

Supporting Information

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Antioxidant Activity of Chemical Constituents Isolated from *Pithecellobium clypearia*

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Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\20121225\HEH-9.d
Method tune_wide_pos.m
Sample Name HEH-9
Comment

Acquisition Date 12/25/2012 2:51:27 PM

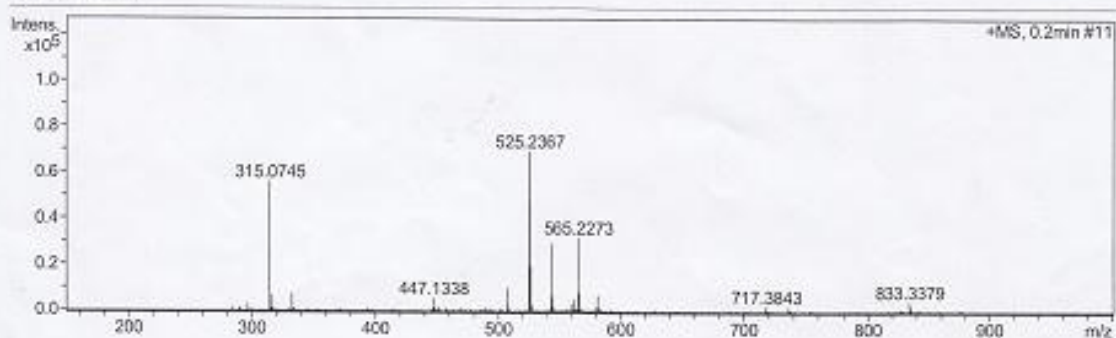
Operator Bryker Customer
Instrument / Ser# micrOTOF-Q 125

Acquisition Parameter

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Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
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Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source

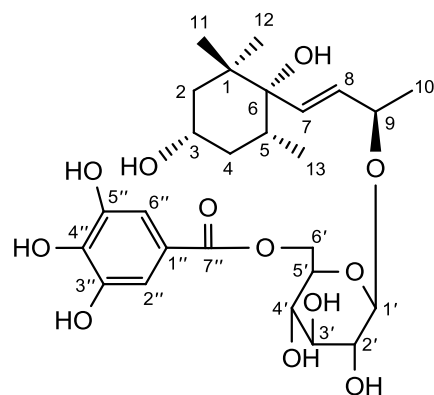
Generate Molecular Formula Parameter

Formula, min.		
Formula, max.		
Measured m/z		
Check Valence	Tolerance	Charge
Nitrogen Rule	Minimum	Maximum
Filter H/C Ratio	Electron Configuration	
Estimate Carbon	Minimum	Maximum

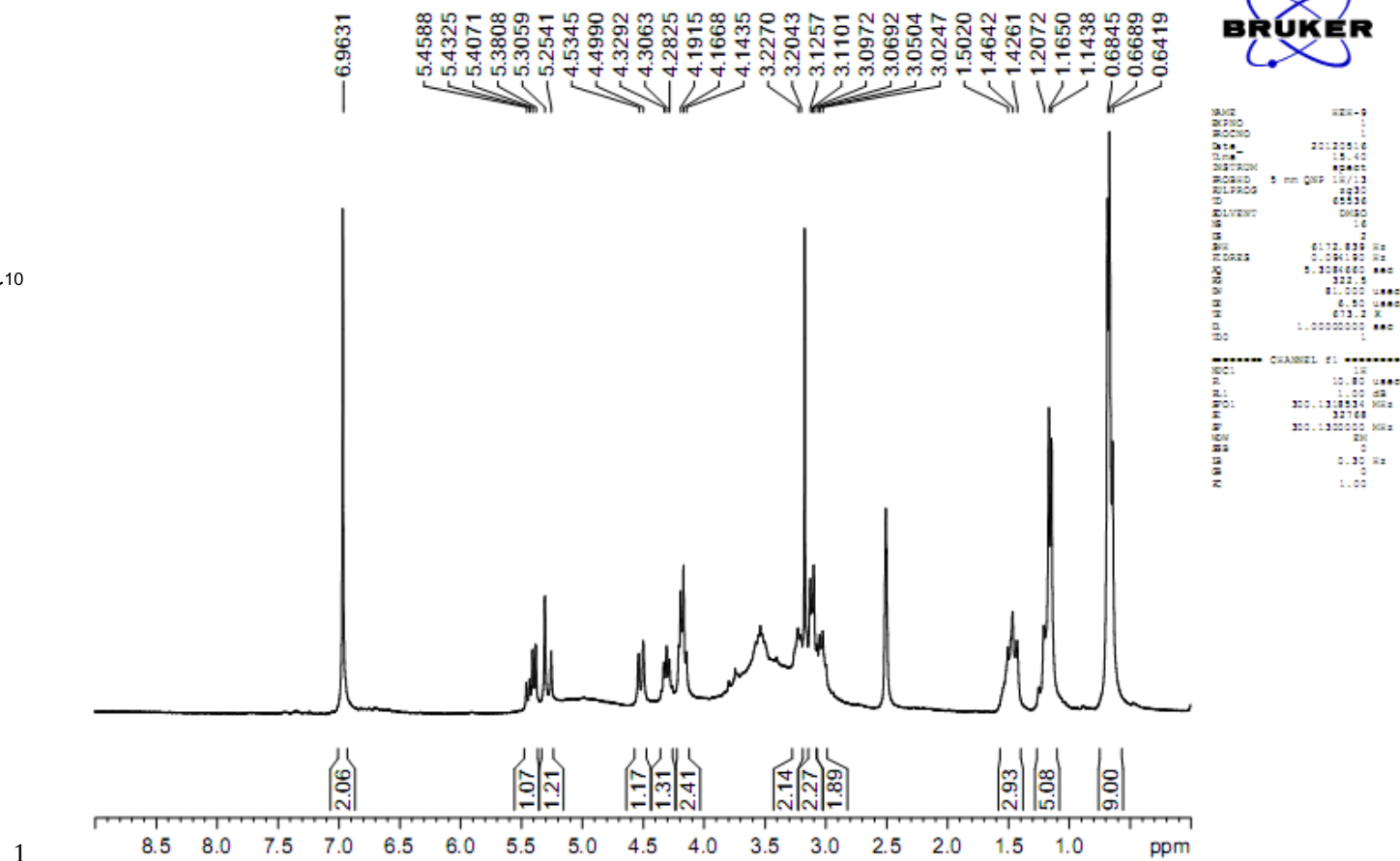


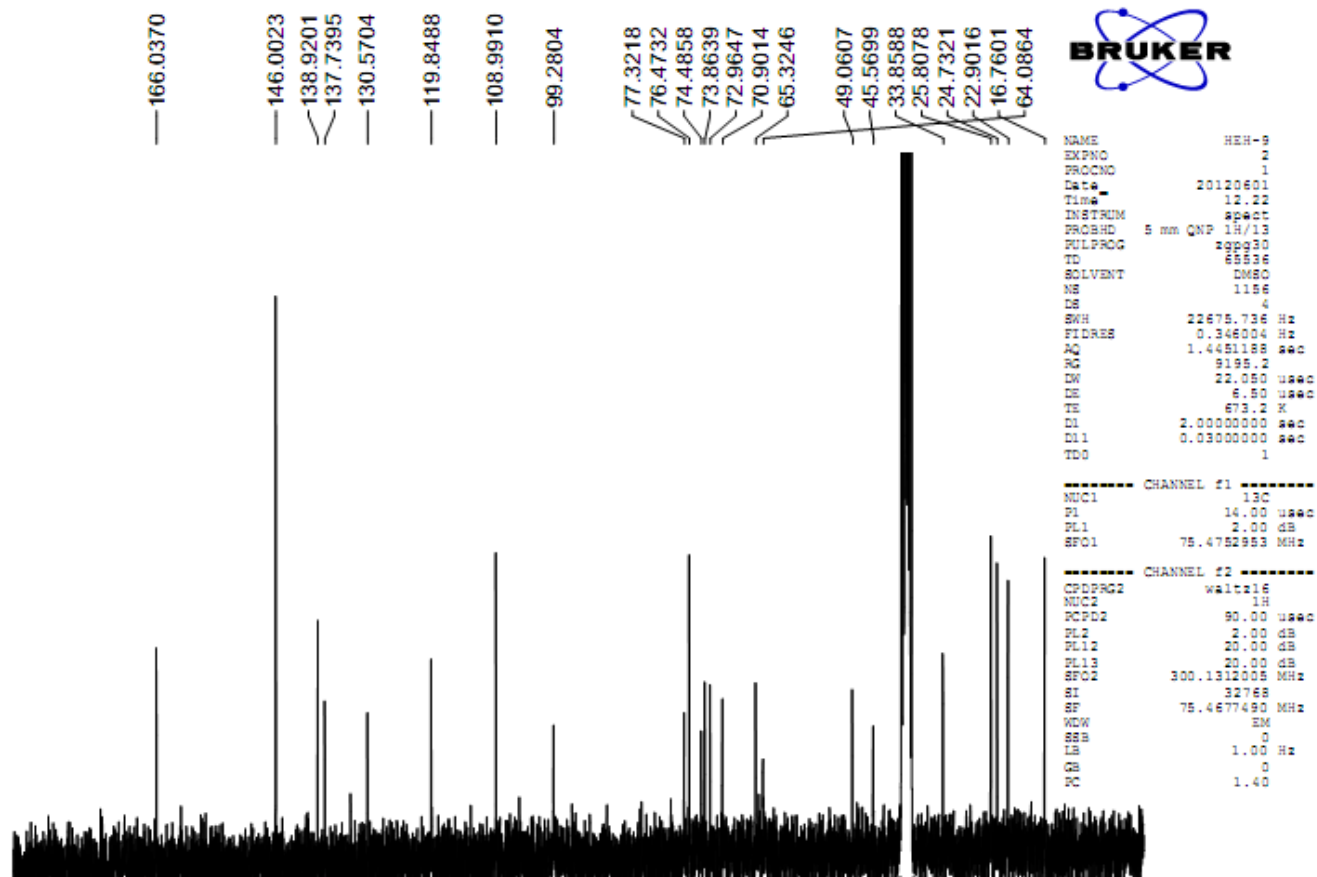
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1	297.0642	2656
2	315.0745	55816
3	316.0785	6556
4	333.0869	7236
5	447.1338	5460
6	507.2227	10108
7	525.2367	69344
8	526.2374	19648
9	527.2379	2797
10	543.2454	29193
11	544.2423	6807
12	560.2708	3064
13	562.2211	4982
14	562.7224	2914
15	565.2273	31897
16	566.2294	7660
17	581.2011	6761
18	833.3379	4142
19	833.8381	2952
20	1107.4607	5017

S1: HRESITOFMS Spectrum of Compound 1

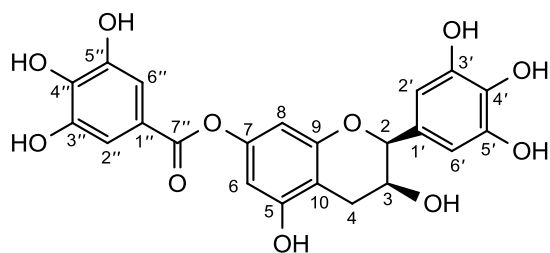


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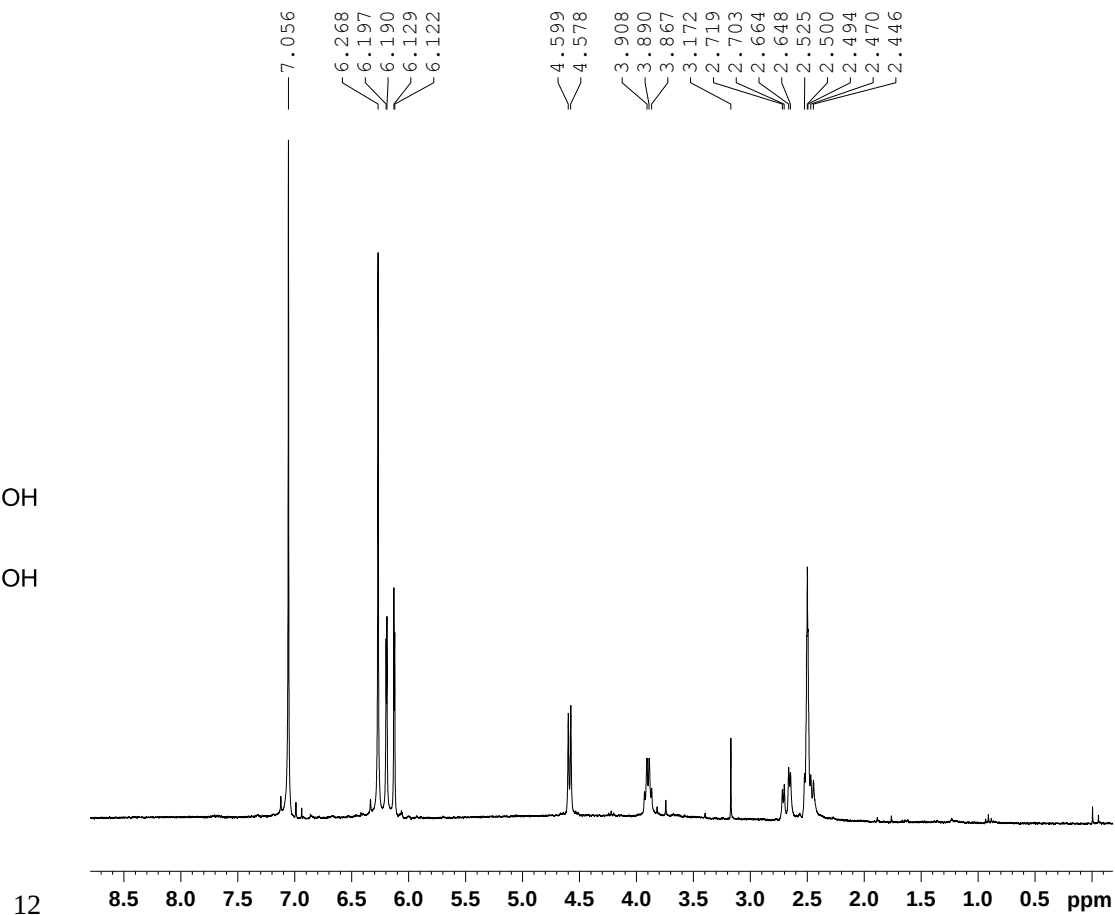




S3: ^{13}C -NMR Spectrum of Compound 1 (75MHz, in DMSO- d_6)



2



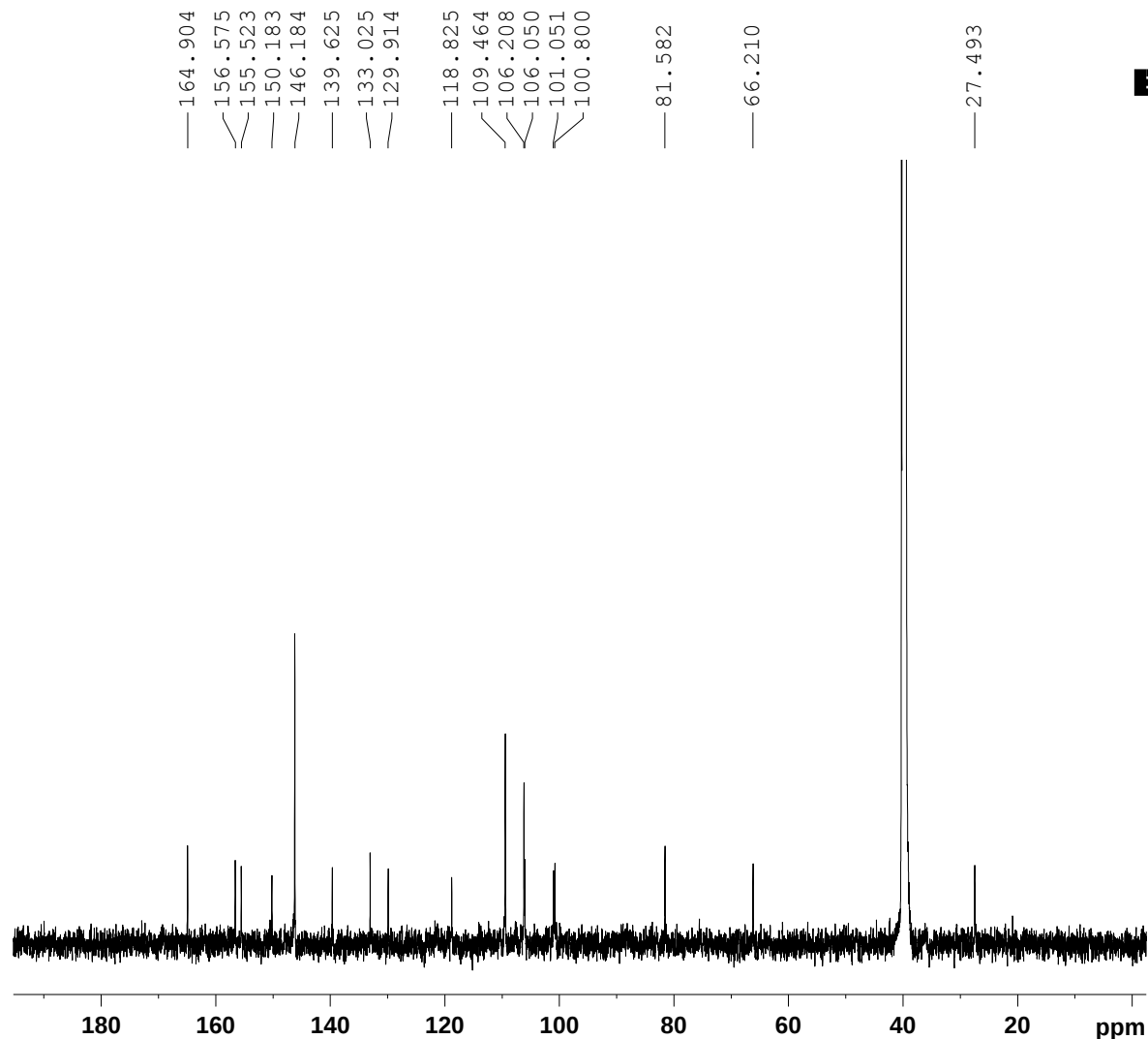
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NAME          HEH-19
EXPNO          1
PROCNO         1
Date_          20121226
Time_          14.11
INSTRUM        spect
PROBHD         5 mm QNP 1H/13
PULPROG        zg30
TD             65536
SOLVENT        DMSO
NS             16
DS             2
SWH            6172.839 Hz
FIDRES         0.094190 Hz
AQ            5.3084660 sec
RG            1024
DW            81.000 usec
DE            6.50 usec
TE            673.2 K
D1            1.00000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1           1H
P1            10.80 usec
PL1           1.00 dB
SFO1          300.1318534 MHz
SI            32768
SF            300.1299995 MHz
WDW            EM
SSB            0
LB            0.30 Hz
GB            0
PC            1.00

```

S5: ¹H-NMR Spectrum of Compound 2 (300MHz, in DMSO-d₆)



```

NAME          HEH-19
EXPNO          2
PROCNO         1
Date_         20130228
Time_          8.23
INSTRUM        spect
PROBHD         5 mm PABBO BB-
PULPROG        zgpg30
TD             65536
SOLVENT        DMSO
NS             469
DS             2
SWH            45454.547 Hz
FIDRES         0.693581 Hz
AQ             0.7209570 sec
RG             18400
DW             11.000 usec
DE             6.50 usec
TE             673.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0            1

```

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===== CHANNEL f1 =====
NUC1           13C
P1             6.00 usec
PL1            1.00 dB
PL1W           83.20243835 W
SFO1           150.9178993 MHz

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===== CHANNEL f2 =====
CPDPRG2        waltz16
NUC2           1H
PCPD2          80.00 usec
PL2            -4.00 dB
PL12           13.16 dB
PL13           16.00 dB
PL2W           34.70265579 W
PL12W          0.66736388 W
PL13W          0.34702653 W
SFO2           600.1324005 MHz
SI             32768
SF             150.9028090 MHz
WDW            EM
SSB            0
LB             3.00 Hz
GB             0
PC             1.40

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S6: ^{13}C -NMR Spectrum of Compound 2 (75MHz, in $\text{DMSO}-d_6$)



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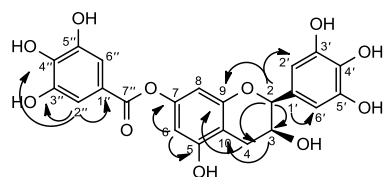
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PROCNO    1
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PULPROG    hsqcpgprsdgk
TD         3274
SOLVENT    MeOH
NS         64
DS         16
SWH         4607.452 Hz
F2FID      4.405012 Hz
AQ          0.1046500 sec
RG          250.00
DE          104.000 umsec
TE          4.50 umsec
YC          252.8 K
CH212      145.0000000
CH213      5.0000000
D0          0.0000000 sec
D1          1.5000000 sec
D2          0.00244826 sec
D6          0.1000000 sec
D16         0.0020000 sec
JBO         0.0000040 sec

===== CHANNEL f1 =====
NUC1        1H
P1          11.10 umsec
P2          22.20 umsec
PL1         -1.00 dB
PL12        24.7024579 dB
STO1        600.1324005 MHz

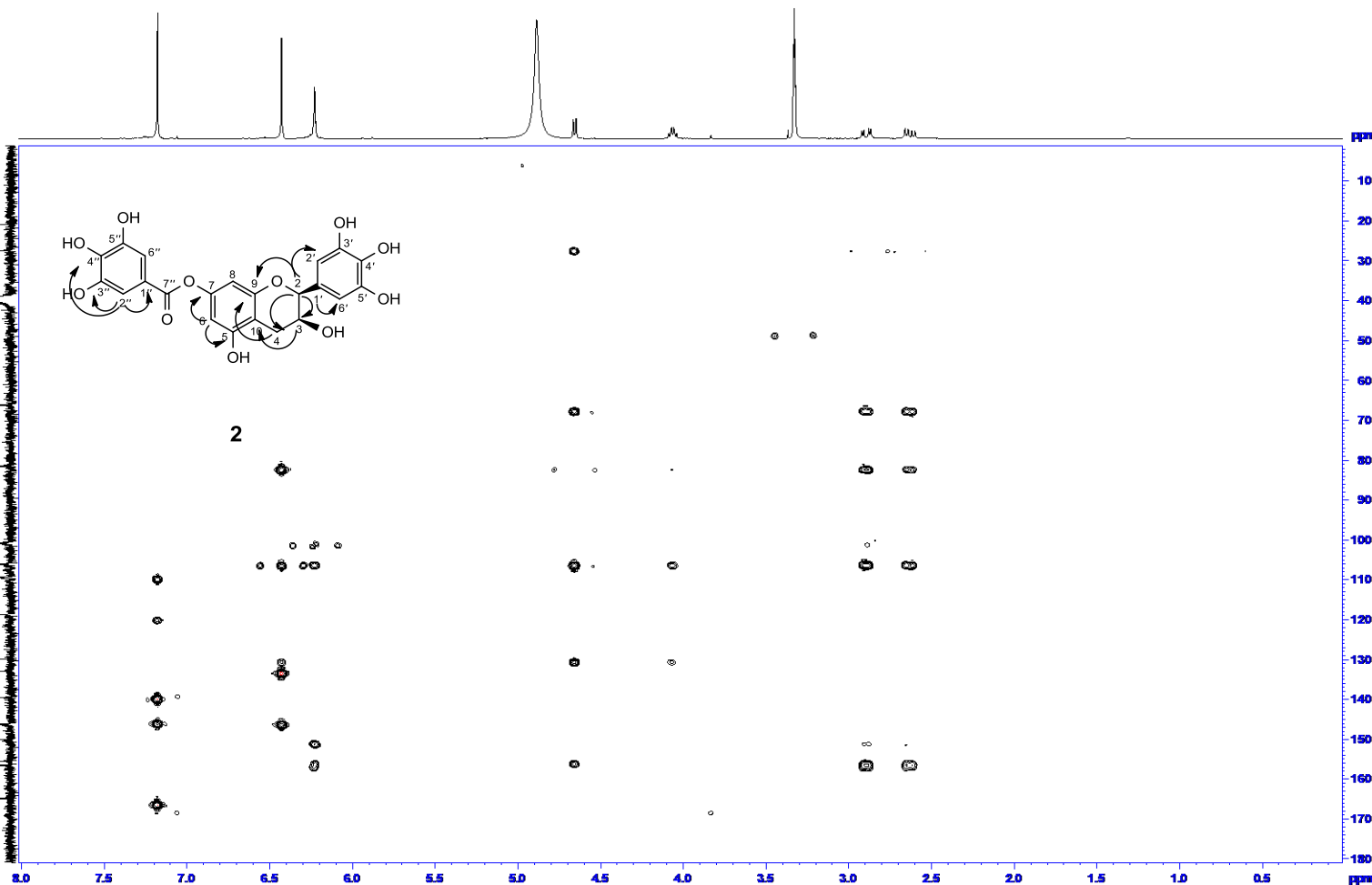
===== CHANNEL f2 =====
NUC2        13C
P3          6.80 umsec
PL2         1.00 dB
PL12        82.26243825 dB
STO2        150.9162903 MHz

===== GRABF2 CHANNEL =====
CPDPRG2     SINE-100
CPDPRG3     SINE-100
CPDPRG4     SINE-100
CPDPRG5     SINE-100
CPDPRG6     SINE-100
CPDPRG7     SINE-100
CPDPRG8     SINE-100
CPDPRG9     SINE-100
CPDPRG10    SINE-100
CPDPRG11    SINE-100
CPDPRG12    SINE-100
CPDPRG13    SINE-100
CPDPRG14    SINE-100
CPDPRG15    SINE-100
CPDPRG16    SINE-100
CPDPRG17    SINE-100
CPDPRG18    SINE-100
CPDPRG19    SINE-100
CPDPRG20    SINE-100
CPDPRG21    SINE-100
CPDPRG22    SINE-100
CPDPRG23    SINE-100
CPDPRG24    SINE-100
CPDPRG25    SINE-100
CPDPRG26    SINE-100
CPDPRG27    SINE-100
CPDPRG28    SINE-100
CPDPRG29    SINE-100
CPDPRG30    SINE-100
CPDPRG31    SINE-100
CPDPRG32    SINE-100
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CPDPRG42    SINE-100
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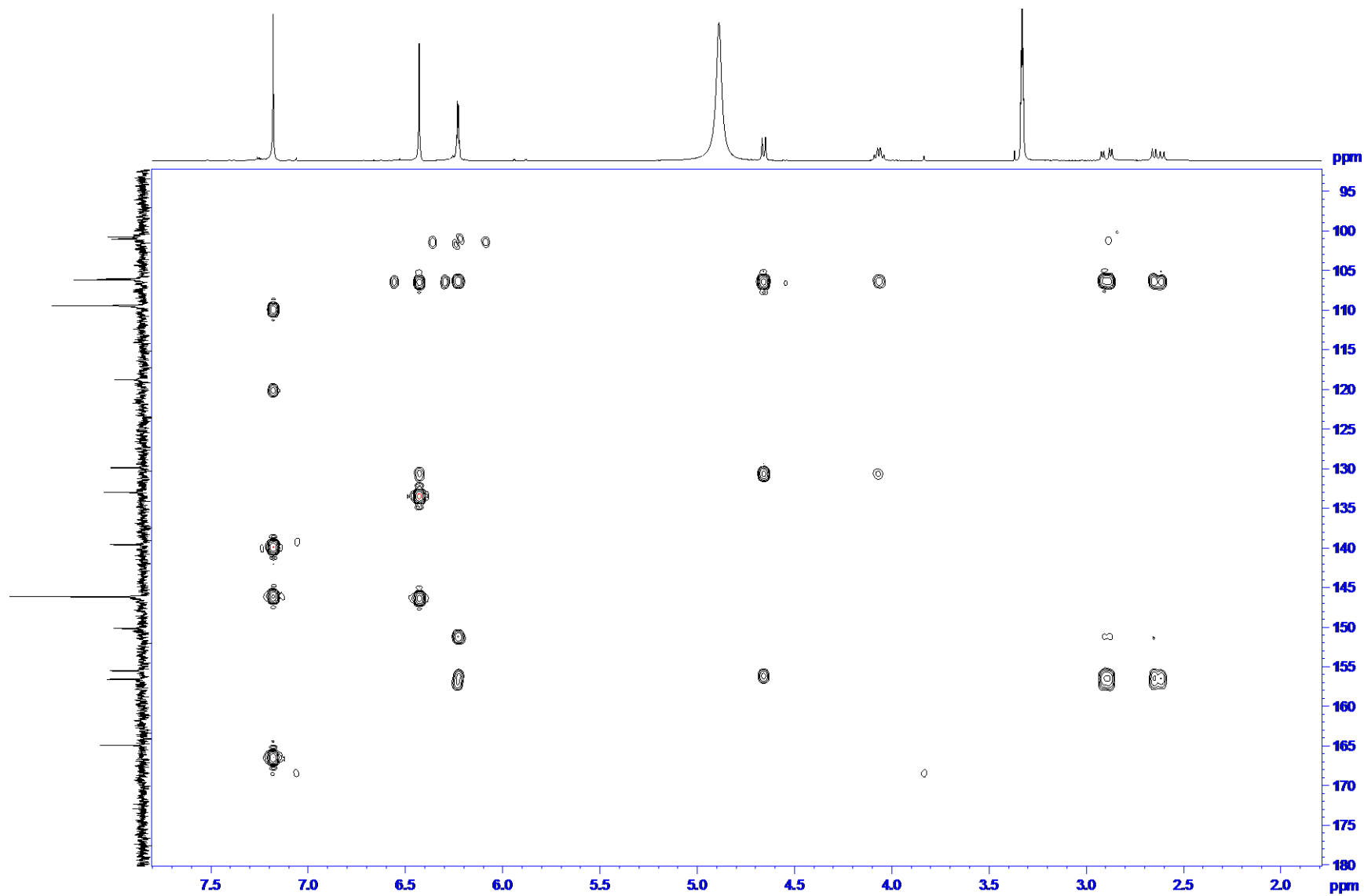
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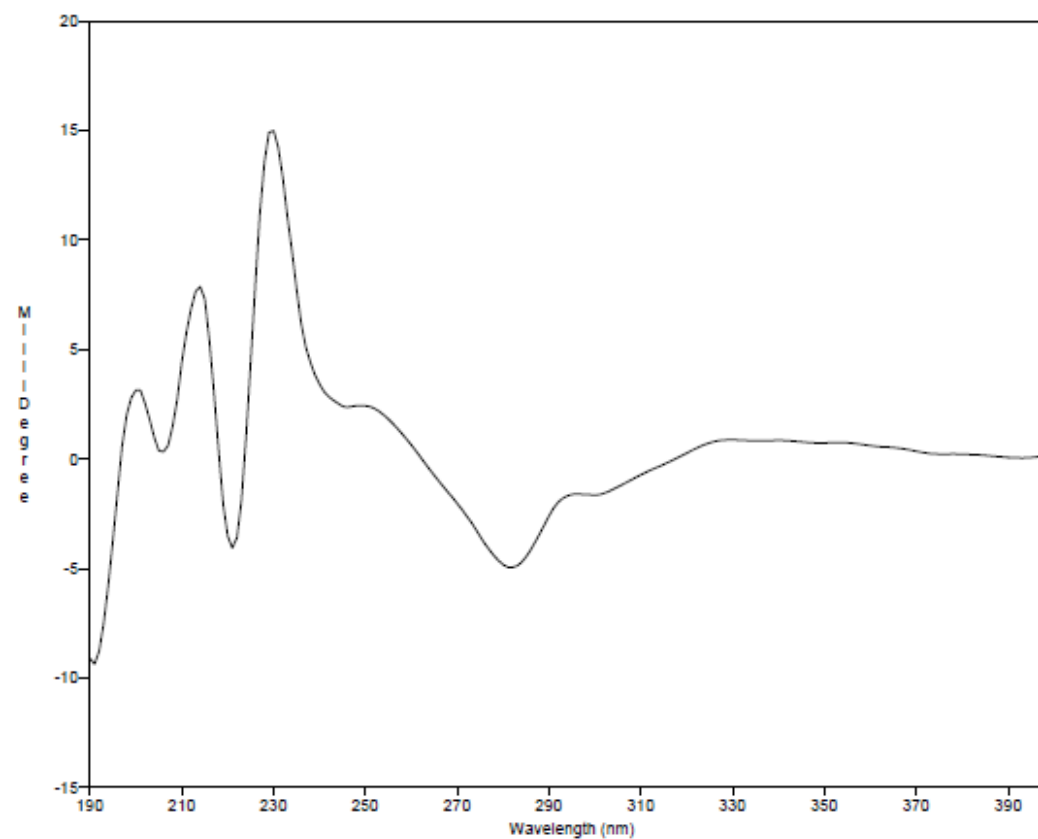
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S7: HMBC Spectrum of Compound 2 (600MHz, in MeOD)



S8: Expansion of the HMBC Spectrum of Compound 2 (600MHz, in MeOD)



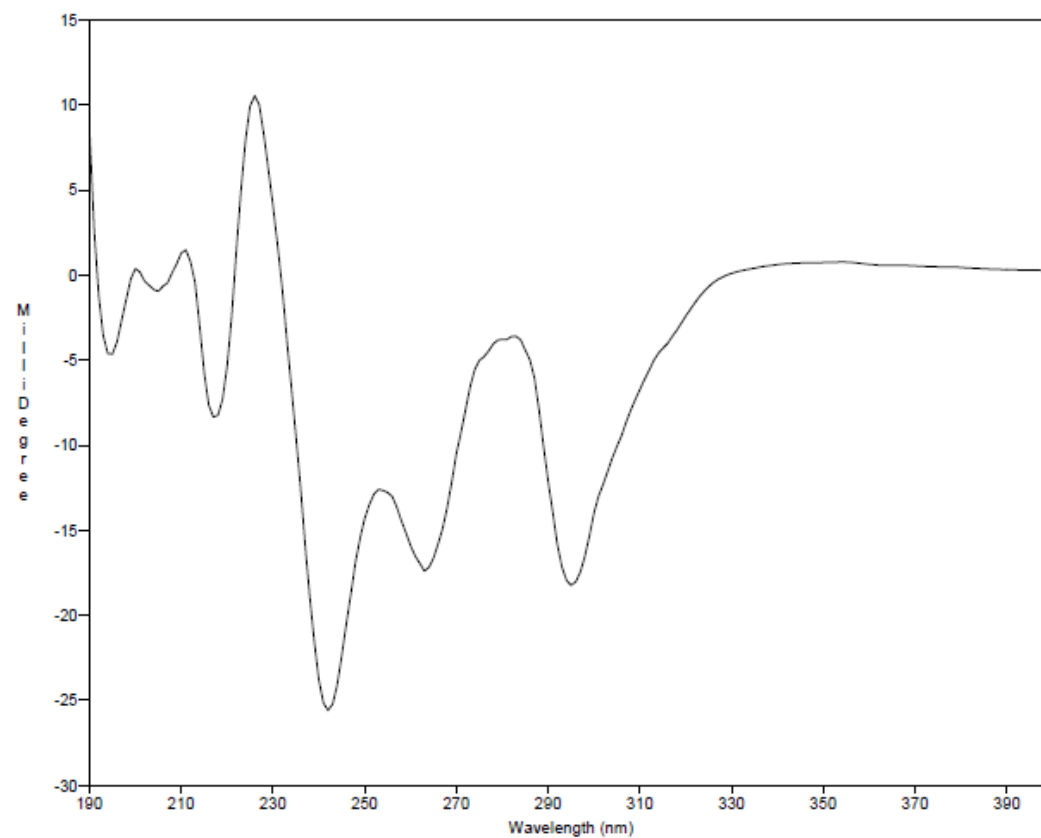
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28

29

S9: The CD spectrum of Compound 2



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30

31

S10: The CD spectrum of Compound 3