

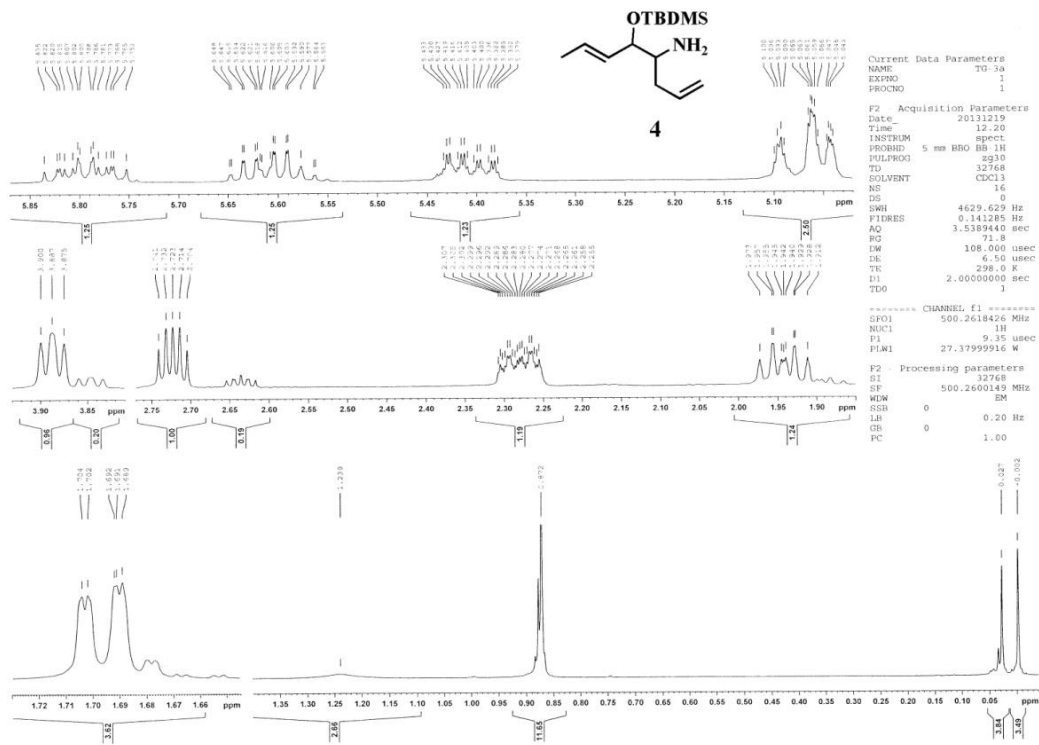
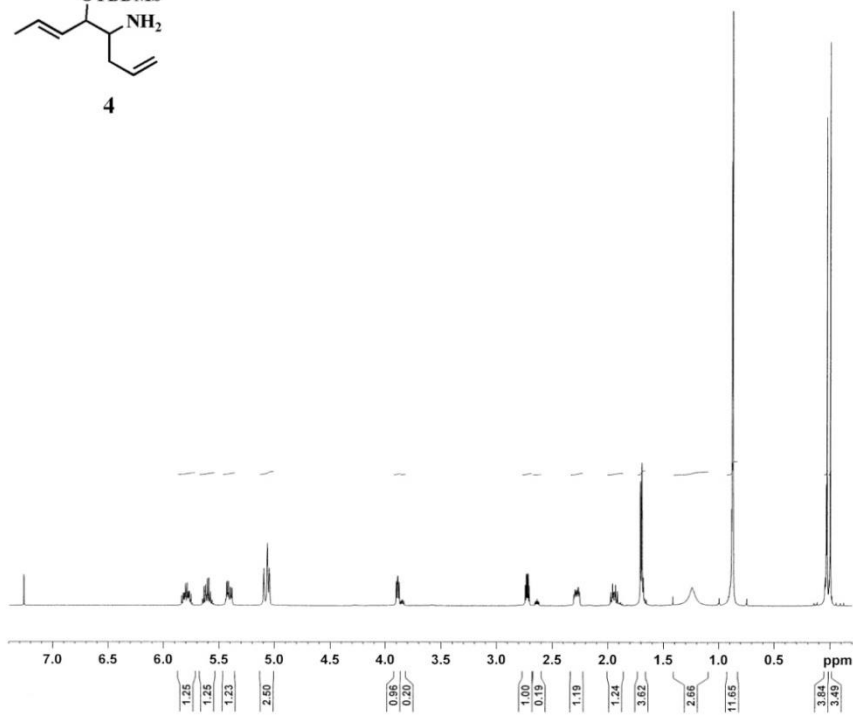
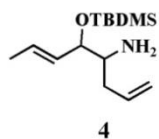
Supplementary data for article:

Tasic, G.; Maslak, V.; Husinec, S.; Todorovic, N.; Savic, V. Study of the Intramolecular Heck Reaction: Synthesis of the Bicyclic Core of Corialstonidine. *Tetrahedron Letters* **2015**, 56 (19), 2529–2532. <https://doi.org/10.1016/j.tetlet.2015.03.129>

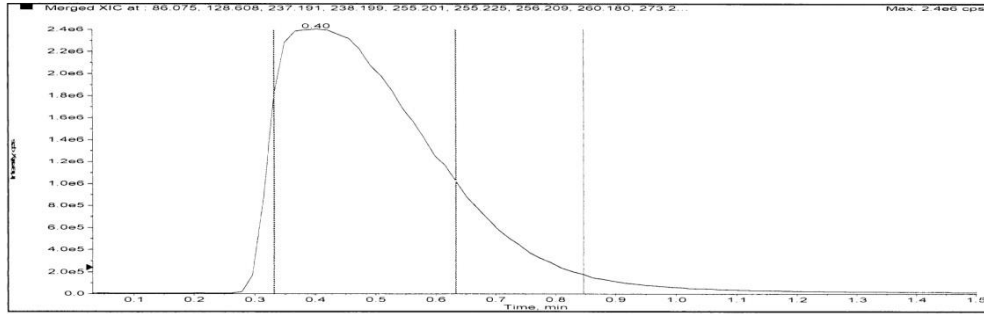
Study of the intramolecular Heck reaction: Synthesis of the Bicyclic Core of Corialstonidine

Gordana Tasic,^a Veselin Maslak,^b Suren Husinec,^c Nina Todorovic,^c Vladimir Savic*^a

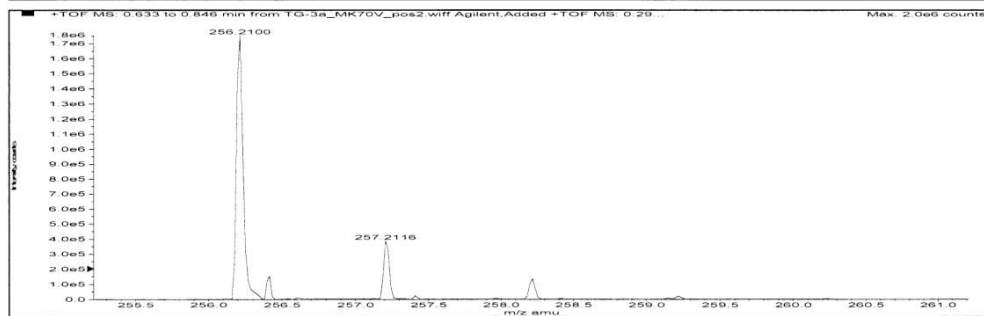
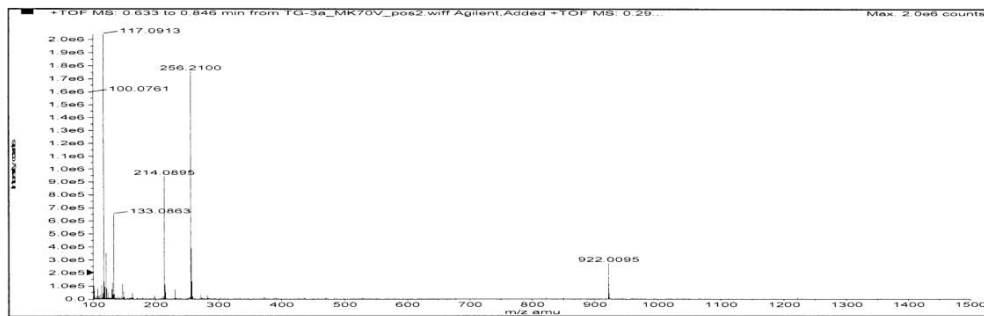
^a Department of Organic Chemistry, Faculty of Pharmacy, University of Belgrade, Vojvode Stepe 450, 11000 Belgrade, Serbia; ^b Faculty of Chemistry, University of Belgrade, Studentski trg 16, 11000 Belgrade, Serbia; ^c Institute for Chemistry, Technology and Metallurgy, P.O. Box 815, Njegoseva 12, 11000 Belgrade, Serbia



Sample Name: **TG-3a** Sample Location: **P1-D7** Sample Id: Operator: **Milka**
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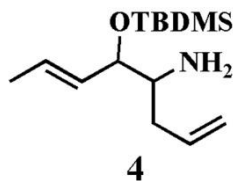


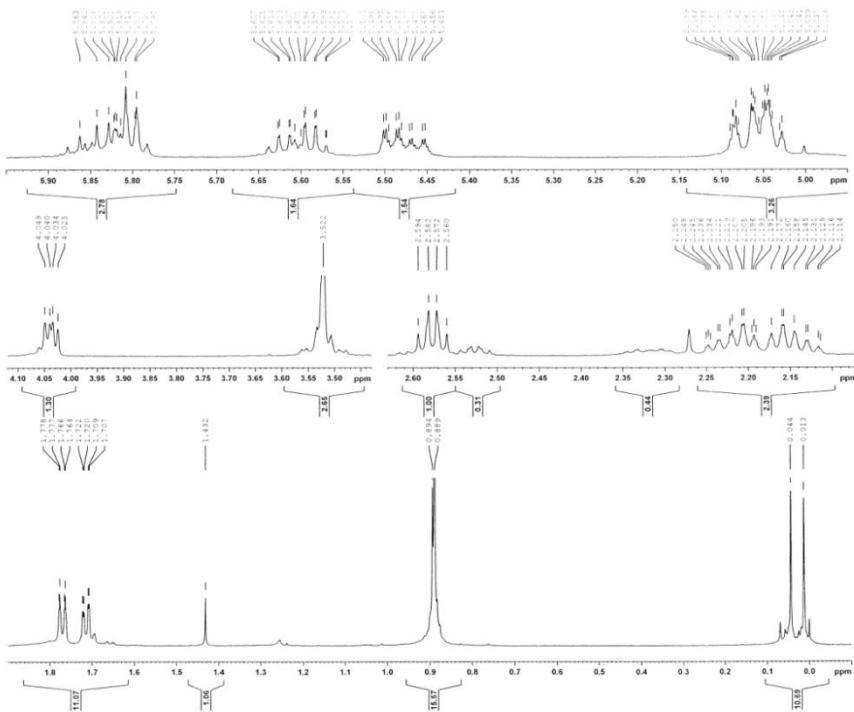
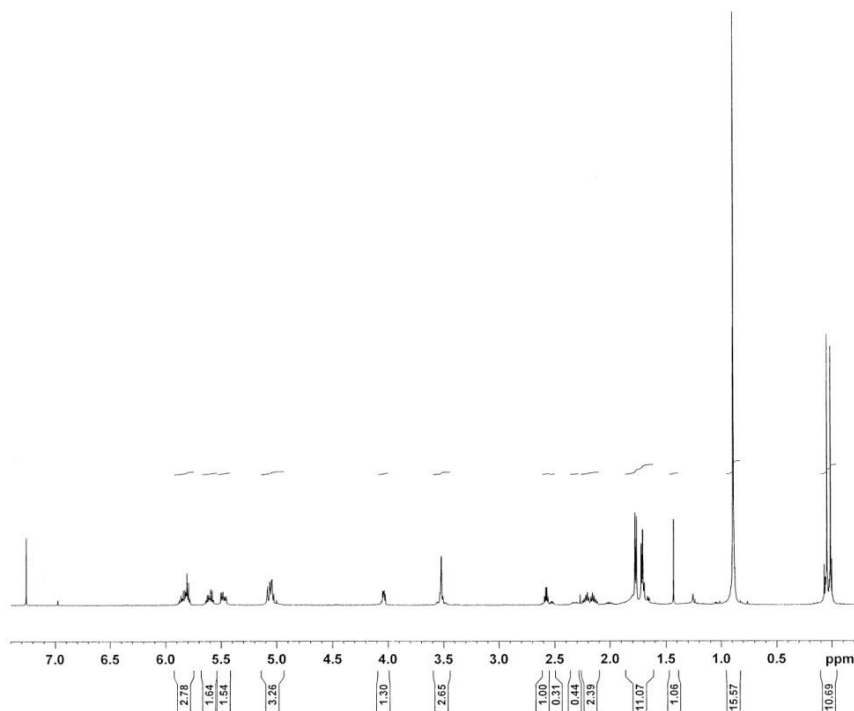
Merged XIC, Period# : 1 Experiment# : 1

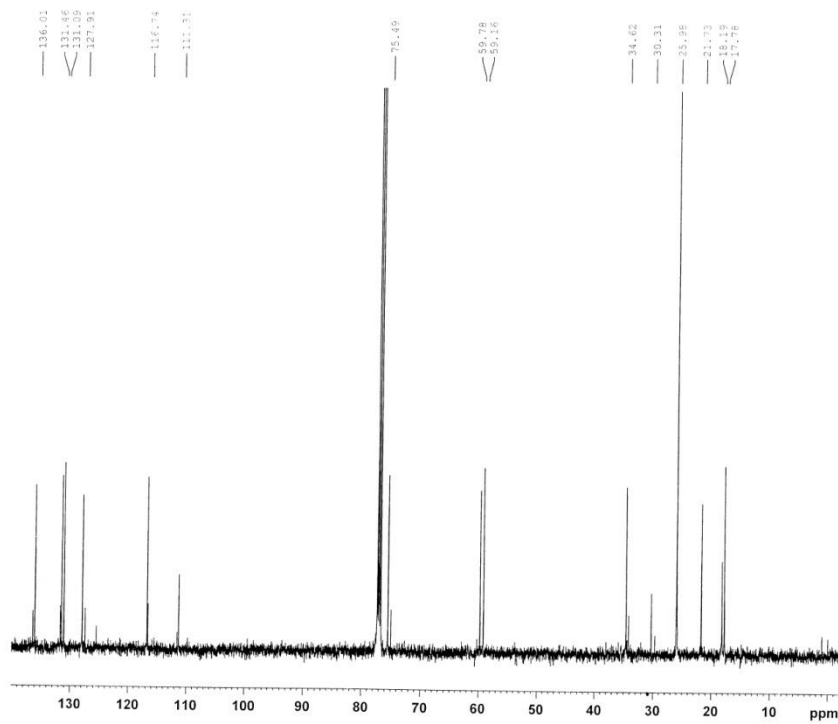


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C14H29NOSi	--	255.20184	0.40	4.36145 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	1778742.32	256.20912	256.20995	0.83685	3.27	--







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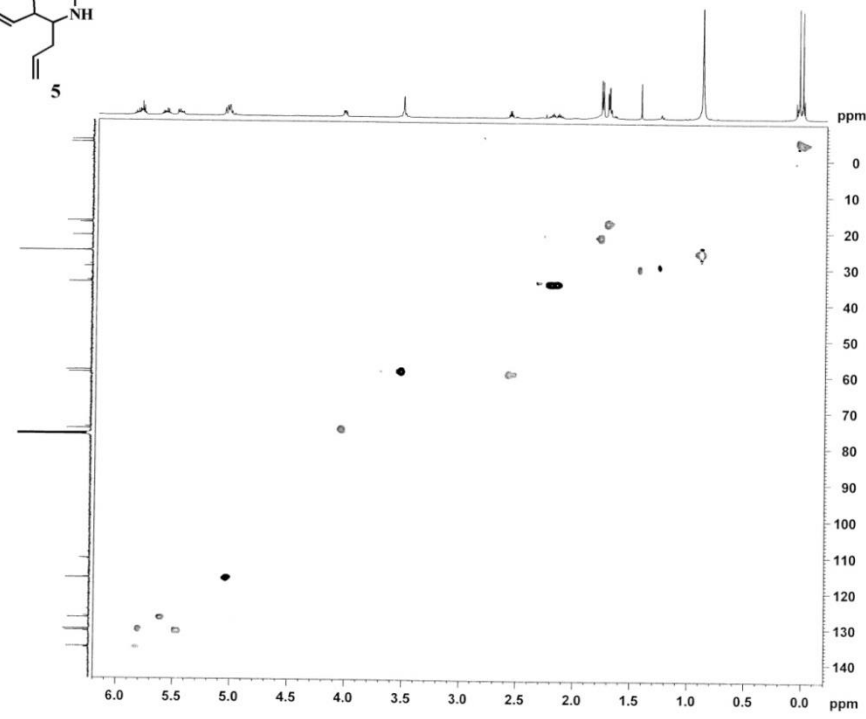
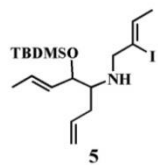
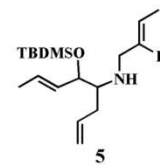
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EXPNO         2
PROCNO        1
Date_         20120203
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INSTRUM       spect
PROBHD        5 mm BBO BB-H
PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            404
DS            4
SNIH          29761.904 Hz
FIDRES        0.908261 Hz
AQ            0.5505524 sec
RG            1030
DW            16.800 usec
DE            6.50 usec
TE            298.0 K
D1            2.0000000 sec
D11           0.0300000 sec
TD0           1
  
```

```

===== CHANNEL f1 =====
NUC1          13C
P1            11.50 usec
PL1           3.00 dB
RG1W         32.2284892 W
SFO1         125.8030560 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2      waitz16
NUC2          1H
PCPD2        80.00 usec
PL2           1.20 dB
PL12         18.40 dB
PL13         18.40 dB
PL2W         20.76952171 W
PL12W        0.39575511 W
PL13W        0.39575511 W
SFO2         500.2618930 MHz
SI            32768
SF           125.7904803 MHz
WDW           EM
SSB           0
LB            1.50 Hz
GB            0
PC            1.40
  
```



```

NAME          TG-273
EXPNO         2
PROCNO        1
Date_         20120203
Time          11.24
INSTRUM       spect
PROBHD        5 mm BBO BB-H
PULPROG       zgpg30
TD            32768
SOLVENT       CDCl3
NS            404
DS            4
SNIH          29761.904 Hz
FIDRES        0.908261 Hz
AQ            0.5505524 sec
RG            1030
DW            16.800 usec
DE            6.50 usec
TE            298.0 K
D1            2.0000000 sec
D11           0.0300000 sec
TD0           1
  
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            9.35 usec
PL1           0.00 dB
PL1W         21.37956230 W
SFO1         500.2618930 MHz
  
```

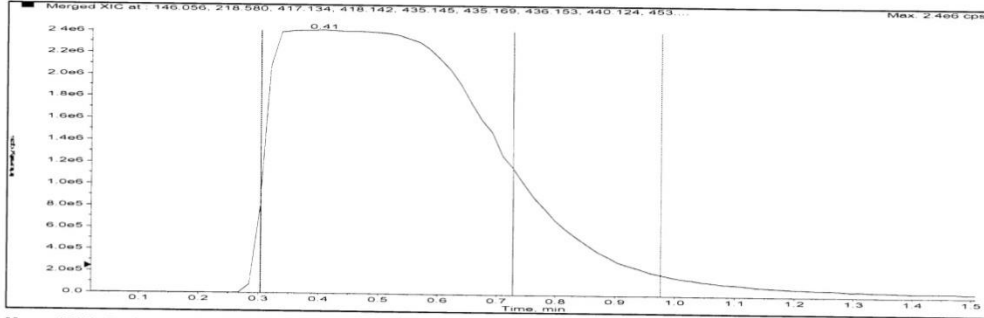
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===== CHANNEL f2 =====
CPDPRG2      waitz16
NUC2          13C
P2            11.50 usec
PL2           3.00 dB
PL2W         32.2284892 W
SFO2         125.7904803 MHz
  
```

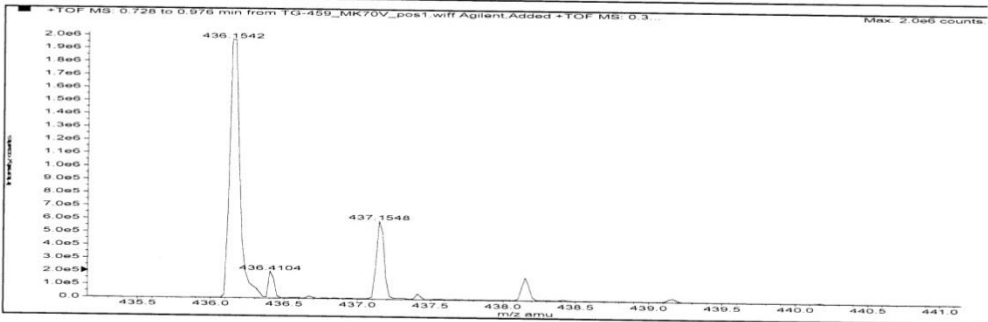
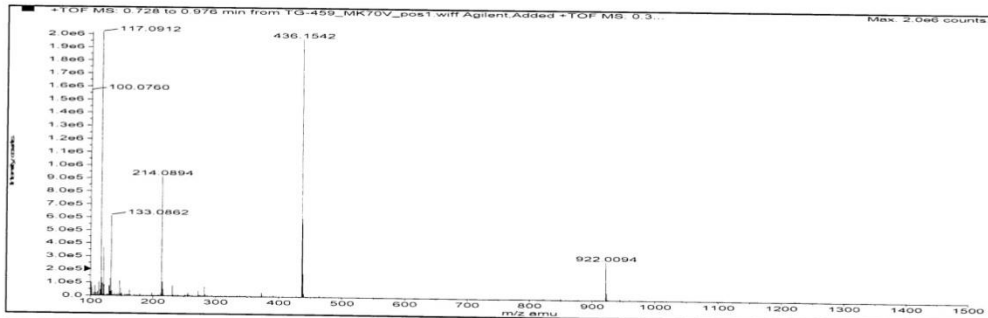
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===== GRADIENT CHANNEL =====
OPRM1        SINE.100
OPRM2        SINE.100
OPRM3        SINE.100
GR1          20.00 u
GR2          80.00 u
GR3          20.10 u
FID          1900.00 usec
RG           2
TD           128
SFO          125.7907 MHz
FIDRES       167.076340 Hz
PR           170.000 PPM
FWDGSE       States-TPPI
SI            1024
SF           900.2603114 MHz
WDW           USINE
SSB           0
LB            0.00 Hz
GB            0
PC            1.40
PC1          1024
PC2          States-TPPI
SF           125.7904822 MHz
WDW           USINE
SSB           0
LB            0.00 Hz
GB            0
  
```

Sample Name: TG-459 Sample Location: P1-D8 Sample Id: Operator: Milka
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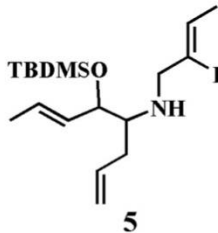


Merged XIC, Period# : 1 Experiment# : 1

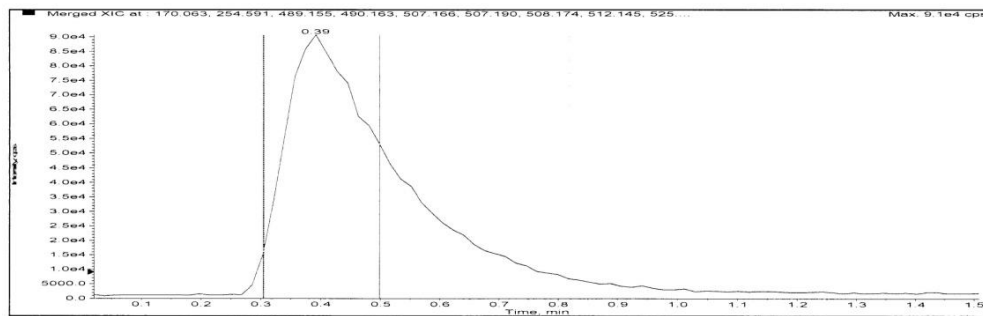


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C ₁₈ H ₃₄ INO ₂	--	435.14543	0.41	6.19840 E7	--

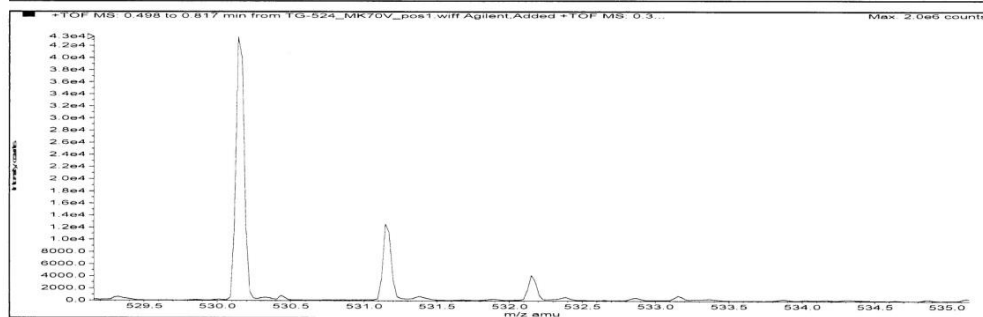
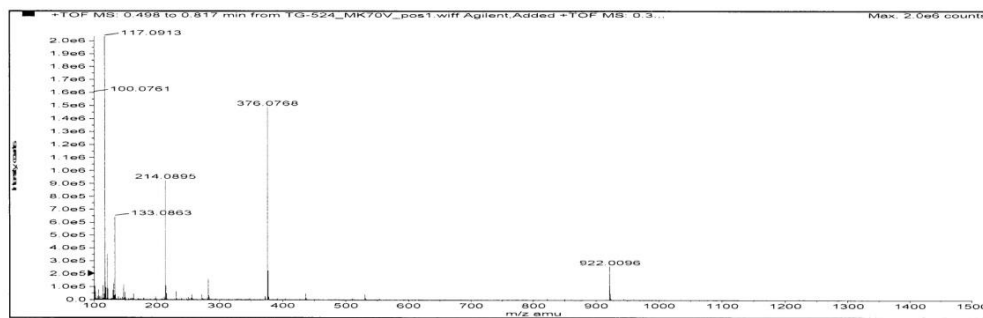
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	2129759.52	436.15271	436.15419	1.47850	3.39	--



Sample Name: TG-524 Sample Location: P1-D9 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Farmaceutski fakultet\Data\TG-524_MK70V_pos1.wiff Acq Time: February 10 2014, 01:04:33
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 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anm\efc.xml

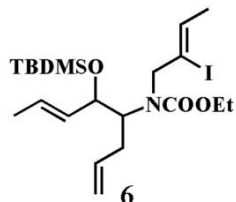


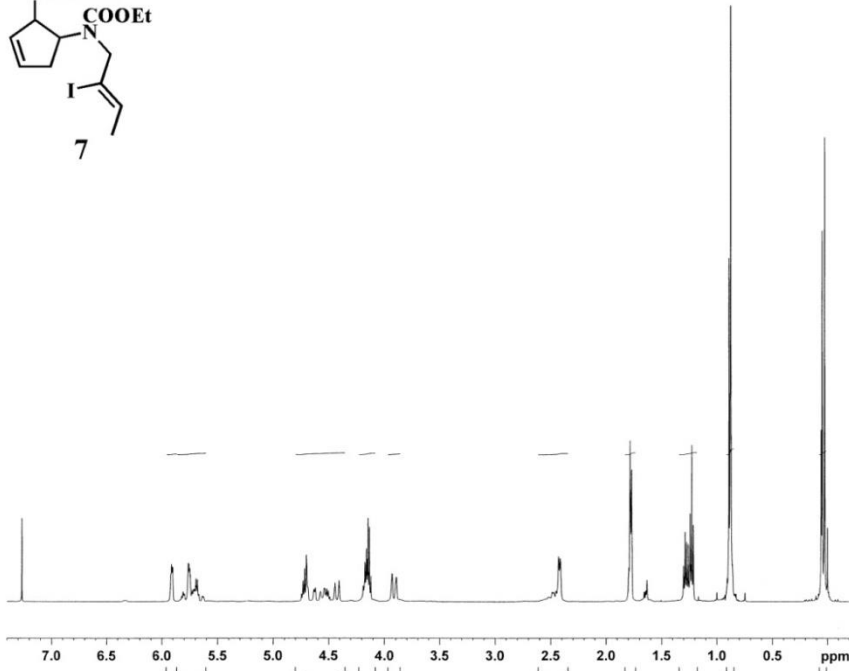
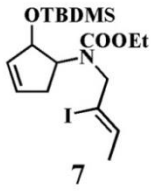
Merged XIC, Period# : 1 Experiment# : 1



Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C21H38NO3Si	--	507.16656	0.39	1.19875 E6	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+Na] ⁺	46265.37	530.15578	530.15521	-0.57050	-1.08	--



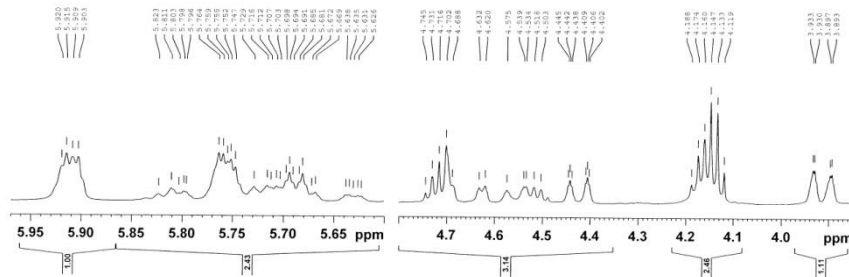


Current Data Parameters
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EXPRO 1
PROCNO 1

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PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 4537.205 Hz
FIDRES 0.138465 Hz
AQ 3.6110337 sec
RG 101
DW 110.200 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
TDO 1

***** CHANNEL f1 *****
SF01 500.2617832 MHz
NUC1 1H
P1 9.35 usec
PLW1 27.37999916 W

F2 - Processing parameters
SI 32768
SF 500.2600118 MHz
WDW EM
SSB 0
LB 0 0.20 Hz
GB 0
PC 1.00

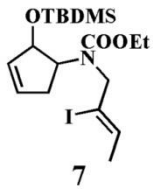
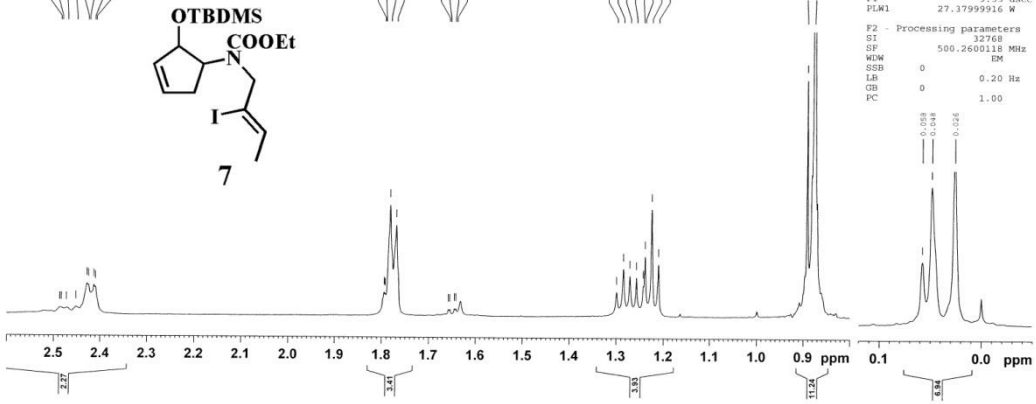


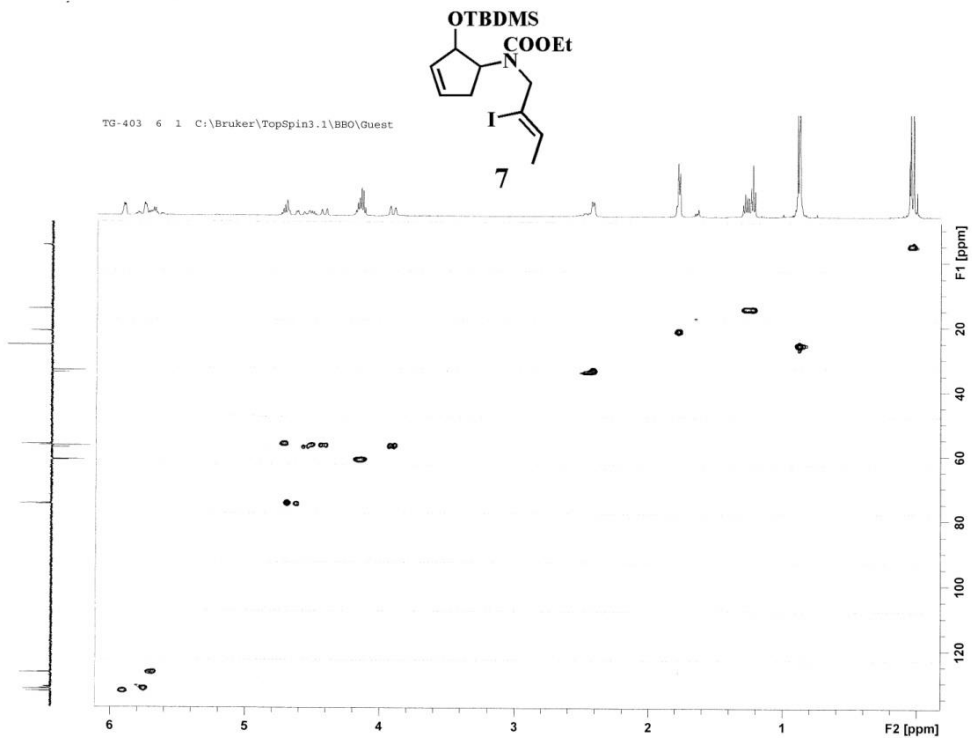
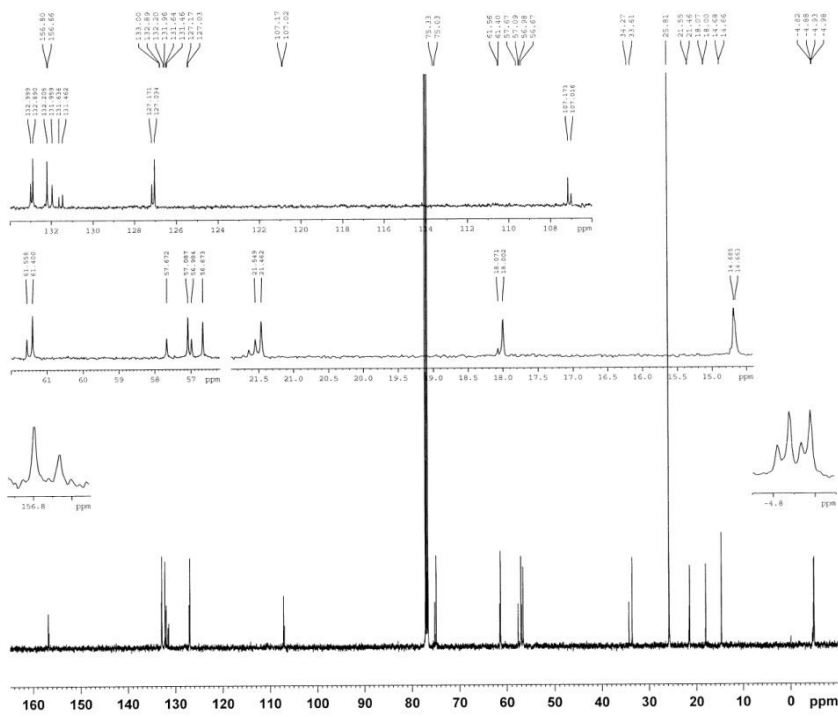
Current Data Parameters
NAME TG-403
EXPRO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130218
Time 10:57
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 4537.205 Hz
FIDRES 0.138465 Hz
AQ 3.6110337 sec
RG 101
DW 110.200 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
TDO 1

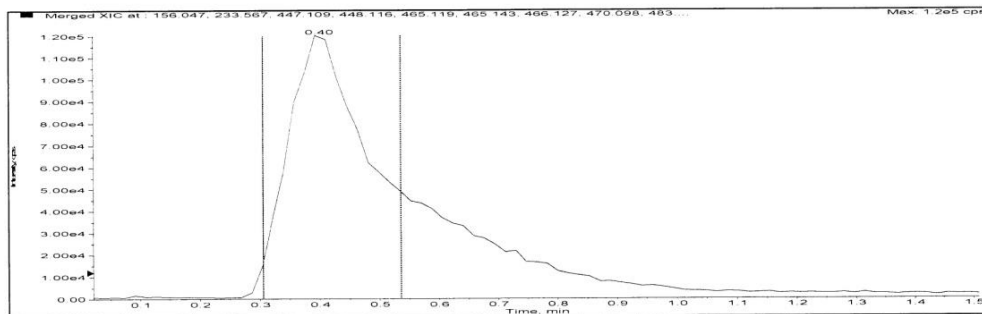
***** CHANNEL f1 *****
SF01 500.2617832 MHz
NUC1 1H
P1 9.35 usec
PLW1 27.37999916 W

F2 - Processing parameters
SI 32768
SF 500.2600118 MHz
WDW EM
SSB 0
LB 0 0.20 Hz
GB 0
PC 1.00

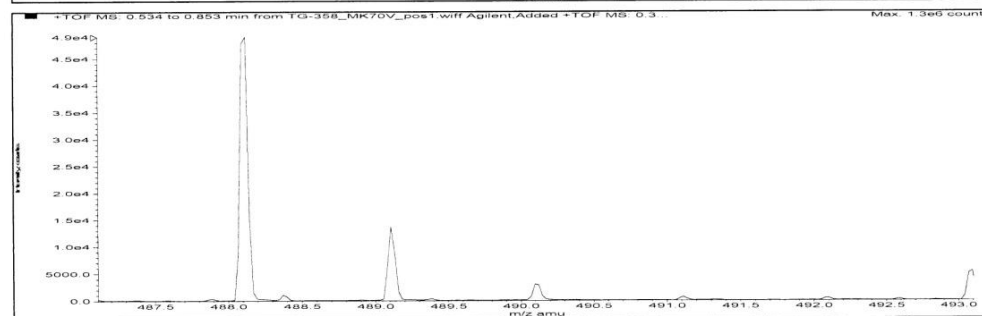
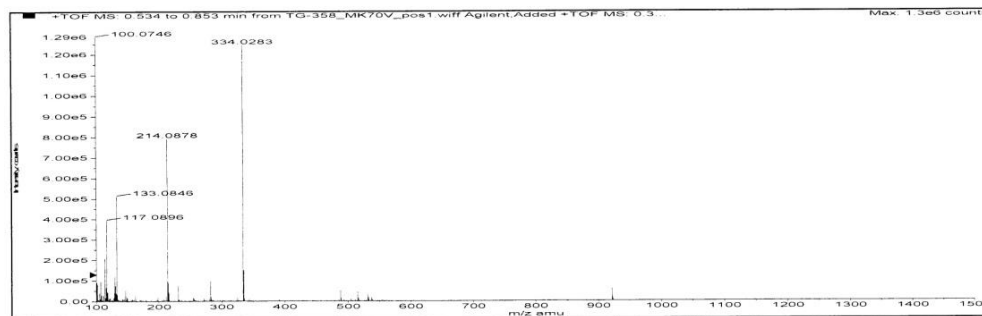




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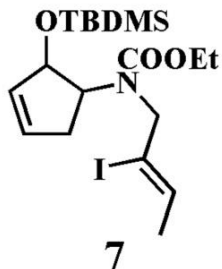


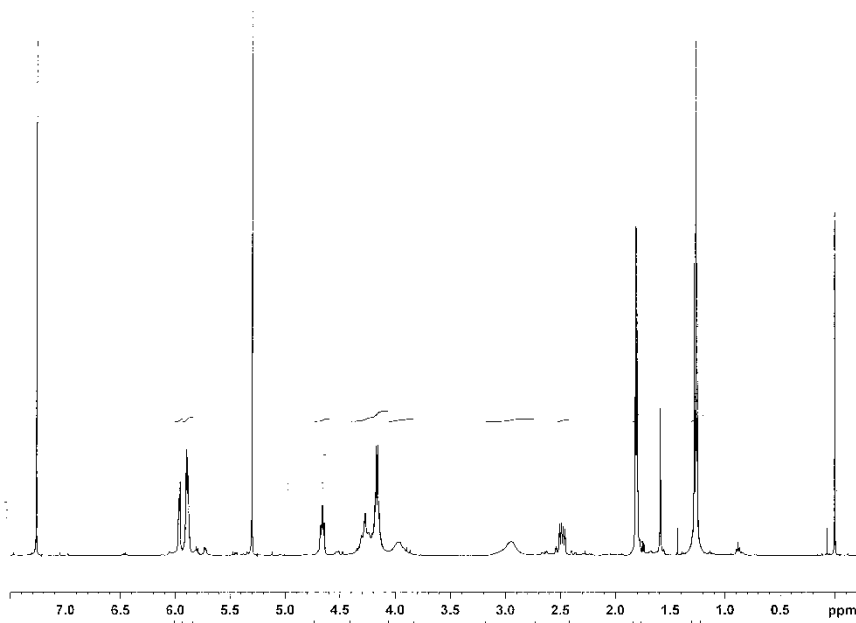
Merged XIC, Period# : 1 Experiment# : 1



Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C18H32INO3Si	--	465.11961	0.40	1.58321 E6	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+Na] ⁺	52806.44	488.10883	488.10699	-1.84894	-3.79	--

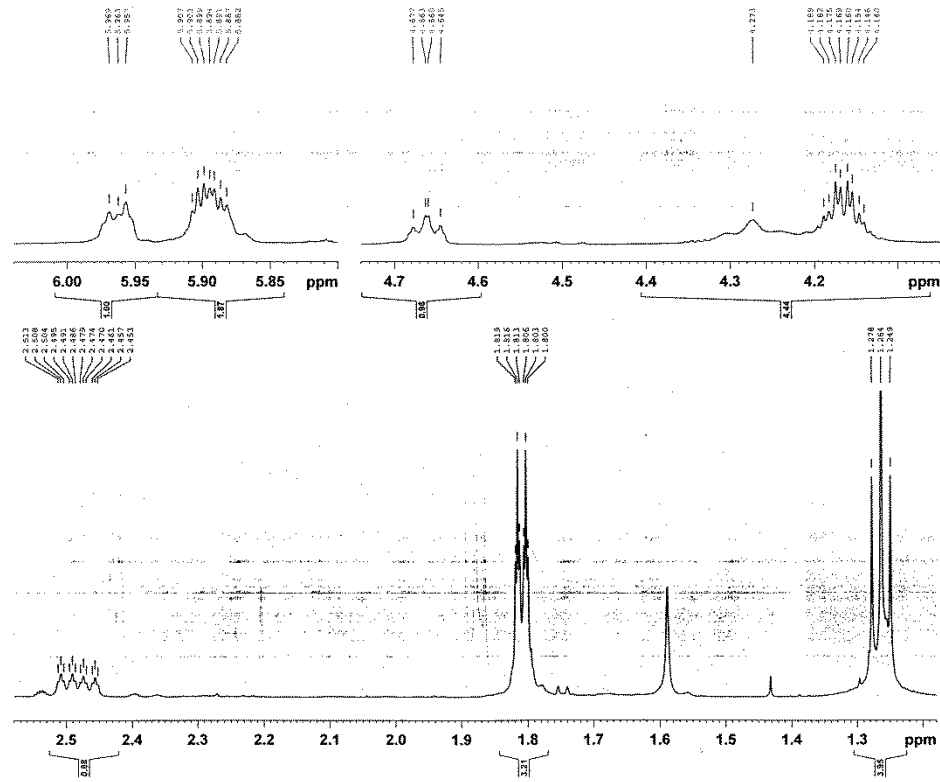
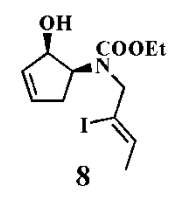




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PULPROG zgpg30
TD 22768
SOLVENT CDCl3
NS 32
DS 0
SWH 4746.835 Hz
FIDRES 0.144852 Hz
AQ 3.4515626 sec
RG 322
DM 105.113 usec
DE 6.50 usec
TE 298.0 K
D1 2.0000000 sec
TD0 1
----- CHANNEL f1 -----
SFO1 500.2617627 MHz
NUC1 1H
P1 9.35 usec
PL1 27.37999916 W
F2 - Processing parameters
SI 32768
SP 500.260133 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00

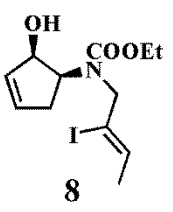
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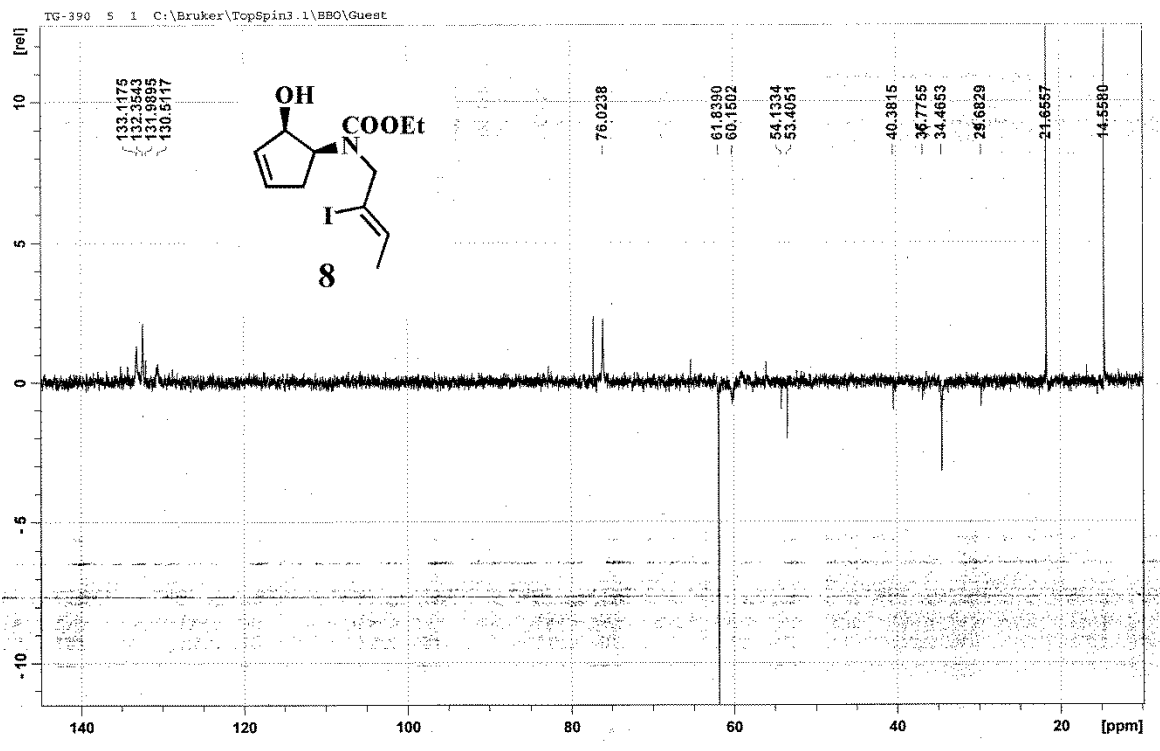
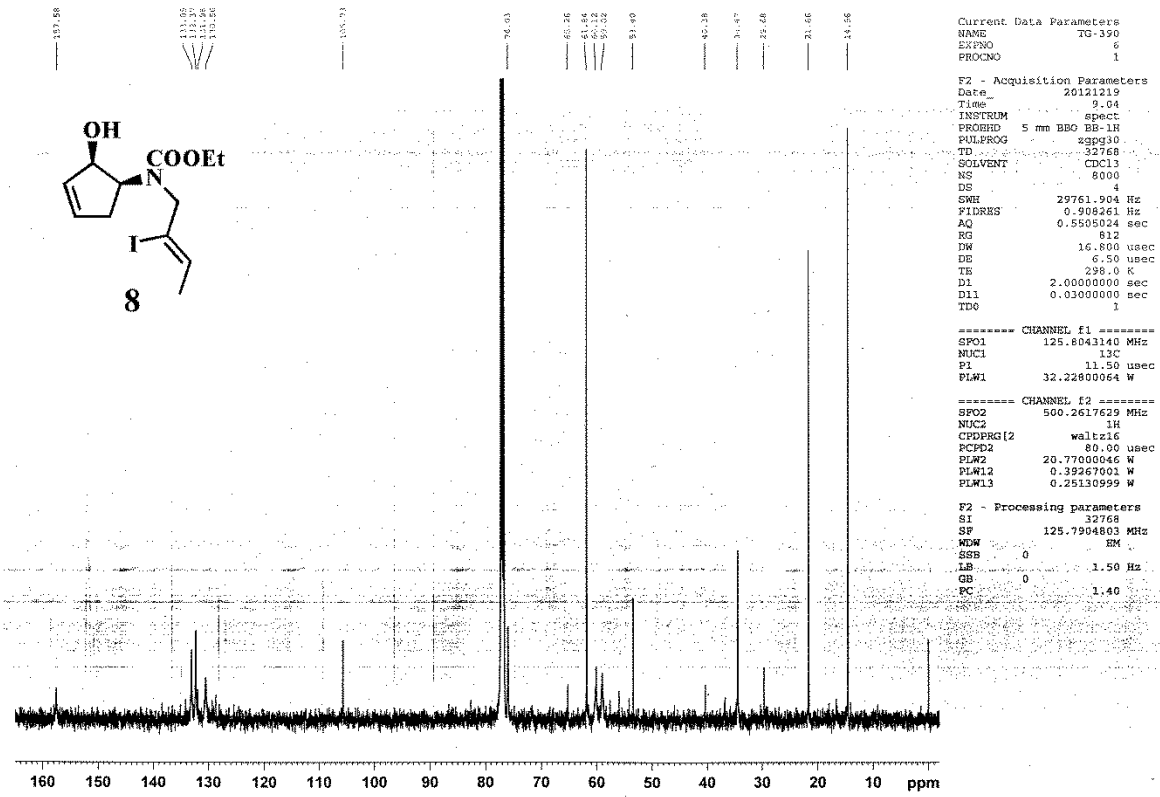


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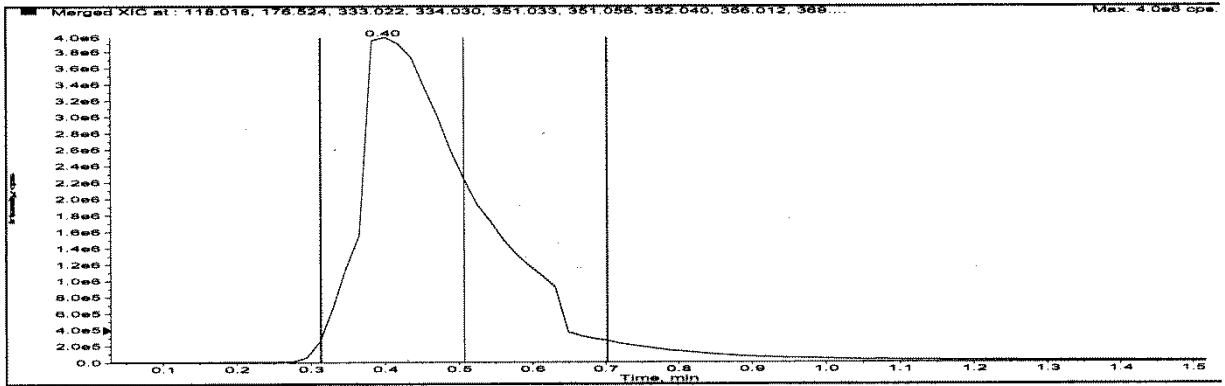
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EXPNO 1
PROCNO 1
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Time 16:05
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 22768
SOLVENT CDCl3
NS 32
DS 0
SWH 4746.835 Hz
FIDRES 0.144852 Hz
AQ 3.4515626 sec
RG 322
DM 105.113 usec
DE 6.50 usec
TE 298.0 K
D1 2.0000000 sec
TD0 1
----- CHANNEL f1 -----
SFO1 500.2617627 MHz
NUC1 1H
P1 9.35 usec
PL1 27.37999916 W
F2 - Processing parameters
SI 32768
SP 500.260133 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00

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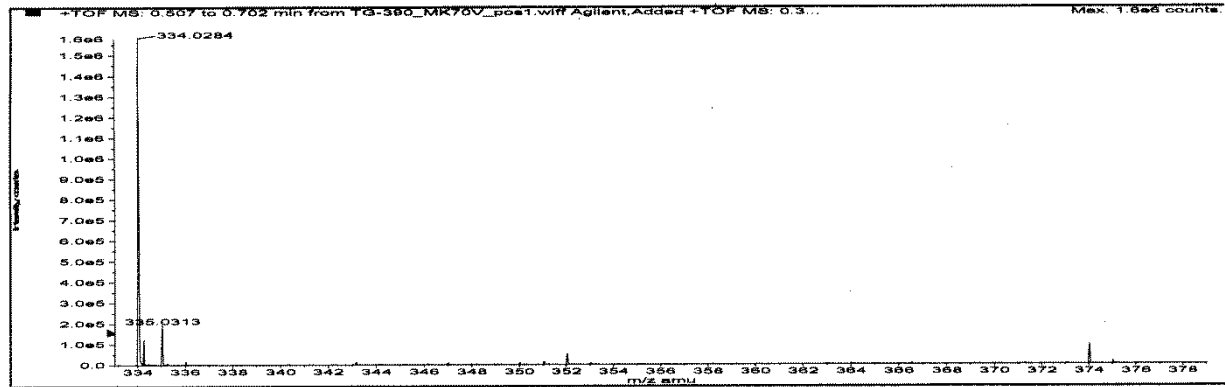
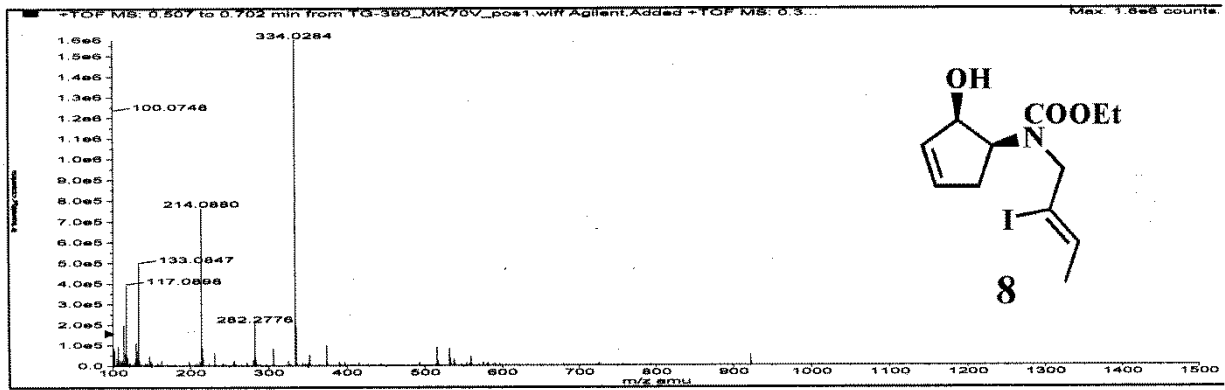




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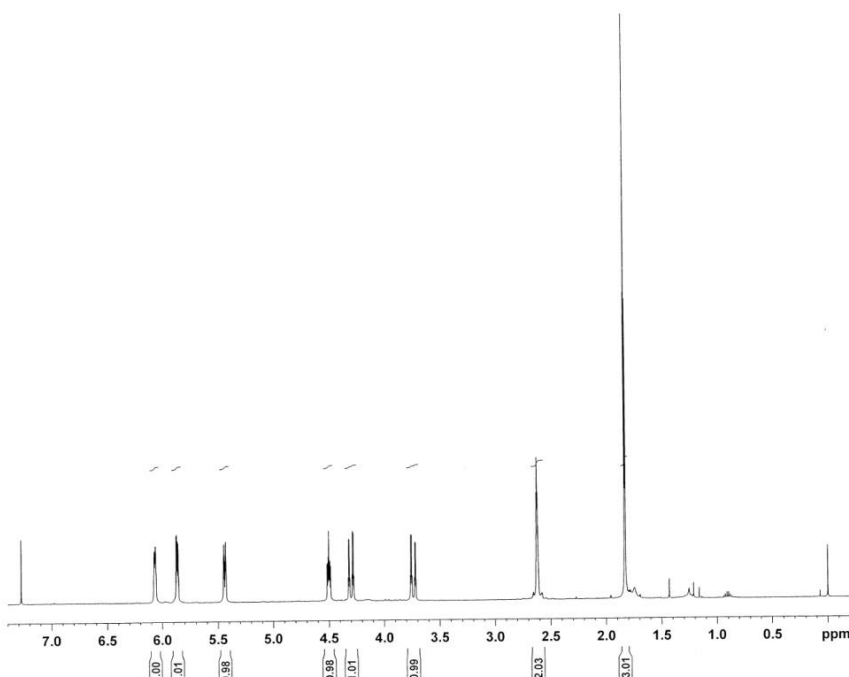


Merged XIC, Period# : 1 Experiment# : 1



Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C ₁₂ H ₁₈ INO ₃	--	351.03314	0.40	4.45853 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H-H ₂ O] ⁺	1583519.18	334.02985	334.02840	-1.44983	-4.34	--
[M+H] ⁺	52715.24	352.04041	352.03920	-1.21567	-3.45	--
[M+Na] ⁺	97745.63	374.02236	374.02062	-1.74007	-4.65	--

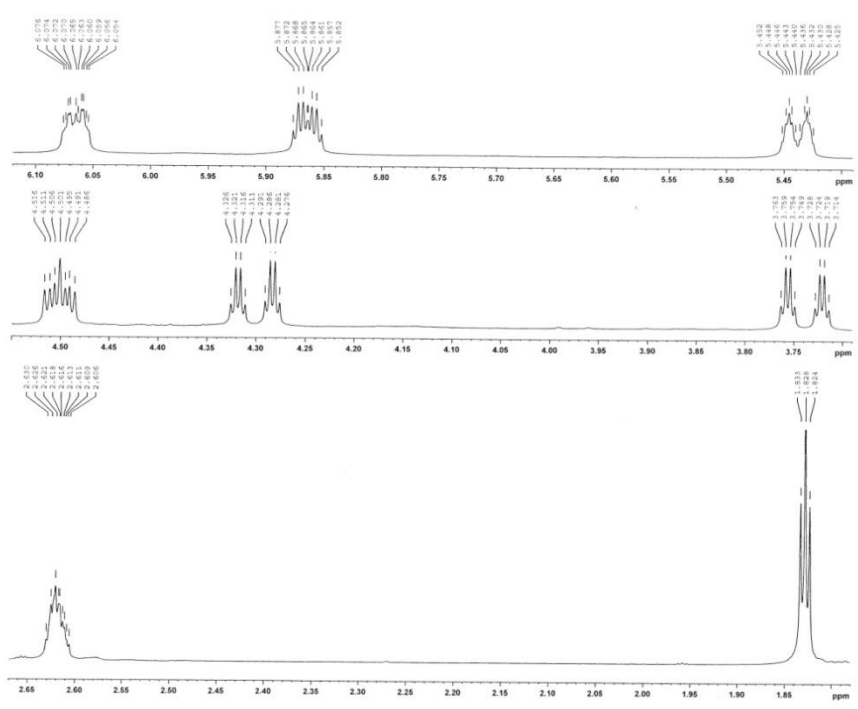
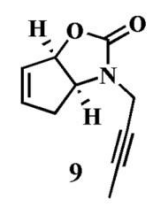


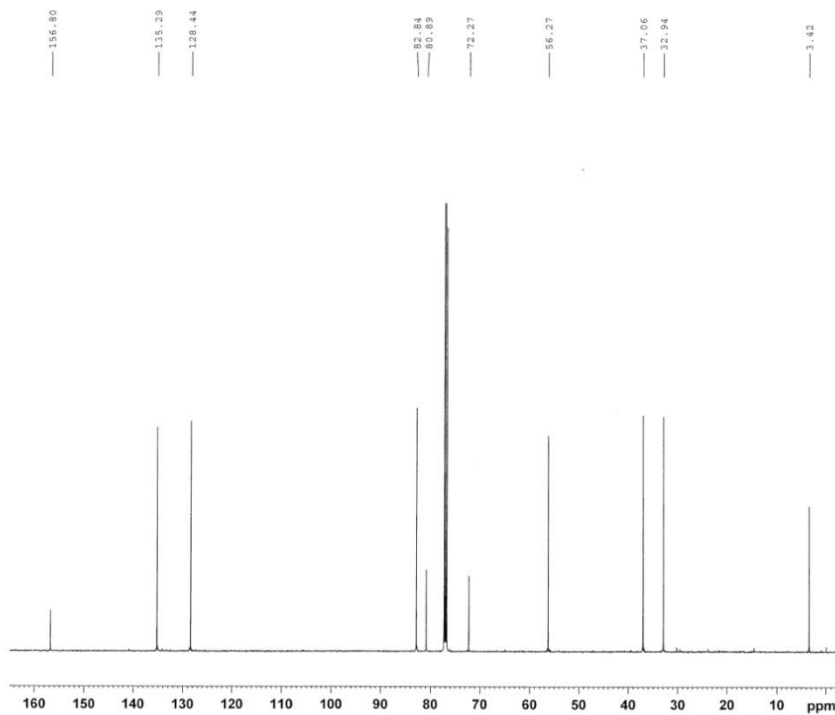
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 PROCNO 1

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 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 4480.287 Hz
 FIDRES 0.136727 Hz
 AQ 3.6569088 sec
 RG 181
 DW 111.600 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.0000000 sec
 TDO 1

----- CHANNEL f1 -----
 SF01 500.2619987 MHz
 NUC1 1H
 P1 9.35 usec
 PLM1 27.37999916 W

F2 - Processing parameters
 SI 32768
 SF 500.2600059 MHz
 WDW RM
 SSB 0
 LB 0 0.20 Hz
 GB 0
 PC 1.00





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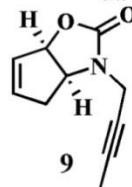
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EXPNO    6
PROCNO   1

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INSTRUM  spect
PROBHD   5 mm BBO BB-1H
PULPROG  zgpg30
TD       32768
SOLVENT  CDCl3
NS       6400
DS       4
SWH      29761.904 Hz
FIDRES   0.908261 Hz
AQ       0.5505024 sec
RG       1030
DM       16.800 usec
DE       6.50 usec
TE       298.0 K
D1       2.00000000 sec
D11      0.03000000 sec
TDO      1

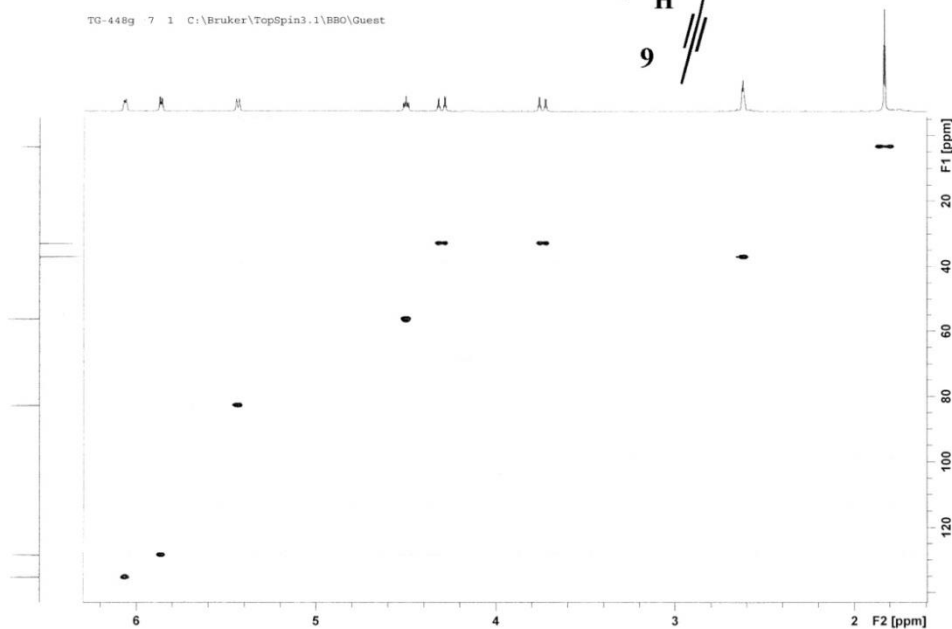
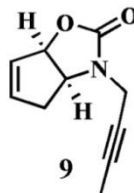
----- CHANNEL f1 -----
SFO1    125.8043140 MHz
NUC1    13C
P1      11.50 usec
PLW1    32.22800064 W

----- CHANNEL f2 -----
SFO2    500.2619985 MHz
NUC2    1H
CPDPRG2 waltz16
PCPD2   80.00 usec
PLW2    20.77000066 W
PLW12   0.39267001 W
PLW13   0.25130999 W

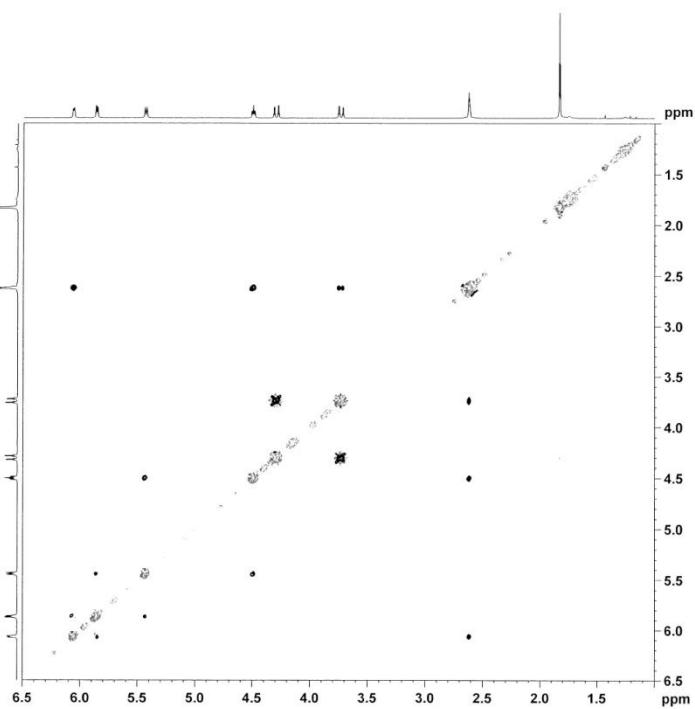
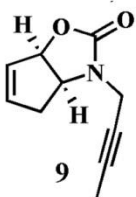
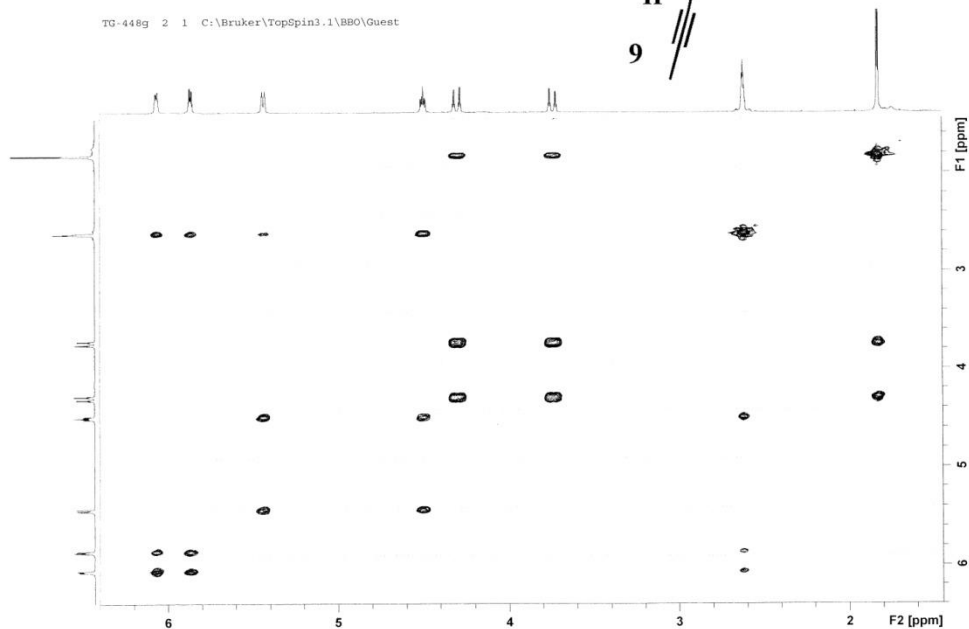
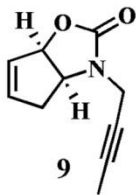
F2 - Processing parameters
SI      32768
SF      125.7904838 MHz
WDW     EM
SSB     0
LB      1.50 Hz
GB      0
PC      1.40
  
```



TG-448g 7 1 C:\Bruker\TopSpin3.1\BBO\Quest



TG-448g 2 1 C:\Bruker\TopSpin3.1\BBO\Guest



```

Current Data Parameters
NAME      TG-448g
EXPROG   1
PROCNO    1

F2 - Acquisition Parameters
Date_     20130625
Time      17.47
INSTRUM   spect
PROBHD    5 mm BBO BH-1H
PULPROG   noesypph
TD         3274
SOLVENT   CDCl3
NS         16
DS         16
SWH        4480.287 Hz
FIDRES    4.375280 Hz
AQ         0.1142784 sec
RG         383
DM         111.600 usec
DE         6.50 usec
TE         298.0 K
DQ         0.0000970 sec
D1         2.0000000 sec
d8         1.0000000 sec
D16        0.0000000 sec
RG         0.00022320 sec
INO        0.00022320 sec

===== CHANNEL f1 =====
SFO1      500.2619945 MHz
NUC1      1H
P1         9.15 usec
P2         18.70 usec
PLM1      27.37999916 W

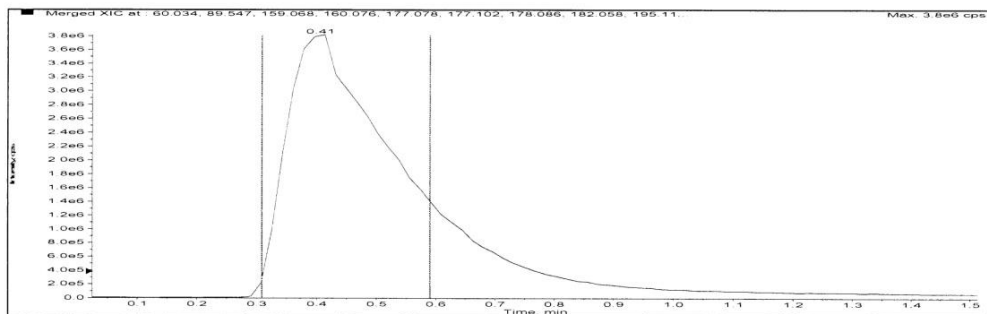
===== GRADIENT CHANNEL =====
GMRM111   SINE:100
CP21      40.00 %
P16        1000.00 usec

F1 - Acquisition parameters
TD         206
SFO1      500.262 MHz
FIDRES    17.501320 Hz
SW         8.956 ppm
FAPCQCE   States-TPP2

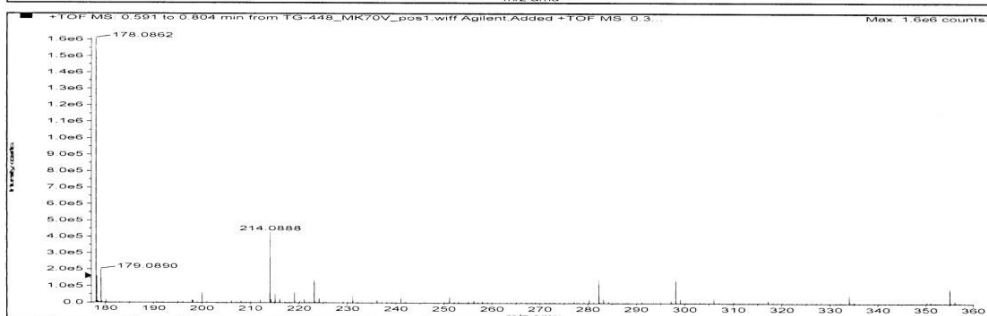
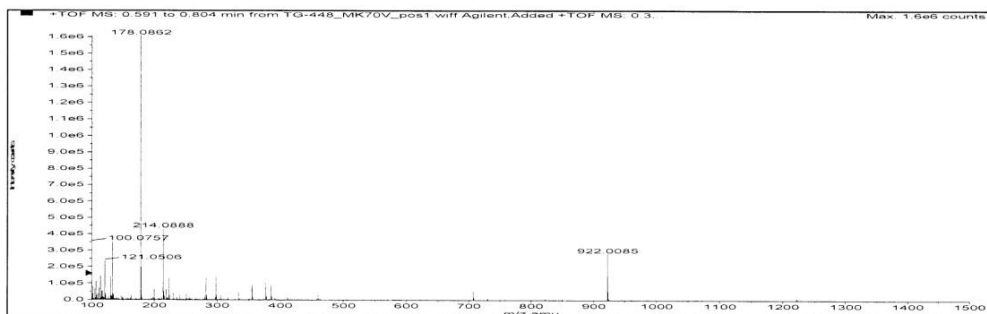
F2 - Processing parameters
SI         312
SF         500.260032 MHz
WDW        COSYB
SSB         2
LB         0 Hz
GB         0
PC         1.00

F1 - Processing parameters
SI         312
SF         500.260032 MHz
WDW        COSYB
SSB         2
LB         0 Hz
GB         0
  
```

Sample Name: TG-448 Sample Location: P1-C5 Sample Id: Operator: Goca
 Data File Name: D:\PE_Sciex_Data\Projects\Farmaceutski fakultet\Data\TG-448_MK70V_pos1.wiff Acq Time: January 31 2014, 03:43:19 PM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.an\lefc.xml

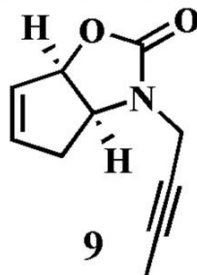


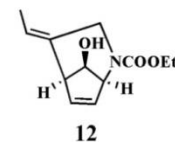
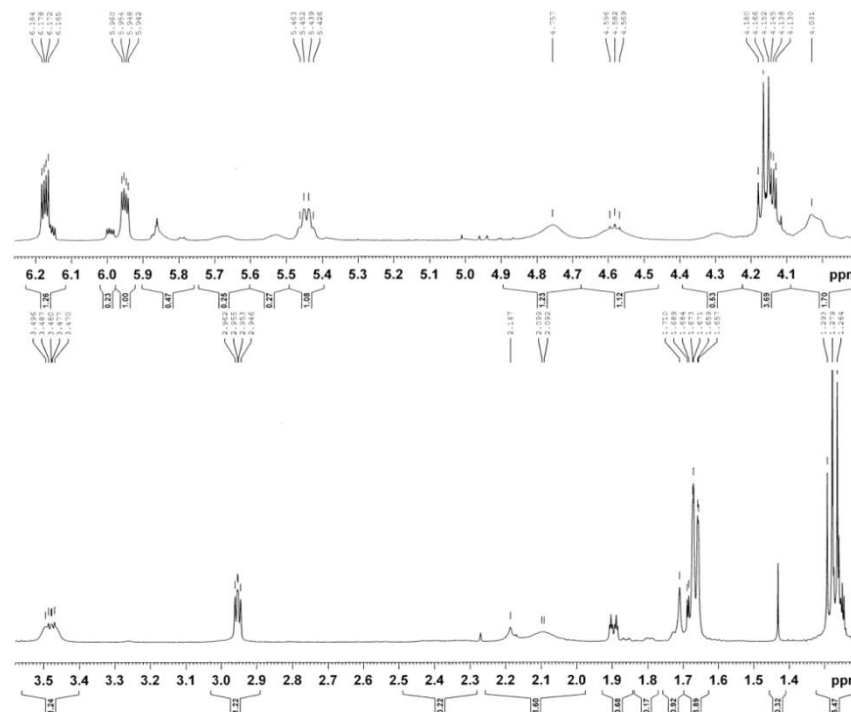
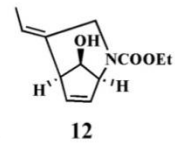
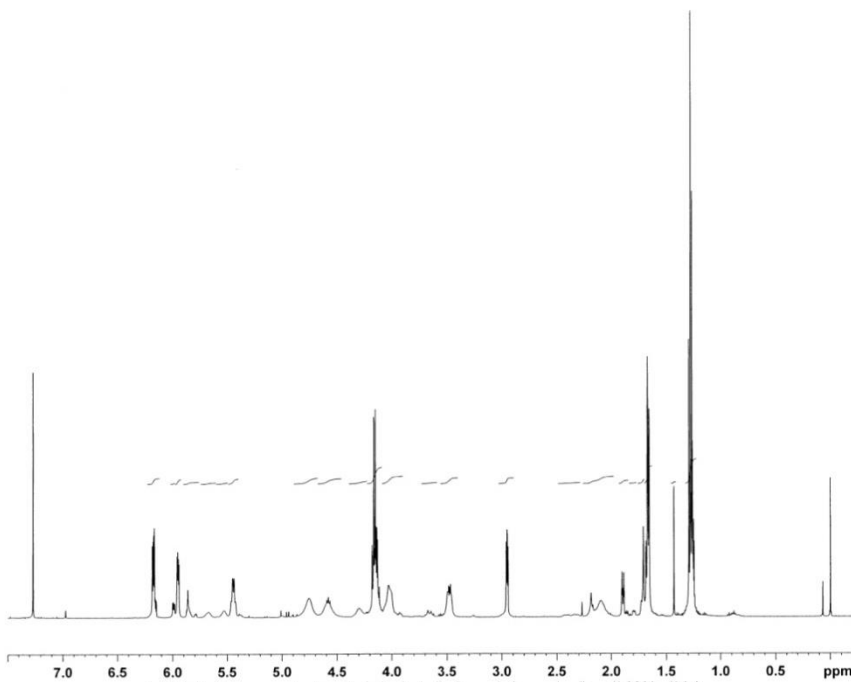
Merged XIC, Period#: 1 Experiment#: 1

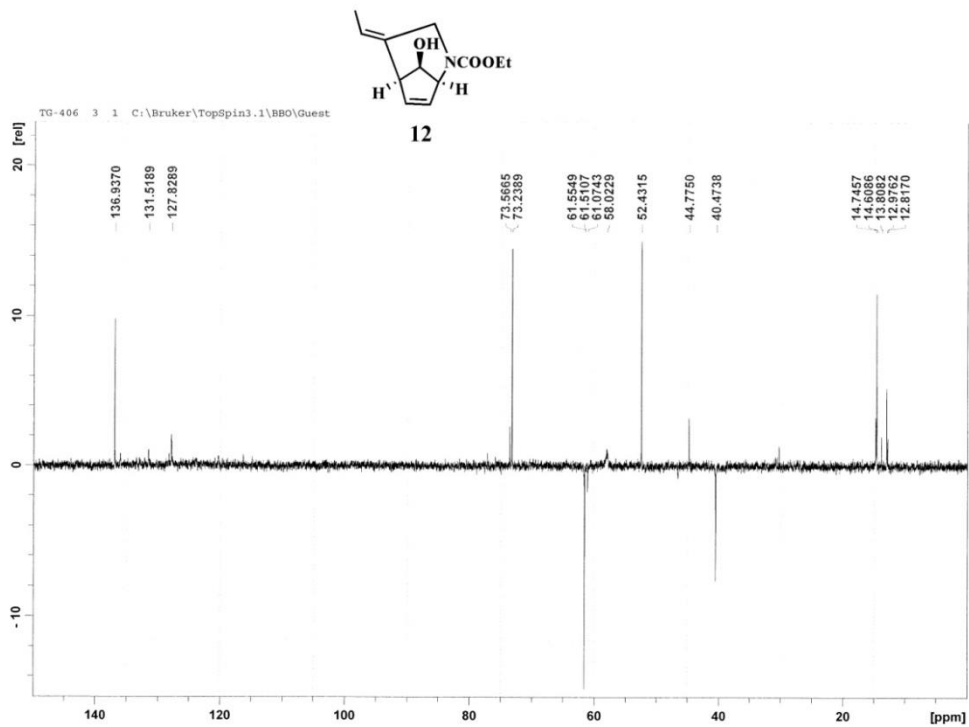
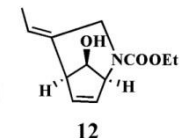
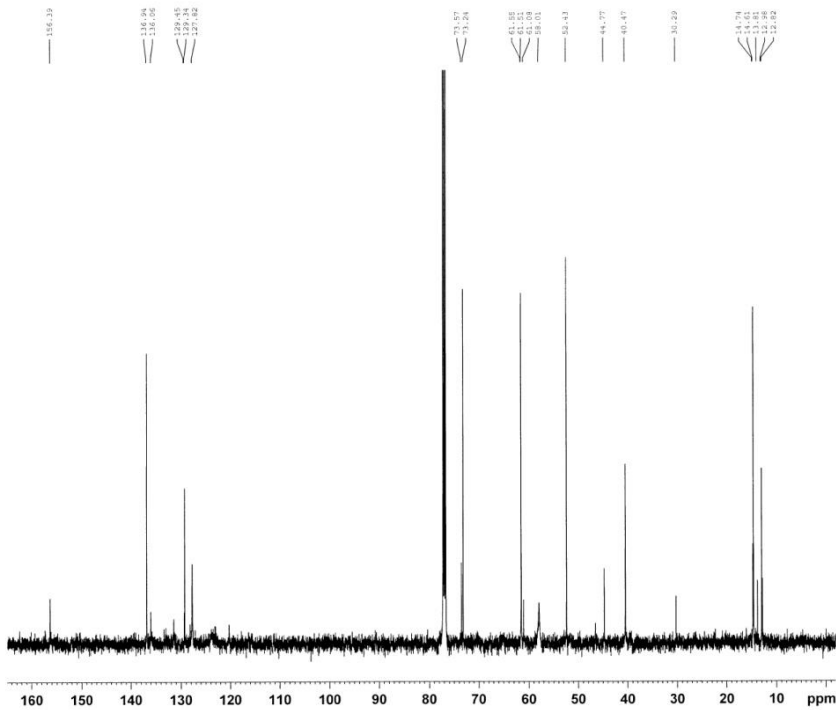


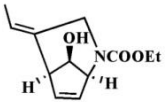
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C10H11NO2	--	177.07898	0.41	5.16923 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	1695105.42	178.08626	178.08623	-0.02215	-0.12	--
[M+Na] ⁺	66711.97	200.06820	200.06751	-0.69036	-3.45	--
[2M+H] ⁺	93907.83	355.16523	355.16453	-0.70577	-1.99	--



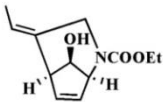
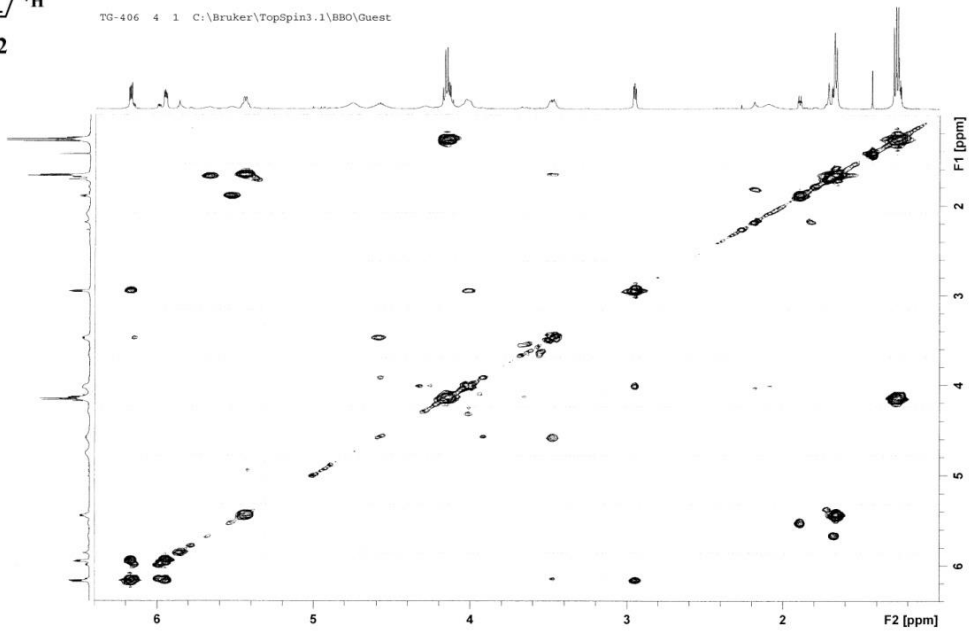




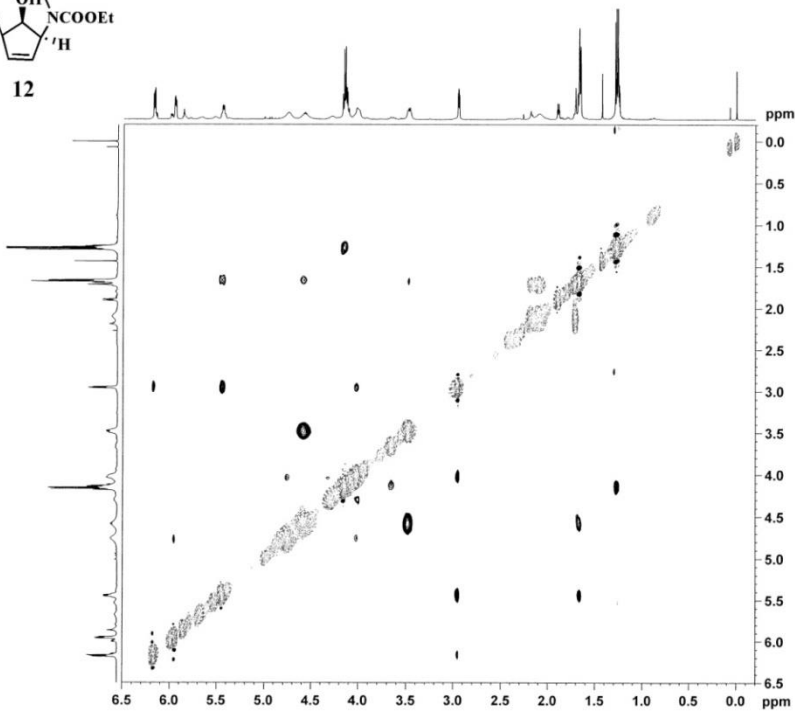


12

TG-406 4 1 C:\Bruker\TopSpin3.1\BBO\Guest



12



```

Current Data Parameters
NAME      TG-406
EXPRO    5
PROCNO   1

F2 - Acquisition Parameters
Date_    2010221
Time     13.18
INSTRUM  spect
PROBHD   5 mm BBO BB-1H
PULPROG  noesygphg
TD       1024
SOLVENT  CDCl3
NS       8
DS       16
SWH      5165.289 Hz
FIDRES   5.044228 Hz
AQ       0.0991212 sec
RG       181
DM       96.800 usec
DE       6.50 usec
TE       298.0 K
DQ       0.0000490 sec
D1       2.0000000 sec
dS1      1.0000000 sec
D16      0.0002000 sec
RG1      0.00019360 sec

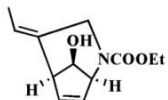
----- CHANNEL f1 -----
SFO1     500.261663 MHz
NUC1     1H
P1       9.35 usec
P2       16.70 usec
PLM1     27.3799916 W

----- GRADIENT CHANNEL -----
GMRM111  8196.100
GFZ1     40.00 k
F16      1500.00 usec

F1 - Acquisition parameters
TD       80
SFO1     500.2616 MHz
FIDRES   64.564116 Hz
SWH      10.125 ppm
PULPROG  States-TPPI

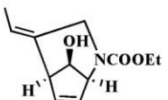
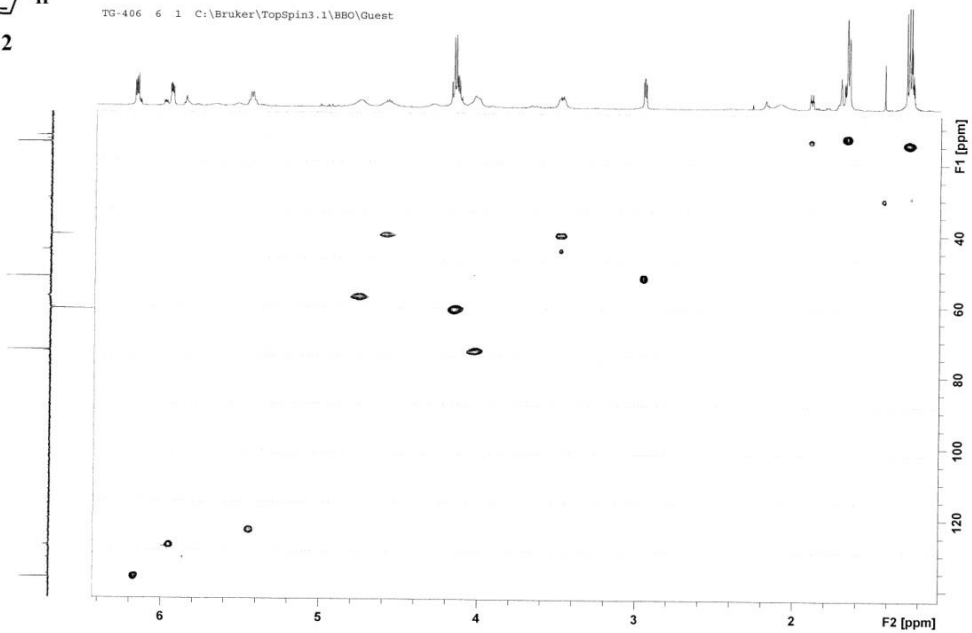
F2 - Processing parameters
SI       512
SF       500.2600036 MHz
WDW      QFINE
SSB      2
LA       0 Hz
GB       0
PC       1.00

F1 - Processing parameters
SI       512
MC2     States-TPPI
SF       500.2600037 MHz
WDW      QFINE
SSB      2
LA       0 Hz
GB       0
  
```

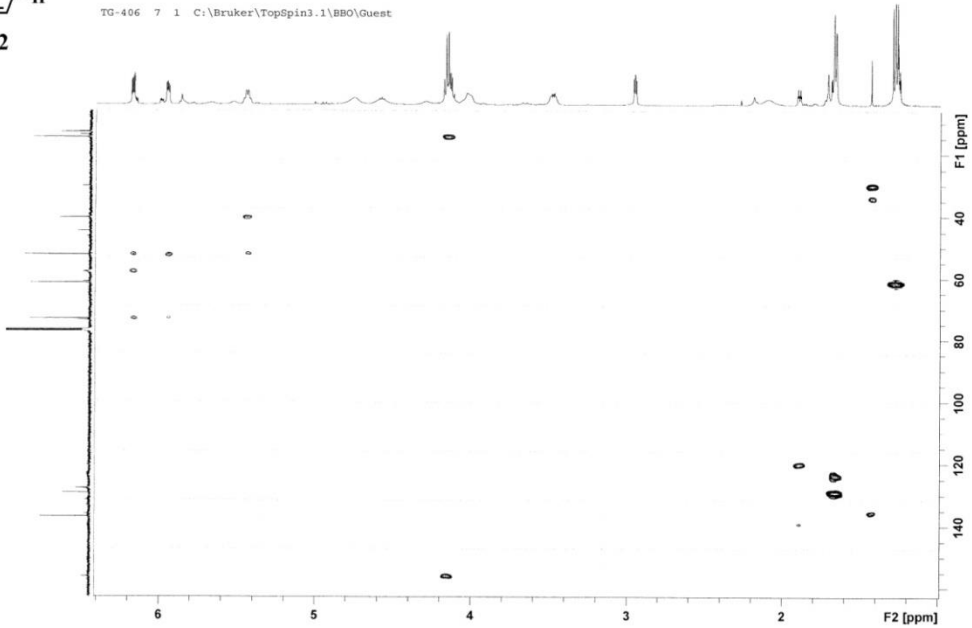
12

TC-406 6 1 C:\Bruker\TopSpin3.1\BBO\Guest

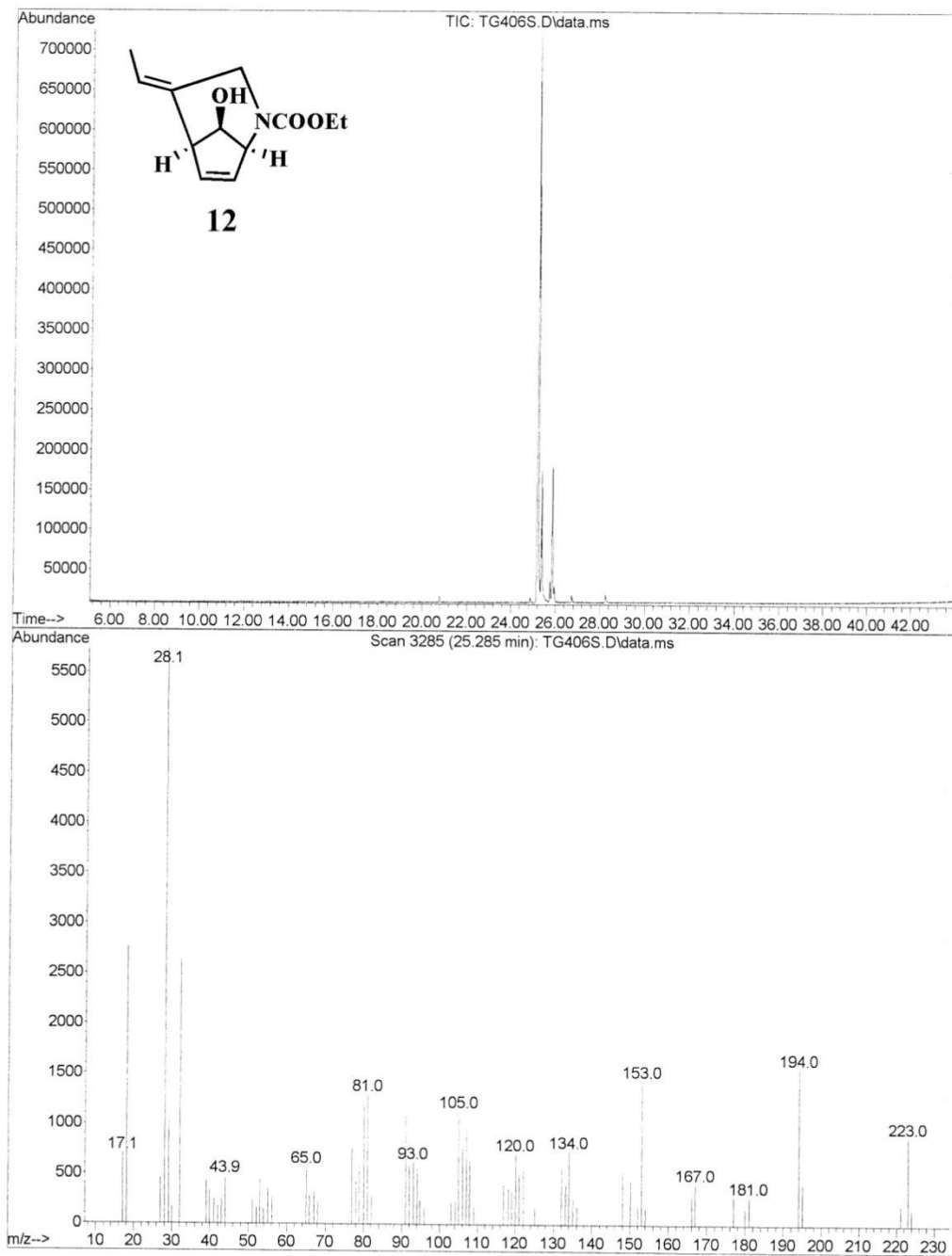


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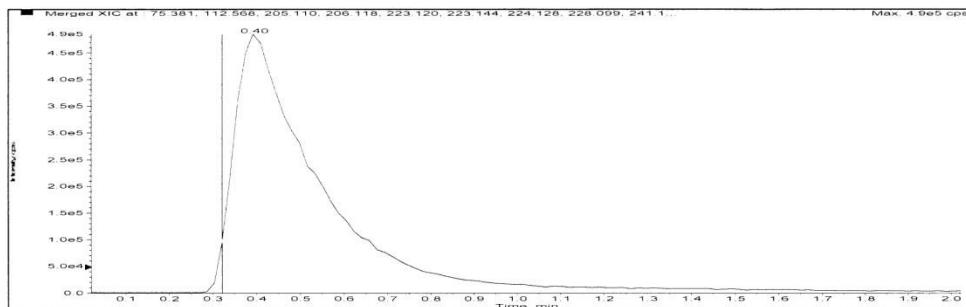
TC-406 7 1 C:\Bruker\TopSpin3.1\BBO\Guest



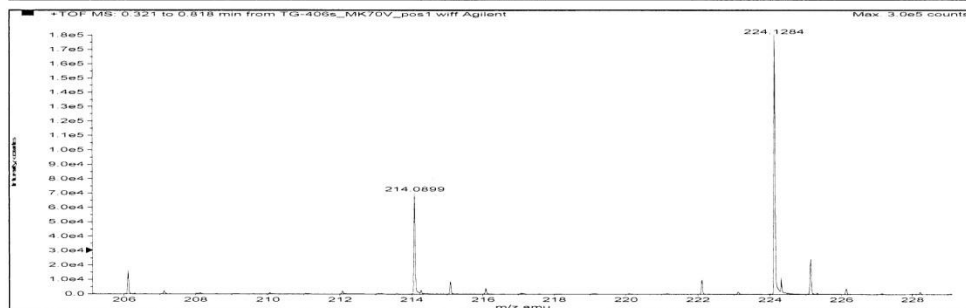
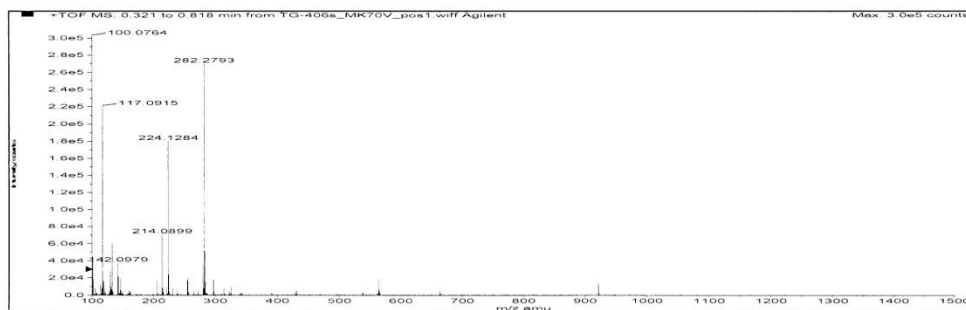
File :D:\DATA\Organska\Goca\TG406S.D
Operator :
Acquired : 10 Dec 2013 11:49 using AcqMethod METODA 44 MIN.M
Instrument : GCMSD
Sample Name:
Misc Info :
Vial Number: 1



Sample Name: TG-406s Sample Location: P1-C3 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Farmaceutski fakultet\Data\TG-406s_MK70V_pos1.wiff Acq Time: December 20 2013, 11:51:33 AM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anm\efc.xml

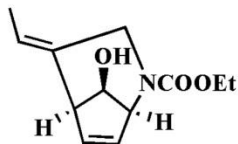


Merged XIC, Period# : 1 Experiment# : 1

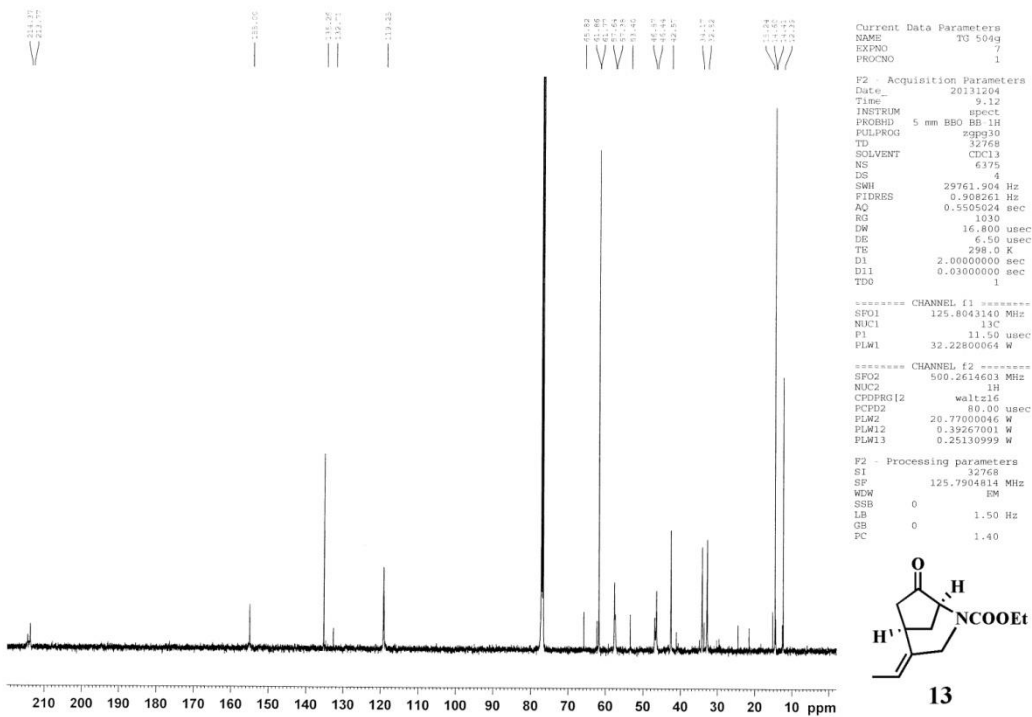
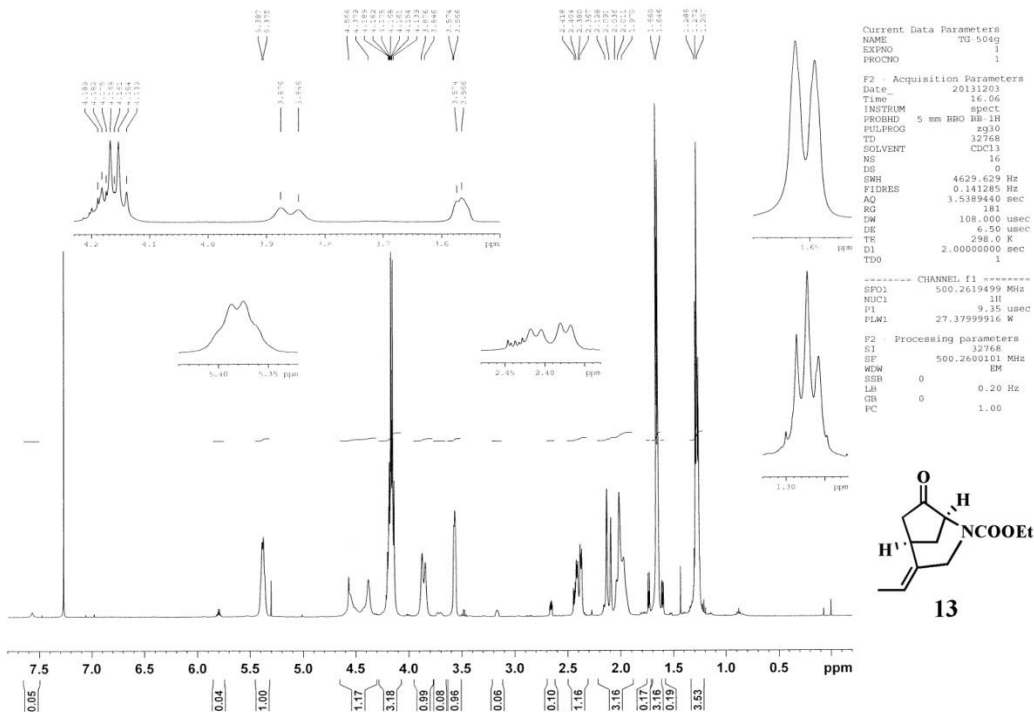


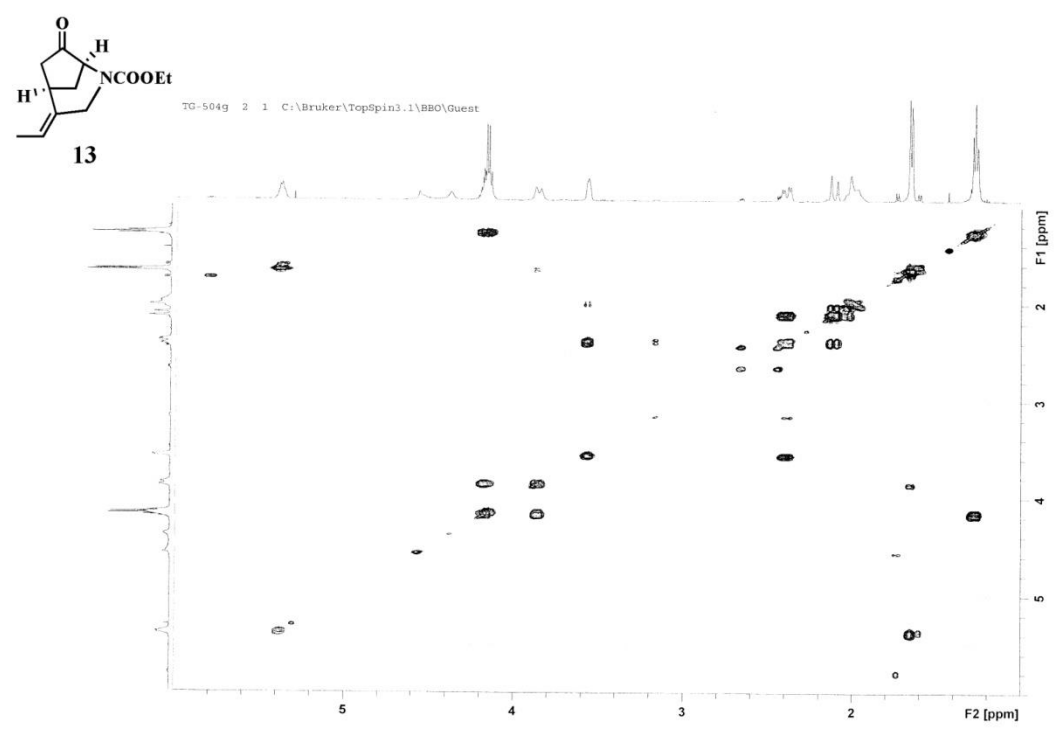
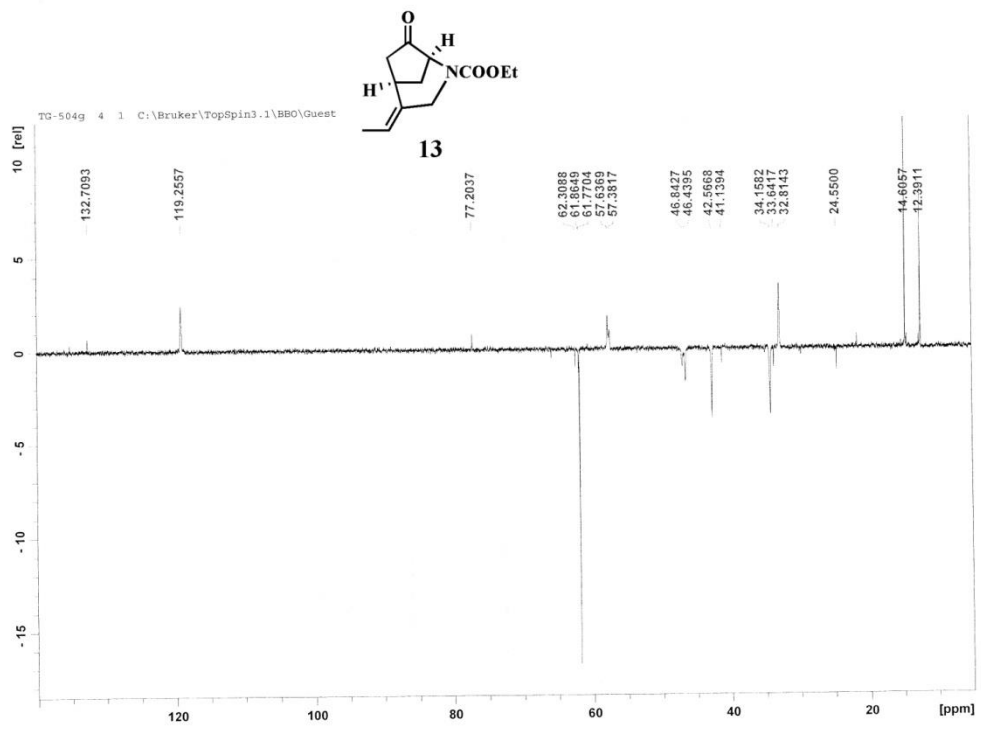
Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C12H17NO3	--	223.12084	0.40	6.17790 E6	--

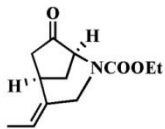
Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H-H2O] ⁺	16173.41	206.11756	206.11806	0.50615	2.46	--
[M+H] ⁺	185377.09	224.12812	224.12844	0.32099	1.43	--



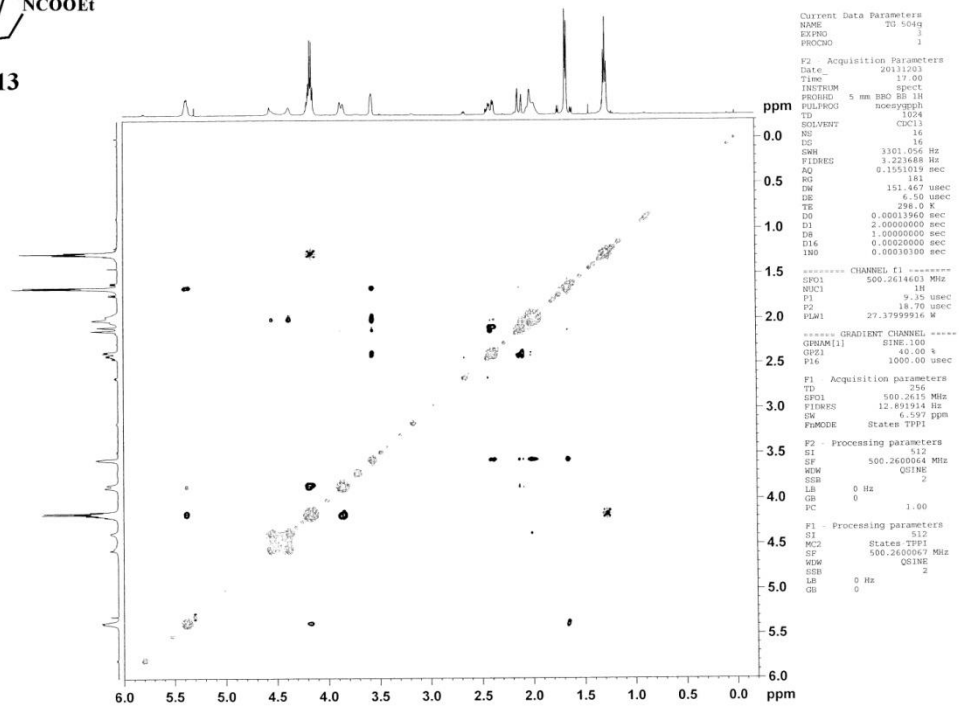
12







13



```

Current Data Parameters
NAME      TG-504g
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    2011103
Time     17.00
INSTRUM  spect
PROBHD   5 mm BBO BB 1H
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       16
SWH      3301.056 Hz
FIDRES   3.221488 Hz
AQ       0.1551019 sec
RG       181
DM       151.467 usec
DE       6.50 usec
TE       298.0 K
DQ       0.0001360 sec
D1       2.0000000 sec
d8       1.0000000 sec
D16      0.0002000 sec
IN0      0.0003000 sec

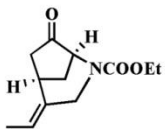
===== CHANNEL C1 =====
SFO1     500.2614603 MHz
NUC1     1H
P1       9.35 usec
P2       18.70 usec
PLM1     27.37899916 M

===== GRADIENT CHANNEL =====
GPROG1   zgpg30
SFO1     500.2614603 MHz
NUC1     1H
P1       9.35 usec
P2       18.70 usec
PLM1     27.37899916 M

===== Acquisition parameters =====
TE       298.2 K
SFO1     500.2615 MHz
FIDRES   12.491914 Hz
SM       6.597 ppm
FAMODE   States TPP1

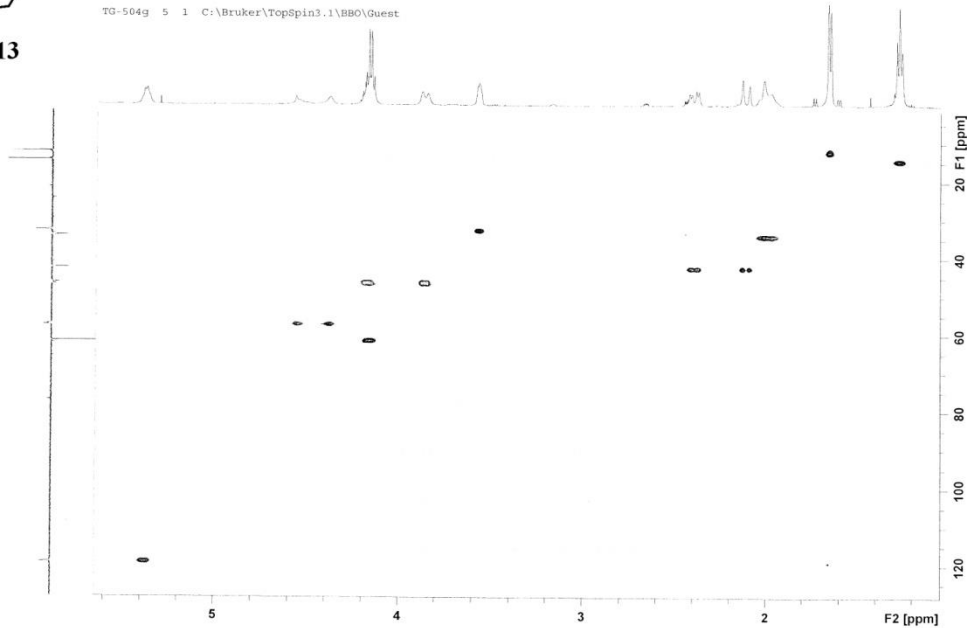
F1 - Processing parameters
SI       312
SF       500.260064 MHz
WDW      COSY
SSB      2
LB       0 Hz
GB       0
PC       1.00

F1 - Processing parameters
SI       312
SF       500.260064 MHz
WDW      COSY
SSB      2
LB       0 Hz
GB       0
  
```

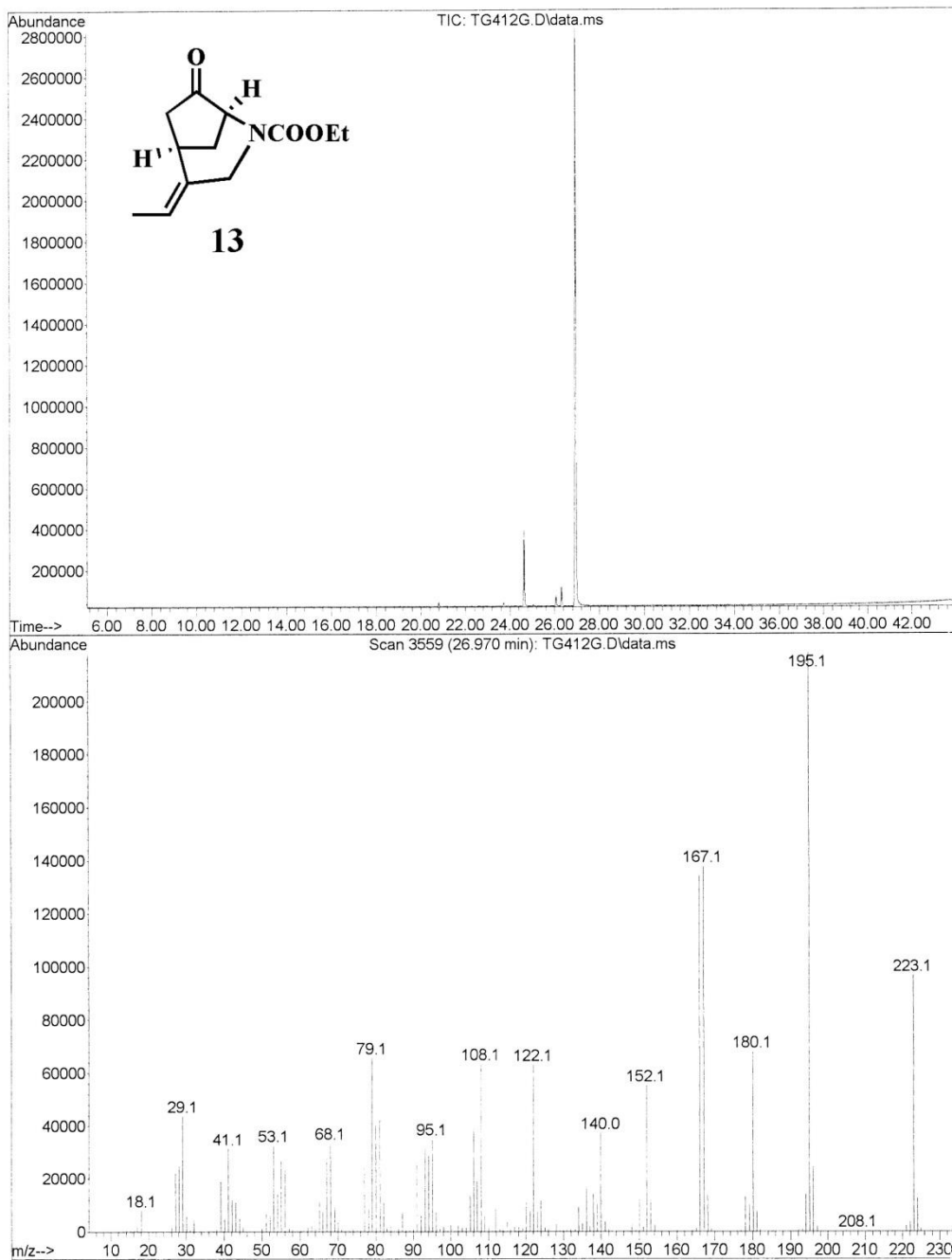


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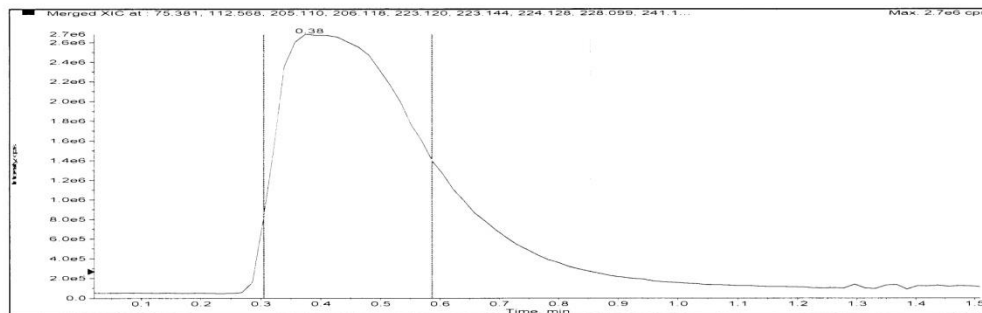
TG-504g 5 1 C:\Bruker\TopSpin3.1\BBO\Guest



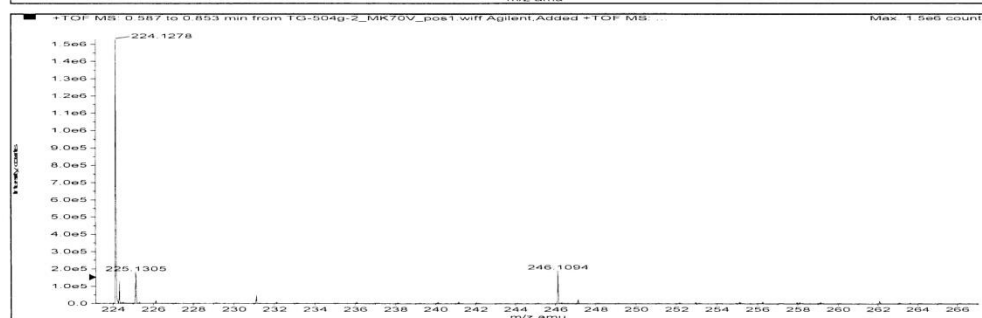
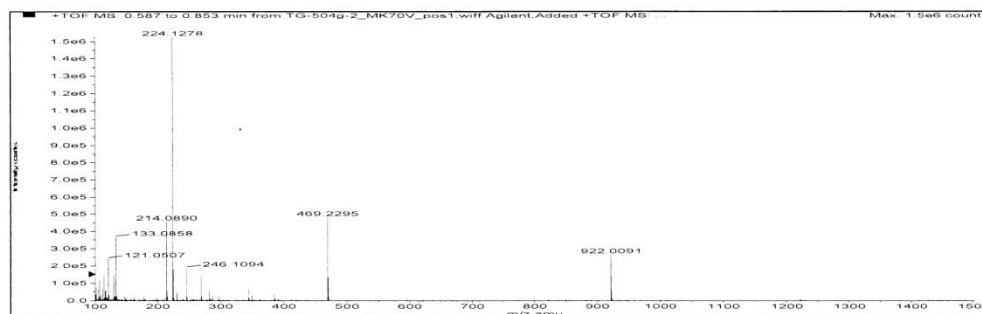
File :D:\DATA\Organska\Goca\TG412G.D
Operator :
Acquired : 7 Feb 2013 13:45 using AcqMethod METODA 44 MIN.M
Instrument : GCMSD
Sample Name:
Misc Info :
Vial Number: 1



Sample Name: TG-504g-2 Sample Location: P1-C7 Sample Id: Operator: Goca
 Data File Name: D:\PE Sciex Data\Projects\Farmaceutski fakultet\Data\TG-504g-2_MK70V_pos1.wiff Acq Time: January 31 2014, 03:48:19 PM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anm\efc.xml

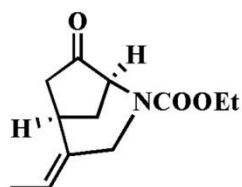


Merged XIC, Period# : 1 Experiment# : 1

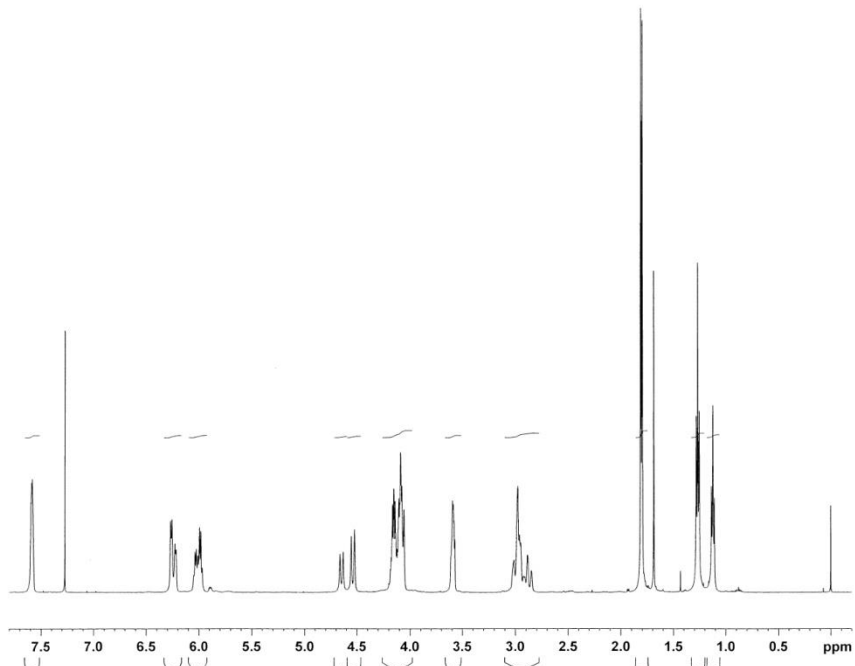


Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C12H17NO3	--	223.12084	0.38	4.71576 E7	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	1529826.79	224.12812	224.12779	-0.32591	-1.45	--
[M+Na] ⁺	190587.70	246.11006	246.10939	-0.67314	-2.74	--
[M+K] ⁺	15457.10	262.08400	262.08389	-0.11152	-0.43	--



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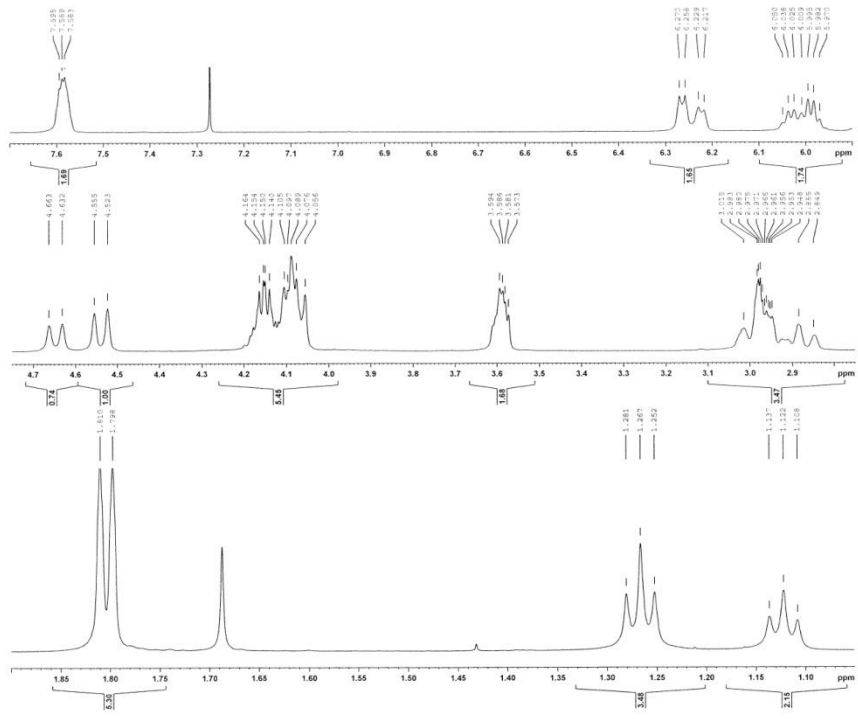
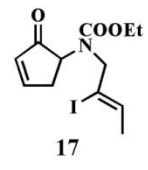
```

Current Data Parameters
NAME          TG-446g
EXPNO        1
PROCNO       1

F2 - Acquisition Parameters
Date_         20130715
Time          14.05
INSTRUM      spect
PROBHD       5 mm BBO BB-1H
PULPROG      zg30
TD            32768
SOLVENT      CDCl3
NS            16
DS            0
SWH           4699.248 Hz
FIDRES       0.143410 Hz
AQ            3.4865153 sec
RG            181
DM            106.400 usec
DE            6.50 usec
TE            298.0 K
D1            2.0000000 sec
TD0           1

----- CHANNEL f1 -----
SFO1          500.2619100 MHz
NUC1          1H
P1            9.35 usec
PLW1          27.37999916 W

F2 - Processing parameters
SI            32768
SF            500.2600081 MHz
WDW           EM
SSB           0
LB            0.20 Hz
GB            0
PC            1.00
  
```



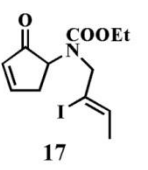
```

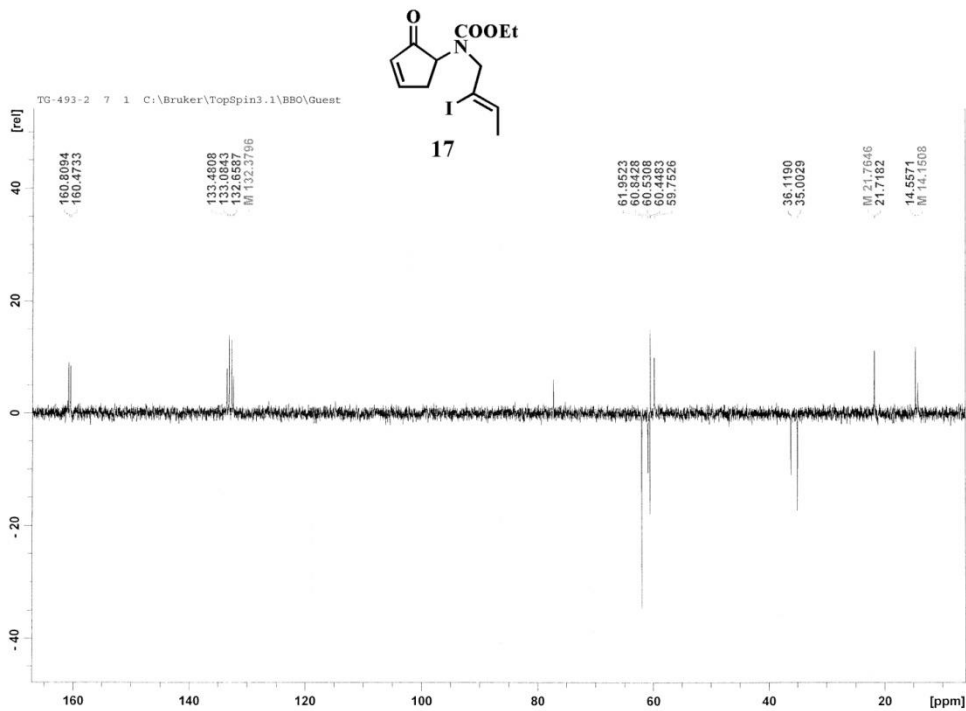
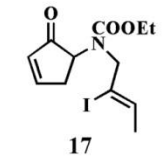
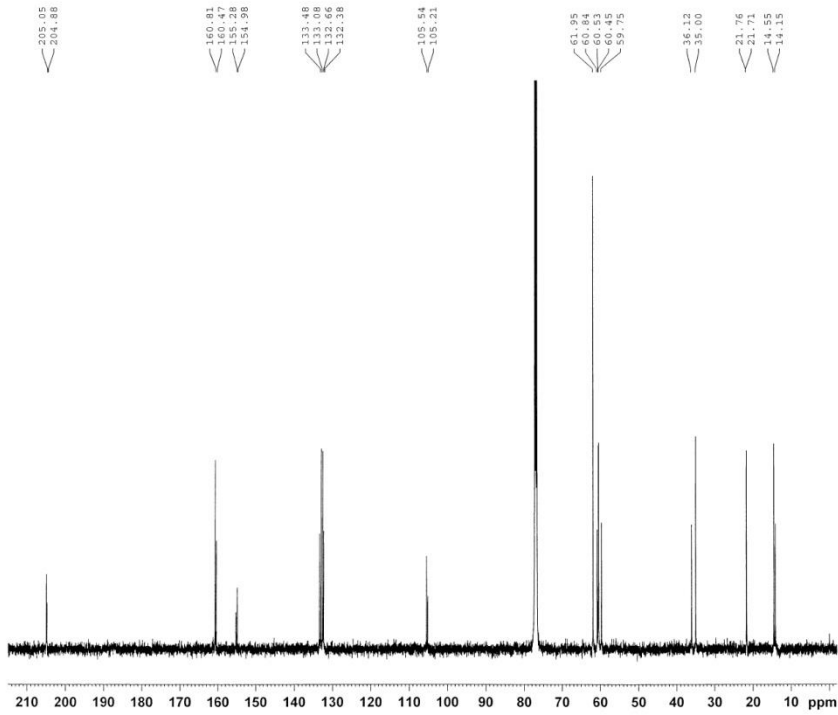
Current Data Parameters
NAME          TG-446g
EXPNO        1
PROCNO       1

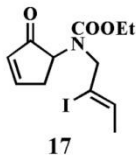
F2 - Acquisition Parameters
Date_         20130715
Time          14.05
INSTRUM      spect
PROBHD       5 mm BBO BB-1H
PULPROG      zg30
TD            32768
SOLVENT      CDCl3
NS            16
DS            0
SWH           4699.248 Hz
FIDRES       0.143410 Hz
AQ            3.4865153 sec
RG            181
DM            106.400 usec
DE            6.50 usec
TE            298.0 K
D1            2.0000000 sec
TD0           1

----- CHANNEL f1 -----
SFO1          500.2619100 MHz
NUC1          1H
P1            9.35 usec
PLW1          27.37999916 W

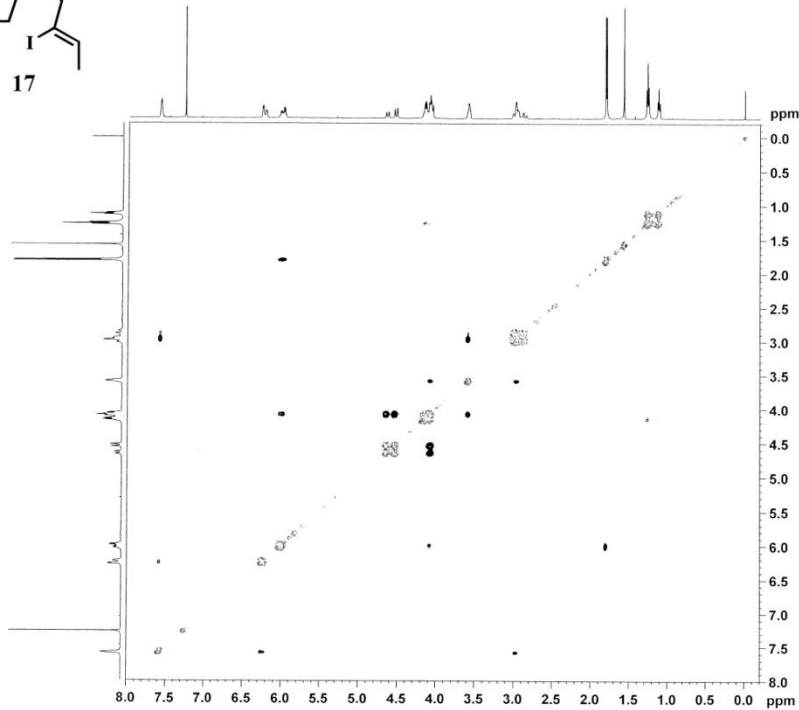
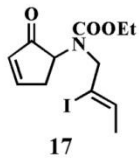
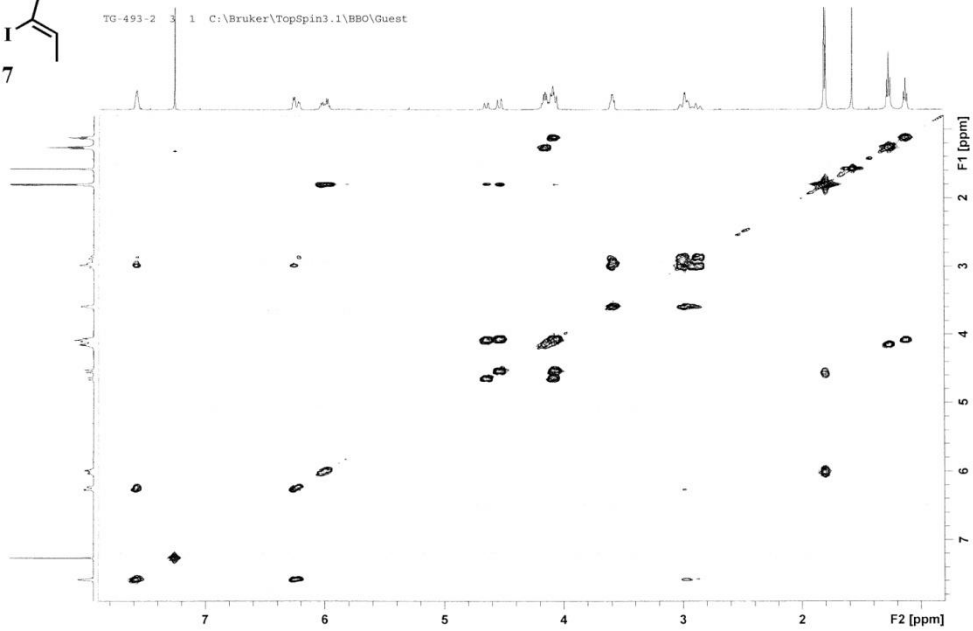
F2 - Processing parameters
SI            32768
SF            500.2600081 MHz
WDW           EM
SSB           0
LB            0.20 Hz
GB            0
PC            1.00
  
```







TG-493-2 3 1 C:\Bruker\TopSpin3.1\BBO\Guest



```

Current Data Parameters
NAME      TG-493-2
EXPRO    4
PROCNO   1

F2 Acquisition Parameters
Date_     2011112
Time      17:09
INSTRUM   spect
PROBHD    5 mm BBO BB-1H
PULPROG   megarpgph
TD         1634
SOLVENT   CDCl3
RG         16
DS         4
SHE        4768.098 Hz
FIDRES    4.597752 Hz
AQ         0.1087488 sec
RG         322
SW         106.200 usec
DE         6.50 usec
TE         298.0 K
DQ         0.00009410 sec
D1         2.00000000 sec
dW         1.00000000 sec
D16        0.00020000 sec
fNO        0.00021240 sec

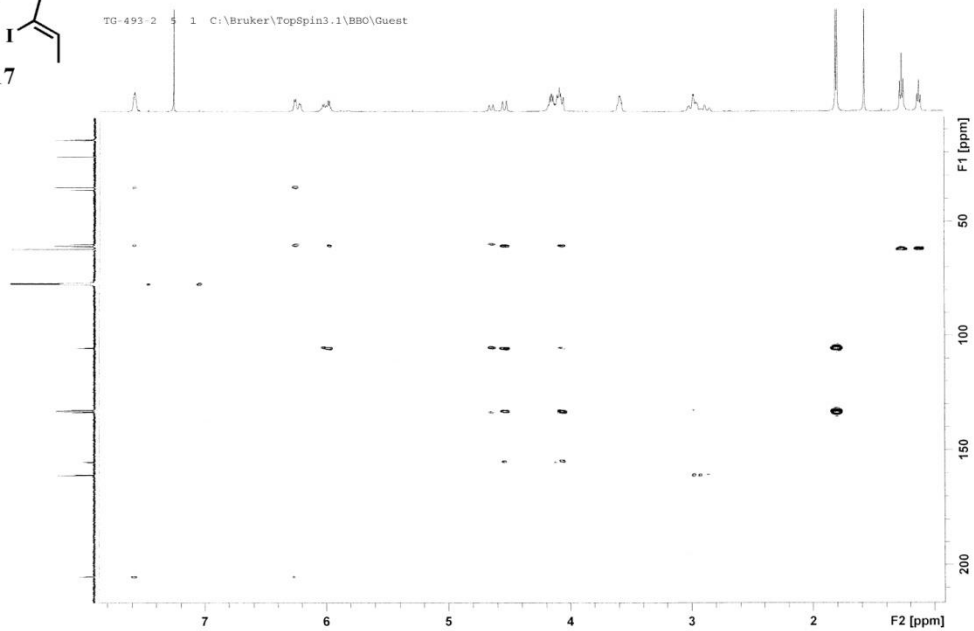
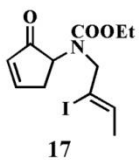
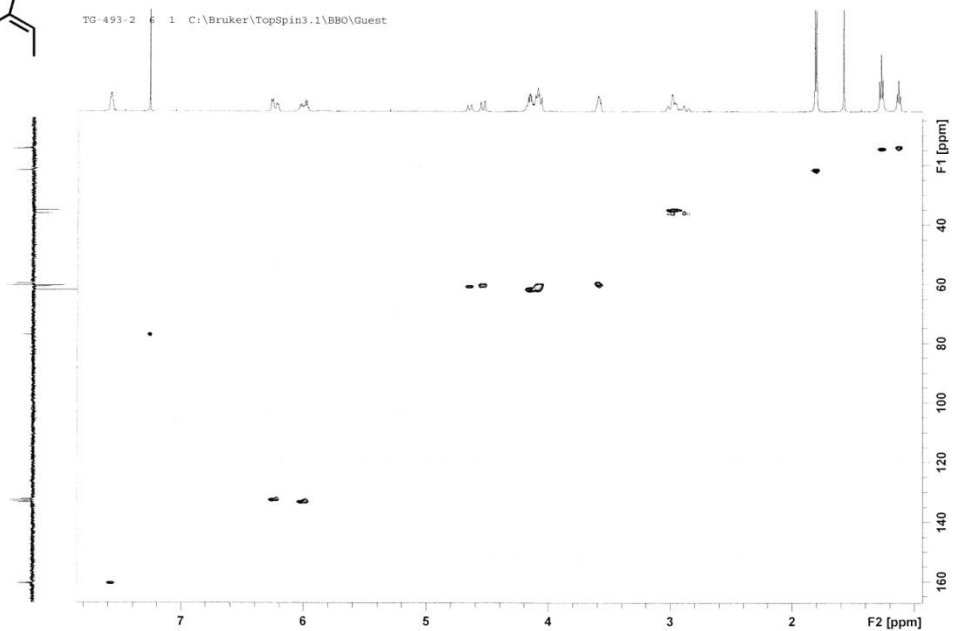
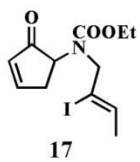
----- CHANNEL f1 -----
SFO1      500.261000 MHz
NUC1       1H
P1         9.15 usec
P2        18.70 usec
PL11      27.37999916 W

----- GRADIENT CHANNEL -----
GPRM11    128.100
GRF1      40.00
G16       1000.00 usec

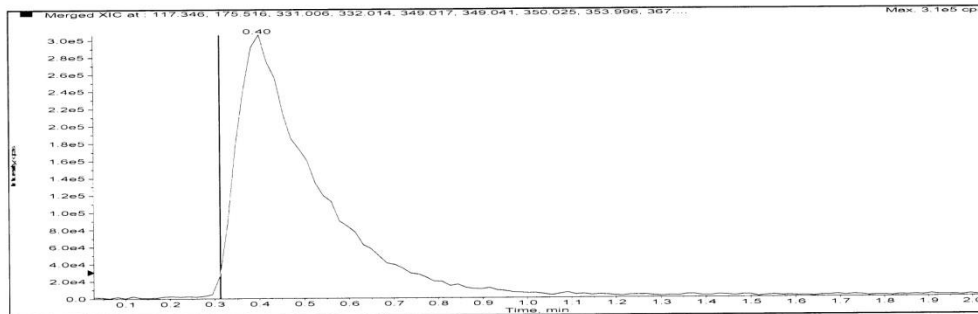
F1 Acquisition parameters
TD         256
SFO1      500.2619 MHz
FIDRES    18.331008 Hz
SW         9.411 ppm
FPMODE    States TPP1

F2 Processing parameters
S1         512
SF         500.260091 MHz
SOLVENT   CDCl3
SOLPROG   2
LB         0 Hz
GB         0
PC         1.00

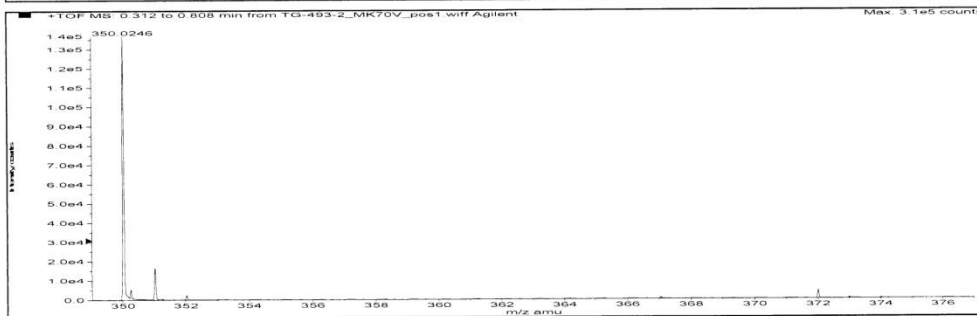
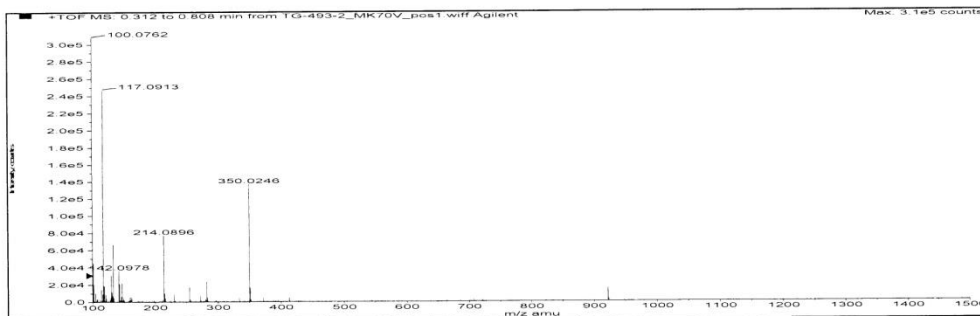
F1 Processing parameters
S1         512
MC2        States TPP1
SF         500.260091 MHz
SOLVENT   CDCl3
SOLPROG   2
LB         0 Hz
GB         0
  
```



Sample Name: TG-493-2 Sample Location: P1-C4 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Farmaceutski fakultet\Data\TG-493-2_MK70V_pos1.wiff Acq Time: December 20 2013,
 11:54:36 AM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anm\efc.xml

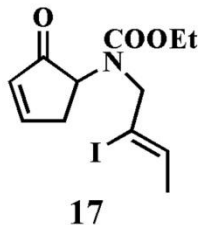


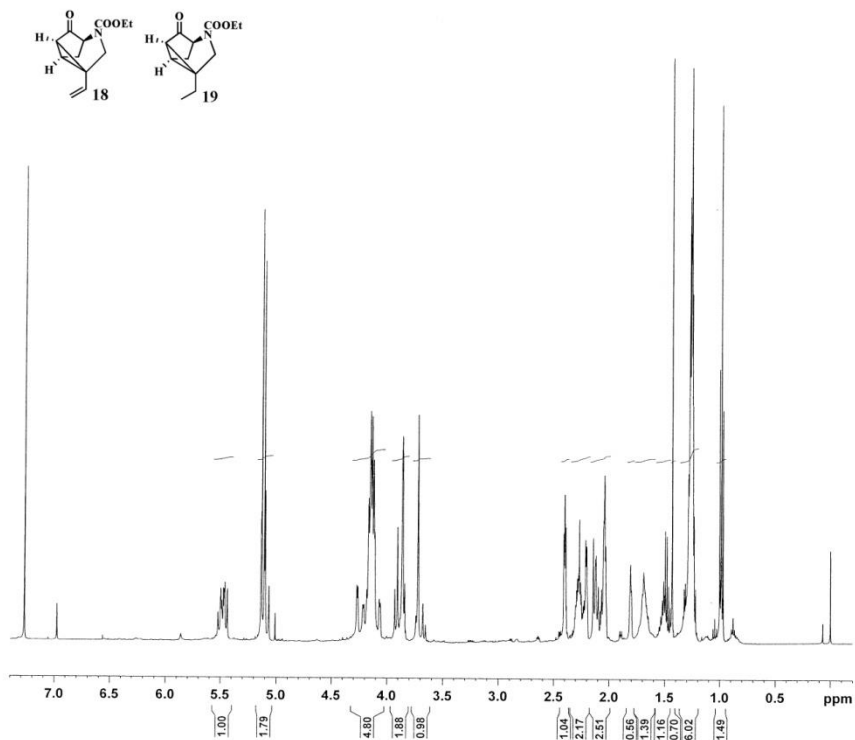
Merged XIC, Period# : 1 Experiment# : 1



Formula	Compound name	Mass	Peak RT (min)	Peak area	Description
C ₁₂ H ₁₆ INO ₃	--	349.01749	0.40	3.68132 E6	--

Species	Abundance (counts)	Ion Mass	Measured Mass	Error (mDa)	Error (ppm)	Ret. Time Error (min)
[M+H] ⁺	139542.58	350.02476	350.02464	-0.12077	-0.35	--
[M+Na] ⁺	4598.95	372.00671	372.00715	0.43833	1.18	--



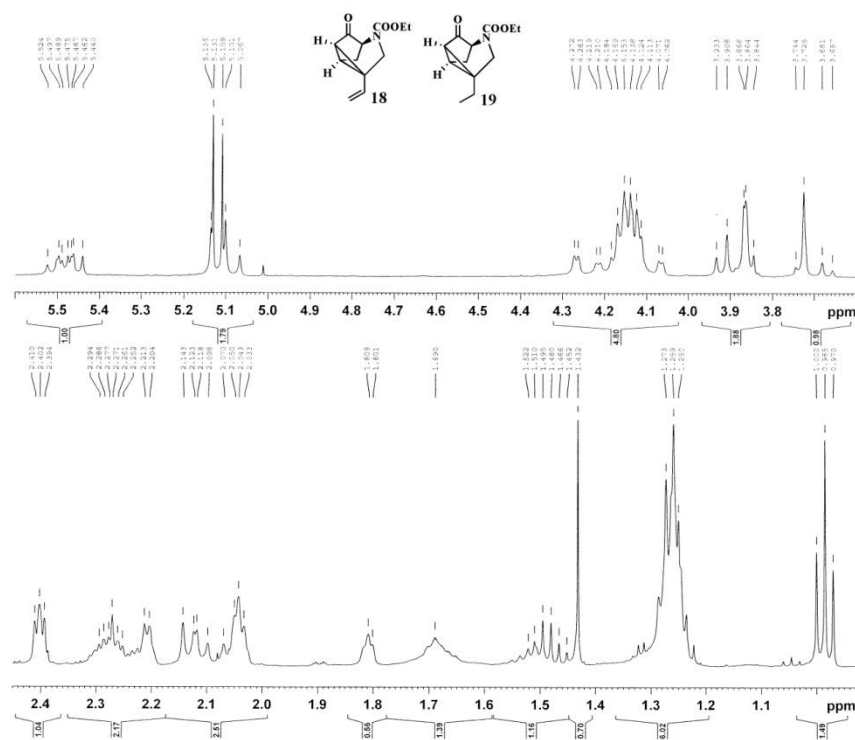


Current Data Parameters
 NAME TG 461g
 EXNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110916
 Time 16:12
 INSTRUM spect
 PROBHD 5 mm BBO BB 1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438017 sec
 RG 181
 DW 111.200 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.0000000 sec
 TDO 1

----- CHANNEL f1 -----
 SFO1 500.2618949 MHz
 NUC1 1H
 P1 9.35 usec
 PLW1 27.37999916 W

F2 - Processing parameters
 SI 32768
 SF 500.2600095 MHz
 NQW DM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

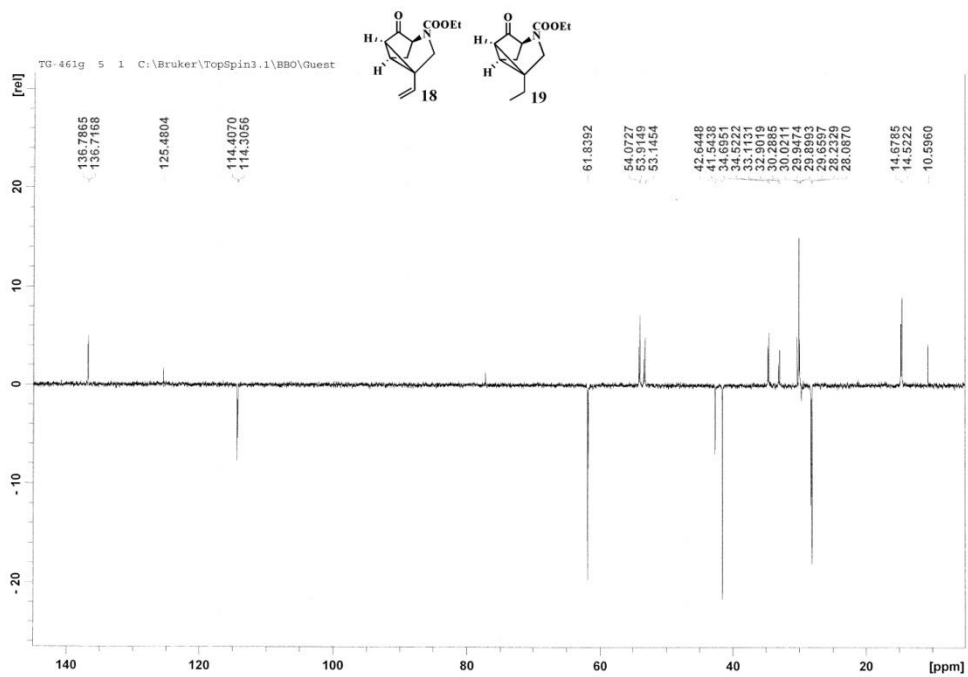
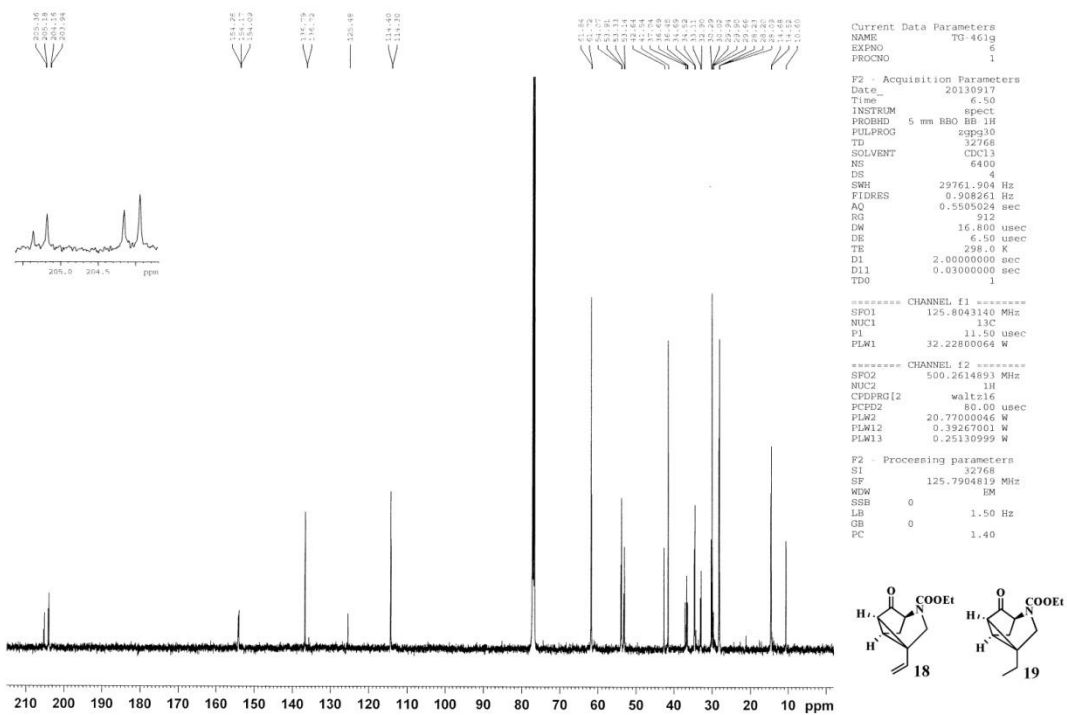


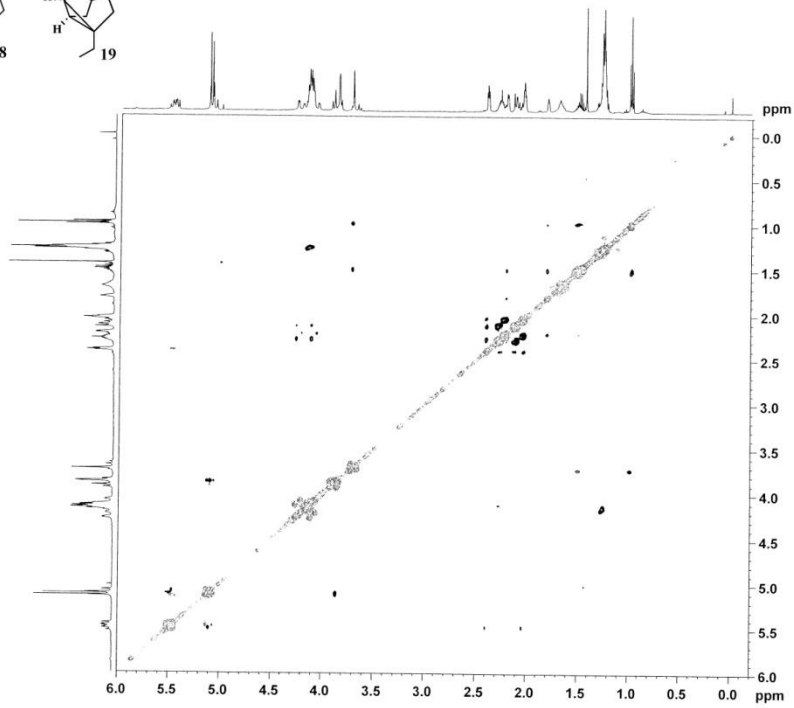
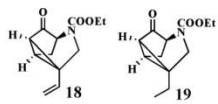
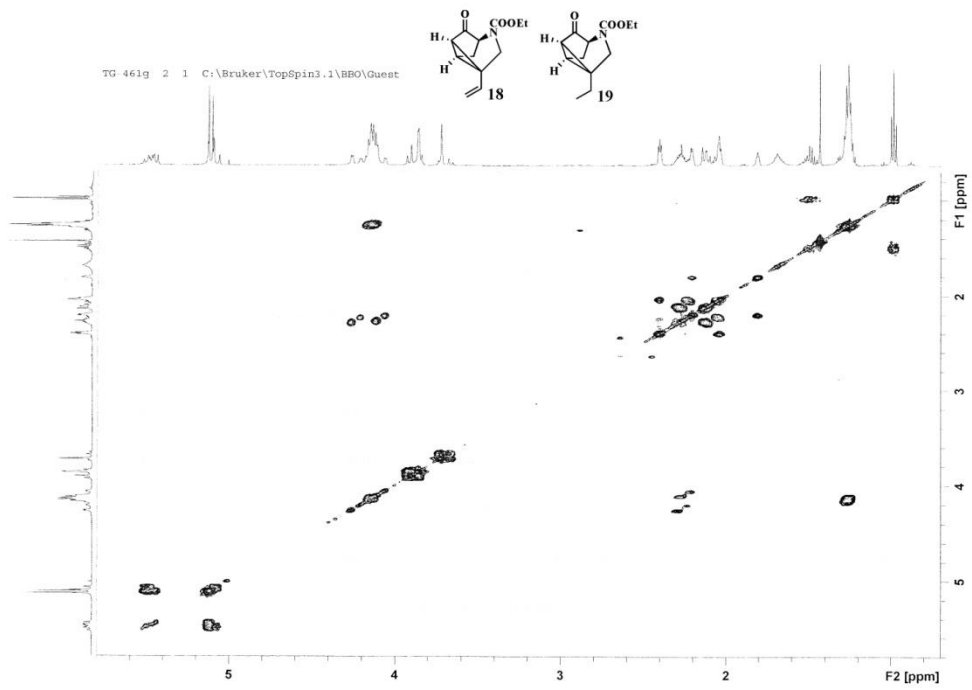
Current Data Parameters
 NAME TG 461g
 EXNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110916
 Time 16:12
 INSTRUM spect
 PROBHD 5 mm BBO BB 1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438017 sec
 RG 181
 DW 111.200 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.0000000 sec
 TDO 1

----- CHANNEL f1 -----
 SFO1 500.2618949 MHz
 NUC1 1H
 P1 9.35 usec
 PLW1 27.37999916 W

F2 - Processing parameters
 SI 32768
 SF 500.2600095 MHz
 NQW DM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00





```

Current Data Parameters
NAME          TG 461g
EXPNO        3
PROCNO       1

F2 - Acquisition Parameters
Date_         20110916
Time          17:04
INSTRUM      spect
PROBHD       5 mm BBO BB-1H
PULPROG      zgpg30
TE           300.2
SOLVENT      CDCl3
NS           16
DS           16
SWH          3255.208 Hz
FIDRES      3.17801e Hz
AQ           0.1572864 sec
RG           181
EM          153.400 usec
DE           6.50 usec
TE           298.0 K
DQ           0.00014170 sec
D1           2.00000000 sec
D8           1.00000000 sec
D16          0.00020000 sec
INQ          0.00030720 sec

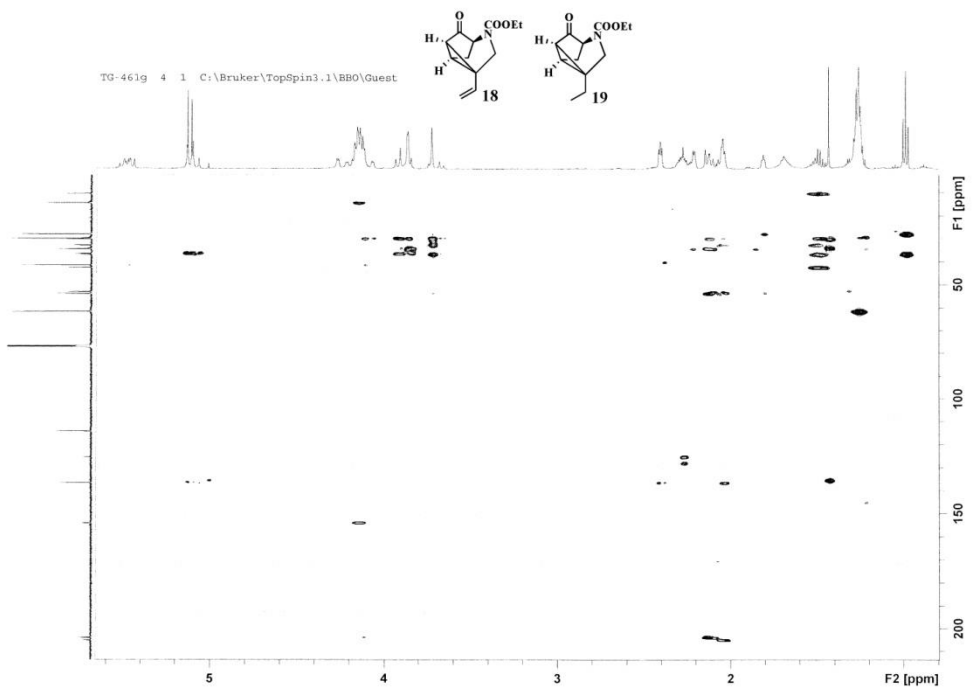
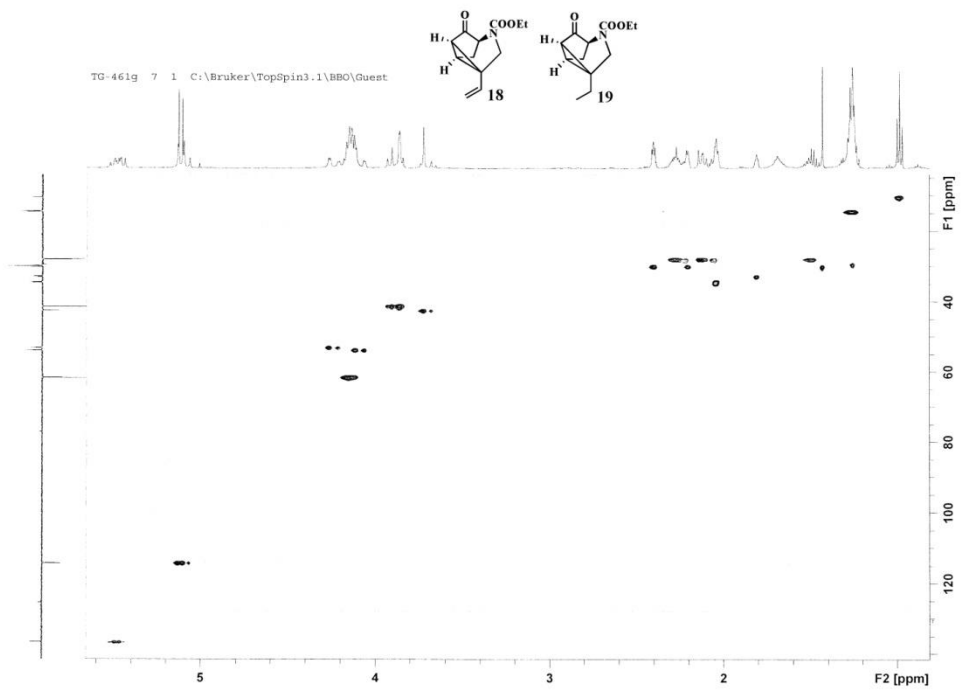
----- CHANNEL f1 -----
SFO1         500.2614893 MHz
NUC1         13C
P1           9.35 usec
P2           18.70 usec
PLM1         27.37999916 M

----- GRADIENT CHANNEL -----
GRAM111     SINE 100
GFC1        80.00 %
P16         1000.00 usec

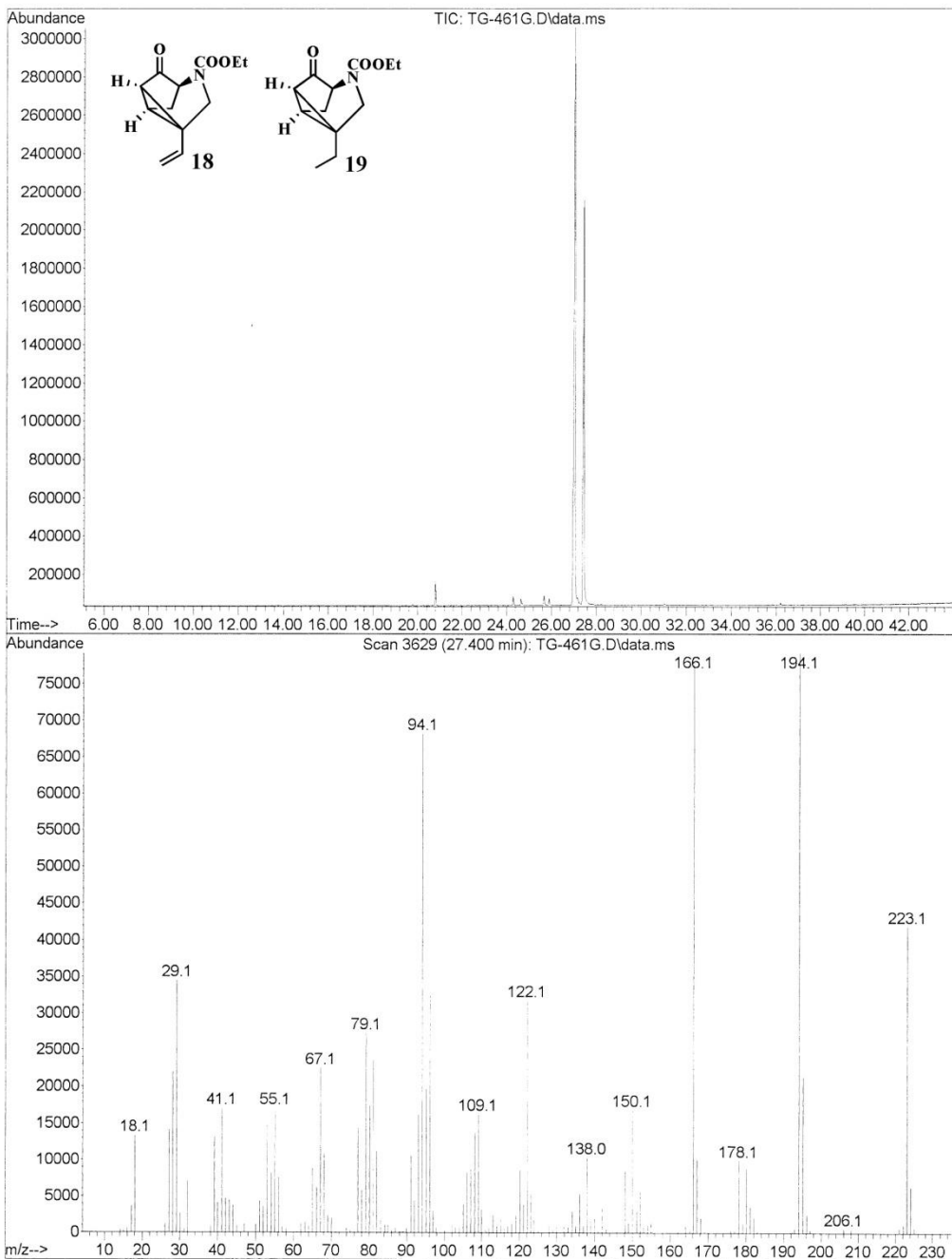
F1 - Acquisition parameters
TD           65536
SFO1         500.2615 MHz
FIDRES      12.715657 Hz
SW          6.507183 MHz
F0MODE      States-TPPI

F2 - Processing parameters
SI           32768
SF           500.2600079 MHz
RG          65536
SSB          0 Hz
CB           0
PC           1.00

F1 - Processing parameters
SI           32768
MC2          States-TPPI
SF           500.2600062 MHz
RG          65536
SSB          0 Hz
CB           0
  
```

File :D:\DATA\Organska\Goca\TG-461G.D
Operator :
Acquired : 19 Sep 2013 10:13 using AcqMethod METODA 44 MIN.M
Instrument : GCMSD
Sample Name:
Misc Info :
Vial Number: 1



File :D:\DATA\Organska\Goca\TG-461G.D
Operator :
Acquired : 19 Sep 2013 10:13 using AcqMethod METODA 44 MIN.M
Instrument : GCMSD
Sample Name :
Misc Info :
Vial Number: 1

