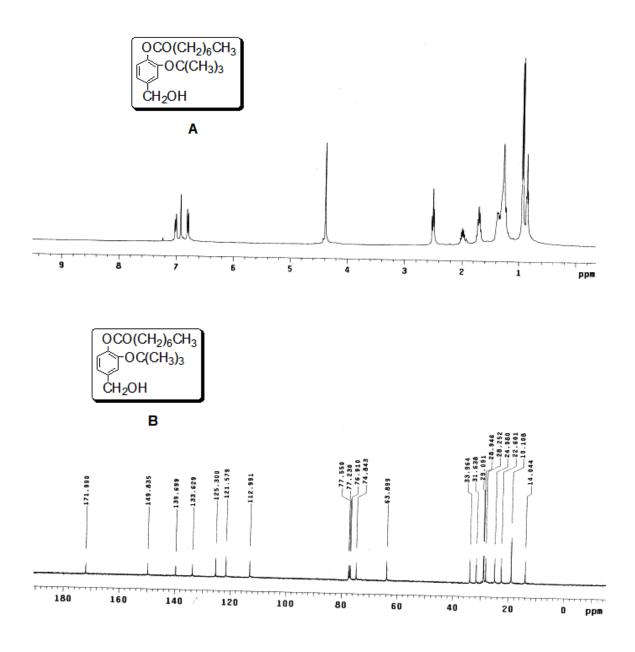


Figure S19: <sup>1</sup>H NMR (A) and <sup>13</sup>C NMR (B) of 5-(hydroxymethyl)-2-methoxyphenyl

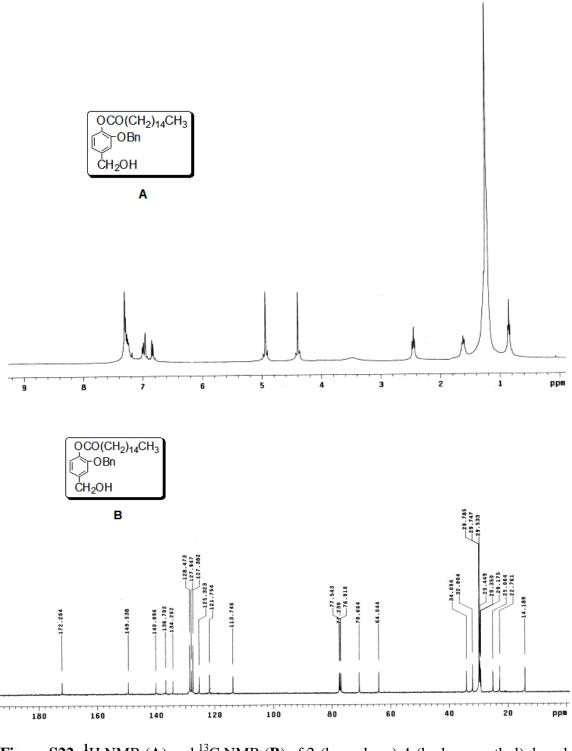
octanoate (10b).



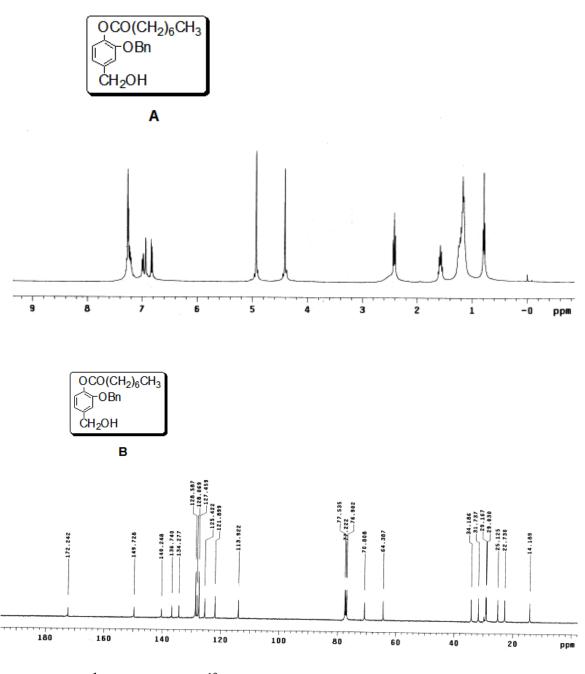
**Figure S20:** <sup>1</sup>H NMR (**A**) and <sup>13</sup>C NMR (**B**) of 2-tert-butoxy-4-(hydroxymethyl)phenyl palmitate (**11a**).



**Figure S21:** <sup>1</sup>H NMR (**A**) and <sup>13</sup>C NMR (**B**) of 2-tert-butoxy-4-(hydroxymethyl)phenyl octanoate (**11b**).



**Figure S22:** <sup>1</sup>H NMR (**A**) and <sup>13</sup>C NMR (**B**) of 2-(benzyloxy)-4-(hydroxymethyl)phenyl palmitate (**12a**).



**Figure S23:** <sup>1</sup>H NMR (**A**) and <sup>13</sup>C NMR (**B**) of 2-(benzyloxy)-4-(hydroxymethyl)phenyl

octanoate (12b).

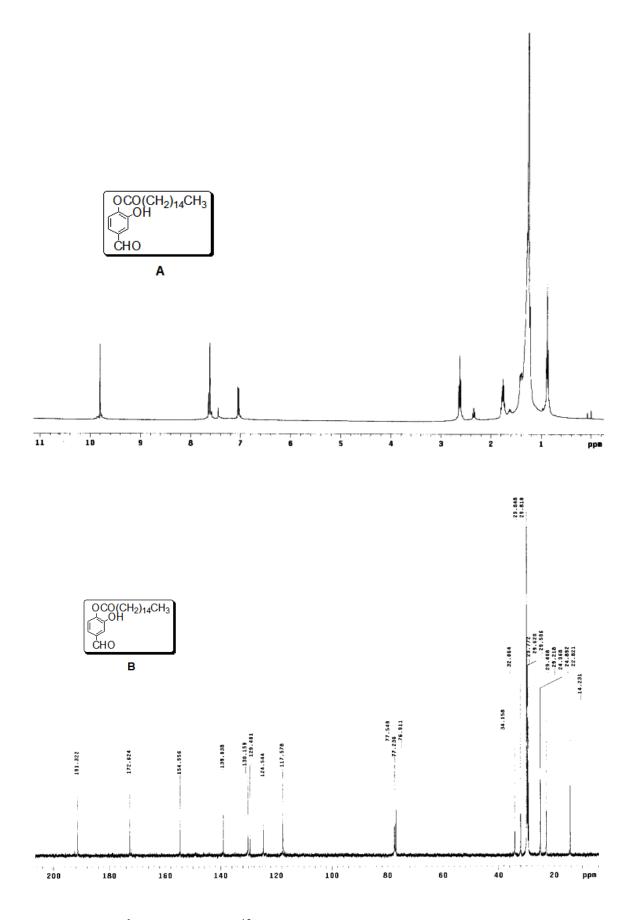


Figure S24: <sup>1</sup>H NMR (A) and <sup>13</sup>C NMR (B) of 4-formyl-2-hydroxyphenyl palmitate.

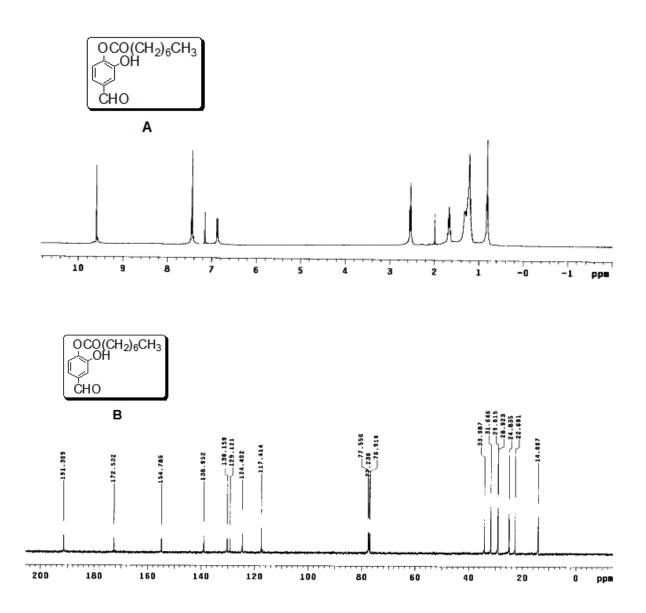
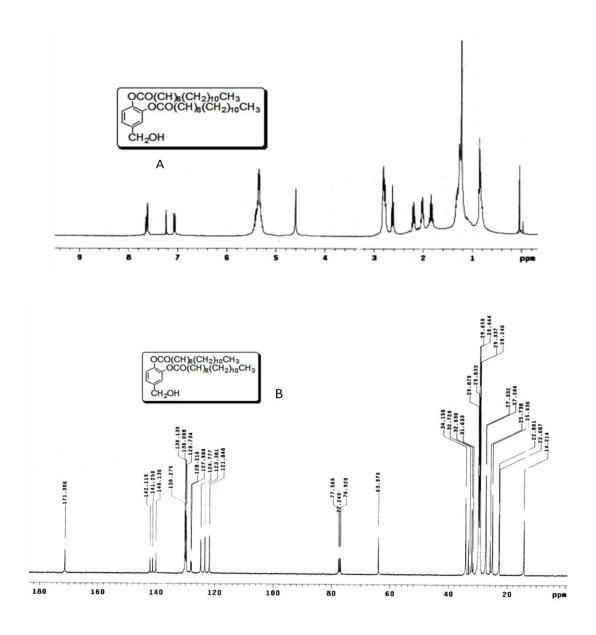
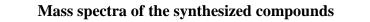


Figure S25: <sup>1</sup>H NMR (A) and <sup>13</sup>C NMR (B) of 4-formyl-2-hydroxyphenyl octanoate.



**Figure S26**: <sup>1</sup>HNMR (**A**) & <sup>13</sup>C NMR (**B**) of 4-(hydroxymethyl)-2-[(5Z,8Z,11Z,14Z)-icosa-

 $5,8,11,14\mbox{-tetraenoyloxy}] phenyl (5Z,8Z,11Z,14Z)\mbox{-icosa-}5,8,11,14\mbox{-tertaenoate}.$ 



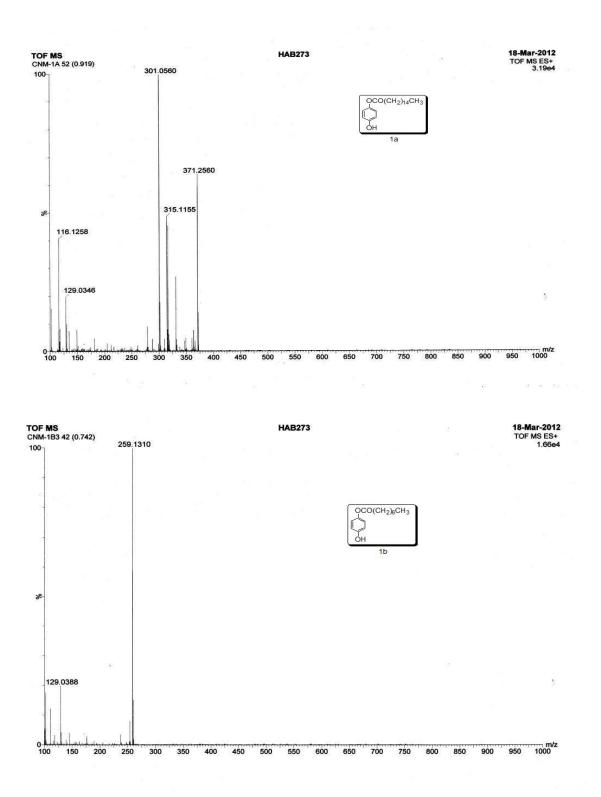


Figure S27: Mass spectrum of compound 1a and 1b.

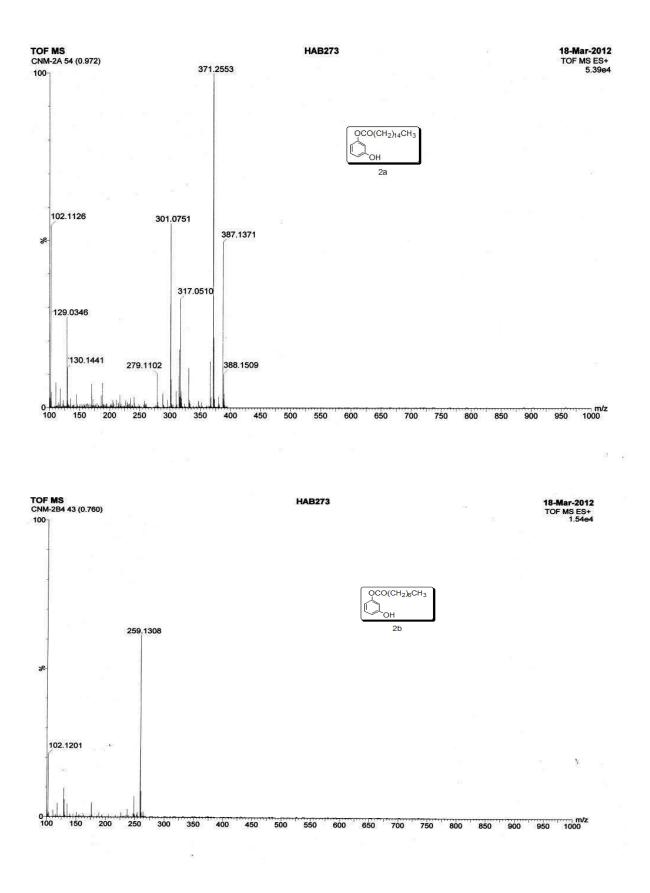


Figure S28: Mass spectrum of compound 2a and 2b.

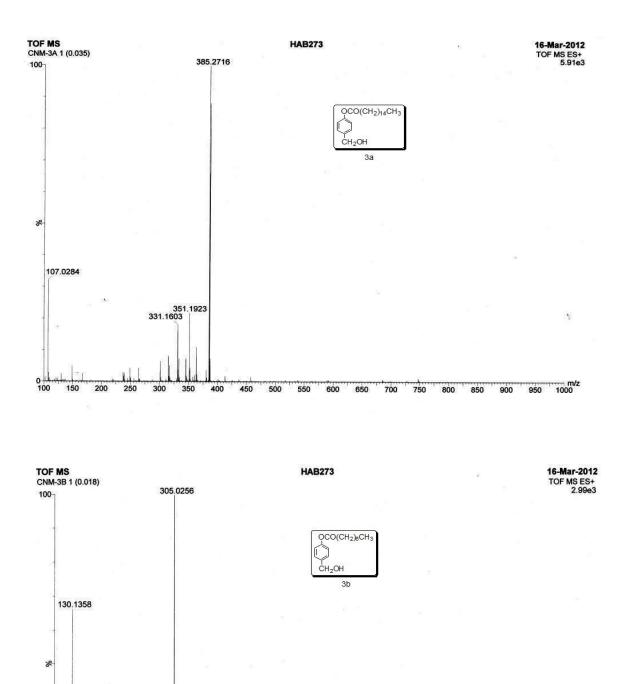


Figure S29: Mass spectrum of compound 3a and 3b.

283.0690

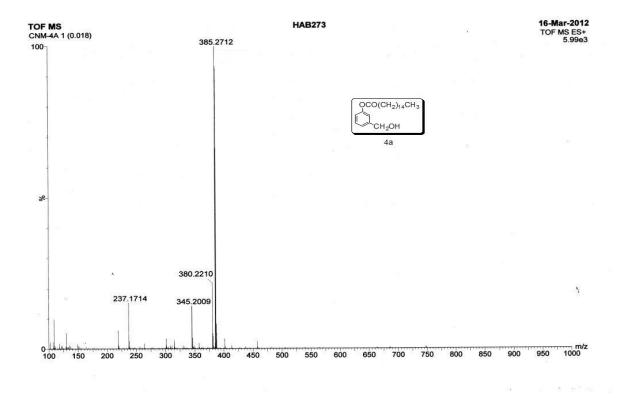
273.1466

315.1221

321.0387

E.

----- m/z 



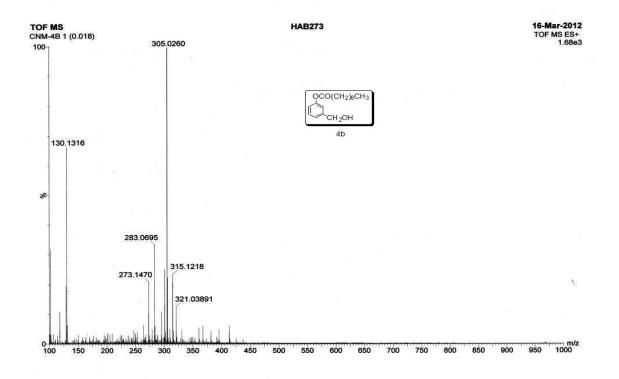


Figure S30: Mass spectrum of compound 4a and 4b.

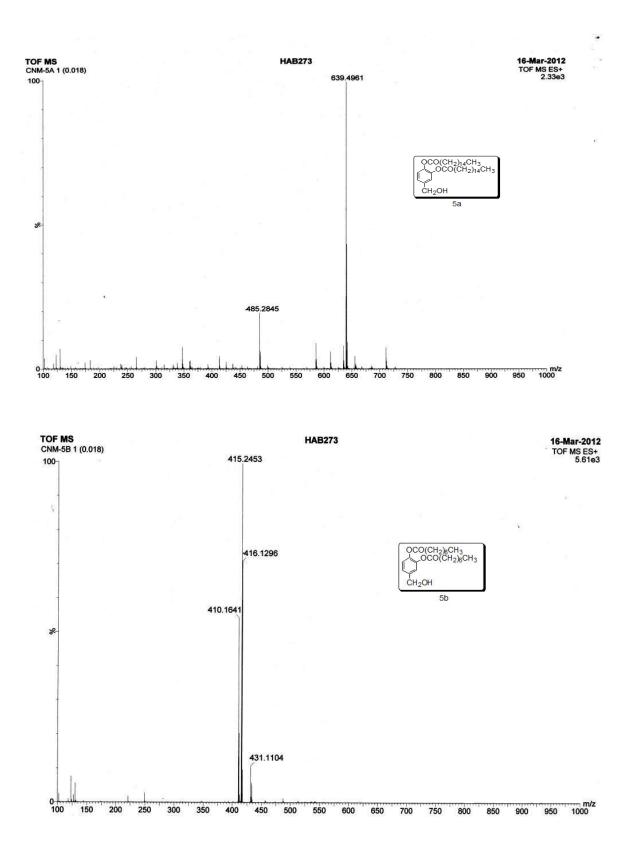


Figure S31: Mass spectrum of compound 5a and 5b.

33

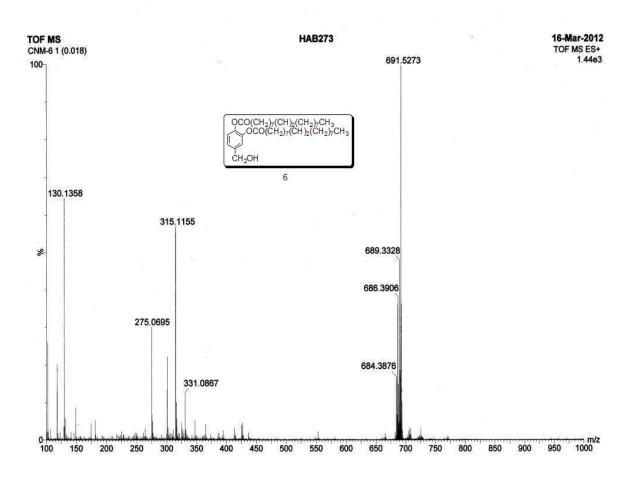


Figure S32: Mass spectrum of compound 6.

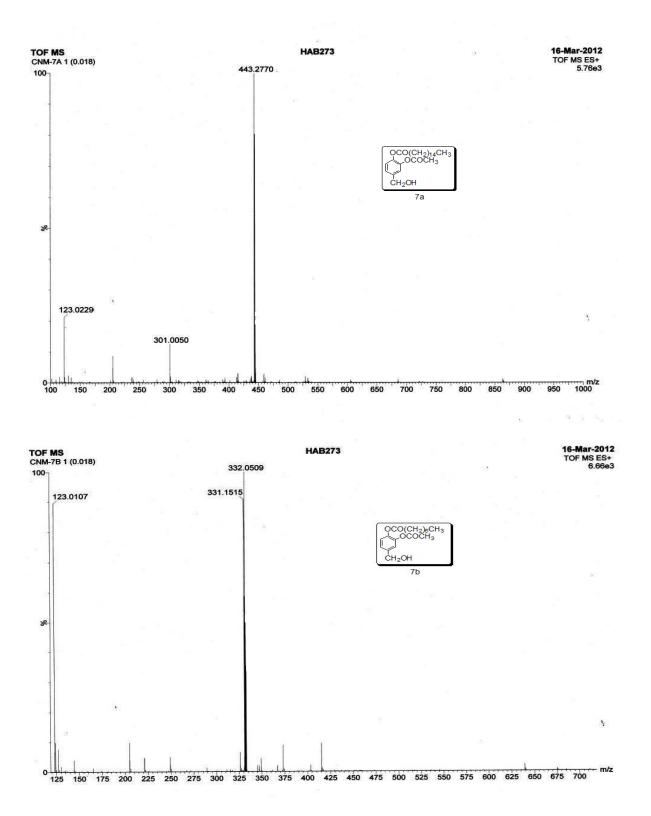
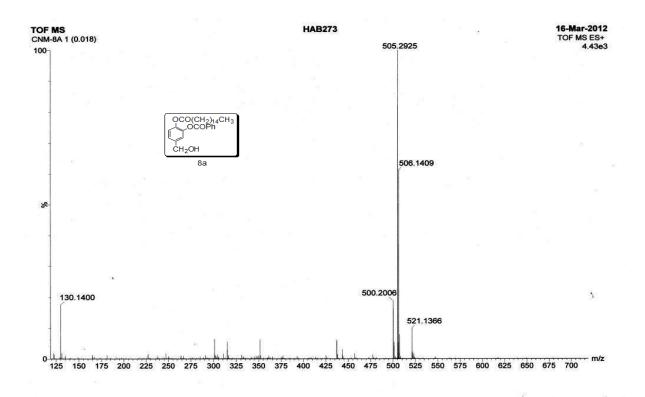


Figure S33: Mass spectrum of compound 7a and 7b.



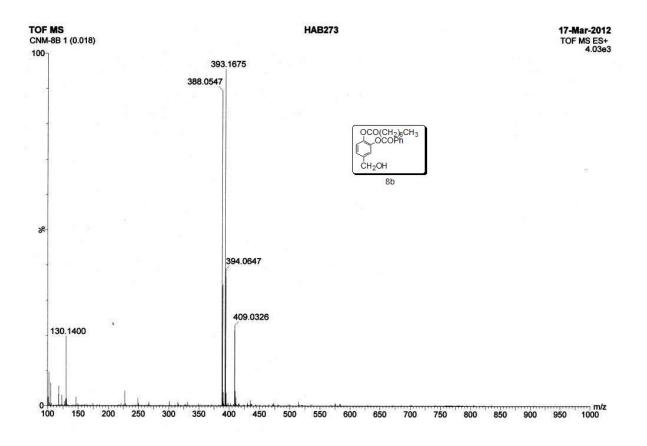


Figure S34: Mass spectrum of compound 8a and 8b.

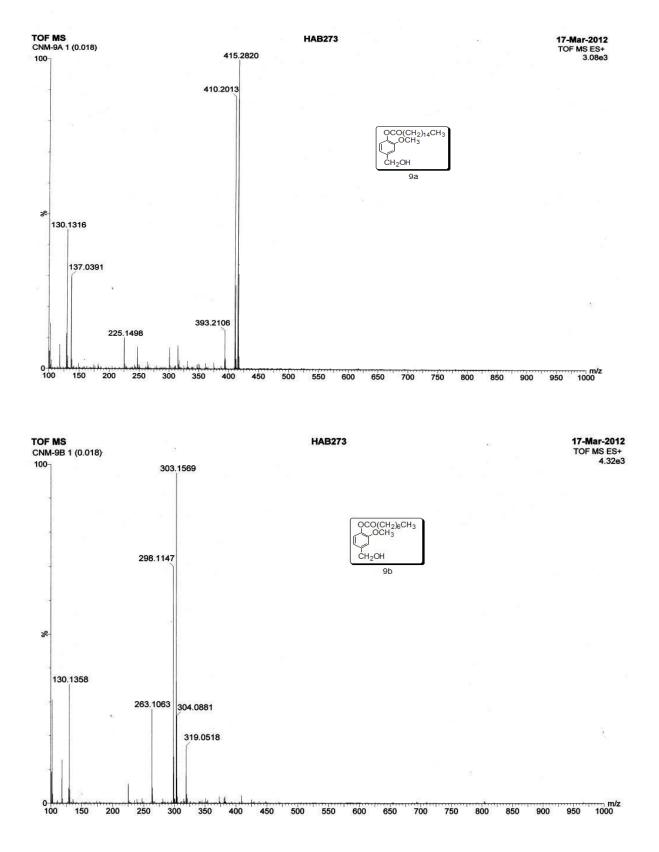


Figure S35: Mass spectrum of compound 9a and 9b.

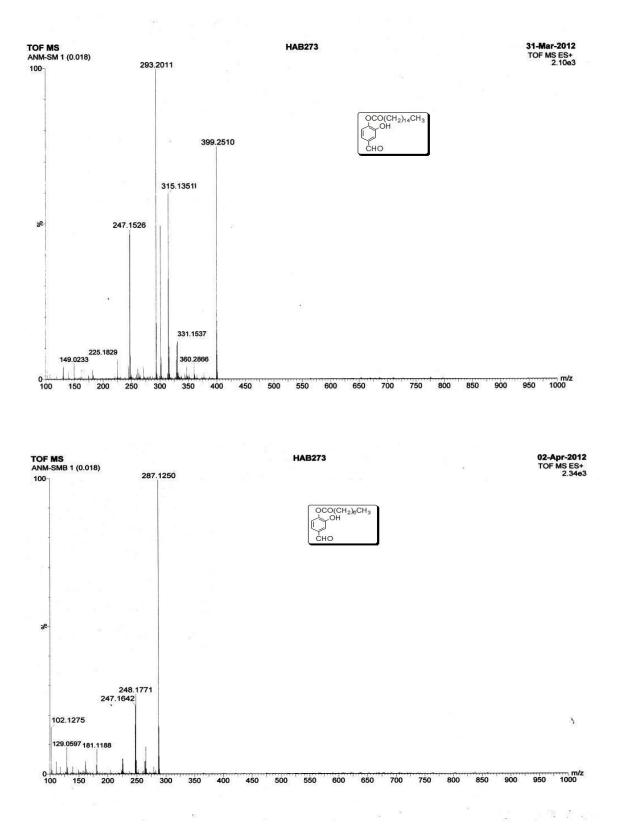


Figure S36: Mass spectrum of 4-formyl-2-hydroxyphenyl palmitate and 4-formyl-2-

hydroxyphenyl octanoate.

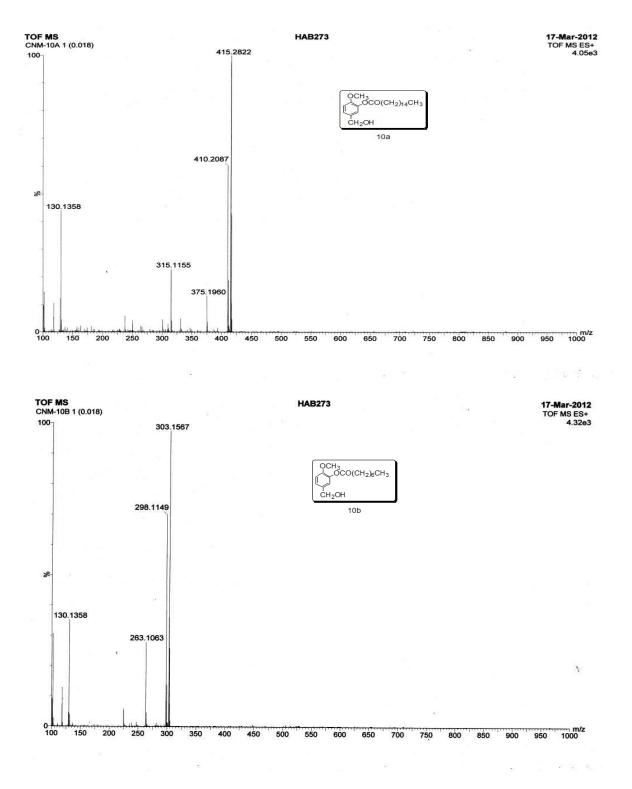


Figure S37: Mass spectrum of compound 10a and 10b.

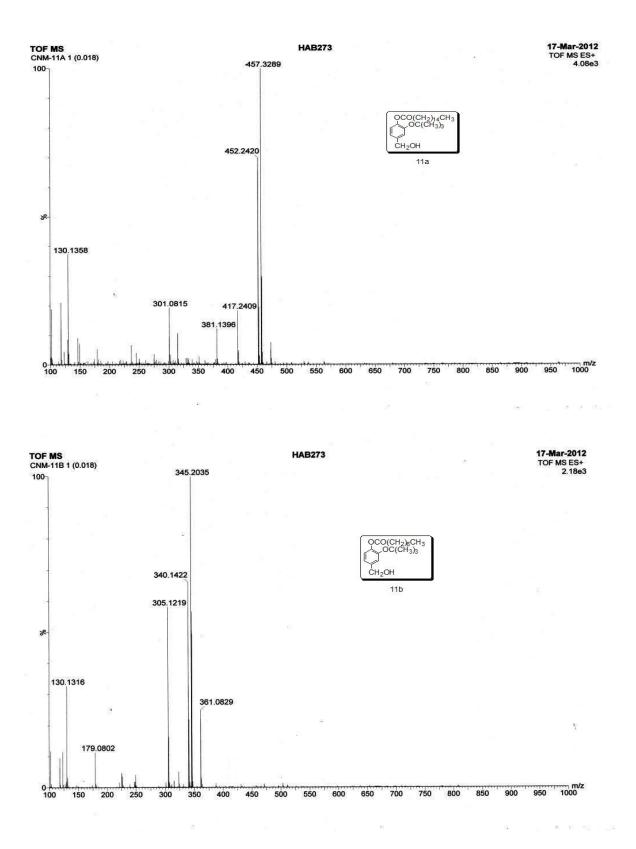


Figure S38: Mass spectrum of compound 11a and 11b.

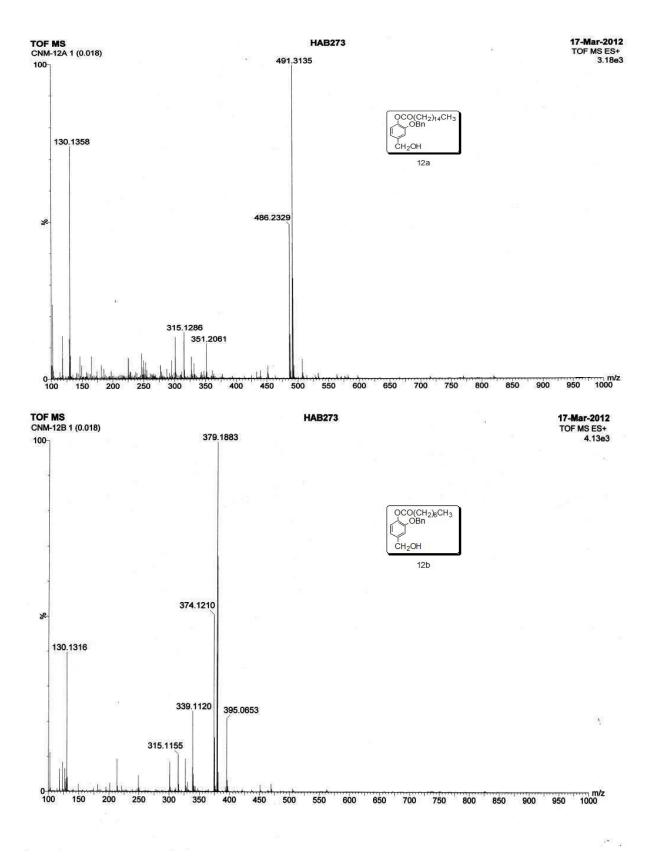


Figure S39: Mass spectrum of compound 12a and 12b.