

Supplementary Material

The synthesis of selected phase II metabolites – *O*-glucuronides and sulfates of drug development candidates

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Dedicated to Rainer Beckert on the occasion of his 60th anniversary

Content

¹ H, ¹³ C NMR spectra and MS data for 7	2
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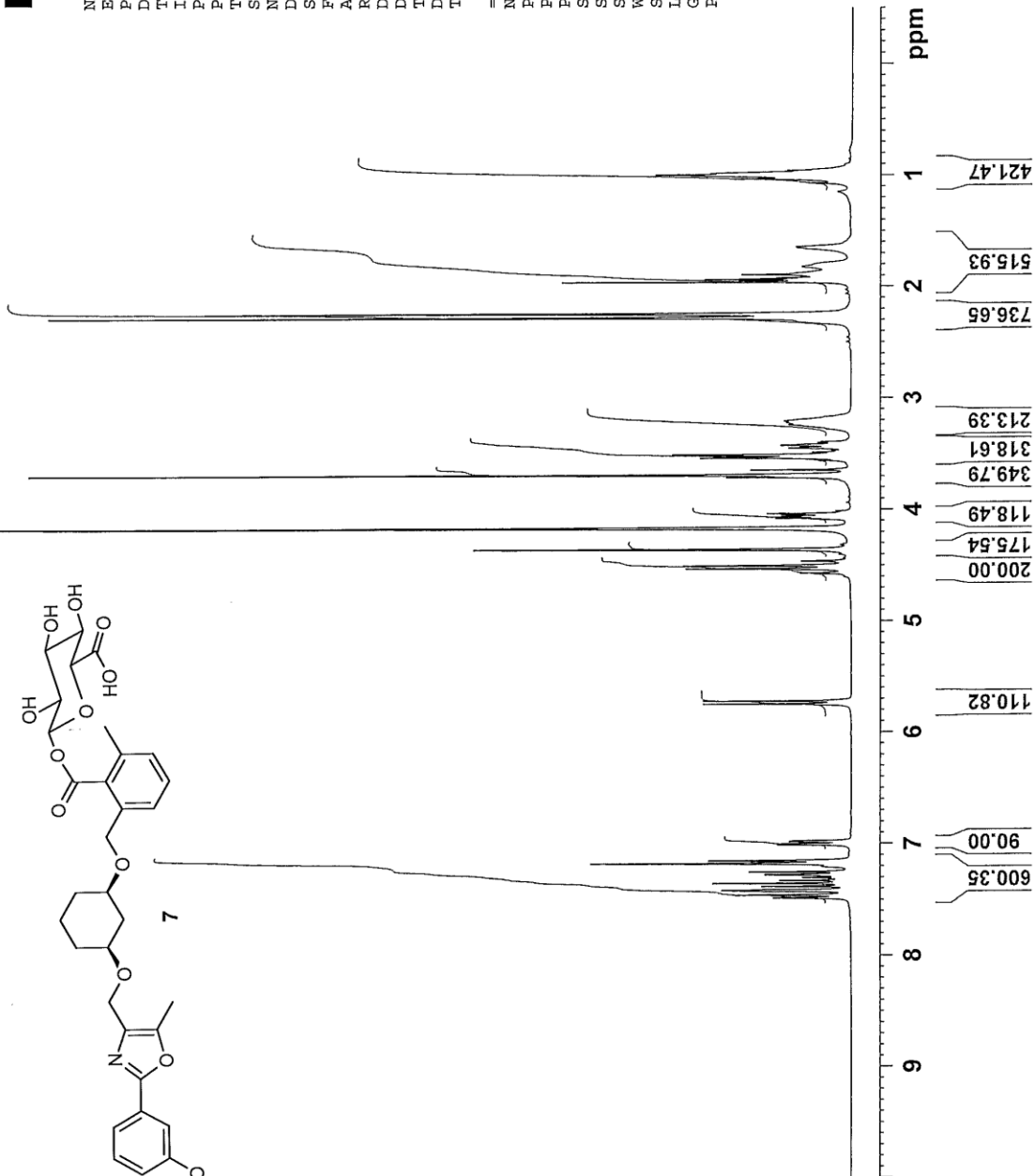
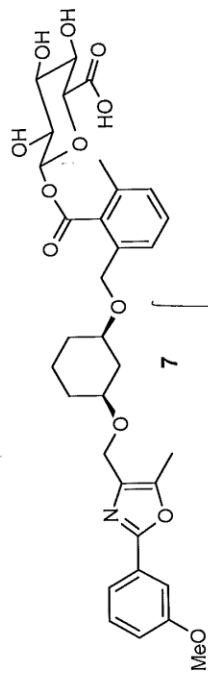
300MHz 1H/B Dr.Az AVE0897-Acylgluc.(OMe)-13Cd3 17 mg ; ACN-d3 : D2O 1 : 1
 proton



```

NAME      atzi8334
EXPNO     30
PROCNO    1
Date_     20110919
Time_     14.16
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CD3CN
NS         128
DS         2
SWH        6188.119 Hz
FIDRES     0.094423 Hz
AQ         5.2953587 sec
RG         181
DE         80.800 usec
TE         6.50 usec
D1         300.0 K
TD0        1.0000000 sec

===== CHANNEL f1 =====
NUC1      1H
P1         12.20 usec
PL1        0.00 dB
PL1W       11.05230045 W
SFO1       300.1318534 MHz
SI         32768
SF         300.1293196 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
```



75MHz 13C/B Dr.Az AVE0897-Acylgluc. (OMe)-13Cd3 17 mg ; ACN-d3 : D2O 1 : 1
c13cpd

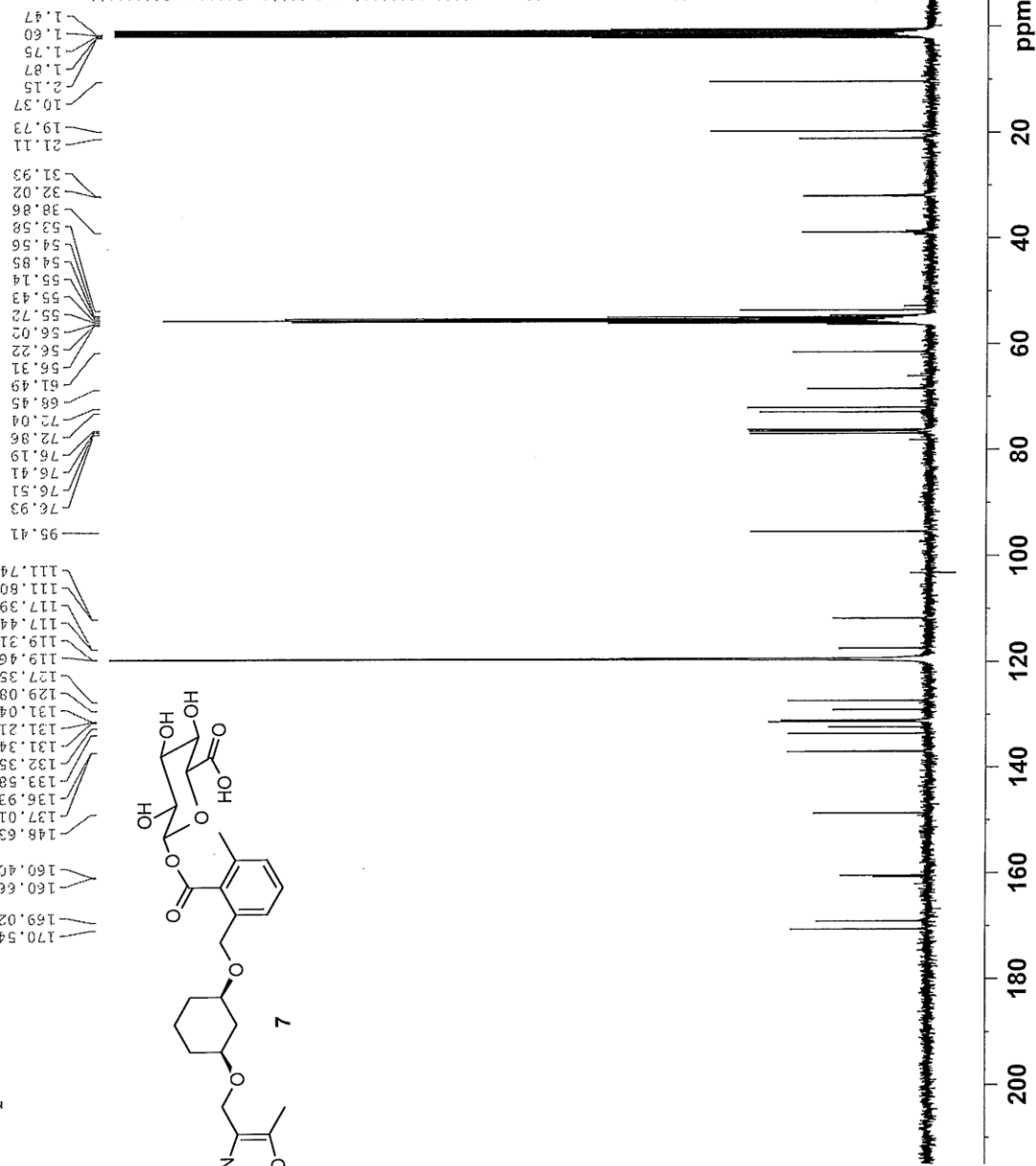


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NAME      atzr8334
EXPNO     32
PROCNO    1
Date_     20110919
Time      21.29
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CD3CN
NS         6000
DS         4
SWH        18028.846 Hz
FIDRES     0.275098 Hz
AQ         1.8175818 sec
RG         32800
DW         27.733 usec
DE         6.50 usec
TE         300.0 K
D1         2.0000000 sec
D11        0.0300000 sec
TDO        1

===== CHANNEL f1 =====
NUC1       13C
P1         8.00 usec
PL1        -2.00 dB
PL1W       54.54068375 W
SF01       75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2         0.00 dB
PL12       16.00 dB
PL13       16.00 dB
PL2W       11.05230045 W
PL12W      0.27762124 W
PL13W      0.27762124 W
SFO2       300.1312005 MHz
SI         32768
SF         75.4675065 MHz
WDM        EM
SSB         0
LB          0
GB          0
PC         1.40
    
```

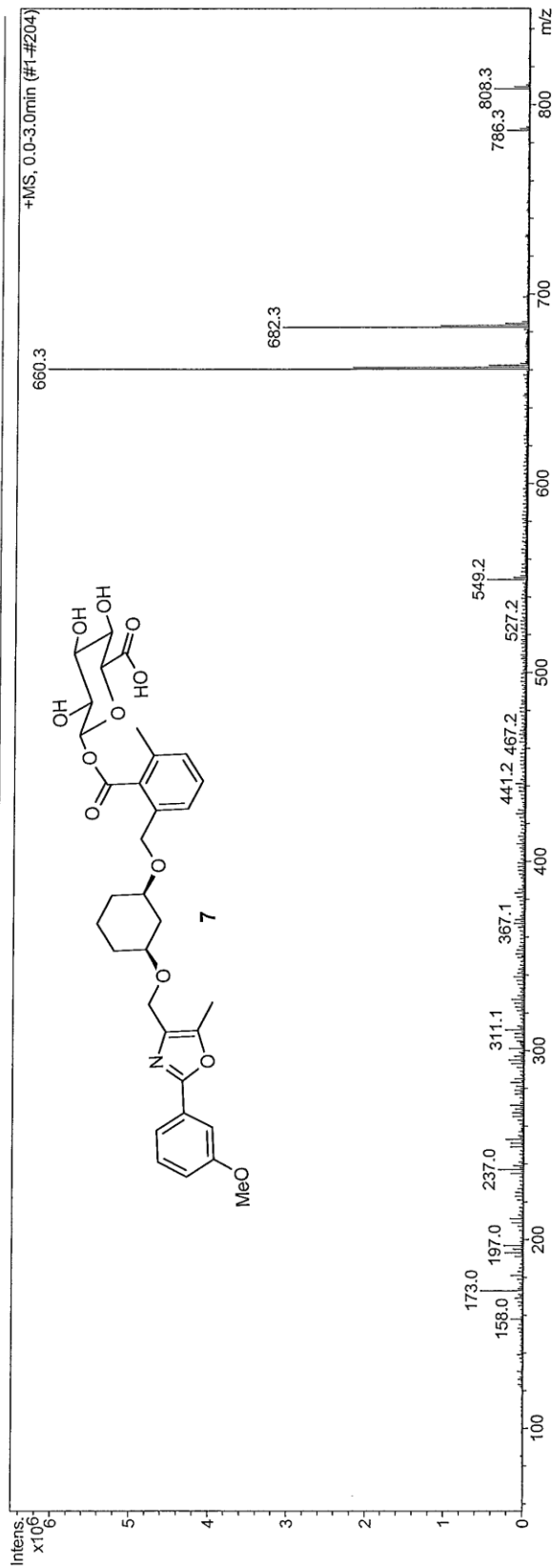


Analysis Info

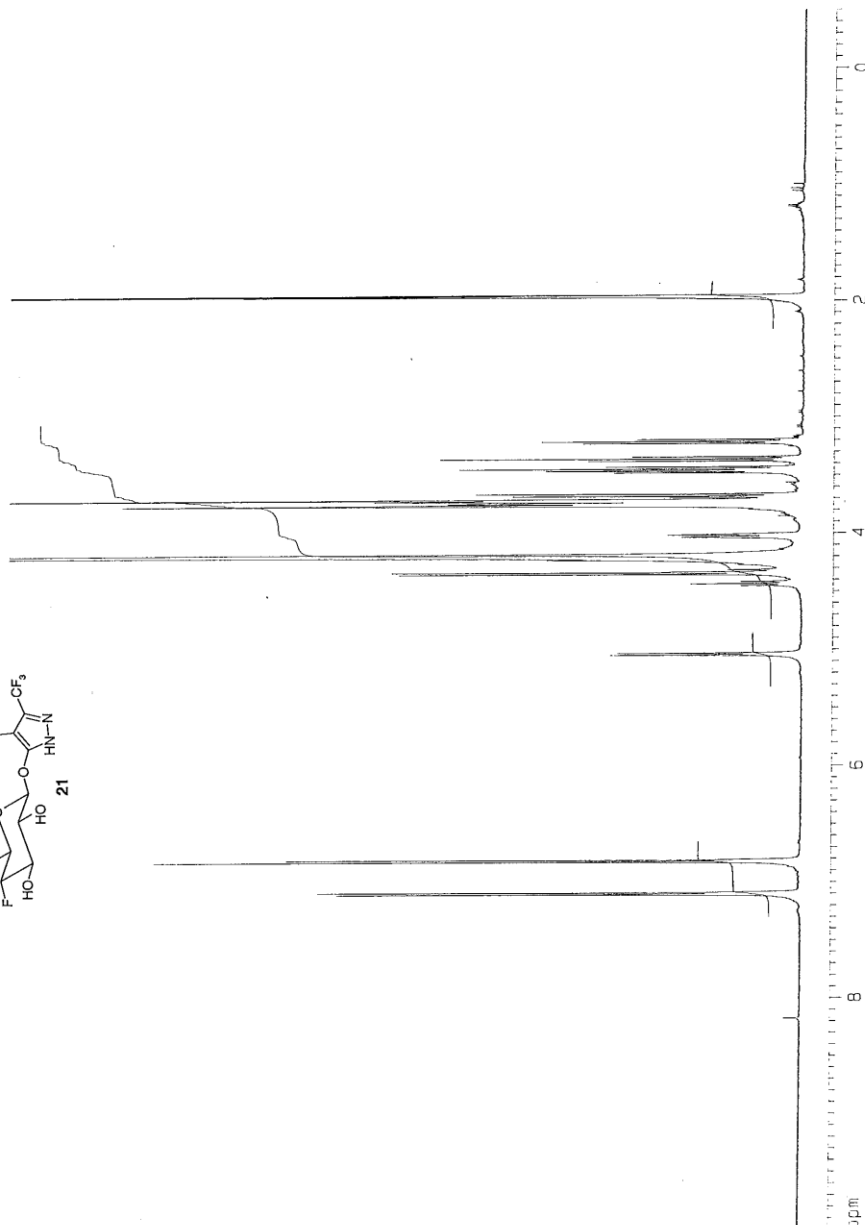
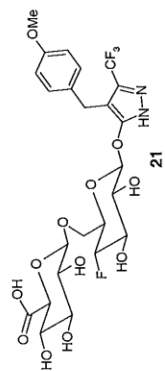
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 Sample Name AVE0897-gluc-OMe 13C,d3
 Comment AVE0897-gluc-OMe 13C,d3
 atzr8334
 ACN : H2O 1 : 1 + HCOOH
 Acquisition Date 09/20/11 15:42:34
 Method Copy of 00 pos.MS
 Administrator esquire3000
 Operator Instrument

MS/MS Parameters

Source/Trap Positive
 Ion Polarity Positive
 Scan Begin 50 m/z
 Scan End 2000 m/z
 ICC Target 30000



500MHz 1H/B gs22895 Dr. Ho SAR7226-M2_Sm_20/25-1 4.8mg; ACN-d3; D20 1:1 +DC000
zg30



```

Current Data Parameters
NAME          R0117460
EXPNO        1
PROCNO       1

F2 - Acquisition Parameters
Date_        20070326
Time         5:22
INSTRUM     spect
PROBHD      5 mm BBO BB-7H
PULPROG     zgpg30
TD          65536
SOLVENT     CDCl3
NS          128
DS          4
SWH         10330.578 Hz
FIDRES     0.157532 Hz
AQ         3.1720407 sec
RG          400
ZM          48.400 us/c
DE          6.00 us/c
TE          300.0 K
D1          1.50000000 sec
dPREST     0.00000000 sec
NCHRG      0.01500000 sec
***** CHANNEL f1 *****
NUC1        1H
P1          17.15 us/c
PL1         0.00 dB
SFO1        500.130884 MHz

F1 - Acquisition parameters
NU0         2
TD          512
SFO1        500.1634 MHz
FIDRES     14.932148 Hz
SOLVENT     States-TTPI

F2 - Processing parameters
SI          32768
SF          500.109998 MHz
RG          0
WDW         EM
SSB         0
LB          0.30 Hz
GB          0
PC          1.00

F1 - Processing parameters
SI          1024
SF          500.160000 MHz
RG          0
WDW         rd
SSB         0
LB          0.30 Hz
GB          0.1

1D NMR plot parameters
CA          20.00 cm
CY          20.00 cm
F1P         10.000 ppm
F1          5001.10 Hz
F2P         -0.500 ppm
F2          -250.05 ppm
PRNCHM     0.52300 ppm/c
          -0.71%
          250.54777 Hz/cm
    
```

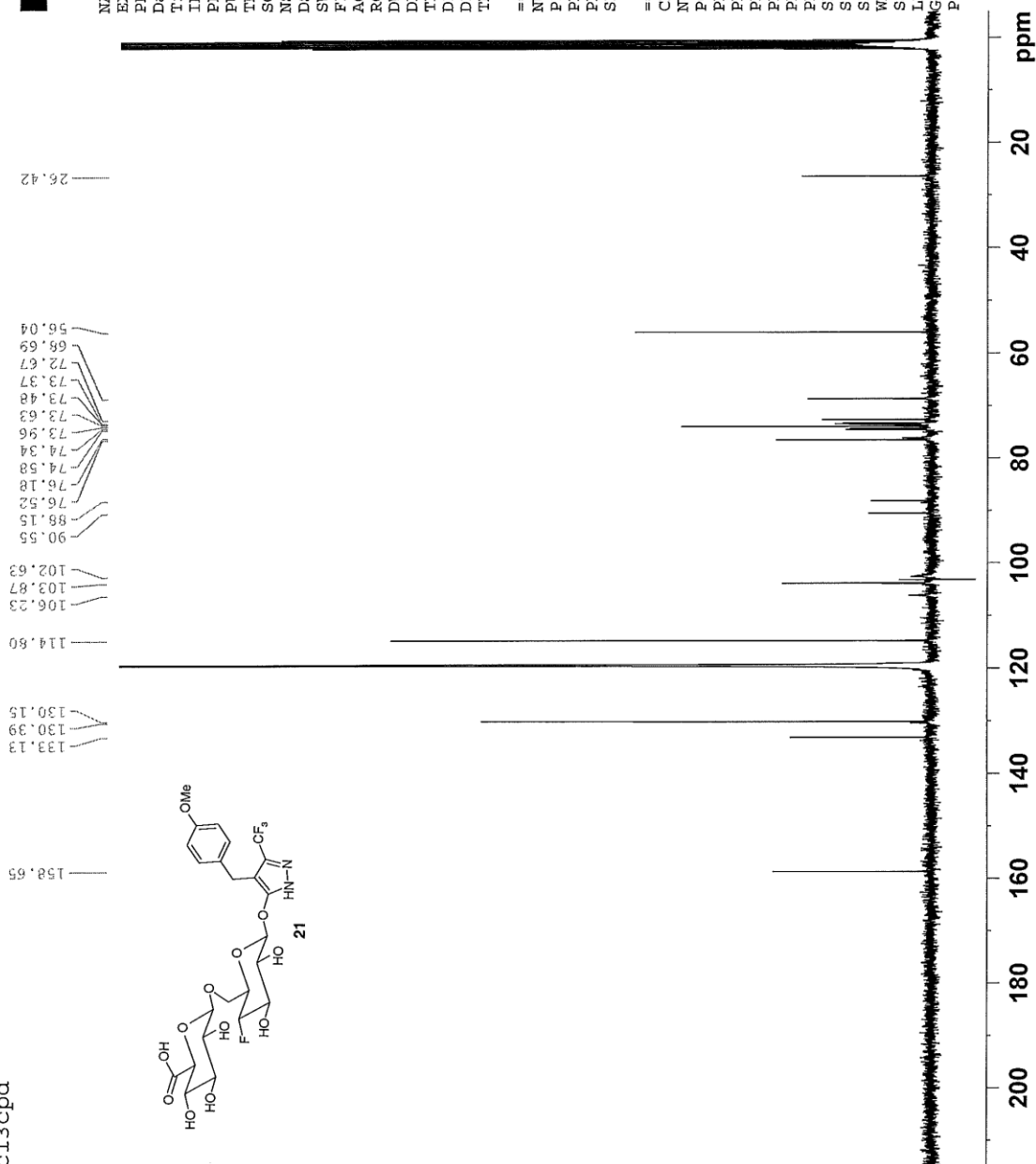
75MHz 13C/B Dr.Ho SAR7226-M2 Sm20/25-3 ; ACN-d3:D2O 1:1
c13cpd



NAME hol17460
EXPNO 21
PROCNO 1
Date 20110914
Time 13.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CD3CN
NS 18432
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 32800
DW 27.733 usec
DE 6.50 usec
TE 300.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TDO 1

==== CHANNEL f1 =====
NUC1 13C
P1 8.00 usec
PL1 -2.00 dB
PL1W 54.54068375 W
SF01 75.4752953 MHZ

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 16.00 dB
PL13 16.00 dB
PL12W 11.05230045 W
PL13W 0.27762124 W
SFO2 300.1312005 MHZ
SI 32768
SF 75.4675066 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Analysis Info

Analysis Name 25x10001.d
 Sample Name SAR7226-M2 Sm 20/25-1
 Comment SAR7226-M2 Sm 20/25-1
 hol17460
 ACN : H2O 1 : 1 + HCOOH

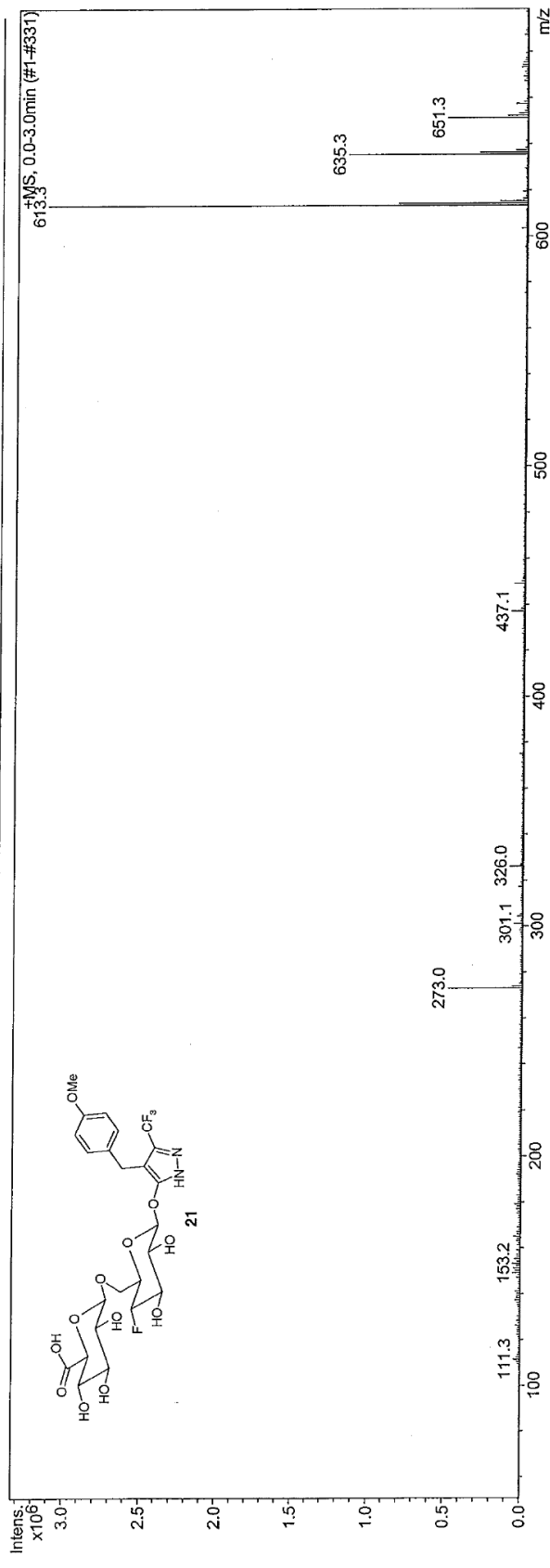
Acquisition Date 03/27/07 14:22:10
 Method Copy of SAR7226+Fr3.MS

Operator
 Instrument

Administrator
 esquire3000

MS/MS Parameters

Source/Trap Positive
 Ion Polarity Positive
 Scan Begin 50 m/z
 Scan End 1000 m/z
 ICC Target 30000

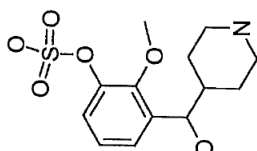


Bruker Daltonics DataAnalysis 3.0

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500MHz 1H/5 9s24833 Dr.De HDL407292 Wb 37.07 (M38007) 0.4mg; DMSO-d₆ 2930



33

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Current Data Parameters
NAME      der0735
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20080325
Time     14:48
INSTRUM  spect
PROBHD   5 mm BBO BB-1H
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
VS        1024
DS        2
SMA       10330.573 Hz
FIDRES    0.157632 Hz
AQ         3.1720007 SEC
RG         600
DM         48.400 usec
DE         6.00 usec
TE         300.0 K
D1         1.50000000 SEC
WDEXT     0.00000000 SEC
WCHIRK    0.01500000 SEC

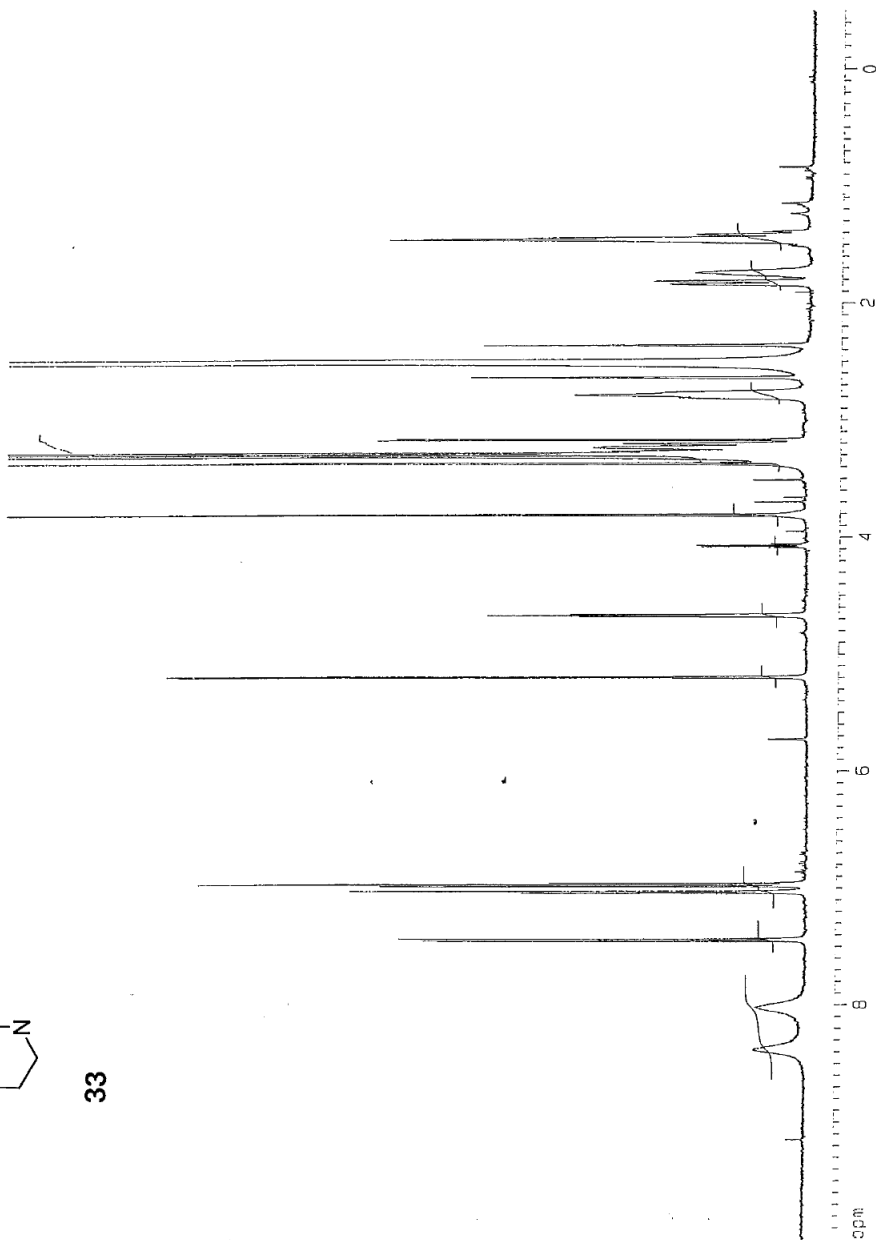
***** CHANNEL f1 *****
NUC1      1H
P1        17.15 usec
PL1       0.00 dB
SFO1      500.130884 MHz

F1 - Acquisition parameters
NUC2      13C
P2        12.00 usec
PL2       1.95 dB
SFO2      125.761170 MHz

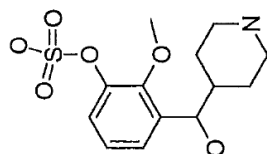
F2 - Processing parameters
SI        32768
SF        500.1099985 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00

F1 - Processing parameters
SI        1024
VC2       TPPI
SF        500.1600000 MHz
WDW       no
SSB       2
LB        0.30 Hz
GB        0.1

1D NMR plot parameters
CX        20.00 cm
CY        1000.00 cm
F1P       10.000 ppm
F1        5001.10 Hz
F2P       -250.05 ppm
F2        -250.05 Hz
SFOCH     0.52500 ppm/cm
AQCH      382.85777 sec/cm
  
```



MDL07292 Compound 33
c13cpd



33

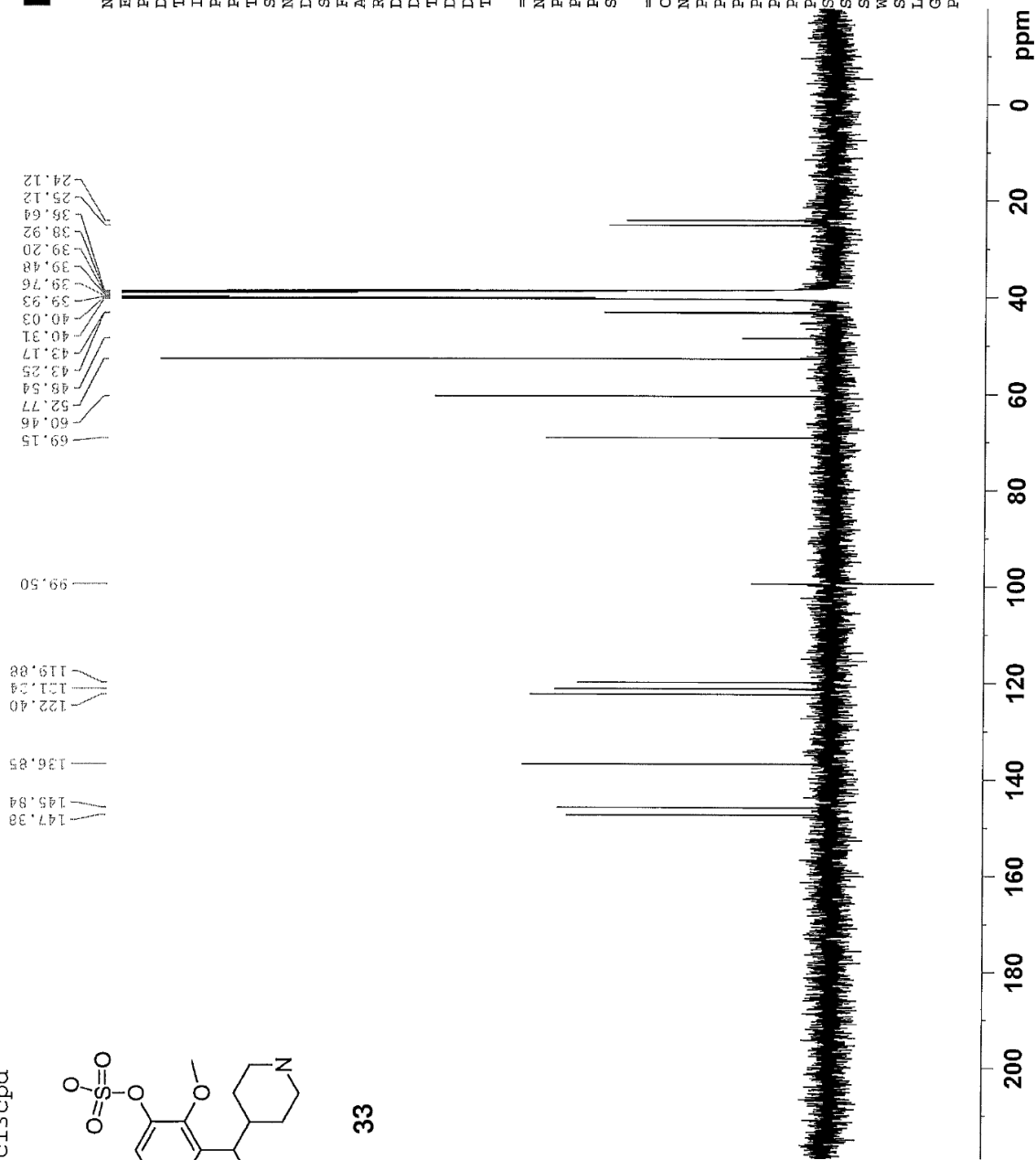


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NAME      derd8345
EXPNO     11
PROCNO    1
Date_     20111020
Time      16.48
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         12288
DS         4
SWH        18028.846 Hz
FIDRES     0.275098 Hz
AQ          1.8175818 sec
RG          32800
DW          27.733 usec
DE          6.50 usec
TE          300.0 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0         1

===== CHANNEL f1 =====
NUC1       13C
P1          8.00 usec
PL1         -2.00 dB
PL1W        54.54068375 W
SFO1        75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2        1H
PCPD2       80.00 usec
PL2          0.00 dB
PL12        16.00 dB
PL13        16.00 dB
PL1W        11.05230045 W
PL12W       0.27762124 W
PL13W       0.27762124 W
SFO2        300.1312005 MHz
SI          32768
SF          75.4677867 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
    
```



Analysis Info

Analysis Name 37x07001.d
 Sample Name MDL107292 M38007
 Comment MDL107292 Wb 37107 M38007
 derd7735
 H2O/ACN 1:1 + HCOOH
 Acquisition Date 03/26/08 14:04:19
 Method Copy of MDL107292-.MS
 Operator Administrator
 Instrument esquire3000

MS/MS Parameters

Source/Trap Ion Polarity Negative
 Scan Begin 50 m/z
 Scan End 2000 m/z
 ICC Target 10000

