

Supporting Information

Amaranzoles B-F, Imidazole-2-carboxy Steroids from the Marine Sponge, *Phorbas amaranthus*. C24-N- and C24-O-Analogs from a Divergent Oxidative Biosynthesis.

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Figure S1. ^1H NMR spectrum for amaranzole B (**2**) in CD_3OD at 600 MHz

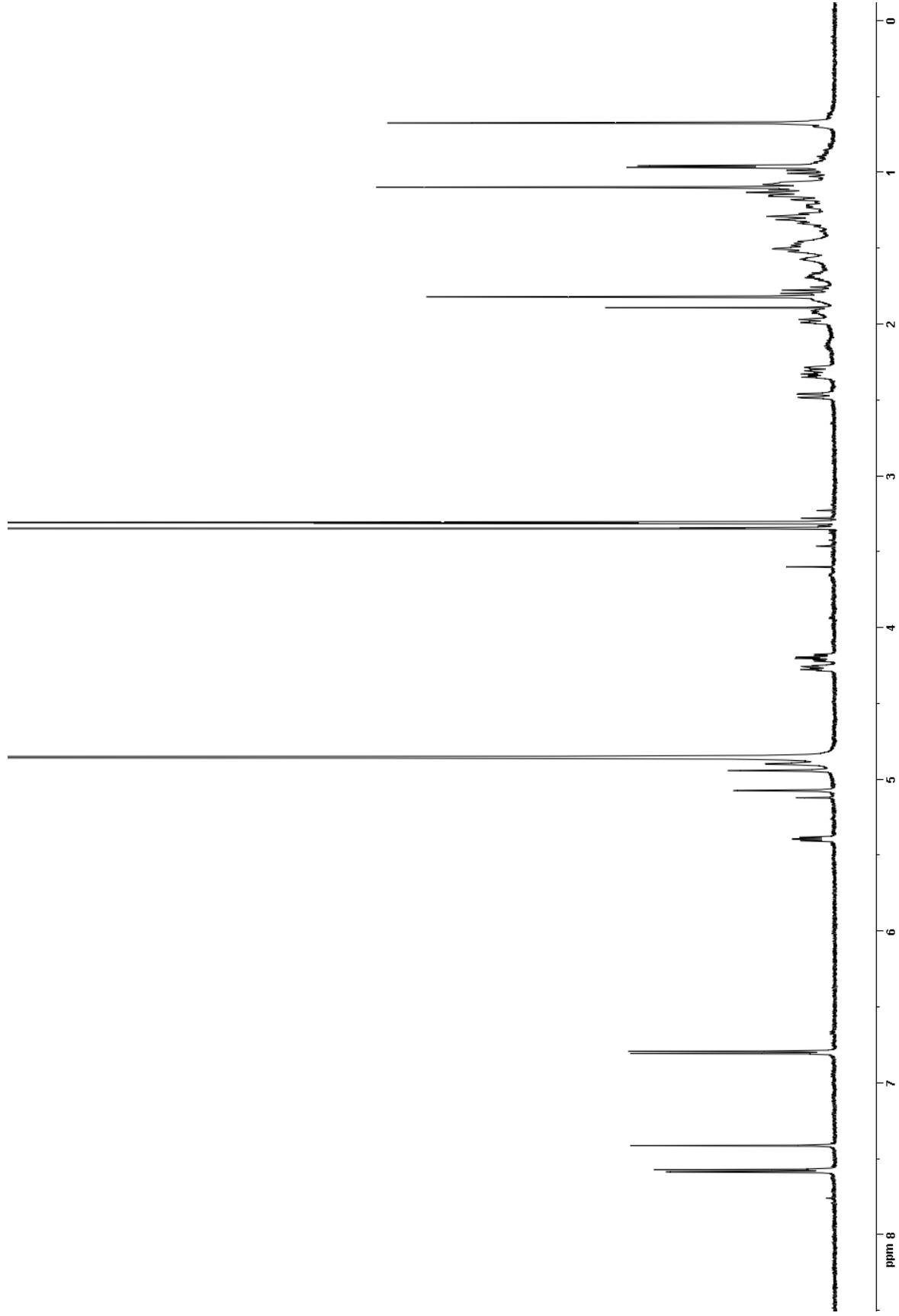


Figure S2. DQF-COSY spectrum for amaranzole B (2) in CD₃OD at 600 MHz

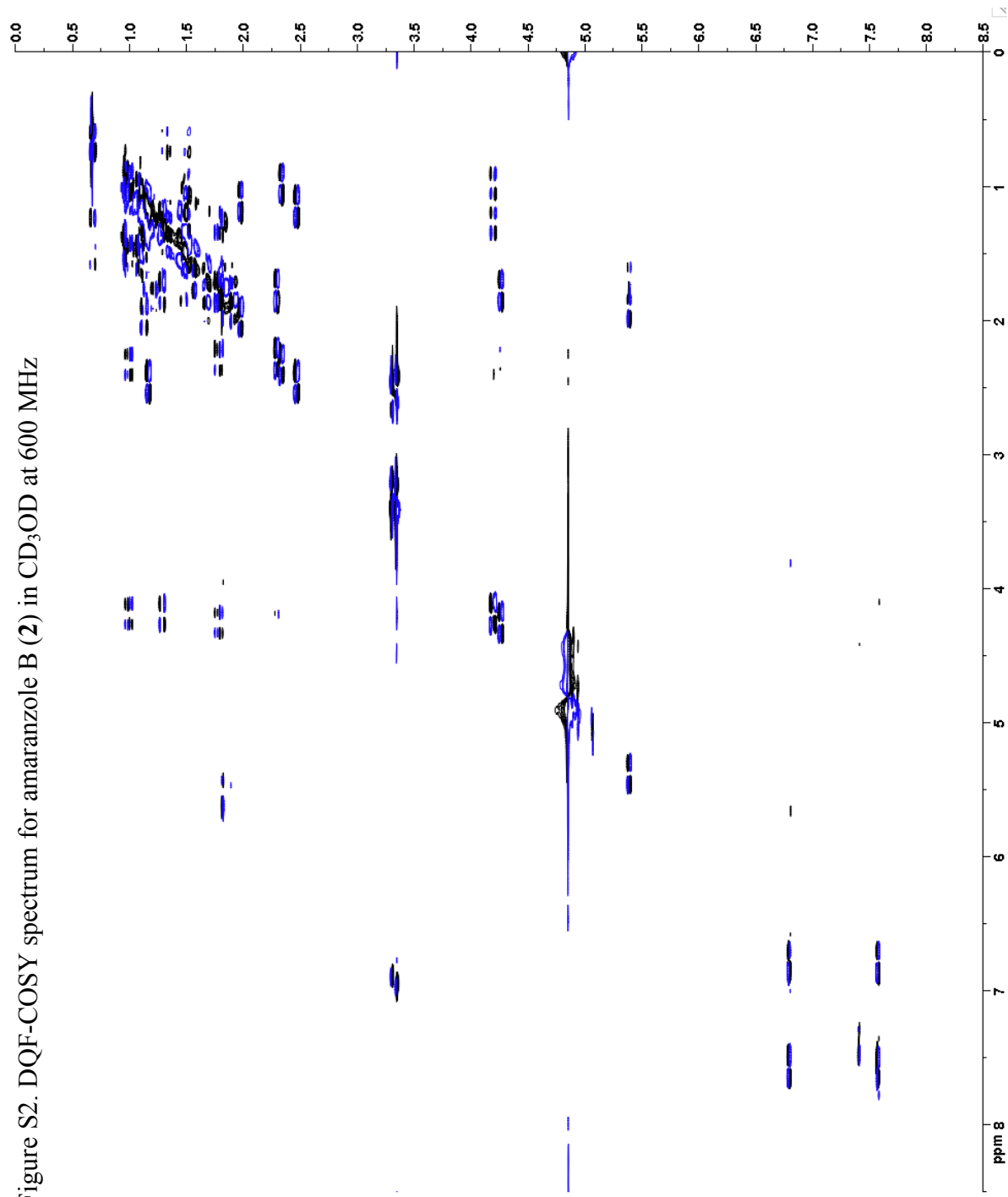


Figure S3. gHSQC spectrum for amaranzole B (2) in CD₃OD at 600 MHz

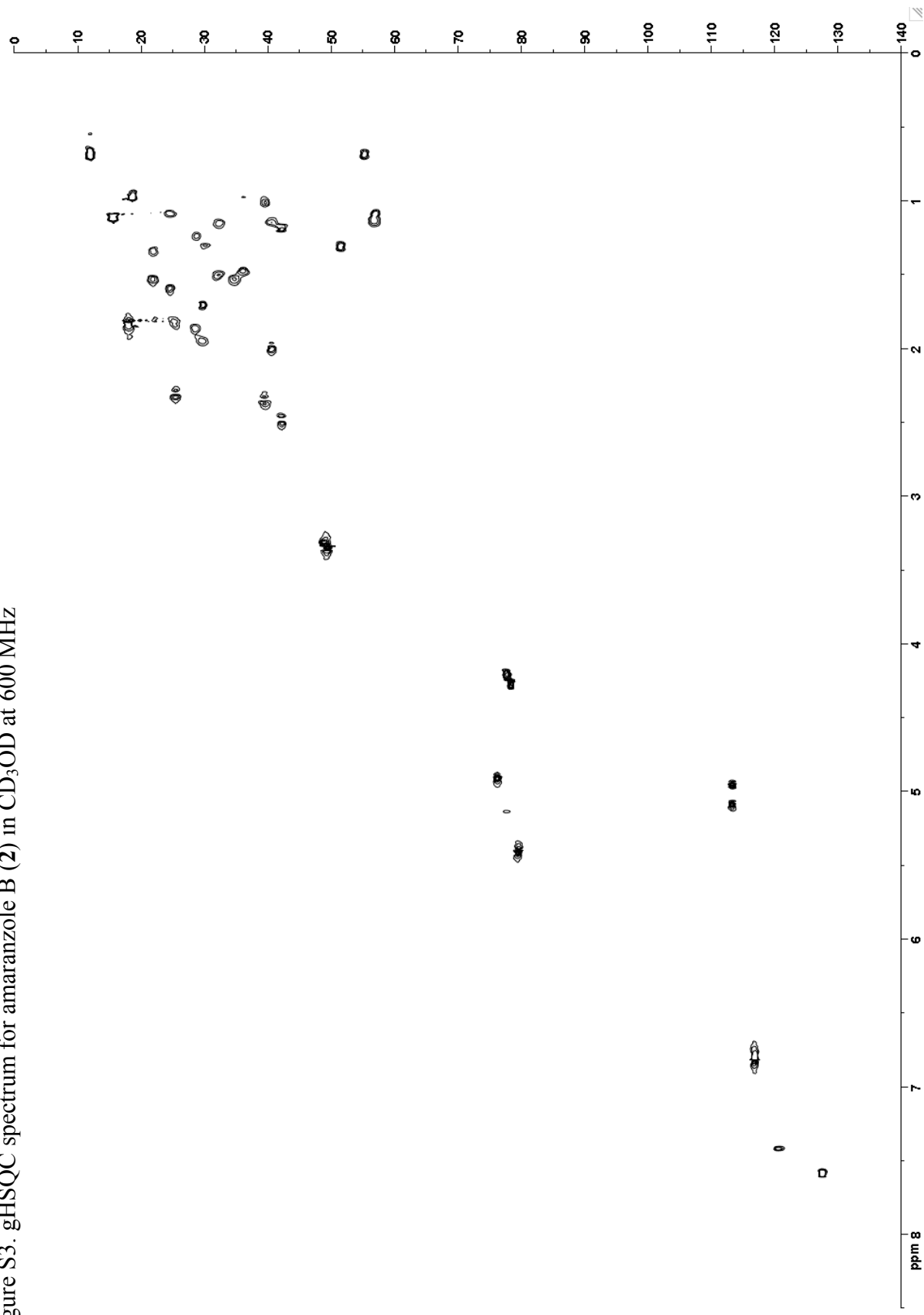


Figure S4. gHMBC spectrum for amaranzole B (2) in CD₃OD at 600 MHz

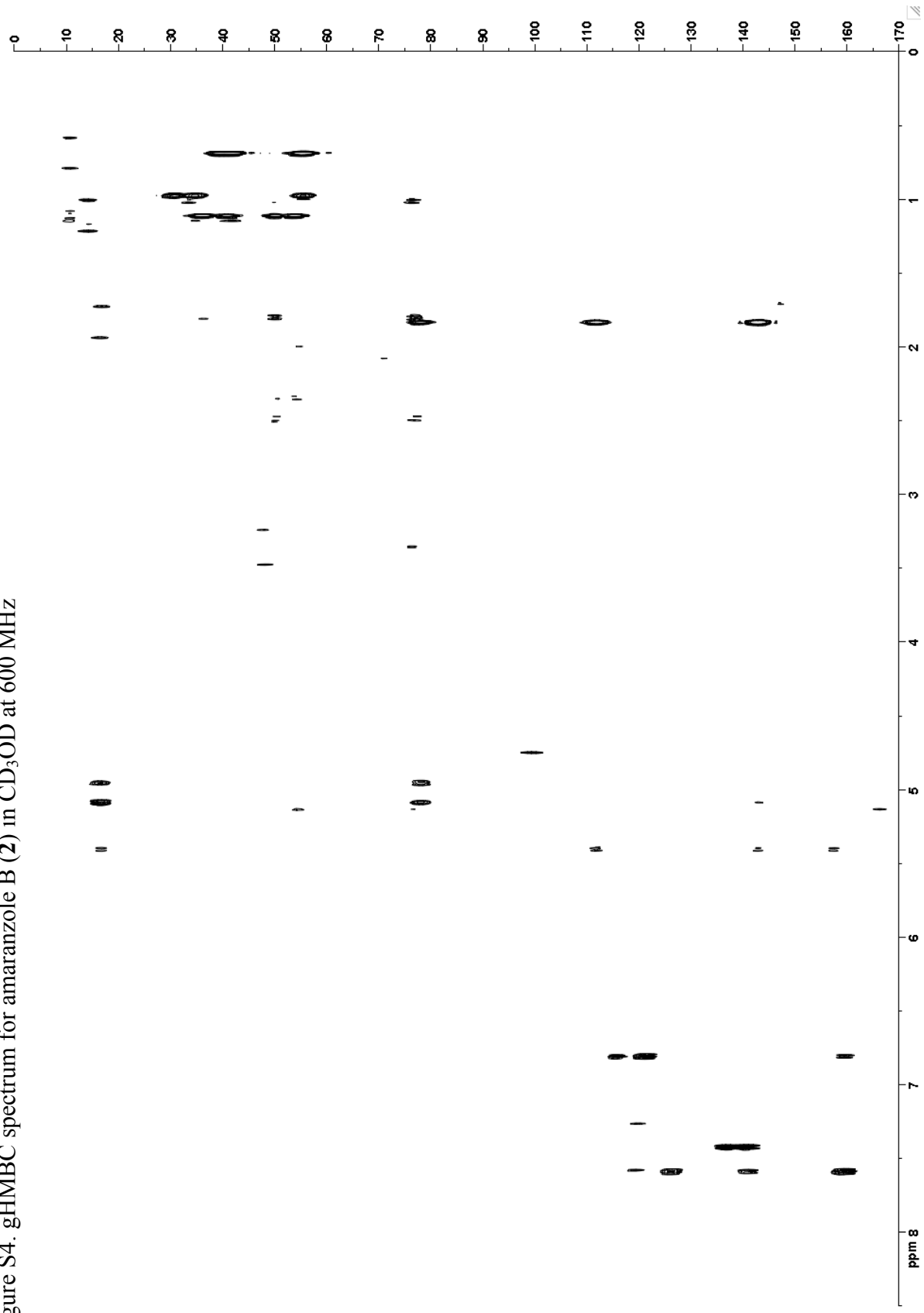


Figure S5. ^1H NMR spectrum for amaranzole C (**3**) in CD_3OD at 600 MHz

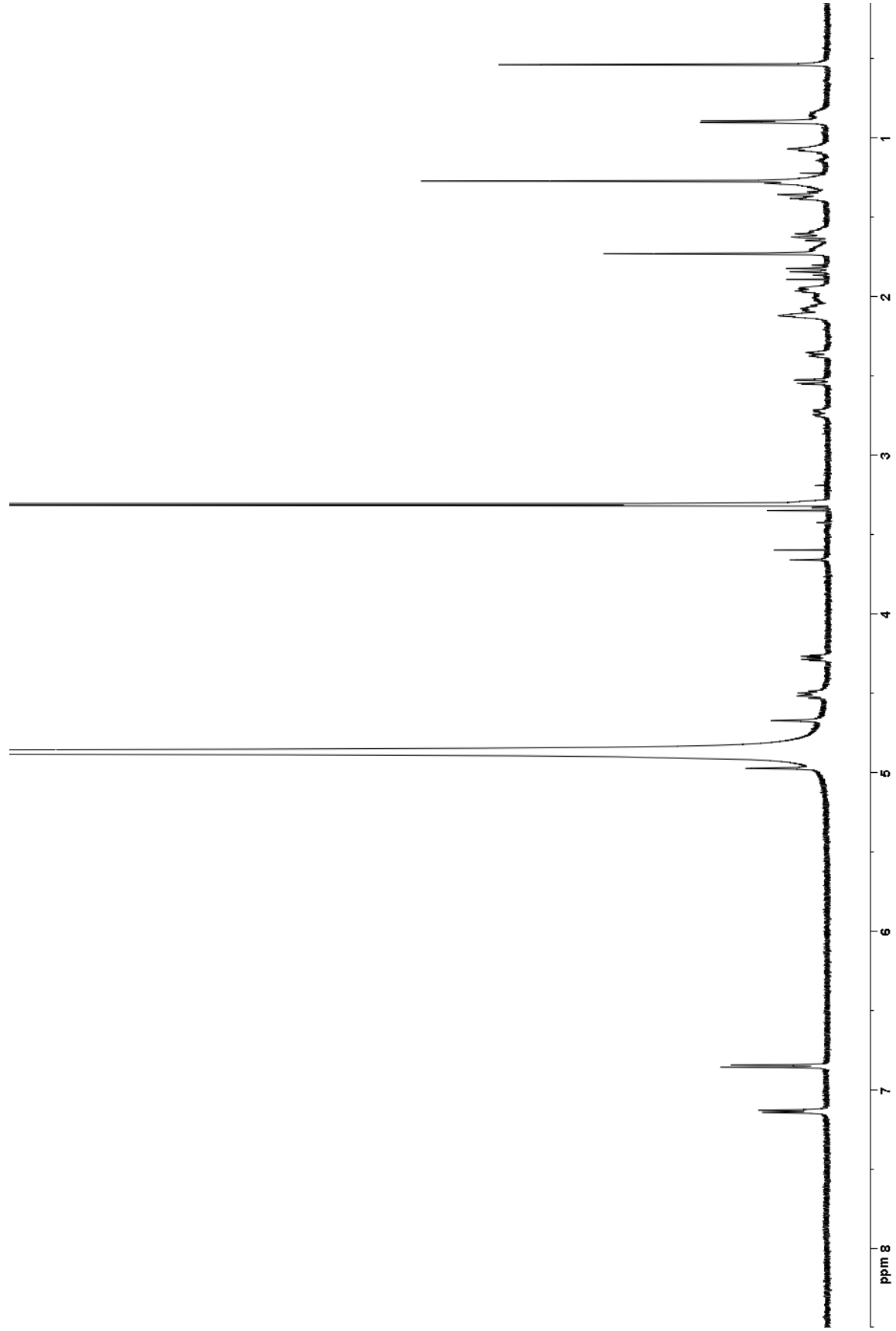


Figure S6. ^1H NMR spectrum for amaranzole D (4) in CD_3OD at 600 MHz

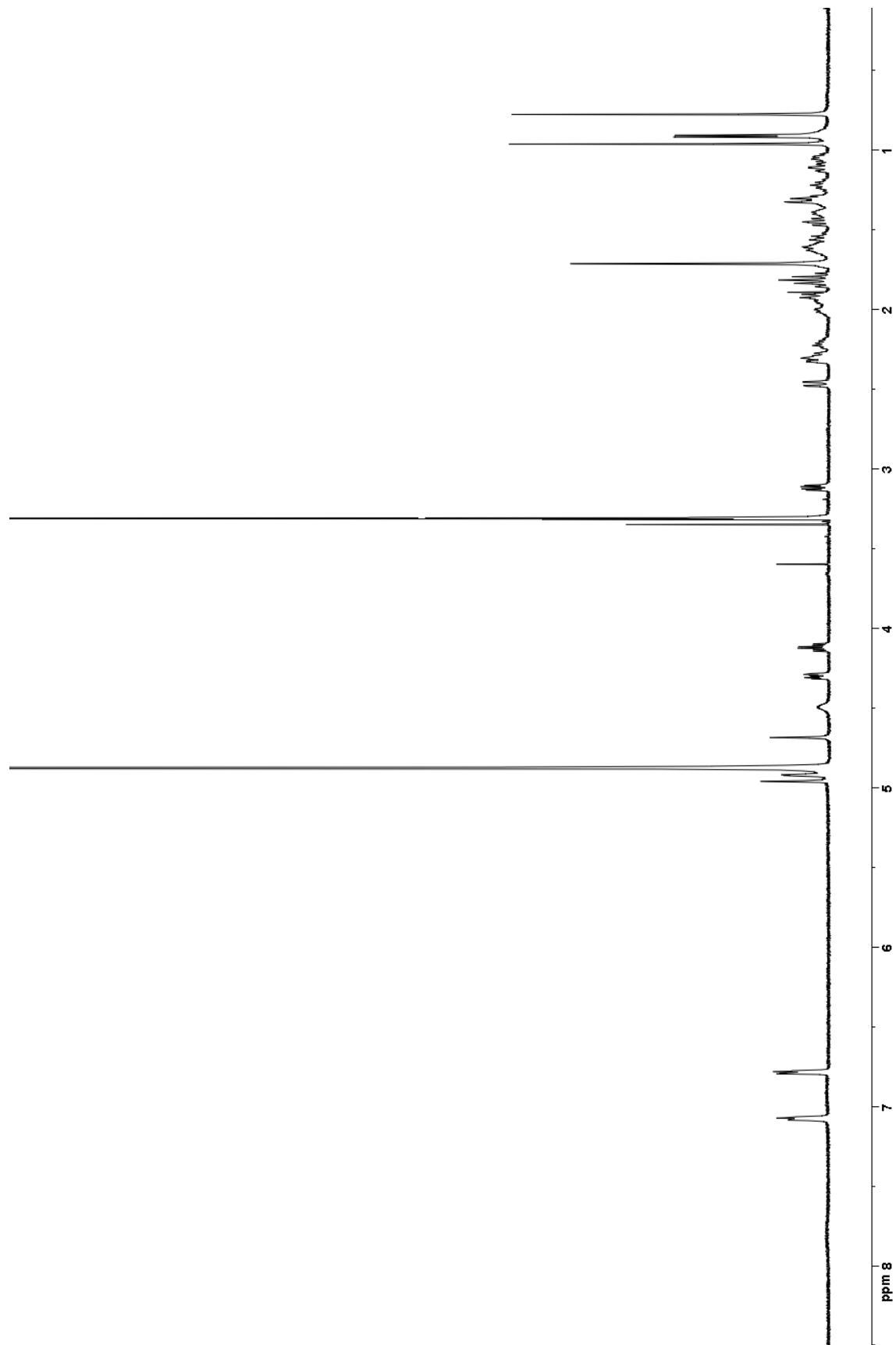


Figure S7. ^1H NMR spectrum for amaranzole E (**5**) in CD_3OD at 600 MHz

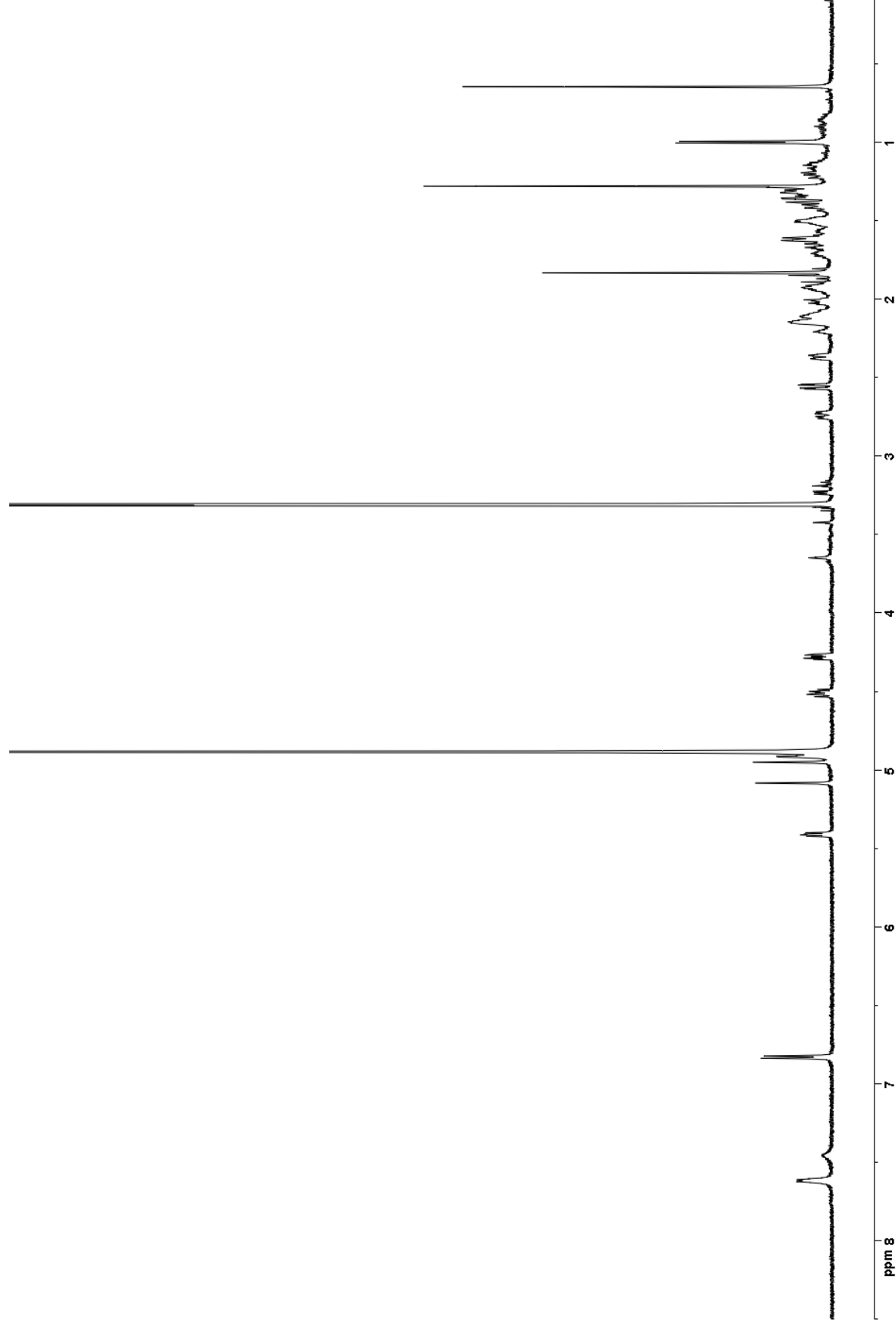


Figure S8. ^1H NMR spectrum for amaranzole F (6) in CD_3OD at 600 MHz

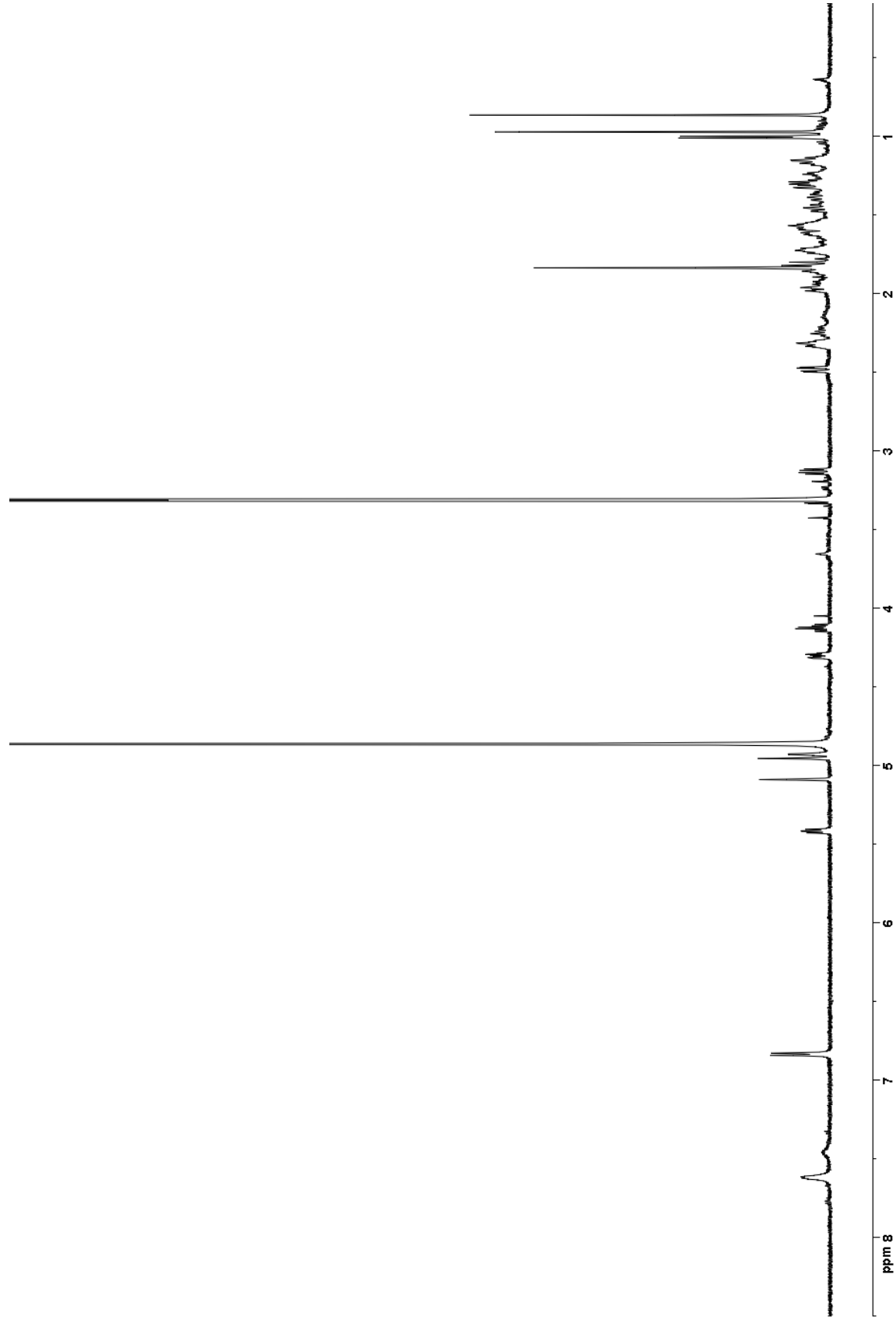


Figure S9. ¹H NMR spectrum for N,O-dimethyl-amaranzole B (7) in CD₃OD at 600 MHz

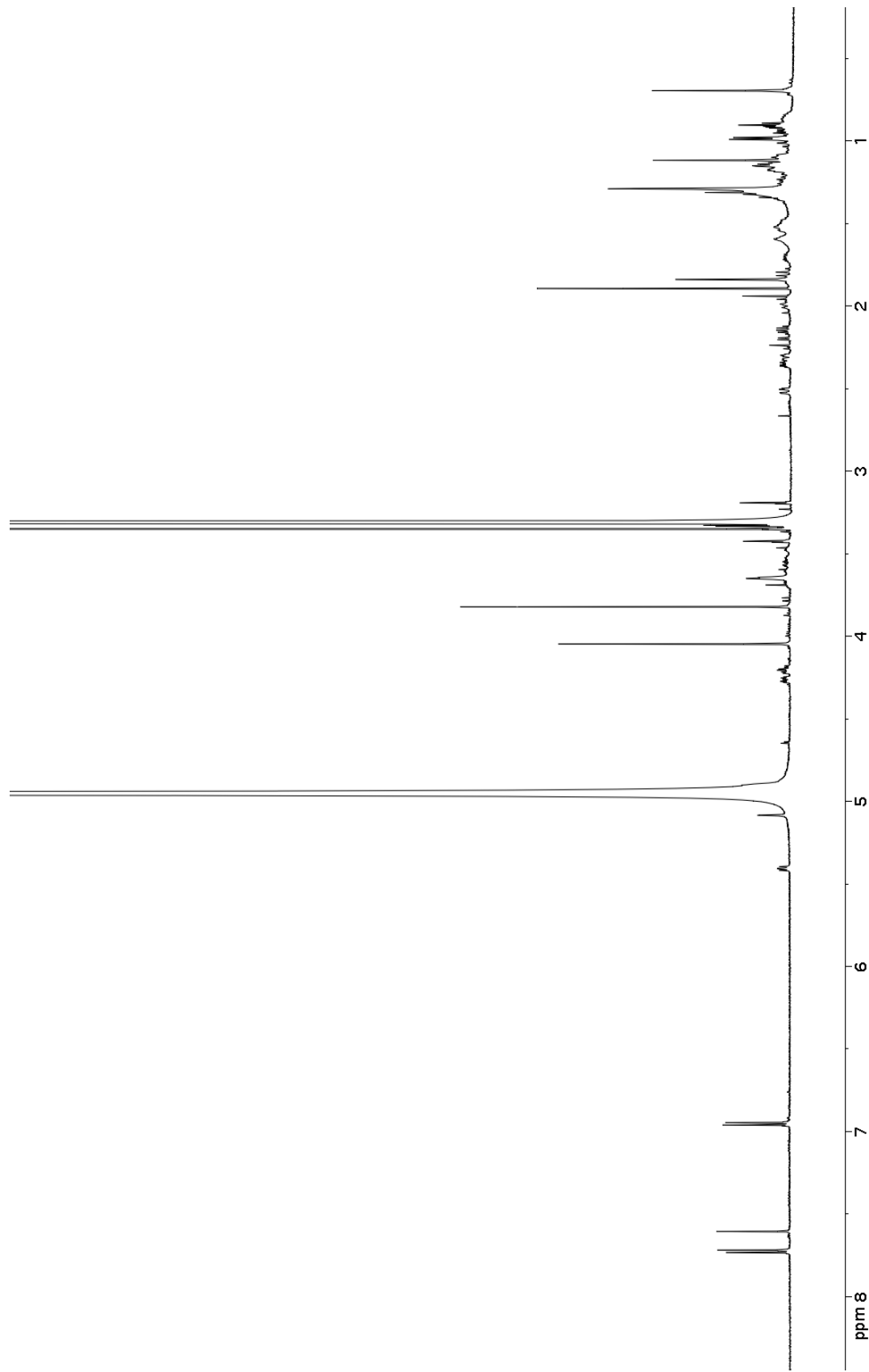


Figure S10. ¹H NMR spectrum for compound 14 in CDCl₃+0.1% TFA-*d* at 400 MHz

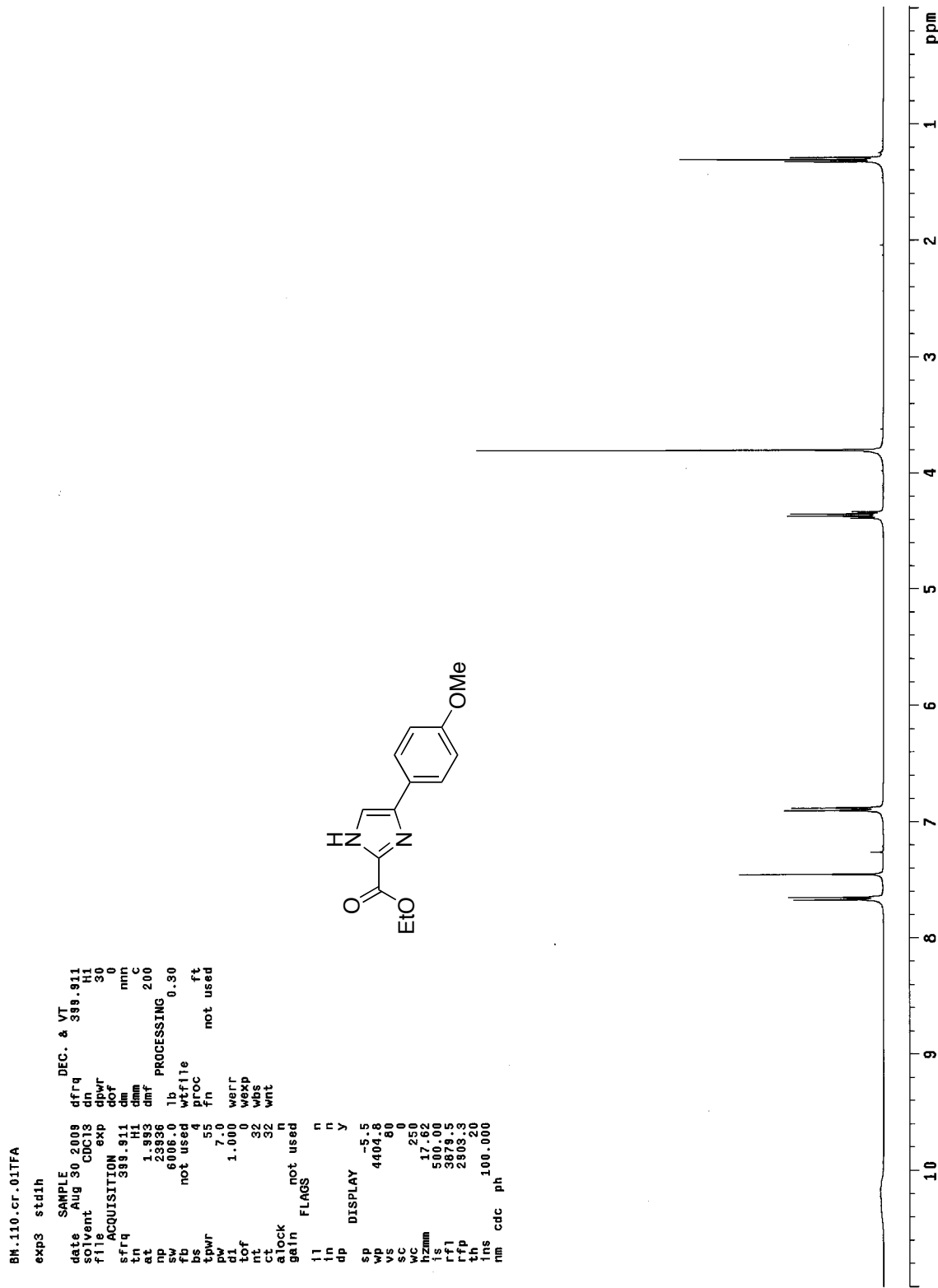


Figure S11. ¹³C NMR spectrum for compound **14** in CDCl₃+0.1% TFA-*d* at 400 MHz

BM.110. cr. 01TFA.13C

Pulse Sequence: s2pu1

Solvent: CDCl₃

Ambient temperature

Mercury-400BB "hg402"

Relax. delay 1.500 sec

Pulse 55.4 degrees

Width 25900.0 Hz

384 repetitions

OBSERVE C13, 100.5572014 MHz

DECOUPLE H1, 399.9110254 MHz

Power 38 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FI size 85536

Total time 18 min, 59 sec

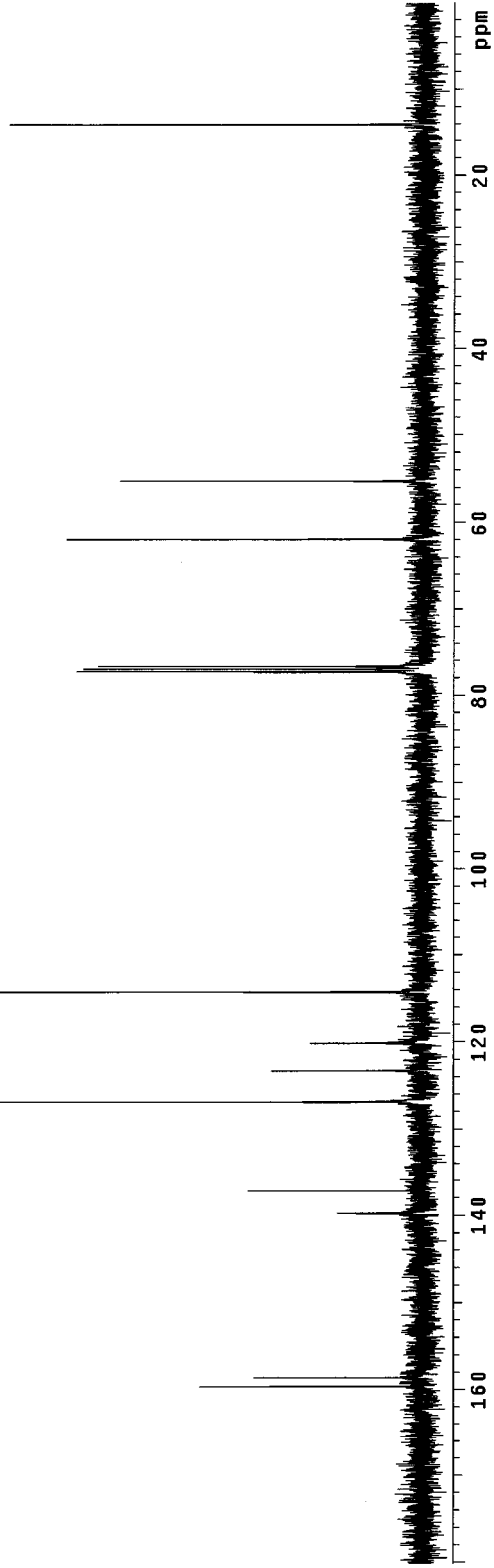
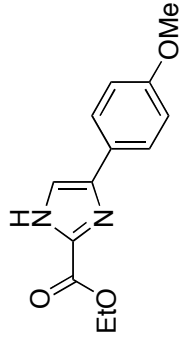


Figure S13. ¹³C NMR spectrum for compound **15a** in CDCl₃ at 400 MHz

13C OBSERVE

Pulse Sequence: s2pu1
Solvent: CDCl₃
Ambient temperature
Mercury-400BB "hg402"

Relax. delay 1.500 sec
Pulse 53.4 degrees
Acq. time 1.139 sec
Width 25000.0 Hz
7000 repetitions
OBSERVE CH, 300.5570011 MHz
PULSE PR, 399.3110254 MHz
Power 98 dB,
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 5 hr, 46 min, 7 sec

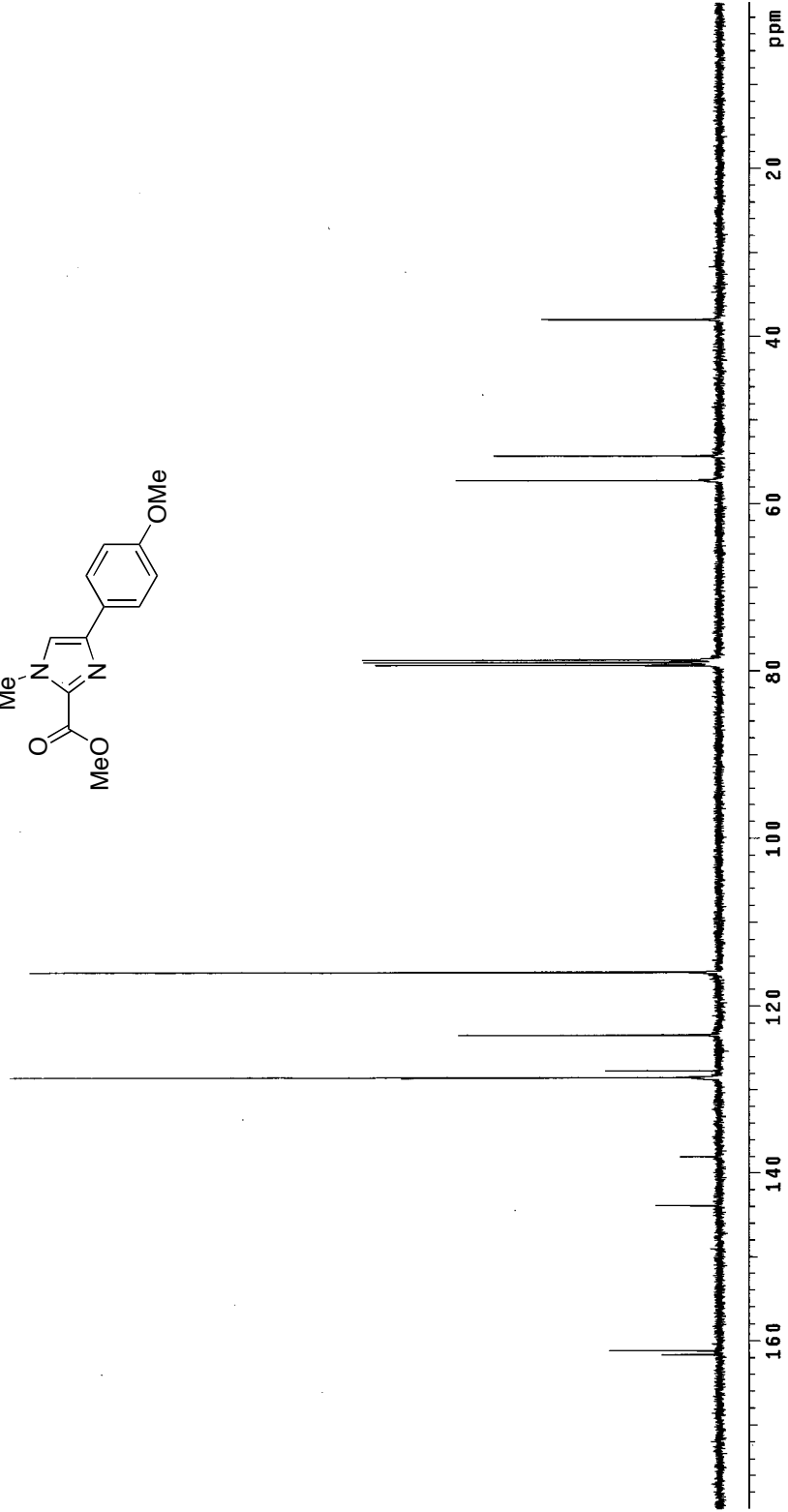
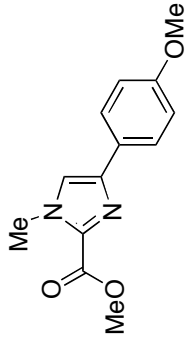


Figure S14. ¹H NMR spectrum for compound **15b** in CDCl₃ at 400 MHz

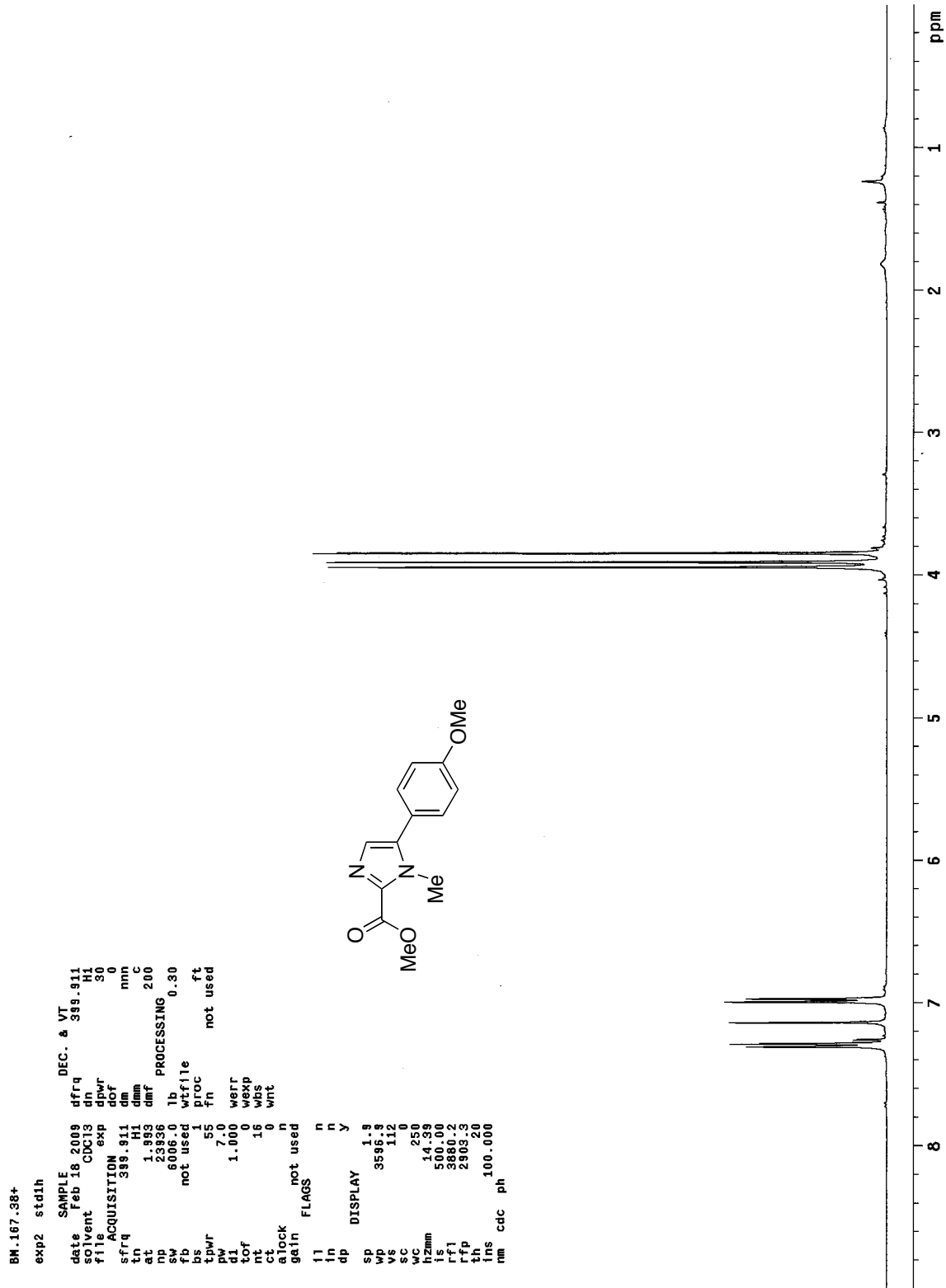


Figure S15. ^{13}C NMR spectrum for compound **15b** in CDCl_3 at 400 MHz

BM-167-38+.13C

Pulse Sequence: s2pu
Solvent: CDCl_3
Ambient temperature
Mercury-400BB "hg402"
Relax. delay 1.500 sec
Pulse 52.4 degrees
Acq. time 1.399 sec
Width 25000.0 Hz
1024 repetitions
OBSERVE C13, 100.5572029 MHz
DECOUPLE H1, 399.9110254 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
File size 65536
Total time 30 min, 37 sec

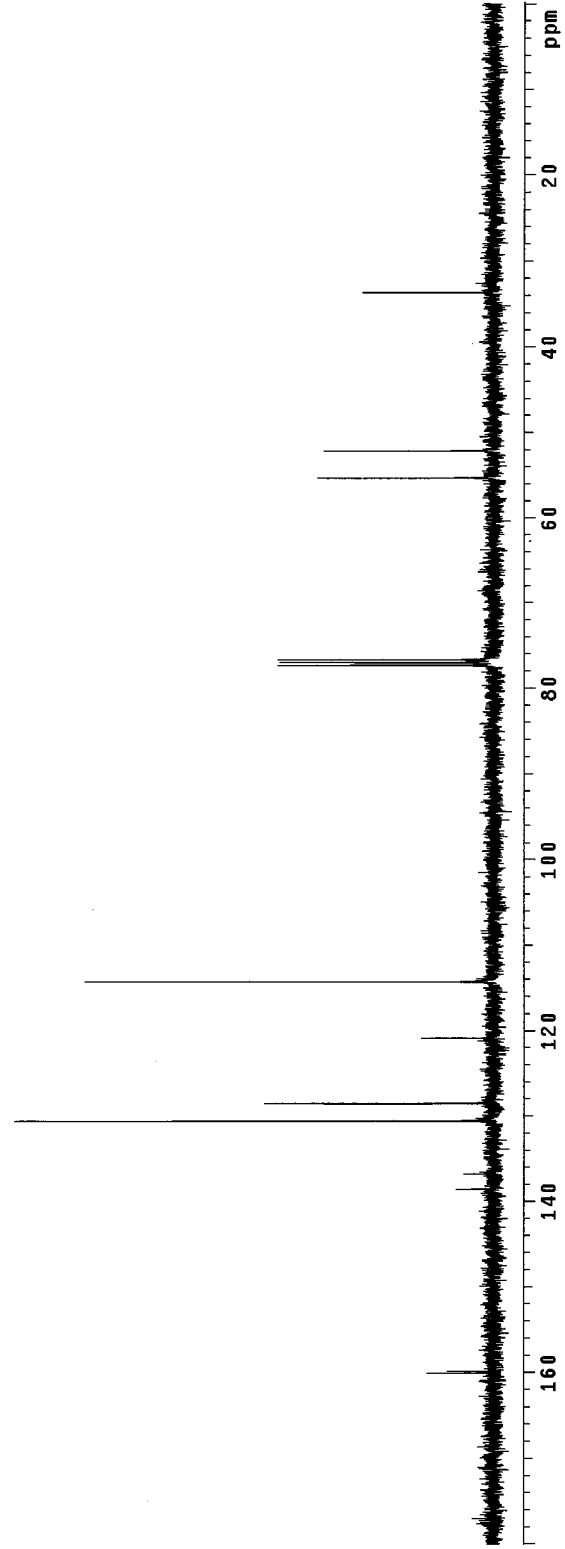
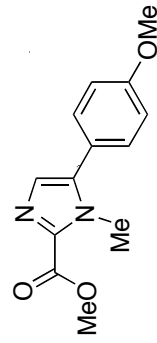


Figure S17. ^{13}C NMR spectrum for compound **10** in $\text{DMSO}-d_6$ at 400 MHz

BM.166.29-37.L10H.13C
Pulse Sequence: s2pul
Solvent: DMSO
Amplitude: 60000
Mercury-400BB "hg402"
Relax. delay 2.000 sec
Pulse 53.4 degrees
Width 38.000 Hz
Width 38.000 Hz
720 repetitions
OBSERVE C13, 100.557200 MHz
DECOUPLE H1, 399.9128250 MHz
Power 38 dB,
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 59 min, 9 sec

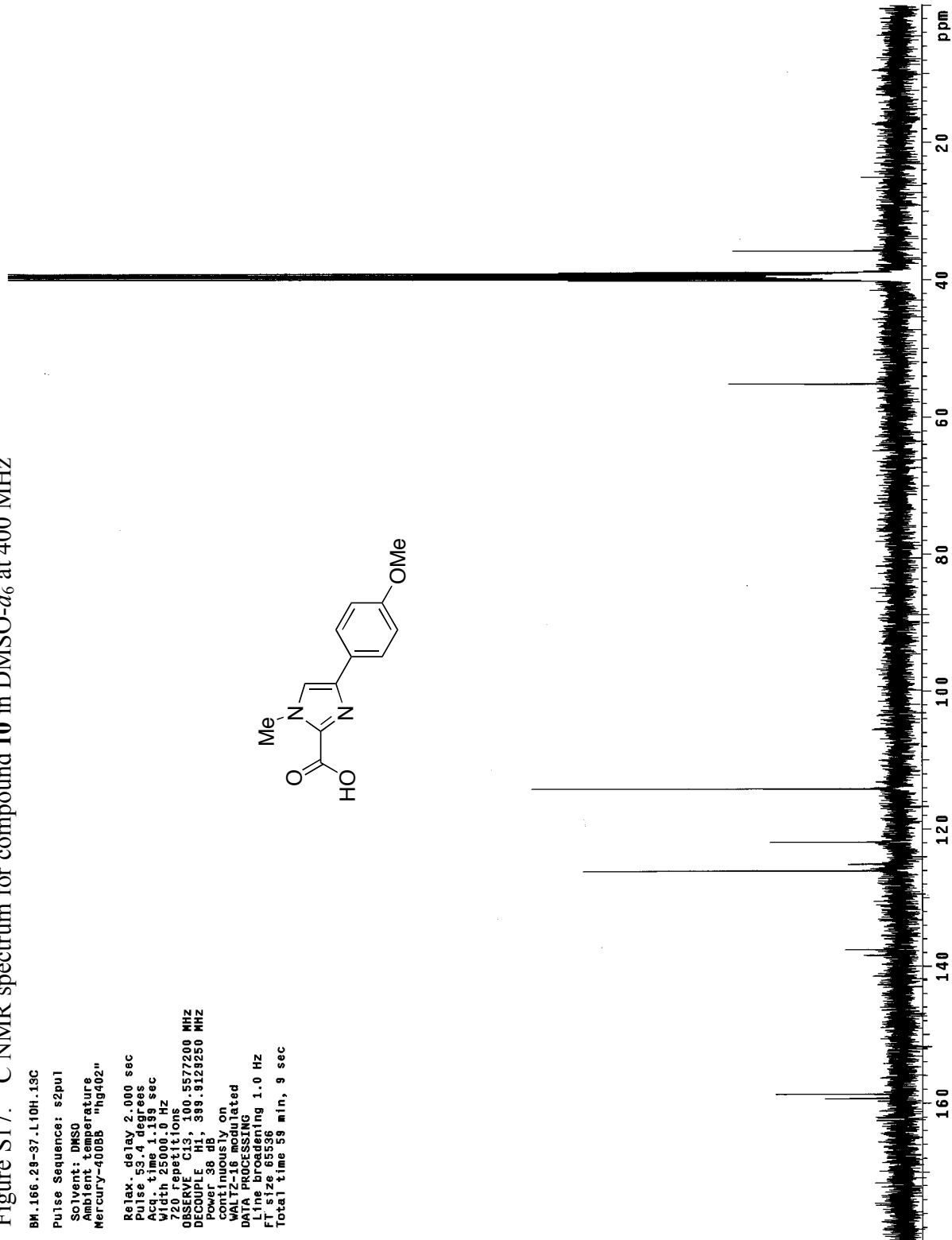
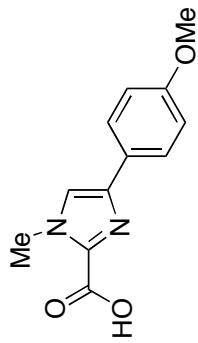


Figure S18. ¹H NMR spectrum for compound (±)-**8** in CD₃OD at 400 MHz

BM.165.25-31.C030D

exp2 std1h

date	SAMPLE	DEC. & VT
Feb 9 2009	Feb	399.913
solvent	cd3od	H1
file	exp	dn
ACQUISITION	exp	dpwr
399.913	0	30
sfreq	dm	dof
399.913	dm	0
at	dmf	min
1.992	dmf	200
np	dmf	PROCESSING
23938	0.30	ft
sw	6006.0	lb
not used	not used	fn
fb	16	proc
bs	55	not used
tpwr	7.0	werr
pw	1.000	wexp
d1	0	wbs
tof	32	wnt
nt	32	
clock	n	
gain	not used	
FLAGS	n	
l1	n	
in	n	
dp	y	
sp	-2.2	DISPLAY
wp	3603.1	
vs	137	
sc	0	
sz	250	
hzmm	14.41	
is	500.00	
rfl	2288.4	
rfp	1323.7	
th	100.000	
ins	cdc	
nm	ph	

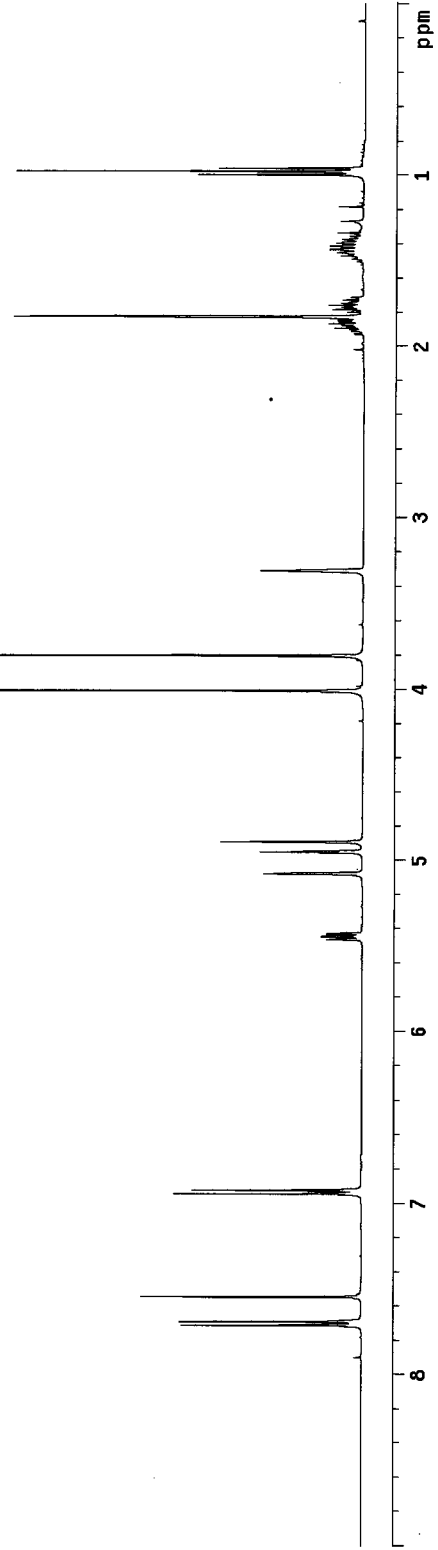
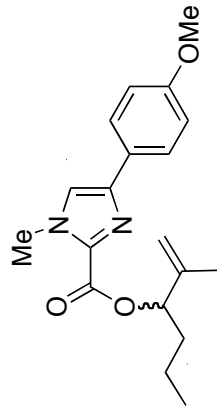


Figure S19. ^{13}C NMR spectrum for compound (\pm)-**8** in CD_3OD at 400 MHz

BM.165.25-31.CD3OD.13C

Pulse Sequence: s2pul
Solvent: CD3OD
Ambient temperature
Mercury-400BB "hg402"

Relax. delay 2.000 sec
Pulse 59.4 degrees
Acq. time 1.189 sec
Width 25000.0 Hz
176 Repetitions
OBSERVE C13, 100.5574523 MHz
DECOUPLE H1, 99.9126011 MHz
Power 38 dB
continuously on
DVT1 FID
MULTI PROCESSED
LINE BROUGHTING 1.0 HZ
FT size 65536
Total time 59 min, 9 sec

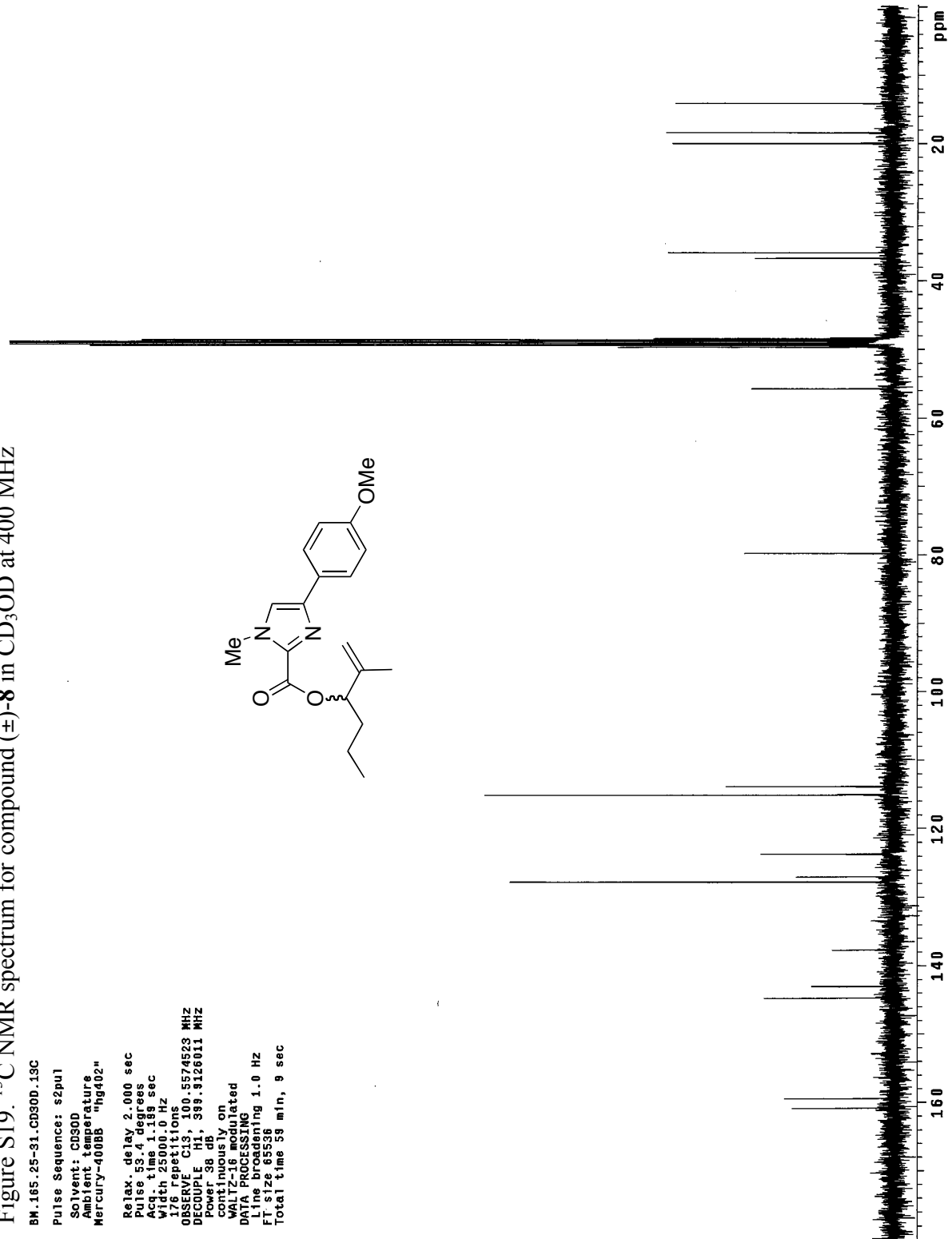
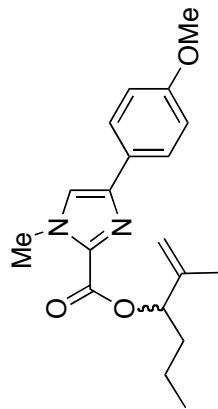


Figure S20. ¹H NMR spectrum for compound (-)-(R)-9 in CD₃OD at 400 MHz

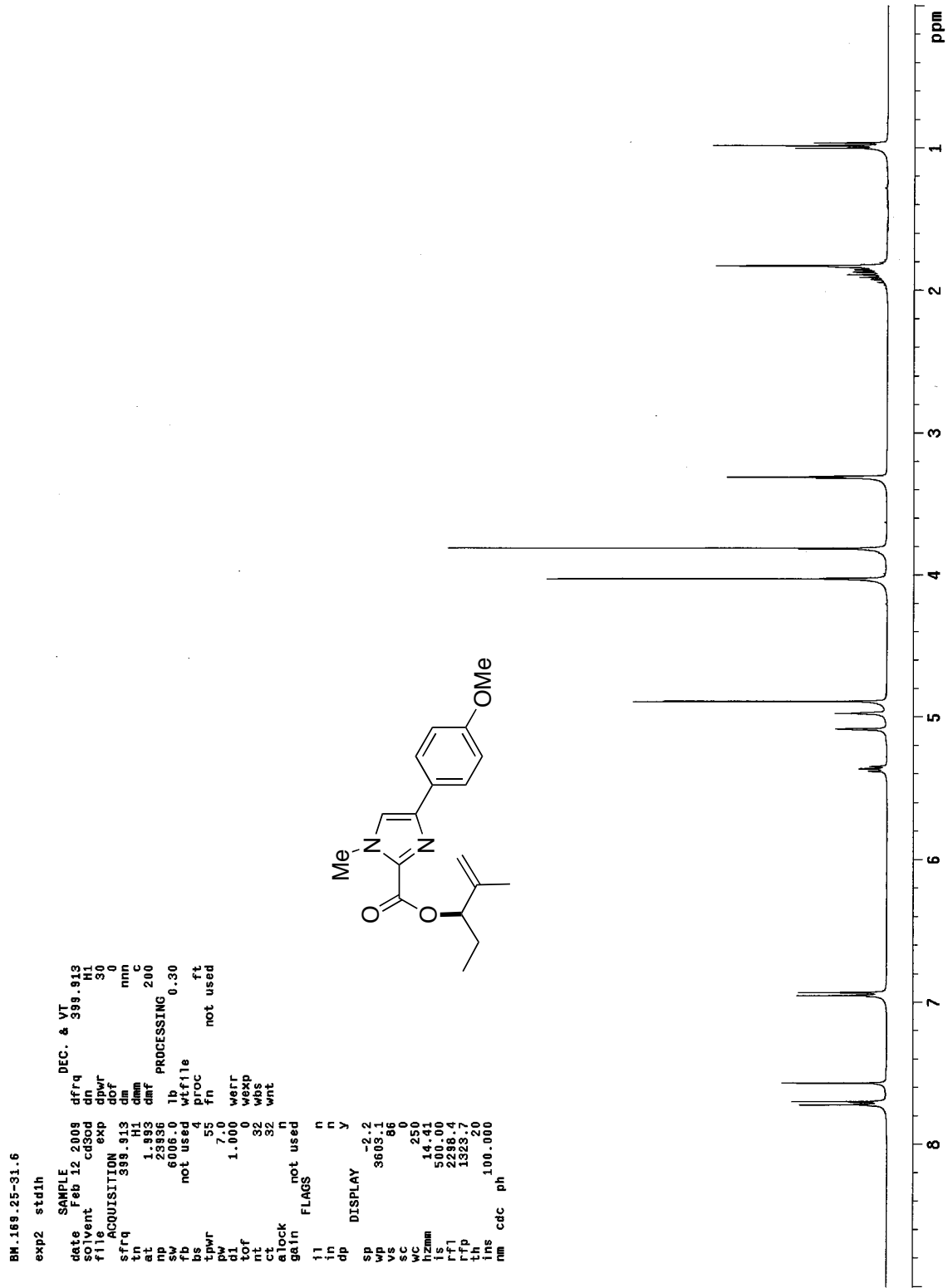


Figure S21. ¹³C NMR spectrum for compound (-)-(R)-9 in CD₃OD at 400 MHz

BN.169.25-31.6.13C

Pulse Sequence: s2pu1
Solvent: cd3od
Ambient temperature
Mercury-400BB "hg402"

Relax. delay 1.500 sec
Pulse 53.4 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
8000 repetitions
OBSERVE C13, 100.5574515 MHz
PCOUPLE H1, 399.8126011 MHz
Continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 6 hr, 35 min, 31 sec

