DiGalactosyl-Glycero-Ether Lipid: synthetic approaches and evaluation as SK3 channel inhibitor.

Charlotte M. Sevrain, a Jean-Pierre Haelters,*a Aurélie Chantôme, b Hélène Couthon-Gourvès,*a Maxime Gueguinou, b Marie Potier-Cartereau, b Christophe Vandier* b and Paul-Alain Jaffrès+a

Summary

ESI-1 Synthesis of compound 5.............................................................................................................. 1
  Figure S1-1: Synthesis of compound ............................................................................................... 1
ESI-2 Spectral data ................................................................................................................................. 2
  Figure S2-1: 1H NMR (CDCl3) spectrum of compound 8................................................................. 2
  Figure S2-2: 13C NMR (CDCl3) spectrum of compound 8.............................................................. 3
  Figure S2-3: 2D NMR - COSY (CDCl3) spectrum of compound 8. ............................................... 4
  Figure S2-4: 2D NMR - HMQC (CDCl3) spectrum of compound 8. .............................................. 5
  Figure S2-5: 2D NMR - HMBC (CDCl3) spectrum of compound 8. .............................................. 6
  Figure S2-6: 1H NMR (CDCl3) spectrum of compound 10............................................................. 7
  Figure S2-7: 13C NMR (CDCl3) spectrum of compound 10............................................................ 8
  Figure S2-8: 1H NMR (CDCl3) spectrum of compound 15.............................................................. 9
  Figure S2-9: 13C NMR (CDCl3) spectrum of compound 15............................................................ 10
  Figure S2-10: 2D NMR - COSY (CDCl3) spectrum of compound 15. ......................................... 11
  Figure S2-11: 2D NMR - HMQC (CDCl3) spectrum of compound 15. ......................................... 12
  Figure S2-12: 2D NMR - HMBC (CDCl3) spectrum of compound 15. ......................................... 13
  Figure S2-13: 1H NMR (CD3OD) spectrum of compound 16........................................................ 14
  Figure S2-14: 13C NMR (CD3OD) spectrum of compound 16. .................................................... 15
  Figure S2-15: 2D NMR - COSY (CD3OD) spectrum of compound 16. ........................................ 16
  Figure S2-16: 2D NMR - HMQC (CD3OD) spectrum of compound 16. ....................................... 17
  Figure S2-17: 2D NMR - HMBC (CDCl3) spectrum of compound 16. ......................................... 18
  Figure S2-18: IR spectrum of compound 16.................................................................................... 19
  Figure S2-19: 1H NMR (CDCl3) spectrum of compound 19. ......................................................... 20
  Figure S2-20: 13C NMR (CDCl3) spectrum of compound 19. ....................................................... 21
ESI-1 Synthesis of compound 5

Figure S1-1: Synthesis of compound 5: a) CH$_3$COONH$_4$, dry DMF, 48 hours, R.T. 85%$^1$ b) Cl$_3$CCN, Cs$_2$CO$_3$, dry THF, 48 hours, R.T. 88%$^2$ c) 3-(hexadecyloxy)-2-methoxypropanol, BF$_3$.Et$_2$O, molecular sieves, dry CH$_2$Cl$_2$, 24 hours, R.T., 53%$^3$ d) K$_2$CO$_3$, dry MeOH, 15 hours, R.T. 86%$^4$

**Figure S2-1:** $^1$H NMR (CDCl$_3$) spectrum of compound 8.
Figure S2-2: $^{13}$C NMR (CDCl$_3$) spectrum of compound 8.
Figure S2-3: 2D NMR - COSY (CDCl₃) spectrum of compound 8.
Figure S2-4: 2D NMR - HMQC (CDCl₃) spectrum of compound 8.
Figure S2-5: 2D NMR - HMBC (CDCl₃) spectrum of compound 8.
Figure S2-6: $^1$H NMR (CDCl$_3$) spectrum of compound 10.
Figure S2-7: $^{13}$C NMR (CDCl$_3$) spectrum of compound 10.
Figure S2-8: $^1$H NMR (CDCl$_3$) spectrum of compound 15.
Figure S2-9: $^{13}$C NMR (CDCl$_3$) spectrum of compound 15.
**Figure S2-10**: 2D NMR - COSY (CDCl₃) spectrum of compound 15.
Figure S2-11: 2D NMR - HMQC (CDCl$_3$) spectrum of compound 15.
**Figure S2-12:** 2D NMR - HMBC (CDCl₃) spectrum of compound 15.
Figure S2-13: $^1$H NMR (CD$_3$OD) spectrum of compound 16.
**Figure S2-14**: $^{13}$C NMR (CD$_3$OD) spectrum of compound 16.
Figure S2-15: 2D NMR - COSY (CD$_3$OD) spectrum of compound 16.
Figure S2-16: 2D NMR - HMQC (CD$_3$OD) spectrum of compound 16.
**Figure S2-17:** 2D NMR - HMBC (CDCl₃) spectrum of compound 16.
Figure S2-18: IR spectrum of compound 16.
Figure S2-19: $^1$H NMR (CDCl$_3$) spectrum of compound 19.
Figure S2-20: $^{13}$C NMR (CDCl₃) spectrum of compound 19.