molecules

MDPI

Supporting information

(-)-Shikimic acid as a chiral building block for the synthesis of new cytotoxic 6-aza-analogues of angucyclinones

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Supplementary Material

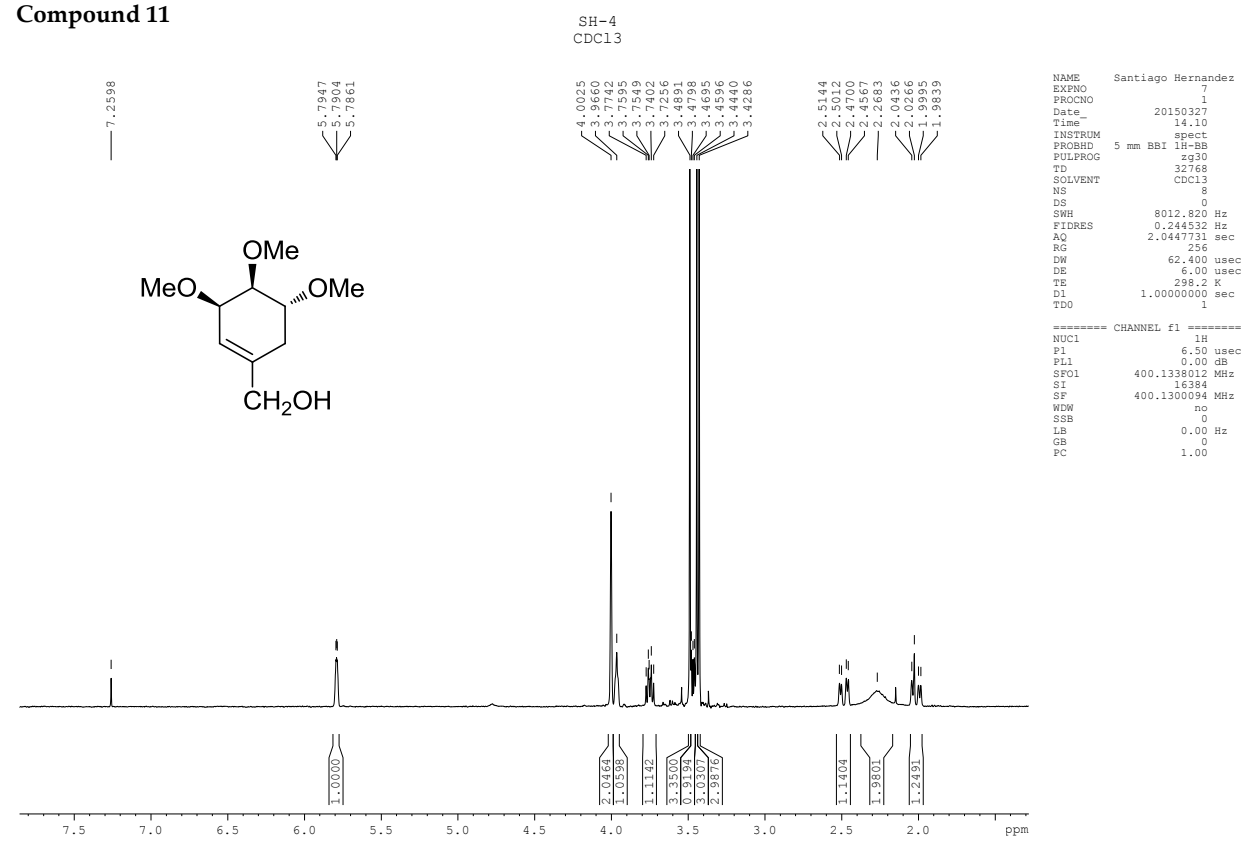
S.1 Nuclear magnetic resonance spectra

S.2 High resolution mass spectrometry

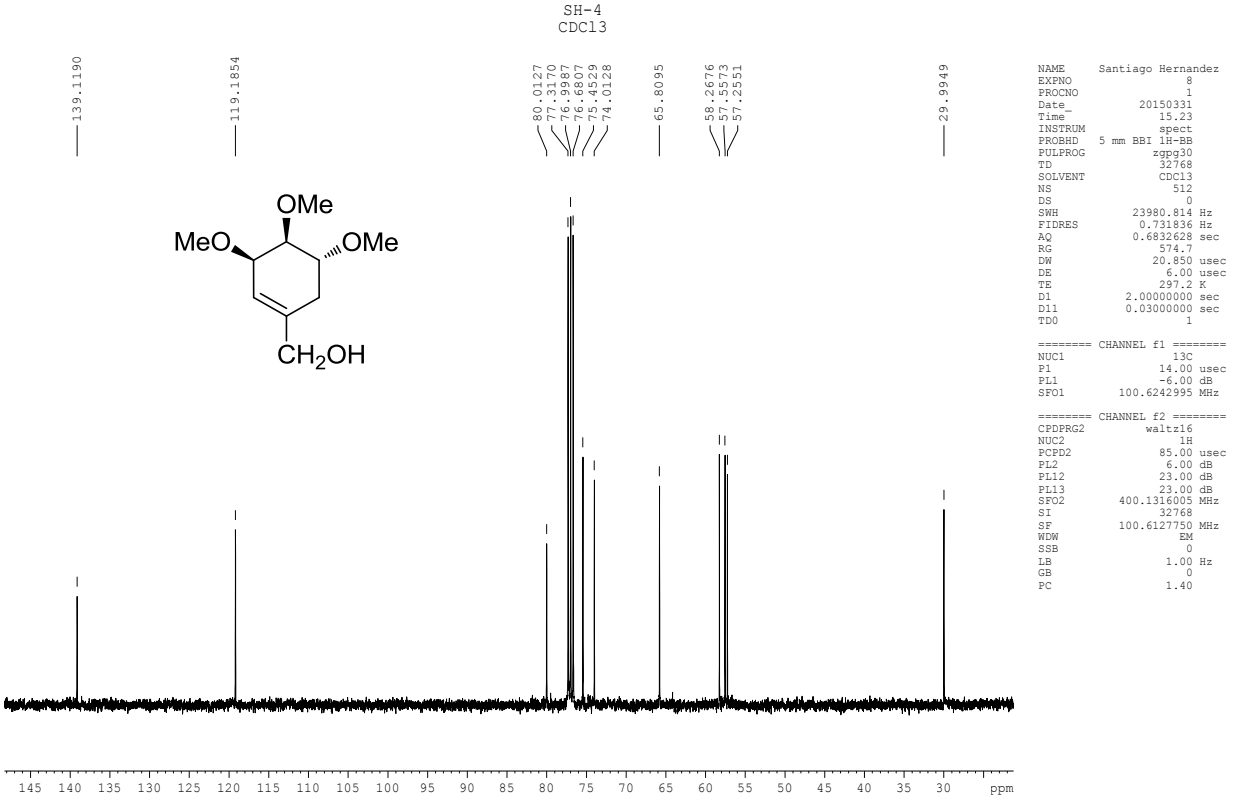
S.3 Infrared spectroscopy

S.1 Nuclear magnetic resonance spectra

Compound 11



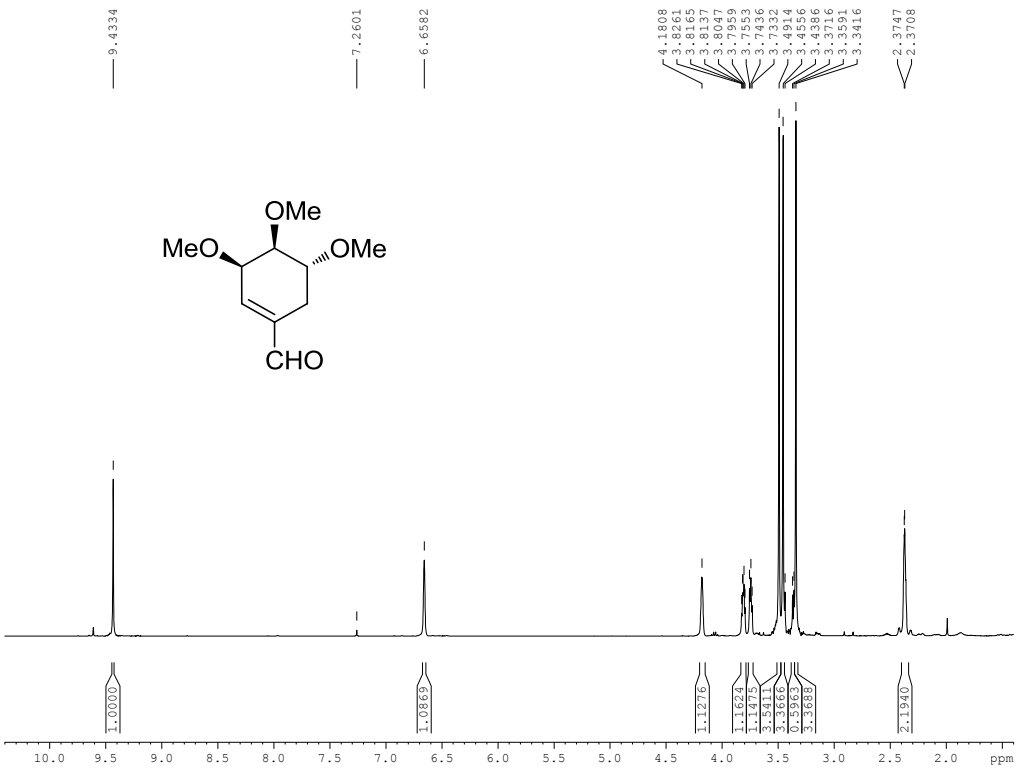

```
NAME      Santiago Hernandez
EXPNO                      7
PROCNO                     1
Date_               20150327
Time                   14.10
INSTRUM                spect
PROBHD   5 mm BBI 1H-BB
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        8
DS                        0
SWH                8012.820 Hz
FIDRES            0.244532 Hz
AQ                2.0447731 sec
RG                      256
DW                   62.400 usec
DE                    6.00 usec
TE                  298.2 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                    6.50 usec
PL1                   0.00 dB
SFO1          400.1338012 MHz
SI                    16384
SF            400.1300094 MHz
WDW                      no
SSB                       0
LB                    0.00 Hz
GB                        0
PC                    1.00
```




```
NAME      Santiago Hernandez
EXPNO                      8
PROCNO                     1
Date_               20150331
Time                   15.23
INSTRUM                spect
PROBHD   5 mm BBI 1H-BB
PULPROG             zgpg30
TD                    32768
SOLVENT               CDCl3
NS                      512
DS                        0
SWH               23980.814 Hz
FIDRES            0.731836 Hz
AQ                0.6832628 sec
RG                    574.7
DW                   20.850 usec
DE                    6.00 usec
TE                  297.2 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     13C
P1                   14.00 usec
PL1                  -6.00 dB
SFO1          100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                      1H
PCPD2                85.00 usec
PL2                   6.00 dB
PL12                 23.00 dB
PL13                 23.00 dB
SFO2          400.1316005 MHz
SI                    32768
SF            100.6127750 MHz
WDW                      EM
SSB                       0
LB                    1.00 Hz
GB                        0
PC                    1.40
```

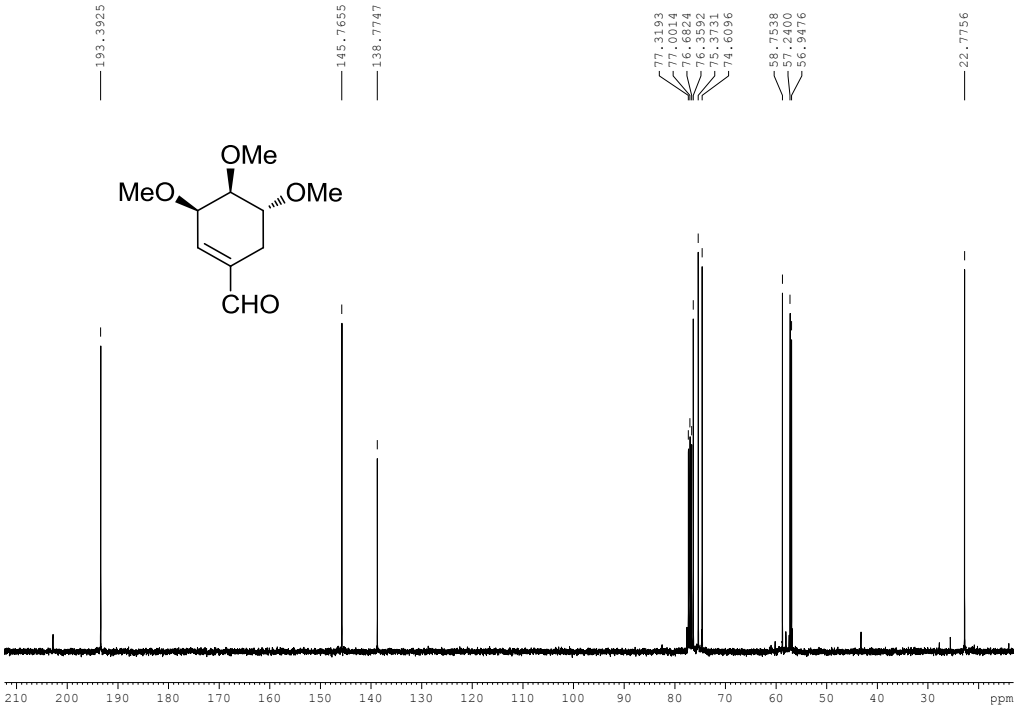
Compound 12

SH-aldehido
CDC13



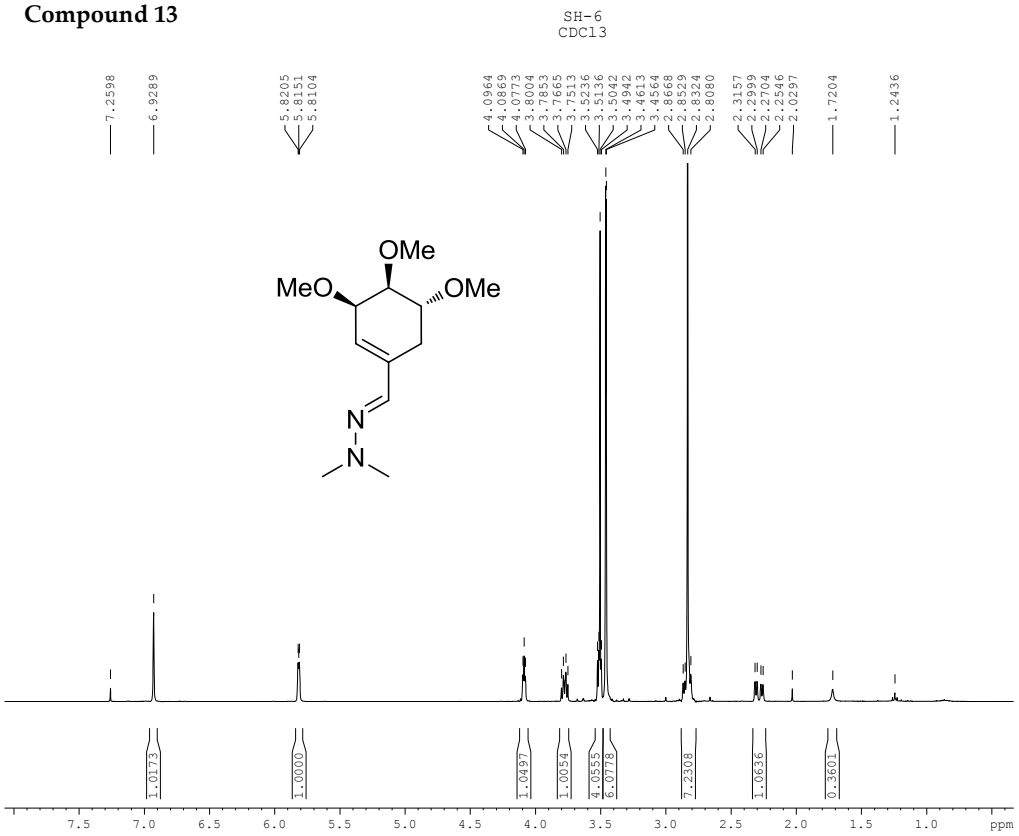

```
NAME      Santiago Hernandez
EXPNO                 14
PROCNO                 1
Date_           20150508
Time_              10.11
INSTRUM             spect
PROBHD   5 mm BBI 1H-BB
PULPROG            zg30
TD                 32768
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             8012.820 Hz
FIDRES             0.244532 Hz
AQ              2.0447731 sec
RG                  71.8
DW                 62.400 usec
DE                  6.00 usec
TE                296.2 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                  6.50 usec
PL1                 0.00 dB
SFO1          400.1338012 MHz
SI                 16384
SF            400.1300089 MHz
WDW                   no
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  1.00
```

SH-aldehido
CDC13

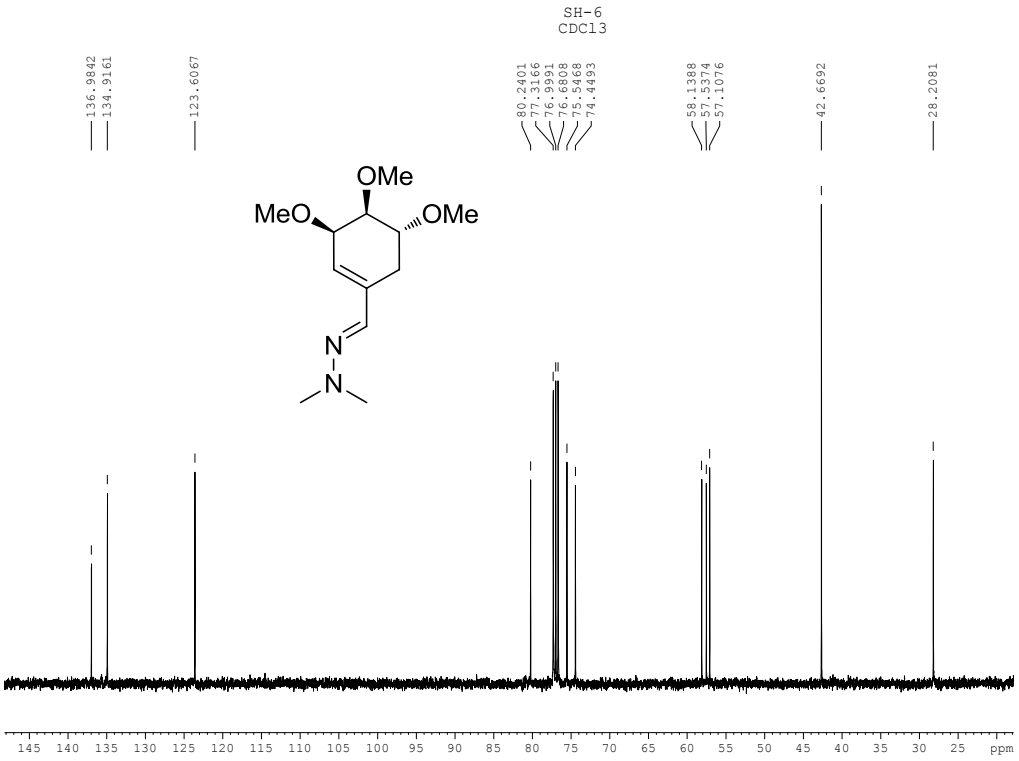



```
NAME      Santiago Hernandez
EXPNO                 23
PROCNO                 1
Date_           20150512
Time_              15.43
INSTRUM             spect
PROBHD   5 mm BBI 1H-BB
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                   512
DS                     0
SWH            23980.814 Hz
FIDRES             0.731836 Hz
AQ              0.6832628 sec
RG                  574.7
DW                 20.850 usec
DE                  6.00 usec
TE                296.2 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 14.00 usec
PL1                -6.00 dB
SFO1         100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              85.00 usec
PL2                 6.00 dB
PL12               23.00 dB
PL13               23.00 dB
SFO2          400.1316005 MHz
SI                 32768
SF            100.6127804 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Compound 13

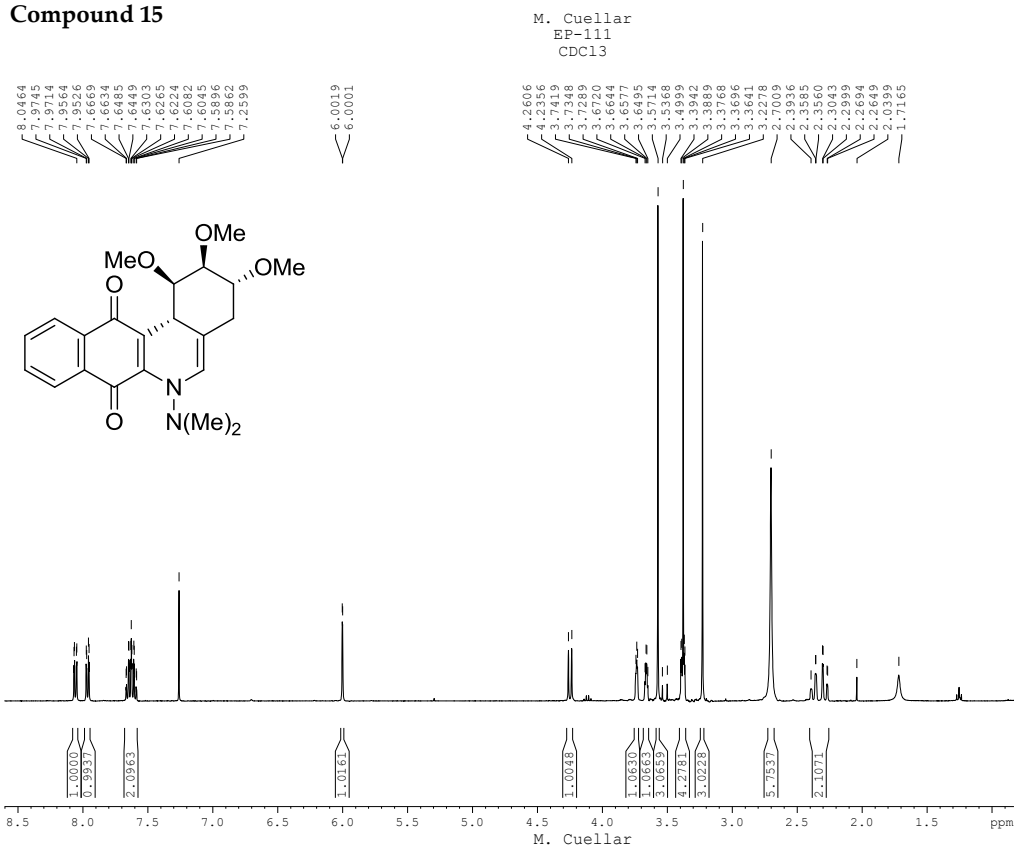



```
NAME          Santiago Hernandez
EXPNO                 19
PROCNO                1
Date_           20150508
Time_             10.41
INSTRUM             spect
PROBHD    5 mm BBI 1H-BB
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             8012.820 Hz
FIDRES             0.244532 Hz
AQ              2.0447731 sec
RG                   181
DW                62.400 usec
DE                 6.00 usec
TE                296.2 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 6.50 usec
PL1                0.00 dB
SFO1         400.1338012 MHz
SI                 16384
SF           400.1300094 MHz
WDW                   no
SSB                    0
LB                 0.00 Hz
GB                     0
PC                 1.00
```

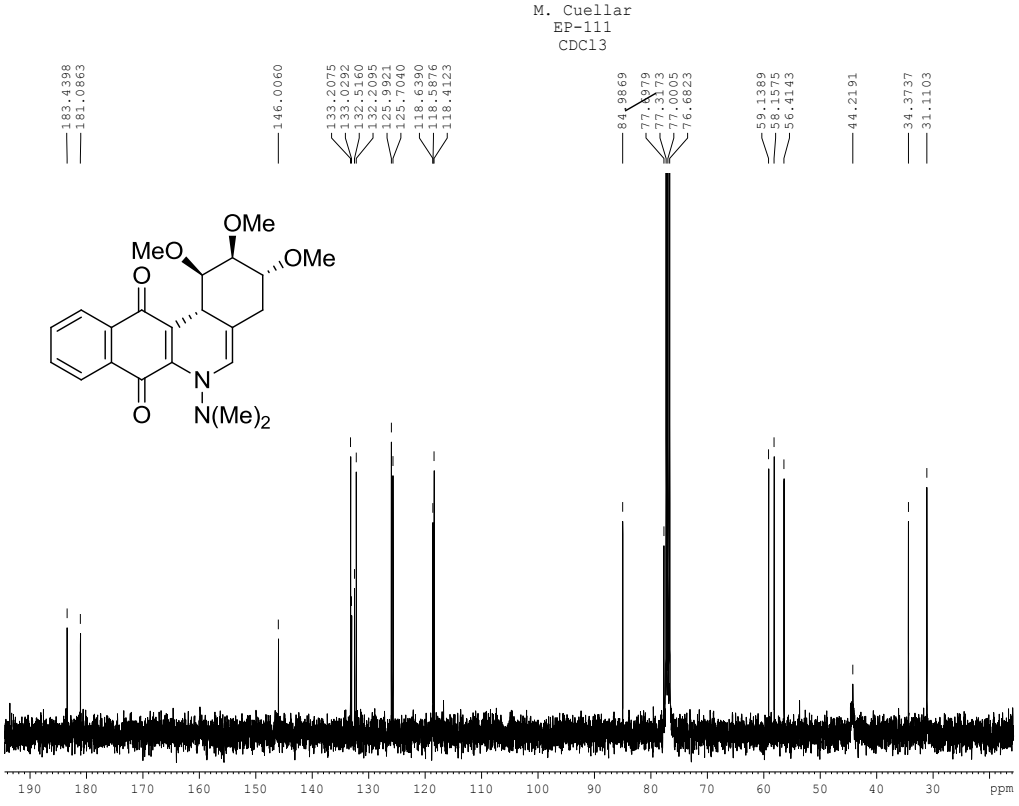



```
NAME          Santiago Hernandez
EXPNO                 20
PROCNO                1
Date_           20150512
Time_             14.52
INSTRUM             spect
PROBHD    5 mm BBI 1H-BB
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                   512
DS                     0
SWH            23980.814 Hz
FIDRES             0.731836 Hz
AQ              0.6832628 sec
RG                 574.7
DW                20.850 usec
DE                 6.00 usec
TE                296.2 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                14.00 usec
PL1               -6.00 dB
SFO1         100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              85.00 usec
PL2                6.00 dB
PL12              23.00 dB
PL13              23.00 dB
SFO2         400.1316005 MHz
SI                 32768
SF           100.6127733 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```

Compound 15

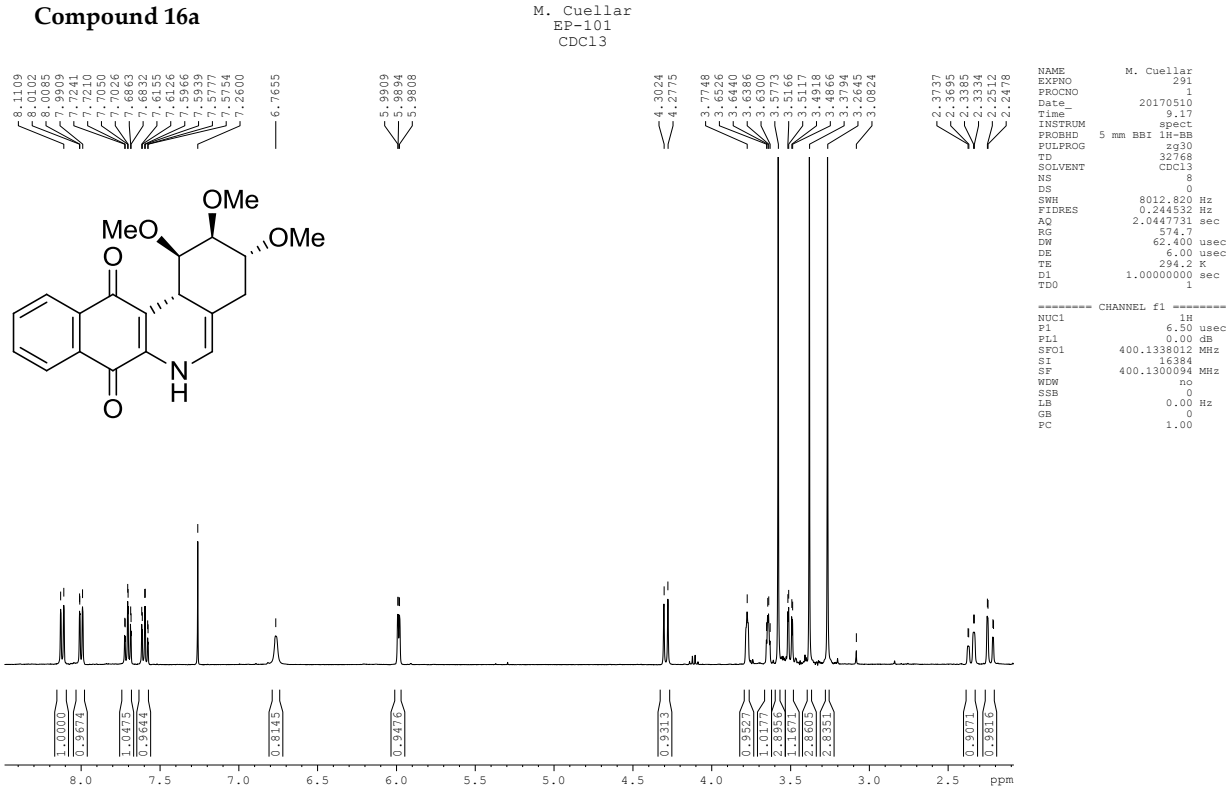



```
NAME          M. Cuellar
EXPNO              302
PROCNO               1
Date_         20170703
Time             16.38
INSTRUM          spect
PROBHD   5 mm BBI 1H-BB
PULPROG          zg30
TD              32768
SOLVENT          CDCl3
NS                   8
DS                   0
SWH           8012.820 Hz
FIDRES           0.244532 Hz
AQ            2.0447731 sec
RG                574.7
DW               62.400 usec
DE                6.00 usec
TE               294.2 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                 1H
P1                6.50 usec
PL1               0.00 dB
SFO1        400.1338012 MHz
SI                16384
SF          400.1300094 MHz
WDW                 no
SSB                  0
LB                0.00 Hz
GB                   0
PC                1.00
```

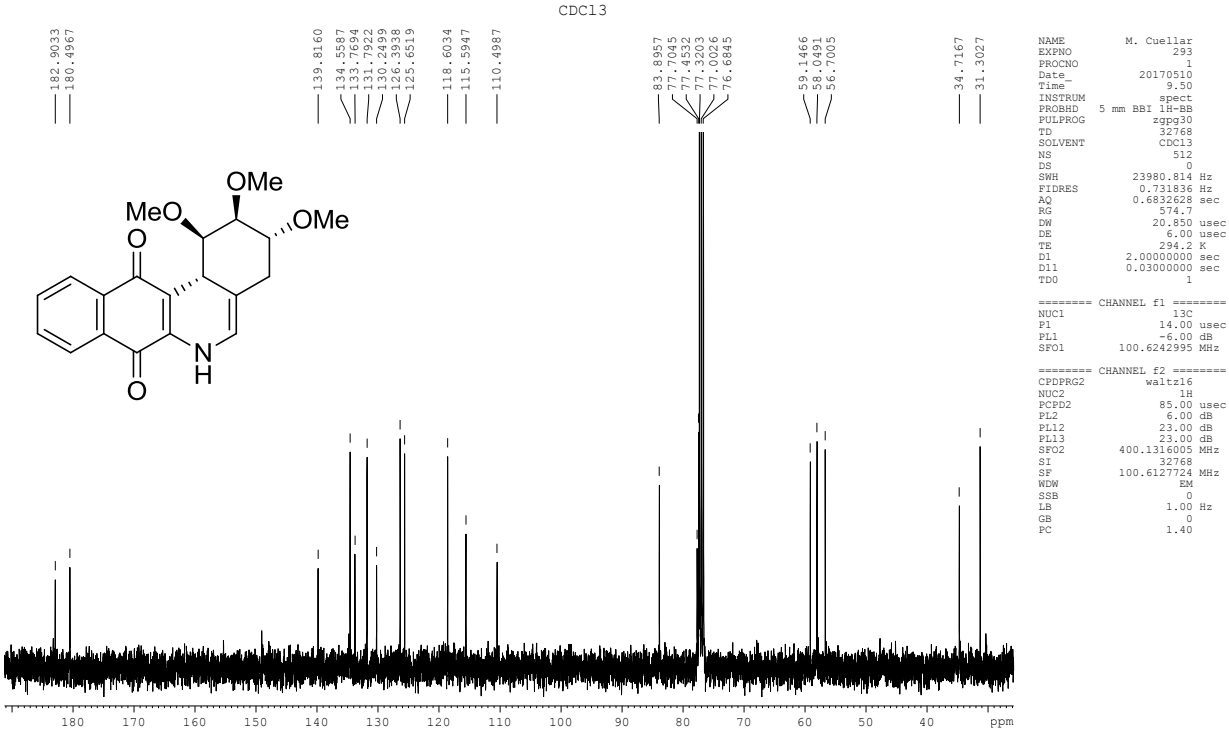



```
NAME          M. Cuellar
EXPNO              303
PROCNO               1
Date_         20170704
Time             16.53
INSTRUM          spect
PROBHD   5 mm BBI 1H-BB
PULPROG          zgpg30
TD              32768
SOLVENT          CDCl3
NS                1024
DS                   0
SWH          23980.814 Hz
FIDRES           0.731836 Hz
AQ            0.6832628 sec
RG                574.7
DW               20.850 usec
DE                6.00 usec
TE               294.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1               14.00 usec
PL1               -6.00 dB
SFO1        100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2            85.00 usec
PL2                6.00 dB
PL12              23.00 dB
PL13              23.00 dB
SFO2        400.1316005 MHz
SI                32768
SF          100.6127724 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```

Compound 16a

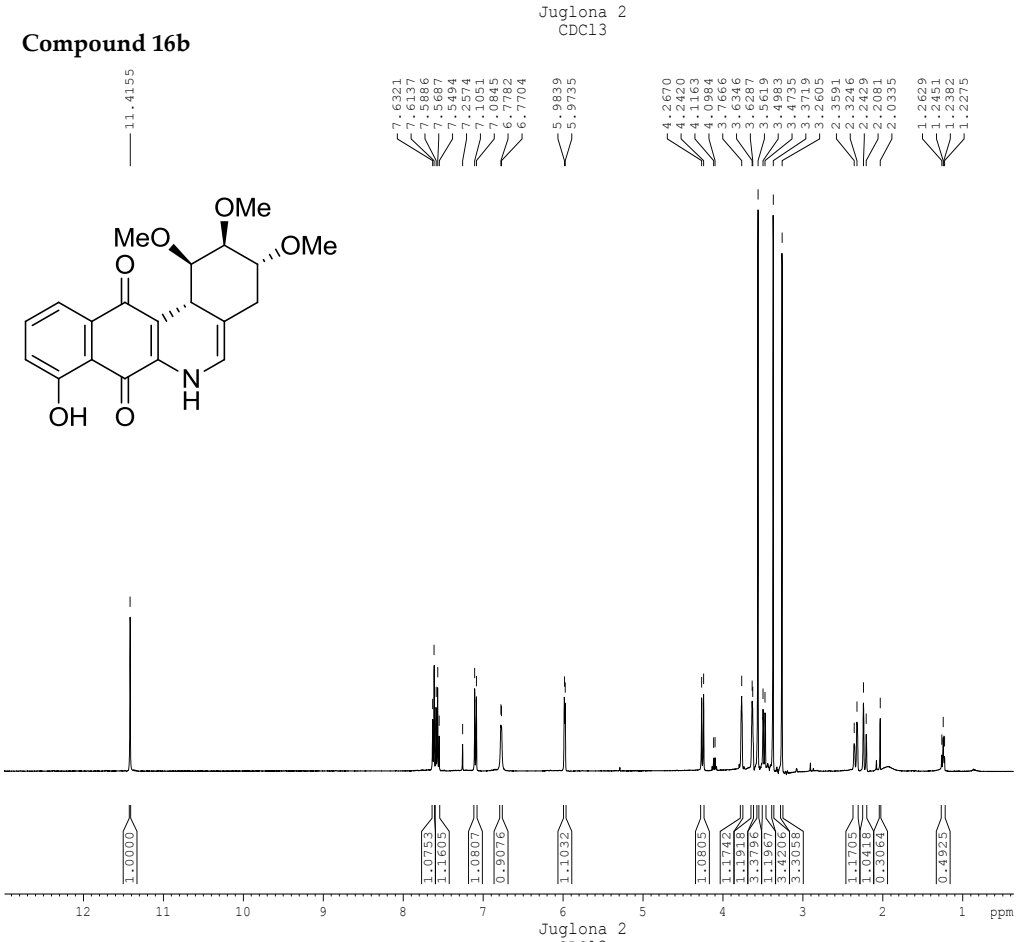



```
NAME          M. Cuellar
EXPNO                291
PROCNO                 1
Date_           20170510
Time                9.17
INSTRUM            spect
PROBHD   5 mm BBI 1H-BB
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ              2.0447731 sec
RG                 574.7
DW                62.400 usec
DE                 6.00 usec
TE                294.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 6.50 usec
PL1                0.00 dB
SFO1          400.1338012 MHz
SI                 16384
SF            400.1300094 MHz
WDW                   no
SSB                    0
LB                 0.00 Hz
GB                     0
PC                 1.00
```

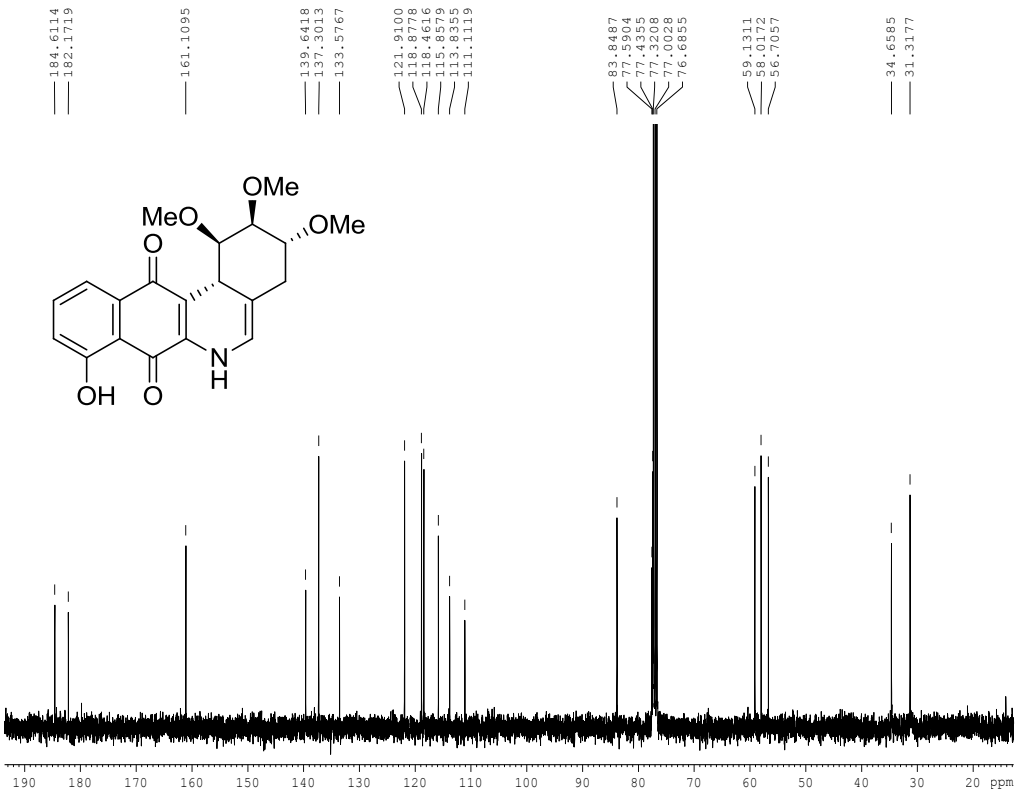



```
NAME          M. Cuellar
EXPNO                293
PROCNO                 1
Date_           20170510
Time                9.50
INSTRUM            spect
PROBHD   5 mm BBI 1H-BB
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                   512
DS                     0
SWH            23980.814 Hz
FIDRES          0.731836 Hz
AQ              0.6832628 sec
RG                 574.7
DW                20.850 usec
DE                 6.00 usec
TE                294.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                14.00 usec
PL1               -6.00 dB
SFO1          100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             85.00 usec
PL2                6.00 dB
PL12              23.00 dB
PL13              23.00 dB
SFO2          400.1316005 MHz
SI                 32768
SF            100.6127724 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```

Compound 16b

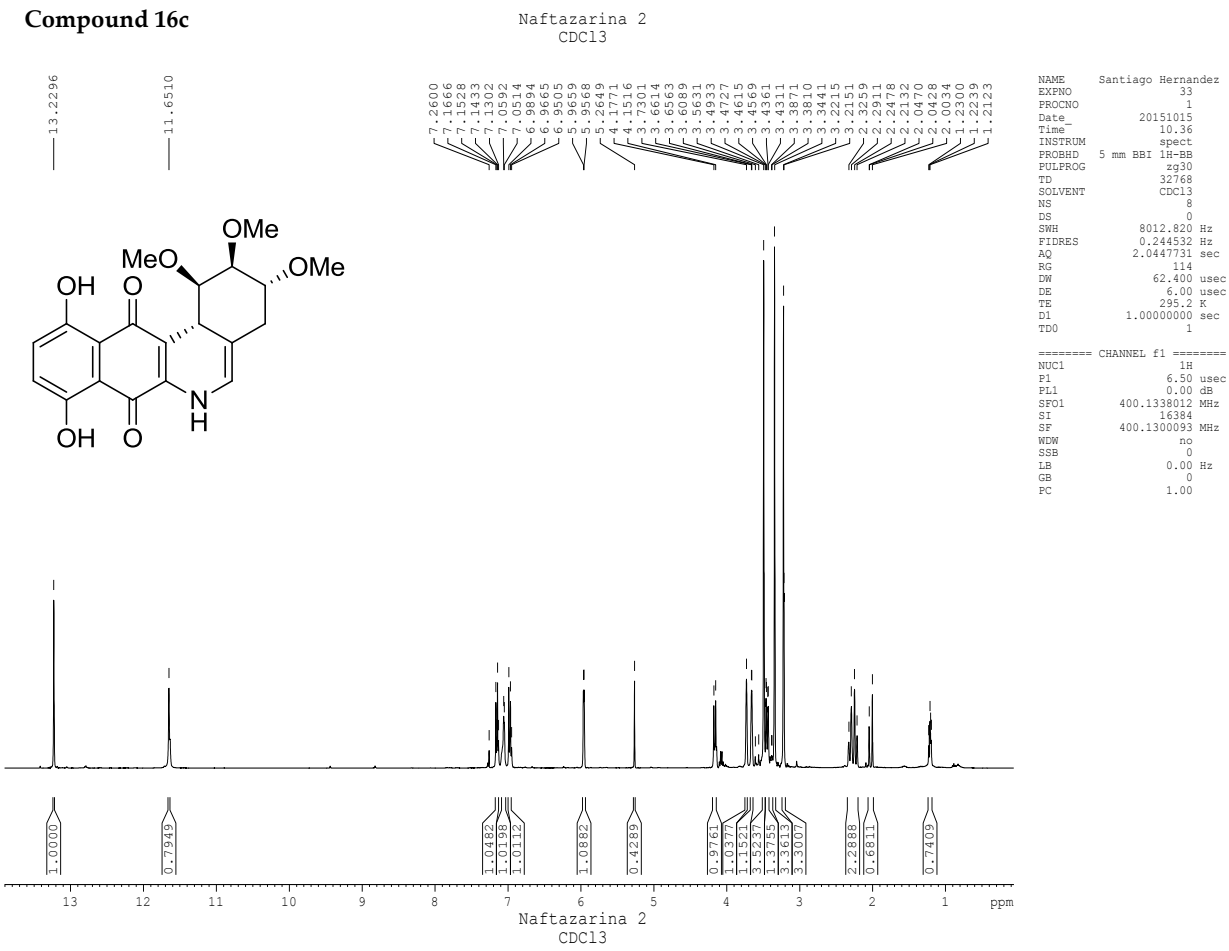



```
NAME      Santiago Hernandez
EXPNO                 28
PROCNO                 1
Date_           20151014
Time_             16.32
INSTRUM           spect
PROBHD   5 mm BBI 1H-BB
PULPROG           zg30
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    0
SWH            8012.820 Hz
FIDRES            0.244532 Hz
AQ             2.0447731 sec
RG                322.5
DW                62.400 usec
DE                 6.00 usec
TE                294.2 K
D1             1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                 6.50 usec
PL1                0.00 dB
SFO1         400.1338012 MHz
SI                16384
SF           400.1300103 MHz
WDW                  no
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 1.00
```



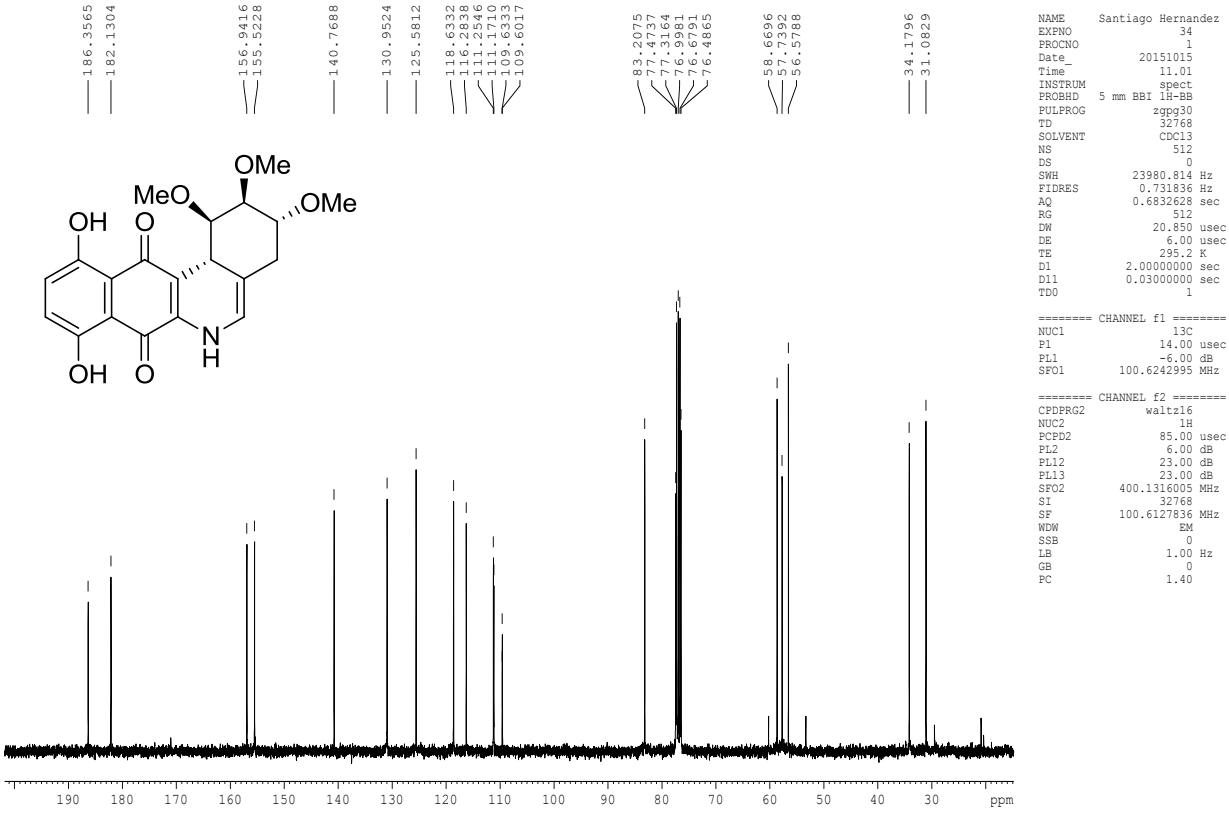

```
NAME      Santiago Hernandez
EXPNO                 32
PROCNO                 1
Date_           20151015
Time_             10.30
INSTRUM           spect
PROBHD   5 mm BBI 1H-BB
PULPROG           zgpg30
TD                32768
SOLVENT           CDCl3
NS                  512
DS                    0
SWH           23980.814 Hz
FIDRES            0.731836 Hz
AQ             0.6832628 sec
RG                574.7
DW                20.850 usec
DE                 6.00 usec
TE                295.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                14.00 usec
PL1               -6.00 dB
SFO1         100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             85.00 usec
PL2                6.00 dB
PL12              23.00 dB
PL13              23.00 dB
SFO2         400.1316005 MHz
SI                32768
SF           100.6127733 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Compound 16c



NAME Santiago Hernandez
EXPNO 33
PROCNO 1
Date_ 20151015
Time 10.36
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 114
DW 62.400 usec
DE 6.00 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 6.50 usec
PL1 0.00 dB
SFO1 400.1338012 MHz
SI 16384
SF 400.1300093 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



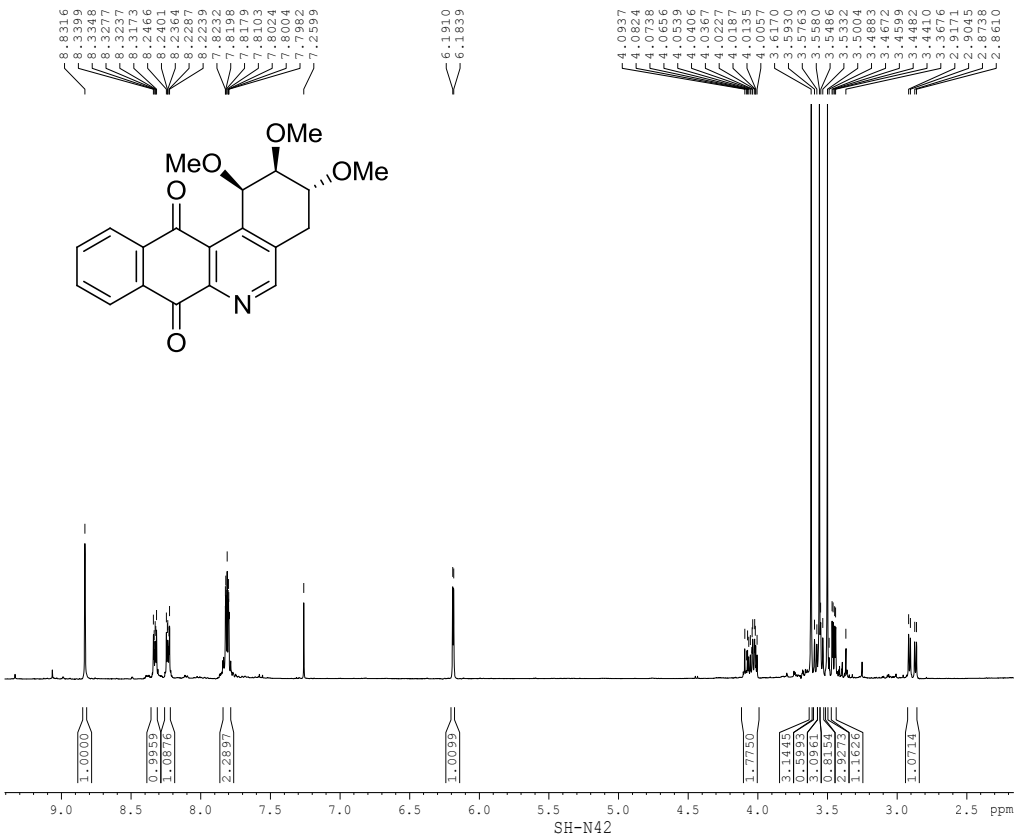
NAME Santiago Hernandez
EXPNO 34
PROCNO 1
Date_ 20151015
Time 11.01
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 512
DS 0
SWH 23980.814 Hz
FIDRES 0.731836 Hz
AQ 0.6832628 sec
RG 512
DW 20.850 usec
DE 6.00 usec
TE 295.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 14.00 usec
PL1 -6.00 dB
SFO1 100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 85.00 usec
PL2 6.00 dB
PL12 23.00 dB
PL13 23.00 dB
SFO2 400.1316005 MHz
SI 32768
SF 100.6127836 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

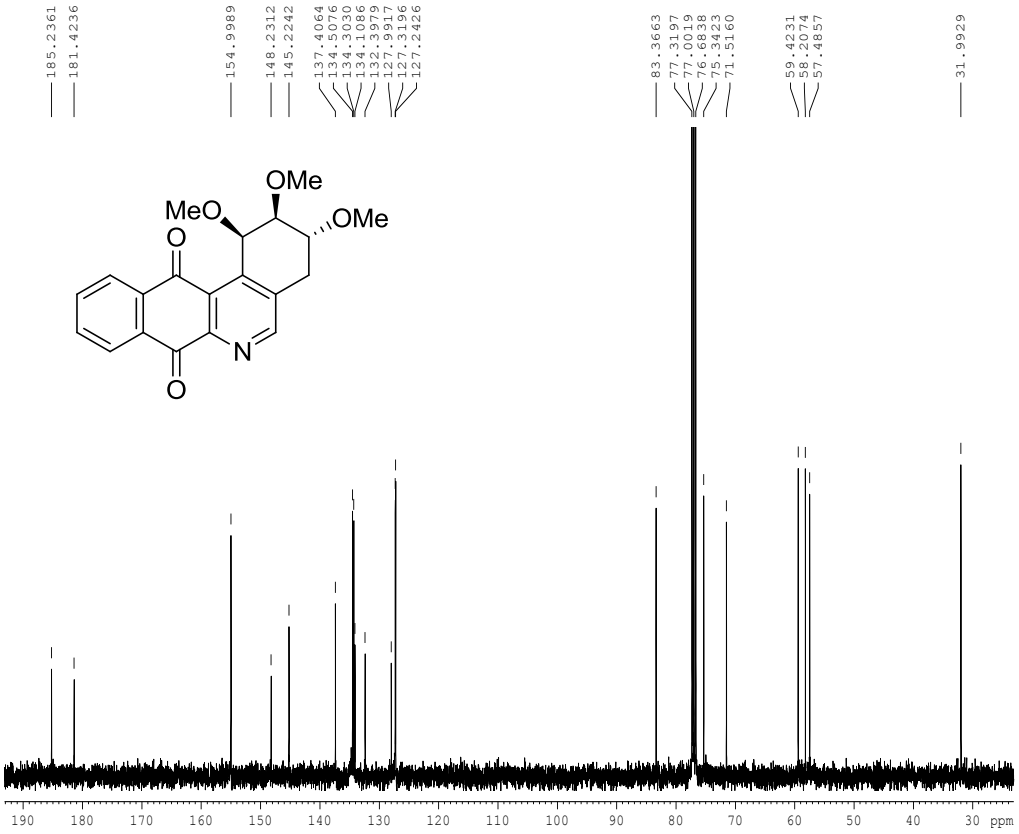
Compound 17

SH-N42
CDCl3




```
NAME      Santiago Hernandez
EXPNO                 65
PROCNO                 1
Date_           20160407
Time                8.46
INSTRUM            spect
PROBHD   5 mm BBI 1H-BB
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             8012.820 Hz
FIDRES             0.244532 Hz
AQ              2.0447731 sec
RG                   256
DW                62.400 usec
DE                 6.00 usec
TE                296.2 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                  6.50 usec
PL1                 0.00 dB
SFO1          400.1338012 MHz
SI                 16384
SF            400.1300094 MHz
WDW                   no
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  1.00
```

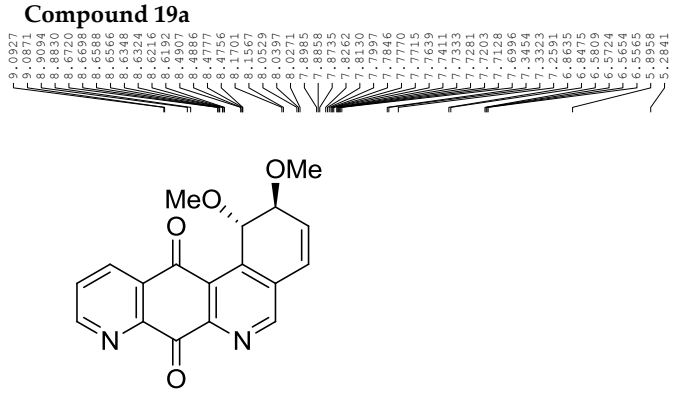
SH-N42
CDCl3

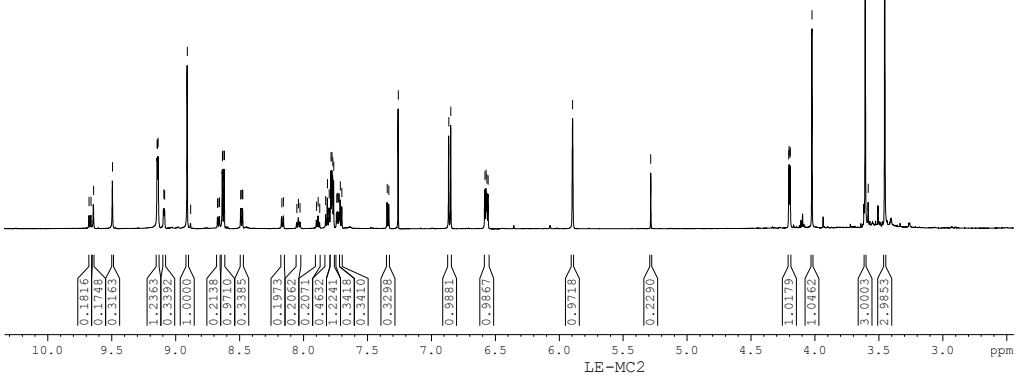



```
NAME      Santiago Hernandez
EXPNO                 68
PROCNO                 1
Date_           20160411
Time               11.13
INSTRUM            spect
PROBHD   5 mm BBI 1H-BB
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                   512
DS                     0
SWH            23980.814 Hz
FIDRES             0.731836 Hz
AQ              0.6832628 sec
RG                 574.7
DW                20.850 usec
DE                 6.00 usec
TE                296.2 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 14.00 usec
PL1                -6.00 dB
SFO1          100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              85.00 usec
PL2                 6.00 dB
PL12               23.00 dB
PL13               23.00 dB
SFO2          400.1316005 MHz
SI                 32768
SF            100.6127745 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

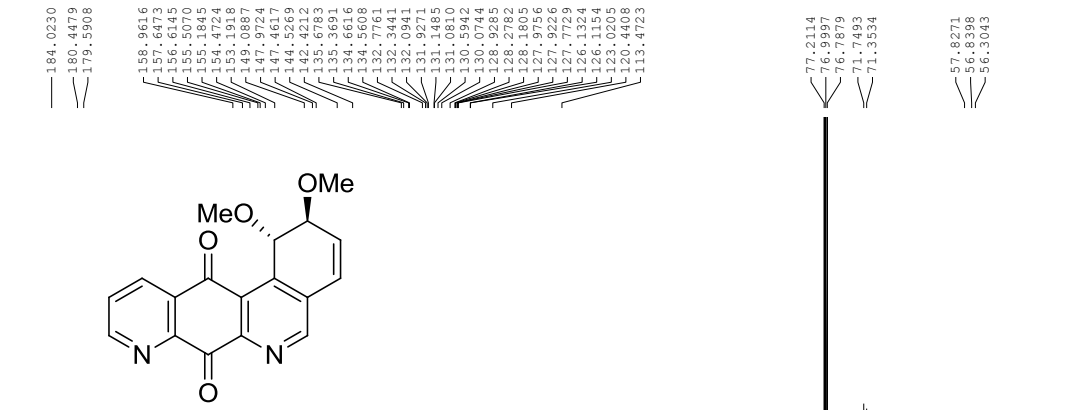
LE-MC2

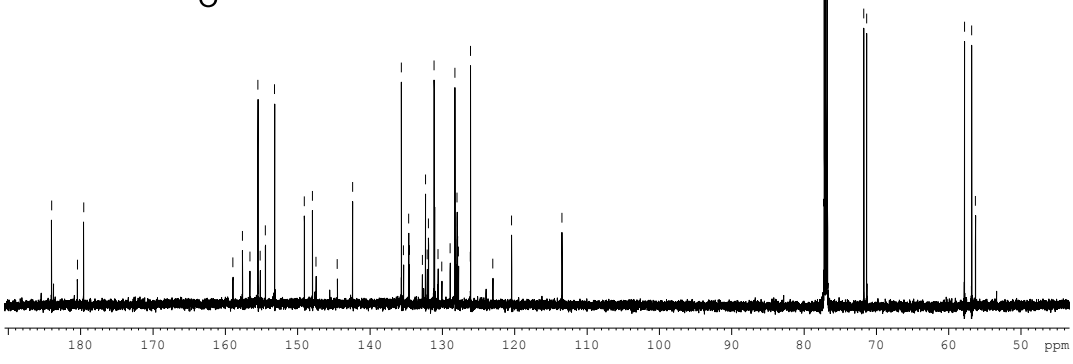
Compound 19a





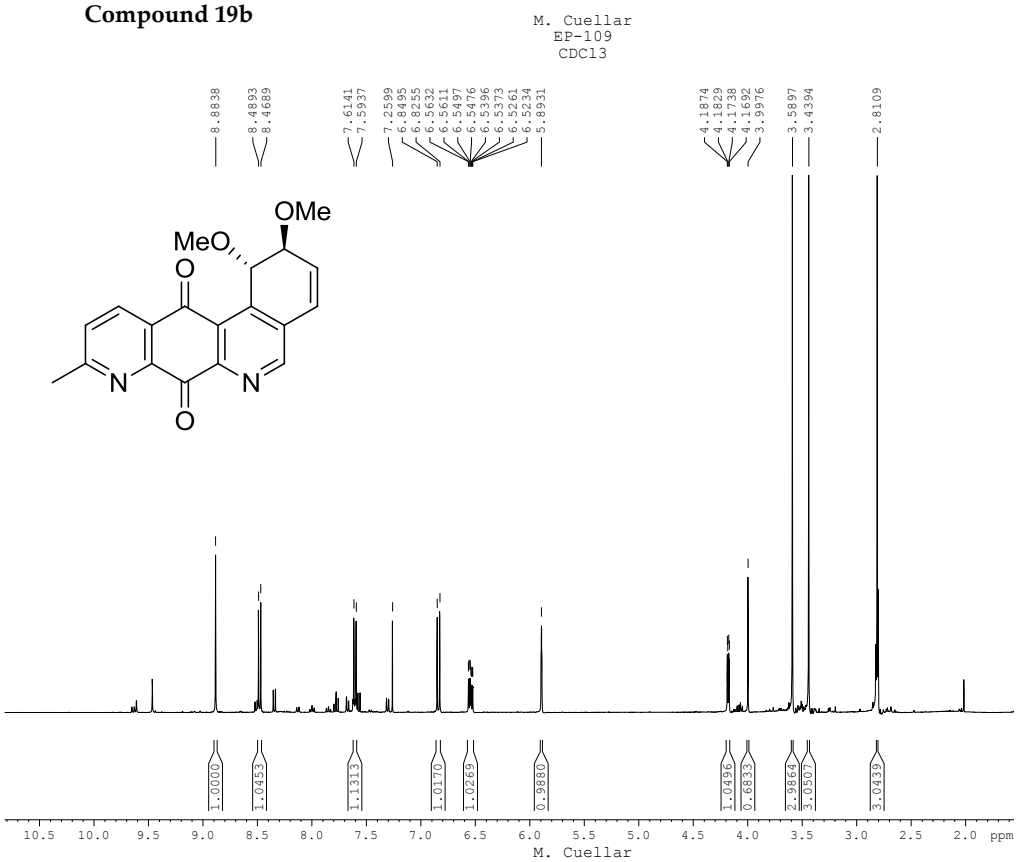

```
NAME              le-mc2
EXPNO                  1
PROCNO                 1
Date_           20171122
Time                7.19
INSTRUM            spect
PROBHD   5 mm CPTCI 1H-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     8
DS                     2
SWH            12019.230 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                  12.7
DW                41.600 usec
DE                20.00 usec
TE                300.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         600.2330011 MHz
NUC1                   1H
P1                  6.60 usec
SI                 65536
SF           600.2300150 MHz
WDW                   no
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  1.00
```



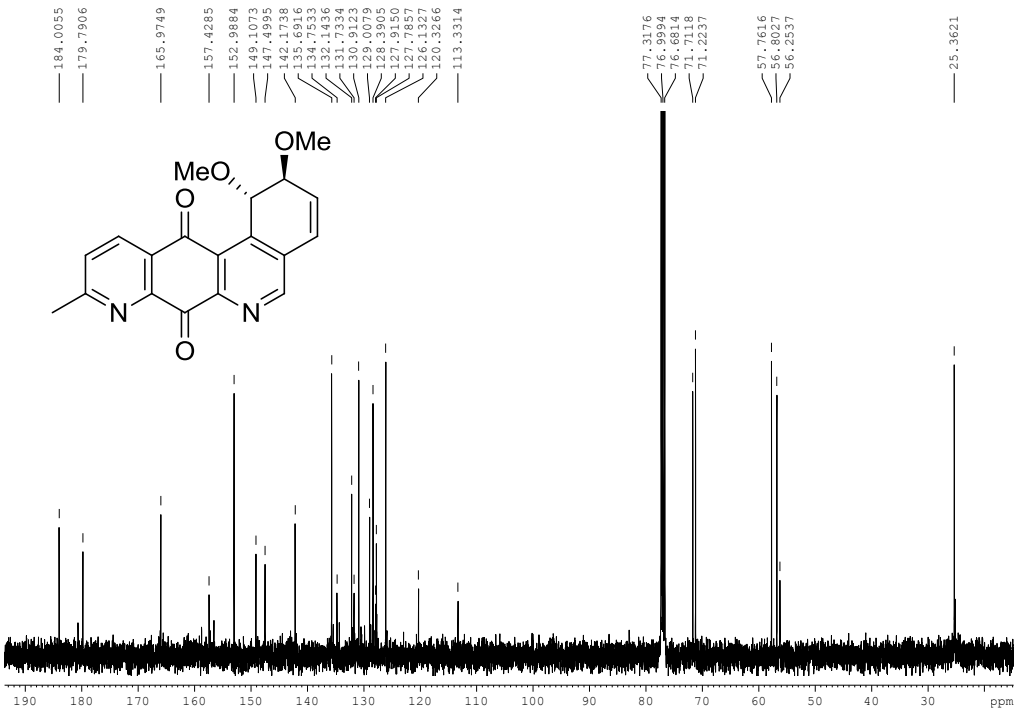



```
NAME              le-mc2
EXPNO                  2
PROCNO                 1
Date_           20171122
Time                7.31
INSTRUM            spect
PROBHD   5 mm CPTCI 1H-
PULPROG         jagzgdc30
TD                 32768
SOLVENT            CDCl3
NS                   268
DS                     0
SWH            34722.223 Hz
FIDRES         1.059638 Hz
AQ             0.4719092 sec
RG                  1290
DW                14.400 usec
DE                15.00 usec
TE                300.0 K
D1             1.50000000 sec
D11            0.03000000 sec

======== CHANNEL f1 ========
SFO1         150.9445561 MHz
NUC1                   13C
P1                  9.50 usec
SI                131072
SF           150.9279599 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.40
```

Compound 19b

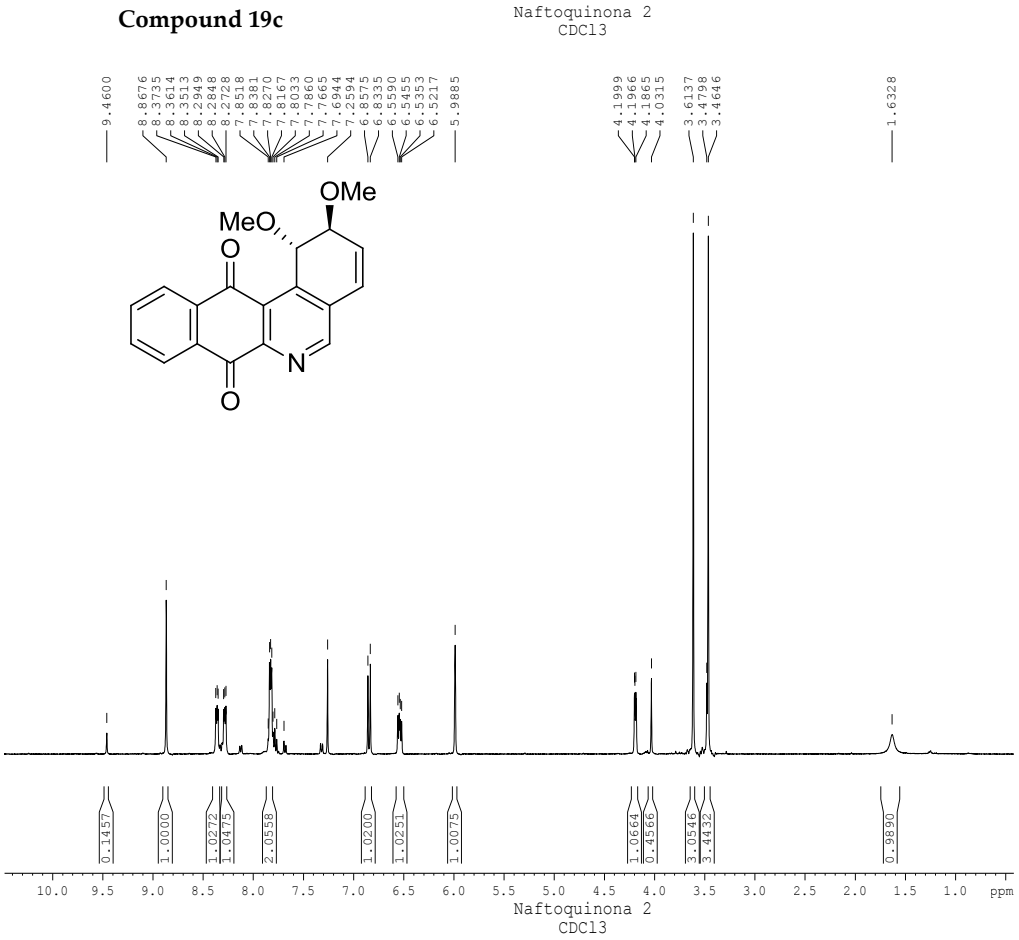



```
NAME          M. Cuellar
EXPNO               311
PROCNO                1
Date_          20170705
Time               15.07
INSTRUM            spect
PROBHD   5 mm BBI 1H-BB
PULPROG            zg30
TD                32768
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             8012.820 Hz
FIDRES             0.244532 Hz
AQ              2.0447731 sec
RG                   362
DW                62.400 usec
DE                 6.00 usec
TE                293.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 6.50 usec
PL1                0.00 dB
SFO1         400.1338012 MHz
SI                 16384
SF           400.1300094 MHz
WDW                   no
SSB                    0
LB                 0.00 Hz
GB                     0
PC                 1.00
```



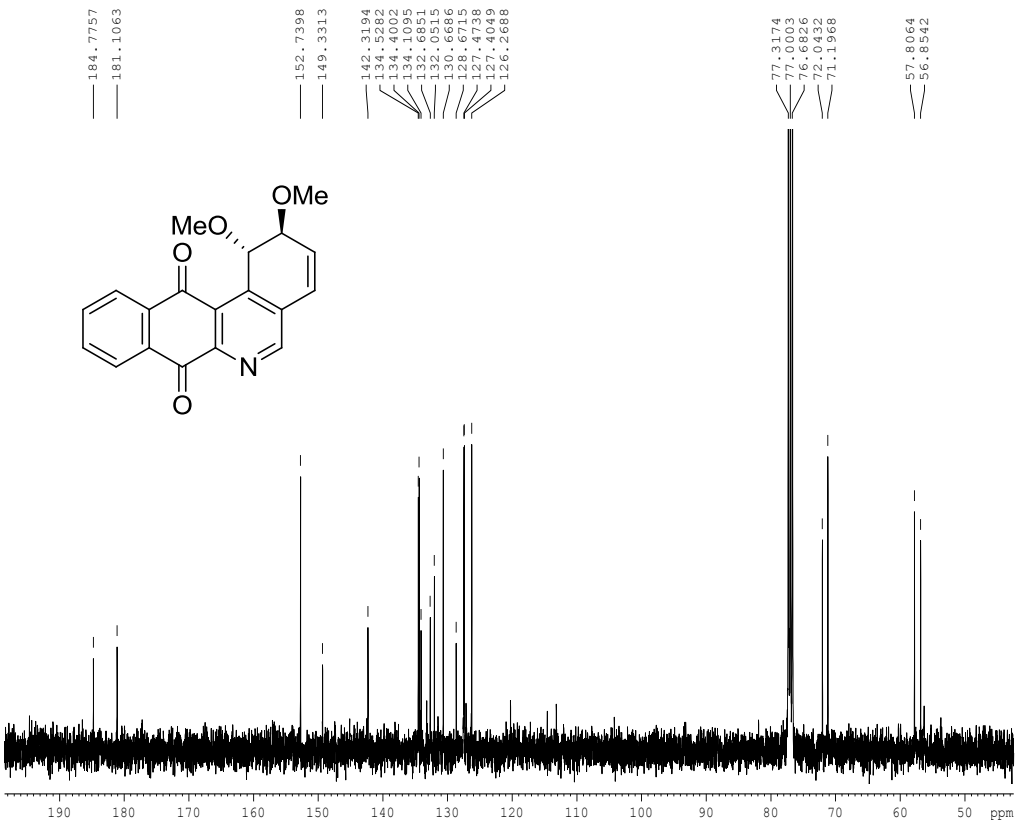

```
NAME          M. Cuellar
EXPNO               312
PROCNO                1
Date_          20170705
Time               15.23
INSTRUM            spect
PROBHD   5 mm BBI 1H-BB
PULPROG          zgpg30
TD                32768
SOLVENT            CDCl3
NS                   512
DS                     0
SWH            23980.814 Hz
FIDRES             0.731836 Hz
AQ              0.6832628 sec
RG                 574.7
DW                20.850 usec
DE                 6.00 usec
TE                294.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                14.00 usec
PL1               -6.00 dB
SFO1         100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             85.00 usec
PL2                6.00 dB
PL12              23.00 dB
PL13              23.00 dB
SFO2         400.1316005 MHz
SI                 32768
SF           100.6127764 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```

Compound 19c



NAME Santiago Hernandez
EXPNO 37
PROCNO 1
Date_ 20151103
Time 12.29
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 1024
DW 62.400 usec
DE 6.00 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 6.50 usec
PL1 0.00 dB
SFO1 400.1338012 MHz
SI 16384
SF 400.1300097 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

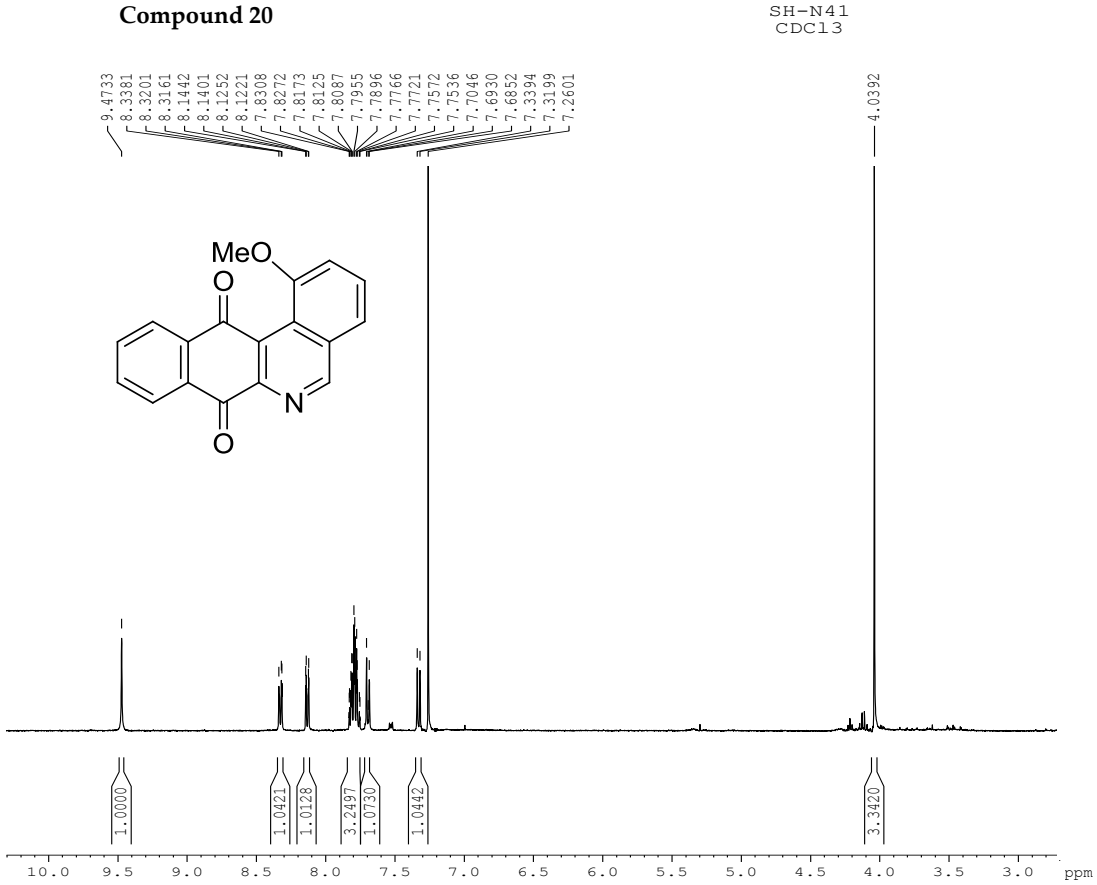


NAME Santiago Hernandez
EXPNO 38
PROCNO 1
Date_ 20151103
Time 12.53
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1536
DS 0
SWH 23980.814 Hz
FIDRES 0.731836 Hz
AQ 0.6832628 sec
RG 574.7
DW 20.850 usec
DE 6.00 usec
TE 297.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

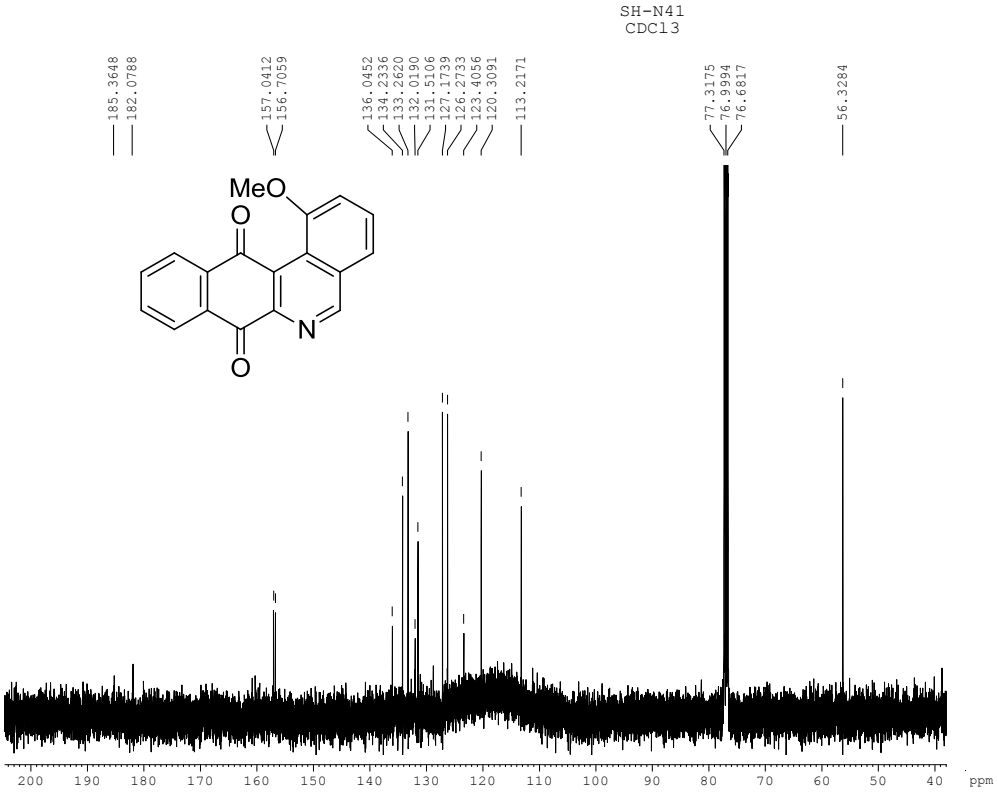
======== CHANNEL f1 ========
NUC1 13C
P1 14.00 usec
PL1 -6.00 dB
SFO1 100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 85.00 usec
PL2 6.00 dB
PL12 23.00 dB
PL13 23.00 dB
SFO2 400.1316005 MHz
SI 32768
SF 100.6127709 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Compound 20

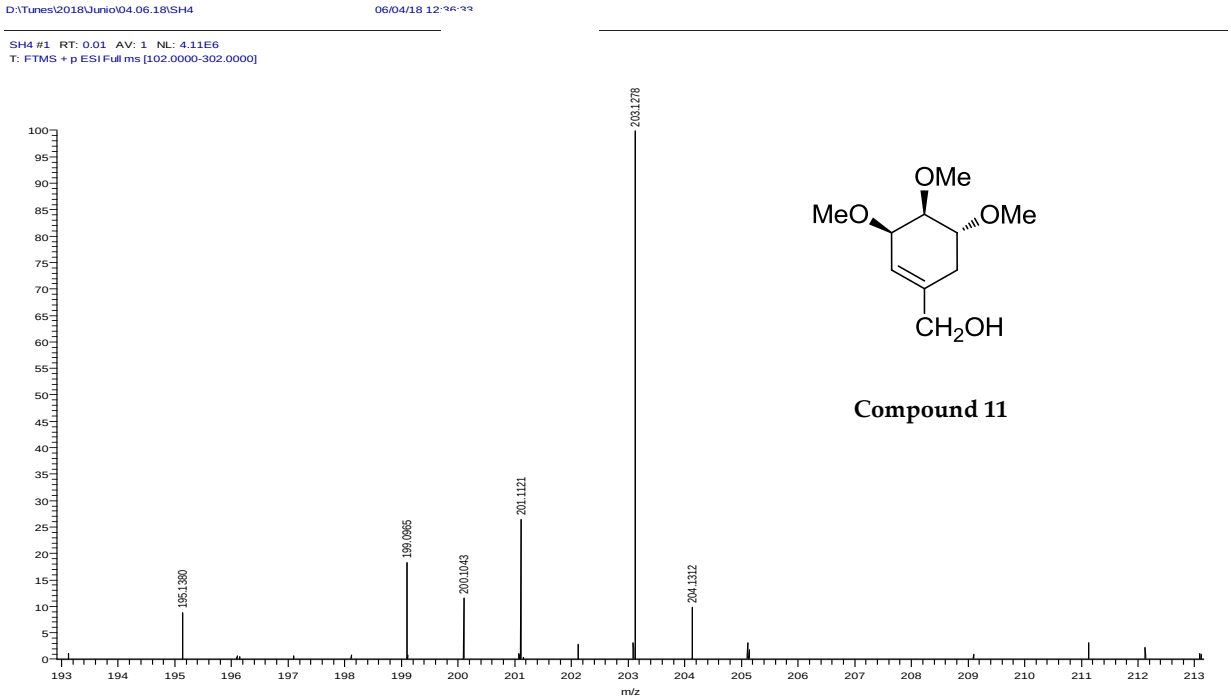



```
NAME      Santiago Hernandez
EXPNO                 83
PROCNO                 1
Date_           20160531
Time                15.15
INSTRUM             spect
PROBHD   5 mm BBI 1H-BB
PULPROG             zg30
TD                 32768
SOLVENT             CDCl3
NS                     8
DS                     0
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ              2.0447731 sec
RG                 812.7
DW                62.400 usec
DE                 6.00 usec
TE                295.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 6.50 usec
PL1                0.00 dB
SFO1        400.1338012 MHz
SI                 16384
SF          400.1300093 MHz
WDW                   no
SSB                    0
LB                 0.00 Hz
GB                     0
PC                 1.00
```

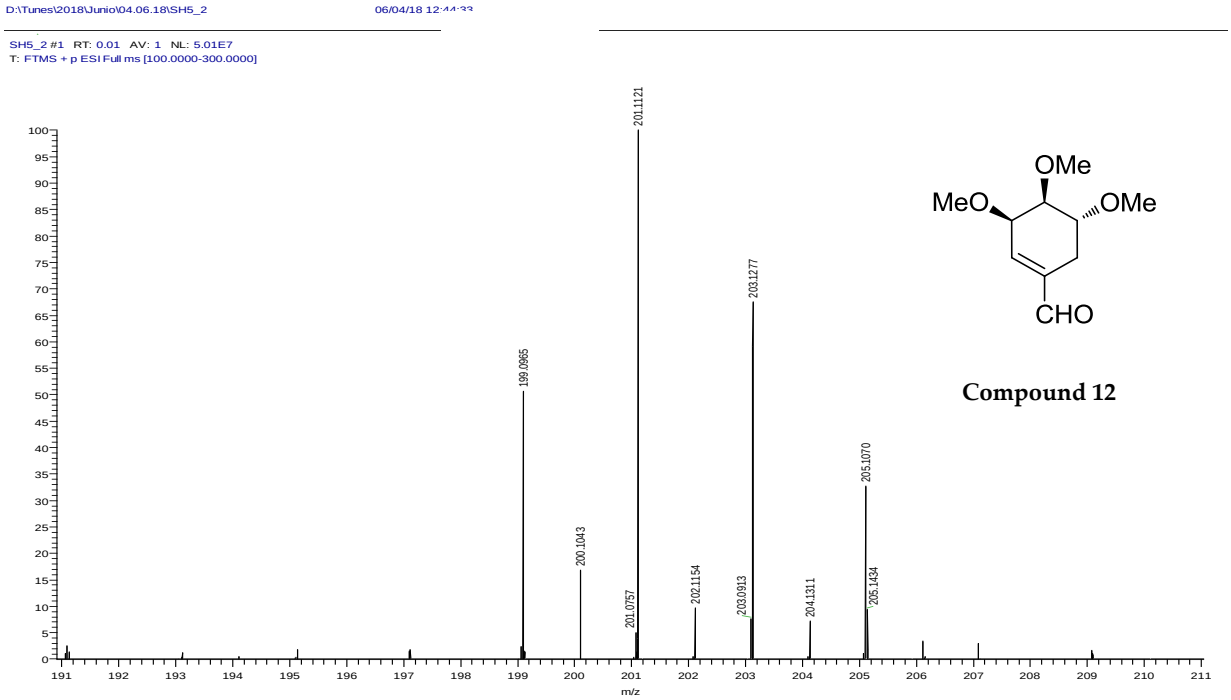



```
NAME      Santiago Hernandez
EXPNO                 87
PROCNO                 1
Date_           20160601
Time                6.05
INSTRUM             spect
PROBHD   5 mm BBI 1H-BB
PULPROG          zgpg30
TD                 32768
SOLVENT             CDCl3
NS                 16000
DS                     0
SWH            23980.814 Hz
FIDRES          0.731836 Hz
AQ              0.6832628 sec
RG                 645.1
DW                20.850 usec
DE                 6.00 usec
TE                297.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                14.00 usec
PL1               -6.00 dB
SFO1       100.6242995 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             85.00 usec
PL2                6.00 dB
PL12              23.00 dB
PL13              23.00 dB
SFO2       400.1316005 MHz
SI                 32768
SF         100.6127699 MHz
WDW                   no
SSB                    0
LB                 0.00 Hz
GB                     0
PC                 1.40
```

S.2 High resolution mass spectroscopy



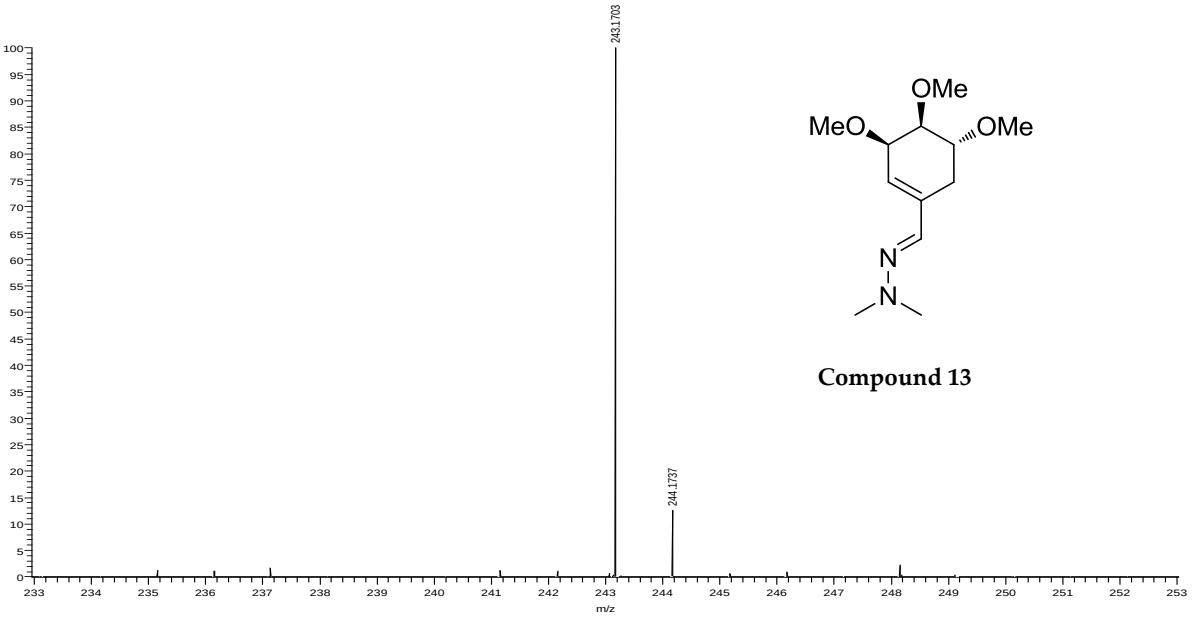
Compound 11



Compound 12

D:\Tunes\2018\Junio\04.06.18\106 06/04/18 12:48:19

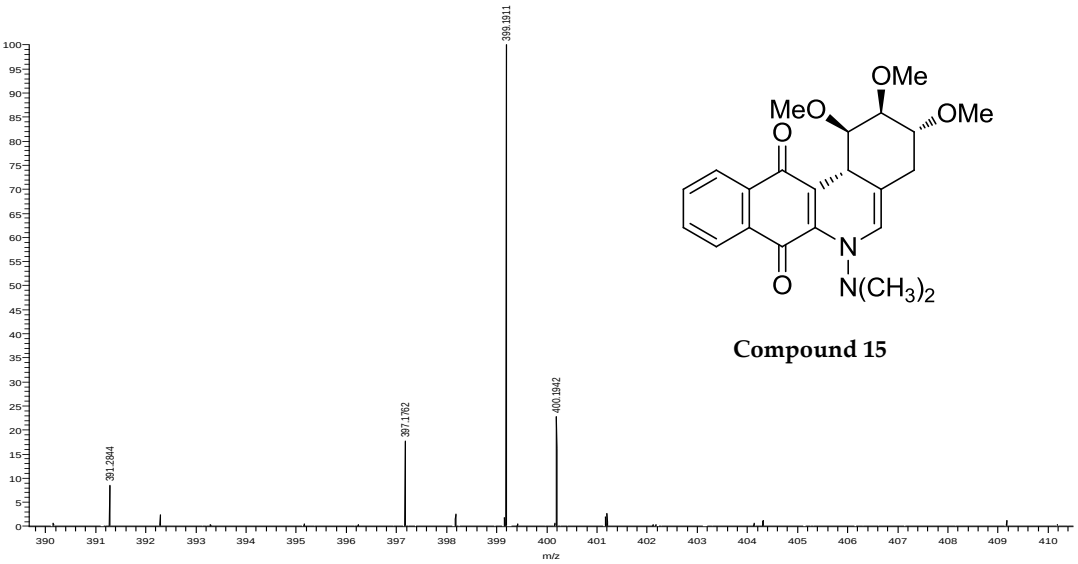
106 #1 RT: 0.01 AV: 1 NL: 5.06E8
T: FTMS + p ESI Full ms [143.0000-343.0000]



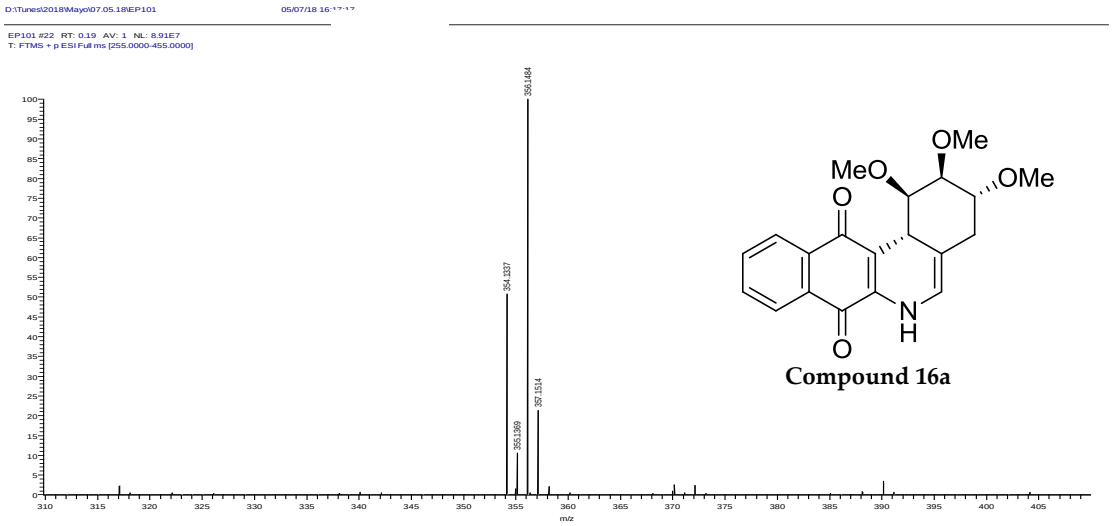
Compound 13

D:\Tunes\2018\Junio\04.06.18\15 06/04/18 12:16:11

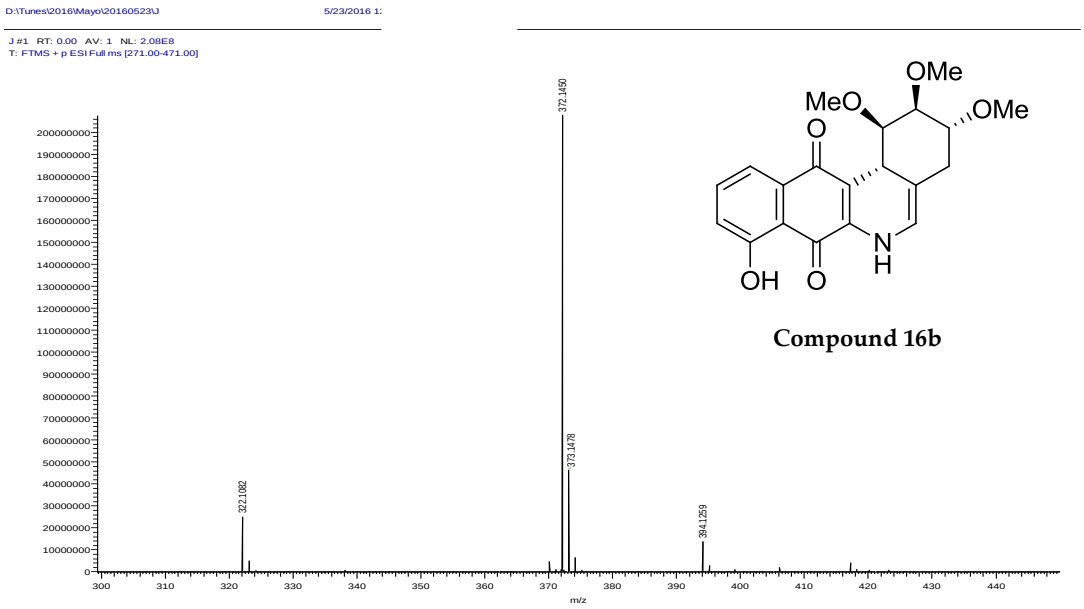
15 #1 RT: 0.01 AV: 1 NL: 6.93E6
T: FTMS + p ESI Full ms [298.0000-498.0000]



Compound 15



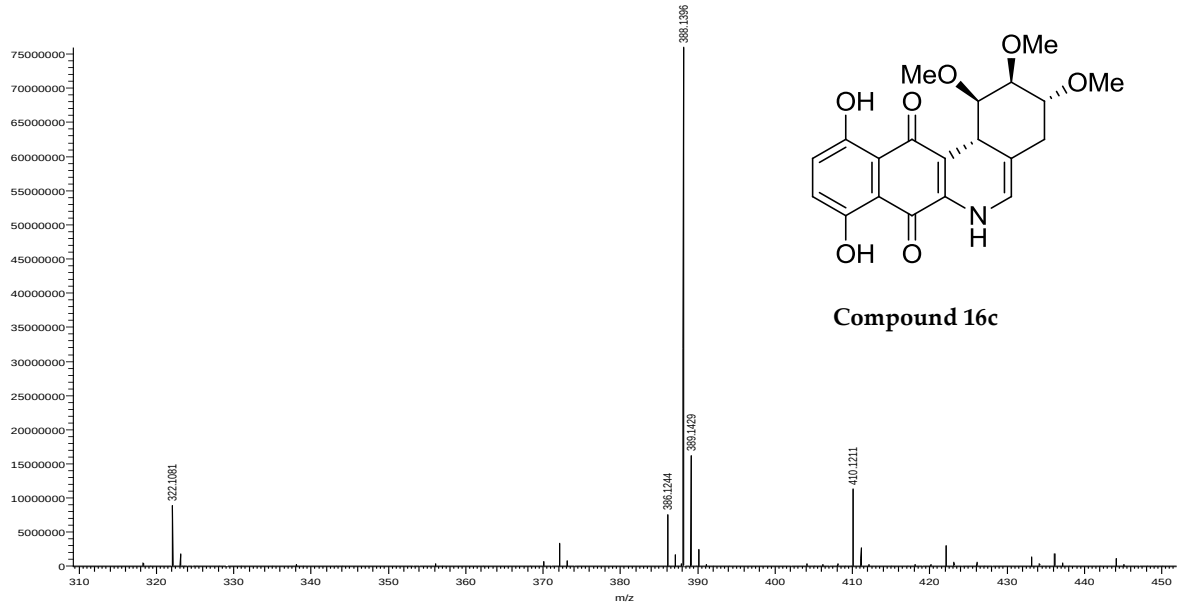
Compound 16a



Compound 16b

D:\Tunes\2016\Mayo\20160523\NZ 5/23/2016 1:

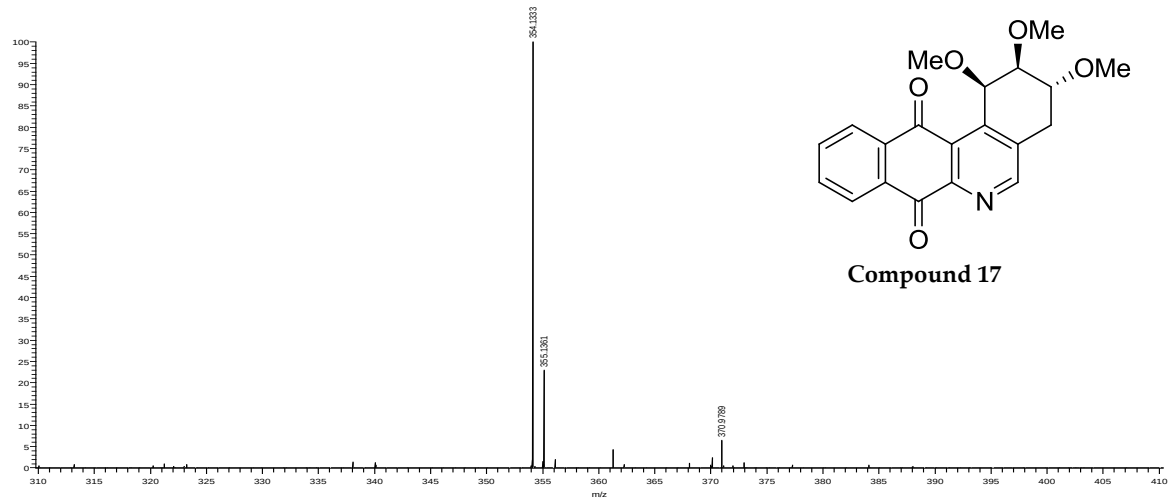
NZ #1 RT: 0.00 AV: 1 NL: 7.60E7
T: FTMS + p ESI Full ms [287.00-487.00]



Compound 16c

D:\Tunes\2018\Mayo\07.05.18\EP106 05/07/18 15:45:13

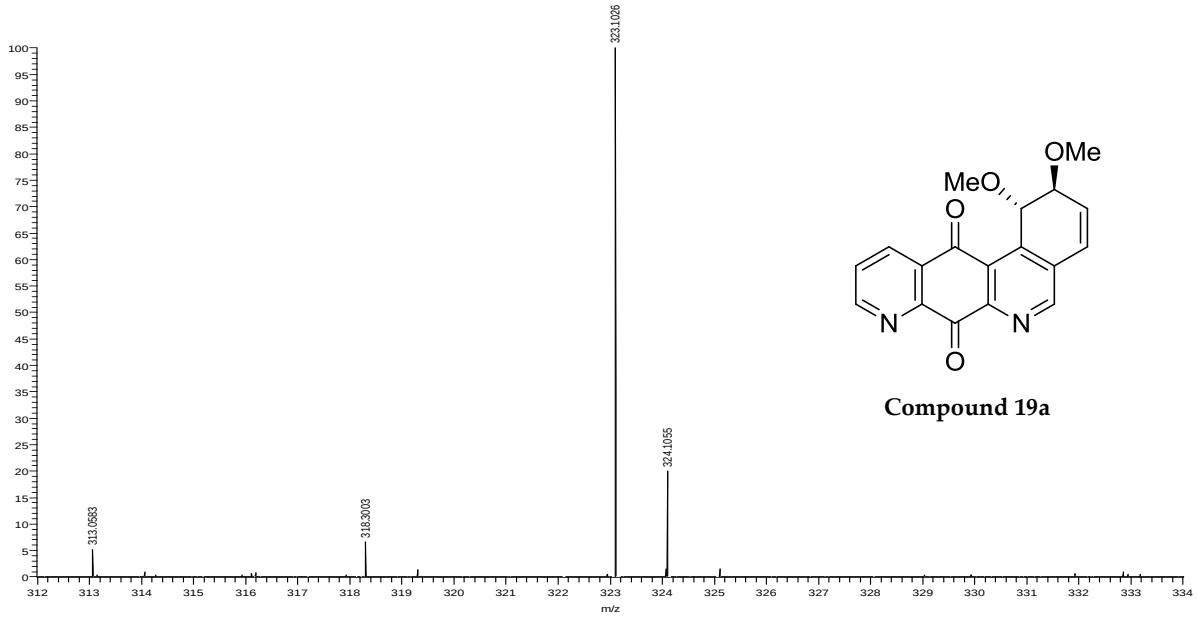
EP106 #1 RT: 0.01 AV: 1 NL: 9.24E7
T: FTMS + p ESI Full ms [255.0000-455.0000]



Compound 17

D:\Tunes\2018\Junio\04.06.18\19a 06/04/18 12:20:16

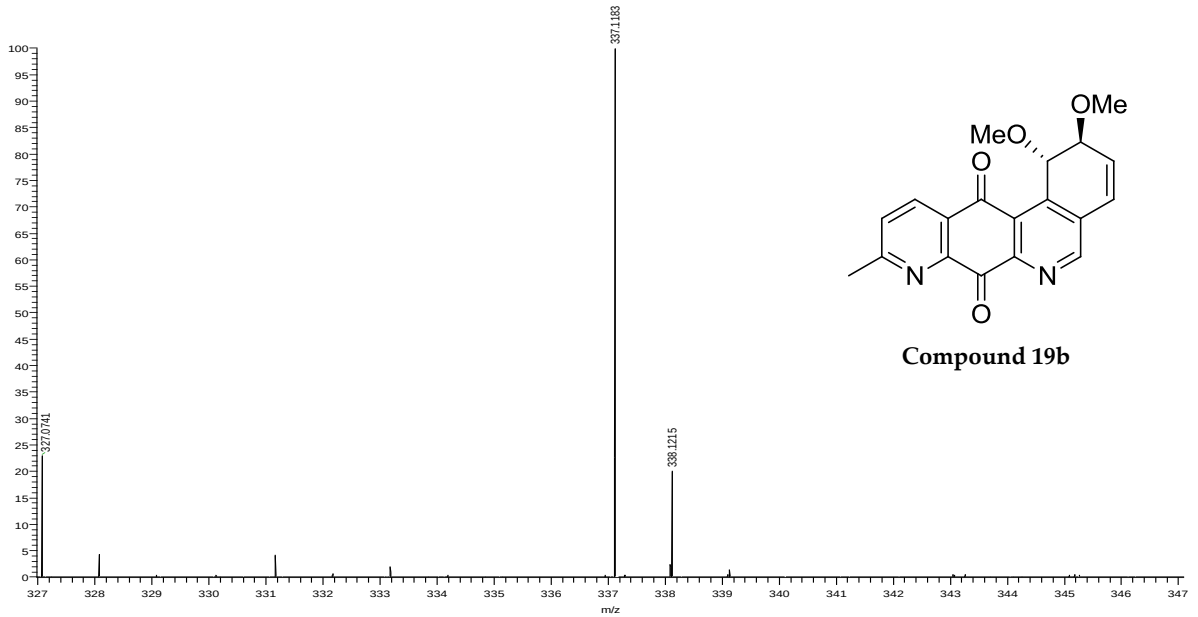
19a #1 RT: 0.01 AV: 1 NL: 1.19E7
T: FTMS + p ESI Full ms [223.0000-423.0000]



Compound 19a

D:\Tunes\2018\Junio\04.06.18\19b 06/04/18 12:23:33

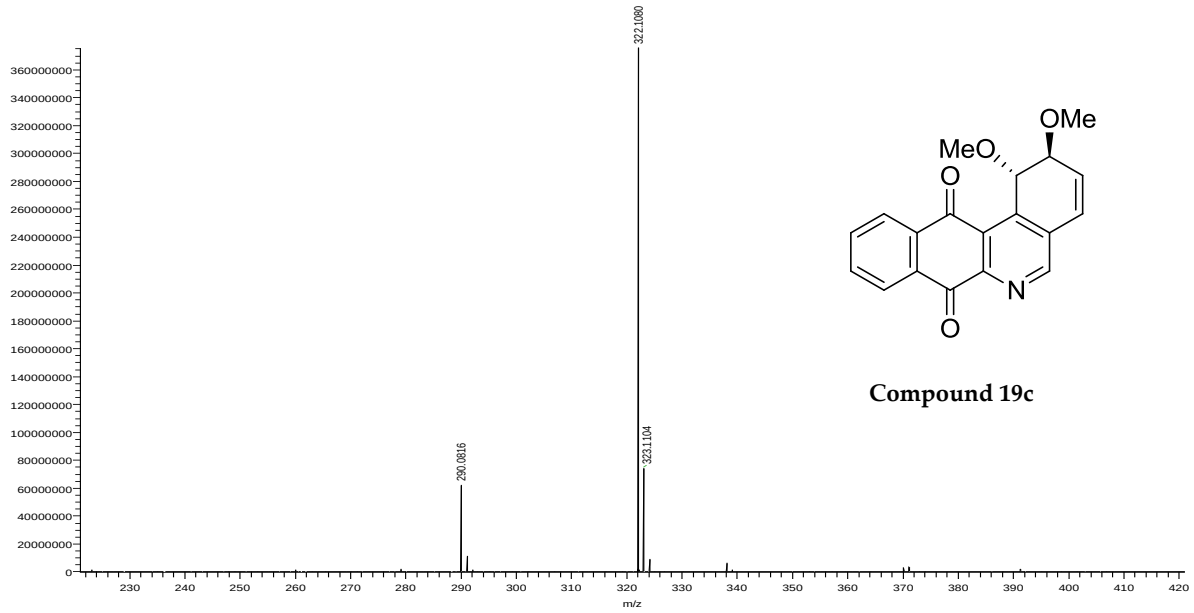
19b #1 RT: 0.01 AV: 1 NL: 1.51E7
T: FTMS + p ESI Full ms [236.0000-436.0000]



Compound 19b

D:\Tunes\2016\Mayo\20160523\NQ 5/23/2016 1:

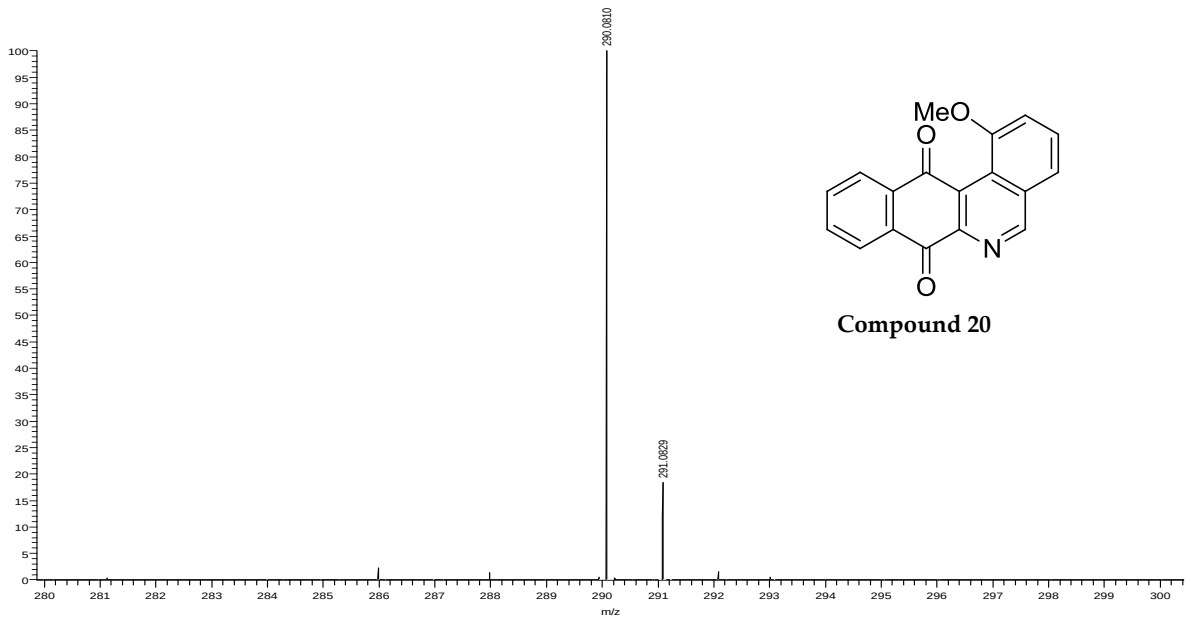
NQ #1 RT: 0.00 AV: 1 NL: 3.75E8
T: FTMS + p ESI Full ms [221.00-421.00]



Compound 19c

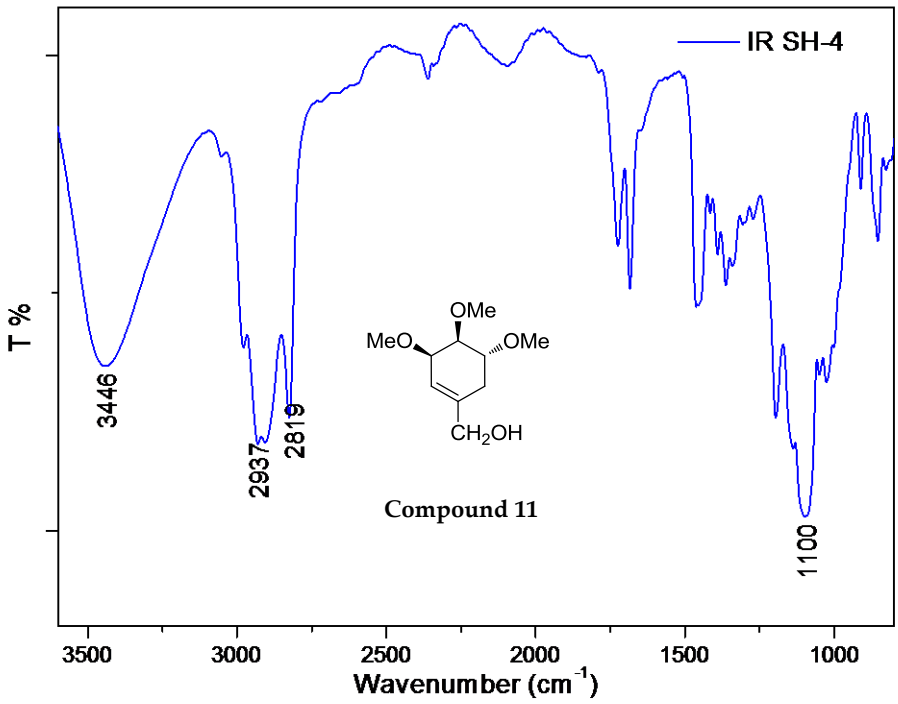
D:\Tunes\2018\Junio\04.06.18\MC20 06/04/18 12:26:51

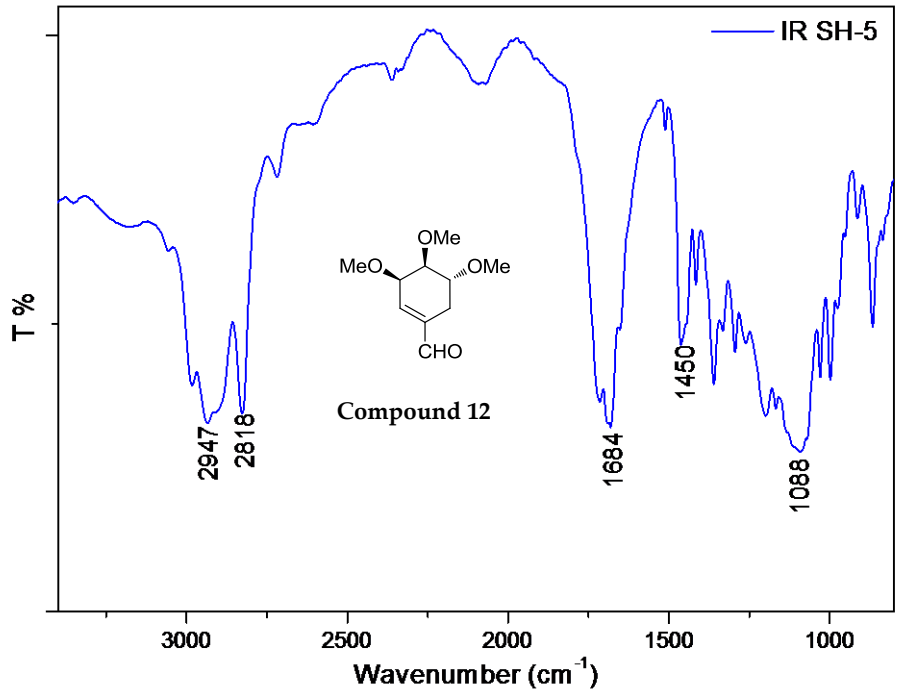
MC20 #1 RT: 0.01 AV: 1 NL: 1.85E8
T: FTMS + p ESI Full ms [189.0000-389.0000]

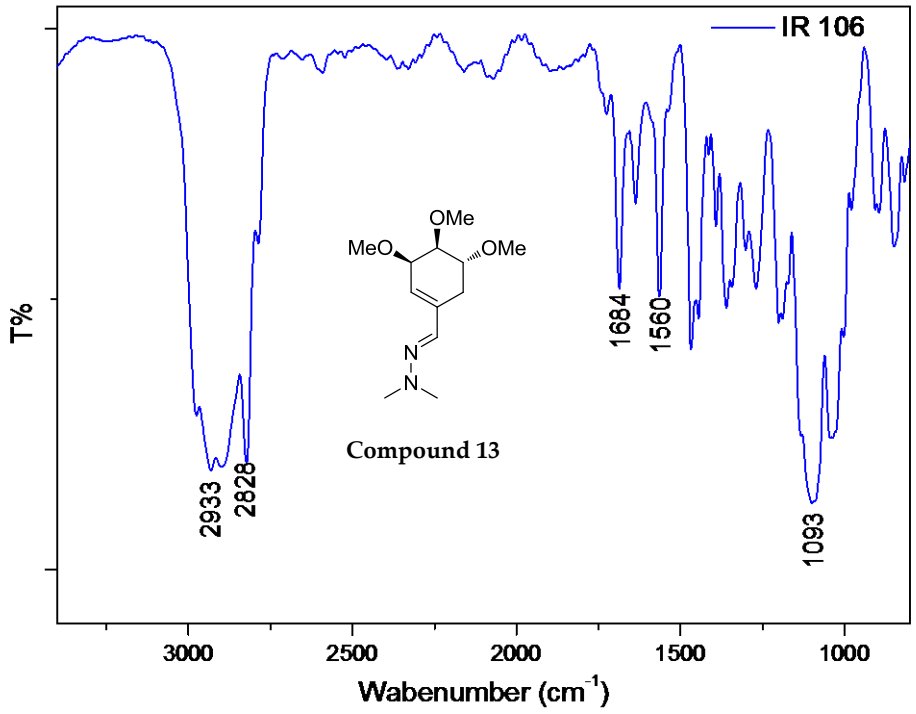


Compound 20

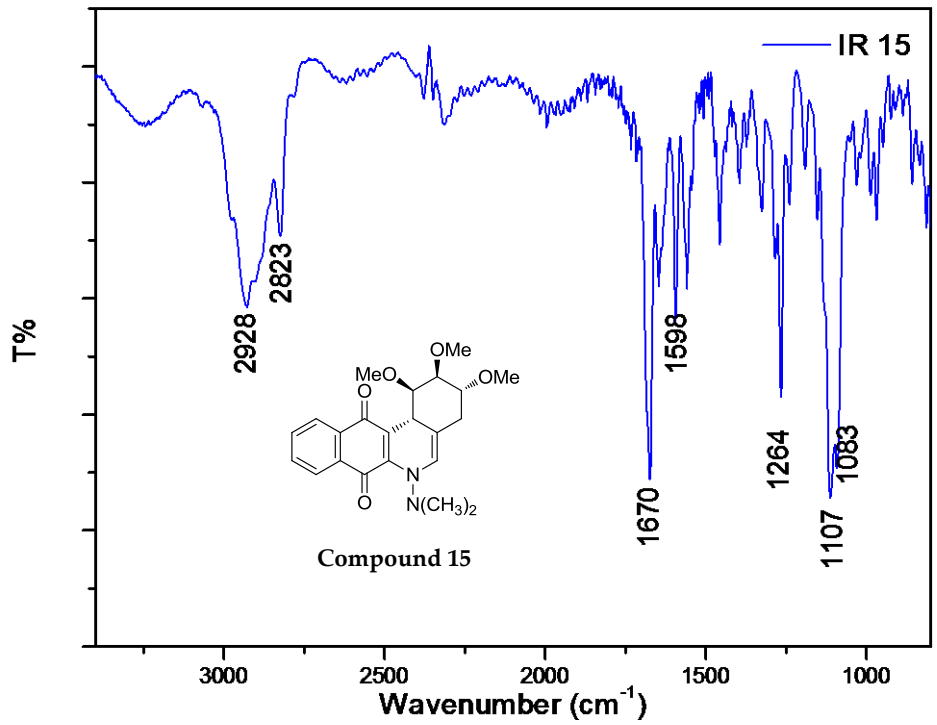
S.3 Infrared spectroscopy



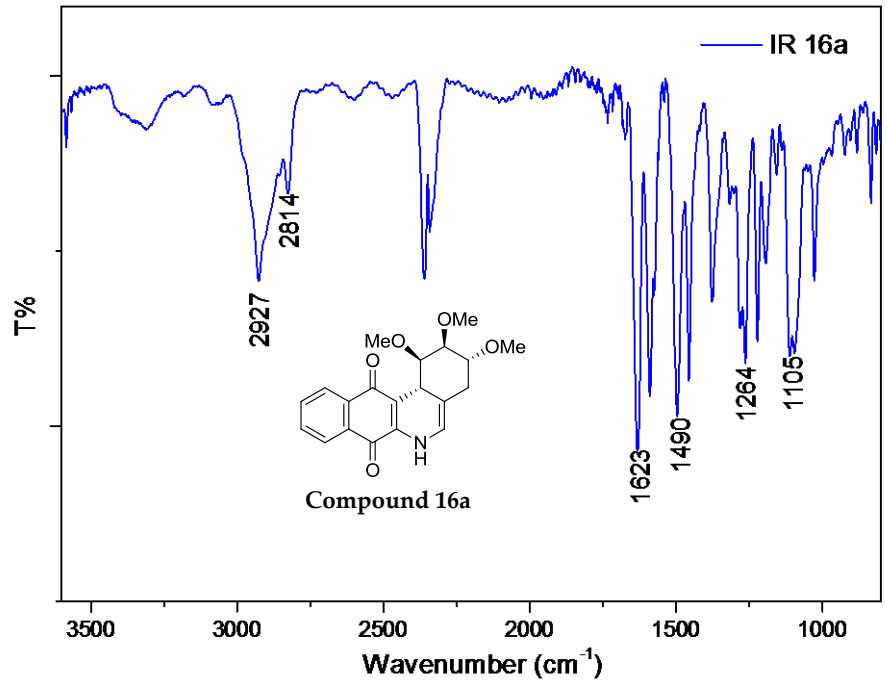




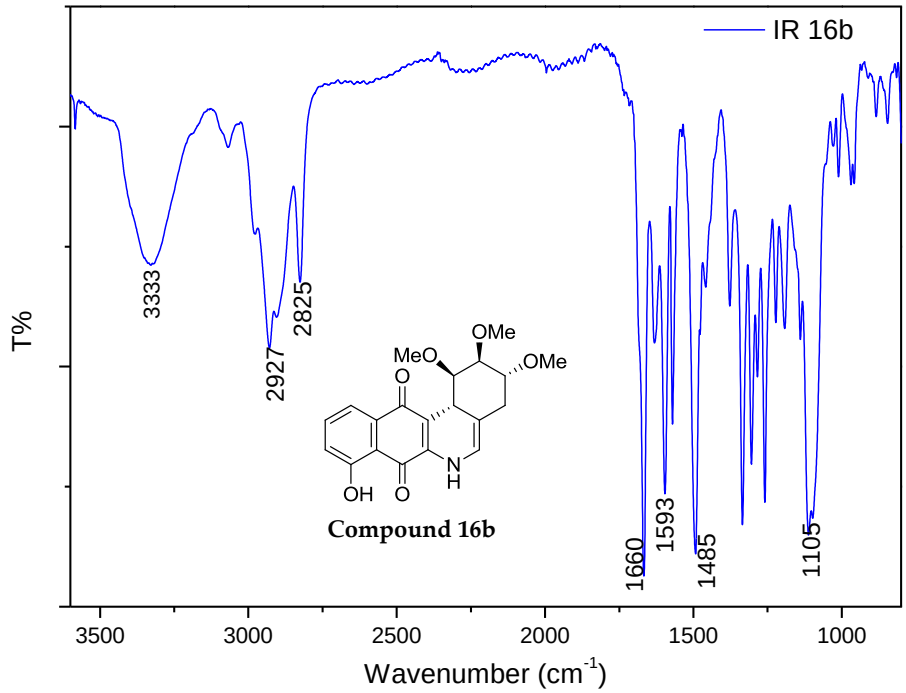
Compound 13



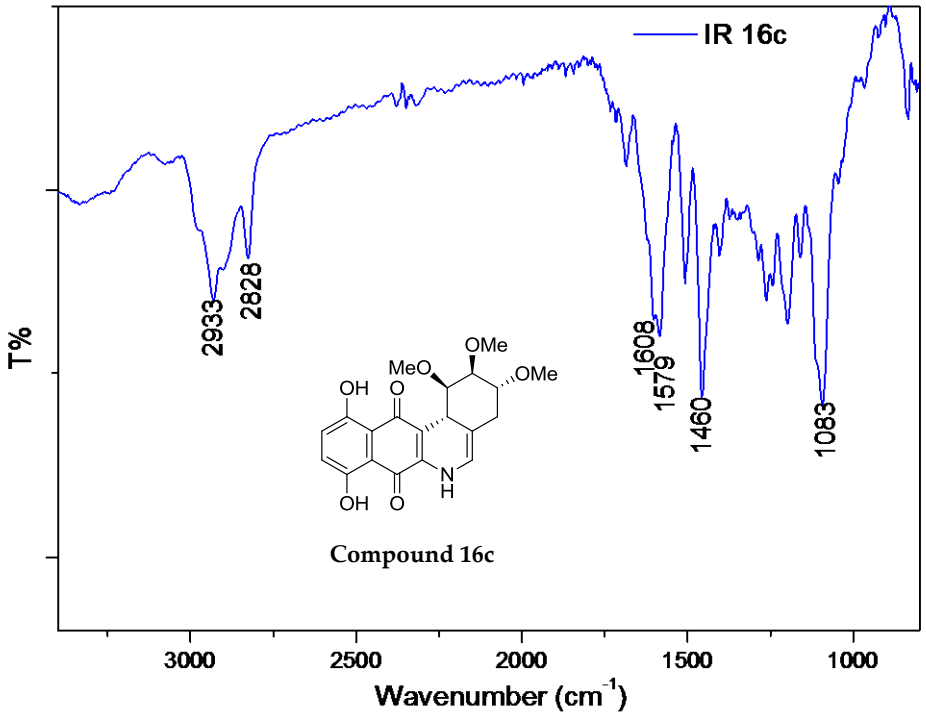
Compound 15



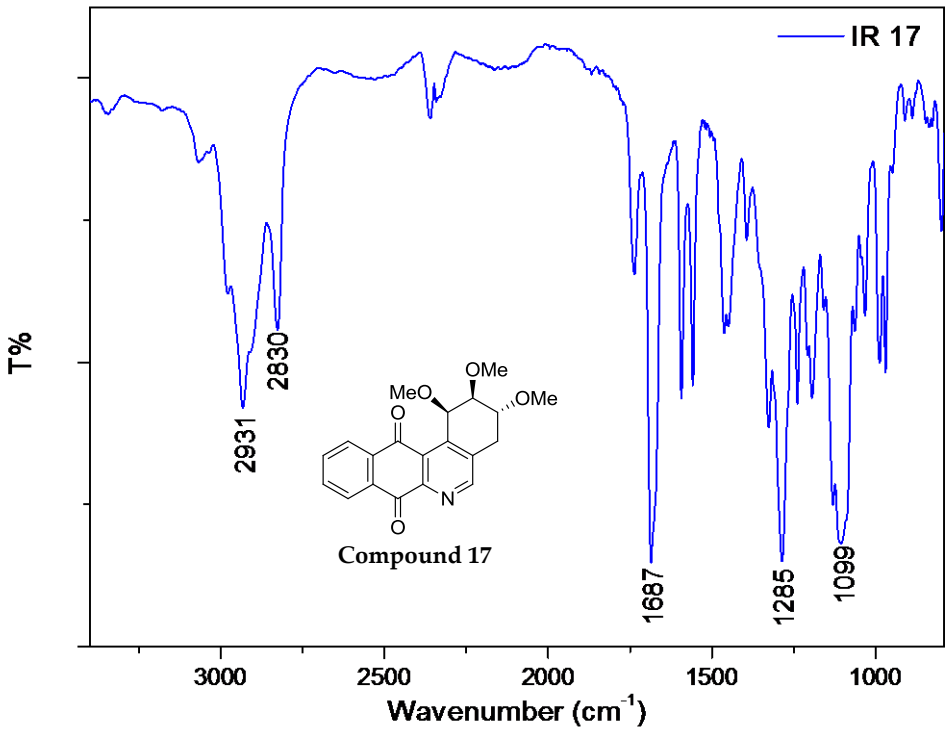
Compound 16a



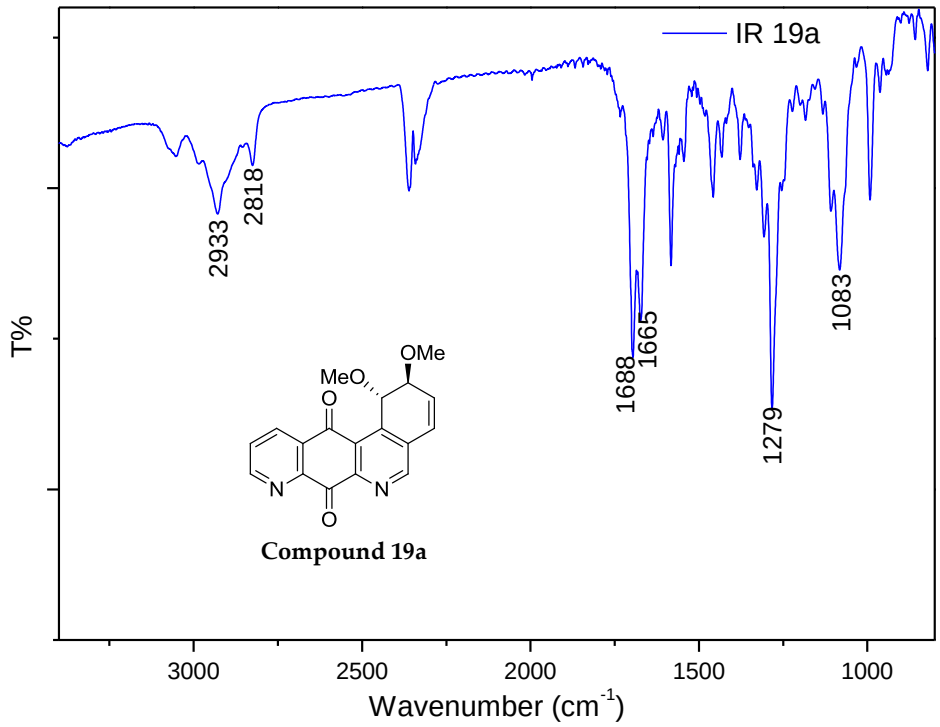
Compound 16b

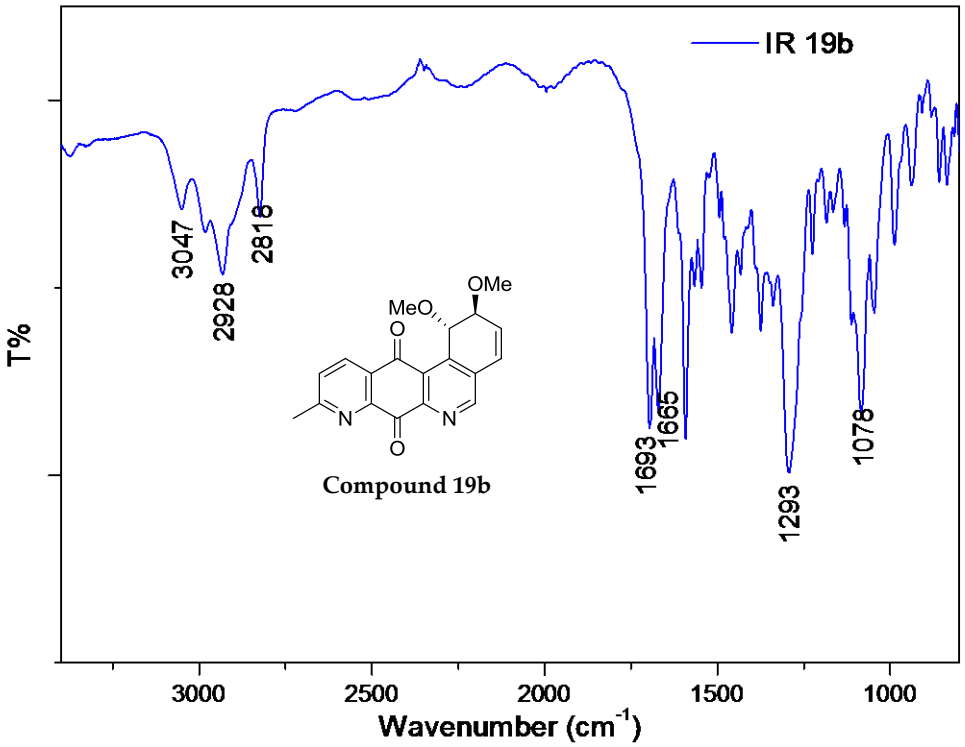


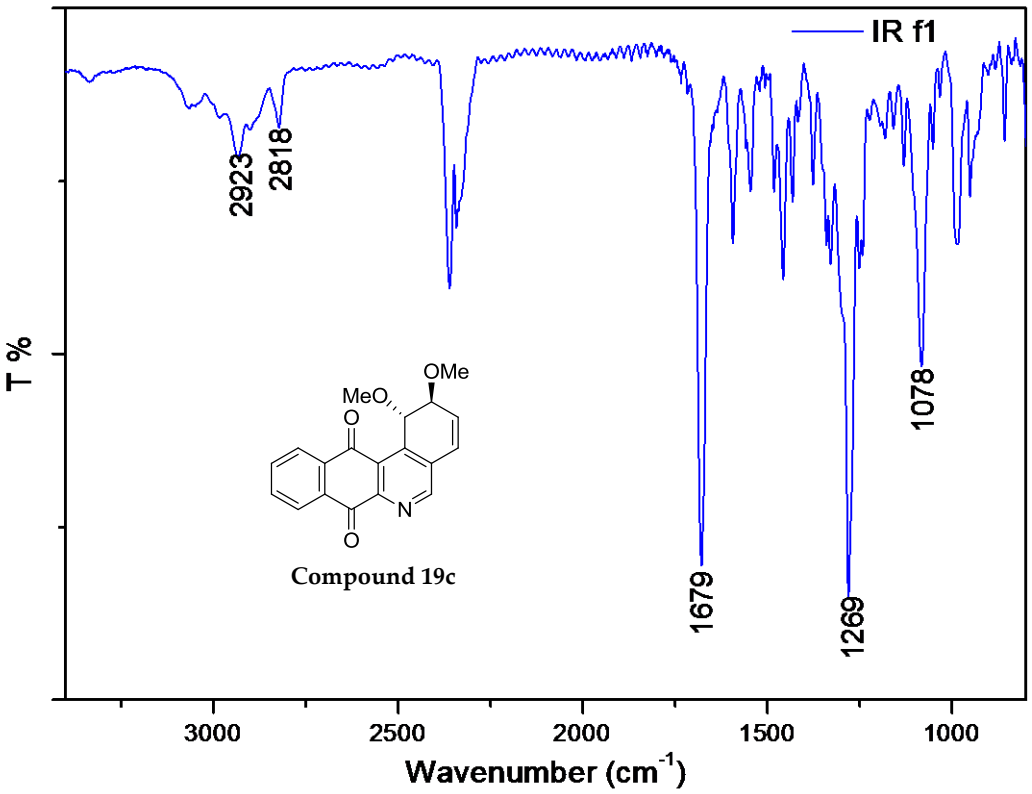
Compound 16c



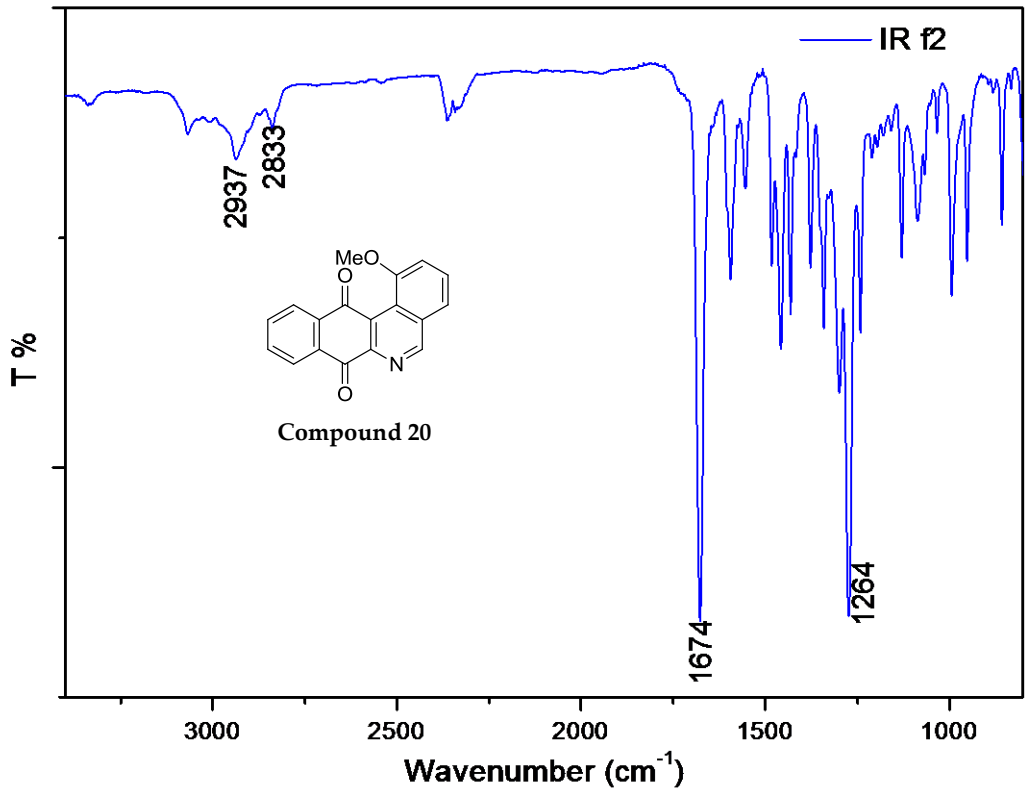
Compound 17


IR 19a
T%
2933
2818
1688
1665
1279
1083
OMe
MeO
O
N
O
Compound 19a
3000
2500
2000
1500
1000
Wavenumber (cm-1)


IR 19b
T%
3047
2928
2818
1693
1665
1293
1078
OMe
MeO
O
N
O
Compound 19b
3000
2500
2000
1500
1000
Wavenumber (cm-1)



Compound 19c



Compound 20