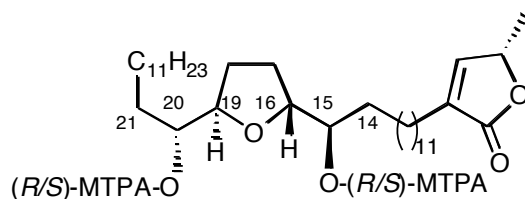


Natural *cis*-Solamin is a Mixture of Tetra-Epimeric Diastereoisomers: Biosynthetic Implications for *Annonaceous* Acetogenins

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Mosher Ester Data

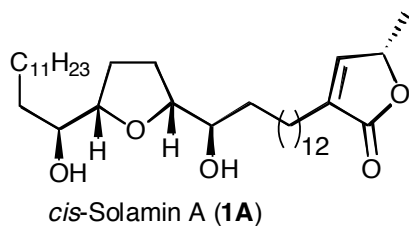
Table 1. Diagnostic ¹H-NMR values (400 MHz, CDCl₃) of (*S*)- and (*R*)-MTPA esters of solamin.



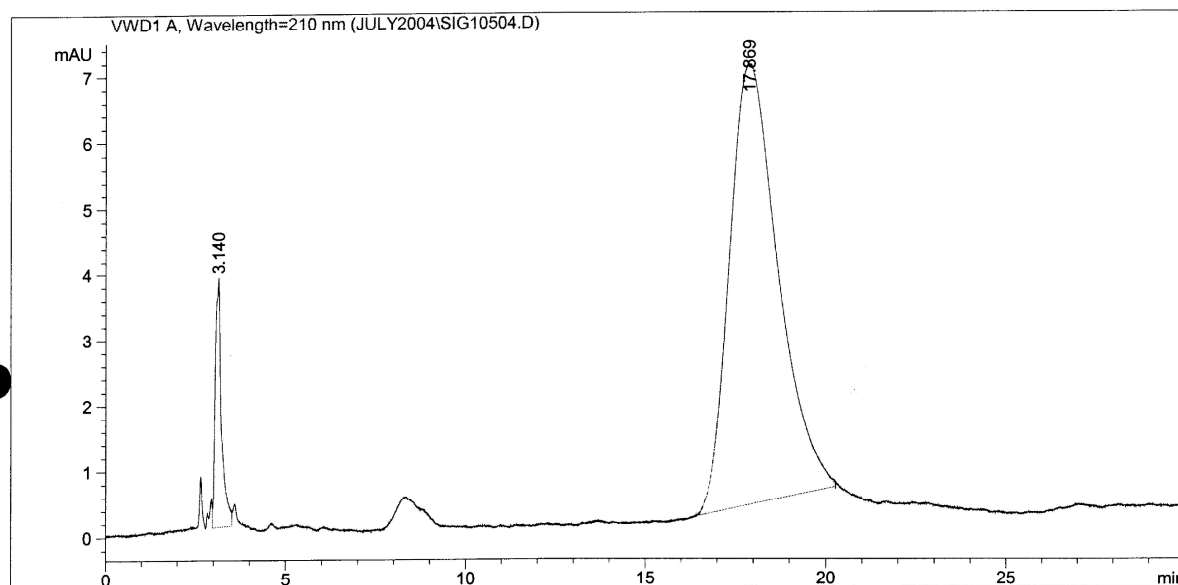
solamin Mosher's ester derivatives

Atom	¹ H δ values for <i>S</i> Mosher's ester (ppm)	¹ H δ values for <i>R</i> Mosher's ester (ppm)	Δδ (<i>S</i> - <i>R</i>)
1	-	-	
2	-	-	
3	2.26 t (7.4 Hz)	2.26 t (7.7 Hz)	
4	1.55 m	1.53 m	
5	1.17-1.36	1.16-1.36	
13	1.30 m	1.16 m	+ 0.14
14	1.28 m	1.51 m	+ 0.07
15	4.96 m	5.03 m	-
16	3.93 m	4.00 m	- 0.07
17,18	1.65 m	1.92 m	- 0.27
17,18	1.35 m	1.56 m	- 0.21
19	3.93 m	4.00 m	- 0.07
20	4.96 m	5.03 m	-
21	1.58 m	1.51 m	+ 0.07
22	1.30 m	1.16 m	+ 0.14
23-30	1.17-1.36	1.16-1.36	
31	1.30 m	1.30 m	
32	0.88 t (6.6 Hz)	0.88 t (6.6 Hz)	
33	6.98 d (1.4 Hz)	6.98 d (1.7 Hz)	
34	4.99 m	4.99 m	
35	1.41 d (6.8 Hz)	1.40 d (6.8 Hz)	
MeO-10	3.52 s	3.54 s	
Ar (5H)	7.58 m and 7.38 m	7.58 m and 7.37 m	

Chiral HPLC trace for a sample of *cis*-solamin A (1A): (Chiral CD-Ph column with gaurd column, eluting with IPA/hexane 15/85 at a flow rate of 1 mL/min. UV detection at 210nm).



Sequence File : D:\HPCHEM\1\SEQUENCE\DEF_LC.S
 Method : C:\HPCHEM\1\METHODS\15IPAHEX.M
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 15% ipa 30 mins



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 Area Percent Report
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Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000

Signal 1: VWD1 A, Wavelength=210 nm

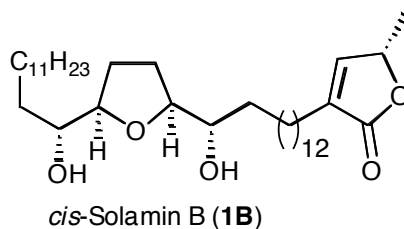
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.140	VB	0.1550	45.67373	3.77930	6.8060
2	17.869	BB	1.0922	625.40936	6.69299	93.1940

Totals : 671.08310 10.47229

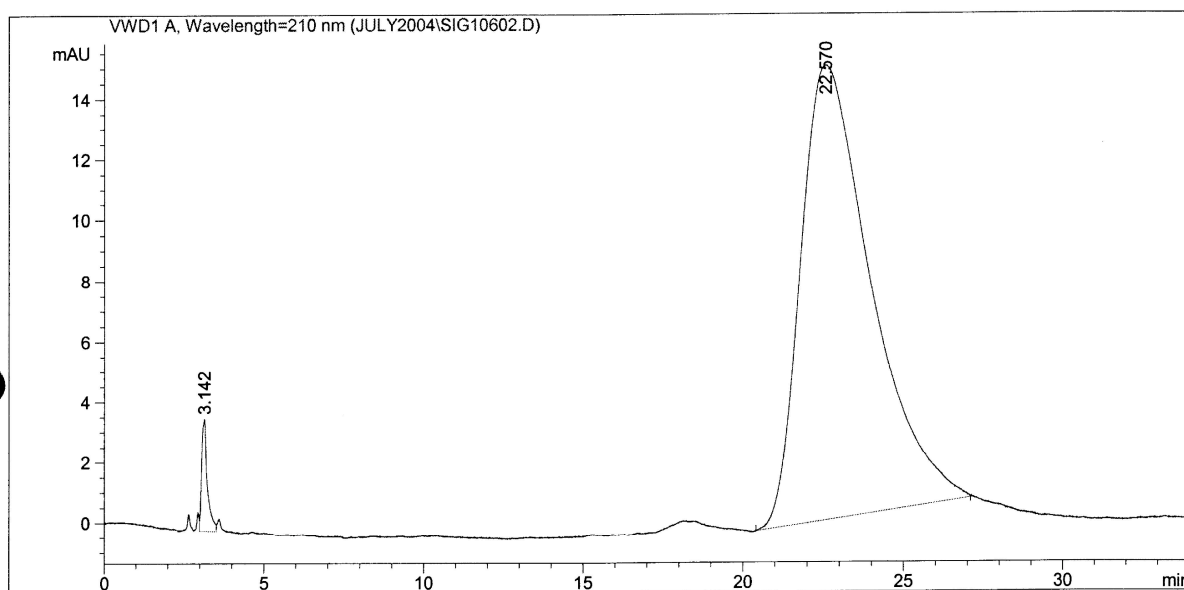
Results obtained with enhanced integrator!

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 *** End of Report ***

Chiral HPLC trace for a sample of *cis*-solamin B (1B): (Chiral CD-Ph column with gaurd column, eluting with IPA/hexane 15/85 at a flow rate of 1 mL/min. UV detection at 210nm).



Sequence File : D:\HPCHEM\1\SEQUENCE\DEF_LC.S
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 15% ipa 30 mins



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 Area Percent Report
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Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000

Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.142	VB	0.1583	45.86706	3.70944	1.9785
2	22.570	PB	1.7674	2272.36548	15.01701	98.0215

Totals : 2318.23254 18.72646

Results obtained with enhanced integrator!

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 *** End of Report ***