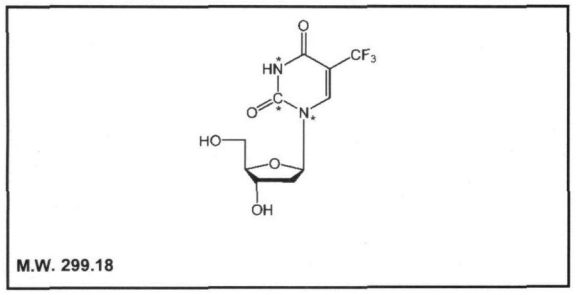
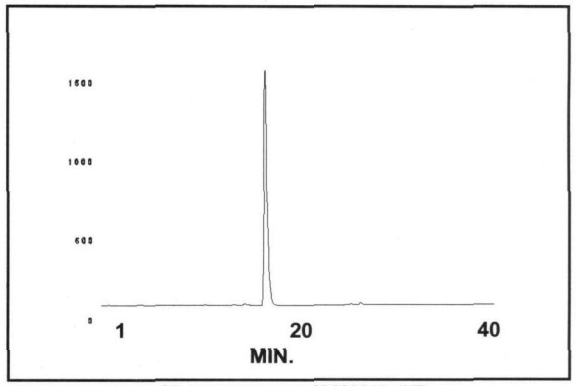
Product Data Sheet

MG-111

5-Trifluoromethyl-2'-deoxyuridine, [2-^{13}C,1,3-^{15}N$_2$]-



M.W. 299.18



HPLC ANALYSIS LOT 249-003-000-A-20120215-JKR
File Name: intX223 Date and Time: 2/16/2012 1:29:07 PM
Unit X UV

Peak #	Area %	Time	Area
1	0.48	14.65330	15.20324
2	99.52	16.76330	3176.20462
Totals	100.00		3191.40786

Lot #: 249-003-000-A-20120215-JKR

Packaged as: Solid

Date of Analysis: February 16, 2012

Chemical Purity @ 260nm : 99.5%

Isotopic Enrichment: 99.4%

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.

Moravek Biochemicals, Inc. 577 Mercury Lane, Brea, California 92821 www.moravek.com info@moravek.com Phone (714) 990-2018 Fax (714) 990-1824

MG-111

5-Trifluoromethyl-2'-deoxyuridine, [2-^{13}C,1,3-$^{15}N_2$]-

Lot 249-003-000-A-20120215-JKR

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

Concentrations and volumes:

Standard solution concentration was 1.0 mg/ml.

5-Trifluoromethyl-2'-deoxyuridine, [2-^{13}C,1,3-$^{15}N_2$]- concentration was 1.0 mg/ml.

Volume of standard alone injection was 3.0 µl.

Volume of **5-Trifluoromethyl-2'-deoxyuridine, [2-^{13}C,1,3-$^{15}N_2$]-** alone injection was 3.0 µl.

Co-injection solution consisted of 3.0 µl **5-Trifluoromethyl-2'-deoxyuridine, [2-^{13}C,1,3-$^{15}N_2$]-** + 3.0 µl standard.

Volume of co-injection was 6.0 µl.

Volume of blank injection was 2.0 µl.

B) Mass spectrometry - Negative mode

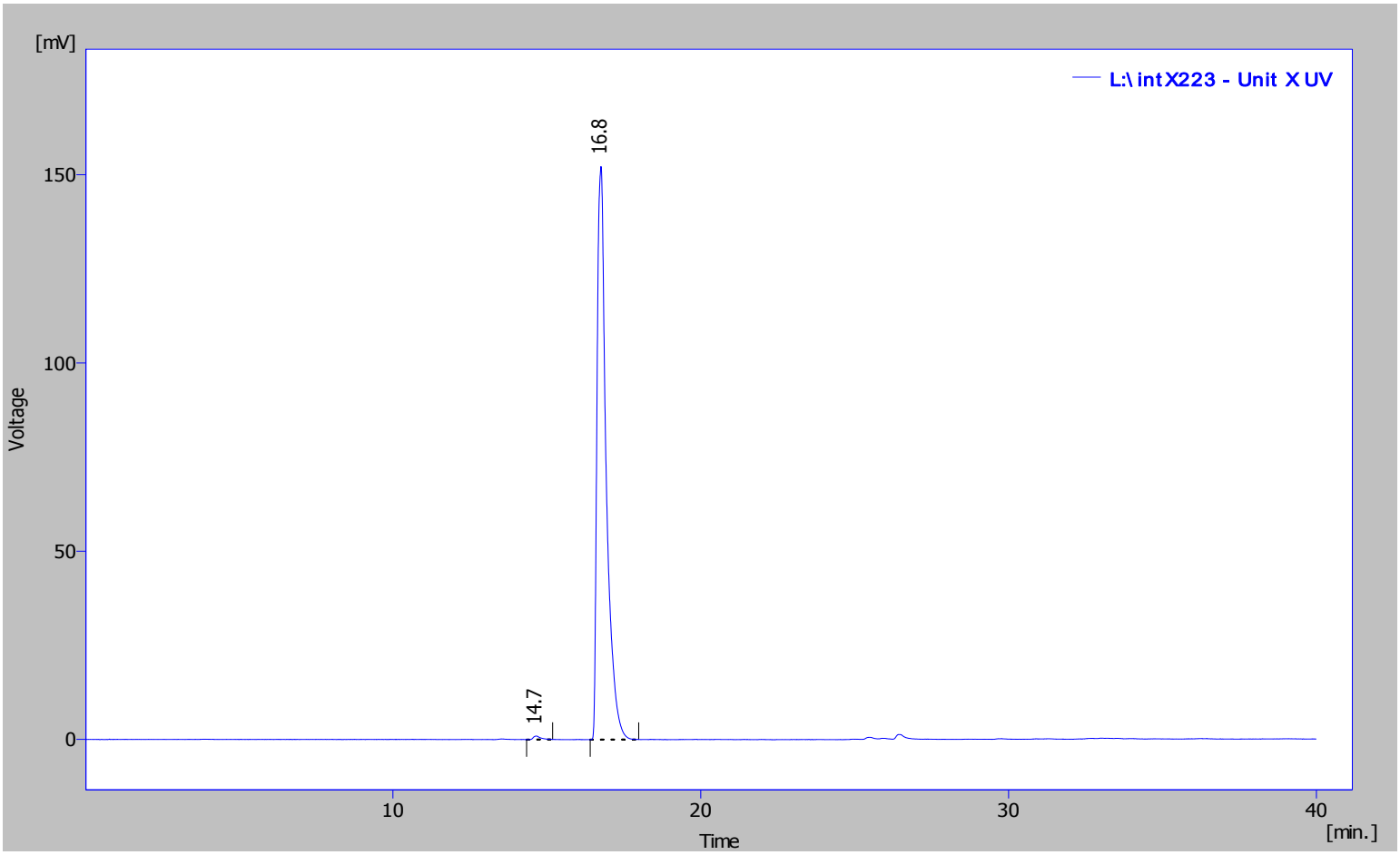
C) NMR - ^{1}H NMR and ^{13}C NMR

MG-111
5-Trifluoromethyl-2'-deoxyuridine, [2-13C,1,3-15N2]-
Lot 249-003-000-A-20120215-JKR

Chromatogram Info:

File Name	: L:\intX223	File Created	: 11/8/2013 3:31:46 PM
Origin	: Acquired, Acquisition started 2/16/2012 12:49:07 PM	Acquired Date	: 2/16/2012 1:29:07 PM
Project	: Test	By	: Administrator

Method	: UnitX-40minrun	By	: Administrator
Description	: UV trace of 13C/15N alone		
Created	: 7/14/2007 11:01 AM	Modified	: 11/8/2013 3:46 PM
Column	:	Detection	: UV 260nm
Mobile Phase	:	Temperature	:
Flow Rate	:	Pressure	:
Note	:		



Result Table (Uncal - L:\intX223 - Unit X UV)

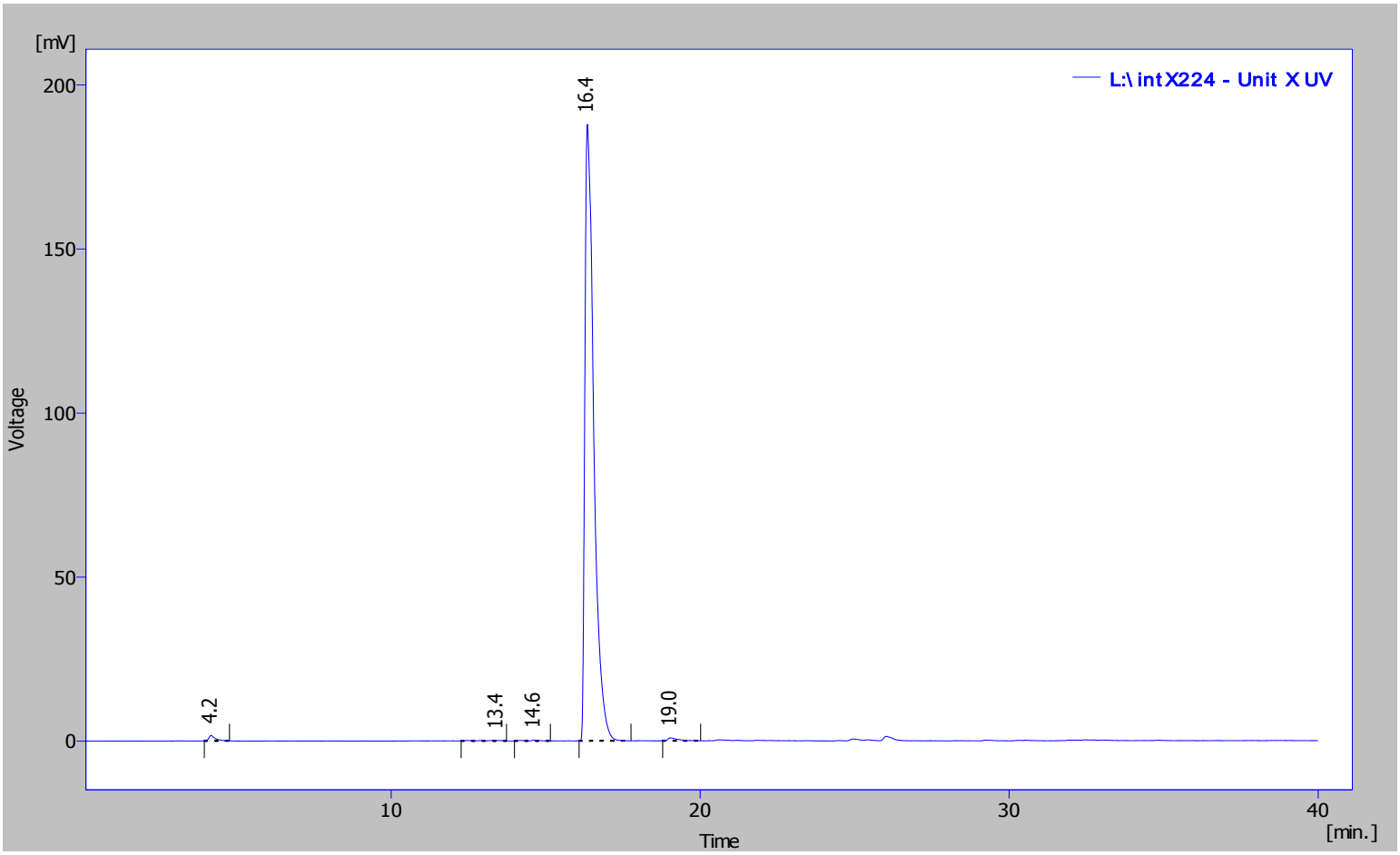
	Compound Name	Reten. Time [min]	Area [%]	Area [mV.s]	Height [mV]	Height [%]	Efficiency [th.pl]
1		14.653	0.48	15.203	0.928	0.606	12800.002
2		16.763	99.52	3176.205	152.259	99.394	9548.125
		Total	100.00	3191.408	153.187	100.000	

MG-111
5-Trifluoromethyl-2'-deoxyuridine, [2-13C,1,3-15N2]-
Lot 249-003-000-A-20120215-JKR

Chromatogram Info:

File Name	: L:\intX224	File Created	: 11/8/2013 3:31:46 PM
Origin	: Acquired, Acquisition started 2/16/2012 2:09:34 PM	Acquired Date	: 2/16/2012 2:49:33 PM
Project	: Test	By	: Administrator

Method	: UnitX-40minrun	By	: Administrator
Description	: UV trace of standard alone		
Created	: 7/14/2007 11:01 AM	Modified	: 11/8/2013 3:46 PM
Column	:	Detection	: UV 260nm
Mobile Phase	:	Temperature	:
Flow Rate	:	Pressure	:
Note	:		



Result Table (Uncal - L:\intX224 - Unit X UV)

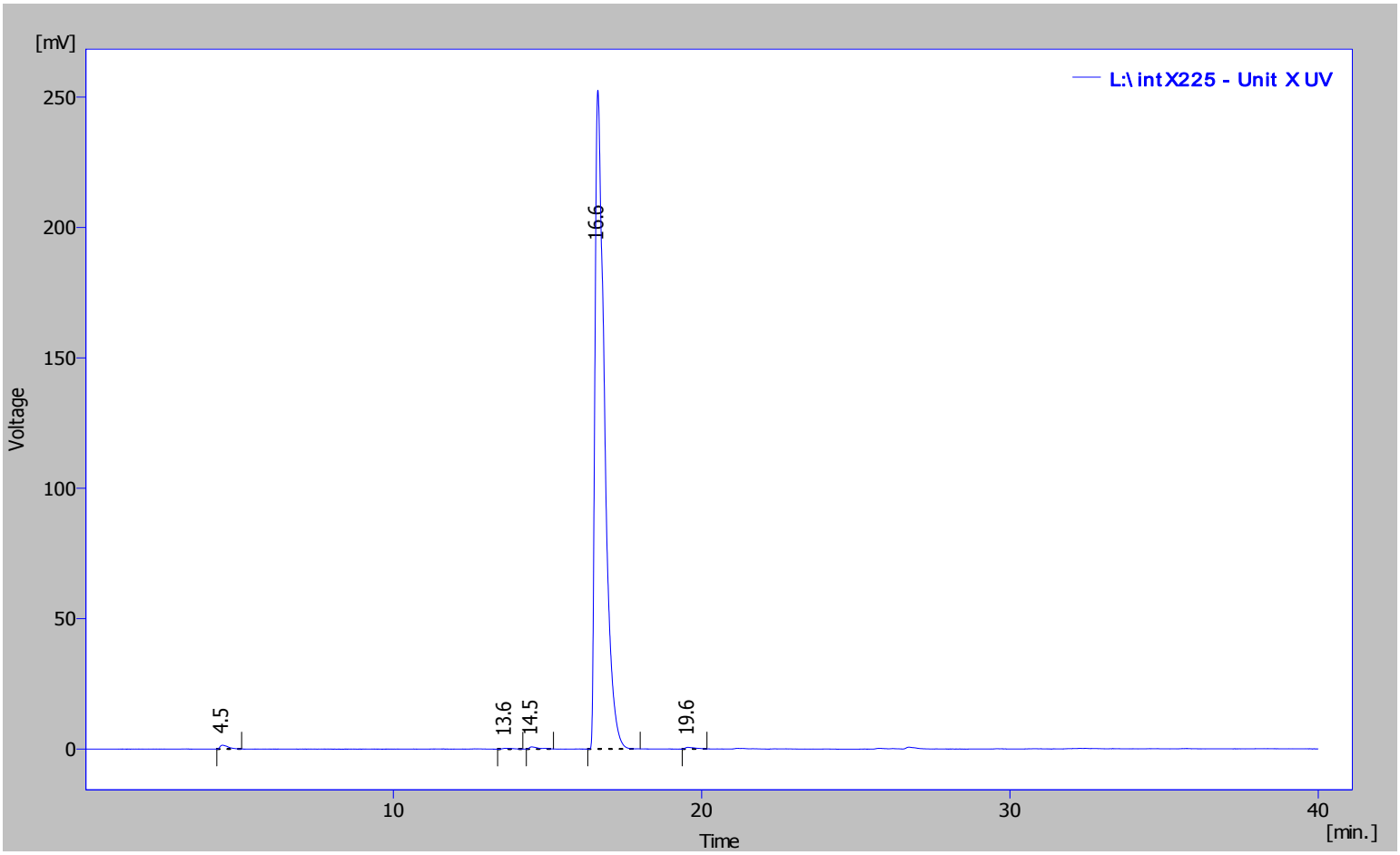
	Compound Name	Reten. Time [min]	Area [%]	Area [mV.s]	Height [mV]	Height [%]	Efficiency [th.pl]
1		4.177	0.65	25.106	1.692	0.886	1005.659
2		13.423	0.21	7.882	0.159	0.083	1072.926
3		14.627	0.19	7.111	0.274	0.144	3107.755
4		16.350	98.41	3780.005	187.902	98.405	10312.662
5		19.043	0.54	20.851	0.920	0.482	7963.122
		Total	100.00	3840.955	190.948	100.000	

MG-111
5-Trifluoromethyl-2'-deoxyuridine, [2-13C,1,3-15N2]-
Lot 249-003-000-A-20120215-JKR

Chromatogram Info:

File Name	: L:\intX225	File Created	: 11/8/2013 3:31:46 PM
Origin	: Acquired, Acquisition started 2/16/2012 3:03:28 PM	Acquired Date	: 2/16/2012 3:43:27 PM
Project	: Test	By	: Administrator

Method	: UnitX-40minrun	By	: Administrator
Description	: UV trace of 13C/15N material co-injected with standard		
Created	: 7/14/2007 11:01 AM	Modified	: 11/8/2013 3:48 PM
Column	:	Detection	: UV 260nm
Mobile Phase	:	Temperature	:
Flow Rate	:	Pressure	:
Note	: Impurities came from standard material		



Result Table (Uncal - L:\intX225 - Unit X UV)

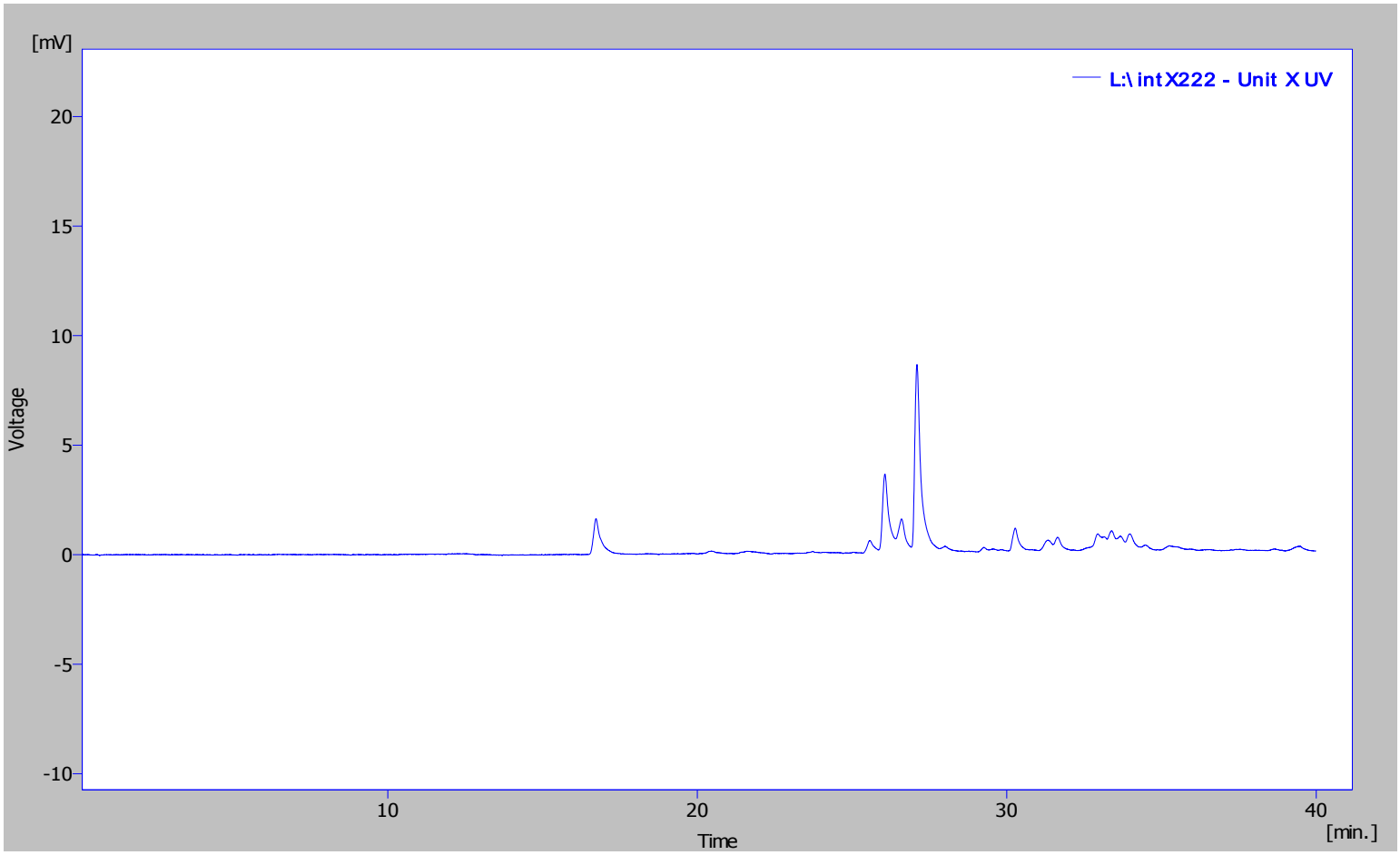
	Compound Name	Reten. Time [min]	Area [%]	Area [mV.s]	Height [mV]	Height [%]	Efficiency [th.pl]
1		4.453	0.50	27.658	1.495	0.584	1081.635
2		13.640	0.12	6.863	0.299	0.117	7673.261
3		14.493	0.31	17.115	0.839	0.328	6284.073
4		16.633	98.80	5438.252	252.621	98.718	9556.898
5		19.563	0.26	14.397	0.647	0.253	14637.463
		Total	100.00	5504.285	255.901	100.000	

MG-111
5-Trifluoromethyl-2'-deoxyuridine, [2-13C,1,3-15N2]-
Lot 249-003-000-A-20120215-JKR

Chromatogram Info:

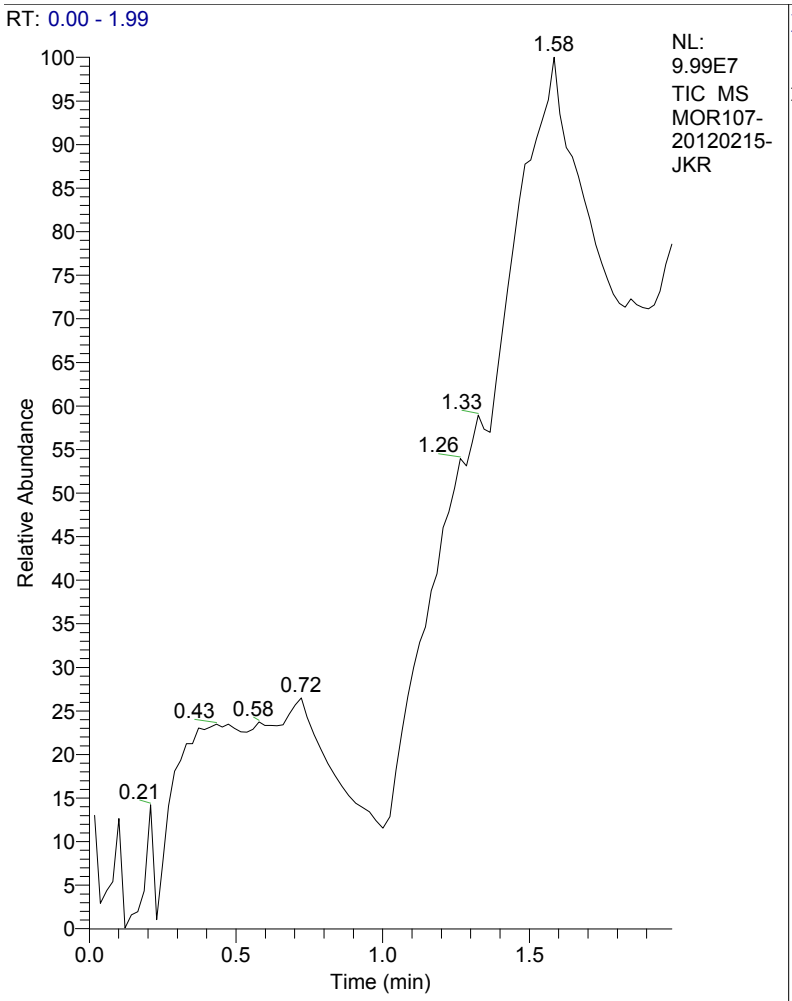
File Name	: L:\intX222	File Created	: 11/8/2013 3:33:41 PM
Origin	: Acquired, Acquisition started 2/16/2012 11:34:23 AM	Acquired Date	: 2/16/2012 12:14:23 PM
Project	: Test	By	: Administrator

Method	: UnitX-40minrun	By	: Administrator
Description	: UV trace of blank injection		
Created	: 7/14/2007 11:01 AM	Modified	: 11/8/2013 3:49 PM
Column	:	Detection	: UV 260nm
Mobile Phase	:	Temperature	:
Flow Rate	:	Pressure	:
Note	:		



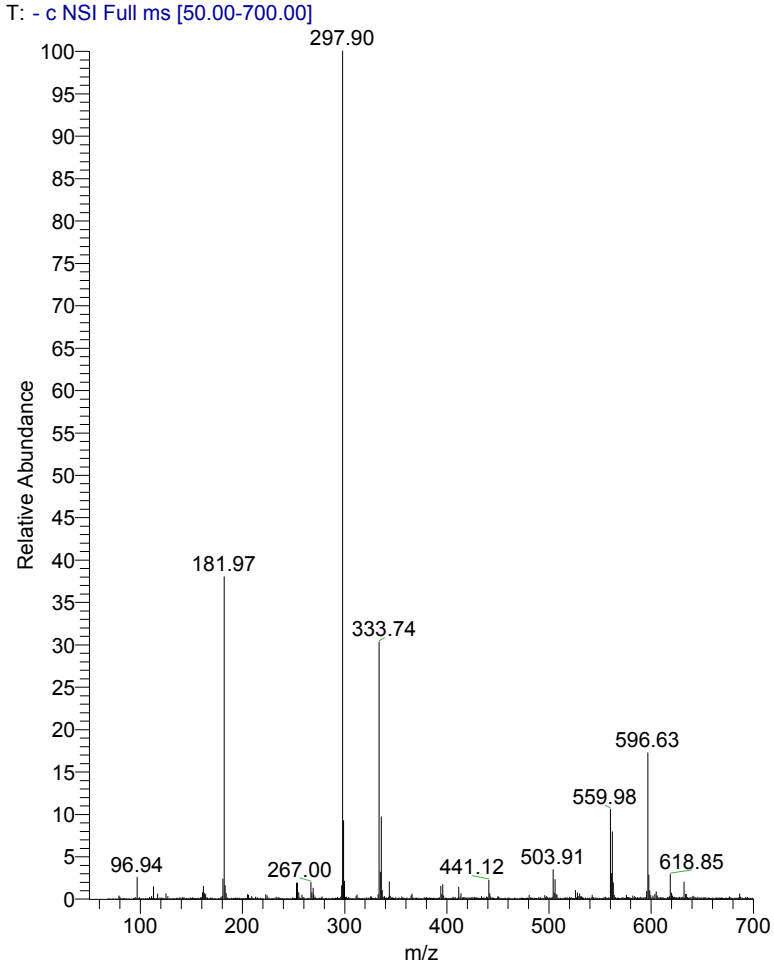
Result Table (Uncal - L:\intX222 - Unit X UV)

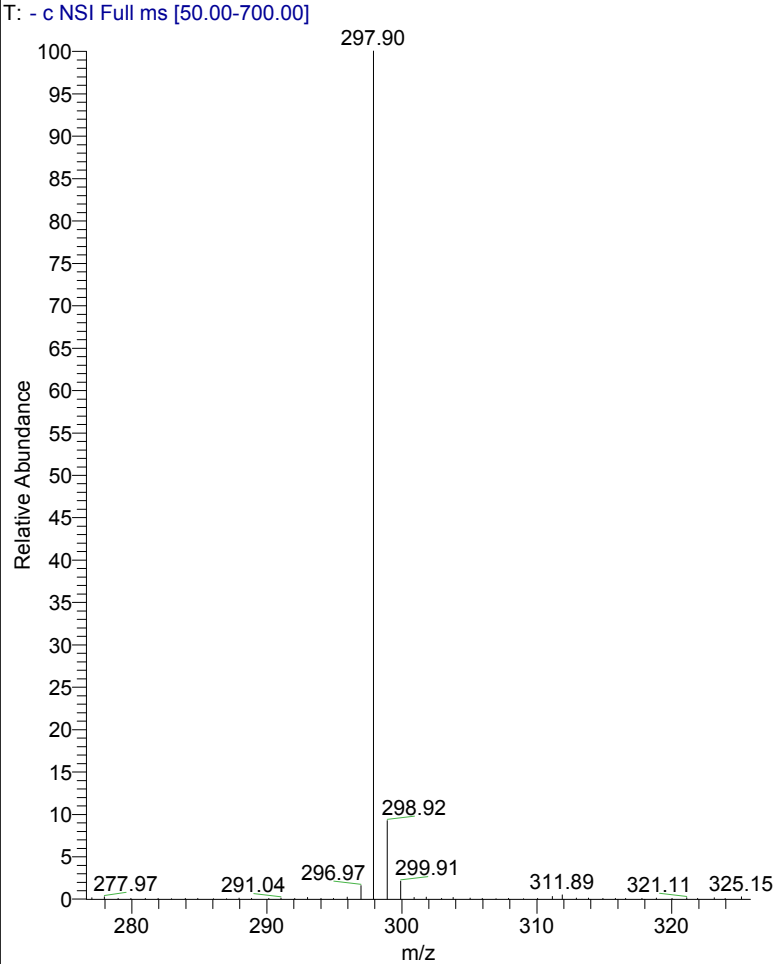
Compound Name	Reten. Time [min]	Area [%]	Area [mV.s]	Height [mV]	Height [%]	Efficiency [th.pl]
No peak to report						



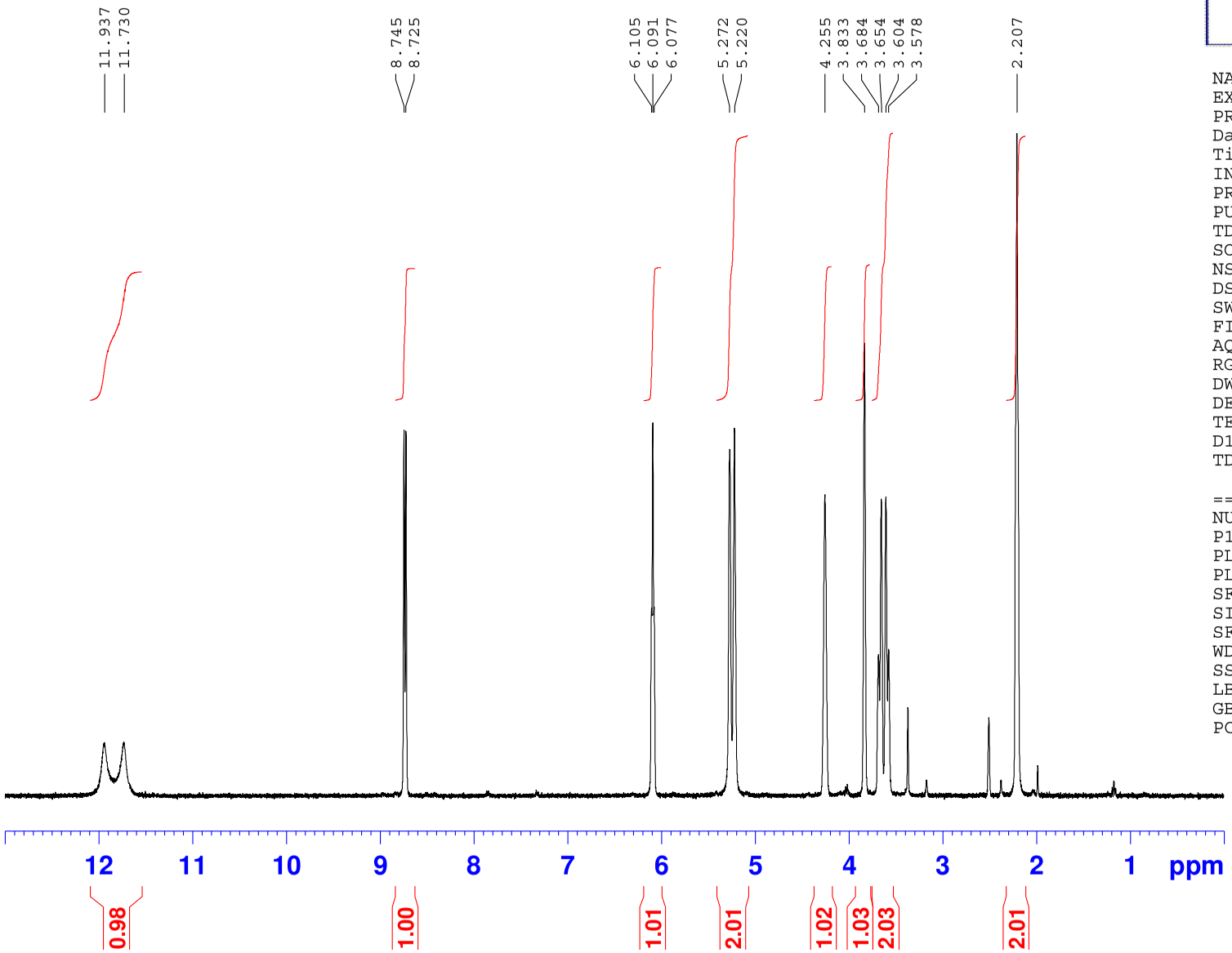
MG111-20120215-JKR #1-96 RT: 0.02-1.99
T: - c NSI Full ms [50.00-700.00]
m/z= 293.90-302.94

m/z	Intensity	Relative
294.02	8137.2	0.07
294.94	6865.9	0.06
295.94	26281.9	0.22
296.97	183027.2	1.55
297.90	11824454.0	100.00
298.92	1092549.3	9.24
299.91	249425.5	2.11
300.91	19247.0	0.16
301.81	23211.0	0.20
302.94	5334.1	0.05



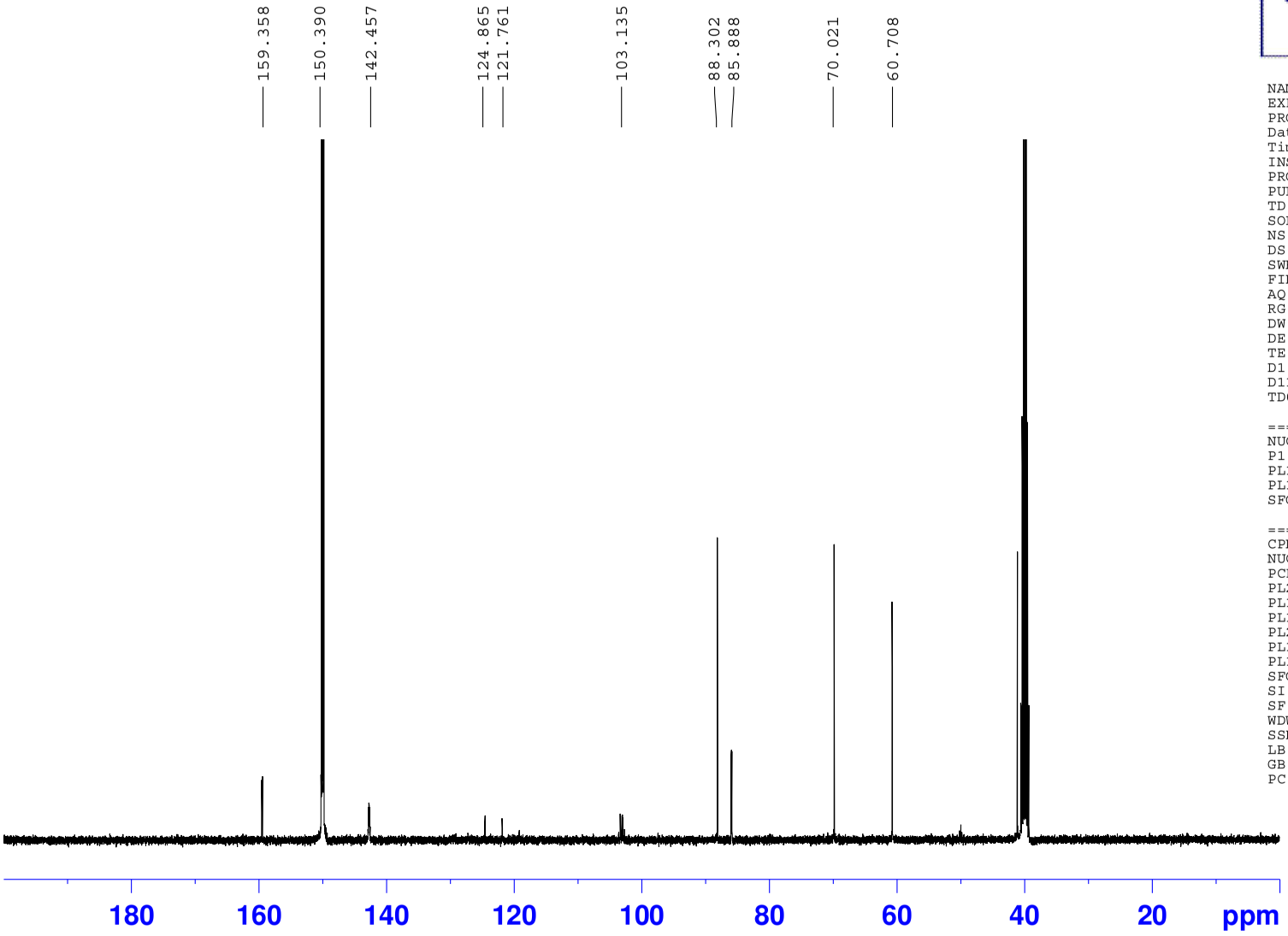


MG111 1H NMR in DMSO-d6
Batch 20120215-JKR



NAME	MG111
EXPNO	2
PROCNO	1
Date_	20120216
Time	15.38
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
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	295.0 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	400.1300000 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

MG111 13C NMR in DMSO-d6
Batch 20120215-JKR



NAME	MG111
EXPNO	1
PROCNO	1
Date_	20120216
Time	15.34
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	4538
DS	4
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	32768
DW	20.850 usec
DE	6.50 usec
TE	295.6 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	7.00 usec
PL1	-3.70 dB
PL1W	84.79348755 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-0.70 dB
PL12	15.16 dB
PL13	15.00 dB
PL2W	10.03411102 W
PL12W	0.26030284 W
PL13W	0.27007160 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.40