

Supplementary Materials

Guaianolide Sesquiterpene Lactones from *Centaurothamnus maximus*

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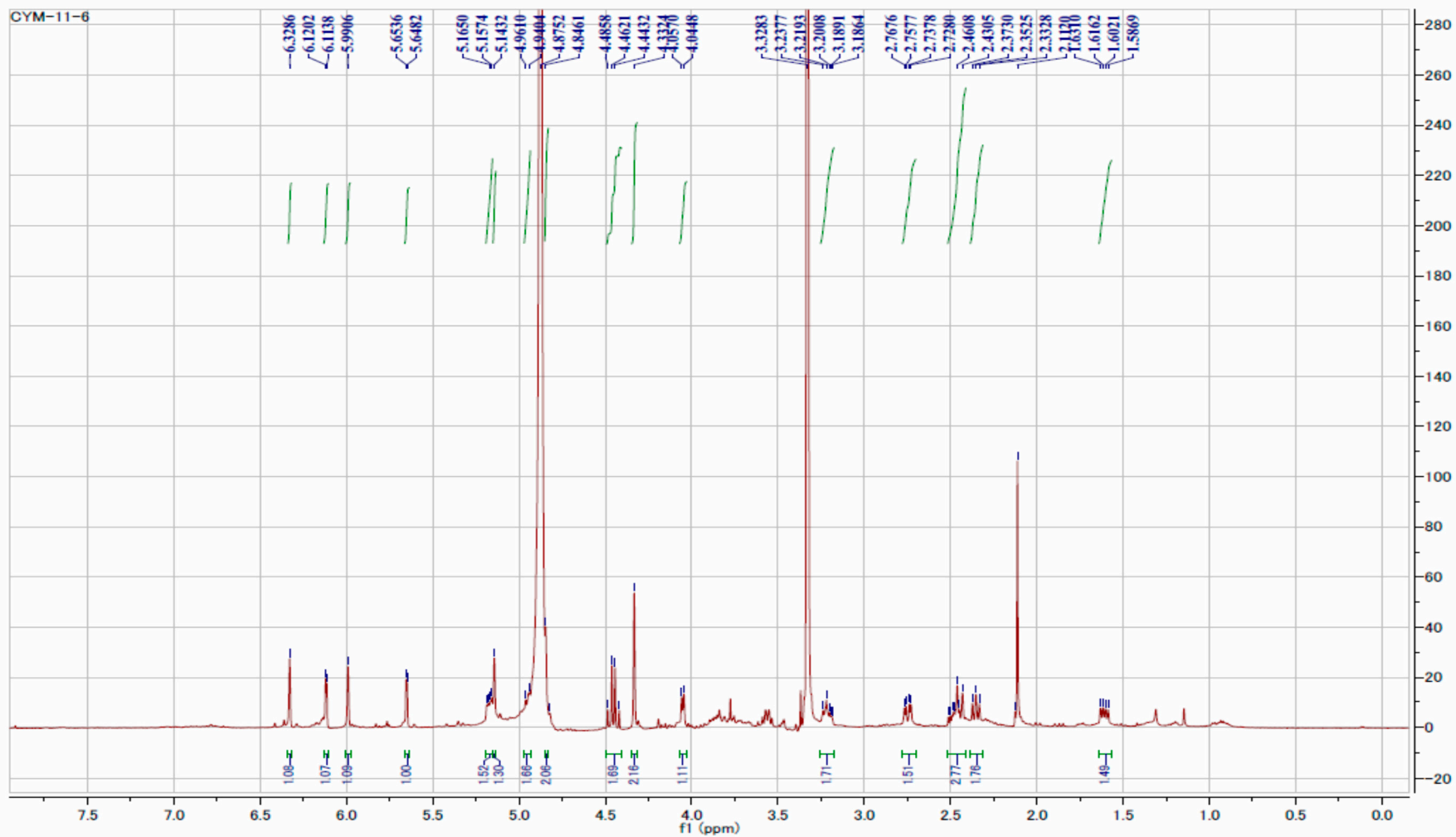
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¹⁰ Department of Pharmaceutical Biology, Institute of Pharmaceutical and Biomedical Sciences, Johannes Gutenberg University, Staudinger Weg 5, 55128 Mainz

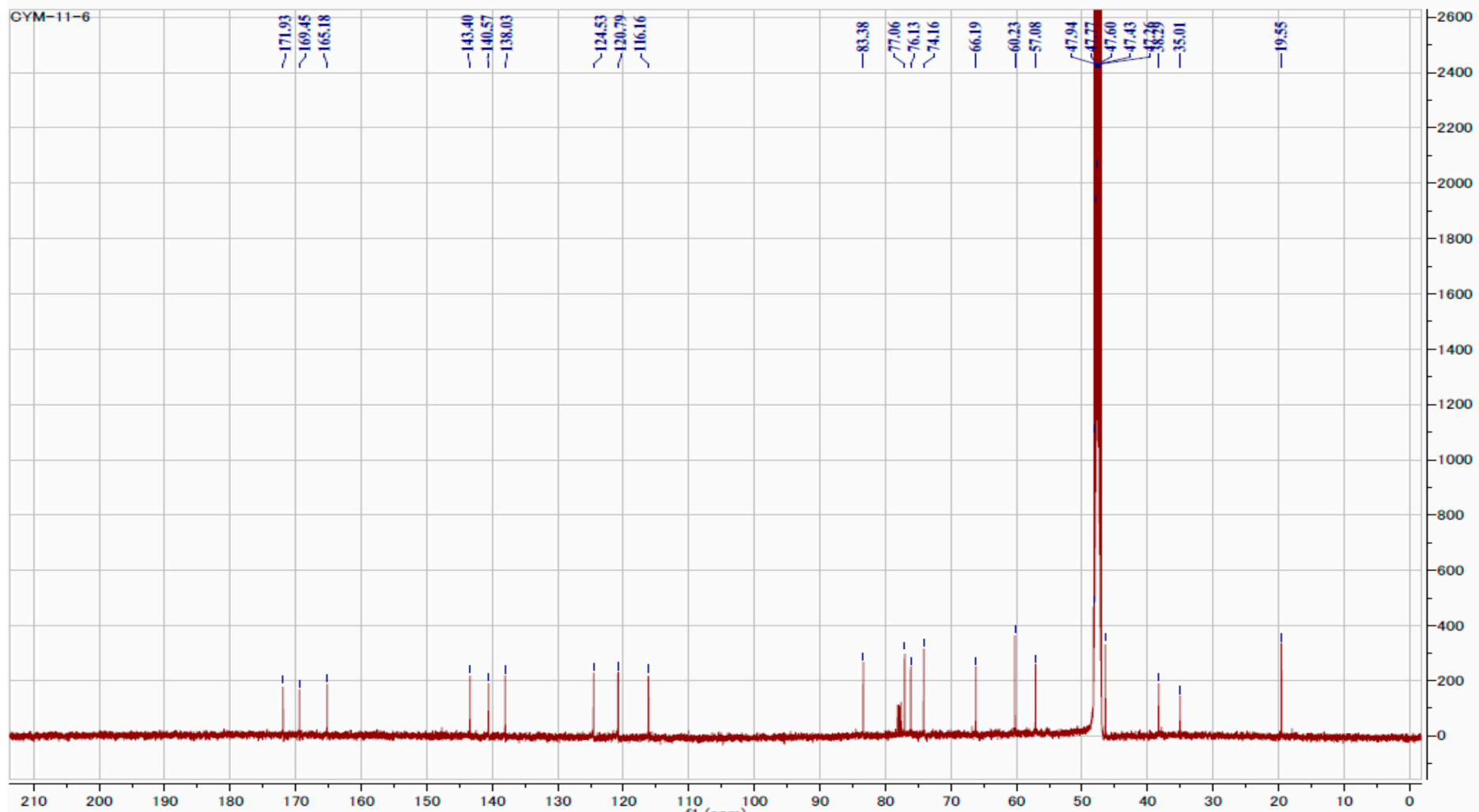
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† These authors contributed equally to this work.

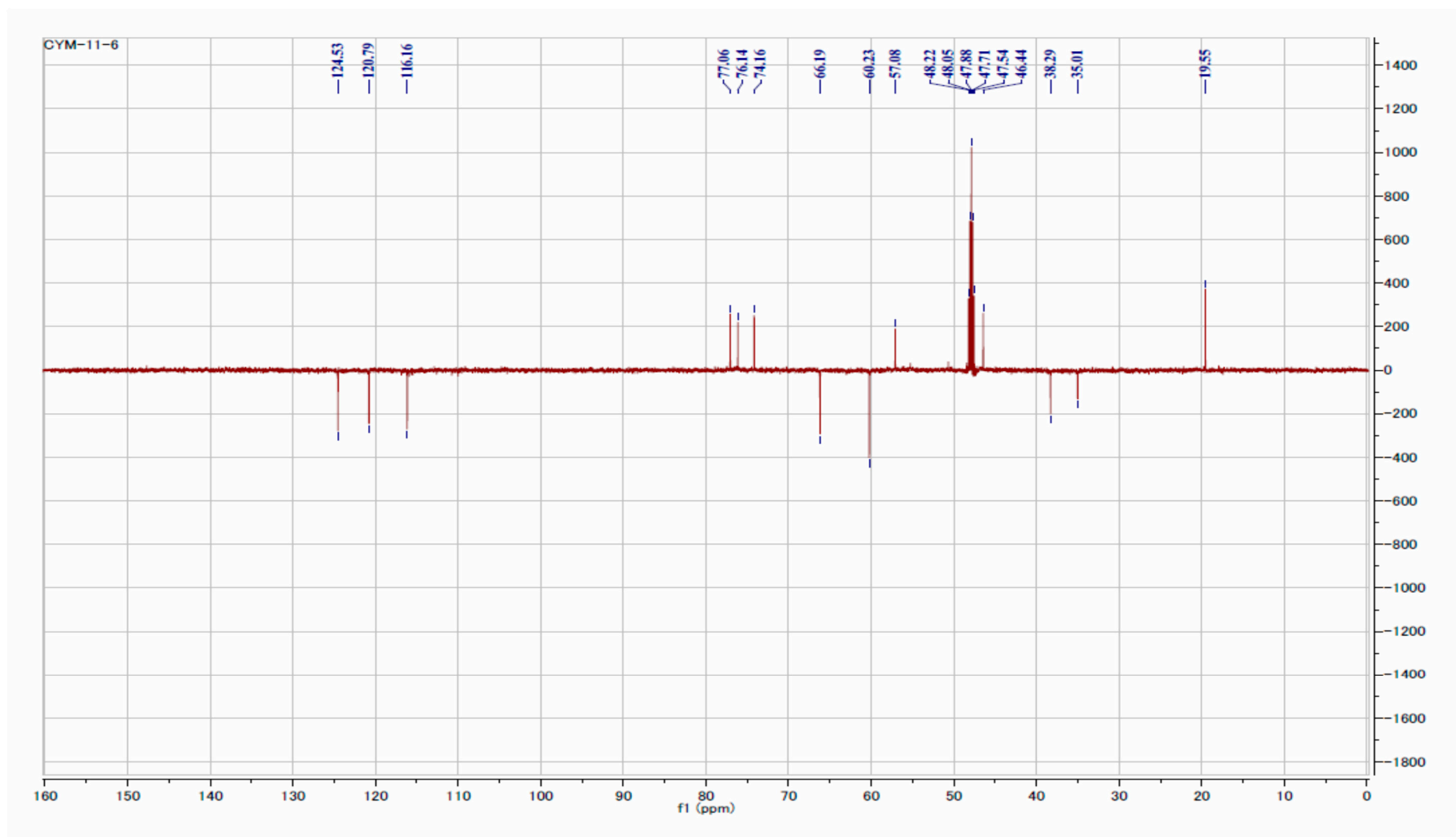
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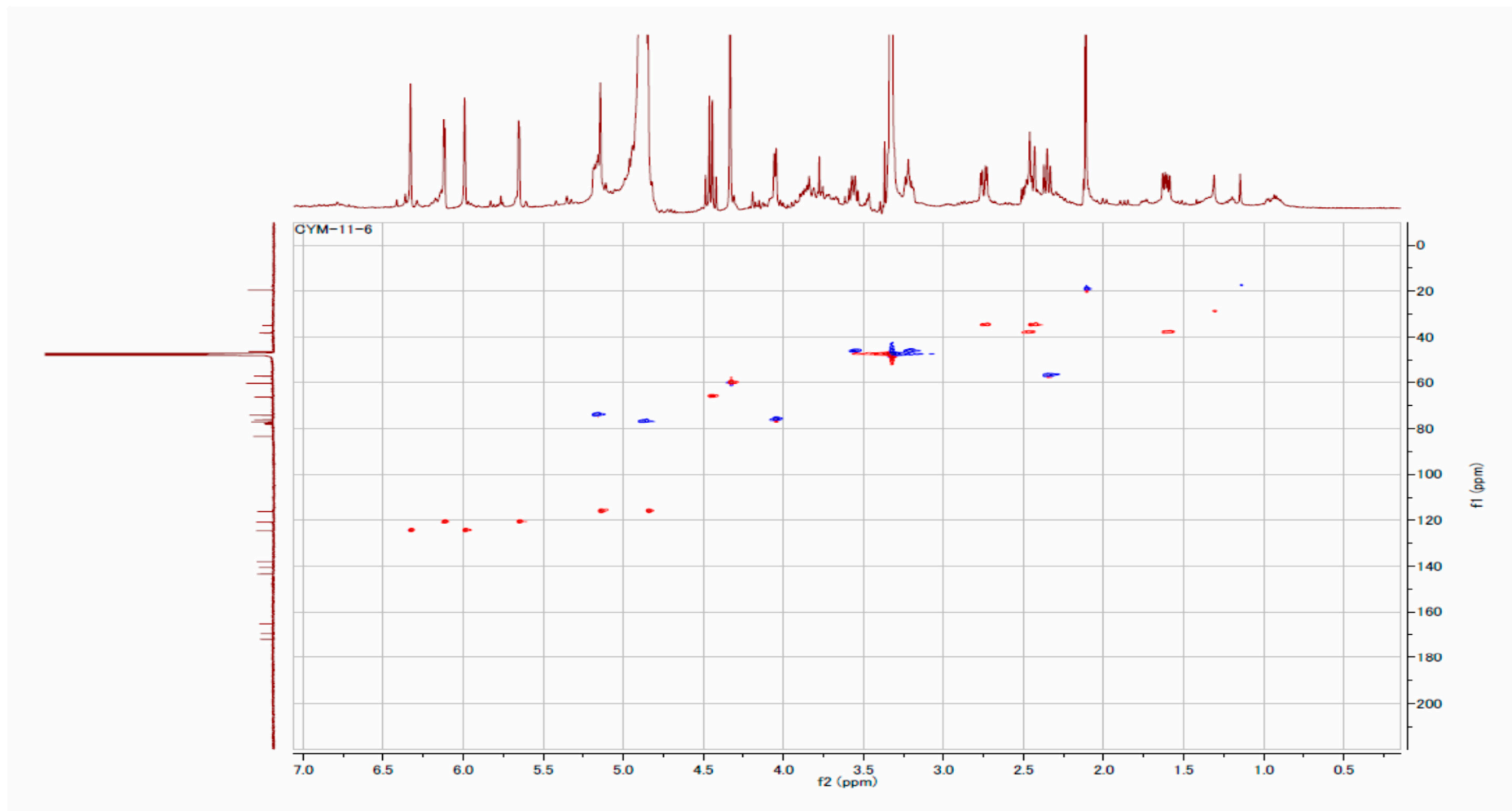
S1: ^1H NMR (CDCl_3 , 500 MHz) of **1**



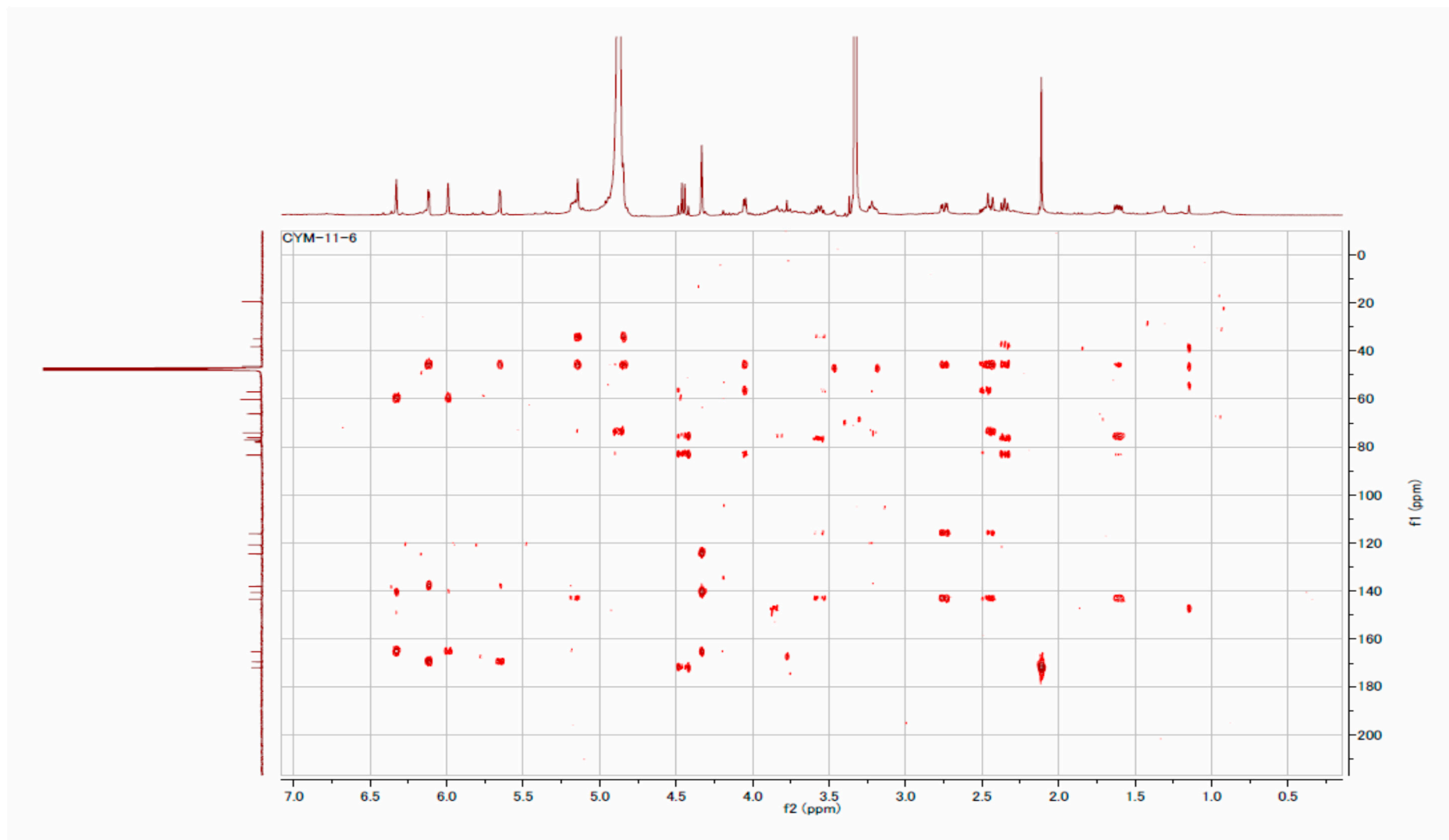
S2: ^{13}C NMR (CDCl_3 , 125 MHz) of **1**



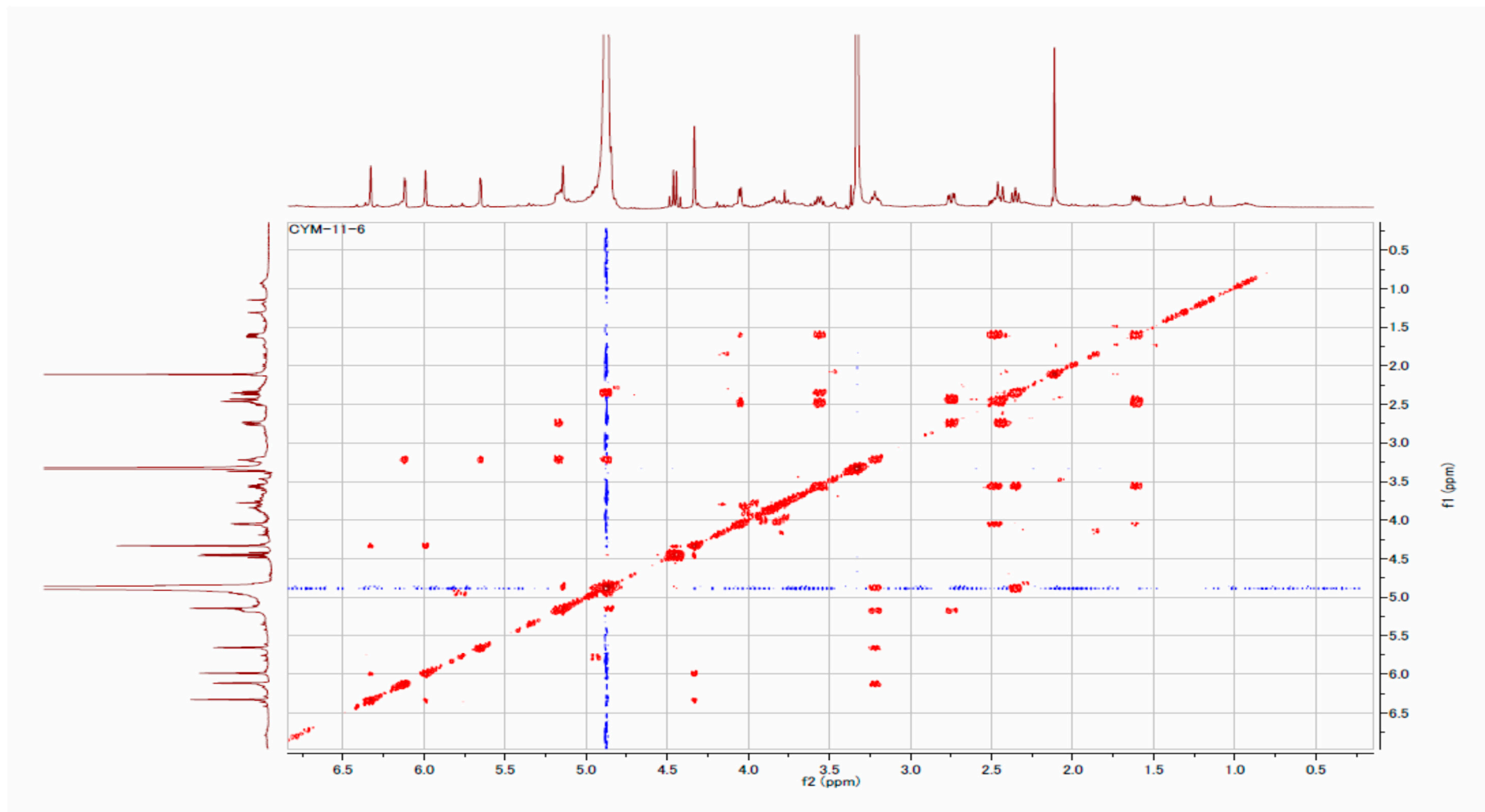
S3:DEPT of 1



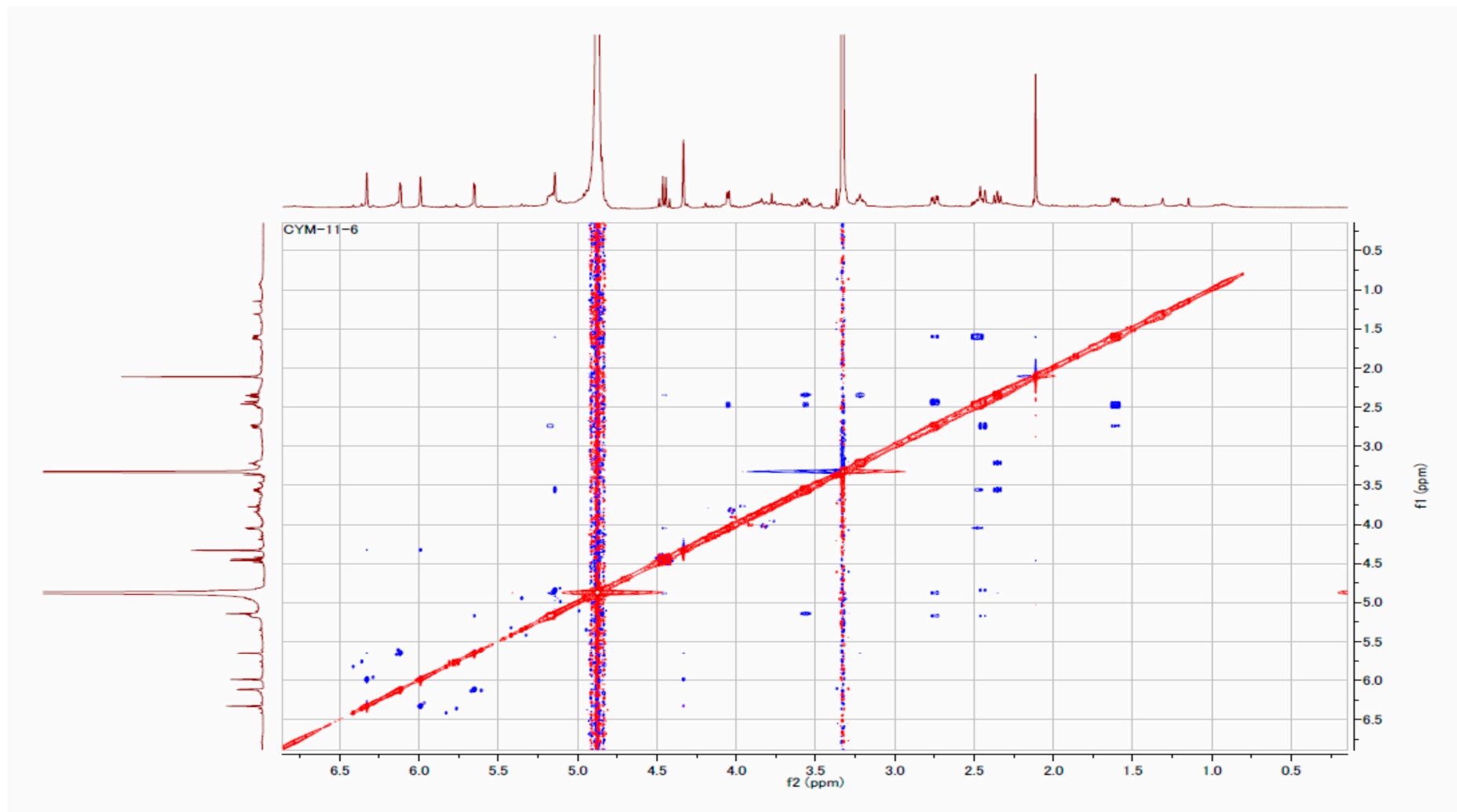
S4:HSQC of 1



S5:HMBC of 1



S6: ^1H ^1H COSY of 1



S7:NOESY of 1

Sample : CyM-11-6

Note : MStation

Inlet : Direct Ion Mode : CI+

RT : 2.11 min Scan# : 56

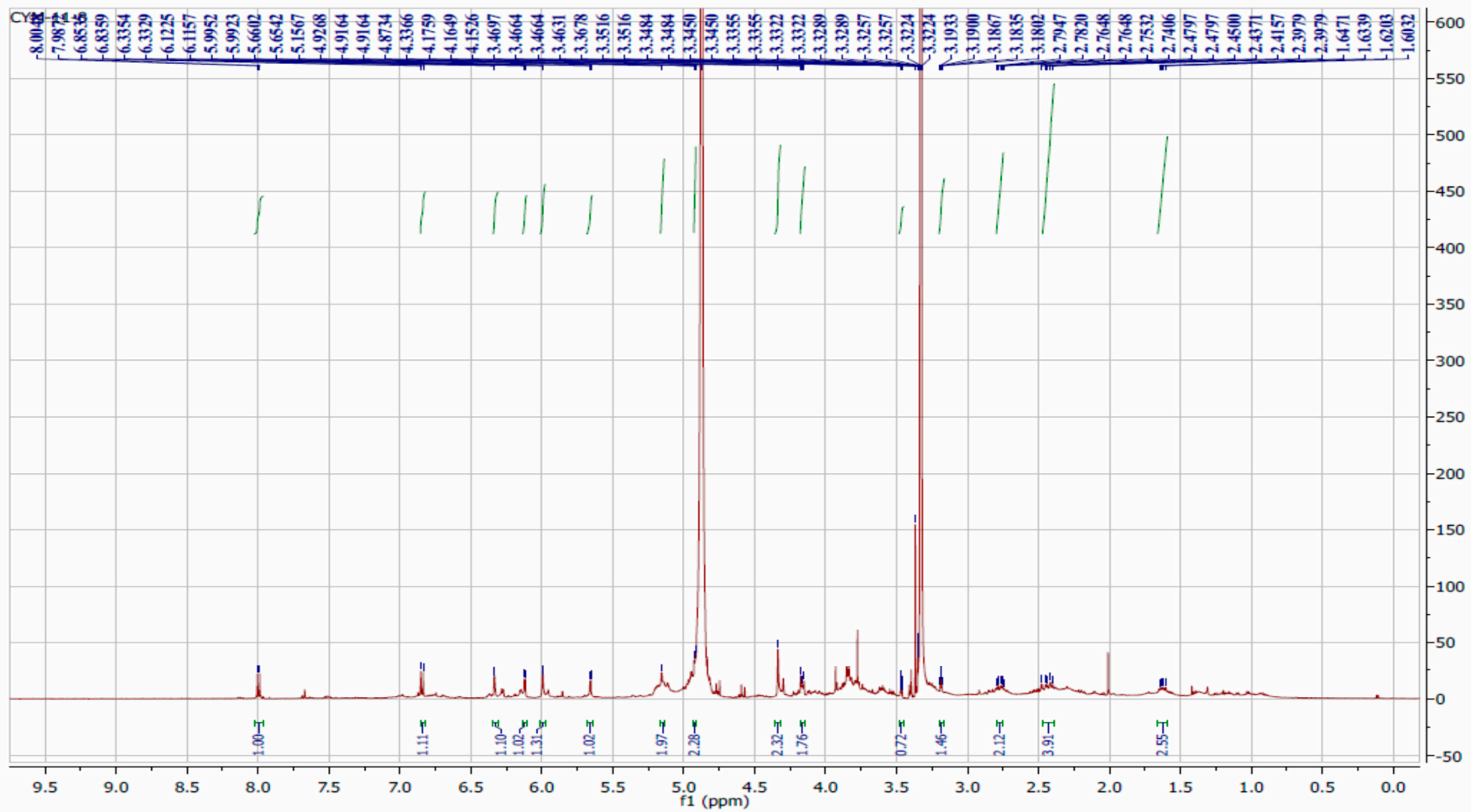
Elements : C 150/0, H 250/0, O 50/0

Mass Tolerance : 5mmu

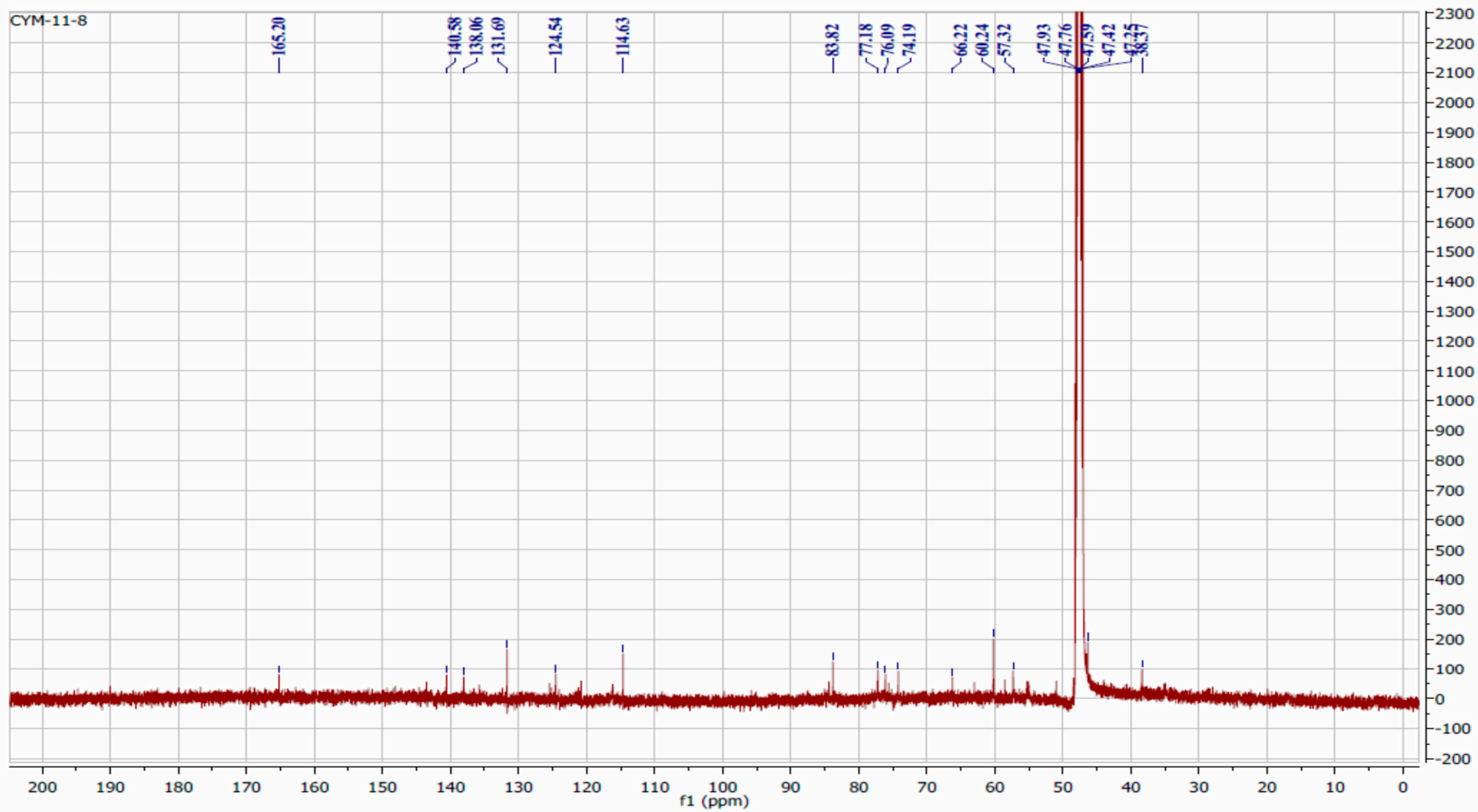
Unsaturation (U.S.) : 0.0 - 15.0

	Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
1	423.1655	18.79	-0.0 / -0.0	8.5 C21 H27 O9

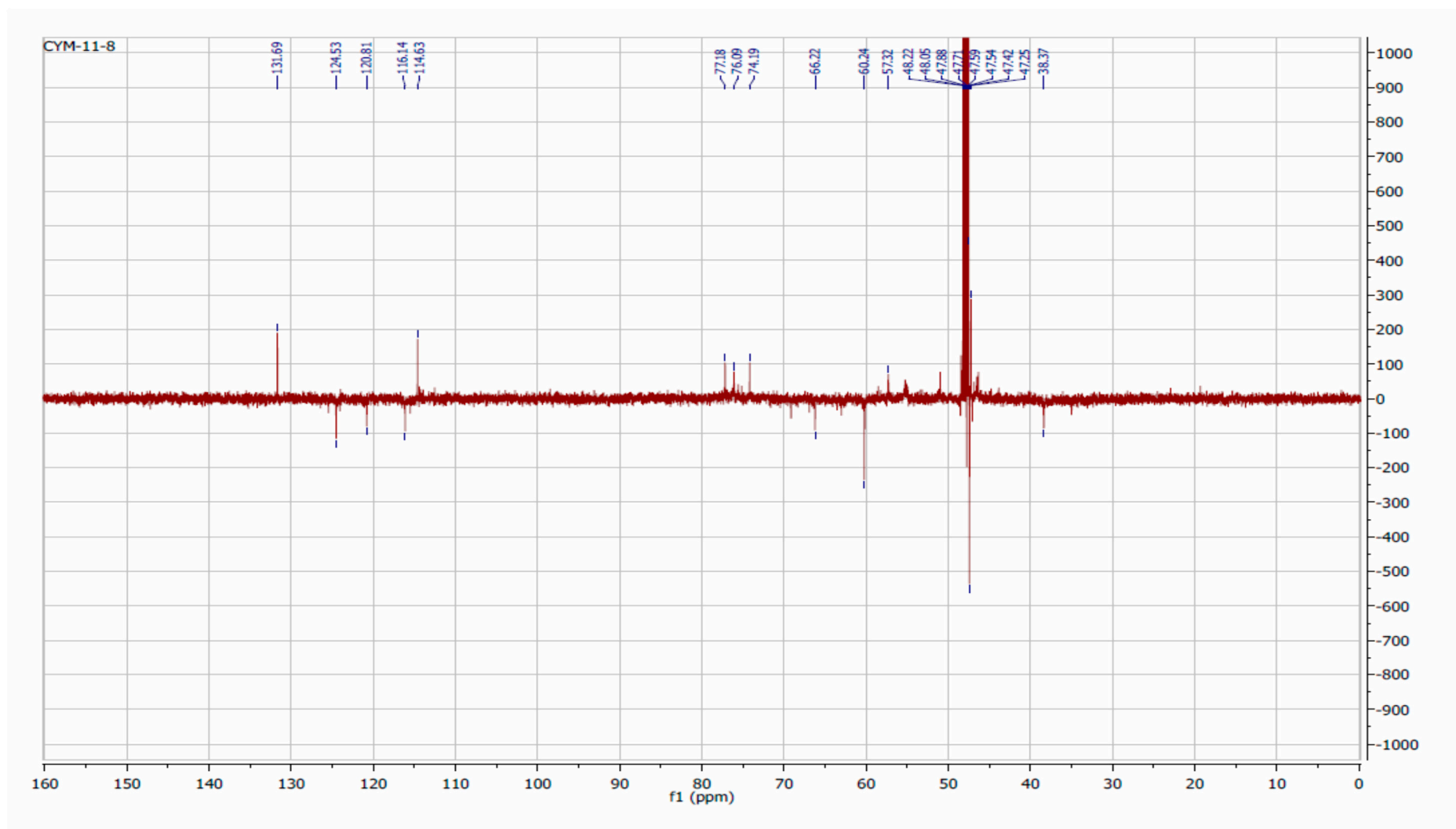
S8: HRCI/mas of 1



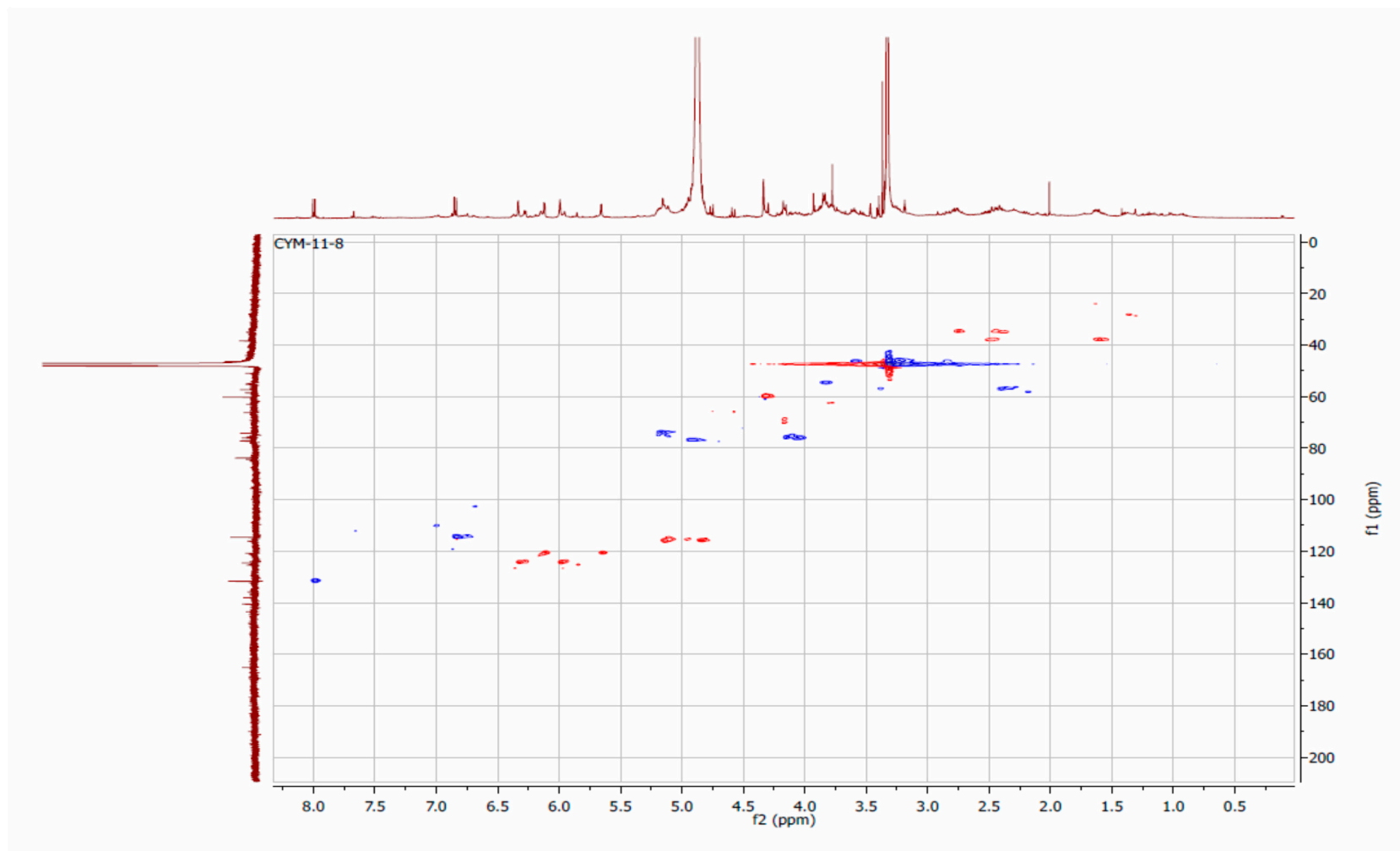
S9: ^1H NMR (CDCl_3 , 500 MHz) of **2**



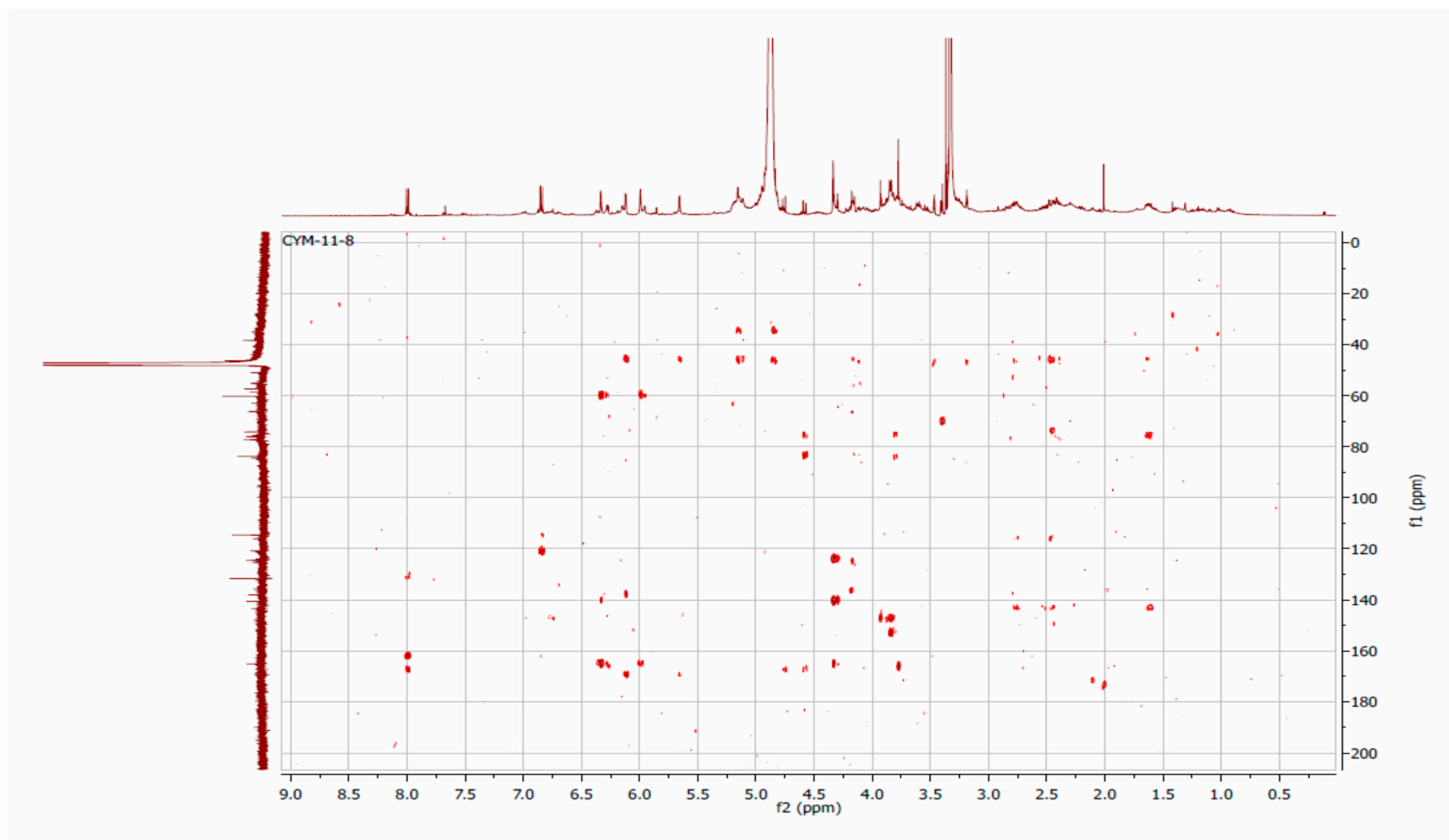
S10: ^{13}C NMR (CDCl_3 , 125 MHz) of **2**



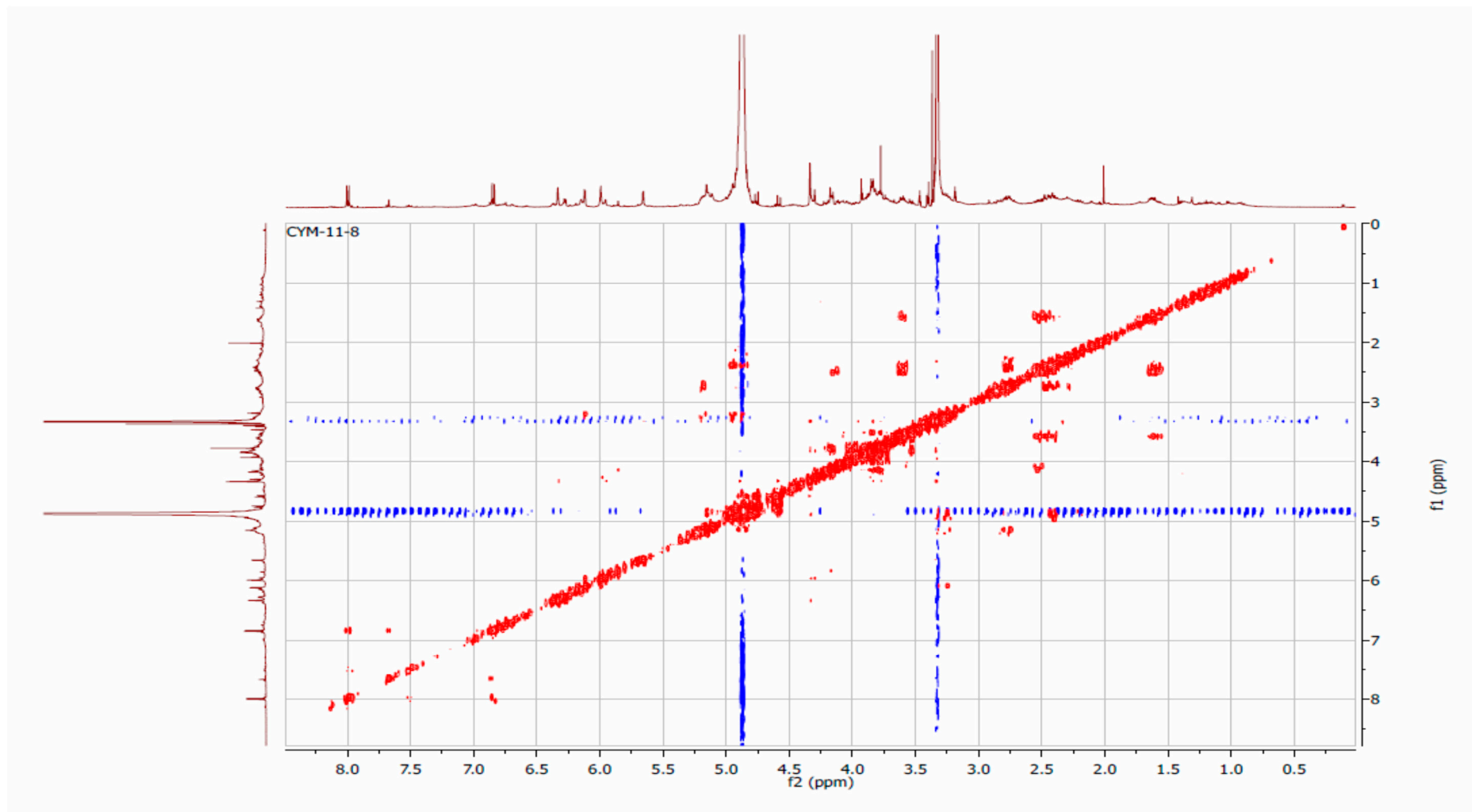
S11:DEPT of 2



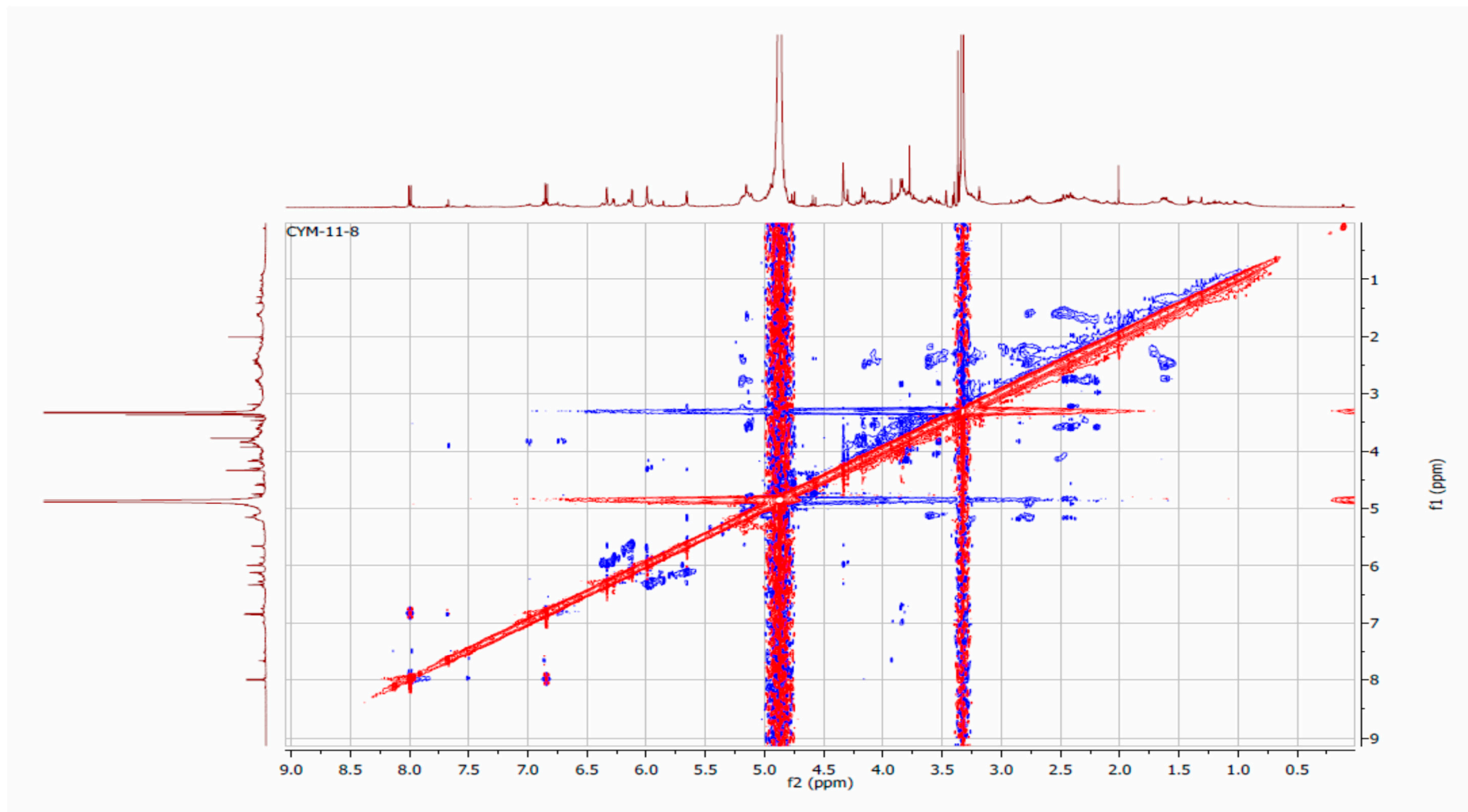
S12:HSQC of 2



S13:HMBC of 2



S14: ^1H ^1H COSY of 2

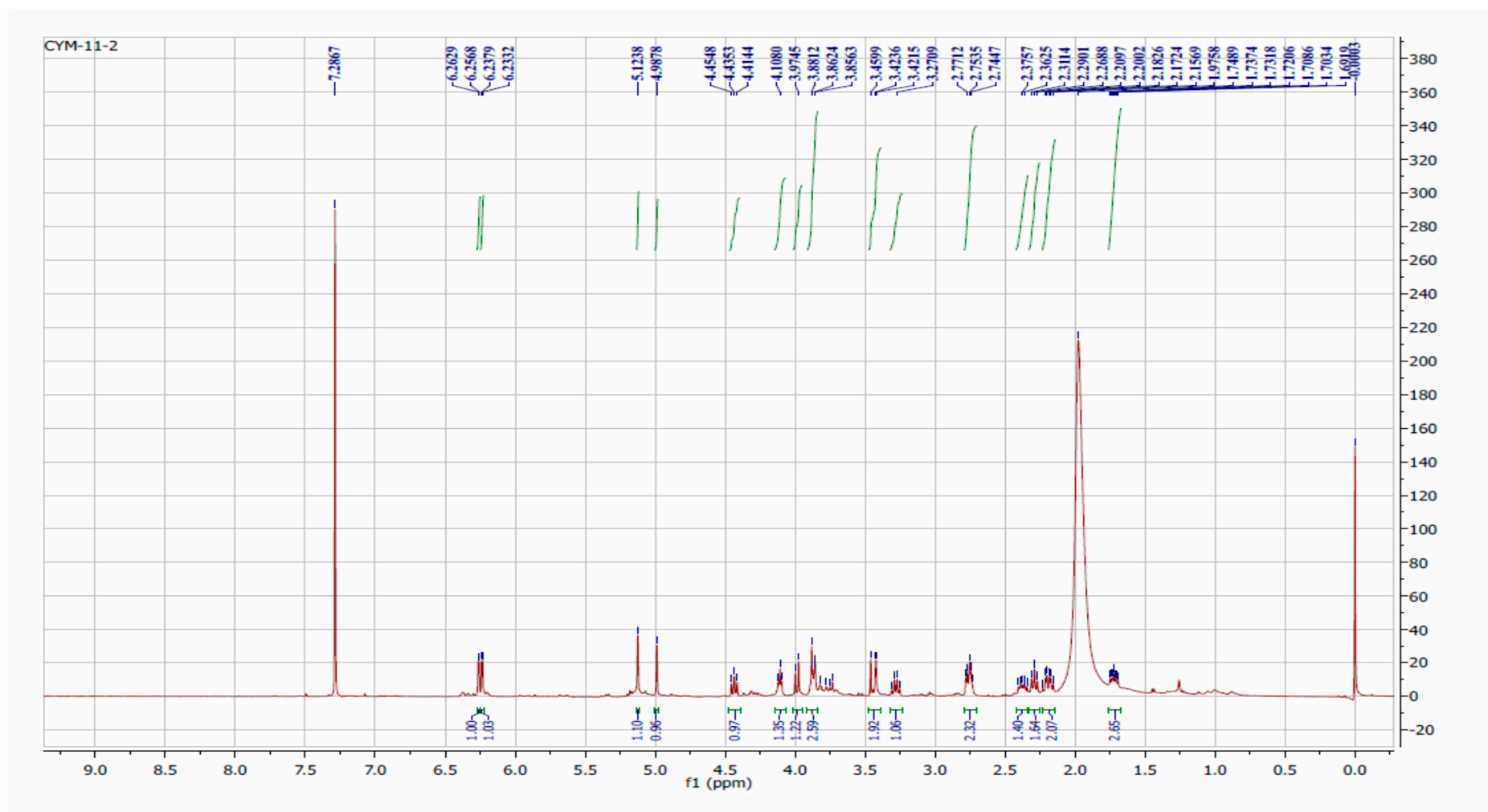


S15:NOESY of 2

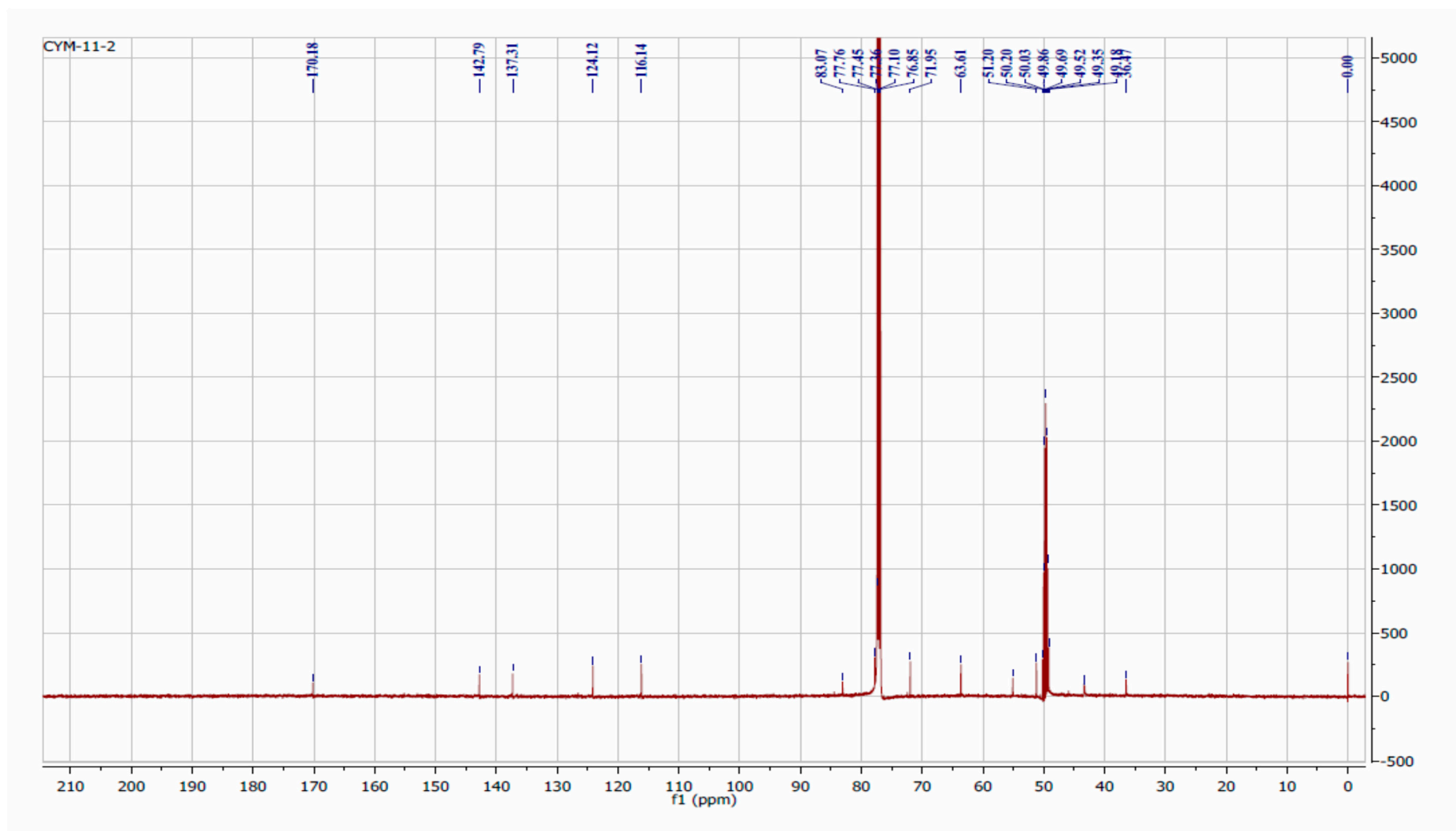
Sample : CyM-11-8
 Note : MStation
 Inlet : Direct Ion Mode : CI+
 RT : 2.26 min Scan# : 60
 Elements : C 150/0, H 250/0, O 50/0
 Mass Tolerance : 5mmu
 Unsaturation (U.S.) : 0.0 - 15.0

	Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
1	472.1758	1.34	+5.2 / +2.5	12.0	C25 H28 O9
2			-7.2 / -3.4	3.0	C18 H32 O14

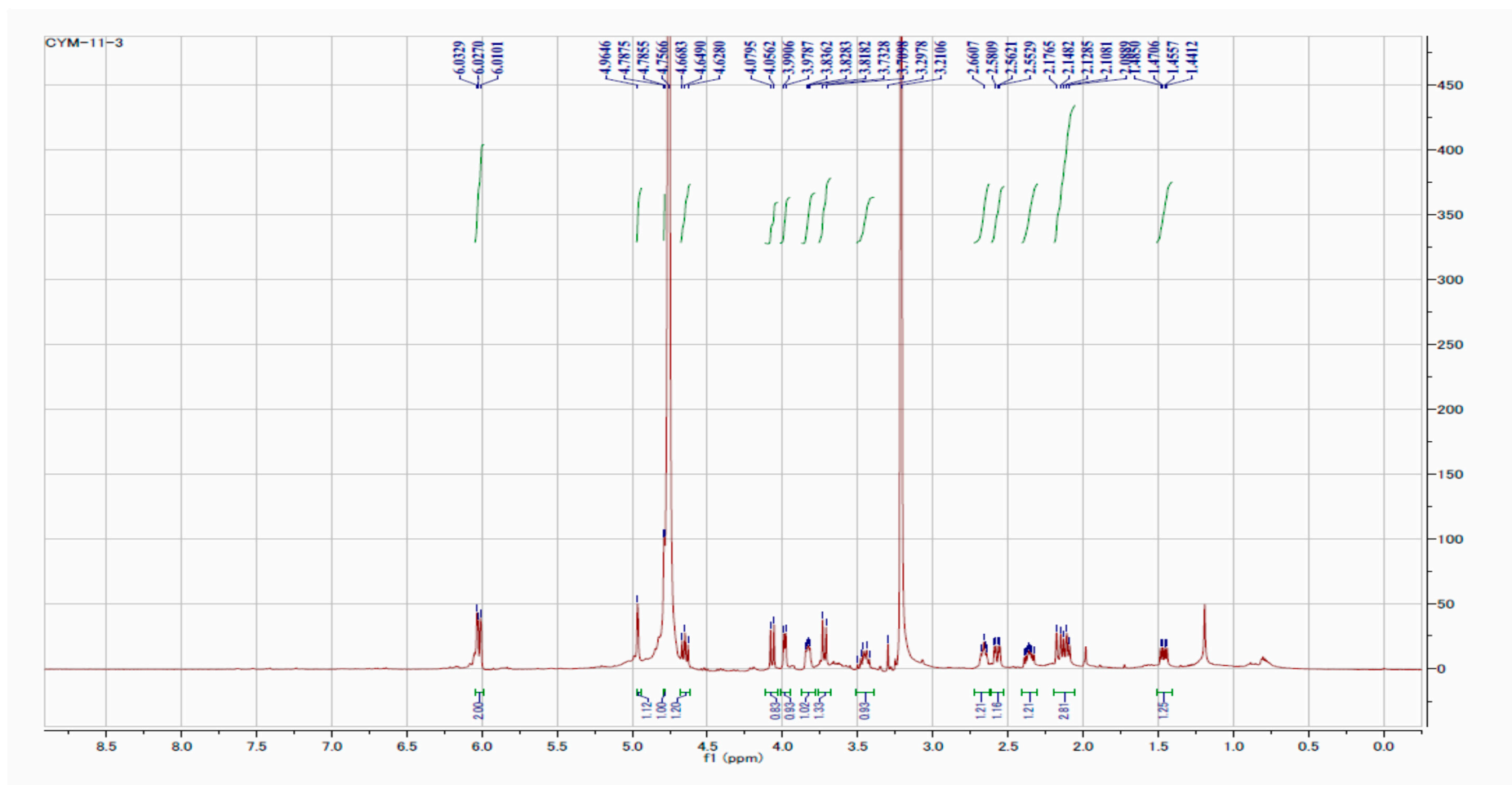
S 16: HRCI/mas of 2



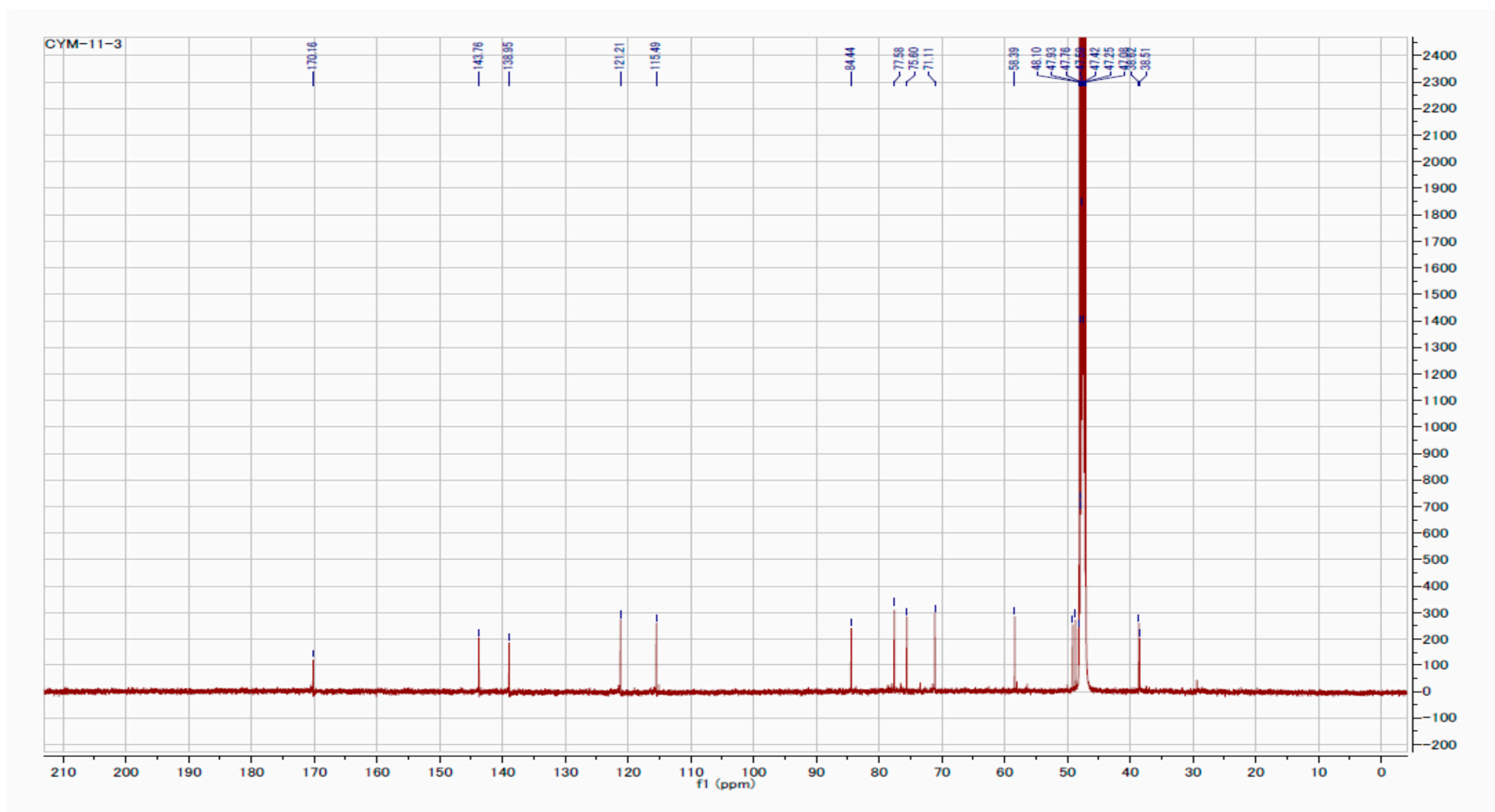
S17: ^1H NMR (CDCl_3 , 500 MHz) of **3**



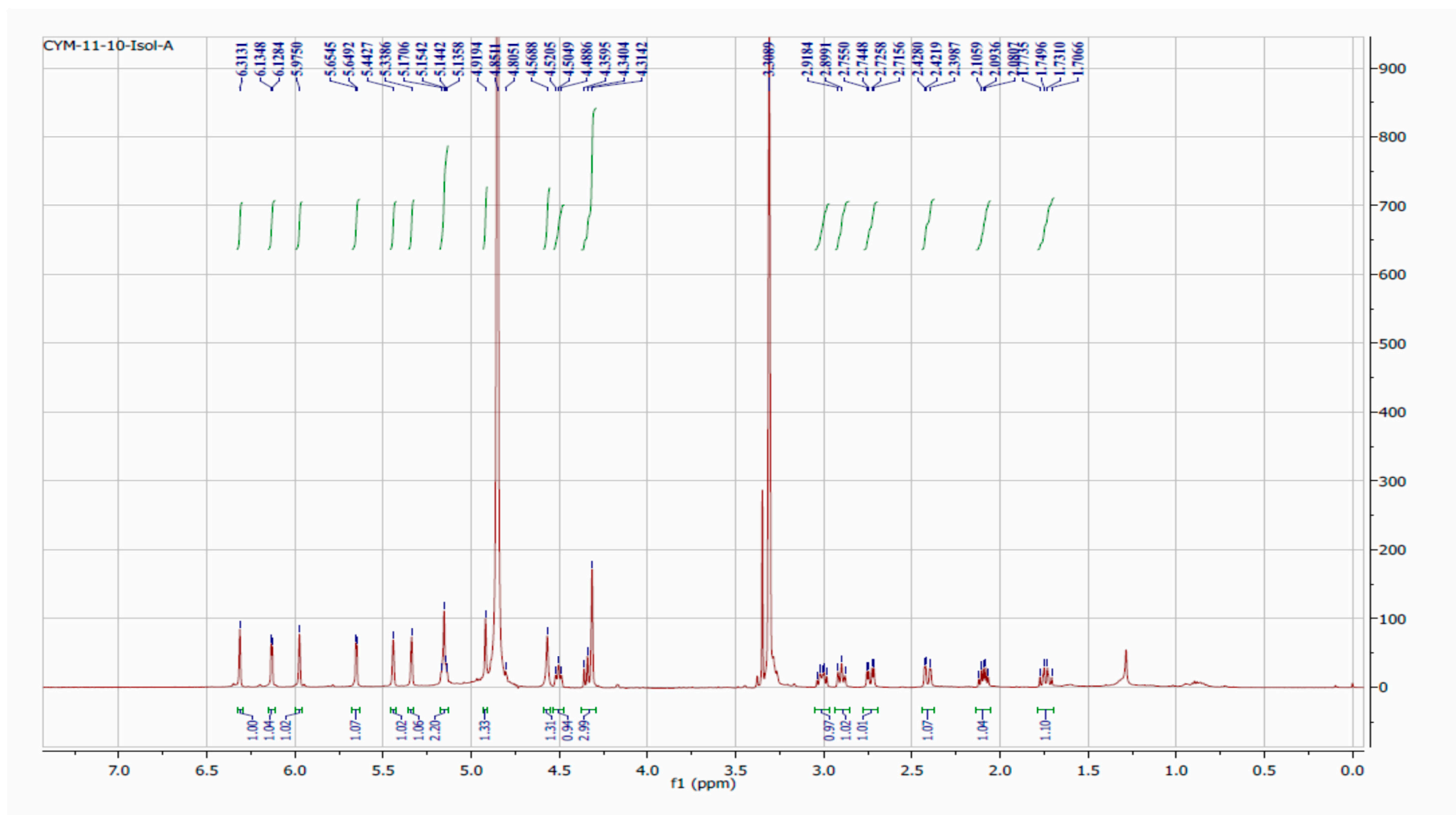
S18: ^{13}C NMR ($\text{C}_5\text{D}_5\text{N}$, 125 MHz) of **3**



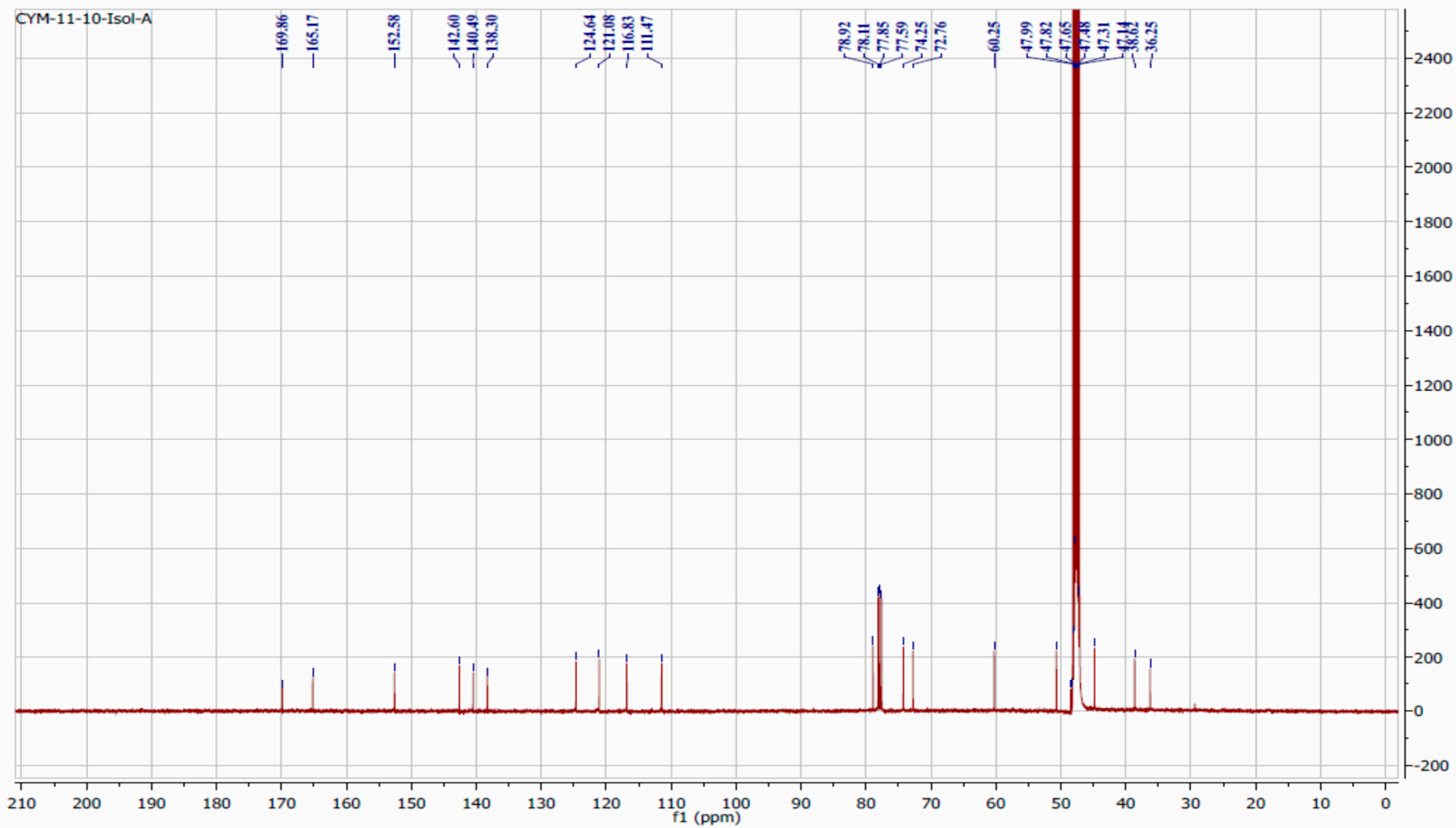
S19: ^1H NMR (CDCl_3 , 500 MHz) of **4**



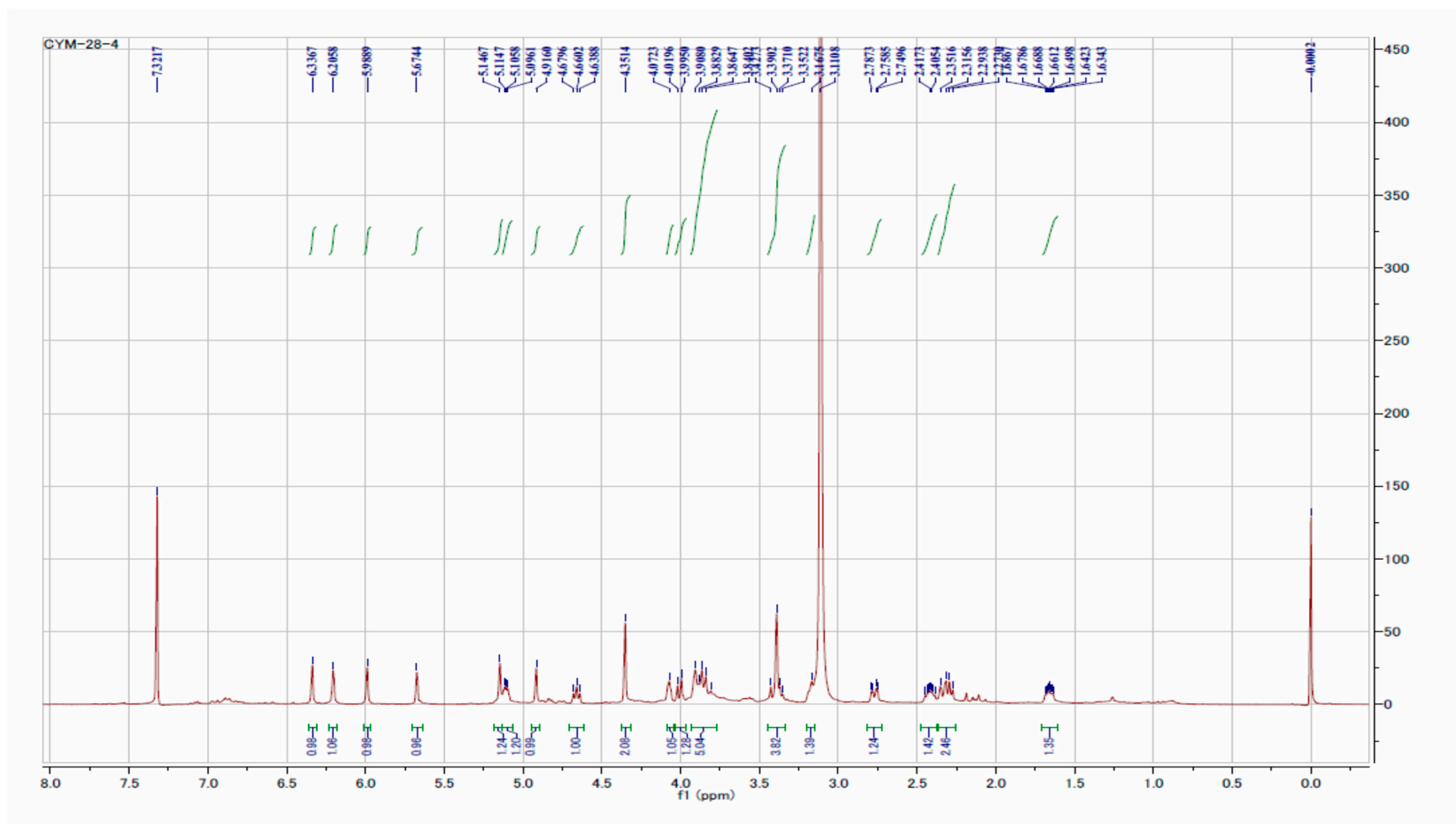
S20: ^{13}C NMR ($\text{C}_5\text{D}_5\text{N}$, 125 MHz) of 4



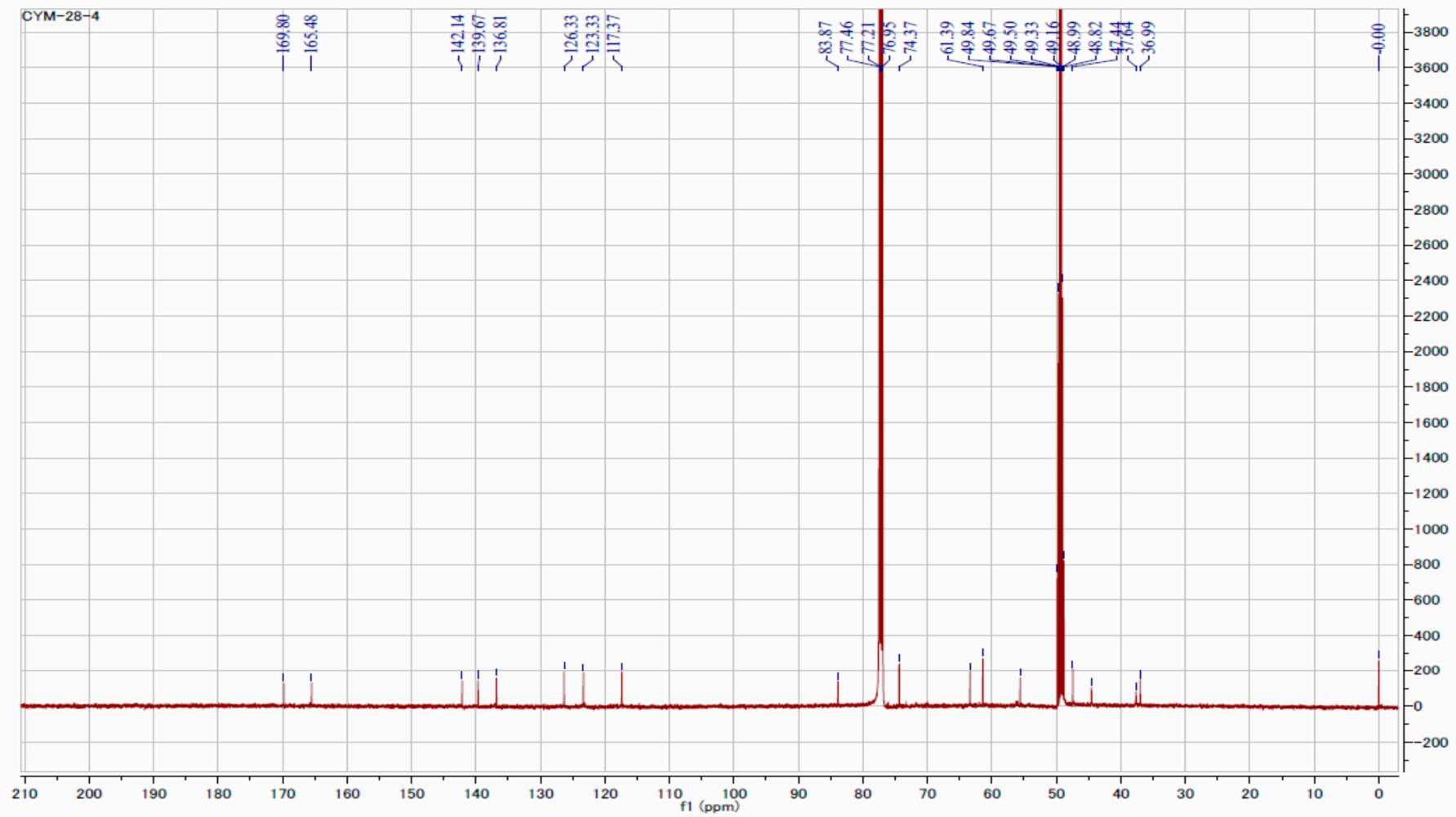
S21:¹H NMR (CDCl₃, 500 MHz) of **5**



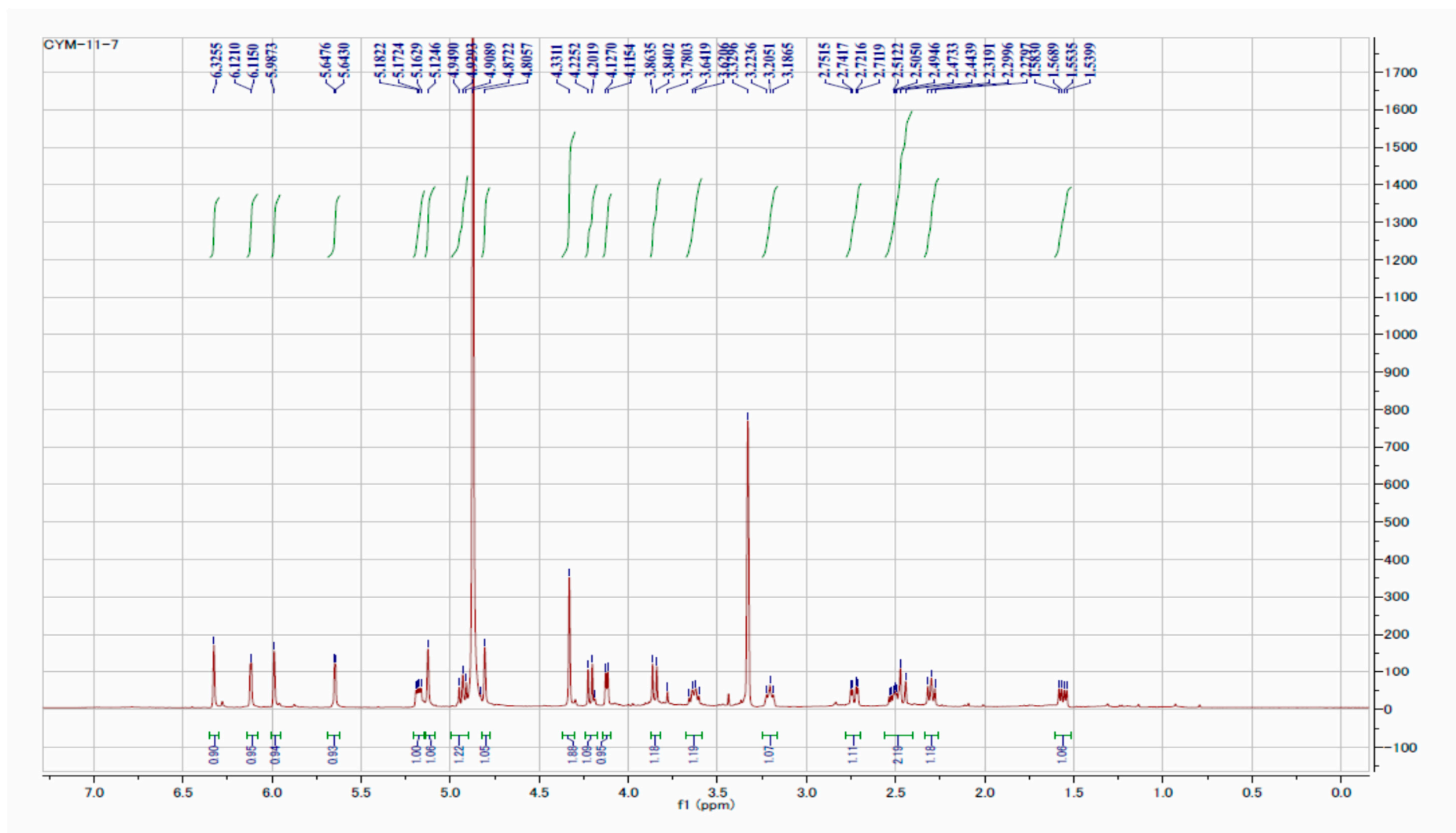
S22: ^{13}C NMR ($\text{C}_5\text{D}_5\text{N}$, 125 MHz) of **5**



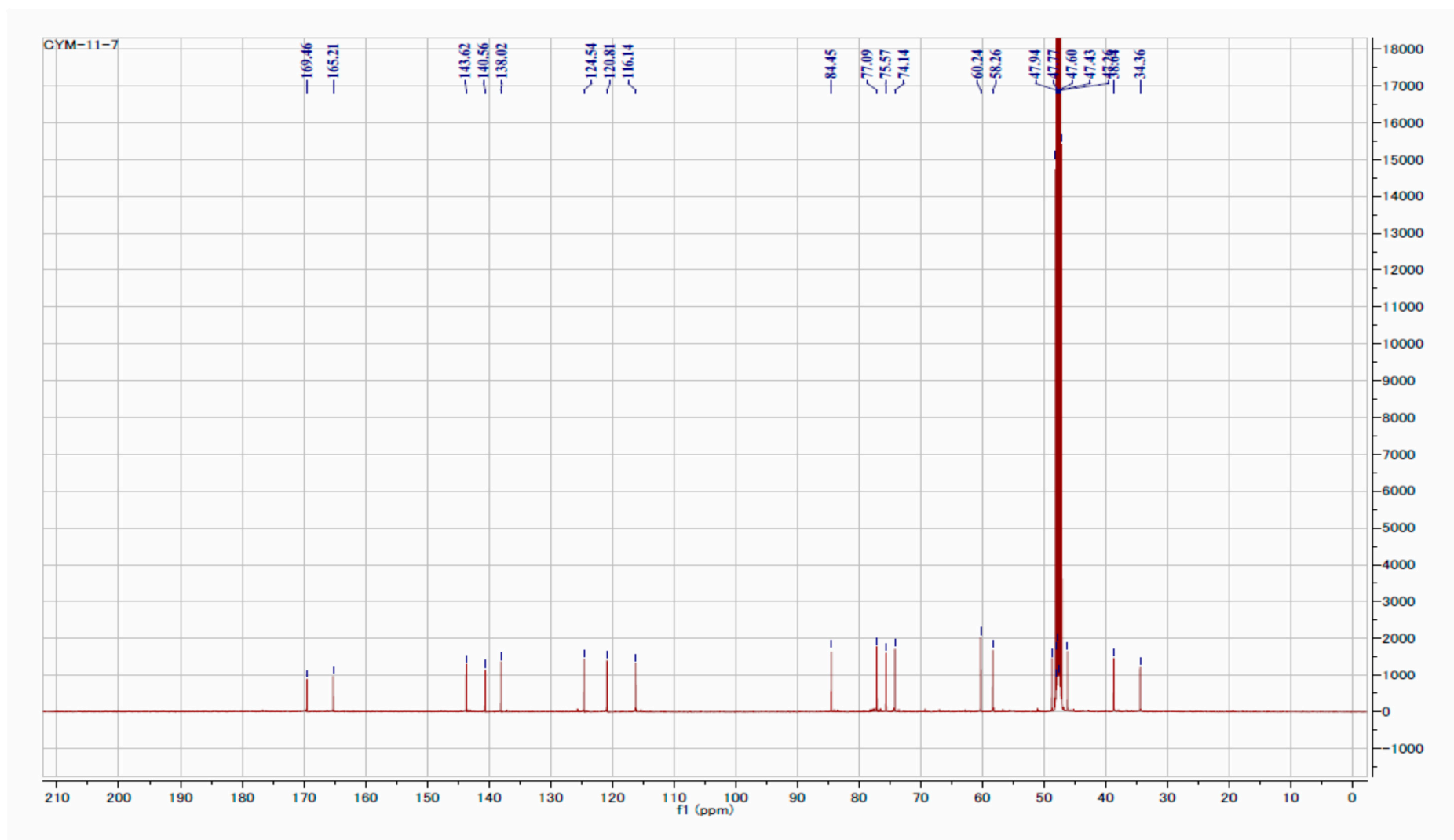
S23: ^1H NMR (CDCl_3 , 500 MHz) of **6**



S24: ^{13}C NMR ($\text{C}_5\text{D}_5\text{N}$, 125 MHz) of **6**



S25: ^1H NMR (CDCl_3 , 500 MHz) of 7



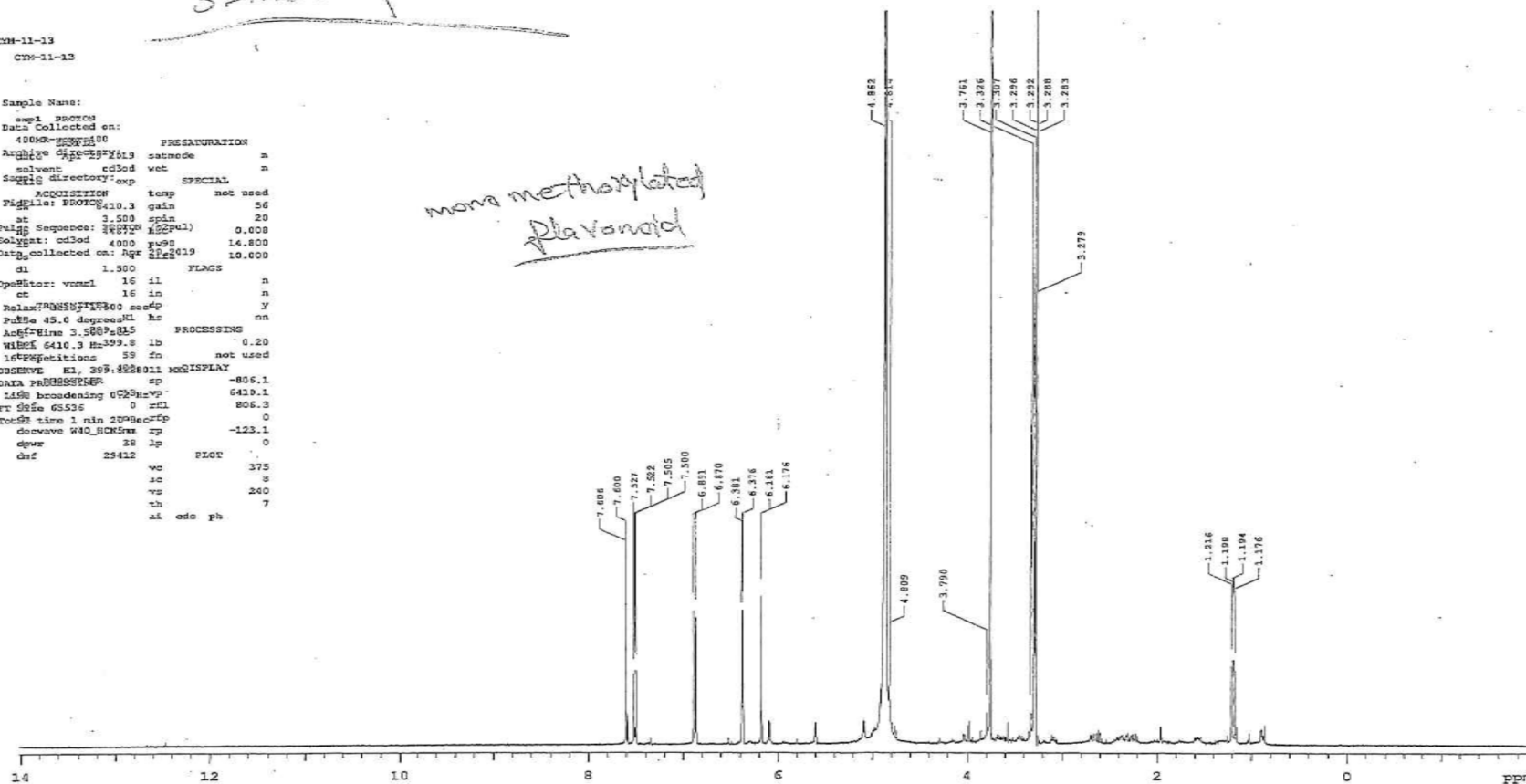
S26: ^{13}C NMR ($\text{C}_5\text{D}_5\text{N}$, 125 MHz) of 7

3-methoxy phenol

CVN-11-13
CVN-11-13

```
Sample Name:
exp1 PROCES
Data Collected on:
4000-xxxxxx00
Acquire Date: 11/13/93
Solvent: cdcl3
Sample directory: exp
ACQUISITION temp not used
Pulse: PROTON 410.3 gain 56
at 1.500 spin 20
Pulse Sequence: zgpg30 (zgpg30) 0.008
Solvent: cdcl3 4000 pw99 14.800
Data collected on: 11/13/93 10.000
d1 1.500
Operator: vnmr1 16 il n
ct 16 in n
Relaxation delay: 3.000 sec Y
Pulse 45.0 degrees kl hc
Acquire time 3.500 hr 0.20
1638 positions 58 fo not used
OBSERVE kl 359.422011 NOISY
DATA PROCESSOR sp -806.1
LINE broadening 0.2 Hz MP 6419.1
FT date 05536 0 x ml 806.3
Total time 1 min 29 sec TP
decouple w40_rfc05m sp -123.1
cpwv 38 lp 0
chf 25412
vc 375
sc 8
vs 240
th
xl odc ph 7
```

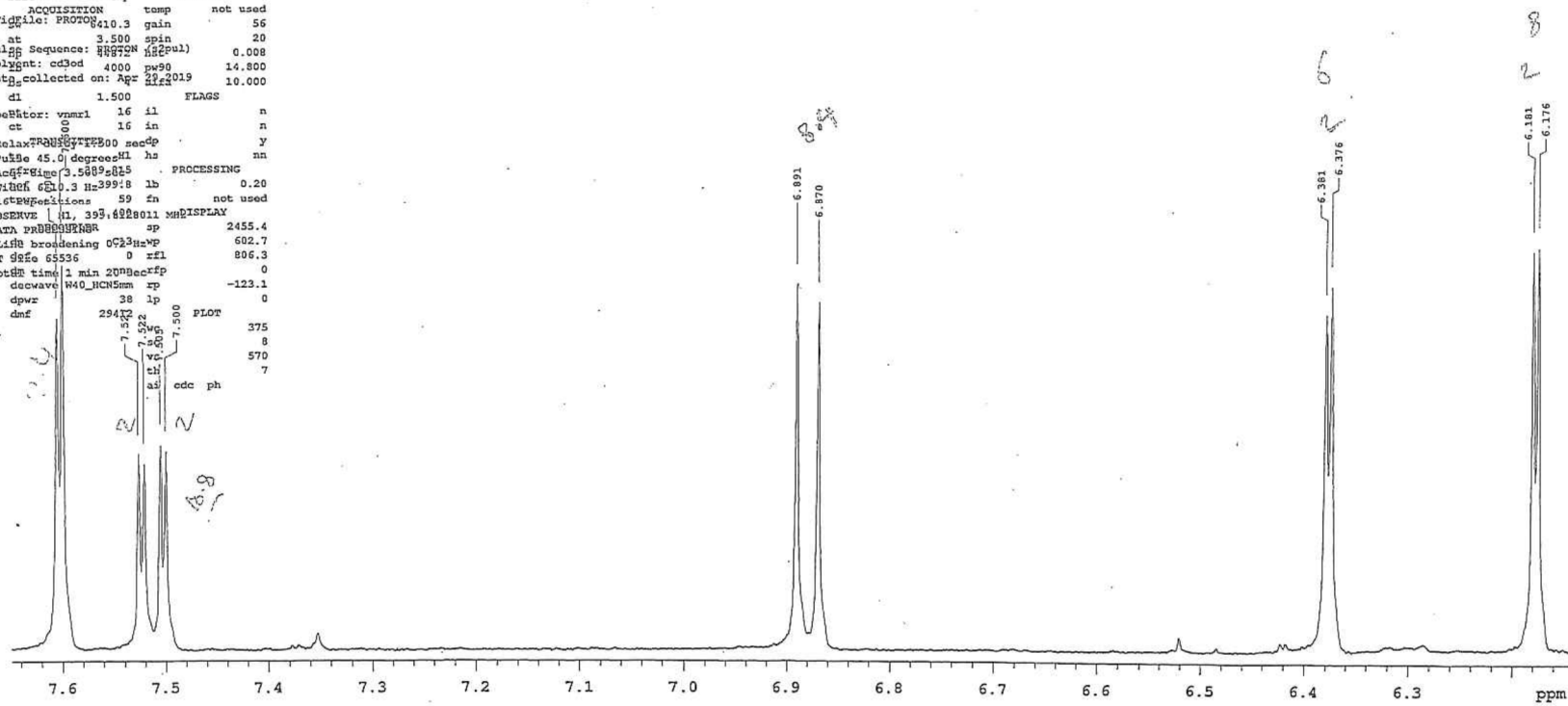
mono methoxylated
flavonoid



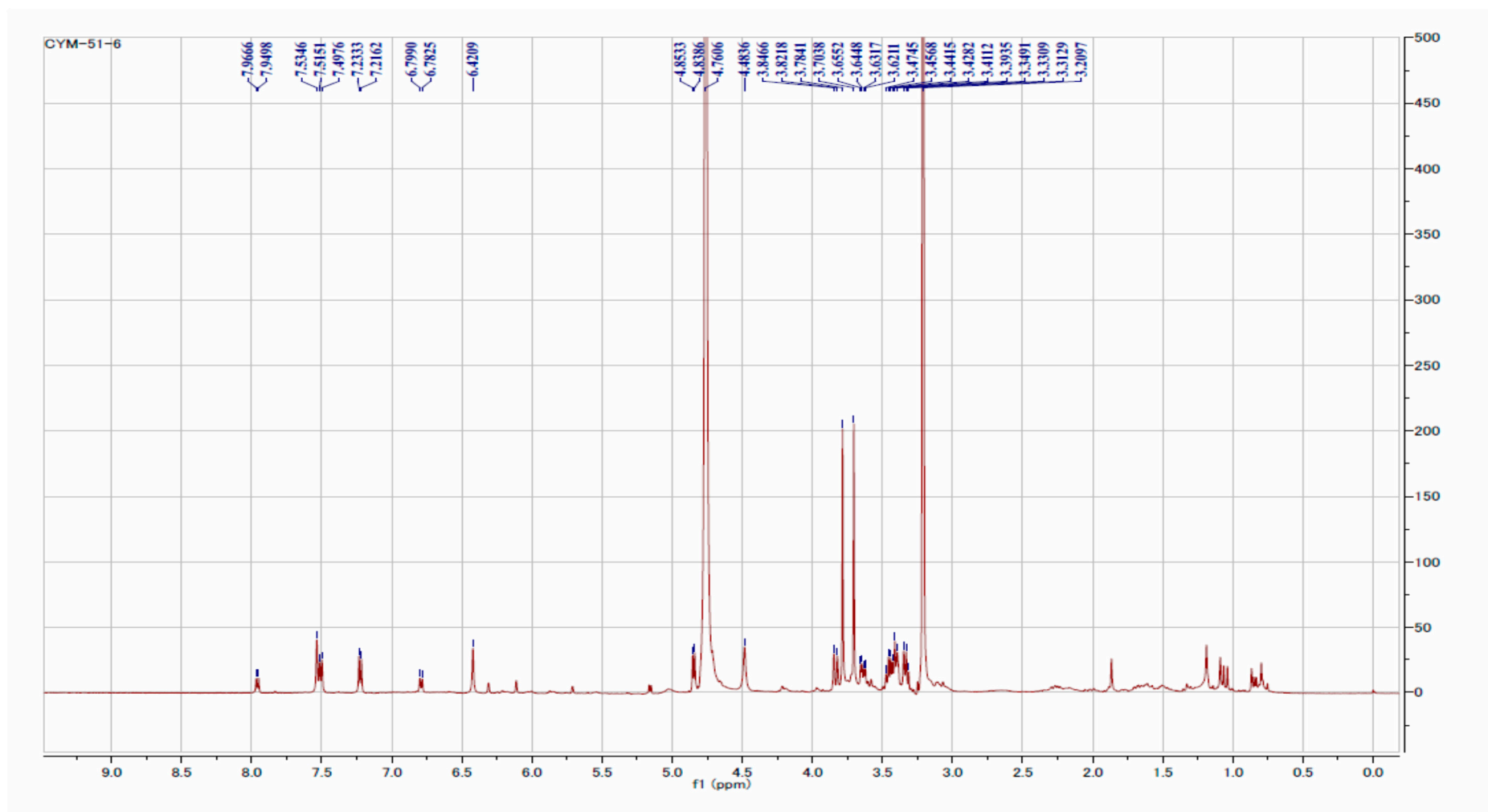
S27: ¹H NMR (CDCl₃, 500 MHz) of 8

CYM-11-13
CYM-11-13

Sample Name:
Data Collection: 400MR-PROTON
Archive directory: cd3od
Sample directory: exp
ACQUISITION temp not used
File: PROTON410.3 gain 56
at 3.500 spin 20
Pulse Sequence: zgpg30 (zgpg30) 0.008
Solvent: cd3od 4000 pw90 14.800
Date collected on: Apr 22 2019 10.000
d1 1.500 FLAGS
Operator: vmm1 16 il n
ct 16 an n
RelaxTime: 1.000 sec y
Pulse 45.0 degree nl hs
AcqTime: 3.500 min
Width: 6.3 Hz
Resolution: 59 fm not used
Observer: JL 193, 41011
Data: 2455.4
Line broadening: 602.7
FT Sfe: 65536 0 xfl 806.3
Total time: 1 min 20 sec
decwave: W40_HCN5mm rp -123.1
dpwr: 38 lp 0
dmf: 2947 PLOT
7.500 375
7.500 8
7.500 570
7.500 7



S27: ^1H NMR ($\text{C}_5\text{D}_5\text{N}$, 125 MHz) of **8**



S28: ^1H NMR (CDCl_3 , 500 MHz) of **9**