

Supporting Information

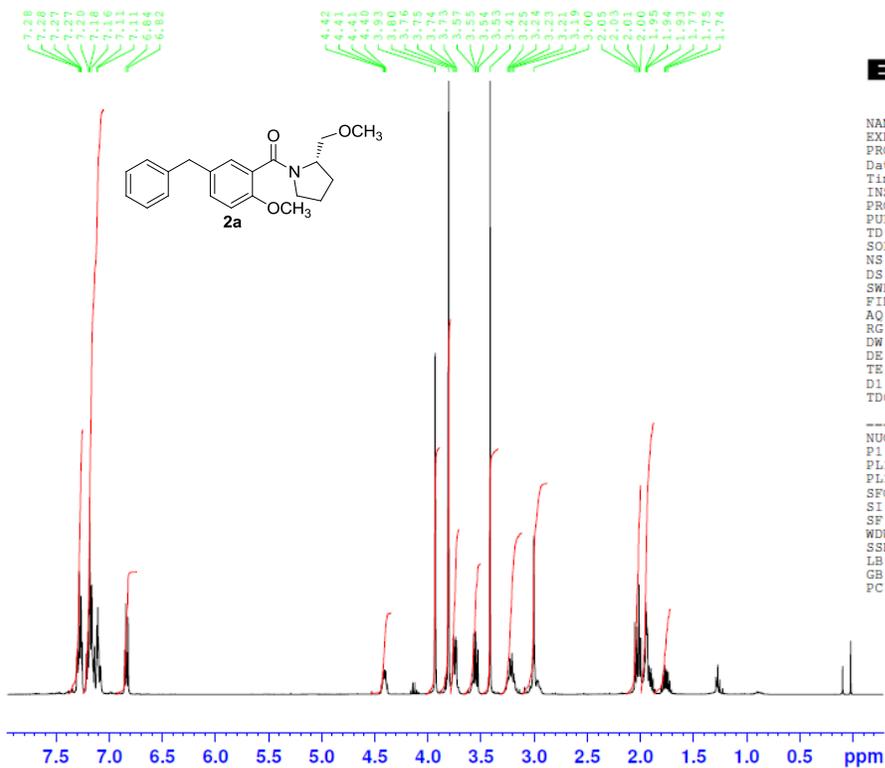
The Enantioselective Construction of Complex Tetracyclic Natural Product Skeletons with Friedel-Crafts Alkylation and Palladium-Catalyzed Cycloalkenylation Reactions

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Department of Chemistry, Bryn Mawr College, Bryn Mawr, Pennsylvania 19010-2899 USA.

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S133-S134	¹ H NMR and ¹³ C NMR for 12e
S135-S137	¹ H NMR, ¹³ C NMR and GC/MS for 13b
S138-S140	¹ H NMR, ¹³ C NMR and GC/MS for 13d
S141-S143	¹ H NMR, ¹³ C NMR and GC/MS for 13e
S144-S146	¹ H NMR, ¹³ C NMR and GC/MS for 14b
S147-S149	¹ H NMR, ¹³ C NMR and GC/MS for 14d
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S188-S193	¹ H NMR, ¹³ C NMR and GC/MS for 21
S194-S198	¹ H NMR and GC/MS for 25-28
S199-S202	¹ H NMR, ¹³ C NMR, GC/MS, COSY, HSQC and NOESY for 26

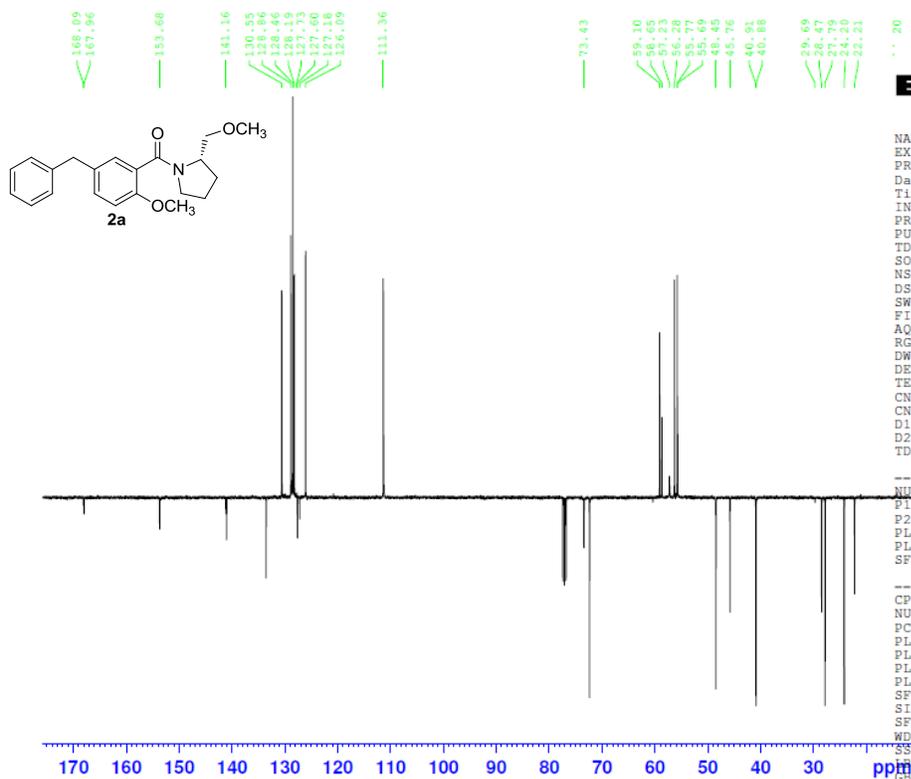


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SOLVENT   CDC13
NS         16
DS         2
SWH        8223.685 Hz
FIDRES    0.125483 Hz
AQ         3.9846387 sec
RG         45.2
DW         60.800 usec
DE         6.50 usec
TE         301.2 K
D1         1.00000000 sec
TDO        1
  
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----- CHANNEL f1 -----
NUC1      1H
P1         12.50 usec
PL1        -2.00 dB
PL1W      12.14226913 W
SFO1      400.1524711 MHz
SI         32768
SF         400.1500000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
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TD         65536
SOLVENT   CDC13
NS         1024
DS         4
SWH        24038.461 Hz
FIDRES    0.366798 Hz
AQ         1.3631988 sec
RG         203
DW         20.800 usec
DE         6.50 usec
TE         301.2 K
CNST2     145.0000000
CNST11    1.0000000
D1         2.00000000 sec
D20        0.00689655 sec
TDO        1
  
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----- CHANNEL f1 -----
NUC1      13C
P1         8.00 usec
P2         16.00 usec
PL1        -2.00 dB
PL1W      56.13311005 W
SFO1      100.6278593 MHz
  
```

```

----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2        -2.00 dB
PL12      14.00 dB
PL2W      12.14226913 W
PL12W     0.30500001 W
SFO2      400.1515629 MHz
SI         32768
SF         100.6177980 MHz
WDW        EM
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Area Percent Report

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Misc :
ALS Vial : 95 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

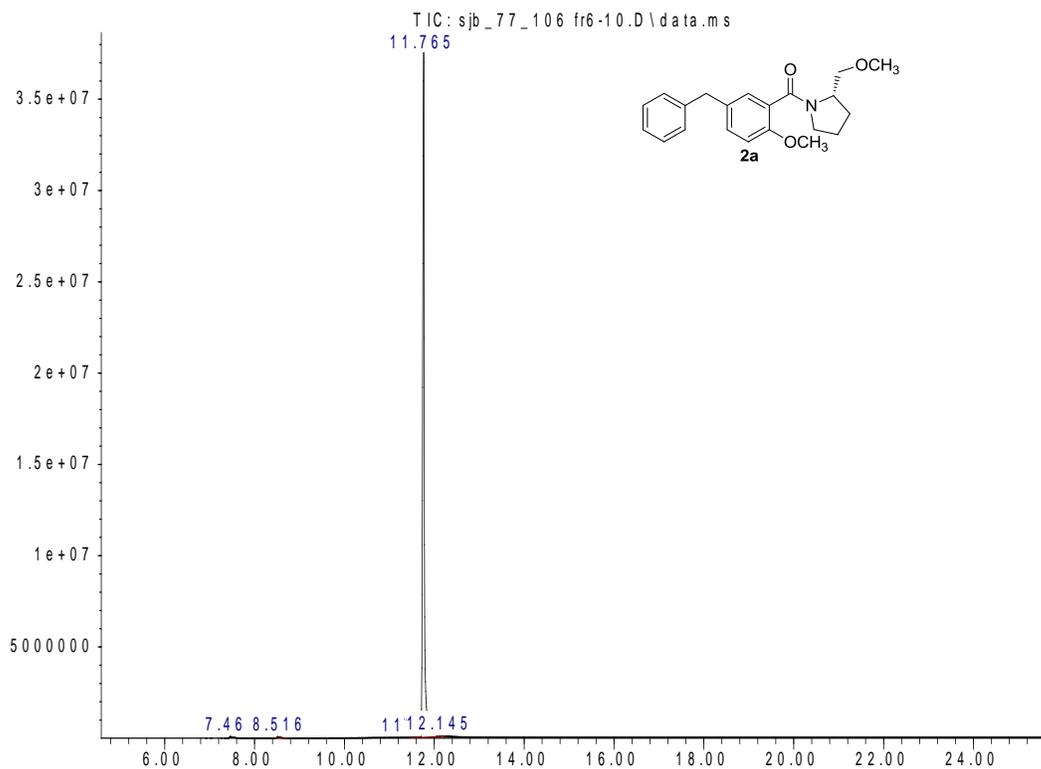
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1	7.462	495	503	539	BV 3	88847	5339264	0.53%	0.524%
2	8.516	679	688	720	BV 3	78689	3977198	0.40%	0.390%
3	11.592	1205	1225	1232	PV 7	20748	714829	0.07%	0.070%
4	11.765	1241	1255	1306	PV 2	38376200	1003659892	100.00%	98.448%
5	12.060	1306	1307	1314	VV 4	119329	2690695	0.27%	0.264%
6	12.107	1314	1315	1321	VV 6	81401	1599566	0.16%	0.157%
7	12.145	1321	1322	1337	VV 9	51004	1503320	0.15%	0.147%

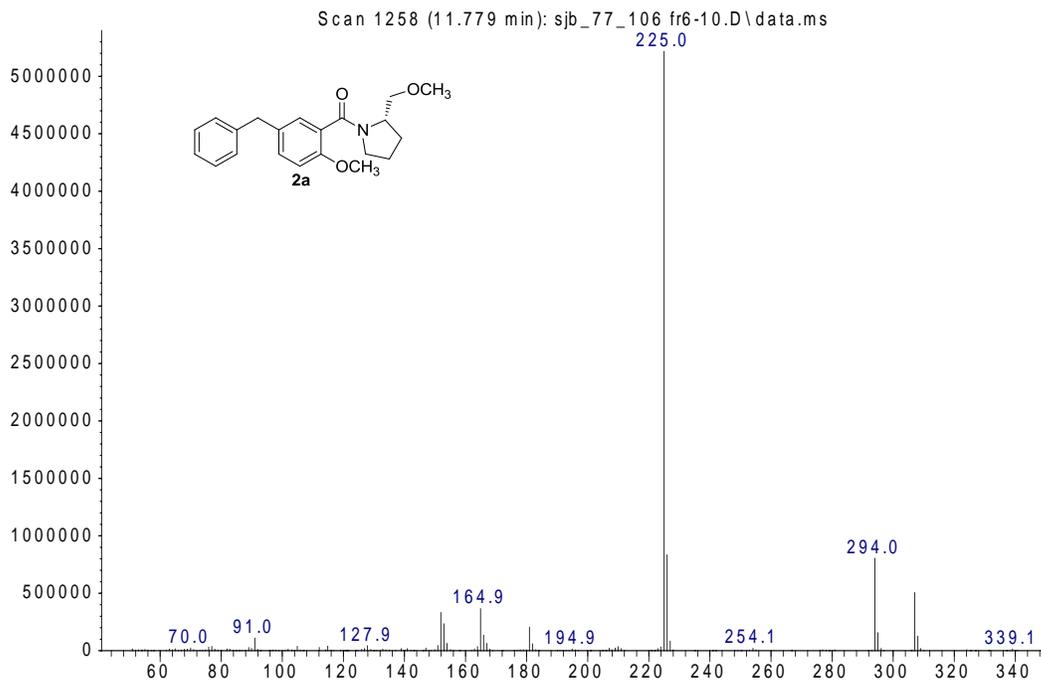
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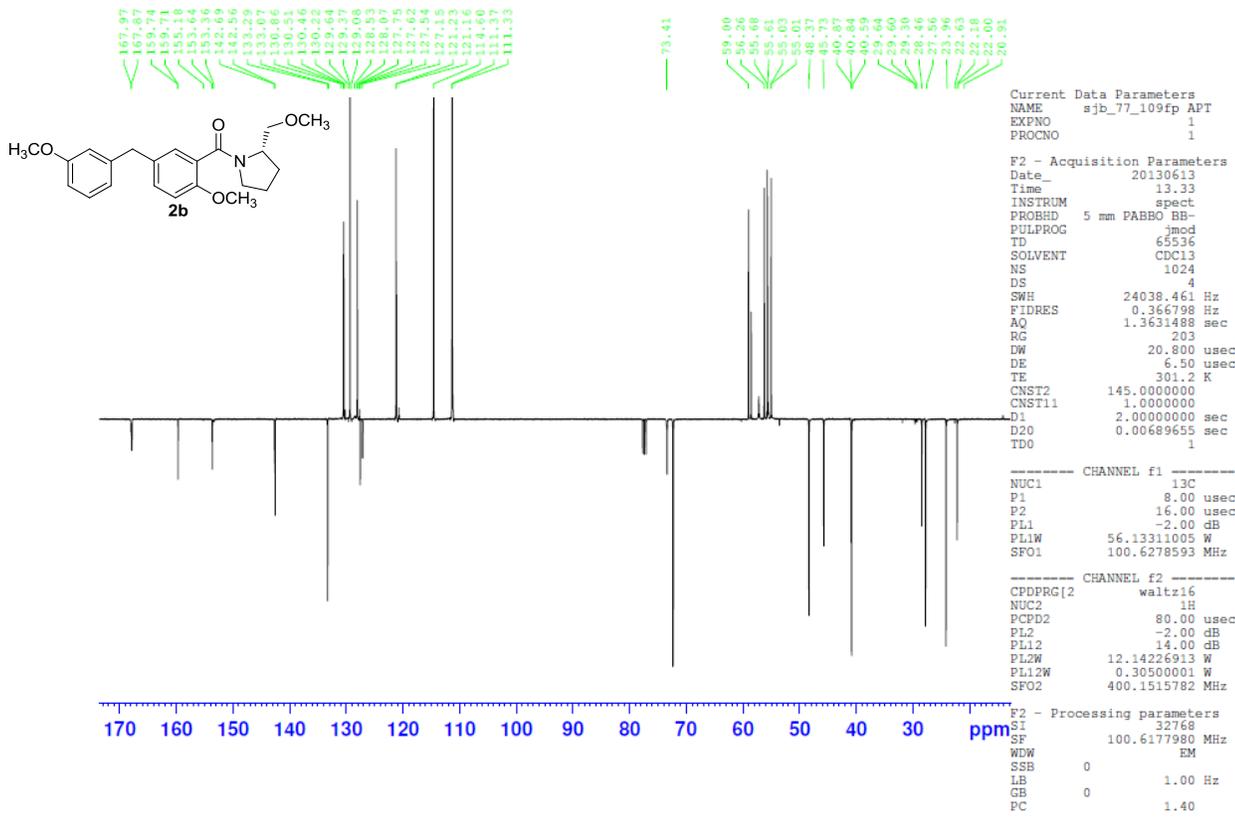
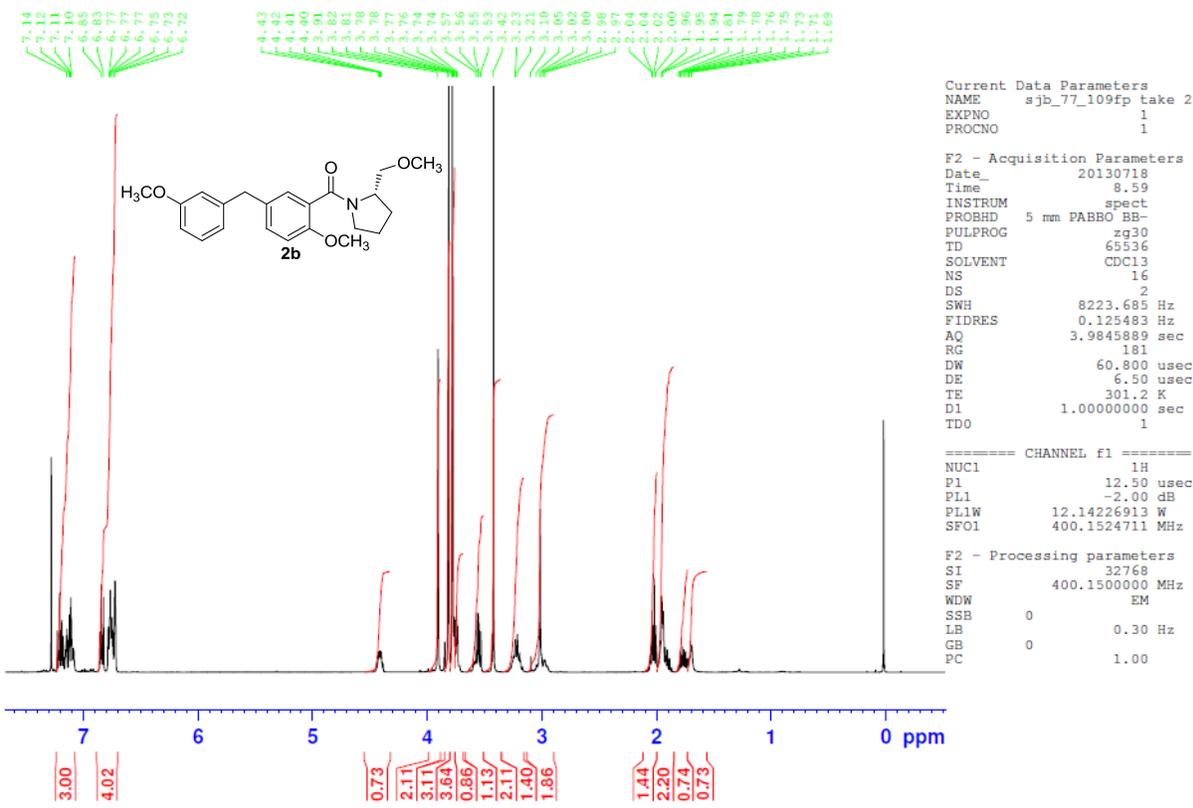


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m/z-->



Area Percent Report

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Acq On : 9 Jul 2013 13:36
Operator : AK
Sample : sjb_77_140fp
Misc :
ALS Vial : 80 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

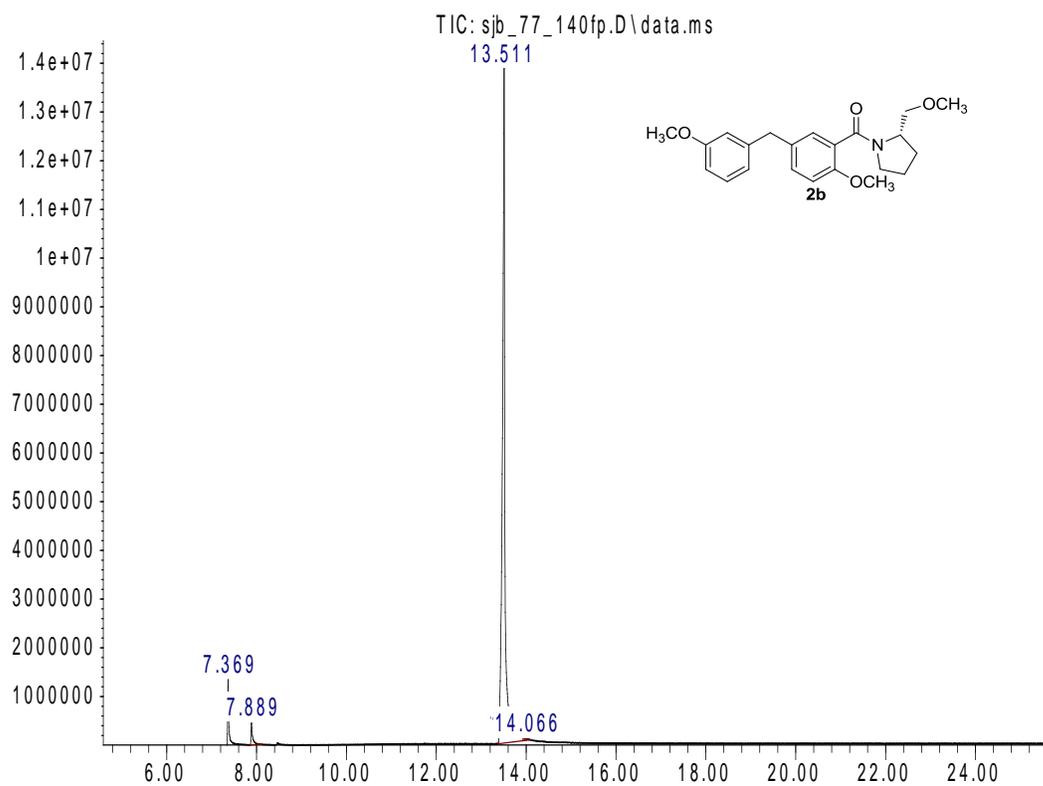
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1	7.369	479	487	520	BV	1310017	25296056	4.59%	4.282%
2	7.889	572	578	614	PV	448612	11314701	2.05%	1.916%
3	13.511	1536	1561	1634	PV	14301284	551191459	100.00%	93.314%
4	13.937	1634	1635	1642	VV 6	65507	1414234	0.26%	0.239%
5	13.986	1642	1644	1649	VV 6	40178	838374	0.15%	0.142%
6	14.025	1649	1650	1656	VV 6	31550	525723	0.10%	0.089%
7	14.066	1656	1658	1660	VV 3	14484	107248	0.02%	0.018%

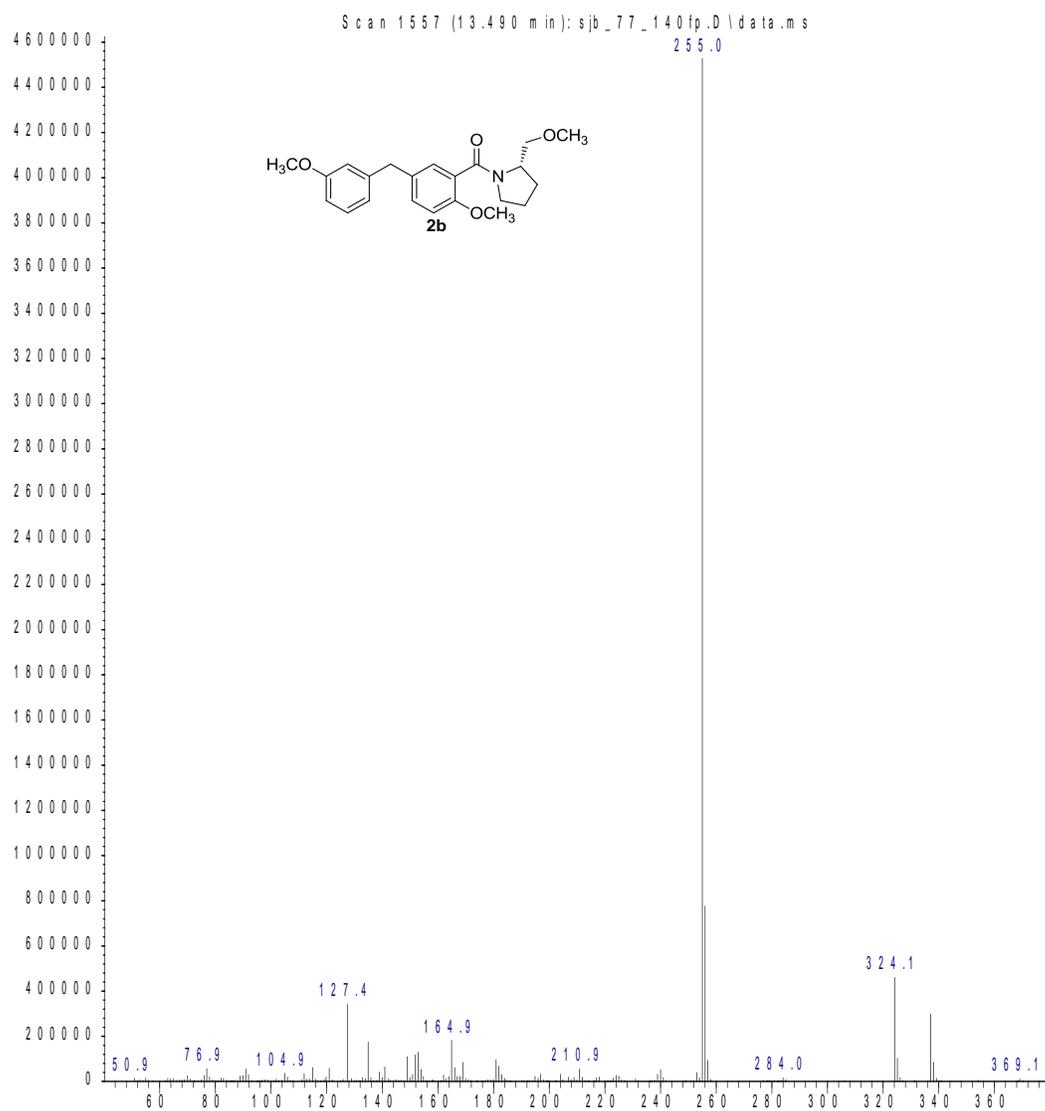
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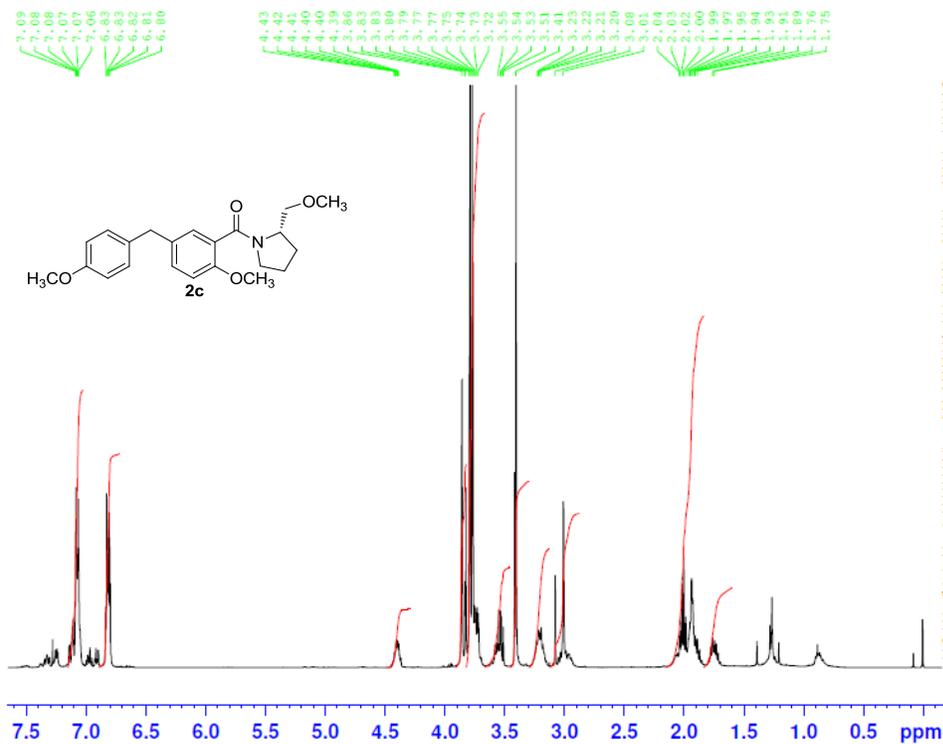


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Abundance



m/z-->

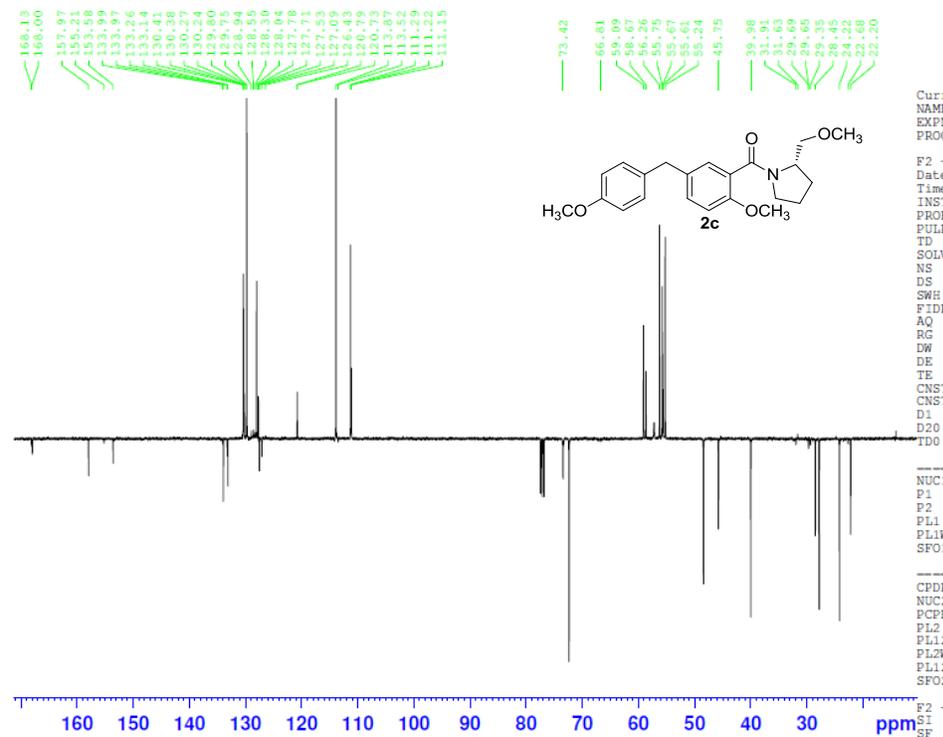


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 PROCNO 1

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 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 40.3
 DW 60.800 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.50 usec
 PL1 -2.00 dB
 PL1W 12.14226913 W
 SFO1 400.1524711 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1500000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME sjb_77_190fp APT2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130923
 Time 10.38
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG jmod
 TD 65536
 SOLVENT CDC13
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 298.2 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 2.00000000 sec
 D20 0.00689655 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.00 usec
 P2 16.00 usec
 PL1 -2.00 dB
 PL1W 56.13311005 W
 SFO1 100.6278593 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 75.00 usec
 PL2 -2.00 dB
 PL12 13.39 dB
 PL2W 12.14226913 W
 PL12W 0.35099408 W
 SFO2 400.1514874 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6177980 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Area Percent Report

Data Path : C:\msdchem\1\DATA\
Data File : sjb_77_190fp.D
Acq On : 10 Sep 2013 9:25
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Sample : sjb_77_190fp
Misc :
ALS Vial : 85 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

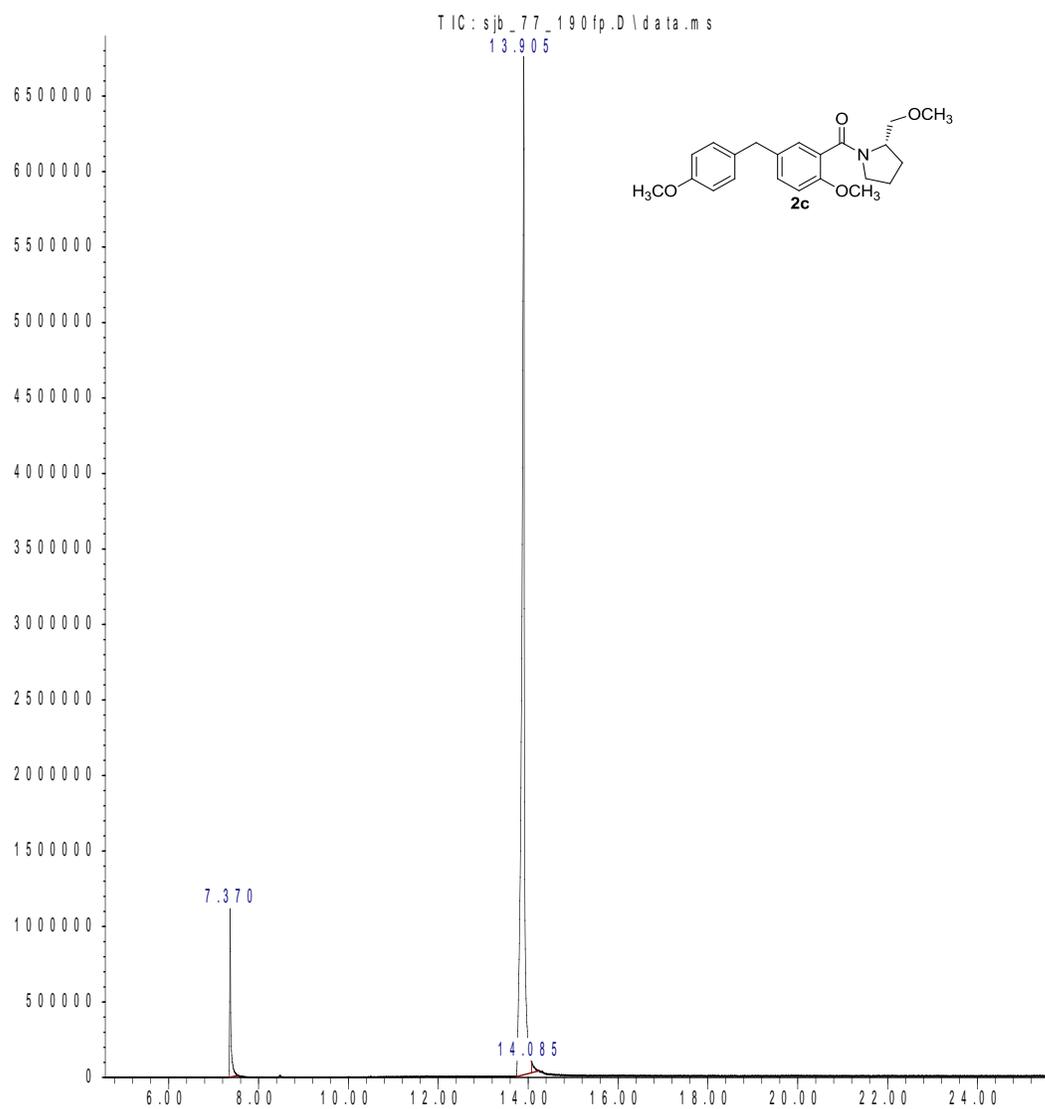
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Signal : TIC: sjb_77_190fp.D\data.ms

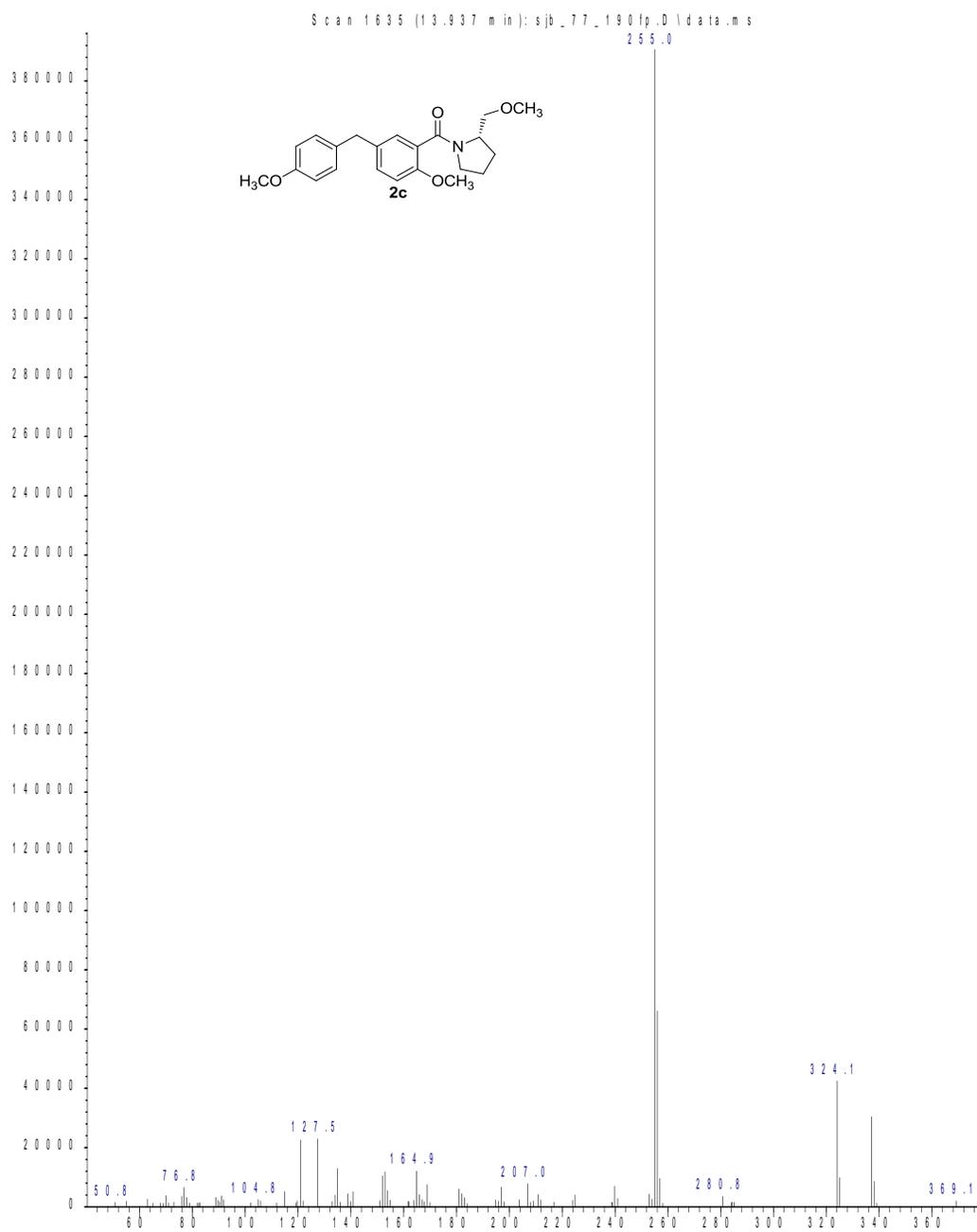
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.370	481	487	517	BV	1069928	19231620	7.04%	6.523%
2	13.905	1598	1629	1660	BV	6770640	273181350	100.00%	92.651%
3	14.085	1660	1661	1687	VV 6	69181	2435562	0.89%	0.826%

Sum of corrected areas: 29484853

Abundance



Abundance



m/z-->

Area Percent Report

Data Path : C:\msdchem\1\DATA\
Data File : sjb_81_015fp2.D
Acq On : 11 Oct 2013 15:54
Operator : sjb
Sample : sjb_81_015fp2
Misc :
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Integration Parameters: atuneWPMar14.e
Integrator: ChemStation

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Title :

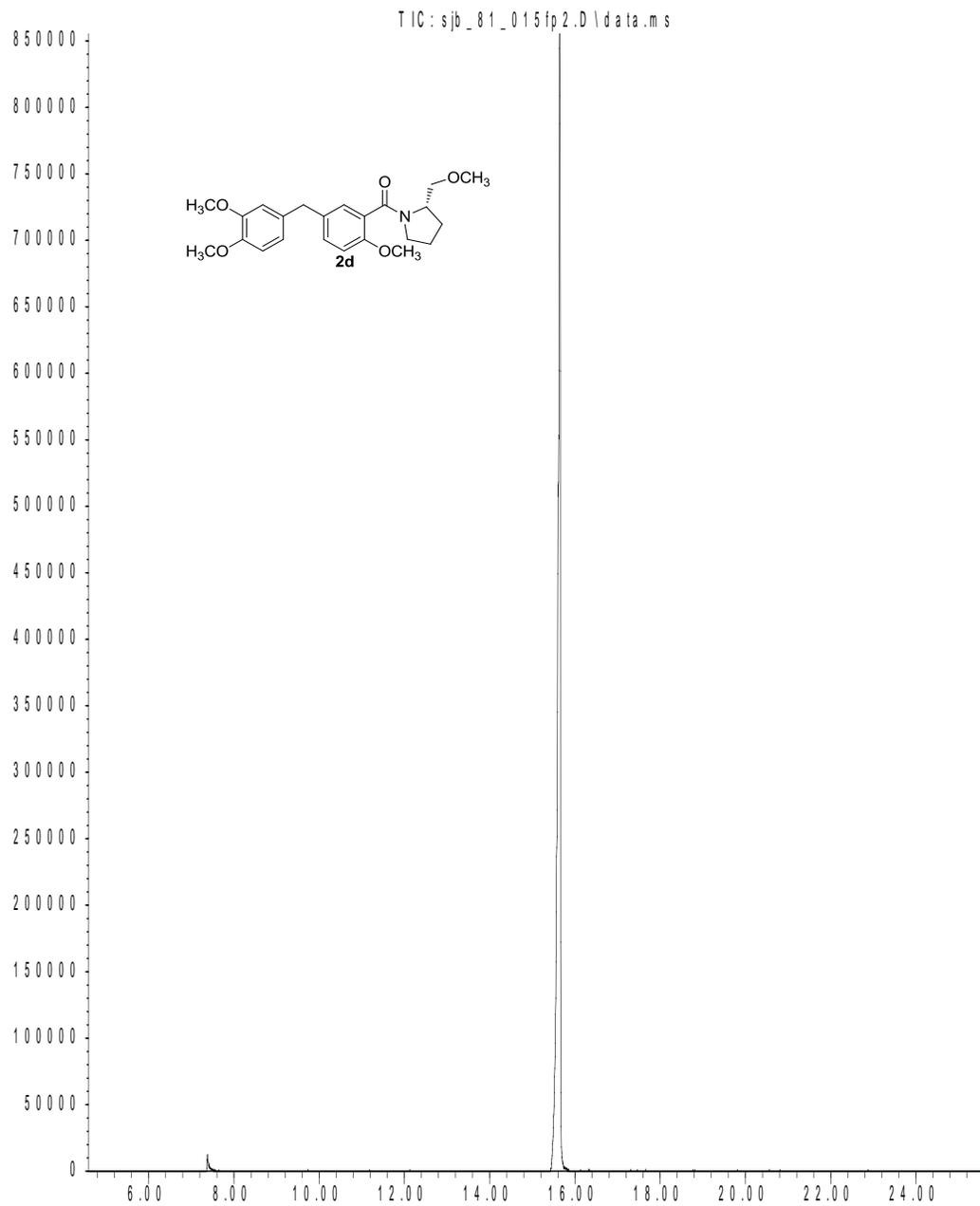
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peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	15.643	1895	1933	1951	BV	864446	36310266	100.00%	100.000%

Sum of corrected areas: 36310266

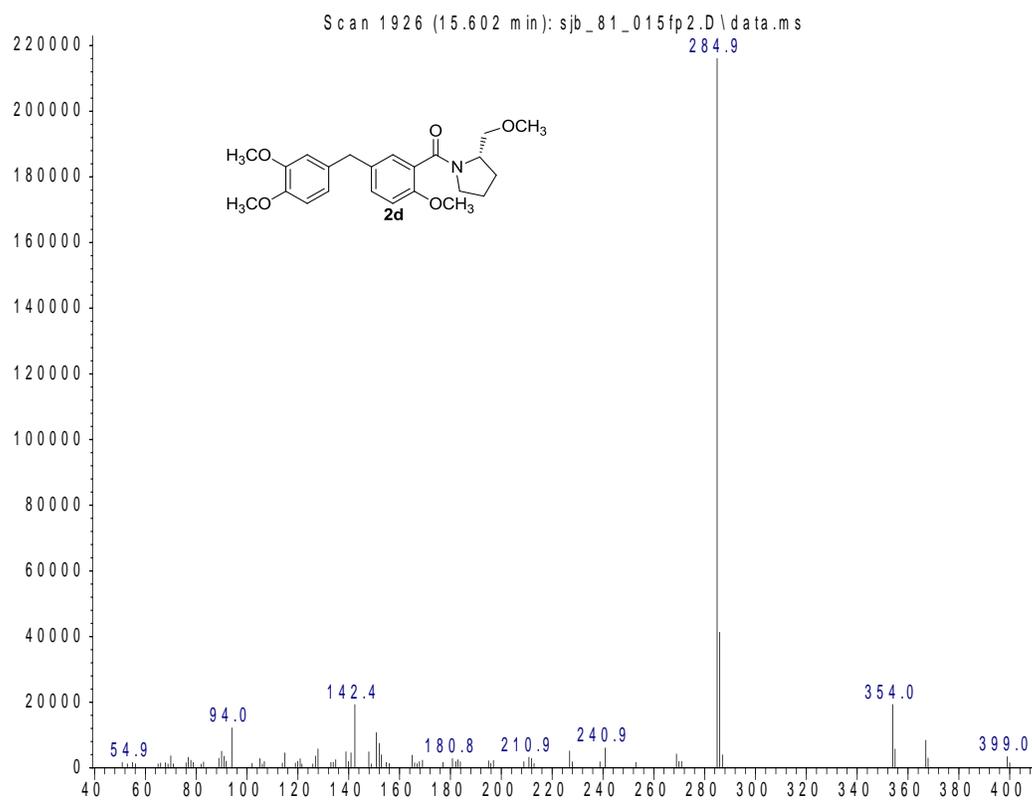
ckr3.m Wed Mar 19 11:39:48 2014

Abundance

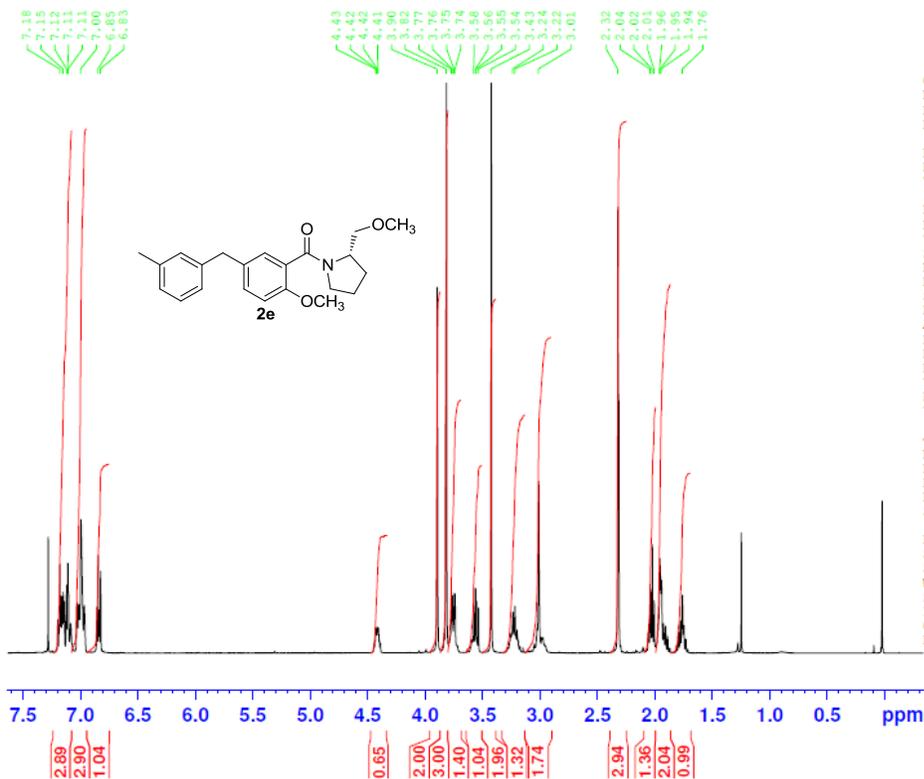


Time-->

Abundance



m/z-->

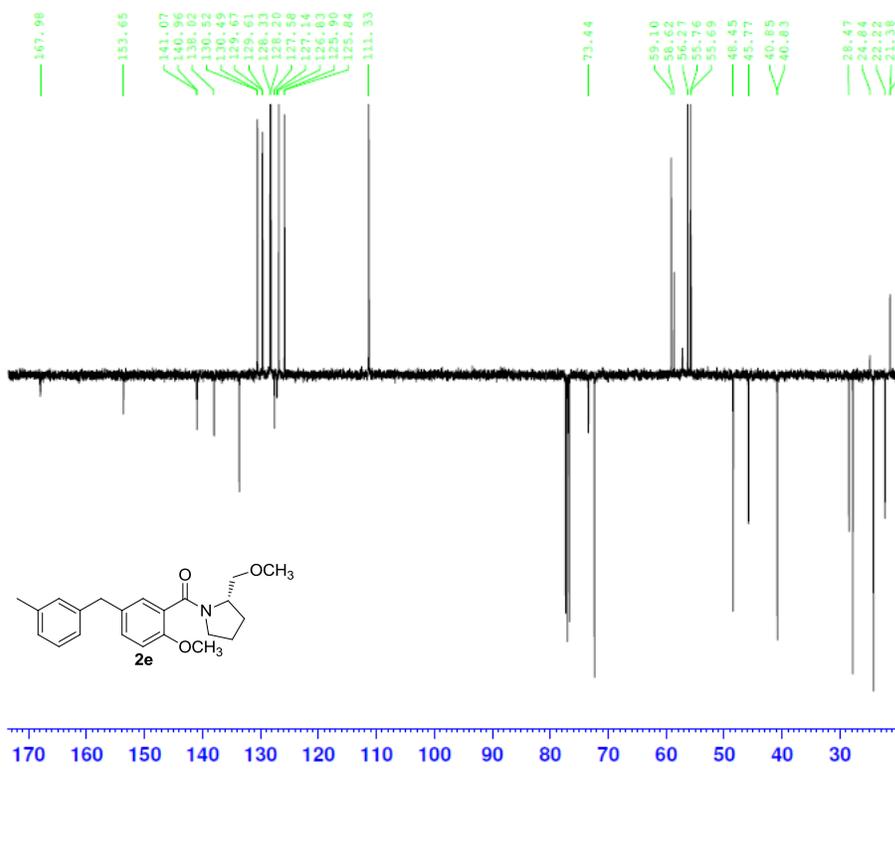


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 PULPROG zg30
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 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 128
 DW 60.800 usec
 DE 6.50 usec
 TE 301.2 K
 D1 1.0000000 sec
 TDO 1

----- CHANNEL f1 -----
 NUC1 1H
 P1 12.50 usec
 PL1 -2.00 dB
 PL1W 12.14226913 W
 SFO1 400.1524711 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1500000 MHz
 WDW EM
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 GB 0
 PC 1.00



Current Data Parameters
 NAME sjb_77_139fp AP13
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130716
 Time 8.42
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG jmod
 TD 65536
 SOLVENT CDCl3
 NS 775
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 301.2 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 2.0000000 sec
 D20 0.00689655 sec
 TDO 1

----- CHANNEL f1 -----
 NUC1 13C
 P1 8.00 usec
 P2 16.00 usec
 PL1 -2.00 dB
 PL1W 56.13311005 W
 SFO1 100.6278593 MHz

----- CHANNEL f2 -----
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -2.00 dB
 PL12 14.00 dB
 PL2W 12.14226913 W
 PL12W 0.30500001 W
 SFO2 400.1517609 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6177980 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Area Percent Report

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Acq On : 8 Jul 2013 9:53
Operator : ep
Sample : sjb_77_139fp
Misc :
ALS Vial : 90 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

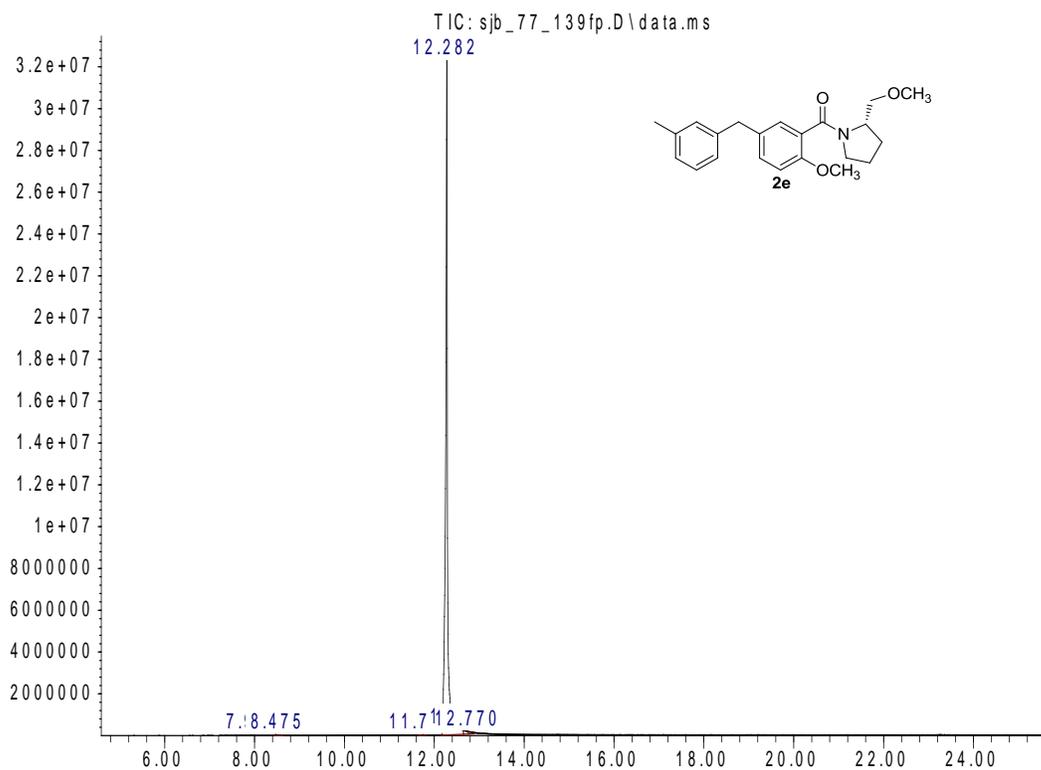
Method : C:\msdchem\1\5973N\PRECISION.M
Title :

Signal : TIC: sjb_77_139fp.D\data.ms

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1	7.929	561	585	599	BV	28577	573288	0.06%	0.056%
2	8.475	675	680	704	BV 3	44818	1476917	0.15%	0.144%
3	11.749	1236	1253	1264	PV 4	20623	556794	0.06%	0.054%
4	12.282	1323	1346	1410	PV 2	33061394	1005291419	100.00%	98.150%
5	12.662	1410	1412	1429	VV 8	191146	9977408	0.99%	0.974%
6	12.770	1429	1431	1452	VB 8	109101	6364368	0.63%	0.621%

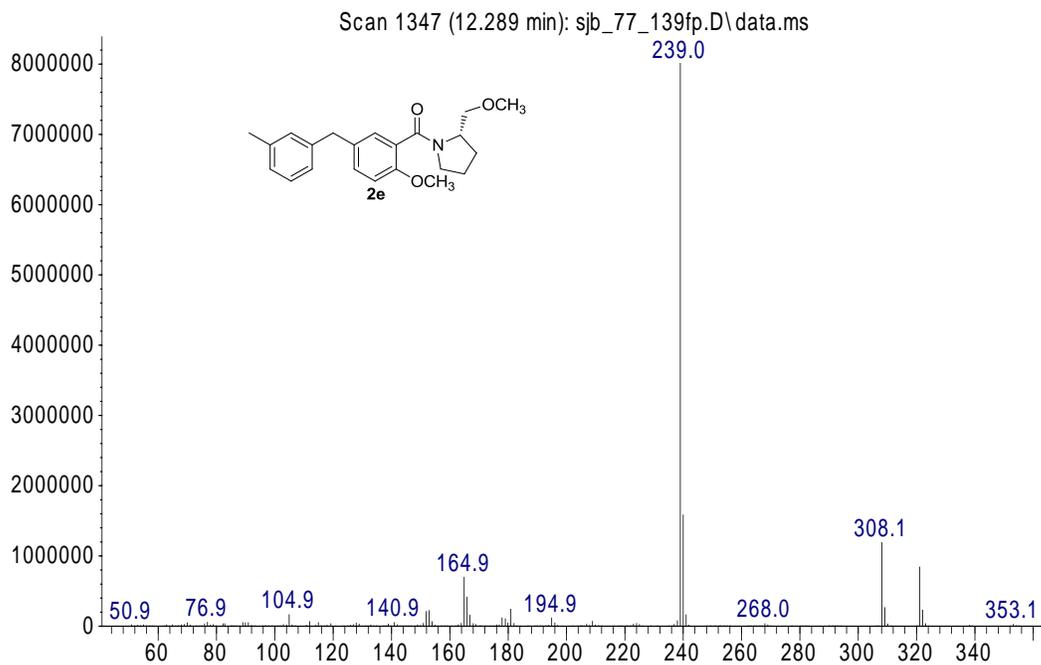
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Abundance



Time-->

Abundance



m/z-->

Area Percent Report

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Operator : sjb
Sample : sjb_74_196fp
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ALS Vial : 5 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\msdchem\1\METHODS\JMB2.m
Title :

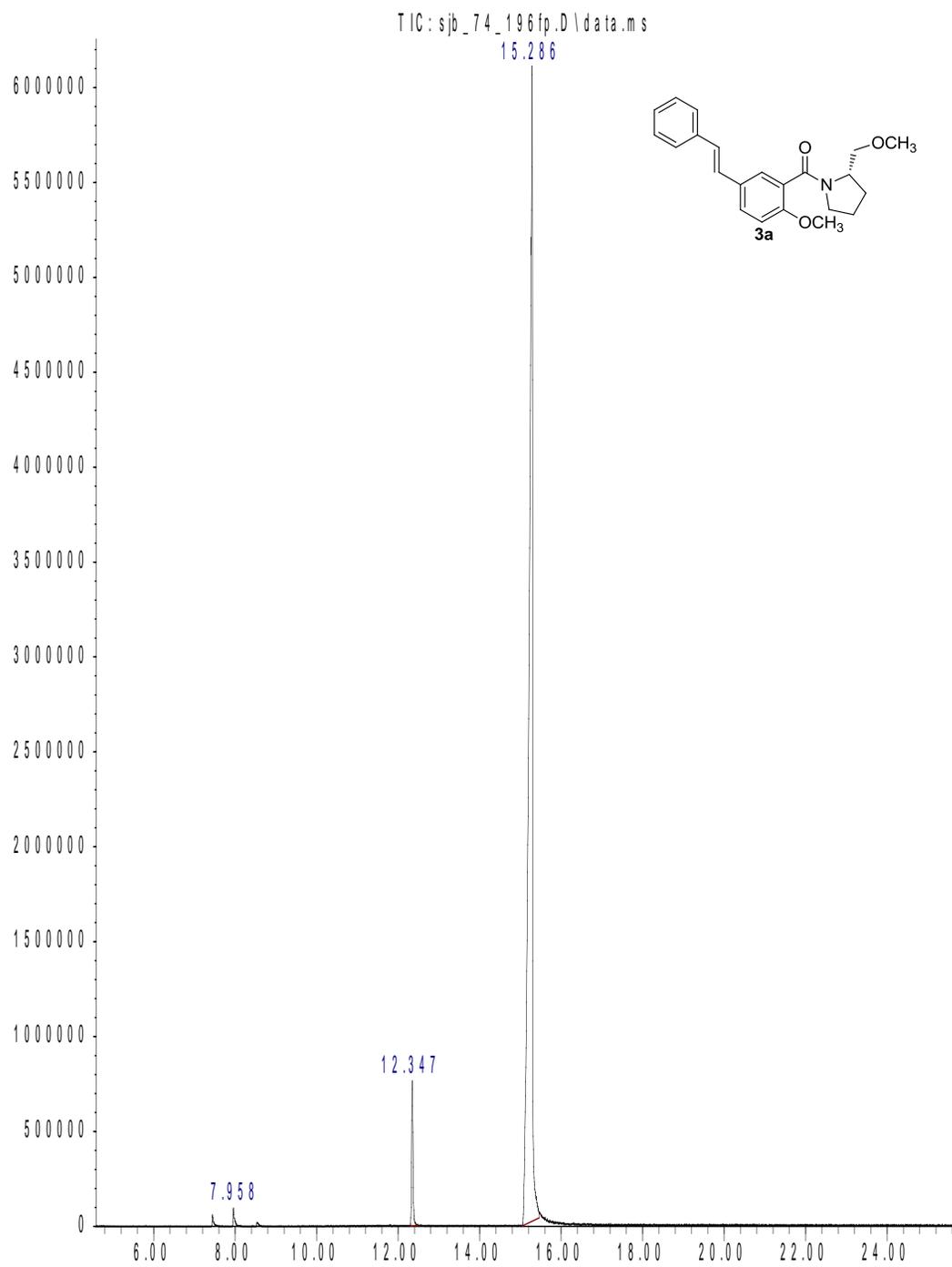
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1	7.958	585	590	614	BV	93249	2391488	0.67%	0.638%
2	12.347	1348	1357	1377	BV 2	754583	16444164	4.62%	4.385%
3	15.286	1828	1871	1901	BV	6269080	356146758	100.00%	94.977%

Sum of corrected areas: 374982409

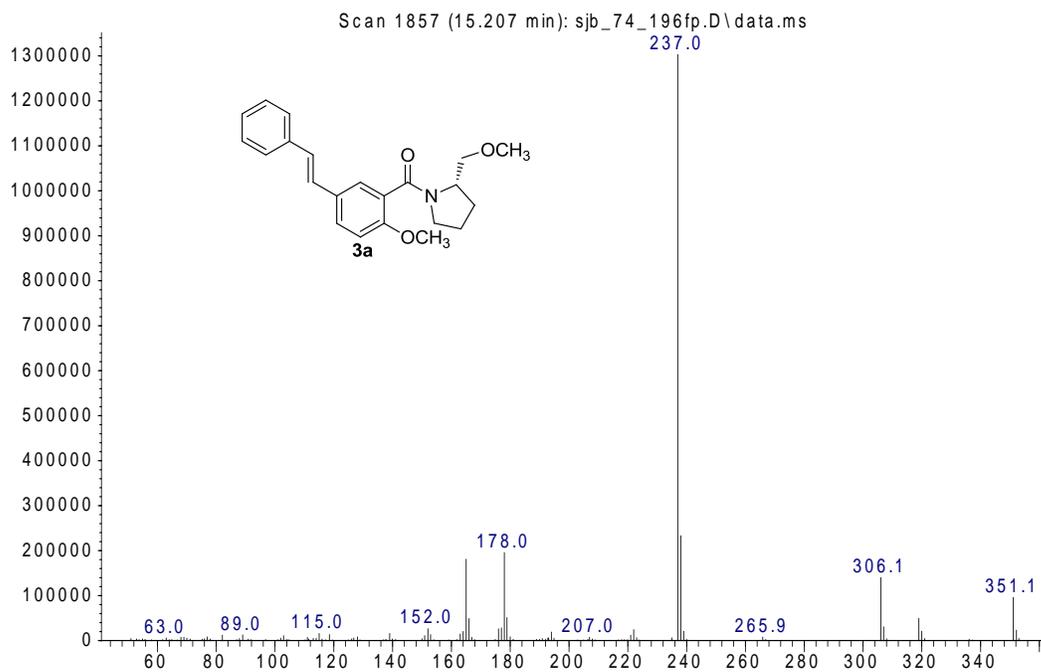
JMB2.m Mon Nov 12 09:46:30 2012

Abundance

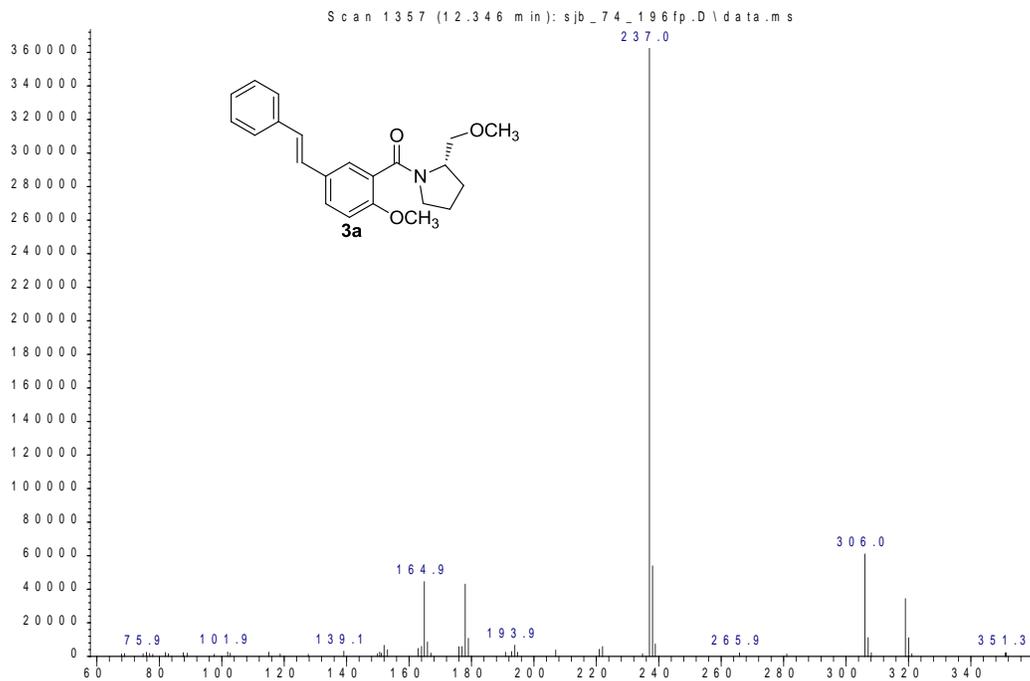


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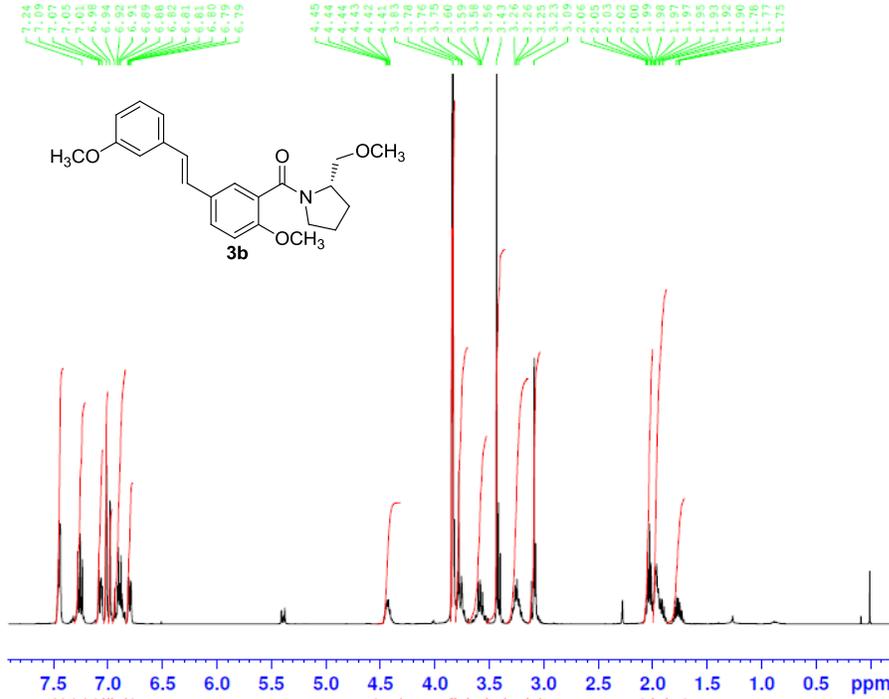
Abundance



m/z-->
Abundance

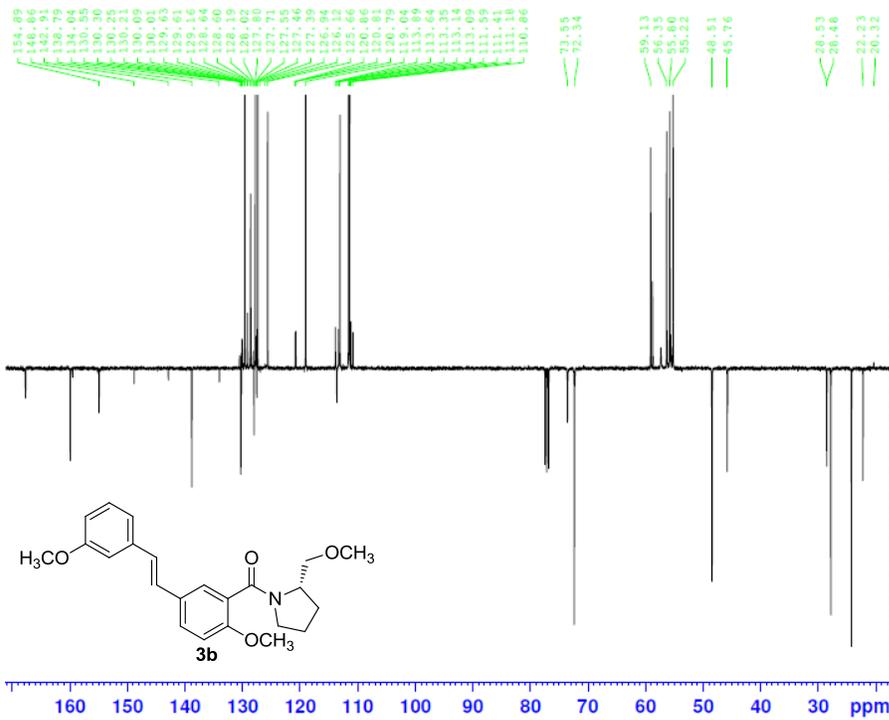


m/z-->



NAME sjb_77_149fp take 2
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PROCNO 1
Date_ 20130718
Time 7.46
INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 40.3
DW 60.800 usec
DE 6.50 usec
TE 301.2 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 12.50 usec
PL1 -2.00 dB
PL1W 12.14226913 W
SFO1 400.1524711 MHz
SI 32768
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME sjb_77_149fp APT
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130718
Time 8.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 987
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 301.2 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TD0 1

CHANNEL f1
NUC1 13C
P1 8.00 usec
P2 16.00 usec
PL1 -2.00 dB
PL1W 56.13311005 W
SFO1 100.6278593 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 14.00 dB
PL2W 12.14226913 W
PL12W 0.30500001 W
SFO2 400.1515527 MHz

F2 - Processing parameters
SI 32768
SF 100.6177980 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Area Percent Report

Data Path : C:\msdchem\1\DATA\
Data File : sjb_74_028fp.D
Acq On : 12 Jun 2012 15:29
Operator : sjb
Sample : sjb_74_028fp
Misc :
ALS Vial : 35 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\msdchem\1\METHODS\JMB2.m
Title :

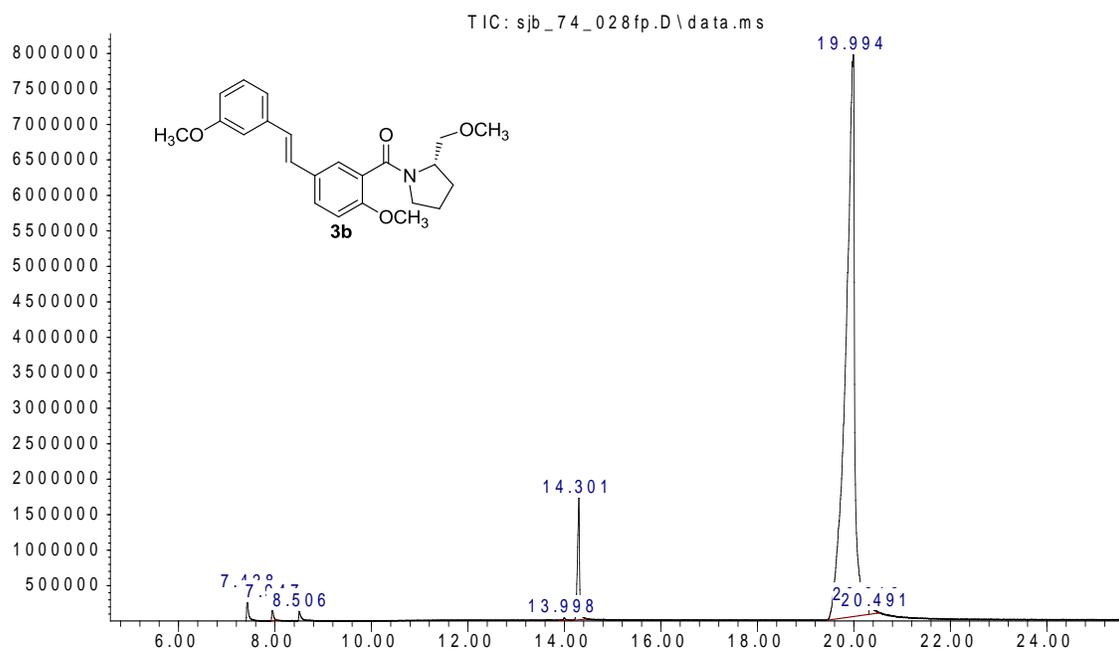
Signal : TIC: sjb_74_028fp.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.428	492	498	537	BV	394397	9499465	0.92%	0.856%
2	7.947	582	588	604	BV	244367	4966452	0.48%	0.447%
3	8.506	678	686	715	PV	133193	4366147	0.42%	0.393%
4	13.998	1627	1646	1657	PV 2	34621	1132361	0.11%	0.102%
5	14.301	1680	1699	1726	PV	1718437	52484842	5.09%	4.727%
6	19.994	2598	2694	2749	PV	8203405	1030243382	100.00%	92.793%
7	20.316	2749	2750	2779	VV 6	124068	7195565	0.70%	0.648%
8	20.491	2779	2781	2788	VV 8	22518	375776	0.04%	0.034%

Sum of corrected areas: 1110263990

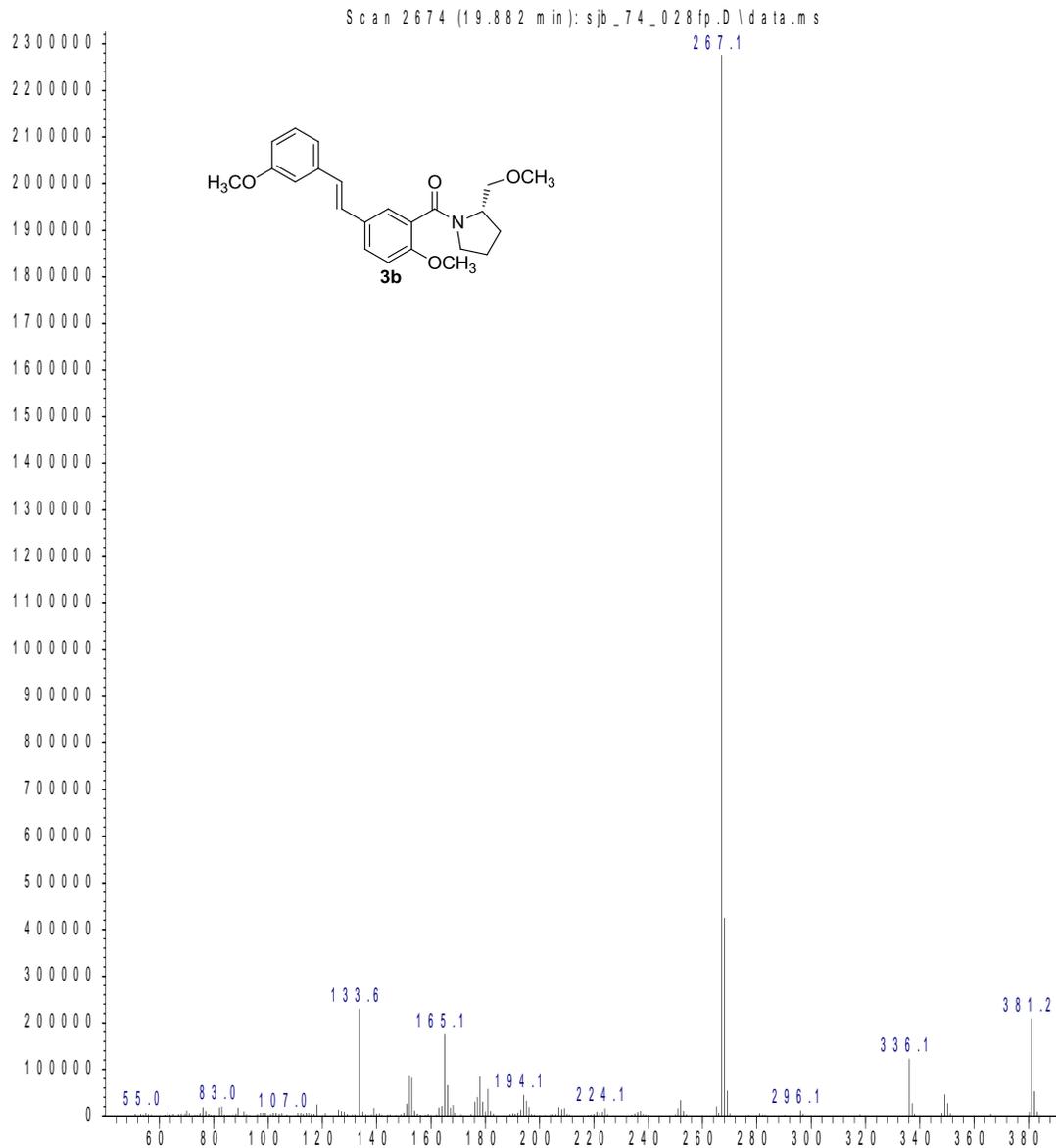
JMB2.m Wed Oct 17 15:12:44 2012

Abundance



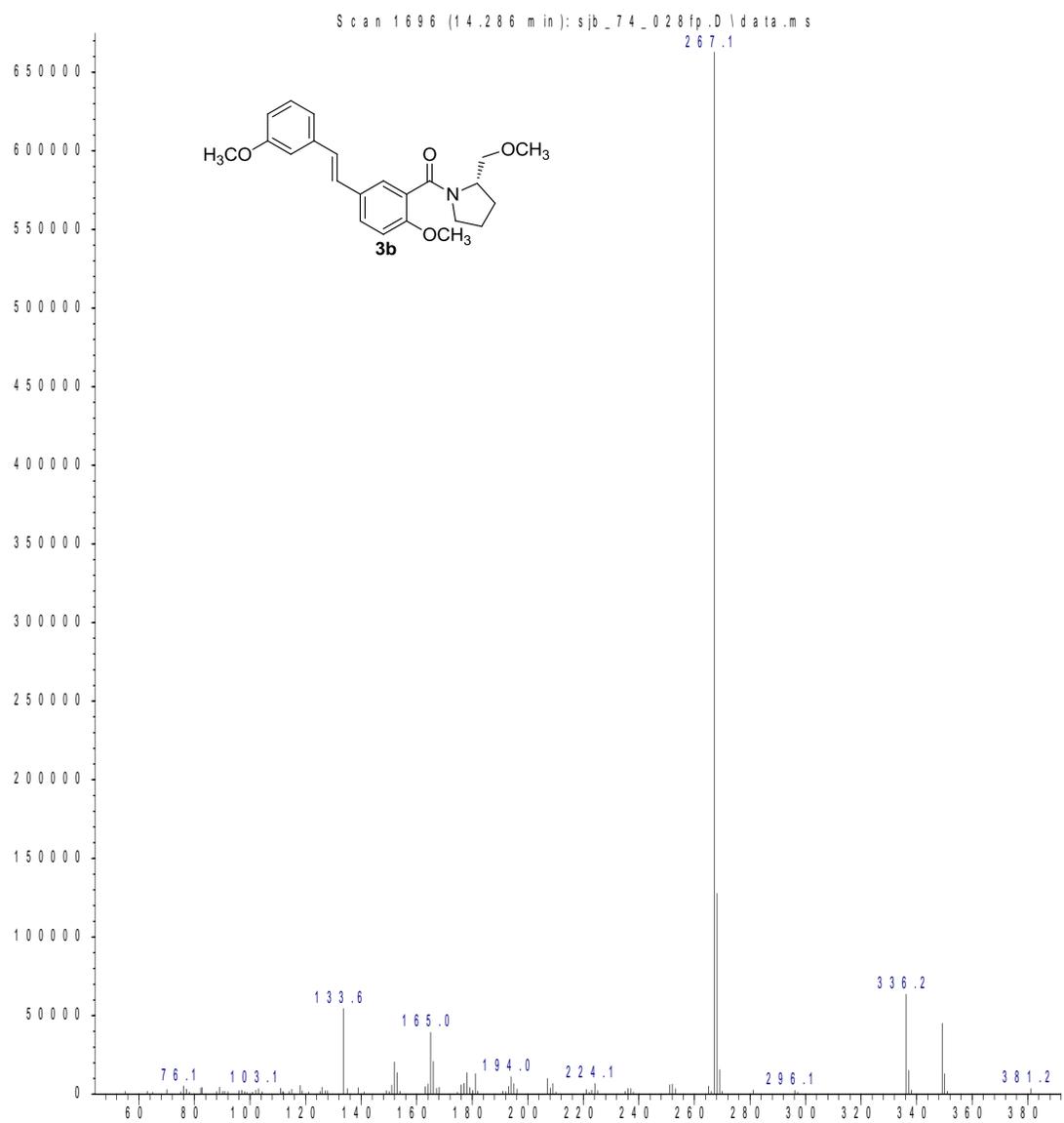
Time-->

Abundance

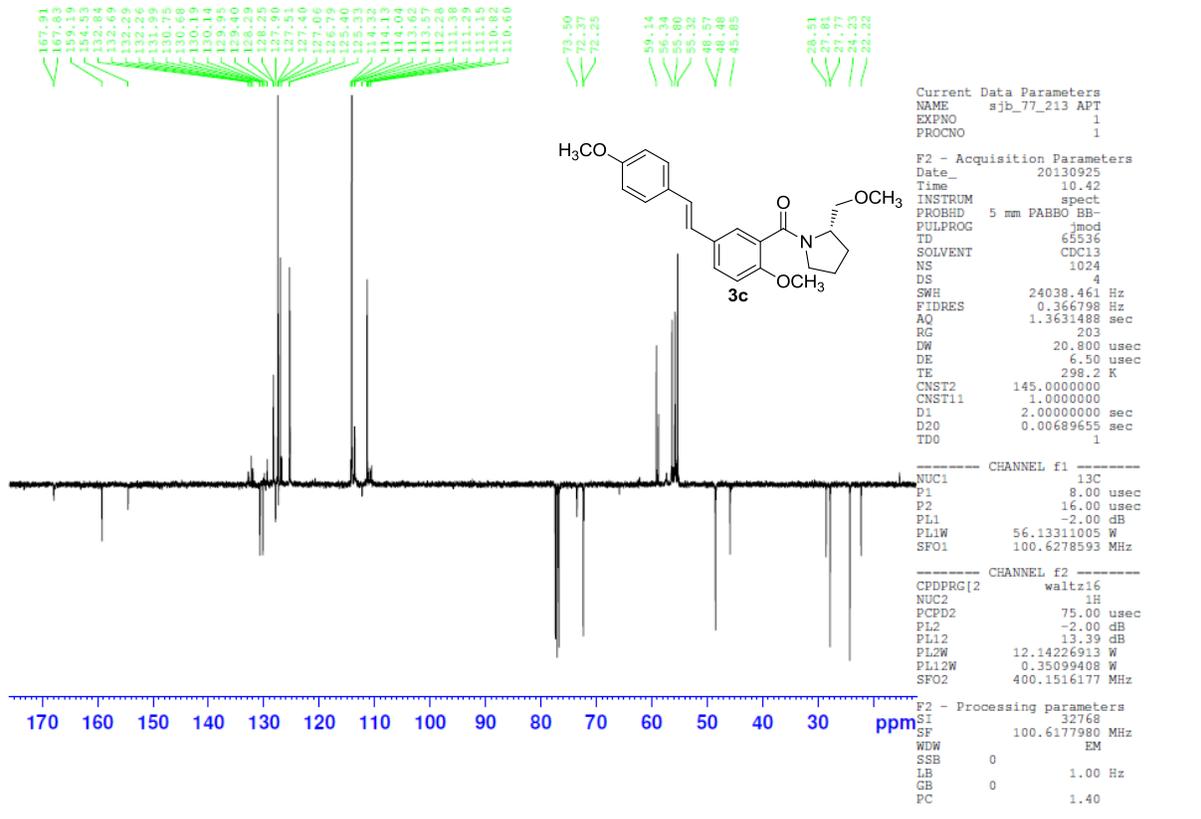
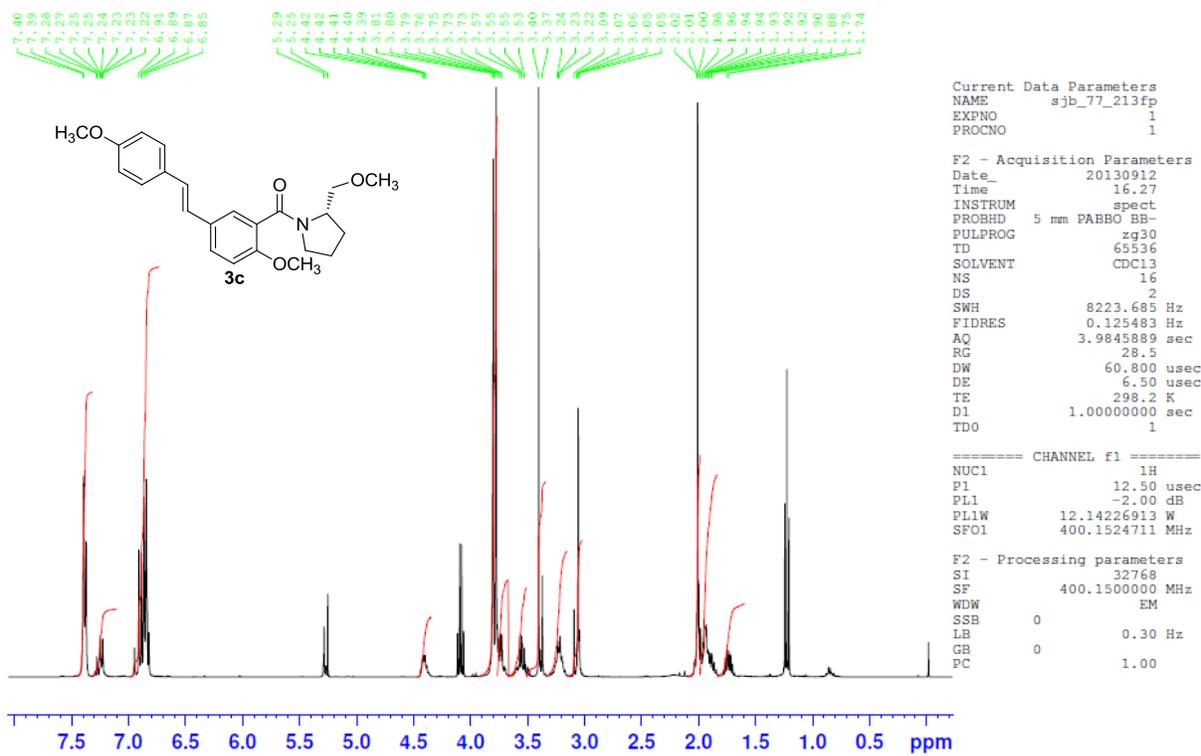


m/z-->

Abundance



m/z-->



Area Percent Report

Data Path : C:\msdchem\1\DATA\
Data File : ra_67_145a.D
Acq On : 16 Jul 2012 10:21
Operator : sm
Sample : ra_67_145a
Misc : Heck cross-coupling 5g scale
ALS Vial : 90 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\msdchem\1\METHODS\JMB2.m
Title :

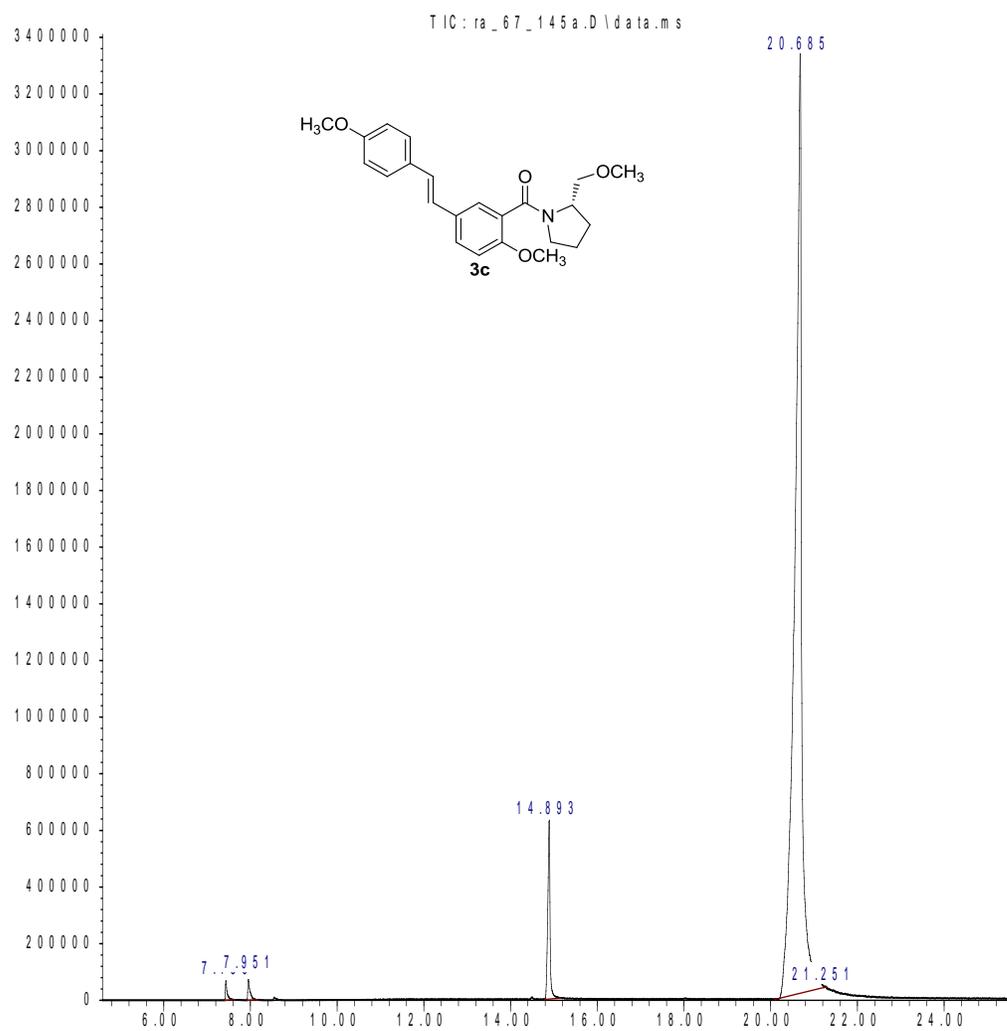
Signal : TIC: ra_67_145a.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.436	493	499	531	BB	68422	1923647	0.52%	0.483%
2	7.951	583	589	625	BB	92384	2825997	0.76%	0.710%
3	14.893	1783	1802	1846	PB	630106	23380433	6.32%	5.873%
4	20.685	2710	2814	2910	PV	3375196	369957456	100.00%	92.923%
5	21.251	2910	2913	2916	VV 3	4131	44728	0.01%	0.011%

Sum of corrected areas: 398132262

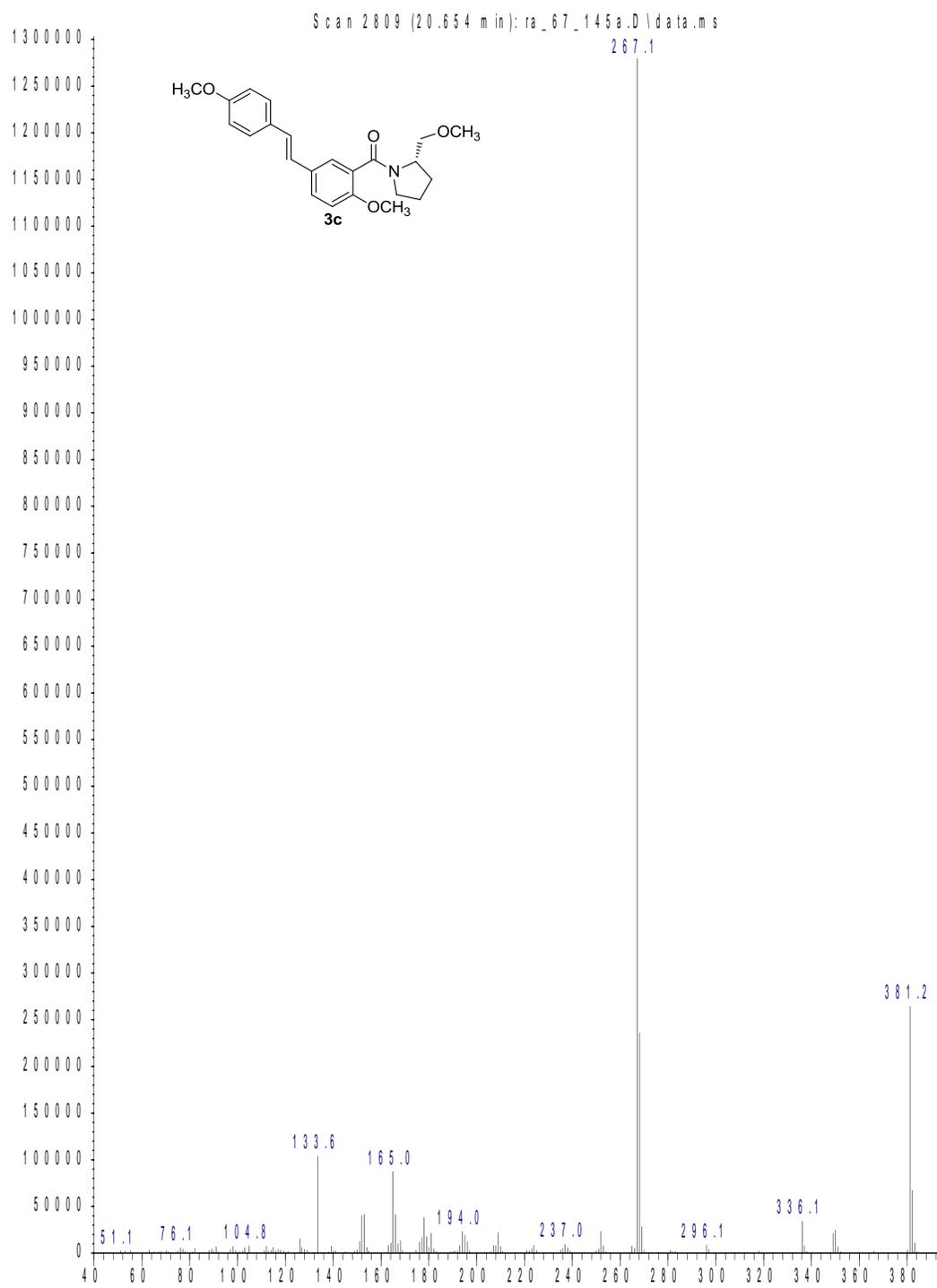
JMB2.m Thu Nov 08 13:39:54 2012

Abundance



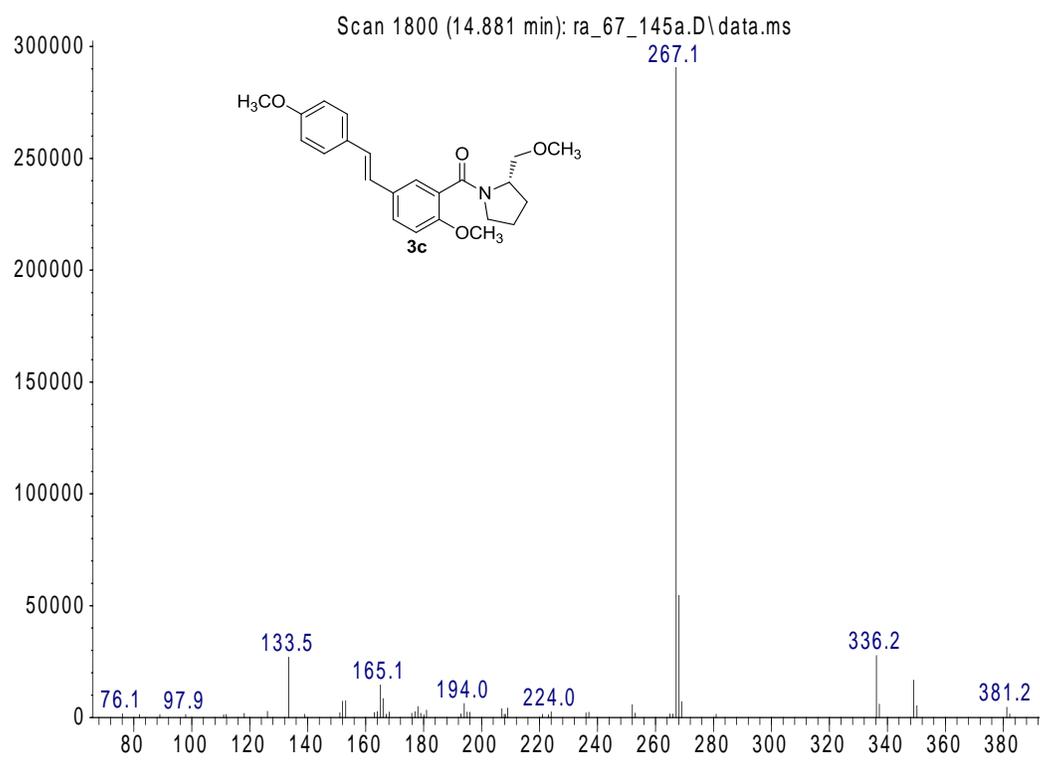
Time-->

Abundance

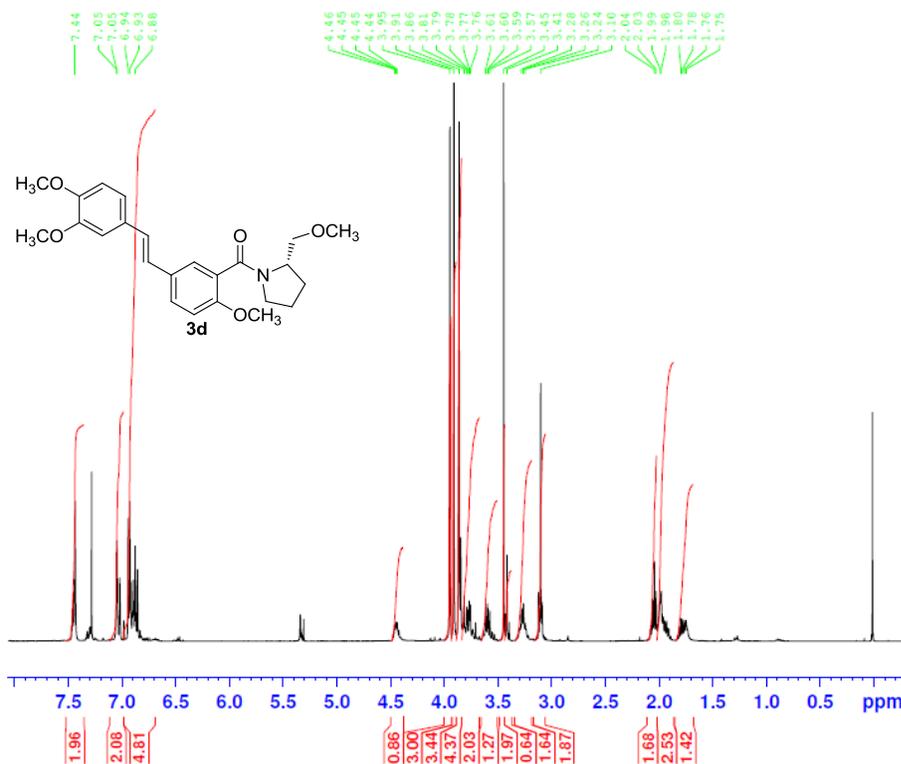


m/z-->

Abundance



m/z-->

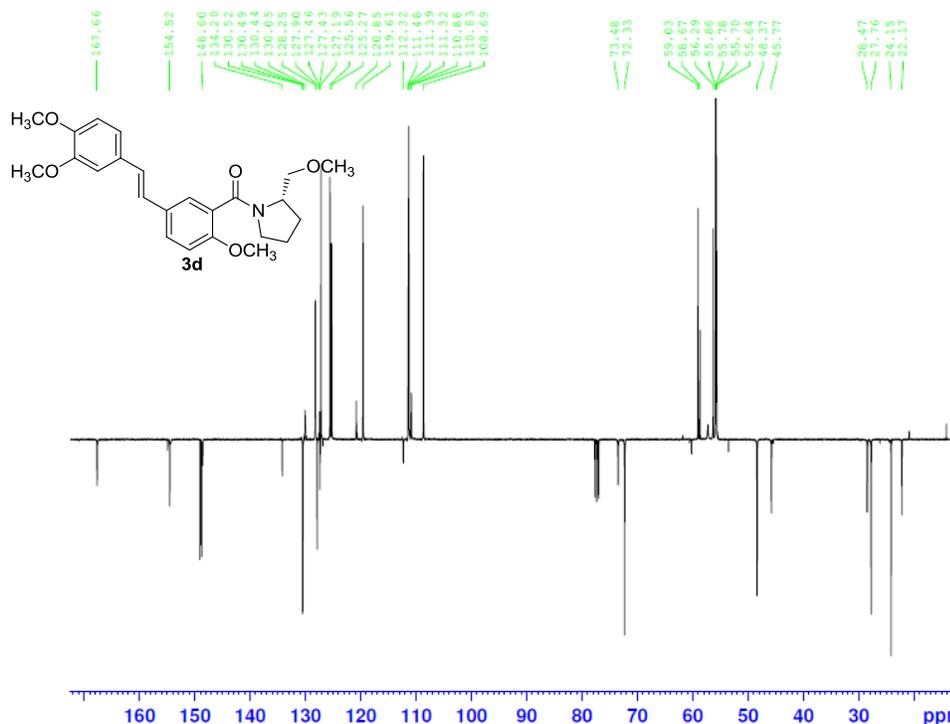


```

NAME      sjb_74_208 take 2
EXPNO    1
PROCNO   1
Date_    20130711
Time     8.57
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       2
SWH      8223.685 Hz
FIDRES   0.125483 Hz
AQ       3.9846387 sec
RG       144
DW       60.800 usec
DE       6.50 usec
TE       301.2 K
D1       1.00000000 sec
TDO     1
  
```

```

----- CHANNEL f1 -----
NUC1     1H
P1       12.50 usec
PL1      -2.00 dB
PL1W     12.14226913 W
SFO1     400.1524711 MHz
SI       32768
SF       400.1500000 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
  
```



```

NAME      sjb_74_208fp APT
EXPNO    1
PROCNO   1
Date_    20121116
Time     15.52
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  jmod
TD       65536
SOLVENT  CDCl3
NS       1024
DS       4
SWH      16233.767 Hz
FIDRES   0.247708 Hz
AQ       2.0185587 sec
RG       203
DW       30.800 usec
DE       6.50 usec
TE       301.2 K
CNST2    145.0000000
CNST11   1.0000000
D1       2.00000000 sec
D20      0.00689655 sec
TDO     1
  
```

```

----- CHANNEL f1 -----
NUC1     13C
P1       8.00 usec
P2       16.00 usec
PL1      -2.00 dB
PL1W     56.13311005 W
SFO1     100.6270320 MHz
  
```

```

----- CHANNEL f2 -----
CPDPRG2  waltz16
NUC2     1H
PCPD2    80.00 usec
PL2      -2.00 dB
PL12     14.00 dB
PL2W     12.14226913 W
PL12W    0.30500001 W
SFO2     400.1515194 MHz
SI       32768
SF       100.6177980 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
  
```

Area Percent Report

Data Path : C:\msdchem\1\DATA\
Data File : sjb_77_169fp.D
Acq On : 7 Aug 2013 10:34
Operator : sjb
Sample : sjb_77_169fp
Misc :
ALS Vial : 85 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

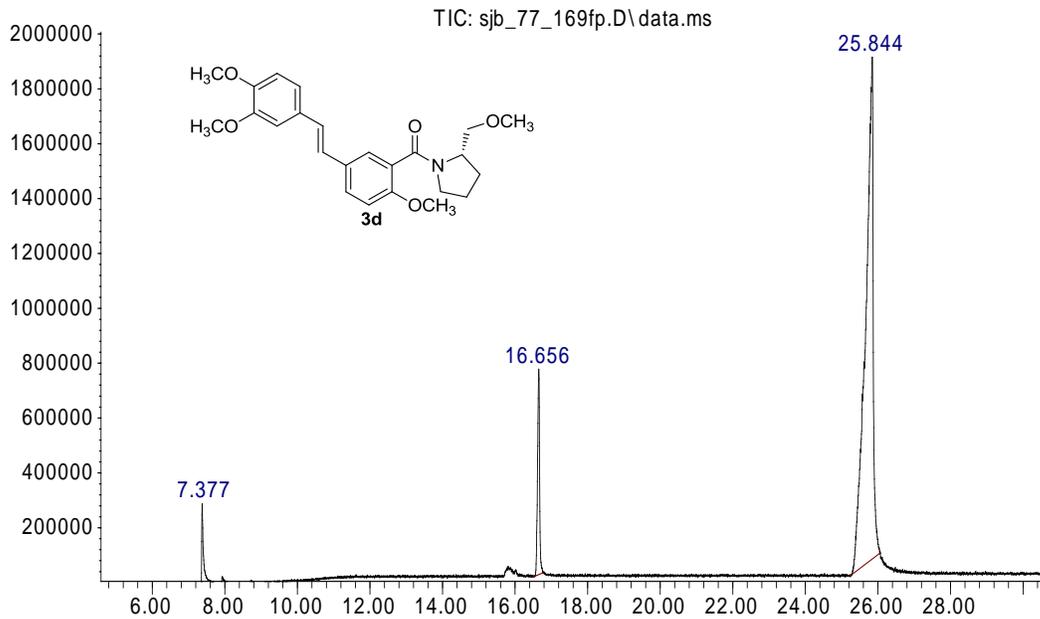
Method : C:\msdchem\1\5973N\PRECISION.M
Title :

Signal : TIC: sjb_77_169fp.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.377	483	489	520	BB	282995	8369318	3.14%	2.755%
2	16.656	2082	2110	2130	PV	744590	29079588	10.92%	9.574%
3	25.844	3611	3716	3752	BV 3	1917900	266290676	100.00%	87.671%

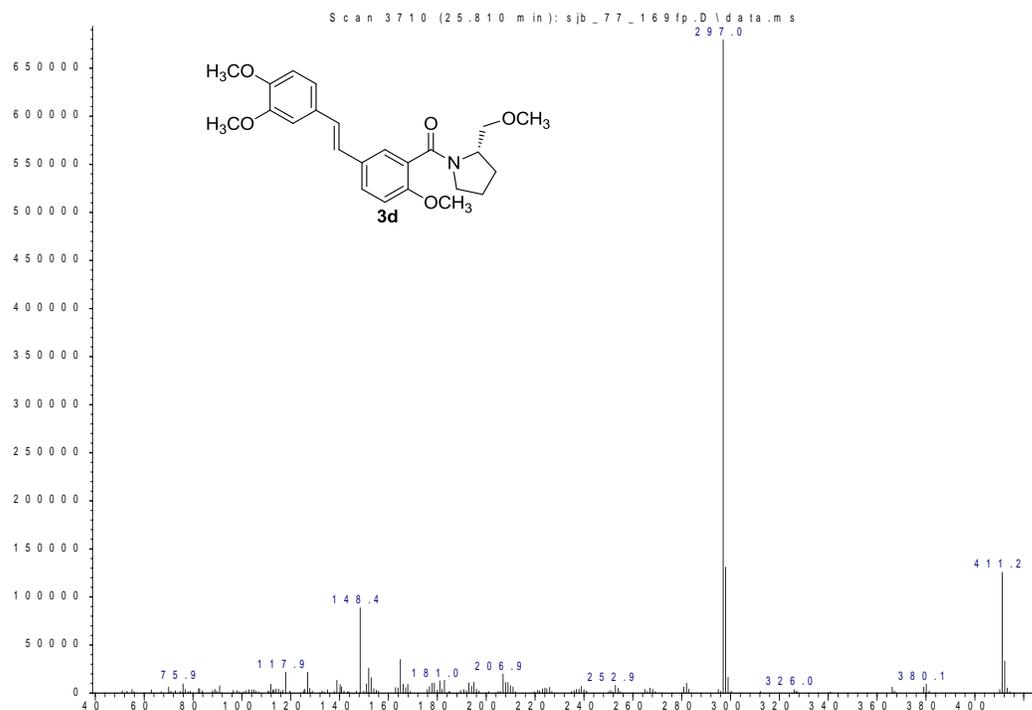
Sum of corrected areas: 303739582

Abundance



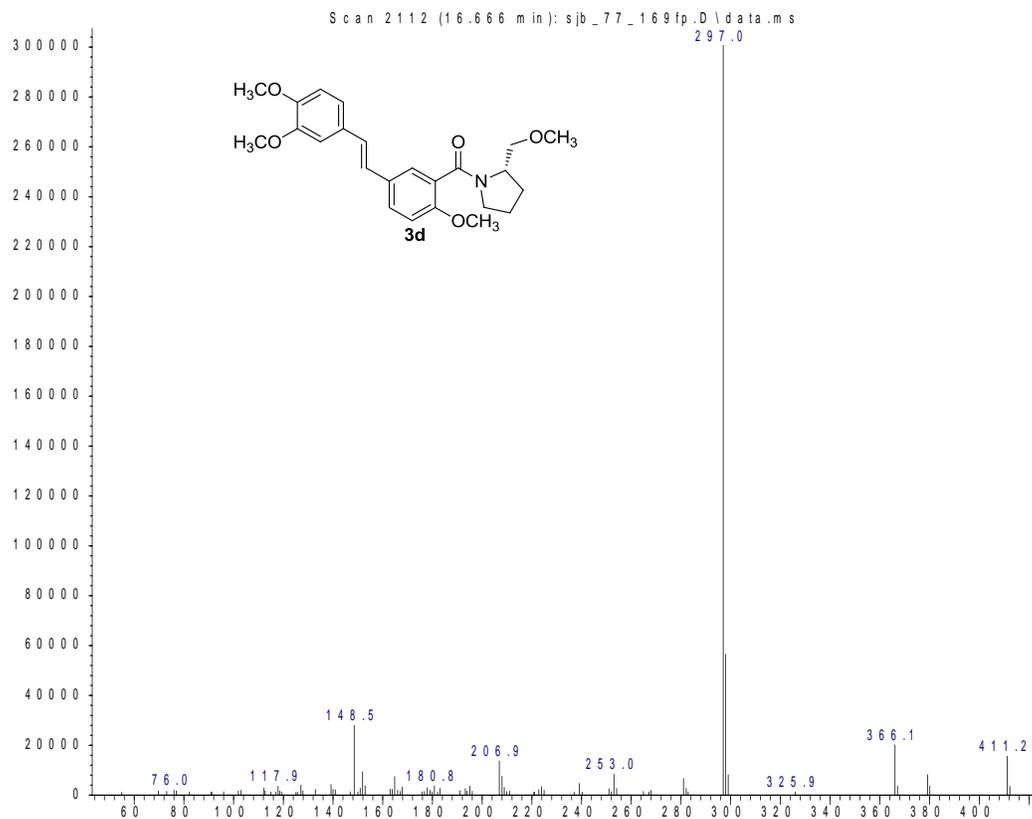
Time-->

Abundance

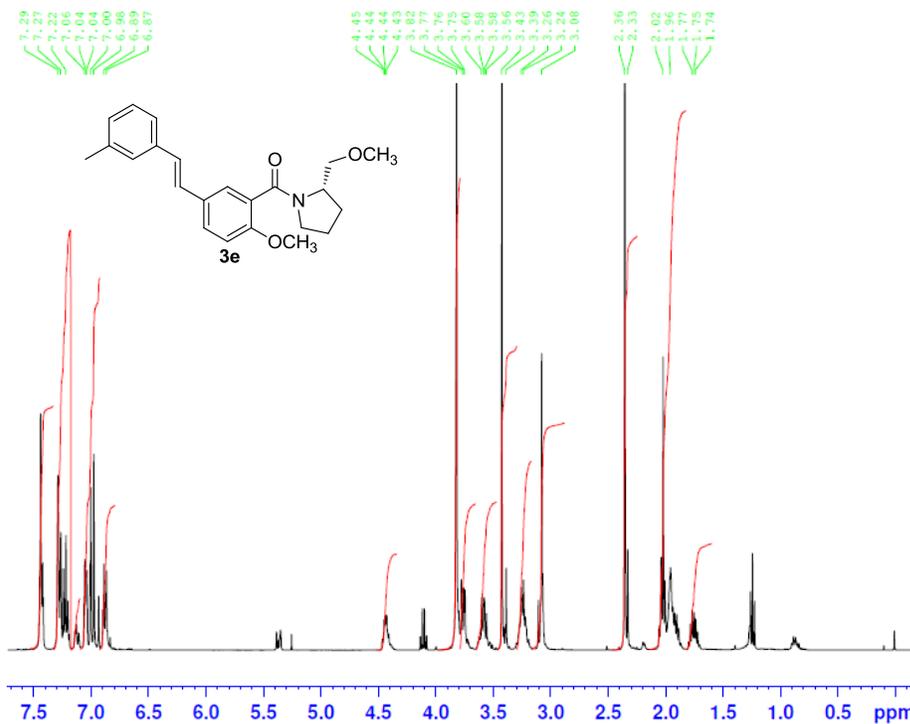


m/z-->

Abundance



m/z-->

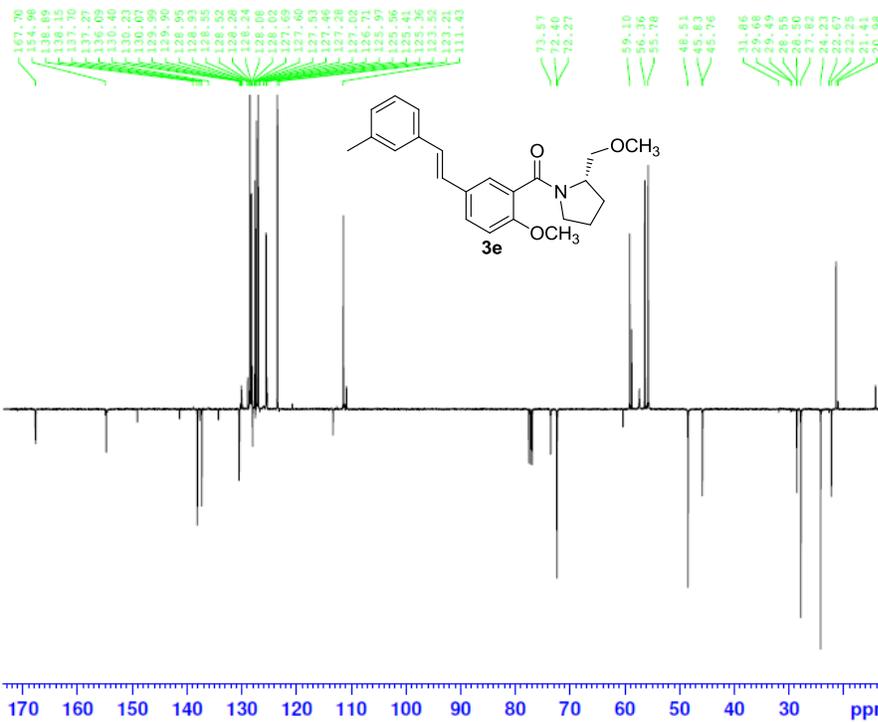


```

NAME      sjb_77_019fp
EXPNO     1
PROCNO    1
Date_     20121219
Time      13.56
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH       8223.685 Hz
FIDRES    0.125483 Hz
AQ         3.9846387 sec
RG         25.4
DW         60.800 usec
DE         6.50 usec
TE         299.4 K
D1         1.00000000 sec
D10        1
TDO        1
  
```

```

===== CHANNEL f1 =====
NUC1      1H
P1        12.50 usec
PL1       -2.00 dB
PL1W      12.14226913 W
SFO1      400.1524711 MHz
SI        32768
SF        400.1500000 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
  
```



```

NAME      sjb_77_019fp APT
EXPNO     1
PROCNO    1
Date_     20121219
Time      15.44
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   jmod
TD         65536
SOLVENT   CDCl3
NS         1024
DS         4
SWH       16304.348 Hz
FIDRES    0.248785 Hz
AQ         2.0098207 sec
RG         203
DW         30.667 usec
DE         6.50 usec
TE         305.2 K
CNST2     145.0000000
CNST11    1.0000000
D1         2.00000000 sec
D20        0.00689655 sec
TDO        1
  
```

```

----- CHANNEL f1 -----
NUC1      13C
P1         8.00 usec
P2        16.00 usec
PL1       -2.00 dB
PL1W      56.13311005 W
SFO1      100.6271040 MHz
  
```

```

----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       -2.00 dB
PL12      14.00 dB
PL2W      12.14226913 W
PL12W     0.30500001 W
SFO2      400.1515120 MHz
SI        32768
SF        100.6177980 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```

Area Percent Report

Data Path : C:\msdchem\1\DATA\
Data File : sjb_77_019fp.D
Acq On : 19 Dec 2012 16:13
Operator : sjb
Sample : sjb_77_019fp
Misc :
ALS Vial : 5 Sample Multiplier: 1

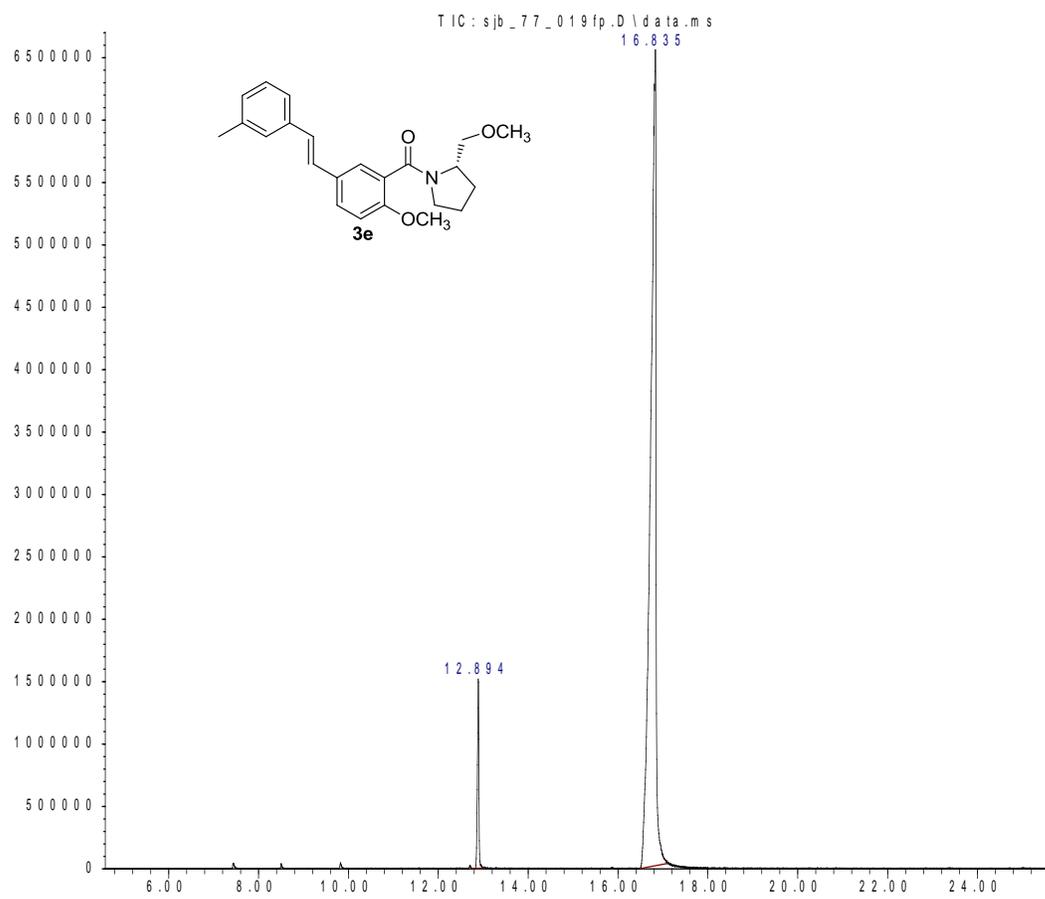
Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\msdchem\1\5973N\PRECISION.M
Title :

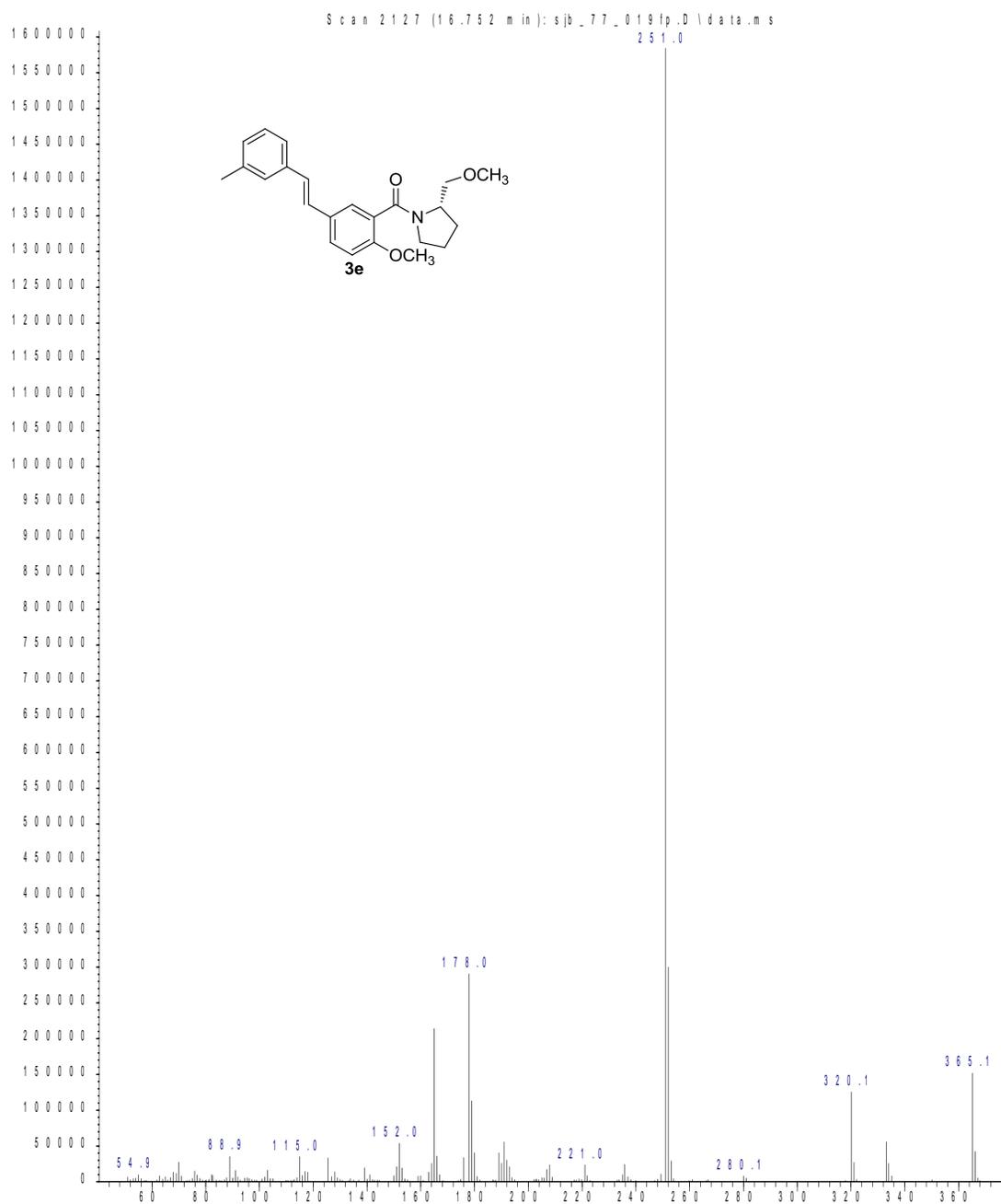
Signal : TIC: sjb_77_019fp.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	12.894	1430	1453	1474	PV	1521351	34495405	6.14%	5.785%
2	16.835	2080	2142	2189	BV 2	6749209	561756588	100.00%	94.215%

Abundance

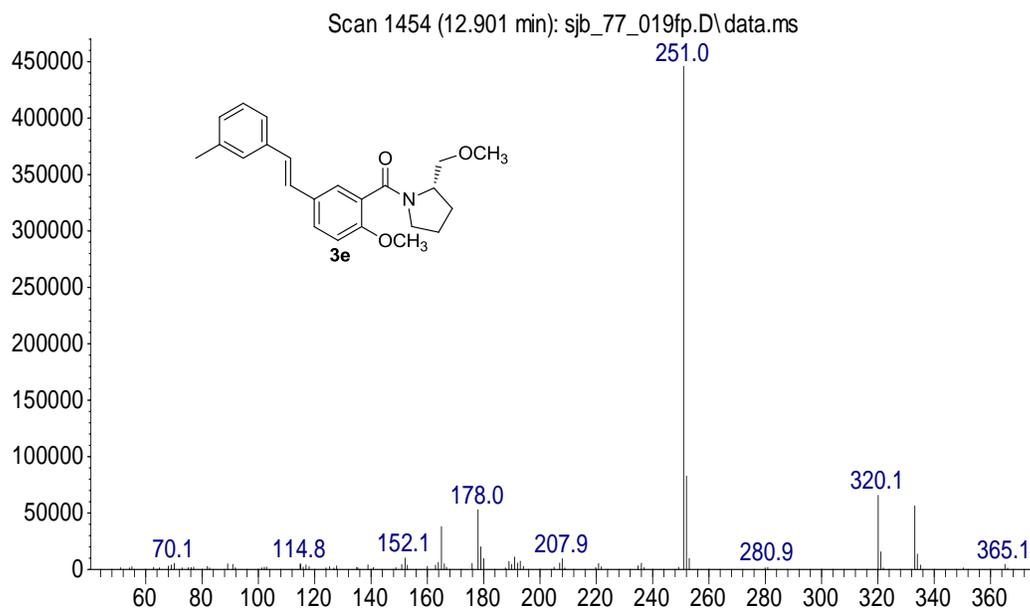


Abundance

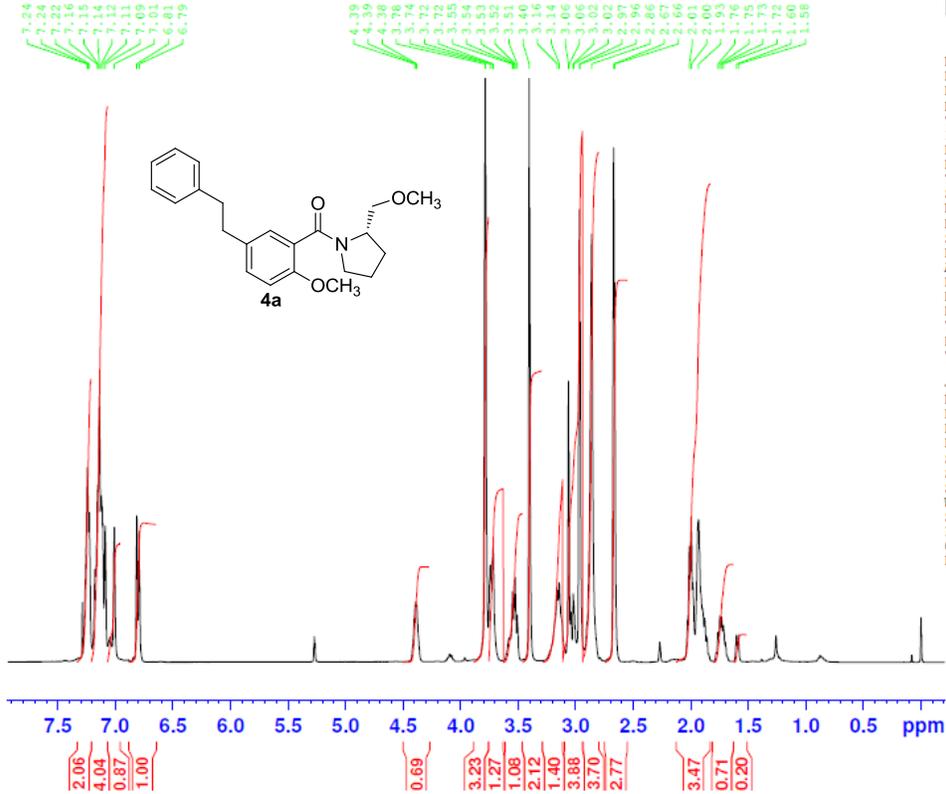


m/z-->

Abundance

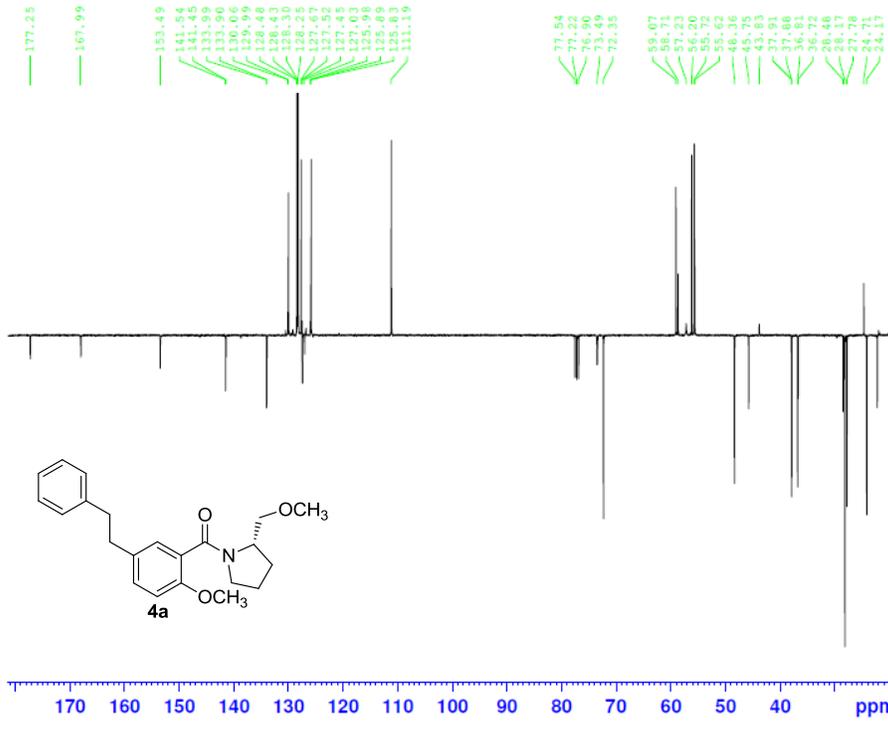


m/z-->



NAME sjb_74_199fp proton
EXPNO 1
PROCNO 1
Date_ 20121109
Time 9.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 28.5
DW 60.800 usec
DE 6.50 usec
TE 301.2 K
D1 1.00000000 sec
TDO 1

CHANNEL f1
NUC1 1H
P1 12.50 usec
PL1 -2.00 dB
PL1W 12.14226913 W
SFO1 400.1524711 MHz
SI 32768
SF 400.1499967 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



NAME sjb_74_199fp APT
EXPNO 1
PROCNO 1
Date_ 20121112
Time 9.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 16339.869 Hz
FIDRES 0.249327 Hz
AQ 2.0054517 sec
RG 203
DW 30.600 usec
DE 6.50 usec
TE 301.2 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TDO 1

CHANNEL f1
NUC1 13C
P1 8.00 usec
P2 16.00 usec
PL1 -2.00 dB
PL1W 56.13311005 W
SFO1 100.6278685 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL2 14.00 dB
PL2W 12.14226913 W
PL12W 0.30500001 W
SFO2 400.1514948 MHz
SI 32768
SF 100.6177980 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Area Percent Report

Data Path : C:\msdchem\1\DATA\
Data File : sjb_74_199fp.D
Acq On : 9 Nov 2012 13:56
Operator : sjb
Sample : sjb_74_199fp
Misc :
ALS Vial : 15 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\msdchem\1\METHODS\JMB2.m
Title :

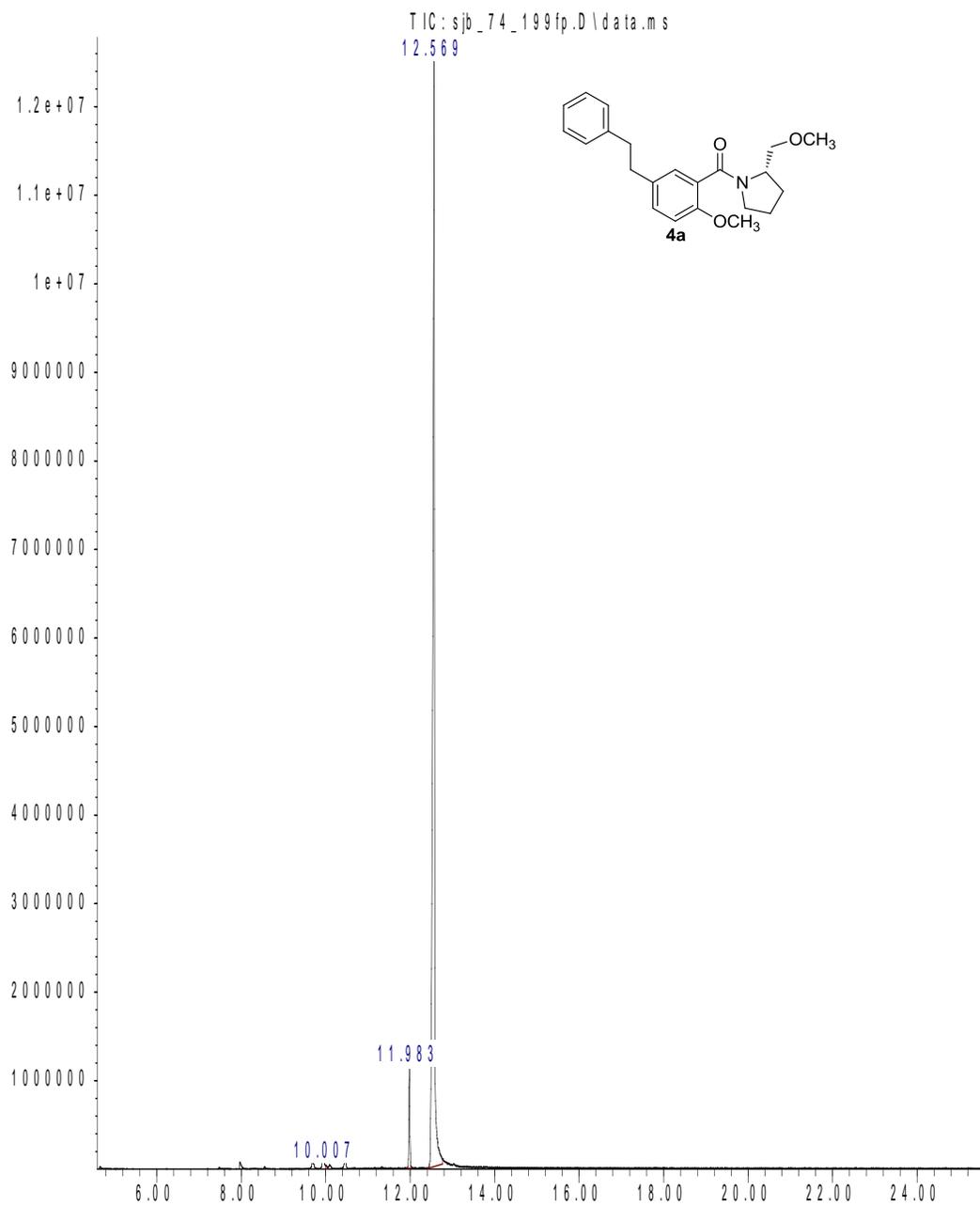
Signal : TIC: sjb_74_199fp.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	10.007	946	948	956	VV 3	41194	970477	0.26%	0.246%
2	11.983	1281	1294	1302	BV	1081831	18401106	4.91%	4.665%
3	12.569	1367	1396	1431	PV	12857242	375088829	100.00%	95.089%

Sum of corrected areas: 394460412

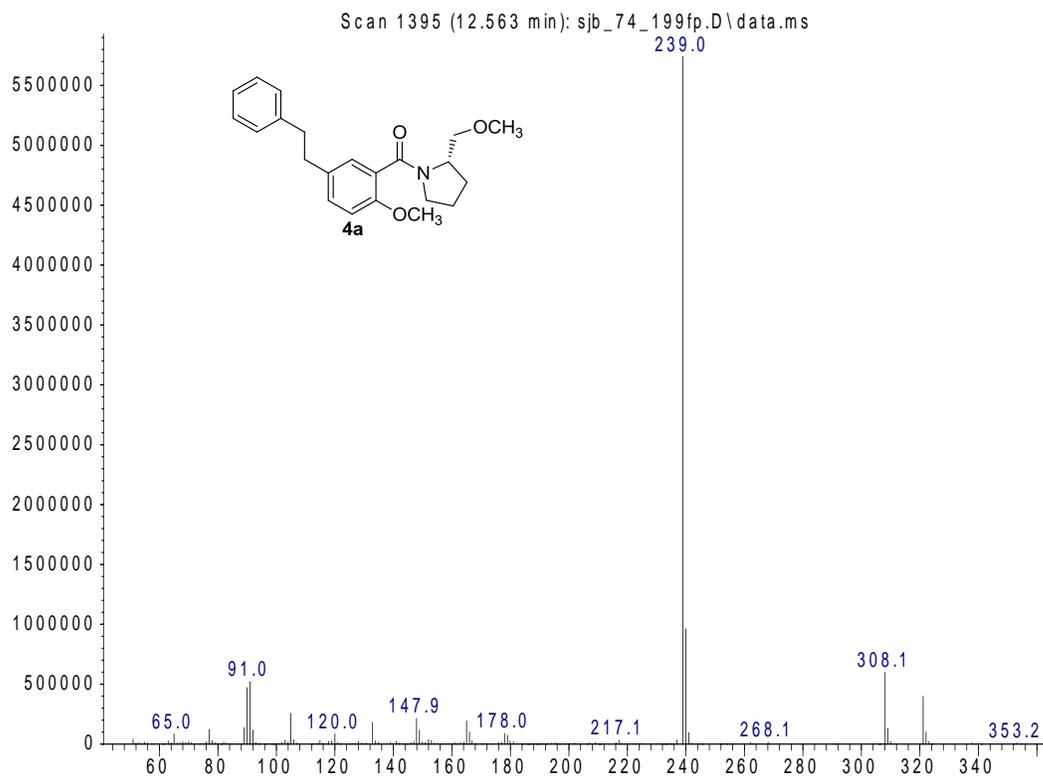
JMB2.m Mon Nov 12 09:44:14 2012

Abundance



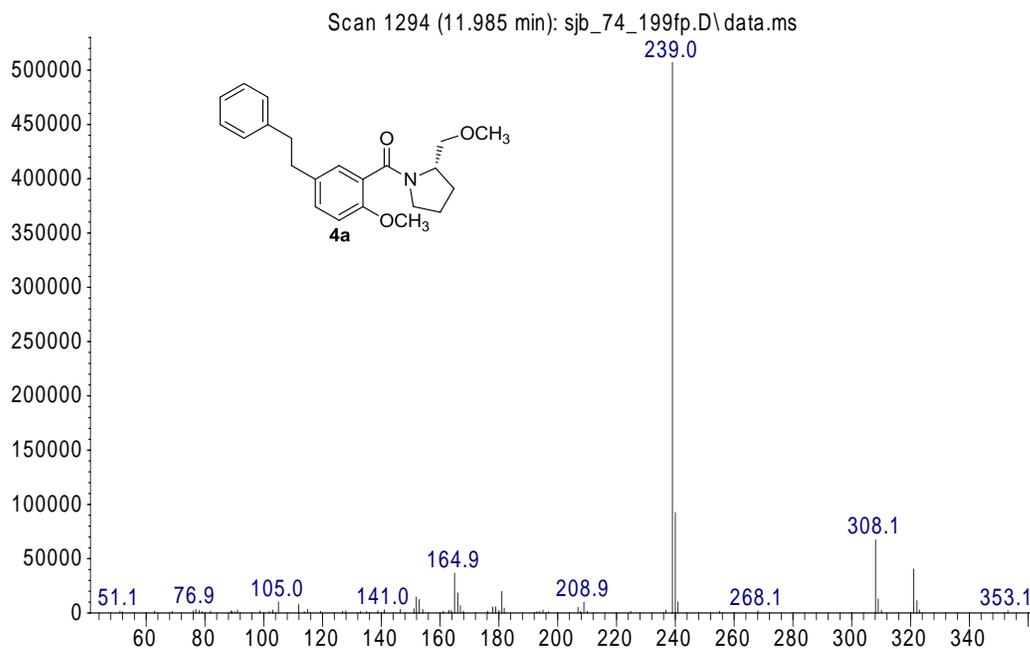
Time-->

Abundance

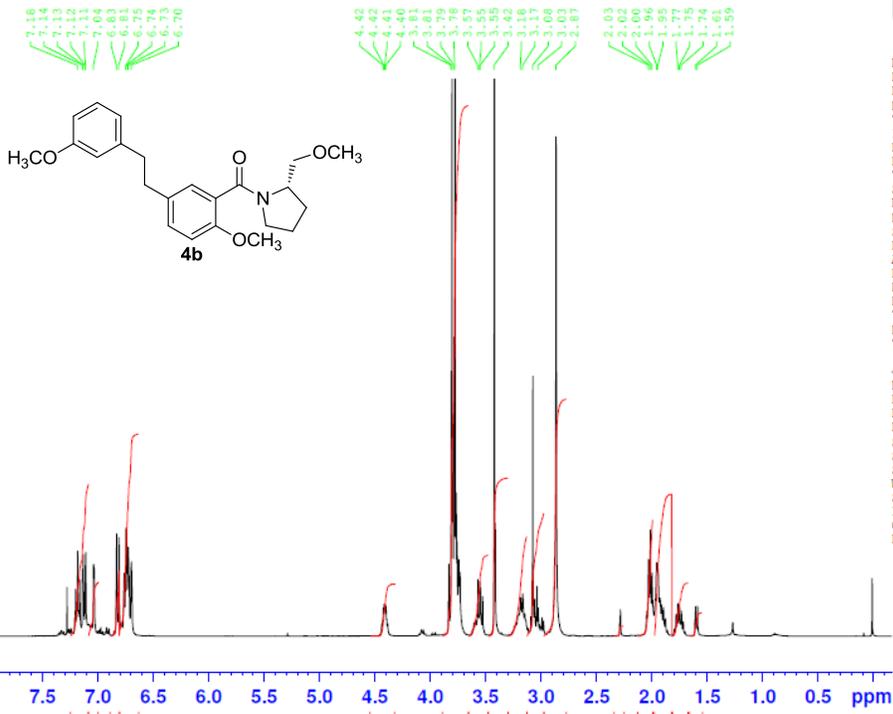


m/z-->

Abundance

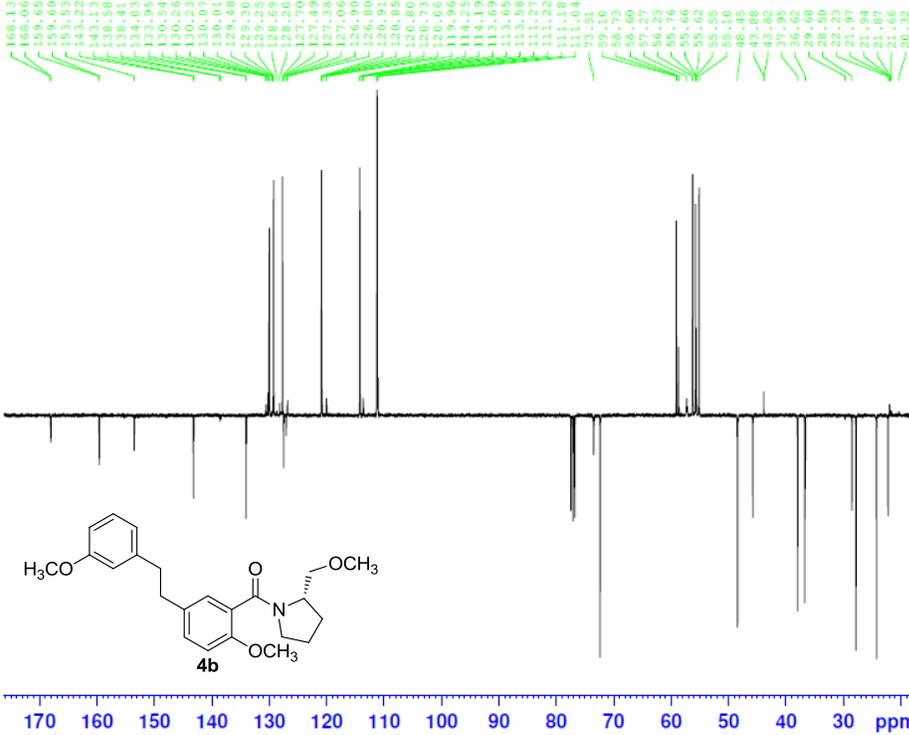


m/z-->



```
NAME      sjb_77_154fp take2
EXPNO     1
PROCNO    1
Date_     20130725
Time      7.53
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        8223.685 Hz
FIDRES    0.125403 Hz
AQ         3.9846387 sec
RG         45.2
DW         60.800 usec
DE         6.50 usec
TE         301.2 K
D1         1.00000000 sec
TDO        1

----- CHANNEL f1 -----
NUC1      1H
P1        12.50 usec
PL1       -2.00 dB
PL1W      12.14226913 W
SFO1      400.1524711 MHz
SI         32768
SF         400.1500000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```



```
Current Data Parameters
NAME      sjb_77_154fp APT
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20130725
Time      8.56
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   jmod
TD         65536
SOLVENT   CDCl3
NS         1024
DS         4
SWH        24038.461 Hz
FIDRES    0.366798 Hz
AQ         1.3631488 sec
RG         203
DW         20.800 usec
DE         6.50 usec
TE         301.2 K
CNST2     145.0000000
CNST11    1.0000000
D1         2.00000000 sec
D20        0.00689655 sec
TDO        1

----- CHANNEL f1 -----
NUC1      13C
P1         8.00 usec
P2        16.00 usec
PL1       -2.00 dB
PL1W      56.13311005 W
SFO1      100.6278593 MHz

----- CHANNEL f2 -----
CPDPRG[2] waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       -2.00 dB
PL12      14.00 dB
PL12W     12.14226913 W
PL12W     0.30500001 W
SFO2      400.1515703 MHz

F2 - Processing parameters
SI         32768
SF         100.6177980 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

Area Percent Report

Data Path : C:\msdchem\1\DATA\
Data File : sjb_74_029fp.D
Acq On : 15 Jun 2012 8:44
Operator : sjb
Sample : sjb_74_029fp
Misc :
ALS Vial : 30 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\msdchem\1\METHODS\JMB2.m
Title :

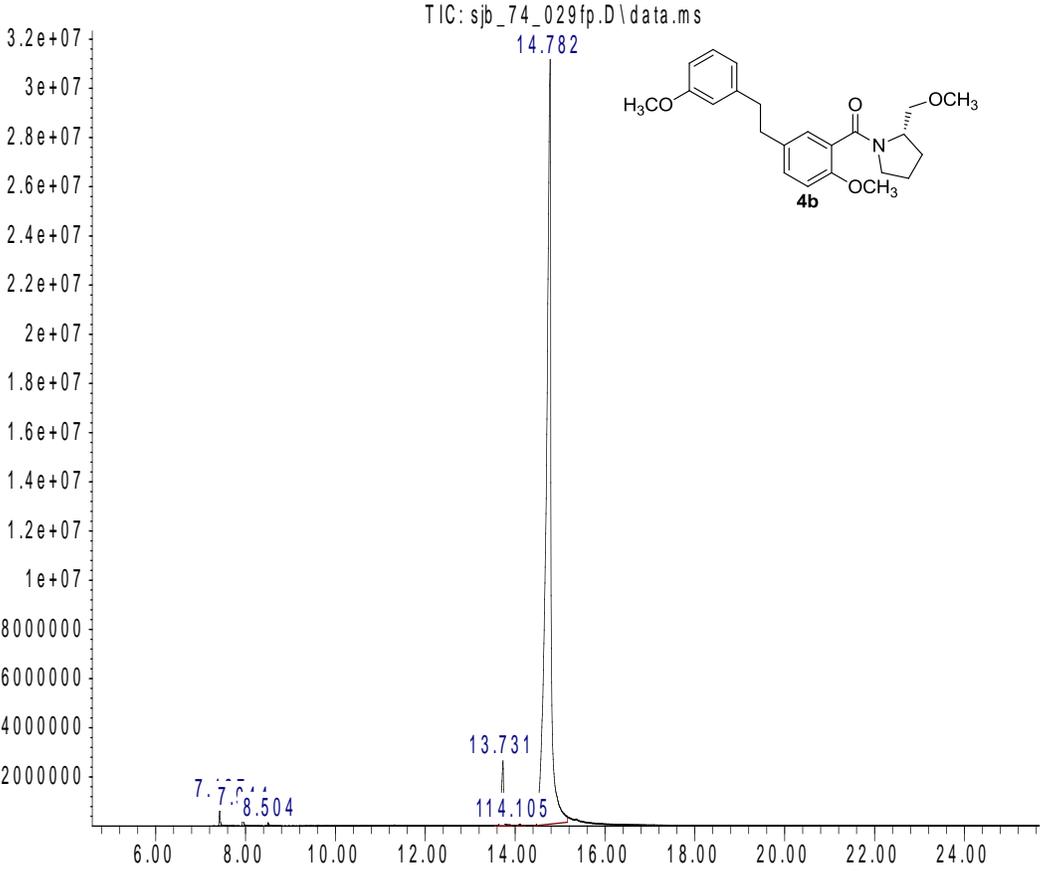
Signal : TIC: sjb_74_029fp.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.427	491	497	525	BV	840988	12778818	0.54%	0.519%
2	7.944	582	588	603	BV	558514	8620398	0.37%	0.350%
3	8.504	680	686	707	PV	130178	2996109	0.13%	0.122%
4	13.731	1566	1599	1622	PV	2596360	88351274	3.77%	3.589%
5	13.881	1622	1625	1634	VV 5	37747	1023498	0.04%	0.042%
6	14.105	1652	1664	1683	VV 4	67239	1888313	0.08%	0.077%
7	14.782	1719	1783	1849	PV 2	31773351	2345930512	100.00%	95.301%

Sum of corrected areas: 2461588922

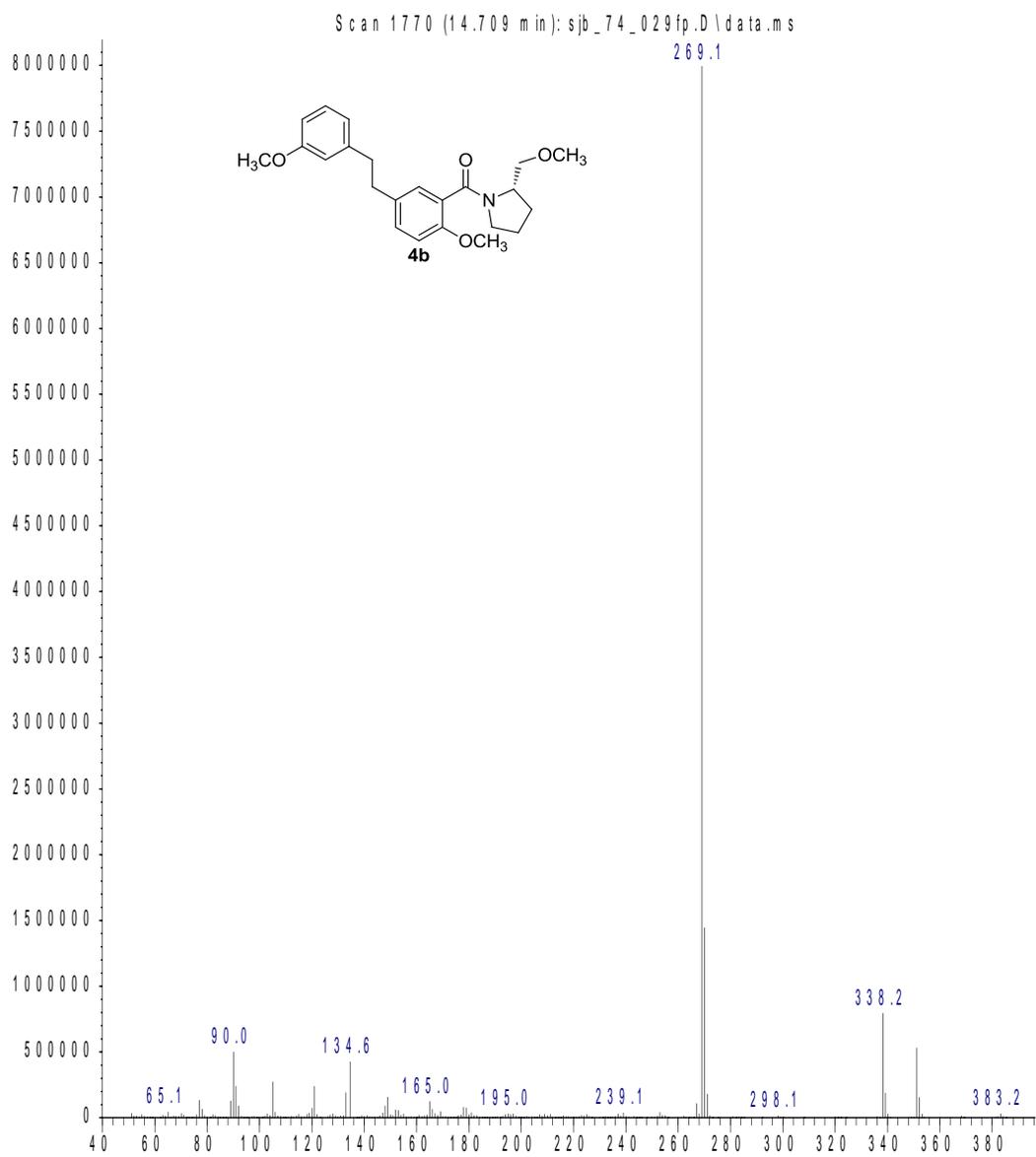
JMB2.m Mon Nov 12 09:52:24 2012

Abundance



Time-->

Abundance

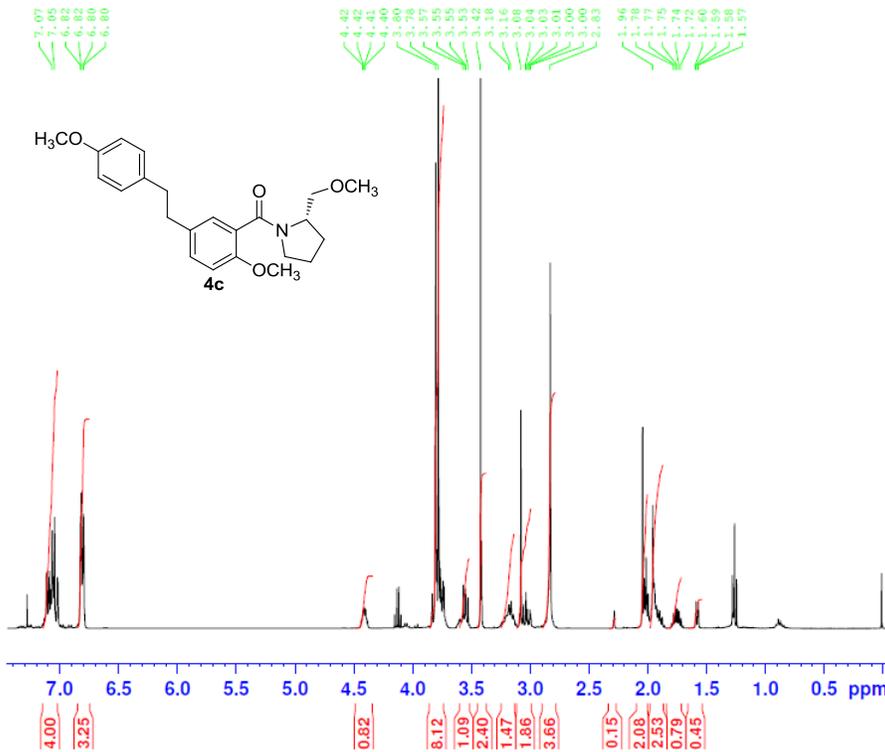


m/z-->

Abundance

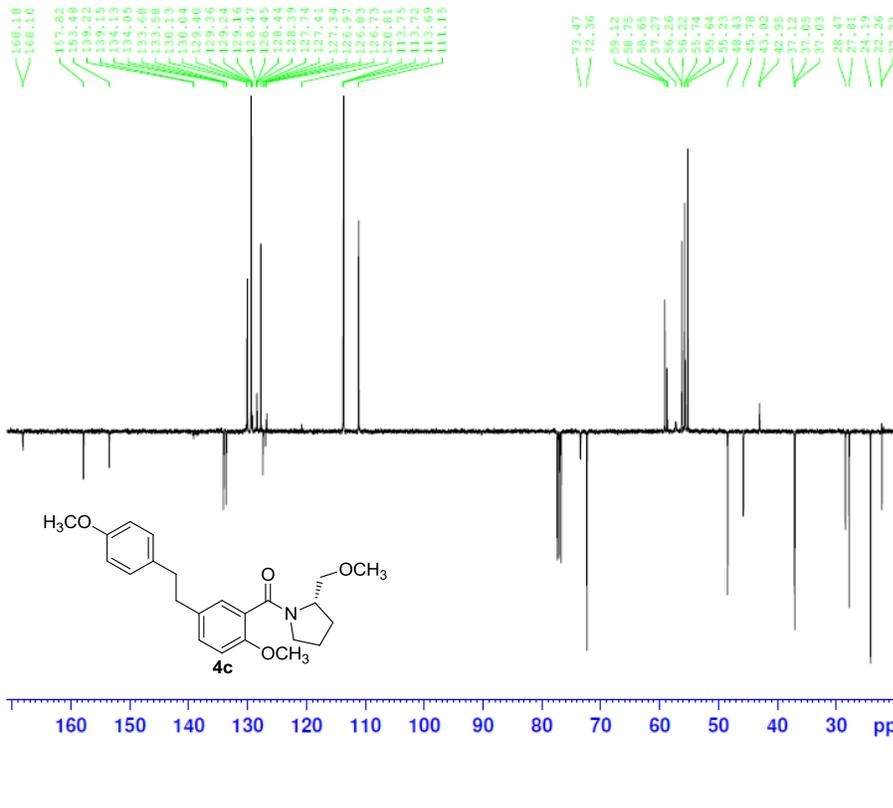


m/z-->



```
NAME ra_67_149pure
EXPNO 1
PROCNO 1
Date_ 20120718
Time 11.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.984637 sec
RG 40.3
DW 60.800 usec
DE 6.50 usec
TE 301.2 K
D1 1.00000000 sec
TDO 1
```

```
===== CHANNEL f1 =====
NUC1 1H
P1 12.50 usec
PL1 -2.00 dB
PL1W 12.14226913 W
SFO1 400.1524711 MHz
SI 32768
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
```



```
Current Data Parameters
NAME sjb_77_217 APT2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20131014
Time 13.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.0000000
CNST11 1.00000000
D1 2.00000000 sec
D20 0.00689655 sec
TDO 1
```

```
===== CHANNEL f1 =====
NUC1 13C
P1 8.00 usec
P2 16.00 usec
PL1 -2.00 dB
PL1W 56.13311005 W
SFO1 100.6278593 MHz
===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 75.00 usec
PL2 -2.00 dB
PL12 13.39 dB
PL2W 12.14226913 W
PL12W 0.35099408 W
SFO2 400.1515863 MHz
```

```
F2 - Processing parameters
SI 32768
SF 100.6177980 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```

Area Percent Report

Data Path : C:\msdchem\1\DATA\
Data File : sjb_77_217fp.D
Acq On : 17 Sep 2013 11:20
Operator : sjb
Sample : sjb_77_217fp
Misc :
ALS Vial : 95 Sample Multiplier: 1

Integration Parameters: atuneWPMMar14.e
Integrator: ChemStation

Method : C:\msdchem\1\METHODS\ckr3.m
Title :

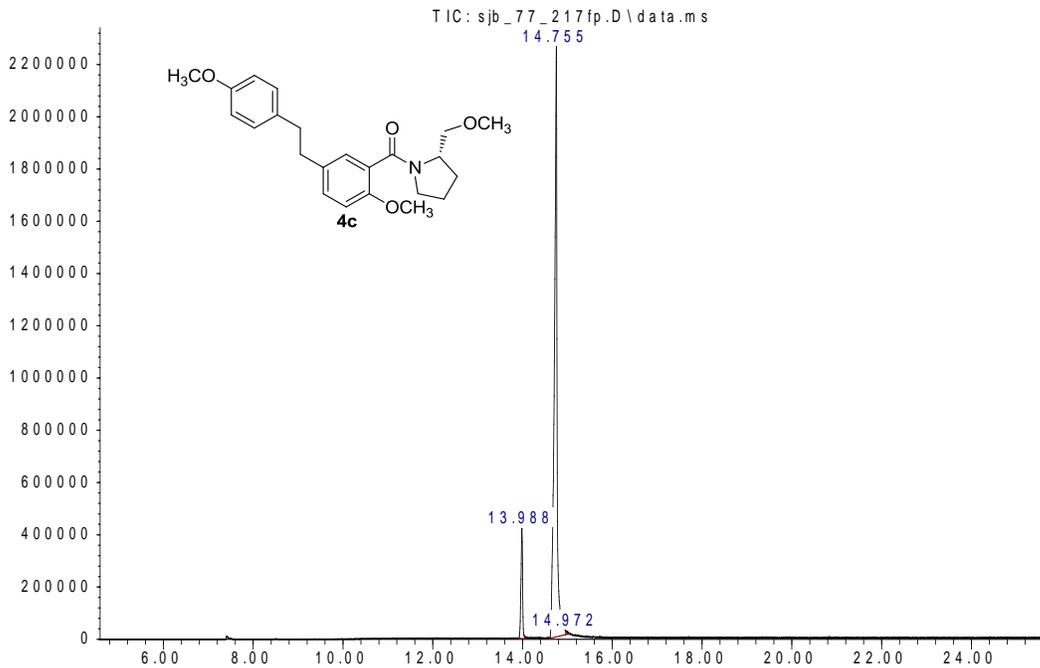
Signal : TIC: sjb_77_217fp.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	13.988	1631	1644	1656	VV	419295	10837930	11.40%	10.200%
2	14.755	1750	1778	1815	PV	2274434	95093596	100.00%	89.494%
3	14.972	1815	1816	1826	VV 6	13174	325675	0.34%	0.306%

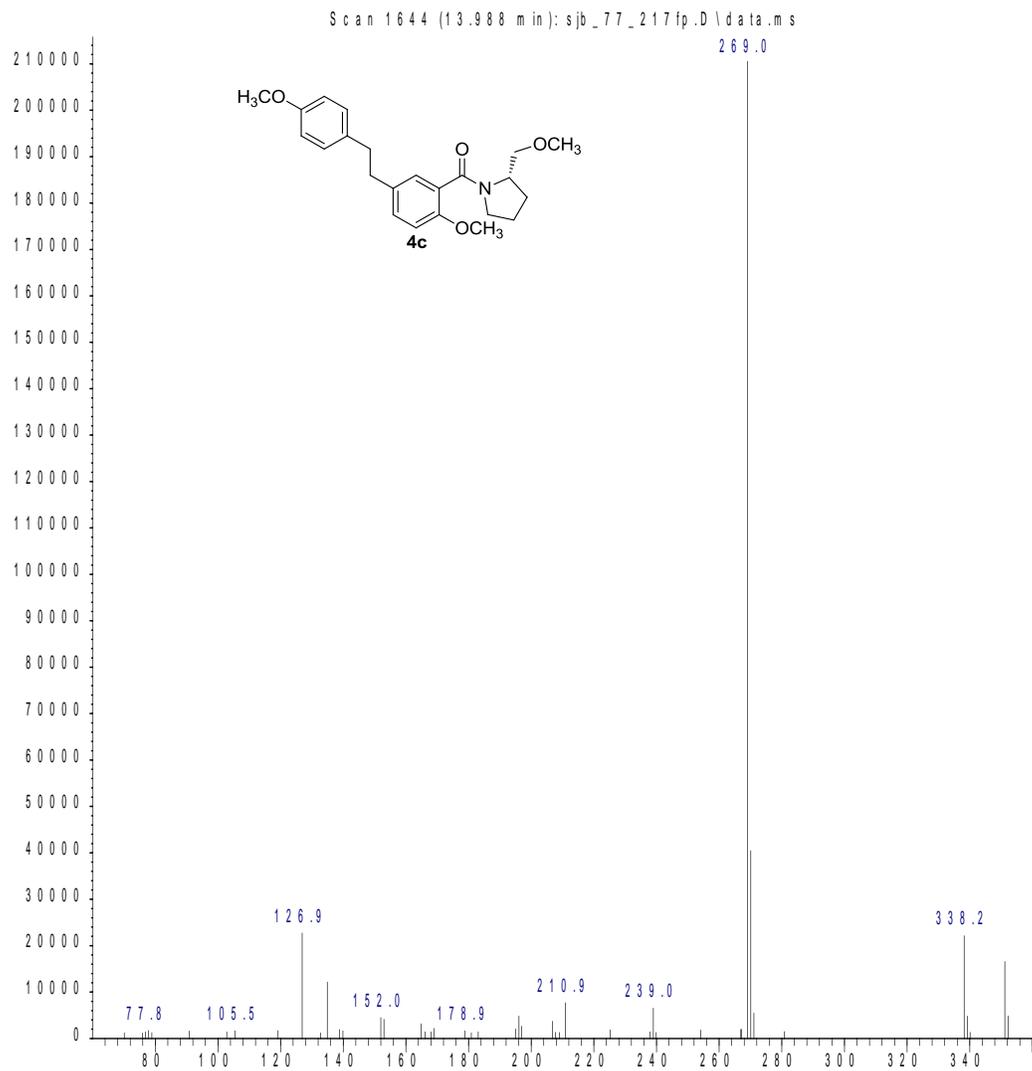
Sum of corrected areas: 106257201

ckr3.m Wed Mar 19 09:43:04 2014

Abundance

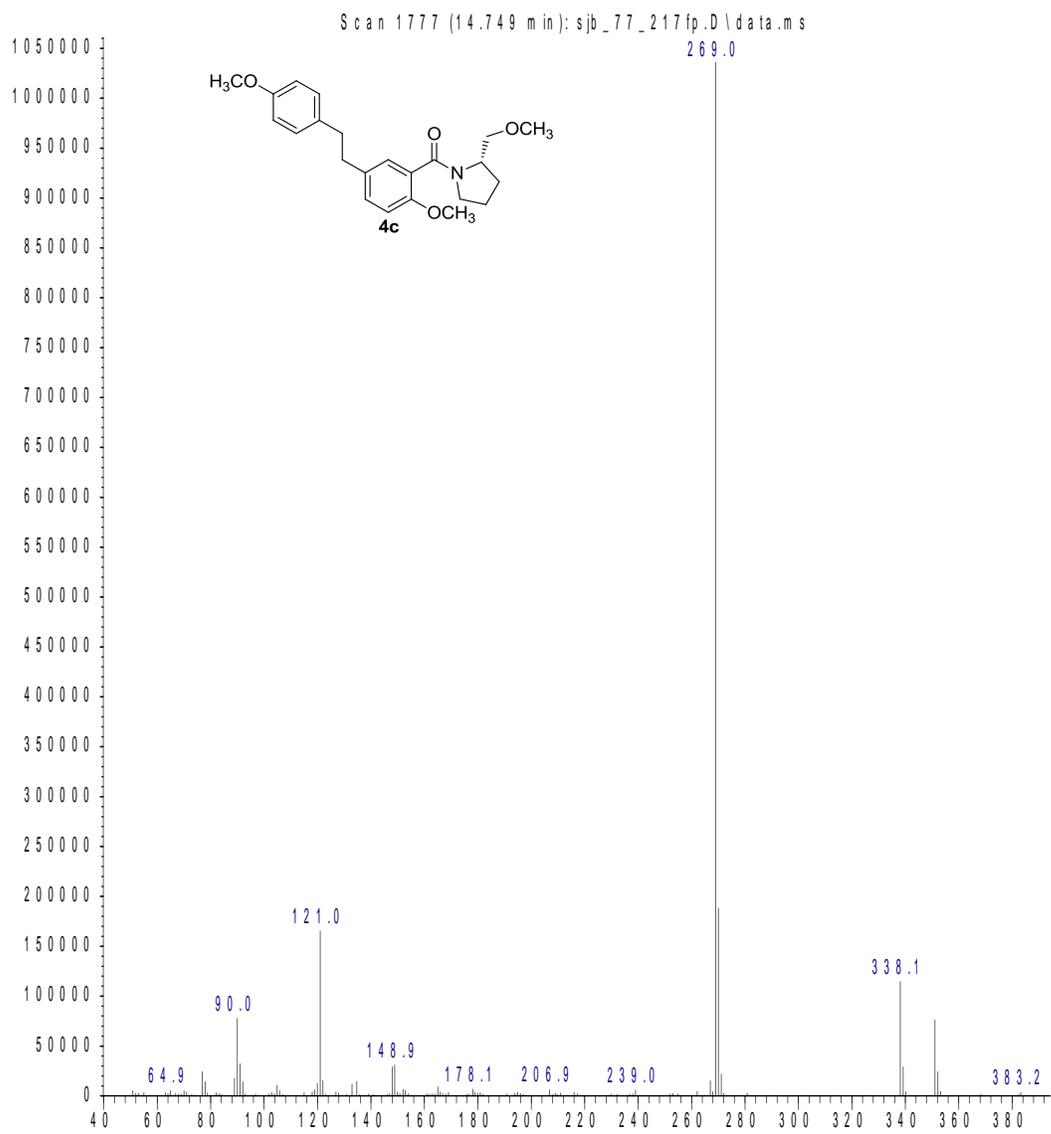


Abundance

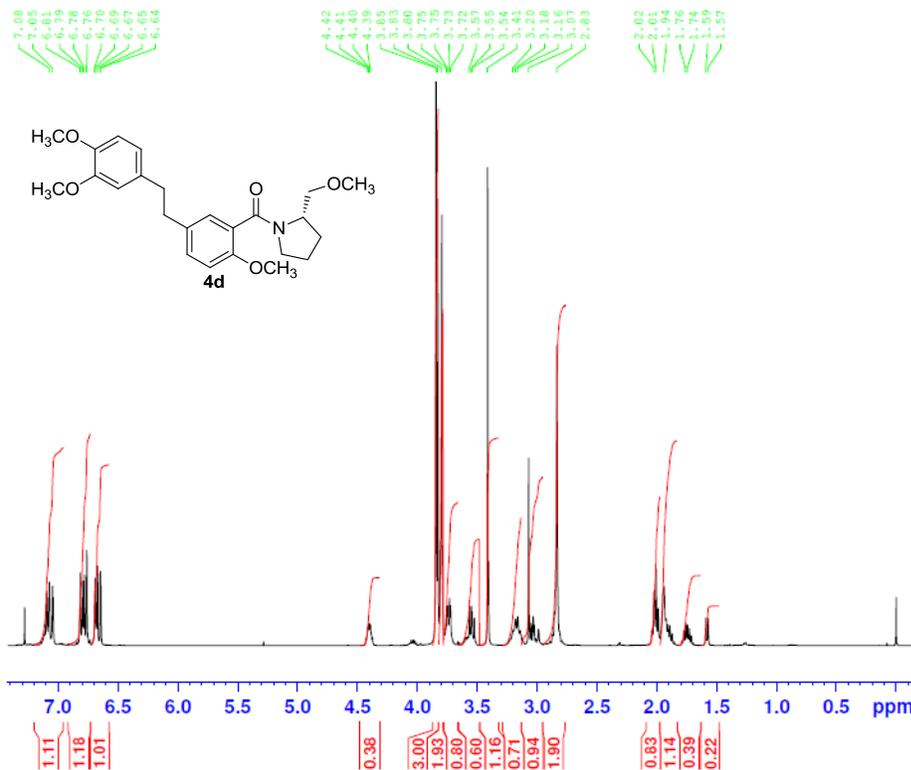


m/z-->

Abundance

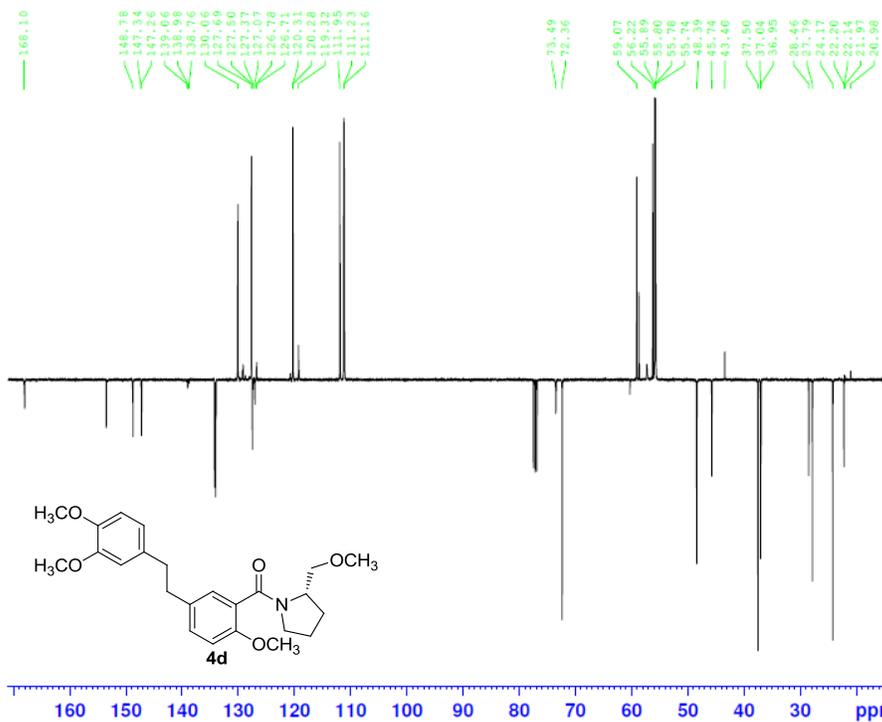


m/z-->



NAME sjb_74_211fp take 2
 EXPNO 1
 PROCNO 1
 Date_ 20130716
 Time 8.57
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 45.2
 DW 60.800 usec
 DE 6.50 usec
 TE 301.2 K
 D1 1.00000000 sec
 TDO 1

CHANNEL f1
 NUC1 1H
 P1 12.50 usec
 PL1 -2.00 dB
 PL1W 12.14226913 W
 SFO1 400.1524711 MHz
 SI 32768
 SF 400.1500000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



NAME sjb_74_211fp 13CAPT
 EXPNO 1
 PROCNO 1
 Date_ 20121127
 Time 9.51
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG jmod
 TD 65536
 SOLVENT CDC13
 NS 1024
 DS 4
 SWH 18750.000 Hz
 FIDRES 0.286102 Hz
 AQ 1.7476766 sec
 RG 203
 DW 26.667 usec
 DE 6.50 usec
 TE 301.2 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 2.00000000 sec
 D20 0.00689655 sec
 TDO 1

CHANNEL f1
 NUC1 13C
 P1 8.00 usec
 P2 16.00 usec
 PL1 -2.00 dB
 PL1W 56.13311005 W
 SFO1 100.6268218 MHz

CHANNEL f2
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -2.00 dB
 PL12 14.00 dB
 PL2W 12.14226913 W
 PL12W 0.30500001 W
 SFO2 400.1514721 MHz
 SI 32768
 SF 100.6177980 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Area Percent Report

Data Path : C:\msdchem\1\DATA\
 Data File : sjb_77_171fp.D
 Acq On : 7 Aug 2013 16:17
 Operator : sjb
 Sample : sjb_77_171fp
 Misc :
 ALS Vial : 100 Sample Multiplier: 1

Integration Parameters: autoint1.e
 Integrator: ChemStation

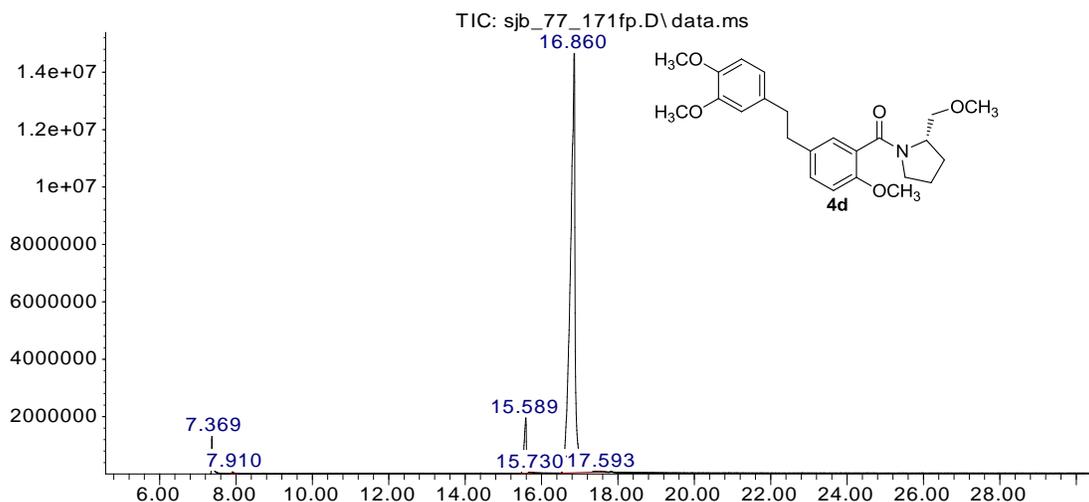
Method : C:\msdchem\1\5973N\PRECISION.M
 Title :

Signal : TIC: sjb_77_171fp.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.369	481	487	521	BV	1282670	30810488	2.37%	2.176%
2	7.910	575	582	600	BV	67415	1896048	0.15%	0.134%
3	15.589	1897	1924	1947	PV	1927063	82443691	6.35%	5.824%
4	15.730	1947	1949	1953	VV 5	27904	466958	0.04%	0.033%
5	16.860	2078	2146	2256	PV	15294204	1299084977	100.00%	91.764%
6	17.501	2256	2258	2260	VV 3	27053	299743	0.02%	0.021%
7	17.520	2260	2261	2272	VV 7	26207	589949	0.05%	0.042%
8	17.593	2272	2274	2278	VV 5	10384	82492	0.01%	0.006%

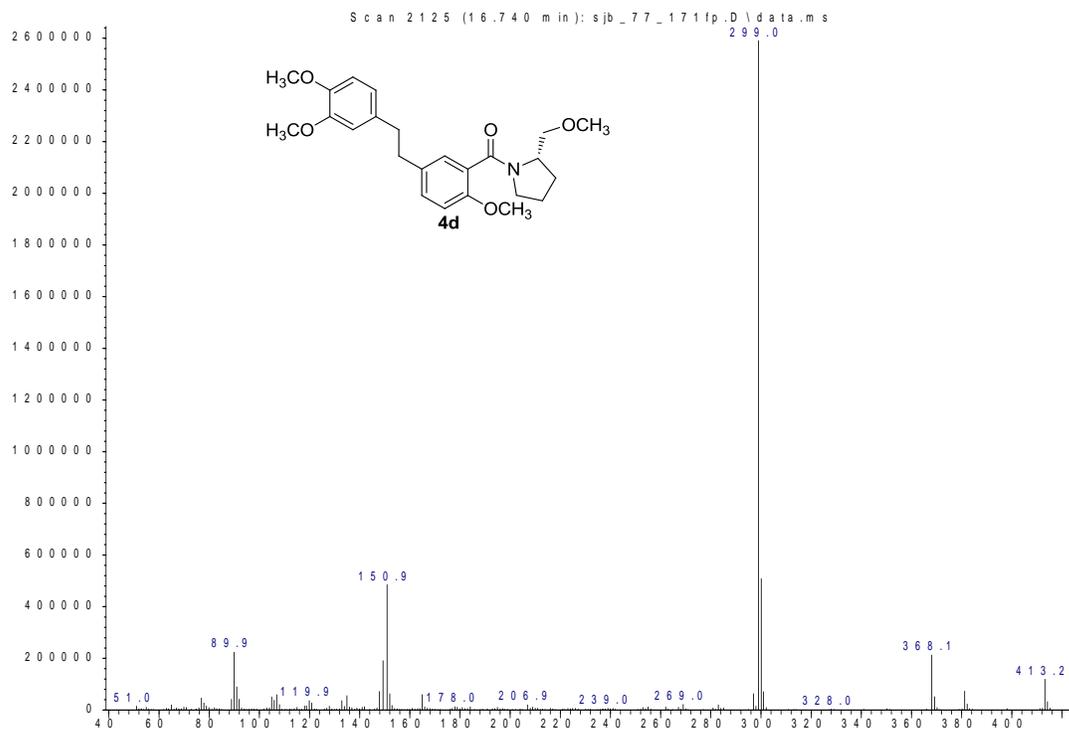
Sum of corrected areas: 1415674346

Abundance

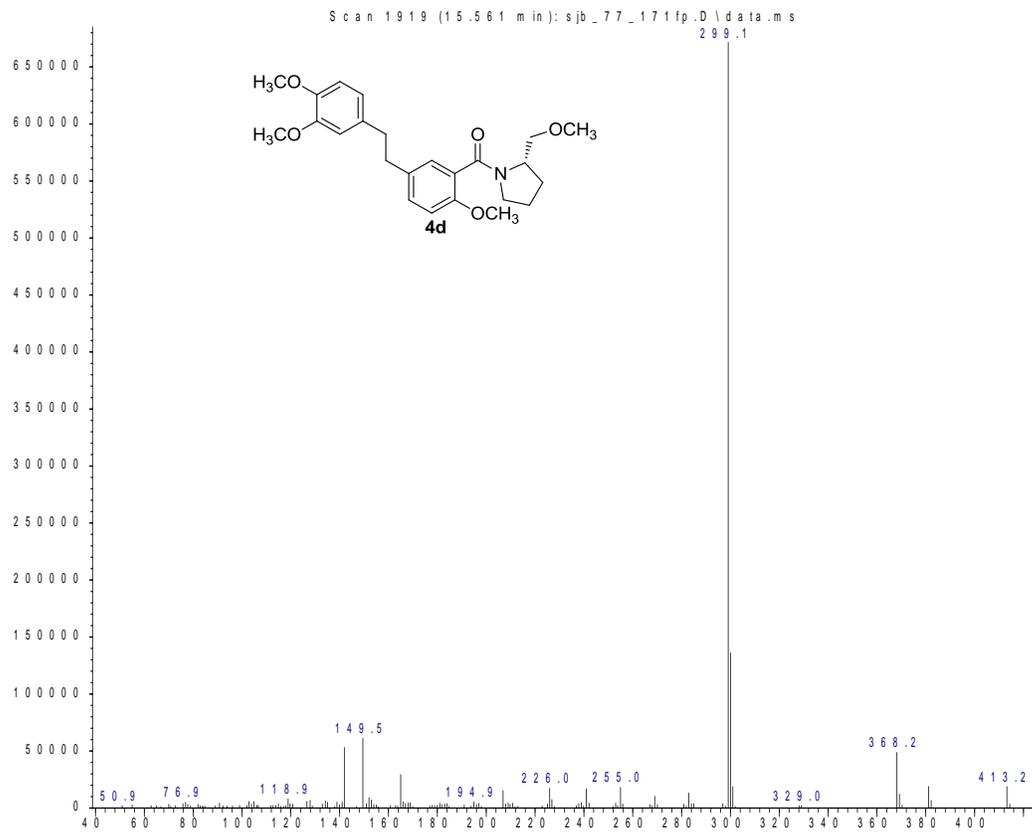


Time-->

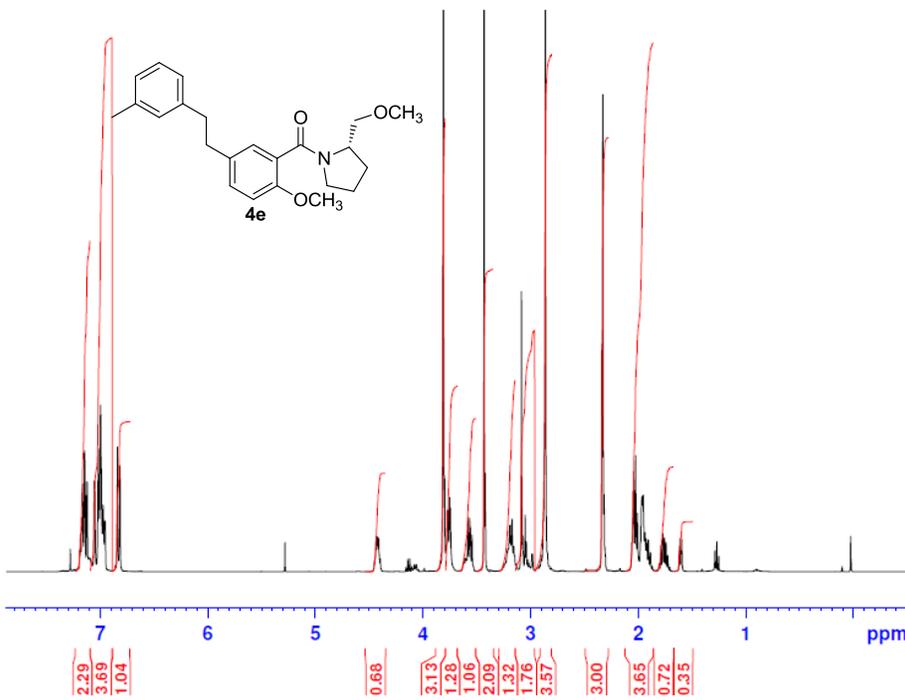
Abundance



m/z-->
Abundance

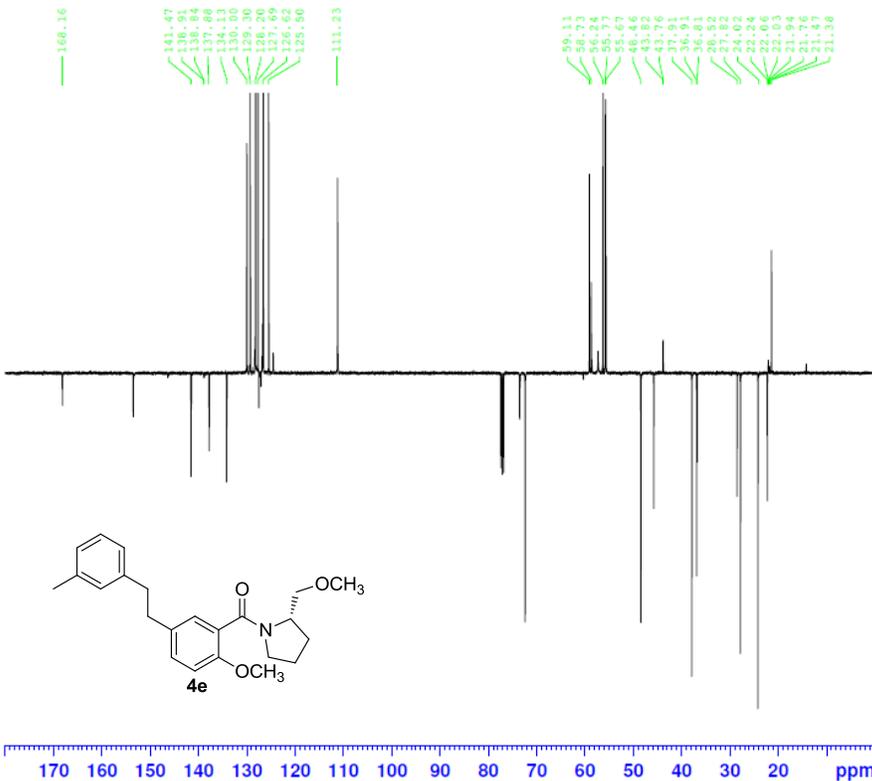


m/z-->



```
NAME      sjb_77_020fp
EXPNO     1
PROCNO    1
Date_     20121221
Time      11.07
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         32
DW         60.800 usec
DE         6.50 usec
TE         303.1 K
D1         1.00000000 sec
TDO        1
```

```
===== CHANNEL f1 =====
NUC1      1H
P1        12.50 usec
PL1       -2.00 dB
PL1W      12.14226913 W
SFO1      400.1524711 MHz
SI         32768
SF        400.1500000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```



```
NAME      sjb_77_020fp 13CAPT
EXPNO     1
PROCNO    1
Date_     20121221
Time      12.46
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   jmod
TD         65536
SOLVENT   CDCl3
NS         1024
DS         4
SWH        18115.941 Hz
FIDRES     0.276427 Hz
AQ         1.8088436 sec
RG         203
DW         27.600 usec
DE         6.50 usec
TE         302.2 K
CNST2     145.0000000
CNST11    1.0000000
D1         2.00000000 sec
D20        0.00689655 sec
TDO        1
```

```
===== CHANNEL f1 =====
NUC1      13C
P1         8.00 usec
P2        16.00 usec
PL1       -2.00 dB
PL1W      56.13311005 W
SFO1      100.6268536 MHz
```

```
===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       -2.00 dB
PL12     14.00 dB
PL2W      12.14226913 W
PL12W     0.30500001 W
SFO2      400.1514742 MHz
SI         32768
SF        100.6177980 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

Area Percent Report

Data Path : C:\msdchem\1\DATA\
Data File : sjb_77_020fp.D
Acq On : 21 Dec 2012 11:20
Operator : sjb
Sample : sjb_77_020fp
Misc :
ALS Vial : 20 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

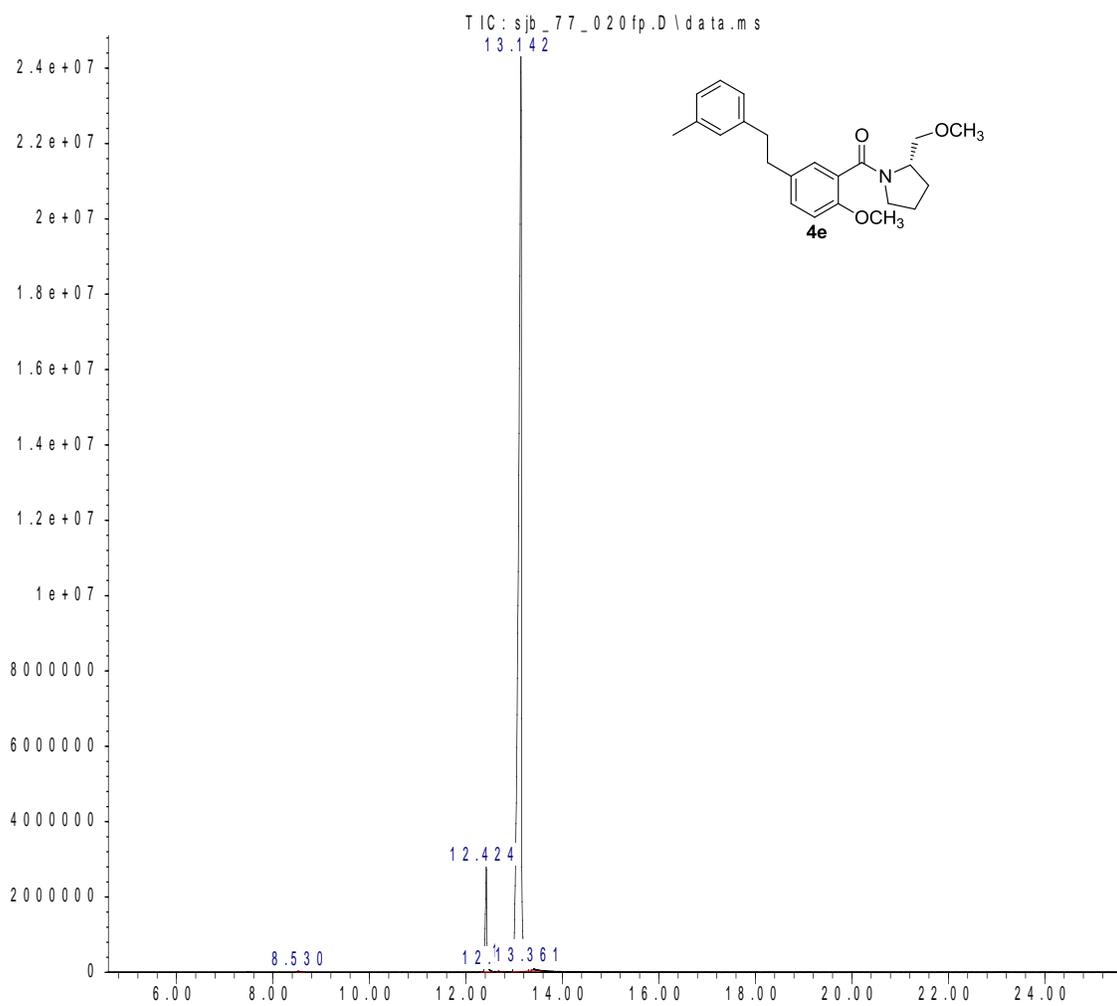
Method : C:\msdchem\1\5973N\PRECISION.M
Title :

Signal : TIC: sjb_77_020fp.D\data.ms

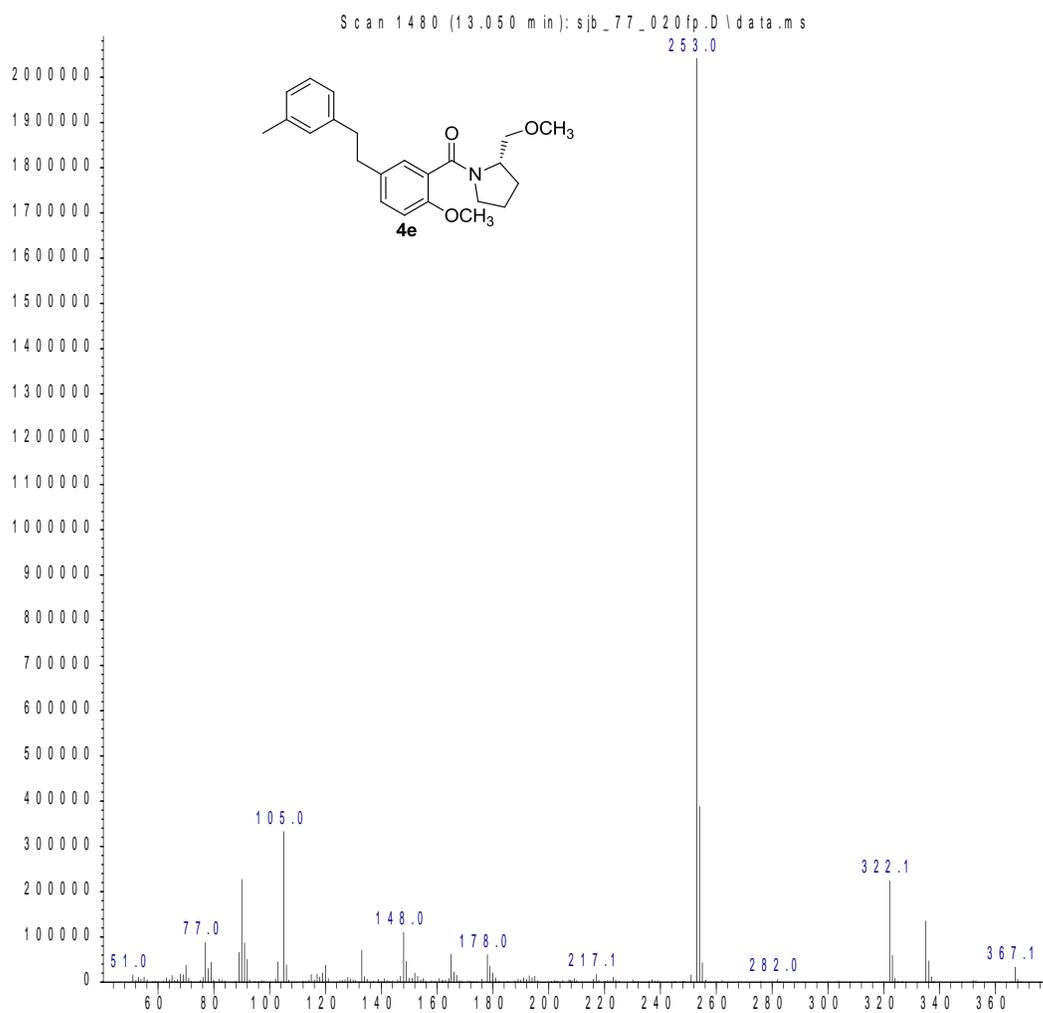
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.530	682	690	708	BV 5	27940	1033448	0.10%	0.092%
2	12.424	1351	1371	1395	PV	2774270	64363753	6.16%	5.746%
3	12.680	1408	1415	1425	VV 2	28357	755335	0.07%	0.067%
4	13.142	1463	1496	1523	PV 2	24682415	1044588528	100.00%	93.256%
5	13.303	1523	1524	1533	VV 6	187569	4711073	0.45%	0.421%
6	13.361	1533	1534	1567	VV 8	94639	4673192	0.45%	0.417%

Sum of corrected areas: 1120125329

Abundance

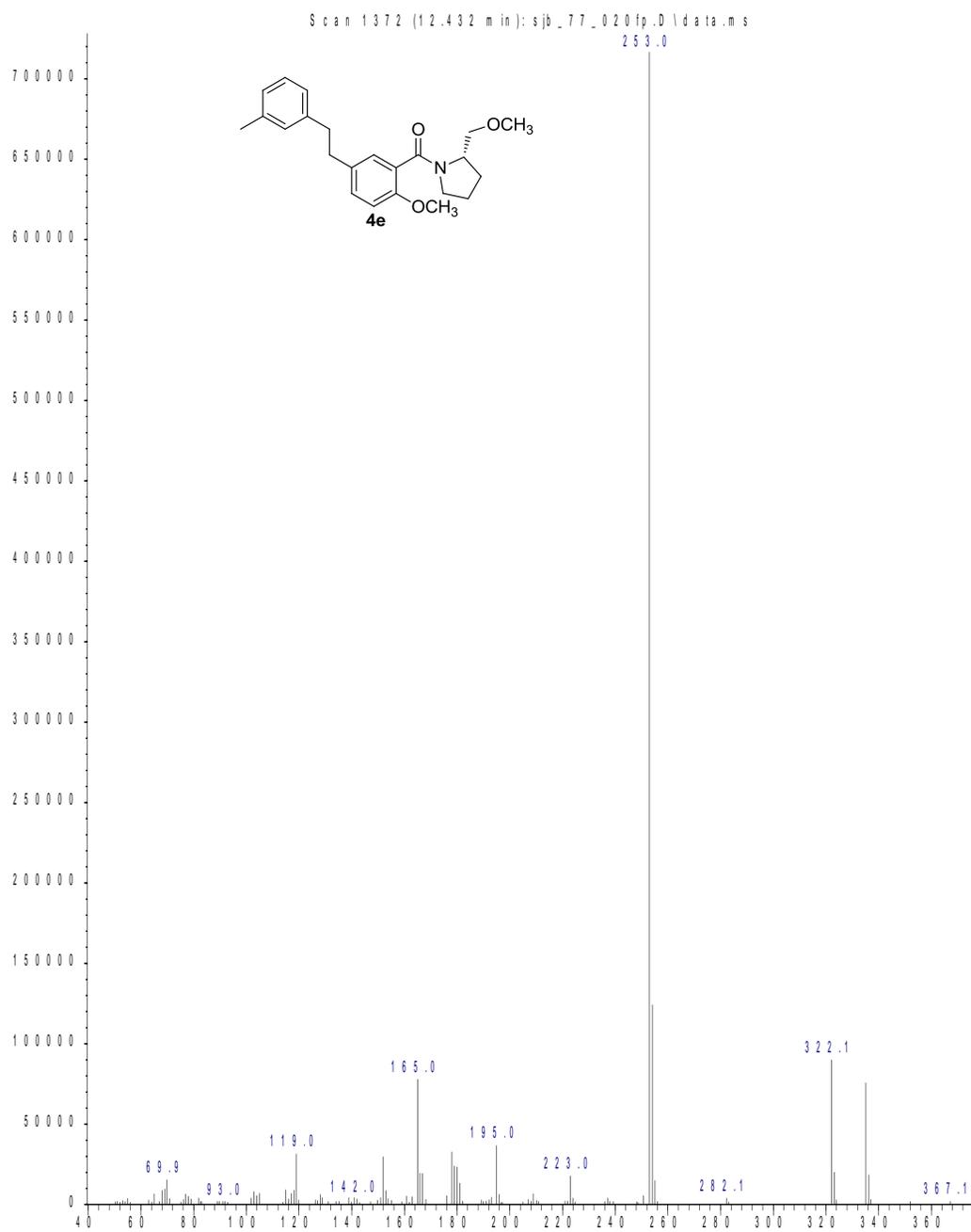


Abundance

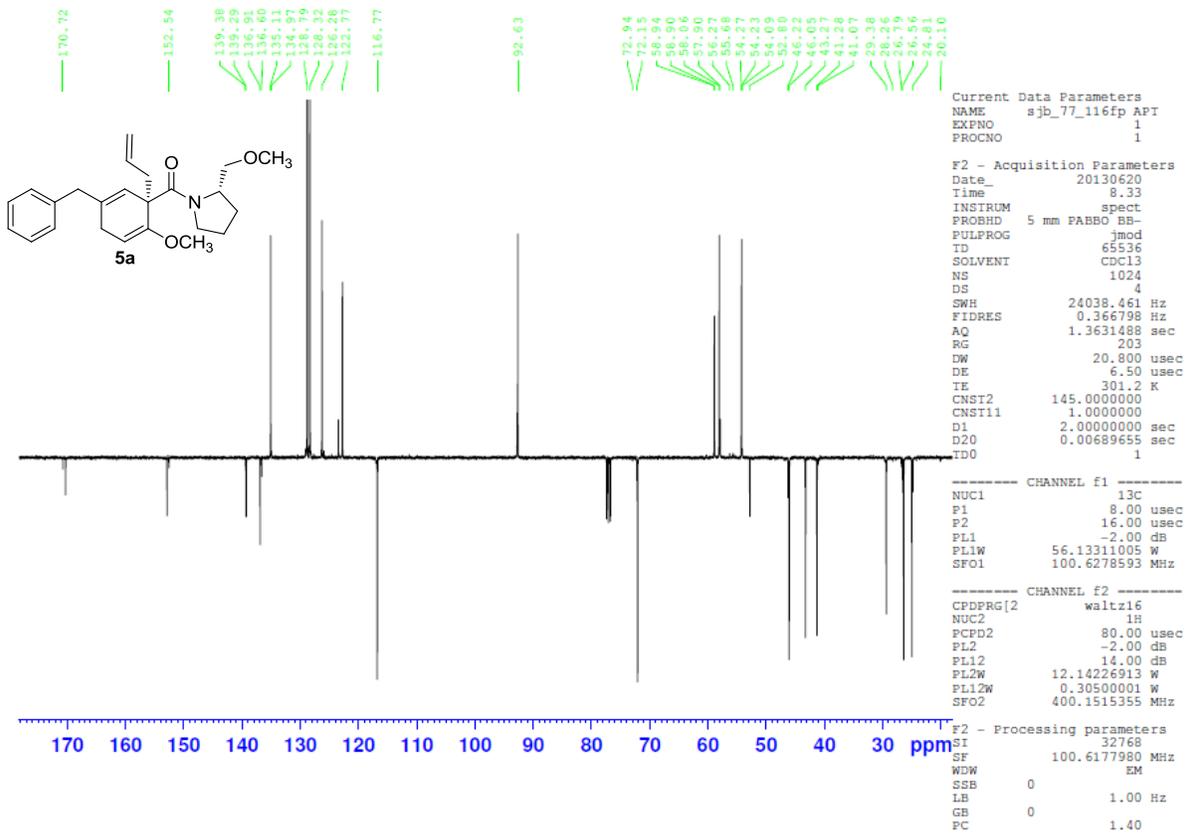
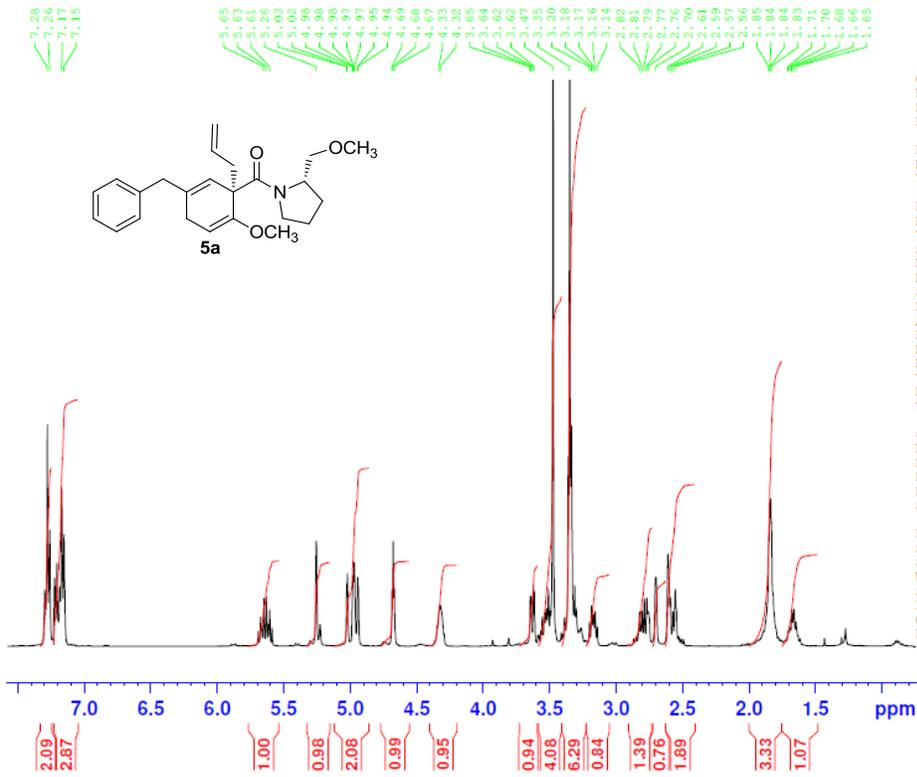


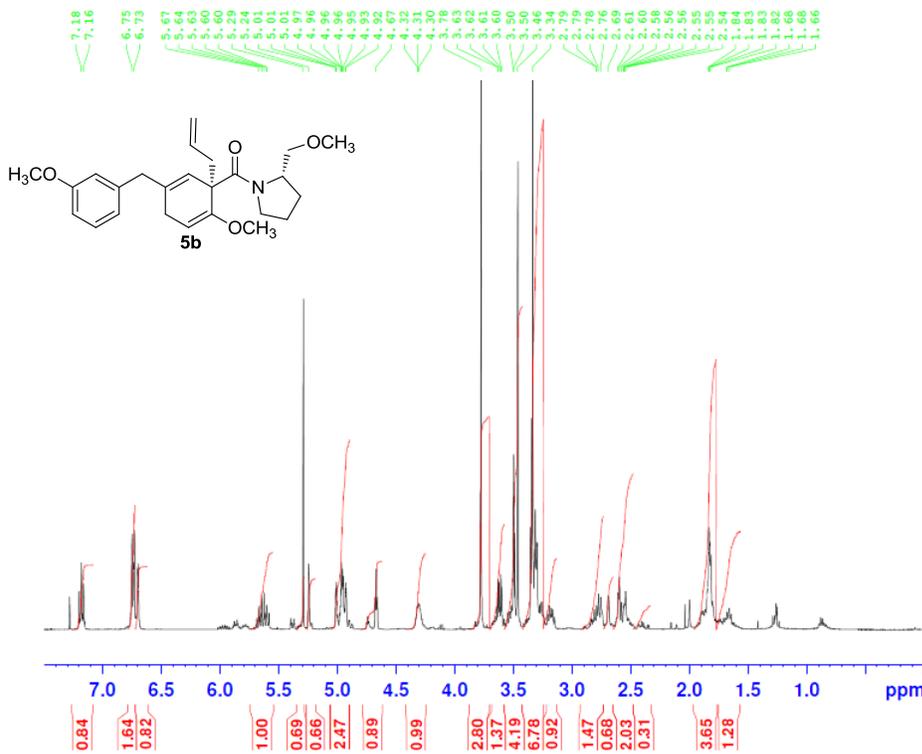
m/z-->

Abundance



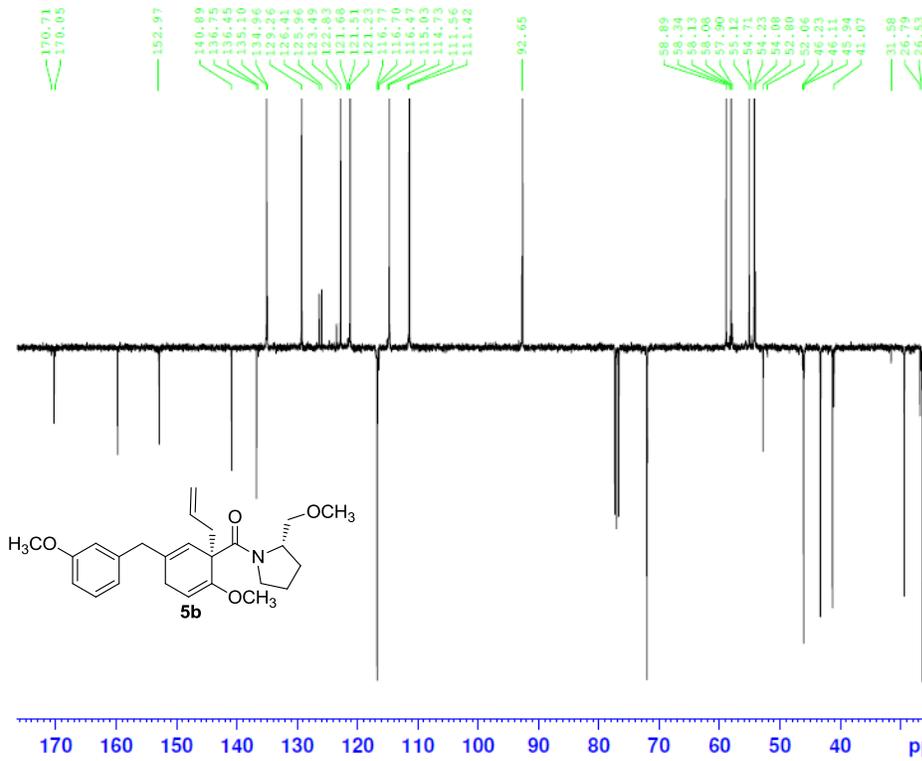
m/z-->





```
NAME sjb_74_152 fr11-19
EXPNO 1
PROCNO 1
Date_ 20121003
Time 9.37
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 36
DW 60.800 usec
DE 6.50 usec
TE 301.2 K
D1 1.0000000 sec
TDO 1
```

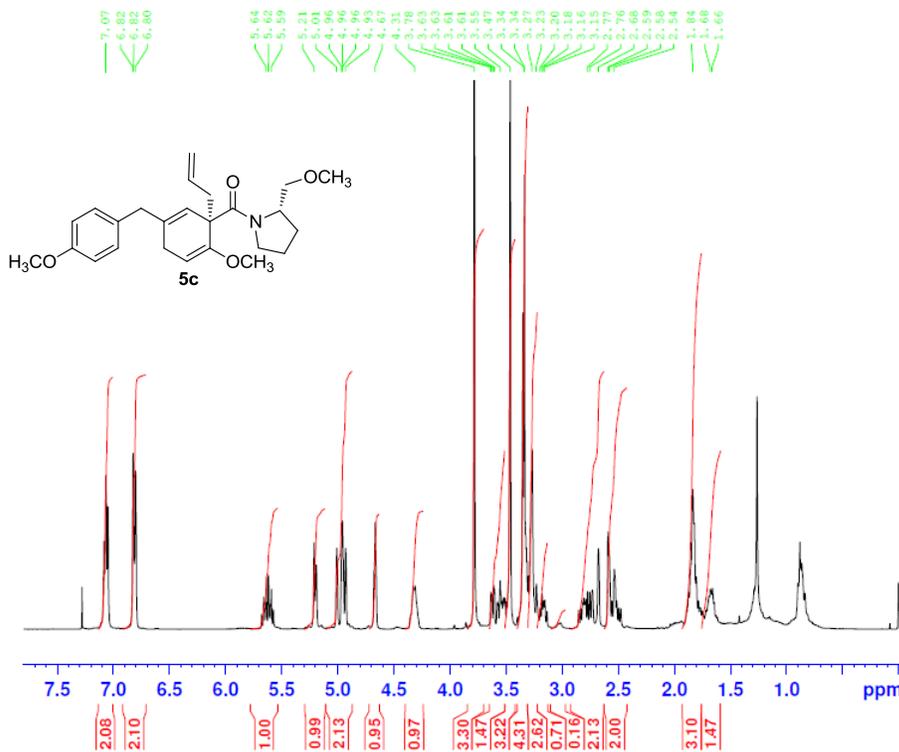
```
===== CHANNEL f1 =====
NUC1 1H
P1 9.80 usec
PL1 -4.00 dB
PLW 19.24419975 W
SFO1 400.1524711 MHz
SI 32768
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
```



```
Current Data Parameters
NAME sjb_77_143fp APT
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130711
Time 8.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT CDC13
NS 922
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 301.2 K
CNST2 145.0000000
CNST1 1.0000000
D1 2.0000000 sec
D20 0.00689655 sec
TDO 1
```

```
===== CHANNEL f1 =====
NUC1 13C
P1 8.00 usec
P2 16.00 usec
PL1 -2.00 dB
PL12 14.00 dB
PL2W 12.14226913 W
PL12W 0.30500001 W
SFO1 100.6278593 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 14.00 dB
PL2W 12.14226913 W
PL12W 0.30500001 W
SFO2 400.1515172 MHz
```

```
F2 - Processing parameters
SI 32768
SF 100.6177980 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```

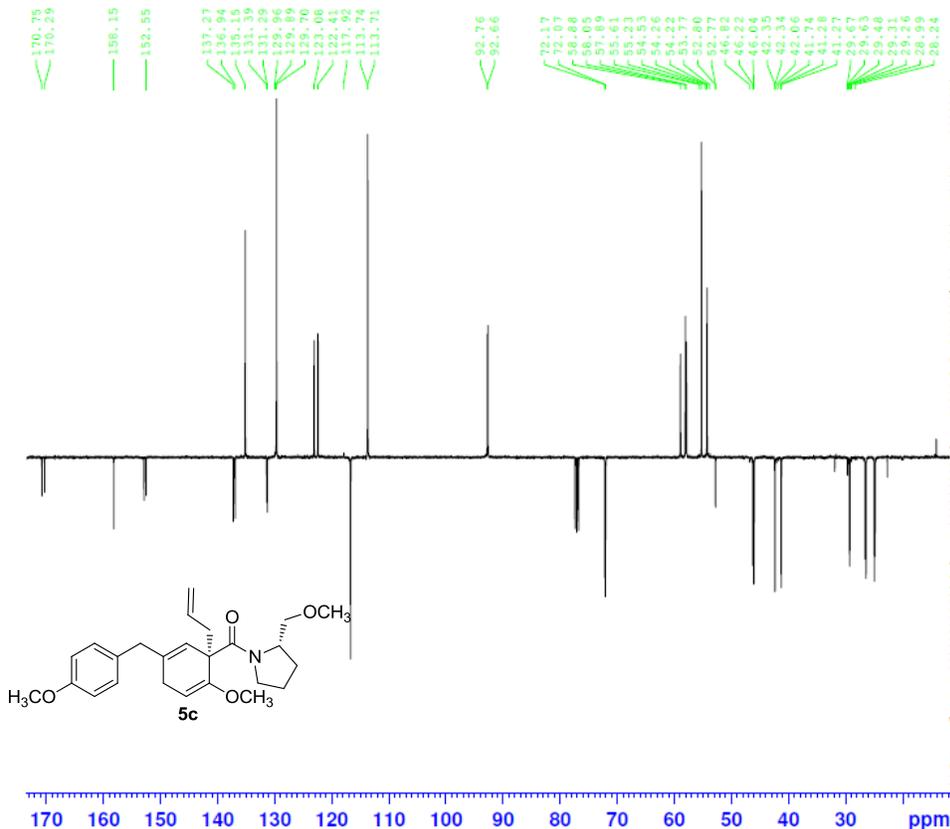


```

NAME      sjb_74_009fp
EXPNO     1
PROCNO    1
Date_     20120531
Time      16.05
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDC13
NS         16
DS         2
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         32
DW         60.800 usec
DE         6.50 usec
TE         301.2 K
D1         1.00000000 sec
TDO        1
  
```

```

===== CHANNEL f1 =====
NUC1      1H
P1        12.50 usec
PL1       -2.00 dB
PL1W      12.14226913 W
SF01      400.1524711 MHz
SI         32768
SF         400.1500000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```



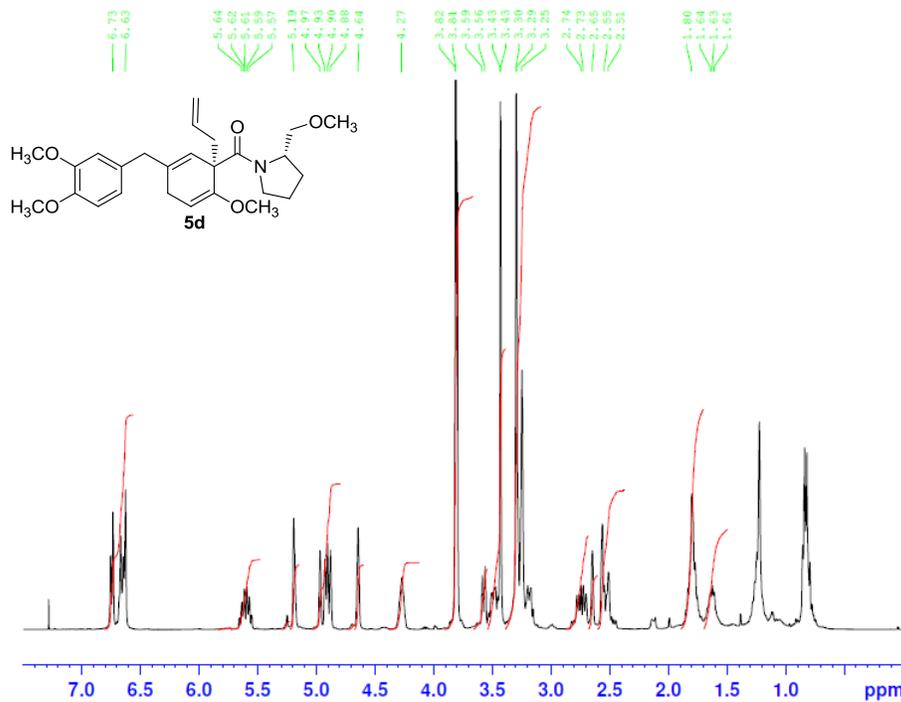
```

NAME      sjb_74_218fp 13CAPT
EXPNO     1
PROCNO    1
Date_     20121206
Time      12.49
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   jmod
TD         65536
SOLVENT   CDC13
NS         1024
DS         4
SWH        18115.941 Hz
FIDRES     0.276427 Hz
AQ         1.8088436 sec
RG         203
DW         27.600 usec
DE         6.50 usec
TE         301.2 K
CNST2     145.0000000
CNST11    1.0000000
D1         2.00000000 sec
D20        0.00689655 sec
TDO        1
  
```

```

===== CHANNEL f1 =====
NUC1      13C
P1         8.00 usec
P2         16.00 usec
PL1        -2.00 dB
PL1W       56.13311005 W
SF01      100.6265472 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2        -2.00 dB
PL12       14.00 dB
PL2W      12.14226913 W
PL12W     0.30500001 W
SF02      400.1515072 MHz
SI         32768
SF         100.6177980 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```



```

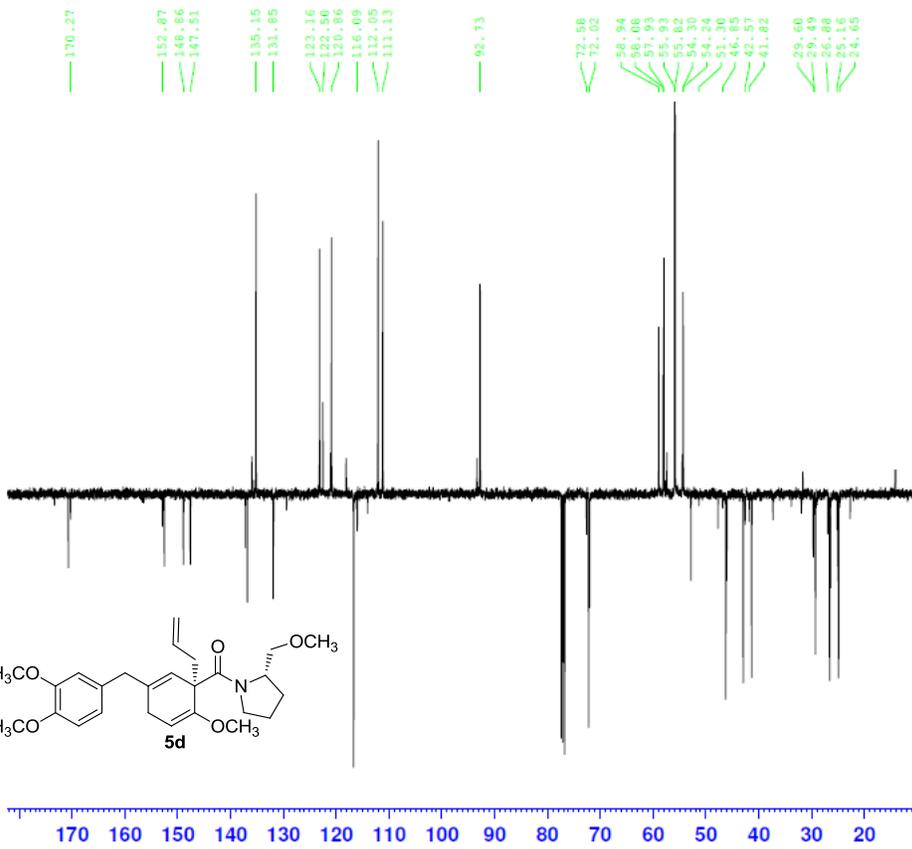
NAME      sjb_74_153fp
EXPNO     1
PROCNO    1
Date_     20121002
Time      16.06
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH       8223.685 Hz
FIDRES    0.125483 Hz
AQ         3.9846387 sec
RG         22.6
DW         60.800 usec
DE         6.50 usec
TE         301.2 K
D1         1.00000000 sec
TDO        1

```

```

===== CHANNEL f1 =====
NUC1      1H
P1         9.80 usec
PL1       -4.00 dB
PL1W      19.24419975 W
SFO1      400.1524711 MHz
SI         32768
SF         400.1500000 MHz
WDW        EM
SSB         0
LB         0.30 Hz
GB         0
PC         1.00

```



```

NAME      sjb_77_119fp APT
EXPNO     1
PROCNO    1
Date_     20130621
Time      8.47
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   jmod
TD         65536
SOLVENT   CDCl3
NS         1024
DS         4
SWH       24038.461 Hz
FIDRES    0.366798 Hz
AQ         1.3631988 sec
RG         203
DW         20.800 usec
DE         6.50 usec
TE         301.2 K
CNST2     145.0000000
CNST11    1.0000000
D1         2.00000000 sec
D20       0.00689655 sec
TDO        1

```

```

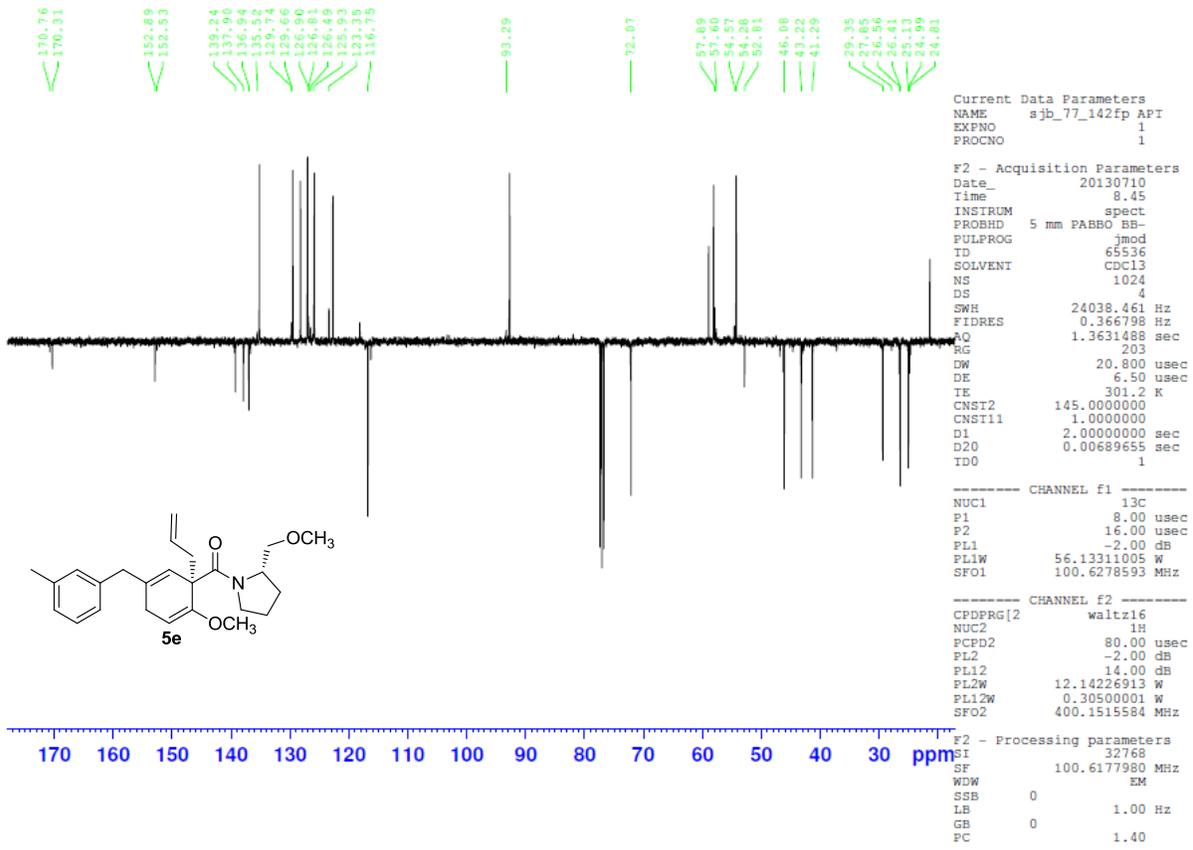
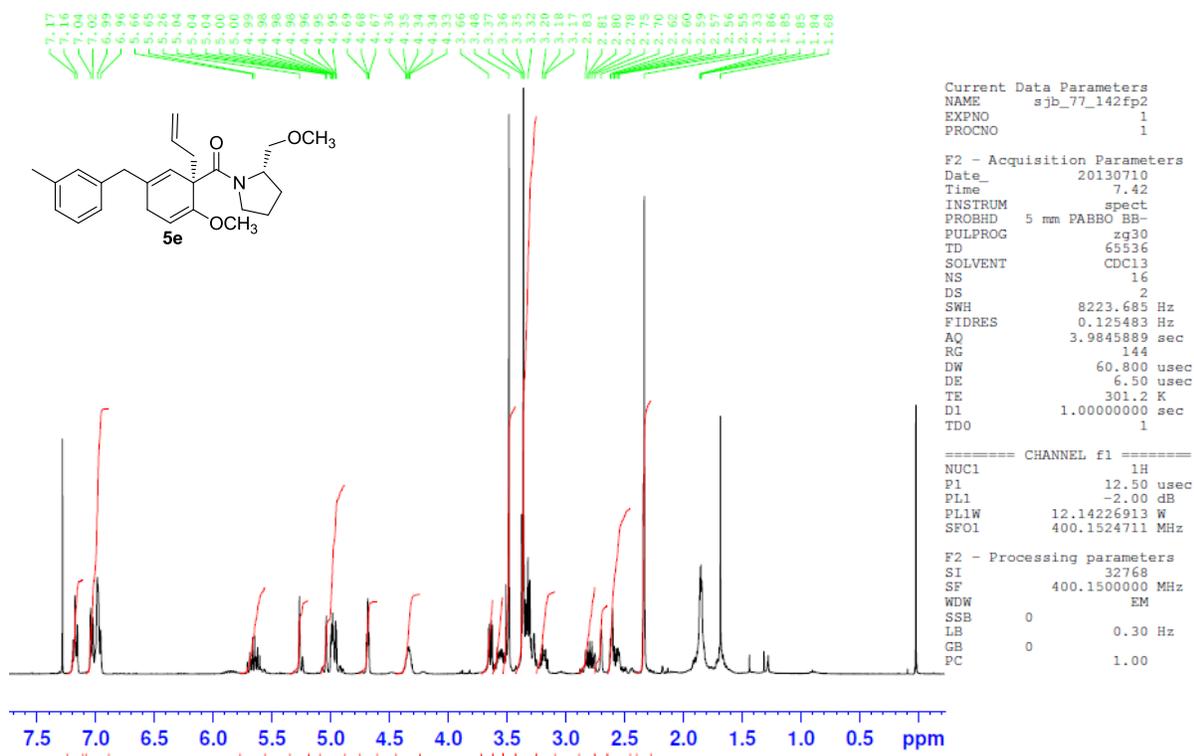
----- CHANNEL f1 -----
NUC1      13C
P1         8.00 usec
P2         16.00 usec
PL1        -2.00 dB
PL1W       56.13311005 W
SFO1      100.6278593 MHz

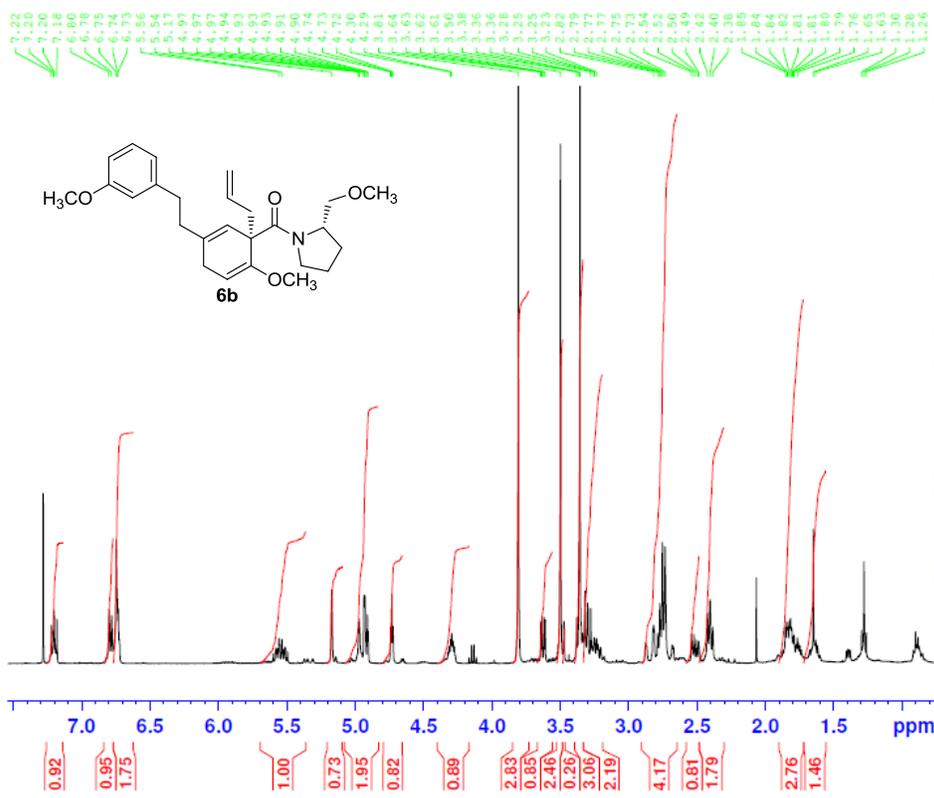
```

```

----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2        -2.00 dB
PL12       14.00 dB
PL12W     12.14226913 W
PL12W     0.30500001 W
SFO2      400.1514270 MHz
SI         32768
SF         100.6177980 MHz
WDW        EM
SSB         0
LB         1.00 Hz
GB         0
PC         1.40

```



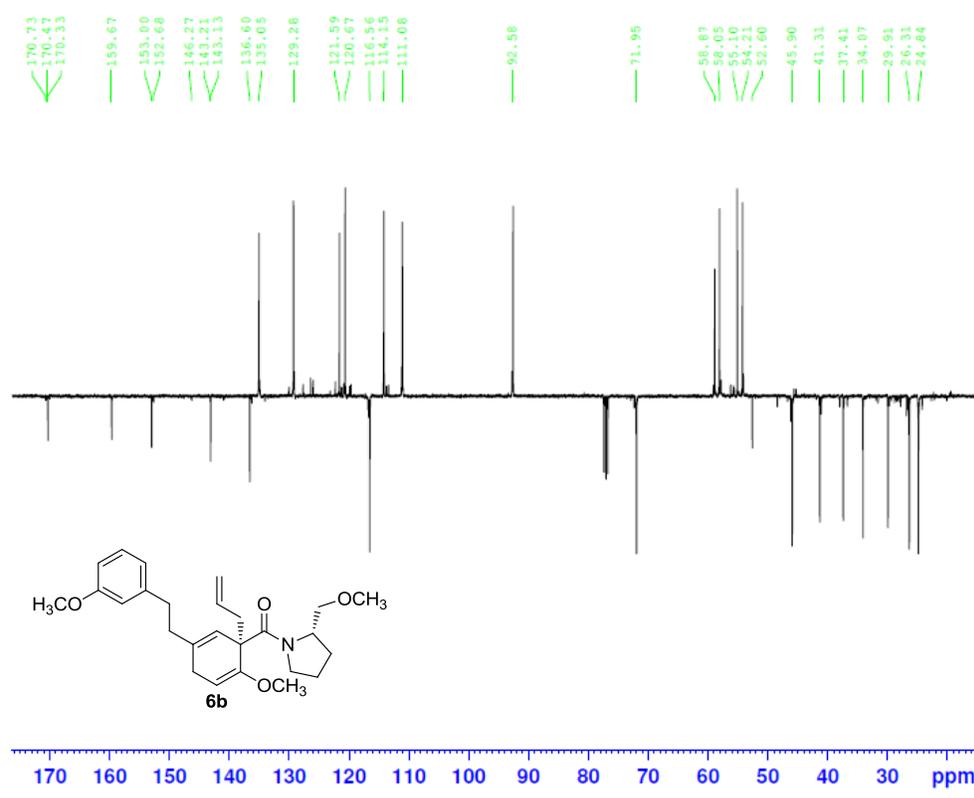


Current Data Parameters
 NAME sjb_81_102fp
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140214
 Time 12.39
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 128
 DW 62.400 usec
 DE 6.50 usec
 TE 296.8 K
 D1 1.0000000 sec
 TDO 1

----- CHANNEL f1 -----
 SFO1 400.1524711 MHz
 NUC1 1H
 P1 12.50 usec
 PLW1 12.14200020 W

F2 - Processing parameters
 SI 65536
 SF 400.1500000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



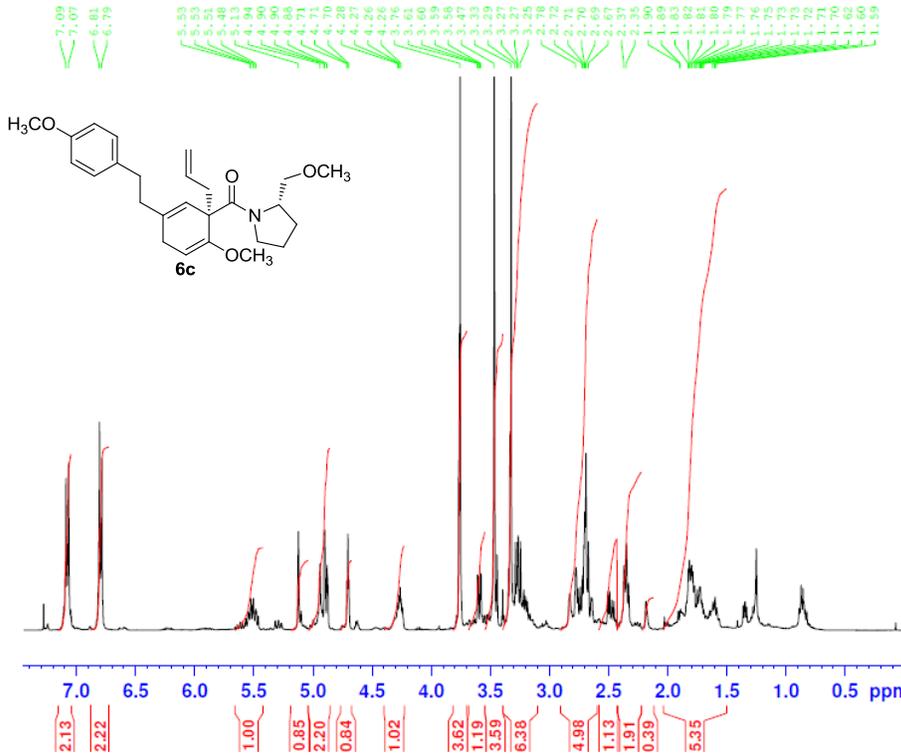
Current Data Parameters
 NAME sjb_81_Birch 666 m methoxy
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140510
 Time 14.31
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG smod
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 301.2 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 2.0000000 sec
 D20 0.00689655 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6298721 MHz
 NUC1 13C
 P1 8.00 usec
 P2 16.00 usec
 PLW1 56.13299942 W

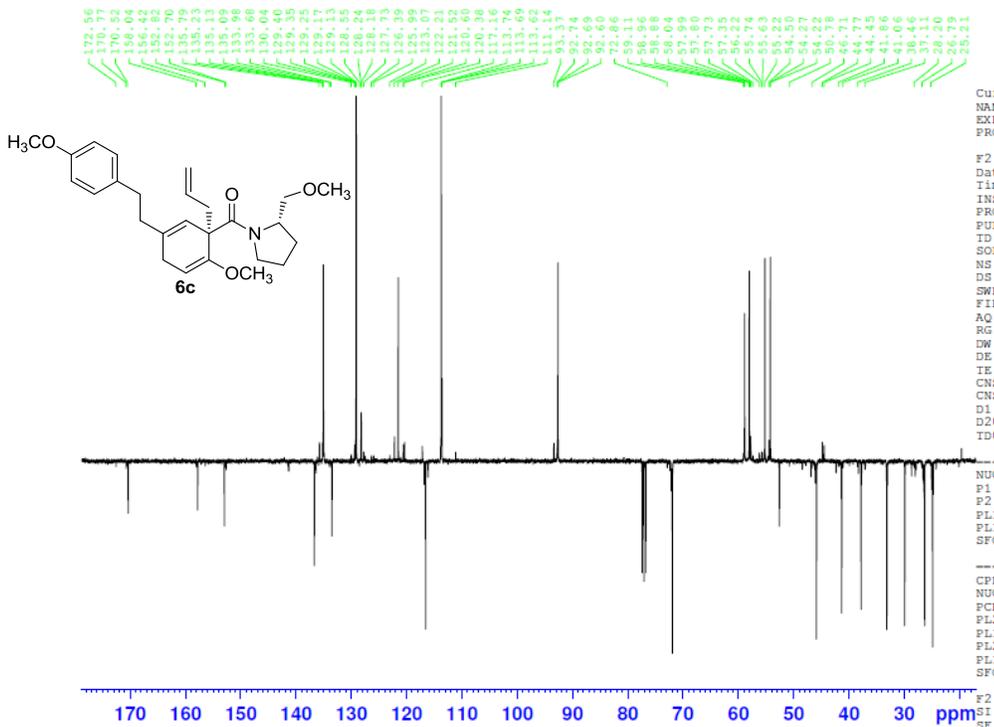
===== CHANNEL f2 =====
 SFO2 400.1516006 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 12.14200020 W
 PLW12 0.24369000 W

F2 - Processing parameters
 SI 32768
 SF 100.6177980 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



NAME ra_67_143pure
EXPNO 1
PROCNO 1
Date_ 20120711
Time 11.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 25.4
DW 60.800 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.50 usec
PL1 -2.00 dB
PL1W 12.14226913 W
SFO1 400.1524711 MHz
SI 32768
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



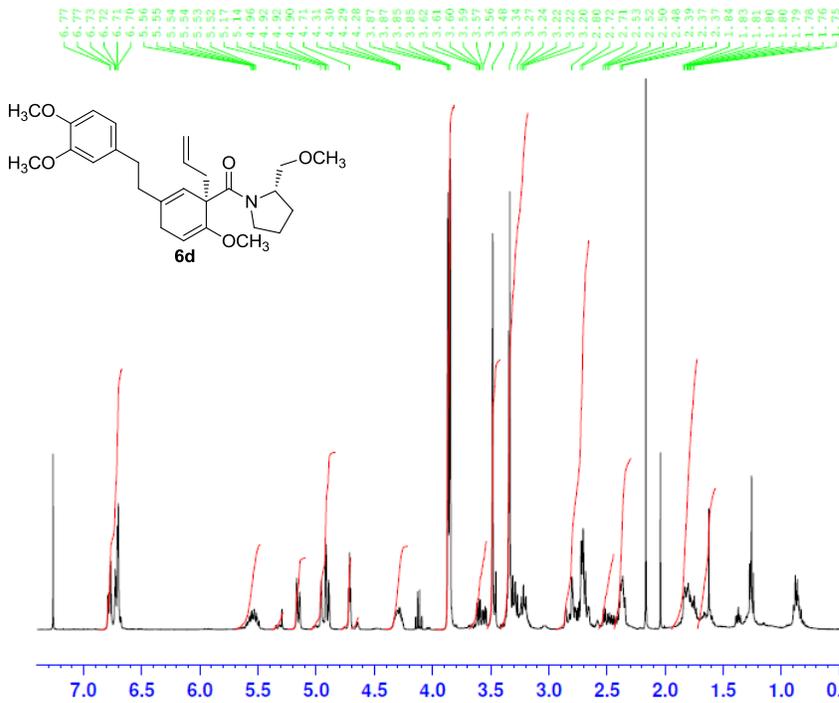
Current Data Parameters
NAME sjb_77_220fp AP1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130924
Time 16.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG 1mod
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.000000
CNST11 1.000000
D1 2.00000000 sec
D20 0.00689655 sec
TD0 1

----- CHANNEL f1 -----
NUC1 13C
P1 8.00 usec
P2 16.00 usec
PL1 -2.00 dB
PL1W 56.13311005 W
SFO1 100.6278593 MHz

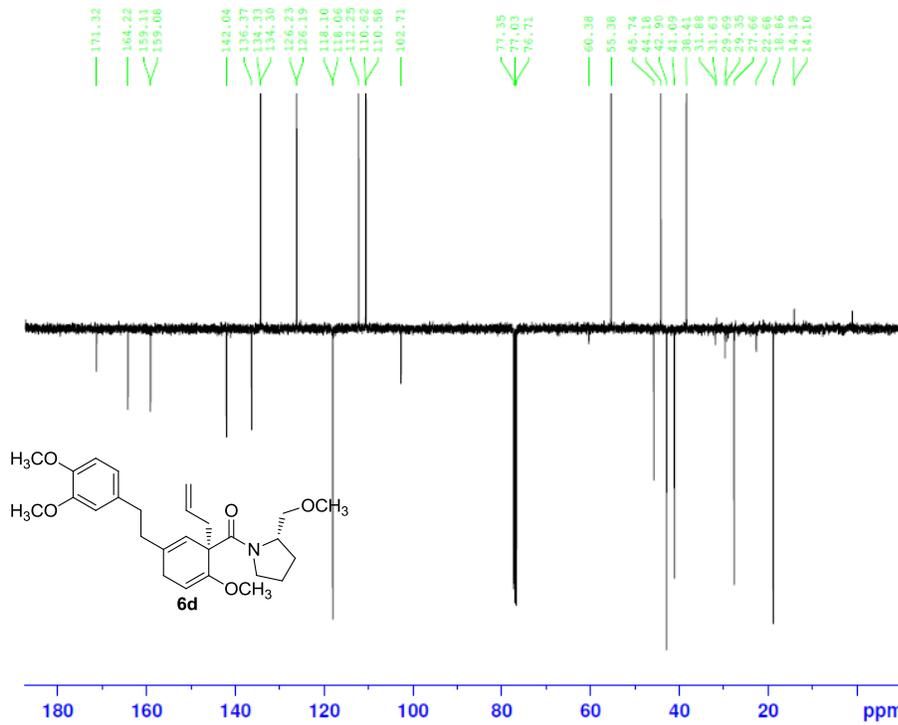
----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 75.00 usec
PL2 -2.00 dB
PL12 13.39 dB
PL2W 12.14226913 W
PL12W 0.35099408 W
SFO2 400.1515013 MHz

F2 - Processing parameters
SI 32768
SF 100.6177980 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



```
NAME      sjb_72_127fp
EXPNO     1
PROCNO    1
Date_     20120220
Time      18.03
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH       8223.685 Hz
FIDRES    0.125483 Hz
AQ         3.9846387 sec
RG         144
DW         60.800 usec
DE         6.50 usec
TE         301.2 K
D1         1.00000000 sec
TDO        1
```

```
===== CHANNEL f1 =====
NUC1      1H
P1        12.50 usec
PL1       -2.00 dB
PL1W      12.14226913 W
SF01      400.1524711 MHz
SI        32768
SF        400.1500066 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
```



```
Current Data Parameters
NAME      sjb_74_174fp 13CAPT
EXPNO     1
PROCNO    1
```

```
F2 - Acquisition Parameters
Date_     20121017
Time      9.19
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   jmod
TD         65536
SOLVENT   CDCl3
NS         1024
DS         4
SWH       20161.291 Hz
FIDRES    0.307637 Hz
AQ         1.6252928 sec
RG         203
DW         24.800 usec
DE         6.50 usec
TE         301.2 K
CNST2     145.0000000
CNST11    1.0000000
D1         2.00000000 sec
D20        0.00689655 sec
TDO        1
```

```
===== CHANNEL f1 =====
NUC1      13C
P1         9.00 usec
P2        18.00 usec
PL1       0 dB
PL1W      35.41759872 W
SF01      100.6268310 MHz
```

```
===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       -3.80 dB
PL12      13.80 dB
PL2W      18.37806702 W
PL12W     0.31937420 W
SF02      400.1514625 MHz
```

```
F2 - Processing parameters
SI        32768
SF        100.6177980 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
```

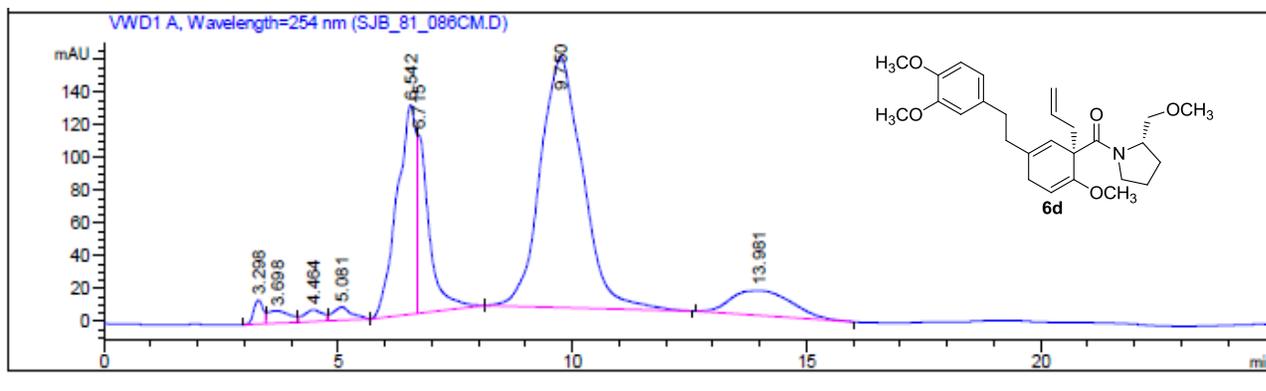
Analysis of stereoselectivity in the Birch reduction-allylation of 4d

1. Enantioselective reaction (LC trace of UV detector reading)

Data File C:\CHEM32\1\DATA\SJB_81_086CM.D

Sample Name: sjb_81_086cm

```
=====
Acq. Operator   : SYSTEM
Acq. Instrument : HPLC
Injection Date  : 1/17/2014 12:22:33 PM
Location       : Vial 1
Inj Volume     : Manually
Method        : C:\CHEM32\1\METHODS\HILIC1.M
Last changed   : 1/17/2014 12:20:27 PM by SYSTEM
                (modified after loading)
Sample Info    : sjb_81_086 crude in 85:15 Hexanes:IPA run in 85:15 Hexanes:IPA at 0.250 mL
                /min for 25 min.
```



Signal 2: WVD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.298	BV	0.2191	203.46292	14.49135	1.1677
2	3.698	VV	0.4577	243.59489	7.32784	1.3980
3	4.464	VV	0.3829	197.91856	7.17767	1.1359
4	5.081	VB	0.4071	224.77737	7.94808	1.2900
5	6.542	BV	0.3841	3654.93994	128.00078	20.9763
6	6.715	VB	0.2498	1885.33069	109.02492	10.8202
7	9.750	BB	0.9449	9656.28906	152.91478	55.4191
8	13.981	BB	1.2294	1357.81055	14.95760	7.7927

Totals : 1.74241e4 441.84302

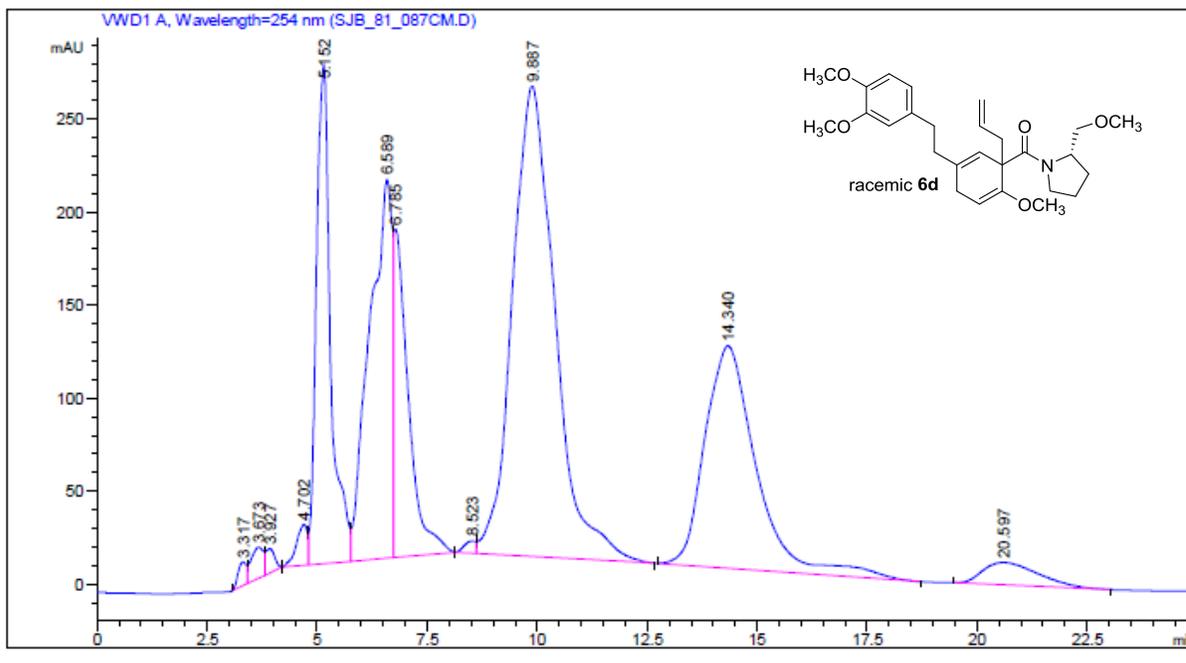
2. Non-enantioselective (LC trace of UV detector reading)

Data File C:\CHEM32\1\DATA\SJB_81_087CM.D

Sample Name: sjb_81_087cm

```
=====
Acq. Operator   : SYSTEM
Acq. Instrument : HPLC
Injection Date  : 1/17/2014 3:35:52 PM
Location        : Vial 1
Inj Volume     : Manually

Method          : C:\CHEM32\1\METHODS\HILIC1.M
Last changed    : 1/17/2014 12:20:27 PM by SYSTEM
                 (modified after loading)
Sample Info     : sjb_81_087cm in 85:15 Hexanes:IPA run in 85:15 Hexanes:IPA at 0.250 mL/min
                 for 25 min.
```



=====
 Area Percent Report
 =====

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

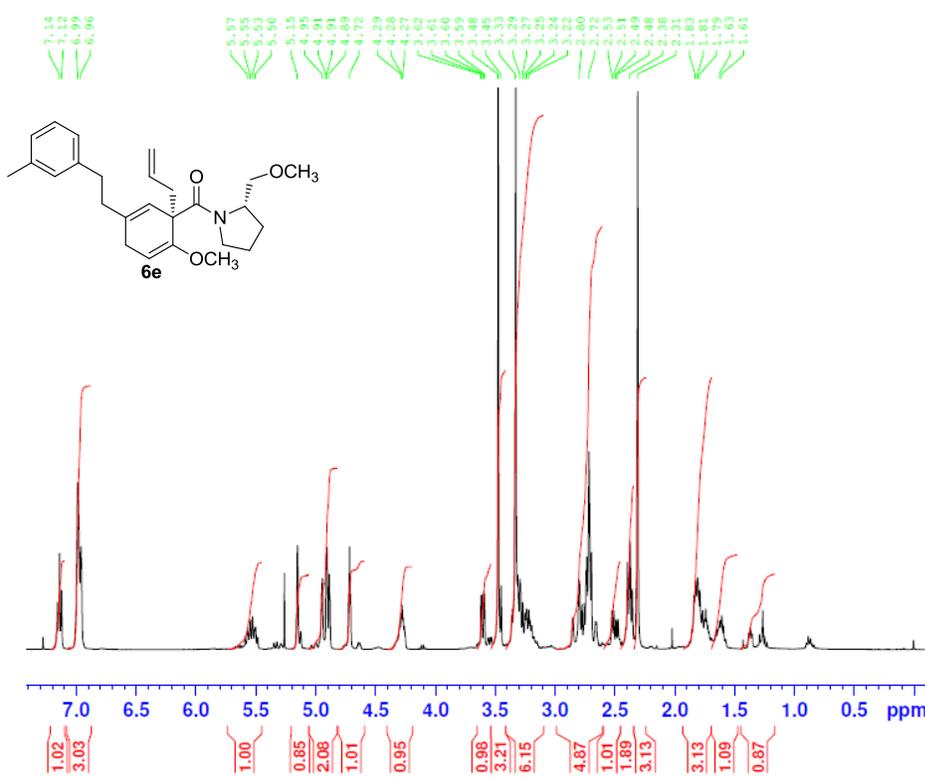
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.317	BV	0.2026	161.71326	12.68614	0.3488
2	3.673	VV	0.2997	329.34979	16.61233	0.7104
3	3.927	VB	0.2226	191.60265	12.91174	0.4133
4	4.702	BV	0.2670	377.67203	22.03365	0.8146
5	5.152	VV	0.3515	6101.32959	268.04456	13.1599
6	6.589	VV	0.4678	7244.44189	203.48740	15.6255
7	6.785	VB	0.3230	4046.57104	176.38852	8.7280
8	8.523	BV	0.2815	114.57014	6.49611	0.2471
9	9.887	VB	0.9084	1.70311e4	252.78012	36.7342
10	14.340	BB	1.2435	9709.70996	119.50664	20.9428
11	20.597	BB	1.2449	1055.00098	11.95725	2.2755

Totals : 4.63631e4 1102.90446

Peak explanation:

retention time (min.)	Compound
5.1	1S enantiomer
6.5-6.7	1R enantiomer
9.8	gamma-alkylation product of Birch reduction
14	unreacted aromatic starting material
20.6	regioisomer of unreacted aromatic starting material

Analysis: Enantioselective reaction shows a small amount of the 1S enantiomer, 1.29%. Therefore the enantioselectivity must be approximately 24:1 (31.8/1.29).

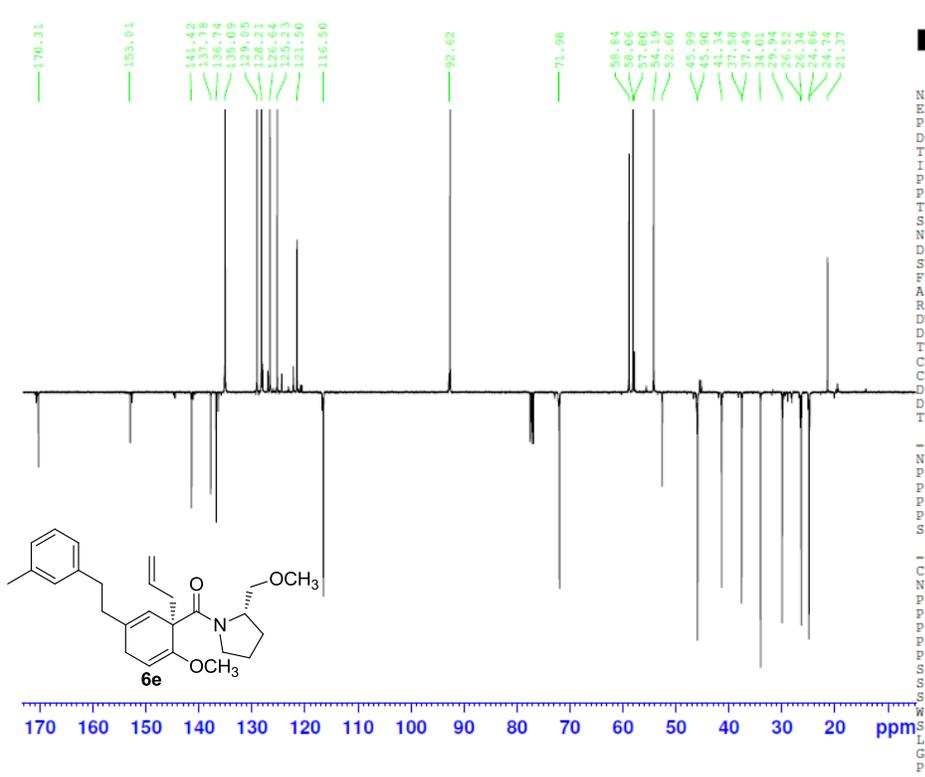


```

NAME      sjb_77_021fp
EXPNO     1
PROCNO    1
Date_     20130103
Time      12.28
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        8223.685 Hz
FIDRES    0.125483 Hz
AQ         3.9846387 sec
RG         18
DW         60.800 usec
DE         6.50 usec
TE         301.9 K
D1         1.00000000 sec
TDO        1
  
```

```

===== CHANNEL f1 =====
NUC1      1H
P1        12.50 usec
PL1       -2.00 dB
PL1W      12.14226913 W
SFO1      400.1524711 MHz
SI         32768
SF         400.1500000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```



```

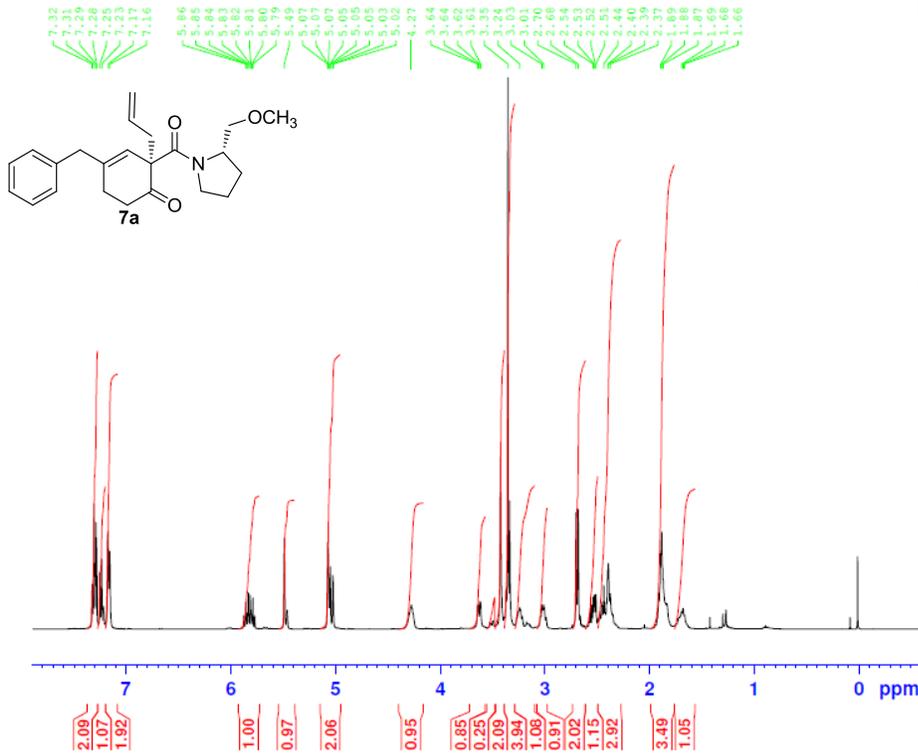
NAME      sjb_77_021fp 13CAPT
EXPNO     1
PROCNO    1
Date_     20130103
Time      15.21
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   jmod
TD         65536
SOLVENT   CDCl3
NS         1024
DS         4
SWH        17006.803 Hz
FIDRES    0.259503 Hz
AQ         1.9268084 sec
RG         203
DW         29.400 usec
DE         6.50 usec
TE         301.1 K
CNST2     145.0000000
CNST11    1.0000000
D1         2.00000000 sec
D20        0.00689655 sec
TDO        1
  
```

```

----- CHANNEL f1 -----
NUC1      13C
P1         8.00 usec
P2        16.00 usec
PL1       -2.00 dB
PL1W      56.13311005 W
SFO1      100.6267471 MHz
  
```

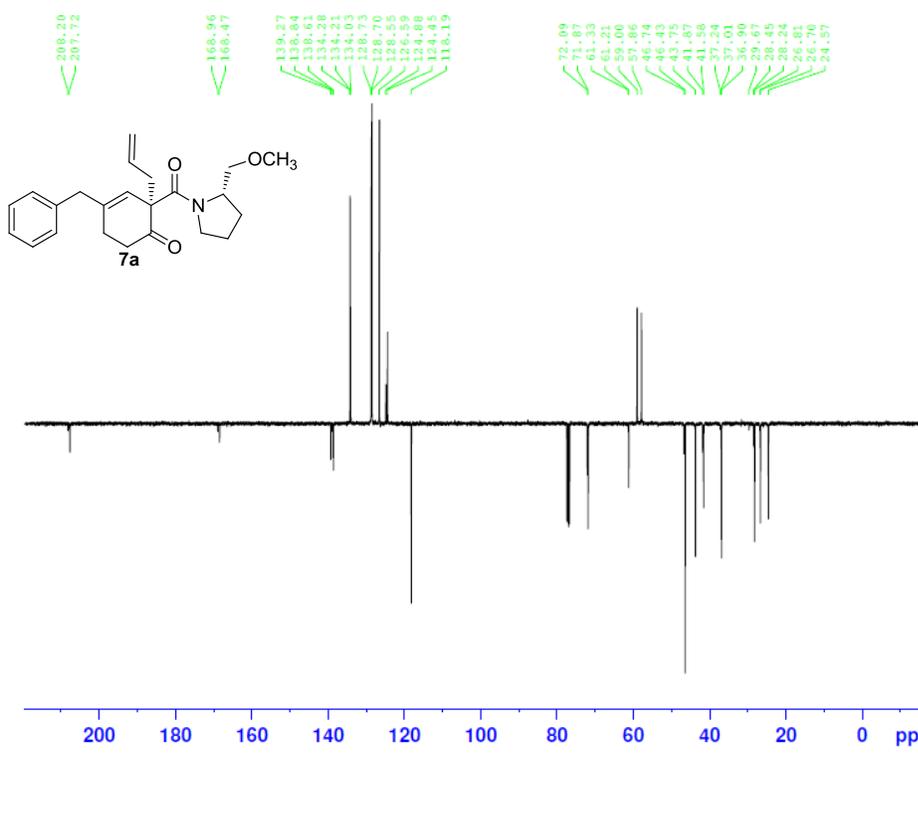
```

----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       -2.00 dB
PL12      14.00 dB
PL2W      12.14226913 W
PL12W     0.30500000 W
SFO2      400.1514615 MHz
SI         32768
SF         100.6177980 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```



NAME sjb_77_120fp2
EXPNO 1
PROCNO 1
Date_ 20130625
Time 9.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 50.8
DW 60.800 usec
DE 6.50 usec
TE 301.2 K
D1 1.00000000 sec
TDO 1

----- CHANNEL f1 -----
NUC1 1H
P1 12.50 usec
PL1 -2.00 dB
PL1W 12.14226913 W
SFO1 400.1524711 MHz
SI 32768
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



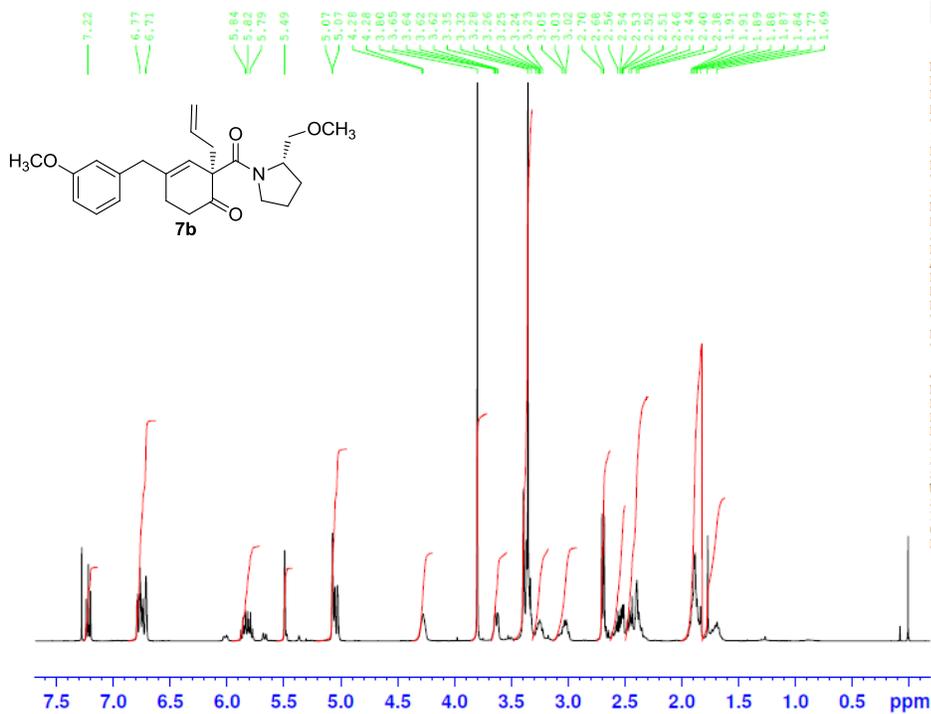
Current Data Parameters
NAME sjb_77_120fp APT
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130625
Time 9.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 301.2 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TDO 1

----- CHANNEL f1 -----
NUC1 13C
P1 8.00 usec
P2 16.00 usec
PL1 -2.00 dB
PL1W 56.13311005 W
SFO1 100.6278593 MHz

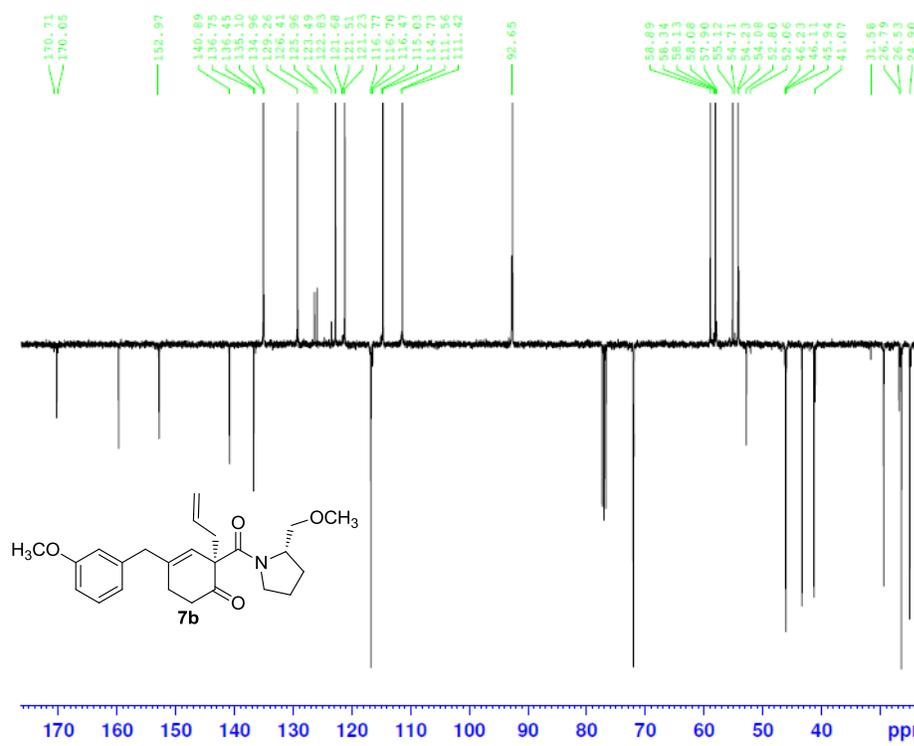
----- CHANNEL f2 -----
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 14.00 dB
PL2W 12.14226913 W
PL12W 0.30500001 W
SFO2 400.1515663 MHz

F2 - Processing parameters
SI 32768
SF 100.6177980 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



NAME sjb_77_145fp take 2
EXPNO 1
PROCNO 1
Date_ 20130717
Time 7.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 101
DW 60.800 usec
DE 6.50 usec
TE 301.2 K
D1 1.00000000 sec
TDO 1

----- CHANNEL f1 -----
NUC1 1H
P1 12.50 usec
PL1 -2.00 dB
PL1W 12.14226913 W
SFO1 400.1524711 MHz
SI 32768
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



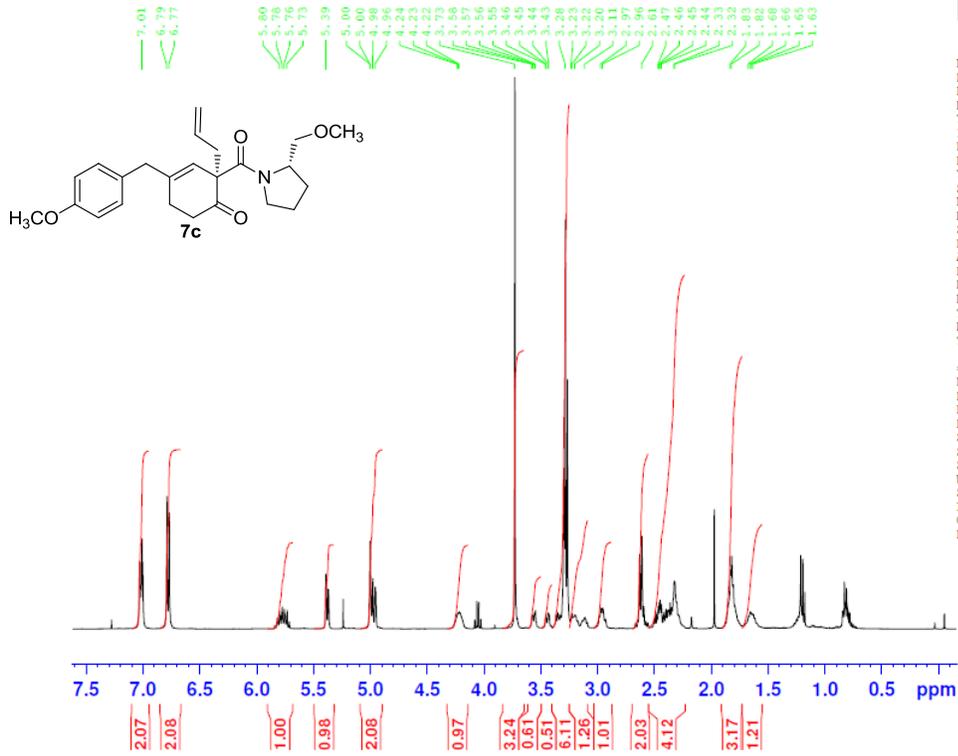
Current Data Parameters
NAME sjb_77_143fp APT
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130711
Time 8.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 922
DS 4
SWH 24038.461 Hz
FIDRES 0.336798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 301.2 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TDO 1

----- CHANNEL f1 -----
NUC1 13C
P1 8.00 usec
P2 16.00 usec
PL1 -2.00 dB
PL1W 56.13311005 W
SFO1 100.6278593 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 14.00 dB
PL2W 12.14226913 W
PL12W 0.30500001 W
SFO2 400.1515172 MHz

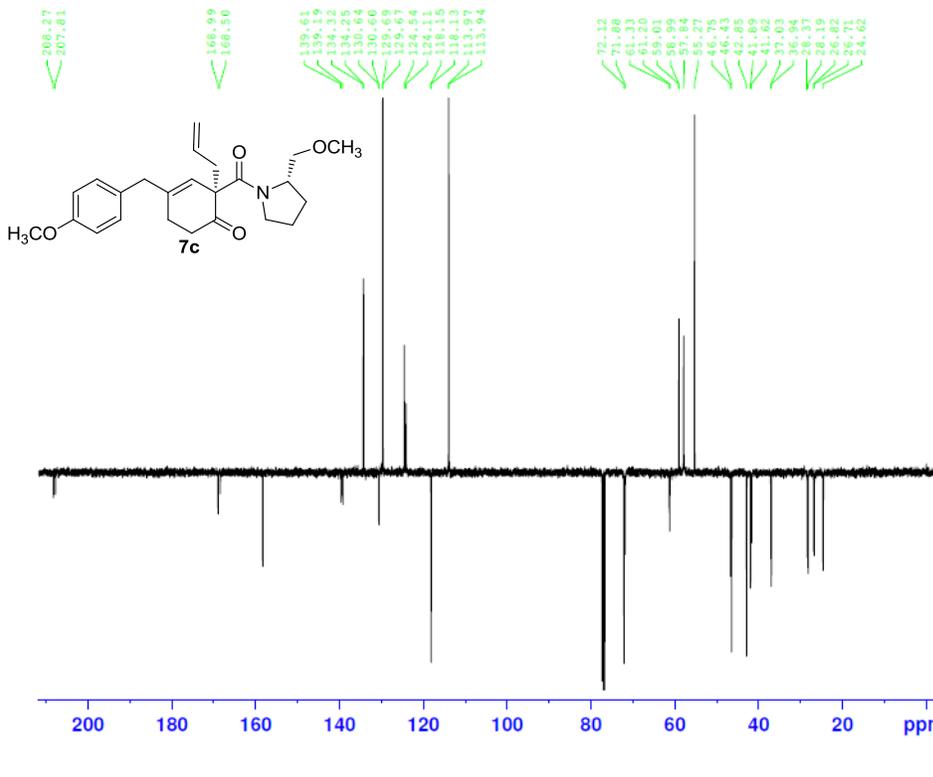
F2 - Processing parameters
SI 32768
SF 100.6177980 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



```

NAME      sjb_74_013fp
EXPNO    1
PROCNO   1
Date_    20120604
Time     11.45
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD       65536
SOLVENT  CDC13
NS       16
DS       2
SWH      8223.685 Hz
FIDRES   0.125483 Hz
AQ       3.9846387 sec
RG       18
DW       60.800 usec
DE       6.50 usec
TE       301.1 K
D1       1.00000000 sec
TDO      1

===== CHANNEL f1 =====
NUC1     1H
P1       12.50 usec
PL1     -2.00 dB
PL1W    12.14226913 W
SFO1    400.1524711 MHz
SI       32768
SF      400.1500000 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
  
```

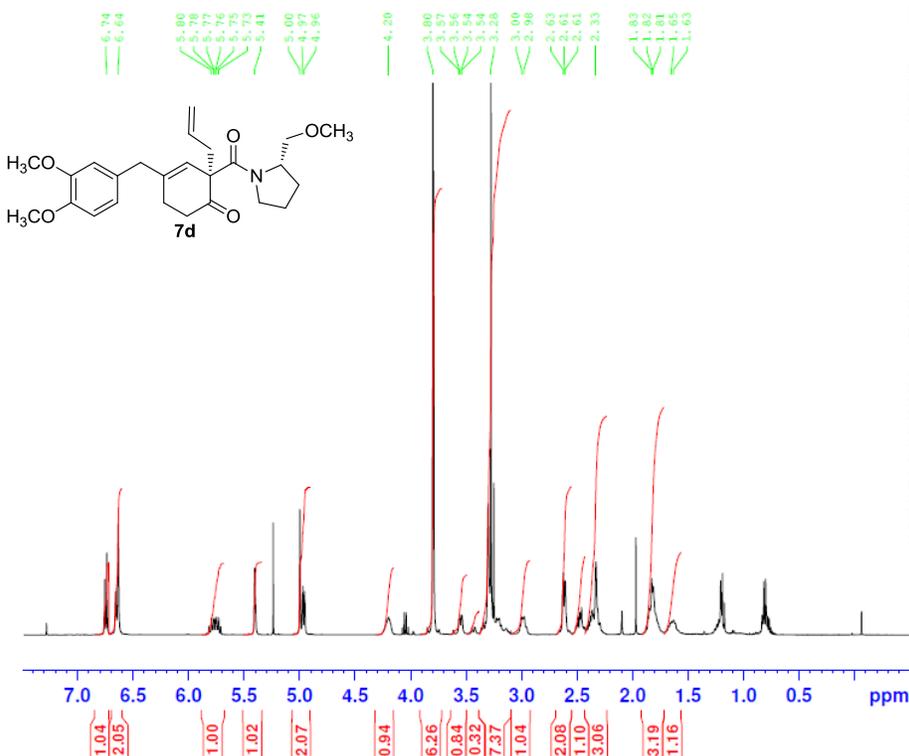


```

NAME      sjb_77_003 13CAPT
EXPNO    1
PROCNO   1
Date_    20121207
Time     12.08
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  jmod
TD       65536
SOLVENT  CDC13
NS       1024
DS       4
SWH      21739.131 Hz
FIDRES   0.331713 Hz
AQ       1.5073780 sec
RG       203
DW       23.000 usec
DE       6.50 usec
TE       301.2 K
CNST2   145.0000000
CNST11  1.0000000
D1       2.00000000 sec
D20     0.00689655 sec
TDO      1

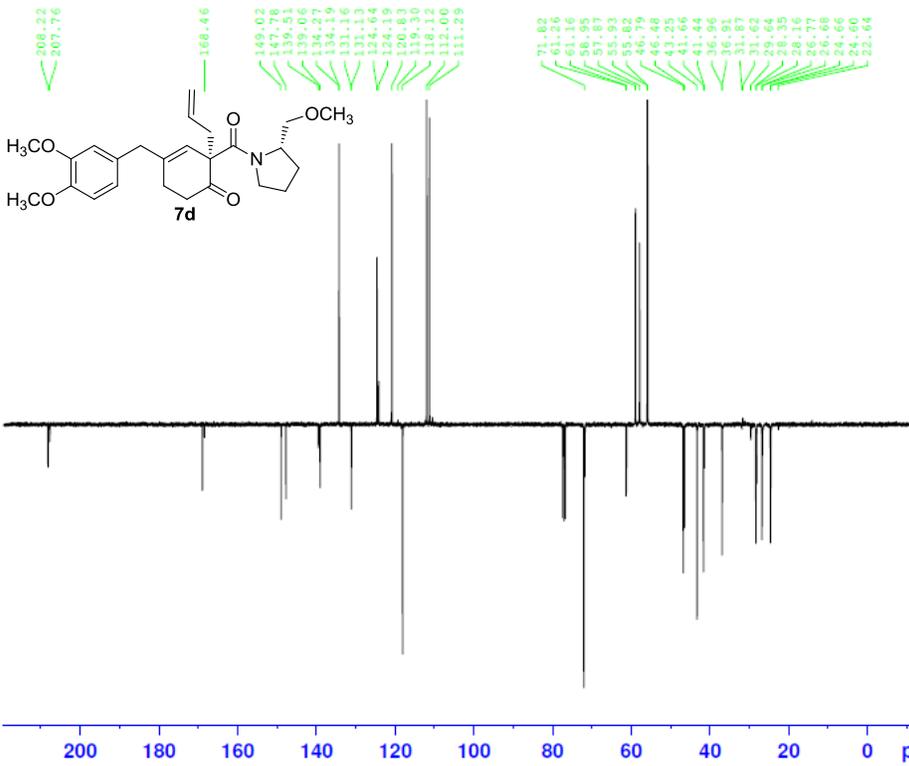
----- CHANNEL f1 -----
NUC1     13C
P1       8.00 usec
P2       16.00 usec
PL1     -2.00 dB
PL1W    56.13311005 W
SFO1    100.6282321 MHz

----- CHANNEL f2 -----
CPDPRG2  waltz16
NUC2     1H
PCPD2   80.00 usec
PL2     -2.00 dB
PL12    14.00 dB
PL2W    12.14226913 W
PL12W   0.30500001 W
SFO2    400.1514774 MHz
SI       32768
SF      100.6177980 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
  
```



```

NAME      sjb_74_157fp
EXPNO     1
PROCNO    1
Date_     20121004
Time      15.05
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         25.4
DW         60.800 usec
DE         6.50 usec
TE         301.2 K
D1         1.00000000 sec
D10        1
===== CHANNEL f1 =====
NUC1      1H
P1        9.80 usec
PL1       -4.00 dB
PL1W      19.24419975 W
SF01      400.1524711 MHz
SI        32768
SF        400.1500000 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
  
```



```

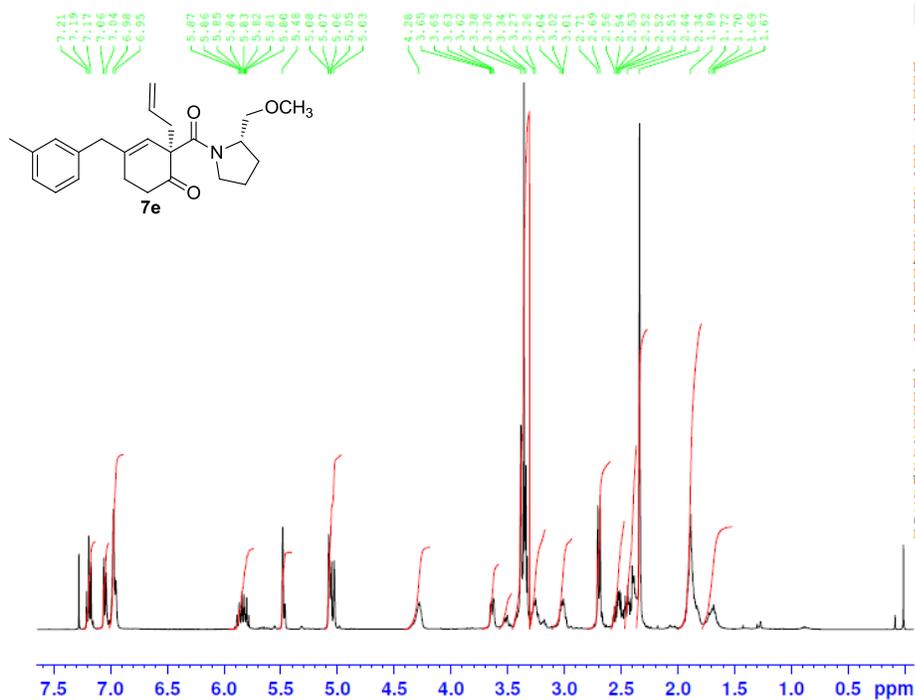
Current Data Parameters
NAME      sjb_77_121fp APT
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20130627
Time      9.00
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   jmod
ID         65536
SOLVENT   CDCl3
NS         968
DS         4
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631488 sec
RG         203
DW         20.800 usec
DE         6.50 usec
TE         301.2 K
CNST12    145.0000000
CNST11    1.0000000
D1         2.00000000 sec
D20        0.00689655 sec
TD0        1

===== CHANNEL f1 =====
NUC1      13C
P1        8.00 usec
P2        16.00 usec
PL1       -2.00 dB
PL1W      56.13311005 W
SF01      100.6278593 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       -2.00 dB
PL12      14.00 dB
PL2W      12.14226913 W
PL12W     0.30500001 W
SF02      400.1514899 MHz

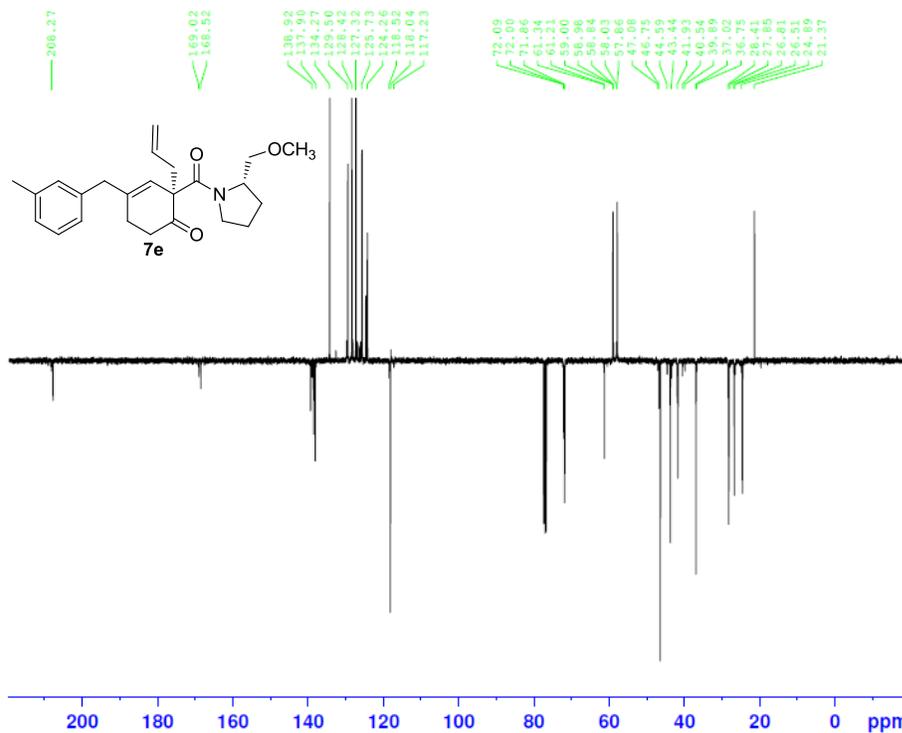
F2 - Processing parameters
SI        32768
SF        100.6177980 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```



```

NAME      sjb_77_144fp2
EXPNO     1
PROCNO    1
Date_     20130715
Time      7.44
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH       8223.685 Hz
FIDRES    0.125483 Hz
AQ         3.9846387 sec
RG         50.8
DW         60.800 usec
DE         6.50 usec
TE         301.2 K
D1         1.00000000 sec
TD0        1

----- CHANNEL f1 -----
NUC1       1H
P1         12.50 usec
PL1        -2.00 dB
PL1W       12.14226913 W
SFO1       400.1524711 MHz
SI         32768
SF         400.1500000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```



```

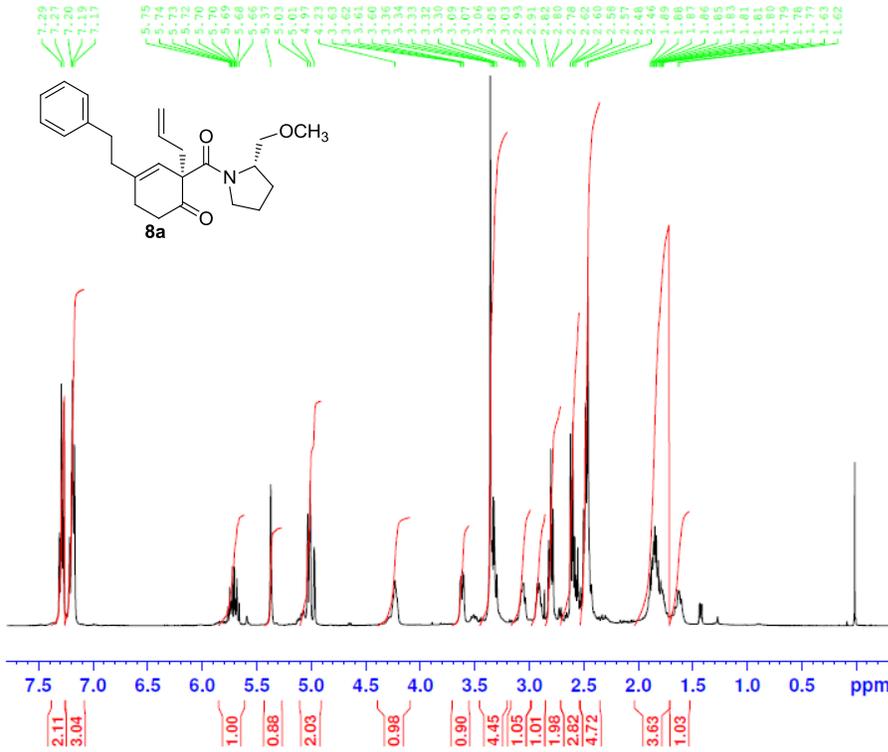
Current Data Parameters
NAME      sjb_77_144fp APT
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20130715
Time      8.48
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   jmod
TD         65536
SOLVENT   CDCl3
NS         1024
DS         4
SWH       24038.461 Hz
FIDRES    0.366798 Hz
AQ         1.3631488 sec
RG         203
DW         20.800 usec
DE         6.50 usec
TE         301.2 K
CNST2     145.000000
CNST11    1.000000
D1         2.00000000 sec
D20        0.00689655 sec
TD0        1

----- CHANNEL f1 -----
NUC1       13C
P1         8.00 usec
P2         16.00 usec
PL1        -2.00 dB
PL1W       56.13311005 W
SFO1       100.6278593 MHz

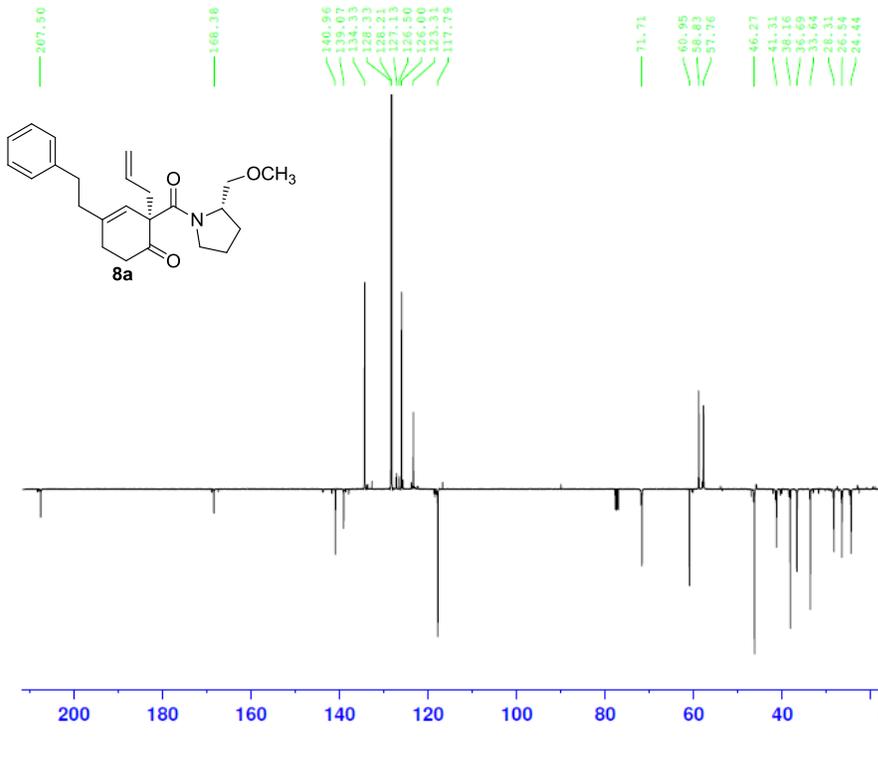
----- CHANNEL F2 -----
CPDPRG[2] waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        -2.00 dB
PL12       14.00 dB
PL2W       12.14226913 W
PL12W      0.30500001 W
SFO2       400.1514776 MHz

F2 - Processing parameters
SI         32768
SF         100.6177980 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```



NAME s_jb_74_205fp take 2
 EXPNO 1
 PROCNO 1
 Date_ 20130801
 Time 10.40
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 50.8
 DW 60.800 usec
 DE 6.50 usec
 TE 301.2 K
 D1 1.0000000 sec
 TDO 1

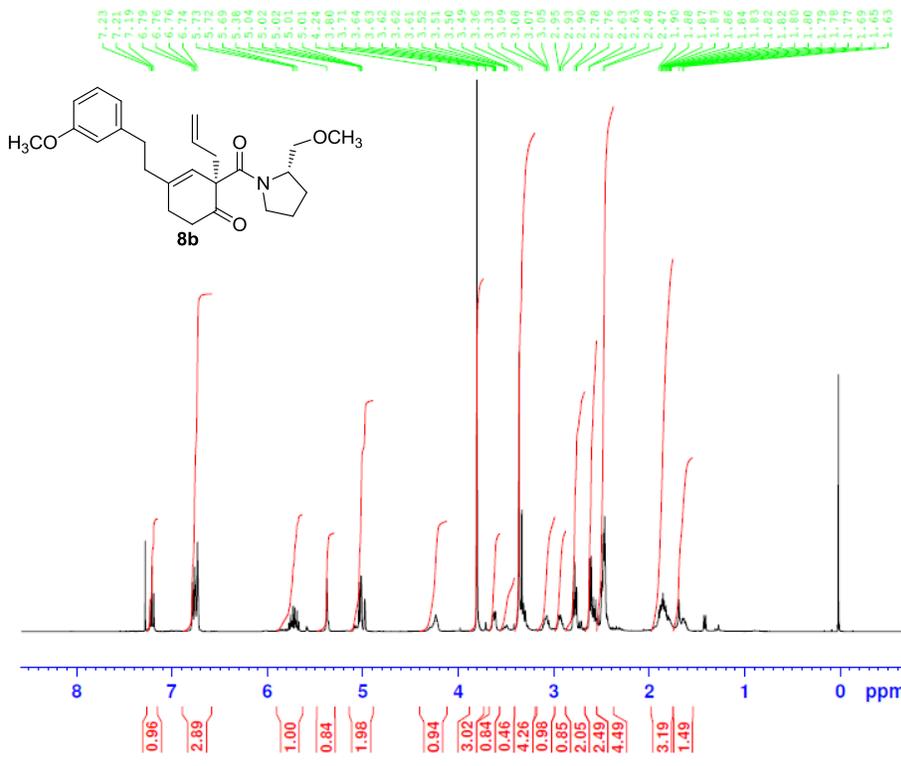
----- CHANNEL f1 -----
 NUC1 1H
 P1 12.50 usec
 PL1 -2.00 dB
 PL1W 12.14226913 W
 SFO1 400.1524711 MHz
 SI 32768
 SF 400.1500000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



NAME s_jb_74_205fp 13CAPT
 EXPNO 1
 PROCNO 1
 Date_ 20121114
 Time 16.58
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG jmod
 TD 65536
 SOLVENT CDC13
 NS 1056
 DS 4
 SWH 20380.436 Hz
 FIDRES 0.310981 Hz
 AQ 1.6078665 sec
 RG 203
 DW 24.533 usec
 DE 6.50 usec
 TE 301.2 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 2.0000000 sec
 D20 0.00689655 sec
 TDO 1

----- CHANNEL f1 -----
 NUC1 13C
 P1 8.00 usec
 P2 16.00 usec
 PL1 -2.00 dB
 PL1W 56.13311005 W
 SFO1 100.6288927 MHz

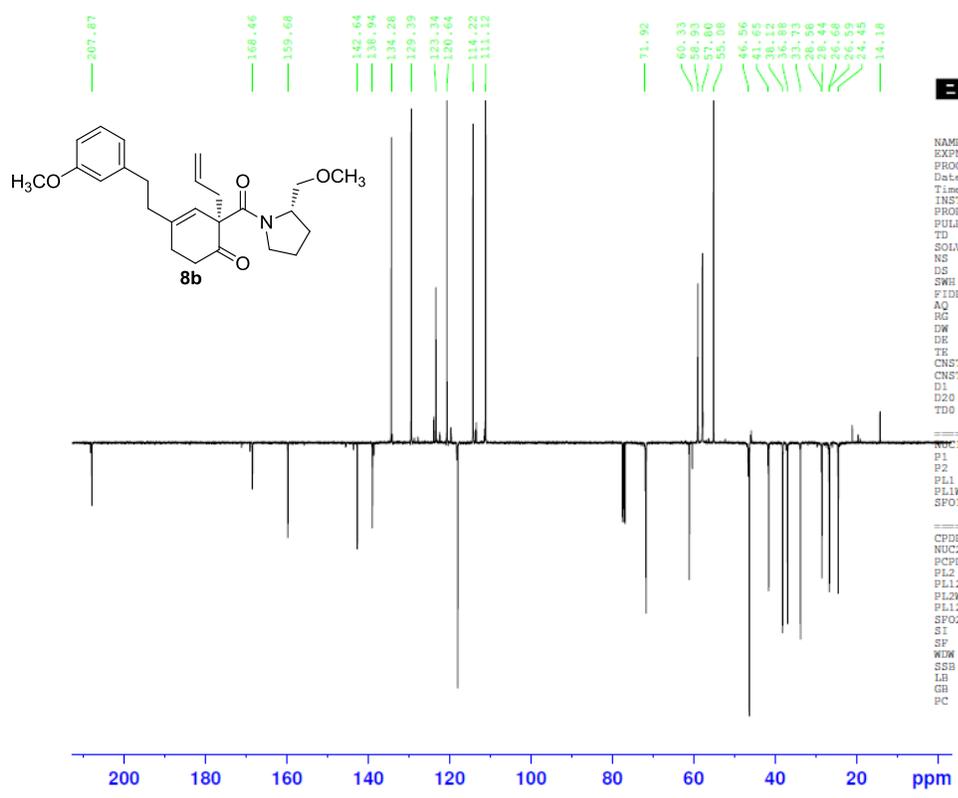
----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -2.00 dB
 PL12 14.00 dB
 PL2W 12.14226913 W
 PL12W 0.30500001 W
 SFO2 400.1514317 MHz
 SI 32768
 SF 100.6177980 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



```

NAME      sjb_77_087fp take 2
EXPNO    1
PROCNO   1
Date_    20130801
Time     10.33
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        2
SWH       8223.685 Hz
FIDRES   0.125483 Hz
AQ        3.9846387 sec
RG        144
DW        60.800 usec
DE        6.50 usec
TE        301.2 K
D1        1.0000000 sec
TDO       1

----- CHANNEL f1 -----
NUC1      1H
P1        12.50 usec
PL1       -2.00 dB
PL1W      12.14226913 W
SFO1      400.1524711 MHz
SI        32768
SF        400.1500000 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
  
```

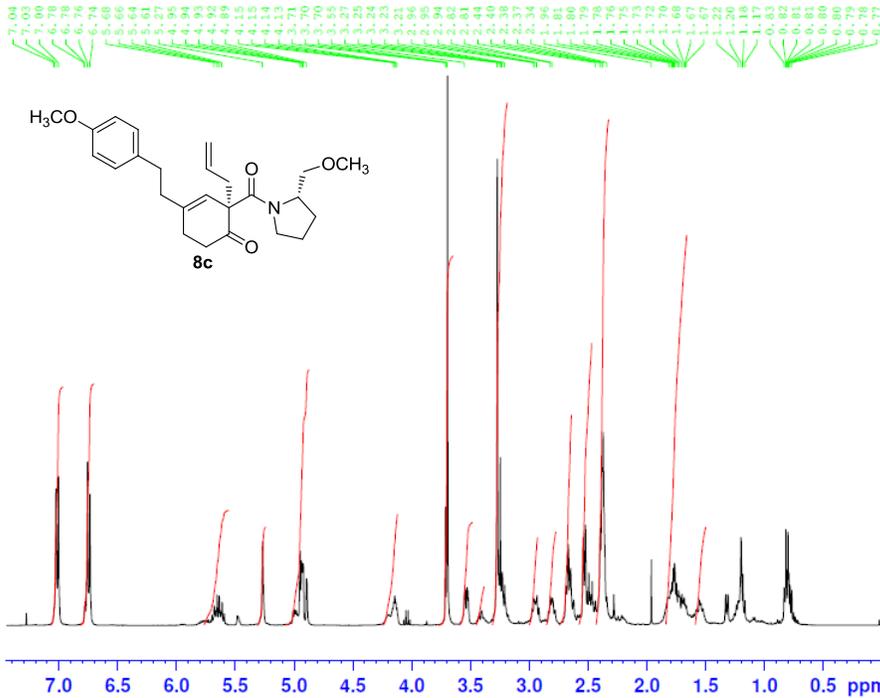


```

NAME      sjb_77_087 Fr9-12 13CAPT
EXPNO    1
PROCNO   1
Date_    20130509
Time     10.40
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  gmod
TD        65536
SOLVENT  CDCl3
NS        1024
DS        4
SWH       21739.131 Hz
FIDRES   0.331713 Hz
AQ        1.5073780 sec
RG        203
DW        23.000 usec
DE        6.50 usec
TE        296.2 K
CNST2    145.0000000
CNST11   1.0000000
D1        2.0000000 sec
D20      0.00689655 sec
TDO       1

===== CHANNEL f1 =====
NUC1      13C
P1        8.00 usec
P2        16.00 usec
PL1       -2.00 dB
PL1W      56.13311005 W
SFO1      100.6283257 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      1H
PCPD2    80.00 usec
PL2       -2.00 dB
PL12     14.00 dB
PL2W     12.14226913 W
PL12W    0.30500001 W
SFO2     400.1514553 MHz
SI        32768
SF        100.6177980 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```

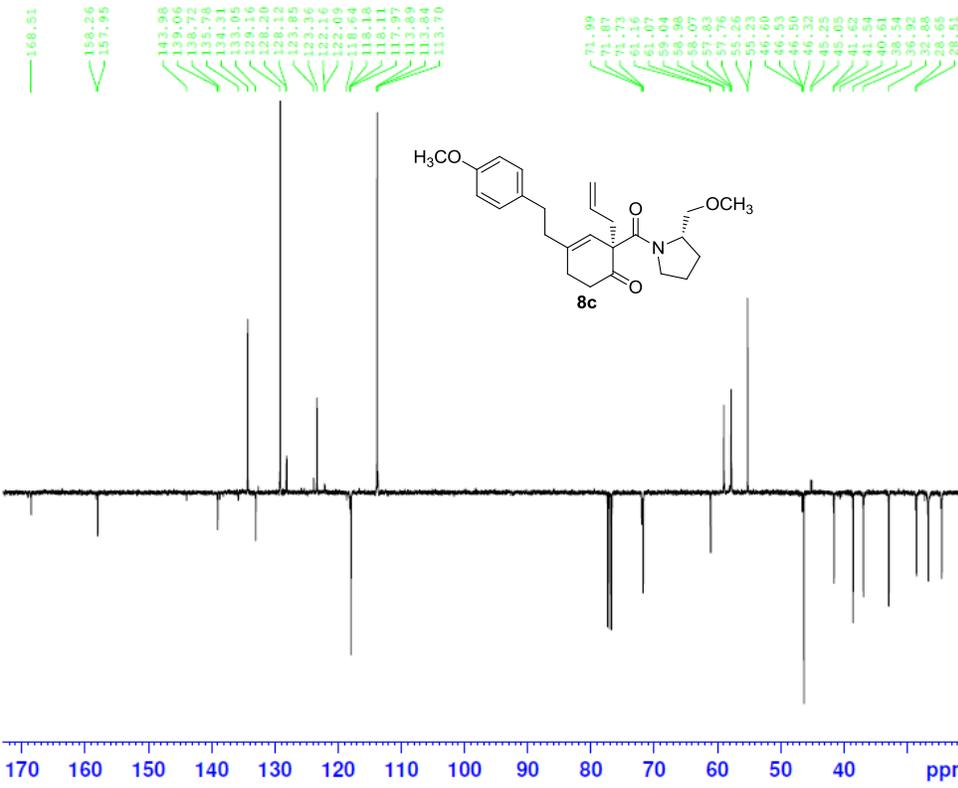


```

NAME ra_67_156column
EXPNO 1
PROCNO 1
Date_ 20120727
Time 14.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 16
DW 60.800 usec
DE 6.50 usec
TE 295.2 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.50 usec
PL1 -2.00 dB
PL1W 12.14226913 W
SFO1 400.1524711 MHz
SI 32768
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

```



```

Current Data Parameters
NAME ajb_77_223fpAPT
EXPNO 1
PROCNO 1

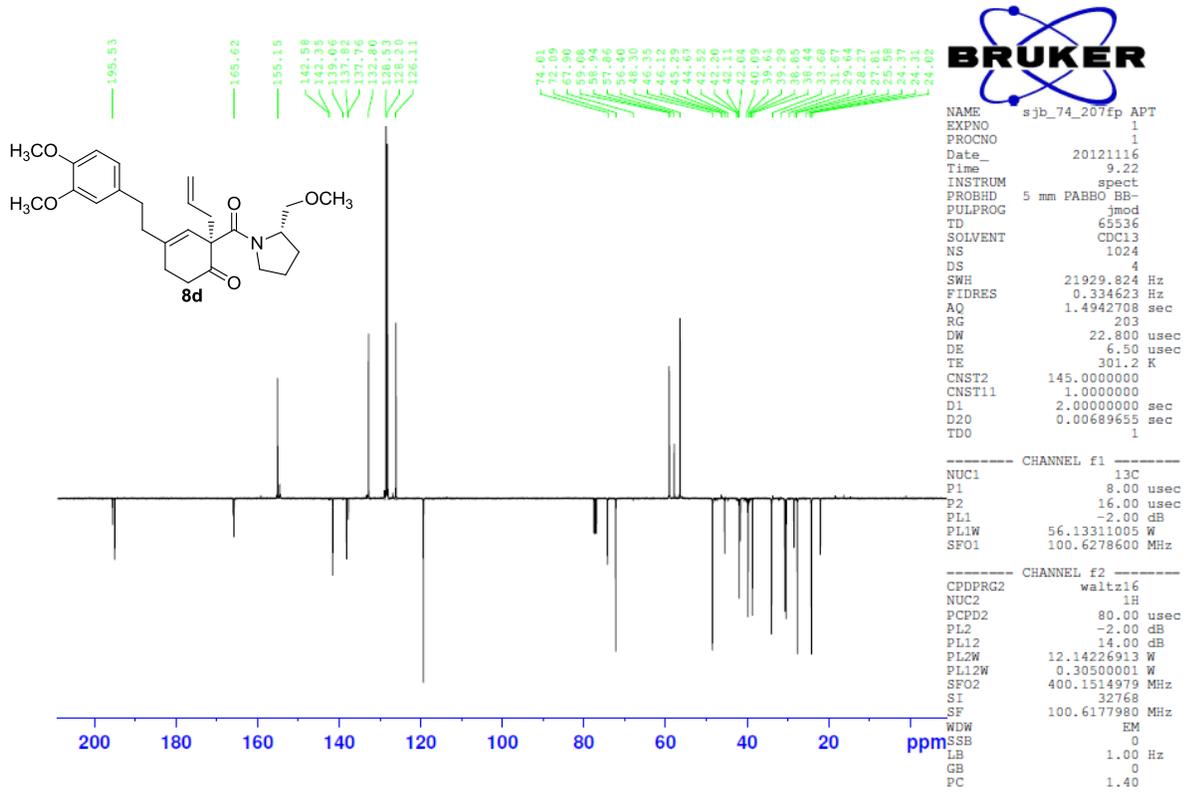
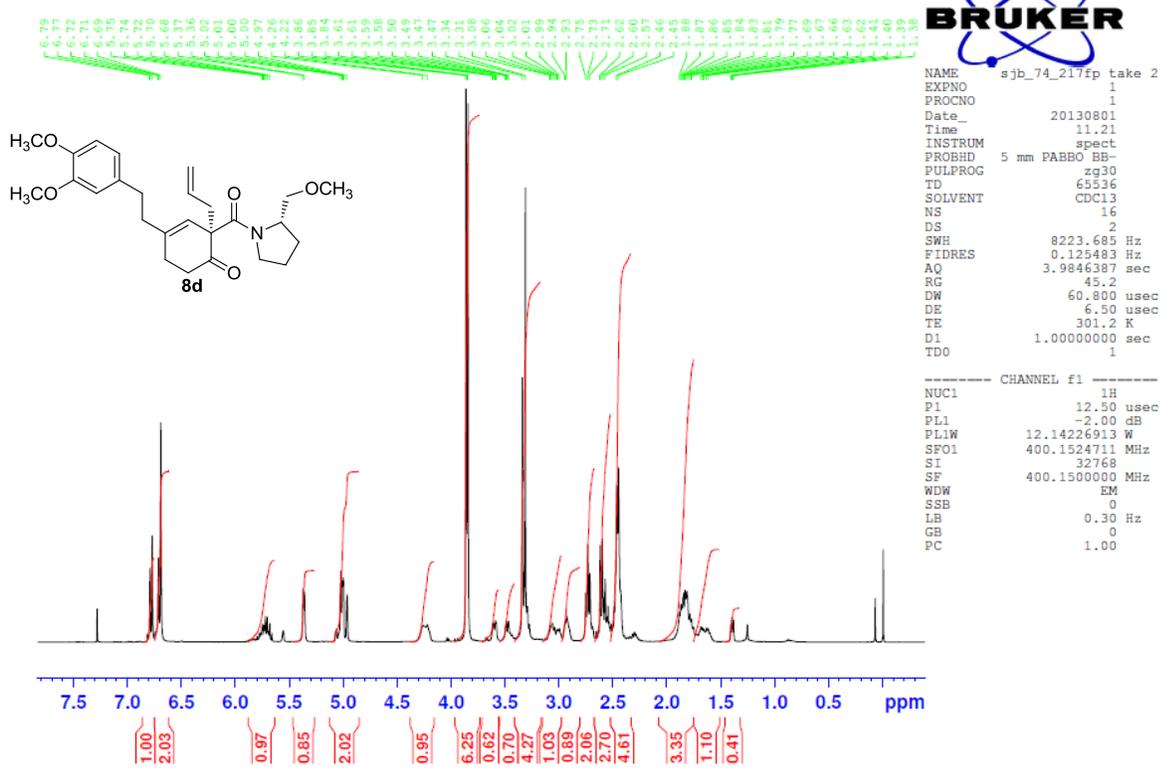
F2 - Acquisition Parameters
Date_ 20130923
Time 16.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TDO 1

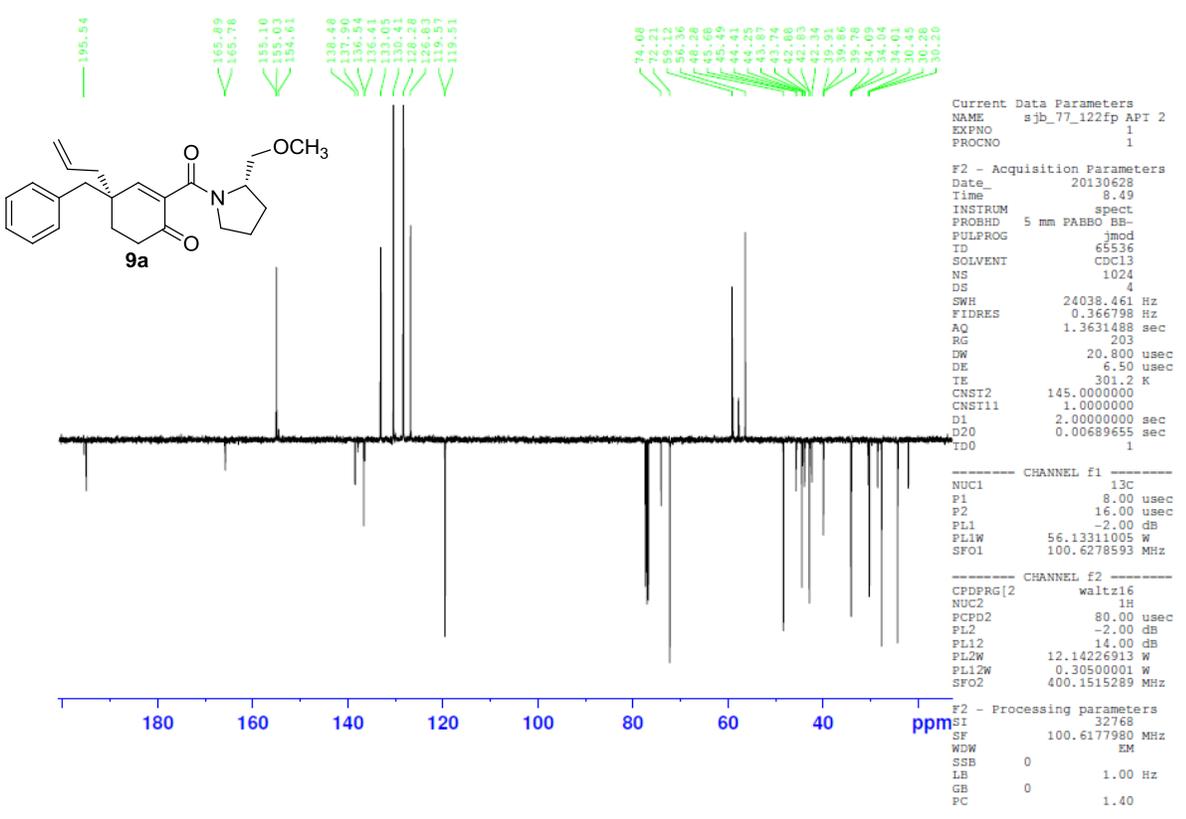
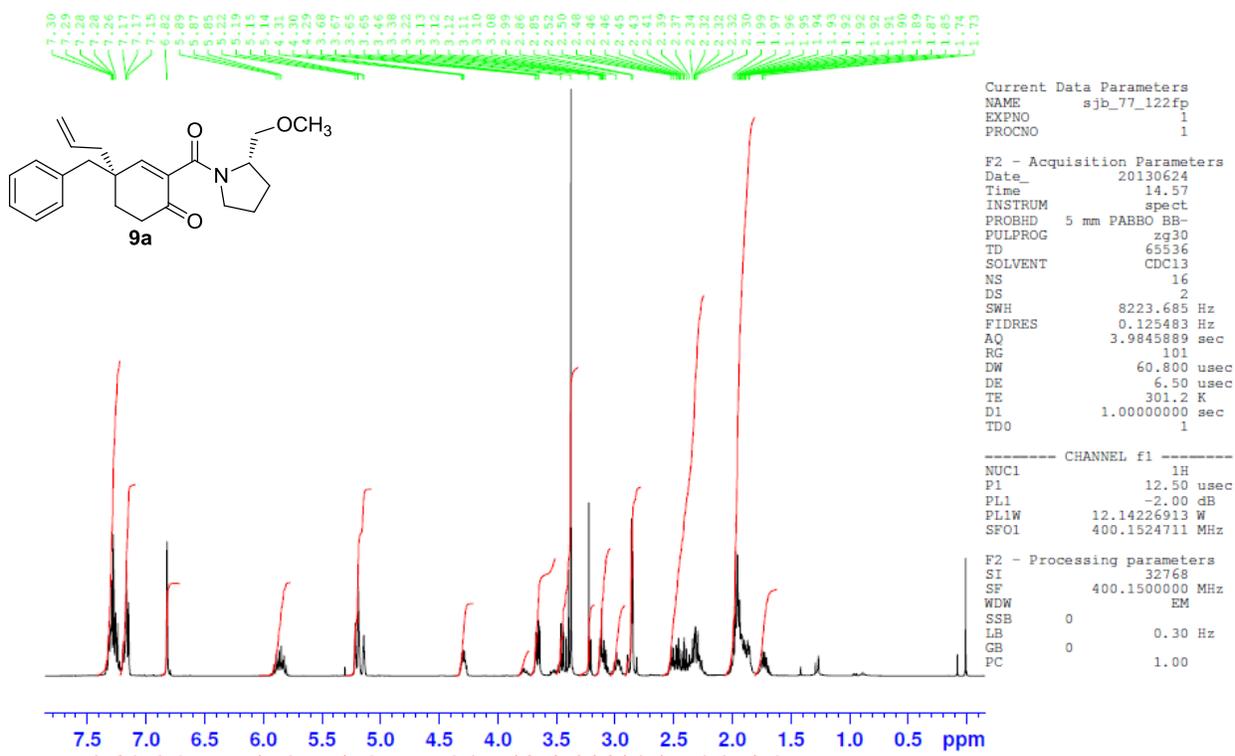
===== CHANNEL f1 =====
NUC1 13C
P1 8.00 usec
P2 16.00 usec
PL1 -2.00 dB
PL1W 56.13311005 W
SFO1 100.6278593 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 75.00 usec
PL2 -2.00 dB
PL12 13.39 dB
PL2W 12.14226913 W
PL12W 0.35099408 W
SFO2 400.1515369 MHz

F2 - Processing parameters
SI 32768
SF 100.6177980 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

```





Area Percent Report

Data Path : C:\msdchem\1\DATA\
Data File : sjb_77_122fp.D
Acq On : 24 Jun 2013 12:57
Operator : JMB
Sample : sjb_77_122fp
Misc :
ALS Vial : 85 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

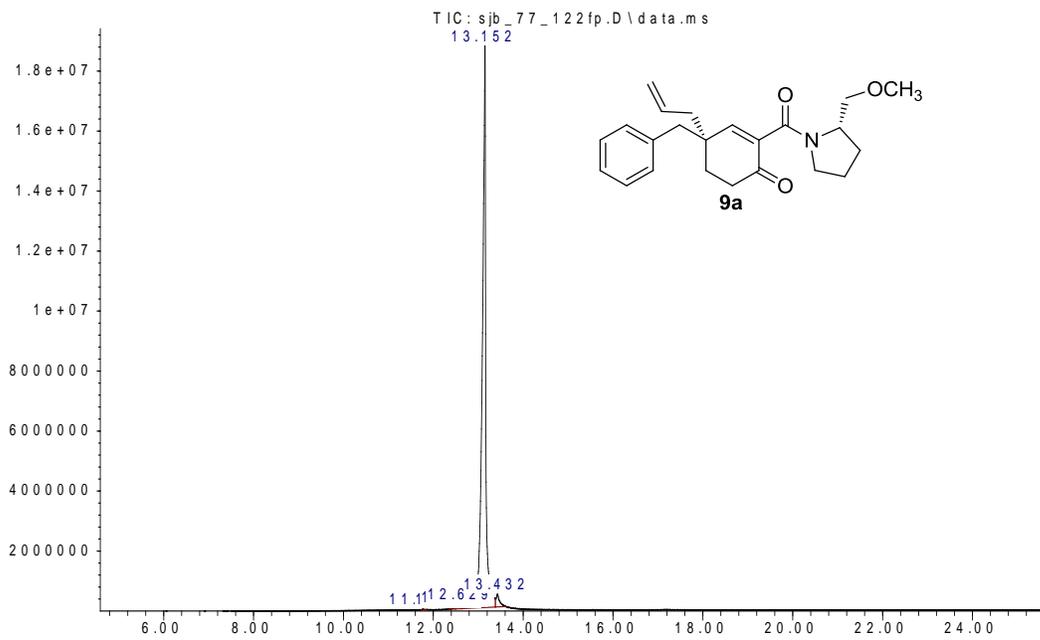
Method : C:\msdchem\1\5973N\PRECISION.M
Title :

Signal : TIC: sjb_77_122fp.D\data.ms

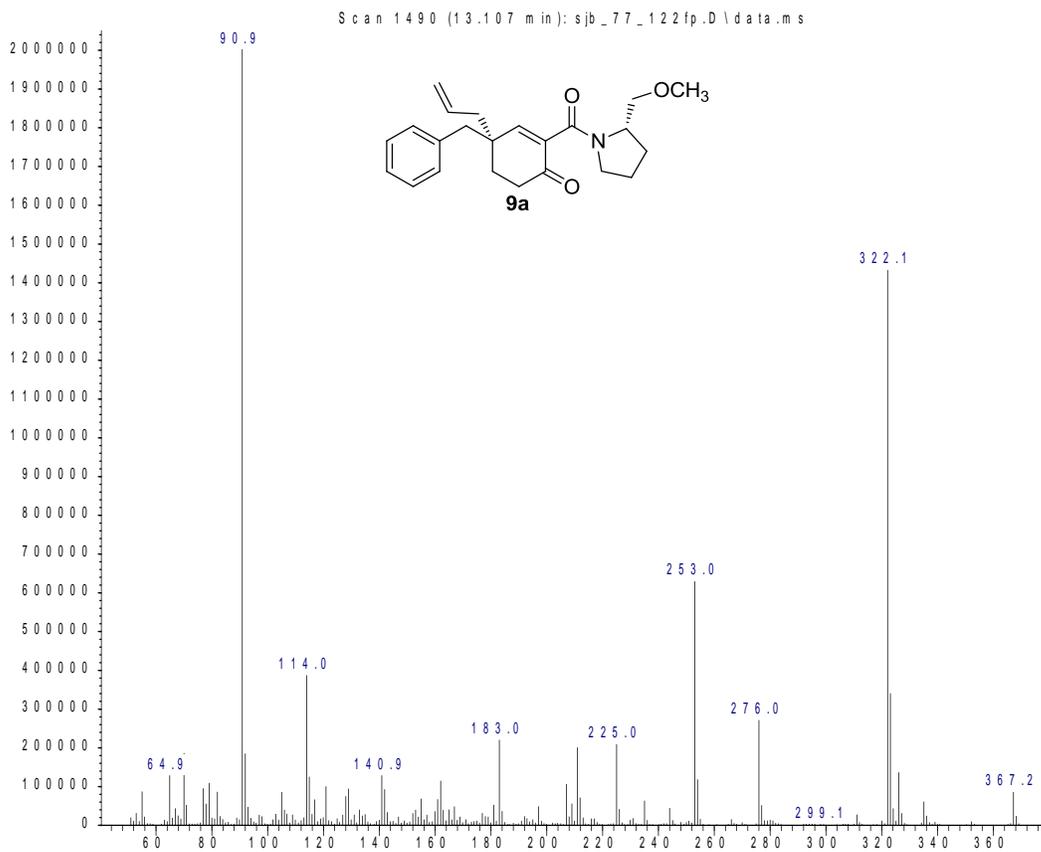
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	11.771	1250	1257	1267	PV 5	23815	610660	0.06%	0.054%
2	12.360	1356	1360	1361	VV 3	14161	144431	0.01%	0.013%
3	12.492	1361	1383	1384	VV 3	45976	1701208	0.16%	0.152%
4	12.629	1384	1407	1408	VV 3	140358	7593364	0.70%	0.677%
5	13.152	1408	1498	1538	VV	19156629	1087462192	100.00%	96.982%
6	13.432	1538	1547	1577	VV 5	422396	23796626	2.19%	2.122%

Sum of corrected areas: 1121308482

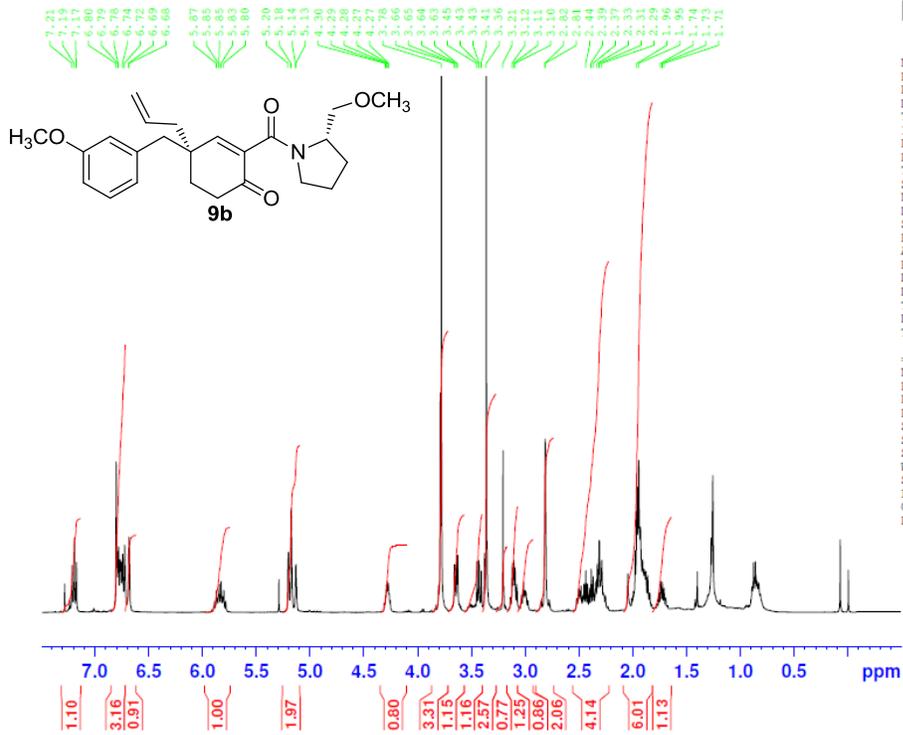
Abundance



Time-->
Abundance



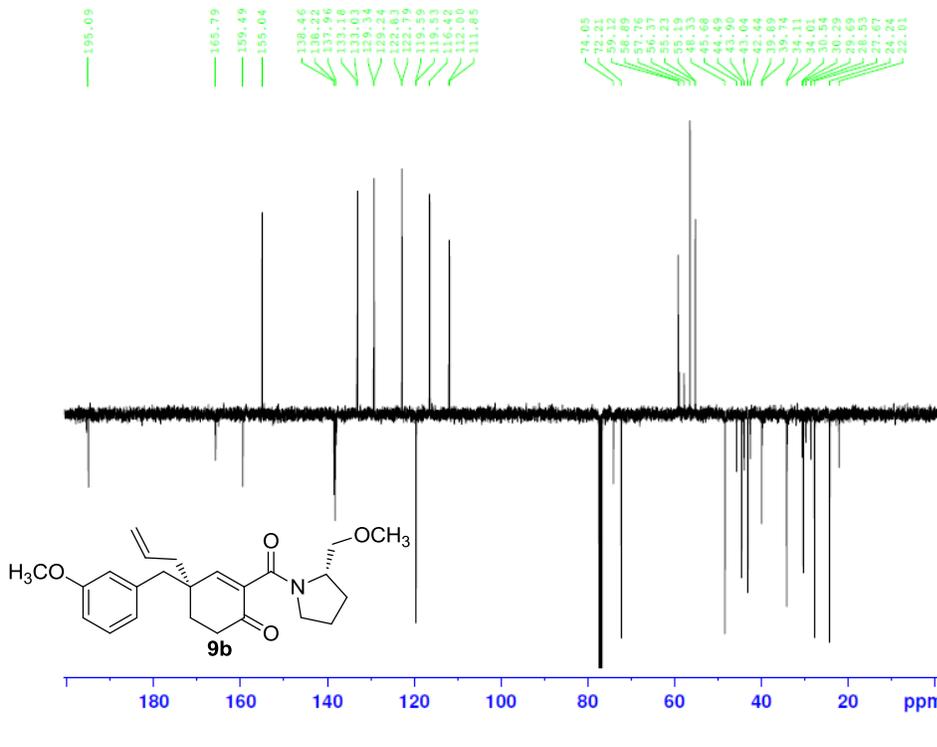
m/z-->



```

NAME      sjb_74_158fp
EXPNO     1
PROCNO    1
Date_     20121005
Time      17.11
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH       8223.685 Hz
FIDRES    0.125483 Hz
AQ         3.9846387 sec
RG         40.3
DW         60.800 usec
DE         6.50 usec
TE         301.2 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1      1H
P1        9.80 usec
PL1       -4.00 dB
PL1W      19.24419975 W
SFO1      400.1524711 MHz
SI         32768
SF         400.1500000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```



```

NAME      sjb_74_158fp APT
EXPNO     1
PROCNO    1
Date_     20121026
Time      9.14
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   jmod
TD         65536
SOLVENT   CDCl3
NS         1024
DS         4
SWH       20380.436 Hz
FIDRES    0.310981 Hz
AQ         1.6078665 sec
RG         203
DW         24.533 usec
DE         6.50 usec
TE         301.2 K
CNST2     145.0000000
CNST11    1.0000000
D1         2.0000000 sec
D20        0.00689655 sec
TD0        1

===== CHANNEL f1 =====
NUC1      13C
P1         9.00 usec
P2         18.00 usec
PL1         0.00 dB
PL1W       35.41759872 W
SFO1       100.6277865 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2     80.00 usec
PL2       -3.80 dB
PL12      13.80 dB
PL2W      18.37806102 W
PL12W     0.31937420 W
SFO2      400.1514268 MHz
SI         32768
SF         100.6177980 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```

Area Percent Report

Data Path : C:\msdchem\1\DATA\
Data File : sjb_74_158fp.D
Acq On : 5 Oct 2012 16:36
Operator : sjb
Sample : sjb_74_158fp
Misc :
ALS Vial : 100 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\msdchem\1\METHODS\JMB2.m
Title :

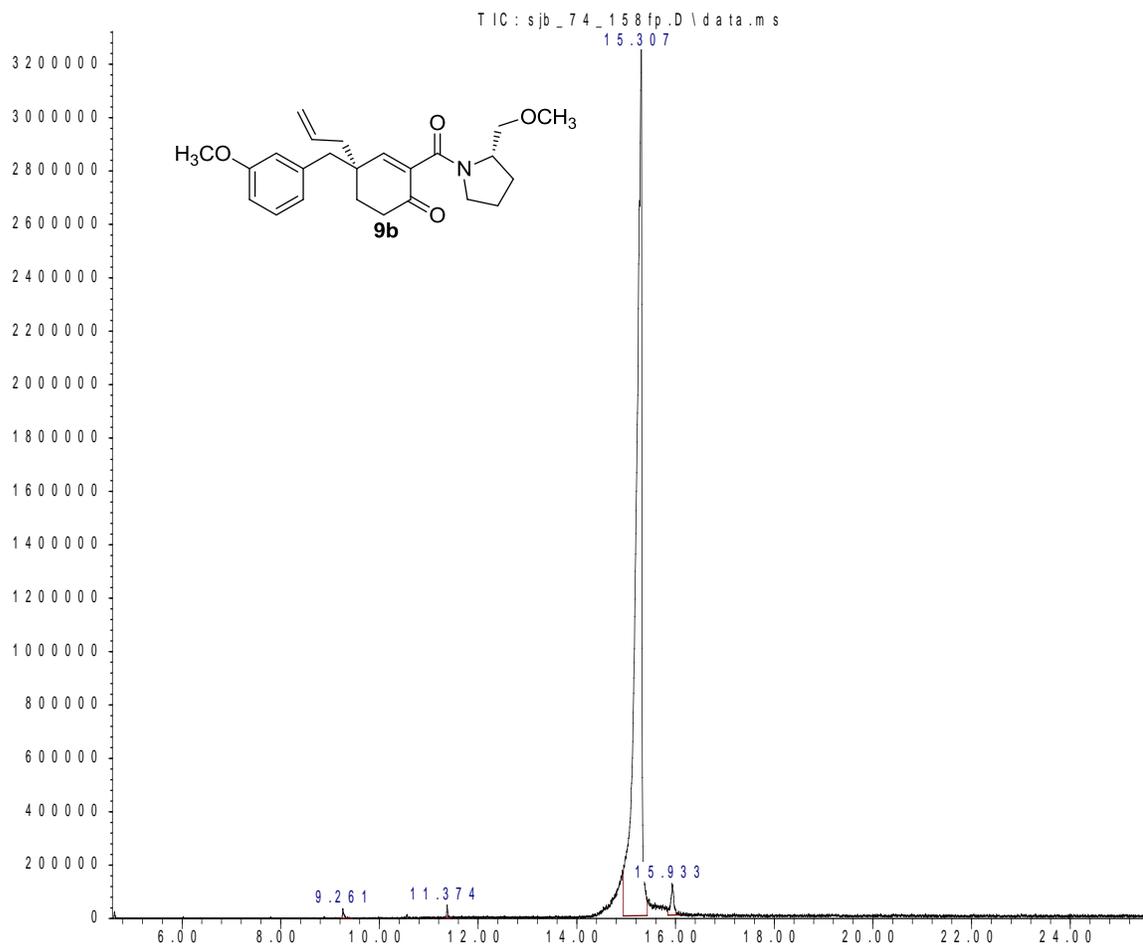
Signal : TIC: sjb_74_158fp.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	9.261	812	818	847	BV 3	35666	858934	0.33%	0.319%
2	11.374	1180	1187	1198	BV 2	45443	646248	0.25%	0.240%
3	15.307	1810	1875	1896	VV 2	3303222	262174800	100.00%	97.492%
4	15.933	1969	1984	2012	VV 7	115524	5238394	2.00%	1.948%

Sum of corrected areas: 268918376

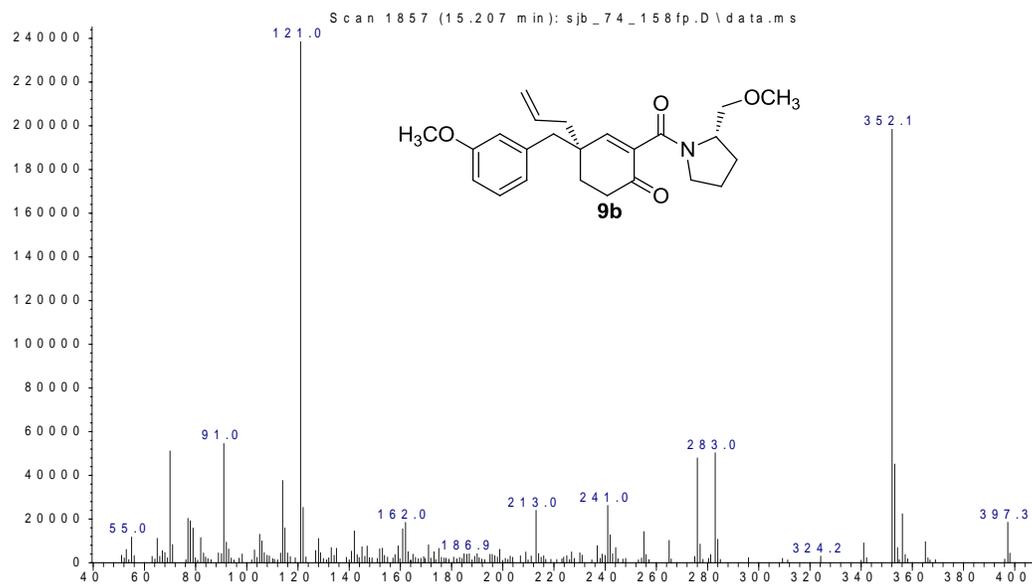
JMB2.m Mon Nov 12 09:53:58 2012

Abundance



Time-->

Abundance



m/z-->

Area Percent Report

Data Path : C:\msdchem\1\DATA\
Data File : sjb_74_015fp.D
Acq On : 5 Jun 2012 12:00
Operator : sjb
Sample : sjb_74_015fp
Misc :
ALS Vial : 30 Sample Multiplier: 1

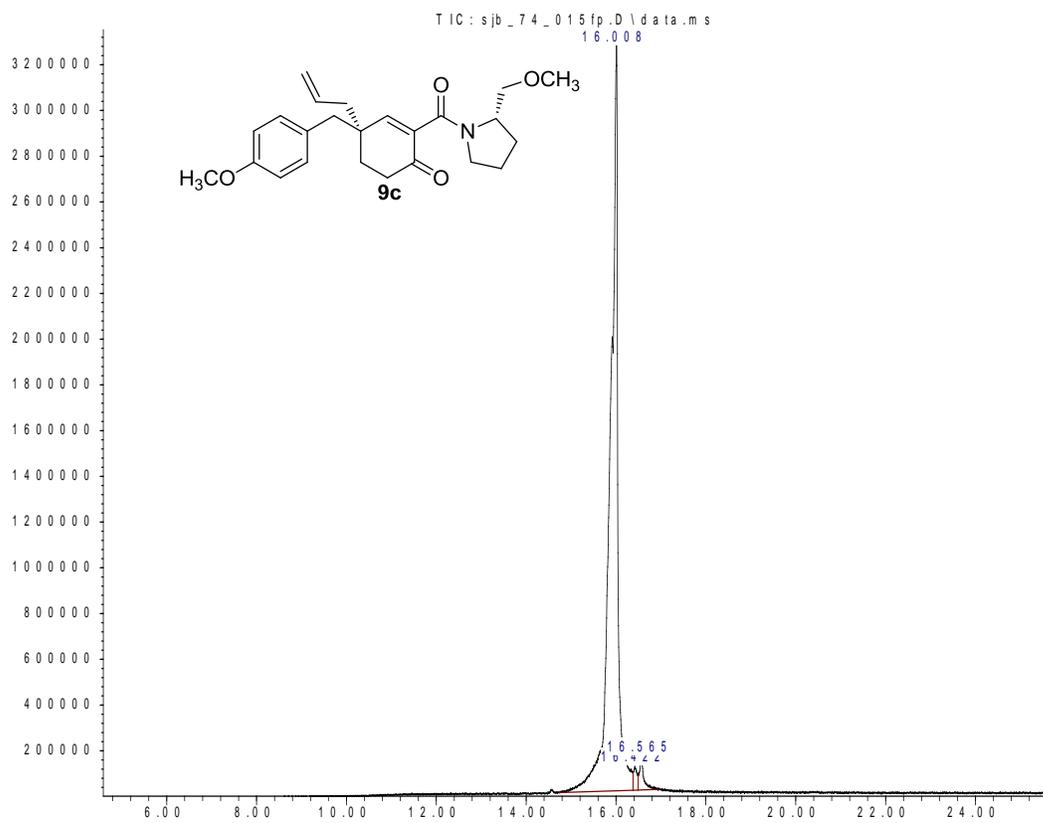
Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\msdchem\1\METHODS\JMB2.m
Title :

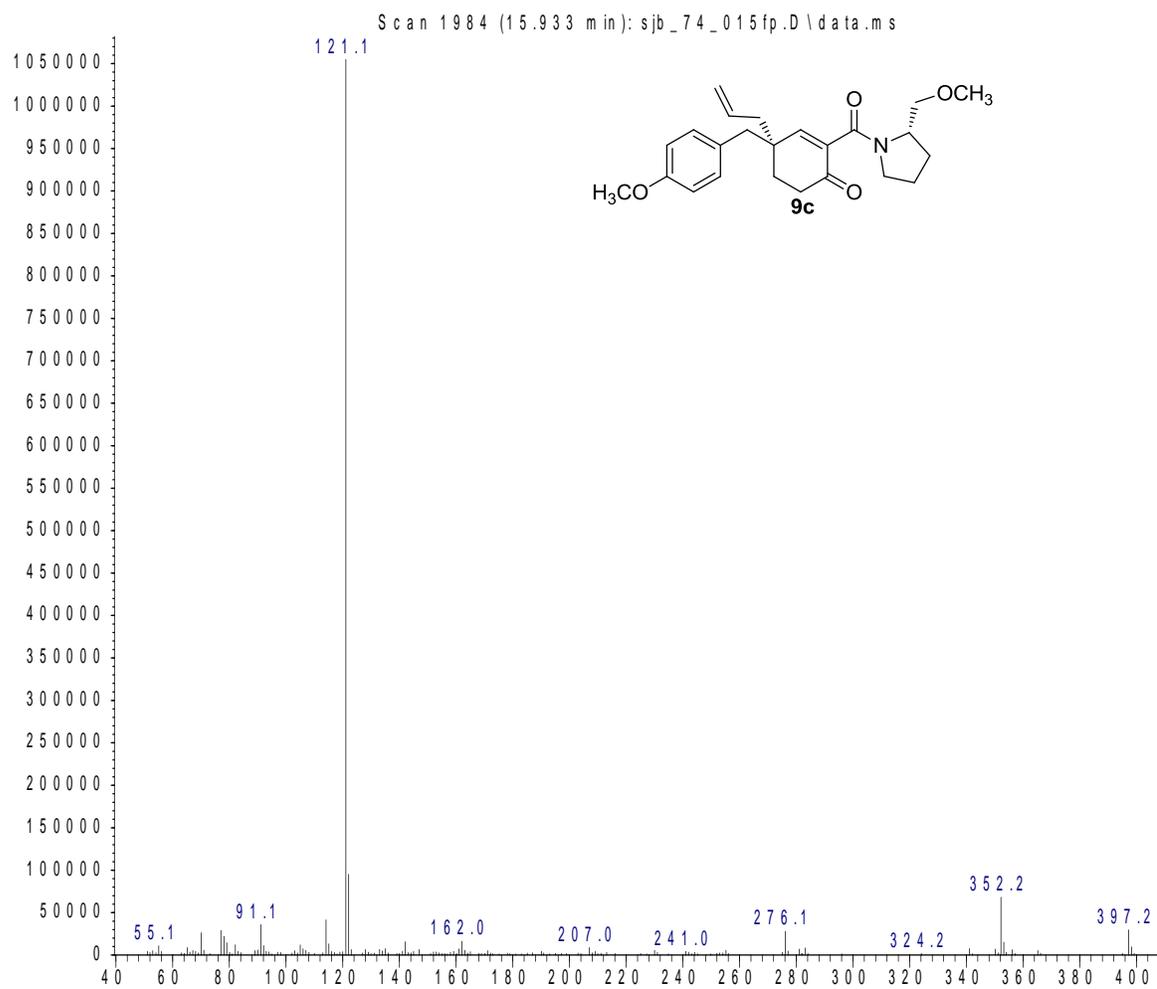
Signal : TIC: sjb_74_015fp.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	16.008	1774	1997	2062	BV	3280944	386191361	100.00%	96.065%
2	16.422	2062	2069	2081	VV 8	101564	5645103	1.46%	1.404%
3	16.565	2081	2094	2159	VB 7	146121	10172724	2.63%	2.530%

Abundance



Abundance



m/z-->

Area Percent Report

Data Path : C:\msdchem\1\DATA\
Data File : sjb_74_159fp.D
Acq On : 5 Oct 2012 11:58
Operator : th
Sample : sjb_74_159fp
Misc :
ALS Vial : 15 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

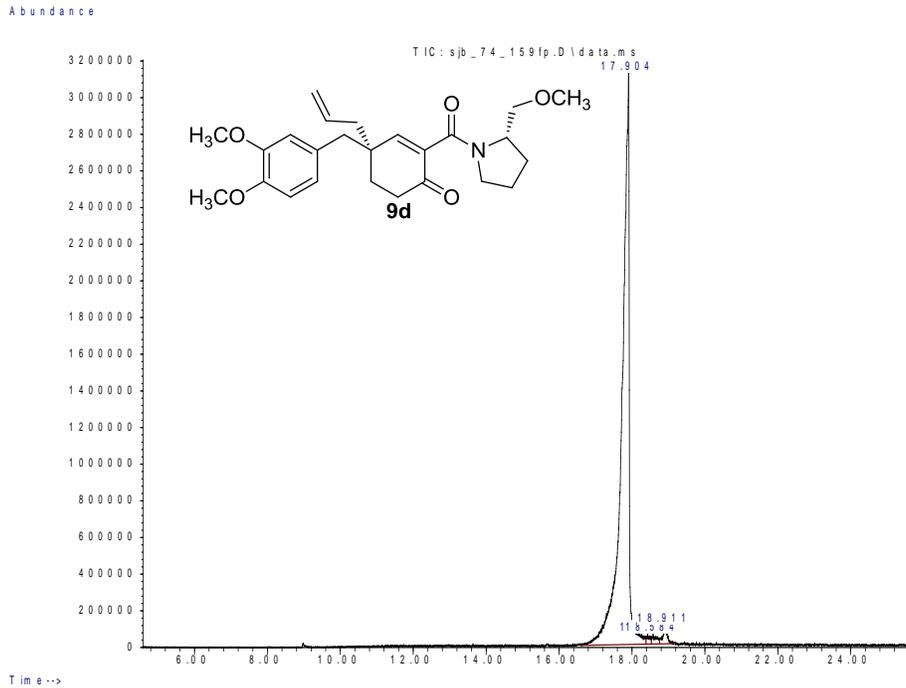
Method : C:\msdchem\1\METHODS\JMB2.m
Title :

Signal : TIC: sjb_74_159fp.D\data.ms

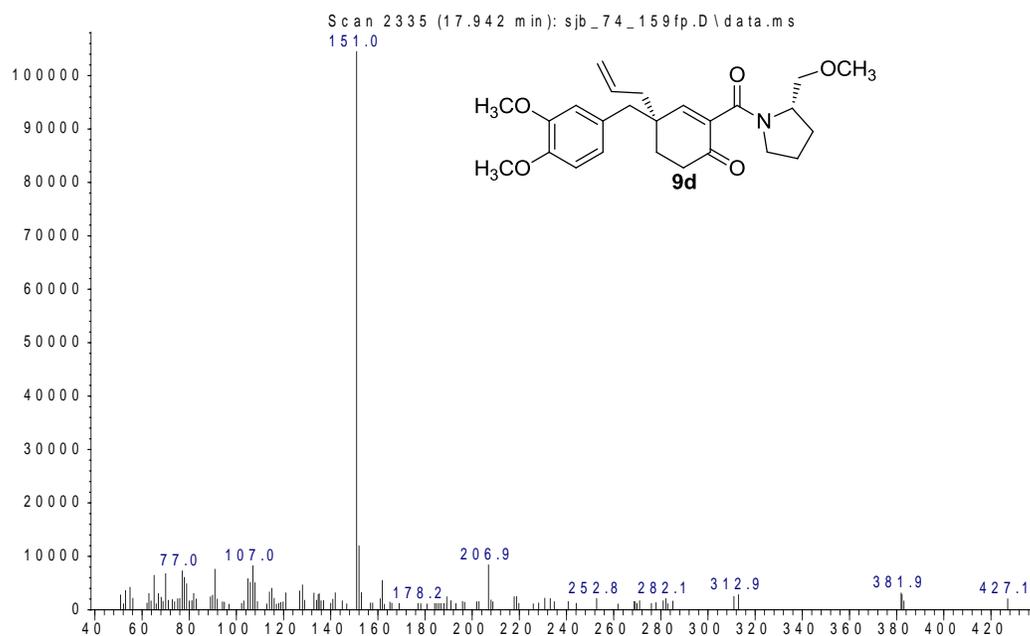
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	17.904	2102	2328	2412	VV	3198330	432129853	100.00%	96.605%
2	18.426	2412	2419	2438	VV	47849	3098396	0.72%	0.693%
3	18.584	2438	2447	2477	VV	50012	4349060	1.01%	0.972%
4	18.911	2477	2504	2546	VV	88199	7737920	1.79%	1.730%

Sum of corrected areas: 447315230

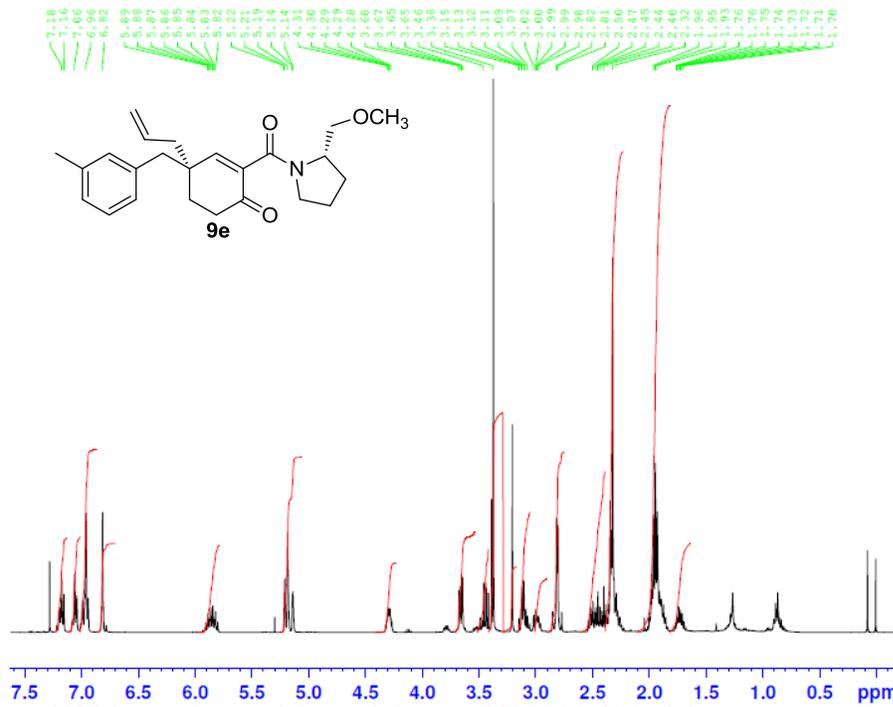
JMB2.m Mon Nov 12 09:56:25 2012



Abundance



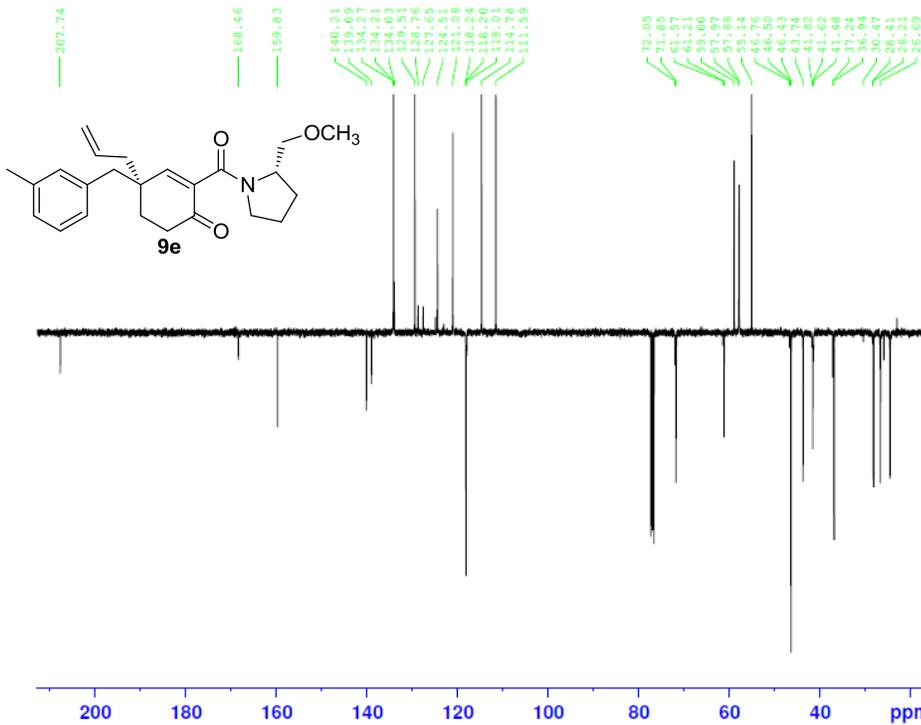
m/z-->



```

NAME      s_jb_77_146fp
EXPNO     1
PROCNO    1
Date_     20130711
Time      12.06
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         45.2
DW         60.800 usec
DE         6.50 usec
TE         301.2 K
D1         1.0000000 sec
TD0        1

----- CHANNEL f1 -----
NUC1      1H
P1        12.50 usec
PL1       -2.00 dB
PL1W      12.14226913 W
SFO1      400.1524711 MHz
SI         32768
SF         400.1500000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```



```

Current Data Parameters
NAME      s_jb_77_145fp APT
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20130717
Time      8.49
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   jmod
TD         65536
SOLVENT   CDCl3
NS         1024
DS         4
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631488 sec
RG         203
DW         20.800 usec
DE         6.50 usec
TE         301.2 K
CNST2     145.0000000
CNST11    1.0000000
D1         2.0000000 sec
D20        0.00689655 sec
TD0        1

----- CHANNEL f1 -----
NUC1      13C
P1         8.00 usec
P2        16.00 usec
PL1       -2.00 dB
PL1W      56.13311005 W
SFO1      100.6278593 MHz

----- CHANNEL f2 -----
CPDPRG[2] waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       -2.00 dB
PL12      14.00 dB
PL2W      12.14226913 W
PL12W     0.30500001 W
SFO2      400.1515122 MHz

F2 - Processing parameters
SI         32768
SF         100.6177980 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```

Data Path : C:\msdchem\1\DATA\
Data File : sjb_77_146fp.D
Acq On : 11 Jul 2013 12:27
Operator : sjb
Sample : sjb_77_146fp
Misc :
ALS Vial : 90 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

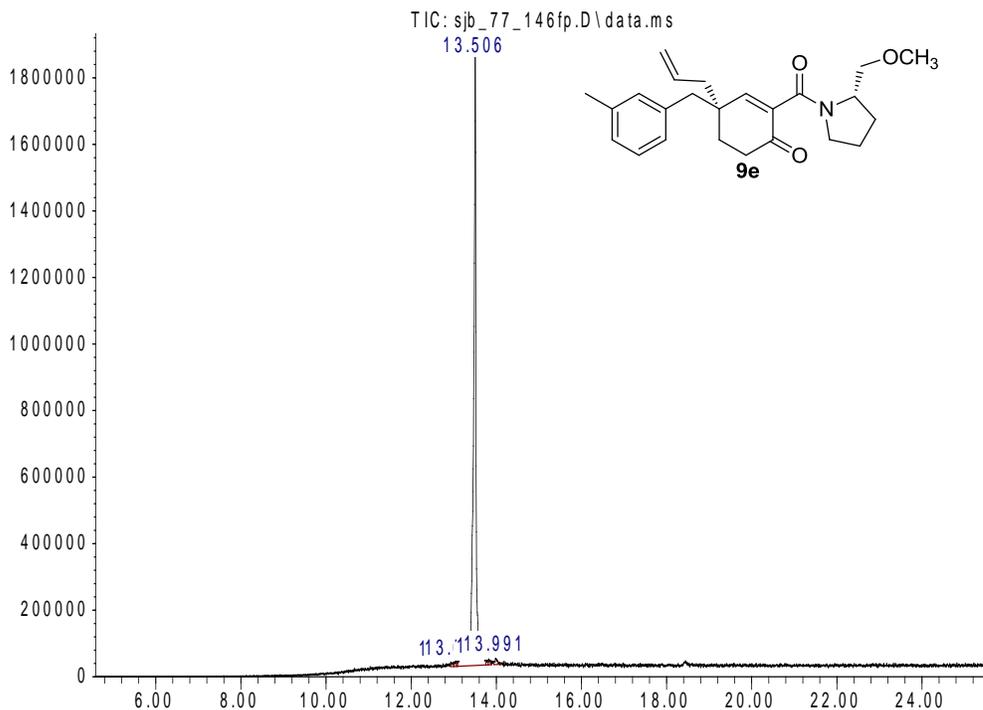
Method : C:\msdchem\1\METHODS\ckr3.m
Title :

Signal : TIC: sjb_77_146fp.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	12.936	1458	1460	1472	VV 7	10298	425396	0.53%	0.517%
2	13.053	1472	1481	1482	VV 7	13961	373159	0.47%	0.453%
3	13.076	1482	1485	1487	VV 4	15082	220310	0.28%	0.268%
4	13.506	1487	1560	1603	VV 2	1898200	79627101	100.00%	96.706%
5	13.762	1603	1604	1613	VV 8	19689	462440	0.58%	0.562%
6	13.823	1613	1615	1623	VV 4	16918	402255	0.51%	0.489%
7	13.991	1635	1645	1661	VV 10	21265	829057	1.04%	1.007%

Sum of corrected areas: 82339717 ckr3.m Wed Mar 19 14:38:32 2014

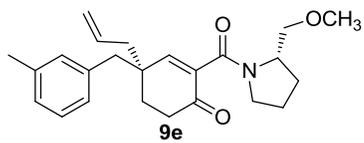
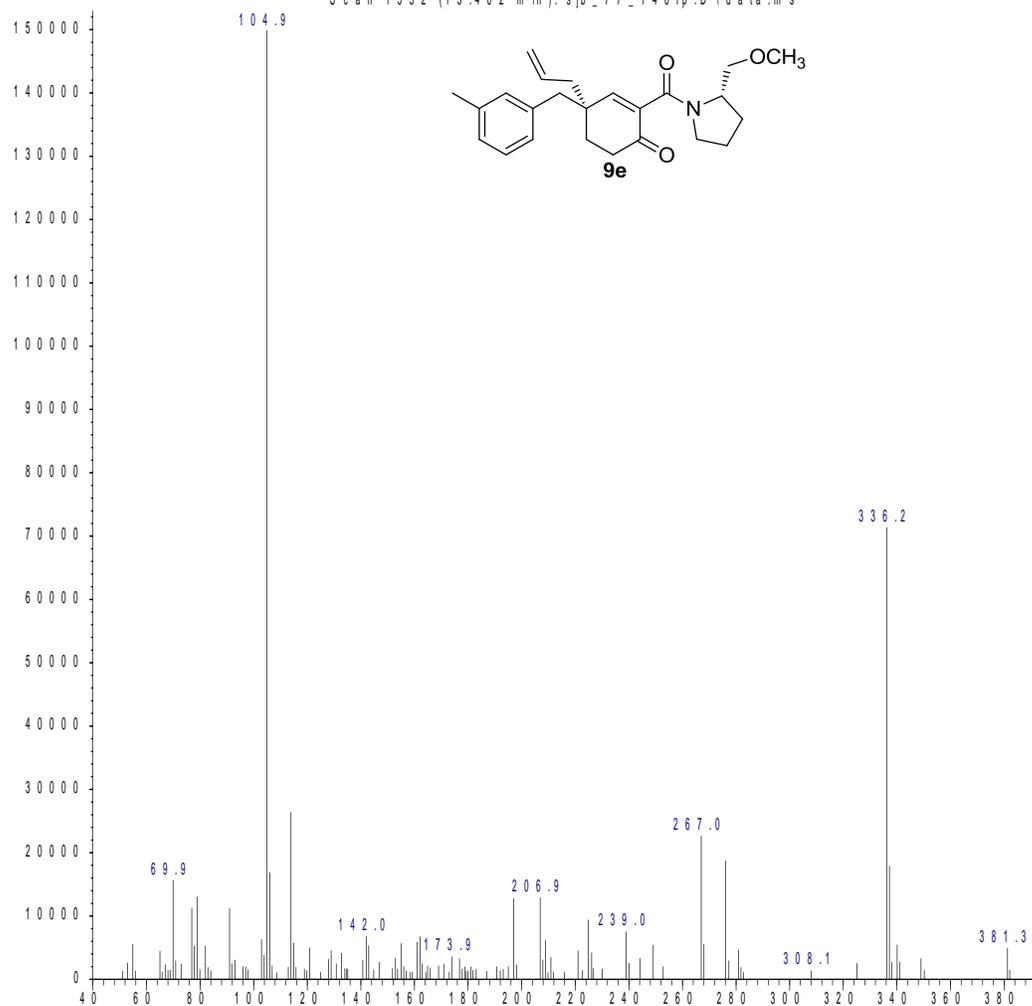
Abundance



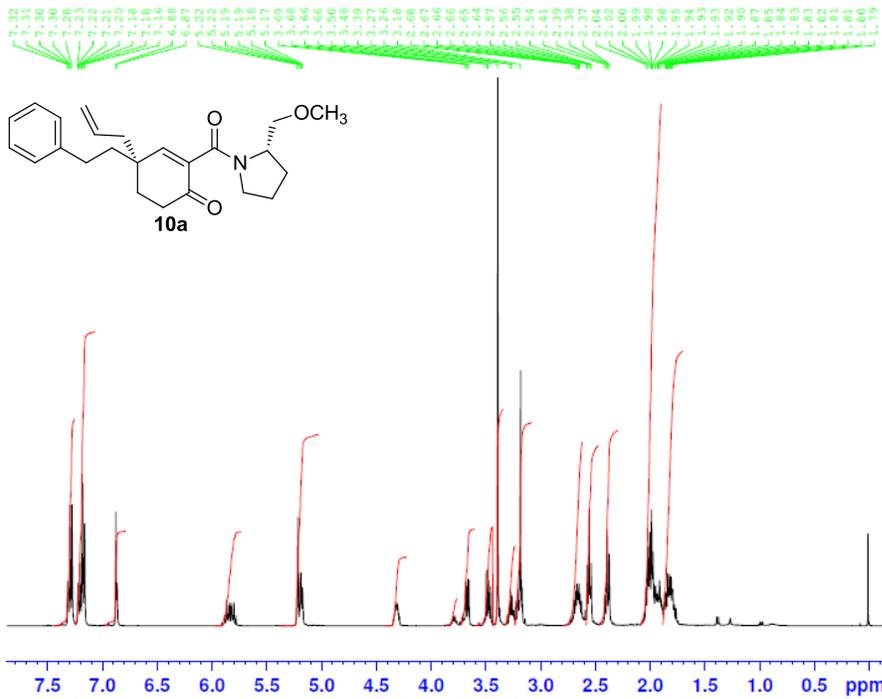
Time-->

Abundance

Scan 1552 (13.462 min): sjb_77_146fp.D\data.ms



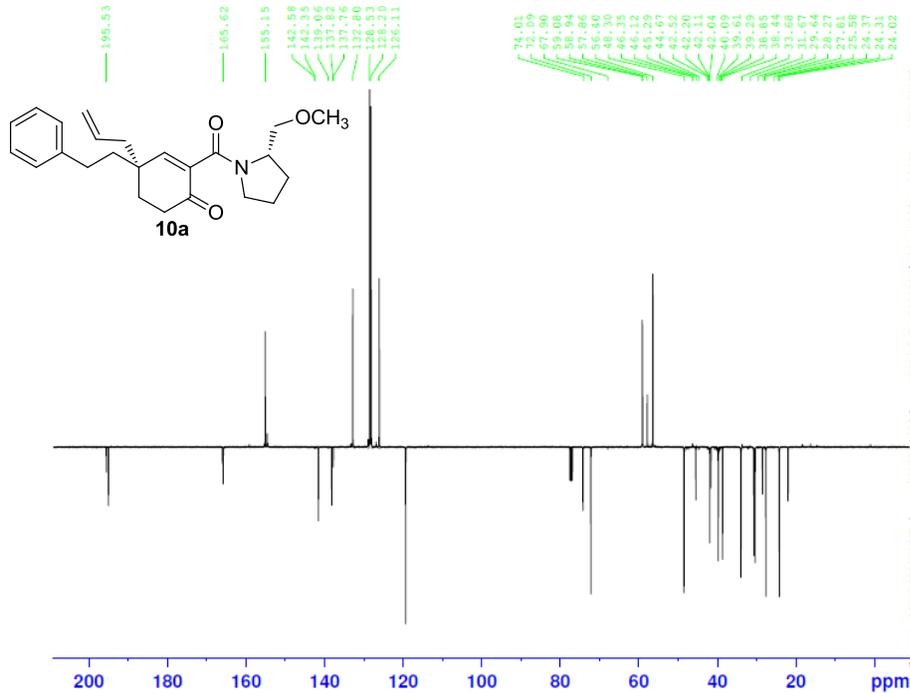
m/z-->



BRUKER

NAME sjb_72_132fp take 2
 EXPNO 1
 PROCNO 1
 Date_ 20130801
 Time 11.14
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 50.8
 DW 60.800 usec
 DE 6.50 usec
 TE 301.2 K
 D1 1.00000000 sec
 TDO 1

----- CHANNEL f1 -----
 NUC1 1H
 P1 12.50 usec
 PL1 -2.00 dB
 PL1W 12.14226913 W
 SFO1 400.1524711 MHz
 SI 32768
 SF 400.1500000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



BRUKER

NAME sjb_74_207fp APT
 EXPNO 1
 PROCNO 1
 Date_ 20121116
 Time 9.22
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG jmod
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 21929.824 Hz
 FIDRES 0.334523 Hz
 AQ 1.4942708 sec
 RG 203
 DW 22.800 usec
 DE 6.50 usec
 TE 301.2 K
 CNST2 145.000000
 CNST11 1.000000
 D1 2.00000000 sec
 D20 0.00689655 sec
 TDO 1

----- CHANNEL f1 -----
 NUC1 13C
 P1 8.00 usec
 P2 16.00 usec
 PL1 -2.00 dB
 PL1W 56.13311005 W
 SFO1 100.6278600 MHz

----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -2.00 dB
 PL12 14.00 dB
 PLW 12.14226913 W
 PL12W 0.30500001 W
 SFO2 400.1514979 MHz
 SI 32768
 SF 100.6177980 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Area Percent Report

Data Path : C:\msdchem\1\DATA\
Data File : sjb_74_207fp.D
Acq On : 15 Nov 2012 17:02
Operator : sjb
Sample : sjb_74_207fp
Misc :
ALS Vial : 5 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\msdchem\1\METHODS\JMB2.m
Title :

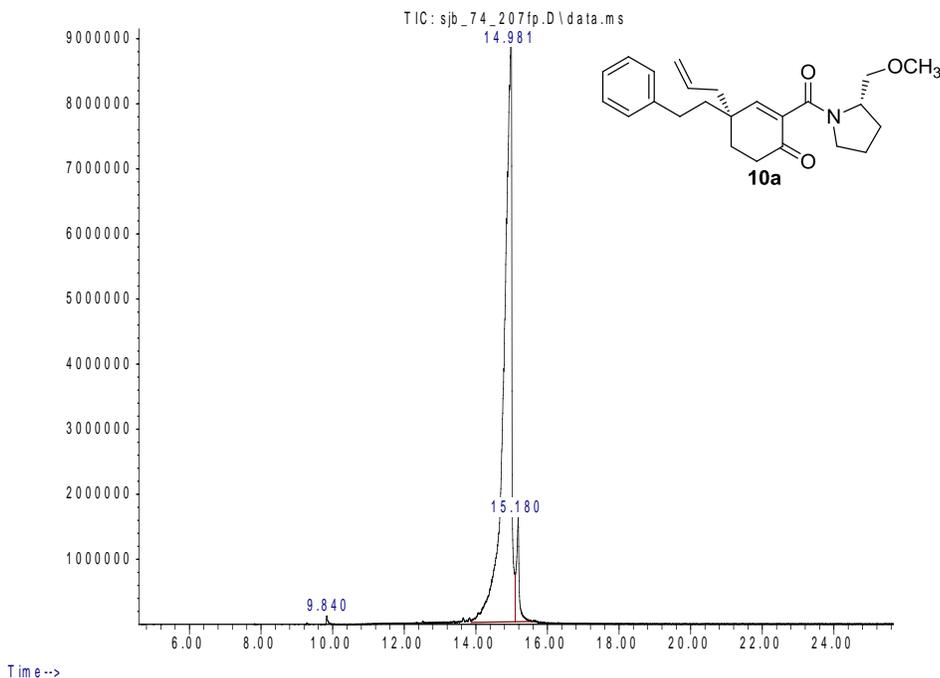
Signal : TIC: sjb_74_207fp.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	9.840	911	919	950	BB 3	122085	3829247	0.28%	0.261%
2	14.981	1623	1817	1838	VV 4	9115287	1373275457	100.00%	93.615%
3	15.180	1838	1852	1921	VV 2	1569203	89832411	6.54%	6.124%

Sum of corrected areas: 1466937115

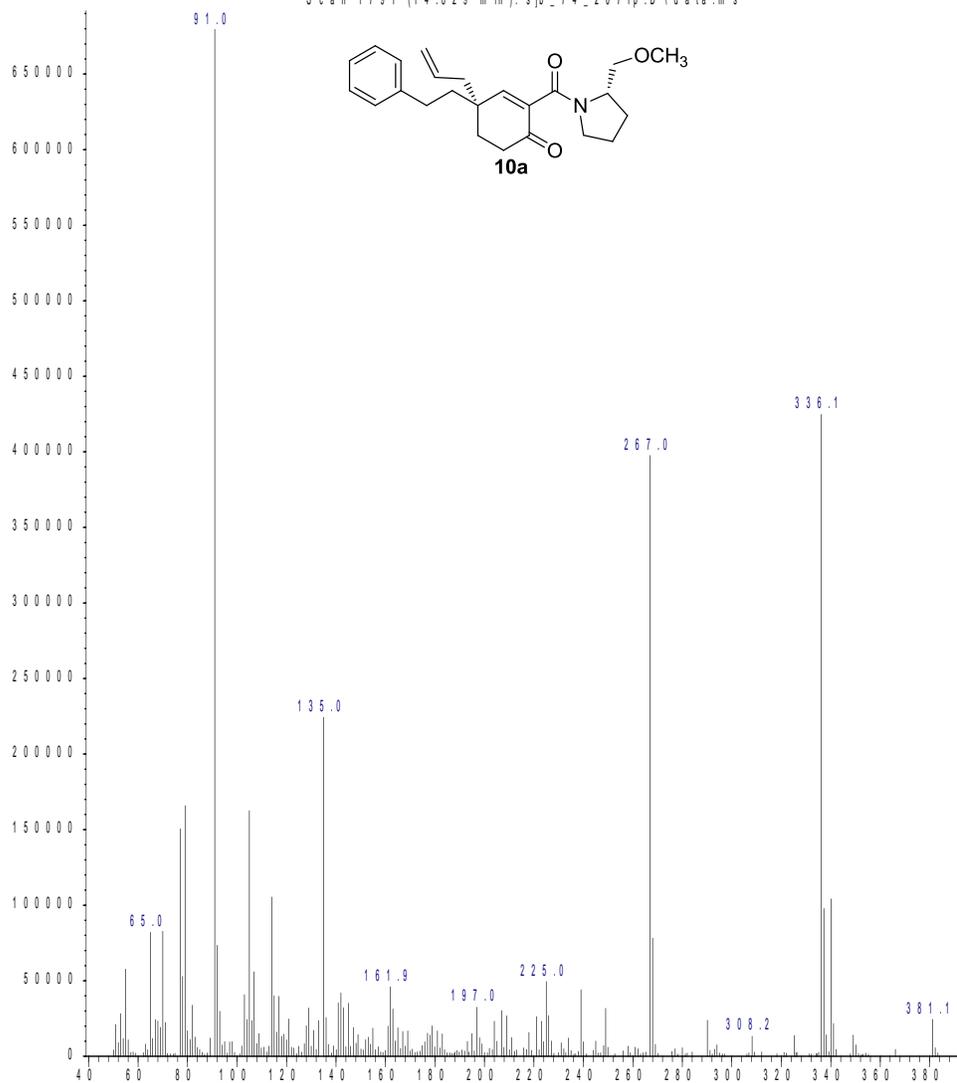
JMB2.m Fri Nov 16 09:07:41 2012

Abundance



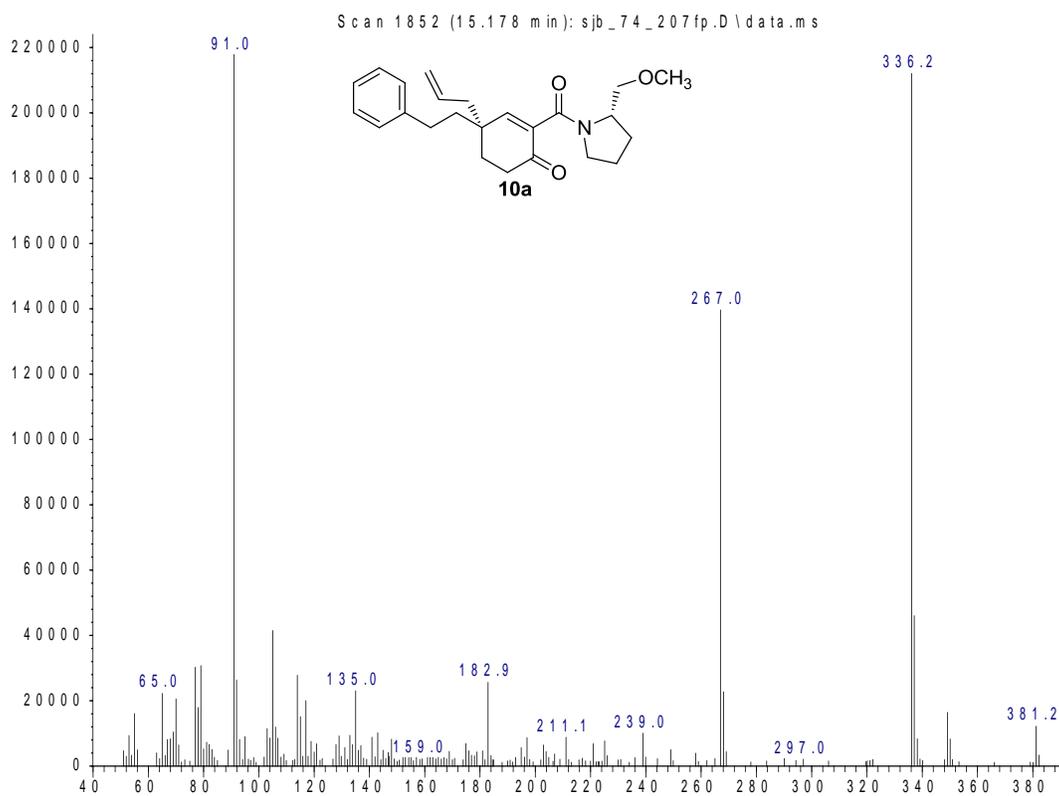
Abundance

Scan 1791 (14.829 min): sjb_74_207fp.D\data.ms



m/z-->

Abundance



m/z-->

Area Percent Report

Data Path : C:\msdchem\1\DATA\
Data File : sjb_77_088fp.D
Acq On : 24 May 2013 15:37
Operator : sjb
Sample : sjb_77_088fp
Misc :
ALS Vial : 90 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

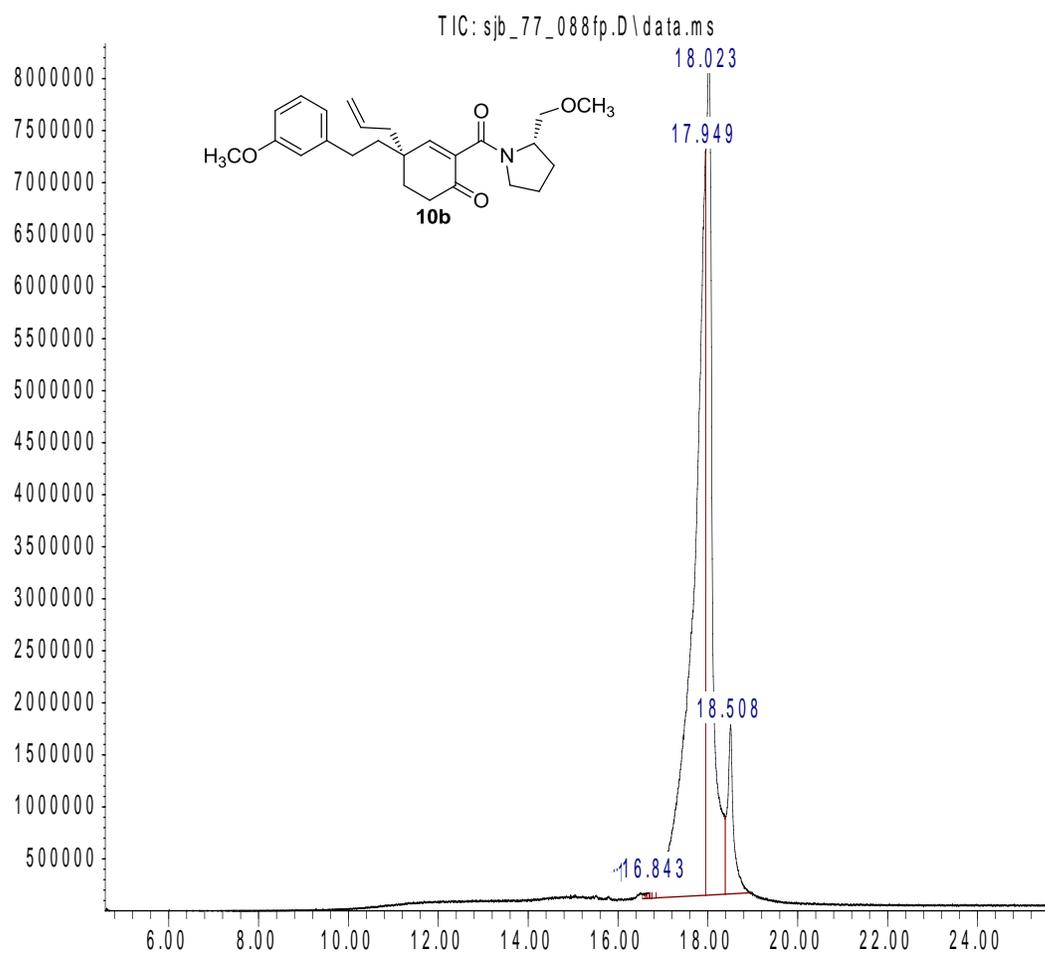
Method : C:\msdchem\1\5973N\PRECISION.M
Title :

Signal : TIC: sjb_77_088fp.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	16.585	2091	2098	2102	VV 10	48273	1551911	0.12%	0.068%
2	16.631	2102	2106	2108	VV 5	53733	828375	0.06%	0.036%
3	16.680	2108	2114	2116	VV 7	59458	1463538	0.11%	0.064%
4	16.701	2116	2118	2121	VV 4	69019	1154890	0.09%	0.051%
5	16.748	2121	2126	2128	VV 6	78916	1822704	0.14%	0.080%
6	16.843	2128	2143	2144	VV 6	121092	5451740	0.42%	0.239%
7	17.949	2144	2336	2337	VV 4	7155601	1309161021	100.00%	57.386%
8	18.023	2337	2349	2413	VV 4	8170841	805405891	61.52%	35.304%
9	18.508	2413	2434	2507	VV 4	1622052	154484566	11.80%	6.772%

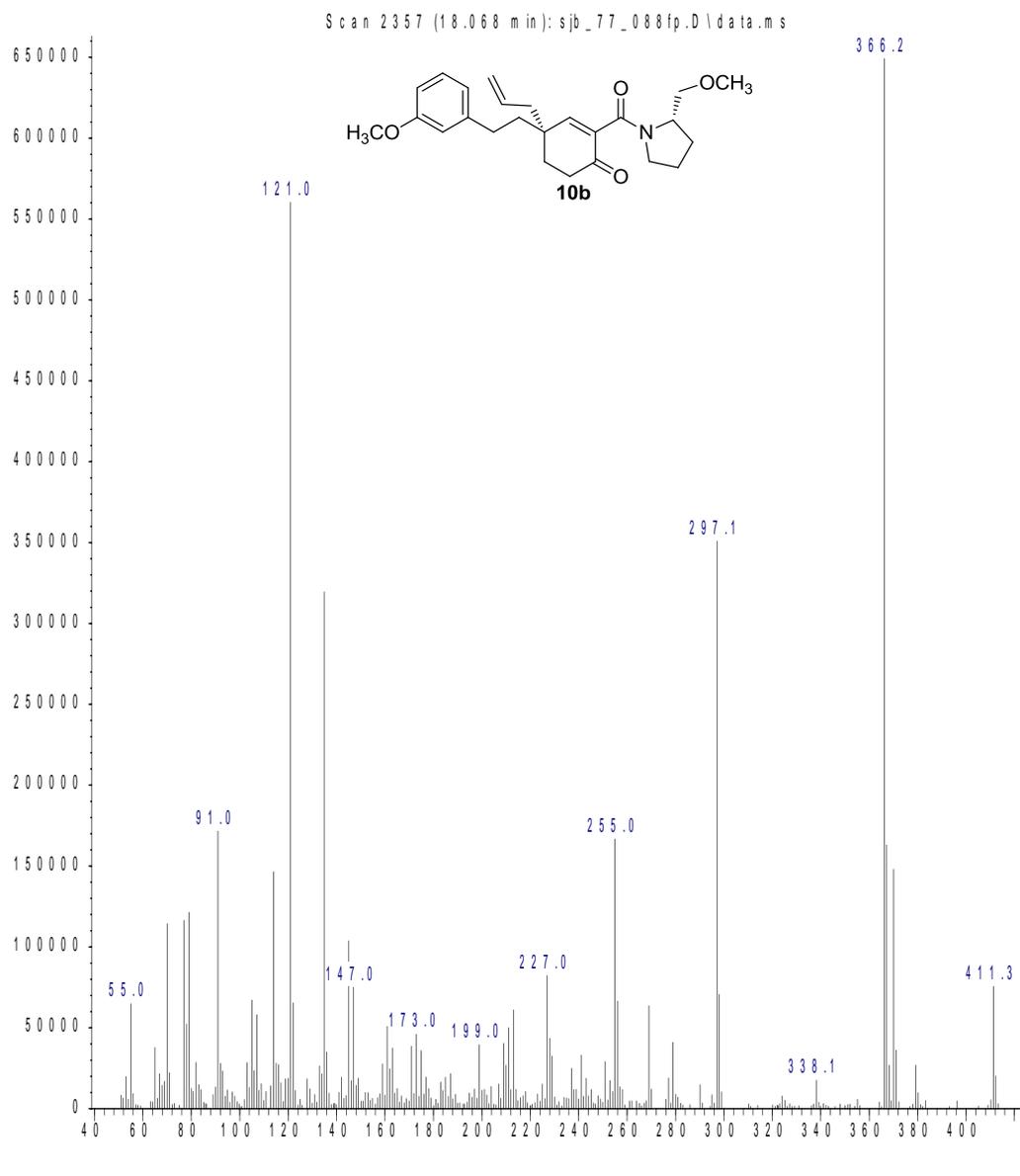
Sum of corrected areas: 2281324637

Abundance

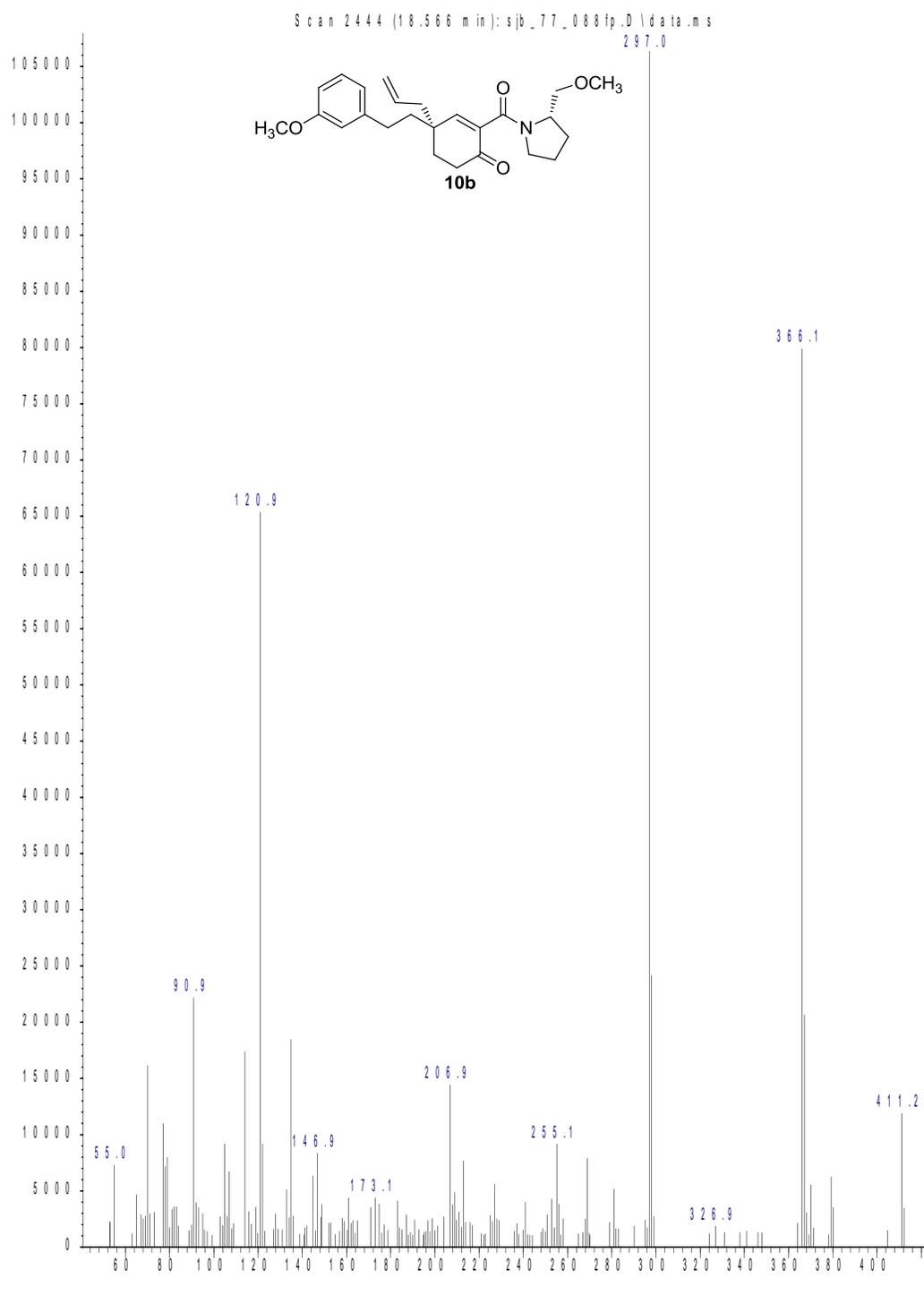


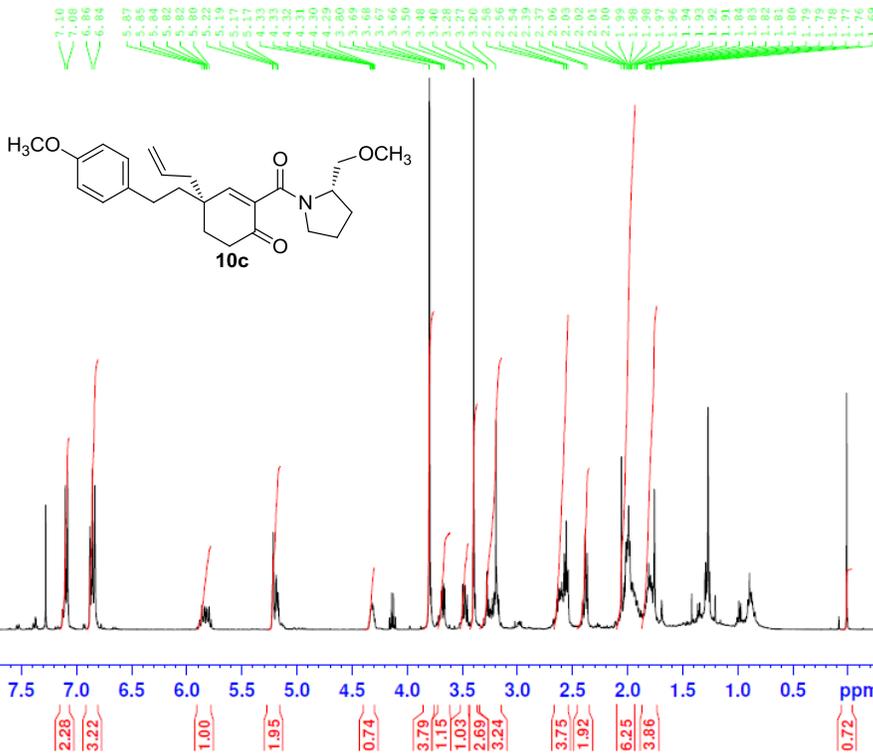
Time-->

Abundance



Abundance





```

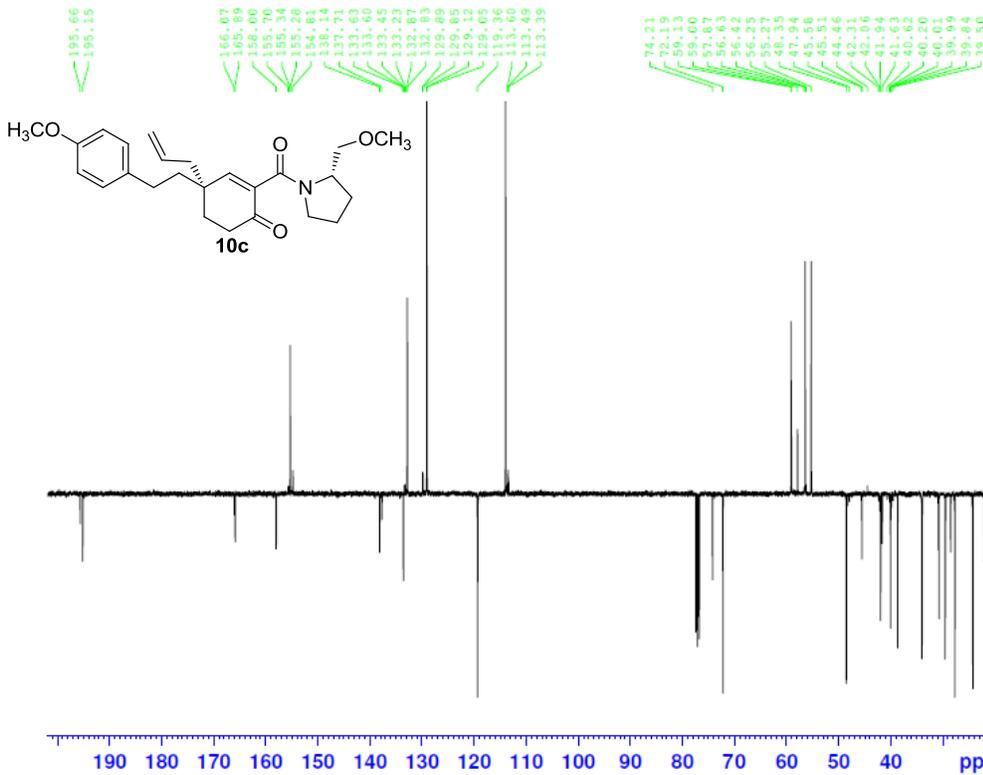
NAME      ra_67_158d
EXPNO     1
PROCNO    1
Date_     20120801
Time      12.50
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         203
DW         60.800 usec
DE         6.50 usec
TE         296.8 K
D1         1.00000000 sec
TDO        1

```

```

===== CHANNEL f1 =====
NUC1      1H
P1         12.50 usec
PL1        -2.00 dB
PL1W      12.14226913 W
SFO1      400.1524711 MHz
SI         32768
SF         400.1500000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00

```



```

Current Data Parameters
NAME      sjb_77_224fAPI
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20130924
Time      10.33
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   jmod
ID         65536
SOLVENT   CDCl3
NS         1024
DS         4
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631488 sec
RG         203
DW         20.800 usec
DE         6.50 usec
TE         298.2 K
CNSI2     145.0000000
CNST11    1.0000000
D1         2.00000000 sec
D20       0.00689655 sec
TD0        1

```

```

----- CHANNEL f1 -----
NUC1      13C
P1         8.00 usec
P2         16.00 usec
PL1        -2.00 dB
PL1W      56.13311005 W
SFO1      100.6278593 MHz

----- CHANNEL f2 -----
CPDPRG[2] waltz16
NUC2      1H
PCPD2     75.00 usec
PL2        -2.00 dB
PL12      13.39 dB
PL2W      12.14226913 W
PL12W     0.35099408 W
SFO2      400.1514893 MHz

```

```

F2 - Processing parameters
SI         32768
SF         100.6177980 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

```

Area Percent Report

Data Path : C:\msdchem\1\DATA\
Data File : sjb_77_224fp2.D
Acq On : 24 Sep 2013 11:10
Operator : sjb
Sample : sjb_77_224fp2
Misc :
ALS Vial : 90 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\msdchem\1\METHODS\ckr3.m
Title :

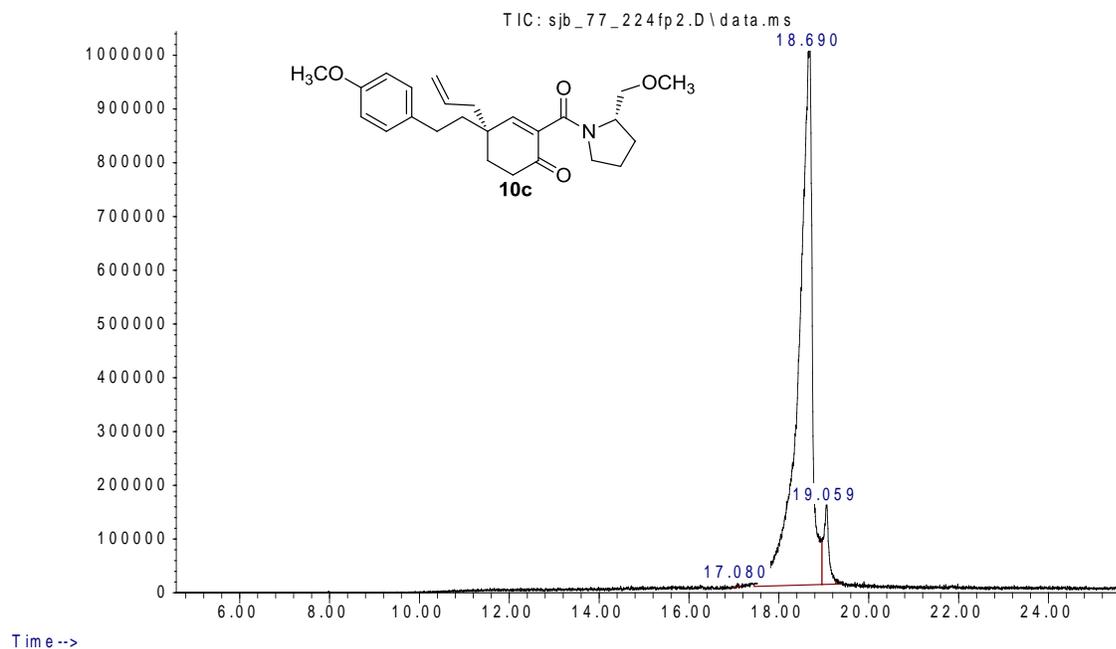
Signal : TIC: sjb_77_224fp2.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	17.080	2166	2184	2195	PV 5	5922	119715	0.06%	0.053%
2	18.690	2249	2466	2513	VV 4	1027532	212733185	100.00%	94.455%
3	19.059	2513	2530	2589	VV 2	146573	12368129	5.81%	5.492%

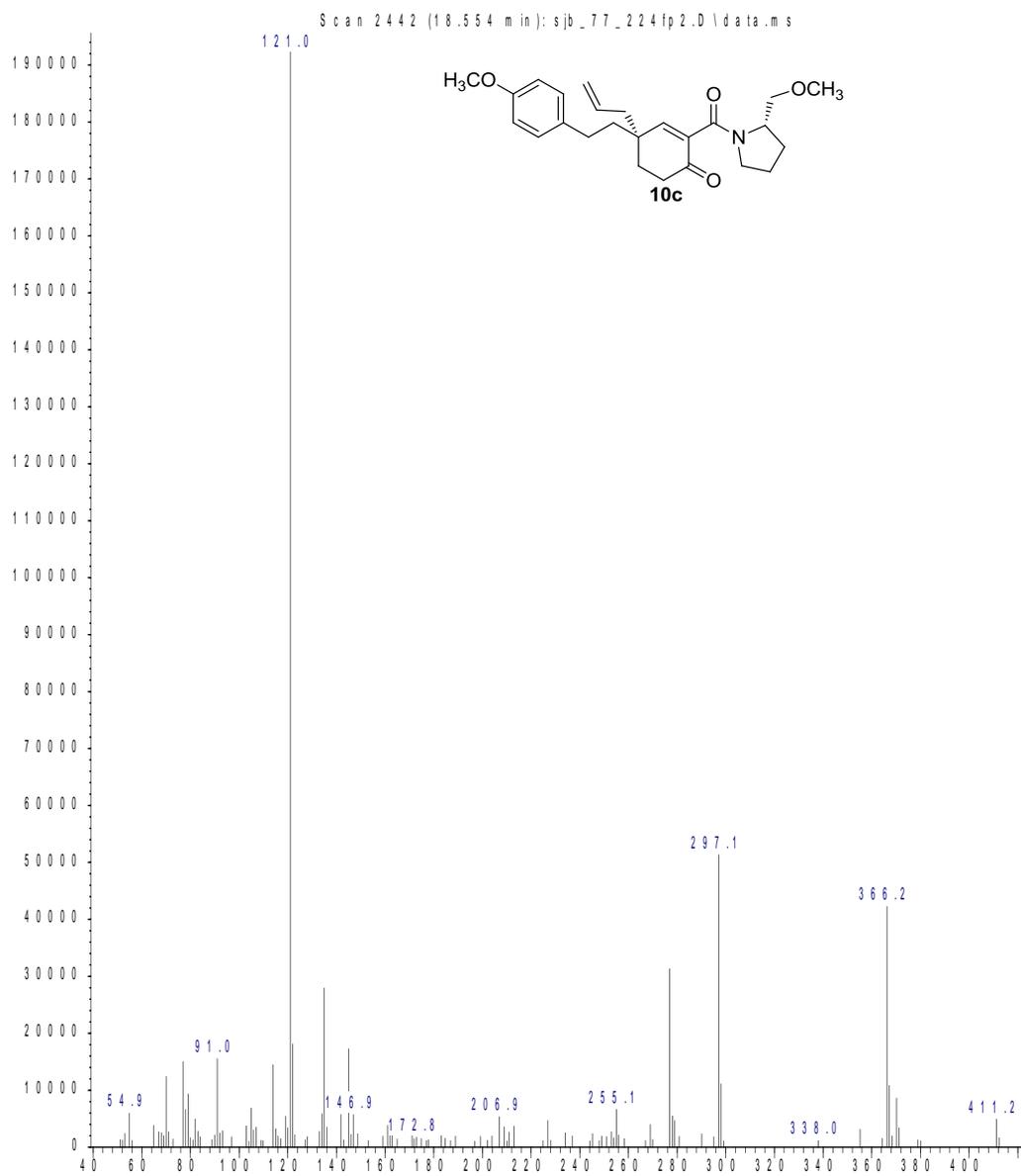
Sum of corrected areas: 225221029

ckr3.m Wed Mar 19 12:16:28 2014

Abundance

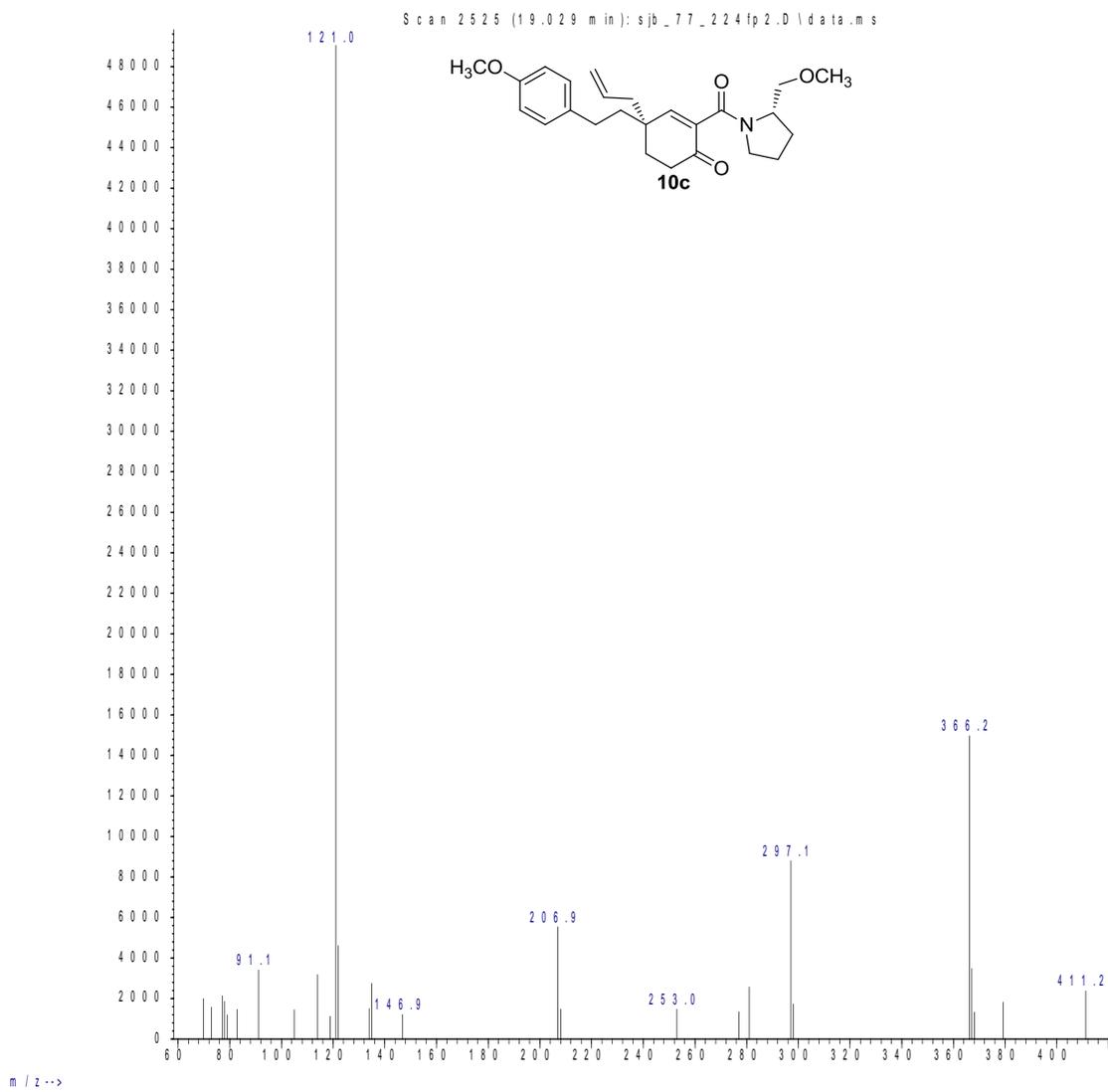


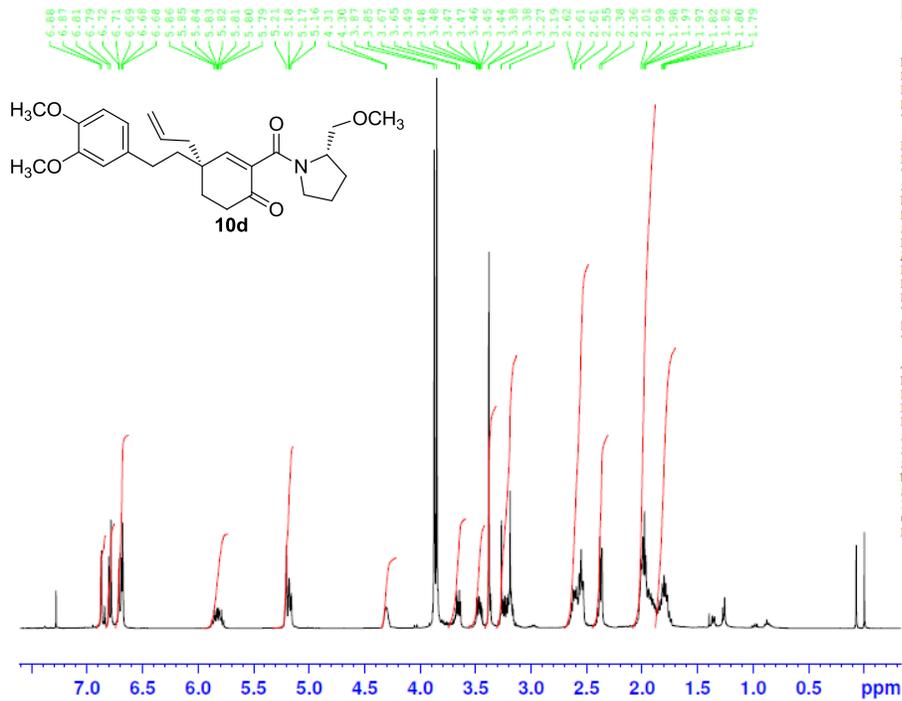
Abundance



m/z-->

Abundance



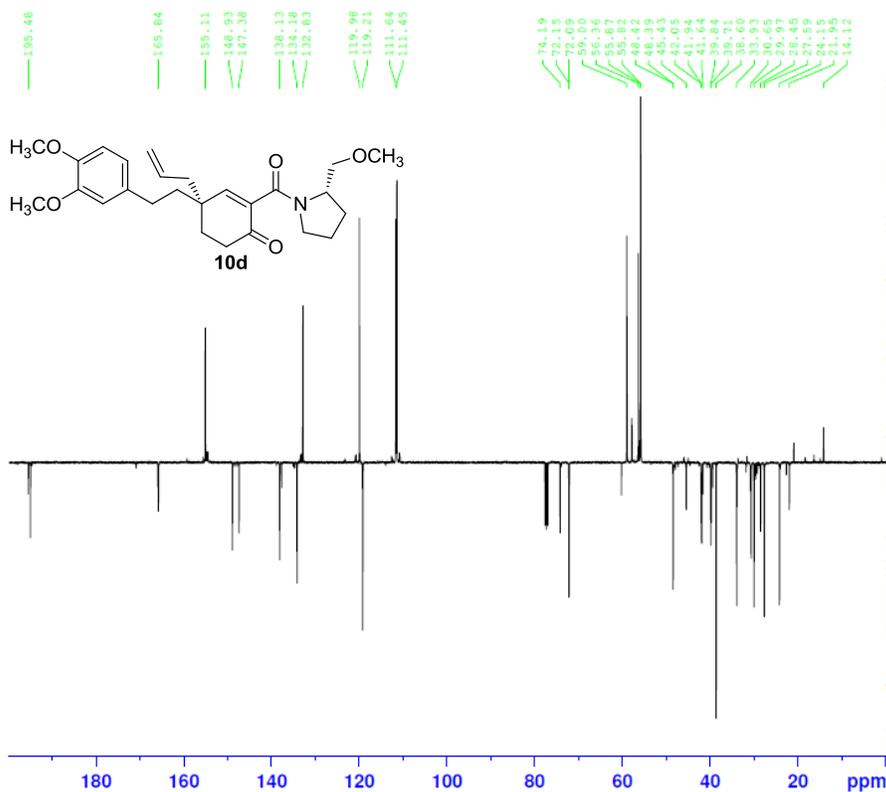


```

NAME      sjb_74_219fp take 2
EXPNO    1
PROCNO   1
Date_    20130801
Time     10.27
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        2
SWH      8223.685 Hz
FIDRES   0.125483 Hz
AQ        3.9846387 sec
RG        50.8
DW        60.800 usec
DE        6.50 usec
TE        301.2 K
D1        1.00000000 sec
TDO       1
  
```

```

----- CHANNEL f1 -----
NUC1     1H
P1       12.50 usec
PL1      -2.00 dB
PL1W     12.14226913 W
SFO1     400.1524711 MHz
SI       32768
SF       400.1500000 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
  
```



```

NAME      sjb_74_219fp APT
EXPNO    1
PROCNO   1
Date_    20121204
Time     13.18
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  jmod
TD        65536
SOLVENT  CDCl3
NS        1024
DS        4
SWH      20380.436 Hz
FIDRES   0.310981 Hz
AQ        1.6078665 sec
RG        203
DW        24.533 usec
DE        6.50 usec
TE        301.2 K
CNST2    145.0000000
CNST11   1.0000000
D1        2.00000000 sec
D20       0.00689655 sec
TDO       1
  
```

```

----- CHANNEL f1 -----
NUC1     13C
P1       8.00 usec
P2       16.00 usec
PL1      -2.00 dB
PL1W     56.13311005 W
SFO1     100.6277079 MHz
  
```

```

----- CHANNEL f2 -----
CPDPRG2  waltz16
NUC2     1H
PCPD2    80.00 usec
PL2      -2.00 dB
PL12     14.00 dB
PL2W     12.14226913 W
PL12W    0.30500001 W
SFO2     400.1514166 MHz
SI       32768
SF       100.6177980 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
  
```

Area Percent Report

Data Path : C:\msdchem\1\DATA\
Data File : sjb_77_178fp.D
Acq On : 13 Aug 2013 14:33
Operator : sjb
Sample : sjb_77_178fp
Misc :
ALS Vial : 100 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\msdchem\1\METHODS\ckr3.m
Title :

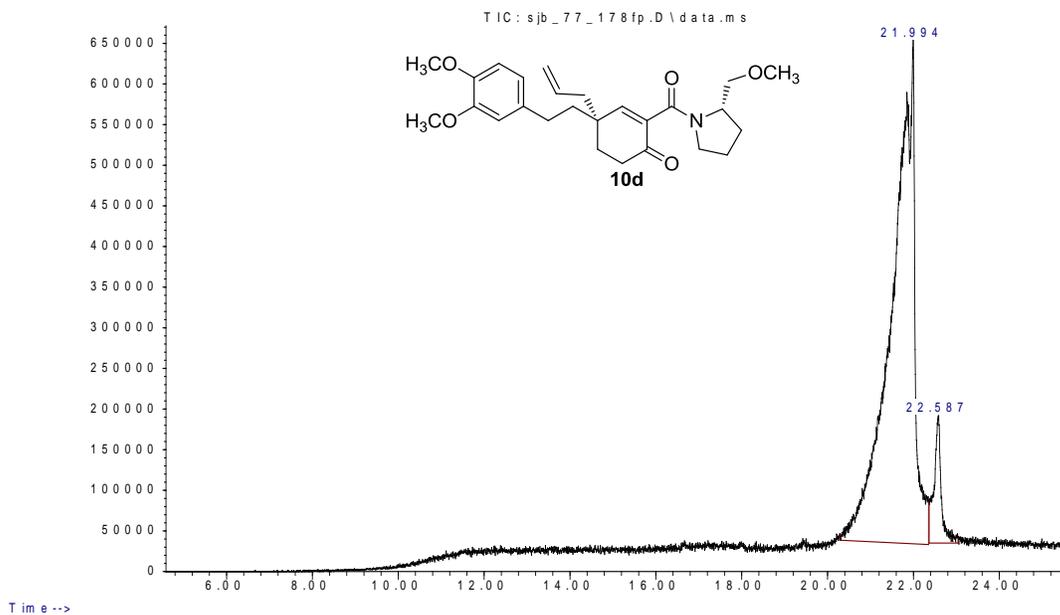
Signal : TIC: sjb_77_178fp.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	21.994	2744	3043	3105	M3	637493	229798336	100.00%	92.496%
2	22.587	3108	3147	3225	M4	157004	18641866	8.11%	7.504%

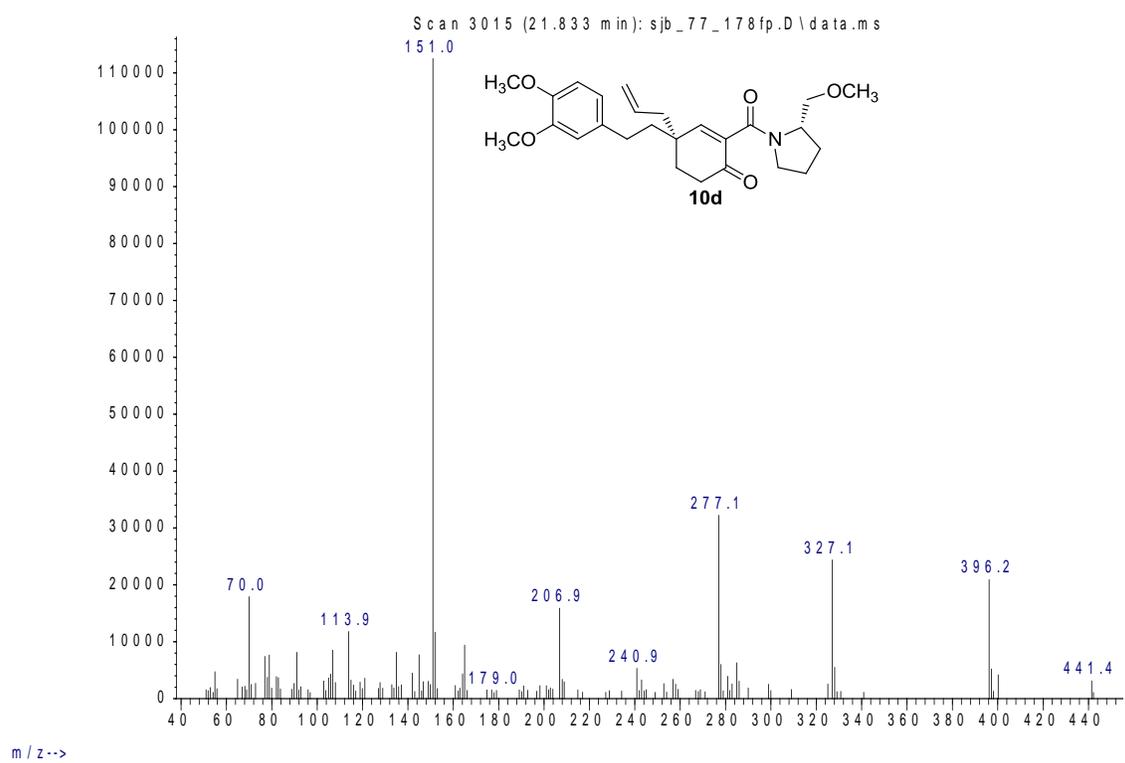
Sum of corrected areas: 248440203

ckr3.m Mon May 12 15:41:13 2014

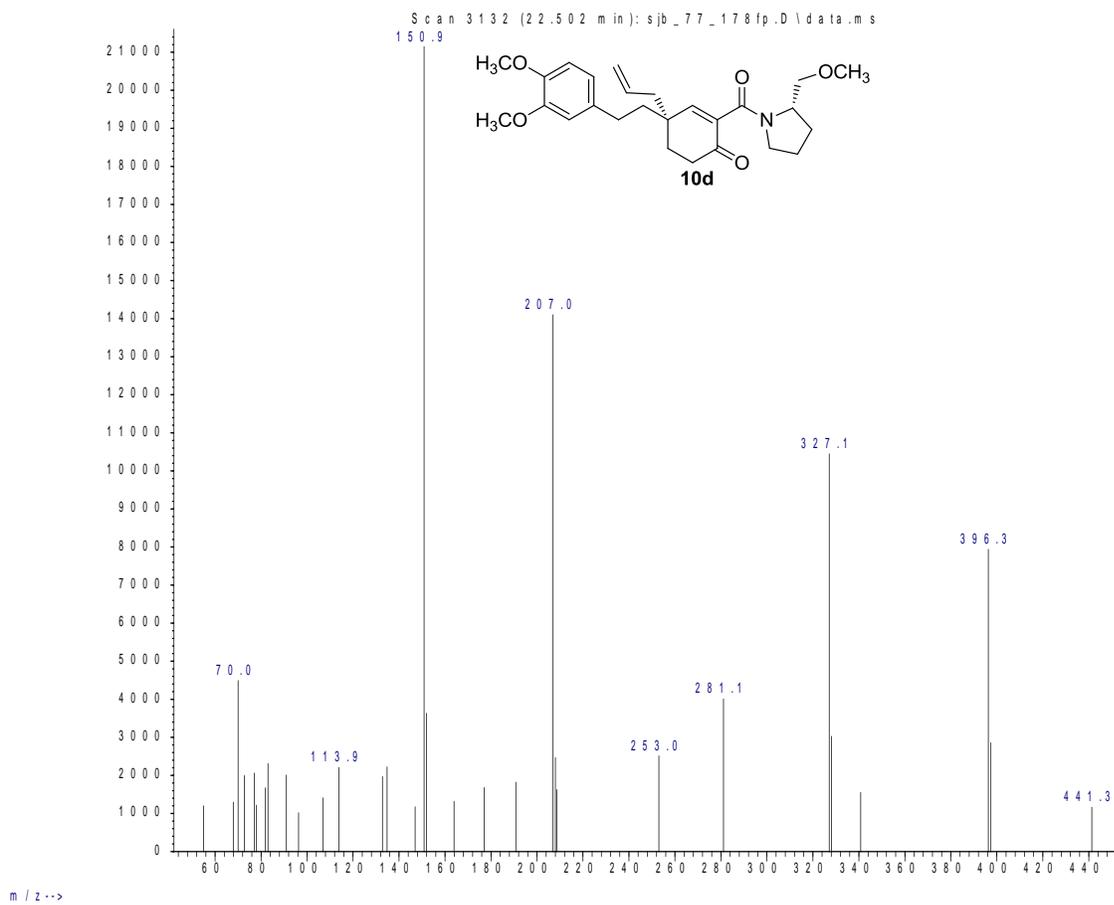
Abundance

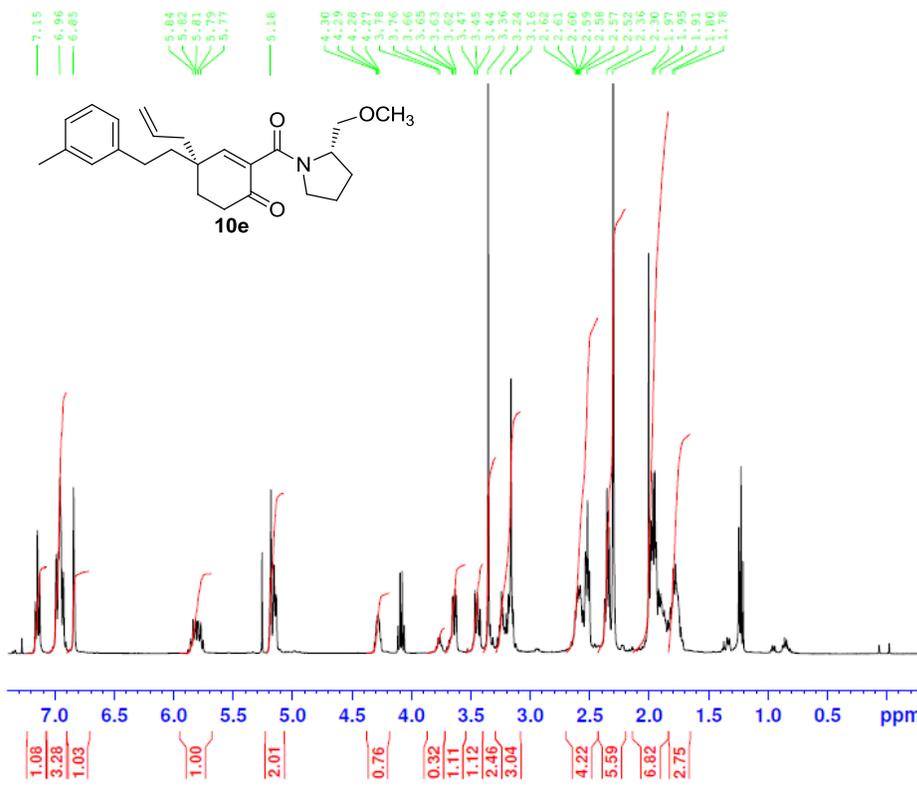


Abundance



Abundance

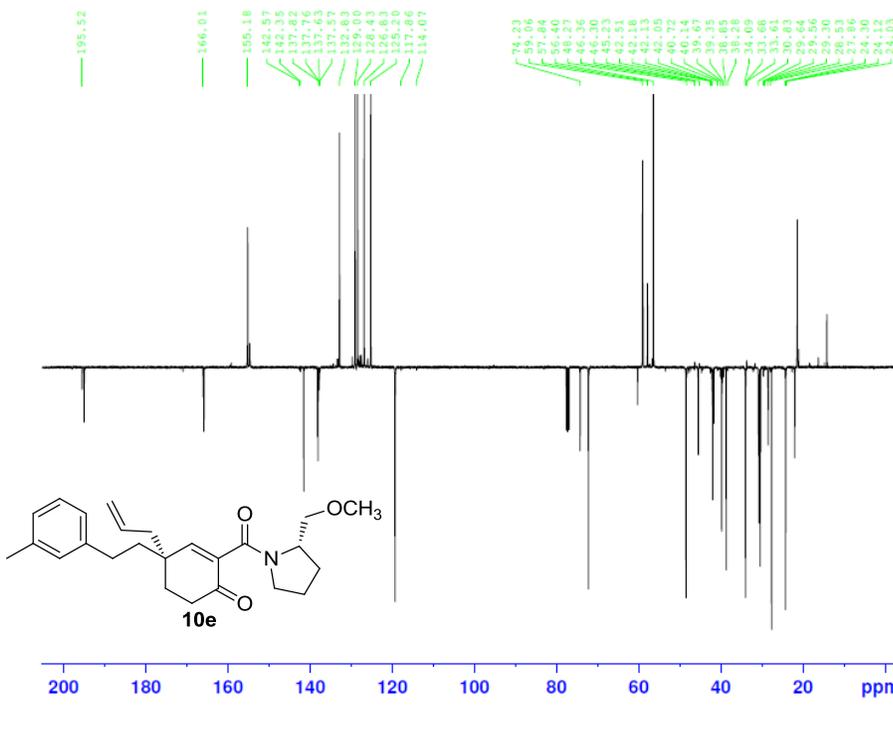




```

NAME      sjb_77_026fp
EXPNO     1
PROCNO    1
Date_     20130108
Time      15.11
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDC13
NS         16
DS         2
SWH       8223.685 Hz
FIDRES    0.125483 Hz
AQ         3.9846387 sec
RG         25.4
DW         60.800 usec
DE         6.50 usec
TE         299.4 K
D1         1.00000000 sec
TDO        1

----- CHANNEL f1 -----
NUC1       1H
P1         12.50 usec
PL1        -2.00 dB
PL1W       12.14226913 W
SF01       400.1524711 MHz
SI         32768
SF         400.1500000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```



```

NAME      sjb_77_026fp 13CAPT
EXPNO     1
PROCNO    1
Date_     20130108
Time      16.42
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   jmod
TD         65536
SOLVENT   CDC13
NS         1024
DS         4
SWH       21008.404 Hz
FIDRES    0.320563 Hz
AQ         1.5598068 sec
RG         203
DW         23.800 usec
DE         6.50 usec
TE         301.6 K
CNST2     145.0000000
CNST11    1.0000000
D1         2.00000000 sec
D20        0.00689655 sec
TDO        1

----- CHANNEL f1 -----
NUC1       13C
P1         8.00 usec
P2         16.00 usec
PL1        -2.00 dB
PL1W       56.13311005 W
SF01       100.6279360 MHz

----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2       1H
PCPD2     80.00 usec
PL2        -2.00 dB
PL12       14.00 dB
PL2W       12.14226913 W
PL12W     0.30500001 W
SF02       400.1514213 MHz
SI         32768
SF         100.6177980 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```

Area Percent Report

Data Path : C:\msdchem\1\DATA\
Data File : sjb_77_026fp.D
Acq On : 8 Jan 2013 15:19
Operator : sjb
Sample : sjb_77_026fp
Misc :
ALS Vial : 5 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\msdchem\1\METHODS\ckr3.m
Title :

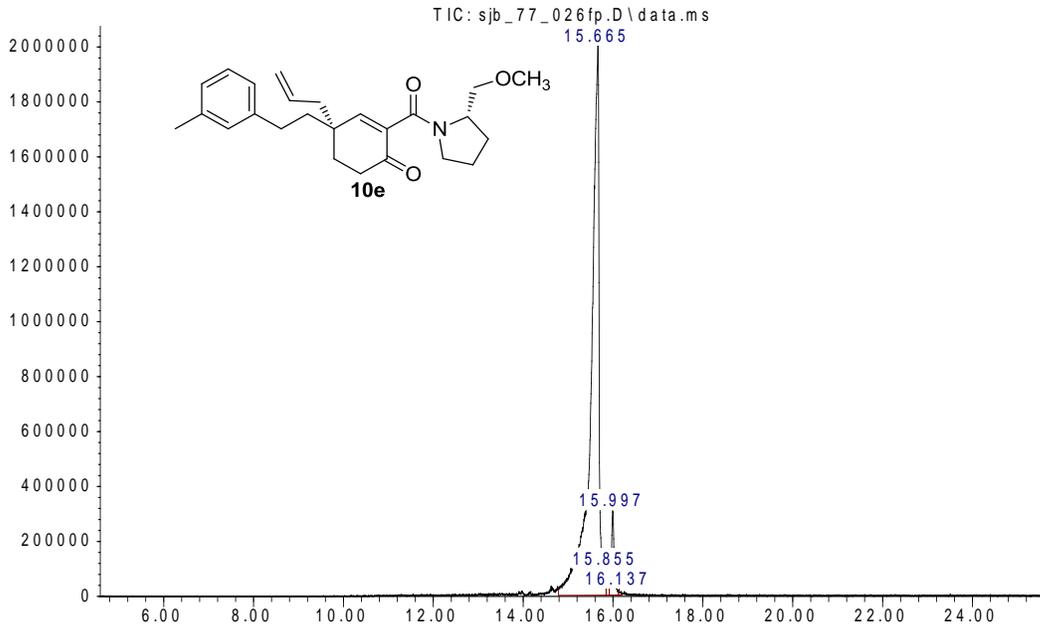
Signal : TIC: sjb_77_026fp.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	15.665	1783	1937	1969	VV 4	2054550	248861067	100.00%	93.344%
2	15.855	1969	1970	1981	VV 8	91613	3553786	1.43%	1.333%
3	15.997	1981	1995	2017	VV 6	301860	13684775	5.50%	5.133%
4	16.137	2017	2020	2030	VV 4	19764	505636	0.20%	0.190%

Sum of corrected areas: 266605263

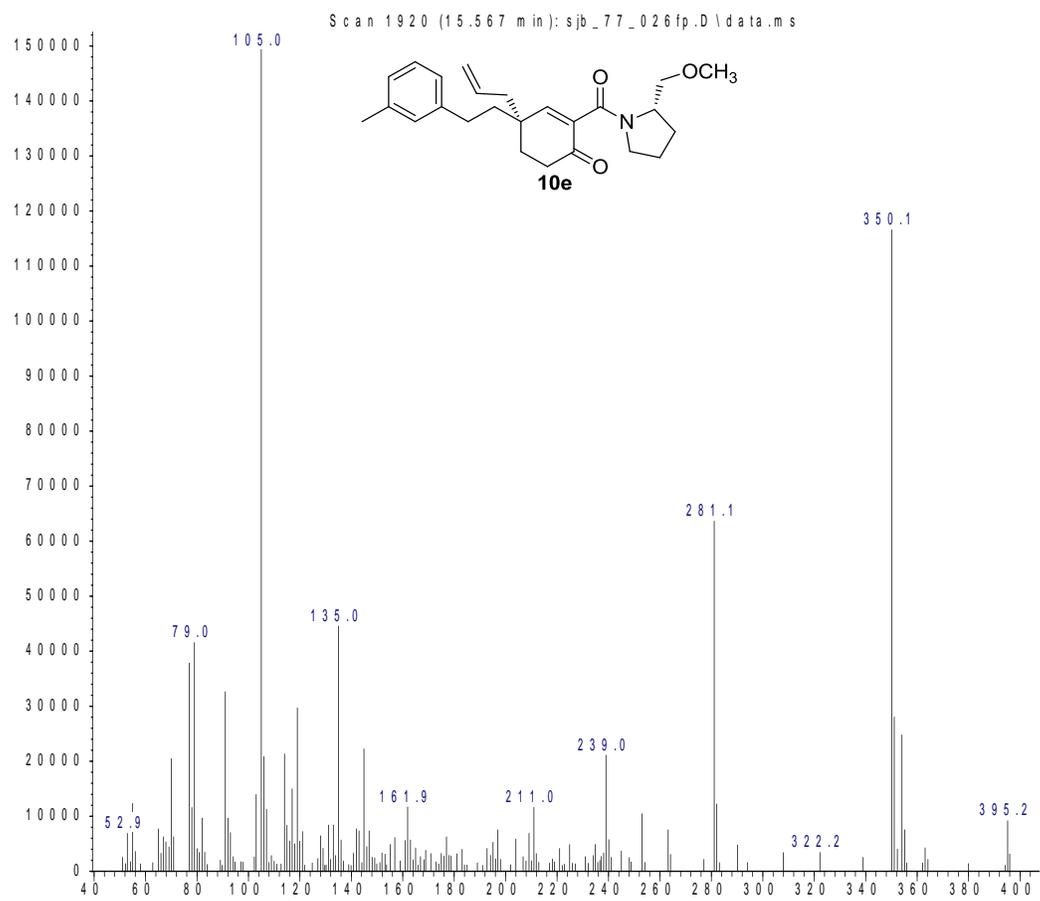
ckr3.m Wed Mar 19 12:22:46 2014

Abundance



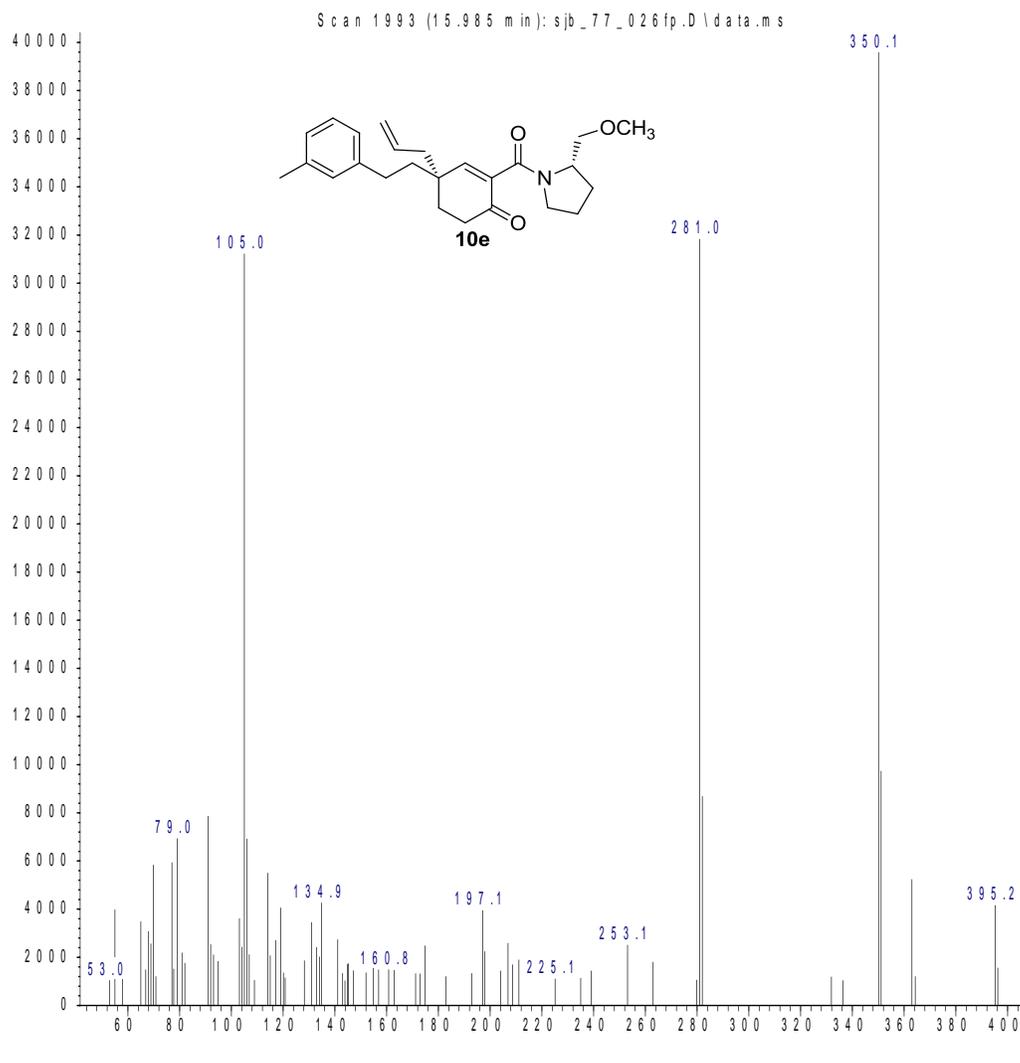
Time-->

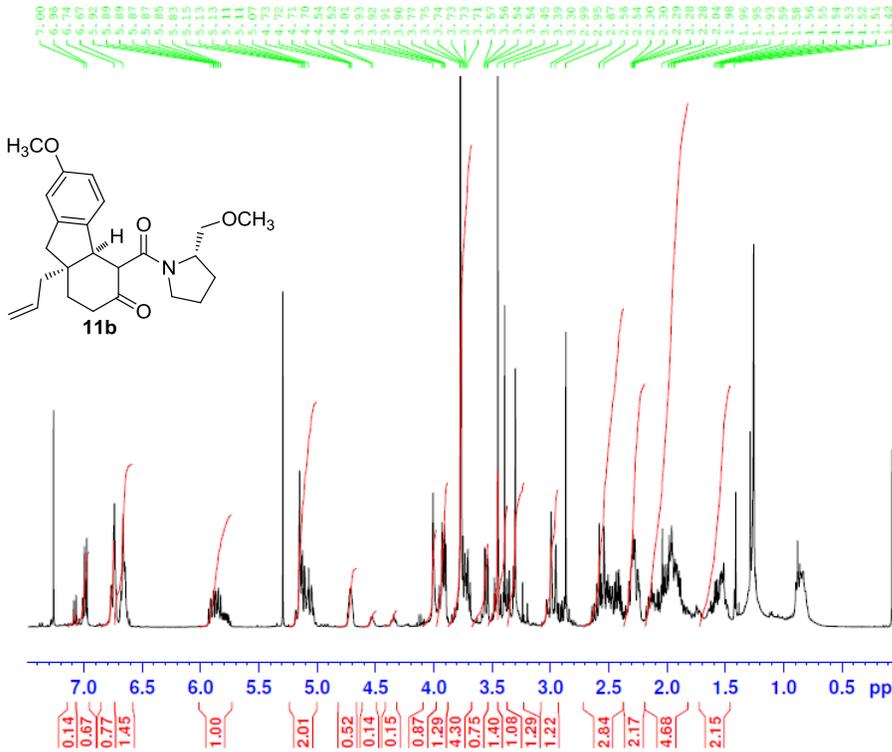
Abundance



m/z-->

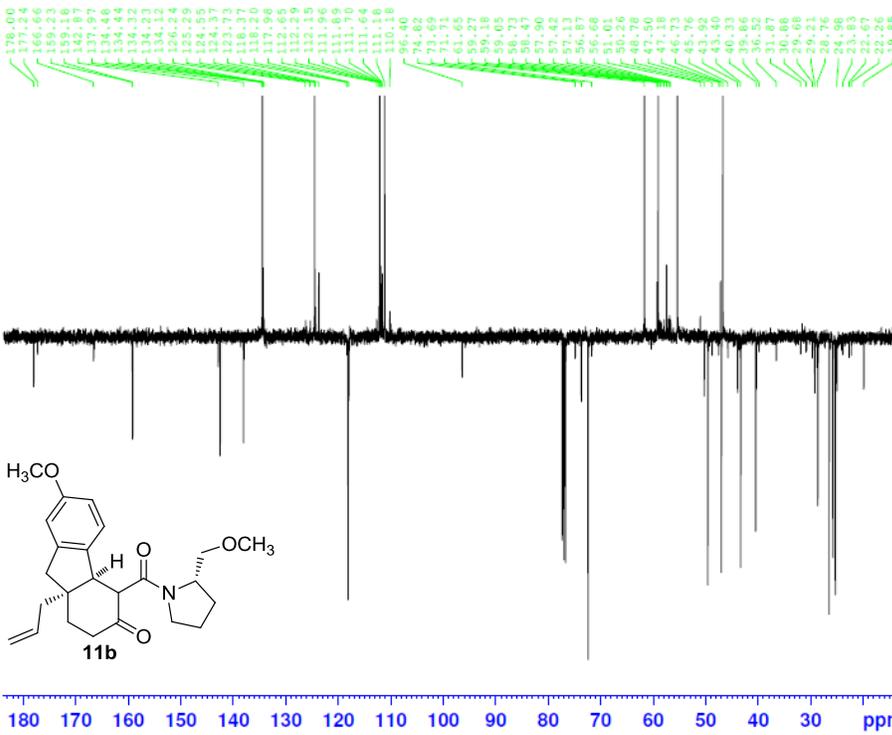
Abundance





```
NAME      sjb_74_172fp
EXPNO     1
PROCNO    1
Date_     20121011
Time      15.16
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   zg30
TD         65536
SOLVENT   CDC13
NS         16
DS         2
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         114
DW         60.800 usec
DE         6.50 usec
TE         301.0 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         9.80 usec
PL1        -4.00 dB
PL1W       19.24419975 W
SFO1       400.1524711 MHz
SI         32768
SF         400.1500077 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```



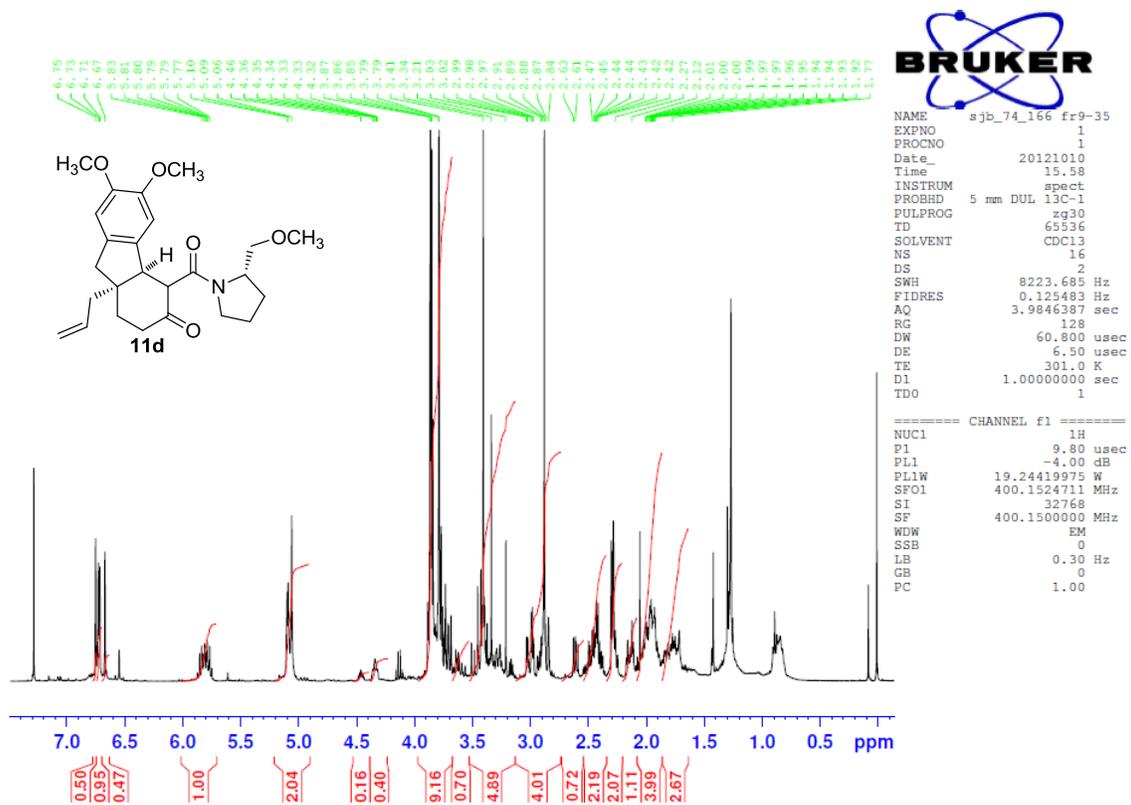
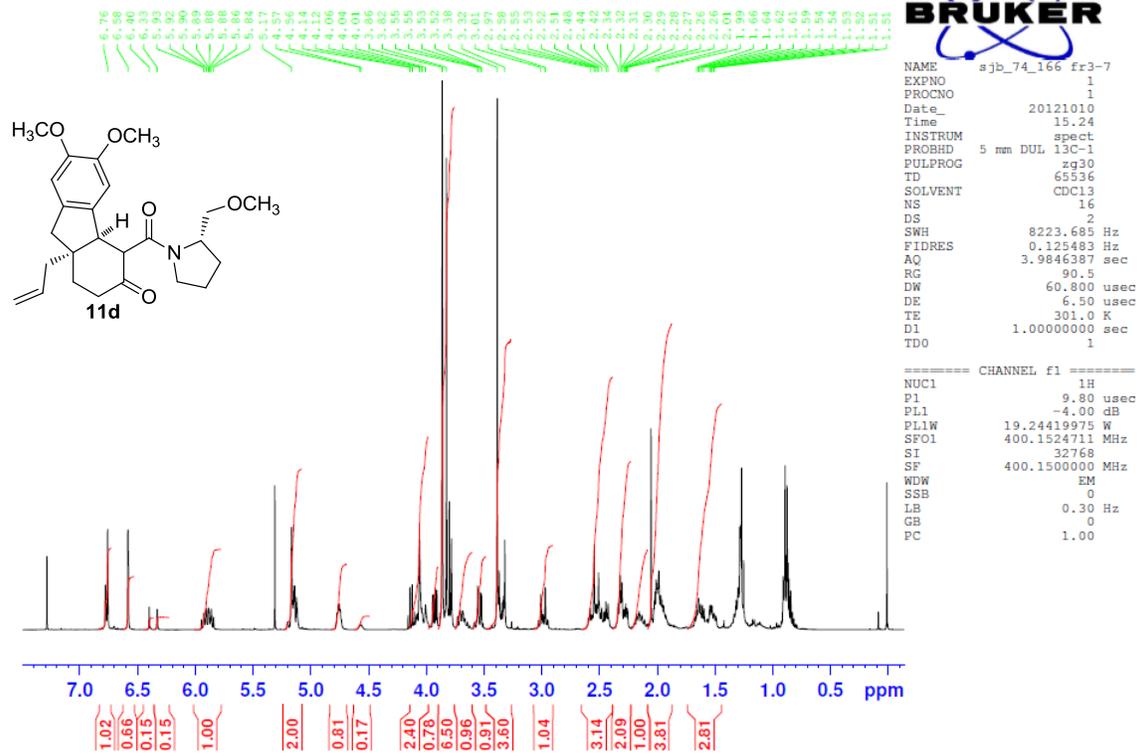
```
Current Data Parameters
NAME      sjb_74_185 APT
EXPNO     1
PROCNO    1

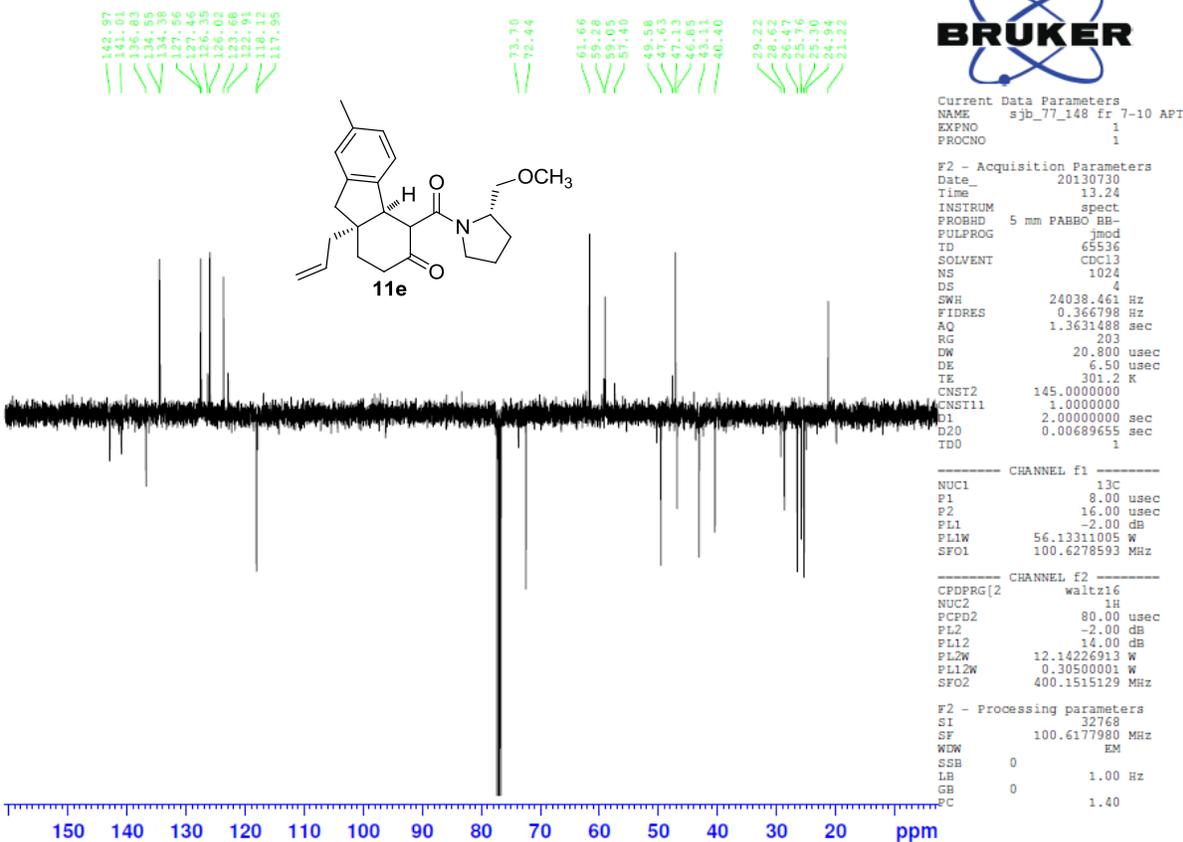
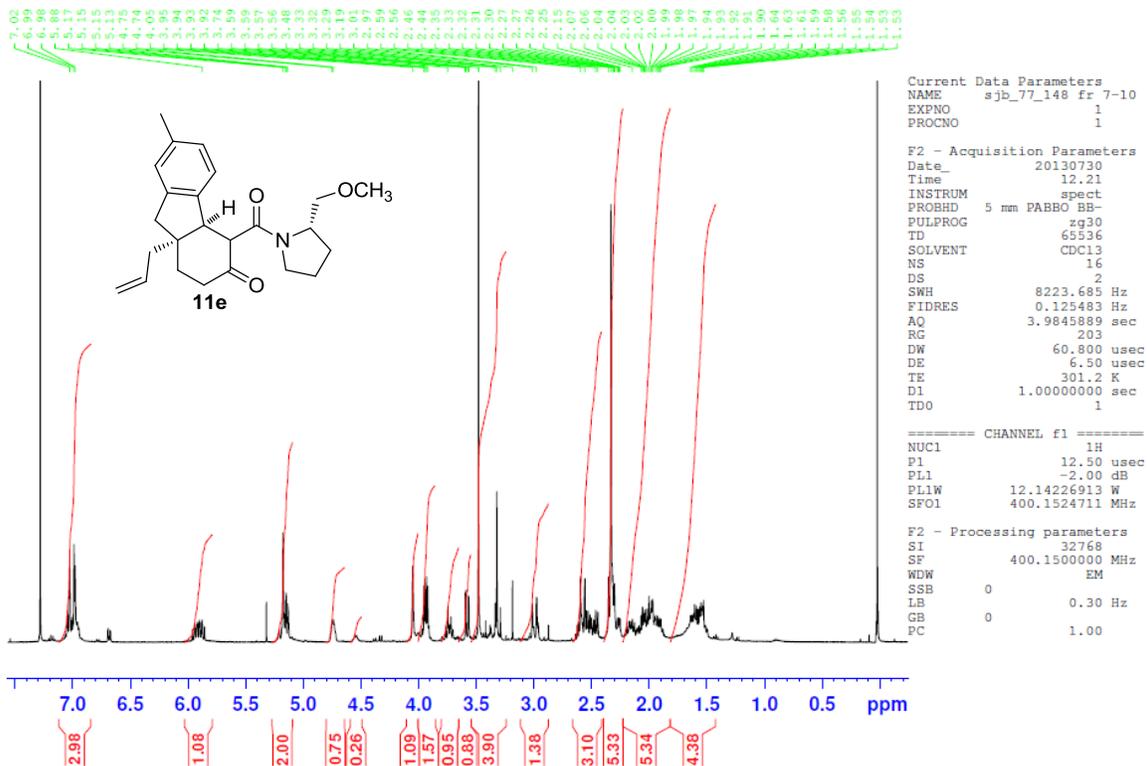
F2 - Acquisition Parameters
Date_     20121024
Time      9.09
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   jmod
TD         65536
SOLVENT   CDC13
NS         1024
DS         4
SWH        19230.770 Hz
FIDRES     0.293438 Hz
AQ         1.7039360 sec
RG         203
DW         26.000 usec
DE         6.50 usec
TE         301.2 K
CNS12     145.0000000
CNS11     1.0000000
D1         2.00000000 sec
D20       0.00689655 sec
TD0        1

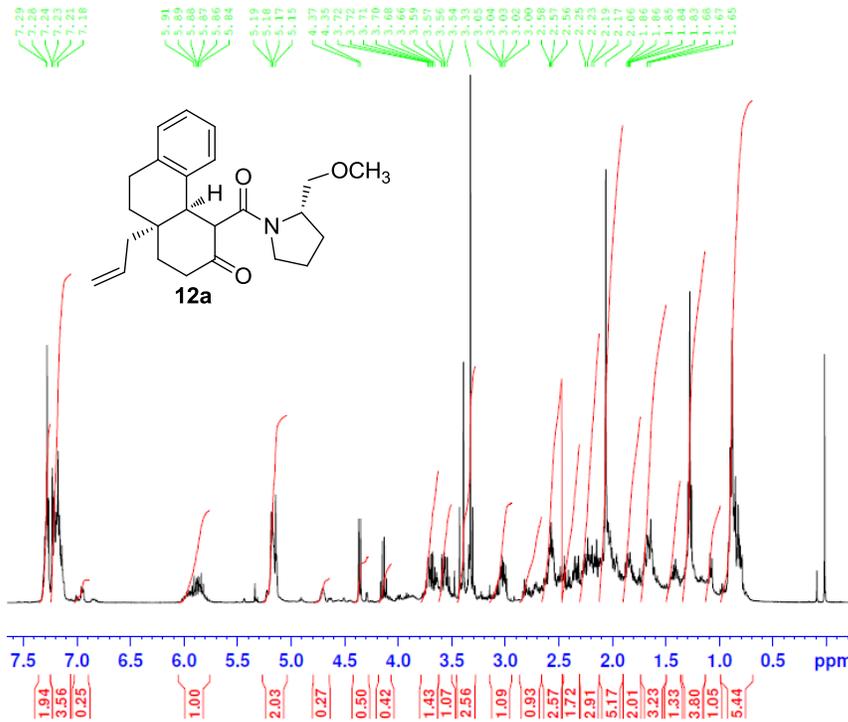
===== CHANNEL f1 =====
NUC1       13C
P1         9.00 usec
P2         18.00 usec
PL1        0 dB
PL1W       35.41759872 W
SFO1       100.6269591 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2       1H
PCPD2     80.00 usec
PL2        -3.80 dB
PL12       13.80 dB
PL2W      18.37806702 W
PL12W     0.31937420 W
SFO2       400.1514663 MHz

F2 - Processing parameters
SI         32768
SF         100.6177980 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```



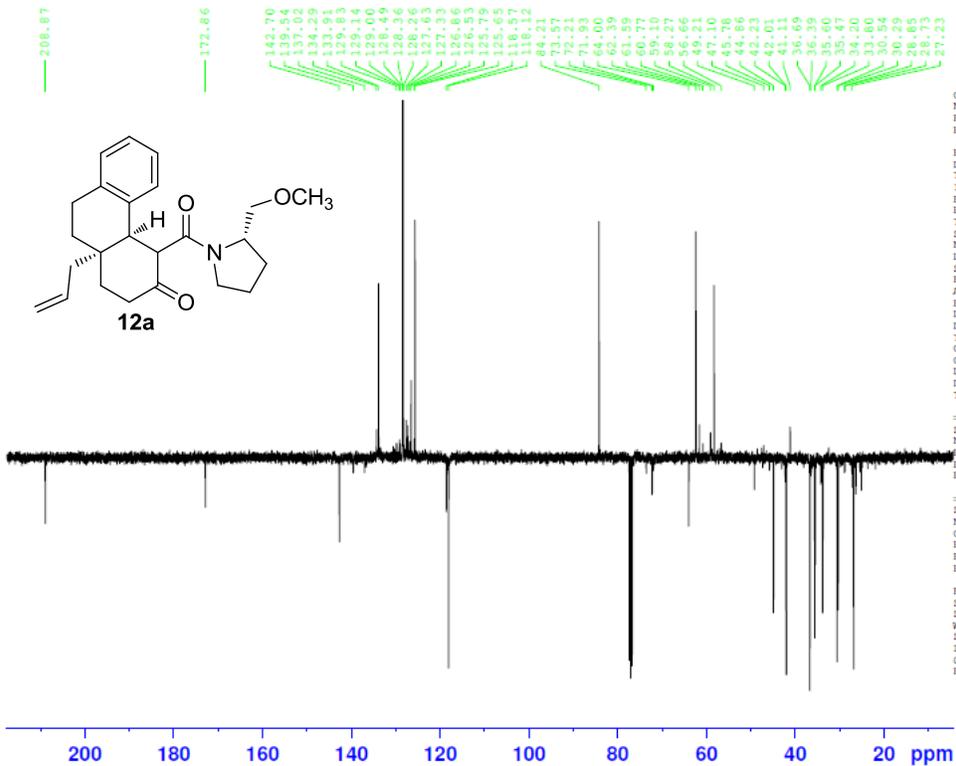




```

NAME      sjb_72_077fp
EXPNO     1
PROCNO    1
Date_     20120118
Time      16.54
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         2
DS         2
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         101
DW         60.800 usec
DE         6.50 usec
TE         297.1 K
D1         1.00000000 sec
TDO        1

===== CHANNEL f1 =====
NUC1       1H
P1         12.50 usec
PL1        -2.00 dB
PL1W       12.14226913 W
SFO1       400.1524711 MHz
SI         32768
SF         400.1500000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```



```

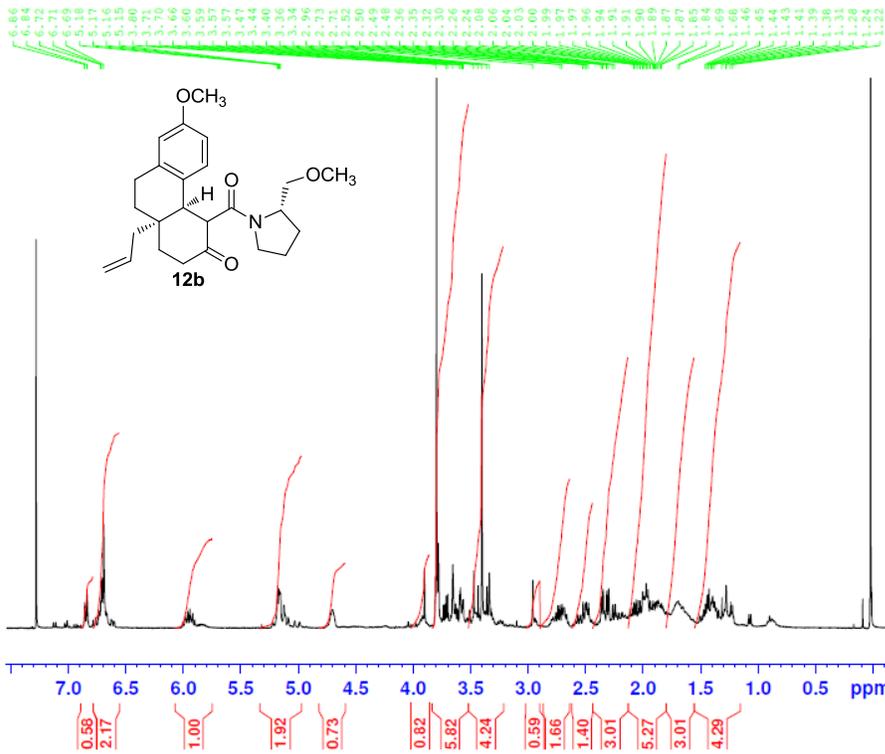
Current Data Parameters
NAME      sjb_210 FC 666 phenyl APT 2
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20140325
Time      19.35
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   jmod
TD         65536
SOLVENT   CDCl3
NS         512
DS         4
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631488 sec
RG         203
DW         20.800 usec
DE         6.50 usec
TE         301.2 K
CNST2     145.0000000
CNST11    1.0000000
D1         2.0000000 sec
D20        0.00689655 sec
TDO        1

===== CHANNEL f1 =====
SFO1       100.6278593 MHz
NUC1       13C
P1         8.00 usec
PL1        16.00 usec
PLW1       56.13299942 W

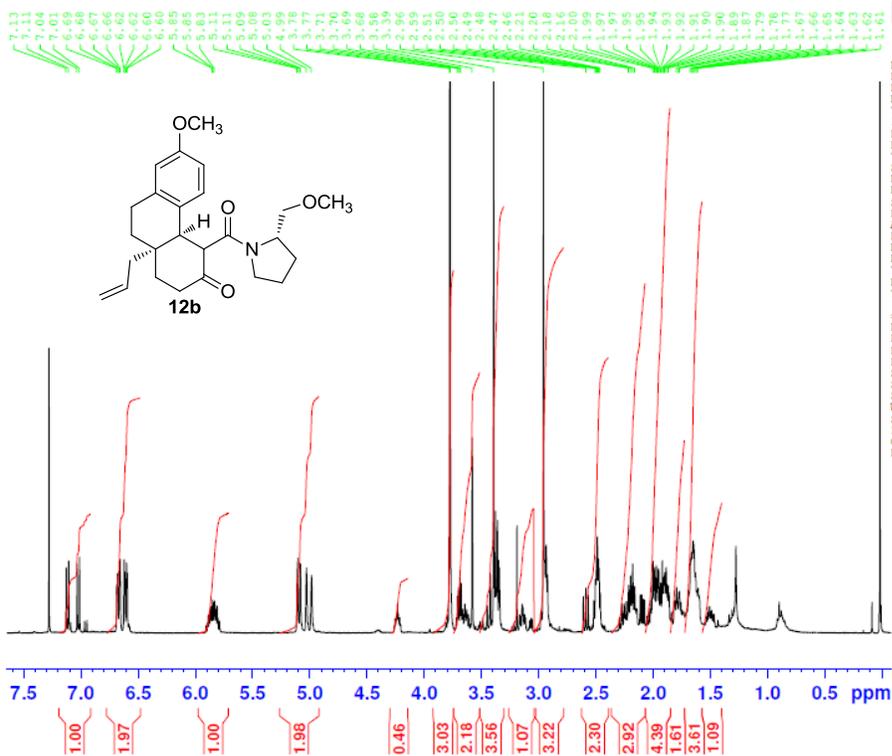
===== CHANNEL f2 =====
SFO2       400.1516006 MHz
NUC2       1H
CPOPC[2]   wait16
PCPO2      90.00 usec
PLW2       12.14200020 W
PLW12      0.24369000 W

F2 - Processing parameters
SI         32768
SF         100.6177980 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```



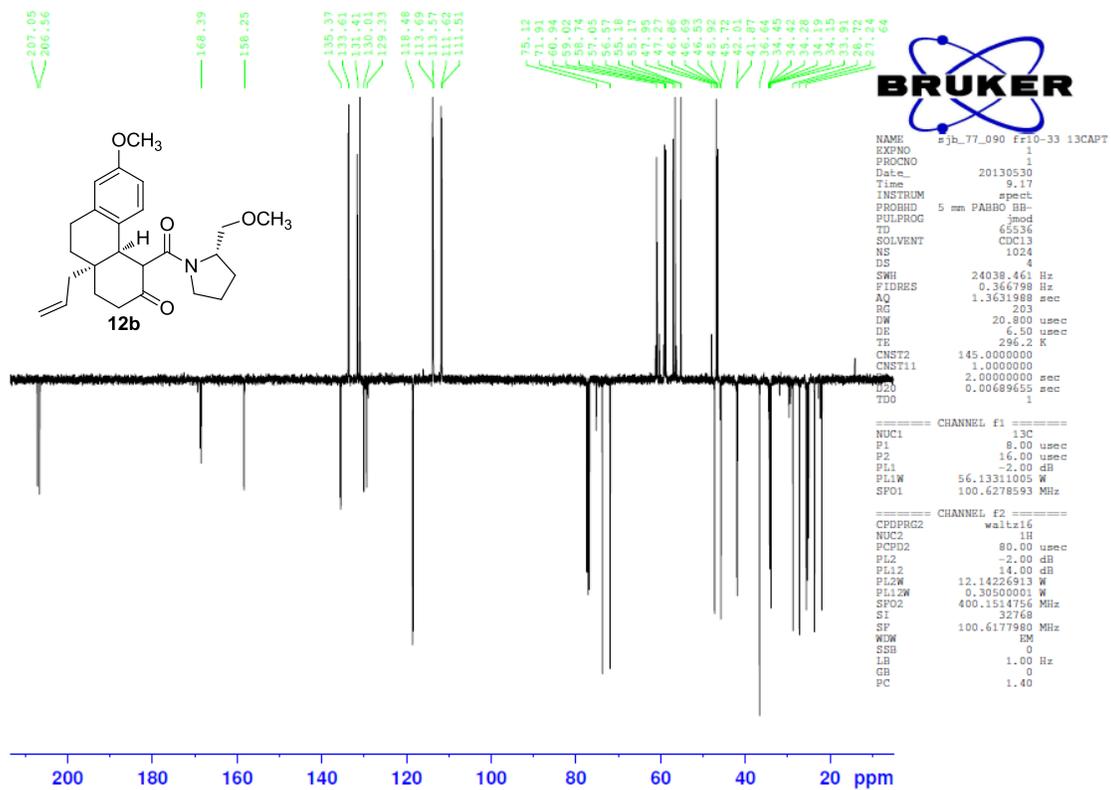
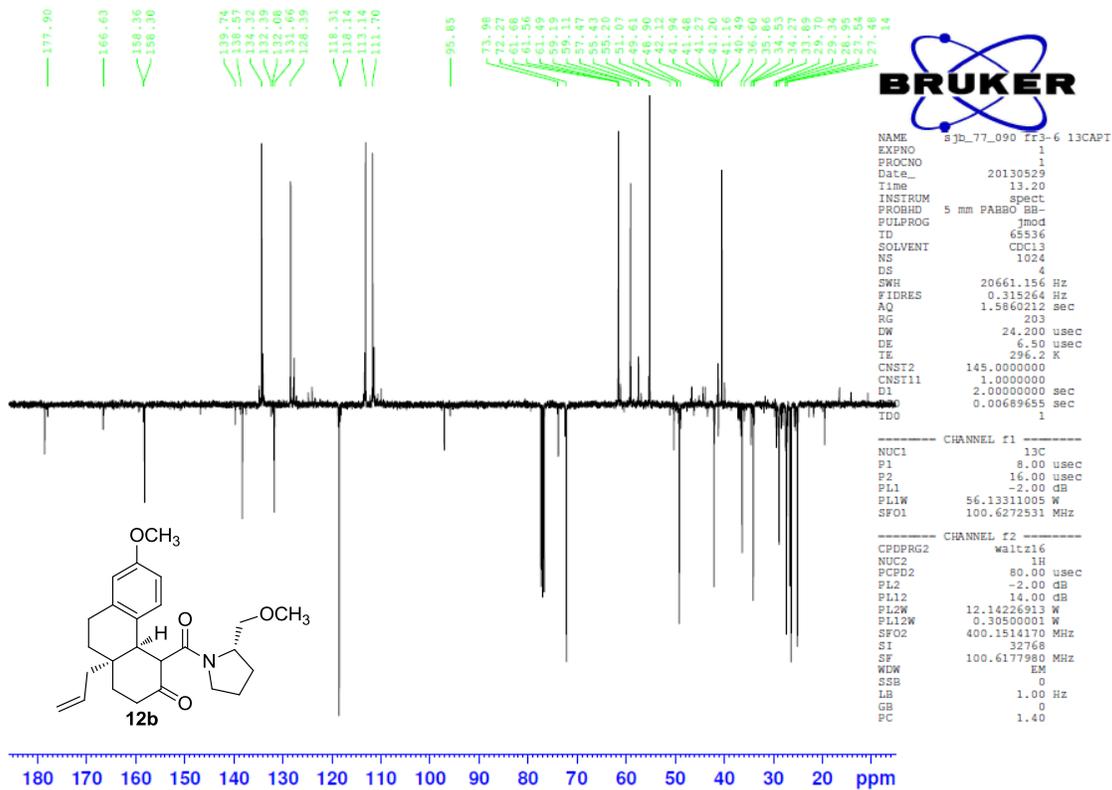
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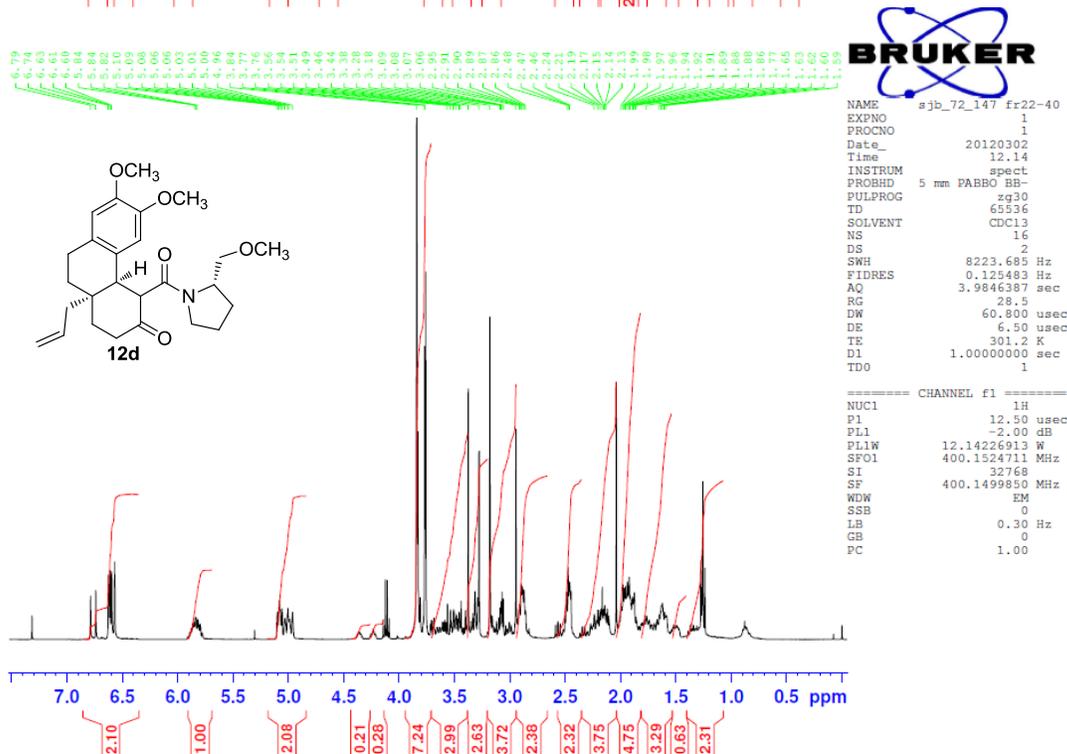
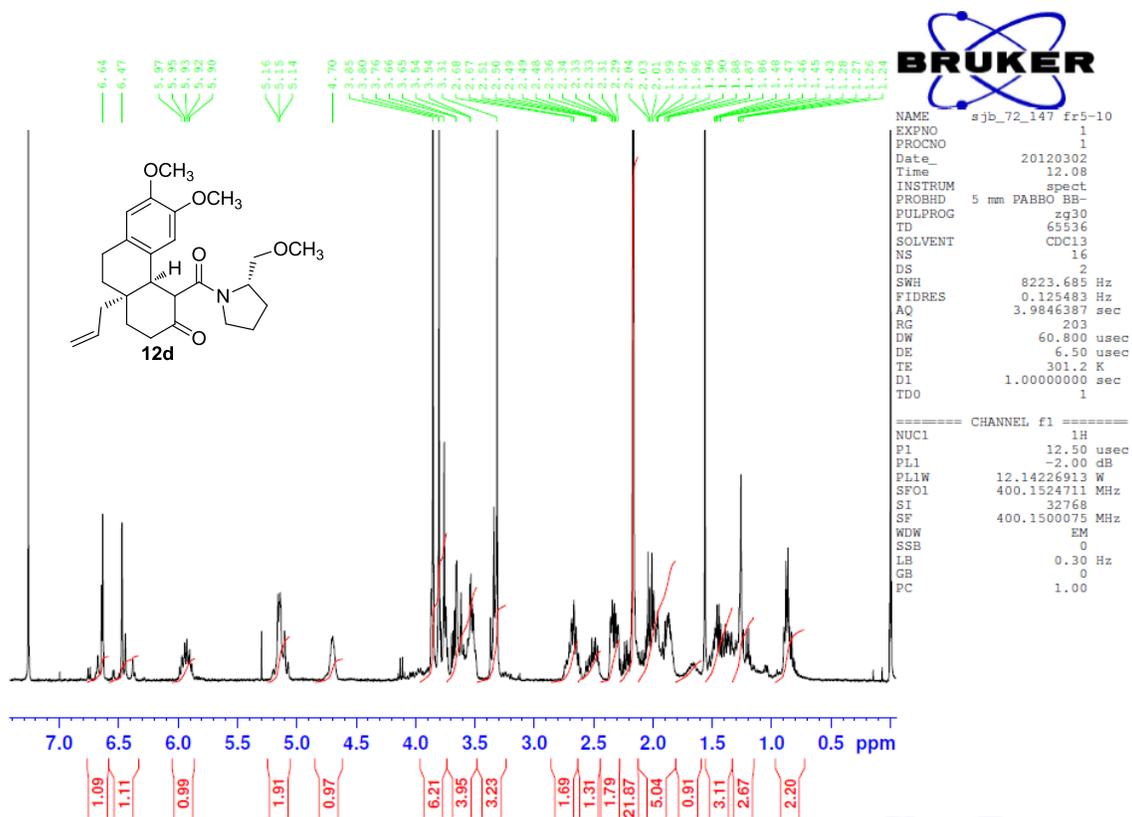
NAME      njb_77_090 fr3-6 fp take2
EXPNO    1
PROCNO   1
Date_    20130802
Time     14.17
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        2
SWH      8223.685 Hz
FIDRES   0.125483 Hz
AQ        3.9846387 sec
RG        203
DW        60.800 usec
DE        6.50 usec
TE        301.2 K
D1        1.00000000 sec
TDO       1
===== CHANNEL f1 =====
NUC1     1H
P1       12.50 usec
PL1      -2.00 dB
PL1W     12.14226913 W
SFO1     400.1524711 MHz
SI       32768
SF       400.1500000 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
  
```

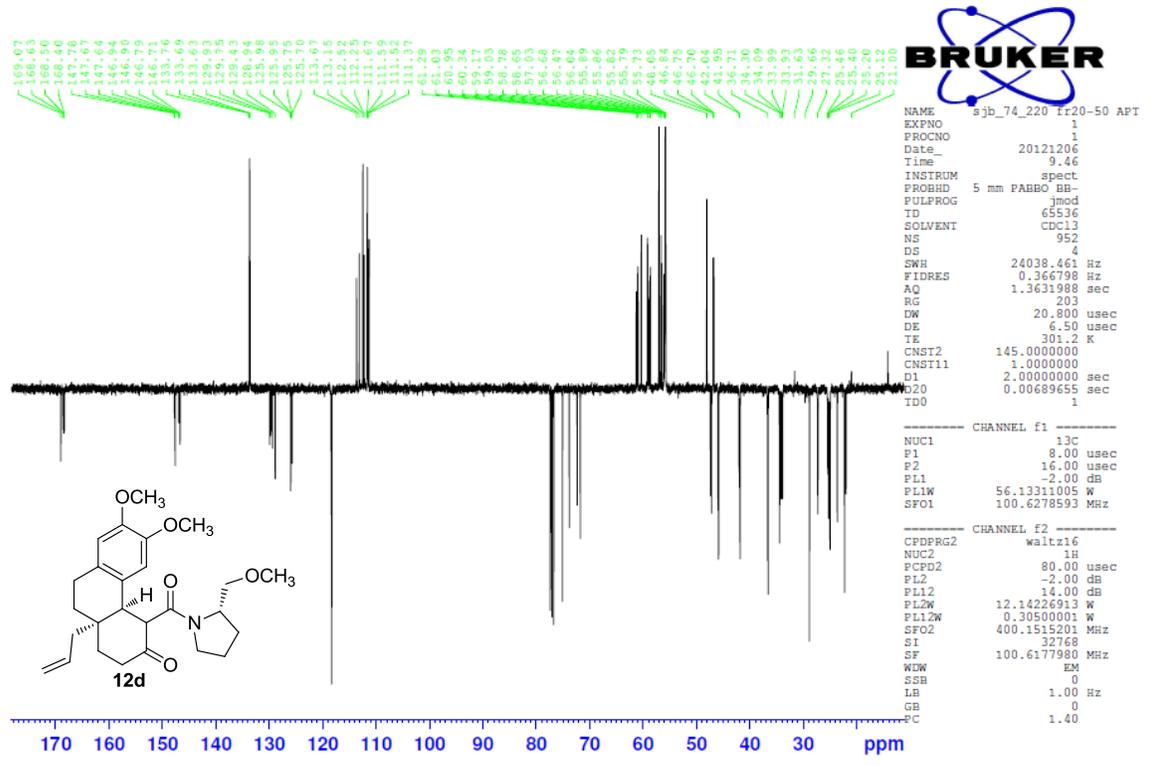
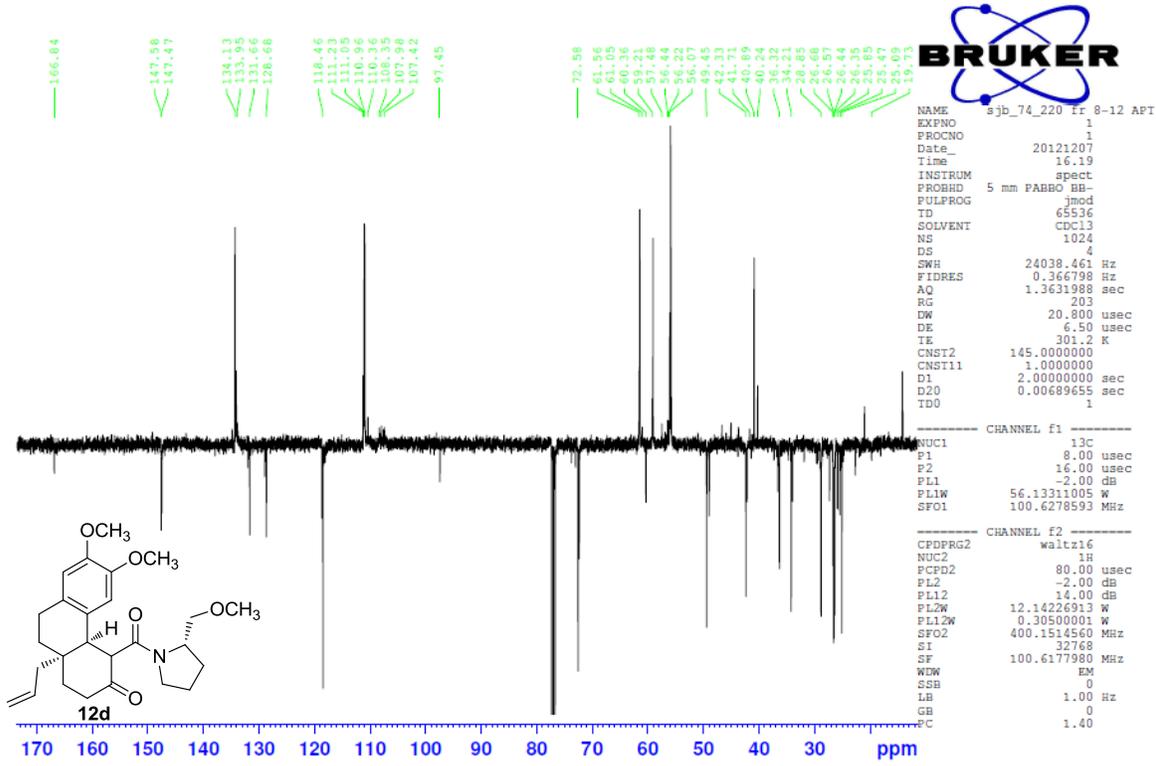


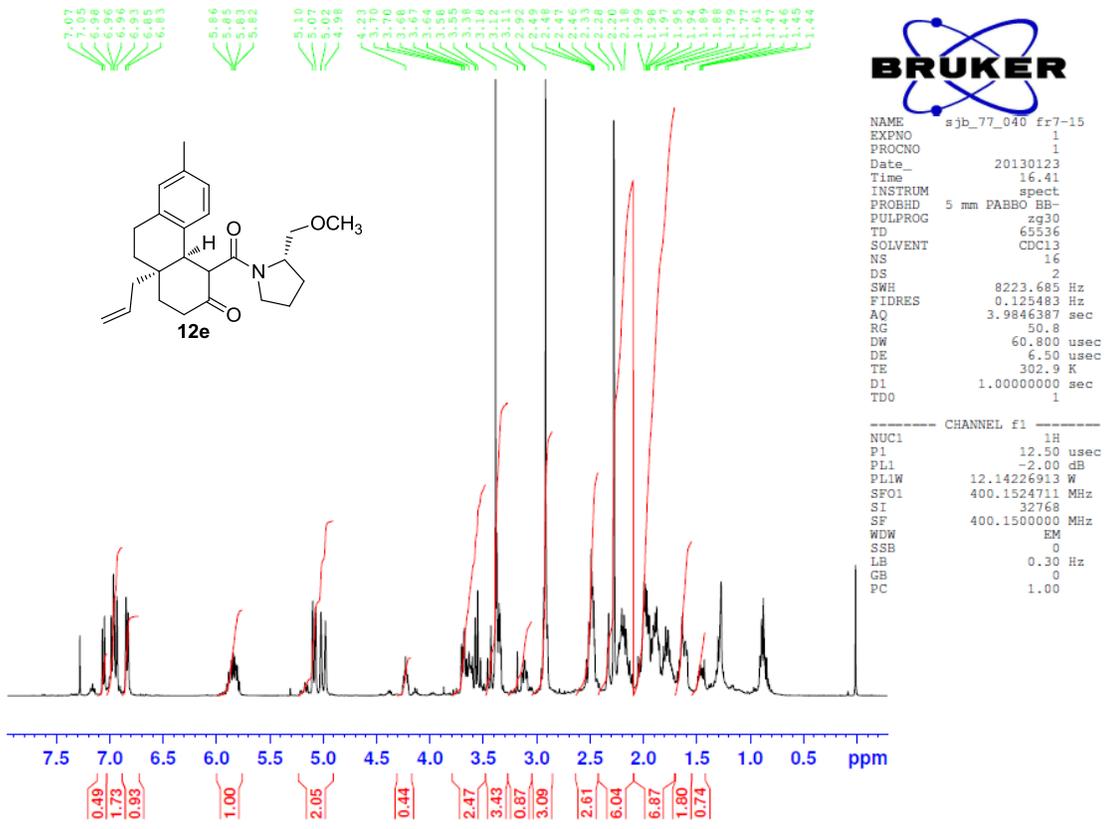
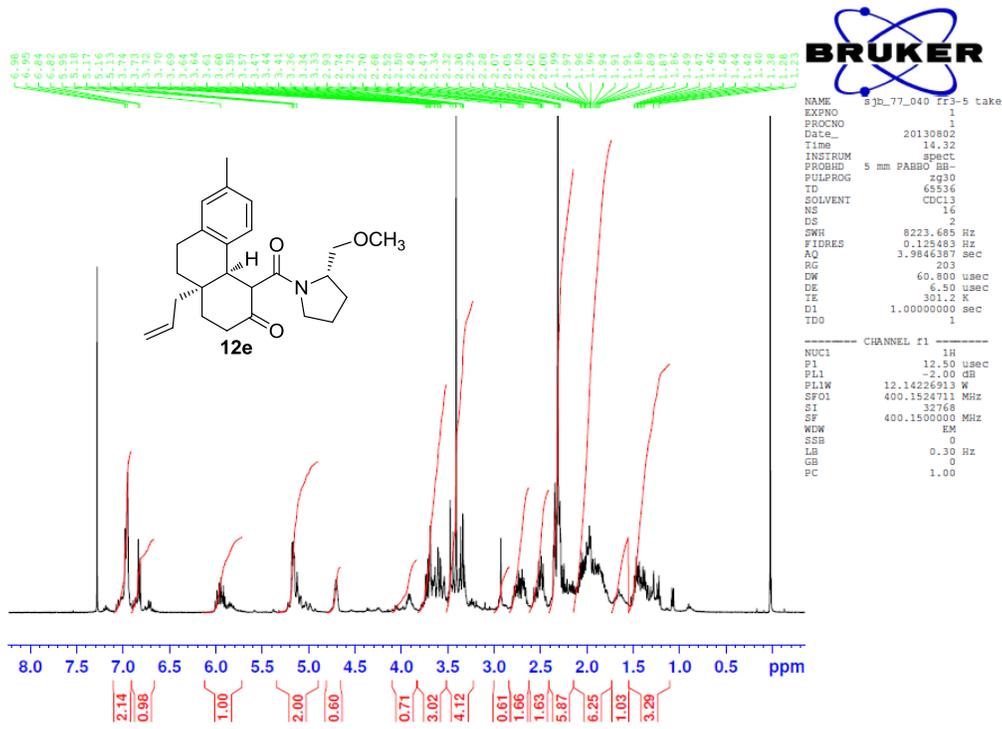
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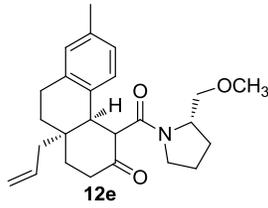
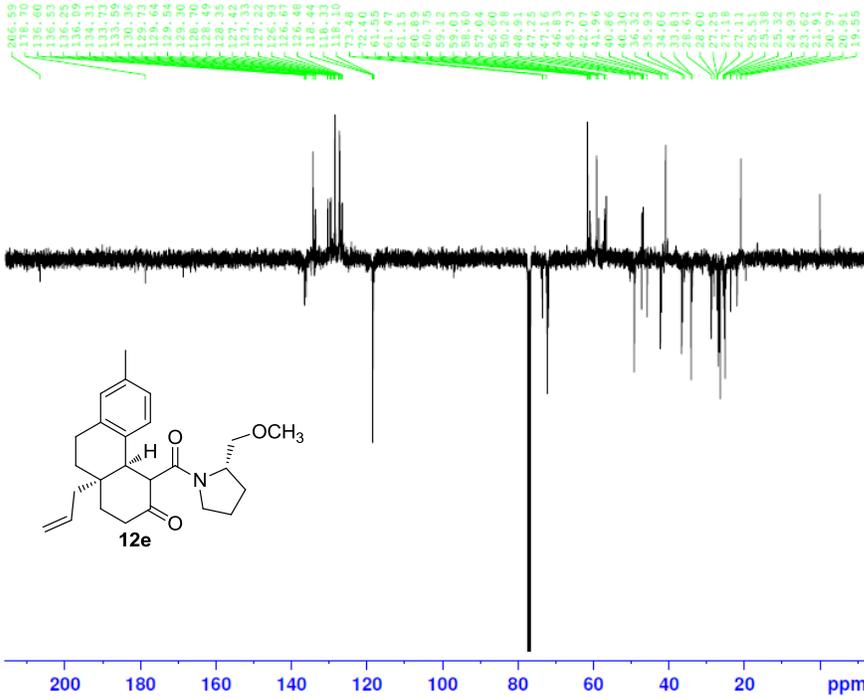
NAME      njb_77_090 fr10-33 take 2
EXPNO    1
PROCNO   1
Date_    20130805
Time     11.21
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        2
SWH      8223.685 Hz
FIDRES   0.125483 Hz
AQ        3.9846387 sec
RG        203
DW        60.800 usec
DE        6.50 usec
TE        301.2 K
D1        1.00000000 sec
TDO       1
===== CHANNEL f1 =====
NUC1     1H
P1       12.50 usec
PL1      -2.00 dB
PL1W     12.14226913 W
SFO1     400.1524711 MHz
SI       32768
SF       400.1500000 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
  
```











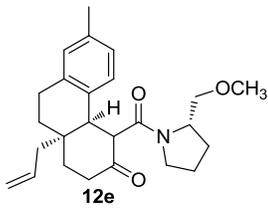
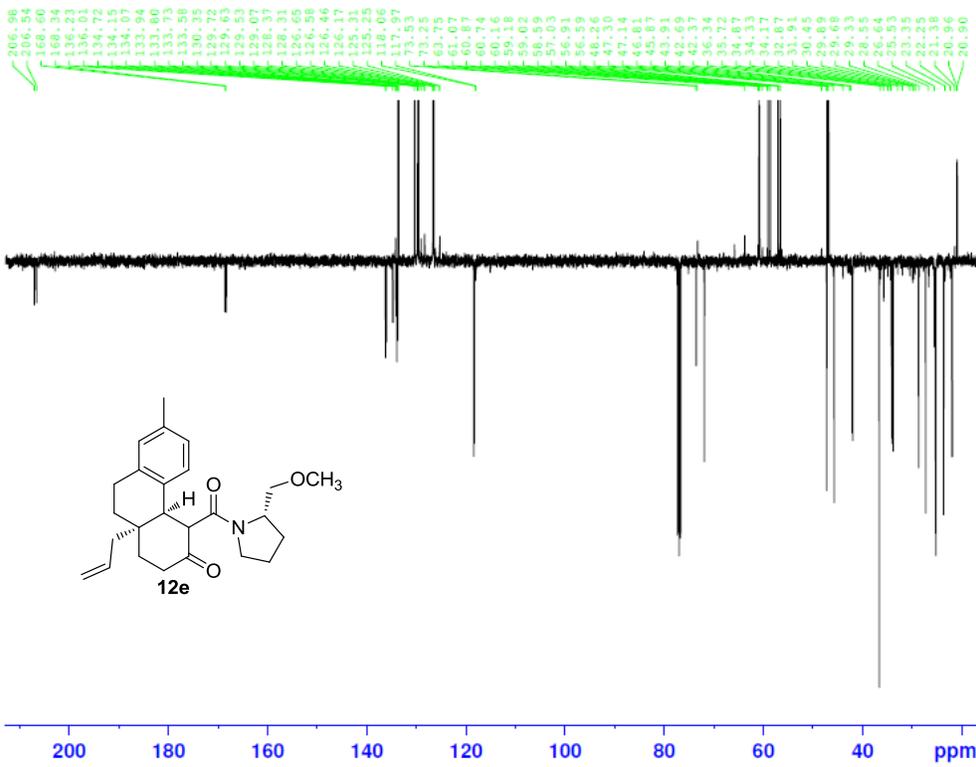
Current Data Parameters
 NAME sjb_77_040 less polar spinor AP1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140326
 Time 7.34
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG 7mod
 ID 65536
 SOLVENT CDCl3
 NS 11962
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 301.2 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 2.0000000 sec
 D20 0.00689655 sec
 TD0 1

----- CHANNEL f1 -----
 SFO1 100.6278593 MHz
 NUC1 13C
 P1 8.00 usec
 P2 16.00 usec
 PL1W 56.13299942 W

----- CHANNEL f2 -----
 SFO2 400.1514505 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PL1W 12.14200020 W
 PL12 0.24349000 W

F2 - Processing parameters
 SI 32768
 SF 100.6177980 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



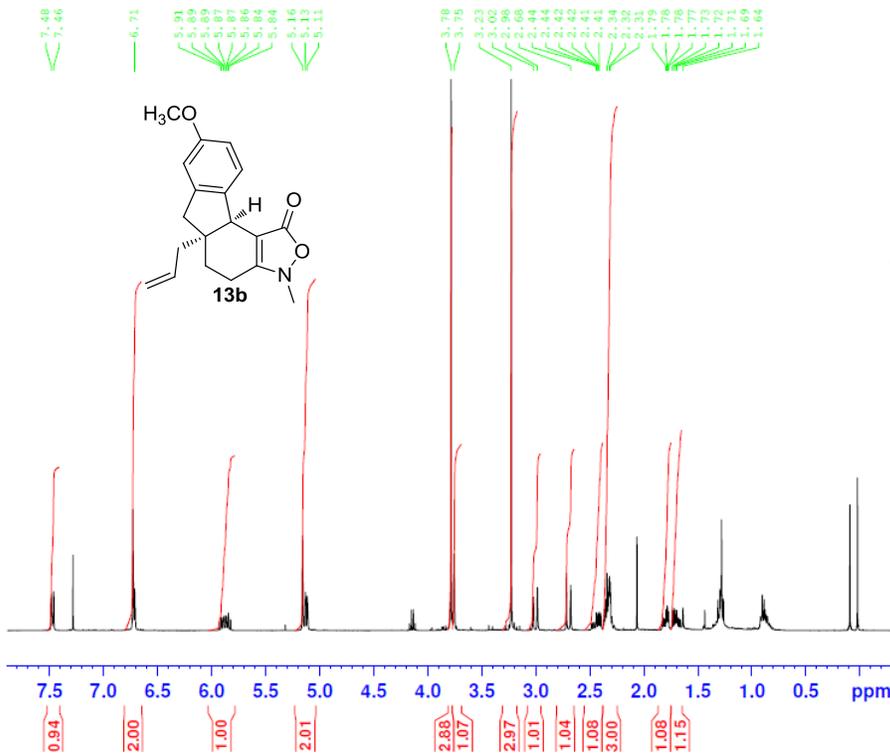
Current Data Parameters
 NAME sjb_77_030 fr7-
 EXPNO 1
 PROCNO 1

F2 - Acquisition Paramet
 Date_ 20130111
 Time 9.19
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG 7mod
 ID 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 24038.461
 FIDRES 0.366798
 AQ 1.3631488 sec
 RG 203
 DW 20.800
 DE 6.50
 TE 302.7
 CNST2 145.0000000
 CNST11 1.0000000
 D1 2.0000000
 D20 0.00689655
 TD0 1

----- CHANNEL f1 -----
 NUC1 13C
 P1 8.00
 P2 16.00
 PL1 -2.00
 PL1W 56.13311005 W
 SFO1 100.6278593

----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00
 PL2 -2.00
 PL12 14.00
 PL2W 12.14226913 W
 PL12W 0.30500001 W
 SFO2 400.1514507

F2 - Processing paramete
 SI 32768
 SF 100.6177980 MHz
 WDW EM
 SSB 0
 LB 1.00
 GB 0
 PC 1.40

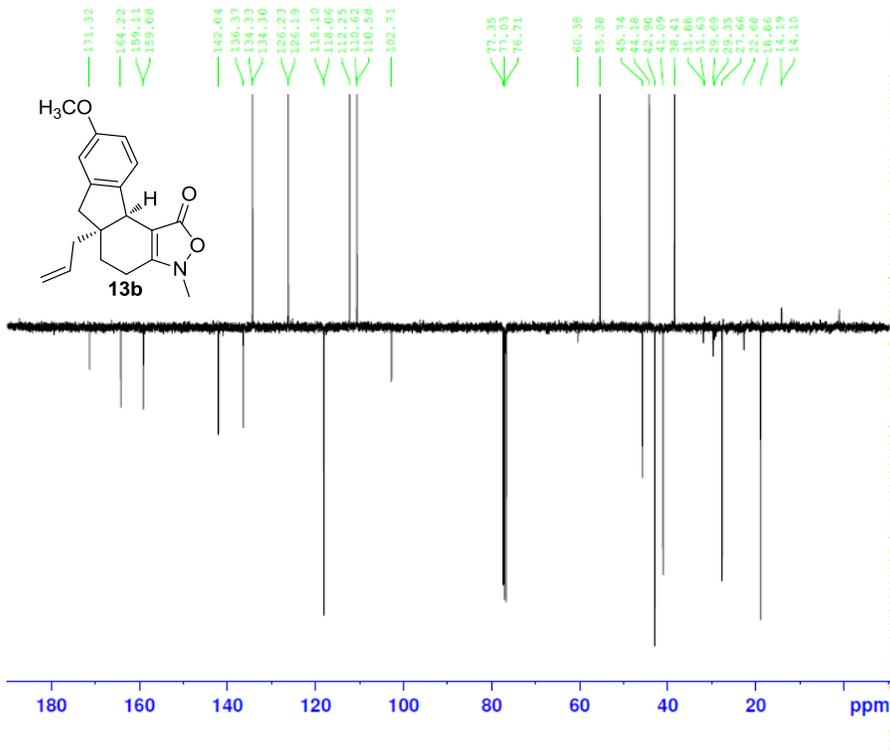


```

NAME      sjb_74_174fp
EXPNO    1
PROCNO   1
Date_    20121012
Time     15.37
INSTRUM  spect
PROBHD   5 mm DUL 13C-1
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        2
SWH      8223.685 Hz
FIDRES   0.125483 Hz
AQ        3.9846387 sec
RG        181
DW        60.800 usec
DE        6.50 usec
TE        301.2 K
D1        1.00000000 sec
TDO       1
  
```

```

===== CHANNEL f1 =====
NUC1      1H
P1        9.80 usec
PL1       -4.00 dB
PL1W      19.24419975 W
SFO1      400.1524711 MHz
SI        32768
SF        400.1500000 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
  
```



```

NAME      sjb_74_174fp 13CAPT
EXPNO    1
PROCNO   1
Date_    20121017
Time     9.19
INSTRUM  spect
PROBHD   5 mm DUL 13C-1
PULPROG  jmod
TD        65536
SOLVENT  CDCl3
NS        1024
DS        4
SWH      20161.291 Hz
FIDRES   0.307637 Hz
AQ        1.6253428 sec
RG        203
DW        24.800 usec
DE        6.50 usec
TE        301.2 K
CNST2    145.0000000
CNST11   1.0000000
D1        2.00000000 sec
D2        0.00689655 sec
TDO       1
  
```

```

===== CHANNEL f1 =====
NUC1      13C
P1        9.00 usec
P2        18.00 usec
PL1       0.00 dB
PL1W      35.41759872 W
SFO1      100.6268310 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       -3.80 dB
PL12      13.80 dB
PL2W      18.37806702 W
SFO2      400.1514525 MHz
SI        32768
SF        100.6177980 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```

Area Percent Report

Data Path : C:\msdchem\1\DATA\
Data File : sjb_74_174fp.D
Acq On : 12 Oct 2012 15:09
Operator : sjb
Sample : sjb_74_174fp
Misc :
ALS Vial : 85 Sample Multiplier: 1

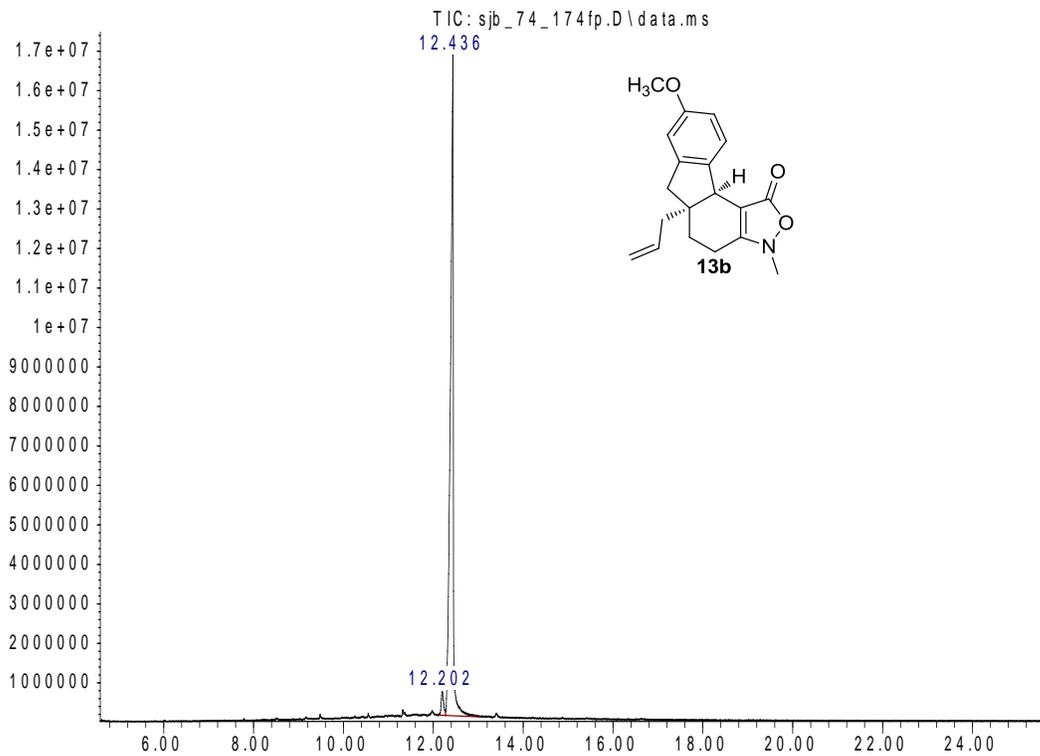
Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\msdchem\1\METHODS\JMB2.m
Title :

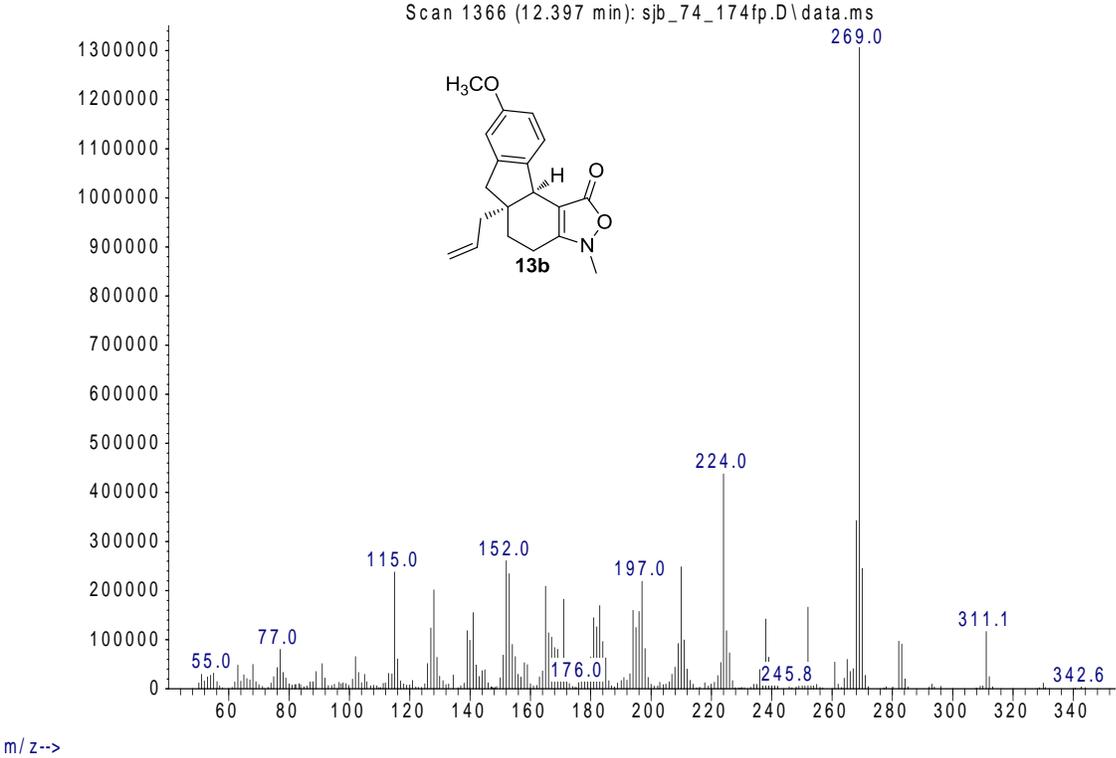
Signal : TIC: sjb_74_174fp.D\data.ms

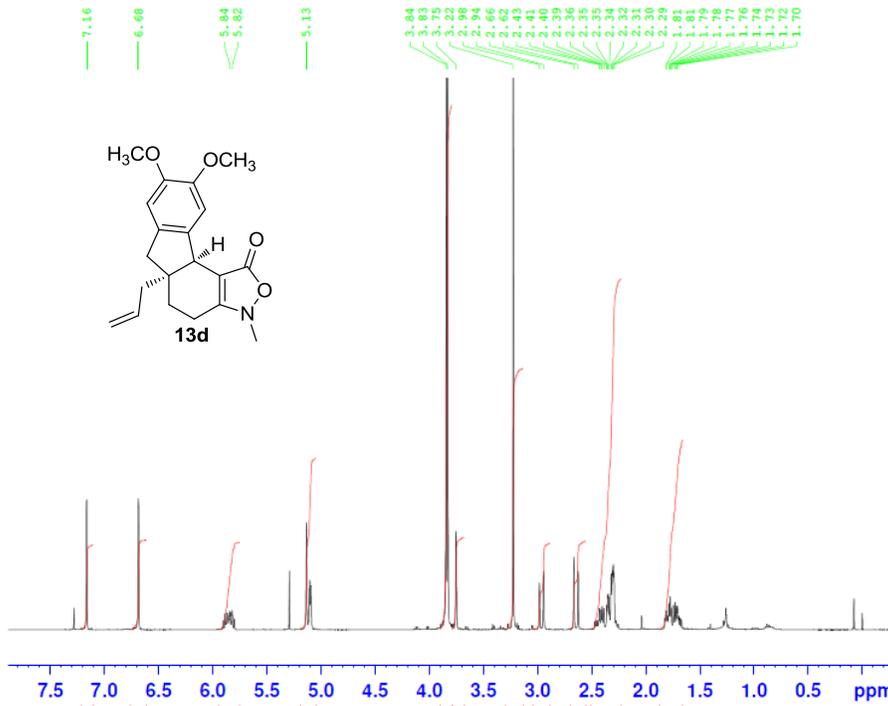
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	12.202	1316	1332	1344	BV 5	600471	23119397	3.01%	2.924%
2	12.436	1344	1373	1479	VB	17087691	767689587	100.00%	97.076%

Abundance



Abundance

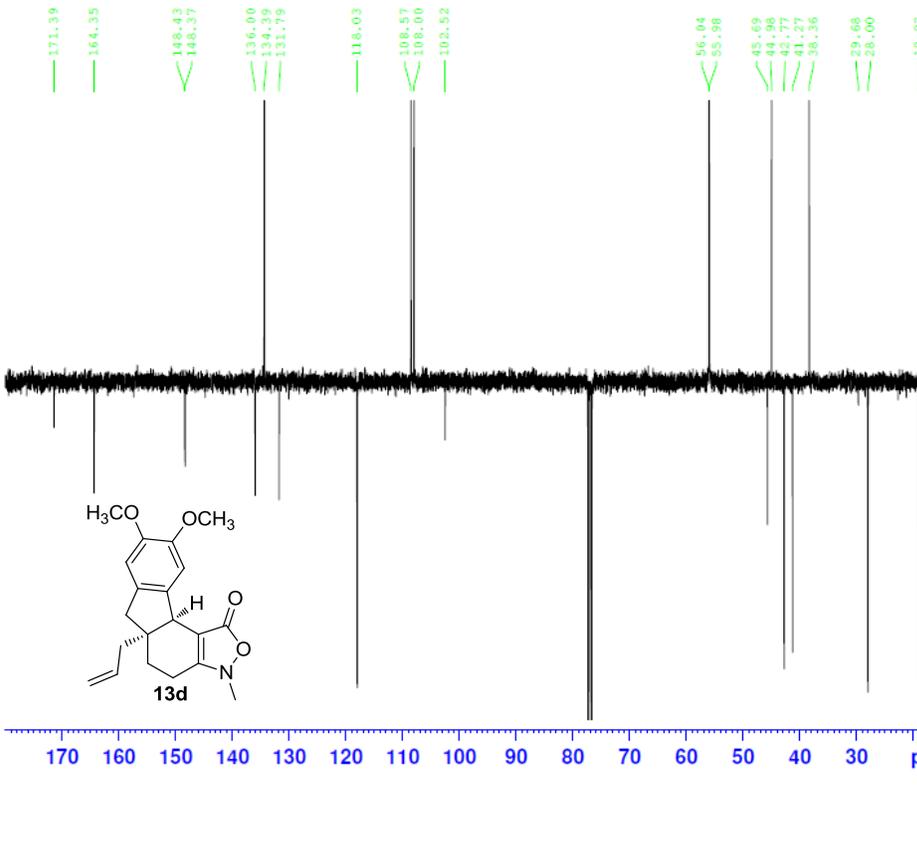




```

NAME      sjb_74_171fp
EXPNO     1
PROCNO    1
Date_     20121011
Time      15.10
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH       8223.685 Hz
FIDRES    0.125483 Hz
AQ         3.9846387 sec
RG         50.8
DW         60.800 usec
DE         6.50 usec
TE         301.1 K
D1         1.0000000 sec
D11        1
D12        1
D13        1
D14        1
D15        1
D16        1
D17        1
D18        1
D19        1
D20        1
D21        1
D22        1
D23        1
D24        1
D25        1
D26        1
D27        1
D28        1
D29        1
D30        1
D31        1
D32        1
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D34        1
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D995       1
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D997       1
D998       1
D999       1
D1000       1

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```

Current Data Parameters
NAME      sjb_81_128fp
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20140325
Time      20.07
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   jmod
TD         65536
SOLVENT   CDCl3
NS         474
DS         4
SWH       24038.461 Hz
FIDRES    0.366798 Hz
AQ         1.3631488 sec
RG         203
DW         20.800 usec
DE         6.50 usec
TE         301.2 K
CNST2     145.0000000
CNST11    1.0000000
D1         2.0000000 sec
D20        0.00689655 sec
D21        1
D22        1
D23        1
D24        1
D25        1
D26        1
D27        1
D28        1
D29        1
D30        1
D31        1
D32        1
D33        1
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D36        1
D37        1
D38        1
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D90        1
D91        1
D92        1
D93        1
D94        1
D95        1
D96        1
D97        1
D98        1
D99        1
D100       1

===== CHANNEL f1 =====
SFO1      100.6278593 MHz
NUC1      13C
P1         8.00 usec
P2         16.00 usec
PLW1      56.13299942 W

===== CHANNEL f2 =====
SFO2      400.1516006 MHz
NUC2      1H
CPDPRG[2] waltz16
PCPD2     90.00 usec
PLW2      12.14200020 W
PLW12     0.24369000 W

F2 - Processing parameters
SI         32768
SF         100.6177980 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

```

Area Percent Report

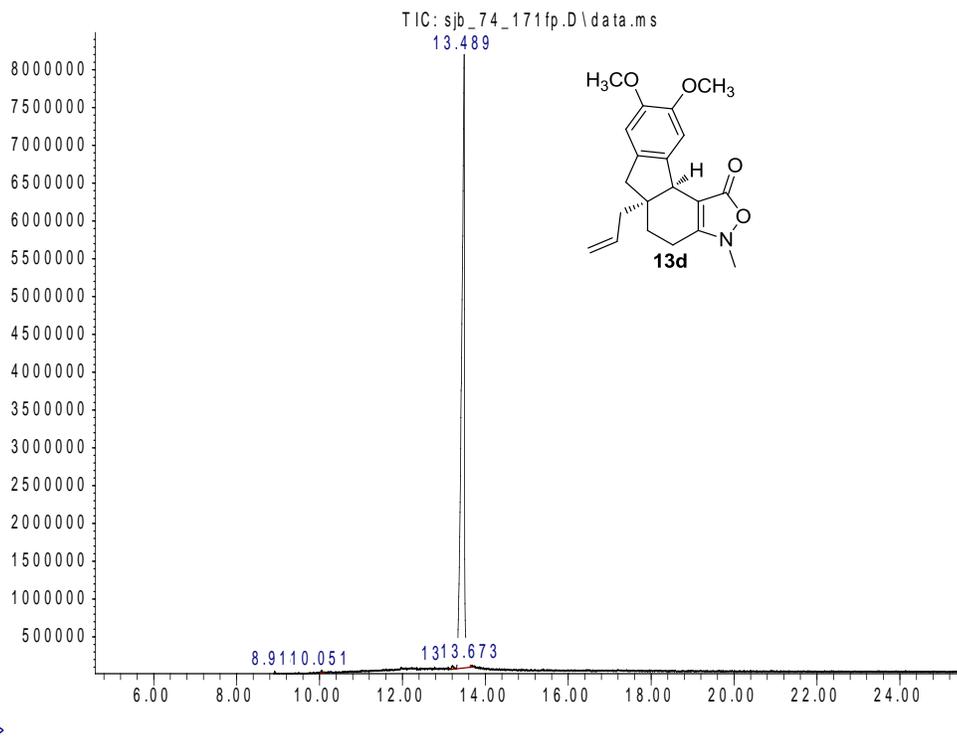
Data Path : C:\msdchem\1\DATA\
 Data File : sjb_74_171fp.D
 Acq On : 11 Oct 2012 12:24
 Operator : sjb
 Sample : sjb_74_171fp
 Misc :
 ALS Vial : 85 Sample Multiplier: 1
 Integration Parameters: autoint1.e
 Integrator: ChemStation
 Method : C:\msdchem\1\METHODS\JMB2.m
 Title :
 Signal : TIC: sjb_74_171fp.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.918	753	758	764	BV 2	35877	546275	0.14%	0.136%
2	10.051	949	956	964	PV 6	33672	718804	0.18%	0.179%
3	13.207	1502	1507	1516	PV 6	42452	1193281	0.30%	0.298%
4	13.489	1522	1557	1582	PV 2	8446940	397073139	100.00%	99.067%
5	13.642	1582	1584	1587	VV 4	63804	727438	0.18%	0.181%
6	13.673	1587	1589	1595	VV 6	37292	555213	0.14%	0.139%

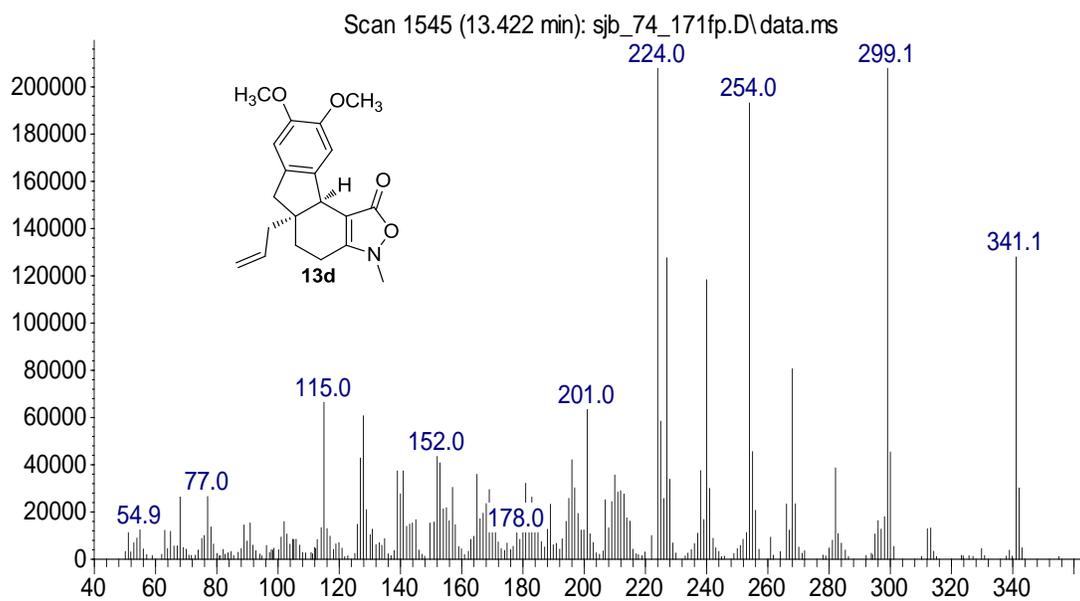
Sum of corrected areas: 400814149

JMB2.m Wed Oct 17 15:09:01 2012

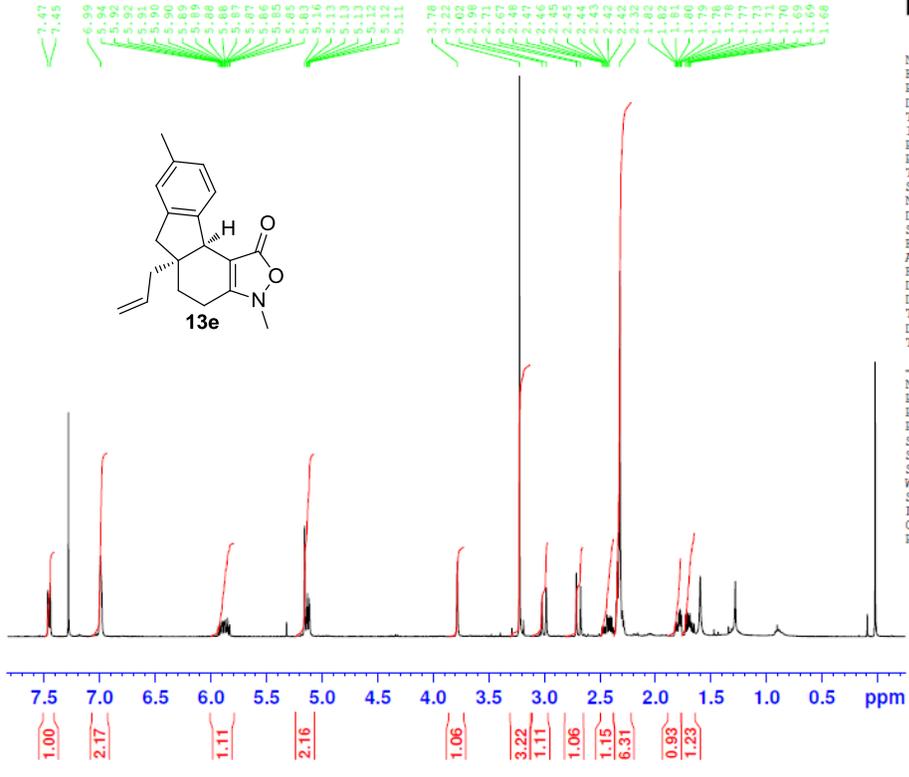
Abundance



Abundance

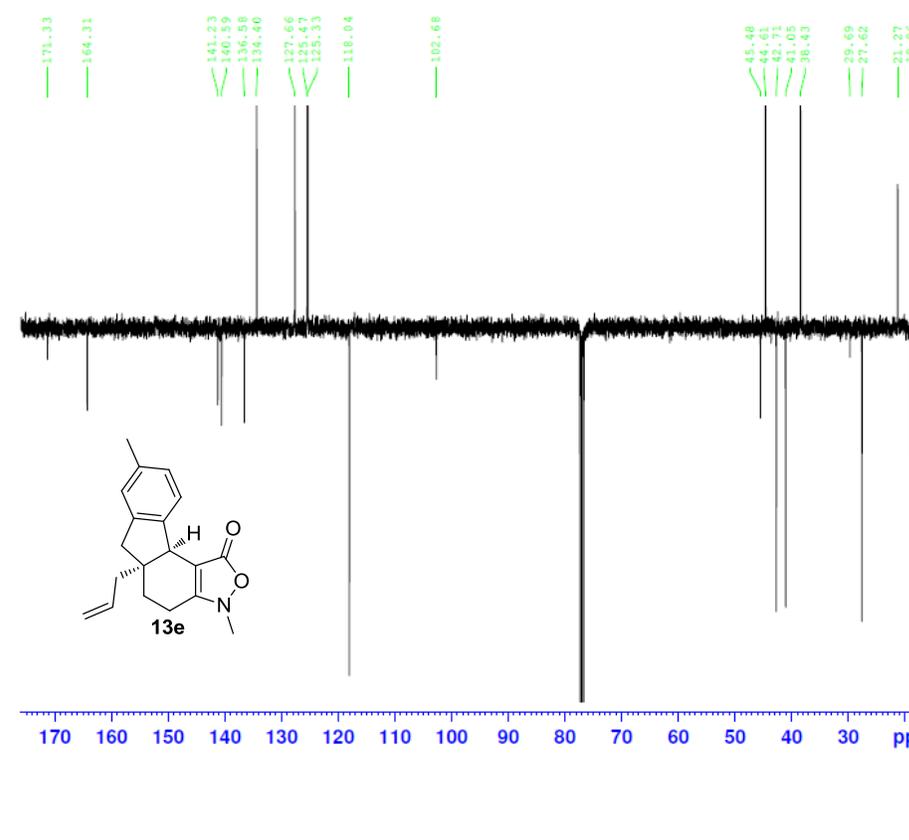


m/z-->



NAME sjb_77_152fp take 2
EXPNO 1
PROCNO 1
Date_ 20130726
Time 8.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 301.2 K
D1 1.00000000 sec
TDO 1

----- CHANNEL f1 -----
NUC1 1H
P1 12.50 usec
PL1 -2.00 dB
PL1W 12.14226913 W
SFO1 400.1524711 MHz
SI 32768
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME sjb_77_152fp APT
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130726
Time 9.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT CDC13
NS 991
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 301.2 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TDO 1

----- CHANNEL f1 -----
NUC1 13C
P1 8.00 usec
F2 16.00 usec
PL1 -2.00 dB
PL1W 56.13311005 W
SFO1 100.6278593 MHz

----- CHANNEL f2 -----
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 14.00 dB
PL2W 12.14226913 W
PL12W 0.30500001 W
SFO2 400.1515990 MHz

F2 - Processing parameters
SI 32768
SF 100.6177980 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Area Percent Report

Data Path : C:\msdchem\1\DATA\
 Data File : sjb_77_152fp.D
 Acq On : 16 Jul 2013 17:41
 Operator : sjb
 Sample : sjb_77_152fp
 Misc :
 ALS Vial : 85 Sample Multiplier: 1
 Integration Parameters: autoint1.e
 Integrator: ChemStation
 Method : C:\msdchem\1\METHODS\ckr3.m
 Title :

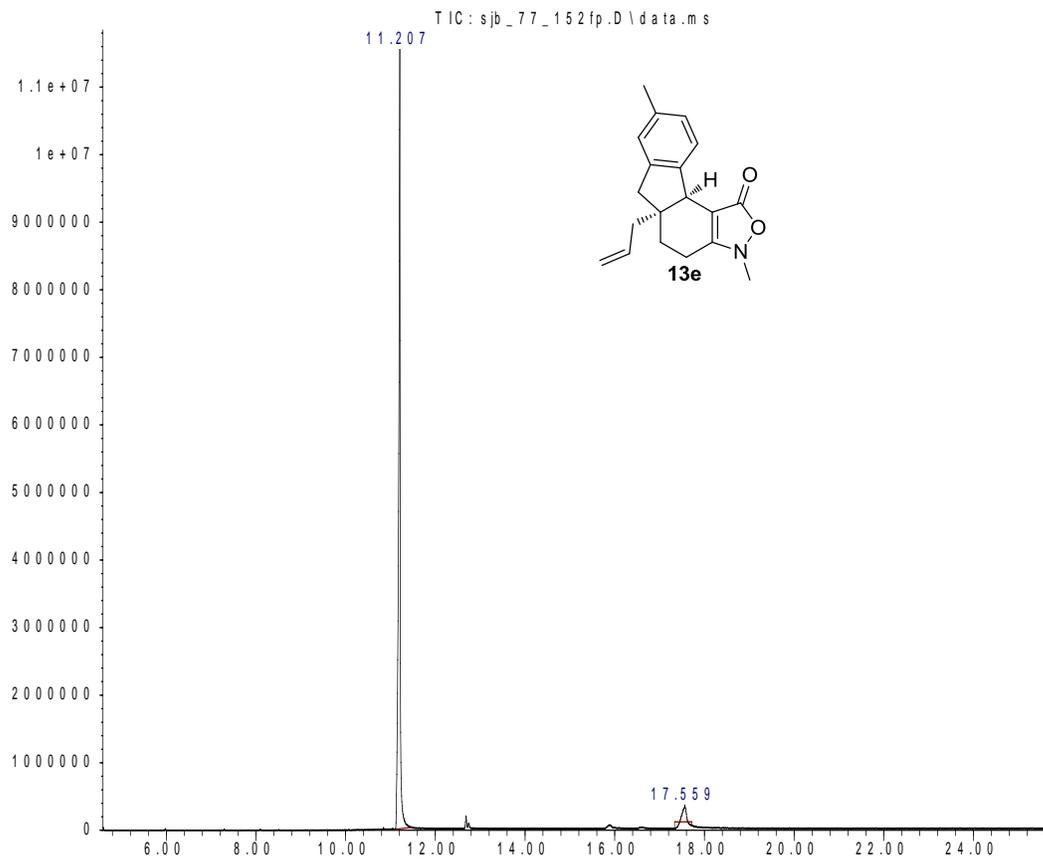
Signal : TIC: sjb_77_152fp.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	11.207	1139	1158	1202	BV	11463397	276482325	100.00%	95.401%
2	17.559	2229	2268	2297	M5	248076	13329377	4.82%	4.599%

Sum of corrected areas: 289811703

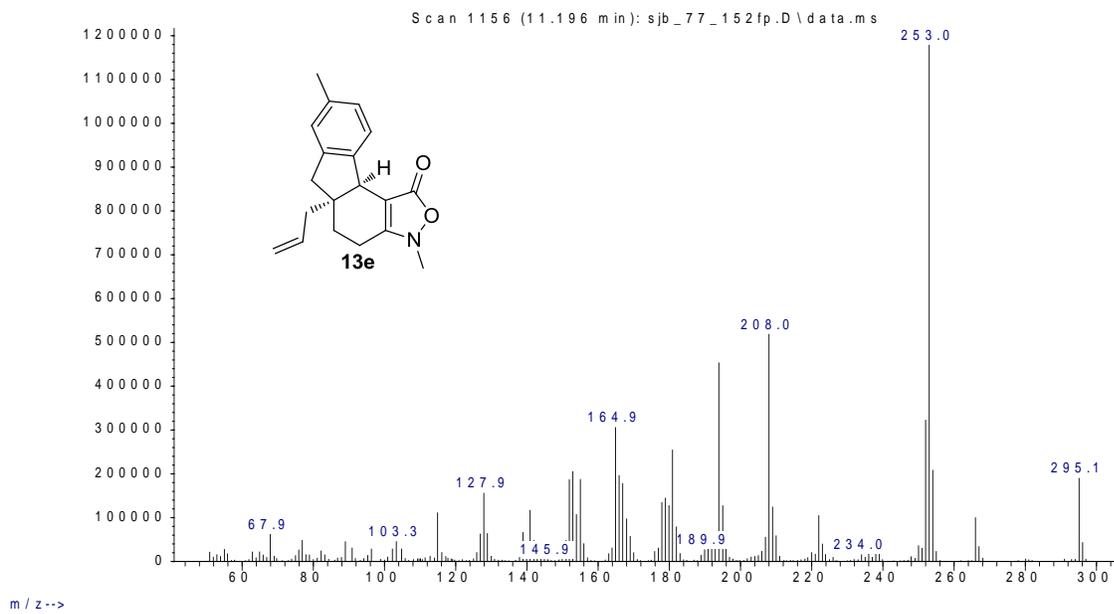
ckr3.m Mon May 12 16:00:02 2014

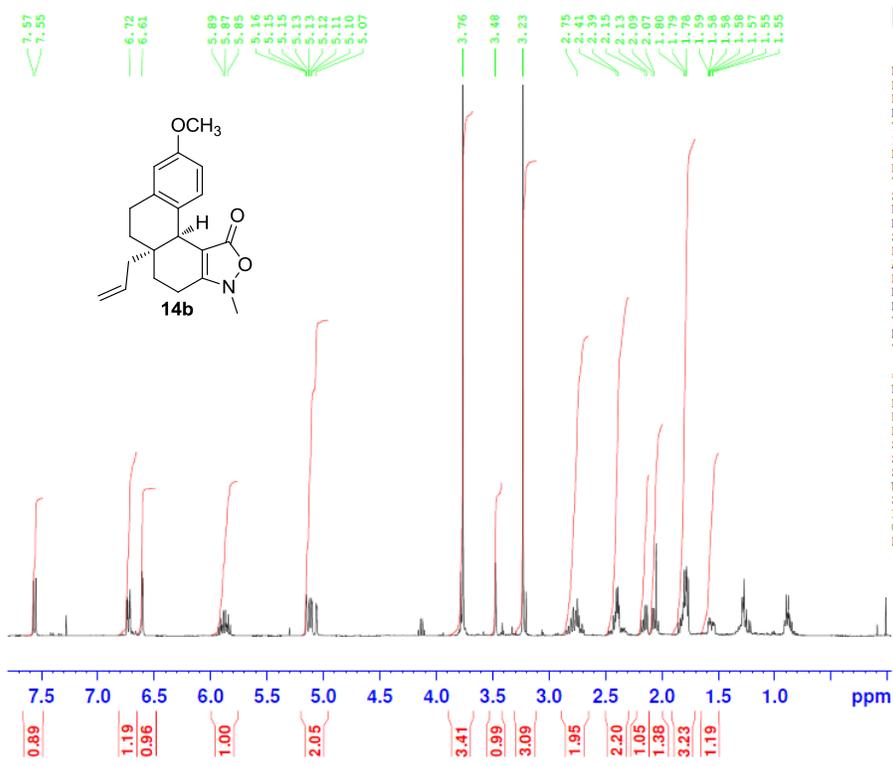
Abundance



Time-->

Abundance

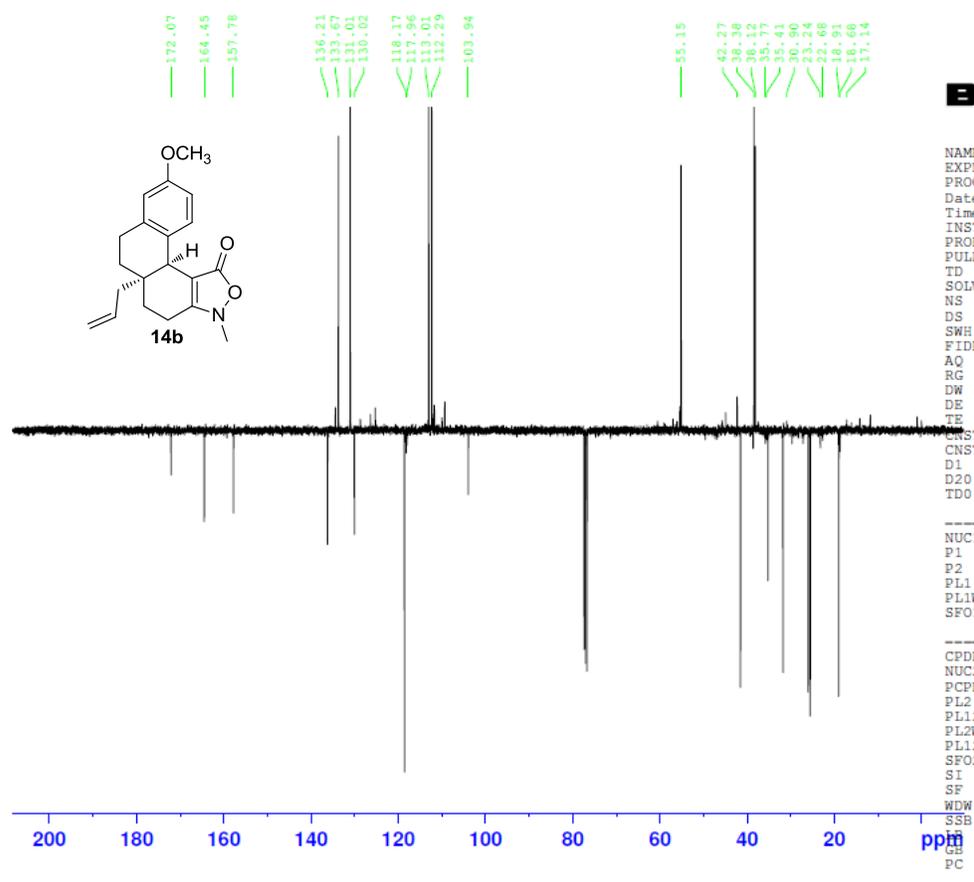




```

NAME      sjb_74_053fp
EXPNO    1
PROCNO   1
Date_    20120703
Time     13.50
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       2
SWH      8223.685 Hz
FIDRES   0.125483 Hz
AQ       3.9846387 sec
RG       40.3
DW       60.800 usec
DE       6.50 usec
TE       301.3 K
D1       1.00000000 sec
TDO      1

===== CHANNEL f1 =====
NUC1     1H
P1       12.50 usec
PL1      -2.00 dB
PL1W     12.14226913 W
SFO1     400.1524711 MHz
SI       32768
SF       400.1500000 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
  
```



```

NAME      sjb_77_094fp 13CAPT
EXPNO    1
PROCNO   1
Date_    20130531
Time     9.22
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  jmod
TD       65536
SOLVENT  CDCl3
NS       1024
DS       4
SWH      21929.824 Hz
FIDRES   0.334623 Hz
AQ       1.4942708 sec
RG       203
DW       22.800 usec
DE       6.50 usec
TE       301.2 K
CNST2    145.0000000
CNST11   1.0000000
D1       2.00000000 sec
D20      0.00689655 sec
TDO      1

----- CHANNEL f1 -----
NUC1     13C
P1       8.00 usec
P2       16.00 usec
PL1      -2.00 dB
PL1W     56.13311005 W
SFO1     100.6277931 MHz

----- CHANNEL f2 -----
CPDPRG2  waltz16
NUC2     1H
PCPD2    80.00 usec
PL2      -2.00 dB
PL12     14.00 dB
PL2W     12.14226913 W
PL12W    0.30500001 W
SFO2     400.1515655 MHz
SI       32768
SF       100.6177980 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
  
```

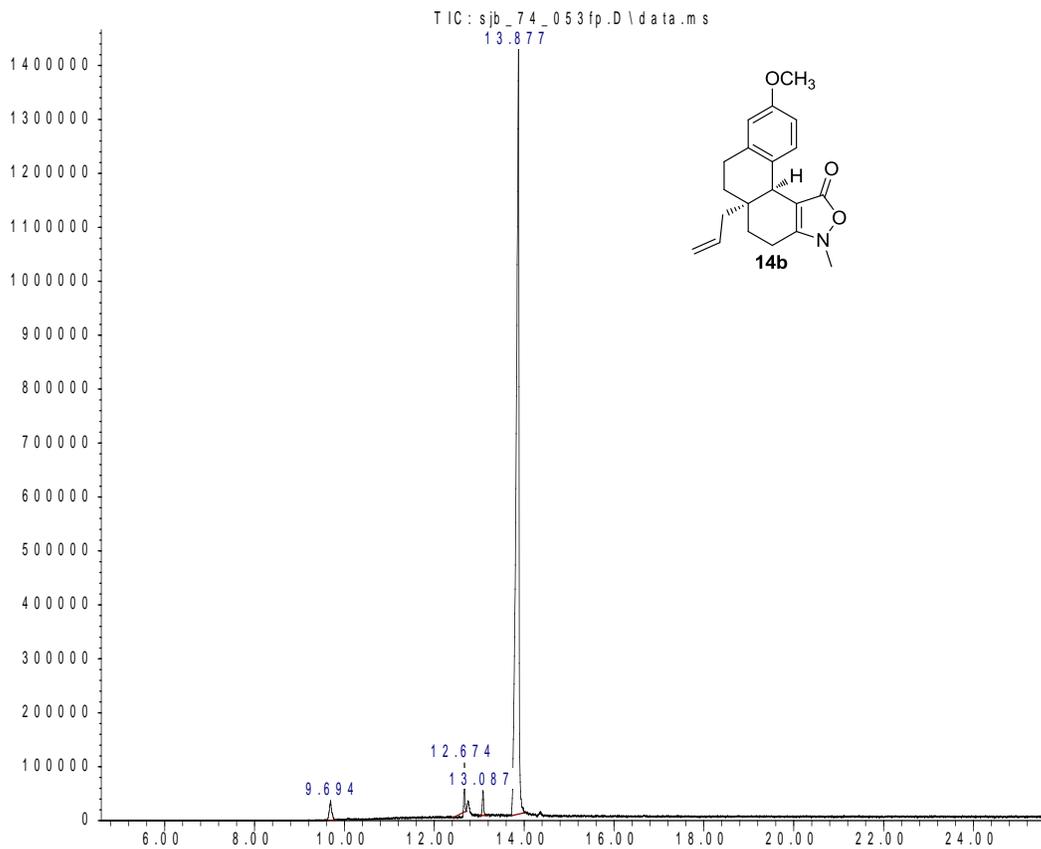
Area Percent Report

Data Path : C:\msdchem\1\DATA\
 Data File : sjb_74_053fp.D
 Acq On : 3 Jul 2012 12:50
 Operator : sjb
 Sample : sjb_74_053fp
 Misc :
 ALS Vial : 100 Sample Multiplier: 1
 Integration Parameters: autoint1.e
 Integrator: ChemStation
 Method : C:\msdchem\1\METHODS\JMB2.m
 Title :
 Signal : TIC: sjb_74_053fp.D\data.ms

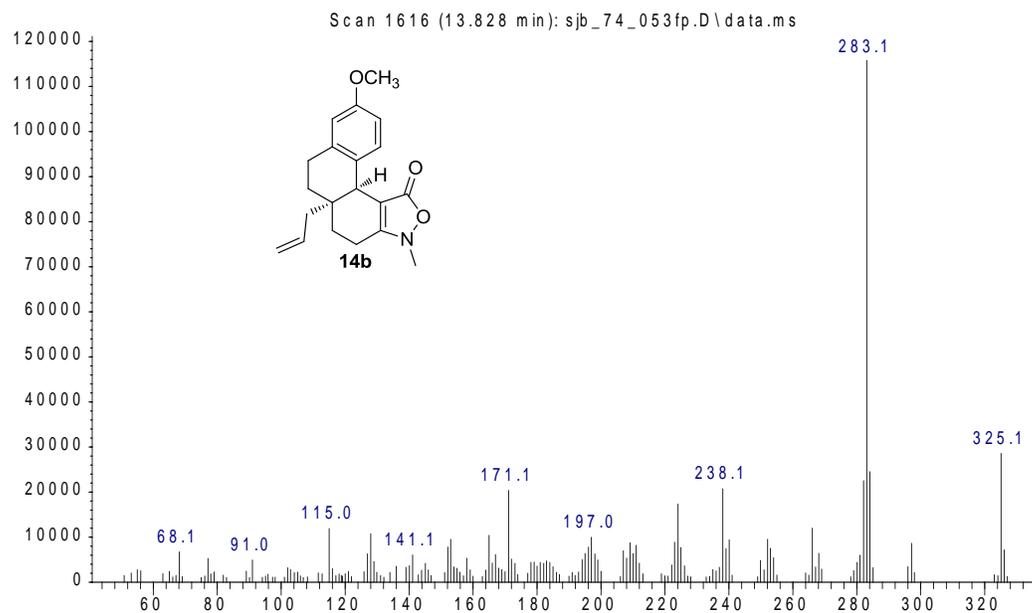
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	9.694	882	894	912	BB	34783	1341908	2.20%	2.098%
2	12.674	1367	1414	1420	BV	87897	861272	1.42%	1.346%
3	13.087	1474	1487	1498	BV 4	45615	902735	1.48%	1.411%
4	13.877	1595	1625	1647	PV 2	1452537	60865753	100.00%	95.145%
Sum of corrected areas:								63971668	

JMB2.m Wed Oct 17 15:30:37 2012

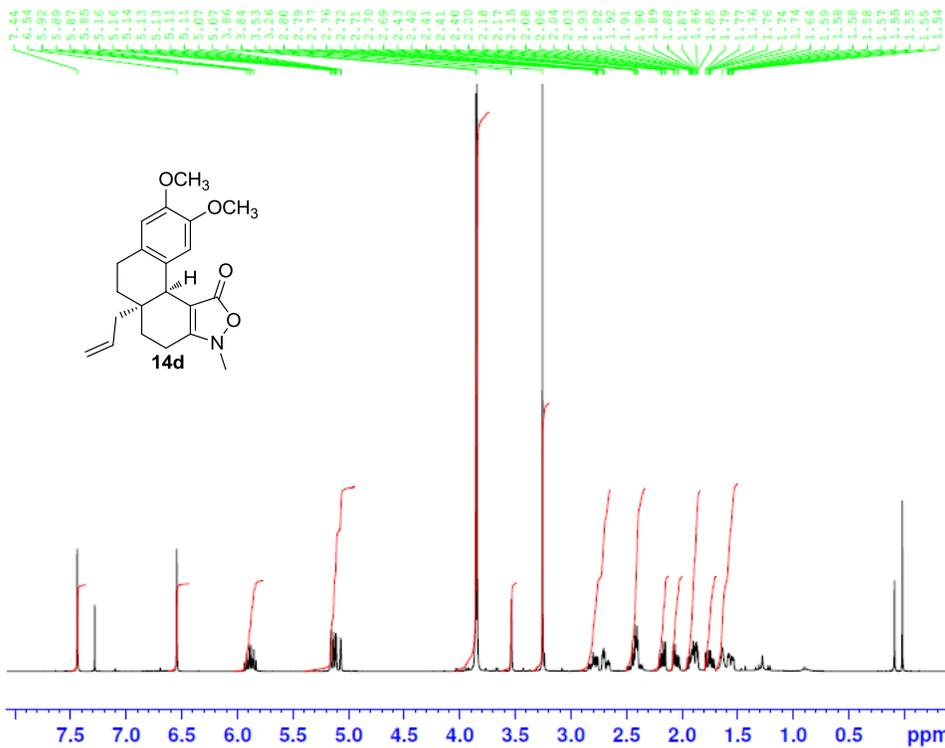
Abundance



Abundance

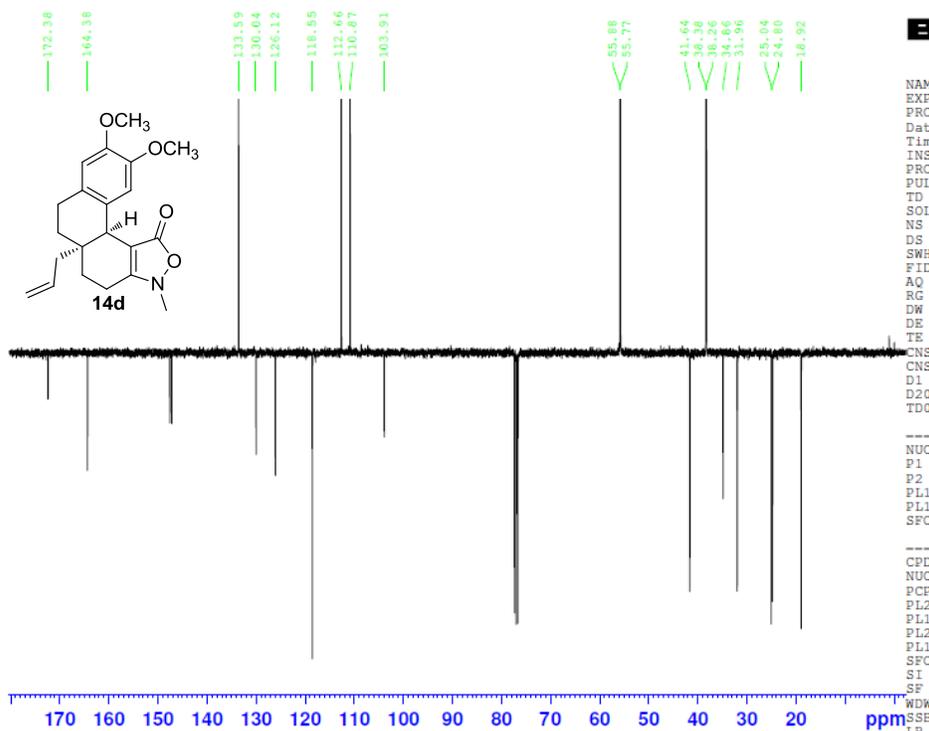


m/z-->



NAME sjb_77_002fp take 2
 EXPNO 1
 PROCNO 1
 Date_ 20130805
 Time 11.14
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 181
 DW 60.800 usec
 DE 6.50 usec
 TE 301.2 K
 D1 1.00000000 sec
 TD0 1

----- CHANNEL f1 -----
 NUC1 1H
 P1 12.50 usec
 PL1 -2.00 dB
 PL1W 12.14226913 W
 SFO1 400.1524711 MHz
 SI 32768
 SF 400.1500000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



NAME sjb_77_002 13CAPT
 EXPNO 1
 PROCNO 1
 Date_ 20121207
 Time 9.37
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG jmod
 TD 65536
 SOLVENT CDC13
 NS 1024
 DS 4
 SWH 18382.354 Hz
 FIDRES 0.280492 Hz
 AQ 1.7826293 sec
 RG 203
 DW 27.200 usec
 DE 6.50 usec
 TE 301.2 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 2.00000000 sec
 D20 0.00689655 sec
 TD0 1

----- CHANNEL f1 -----
 NUC1 13C
 P1 8.00 usec
 P2 16.00 usec
 PL1 -2.00 dB
 PL1W 56.13311005 W
 SFO1 100.6267469 MHz

----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -2.00 dB
 PL12 14.00 dB
 PL2W 12.14226913 W
 PL12W 0.30500001 W
 SFO2 400.1514987 MHz
 SI 32768
 SF 100.6177980 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Area Percent Report

Data Path : C:\msdchem\1\DATA\
Data File : sjb_72_195fp.D
Acq On : 1 May 2012 17:23
Operator : sjb
Sample : sjb_72_195fp
Misc :
ALS Vial : 45 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

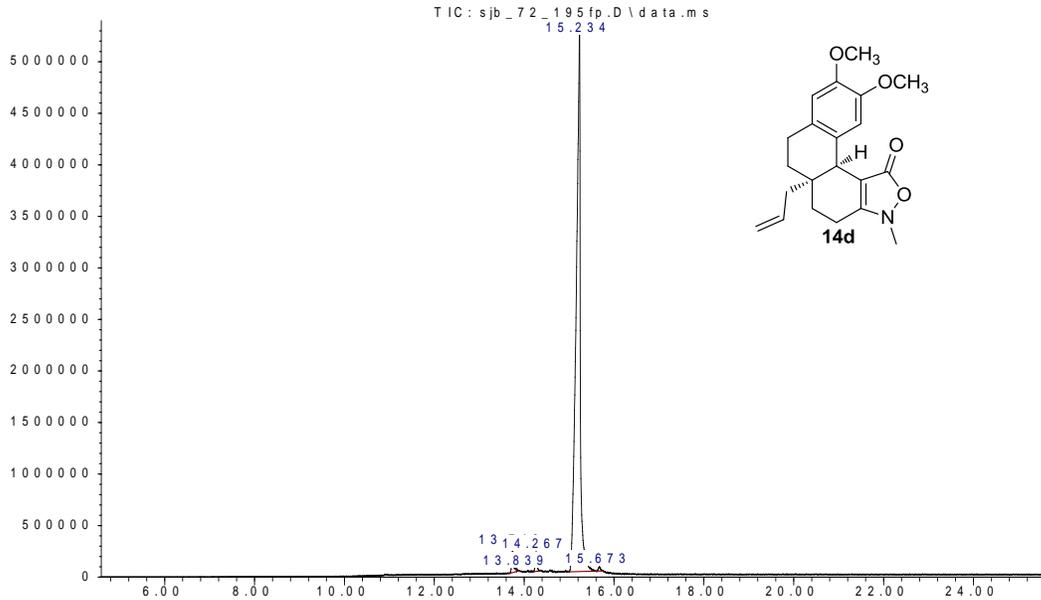
Method : C:\msdchem\1\METHODS\JMB2.m
Title :

Signal : TIC: sjb_72_195fp.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	13.743	1587	1601	1616	PV 9	232062	6716431	2.01%	1.928%
2	13.839	1616	1618	1624	VV 6	23517	354612	0.11%	0.102%
3	14.267	1683	1693	1708	PV 6	188248	5335080	1.59%	1.531%
4	15.234	1817	1862	1912	PV	5381726	334739484	100.00%	96.071%
5	15.673	1921	1938	1951	PV 10	40476	1284013	0.38%	0.369%

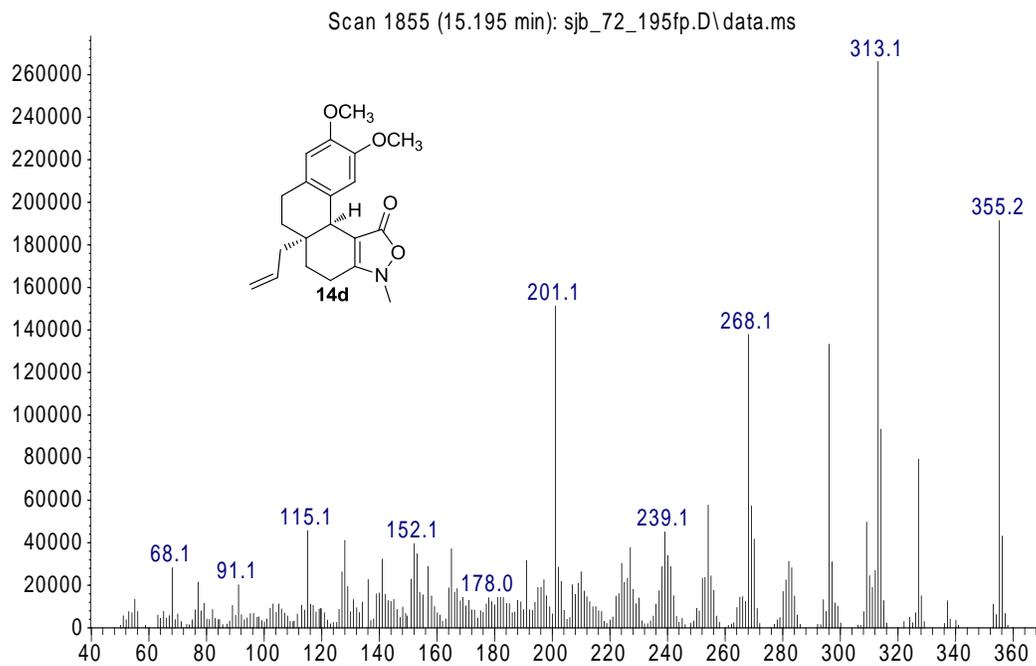
Sum of corrected areas: 348429620

Abundance

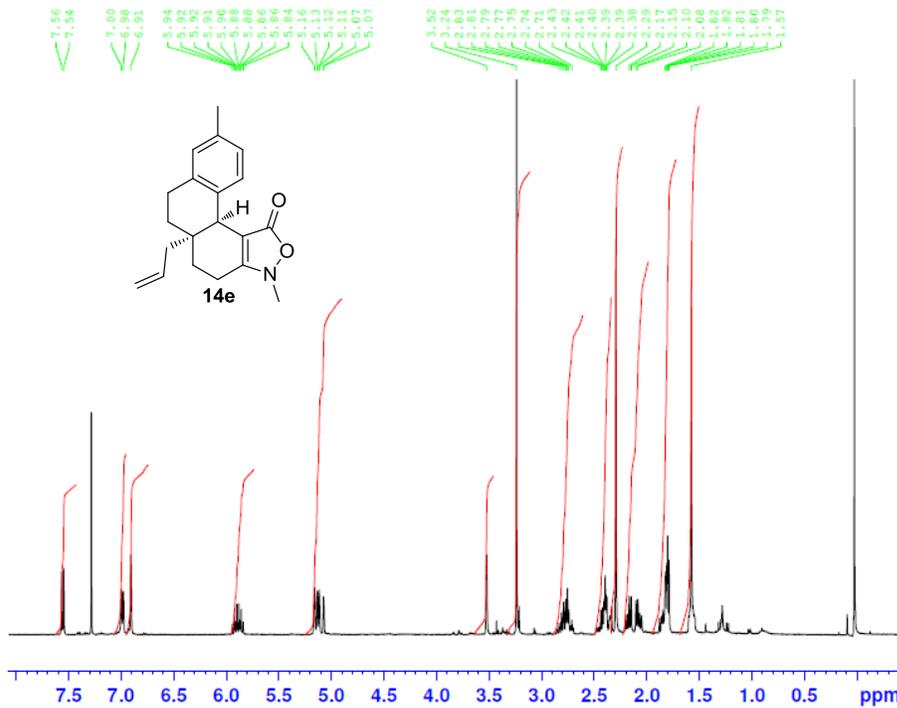


Time-->

Abundance

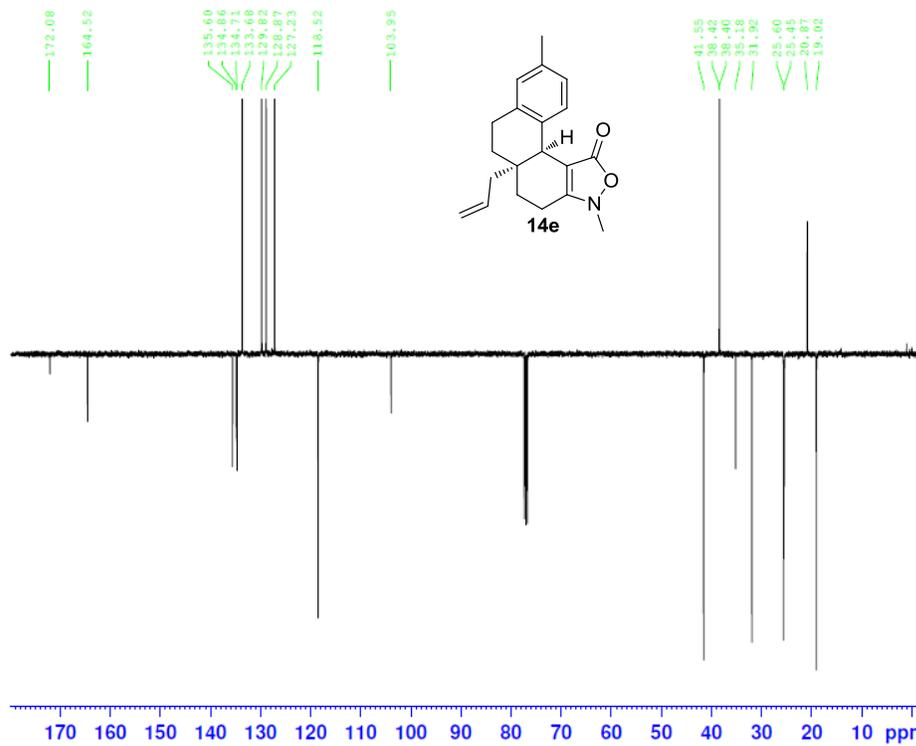


m/z-->



NAME sjb_77_041fp take 2
EXPNO 1
PROCNO 1
Date_ 20130802
Time 14.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 301.2 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 1H
P1 12.50 usec
PL1 -2.00 dB
PL1W 12.14226913 W
SFO1 400.1524711 MHz
SI 32768
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME sjb_77_032fp APT
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130115
Time 13.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 18382.354 Hz
FIDRES 0.280492 Hz
AQ 1.7825792 sec
RG 203
DW 27.200 usec
DE 6.50 usec
TE 299.5 K
CNST2 145.0000000
CNST11 1.0000000
D1 2.00000000 sec
D20 0.00689655 sec
TD0 1

----- CHANNEL f1 -----
NUC1 13C
P1 8.00 usec
P2 16.00 usec
PL1 -2.00 dB
PL1W 56.13311005 W
SFO1 100.6266983 MHz

----- CHANNEL f2 -----
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 14.00 dB
PL2W 12.14226913 W
PL12W 0.30500001 W
SFO2 400.1515831 MHz

F2 - Processing parameters
SI 32768
SF 100.6177980 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Area Percent Report

Data Path : C:\msdchem\1\DATA\
 Data File : sjb_77_041fp.D
 Acq On : 24 Jan 2013 16:52
 Operator : sjb
 Sample : sjb_77_041fp
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Integration Parameters: autoint1.e
 Integrator: ChemStation

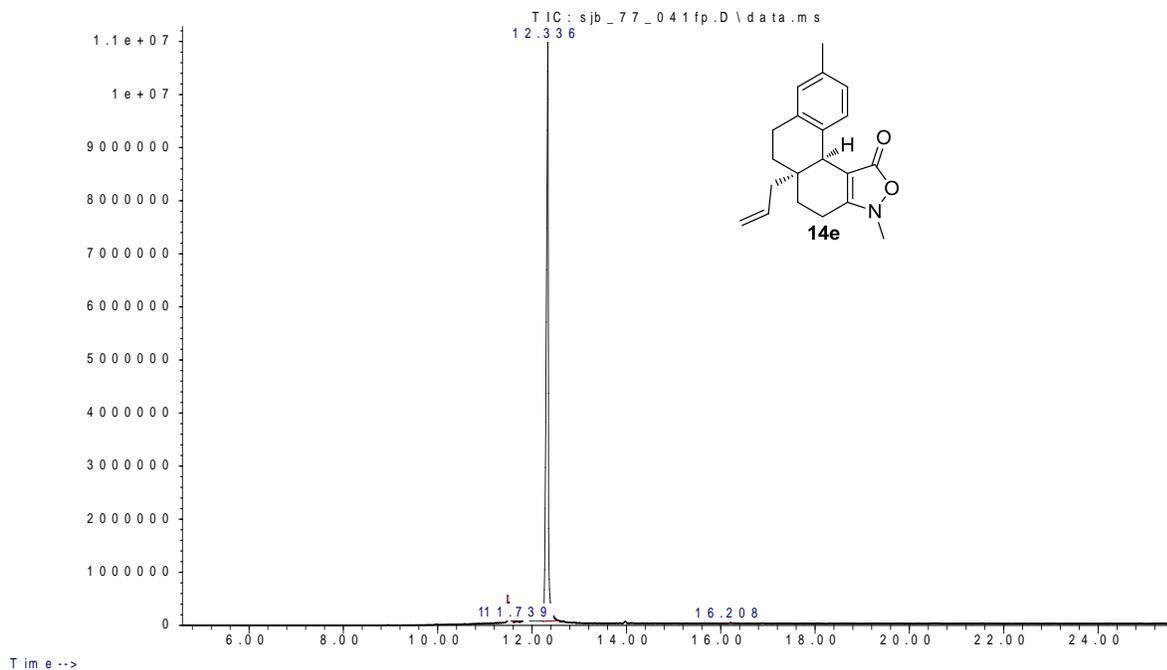
Method : C:\msdchem\1\5973N\PRECISION.M
 Title :

Signal : TIC: sjb_77_041fp.D\data.ms

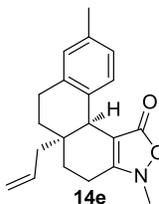
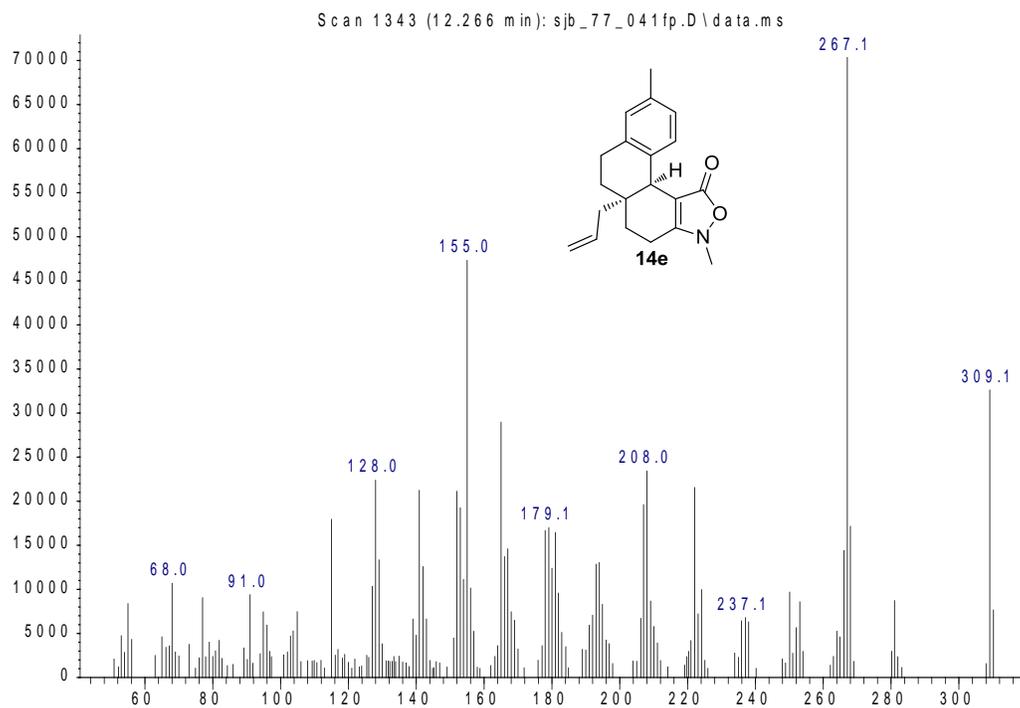
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	11.479	1205	1205	1205	M	-467102	0	0.00%	0.000%
2	11.616	1227	1229	1232	VV 3	33842	476512	0.14%	0.141%
3	11.739	1249	1251	1254	VV 4	30352	427668	0.13%	0.127%
4	11.815	1264	1264	1264	M4	-204808	0	0.00%	0.000%
5	12.336	1336	1355	1392	VV	11066989	336059983	100.00%	99.591%
6	16.208	2026	2032	2041	PV 10	18378	475433	0.14%	0.141%

Sum of corrected areas: 337439597

Abundance



Abundance



m/z-->

Area Percent Report

Data Path : C:\msdchem\1\DATA\
Data File : sjb_74_193fp.D
Acq On : 26 Oct 2012 9:51
Operator : sjb
Sample : sjb_74_193fp
Misc :
ALS Vial : 25 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\msdchem\1\METHODS\JMB2.m
Title :

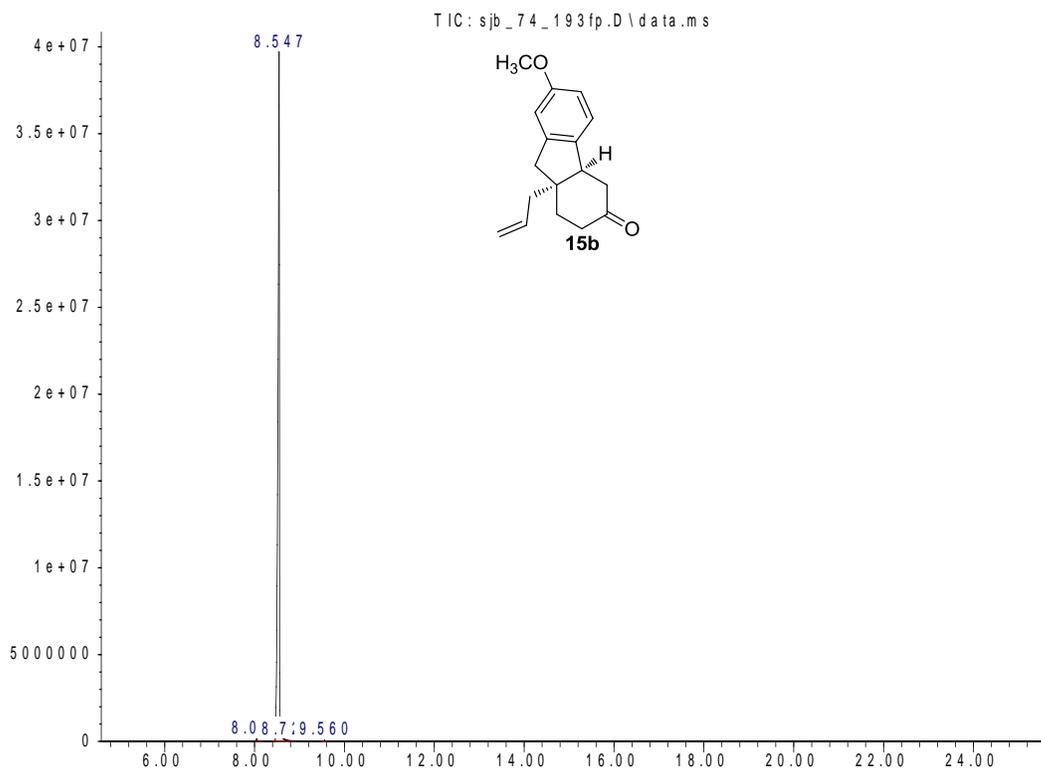
Signal : TIC: sjb_74_193fp.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.048	601	606	619	BB 2	136209	1898997	0.21%	0.206%
2	8.547	670	693	720	BV	40169943	918832725	100.00%	99.531%
3	8.720	720	723	739	VV 7	61335	1679808	0.18%	0.182%
4	9.560	862	870	875	BV 3	63401	749249	0.08%	0.081%

Sum of corrected areas: 923160778

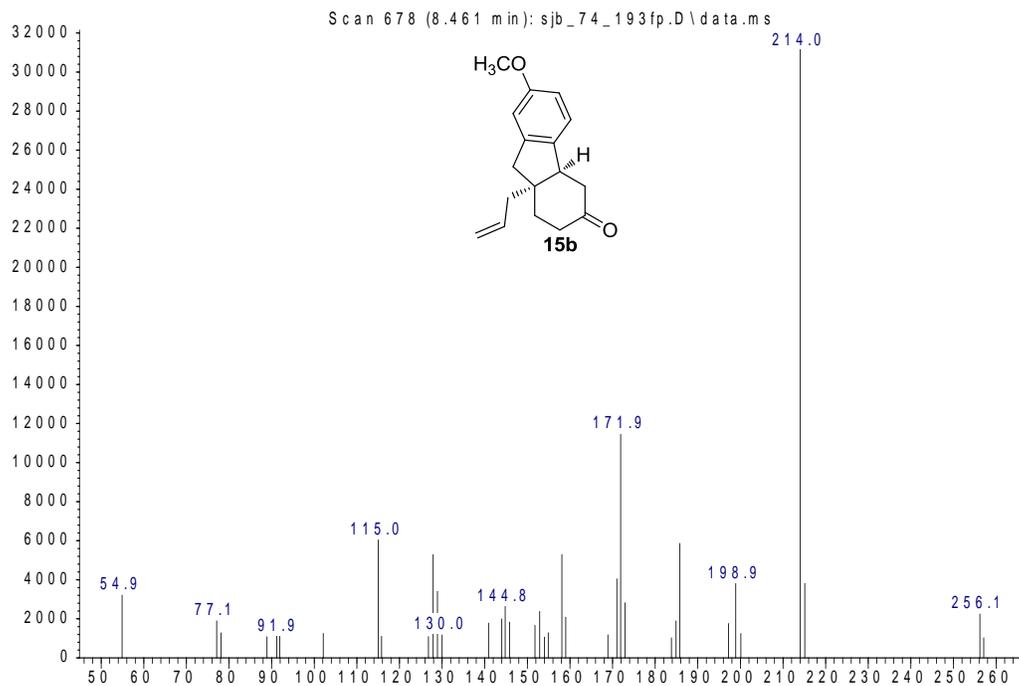
JMB2.m Thu Nov 08 10:08:59 2012

Abundance

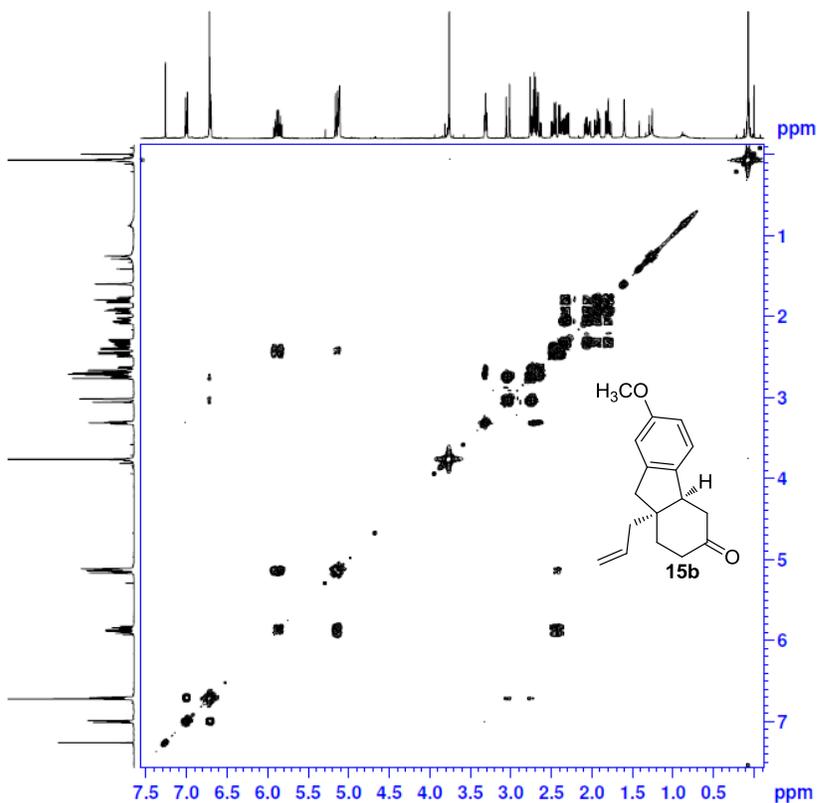


Time-->

Abundance



m/z-->



```

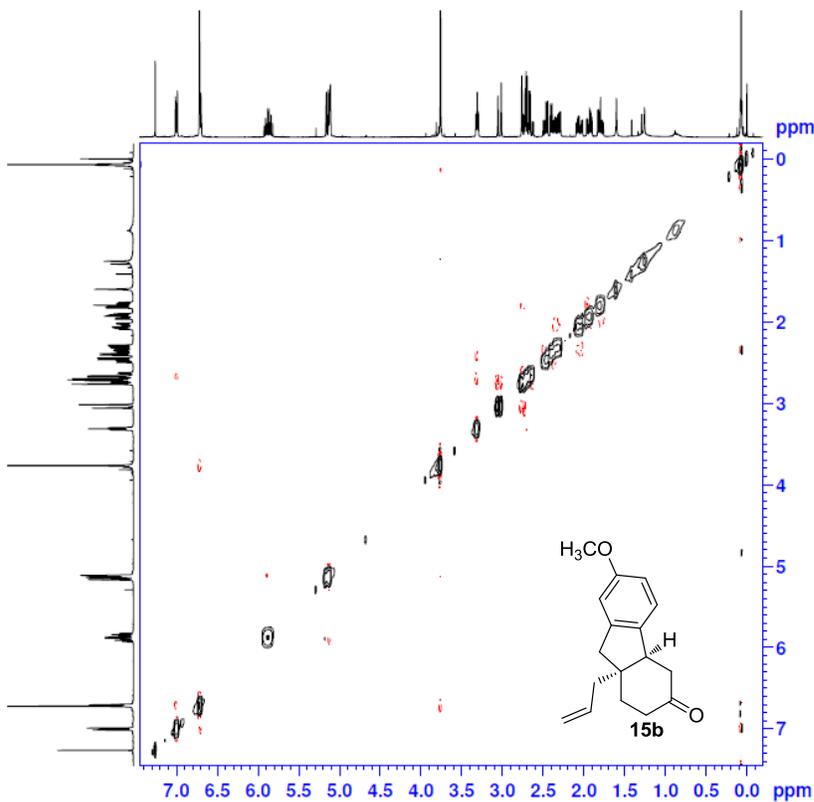
NAME      sjb_74_193fp
EXPNO     3
PROCNO    1
Date_     20121031
Time      8.47
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   cosyppgf
TD         2048
SOLVENT   CDCl3
NS         3
DS         8
SWH        3078.818 Hz
FIDRES     1.503329 Hz
AQ         0.3326452 sec
RG         64
DW         162.400 usec
DE         6.50 usec
TE         301.1 K
DO         0.00000300 sec
D1         1.4869198 sec
D13        0.00000400 sec
D16        0.00020000 sec
IN0        0.00032480 sec
  
```

```

----- CHANNEL f1 -----
NUC1      1H
P1        9.80 usec
PL1       -4.00 dB
PL1W      19.24419975 W
SF01      400.1515004 MHz
  
```

```

----- GRADIENT CHANNEL -----
GPNAM1    SINE.100
GP21      10.00 %
P16       1000.00 usec
NDO       1
TD         128
SF01      400.1515 MHz
FIDRES     24.052856 Hz
SW         7.694 ppm
FMODE     CF
SI         1024
SF         400.1500105 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0
PC         1.00
SI         1024
MC2       CF
SF         400.1500105 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0
  
```

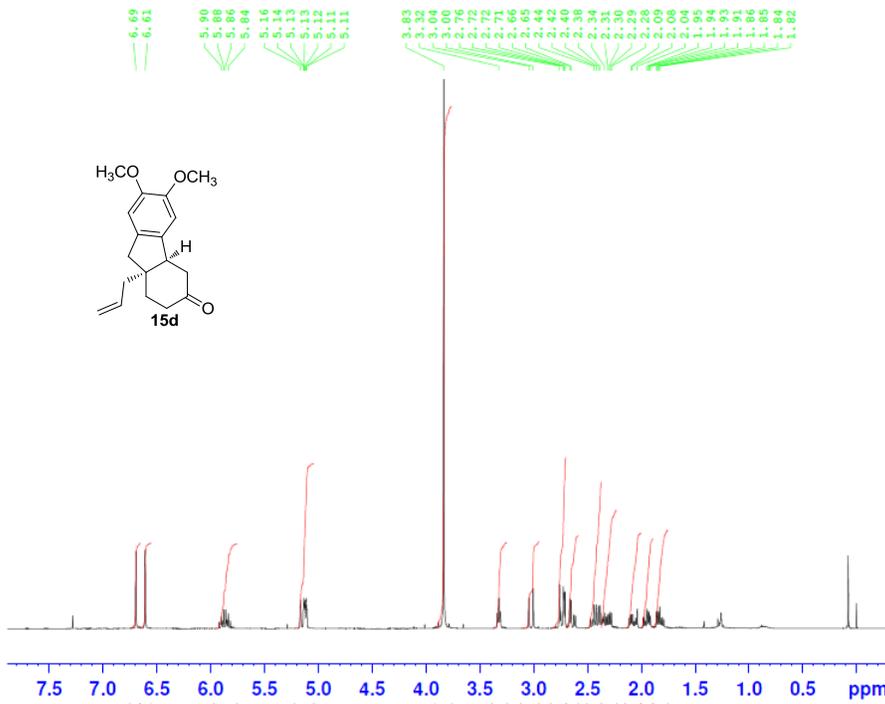


```

NAME      sjb_74_193fp
EXPNO     2
PROCNO    1
Date_     20121029
Time      11.33
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   noesyph
TD         2048
SOLVENT   CDCl3
NS         8
DS         4
SWH        3059.976 Hz
FIDRES     1.494129 Hz
AQ         0.3346932 sec
RG         203
DW         163.400 usec
DE         6.50 usec
TE         301.2 K
DO         0.00015092 sec
D1         2.00000000 sec
D8         0.69999999 sec
IN0        0.00032680 sec
  
```

```

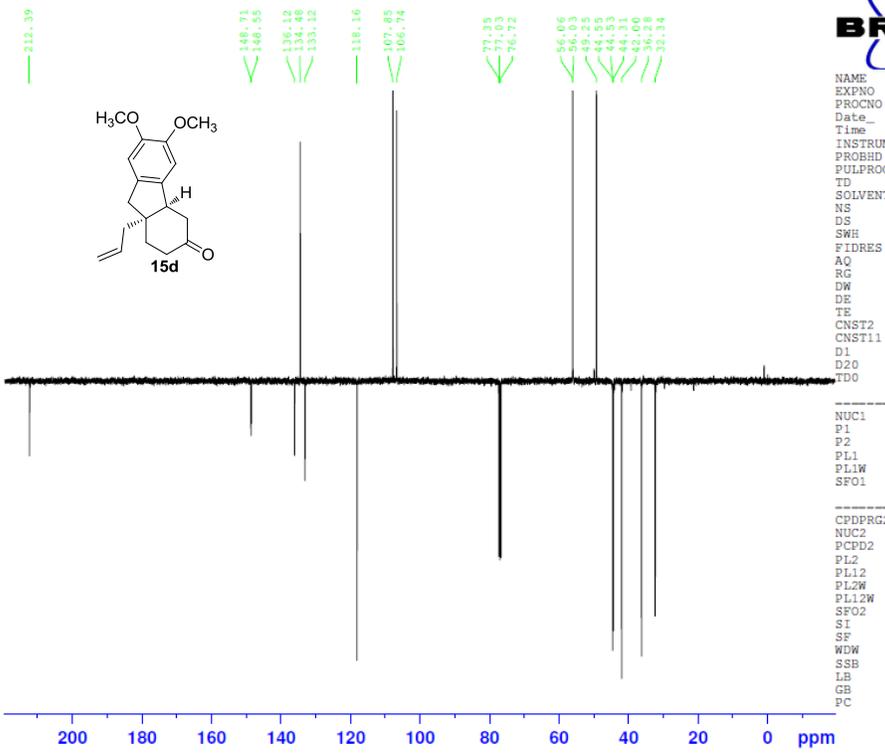
----- CHANNEL f1 -----
NUC1      1H
P1        9.80 usec
PL1       -4.00 dB
PL1W      19.24419975 W
SF01      400.1514624 MHz
NDO       1
TD         128
SF01      400.1515 MHz
FIDRES     23.905924 Hz
SW         7.647 ppm
FMODE     States-TPII
SI         1024
SF         400.1500105 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
PC         1.00
SI         1024
MC2       States-TPII
SF         400.1500105 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
  
```



```

NAME      sjb_74_170fp
EXPNO     1
PROCNO    1
Date_     20121012
Time      11.27
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   zg30
TD        65536
SOLVENT   CDCl3
NS        16
DS        2
SWH       8223.685 Hz
FIDRES    0.125483 Hz
AQ        3.9846387 sec
RG        45.2
DW        60.800 usec
DE        6.50 usec
TE        301.2 K
D1        1.00000000 sec
TD0       1

===== CHANNEL f1 =====
NUC1      1H
P1        9.80 usec
PL1       -4.00 dB
PL1W      19.24419975 W
SFO1      400.1524711 MHz
SI        32768
SF        400.1500000 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
  
```



```

NAME      sjb_74_170fp 13CAPT
EXPNO     1
PROCNO    1
Date_     20121017
Time      17.13
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   jmod
TD        65536
SOLVENT   CDCl3
NS        1024
DS        4
SWH       24038.461 Hz
FIDRES    0.366798 Hz
AQ        1.3631988 sec
RG        203
DW        20.800 usec
DE        6.50 usec
TE        301.2 K
CNST2     145.0000000
CNST11    1.0000000
D1        2.00000000 sec
D20       0.00689655 sec
TD0       1

----- CHANNEL f1 -----
NUC1      13C
P1        9.00 usec
P2        18.00 usec
PL1       0.00 dB
PL1W      35.41759872 W
SFO1      100.6278593 MHz

----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       -3.80 dB
PL12      13.80 dB
PL2W      18.37806702 W
PL12W     0.31937420 W
SFO2      400.1514620 MHz
SI        32768
SF        100.6177980 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```

Area Percent Report

Data Path : C:\msdchem\1\DATA\
Data File : sjb_74_170fp.D
Acq On : 12 Oct 2012 11:58
Operator : th
Sample : sjb_74_170fp
Misc :
ALS Vial : 10 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\msdchem\1\METHODS\JMB2.m
Title :

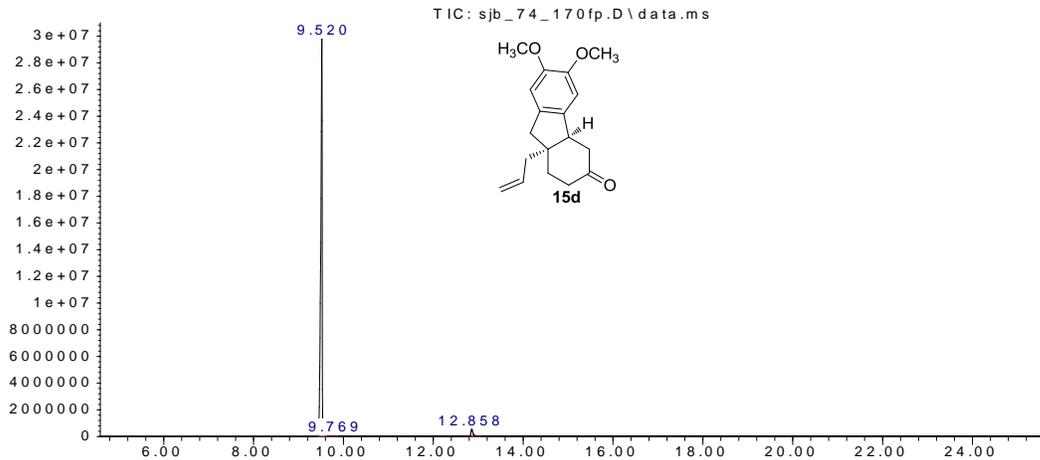
Signal : TIC: sjb_74_170fp.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	9.520	845	863	903	BV	30303782	659142387	100.00%	97.384%
2	9.769	903	907	921	VV 6	35305	957519	0.15%	0.141%
3	12.858	1437	1447	1475	VV 3	525720	16747955	2.54%	2.474%

Sum of corrected areas: 676847861

JMB2.m Wed Oct 17 14:59:13 2012

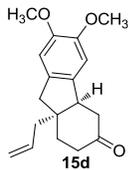
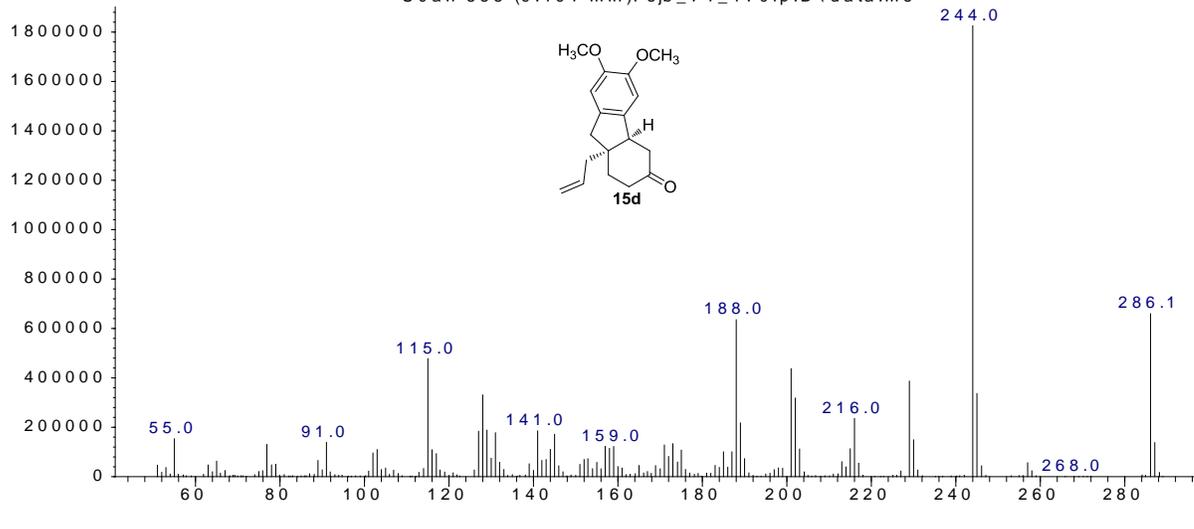
Abundance



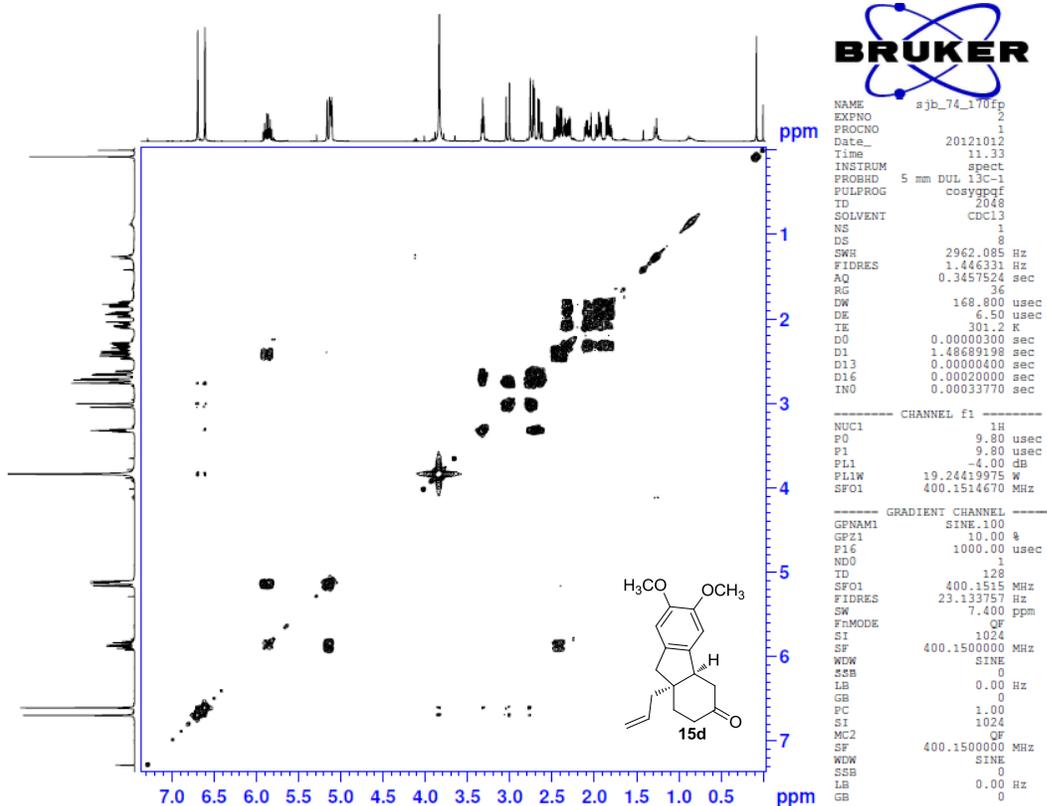
Time-->

Abundance

Scan 858 (9.491 min): sjb_74_170fp.D\data.ms



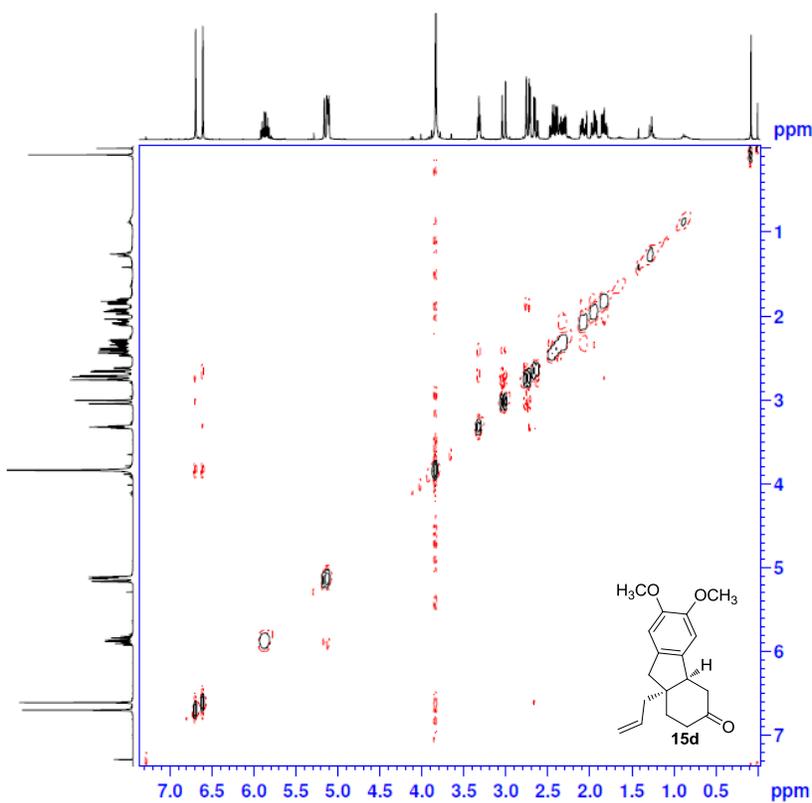
m/z-->



```
NAME sjb_74_170fp
EXPNO 2
PROCNO 1
Date_ 20121012
Time 11.33
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG cosygpqf
TD 2048
SOLVENT CDCl3
NS 1
DS 1
SWH 2962.085 Hz
FIDRES 1.446331 Hz
AQ 0.3457524 sec
RG 36
DW 168.800 usec
DE 6.50 usec
TE 301.2 K
D0 0.0000300 sec
D1 1.48689198 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00033770 sec

----- CHANNEL f1 -----
NUC1 1H
P0 9.80 usec
P1 9.80 usec
PL1 -4.00 dB
PL1W 19.24419975 W
SFO1 400.1514670 MHz

----- GRADIENT CHANNEL -----
GPNAM1 SINE.100
GPZ1 10.00 %
PlG 1000.00 usec
ND0 1
SFO1 400.1515 MHz
FIDRES 23.133757 Hz
SW 7.400 ppm
FIRMODE QF
SI 1024
SF 400.1500000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
SI 1024
MC2 QF
SF 400.1500000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
```



```

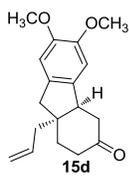
NAME      sjb_74_170fp
EXPNO     3
PROCNO    1
Date_     20121012
Time      11.56
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   noesyph
TD         2048
SOLVENT   CDCl3
NS         8
DS         4
SWH        2962.085 Hz
FIDRES     1.446331 Hz
AQ         0.3457524 sec
RG         25.4
DW         168.800 usec
DE         6.50 usec
TE         301.2 K
DO         0.00015638 sec
D1         2.00000000 sec
D8         0.69999999 sec
INO        0.00033770 sec

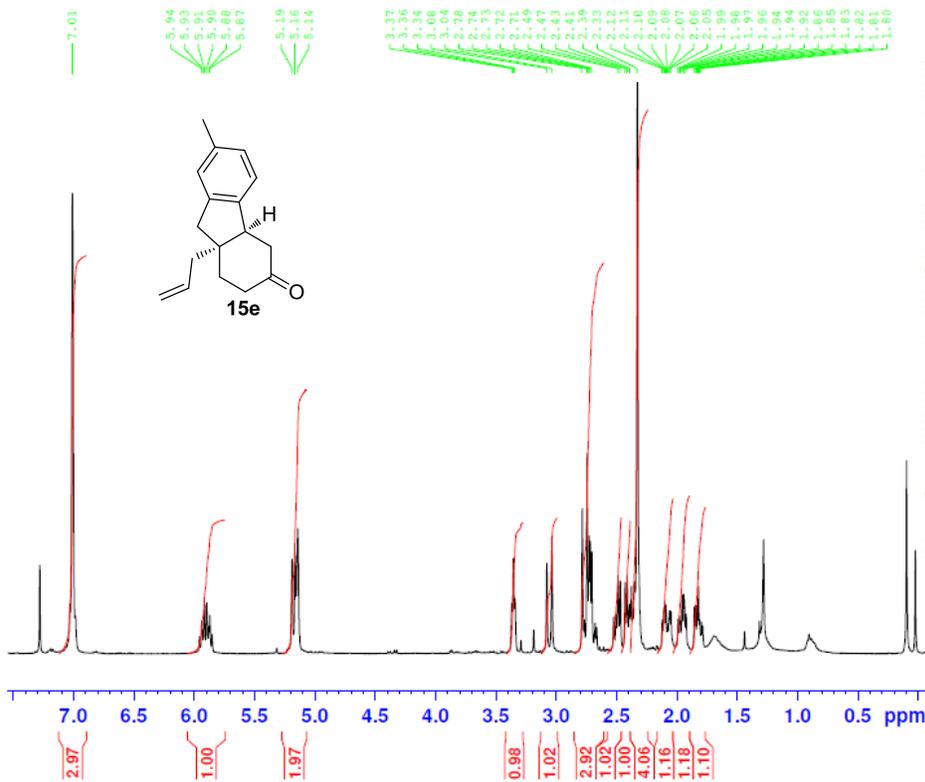
```

```

----- CHANNEL f1 -----
NUC1      1H
P1        9.80 usec
PL1       -4.00 dB
PL1W      19.24419975 W
SFO1      400.1514670 MHz
NDO       1
TD        128
SFO1      400.1515 MHz
FIDRES    23.133757 Hz
SW        7.400 ppm
FnMODE    States-TPPI
SI        1024
SF        400.1500000 MHz
WDW       QSINE
SSB       2
LB        0.00 Hz
GB        0
PC        1.00
SI        1024
MC2       States-TPPI
SF        400.1500000 MHz
WDW       QSINE
SSB       2
LB        0.00 Hz
GB        0

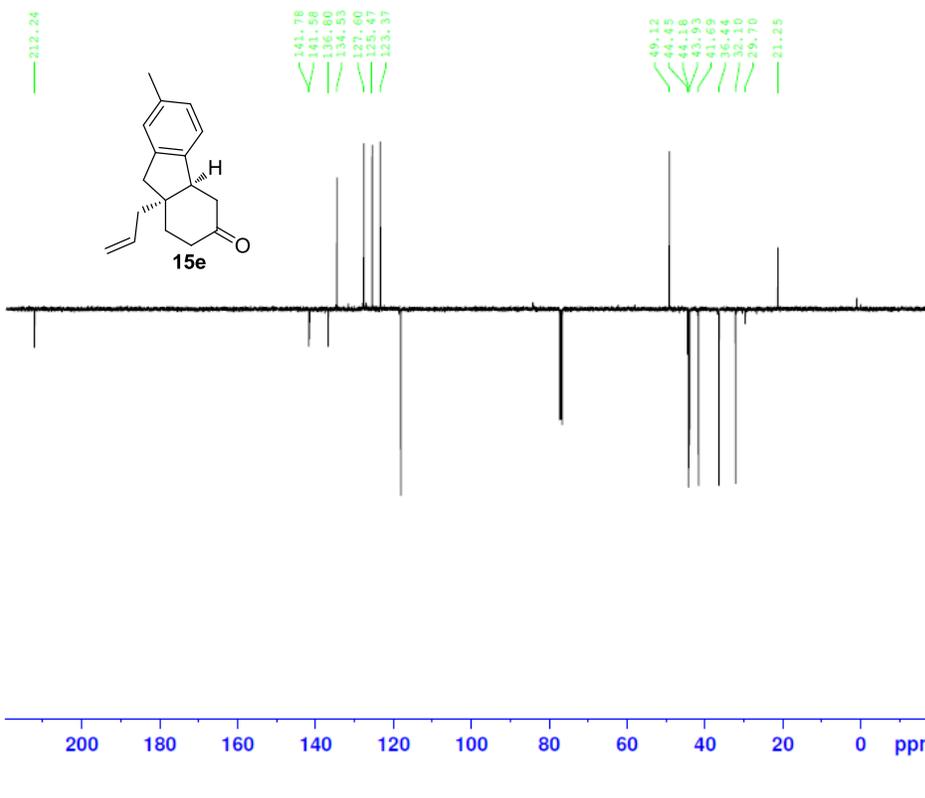
```





```

NAME      sjb_77_155fp take 2
EXPNO    1
PROCNO   1
Date_    20130730
Time     9.33
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        2
SWH       8223.685 Hz
FIDRES   0.125483 Hz
AQ        3.9846387 sec
RG        144
DW        60.800 usec
DE        6.50 usec
TE        301.2 K
D1        1.0000000 sec
TDO       1
----- CHANNEL f1 -----
NUC1      1H
P1        12.50 usec
PL1       -2.00 dB
PL1W      12.14226913 W
SFO1      400.1524711 MHz
SI        32768
SF        400.1500000 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
  
```



```

NAME      sjb_77_155fp APT
EXPNO    1
PROCNO   1
Date_    20130730
Time     10.38
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  jmod
TD        65536
SOLVENT  CDCl3
NS        1024
DS        4
SWH       24038.461 Hz
FIDRES   0.366798 Hz
AQ        1.3631988 sec
RG        203
DW        20.800 usec
DE        6.50 usec
TE        301.2 K
CNST2    145.0000000
CNST11   1.0000000
D1        2.0000000 sec
D20       0.00689655 sec
TDO       1
----- CHANNEL f1 -----
NUC1      13C
P1        8.00 usec
P2        16.00 usec
PL1       -2.00 dB
PL1W      56.13311005 W
SFO1      100.6278593 MHz
----- CHANNEL f2 -----
CPDPRG2  waltz16
NUC2      1H
PCPD2    80.00 usec
PL2       -2.00 dB
PL12     14.00 dB
PL2W     12.14226913 W
PL12W    0.30500001 W
SFO2     400.1514963 MHz
SI        32768
SF        100.6177980 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```

Area Percent Report

Data Path : C:\msdchem\1\DATA\
Data File : sjb_77_155fp.D
Acq On : 17 Jul 2013 19:26
Operator : JMB
Sample : sjb_77_155fp
Misc :
ALS Vial : 70 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

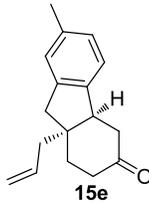
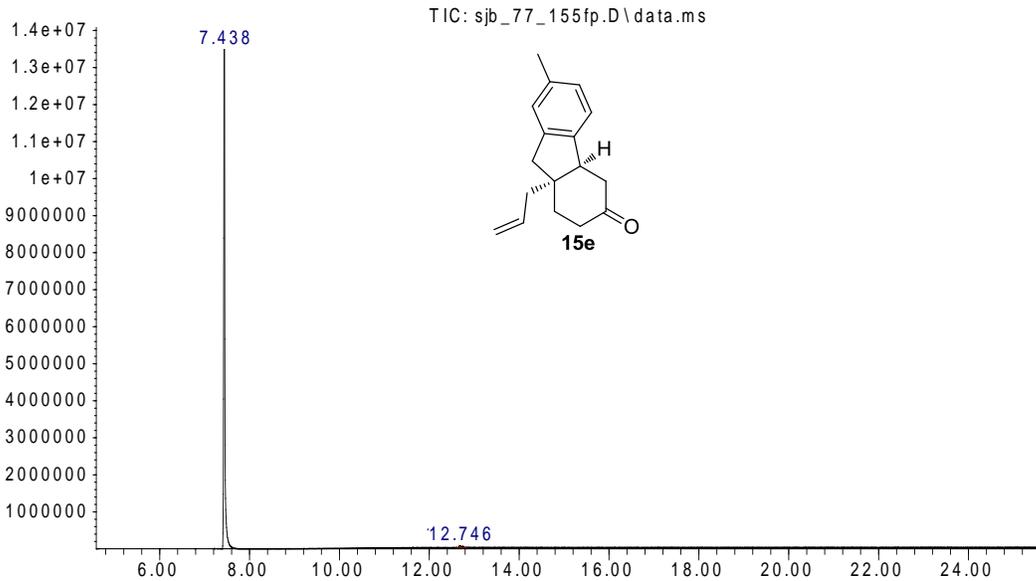
Method : C:\msdchem\1\5973N\PRECISION.M
Title :

Signal : TIC: sjb_77_155fp.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.438	485	499	557	PV	17547844	273377835	100.00%	99.173%
2	12.685	1406	1416	1423	BV 3	71876	1506033	0.55%	0.546%
3	12.746	1423	1427	1438	VV 6	38668	772660	0.28%	0.280%

Sum of corrected areas: 275656527

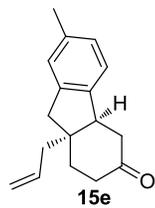
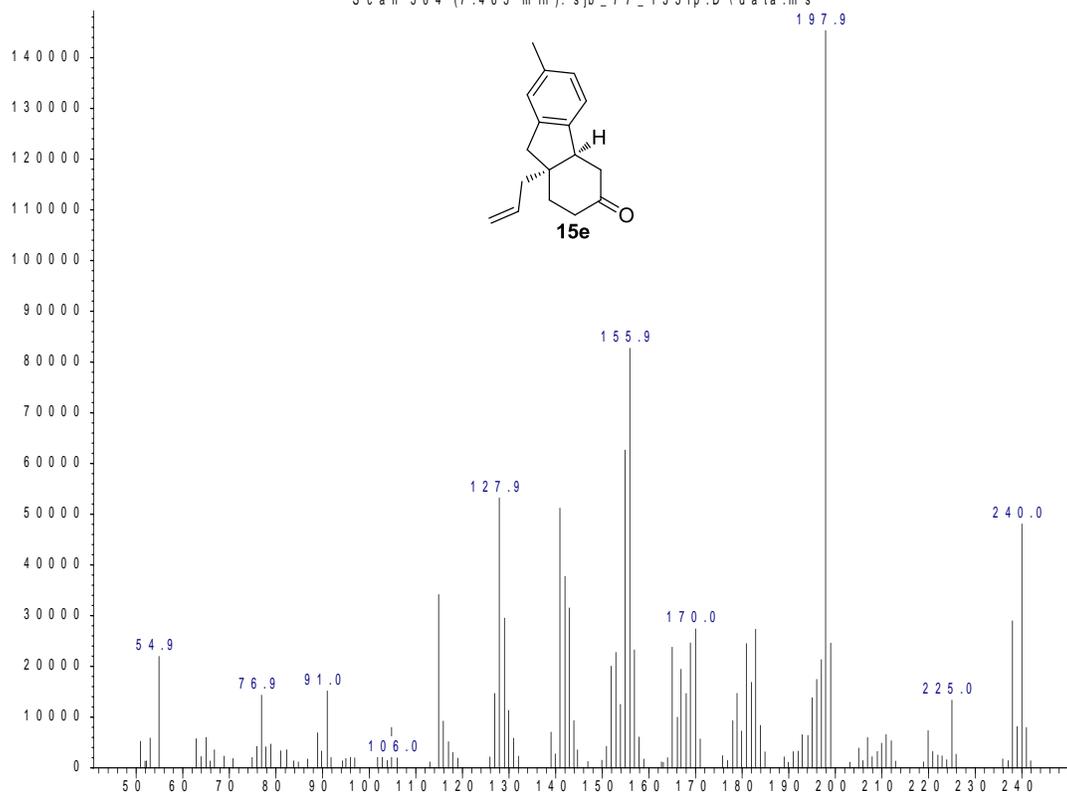
Abundance



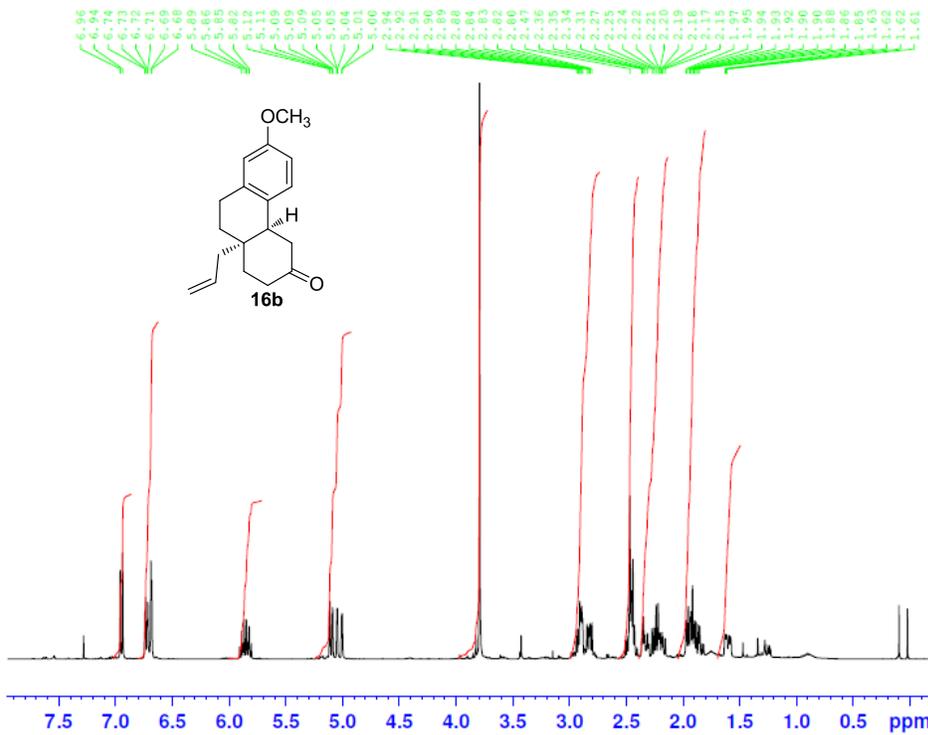
Time-->

Abundance

Scan 504 (7.465 min): sjb_77_155fp.D\data.ms



m/z-->

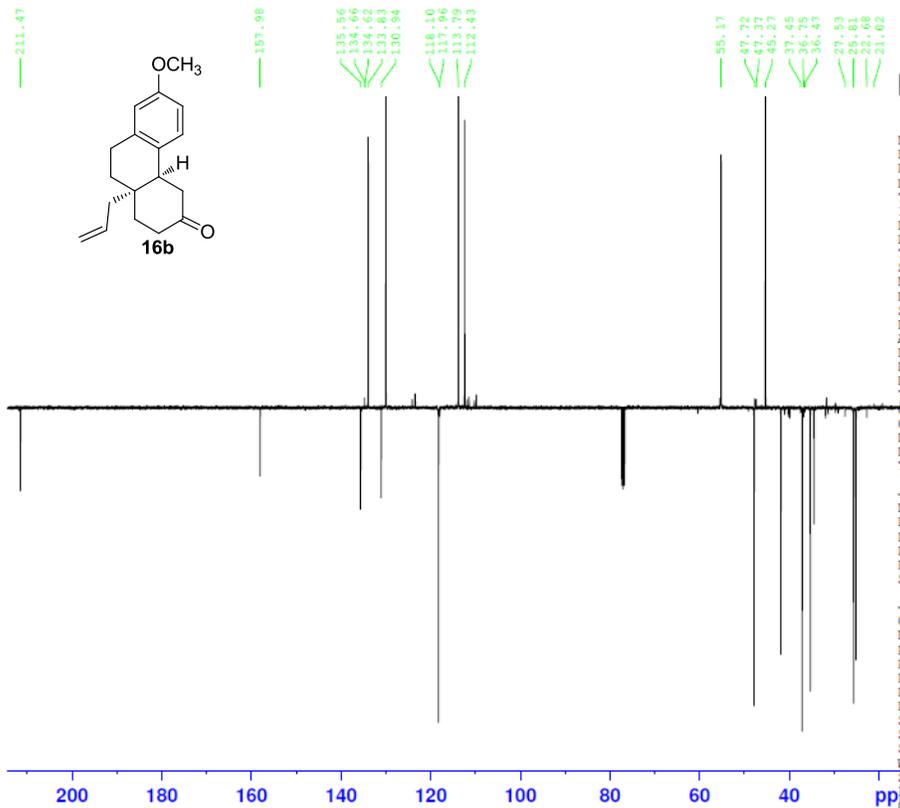


```

NAME      sjb_77_098fp take 2
EXPNO    1
PROCNO   1
Date_    20130805
Time     11.07
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       2
SWH      8223.685 Hz
FIDRES   0.125483 Hz
AQ       3.9846387 sec
RG       50.8
DW       60.800 usec
DE       6.50 usec
TE       301.2 K
D1       1.0000000 sec
TDO      1
  
```

```

----- CHANNEL f1 -----
NUC1     1H
P1       12.50 usec
PL1      -2.00 dB
PL1W    12.14226913 W
SFO1     400.1524711 MHz
SI       32768
SF       400.1500000 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
  
```



```

NAME      sjb_77_098fp APT
EXPNO    1
PROCNO   1
Date_    20130605
Time     9.21
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  jmod
TD       65536
SOLVENT  CDCl3
NS       1024
DS       4
SWH      24038.461 Hz
FIDRES   0.366798 Hz
AQ       1.3631988 sec
RG       203
DW       20.800 usec
DE       6.50 usec
TE       301.2 K
D1       145.0000000 sec
D2       2.0000000 sec
D3       0.00689655 sec
TDO      1
  
```

```

----- CHANNEL f1 -----
NUC1     13C
P1       8.00 usec
P2       16.00 usec
PL1      -2.00 dB
PL1W    56.13311005 W
SFO1     100.6278593 MHz
  
```

```

----- CHANNEL f2 -----
CPDPRG2  waltz16
NUC2     1H
PCPD2    80.00 usec
PL2      -2.00 dB
PL12     14.00 dB
PL2W    12.14226913 W
PL12W   0.30500001 W
SFO2     400.1515253 MHz
SI       32768
SF       100.6177980 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
  
```

Area Percent Report

Data Path : C:\msdchem\1\DATA\
Data File : sjb_74_055fp.D
Acq On : 5 Jul 2012 11:31
Operator : sjb
Sample : sjb_74_055fp
Misc :
ALS Vial : 100 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\msdchem\1\METHODS\JMB2.m
Title :

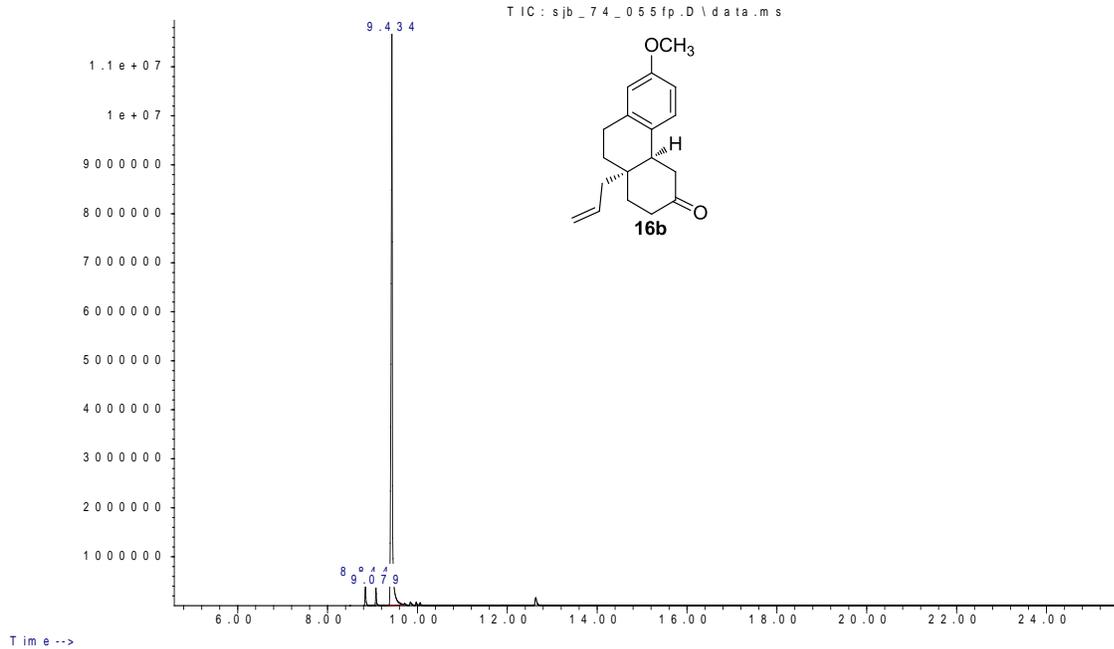
Signal : TIC: sjb_74_055fp.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.844	737	745	759	BB	519105	7434595	3.19%	3.034%
2	9.079	779	786	796	BV	347741	4764015	2.05%	1.944%
3	9.434	833	848	892	BV	11665755	232806835	100.00%	95.021%

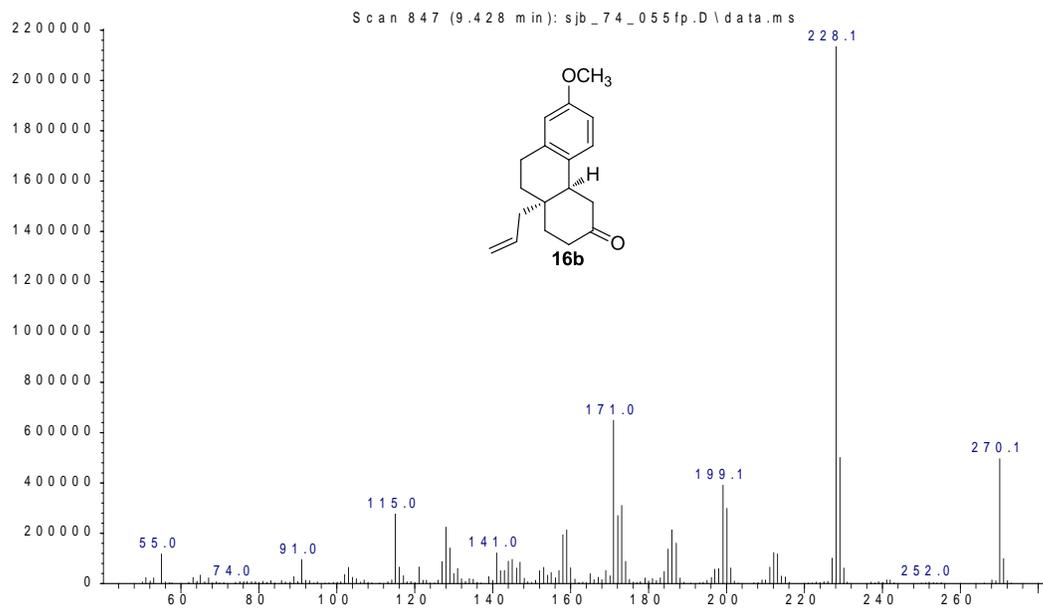
Sum of corrected areas: 245005445

JMB2.m Mon Nov 12 10:09:42 2012

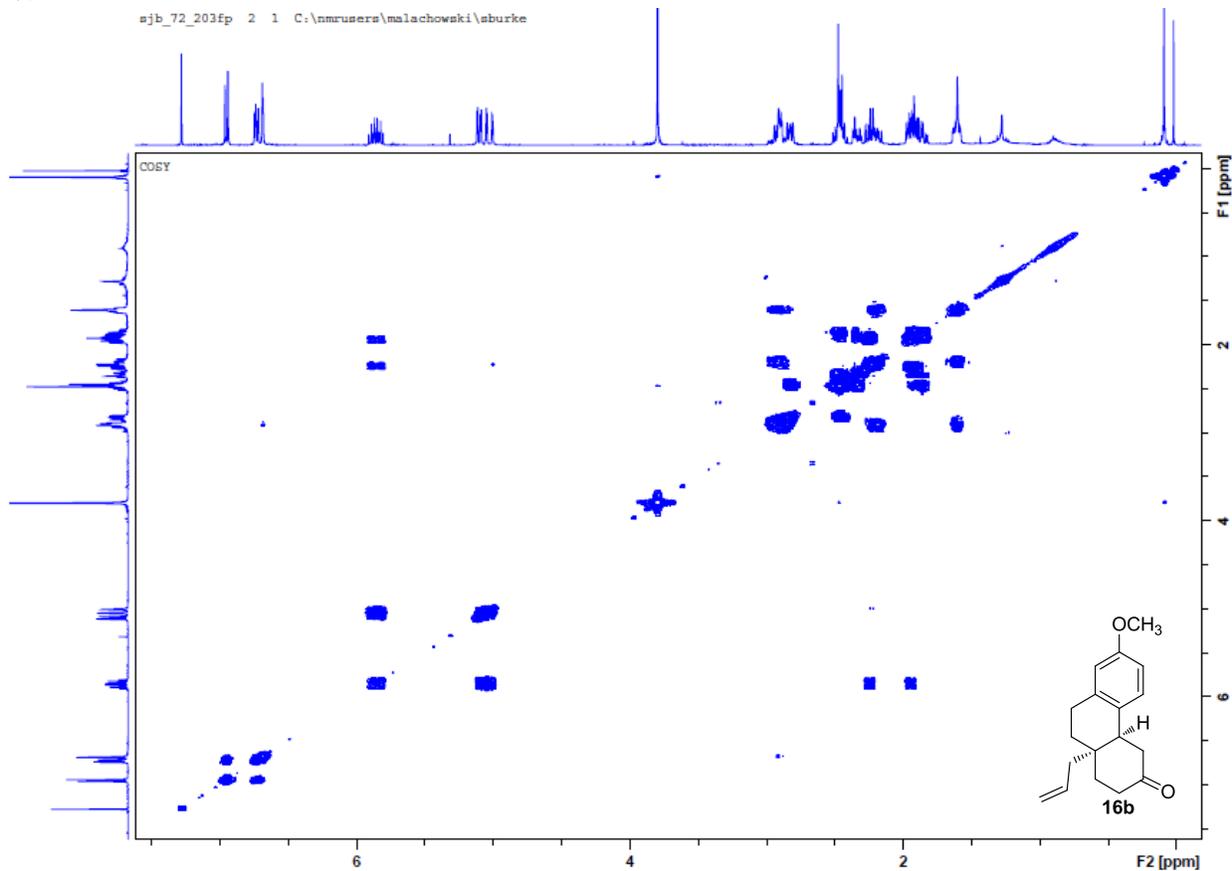
Abundance



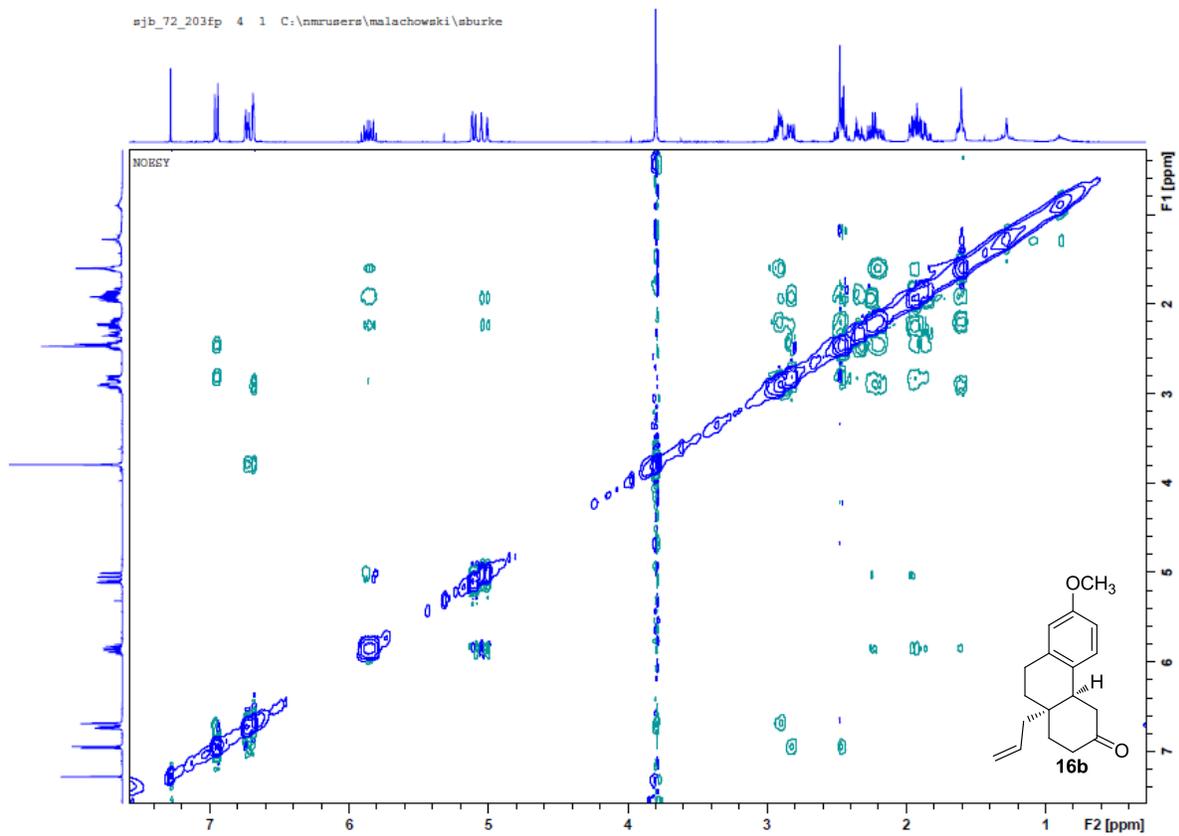
Abundance



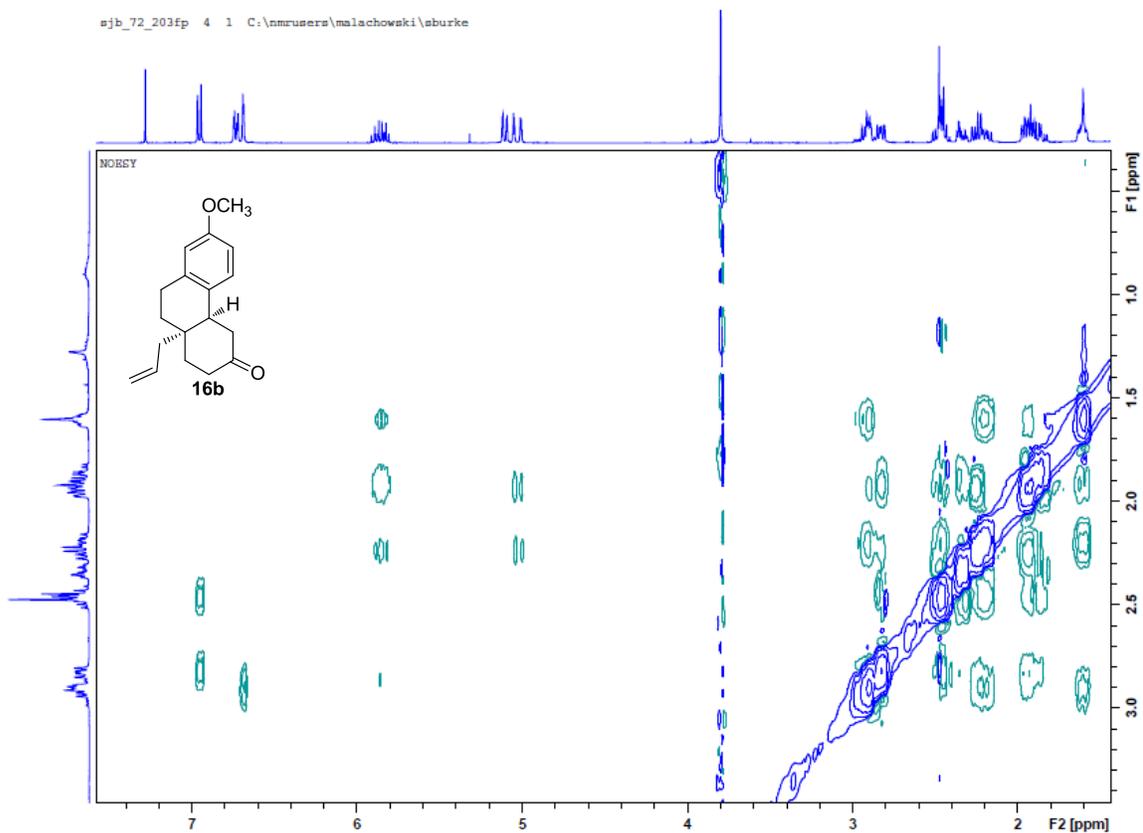
m/z-->

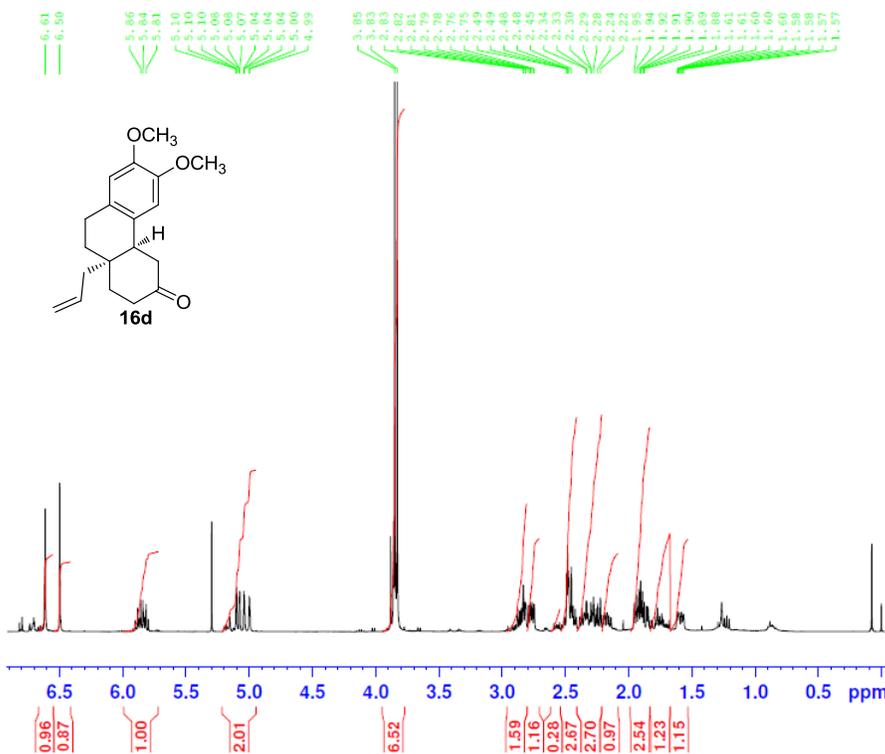


sjb_72_203fp 4 1 C:\nmrusers\malachowski\aburke



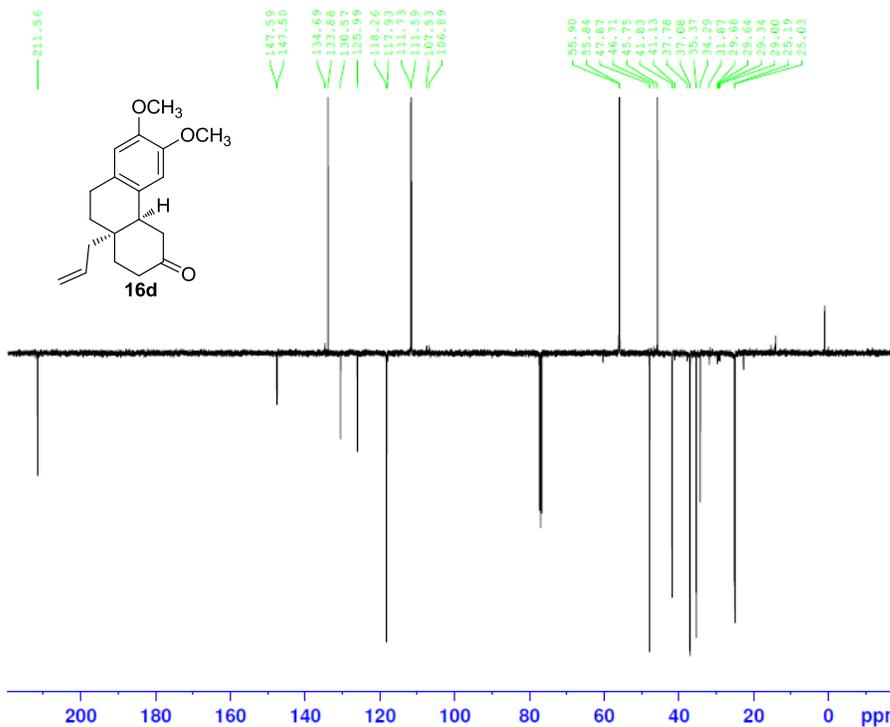
sjb_72_203fp 4 1 C:\nmrusers\malachowski\aburke





NAME sjb_72_198fp
 EXPNO 1
 PROCNO 1
 Date_ 20120503
 Time 11.39
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 40.3
 DW 60.800 usec
 DE 6.50 usec
 TE 301.2 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 12.50 usec
 PL1 -2.00 dB
 PL1W 12.14226913 W
 SFO1 400.1524711 MHz
 SI 32768
 SF 400.1500000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



NAME sjb_77_005fp APT
 EXPNO 1
 PROCNO 1
 Date_ 20121210
 Time 9.30
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG jmod
 TD 65536
 SOLVENT CDC13
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 301.2 K
 CNST2 145.0000000
 CNST11 1.0000000
 D1 2.00000000 sec
 D20 0.00689655 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 8.00 usec
 P2 16.00 usec
 PL1 -2.00 dB
 PL1W 56.13311005 W
 SFO1 100.6278593 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -2.00 dB
 PL12 14.00 dB
 PL2W 12.14226913 W
 PL12W 0.30500001 W
 SFO2 400.1514495 MHz
 SI 32768
 SF 100.6177980 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Area Percent Report

Data Path : C:\msdchem\1\DATA\
 Data File : sjb_72_198fp.D
 Acq On : 3 May 2012 11:59
 Operator : sjb
 Sample : sjb_72_198fp
 Misc :
 ALS Vial : 55 Sample Multiplier: 1

Integration Parameters: autoint1.e
 Integrator: ChemStation

Method : C:\msdchem\1\METHODS\JMB2.m
 Title :

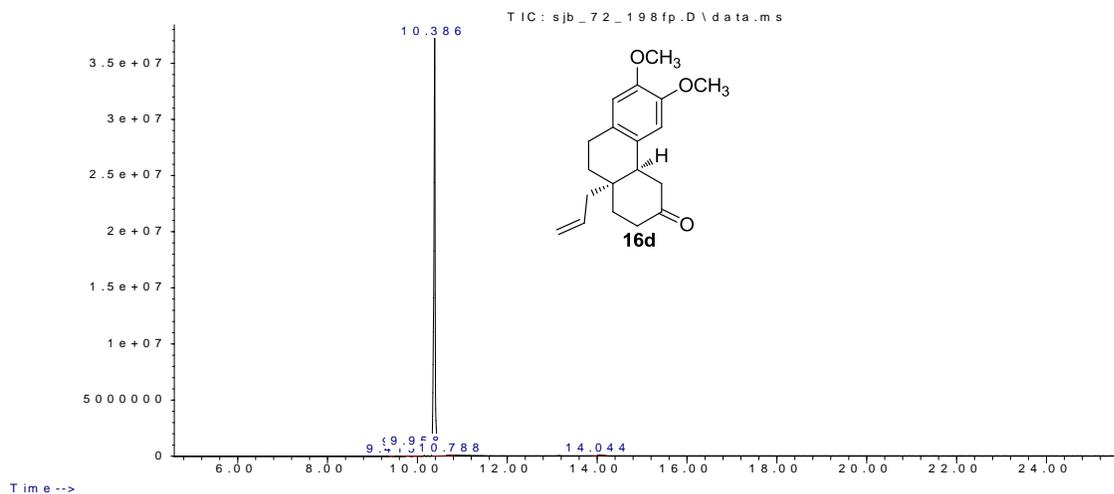
Signal : TIC: sjb_72_198fp.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	9.415	838	845	854	PV 3	35843	523833	0.06%	0.060%
2	9.771	888	907	926	PV	639609	9434624	1.12%	1.081%
3	9.958	926	940	964	VV 3	682972	12270772	1.45%	1.406%
4	10.386	999	1015	1076	PV	37735401	845131612	100.00%	96.870%
5	10.748	1076	1078	1083	VV 5	44991	946871	0.11%	0.109%
6	10.788	1083	1085	1090	VV 5	27602	321745	0.04%	0.037%
7	14.044	1628	1654	1680	VV 5	82632	3807415	0.45%	0.436%

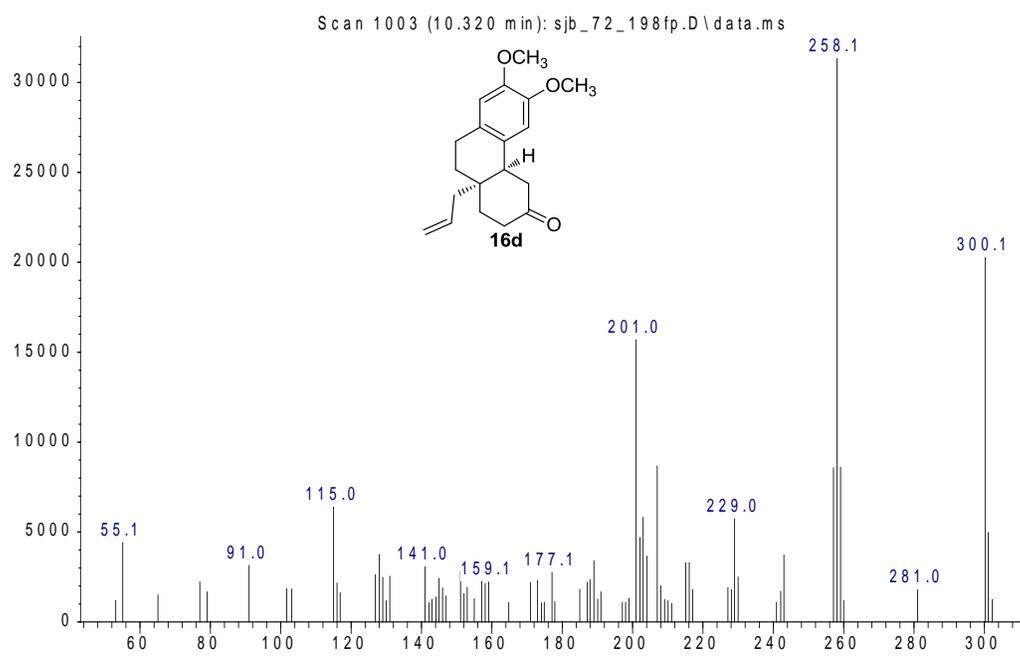
Sum of corrected areas: 872436873

JMB2.m Thu Nov 08 10:05:52 2012

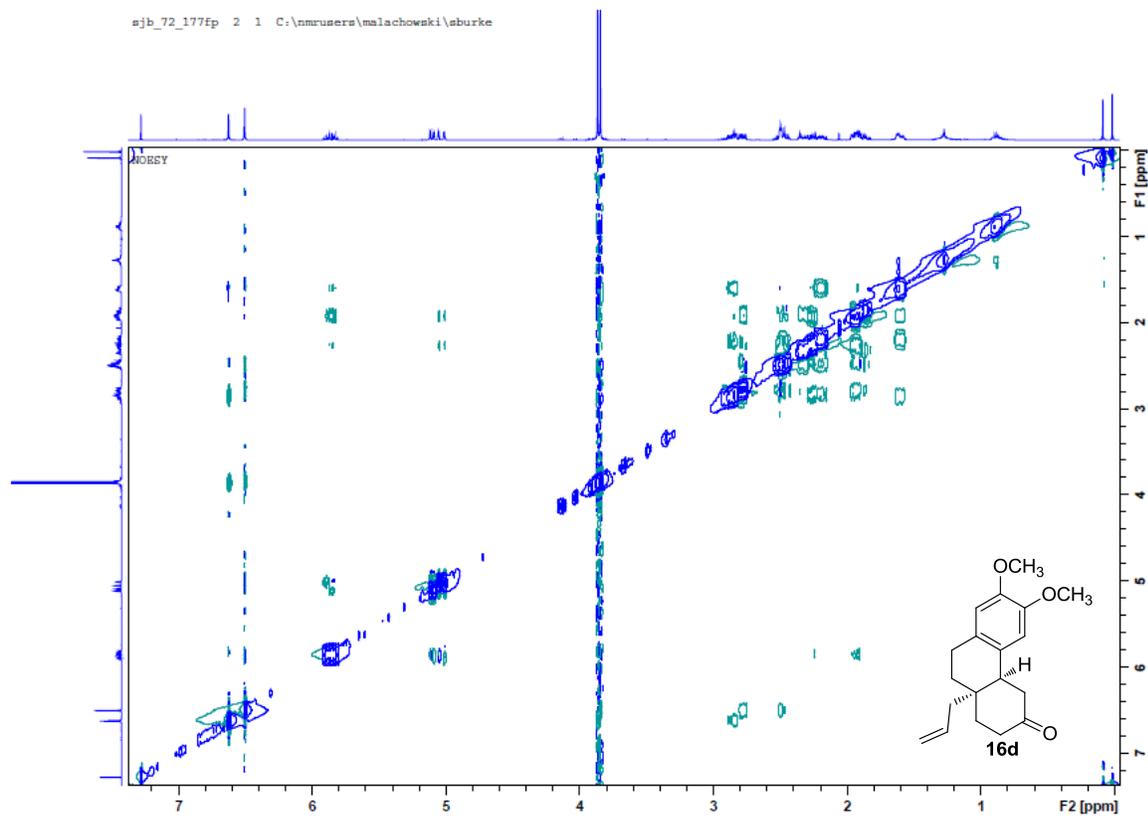
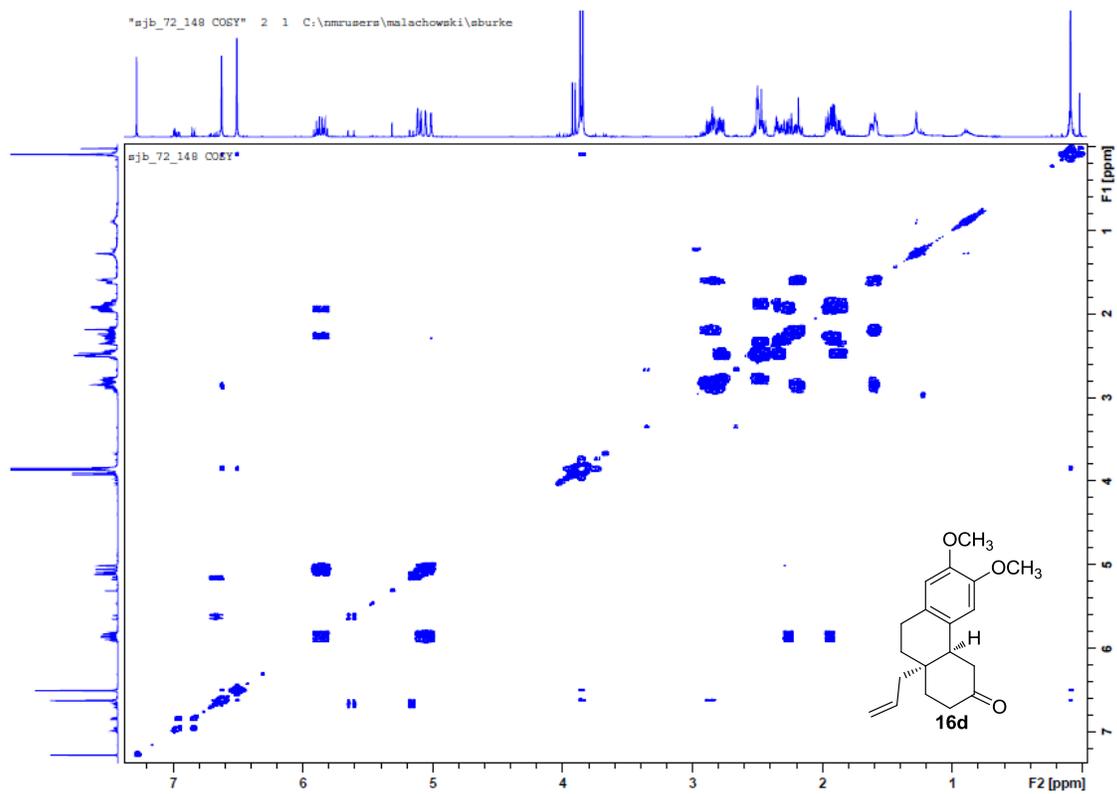
Abundance

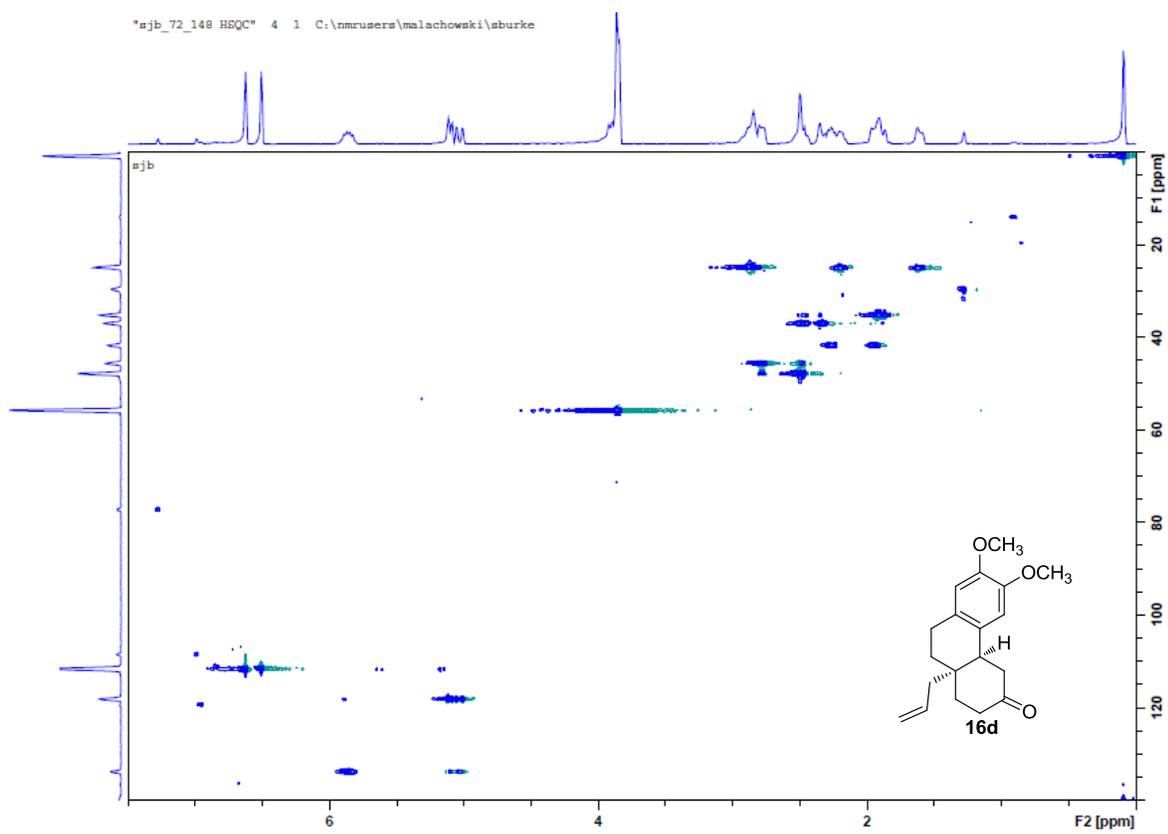
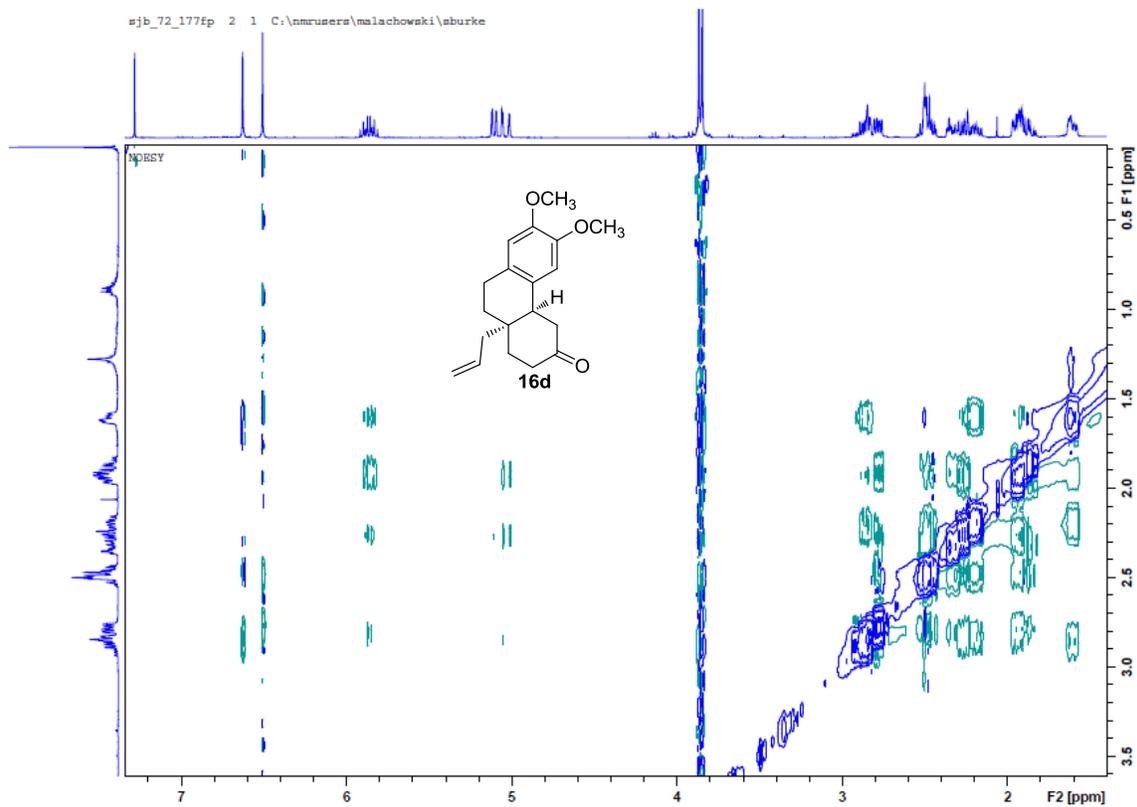


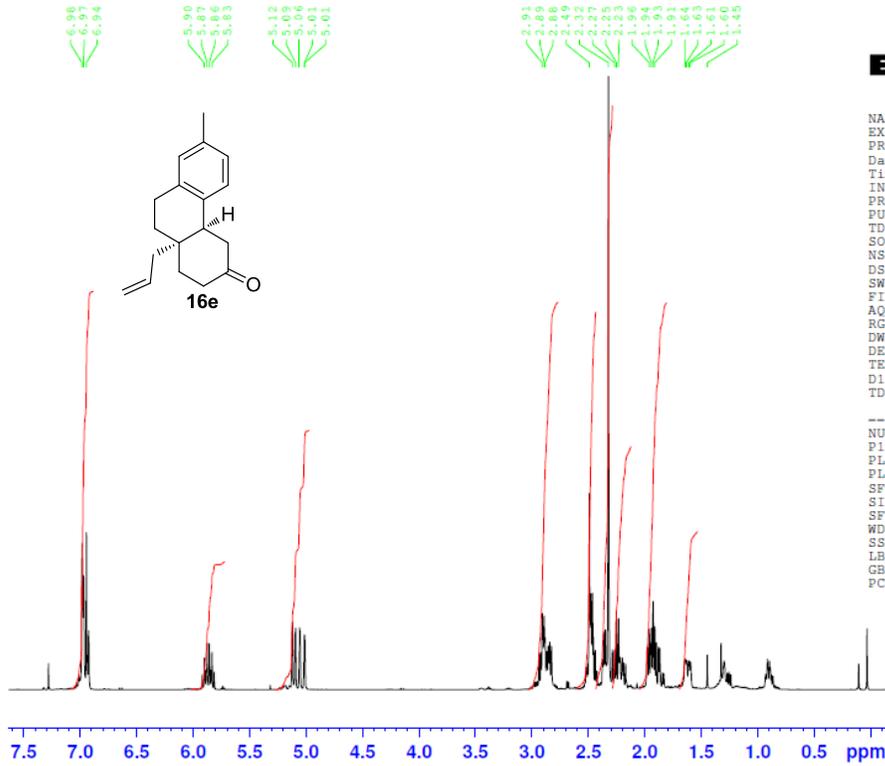
Abundance



m/z-->

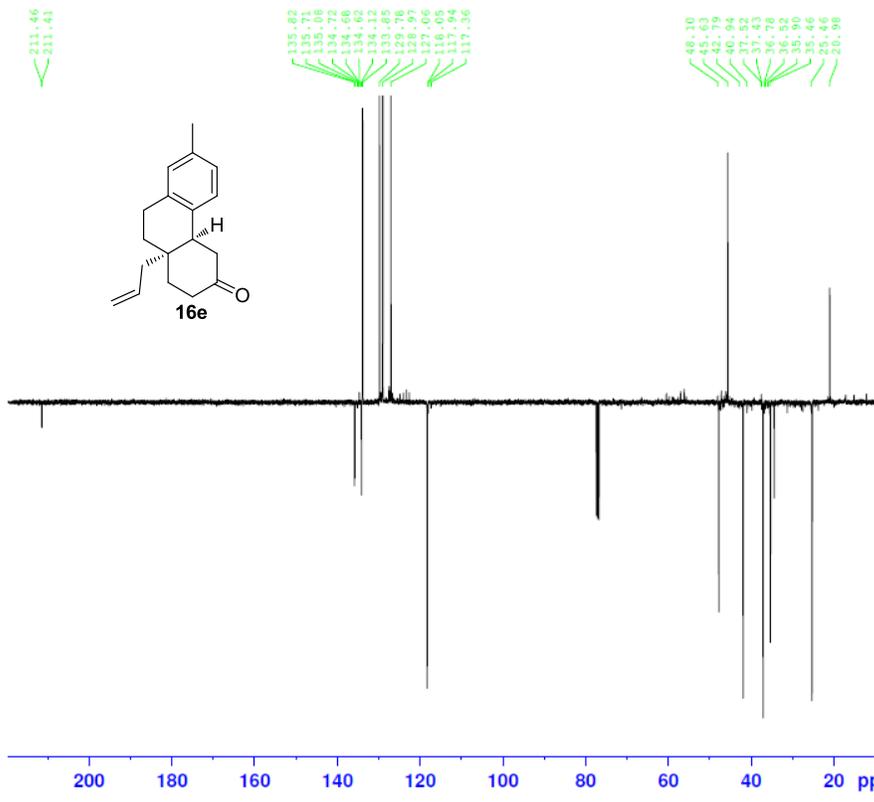






NAME sjb_77_045 fr10
 EXPNO 1
 PROCNO 1
 Date_ 20130125
 Time 14.10
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.695 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 50.8
 DW 60.800 usec
 DE 6.50 usec
 TE 304.9 K
 D1 1.00000000 sec
 TDO 1

----- CHANNEL f1 -----
 NUC1 1H
 P1 12.50 usec
 PL1 -2.00 dB
 PL1W 12.14226913 W
 SFO1 400.1524711 MHz
 SI 32768
 SF 400.1500000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



NAME sjb_77_035APT
 EXPNO 1
 PROCNO 1
 Date_ 20130118
 Time 13.23
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG jmod
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 304.6 K
 SFO2 145.0000000 MHz
 CNST11 1.0000000
 D1 2.00000000 sec
 D20 0.00689655 sec
 TDO 1

----- CHANNEL f1 -----
 NUC1 13C
 P1 8.00 usec
 P2 16.00 usec
 PL1 -2.00 dB
 PL1W 56.13311005 W
 SFO1 100.6278593 MHz

----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -2.00 dB
 PL12 14.00 dB
 PL2W 12.14226913 W
 PL12W 0.30500001 W
 SFO2 400.1514921 MHz
 SI 32768
 SF 100.6177980 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Area Percent Report

Data Path : C:\msdchem\1\DATA\
Data File : sjb_77_035fp.D
Acq On : 17 Jan 2013 9:18
Operator : sjb
Sample : sjb_77_035fp
Misc :
ALS Vial : 15 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

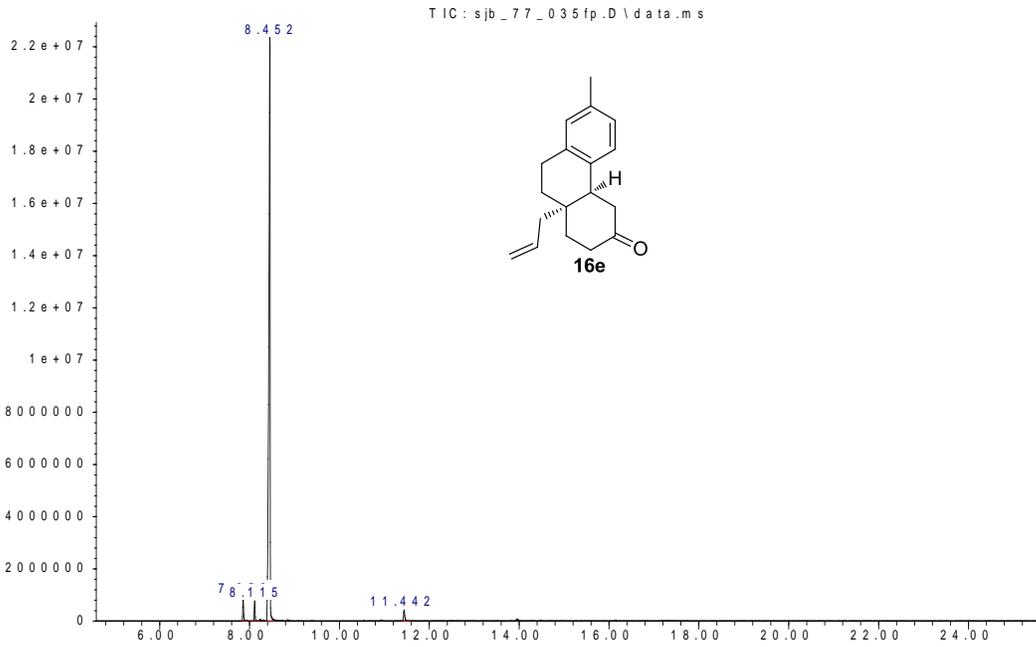
Method : C:\msdchem\1\5973N\PRECISION.M
Title :

Signal : TIC: sjb_77_035fp.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.859	567	573	586	BV	921047	12330088	2.82%	2.645%
2	8.115	602	618	630	BV 2	742118	9405778	2.15%	2.017%
3	8.452	662	677	691	VV	22818856	436485499	100.00%	93.619%
4	11.442	1191	1199	1218	PV 3	413116	8016772	1.84%	1.719%

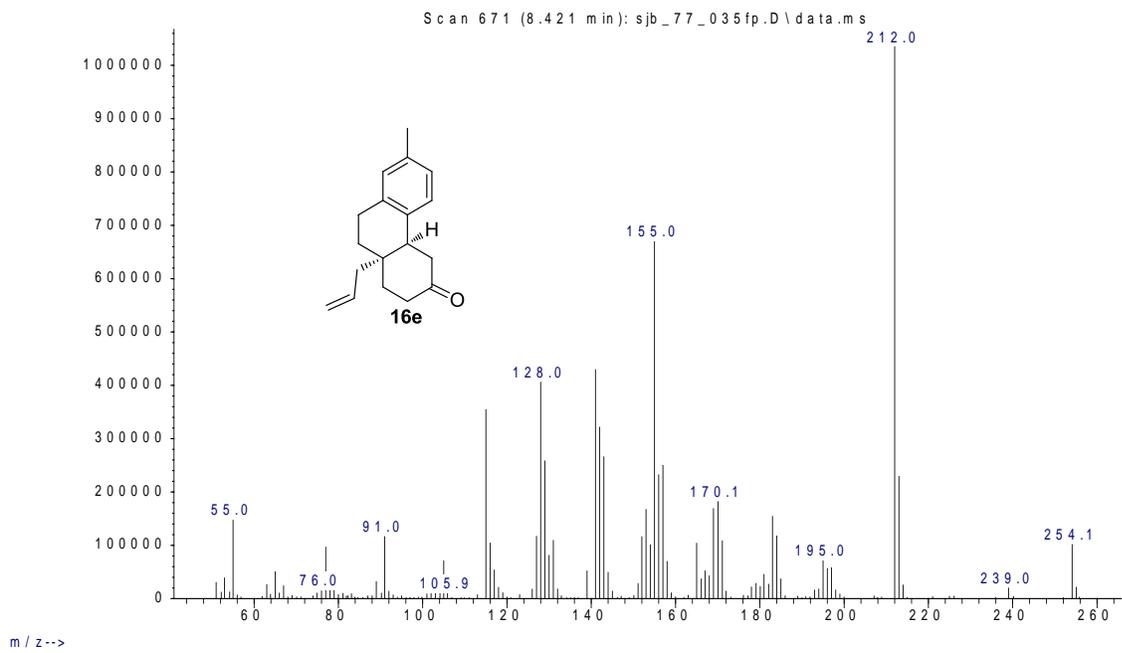
Sum of corrected areas: 466238136

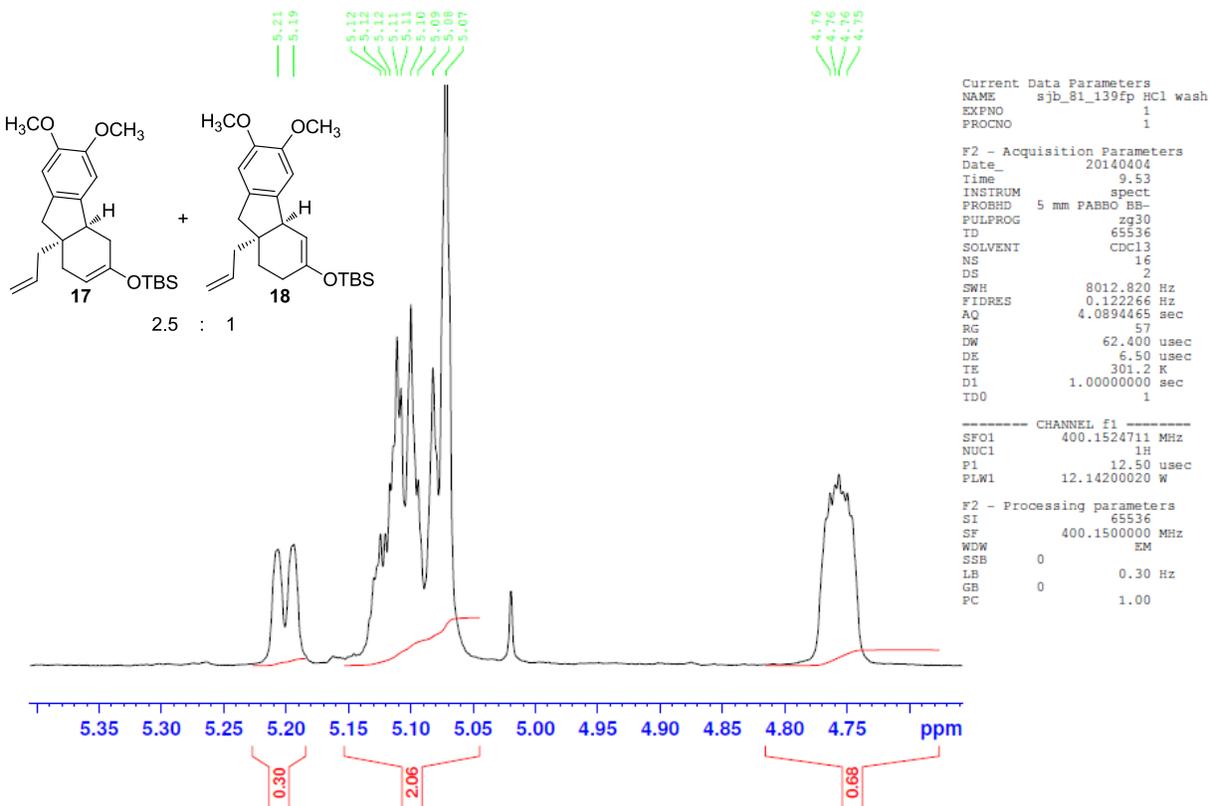
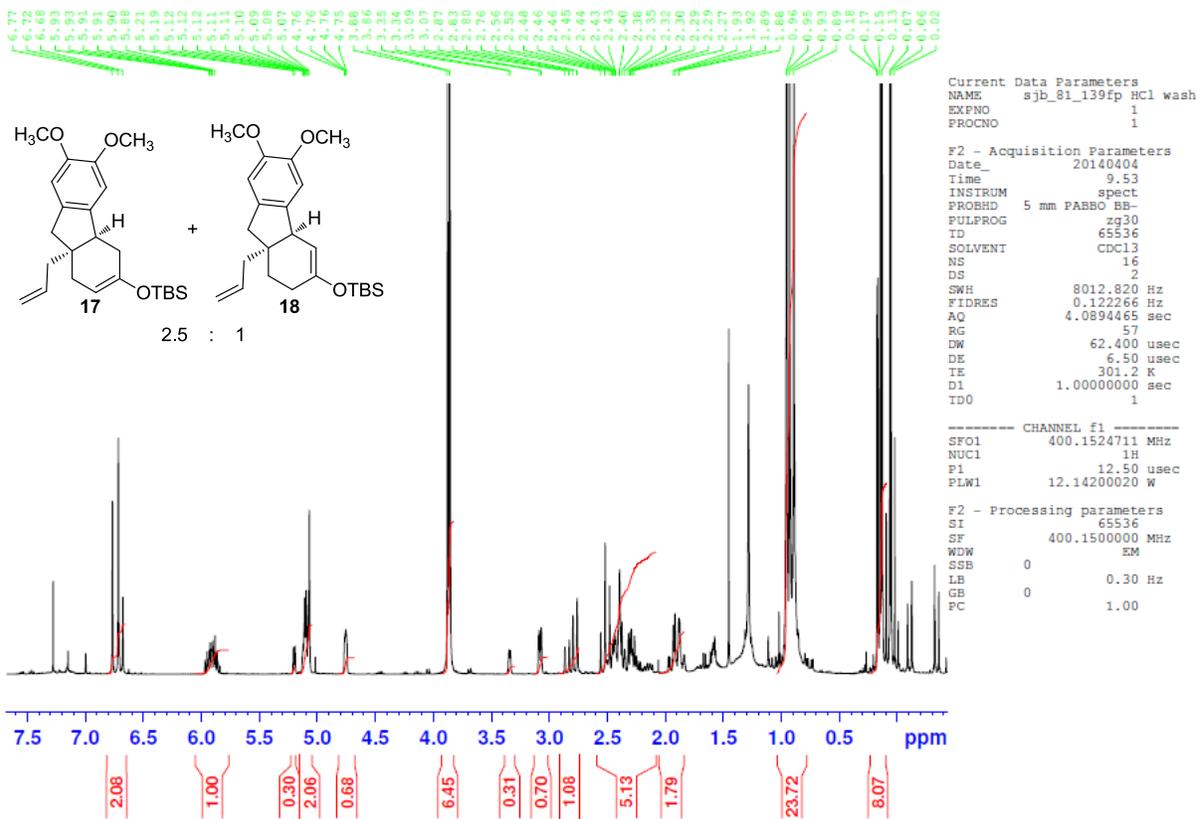
Abundance

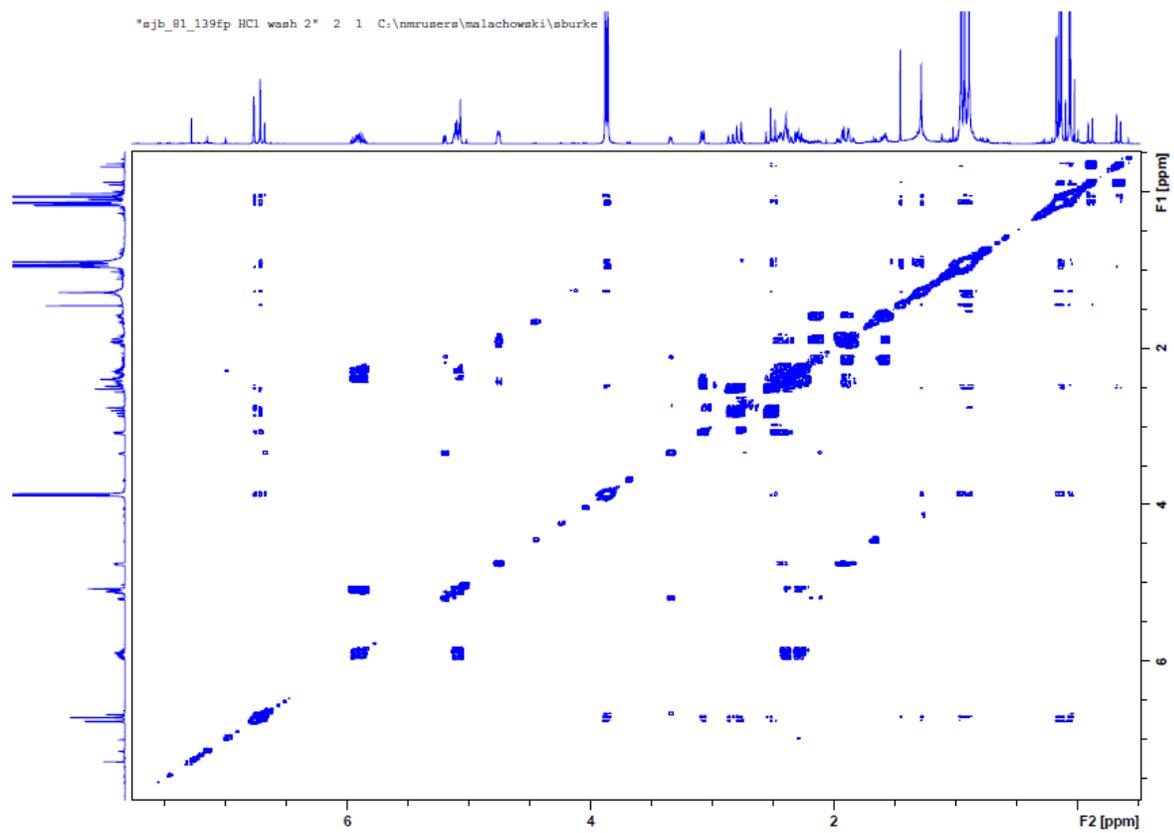
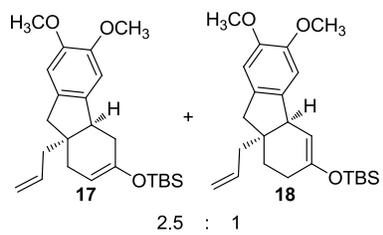


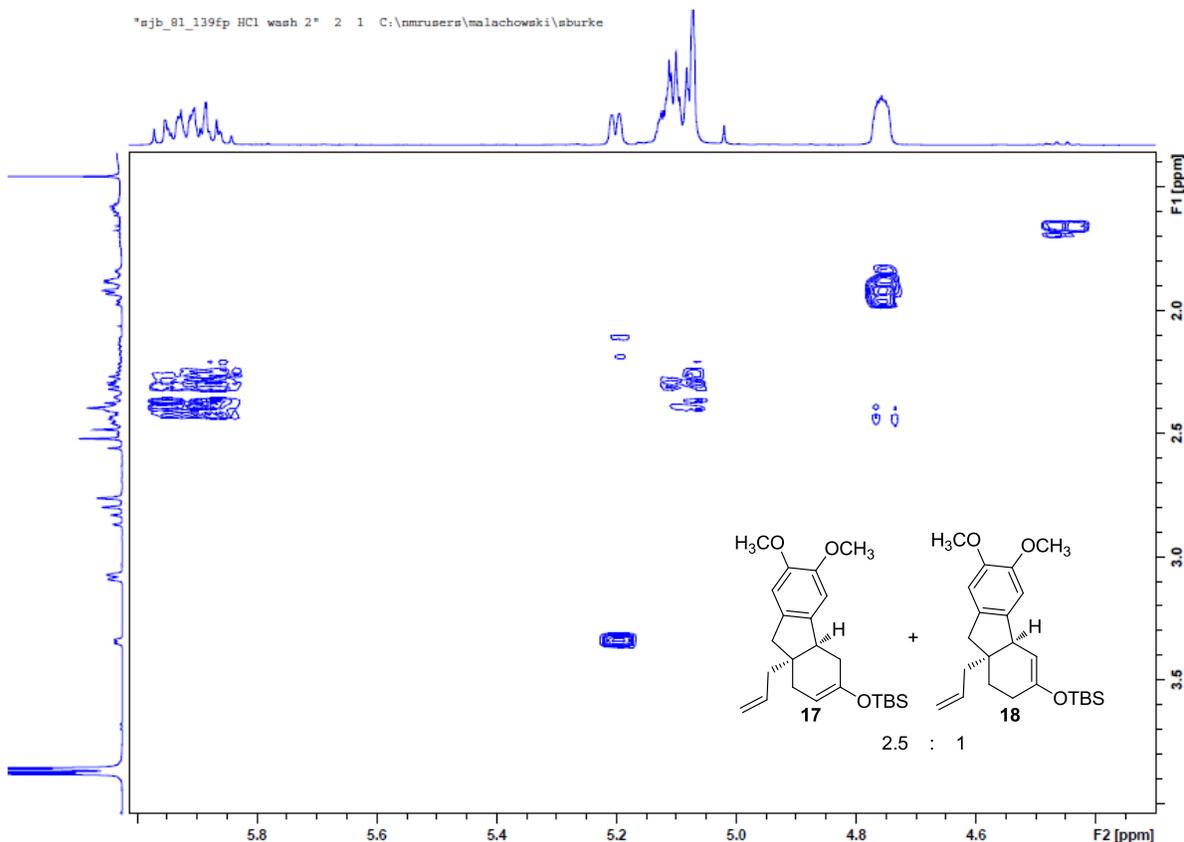
Time-->

Abundance









Area Percent Report

Data Path : C:\msdchem\1\DATA\
 Data File : sjb_81_139fp.D
 Acq On : 4 Apr 2014 10:33
 Operator : sjb
 Sample : sjb_81_139fp
 Misc :
 ALS Vial : 100 Sample Multiplier: 1

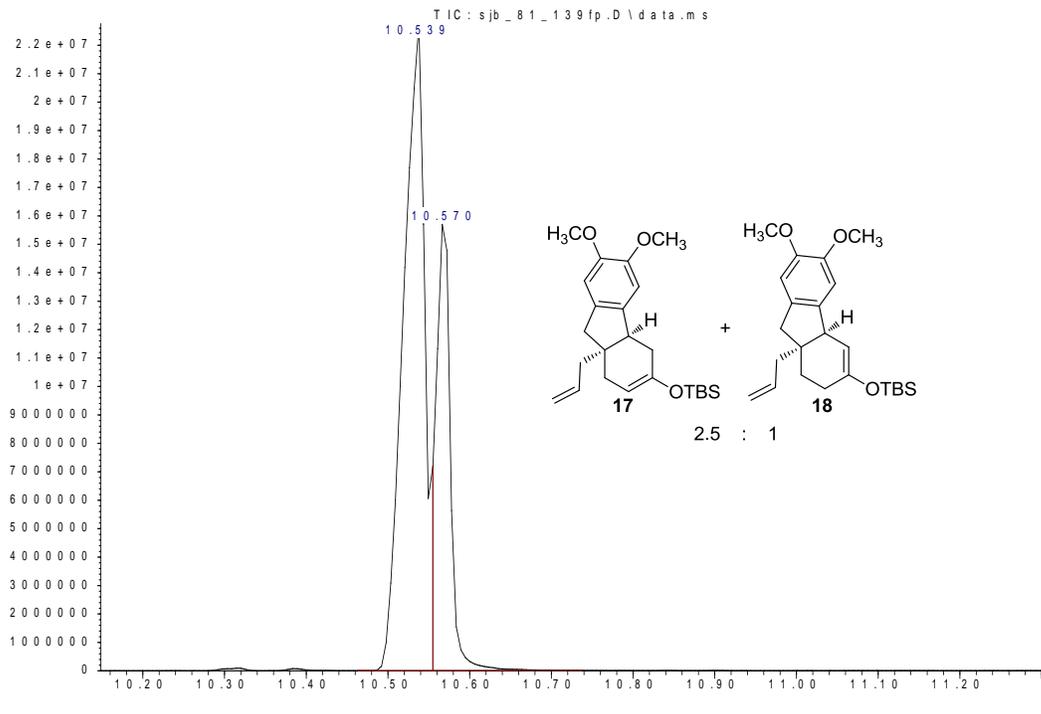
Integration Parameters: autoint1.e
 Integrator: ChemStation

Method : C:\msdchem\1\METHODS\ckr3.m
 Title :

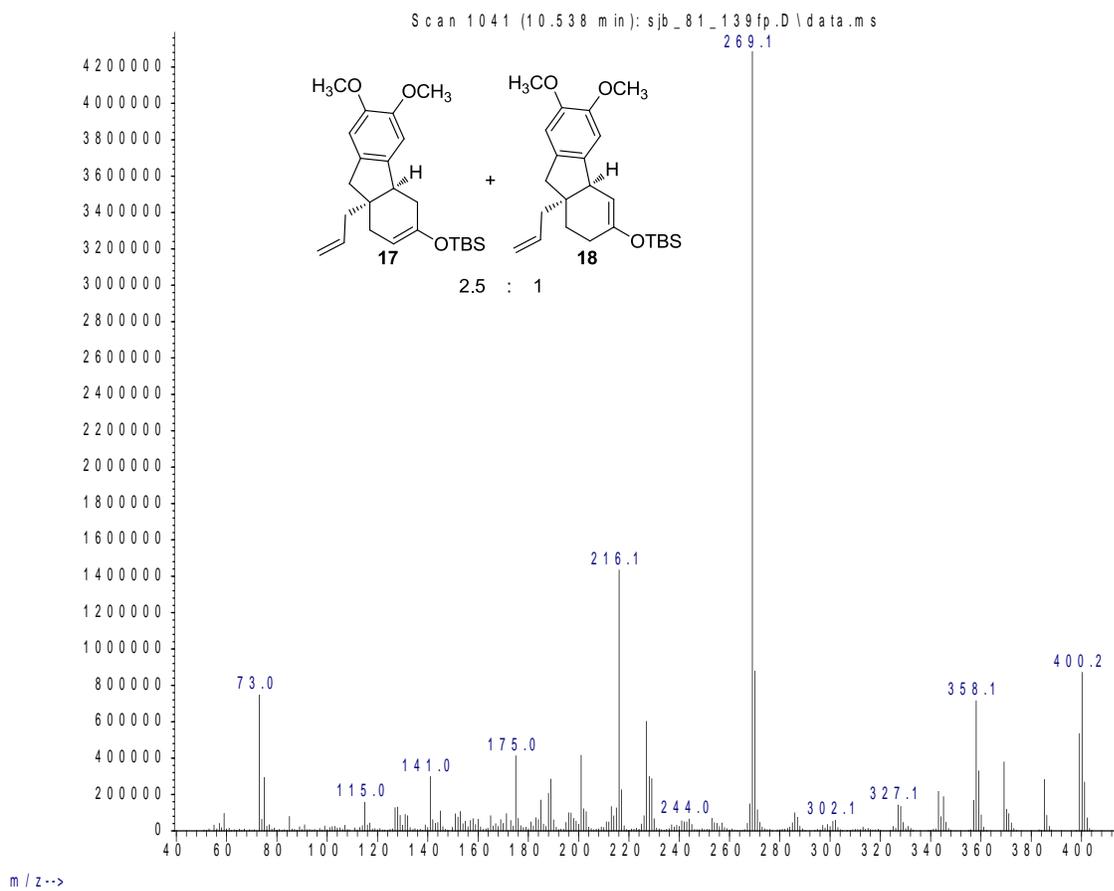
Signal : TIC: sjb_81_139fp.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.833	737	743	748	BV	449693	5482203	1.36%	0.899%
2	10.539	1028	1041	1044	BV	22326971	404324493	100.00%	66.320%
3	10.570	1044	1047	1076	VB	15532325	199850556	49.43%	32.781%

Abundance

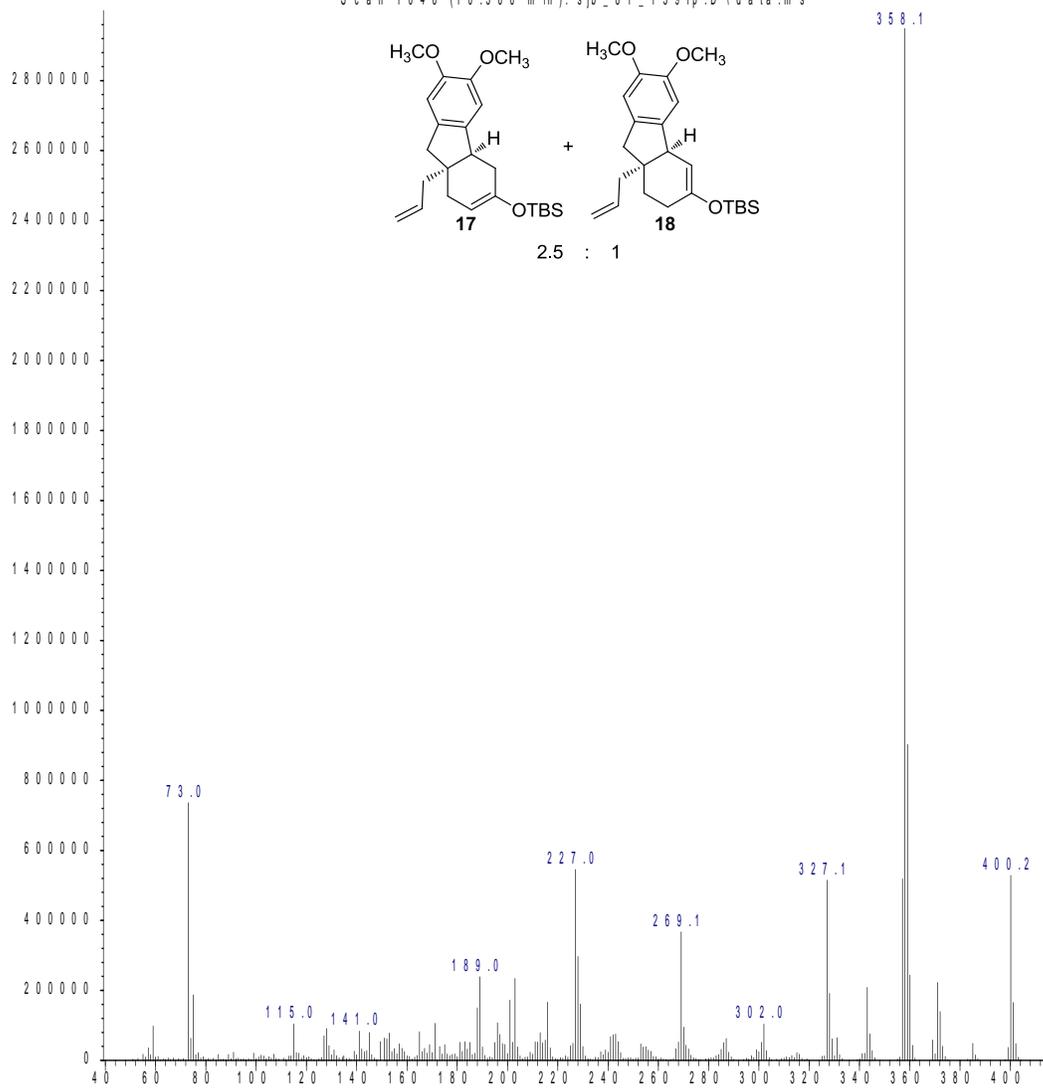


Abundance

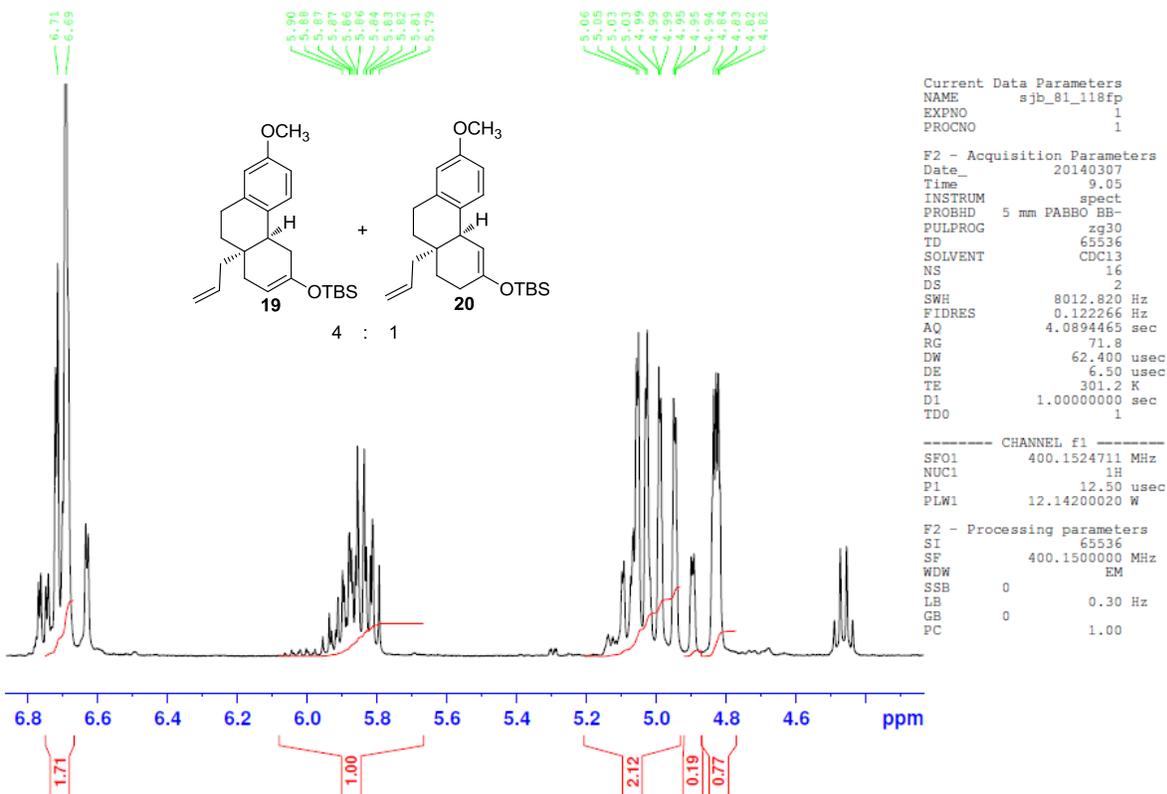
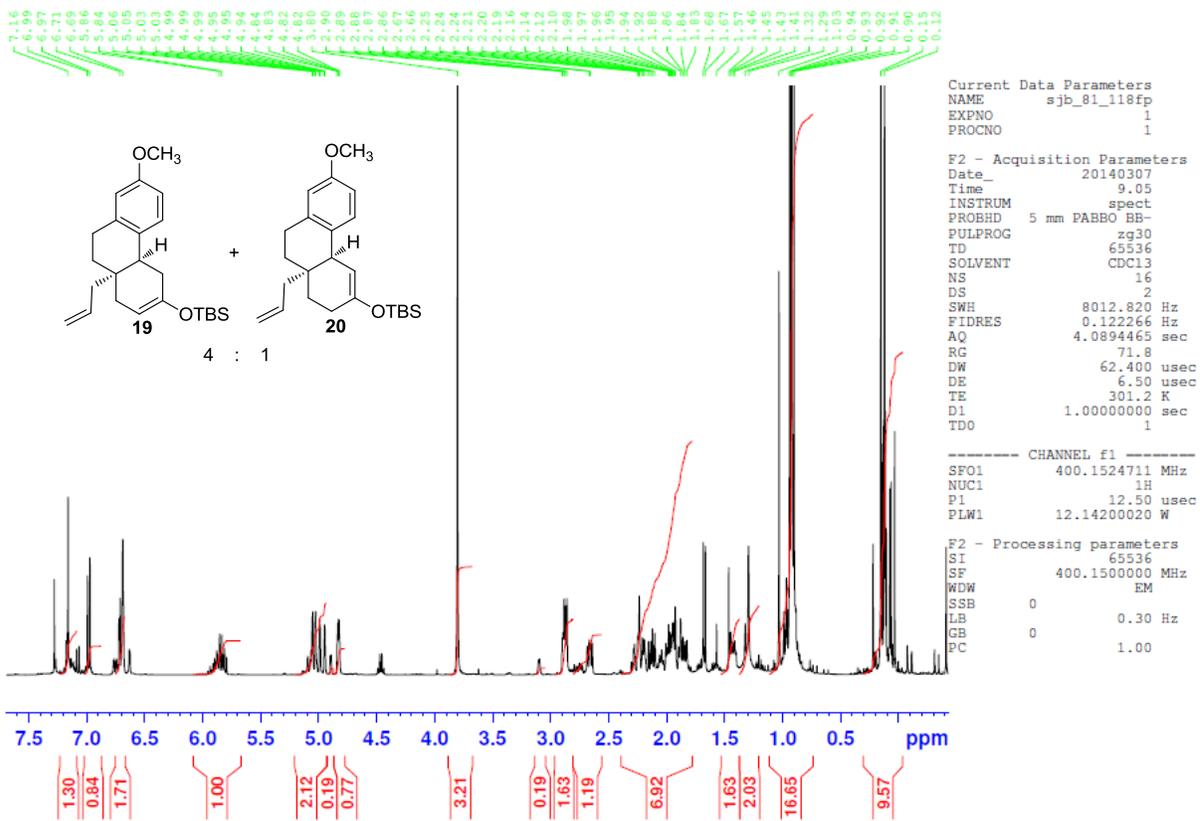


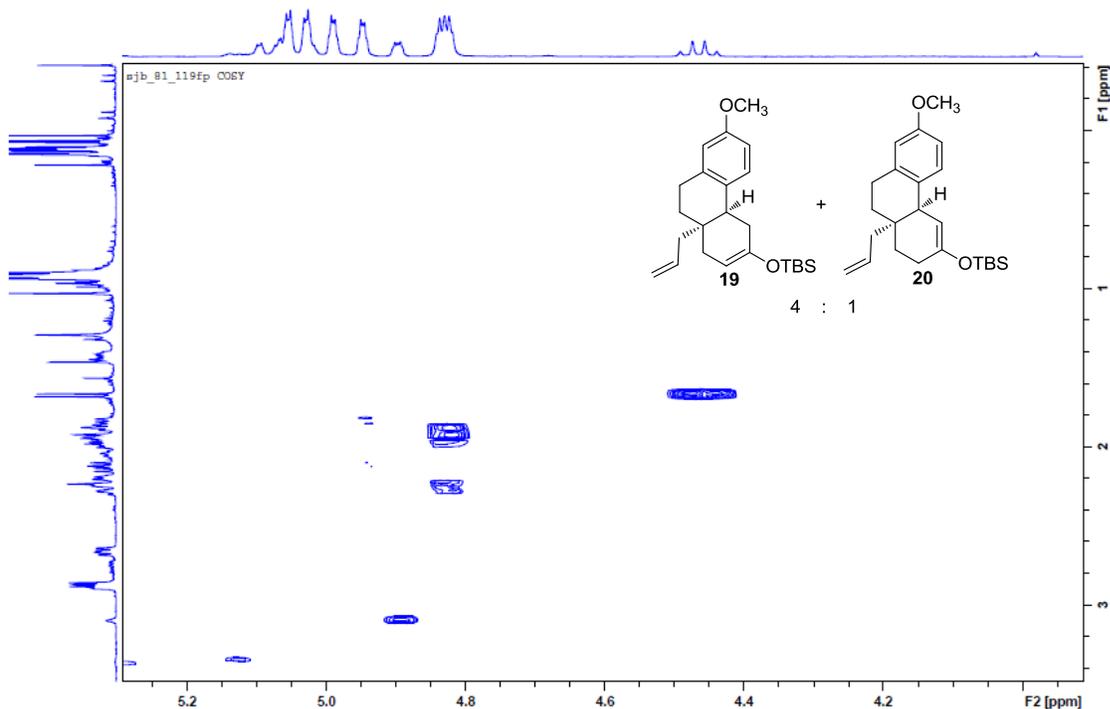
Abundance

Scan 1046 (10.566 min): sjb_81_139fp.D\data.ms



m/z-->





Area Percent Report

Data Path : C:\msdchem\1\DATA\
 Data File : sjb_81_118fp2.D
 Acq On : 7 Mar 2014 10:09
 Operator : sjb
 Sample : sjb_81_118fp2
 Misc :
 ALS Vial : 85 Sample Multiplier: 1

Integration Parameters: autoint1.e
 Integrator: ChemStation

Method : C:\msdchem\1\METHODS\ckr3.m
 Title :

Signal : TIC: sjb_81_118fp2.D\data.ms

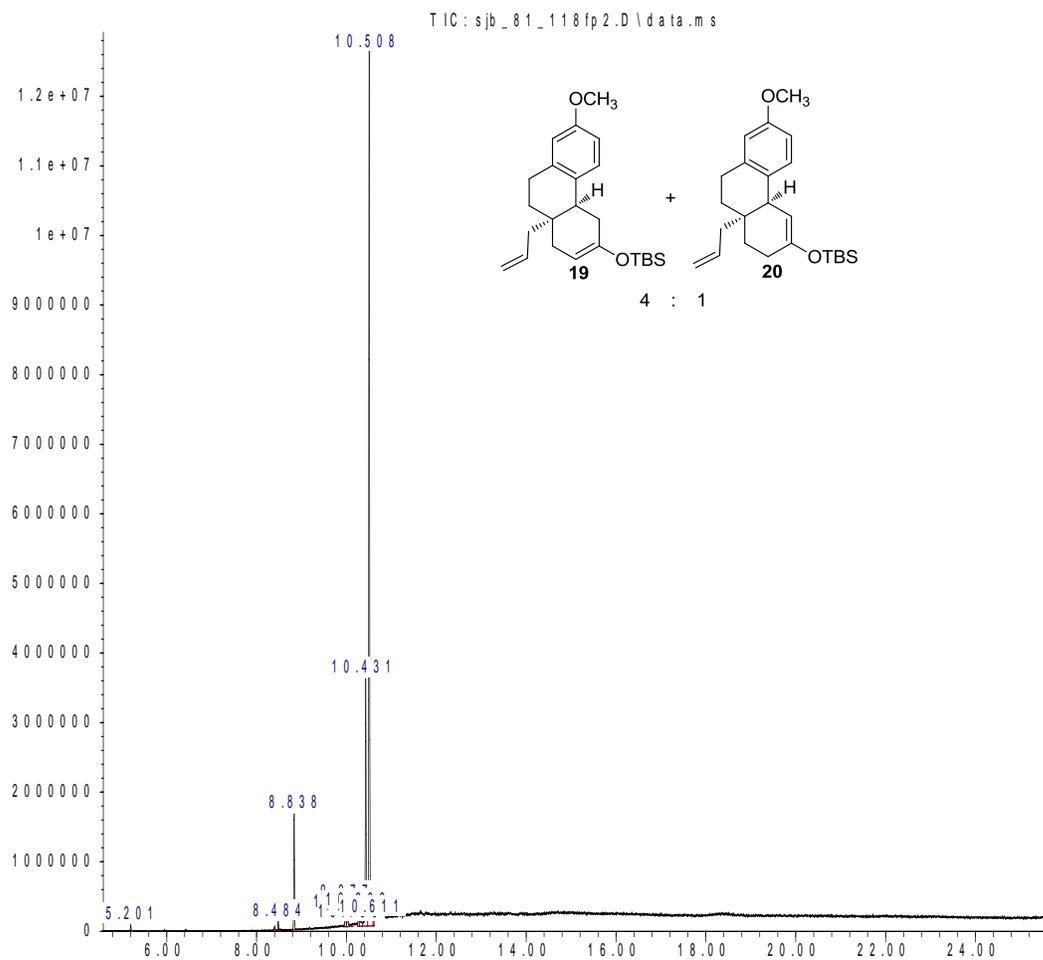
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.201	104	108	114	PB 2	87210	899707	0.52%	0.342%
2	8.484	674	682	687	PV	120399	1516861	0.87%	0.577%
3	8.838	736	744	755	PV	1657895	20458627	11.73%	7.776%
4	9.977	936	943	948	VV 2	341301	4863739	2.79%	1.849%
5	10.028	948	952	961	VV	193154	3209783	1.84%	1.220%

6	10.130	965	970	973	VV 6	39706	723550	0.41%	0.275%
7	10.273	990	995	997	VV 5	131194	1980406	1.14%	0.753%
8	10.302	997	1000	1010	VV 2	213577	4417680	2.53%	1.679%
9	10.431	1010	1022	1030	VV	3434232	48673209	27.91%	18.499%
10	10.508	1030	1036	1050	VV	13009865	174420154	100.00%	66.291%
11	10.611	1050	1054	1056	VV 5	112236	1948724	1.12%	0.741%

Sum of corrected areas: 263112441

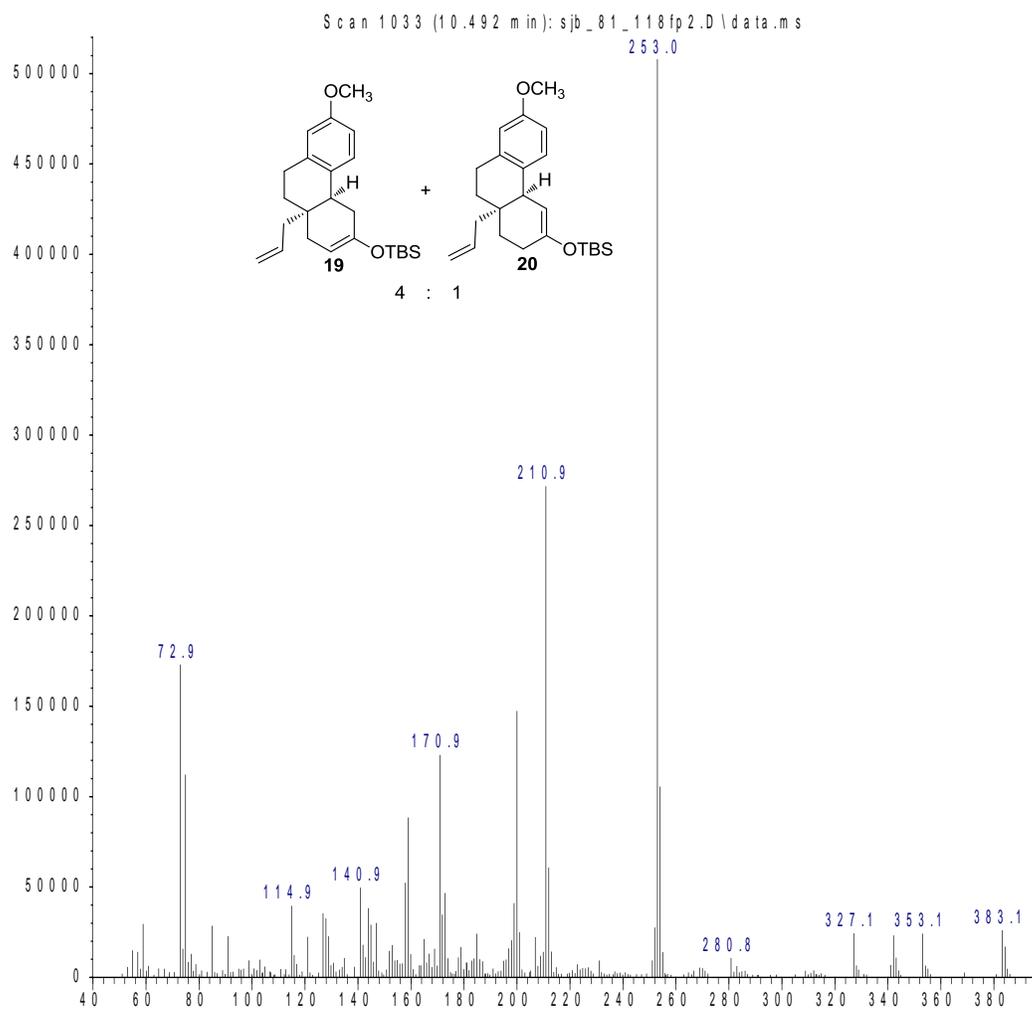
ckr3.m Tue Mar 25 16:57:32 2014

Abundance



Time -->

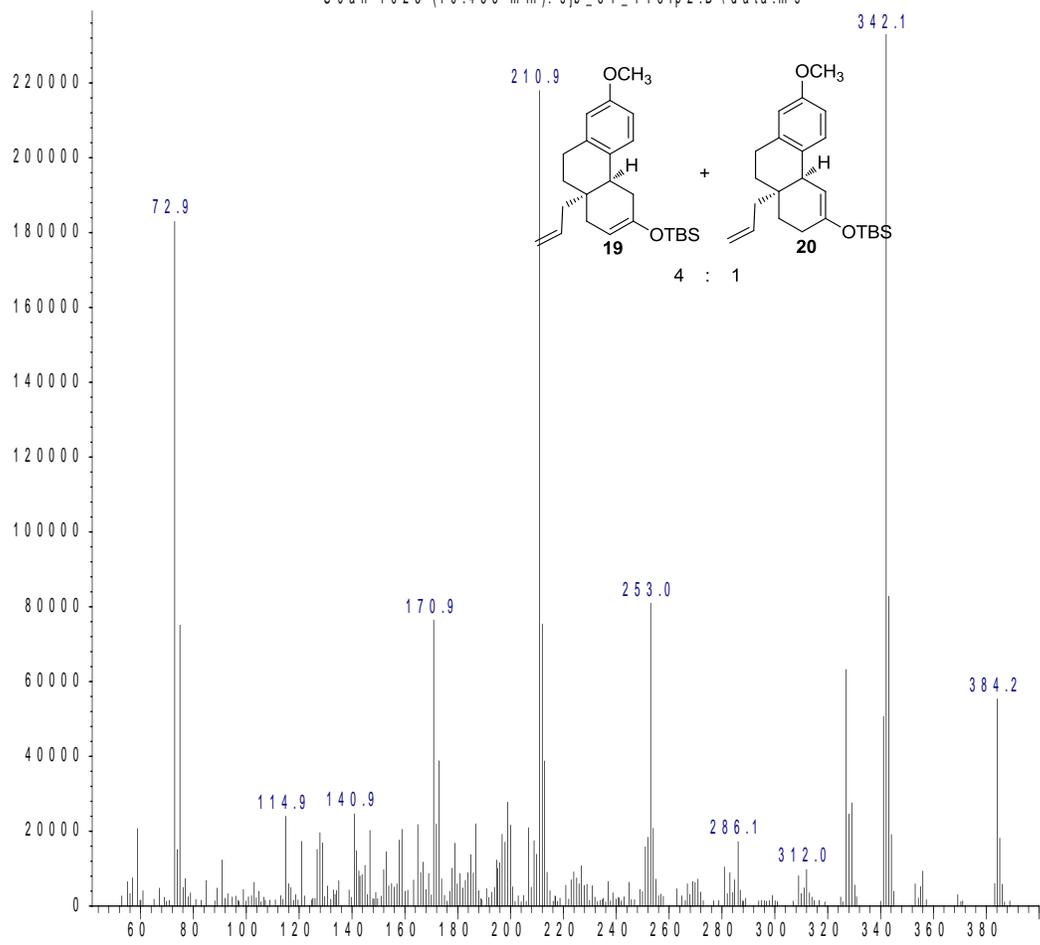
Abundance

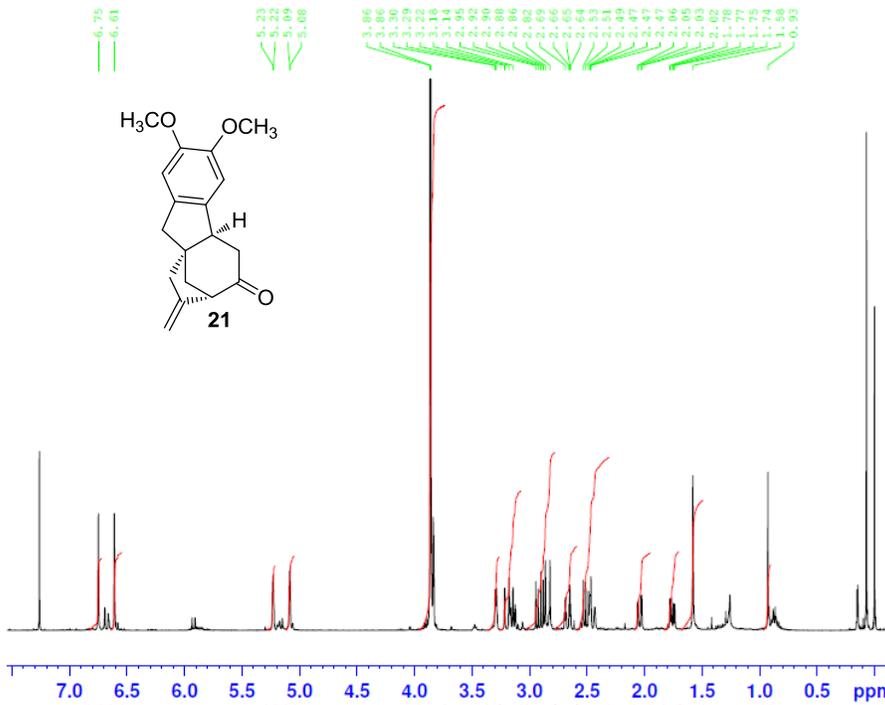


m/z-->

Abundance

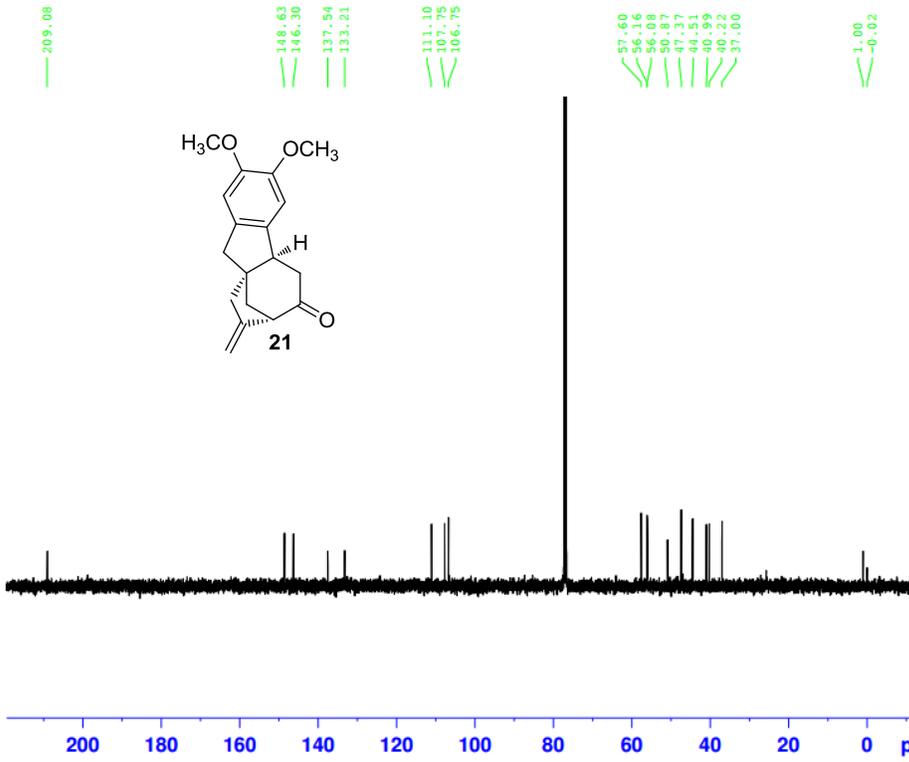
Scan 1023 (10.435 min): sjb_81_118fp2.D\data.ms





NAME sjb_74_180 fr3-5
EXPNO 1
PROCNO 1
Date_ 20121022
Time 10.12
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 301.2 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.80 usec
PL1 -4.00 dB
PL1W 19.24419975 W
SFO1 400.1524711 MHz
SI 32768
SF 400.1500084 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME sjb_74_180 fr 3-5 13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121022
Time 11.38
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 301.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 0 dB
PL1W 35.41759872 W
SFO1 100.6278593 MHz
===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.80 dB
PL12 13.80 dB
PL13 13.80 dB
PL2W 18.37806702 W
PL12W 0.31937420 W
PL13W 0.31937420 W
SFO2 400.1516006 MHz

F2 - Processing parameters
SI 32768
SF 100.6177980 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Area Percent Report

Data Path : C:\msdchem\1\DATA\
Data File : sjb_74_180 fr3-5.D
Acq On : 19 Oct 2012 11:34
Operator : sjb
Sample : sjb_74_180 fr3-5
Misc :
ALS Vial : 10 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\msdchem\1\METHODS\ckr3.m
Title :

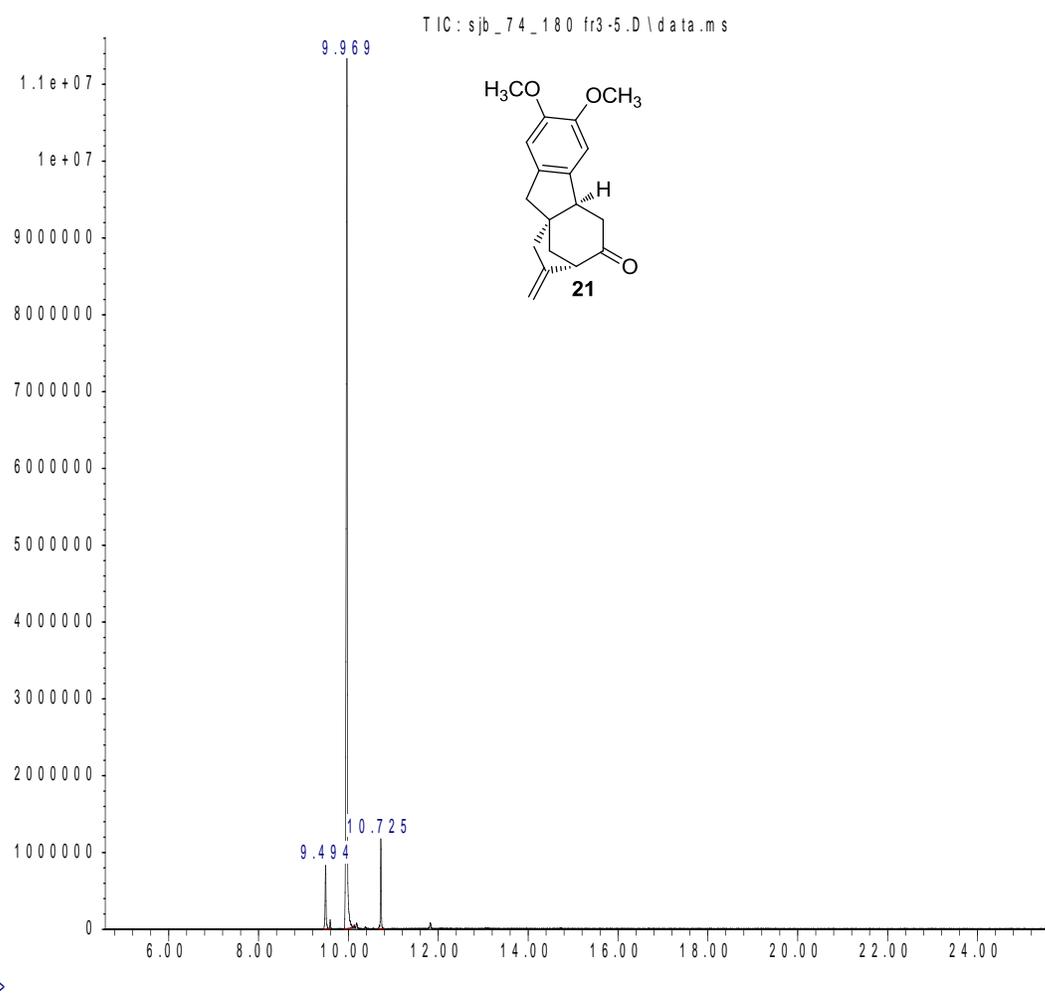
Signal : TIC: sjb_74_180 fr3-5.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	9.494	850	859	872	BV	798947	11914481	5.98%	5.277%
2	9.969	931	942	967	BV	11427409	199102091	100.00%	88.184%
3	10.725	1063	1074	1082	BV	1129946	14764330	7.42%	6.539%

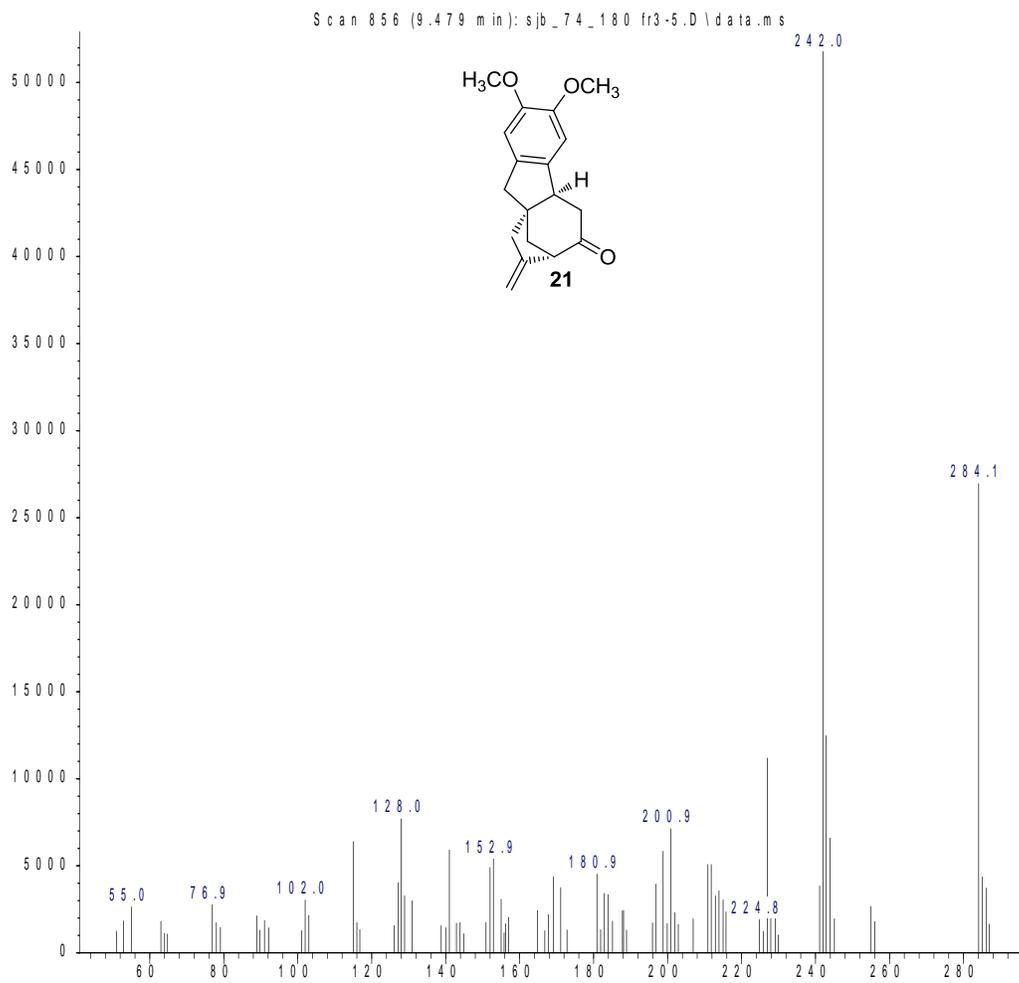
Sum of corrected areas: 225780902

ckr3.m Mon Apr 07 17:09:08 2014

Abundance

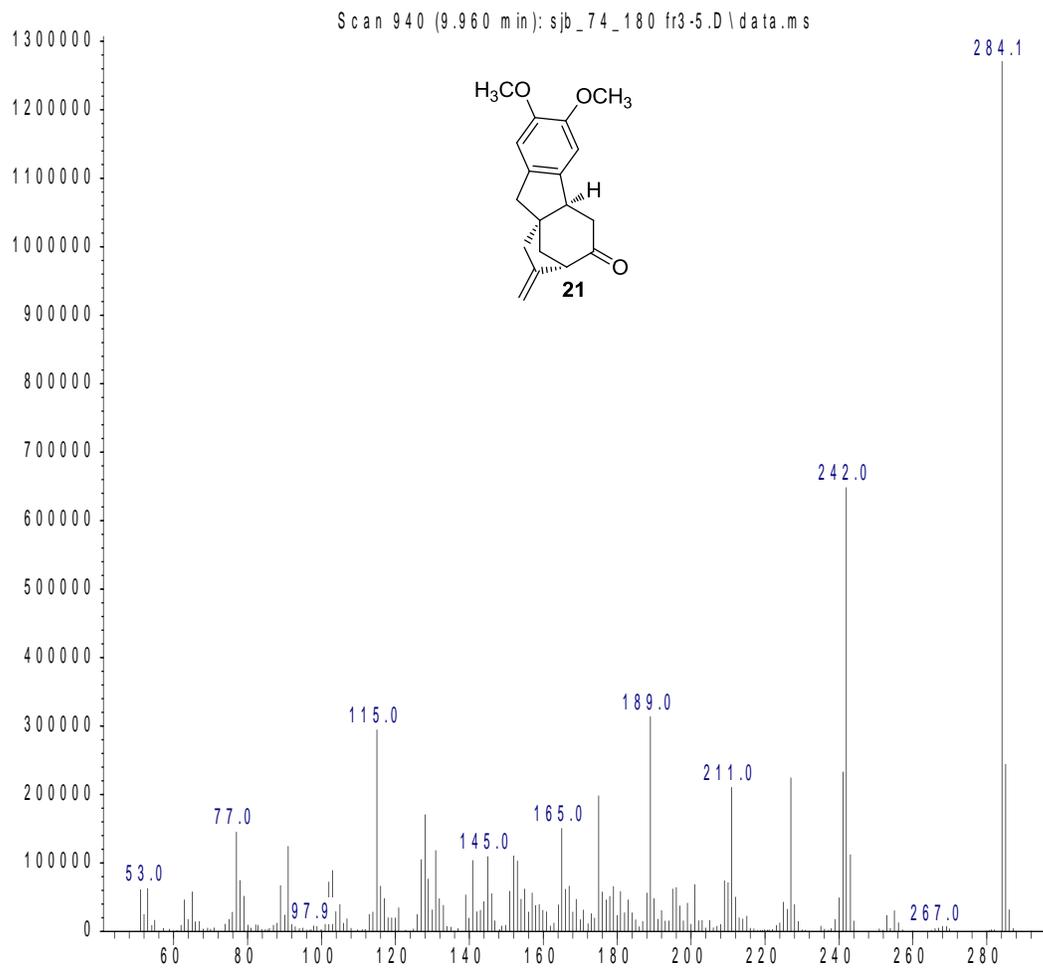


Abundance



m/z-->

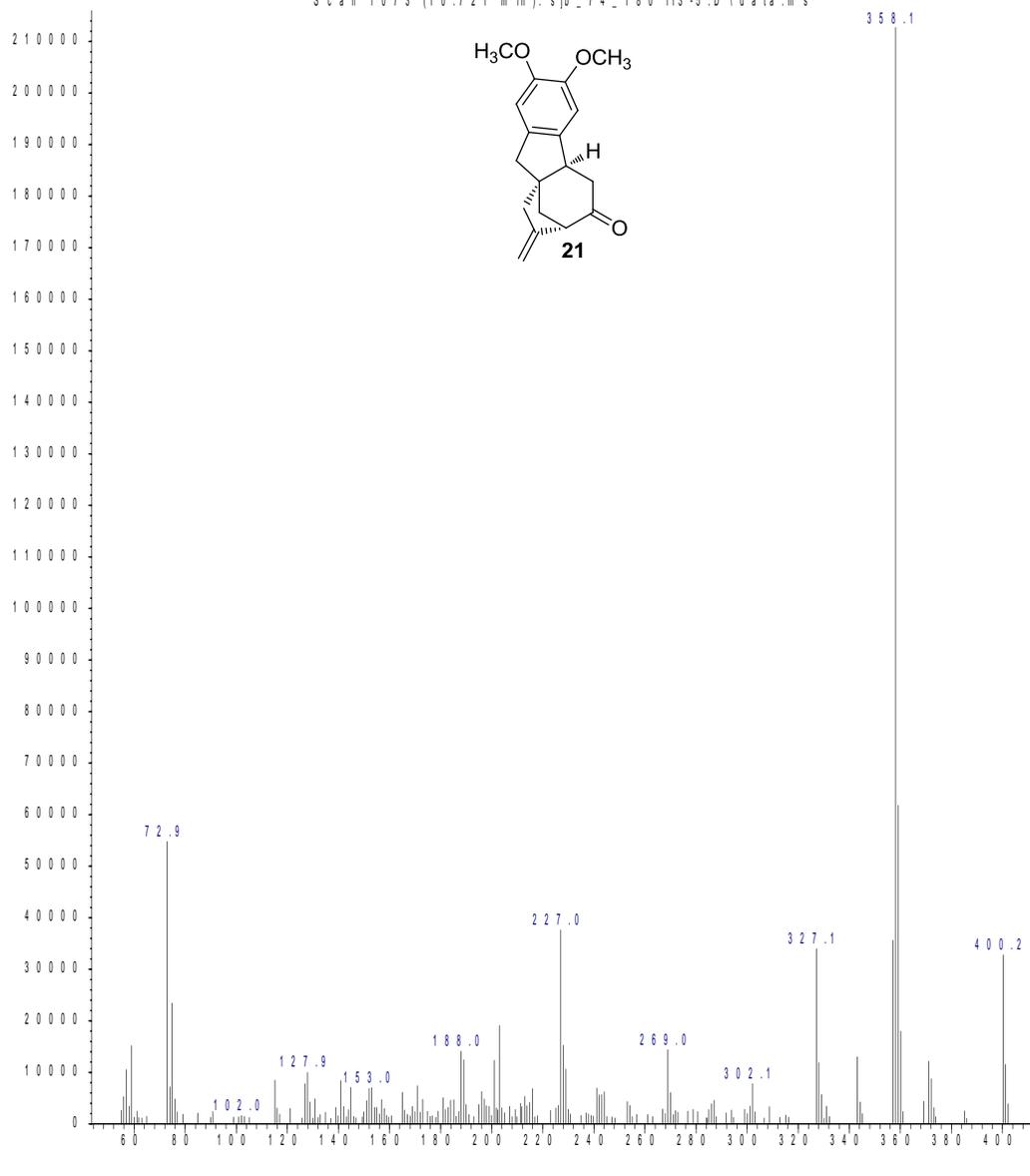
Abundance

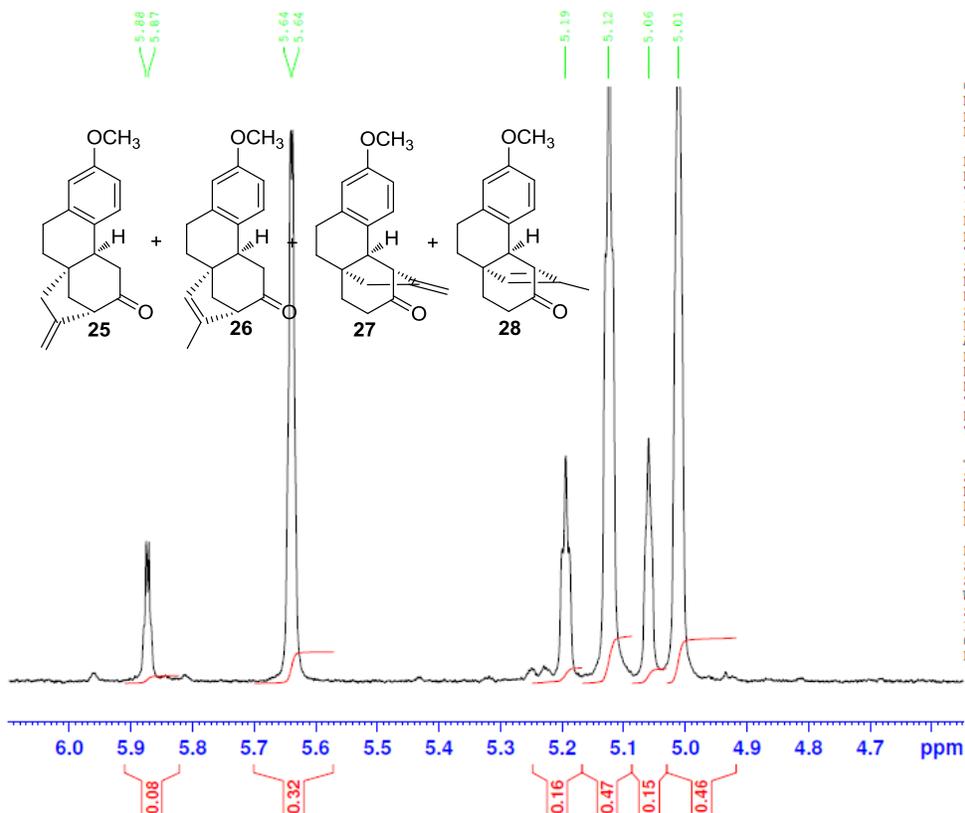
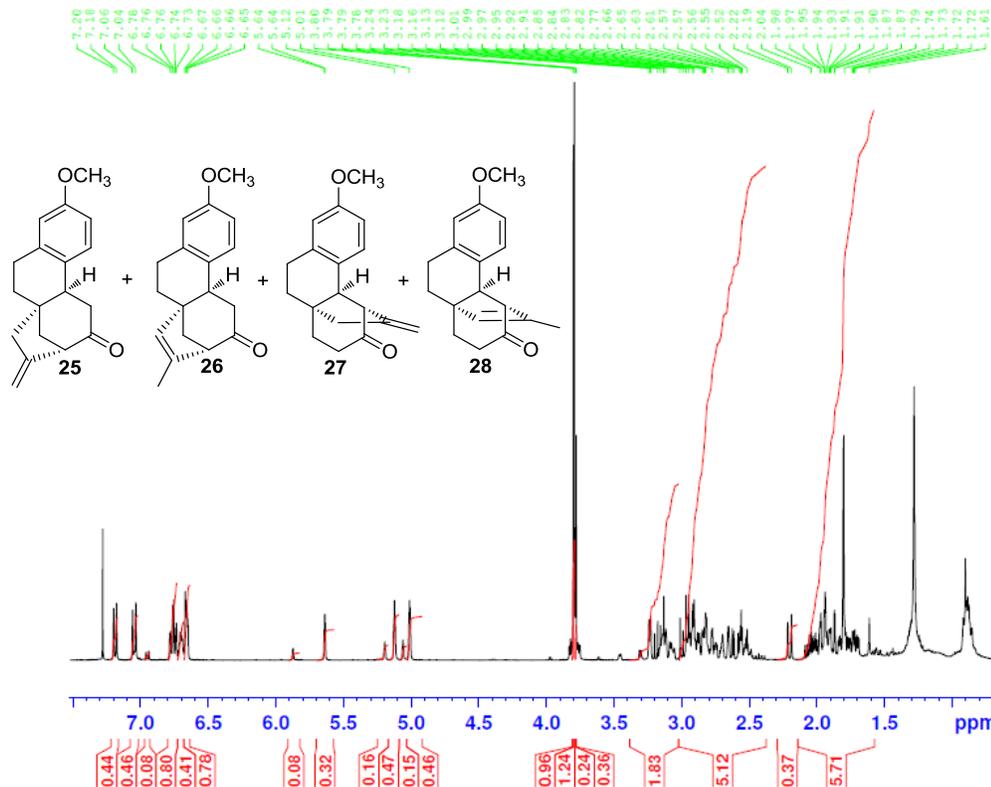


m/z-->

Abundance

Scan 1073 (10.721 min): sjb_74_180 fr3-5.D\data.ms





Area Percent Report

Data Path : C:\msdchem\1\DATA\
Data File : sjb_81_121fp.D
Acq On : 14 Mar 2014 9:05
Operator : sjb
Sample : sjb_81_121fp
Misc :
ALS Vial : 90 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\msdchem\1\METHODS\ckr3.m
Title :

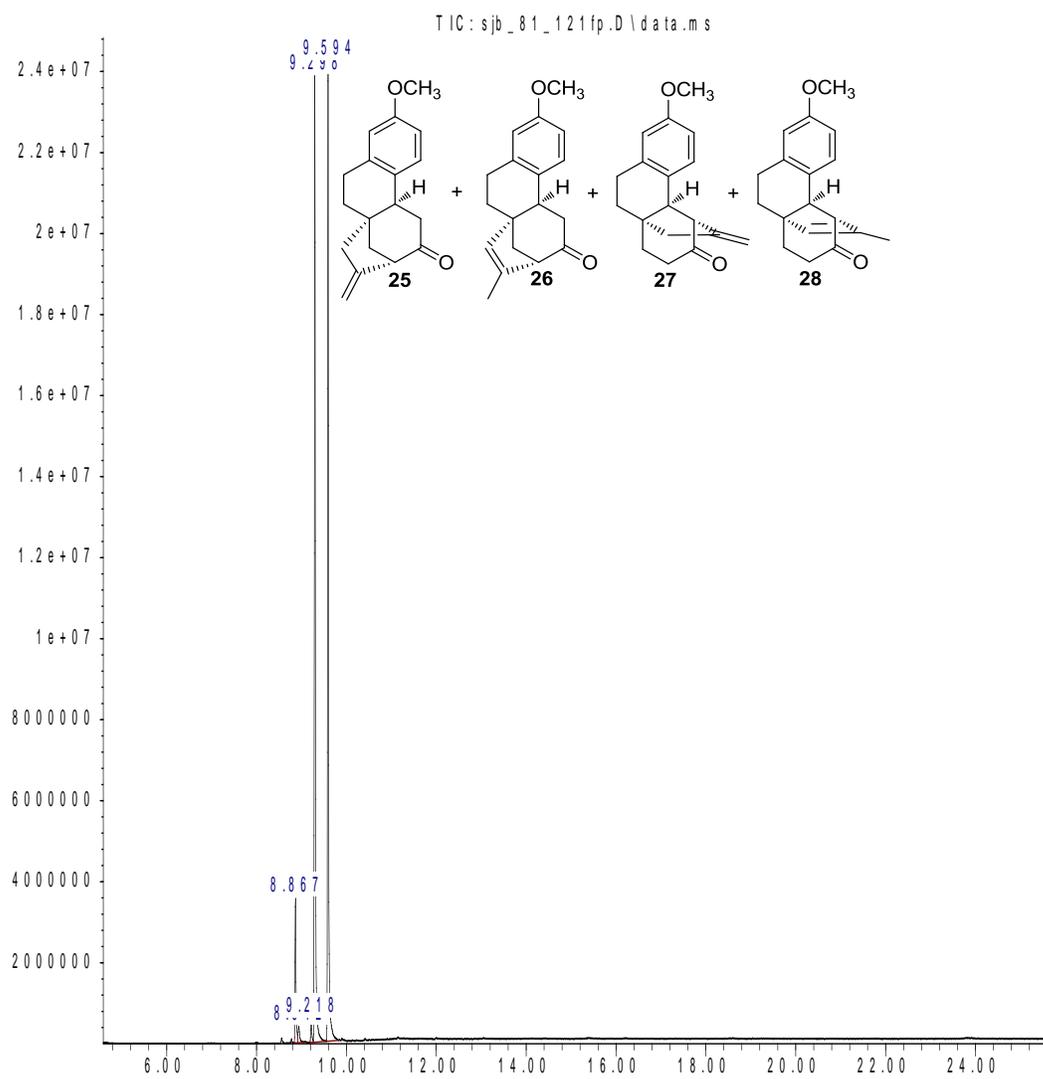
Signal : TIC: sjb_81_121fp.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.867	743	749	758	BV	3522428	56027446	14.44%	6.629%
2	8.942	758	762	782	VB 4	398136	10292277	2.65%	1.218%
3	9.218	805	810	818	BV 2	561113	10095541	2.60%	1.195%
4	9.298	818	824	863	VV 2	22894893	387965102	100.00%	45.906%
5	9.594	867	876	917	VV	24458757	380749882	98.14%	45.052%

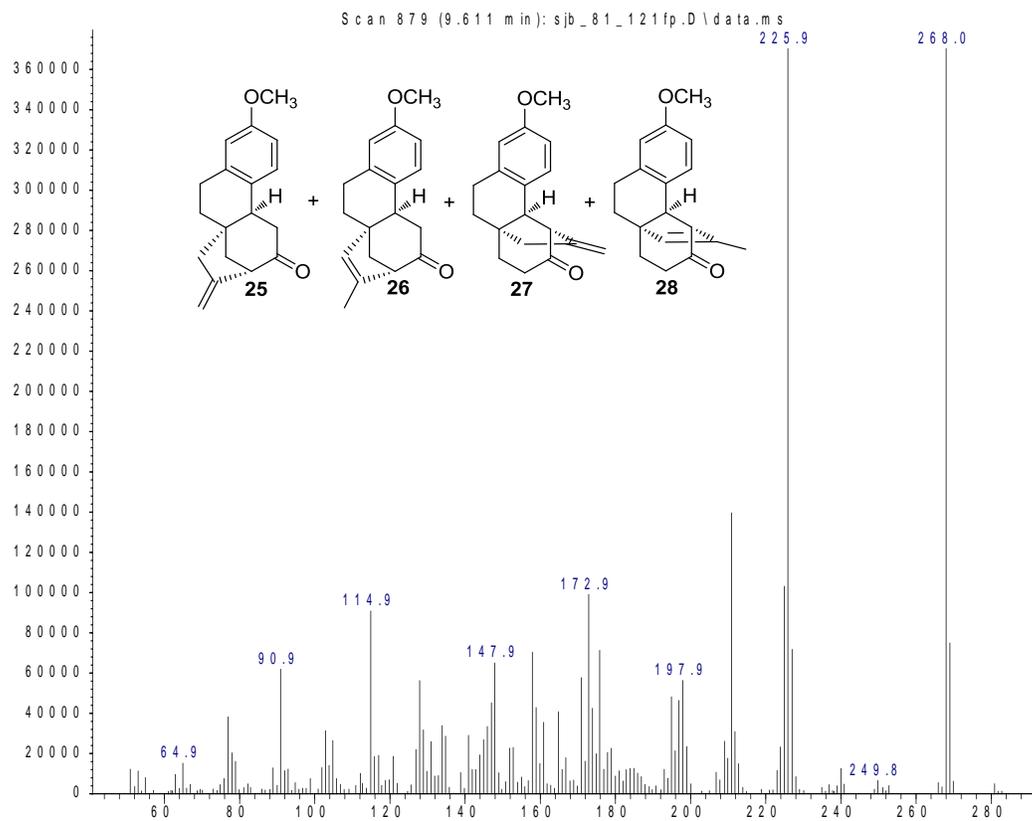
Sum of corrected areas: 845130248

ckr3.m Thu Mar 27 12:26:01 2014

Abundance

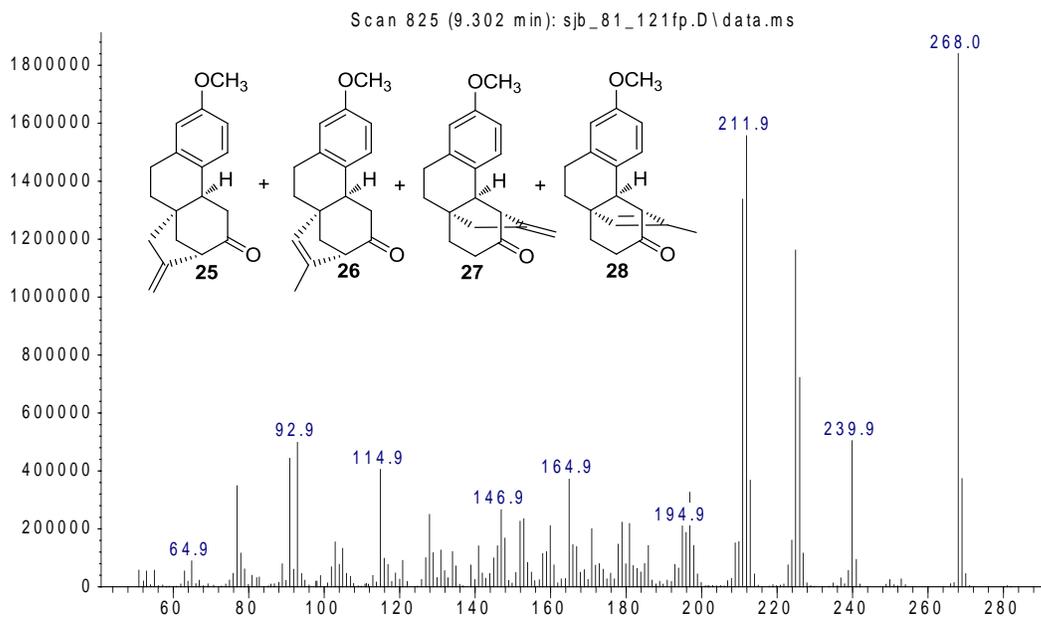


Abundance



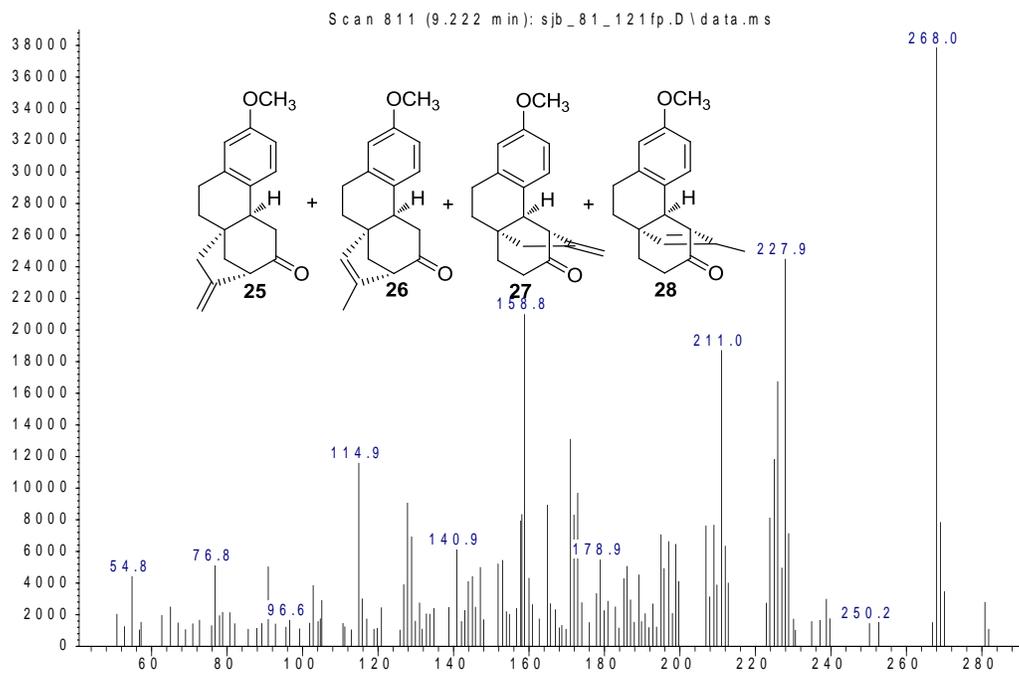
m/z-->

Abundance

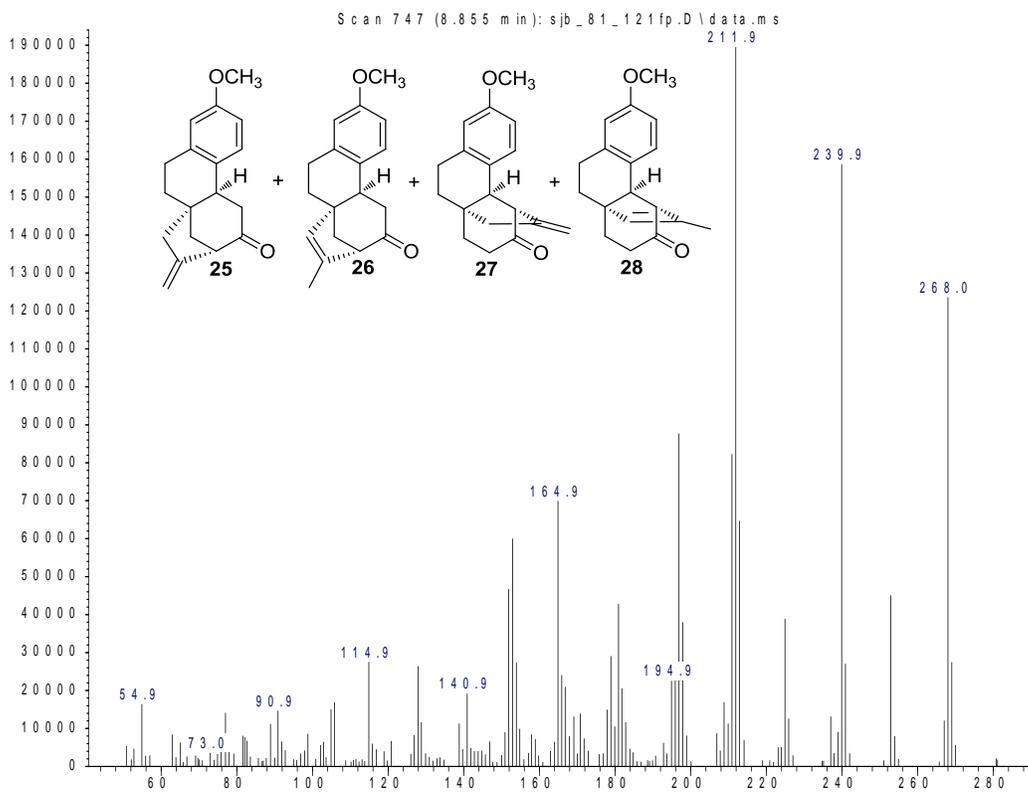


m/z-->

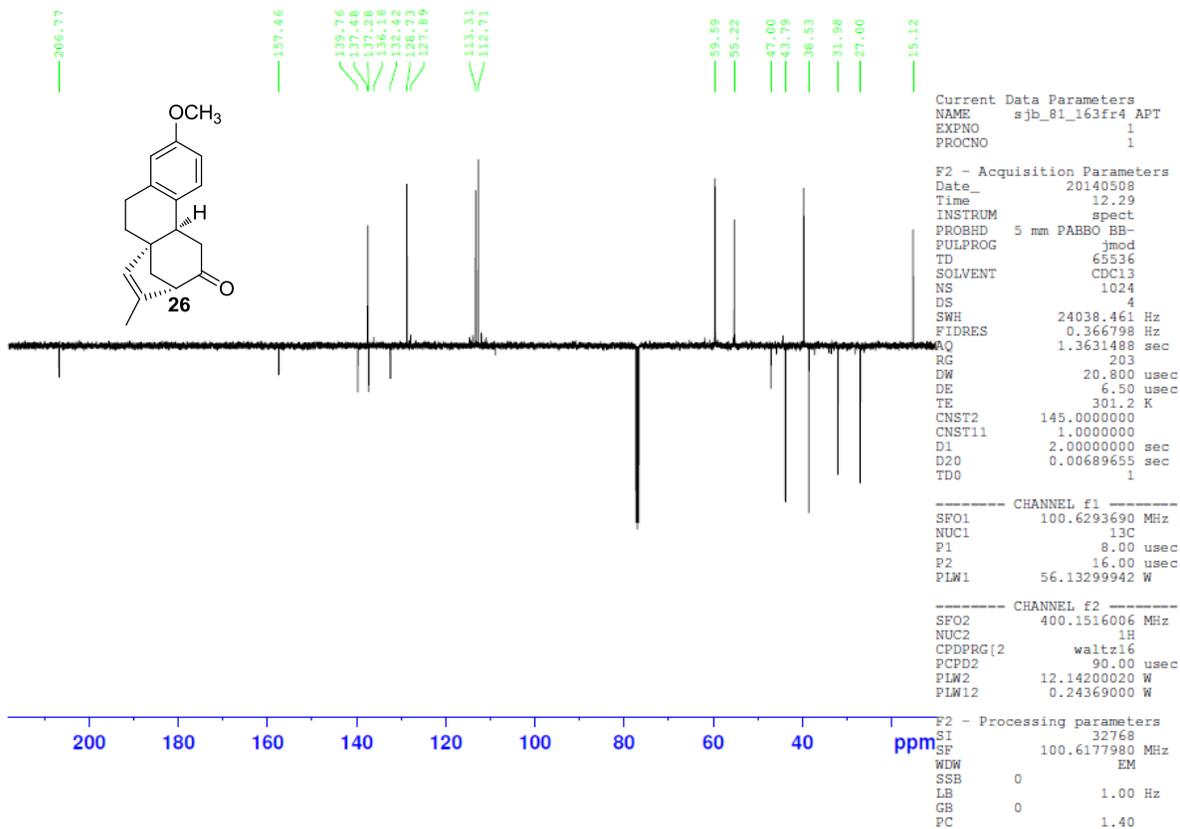
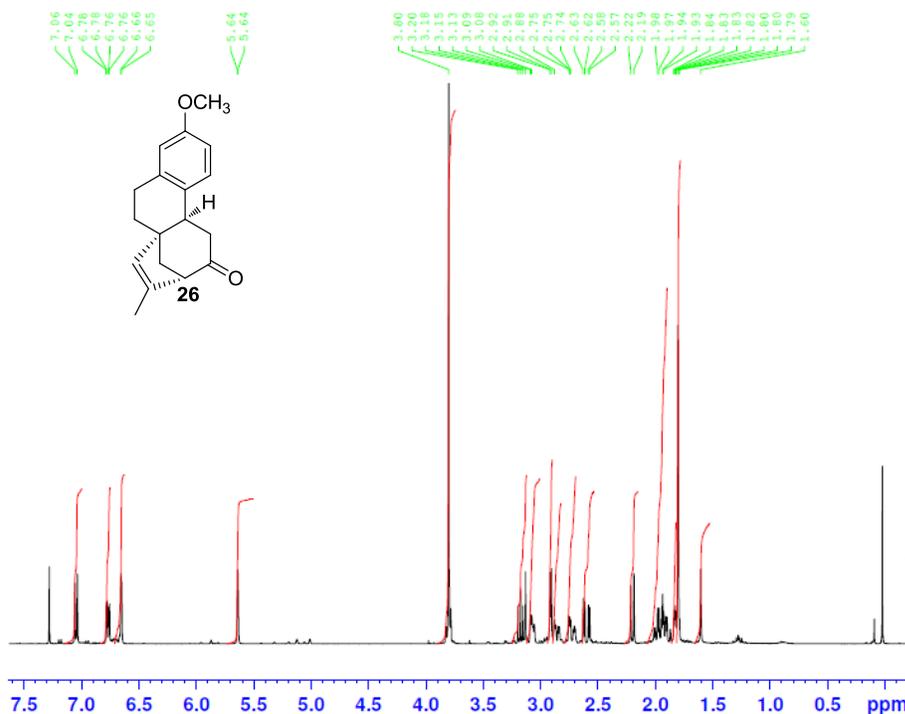
Abundance



m/z-->
Abundance



m/z-->



Area Percent Report

Data Path : C:\msdchem\1\DATA\
Data File : sjb_81_163 fr4.D
Acq On : 7 May 2014 16:54
Operator : sjb
Sample : sjb_81_163 fr4
Misc :
ALS Vial : 100 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\msdchem\1\METHODS\ckr3.m
Title :

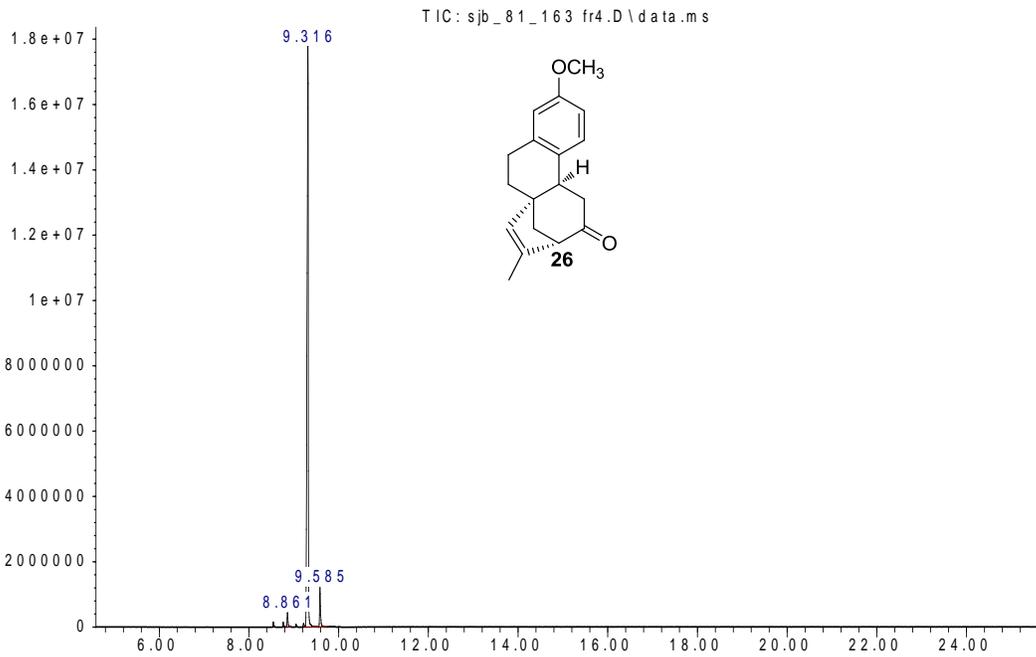
Signal : TIC: sjb_81_163 fr4.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.861	743	748	757	BV	436595	6037089	1.74%	1.626%
2	9.316	817	827	862	VB	18042696	347130619	100.00%	93.508%
3	9.585	867	875	897	BB	1151425	18062141	5.20%	4.865%

Sum of corrected areas: 371229849

ckr3.m Mon May 12 15:24:00 2014

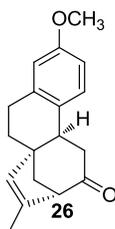
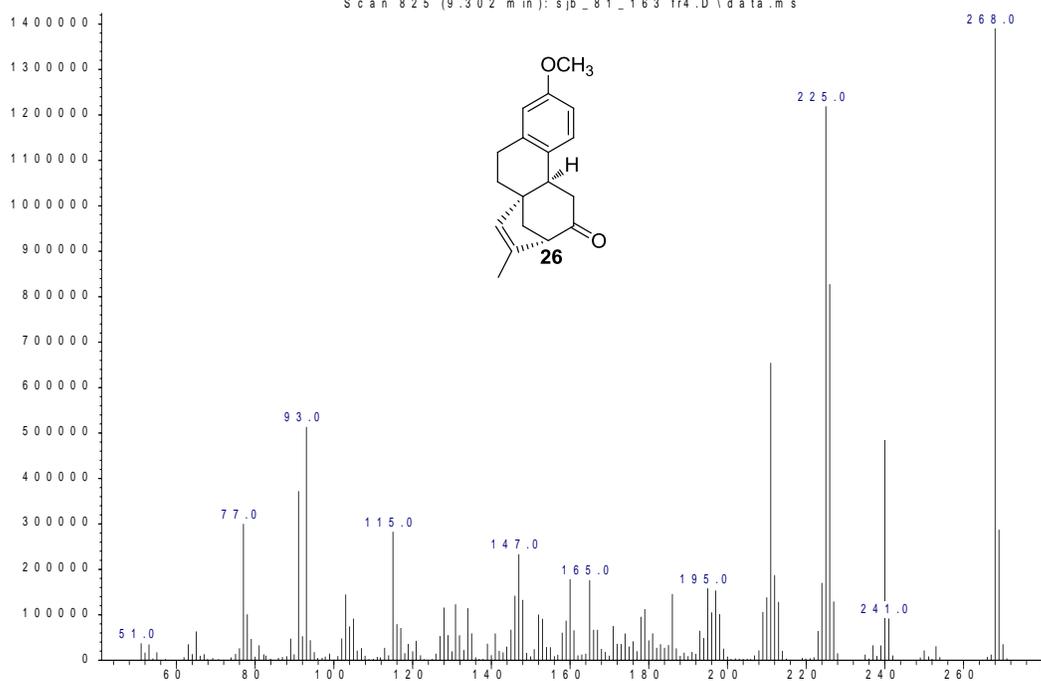
Abundance



Time-->

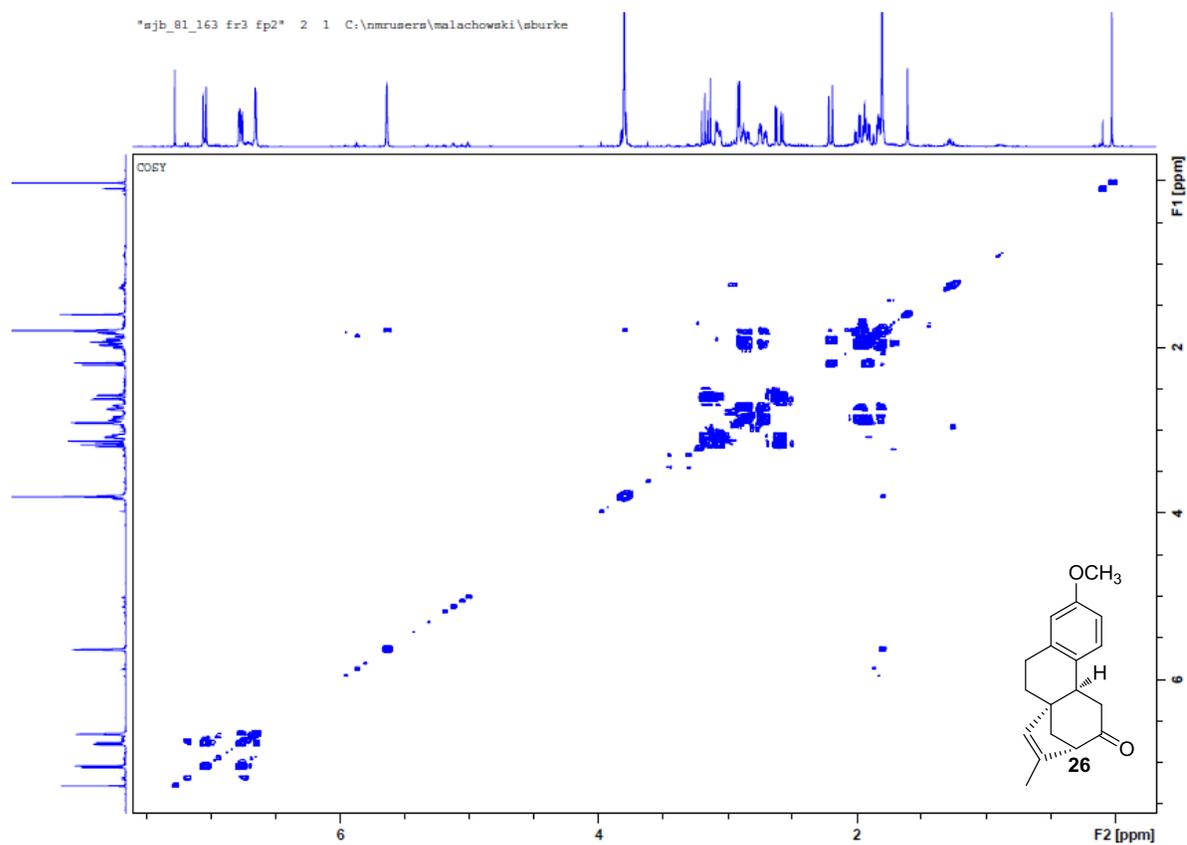
Abundance

Scan 825 (9.302 min): sjb_81_163 fr4.D\data.ms



m/z-->

"sjb_81_163 fr3 Ep2" 2 1 C:\nmruser\malachowski\sburke



"ejb_01_163 Fz3 fp3" 2 1 C:\nmrusers\malachowski\aburke

