



Supporting Information

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## Supporting Information

for

### **Benzopyrenomycin, a Cytotoxic Bacterial Polyketide Metabolite with an Unprecedented Benzo[a]pyrene-Type Carbacyclic Ring System**

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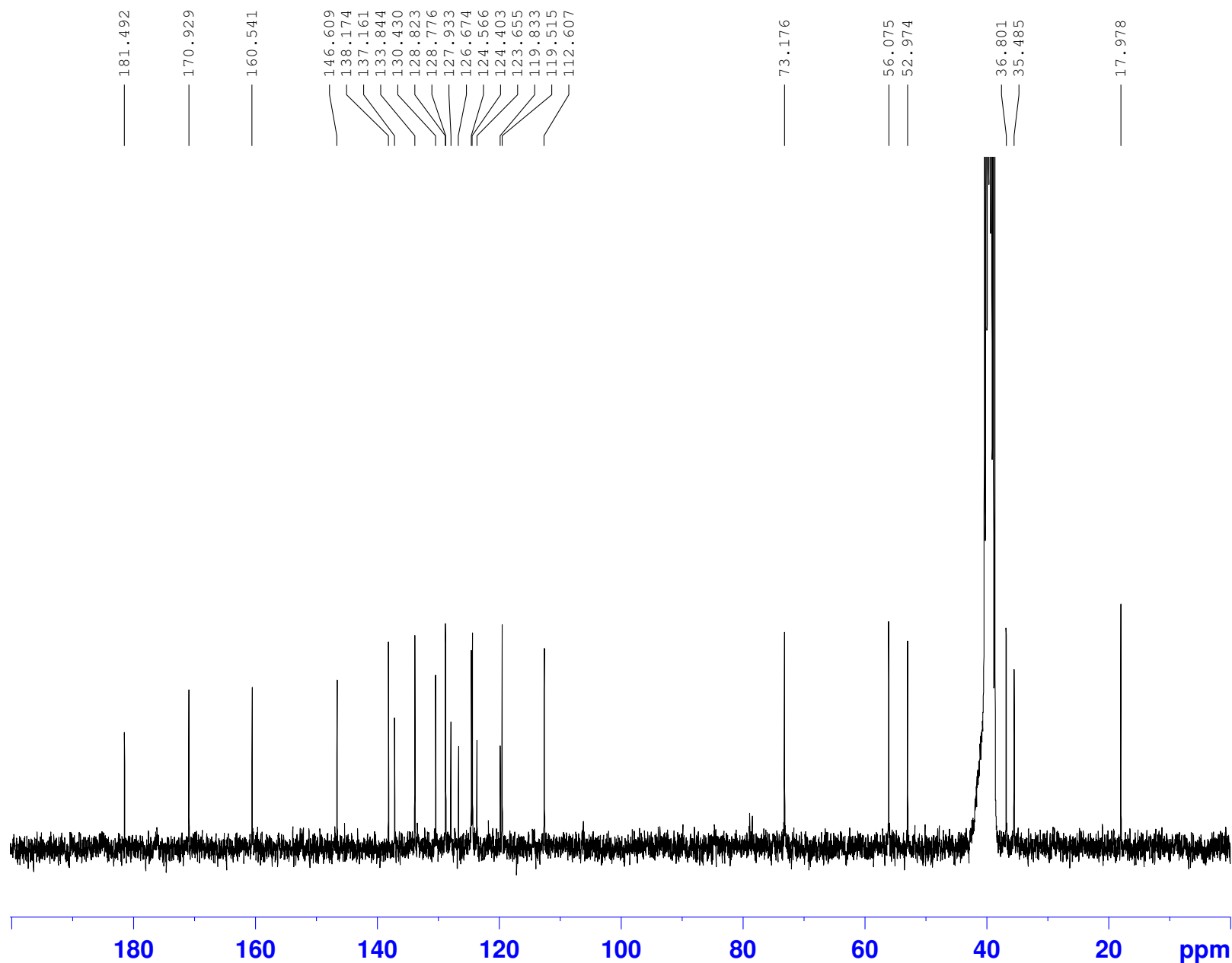
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Fig. 1 <sup>13</sup>C NMR spectrum of benzpyrenomycin (1)



CHE061/DMSO-d6/He/<sup>13</sup>C

Current Data Parameters  
NAME CHE061CA  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
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PULPROG zgpg  
TD 32768  
SOLVENT DMSO  
NS 49164  
DS 2  
SWH 18939.395 Hz  
FIDRES 0.577984 Hz  
AQ 0.8651252 sec  
RG 8192  
DW 26.400 usec  
DE 5.00 usec  
TE 300.0 K  
D1 0.4000001 sec  
D11 0.0300000 sec  
D12 0.0000200 sec

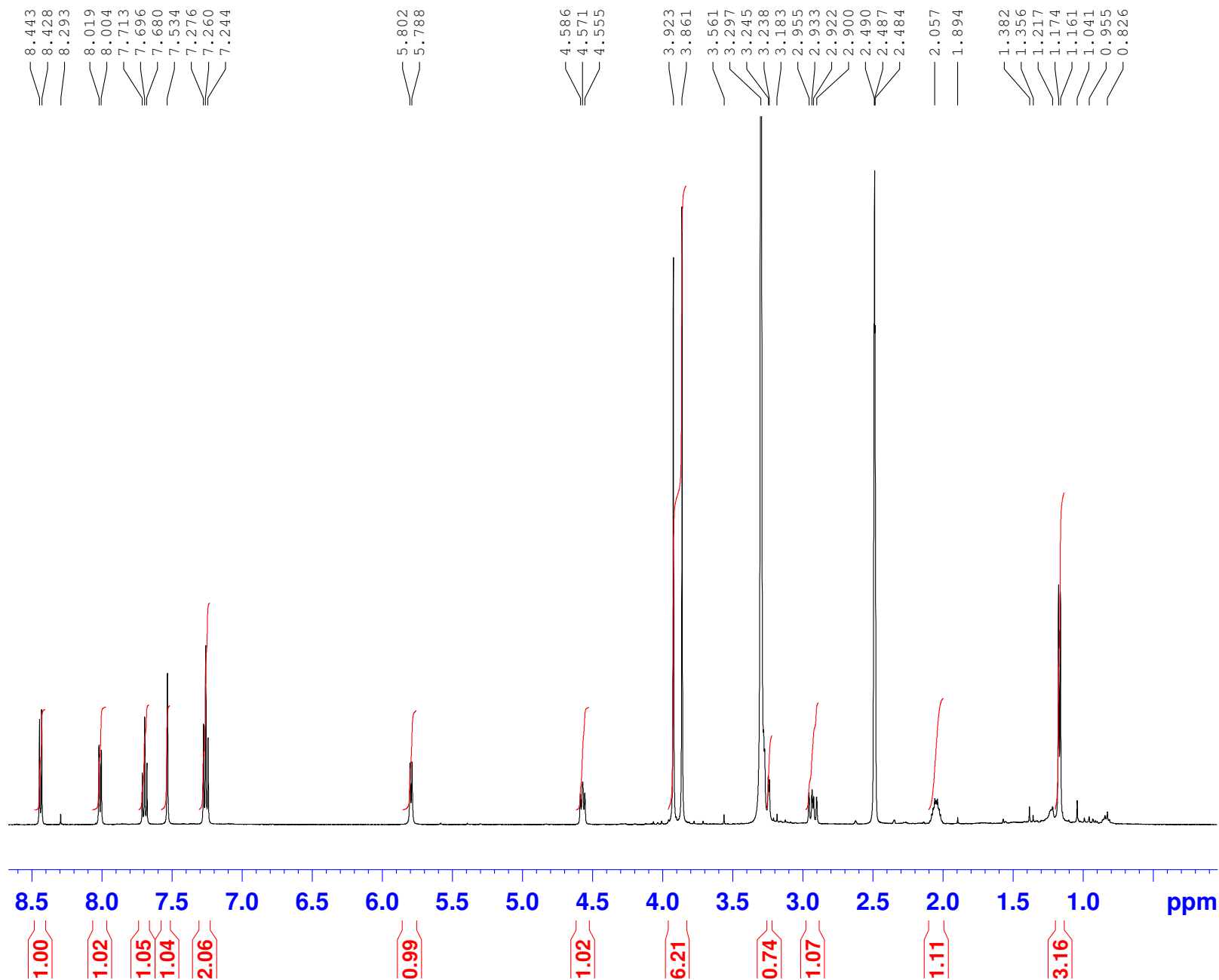
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PL1 -3.00 dB  
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NUC2 <sup>1</sup>H  
PCPD2 87.00 usec  
PL2 120.00 dB  
PL12 17.00 dB  
PL13 24.00 dB  
SFO2 300.1312829 MHz

F2 - Processing parameters  
SI 32768  
SF 75.4677892 MHz  
WDW EM  
SSB 0  
LB 1.50 Hz  
GB 0  
FC 1.40

Fig. 2 <sup>1</sup>H NMR spectrum of benzpyrenomycin (1)

CHE061/DMSO-d<sub>6</sub>/He/1H  
GT61324



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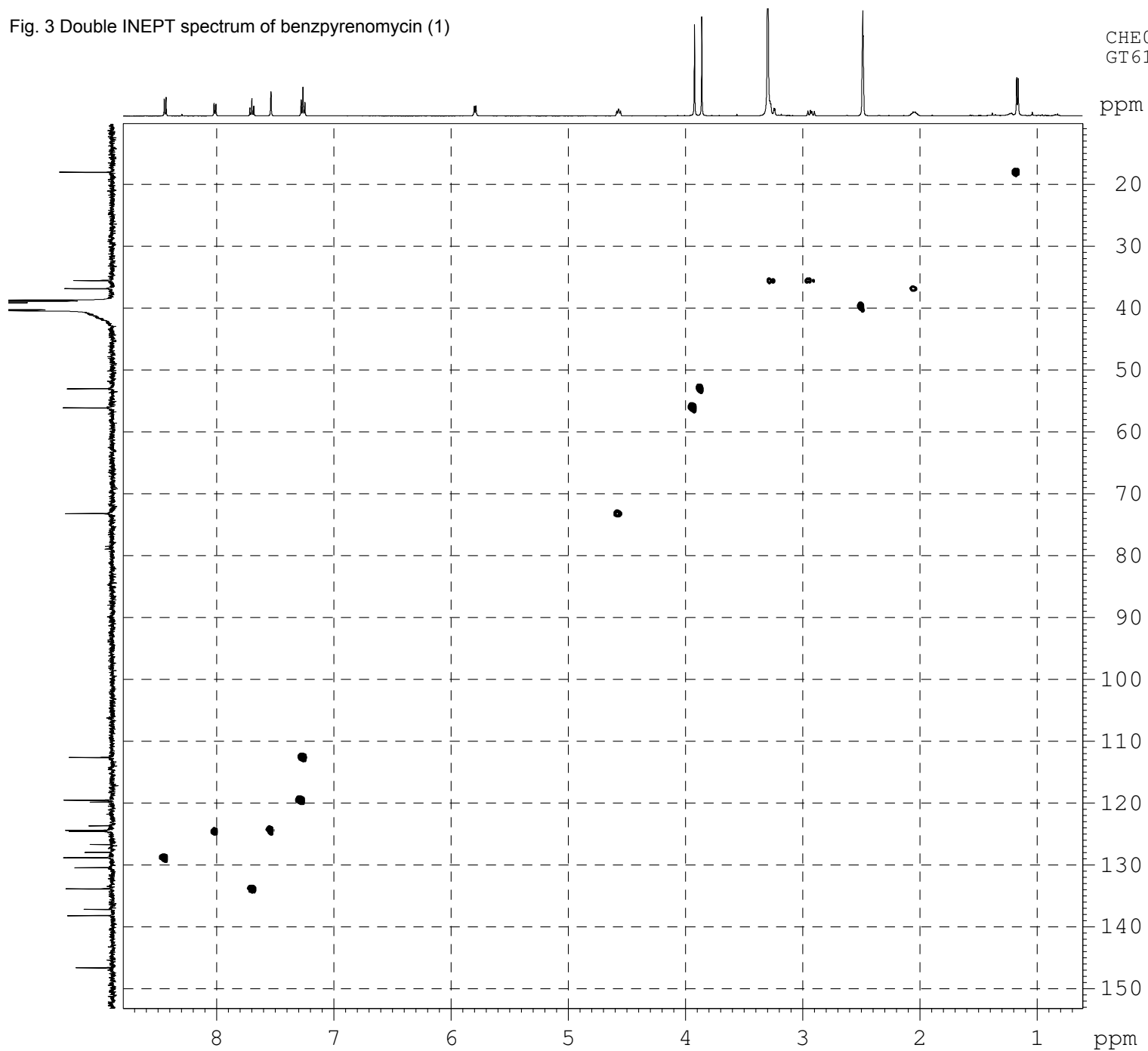
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PULPROG  zg30
TD        32768
SOLVENT  DMSO
NS        128
DS         0
SWH       4734.849 Hz
FIDRES    0.144496 Hz
AQ        3.4603508 sec
RG         574.7
DW        105.600 usec
DE         4.50 usec
TE        303.0 K
D1        1.0000000 sec

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PL1       2.00 dB
SFO1     500.1323268 MHz

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SF        500.1300111 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        3.00
    
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Fig. 3 Double INEPT spectrum of benzpyrenomycin (1)



CHE061/DMSO-d6/He/Double INEPT  
GT61324

```

Current Data Parameters
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EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20010321
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INSTRUM       spect
PROBHD        5 mm TXI 13C
PULPROG       invieagssi
TD            2048
SOLVENT       DMSO
NS            32
DS            64
SWH           4734.849 Hz
FIDRES        2.311938 Hz
AQ            0.2163188 sec
RG            8192
DW            105.600 usec
DE            4.50 usec
TE            303.0 K
CNSTO         1.0000000
D0            0.00000300 sec
D1            1.00000000 sec
D4            0.00172500 sec
D11           0.03000000 sec
D13           0.00000300 sec
D16           0.00020000 sec
d20           0.00128100 sec
d21           0.00120700 sec
D24           0.00114940 sec
IN0           0.00002126 sec
I3            256

===== CHANNEL f1 =====
NUC1           1H
P1             12.25 usec
P2             25.00 usec
P28            2000.00 usec
PL1            4.00 dB
SFO1           500.1323270 MHz

===== CHANNEL f2 =====
CPDPRG2        garp
NUC2           13C
P3             11.30 usec
P4             22.60 usec
PCPD2          75.00 usec
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PL12           17.50 dB
SFO2           125.7701890 MHz

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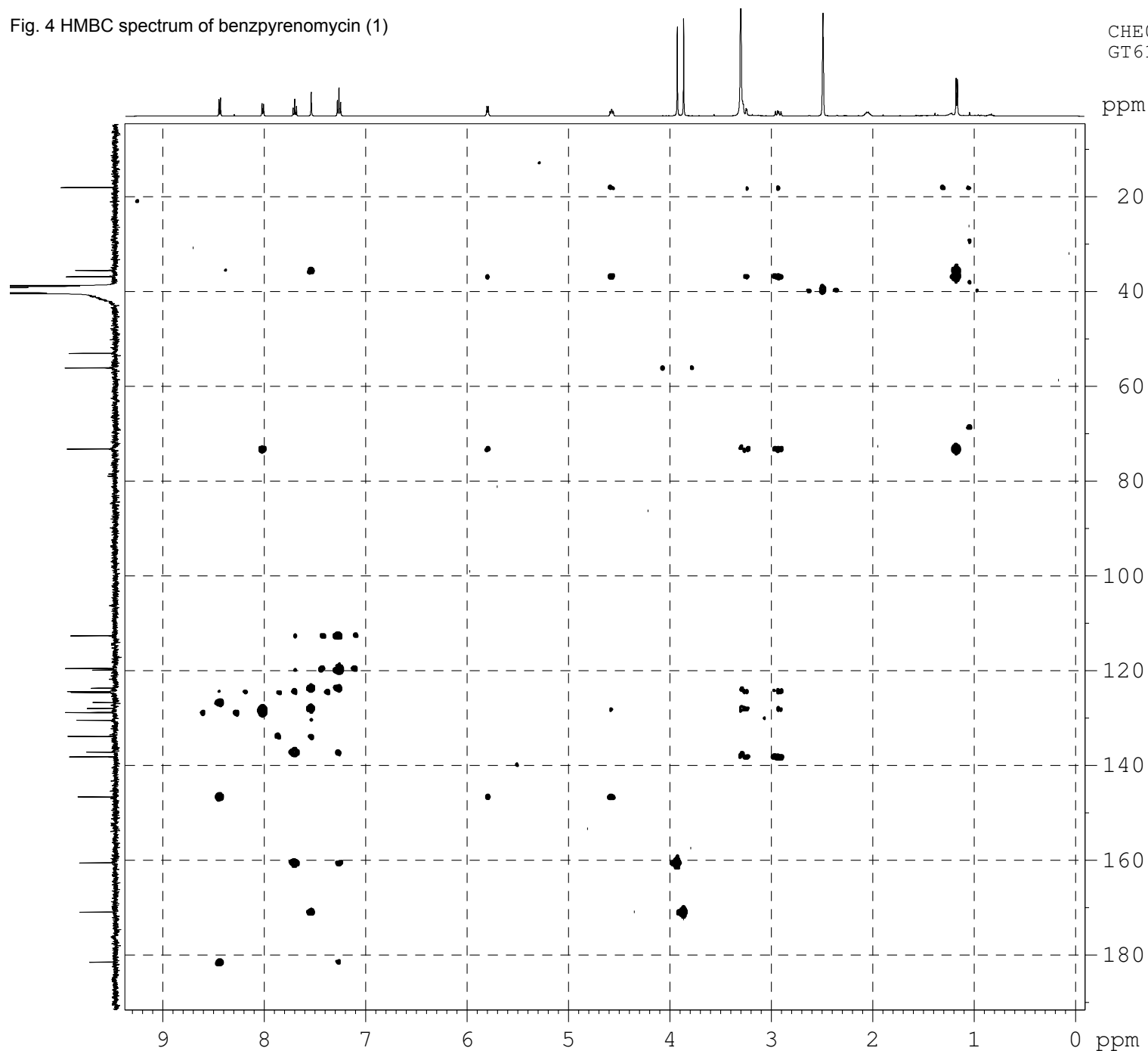
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FnMODE         undefined

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SI             2048
SF             500.1300043 MHz
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SSB            0
LB             1.00 Hz
GB             0
PC             3.00

F1 - Processing parameters
SI             1024
MC2            echo-antiecho
SF             125.7578422 MHz
WDW            QSINE
SSB            2
LB             0.00 Hz
GB             0
    
```

Fig. 4 HMBC spectrum of benzpyrenomycin (1)

CHE061/DMSO-d6/He/HMBC  
GT61324



```

Current Data Parameters
NAME          CHE061MU
EXPNO         2
PROCNO        1

F2 - Acquisition Parameters
Date_         20010321
Time          21.01
INSTRUM       spect
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PULPROG       inv4gsplrnd
TD            2048
SOLVENT       CDCl3
NS            64
DS            16
SWH           4734.849 Hz
FIDRES        2.311938 Hz
AQ            0.2163188 sec
RG            8192
DW            105.600 usec
DE            4.50 usec
TE            303.0 K
D0            0.00000300 sec
D1            1.50000000 sec
D2            0.00345000 sec
D6            0.06500000 sec
D13           0.00000300 sec
D16           0.00020000 sec
IN0           0.00002126 sec

===== CHANNEL f1 =====
NUC1          1H
P1            12.50 usec
P2            25.00 usec
PL1           4.00 dB
SFO1          500.1323270 MHz

===== CHANNEL f2 =====
NUC2          13C
P3            11.30 usec
PL2           1.00 dB
SFO2          125.7701890 MHz

===== GRADIENT CHANNEL =====
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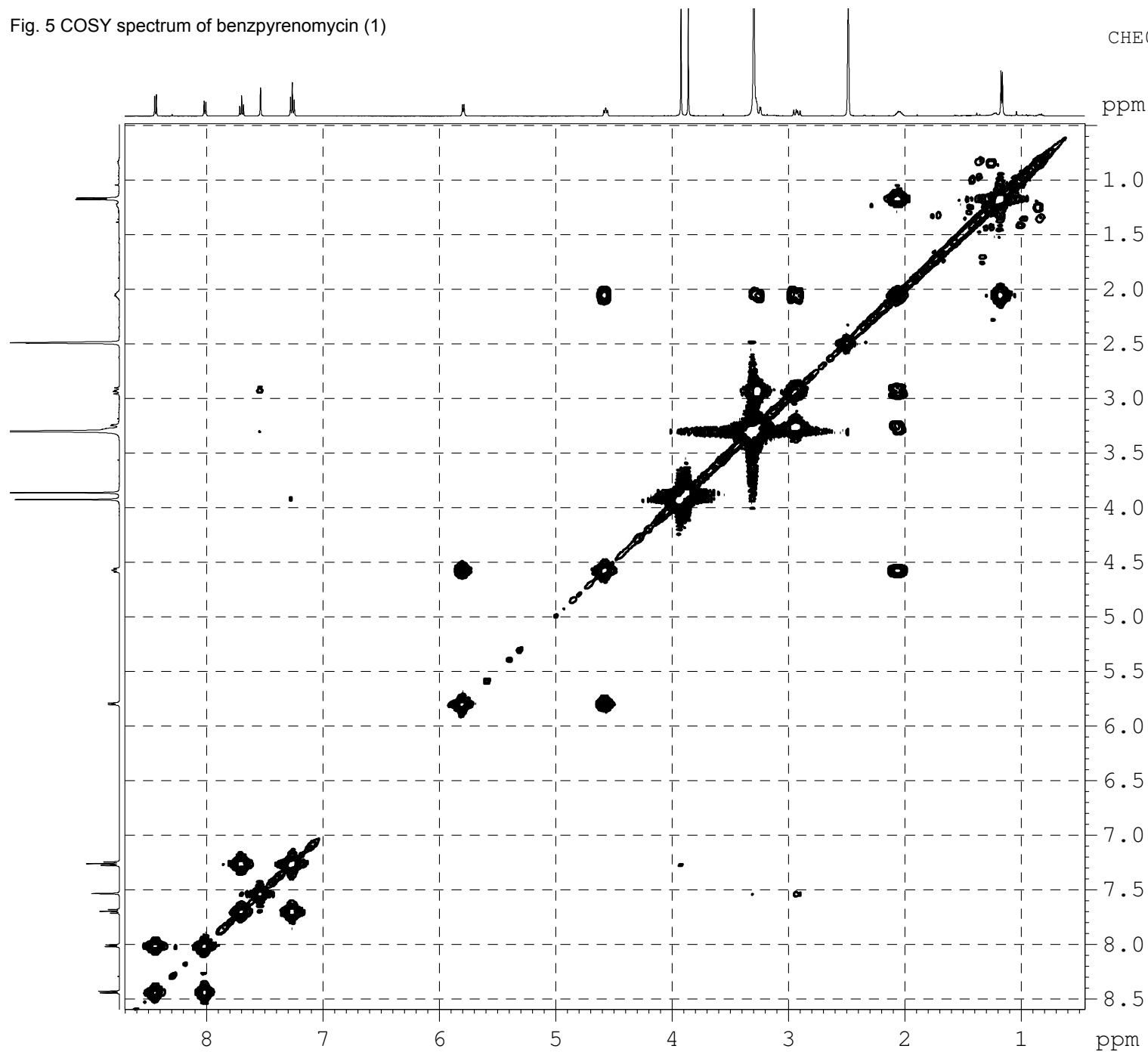
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ND0           2
TD            256
SFO1          125.7702 MHz
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FnMODE        undefined

F2 - Processing parameters
SI            2048
SF            500.1300060 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
PC            1.40

F1 - Processing parameters
SI            1024
MC2           QF
SF            125.7578526 MHz
WDW           SINE
SSB           0
LB            0.00 Hz
GB            0
    
```

Fig. 5 COSY spectrum of benzpyrenomycin (1)

CHE061/DMSO-d6/He/COSY



Current Data Parameters  
NAME CHE061CO  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20010516  
Time 8.23  
INSTRUM spect  
PROBHD 5 mm TXI 13C  
PULPROG cosygs  
TD 1024  
SOLVENT DMSO  
NS 4  
DS 4  
SWH 5000.000 Hz  
FIDRES 4.882813 Hz  
AQ 0.1024500 sec  
RG 256  
DW 100.000 usec  
DE 4.50 usec  
TE 303.0 K  
D0 0.00000300 sec  
D1 1.00000000 sec  
D13 0.00000300 sec  
D16 0.00020000 sec  
IN0 0.00019995 sec

===== CHANNEL f1 =====  
NUC1 1H  
P0 6.28 usec  
P1 12.55 usec  
PL1 2.00 dB  
SFO1 500.1320800 MHz

===== GRADIENT CHANNEL =====  
P16 1000.00 usec

F1 - Acquisition parameters  
ND0 1  
TD 256  
SFO1 500.1321 MHz  
FIDRES 19.536135 Hz  
SW 10.000 ppm  
FnMODE undefined

F2 - Processing parameters  
SI 1024  
SF 500.1300071 MHz  
WDW SINE  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 3.00

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 500.1300068 MHz  
WDW SINE  
SSB 0  
LB 0.00 Hz  
GB 0



Fig. 6 EI-MS spectrum of benzpyrenomycin (1)

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of Mi, 08.12.1900, 11:29 h  
Spectrum 8

Comment: He

<n> = basepeak

<g> = 1.00

<d> = user

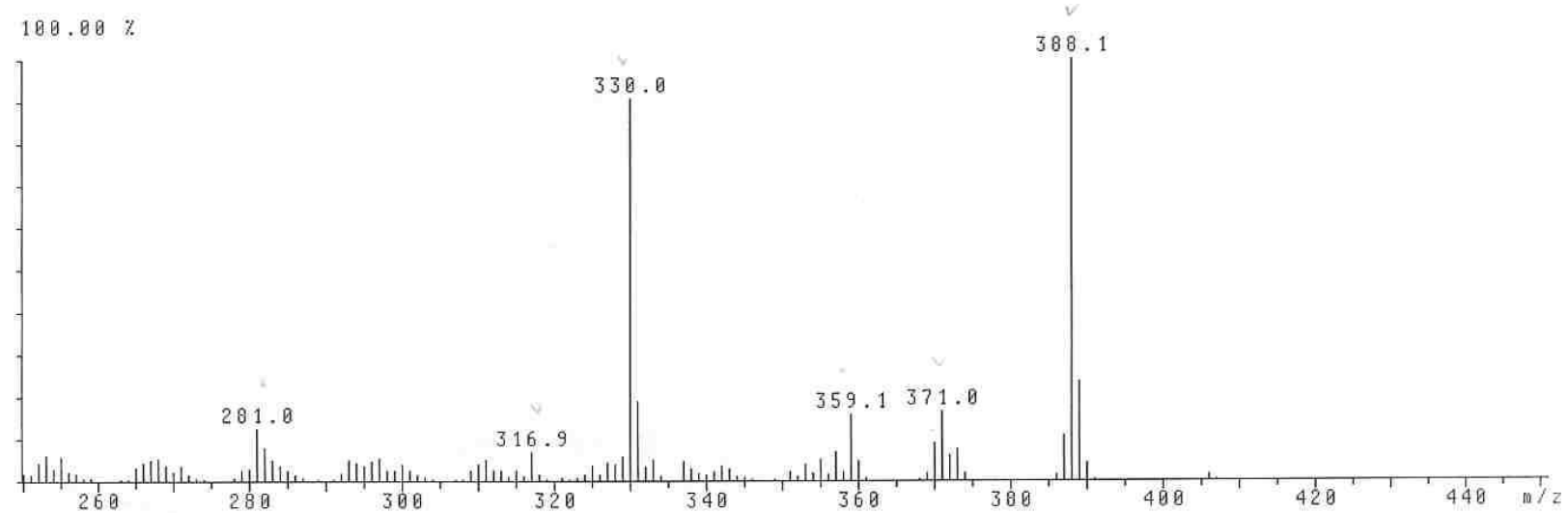
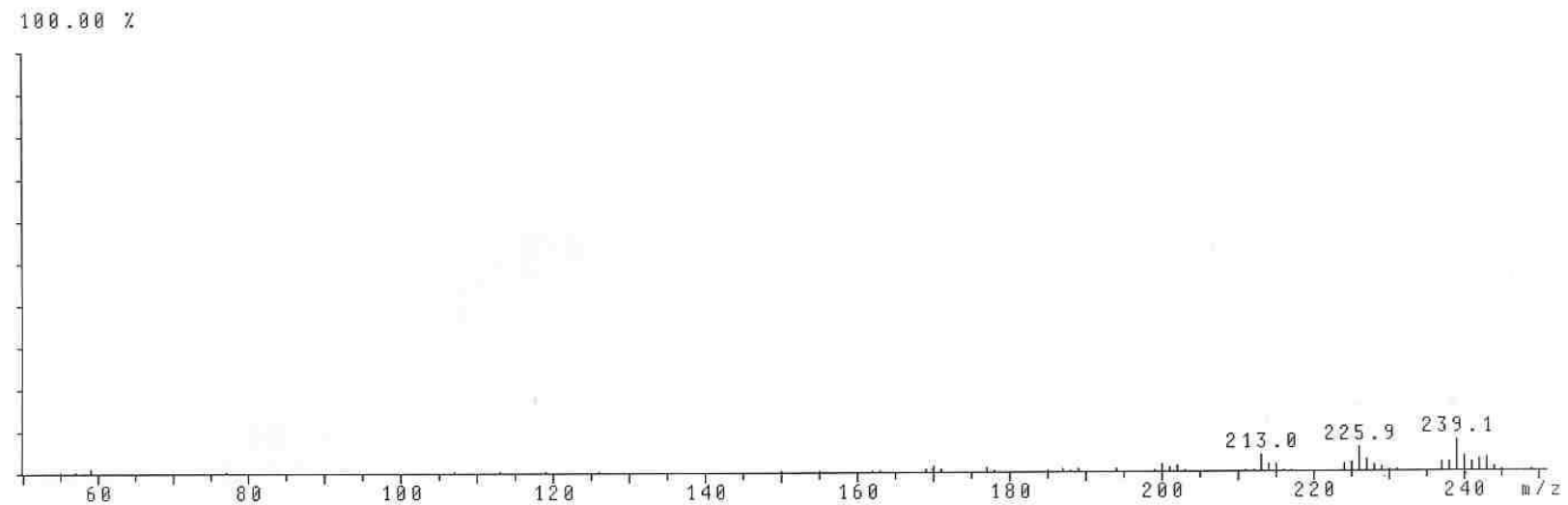


Fig. 7 HR-MS data of benzpyrenomycin (1)

Simulated:

m/z= 383.13-393.13				
m/z	Theo. Mass	Delta (mmu)	RDB equiv.	Composition
388.1300	388.1305	-0.53	15.0	C <sub>24</sub> H <sub>20</sub> O <sub>5</sub>
	388.1292	0.82	15.5	C <sub>22</sub> H <sub>18</sub> O <sub>4</sub> N <sub>3</sub>
	388.1319	-1.86	20.0	C <sub>25</sub> H <sub>16</sub> O <sub>1</sub> N <sub>4</sub>
	388.1324	-2.38	2.0	C <sub>12</sub> H <sub>24</sub> O <sub>12</sub> N <sub>2</sub>
	388.1332	-3.21	19.5	C <sub>27</sub> H <sub>18</sub> O <sub>2</sub> N <sub>1</sub>
	388.1265	3.50	11.0	C <sub>19</sub> H <sub>20</sub> O <sub>7</sub> N <sub>2</sub>
	388.1351	-5.06	6.5	C <sub>15</sub> H <sub>22</sub> O <sub>9</sub> N <sub>3</sub>
	388.1247	5.35	24.0	C <sub>31</sub> H <sub>16</sub>
	388.1238	6.18	6.5	C <sub>16</sub> H <sub>22</sub> O <sub>10</sub> N <sub>1</sub>
	388.1364	-6.40	6.0	C <sub>17</sub> H <sub>24</sub> O <sub>10</sub>
	388.1225	7.52	7.0	C <sub>14</sub> H <sub>20</sub> O <sub>9</sub> N <sub>4</sub>
	388.1377	-7.74	11.0	C <sub>18</sub> H <sub>20</sub> O <sub>6</sub> N <sub>4</sub>
	388.1391	-9.08	10.5	C <sub>20</sub> H <sub>22</sub> O <sub>7</sub> N <sub>1</sub>
	388.1206	9.37	20.0	C <sub>26</sub> H <sub>16</sub> O <sub>2</sub> N <sub>2</sub>
	388.1198	10.20	2.5	C <sub>11</sub> H <sub>22</sub> O <sub>12</sub> N <sub>3</sub>
	388.1418	-11.76	15.0	C <sub>23</sub> H <sub>20</sub> O <sub>4</sub> N <sub>2</sub>
	388.1179	12.05	15.5	C <sub>23</sub> H <sub>18</sub> O <sub>5</sub> N <sub>1</sub>
	388.1166	13.39	16.0	C <sub>21</sub> H <sub>16</sub> O <sub>4</sub> N <sub>4</sub>
	388.1436	-13.61	2.0	C <sub>11</sub> H <sub>24</sub> O <sub>11</sub> N <sub>4</sub>
	388.1444	-14.44	19.5	C <sub>26</sub> H <sub>18</sub> O <sub>1</sub> N <sub>3</sub>