

CHEM**BIO**CHEM

Supporting Information

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Supporting Information

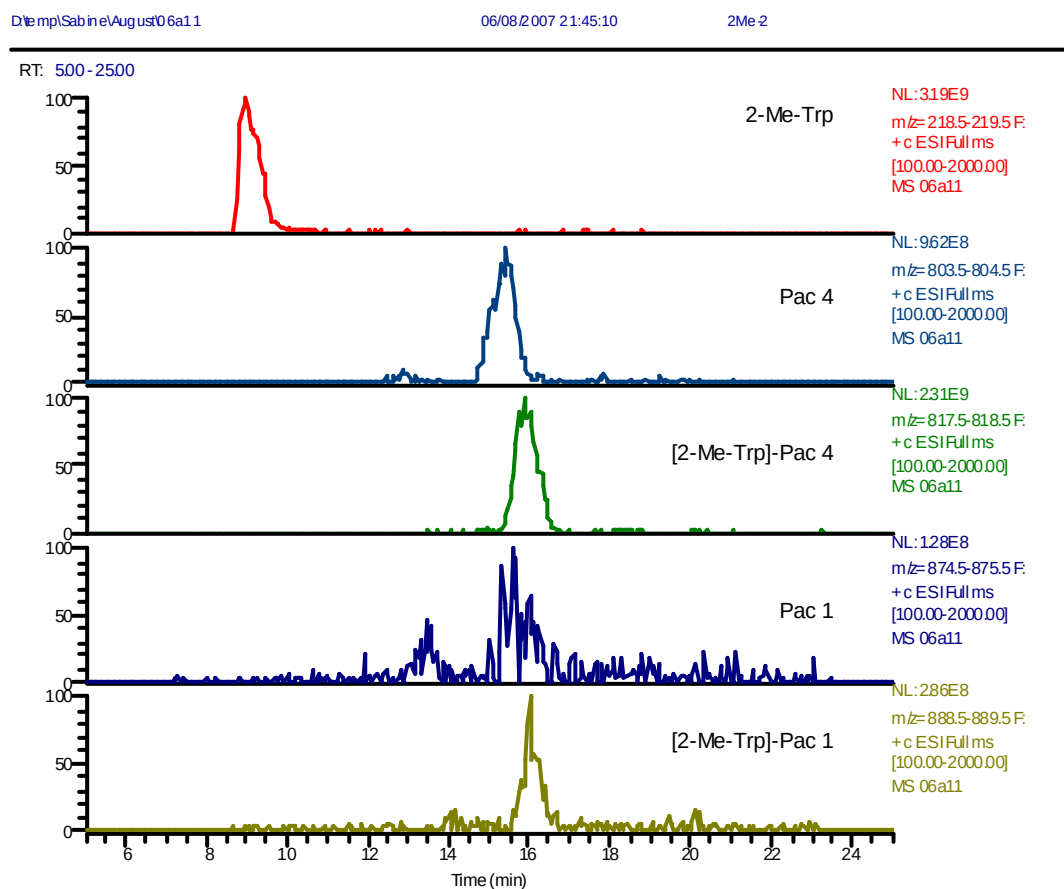
for

New Pacidamycin Antibiotics Through Precursor-Directed Biosynthesis

Sabine Gröschow, Emma J. Rackham, Benjamin Elkins, Philip L. A. Newill,
Lionel M. Hill, and Rebecca J. M. Goss*

Extracted ion chromatograms

Supplementation with 2-methyltryptophan

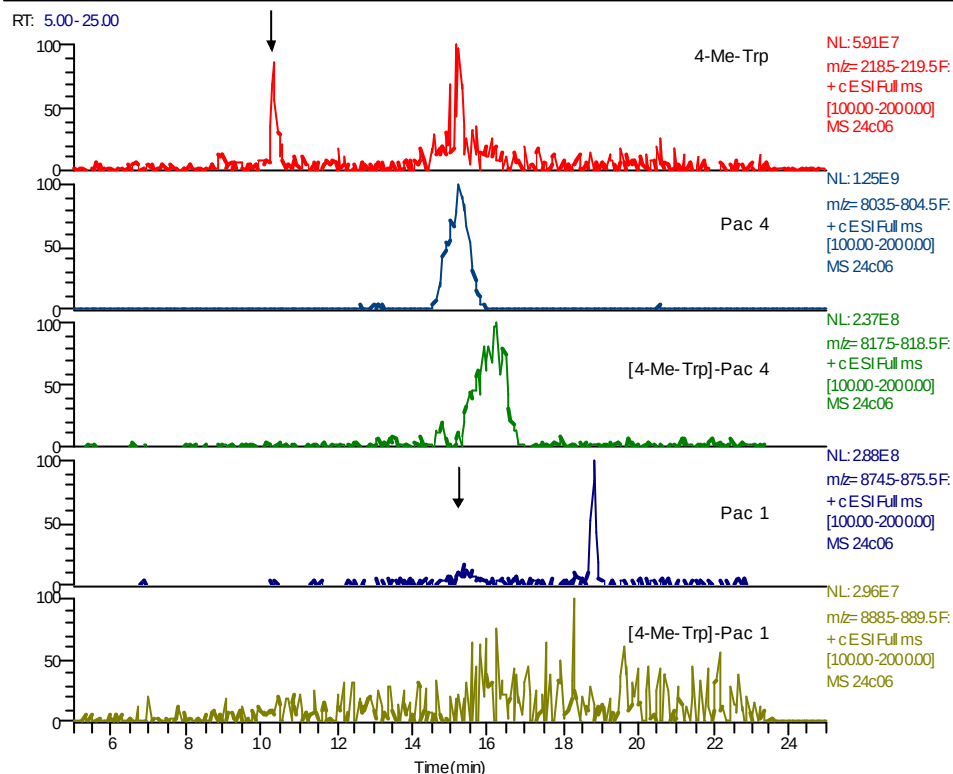


Supplementation with 4-methyltryptophan

D:\temp\Sabin e\Aug ust24 c06

24/08/2007 20:51:50

4Me-2

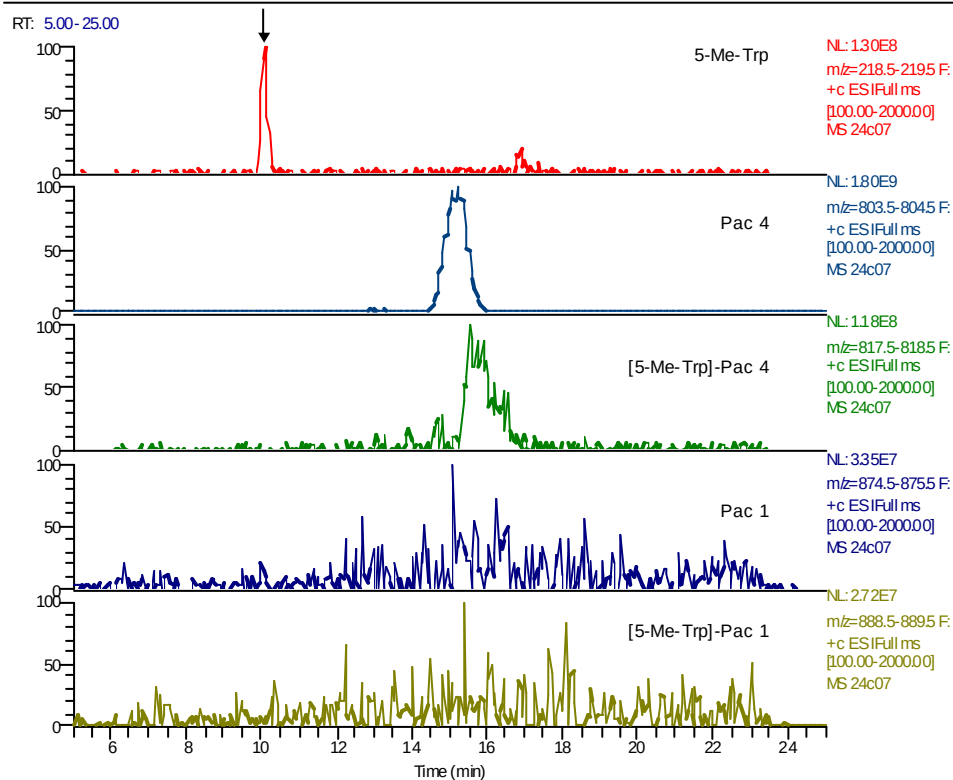


Supplementation with 5-methyltryptophan

D:\temp\Sabin e\August24c07

24/08/2007 21:24:06

5Me-1



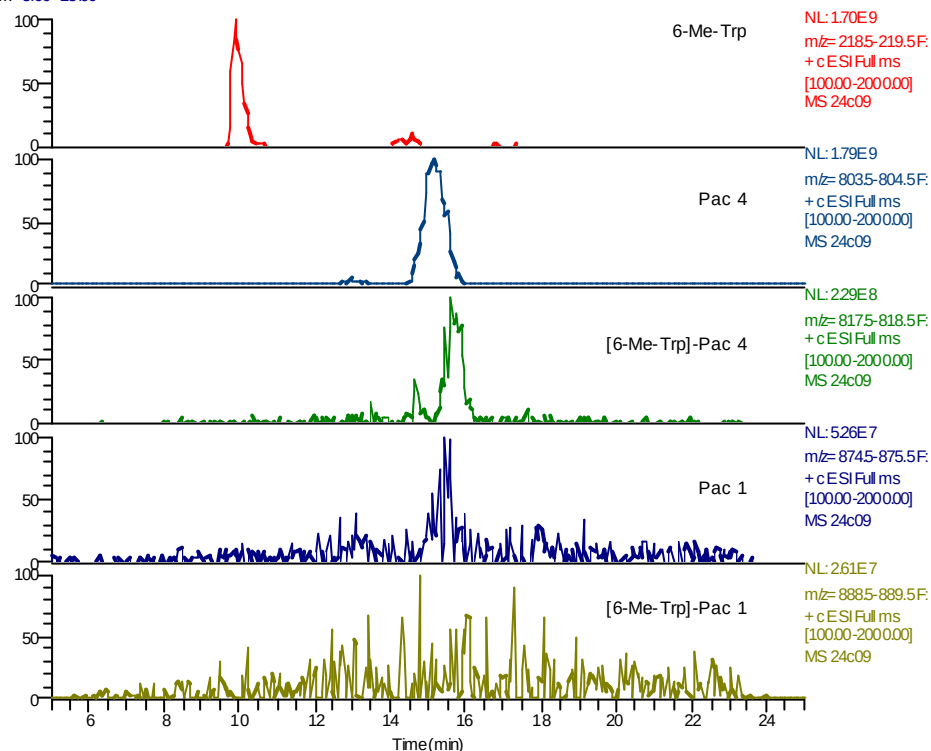
Supplementation with 6-methyltryptophan

D:\temp\Sabin e\Aug ust24 09

24/08/2007 22:28:55

6Me-1

RT: 5.00-25.00



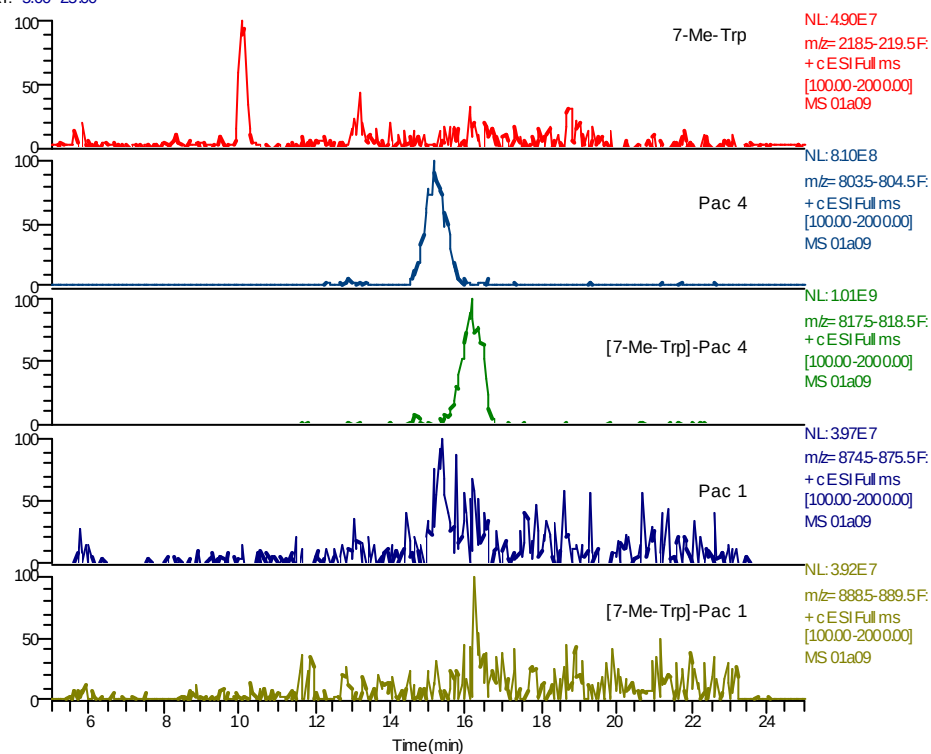
Supplementation with 7-methyltryptophan

D:\temp\Sabin e\01a 09

01/08/2007 22:25:47

7Me

RT: 5.00-25.00



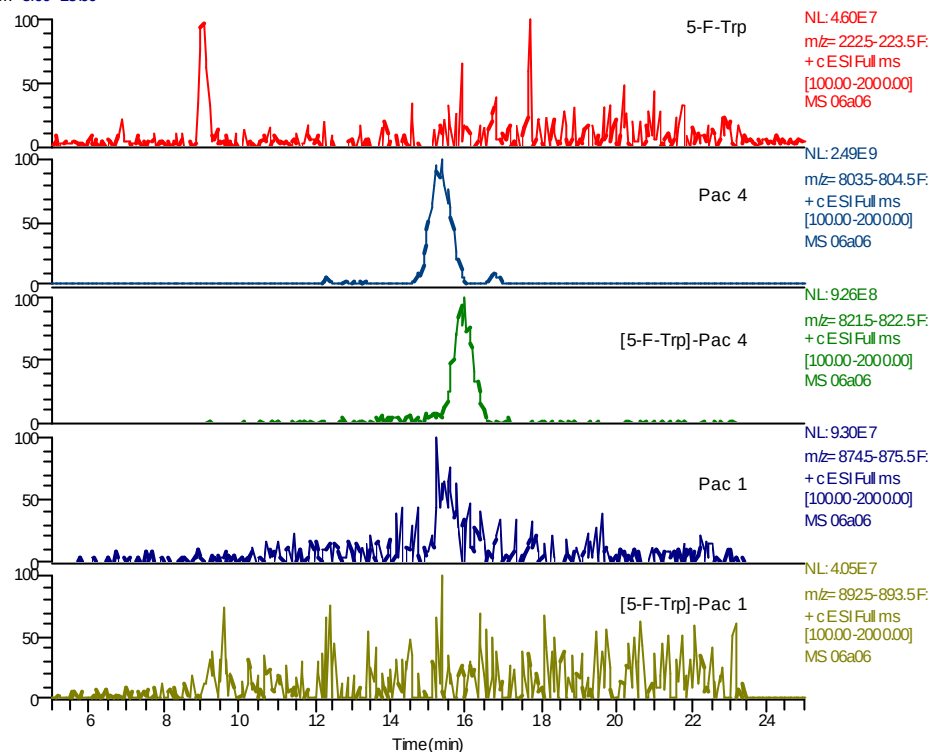
Supplementation with 5-fluorotryptophan

D:\temp\Sabin e\Aug ust06 a06

06/08/2007 19:03:24

5F-2

RT: 5.00-25.00



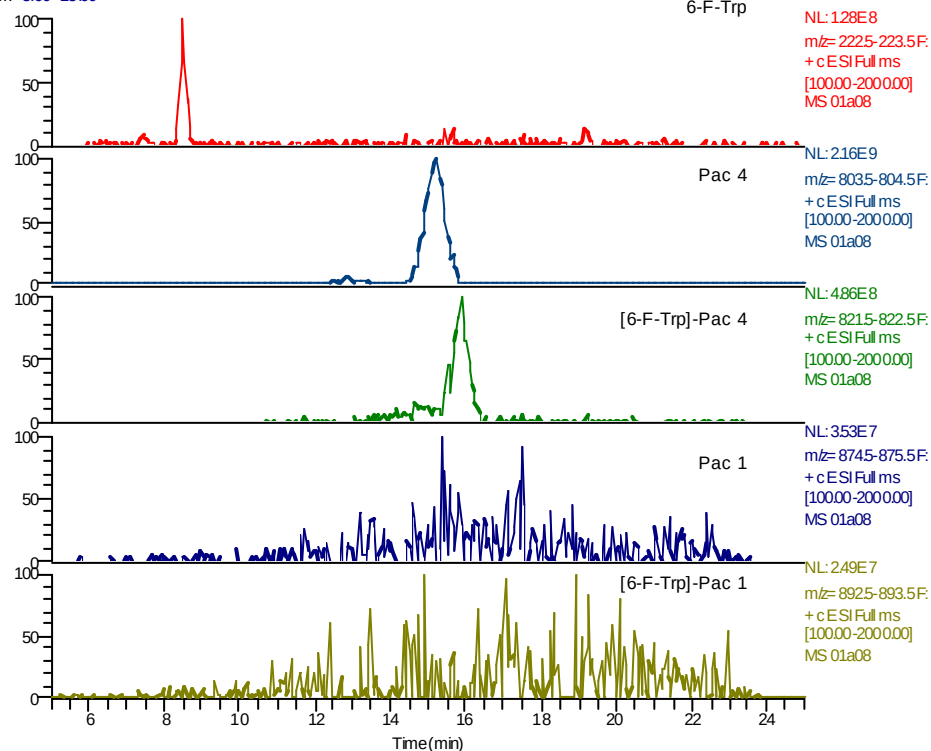
Supplementation with 6-fluorotryptophan

D:\temp\Sabin e\01a 08

01/08/2007 21:53:26

6F

RT: 5.00-25.00



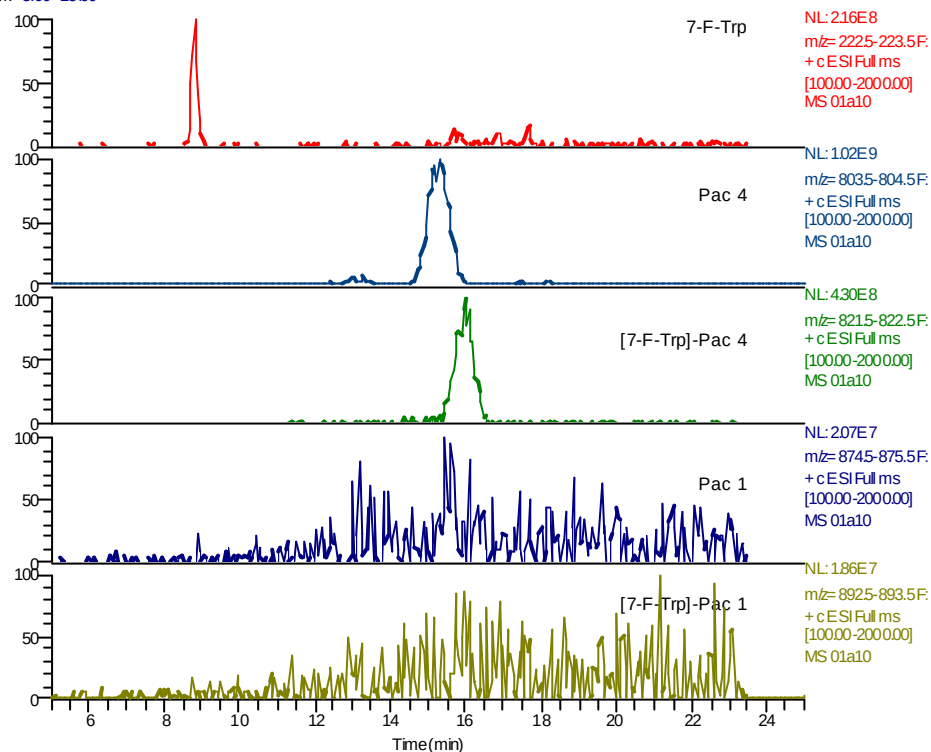
Supplementation with 7-fluorotryptophan

D:\temp\Sabin e01a 10

01/08/2007 22:58:12

7F

RT: 5.00-25.00



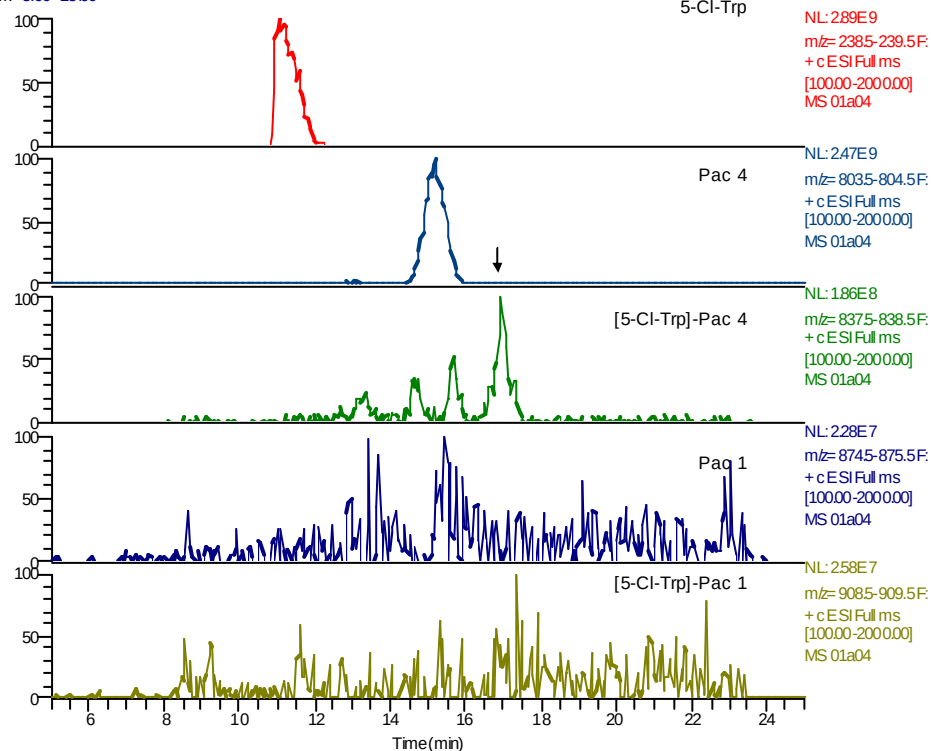
Supplementation with 5-chlorotryptophan

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01/08/2007 19:43:54

5CI

RT: 5.00-25.00



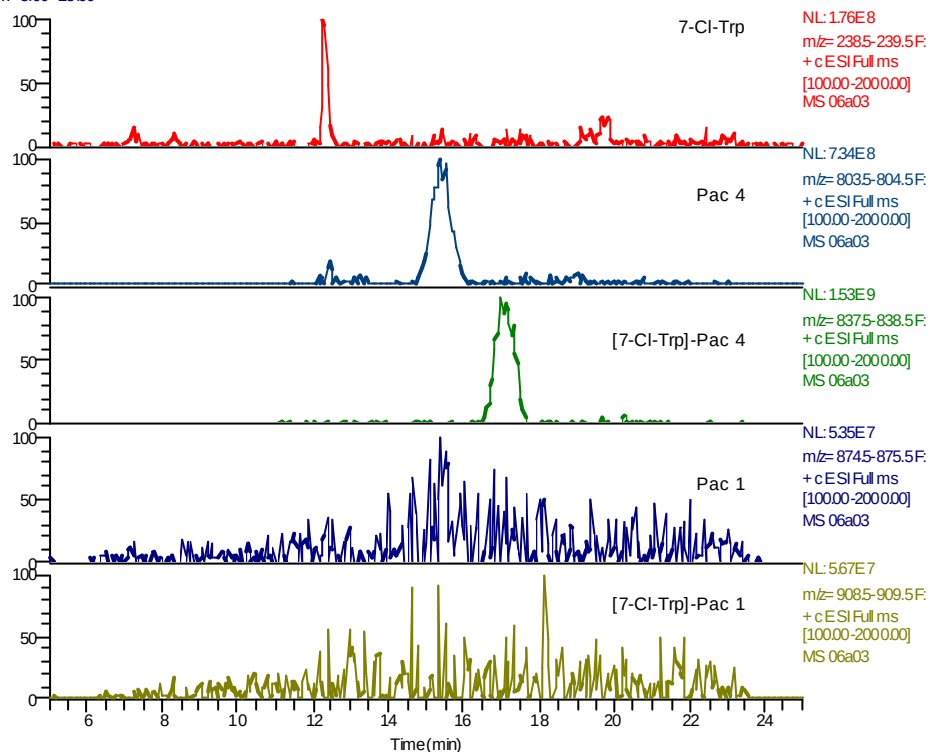
Supplementation with 7-chlorotryptophan

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7Cl2

RT: 5.00-25.00



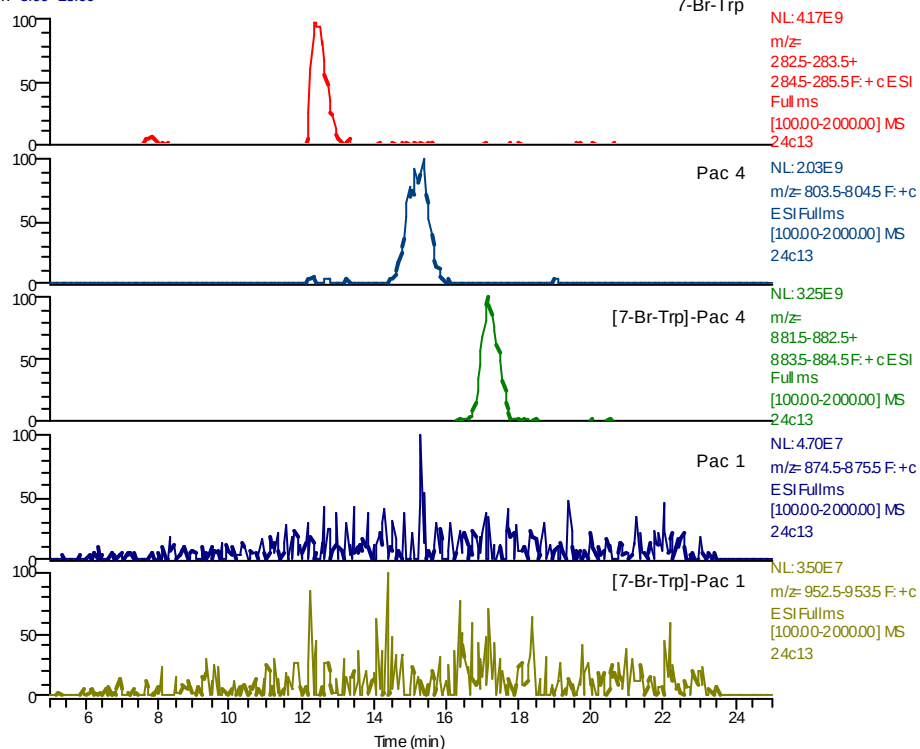
Supplementation with 7-bromotryptophan

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25/08/2007 00:37:59

7Br3

RT: 5.00-25.00



Mass spectra and MS/MS analysis

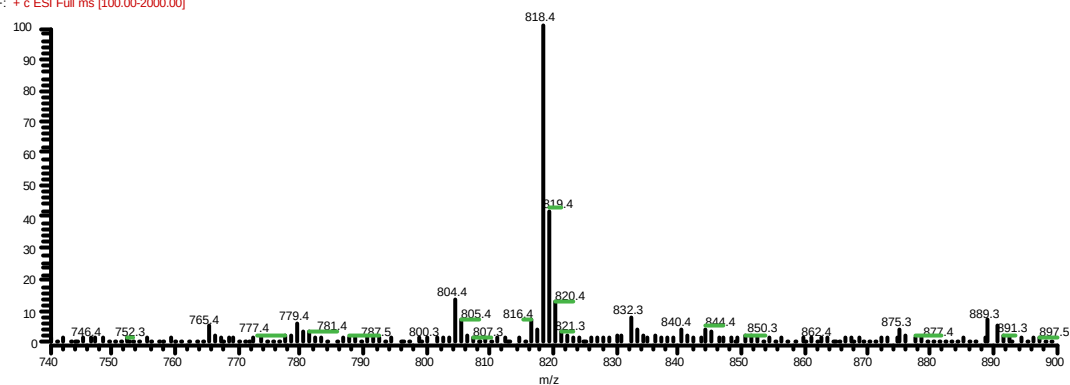
[2-Me-Trp]-pacidamycin 4

D:\templSabine\August06a11

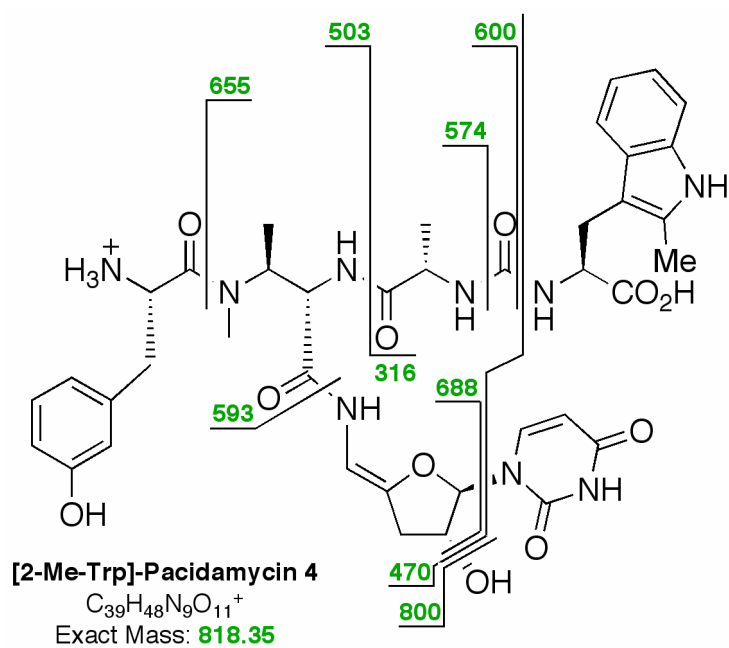
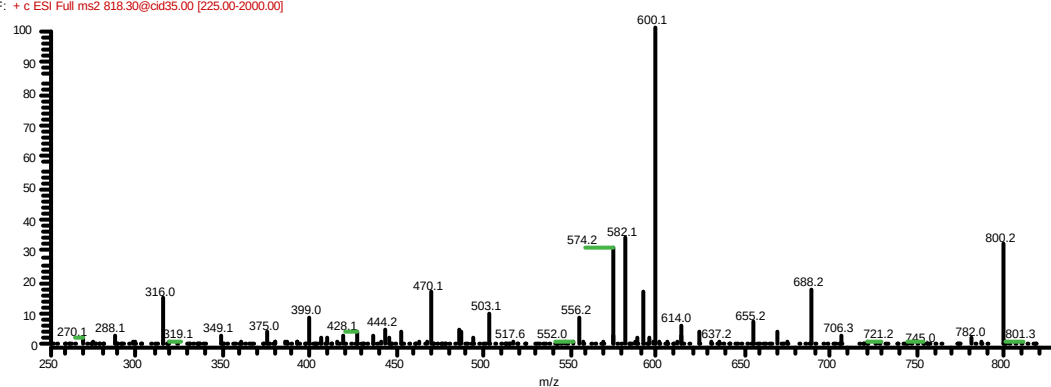
06/08/2007 21:45:10

2Me-2

06a11 #1308-1358 RT: 15.59-16.16 AV: 13 NL: 1.72E9
F: + c ESI Full ms [100.00-2000.00]



06a11 #1290-1395 RT: 15.37-16.60 AV: 14 NL: 2.08E7
F: + c ESI Full ms2 818.30@cid35.00 [225.00-2000.00]



[2-Me-Trp]-pacidamycin 1

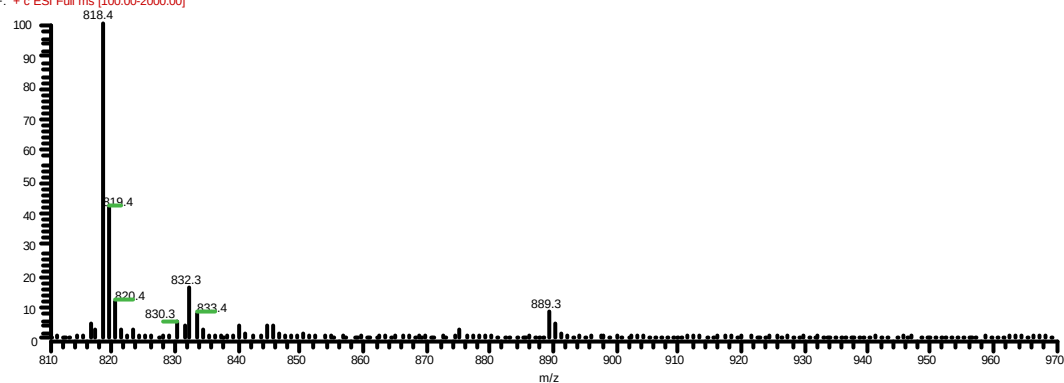
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2Me-2

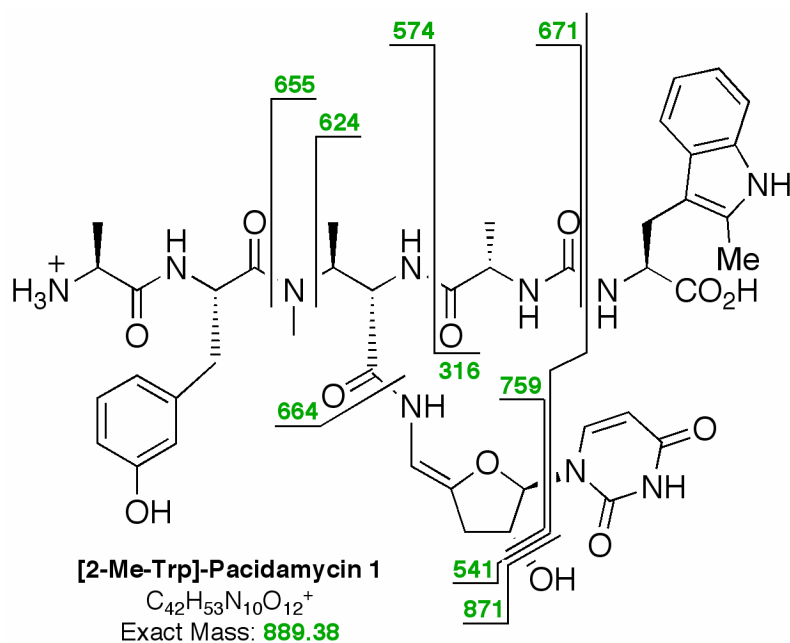
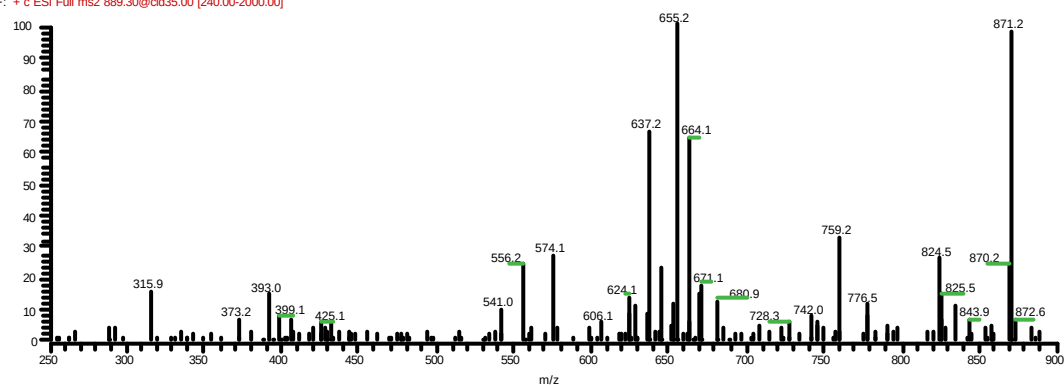
06a11 # 1320-1369 RT: 15.74-16.31 AV: 13 NL: 1.68E9

F: + c ESI Full ms [100.00-2000.00]

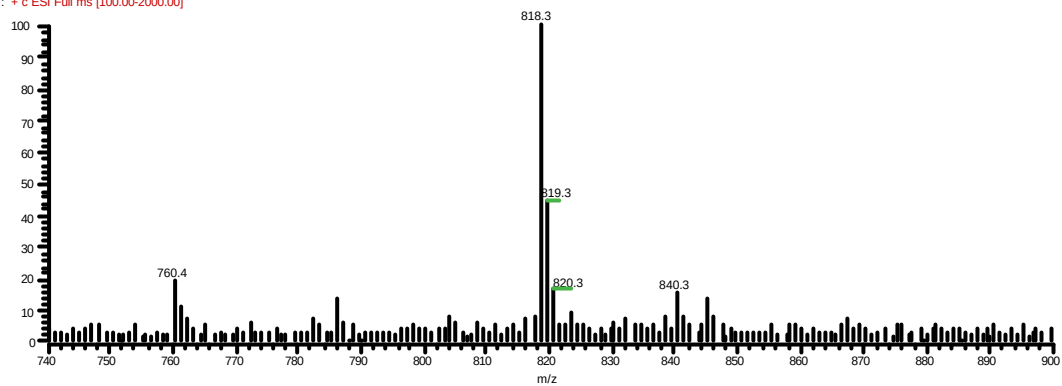


06a11 # 1349-1372 RT: 16.15-16.34 AV: 3 NL: 4.19E6

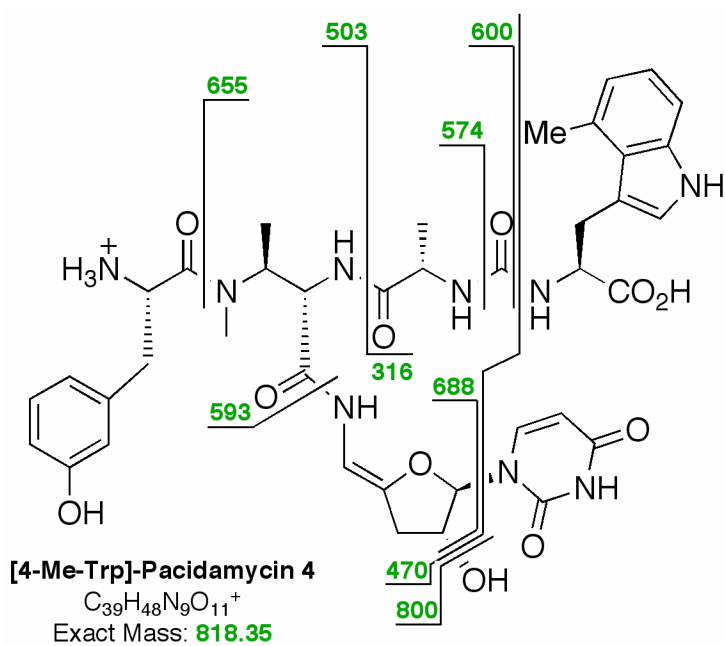
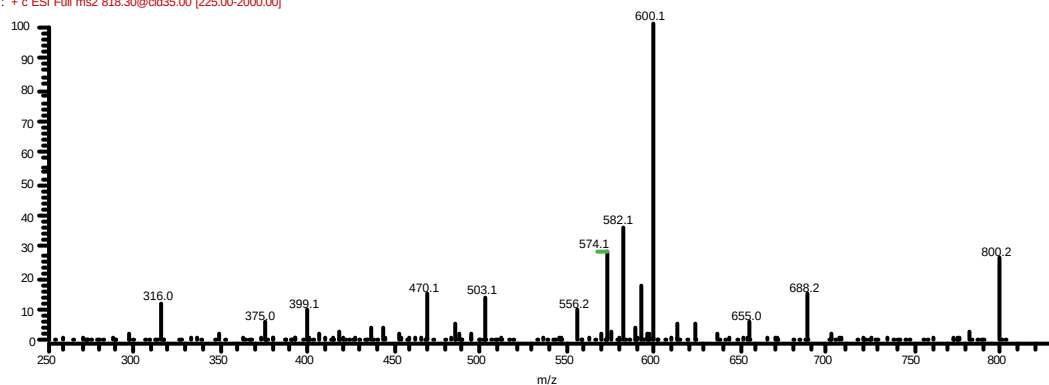
F: + c ESI Full ms2 889.30@cid35.00 [240.00-2000.00]



24c06 #1320-1373 RT: 15.85-16.47 AV: 14 NL: 1.74E8
F: + c ESI Full ms [100.00-2000.00]



24c06 #1331-1378 RT: 16.05-16.53 AV: 6 NL: 3.48E7
F: + c ESI Full ms2 818.30@cid35.00 [225.00-2000.00]



[4-Me-Trp]-pacidamycin 4

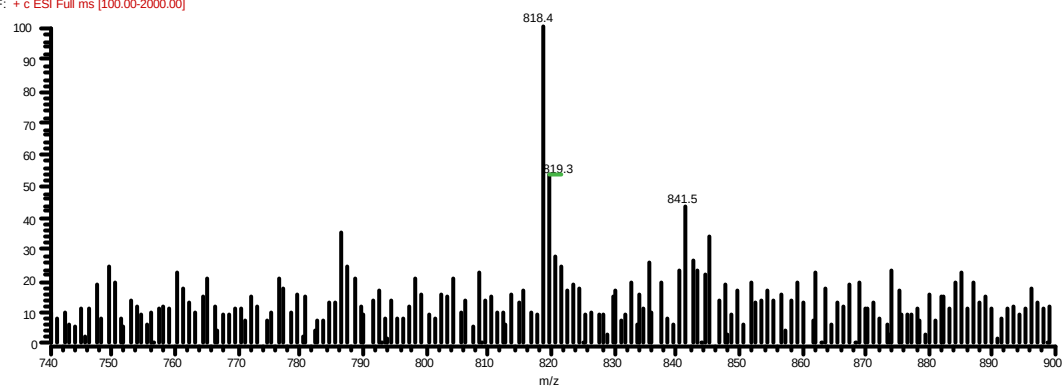
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D:\temp\Sabine\August\24\c07

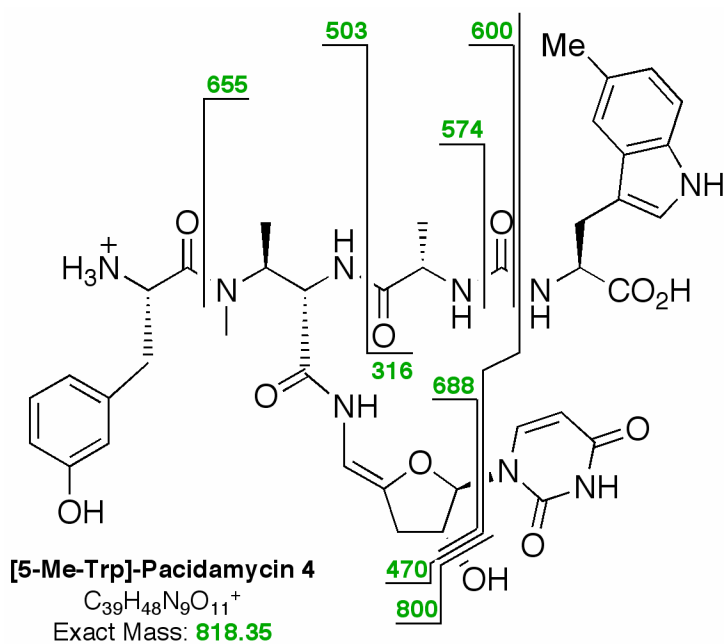
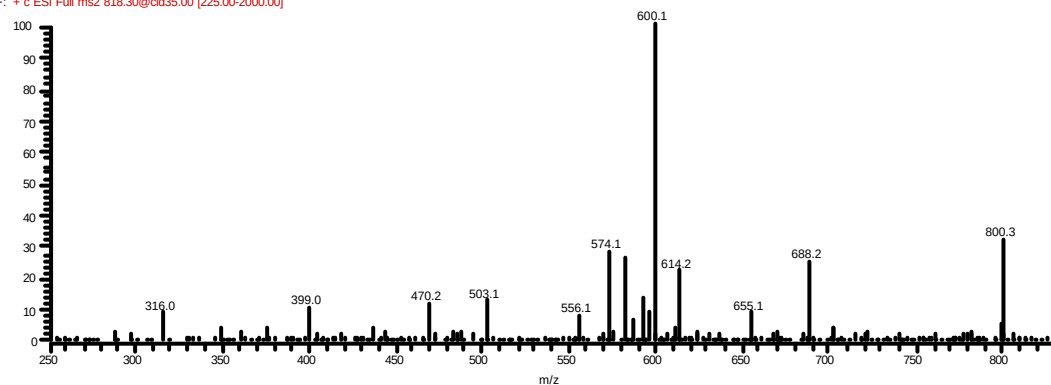
24/08/2007 21:24:06

5Me-1

24c07 #1332-1384 RT: 16.02-16.60 AV: 13 NL: 4.05E7
F: + c ESI Full ms [100.00-2000.00]



24c07 #1332-1395 RT: 16.08-16.76 AV: 8 NL: 5.24E6
F: + c ESI Full ms2 818.30@cid35.00 [225.00-2000.00]



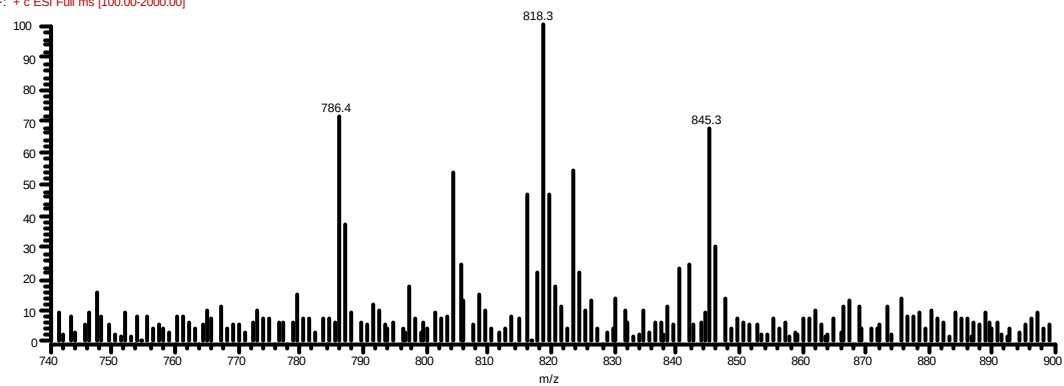
[6-Me-Trp]-pacidamycin 4

D:\temp\Sabine\August\24\09

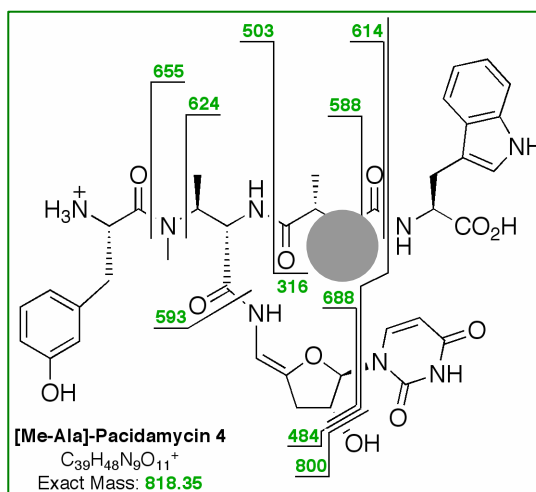
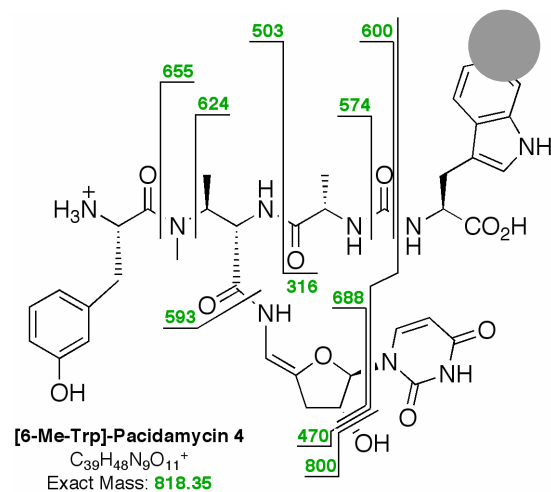
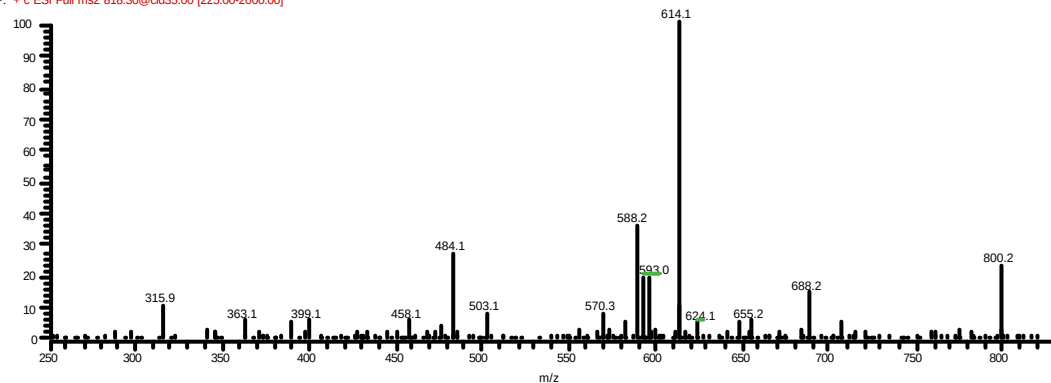
24.08/2007 22:28:55

6 Me-1

24c09 #1317-1341 RT: 15.81-16.10 AV: 7 NL: 9.10E7
F: + c ESI Full ms [100.00-2000.00]



24c09 #1330-1354 RT: 15.97-16.27 AV: 4 NL: 9.47E6
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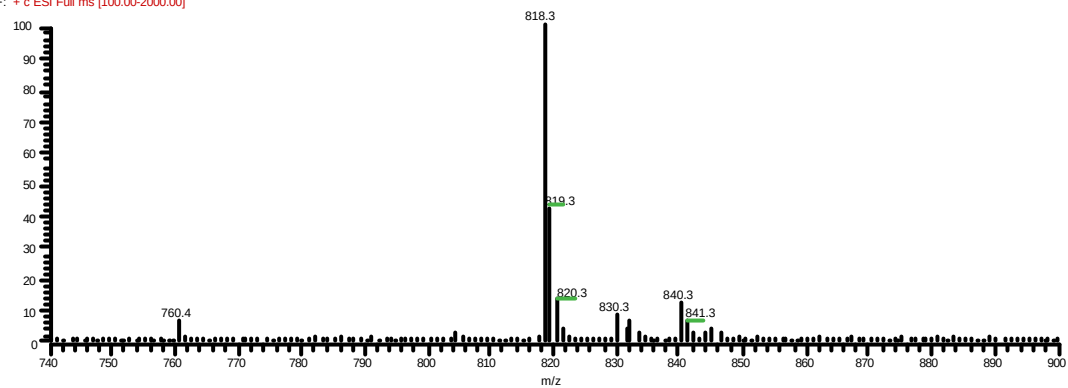
[7-Me-Trp]-pacidamycin 4

D:\temp\Sabine\01a09

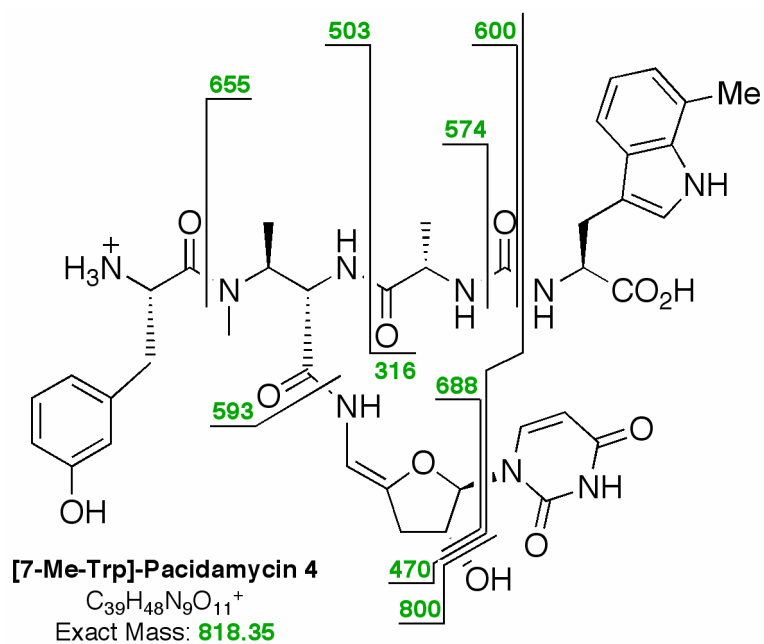
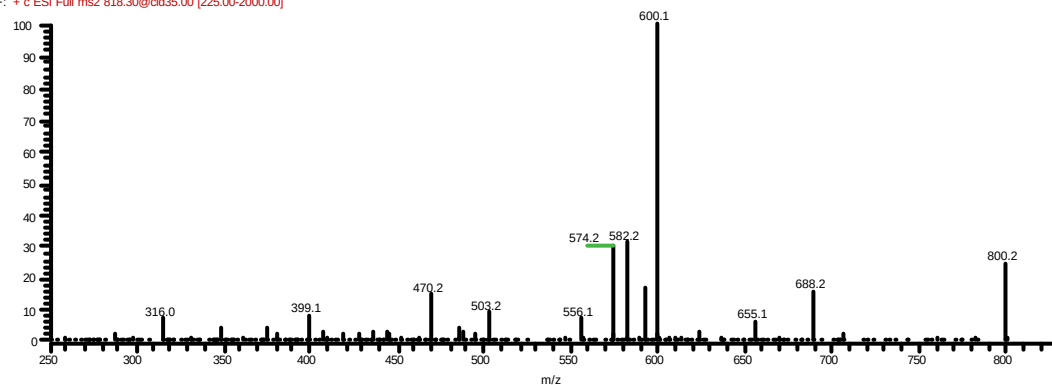
01.08/2007 22:25:47

7Me

01a09 #1337-1386 RT: 15.94-16.50 AV: 13 NL: 7.34E8
F: + c ESI Full ms [100.00-2000.00]



01a09 #1340-1394 RT: 16.05-16.61 AV: 7 NL: 9.70E7
F: + c ESI Full ms2 818.30@cid35.00 [225.00-2000.00]



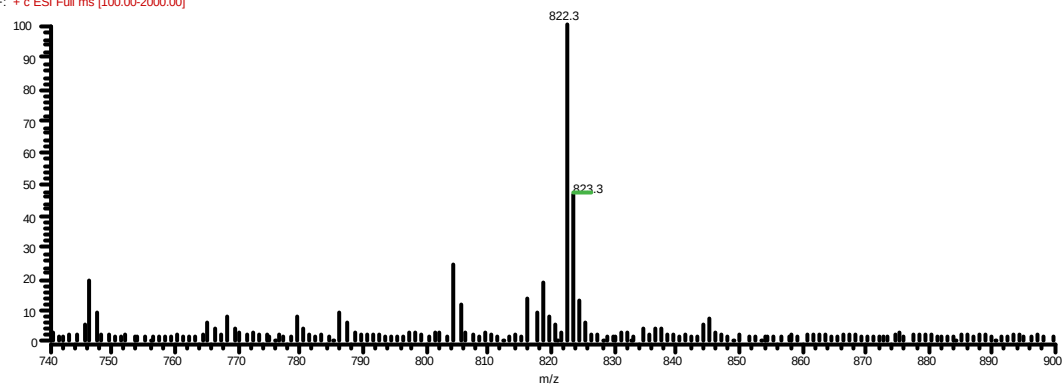
[5-F-Trp]-pacidamycin 4

D:\temp\Sabine\August\06a06

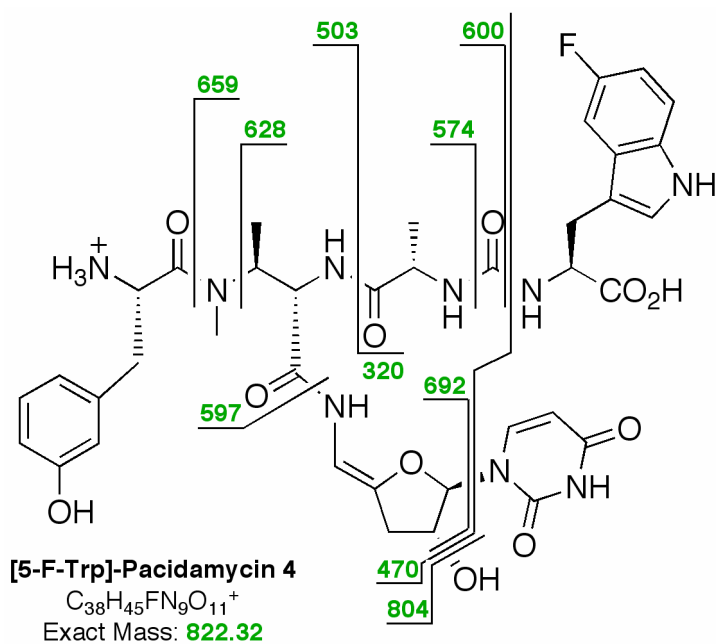
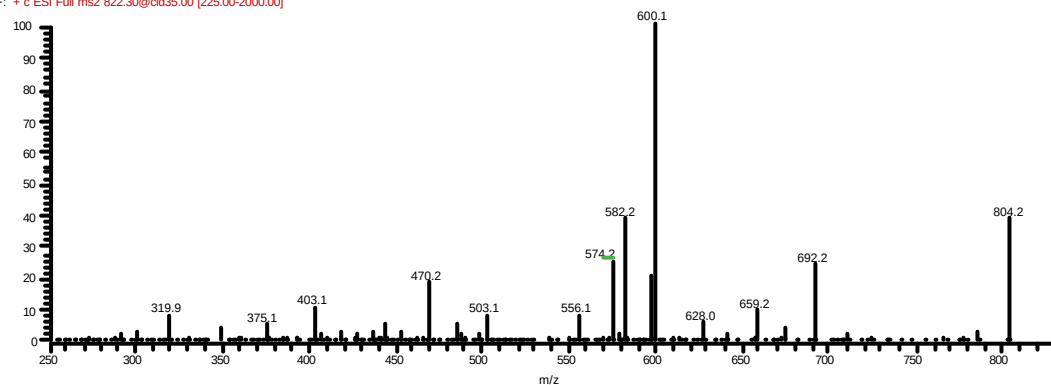
06/08/2007 19:03:24

5F2

06a06 #1320-1358 RT: 15.77-16.19 AV: 10 NL: 7.14E8
F: + c ESI Full ms [100.00-2000.00]



06a06 #1305-1352 RT: 15.60-16.06 AV: 6 NL: 8.45E7
F: + c ESI Full ms2 822.30@cid35.00 [225.00-2000.00]



[6-F-Trp]-pacidamycin 4

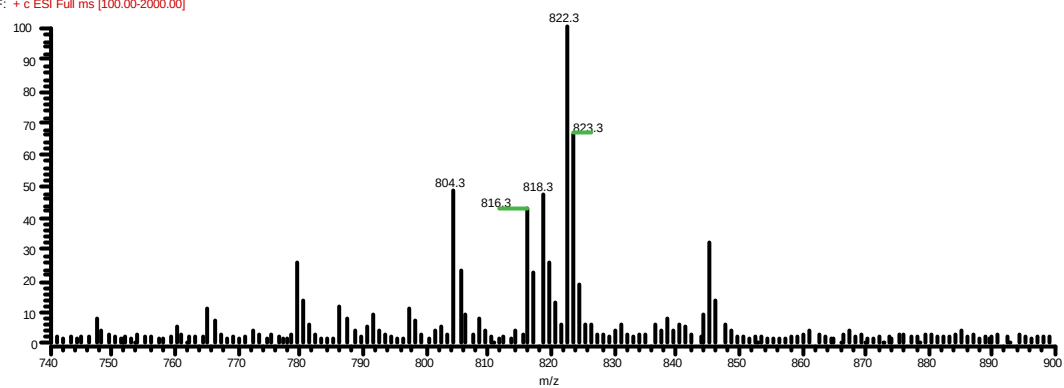
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6F

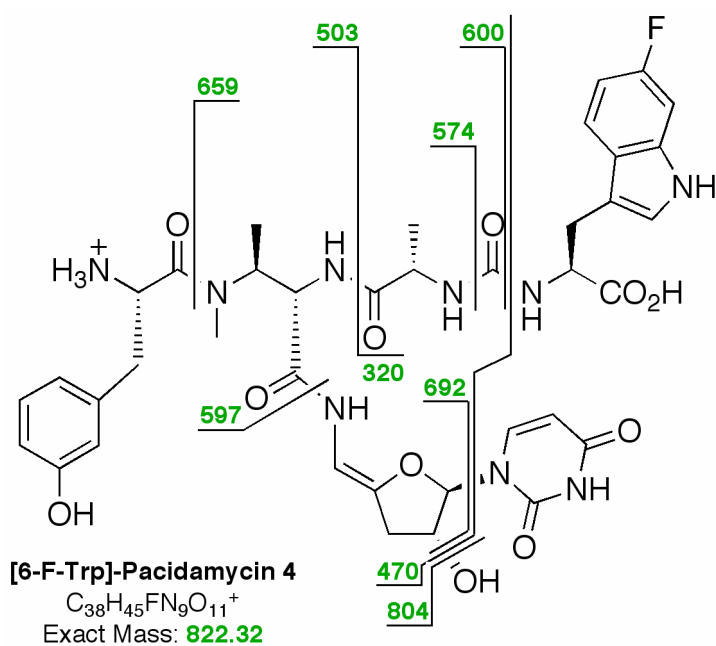
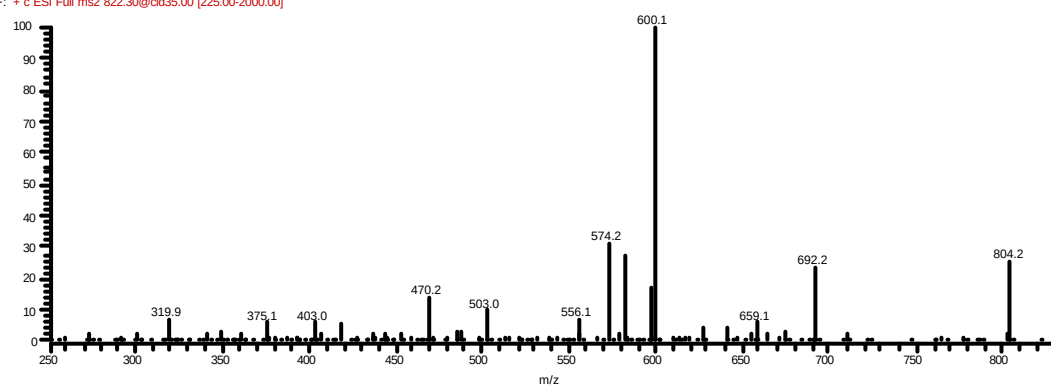
01a08 #1293-1337 RT: 15.61-16.13 AV: 12 NL: 3.12E8

F: + c ESI Full ms [100.00-2000.00]



01a08 #1290-1337 RT: 15.58-16.06 AV: 6 NL: 5.60E7

F: + c ESI Full ms2 822.30@cid35.00 [225.00-2000.00]



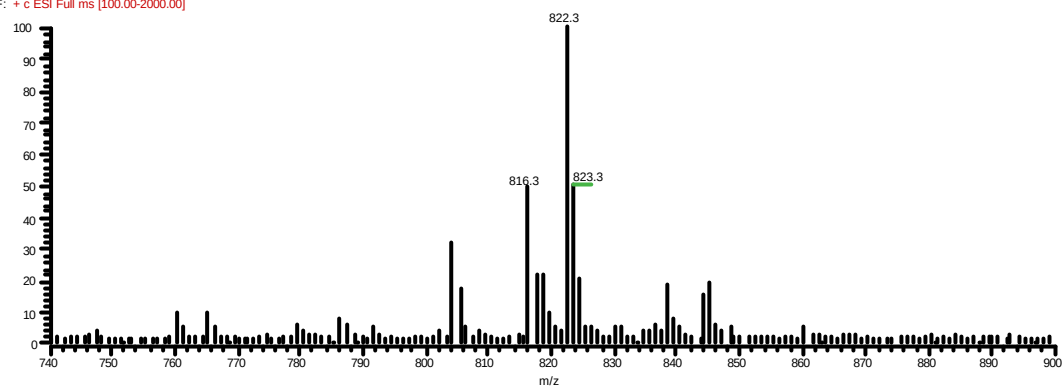
[7-F-Trp]-pacidamycin 4

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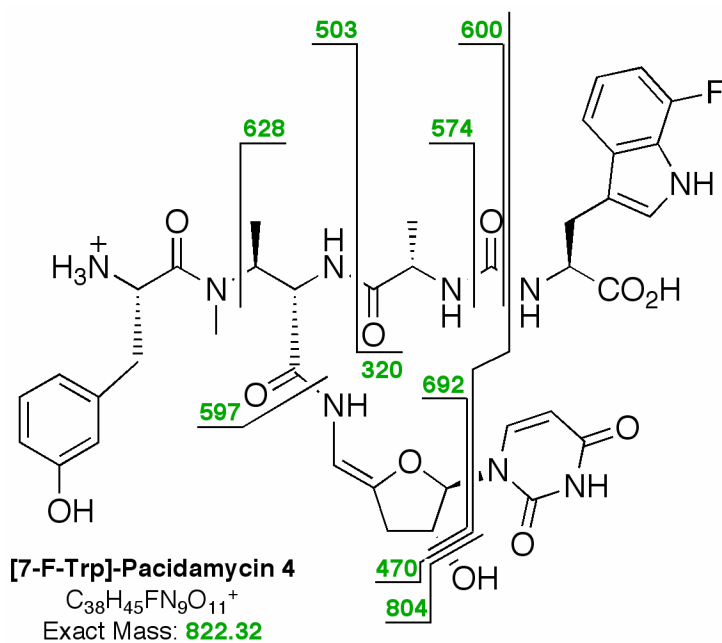
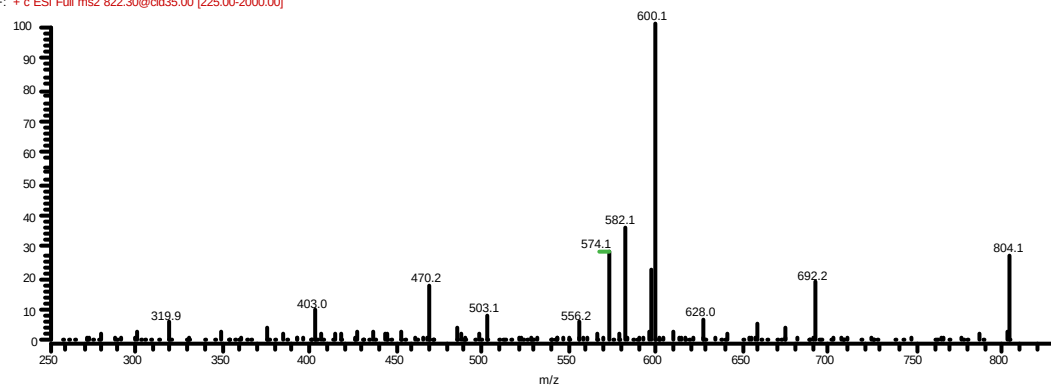
01/08/2007 22:58:12

7F

01a10 # 1312-1363 RT: 15.67-16.25 AV: 13 NL: 3.03E8
F: + c ESI Full ms [100.00-2000.00]



01a10 # 1309-1363 RT: 15.68-16.26 AV: 7 NL: 5.16E7
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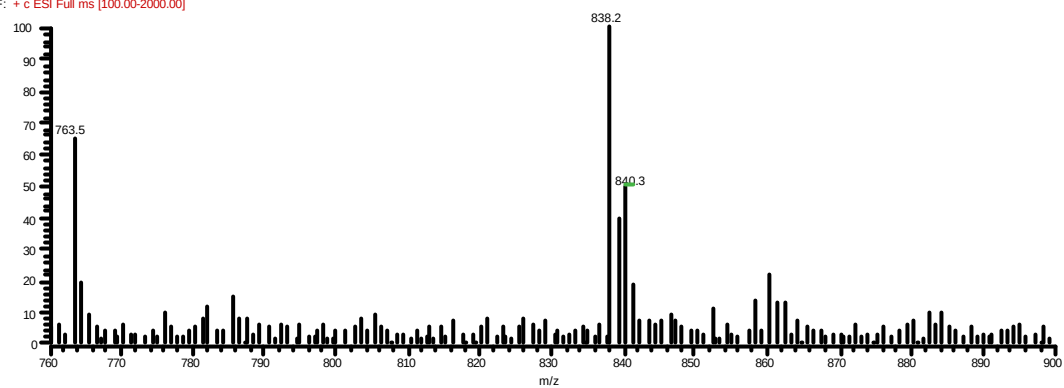
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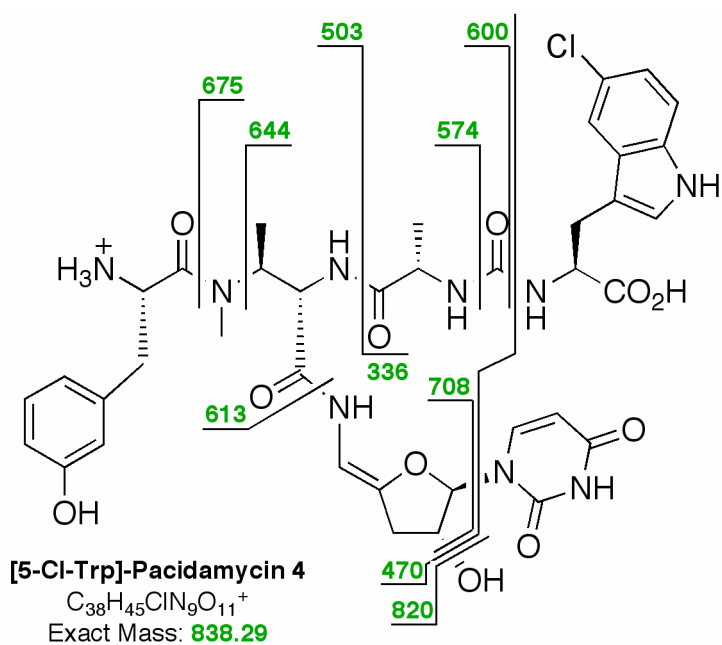
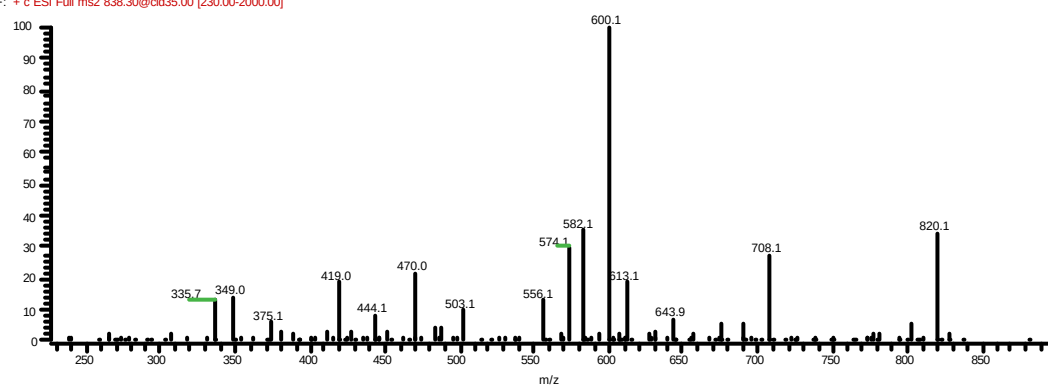
01/08/2007 19:43:54

50

01a04 #1405-1439 RT: 16.75-17.13 AV: 9 NL: 1.10E8
F: + c ESI Full ms [100.00-2000.00]



01a04 #1399-1445 RT: 16.72-17.20 AV: 6 NL: 1.34E7
F: + c ESI Full ms2 838.30@cid35.00 [230.00-2000.00]



[7-Cl-Trp]-pacidamycin 4

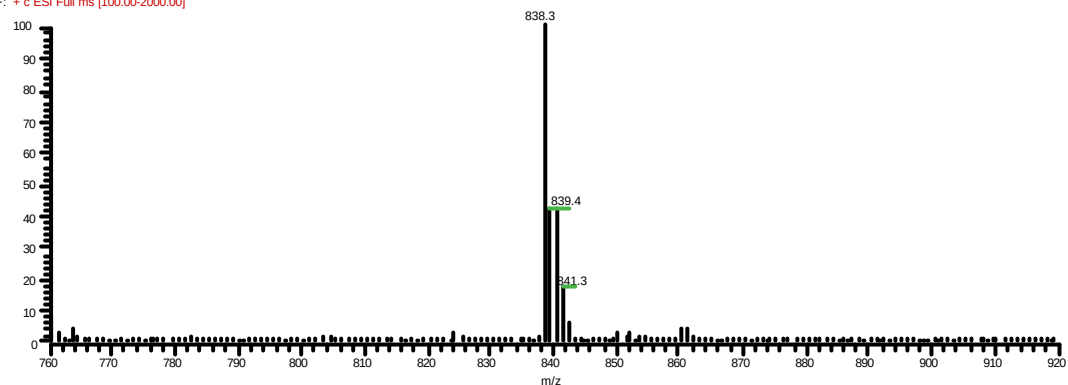
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06/08/2007 17 26:14

7Cl-2

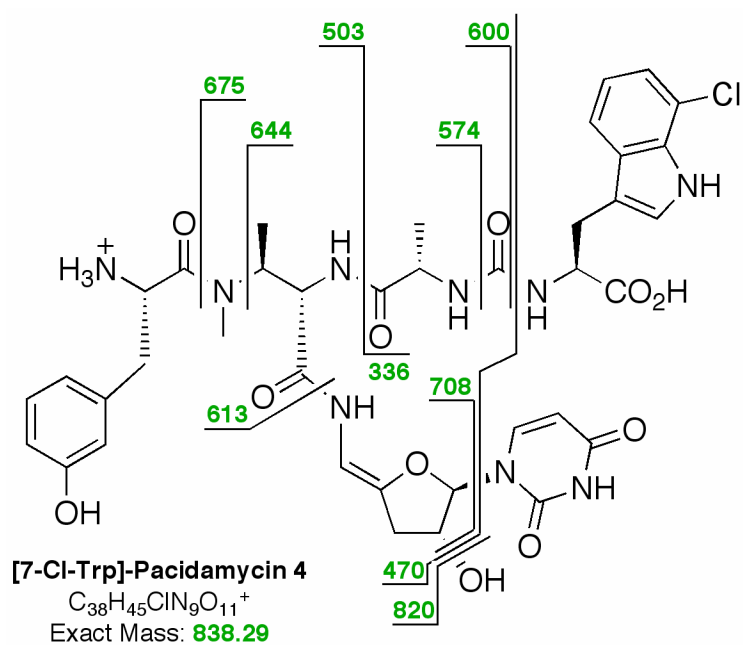
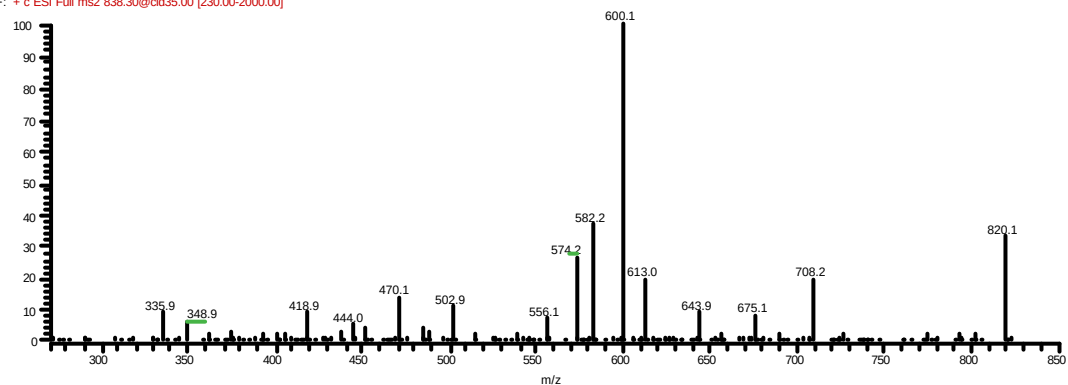
06a03 #1406-1459 RT: 16.81-17.37 AV: 13 NL: 1.22E9

F: + c ESI Full ms [100.00-2000.00]



06a03 #1389-1479 RT: 16.65-17.59 AV: 11 NL: 1.65E7

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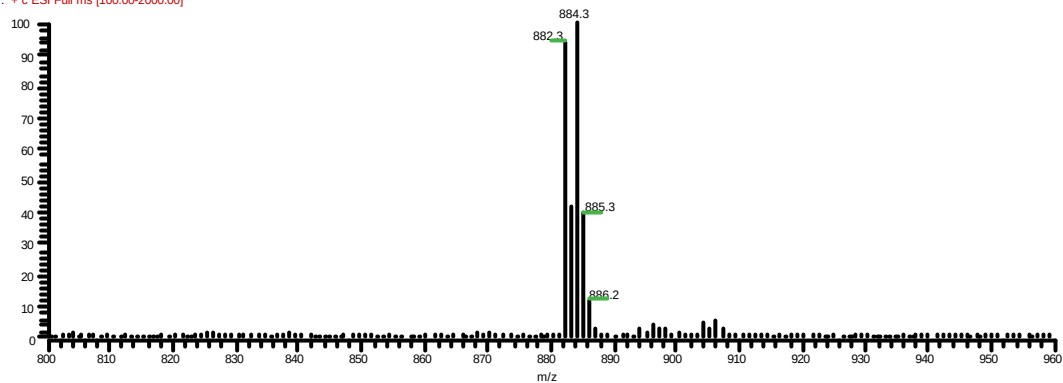
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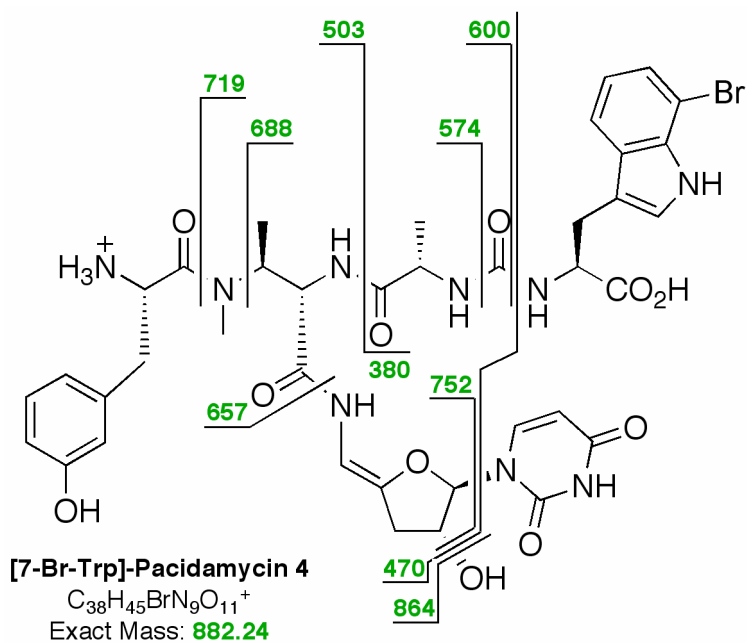
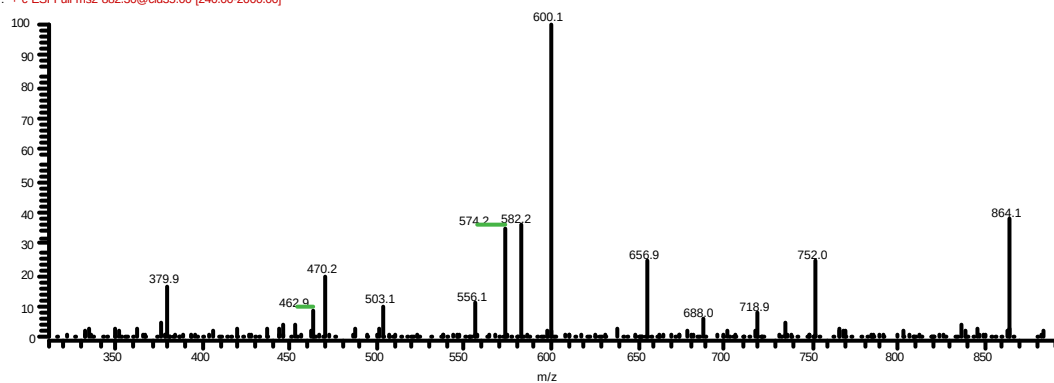
25/08/2007 00:37:59

7Br3

24c13 #1407-1467 RT: 16.84-17.51 AV: 15 NL: 1.11E9
F: + c ESI Full ms [100.00-2000.00]



24c13 #1387-1499 RT: 16.67-17.91 AV: 14 NL: 5.53E6
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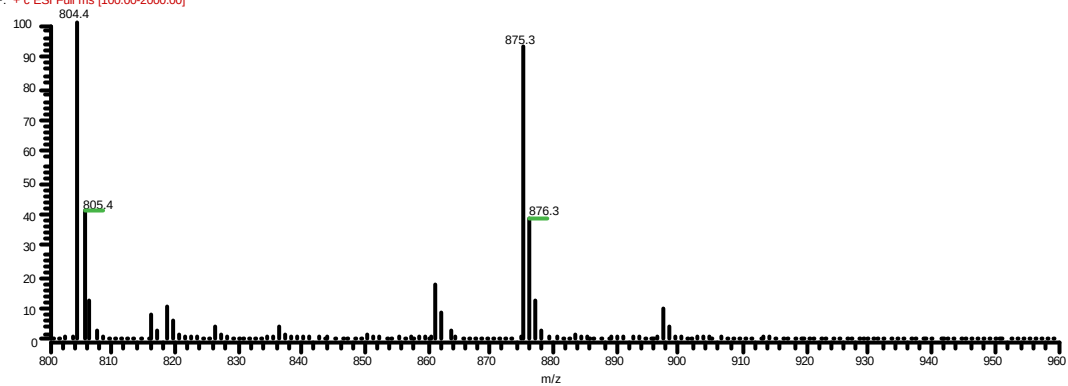
Pacidamycin 1

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26.04/2007 20 36:18

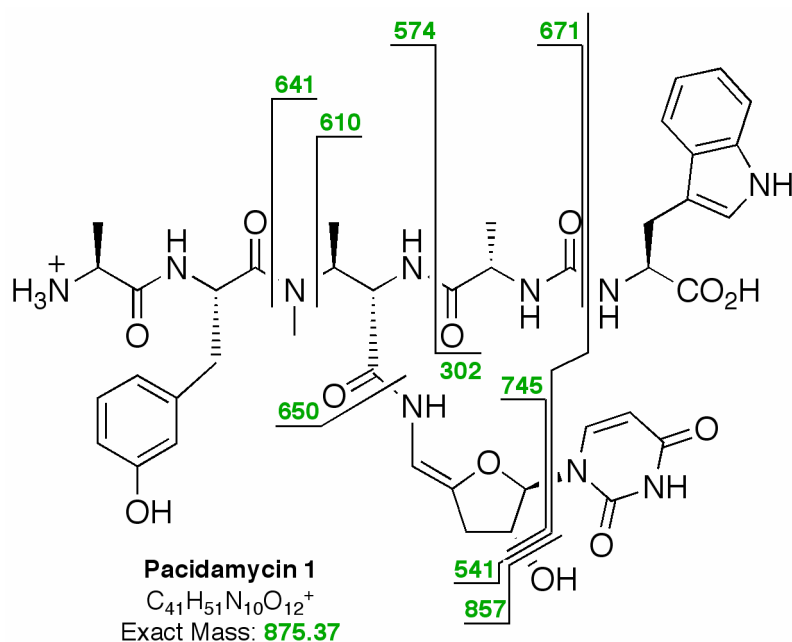
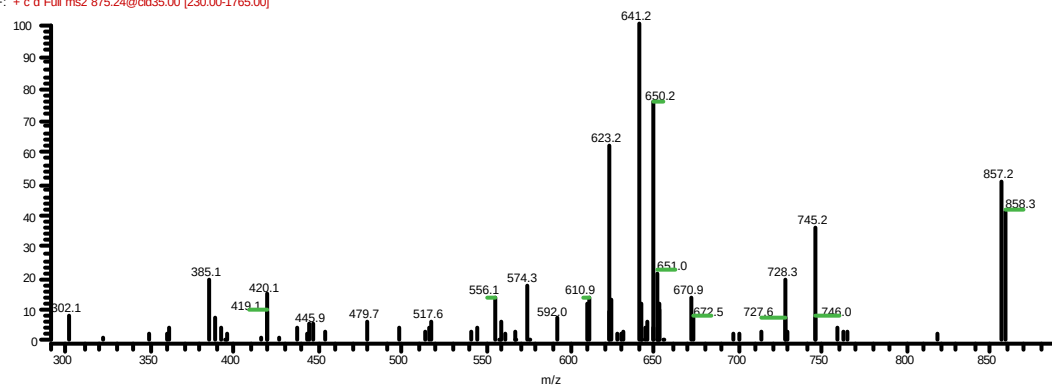
26c04 #846-895 RT: 11.12-11.77 AV: 17 NL: 4.96E8

F: + c ESI Full ms [100.00-2000.00]



26c04 #862 RT: 11.35 AV: 1 NL: 2.54E7

F: + c d Full ms2 875.24@cid35.00 [230.00-1765.00]

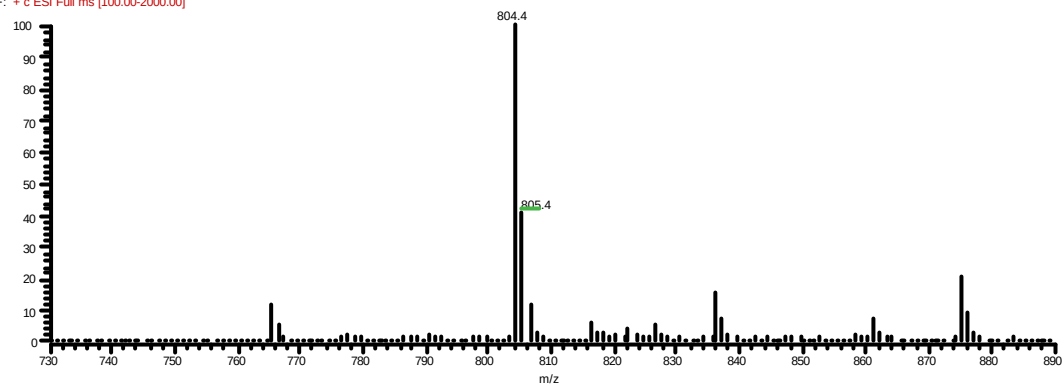


Pacidamycin 4

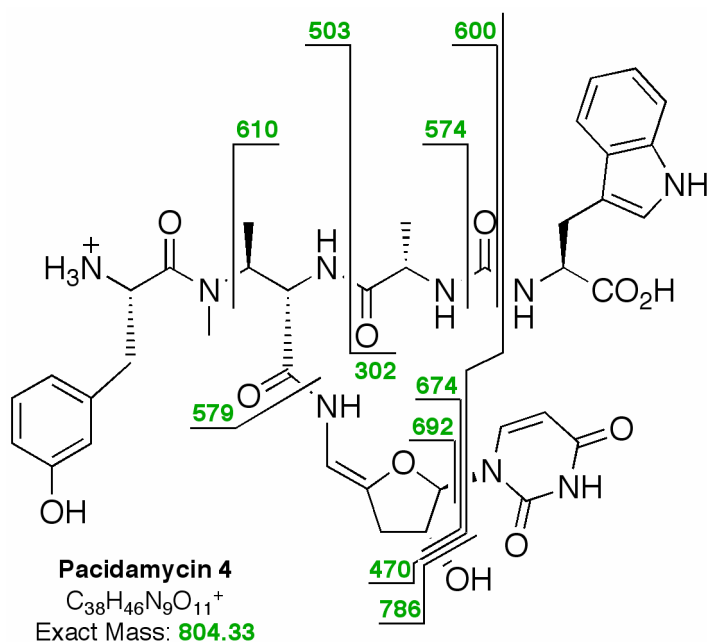
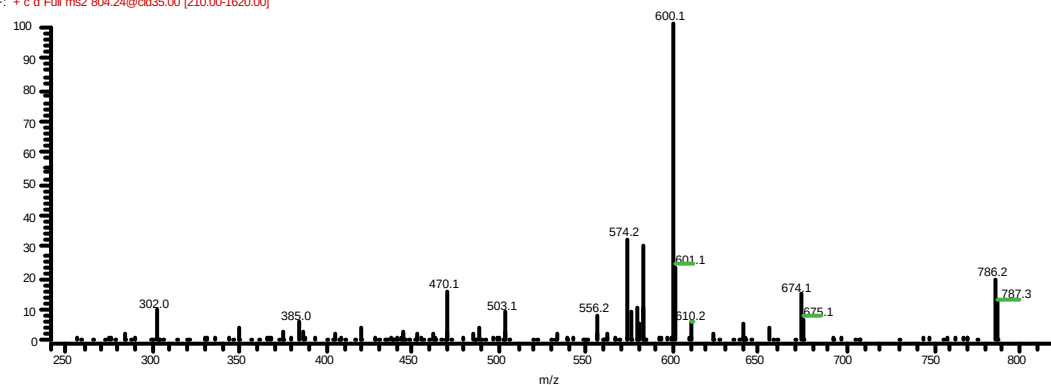
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26.04/2007 20:36:18

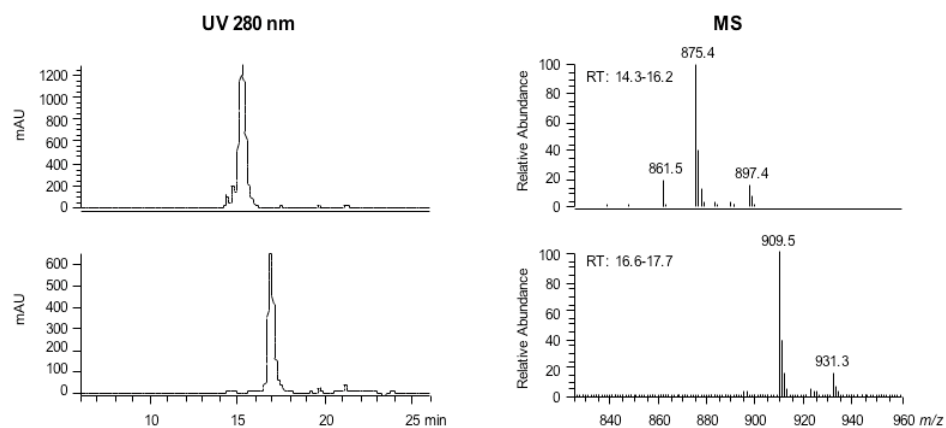
26c04 #794-850 RT: 10.44-11.16 AV: 19 NL: 5.54E8
F: + c ESI Full ms [100.00-2000.00]



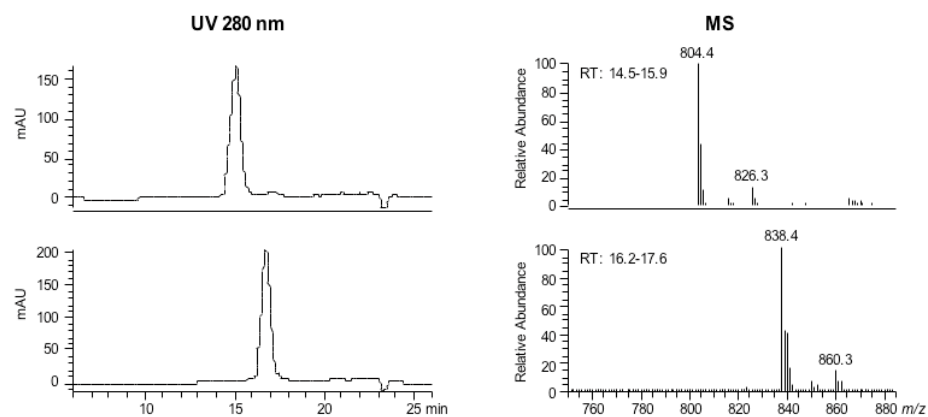
26c04 #779-890 RT: 10.30-11.47 AV: 6 NL: 4.61E7
F: + c d Full ms2 804.24@cid35.00 [210.00-1620.00]



Isolation of pacidamycins



UV chromatogram and MS spectrum for isolated pacidamycin 1 (top, m/z 875.4 $M+H^+$, 897.4 $M+Na^+$) and [7-Cl-Trp]-pacidamycin 1 (bottom, m/z 909.5 $M+H^+$, 931.3 $M+Na^+$).

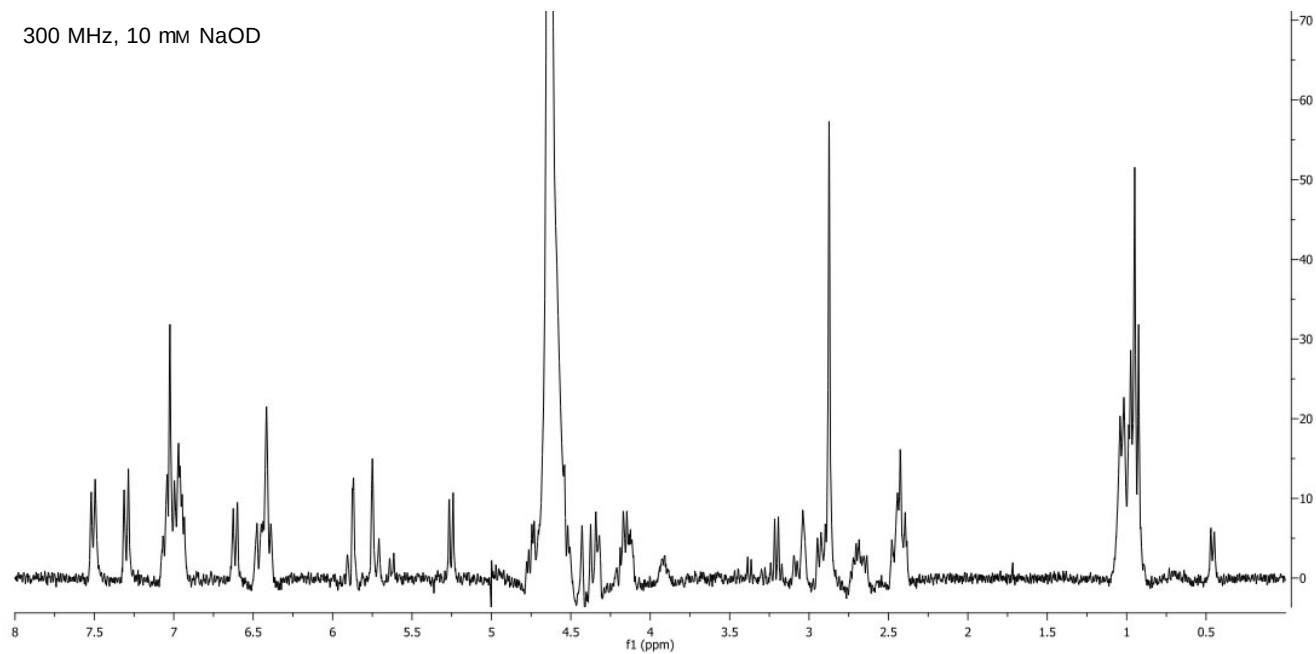


UV chromatogram and MS spectrum for isolated pacidamycin 4 (top, m/z 804.4 $M+H^+$, 826.3 $M+Na^+$) and [7-Cl-Trp]-pacidamycin 4 (bottom, m/z 838.4 $M+H^+$, 860.3 $M+Na^+$).

NMR spectra

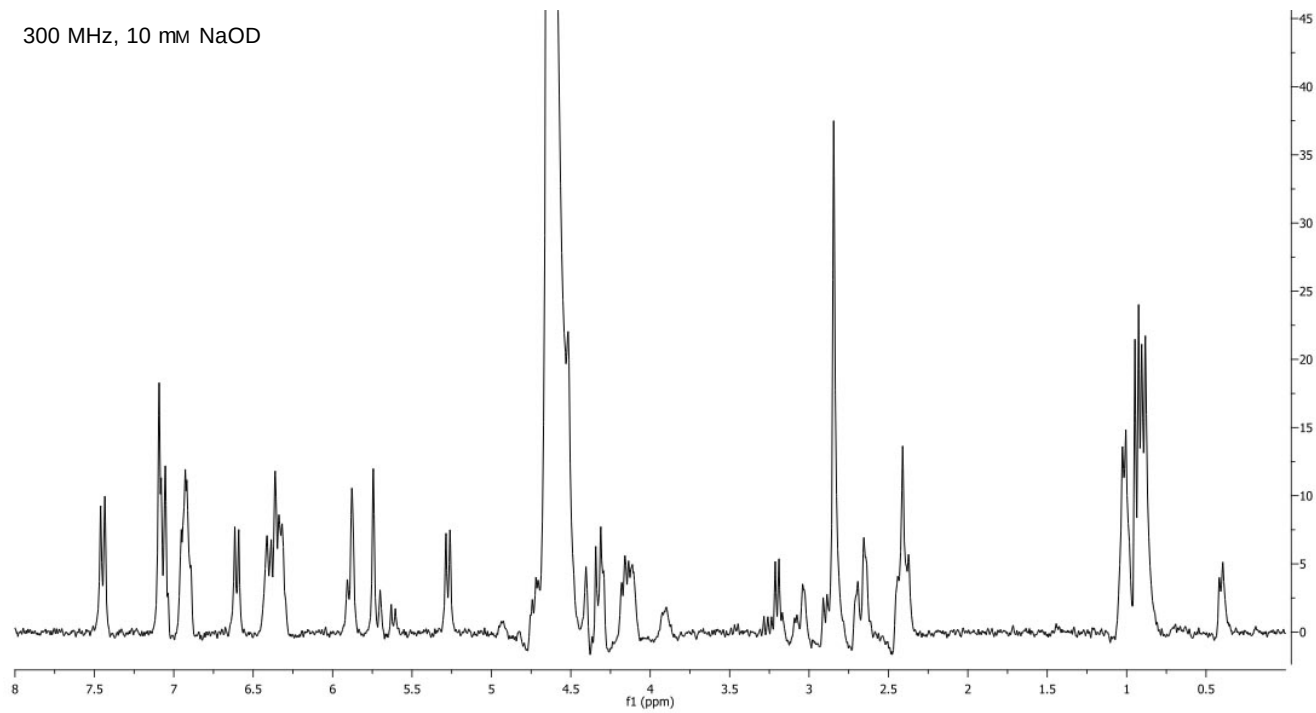
Pacidamycin 1

300 MHz, 10 mM NaOD



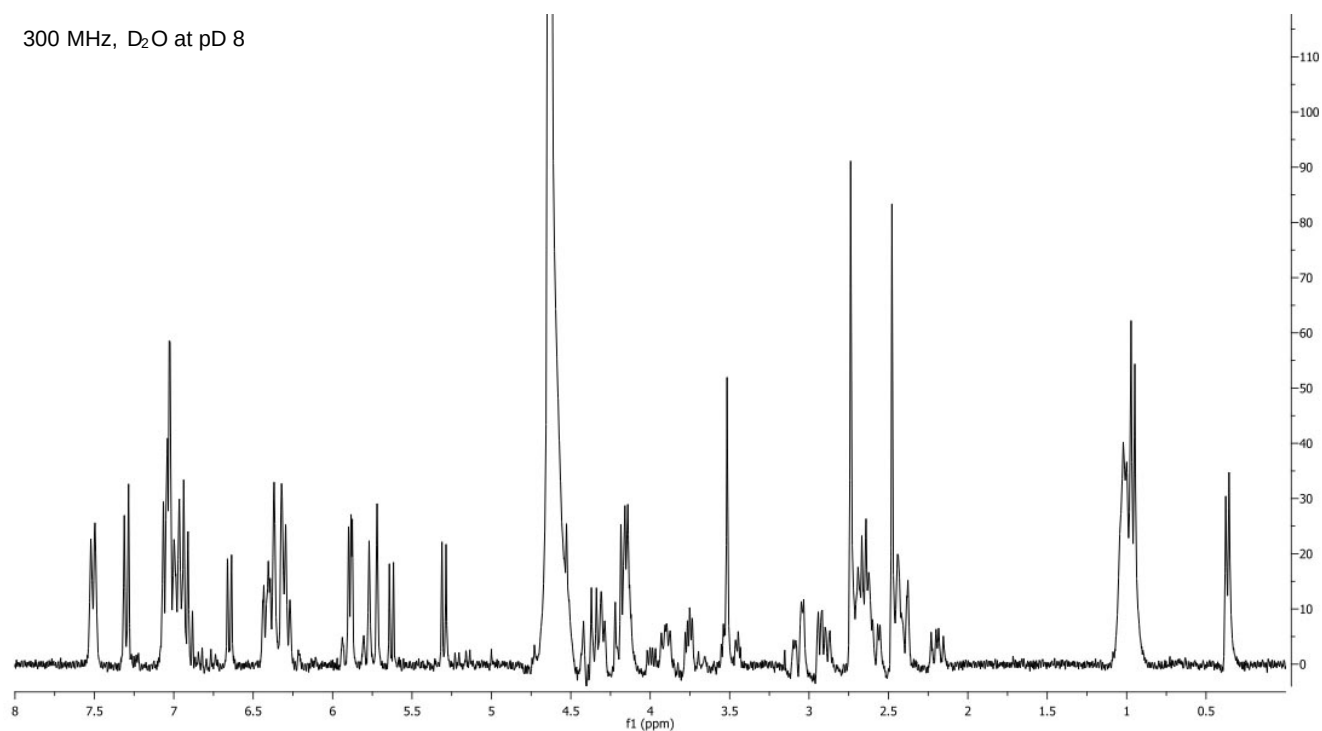
[7-Cl-Trp]-pacidamycin 1

300 MHz, 10 mM NaOD



Pacidamycin 4

300 MHz, D₂O at pD 8



[7-Cl-Trp]-pacidamycin 4

300 MHz, D₂O at pD 8

