

Bioassay Guided Isolation and Docking studies of a Potential β - Lactamase Inhibitor from *Clutia myricoides*

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733-110

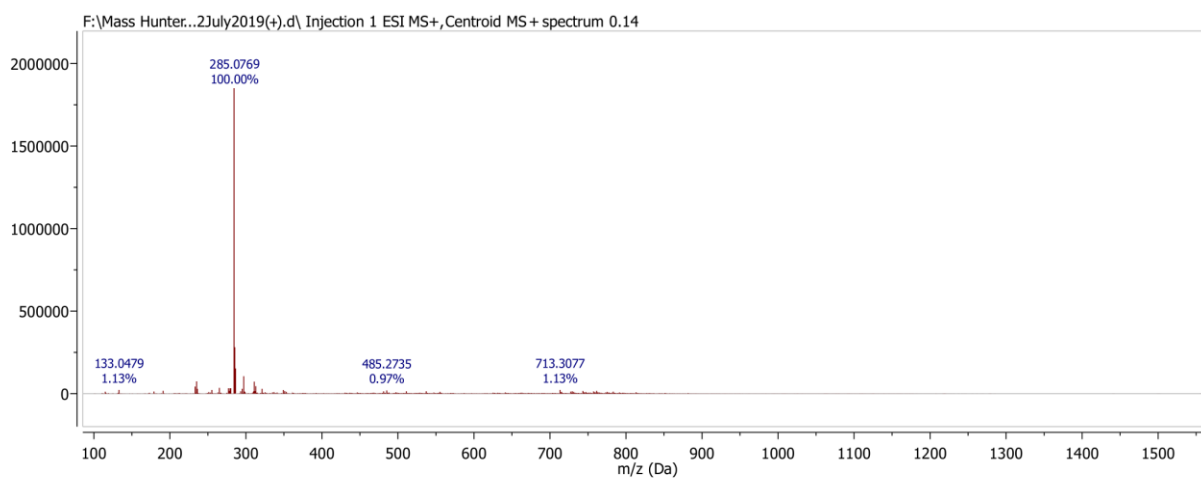


Figure S1: HRESIMS spectrum of compound **2**.

Dr. Hossam
Sample : CLMC-6-1 CDCl₃

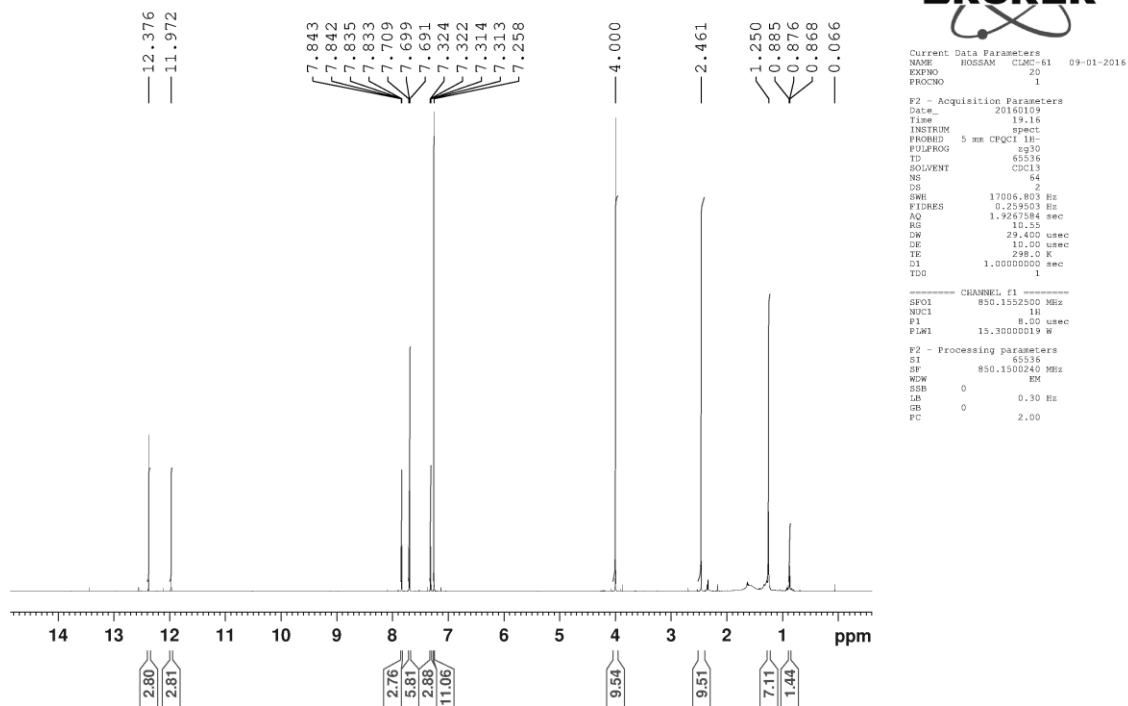
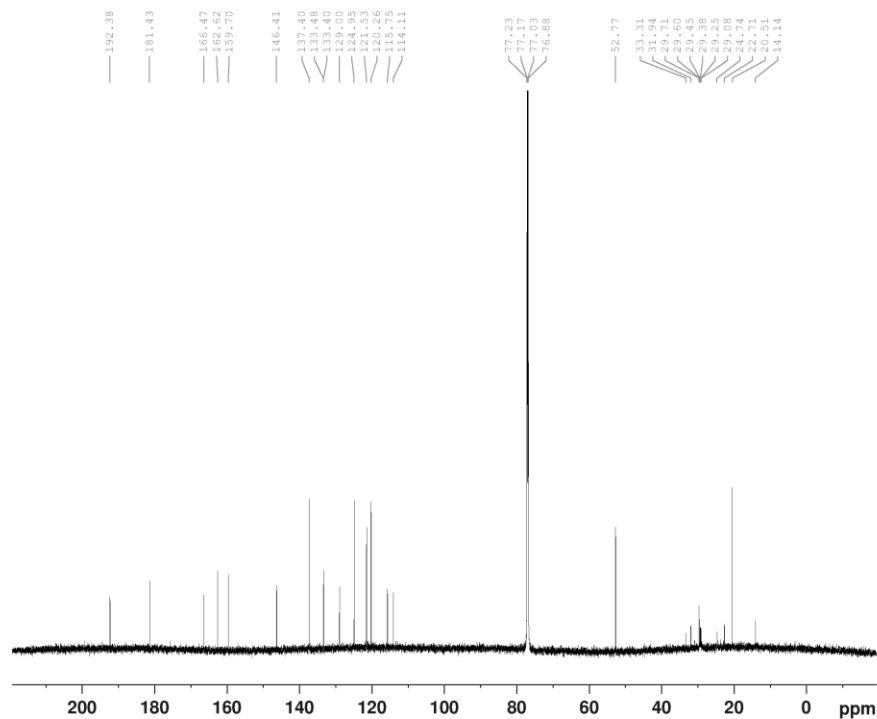


Figure S2: ¹H NMR spectrum of compound 2 (850 MHz, CDCl₃).

Dr.Hossam
Sample : CLMC-6-1

CDCL3



```
Current Data Parameters
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EXPNO    10
PROCNO   1

F2 - Acquisition Parameters
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PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       1116
DS       4
SWH      51020.406 Hz
FIDRES   0.778510 Hz
AQ       0.6422528 sec
RG       185.83
DM       9.800 usec
DE       18.00 usec
TE       298.0 K
D1       2.00000000 sec
D11      0.03000000 sec
TDO      1

===== CHANNEL f1 =====
SFO1     213.7917636 MHz
NUC1     13C
P1       12.00 usec
PLM1     130.00000000 W

===== CHANNEL f2 =====
SFO2     850.1534006 MHz
NUC2     1H
CPDPRG2  waltz16
PCPD2    80.00 usec
PLM2     13.80000019 W
PLM3     0.13800000 W
PLM3     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
```

Figure S3: ^{13}C NMR spectrum of compound 2 (214 MHz, CDCl_3).

Dr. Hossam
Sample :

CLMC-61 CDCL3

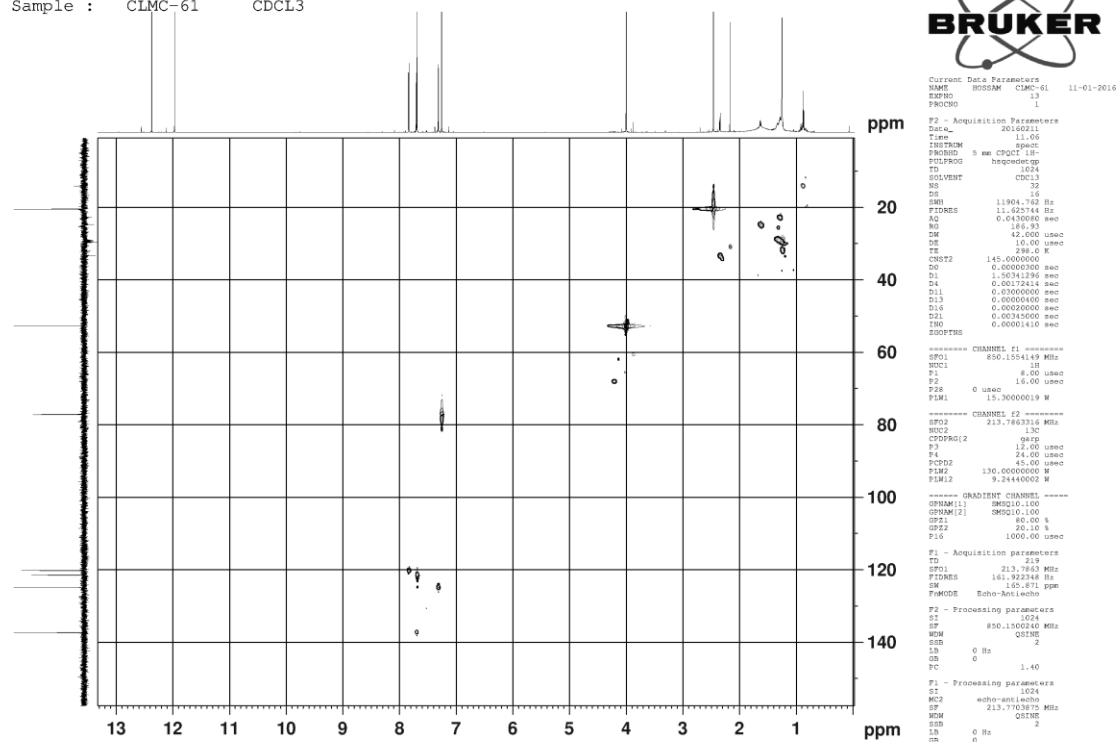


Figure S4: HSQC spectrum of compound 1 (CDCl₃).

Dr. Hossam
Sample : CLMC-61 CDCL3

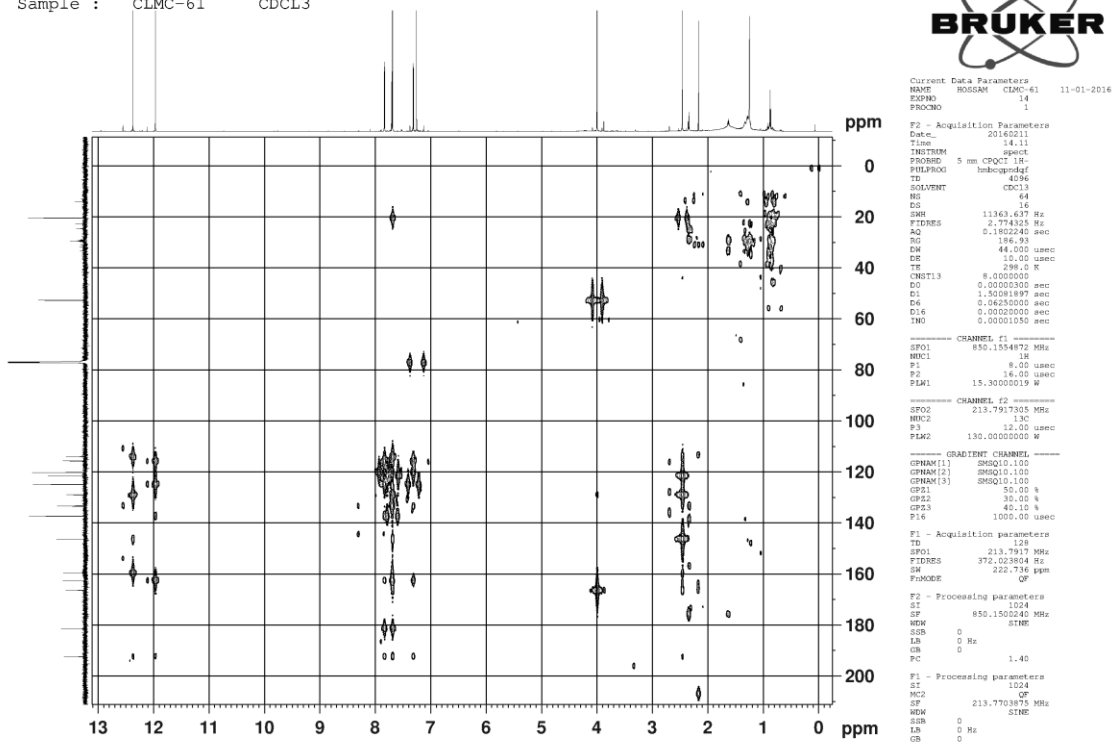


Figure S5: HMBC spectrum of compound 1 (CDCl₃).

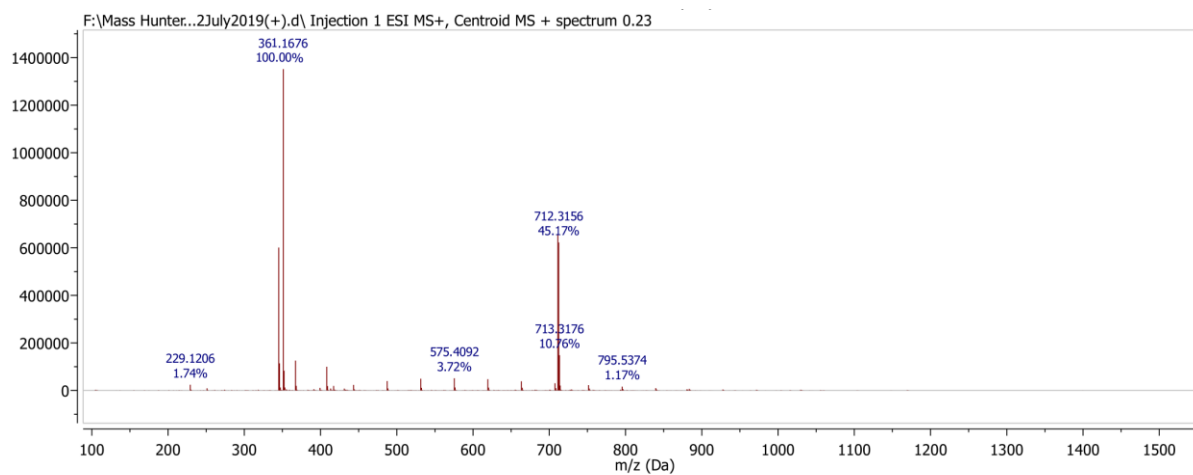


Figure S6: HRESIMS spectrum of compound **5**.

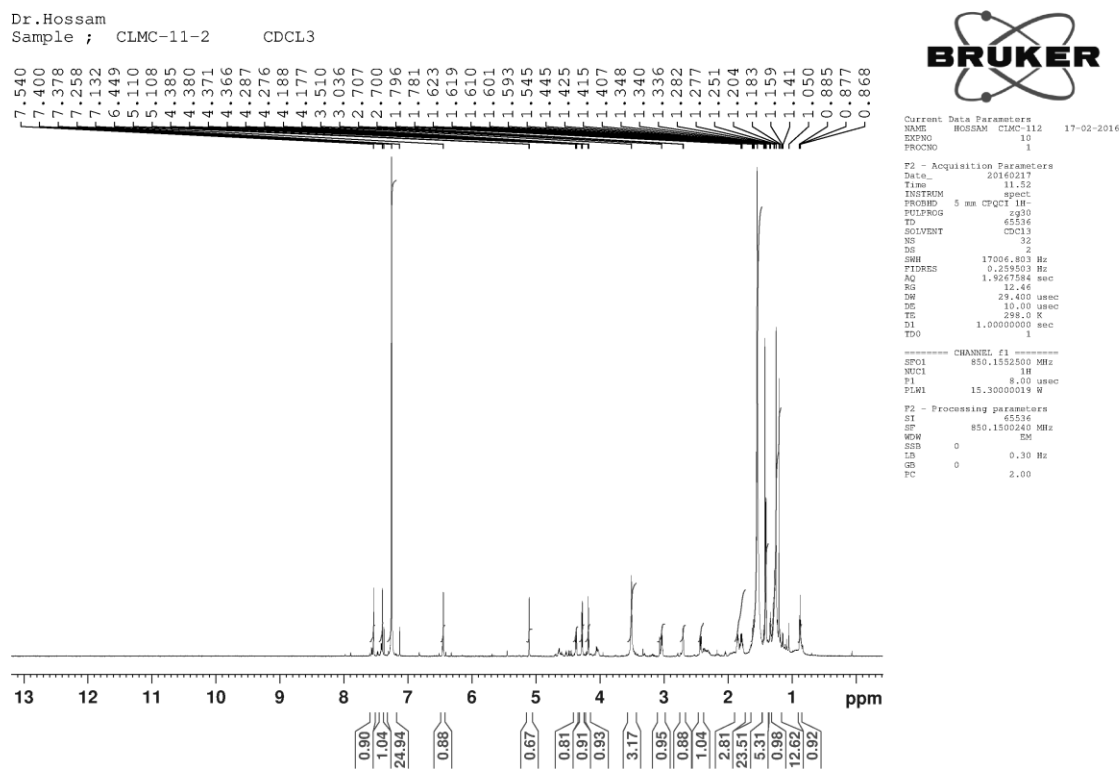
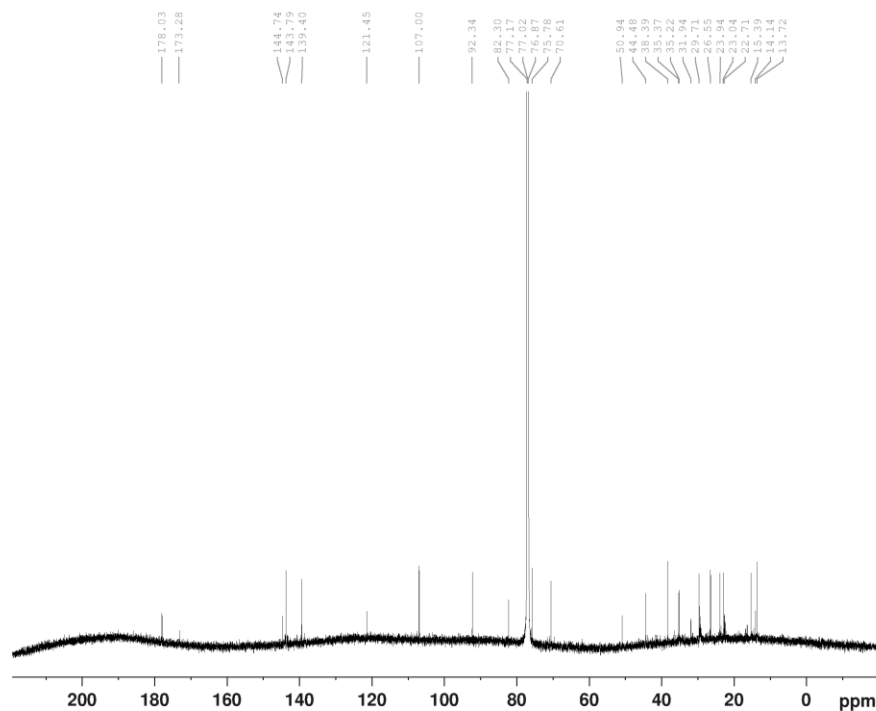


Figure S7. ¹H NMR spectrum of compound 5 (850 MHz, CDCl₃).

Dr. Hossam
Sample : CLMC-11-2

CDCL₃



```
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PROCNO   1

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PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        14336
DS        4
SWH       51020.406 Hz
FIDRES   0.778510 Hz
AQ        0.6482258 sec
RG         186.93
DE         9.500 usec
TE        298.0 K
D1        2.0000000 sec
D11       0.0300000 sec
TD0       1

===== CHANNEL f1 =====
RF01     213.7917436 MHz
NUC1      13C
P1        12.00 usec
PLW1     130.0000000 W

===== CHANNEL f2 =====
RF02     850.1334006 MHz
NUC2      1H
CPDPRG2  waltz16
PCPD2    80.00 usec
PLW2     13.8000019 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
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Figure S8: ¹³C NMR spectrum of compound 5 (214 MHz, CDCl₃).

Dr. Hossam
Sample : CLMC-11-2 CDCL3

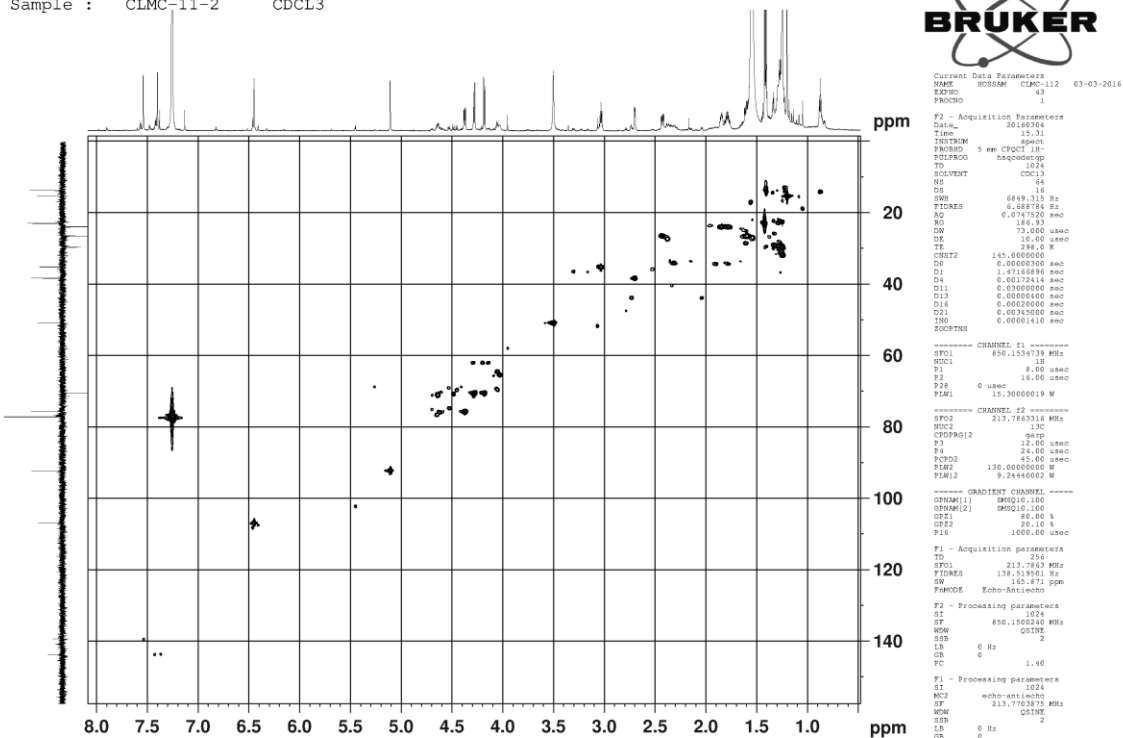


Figure S9: HSQC spectrum of compound 5 (CDCl₃).

Dr. Hossam
Sample : CLMC-11-2 CDCL3

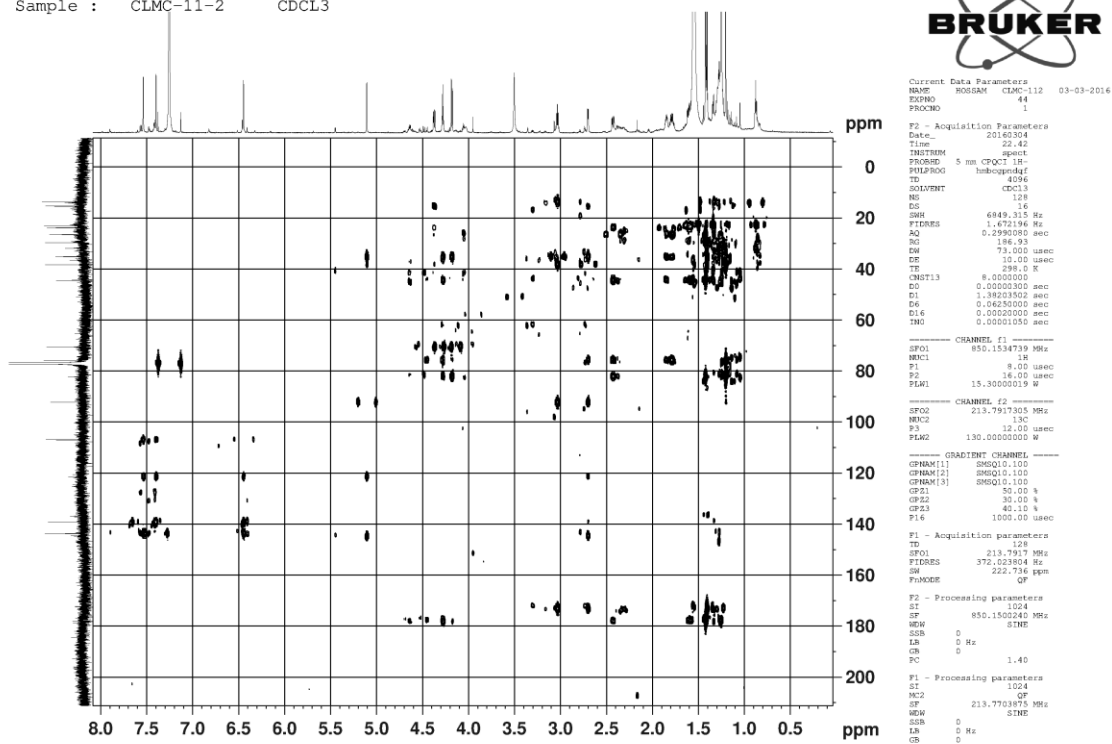


Figure S10: HMBC spectrum of compound 5 (CDCl₃).

Dr.Hossam
Sample : CLMC-11-2 CDCL3
NOESYPHSW CDCL3 D:\ nmr

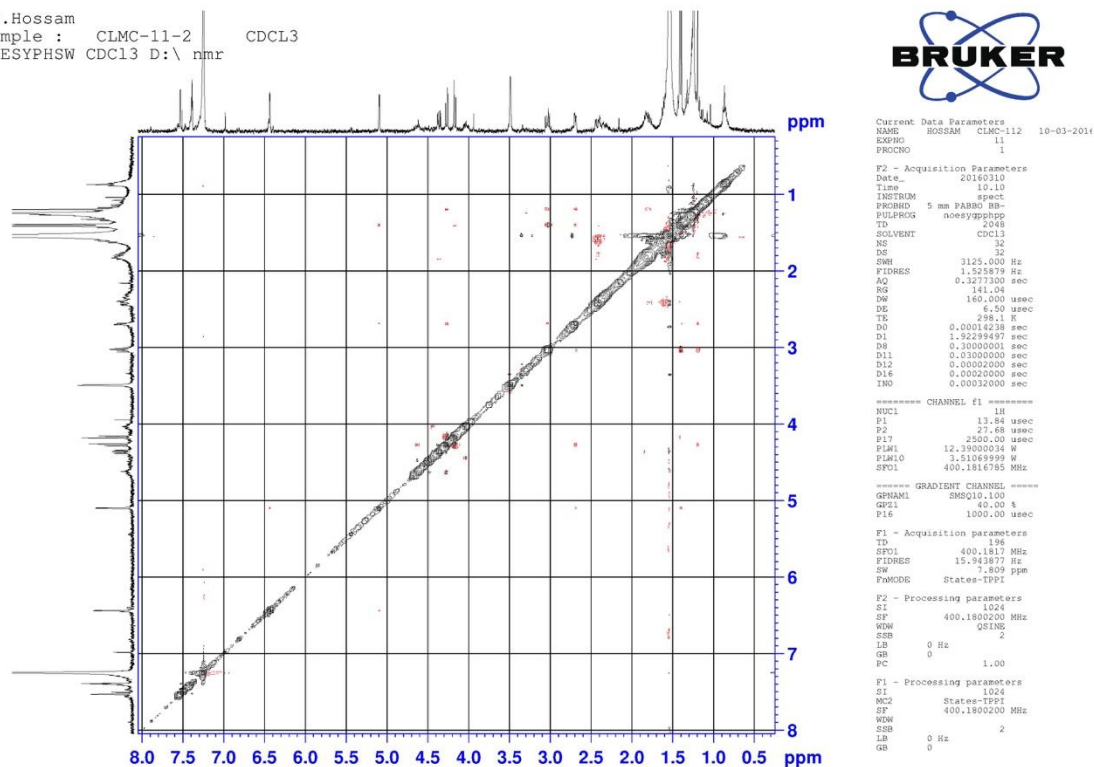


Figure S11: NOESY spectrum of compound 5 (CDCl₃).