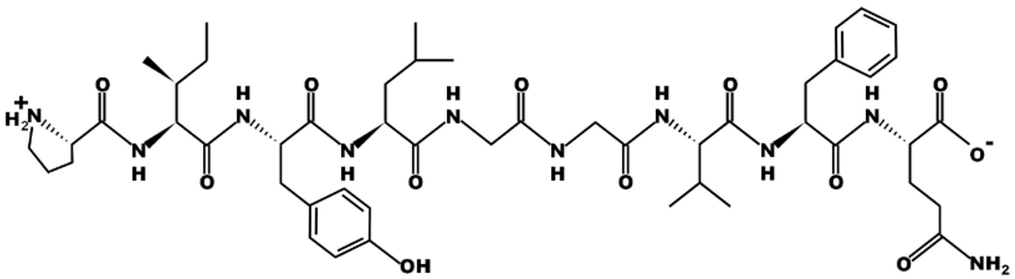
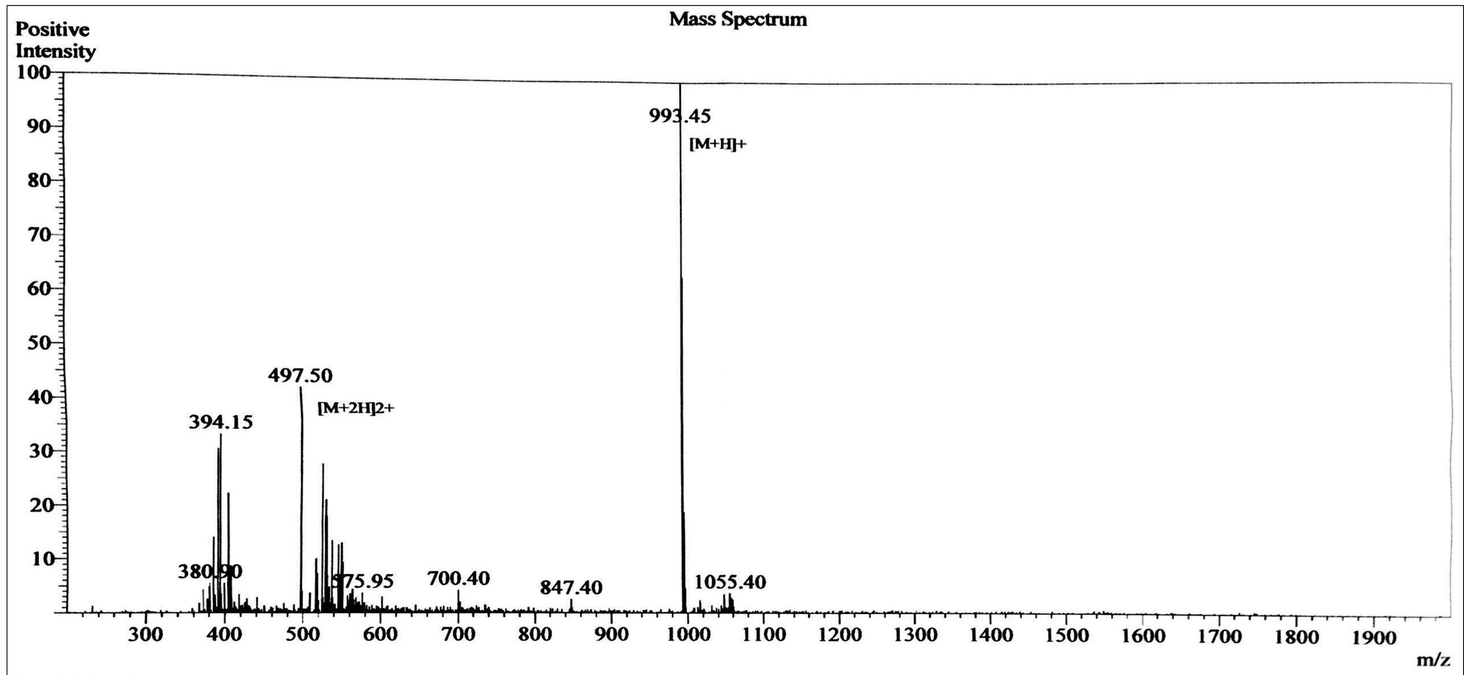
Figure S2.

A



B



Sample Information

Acquired by :	Gary
Month-Day Processed :	10/10/15
Time Processed :	9:01:34
Injection Volume :	0.2
Sample Name :	2
Sample ID :	716547-1
Theoretical MW :	993.16
Observed MW :	992.45

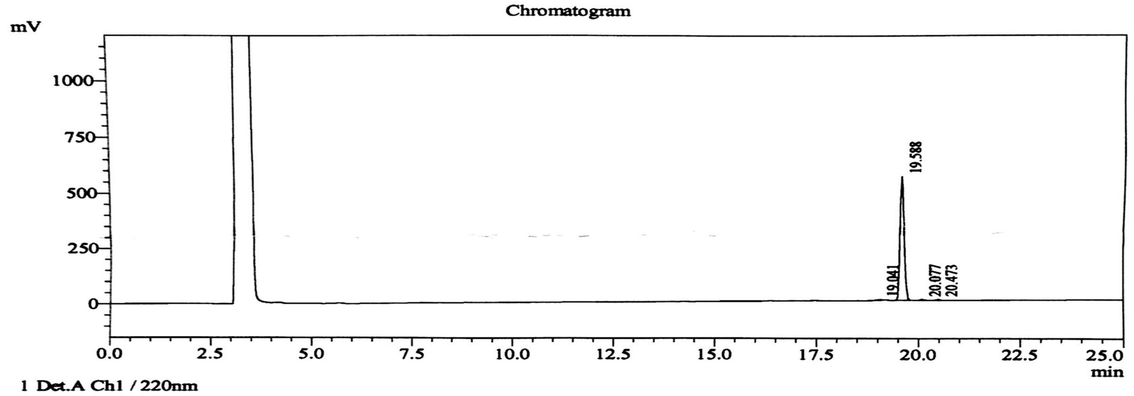
Interface	:ESI	Interface Bias	: +4.5 kV
Nebulizing Gas Flow	:1.5L/min	Drying Gas Flow	:5 L/min
CDL Temp	:250℃	T.Flow	:0.2 ml/min
Block Temp	:200℃	B.conc	:50%H2O/50%MeOH

C

Pump A : 0.065% trifluoroacetic in 100% water (v/v)
Pump B : 0.05% trifluoroacetic in 100% acetonitrile (v/v)
Total Flow:1 ml/min
Wavelength:220 nm

Time	Unit	Command	Value	Comment
0.01	Pumps	Pump A B.Conc	5	
25.00	Pumps	Pump A B.Conc	65	
25.01	Pumps	Pump A B.Conc	95	
31.00	Pumps	Pump A B.Conc	95	
31.01	Pumps	Pump A B.Conc	5	
40.00	Pumps	Pump A B.Conc	5	
40.01	Controller	Stop		

<<Column Performance>>
<Detector A>
Column : AlltimaTM C18 4.6 x 250 mm



Peak Table

Detector A Ch1 220nm

Peak#	Ret. Time	Area	Height	Area %
1	19.041	28680	3698	0.726
2	19.588	3888680	555298	98.395
3	20.077	16322	3069	0.413
4	20.473	18409	3338	0.466
Total		3952092	565403	100.000