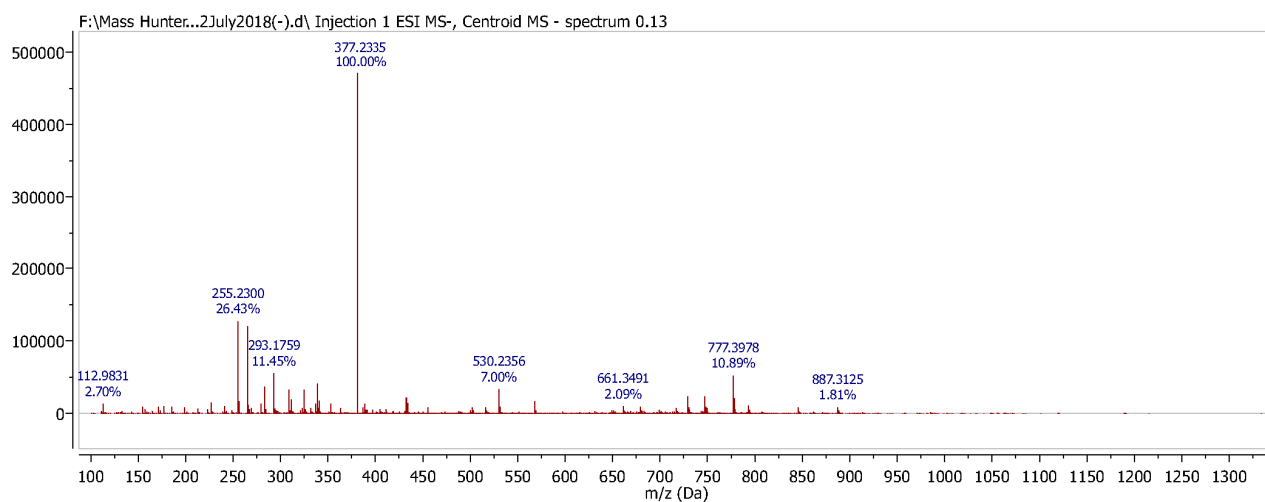


Nitric oxide-mediated vasodilation of bioactive compounds isolated from *Hypericum revolutum*

. Abdallah^{1,2,*}, Noha Z.Hossam M

Timraz¹, Sabrin R. M. Ibrahim^{3,4}, Ali M El-Halawany^{1,2}, Azizah M. Malebari⁵, Ibrahim A. Shehata^{1,2}, Hany M El-Bassossy^{6,7}

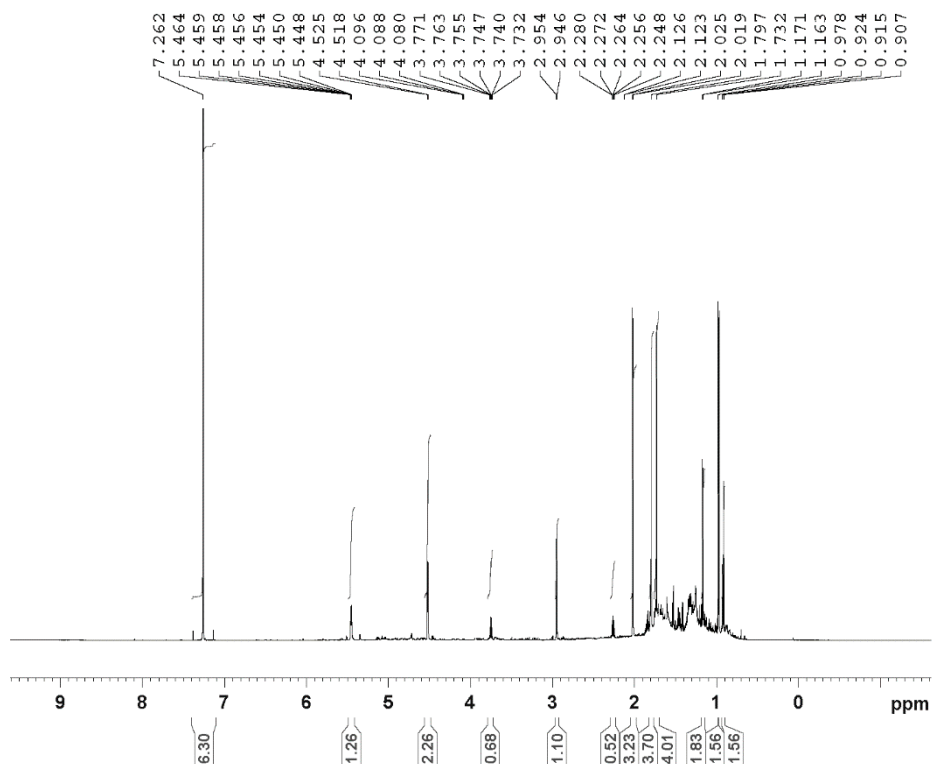
Supplementary Figures



Supplementary Figure S1. HR- ESI, Mass spectrometry spectrum of compound **1**.

Dr. Hossam
Sample :

HR-8-2 CDCl₃



Current Data Parameters
NAME HOSSAM HR-82 16-01-2017
EXPNO 40
PROCNO 1

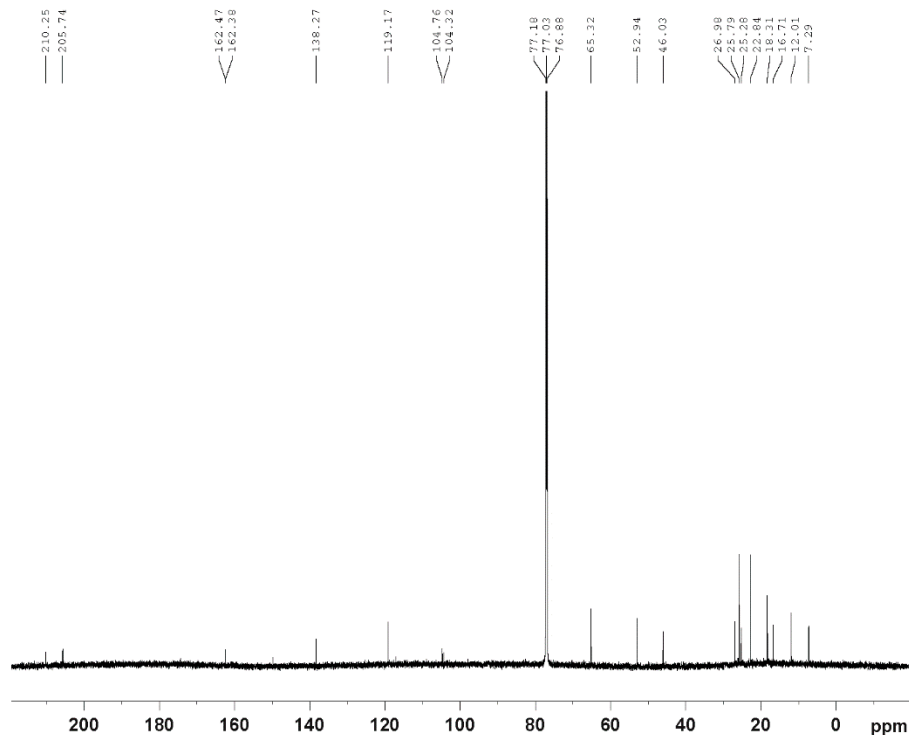
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Date_ 20170116
Time 10.22
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PROBHD 5 mm CPQCI 1H-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 64
DS 2
SWH 17006.803 Hz
FIDRES 0.259503 Hz
AQ 1.9267584 sec
RG 10.55
DW 29.400 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
SF01 850.1582500 MHz
NUC1 1H
P1 8.00 usec
PLW1 15.30000019 W

F2 - Processing parameters
SI 65536
SF 850.1500200 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00

Supplementary Figure S2. ¹H NMR spectrum of compound **1** (CDCl₃, 850 Hz).

Dr. Hossam
Sample : HR-82 CDCl₃



Current Data Parameters
NAME HOSSAM HR-82 18-01-2017
EXPNO 40
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170118
Time 14.25
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PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 2560
DS 4
SWH 51020.406 Hz
FIDRES 0.773510 Hz
AQ 0.6422528 sec
RG 186.93
DM 9.900 usec
DE 19.00 usec
TE 299.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL f1 =====
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NUC1 13C
P1 12.00 usec
PL1 130.0000000 W

===== CHANNEL f2 =====
SFO2 850.1534006 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 13.80000019 W
PLW12 0.13800000 W
PLW13 0.08833000 W

F2 - Processing parameters
SI 32768
SF 213.7703875 MHz
WDW HN
SSB 0
LB 1.50 Hz
GB 0
PC 2.00

Supplementary Figure S3. ¹³C NMR spectrum of compound **1** (CDCl₃, 214 Hz).

Dr.Hossam
Sample : HR-8-2

CDCL3



Current Data Parameters
NAME HOSSAM HR-8-2
EXPNO 23
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170322
Time 16.01
INSTRUM spect
PROBHD 5 mm CPQCI 1H-
PULPROG hsqc-rectop
TD 1024
SOLVENT CDCL3
RG 22
DE 1.6
B0H 989.922 Hz
FIDRES 0.571442 Hz
AQ 0.0322249 sec
RG 166.53
DE 51.000 usec
DM 10.00 usec
TE 298.0 K
COST2 145.000000
DO 0.0000000 sec
D1 1.48419701 sec
D4 0.00172414 sec
D11 0.00000000 sec
D13 0.00000000 sec
D16 0.00000000 sec
D21 0.00345000 sec
D22 0.00001410 sec
EQUPTS 0.00001410 sec

===== CHANNEL f1 =====
NUC1 13C
P1 8.00 usec
P2 16.00 usec
P4H 11.50000019 Hz

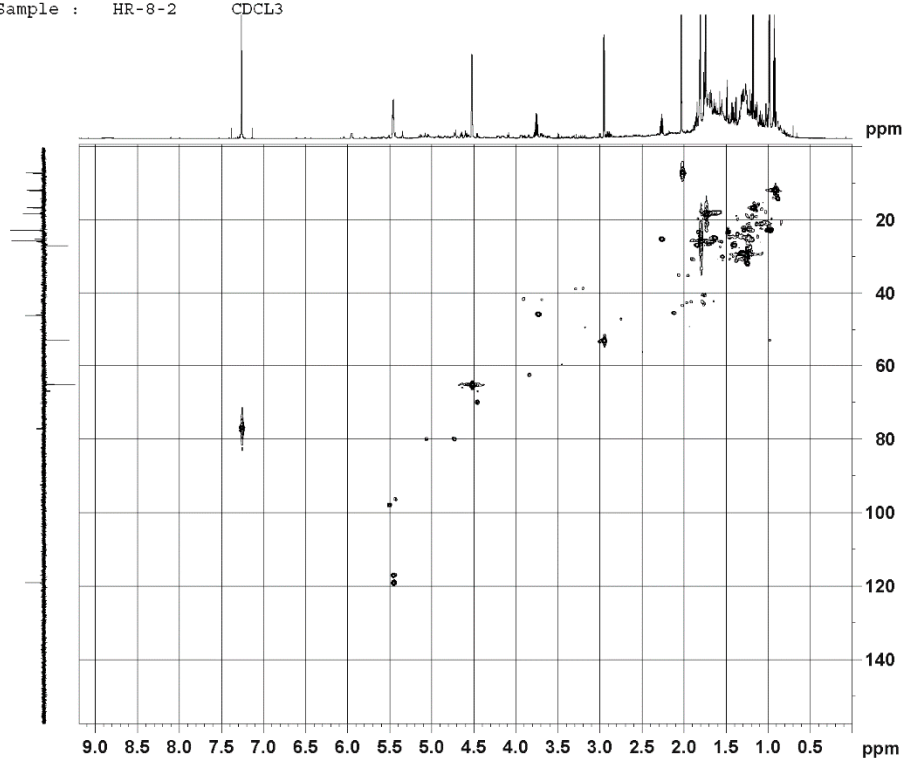
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NUC2 13C
CPDPRG2 gmp
P3 15.00 usec
P4 24.00 usec
P5 15.00 usec
P6H2 130.00000000 Hz
P6H12 9.24440002 Hz

===== GRADIENT CHANNEL =====
GPRAM11 SMC10.100
GPRAM12 SMC10.100
GPR1 20.00 Hz
GPR2 20.00 Hz
P15 1000.00 usec

F1 - Acquisition parameters
TD 256
SFO1 213.7863 MHz
FIDRES 134.519301 Hz
B0 151.873 ppm
FAMCDS Echo-NotEcho

F2 - Processing parameters
ET 1024
SF 450.1500000 MHz
NCH QTHS
LA 0 Hz
GB 0
PC 1.40

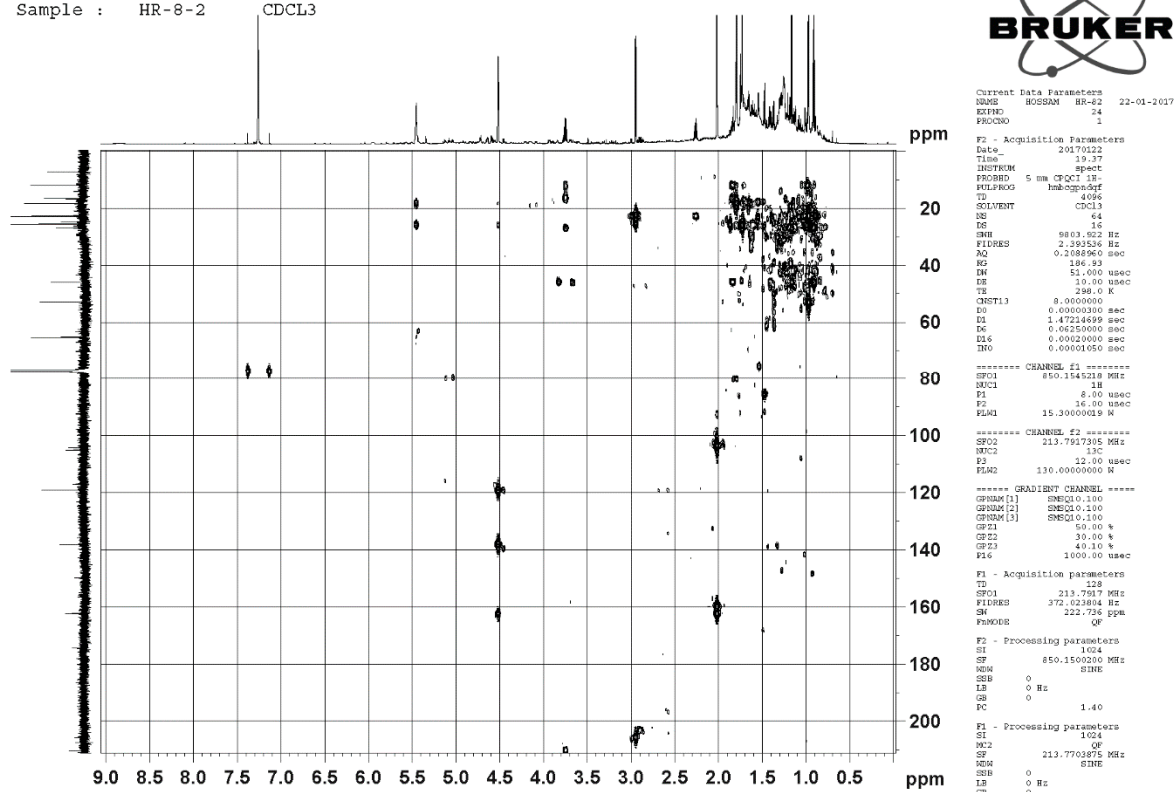
F1 - Processing parameters
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NCH echo-notecho
SF 213.7703875 MHz
NCH QTHS
LA 0 Hz
GB 0



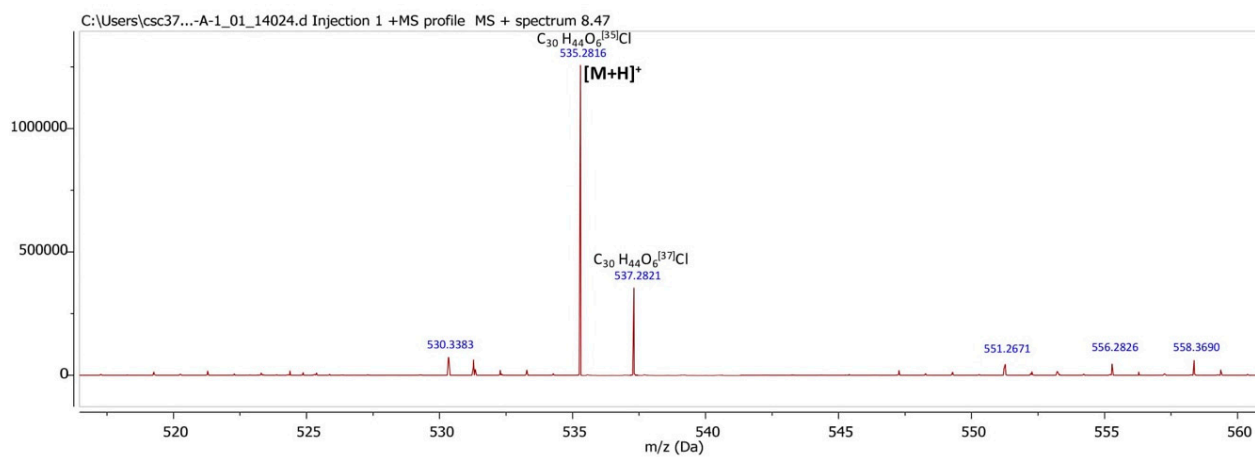
Supplementary Figure S4. HSQC spectrum of compound 1

Dr. Hossam
Sample : HR-8-2

CDCL3



Supplementary Figure S5. HMBC spectrum of compound 1.

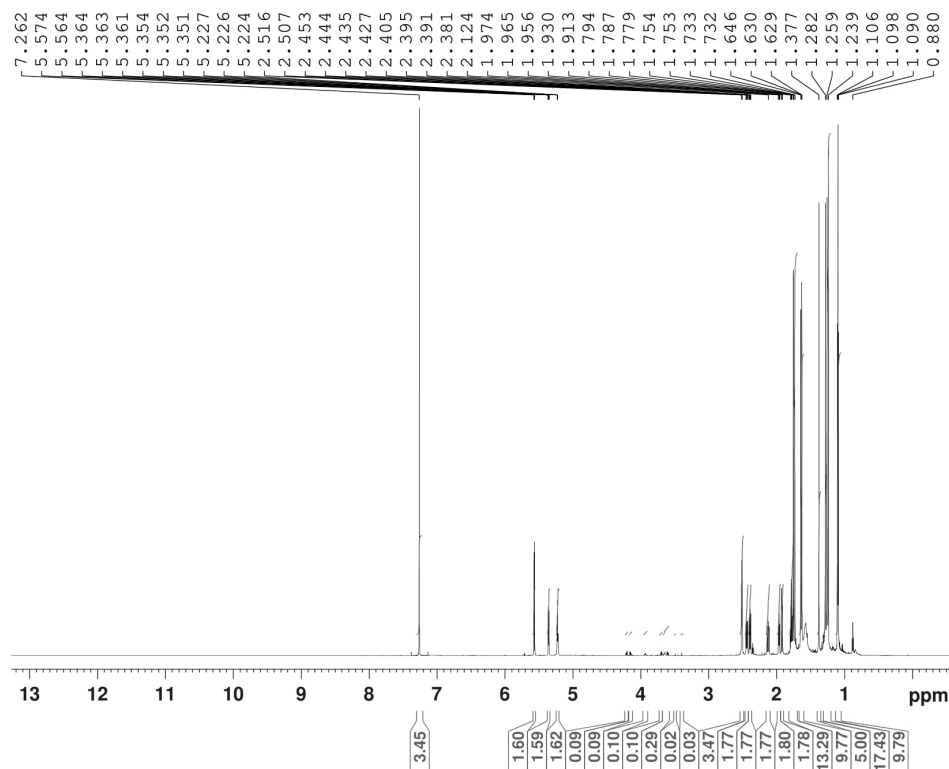


Supplementary Figure S6. HR- ESI, Mass spectrometry spectrum of compound **2**.

Dr.Hossam
Sample :

HR-8-3

CDCL₃



Current Data Parameters
NAME HOSSAM HR-83 16-01-2017
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170116
Time 10.15
INSTRUM spect
PROBHD 5 mm CPQCI 1H-
PULPROG zg30
TD 65536
SOLVENT CDCL3
NS 64
DS 2
SWH 17006.803 Hz
FIDRES 0.259503 Hz
AQ 1.9267584 sec
RG 10.55
DW 29.400 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

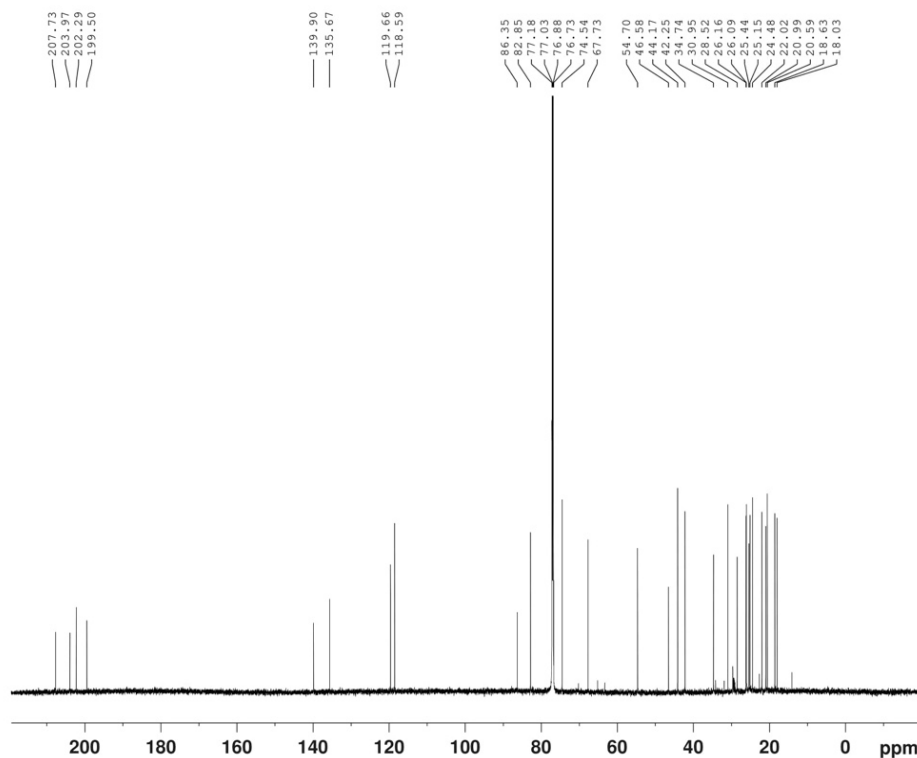
===== CHANNEL f1 =====
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NUC1 1H
P1 8.00 usec
PLW1 15.30000019 W

F2 - Processing parameters
SI 65536
SF 850.1500200 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00

Supplementary Figure S7. ¹H NMR spectrum of compound **2** (CDCl₃, 850 Hz).

Dr.Hossam

Sample : HR-83 CDCL₃



```

Current Data Parameters
NAME      HOSSAM   HR-83   18-01-2017
EXPNO     10
PROCNO    1

F2 - Acquisition Parameters
Date_     20170118
Time      11.59
INSTRUM   spect
PROBHD    5 mm CPQCI 1H-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         993
DS         4
SWH        51020.406 Hz
FIDRES     0.778510 Hz
AQ         0.6422528 sec
RG         186.93
DW         9.800 usec
DE         18.00 usec
TE         298.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TDO        1

===== CHANNEL f1 =====
SF01       213.7917636 MHz
NUC1       13C
P1         12.00 usec
PLW1       130.0000000 W

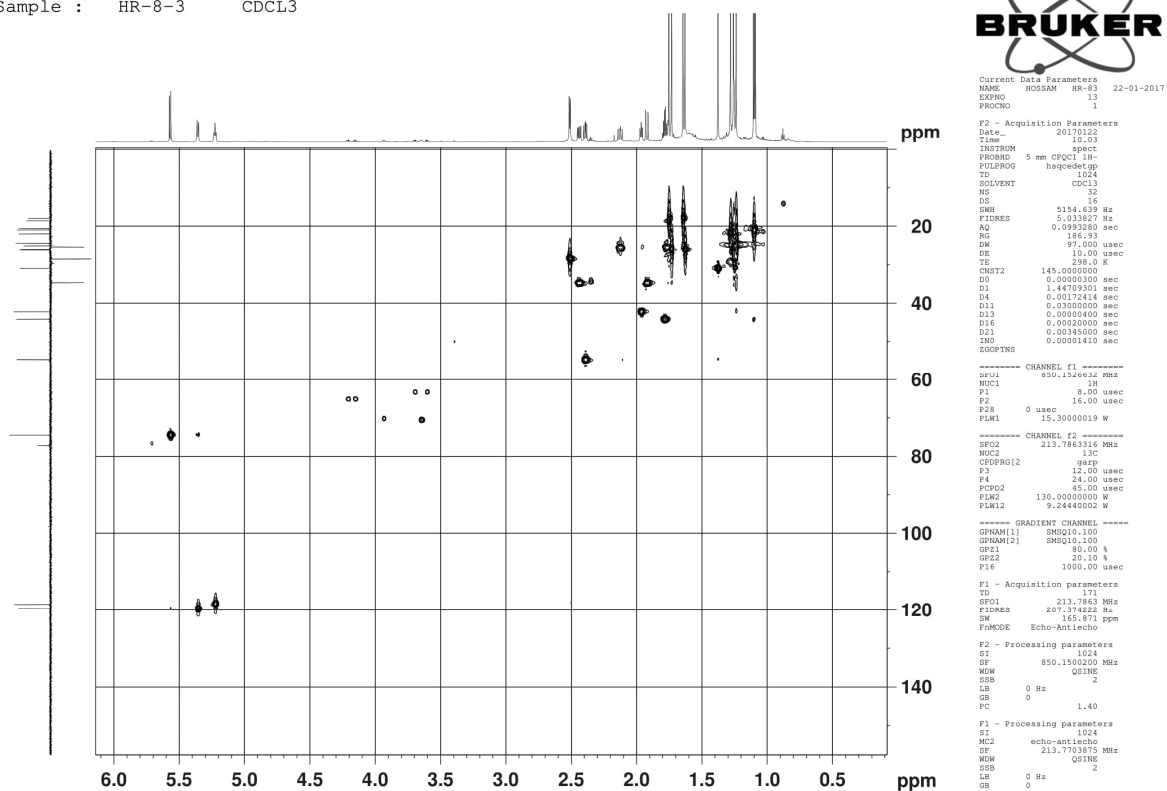
===== CHANNEL f2 =====
SF02       850.1534006 MHz
NUC2       1H
CPDPRG2    Waltz16
PCPD2      80.00 usec
PLW2       13.80000019 W
PLW12      0.13800000 W
PLW13      0.08832000 W

F2 - Processing parameters
SI         32768
SF         213.7703875 MHz
WDW        EM
SSB        0
LB         1.50 Hz
GB         0
PC         2.00

```

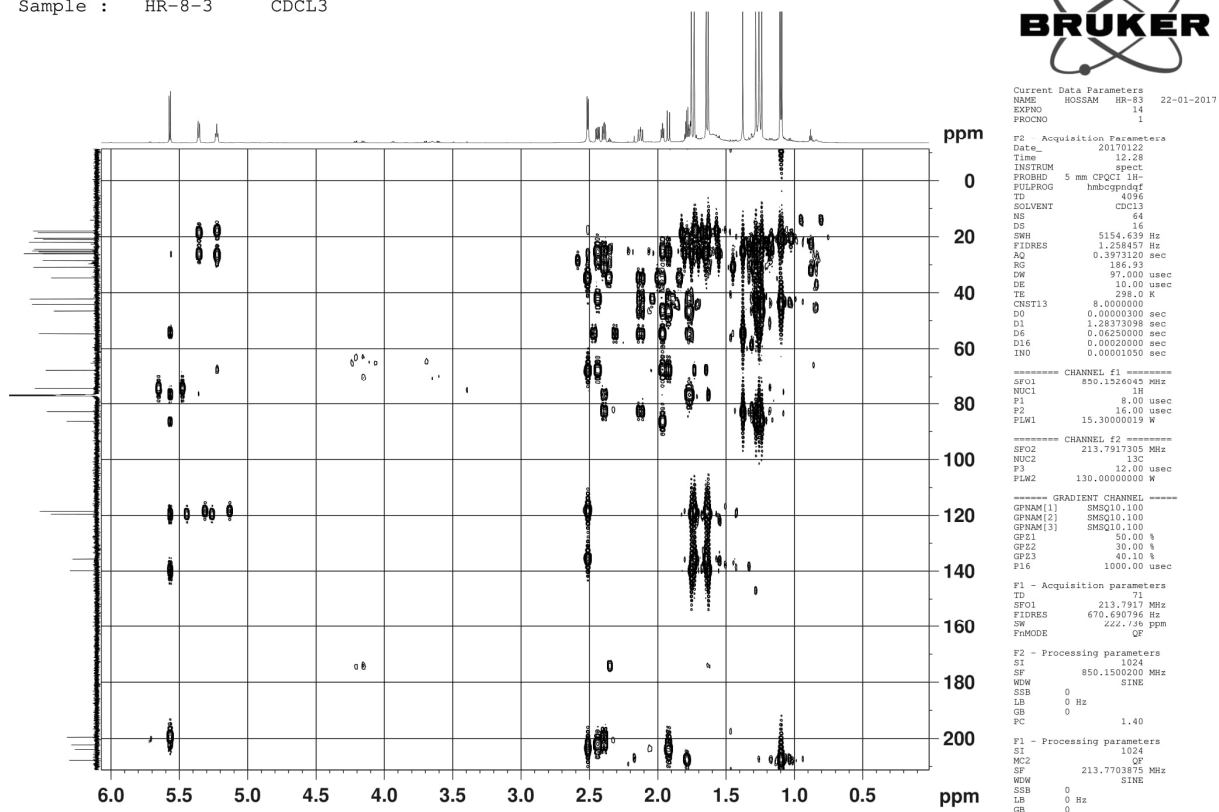
Supplementary Figure S8. ¹³C NMR spectrum of compound **2** (CDCl₃, 214 Hz).

Dr.Hossam
Sample : HR-8-3 CDCL3



Supplementary Figure S9. HSQC spectrum of compound 2

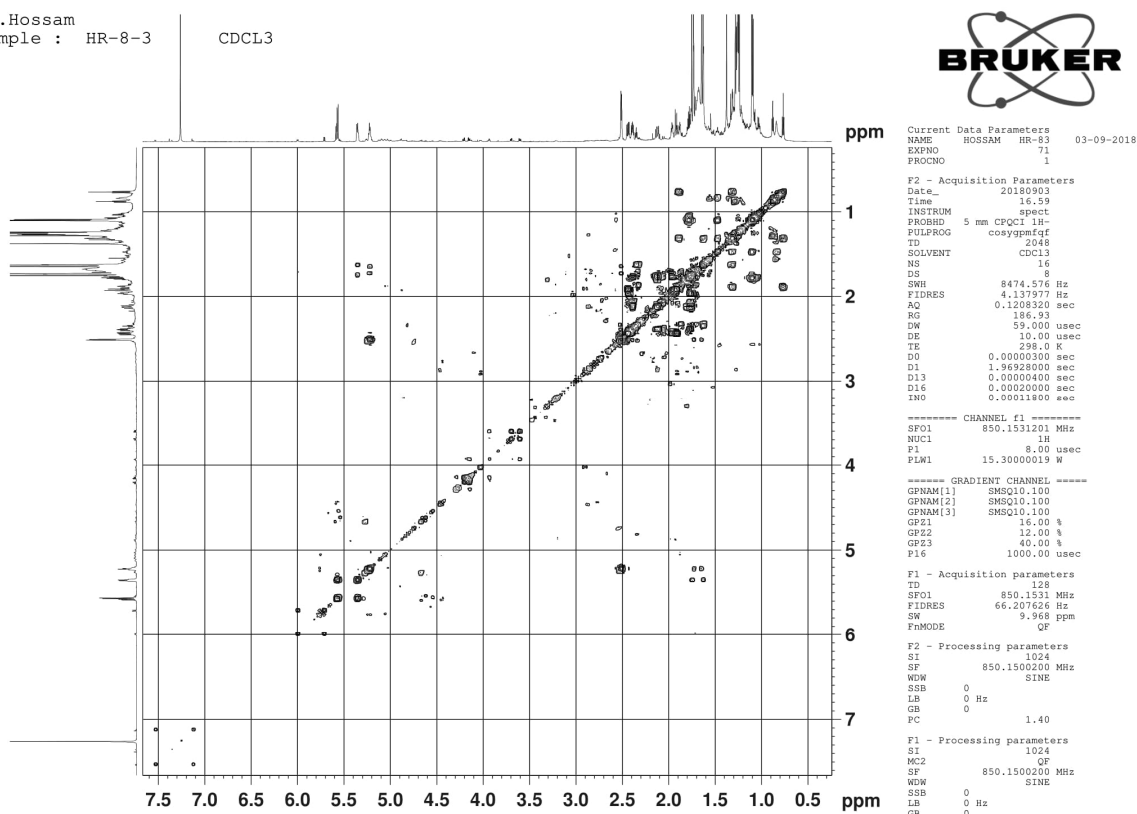
Dr. Hossam
Sample : HR-8-3 CDCL₃



Supplementary Figure S10. HMBC spectrum of compound 2

Dr.Hossam
Sample : HR-8-3

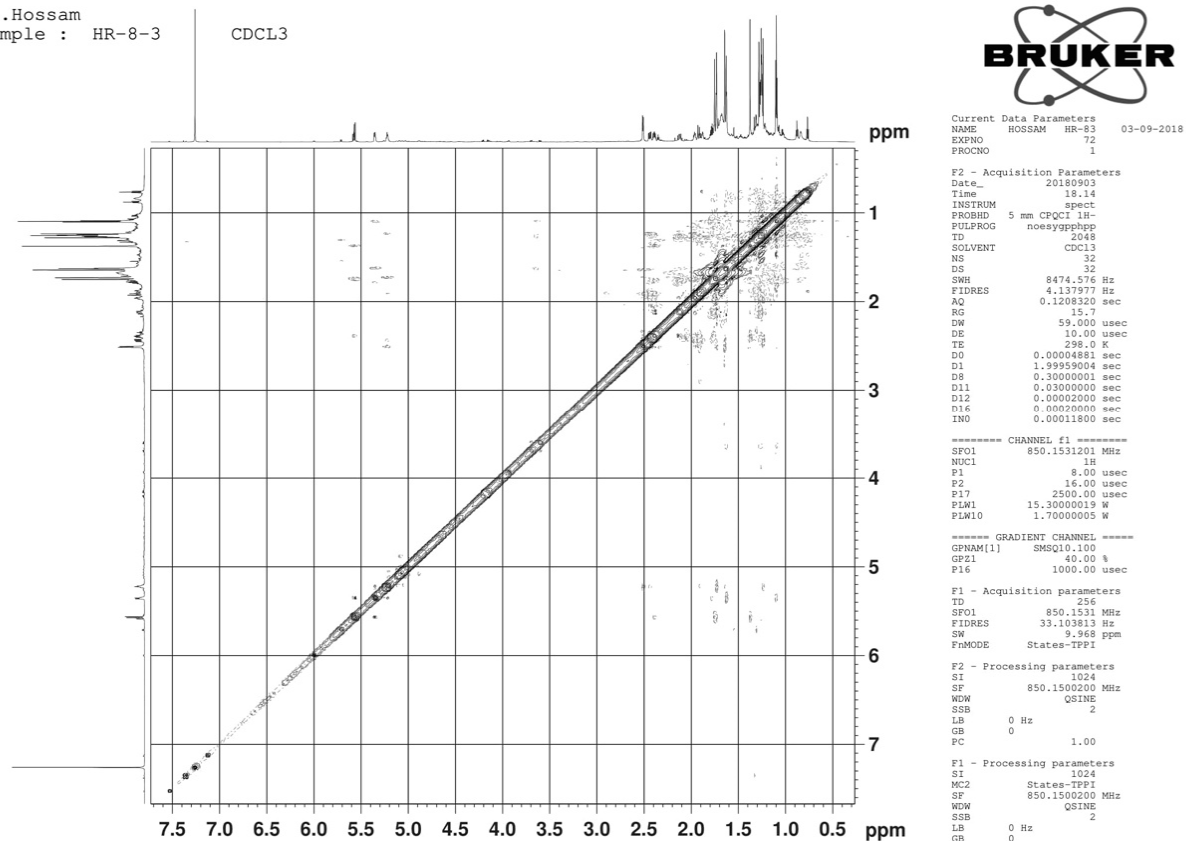
CDCL3



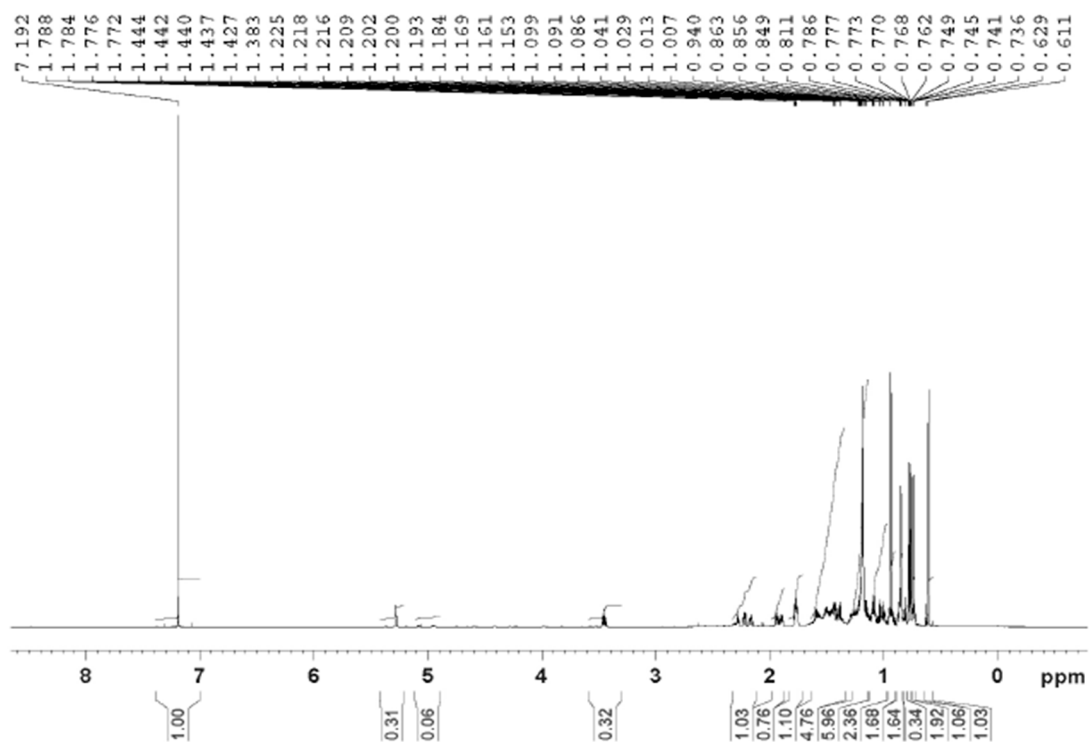
Supplementary Figure S11. COSY spectrum of compound **2**

Dr.Hossam
Sample : HR-8-3

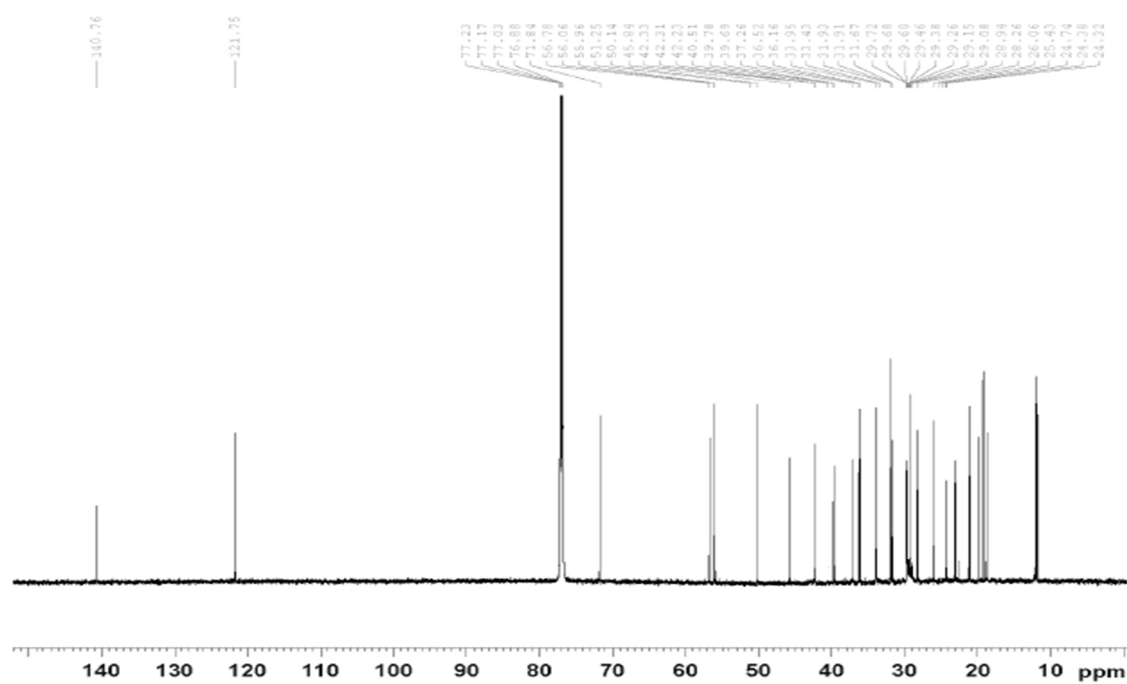
CDCL3



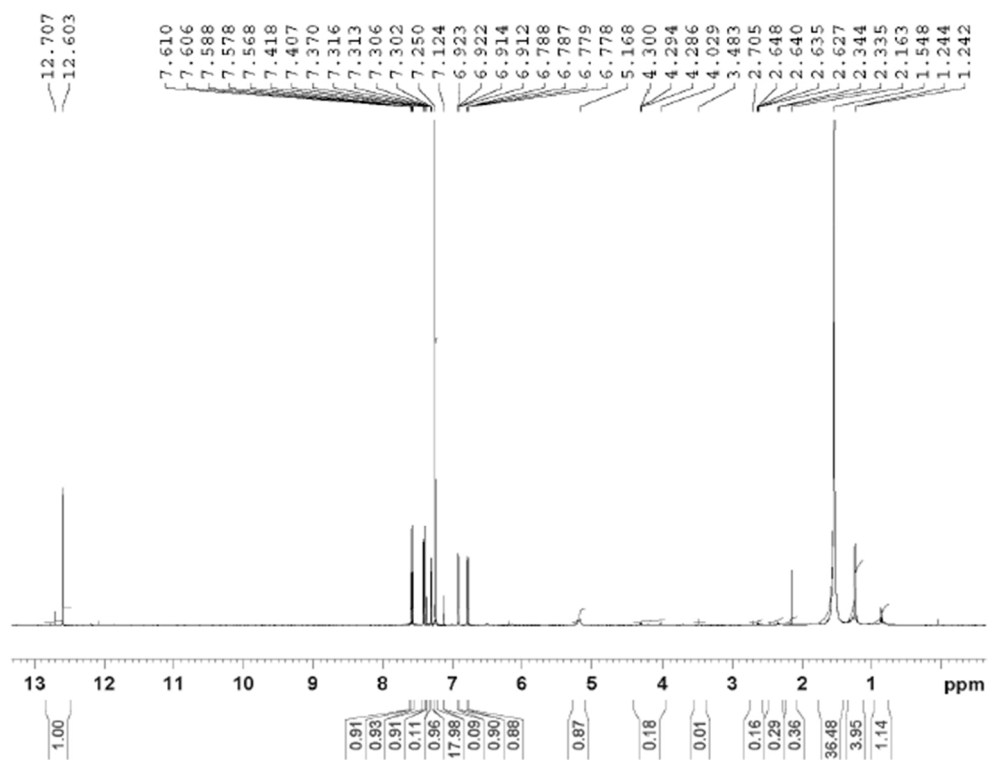
Supplementary Figure S12. NOESY spectrum of compound 2



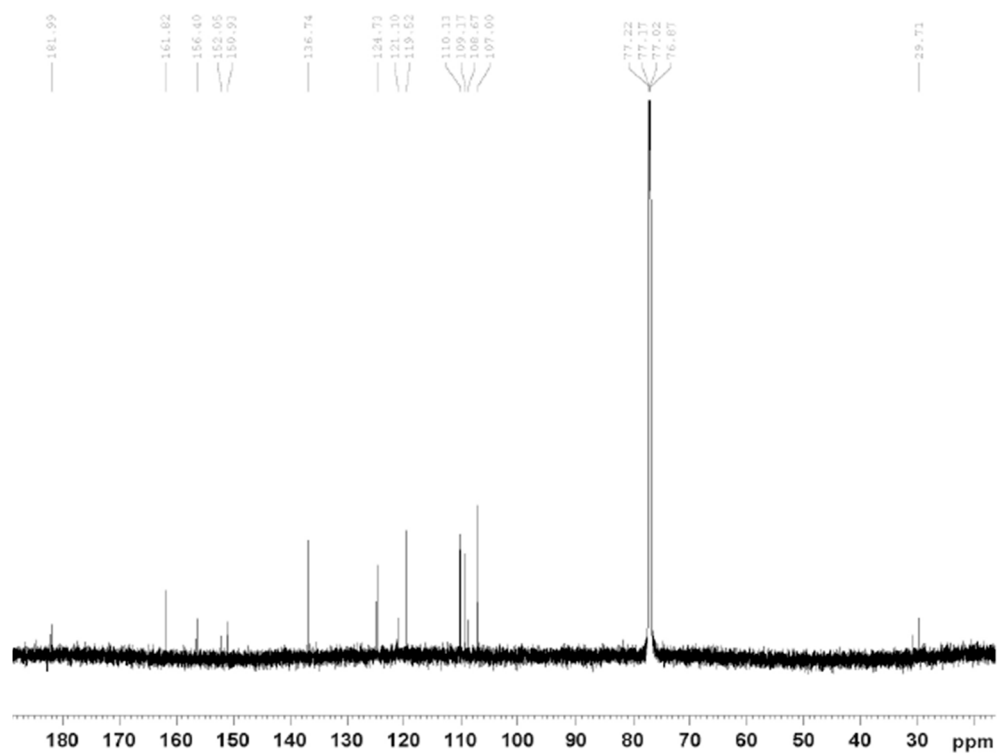
Supplementary Figure S13: ^1H NMR spectrum of compound **3** (CDCl_3 , 850 Hz).



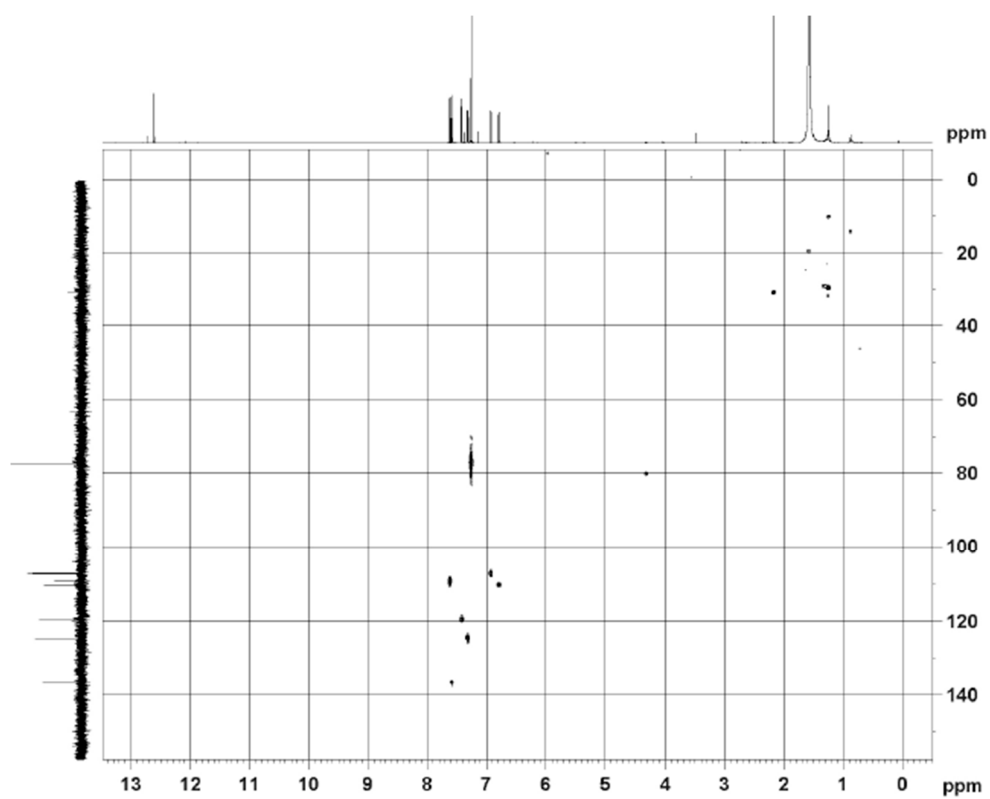
Supplementary Figure S14: ^{13}C NMR spectrum of compound **3** (CDCl_3 , 214 Hz).



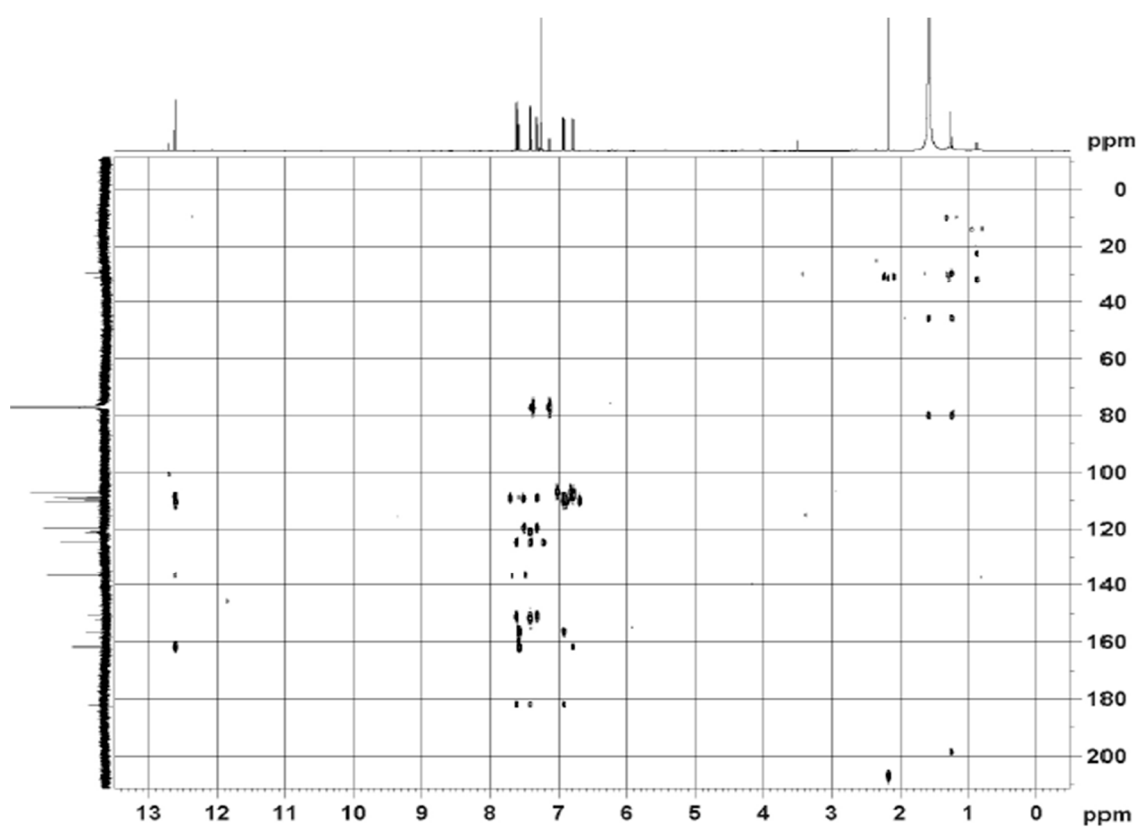
Supplementary Figure S15: ^1H NMR spectrum of compound 4 (euxanthone) (CDCl_3 , 850 Hz).



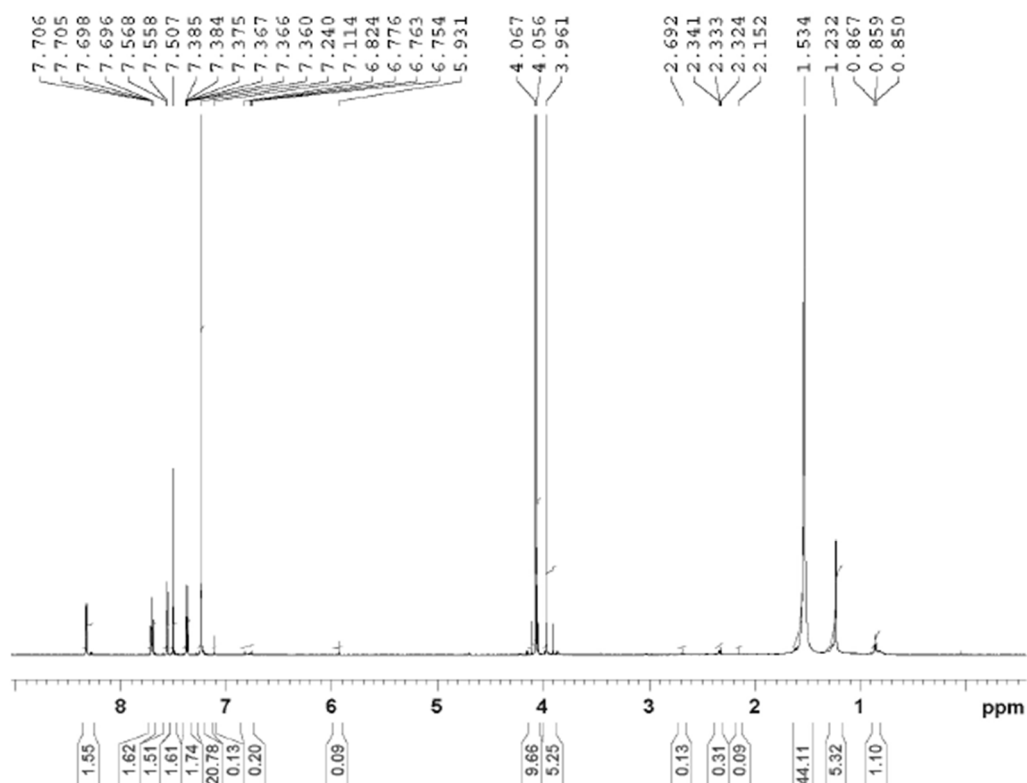
Supplementary Figure S16: ¹³C NMR spectrum of compound **4** (euxanthone) (CDCl₃, 214 Hz).



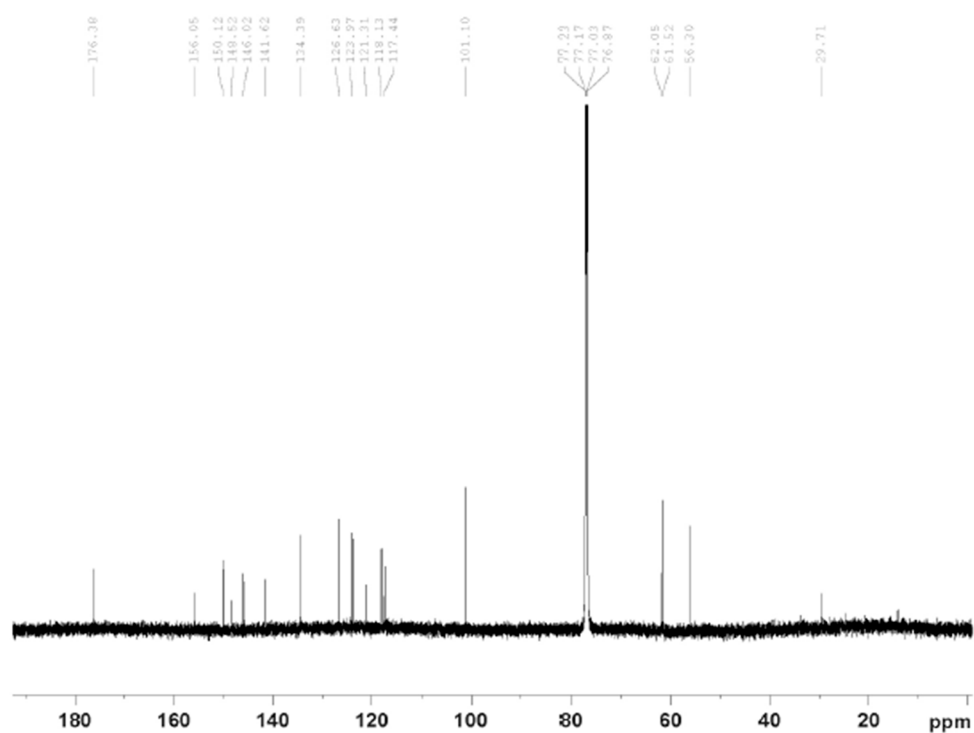
Supplementary Figure S17: HSQC spectrum of compound **4** (euxanthone)



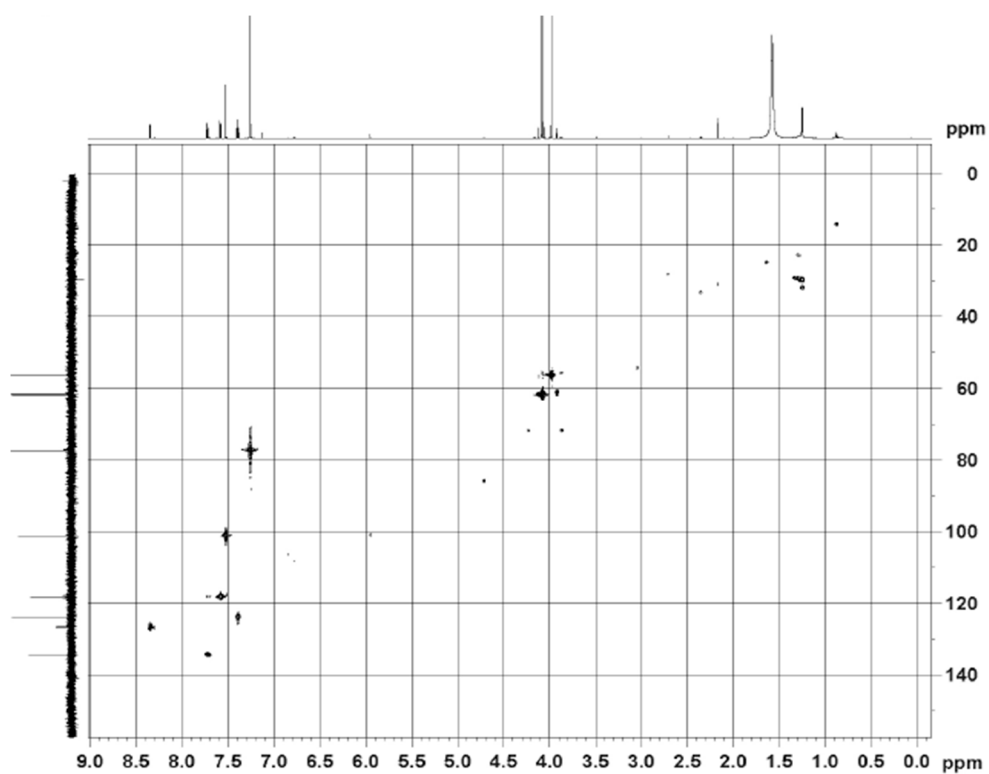
Supplementary Figure S18: HMBC spectrum of compound **4** (euxanthone)



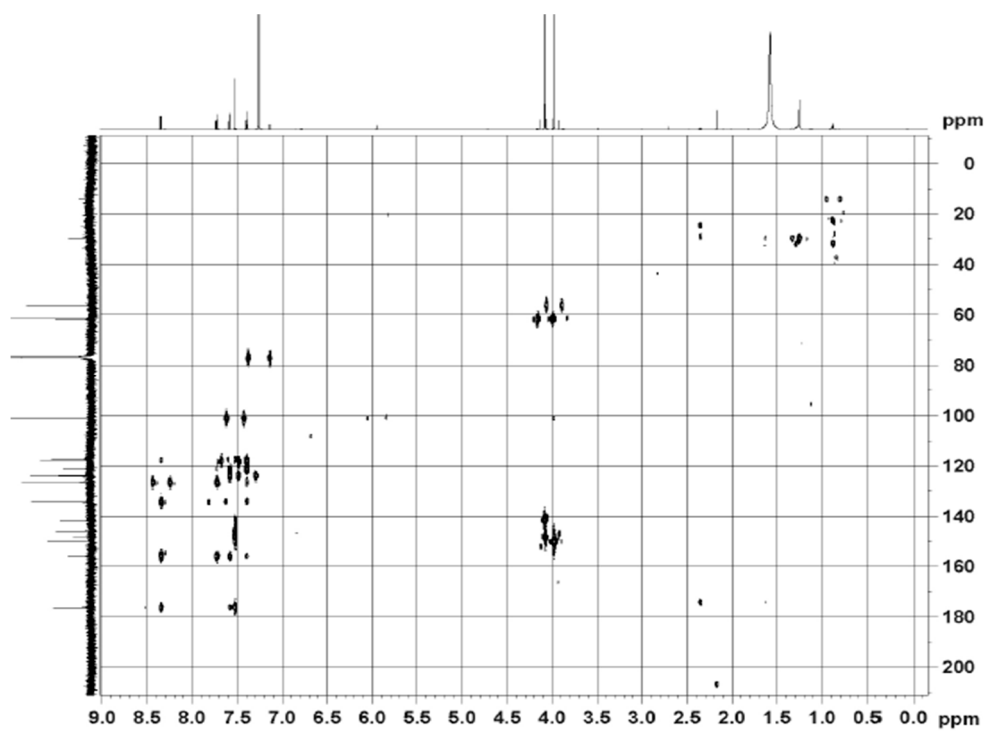
Supplementary Figure S19: ¹H NMR spectrum of compound **5** (2,3,4-trimethoxy xanthone) (CDCl₃, 850 Hz).



Supplementary Figure S20: ¹³C NMR spectrum of compound **5** (2,3,4-trimethoxy xanthone) (CDCl₃, 214 Hz).



Supplementary Figure S21: HSQC spectrum of compound **5** (2,3,4-trimethoxy xanthone)



Supplementary Figure S22: HMBC spectrum of compound **5** (2,3,4-trimethoxy xanthone)

Supplementary Tables

Supplementary Table S1: NMR data of compound **3** (CDCl₃, 850 and 214 Hz).

No.	δ_{H} [mult., <i>J</i> (Hz)]	δ_{C} (mult.)
1	1.83, 1.07 m	37.3 CH ₂
2	1.45, 1.23 m	31.9 CH ₂
3	3.45 m	71.8 CH
4	1.95, 1.83 m	42.3 CH ₂
5	-	140.8 C
6	5.28 m	121.8 CH
7	1.97, 1.83 m	31.7 CH ₂
8	1.51 m	31.9 CH
9	0.92 m	50.1 CH
10	-	36.5 C
11	1.45 m	21.1 CH ₂
12	1.99, 1.51 m	39.7 CH ₂
13	2.28, 2.23 m	42.3 CH ₂
14	0.98 m	56.8 CH
15	1.58, 1.03 m	24.3 CH ₂
16	1.84, 1.25 m	28.3 CH ₂
17	1.09 m	56.1 CH
18	0.61 s	11.9 CH ₃
19	0.94 s	19.4 CH ₃
20	1.38 m	36.2 CH
21	0.84 d (6.4)	19.0 CH ₃
22	1.32, 1.11 m	34.0 CH ₂
23	1.13 m	26.1 CH ₂
24	0.93 m	45.8 CH
25	1.65 m	29.2 CH
26	0.74 d (6.7)	18.8 CH ₃
27	0.76 d (6.7)	19.8 CH ₃
28	-	23.1 CH ₂
29	0.77 t (6.9)	12.0 CH ₃

Supplementary Table S2: NMR data of compound **4** (euxanthone) (CDCl₃, 850 and 214 Hz).

No.	δ_{H} [mult., J (Hz)]	δ_{C} (mult.)	HMBC
1	-	161.8 C	-
2	6.78 dd (2.1, 8.5)	110.1 CH	1, 2, 8b
3	7.58 t (8.5)	136.7 CH	1, 4a, 8b
4	6.92 dd (2.1, 8.5)	107.0 CH	2, 4a, 8b
4a	-	156.4 C	-
4b	-	150.9 C	-
5	7.41 d (8.5)	119.5 CH	6, 7, 8a
6	7.31 dd (2.5, 8.5)	124.7 CH	5, 8, 4b
7	-	152.1 C	-
8	7.61 d (2.5)	109.2 CH	-
8a	-	121.1C	-
8b	-	108.7 C	-
9	-	182.0 C	
1-OH	12.6 s	-	1, 3, 4a, 8b

Supplementary Table S3: NMR data of compound **5** (2,3,4-trimethoxy xanthone) (CDCl₃, 850 and 214 Hz).

No.	δ_{H} [mult., <i>J</i> (Hz)]	δ_{C} (mult.)	HMBC
1	7.51 s	101.1 CH	3, 4a, 9
2	-	141.6 C	-
3	-	148.5 C	-
4	-	150.1 C	-
4a	-	146.2 C	-
4b	-	156.1 C	-
5	7.56 brd (8.5)	118.1 CH	7, 8a
6	7.71 dt (1.7, 8.5)	134.4 CH	8, 4b
7	7.38 t (8.5)	124.0 CH	3, 5, 8a
8	8.32 dd (1.7, 8.5)	126.6 CH	4b, 6
8a	-	121.1 Cs	-
8b	-	117.4 C	-
9	-	176.4 C	-
2-OCH ₃	4.07 s	56.3 CH ₃	2, 8b
3-OCH ₃	4.06 s	61.5 CH ₃	3, 4a
4-OCH ₃	3.96 s	61.1 CH ₃	4, 8b