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Supporting Information

for

Synthesis and Esterolytic Activity of Catalytic Peptide Dendrimers

By

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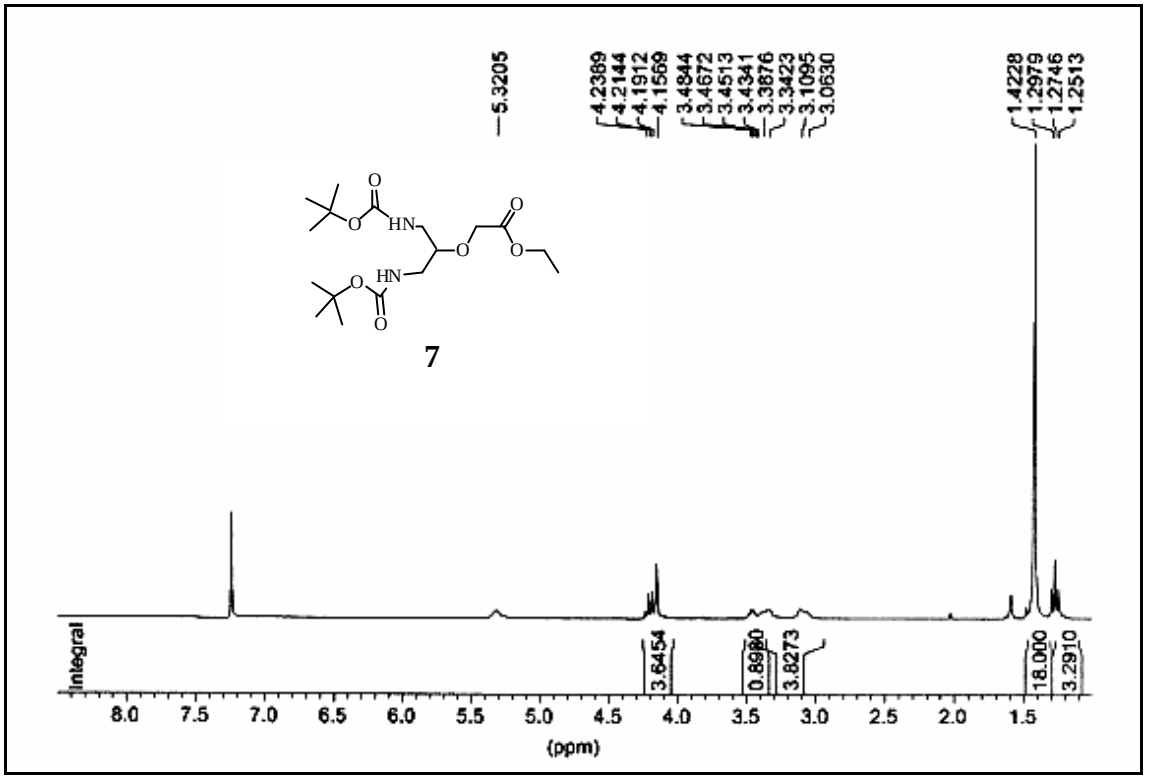
^{1}H and ^{13}C NMR for intermediates and linkers 1, 2; capping unit 4; quinolinium substrates 15-17 and 19-21.

Analytical HPLC profiles and Mass spectra (ESI MS) data for the monomeric and dimeric peptide dendrimers

Analytical HPLC columns: Vydac 218TP-54 C_{18}, pore size 300 Å, 0.45 × 22 cm, flow 1.5 mL.min^{-1} or Chromolith Performance RP-18e , 0.46 × 10 cm, flow 5 mL.min^{-1}; detection by UV at 214 nm, solvent systems: A = 0.1% TFA in H_2O; B = 40% H_2O / 60% CH_3CN, 0.1% TFA.
Starting conditions: for dendrimers with linkers **1**, **2**, **3**: 80% A / 20% B, gradient +1% B / min; for hydrophobic dendrimers: 20% B to 100% B in 5 min.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3.0630
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1.2746
1.2513
Integral
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0.8980
3.8273
18.000
3.2910
8.0
7.5
7.0
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2.5
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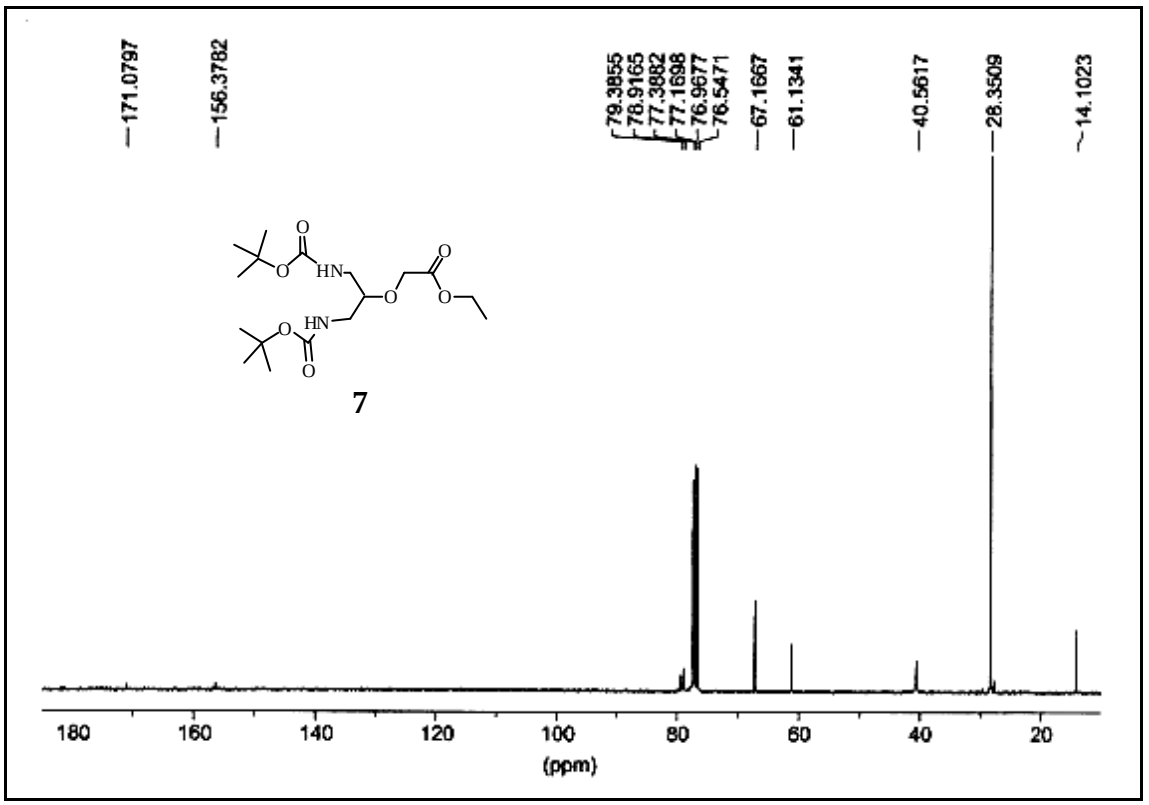
(ppm)

7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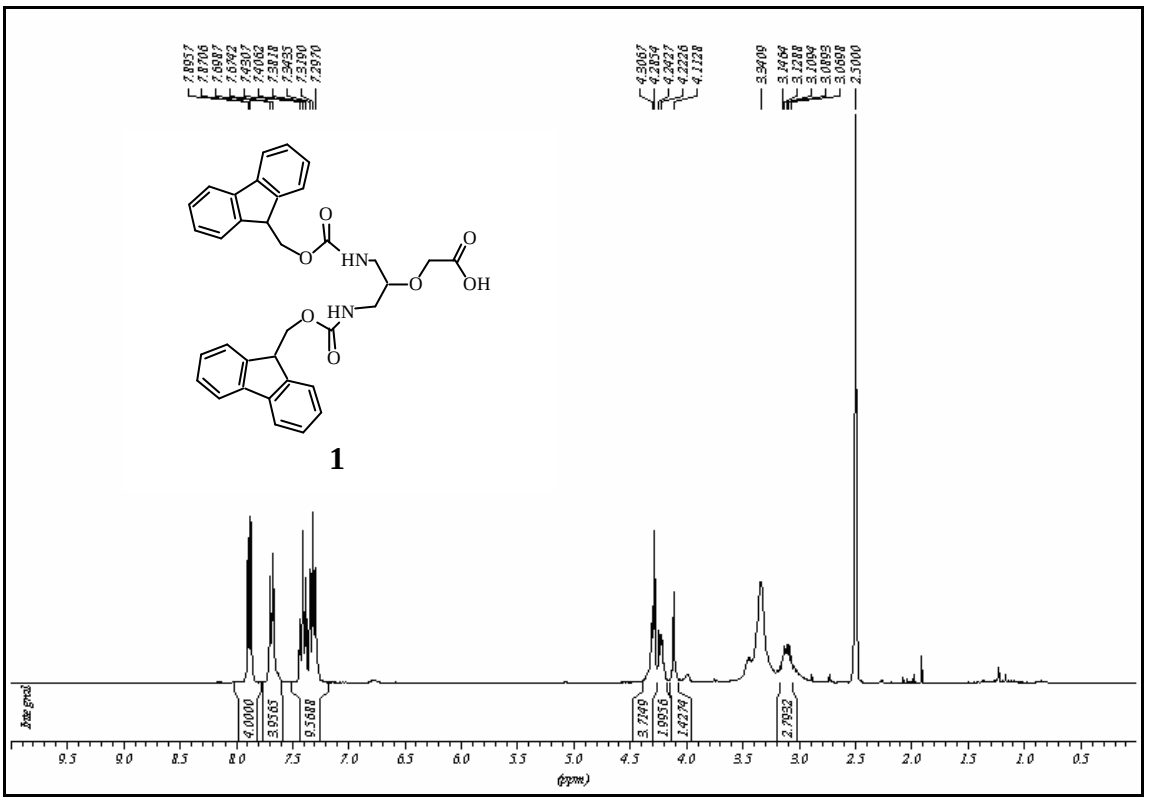
20
(ppm)

7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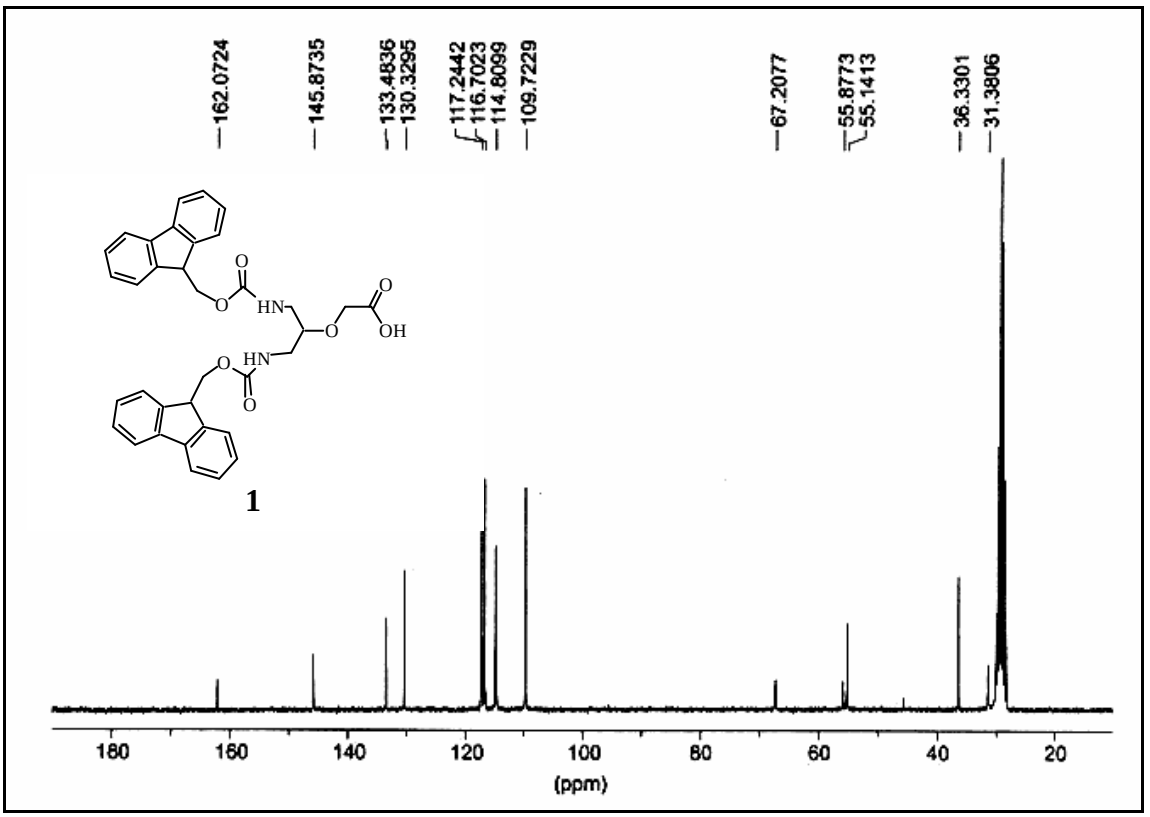
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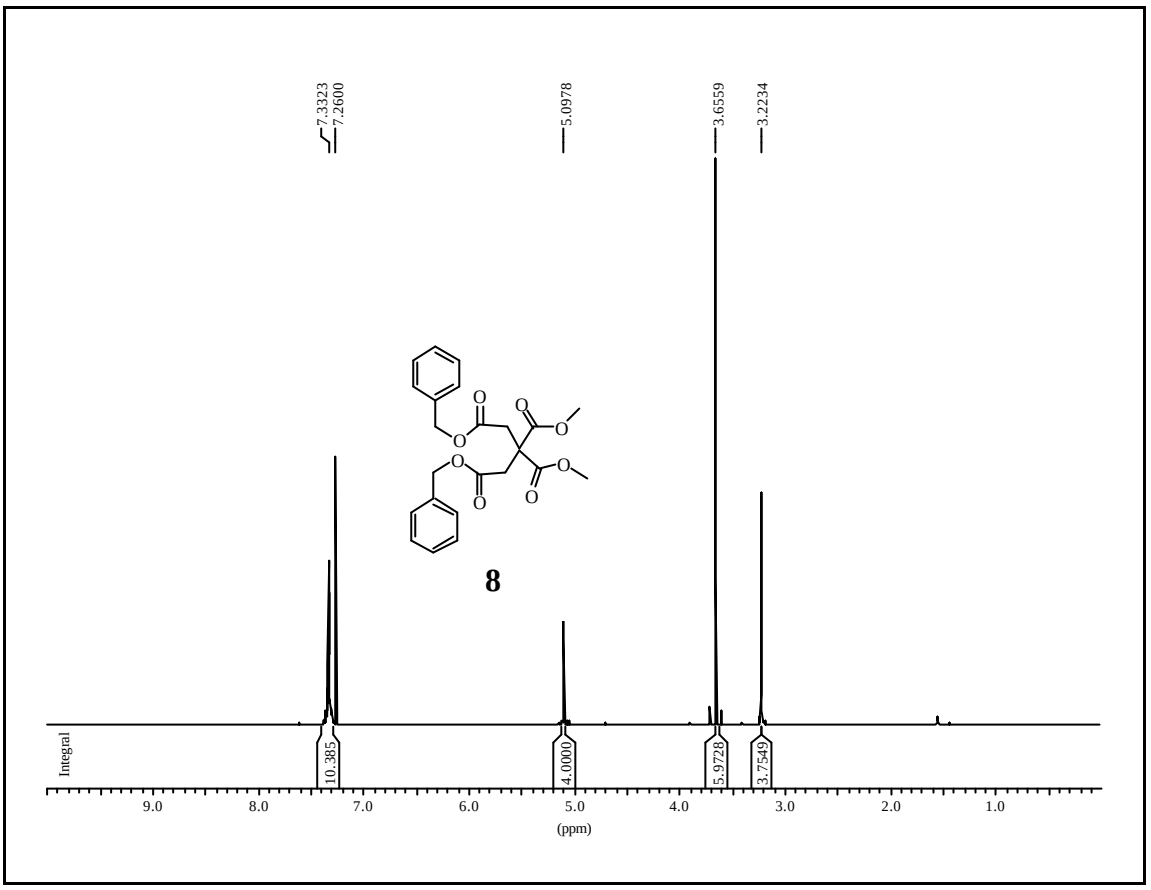
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4.0
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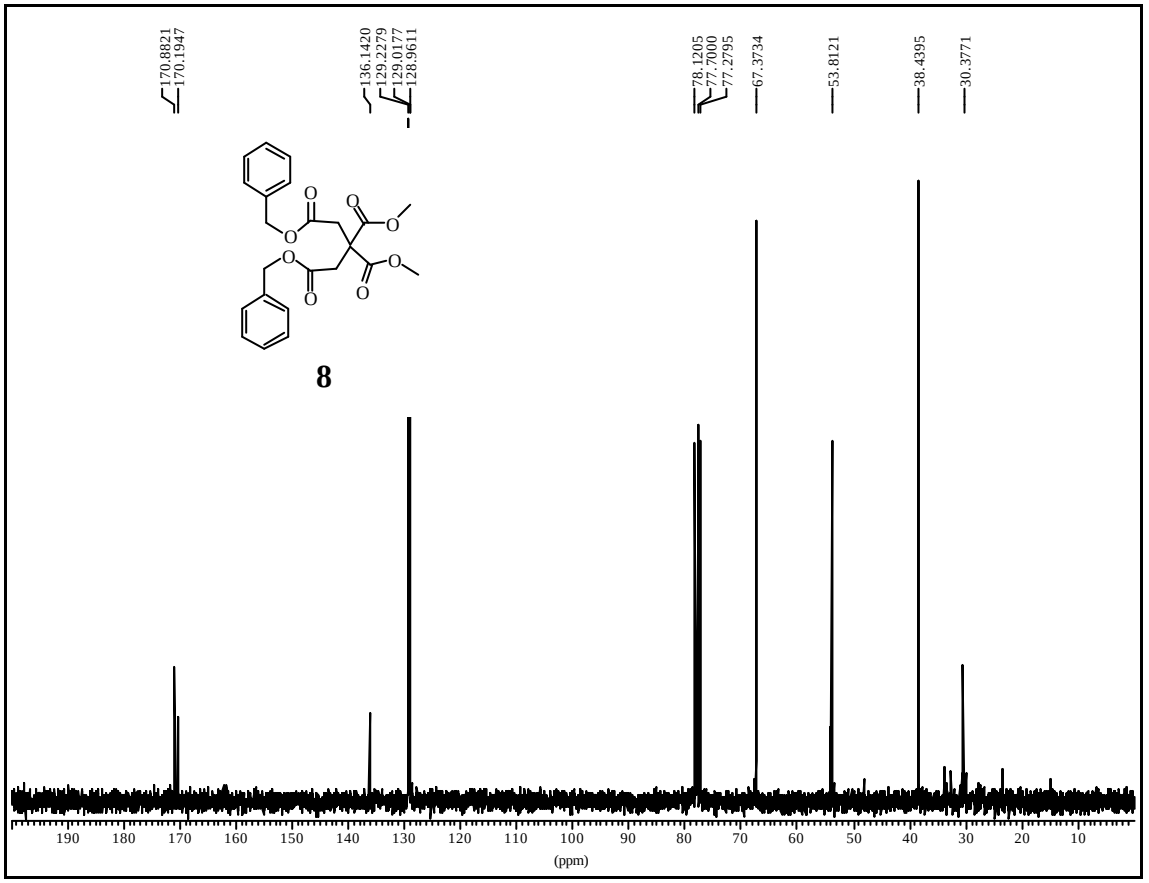
1.0
(ppm)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8
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130
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110
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90
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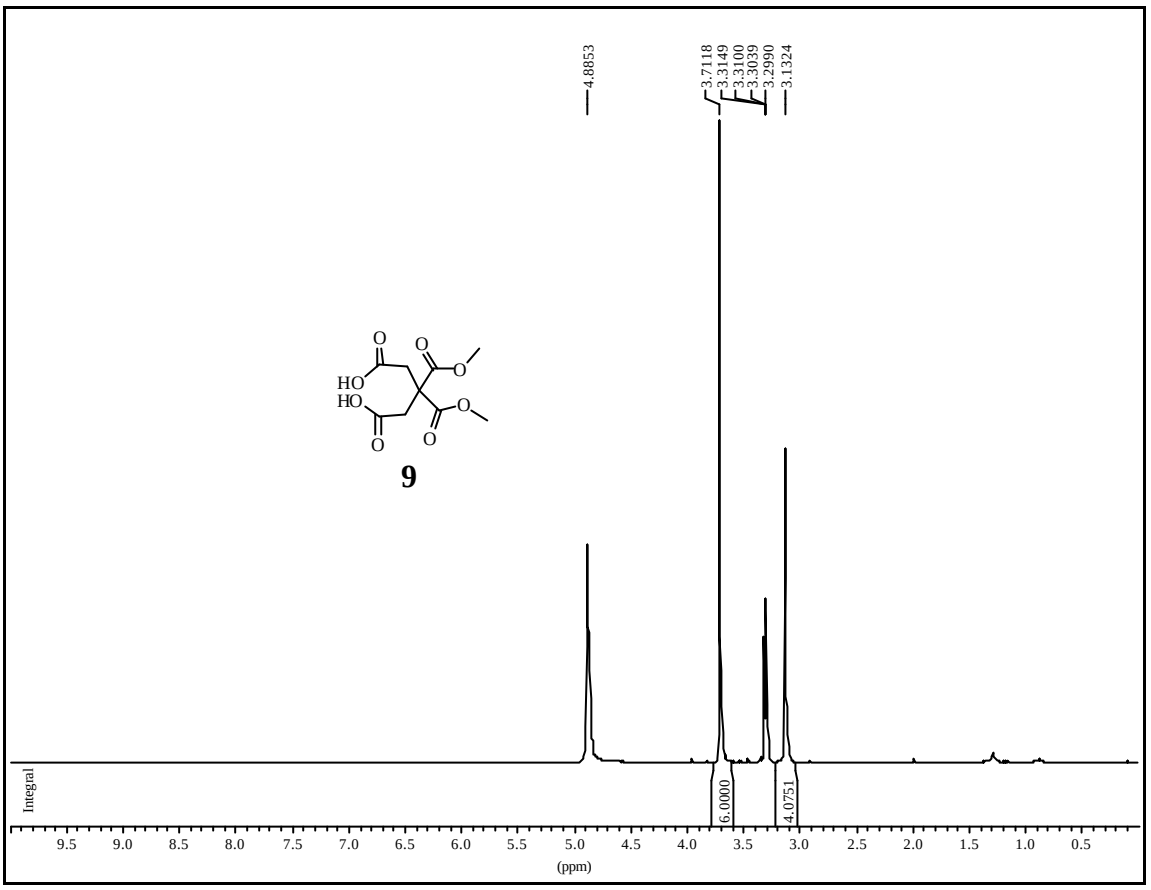
20
10
(ppm)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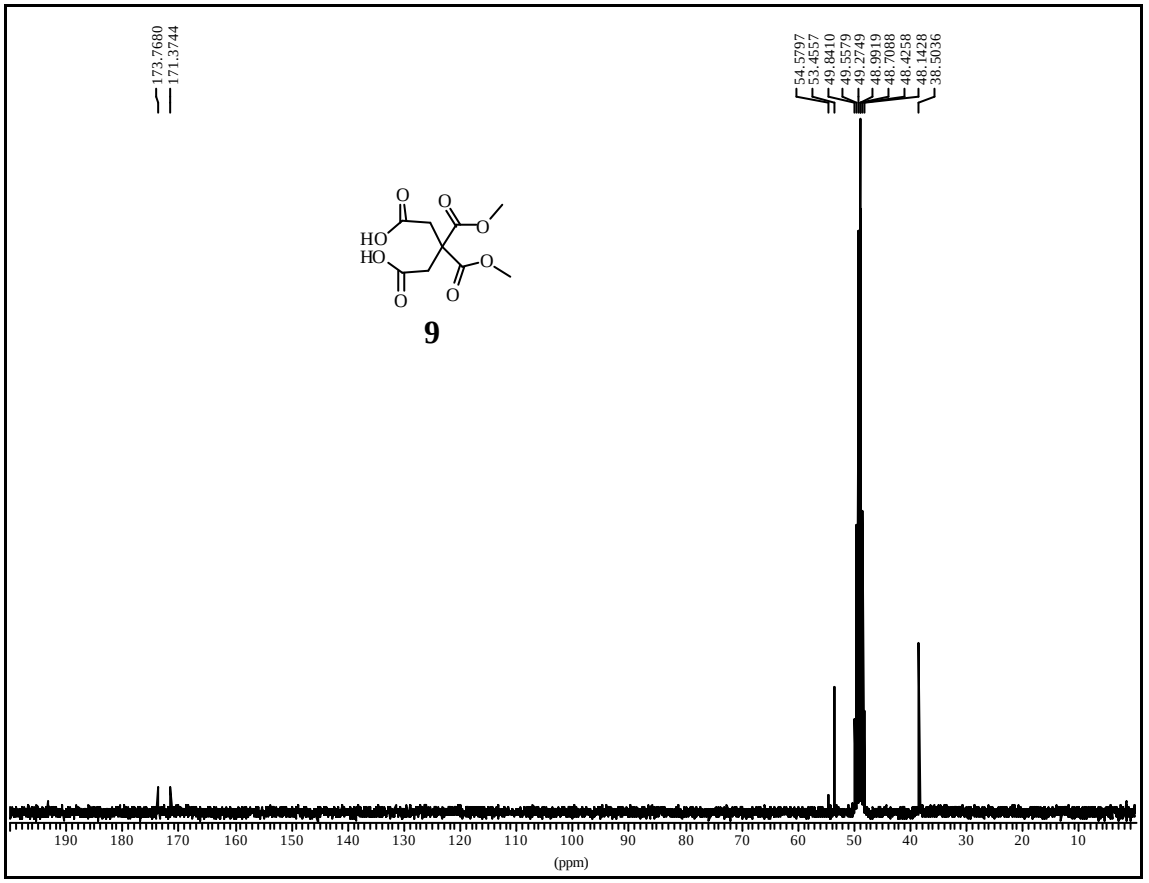
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HO
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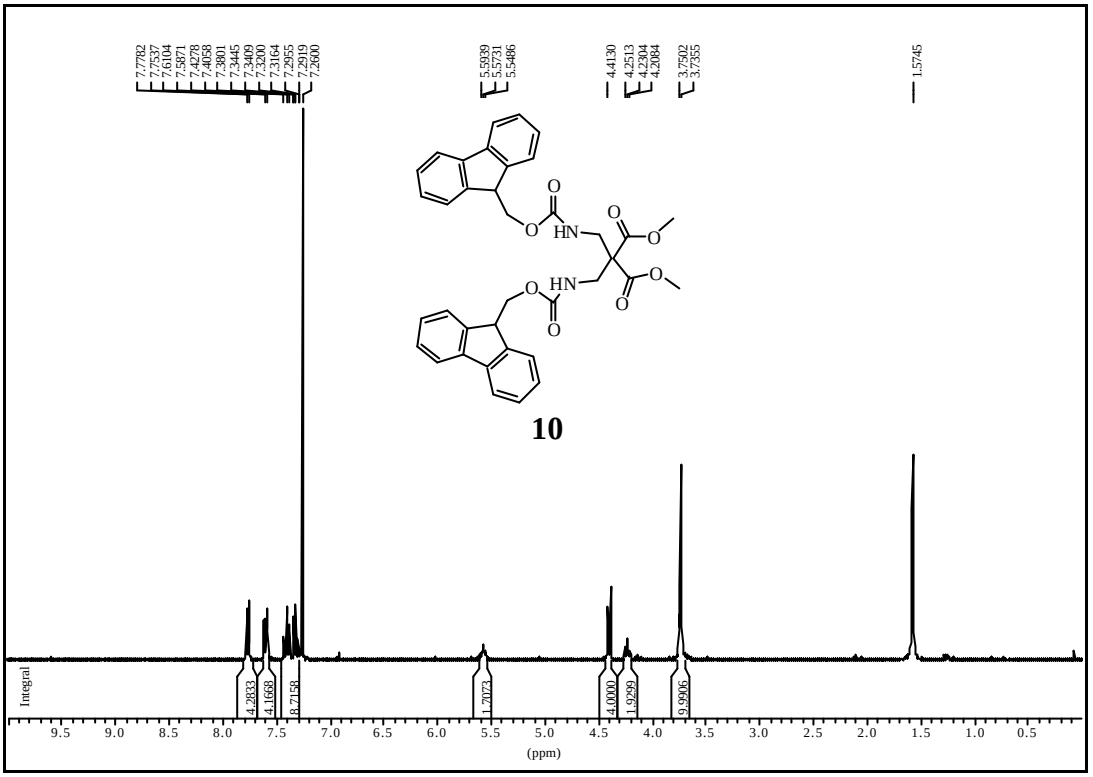
(ppm)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5.5486
4.4130
4.2513
4.2304
4.2084
3.7502
3.7355
1.5745
Integral
4.2833
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1.9299
9.9906
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
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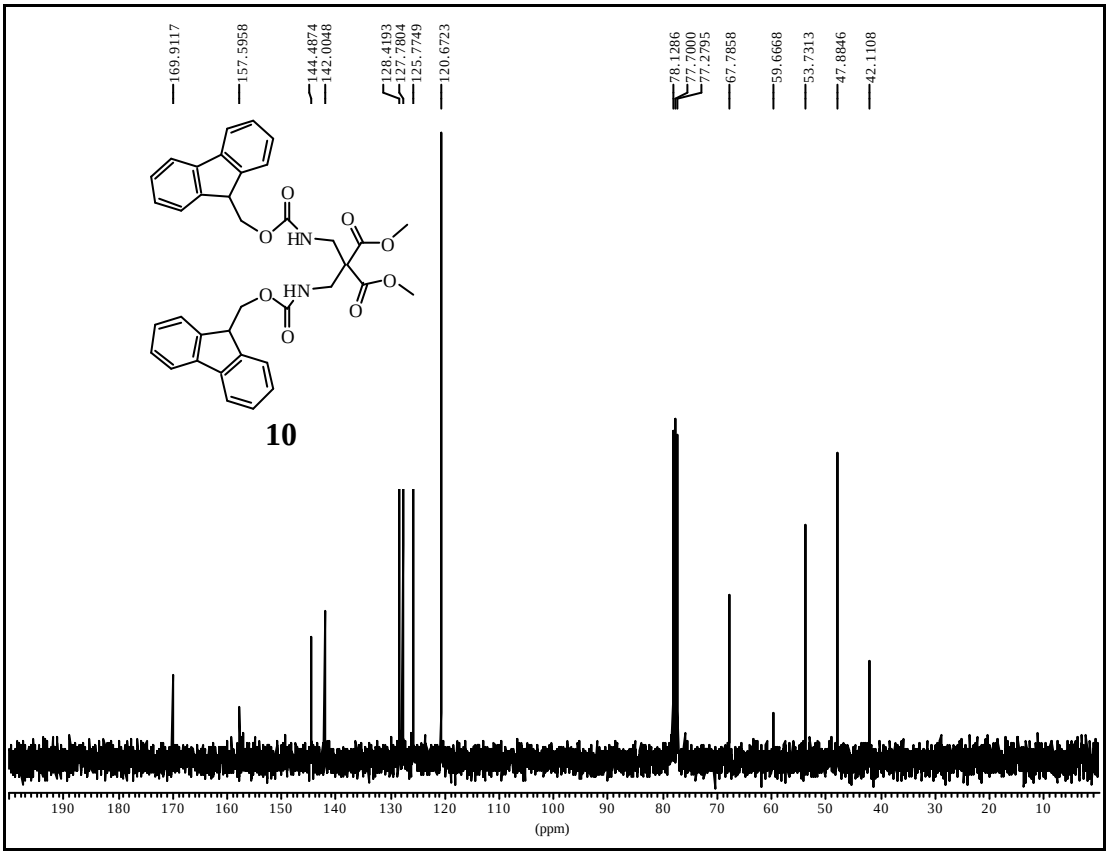
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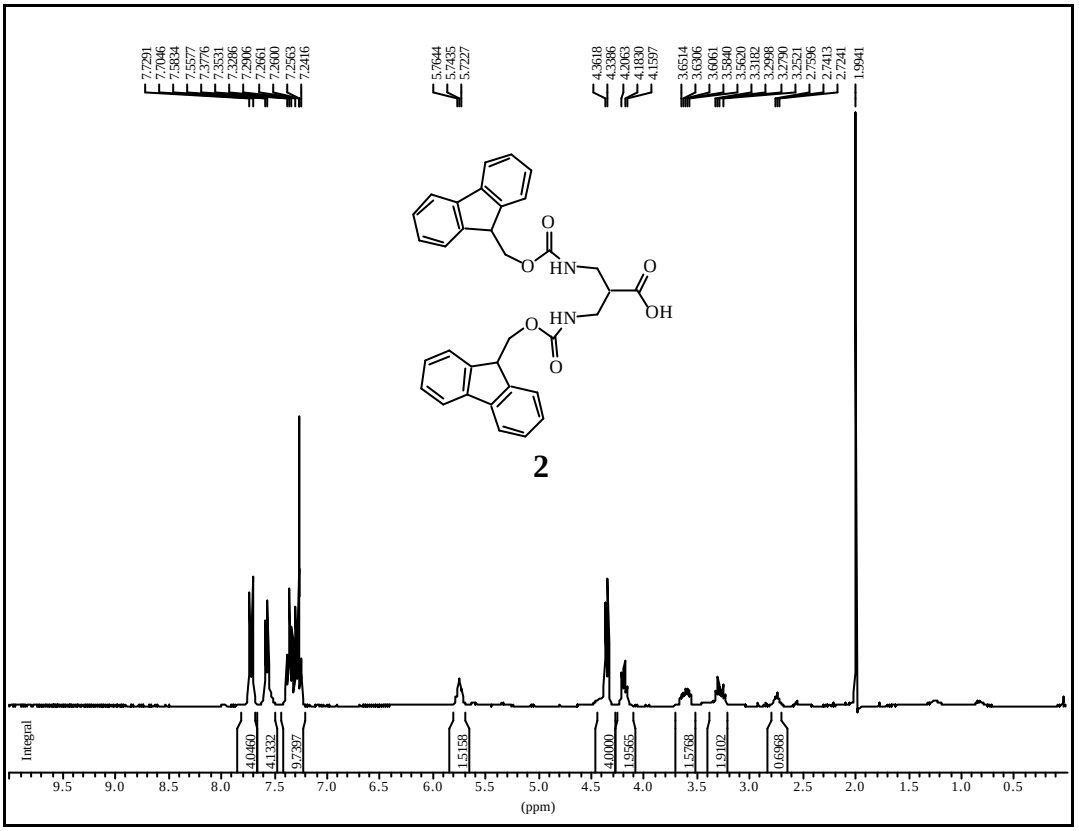
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2.7241
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OH
O
HN
O
O
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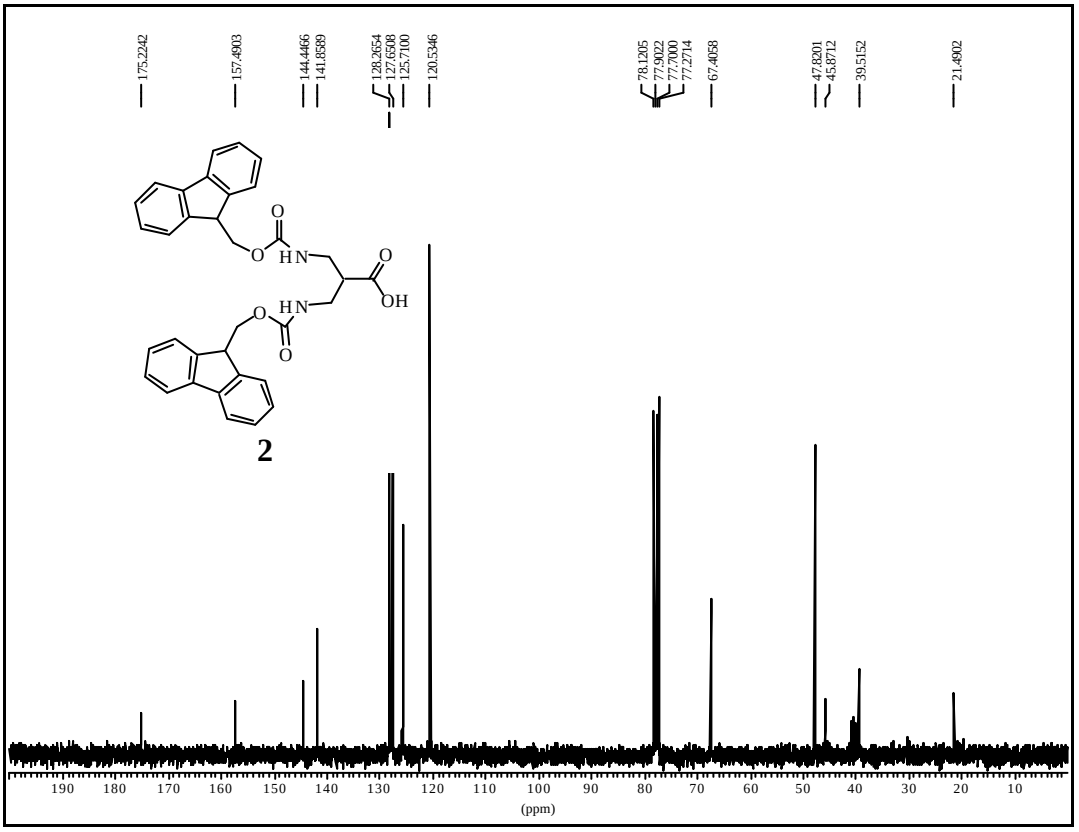
(ppm)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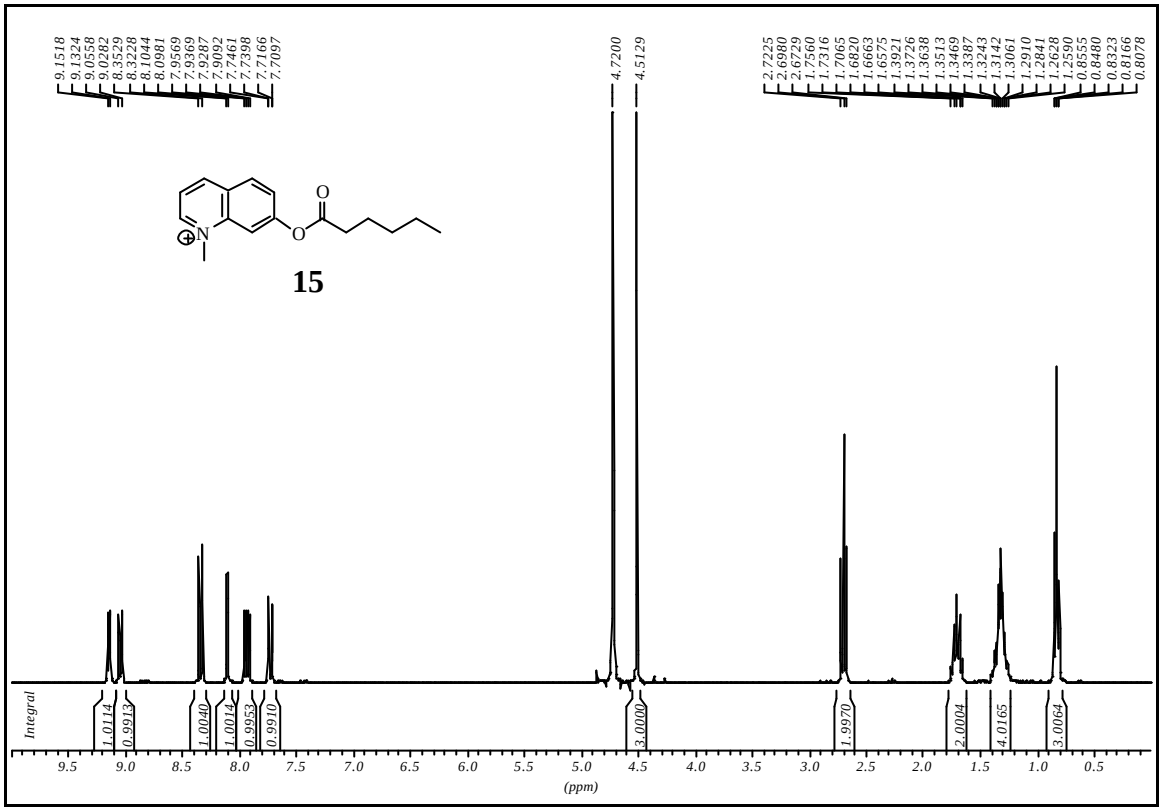
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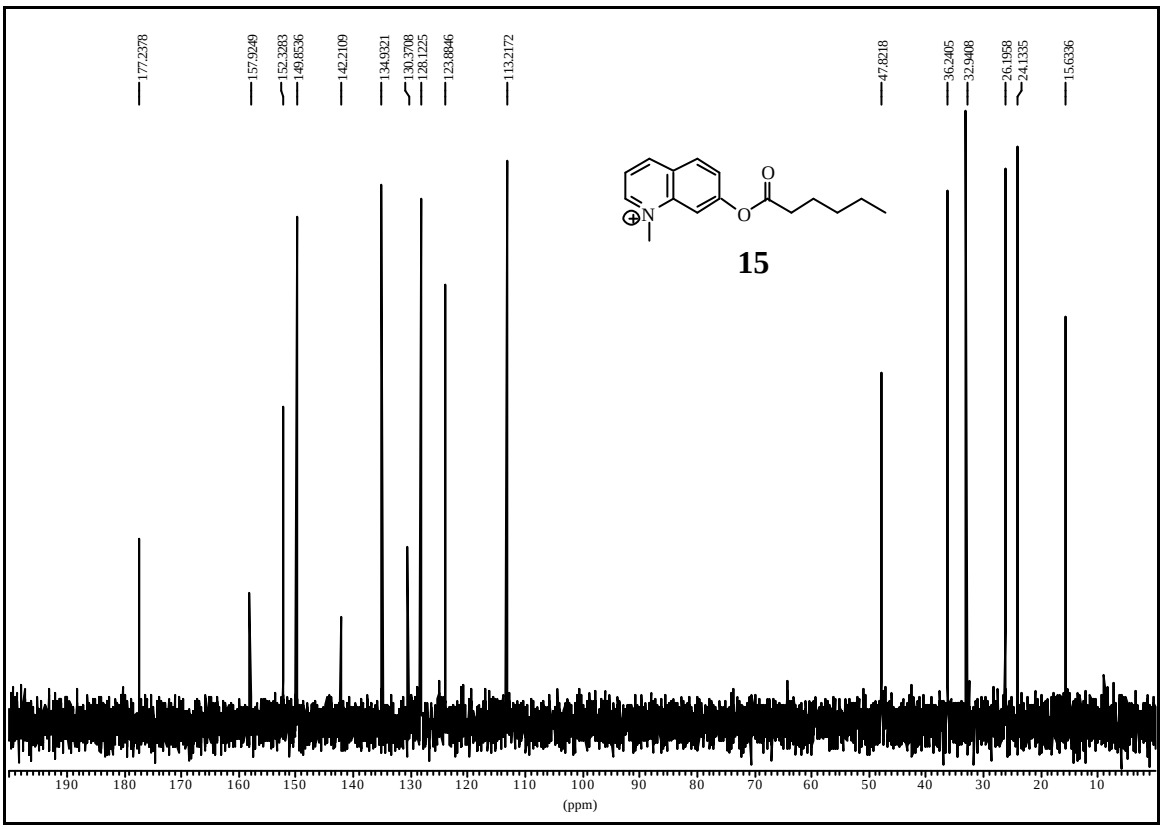
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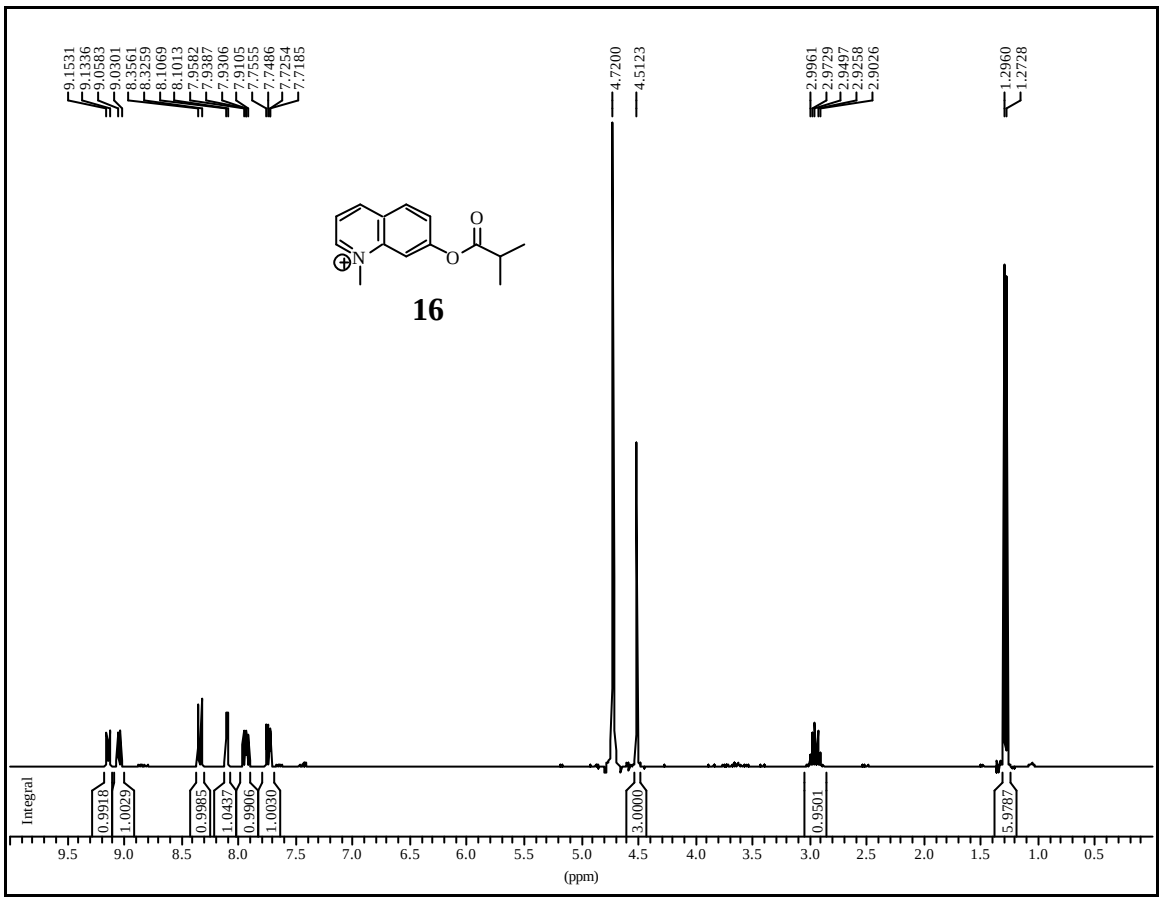
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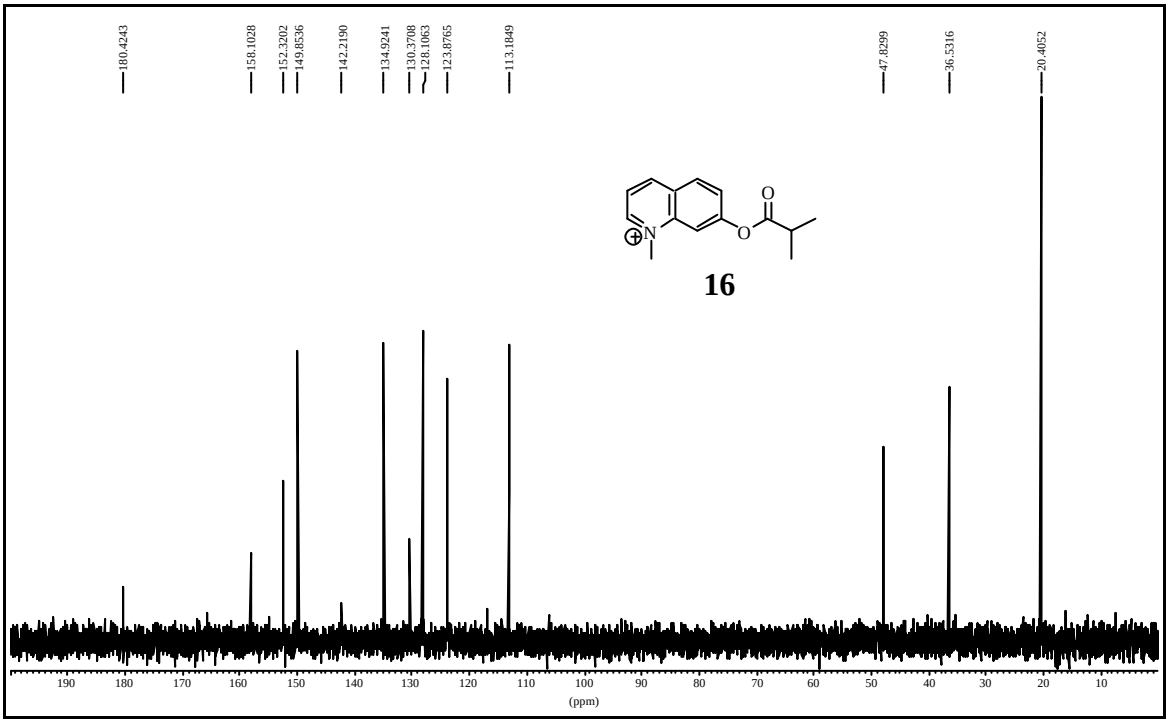
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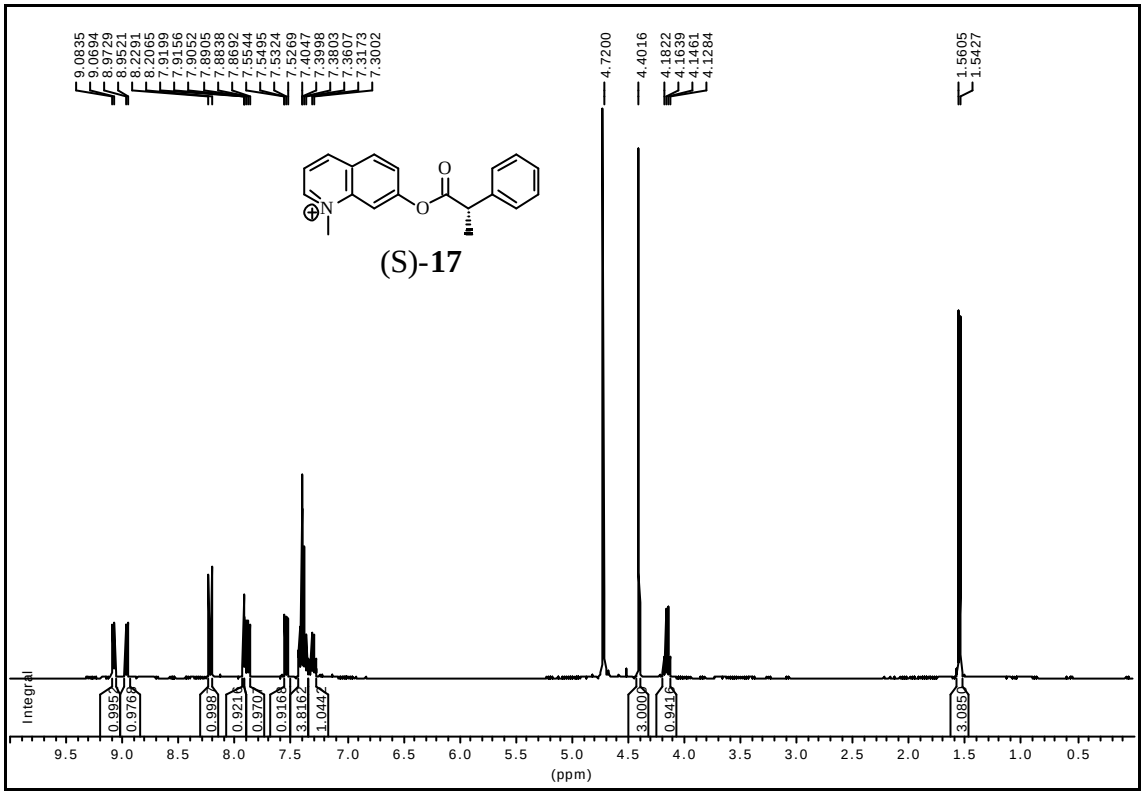
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7.8692
7.5544
7.5495
7.5324
7.5269
7.4047
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7.3803
7.3607
7.3173
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4.7200
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4.1461
4.1284
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Integral
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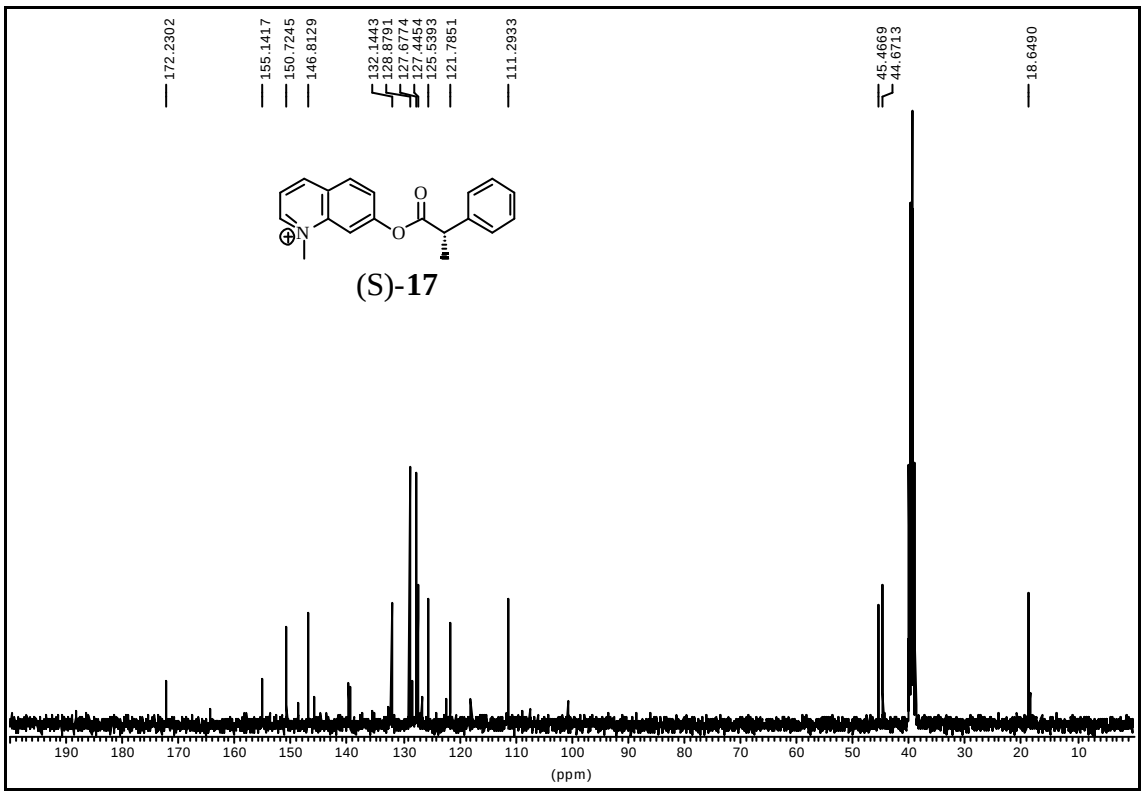
(S)-**17**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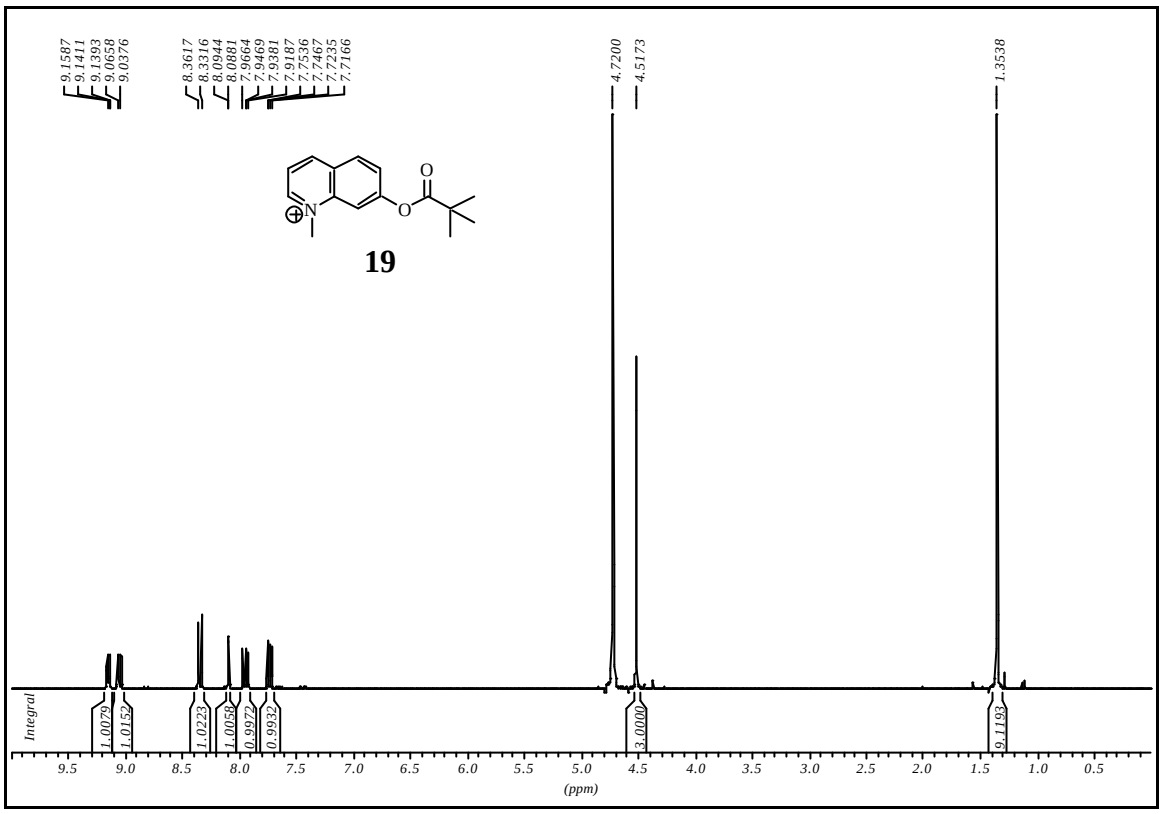
(S)-**17**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7.7536
7.7467
7.7235
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19
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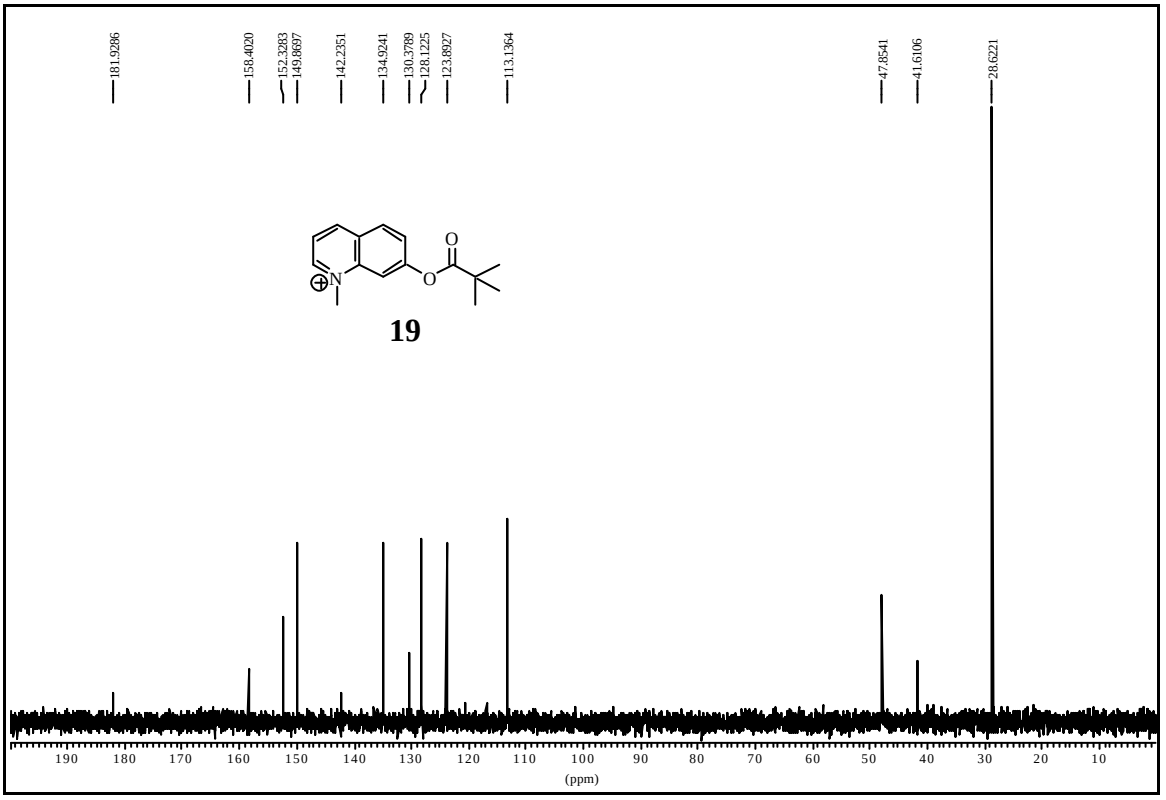
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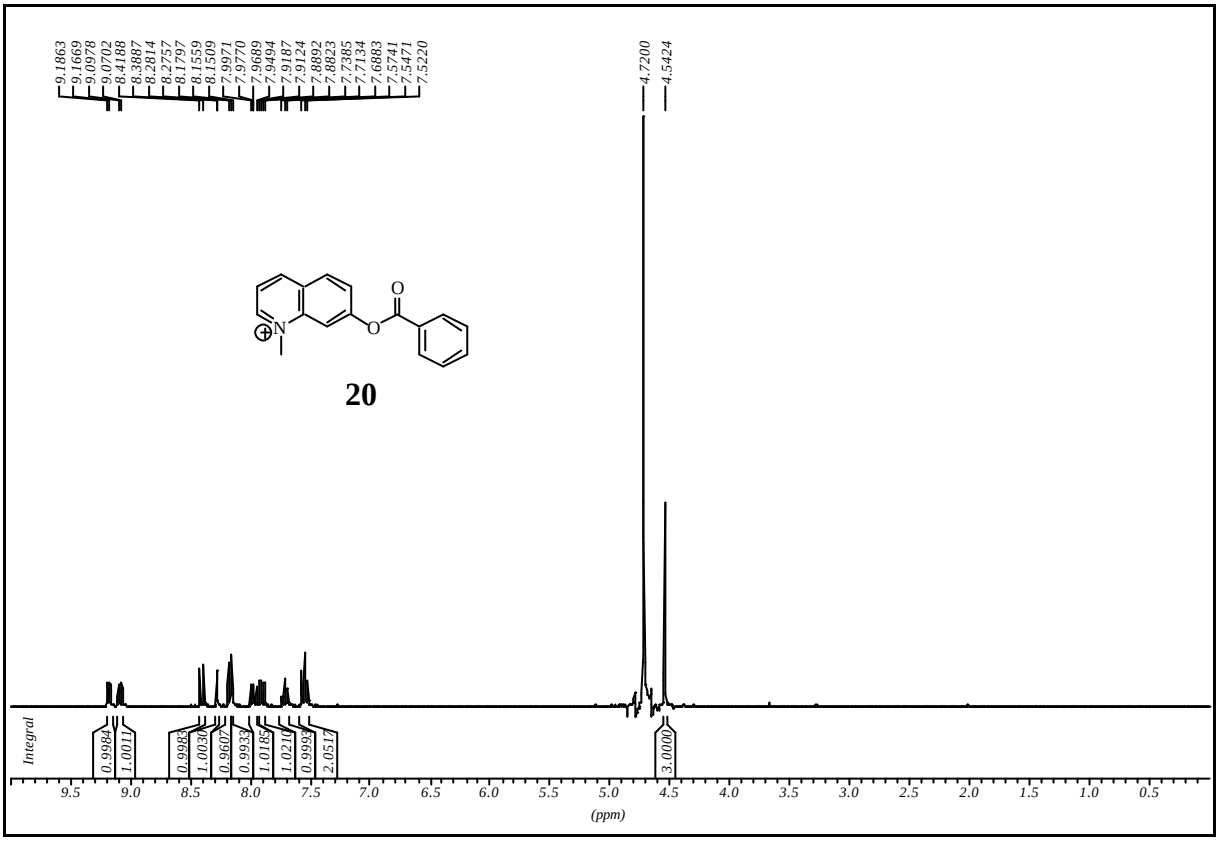
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O
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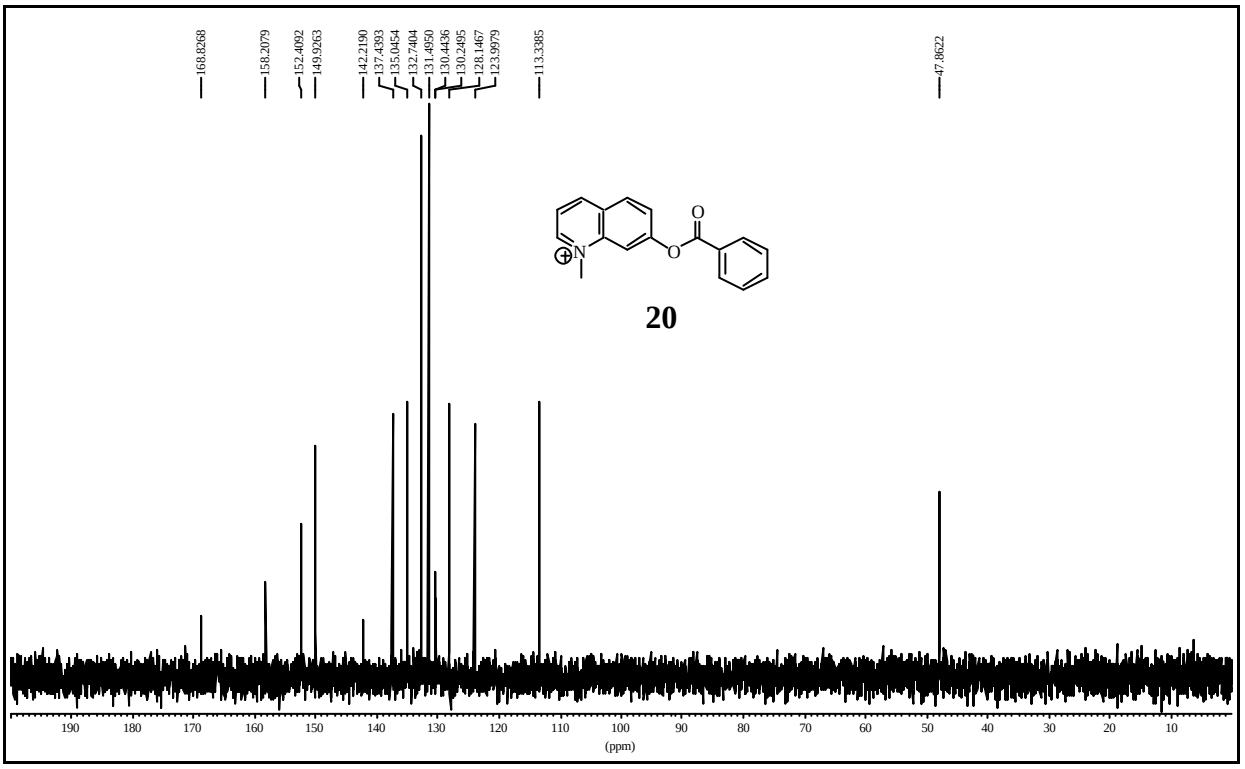
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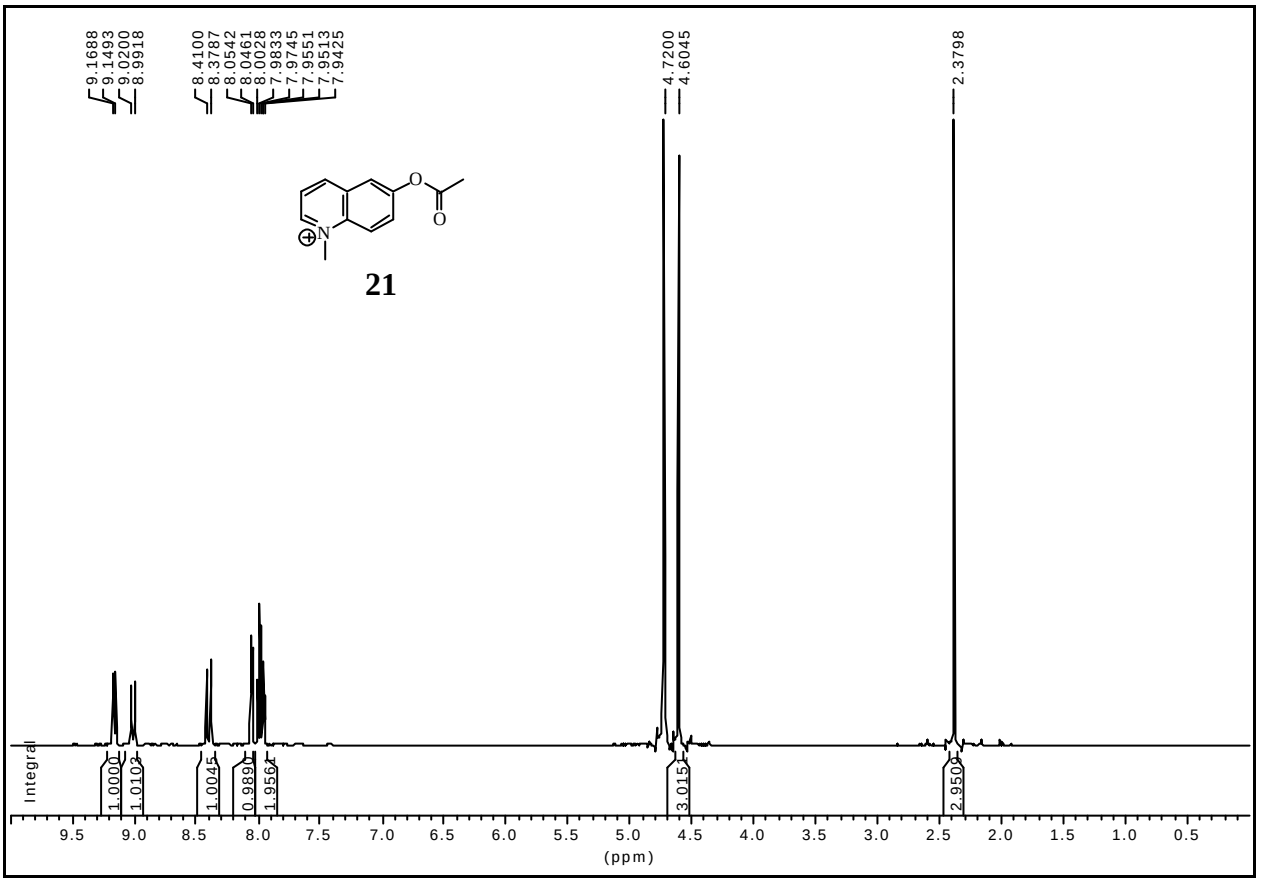
(ppm)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7.9513
7.9425
4.7200
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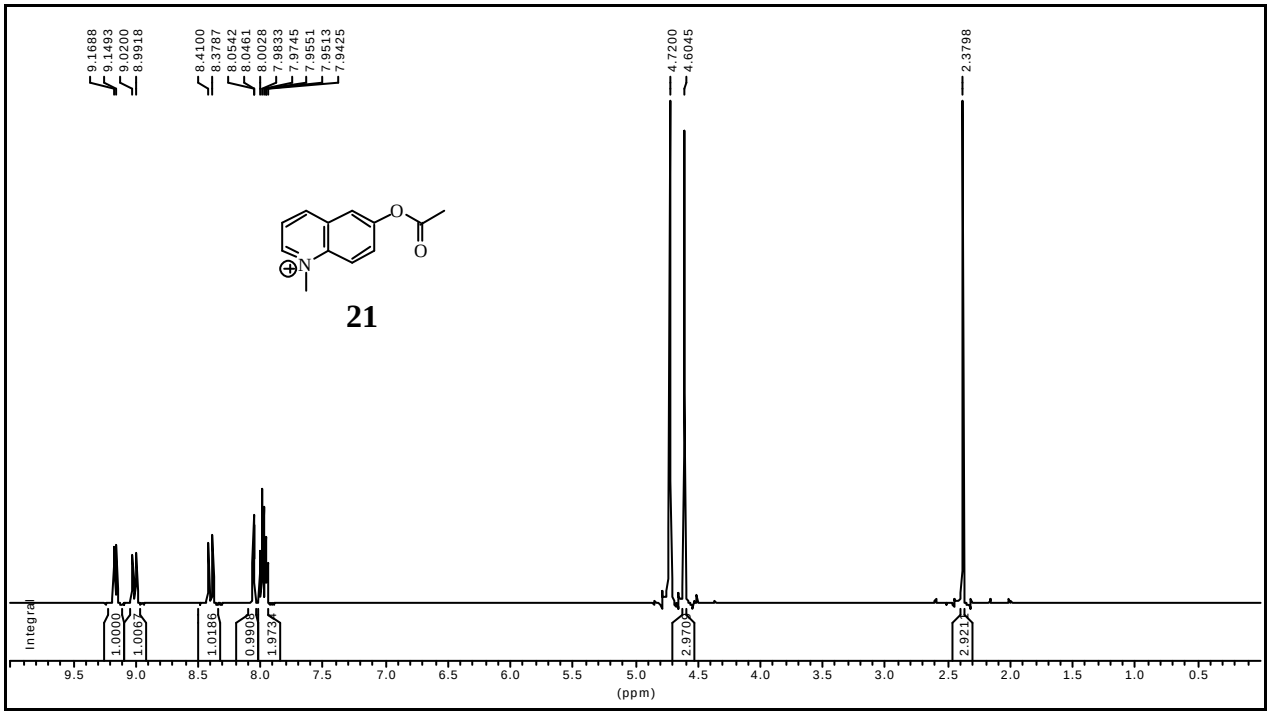
21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7.9551
7.9513
7.9425
4.7200
4.6045
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Integral
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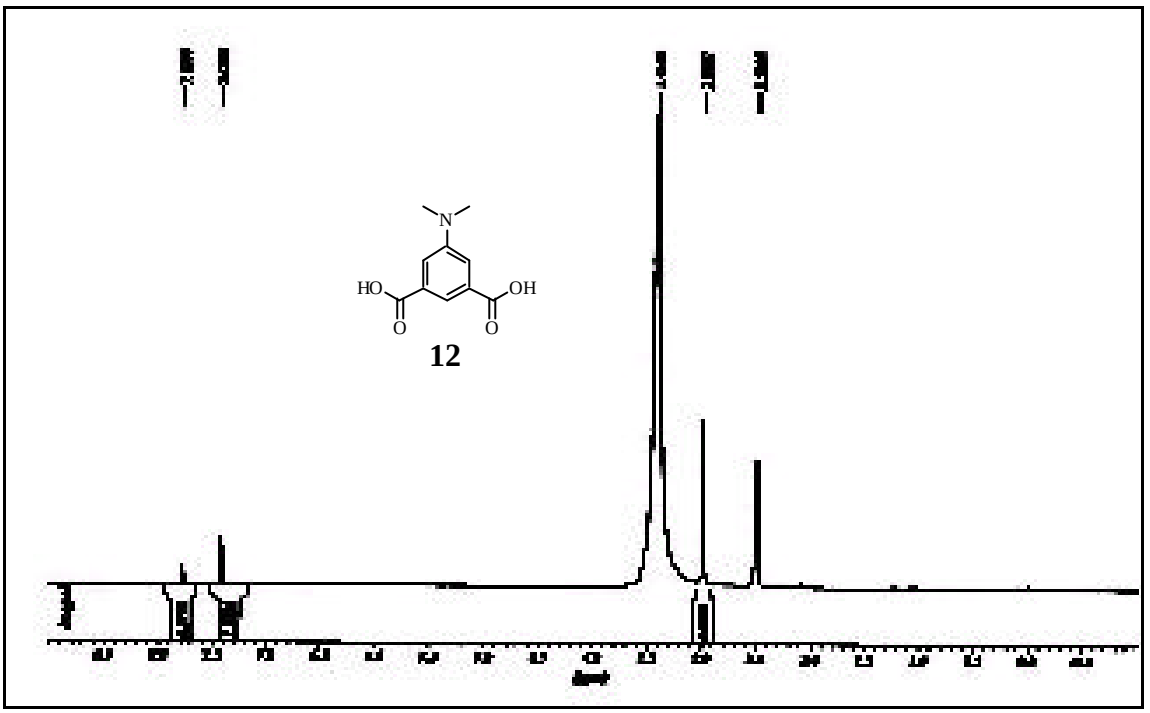
21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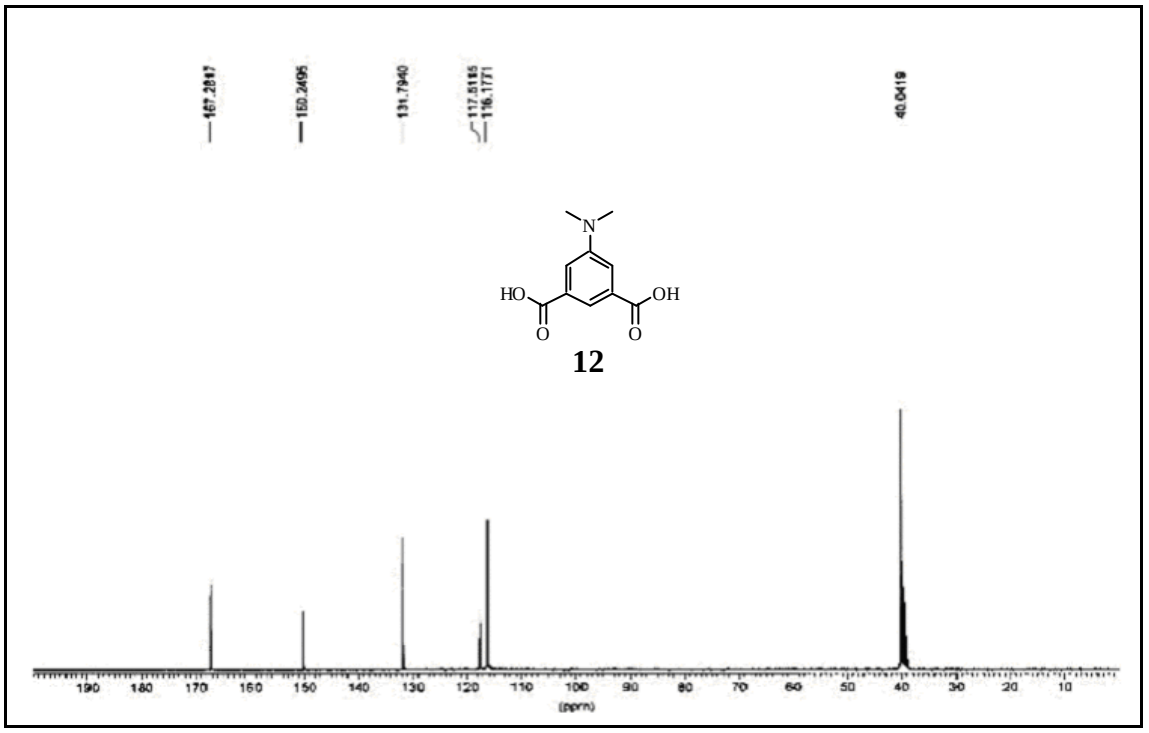
O
N

12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117.5185
116.1771
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HO
OH
O
O
N
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180
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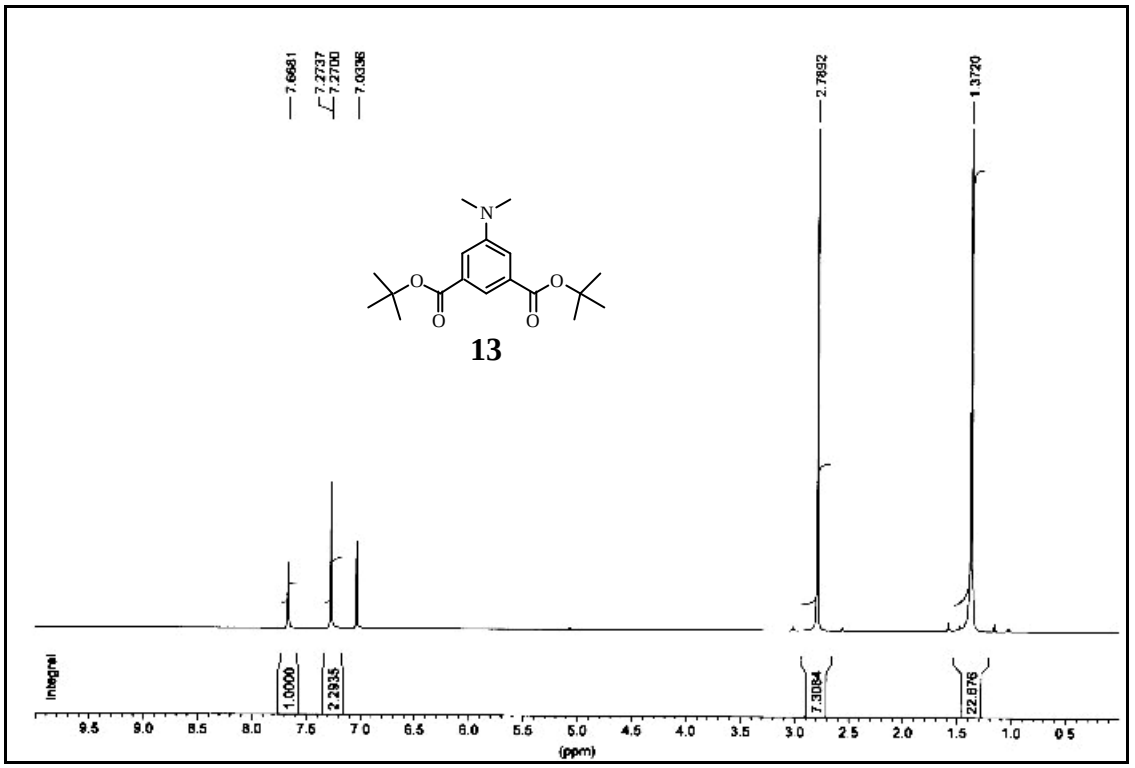
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
(ppm)

12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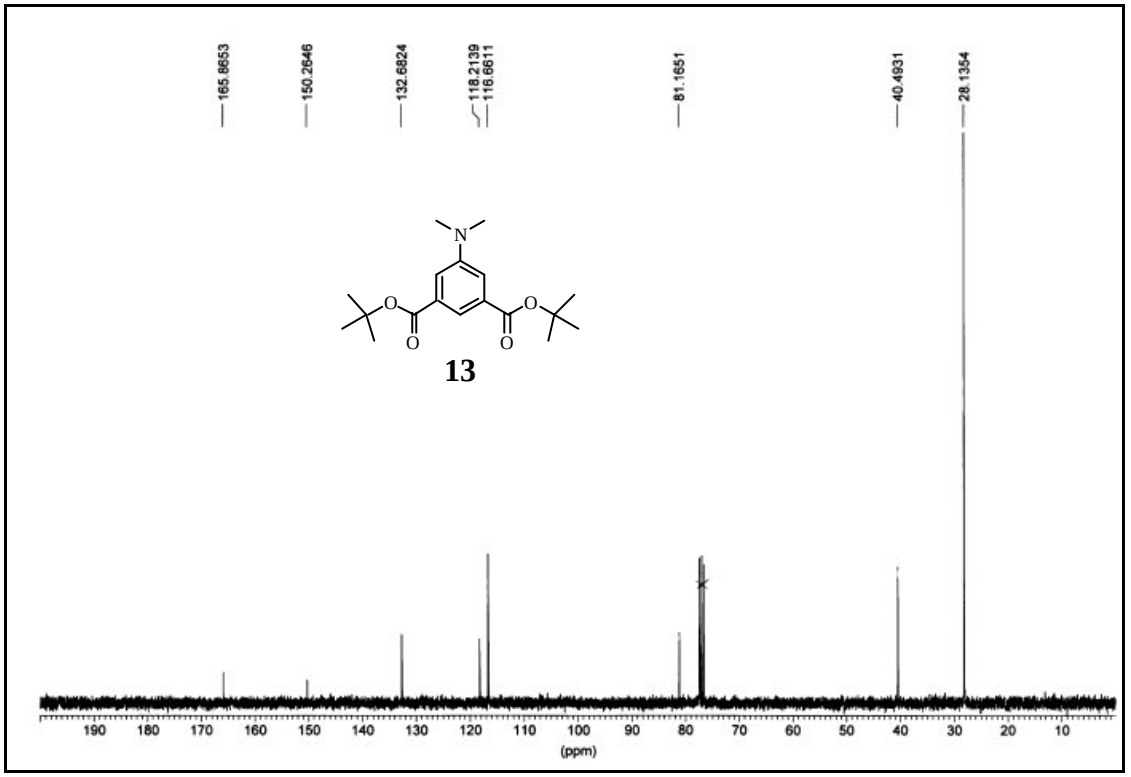
7.2737
7.2700
7.0336
2.7892
1.3720
13
Integral
1.0000
2.2935
7.3084
22.676
(ppm)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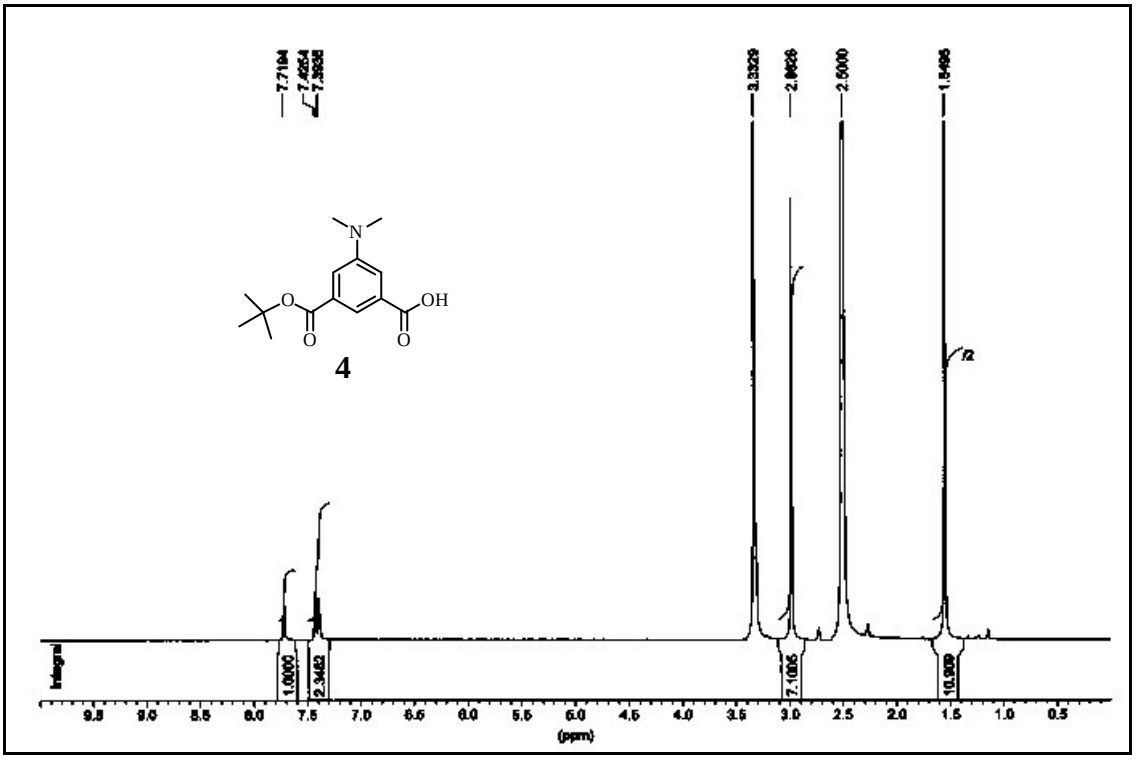
150.2646
132.6824
118.2139
116.6811
81.1651
40.4931
28.1354
13
(ppm)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7.4254
7.3938
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2.5000
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I2
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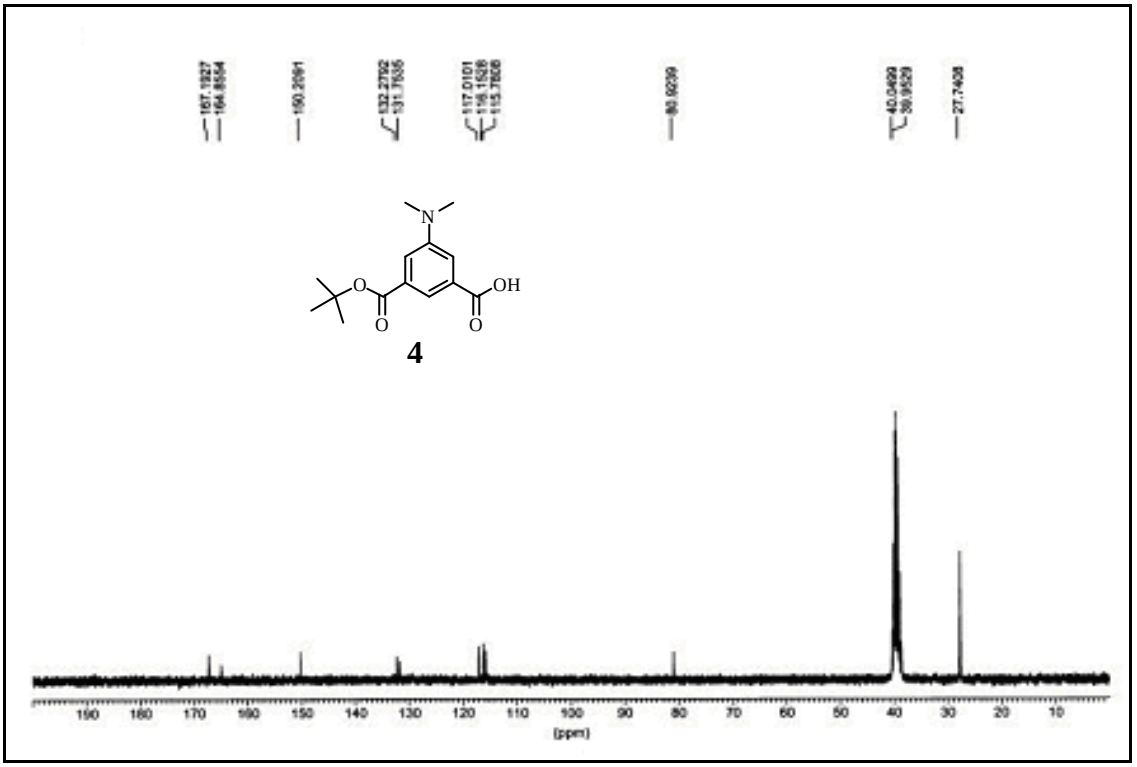
(ppm)

4


167.1827
164.8554
150.2091
132.2792
131.7535
117.0101
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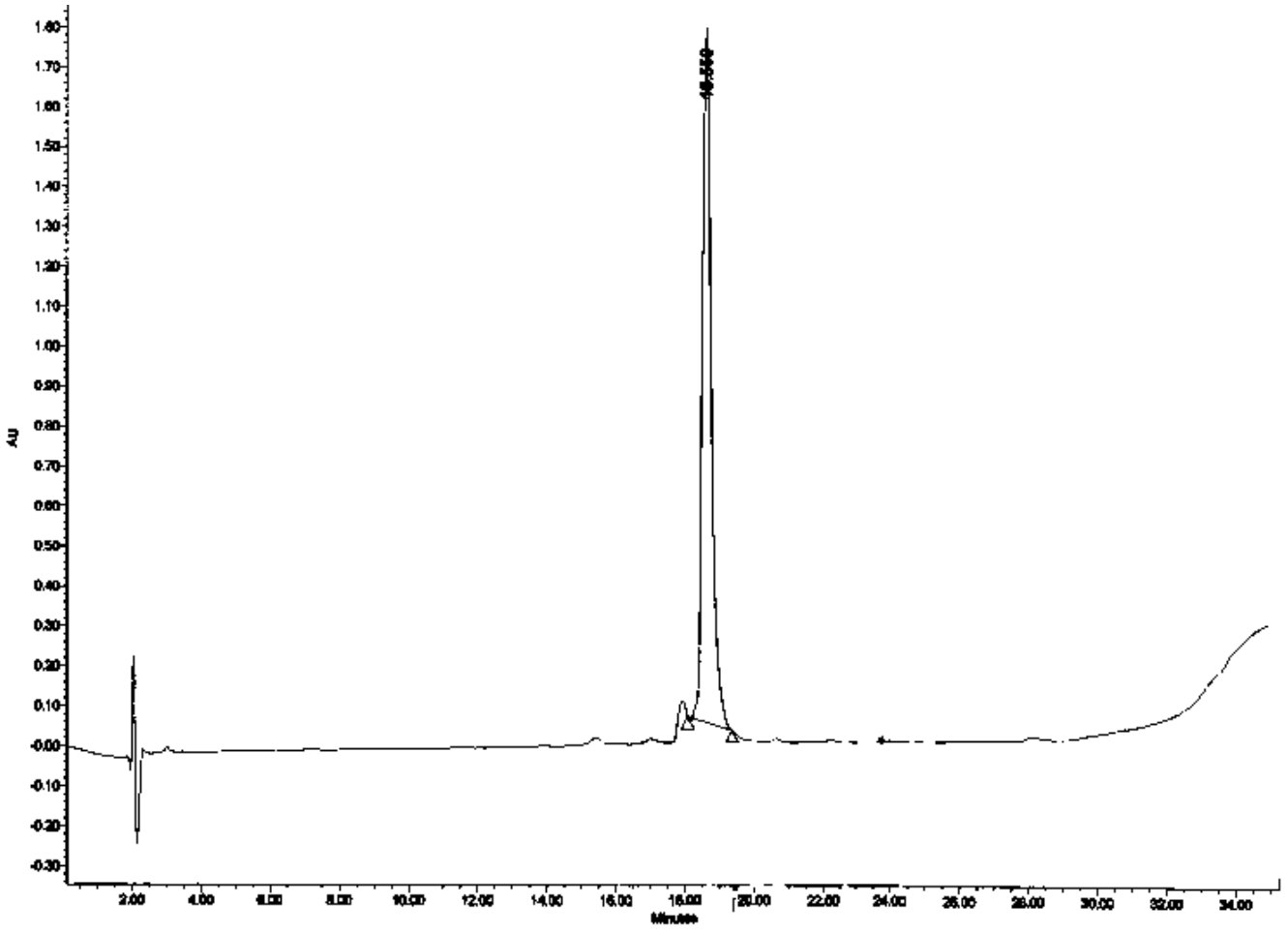
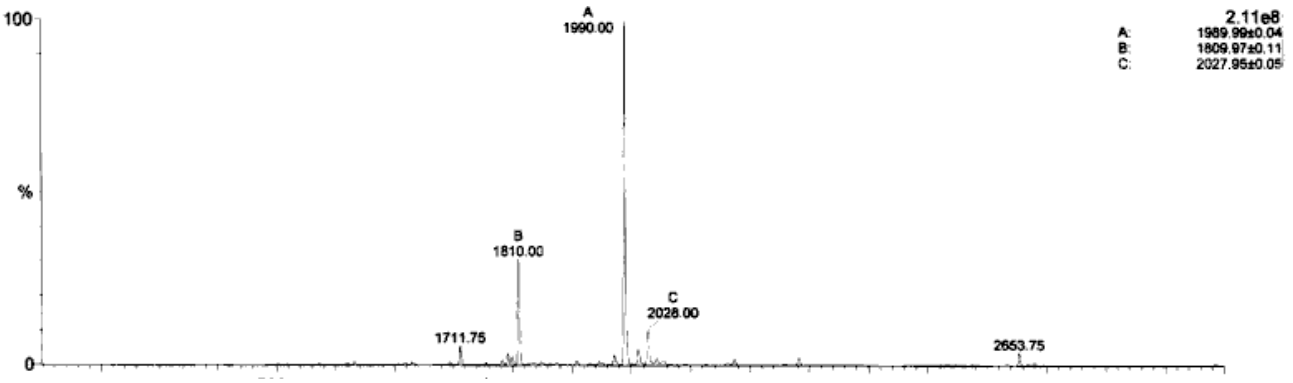
115.7806
80.9239
40.0499
39.9529
27.7408
(ppm)

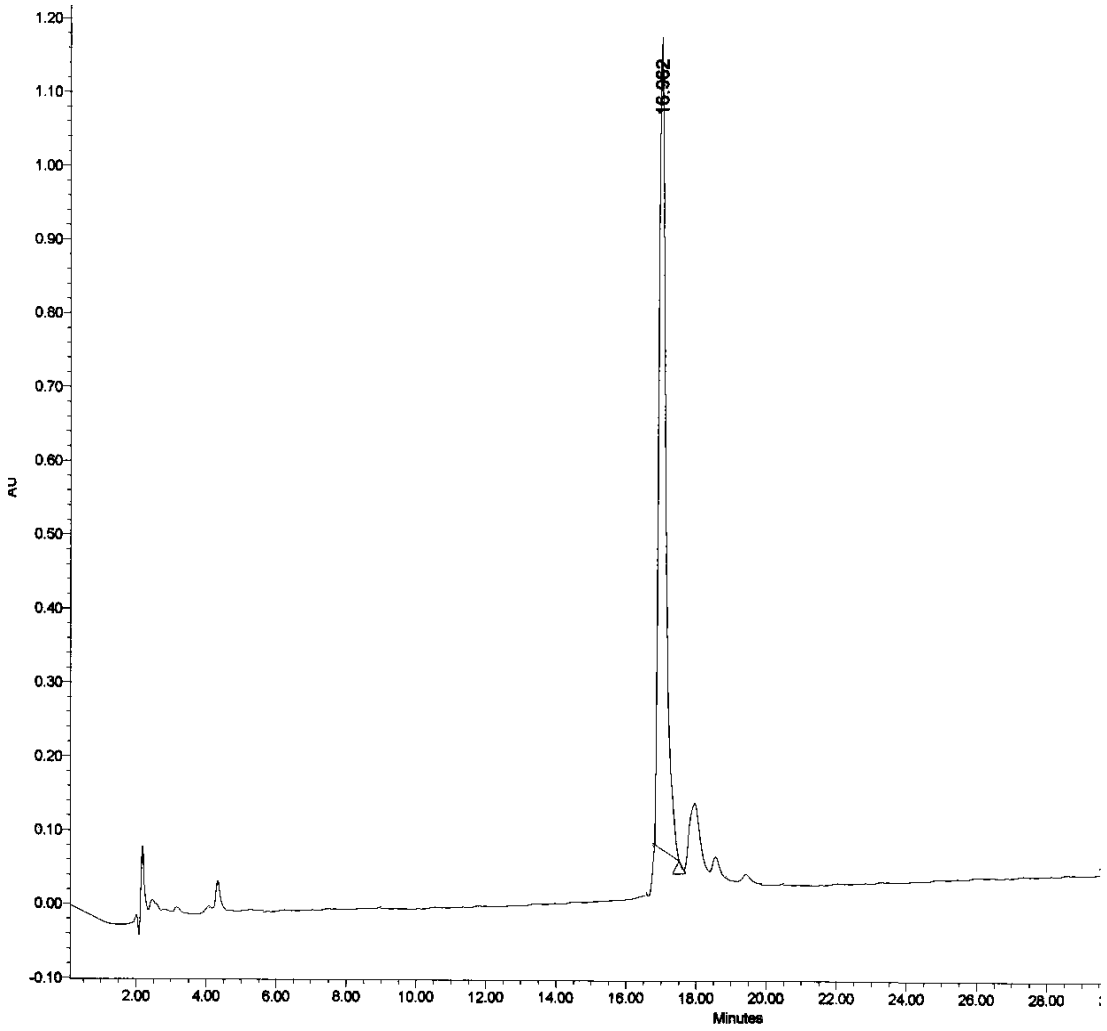
4

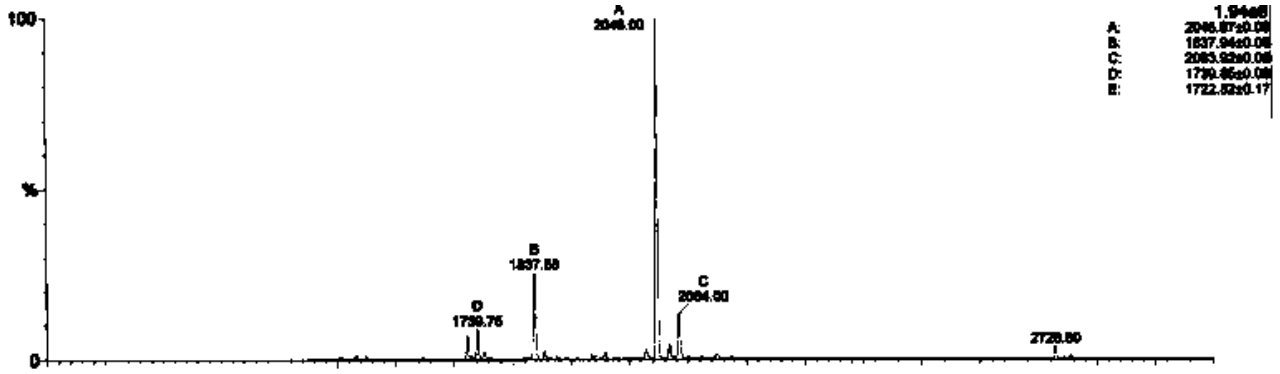
Dendrimer A_1



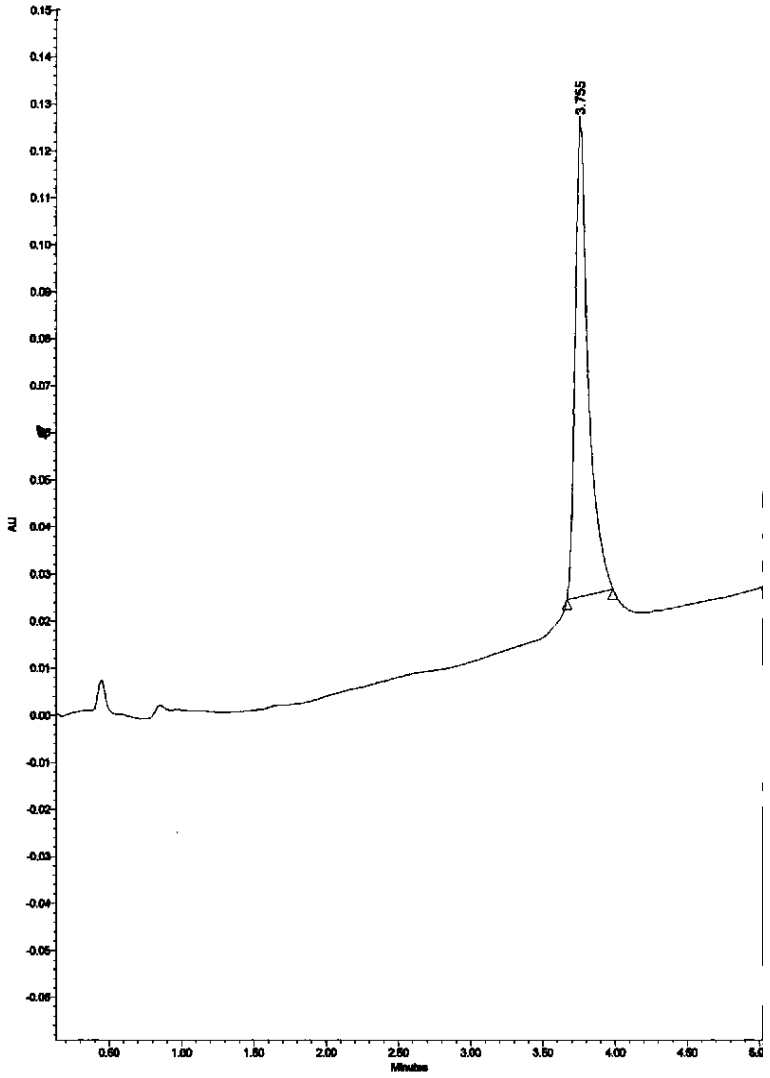


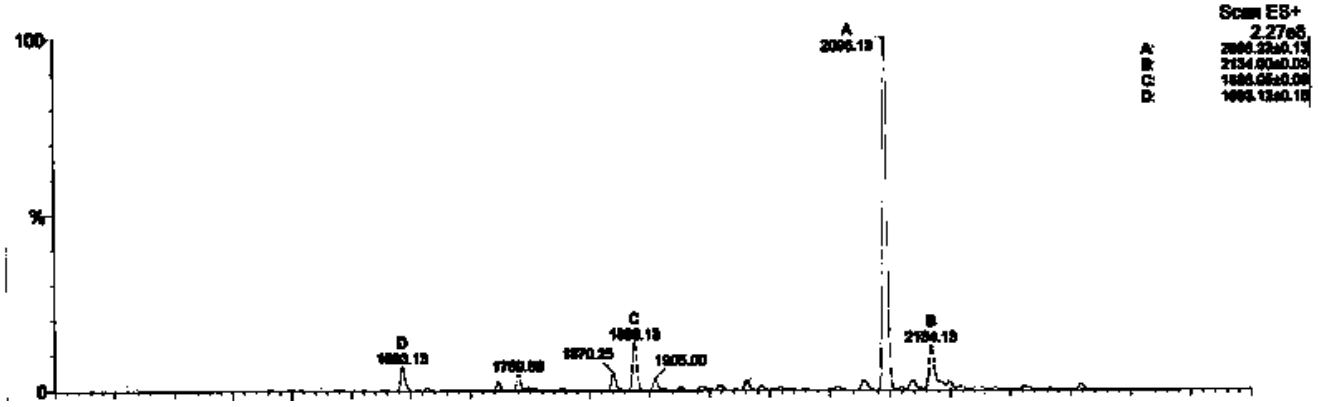
Dendrimer B_1



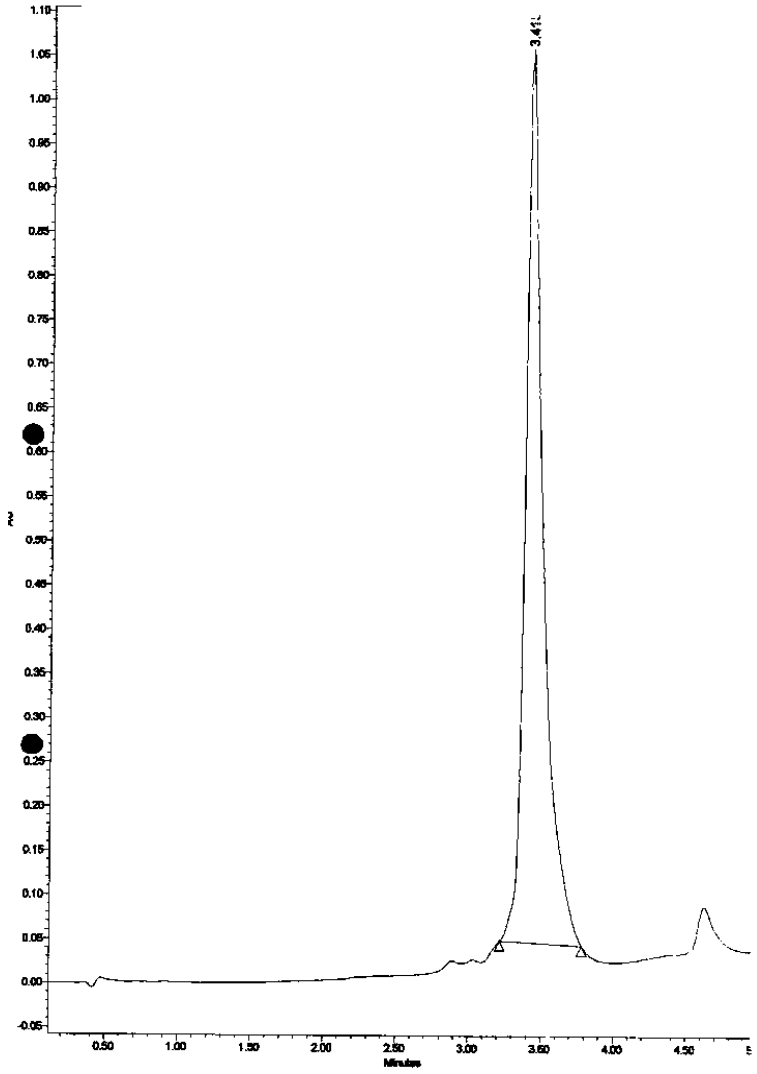


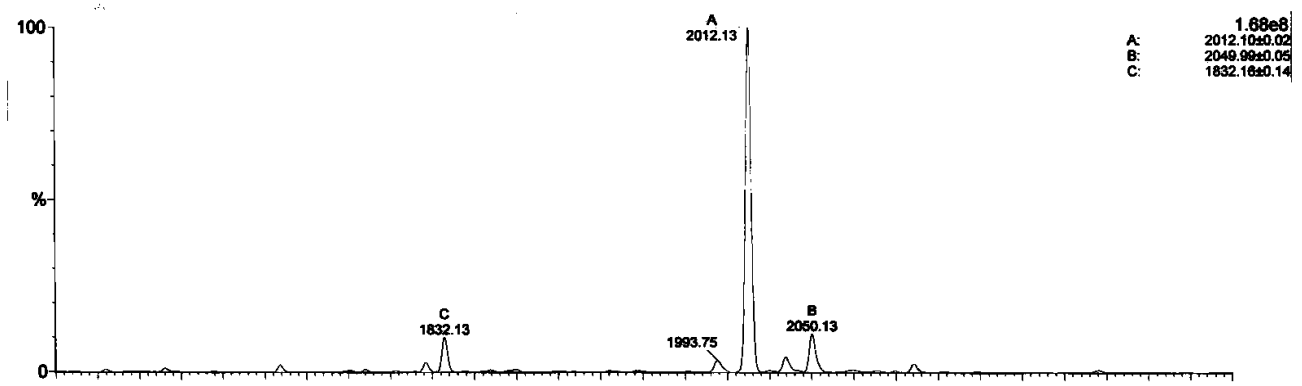
Dendrimer C_1



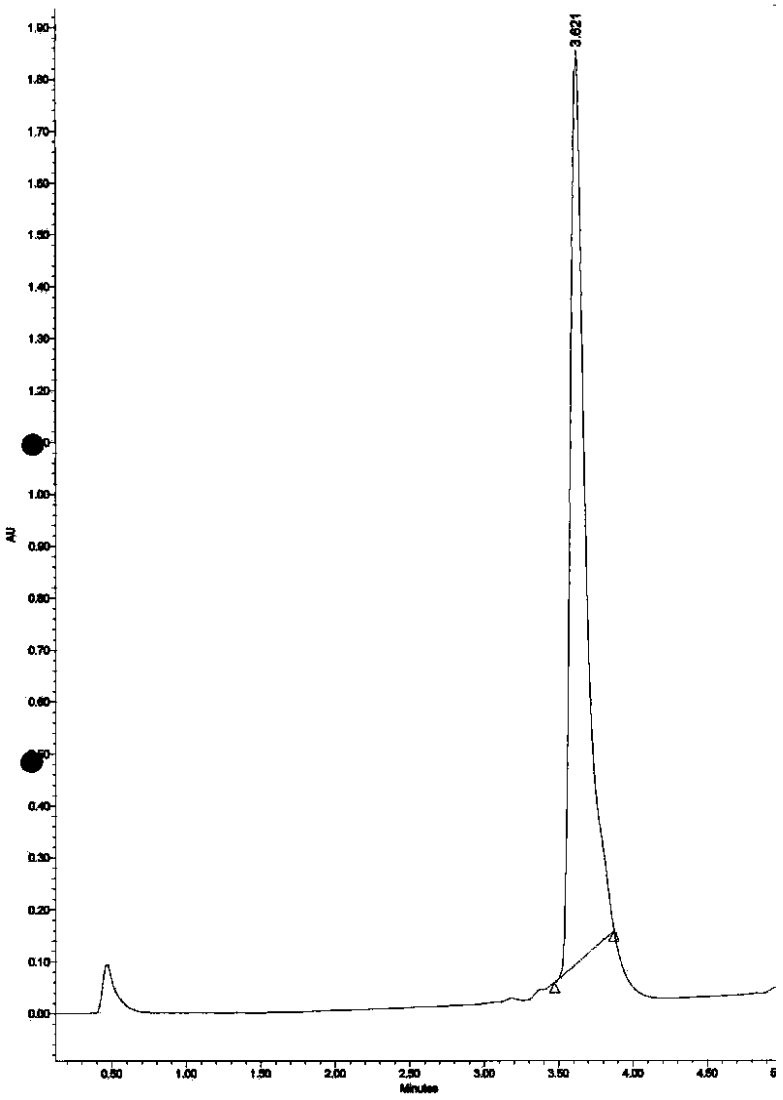


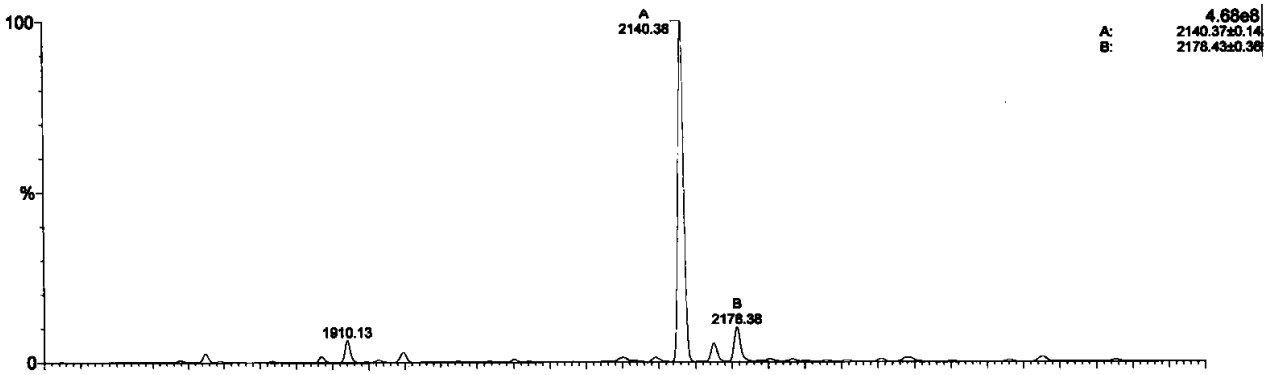
Dendrimer D_1



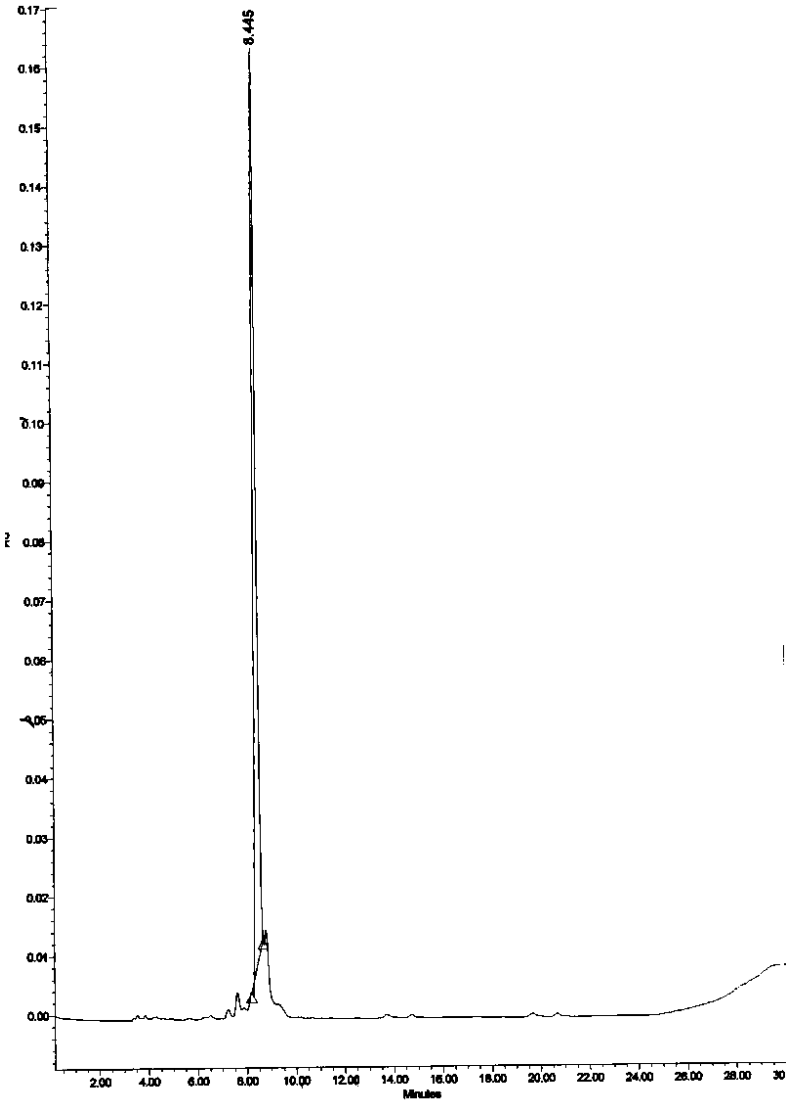


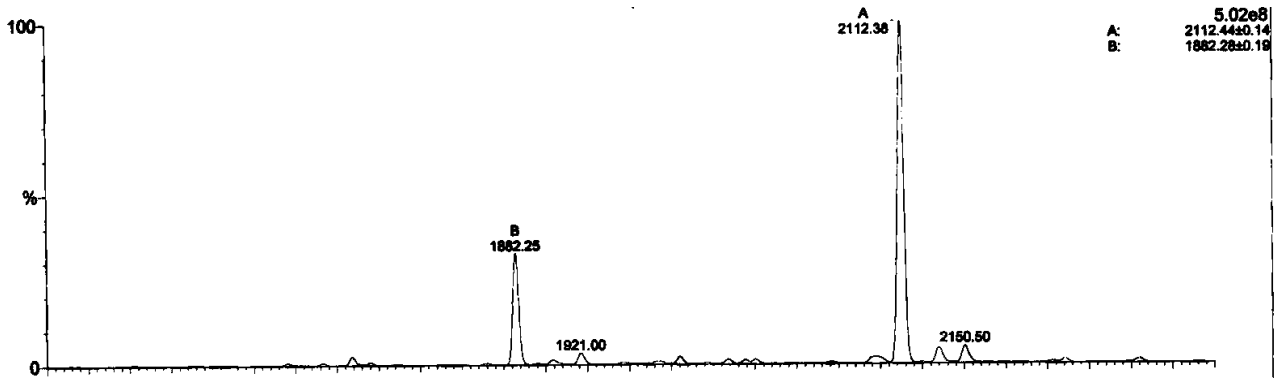
Dendrimer E_1



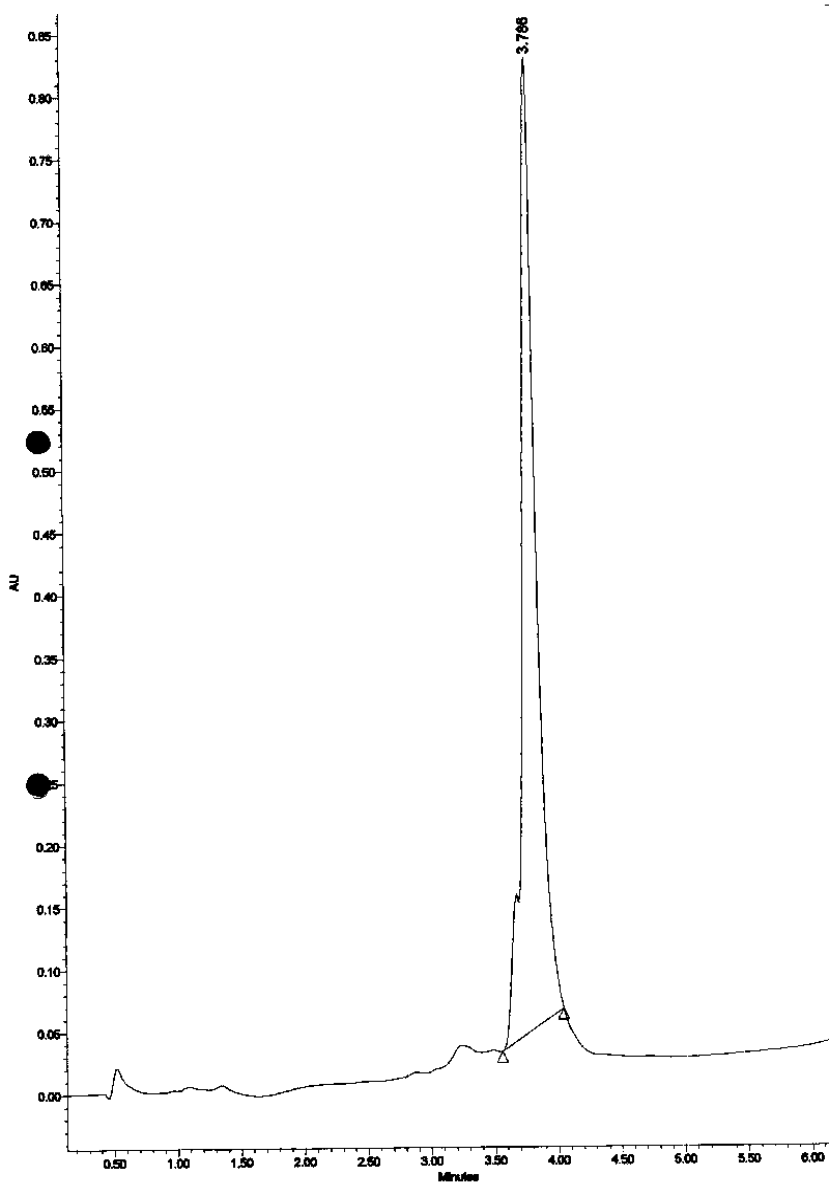


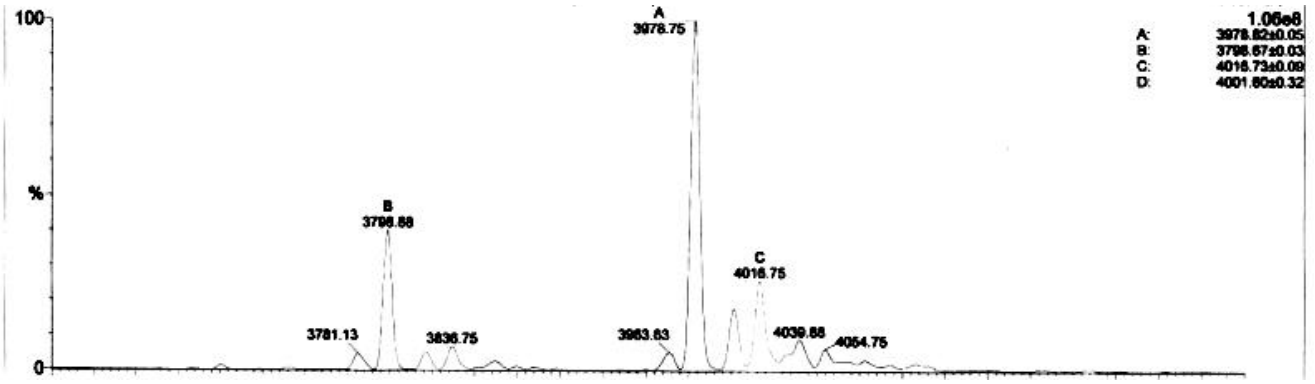
Dendrimer F_1



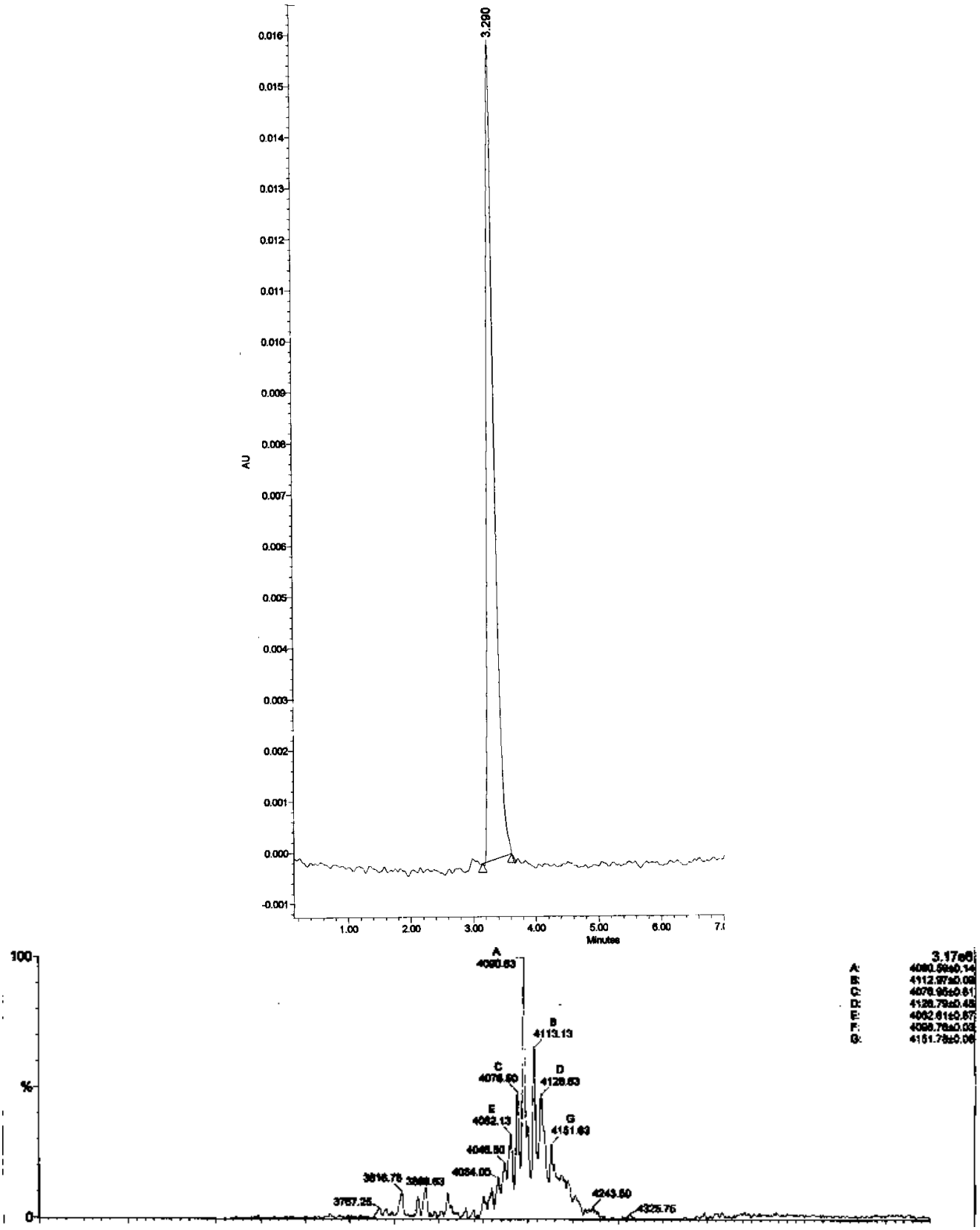


Dendrimer A_1-A_1

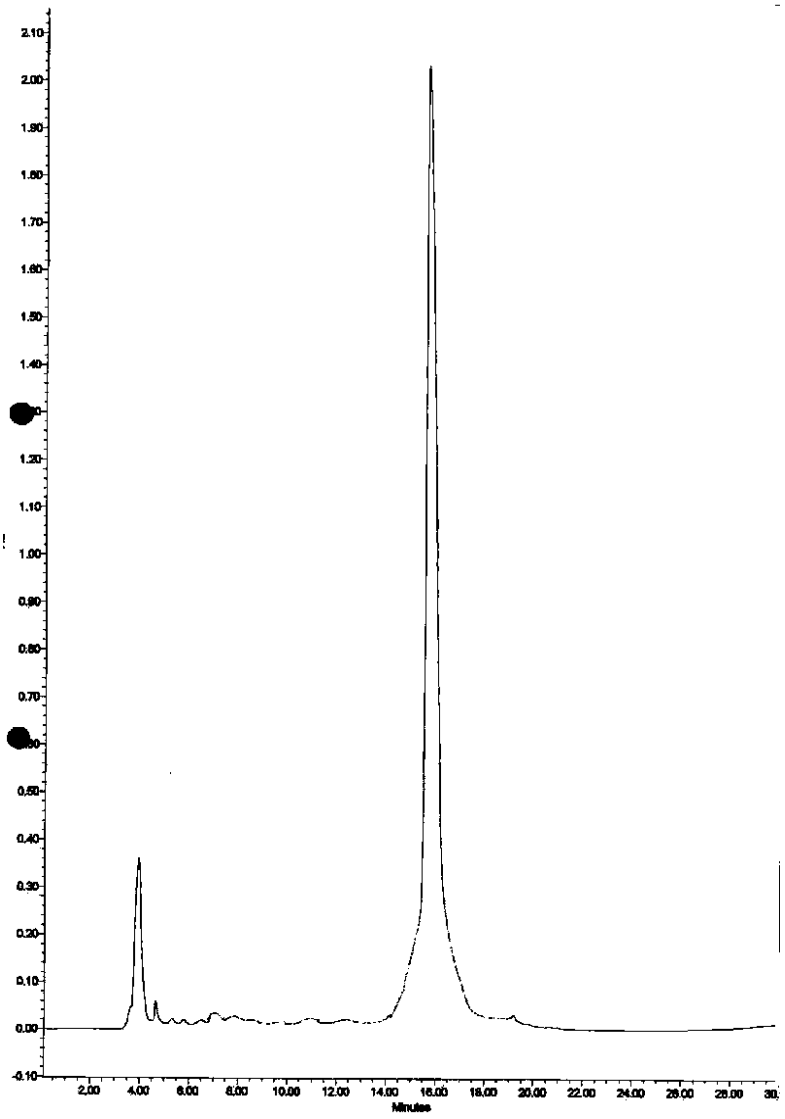


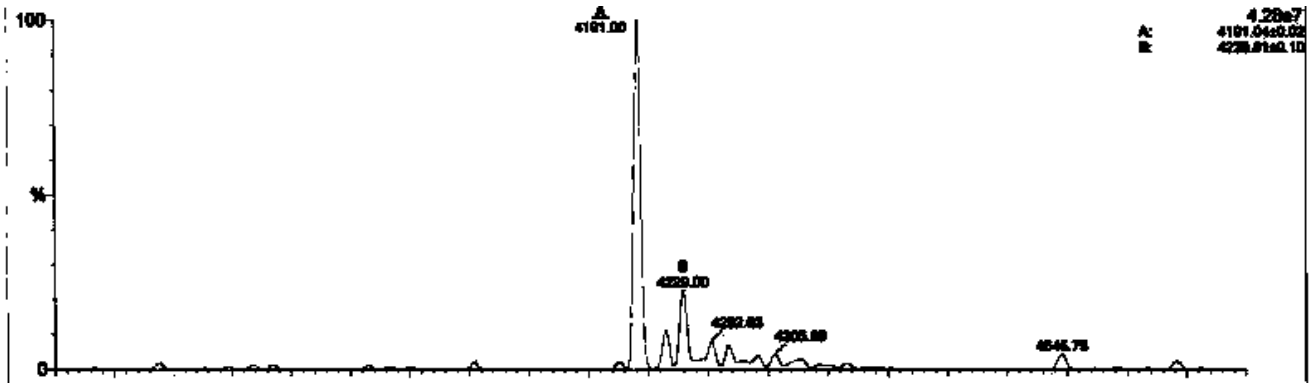


Dendrimer B_1-B_1

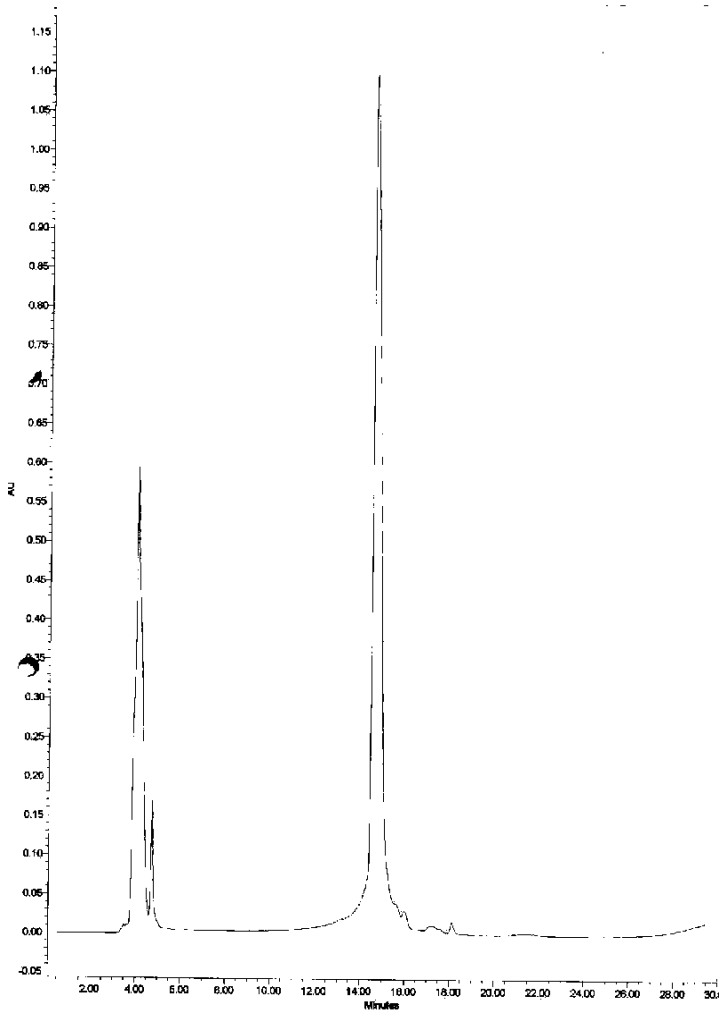


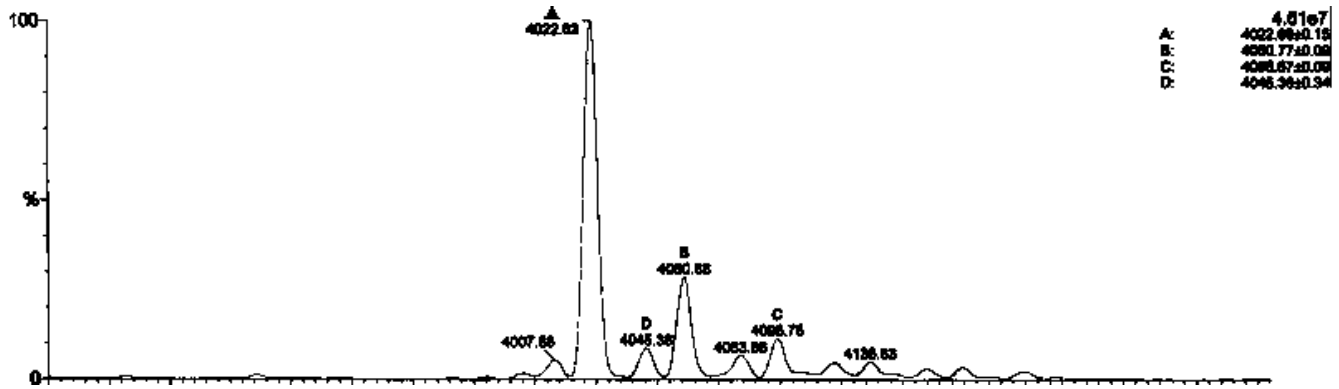
Dendrimer C_1-C_1



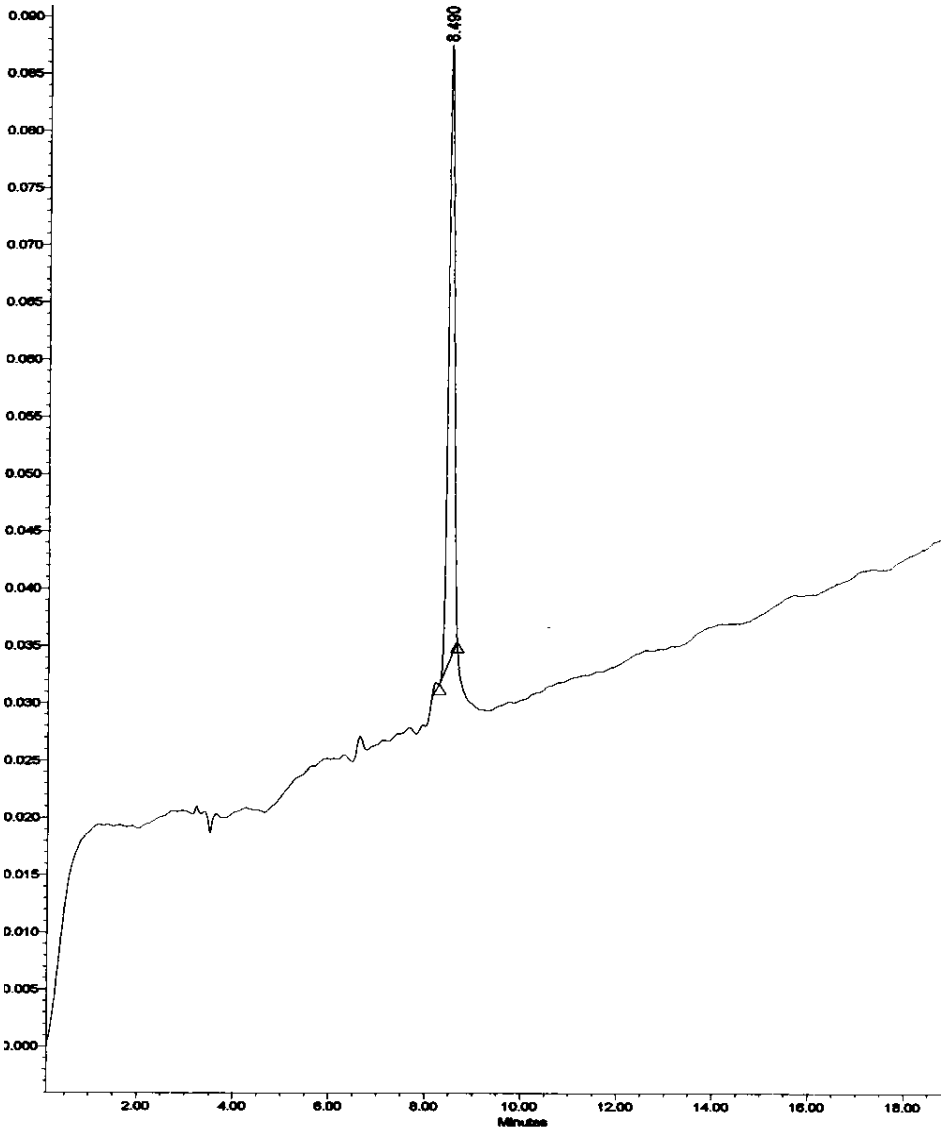


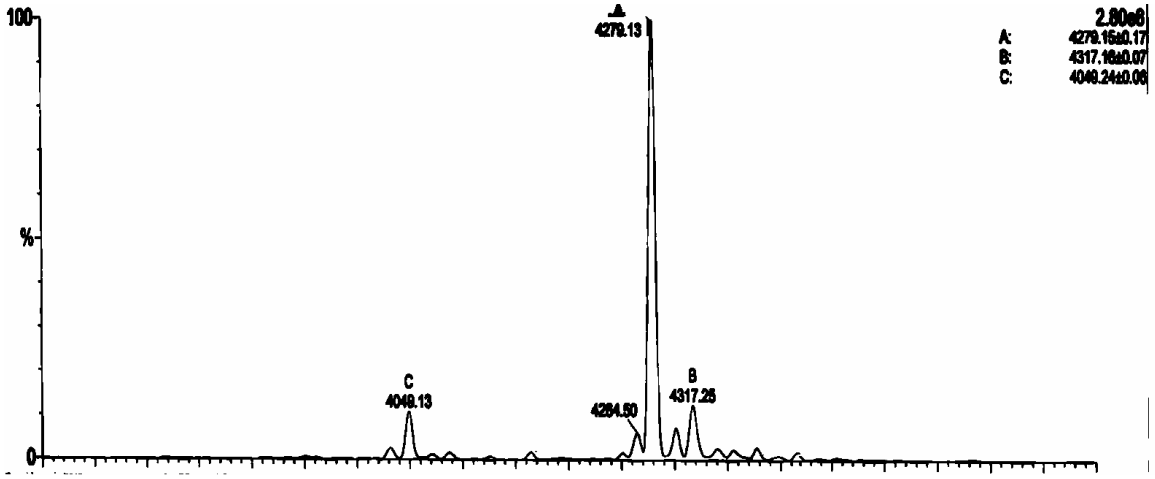
Dendrimer D_1-D_1



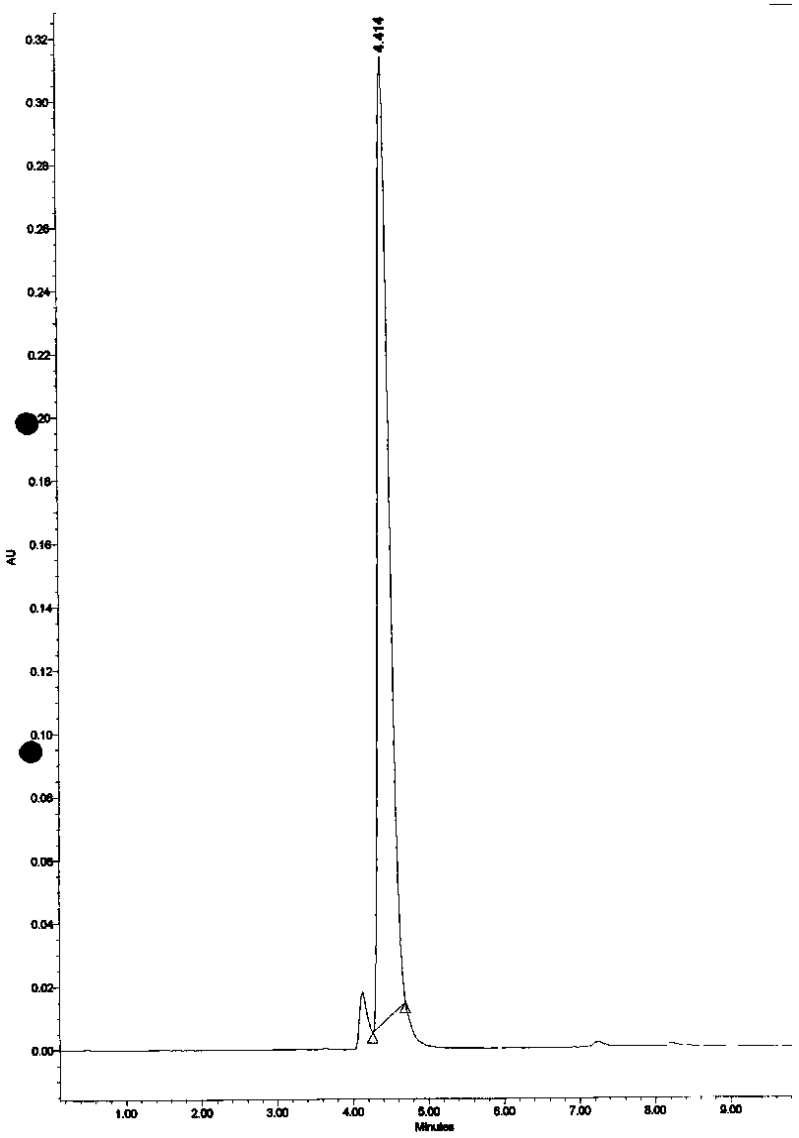


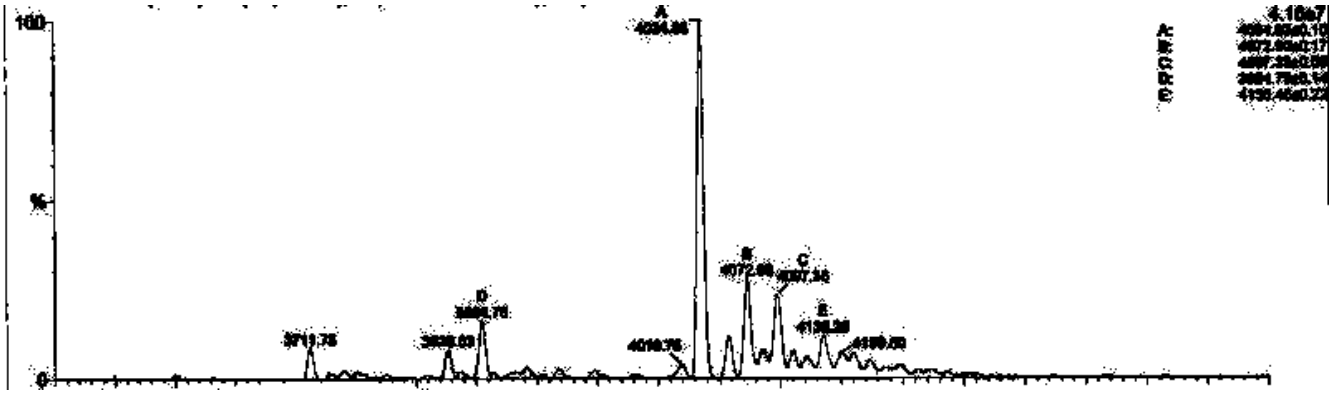
Dendrimer E_1-E_1



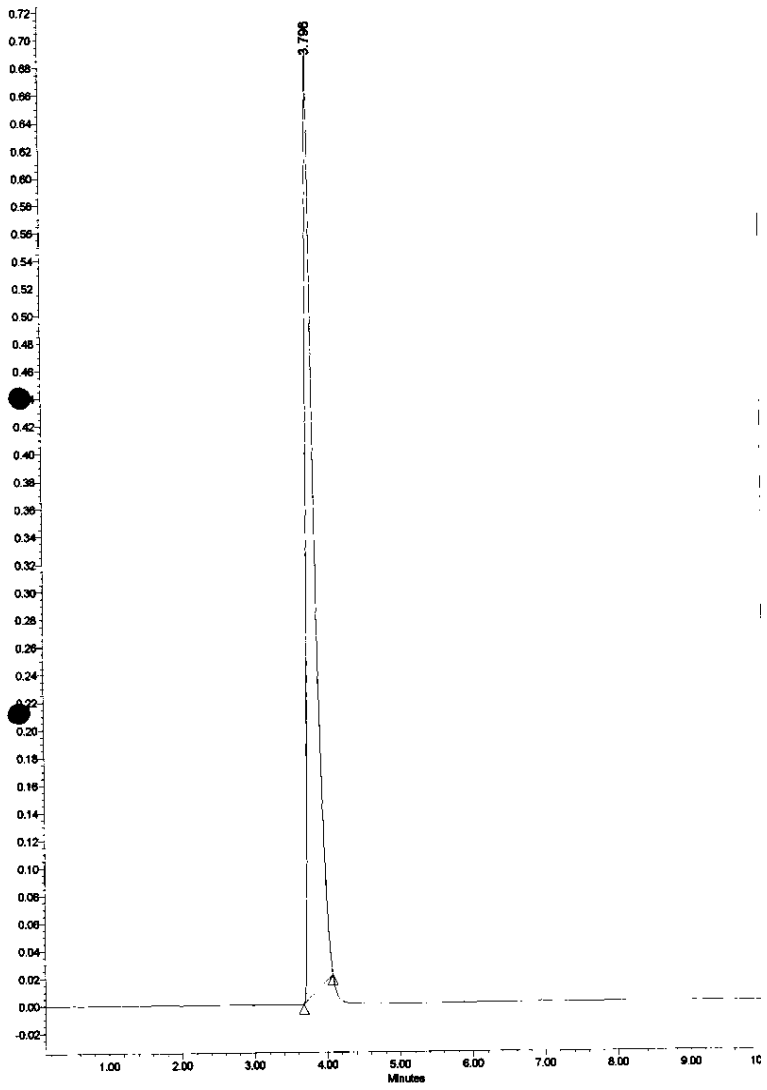


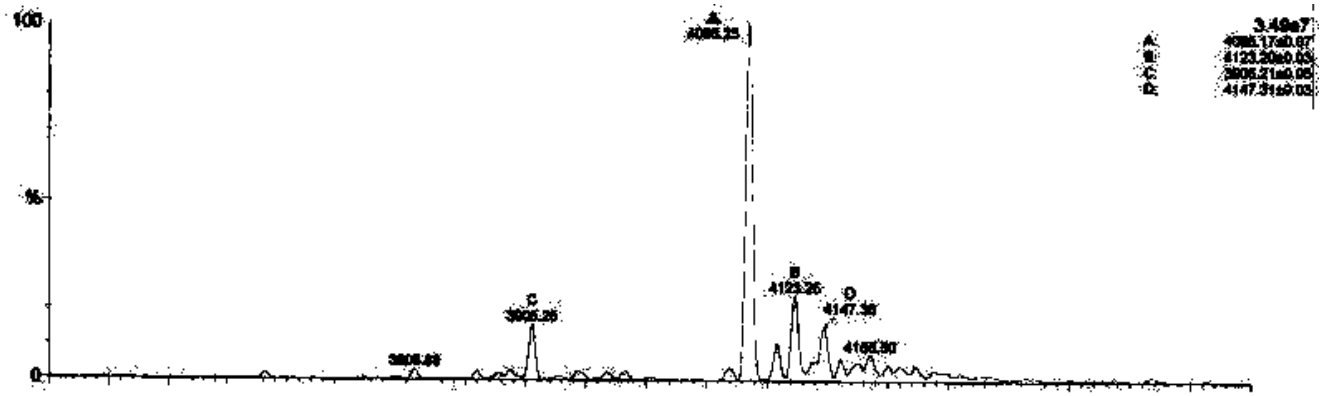
Dendrimer A_1-B_1



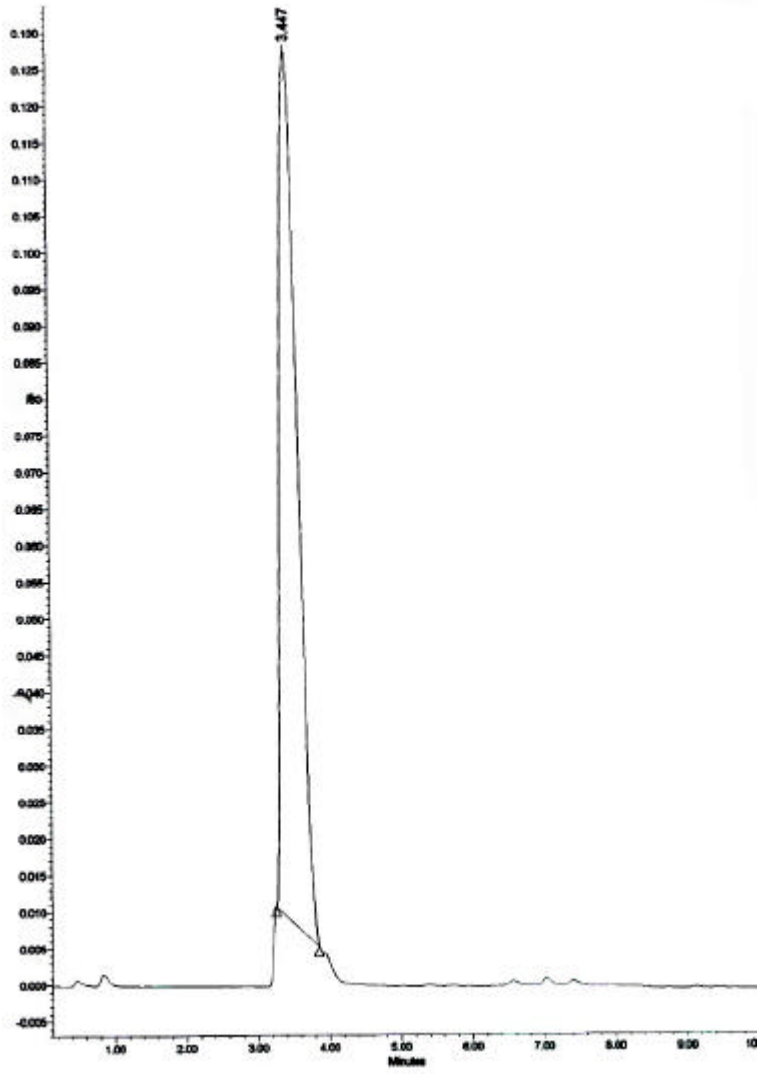


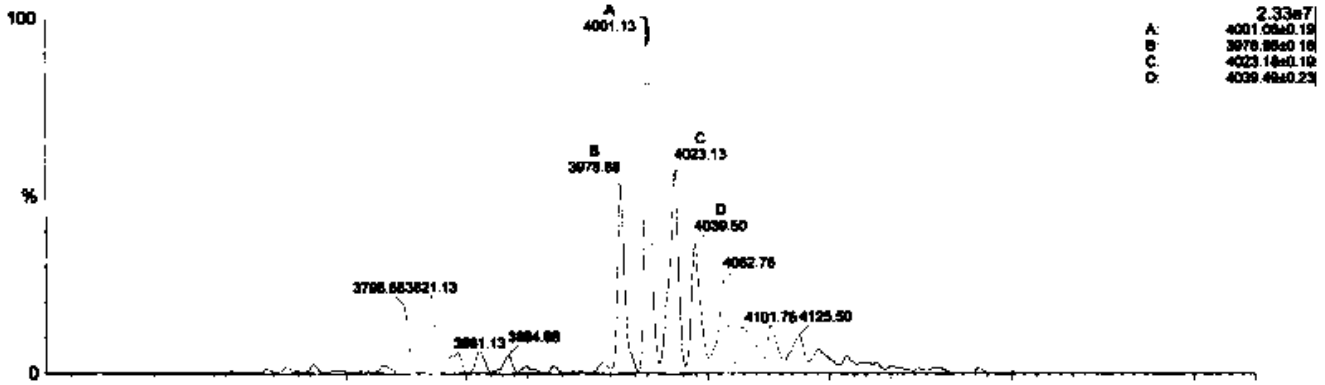
Dendrimer A_1-C_1



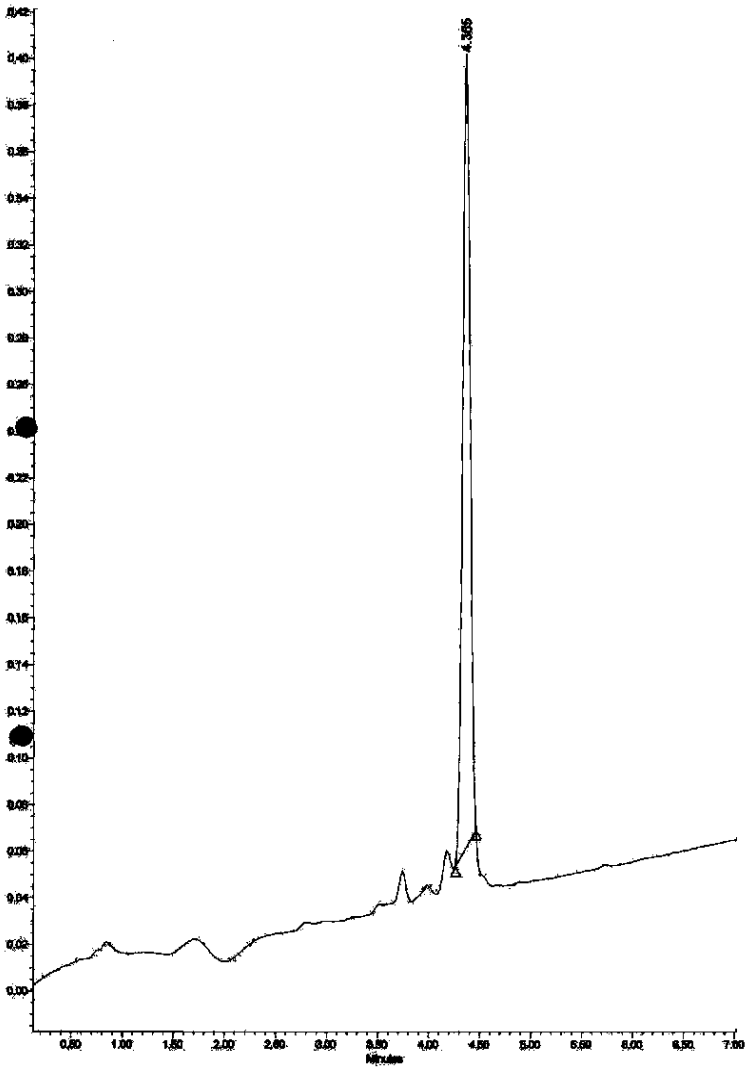


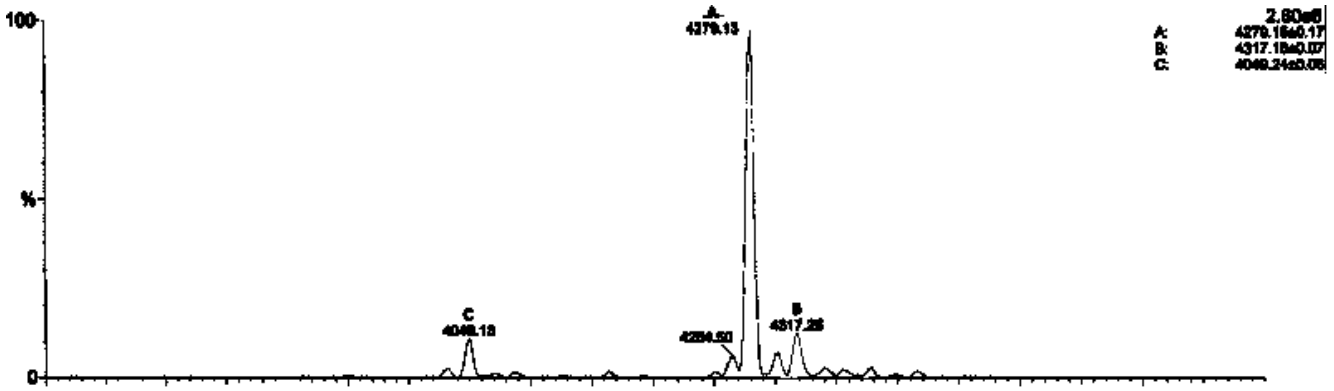
Dendrimer A_1-D_1



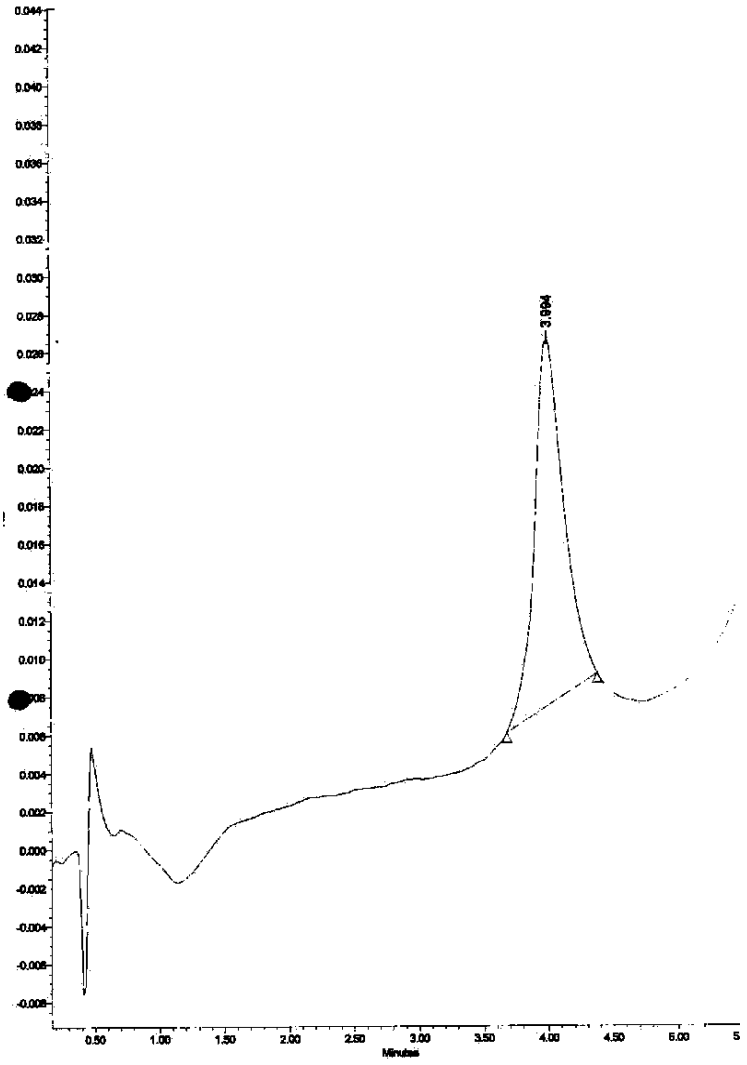


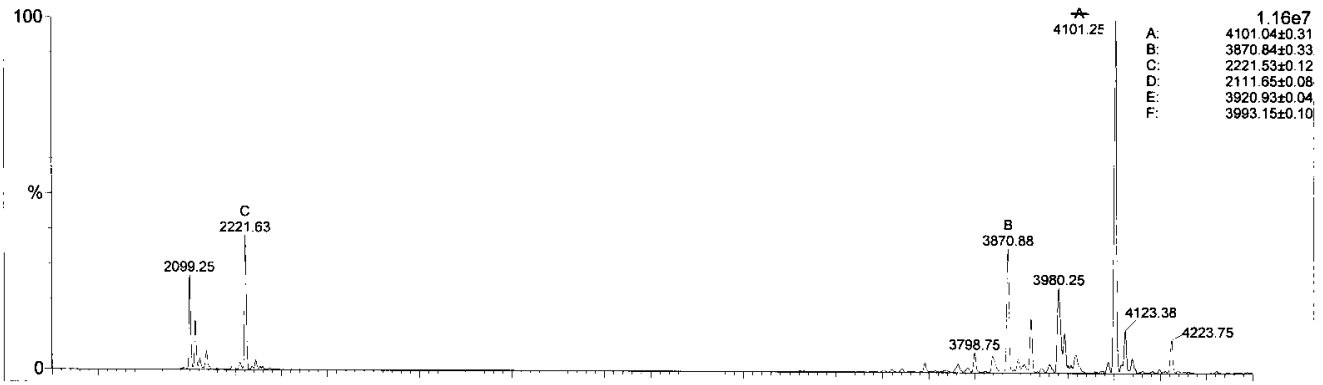
Dendrimer A_1-E_1





Dendrimer A_1-F_1





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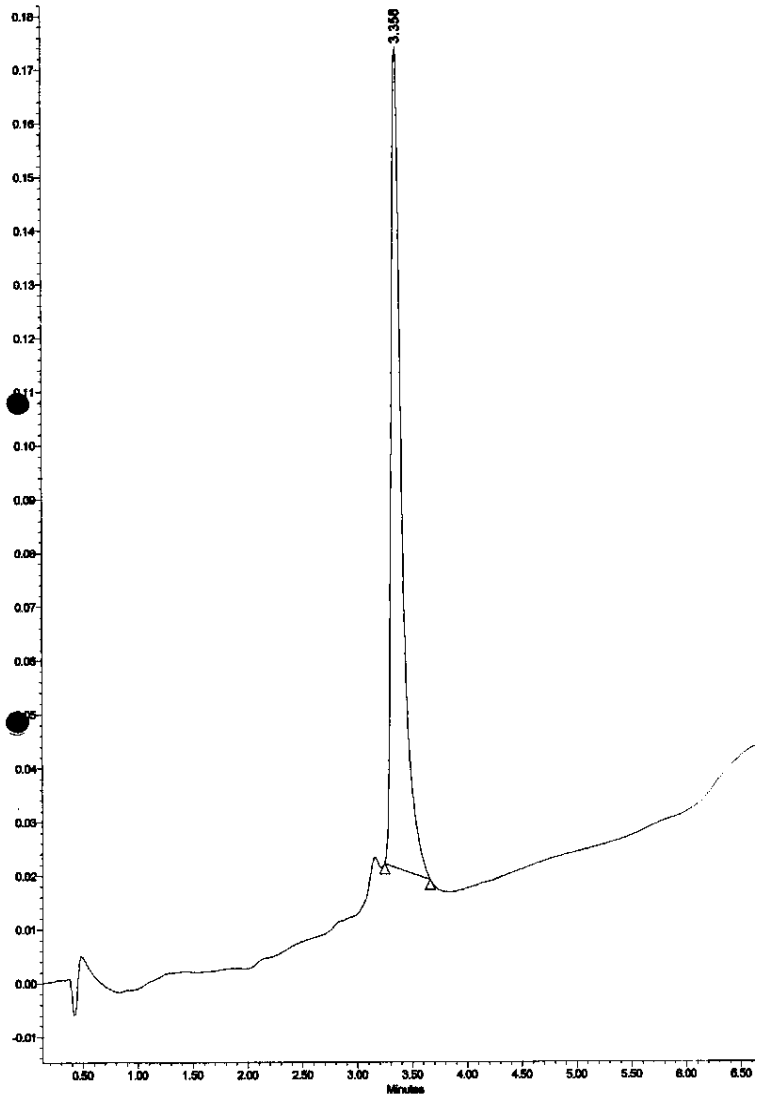

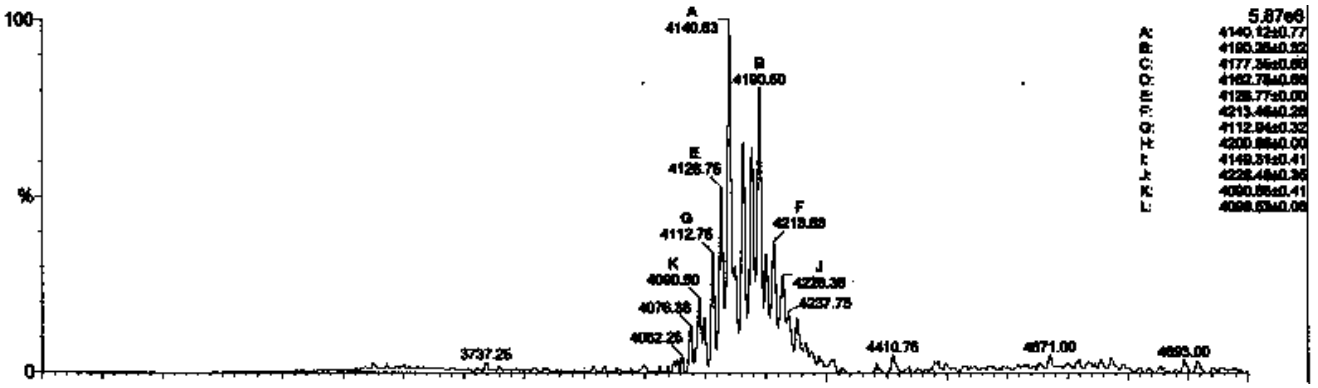

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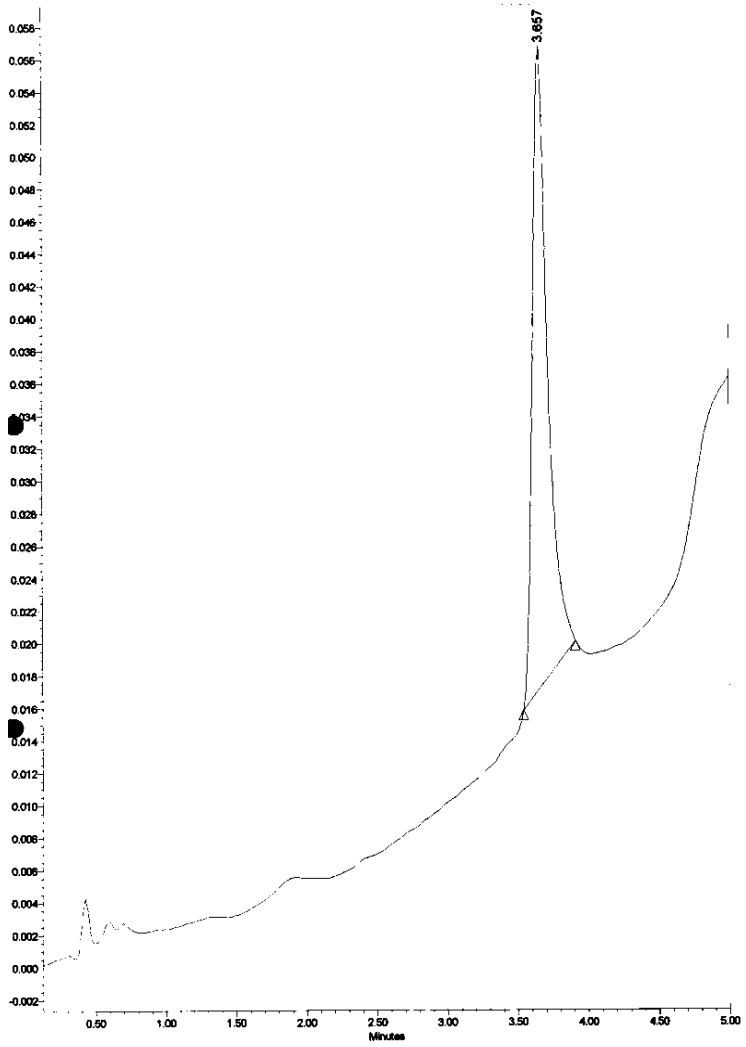

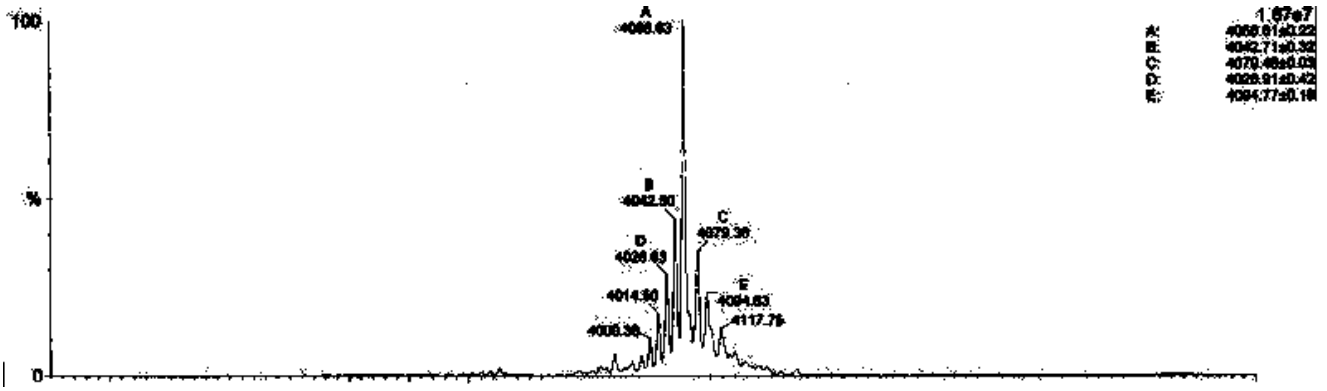

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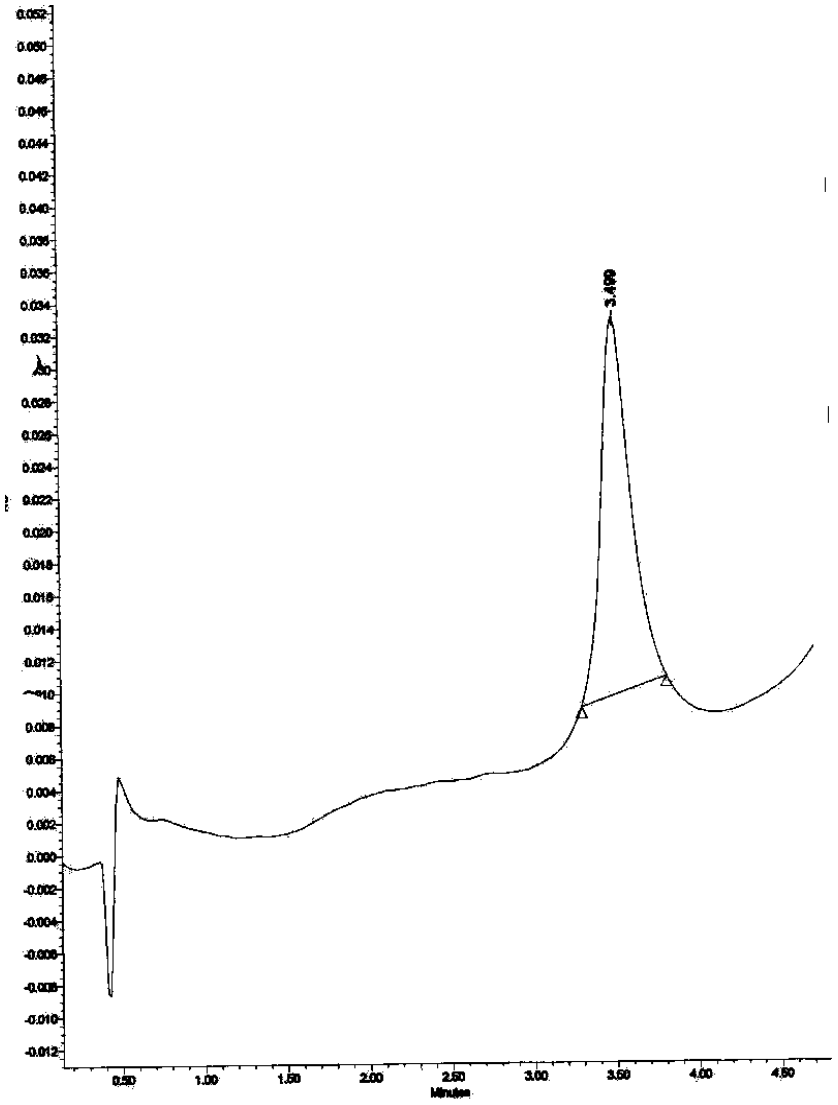
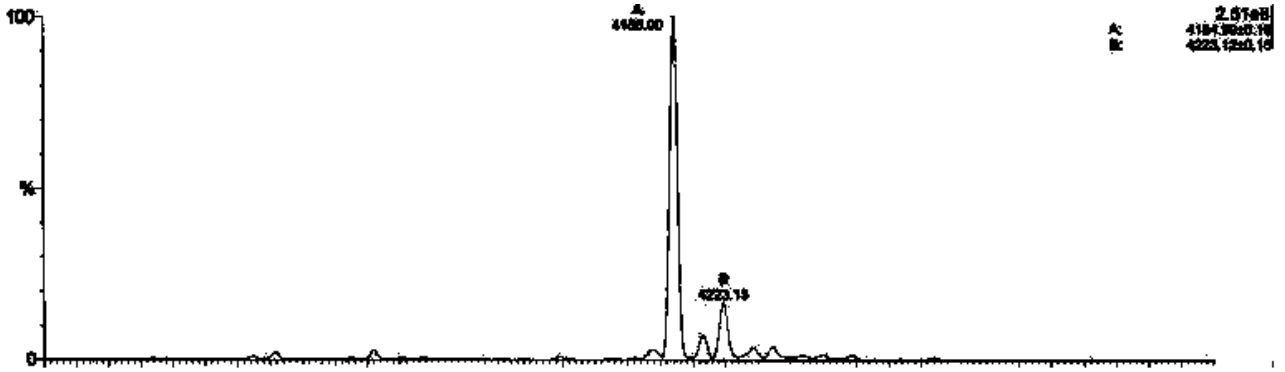
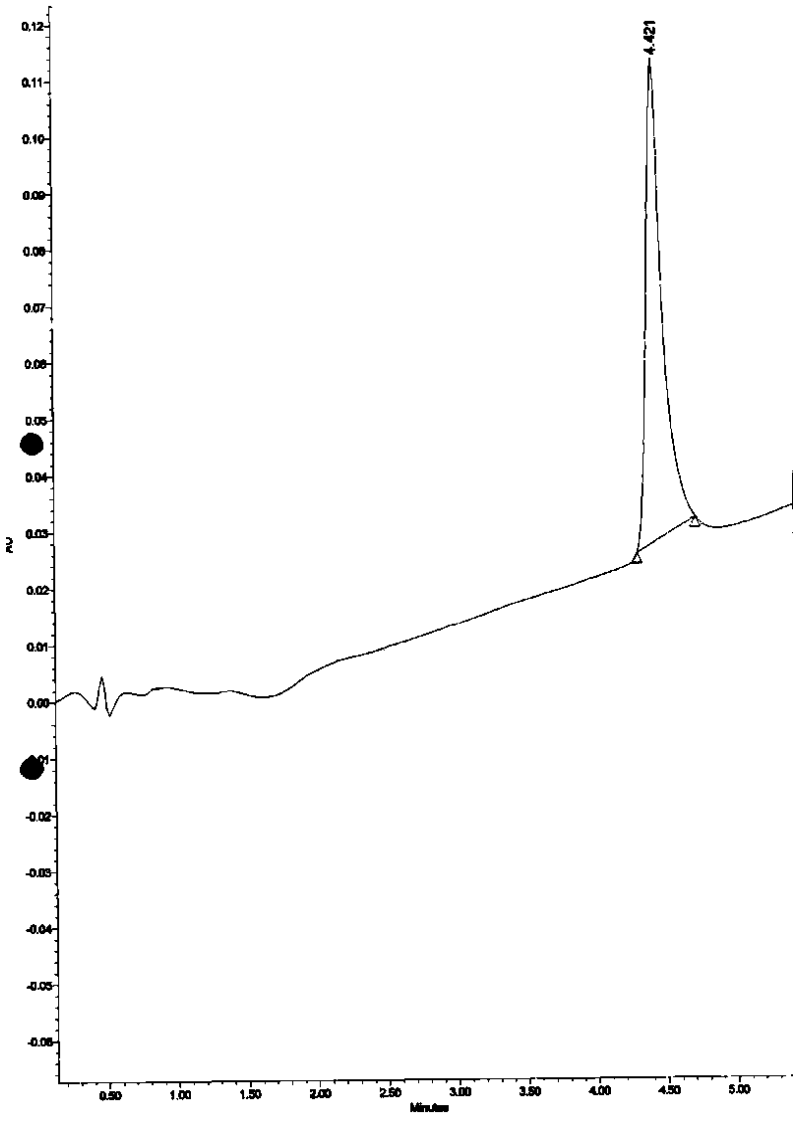
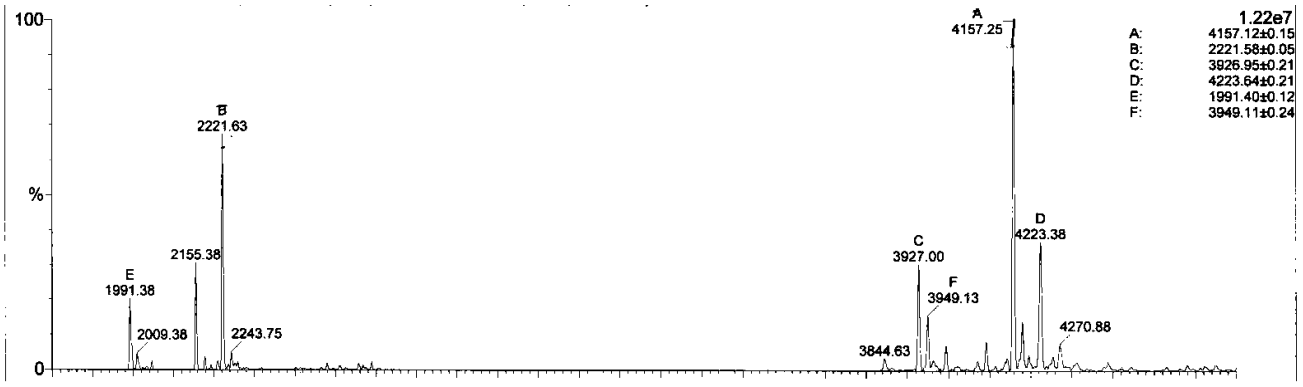


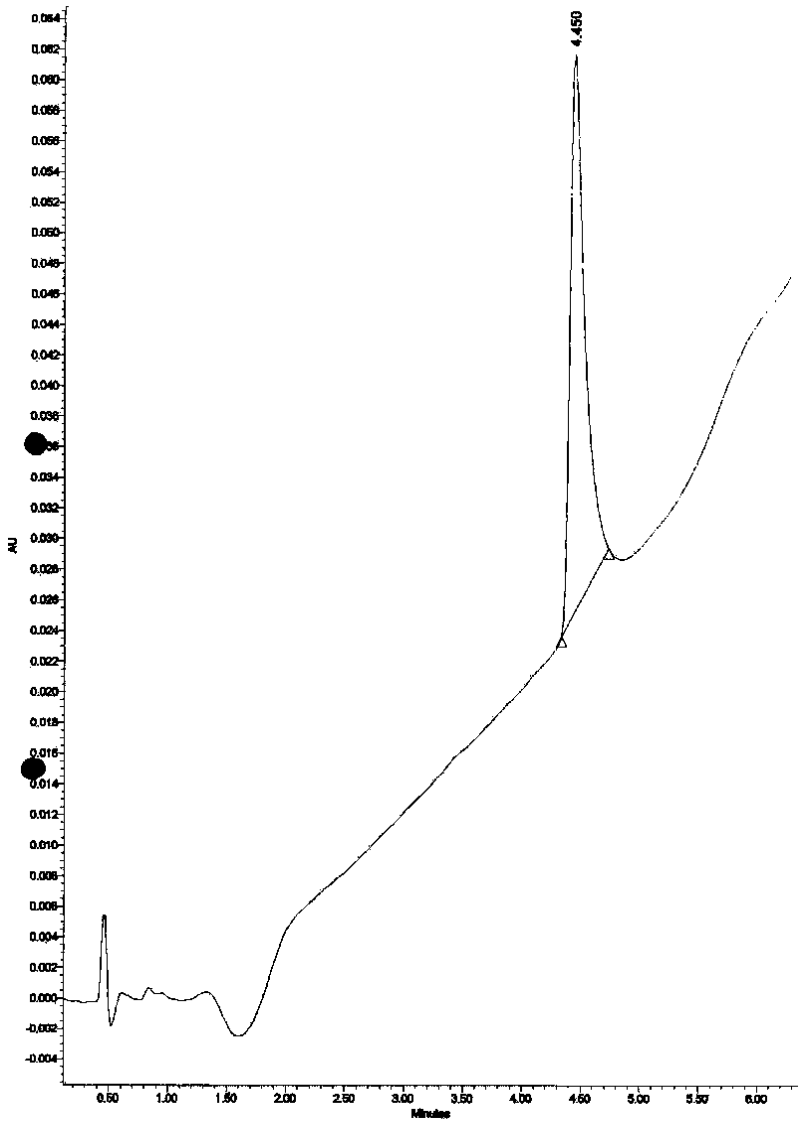


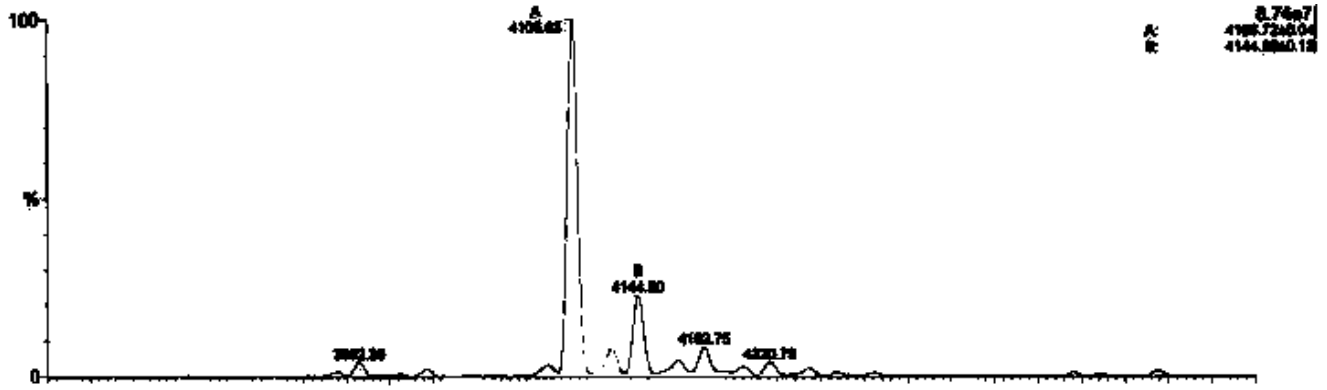
Dendrimer B_1-F_1



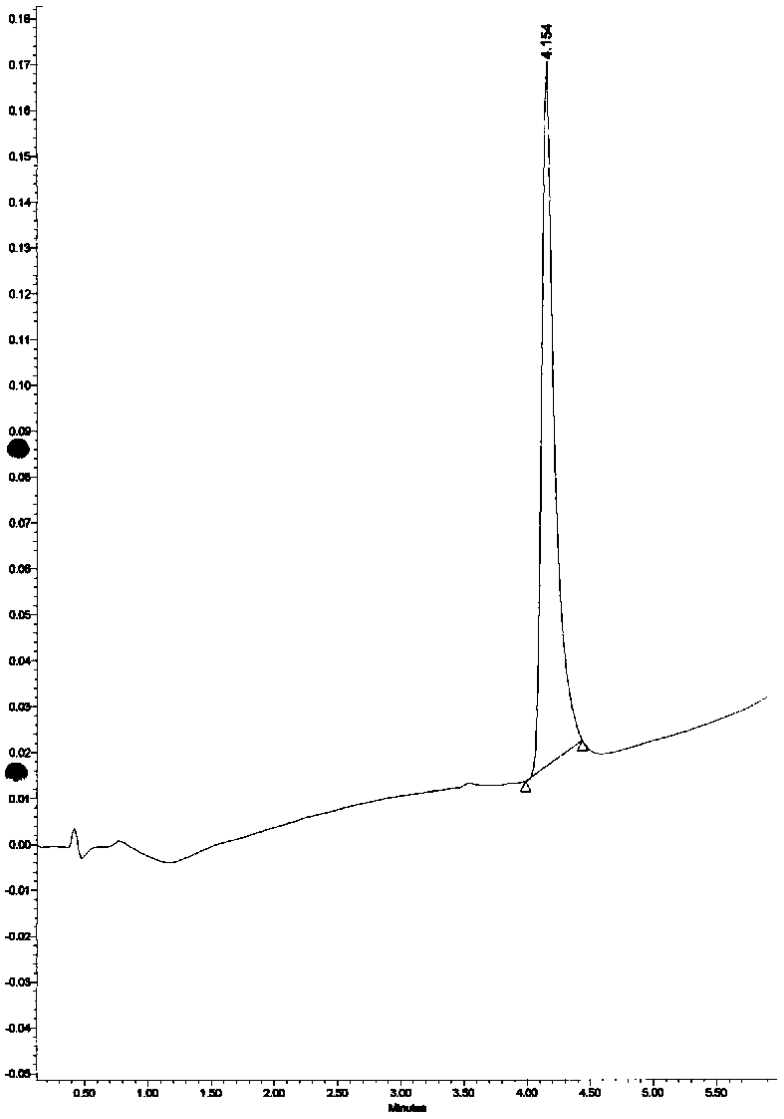


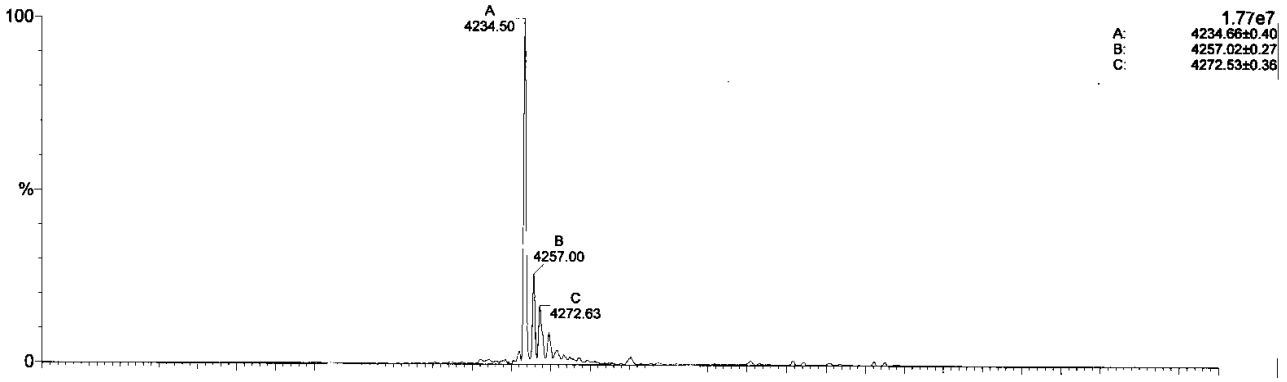
Dendrimer C_1-D_1



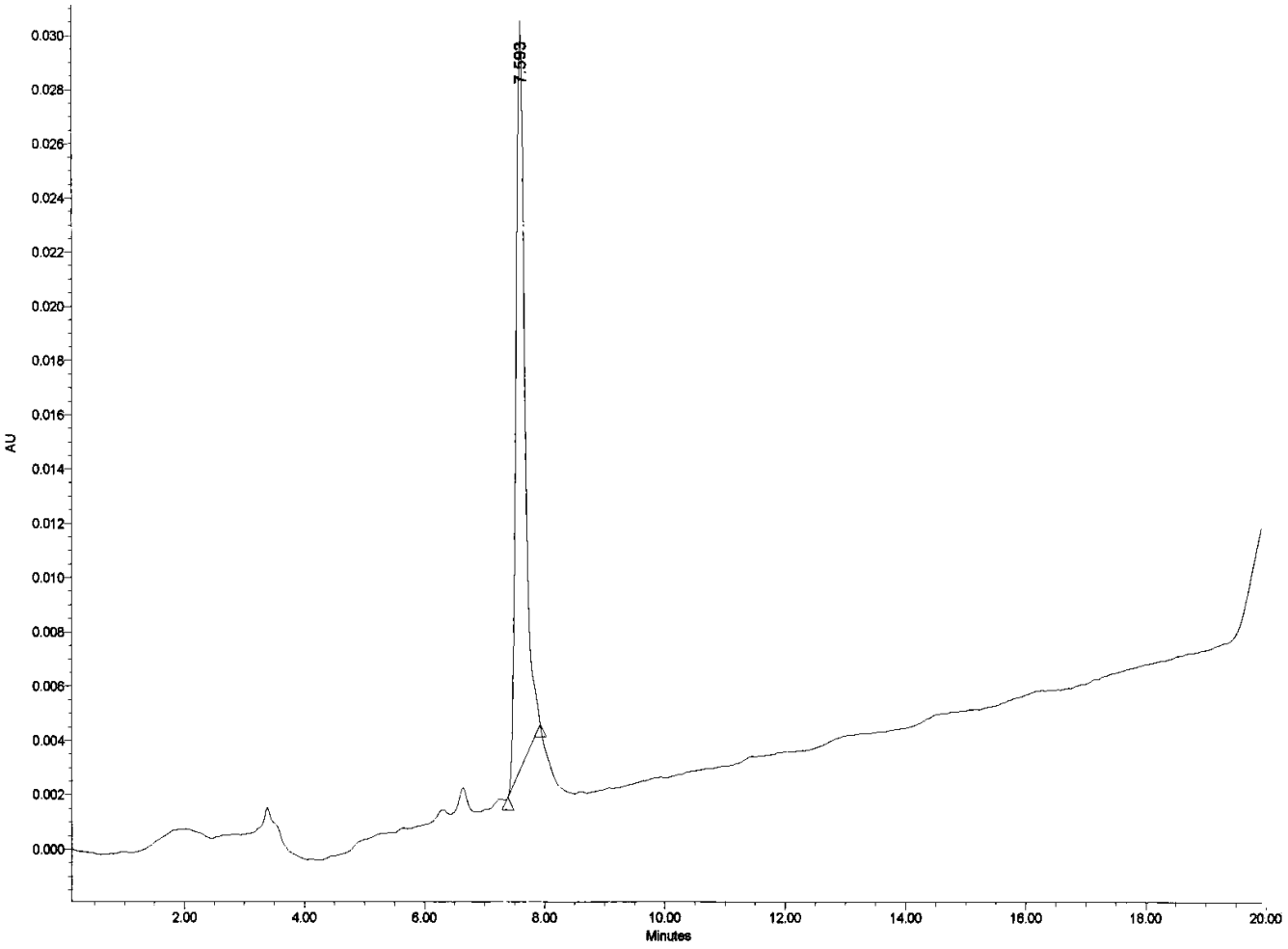


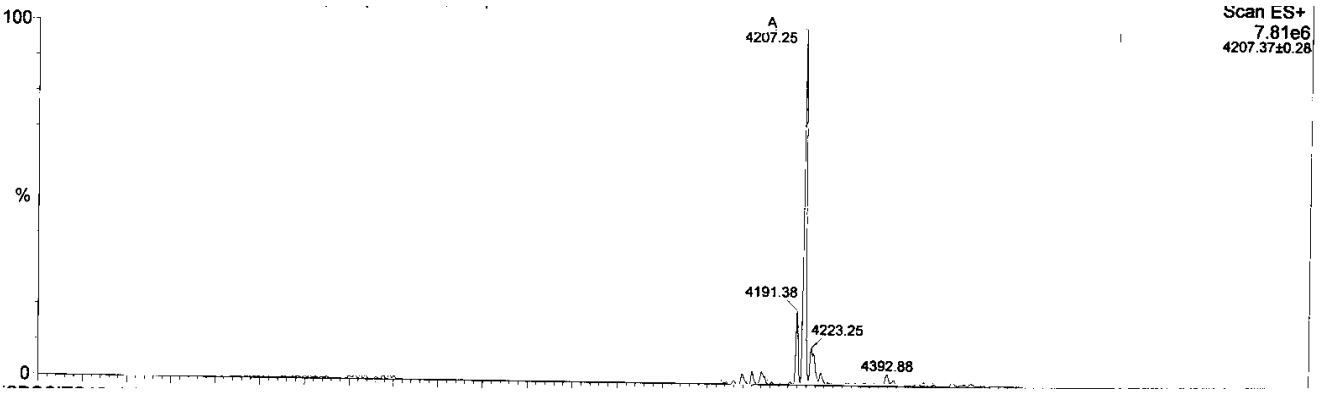
Dendrimer C_1-E_1



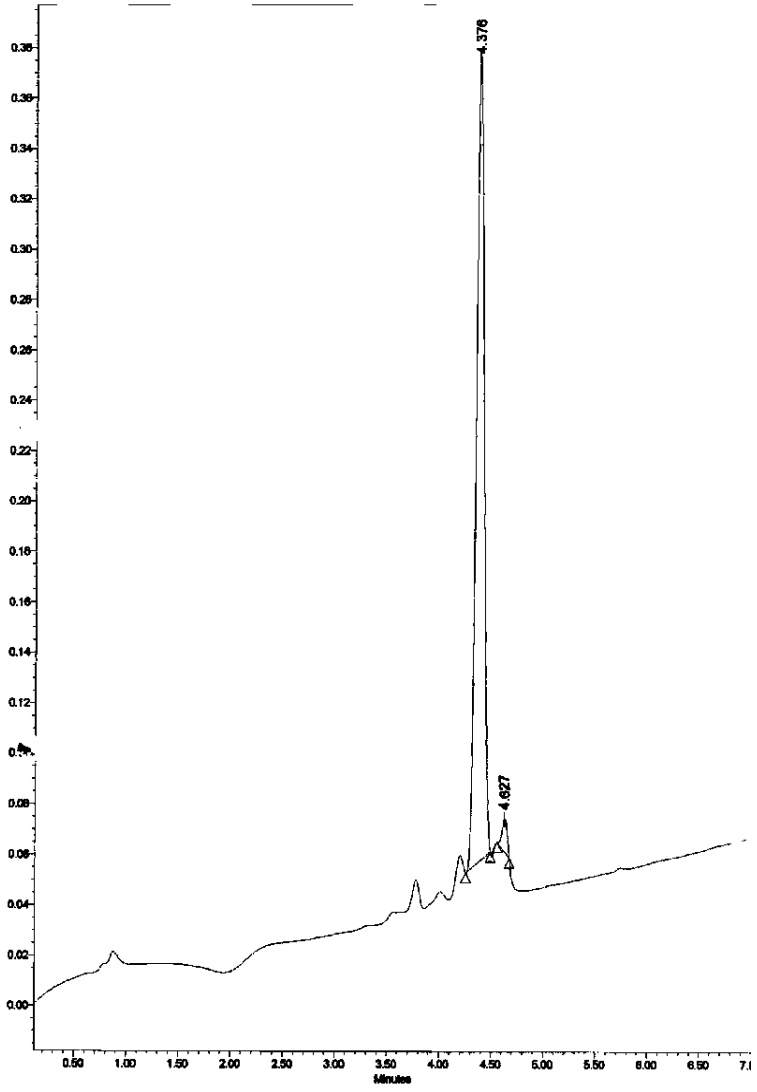


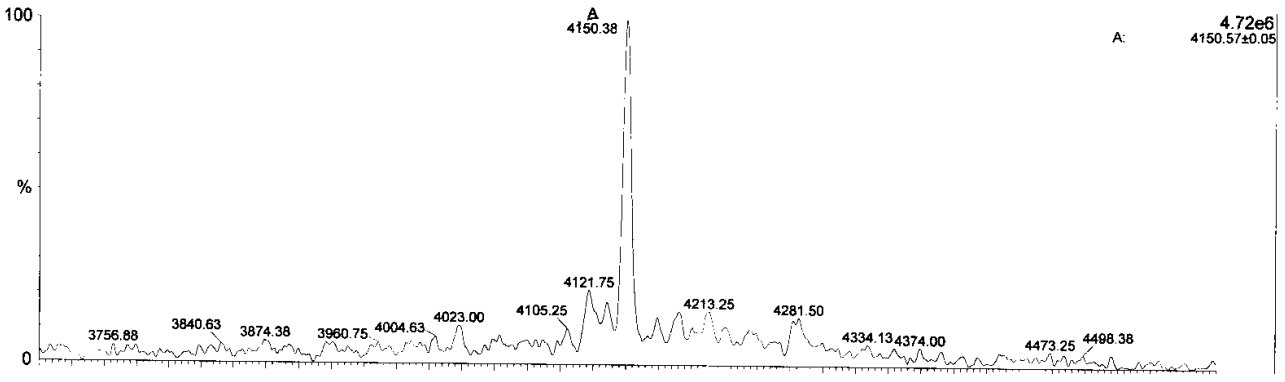
Dendrimer C_1-F_1



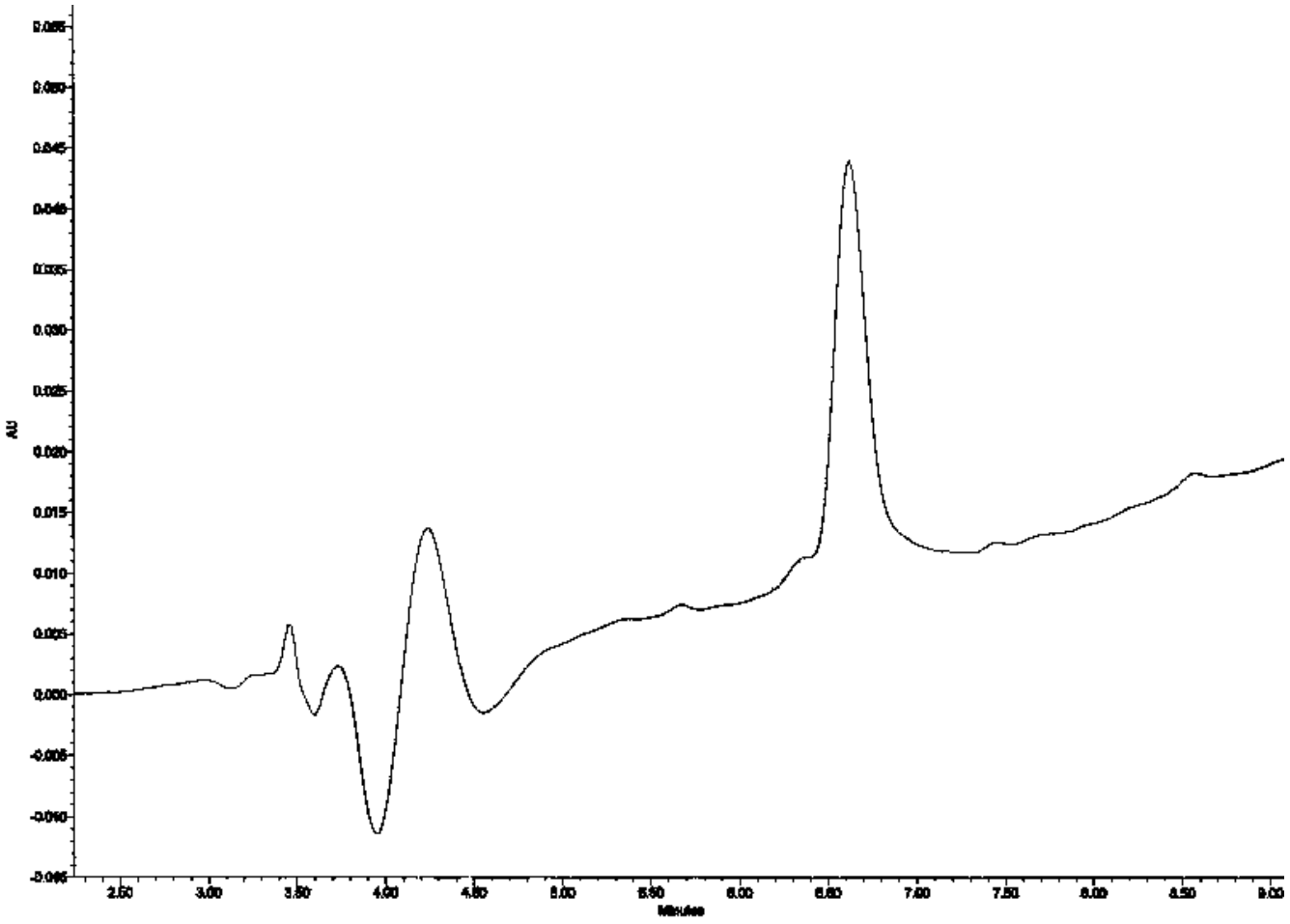


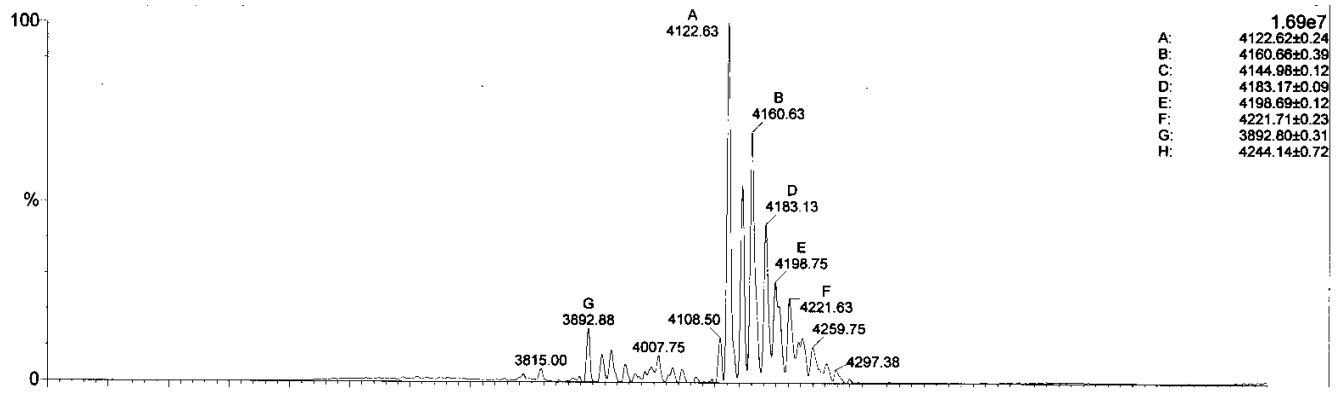
Dendrimer D_1-E_1



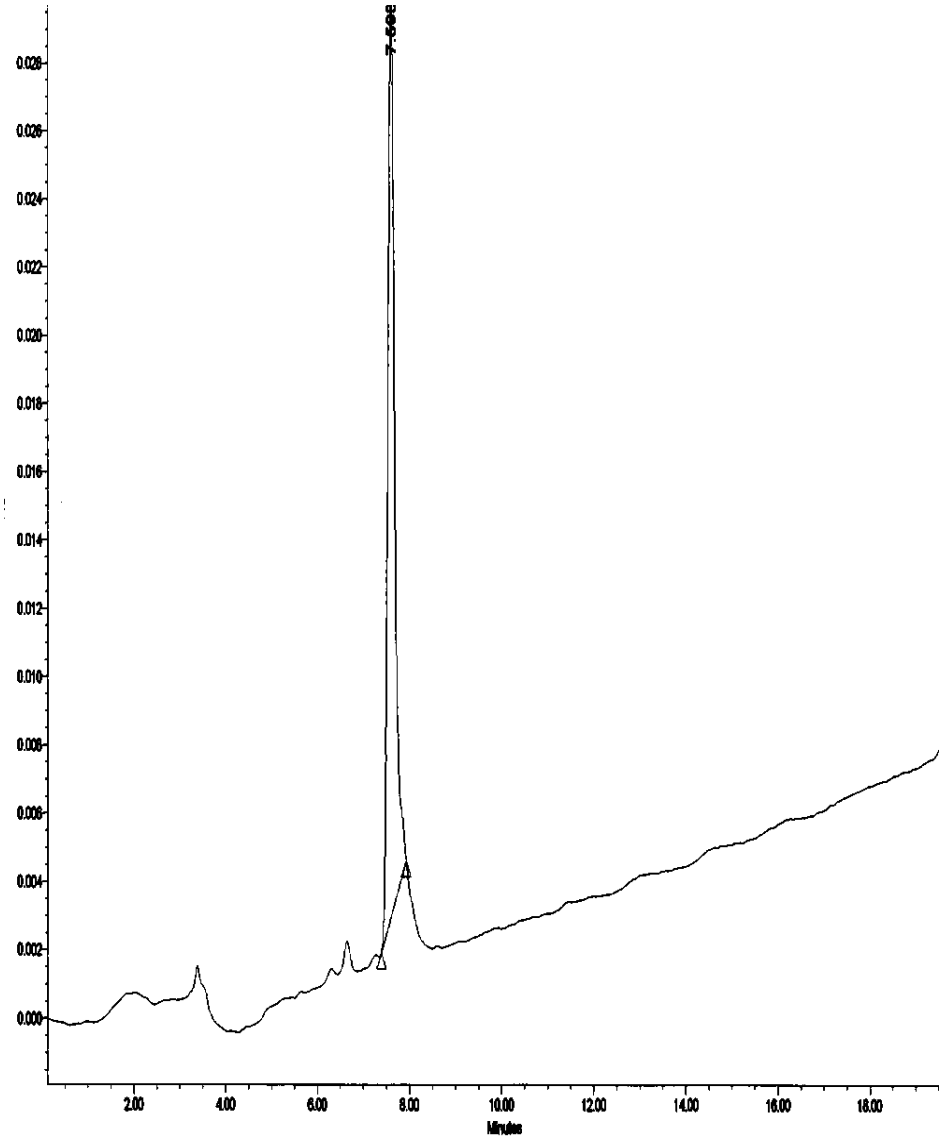


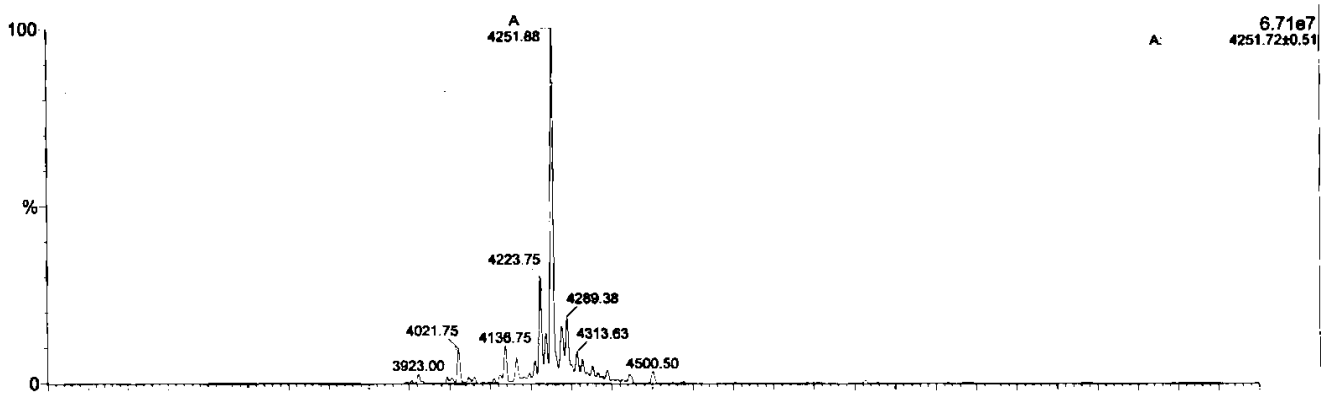
Dendrimer D_1-F_1



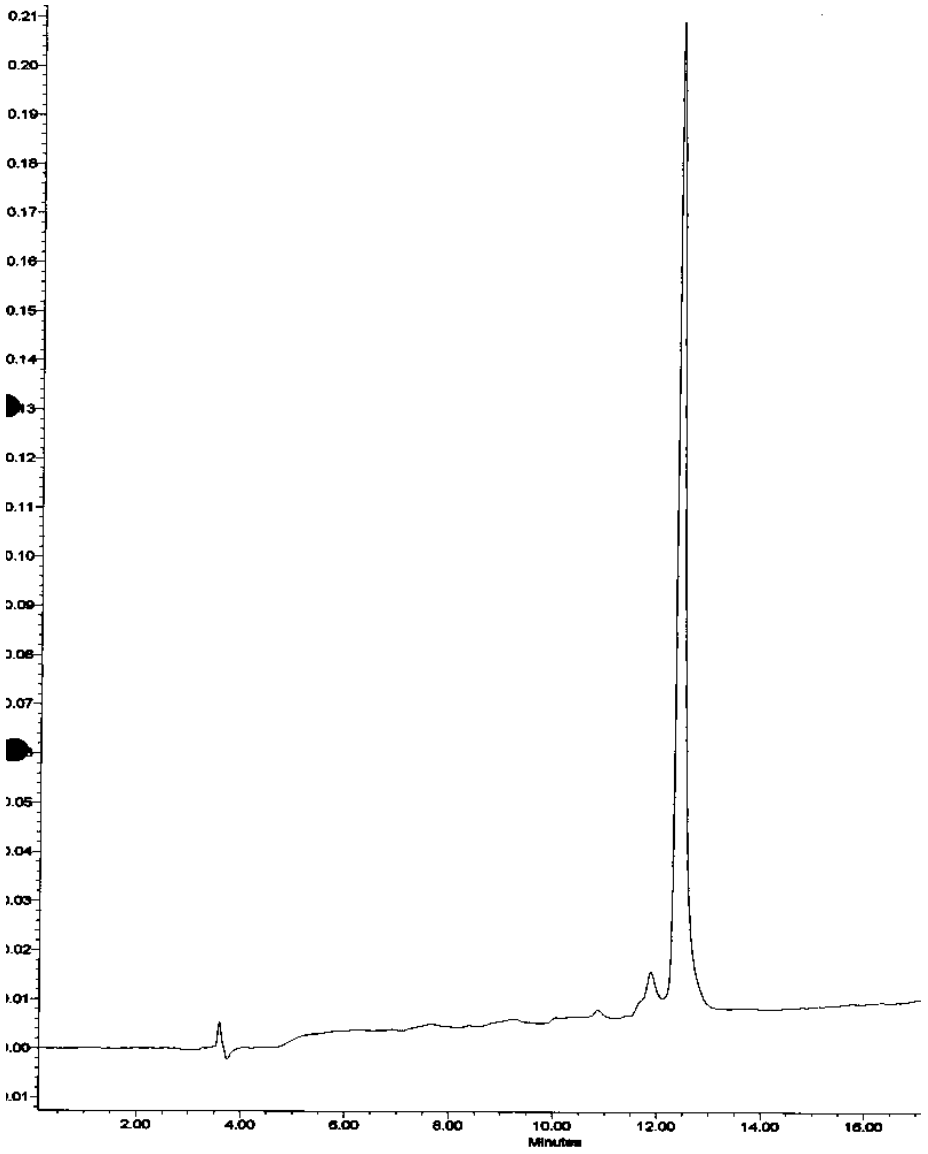


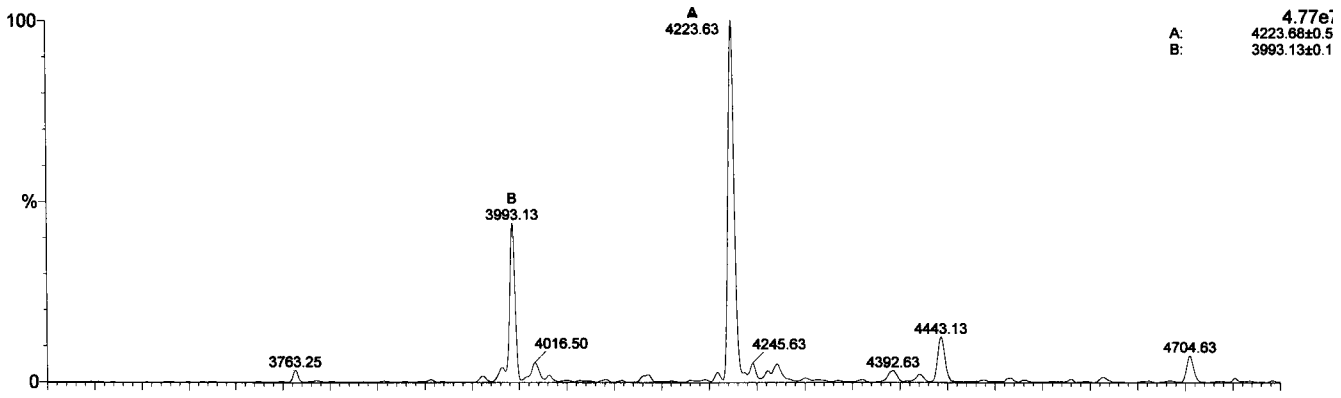
Dendrimer E_1-F_1



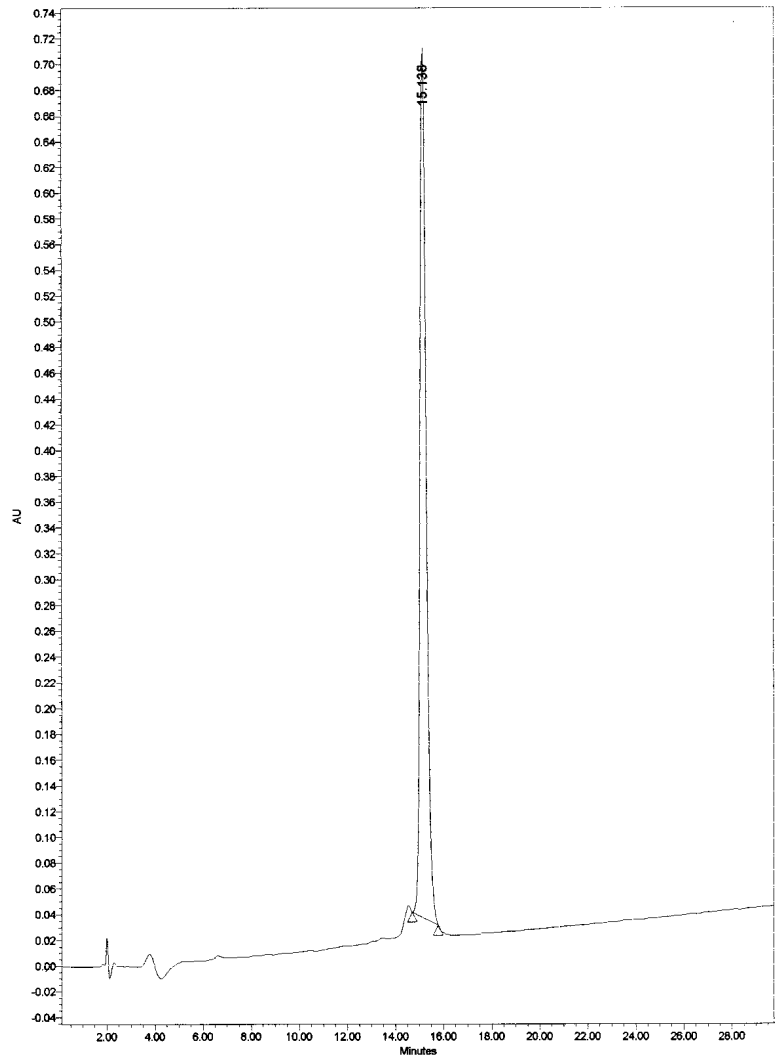


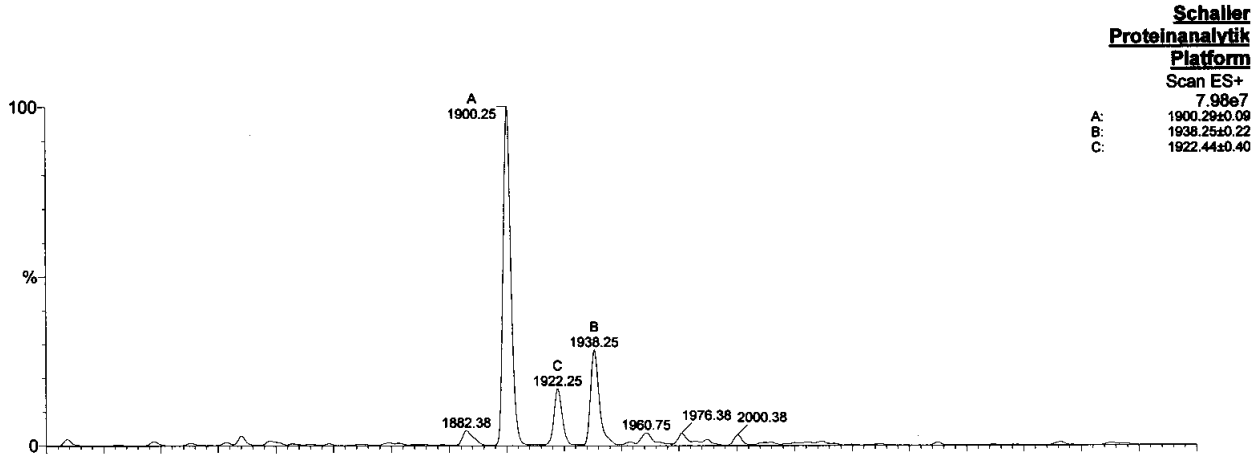
Dendrimer F_1-F_1





Dendrimer A_2





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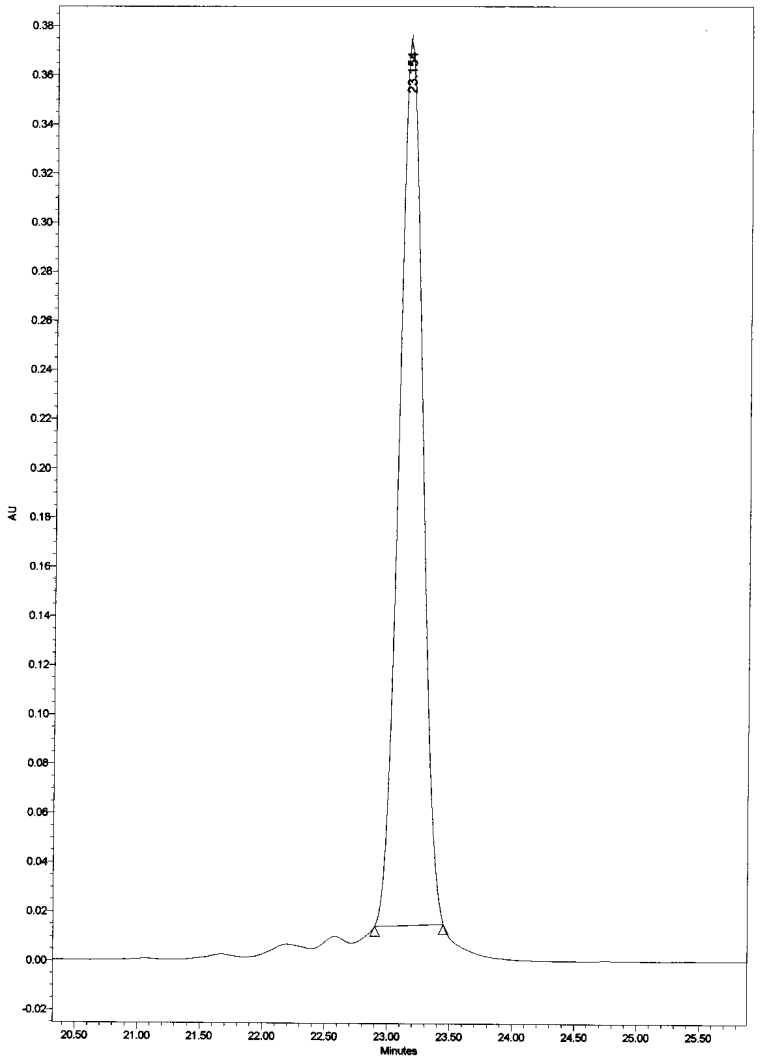
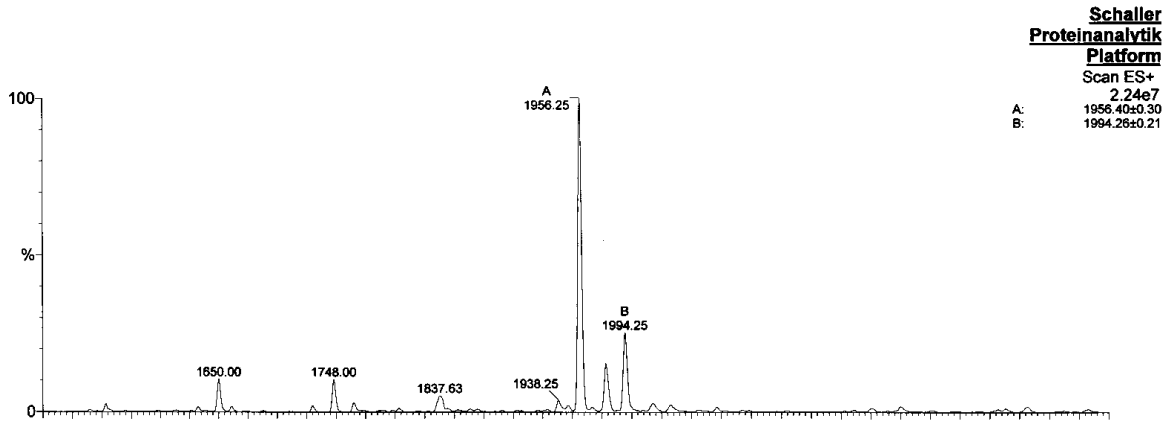
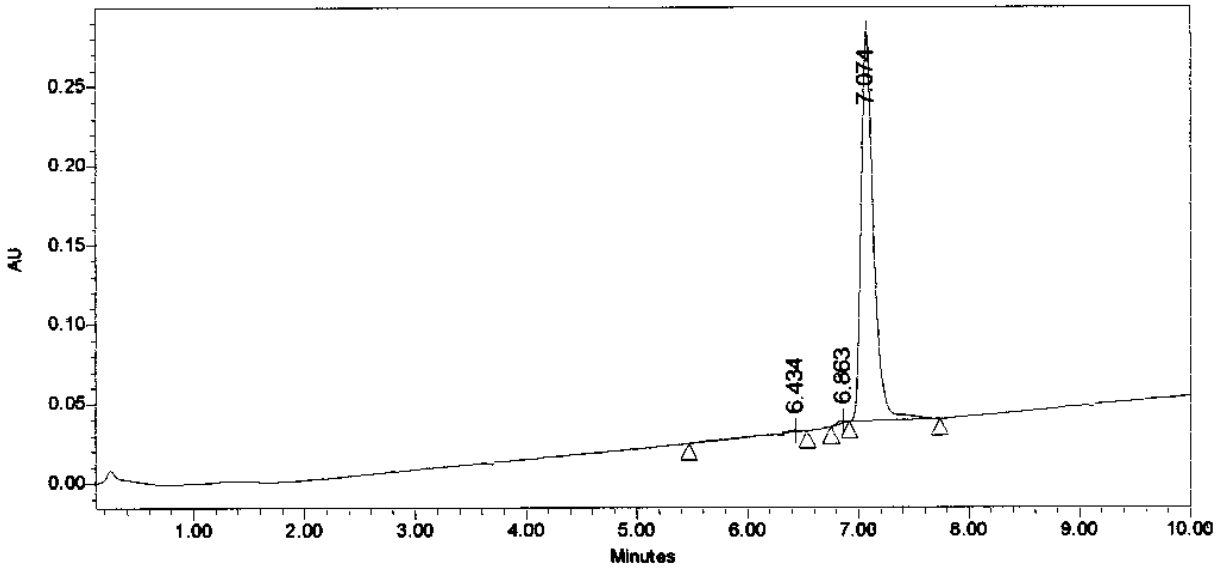
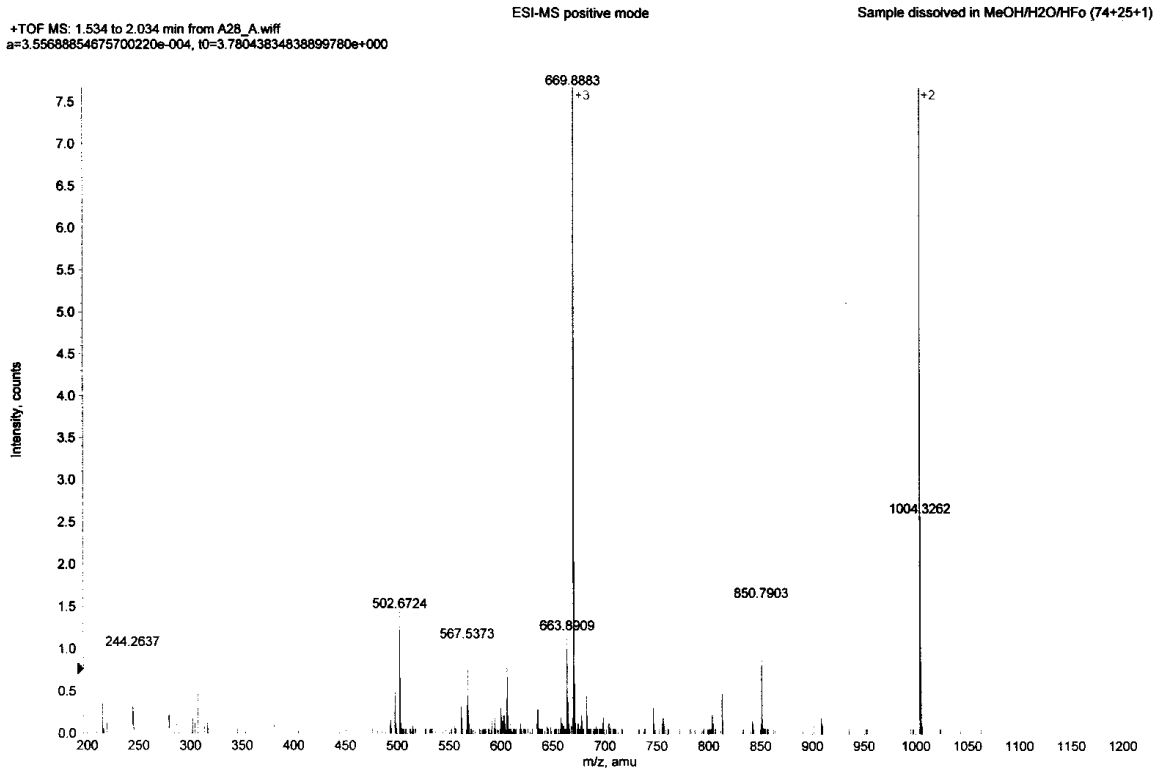


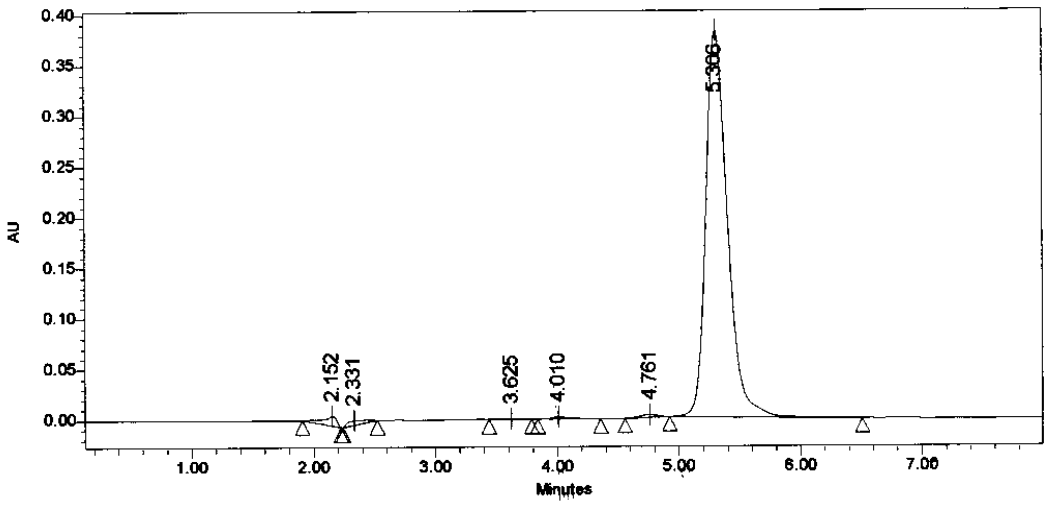


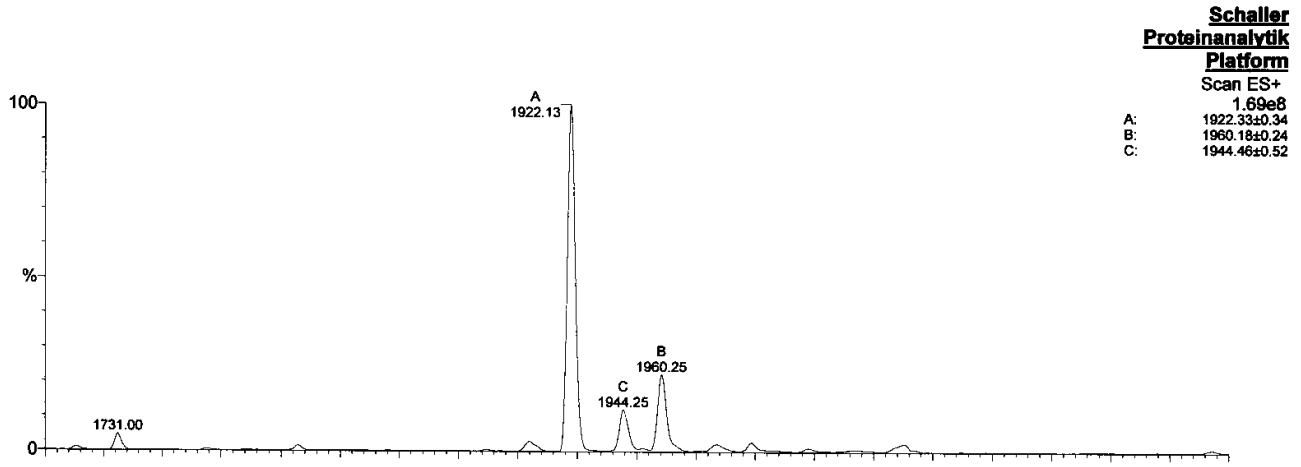
Dendrimer C_2





Dendrimer D_2





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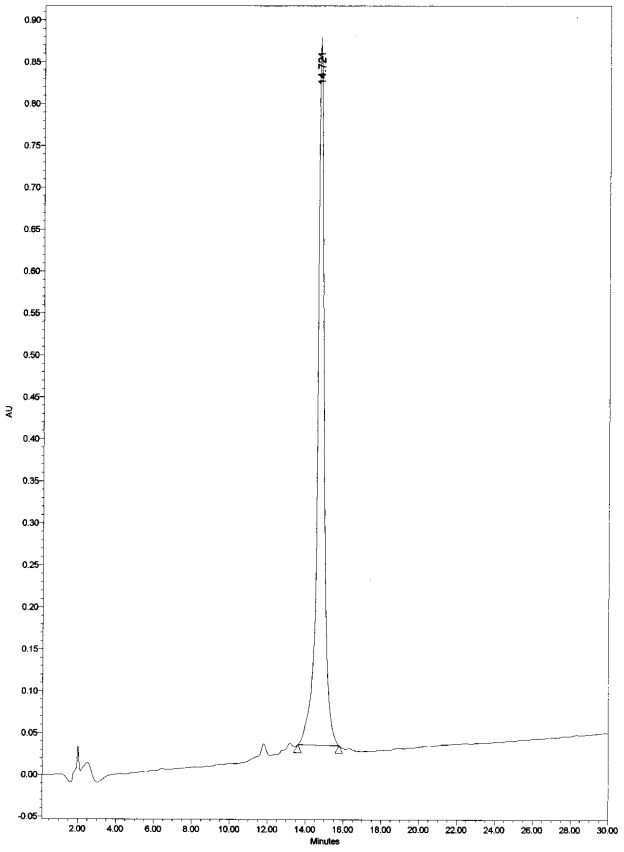
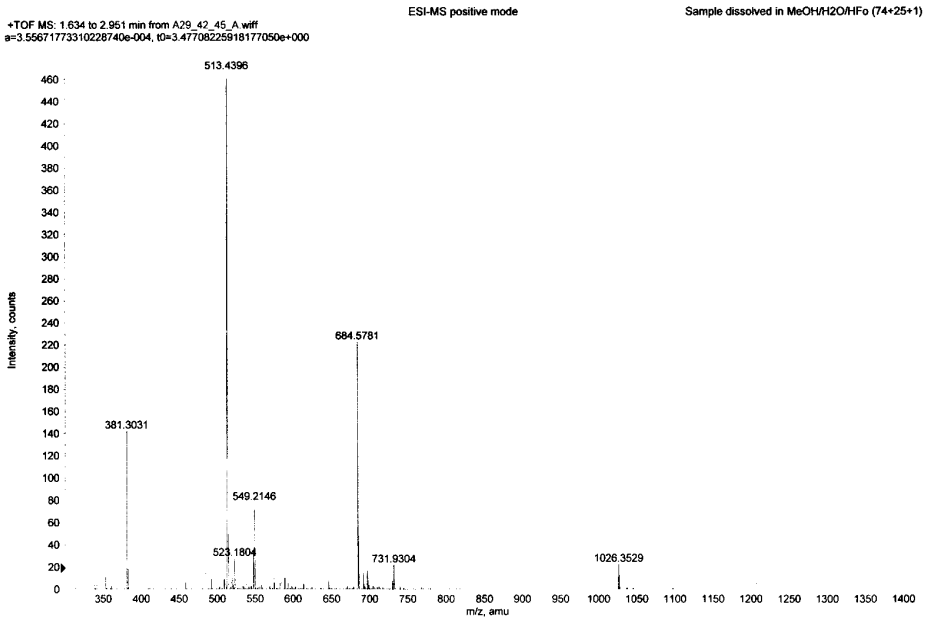
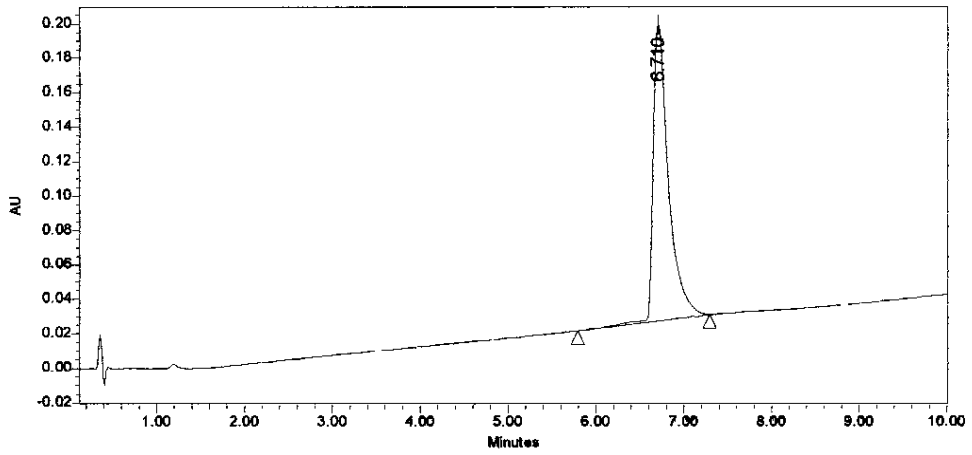
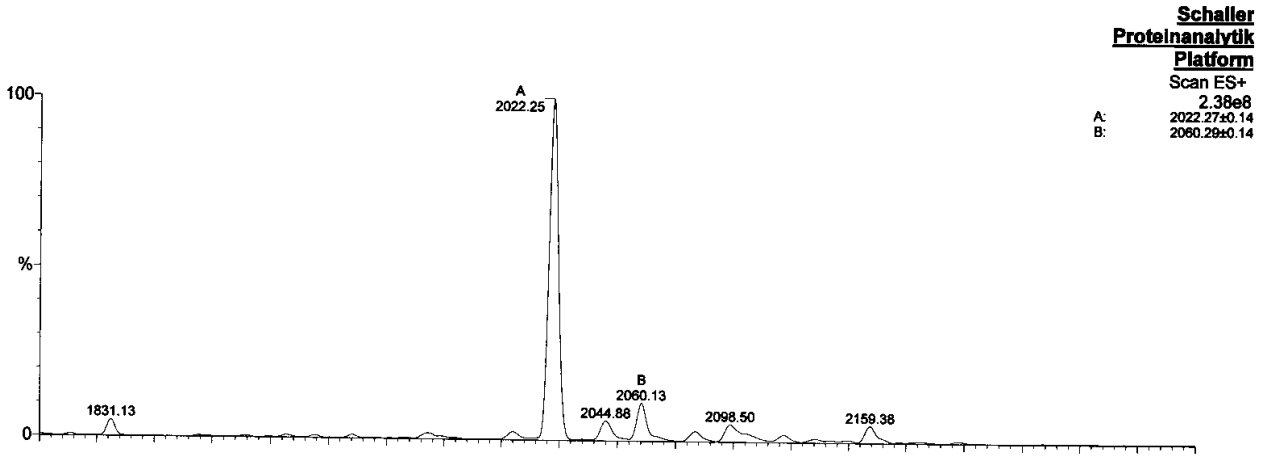


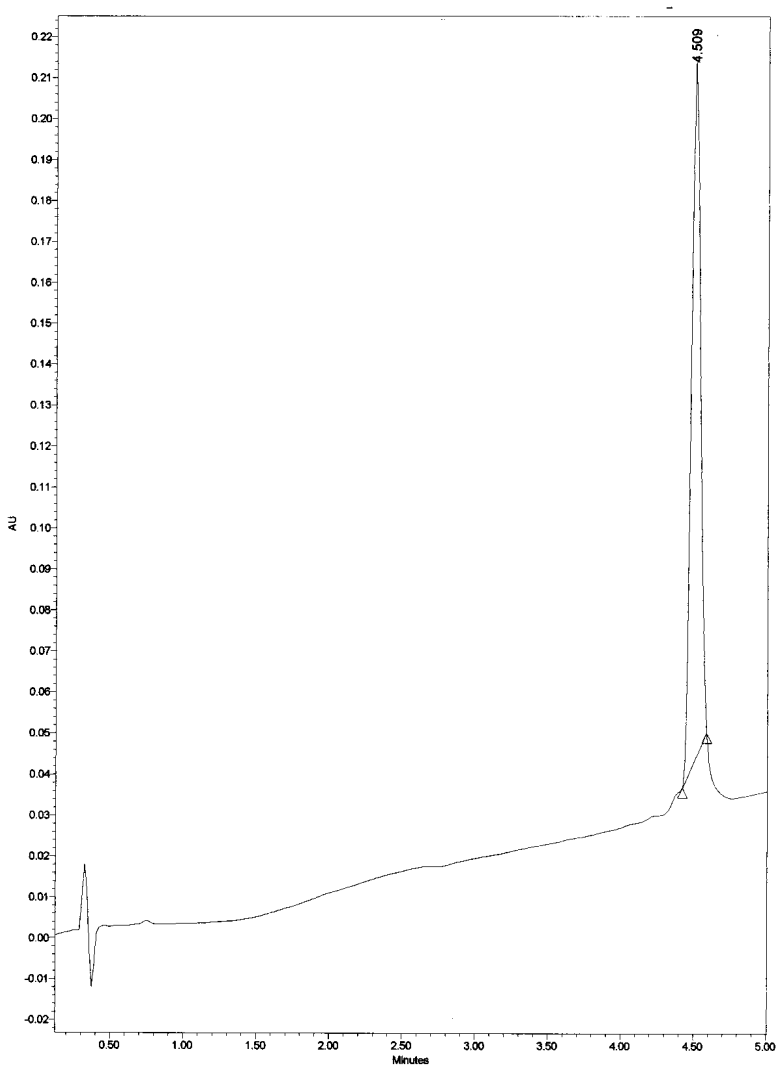


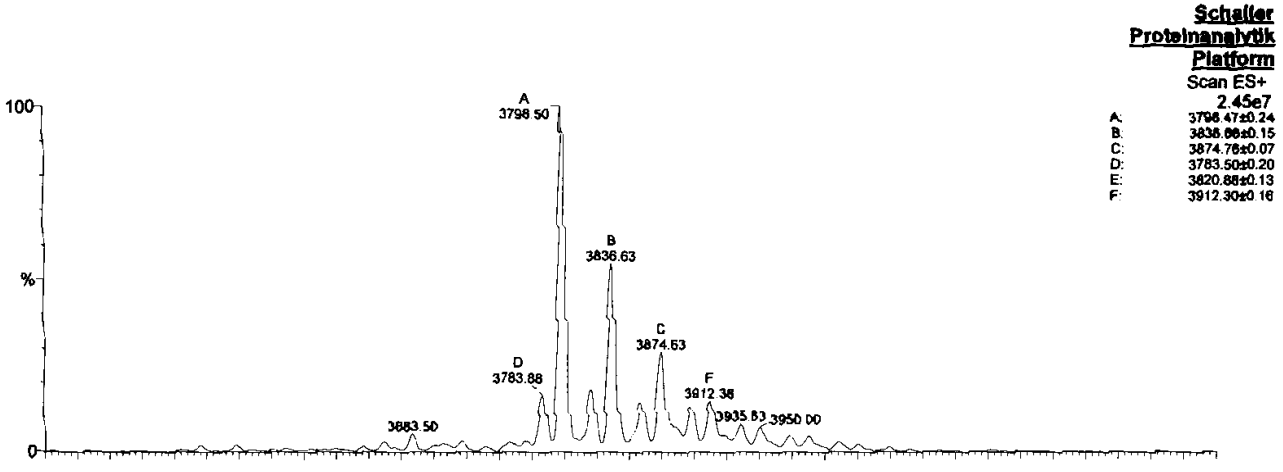
Dendrimer F_2



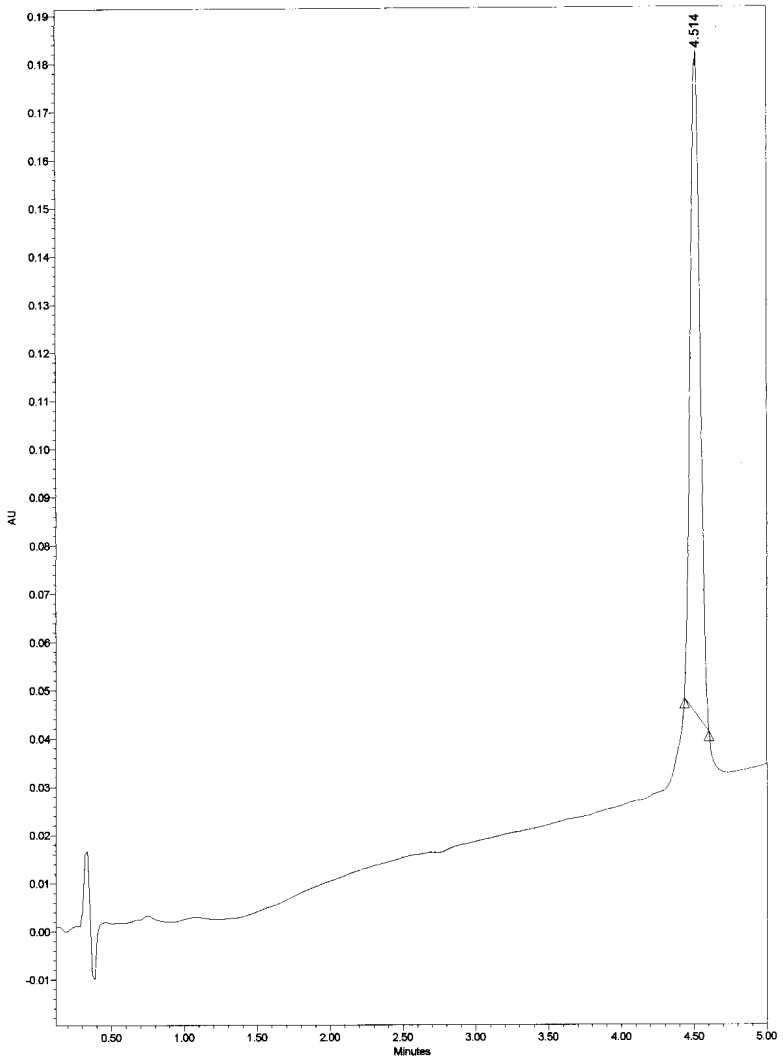


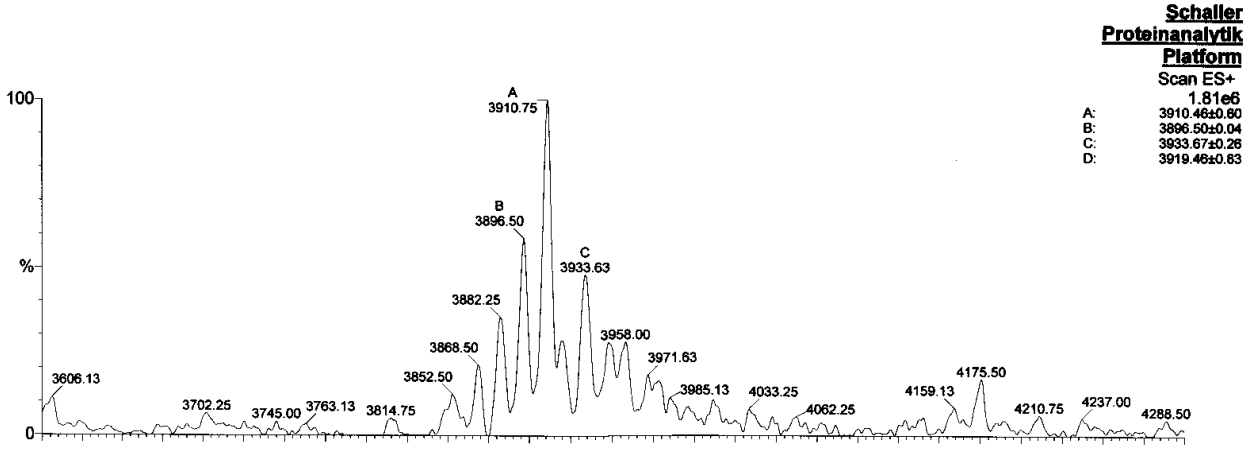
Dendrimer A_2-A_2



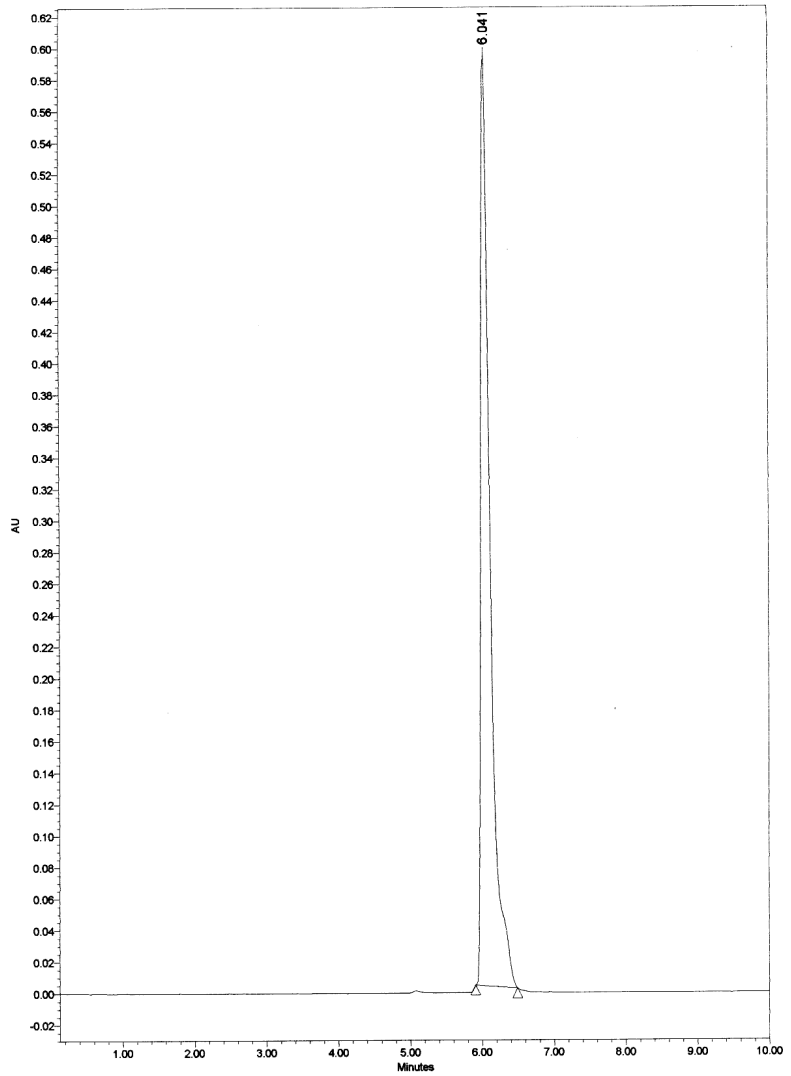


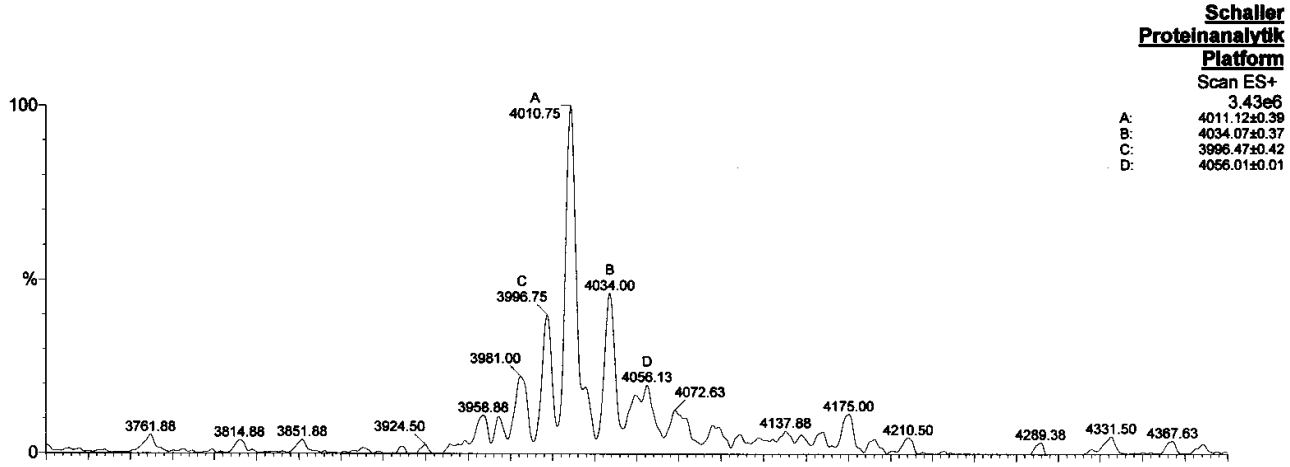
Dendrimer B_2-B_2



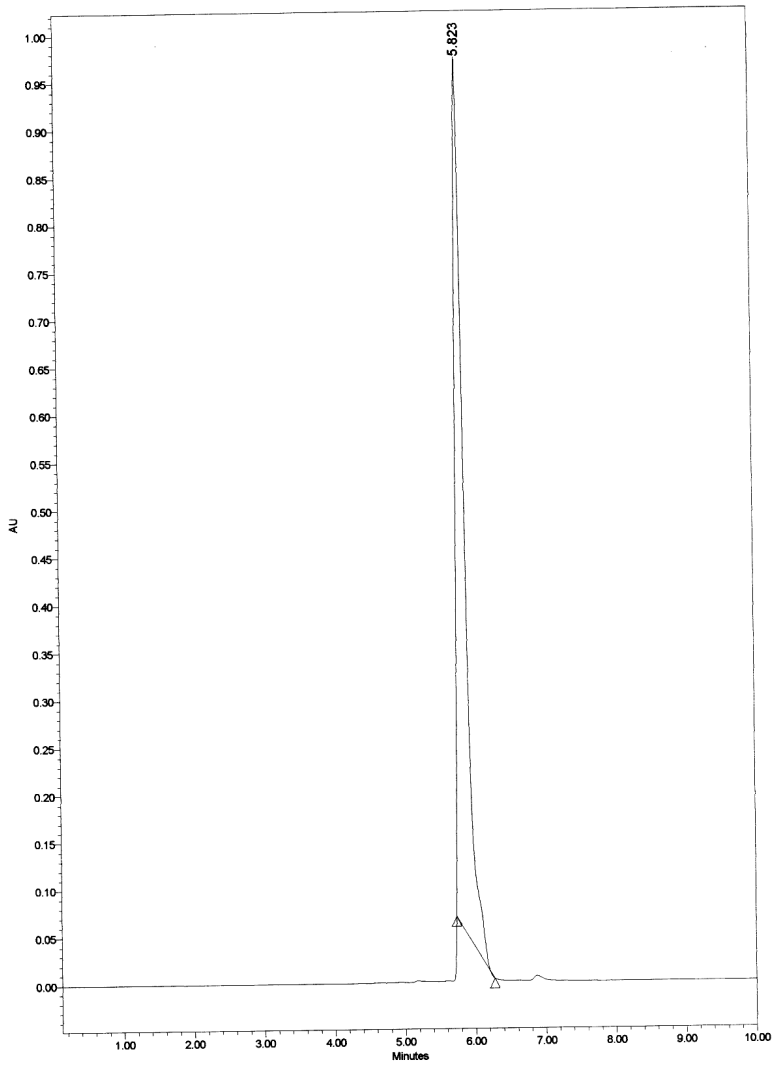


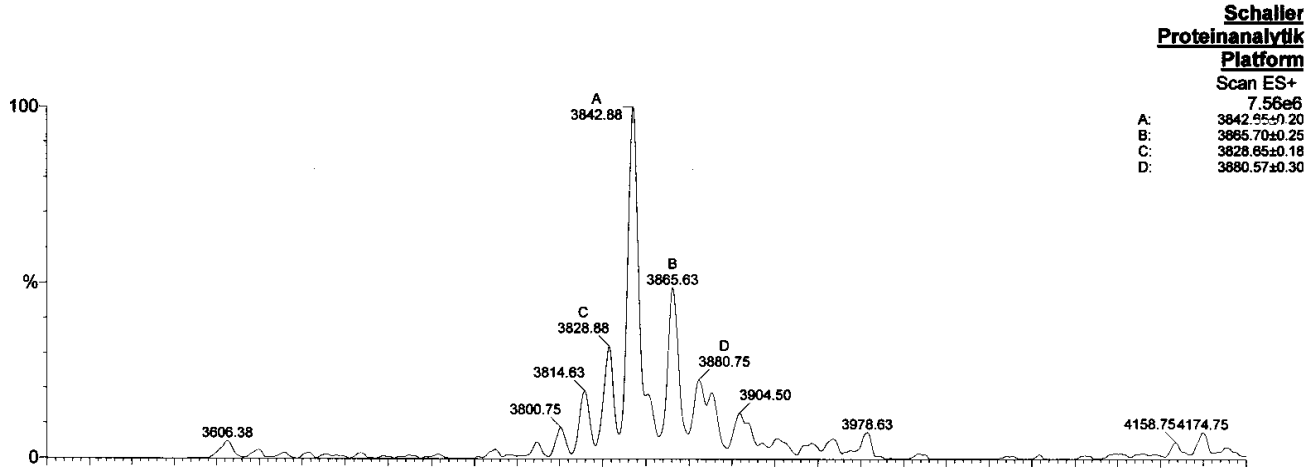
Dendrimer C_2-C_2



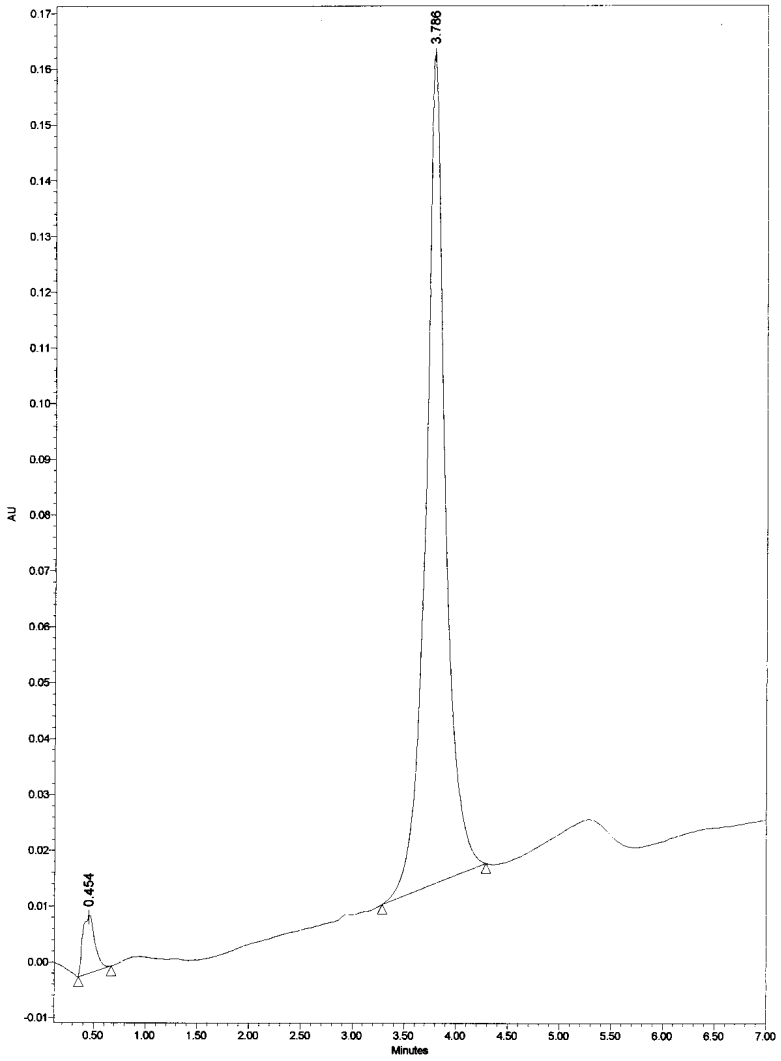


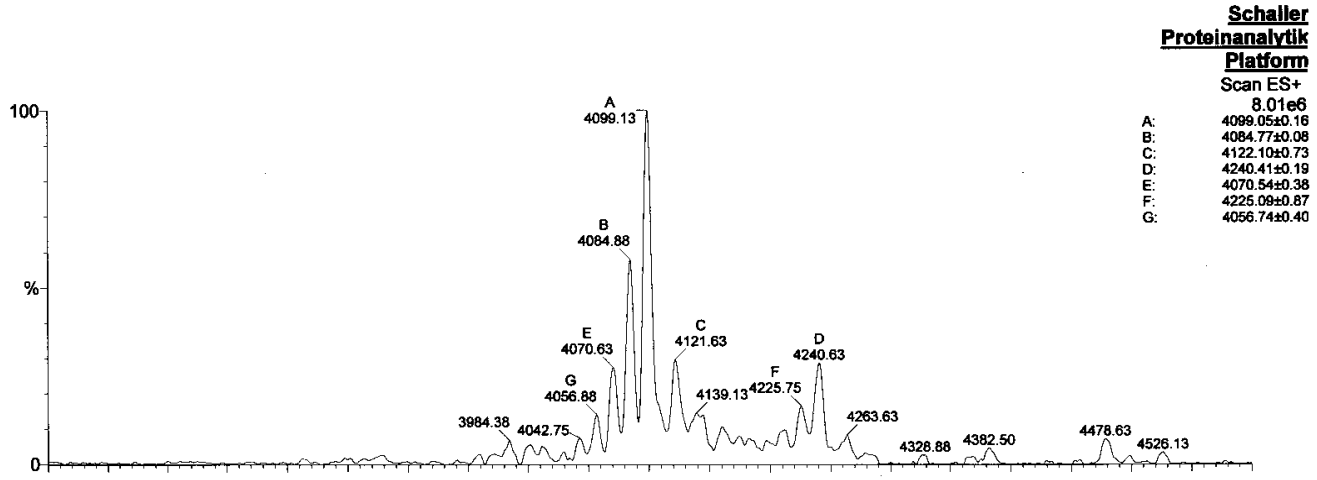
Dendrimer D_2-D_2



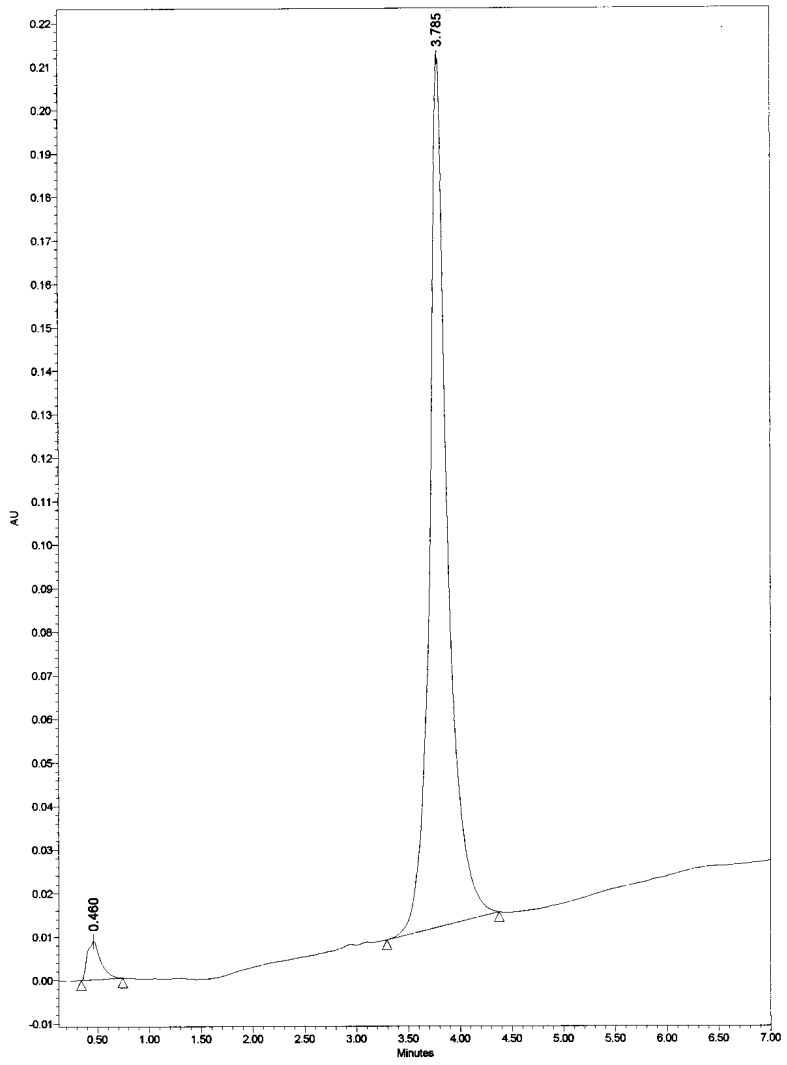


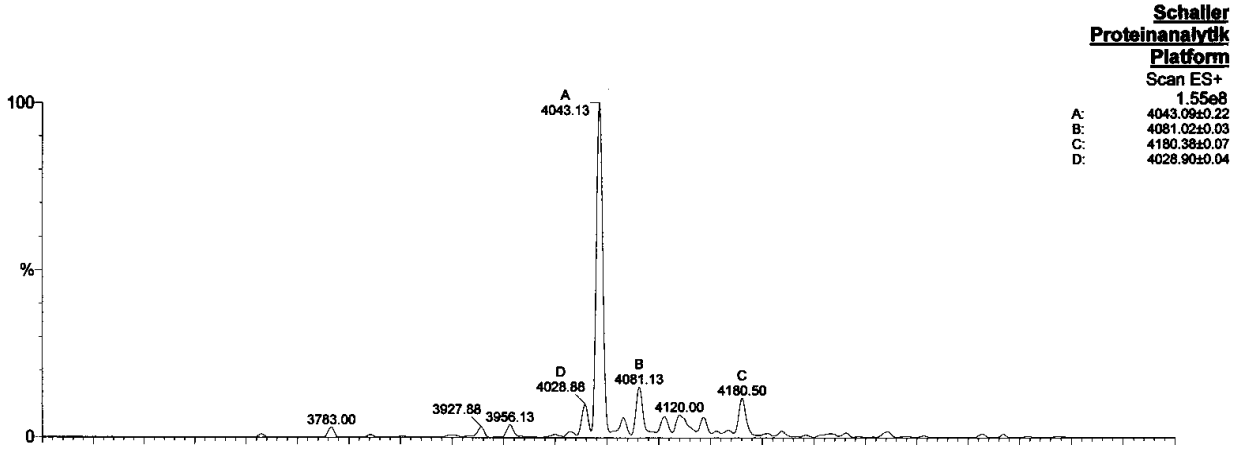
Dendrimer E_2-E_2



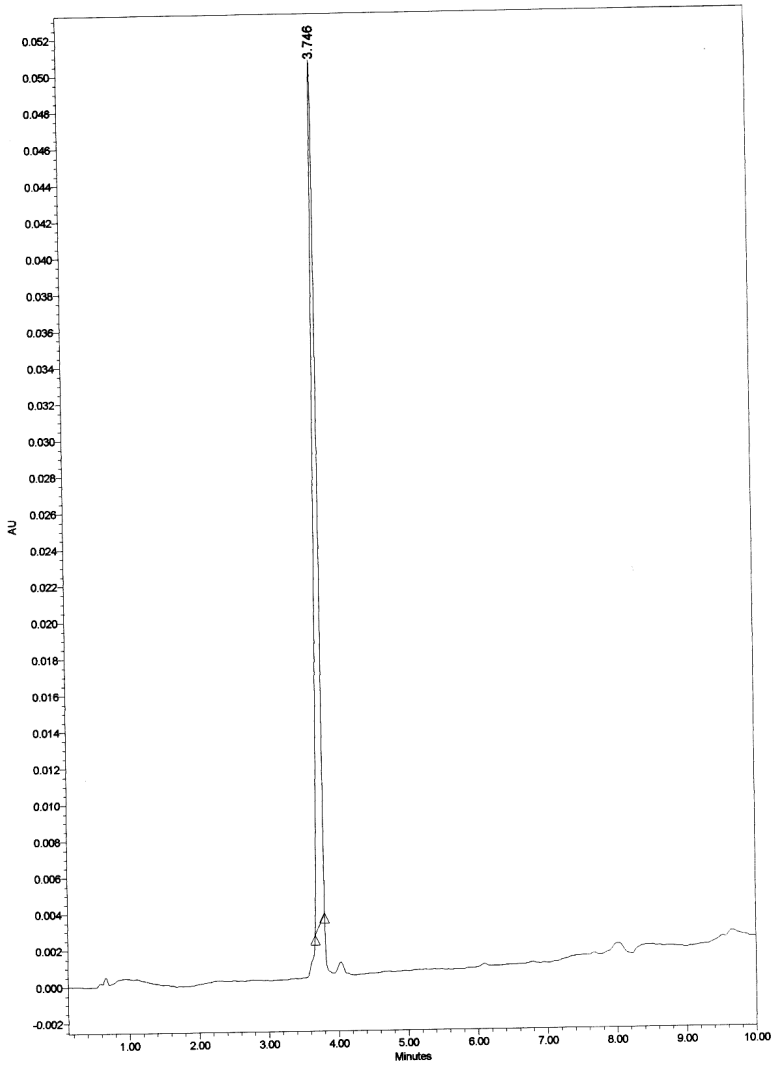


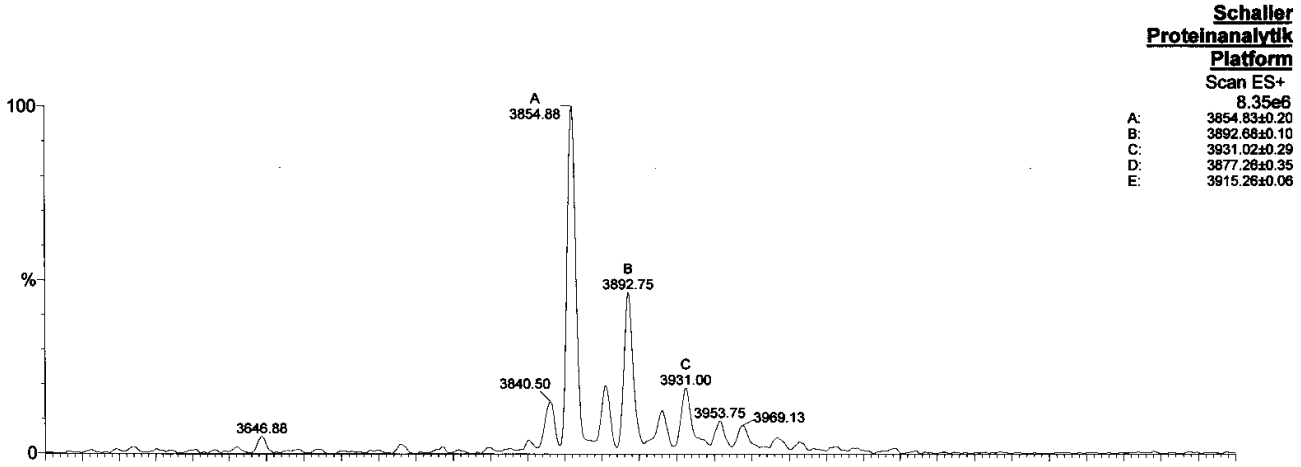
Dendrimer F_2-F_2



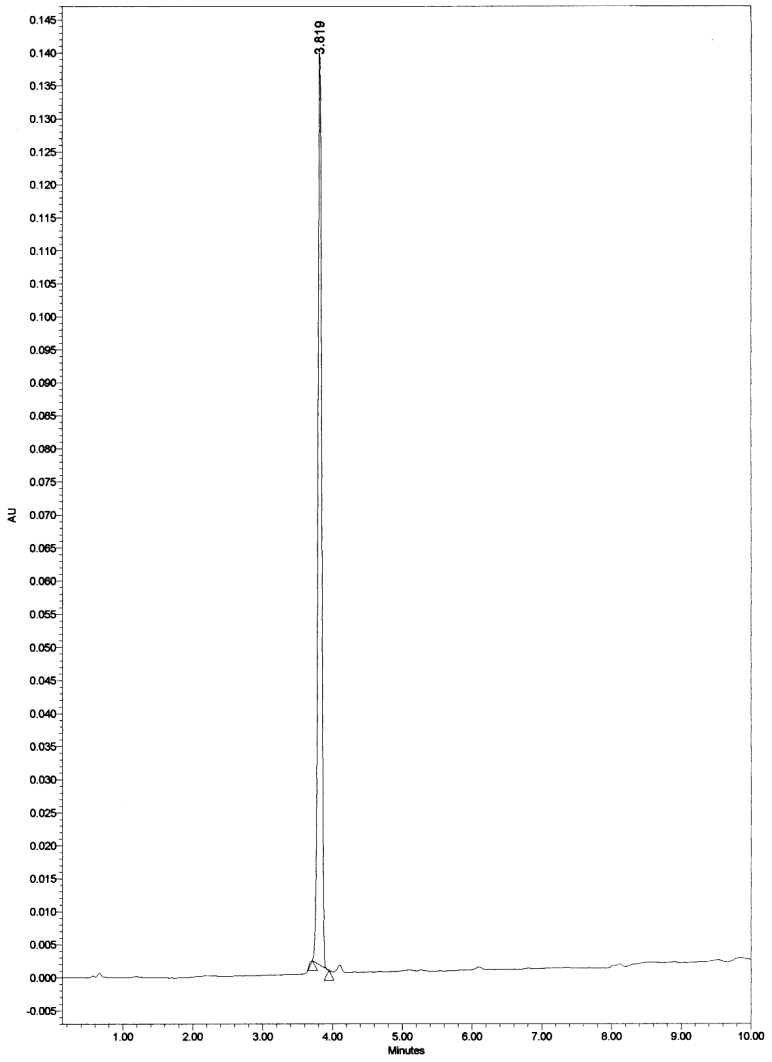


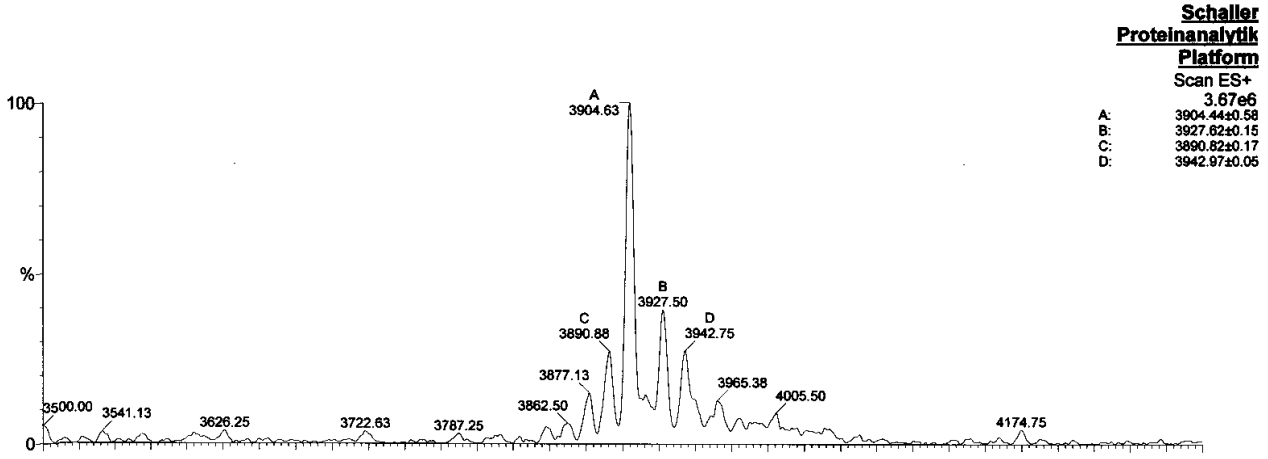
Dendrimer A_2-B_2





Dendrimer A_2-C_2





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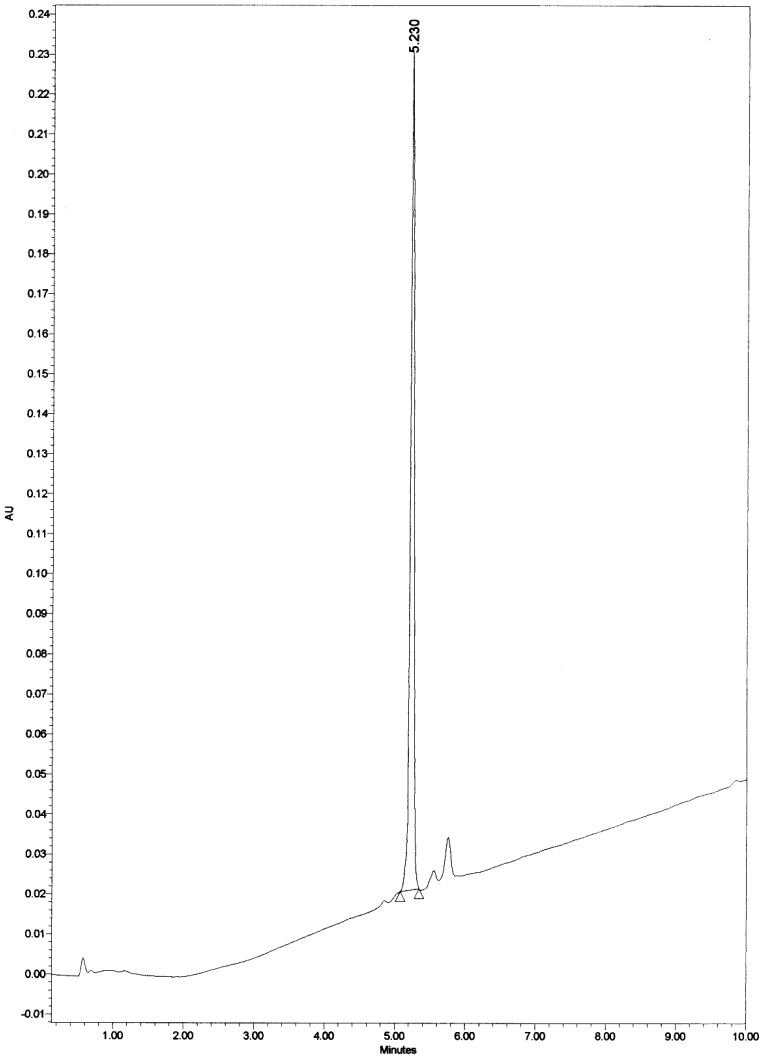

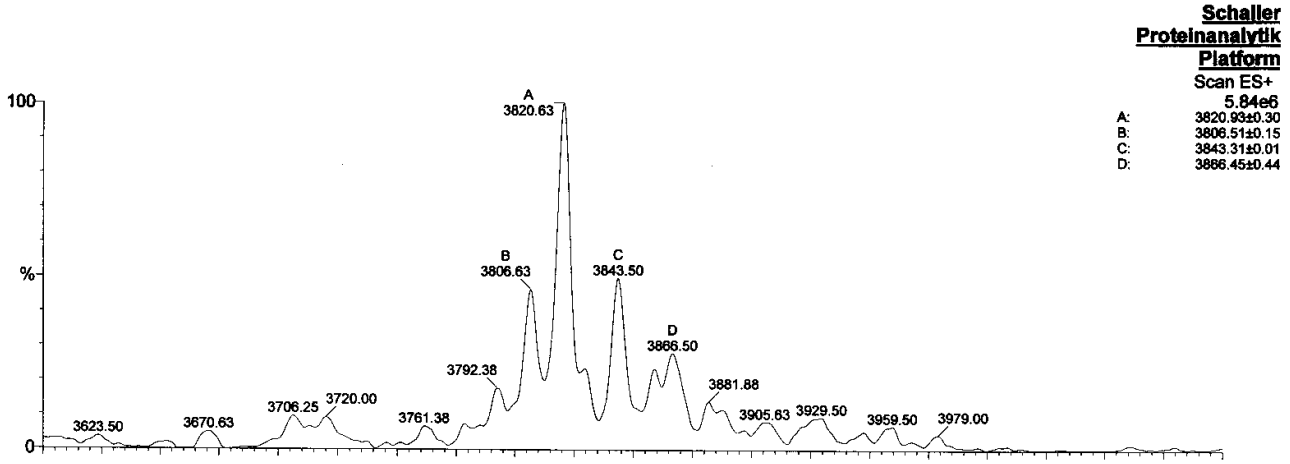

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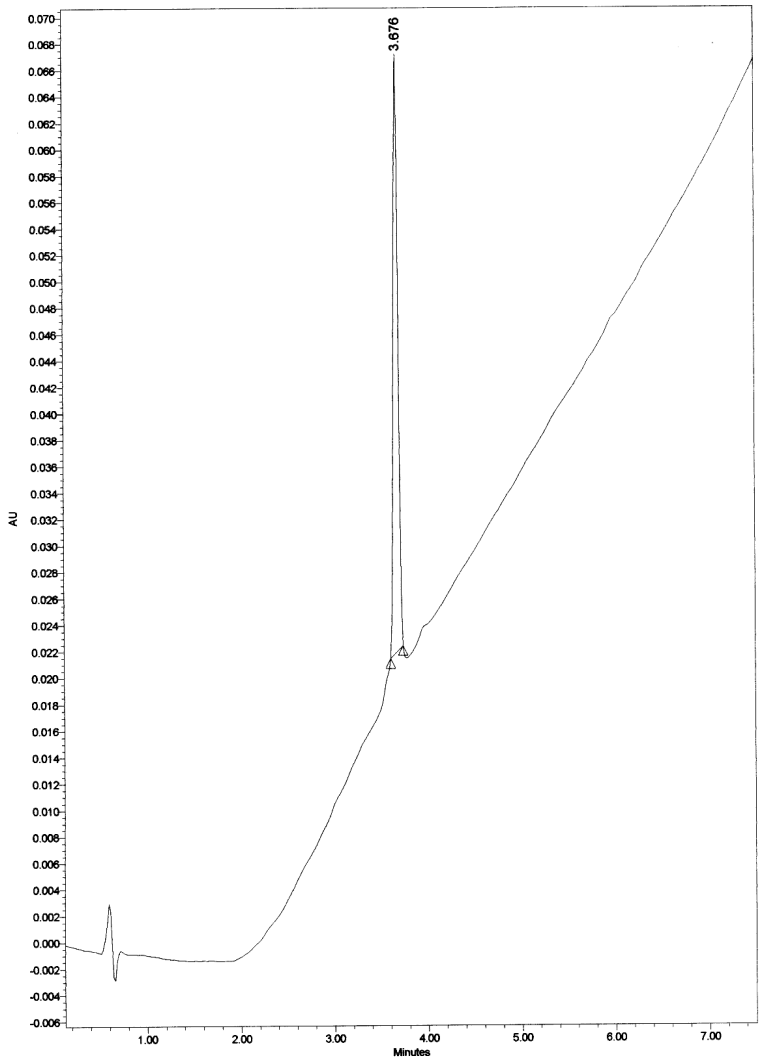

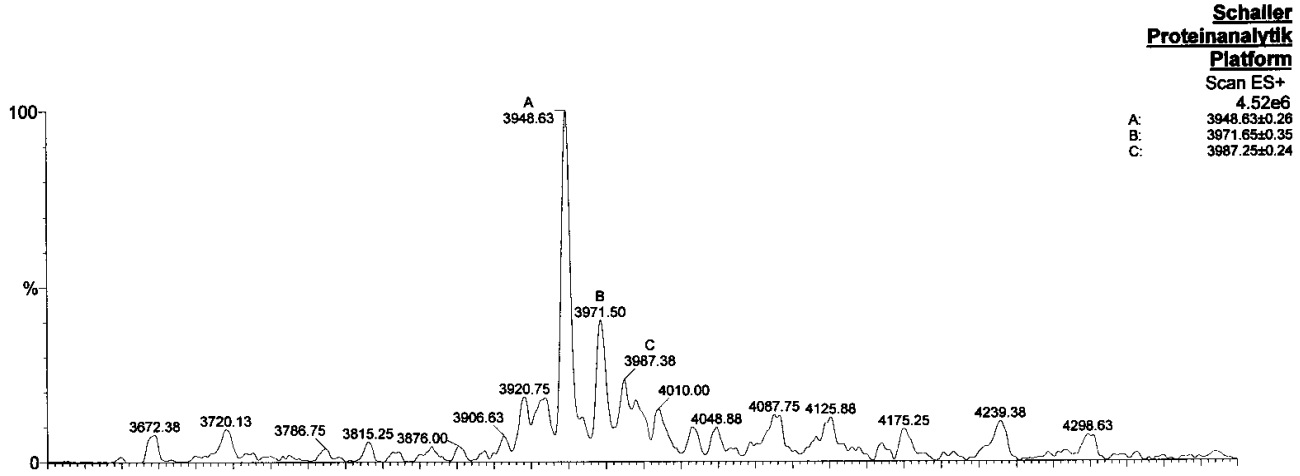

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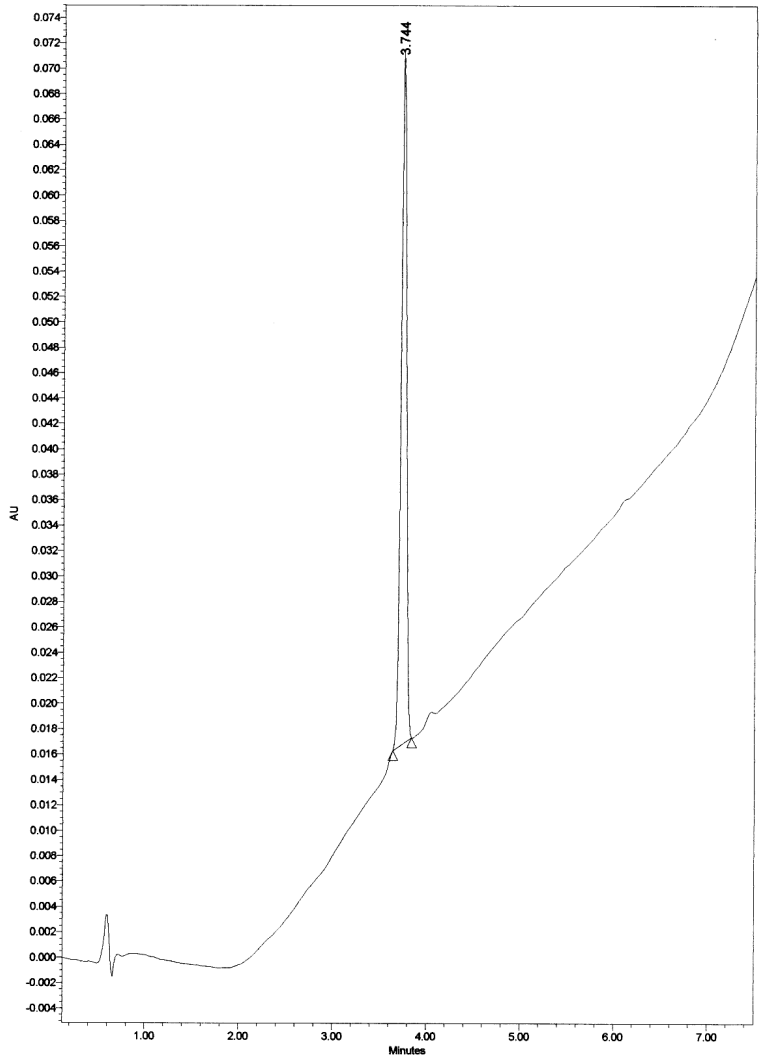

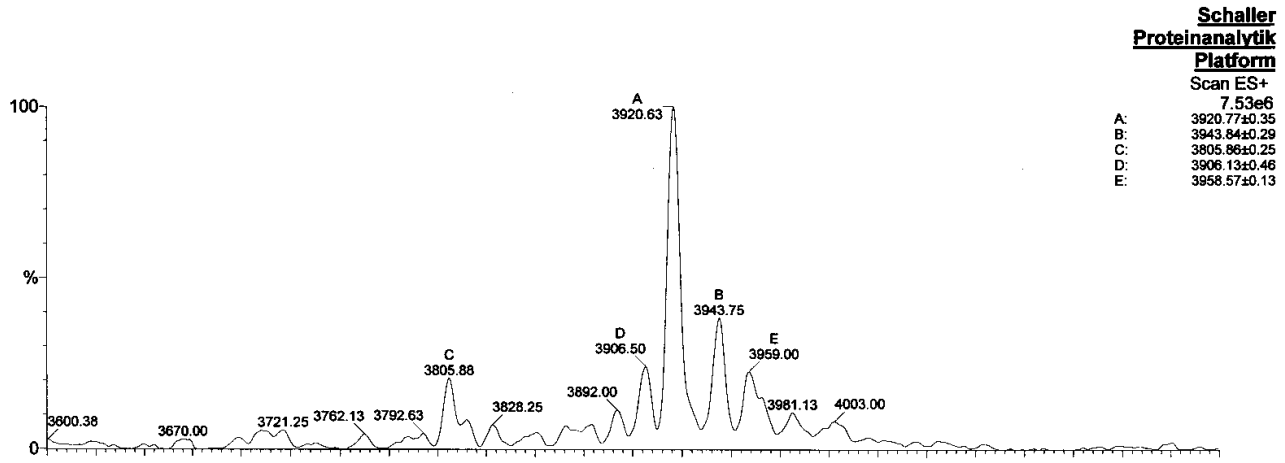

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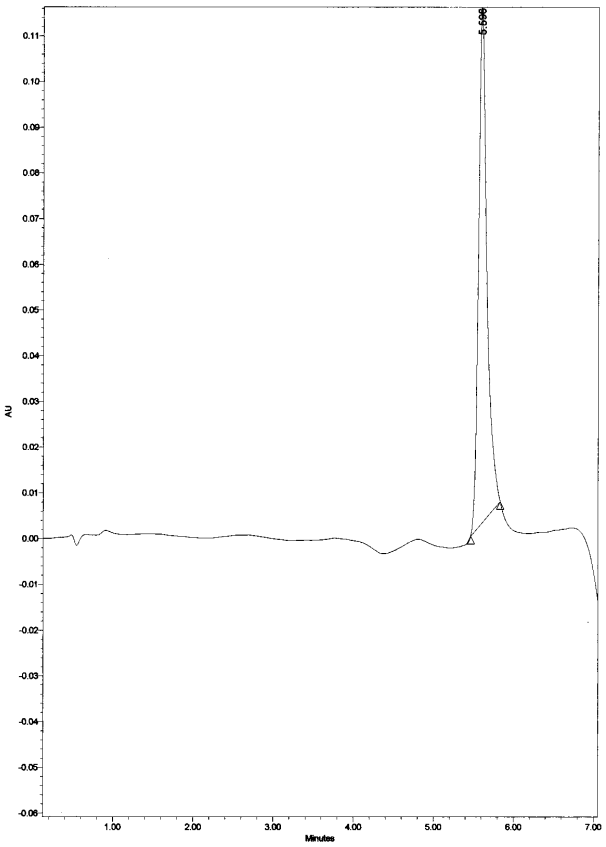

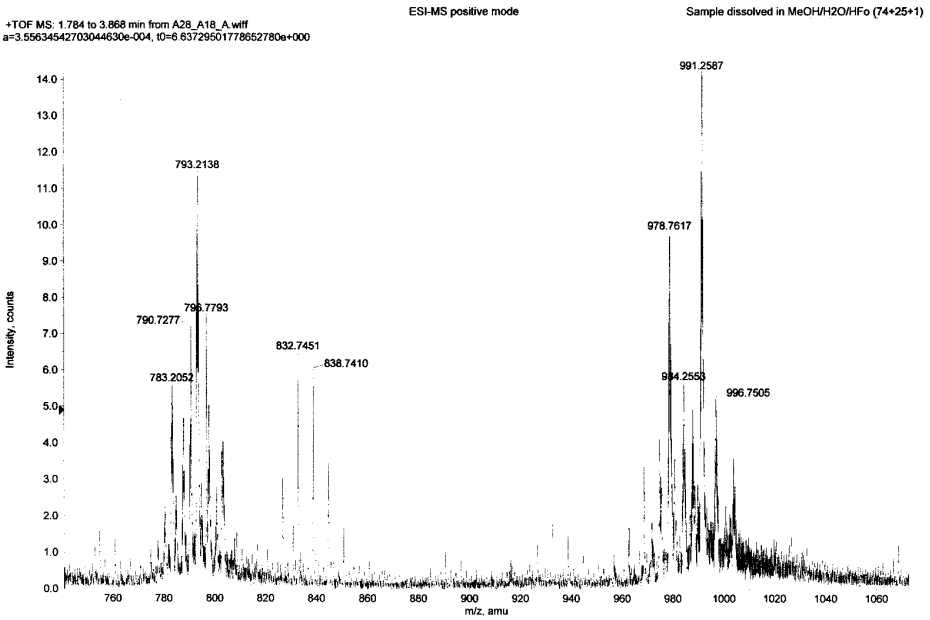

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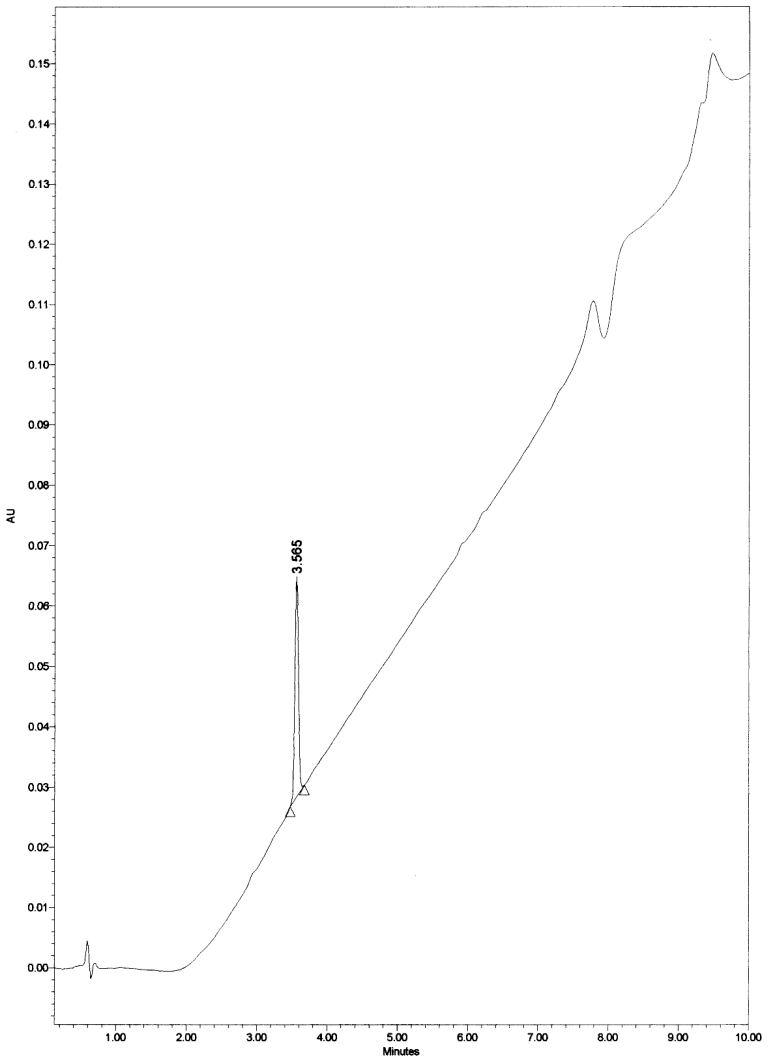

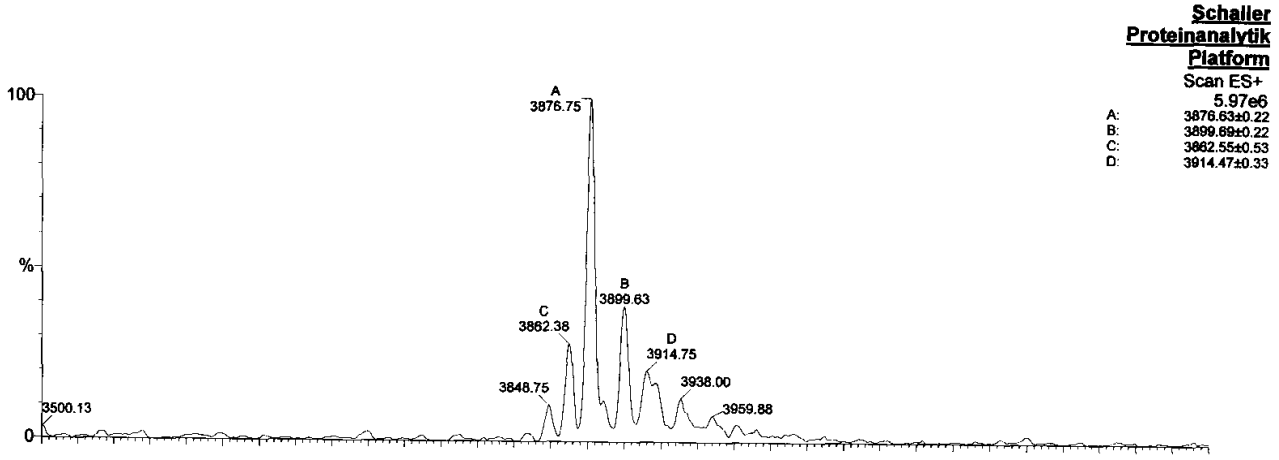

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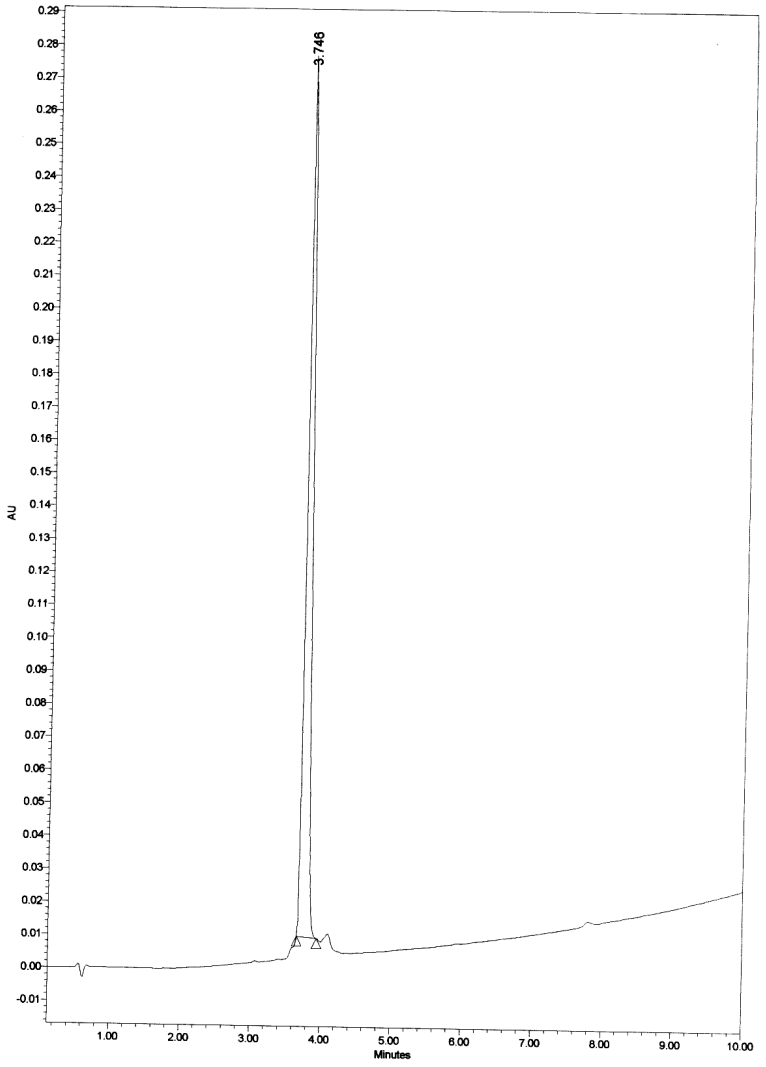
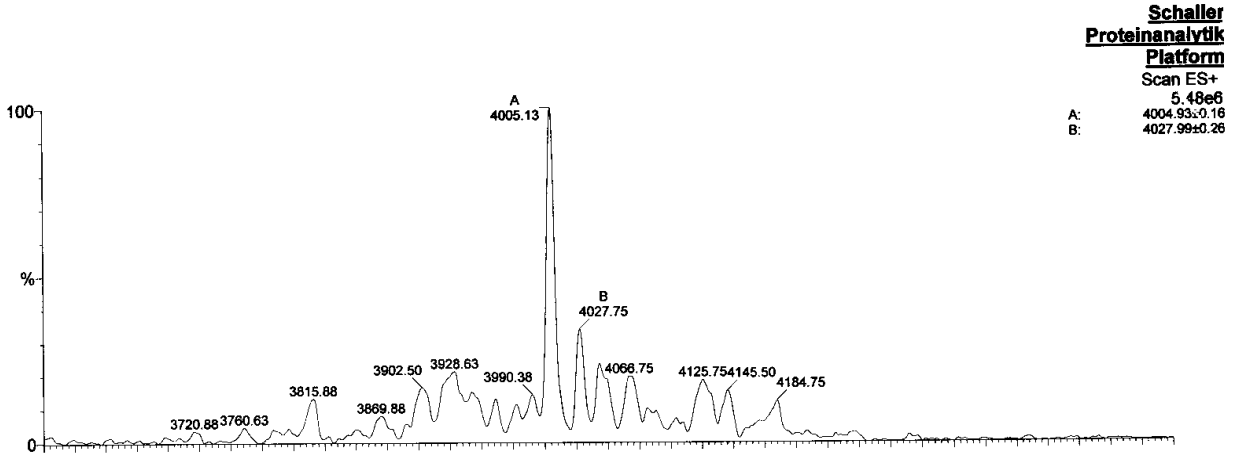
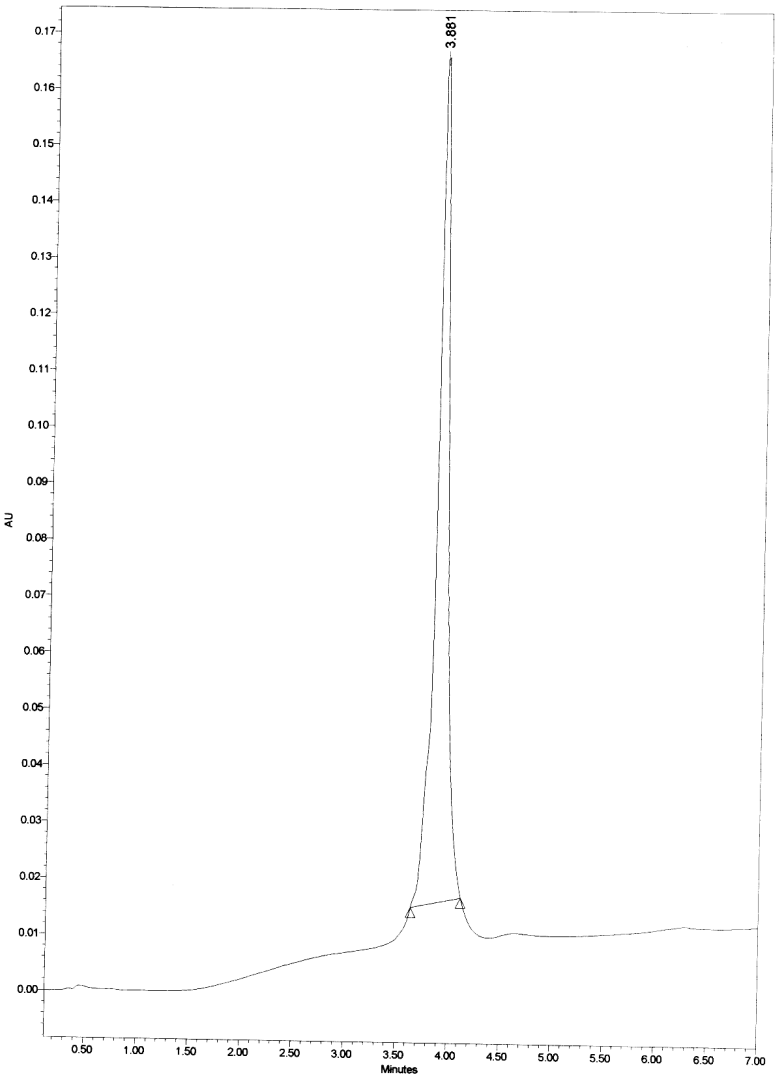
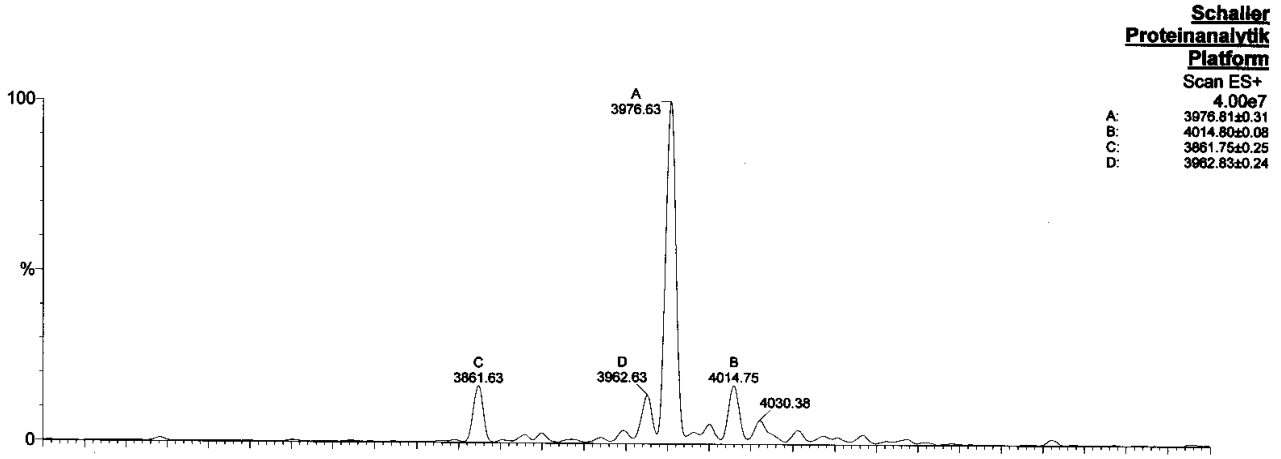


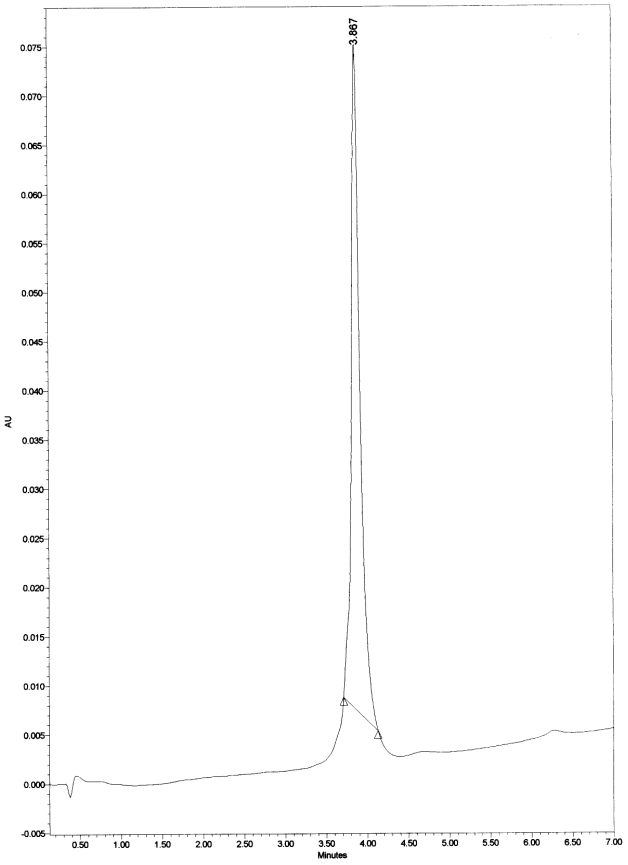


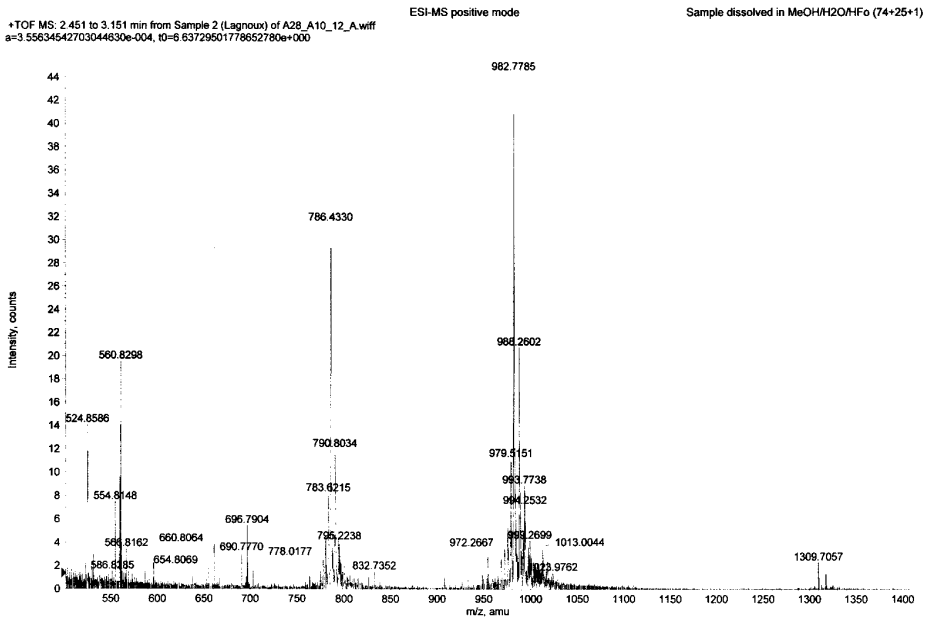
Dendrimer B_2-F_2





Dendrimer C_2-D_2





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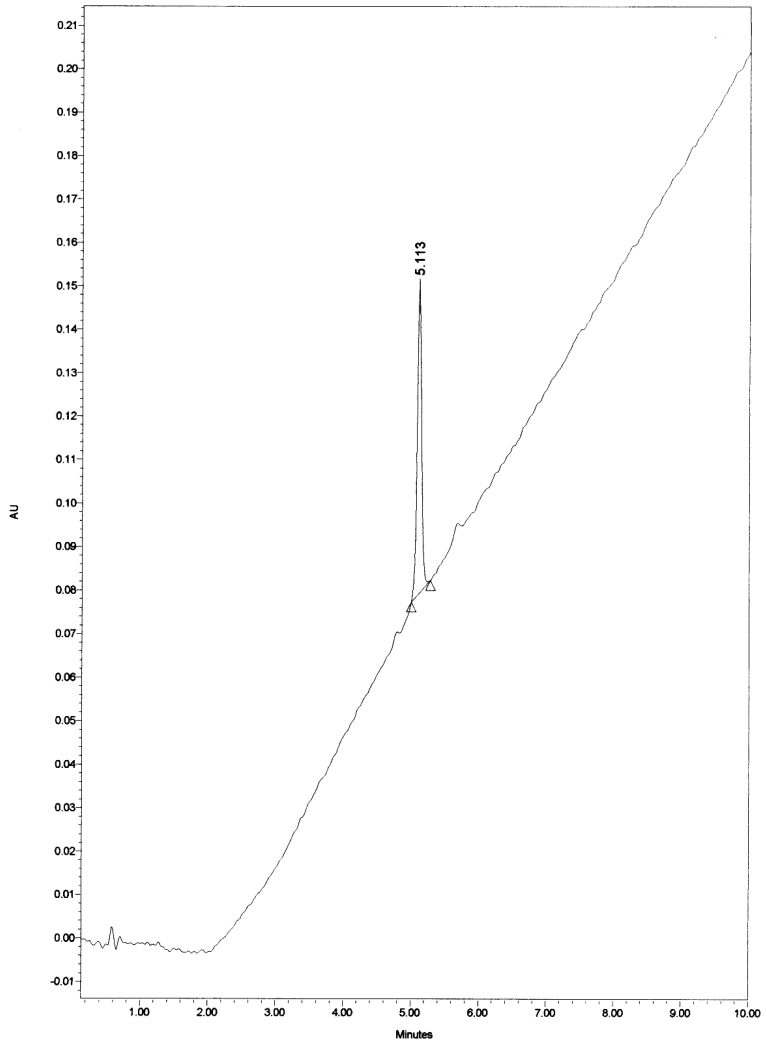
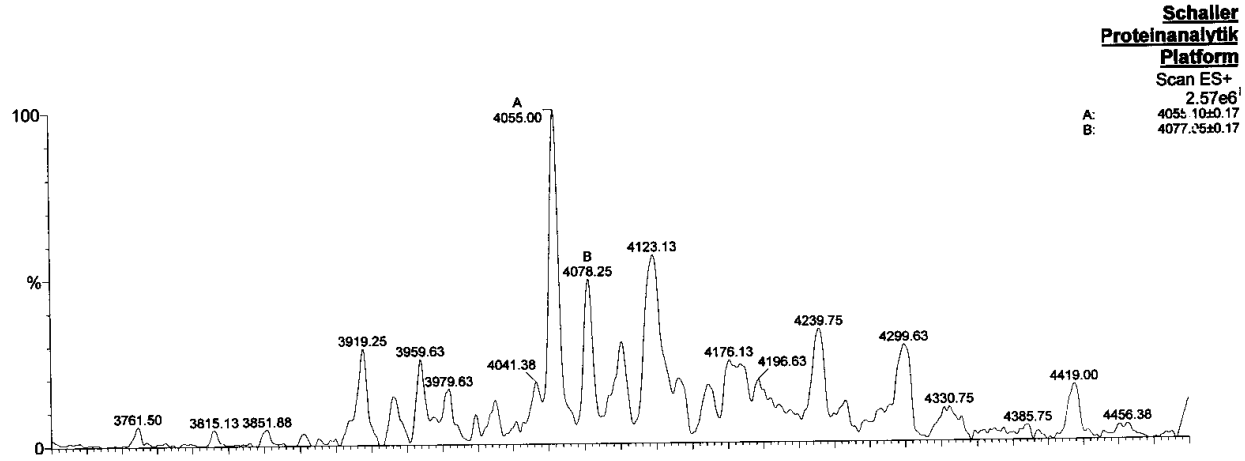
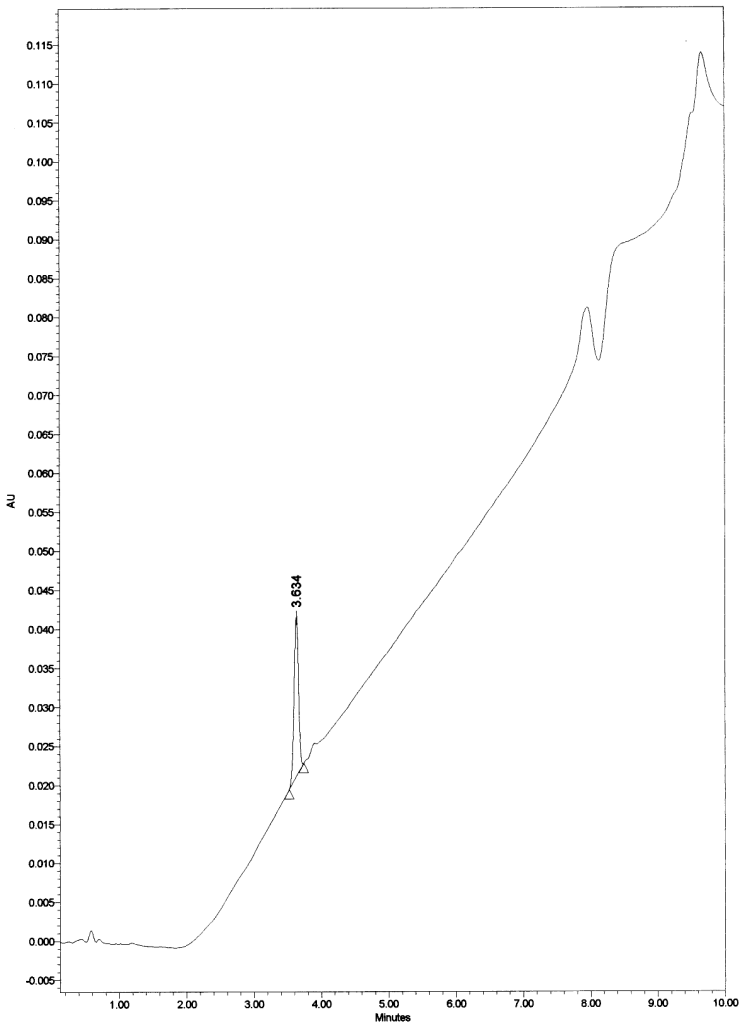
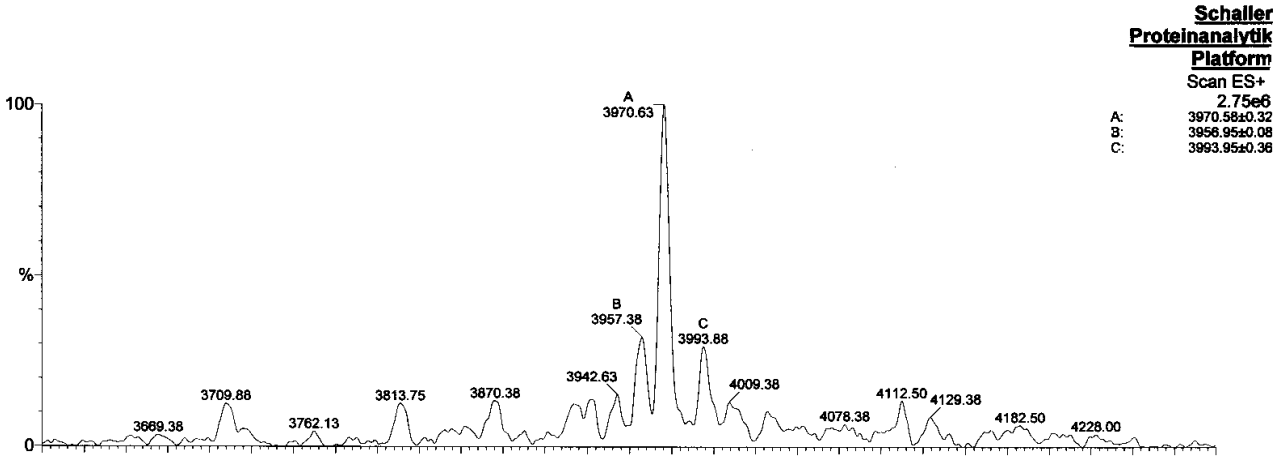




Dendrimer D_2-E_2





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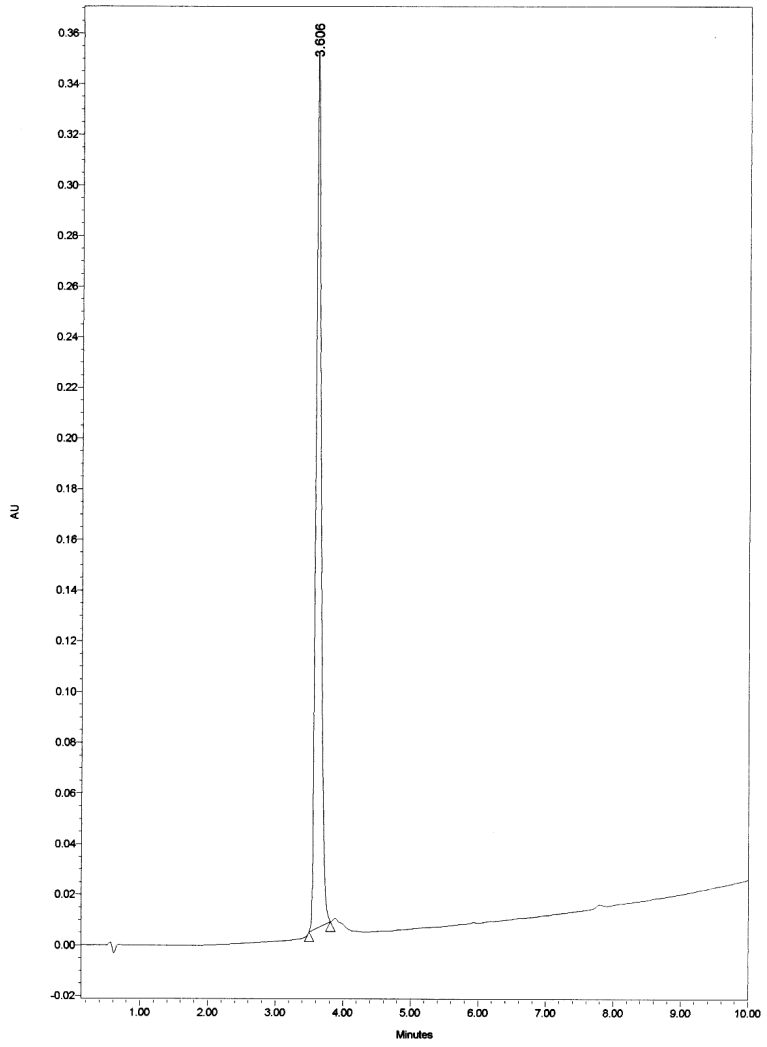
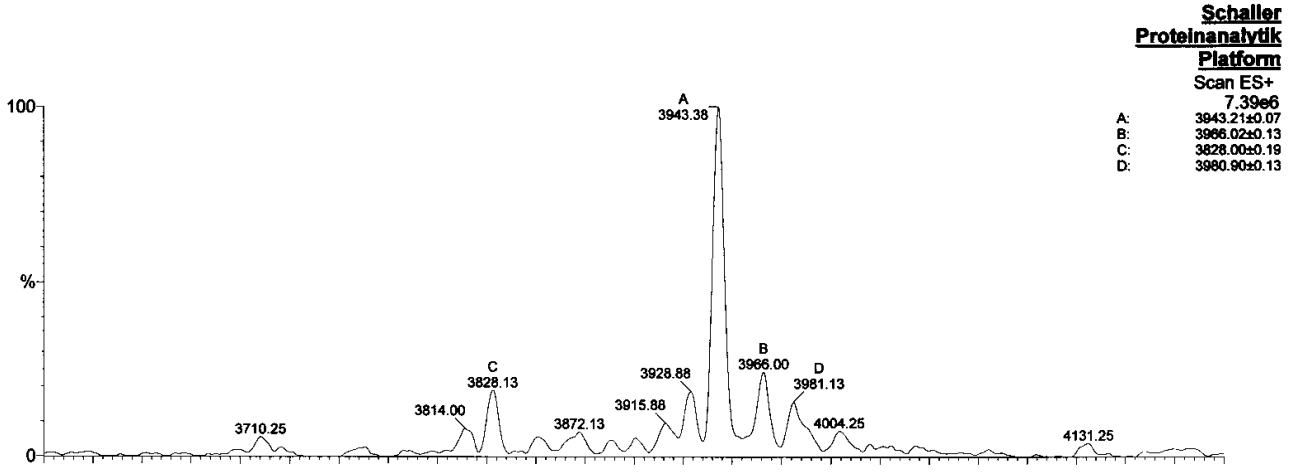
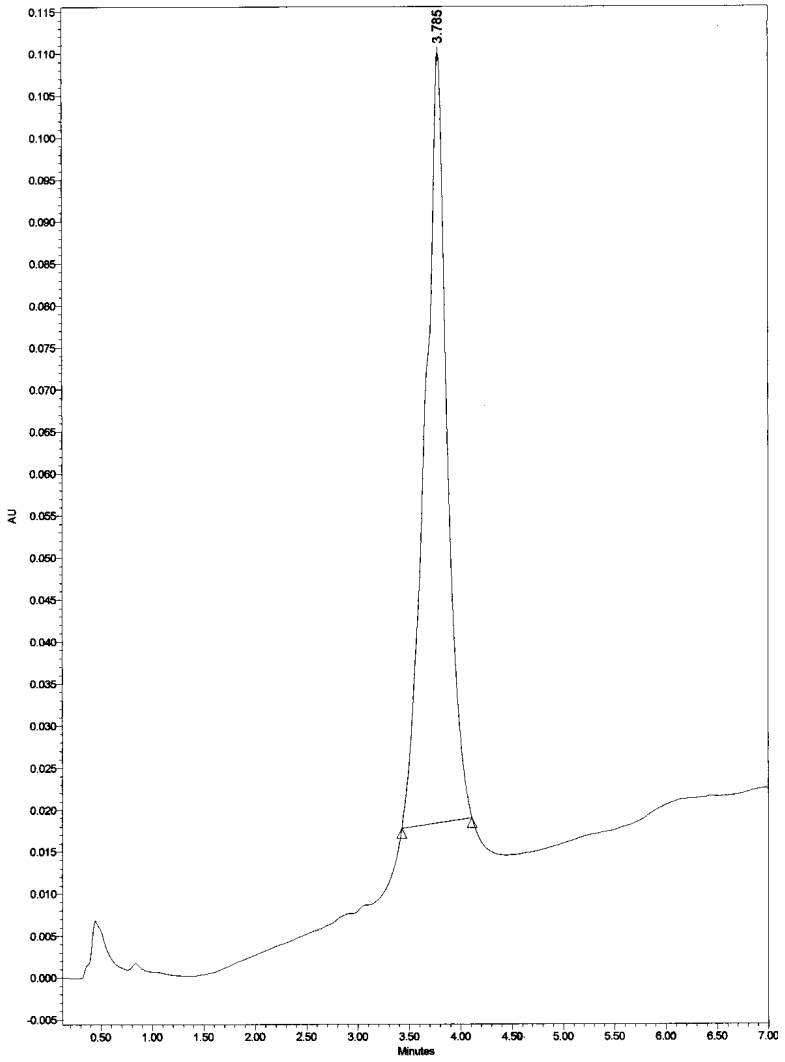
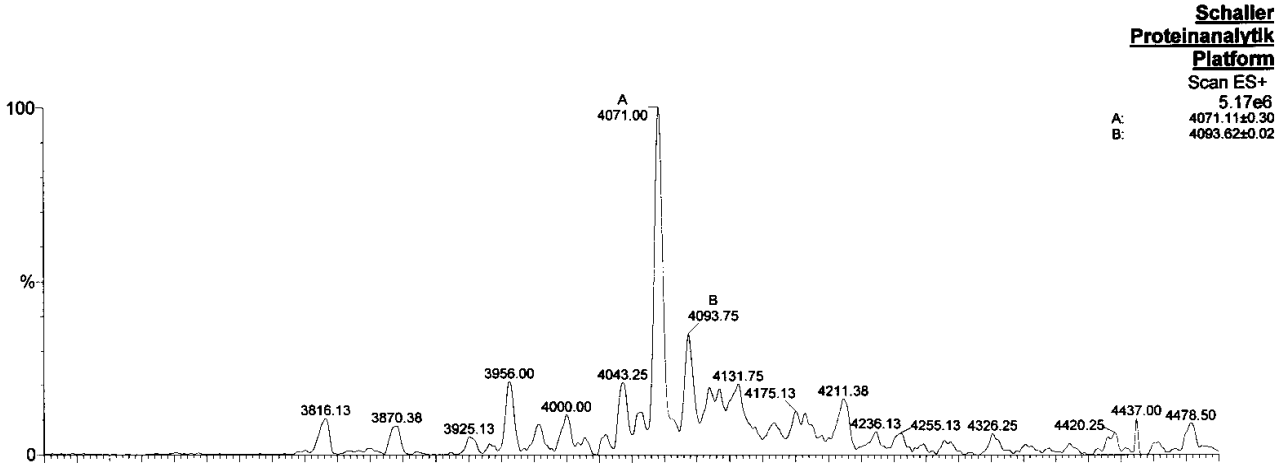
Dendrimer D_2-F_2



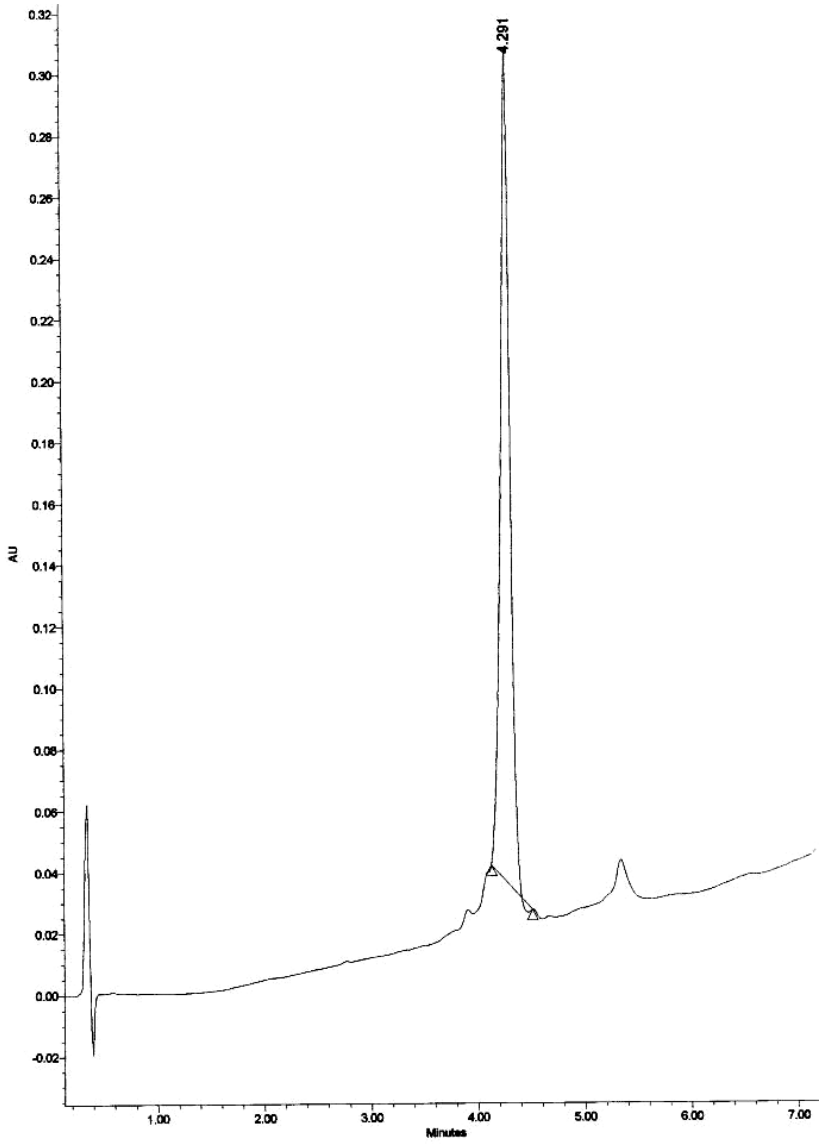


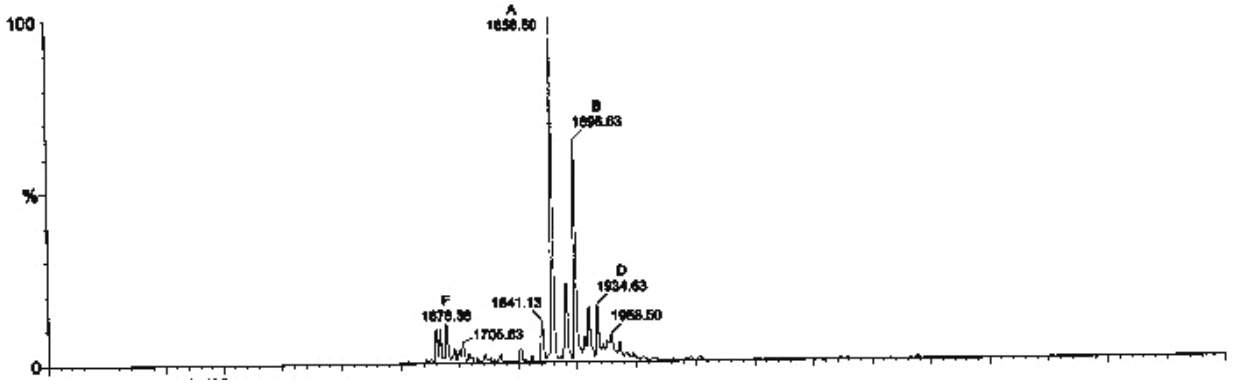
Dendrimer E_2-F_2



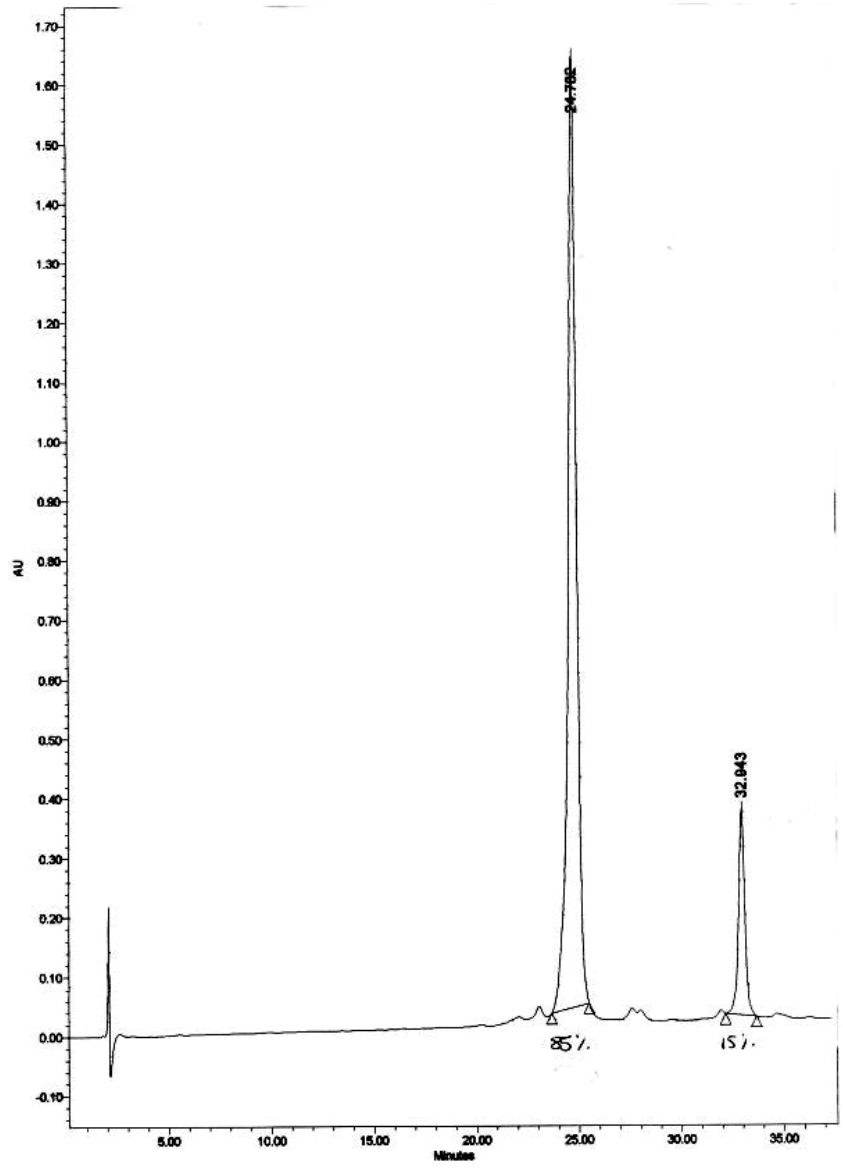


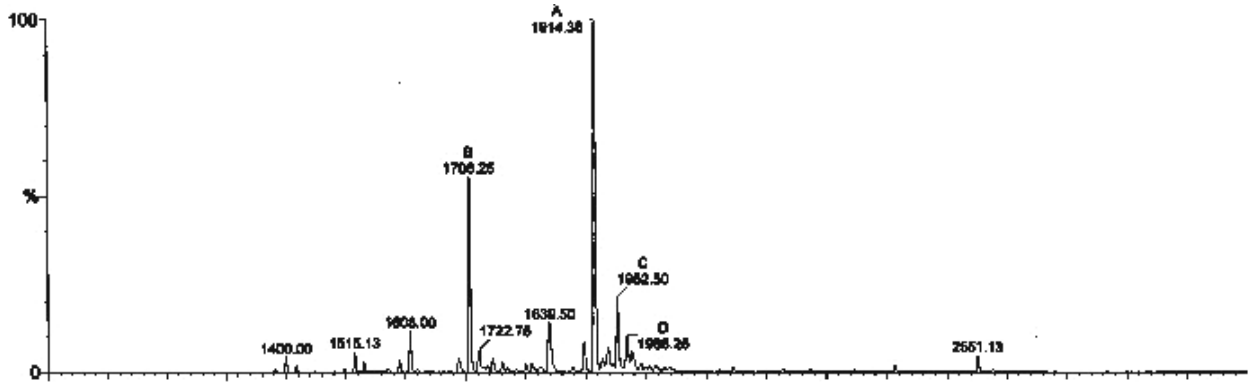
Dendrimer A_3



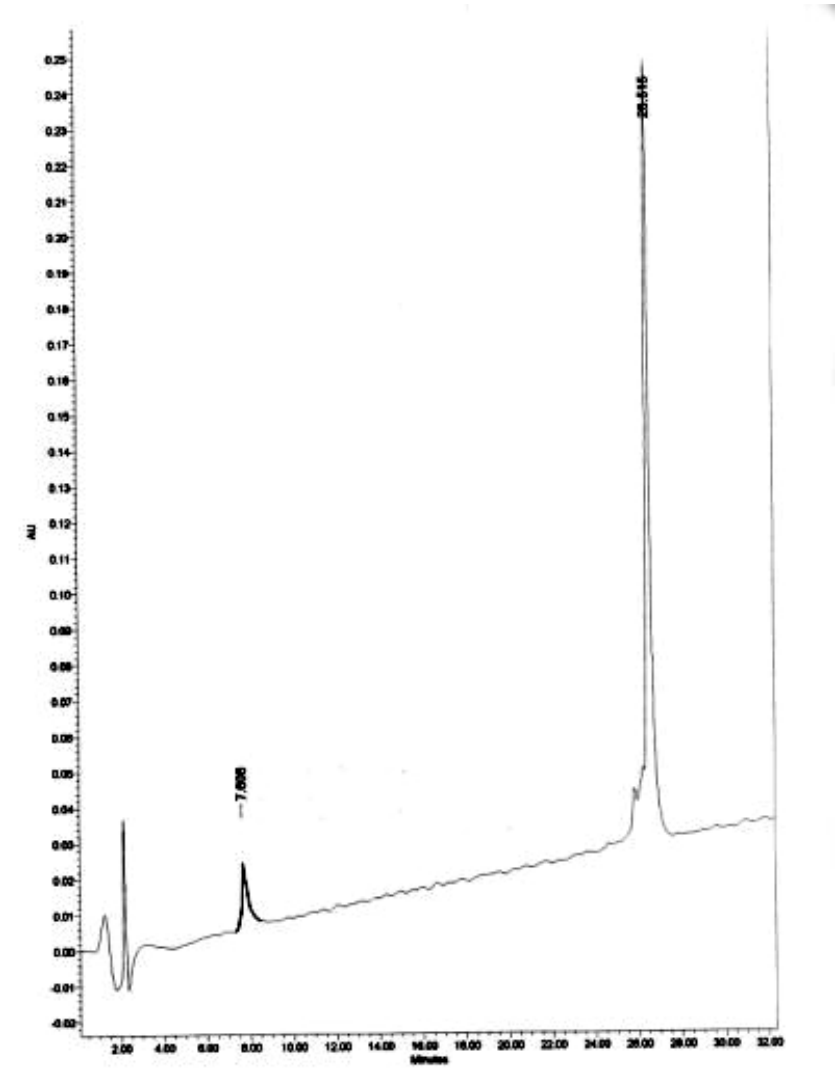


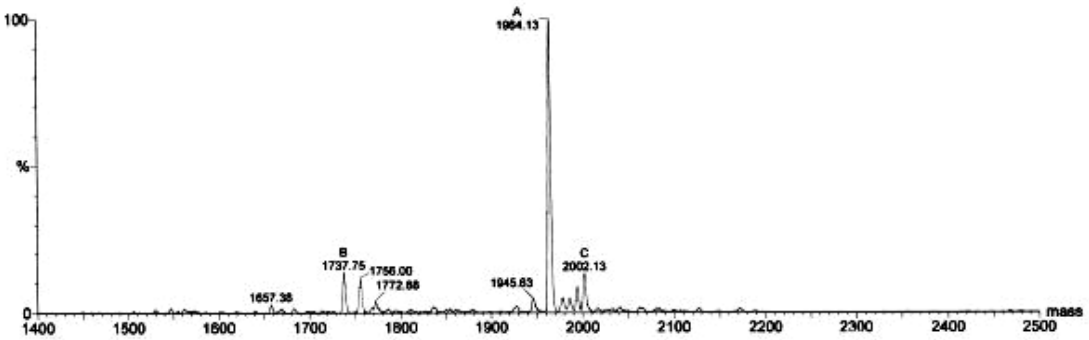
Dendrimer B_3



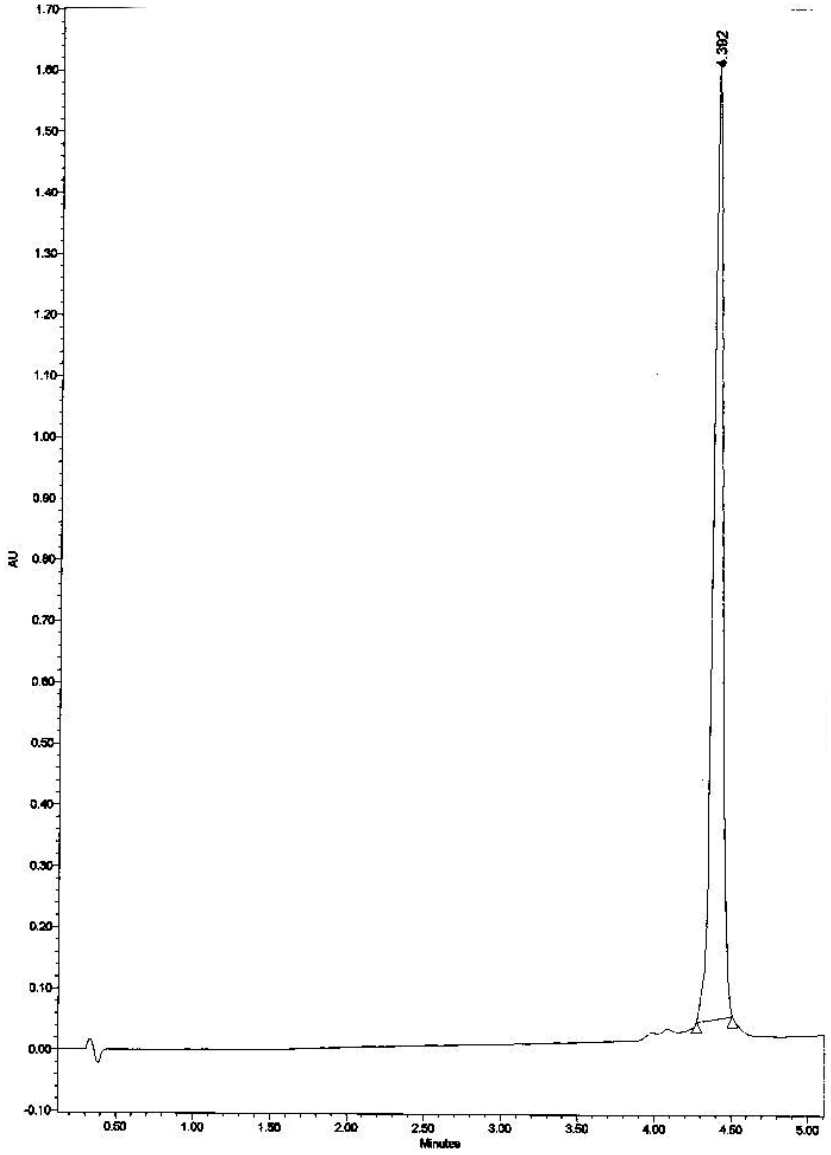


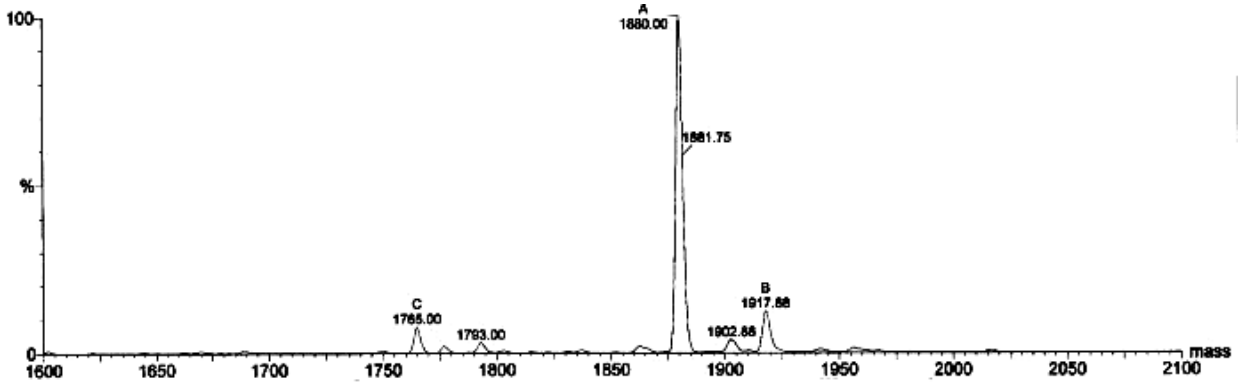
Dendrimer C_3





Dendrimer D_3





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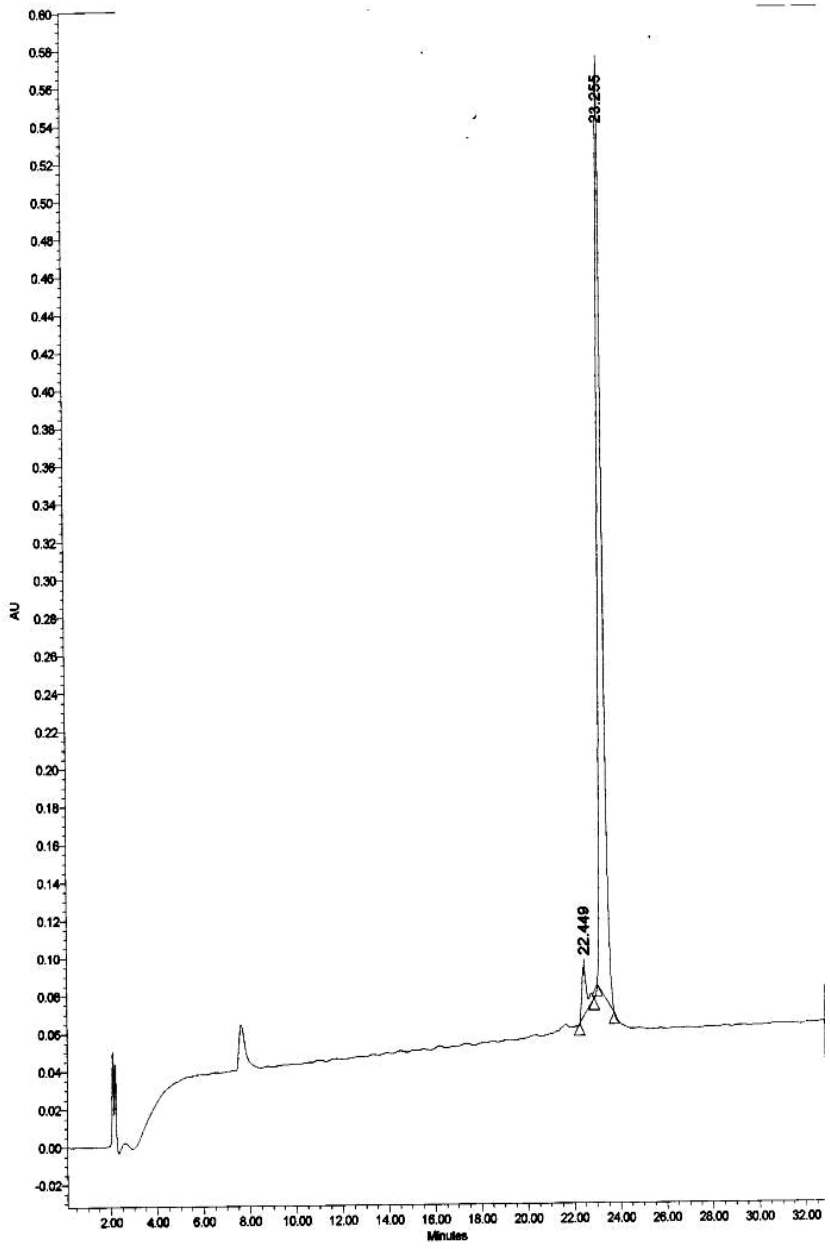

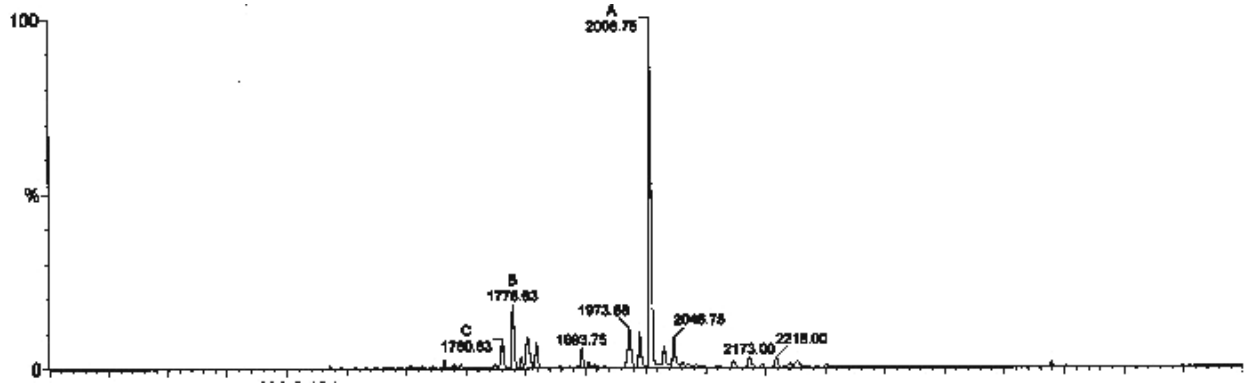

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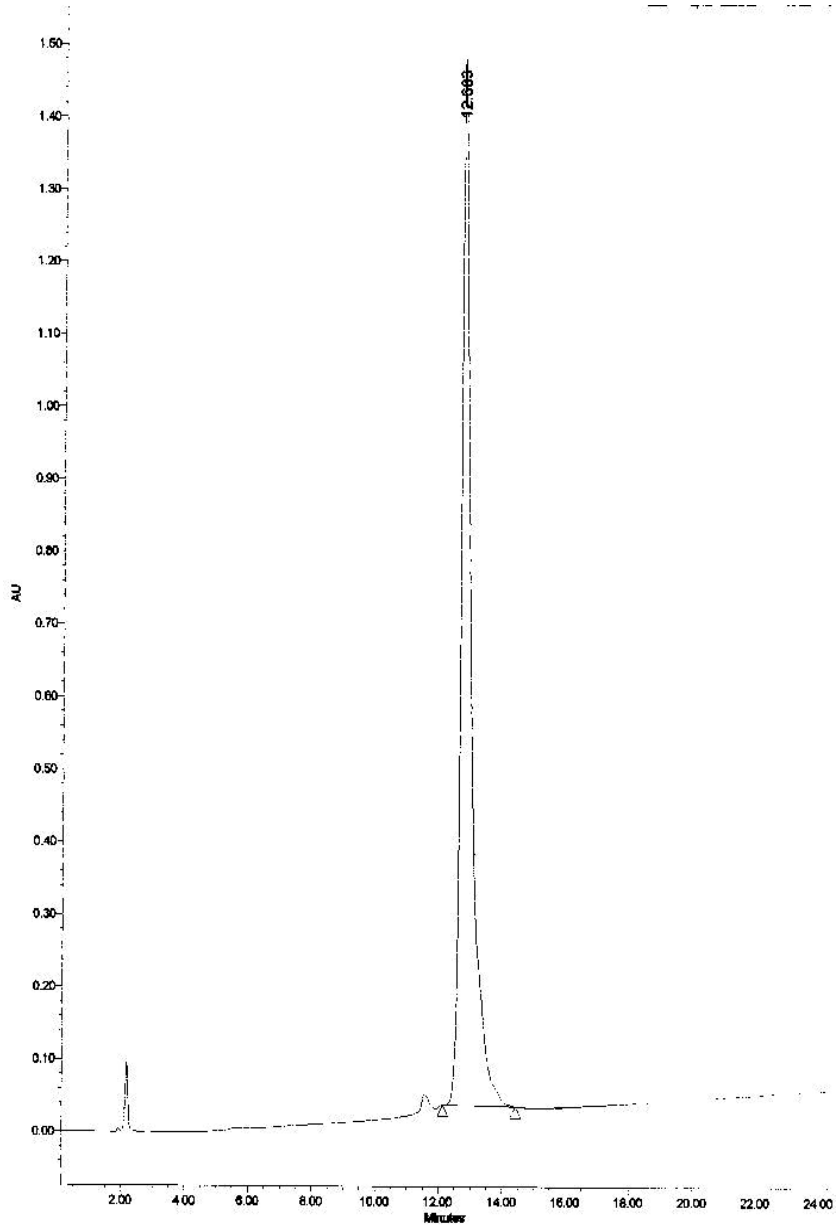

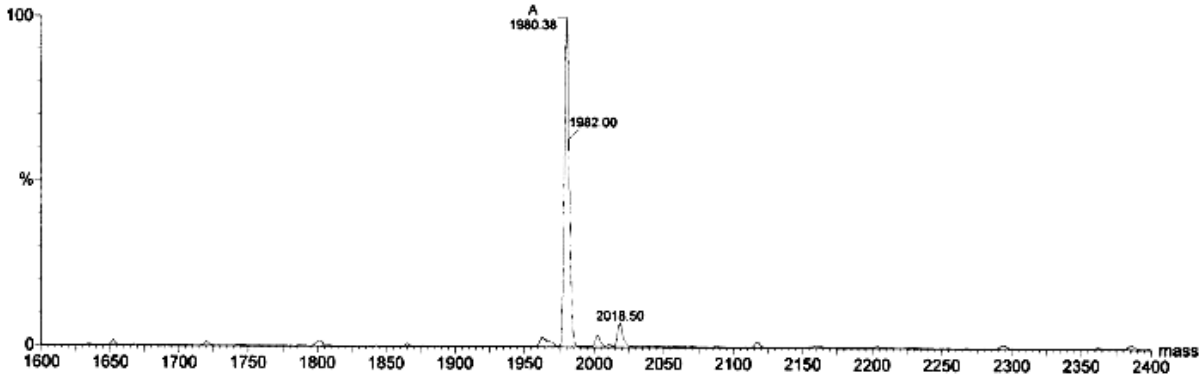

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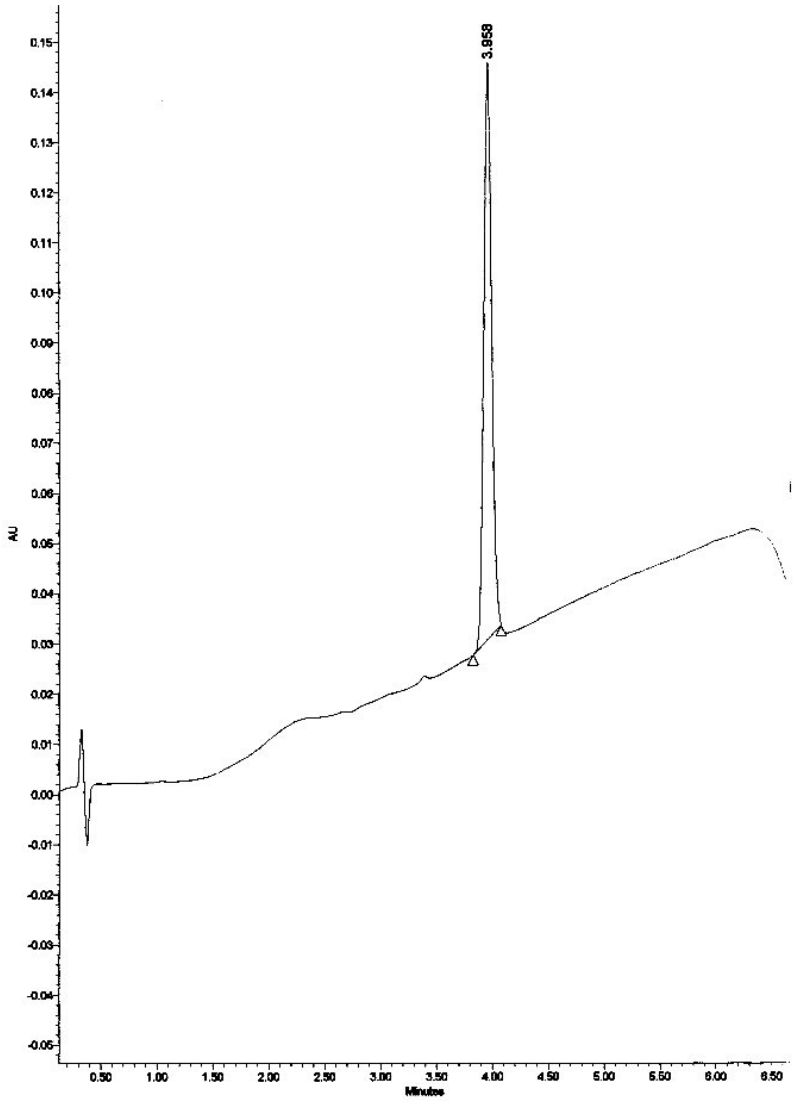

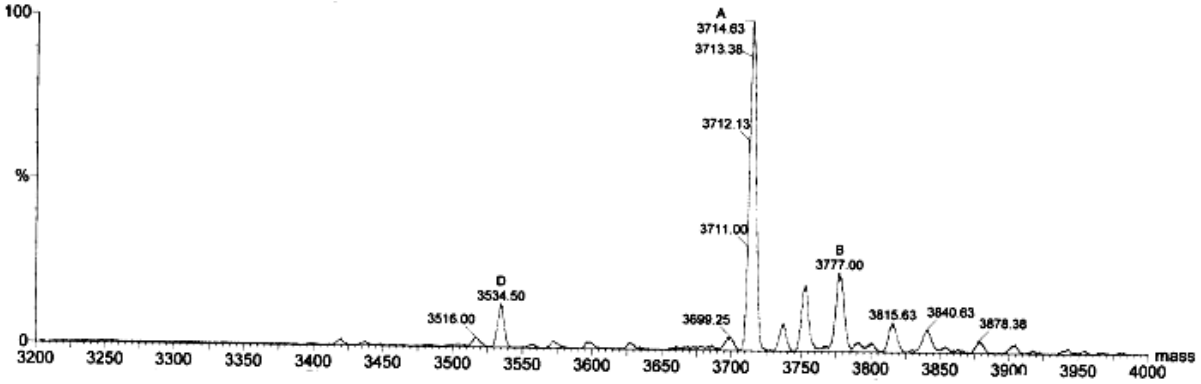

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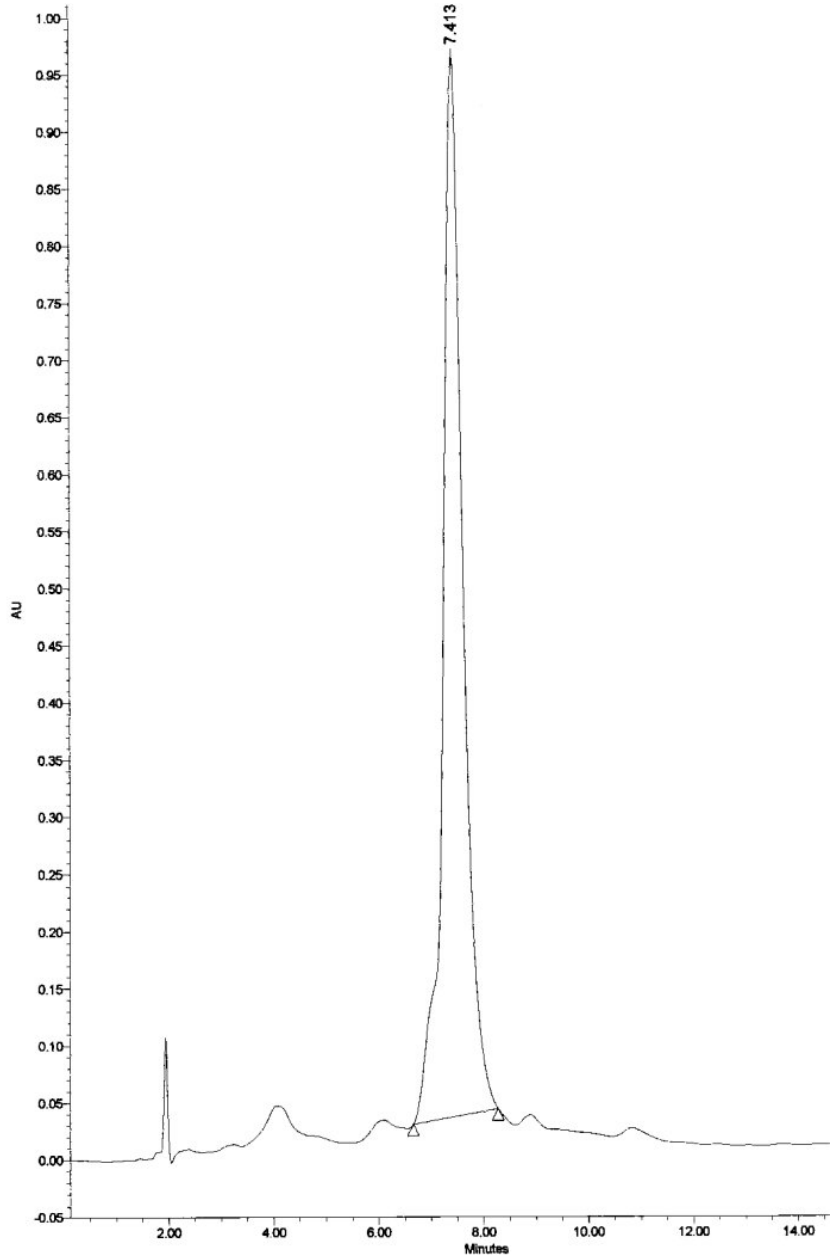

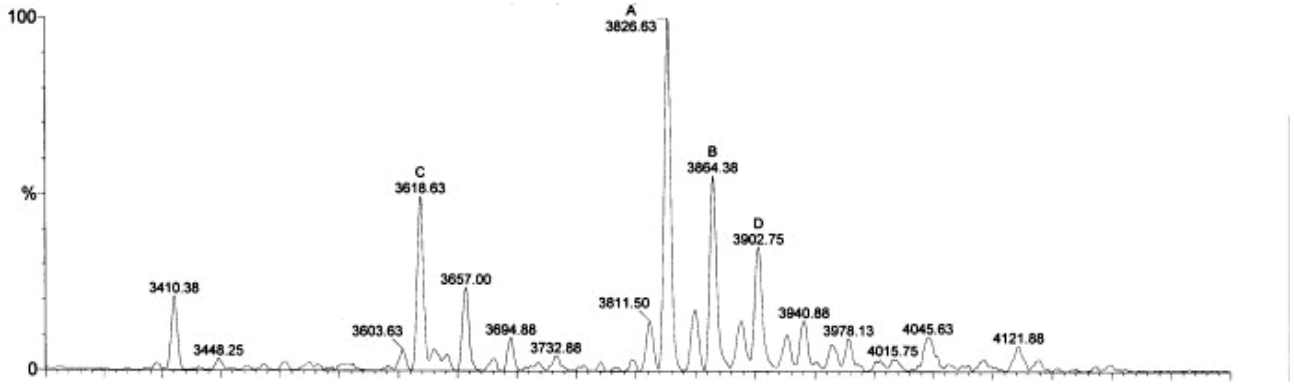

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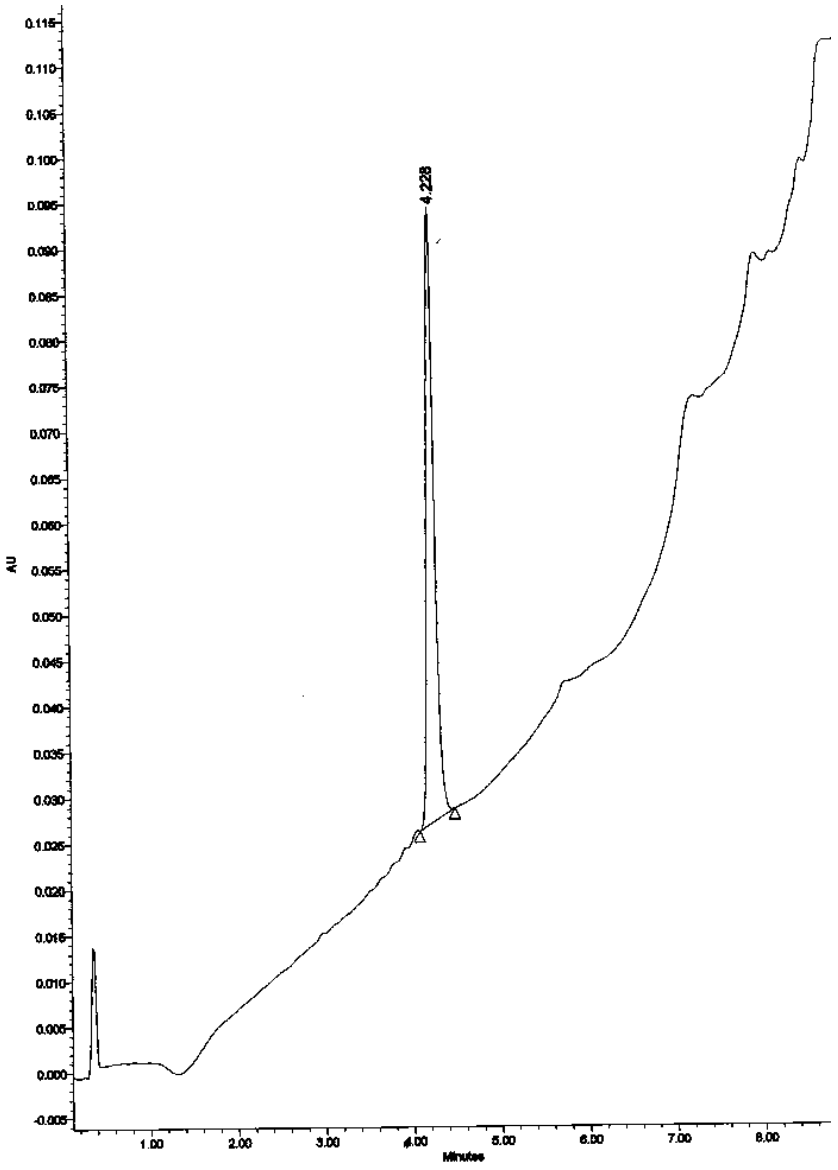

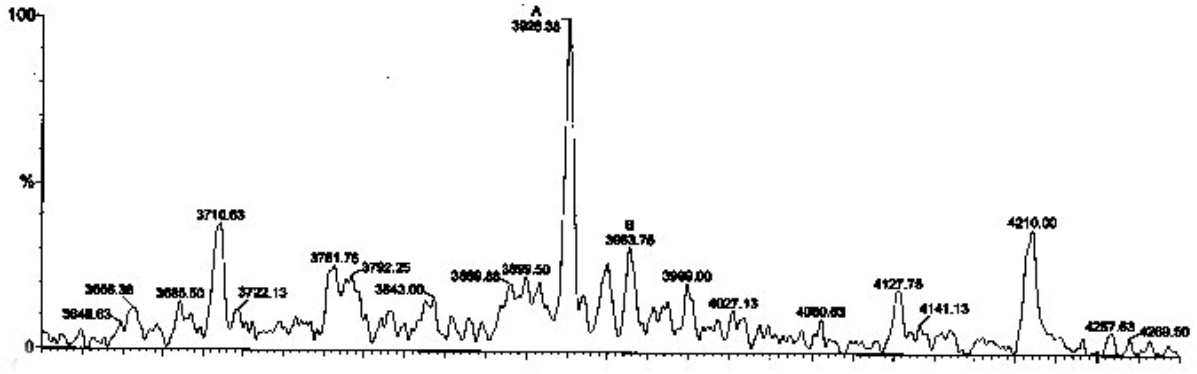

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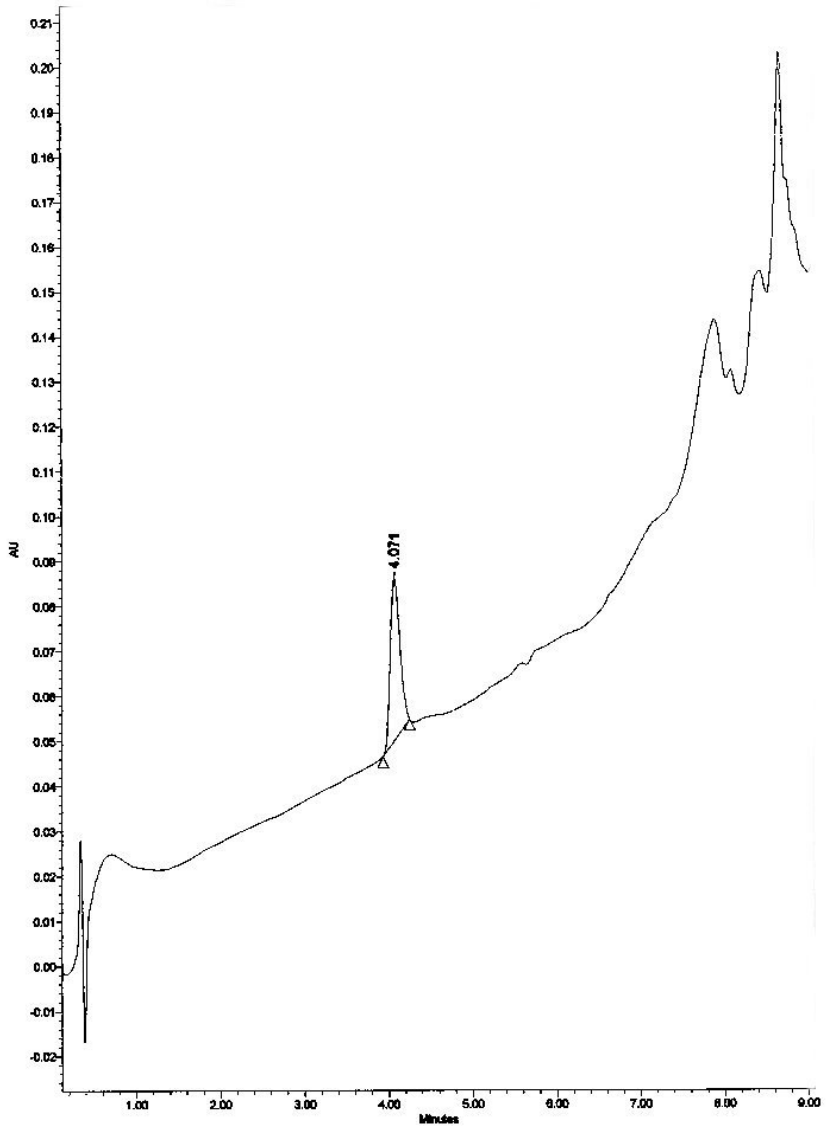

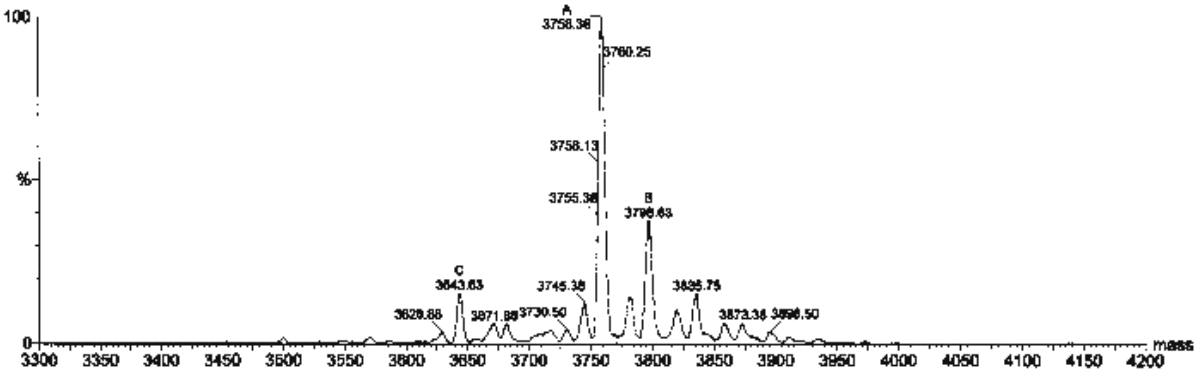

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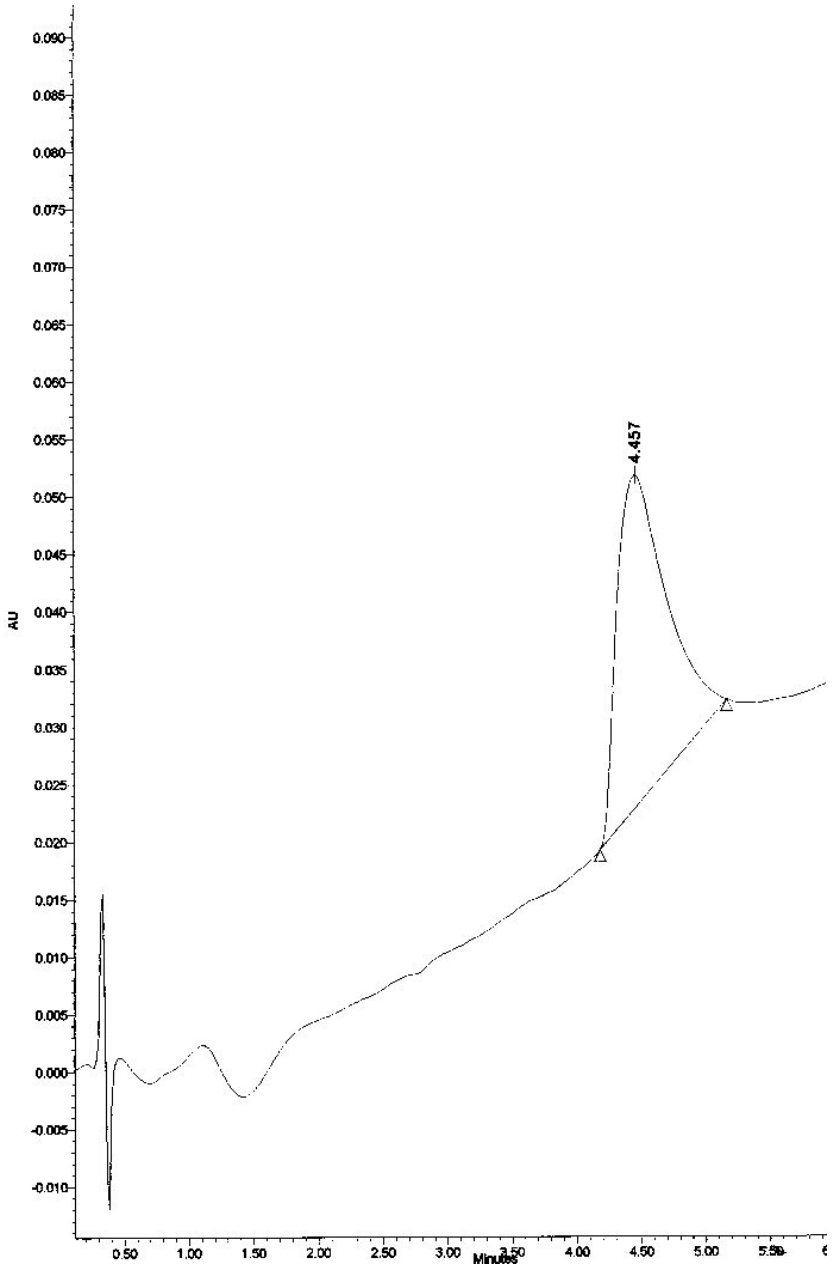

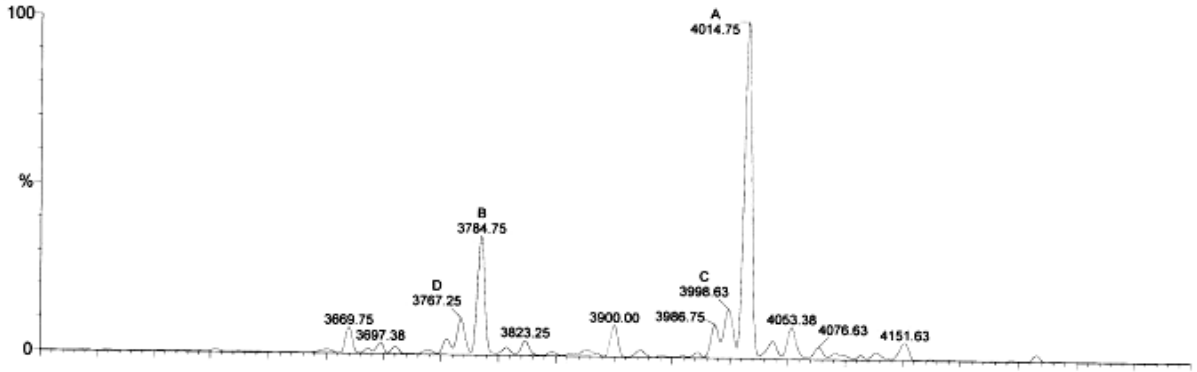

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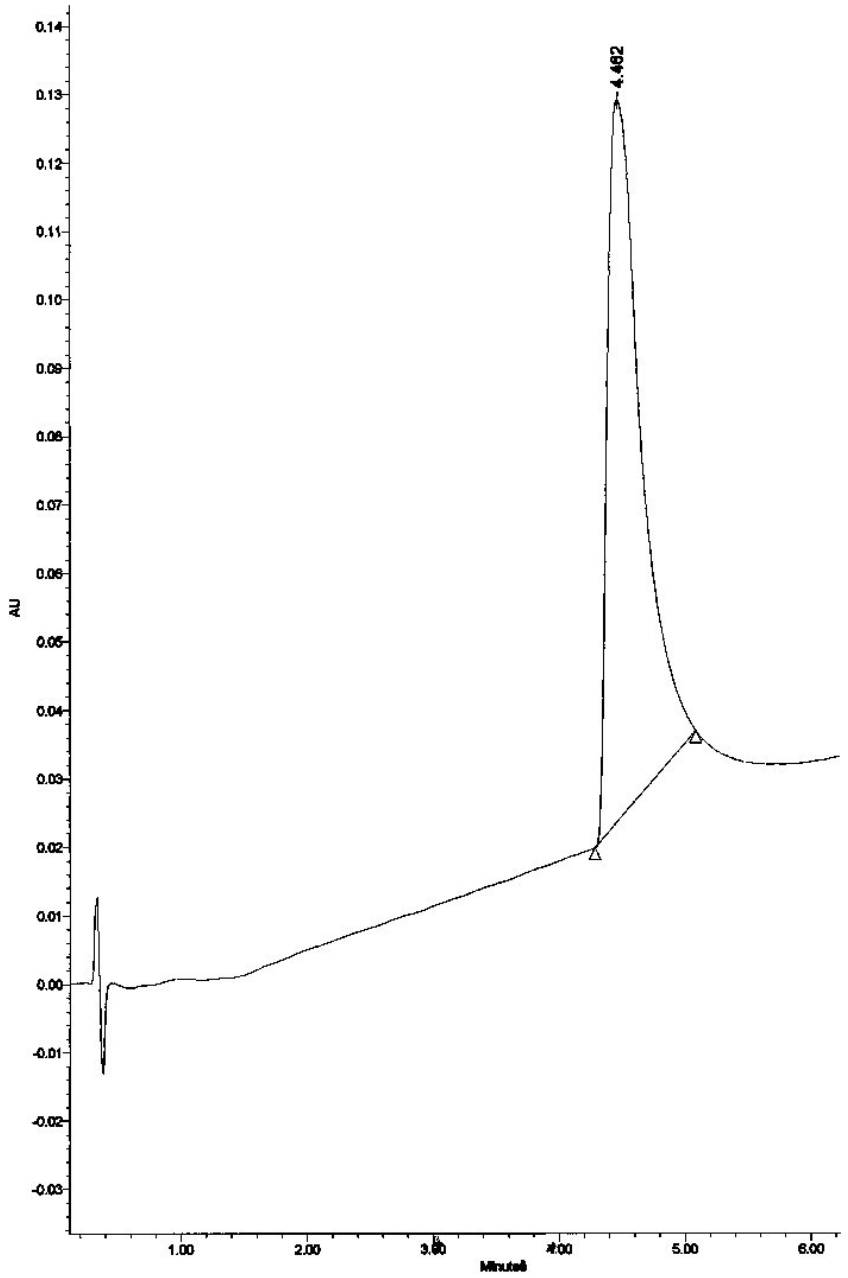

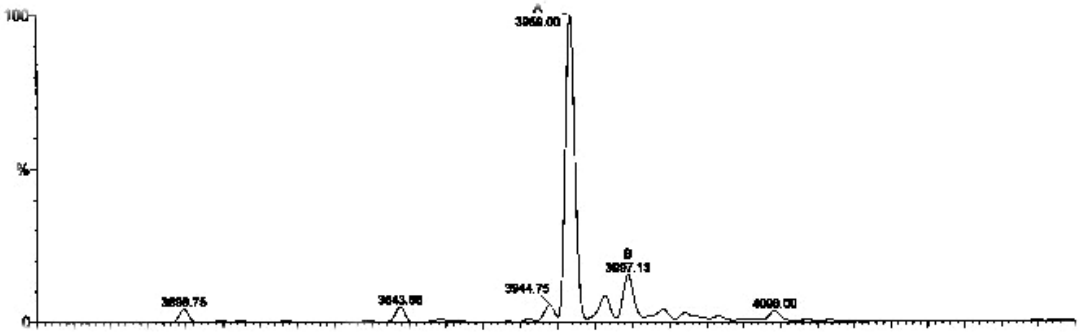

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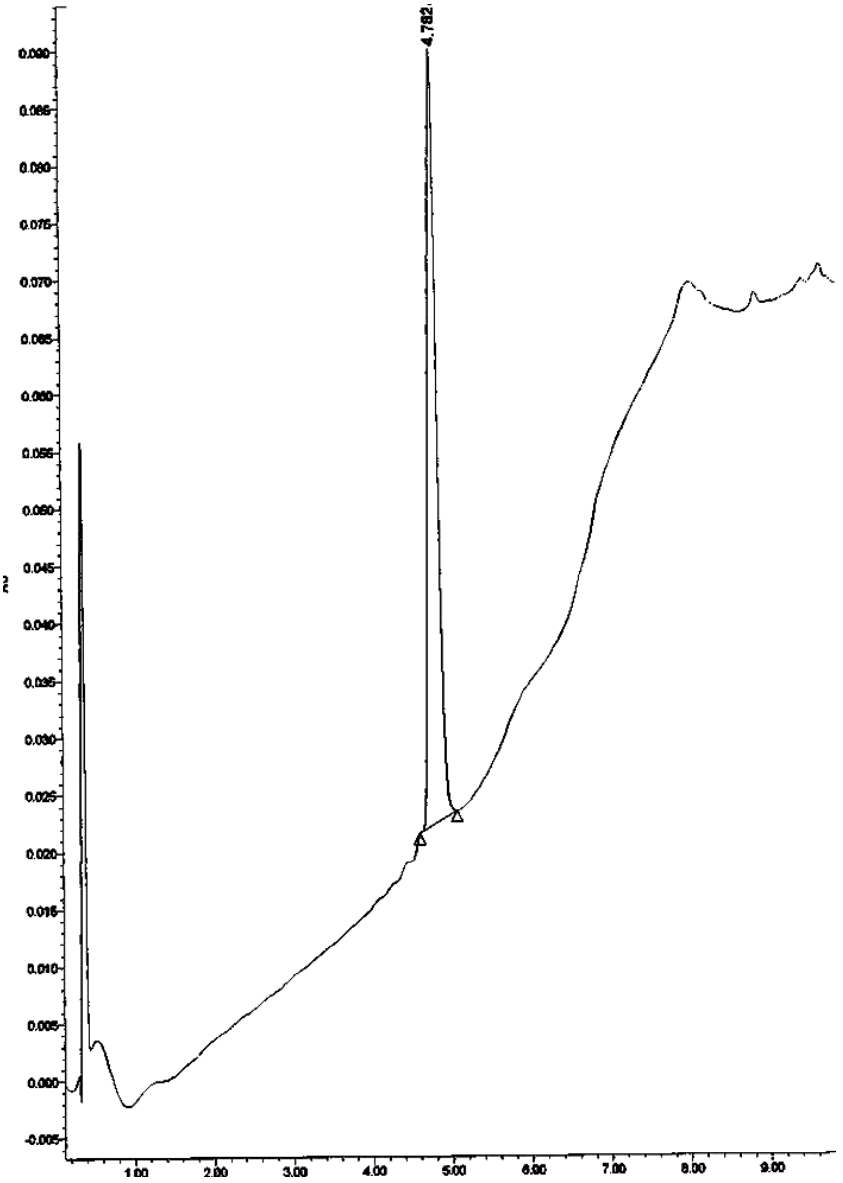

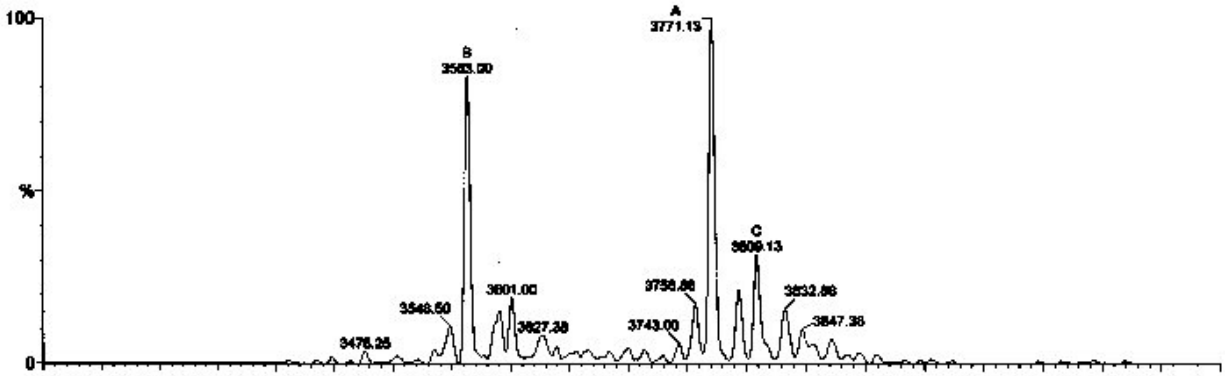

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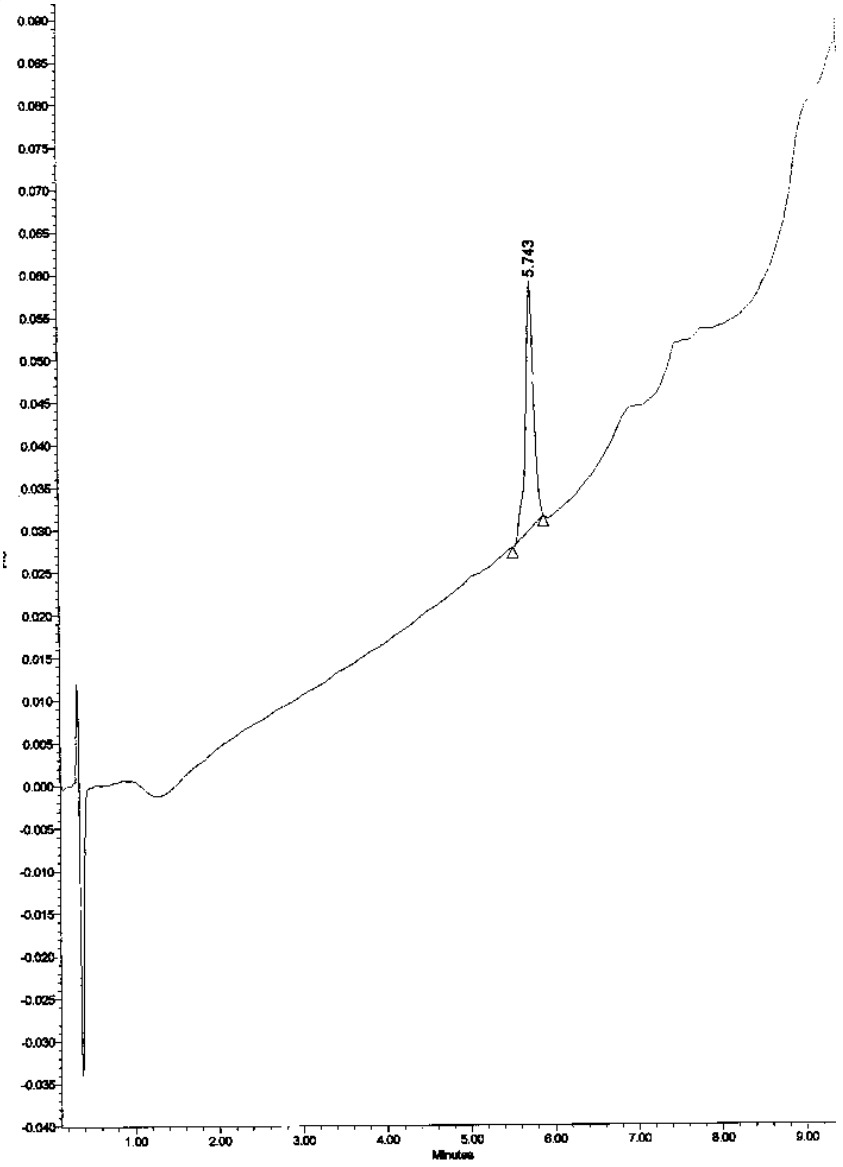

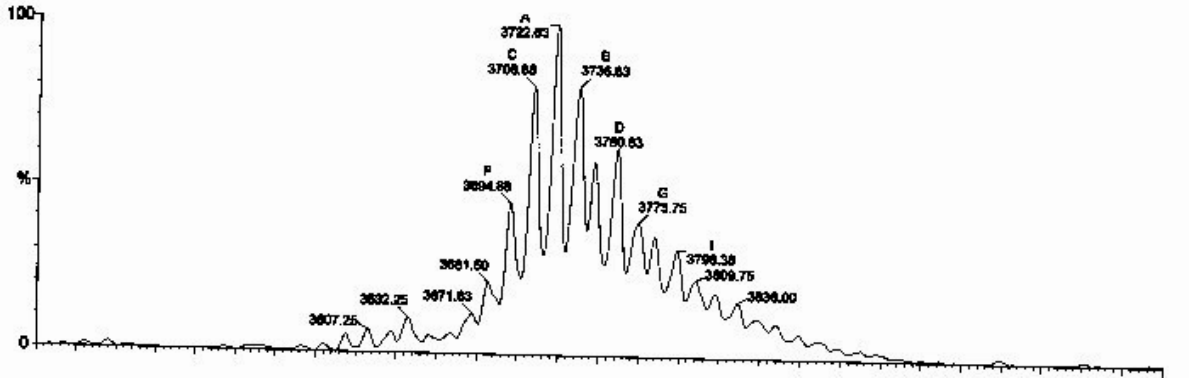

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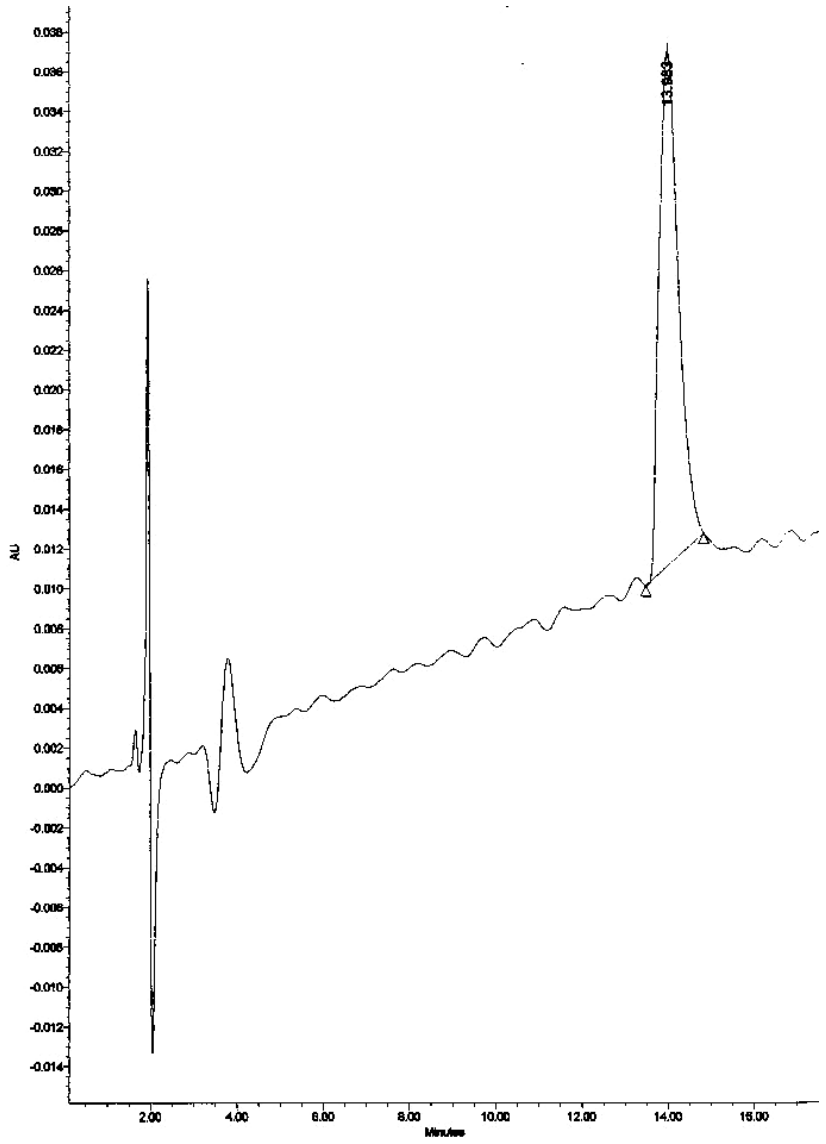

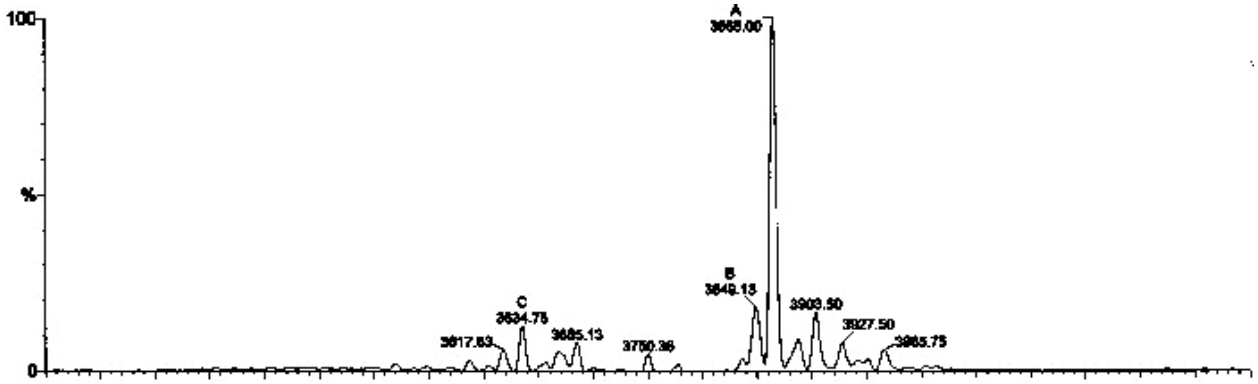

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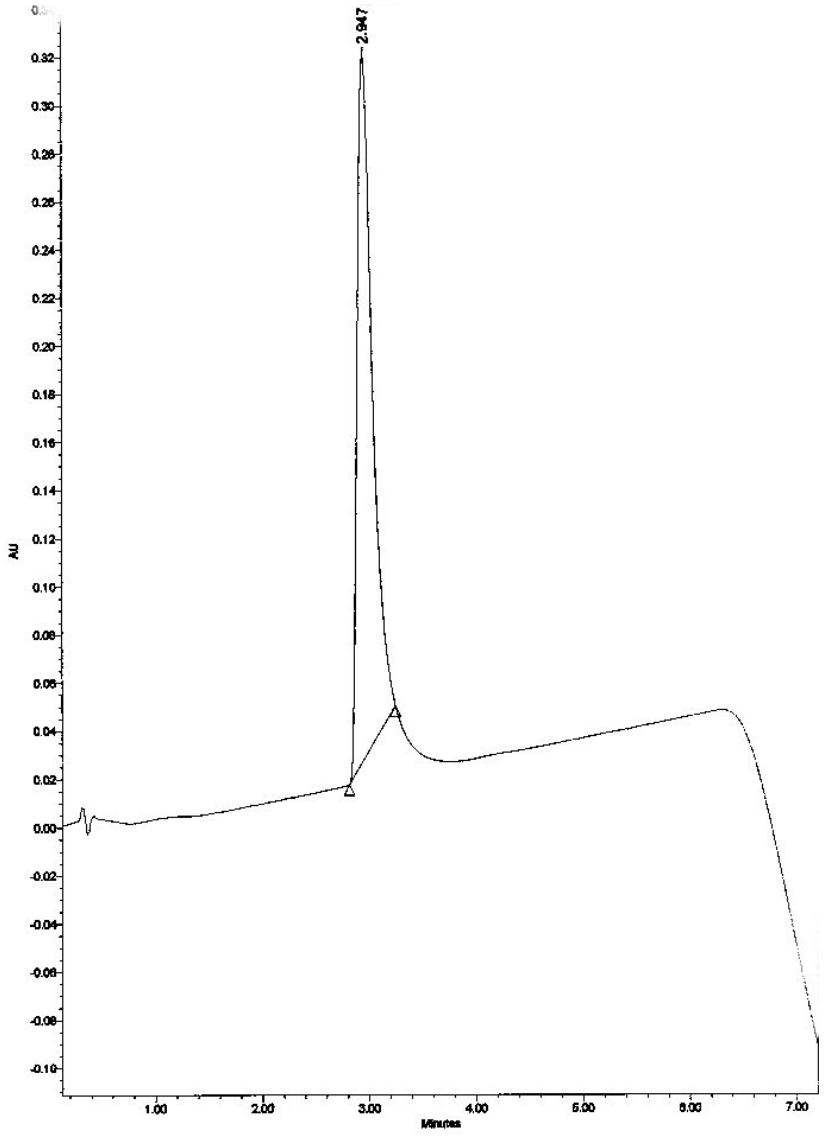

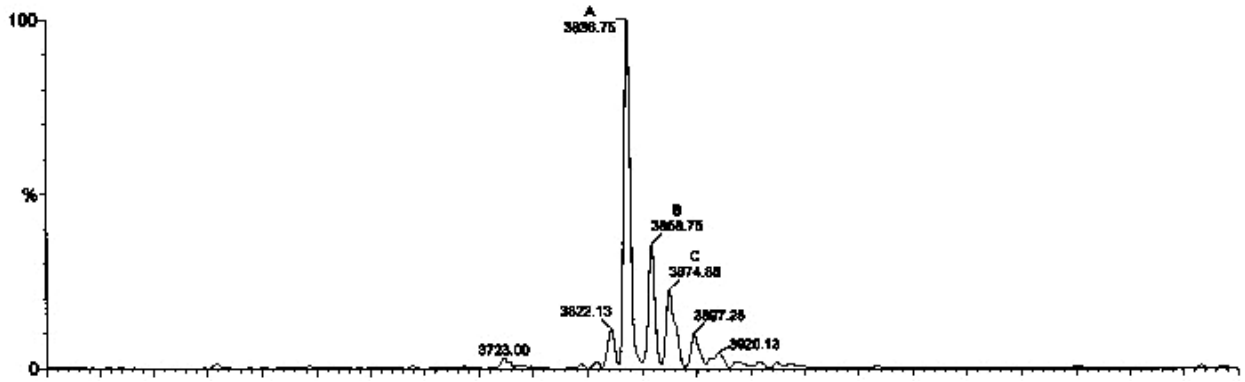

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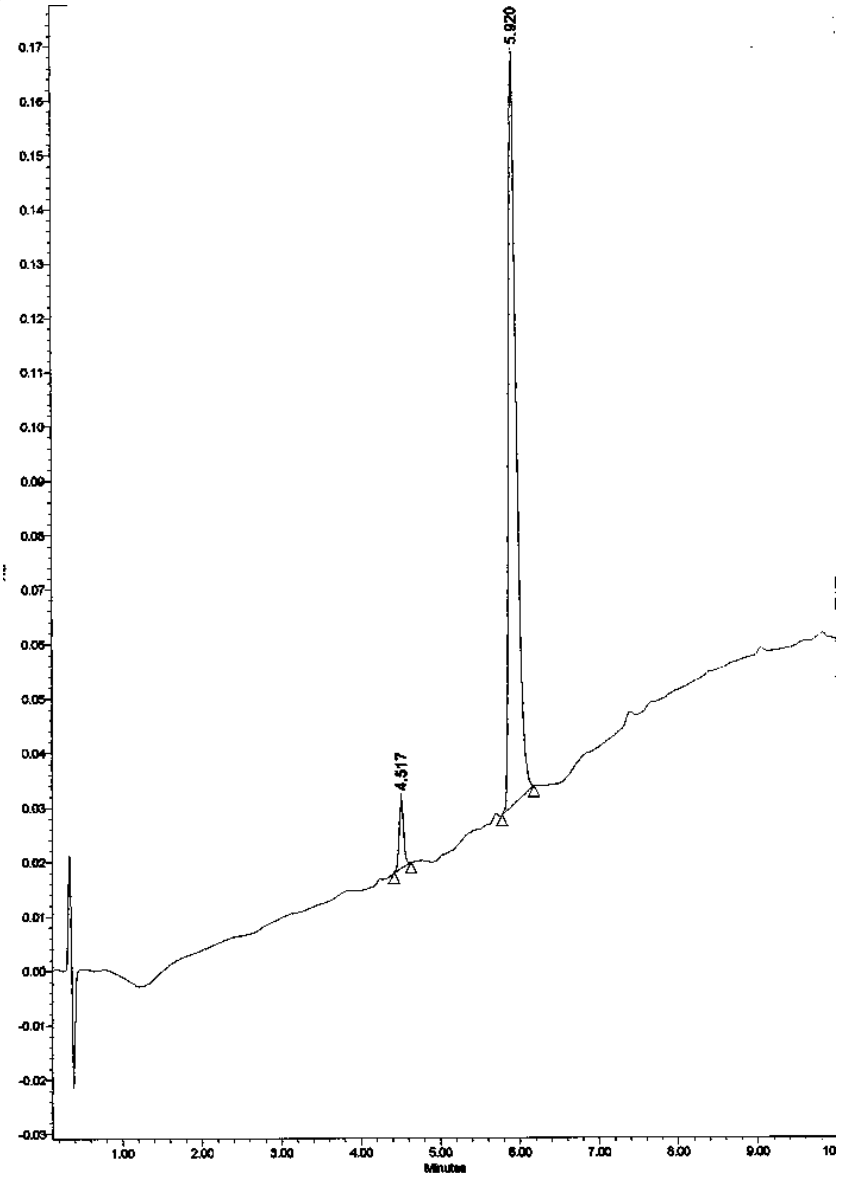

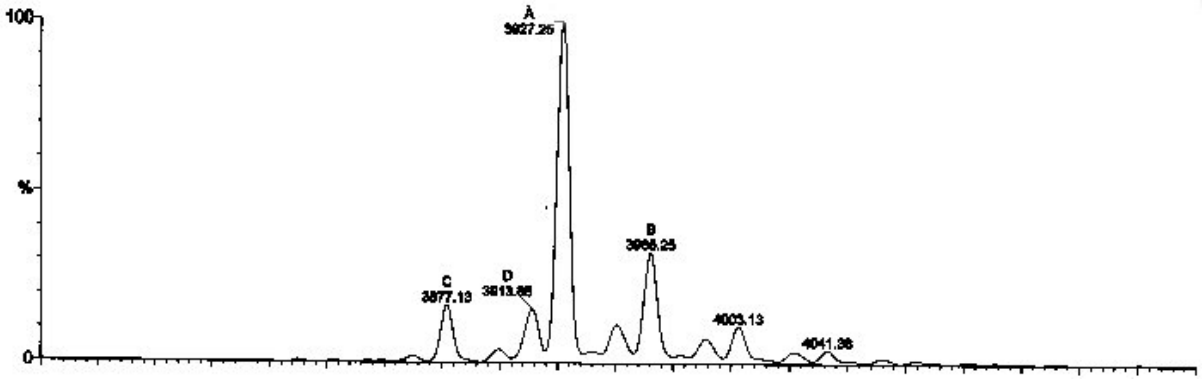

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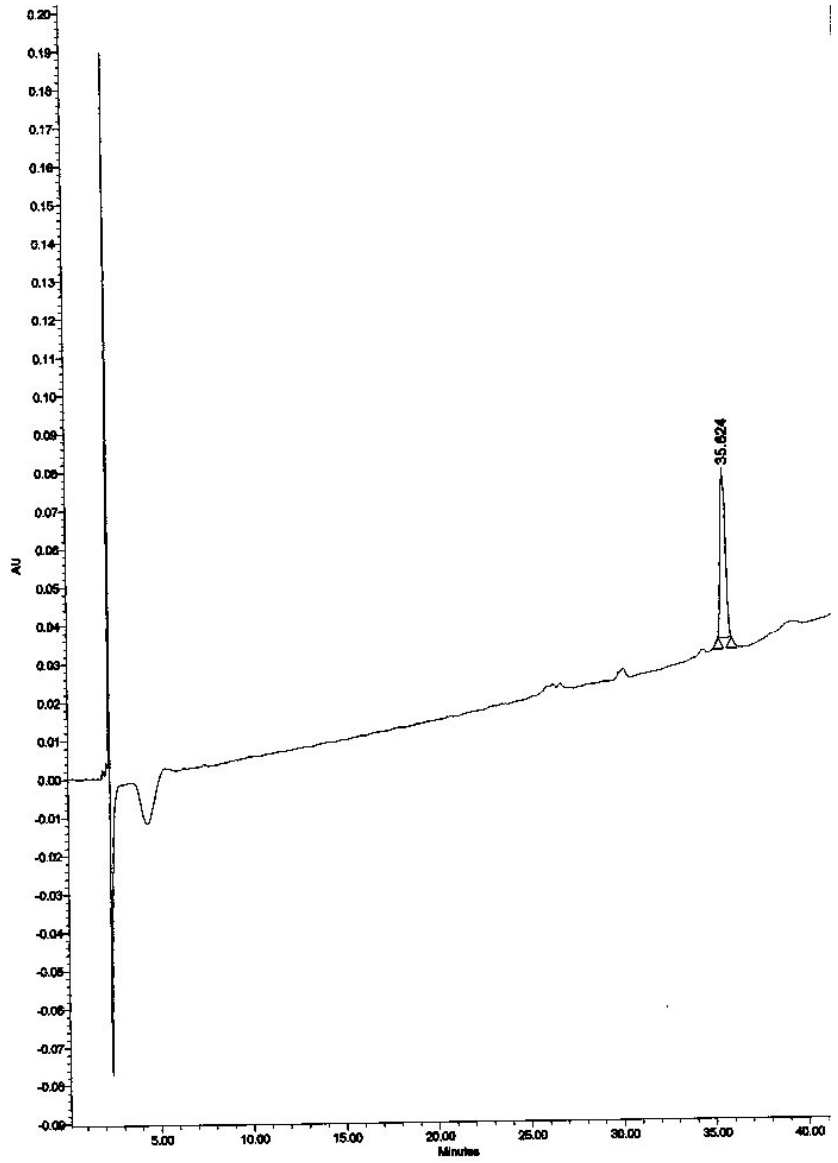

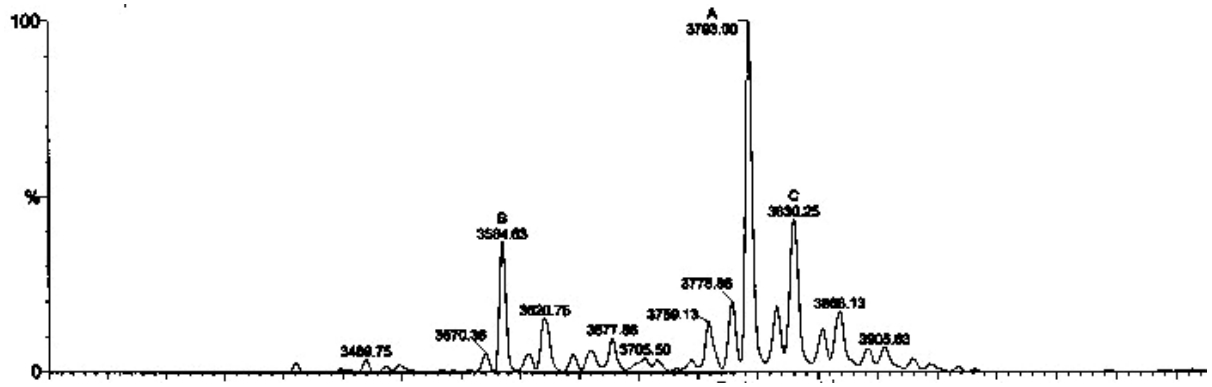

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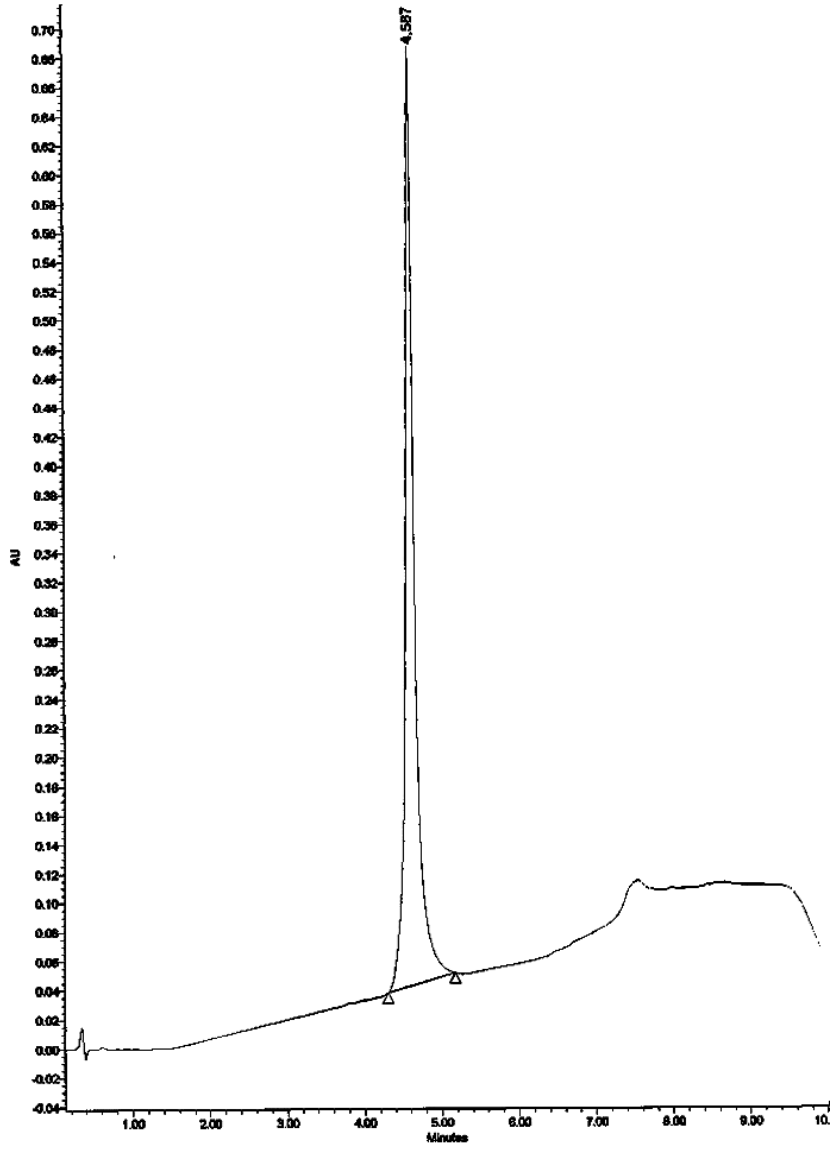

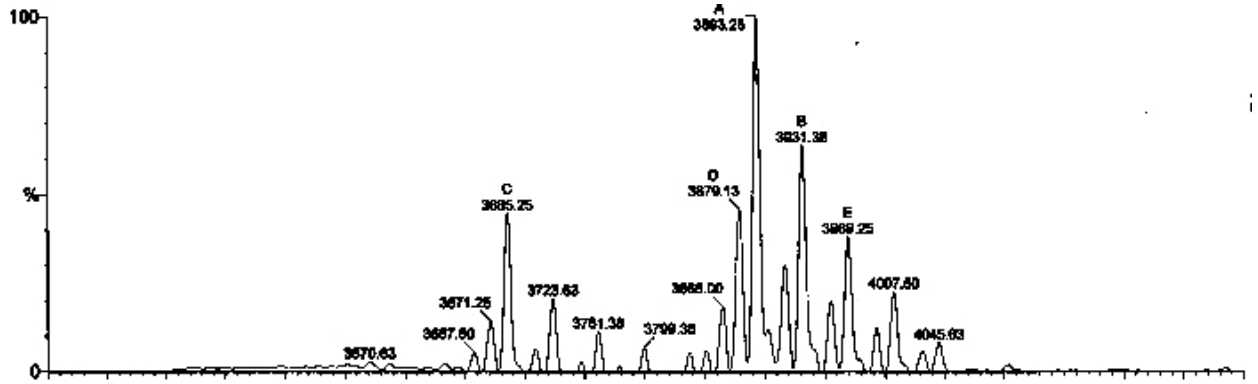

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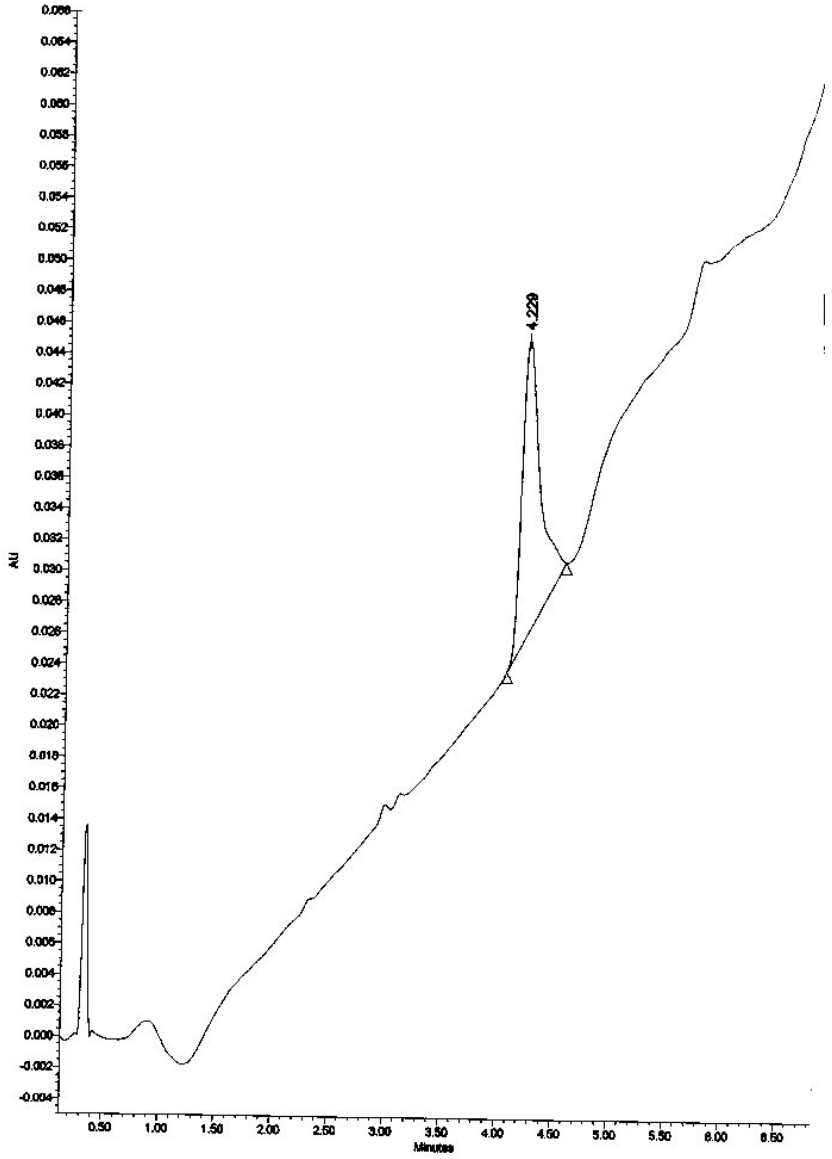

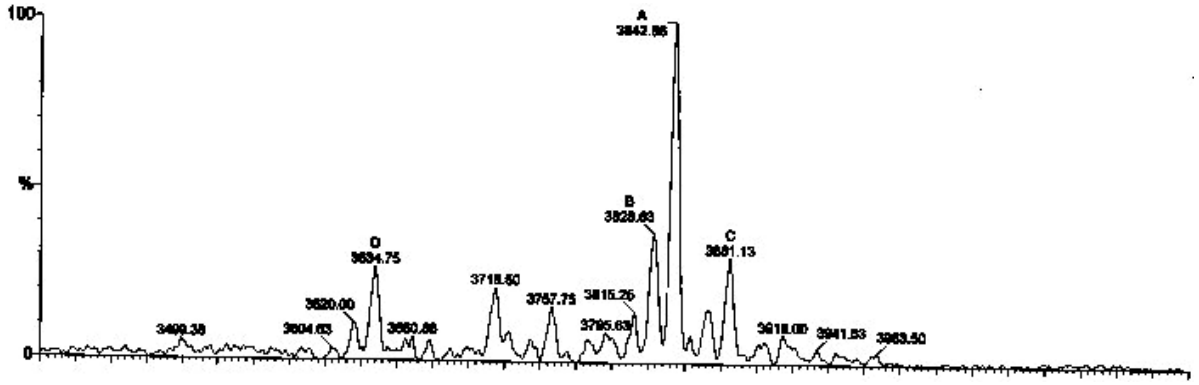

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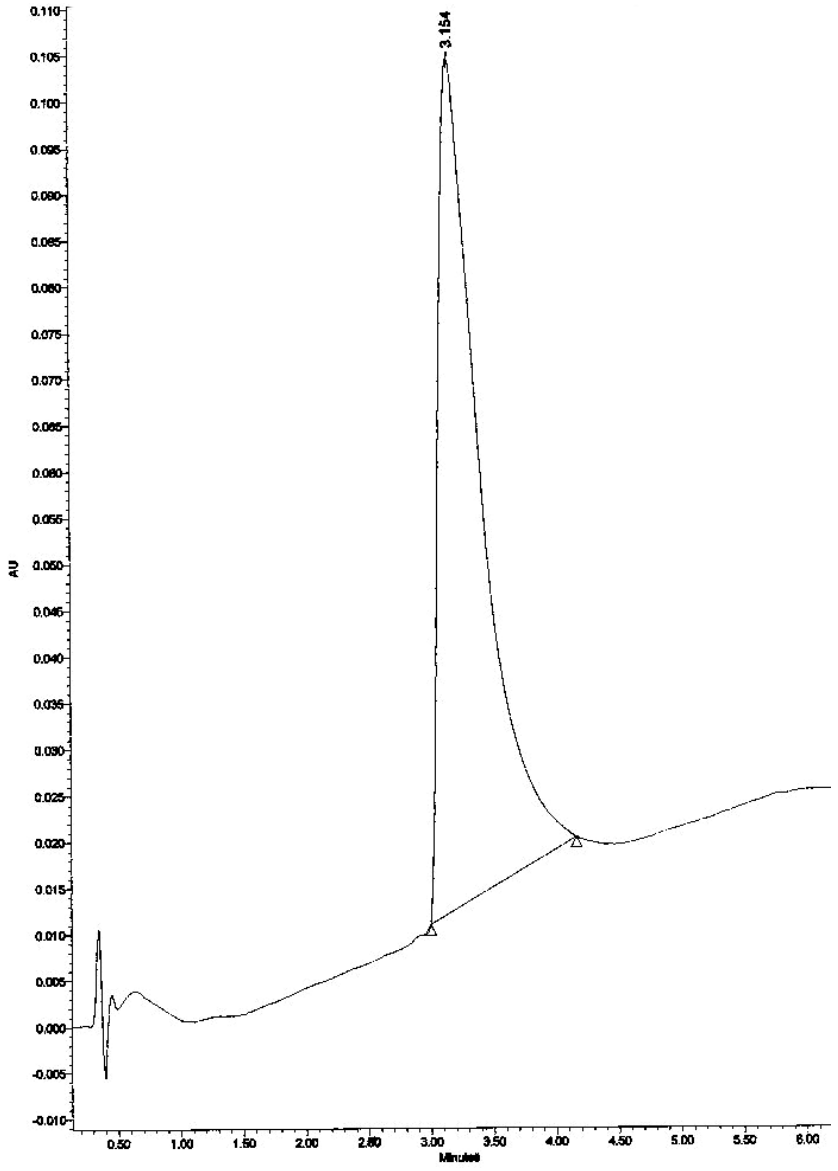

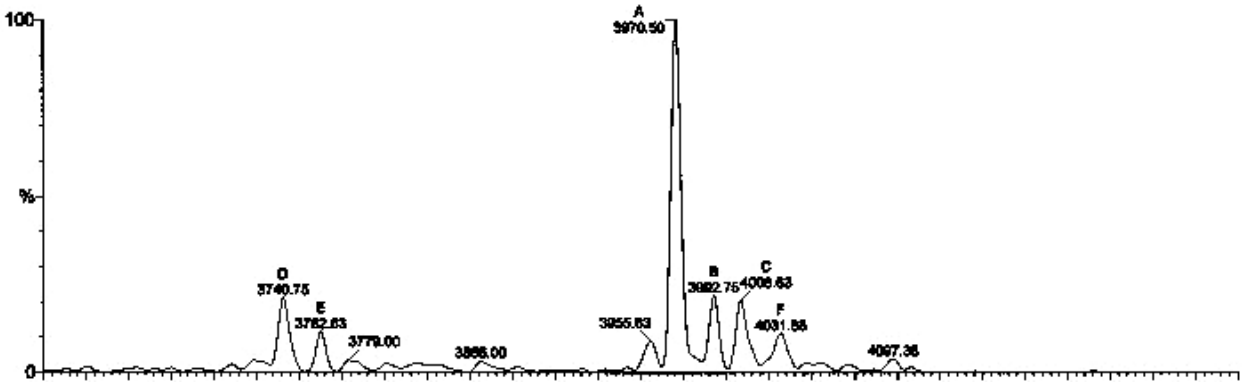

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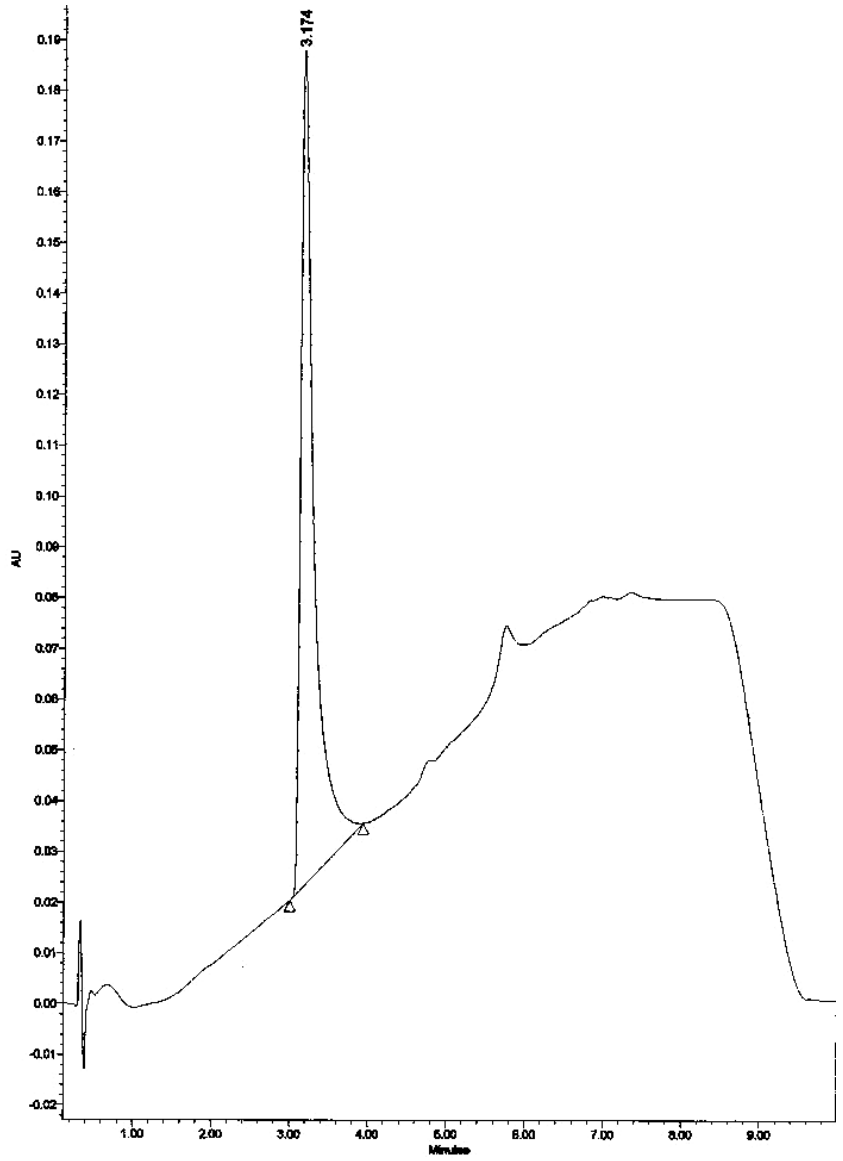

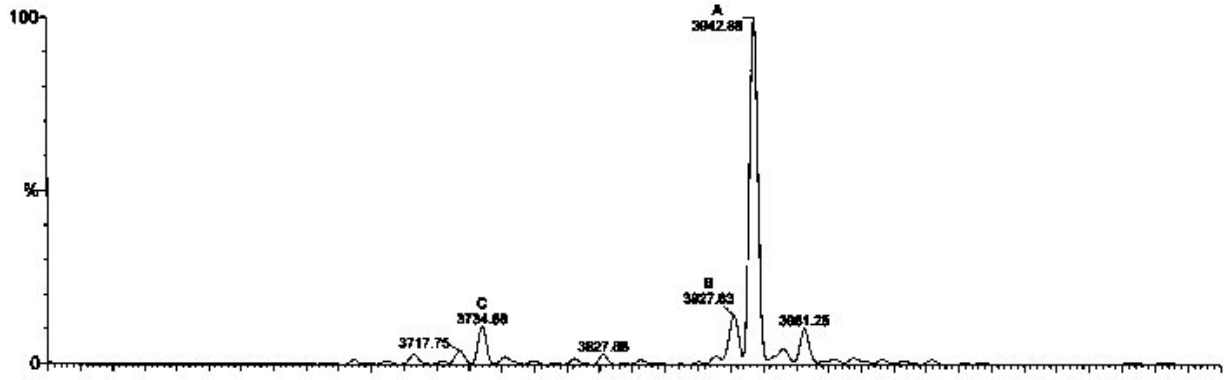

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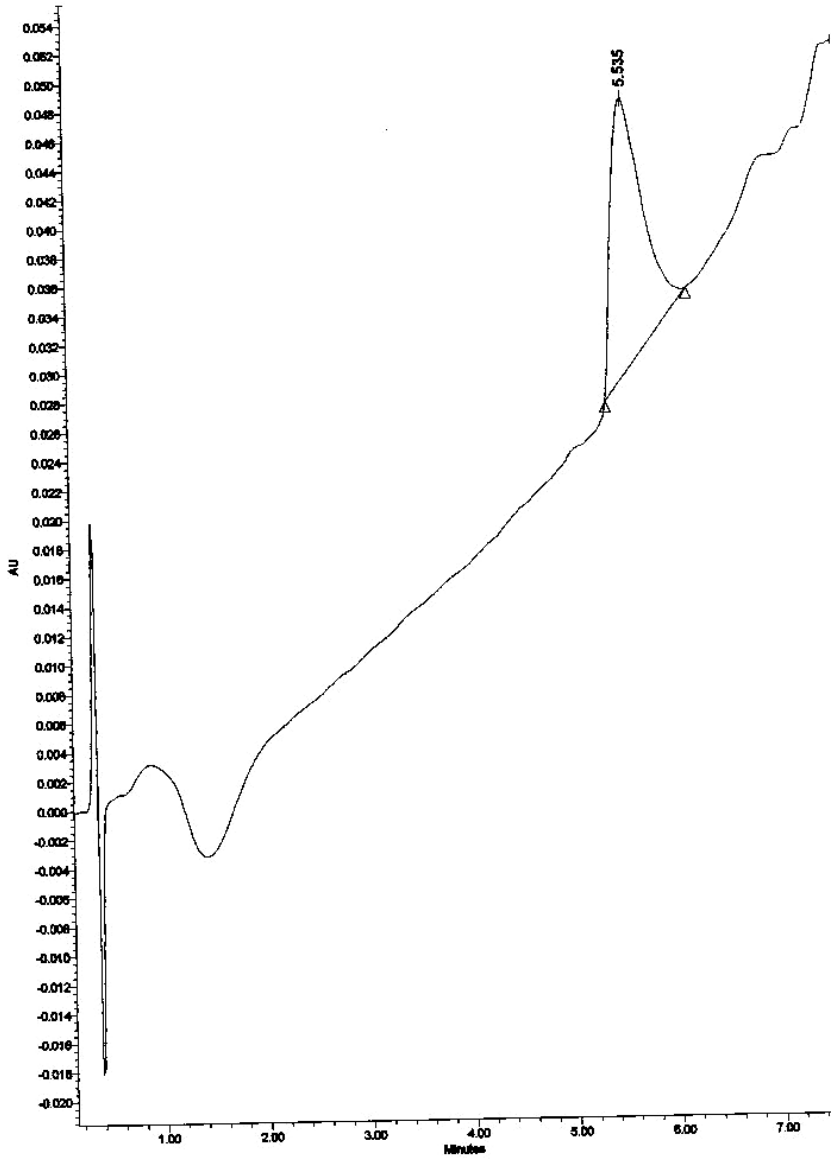

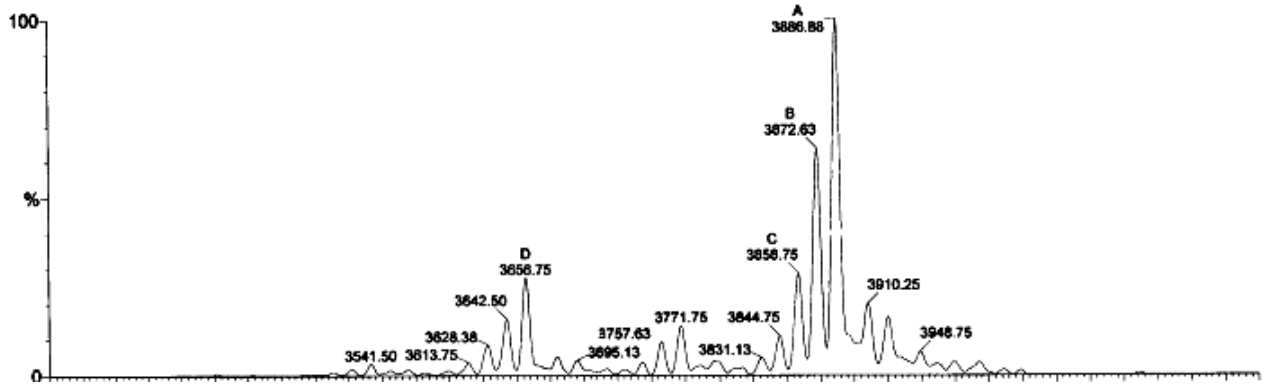

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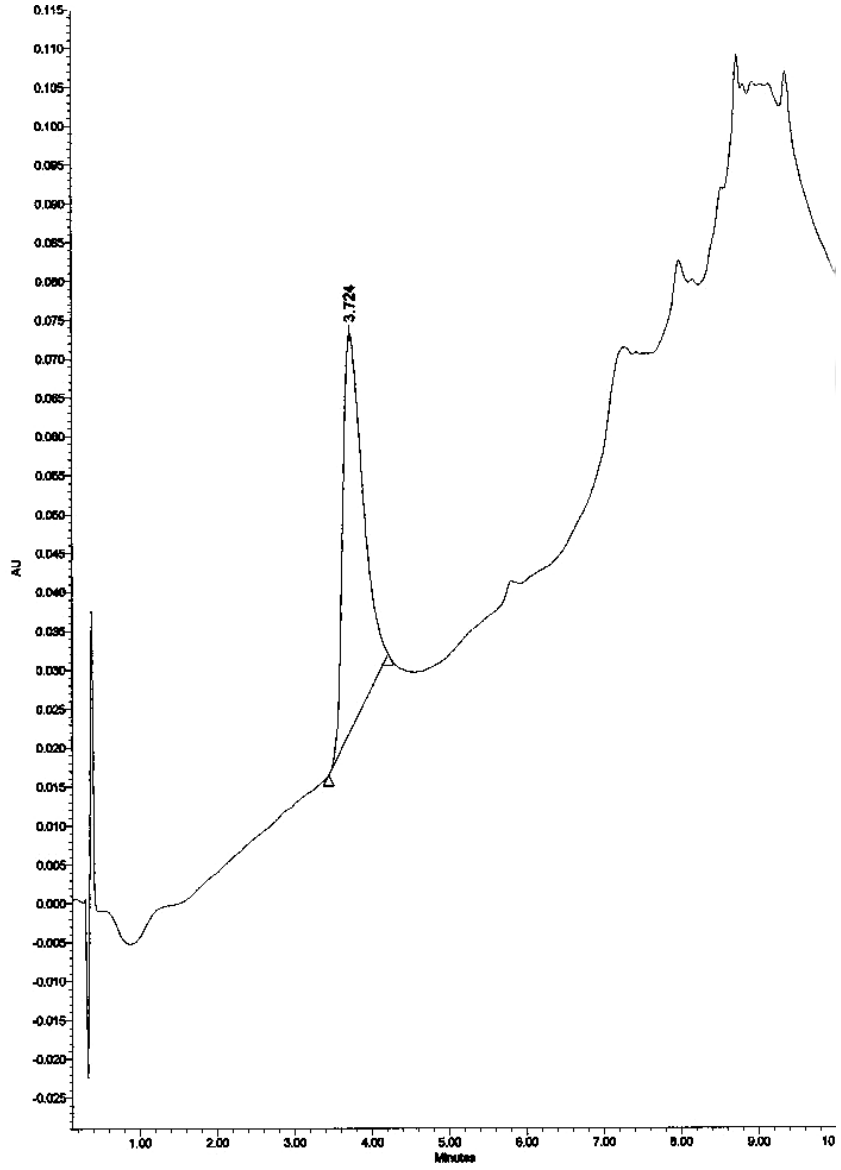

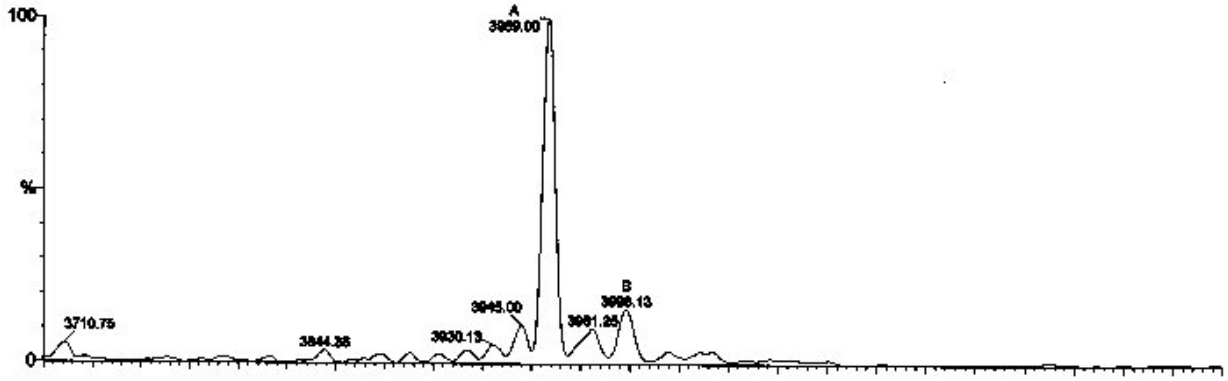

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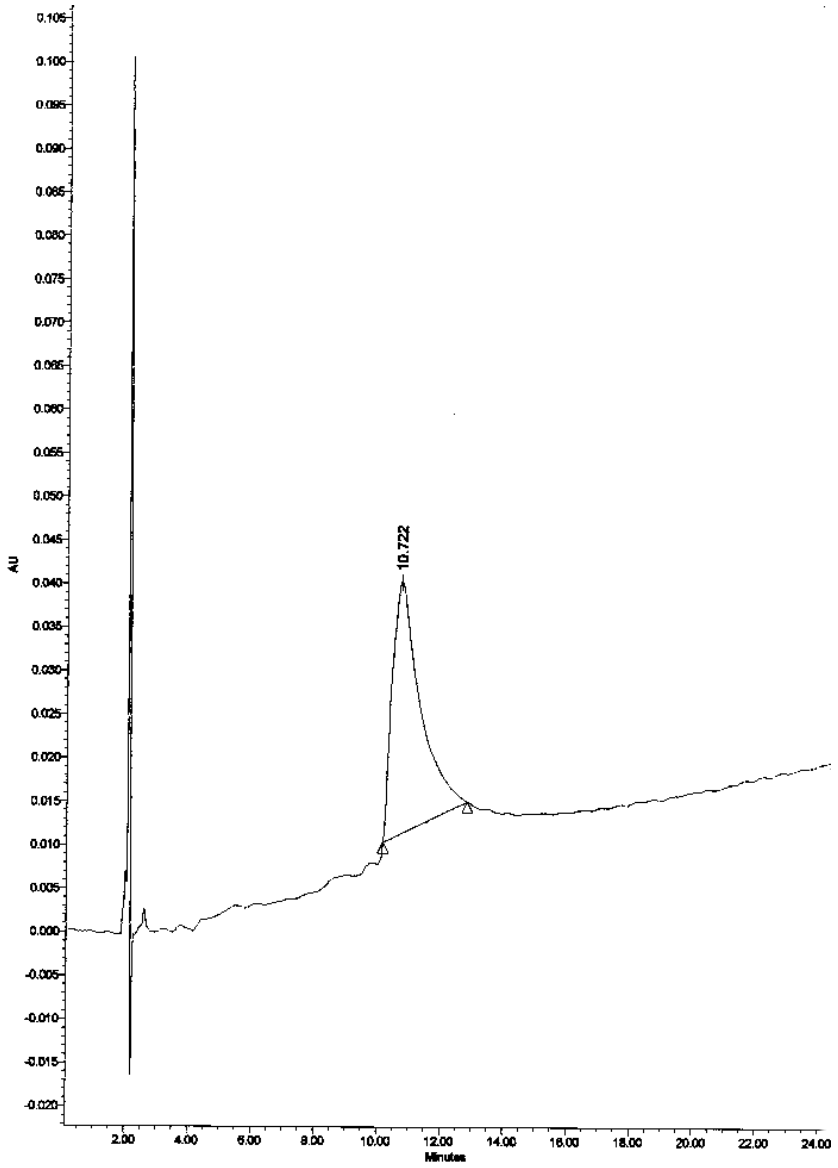
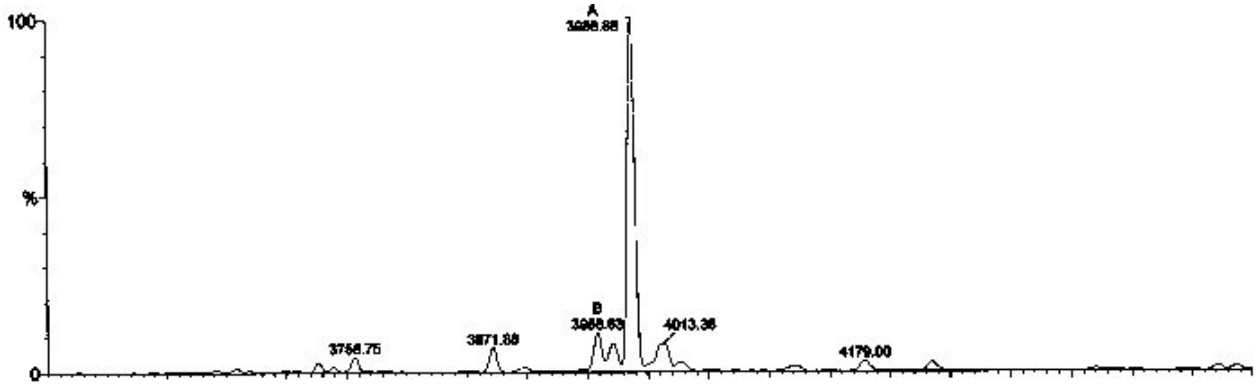
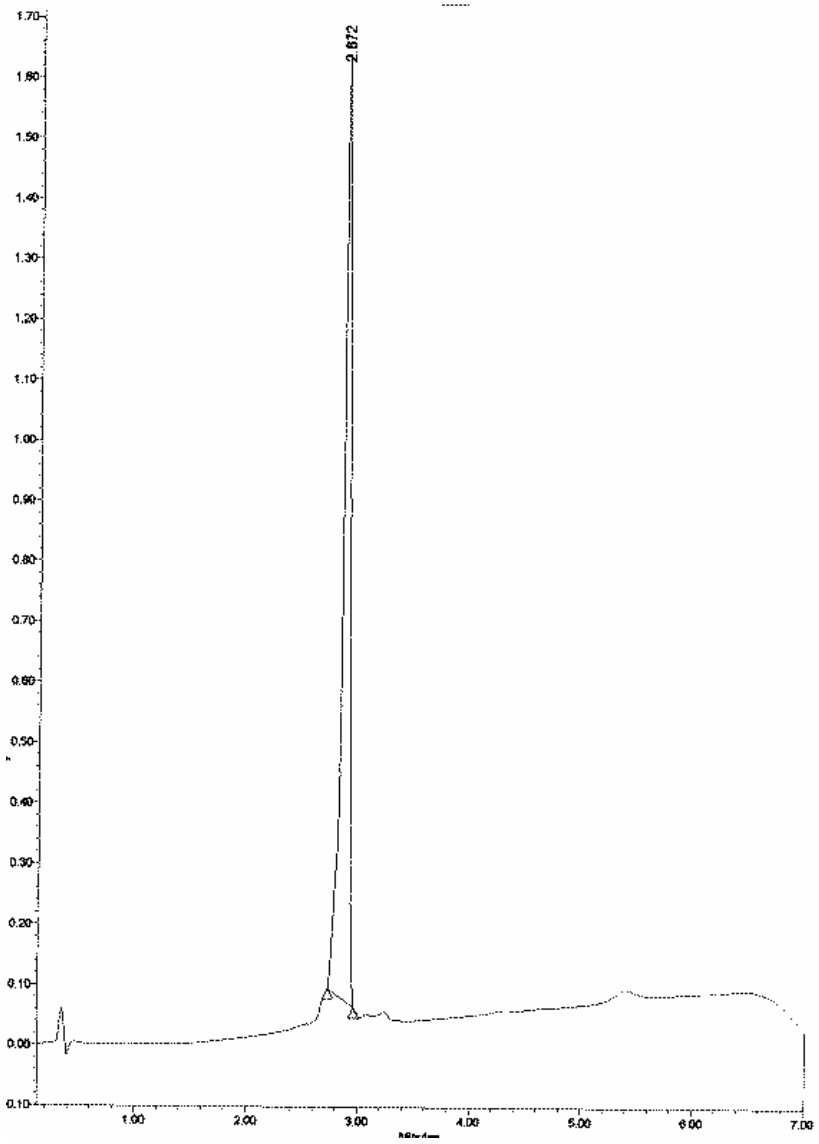




Monomer DHL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1.30
1.20
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0.60
0.50
0.40
0.30
0.20
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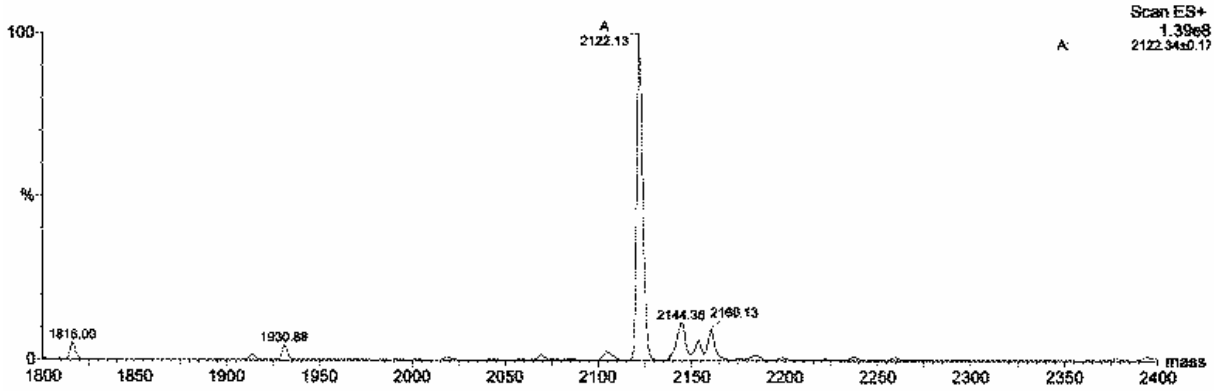
0.00
-0.10
1.00
2.00
3.00
4.00
5.00
6.00
7.00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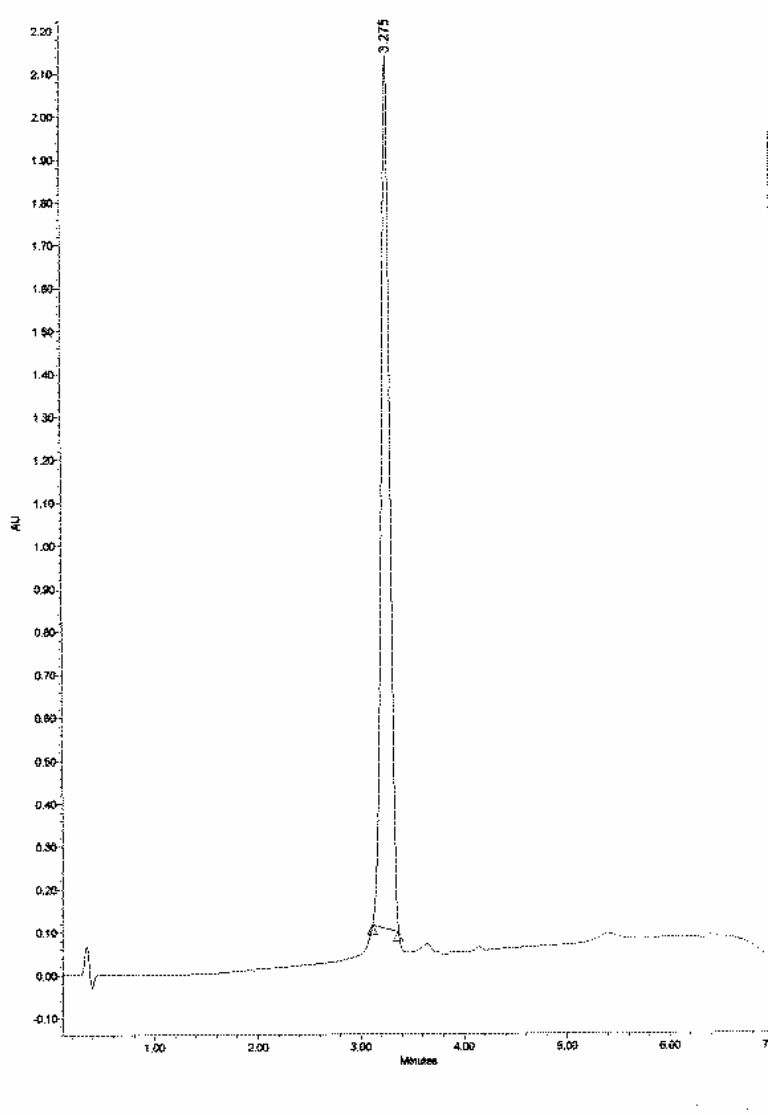
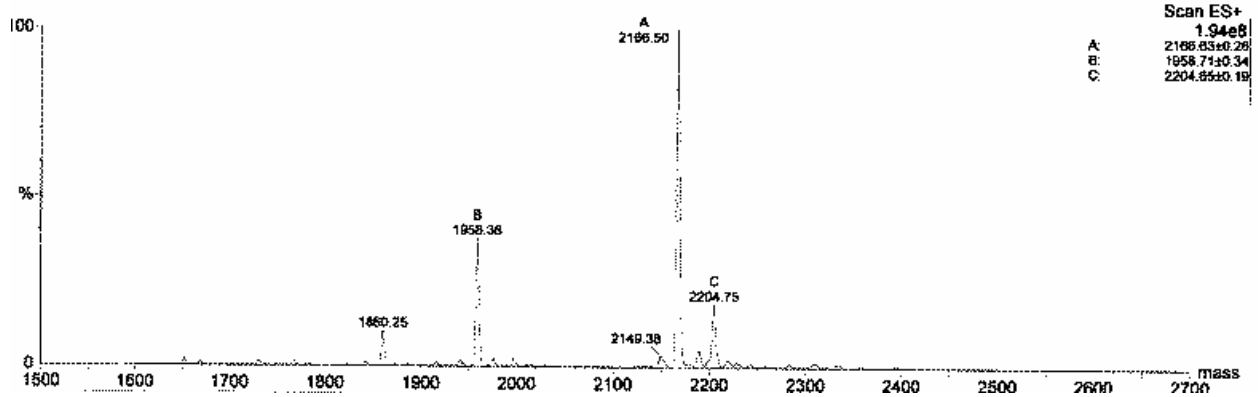
1.39e8
A
2122.13
A:
2122.34±0.17
100
%
0
1816.09
1930.88
2144.36
2168.13
1800
1850
1900
1950
2000
2050
2100
2150
2200
2250
2300
2350
2400
mass

Monomer DFH


3.275
AU
Minutes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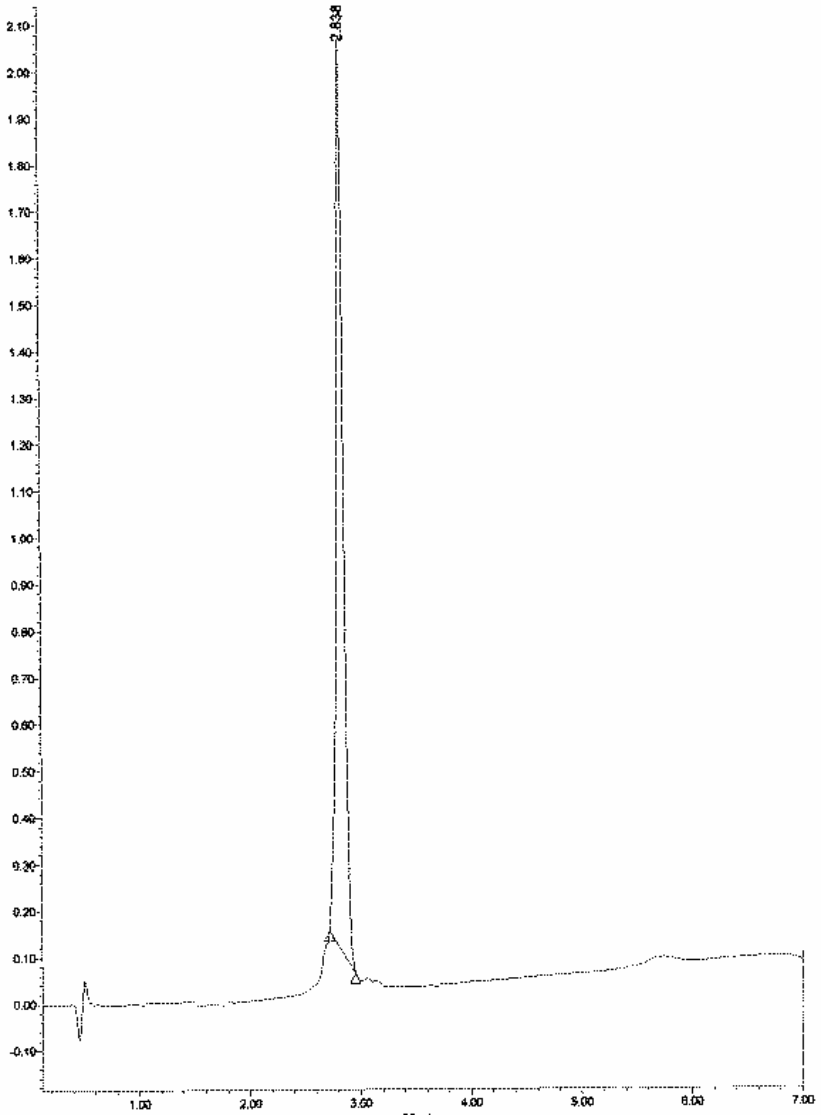
A: 2166.63±0.26
B: 1958.71±0.34
C: 2204.65±0.19
A
2166.50
B
1958.38
C
2204.75
1660.25
2149.38
%
mass

Monomer HWS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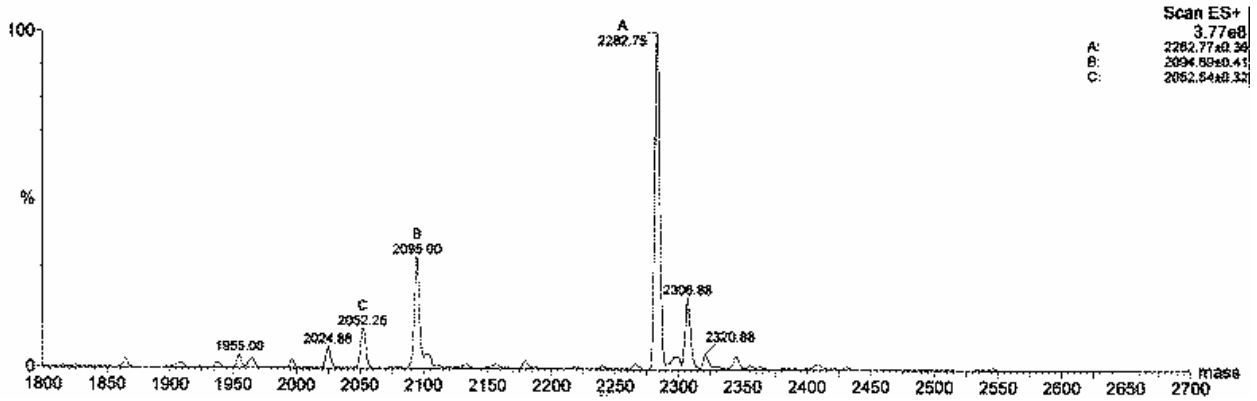
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2095.00
C
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2320.88
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%
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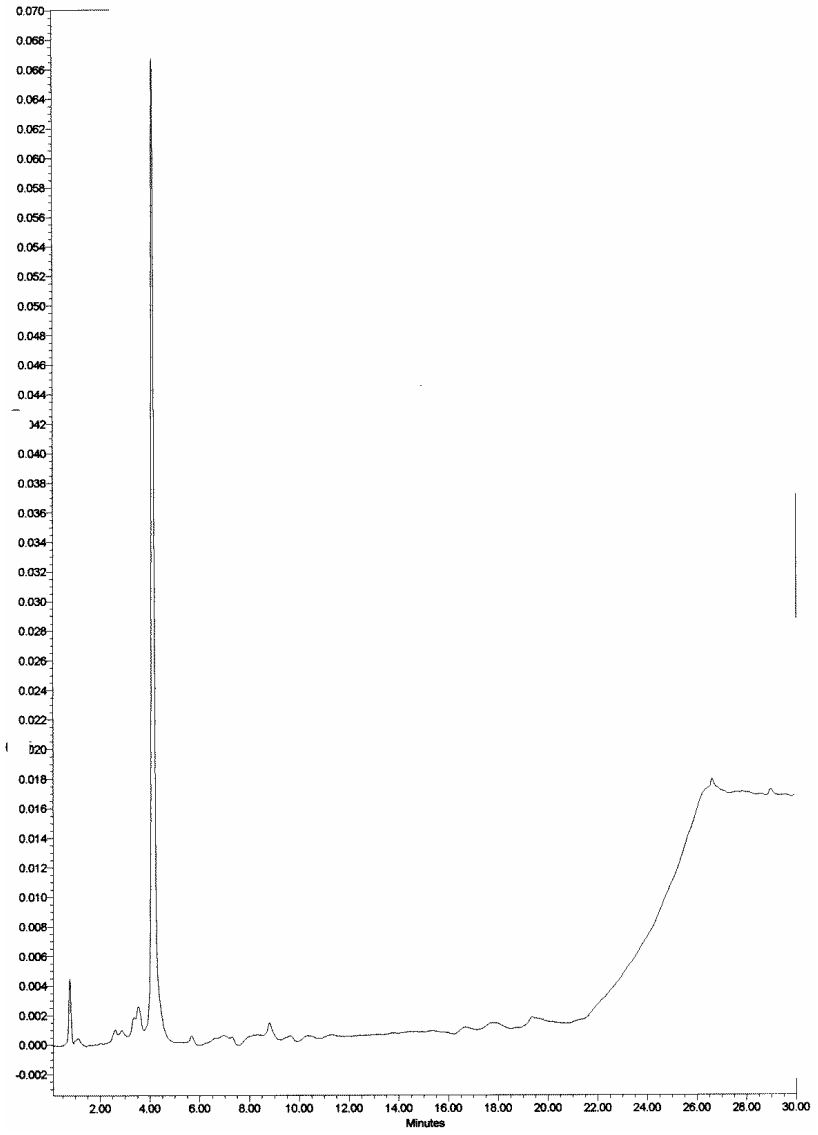
mass

Monomer HHH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4.00
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8.00
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24.00
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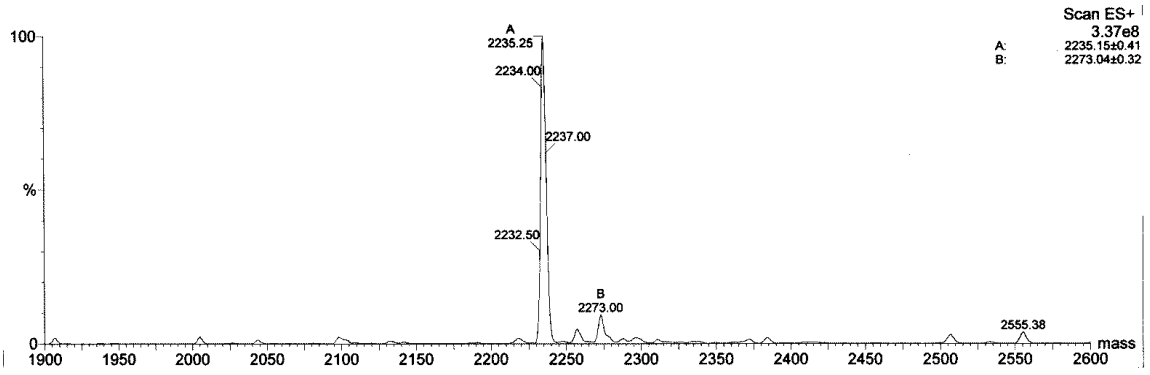
28.00
30.00
Minutes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%
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2232.50
B
2273.00
2555.38
mass
1900
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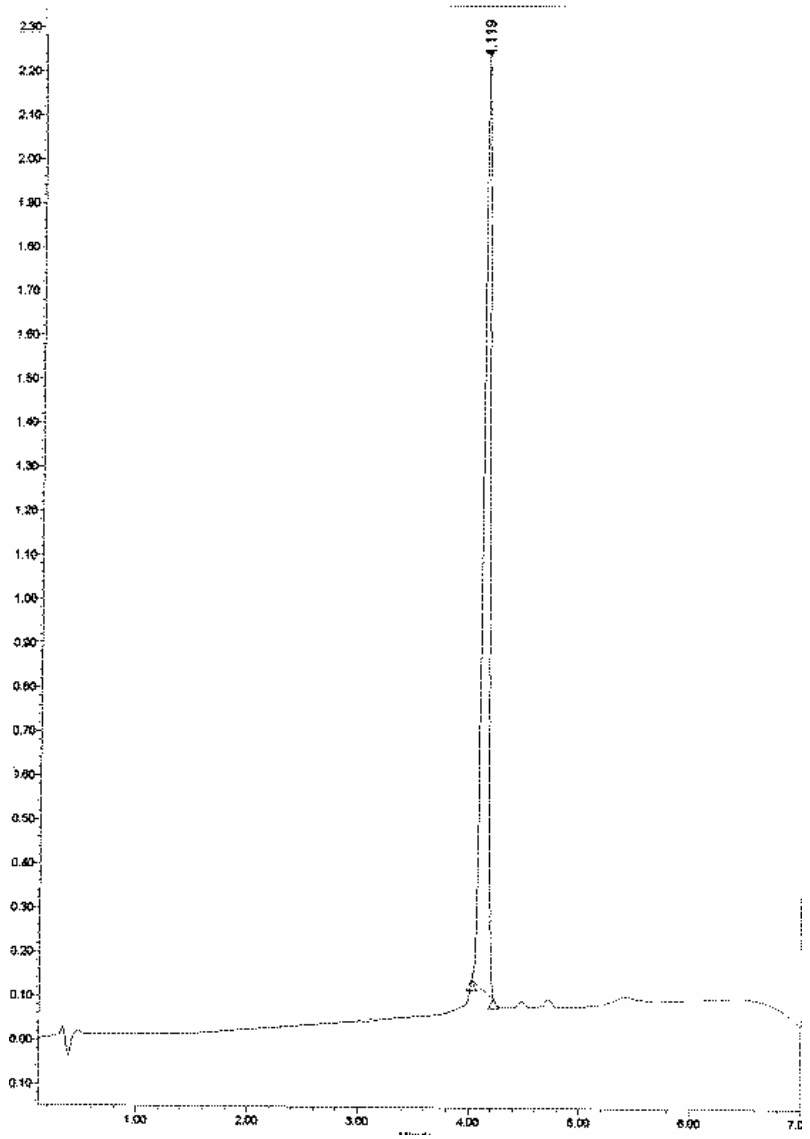
MonomerLRH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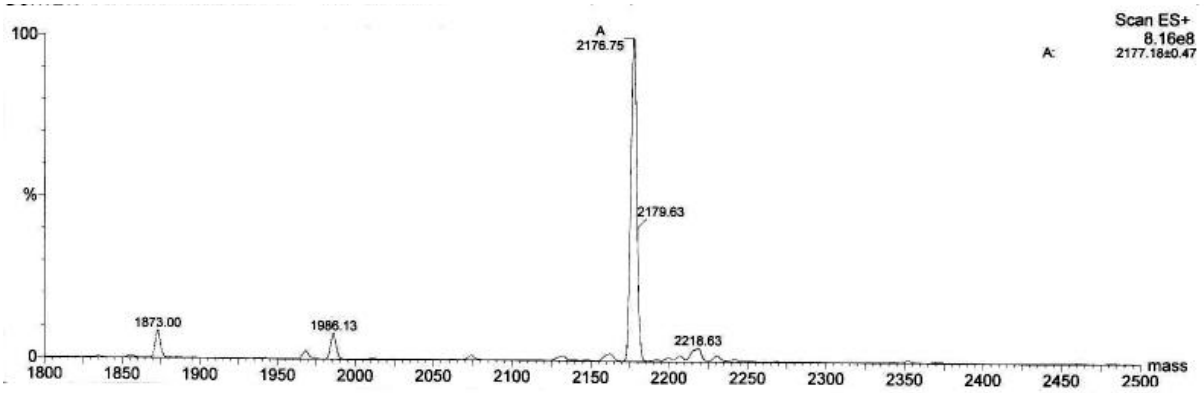
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A
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100
%
0
1800
1850
1900
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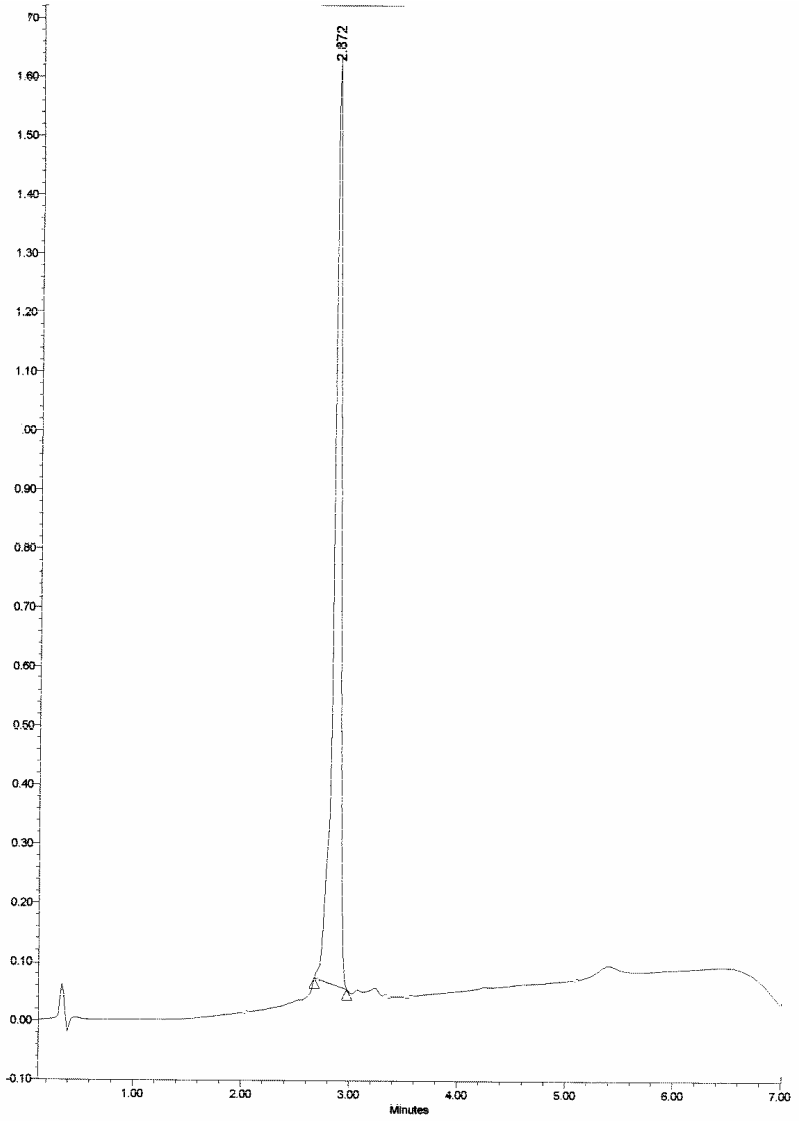
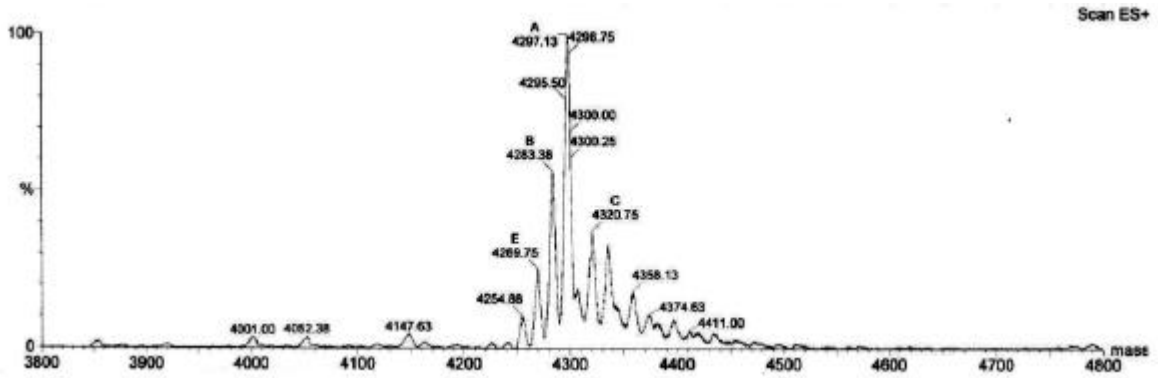
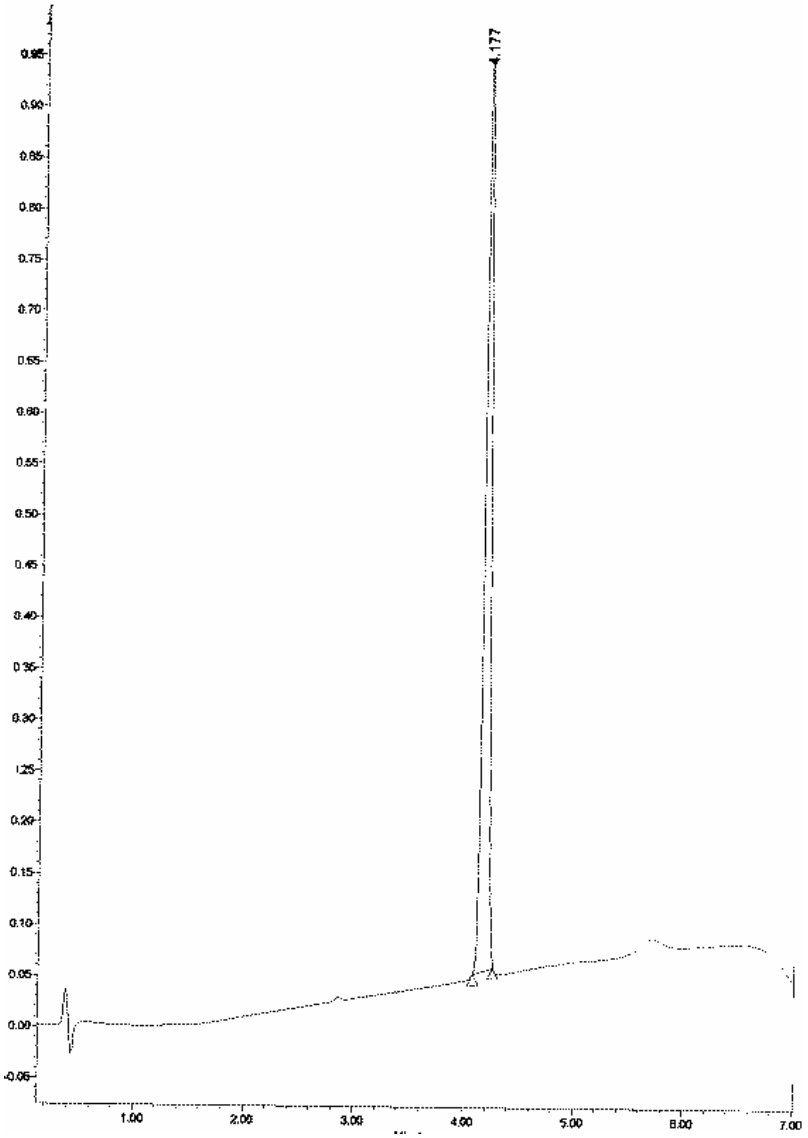
mass

Dendrimer LRH-DHL





Dendrimer LRH-HSD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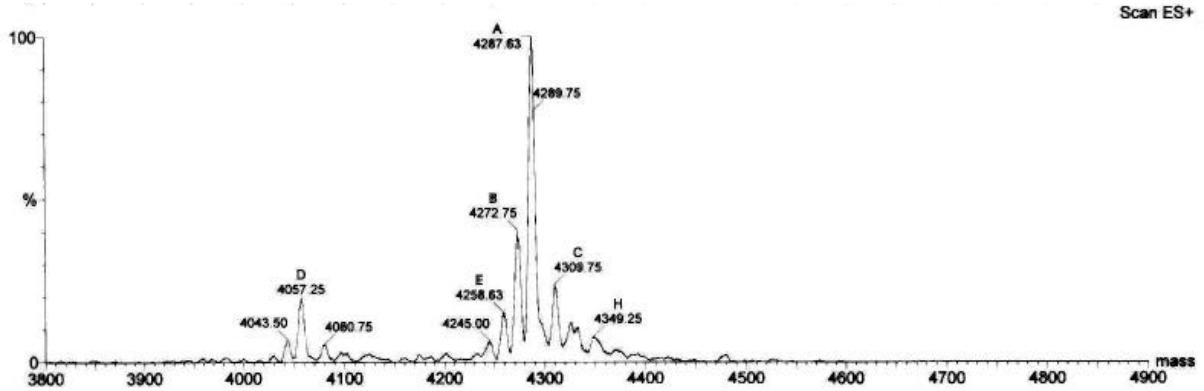
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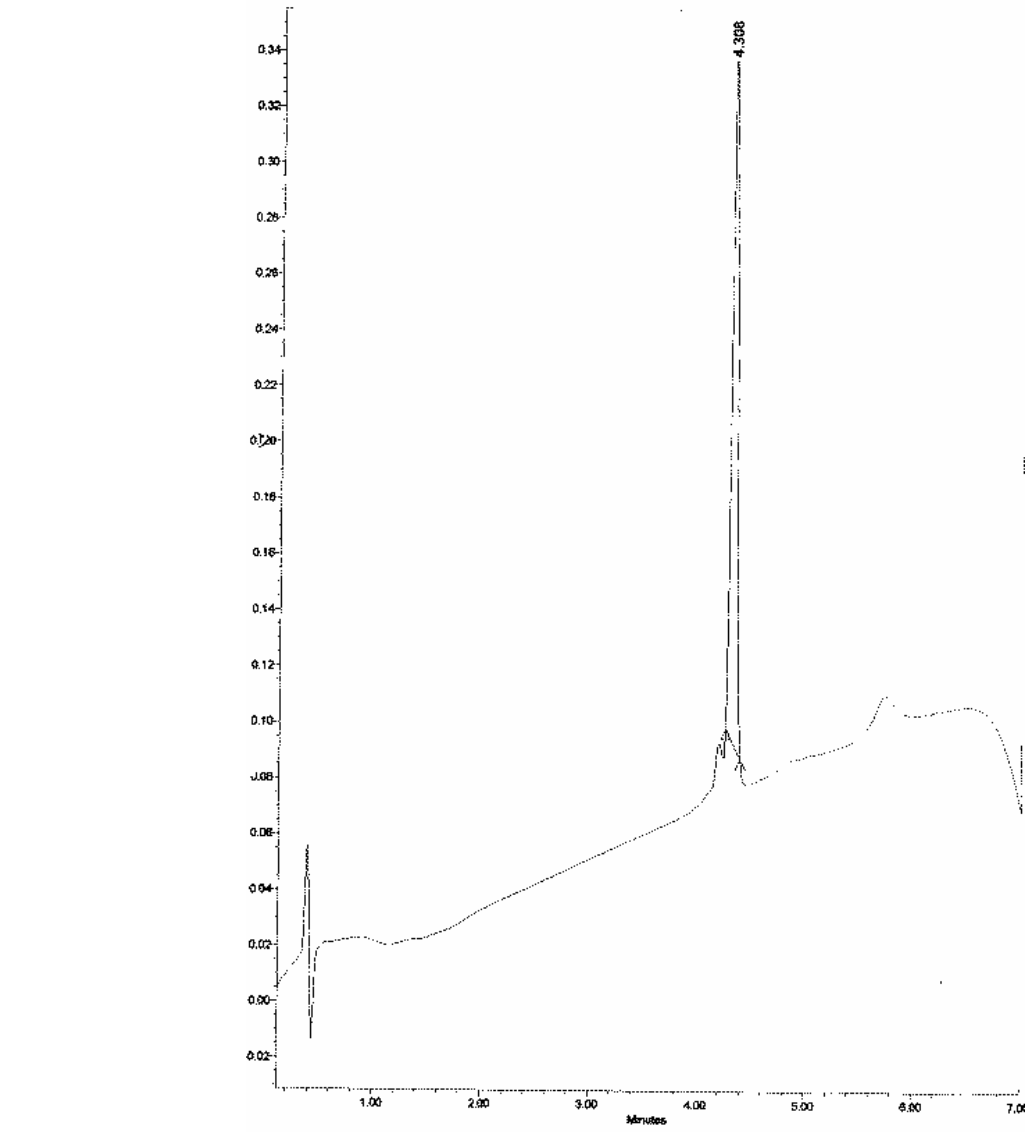
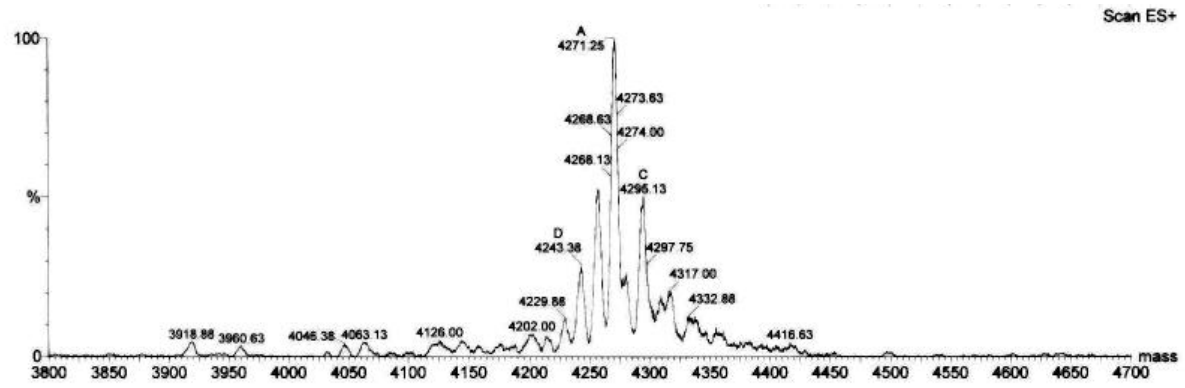
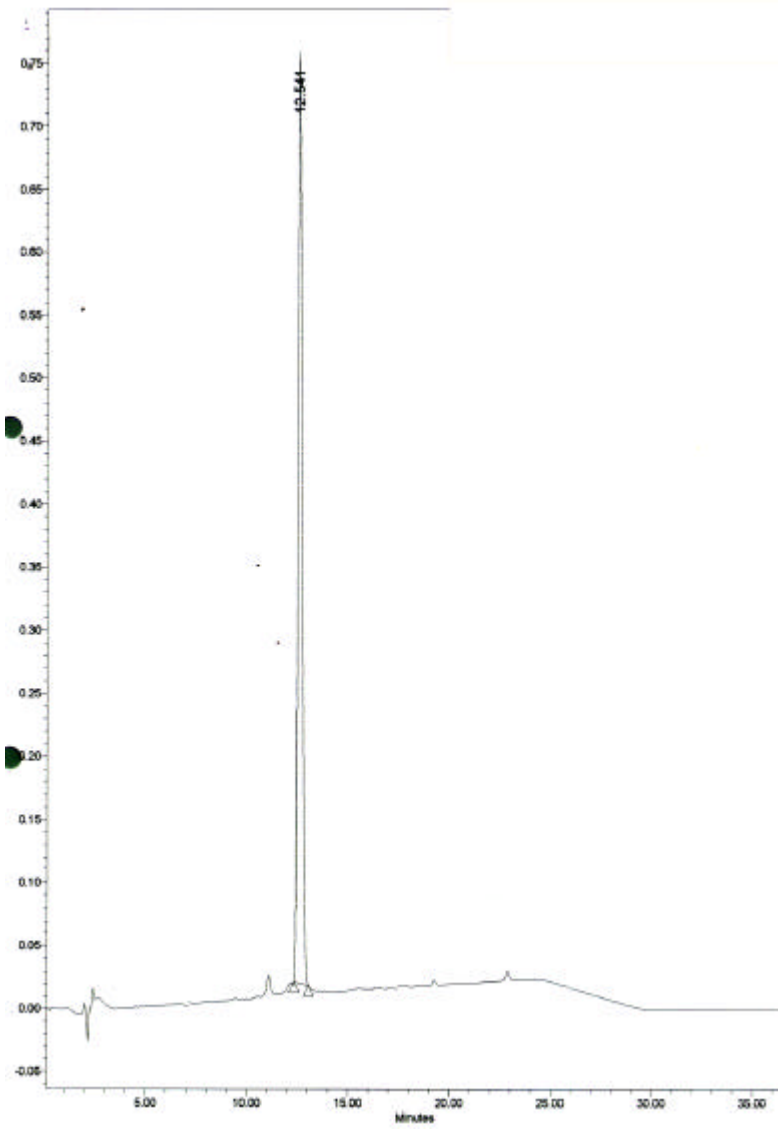
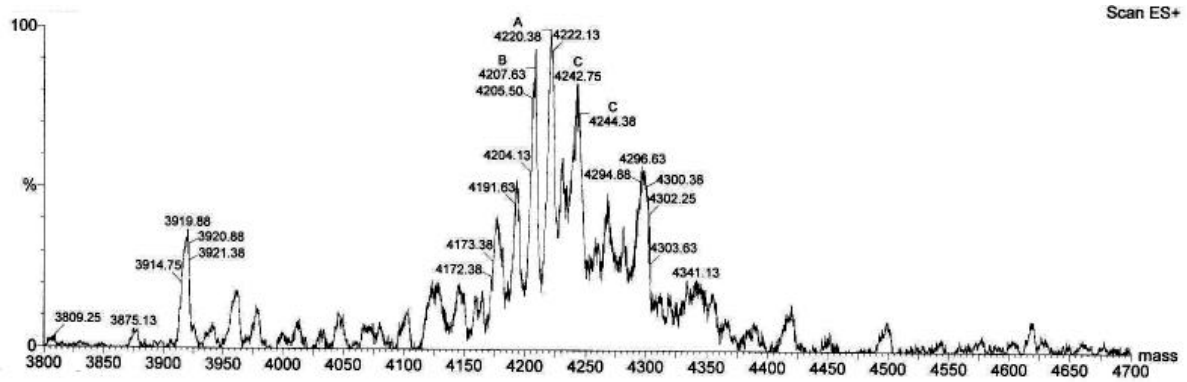
Dendrimer LRH-DHS



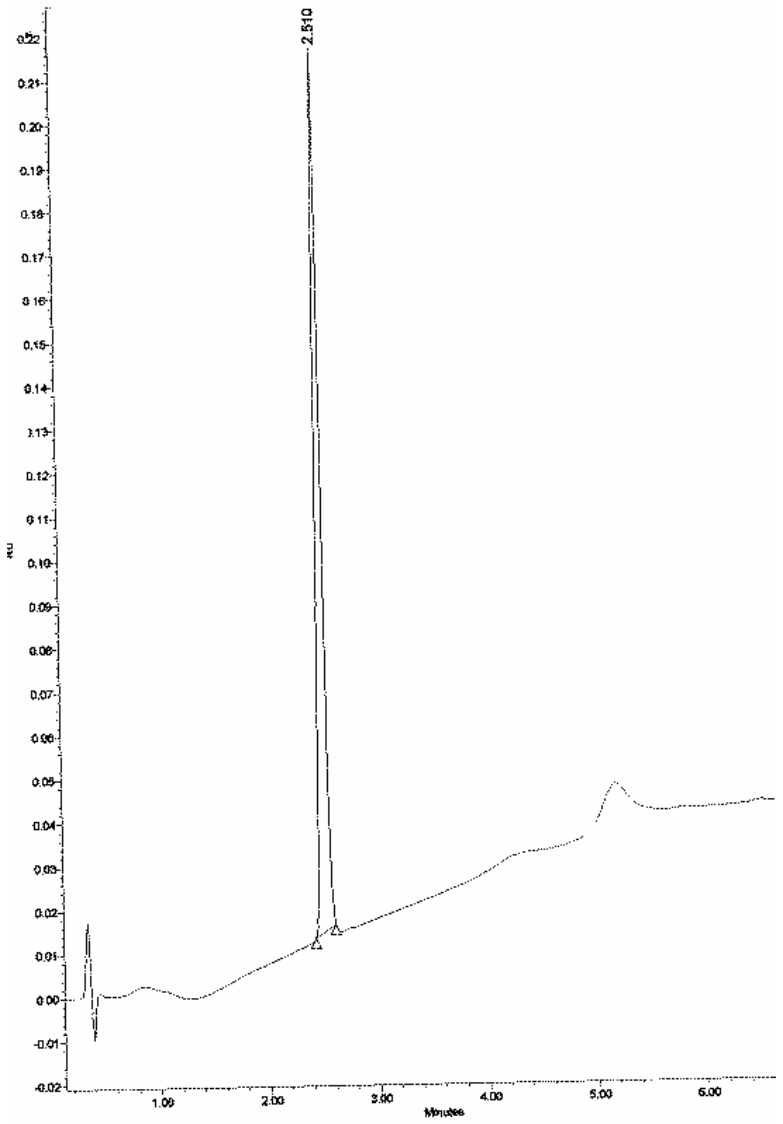


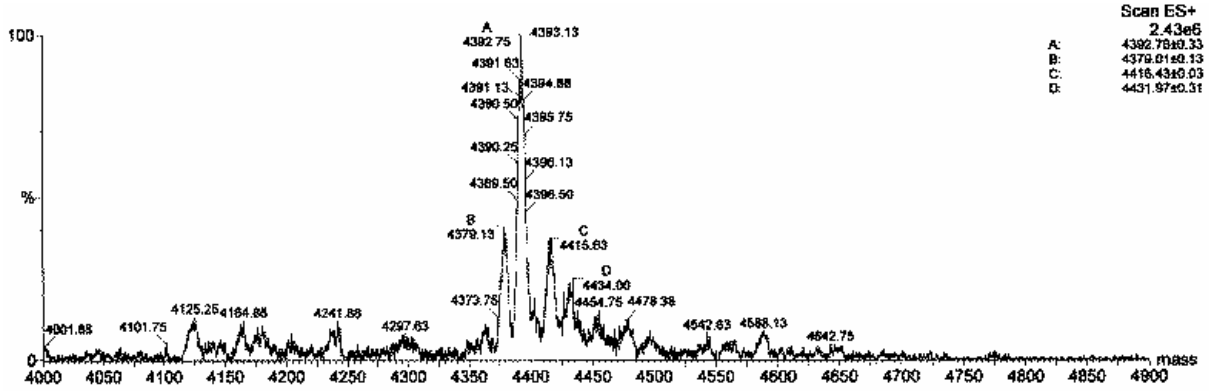
Dendrimer LRH-DSH





Dendrimer HWS-HSD





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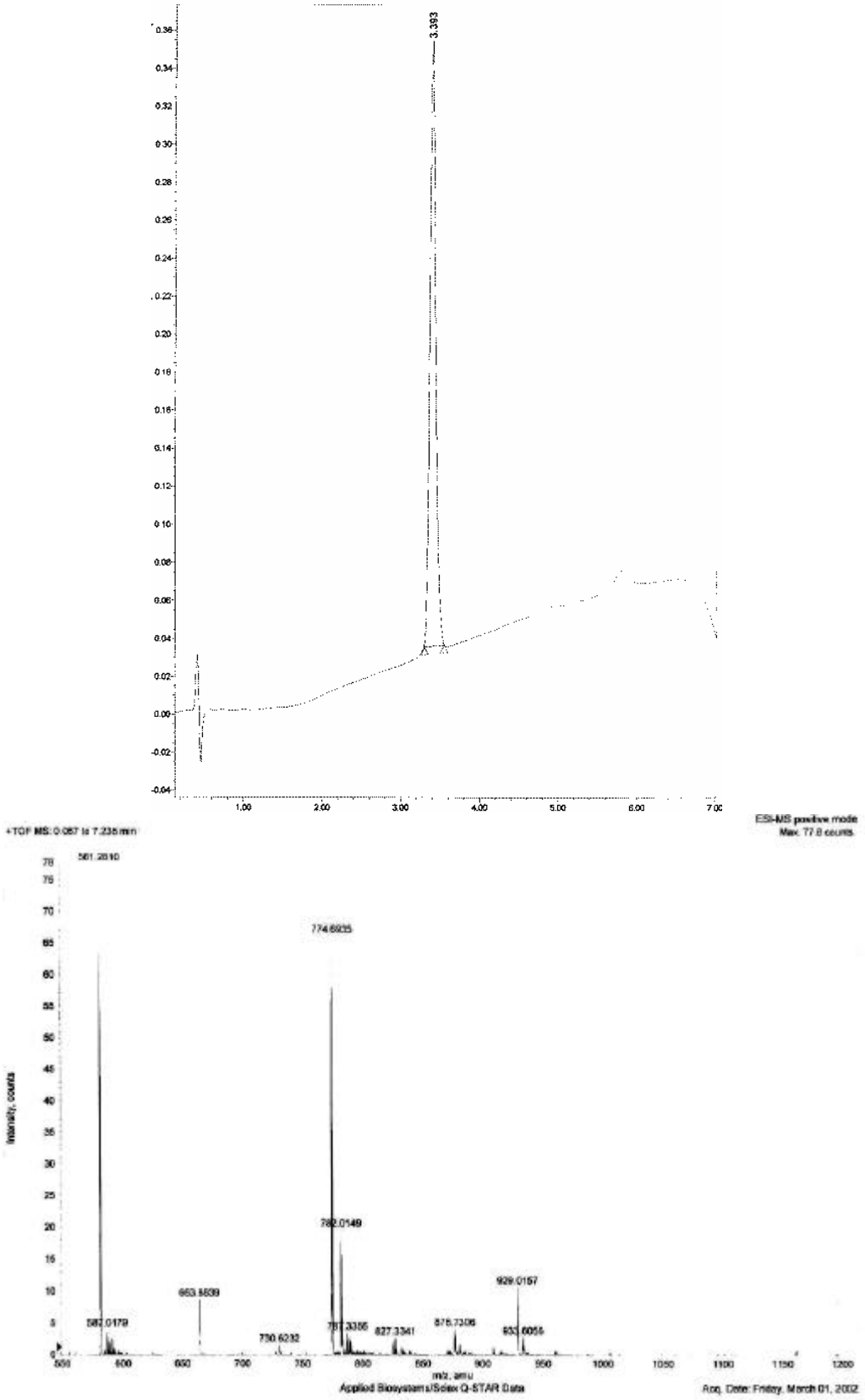

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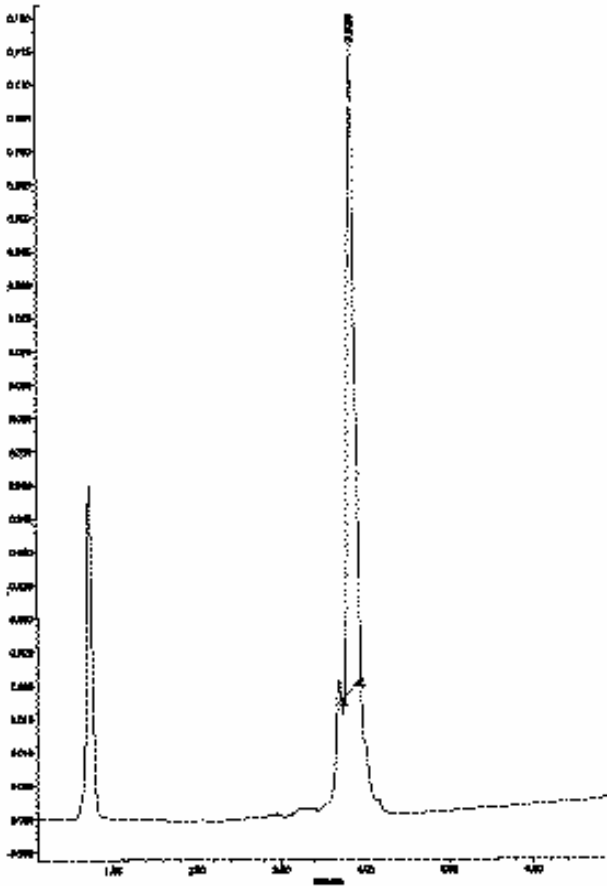

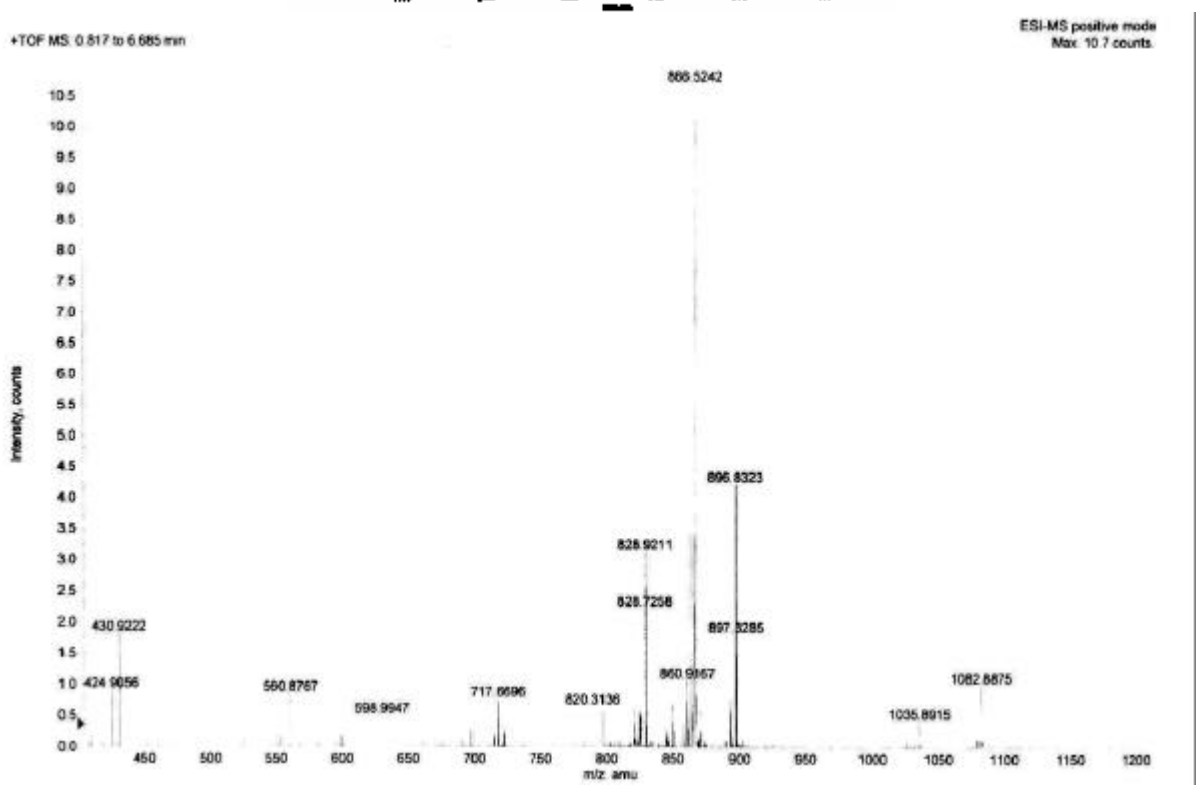

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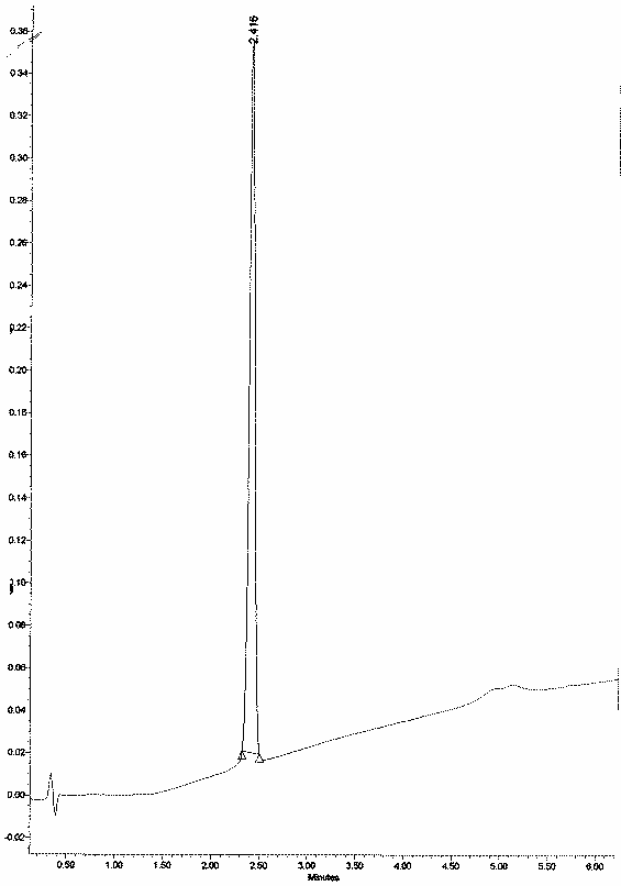

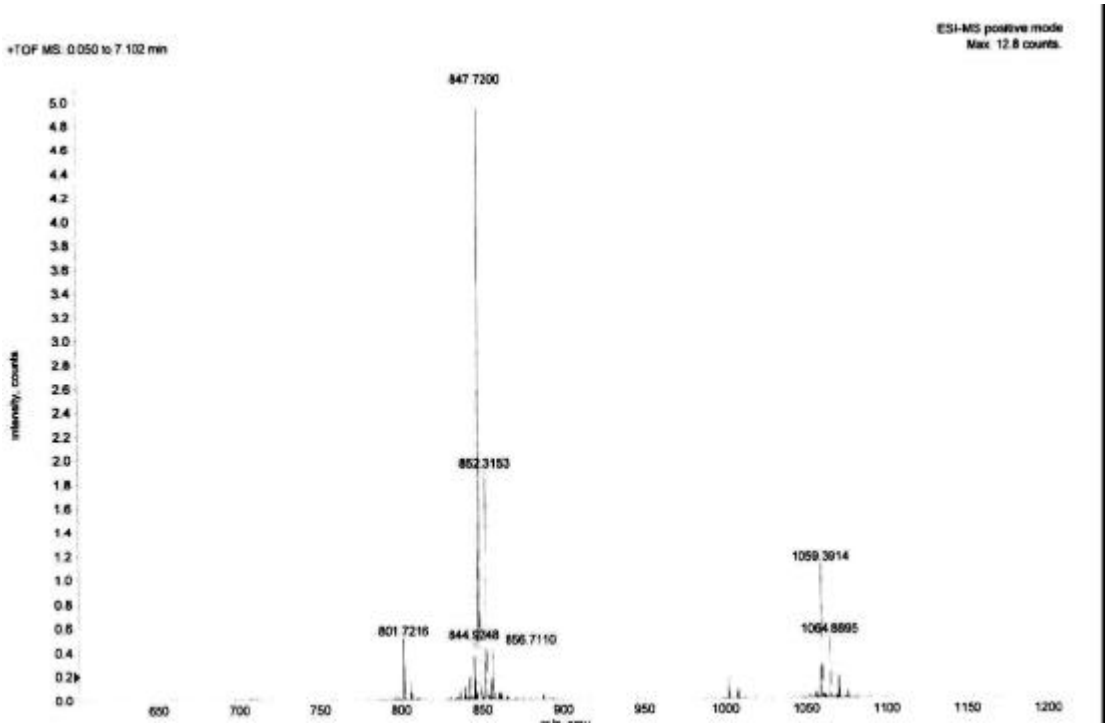

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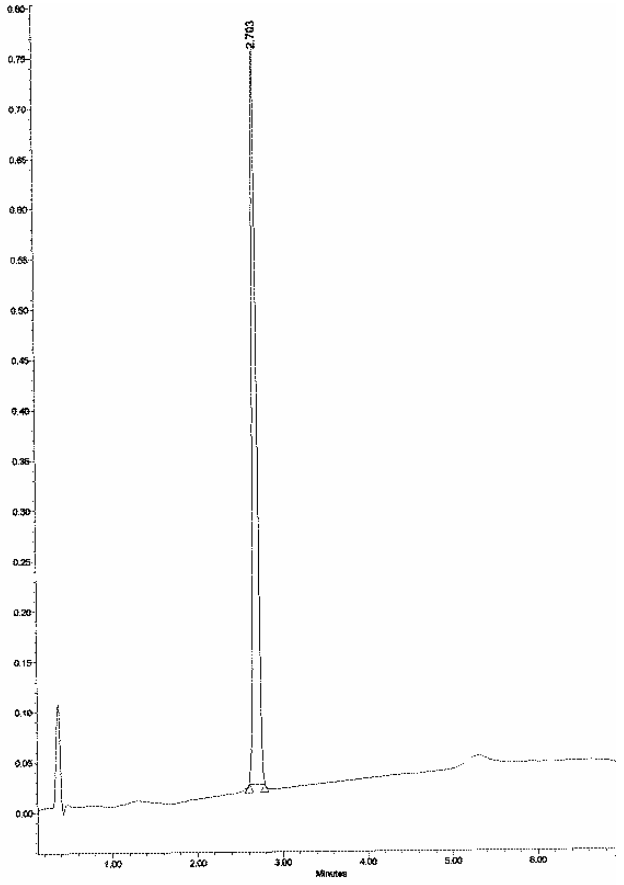

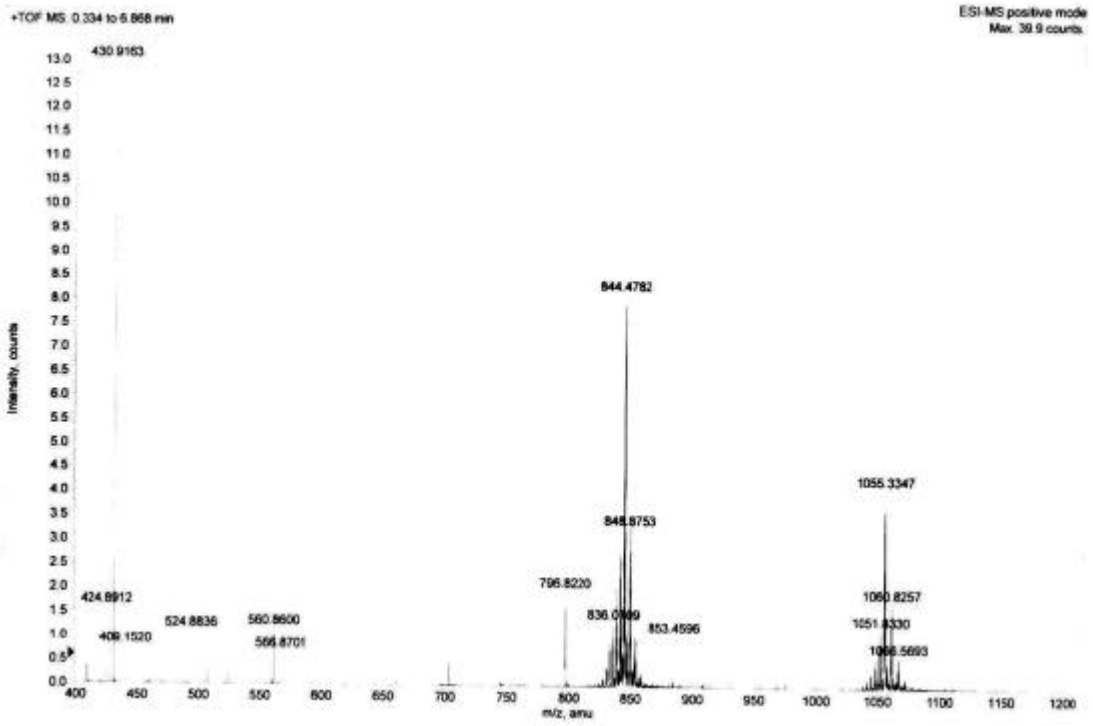

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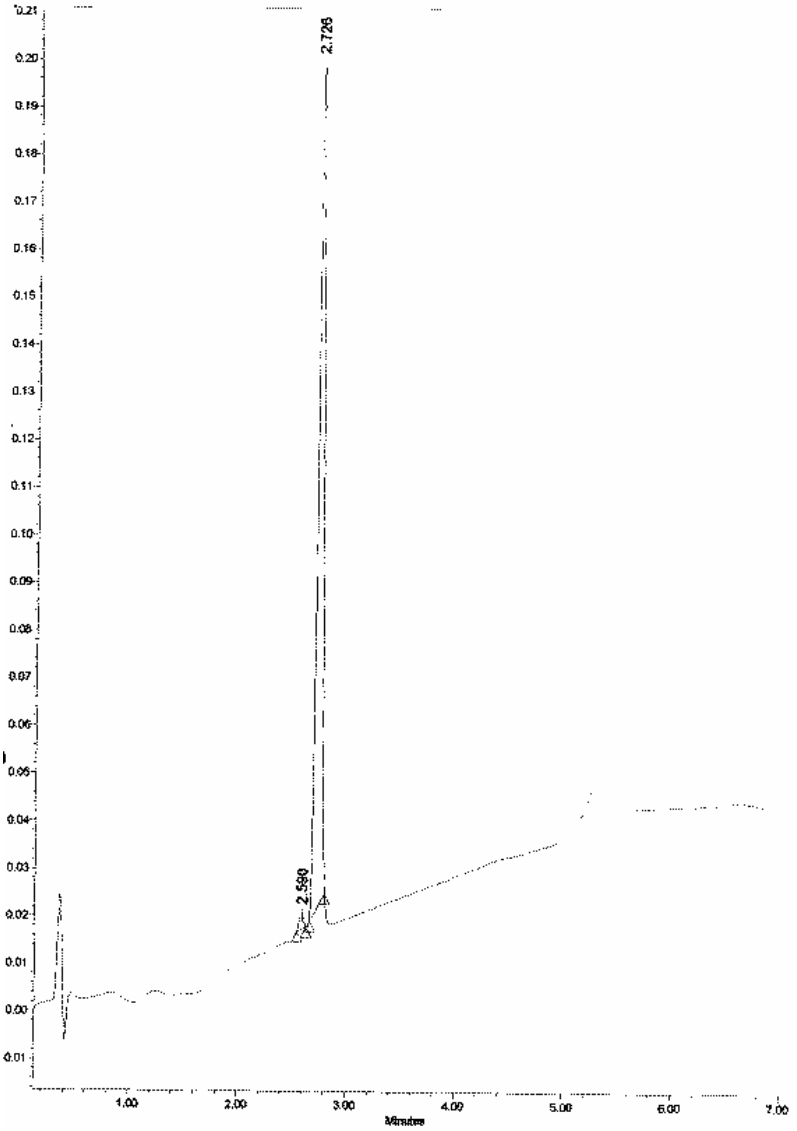

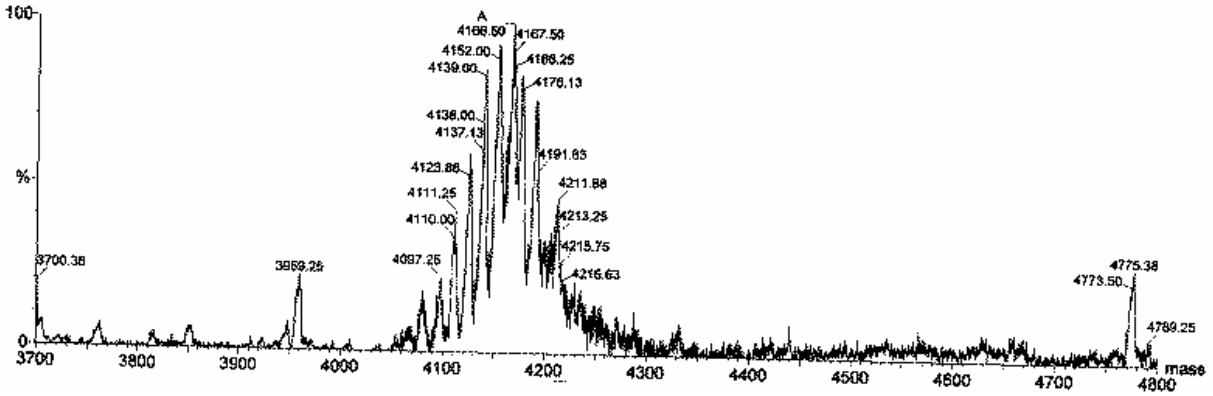

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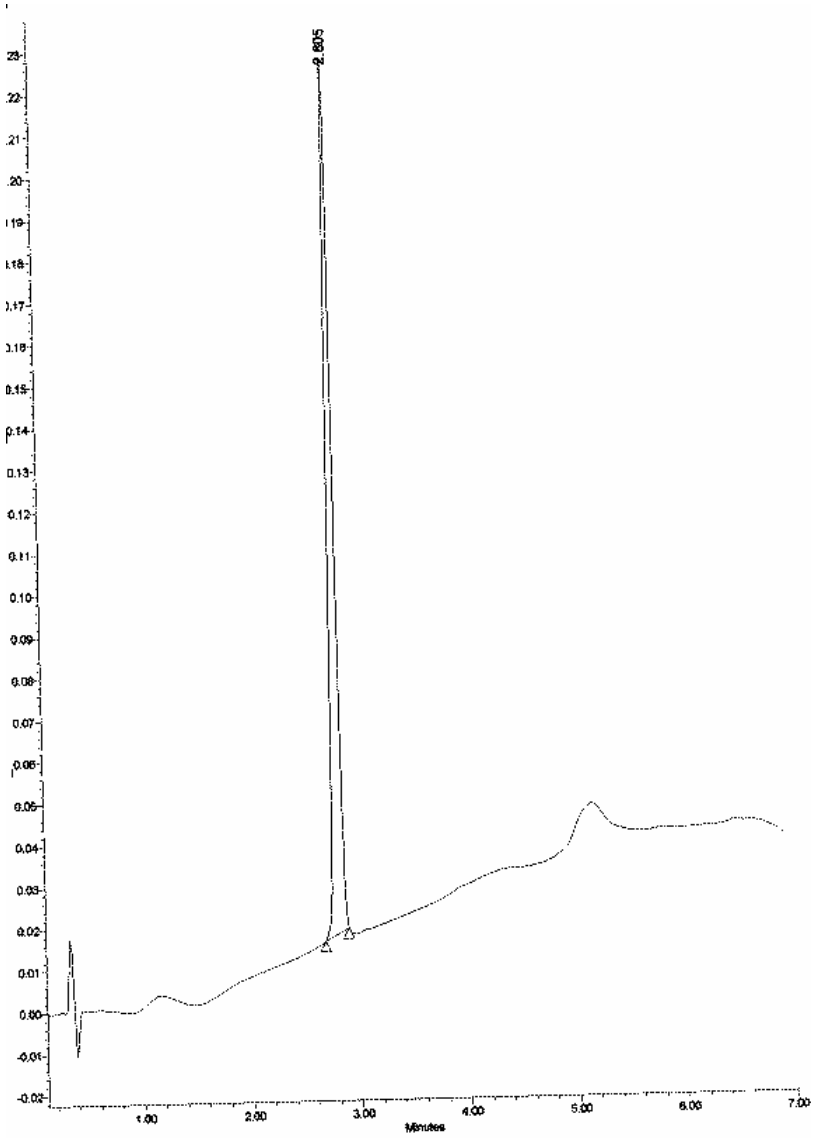

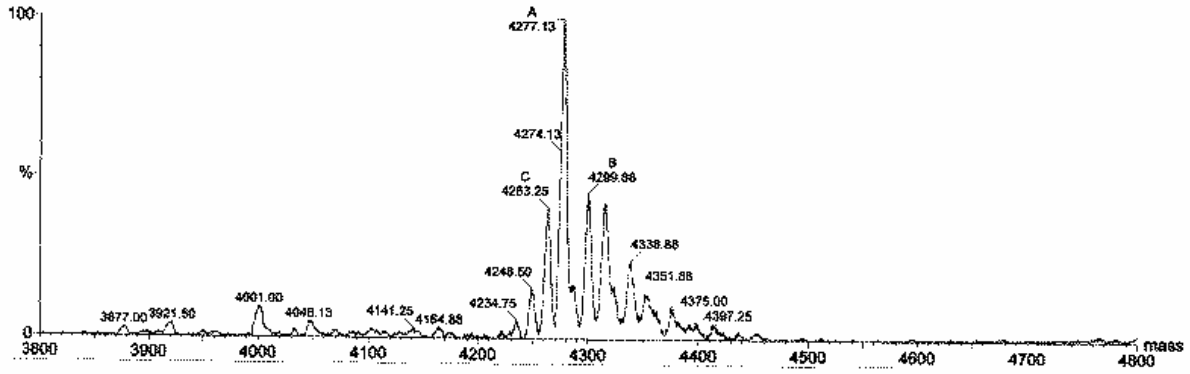

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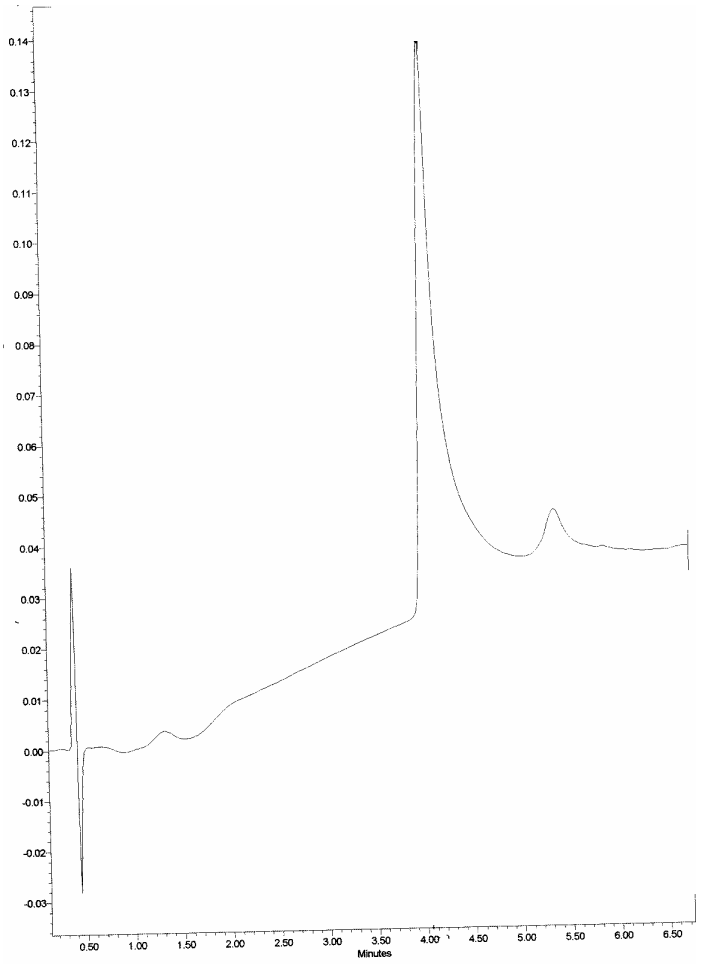

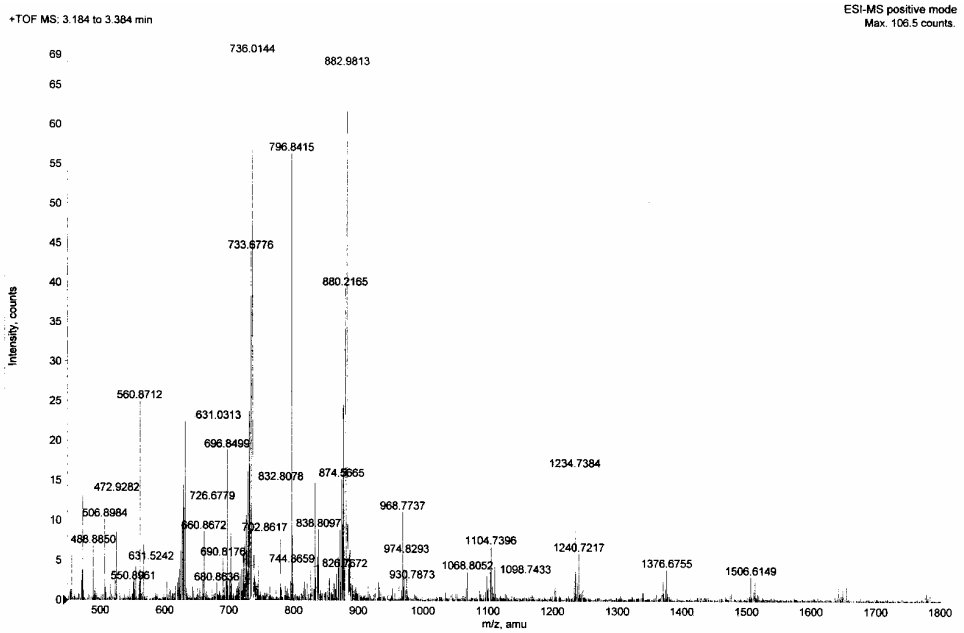

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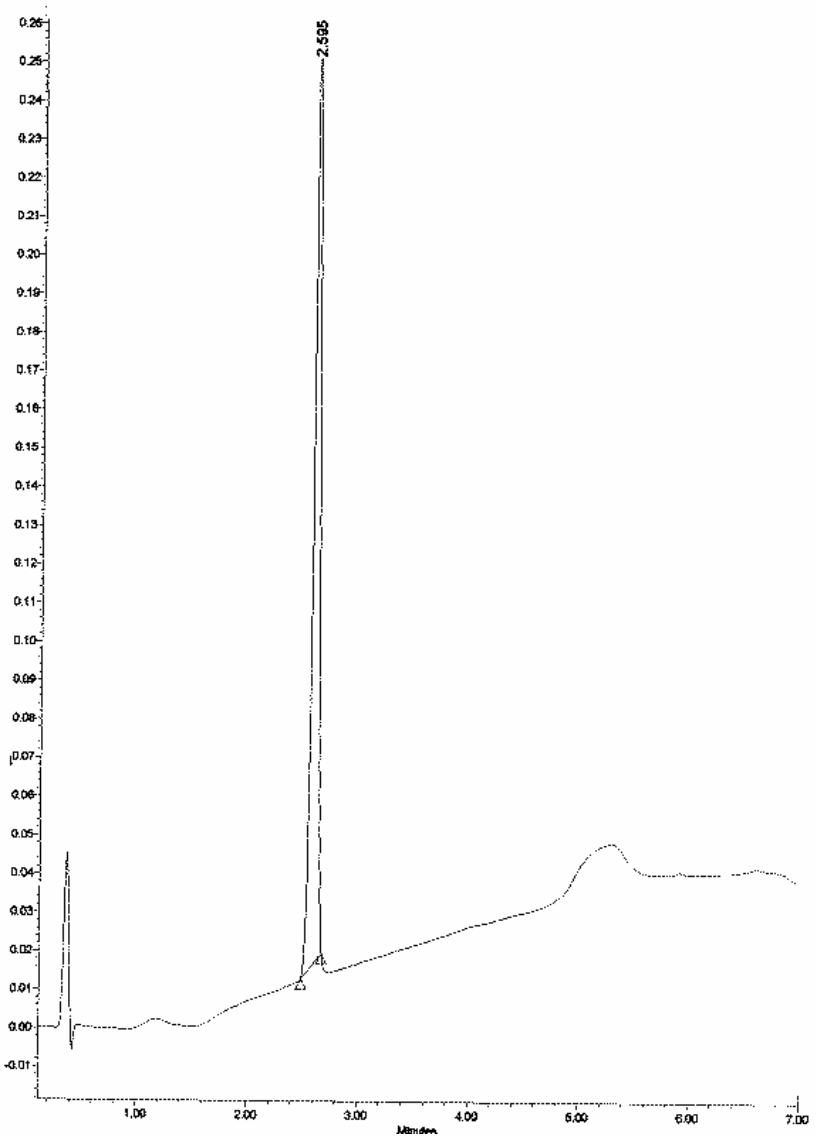

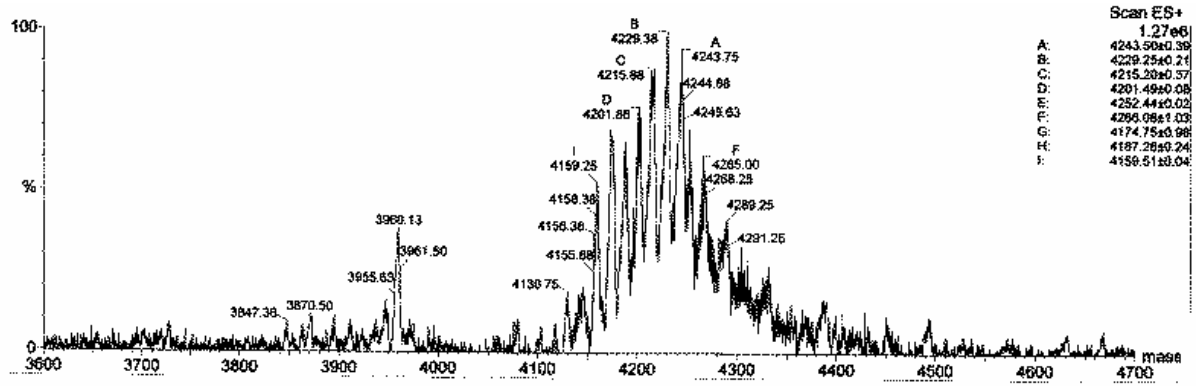

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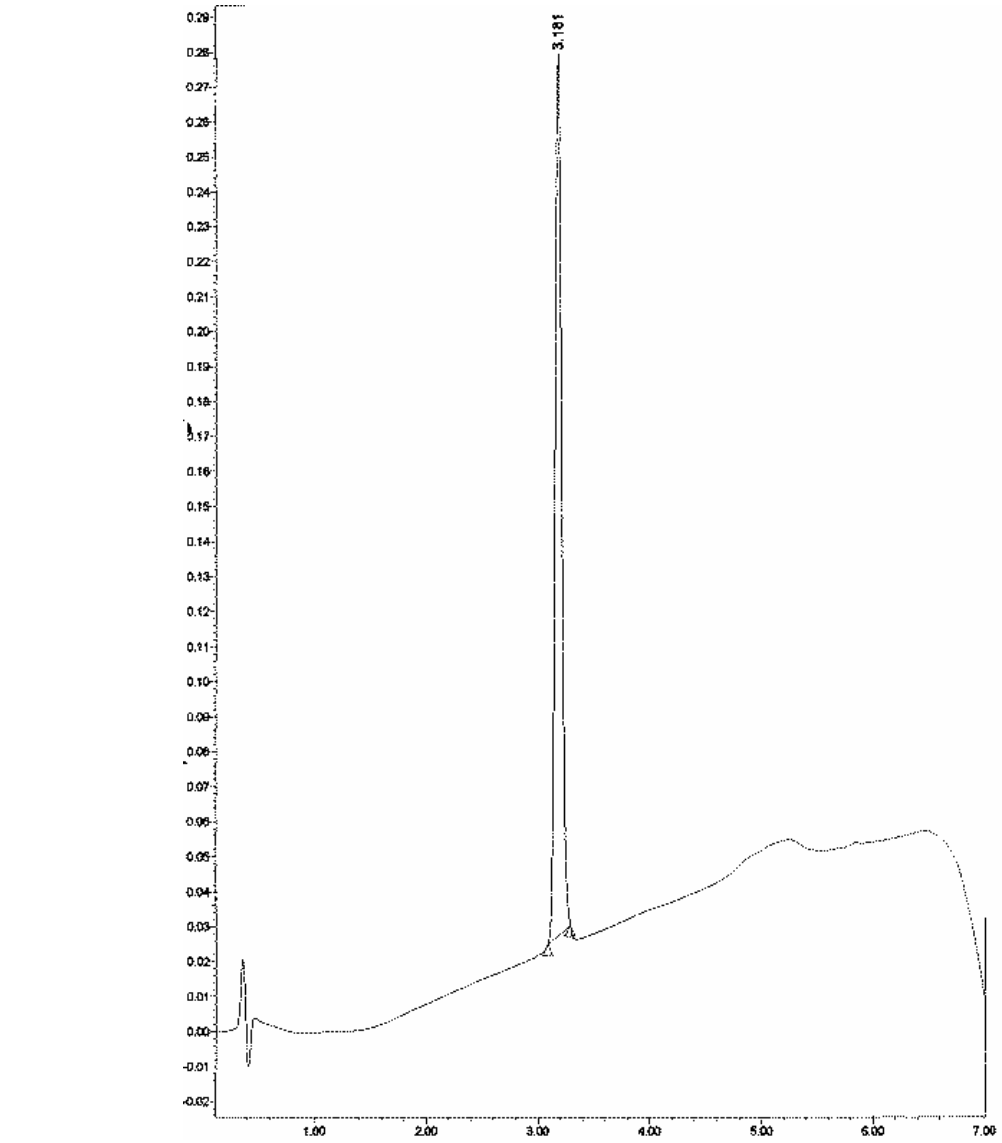

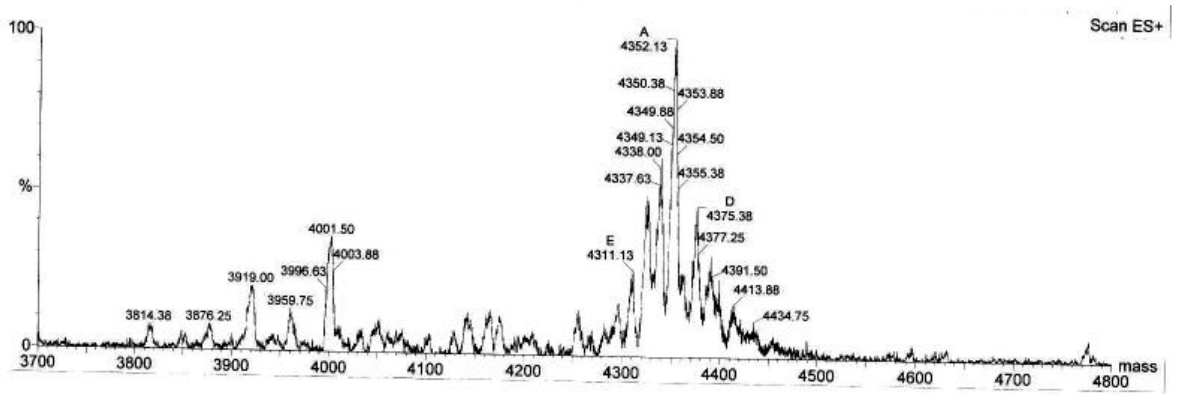

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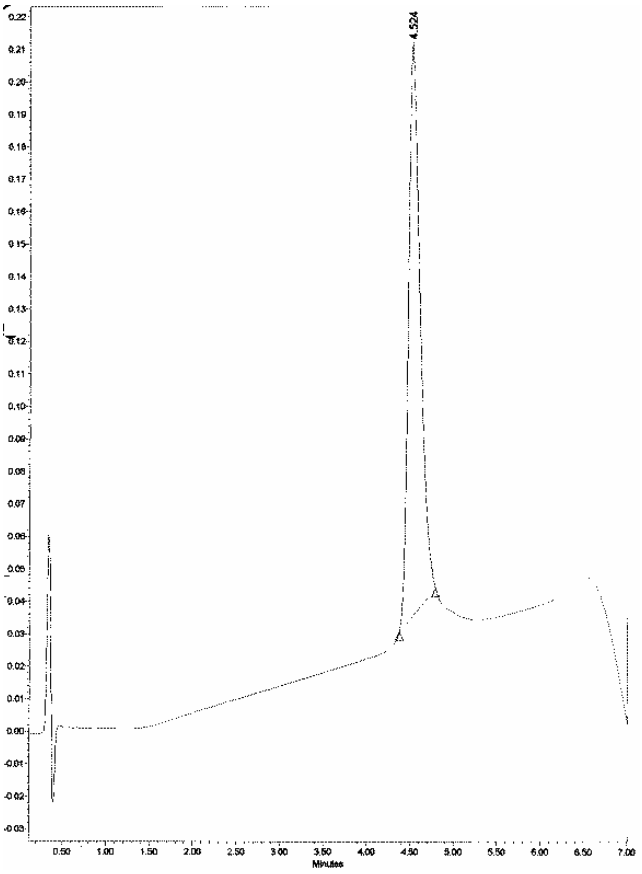

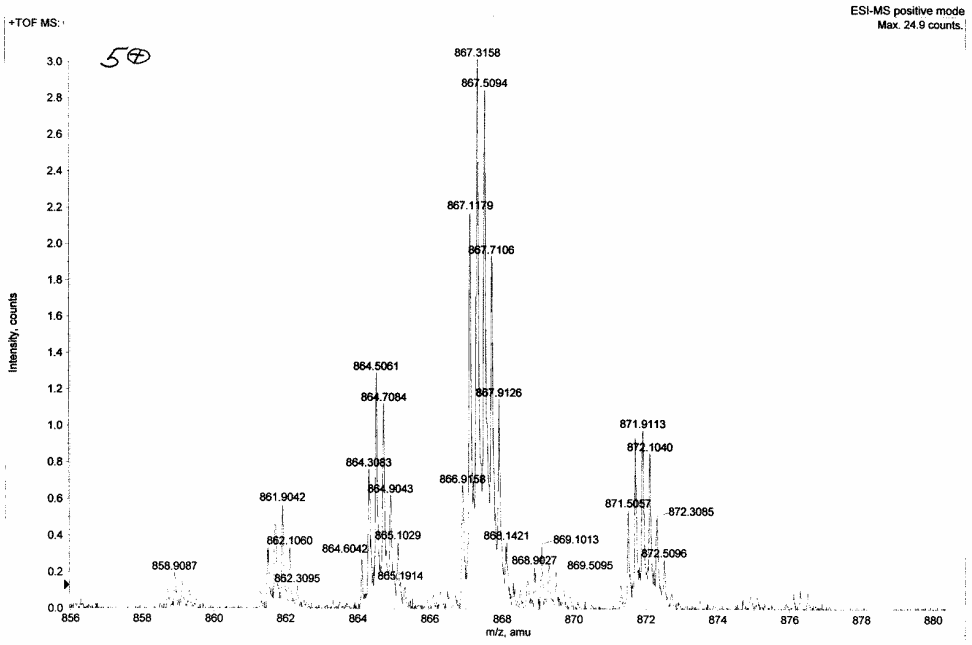

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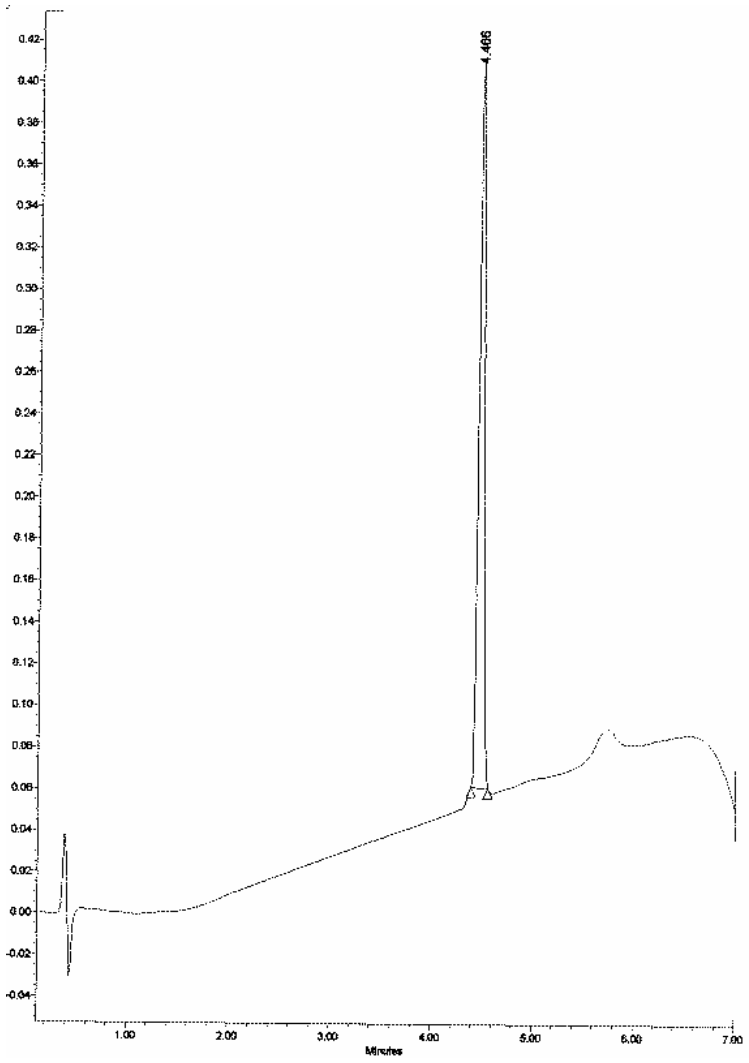

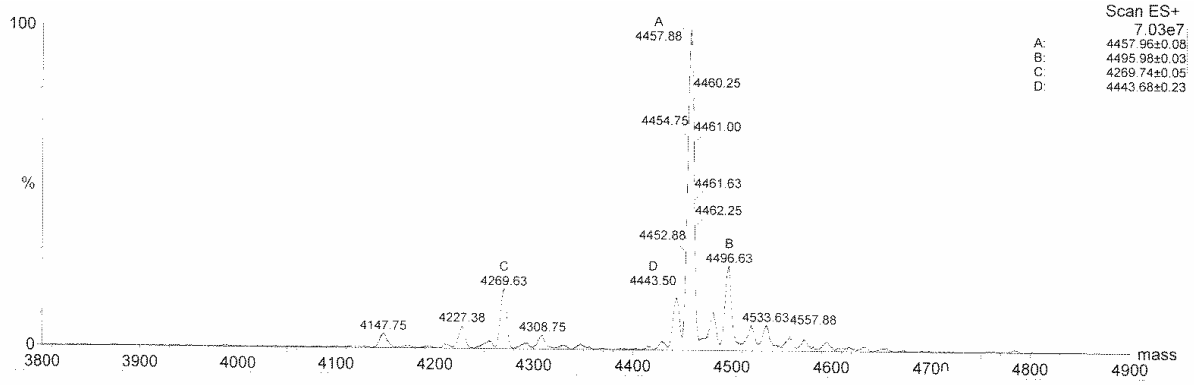

Dendrimer LRH-DFH