

Supporting information for

Total synthesis of four stereoisomers of methyl 4,8,12-trimethylpentadecanoate, major component of the sex pheromone of the stink bug *Edessa meditabunda*.

Daiane Szczerbowski^{a,b}, Stefan Schulz^b and Paulo Henrique Gorgatti Zarbin^{a,*}

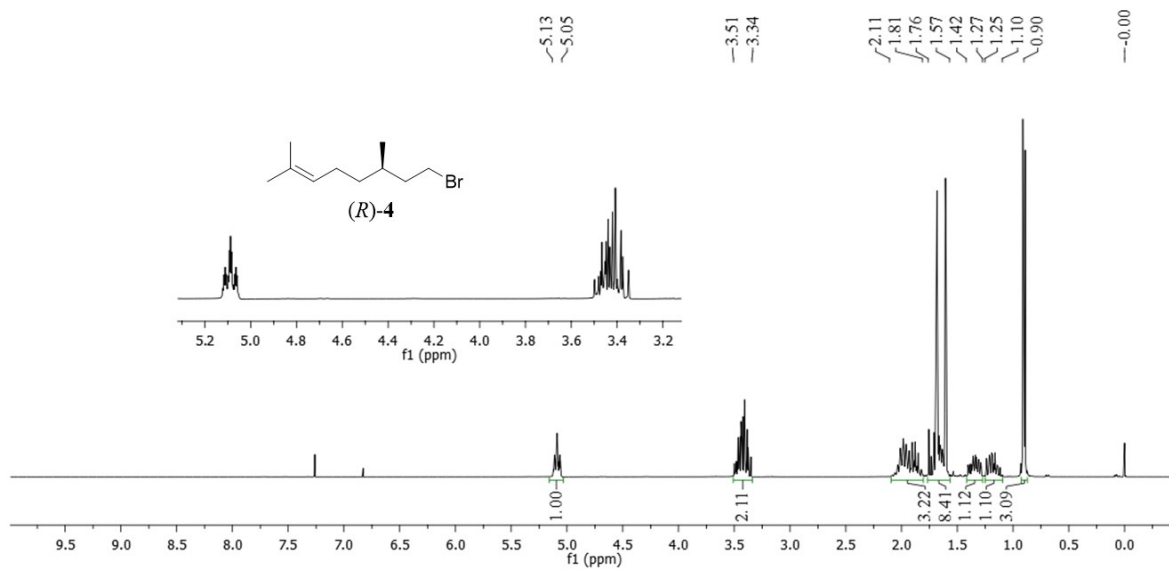
^a Laboratório de Semioquímicos, Chemistry Department, Federal University of Paraná, 81531-990 Curitiba, Brazil

^b Institute of Organic Chemistry, Technische Universität Braunschweig, 38106 Braunschweig, Germany

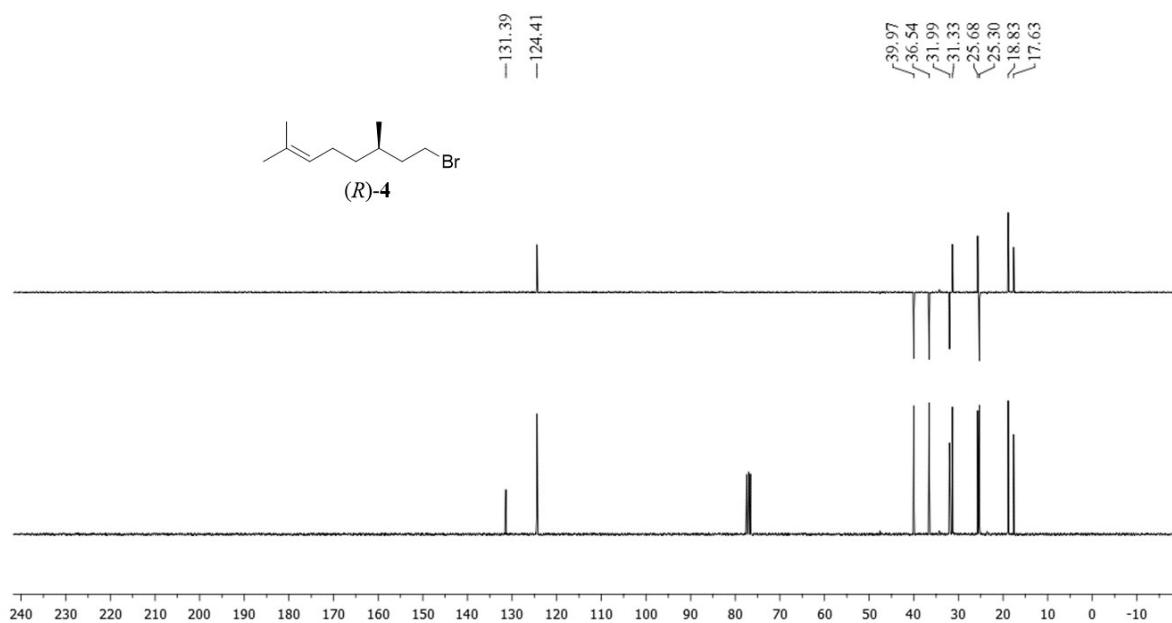
[*pzarbin@ufpr.br](mailto:pzarbin@ufpr.br)

Copy of NMR, IR and mass spectra of selected stereoisomers.

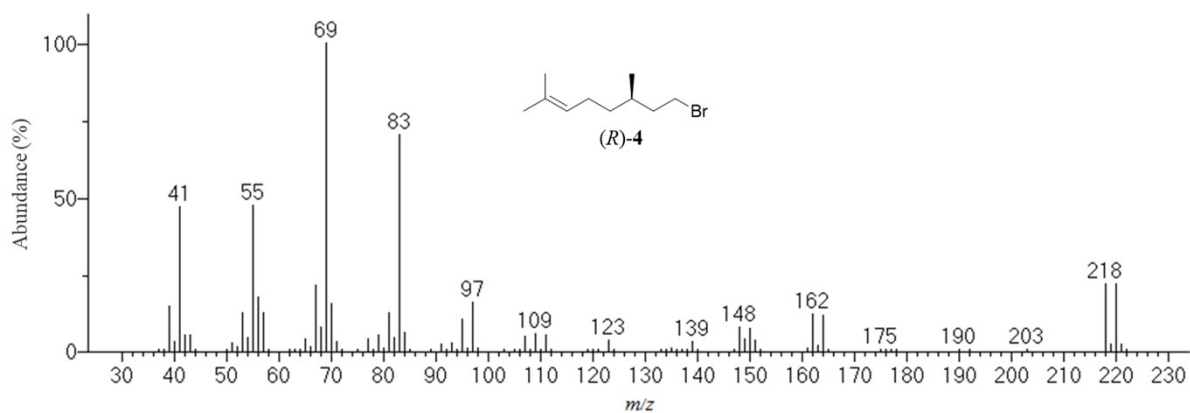
^1H NMR (300 MHz, CDCl_3) of compound (*R*)-4



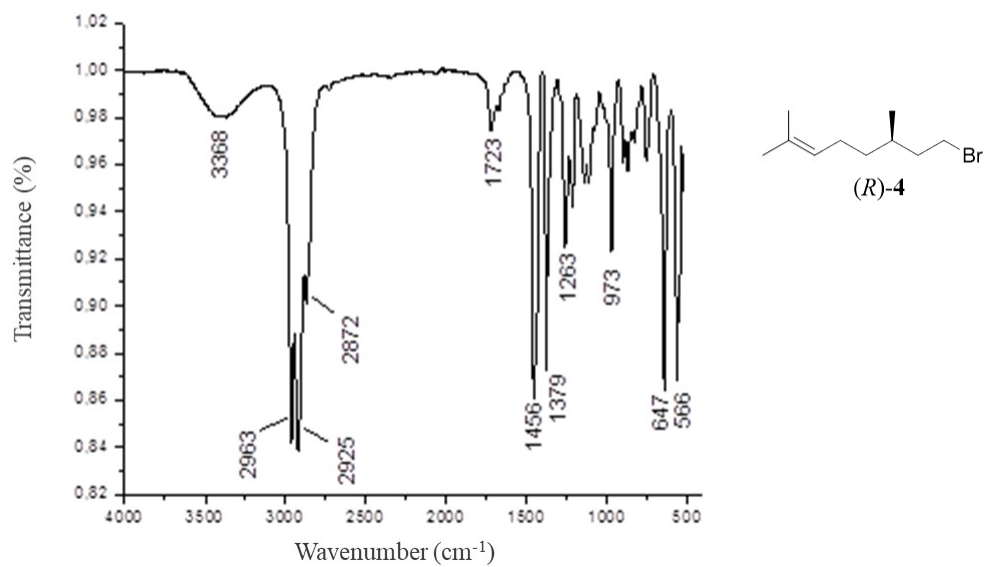
^{13}C NMR (75 MHz, CDCl_3) and DEPT 135 (superior) of compound (*R*)-4



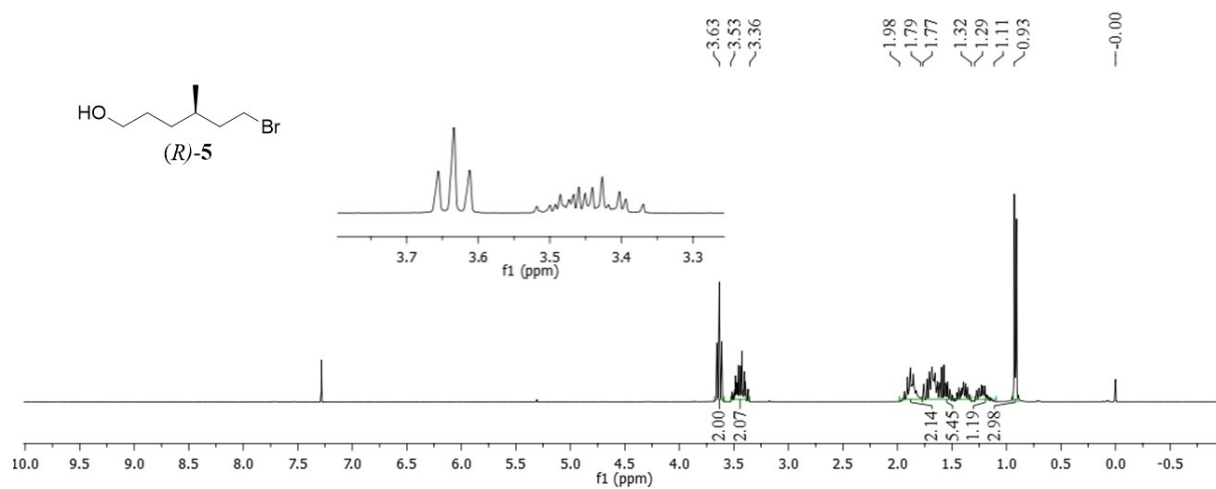
Mass spectrum (EI, 70 eV) of compound (R)-4



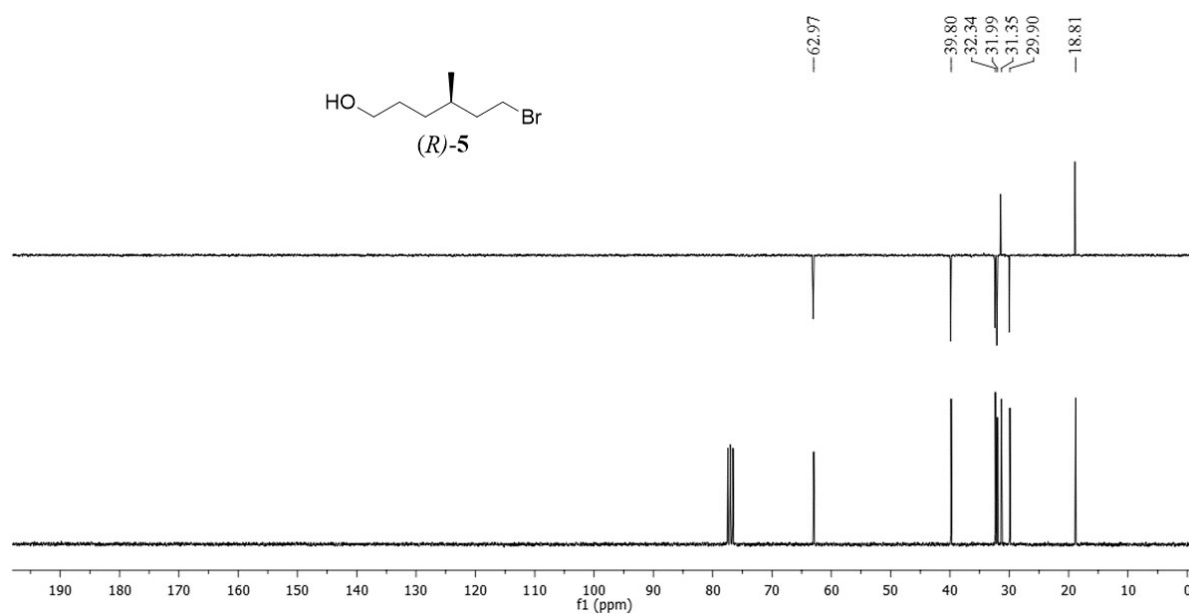
Infrared spectrum of compound (R)-4



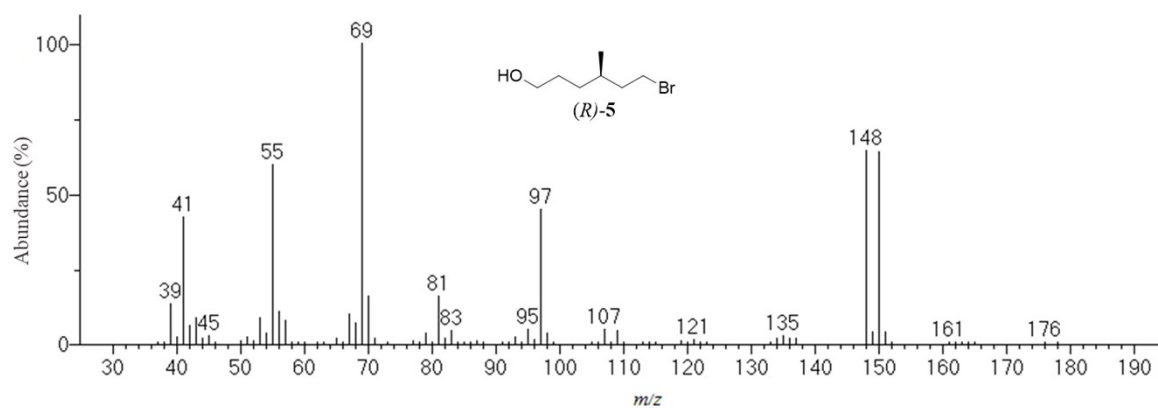
^1H NMR (300 MHz, CDCl_3) of compound (*R*)-**5**



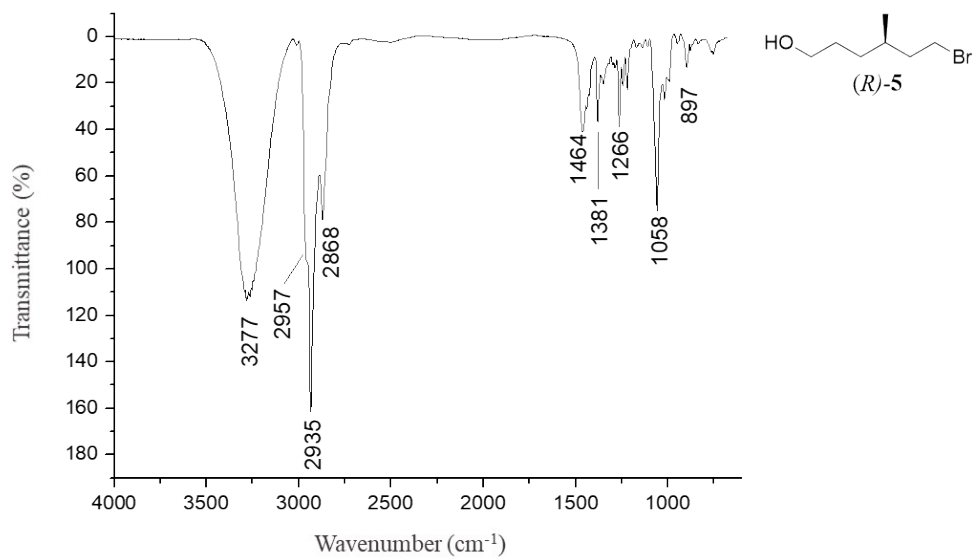
^{13}C NMR (75 MHz, CDCl_3) and DEPT 135 (superior) of compound (*R*)-**5**



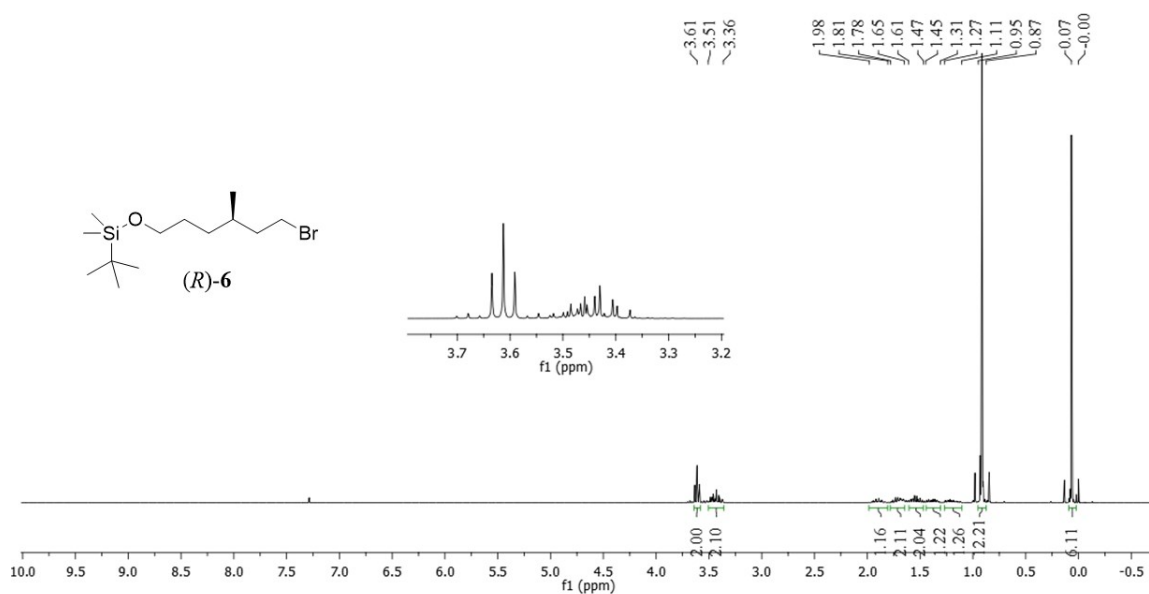
Mass spectrum (EI, 70 eV) of compound (*R*)-**5**



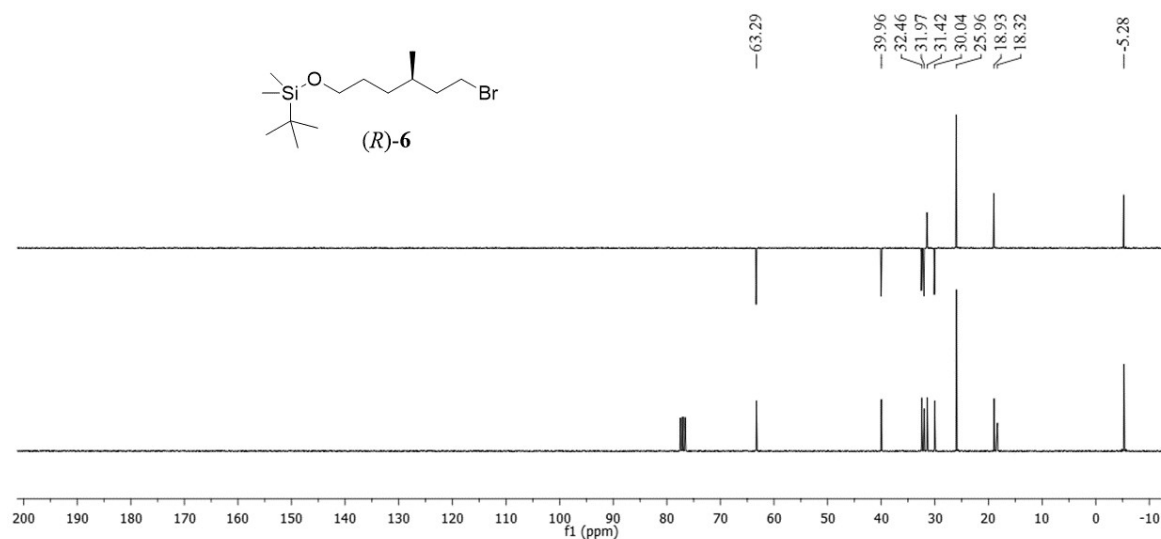
Infrared spectrum of compound (*R*)-**5**



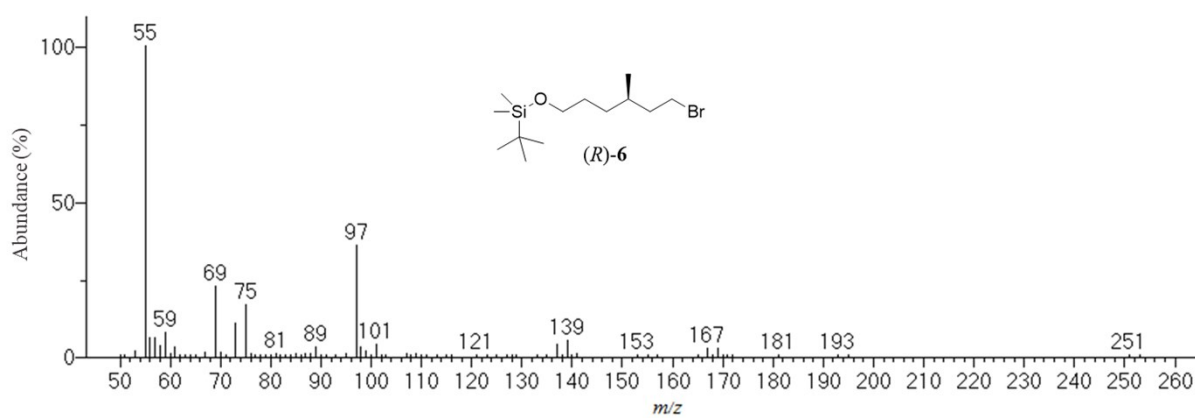
^1H NMR (300 MHz, CDCl_3) of compound (*R*)-**6**



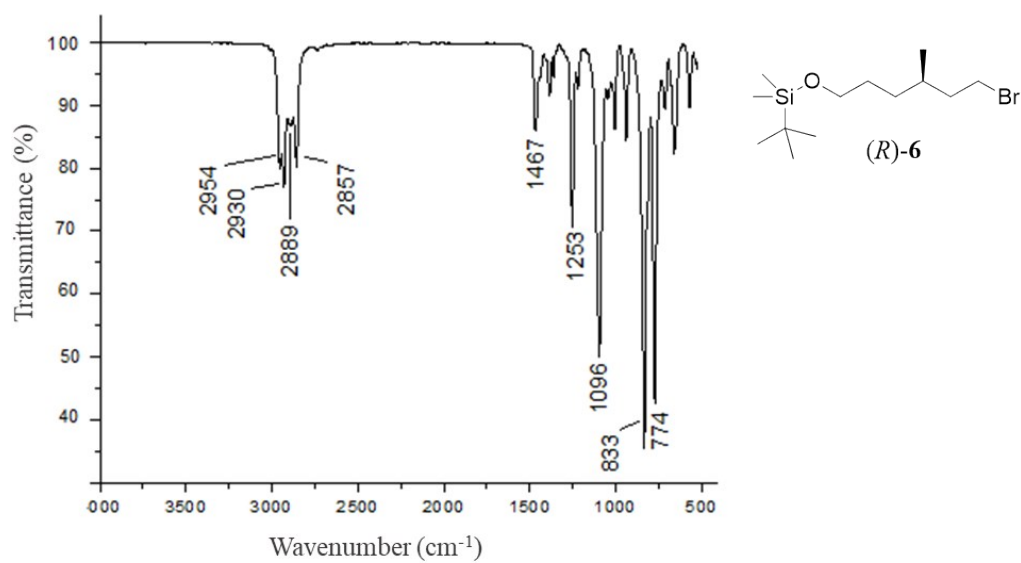
^{13}C NMR (75 MHz, CDCl_3) e DEPT 135 (superior) of compound (*R*)-**6**



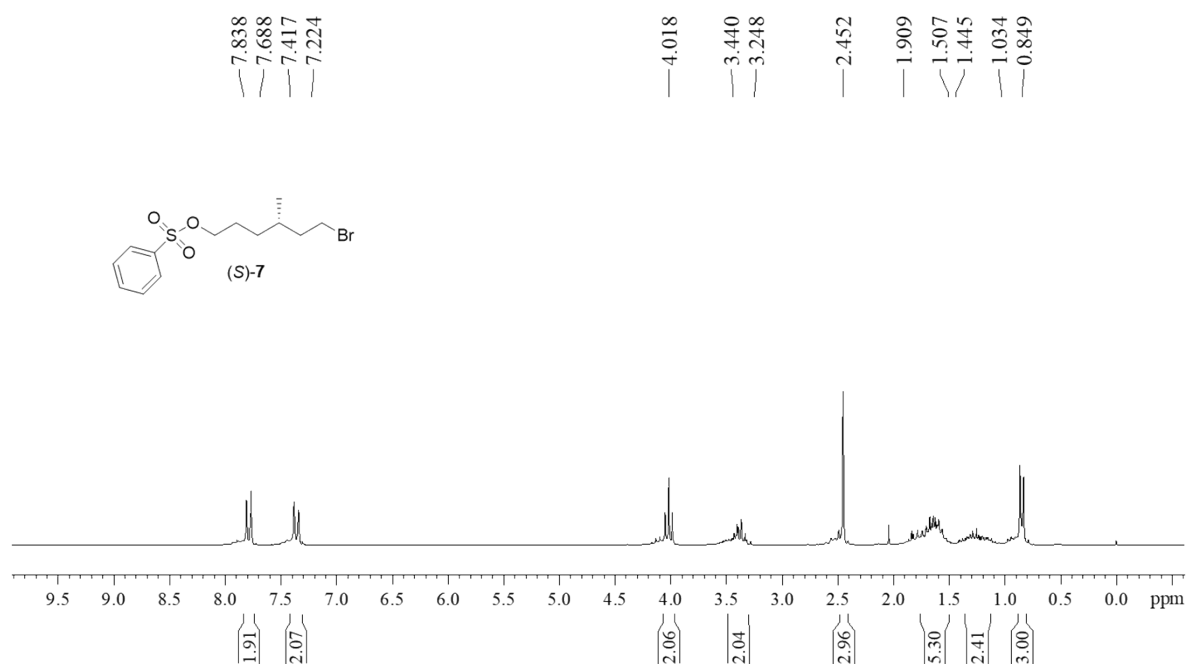
Mass spectrum (EI, 70 eV) of compound (*R*)-6



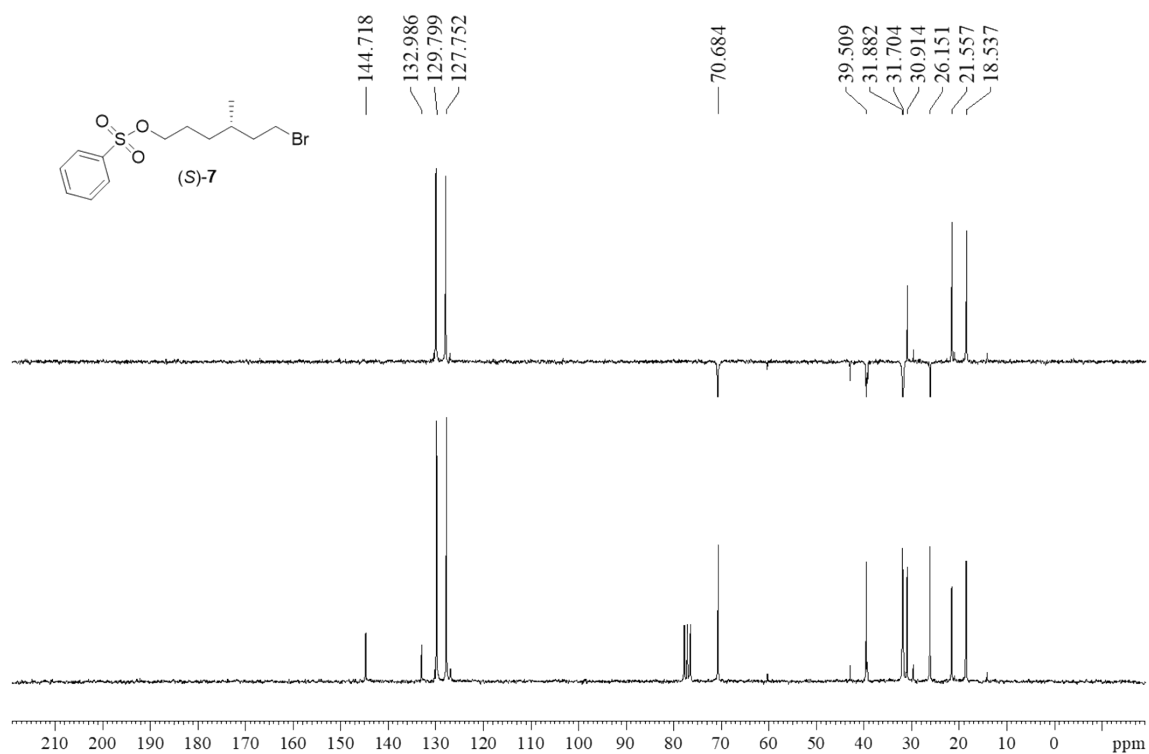
Infrared spectrum of compound (*R*)-6



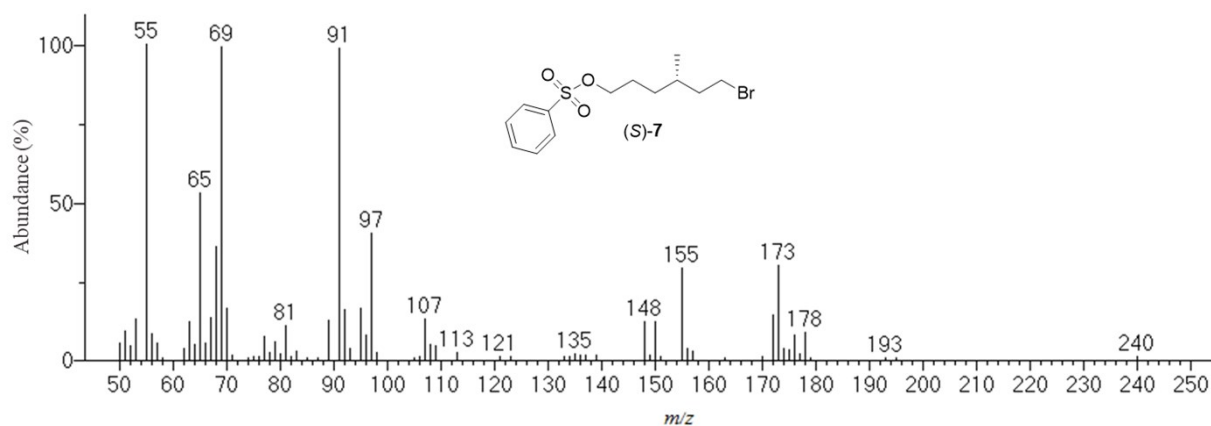
^1H NMR (200 MHz, CDCl_3) of compound (*S*)-7



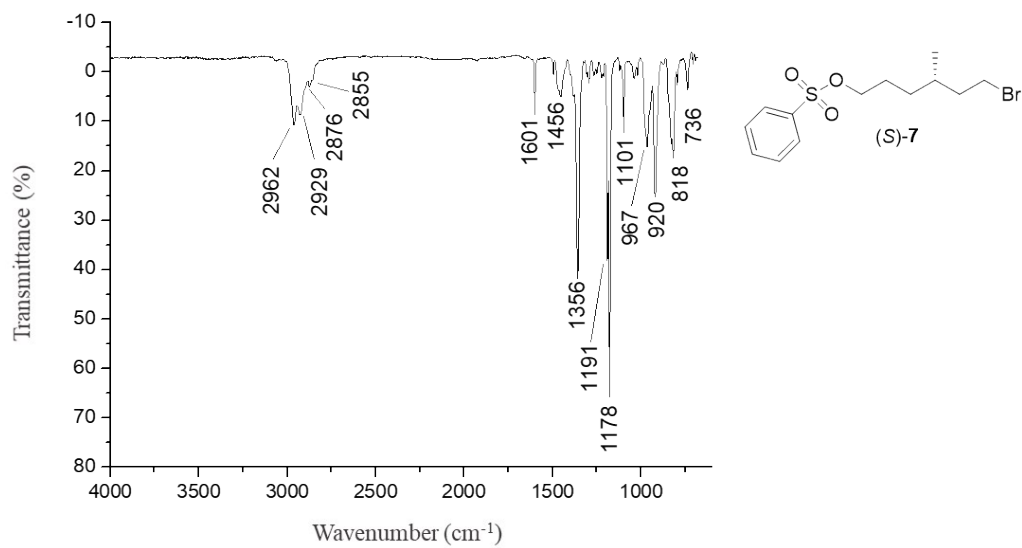
^{13}C NMR (50 MHz, CDCl_3) of compound (*S*)-7



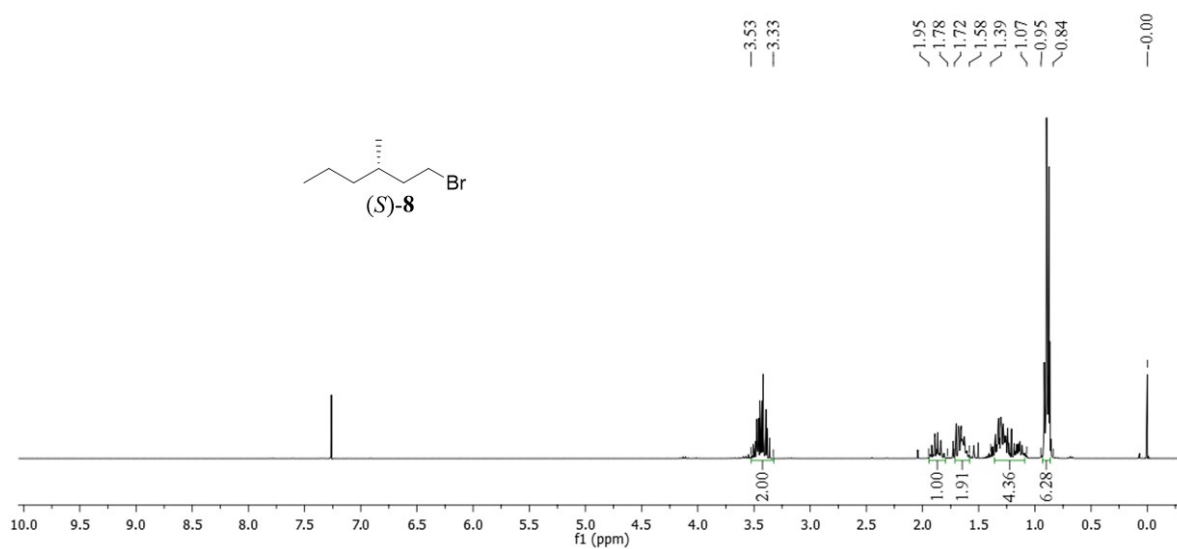
Mass spectrum (EI, 70 eV) of compound (S)-7



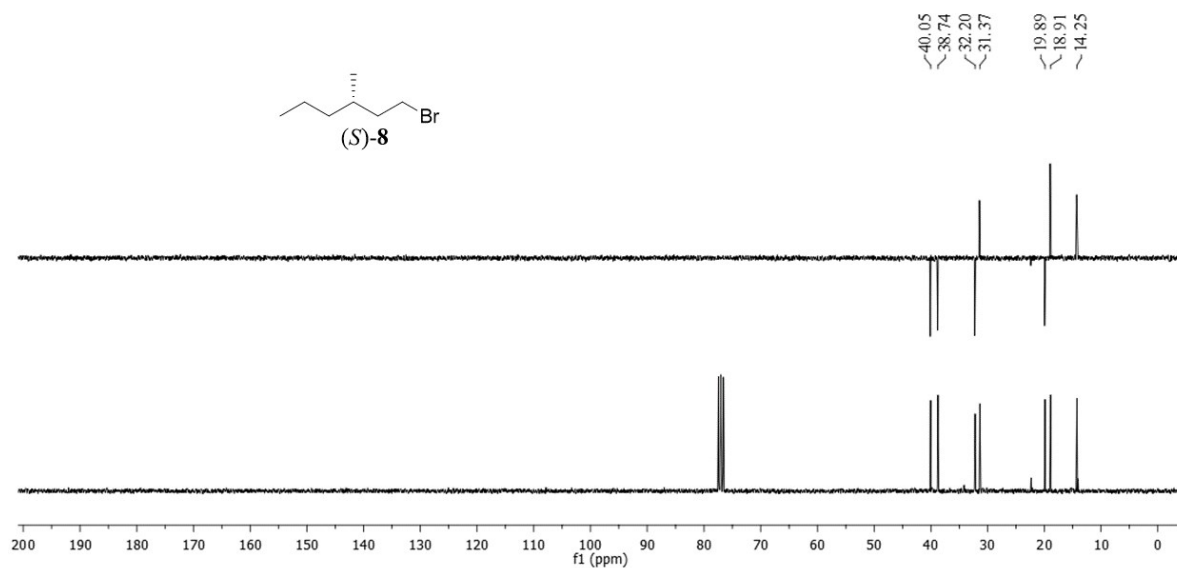
Infrared spectrum of compound (S)-7



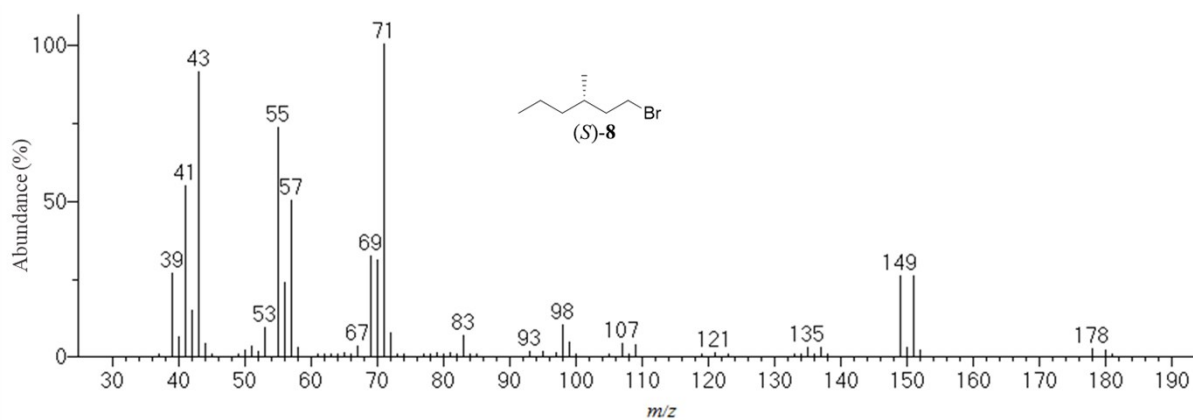
^1H NMR (300 MHz, CDCl_3) of compound (*S*)-**8**



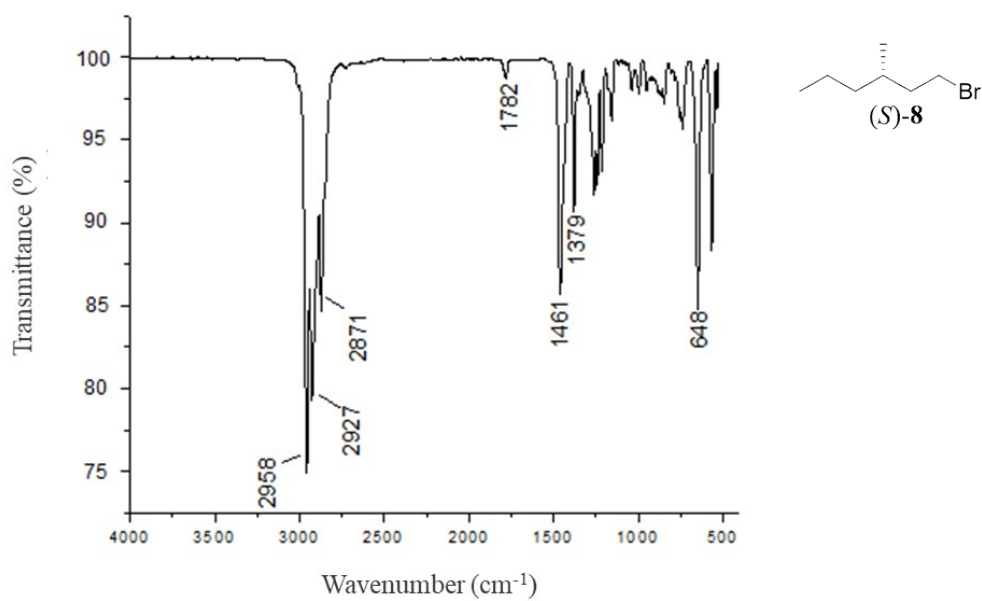
^{13}C NMR (75 MHz, CDCl_3) and DEPT 135 (superior) of compound (*S*)-**8**



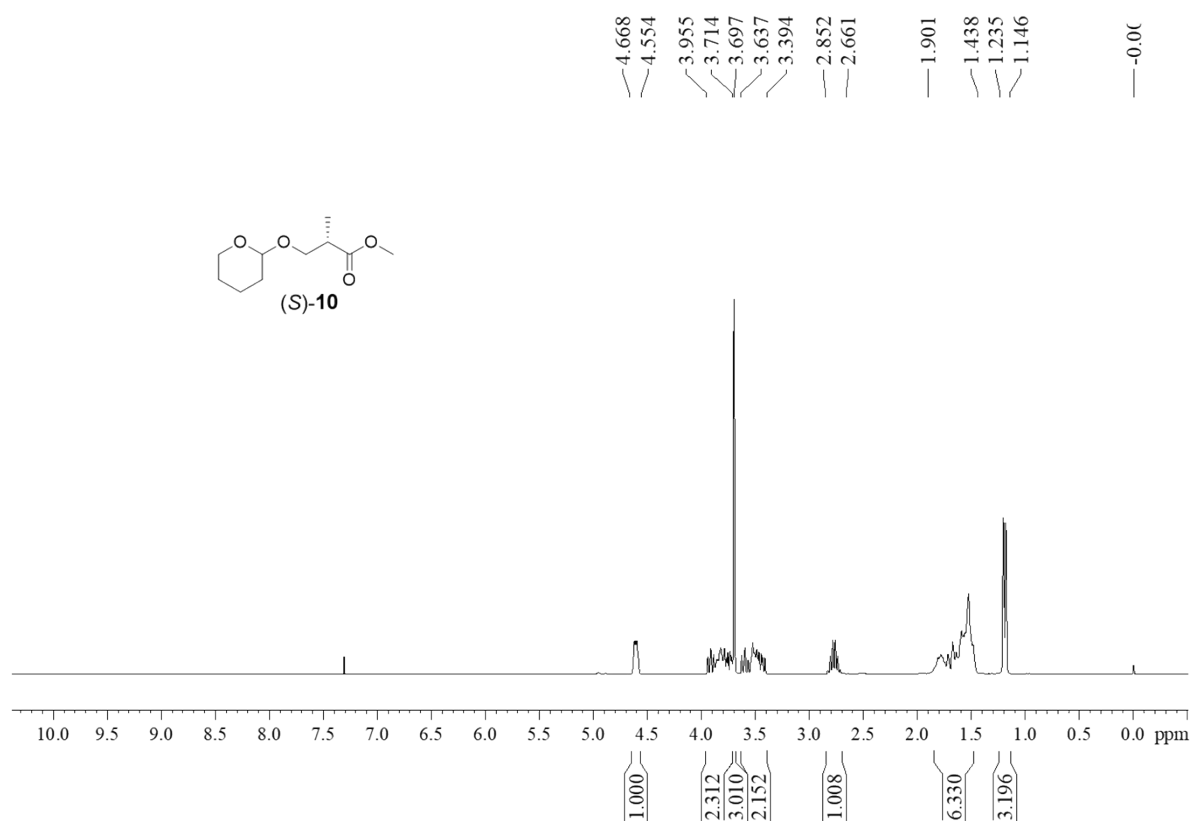
Mass spectrum (EI, 70 eV) of compound (*S*)-**8**



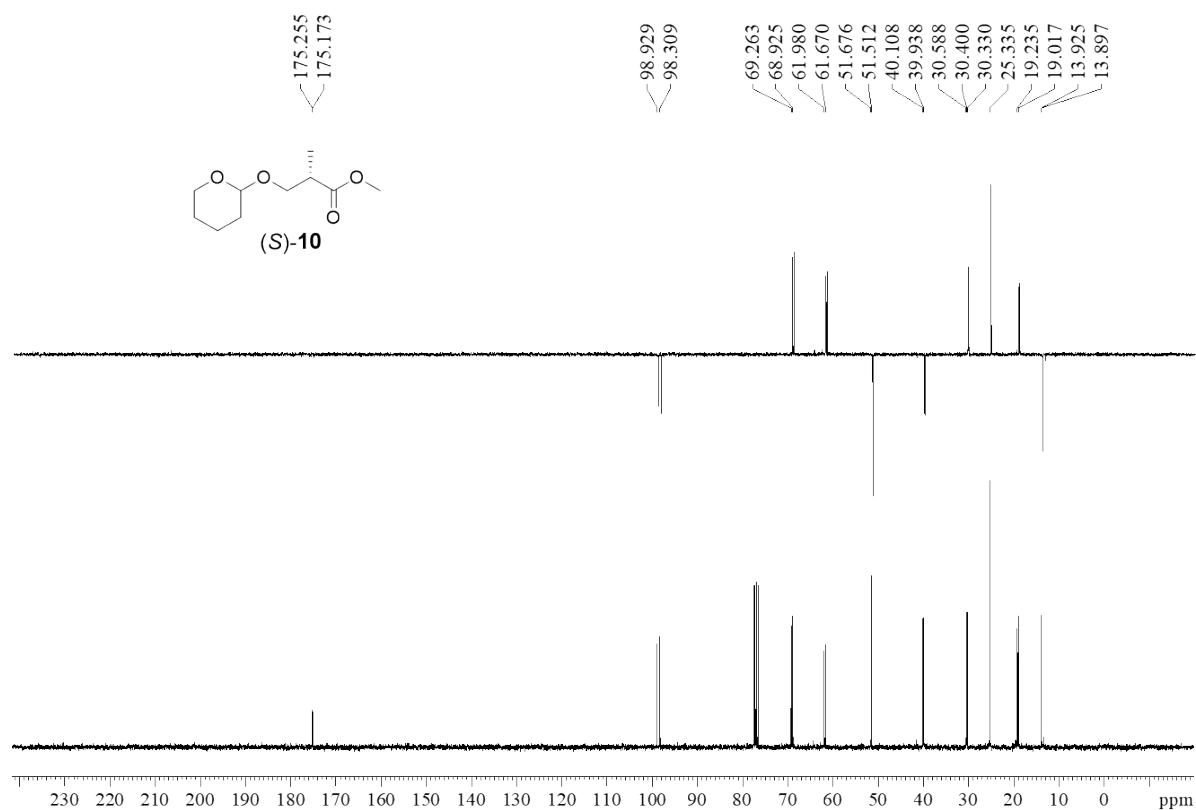
Infrared spectrum of compound (*S*)-**8**



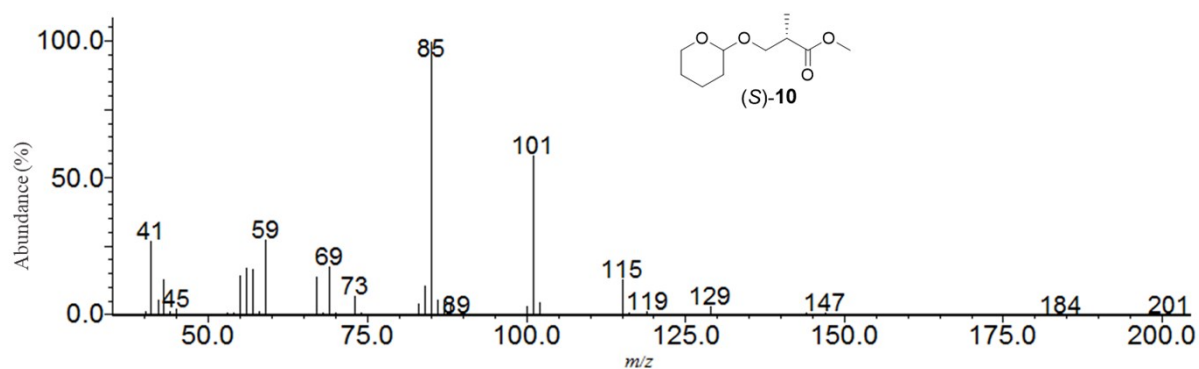
^1H NMR (300 MHz, CDCl_3) of compound (*S*)-**10**



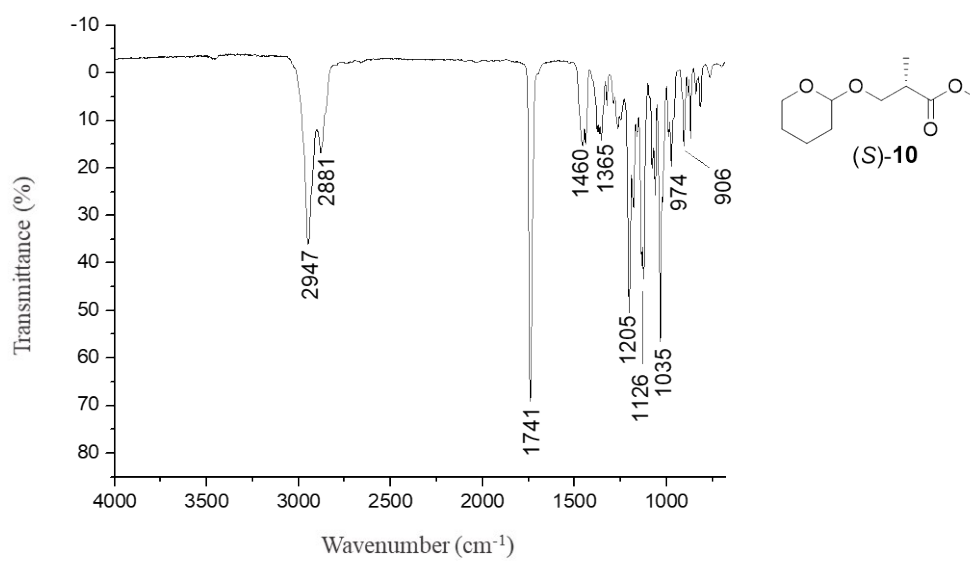
^{13}C NMR (75 MHz, CDCl_3) of compound (*S*)-**10**



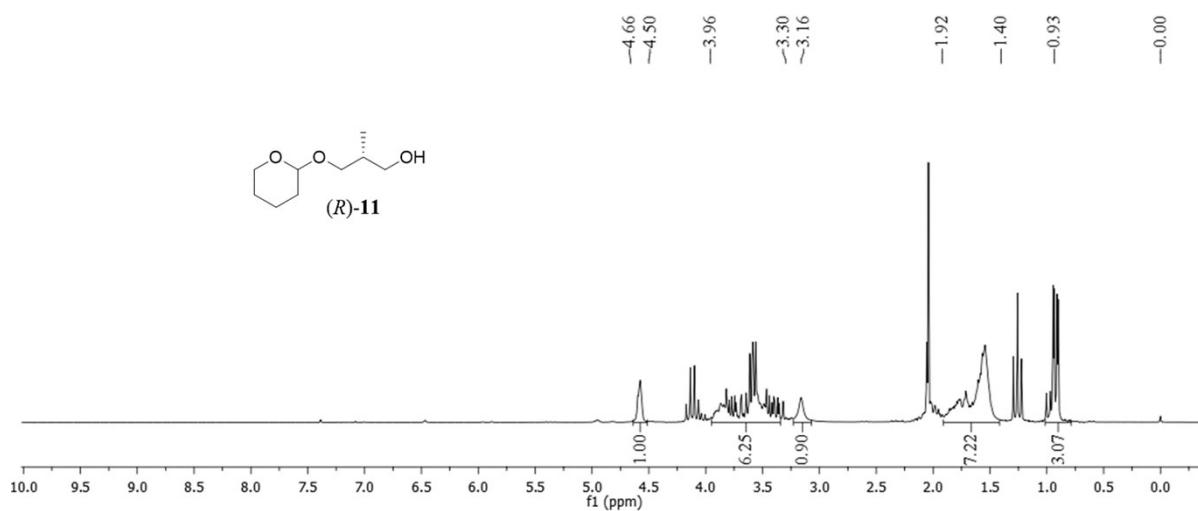
Mass spectrum (EI, 70 eV) of compound (S)-10



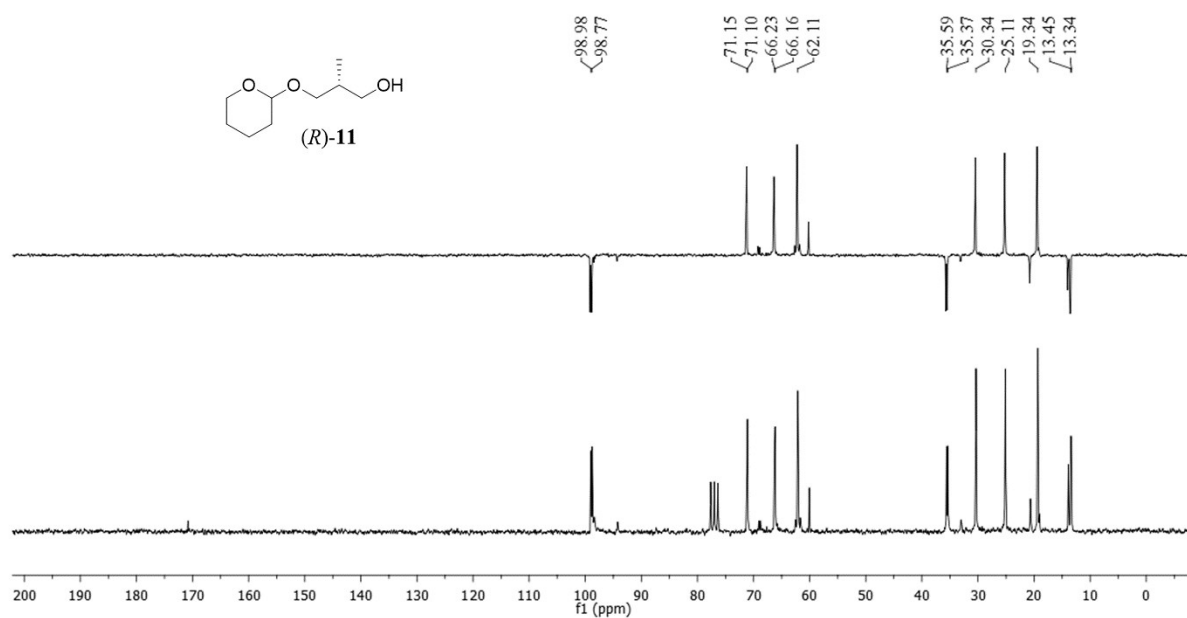
Infrared spectrum of compound (S)-10



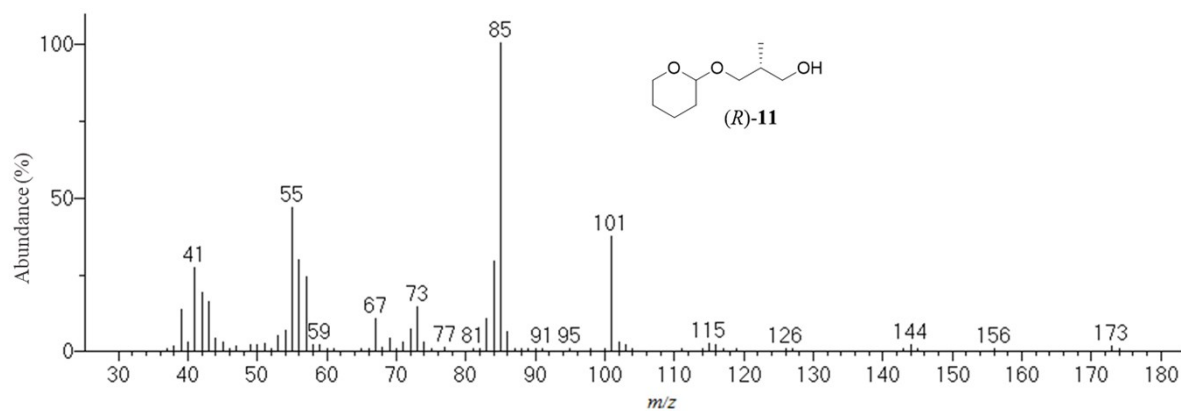
^1H NMR (300 MHz, CDCl_3) of compound (*R*)-**11**



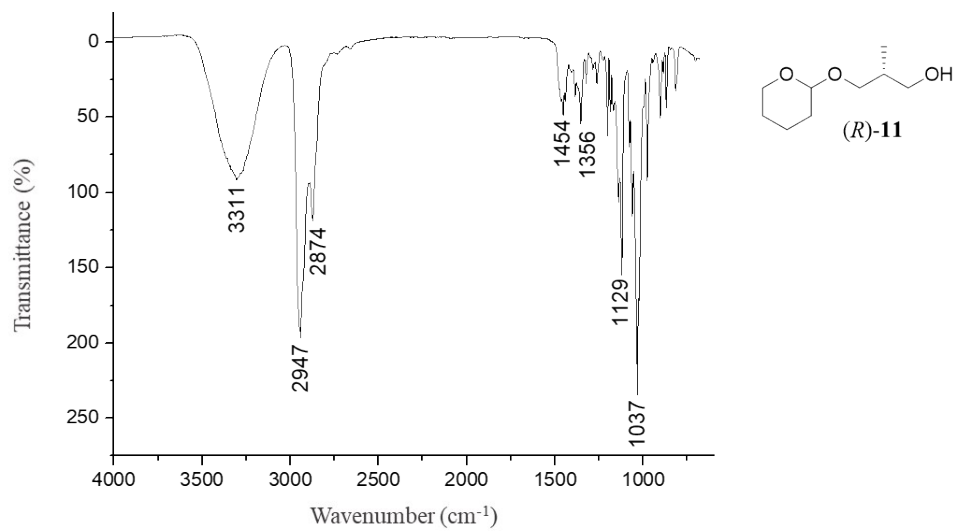
^{13}C NMR (75 MHz, CDCl_3) and DEPT 135 (superior) of compound (*R*)-**11**



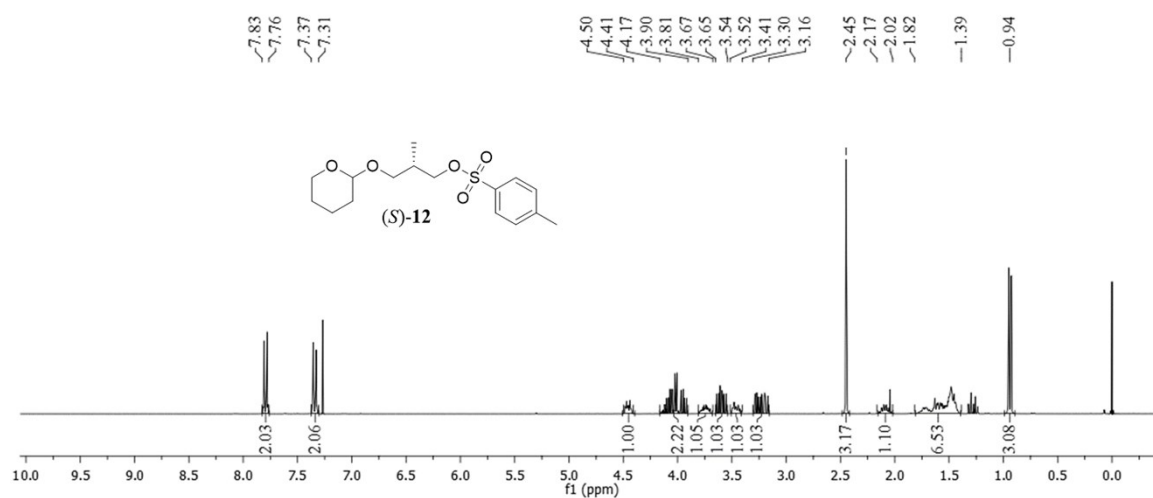
Mass spectrum (EI, 70 eV) of compound (*R*)-**11**



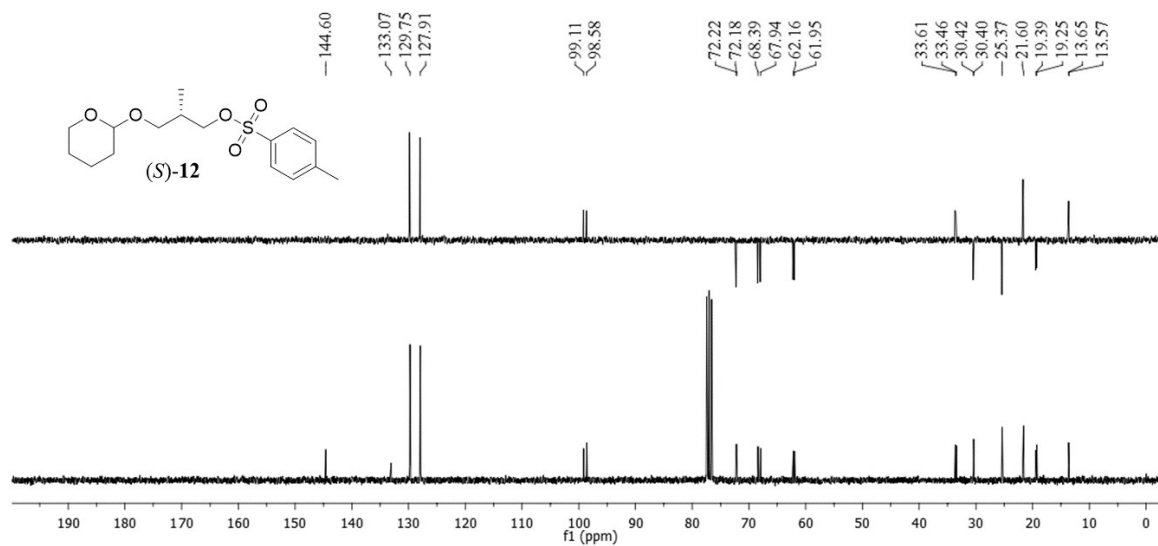
Infrared spectrum of compound (*R*)-**11**



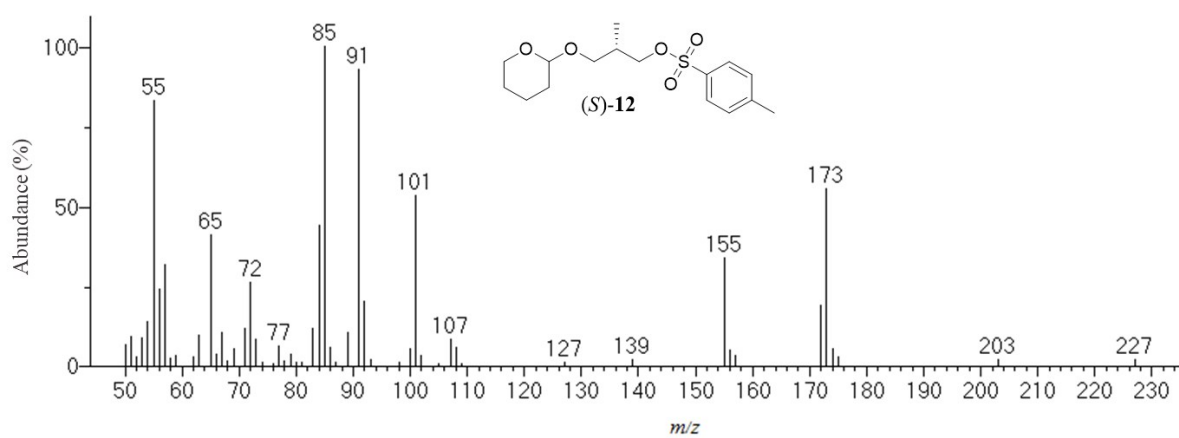
^1H NMR (300 MHz, CDCl_3) of compound (*S*)-**12**



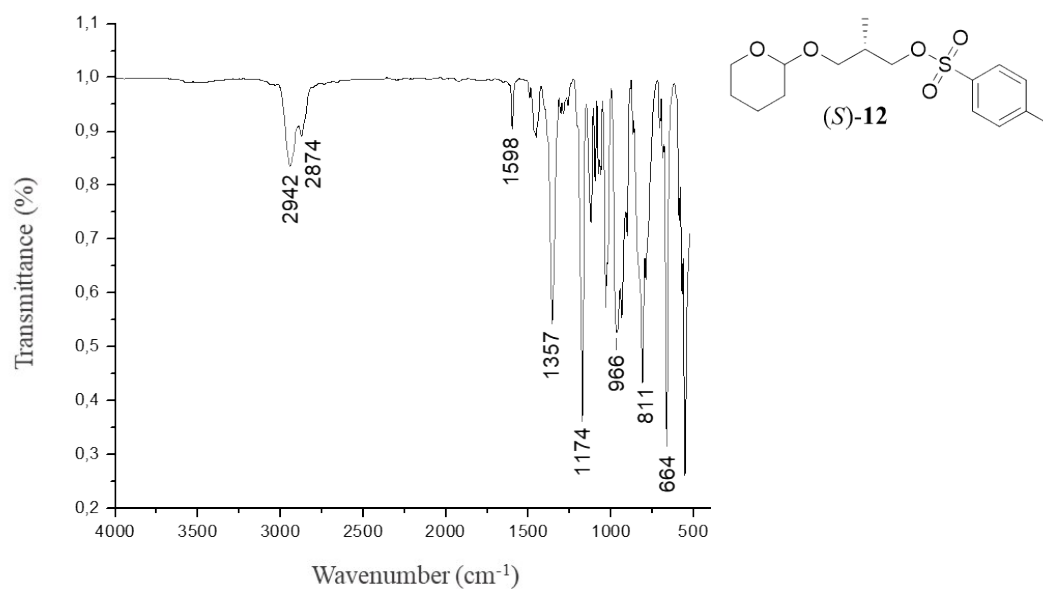
^{13}C NMR (75 MHz, CDCl_3) and DEPT 135 (superior) of compound (*S*)-**12**



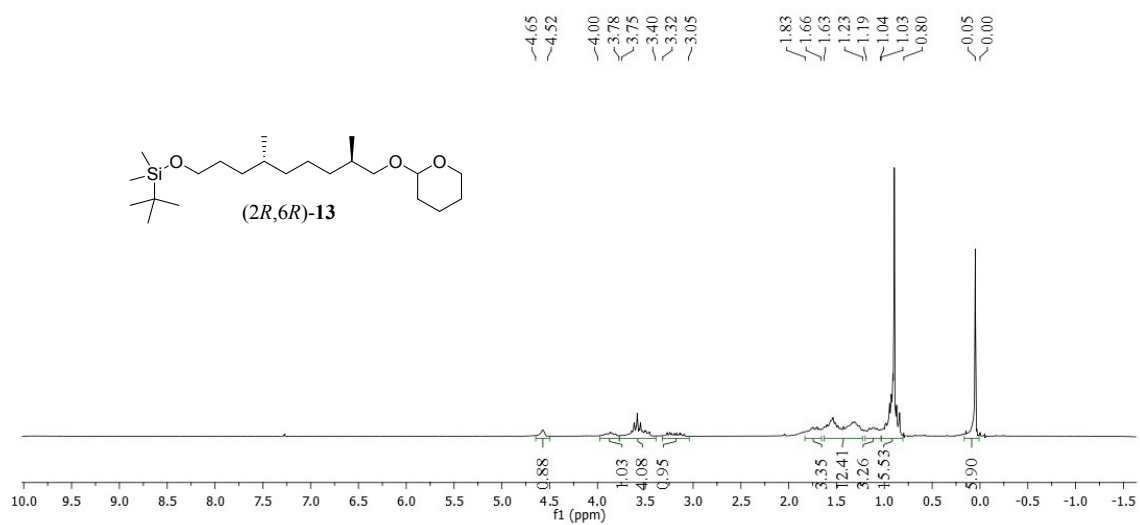
Mass spectrum (EI, 70 eV) of compound (S)-12



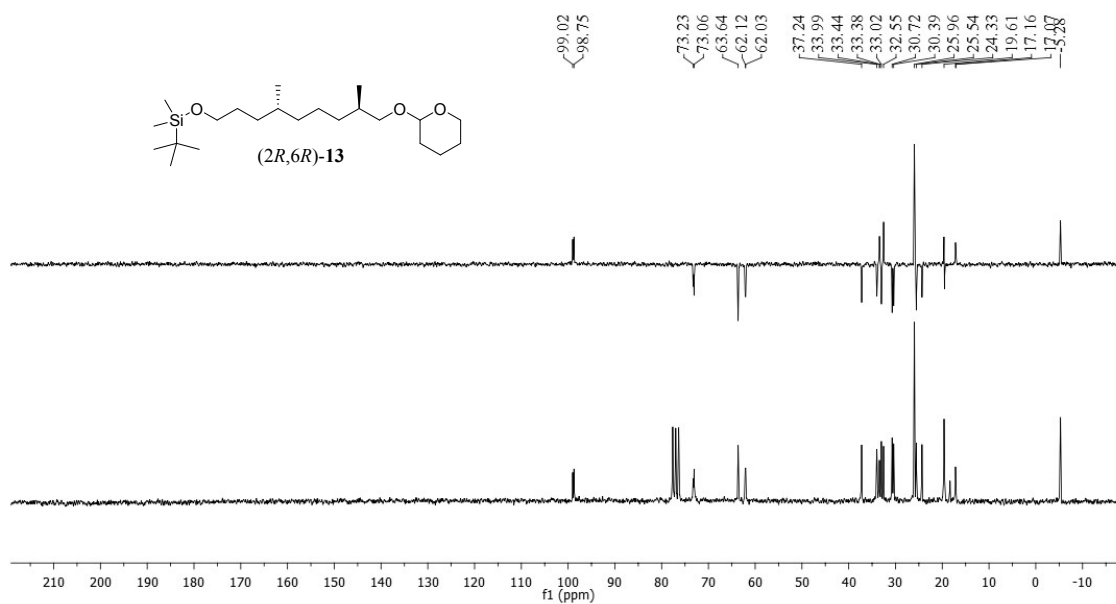
Infrared spectrum of compound (S)-12



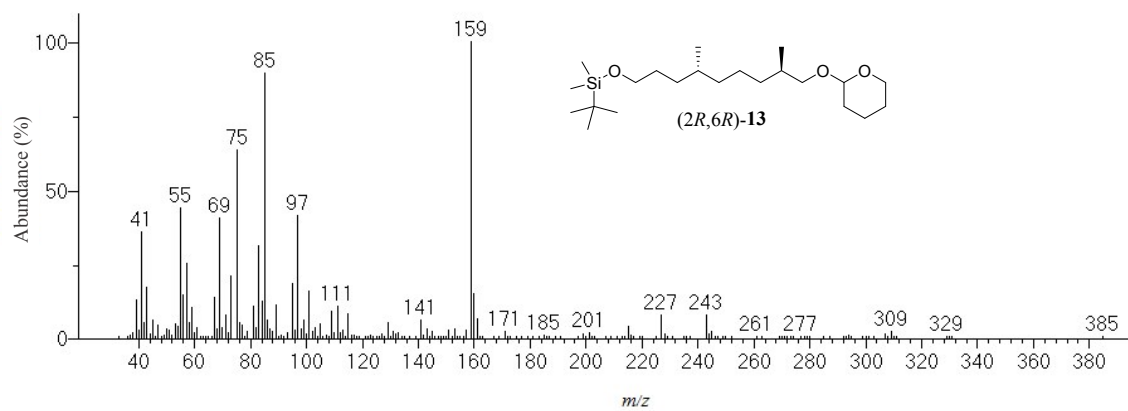
^1H NMR (200 MHz, CDCl_3) of compound (2*R*,6*R*)-**13**



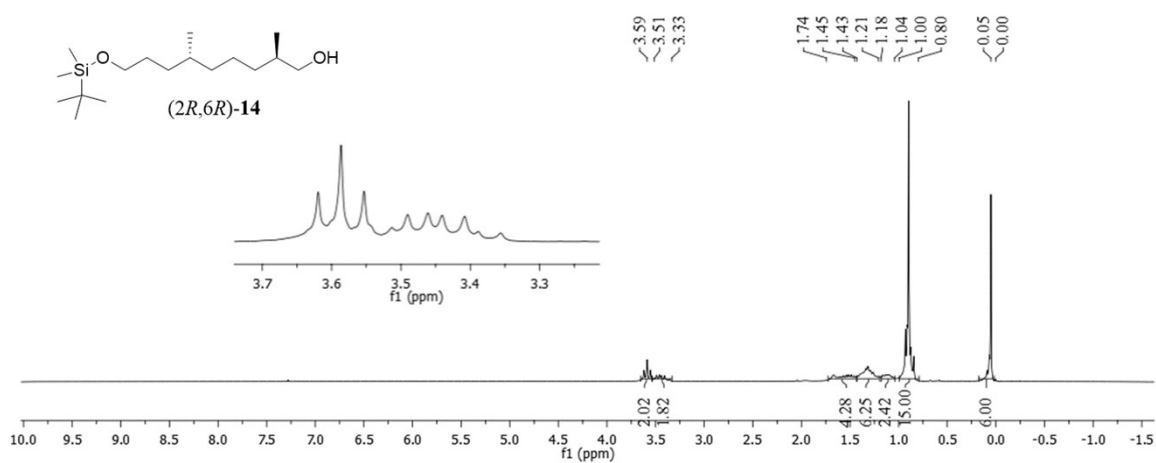
^{13}C NMR (50 MHz) and DEPT 135 (superior) of compound (2*R*,6*R*)-**13**



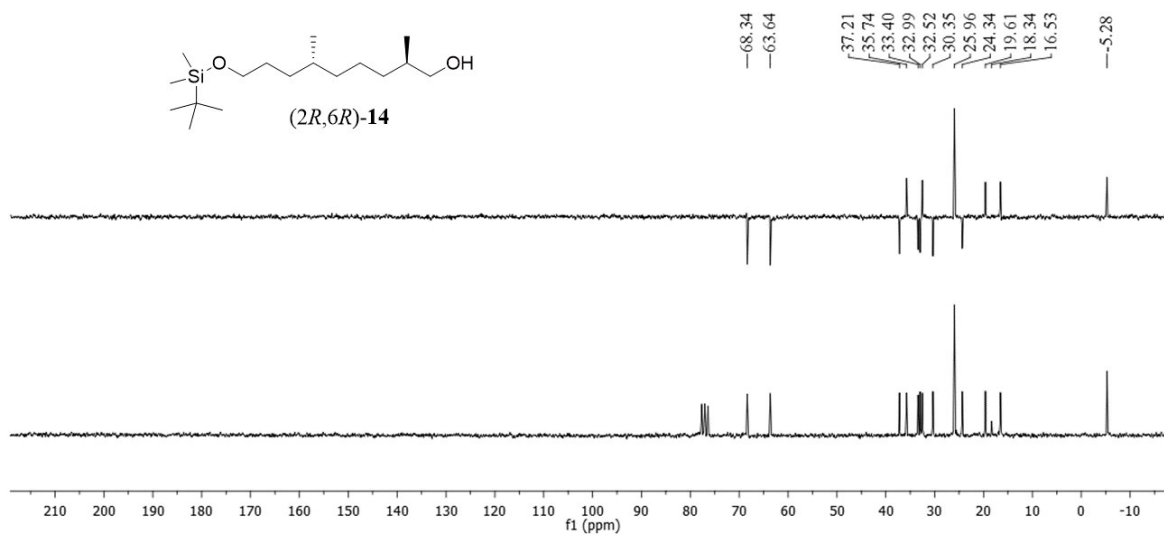
Mass spectrum (EI, 70 eV) of compound (2*R*,6*R*)-**13**



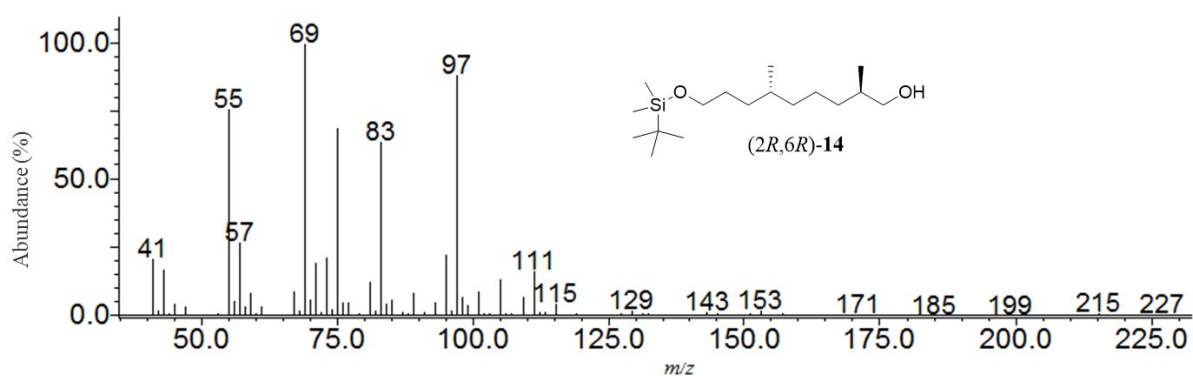
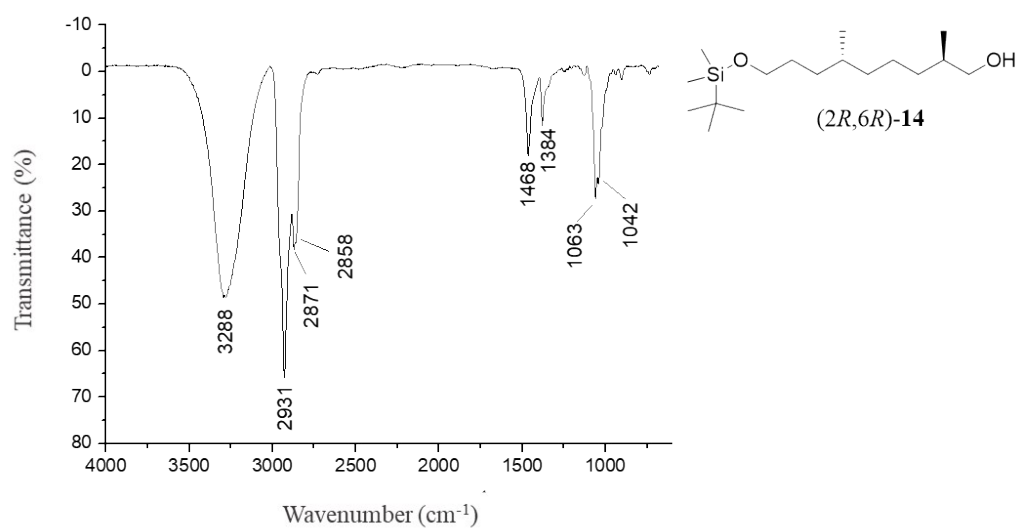
^1H NMR (200 MHz, CDCl_3) of compound (2*R*,6*R*)-**14**



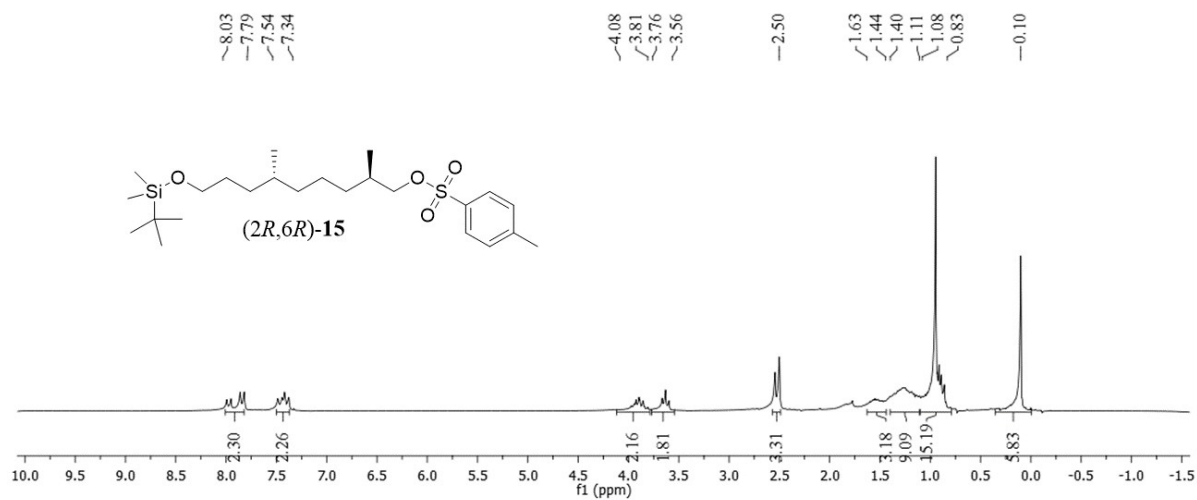
^{13}C NMR (50 MHz, CDCl_3) and DEPT 135 (superior) of compound (2*R*,6*R*)-**14**



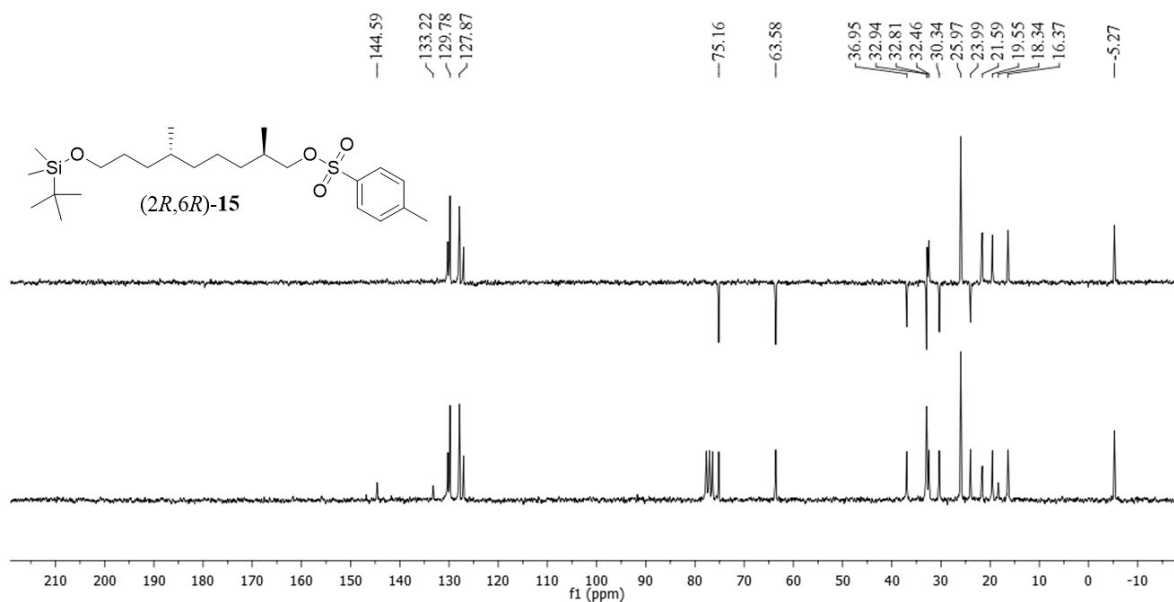
Mass spectrum (EI, 70 eV) of compound (2*R*,6*R*)-**14**

Infrared spectrum of compound (2*R*,6*R*)-**14**

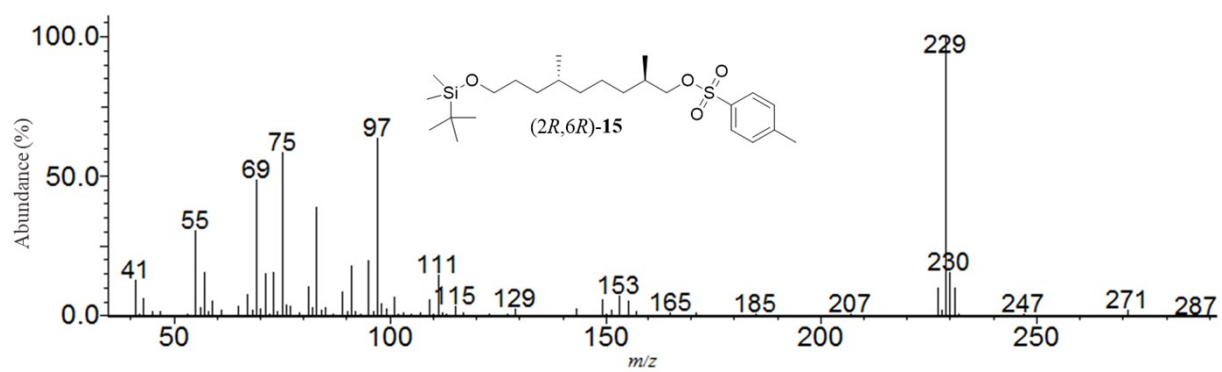
^1H NMR (200 MHz, CDCl_3) of compound (2*R*,6*R*)-**15**



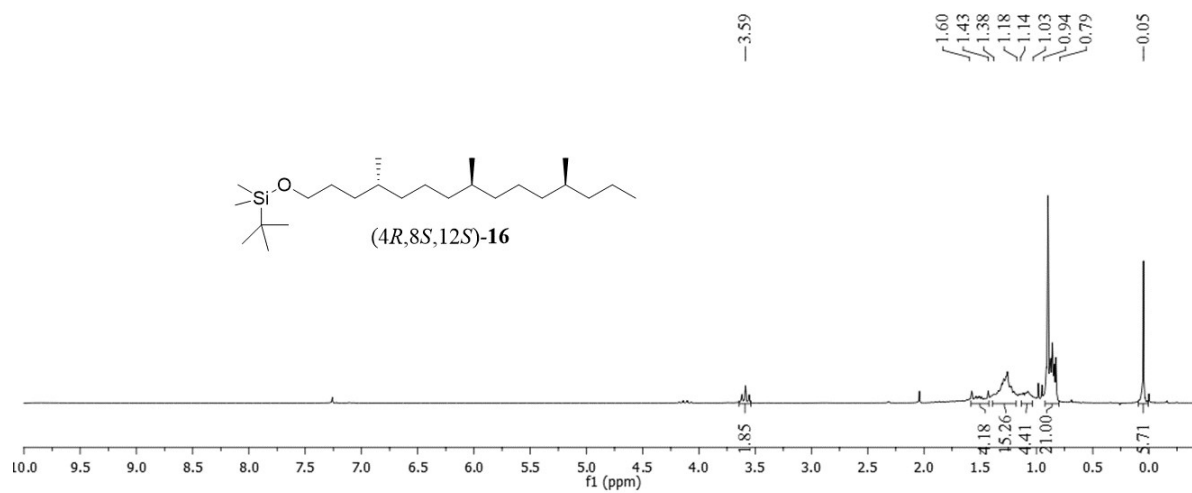
^{13}C NMR (50 MHz, CDCl_3) and DEPT 135 (superior) of compound (2*R*,6*R*)-**15**



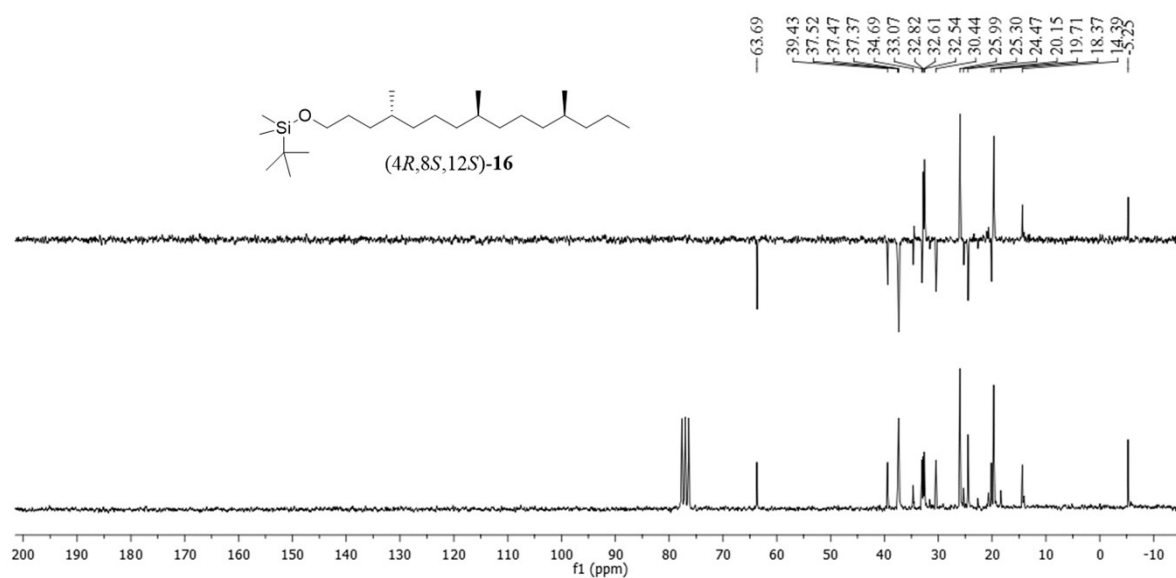
Mass spectrum (EI, 70 eV) of compound (2*R*,6*R*)-15



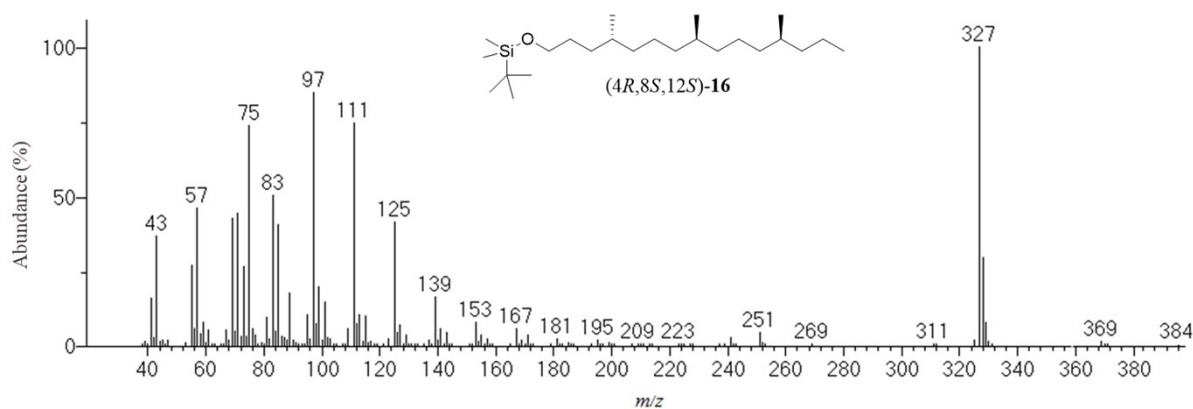
^1H NMR (200 MHz, CDCl_3) of compound (4*R*,8*S*,12*S*)-**16**



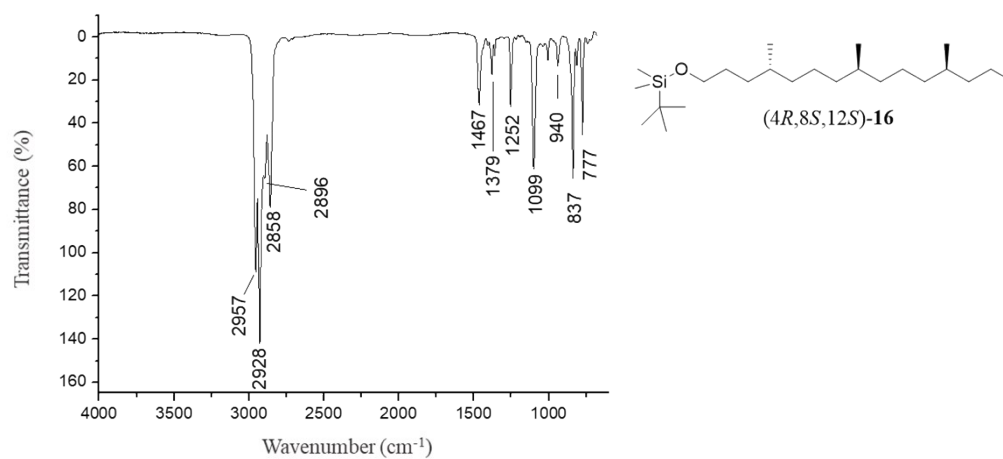
^{13}C NMR (50 MHz, CDCl_3) and DEPT 135 (superior) of compound (4*R*,8*S*,12*S*)-**16**



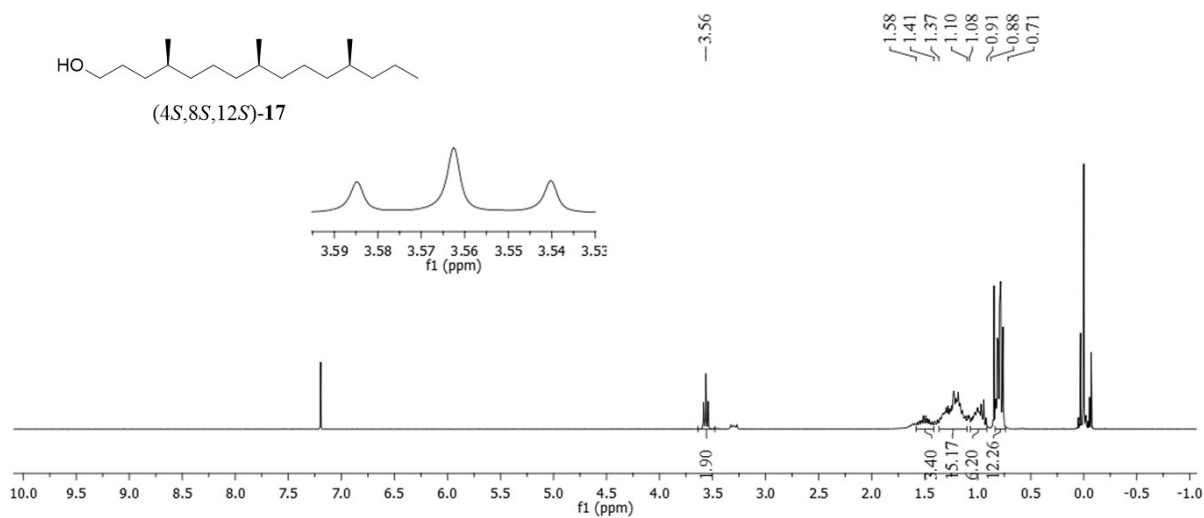
Mass spectrum (EI, 70 eV) of compound (4*R*,8*S*,12*S*)-**16**



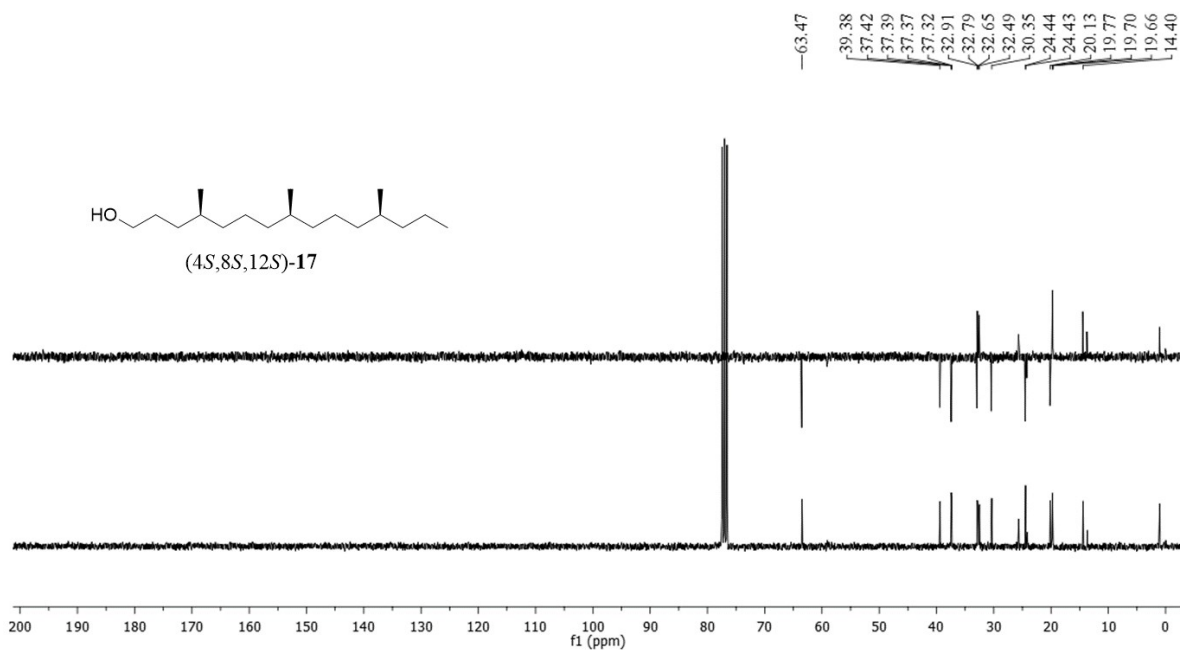
Infrared spectrum of compound (4*R*,8*S*,12*S*)-**16**



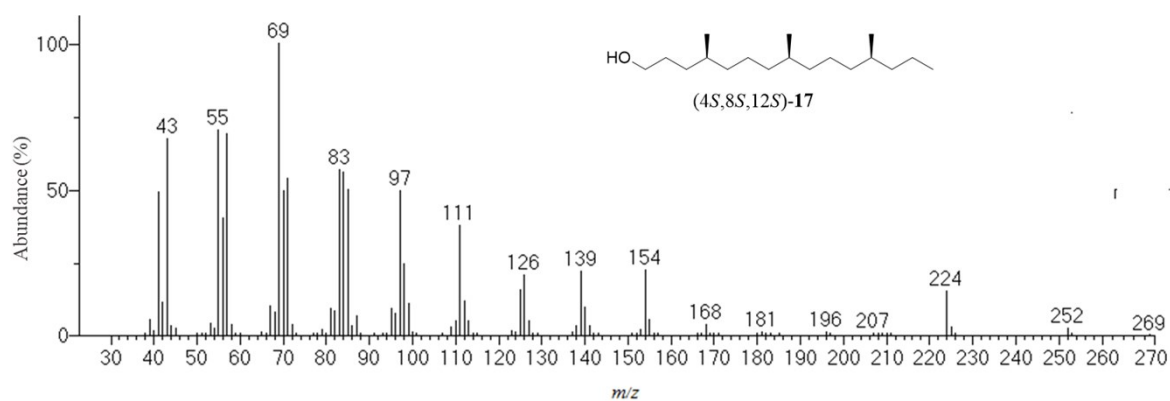
^1H NMR (300 MHz, CDCl_3) of compound (4*S*,8*S*,12*S*)-**17**



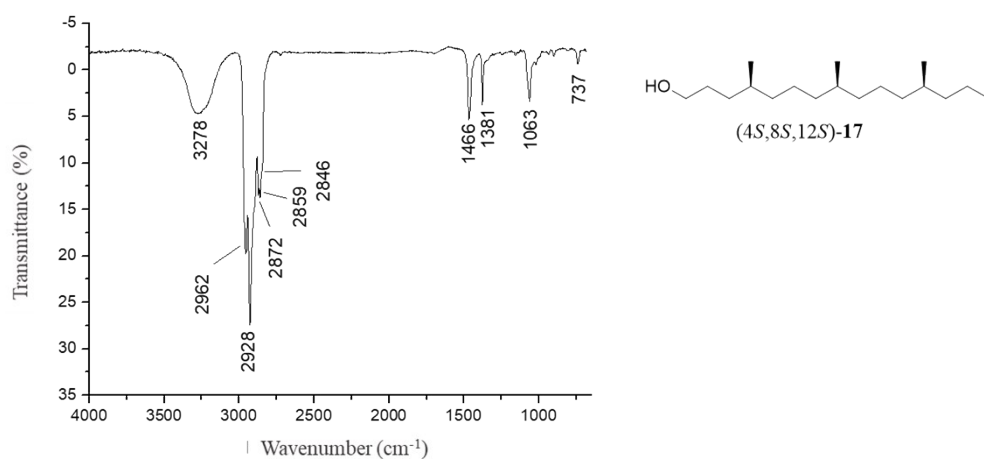
^{13}C NMR (75 MHz, CDCl_3) and DEPT 135 (superior) of compound (4*S*,8*S*,12*S*)-**17**



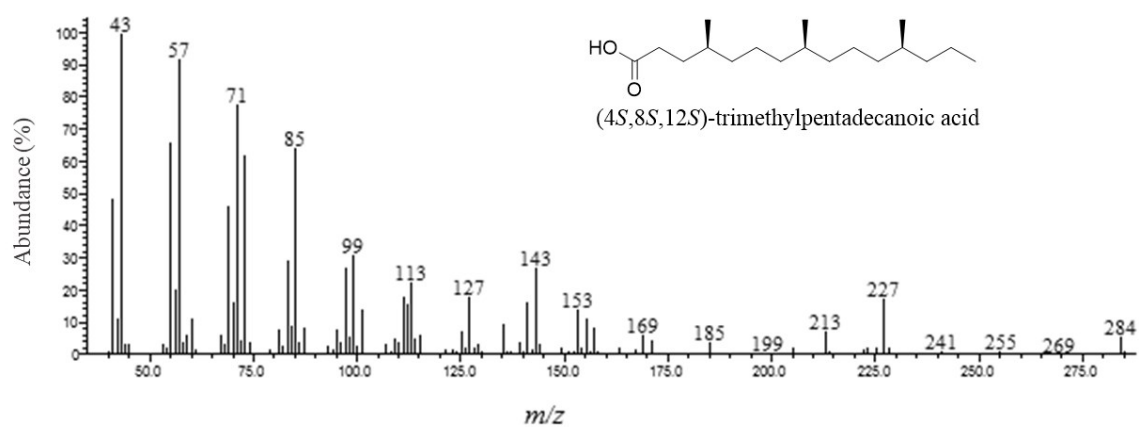
Mass spectrum (EI, 70 eV) of compound (4*S*,8*S*,12*S*)-**17**



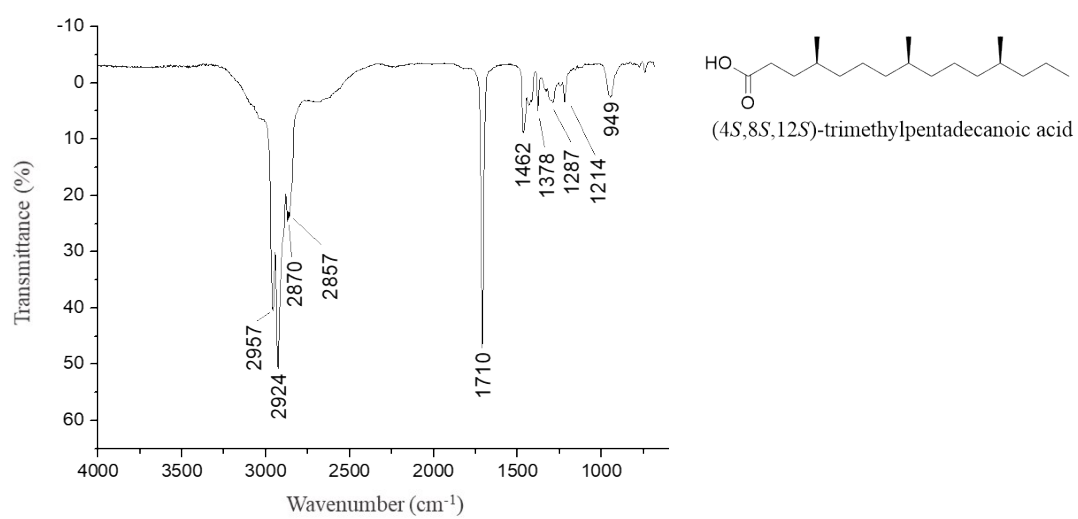
Infrared spectrum of compound (4*S*,8*S*,12*S*)-**17**



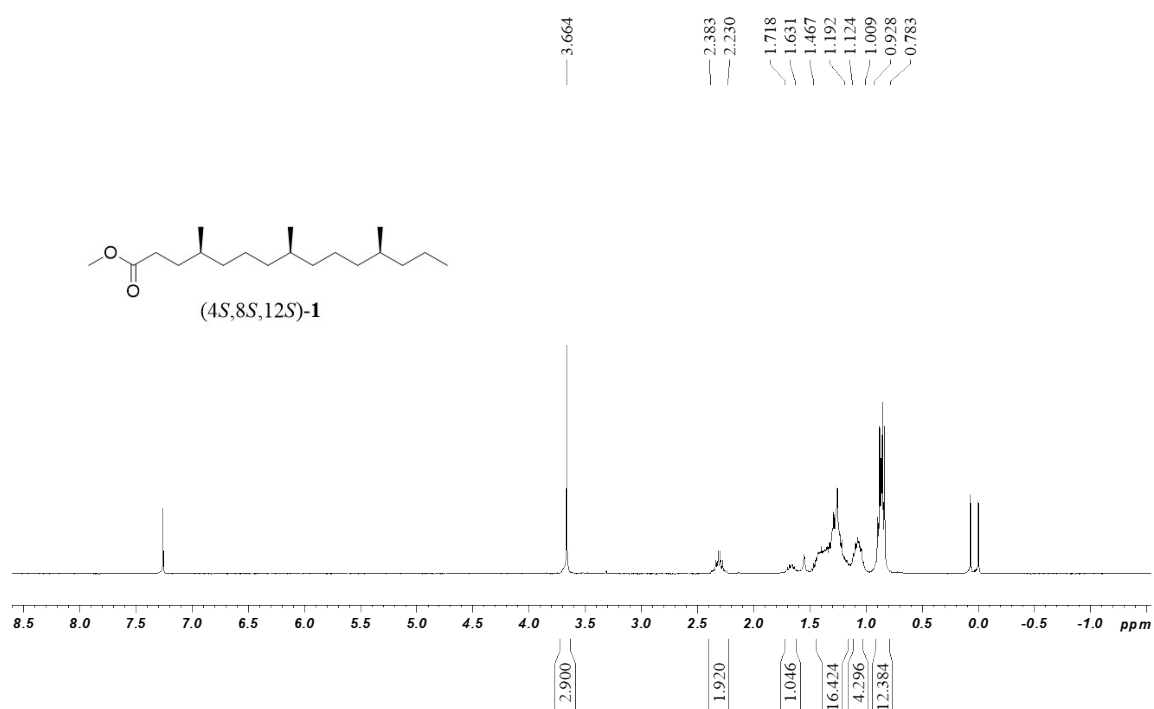
Mass spectrum (EI, 70 eV) of (4*S*,8*S*,12*S*)-trimethylpentadecanoic acid



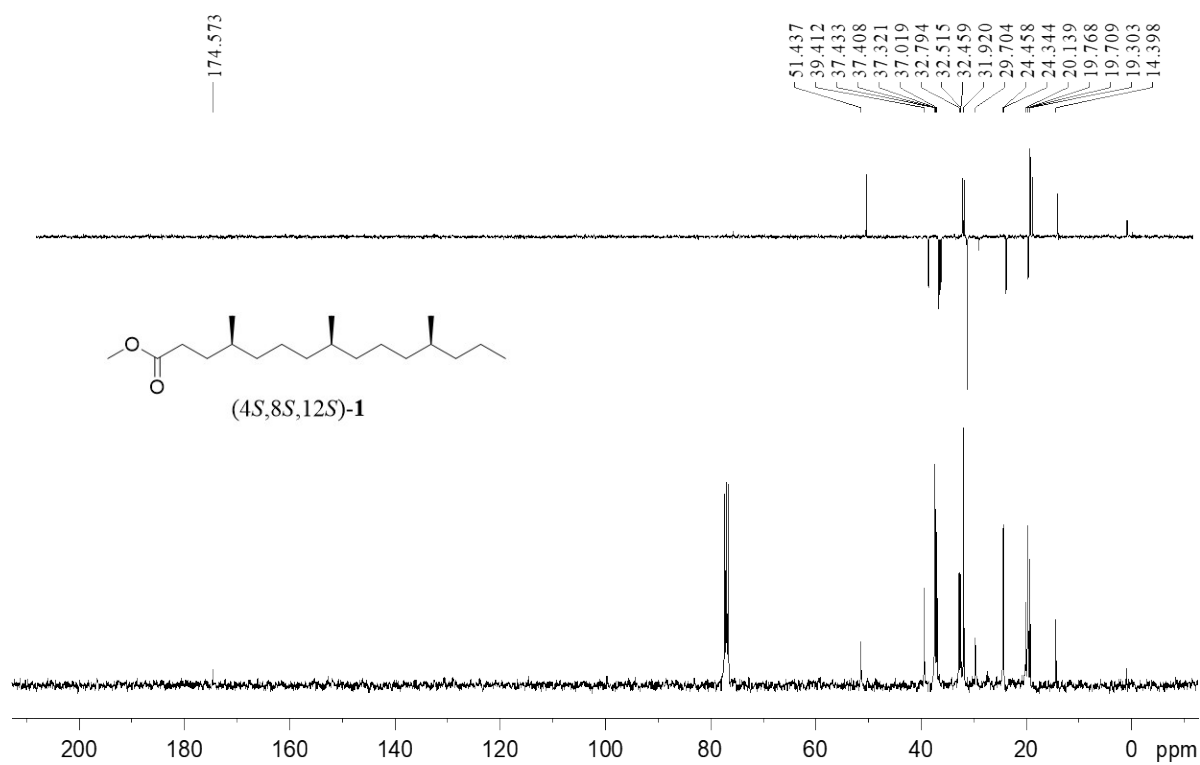
Infrared spectrum of compound (4*S*,8*S*,12*S*)-trimethylpentadecanoic acid



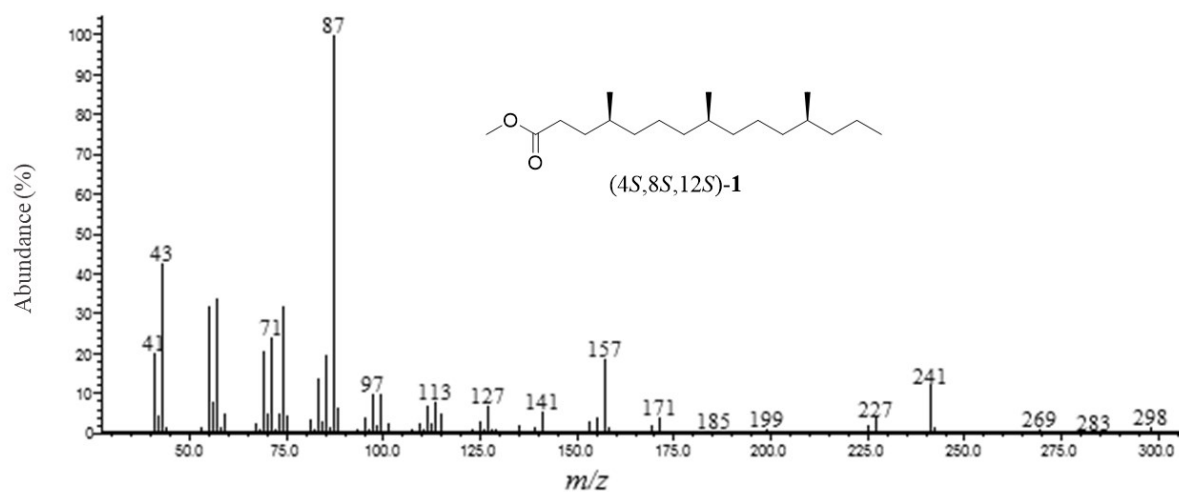
^1H NMR (200 MHz, CDCl_3) of compound (4*S*,8*S*,12*S*)-1



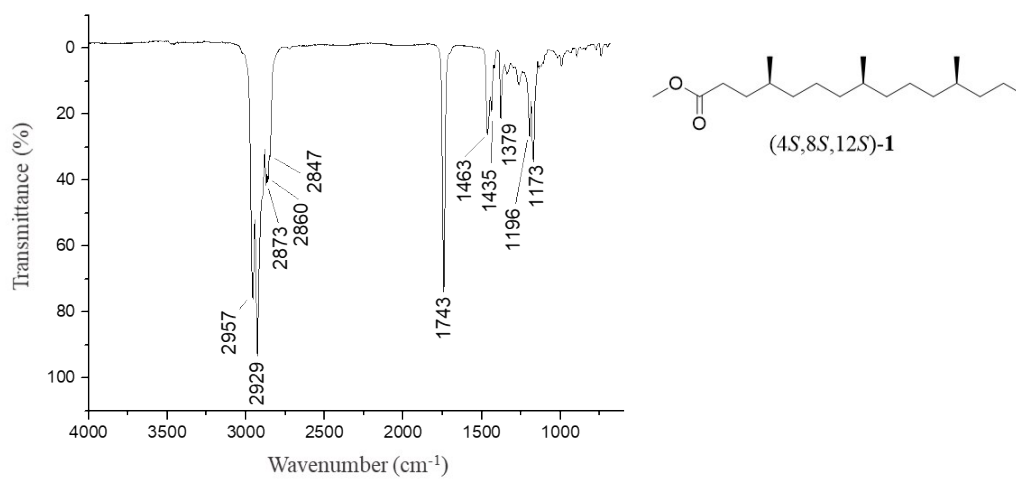
^{13}C NMR (50 MHz, CDCl_3) and DEPT 135 (superior) of compound (4*S*,8*S*,12*S*)-1



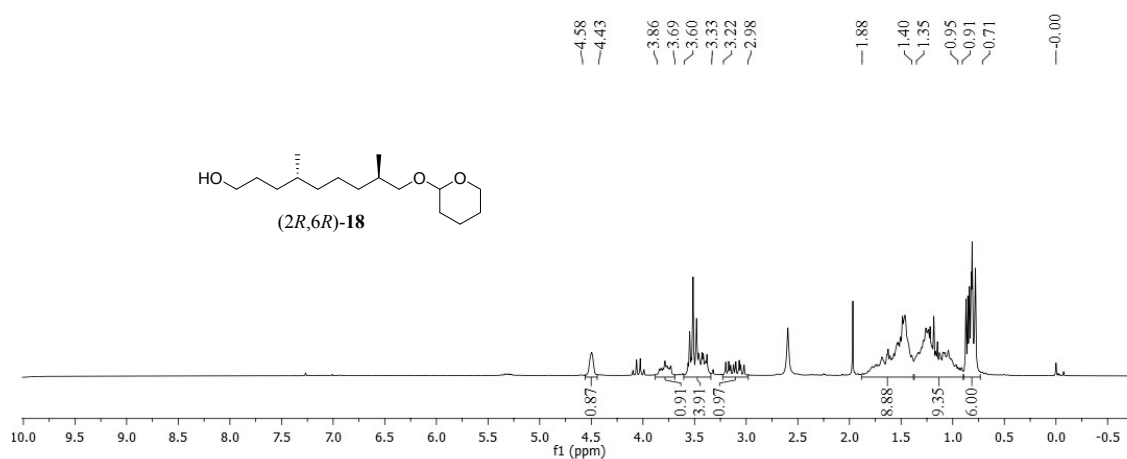
Mass spectrum (EI, 70 eV) of compound (4*S*,8*S*,12*S*)-1



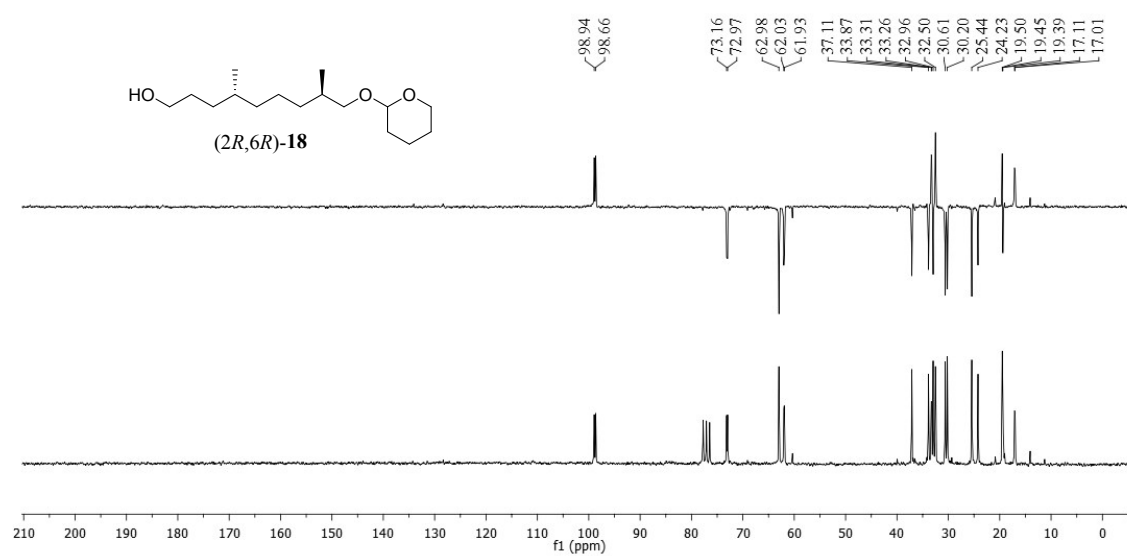
Infrared spectrum of compound (4*S*,8*S*,12*S*)-1



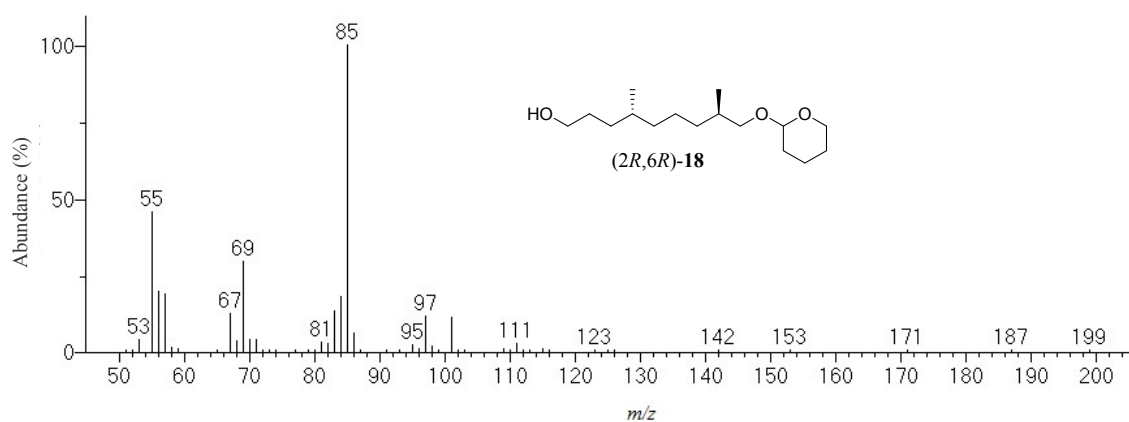
^1H NMR (200 MHz, CDCl_3) of compound (2*R*,6*R*)-**18**



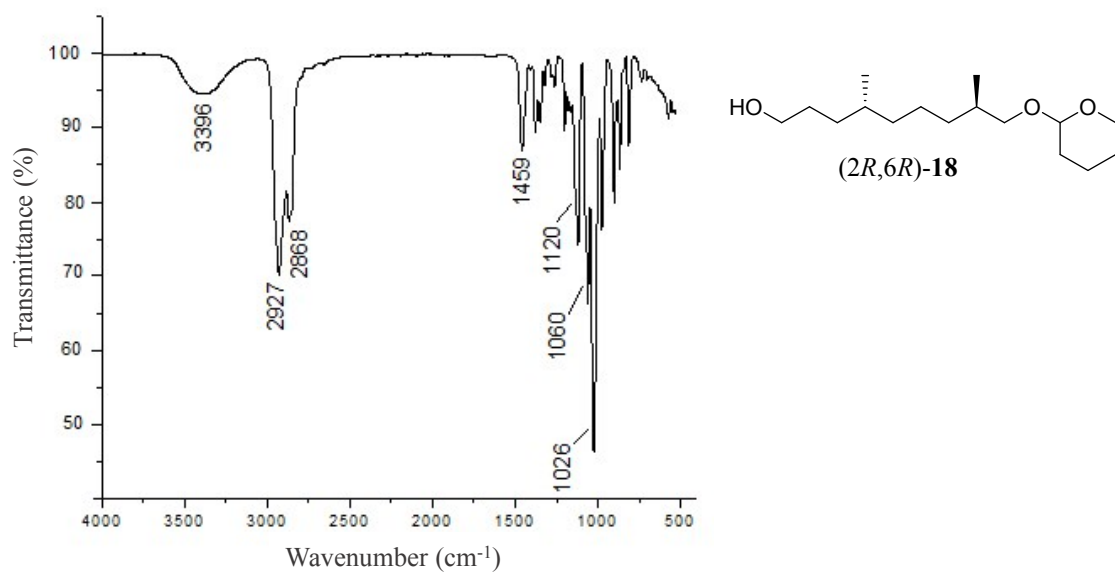
^{13}C NMR (50 MHz, CDCl_3) and DEPT 135 (superior) of compound (2*R*,6*R*)-**18**



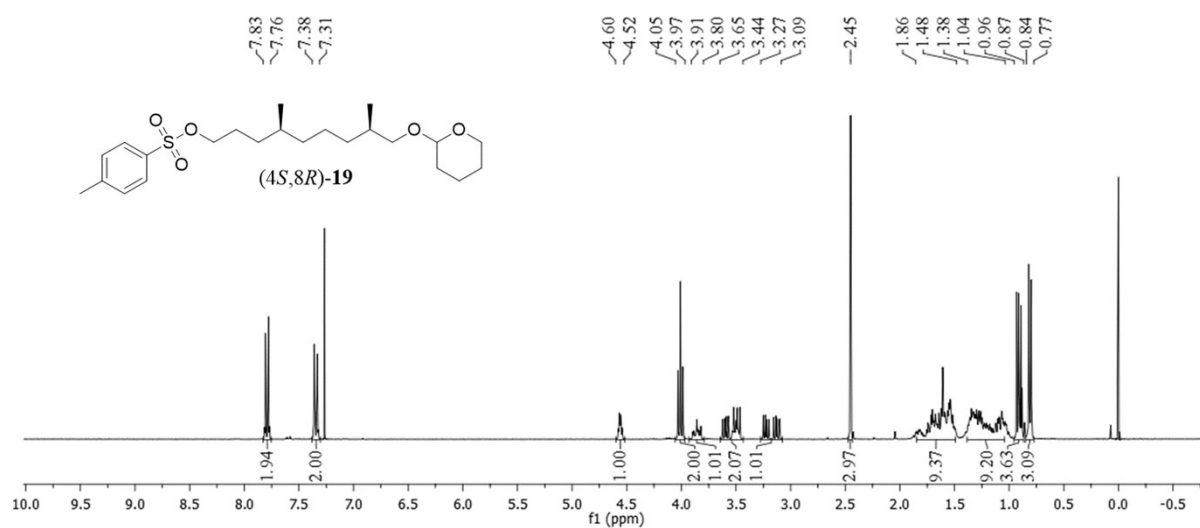
Mass spectrum (EI, 70 eV) of compound (2*R*,6*R*)-**18**



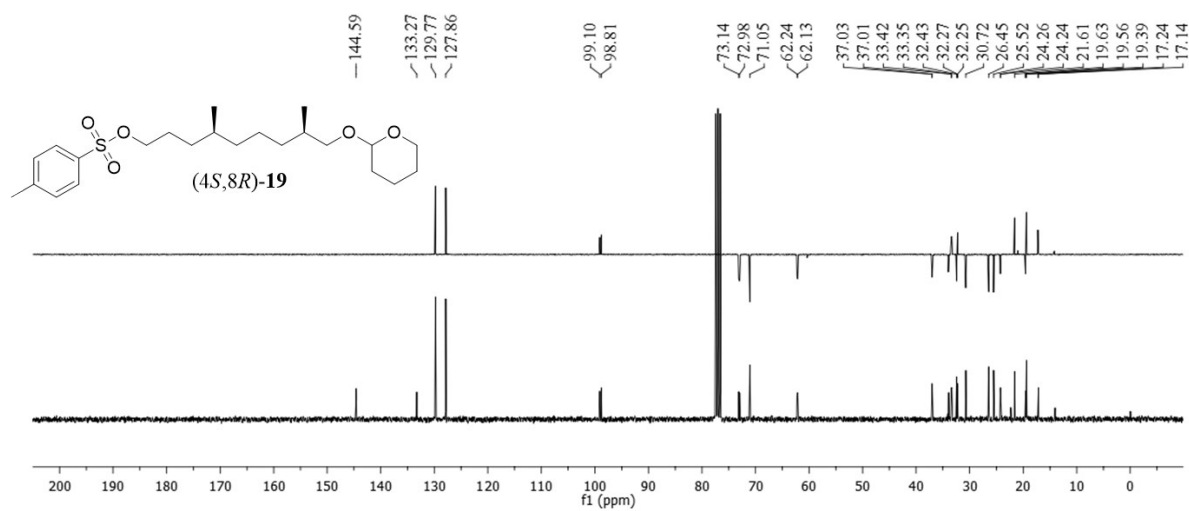
Infrared spectrum of compound (2*R*,6*R*)-**18**



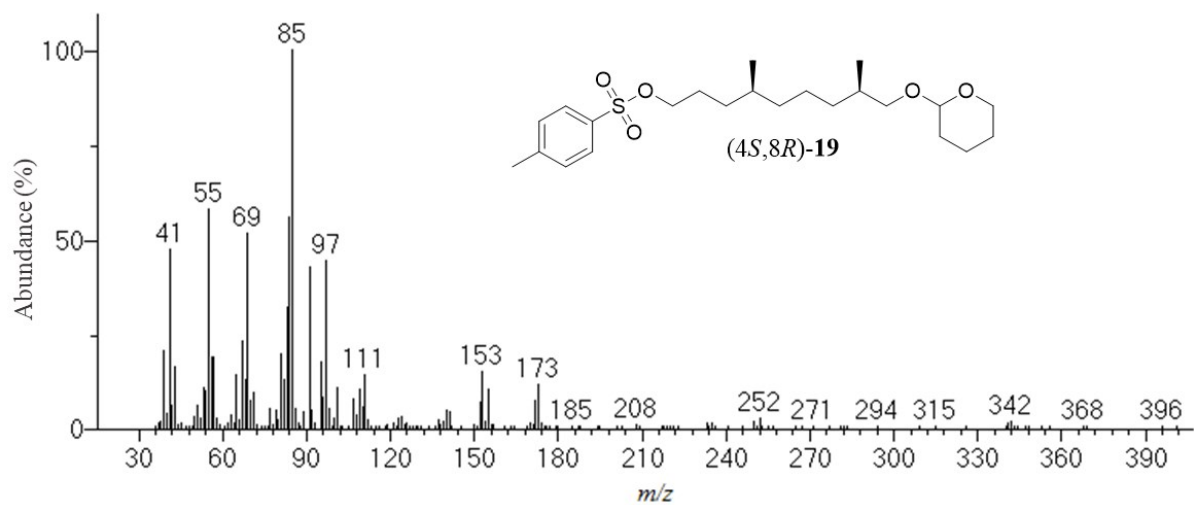
^1H NMR (300 MHz, CDCl_3) of compound (4*S*,8*R*)-**19**



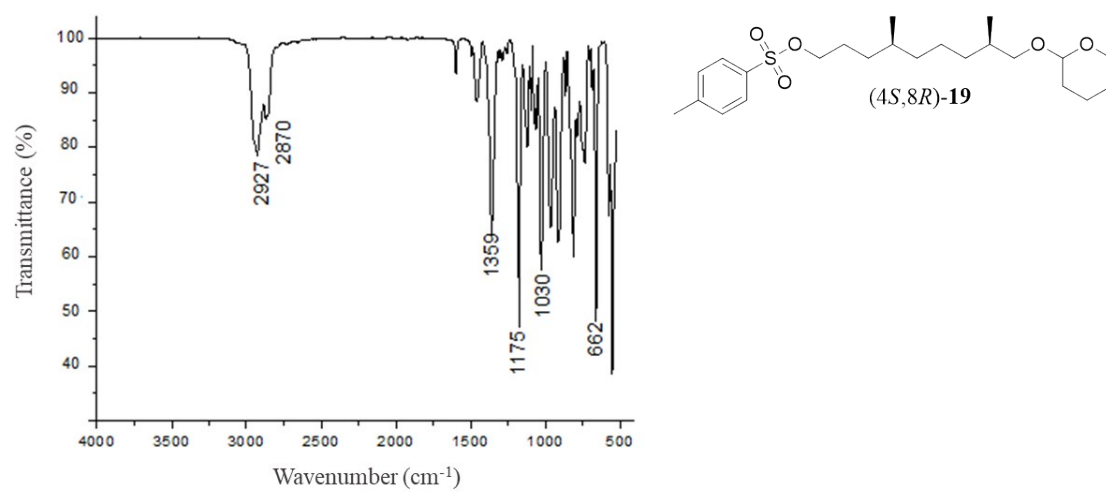
^{13}C NMR (75 MHz, CDCl_3) and DEPT 135 (superior) of compound (4*S*,8*R*)-**19**



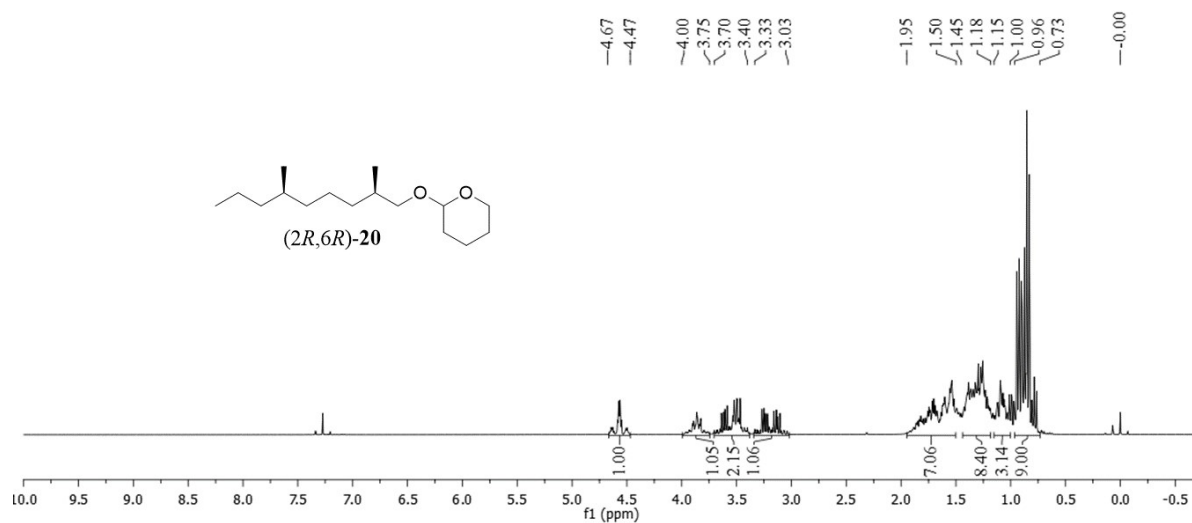
Mass spectrum (EI, 70 eV) of compound (4*S*,8*R*)-**19**



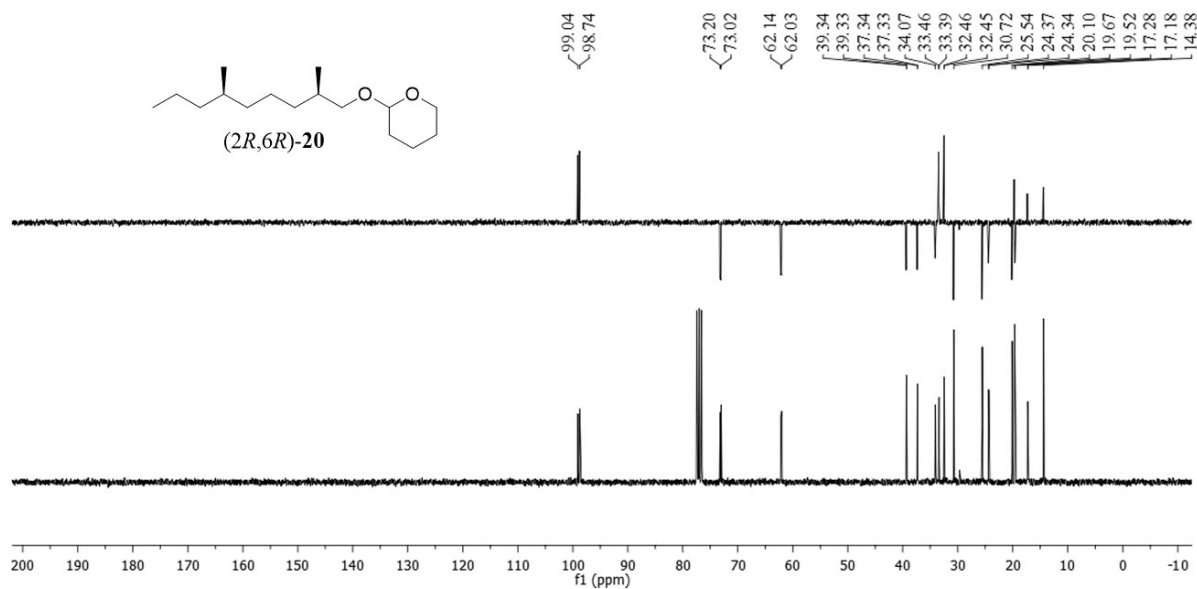
Infrared spectrum of compound (4*S*,8*R*)-**19**



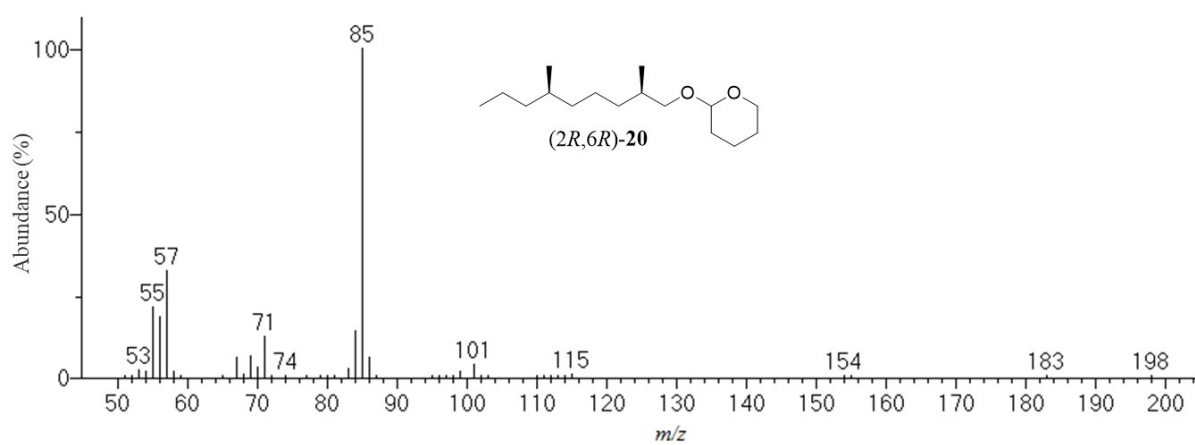
^1H NMR (300 MHz, CDCl_3) of compound (2*R*,6*R*)-**20**



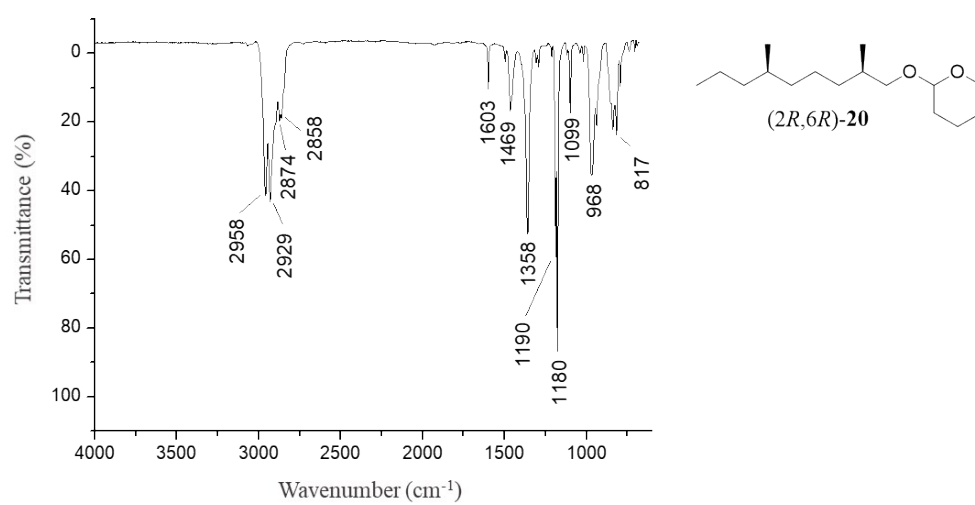
^{13}C NMR (50 MHz, CDCl_3) and DEPT 135 (superior) of compound (2*R*,6*R*)-**20**



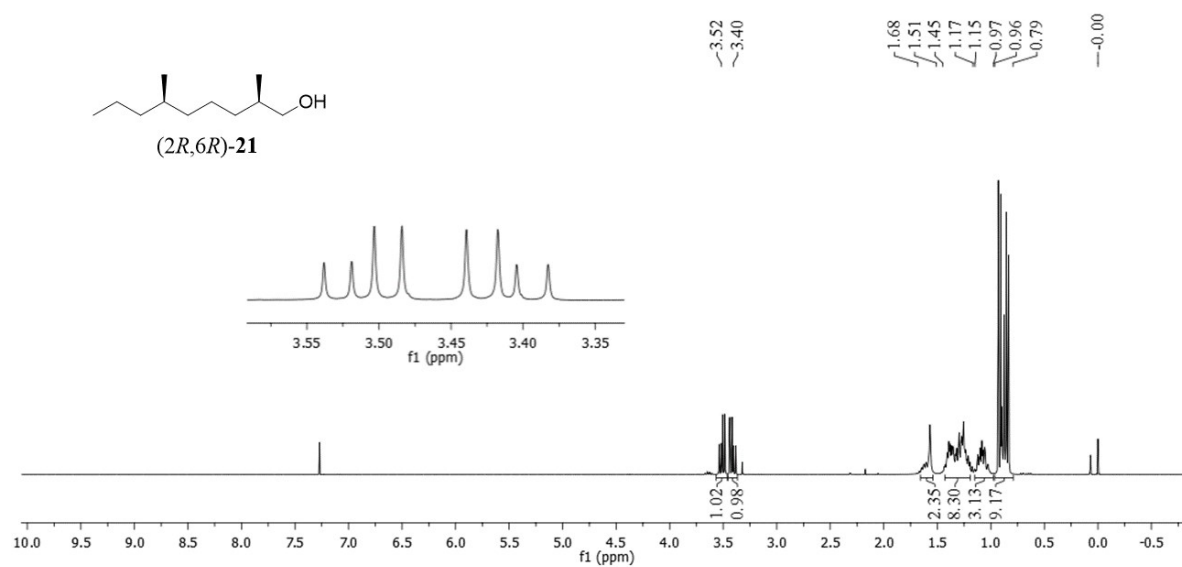
Mass spectrum (EI, 70 eV) of compound (2*R*,6*R*)-**20**



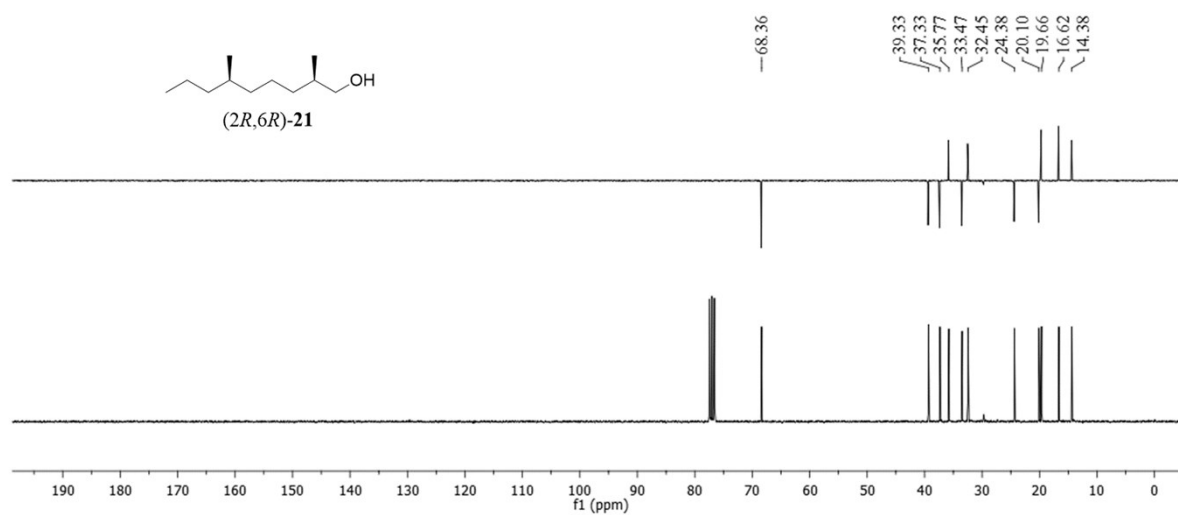
Infrared spectrum of compound (2*R*,6*R*)-**20**



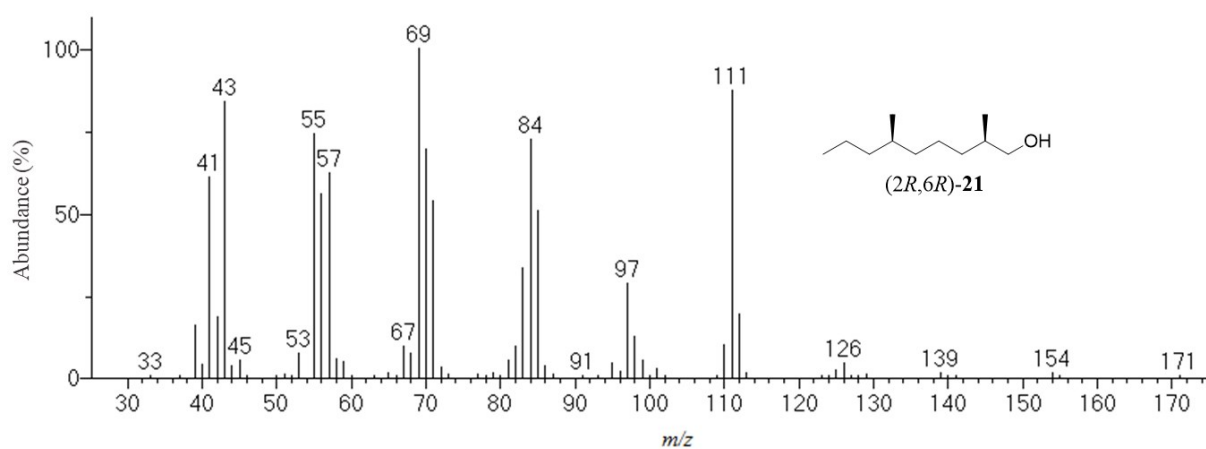
^1H NMR (300 MHz, CDCl_3) of compound (2*R*,6*R*)-**21**



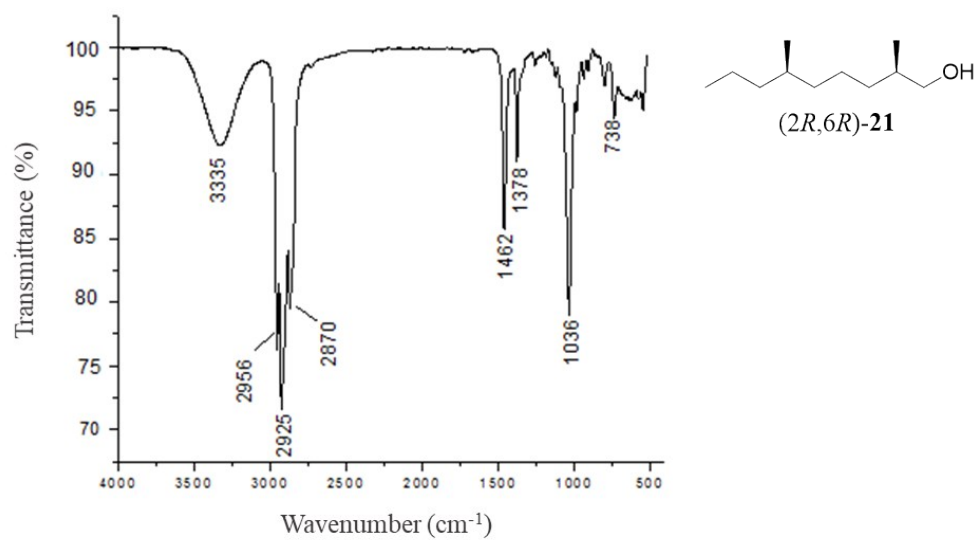
^{13}C NMR (75 MHz, CDCl_3) and DEPT 135 (superior) of compound (2*R*,6*R*)-**21**



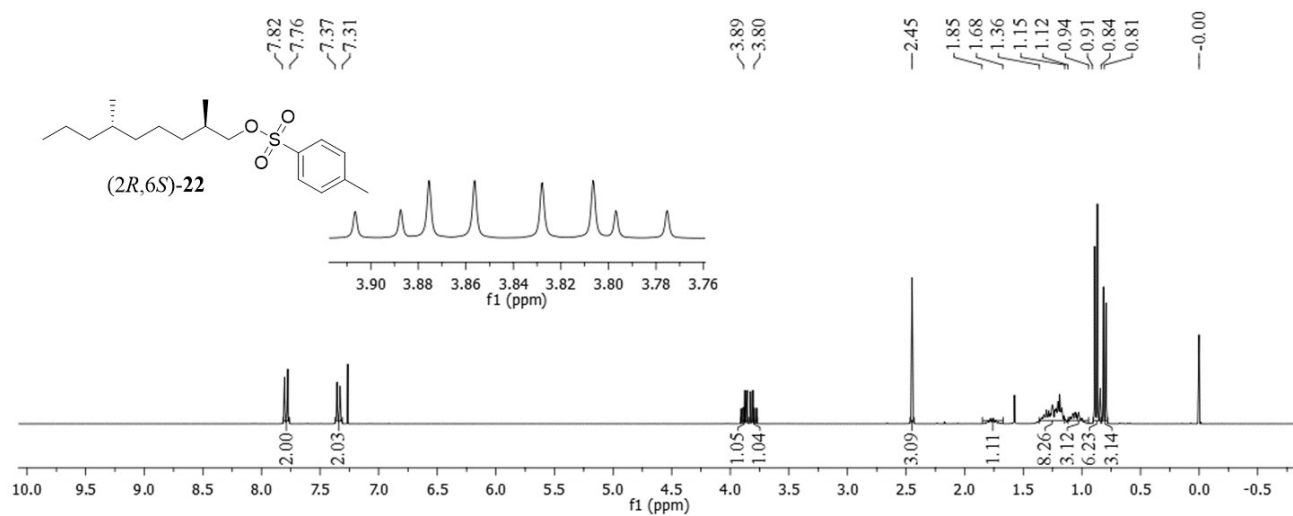
Mass spectrum (EI, 70 eV) of compound (2*R*,6*R*)-**21**



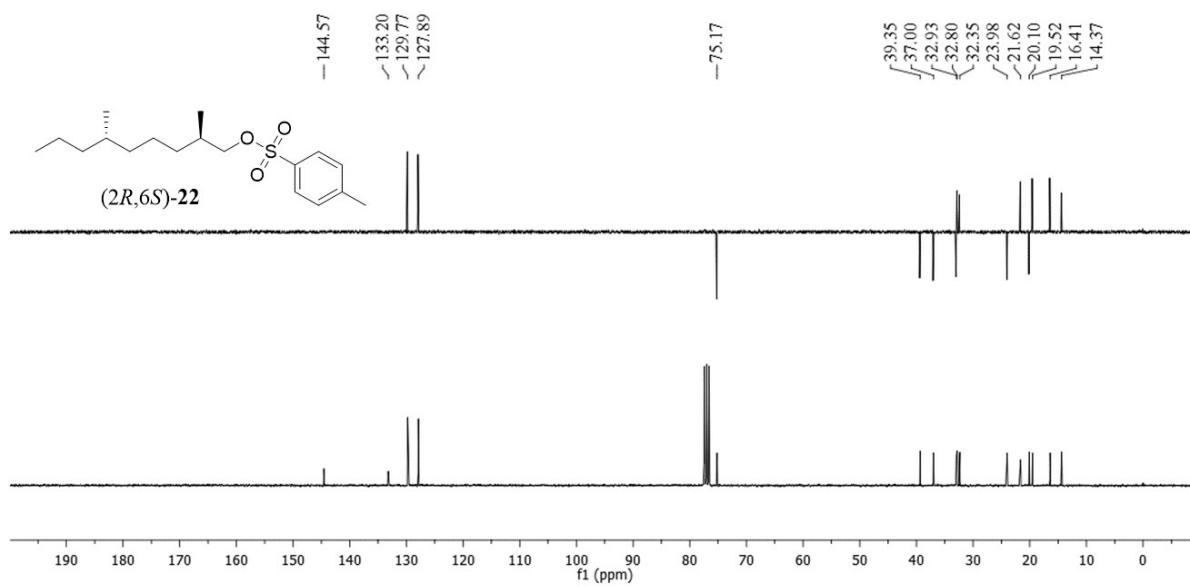
Infrared spectrum of compound (2*R*,6*R*)-**21**



^1H NMR (300 MHz, CDCl_3) of compound (2*R*,6*S*)-**22**



^{13}C NMR (75 MHz, CDCl_3) and DEPT 135 (superior) of compound (2*R*,6*S*)-**22**



Mass spectrum (EI, 70 eV) of compound (2*R*,6*S*)-**22**

