SUPPORTING INFORMATION

Total Synthesis of (–)-Sacidumlignans B and D

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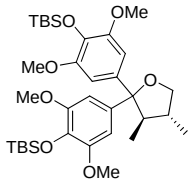
9	 **16**	^{1}H NMR Spectrum	S29
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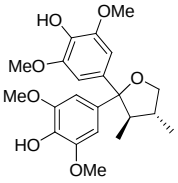
10	 **4**	^{1}H NMR Spectrum	S34
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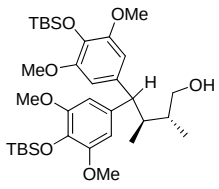
11	 **7**	^{1}H NMR Spectrum	S41
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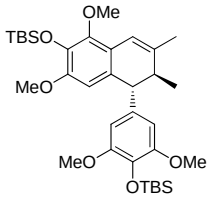
12	 **8**	^{1}H NMR Spectrum	S46
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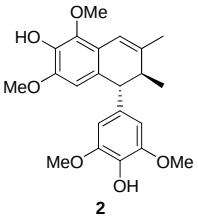
13	 **2**	^{1}H NMR Spectrum	S51
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		DEPT Spectrum	S54
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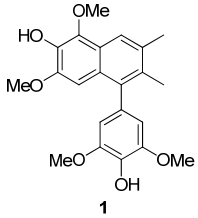
14	 **1**	^{1}H NMR Spectrum	S59
		^{13}C NMR Spectrum	S60
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		Mass Spectra	S62, S63

TABLE 1: Comparative ^{1}H & ^{13}C Coupling Constants (*J*) and/or Chemical Shifts for Natural and Synthetic Sacidumlignan A

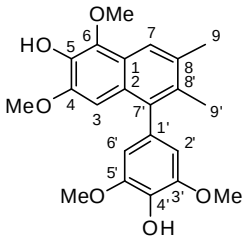
 Sacidumlignan A **1**	***Natural***		***Synthetic***	
	δ_H, *J* (Hz)	δ_C	δ_H, *J* (Hz)	δ_C
1		123.9		123.9
2		127.4		127.4
3	6.56 (1H, s)	101.8	6.58 (1H, s)	101.8
4		149.1		149.1
5		138.0		138.1
6		140.6		140.7
7	7.74 (1H, s)	120.4	7.77 (1H, s)	120.5
8		133.7		133.7
9	2.43	21.3	2.45 (3H, s)	21.4
1’		131.7		131.7
2’, 6’	6.47 (2H, s)	108.2	6.49 (2H, s)	108.2
3’, 5’		148.8		148.9
4’		135.6		135.7
7’		138.6		138.7
8’		131.7		131.8
9’	2.09	17.5	2.11 (3H, s)	17.6
6-OMe	3.95	60.7	3.97 (3H, s)	60.7
3’, 5’-OMe	3.82 (6H, s)	56.7	3.84 (6H, s)	56.7
4-OMe	3.66	55.9	3.67 (3H, s)	55.9
4’, 5-OH	*Not observed*		7.32 (1H, s), 7.73 (1H, s)	

TABLE 2: Comparative ^{1}H & ^{13}C Coupling Constants (*J*) and/or Chemical Shifts for Natural and Synthetic Sacidumlignan B

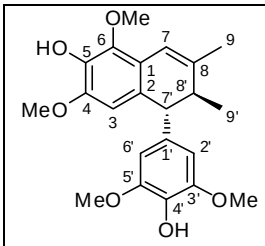
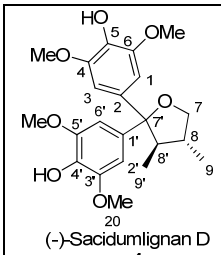
 (-)-Sacidumlignan B **2**	***Natural***		***Synthetic***	
	δ_H, ***J* (Hz)**	δ_C	δ_H, ***J* (Hz)**	δ_C
1		121.3		121.4
2		127.1		127.1
3	6.47 (1H, s)	109.5	6.50 (1H, s)	109.4
4		147.8		147.8
5		138.7		138.8
6		143.9		143.9
7	6.43 (1H, d, 1.2)	116.0	6.46 (1H, d, 1.2)	116.1
8		139.1		139.1
9	1.80 (3H, d, 1.2)	22.6	1.82 (3H, d, 1.2)	22.7
1’		137.1		137.1
2’, 6’	6.39 (2H, s)	106.0	6.42 (2H, s)	105.9
3’, 5’		148.3		148.3
4’		135.0		135.1
7’	3.64 (1H, d, 3.0)	51.9	3.67 (1H, d, 3.0)	52.0
8’	2.04 (1H, dq, 7.0, 3.0)	42.4	2.41 (1H, dq, 7.0, 3.0)	42.5
9’	1.02 (3H, d, 7.0)	18.8	1.05 (3H, d, 7.0)	18.9
6-OMe	3.79 (3H, s)	60.9	3.81 (3H, s)	60.9
3’, 5’-OMe	3.68 (6H, s)	56.5	3.71 (6H, s)	56.4
4-OMe	3.72 (3H, s)	51.9	3.74 (3H, s)	52.0
4’, 5-OH	*Not observed*		6.95 (1H, s), 7.31(1H, s)	

TABLE 3: Comparative ^{1}H & ^{13}C Coupling Constants (*J*) and/or Chemical Shifts for Natural and Synthetic Sacidumlignan D

 (-)-Sacidumlignan D **4**	***Natural***		***Synthetic***	
	δ_H, *J* (Hz)	**δ_C**	**δ_H, *J* (Hz)**	**δ_C**
1,3	6.50 (2H, s)	106.6	6.53 (2H, s)	106.4
2		137.1		137.1
4, 6		148.1		148.0
5		135.8		135.7
7	**7α**: 3.20 (1H, dd, 10.0, 8.0) **7β:** 4.25 (1H, dd, 8.0, 7.7)	74.3	**7α:** 3.33 (1H, dd, 10.1, 8.2) **7β:** 4.26 (1H, t, 7.7)	74.2
8	2.00 (1H, m)	42.3	1.99 (1H, m)	42.3
9	0.96 (3H,d, 6.5)	15.4	0.98 (3H,d, 6.5)	15.4
1’		139.4		139.4
2’, 6’	6.76 (2H, s)	106.3	6.78 (2H, s)	106.0
3’, 5’		148.5		148.4
4’		136.2		136.2
7’		91.7		91.5
8’	2.40 (1H, dq, 9.6, 6.9)	51.2	2.42 (1H, dq, 9.6, 6.9)	51.2
9’	0.85 (3H, d, 6.9)	17.0	0.86 (3H, d, 6.9)	17.0
4,6-OMe	3.72 (6H, s)	57.0	3.73 (6H, s)	56.9
3’, 5’-OMe	3.78 (6H, s)	57.2	3.80 (6H, s)	57.1
4’, 5-OH	*Not observed*		7.06 (1H, s), 7.17 (1H, s)	

Acquisition Time (sec)	4.0894	***Comment***	Jeetendra			***Date***	11/05/2011 15:30:24
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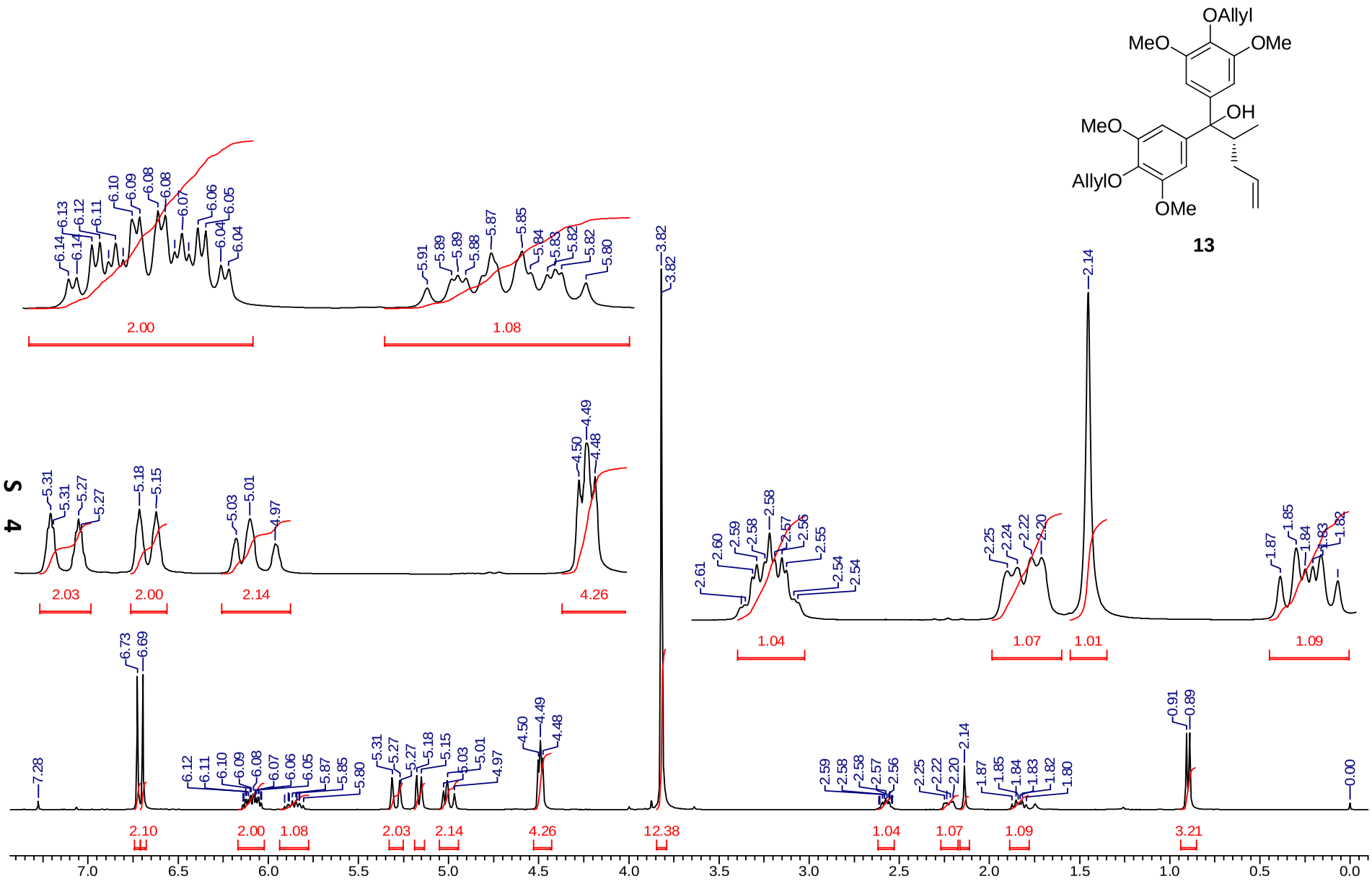
Temperature (grad C)	0.000						



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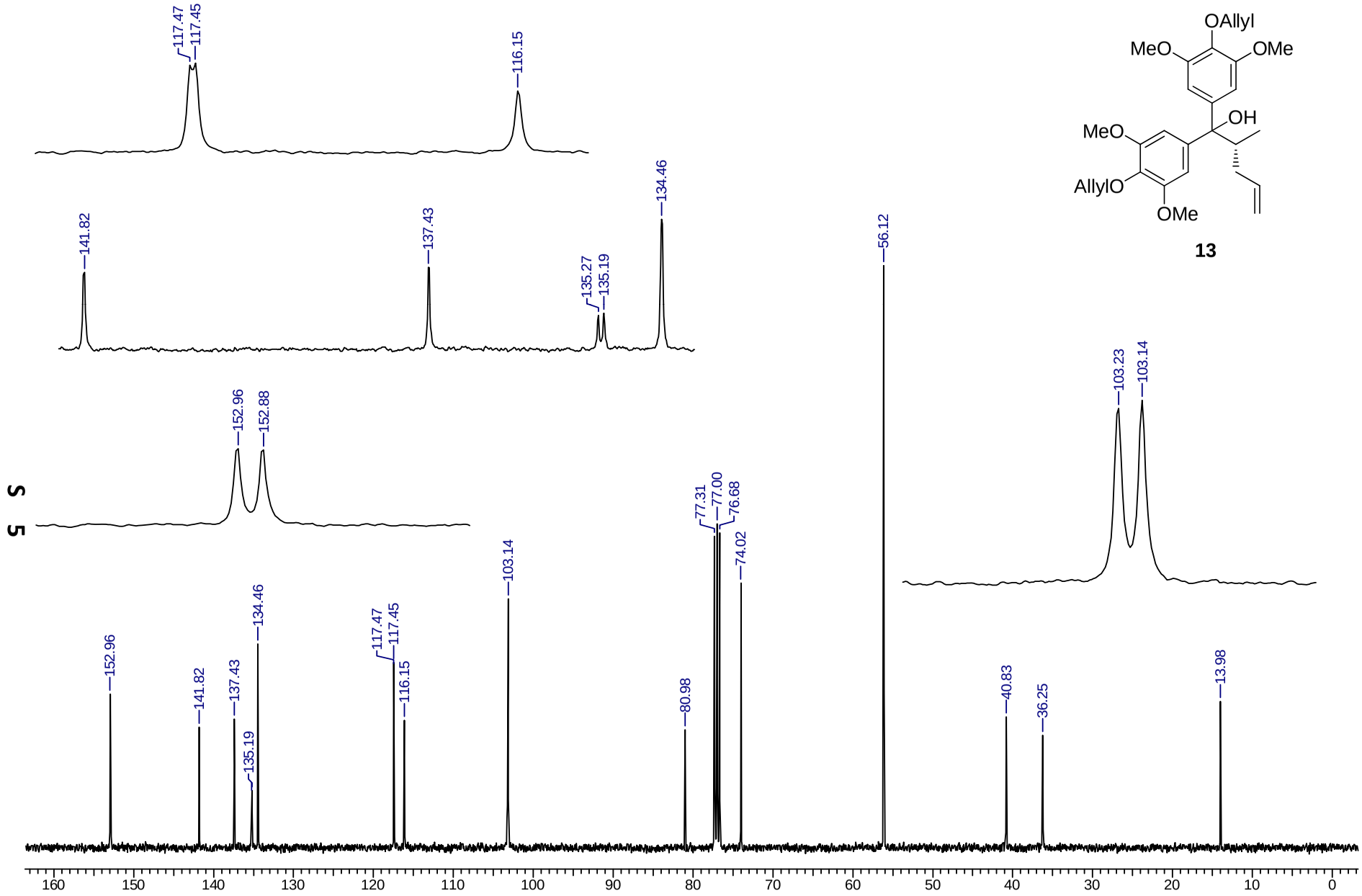

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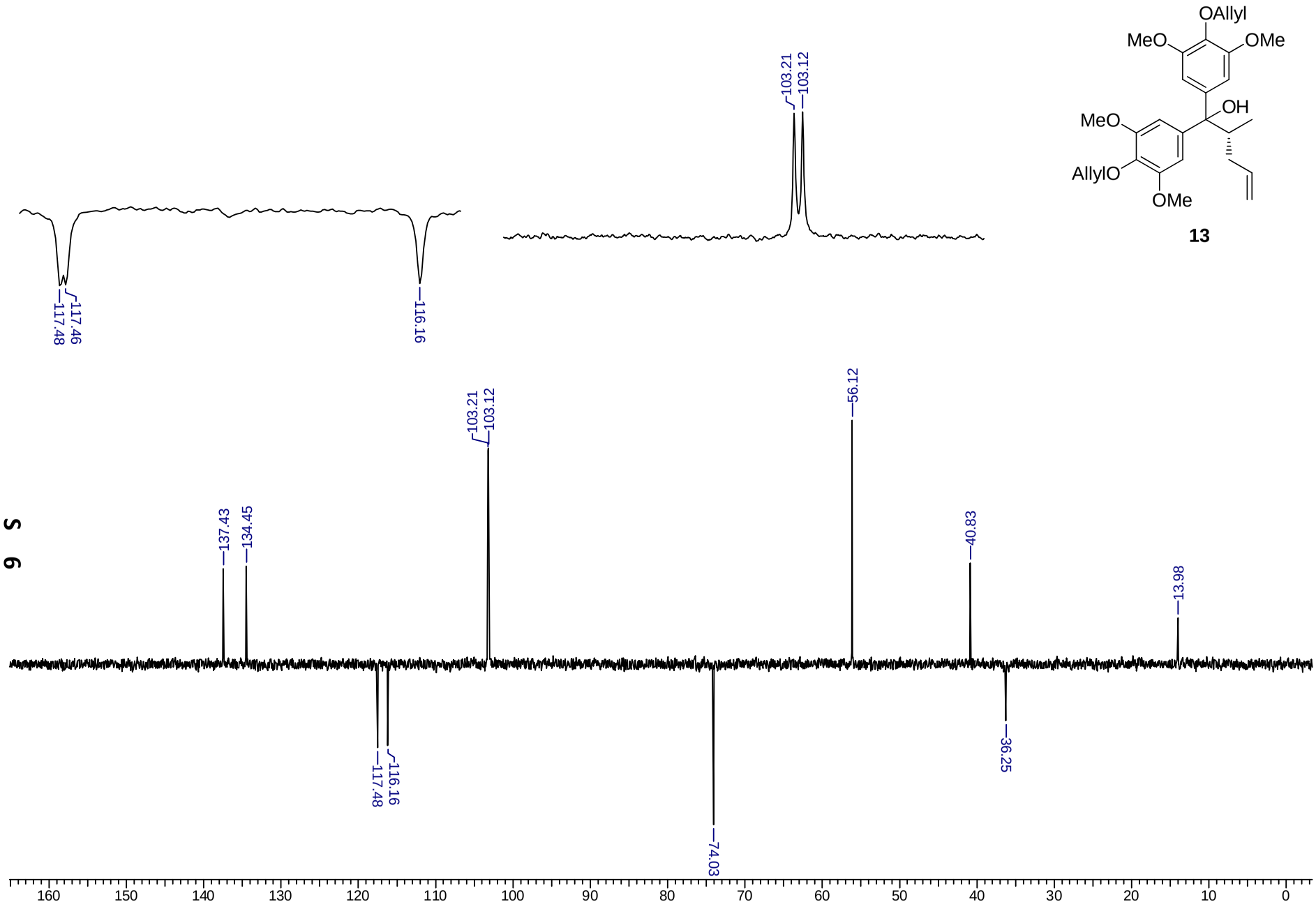

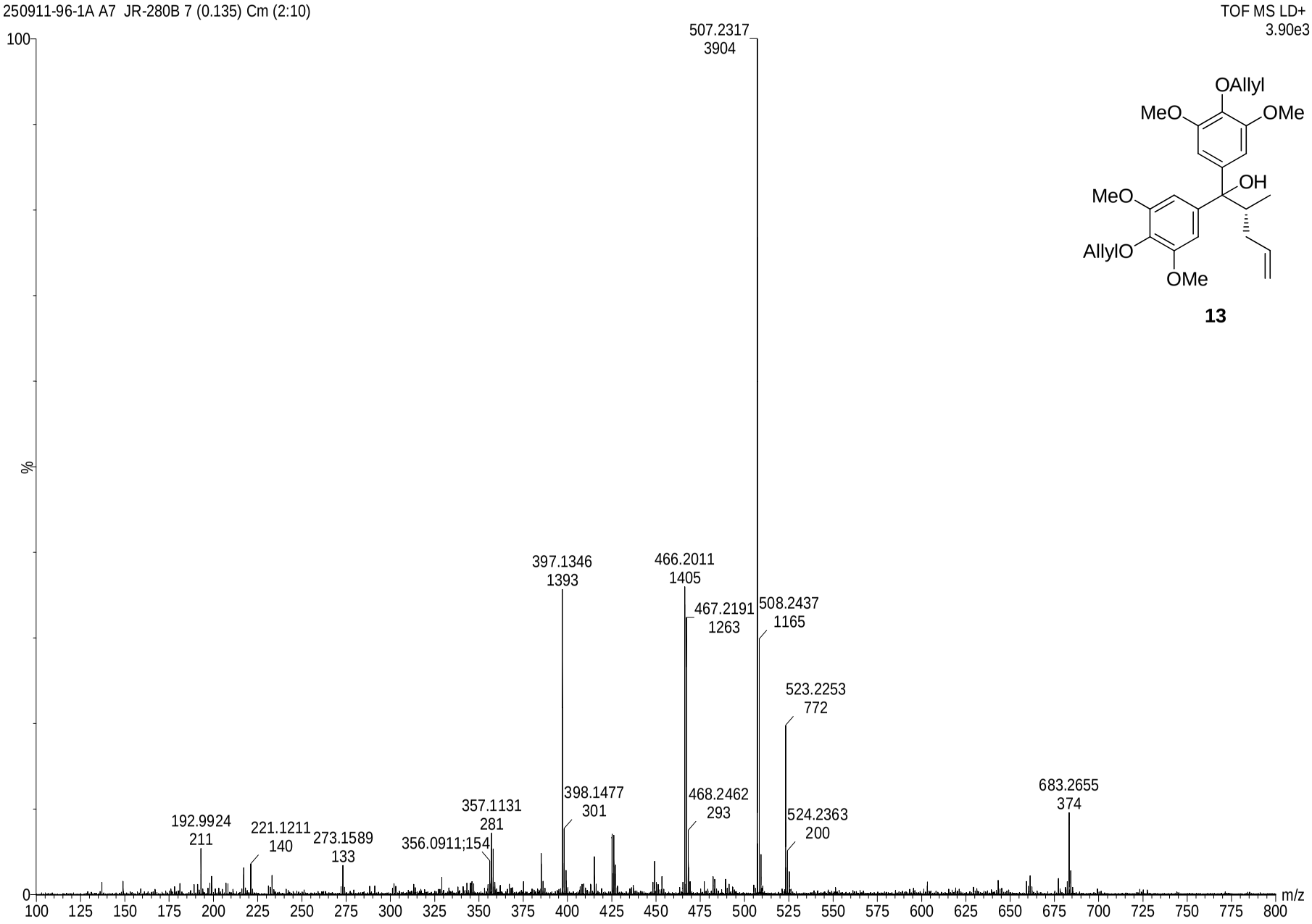
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%
0
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397.1346
1393
466.2011
1405
467.2191
1263
508.2437
1165
523.2253
772
683.2655
374
398.1477
301
468.2462
293
524.2363
200
357.1131
281
192.9924
211
221.1211
140
273.1589
133
356.0911;154
100 125 150 175 200 225 250 275 300 325 350 375 400 425 450 475 500 525 550 575 600 625 650 675 700 725 750 775 800
m/z
OAllyl
MeO
OMe
OH
MeO
AllylO
OMe
13

F:\DATA\RAMANA\JR260-D 2/24/2011 3:27:20 PM

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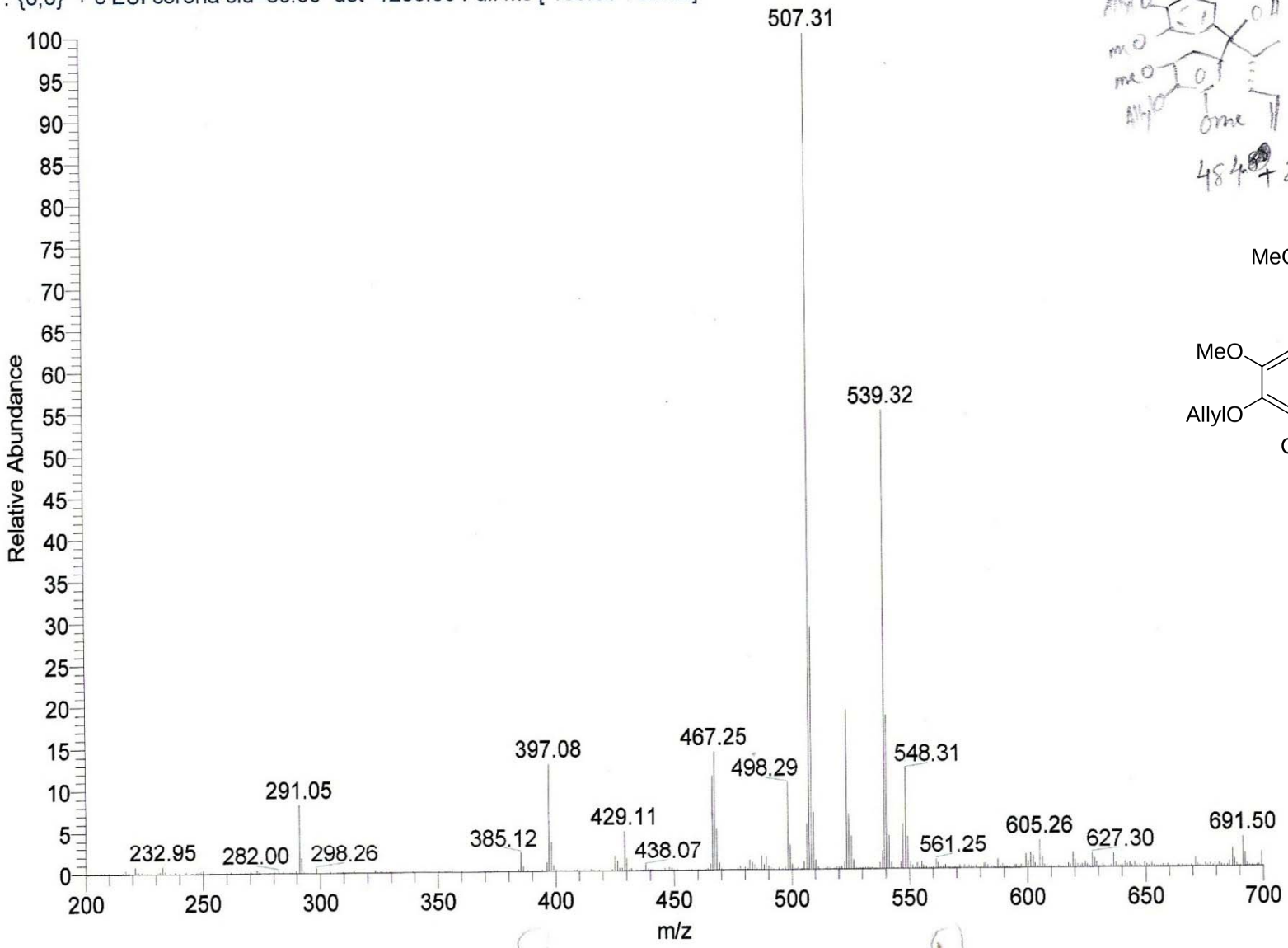

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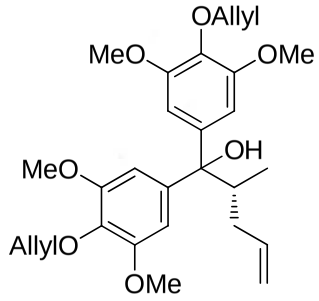

13

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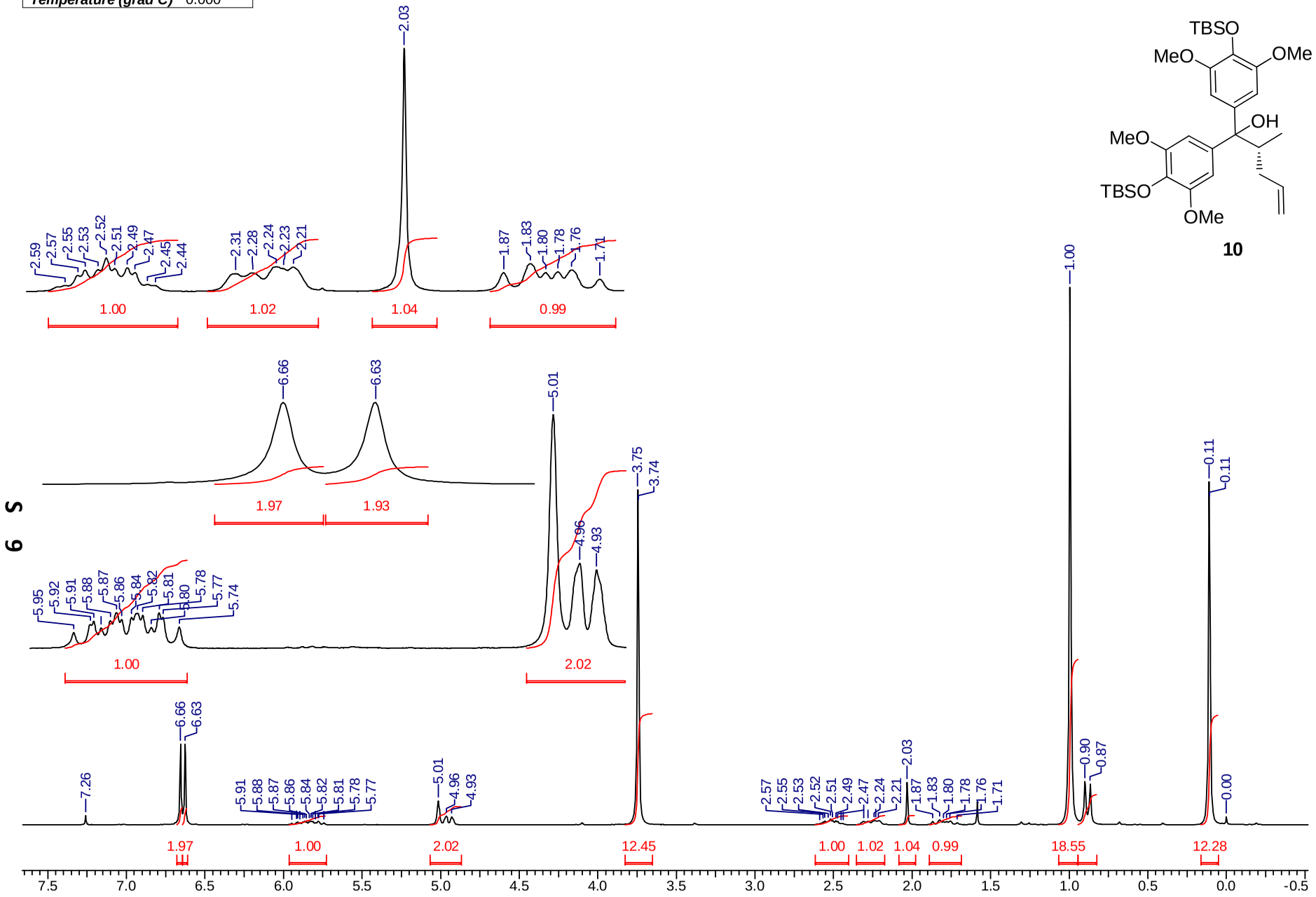
Temperature (grad C)	0.000						



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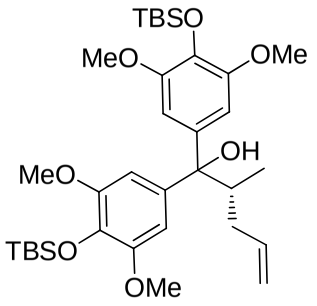
Temperature (grad C)	0.000						



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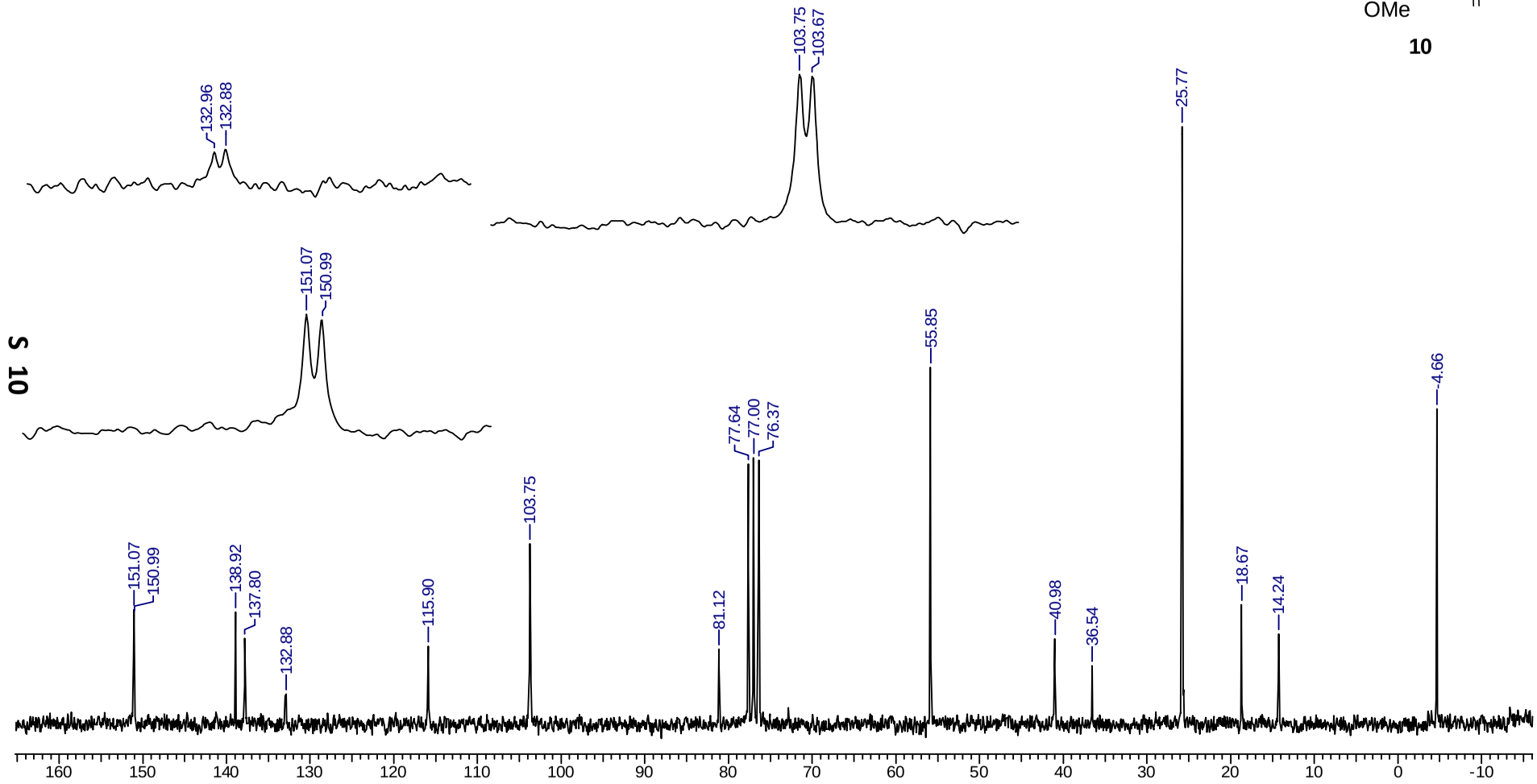

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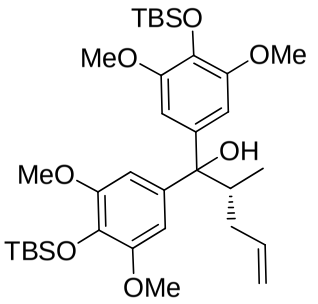
Temperature (grad C)	0.000						



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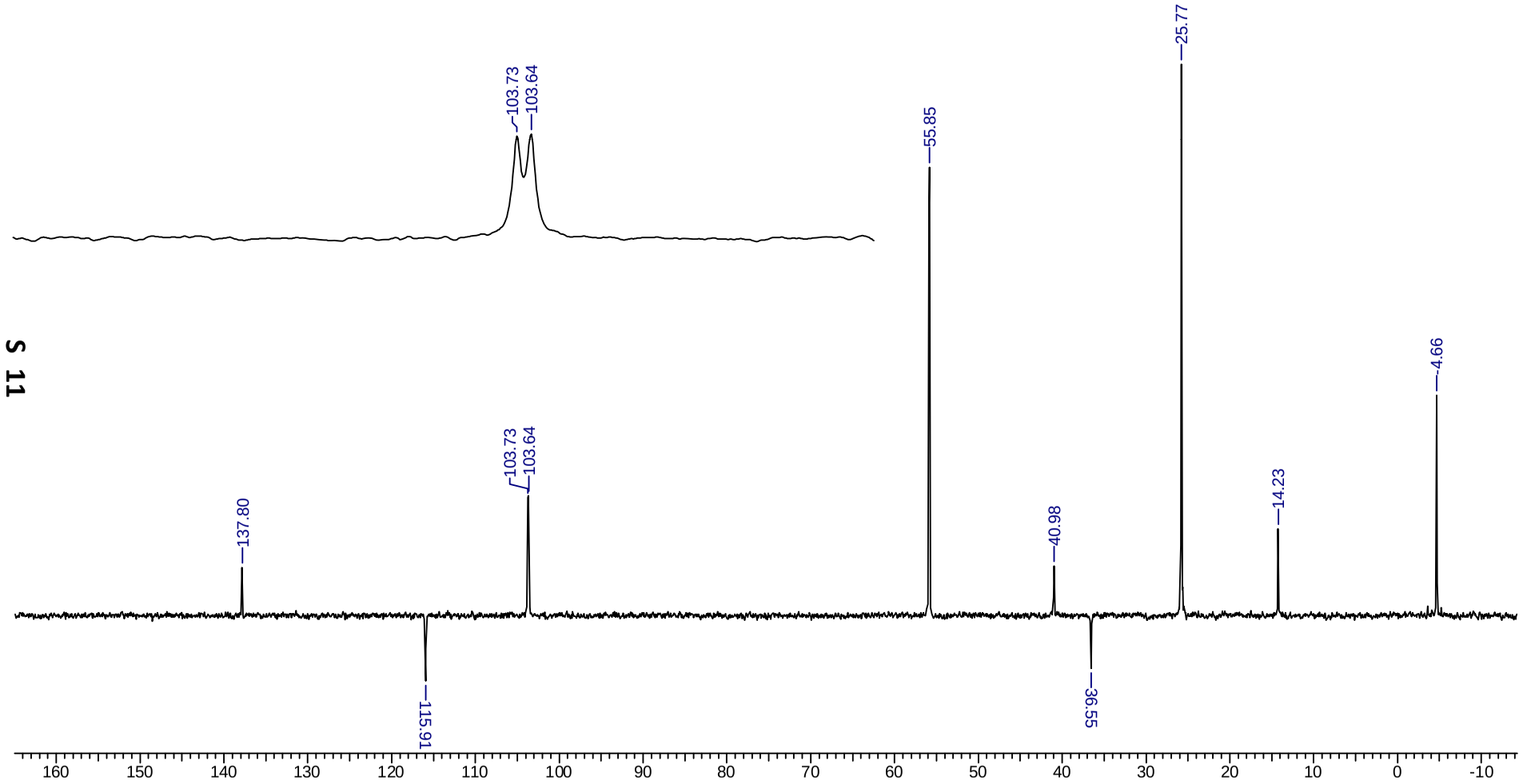

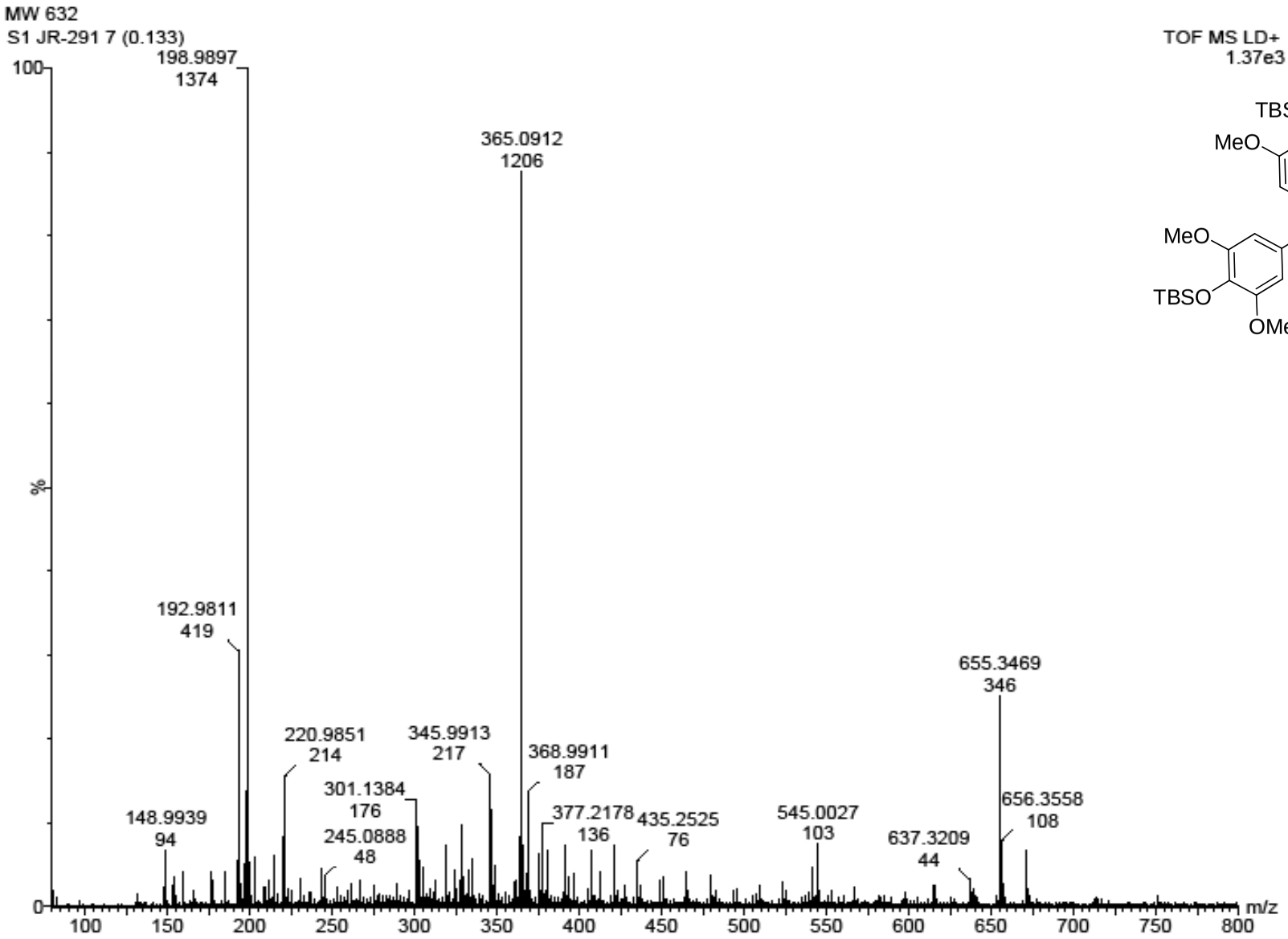
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1206
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419
220.9851
214
345.9913
217
368.9911
187
301.1384
176
148.9939
94
245.0888
48
377.2178
136
435.2525
76
545.0027
103
637.3209
44
655.3469
346
656.3558
108
100
%
0
100
150
200
250
300
350
400
450
500
550
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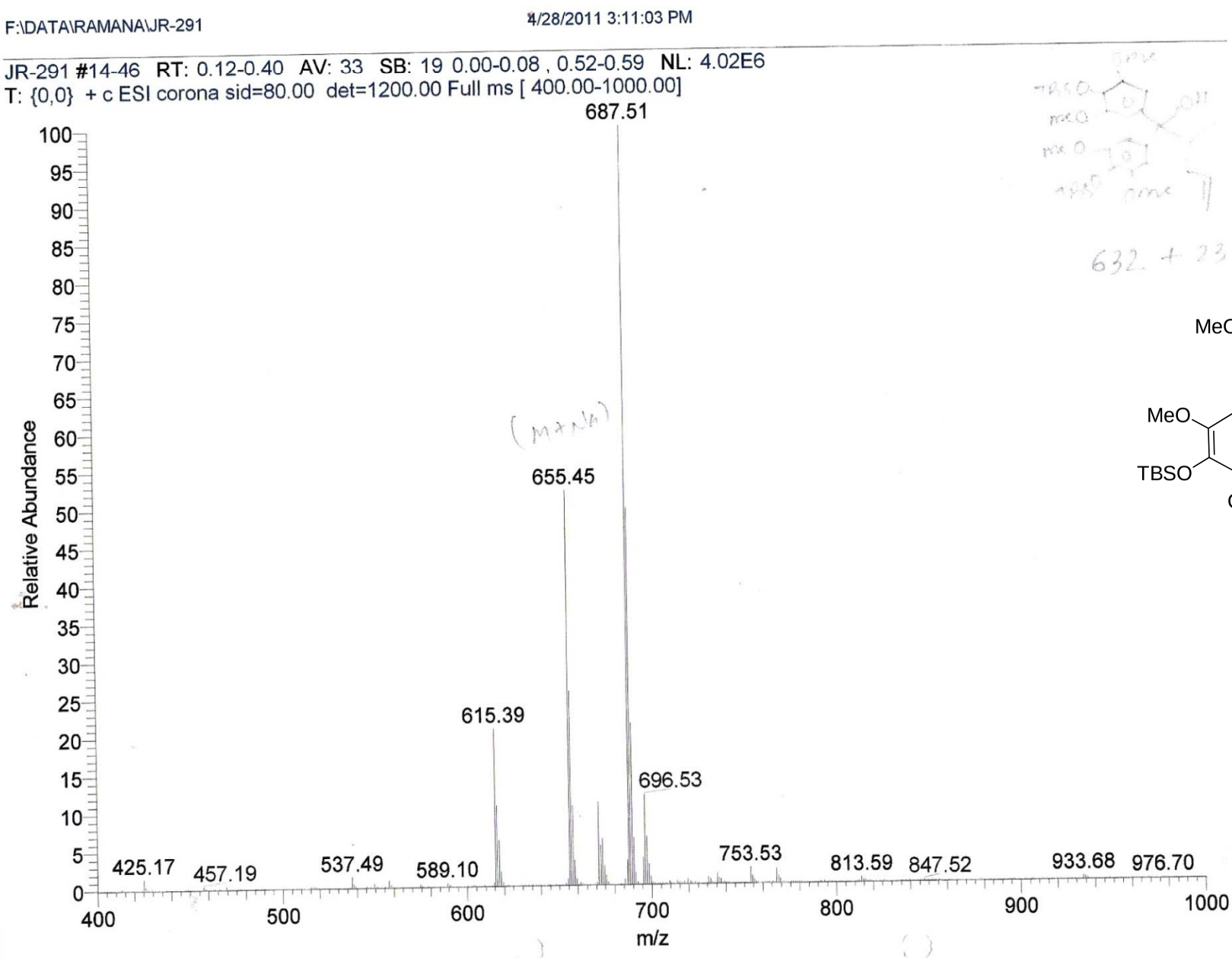
650
700
750
800
m/z
TBSO
MeO
OMe
OH
MeO
TBSO
OMe

10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687.51
655.45
615.39
696.53
425.17
457.19
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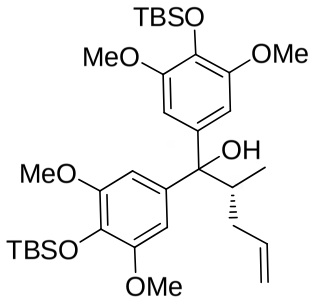
Relative Abundance
m/z
632 + 23 = 655
(M+Na)


TBSO
MeO
OMe
OH
MeO
TBSO
OMe

10

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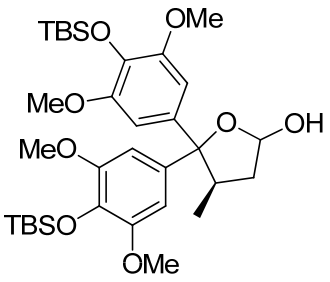
Temperature (grad C)	0.000						



15

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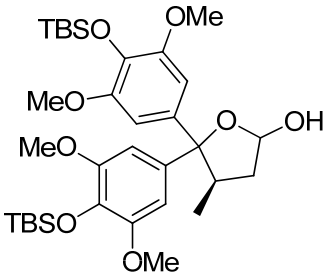

15

S 15

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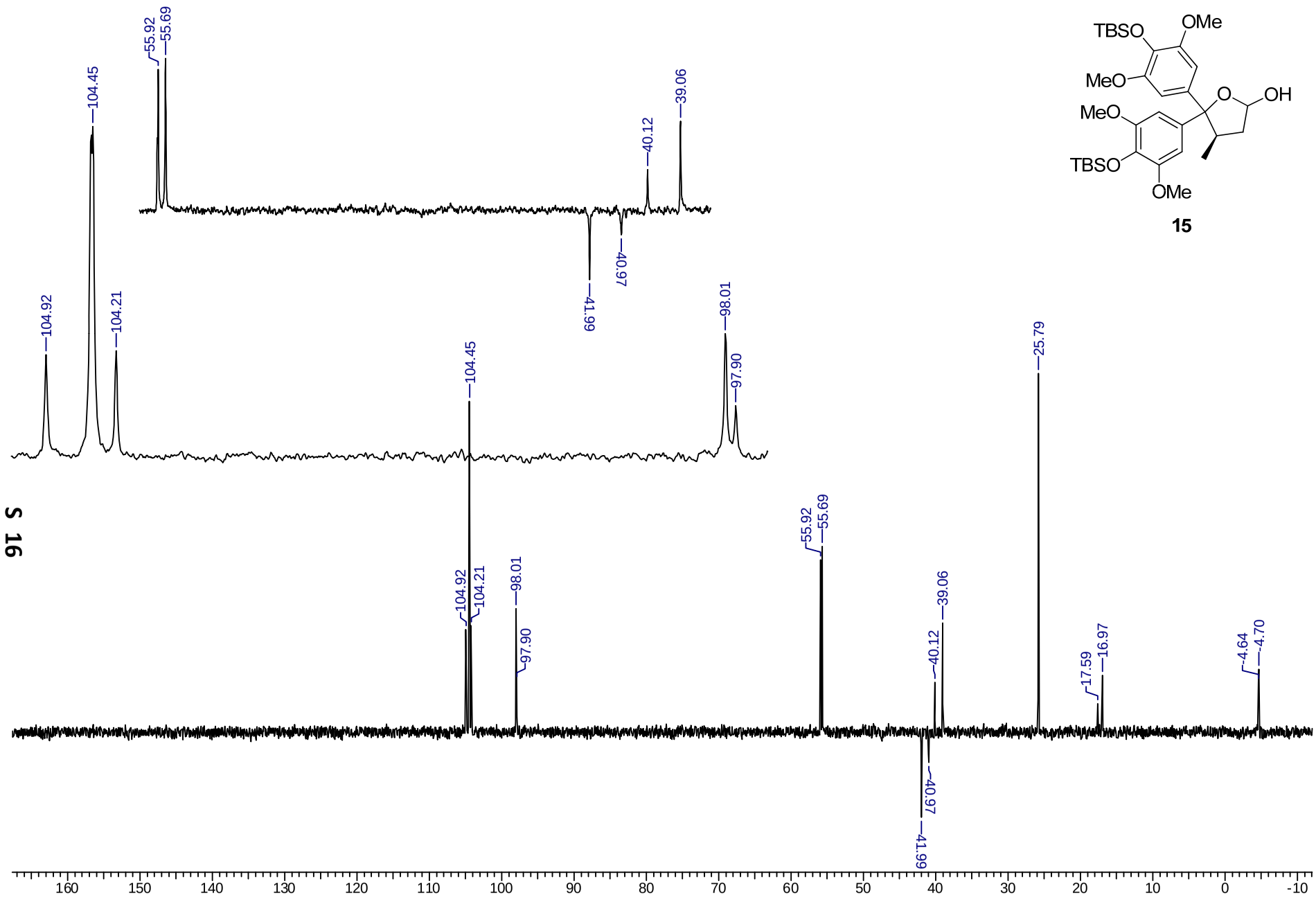

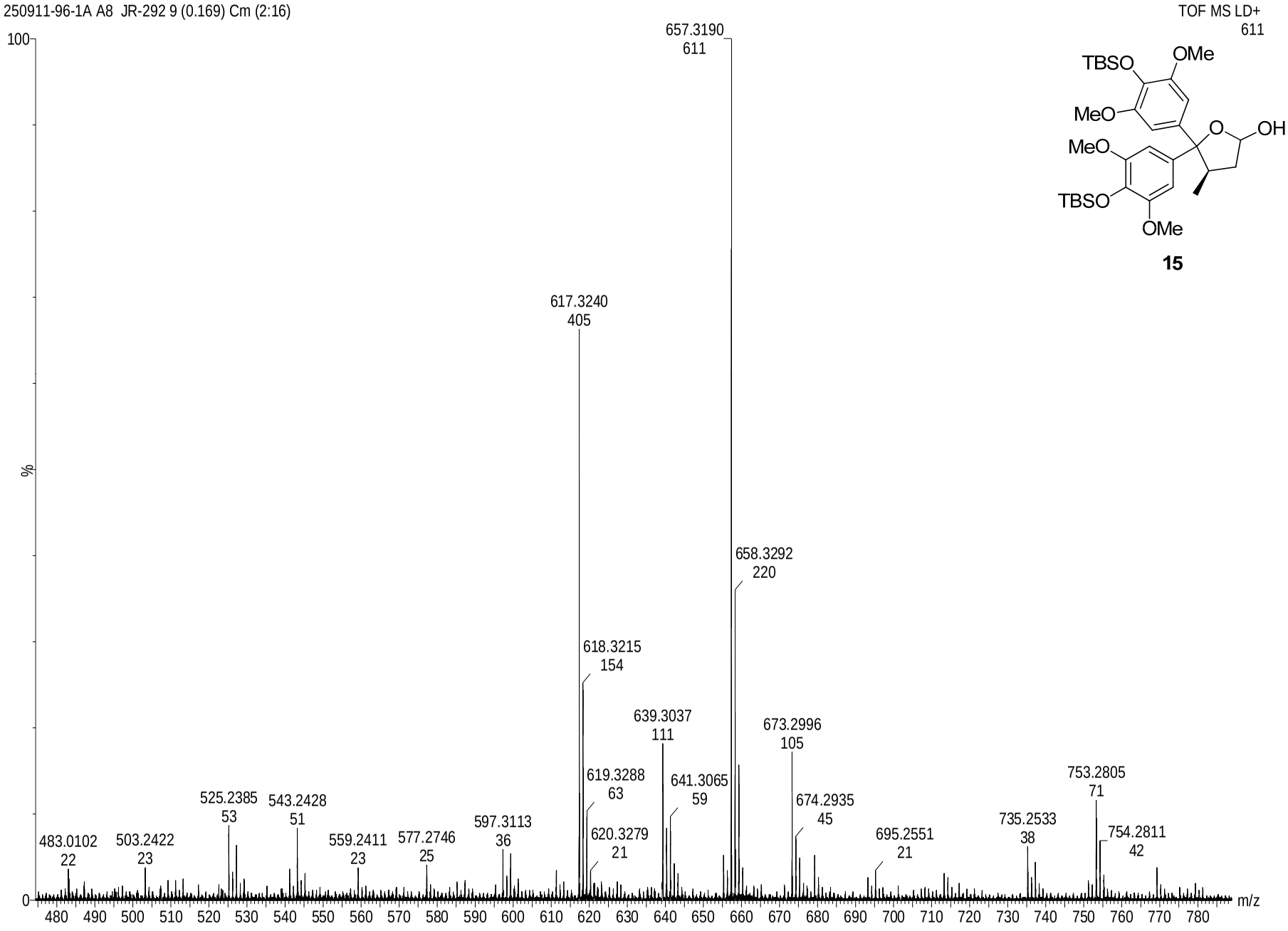
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%
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617.3240
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658.3292
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618.3215
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639.3037
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673.2996
105
619.3288
63
641.3065
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674.2935
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753.2805
71
525.2385
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543.2428
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597.3113
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620.3279
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735.2533
38
754.2811
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483.0102
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503.2422
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559.2411
23
577.2746
25
695.2551
21
480 490 500 510 520 530 540 550 560 570 580 590 600 610 620 630 640 650 660 670 680 690 700 710 720 730 740 750 760 770 780
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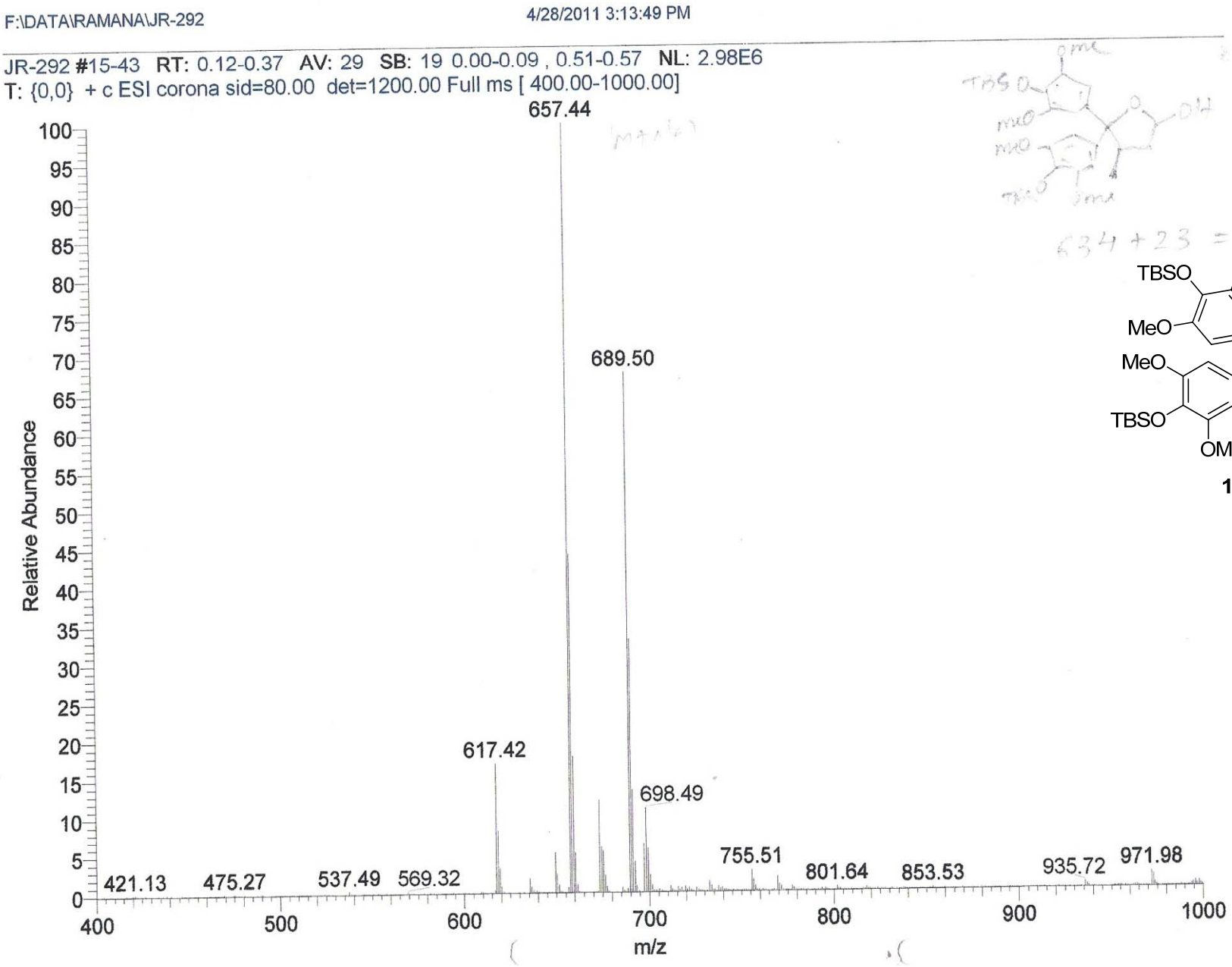
OMe
MeO
O
OH
MeO
TBSO
OMe
15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689.50
617.42
698.49
421.13
475.27
537.49
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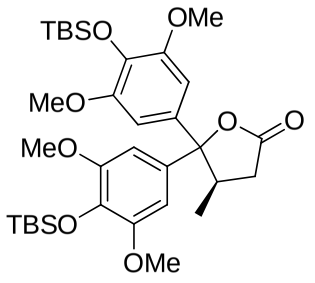
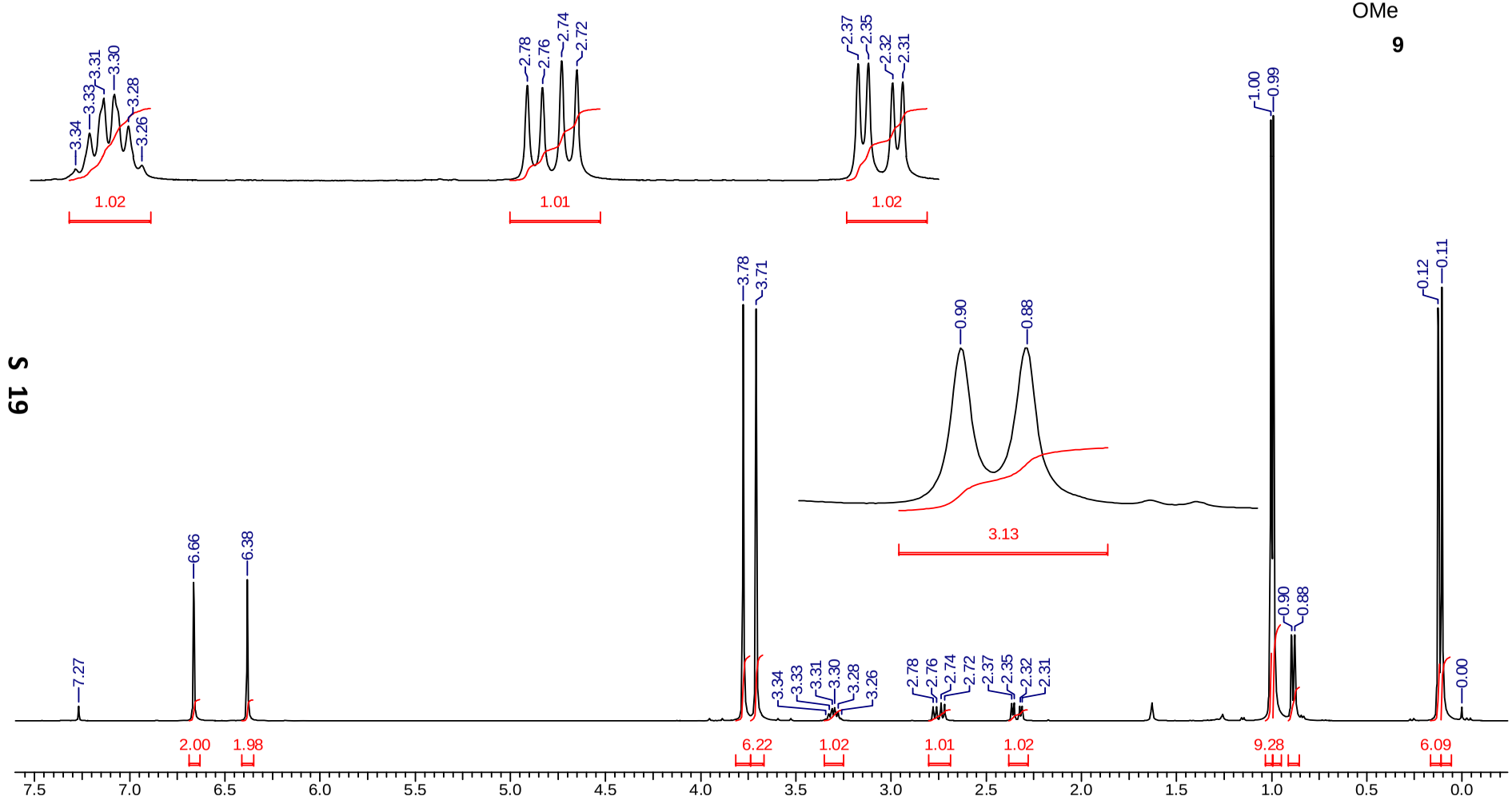
755.51
801.64
853.53
935.72
971.98
Relative Abundance
m/z
TBSO
OMe
MeO
O
OH
MeO
TBSO
OMe

15

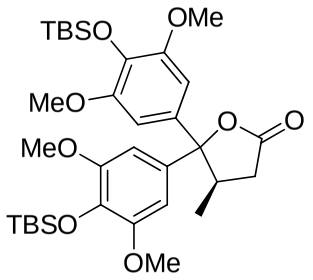
Acquisition Time (sec)	4.0894	***Comment***	Jeetendra		***Date***	11/05/2011 15:54:28	
Frequency (MHz)	400.13	***Nucleus***	1H	***Original Points Count*** 32768	***Points Count***	32768	***Sweep Width (Hz)*** 8012.82
Temperature (grad C)	0.000						



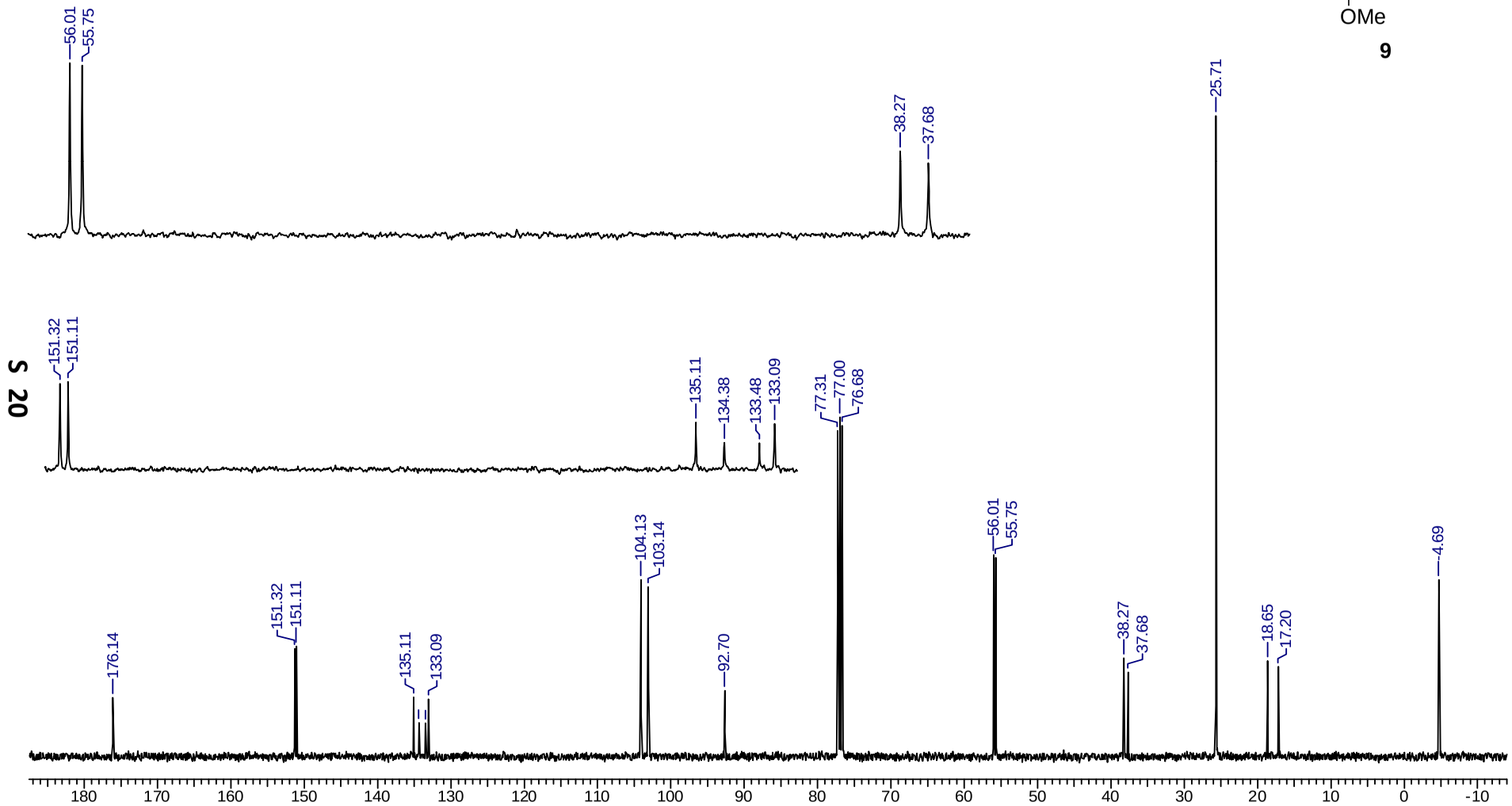
9



Acquisition Time (sec)	1.3631	***Date***	11/05/2011 16:23:34	***Frequency (MHz)***	100.61	***Nucleus***	13C
Original Points Count	32768	***Points Count***	32768	***Sweep Width (Hz)***	24038.46	***Temperature (grad C)***	0.000

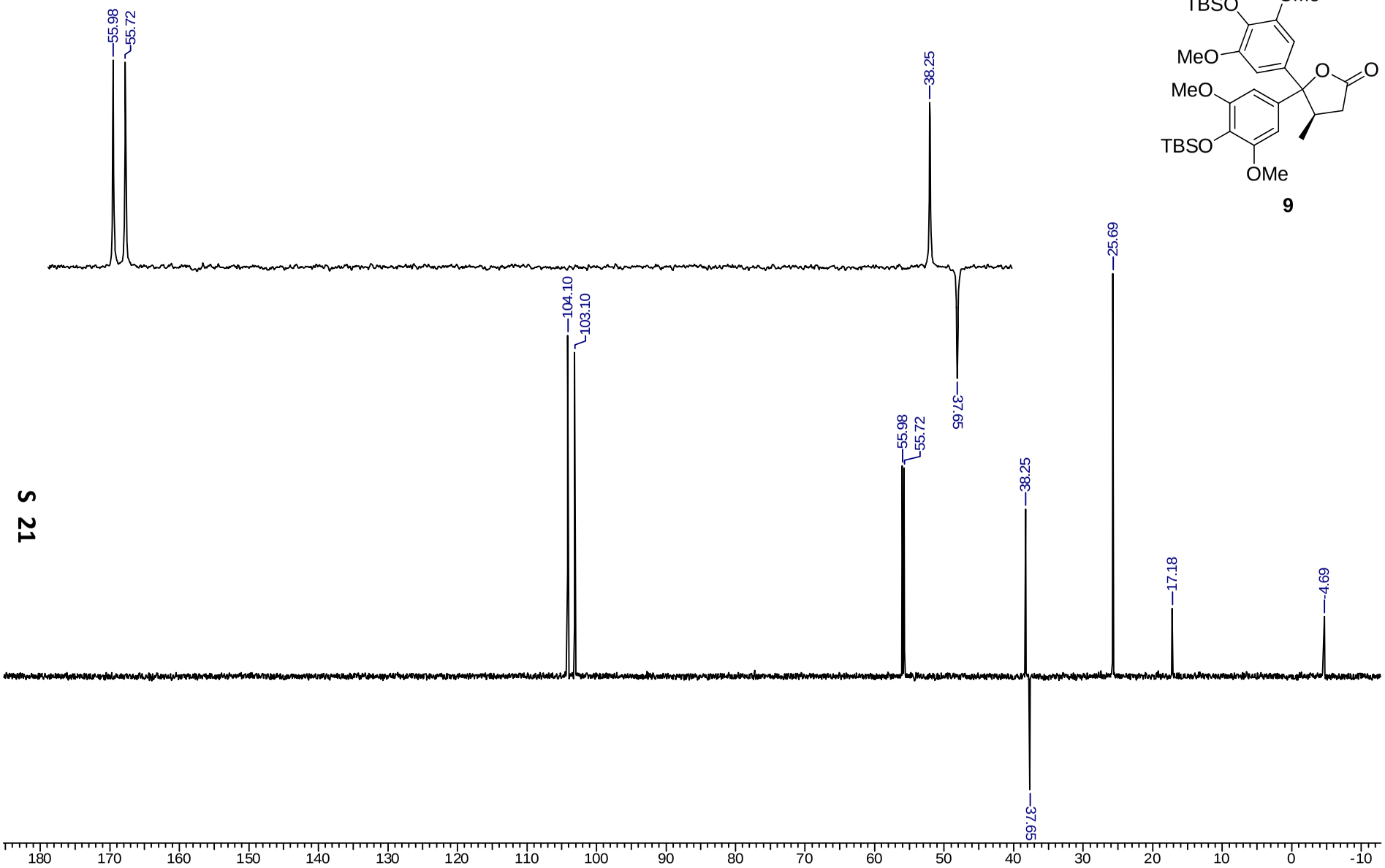


9

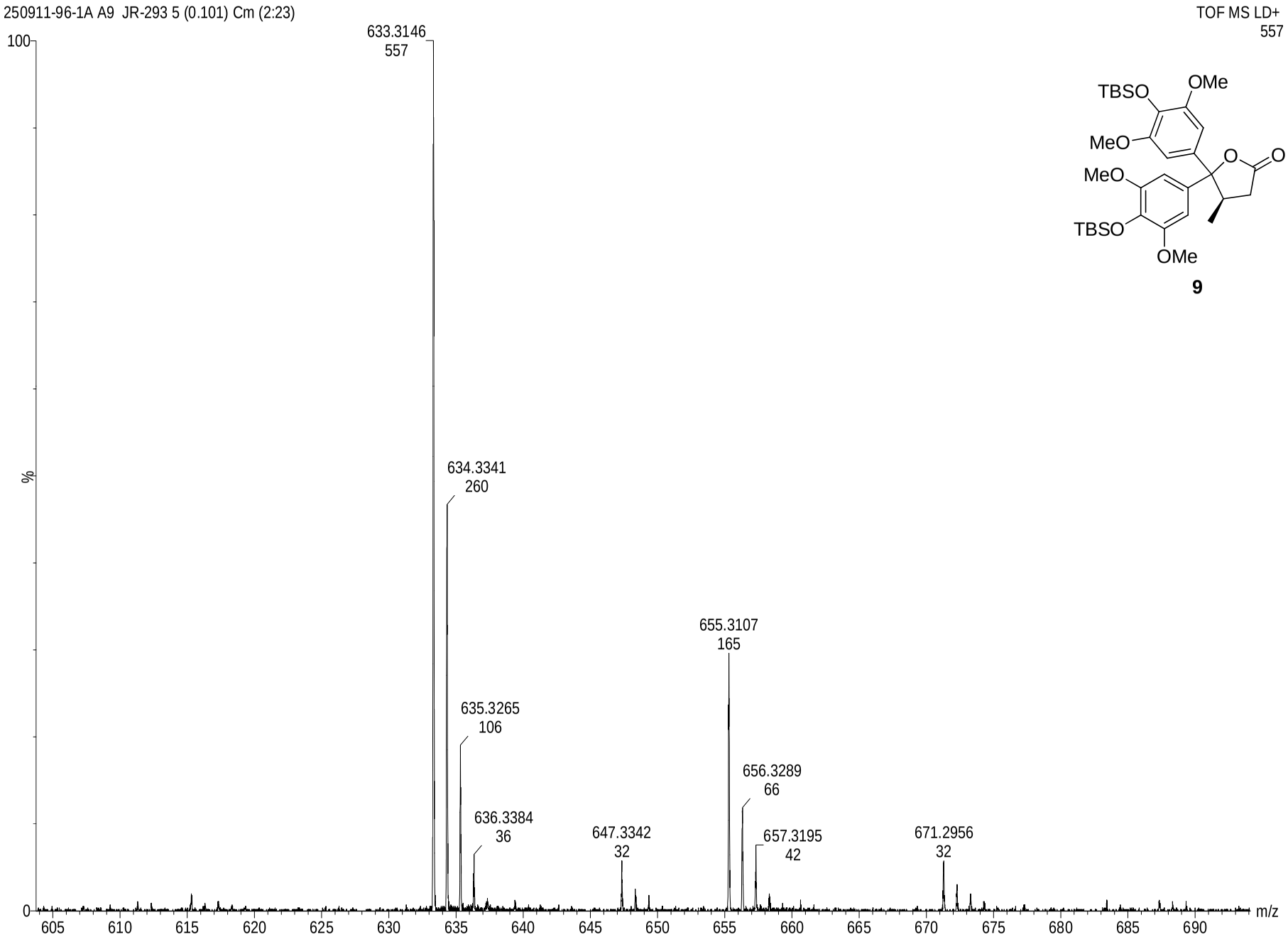


20 May 2011

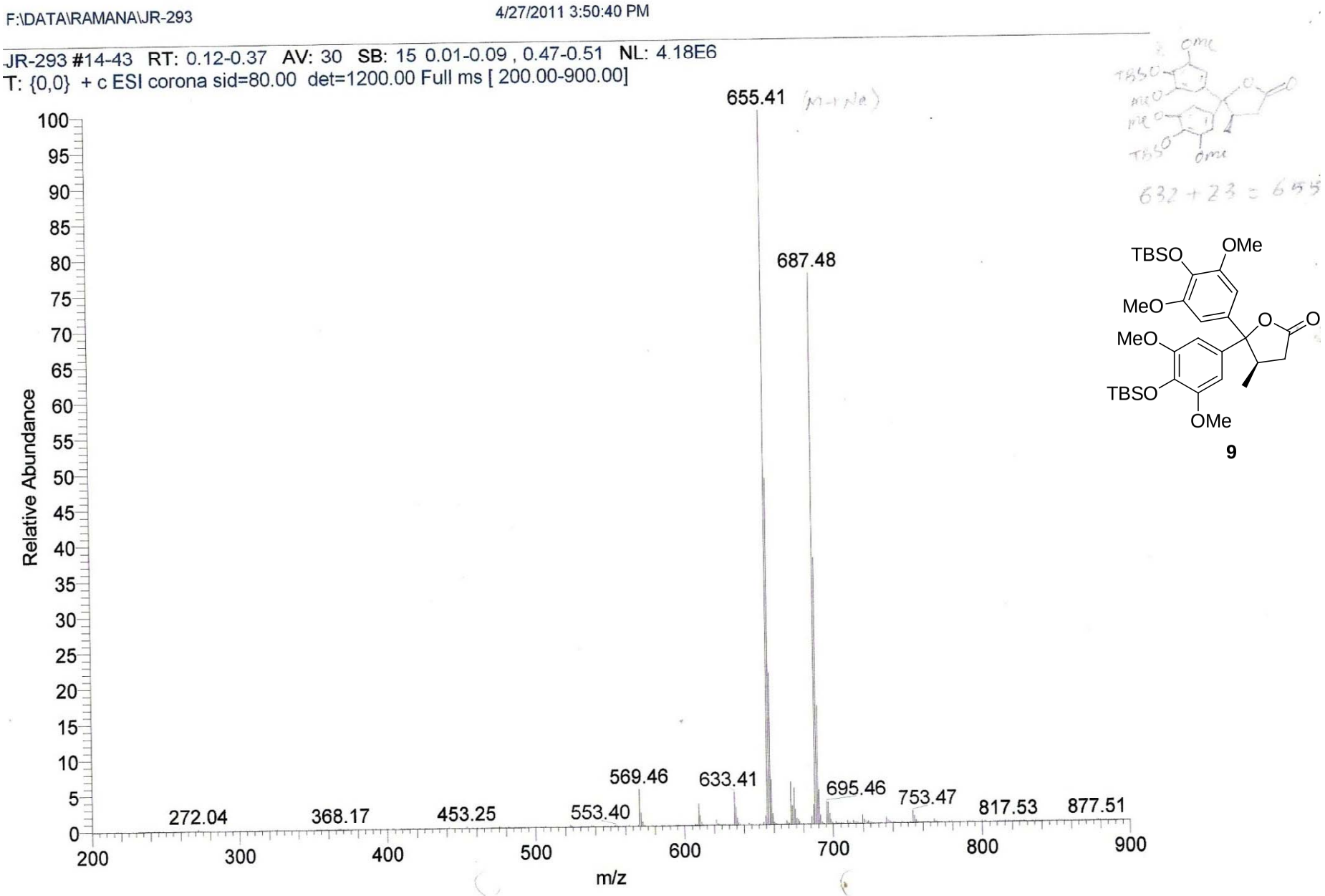
Acquisition Time (sec) 1.3631	***Date***	11/05/2011 16:23:02		***Frequency (MHz)***	100.61	***Nucleus***	13C
Original Points Count 32768	***Points Count***	32768	***Sweep Width (Hz)*** 24038.46			***Temperature (grad C)***	0.000



9

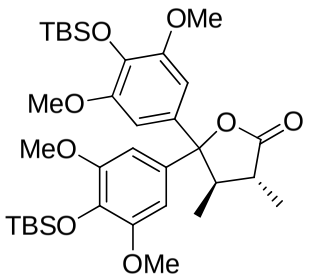

250911-96-1A A9 JR-293 5 (0.101) Cm (2:23)
TOF MS LD+
557
100
%
0
633.3146
557
634.3341
260
635.3265
106
636.3384
36
647.3342
32
655.3107
165
656.3289
66
657.3195
42
671.2956
32
m/z
605
610
615
620
625
630
635
640
645
650
655
660
665
670
675
680
685
690
TBSO
OMe
MeO
O
O
MeO
TBSO
OMe

9


F:\DATA\RAMANA\JR-293
4/27/2011 3:50:40 PM
JR-293 #14-43 RT: 0.12-0.37 AV: 30 SB: 15 0.01-0.09 , 0.47-0.51 NL: 4.18E6
T: {0,0} + c ESI corona sid=80.00 det=1200.00 Full ms [200.00-900.00]
655.41
687.48
569.46
633.41
695.46
753.47
817.53
877.51
272.04
368.17
453.25
553.40
Relative Abundance
m/z
632 + 23 = 655
TBSO
OMe
MeO
MeO
TBSO
OMe
O
O

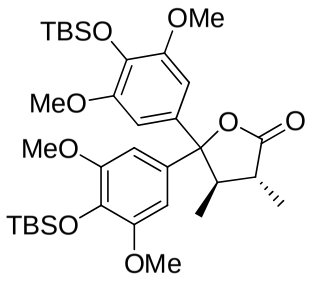
9

Acquisition Time (sec)	4.0894	***Comment***	1H/	***Date***	24/04/2011 12:55:22	***Frequency (MHz)***	400.13
Nucleus	1H	***Original Points Count***	32768	***Points Count***	32768	***Sweep Width (Hz)***	8012.82
Temperature (grad C)	0.000						

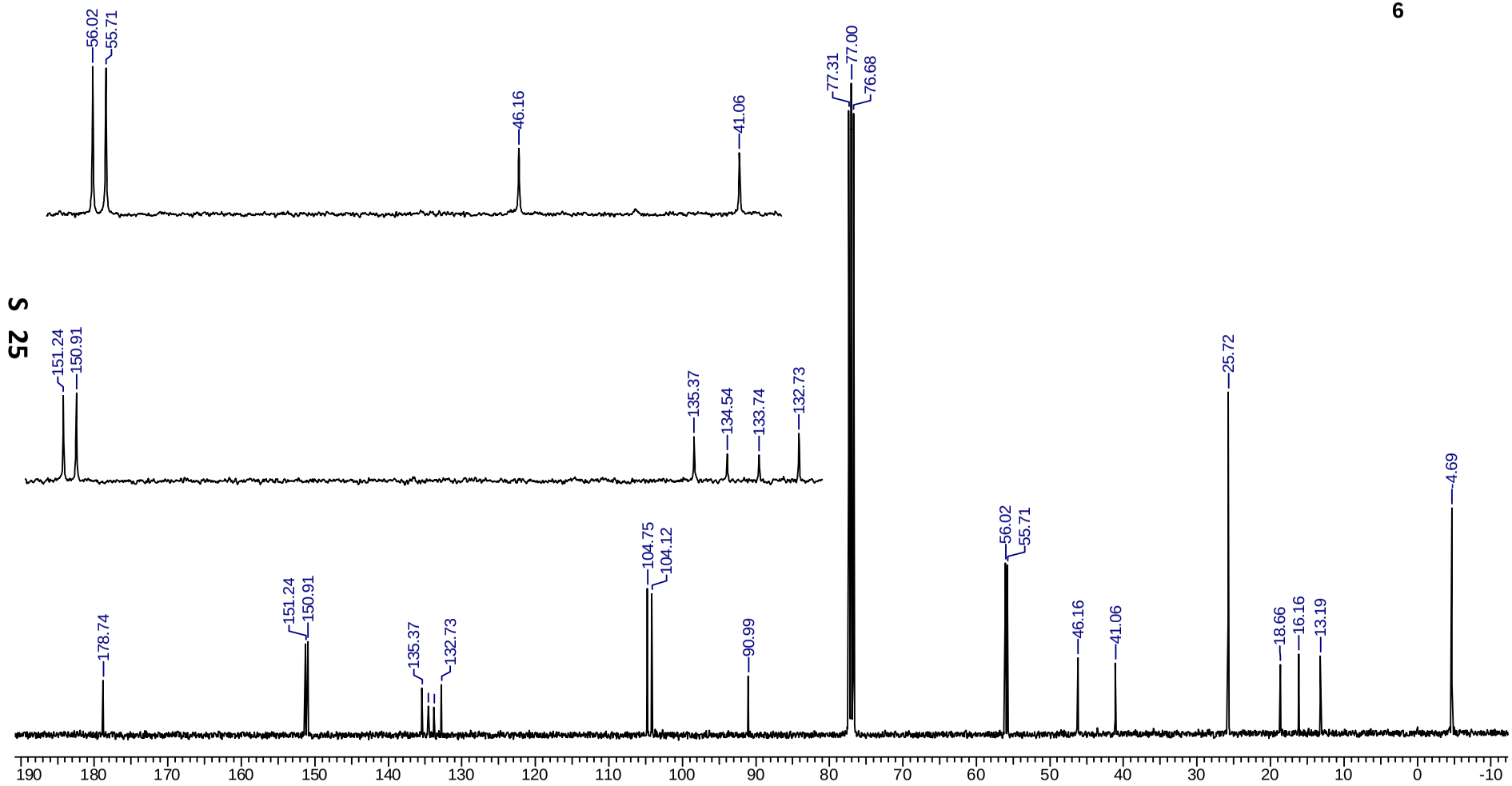


6

Acquisition Time (sec) 1.2976	***Date***	24/04/2011 13:49:42		***Frequency (MHz)***	100.61	***Nucleus***	13C
Original Points Count 32768	***Points Count***	32768	***Sweep Width (Hz)*** 25252.53			***Temperature (grad C)***	0.000

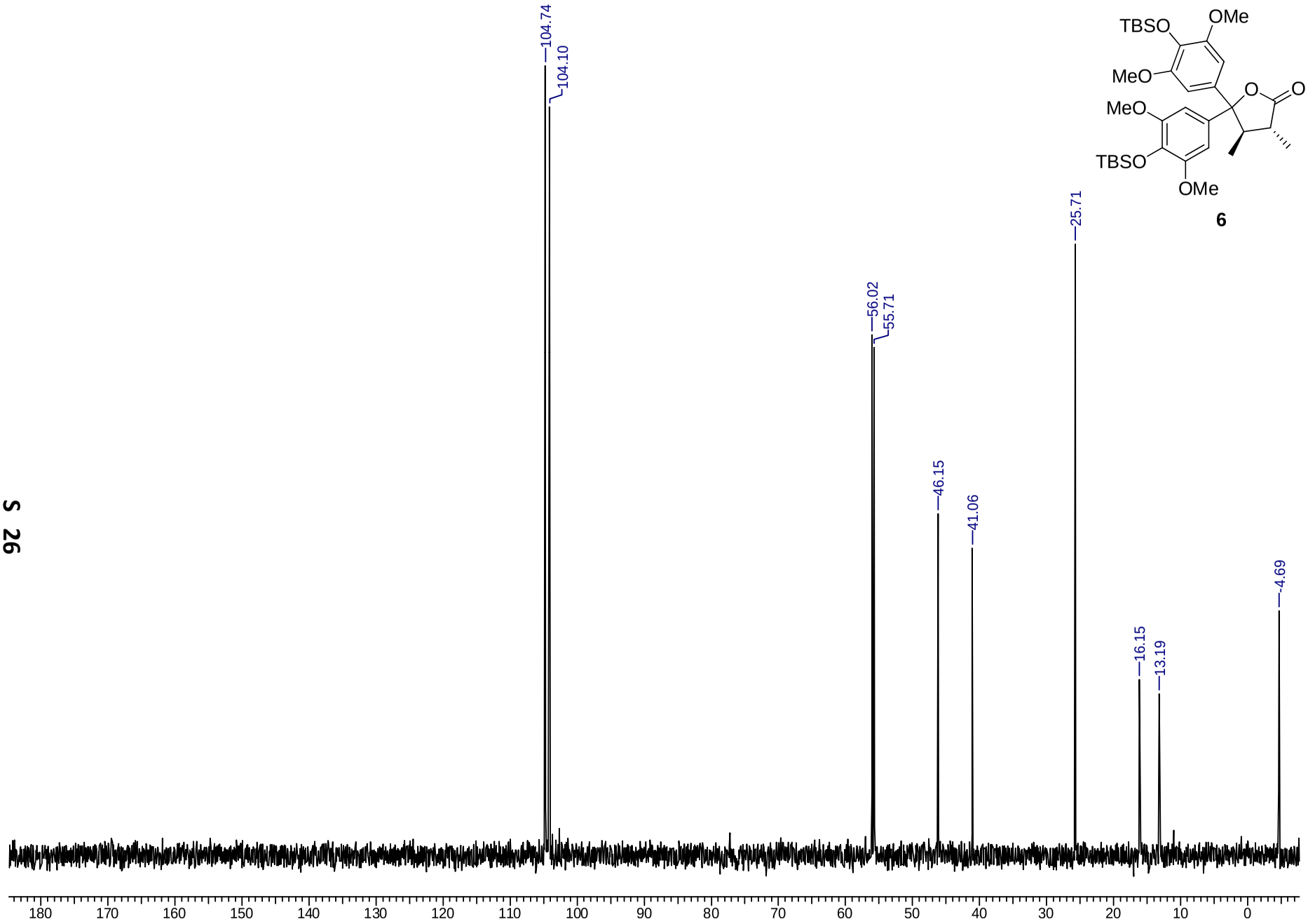


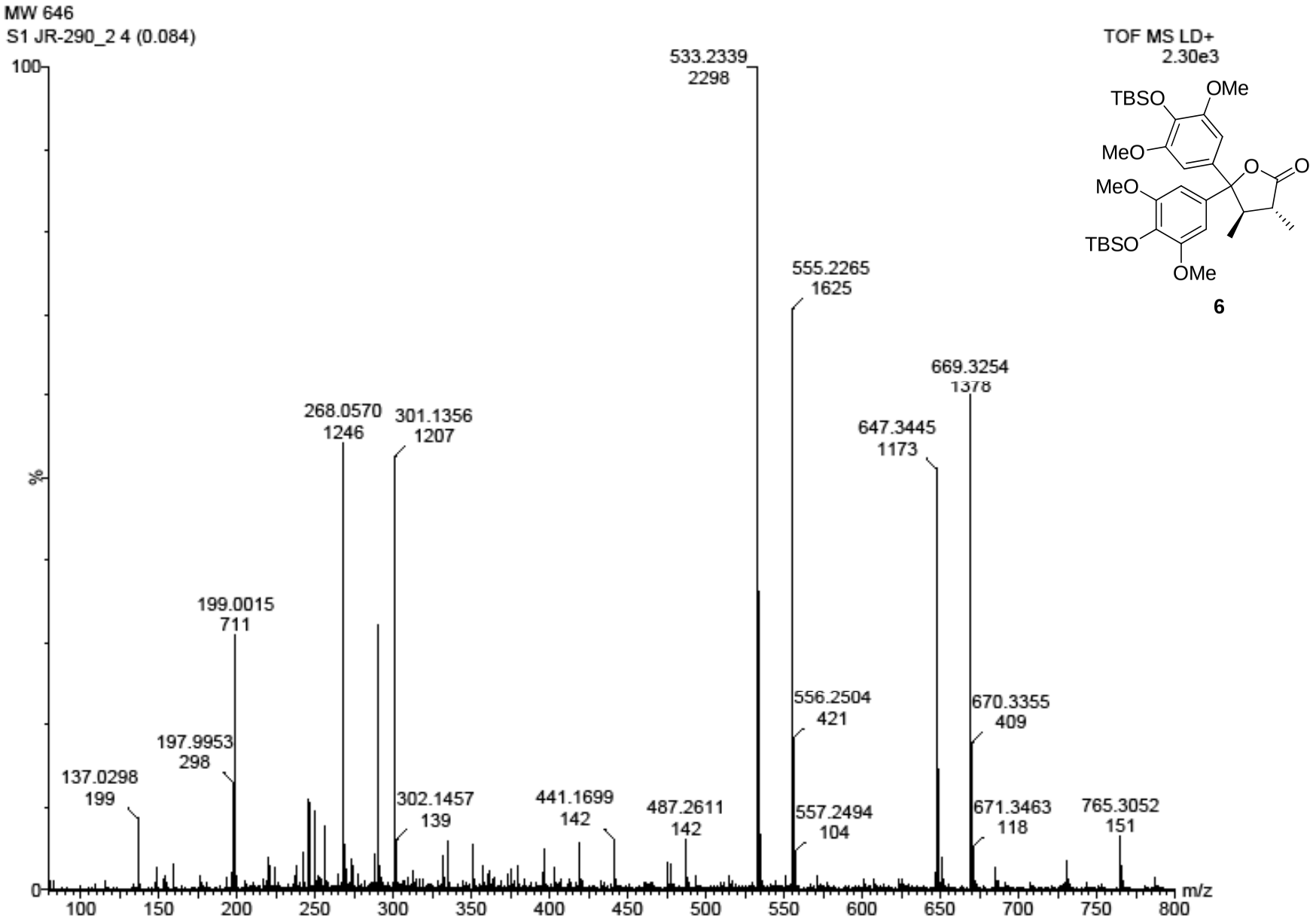
6



S 25

Acquisition Time (sec) 1.2976	***Date***	24/04/2011 13:47:54		***Frequency (MHz)***	100.61	***Nucleus***	13C
Original Points Count 32768	***Points Count***	32768	***Sweep Width (Hz)*** 25252.53			***Temperature (grad C)***	0.000

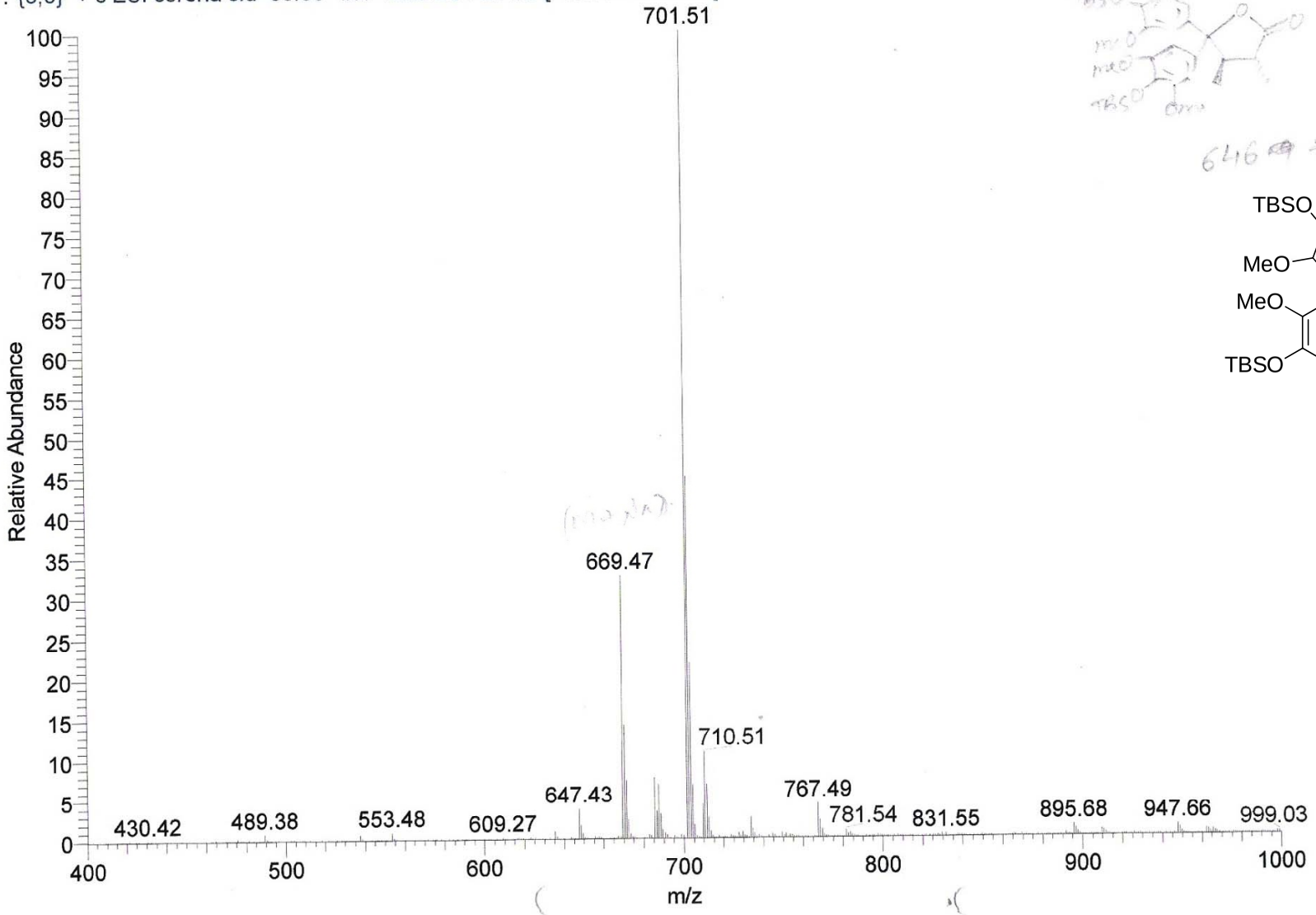



MW 646
S1 JR-290_2 4 (0.084)
TOF MS LD+
2.30e3
533.2339
2298
555.2265
1625
669.3254
1378
268.0570
1246
301.1356
1207
647.3445
1173
199.0015
711
556.2504
421
670.3355
409
197.9953
298
137.0298
199
302.1457
139
441.1699
142
487.2611
142
557.2494
104
671.3463
118
765.3052
151
%
m/z
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
TBSO
OMe
MeO
MeO
TBSO
OMe
O
O

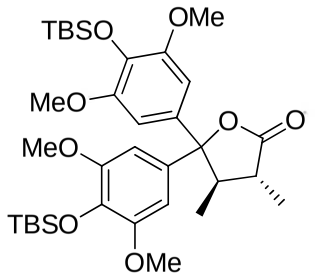
6

F:\DATA\RAMANA\JR-290 4/28/2011 3:08:11 PM

JR-290 #14-48 RT: 0.12-0.42 AV: 35 SB: 22 0.00-0.08 , 0.52-0.62 NL: 3.23E6
T: {0,0} + c ESI corona sid=80.00 det=1200.00 Full ms [400.00-1000.00]

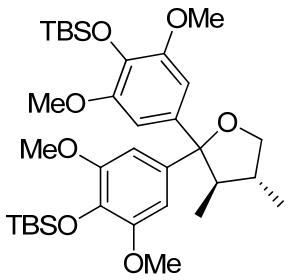


646 + 23 = 669

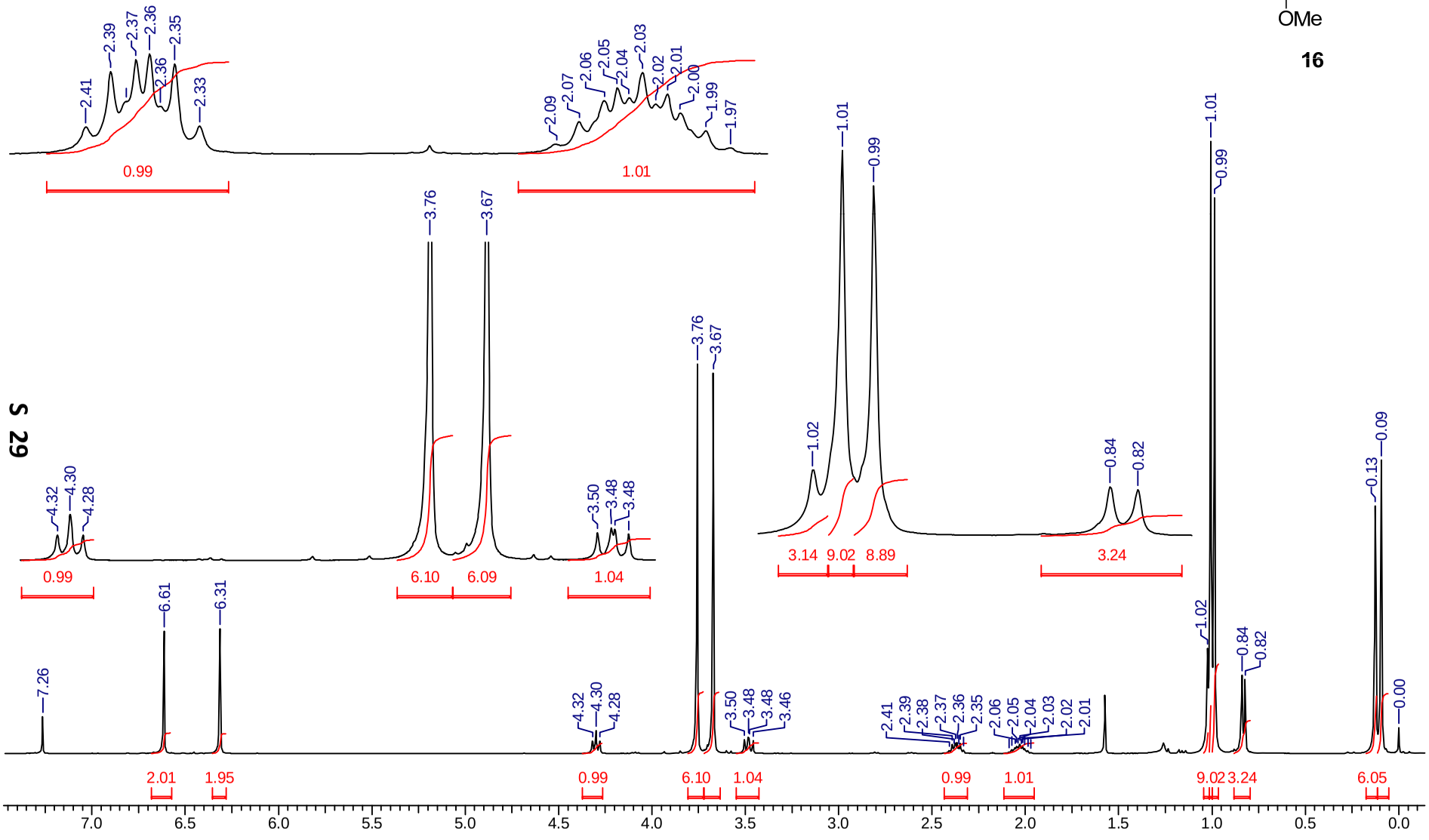


6

Acquisition Time (sec)	4.0894	***Comment***	1H/	***Date***	24/04/2011 20:55:00	***Frequency (MHz)***	400.13
Nucleus	1H	***Original Points Count***	32768	***Points Count***	32768	***Sweep Width (Hz)***	8012.82
Temperature (grad C)	0.000						

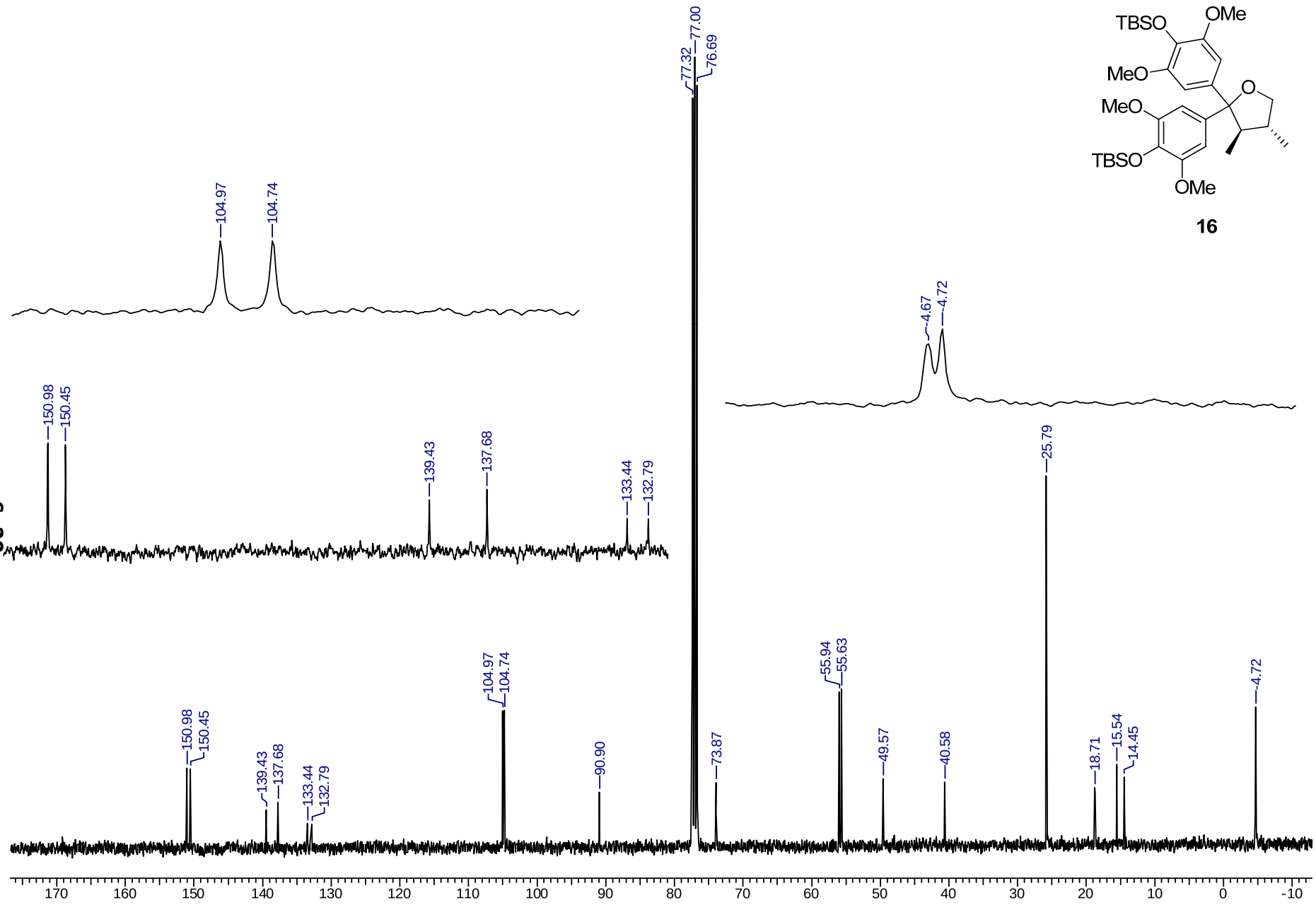


16

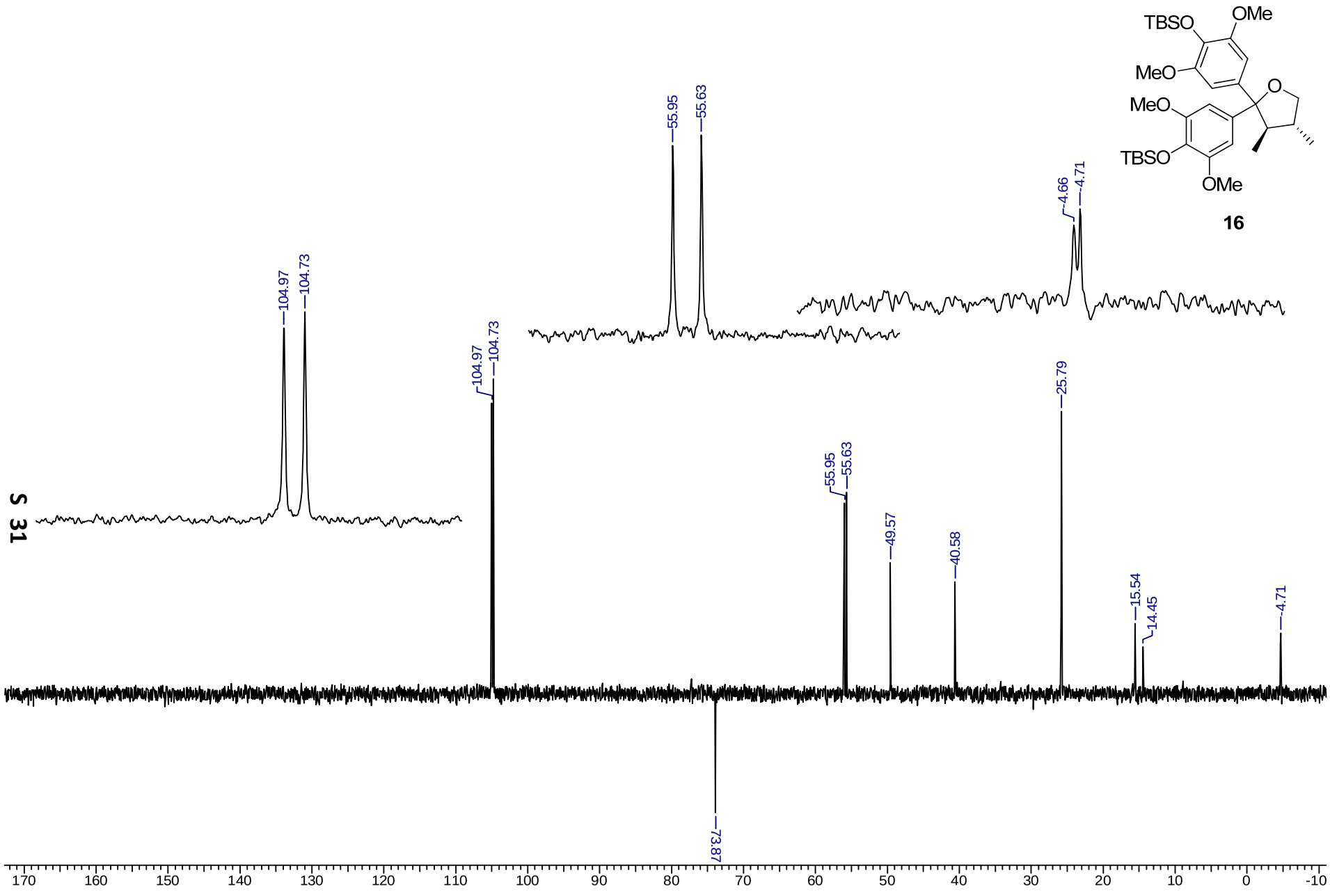


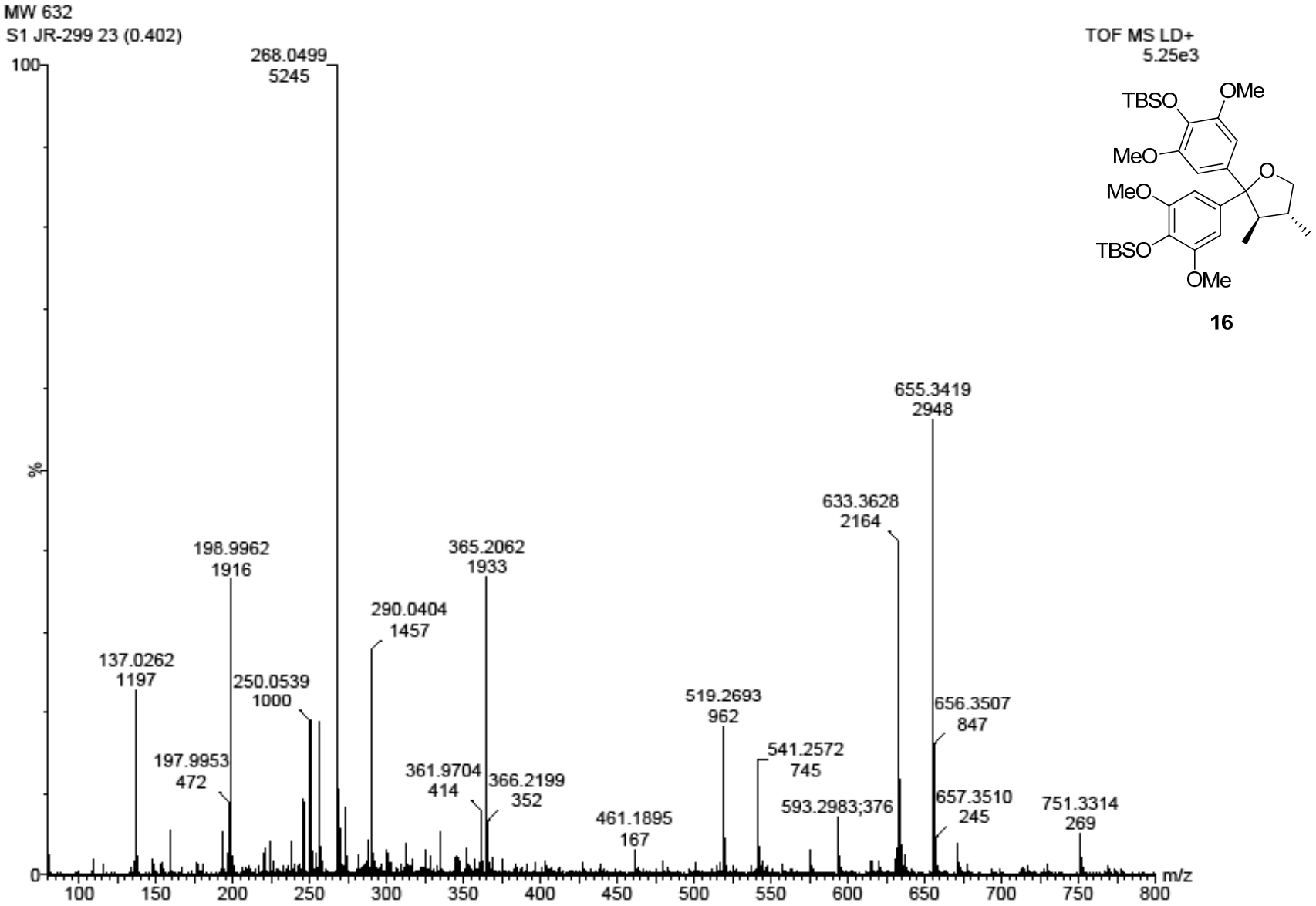
S 29

Acquisition Time (sec)	1.2976	***Date***	24/04/2011 20:57:28	***Frequency (MHz)***	100.61	***Nucleus***	13C
Original Points Count	32768	***Points Count***	32768	***Sweep Width (Hz)***	25252.53	***Temperature (grad C)***	0.000



Acquisition Time (sec) 1.2976	***Date***	24/04/2011 20:55:26		***Frequency (MHz)***	100.61	***Nucleus***	13C
Original Points Count 32768	***Points Count***	32768	***Sweep Width (Hz)*** 25252.53			***Temperature (grad C)***	0.000

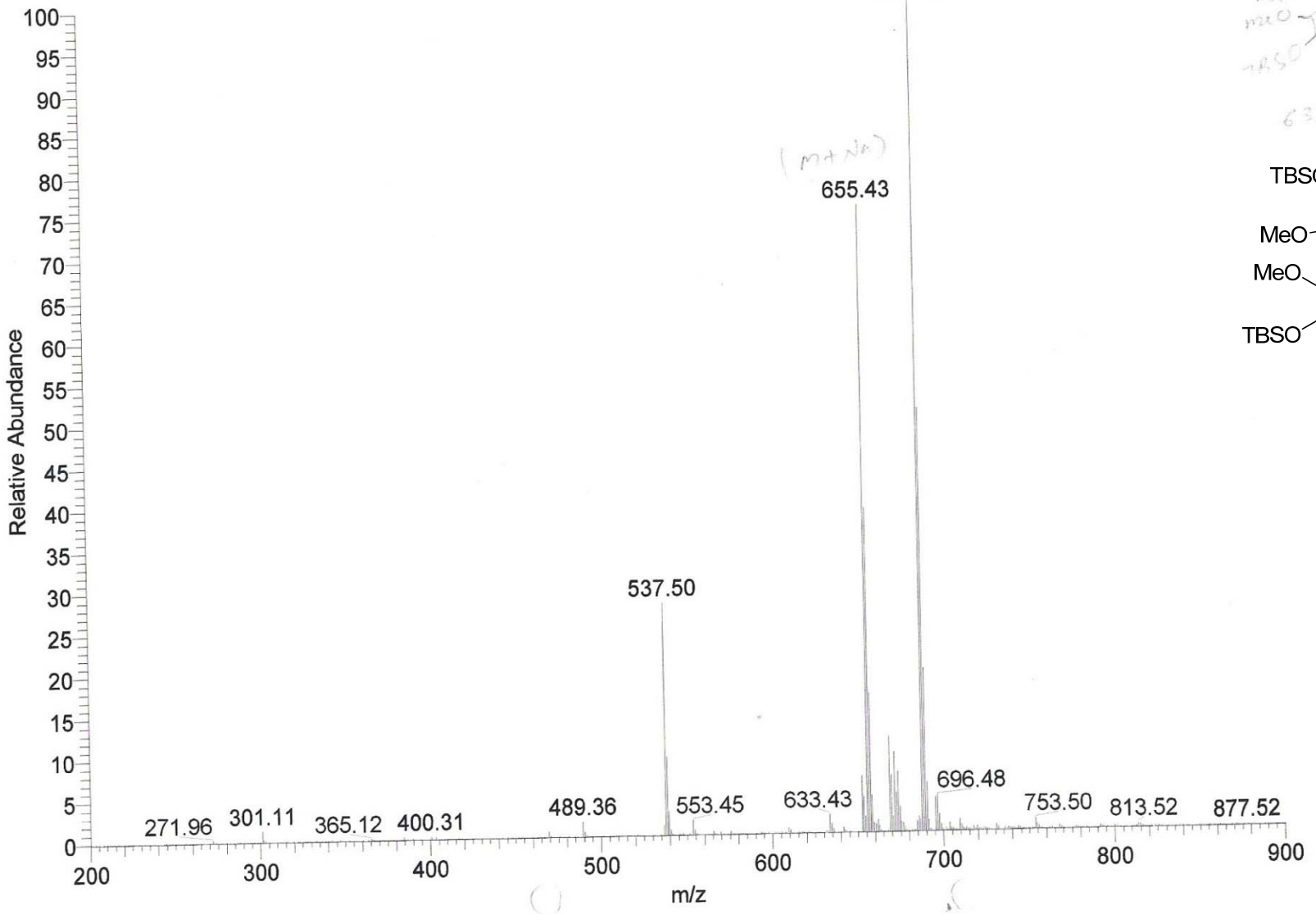


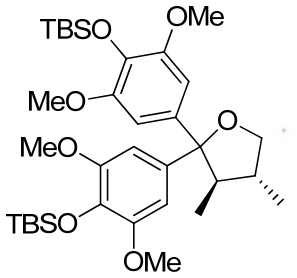

MW 632
S1 JR-299 23 (0.402)
TOF MS LD+
5.25e3
268.0499
5245
655.3419
2948
633.3628
2164
198.9962
1916
365.2062
1933
290.0404
1457
137.0262
1197
250.0539
1000
519.2693
962
656.3507
847
541.2572
745
197.9953
472
361.9704
414
366.2199
352
593.2983;376
657.3510
245
751.3314
269
461.1895
167
100
%
0
m/z
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
TBSO
OMe
MeO
MeO
TBSO
OMe
O

16

F:\DATA\RAMANA\JR-299 4/27/2011 3:55:26 PM

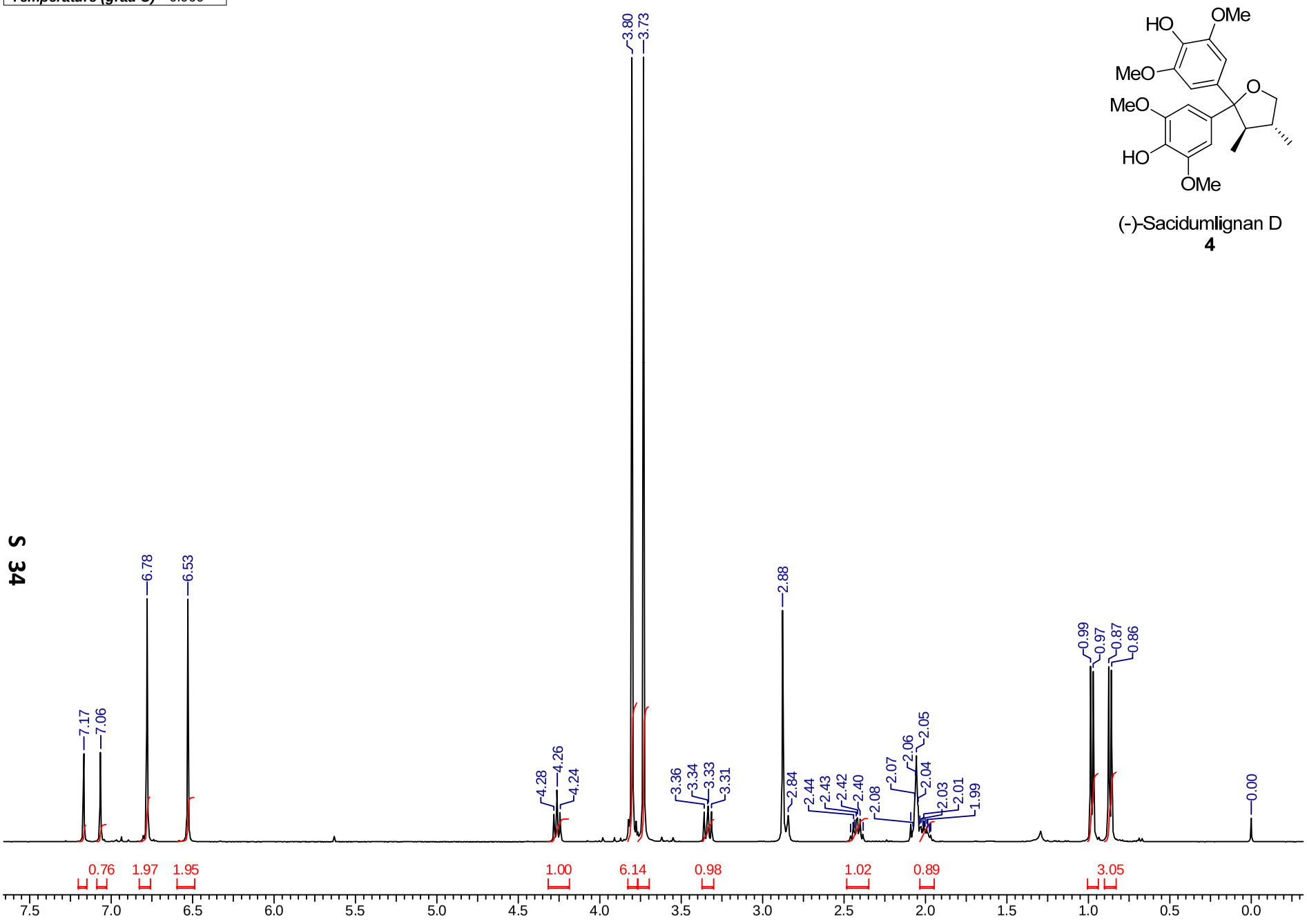
JR-299 #13-58 RT: 0.11-0.51 AV: 46 SB: 18 0.00-0.07 , 0.59-0.66 NL: 3.59E6
T: {0,0} + c ESI corona sid=80.00 det=1200.00 Full ms [200.00-900.00]





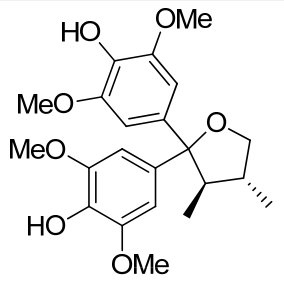
16

Acquisition Time (sec)	4.0894	***Comment***	Sunil	***Date***	23/04/2011 09:29:38			***Frequency (MHz)***	400.13
Nucleus	1H	***Original Points Count***	32768	***Points Count***	32768	***Sweep Width (Hz)***	8012.82		
Temperature (grad C)	0.000								



(-)-Sacidumlignan D
4

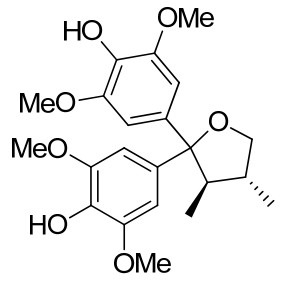
Acquisition Time (sec)	1.2976	***Comment***	13C	***Date***	23/04/2011 10:44:06	***Frequency (MHz)***	100.61
Nucleus	13C	***Original Points Count***	32768	***Points Count***	32768	***Sweep Width (Hz)***	25252.53
Temperature (grad C)	0.000						



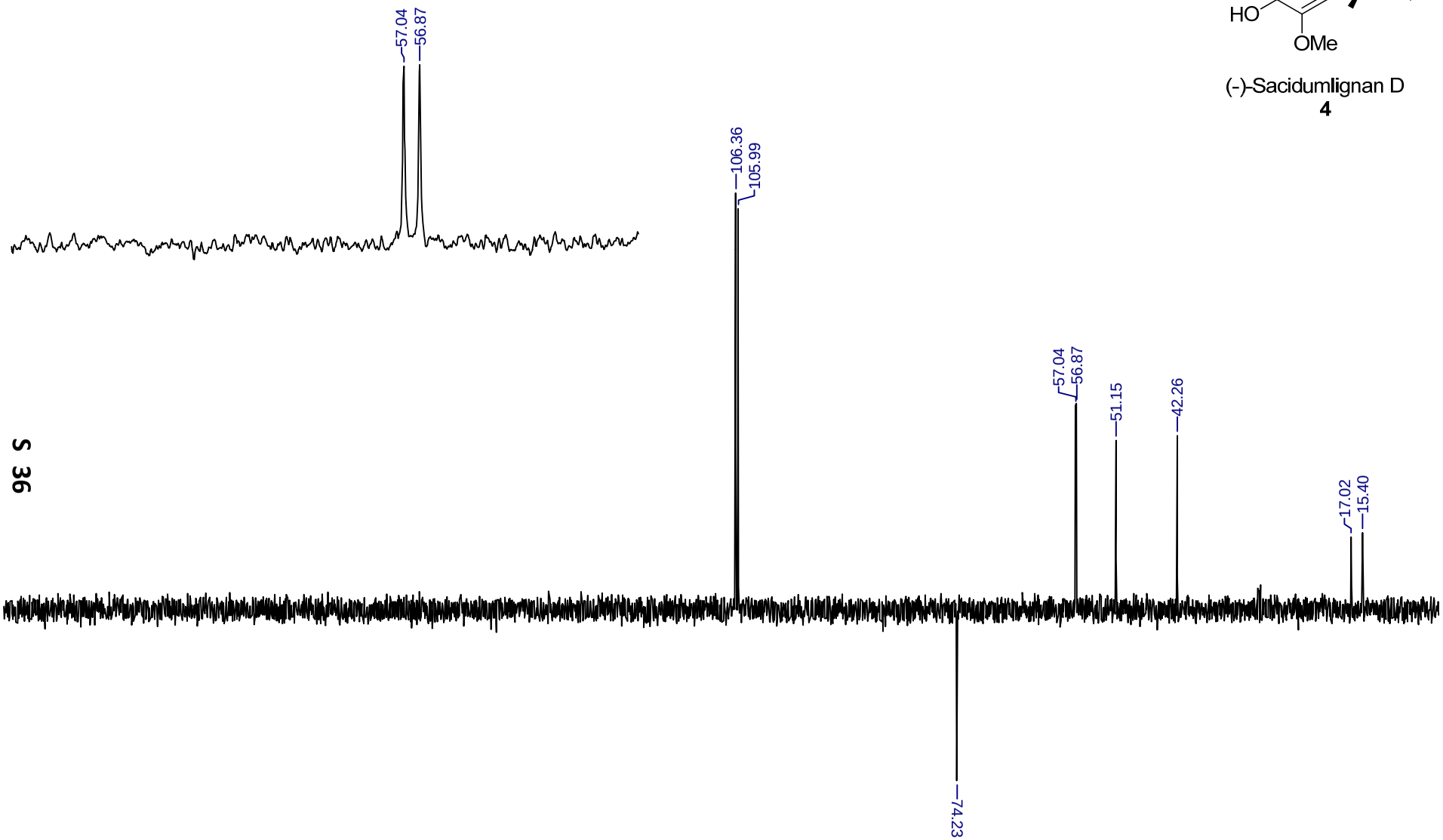
(-)-Sacidumlignan D

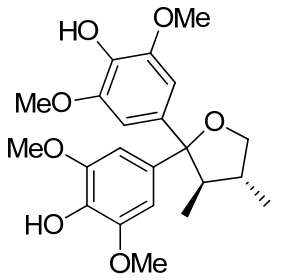
4

Acquisition Time (sec)	1.2976	***Comment***	Dept	***Date***	23/04/2011 09:38:50			***Frequency (MHz)***	100.61
Nucleus	13C	***Original Points Count***	32768	***Points Count***	32768	***Sweep Width (Hz)***	25252.53		
Temperature (grad C)	0.000								



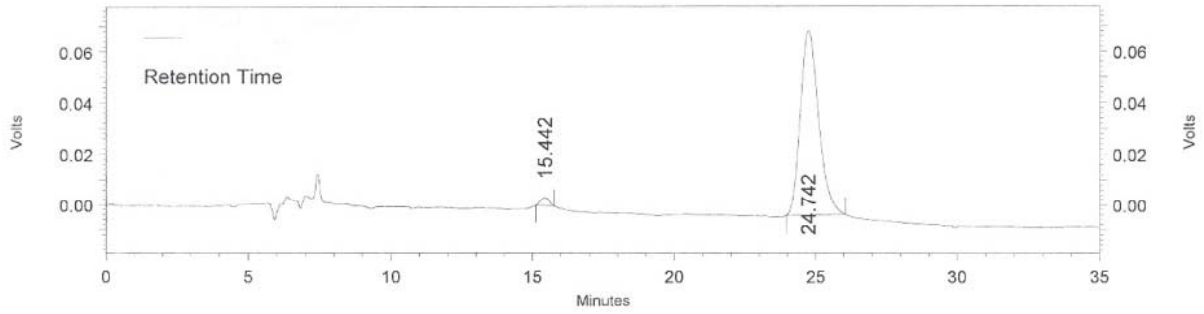
(-)-Sacidumlignan D
4





(-)-Sacidumlignan D
4

Shimadzu CLASS-VP V6.12 SP5
Method Name: C:\CLASS-VP\Method ch 2.met
Data Name: C:\CLASS-VP\Data\General\Gen1303
User: System
Acquired: 4/21/11 3:13:21 PM
Printed: 4/21/11 3:54:34 PM
Sample Name JR-303-Chiral

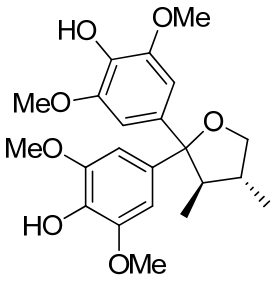


Detector A - 1 (254nm)

Retention Time	C Area	Area %
15.442	69053	2.074
24.742	3260147	97.926

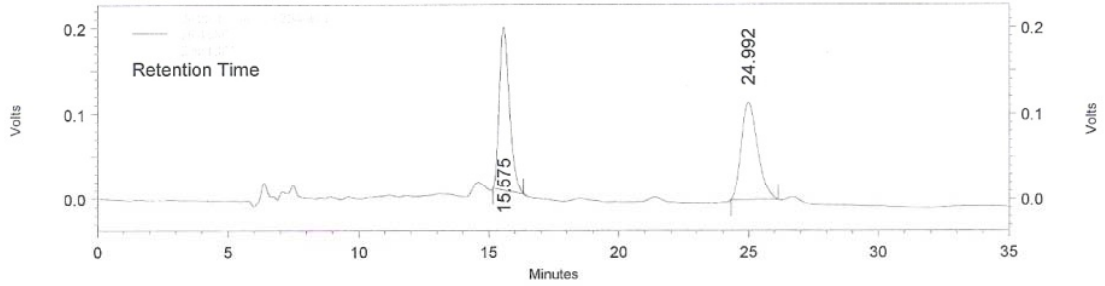
Totals	3329200	100.000

Project Leader : Dr.C.V. RAMANA
Column :Kromasil 5-AmyCoat (250x4.6mm)
Mobile Phase :Ethanol:n-Hexane (40:60)
Wavelength : 254nm
Flow Rate : 0.5ml/min 44 kgf
Inj vol- :5ul
Kunte



(±)-Sacidumlignan D

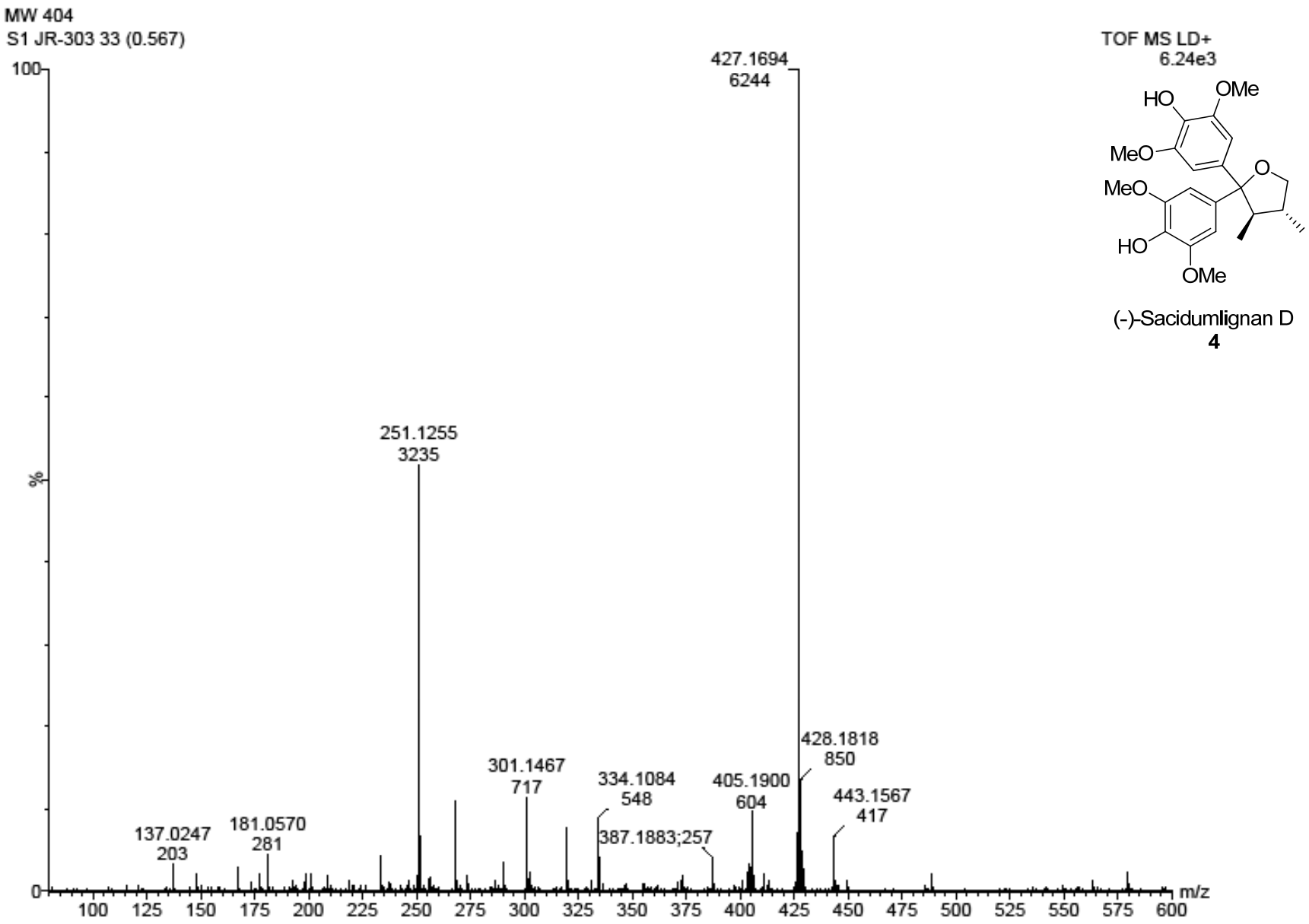
Shimadzu CLASS-VP V6.12 SP5
Method Name: C:\CLASS-VP\Method ch 2.met
Data Name: C:\CLASS-VP\Data\General\Gen1302
User: System
Acquired: 4/21/11 2:35:49 PM
Printed: 4/21/11 3:11:58 PM
Sample Name JR-RAC

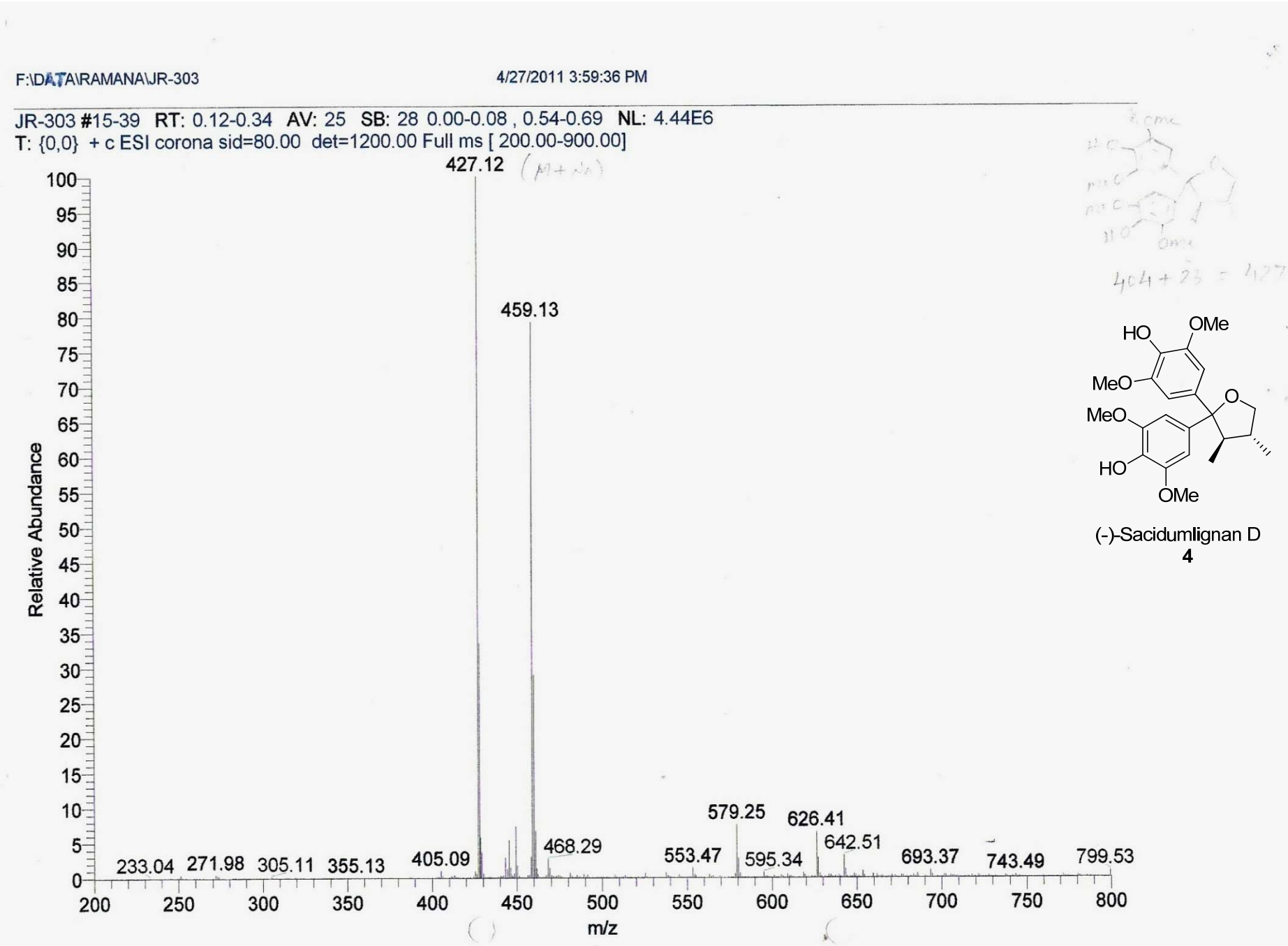


Detector A - 1 (254nm)

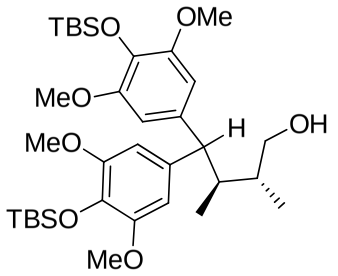
Retention Time	C Area	Area %
15.575	5139051	50.498
24.992	5037702	49.502
Totals	10176753	100.000

Project Leader : Dr.C.V. RAMANA
Column :Kromasil 5-AmyCoat (250x4.6mm)
Mobile Phase :Ethanol:n-Hexane (40:60)
Wavelength : 254nm
Flow Rate : 0.5ml/min 44 kgf
Inj vol- :5ul
Kunte

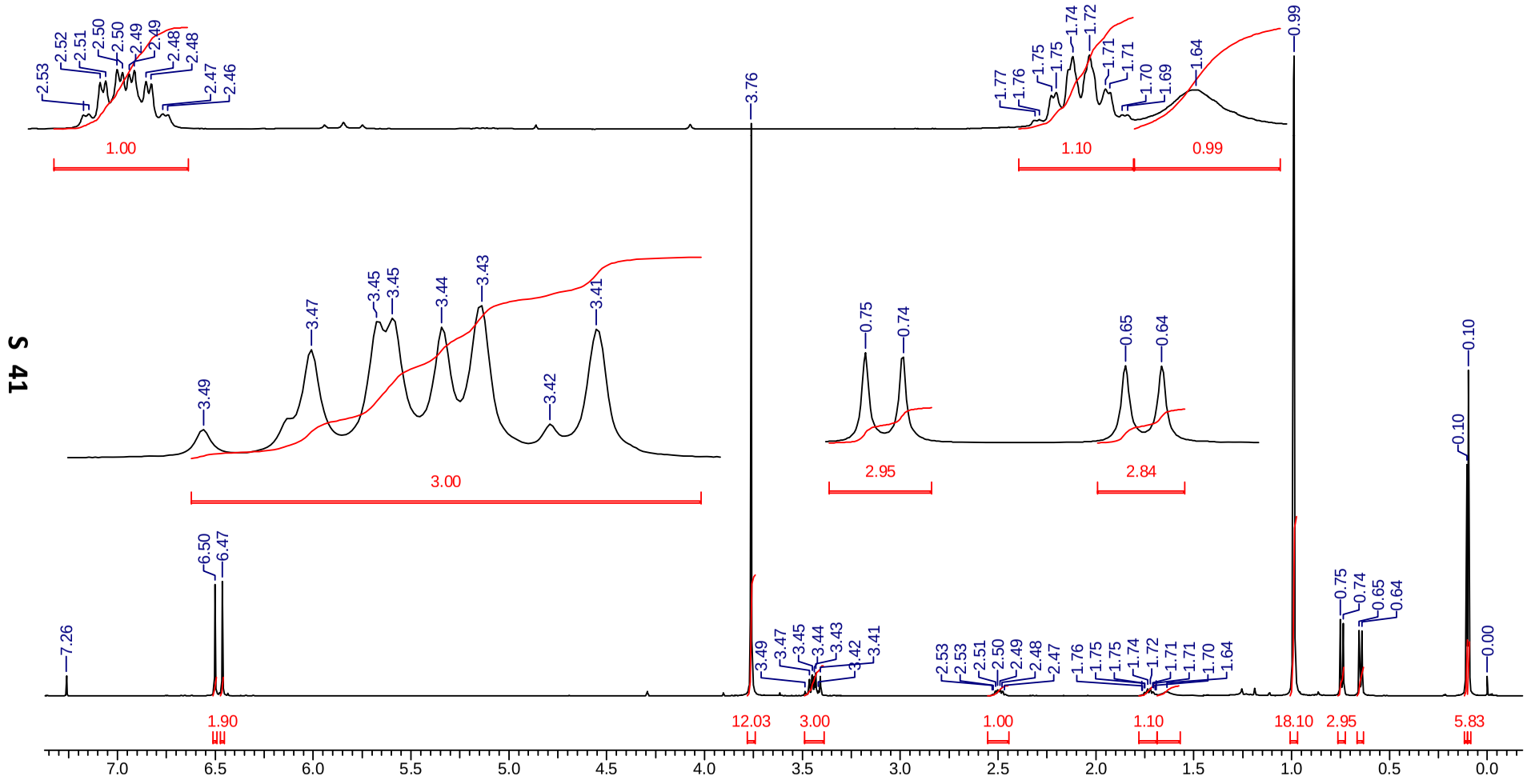

MW 404
S1 JR-303 33 (0.567)
TOF MS LD+
6.24e3
427.1694
6244
251.1255
3235
301.1467
717
334.1084
548
405.1900
604
428.1818
850
443.1567
417
387.1883;257
137.0247
203
181.0570
281
%
m/z
HO
OMe
MeO
MeO
O
HO
OMe
(-)-Sacidumlignan D
4


F:\DATA\RAMANA\JR-303
4/27/2011 3:59:36 PM
JR-303 #15-39 RT: 0.12-0.34 AV: 25 SB: 28 0.00-0.08 , 0.54-0.69 NL: 4.44E6
T: {0,0} + c ESI corona sid=80.00 det=1200.00 Full ms [200.00-900.00]
427.12
459.13
Relative Abundance
m/z
233.04
271.98
305.11
355.13
405.09
468.29
553.47
579.25
595.34
626.41
642.51
693.37
743.49
799.53
HO
OMe
MeO
O
MeO
HO
OMe
(-)-Sacidumlignan D
4

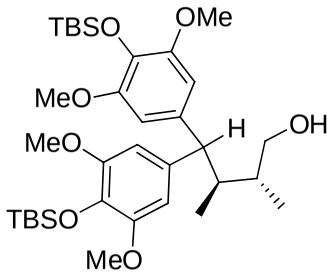
Acquisition Time (sec)	3.2768	***Comment***	1H	***Date***	19/07/2011 18:54:28	***Frequency (MHz)***	500.13
Nucleus	1H	***Original Points Count***	32768	***Points Count***	32768	***Sweep Width (Hz)***	10000.00
Temperature (grad C)	0.000						



7

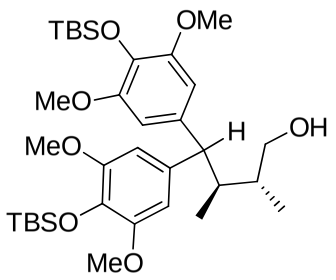


Acquisition Time (sec)	1.1010	***Comment***	13C	***Date***	19/07/2011 20:48:16	***Frequency (MHz)***	125.76
Nucleus	13C	***Original Points Count***	32768	***Points Count***	32768	***Sweep Width (Hz)***	29761.90
Temperature (grad C)	0.000						

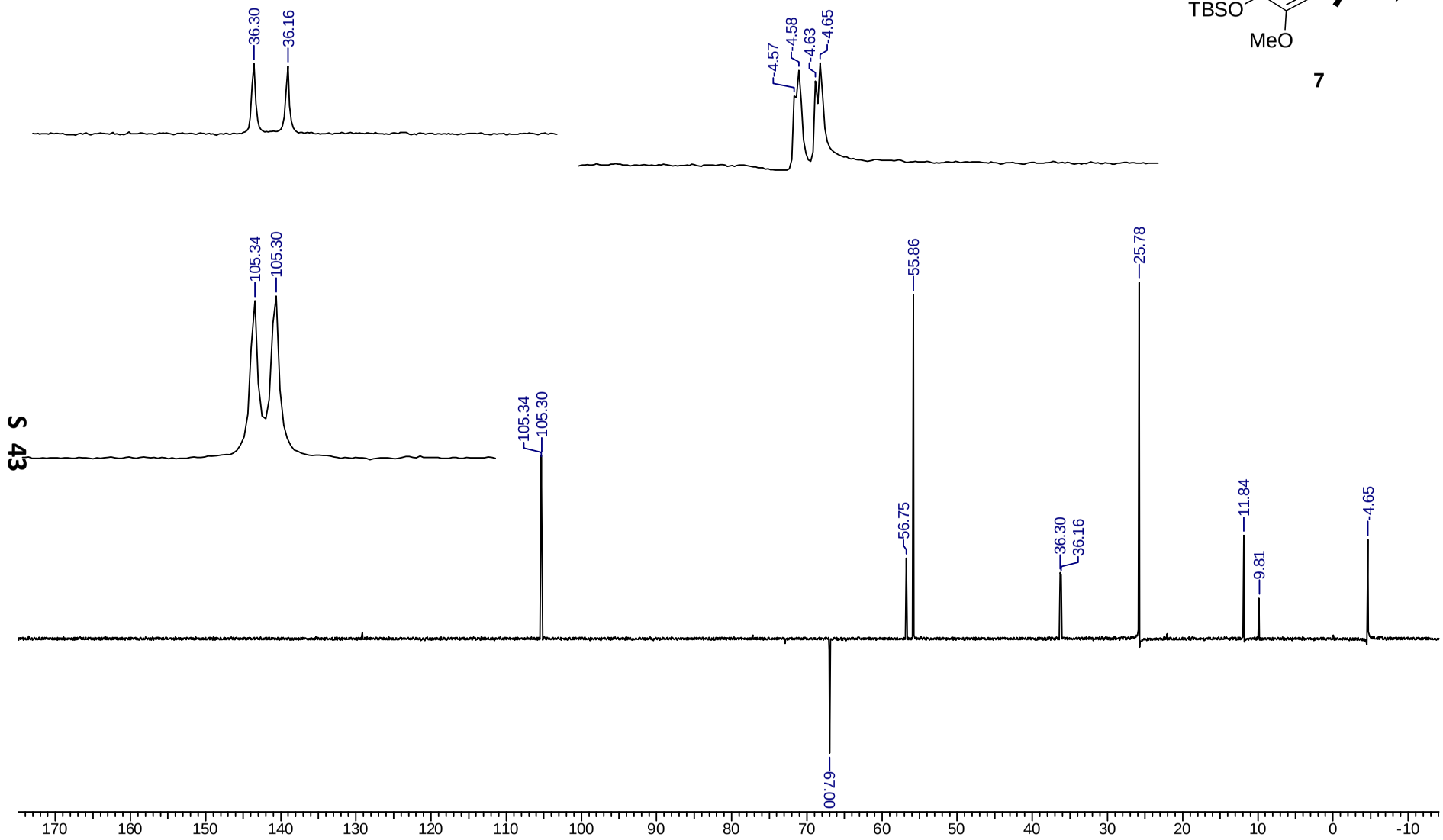


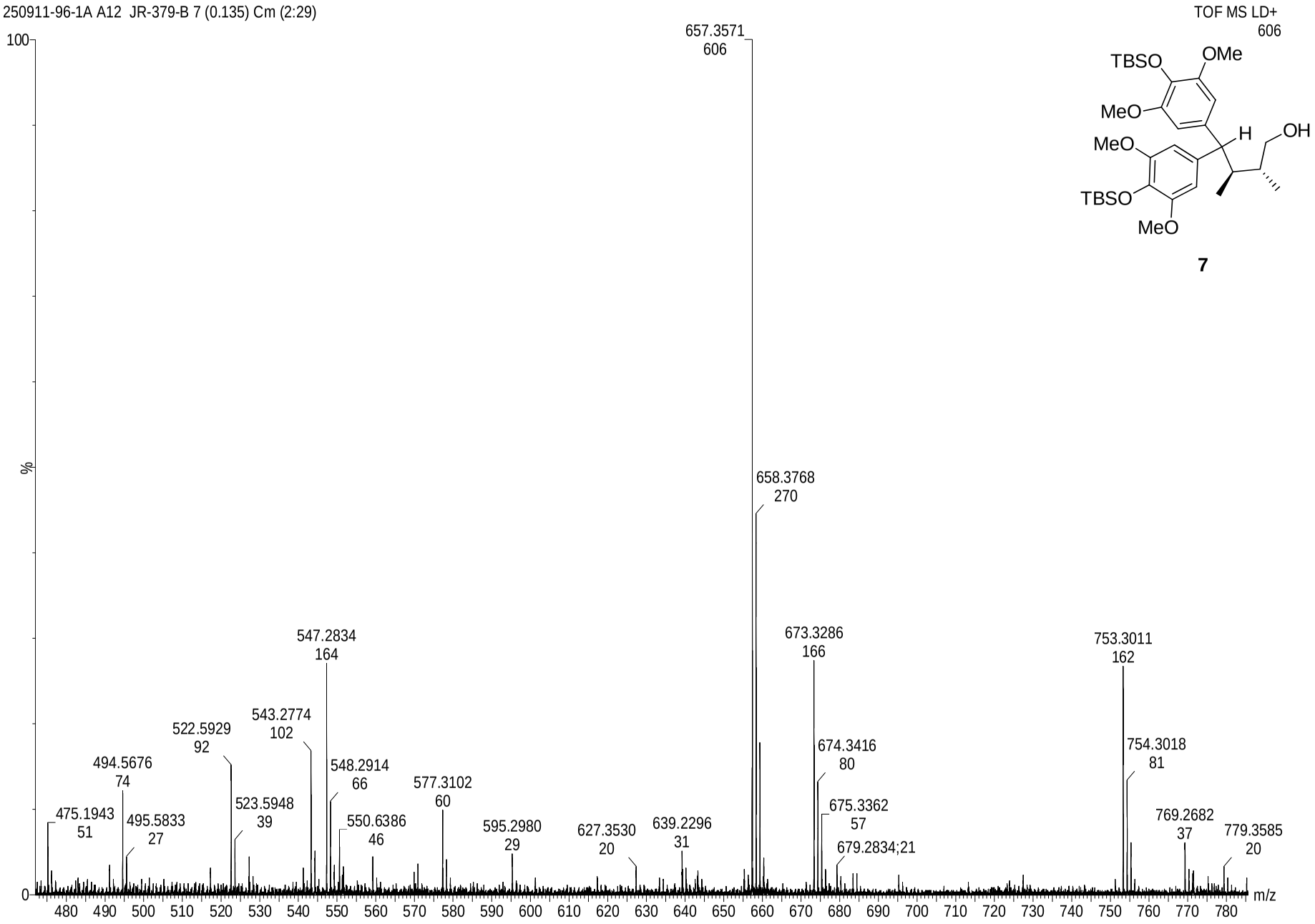
7

Acquisition Time (sec)	1.1010	***Comment***	DEPT135		***Date***	19/07/2011 20:47:58	
Frequency (MHz)	125.76	***Nucleus***	13C	***Original Points Count*** 32768	***Points Count***	32768	***Sweep Width (Hz)*** 29761.90
Temperature (grad C)	0.000						



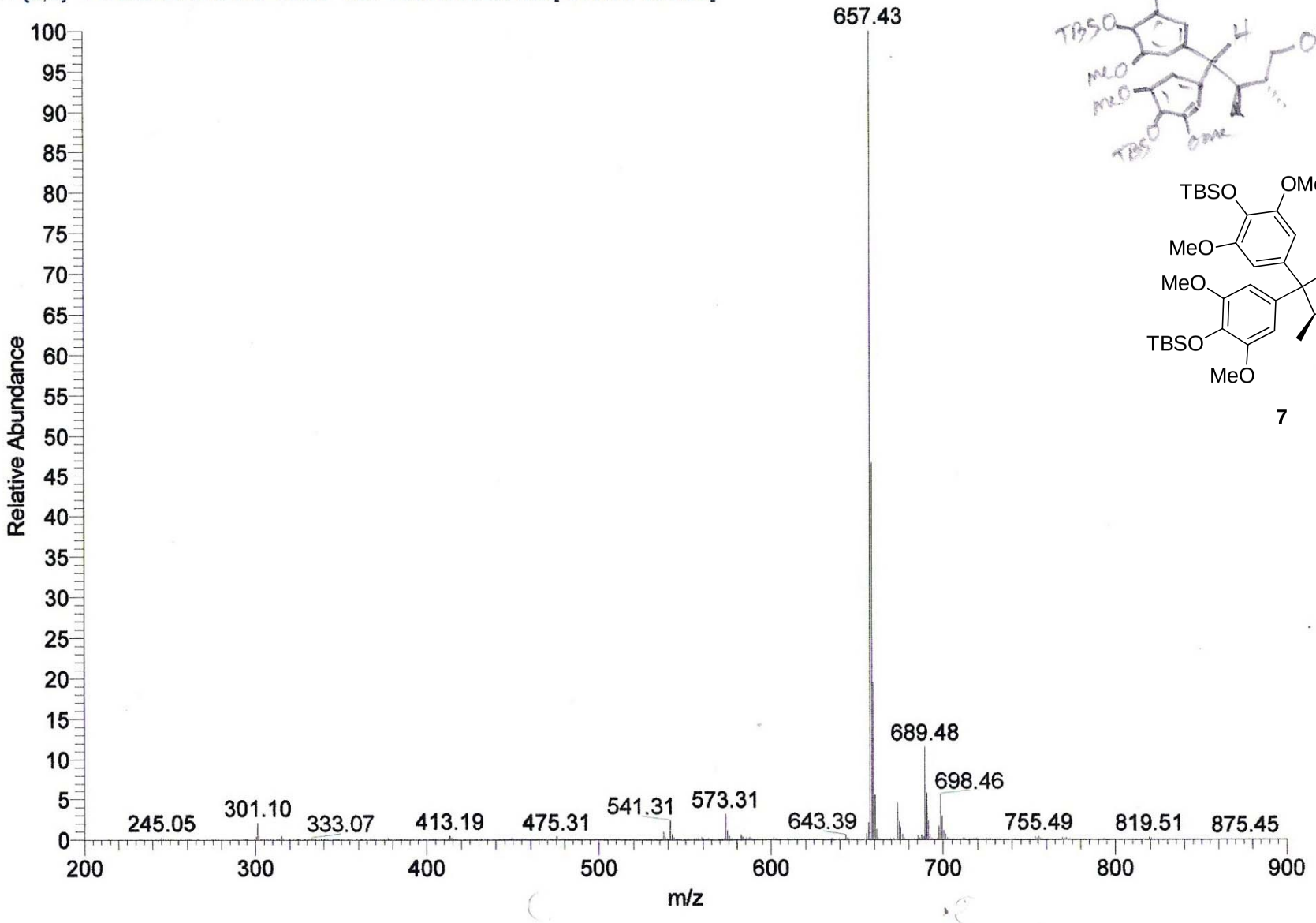
7




250911-96-1A A12 JR-379-B 7 (0.135) Cm (2:29)
TOF MS LD+
606
100
%
0
657.3571
606
658.3768
270
547.2834
164
543.2774
102
522.5929
92
494.5676
74
548.2914
66
577.3102
60
673.3286
166
753.3011
162
674.3416
80
754.3018
81
675.3362
57
769.2682
37
779.3585
20
679.2834;21
475.1943
51
495.5833
27
523.5948
39
550.6386
46
595.2980
29
627.3530
20
639.2296
31
480 490 500 510 520 530 540 550 560 570 580 590 600 610 620 630 640 650 660 670 680 690 700 710 720 730 740 750 760 770 780
m/z
TBSO
OMe
MeO
H
OH
MeO
TBSO
MeO
7

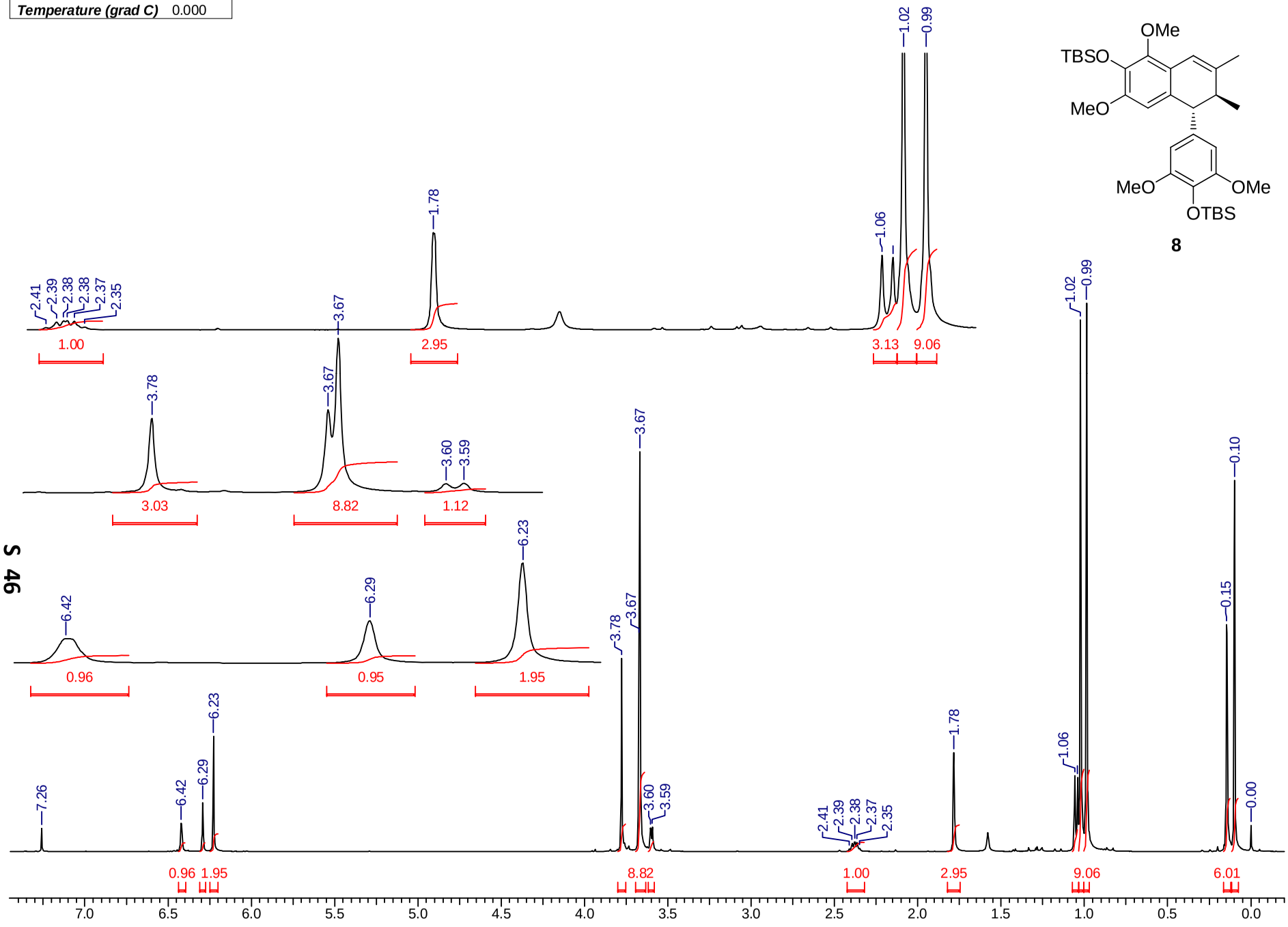
F:\DATA\RAMANA\JR363 7/4/2011 4:09:29 PM

JR363 #14-47 RT: 0.12-0.41 AV: 34 SB: 18 0.00-0.08 , 0.52-0.58 NL: 5.28E6
T: {0,0} + c ESI corona sid=80.00 det=1200.00 Full ms [200.00-900.00]

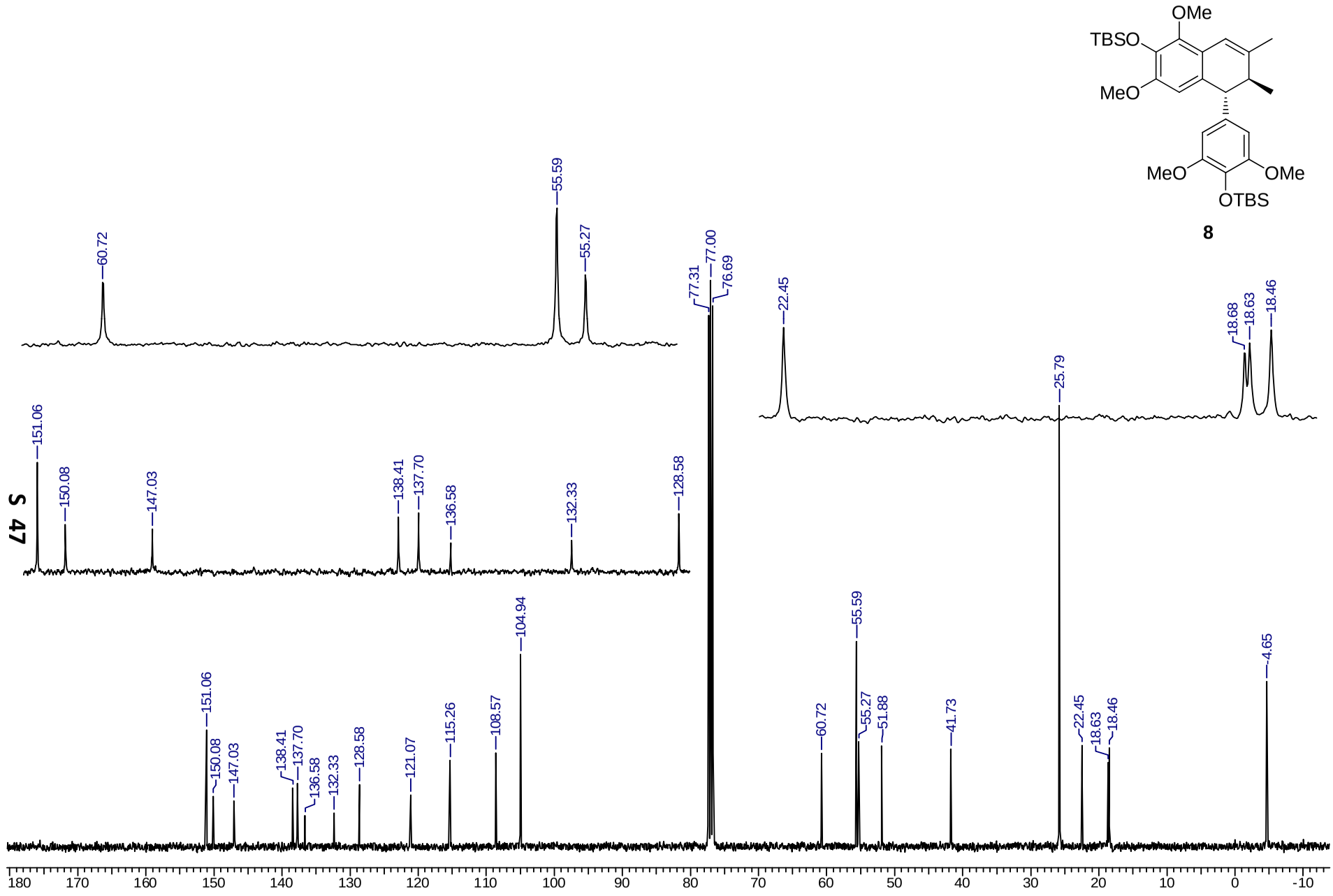


7

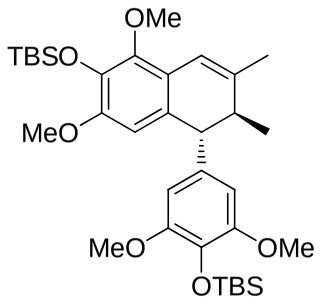
Acquisition Time (sec)	5.4526	***Comment***	Jeetendra		***Date***	21/07/2011 10:24:00	
Frequency (MHz)	400.13	***Nucleus***	1H	***Original Points Count*** 32768	***Points Count***	32768	***Sweep Width (Hz)*** 6009.62
Temperature (grad C)	0.000						



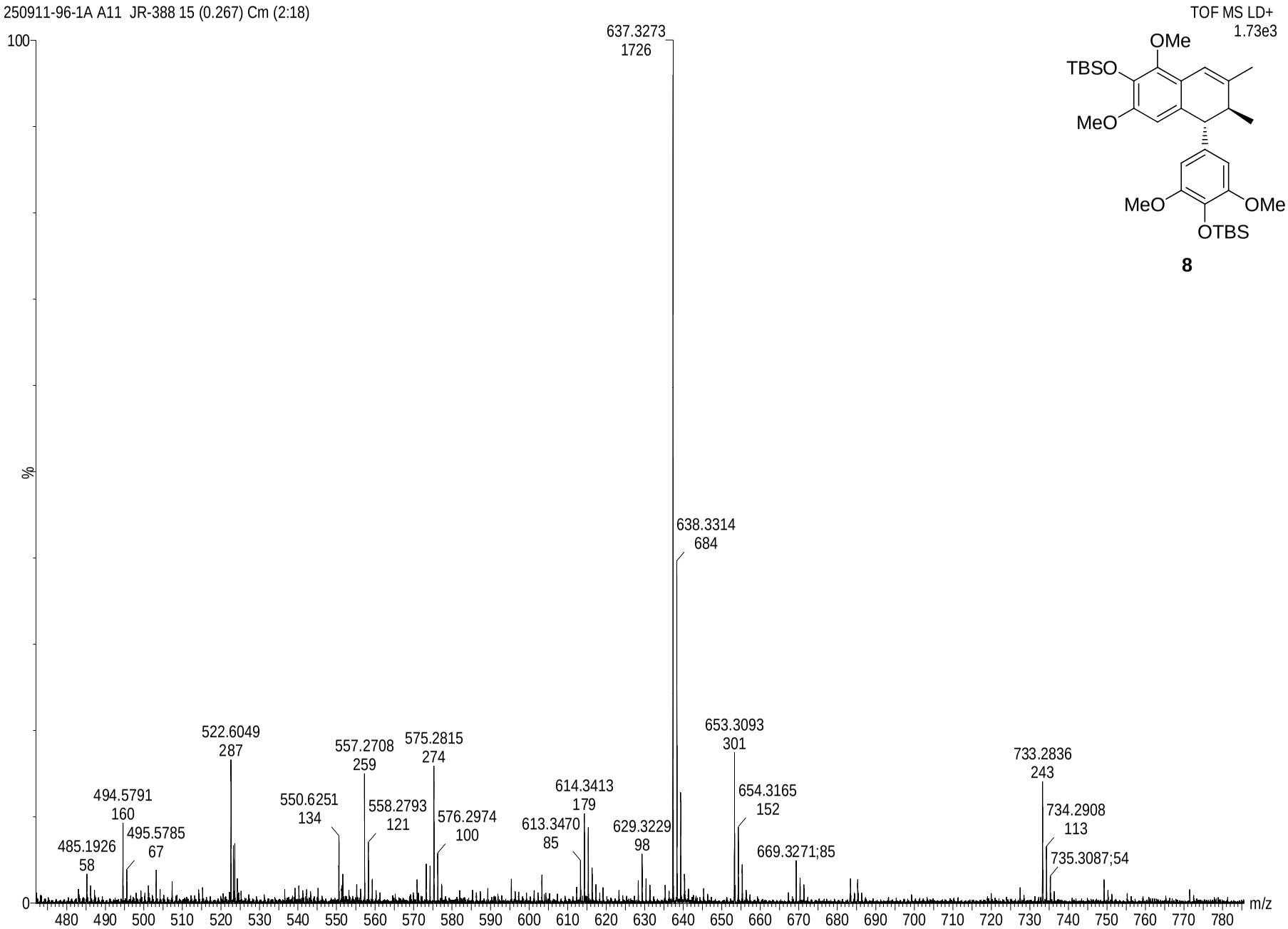
Acquisition Time (sec) 1.2976	***Date***	21/07/2011 11:33:38		***Frequency (MHz)***	100.61	***Nucleus***	13C
Original Points Count 32768	***Points Count***	32768	***Sweep Width (Hz)*** 25252.53			***Temperature (grad C)***	0.000



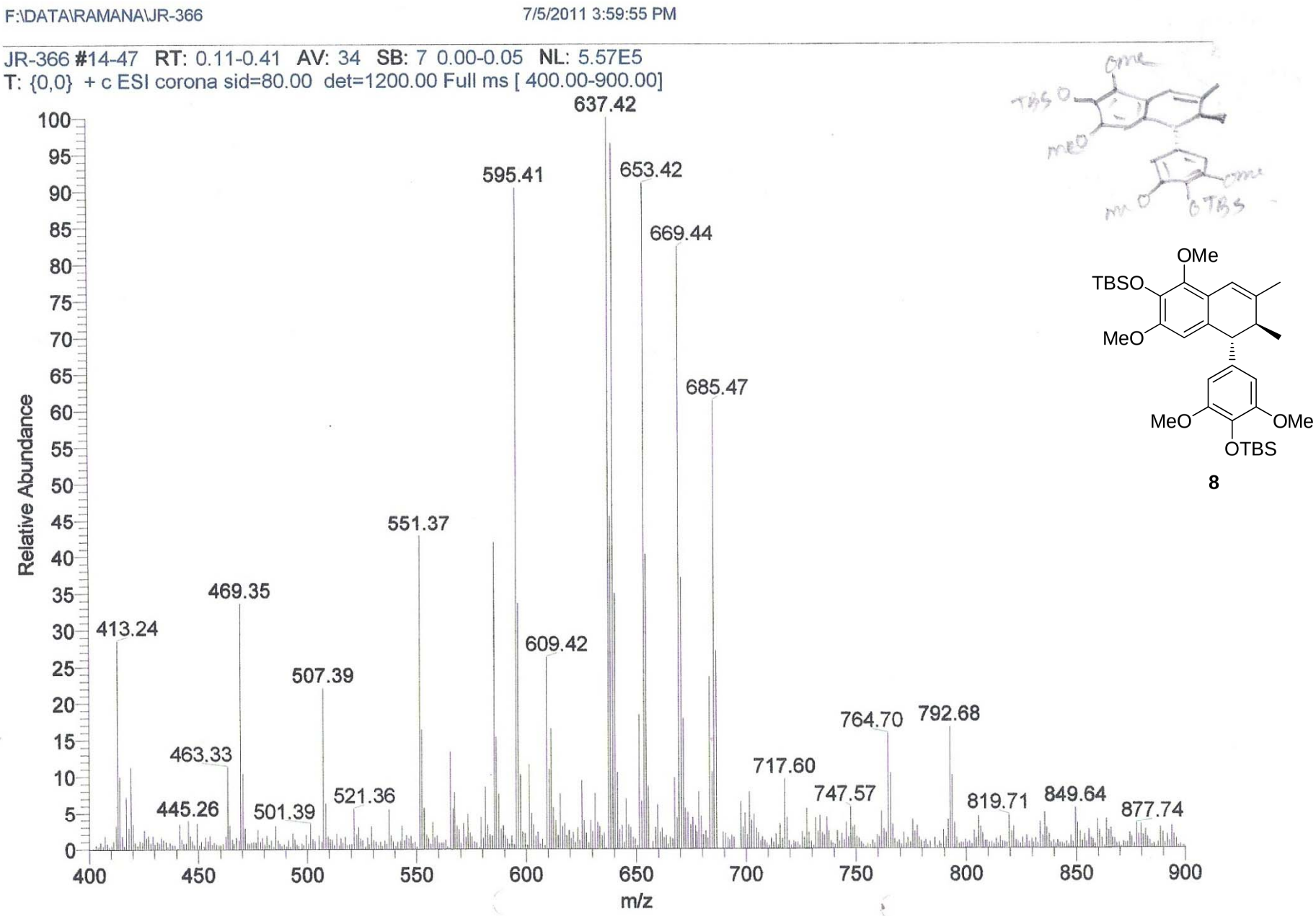
Acquisition Time (sec) 1.3631	***Date***	21/07/2011 10:58:52		***Frequency (MHz)***	100.61	***Nucleus***	13C
Original Points Count 32768	***Points Count***	32768	***Sweep Width (Hz)*** 24038.46			***Temperature (grad C)***	0.000



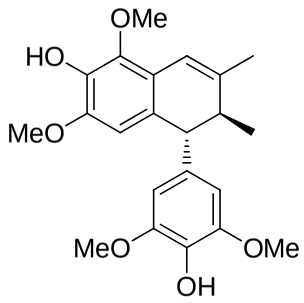
8


250911-96-1A A11 JR-388 15 (0.267) Cm (2:18)
TOF MS LD+
1.73e3
100
%
0
637.3273
1726
638.3314
684
653.3093
301
654.3165
152
669.3271;85
733.2836
243
734.2908
113
735.3087;54
522.6049
287
557.2708
259
575.2815
274
550.6251
134
558.2793
121
576.2974
100
494.5791
160
495.5785
67
485.1926
58
614.3413
179
613.3470
85
629.3229
98
480 490 500 510 520 530 540 550 560 570 580 590 600 610 620 630 640 650 660 670 680 690 700 710 720 730 740 750 760 770 780
m/z
OMe
TBSO
MeO
MeO
OMe
OTBS

8


F:\DATA\RAMANA\JR-366
7/5/2011 3:59:55 PM
JR-366 #14-47 RT: 0.11-0.41 AV: 34 SB: 7 0.00-0.05 NL: 5.57E5
T: {0,0} + c ESI corona sid=80.00 det=1200.00 Full ms [400.00-900.00]
Relative Abundance
m/z
637.42
595.41
653.42
669.44
685.47
551.37
469.35
413.24
609.42
507.39
463.33
445.26
501.39
521.36
764.70
792.68
717.60
747.57
819.71
849.64
877.74
OMe
TBSO
MeO
MeO
OMe
OTBS
8

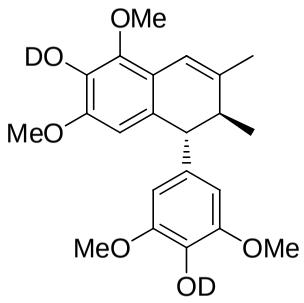
Acquisition Time (sec)	3.9846	***Comment***	Jeetendra			***Date***	24/07/2011 10:09:50
Frequency (MHz)	400.13	***Nucleus***	1H	***Original Points Count***	32768	***Points Count***	32768	***Sweep Width (Hz)***	8223.68
Temperature (grad C)	0.000						



(-)-Sacidumlignan B

2

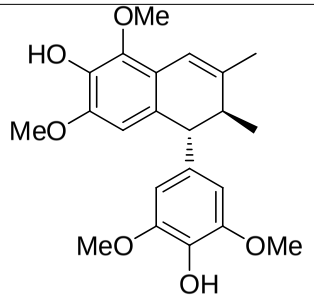
Acquisition Time (sec)	4.8234	***Comment***	Jeetendra			***Date***	27/07/2011 10:10:22
Frequency (MHz)	400.13	***Nucleus***	1H	***Original Points Count***	32768	***Points Count***	32768
Temperature (grad C)	0.000					***Sweep Width (Hz)***	6793.48



(-)-Sacidumlignan B

2

Acquisition Time (sec) 1.2976	***Date***	24/07/2011 18:20:56		***Frequency (MHz)***	100.61	***Nucleus***	13C
Original Points Count 32768	***Points Count***	32768	***Sweep Width (Hz)*** 25252.53			***Temperature (grad C)***	0.000



(-)-Sacidumlignan B

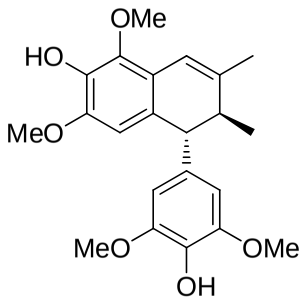
2

S 53

206.21
60.87
56.45
51.98
42.48
105.93
29.80
29.99
29.61
127.15
121.36
116.10
109.38
148.27
147.79
143.95
139.10
138.78
137.08
135.11
22.69
18.88

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

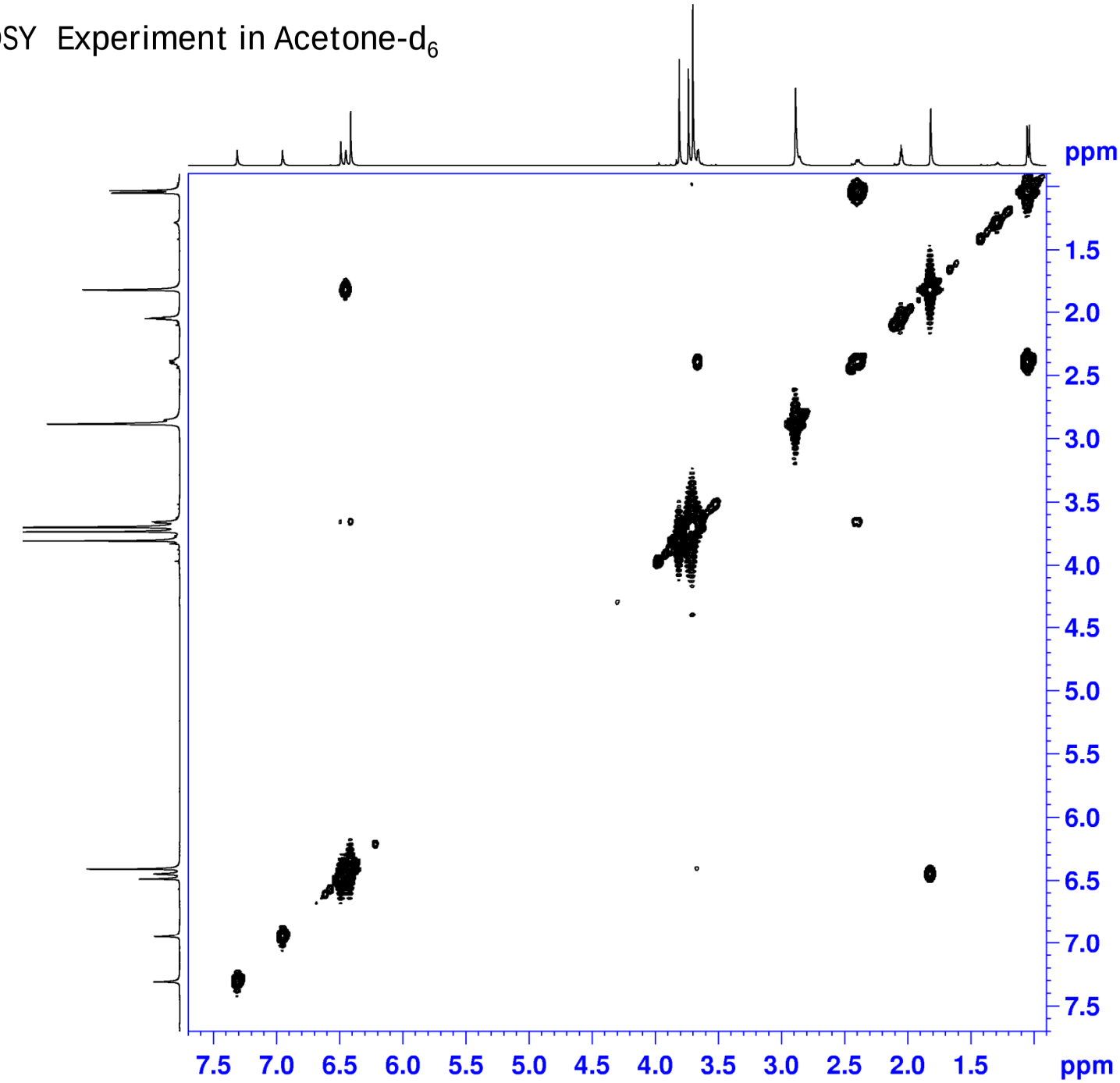
Acquisition Time (sec) 1.3631	***Date***	24/07/2011 18:36:12		***Frequency (MHz)***	100.61	***Nucleus***	13C
Original Points Count 32768	***Points Count***	32768	***Sweep Width (Hz)*** 24038.46			***Temperature (grad C)***	0.000

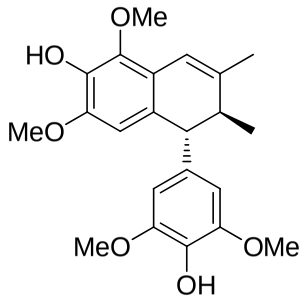


(-)-Sacidumlignan B

2

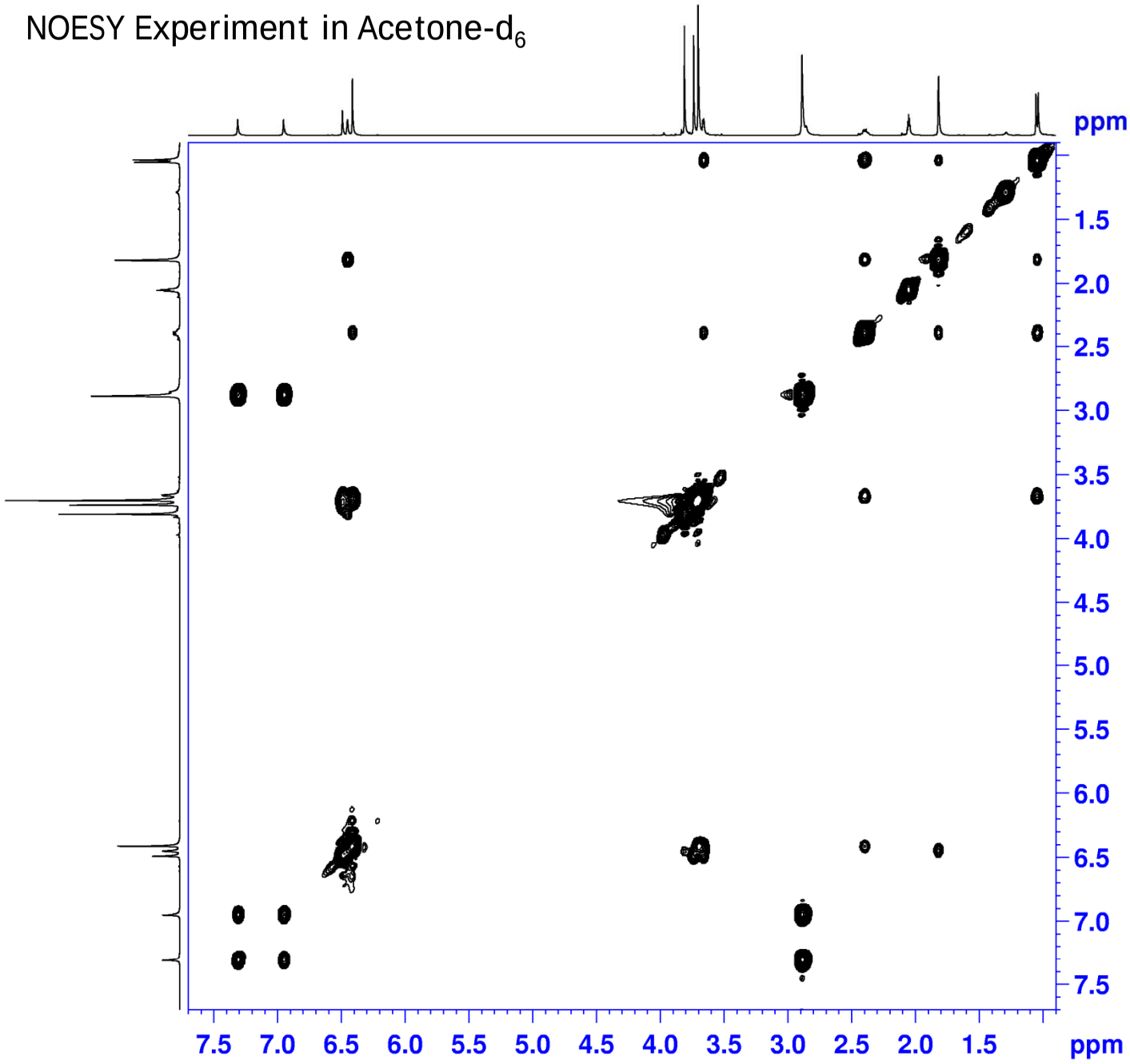
COSY Experiment in Acetone-d_6

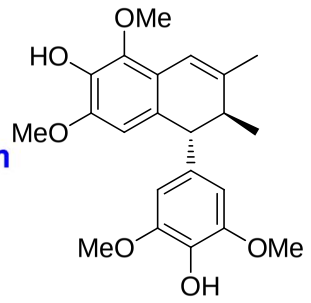




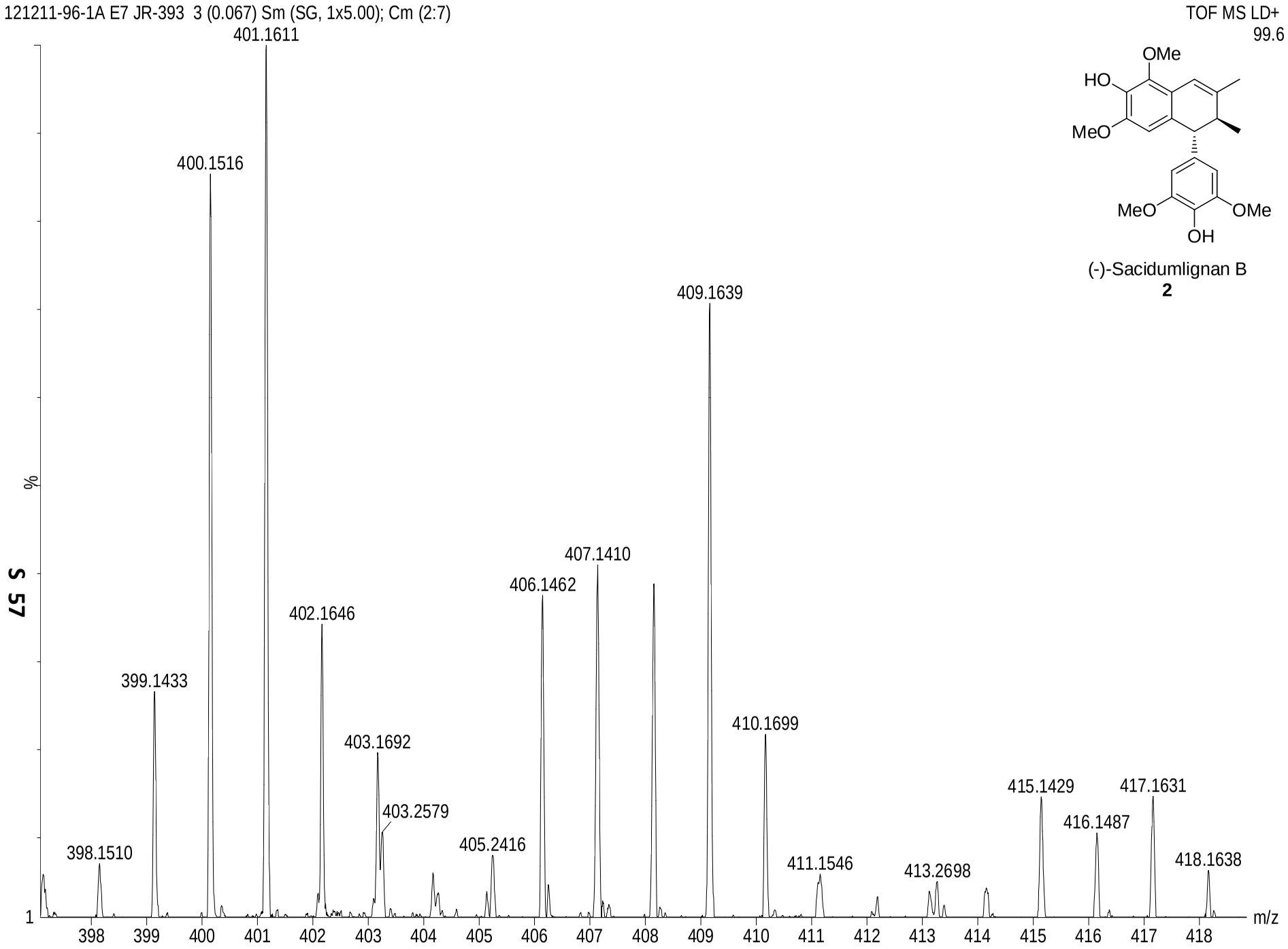
(-)-Sacidumlignan B
2

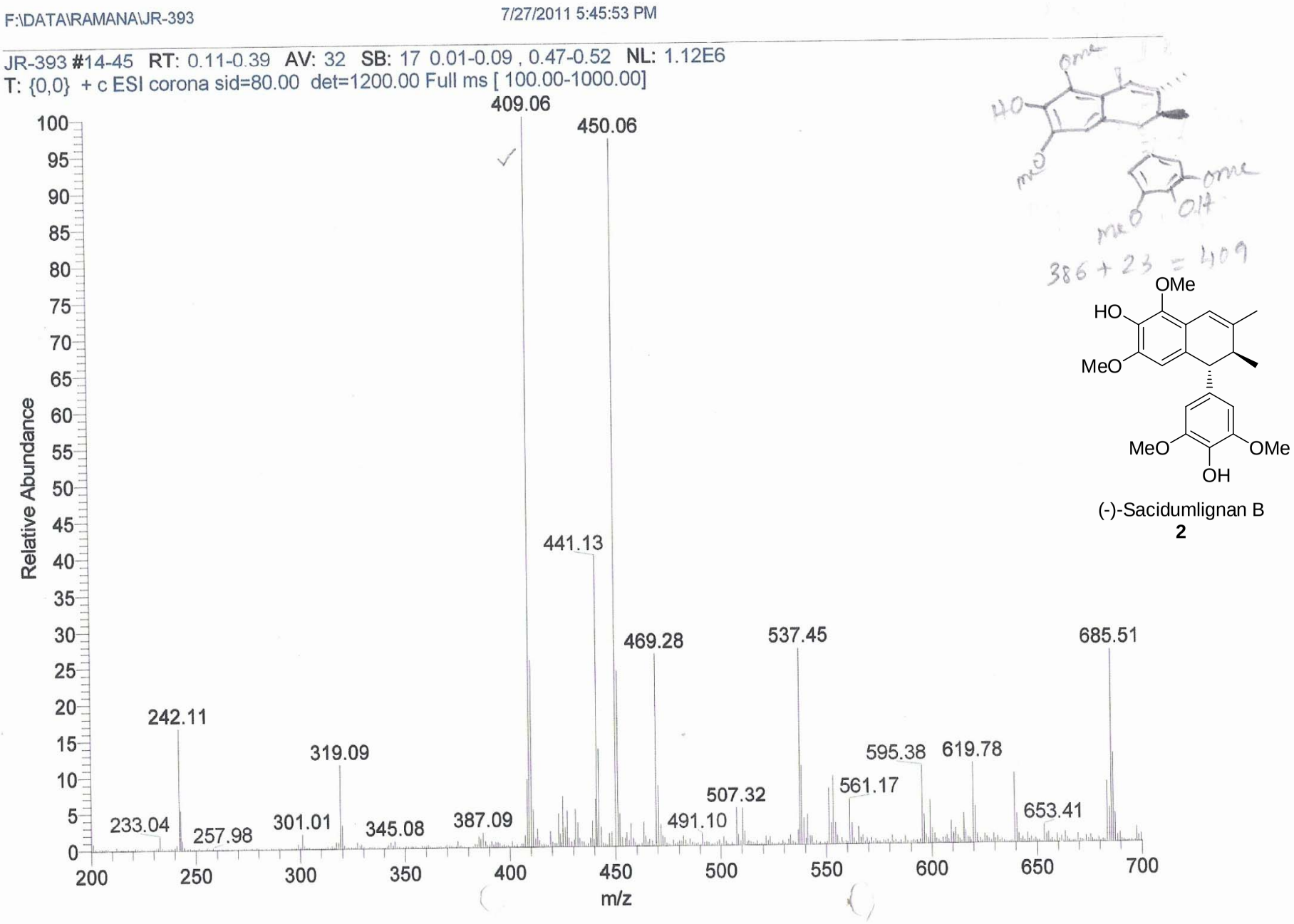
NOESY Experiment in Acetone-d_6



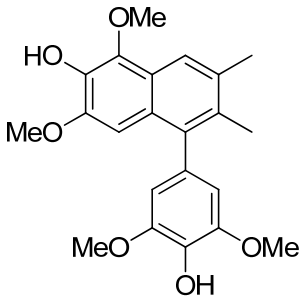


(-)-Sacidumlignan B
2


121211-96-1A E7 JR-393 3 (0.067) Sm (SG, 1x5.00); Cm (2:7)
TOF MS LD+
99.6
401.1611
400.1516
409.1639
407.1410
406.1462
402.1646
399.1433
403.1692
403.2579
410.1699
405.2416
415.1429
417.1631
416.1487
418.1638
411.1546
413.2698
398.1510
%
S 57
1
m/z
398
399
400
401
402
403
404
405
406
407
408
409
410
411
412
413
414
415
416
417
418
OMe
HO
MeO
MeO
OMe
OH
(-)-Sacidumlignan B
2

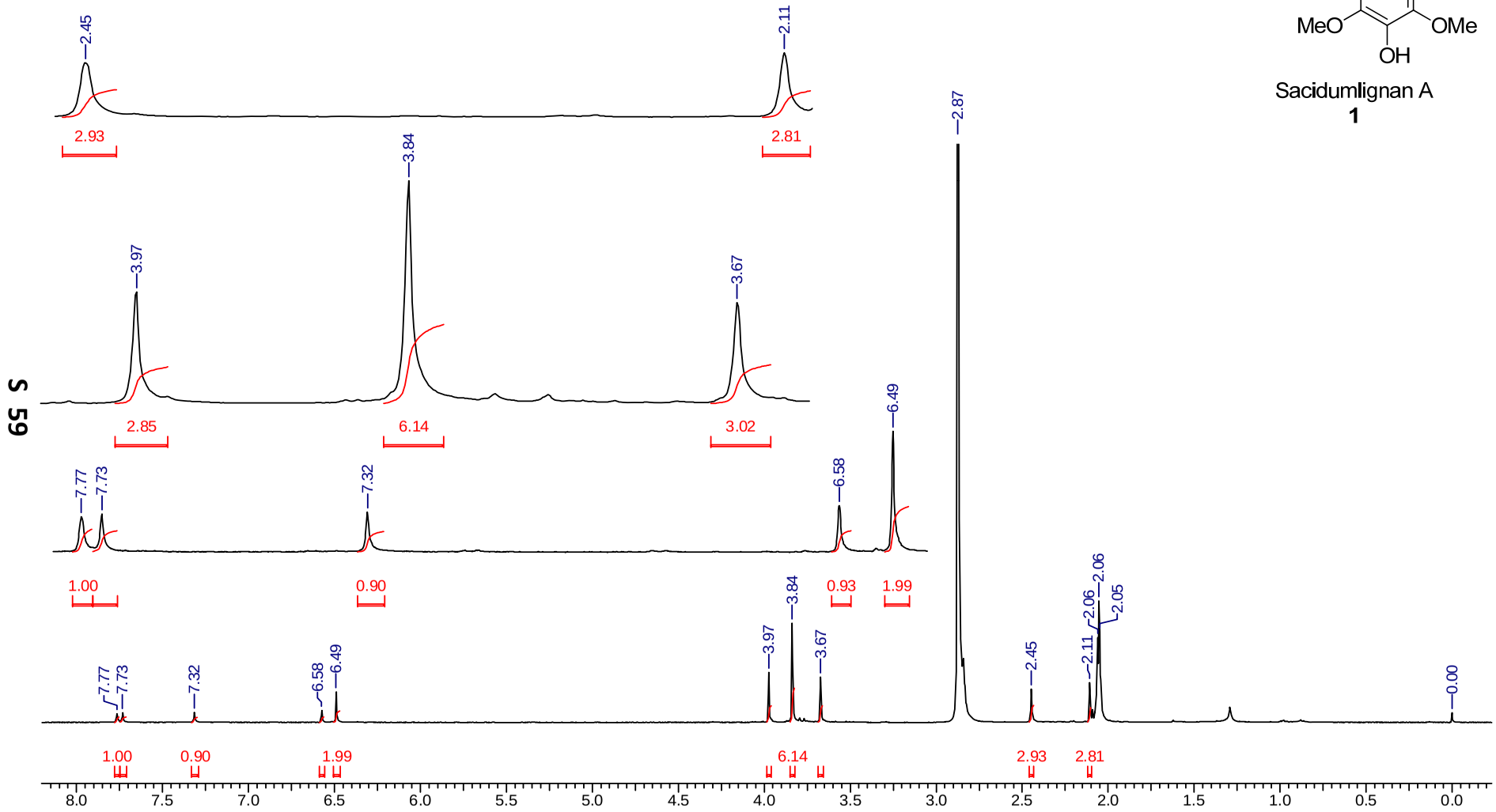

F:\DATA\RAMANA\JR-393
7/27/2011 5:45:53 PM
JR-393 #14-45 RT: 0.11-0.39 AV: 32 SB: 17 0.01-0.09 , 0.47-0.52 NL: 1.12E6
T: {0,0} + c ESI corona sid=80.00 det=1200.00 Full ms [100.00-1000.00]
409.06
450.06
441.13
469.28
537.45
685.51
242.11
319.09
595.38
619.78
561.17
507.32
653.41
233.04
257.98
301.01
345.08
387.09
491.10
Relative Abundance
m/z
386 + 23 = 409
OMe
HO
MeO
MeO
OMe
OH
(-)-Sacidumlignan B
2

Acquisition Time (sec)	3.9846	***Comment***	Jeetendra			***Date***	13/08/2011 14:49:32	
Frequency (MHz)	400.13	***Nucleus***	1H	***Original Points Count***	32768	***Points Count***	32768	***Sweep Width (Hz)***	8223.68
Temperature (grad C)	0.000								



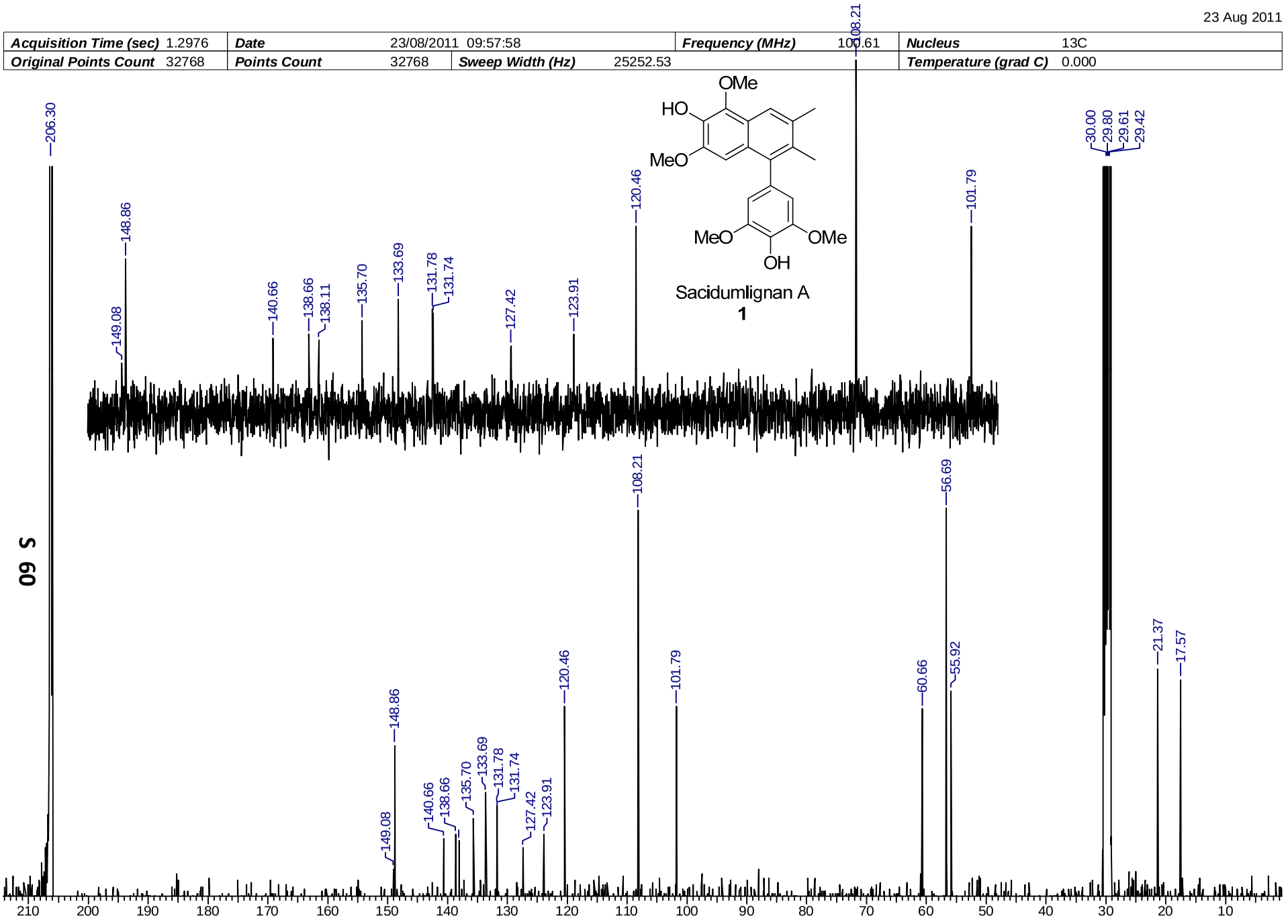
Sacidumlignan A

1



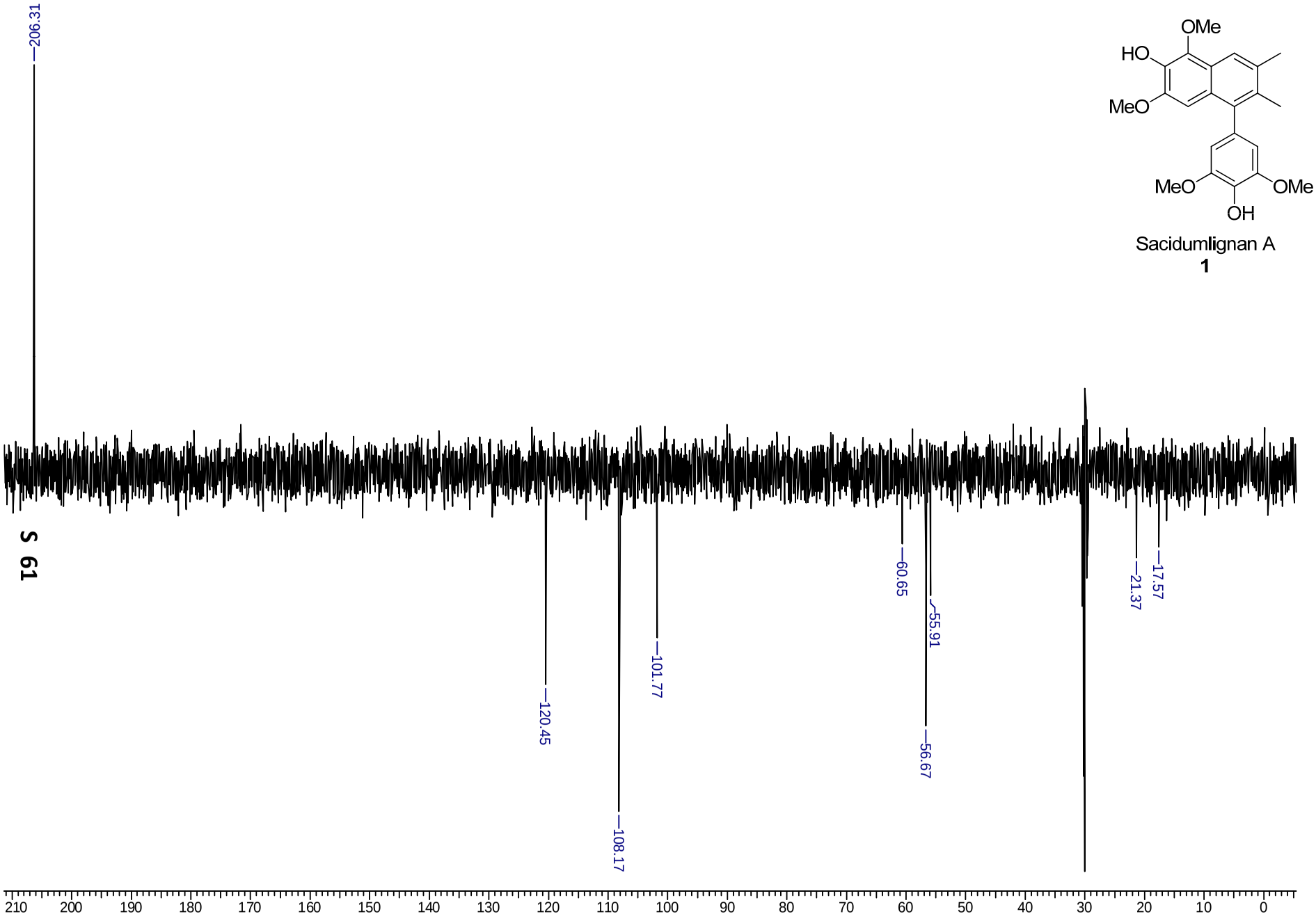
23 Aug 2011

Acquisition Time (sec)	1.2976	***Date***	23/08/2011 09:57:58	***Frequency (MHz)***	100.61	***Nucleus***	13C
Original Points Count	32768	***Points Count***	32768	***Sweep Width (Hz)***	25252.53	***Temperature (grad C)***	0.000



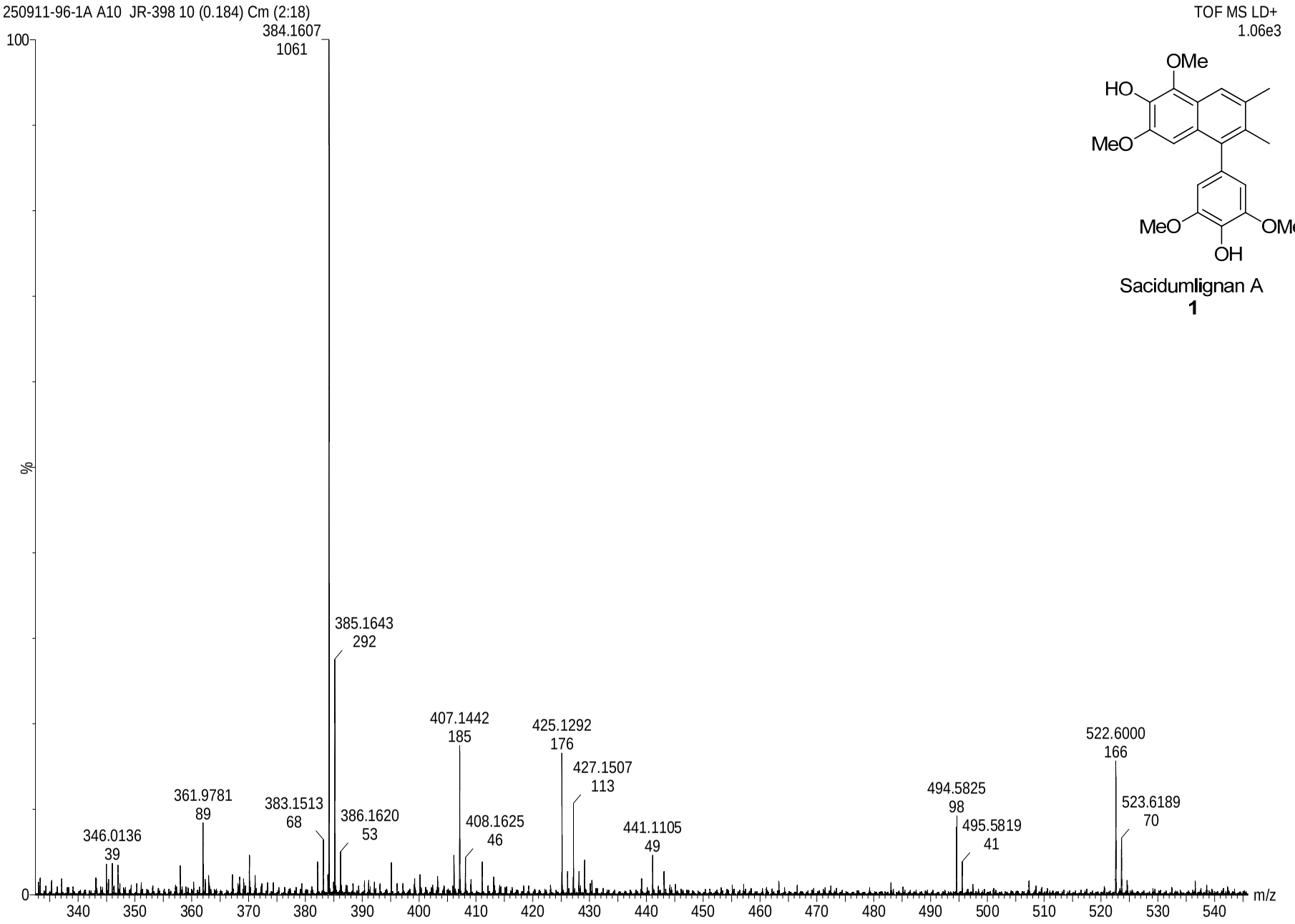
23 Aug 2011

Acquisition Time (sec)	1.3631	***Date***	23/08/2011 09:58:22	***Frequency (MHz)***	100.61	***Nucleus***	13C
Original Points Count	32768	***Points Count***	32768	***Sweep Width (Hz)***	24038.46	***Temperature (grad C)***	0.000



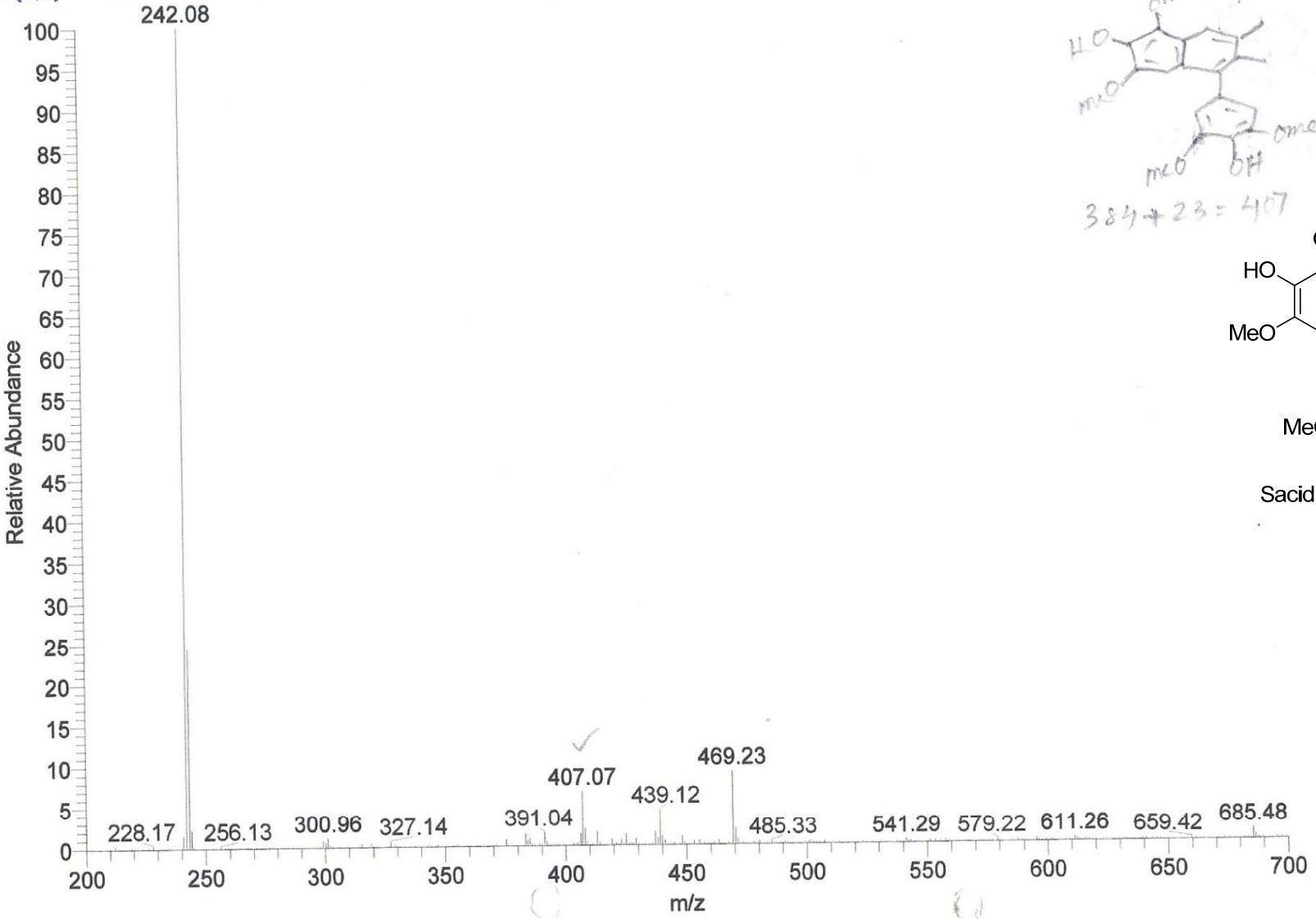
Sacidumlignan A

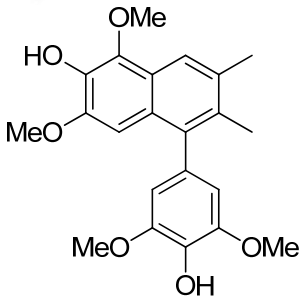
1


250911-96-1A A10 JR-398 10 (0.184) Cm (2:18)
TOF MS LD+
1.06e3
100
%
0
384.1607
1061
385.1643
292
407.1442
185
425.1292
176
427.1507
113
522.6000
166
361.9781
89
383.1513
68
386.1620
53
408.1625
46
441.1105
49
494.5825
98
495.5819
41
523.6189
70
346.0136
39
340
350
360
370
380
390
400
410
420
430
440
450
460
470
480
490
500
510
520
530
540
m/z
OMe
HO
MeO
MeO
OMe
OH
Sacidumlignan A
1

F:\DATA\RAMANA\JR-395 7/27/2011 5:48:24 PM

JR-395 #14-44 RT: 0.11-0.38 AV: 31 SB: 17 0.01-0.08 , 0.46-0.52 NL: 2.11E6
T: {0,0} + c ESI corona sid=80.00 det=1200.00 Full ms [100.00-1000.00]





Sacidumlignan A
1