

Supplementary material

Table S1: Analytical data for compounds used in the study.

Code	Compound	Experimental Molecular weight	HPLC peak (min)	Purity %
5	H-Arg-[3-amino-3(1-naphthyl)-propionic acid]-Phe-OH	519.4	14.55	99
6(S)	H-Arg-[3-amino-3(1-naphthyl)-propionic acid]-Tyr-OH	535.3	11.58	98
6(R)	H-Arg-[3-amino-3(1-naphthyl)-propionic acid]-Tyr-OH	535.3	10.0	99
7(S)	H-Arg-[3-amino-3(1-naphthyl)-propionic acid]-Asp-OH	487.2	11.68	96
7(R)	H-Arg-[3-amino-3(1-naphthyl)-propionic acid]-Asp-OH	487.3	13.53	93
8(S)	H-Arg-[3-amino-3(1-naphthyl)-propionic acid]-[3-amino-3(1-naphthyl)-propionic acid]-OH	569	5.02	95
9(S)	H-Arg-[3-amino-3(1-naphthyl)-propionic acid]-Phe-Asp-OH	636	7.88	99
10(S)	H-Arg-[3-amino-3(biphenyl)-propionic acid]-Phe-OH	545.3	12.93	99
10(R)	H-Arg-[3-amino-3(biphenyl)-propionic acid]-Phe-OH	545.3	14.10	98
11(S)	H-Lys-[3-amino-3(biphenyl)-propionic acid]-Phe-OH	517.2	14.583	98
11(R)	H-Lys-[3-amino-3(biphenyl)-propionic acid]-Phe-OH	517.2	15.42	98
12(S)	H-Arg-Pro-[3-amino-3(1-naphthyl)-propionic acid]-Phe-OH	615.34	8.92	98
12(R)	H-Arg-Pro-[3-amino-3(1-naphthyl)-propionic acid]-Phe-OH	615.28	12.92	98
13(S)	H-Arg-Pro-[3-amino-3(1-naphthyl)-propionic acid]-Tyr-OH	632.6	11.27	96
13(R)	H-Arg-Pro-[3-amino-3(1-naphthyl)-propionic acid]-Tyr-OH	632.5	12.08	95
14(S)	Cyclo (1,4) Arg ¹ -Pro ² -[3-amino-3(1-naphthyl)-propionic acid] ³ -Phe ⁴	597.88	11.15	96
15(S)	Cyclo (1,5) Arg ¹ -Pro ² -[3-amino-3(1-naphthyl)-propionic acid] ³ -Phe ⁴	862.98	14.88	98

	acid] ³ -Phe ⁴ -DBF ⁵			
16(S)	Ac- Arg-[3-amino-3(1-naphthyl)-propionic acid]-Phe-NH ₂	560.4	16.13	99
16(R)	Ac- Arg-[3-amino-3(1-naphthyl)-propionic acid]-Phe-NH ₂	560.3	19.53	99
17(S)	H-Arg-[3-amino-3(1-naphthyl)-propionic acid]-Phe-Cys-OH	622.3	15.83	97
17(R)	H-Arg-[3-amino-3(1-naphthyl)-propionic acid]-Phe-Cys-OH	622.4	18.60	96
FITC-5	FITC-Aminocaproicacid-Arg-[3-amino-3(1-naphthyl)-propionic acid]-Phe-OH	1020.9	13.92	95

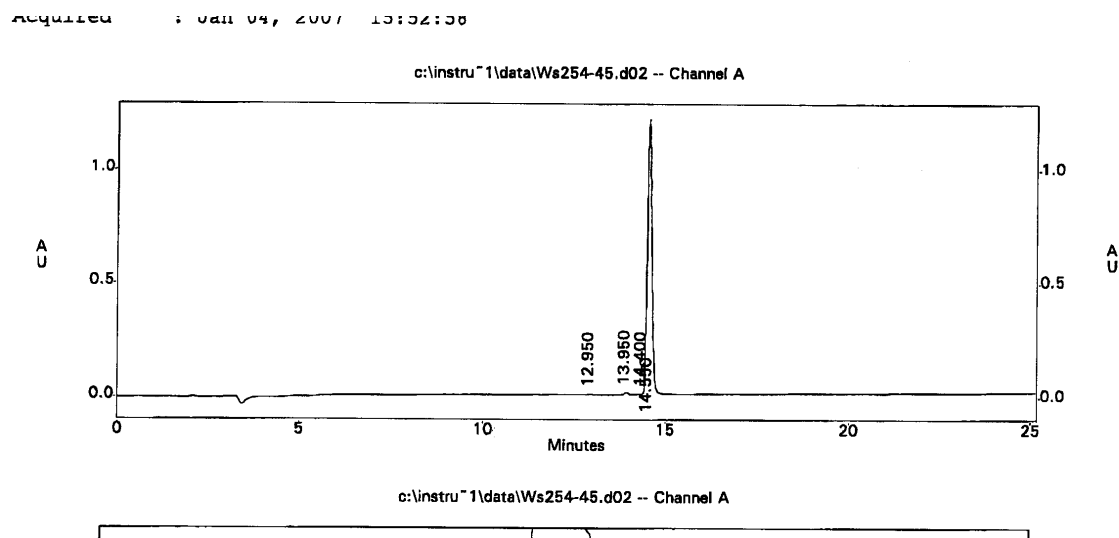


Fig. 1. HPLC of compound 5

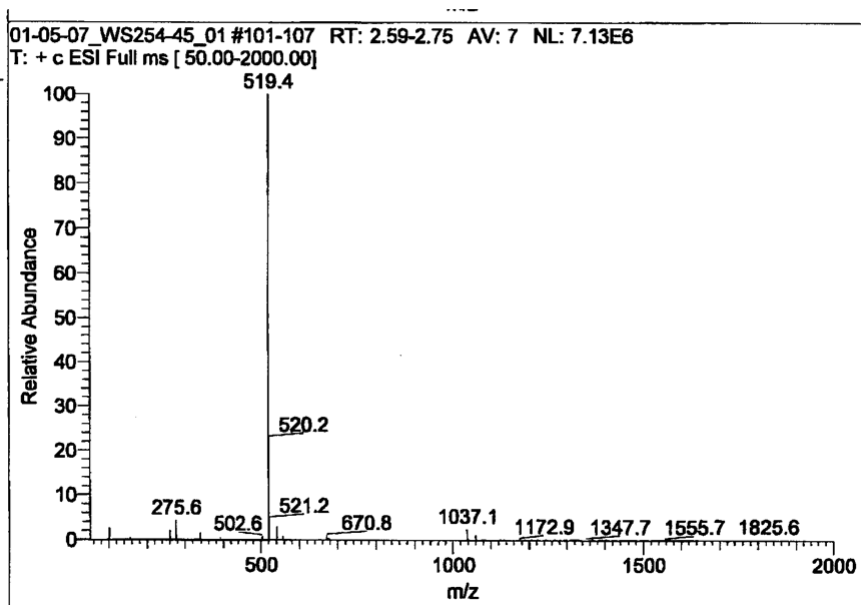
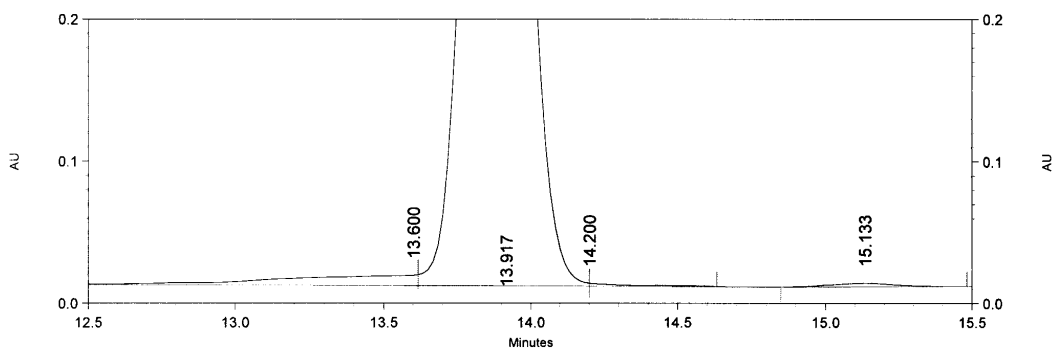
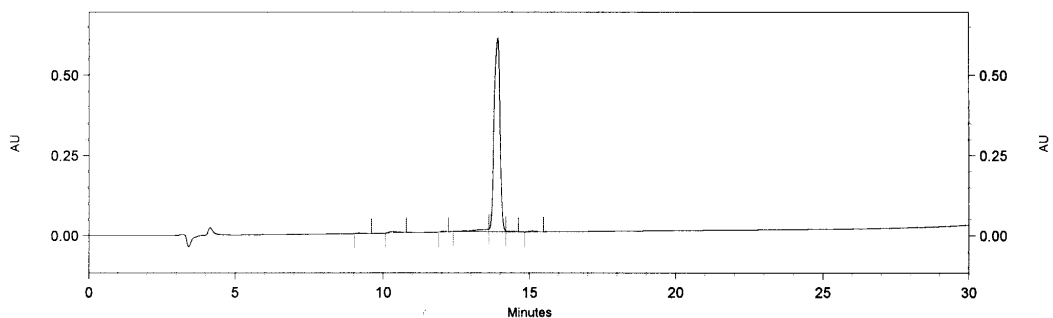


Fig. 2. Mass Spectrum of compound 5

Sample ID: AAF131 // 287095-11(11-12) in ACN/H2O
System: BECKMAN
Column: YMC C18, 4.6 X 250mm 60°C
Solvent: A=0.1%TFA/H2O, B=0.1%TFA/ACN
Flow: 1ml/min
Detector: 215nm
Method: C:\32Karat\Projects\Default\Method\35-65%B in 30 min.met
Filename: C:\32Karat\Projects\Default\Data\HPLC 1\AAF131.D113.dat
Acquisition Date: 9/20/2010 9:06:50 AM



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Results

Pk #	Retention Time	Area	Area Percent	Height
1	9.18	16990	0.19	1166
2	10.33	85597	0.97	4114
3	12.08	14753	0.17	1269
4	13.60	240568	2.74	7238
5	13.92	8381756	95.29	602994
6	14.20	18650	0.21	2001
7	15.13	37571	0.43	2462
Totals		8795885	100.00	621244

Fig. 3. HPLC of FITC-5

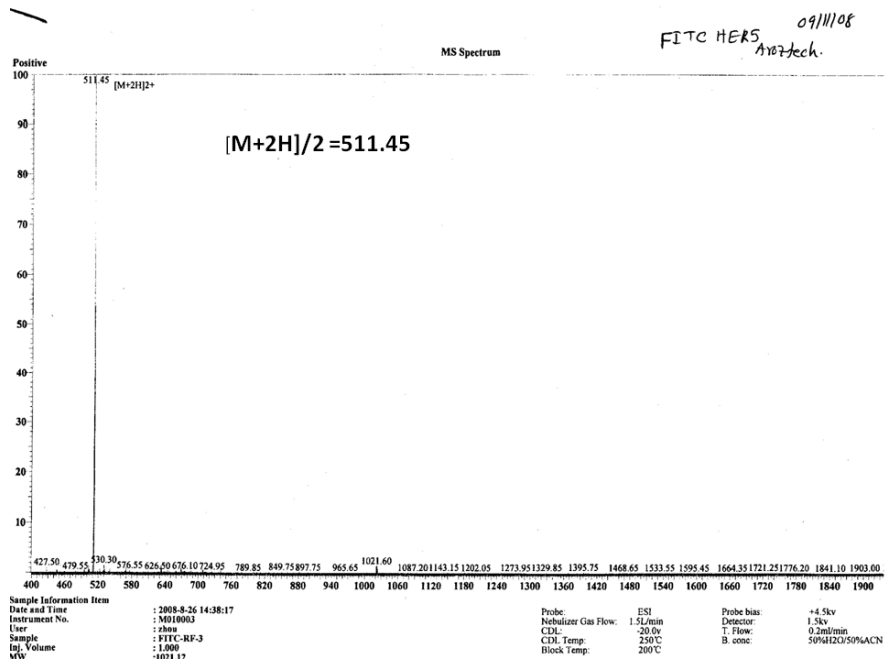


Fig. 4. Mass Spectrum of FITC-5

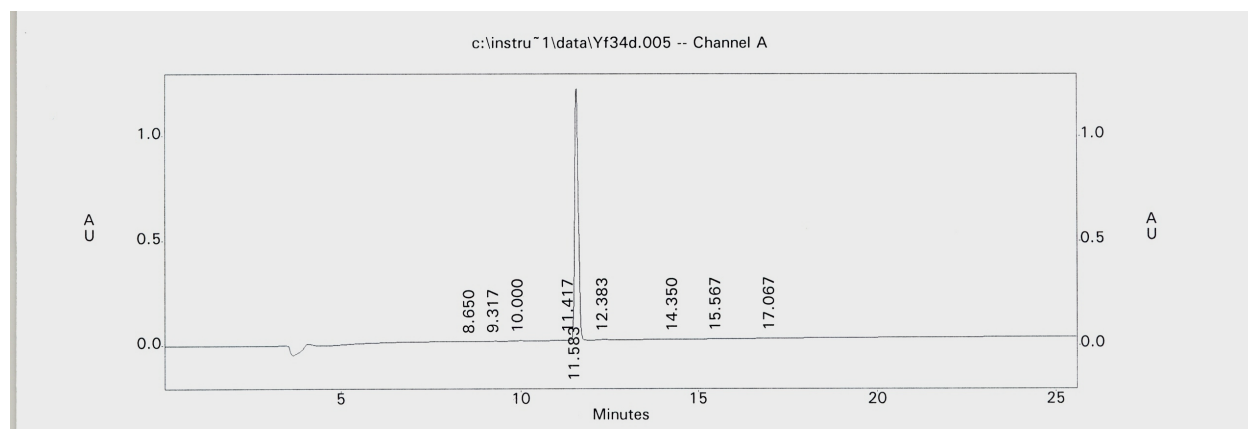


Fig. 5. HPLC of compound 6(S)

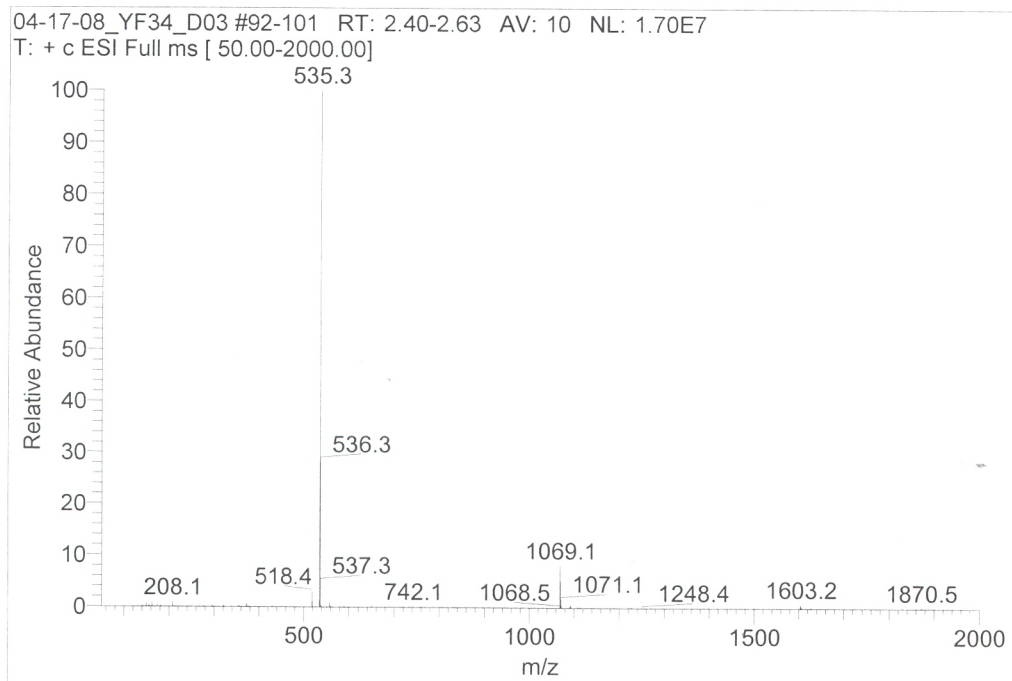


Fig 6. Mass spectrum of compound 6(S)

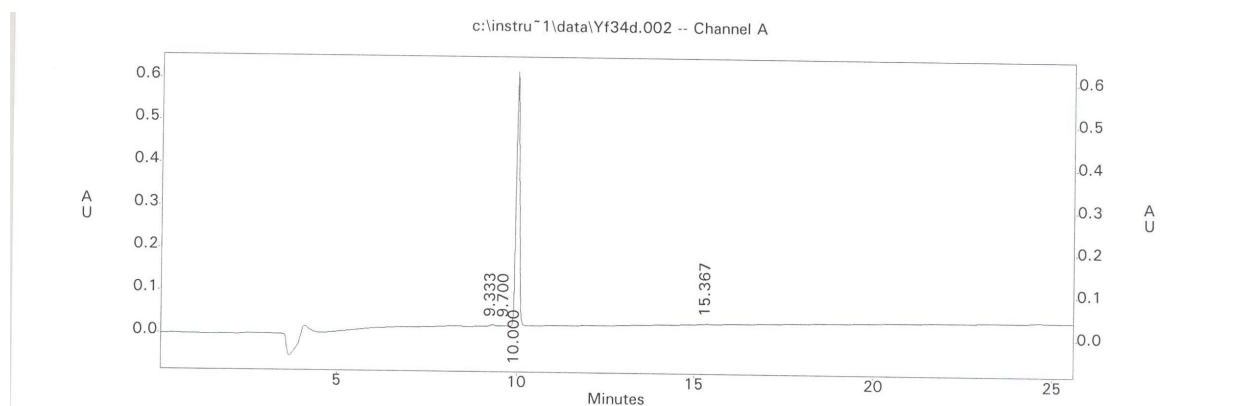


Fig. 7. HPLC of compound 6(R)

04-17-08_YF34_D01 #86-96 RT: 2.23-2.48 AV: 11 NL: 2.82E7
T: + c ESI Full ms [50.00-2000.00]

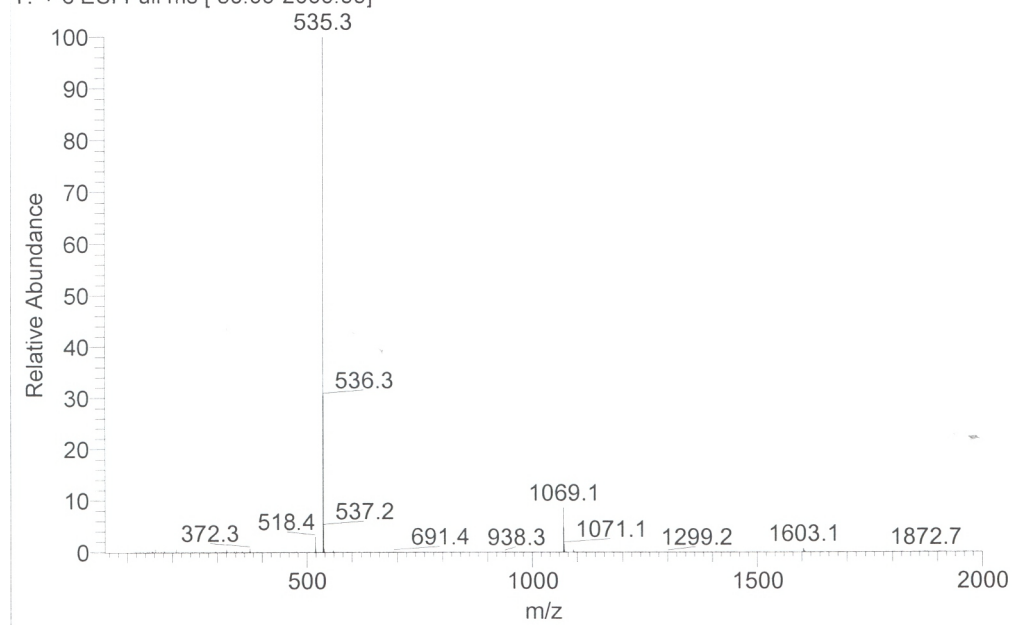


Fig. 8. Mass spectrum of compound 6(R)

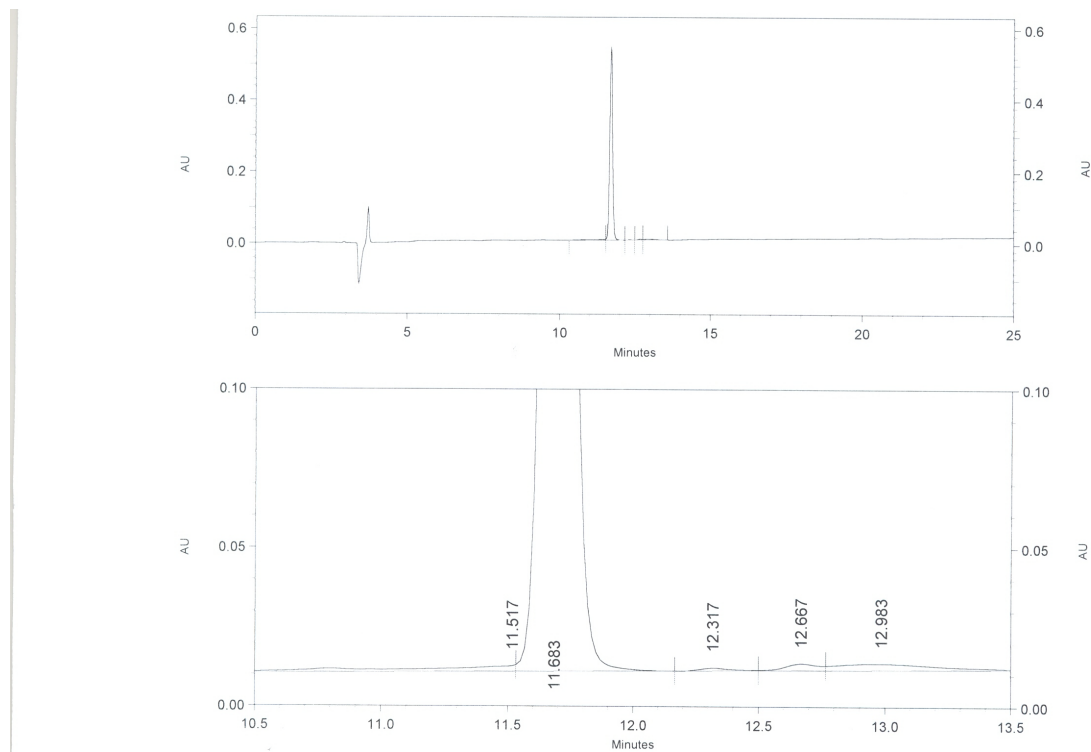


Fig. 9. HPLC of compound 7(S)

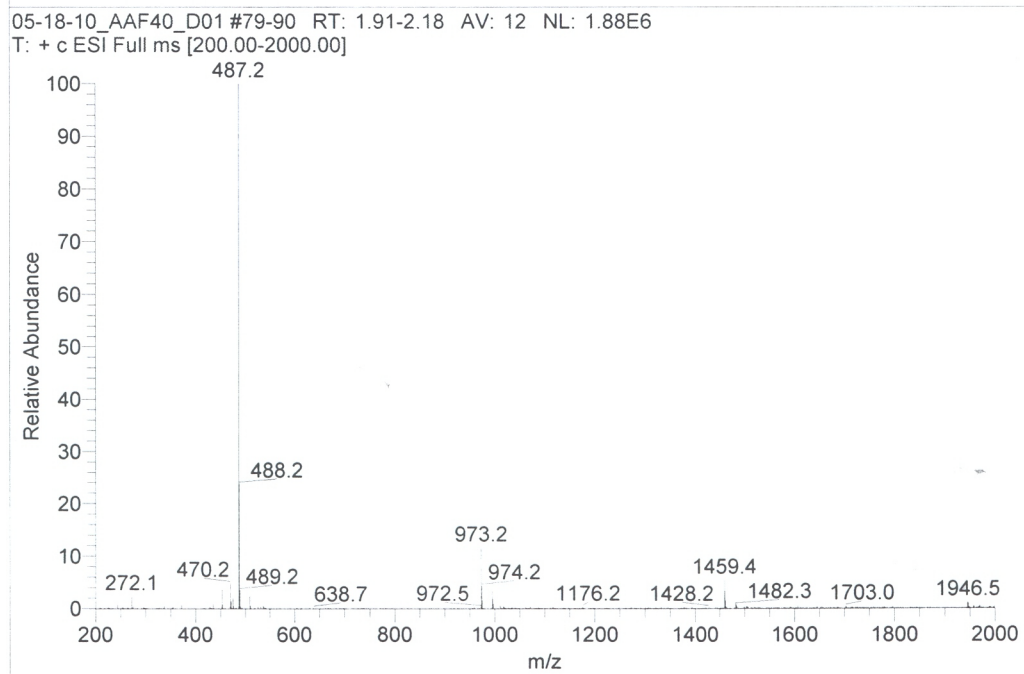


Fig. 10. Mass spectrum of compound 7(S)

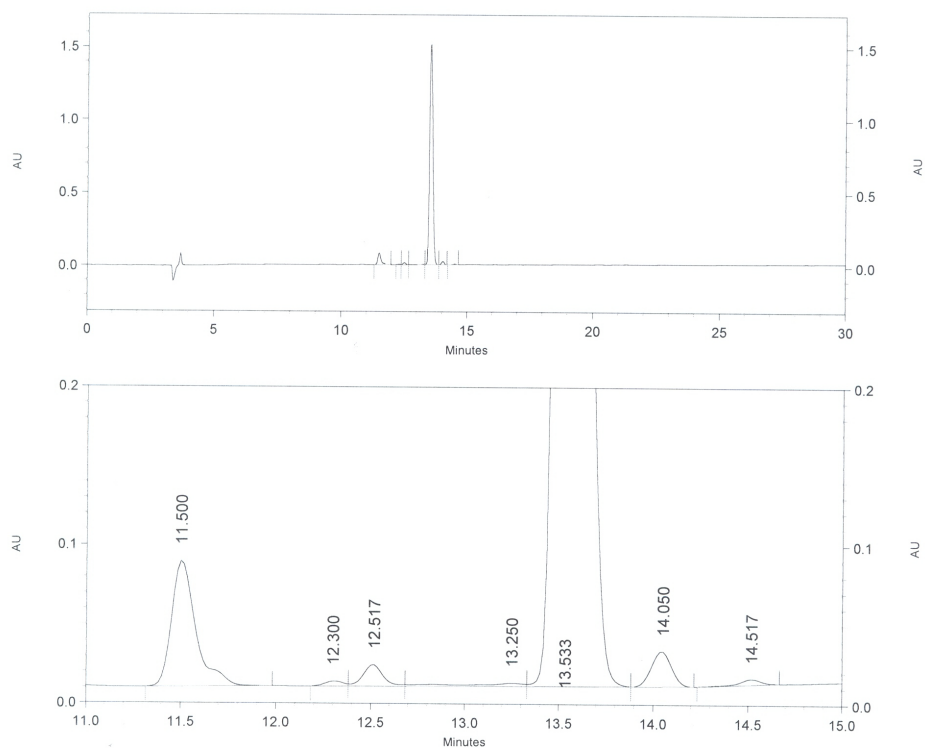


Fig. 11. HPLC of compound 7(R)

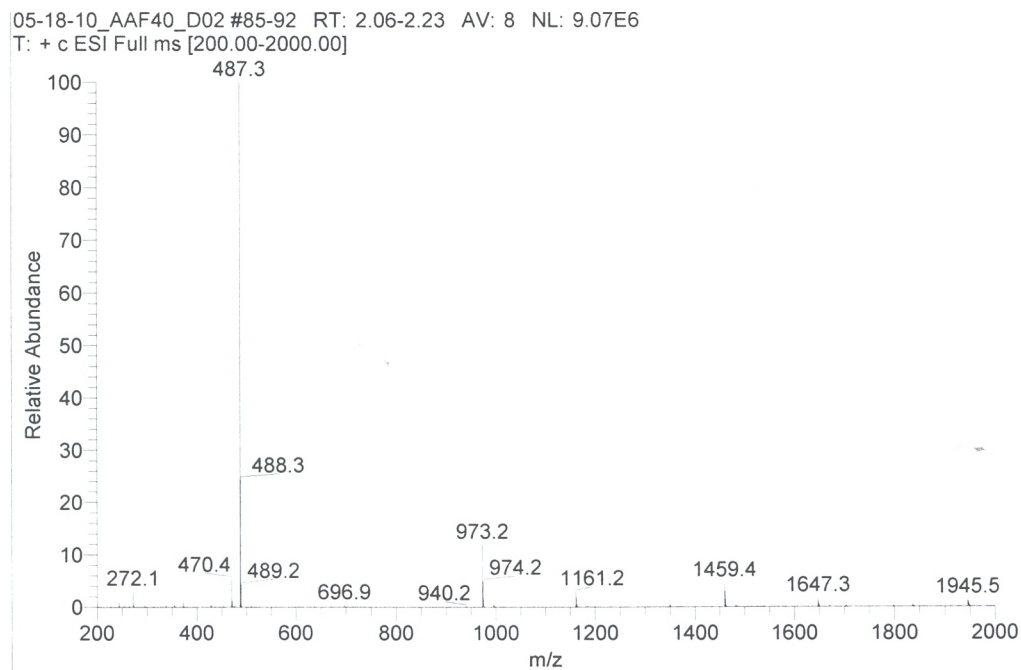


Fig. 12. Mass spectrum of compound 7(R)

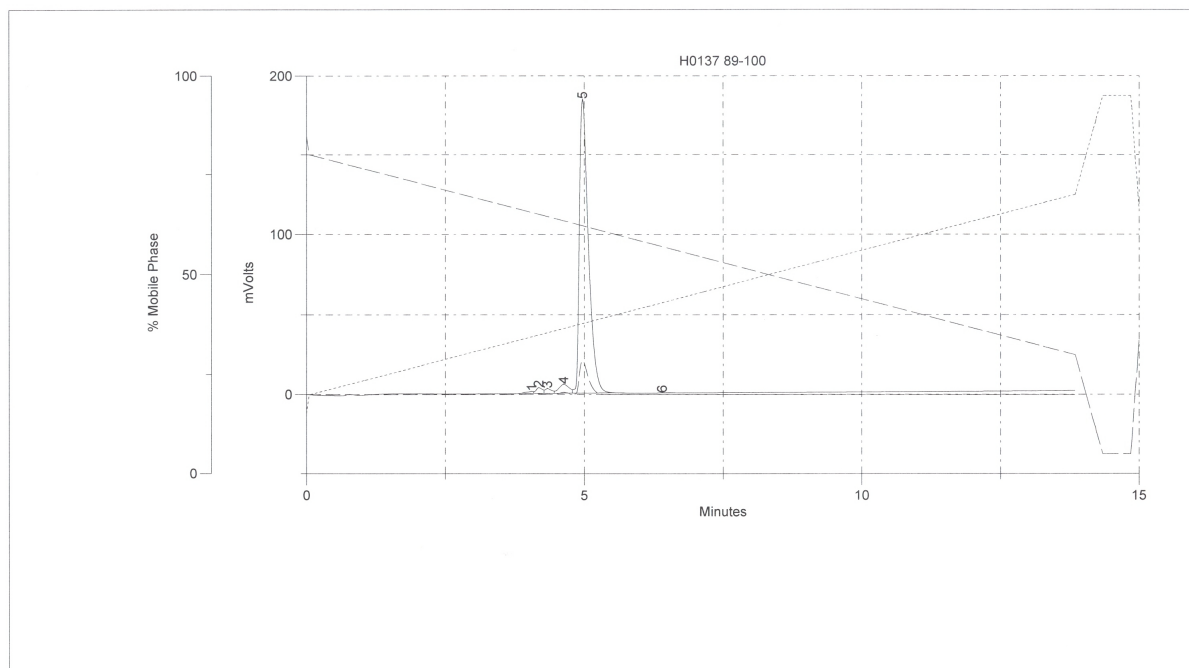


Fig. 13. HPLC of compound 8(S)

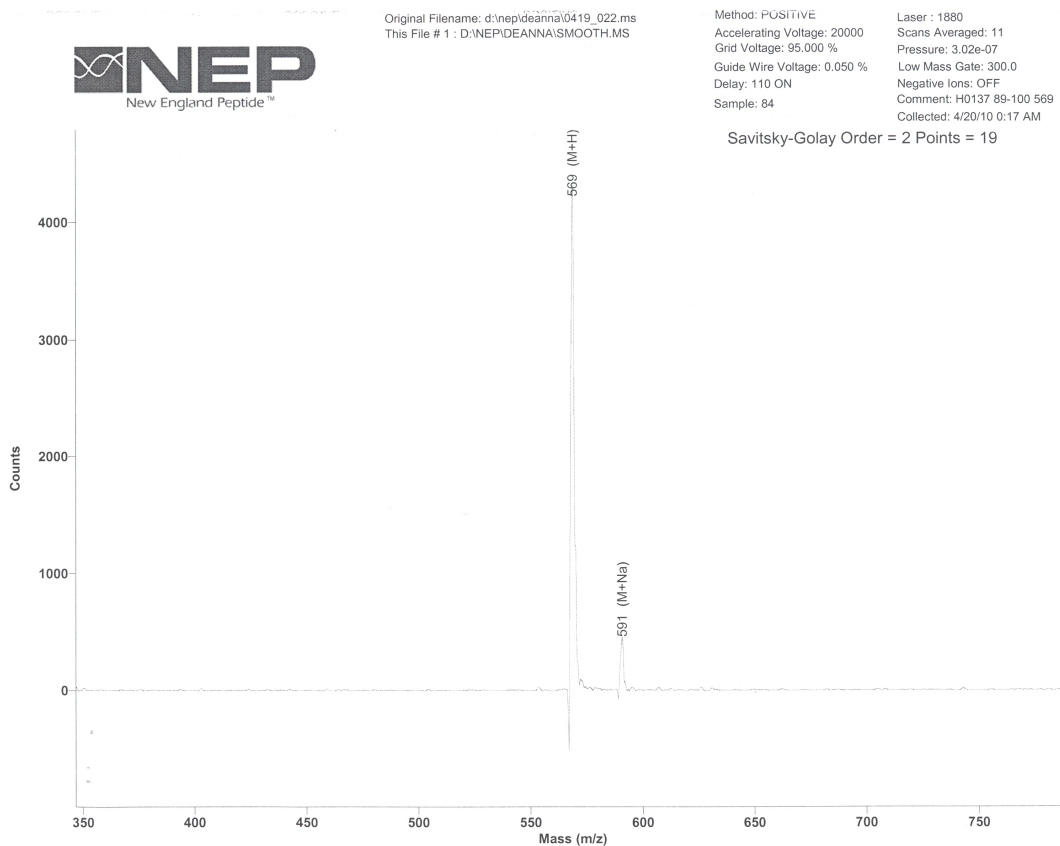


Fig. 14. Mass spectrum of compound 8(S)

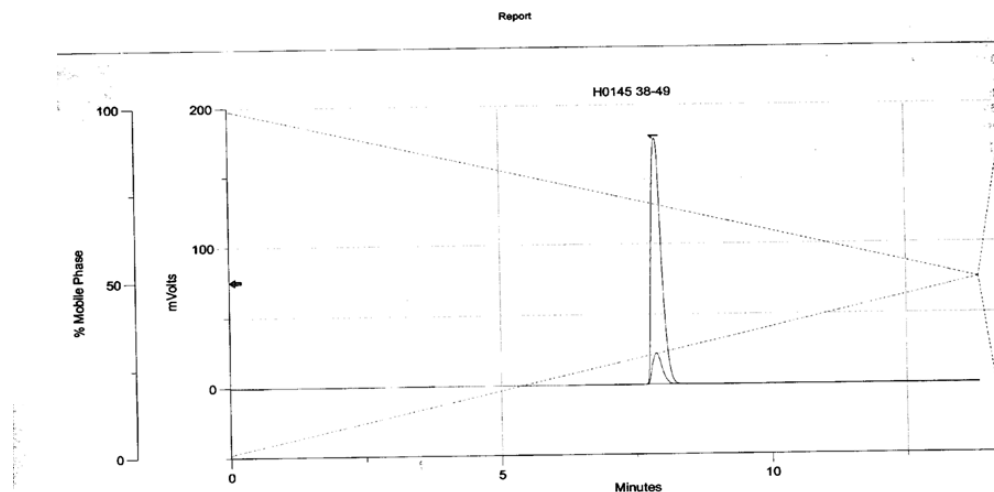


Fig. 15. HPLC of 9 compound (S)

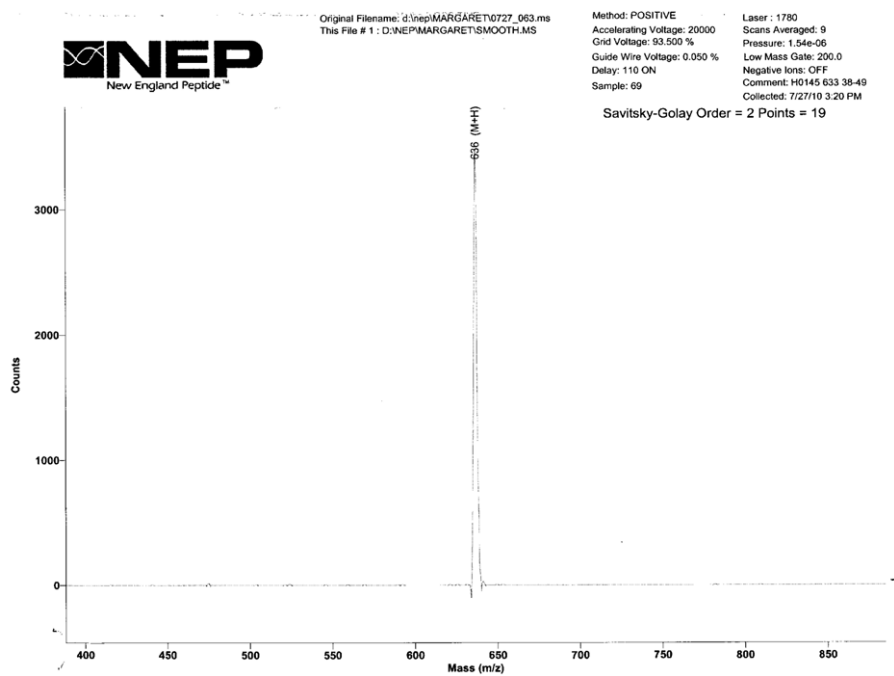


Fig. 16. Mass spectrum of compound 9(S)

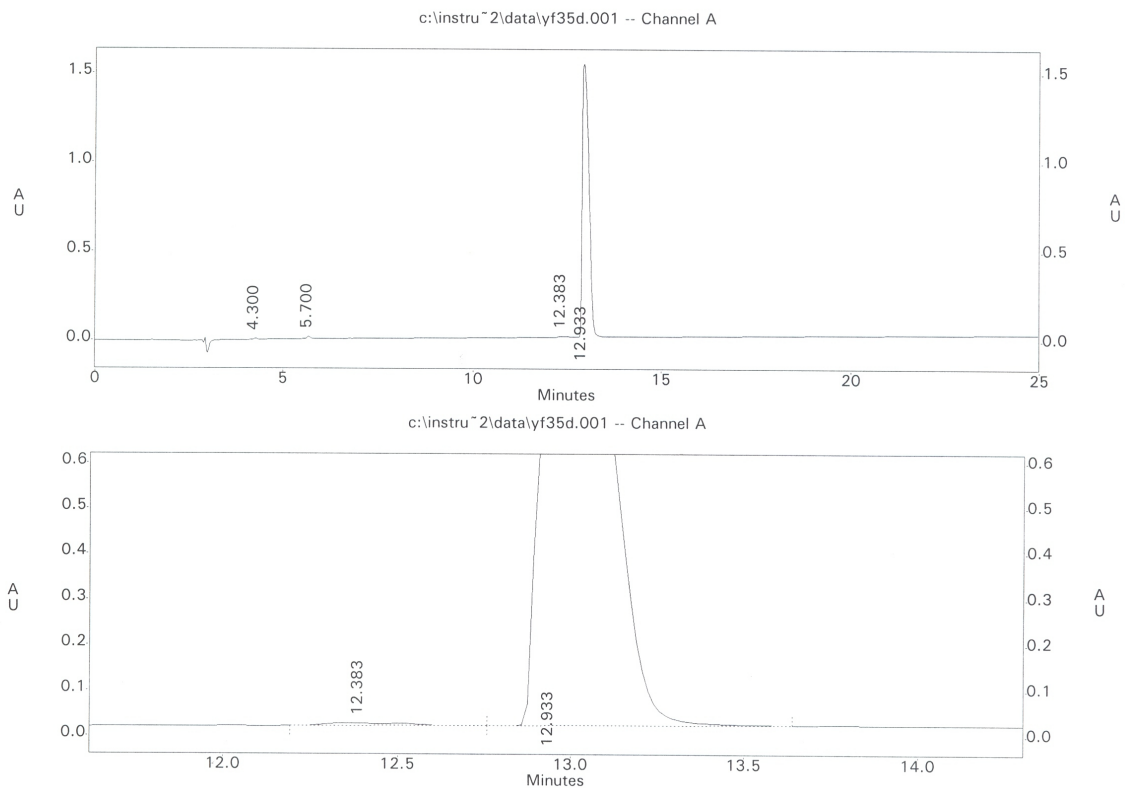


Fig. 17. HPLC of compound 10(S)

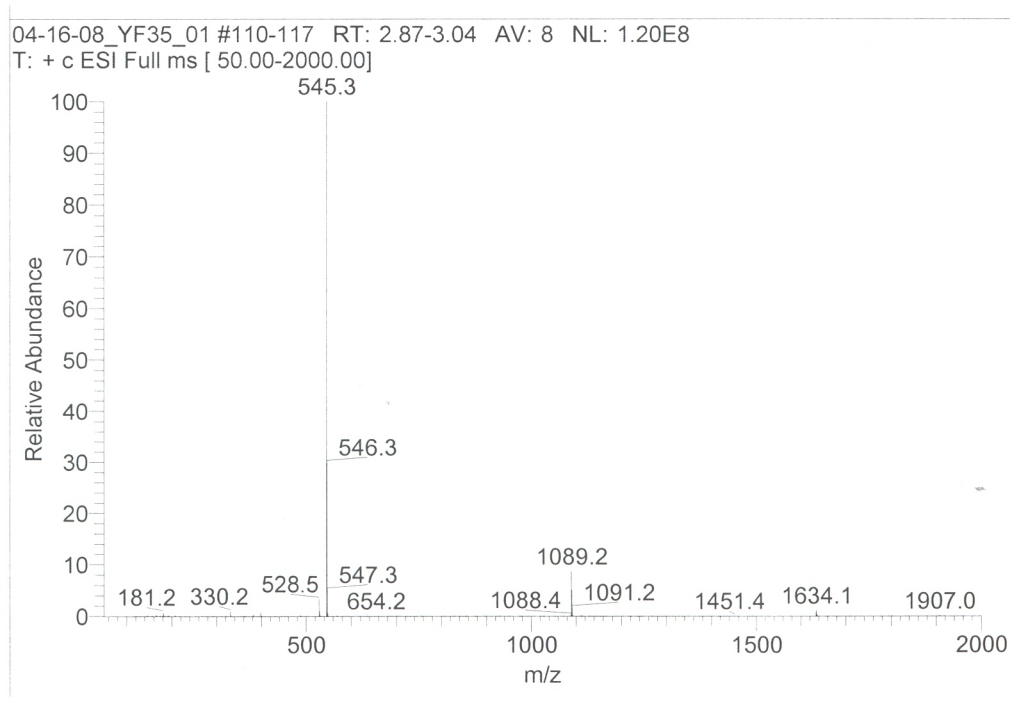


Fig. 18. Mass spectrum of compound 10(S)

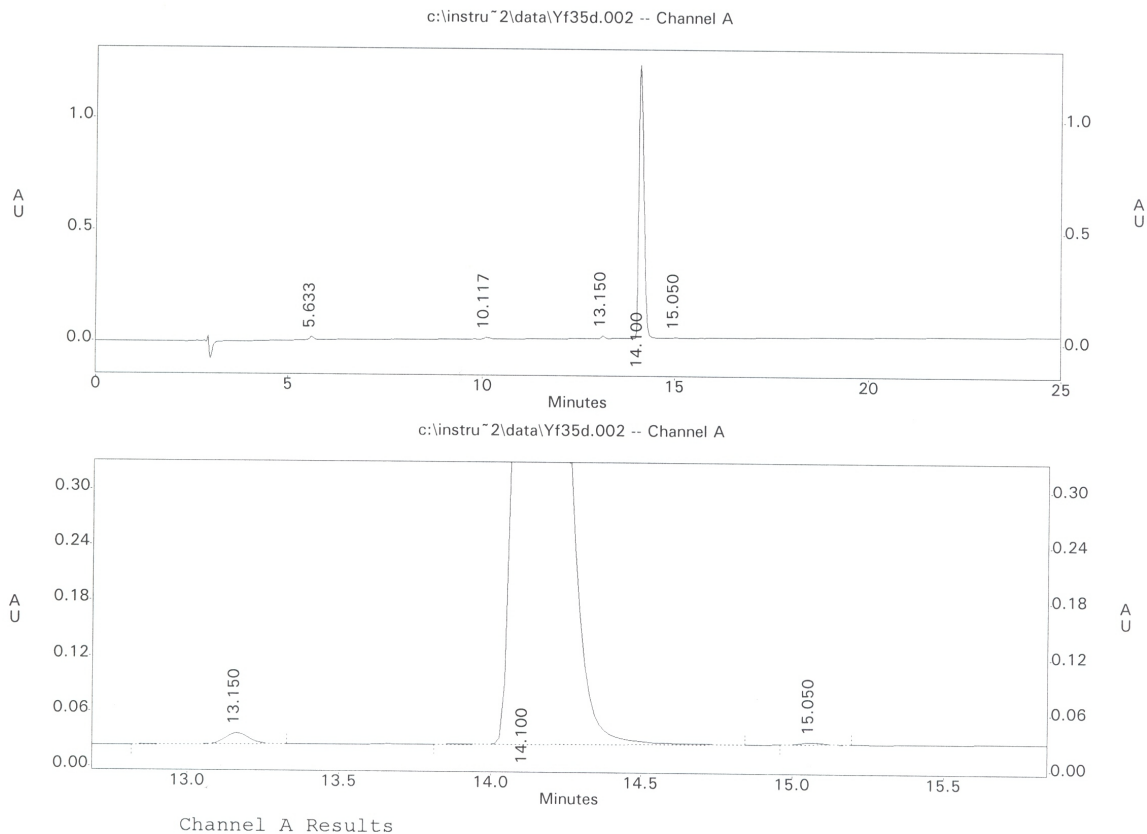


Fig. 19. HPLC of compound 10(R)

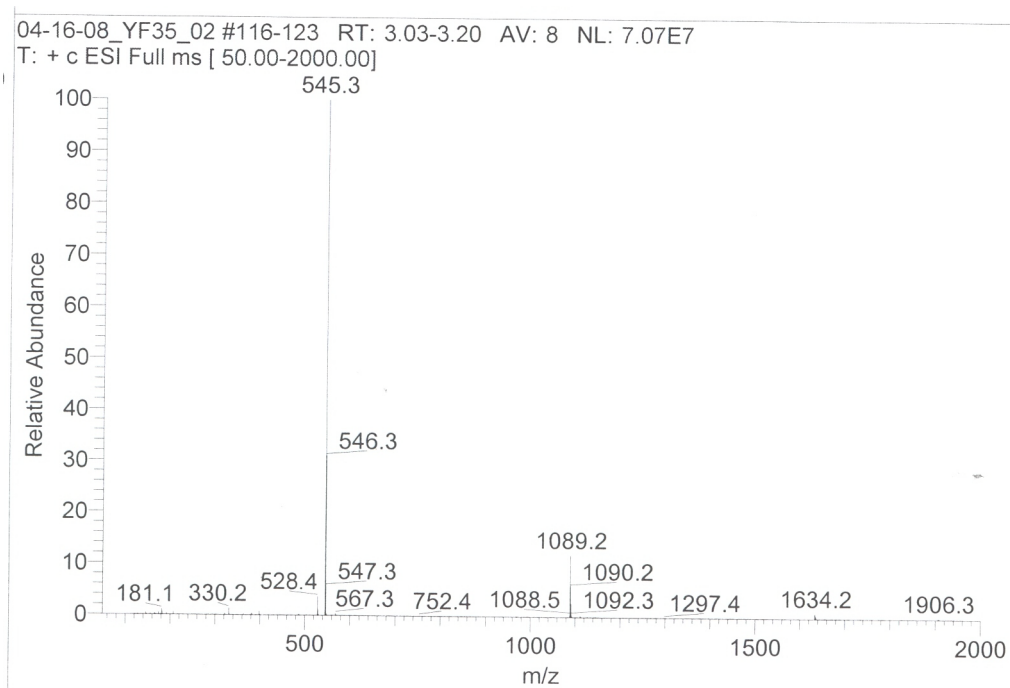


Fig. 20. Mass spectrum of compound 10(R)

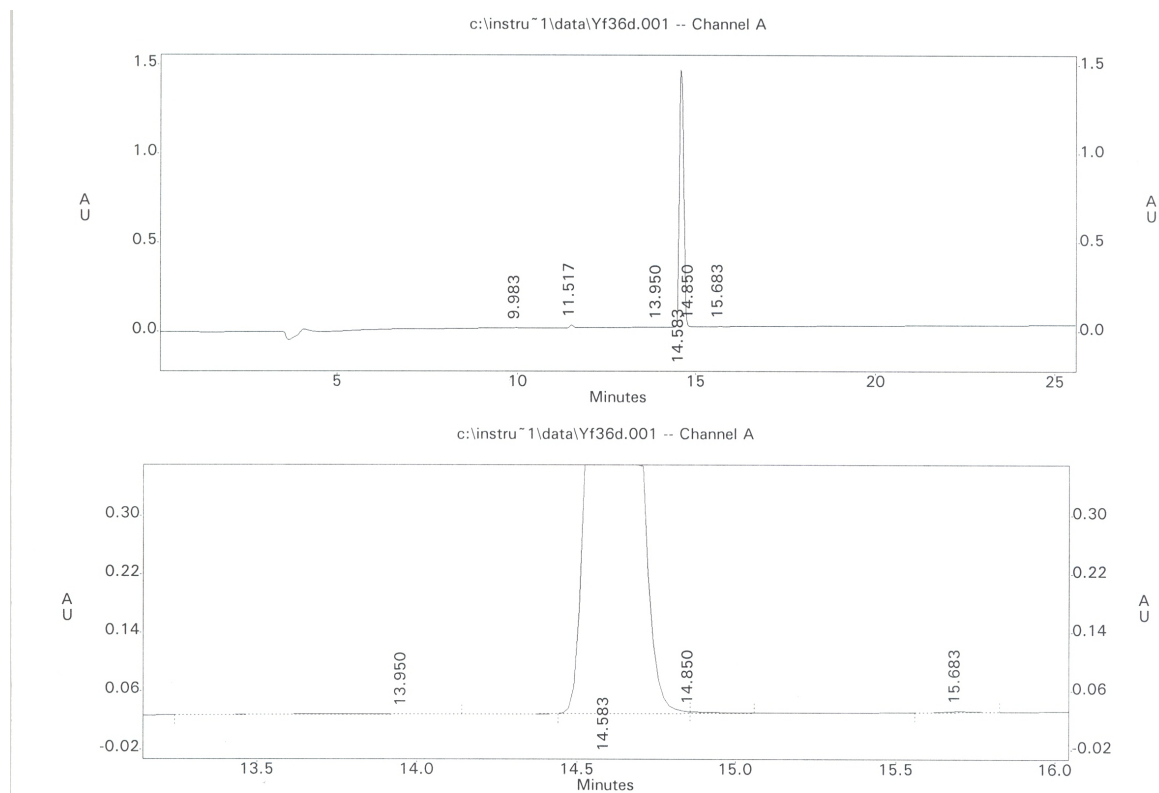


Fig. 21. HPLC of compound 11(S)

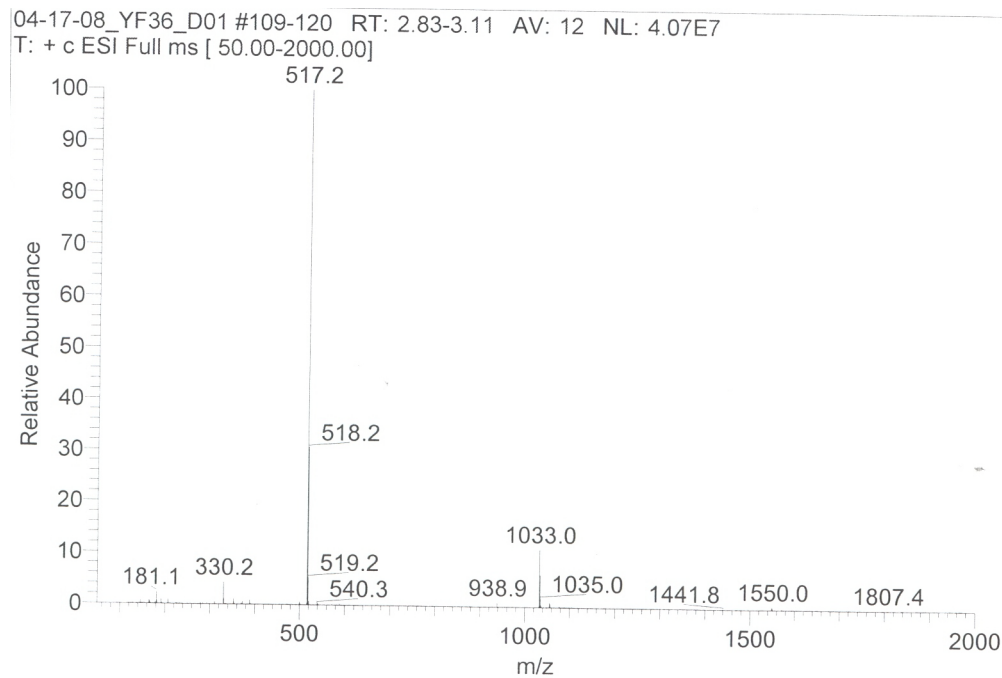


Fig. 22. Mass spectrum of compound 11(S)

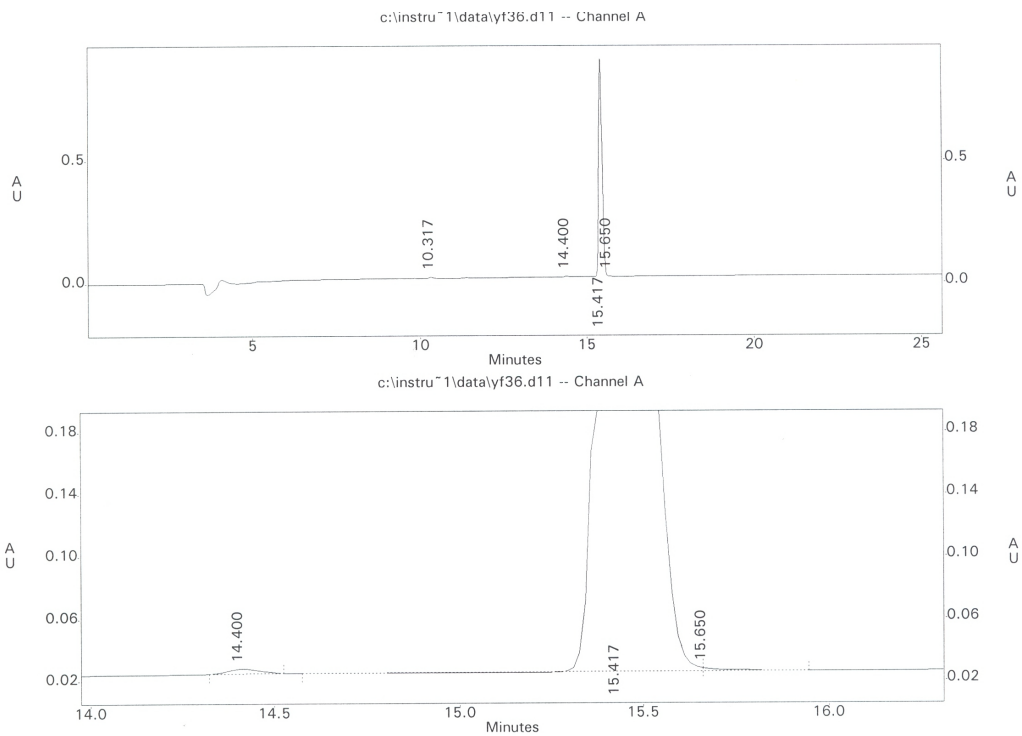


Fig. 23. HPLC of compound 11(R)

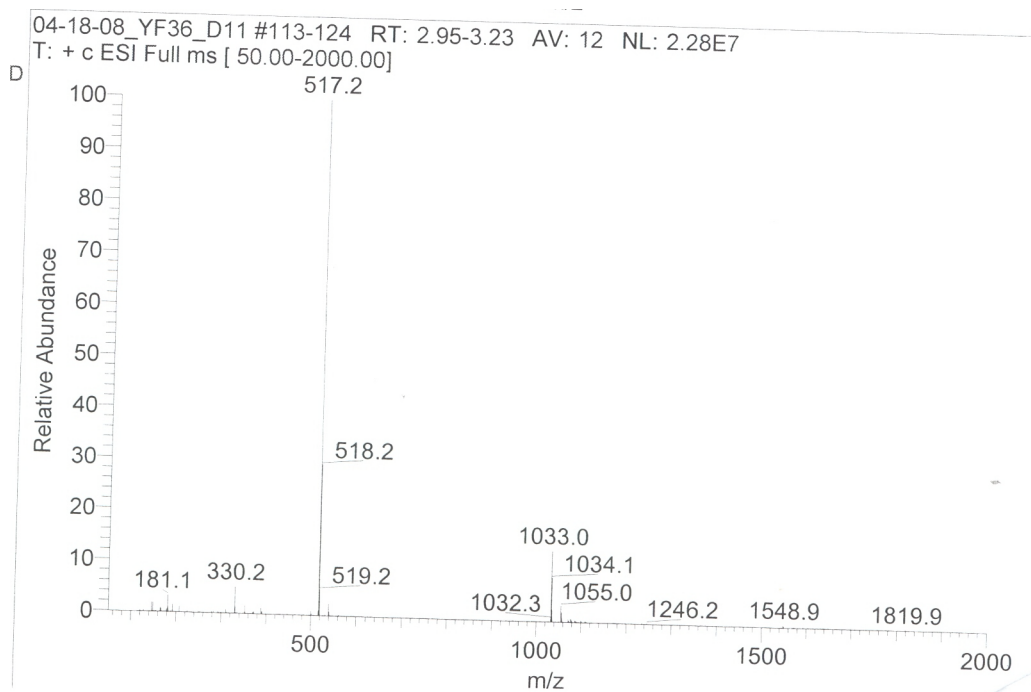
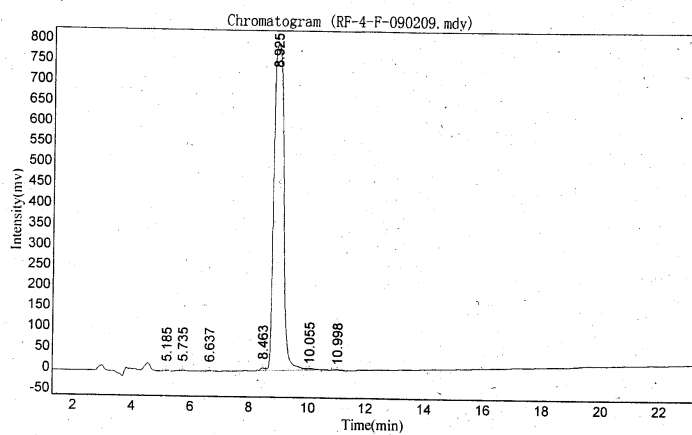


Fig. 24. Mass spectrum of compound 11(R)

Volume : 5ul



Results

Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		5.185	2034.454	17105.600	0.0927
2		5.735	2000.000	15728.002	0.0852
3		6.637	2024.648	16143.999	0.0875
4		8.463	6112.589	65516.766	0.3551
5		8.925	790578.125	18260086.000	98.9634
6		10.055	3074.224	55562.207	0.3011
7		10.998	1644.108	21216.004	0.1150
Total			807468.148	18451358.577	100.0000

Fig. 25. HPLC of compound 12(S)

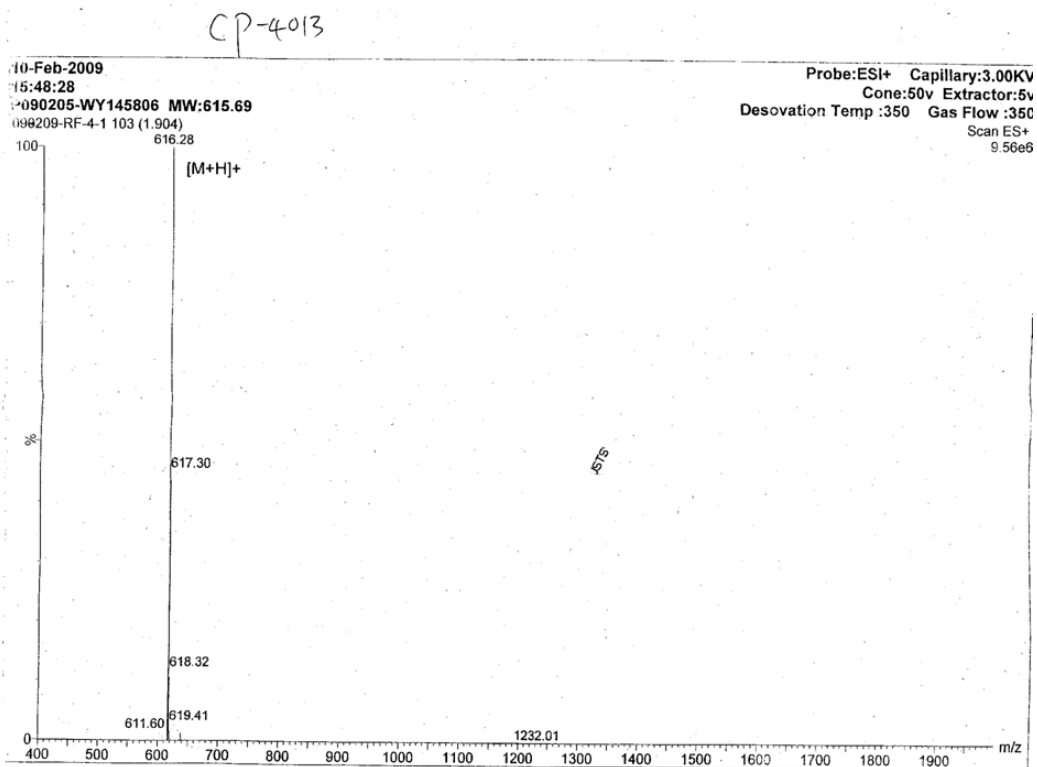
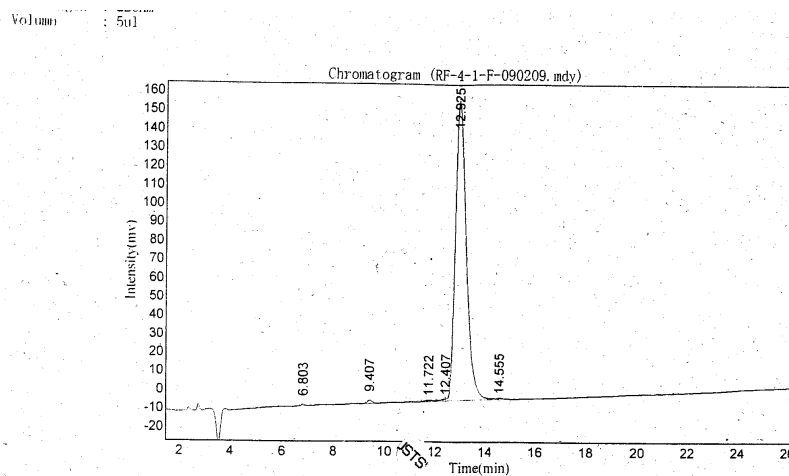


Fig. 26. Mass spectrum of compound 12(S)



Results

Peak No.	Peak ID	Ret Time	Height	Area	Conc.
1		6.803	748.351	6118.394	0.1226
2		9.407	1827.459	21246.398	0.4258
3		11.722	661.096	14848.227	0.2976
4		12.407	1094.085	15201.640	0.3046
5		12.925	161319.844	4917201.000	98.5390
6		14.555	554.265	15493.111	0.3105
Total			166205.100	4990108.770	100.0000

Fig. 27. HPLC of compound 12(R)

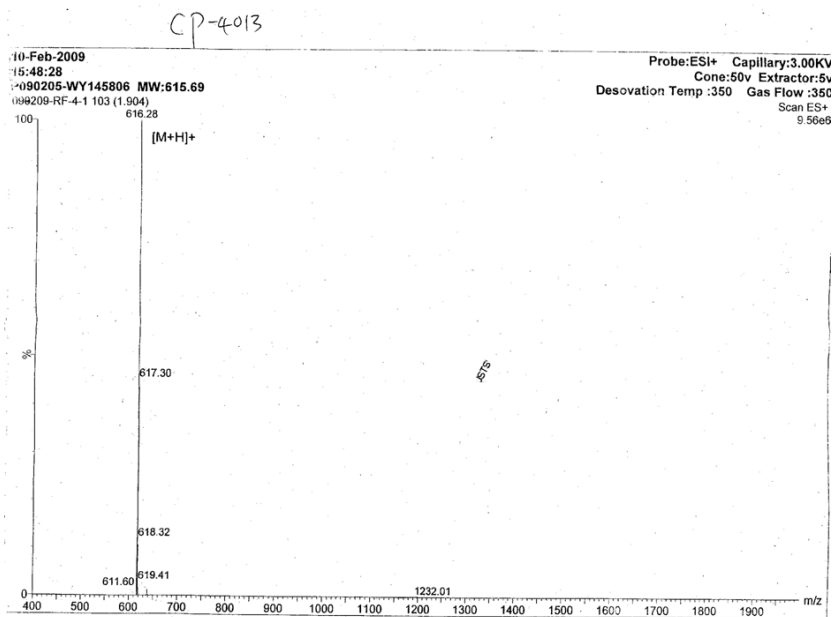


Fig. 28. Mass spectrum of compound 12(R)

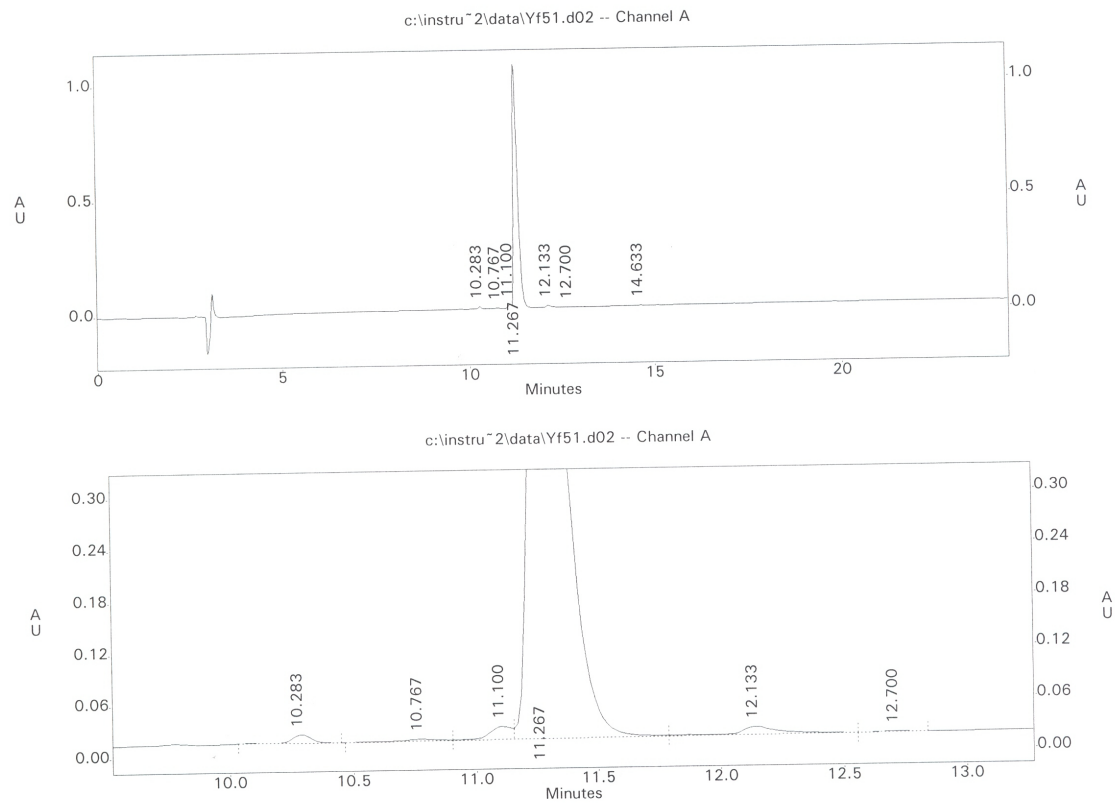


Fig. 29. HPLC of compound 13(S)

06-03-08_YF51_01 #92-99 RT: 2.34-2.52 AV: 8 NL: 4.26E6
T: + c ESI Full ms [50.00-2000.00]

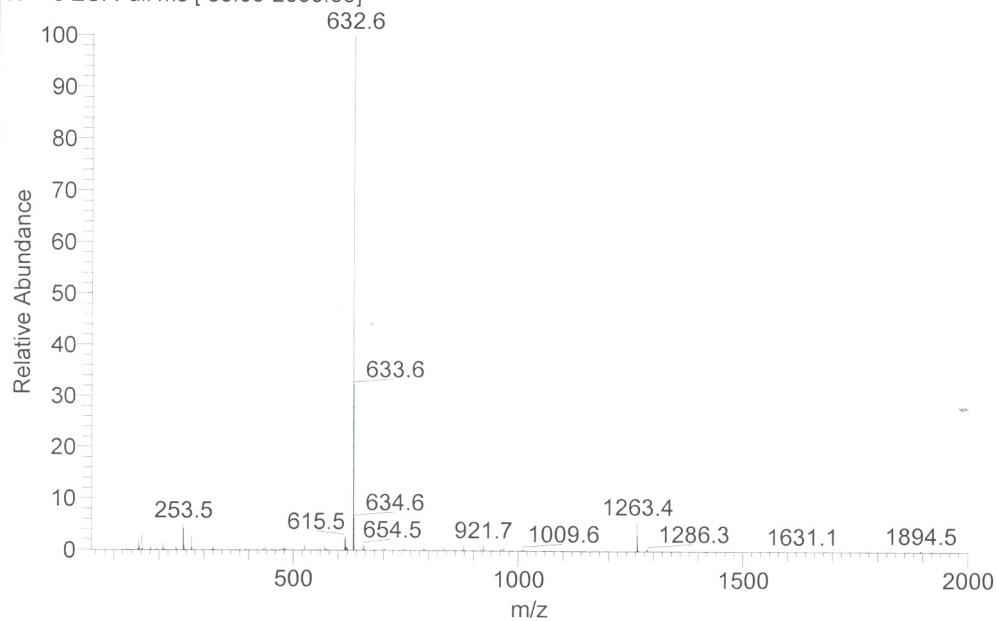


Fig. 30. Mass spectrum of compound 13(S)

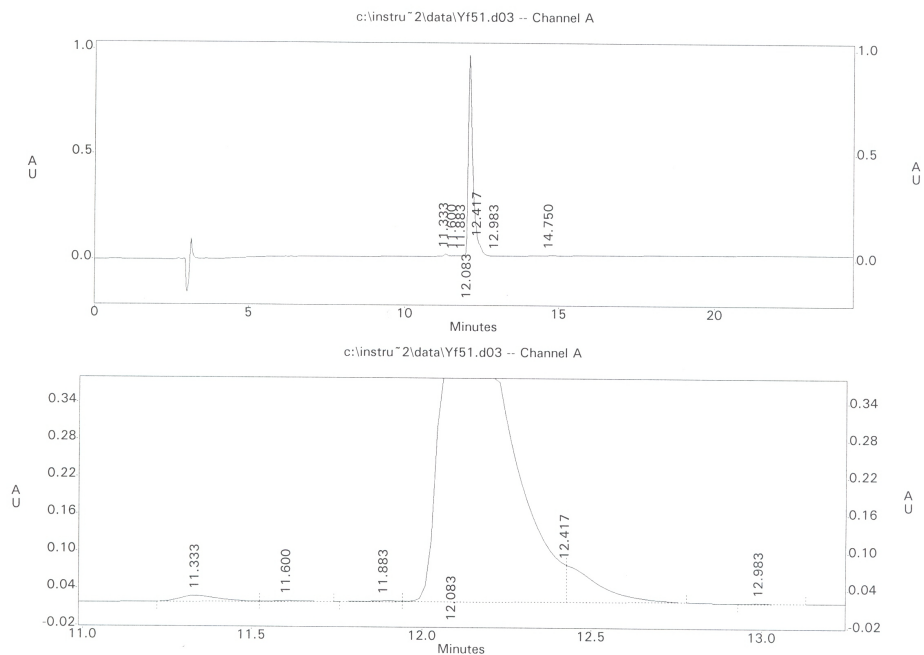


Fig. 31. HPLC of compound 13(R)

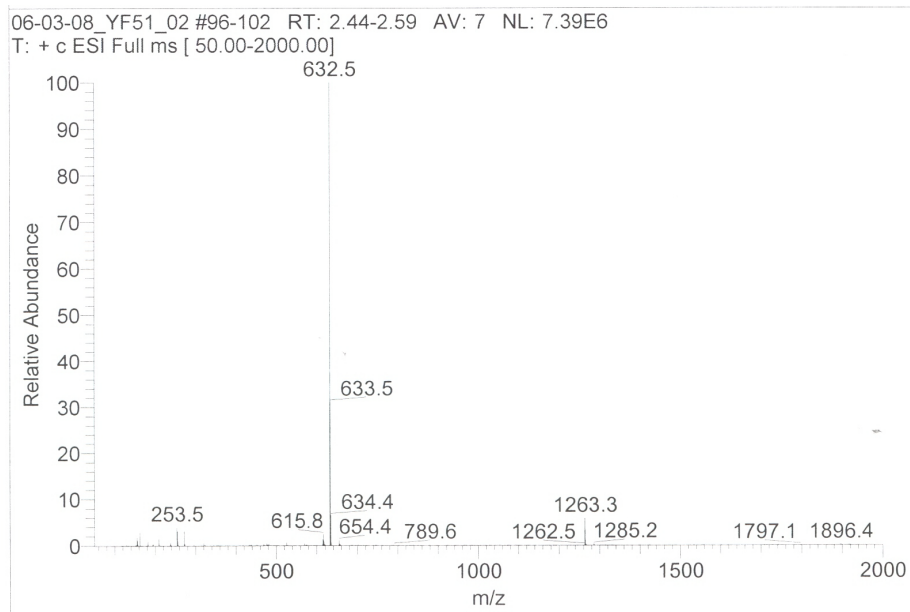


Fig. 32. Mass spectrum of compound 13(R)

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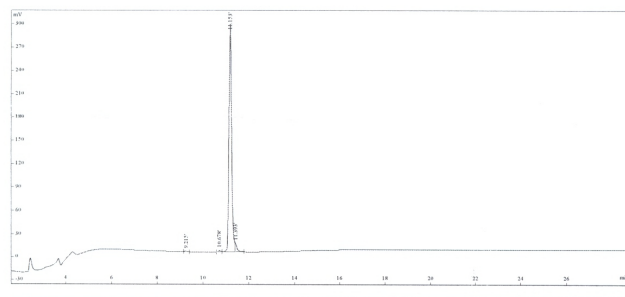


Fig. 33. HPLC of compound 14(S)

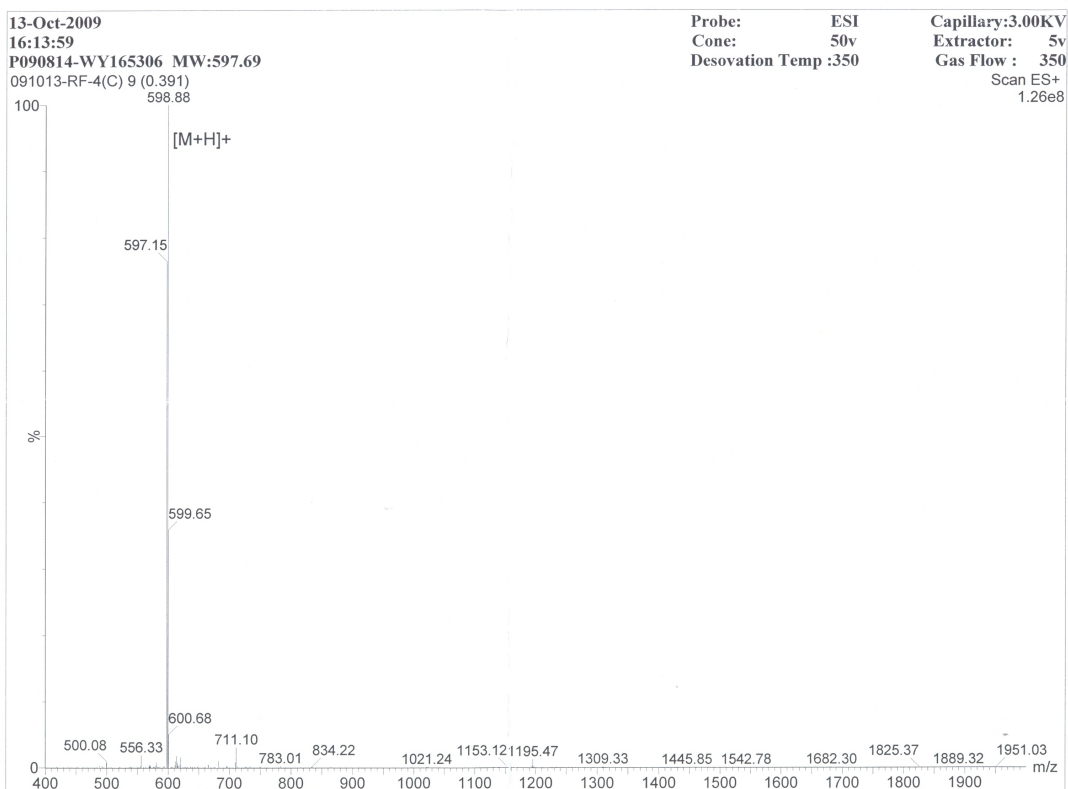


Fig. 34. Mass spectrum of compound 14(S)

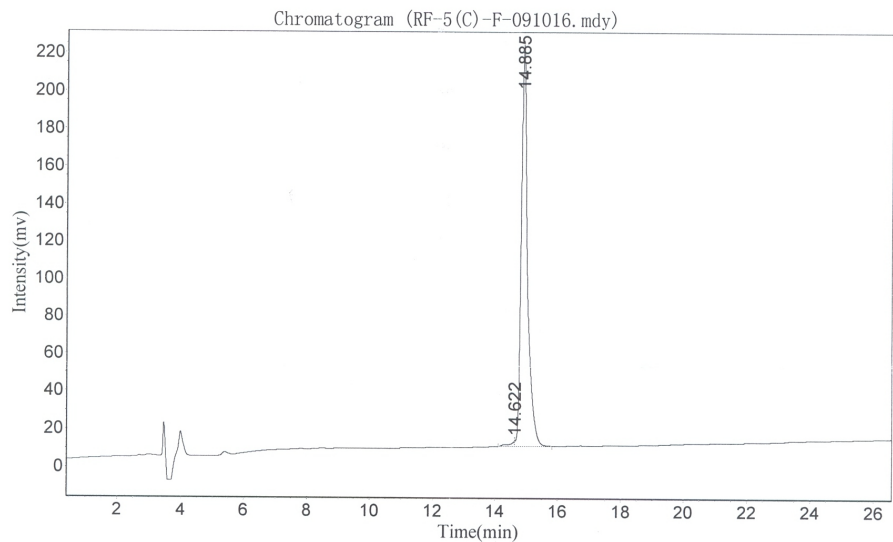
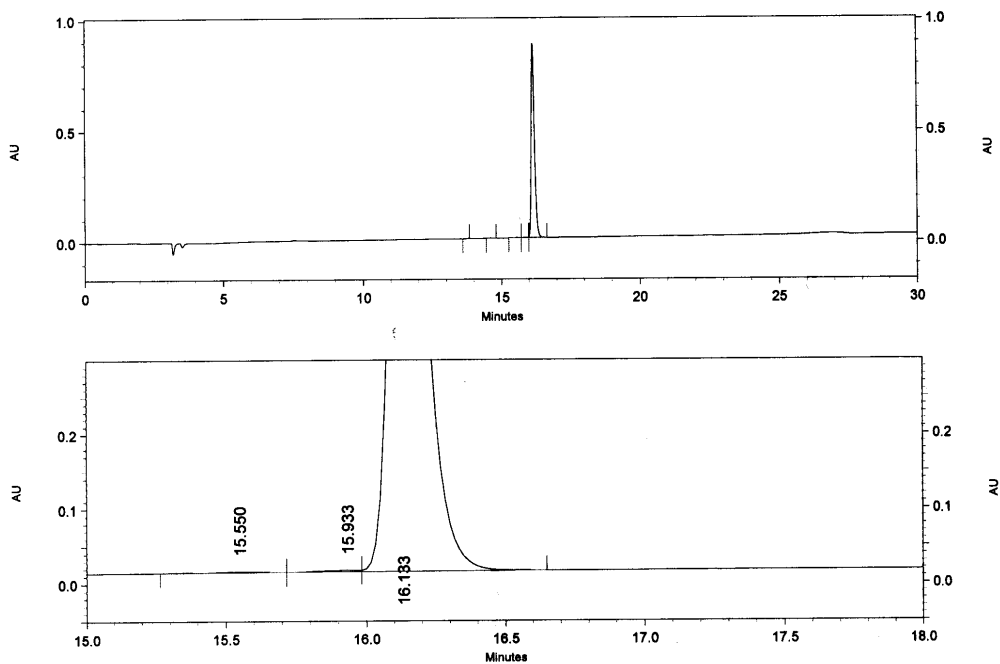


Fig. 35. HPLC of compound 15(S)



Fig. 36. Mass Spectrum of 15(S)



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Fig. 37. HPLC of compound 16(S)

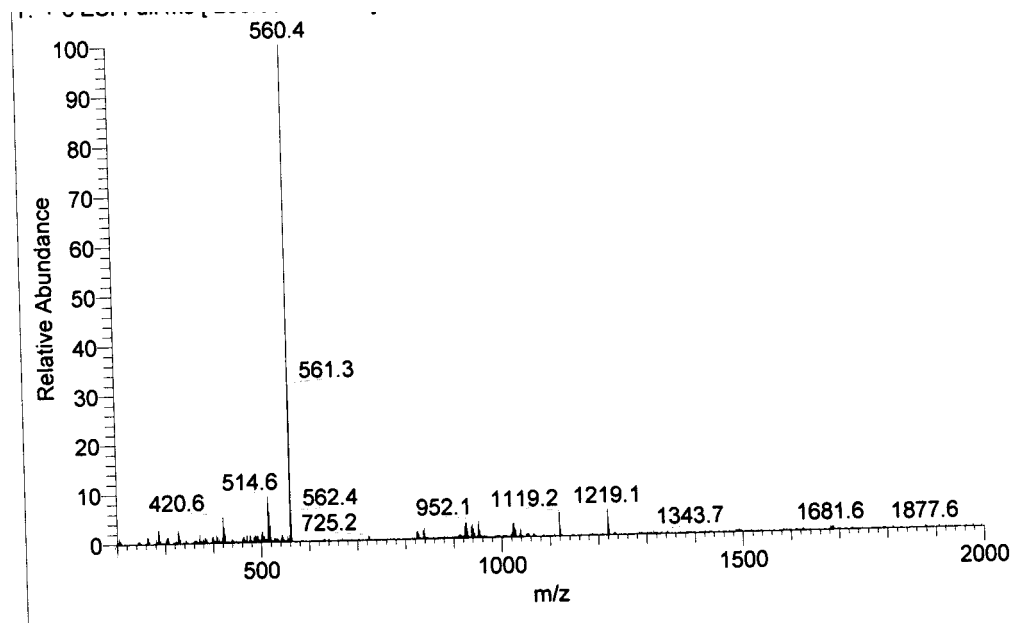


Fig. 38. Mass Spec of compound 16(S)

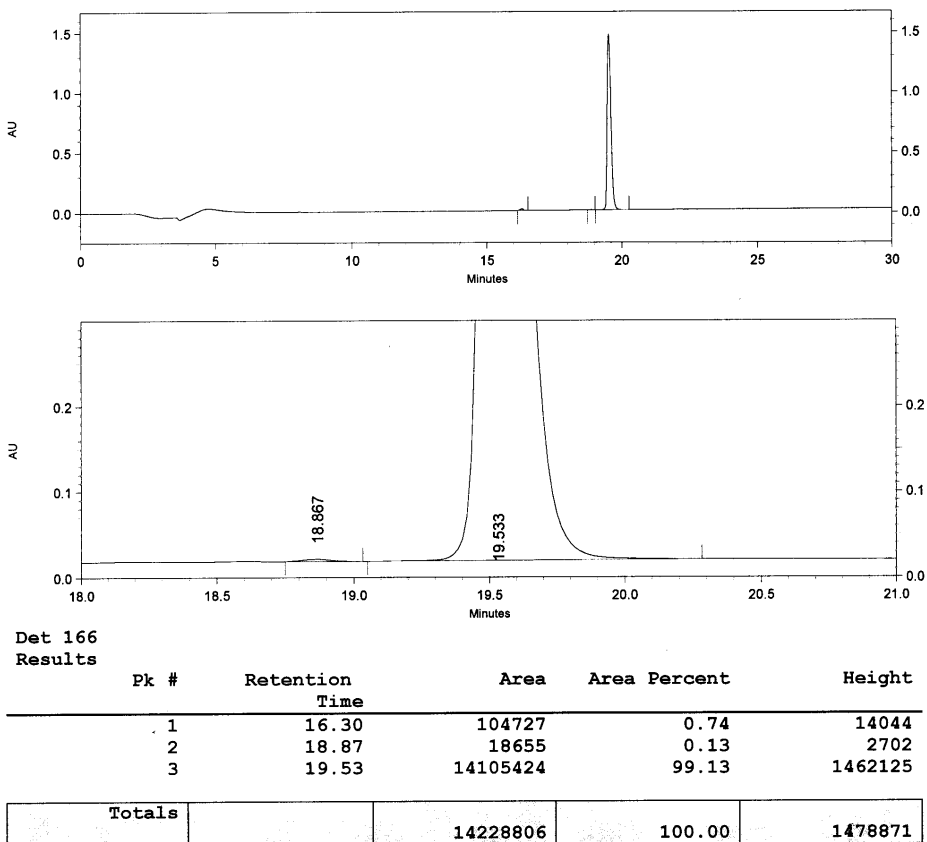


Fig. 39. HPLC of compound 16(R)

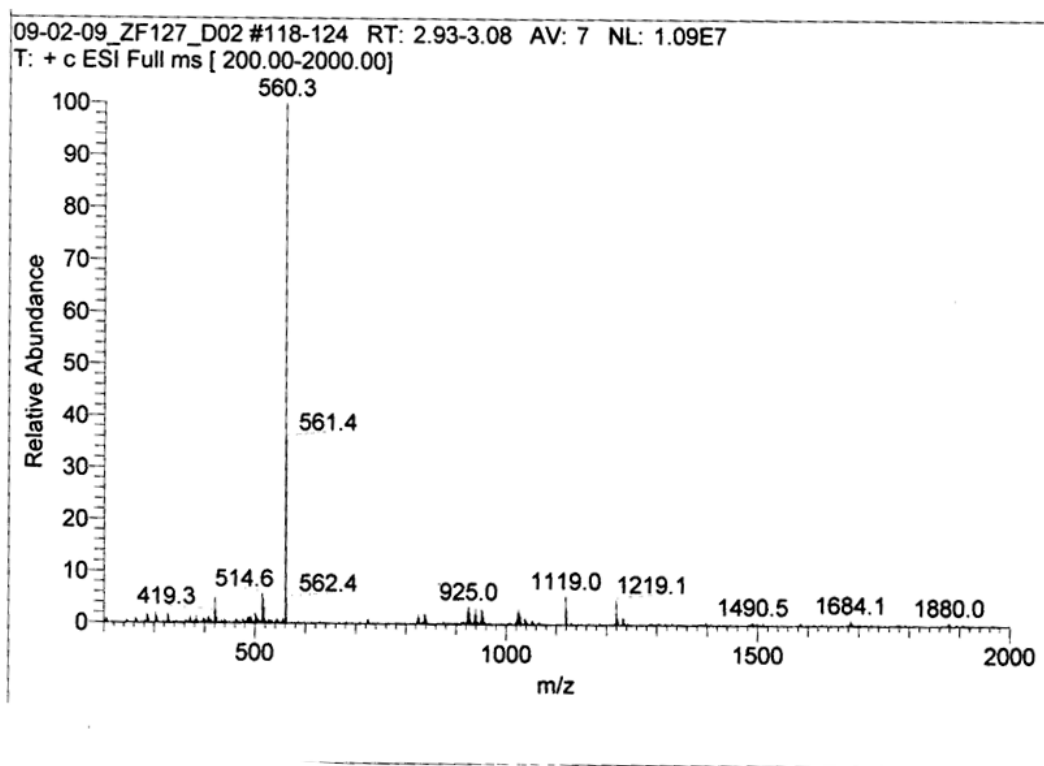


Fig. 40. Mass spectrum compound 16(R)

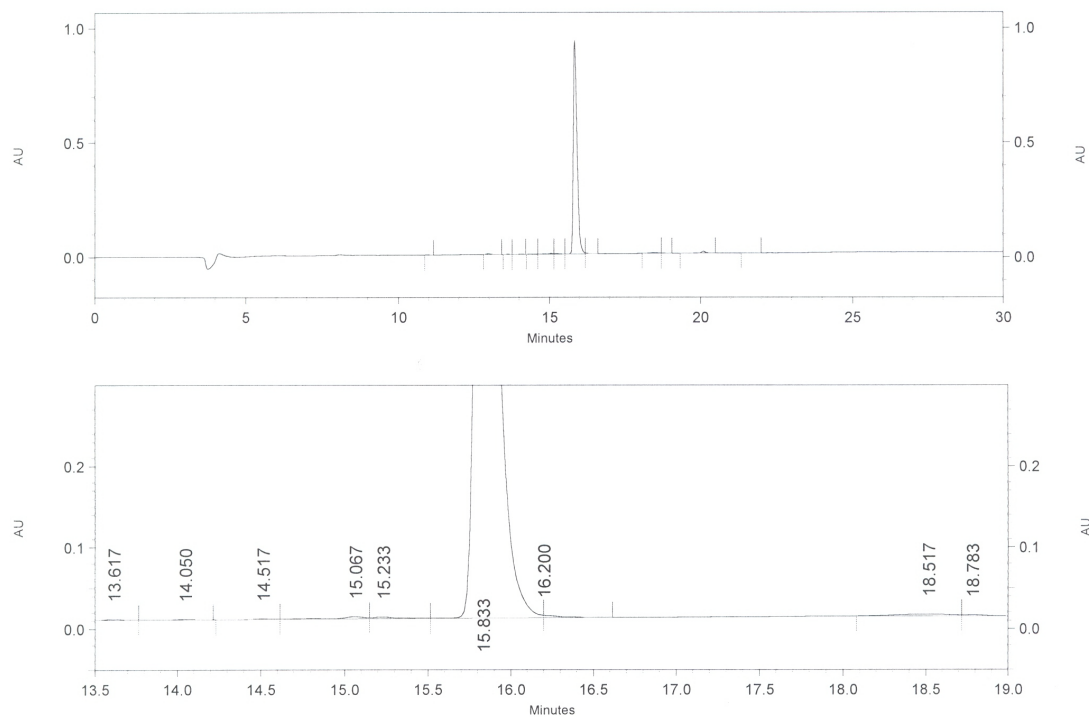


Fig. 41. HPLC of compound 17(S)

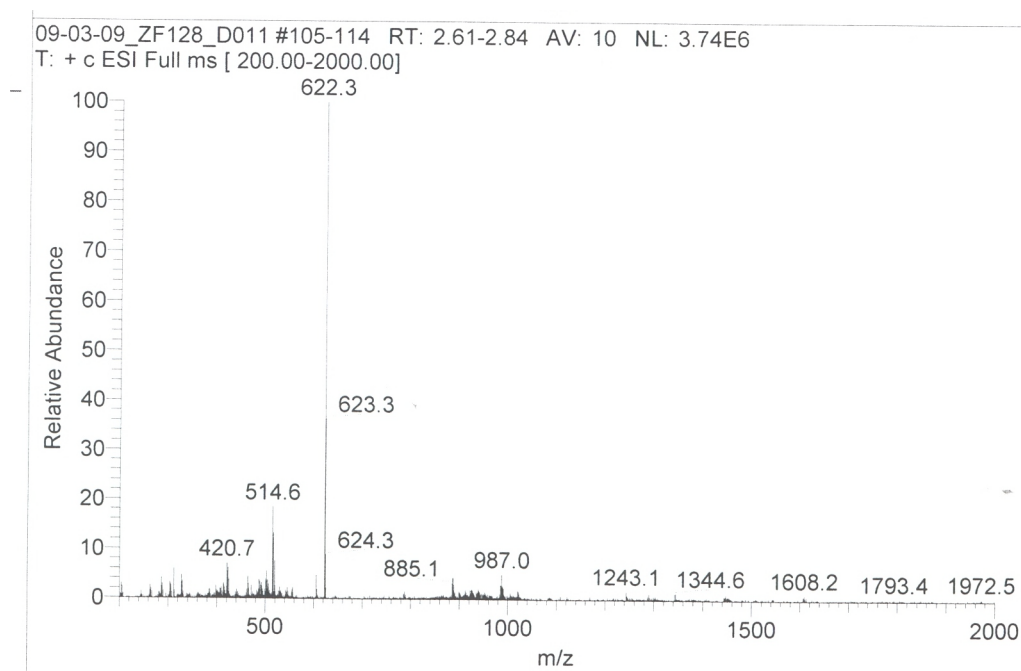


Fig. 42. Mass spectrum of 17(S)

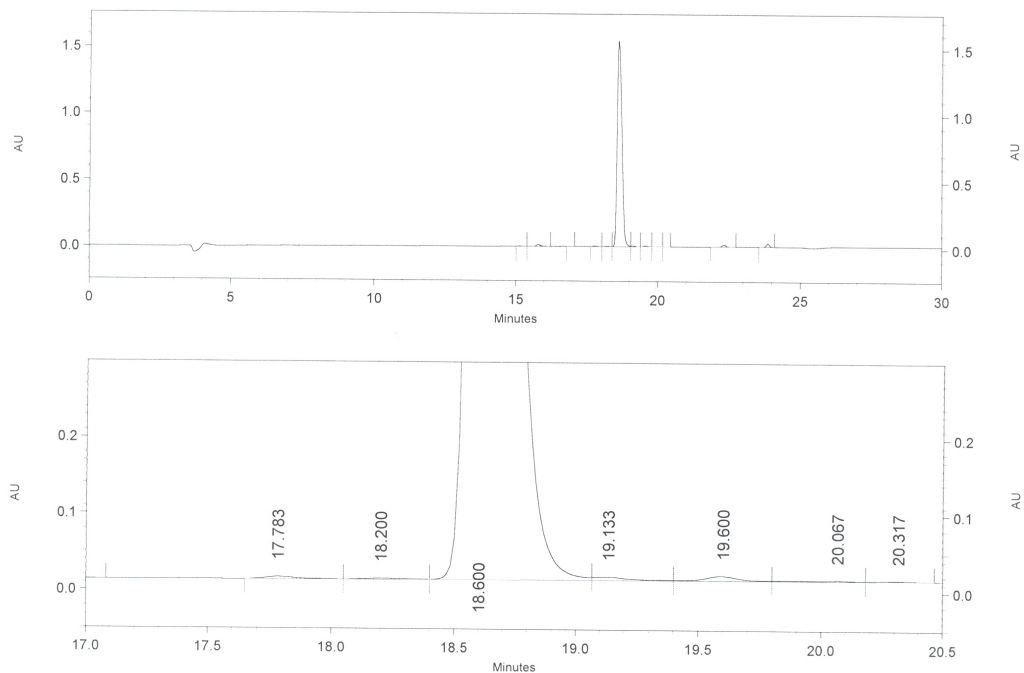


Fig. 43. HPLC of compound 17(R)

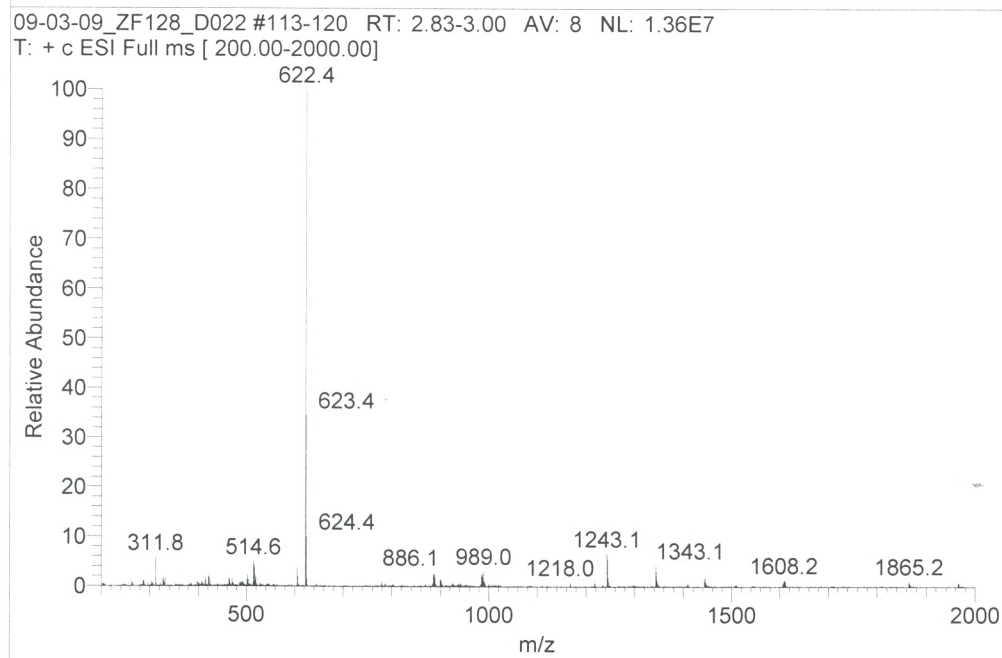
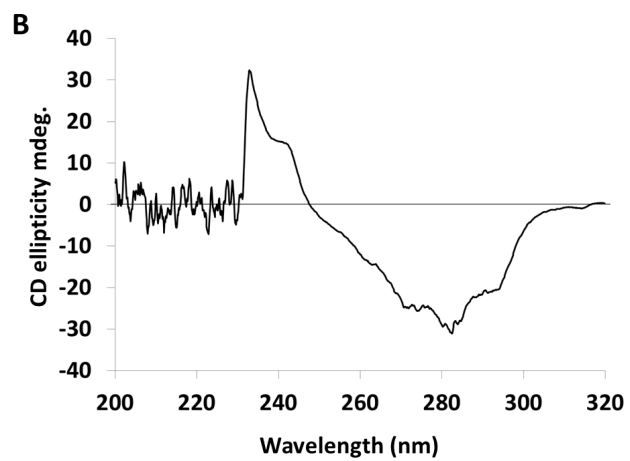
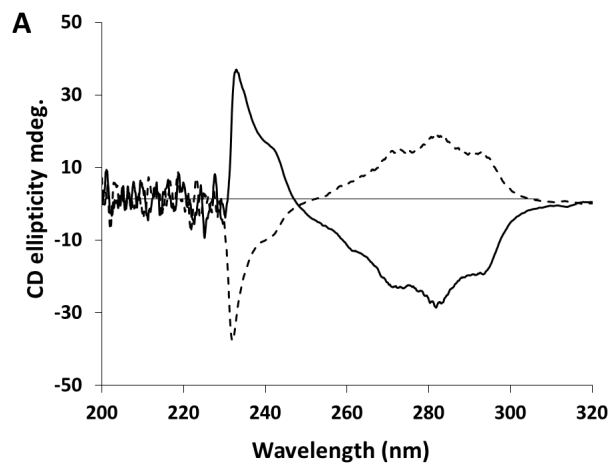
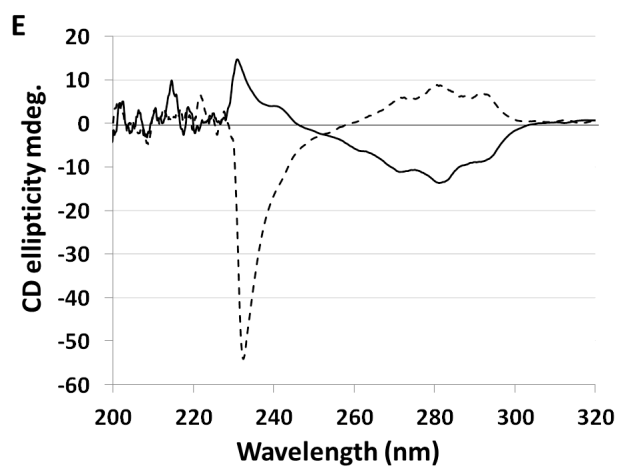
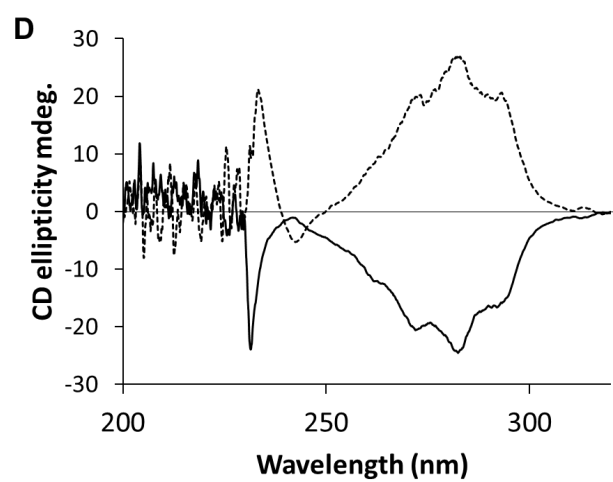
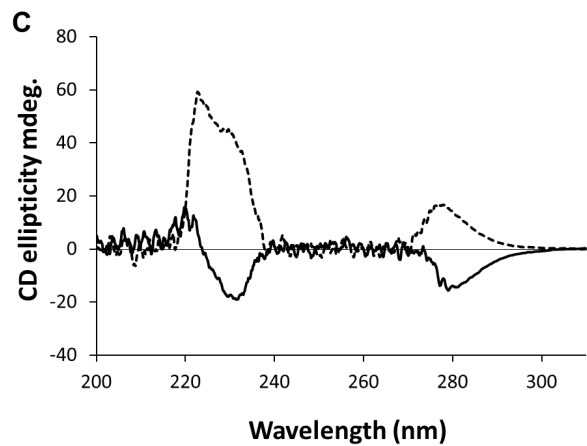


Fig. 44. Mass spectrum 17(R)





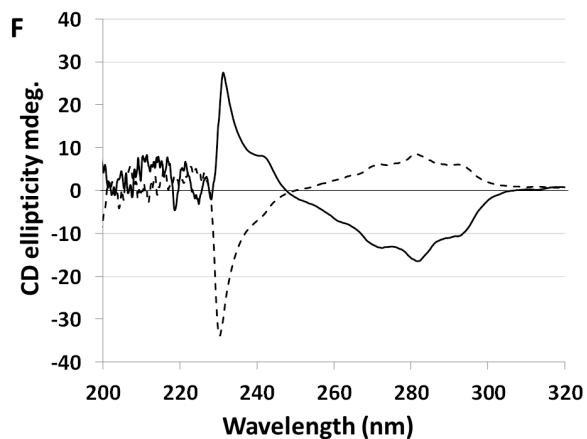


Fig. 45. CD spectra of compound **5** and its analogs in water. For synthesis of compounds **5**, **9**, **14** and **15** β -amino acid used had *S* chirality. For other compounds described in this report, β -amino acid used was a racemic mixture. During purification by HPLC, the epimers could be separated. Chirality of the epimers was identified by CD spectra. For reference CD spectra of compound **5** was used. A) compound **5**, solid line represents the spectra of compound with *S* chirality at β -amino acid. Dashed line represents CD spectra of compound **5** with *R* chirality at β -amino acid. B) compound **9(S)**, C) compounds **10(S)** and **10(R)**, D) **12(S)** and **12(R)**, E) **16(S)** and **16(R)** F) **17(S)** and **17(R)**. Dashed lines represent compounds with *R* configuration at the β -amino acid.

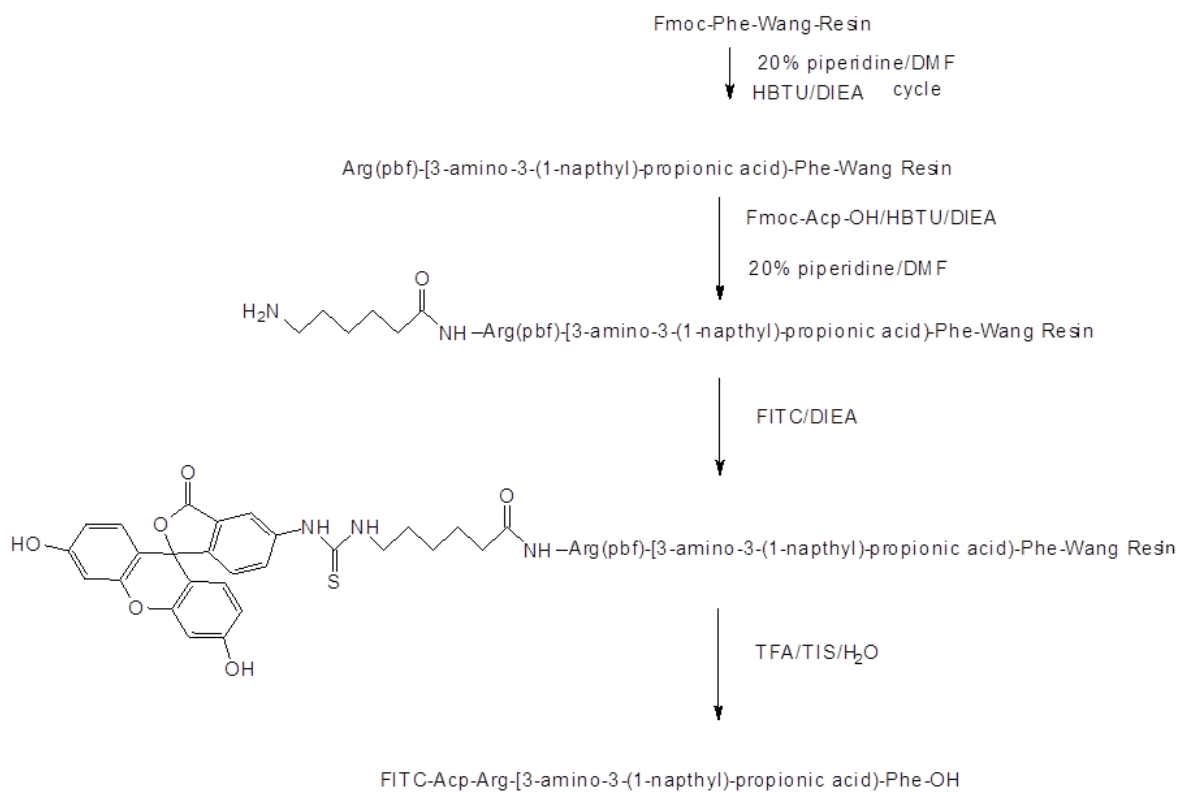


Fig. 46. Schematic diagram of synthesis of FITC-5. Amino acids used had L-chirality.