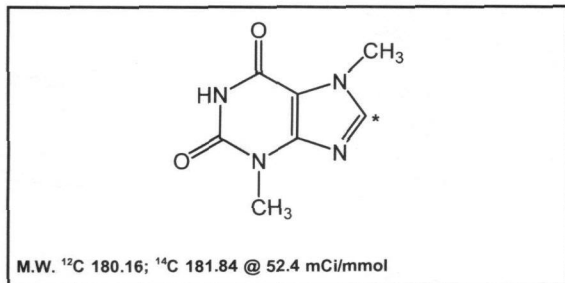




## Product Data Sheet

**MC-1104**

**Theobromine, [8-<sup>14</sup>C]-**



**Lot #:** 194-134-0524-A-20100701-NT

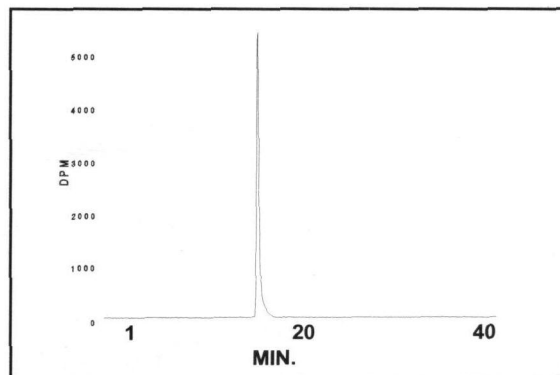
**Specific Activity:** 52.4 mCi/mmol

**Concentration:** 0.1 mCi/ml; 347.02 µg/ml

**Packaged in:** Ethanol : water (1 : 1) solution

**Date of Analysis:** August 06, 2010

**Radiochemical Purity:** 99.5%



HPLC ANALYSIS LOT 194-134-0524-A-20100701-NT  
File Name: int20637 Date and Time: 8/6/2010 3:58:15 PM  
Unit 2 Radio

Peak #	Area %	Time	Area
1	0.20	15.26670	20.85653
2	99.54	15.70330	10353.39180
3	0.13	16.90330	13.27218
4	0.13	17.88670	13.38480
Totals	100.00		10400.90531

**Stability and Storage Recommendation:** Store at -20°C.

**Product Warranty:** Stated on the reverse side of this Product Data Sheet.

**Caution:** Not For Use In Humans Or Clinical Diagnosis. This product is intended for investigational or manufacturing use only. It is pharmaceutically unrefined and is not intended for use in humans. Responsibility for its use in humans, as a diagnostic reagent, and compliance with federal laws rests solely with the purchaser.

**MC-1104**

**Theobromine, [8-<sup>14</sup>C]-**

**Lot 194-134-0524-A-20100701-NT**

**A) All chromatograms were run using the HPLC method described on the Product Data Sheet.**

**Concentrations and volumes:**

Standard solution concentration was 0.5 mg/ml.

**Theobromine, [8-<sup>14</sup>C]-** concentration was 50.0 µCi/ml.

Volume of standard alone injection was 2.0 µl.

Volume of **Theobromine, [8-<sup>14</sup>C]-** alone injection was 2.0 µl.

Co-injection solution consisted of 2.0 µl **Theobromine, [8-<sup>14</sup>C]-** + 1.0 µl standard.

Volume of co-injection was 3.0 µl.

Volume of blank injection was 2.0 µl.

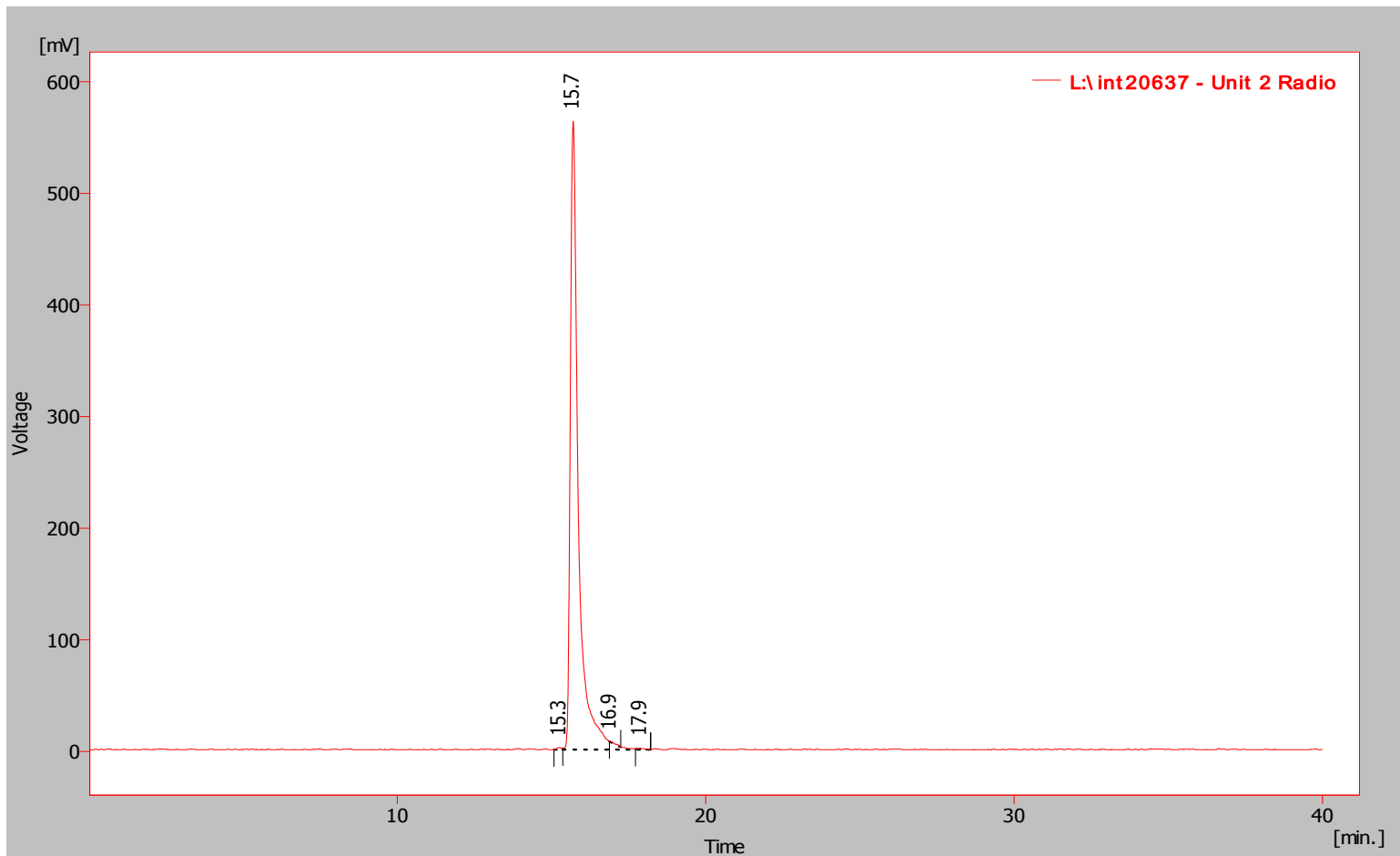
**B) Mass spectrometry – Positive mode**

**C) NMR**

**MC-1104**  
**Theobromine, [8-14C]-**  
**Lot 194-134-0524-A-20100701-NT**

## Chromatogram Info:

File Name	: L:\int20637	File Created	: 10/30/2013 1:54:54 PM
Origin	: Acquired, Acquisition started 8/6/2010 3:18:16 PM	Acquired Date	: 8/6/2010 3:58:15 PM
Project	: Test	By	: Administrator
Method	: Unit2-40minrun	By	: Administrator
Description	: Radiochemical trace of 14C material alone	Modified	: 10/30/2013 2:07 PM
Created	: 6/16/2007 8:19 AM	Detection	: Radiochemical
Column	:	Temperature	:
Mobile Phase	:	Pressure	:
Flow Rate	:	Note	:



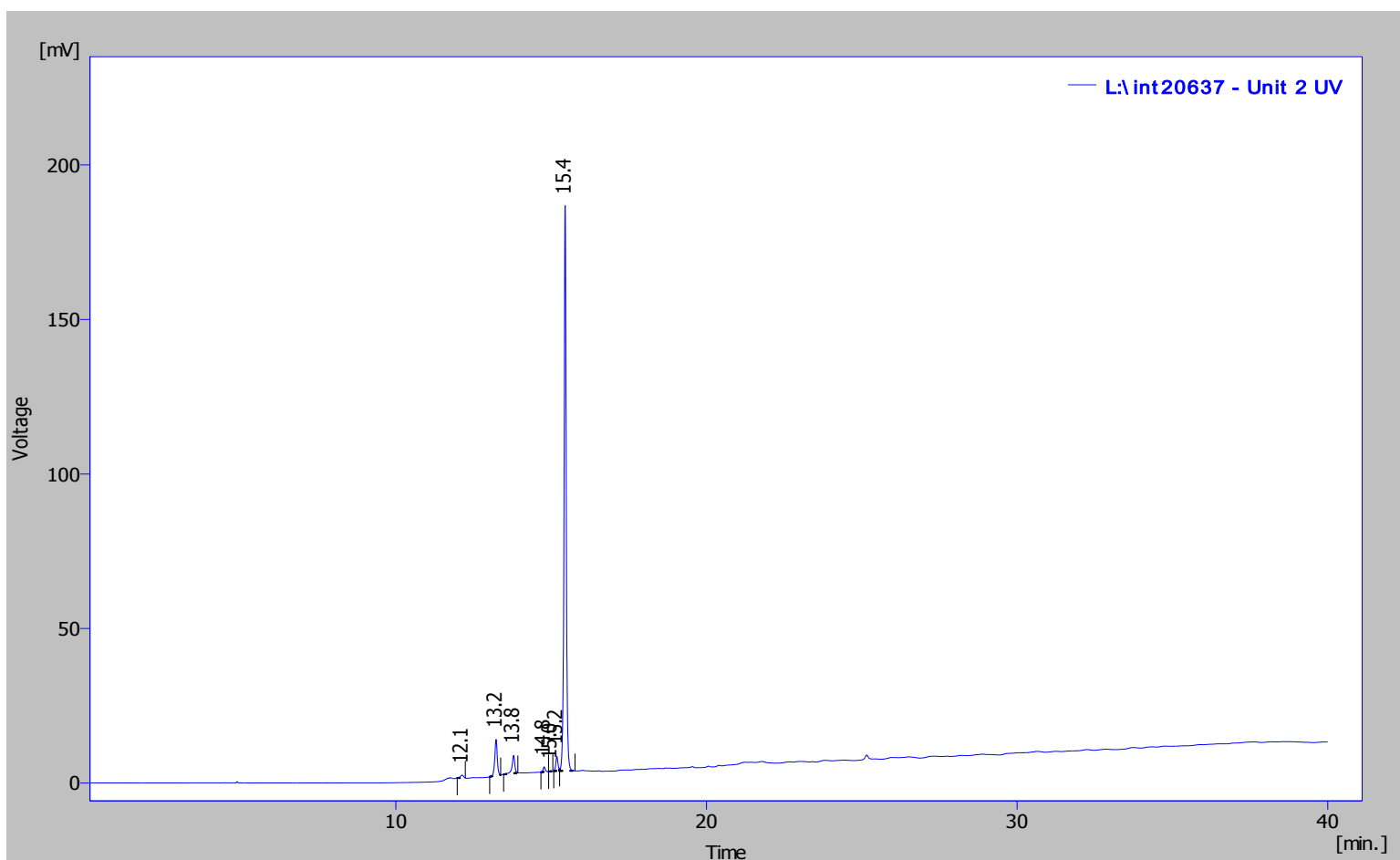
Result Table (Uncal - L:\int20637 - Unit 2 Radio)

	Compound Name	Reten. Time [min]	Area [%]	Area [mV.s]	Height [mV]	Height [%]	Efficiency [th.pl]
1		15.267	0.20	20.857	1.971	0.348	33383.871
2		15.703	99.54	10353.392	562.883	99.357	23717.613
3		16.903	0.13	13.272	0.548	0.097	1424613.271
4		17.887	0.13	13.385	1.121	0.198	47419.297
		Total	100.00	10400.905	566.524	100.000	

**MC-1104**  
**Theobromine, [8-14C]-**  
**Lot 194-134-0524-A-20100701-NT**

Chromatogram Info:

File Name	: L:\int20637	File Created	: 10/30/2013 1:54:54 PM
Origin	: Acquired, Acquisition started 8/6/2010 3:18:16 PM	Acquired Date	: 8/6/2010 3:58:15 PM
Project	: Test	By	: Administrator
Method	: Unit2-40minrun	By	: Administrator
Description	: UV trace of 14C material alone	Modified	: 10/30/2013 2:08 PM
Created	: 6/16/2007 8:19 AM	Detection	: UV 273nm
Column	:	Temperature	:
Mobile Phase	:	Pressure	:
Flow Rate	:	Note	:



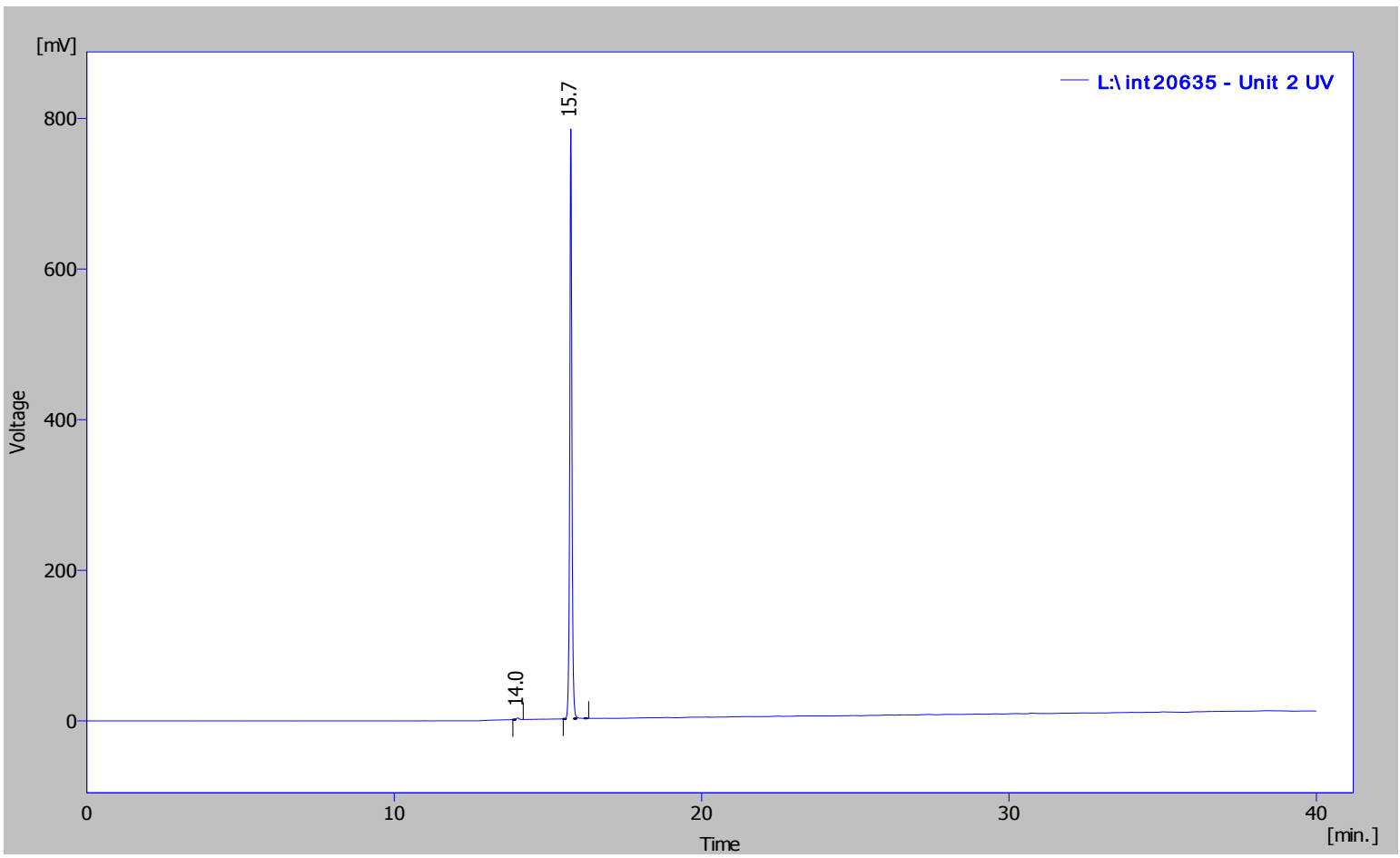
Result Table (Uncal - L:\int20637 - Unit 2 UV)

	Compound Name	Reten. Time [min]	Area [%]	Area [mV.s]	Height [mV]	Height [%]	Efficiency [th.pl]
1		12.133	0.68	7.063	0.964	0.463	56637.951
2		13.227	6.32	66.082	11.687	5.617	129034.664
3		13.790	3.43	35.795	5.798	2.787	151705.312
4		14.773	0.72	7.502	1.647	0.791	224834.994
5		14.987	0.12	1.267	0.363	0.175	345634.718
6		15.183	2.24	23.388	4.695	2.256	199555.657
7		15.450	86.50	903.771	182.904	87.910	245903.030
		Total	100.00	1044.867	208.058	100.000	

**MC-1104**  
**Theobromine, [8-14C]-**  
**Lot 194-134-0524-A-20100701-NT**

Chromatogram Info:

File Name	: L:\int20635	File Created	: 10/30/2013 1:54:54 PM
Origin	: Acquired, Acquisition started 8/9/2010 9:38:49 AM	Acquired Date	: 8/9/2010 10:24:43 AM
Project	: Test	By	: Administrator
Method	: Unit2-40minrun	By	: Administrator
Description	: UV trace of standard material alone	Modified	: 10/30/2013 2:09 PM
Created	: 6/16/2007 8:19 AM	Detection	: UV 273nm
Column	:	Temperature	:
Mobile Phase	:	Pressure	:
Flow Rate	:	Note	:



Result Table (Uncal - L:\int20635 - Unit 2 UV)

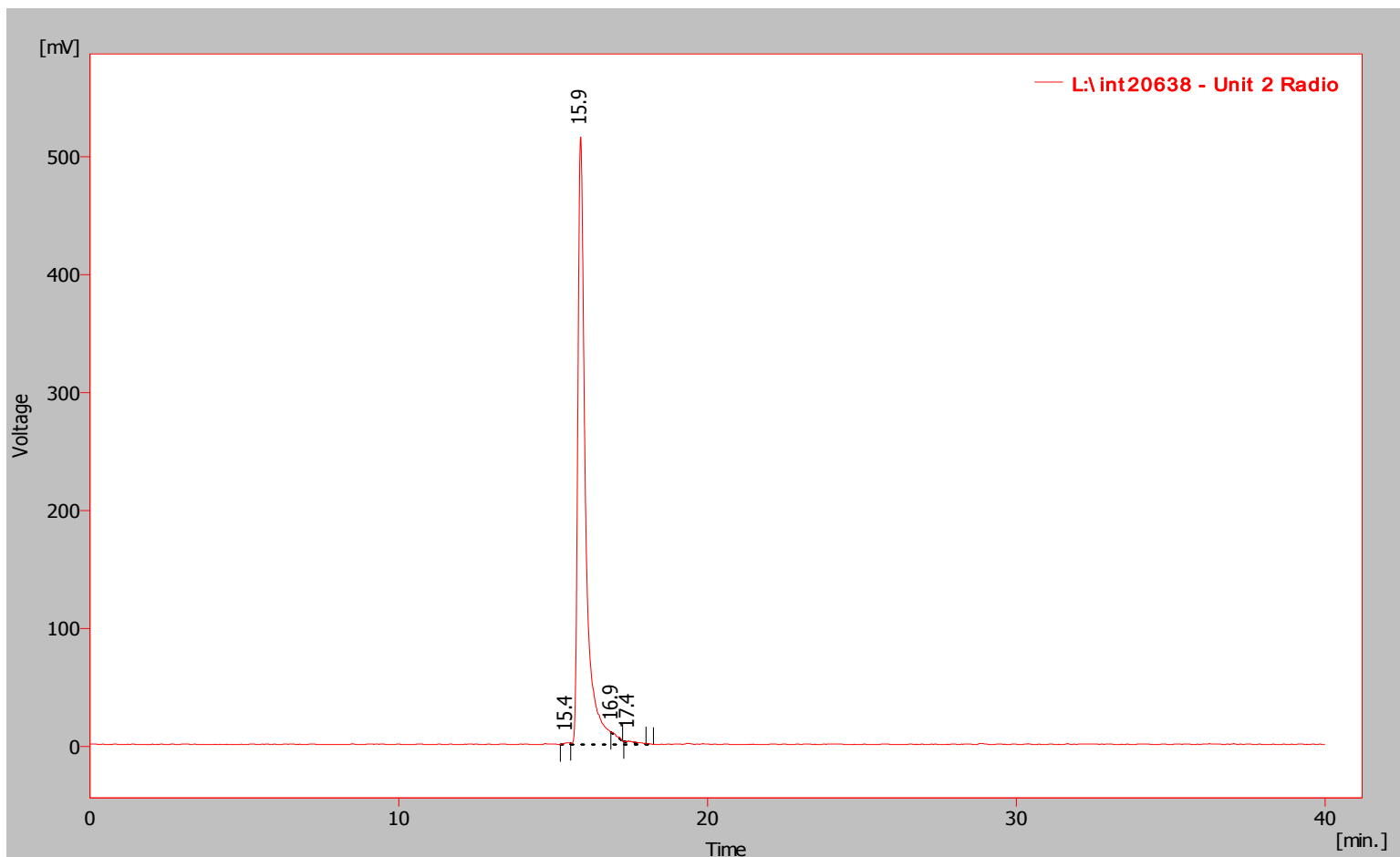
	Compound Name	Reten. Time [min]	Area [%]	Area [mV.s]	Height [mV]	Height [%]	Efficiency [th.pl]
1		14.017	0.32	12.131	2.222	0.283	156733.470
2		15.743	99.68	3798.883	783.241	99.717	255329.088
		Total	100.00	3811.014	785.463	100.000	



**MC-1104**  
**Theobromine, [8-14C]-**  
**Lot 194-134-0524-A-20100701-NT**

Chromatogram Info:

File Name	: L:\int20638	File Created	: 10/30/2013 1:54:54 PM
Origin	: Acquired, Acquisition started 8/9/2010 10:48:41 AM	Acquired Date	: 8/9/2010 11:28:40 AM
Project	: Test	By	: Administrator
Method	: Unit2-40minrun	By	: Administrator
Description	: Radiochemical trace of 14C material co-injected with standard	Modified	: 10/30/2013 2:10 PM
Created	: 6/16/2007 8:19 AM		
Column	:	Detection	: Radiochemical
Mobile Phase	:	Temperature	:
Flow Rate	:	Pressure	:
Note	:		



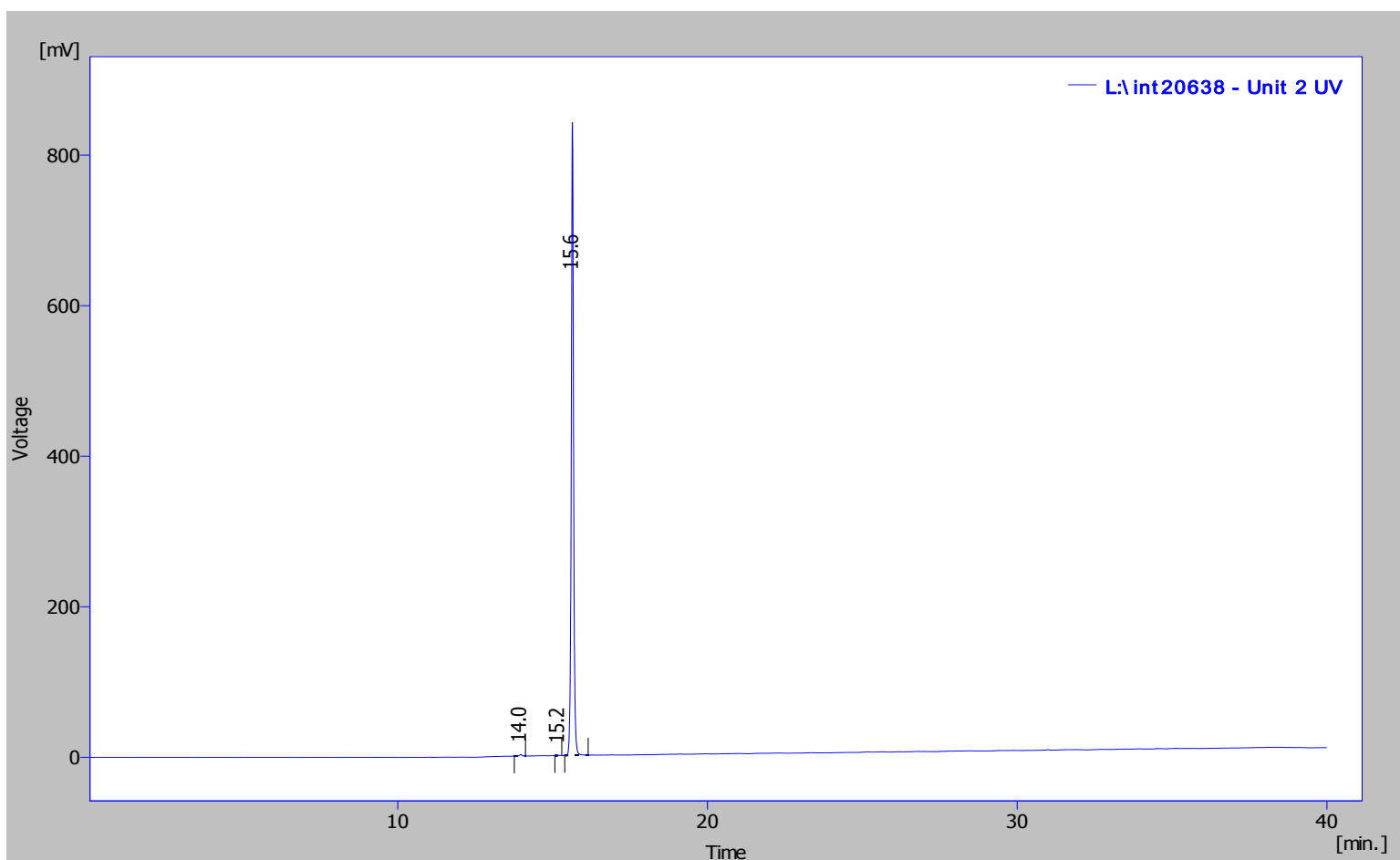
Result Table (Uncal - L:\int20638 - Unit 2 Radio)

	Compound Name	Reten. Time [min]	Area [%]	Area [mV.s]	Height [mV]	Height [%]	Efficiency [th.pl]
1		15.427	0.22	20.453	1.536	0.296	22889.245
2		15.893	99.36	9136.758	515.151	99.312	24295.020
3		16.907	0.21	19.639	0.883	0.170	210824.733
4		17.440	0.20	18.417	1.151	0.222	592386.660
		Total	100.00	9195.268	518.721	100.000	

**MC-1104**  
**Theobromine, [8-14C]-**  
**Lot 194-134-0524-A-20100701-NT**

Chromatogram Info:

File Name	: L:\int20638	File Created	: 10/30/2013 1:54:54 PM
Origin	: Acquired, Acquisition started 8/9/2010 10:48:41 AM	Acquired Date	: 8/9/2010 11:28:40 AM
Project	: Test	By	: Administrator
Method	: Unit2-40minrun	By	: Administrator
Description	: UV trace of 14C material co-injected with standard	Modified	: 10/30/2013 2:11 PM
Created	: 6/16/2007 8:19 AM		
Column	:	Detection	: UV 273nm
Mobile Phase	:	Temperature	:
Flow Rate	:	Pressure	:
Note	:		



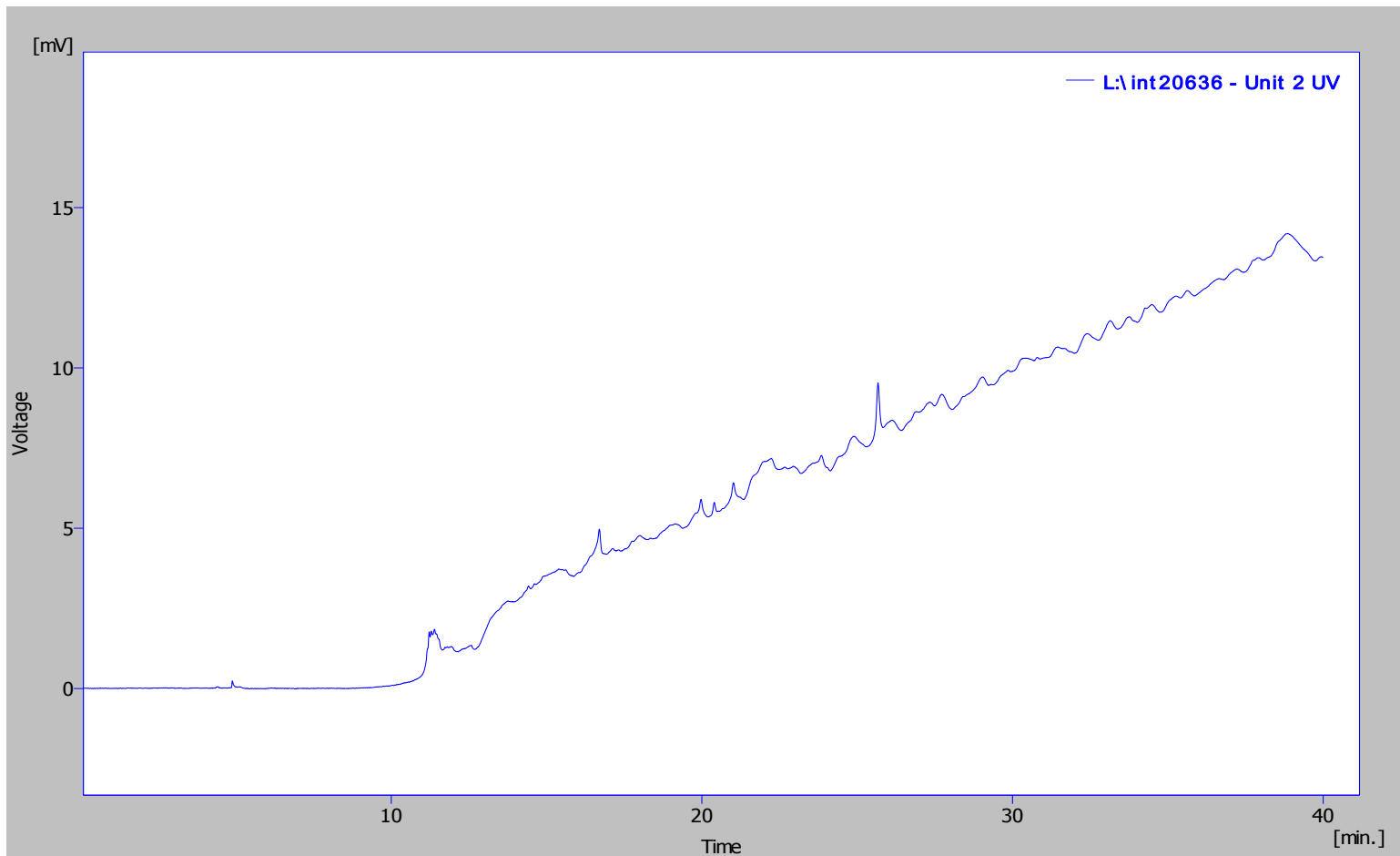
Result Table (Uncal - L:\int20638 - Unit 2 UV)

	Compound Name	Reten. Time [min]	Area [%]	Area [mV.s]	Height [mV]	Height [%]	Efficiency [th.pl]
1		13.967	0.28	12.290	2.074	0.246	133416.727
2		15.190	0.04	1.732	0.396	0.047	260873.060
3		15.637	99.68	4325.070	840.456	99.707	230454.376
	Total		100.00	4339.092	842.927	100.000	

**MC-1104**  
**Theobromine, [8-14C]-**  
**Lot 194-134-0524-A-20100701-NT**

## Chromatogram Info:

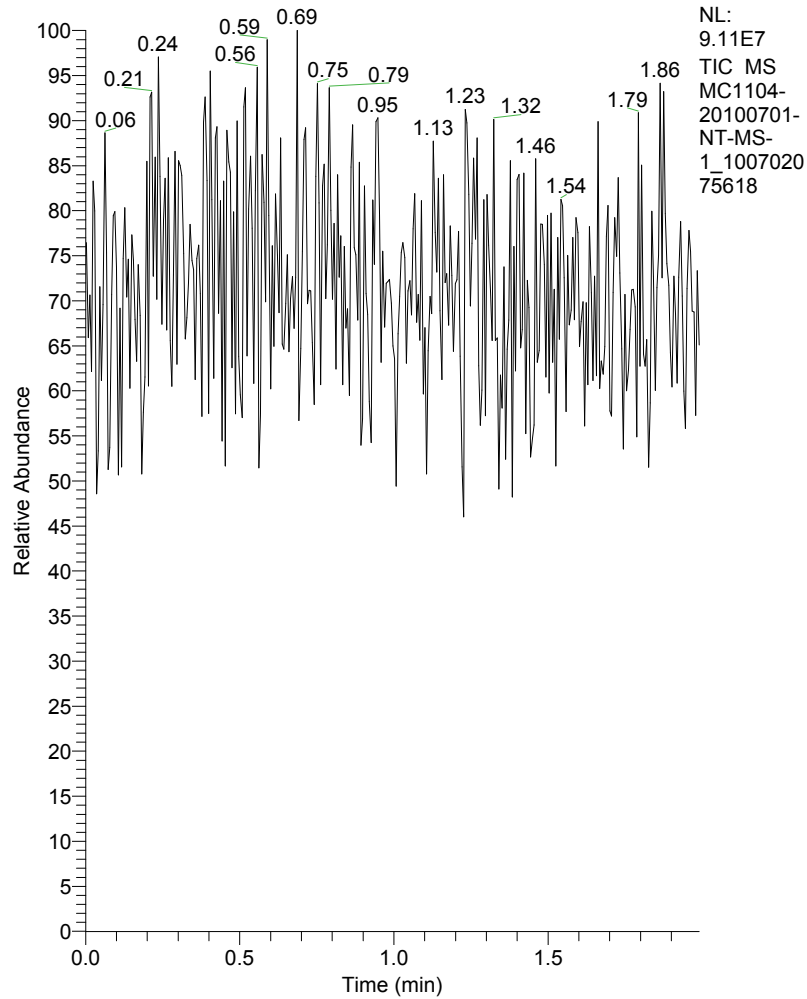
File Name	: L:\int20636	File Created	: 10/30/2013 1:54:54 PM
Origin	: Acquired, Acquisition started 8/6/2010 12:10:38 PM	Acquired Date	: 8/6/2010 12:50:37 PM
Project	: Test	By	: Administrator
Method	: Unit2-40minrun	By	: Administrator
Description	: UV trace of blank injection	Modified	: 10/30/2013 2:12 PM
Created	: 6/16/2007 8:19 AM		
Column	:	Detection	: UV 273nm
Mobile Phase	:	Temperature	:
Flow Rate	:	Pressure	:
Note	:		



*Result Table (Uncal - L:\int20636 - Unit 2 UV)*

Compound Name	Reten. Time [min]	Area [%]	Area [mV.s]	Height [mV]	Height [%]	Efficiency [th.p]
No peak to report						

RT: 0.00 - 1.99



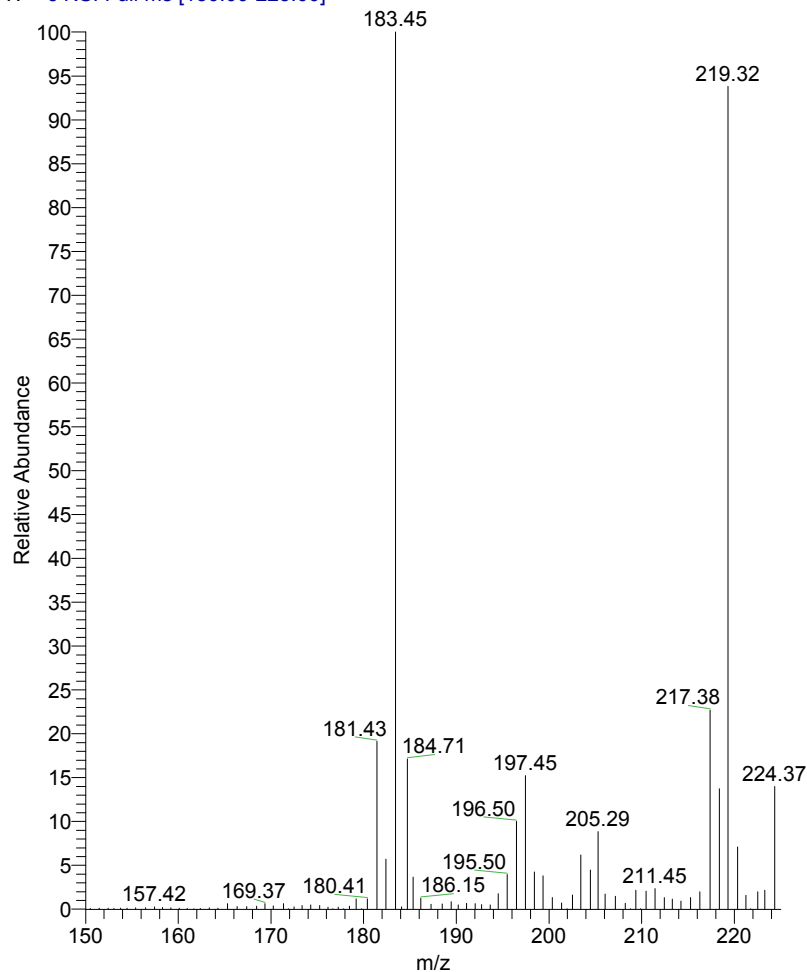
MC1104-20100701-NT-MS-1\_100702075618#1-366

T: + c NSI Full ms [150.00-225.00]

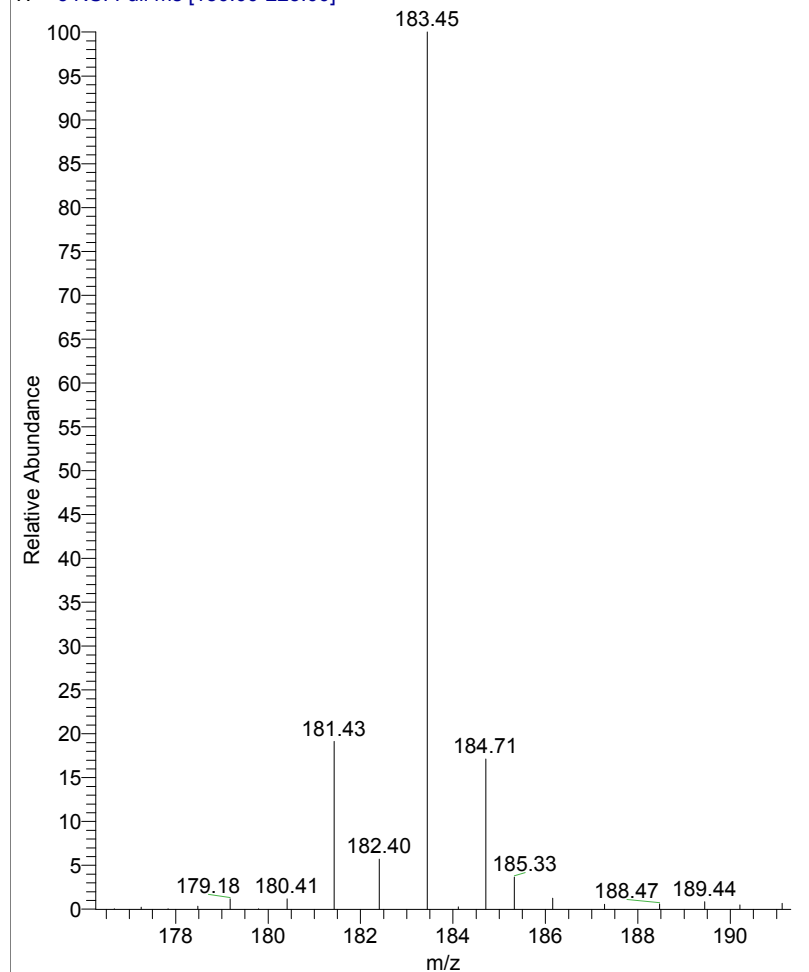
m/z = 180.92-184.19

m/z	Intensity	Relative
181.43	3142008.0	19.08
182.40	936372.5	5.69
183.45	16465581.9	100.00
184.12	40756.7	0.25

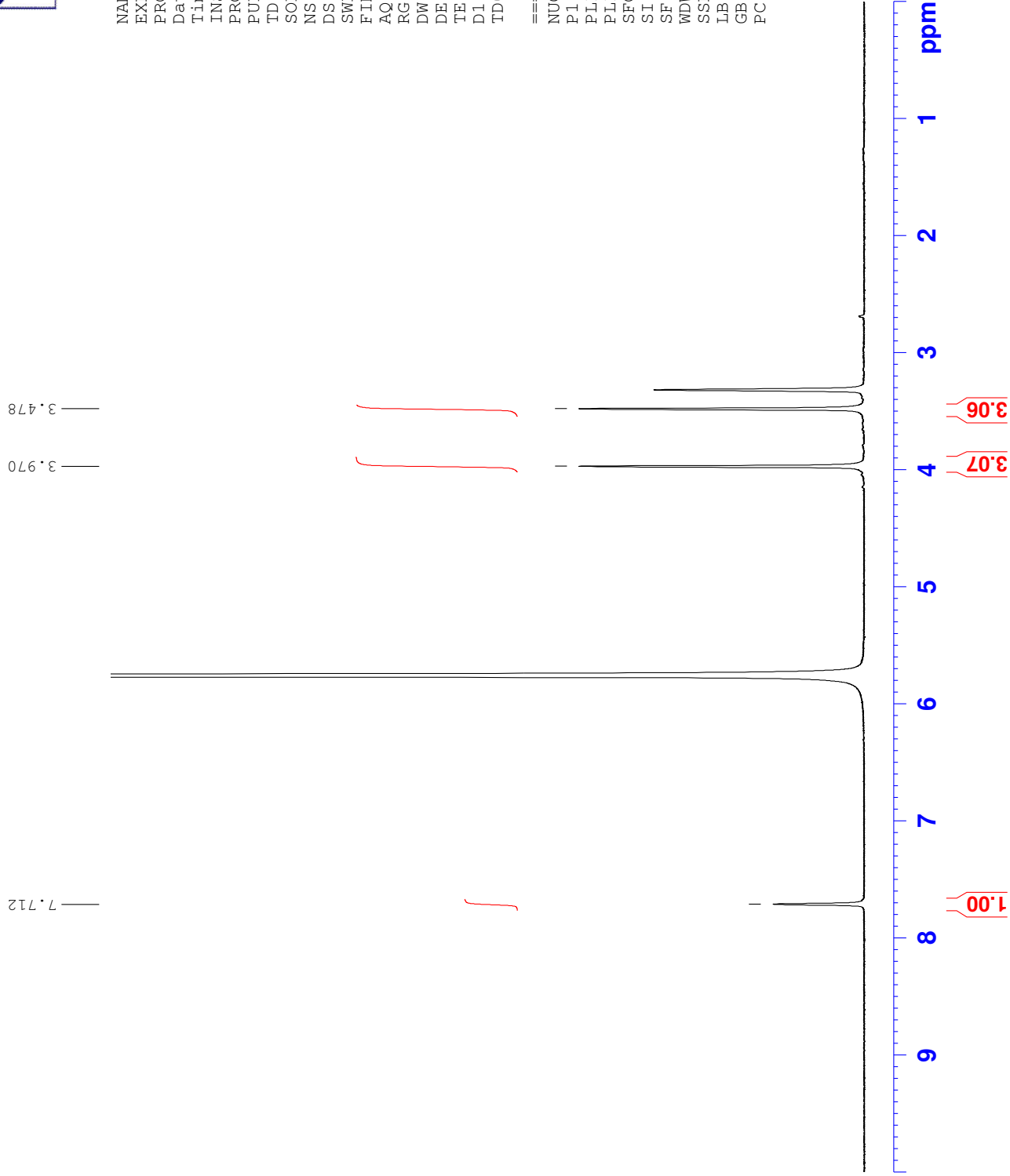
MC1104-20100701-NT-MS-1\_100702075618 #1-366 RT: 0.00-1.99 AV: 366 NL: T: + c NSI Full ms [150.00-225.00]



MC1104-20100701-NT-MS-1\_100702075618 #1-366 RT: 0.00-1.99 AV: 366 NL: T: + c NSI Full ms [150.00-225.00]



MC1104 1H NMR in MeOD/NaOD  
Batch 20100701-NT



NAME MC1104-20100701-NT  
EXPNO 1  
PROCNO 1  
Date\_ 20100809  
Time 12.10  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT MeOD  
NS 512  
DS 2  
SWH 8278.146 Hz  
FIDRES 0.126314 Hz  
AQ 3.9584243 sec  
RG 4  
DW 60.400 usec  
DE 6.50 usec  
TE 294.4 K  
D1 1.00000000 sec  
TD0 1  
===== CHANNEL f1 =====  
NUC1 1H  
P1 14.50 usec  
PL1 -0.70 dB  
PL1W 10.03411102 W  
SFO1 400.1324710 MHz  
SI 32768  
SF 400.1300062 MHz  
WDW no  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00