Supplementary Material

Concise Asymmetric Syntheses of (*S*)-ethyl 4-methyloctanoate and its Acid: Aggregation Pheromones of Rhinoceros Beetles of the Genus *Oryctes*

Rachana Pandey and Ranjana Prakash*

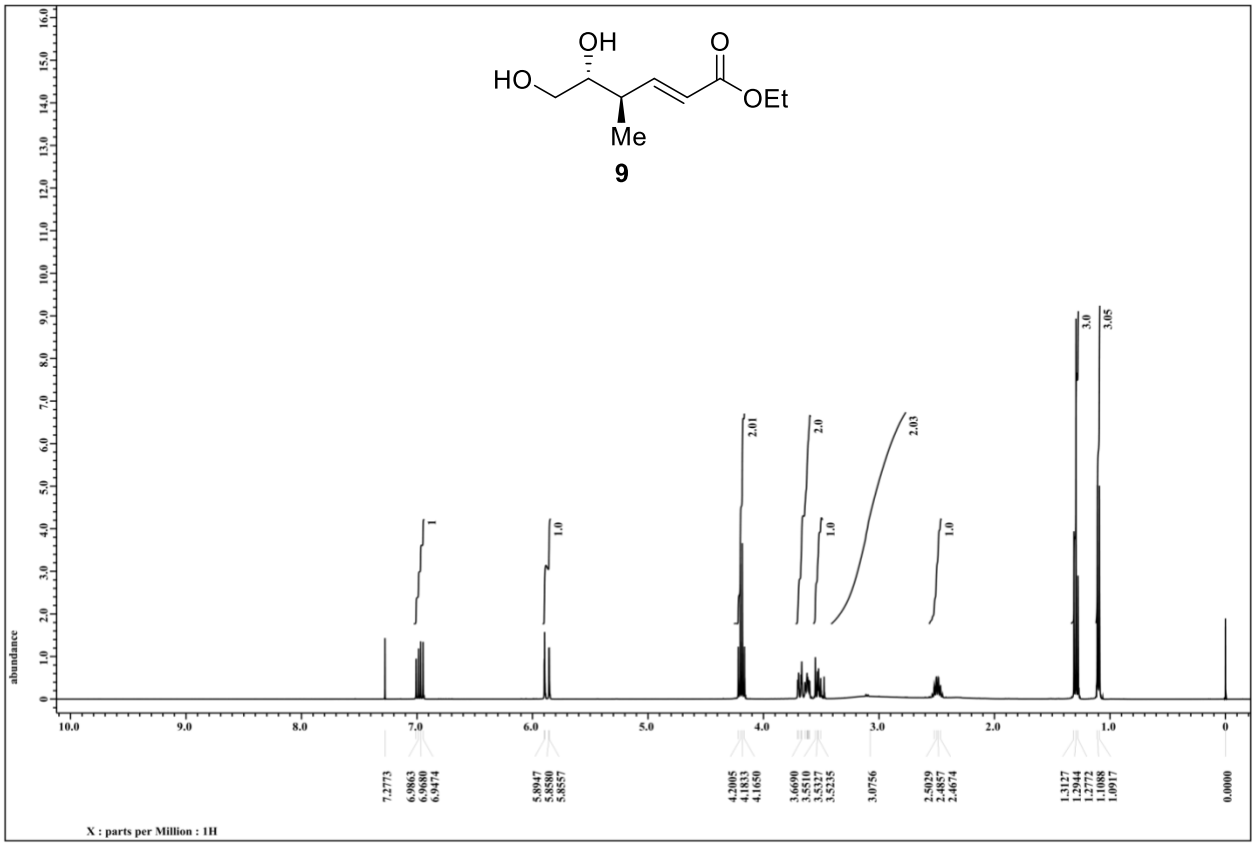
School of Chemistry and Biochemistry, Thapar Institute of Engineering and Technology, Patiala 147 001, India.
**Corresponding Author: Phone: +91-175-239-3832, Fax No. +91-175-236-4498*
E-mail: rprakash@thapar.edu

Table of contents

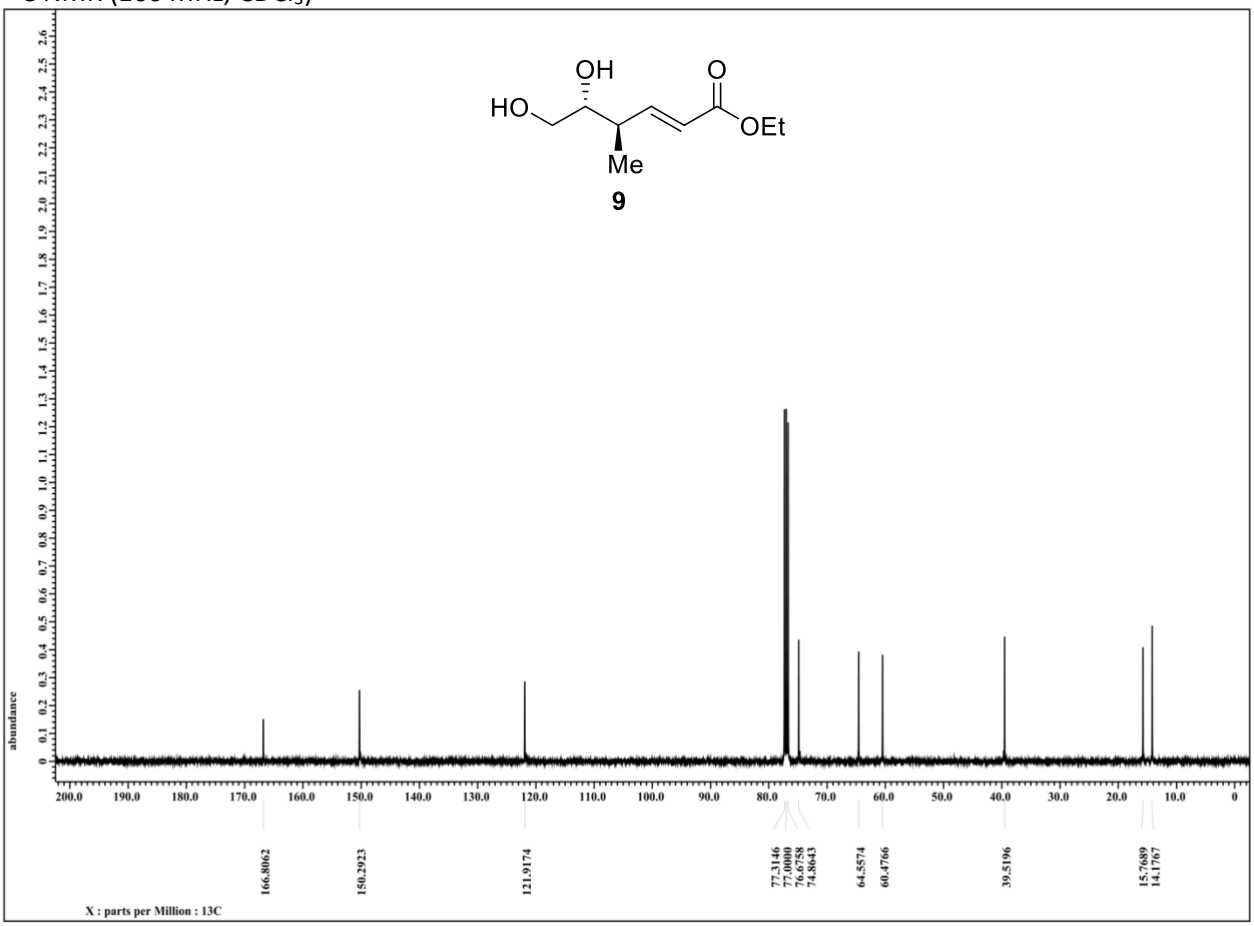
Materials and methods

All reactions were carried out under argon or nitrogen in oven-dried glassware using standard glass syringes and septa. The solvents and chemicals were purchased from Merck and Sigma Aldrich chemical company. Solvents and reagents were purified and dried by standard methods prior to use. Progress of the reactions was monitored by TLC using precoated aluminium plates of Merck kieselgel 60 F254. Column chromatography was performed on silica gel (60-120 and 100-200 mesh) using a mixture of *n*-hexane and ethyl acetate. Optical rotations were measured on automatic polarimeter AA-65. ^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ (unless otherwise mentioned) on JEOL ECS operating at 400 and 100 MHz, respectively. Chemical shifts are reported in δ (ppm), referenced to TMS. HRMS were recorded on Agilent 6530 Accurate-Mass Q-TOF using Electron Spray Ionization. IR spectra were recorded on Agilent resolution Pro 600 FT-IR spectrometer, fitted with a beam condensing ATR accessory.

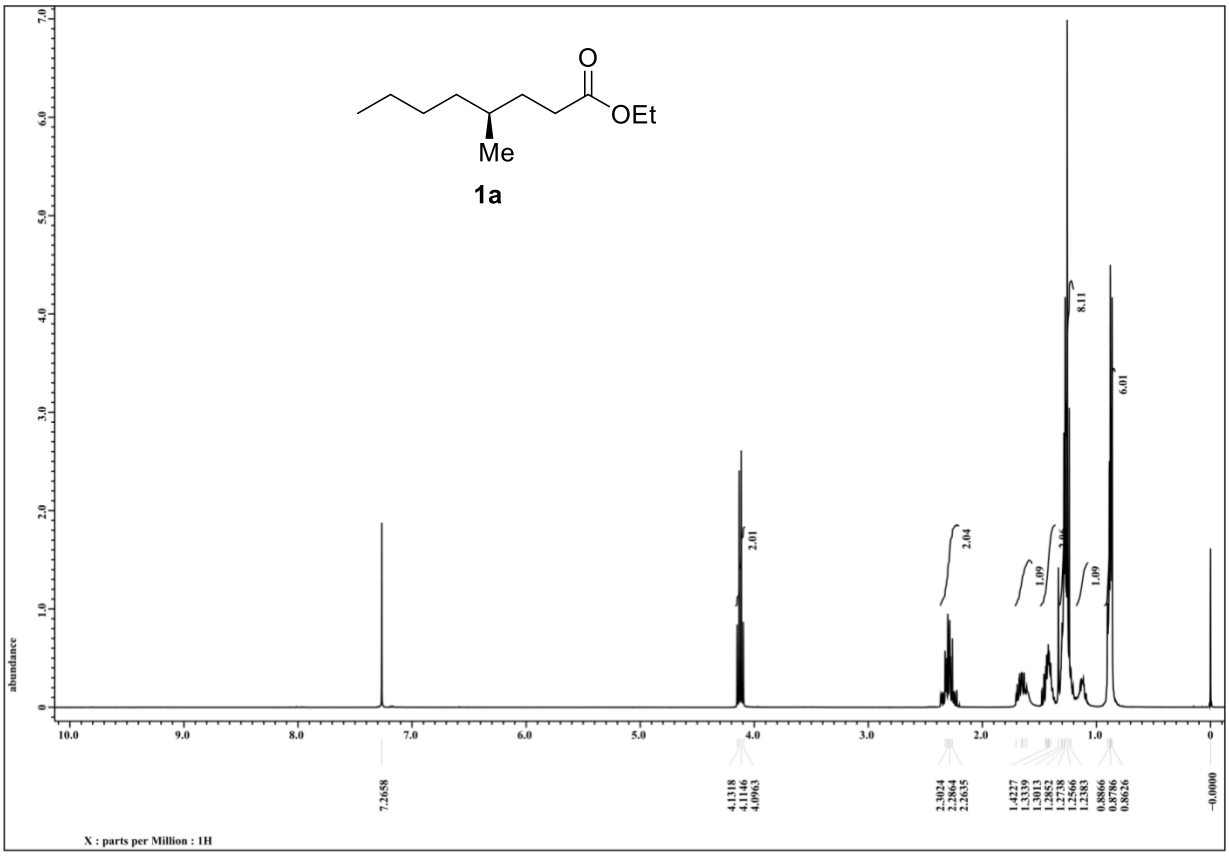
^{1}H NMR (400 MHz, $CDCl_3$/TMS)



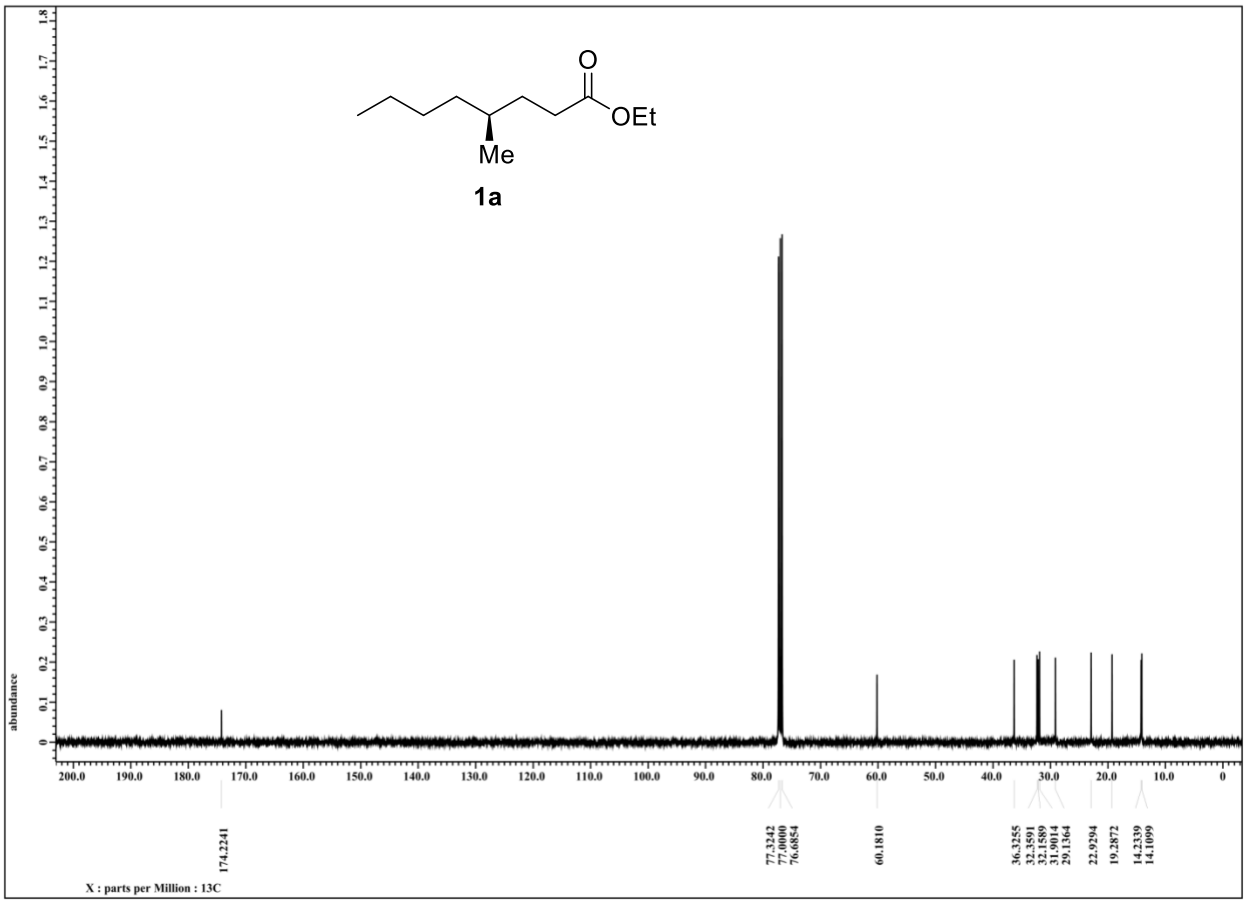
^{13}C NMR (100 MHz, $CDCl_3$)



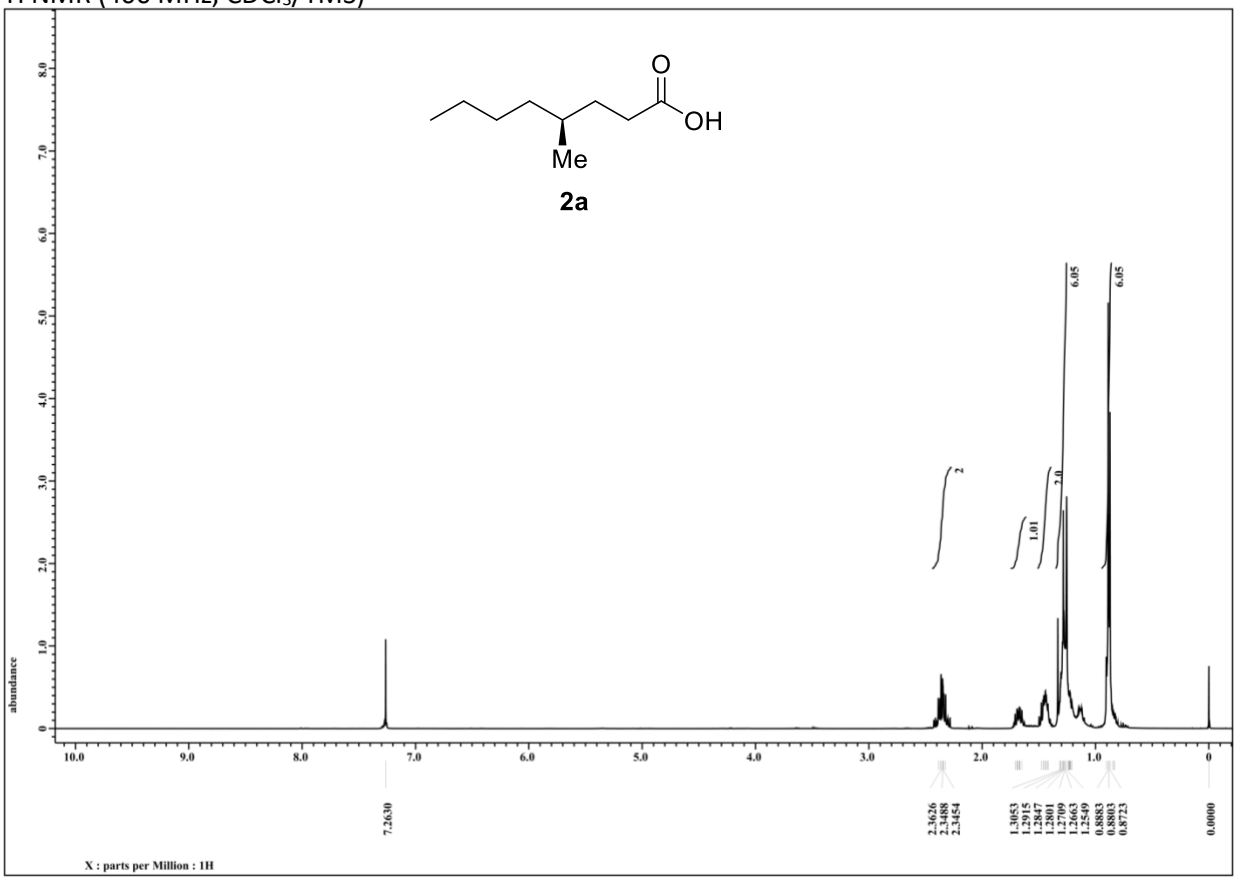
^{1}H NMR (400 MHz, $CDCl_3$/TMS)



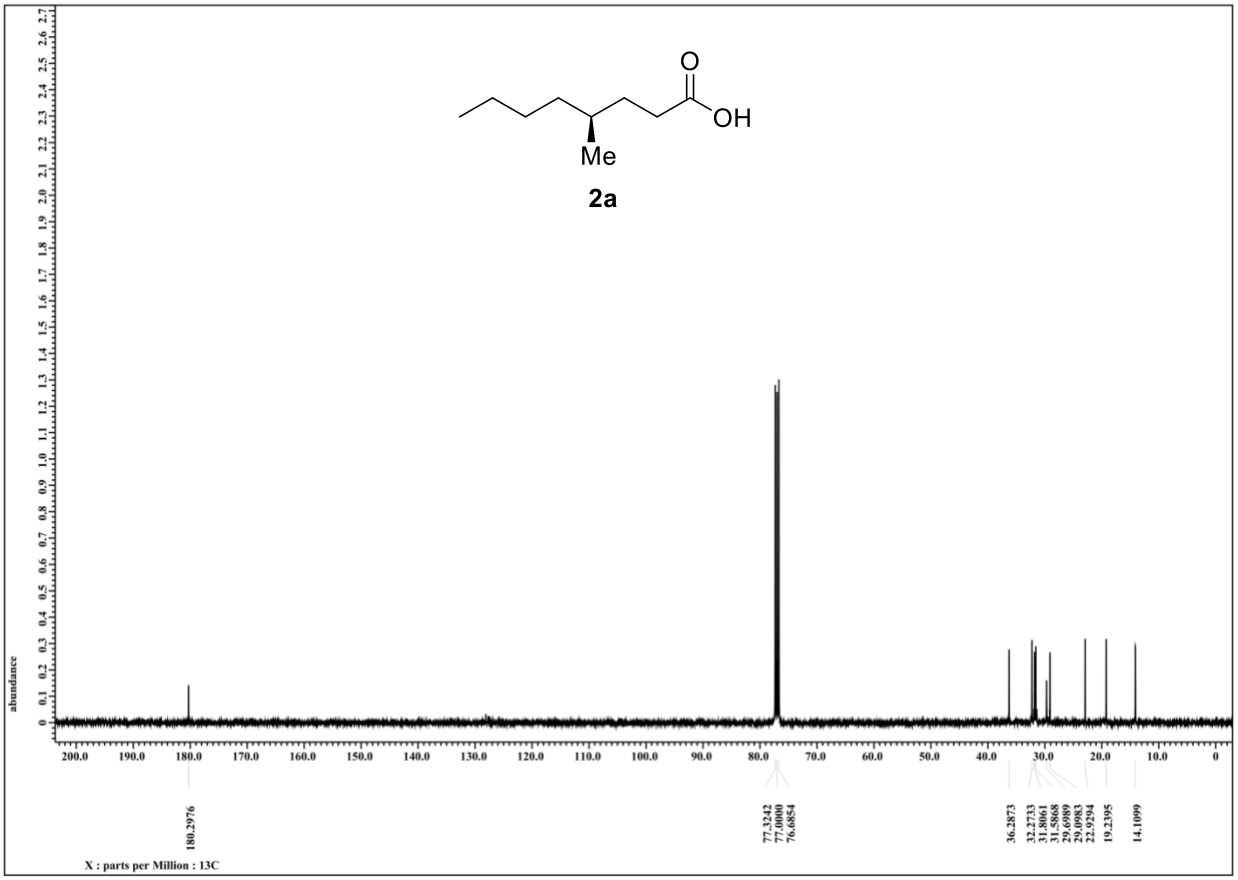
^{13}C NMR (100 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$/TMS)



^{13}C NMR (100 MHz, $CDCl_3$)



D-7000 HPLC System Manager Report

Analyzed: 03/16/18 02:54 PM

Reported: 03/16/18 03:25 PM
Processed: 03/16/18 03:25 PM

Data Path: C:\WIN32APP\HSM\HPLC\DATA\0094\

D-7000 HPLC System Manager Report

Analyzed: 03/16/18 02:29 PM

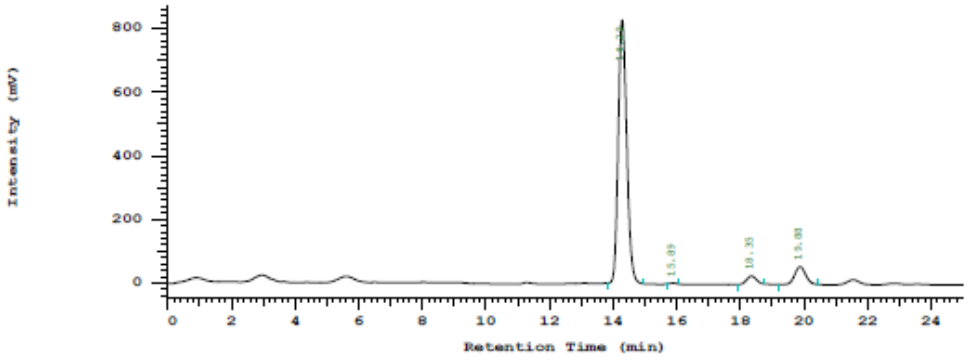
Reported: 03/16/18 03:27 PM
Processed: 03/16/18 03:26 PM

Data Path: C:\WIN32APP\HSM\HPLC\DATA\0093\
Processing Method: cal

System(acquisition): Sys 1
Application: HPLC
Sample Name: R2 (Chiral)
Injection from this vial: 1 of 1
Sample Description: PET:ETOH(99:1)

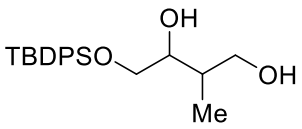
Series:0093
Volume: 10.0 ul

Chrom Type: HPLC Channel : 1

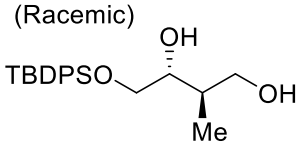


No.	RT	Area	Conc 1	BC
1	14.29	15250441	89.041	BB
2	15.89	27761	0.162	BB
3	18.35	531220	3.102	BB
4	19.88	1317927	7.695	BB
		17127349	100.000	

Peak rejection level: 0



(Racemic)




```
Project Leader: Dr.TRIPATHI.P.K
Column        :Chiralpak IB (250 mm x 4.6mm)
Mobile Phase  :Petether:EtoH(99:01)
Wavelength : 220nm
Flow       : 1.0 ml/min.
Inject vol: 2ul
```

D-7000 HPLC System Manager Report

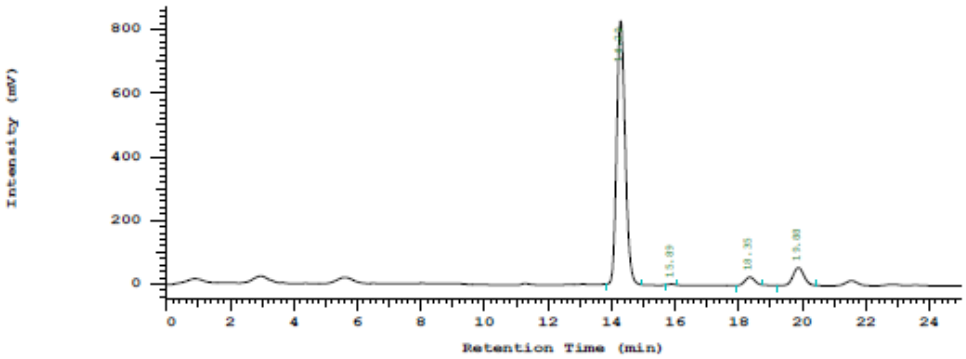
Analyzed: 03/16/18 02:29 PM
Reported: 03/16/18 03:27 PM
Processed: 03/16/18 03:26 PM

Data Path: C:\WIN32APP\HSM\HPLC\DATA\0093\
Processing Method: cal

System(acquisition): Sys 1
Application: HPLC
Sample Name: R2 (Chiral)
Injection from this vial: 1 of 1
Sample Description: PET:ETOH(99:1)

Series:0093
Volume: 10.0 ul

Chrom Type: HPLC Channel : 1



No.	RT	Area	Conc 1	BC
1	14.29	15250441	89.041	BB
2	15.89	27761	0.162	BB
3	18.35	531220	3.102	BB
4	19.88	1317927	7.695	BB
		17127349	100.000	

Peak rejection level: 0

```
Project Leader: Dr.TRIPATHI.P.K
Column        :Chiralpak IB (250 mm x 4.6mm)
Mobile Phase  :Petether:EtoH(99:01)
Wavelength : 220nm
Flow       : 1.0 ml/min.
Inject vol: 2ul
```