

Supplementary data for article:

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A highly regioselective, protecting group controlled, synthesis of bicyclic compounds via Pd-catalysed intramolecular cyclisations

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SUPPLEMENTARY INFORMATION

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1. General

The NMR spectra were recorded on a Bruker Avance III (500 MHz) spectrometer. Chemical shifts are given in parts per million (δ) downfield from tetramethylsilane as the internal standard. Deuteriochloroform was used as a solvent, unless otherwise stated. Mass spectral data were recorded using Agilent MSD TOF spectrometer coupled with Agilent 1200 HPLC. IR spectra were recorded on a IR Termo Scientific NICOLET iS10 (4950) spectrometer. Flash chromatography employed silica gel 60 (230-400 mesh) while thin layer chromatography was carried out using alumina plates with 0.25mm silica layer (Kieselgel 60 F₂₅₄, Merck). The solvents were purified by distillation before use.

2. Synthetic procedures

2.1 General procedure for the synthesis of compound **11** (table 1)

A mixture of compound **5** (30mg, 0.066mmol), Pd(OAc)₂ (1.5mg, 0.0066mmol), PPh₃ (3.5mg, 0.0131mmol), base (2 eq) in toluene (6.5 mL) was refluxed under nitrogen atmosphere for 15h. The solvent was evaporated under reduced pressure and the residue was dissolved in DCM (20 mL), washed with water, dried (Na₂SO₄) and filtered. The solvent was then evaporated under reduced pressure and the residue was purified by flash chromatography (SiO₂, 8:2 v/v petroleum ether-ether) to afford the product **11** as light yellow oil.

IR ν_{\max} : 2927, 2856, 1615, 1390, 776, 740

¹H NMR (500 MHz, CDCl₃) δ -0.12, 0.03 (2s, 6H, 2CH₃ from TBDMS), 0.63 (s, 9H, C(CH₃)₃ from TBDMS), 3.25 (s, 3H, N-CH₃), 3.61 (dd, 1H, $J=6.5\text{Hz}$, $J=3.5\text{Hz}$, CH-C₆H₄), 3.97 (dd, 1H, $J=6.5\text{Hz}$, $J=3\text{Hz}$, NCH-CH(OTBDMS)), 4.55 (t, 1H, $J=6.5\text{Hz}$, CH(OTBDMS)), 5.83(dd, 1H, $J=6\text{Hz}$, $J=3\text{Hz}$, CH(C₆H₄)CH=CH), 6.06 (dd, 1H, $J=6\text{Hz}$, $J=3.5\text{Hz}$, CH(C₆H₄)CH=CH), 7.10 (dd, 1H, ArH), 7.26-7.34 (m, 2H, ArH), 8.57 (dd, 1H, ArH)

¹³C NMR (125 MHz, CDCl₃) δ -5.0, -4.96, 17.63, 25.3, 40.03, 56.02, 66.5, 69.6, 126.5, 127.4, 129.21, 130.8, 133.9, 134.71, 138.32, 139.51, 167.83

m/z (EI) 329.1 (M⁺), 314.1, 272.1, 215.0, 198.1, 156

HRMS (ESI): calculated for C₁₉H₂₇NO₂Si (M+H)⁺ 330.18838, found 330.18711

2.2 General procedure for the synthesis of compound **13** and **14** (table 2)

A mixture of compound **12** (104mg, 0.303mmol), Pd(OAc)₂ (6.8mg, 0.0303mmol), PPh₃ (15.9mg, 0.0606mmol), base (2 eq) in toluene (30.3 mL) was refluxed under nitrogen atmosphere for 15h. The solvent was evaporated under reduced pressure and the residue was dissolved in DCM (50 mL), washed with water, dried (Na₂SO₄) and filtered. The solvent was then evaporated under reduced pressure and the

residue was purified by flash chromatography (SiO₂, 9:1 v/v ether-petroleum ether) to afford the product **13**. Further elution (95:5 v/v ether-petroleum ether) afforded the product **14** as light yellow oil.

Compound 13

IR ν_{\max} : 1745, 1615, 1387, 1264, 1241, 703

¹H NMR (500 MHz, CDCl₃) δ 2.34 (dd, 1H, $J=14.5\text{Hz}$, $J=3\text{Hz}$, CH₂CH-N), 2.52 (dd, 1H, $J=19\text{Hz}$, $J=3\text{Hz}$, CH₂C=O), 2.58-2.64 (m, 1H, CH₂CH-N), 2.78 (dd, 1H, $J=19\text{Hz}$, $J=8.5\text{Hz}$, CH₂C=O), 3.36 (s, 3H, N-CH₃), 3.76 (t, 1H, $J=7.5\text{Hz}$, CH-C₆H₄), 3.81 (d, 1H, $J=8\text{Hz}$, CH-N), 7.22 (dd, 1H, ArH), 7.24-7.42 (m, 2H, ArH), 8.57 (dd, 1H, ArH)

¹³C NMR (125 MHz, CDCl₃) δ 33.8, 40.2, 42.4, 48.2, 63.3, 127.1, 129.0, 130.54, 131.7, 135.0, 143.9, 165.8, 212.0

m/z (EI) 215.1 (M⁺), 197.1, 172.1, 158.1, 144.1, 131.1

HRMS (ESI): calculated for C₁₃H₁₃NO₂ (M+H)⁺ 216.10191 found 216.10168

Compound 14

IR ν_{\max} : 1610, 1593, 1389, 1251, 761, 739

¹H NMR (500 MHz, CDCl₃) δ 2.1 (d, 1H, $J=12.5\text{Hz}$, CH₂ from ring), 2.46 (dt, 1H, $J=12.5\text{Hz}$, CH₂ from ring), 3.27 (s, 3H, N-CH₃), 3.75 (dd, 1H, $J=6.5\text{Hz}$, $J=3\text{Hz}$, CH-C₆H₄), 4.31 (dd, 1H, $J=7.5\text{Hz}$, $J=2.5\text{Hz}$, CH-N), 5.88 (dd, 1H, $J=5.5\text{Hz}$, $J=2.5\text{Hz}$, =CH-CH-N), 6.05 (dd, 1H, $J=5.5\text{Hz}$, $J=3\text{Hz}$, CH=CH-CH-N), 7.22 (dd, 1H, ArH), 7.26-7.30 (m, 1H, ArH), 7.32-7.35 (m, 1H, ArH), 8.6 (dd, 1H, ArH)

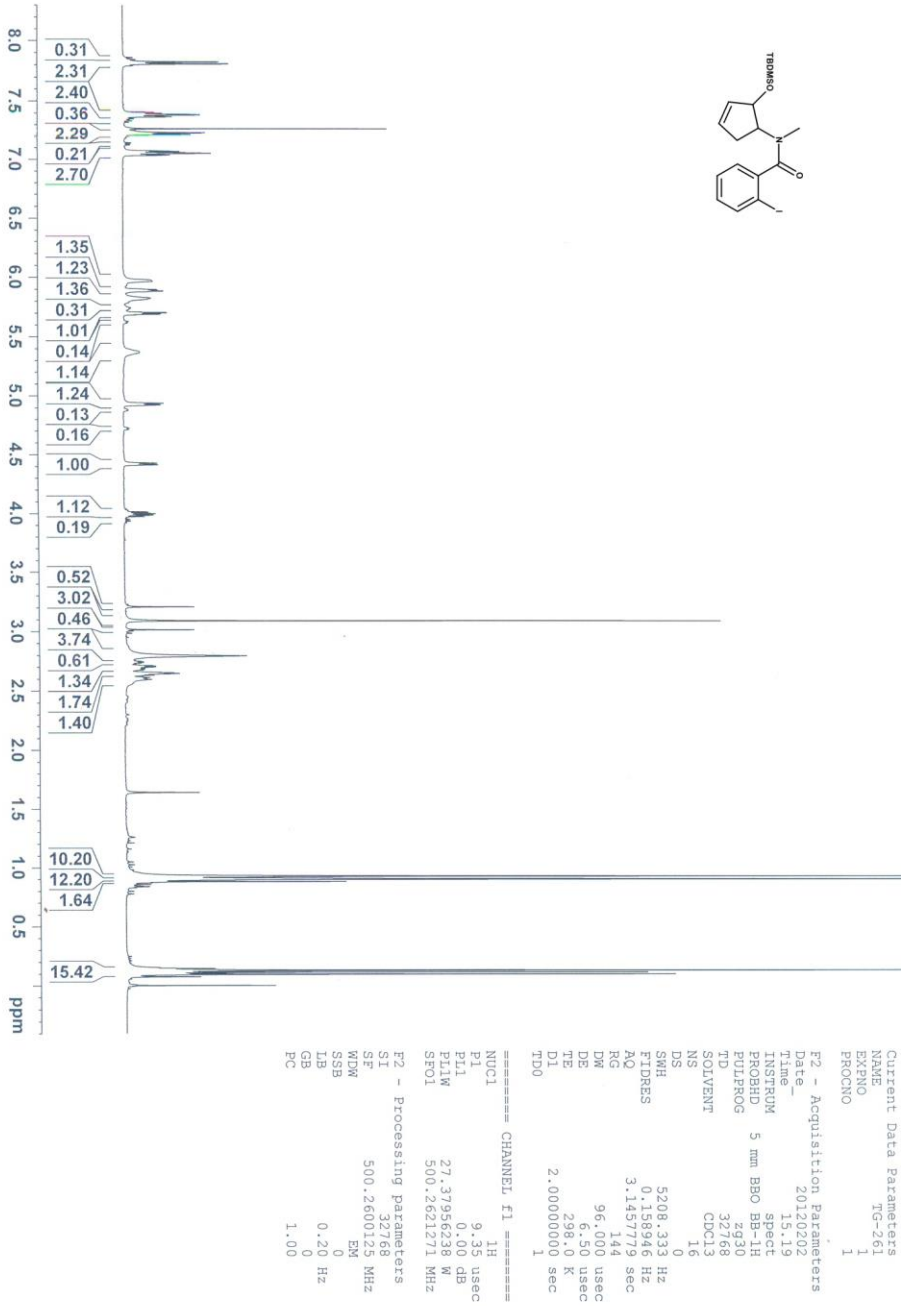
¹³C NMR (125 MHz, CDCl₃) δ 37.1, 39.0, 51.4, 65.3, 126.5, 127.9, 128.11, 131.02, 132.0, 135.6, 138.13, 144.44, 166.4

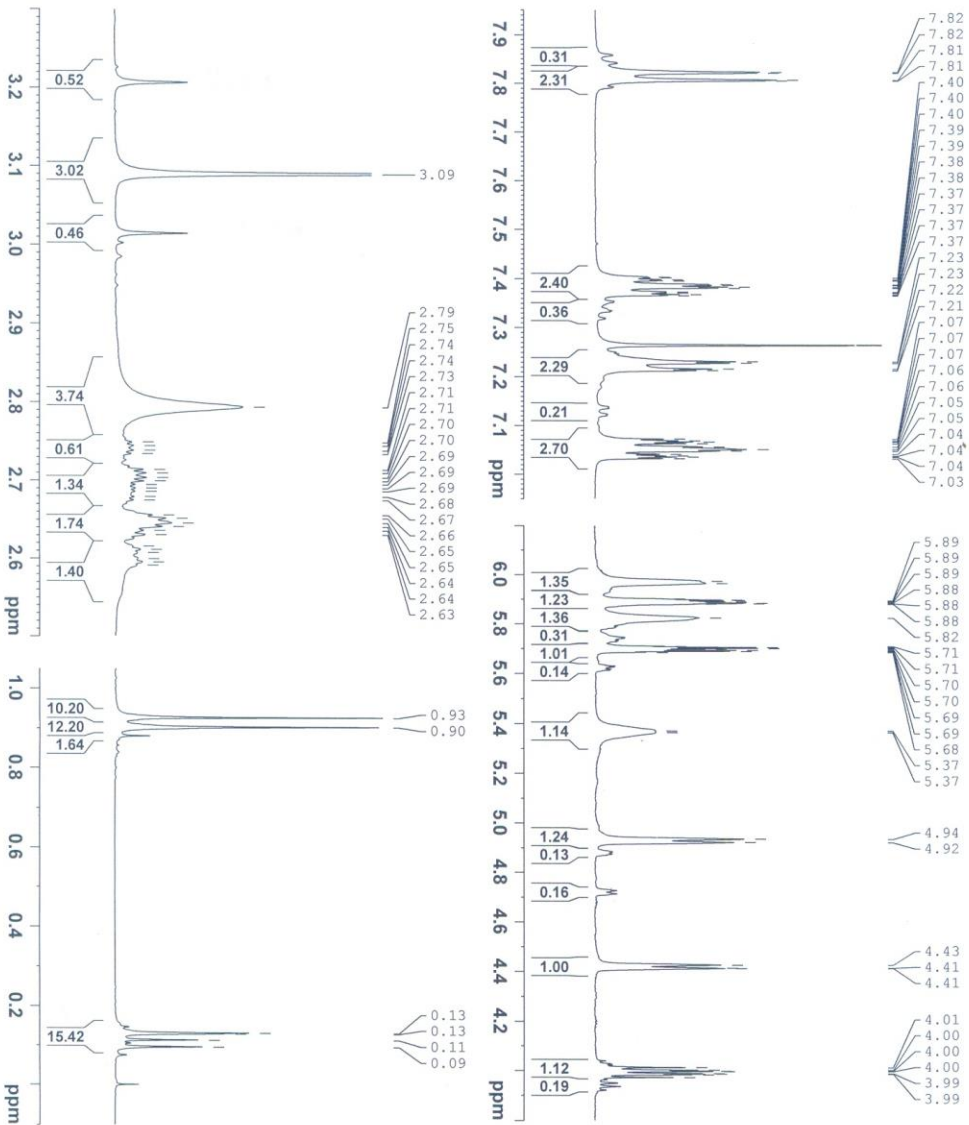
m/z (EI) 199.1 (M⁺), 184.0, 170.0, 141.0, 128.1, 115.0

HRMS (ESI): calculated for C₁₃H₁₃NO (M+H)⁺ 200.10699, found 200.10611

3. Spectral data for key compounds and products

Spectral data for compound 5 (isolated as a mixture of diastereomers):





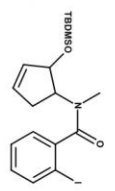
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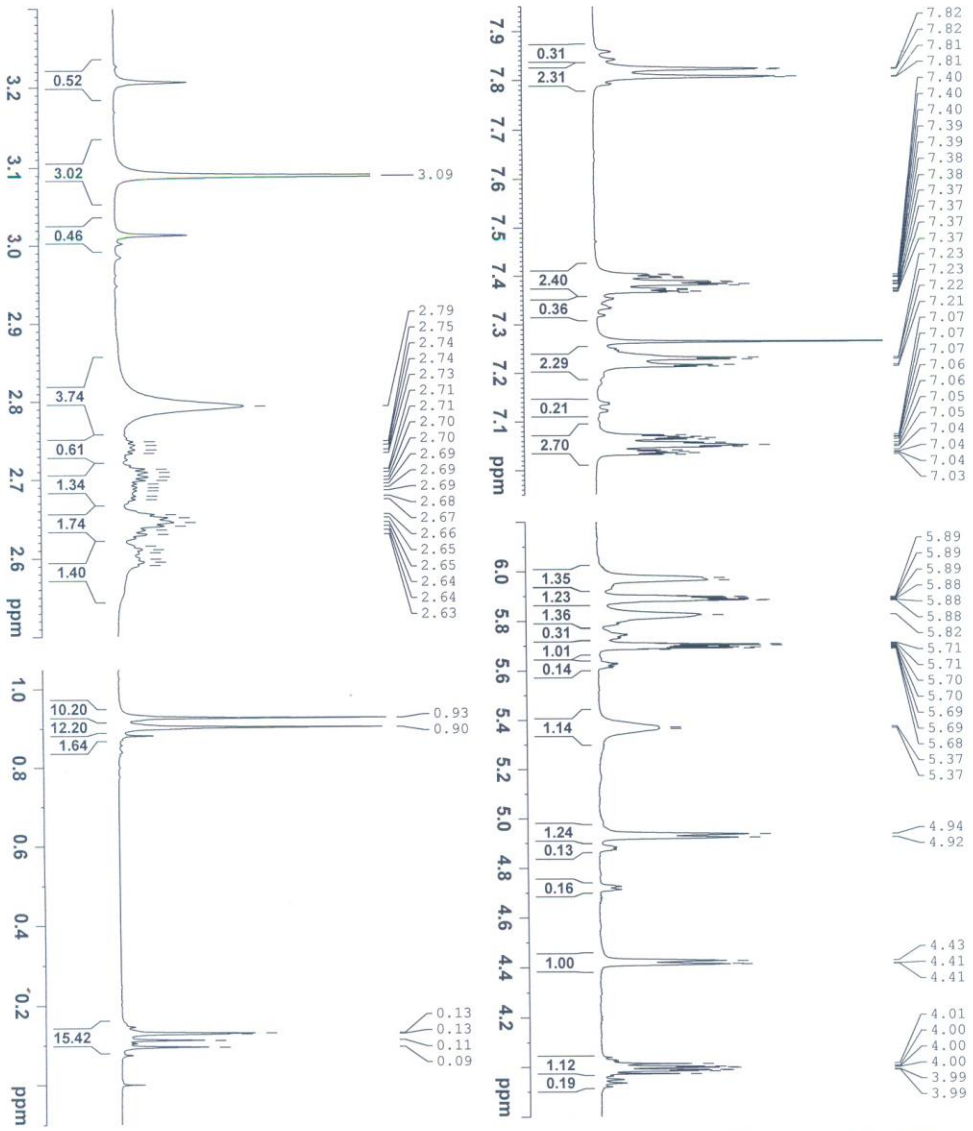
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PROCNO    1

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FIDRES     0.158946 Hz
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TE         298.0 K
D1         2.00000000 sec
TD0        1

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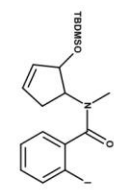


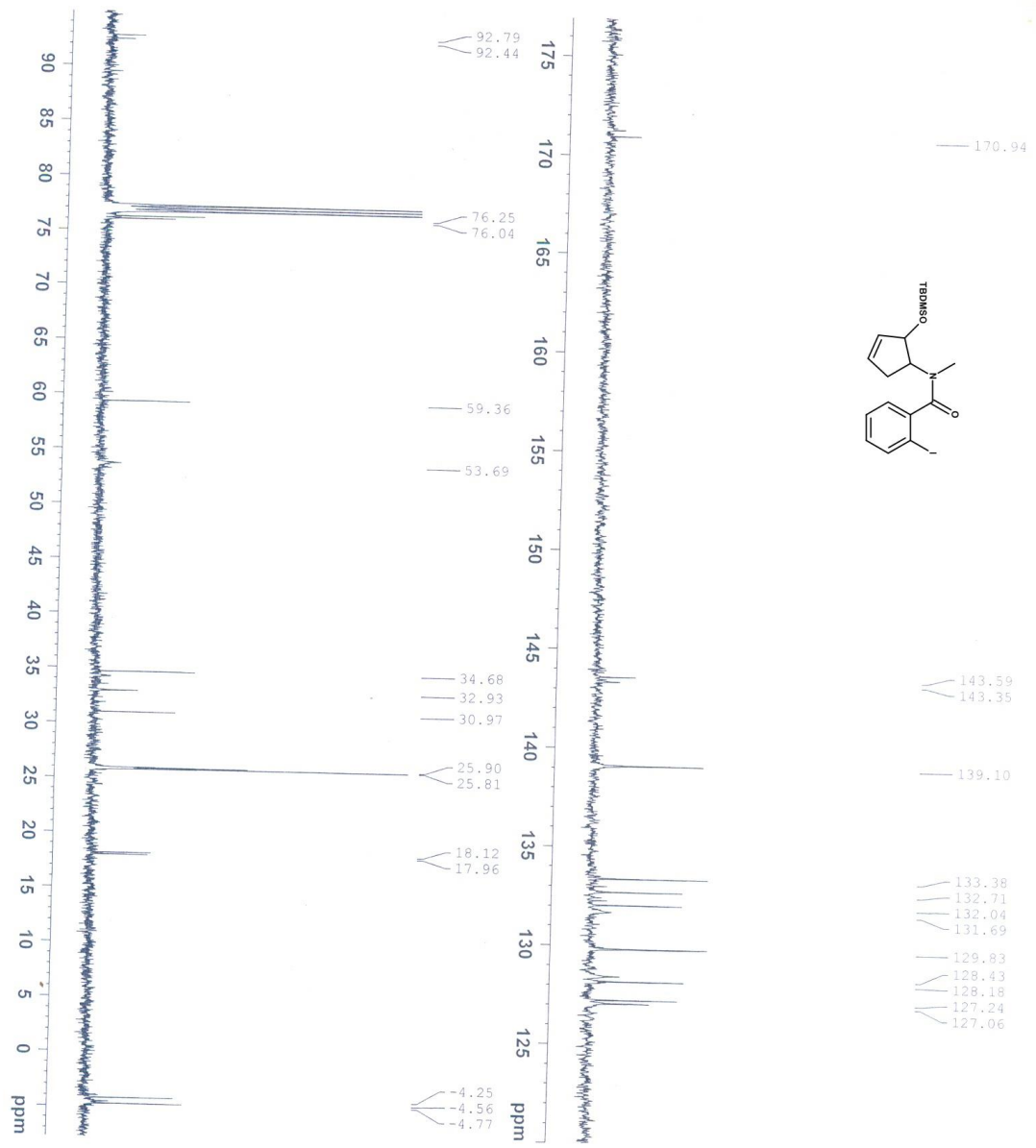
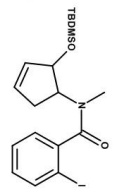
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 DS 0
 SWH 5208.333 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457719 sec
 RG 144
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 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 TD0 1

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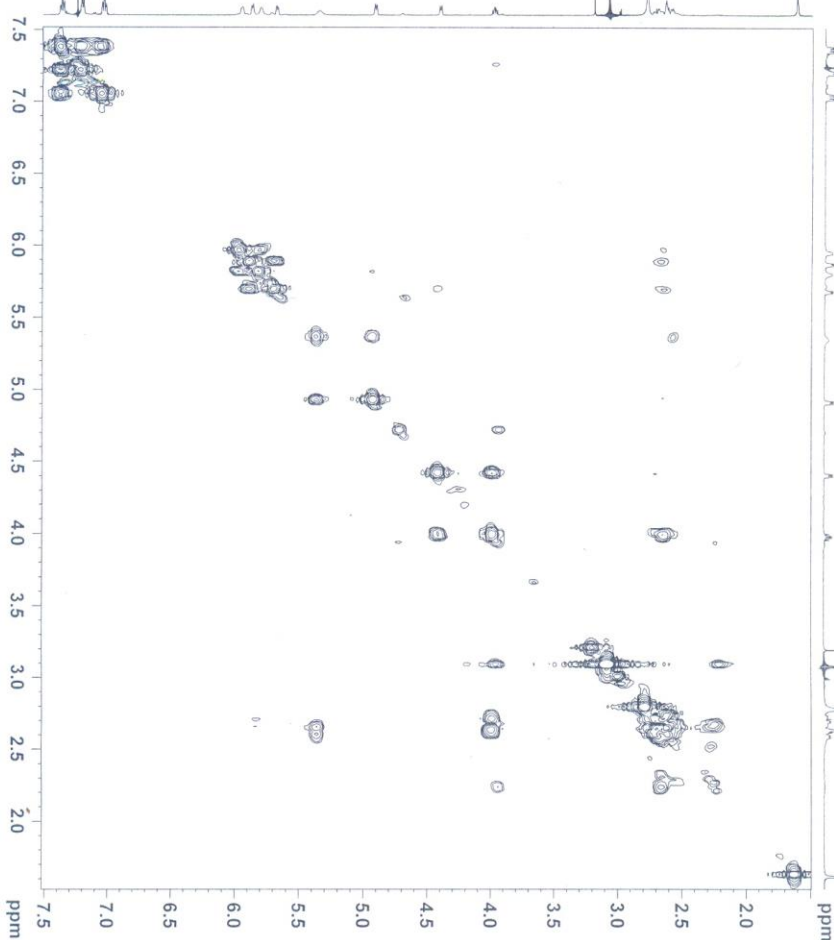


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NS           603
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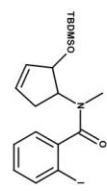
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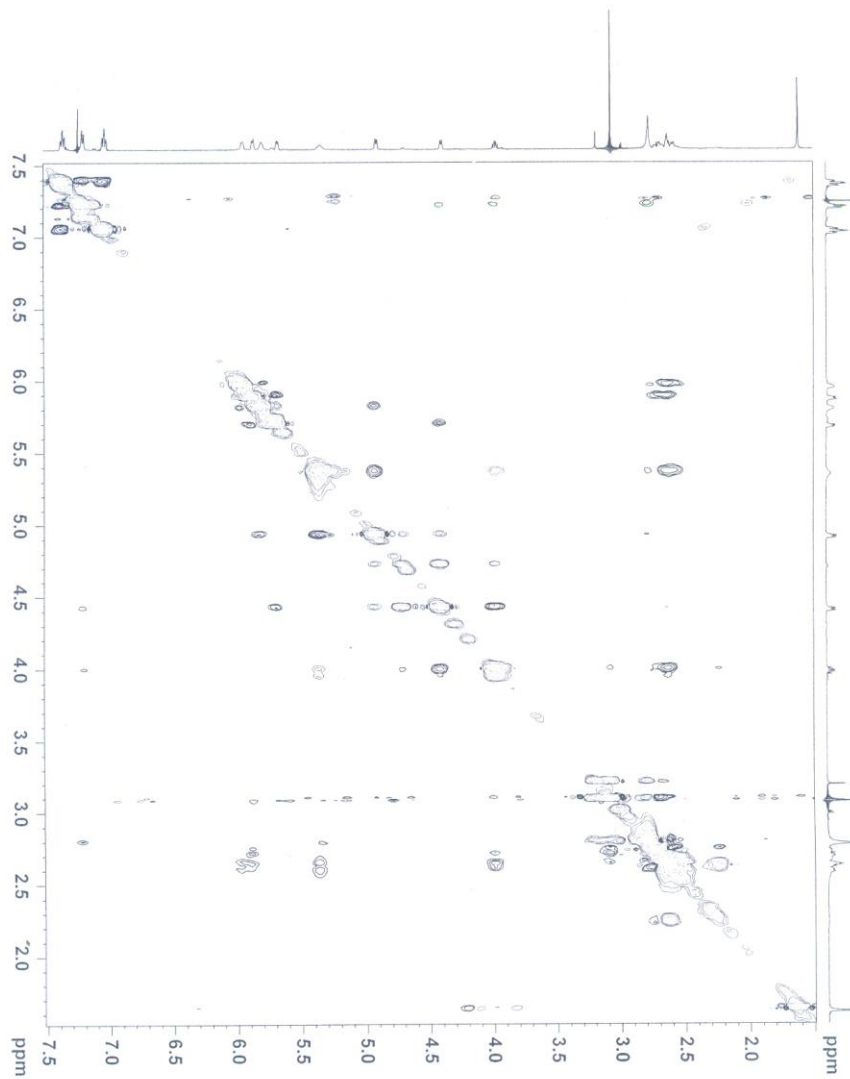
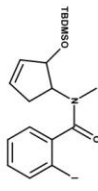



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 NUC2: 13C
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 RG: 111.000 usec
 DW: 111.000 usec
 DE: 6.50 usec
 TE: 298.0 K
 TD: 0.0000300 sec
 D1: 0.0000100 sec
 D13: 0.00000400 sec
 D16: 0.0002000 sec
 IN0: 0.0002210 sec

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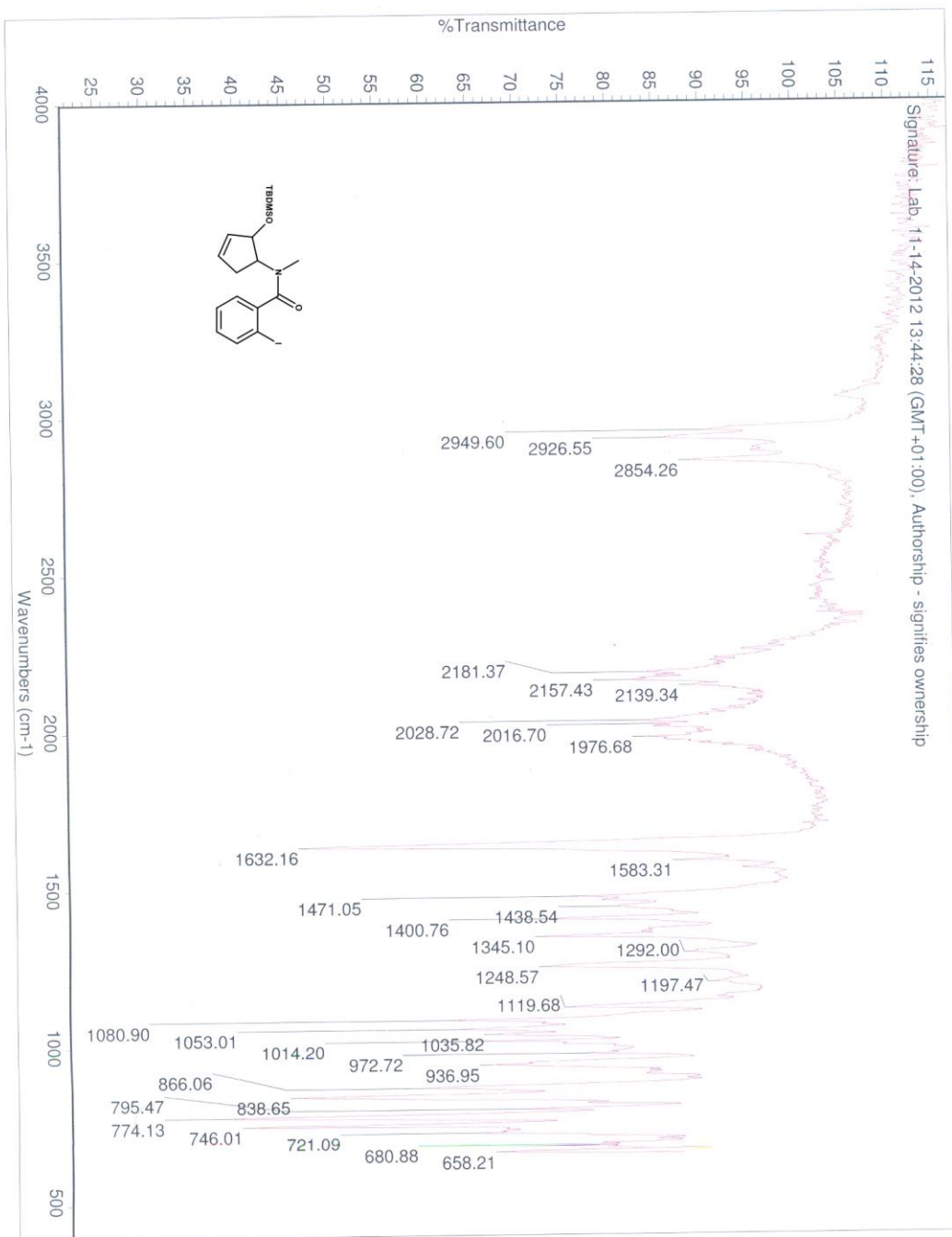
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 SN: 9.000 ppm
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 FREQS2: 500.2620010 MHz
 ST: 5
 KW: 0.00 Hz
 SSB: 0.00 Hz
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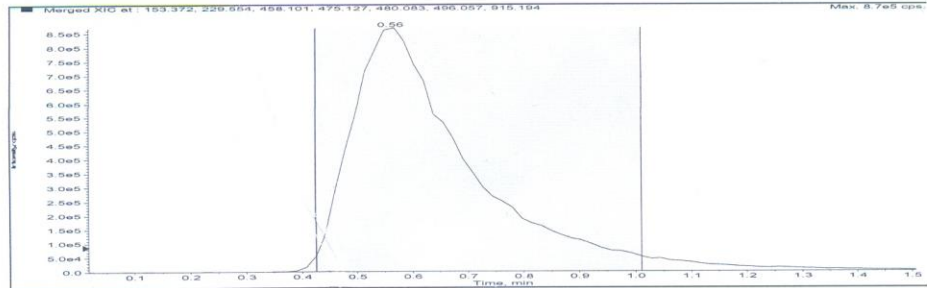
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DE           6.50 usec
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D1           1.0000000 sec
D2           0.00022210 sec
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SFO1         States-TFPI
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SFO1         0.00 Hz
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GB           1.00
SFO1         1.512
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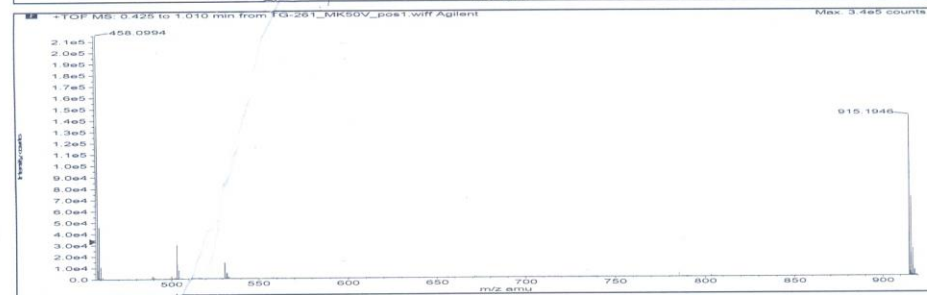
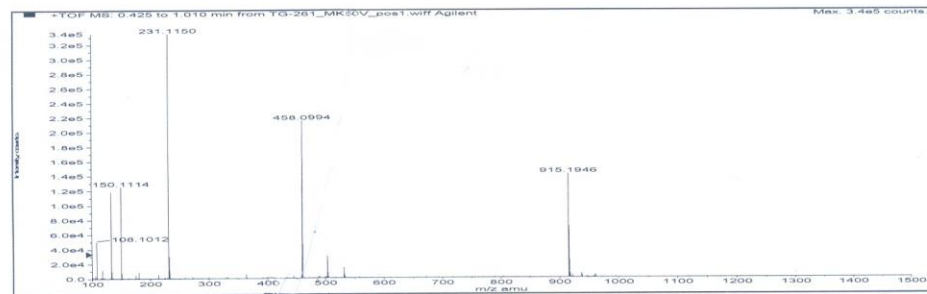



Signature: Lab_11-14-2012 13:44:28 (GMT+01:00), Authorship - signifies ownership

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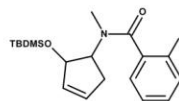


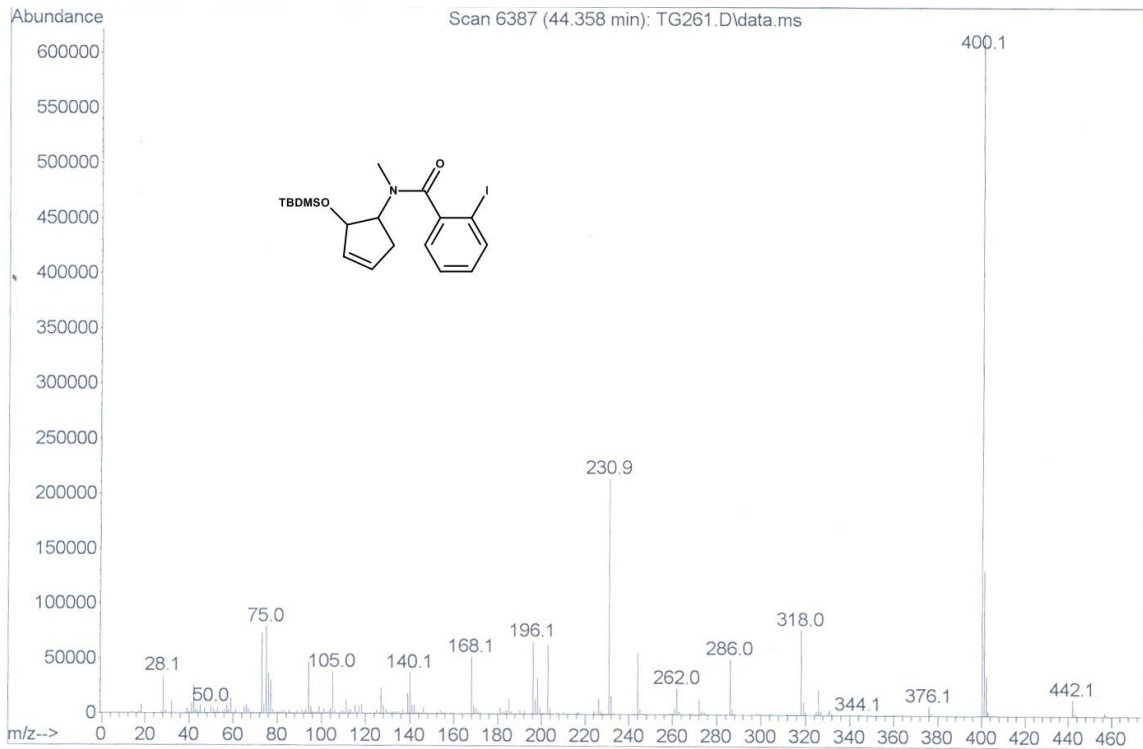
Merged XIC, Period# : 1 Experiment# : 1



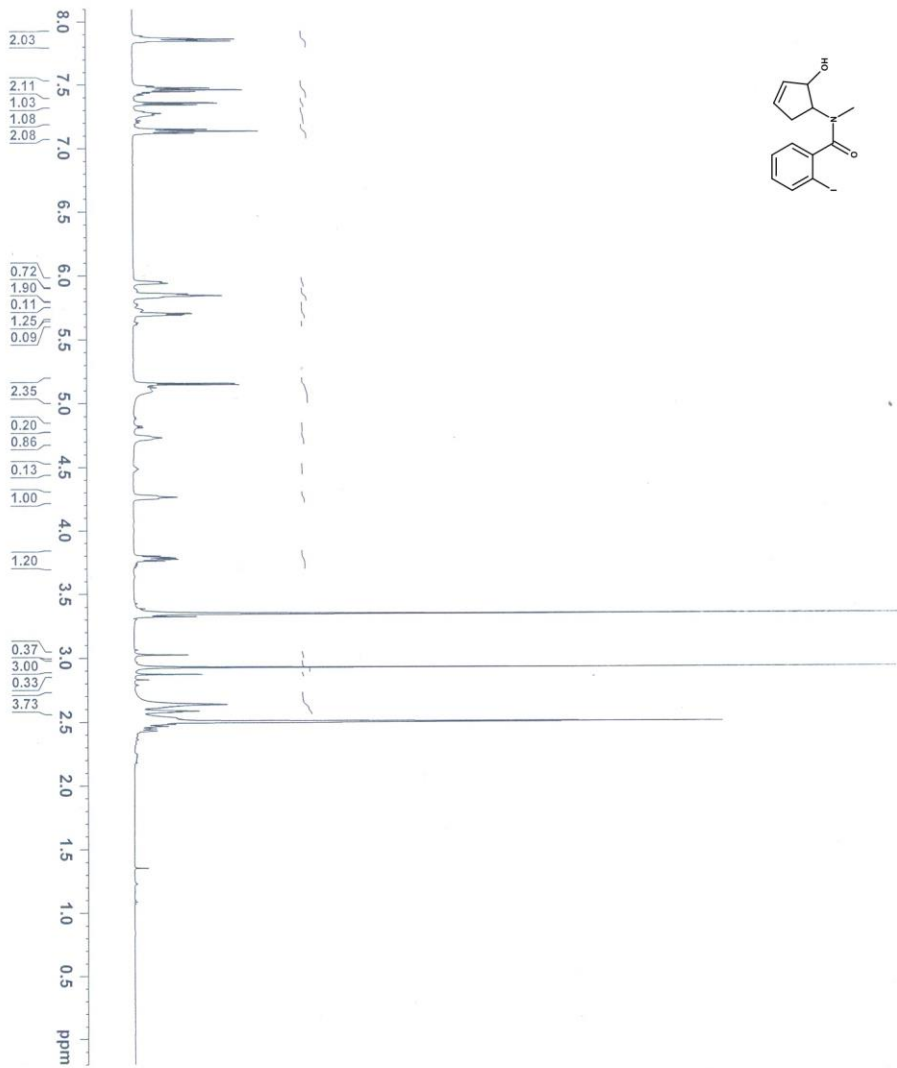
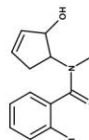
| Formula | Compound name | Mass | Peak RT (min) | Peak area | Description |
|--------------|---------------|-----------|---------------|------------|-------------|
| C19H28INO2Si | -- | 457.09340 | 0.56 | 1.28058 E7 | -- |

| Species | Abundance (counts) | Ion Mass | Measured Mass | Error (mDa) | Error (ppm) | Ret. Time Error (min) |
|---------------------|--------------------|-----------|---------------|-------------|-------------|-----------------------|
| [M+H] ⁺ | 224554.37 | 458.10068 | 458.09941 | -1.26829 | -2.77 | -- |
| [2M+H] ⁺ | 147607.53 | 915.19407 | 915.19464 | 0.56491 | 0.62 | -- |





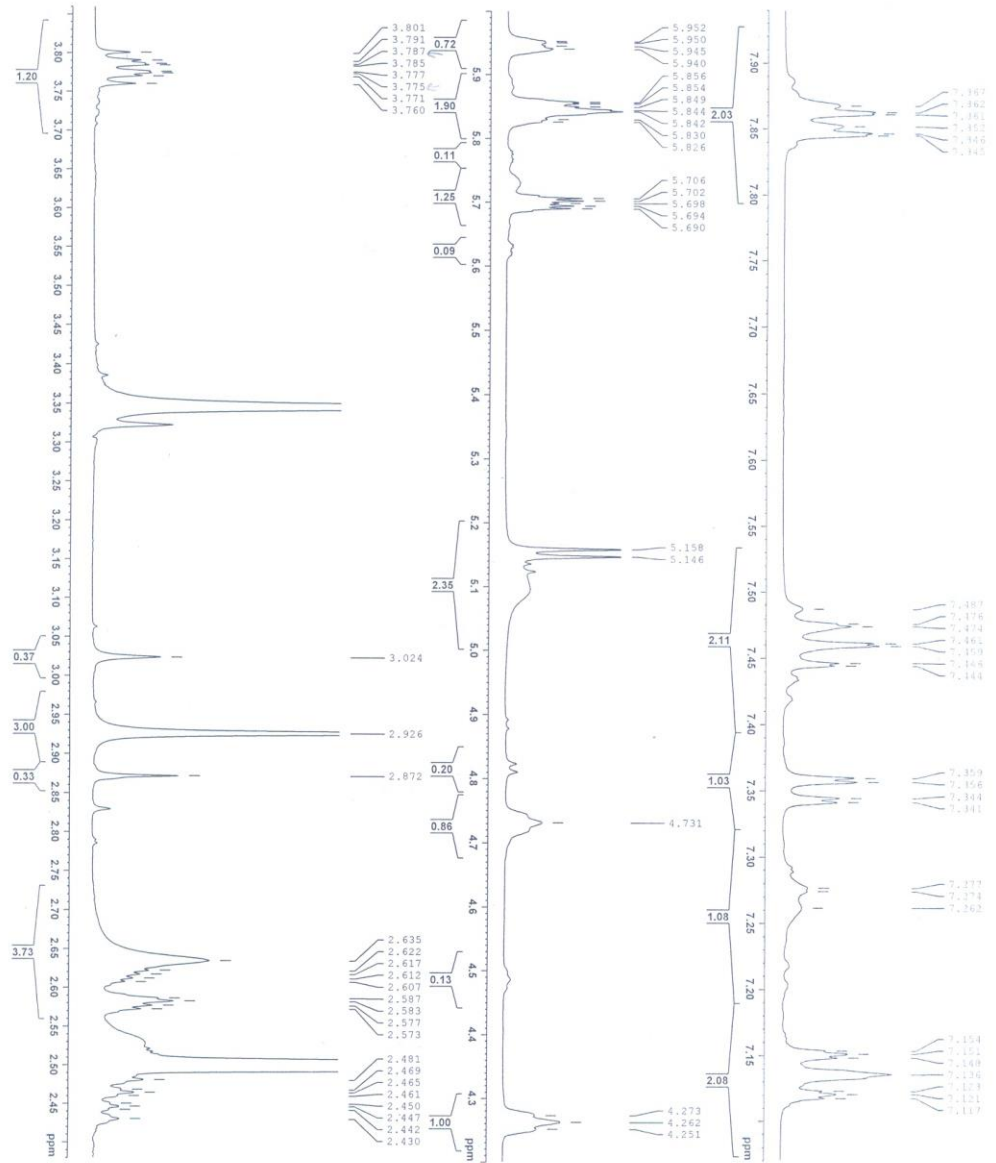
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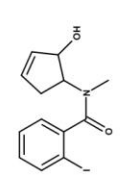
CHANNEL F1

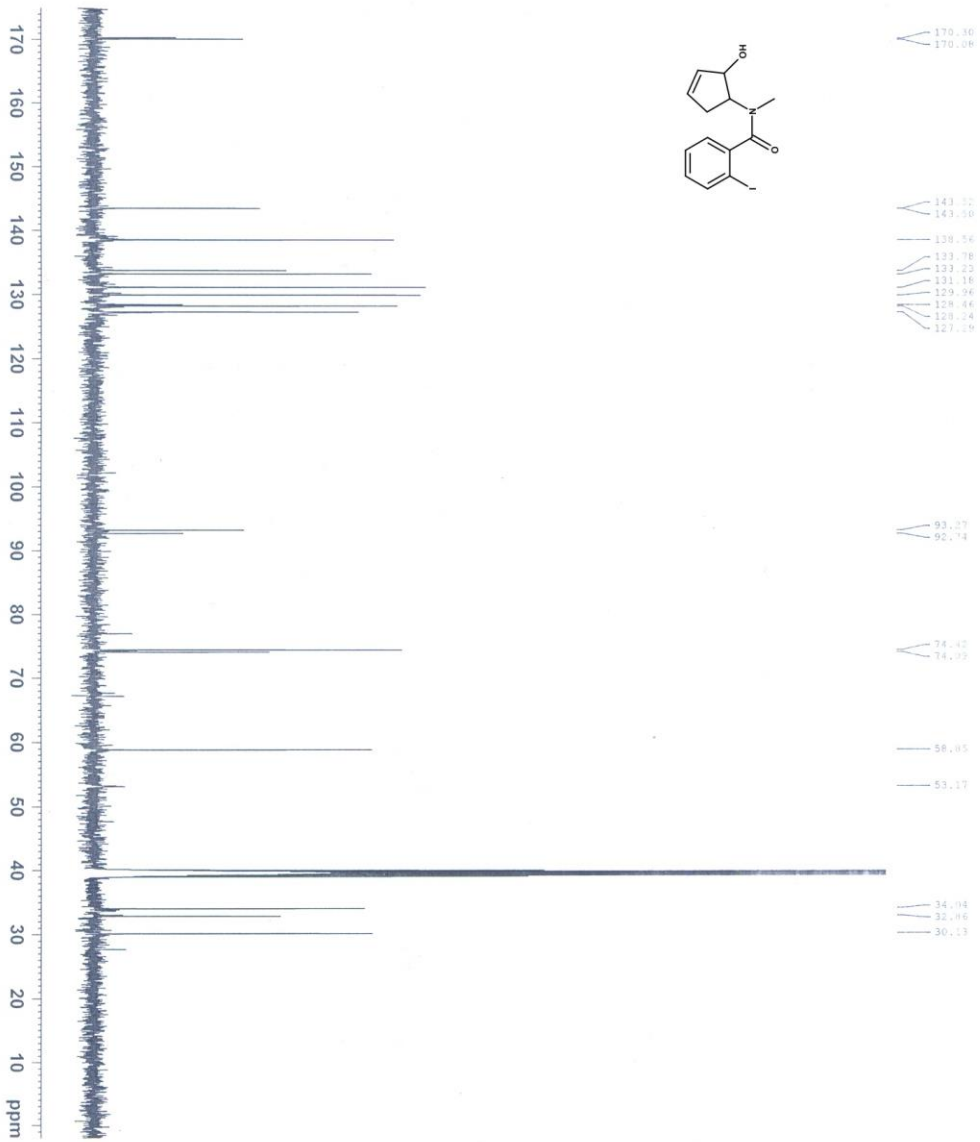
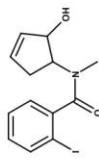
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 SF: 500.260063 MHz
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 SSB: 0
 LB: 0.20 Hz
 GB: 0
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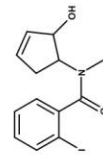


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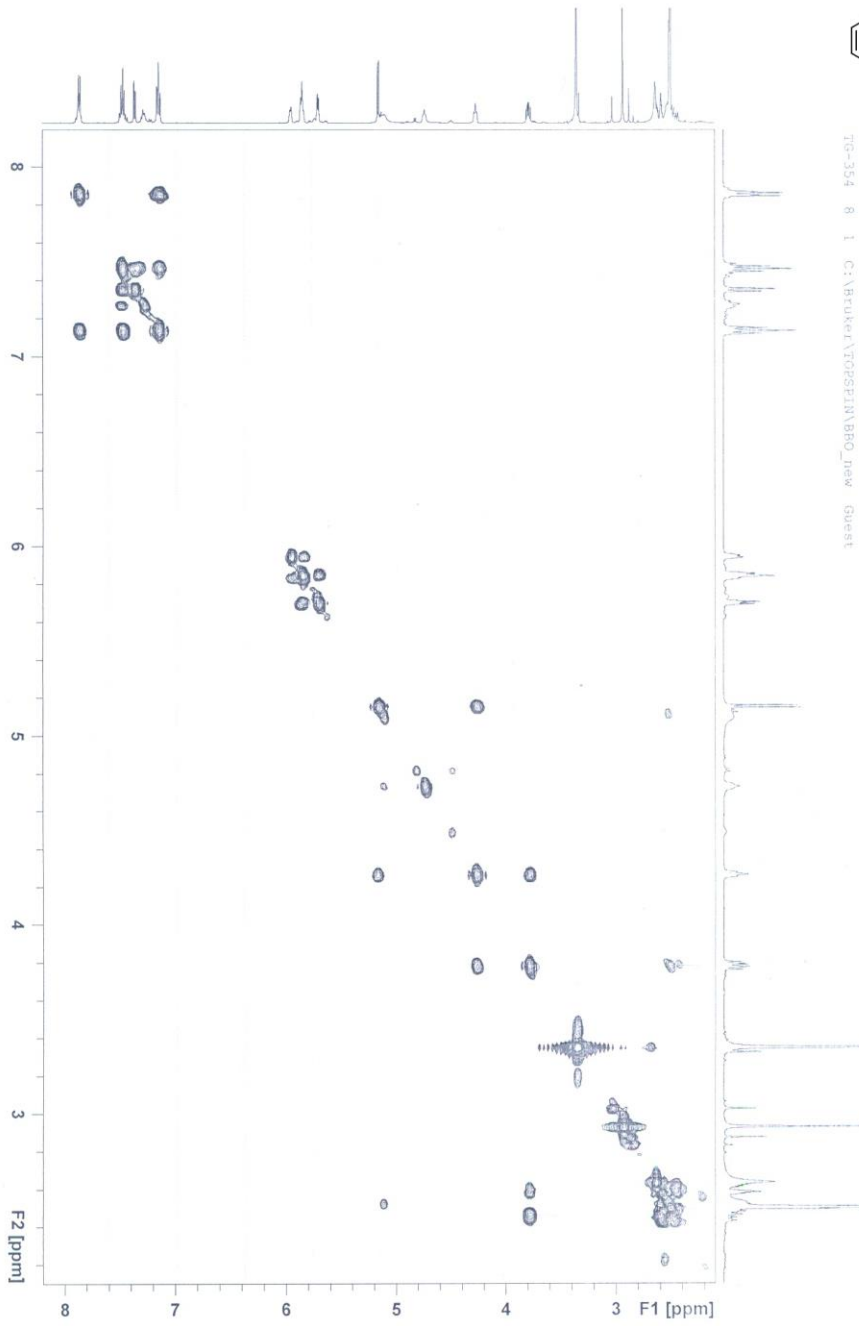
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D11           0.03000000 sec
TD0           1

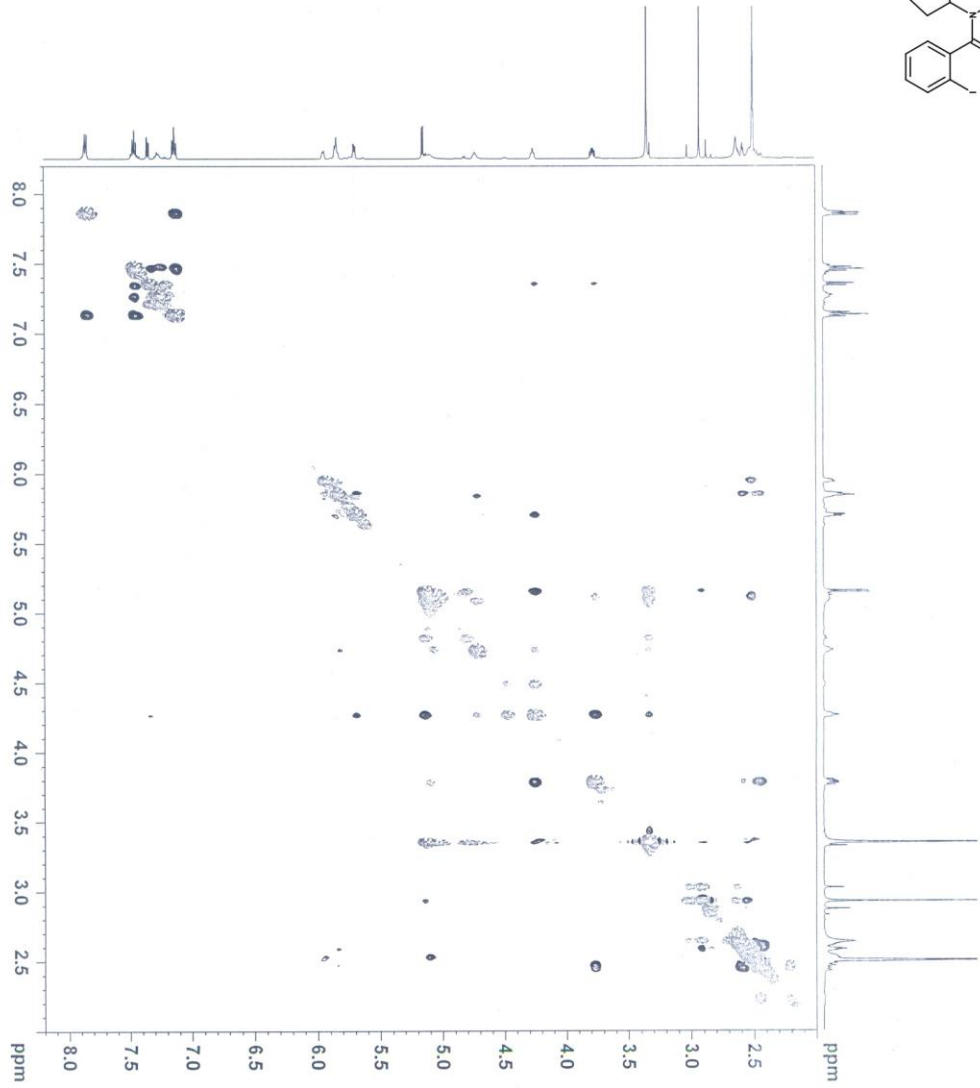
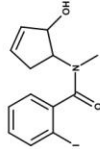
===== CHANNEL f1 =====
NUC1          13C
P1            11.50 usec
PL1           3.00 dB
PL1W          32.22848892 W
SFO1          125.8043140 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           1.20 dB
PL2W          18.40 dB
PL3           18.40 dB
PL3W          20.76952171 W
PL4W          0.39575511 W
PL5W          0.39575511 W
SFO2          500.2620105 MHz
SI            32768
SF            125.7905379 MHz
WDW           EX
SSB           0
LB            1.50 Hz
GB            0
PC            1.40
  
```



T0-354 0 1 C:\Bruker\TOPSPIN\BRO_new Guest

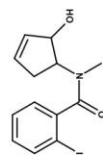




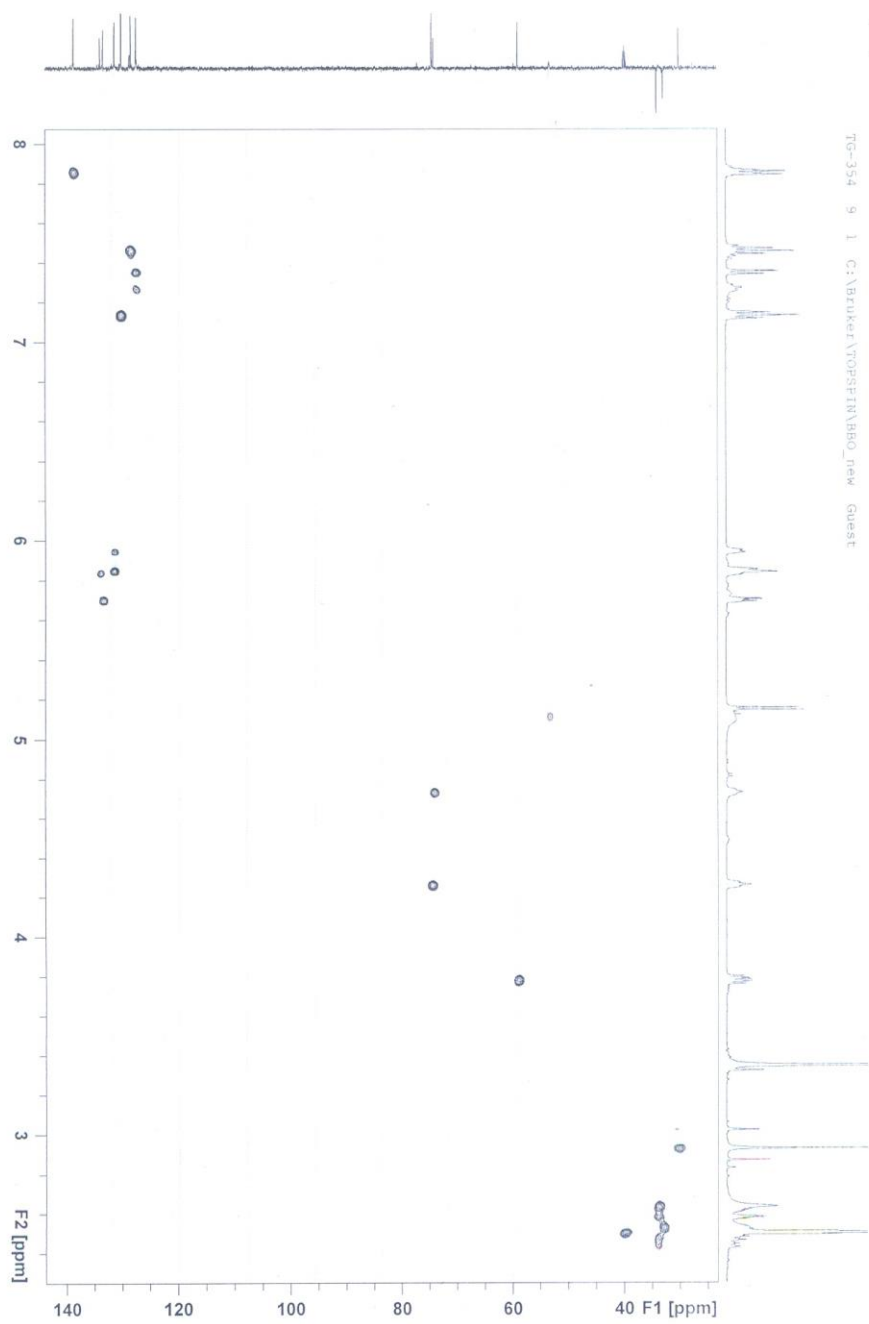
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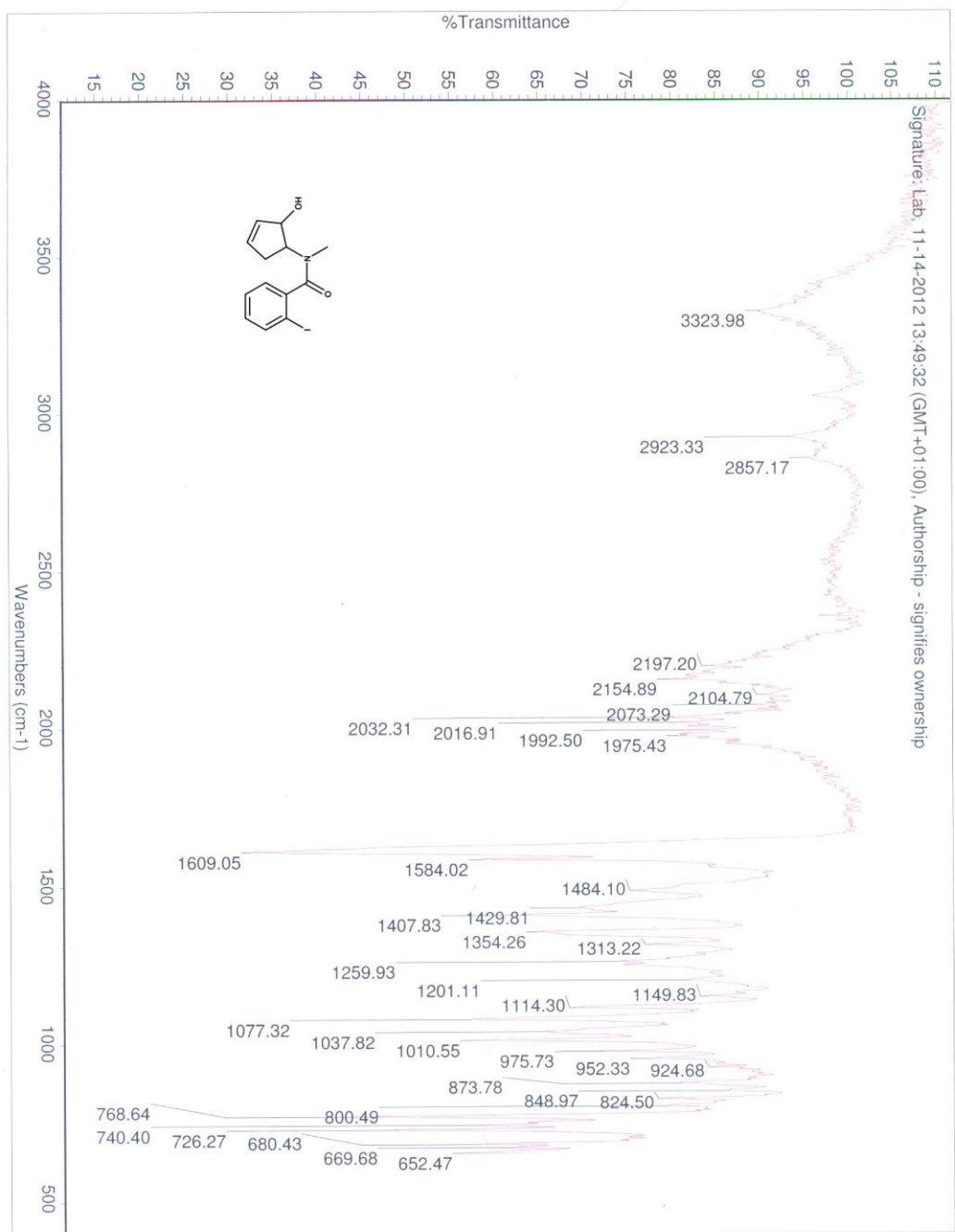
=====
NAME          TG-164
EXPNO         10
PROCNO        1
Date_         20111025
Time          14.42
INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       zgpg30
F2H2PRG2     hsqcyaq3h
SOLVENT       DMSO
NS            8
DS            2
SF            498.132 MHz
AQ            0.1027231 sec
RG            144
WDW           EM
SSB           0
LB            1.00
GB            0
PC            1.00
ST2           ST2
SF2           500.2600056 MHz
WDW           QSIINE
SSB           0
LB            0.00 Hz
GB            0
=====
CHANNEL #1
NUC1          13C
P1            9.31 usec
F2            18.70 usec
PL1          0.00 dB
PL2          27.37956238 W
SFO1         500.2620105 MHz
=====
GRABNAME      SINE.100
GPRM1        40.00 %
GPRM2        1000.00 usec
TD           160
SFO1         500.262 MHz
F2H2PRG2     zgpg30
PULPROG       zgpg30
SOLVENT       DMSO
SI           512
SF           500.2600018 MHz
WDW           QSIINE
SSB           0
LB            0.00 Hz
GB            0
PC            1.00
ST2           ST2
SF2           500.2600056 MHz
WDW           QSIINE
SSB           0
LB            0.00 Hz
GB            0
=====

```

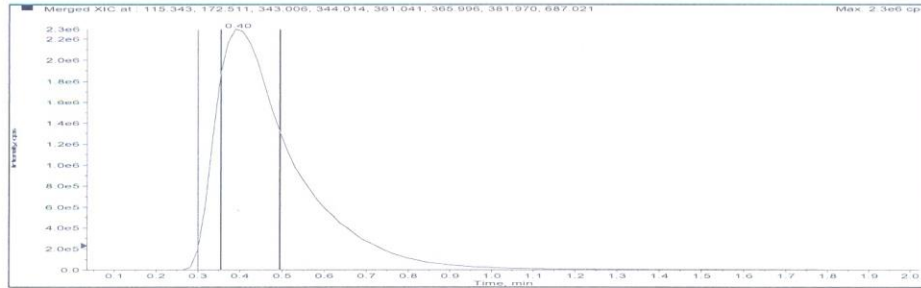


TG-354 9 1 C:\BIOKET\TOPSPIN\RB0_new Guest

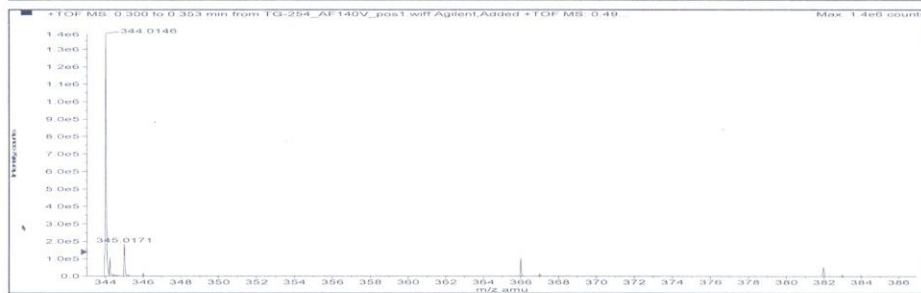
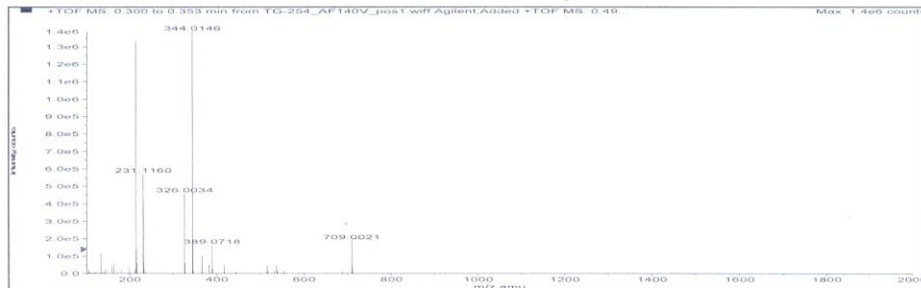




Sample Name: TG-254 Sample Location: P1-C8 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Farmaceutski fakulteti\Data\TG-254_AF140V_pos1.wiff Acq Time: December 29 2011,
 12:40:30 PM
 Method: D:\TOF_Data\damethods\Night_Seq_Comp_ident1.anml\efc.xml

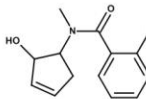


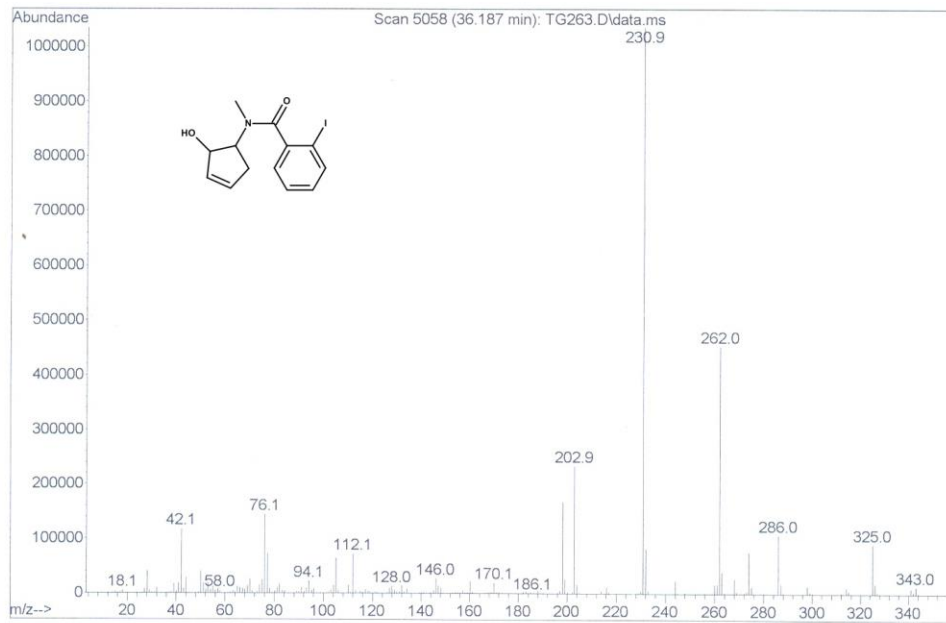
Merged XIC, Period# : 1 Experiment# : 1



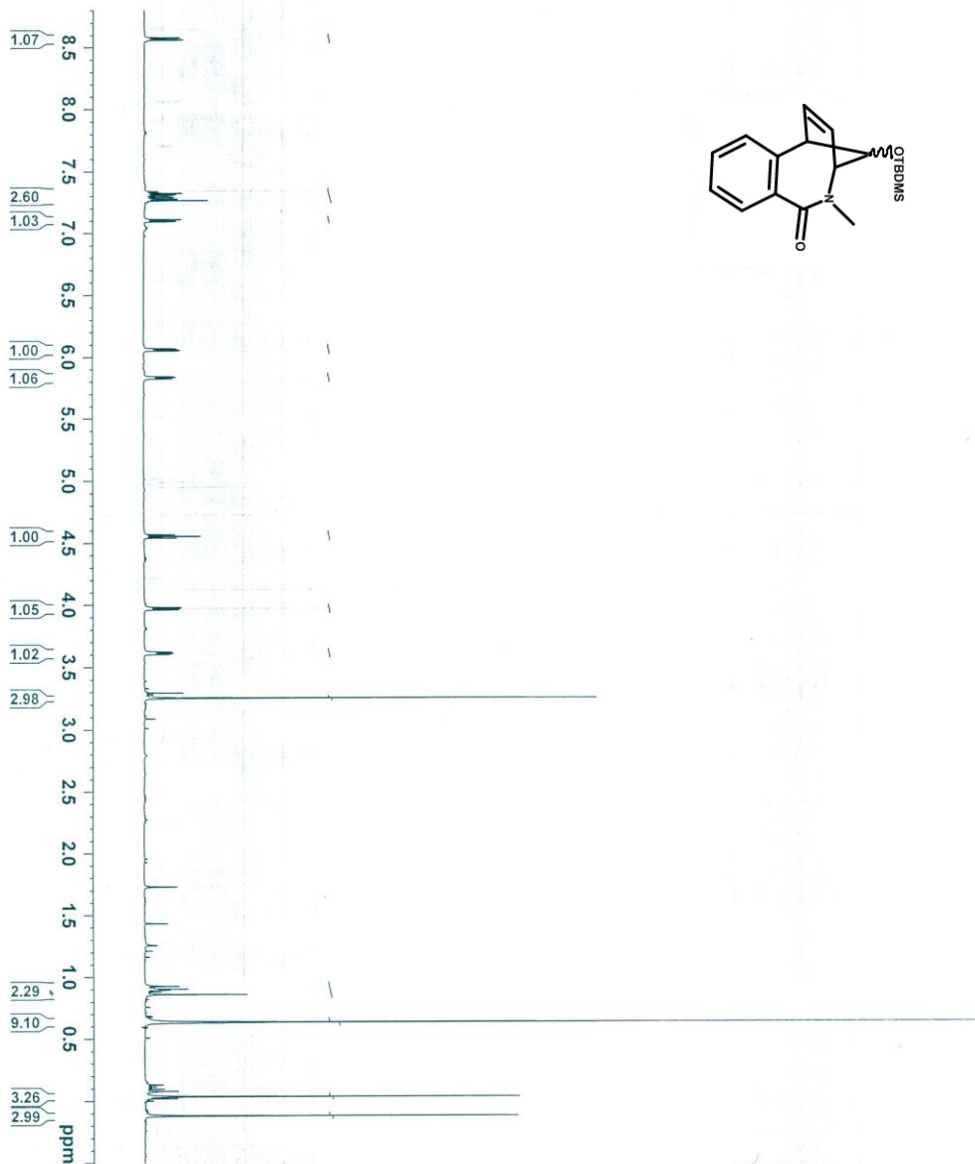
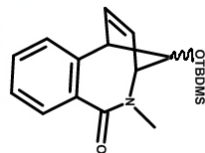
| Formula | Compound name | Mass | Peak RT (min) | Peak area | Description |
|-----------|---------------|-----------|---------------|------------|-------------|
| C13H14NO2 | -- | 343.00692 | 0.40 | 2.95065 E7 | -- |

| Species | Abundance (counts) | Ion Mass | Measured Mass | Error (mDa) | Error (ppm) | Ret. Time Error (min) |
|---------------------|--------------------|-----------|---------------|-------------|-------------|-----------------------|
| [M+H] ⁺ | 1390280.79 | 344.01420 | 344.01458 | 0.37701 | 1.10 | -- |
| [M+Na] ⁺ | 104798.06 | 365.99614 | 365.99588 | -0.26409 | -0.72 | -- |
| [M+K] ⁺ | 53656.88 | 381.97008 | 381.96972 | -0.36353 | -0.95 | -- |





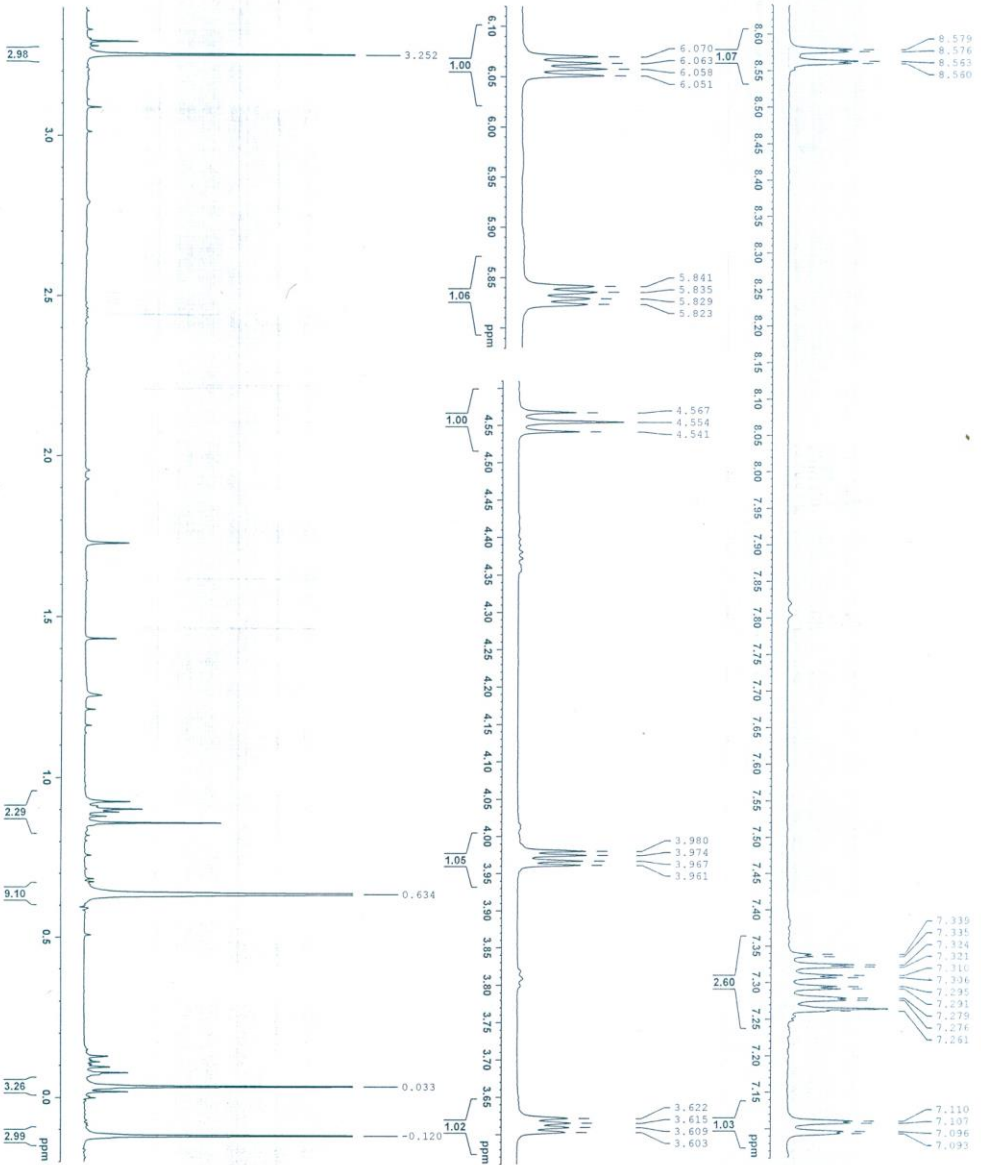
Spectral data for compound 11



```

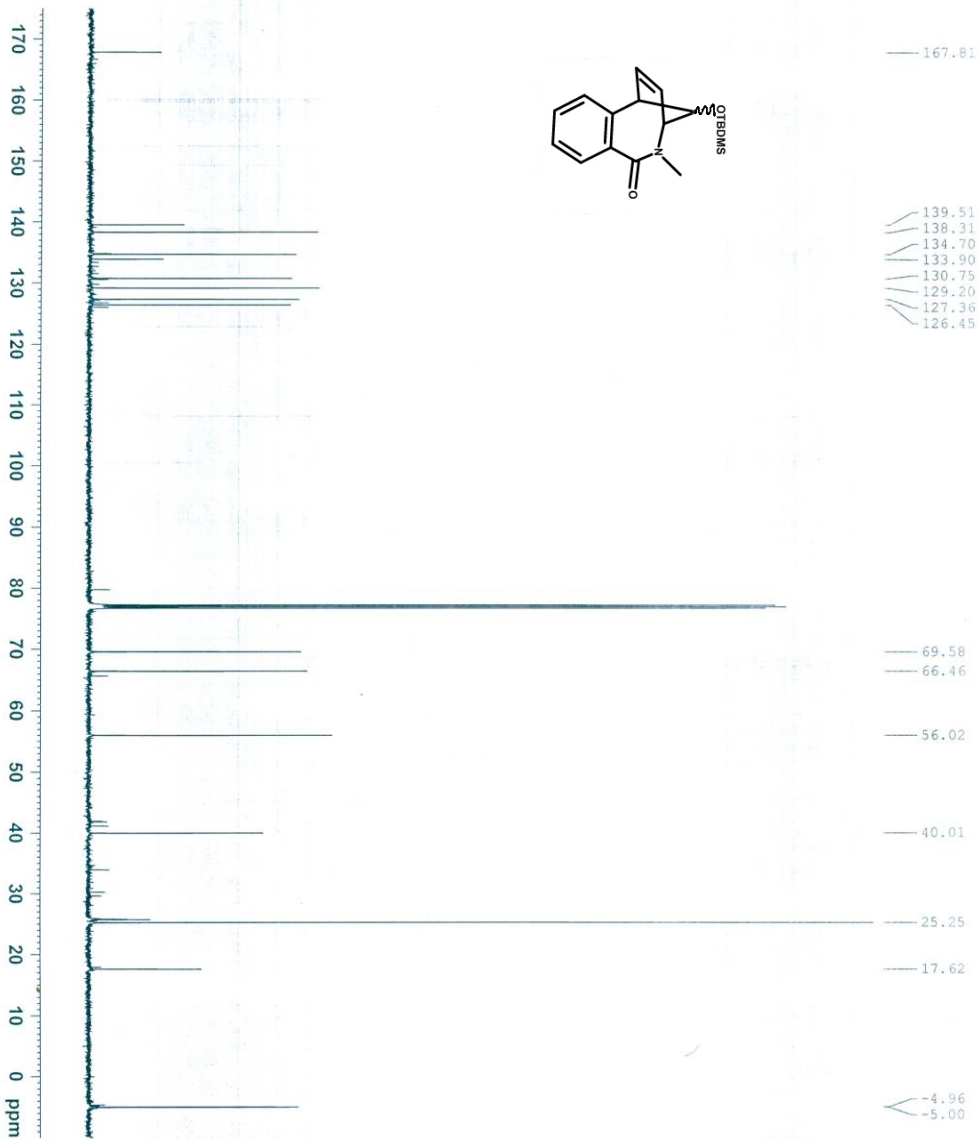
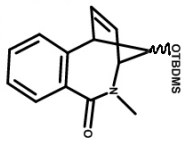
NAME          75-366
EXPNO         1
PROCNO        1
Time          20121121
Time         14.34
INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       zgpg30
TD            32769
SOLVENT       CDCl3
NS           12
DS            0
SWH           5208.333 Hz
FIDRES        0.158946 Hz
AQ            3.145779 sec
RG            64
DM            96.000 usec
DE            288.0 K
TE            298.0 K
D1            2.00000000 sec
TDO           1

===== CHANNEL f1 =====
NUC1          1H
P1            9.700 usec
PL1           0.00 dB
PL12          27.37956238 W
SFO1          500.2621302 MHz
SI            32768
SF            500.2600124 MHz
WDW           EM
SSB           0
GB            0
PC            1.00
  
```

```

NAME          TG-366
EXPNO         1
PROCNO        1
Date_         20121121
Time          14.34
INSTRUM       S
PROBHD        5 mm BBO BB-1H
PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            16
DS            0
SWH           5208.333 Hz
FIDRES       0.158946 Hz
AQ           3.143772 sec
RG           96.000
DE           6.500 usec
TE           298.0 K
D1           2.00000000 sec
D10          1
===== CHANNEL f1 =====
NUC1          1H
P1           9.35 usec
PL1          0.00 dB
PL1W         27.37956238 W
SFO1         500.2621302 MHz
SI           32768
SF           500.2600124 MHz
WDW          EM
SSB          0
LB           0.20 Hz
GB           0
PC           1.00
  
```



167.81
139.51
138.31
134.70
133.90
130.75
129.20
127.36
126.45

69.58
66.46
56.02
40.01
25.25
17.62

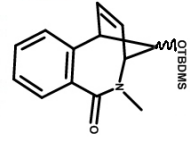
4.96
5.00

```

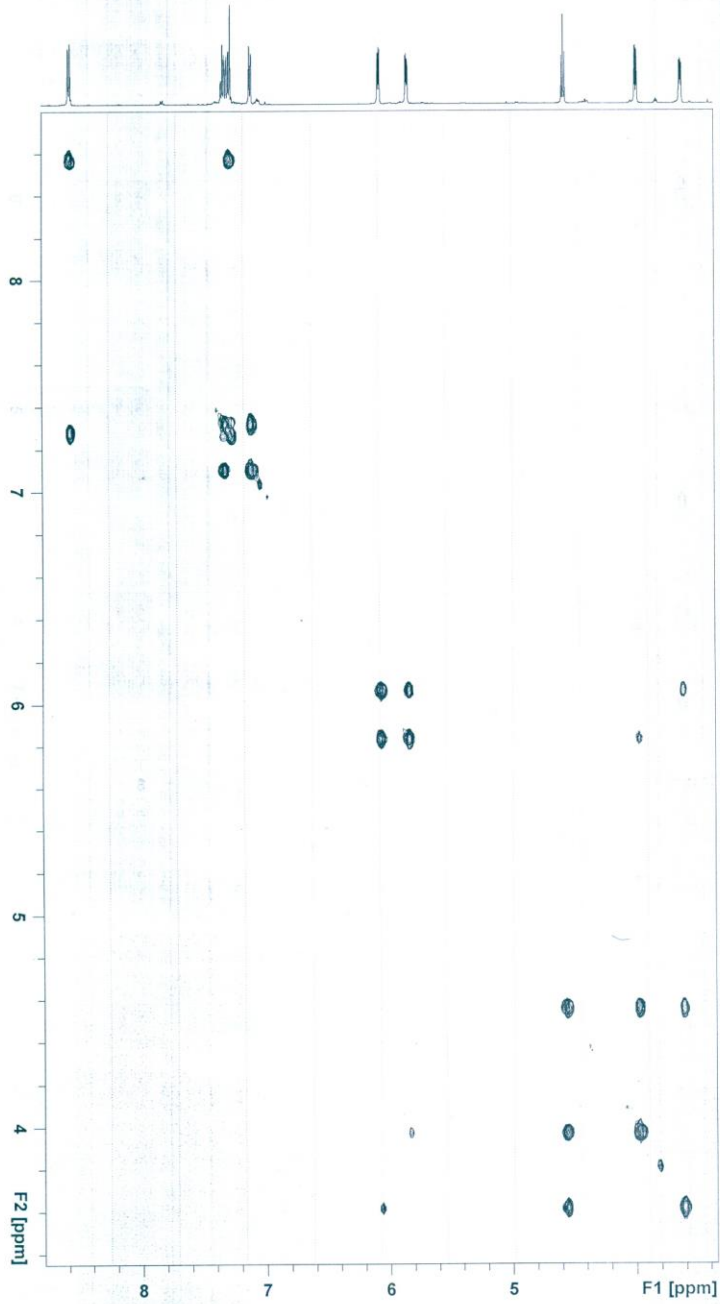
NAME          TG-166
EXPNO         2
PROCNO        1
PROCRES       20121121
Time         14:32
INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS           832
DS           4
SWH          29761.904 Hz
FIDRES       0.508261 Hz
AQ          0.5301034 sec
RG           16.800 usec
DE           6.50 usec
TE           298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0          1

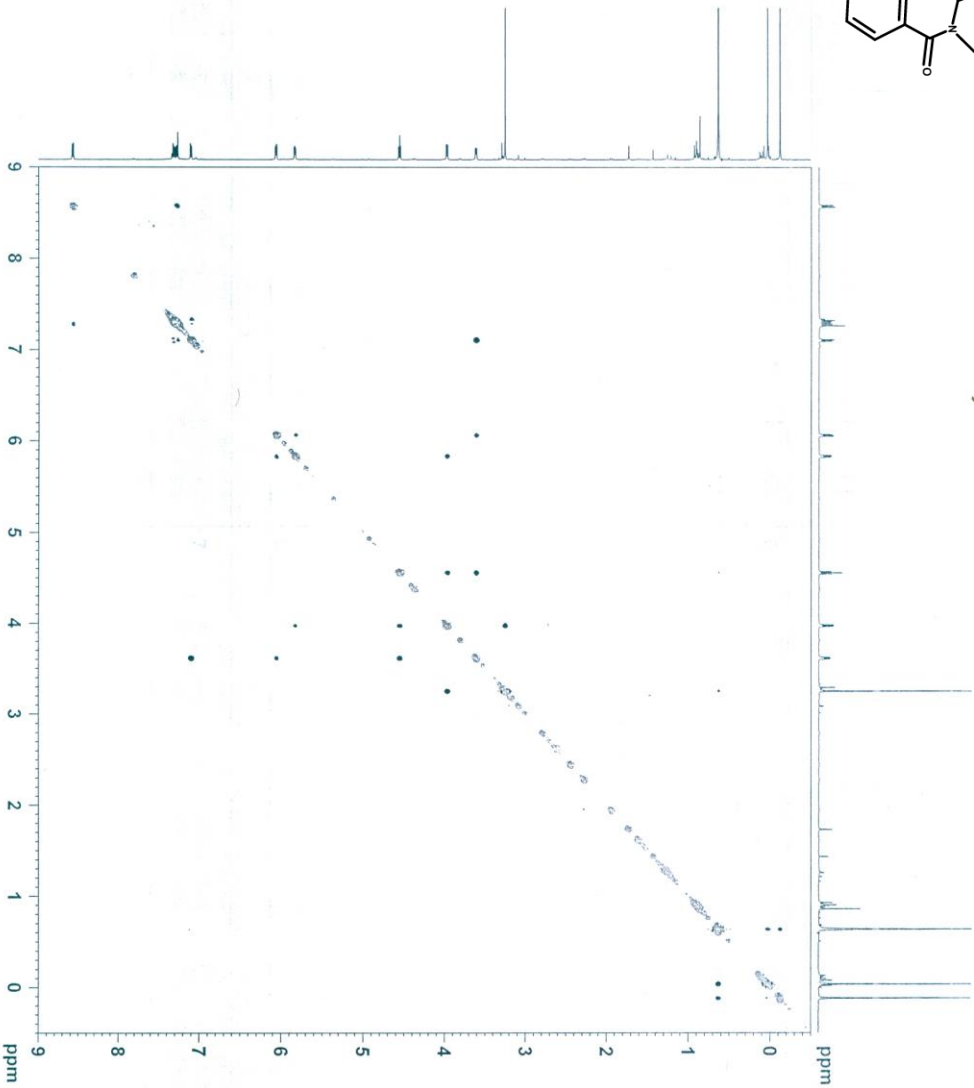
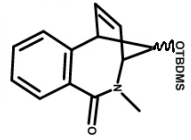
===== CHANNEL f1 =====
NUC1          13C
P1           11.50 usec
PL1          1.20 dB
SFO1         125.8030560 MHz

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2        80.00 usec
PL2          1.20 dB
PL12         18.40 dB
PL13         18.40 dB
PL14         20.76624511 M
PL15         0.38575511 W
PL16         0.38575511 W
PL17         500.2621301 MHz
SFO2         500.2621301 MHz
SI           32768
SF           125.7904824 MHz
WDW          EM
SSB          0
LB           1.50 Hz
GB           0
PC           1.40
  
```



TG-366 4 1 C:\Bruker\TOPSPIN\BPO_new Guest



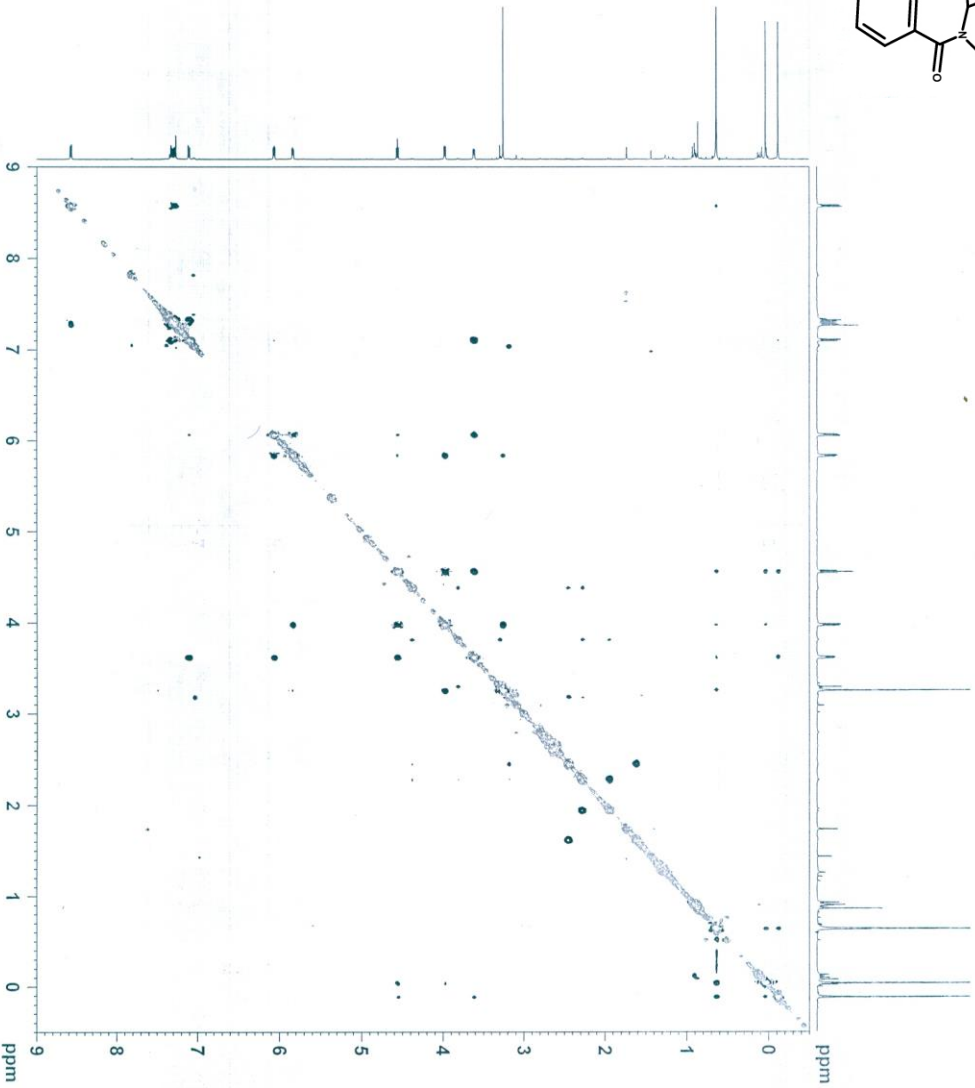
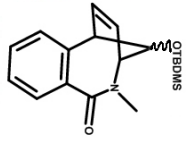


```

NAME          TG-346
EXPNO         2
PROCNO        1
Date_         20121122
Time         0.15
INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS           16
DS           16
SWH           5208.315 Hz
FIDRES       5.086263 Hz
AQ           0.0983940 sec
RG           64
RG2          64
AQ2          96.00 usec
DE           6.50 usec
TE           298.0 K
D0           0.00008410 sec
D1           2.00000000 sec
D2           0.00000000 sec
D3           0.00000000 sec
D4           0.00000000 sec
D5           0.00000000 sec
D6           0.00019200 sec
IND          0.00019200 sec

***** CHANNEL f1 *****
NUC1          1H
P1           9.35 usec
P2           18.70 usec
FL1          23.3796238 MHz
FL2          500.2611991 MHz
SFO1          500.2611991 MHz

***** GRADIENT CHANNEL *****
GENGR1       SINE 100 %
P1           100.00 usec
P2           1
NUC2          13C
TD           256
SFO1         500.2611991 MHz
SFO2         20.104111111 MHz
SW           20.104111111 MHz
F2MODE       States-pp1
SI           512
SF           500.260091 MHz
KERN         QSI13C
SSB          2
LB           0.00 Hz
GB           0
PC           1.00
SI           512
MCZ          States-pp1
SF           500.2600091 MHz
QSI13C
KERN         QSI13C
LB           0.00 Hz
GB           0
  
```

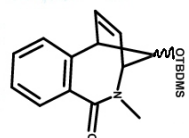


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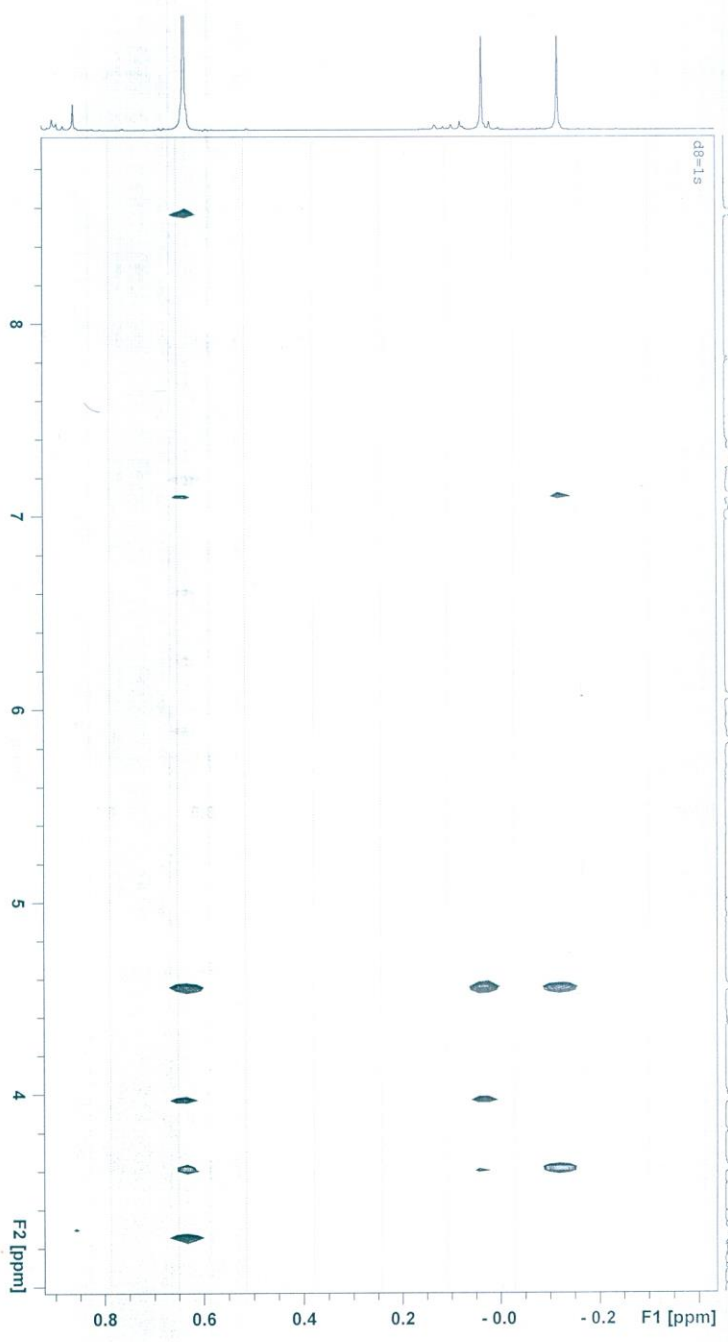
NAME          TS-366
EXPNO         2
PROCNO       2
Date_        20121122
Time         0.15
INSTRUM      spect
PROBHD       5 mm BBO BB-1H
PULPROG      zgpg30
TD           1024
SOLVENT      CDCl3
NS           16
DS           1
SFHM         5208.333 Hz
FIDRES      3.086273 Hz
AQ          0.0983544 sec
RG           64
AQ          96.000 usec
DE           6.50 usec
TE           298.10 K
D1           0.00000000 sec
D2           2.00000000 sec
D3           1.00000000 sec
D4           0.00020000 sec
D5           0.00020000 sec
D6           0.00019200 sec
D7           0.00019200 sec
D8           0.00019200 sec
D9           0.00019200 sec
D10          0.00019200 sec
D11          0.00019200 sec
D12          0.00019200 sec
D13          0.00019200 sec
D14          0.00019200 sec
D15          0.00019200 sec
D16          0.00019200 sec
D17          0.00019200 sec
D18          0.00019200 sec
D19          0.00019200 sec
D20          0.00019200 sec
D21          0.00019200 sec
D22          0.00019200 sec
D23          0.00019200 sec
D24          0.00019200 sec
D25          0.00019200 sec
D26          0.00019200 sec
D27          0.00019200 sec
D28          0.00019200 sec
D29          0.00019200 sec
D30          0.00019200 sec
D31          0.00019200 sec
D32          0.00019200 sec
D33          0.00019200 sec
D34          0.00019200 sec
D35          0.00019200 sec
D36          0.00019200 sec
D37          0.00019200 sec
D38          0.00019200 sec
D39          0.00019200 sec
D40          0.00019200 sec
D41          0.00019200 sec
D42          0.00019200 sec
D43          0.00019200 sec
D44          0.00019200 sec
D45          0.00019200 sec
D46          0.00019200 sec
D47          0.00019200 sec
D48          0.00019200 sec
D49          0.00019200 sec
D50          0.00019200 sec
D51          0.00019200 sec
D52          0.00019200 sec
D53          0.00019200 sec
D54          0.00019200 sec
D55          0.00019200 sec
D56          0.00019200 sec
D57          0.00019200 sec
D58          0.00019200 sec
D59          0.00019200 sec
D60          0.00019200 sec
D61          0.00019200 sec
D62          0.00019200 sec
D63          0.00019200 sec
D64          0.00019200 sec
D65          0.00019200 sec
D66          0.00019200 sec
D67          0.00019200 sec
D68          0.00019200 sec
D69          0.00019200 sec
D70          0.00019200 sec
D71          0.00019200 sec
D72          0.00019200 sec
D73          0.00019200 sec
D74          0.00019200 sec
D75          0.00019200 sec
D76          0.00019200 sec
D77          0.00019200 sec
D78          0.00019200 sec
D79          0.00019200 sec
D80          0.00019200 sec
D81          0.00019200 sec
D82          0.00019200 sec
D83          0.00019200 sec
D84          0.00019200 sec
D85          0.00019200 sec
D86          0.00019200 sec
D87          0.00019200 sec
D88          0.00019200 sec
D89          0.00019200 sec
D90          0.00019200 sec
D91          0.00019200 sec
D92          0.00019200 sec
D93          0.00019200 sec
D94          0.00019200 sec
D95          0.00019200 sec
D96          0.00019200 sec
D97          0.00019200 sec
D98          0.00019200 sec
D99          0.00019200 sec
D100         0.00019200 sec
  
```

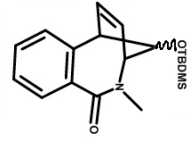
```

GRABP1       1H
GRABP2       13C
GRABP3       1H
GRABP4       13C
GRABP5       1H
GRABP6       13C
GRABP7       1H
GRABP8       13C
GRABP9       1H
GRABP10      13C
GRABP11      1H
GRABP12      13C
GRABP13      1H
GRABP14      13C
GRABP15      1H
GRABP16      13C
GRABP17      1H
GRABP18      13C
GRABP19      1H
GRABP20      13C
GRABP21      1H
GRABP22      13C
GRABP23      1H
GRABP24      13C
GRABP25      1H
GRABP26      13C
GRABP27      1H
GRABP28      13C
GRABP29      1H
GRABP30      13C
GRABP31      1H
GRABP32      13C
GRABP33      1H
GRABP34      13C
GRABP35      1H
GRABP36      13C
GRABP37      1H
GRABP38      13C
GRABP39      1H
GRABP40      13C
GRABP41      1H
GRABP42      13C
GRABP43      1H
GRABP44      13C
GRABP45      1H
GRABP46      13C
GRABP47      1H
GRABP48      13C
GRABP49      1H
GRABP50      13C
GRABP51      1H
GRABP52      13C
GRABP53      1H
GRABP54      13C
GRABP55      1H
GRABP56      13C
GRABP57      1H
GRABP58      13C
GRABP59      1H
GRABP60      13C
GRABP61      1H
GRABP62      13C
GRABP63      1H
GRABP64      13C
GRABP65      1H
GRABP66      13C
GRABP67      1H
GRABP68      13C
GRABP69      1H
GRABP70      13C
GRABP71      1H
GRABP72      13C
GRABP73      1H
GRABP74      13C
GRABP75      1H
GRABP76      13C
GRABP77      1H
GRABP78      13C
GRABP79      1H
GRABP80      13C
GRABP81      1H
GRABP82      13C
GRABP83      1H
GRABP84      13C
GRABP85      1H
GRABP86      13C
GRABP87      1H
GRABP88      13C
GRABP89      1H
GRABP90      13C
GRABP91      1H
GRABP92      13C
GRABP93      1H
GRABP94      13C
GRABP95      1H
GRABP96      13C
GRABP97      1H
GRABP98      13C
GRABP99      1H
GRABP100     13C
  
```

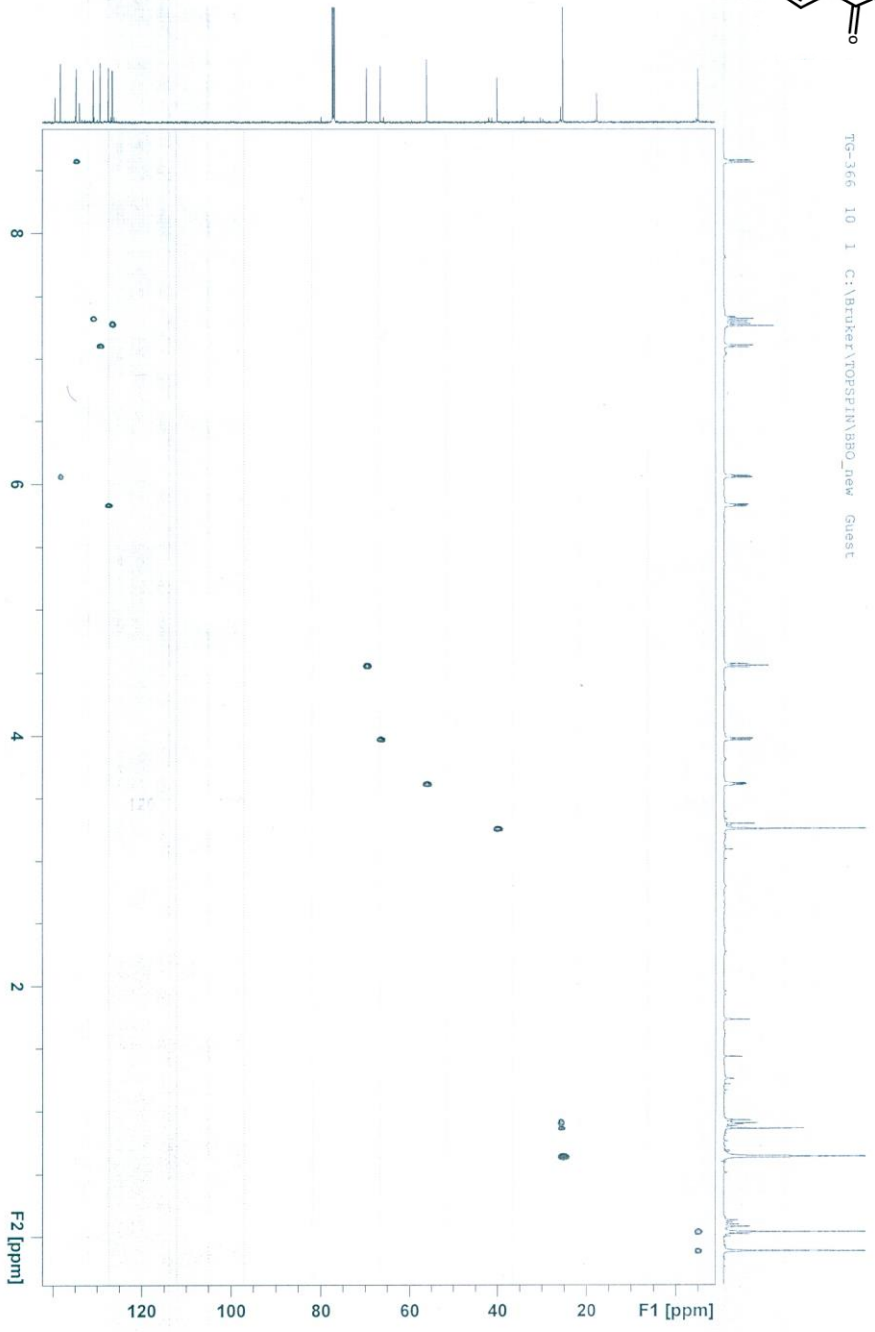


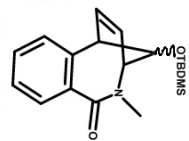
TG-366 7 2 C:\Bruker\TOPSPIN\BBO_new Guest





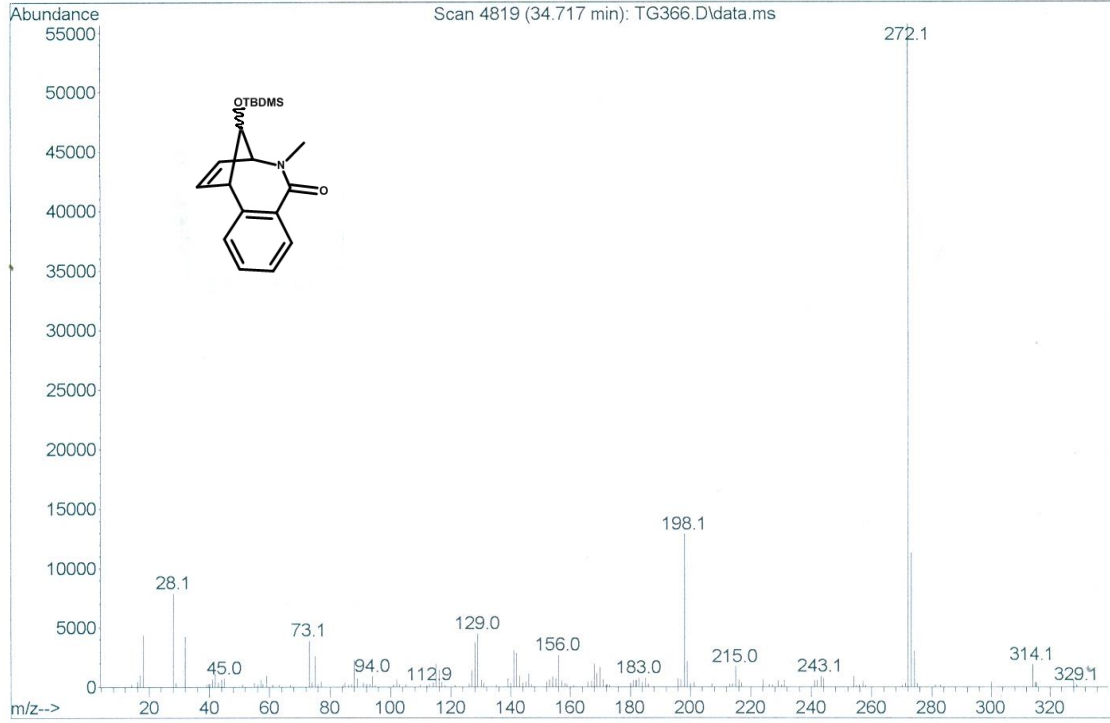
TG-366 10 1 C:\Bruker\TOPSPIN\BBO_new Guest

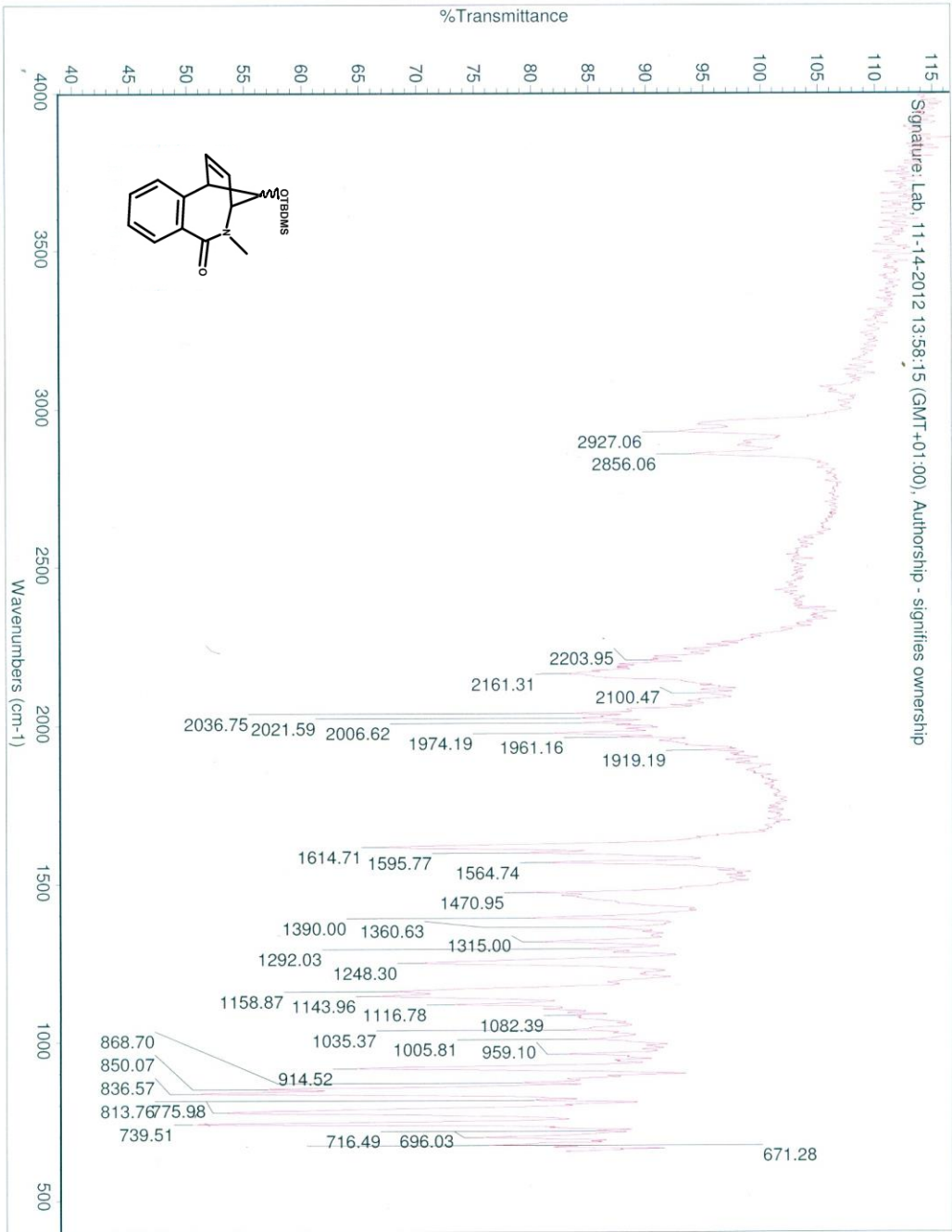




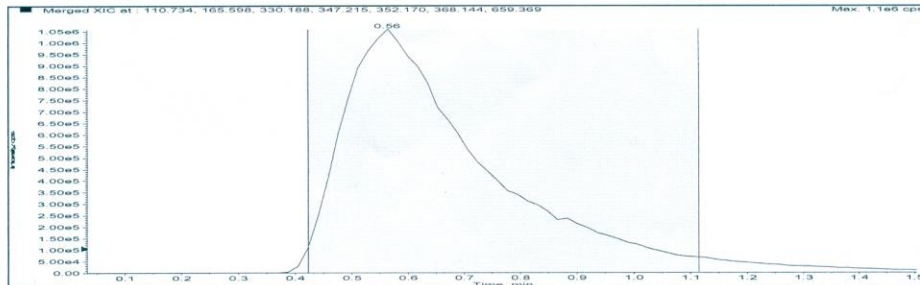
TG-366 9 1 C:\Bruker\TOPSPIN\BRO_new Guest



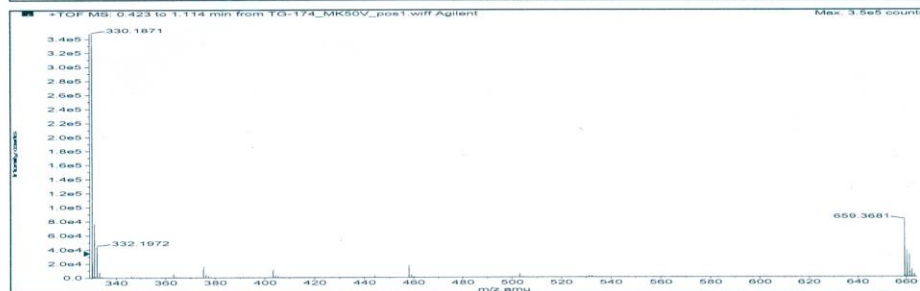
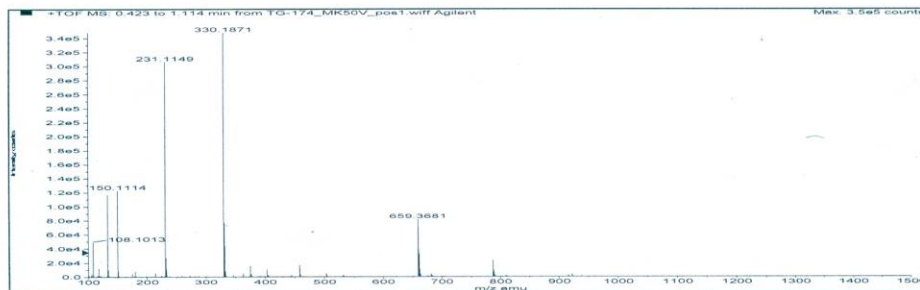




Sample Name: TG-174 Sample Location: P1-C2 Sample Id: Operator: Gordana
 Data File Name: D:\PE Sciex Data\Projects\Farmaceutski fakultet\Data\TG-174_MK50V_pos1.wiff Acq Time: November 13 2012, 11:19:15 AM
 Method: d:\TOF Software\damethods\Night_Seq_Comp_ident1.anm\efc.xml

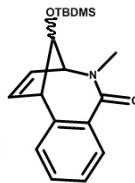


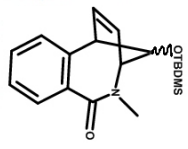
Merged XIC, Period# : 1 Experiment# : 1



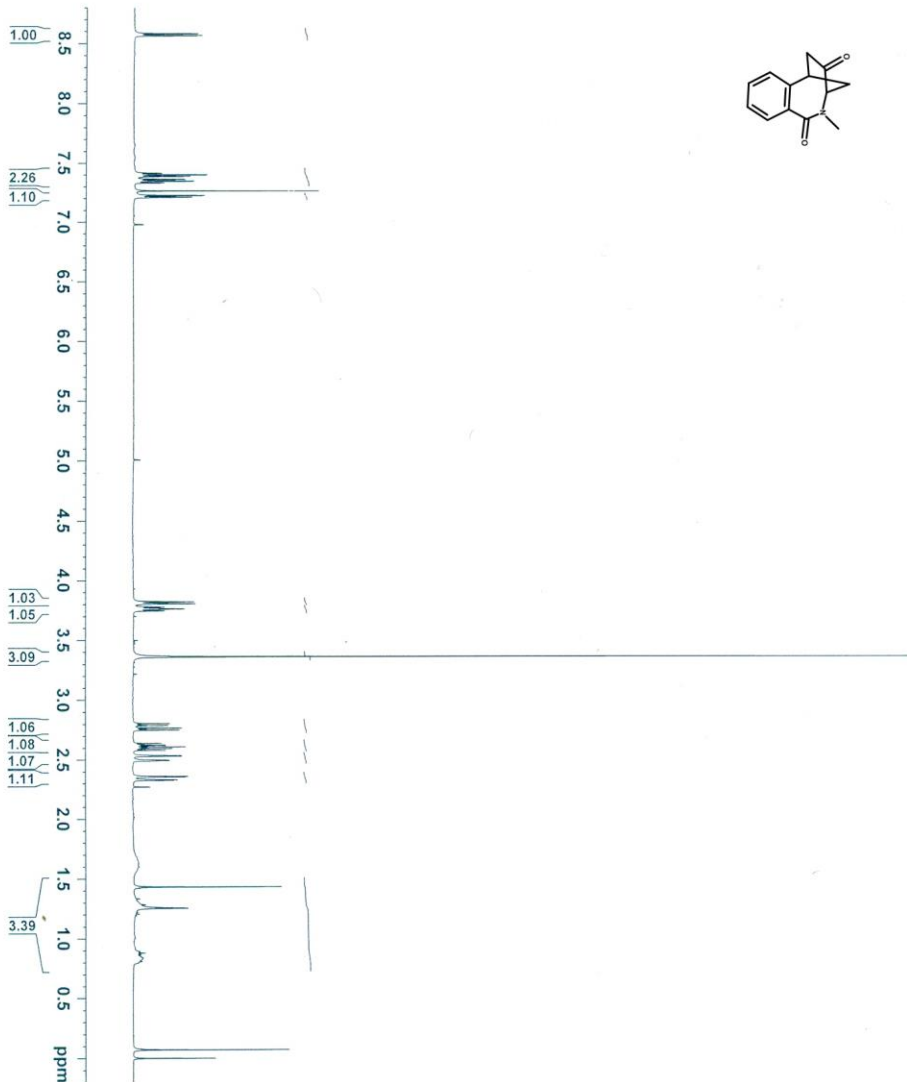
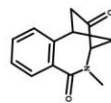
| Formula | Compound name | Mass | Peak RT (min) | Peak area | Description |
|-------------|---------------|-----------|---------------|------------|-------------|
| C19H27NO2Si | -- | 329.18111 | 0.56 | 1.86376 E7 | -- |

| Species | Abundance (counts) | Ion Mass | Measured Mass | Error (mDa) | Error (ppm) | Ret. Time Error (min) |
|---------------------|--------------------|-----------|---------------|-------------|-------------|-----------------------|
| [M+H] ⁺ | 362047.44 | 330.18838 | 330.18711 | -1.27458 | -3.86 | -- |
| [2M+H] ⁺ | 81932.05 | 659.36949 | 659.36808 | -1.41020 | -2.14 | -- |





Spectral data for compound 13



```

NAME      TG-2103
EXPNO     1
PROCNO    1
Date_     20111019
Time      11.39
INSTRUM   spect
PROBHD    5 mm BBO
PULPROG   zg30
TD        32768
SOLVENT   CDCl3
DS        16
SWH       5357.143 Hz
AQ        0.163487 Hz
RG        3.0683966 sec
DE        93.236 usec
TE        298.0 K
D1        1.50000000 sec
TD0       1

===== CHANNEL f1 =====
NUC1      1H
P1        9.35 usec
PL1       0.00 dB
SFO1      500.2622088 MHz
SI        16384
SF        500.2600131 MHz
WDW       EM
SSB       0
GB        0
PC        1.00
    
```

8.582
8.579
8.566
8.563

7.416
7.413
7.401
7.396
7.386
7.383
7.363
7.347
7.344
7.332
7.329

7.226
7.223
7.217
7.208

3.822
3.806
3.778
3.763
3.748

3.362

2.806
2.805
2.788
2.785
2.767
2.752

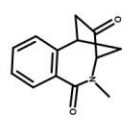
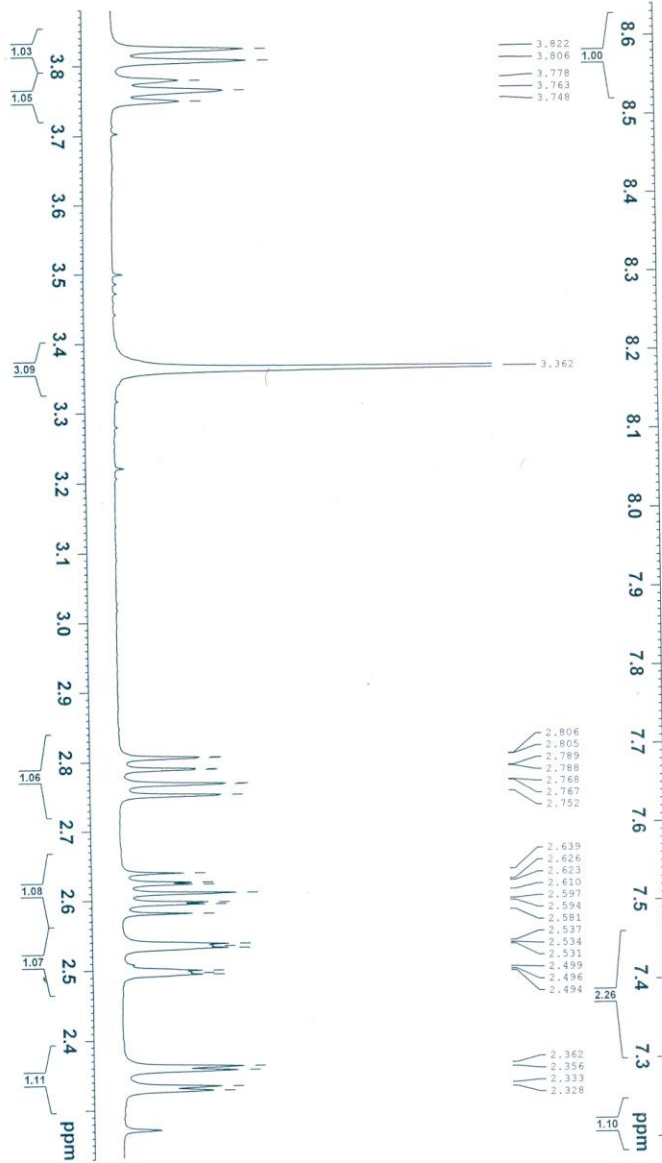
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2.626
2.623
2.619
2.597
2.594
2.581
2.575

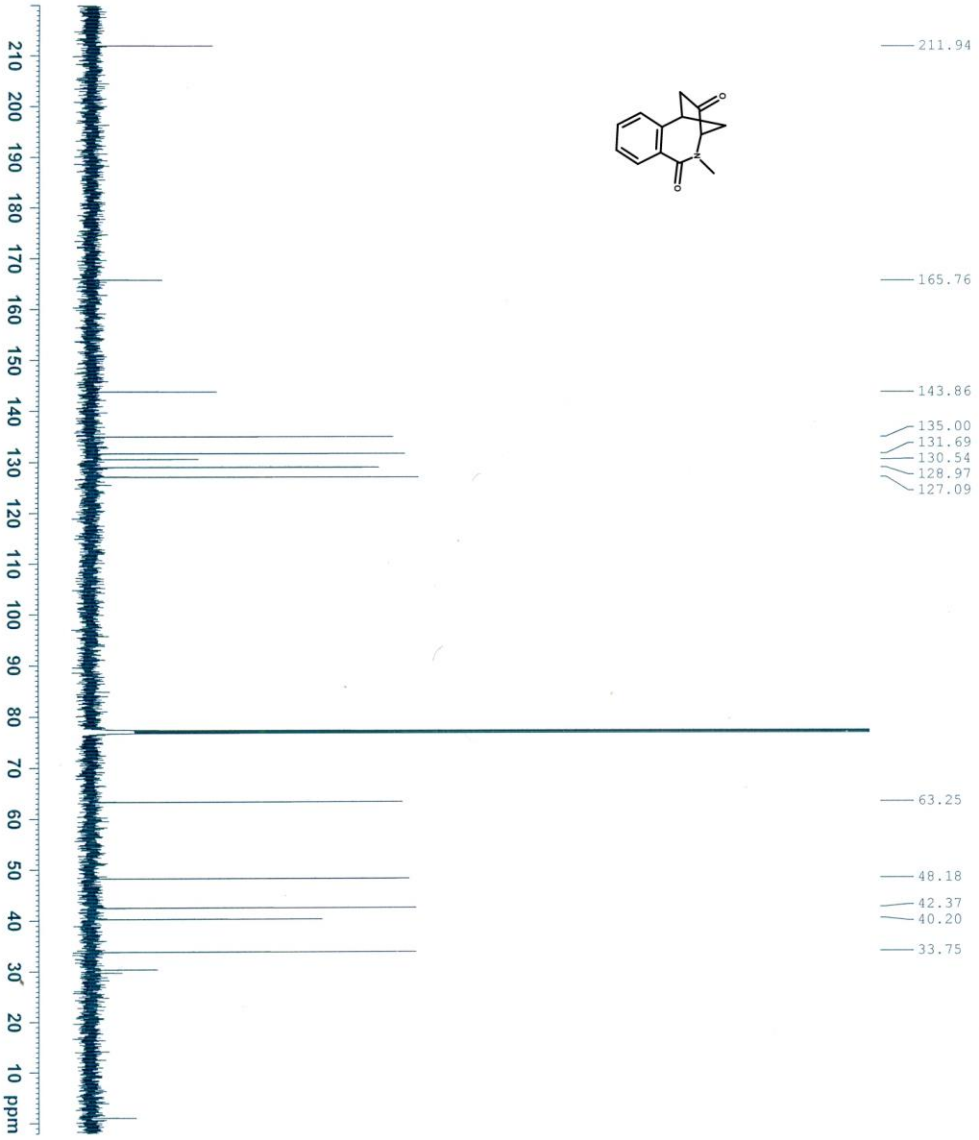
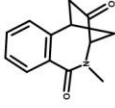
2.534
2.531
2.514
2.496
2.494

2.362
2.356
2.333
2.328

NAME TG-2109
PROCNO 1
Date 20111019
Time 11.39
INSTRUM spect
PROBHD 5 mm BBO BB-71H
PULPROG zgpg30
SOLVENT CDCl3
NS 16
DS 0
SWH 5357.143 Hz
FIDRES 0.163467 Hz
AQ 3.0983256 sec
RG 93.333 usec
DE 6.50 usec
TE 298.0 K
D1 1.50000000 sec
TD0 1

CHANNEL F1
NUC1 1H
P1 9.35 usec
PL 0.00 dB
FLL 27.37956238 W
ELLW 500.2622088 MHz
SFO1 500.2622088 MHz
SI 16394
SF 500.2622088 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





211.94
 165.76
 143.86
 135.00
 131.69
 130.54
 128.97
 127.09

63.25
 48.18
 42.37
 40.20
 33.75

NAME TG-210a
 EXPNO 2
 PROCNO 1
 Date_ 20111019
 Time 11:49
 INSTRUM spect
 PROBRD 5 mm BBO Bp1H
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 520
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 0.550524 sec
 RG 1630
 RM 1.920 usec
 DR 4.50 usec
 TE 298.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TDO 1

===== CHANNEL F1 =====
 NUCL 13C
 P1 11.50 usec
 P11 3.00 dB
 P11W 32.22848852 W
 SFO1 129.8043140 MHz

===== CHANNEL F2 =====
 CDPRG2 waltz16
 NUCL2 1H
 PCPD2 80.00 usec
 P12 1.20 dB
 P112 18.40 dB
 P113 18.40 dB
 P12W 20.76952171 W
 P113W 0.38272511 W
 P113M 0.38272511 W
 SFO2 500.3622068 MHz
 SF 32768
 WDM 125.7904810 MHz
 SSB EM
 LB 0
 GB 1.50 Hz
 PC 0
 1.40

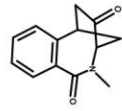
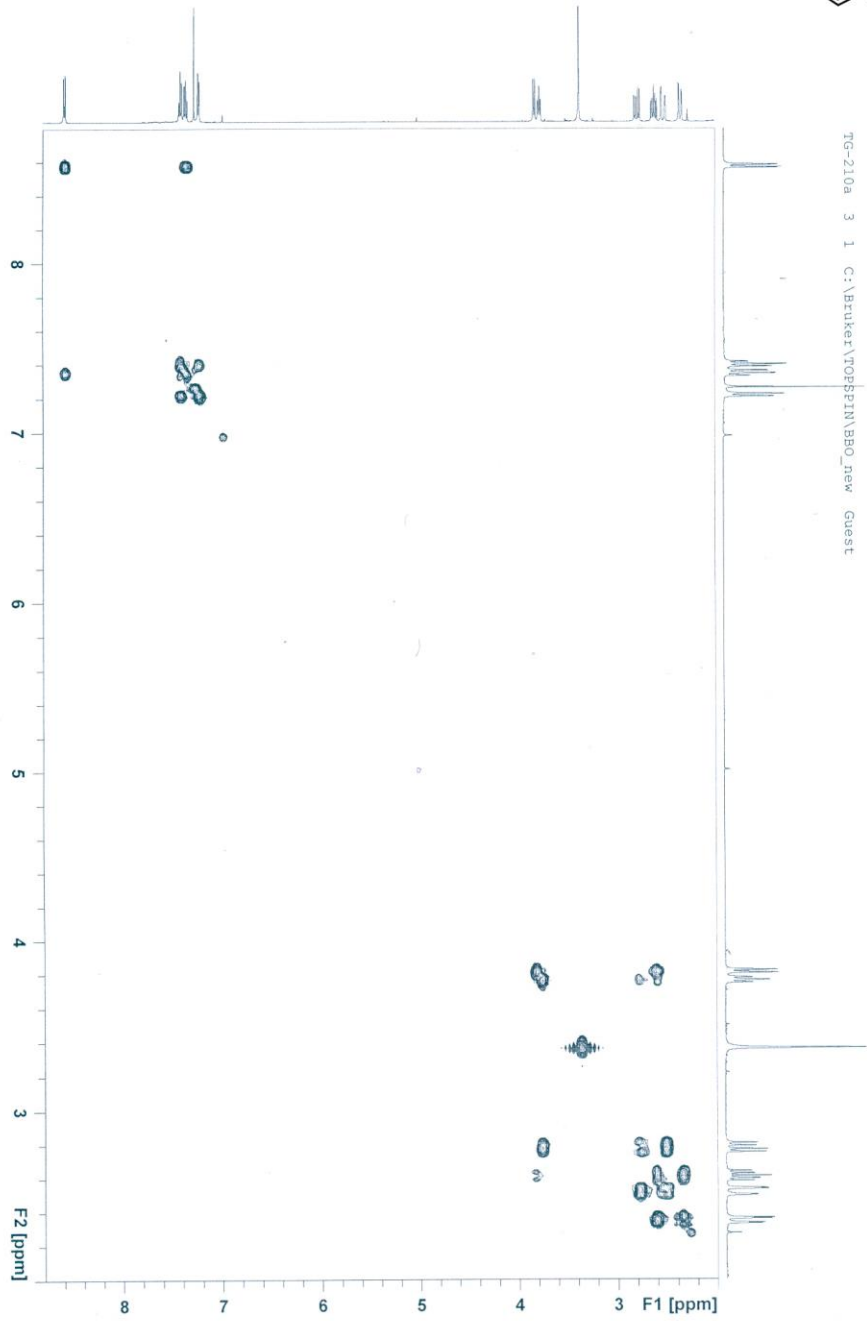
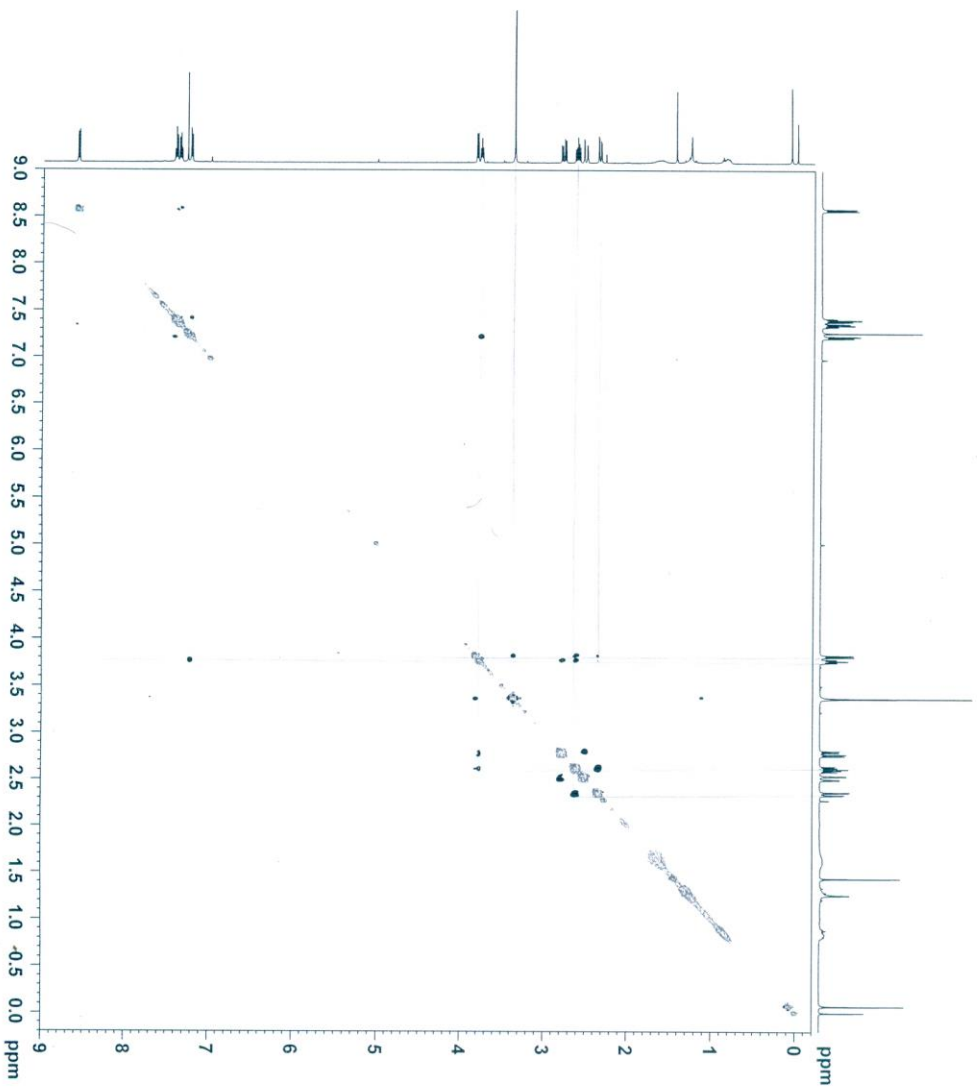
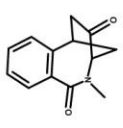


Fig-210a 3 1 C:\Bruker\TOPSPIN\BBO_new Guest

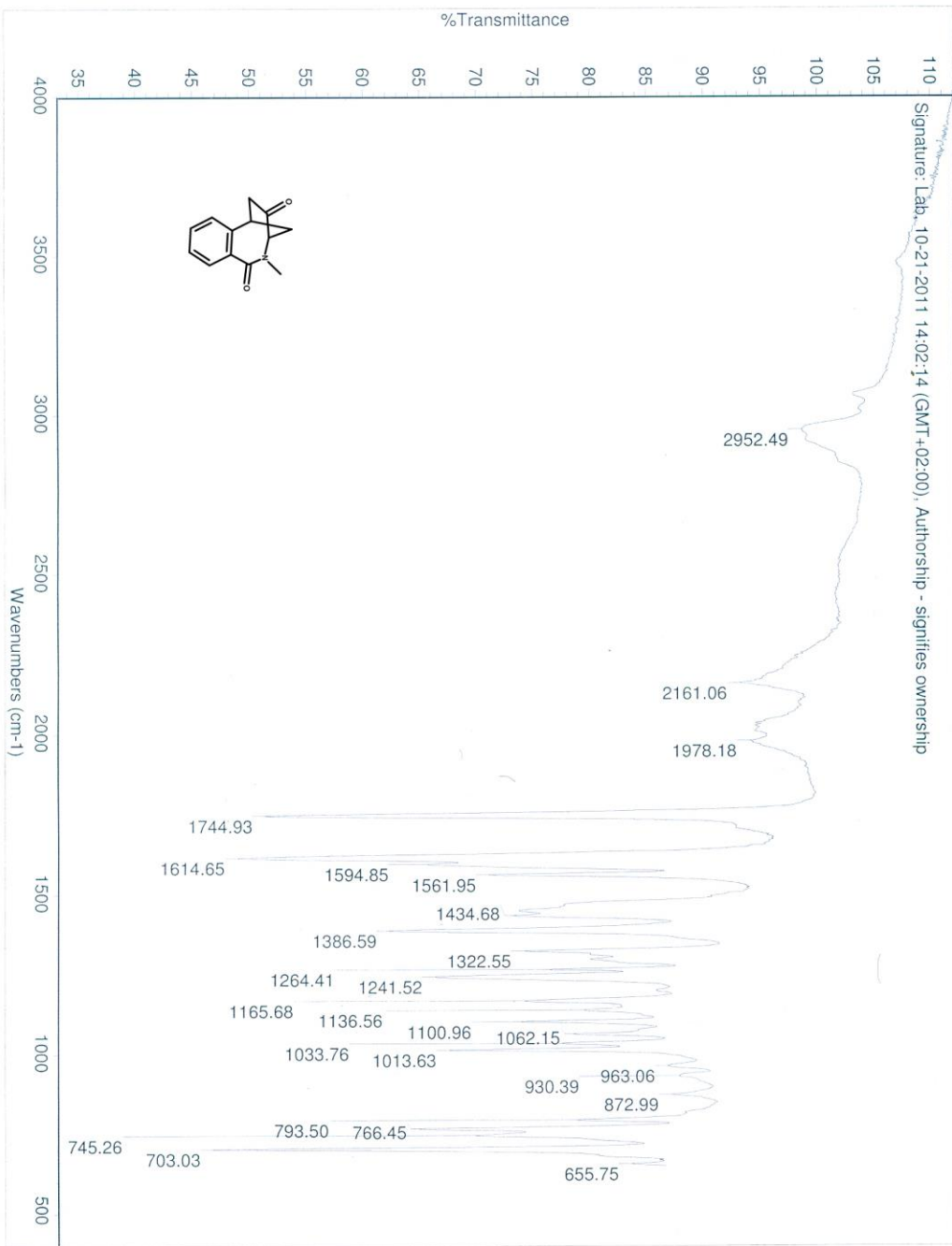




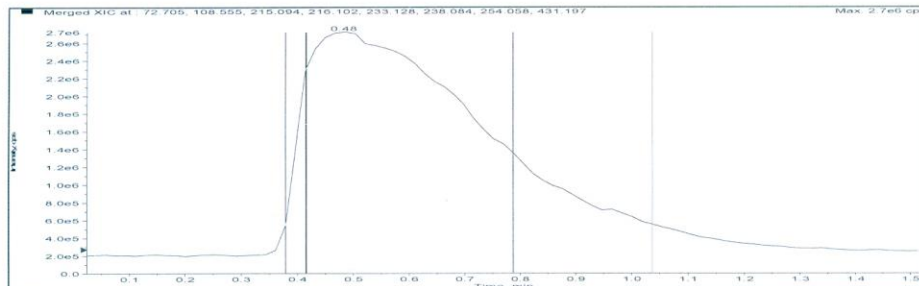
NAME TS-210a
 EXPNO 5
 PROCNO 1
 20111011
 Time 12:19
 INSTRUM spect
 PROBD 5 mm BBO BB-1H
 PULPROG zgpg30
 SOLVENT noesyppm
 NS 1024
 DS 8
 SMH 5357.143 Hz
 FIDRES 0.331293 Hz
 AQ 0.0594228 sec
 RG 228
 DW 93.333 usec
 DE 6.50 usec
 DS 288.0 K
 DI 0.00000000 sec
 D1 2.00000000 sec
 D8 0.80000001 sec
 INO 0.00018665 sec
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 9.35 usec
 PL1 0.00 dB
 PL1W 27.37956238 W
 SFO1 500.2622086 MHz
 TD 256
 SF 500.2622086 MHz
 FIDRES 20.326397 Hz
 SW 10.709 ppm
 SHMOPR States-1024
 SF 500.2600107 MHz
 WDW OSINE
 SSB 2
 GB 0.00 Hz
 PC 1.00
 SI 1024
 MC2 States-TPI
 SF 500.2600111 MHz
 SSB 2
 LB 0.00 Hz
 GB 0



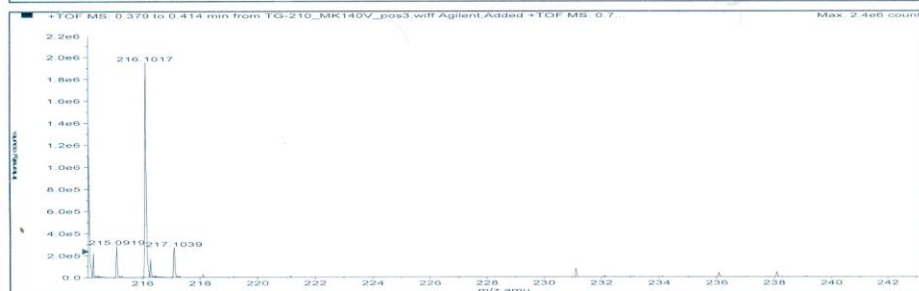
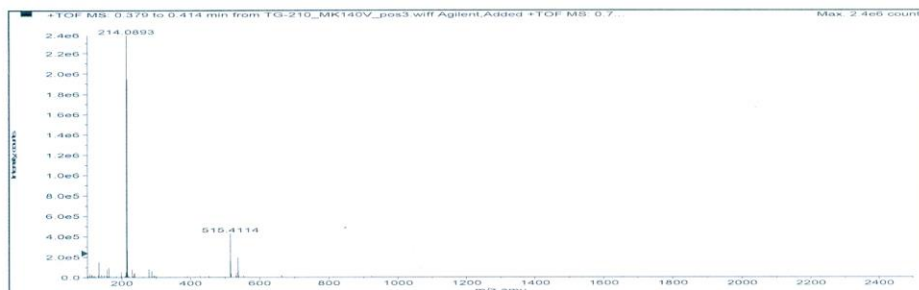
TG 210



Sample Name: TG-210 Sample Location: P1-E2 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Farmaceutski fakulteti\Data\TG-210_MK140V_pos3.wiff Acq Time: October 26 2011,
 01:29:25 PM
 Method: D:\TOF_Data\damethods\Night_Seq_Comp_ident1.anmlefc.xml

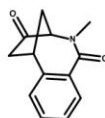


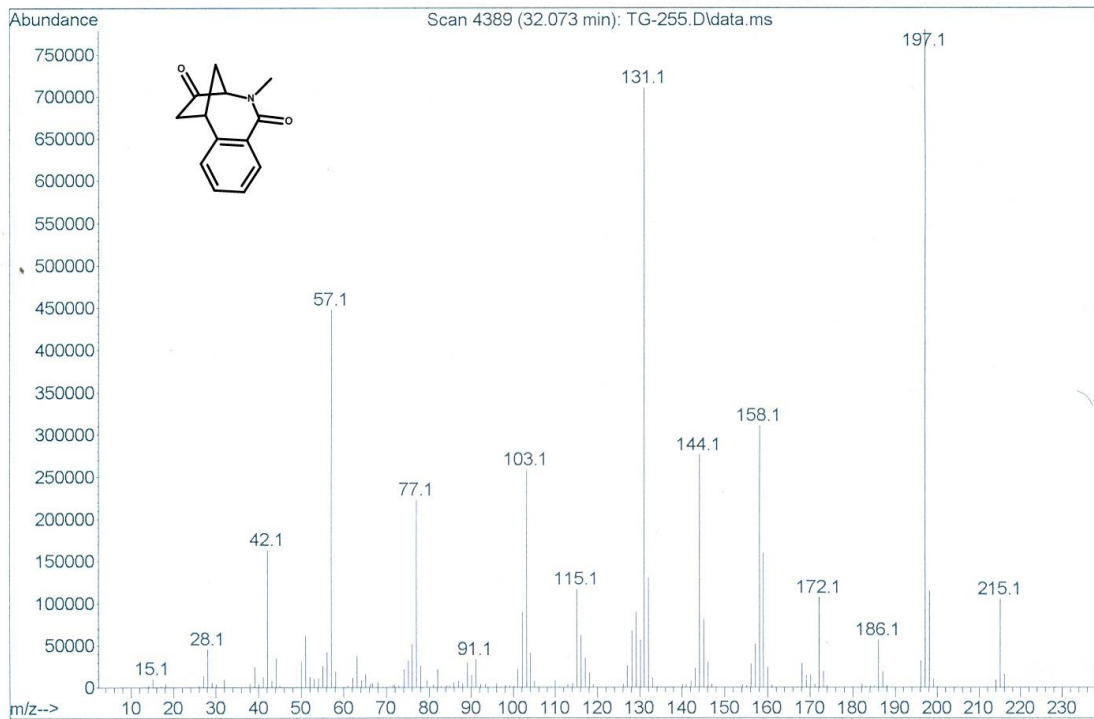
Merged XIC, Period# : 1 Experiment# : 1



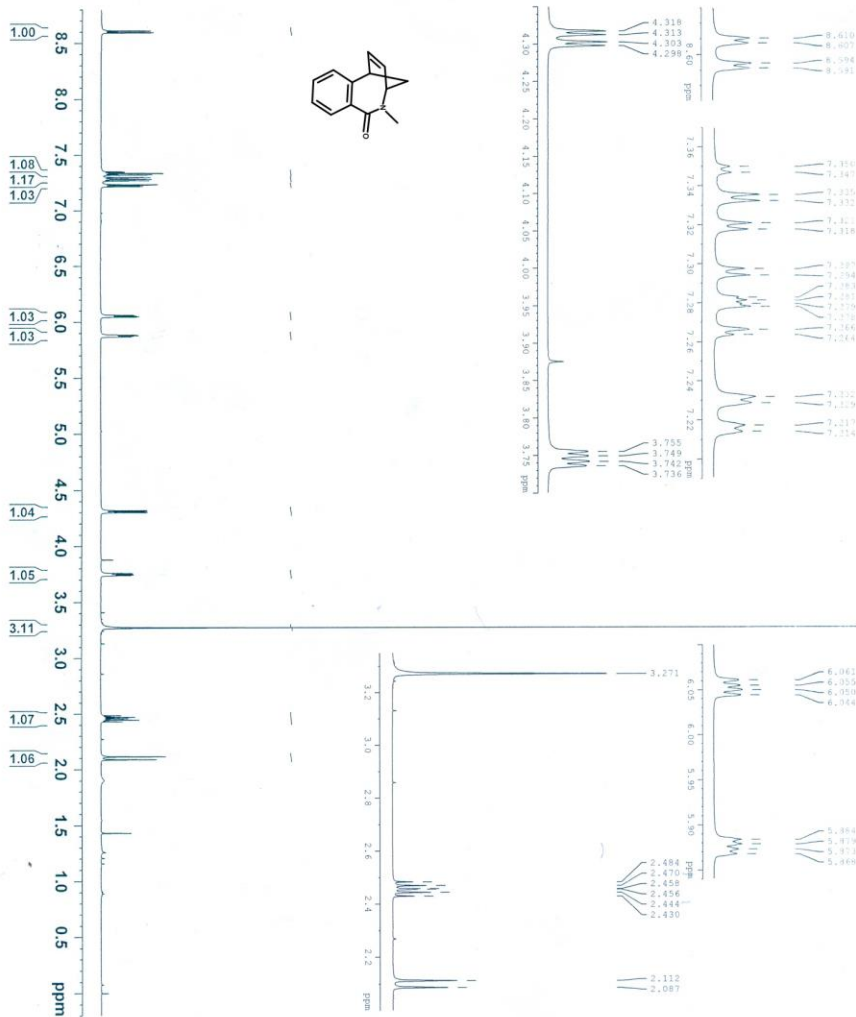
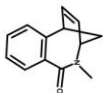
| Formula | Compound name | Mass | Peak RT (min) | Peak area | Description |
|---|---------------|-----------|---------------|------------|-------------|
| C ₁₃ H ₁₃ NO ₂ | -- | 215.09463 | 0.48 | 5.92442 E7 | -- |

| Species | Abundance (counts) | Ion Mass | Measured Mass | Error (mDa) | Error (ppm) | Ret. Time Error (min) |
|---------------------|--------------------|-----------|---------------|-------------|-------------|-----------------------|
| M+ | 287271.65 | 215.09408 | 215.09187 | -2.21182 | -10.28 | -- |
| [M+H] ⁺ | 1954138.71 | 216.10191 | 216.10168 | -0.22443 | -1.04 | -- |
| [M+Na] ⁺ | 45383.50 | 238.08385 | 238.08315 | -0.70133 | -2.95 | -- |



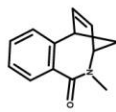


Spectral data for compound 14

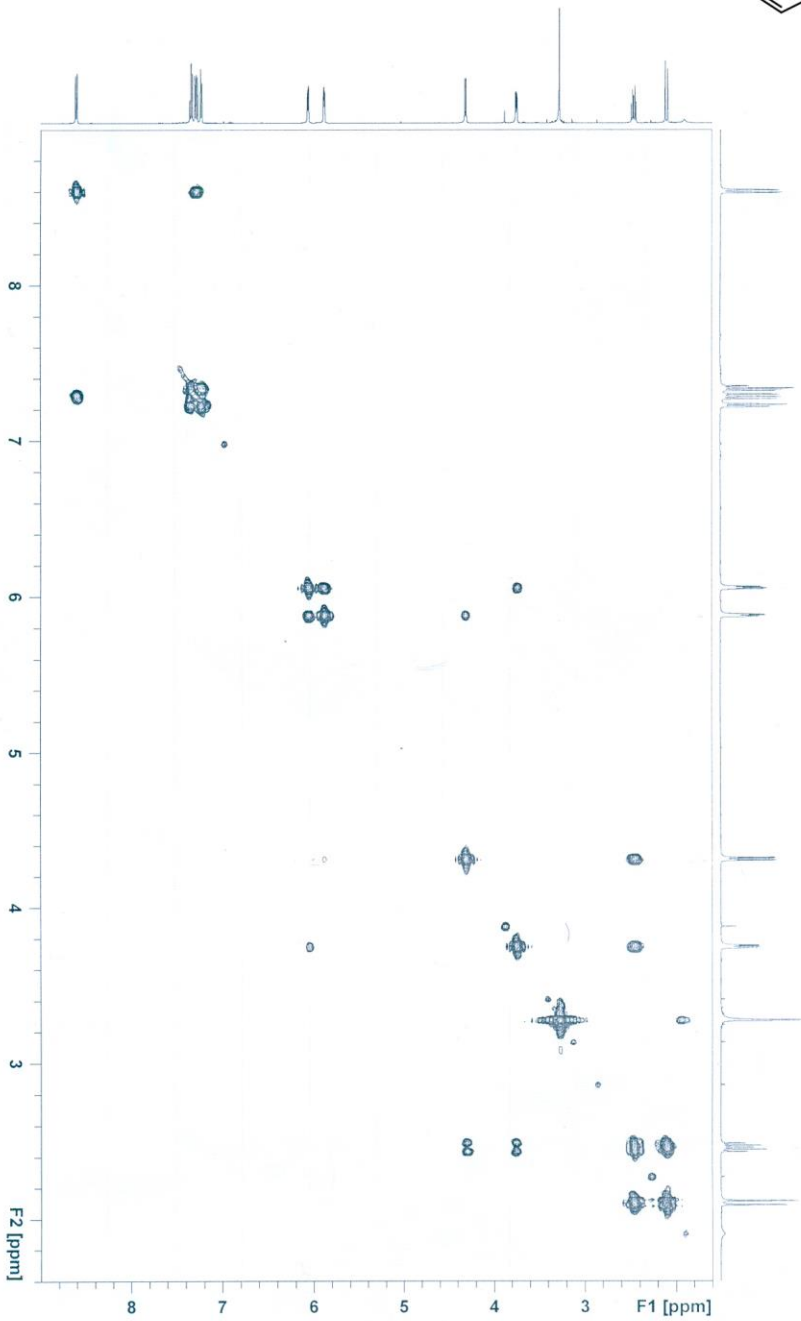


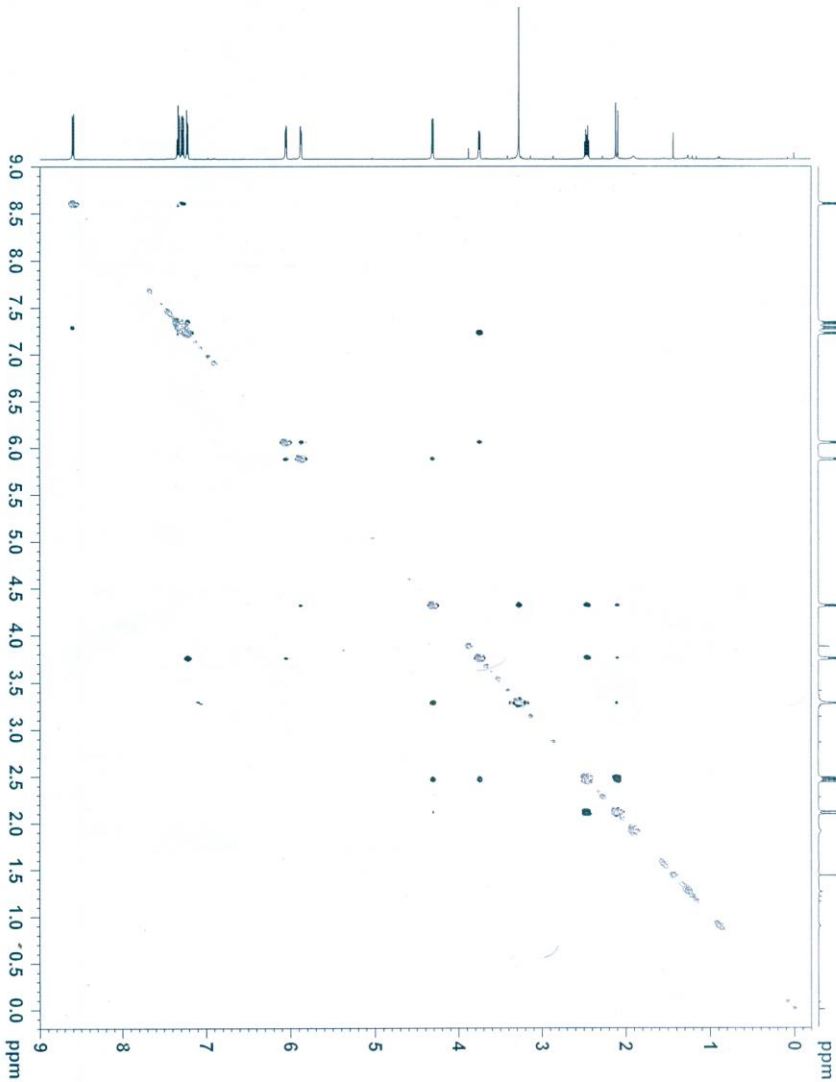
NAME: 709-3117
 EXPNO: 1
 PROCNO: 1
 Date_: 20121015
 INSTRUM: spect
 PROBHD: 5 mm BBO BB-1H
 PULPROG: zgpg30
 SOLVENT: DMSO
 NS: 16
 DSF: 0
 FIDRES: 5116.498 Hz
 AQ: 0.156768 sec
 RG: 3.1894686
 EQ: 80.0 usec
 DE: 97.0 usec
 TE: 298.0 K
 D1: 2.0000000 sec
 T00: 1

CHANNEL F1
 NUC1: 13C
 P1: 9.1H
 PL1: 0.20 usec
 PL1W: 27.37956238 W
 SFO1: 500.2623169 MHz
 SF: 500.2623169 MHz
 KW: 500.2623169 MHz
 SSB: 0
 LB: 0.20 Hz
 GB: 0
 PC: 1.00



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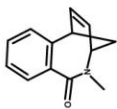


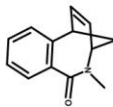


NAME: TG-3119
 EXPNO: 5
 PROCNO: 1
 DATE_UTC: 20121012
 TIME: 11:15
 INSTRUM: spect
 F2PROB: 5 mm BBO BB-1H
 PULPROG: noesygprb
 SOLVENT: CDCl3
 NS: 4
 DS: 4
 SM: 132.916 Hz
 SFO1: 500.136180 MHz
 STRSSES: 0.0597193 sec
 AQ: 0.0597193 sec
 RG: 80.6
 RC: 97.333 usec
 DM: 298.0 K usec
 TE: 298.0 K usec
 D0: 0.00008543 sec
 D1: 2.00000000 sec
 D8: 1.00000000 sec
 D11: 0.00000000 sec
 I10: 0.00019465 sec

CHANNEL F1
 NU1: 1H 10 usec
 P1: 9.18 usec
 P2: 18.70 usec
 PL1: 0.00 dB
 PL1W: 27.31956238 W
 SFO1: 500.2623167 MHz

GRADIENT CHANNEL
 GPRM1: SINE:100
 GE21: 40.00 %
 N1: 10.00 usec
 N10: 1000.00 usec
 TD: 256
 SFO1: 500.2623 MHz
 FIDRES: 20.06363 Hz
 FWHM: 0.70354 ppm
 FIMODE: States-TPI
 SI: 512
 SF: 500.2600048 MHz
 K1: 8
 K2: 2
 LB: 0.00 Hz
 GB: 0
 EC: 1.00
 FC: 1.00
 MCK: States-TPI
 SF: 500.2600064 MHz
 WTR: OSINE
 SSB: 0
 GB: 0.00 Hz





166.39
144.44
138.13
135.60
131.95
131.02
128.11
127.89
126.48
65.28
51.35
38.98
37.09

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

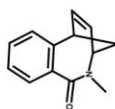


```

NAME          TG-371g
EXPNO         2
PROCNO        1
Date_         20121015
Time          11:31
INSTRUM       5 mm BBO BB-1H
PROBHD        BB-1H
PULPROG       zgpg30
TD            655368
SOLVENT       CDCl3
NS            404
DS            4
SWH           29761.904 Hz
FIDRES        0.908261 Hz
AQ            0.5505524 sec
RG            1620
DM            16.800 usec
DE            6.30 usec
TE            293.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TDO           1

===== CHANNEL F1 =====
NUC1           13C
P1            11.50 usec
PL1           3.00 dB
PL1W          32.22848892 W
SFO1          125.8043140 MHz

===== CHANNEL F2 =====
CDEPRG2       waltz16
NUC2           1H
PCPD2         80.00 usec
P2           1.20 dB
PL12          18.40 dB
PL13          18.40 dB
PL1W          20.76952171 W
PL2W          0.38575511 W
PL13W         0.38575511 W
SFO2          500.2621167 MHz
SI            1
RFW          125.7904884 MHz
SSB           0
LB            1.50 Hz
GB            0
PC            1.40
  
```



NAME: 20-319
 EXPNO: 1
 Date_: 20121015
 TIME: 16:45:29
 INSTRUM: spect
 F2PRG2: 3 line BBO BR-1H
 F2FREQ: 125.760474 MHz
 TO: 1024
 SOLVENT: CDCl3
 NS: 16
 DS: 2
 SFR: 3136.886 Hz
 AQCROSS: 0.0097193 sec
 ACQ: 9.7050 usec
 MD: 9.7050 usec
 DE: 6.50 usec
 TE: 298.0 K
 TD: 65536
 GB: 0
 PC: 2.0000000 sec
 D1: 2.0000000 sec
 D11: 0.0300000 sec
 D12: 0.0300000 sec
 D13: 0.0300000 sec
 D21: 0.00184616 sec
 D22: 0.00184616 sec
 D23: 0.0002210 sec
 INO: 0.0002210 sec

===== CHANNEL f1 =====
 NUCL1: 1H
 F1: 9.14 usec
 P1: 18.70 usec
 PL1: 27.3748 0.00 dB
 SFO1: 500.262167 MHz

===== CHANNEL f2 =====
 CPDPRG2: 2zap
 NUCL2: 13C
 F2: 11.36 usec
 P2: 21.00 usec
 PL2: 19.00 dB
 SFO2: 125.760474 MHz

===== CHANNEL f3 =====
 CPDPRG3: 2zap
 NUCL3: 15N
 F3: 9.14 usec
 P3: 18.70 usec
 PL3: 27.3748 0.00 dB
 SFO3: 500.262167 MHz

===== CHANNEL f4 =====
 CPDPRG4: 2zap
 NUCL4: 13C
 F4: 11.36 usec
 P4: 21.00 usec
 PL4: 19.00 dB
 SFO4: 125.760474 MHz

===== CHANNEL f5 =====
 CPDPRG5: 2zap
 NUCL5: 15N
 F5: 9.14 usec
 P5: 18.70 usec
 PL5: 27.3748 0.00 dB
 SFO5: 500.262167 MHz

===== CHANNEL f6 =====
 CPDPRG6: 2zap
 NUCL6: 13C
 F6: 11.36 usec
 P6: 21.00 usec
 PL6: 19.00 dB
 SFO6: 125.760474 MHz

===== CHANNEL f7 =====
 CPDPRG7: 2zap
 NUCL7: 15N
 F7: 9.14 usec
 P7: 18.70 usec
 PL7: 27.3748 0.00 dB
 SFO7: 500.262167 MHz

===== CHANNEL f8 =====
 CPDPRG8: 2zap
 NUCL8: 13C
 F8: 11.36 usec
 P8: 21.00 usec
 PL8: 19.00 dB
 SFO8: 125.760474 MHz

===== CHANNEL f9 =====
 CPDPRG9: 2zap
 NUCL9: 15N
 F9: 9.14 usec
 P9: 18.70 usec
 PL9: 27.3748 0.00 dB
 SFO9: 500.262167 MHz

===== CHANNEL f10 =====
 CPDPRG10: 2zap
 NUCL10: 13C
 F10: 11.36 usec
 P10: 21.00 usec
 PL10: 19.00 dB
 SFO10: 125.760474 MHz

===== CHANNEL f11 =====
 CPDPRG11: 2zap
 NUCL11: 15N
 F11: 9.14 usec
 P11: 18.70 usec
 PL11: 27.3748 0.00 dB
 SFO11: 500.262167 MHz

===== CHANNEL f12 =====
 CPDPRG12: 2zap
 NUCL12: 13C
 F12: 11.36 usec
 P12: 21.00 usec
 PL12: 19.00 dB
 SFO12: 125.760474 MHz

===== CHANNEL f13 =====
 CPDPRG13: 2zap
 NUCL13: 15N
 F13: 9.14 usec
 P13: 18.70 usec
 PL13: 27.3748 0.00 dB
 SFO13: 500.262167 MHz

===== CHANNEL f14 =====
 CPDPRG14: 2zap
 NUCL14: 13C
 F14: 11.36 usec
 P14: 21.00 usec
 PL14: 19.00 dB
 SFO14: 125.760474 MHz

===== CHANNEL f15 =====
 CPDPRG15: 2zap
 NUCL15: 15N
 F15: 9.14 usec
 P15: 18.70 usec
 PL15: 27.3748 0.00 dB
 SFO15: 500.262167 MHz

===== CHANNEL f16 =====
 CPDPRG16: 2zap
 NUCL16: 13C
 F16: 11.36 usec
 P16: 21.00 usec
 PL16: 19.00 dB
 SFO16: 125.760474 MHz

===== CHANNEL f17 =====
 CPDPRG17: 2zap
 NUCL17: 15N
 F17: 9.14 usec
 P17: 18.70 usec
 PL17: 27.3748 0.00 dB
 SFO17: 500.262167 MHz

===== CHANNEL f18 =====
 CPDPRG18: 2zap
 NUCL18: 13C
 F18: 11.36 usec
 P18: 21.00 usec
 PL18: 19.00 dB
 SFO18: 125.760474 MHz

===== CHANNEL f19 =====
 CPDPRG19: 2zap
 NUCL19: 15N
 F19: 9.14 usec
 P19: 18.70 usec
 PL19: 27.3748 0.00 dB
 SFO19: 500.262167 MHz

===== CHANNEL f20 =====
 CPDPRG20: 2zap
 NUCL20: 13C
 F20: 11.36 usec
 P20: 21.00 usec
 PL20: 19.00 dB
 SFO20: 125.760474 MHz

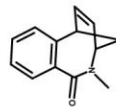
===== CHANNEL f21 =====
 CPDPRG21: 2zap
 NUCL21: 15N
 F21: 9.14 usec
 P21: 18.70 usec
 PL21: 27.3748 0.00 dB
 SFO21: 500.262167 MHz

===== CHANNEL f22 =====
 CPDPRG22: 2zap
 NUCL22: 13C
 F22: 11.36 usec
 P22: 21.00 usec
 PL22: 19.00 dB
 SFO22: 125.760474 MHz

===== CHANNEL f23 =====
 CPDPRG23: 2zap
 NUCL23: 15N
 F23: 9.14 usec
 P23: 18.70 usec
 PL23: 27.3748 0.00 dB
 SFO23: 500.262167 MHz

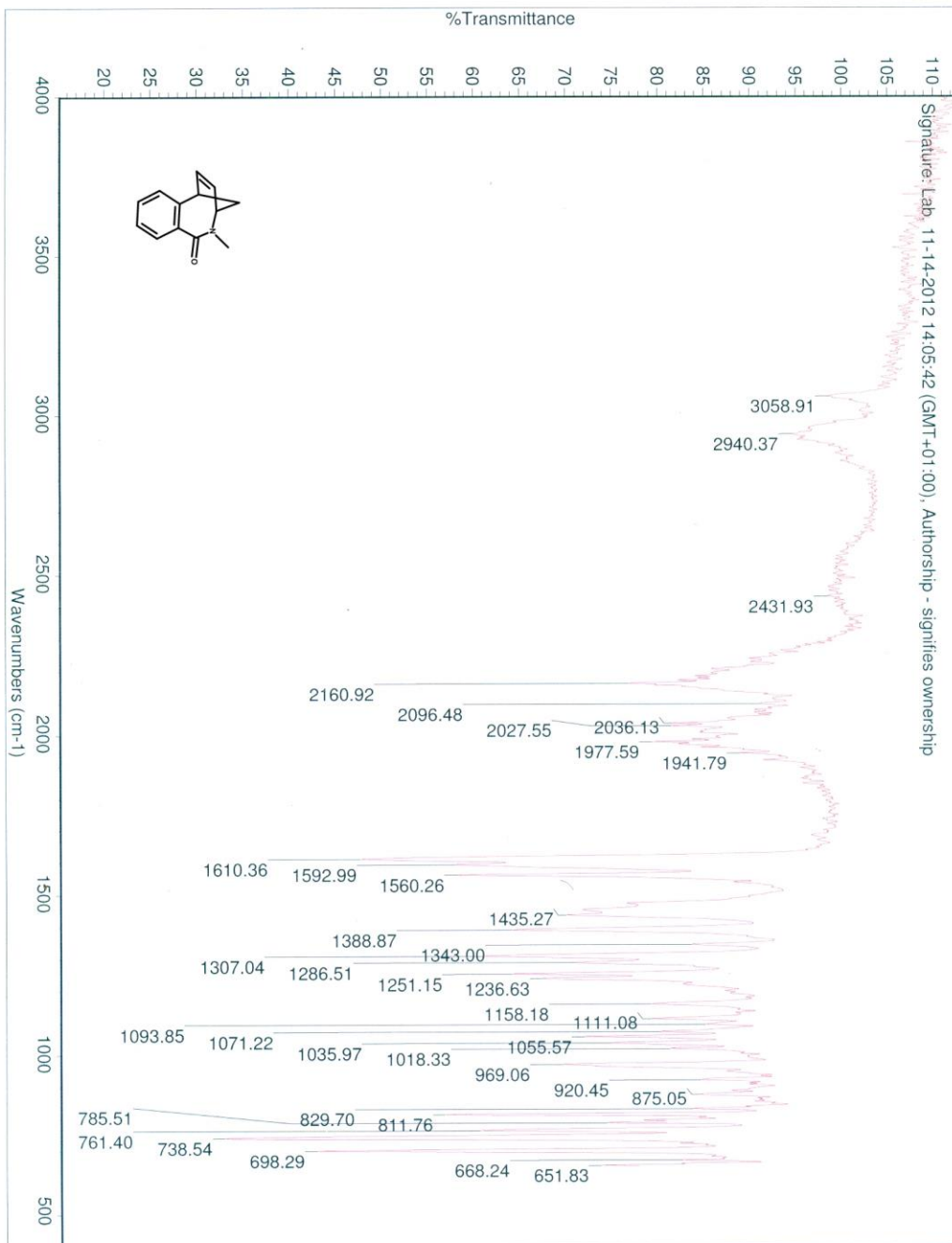
===== CHANNEL f24 =====
 CPDPRG24: 2zap
 NUCL24: 13C
 F24: 11.36 usec
 P24: 21.00 usec
 PL24: 19.00 dB
 SFO24: 125.760474 MHz

===== CHANNEL f25 =====
 CPDPRG25: 2zap
 NUCL25: 15N
 F25: 9.14 usec
 P25: 18.70 usec
 PL25: 27.3748 0.00 dB
 SFO25: 500.262167 MHz

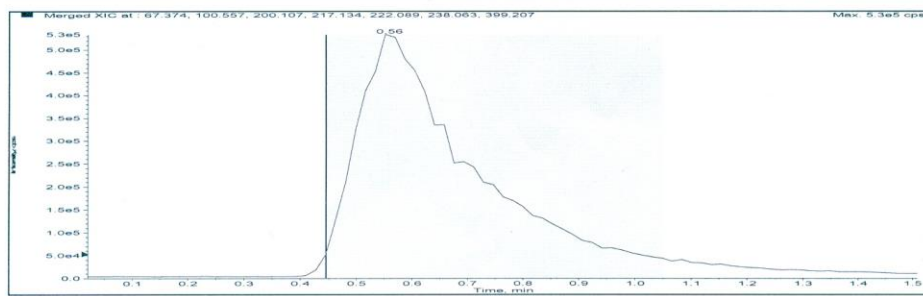


TG-371g 4 1 C:\Bruker\TOPSPIN\BBO_new Guest

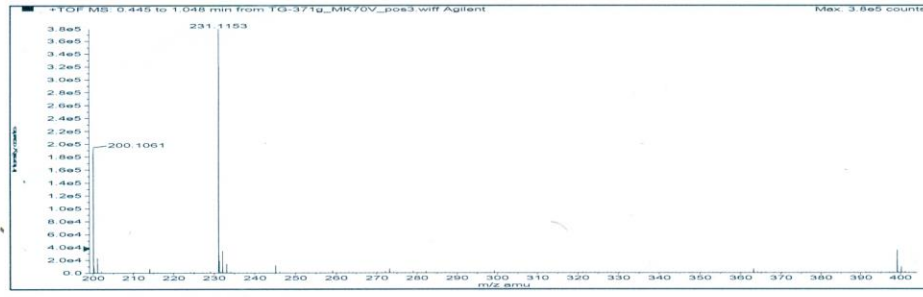
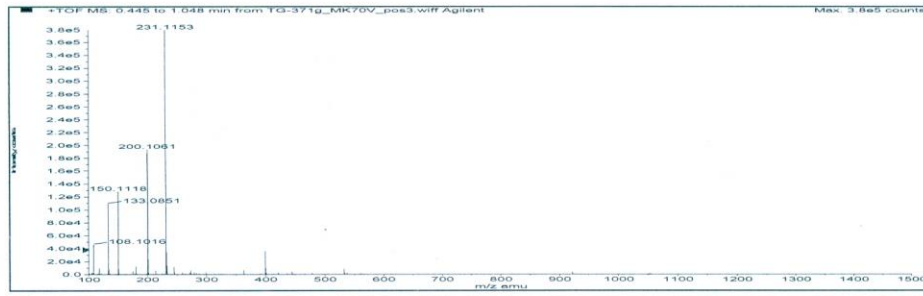




Sample Name: **TG-371g** Sample Location: **P1-C4** Sample Id: Operator: **Gordana**
 Data File Name: **D:\PE Sciex Data\Projects\Farmaceutski fakultet\Data\TG-371g_MK70V_pos3.wiff** Acq Time: **November 13 2012, 11:36:19 AM**
 Method: **d:\TOF Software\damethods\Night_Seq_Comp_ident1.anm\efc.xml**



Merged XIC, Period# : 1 Experiment# : 1



| Formula | Compound name | Mass | Peak RT (min) | Peak area | Description |
|----------|---------------|-----------|---------------|------------|-------------|
| C13H13NO | -- | 199.09971 | 0.56 | 7.83144 E6 | -- |

| Species | Abundance (counts) | Ion Mass | Measured Mass | Error (mDa) | Error (ppm) | Ret. Time Error (min) |
|---------------------|--------------------|-----------|---------------|-------------|-------------|-----------------------|
| [M+H] ⁺ | 201225.00 | 200.10699 | 200.10611 | -0.88493 | -4.42 | -- |
| [2M+H] ⁺ | 37255.90 | 399.20670 | 399.20556 | -1.13971 | -2.85 | -- |

