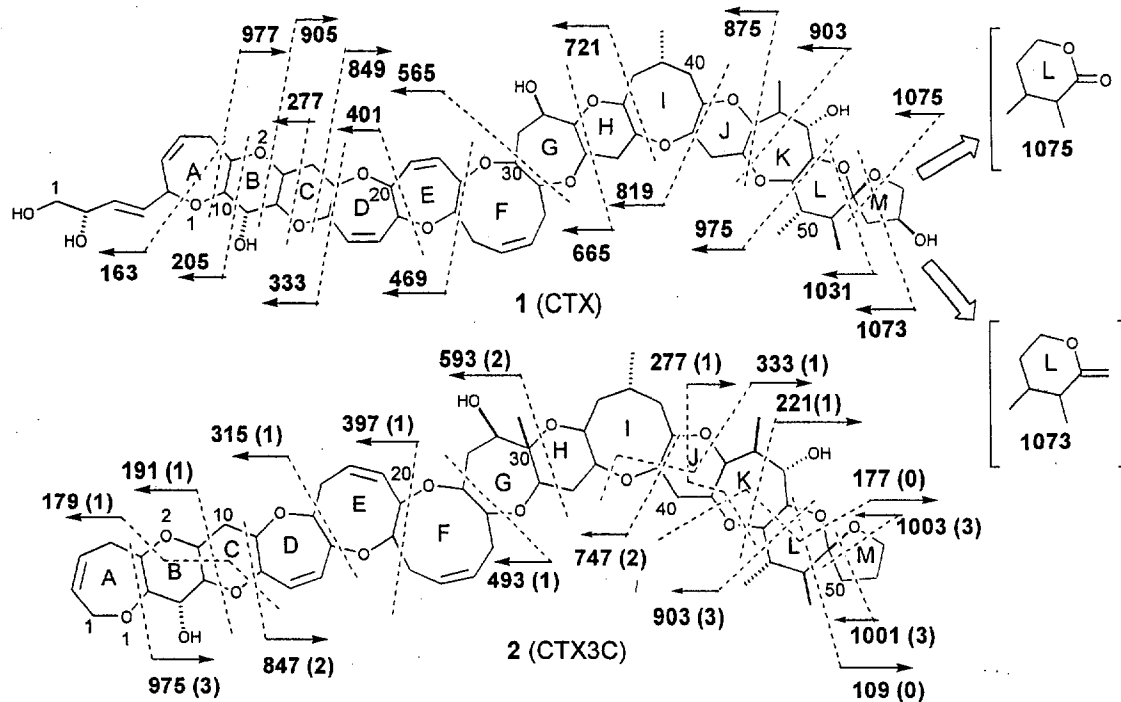


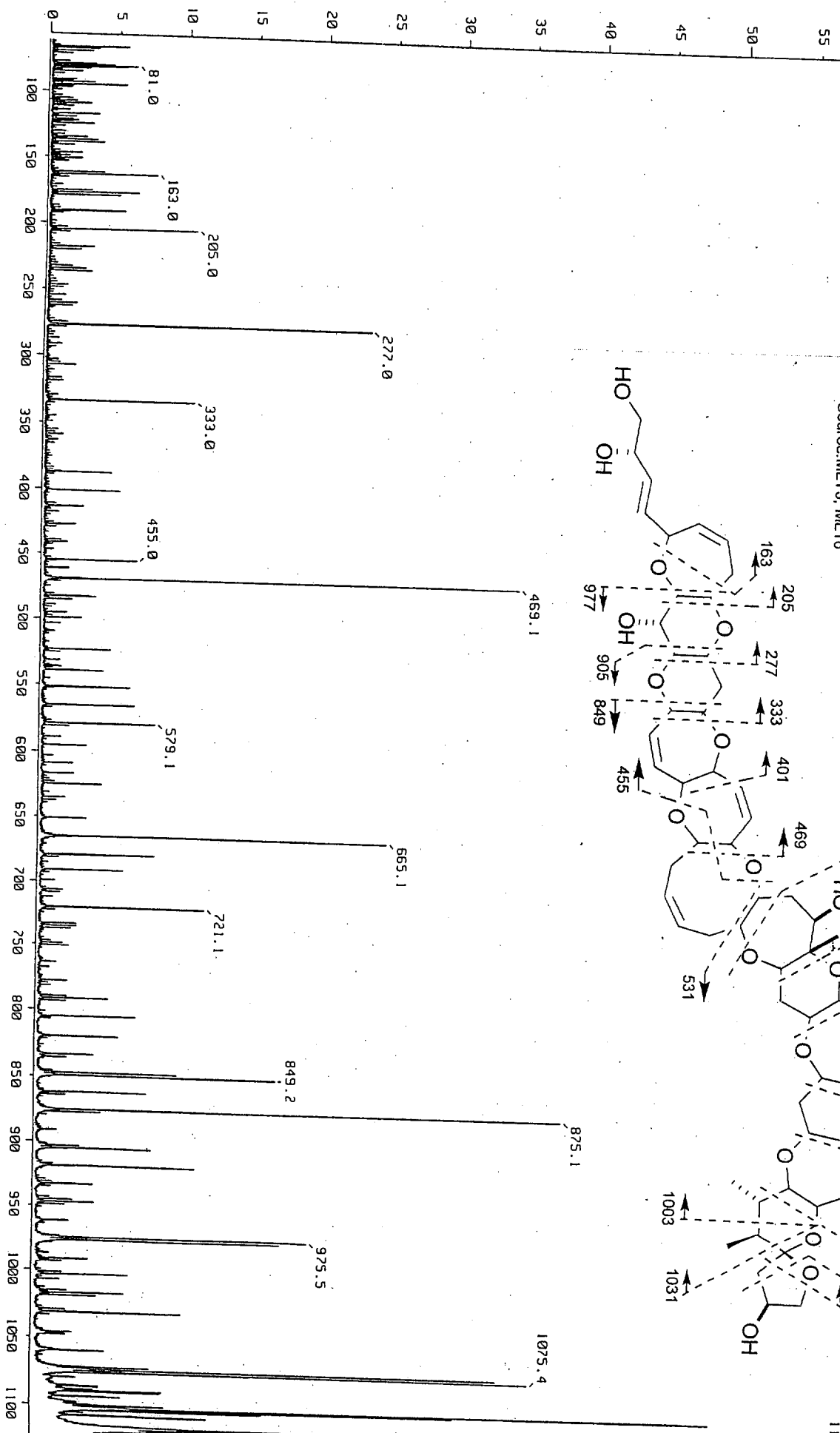
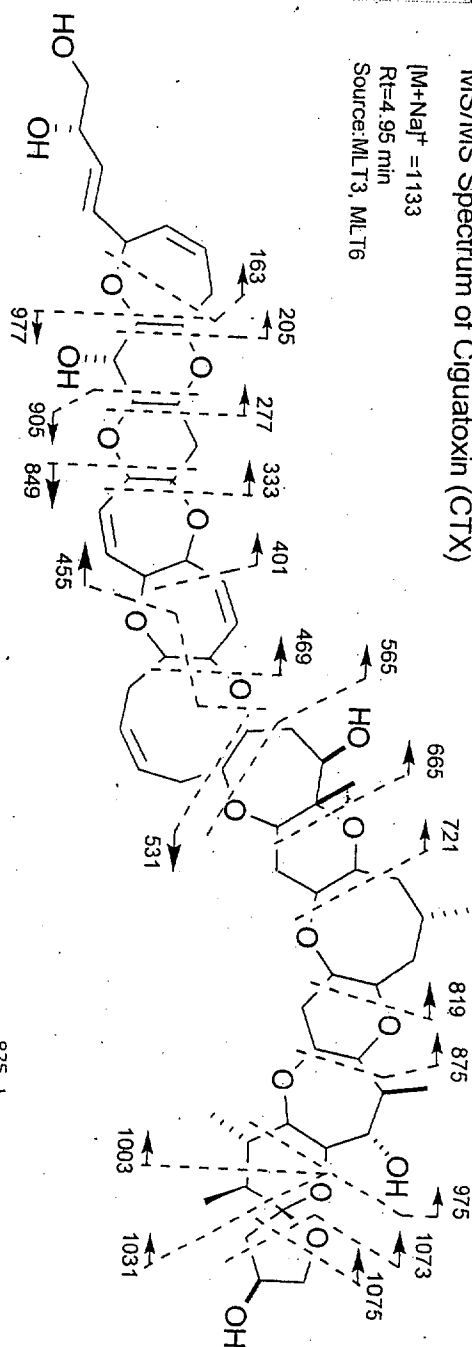


Structures and characteristic fragments of CTX (1) and CTX3C (2). Numbers in parentheses on the fragments of 2 denote the increase in mu after replacing hydroxyl protons with deuterium. The mass units indicated are those of Na-adduct ions. For clarity not all fragments are shown.

[Mass Spectrum]
 Date :
 Sample : CTX-1B
 Note : Array Detector Data
 Inlet : Direct
 Spectrum Type : Product (m/z 1133.50, 3rd FF)
 RI : 0.00 min Scan# : 1
 BP : m/z 1133.2761 Int. : 28.82
 Output m/z range : 52.0425 to 1143.0225
 170196

MS/MS Spectrum of Ciguatoxin (CTX)

[M+Na]⁺ = 1133
 Rt=4.95 min
 Source:MLT3, MLT6



[Mass Spectrum]
 Date : post3e
 Sample : CTX-3C
 Note : Array Detector Data
 Inlet : Direct
 Spectrum Type : Product (m/z 1045.50, 3rd FFR, FC: 8.00kV)
 RT : 0.00 min
 BP : m/z 1044.1864 Int. : 30.10
 Output m/z range : 36.8150 to 1048.1161
 267491

Date : 06-Aug-98 11:11

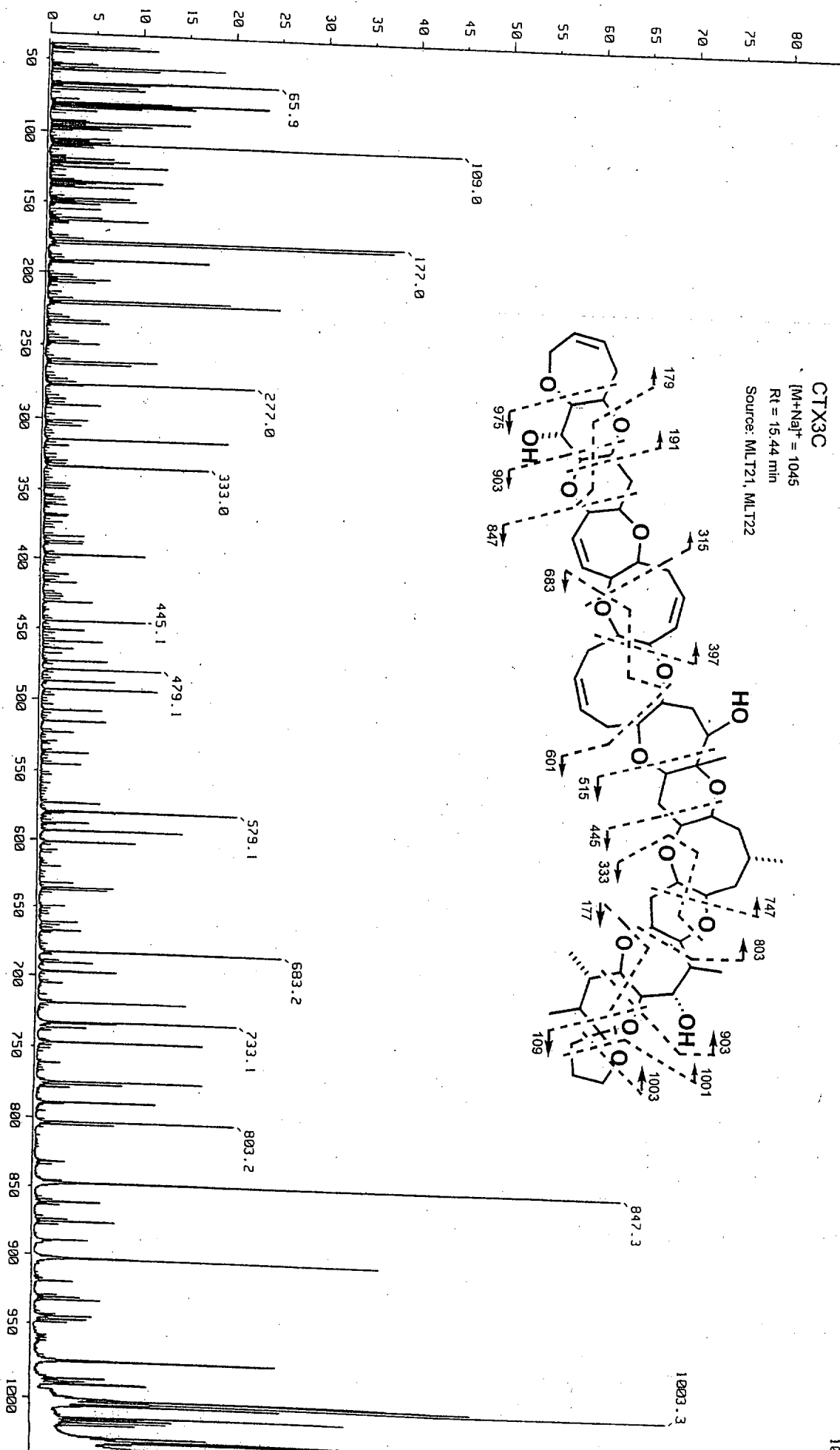
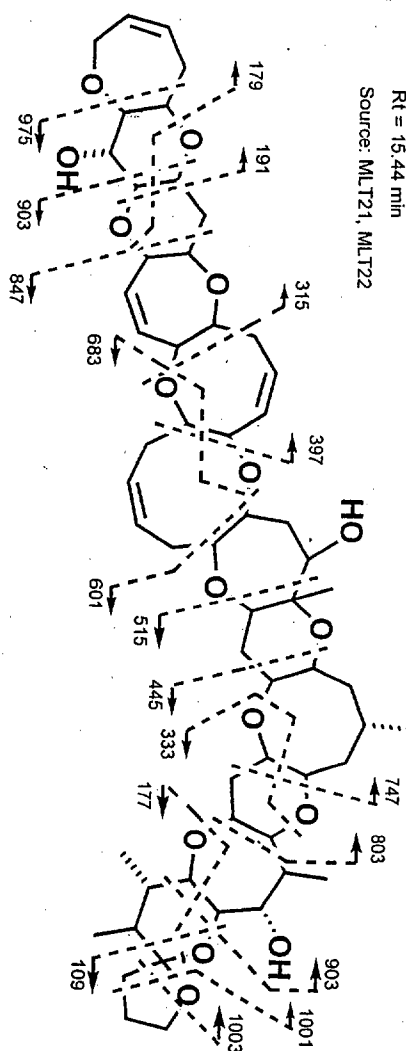
Cut Level : 0.00 %

CTX3C

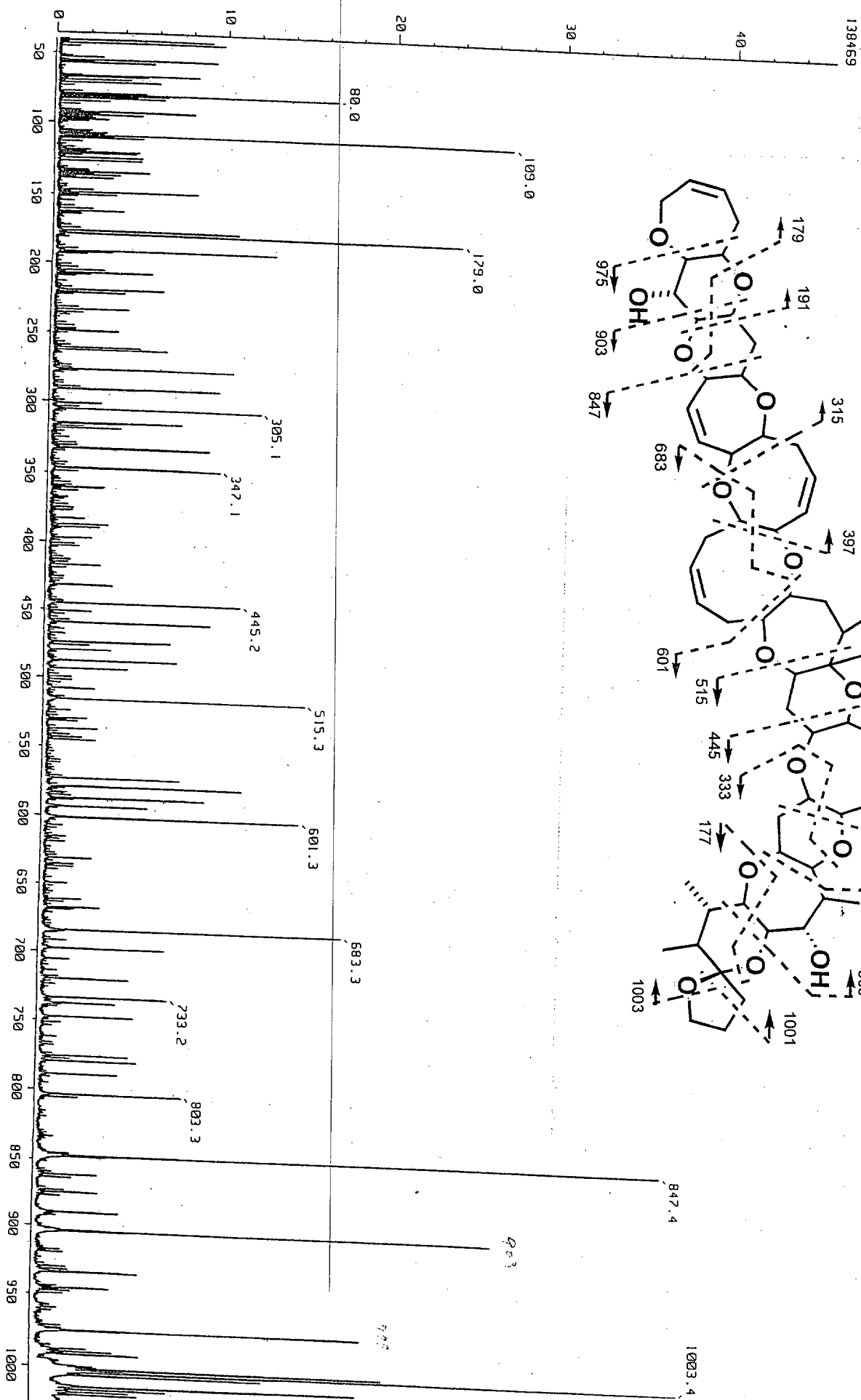
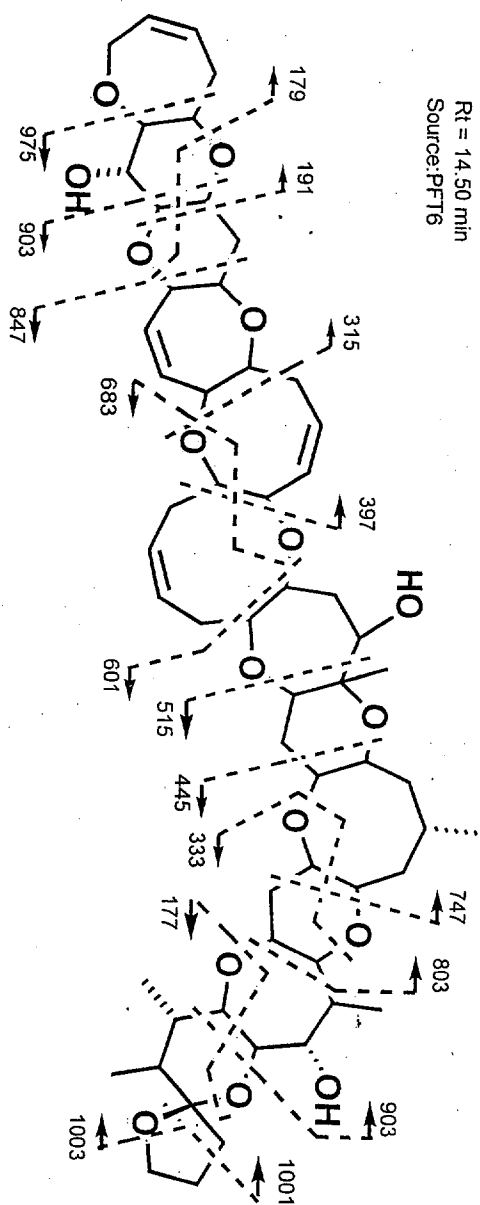
[M+Na]⁺ = 1045

Rt = 15.44 min

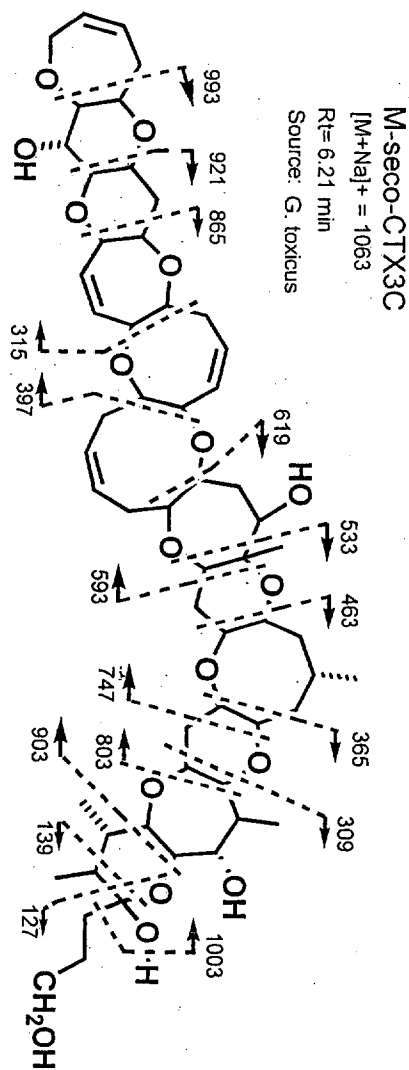
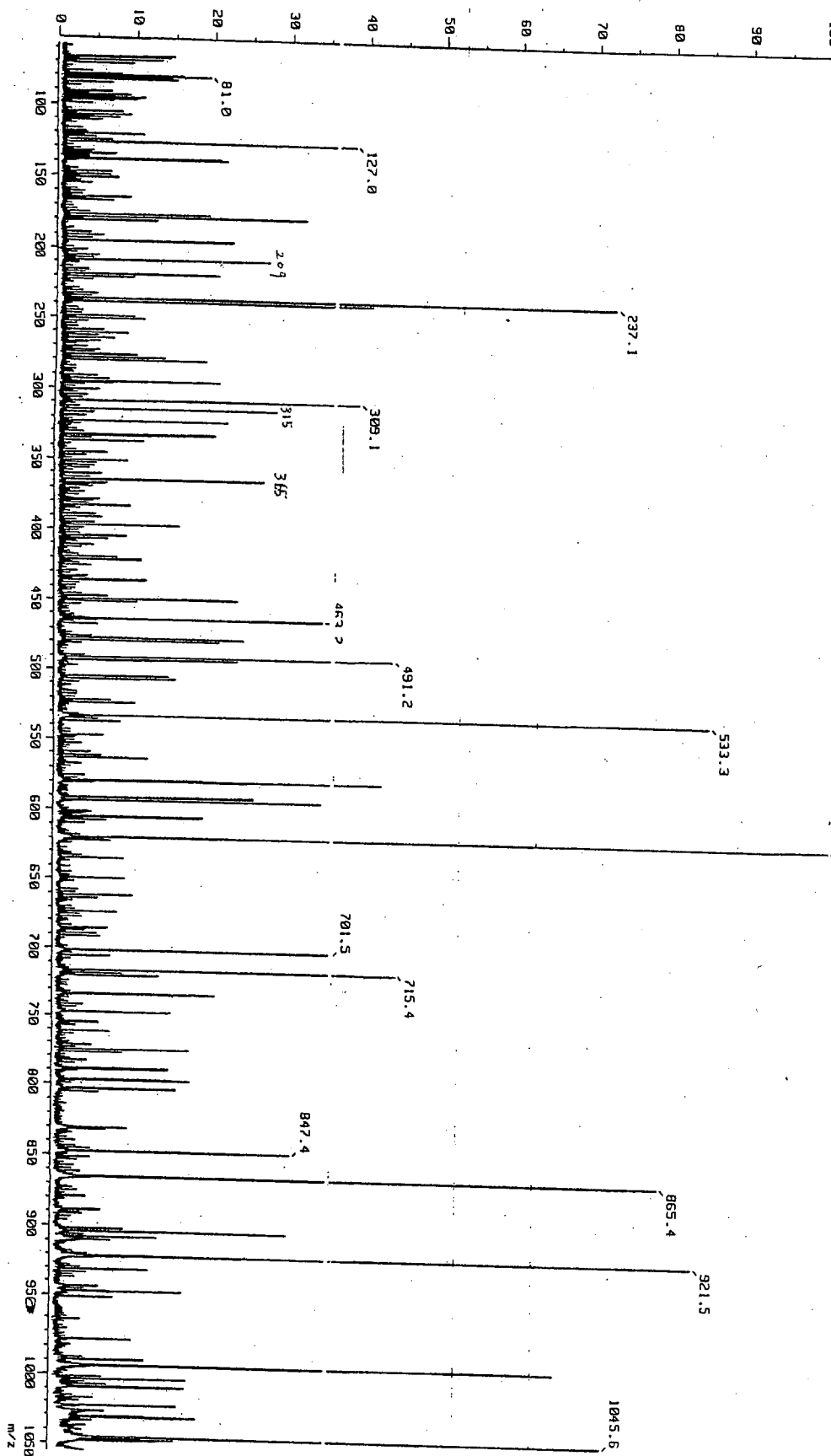
Source: MLT21, MLT22



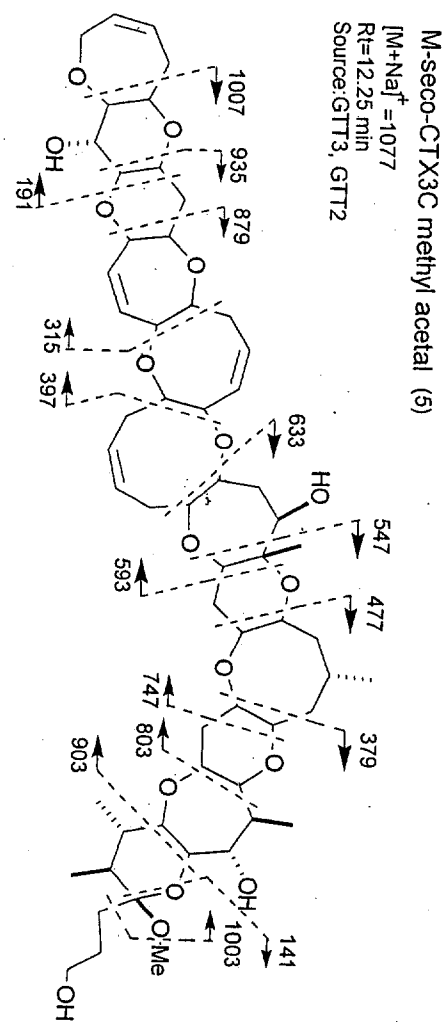
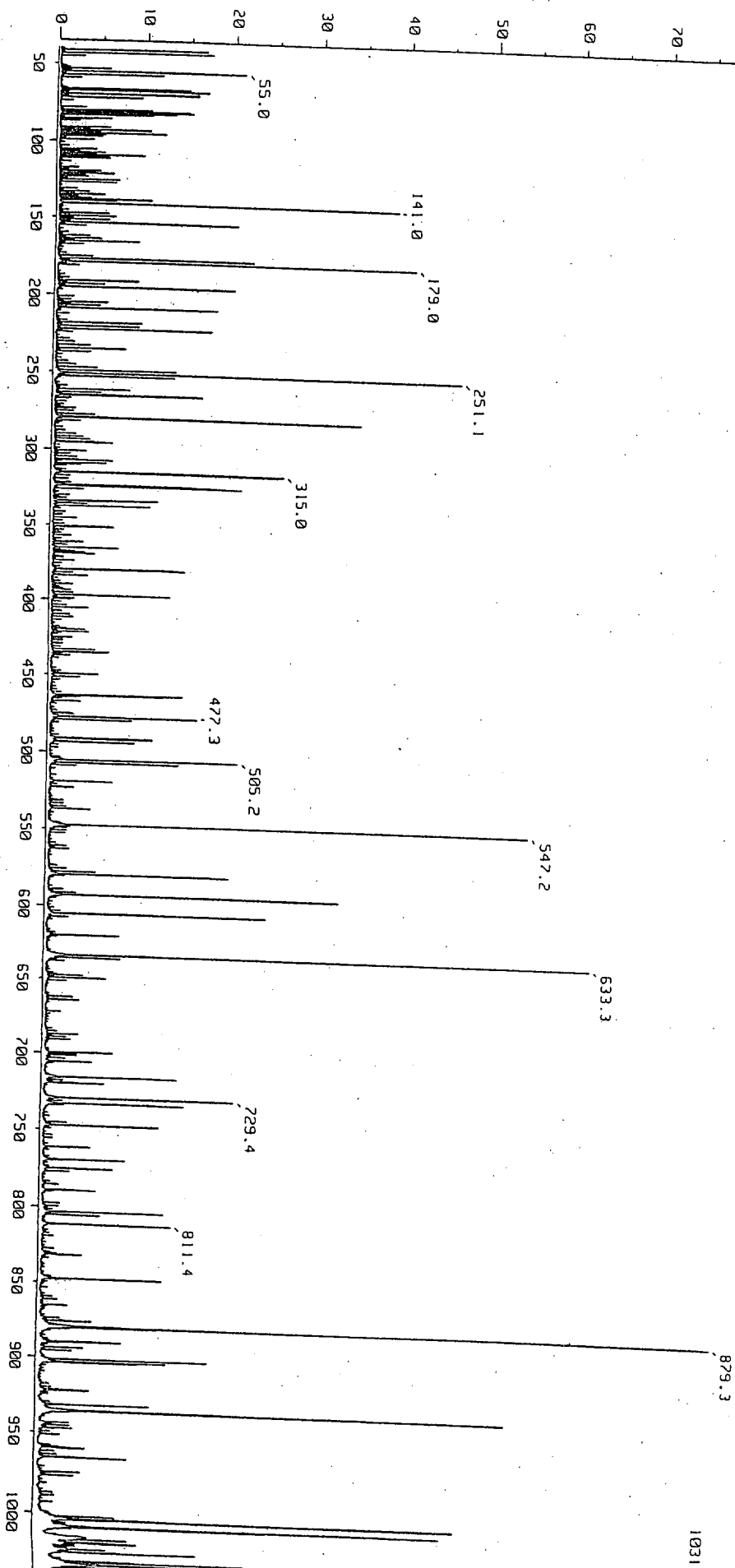
49
52-epi-CTX3C
[M+Na]⁺ = 1045
Rt = 14.50 min
Source: PFT6



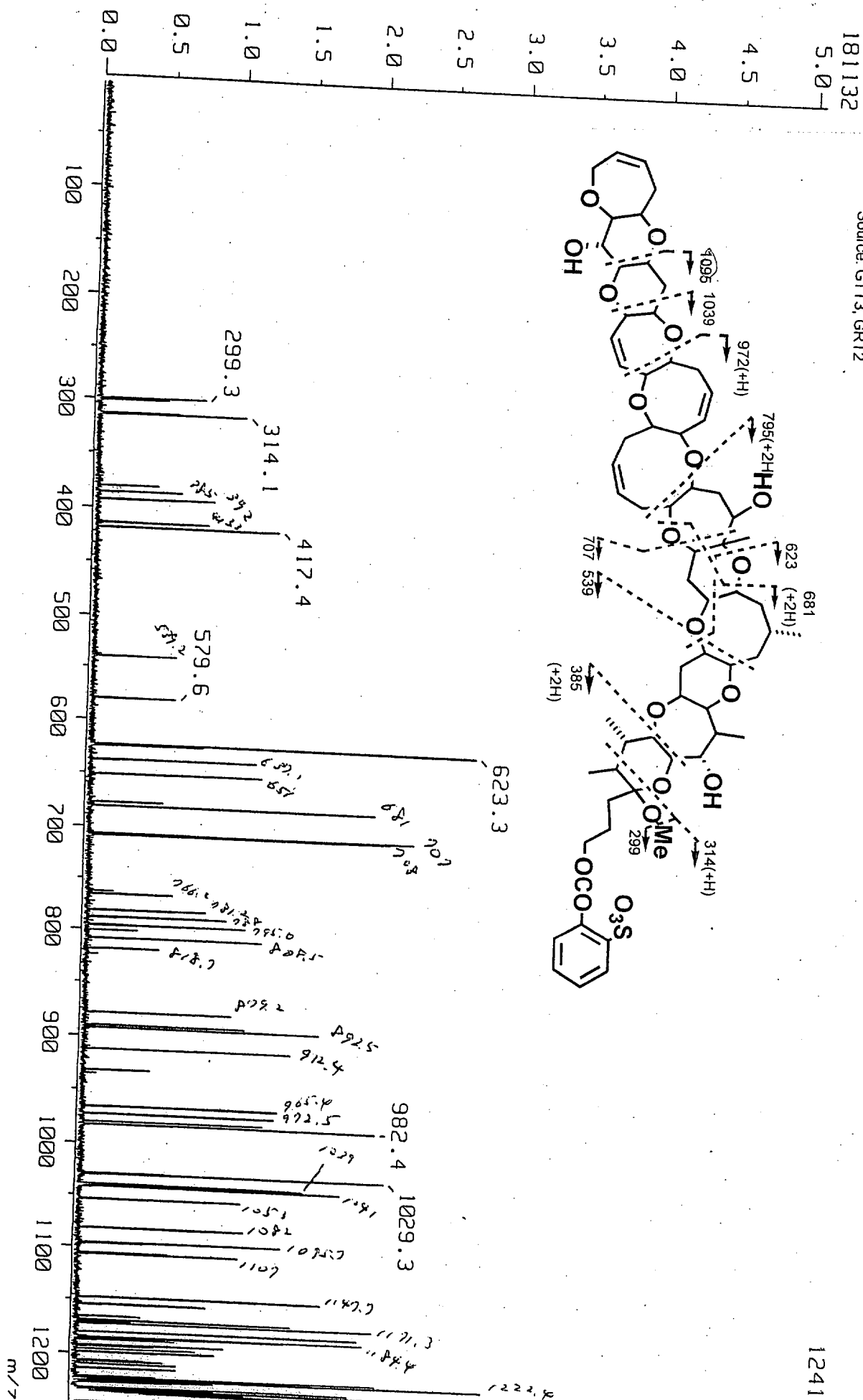
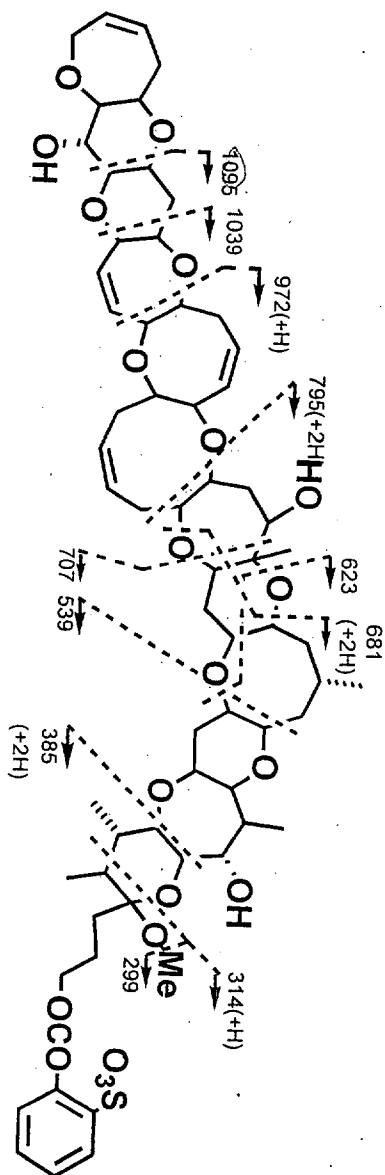
[Mass Spectrum]
 Date : 13-Dec-99 15:39
 Sample : seco CTX3C
 Note : Array Detector Data
 Inlet : Direct
 Spectrum Type : Product (m/z 1063.60, 3rd FFR, FC: 8.00kV)
 RT : 0.00 min Scan# : 1
 BP : m/z 619.2738 Int. : 5.25
 Output m/z range : 57.9739 to 1065.5800 Cut Level : 0.00 %
 55102



[Mass Spectrum]
 Date : 15-Oct-98 18:13
 Sample : CTX-GT-172
 Note : Array Detector Data
 Inlet : Direct
 Spectrum Type : Product (m/z 1077.50, 3rd FFR, FC: 8.00kV)
 RT : 0.00 min Scan# : 1
 BP : m/z 1073.7288 Int. : 26.64
 Output m/z range : 39.2462 to 1074.8462
 Cut Level : 0.00 %



M-seco-CTX3C methyl acetal sulfobenzoate (Linked scan LC/MS/MS)
 [M-H]⁻ = 1237
 Source: GTT3, GRT2

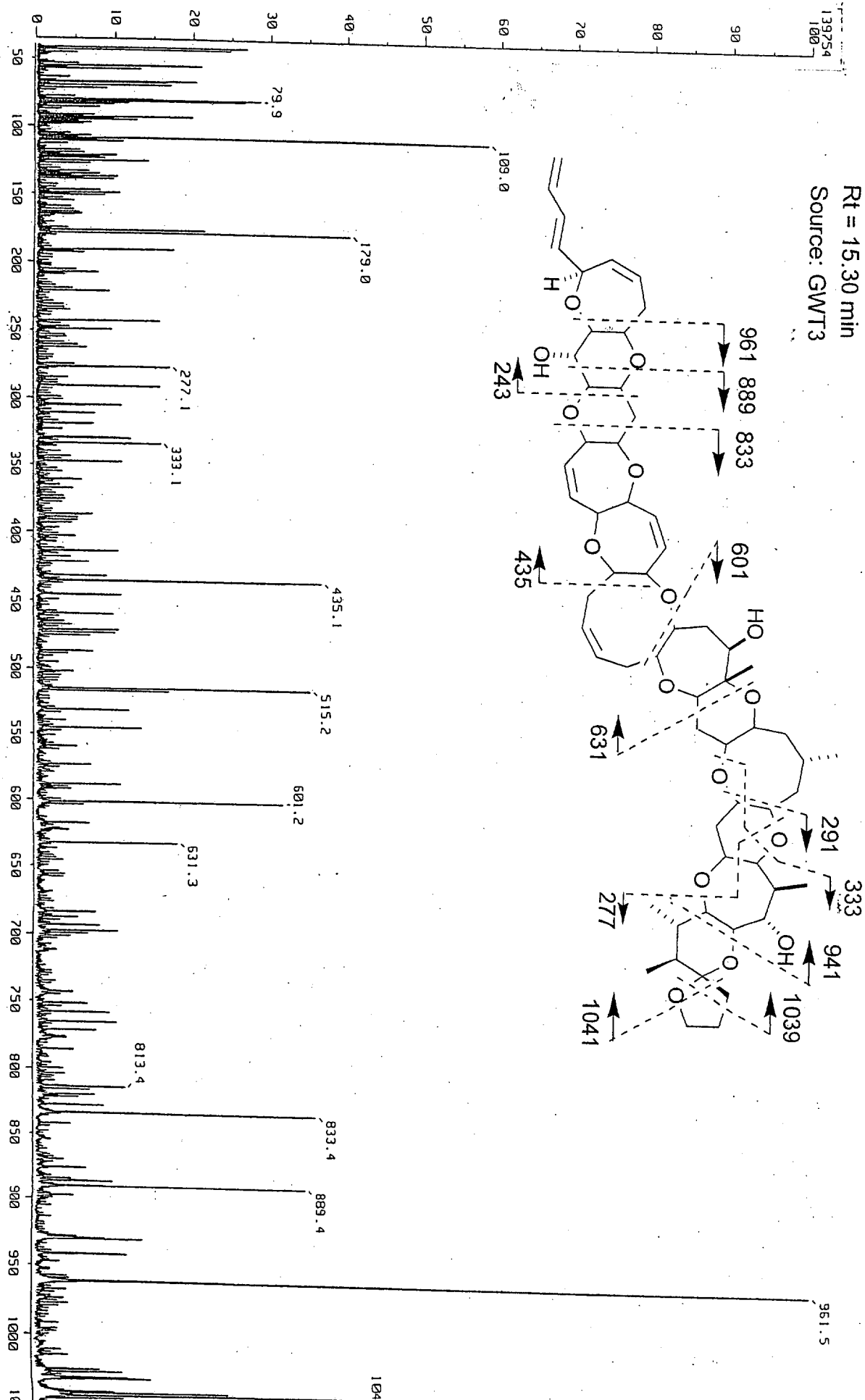


CTX4A

[M+Na]⁺ = 1083

Rt = 15.30 min

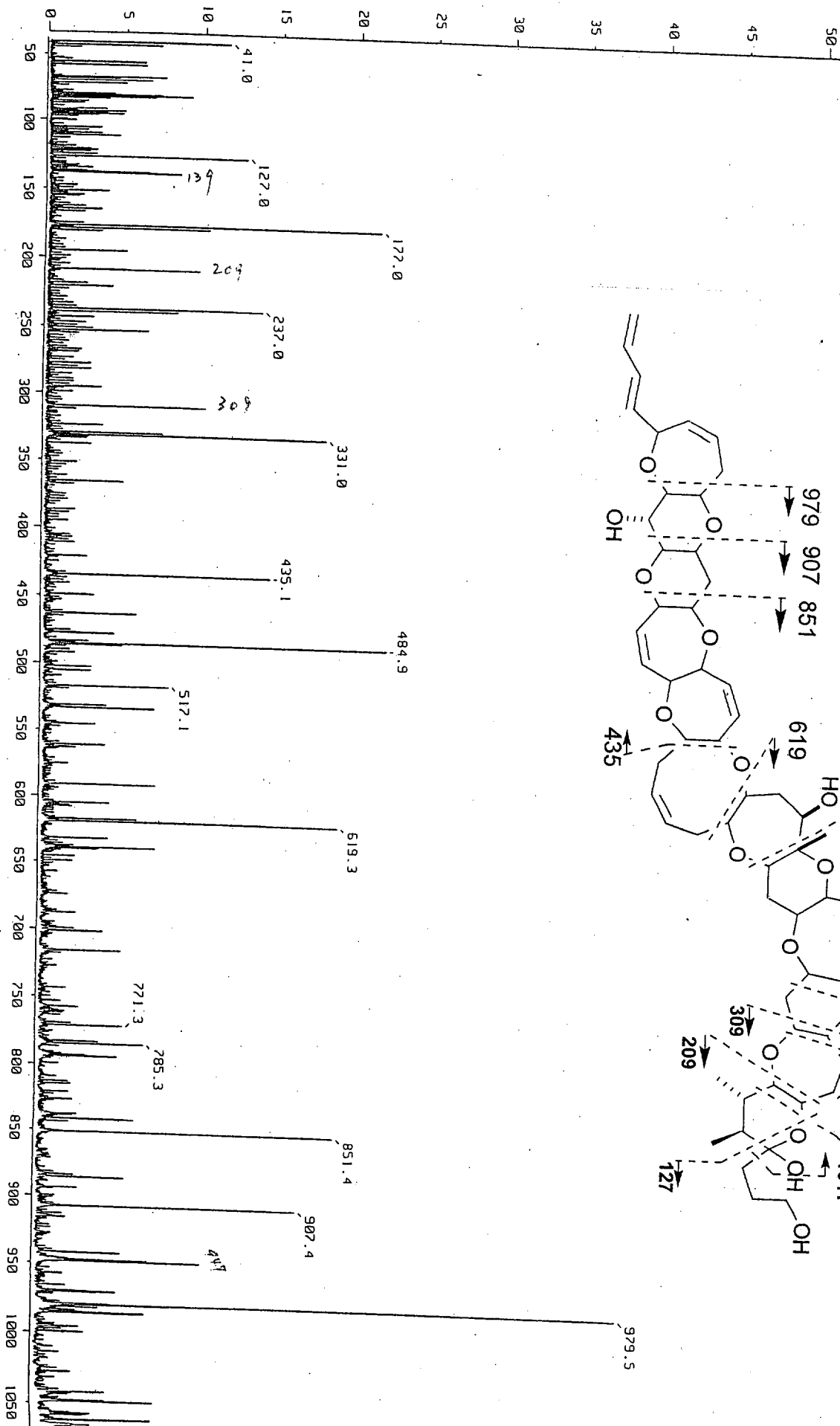
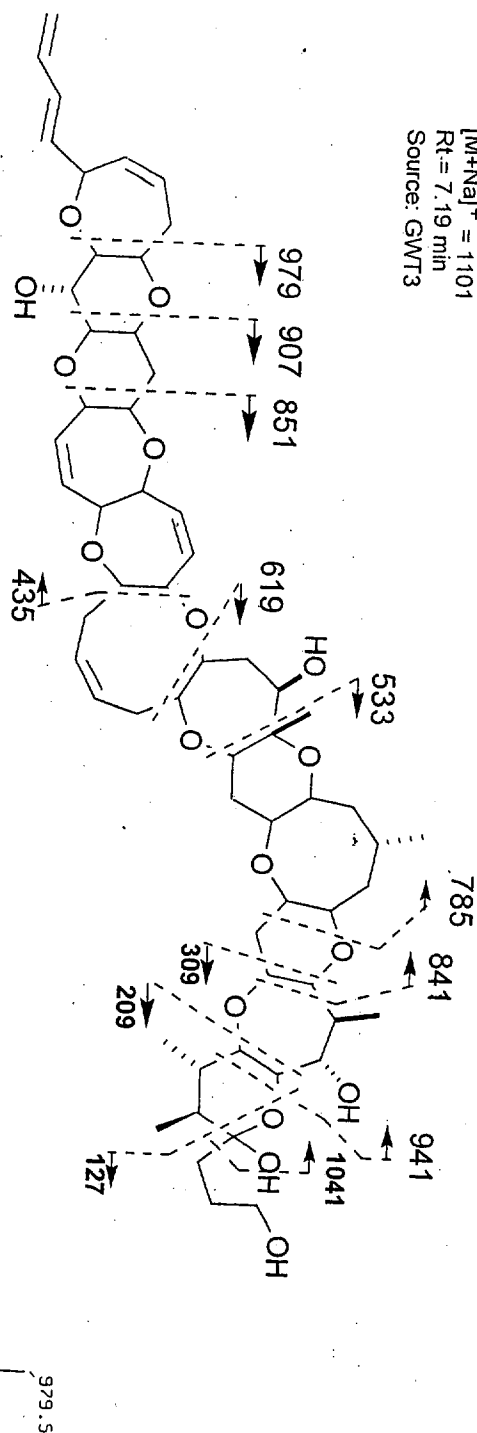
Source: GWT3



[Mass Spectrum]
 Data : 13b
 Sample: CTX-13
 Note : Array Detector Data
 Inlet : Direct
 Spectrum Type : Product (m/z 1101.50)
 RT : 0.00 min Scan# : 1
 BP : m/z 1099.9990 Int. : 27.45
 Output m/z range : 38.6348 to 1099.63
 146976

M-seco-CTX4A (or 4B)

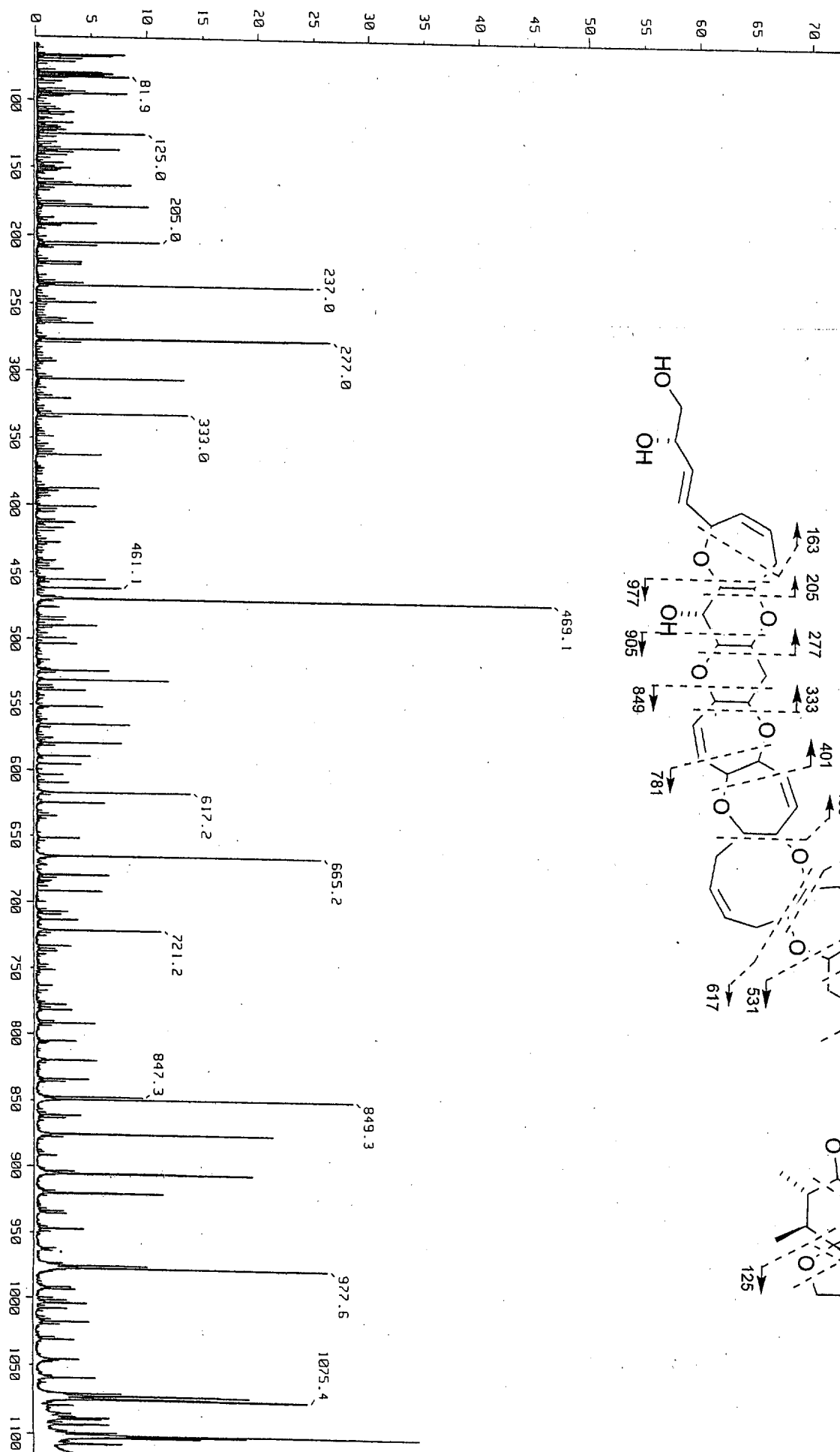
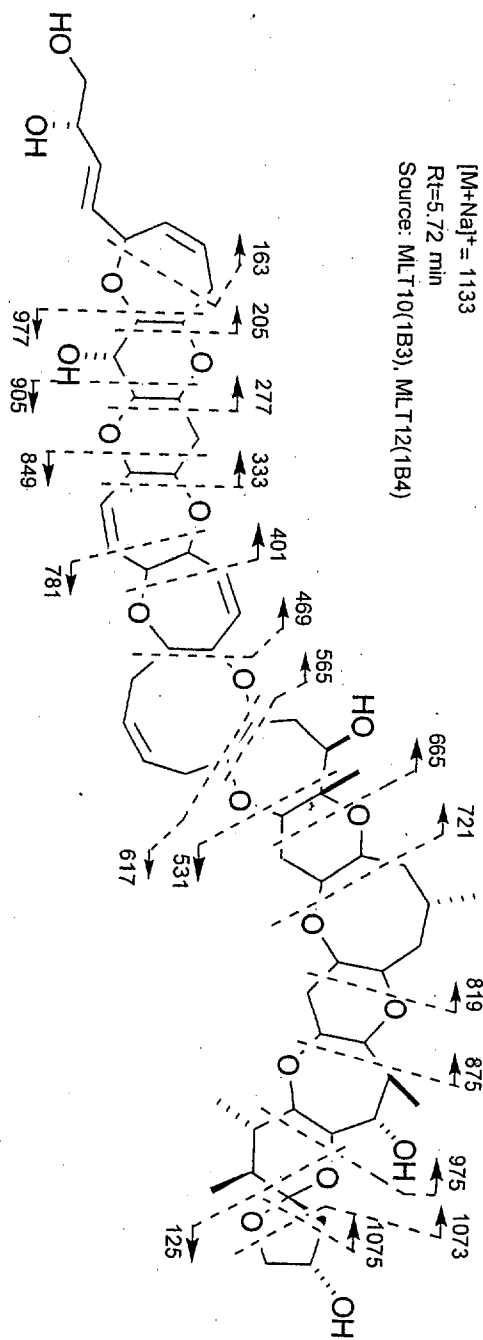
[M+Na]⁺ = 1101
 Rt = 7.19 min
 Source: GWT3



[Mass Spectrum]
 Date : 1b21b
 Sample: CTX-1B2.1
 Note: Array Detector Data
 Inlet: Direct
 Spectrum Type: Product (m/z 1133.50, 3rd
 RT: 0.00 min Scan#: 1
 BP: m/z 1132.7137 Int.: 28.86
 Output m/z range: 57.2512 to 1137.8912
 219041

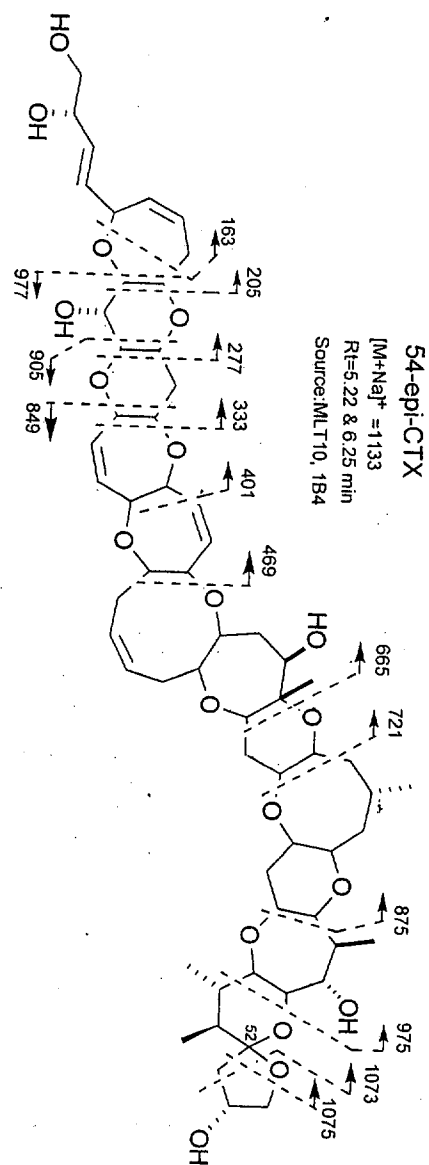
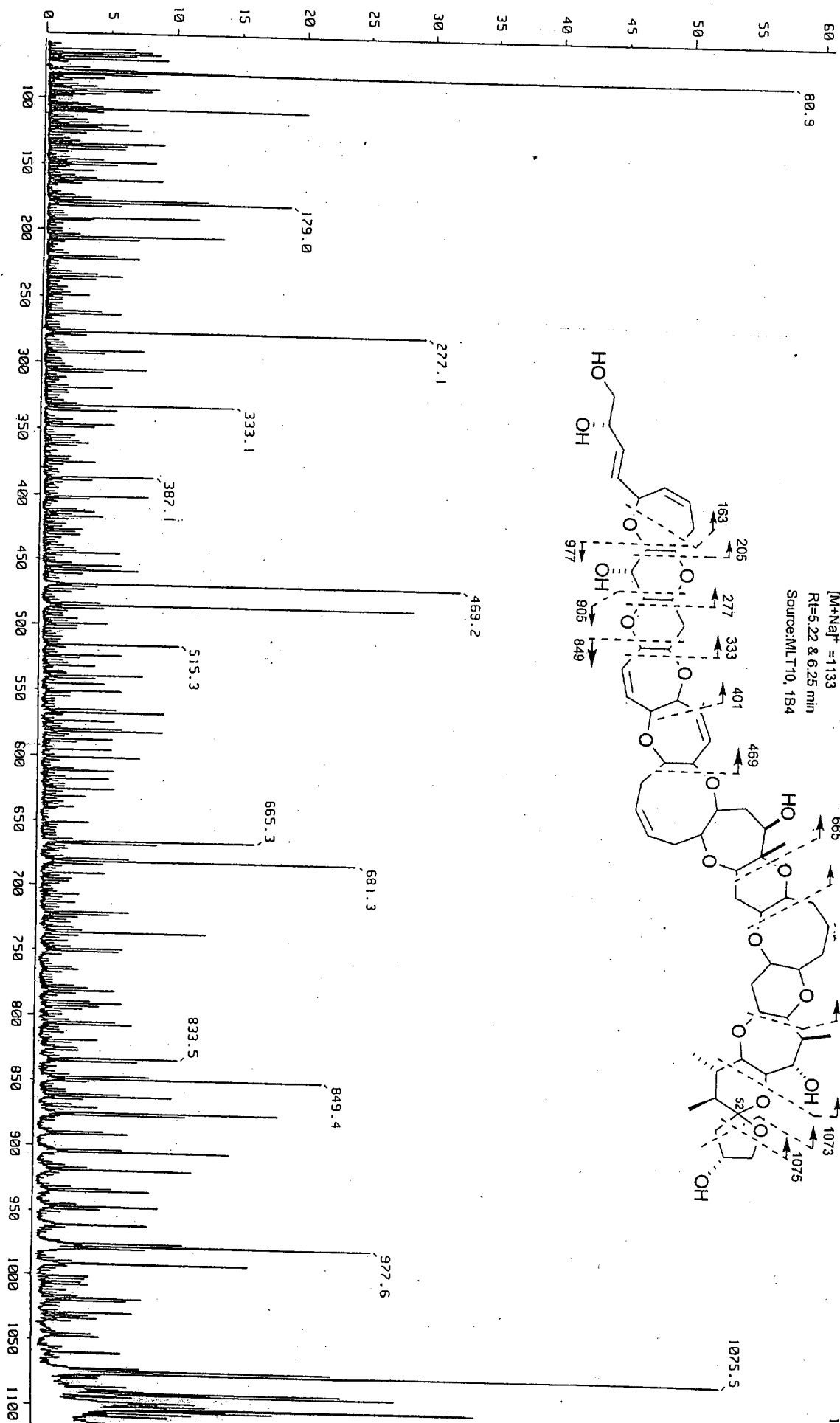
MS/MS Spectrum of 52-epi-CTX

[M+Na]⁺ = 1133
 Rt=5.72 min
 Source: MLT10(1B3), MLT12(1B4)



[Mass Spectrum]
Date : 1b4a
Sample: CTX-1B4
Note: Array Detector Data
Inlet : Direct
Spectrum Type : Product (m/z 1133.50, 3rd FFR, FC: 8.00kV)
RT : 0.00 min Scan# : 1
BP : m/z 1132.8728 Int. : 28.92
Output m/z range : 55.6393 to 1136.4193
183909

Date : 24-Sep-98 15:27

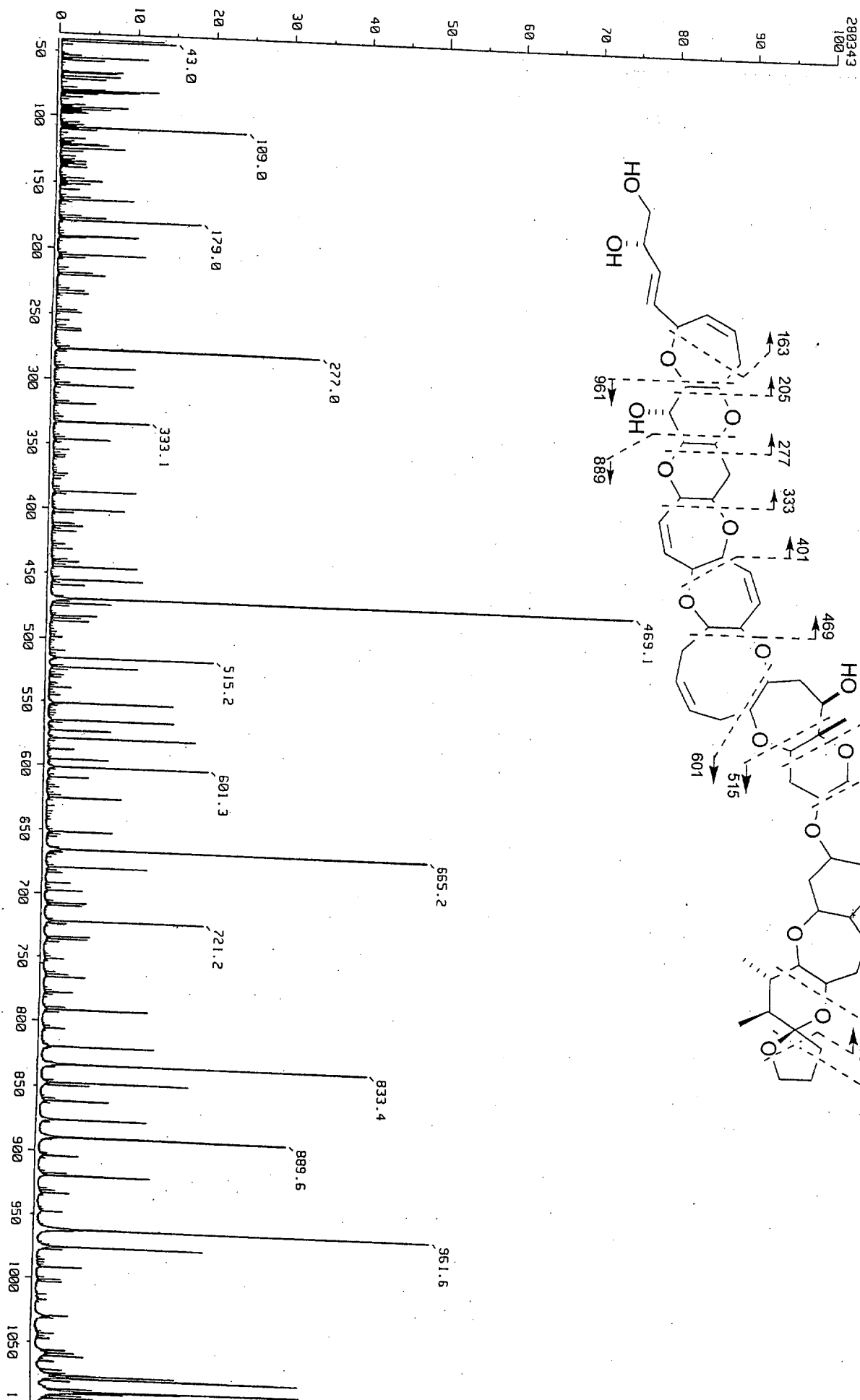
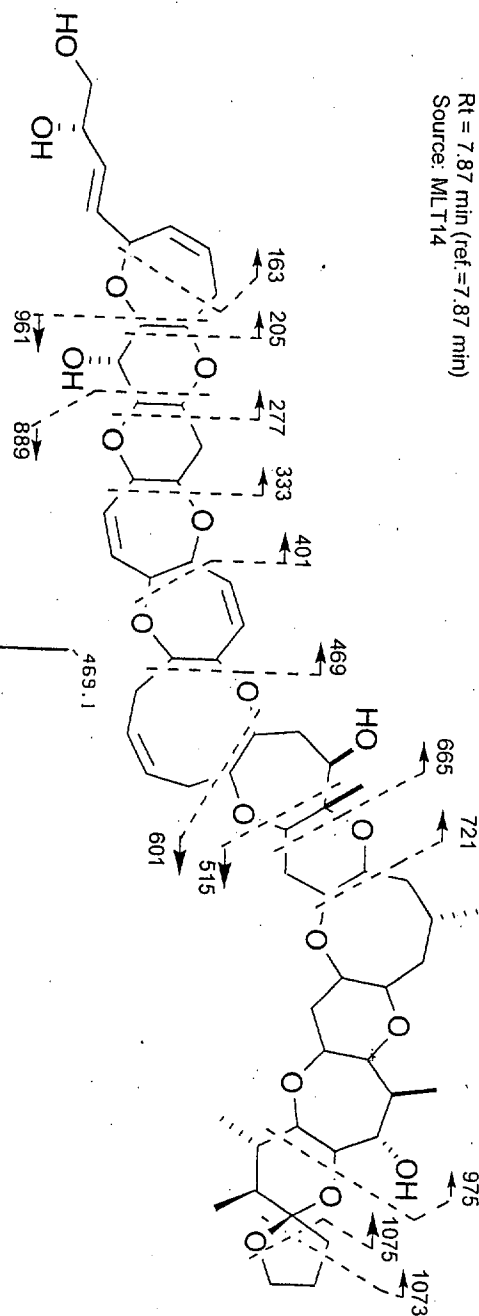


52-*epi*-54-deoxy-CTX

[M+Na]⁺ = 1117

Rt = 7.87 min (ref. = 7.87 min)

Source: ML T14

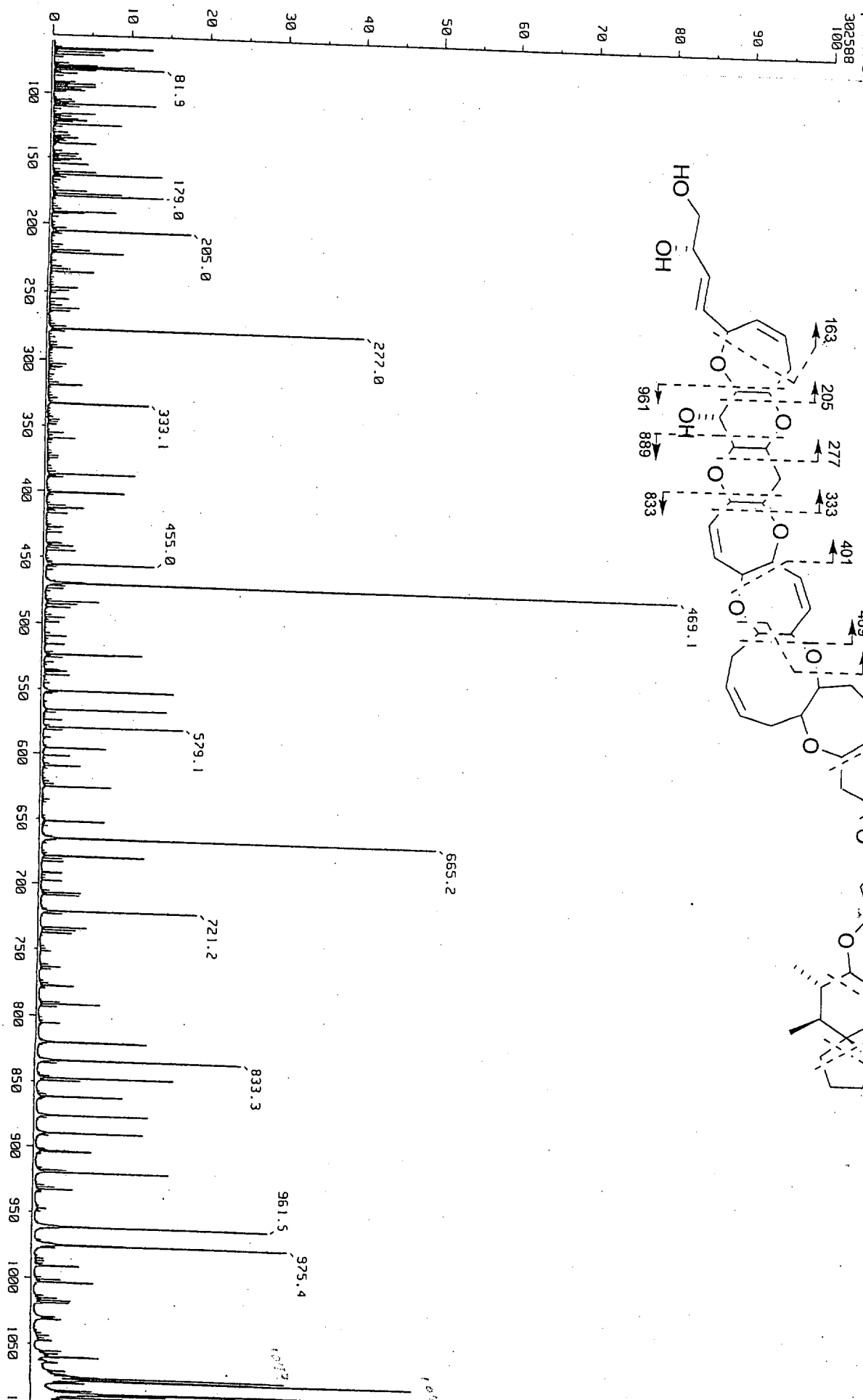
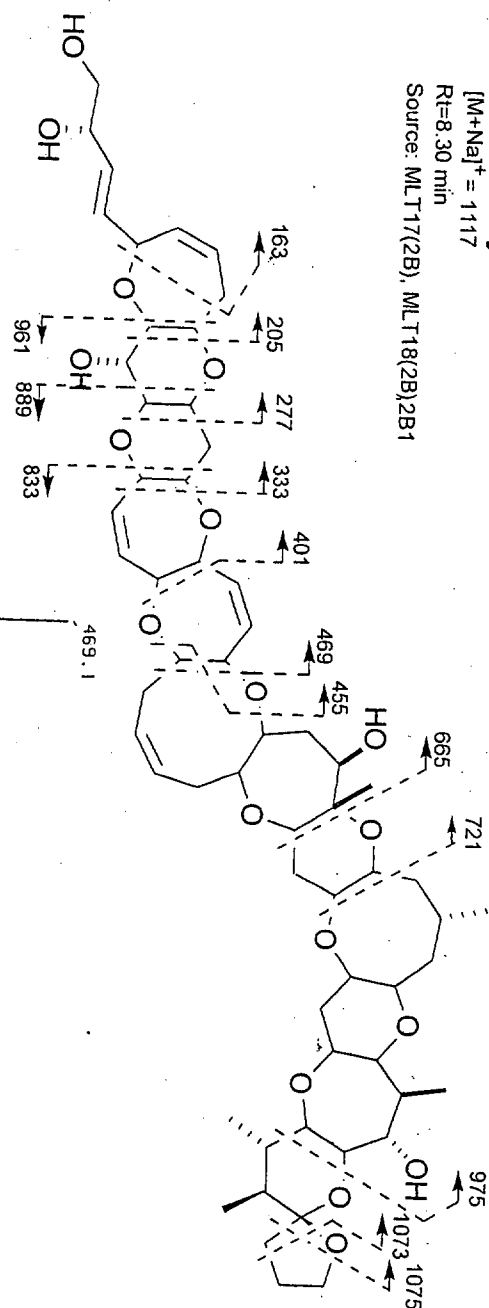


54-deoxy-CTX

[M+Na]⁺ = 1117

RT=8.30 min

Source: MLT17(2B), MLT18(2B)2B1



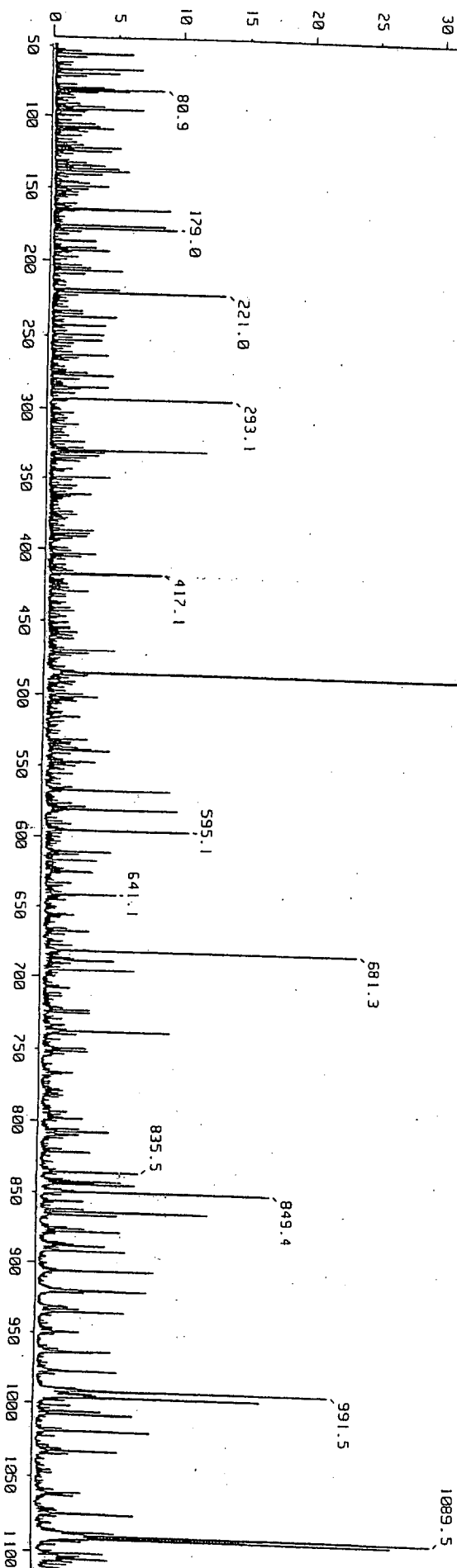
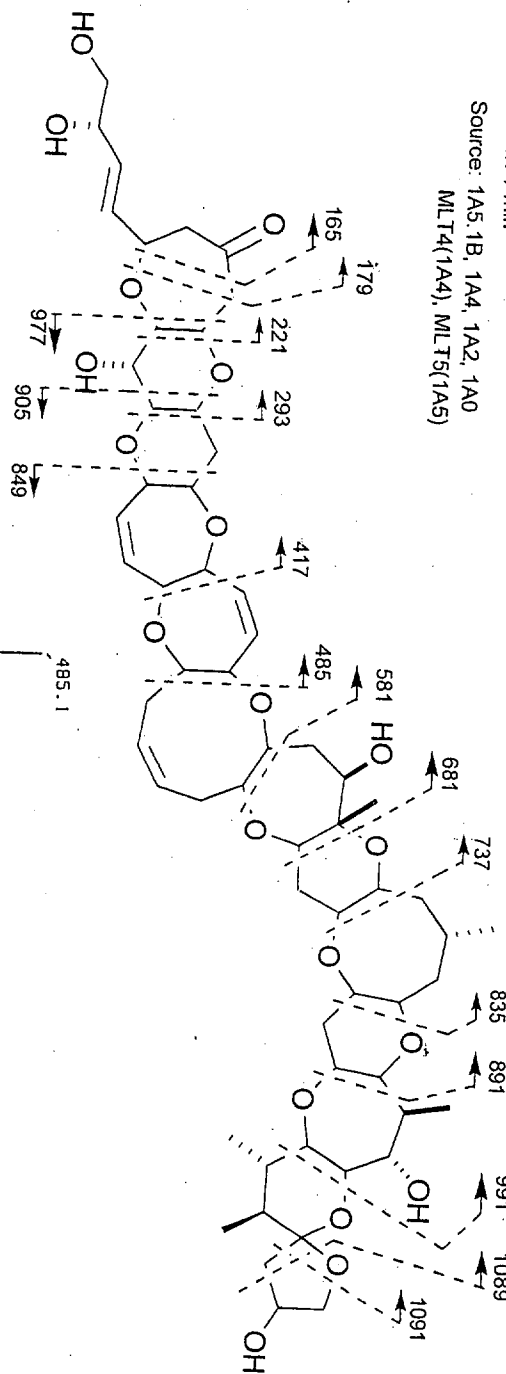
7-Oxo-CTX (MNa=1149)

[M+Na]⁺ = 1149

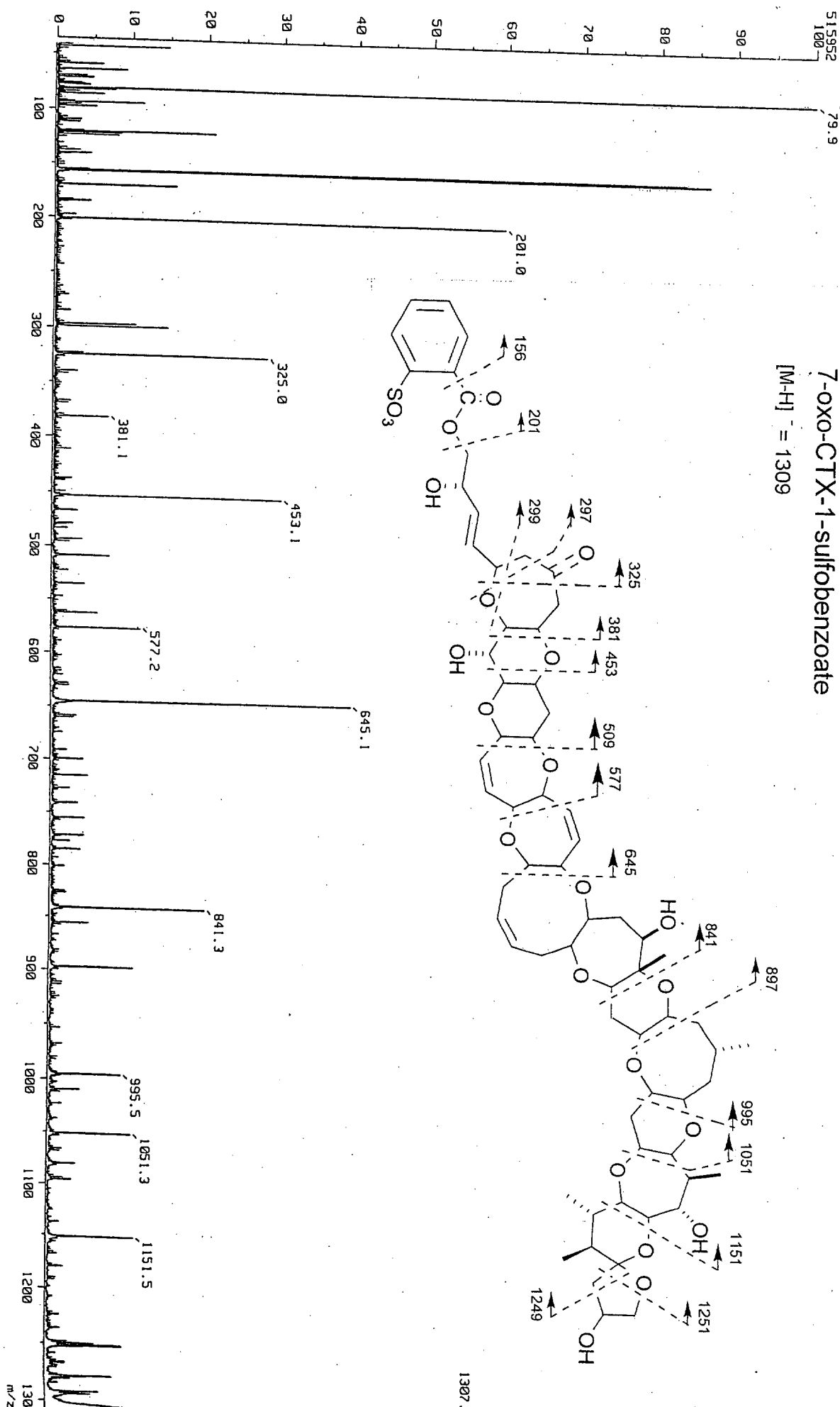
Rt = 4.71 min

Source: 1A5, 1B, 1A4, 1A2, 1A0

MLT4(1A4), MLT5(1A5)

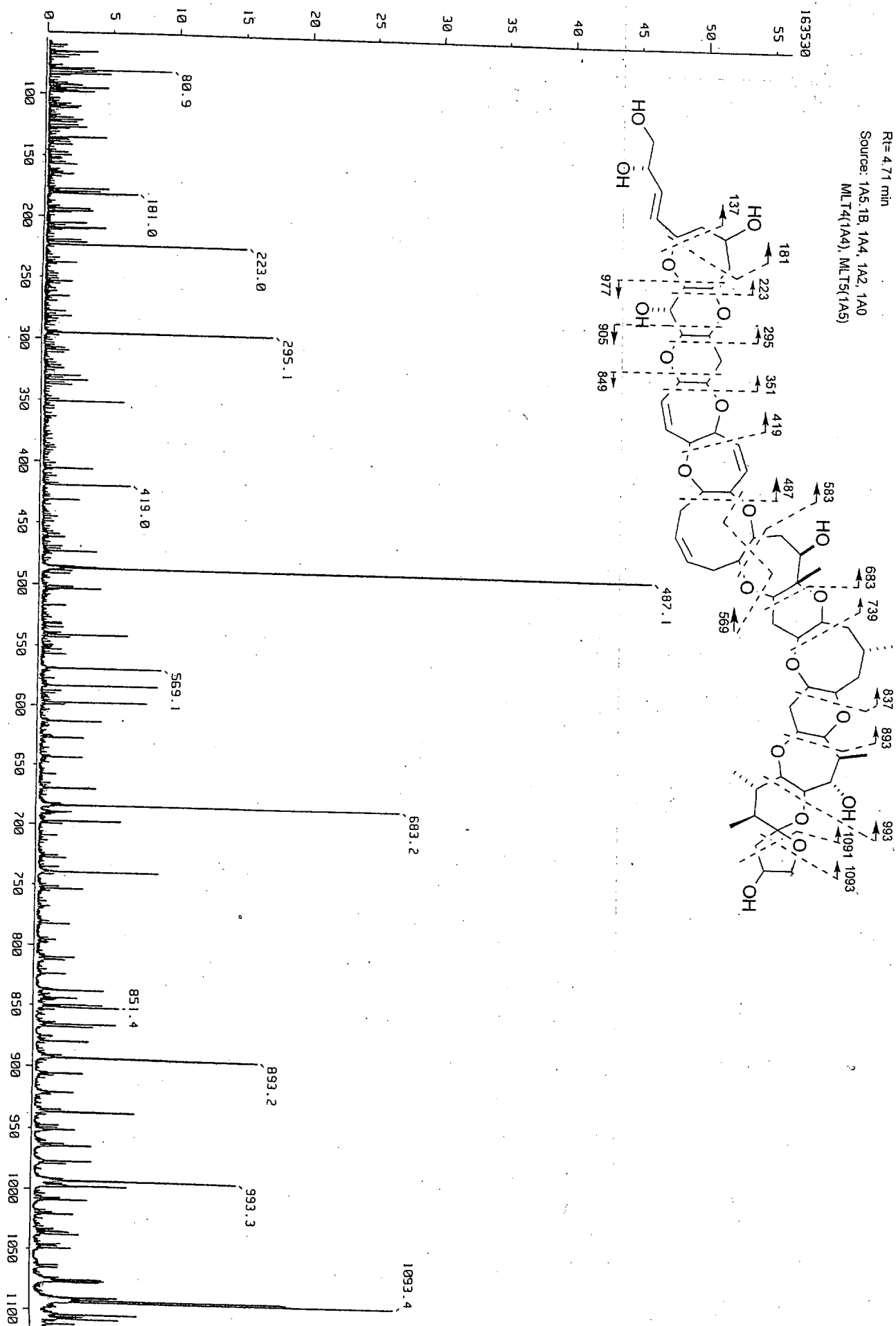


7-oxo-CTX-1-sulfobenzoate
[M-H]⁻ = 1309



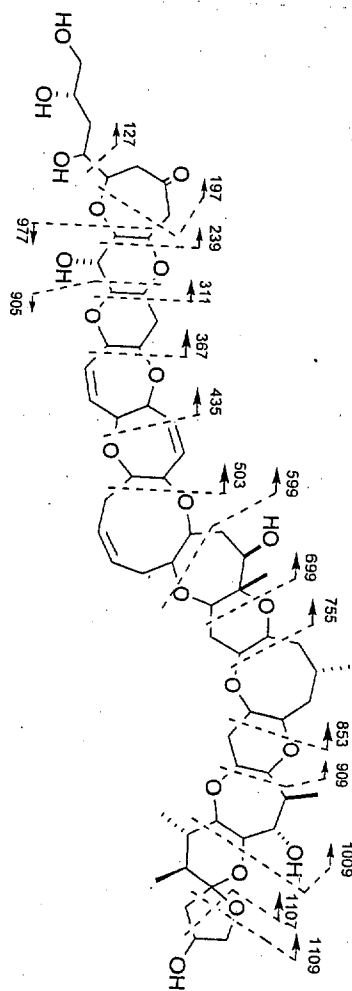
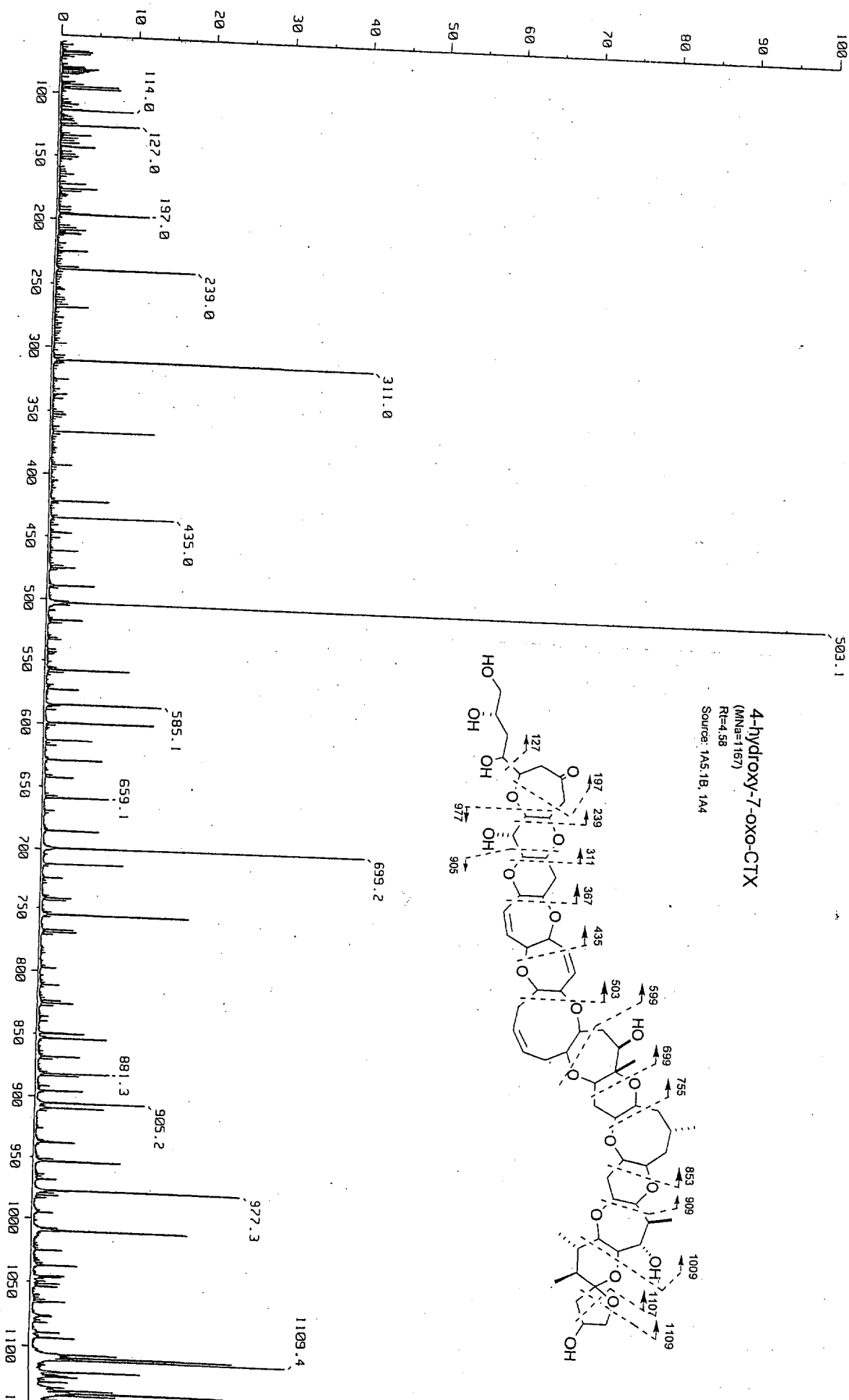
Rt= 4.71 min

Source: 1A5.1B, 1A4, 1A2, 1A0
MLT4(1A4), MLT5(1A5)



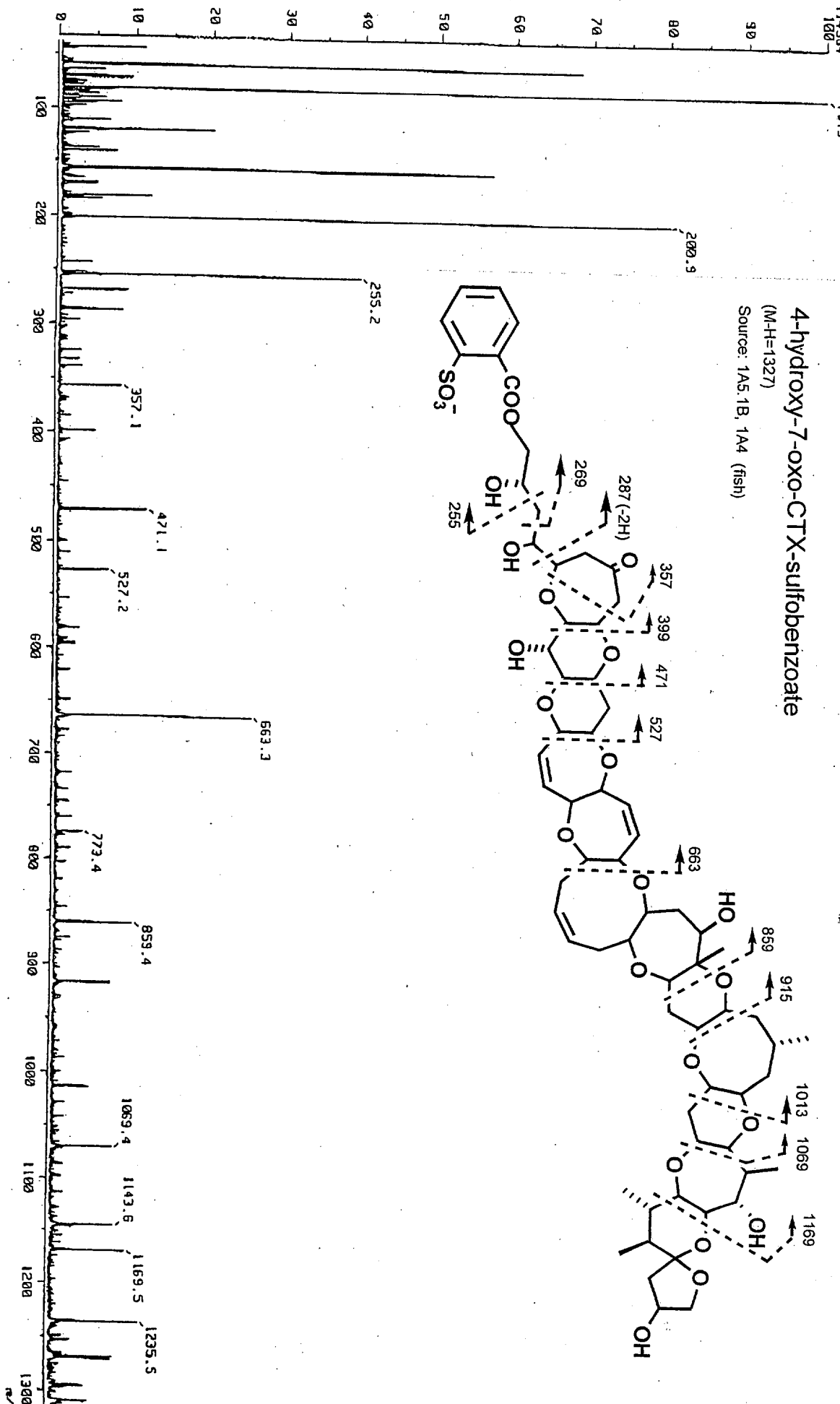
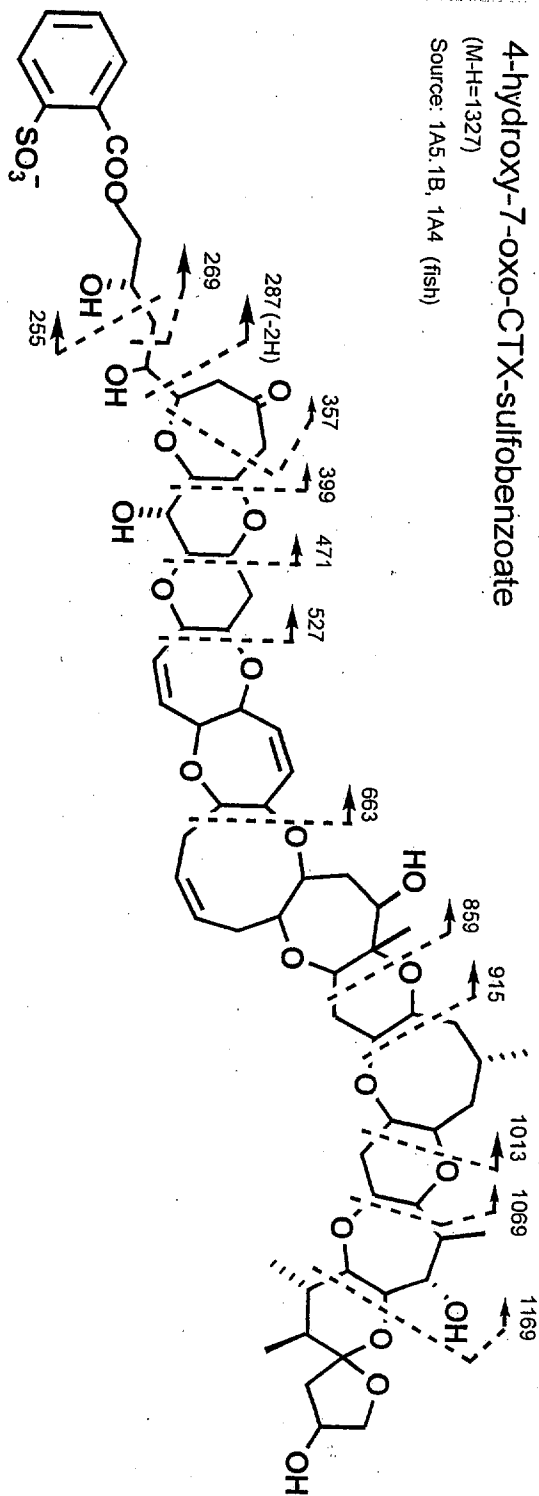
[Mass Spectrum]
 Date : 1a5a
 Sample: CTX-1165.1B
 Note : Array Detector Data
 Inlet : Direct
 Spectrum Type : Product (m/z 1167.50, 3rd FFR, FC: 8.00kV)
 RT : 0.00 min Scan# : 1
 BP : m/z 503.0646 Int. : 40.47
 Output m/z range : 58.8960 to 1170.5959
 424401
 Cut Level : 0.00 %

Date : 28-Aug-98 11:49



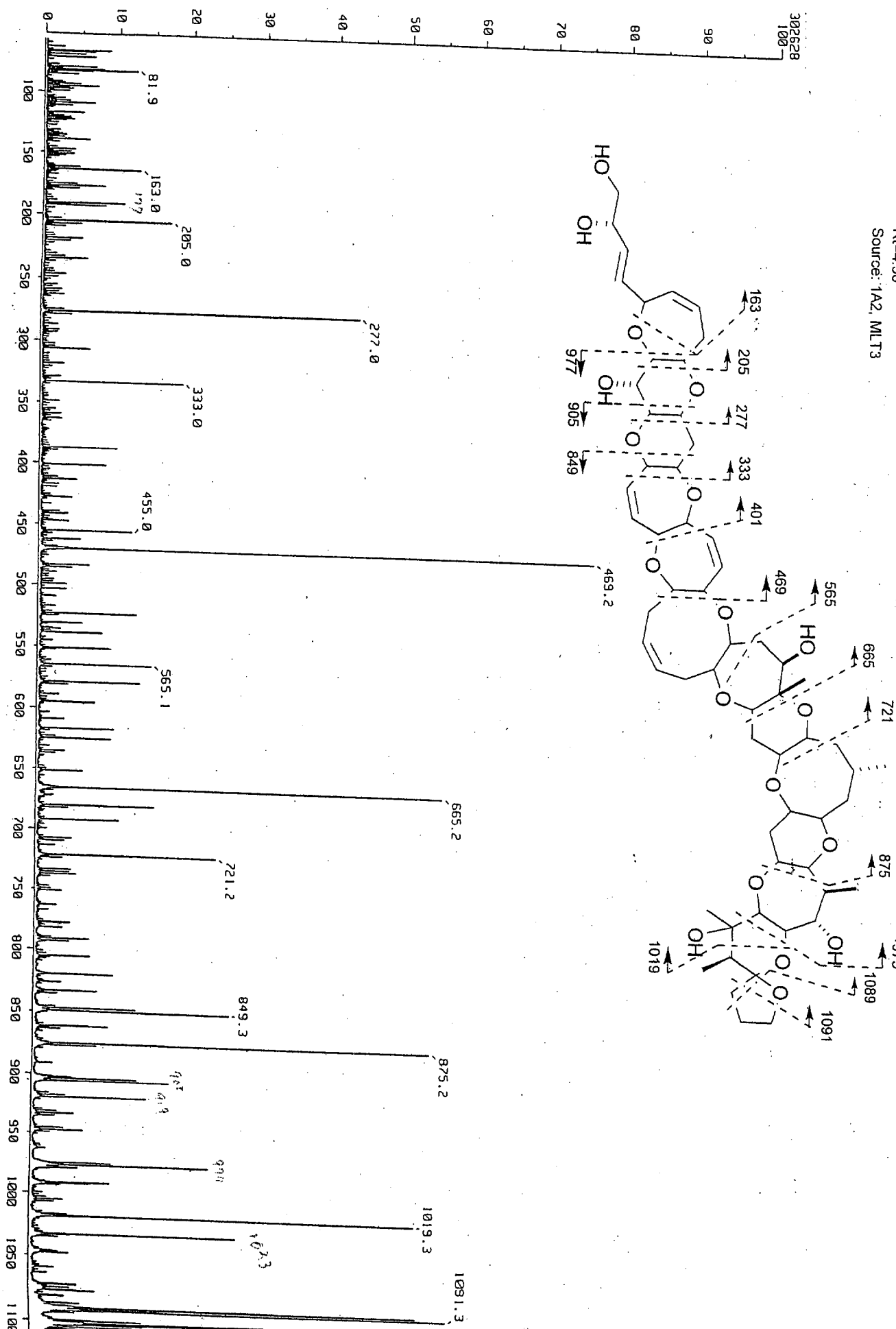
(Mass Spectrum)
 Date : 08-Sep-99 18:33
 Sample: Sulfo CTX-1
 Note: Array Detector Data
 Inlet : Direct
 Spectrum Type : Product (m/z 1327.50, 3rd FFR, FC: 0.00kV)
 RT : 0.00 min Scan# : 1
 BP : m/z 79.9077 Ion : 10.91
 Output m/z range : 38.3950 to 1322.6150 Out Level : 0.00 %

4-hydroxy-7-oxo-CTX-sulfobenzoate
 (M-H=1327)
 Source: 1A5.1B, 1A4 (fish)

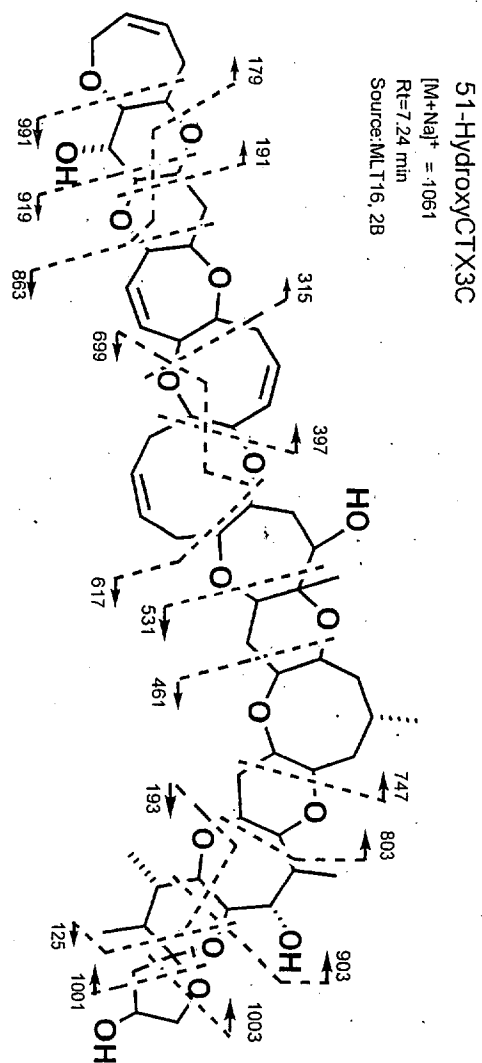
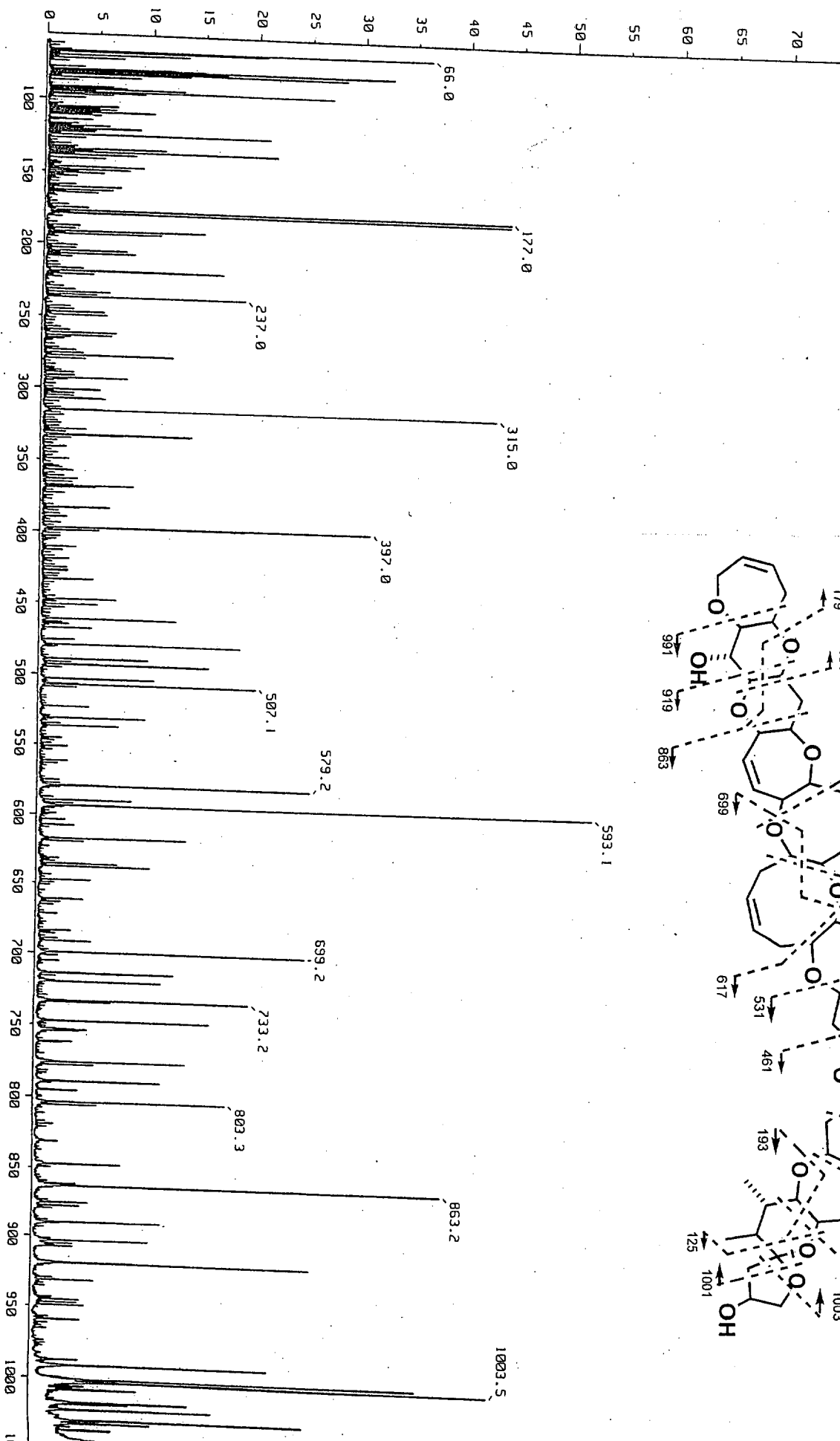


Rt=4.90

Source: 1A2, MLT3

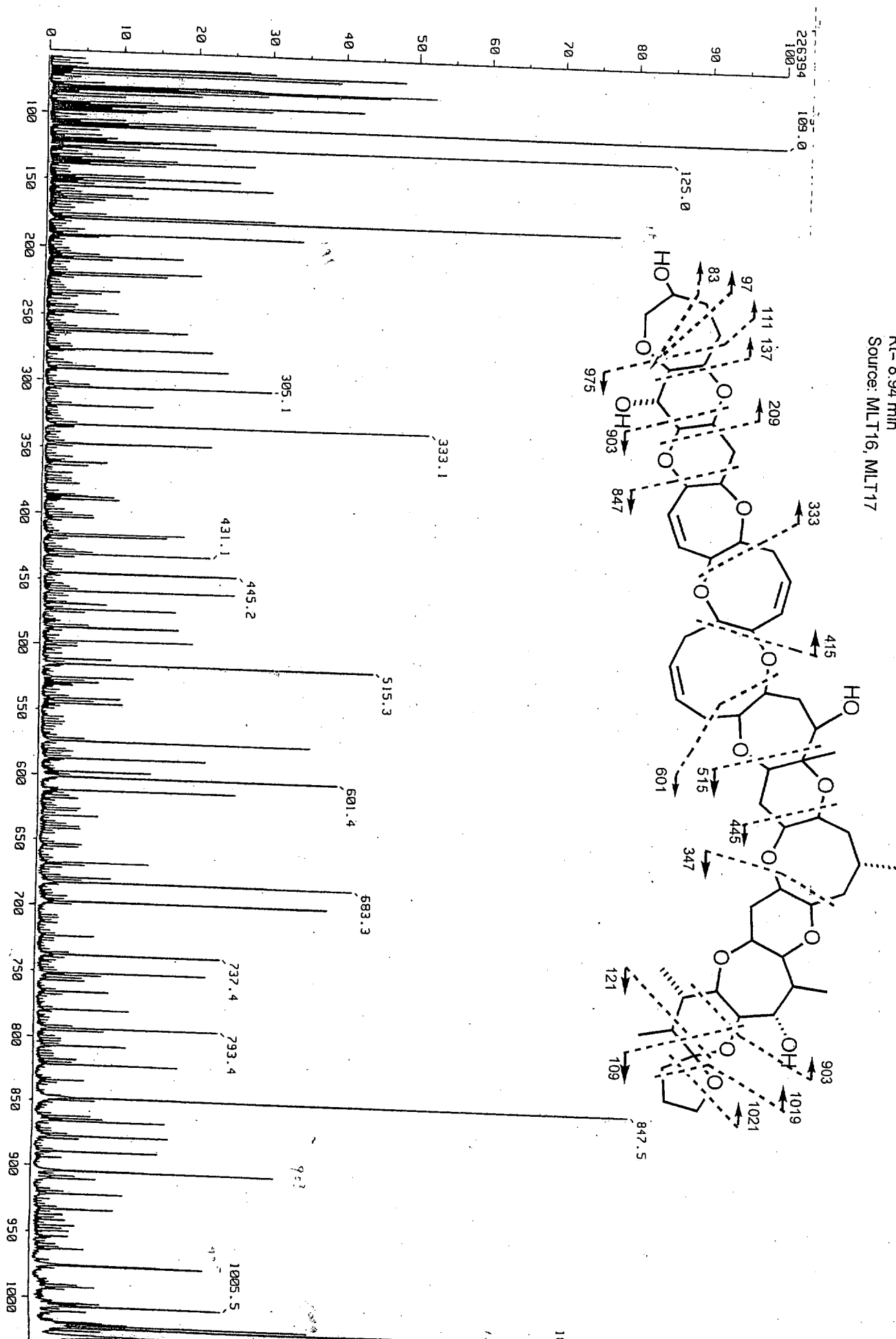


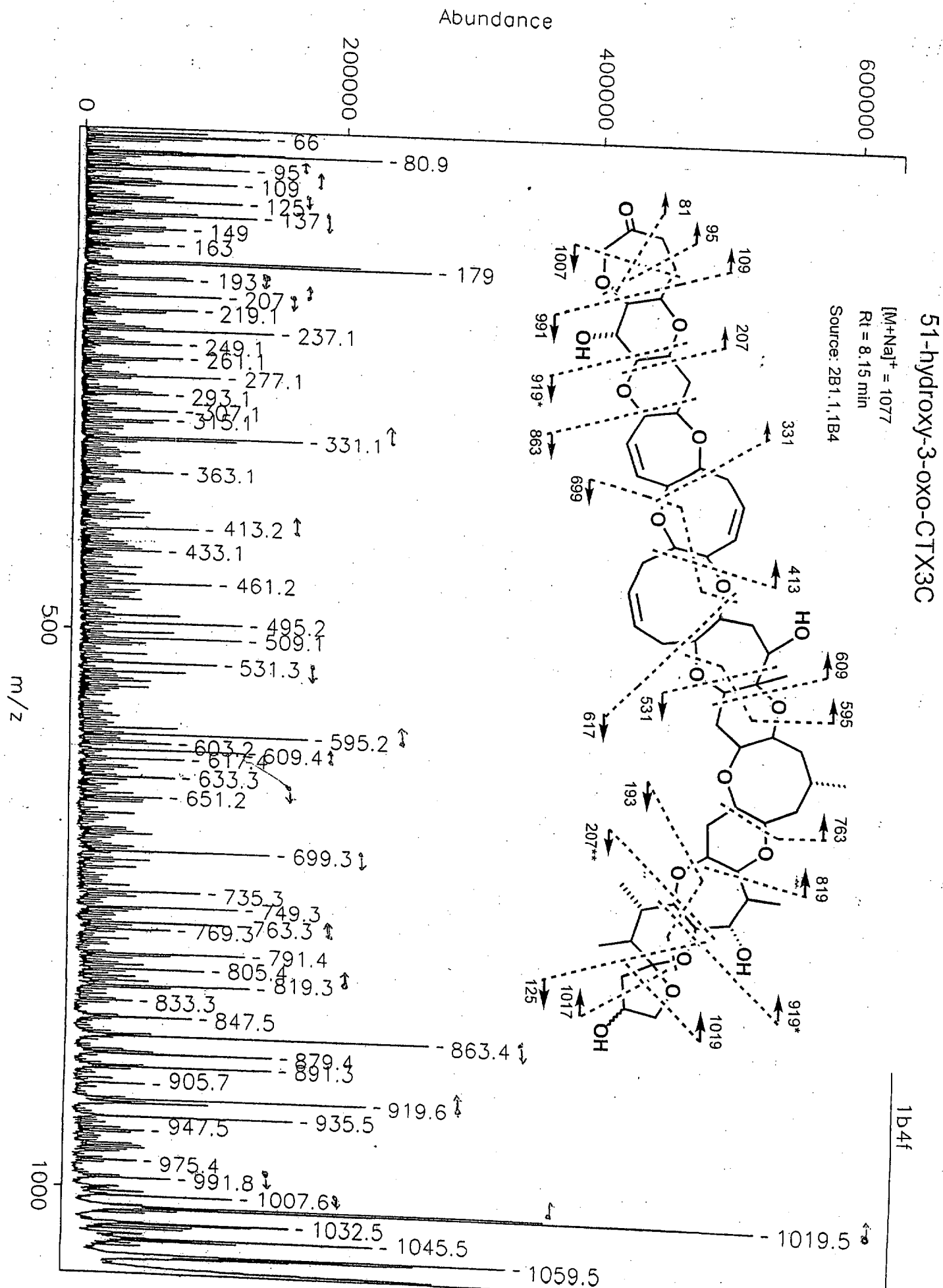
[Mass Spectrum]
 Date : 28-Aug-98 16:28
 Sample : CTX-2B
 Note : Array Detector Data
 Inlet : Direct
 Spectrum Type : Product (m/z 1061.50, 3rd FFR, FC: 8.00kV)
 RT : 0.00 min Scan# : 1
 BP : m/z 1058.9960 Int. : 28.85
 Output m/z range : 59.4322 to 1064.5122 Cut Level : 0.00 %
 224303



2-hydroxy-CTX3C

[M+Na]⁺ = 1063
 Rt = 8.94 min
 Source: MLT16, MLT17



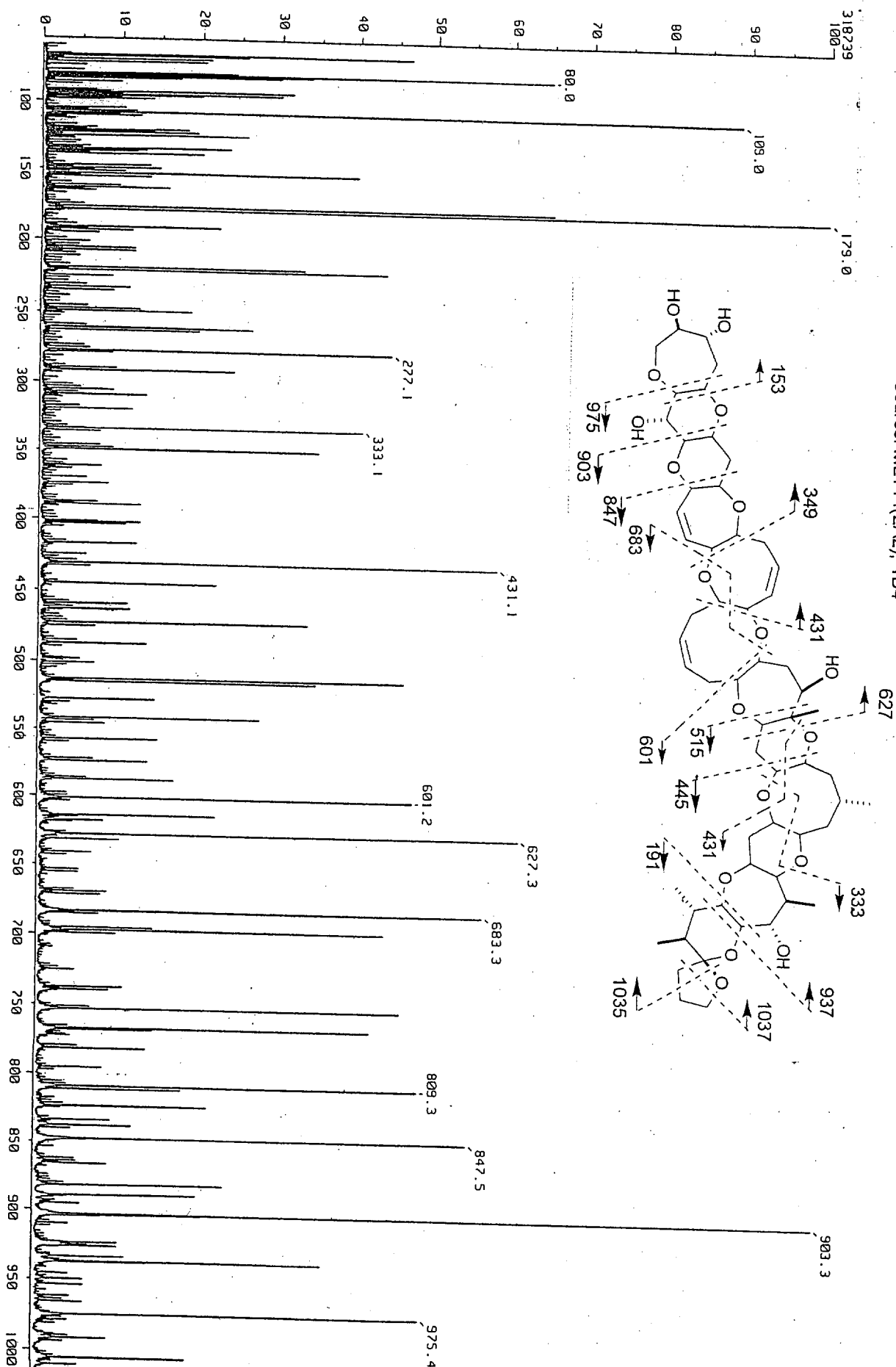


2.3-dihydroxy-CTX3C

[M+Na]⁺ = 1079

Rt = 7.80 min (ref. 7.66 min)

Source: MLT14(2A2), 1B4



[Mass Spectrum]
 Date : 1a8b
 Sample: CTX-1R0
 Note : Array Detector Data
 Inlet : Direct
 Spectrum Type : Product (m/z 1095.50, 3rd scan)
 RT : 0.00 min Scan# : 1
 BP : m/z 1093.5204 Ion : 28.86
 Output m/z range : 58.2979 to 1096.2780
 226968

Date : 28-Aug-98 15:36

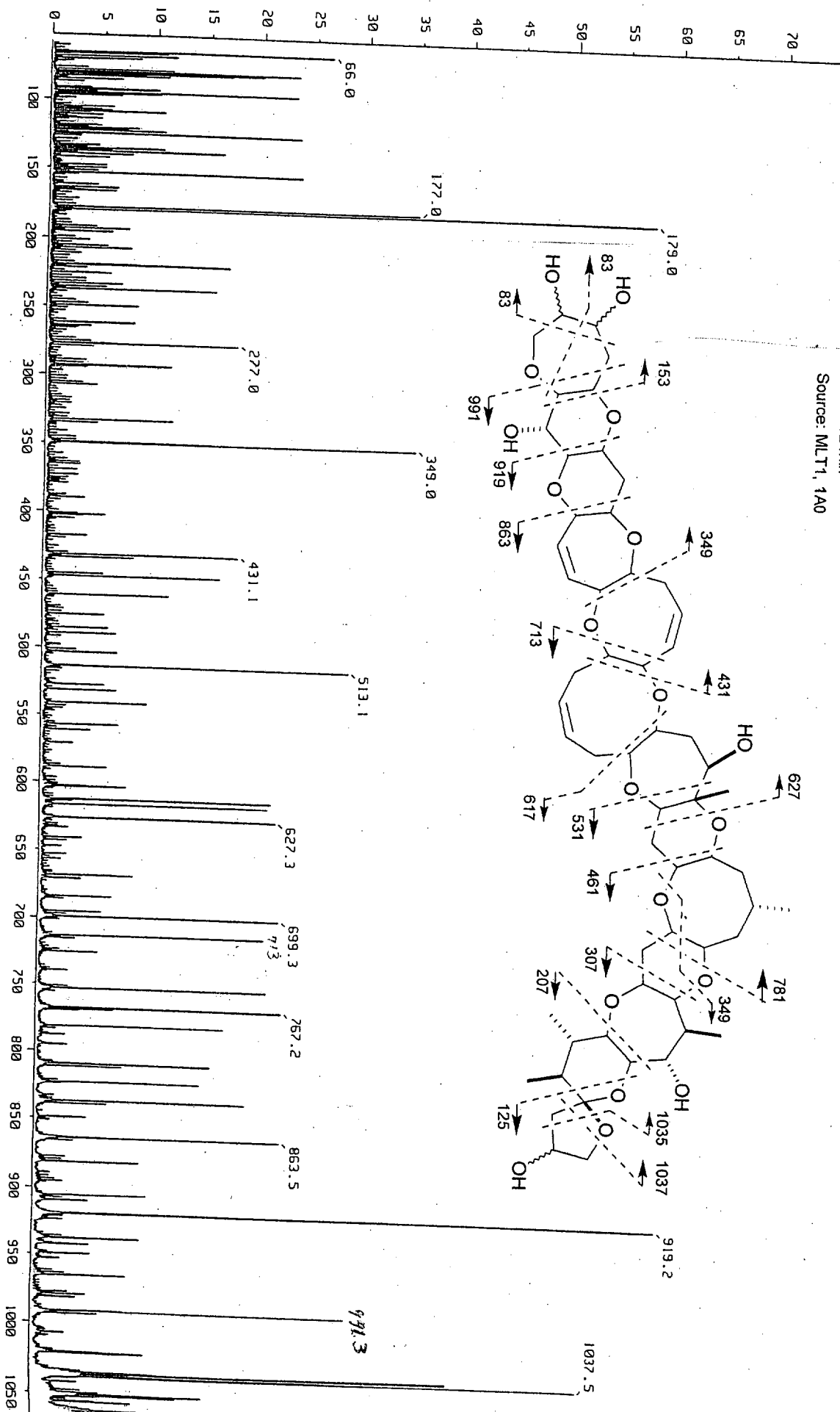
Ion Mode : FAB+

2,3,5,1-trihydroxy-CTX3C

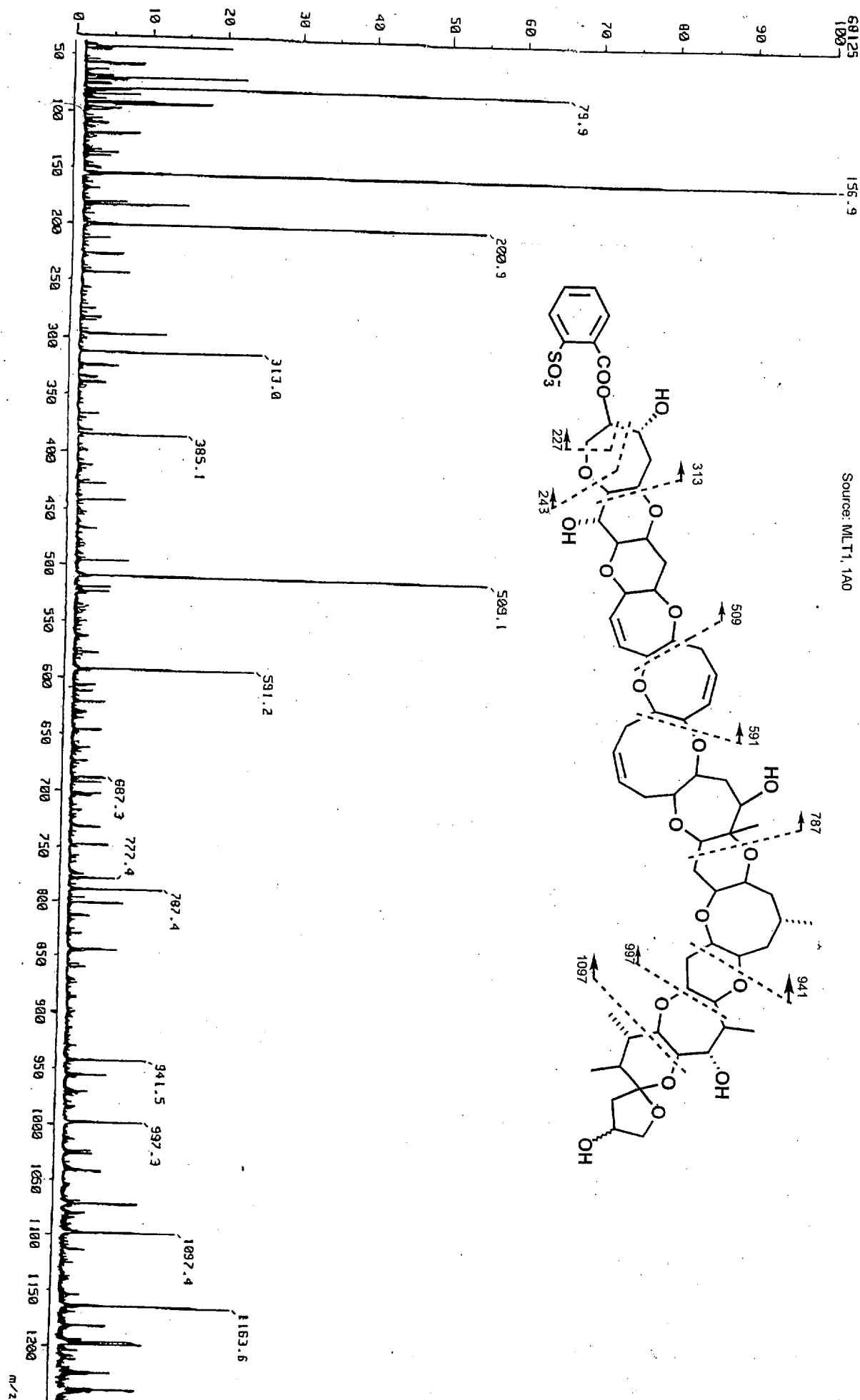
[M+Na]⁺ = 1095

Rt = 4.52 min

Source: MLT1, 1A0



2,3,5-trihydroxy-CTX3C-sulfobenzozite
 [M-H]⁻ = 1225
 Source: MLT1, 1A0



[Mass Spectrum]

Date : 1a4c
 Sample: CTX-1A4
 Note : Array Detector Data
 Inlet : Direct
 Spectrum Type : Product (m/z)
 RT : 0.00 min Scan#
 BP : m/z 1029.6907 Int.
 Output m/z range : 57.5138 to 111354

Date : 28-Aug-98 14:14

Ion Mode : ESI+

A-seco-51-hydroxy-CTX3C

[M+Na]⁺ = 1081

RT = 4.75 min

Source: 1A4

