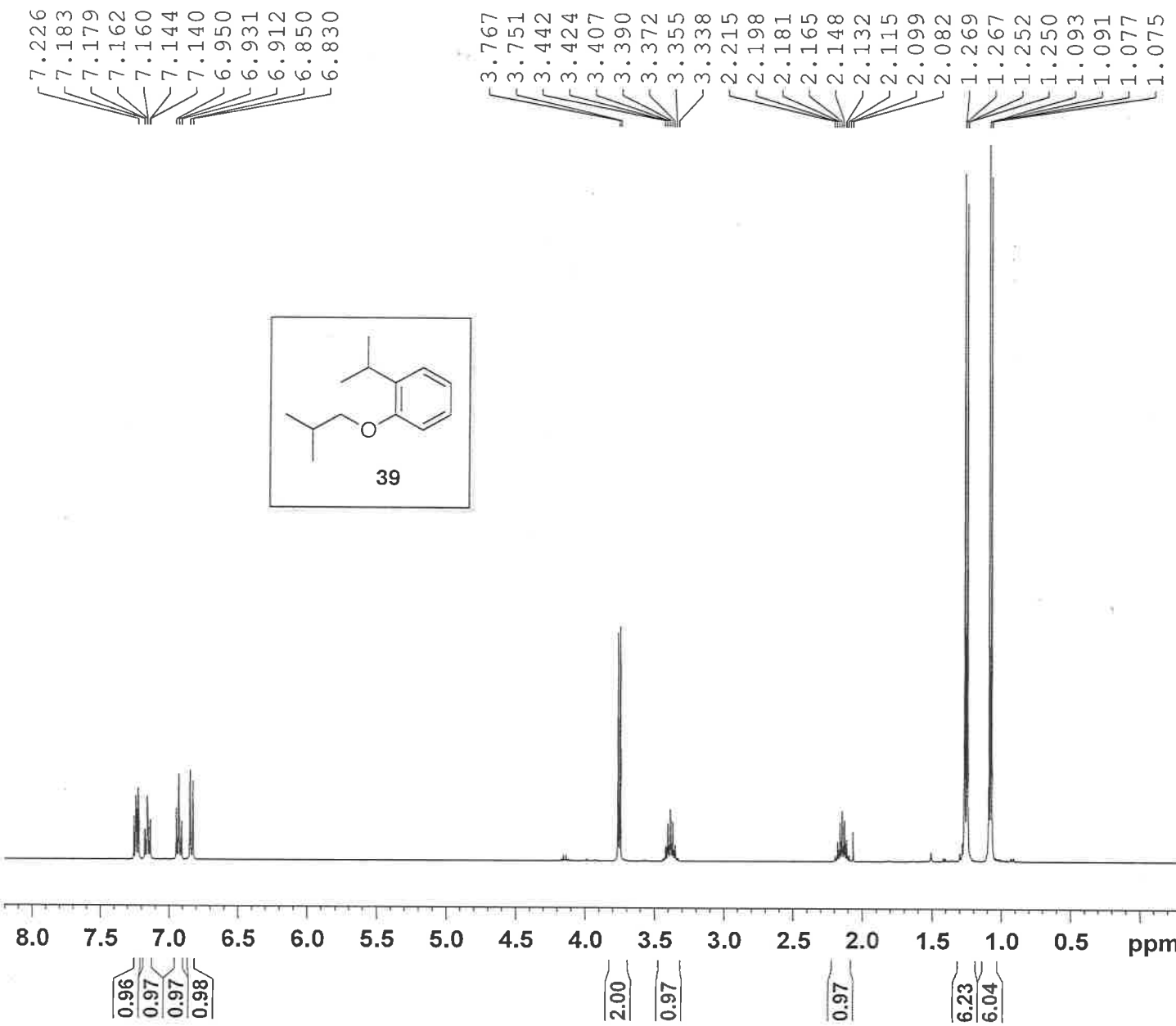
Supporting Information for **Modeling, Synthesis and Biological Evaluation of Potential Retinoid-X-Receptor (RXR) Selective Agonists: Analogs of 4-[1-(3,5,5,8,8-Pentamethyl-5,6,7,8-tetrahydro-2-naphthyl)ethynyl]benzoic Acid (Bexarotene) and 6-(Ethyl(4-isobutoxy-3-isopropylphenyl)amino)nicotinic Acid (NEt-4IB)**:

^{1}H- and ^{13}C-NMR for all reported compounds

Representative HPLC Method for compound **33**

HPLC Traces for compounds **25-36, 37a** and **37b**

CWV-195

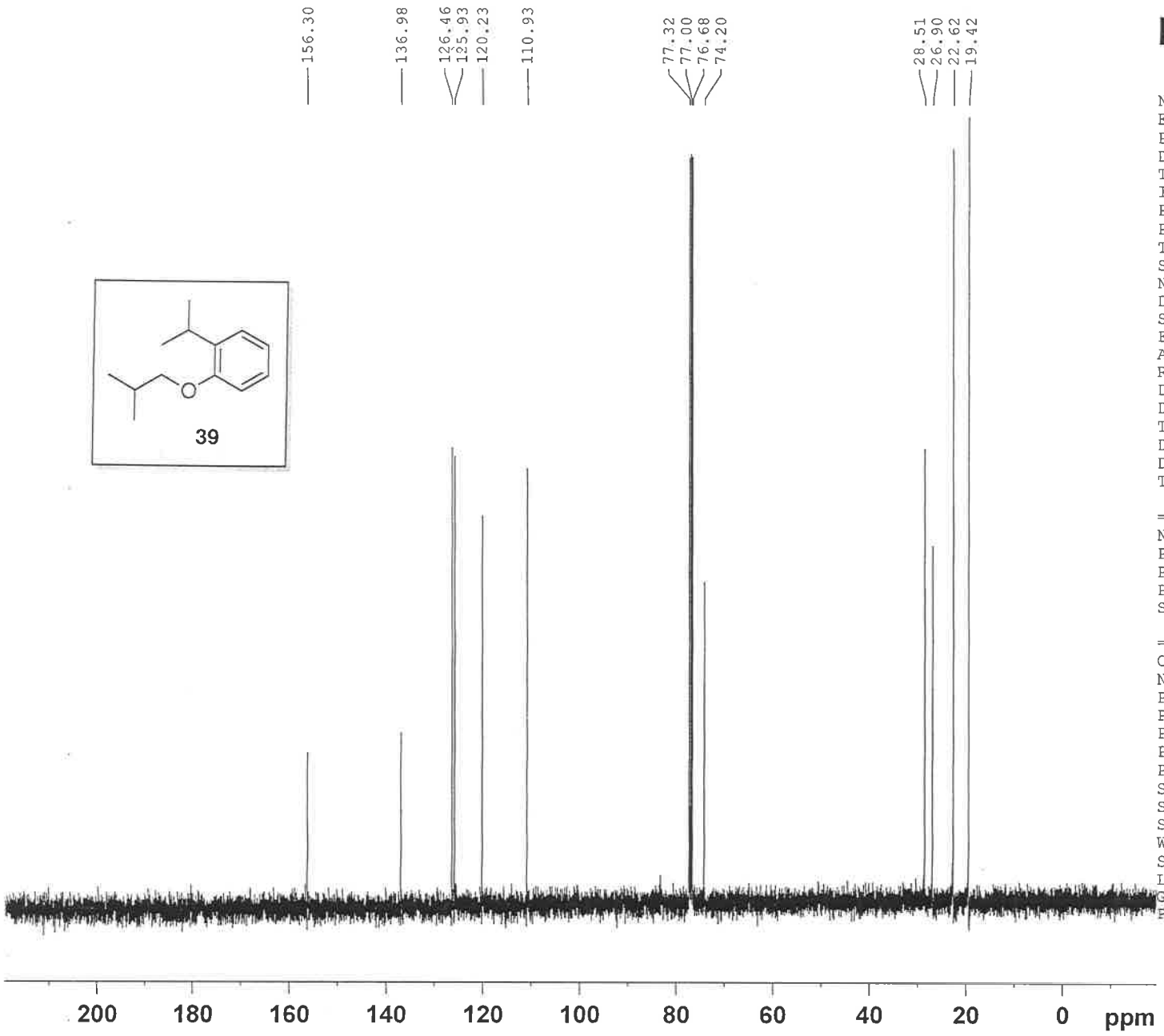


NAME	CWV-195
EXPNO	1
PROCNO	1
Date_	20141227
Time	15.46
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	298.2 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	1H
P1	14.00 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300096 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

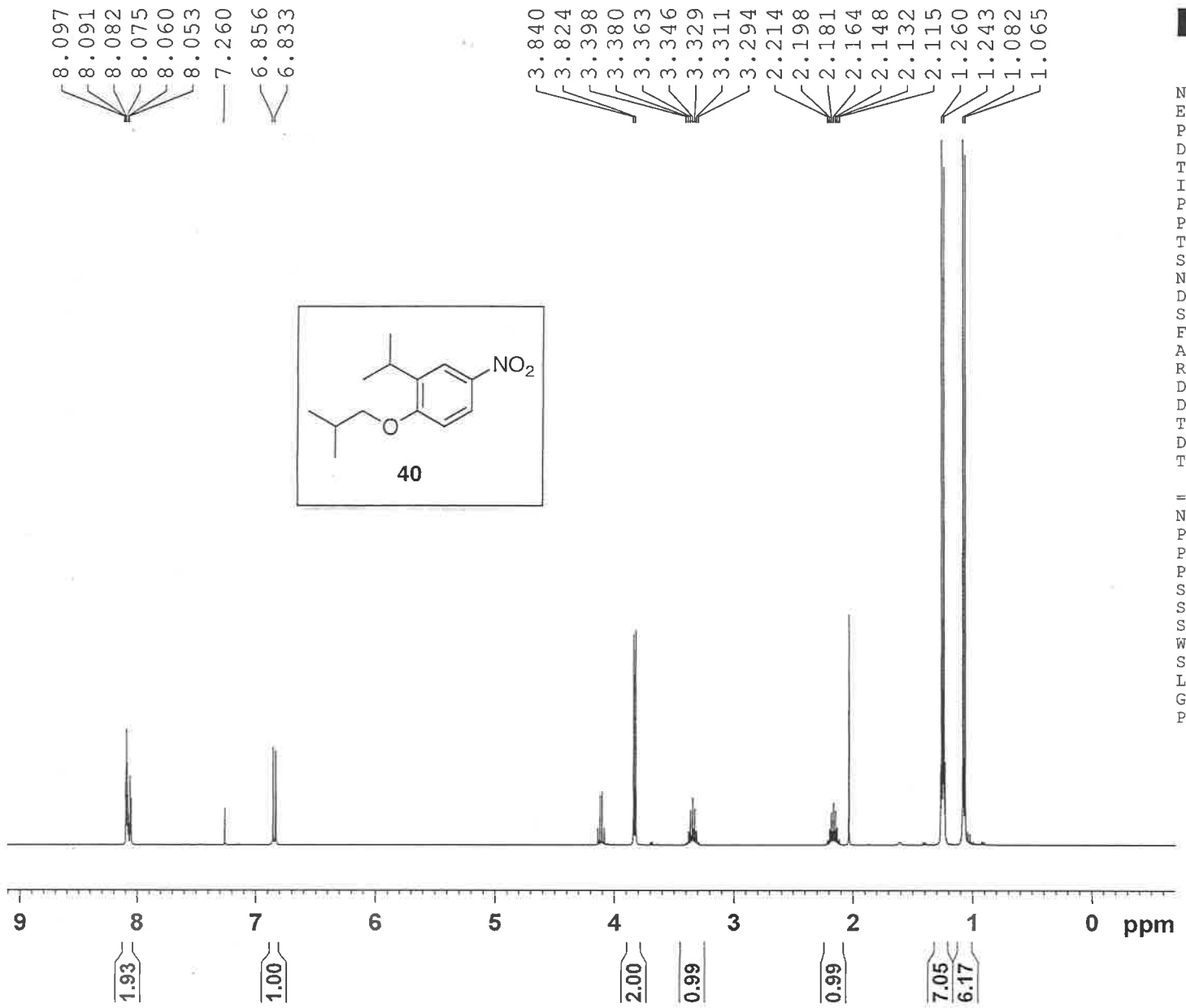
CWV-195



BRUKER

NAME	CWV-195
EXPNO	2
PROCNO	1
Date_	20141227
Time	15.53
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	51
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	298.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127722 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

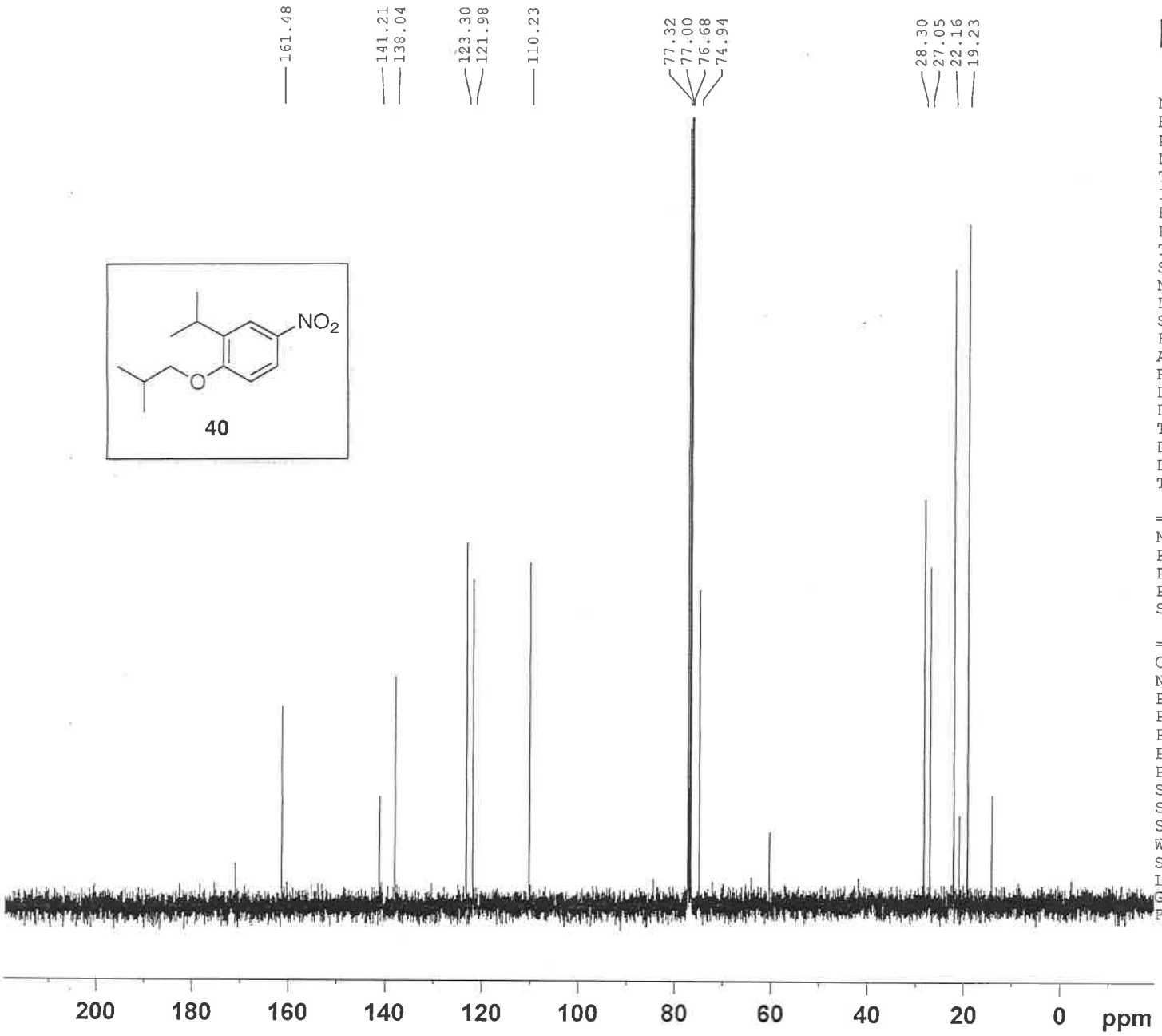
CWV-197 bottom spot



BRUKER

NAME	CWV-197
EXPNO	7
PROCNO	1
Date_	20150108
Time	9.47
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	298.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.00 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300099 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

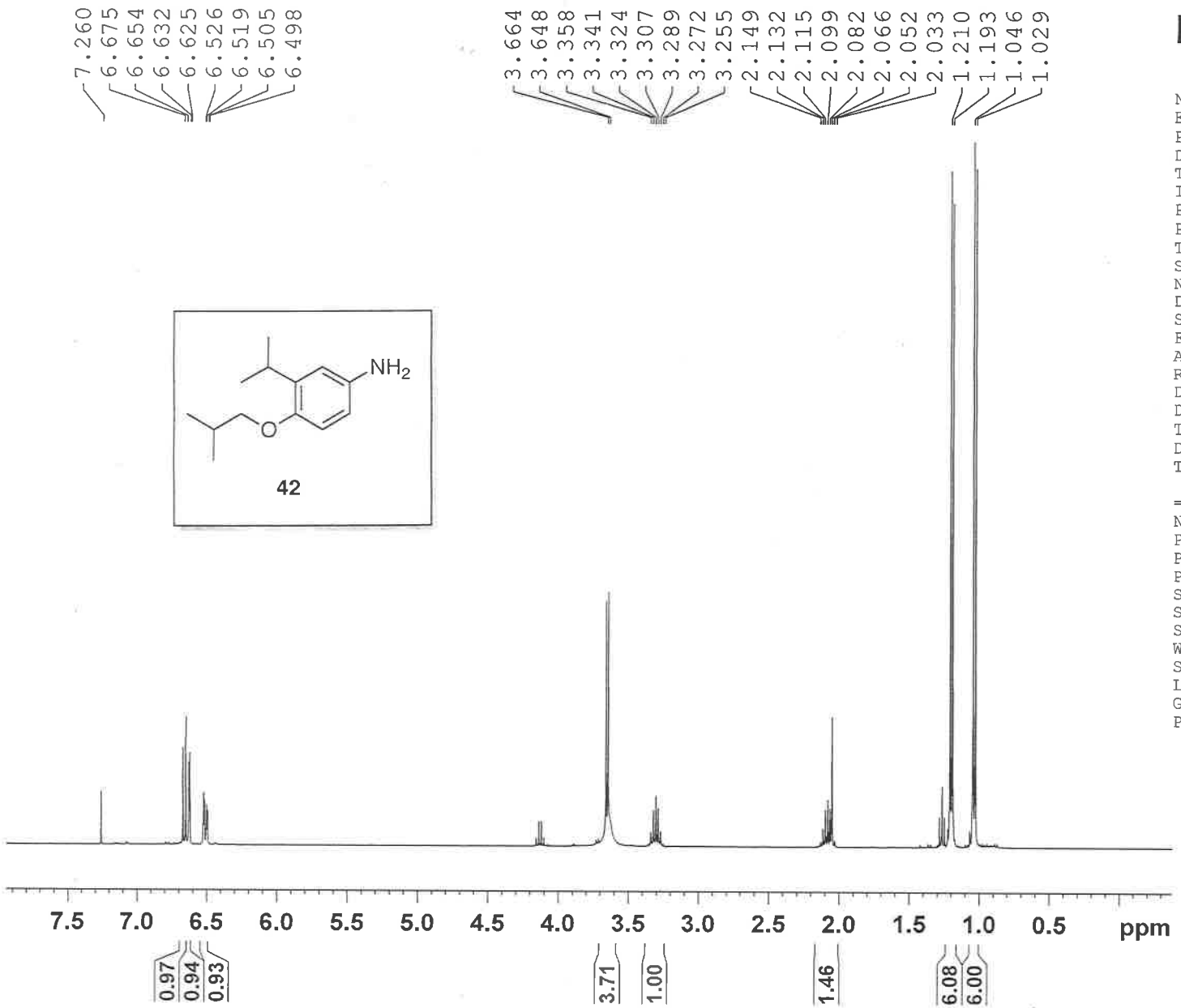
CWV-197 bottom spot



BRUKER

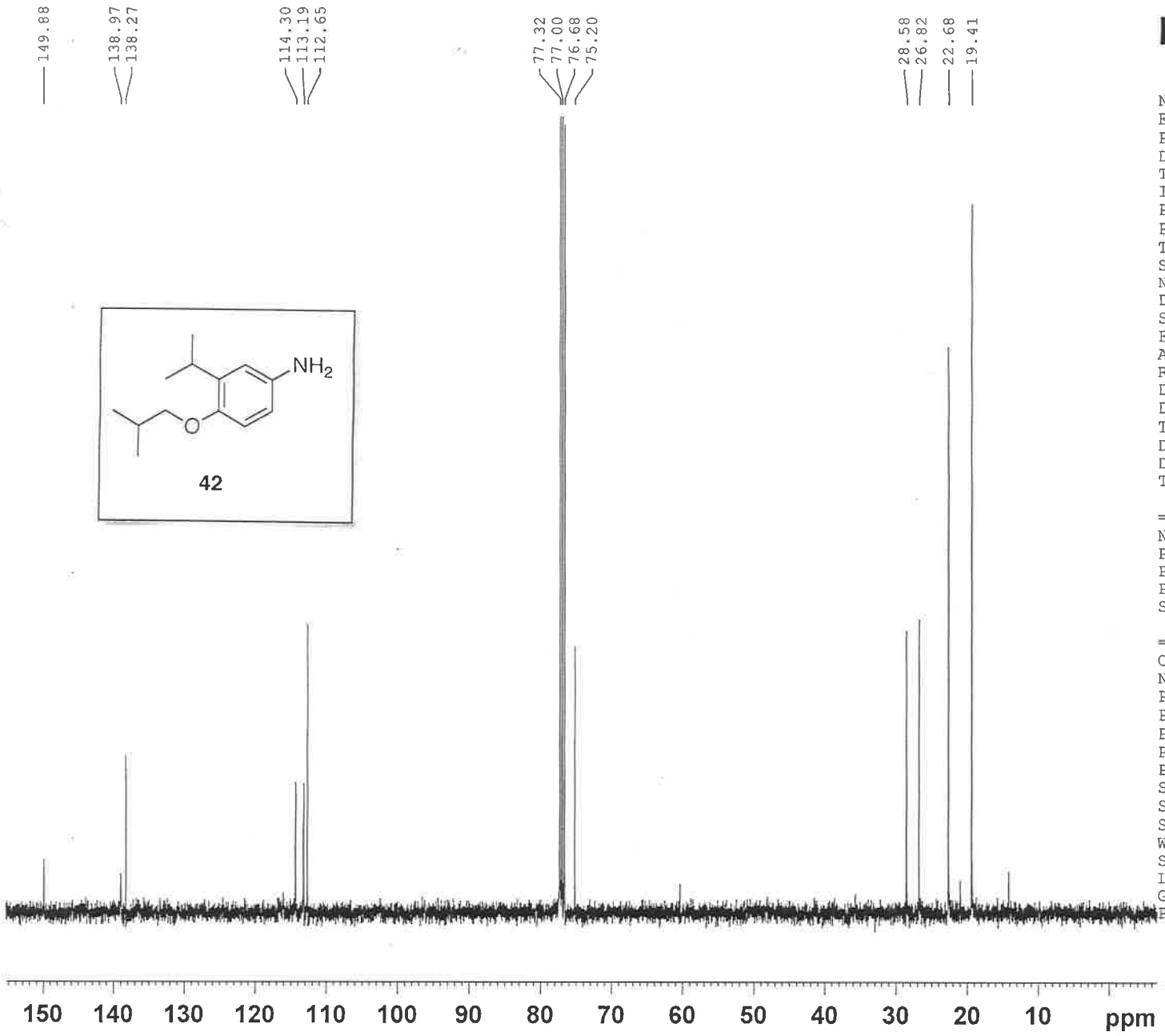
NAME	CWV-197
EXPNO	8
PROCNO	1
Date_	20150108
Time	9.54
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	63
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	298.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127722 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

CWV-199



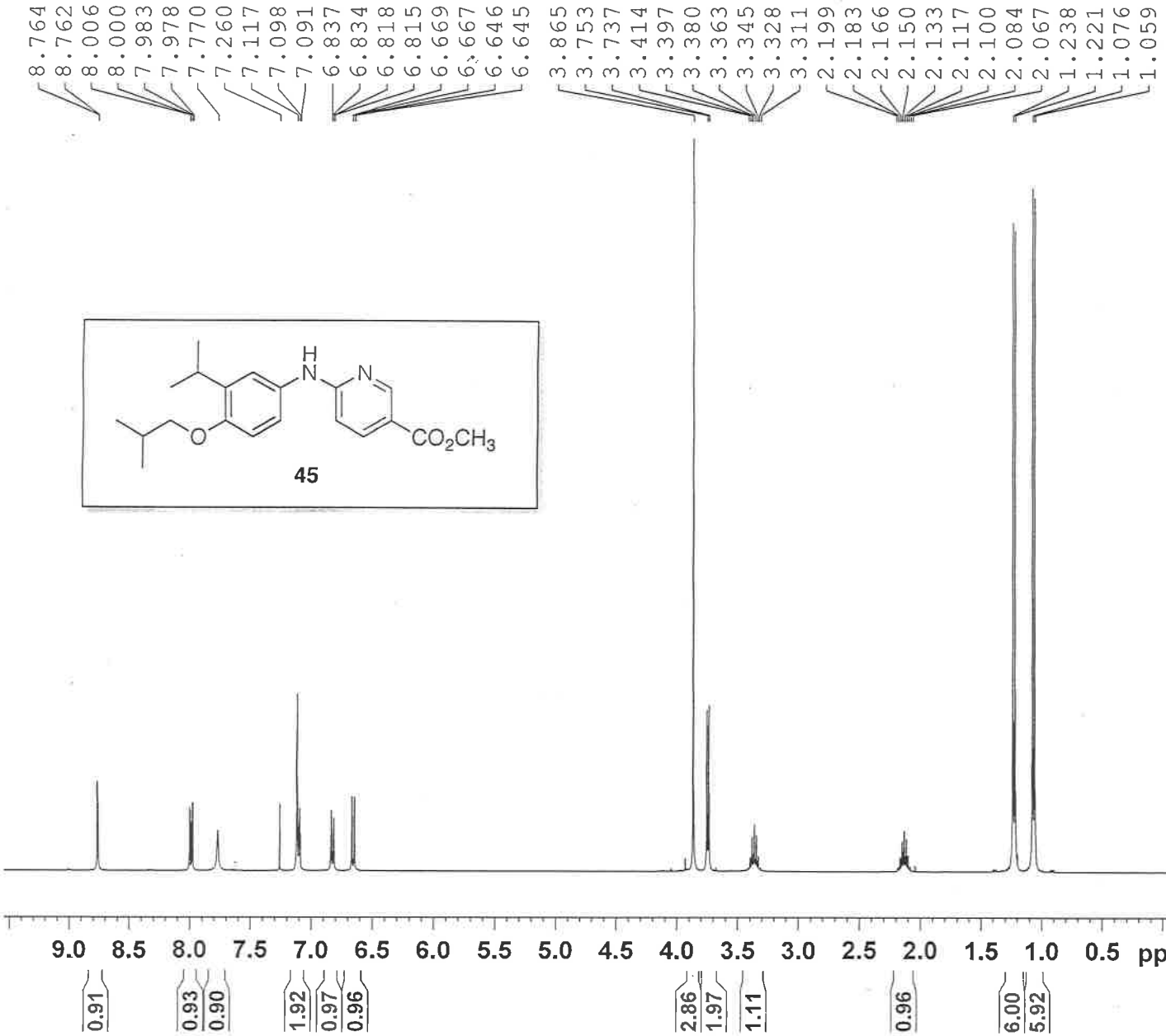
NAME	CWV-199
EXPNO	1
PROCNO	1
Date_	20150112
Time	15.06
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	298.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.00 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300099 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWV-199



NAME	CWV-199
EXPNO	2
PROCNO	1
Date_	20150112
Time	15.22
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	160
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	298.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127729 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

CWV-219



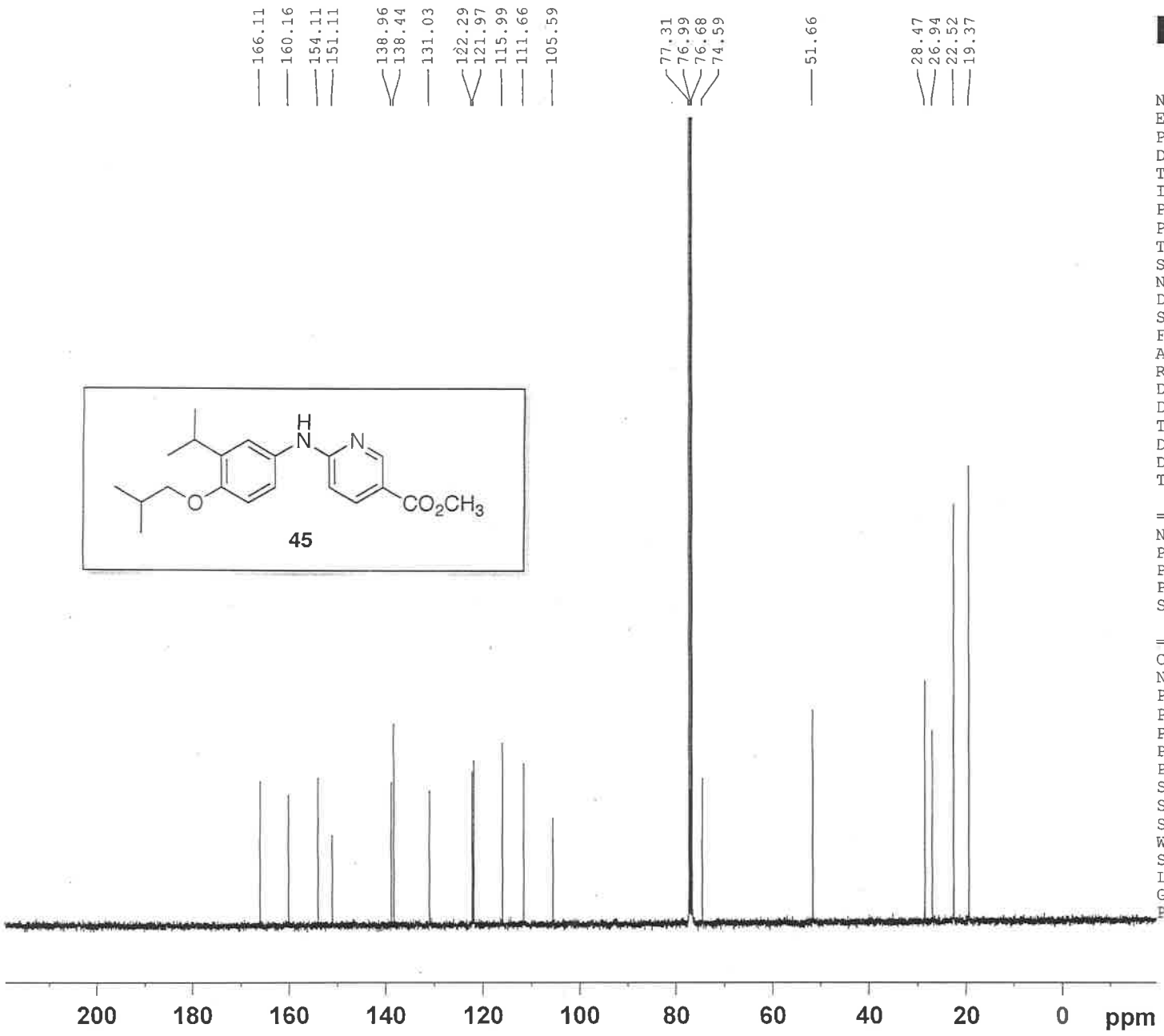
BRUKER

NAME	CWV-219
EXPNO	1
PROCNO	1
Date_	20150331
Time	12.26
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	298.2 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========

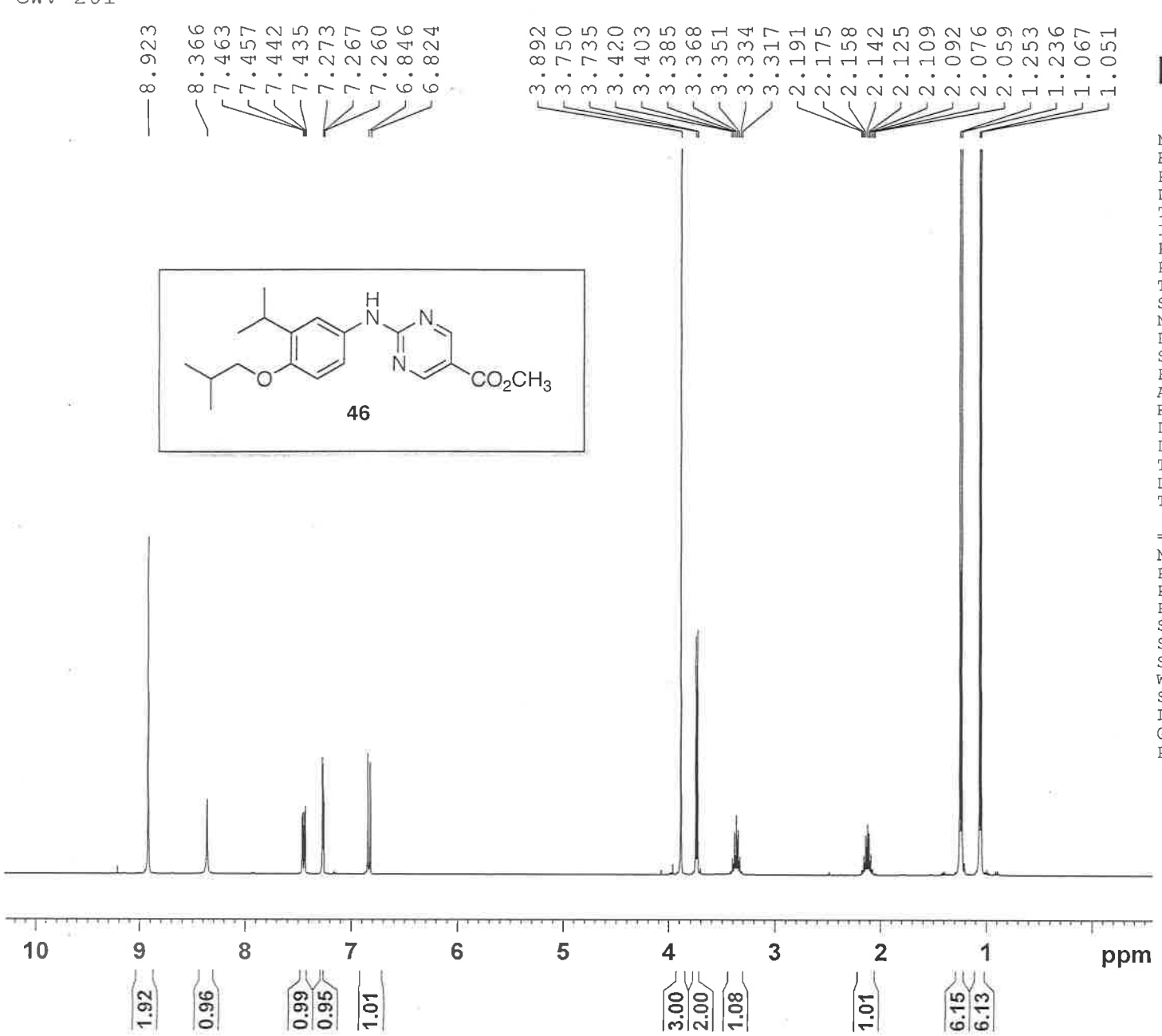
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300096 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWV-219



NAME	CWV-219
EXPNO	2
PROCNO	1
Date_	20150331
Time	12.32
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	298.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127729 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

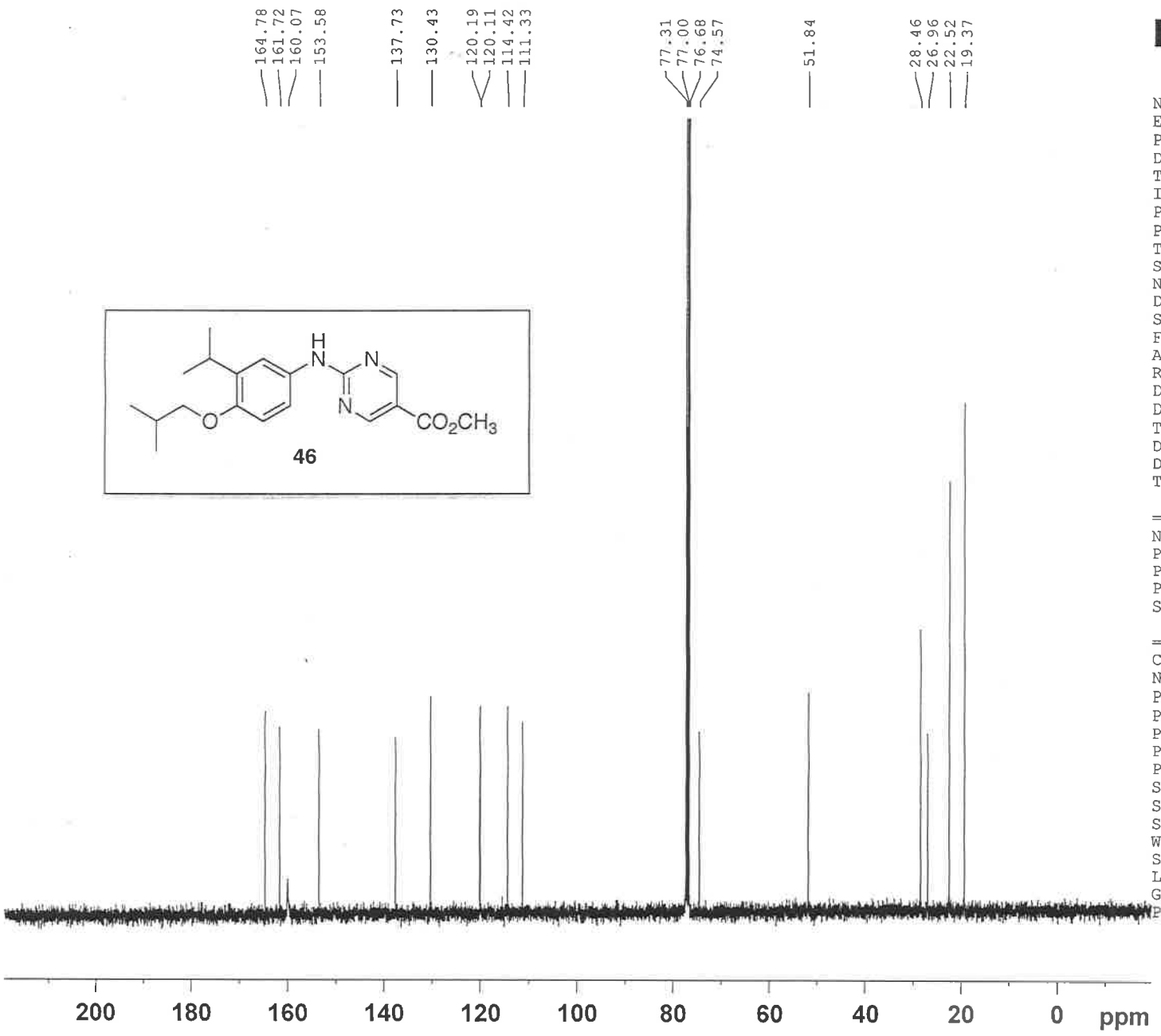
CWV-201



BRUKER

NAME	CWV-201
EXPNO	1
PROCNO	1
Date_	20150116
Time	16.58
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	298.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.00 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300099 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWV-201



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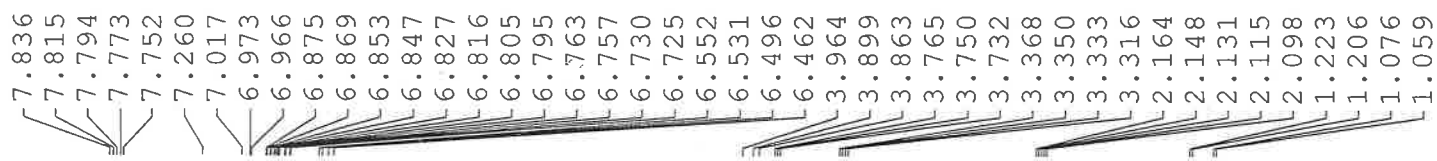
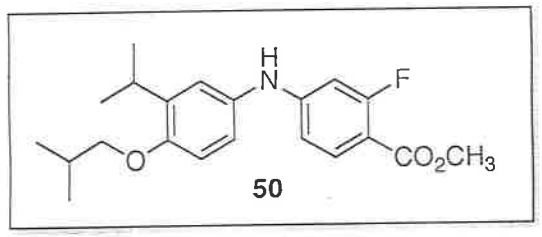
NAME	CWV-201
EXPNO	2
PROCNO	1
Date_	20150116
Time	17.07
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	208
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	298.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127736 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

CWV-215

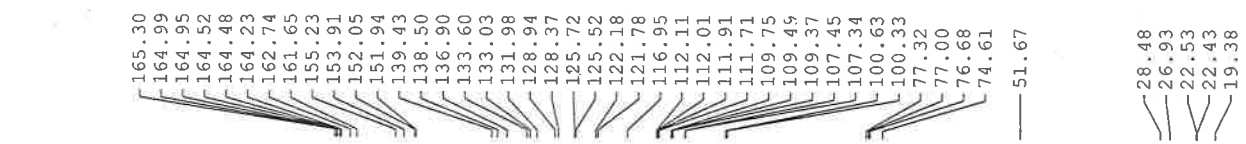


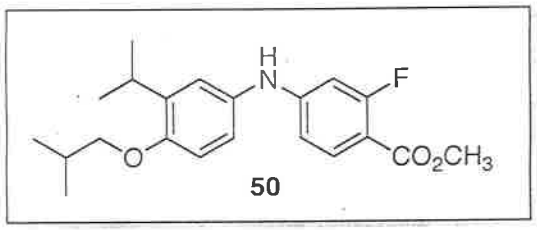


50

NAME	CWV-215
EXPNO	1
PROCNO	1
Date_	20150331
Time	13.42
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300096 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWV-215

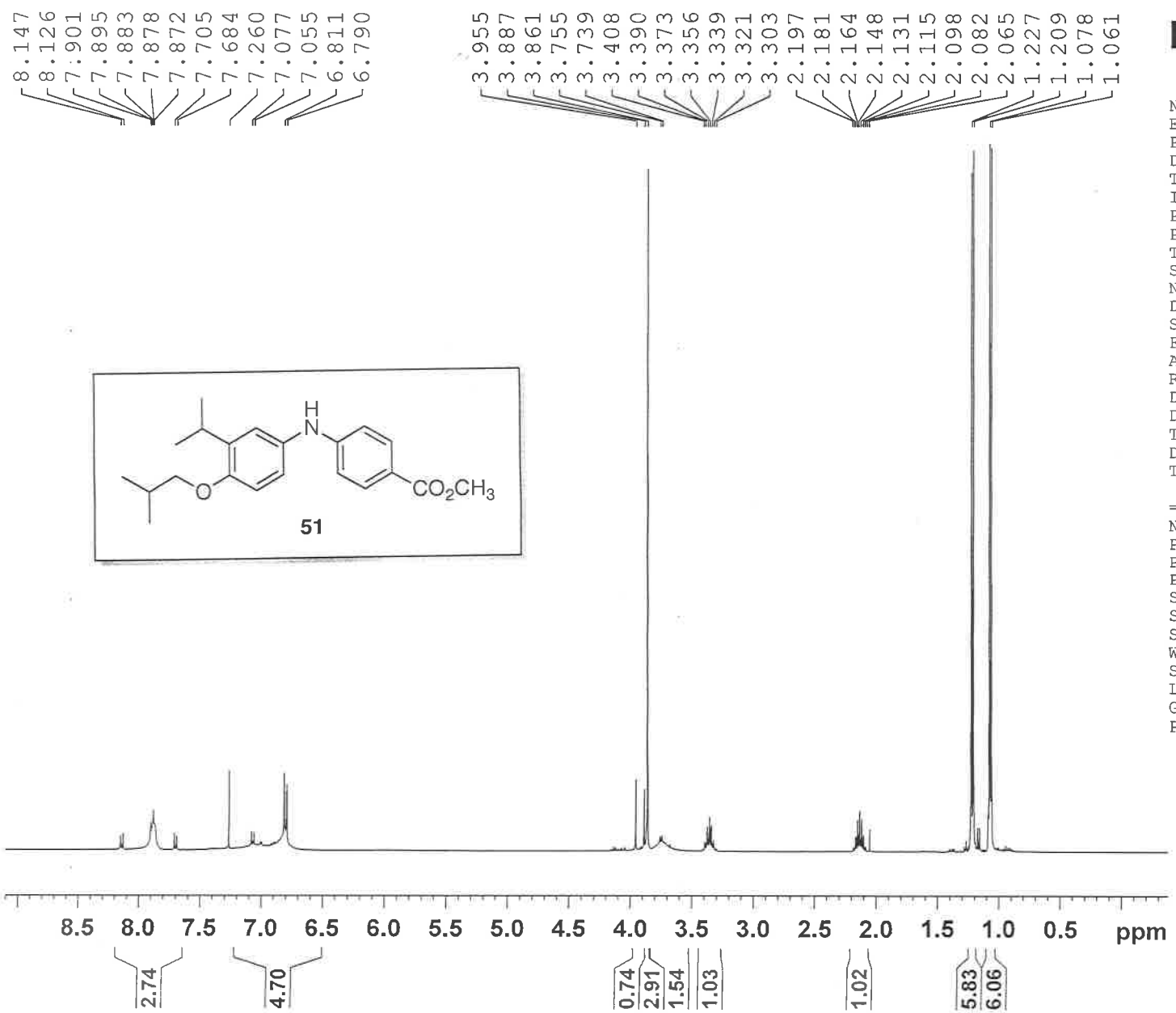




50

NAME	CWV-215
EXPNO	4
PROCNO	1
Date_	20150401
Time	8.55
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	2048
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	298.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127722 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

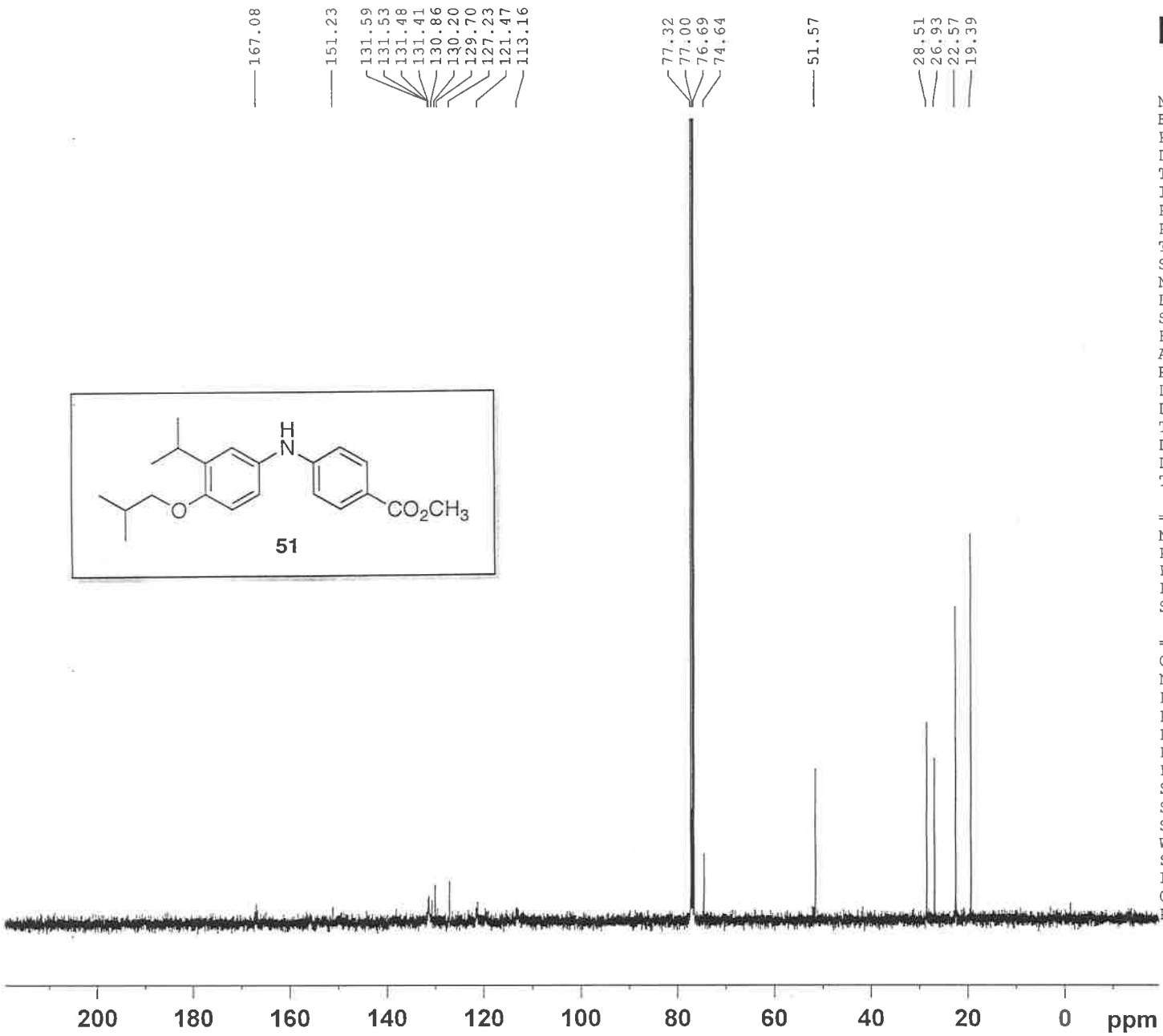
CWV-217



BRUKER

NAME	CWV-217
EXPNO	1
PROCNO	1
Date_	20150325
Time	17.50
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	298.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300096 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

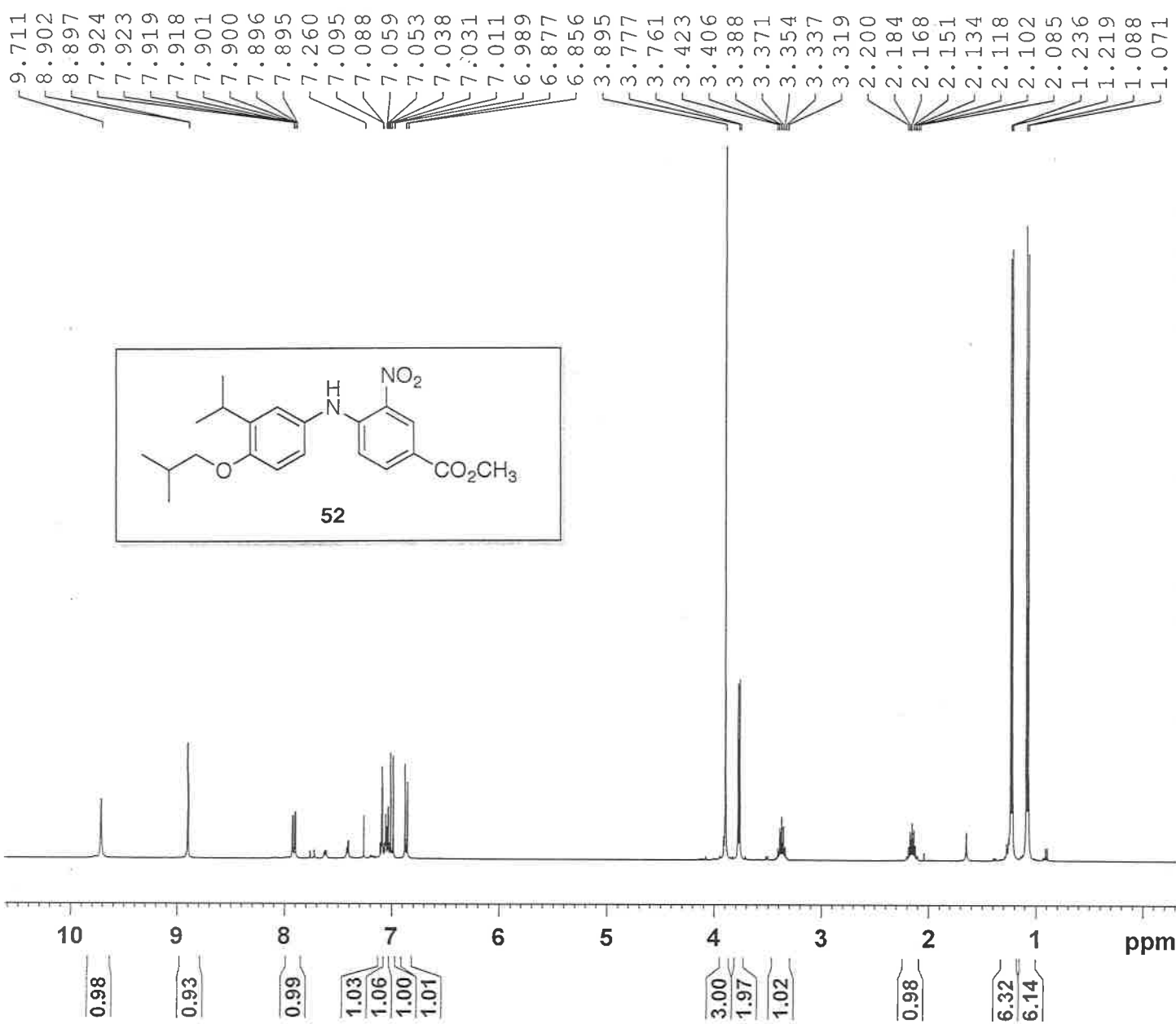
CWV-217



51

NAME	CWV-217
EXPNO	2
PROCNO	1
Date_	20150325
Time	18.20
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	365
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	298.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127722 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

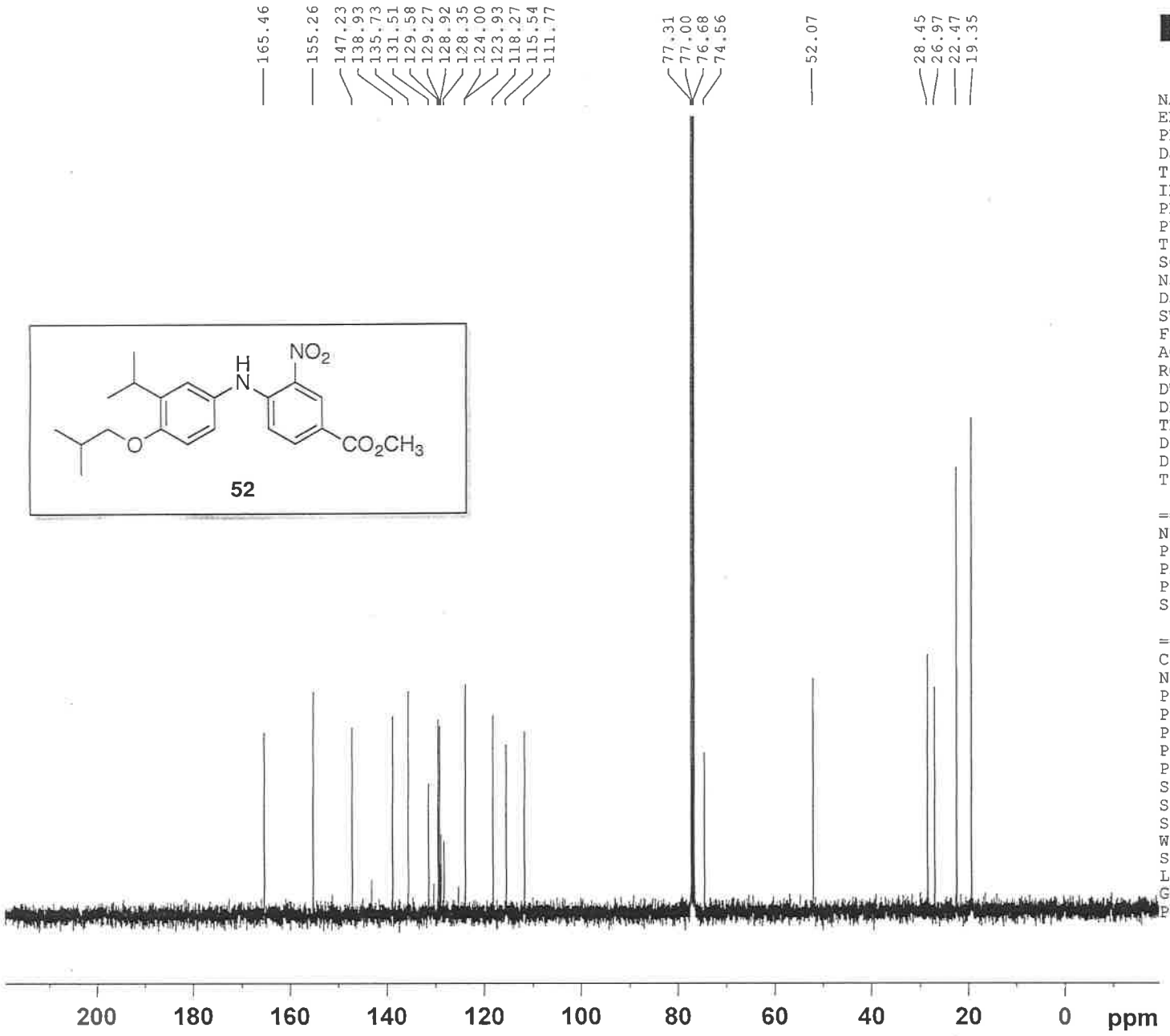
CWV-231



52

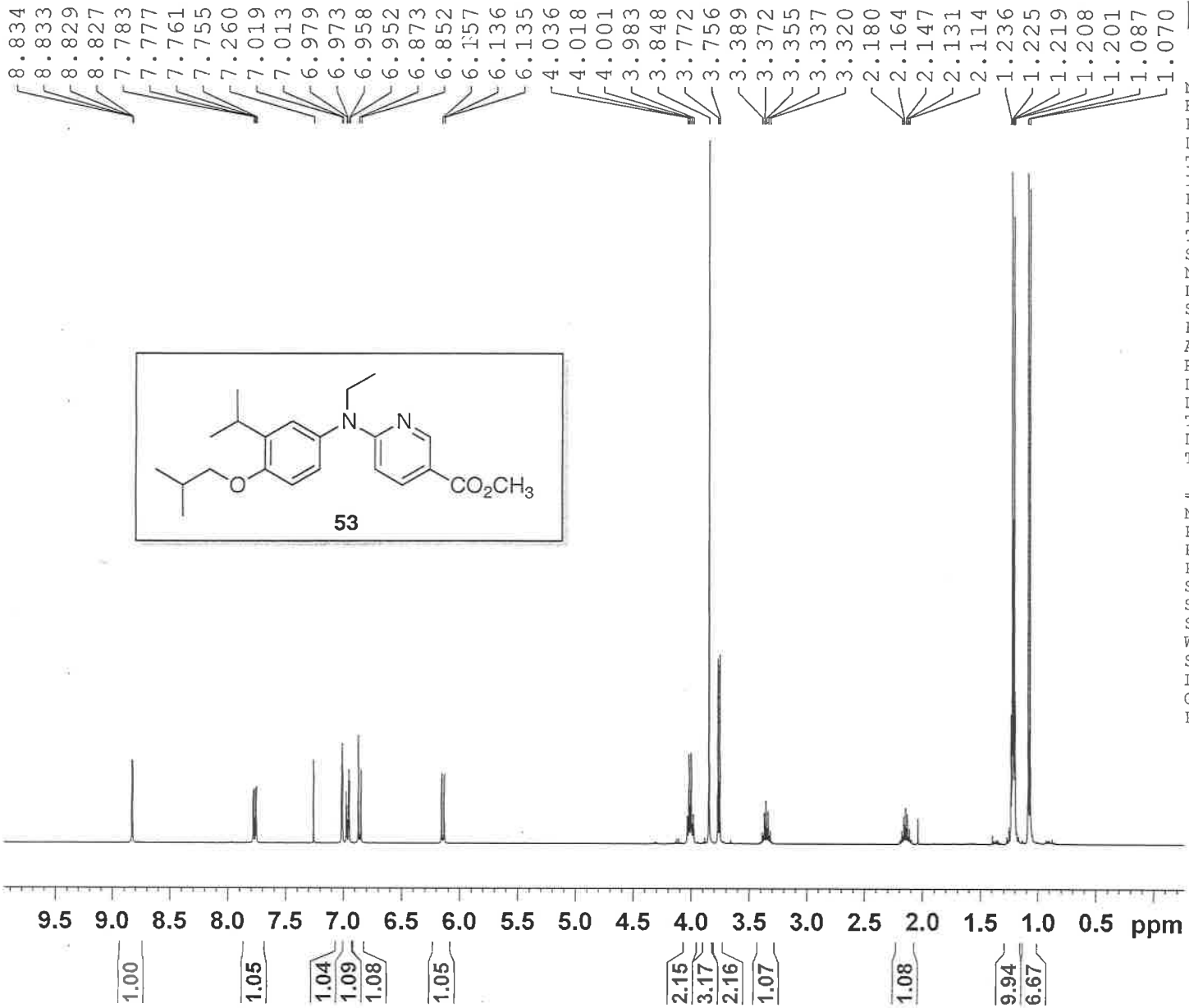
NAME	CWV-231
EXPNO	1
PROCNO	1
Date_	20150706
Time	9.23
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	298.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300099 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWV-231



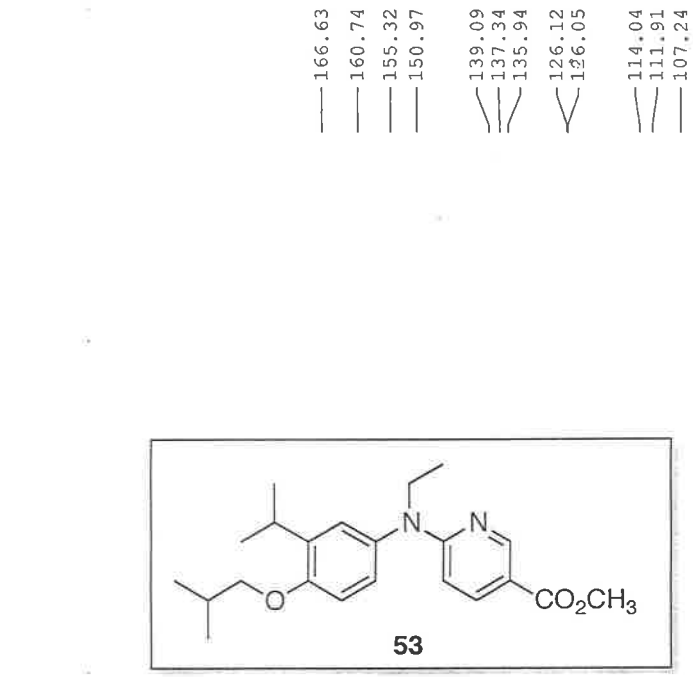
NAME	CWV-231
EXPNO	2
PROCNO	1
Date_	20150706
Time	9.32
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	158
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	298.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127736 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

CWV-221



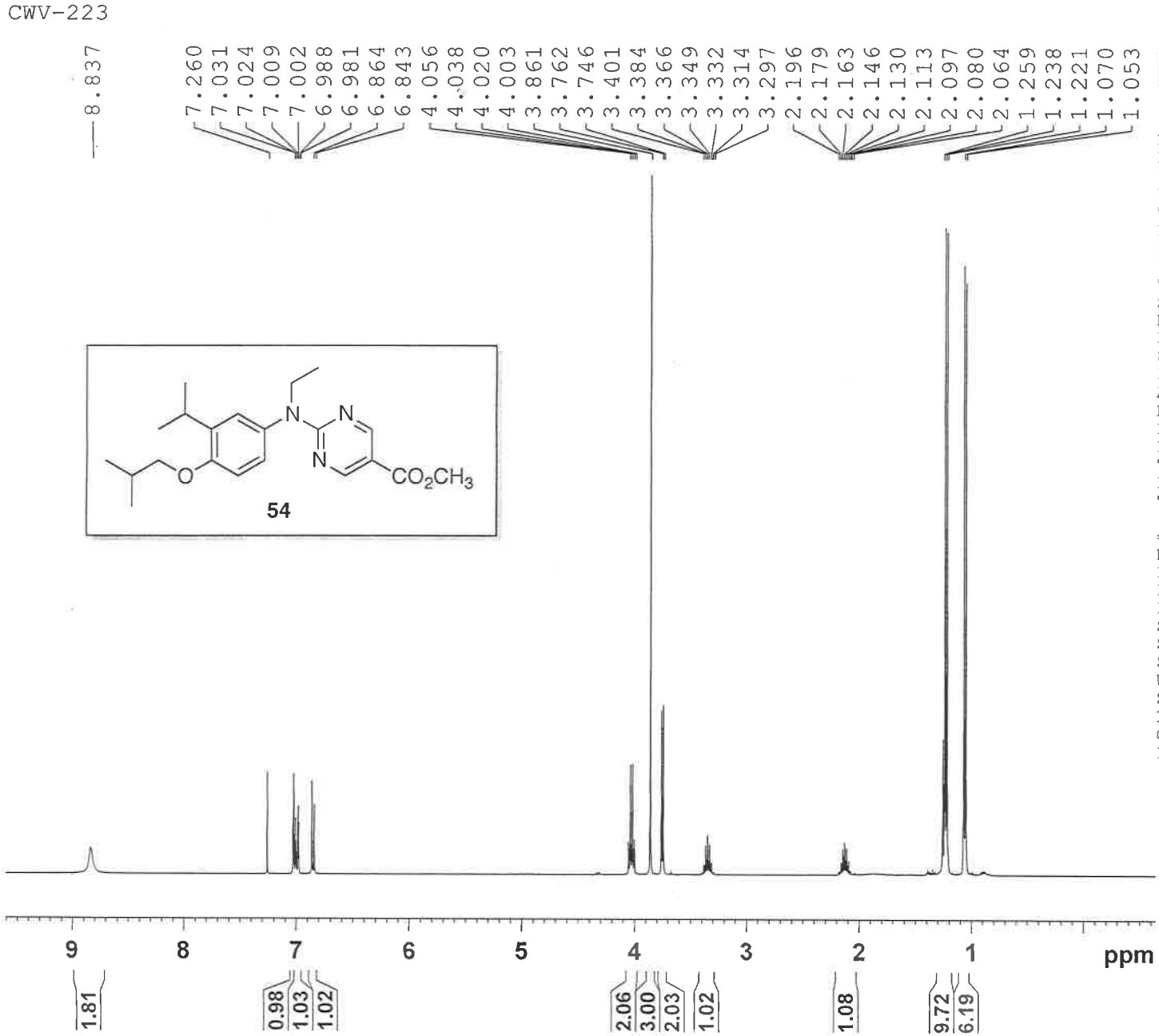
NAME	CWV-221
EXPNO	1
PROCNO	1
Date_	20150420
Time	13.00
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300096 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWV-221



NAME	CWV-221
EXPNO	2
PROCNO	1
Date_	20150420
Time	13.16
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	464
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	298.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127714 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

CWV-223



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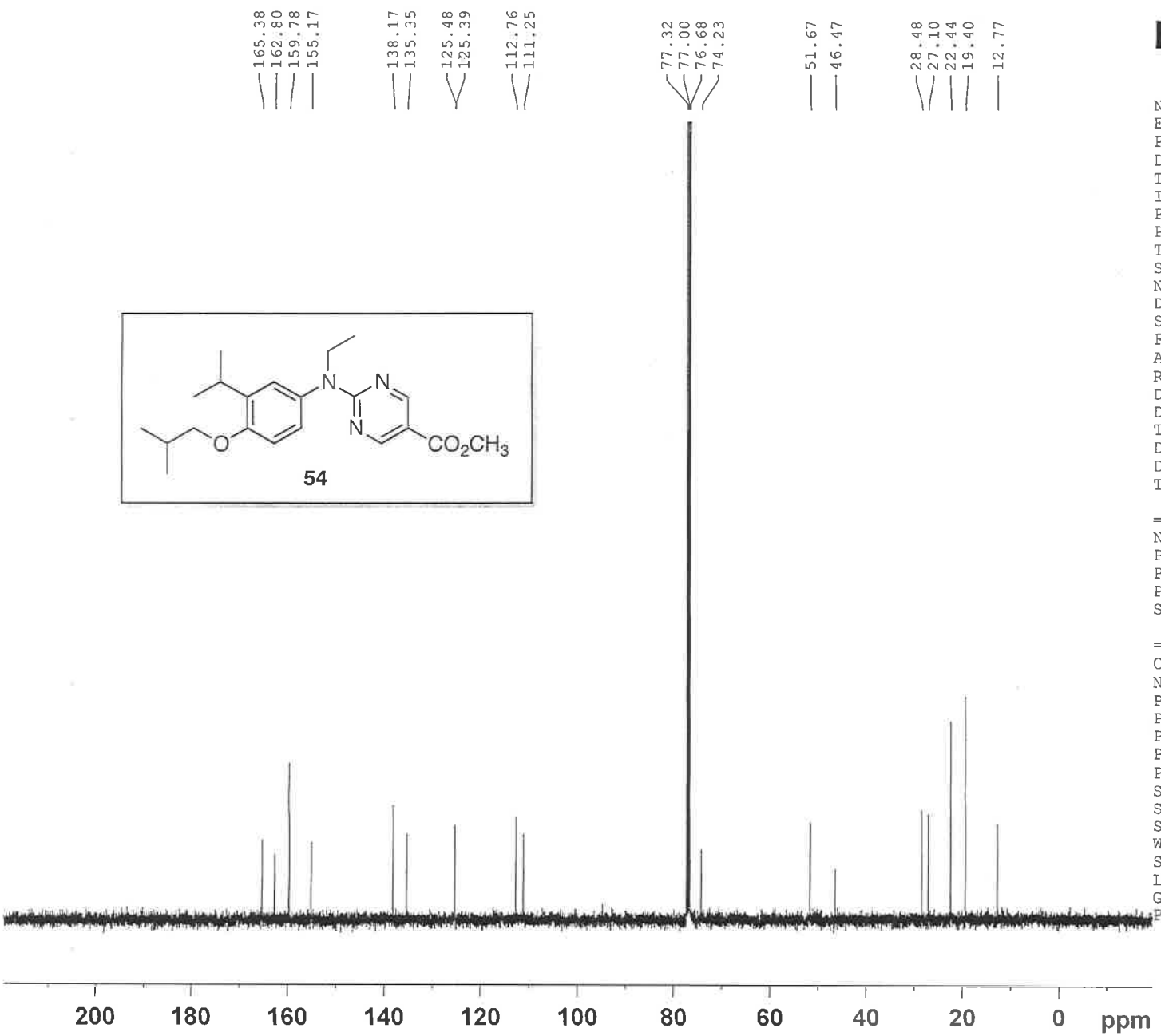
NAME	CWV-223
EXPNO	1
PROCNO	1
Date_	20150413
Time	12.17
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	298.2 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300096 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWV-223



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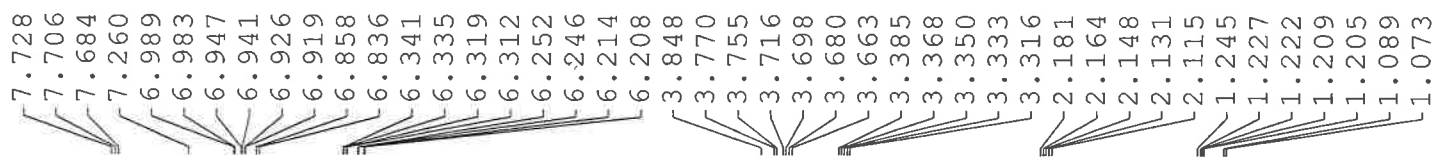
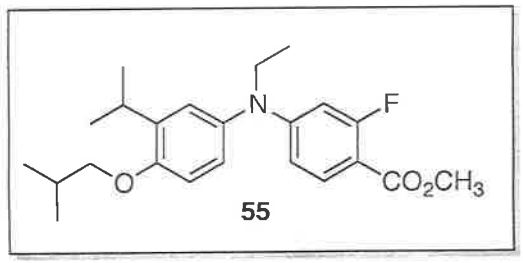
BRUKER

NAME	CWV-223
EXPNO	2
PROCNO	1
Date_	20150413
Time	12.37
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	284
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	298.6 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127714 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

CWV-229





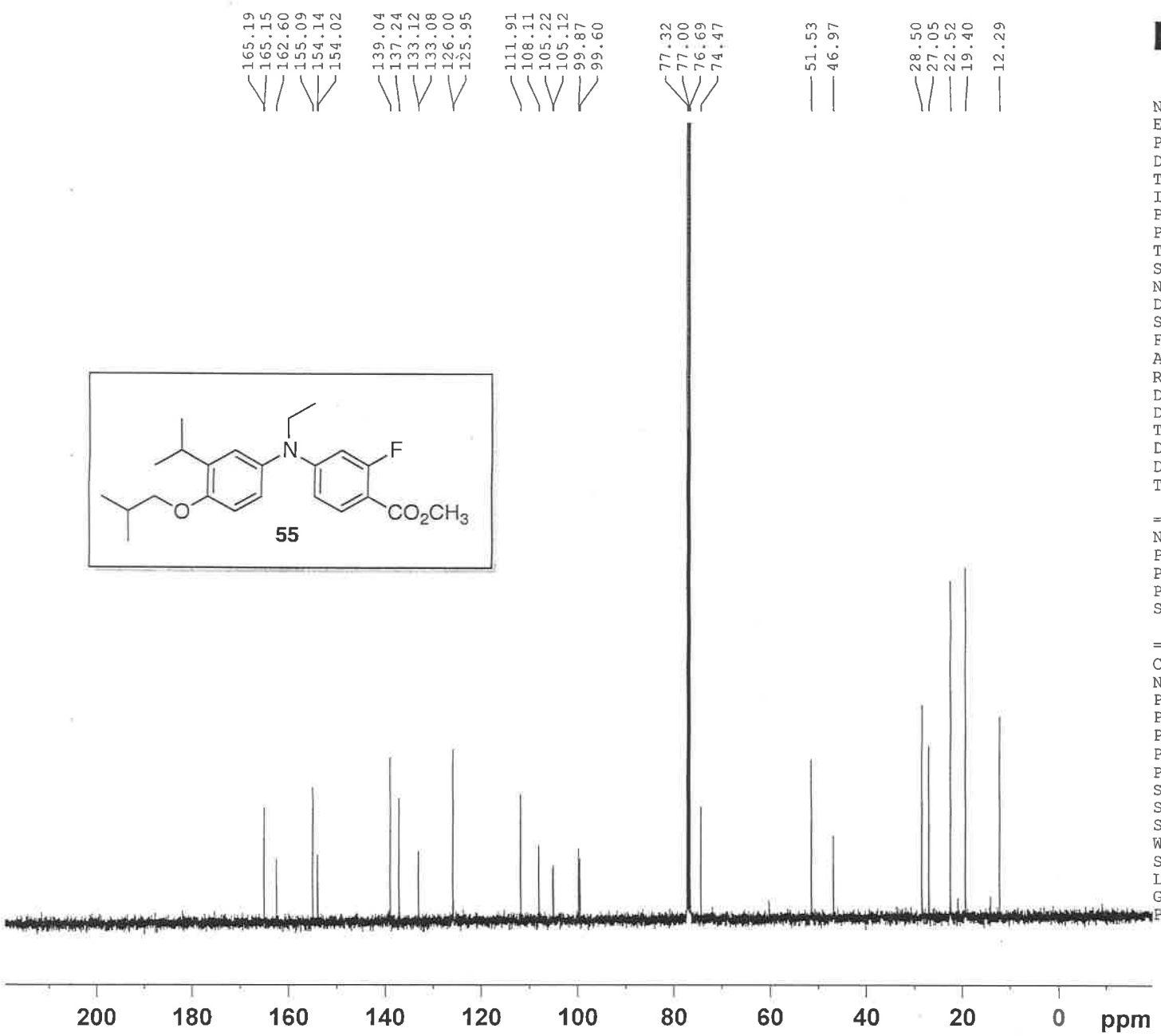
55

NAME	CWV-229
EXPNO	1
PROCNO	1
Date_	20150420
Time	11.56
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	298.2 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300096 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

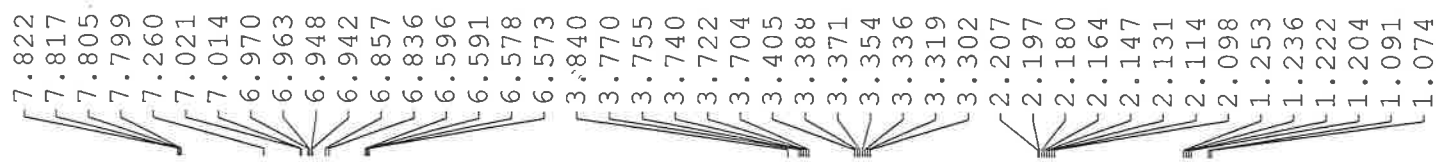
CWV-229

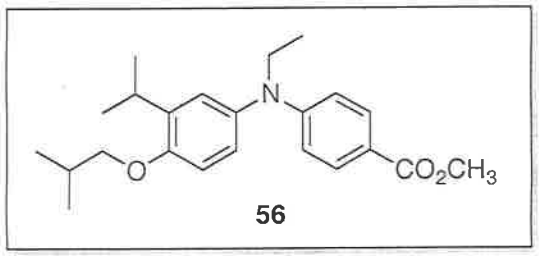


BRUKER

NAME	CWV-229
EXPNO	2
PROCNO	1
Date_	20150420
Time	12.14
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	376
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	298.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127714 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

CWV-227

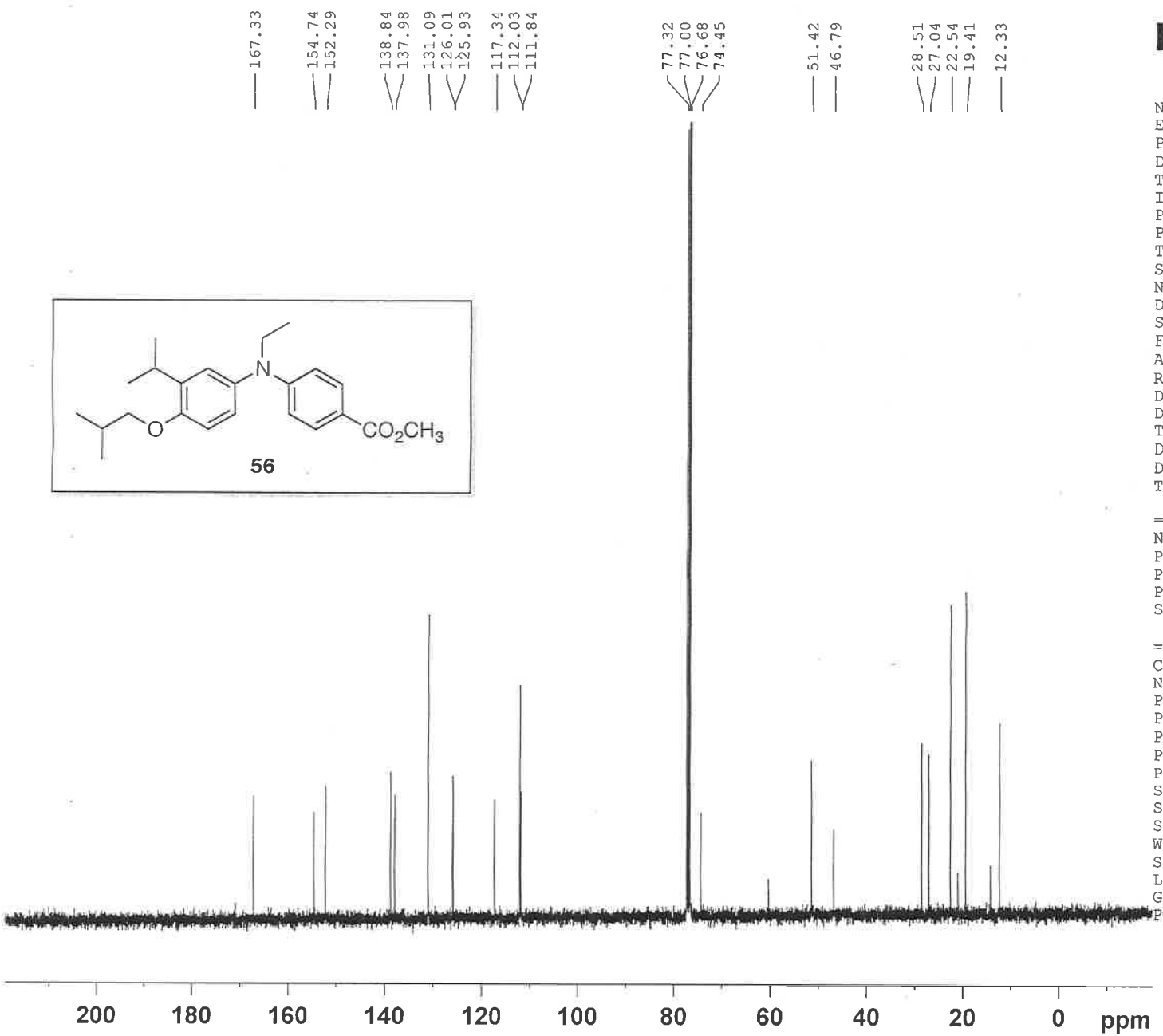




56

NAME	CWV-227
EXPNO	1
PROCNO	1
Date_	20150420
Time	12.27
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300096 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWV-227



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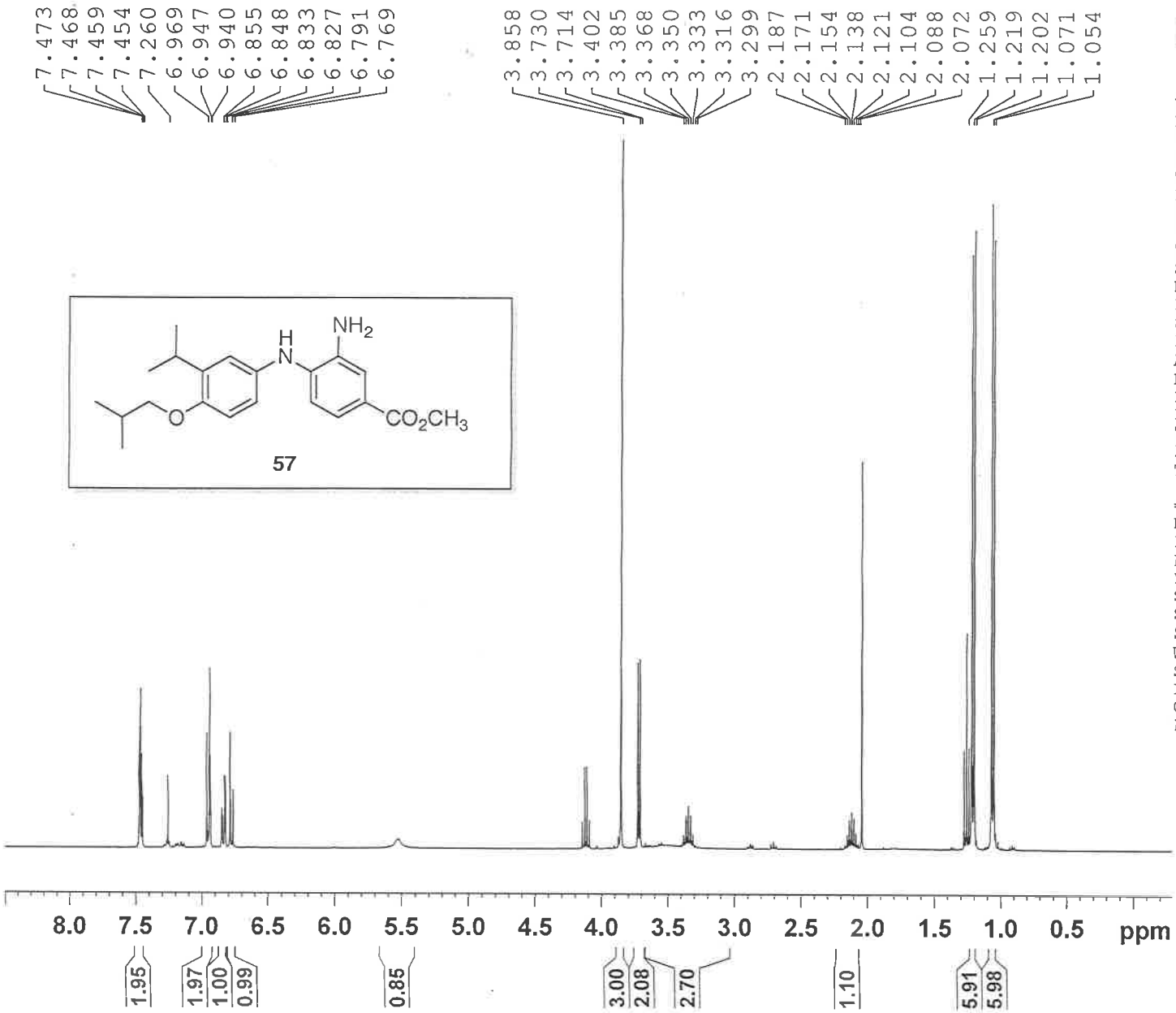
BRUKER

NAME	CWV-227
EXPNO	2
PROCNO	1
Date_	20150420
Time	12.45
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	267
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	298.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127722 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

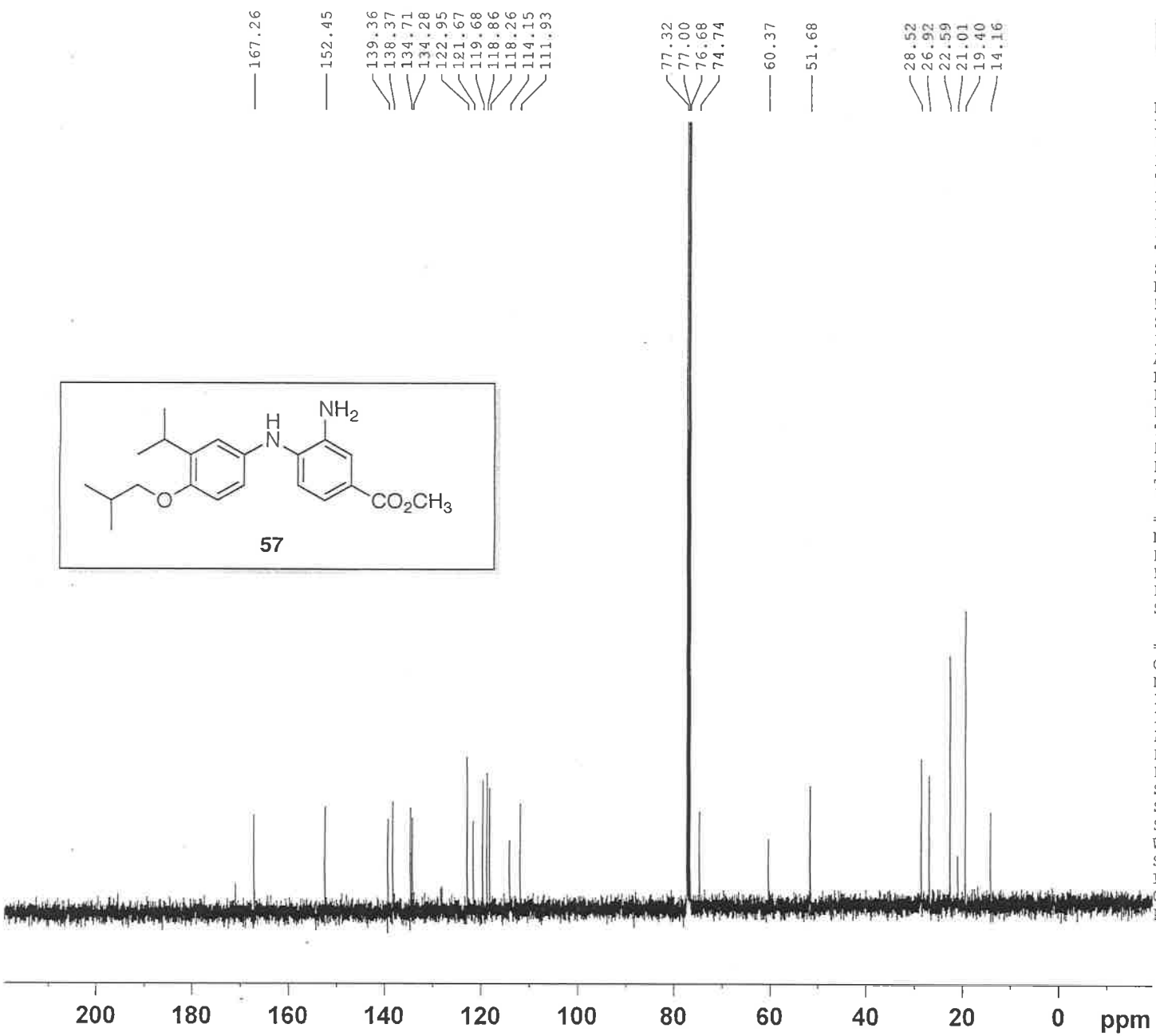
CWV-235



BRUKER

NAME	CWV-235
EXPNO	1
PROCNO	1
Date_	20150706
Time	15.52
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	298.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300099 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWV-235



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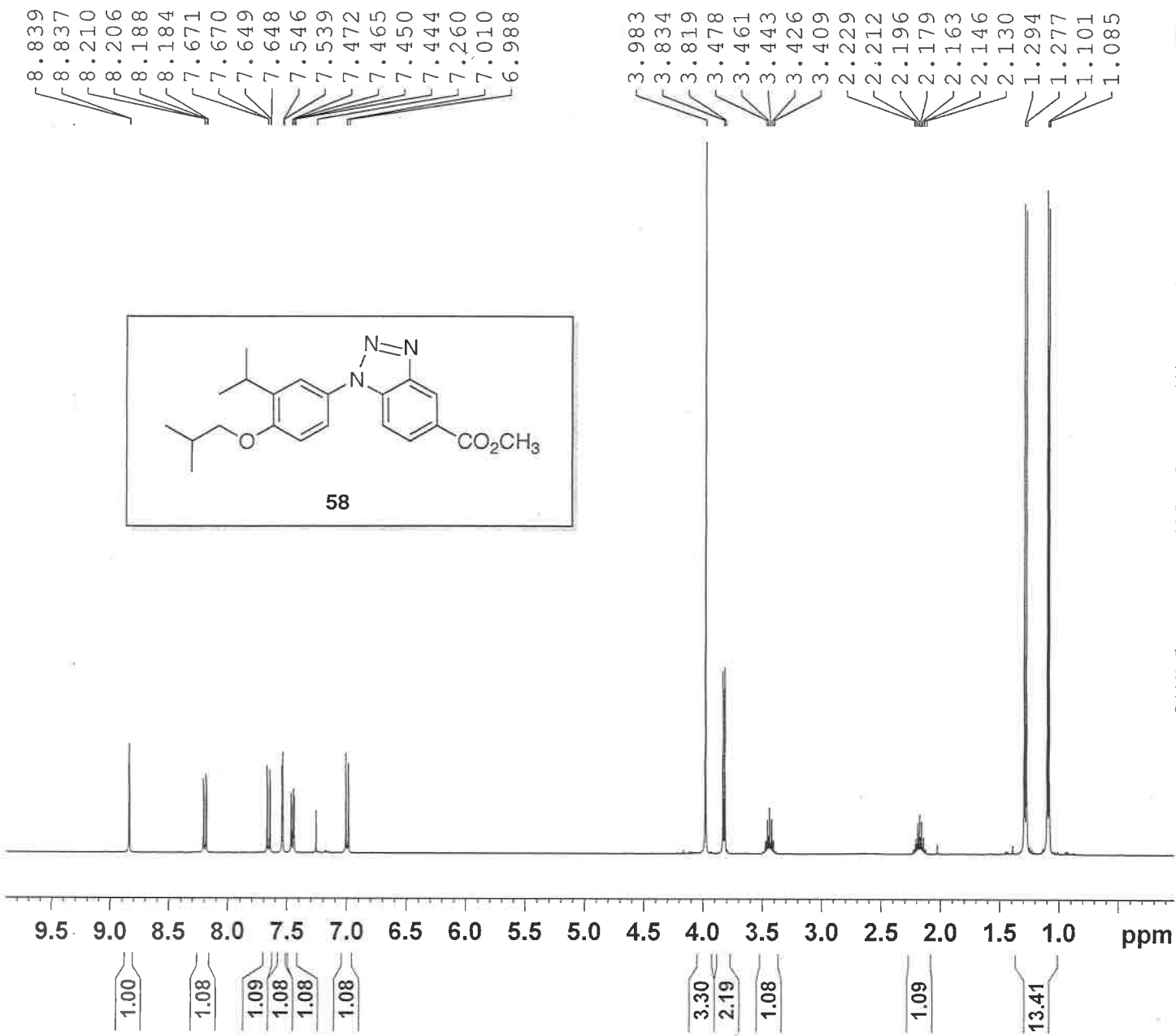
BRUKER

NAME	CWV-235
EXPNO	2
PROCNO	1
Date_	20150706
Time	15.59
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	118
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	298.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127729 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

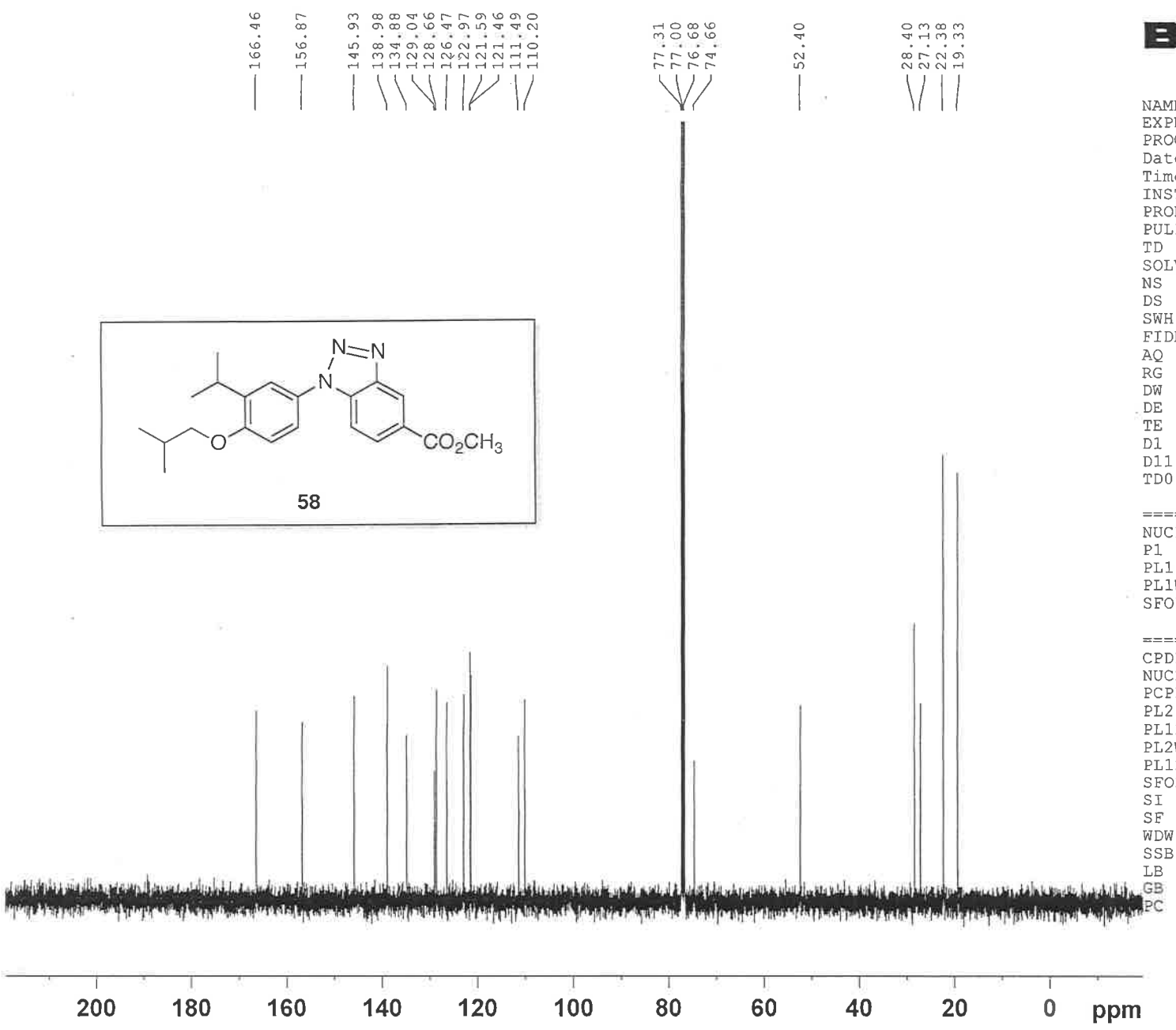
CWI-237



BRUKER

NAME	CWV-237
EXPNO	1
PROCNO	1
Date_	20150805
Time	16.05
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	298.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300096 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

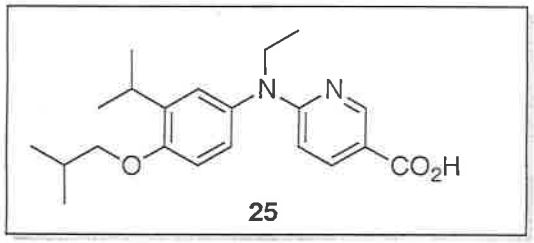
CWI-237



NAME	CWV-237
EXPNO	2
PROCNO	1
Date_	20150805
Time	16.20
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	63
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	298.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127744 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

CWV-253

8.927 8.922 8.921 7.842 7.836 7.819 7.813 7.260 7.030 7.024 6.991 6.985 6.970 6.964 6.886 6.865 6.187 6.164 4.064 4.046 4.029 4.011 3.779 3.763 3.397 3.380 3.362 3.345 3.328 3.311 2.202 2.186 2.169 2.153 2.136 2.120 2.103 1.258 1.240 1.235 1.222 1.217 1.091 1.075



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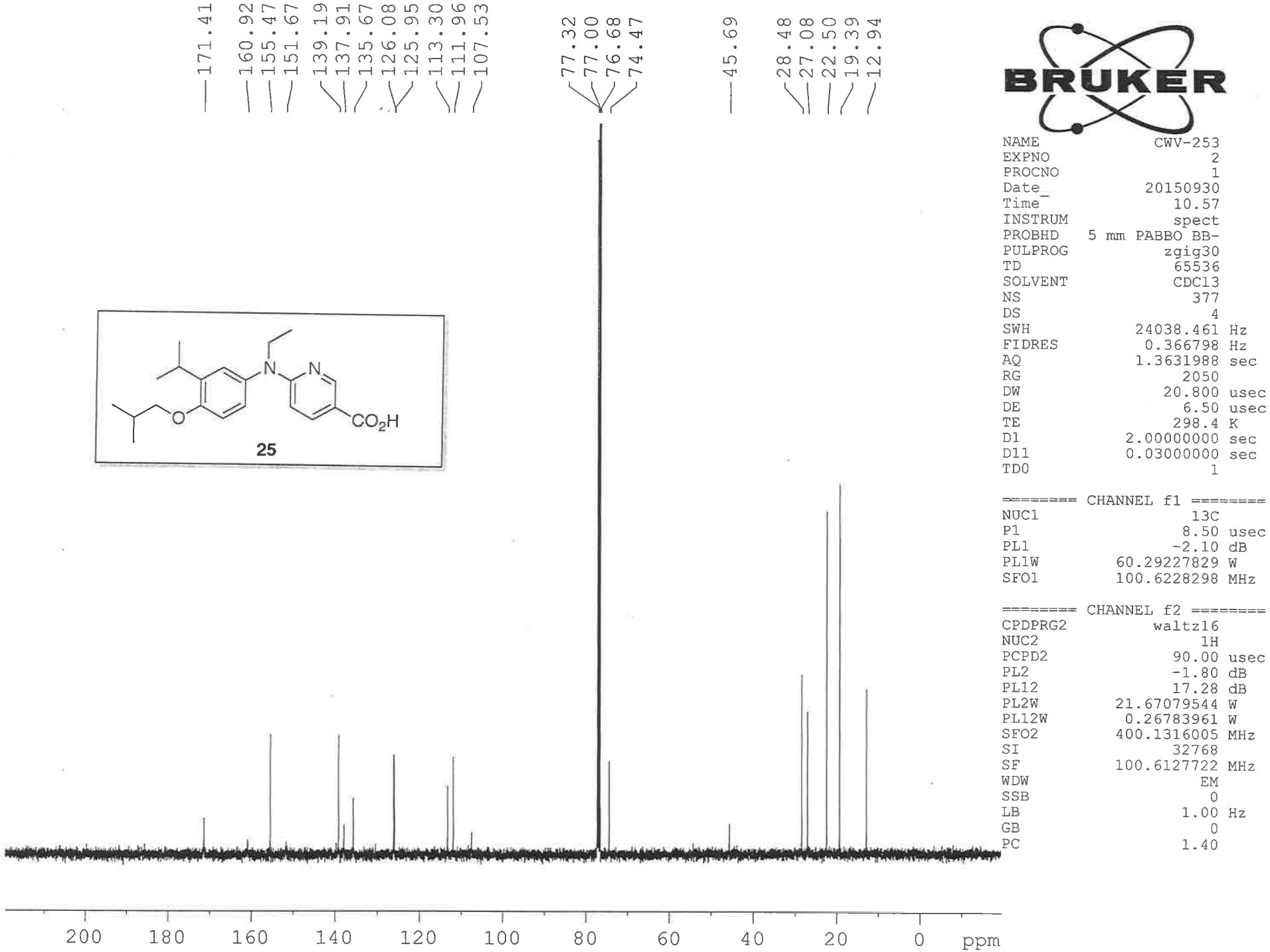
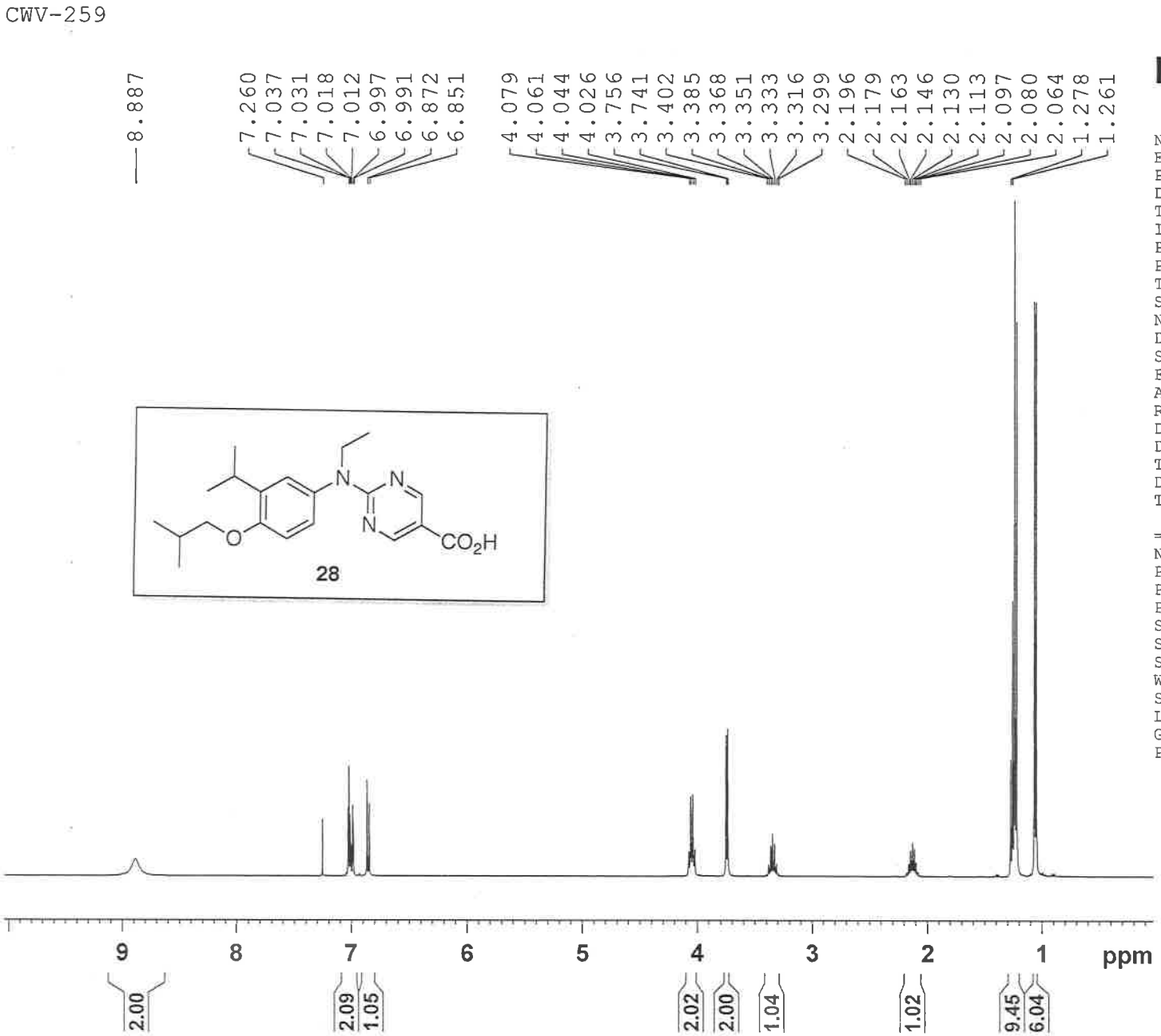
NAME	CWV-253
EXPNO	1
PROCNO	1
Date_	20150930
Time	10.46
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	298.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300099 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWV-253



NAME	CWV-253
EXPNO	2
PROCNO	1
Date_	20150930
Time	10.57
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	377
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	298.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127722 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

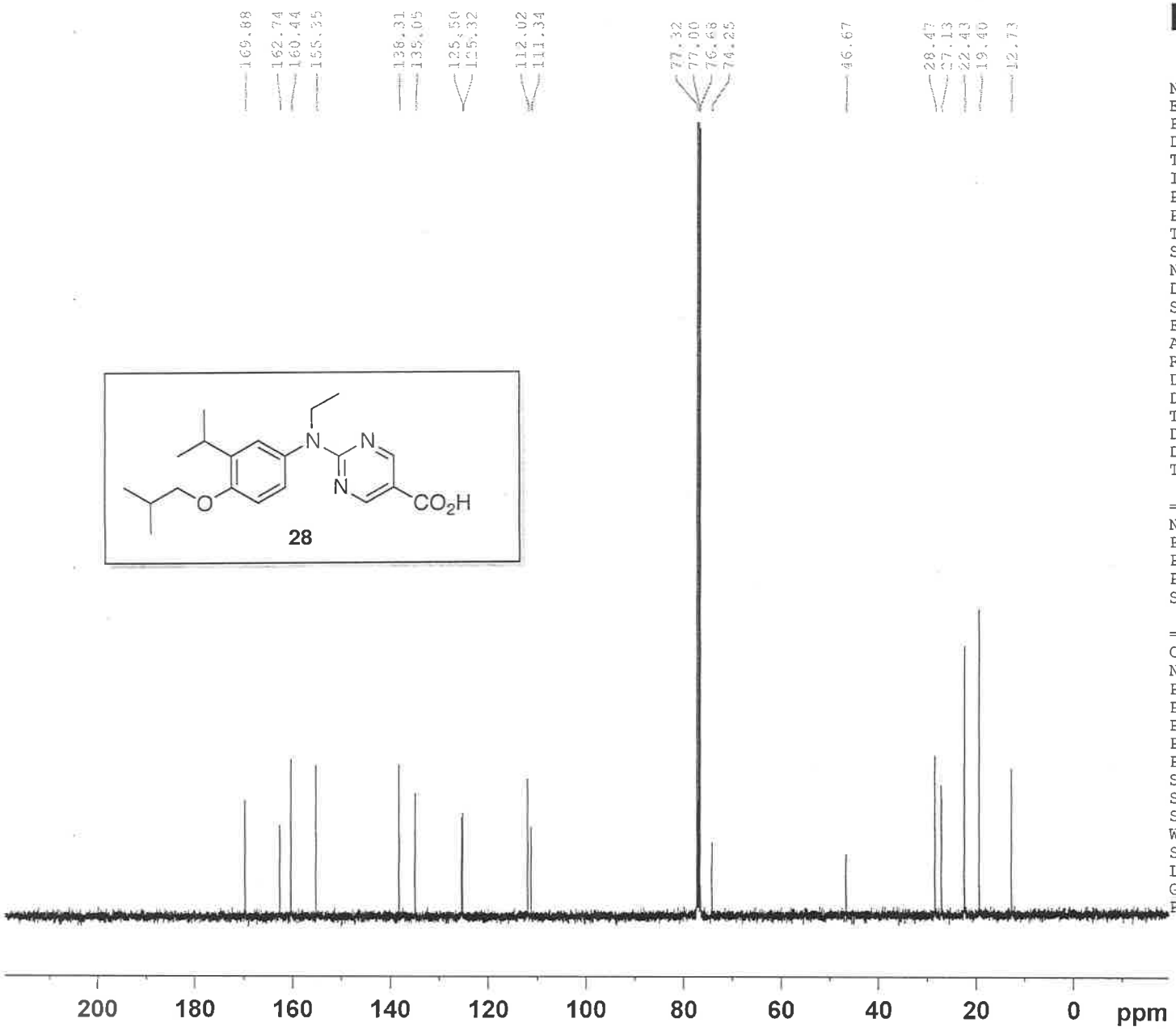
CWV-259



BRUKER

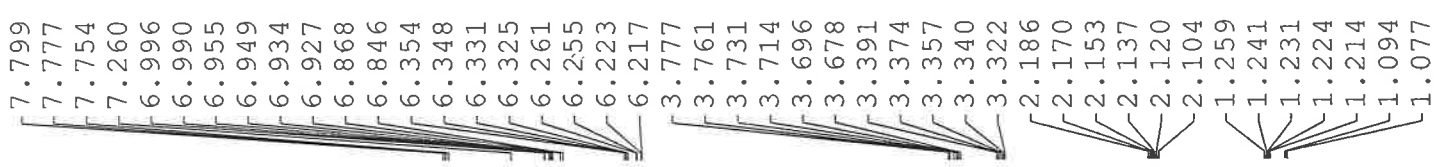
NAME	CWV-259
EXPNO	1
PROCNO	1
Date_	20150930
Time	11.15
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300096 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

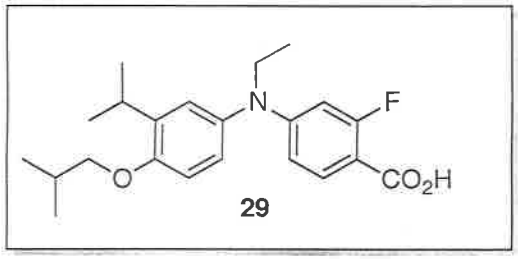
CWV-259



NAME	CWV-259
EXPNO	2
PROCNO	1
Date_	20150930
Time	11.36
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	467
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	298.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127722 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

CWV-265

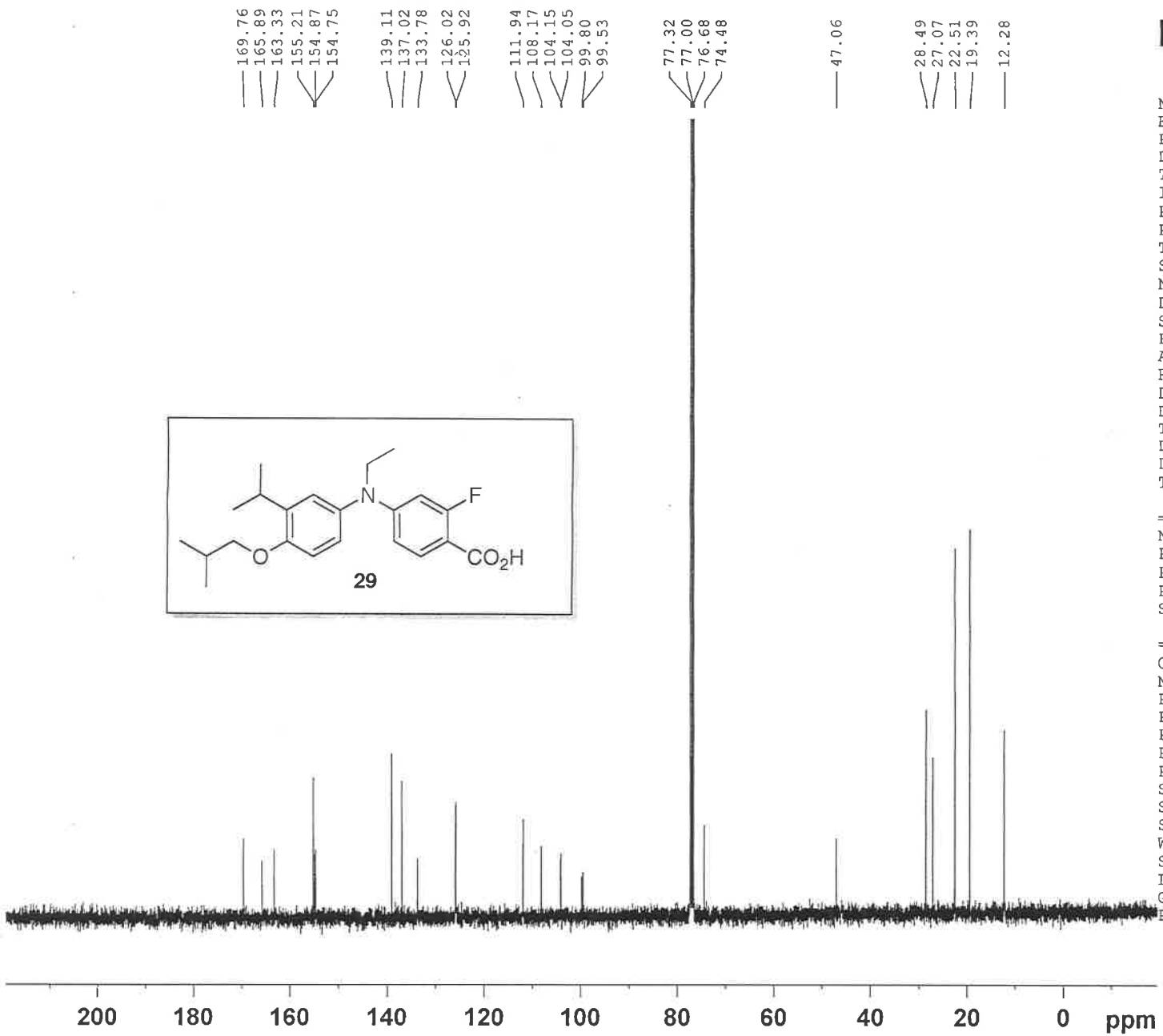




29

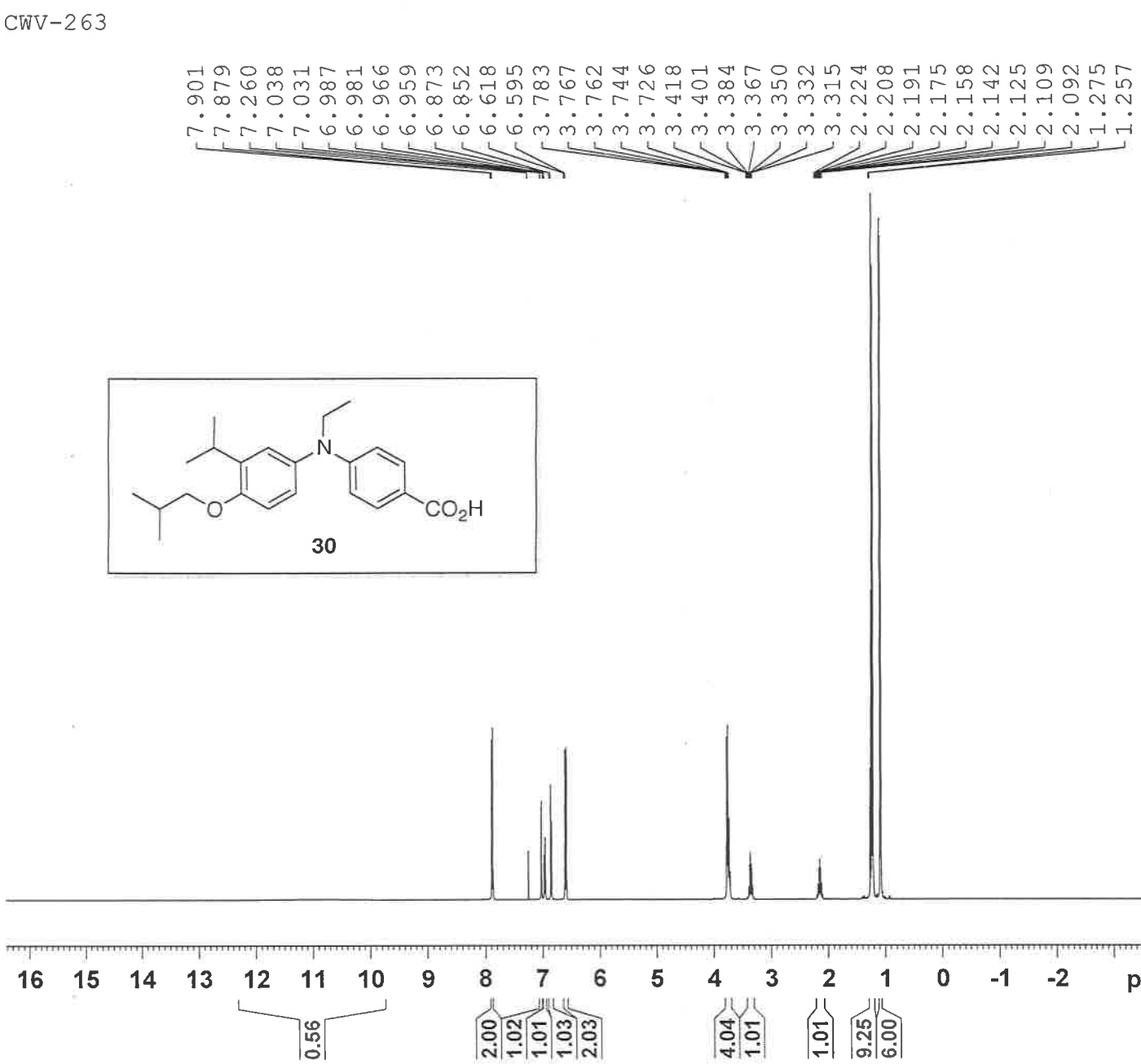
NAME	CWV-265
EXPNO	1
PROCNO	1
Date_	20150930
Time	12.28
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	298.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300099 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWV-265



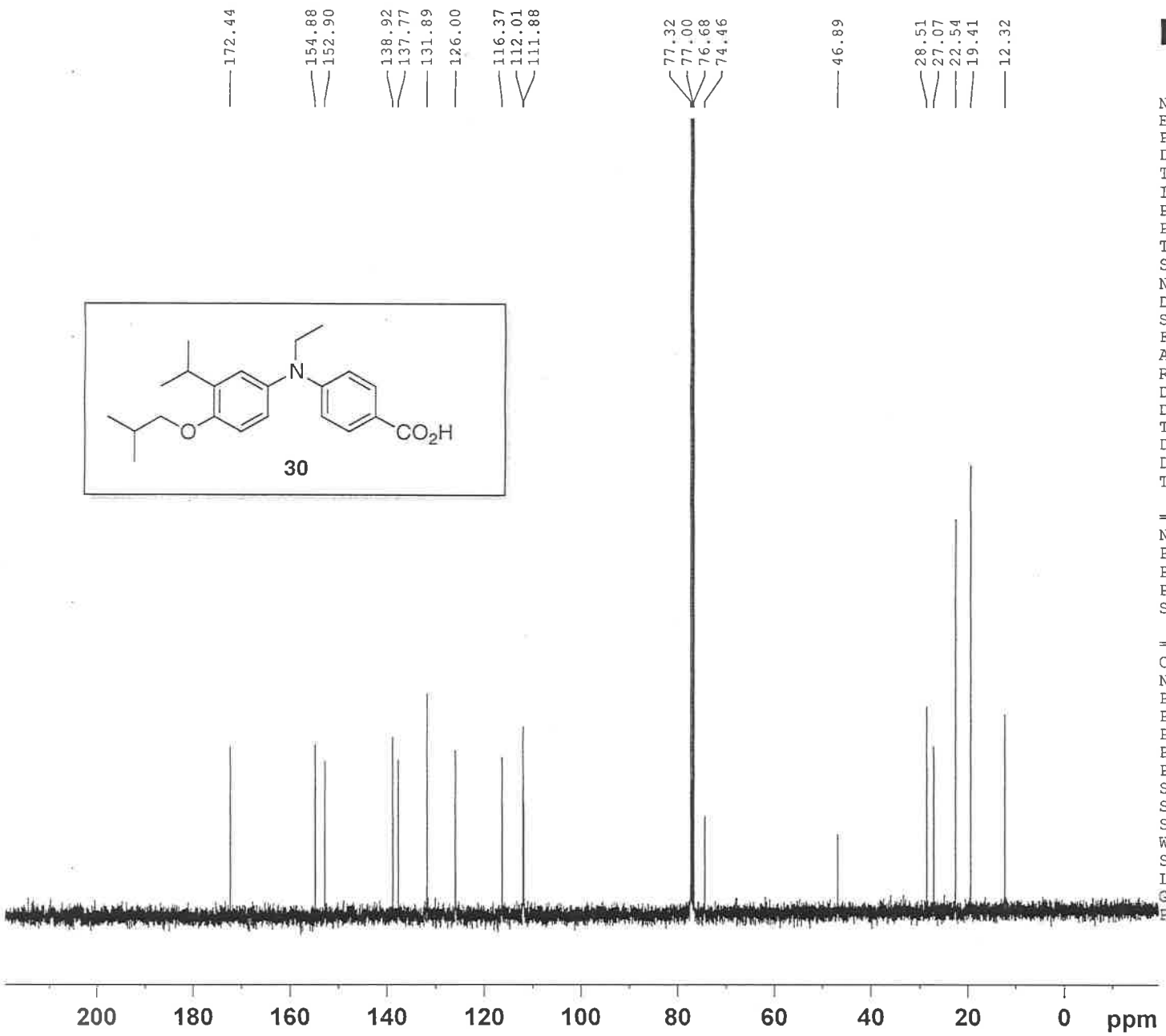
NAME	CWV-265
EXPNO	2
PROCNO	1
Date_	20150930
Time	12.37
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	207
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	298.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127722 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

CWV-263



NAME	CWV-263
EXPNO	1
PROCNO	1
Date_	20150930
Time	11.54
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	297.9 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300099 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

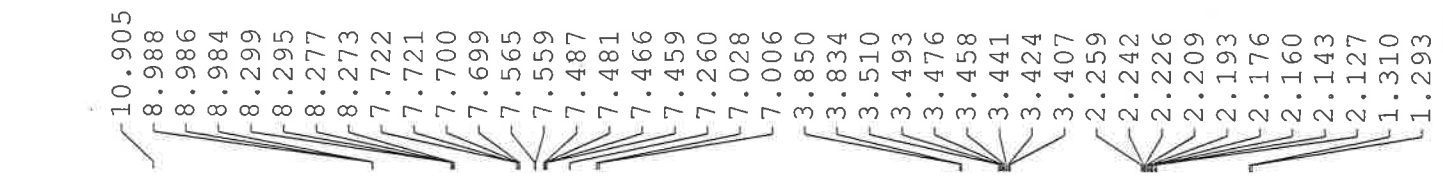
CWV-263

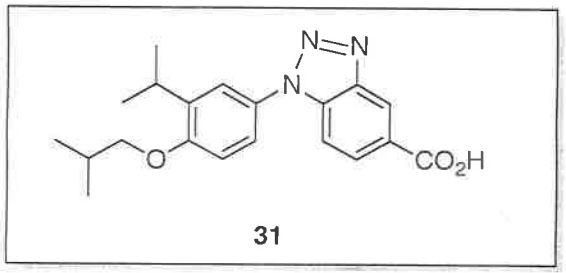


BRUKER

NAME	CWV-263
EXPNO	3
PROCNO	1
Date_	20150930
Time	12.13
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	155
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	298.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127729 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

CWV-267

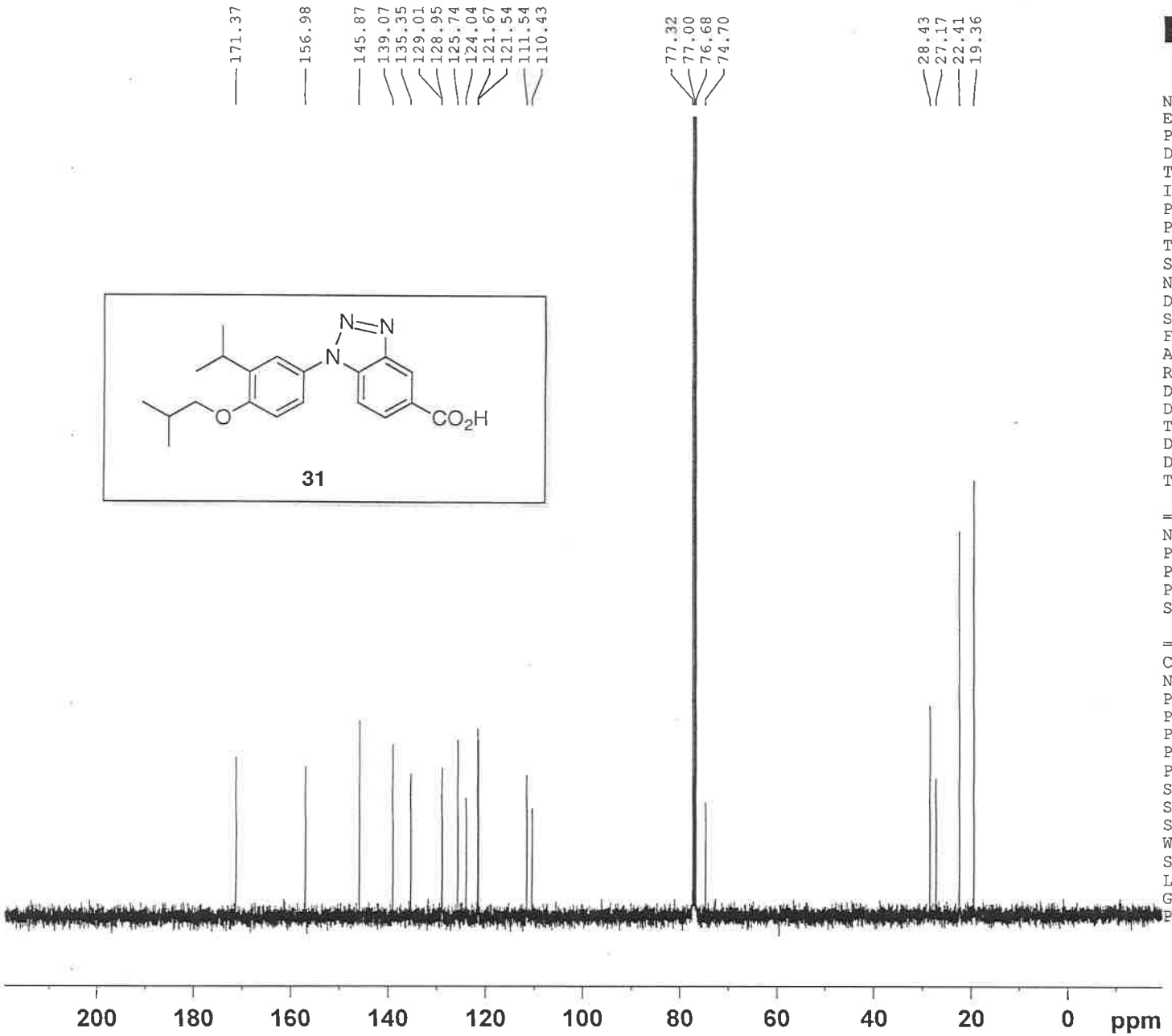




31

NAME	CWV-267
EXPNO	1
PROCNO	1
Date_	20150930
Time	12.47
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	298.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300096 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

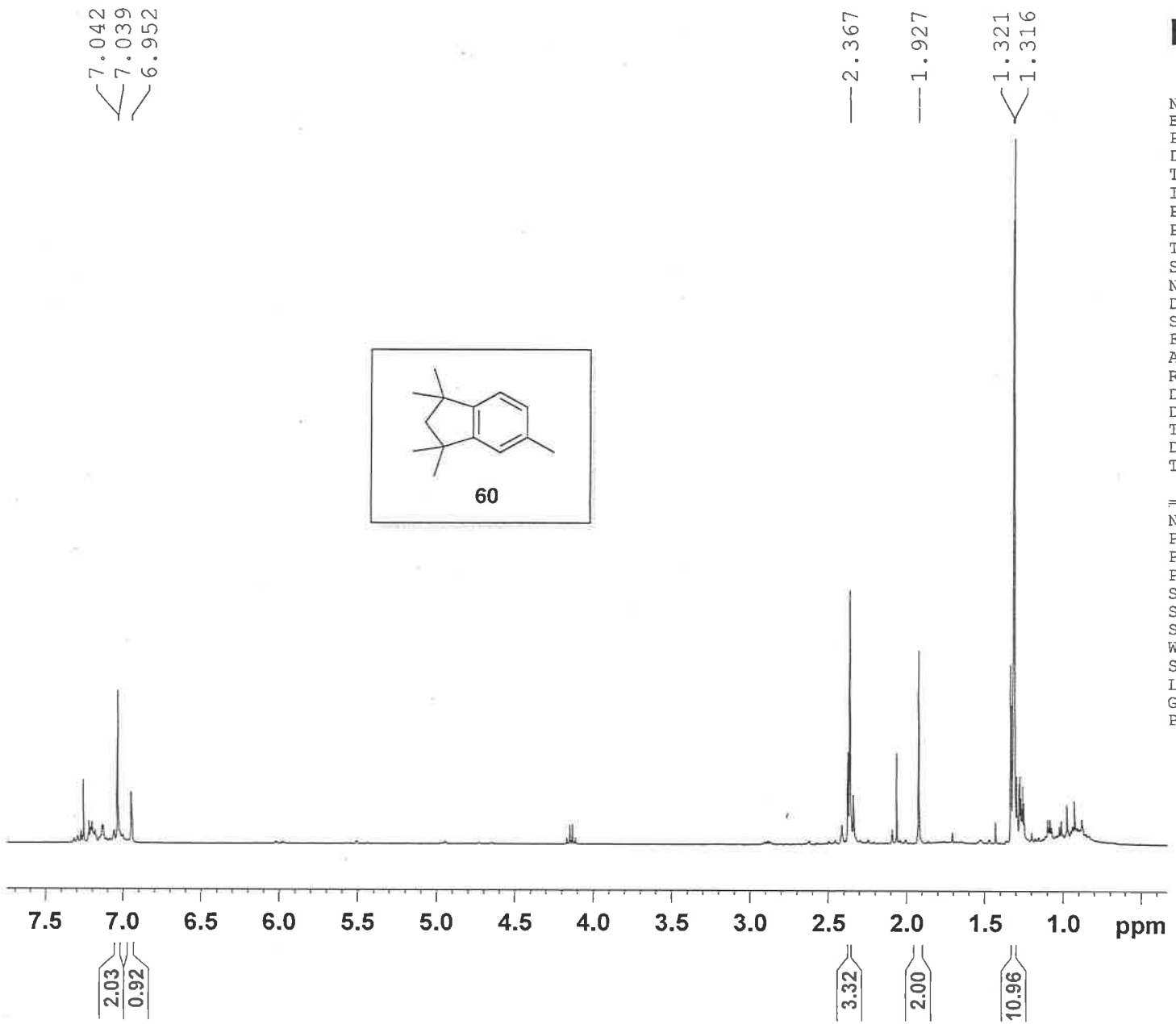
CWV-267



BRUKER

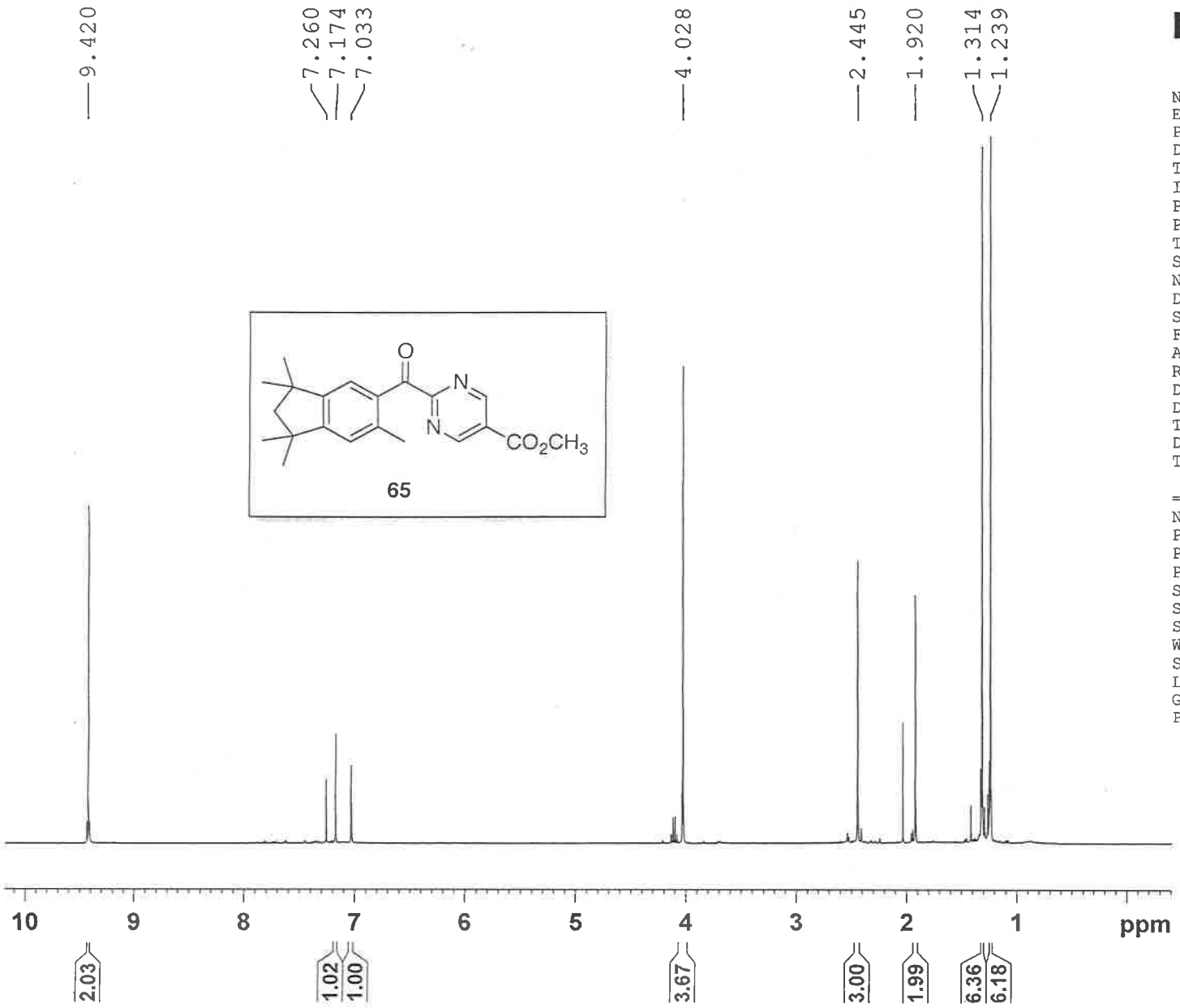
NAME	CWV-267
EXPNO	2
PROCNO	1
Date_	20150930
Time	12.55
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	148
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	298.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127729 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

CWV-247



NAME	CWV-247
EXPNO	1
PROCNO	1
Date_	20150723
Time	12.22
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	298.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300096 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWV-249 f7-11

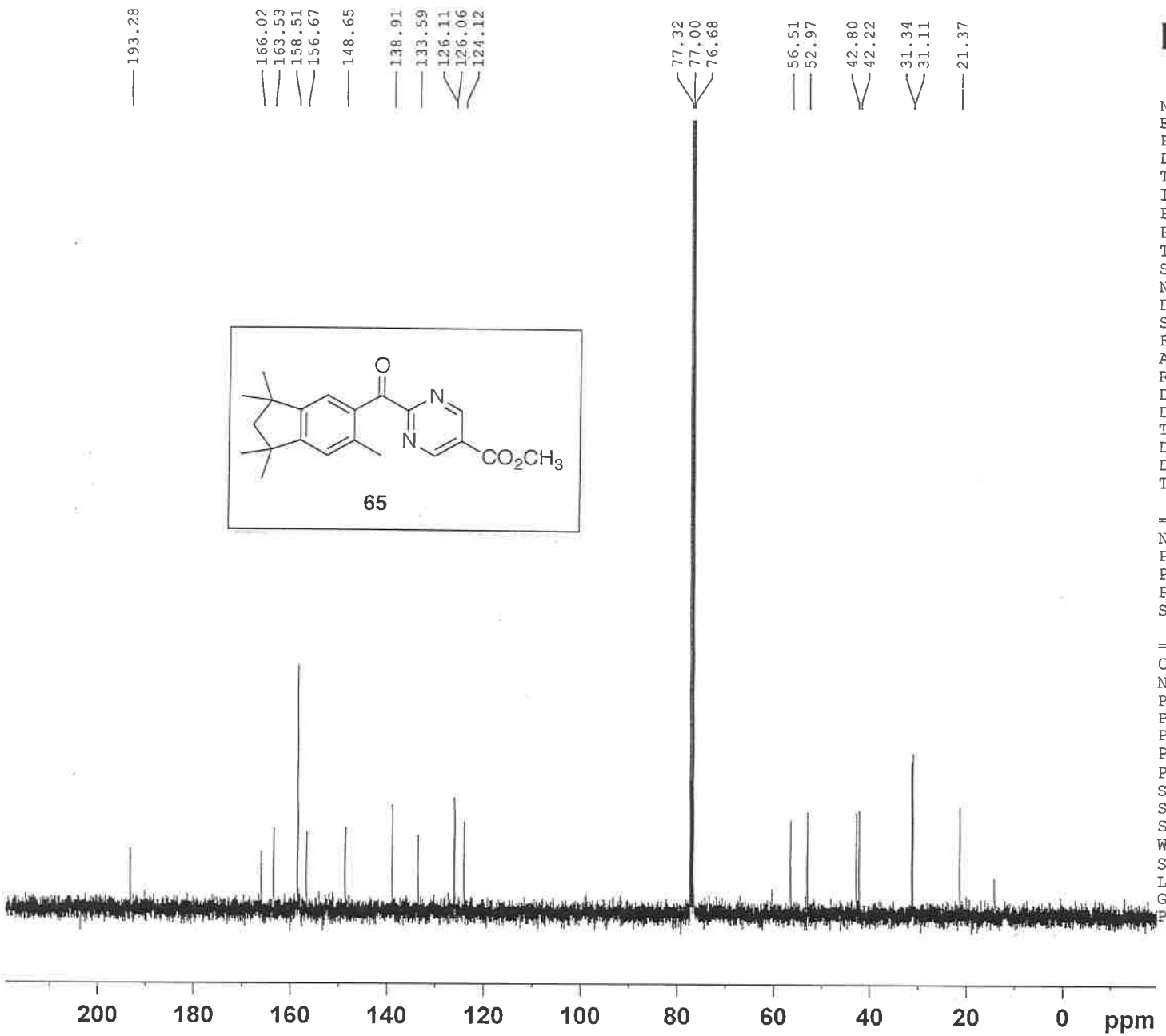


NAME	CWV-249
EXPNO	1
PROCNO	1
Date_	20150730
Time	10.31
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	298.2 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300099 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWV-249 f7-11



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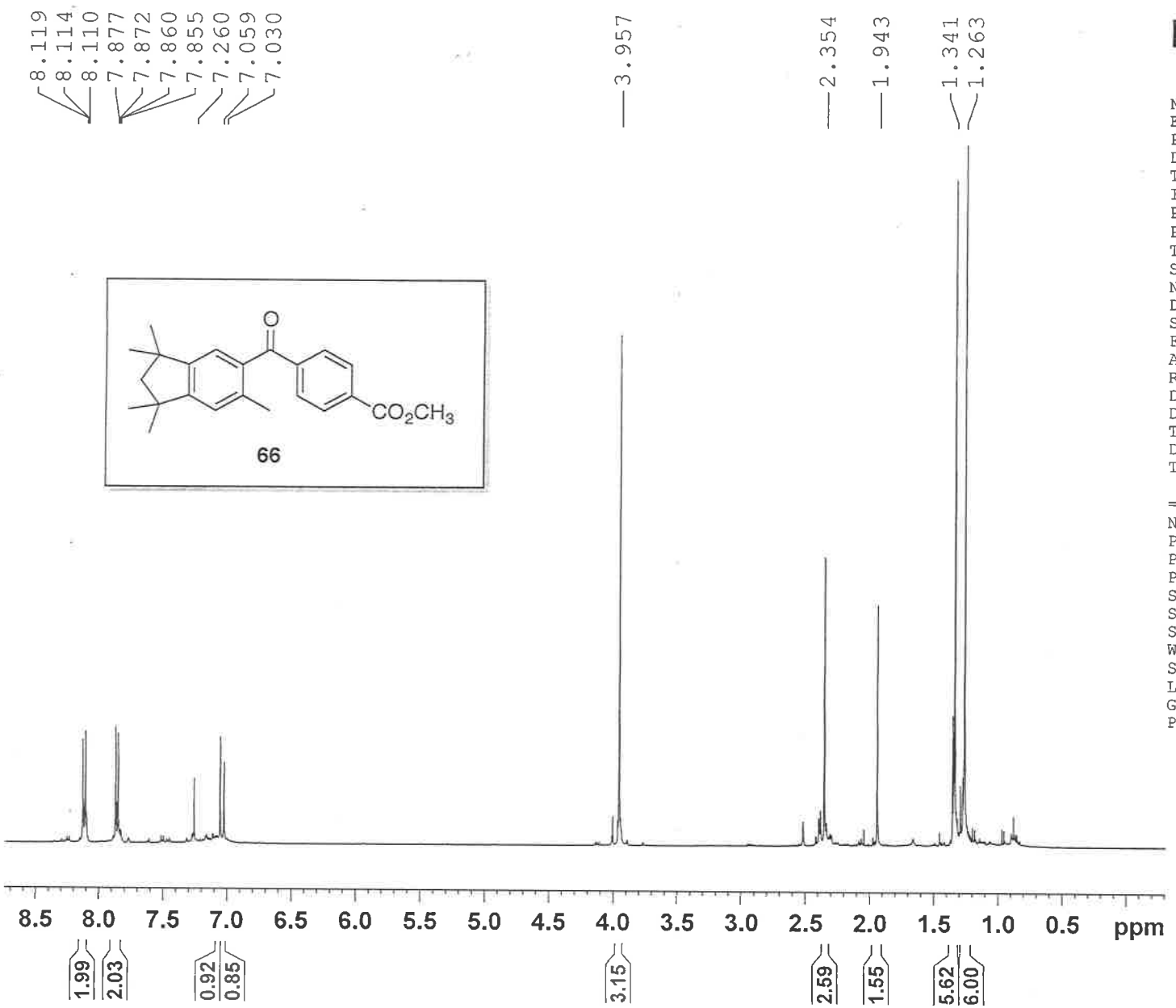
NAME	CWV-249	
EXPNO	2	
PROCNO	1	
Date_	20150730	
Time_	10.40	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgig30	
TD	65536	
SOLVENT	CDCl3	
NS	110	
DS	4	
SWH	24038.461	Hz
FIDRES	0.366798	Hz
AQ	1.3631988	sec
RG	2050	
DW	20.800	usec
DE	6.50	usec
TE	298.4	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	8.50	usec
PL1	-2.10	dB
PL1W	60.29227829	W
SFO1	100.6228298	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	90.00	usec
PL2	-1.80	dB
PL12	17.28	dB
PL2W	21.67079544	W
PL12W	0.26783961	W
SFO2	400.1316005	MHz
SI	32768	
SF	100.6127729	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

CWVI-027 f4



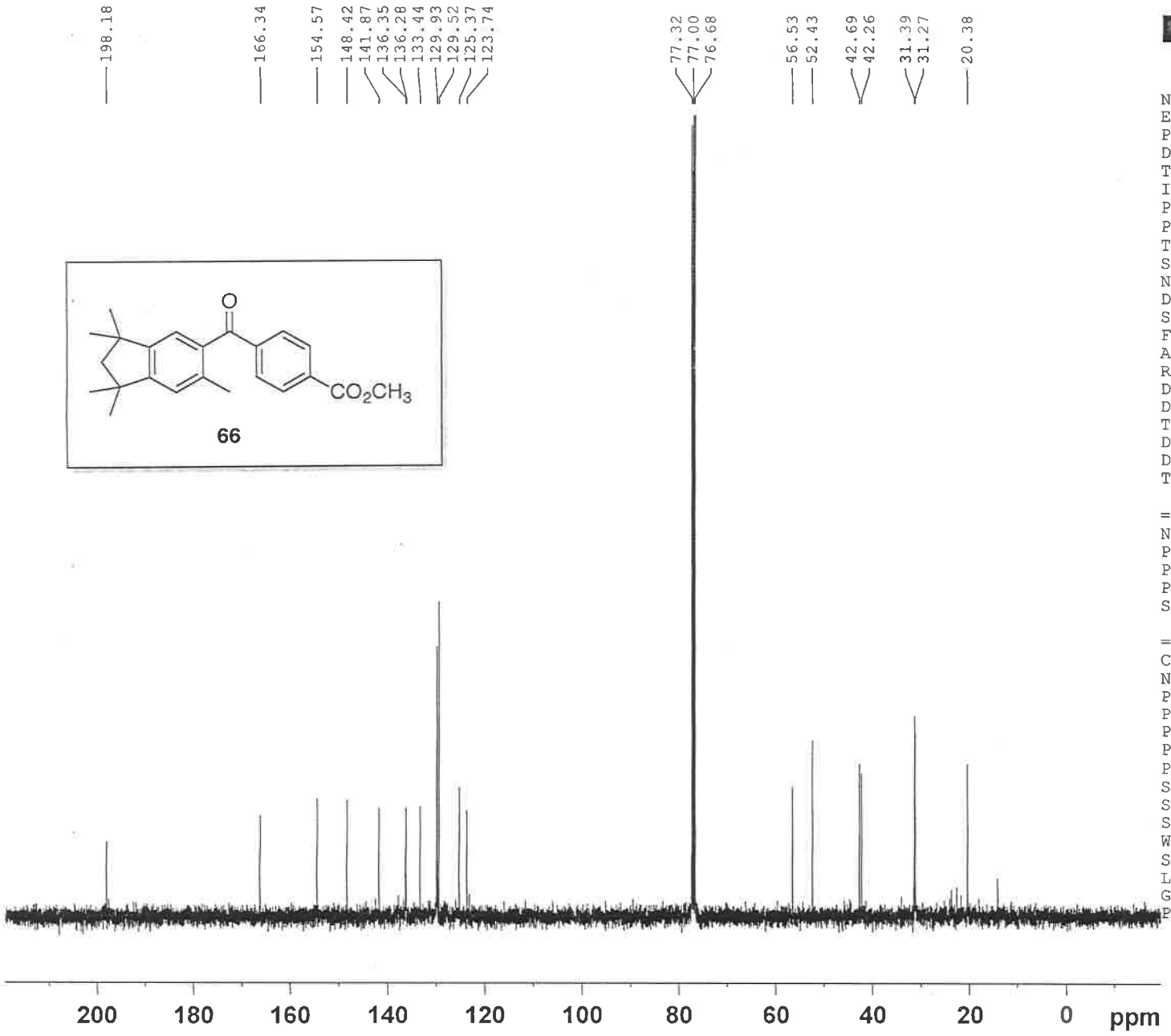
BRUKER

NAME	CWVI-027
EXPNO	1
PROCNO	1
Date_	20160520
Time	12.05
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	673.2 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300101 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

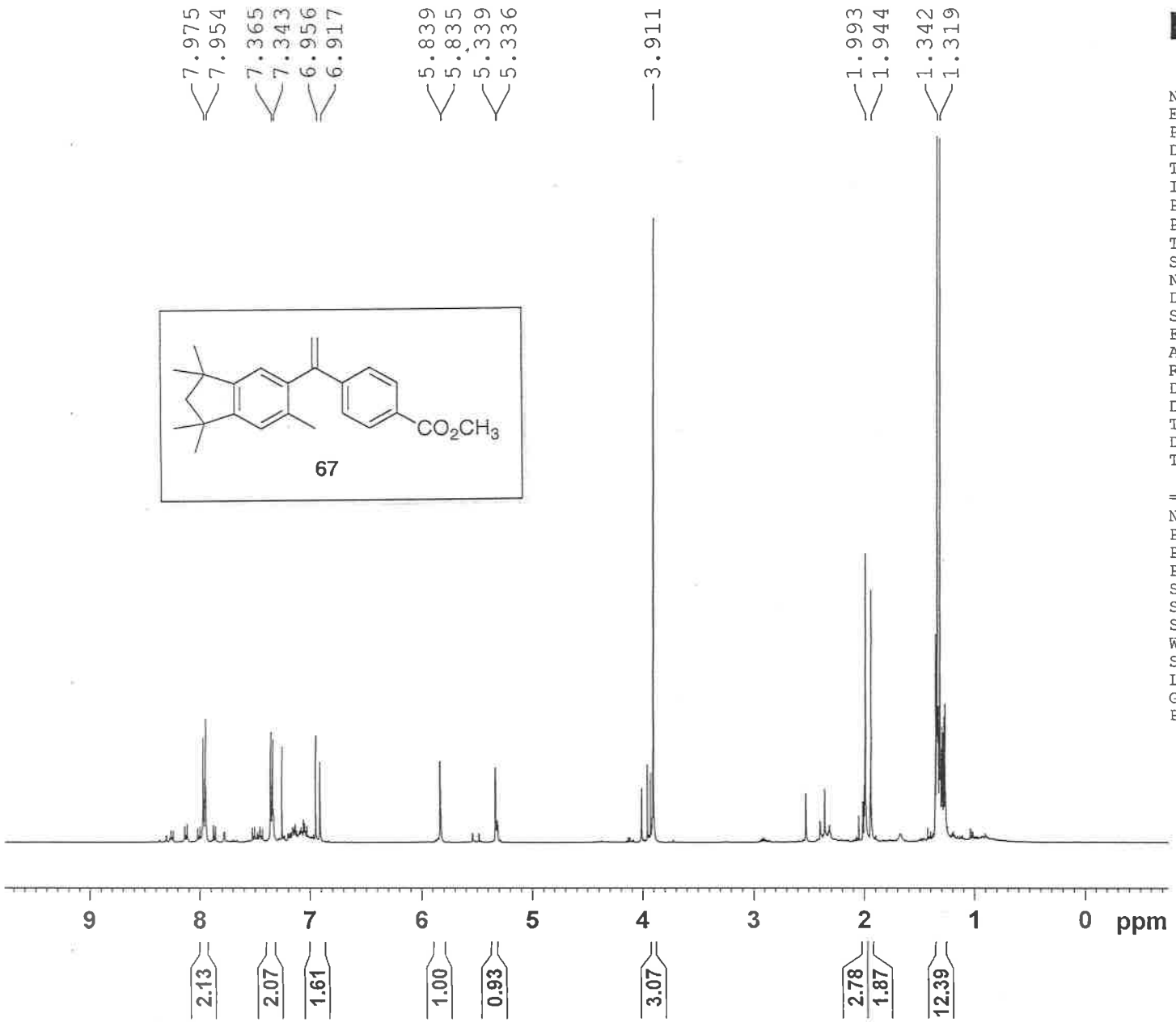
CWVI-027 f4



BRUKER

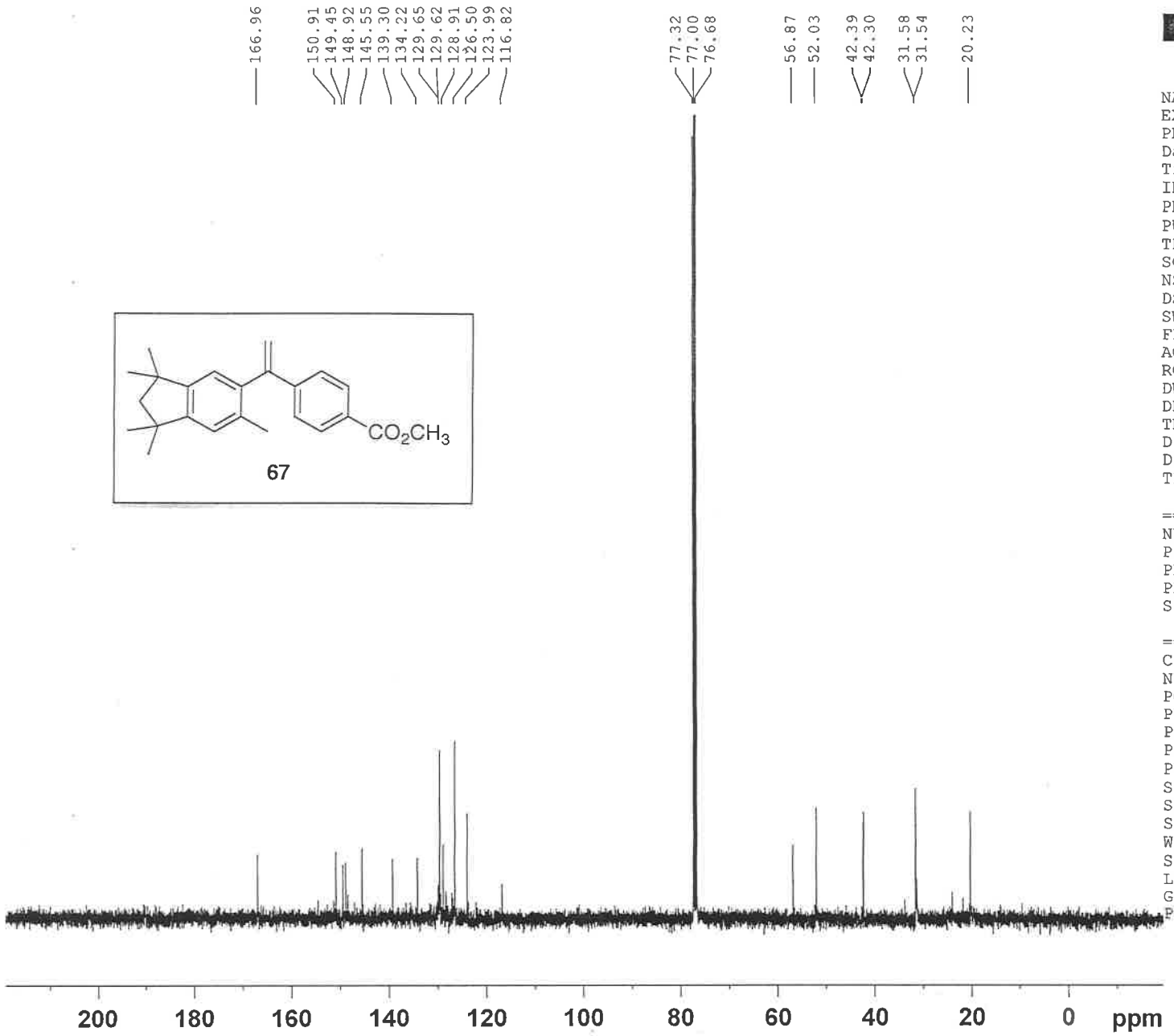
NAME	CWVI-027
EXPNO	2
PROCNO	1
Date_	20160520
Time	12.15
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	141
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	673.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127751 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

CWVI-031



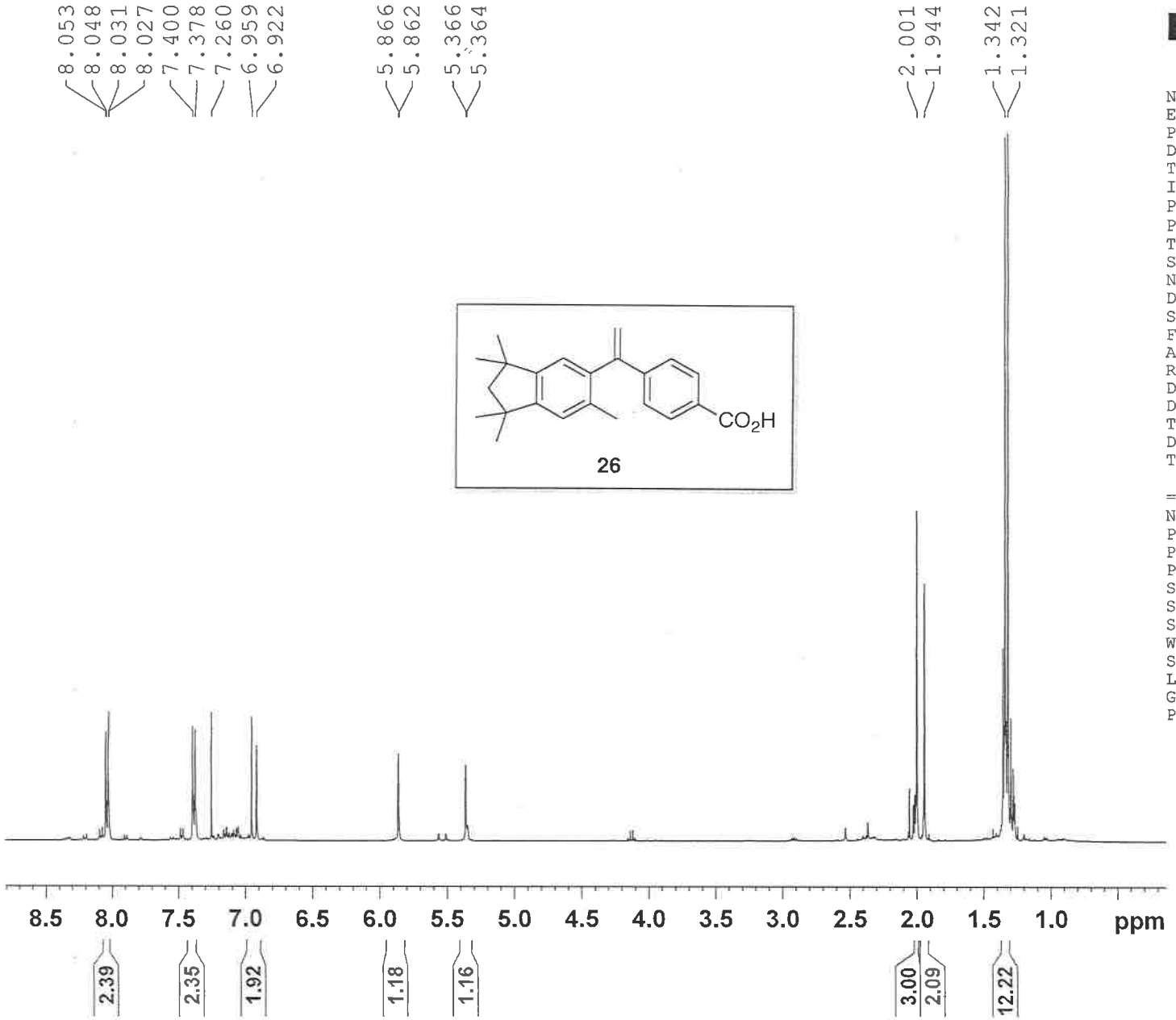
NAME	CWVI-031
EXPNO	1
PROCNO	1
Date_	20160718
Time	12.25
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	294.9 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300101 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWVI-031



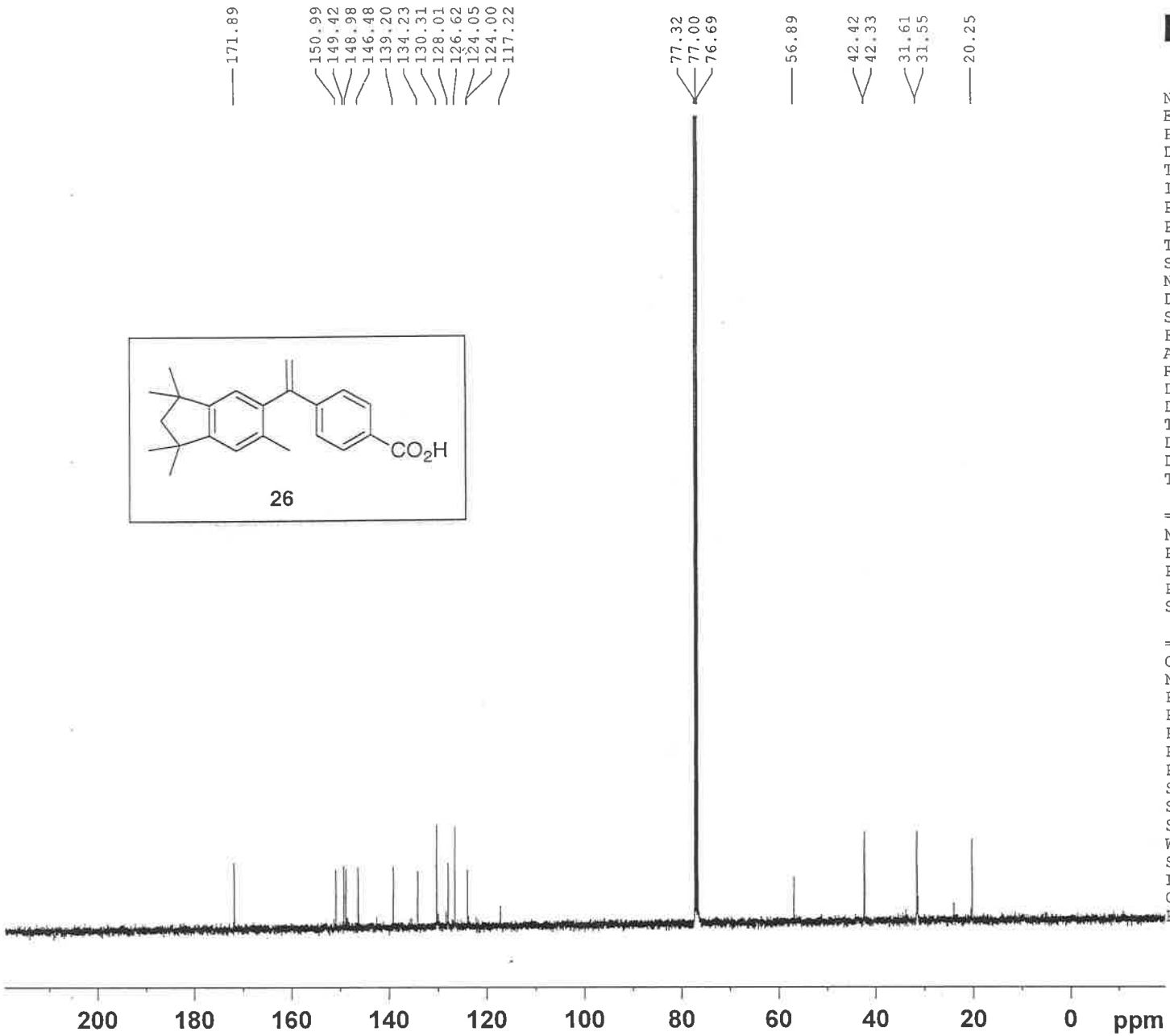
NAME	CWVI-031
EXPNO	2
PROCNO	1
Date_	20160718
Time	12.40
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	209
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	295.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127736 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

CWVI-035



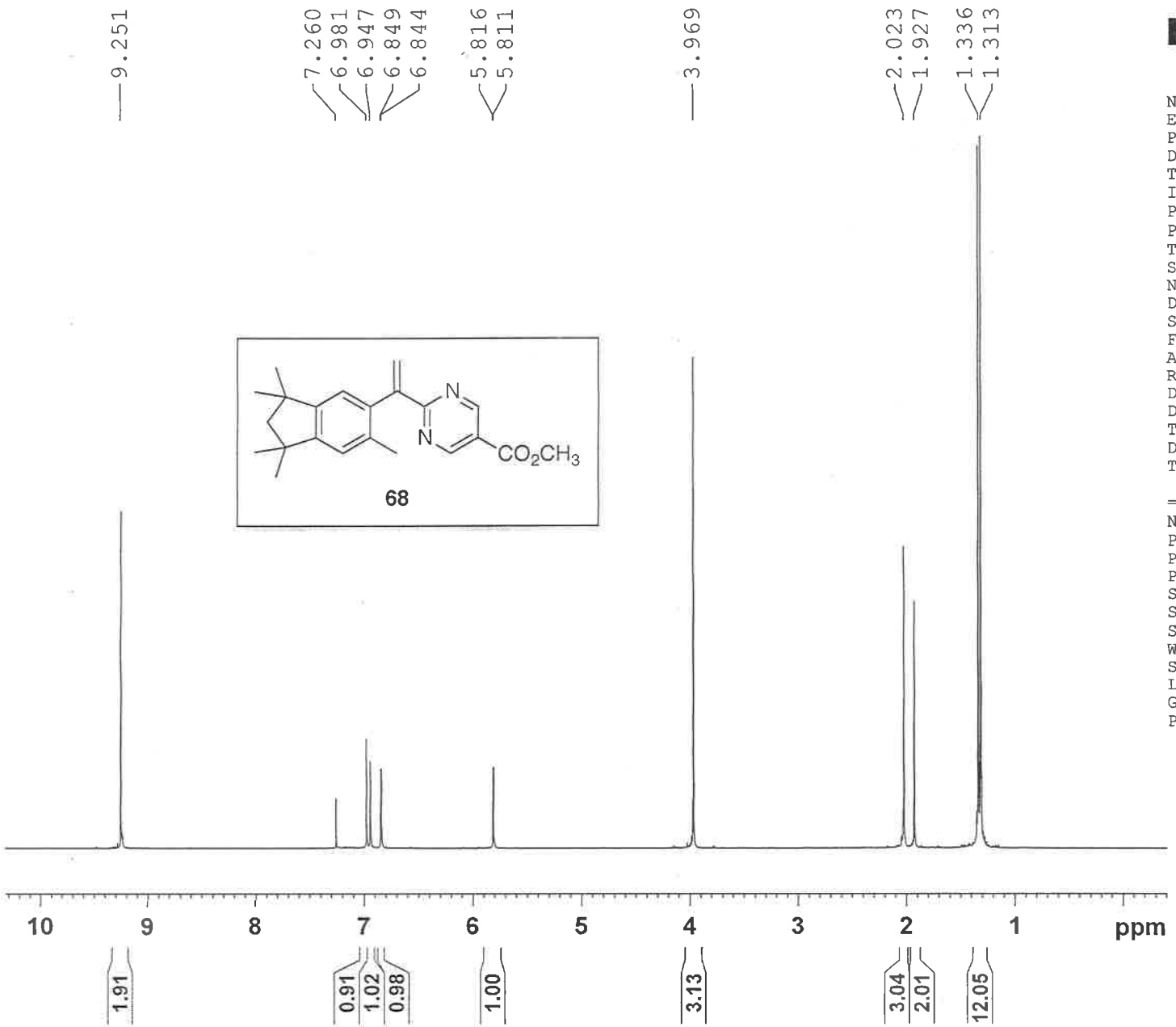
NAME	CWVI-035
EXPNO	1
PROCNO	1
Date_	20160729
Time	12.24
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	295.7 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300104 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWVI-035



NAME	CWVI-035
EXPNO	2
PROCNO	1
Date_	20160729
Time	13.04
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	731
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	296.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127714 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

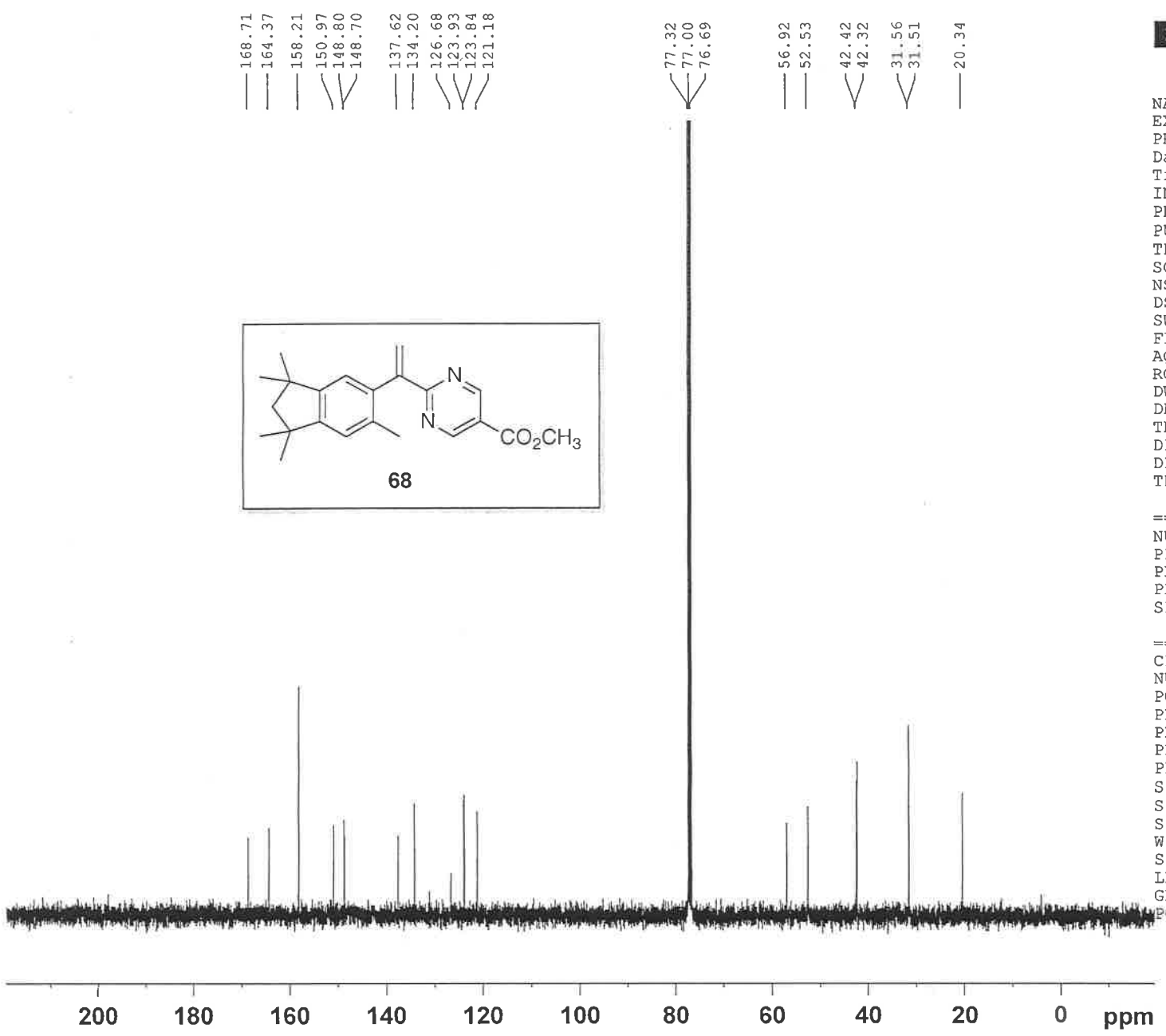
CWV-251



BRUKER

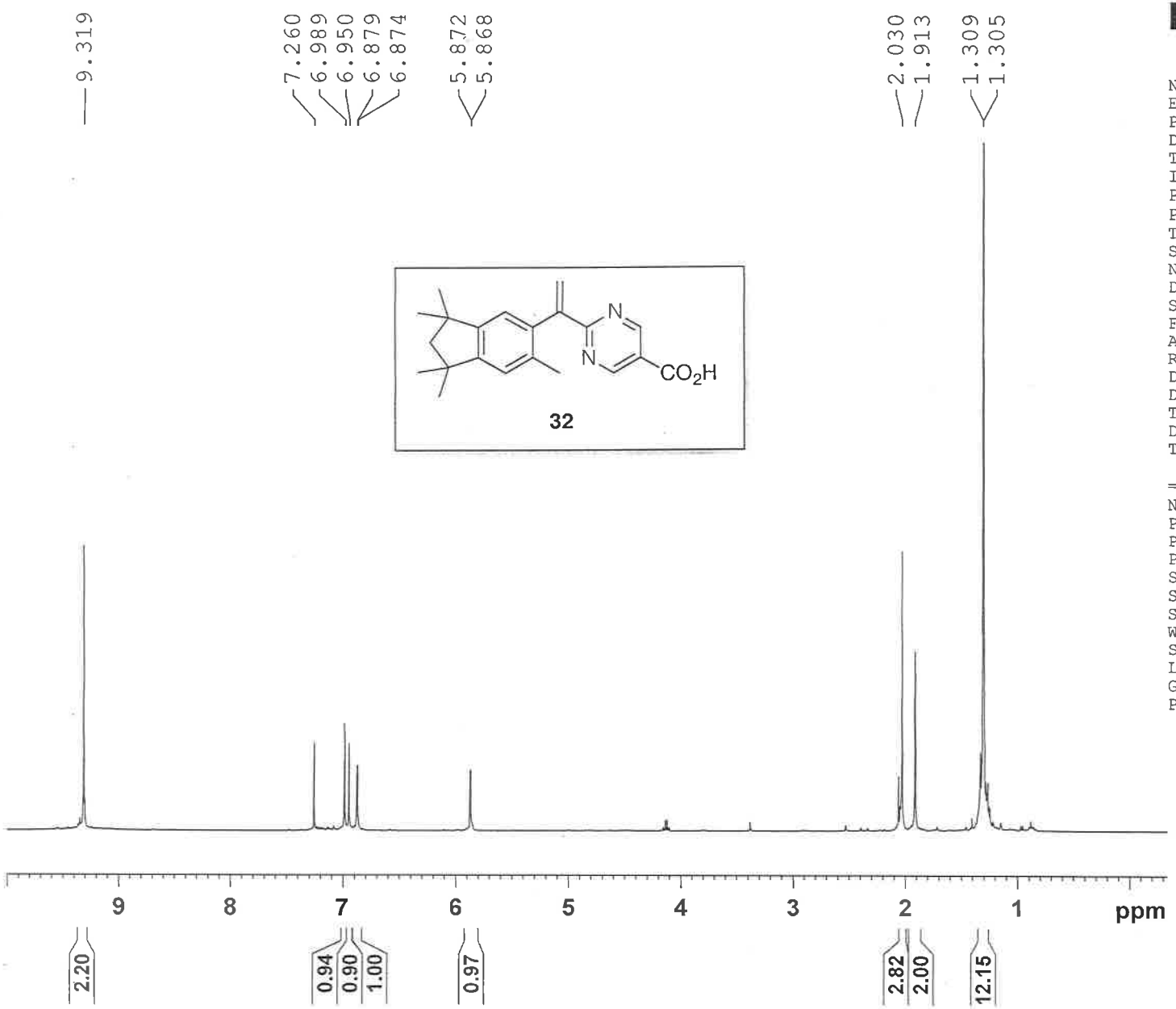
NAME	CWV-251
EXPNO	1
PROCNO	1
Date_	20150902
Time	11.41
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	299.3 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300099 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWV-251



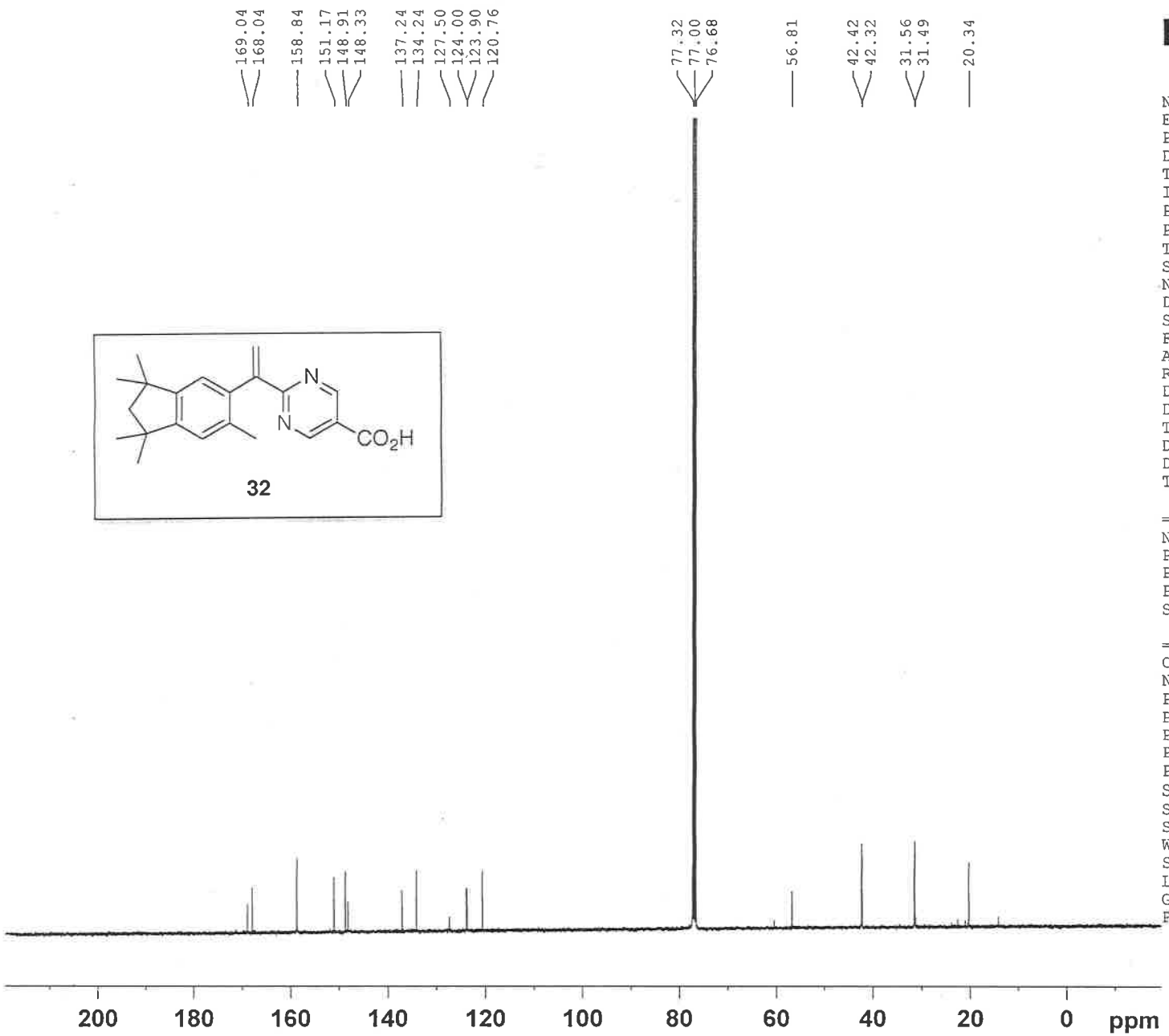
NAME	CWV-251
EXPNO	2
PROCNO	1
Date_	20150902
Time	11.50
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	139
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127714 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

CWVI-007



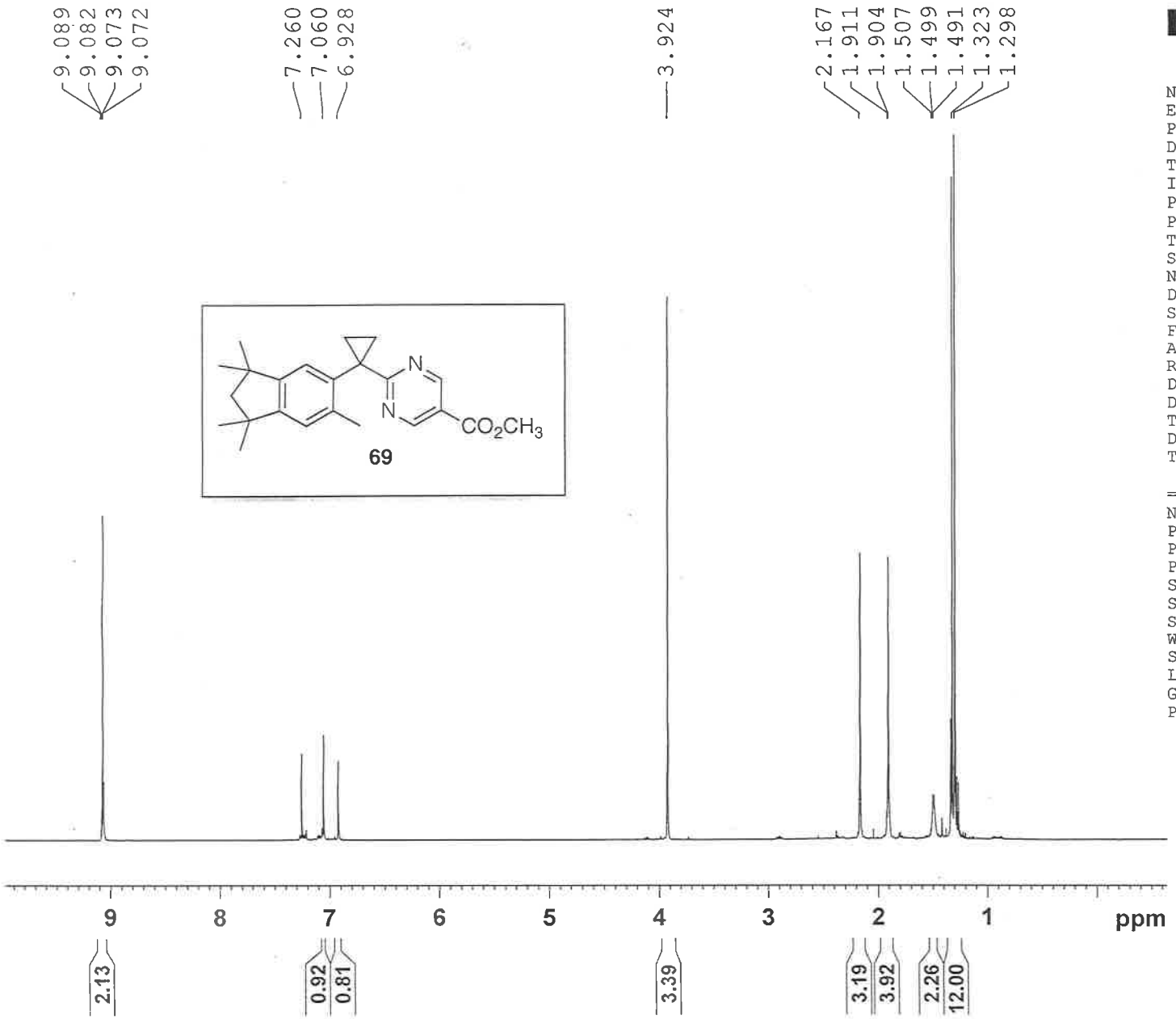
NAME	CWVI-007
EXPNO	1
PROCNO	1
Date_	20160328
Time	10.49
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	673.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300101 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWVI-007



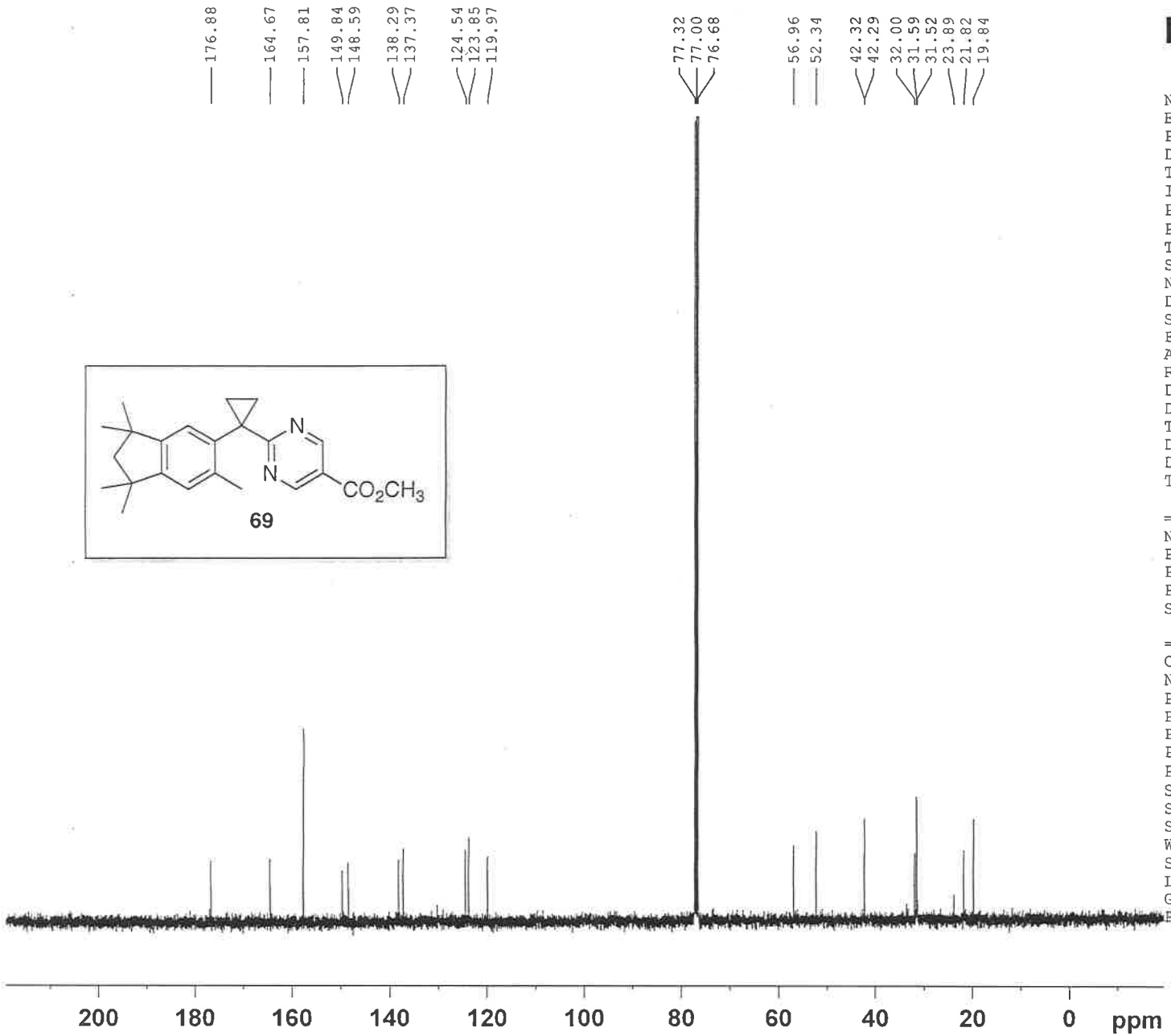
NAME	CWVI-007
EXPNO	2
PROCNO	1
Date_	20160328
Time	11.08
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	3620
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	673.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127729 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

CWV-271



NAME	CWV-271
EXPNO	1
PROCNO	1
Date_	20151009
Time	10.50
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	298.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300099 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWV-271



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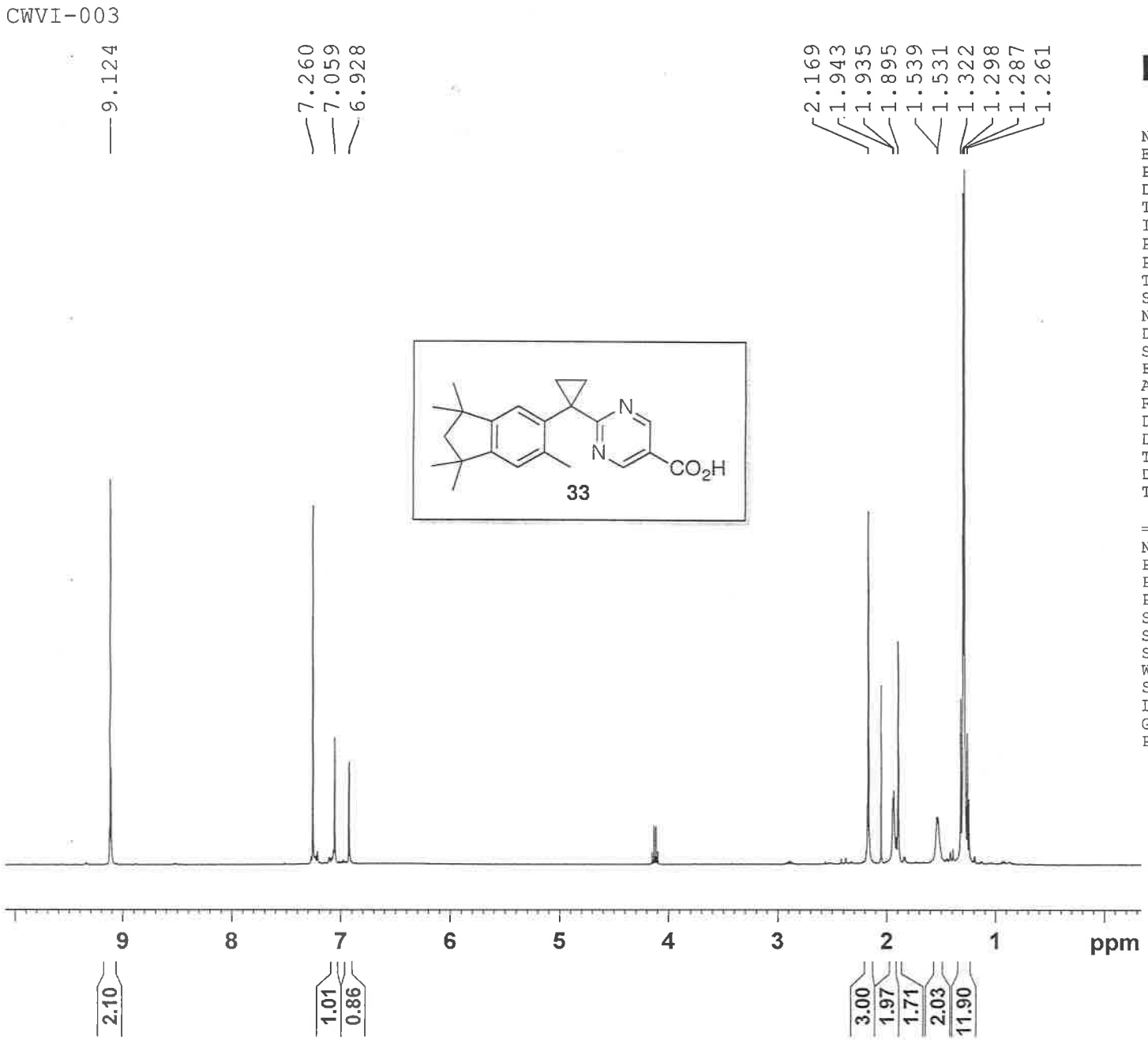
NAME	CWV-271
EXPNO	2
PROCNO	1
Date_	20151009
Time	11.00
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	282
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	298.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127714 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

CWVI-003

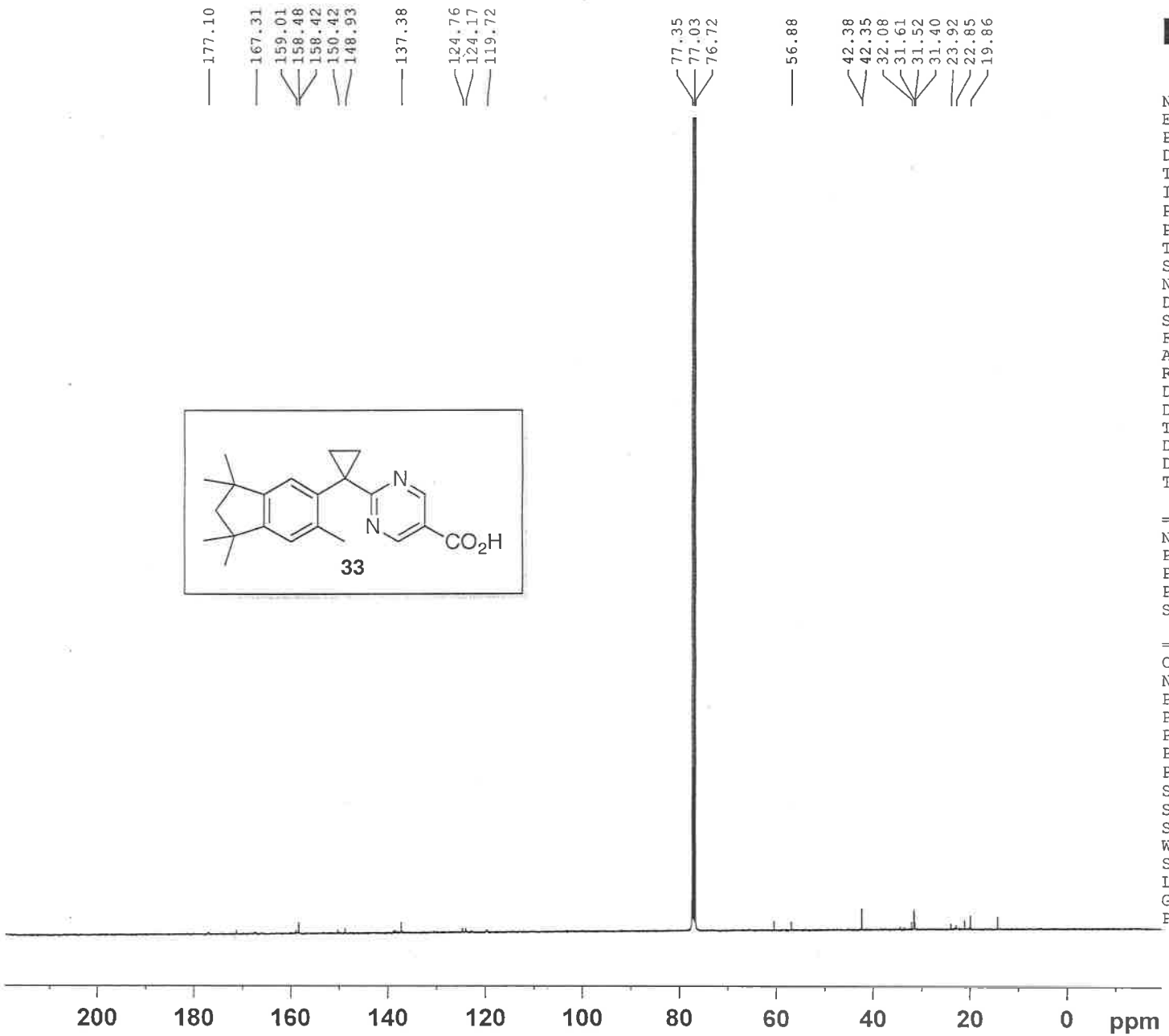


NAME	CWVI-003
EXPNO	1
PROCNO	1
Date_	20160328
Time	10.43
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	673.2 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========

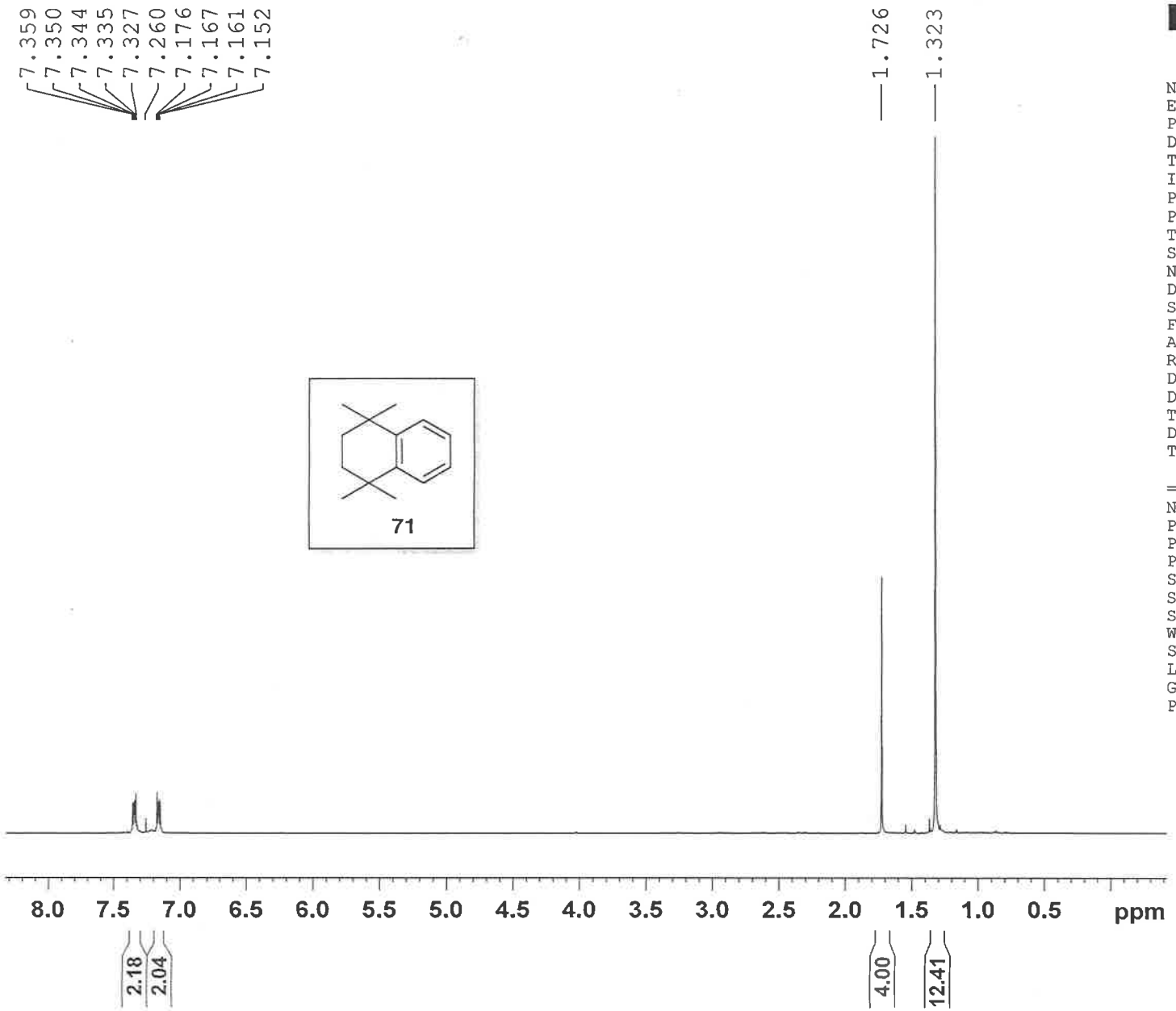
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300101 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWVI-003



NAME	CWVI-003
EXPNO	2
PROCNO	1
Date_	20160330
Time	14.39
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	19951
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	673.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

CWIII-121

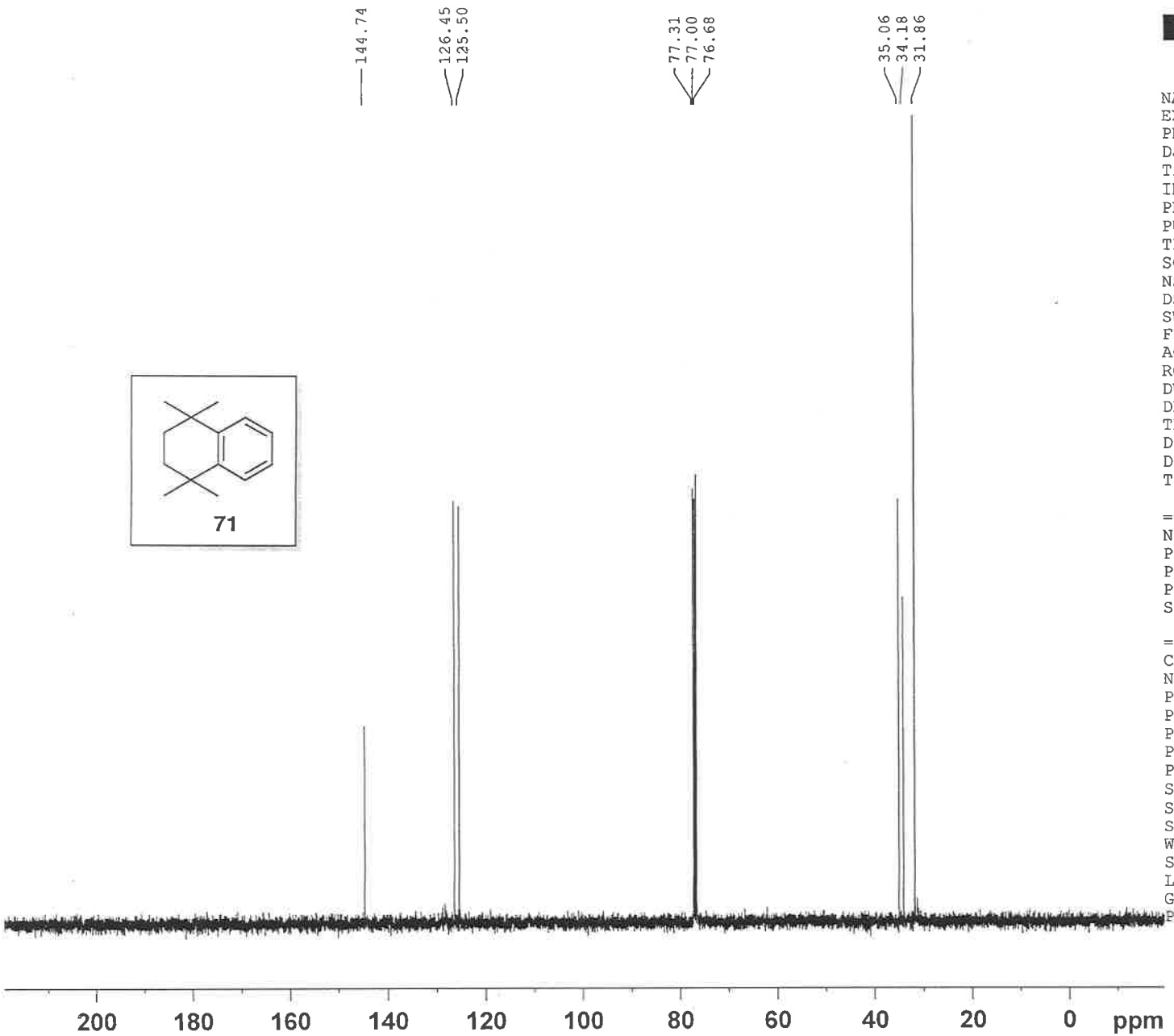


NAME	CWIII-121
EXPNO	1
PROCNO	1
Date_	20100609
Time	11.35
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	291.2 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========

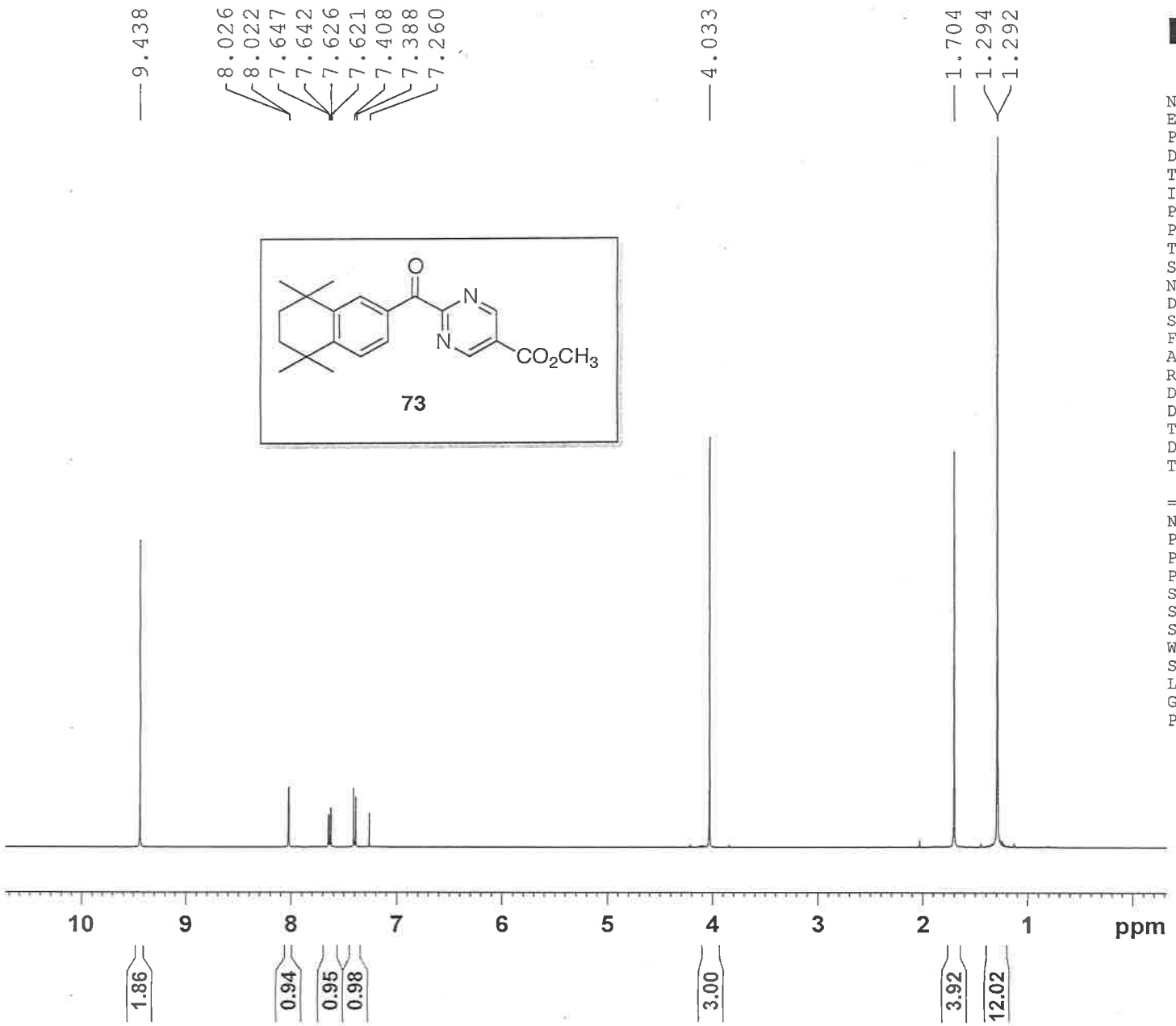
NUC1	1H
P1	10.00 usec
PL1	-1.80 dB
PL1W	21.67079544 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300104 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWIII-121



NAME	CWIII-121
EXPNO	2
PROCNO	1
Date_	20100609
Time	11.43
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	41
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	291.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-1.50 dB
PL1W	52.51238251 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127766 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

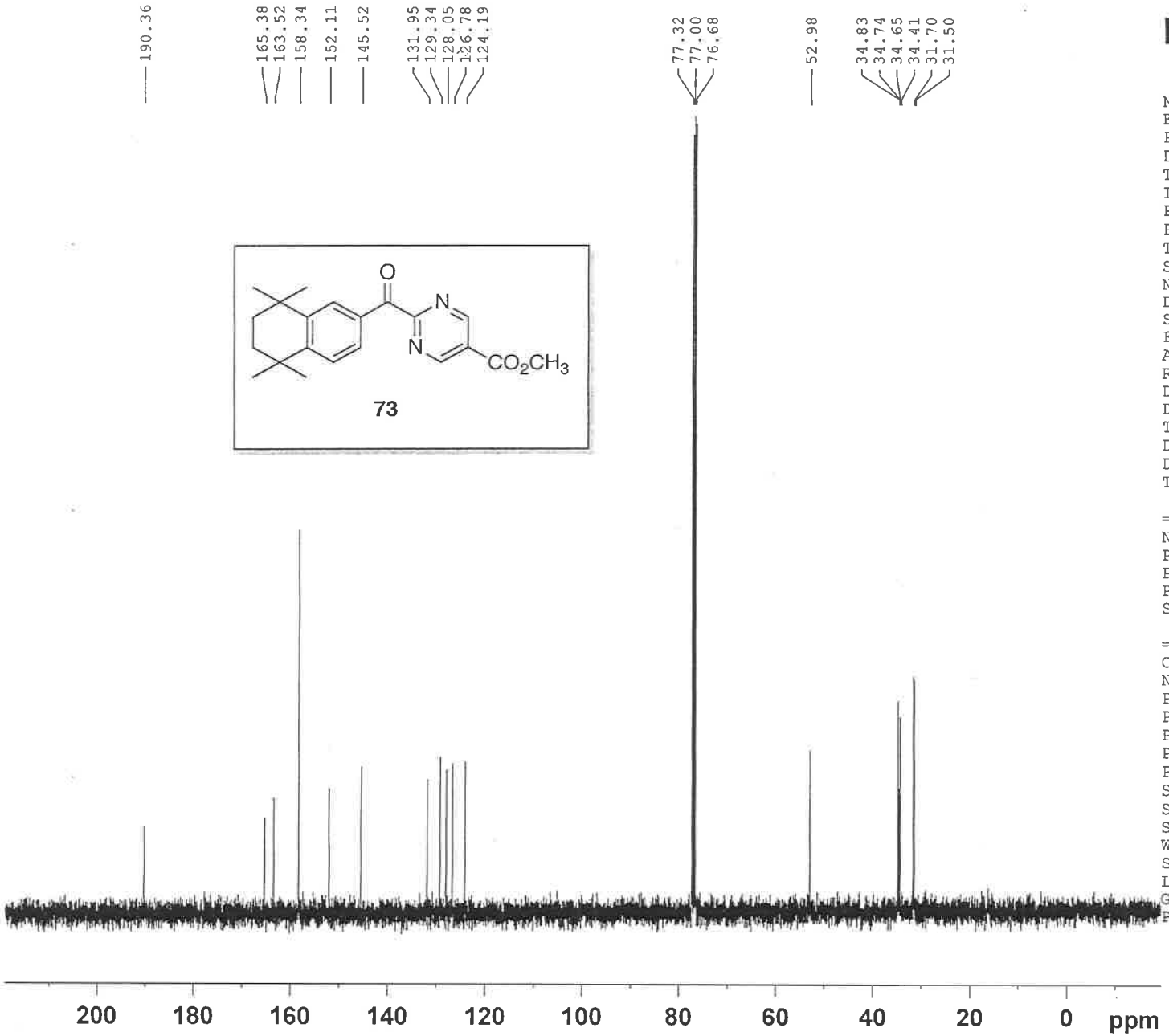
CWV-297



BRUKER

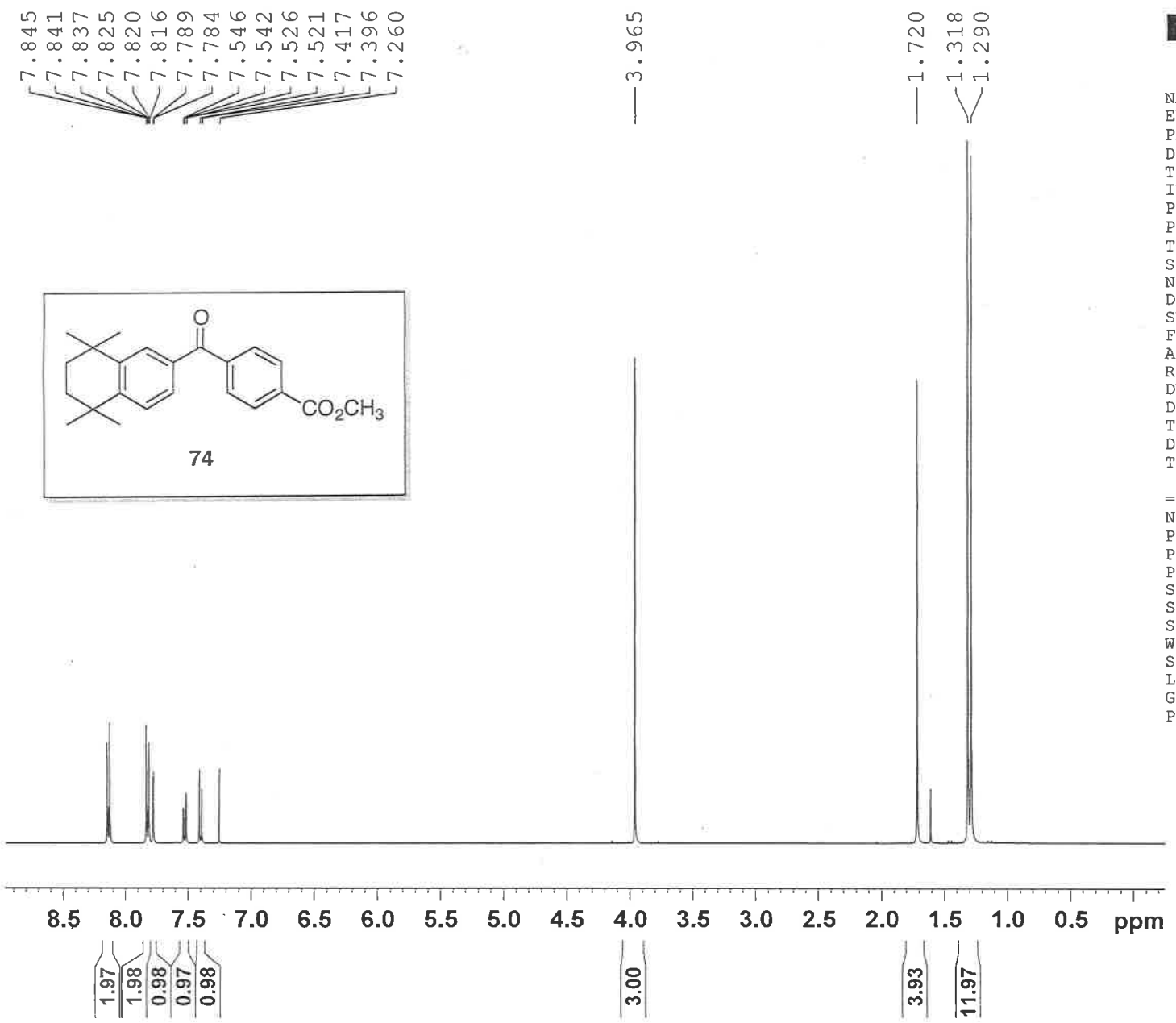
NAME	CWV-297
EXPNO	1
PROCNO	1
Date_	20151224
Time	15.10
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	298.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300096 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWV-297



NAME	CWV-297
EXPNO	2
PROCNO	1
Date_	20151224
Time	15.15
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	64
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	298.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127736 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

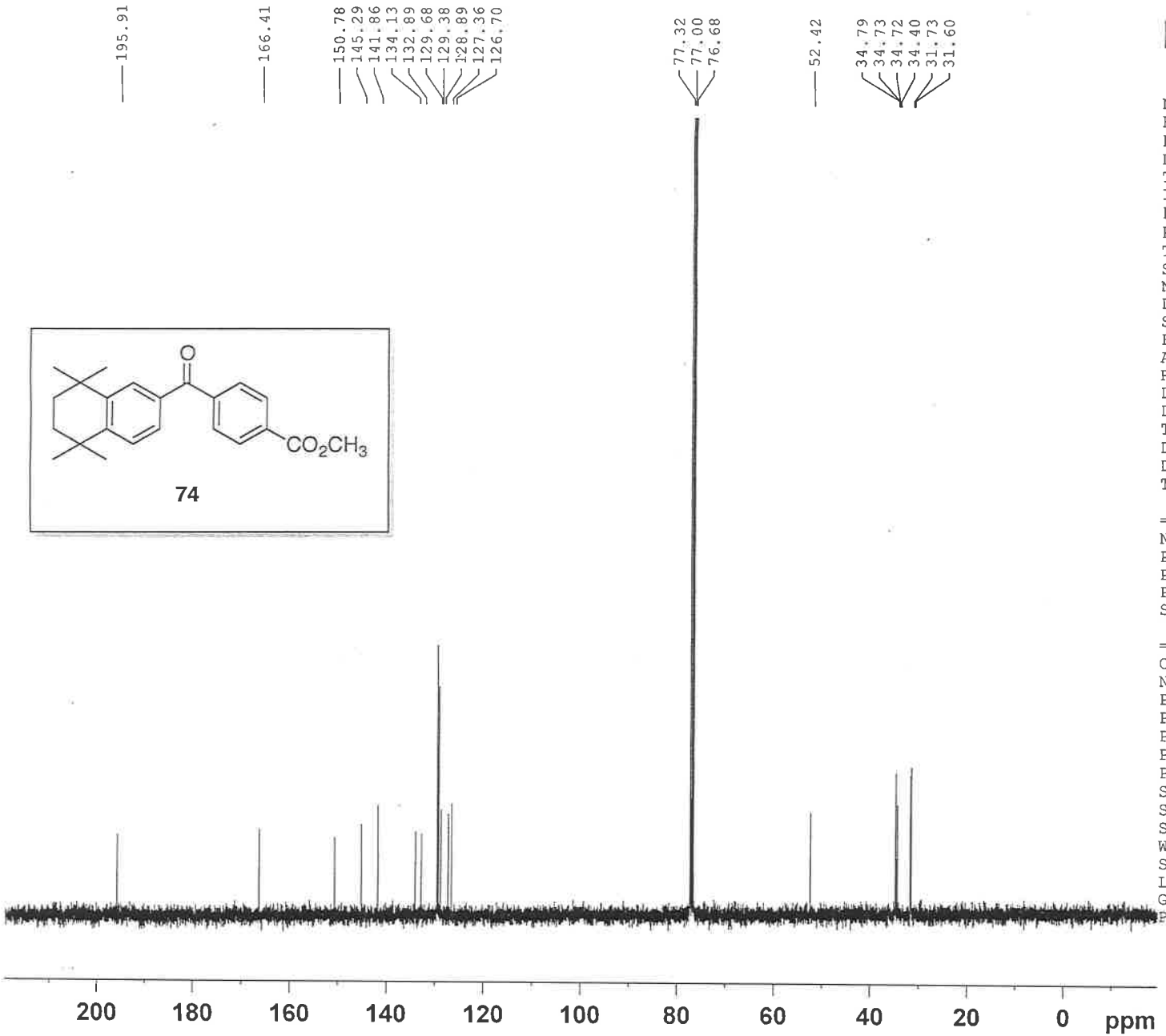
CWVI-017



BRUKER

NAME	CWVI-017
EXPNO	1
PROCNO	1
Date_	20160728
Time	14.54
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	673.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300104 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

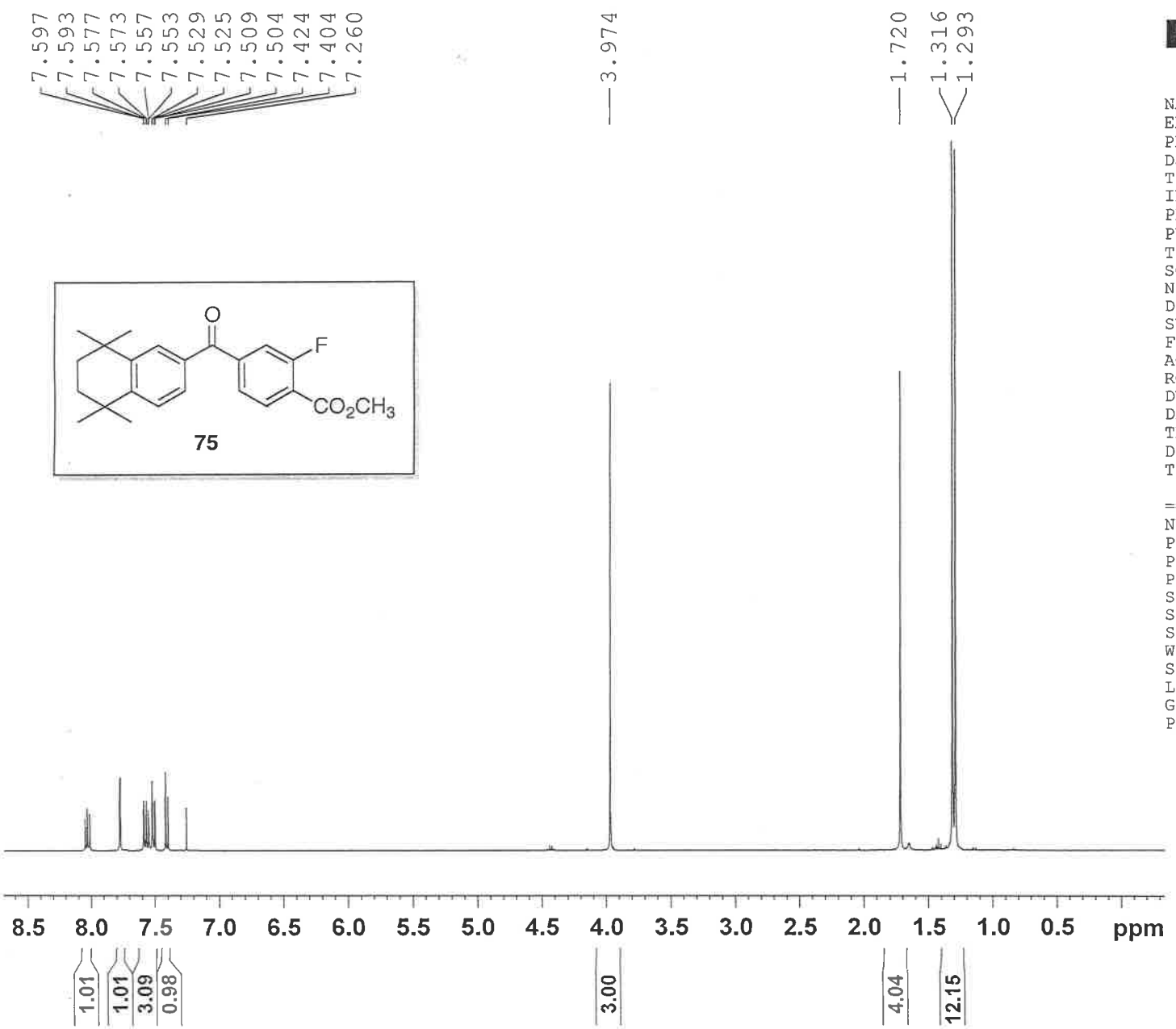
CWVI-017



BRUKER

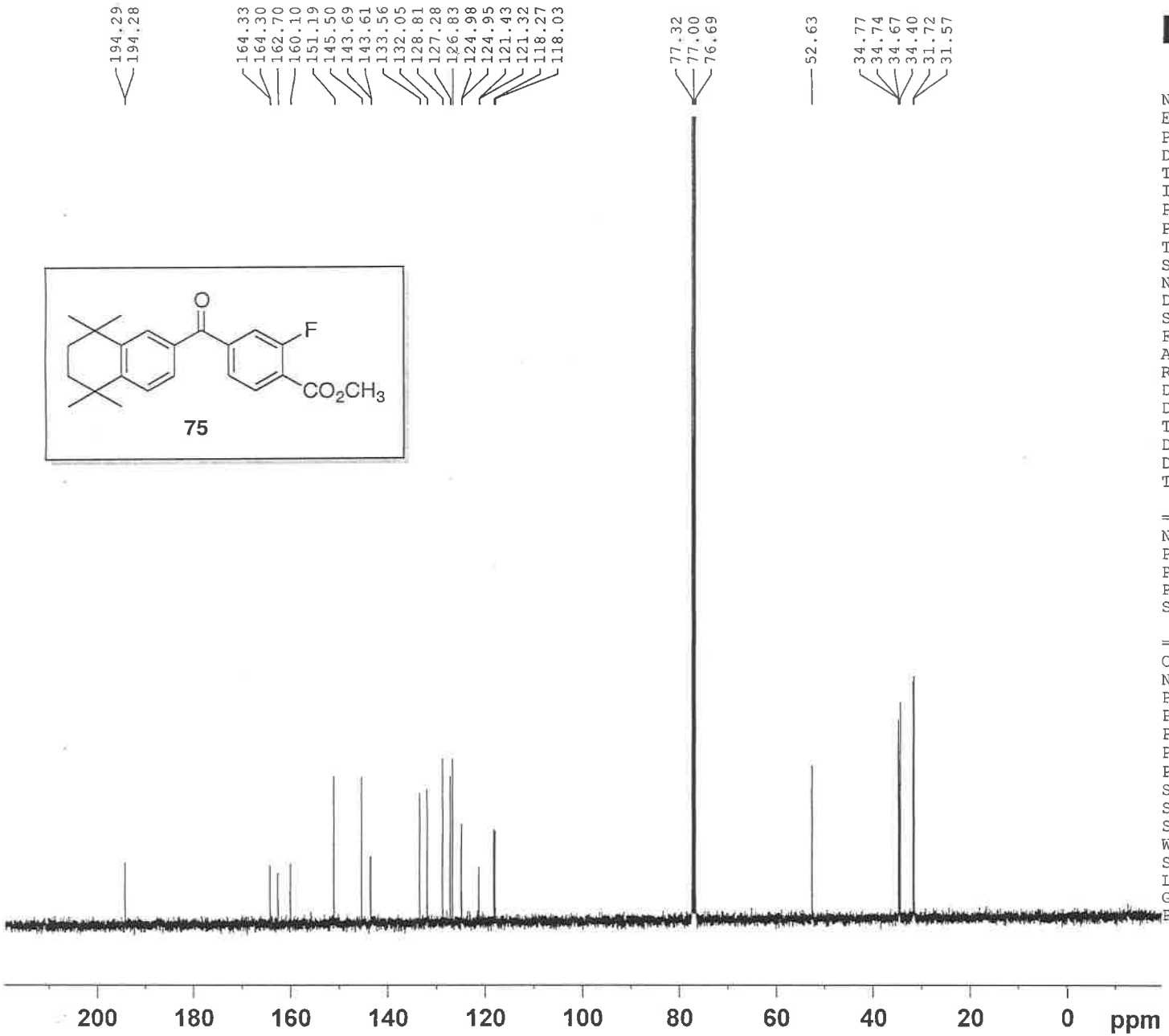
NAME	CWVI-017
EXPNO	2
PROCNO	1
Date_	20160728
Time	15.00
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	157
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	673.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127722 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

CWVI-015



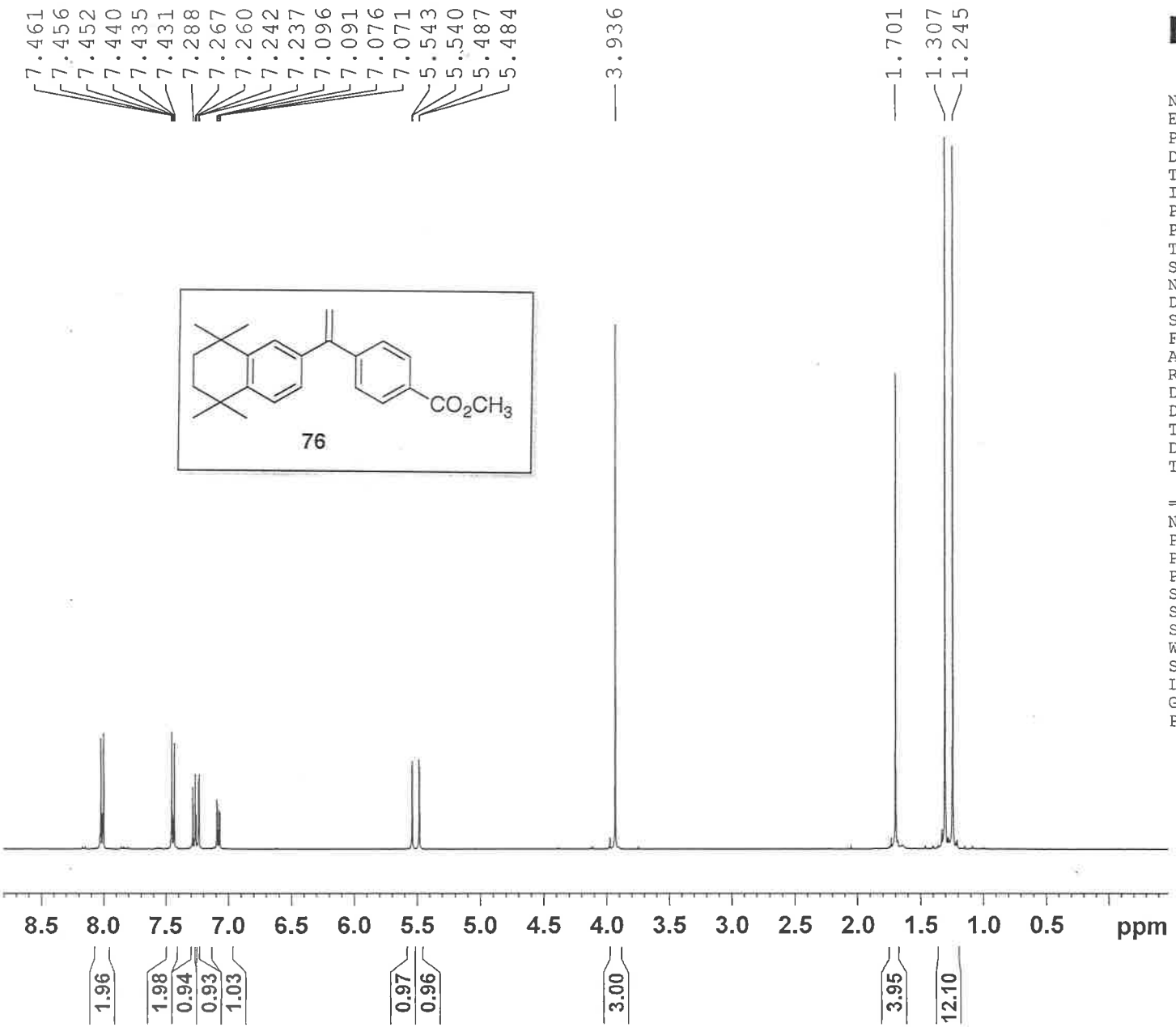
NAME	CWVI-015
EXPNO	1
PROCNO	1
Date_	20160728
Time	14.27
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	673.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300104 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWVI-015



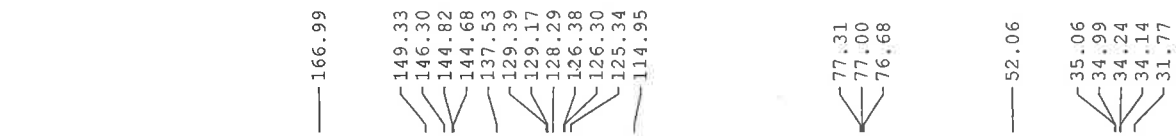
NAME	CWVI-015
EXPNO	2
PROCNO	1
Date_	20160728
Time	14.46
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	360
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	673.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127729 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

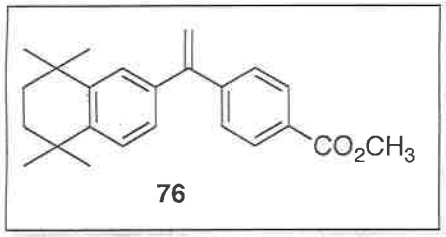
CWVI-021



NAME	CWVI-021
EXPNO	1
PROCNO	1
Date_	20160728
Time	15.29
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	295.5 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300101 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

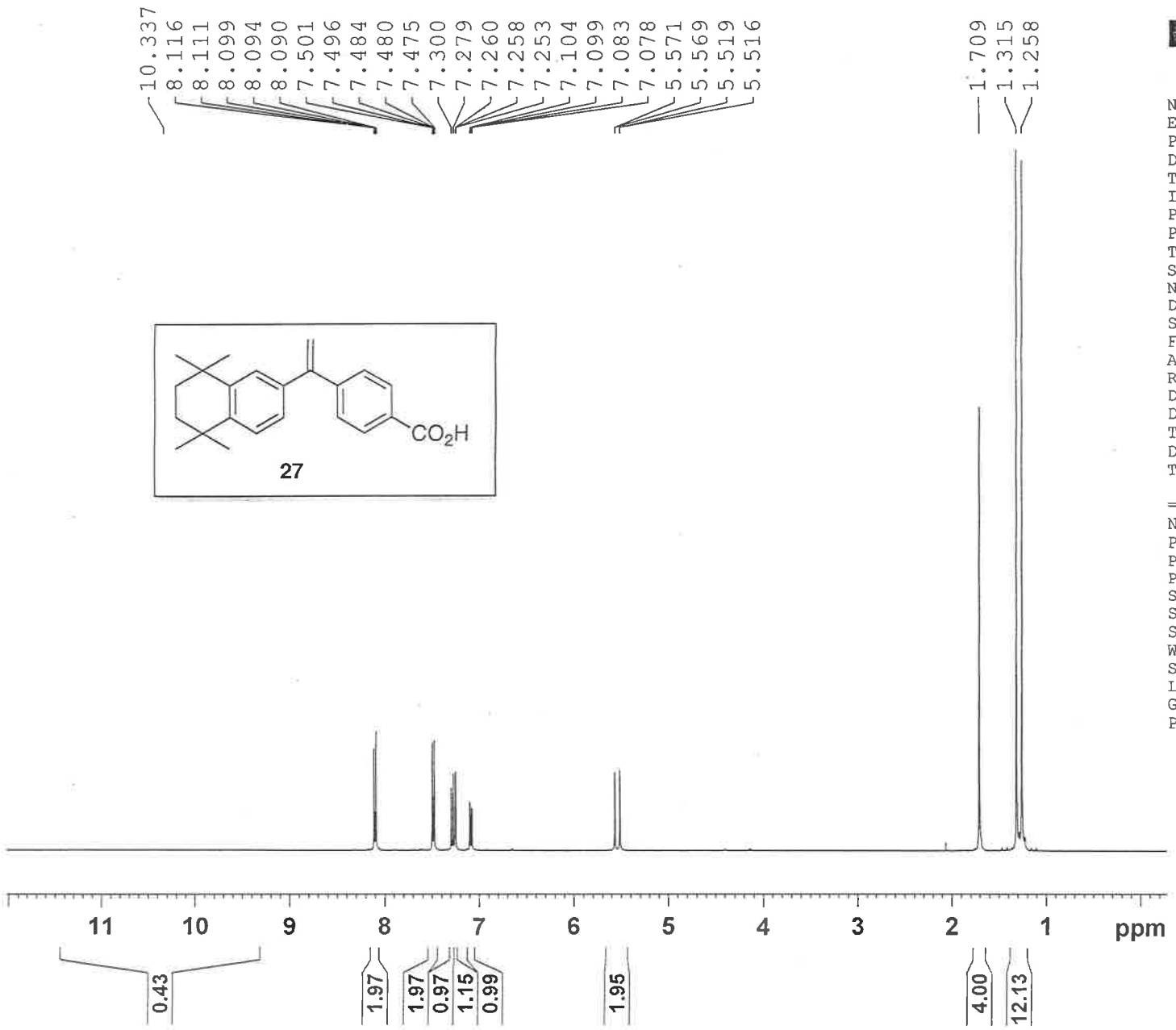
CWVI-021





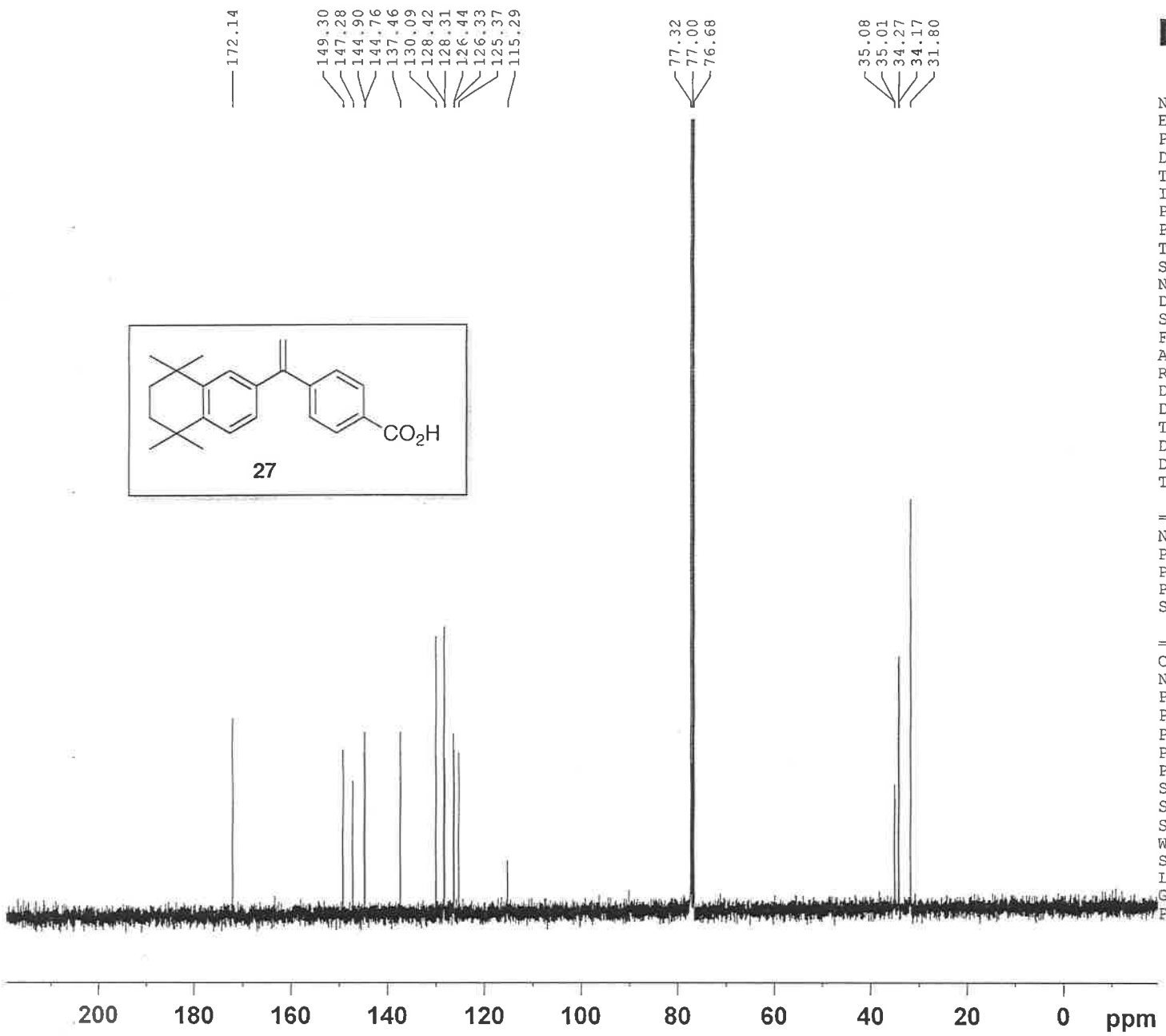
NAME	CWVI-021
EXPNO	2
PROCNO	1
Date_	20160728
Time	15.33
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	145
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	295.7 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127744 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

CWVI-025



NAME	CWVI-025
EXPNO	1
PROCNO	1
Date_	20160729
Time	13.33
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	295.8 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300104 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

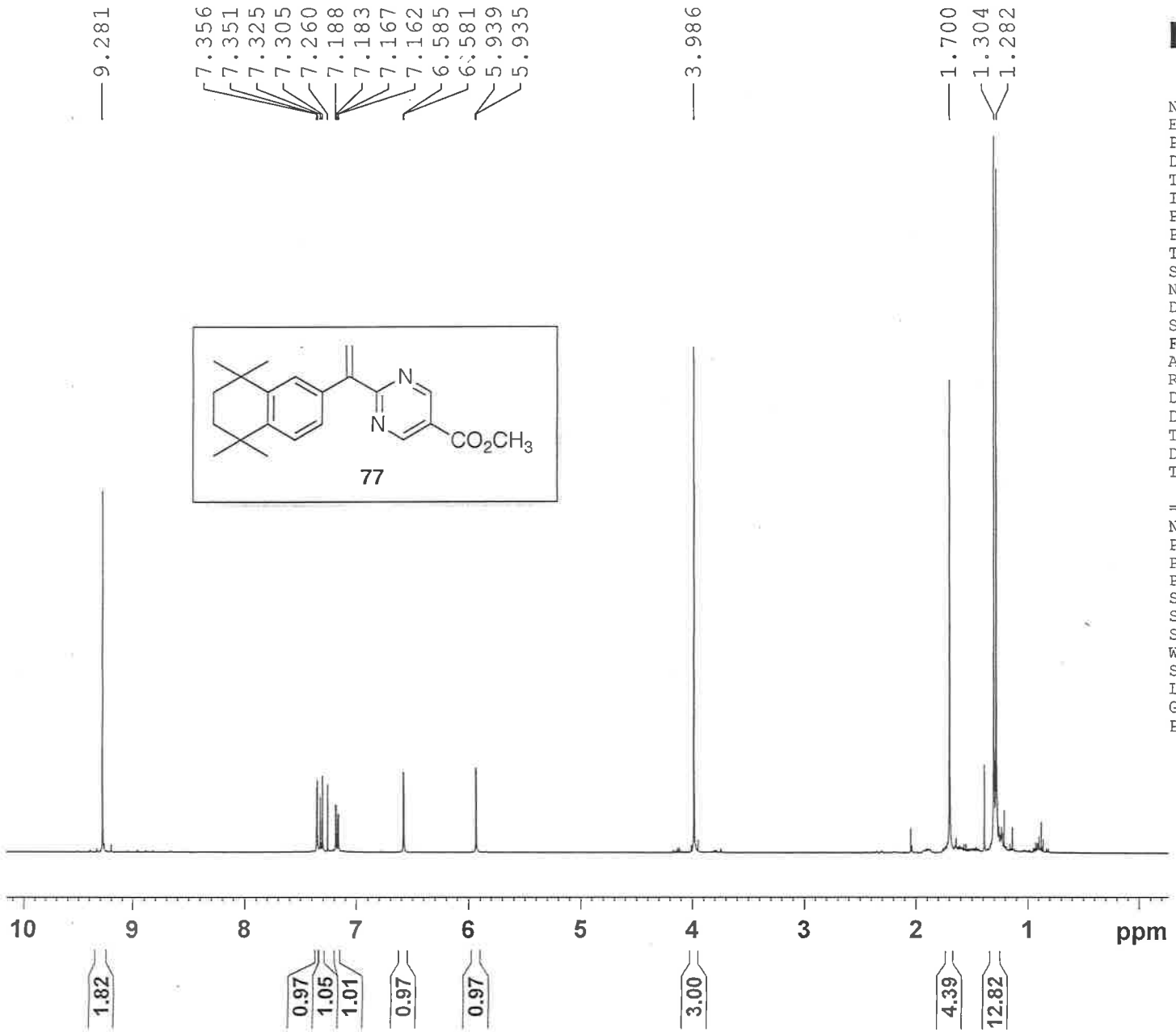
CWVI-025



BRUKER

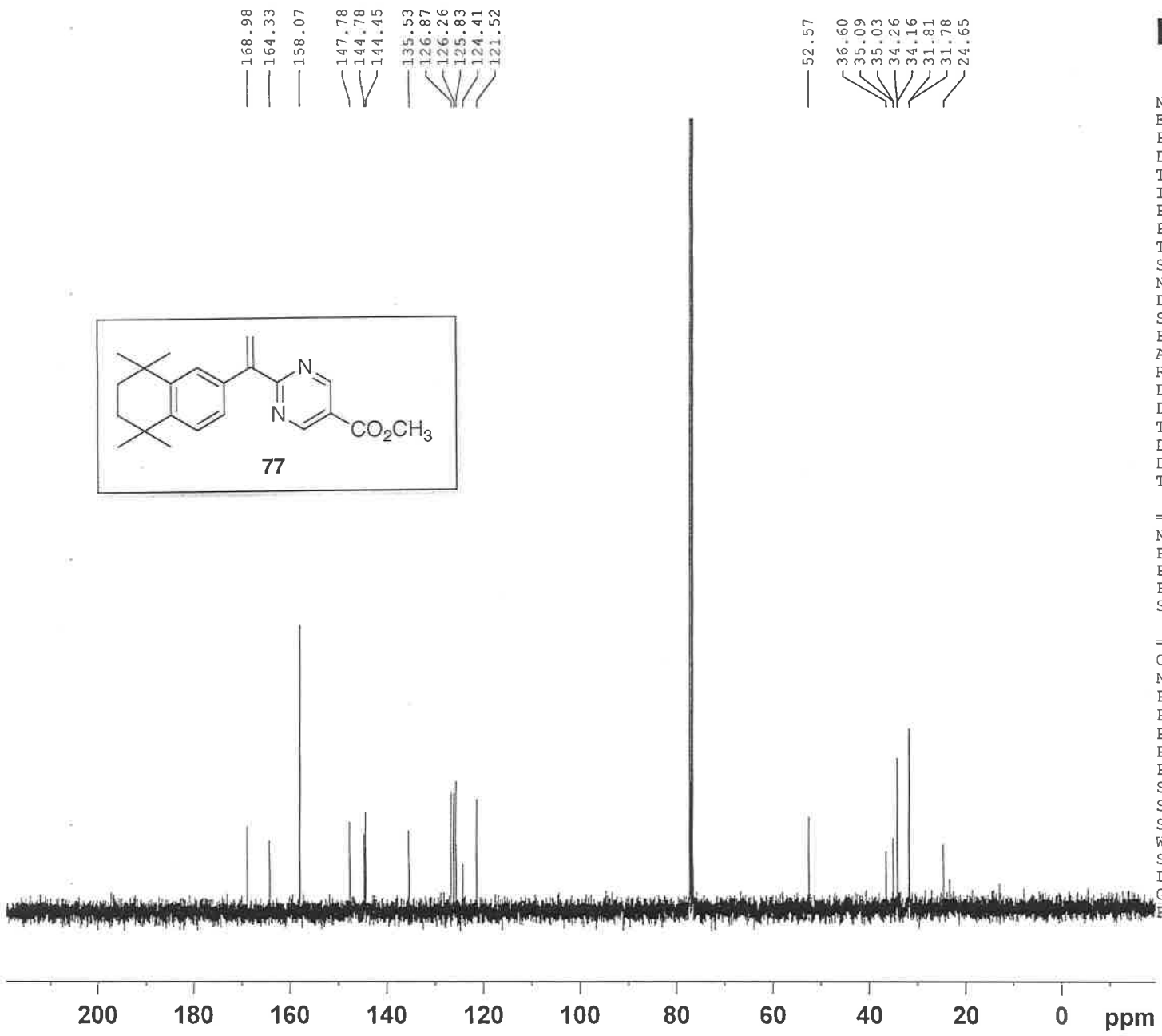
NAME	CWVI-025
EXPNO	2
PROCNO	1
Date_	20160729
Time	13.38
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	173
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	296.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127729 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

CWV-301



NAME	CWV-301
EXPNO	2
PROCNO	1
Date_	20151224
Time	16.17
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	298.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300096 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

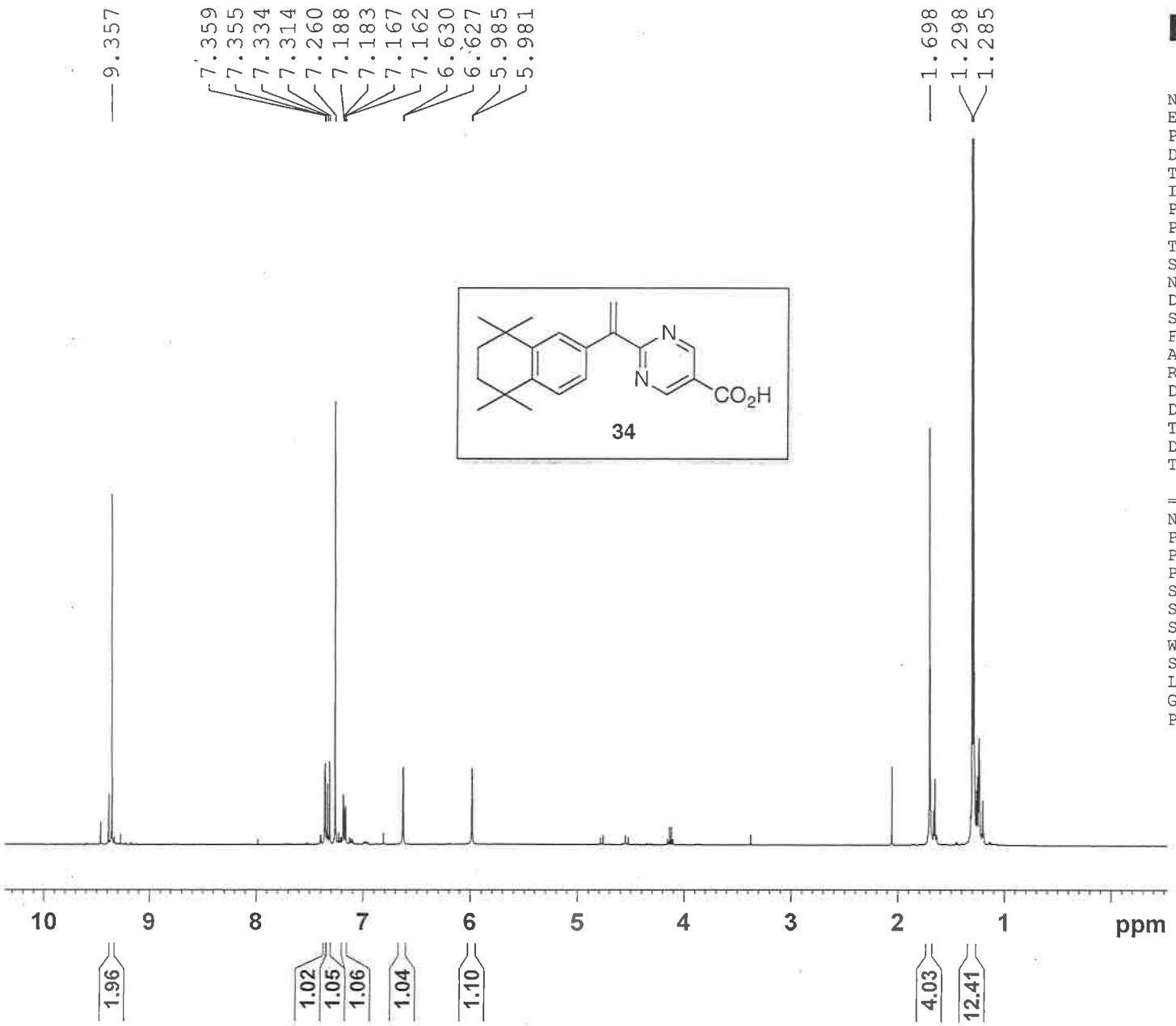
CWV-301



BRUKER

NAME	CWV-301
EXPNO	3
PROCNO	1
Date_	20151224
Time	16.22
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	112
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	298.3 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127729 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

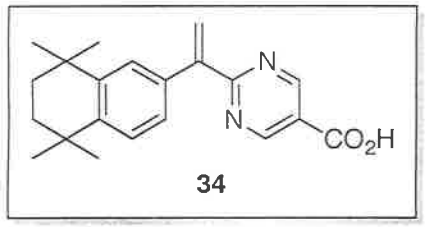
CWVI-009 from EtOAc



BRUKER

NAME	CWVI-009
EXPNO	2
PROCNO	1
Date_	20160331
Time	9.32
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	673.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300101 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWVI-009 from EtOAc



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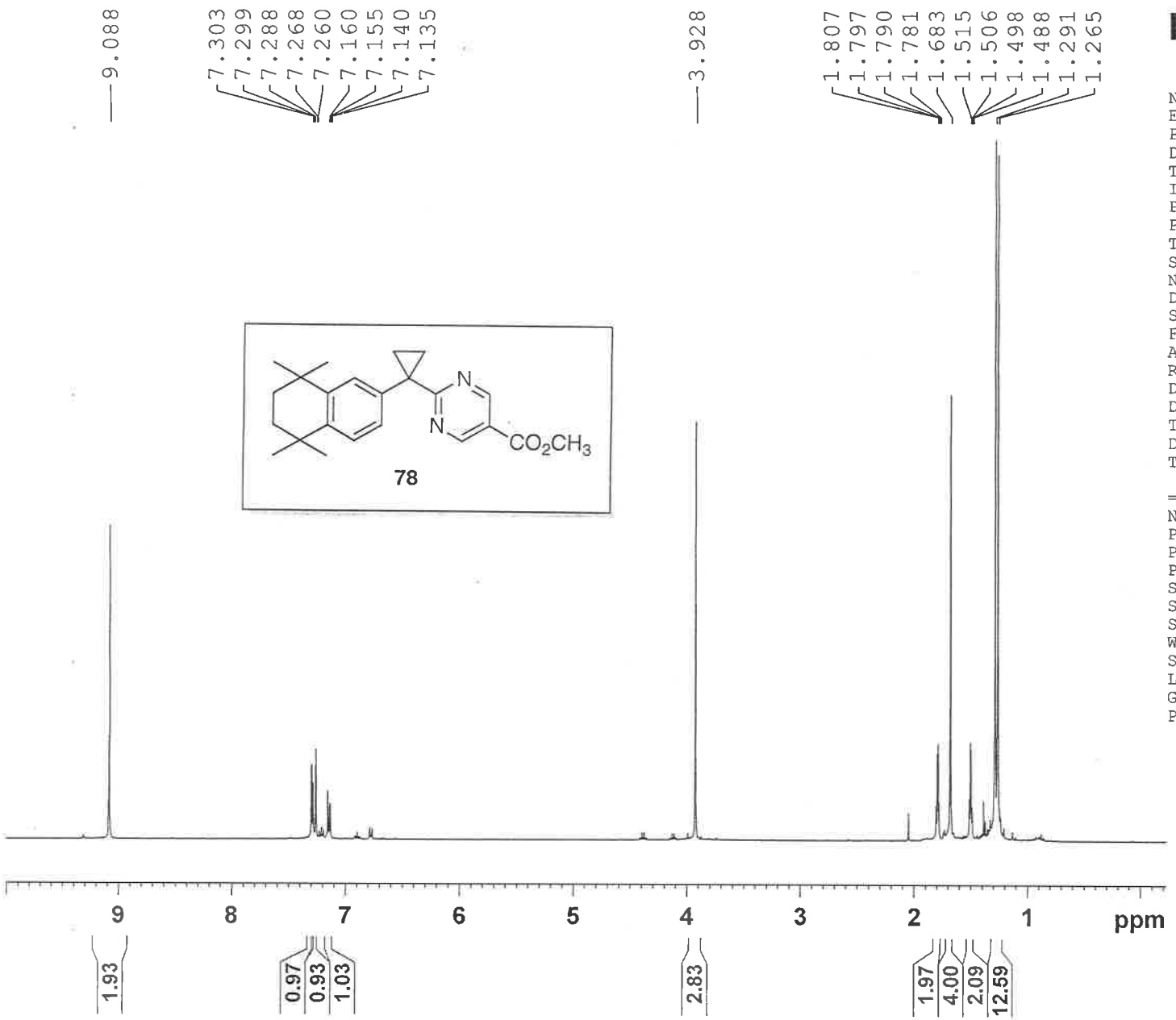
NAME	CWVI-009
EXPNO	3
PROCNO	1
Date_	20160401
Time	16.13
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	32372
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	673.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127722 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

CWVI-011



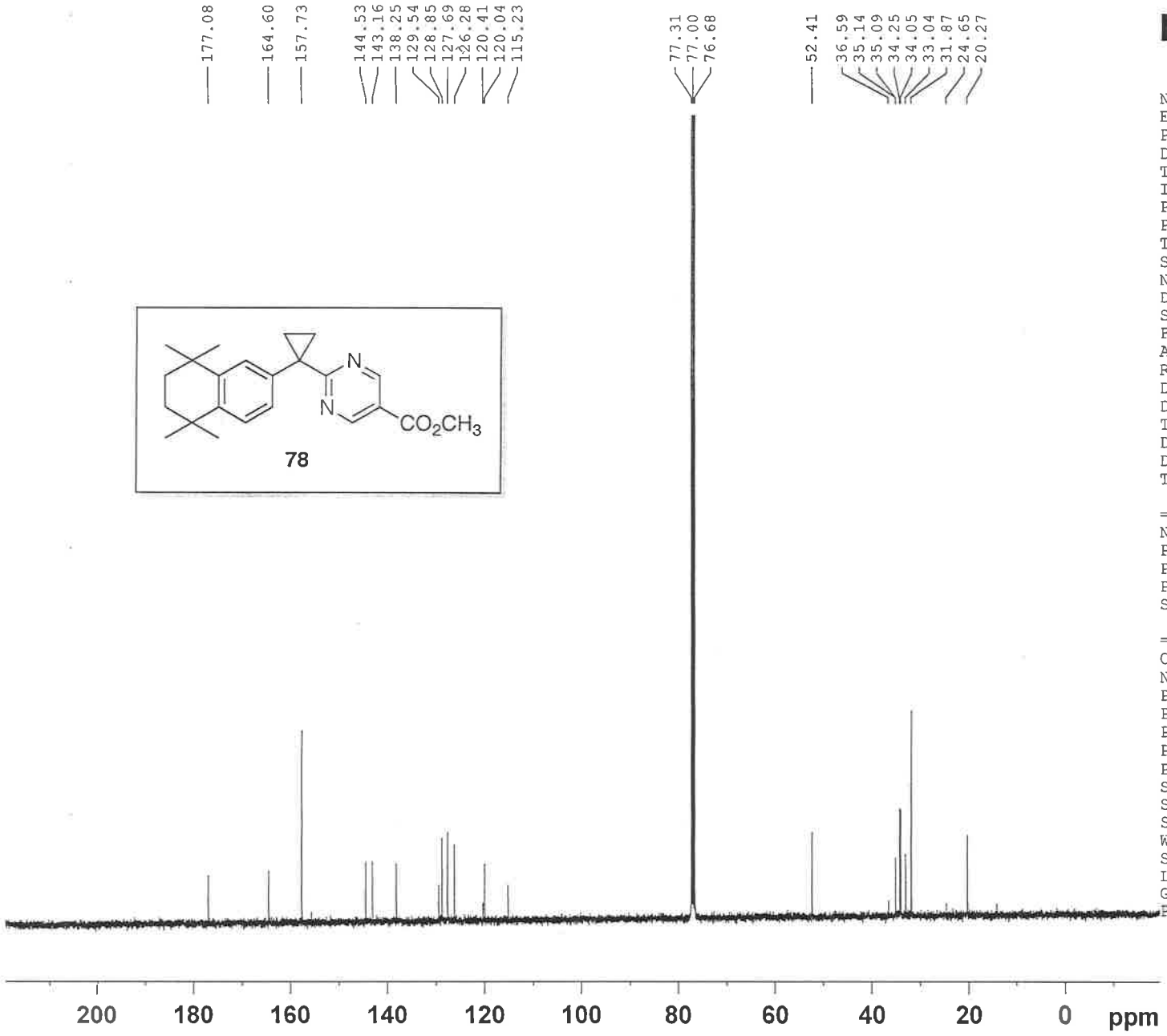
BRUKER

NAME	CWVI-011
EXPNO	1
PROCNO	1
Date_	20160317
Time	11.11
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	673.2 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300099 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

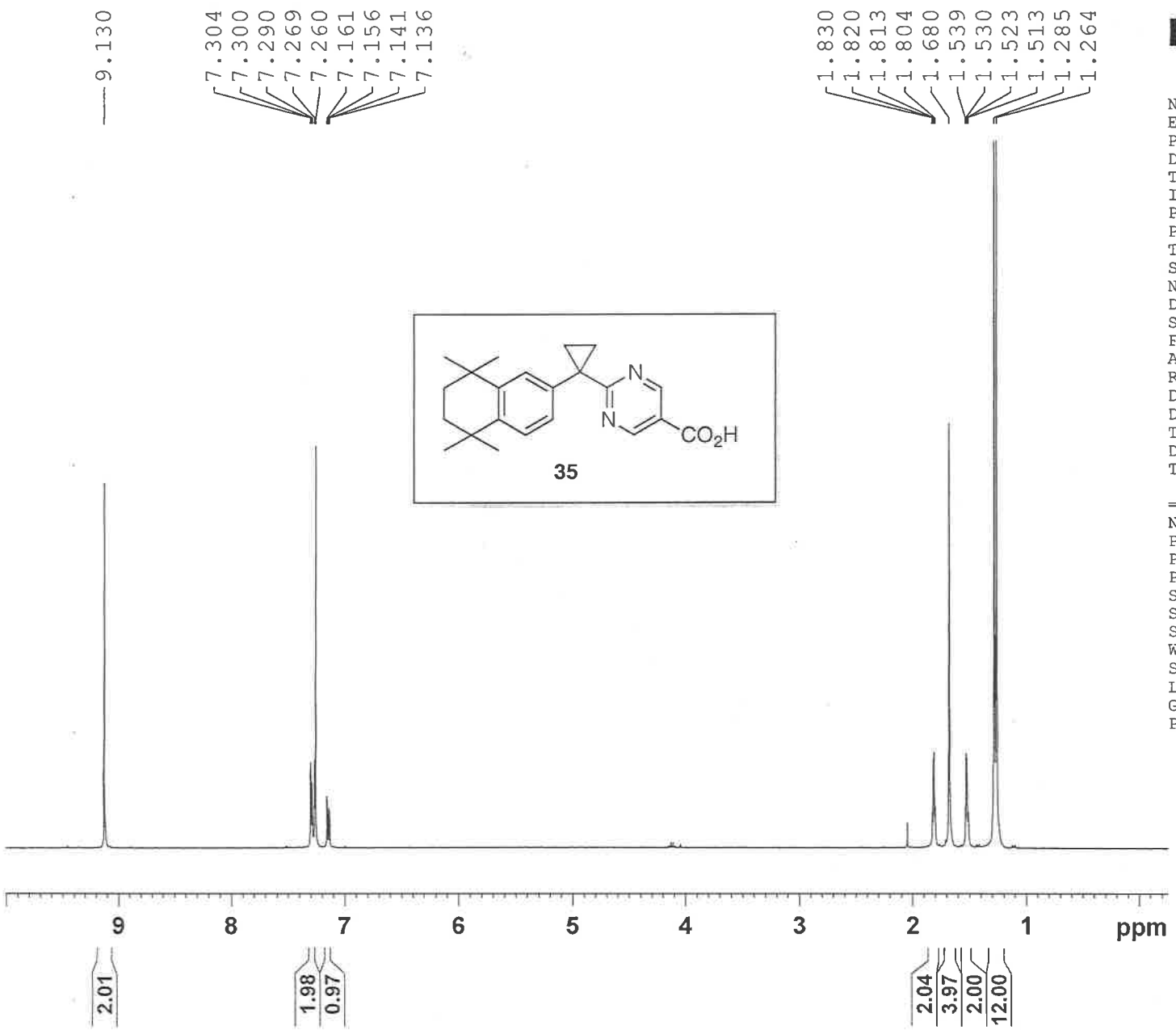
CWVI-011



BRUKER

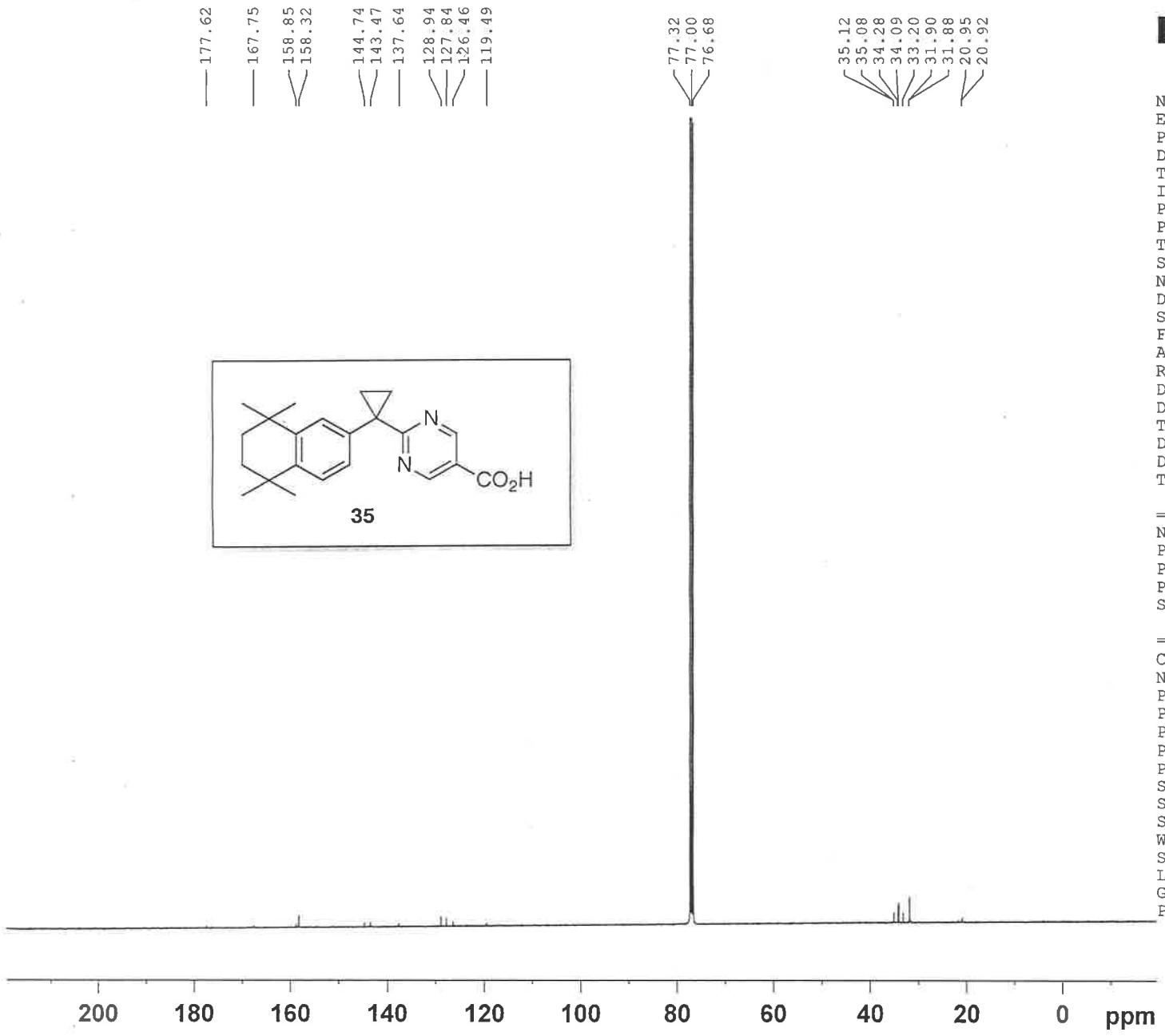
NAME	CWVI-011
EXPNO	2
PROCNO	1
Date_	20160317
Time	12.08
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	673.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127736 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

CWVI-013



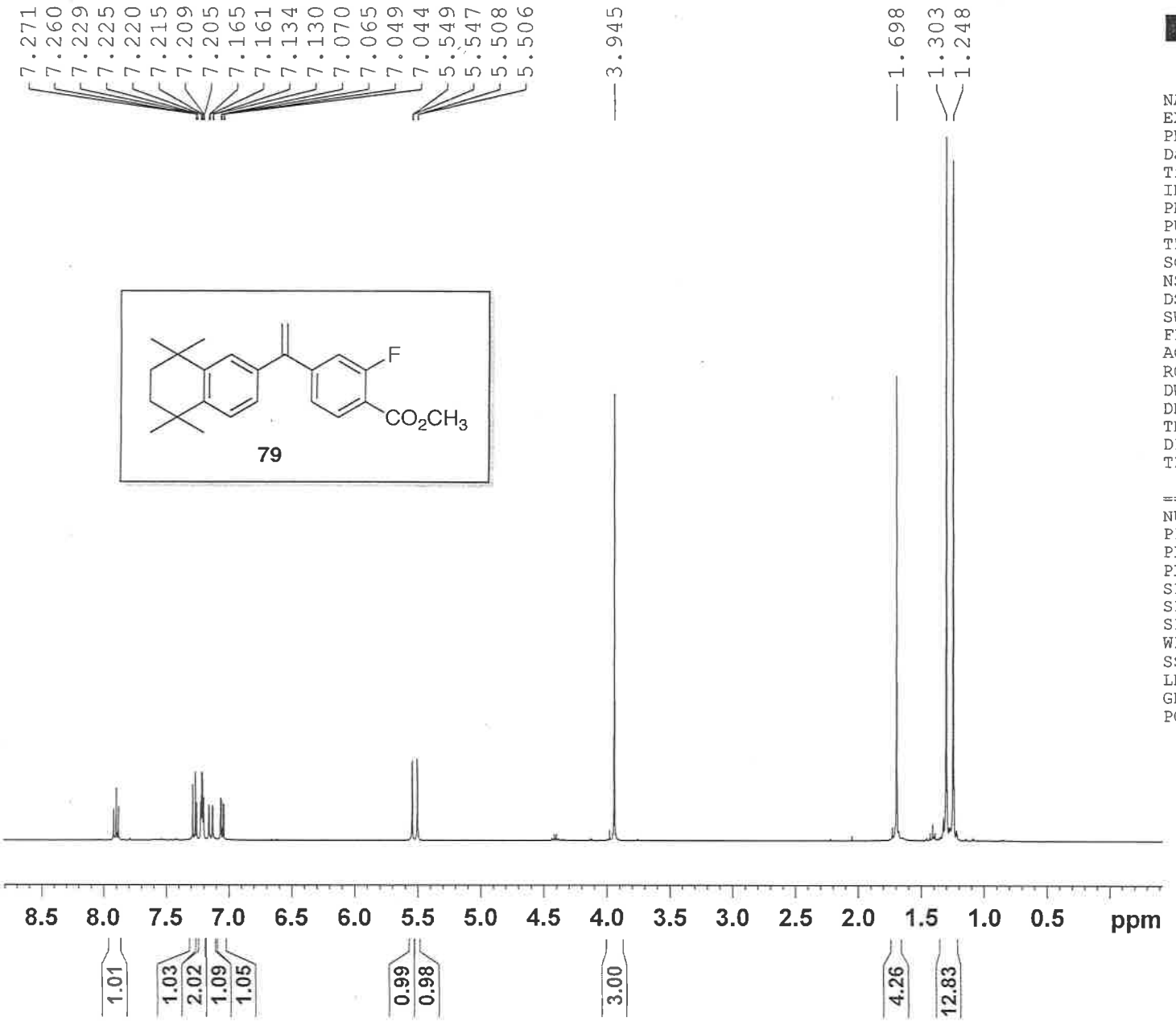
NAME	CWVI-013
EXPNO	1
PROCNO	1
Date_	20160323
Time	17.00
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	673.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300101 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWVI-013



NAME	CWVI-013
EXPNO	5
PROCNO	1
Date_	20160329
Time	10.19
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	29547
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	673.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127722 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

CWVI-019



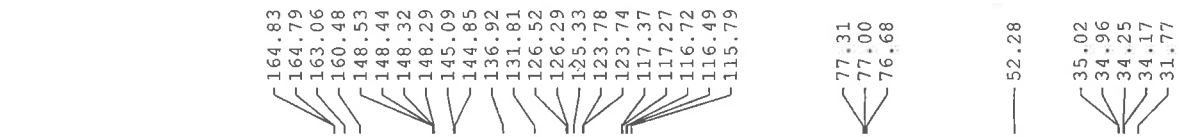
BRUKER

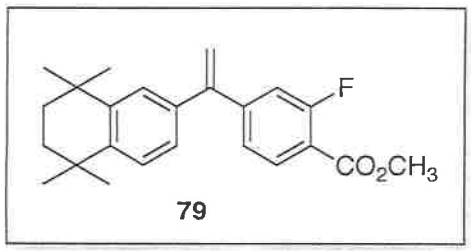
NAME	CWVI-019
EXPNO	1
PROCNO	1
Date_	20160728
Time	15.10
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	673.2 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300104 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWVI-019





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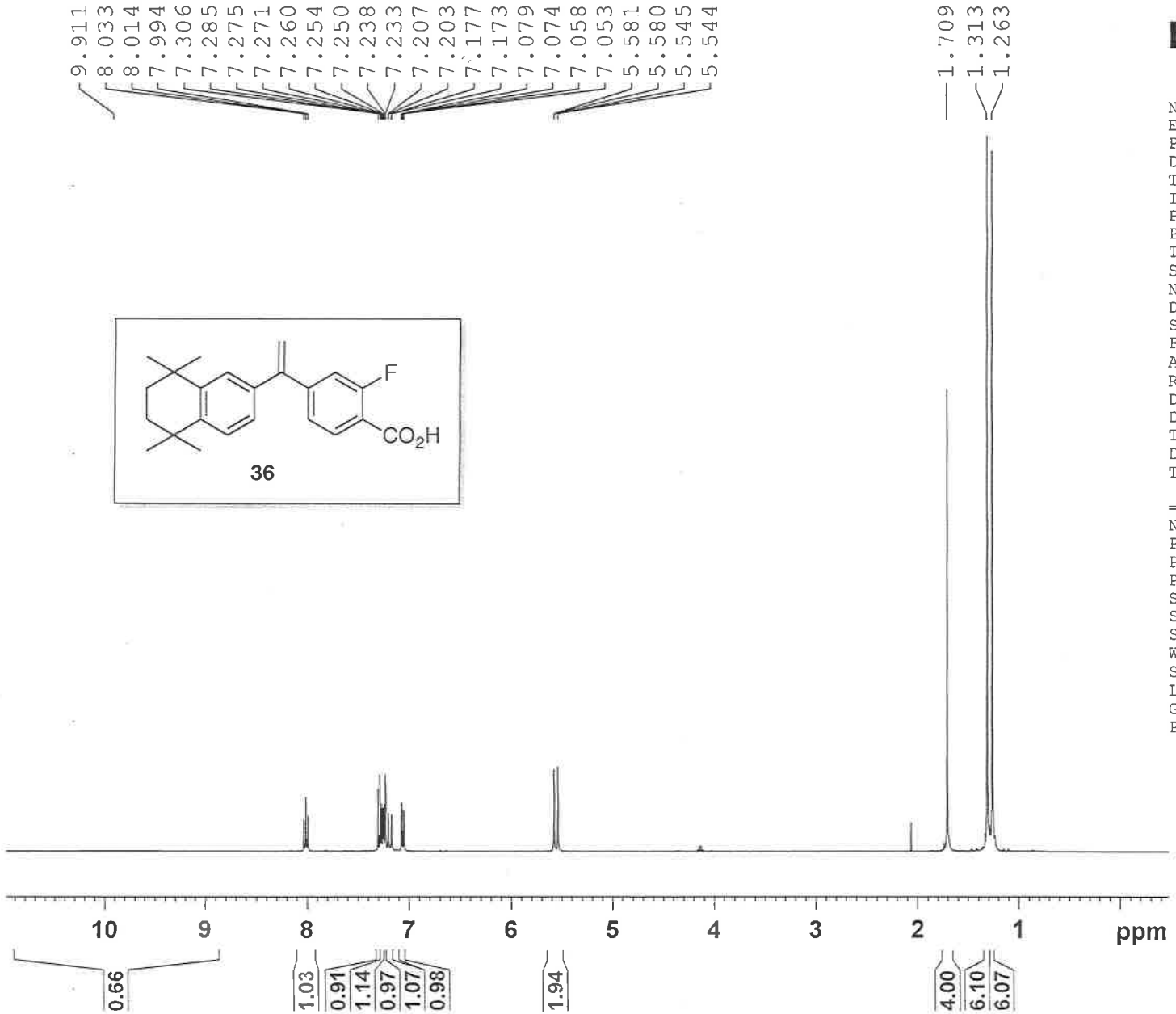
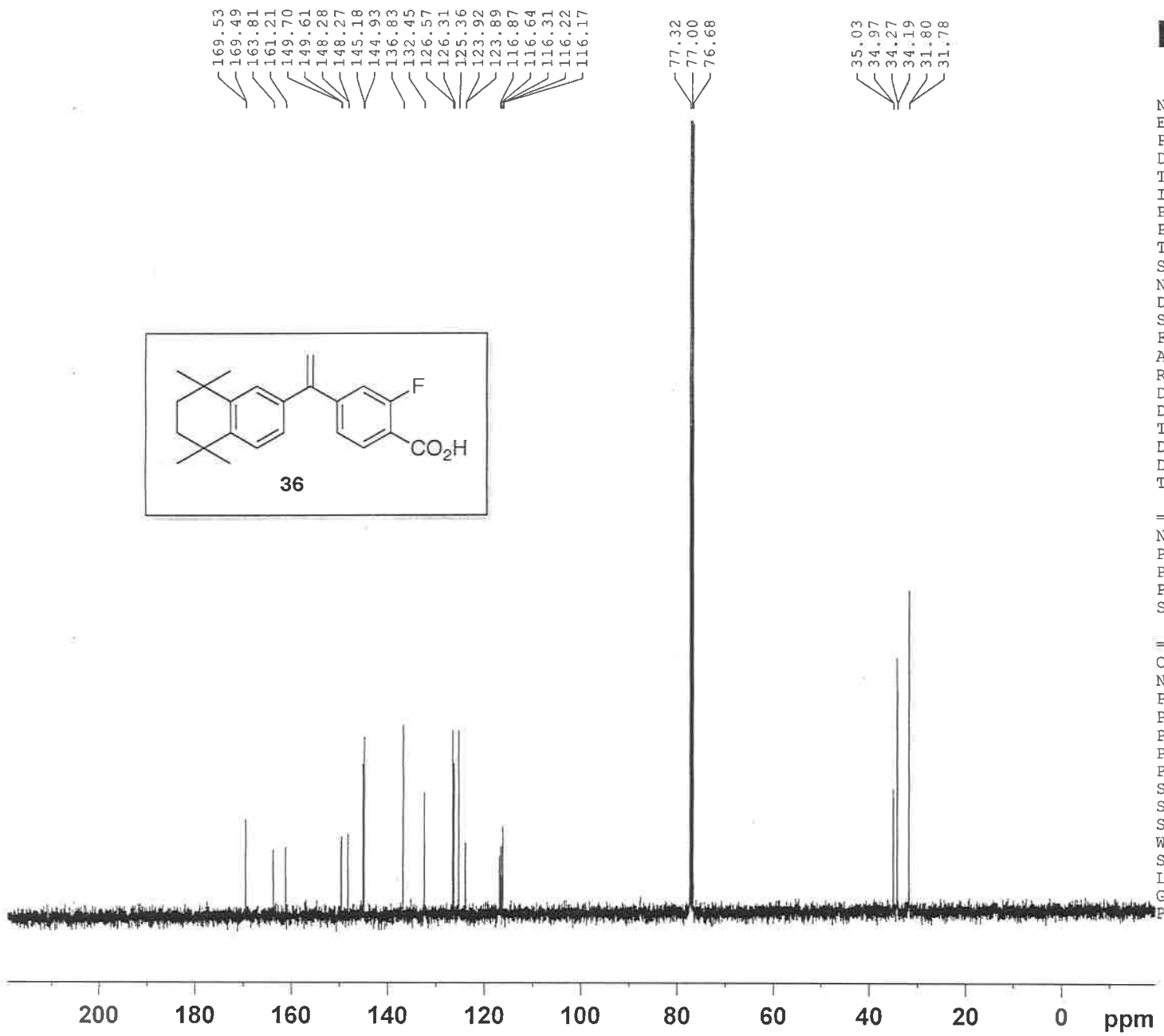
NAME	CWVI-019
EXPNO	2
PROCNO	1
Date_	20160728
Time	15.17
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	219
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	673.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127736 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

CWVI-023



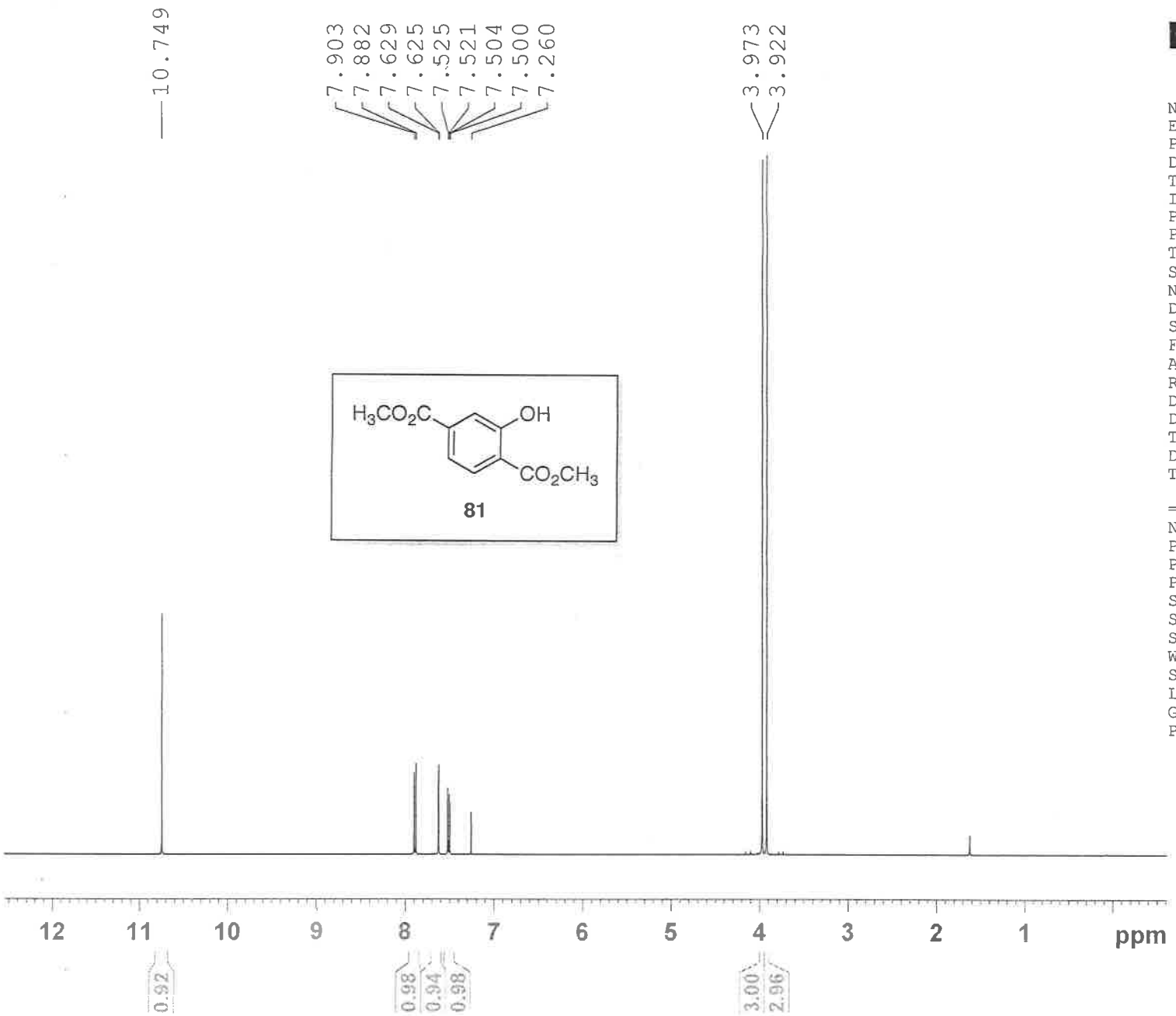
NAME	CWVI-023
EXPNO	1
PROCNO	1
Date_	20160729
Time	13.15
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	295.8 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300104 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWVI-023



NAME	CWVI-023
EXPNO	2
PROCNO	1
Date_	20160729
Time	13.21
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	201
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	296.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127729 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

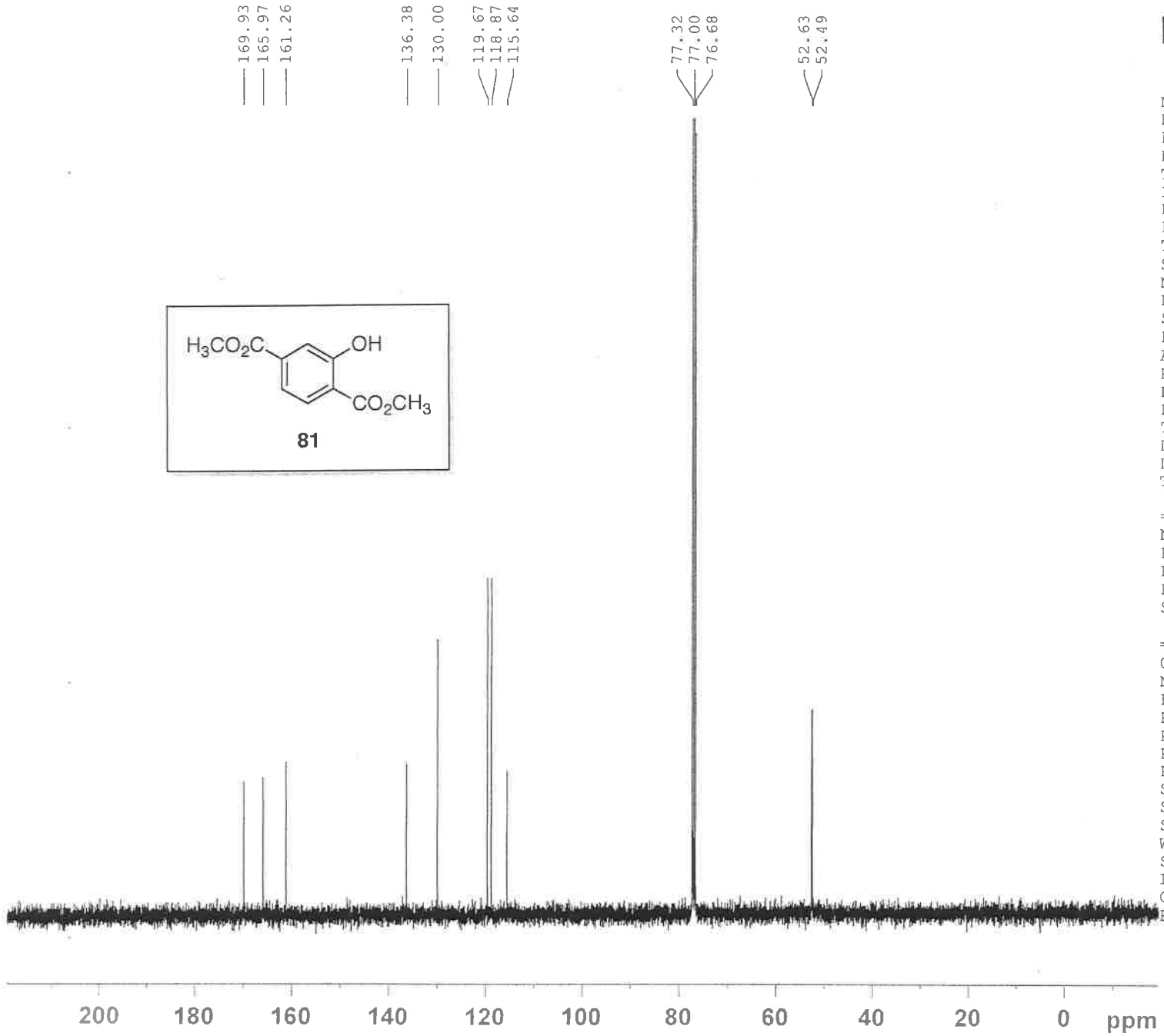
CWVI-053



BRUKER

NAME	CWVI-053
EXPNO	1
PROCNO	1
Date_	20161021
Time	10.55
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	673.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300101 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWVI-053



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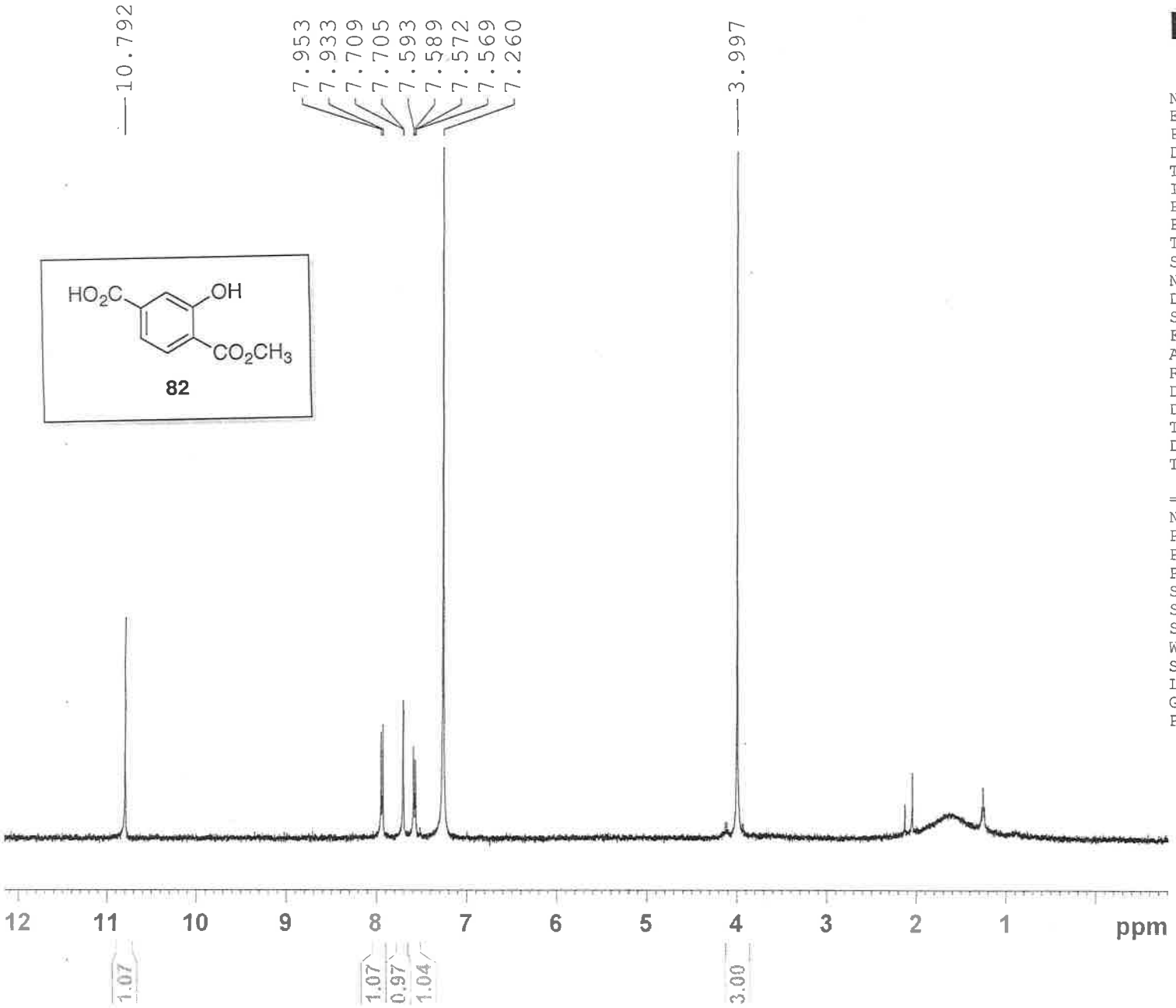
NAME	CWVI-053
EXPNO	2
PROCNO	1
Date_	20161021
Time	11.09
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	118
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	673.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127729 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

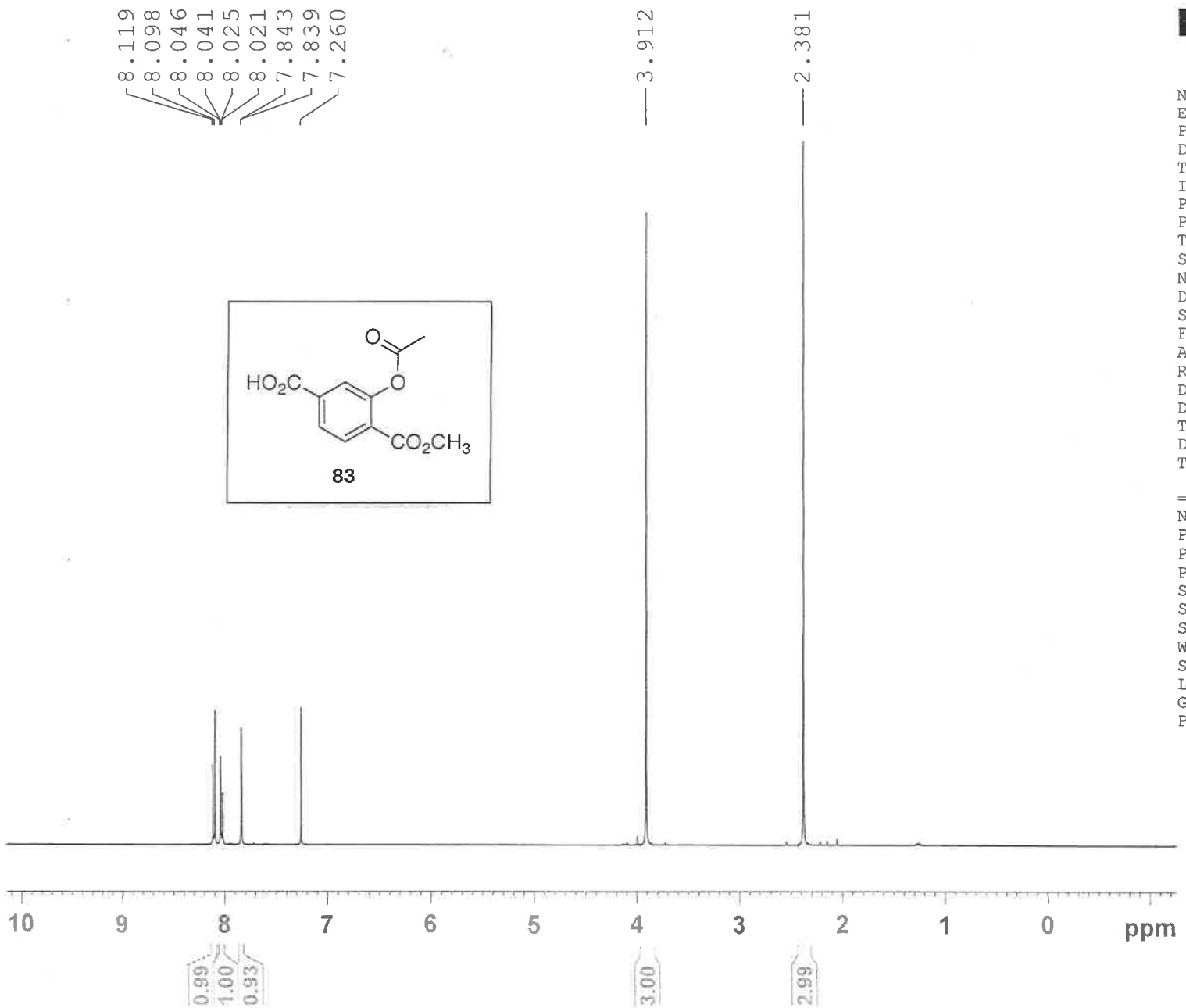
CWVI-059 Middle Spot



BRUKER

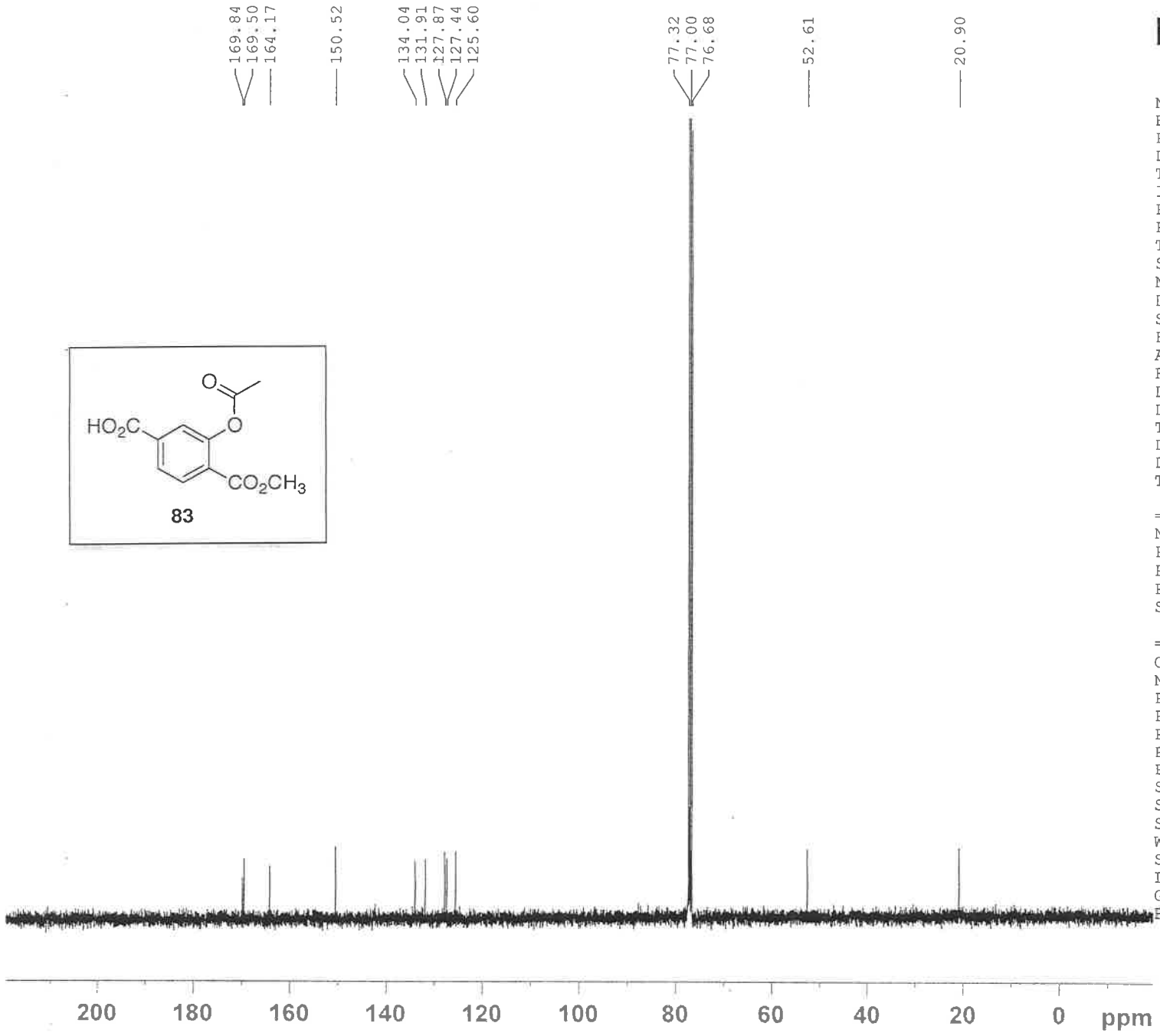
NAME	CWVI-059
EXPNO	2
PROCNO	1
Date_	20161107
Time	14.30
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	673.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300104 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWVI-061 f12-16



NAME	CWVI-061
EXPNO	2
PROCNO	1
Date_	20161122
Time	12.21
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	673.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300104 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWVI-061 f12-16



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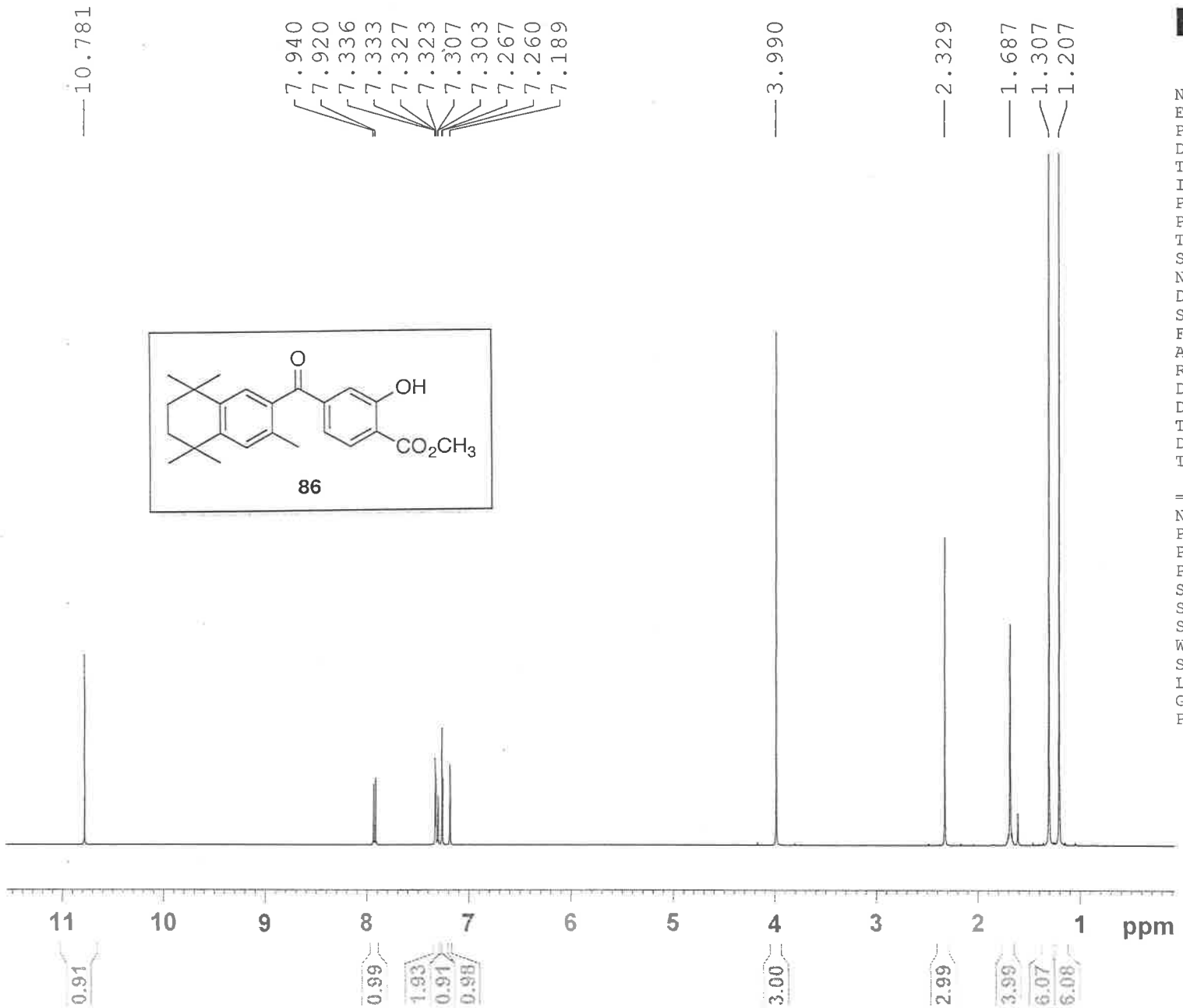
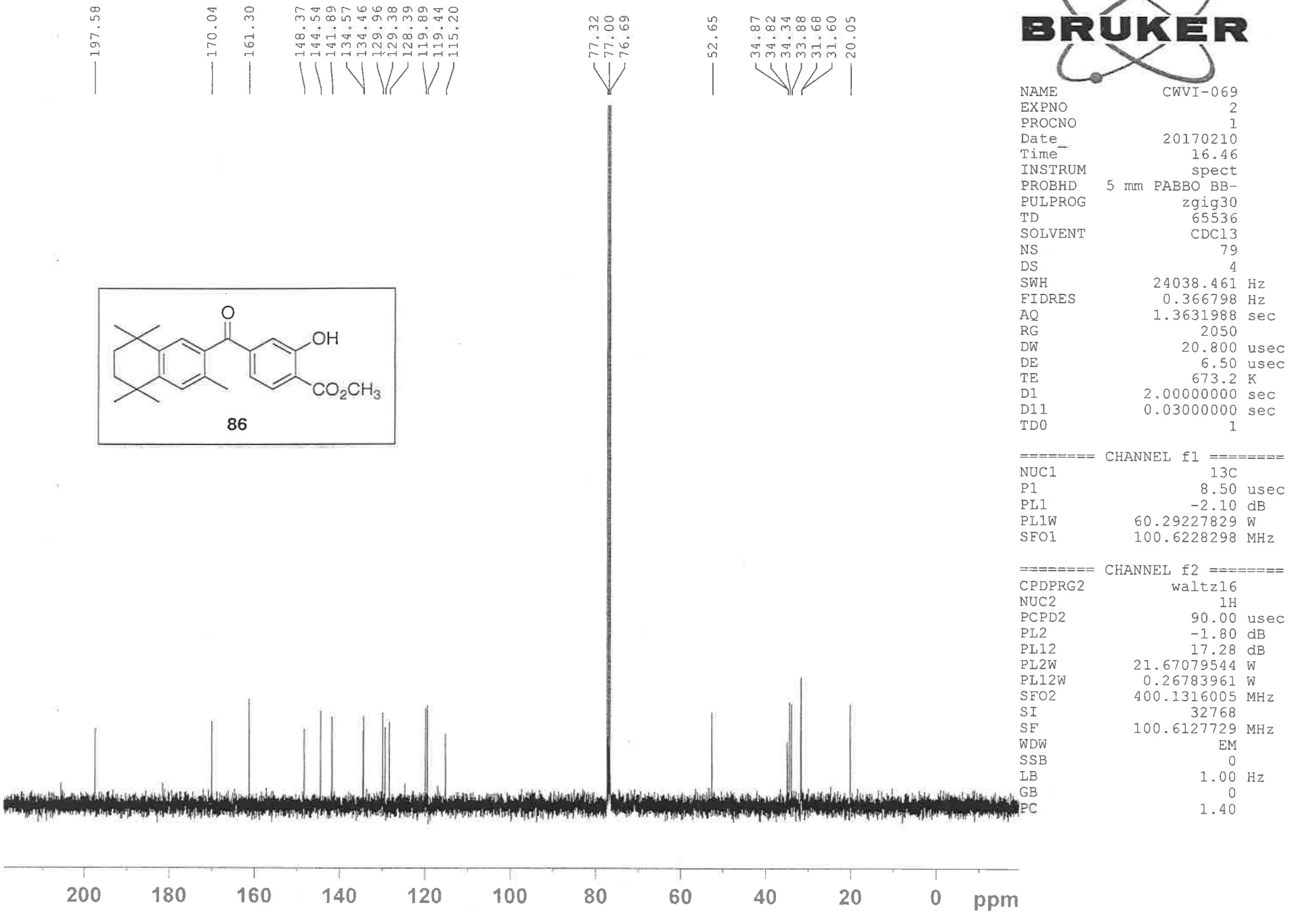
NAME	CWVI-061
EXPNO	3
PROCNO	1
Date_	20161122
Time	12.31
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	271
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	673.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127722 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

CWVI-069 f5-9



NAME	CWVI-069
EXPNO	1
PROCNO	1
Date_	20170210
Time	16.38
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	673.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300104 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

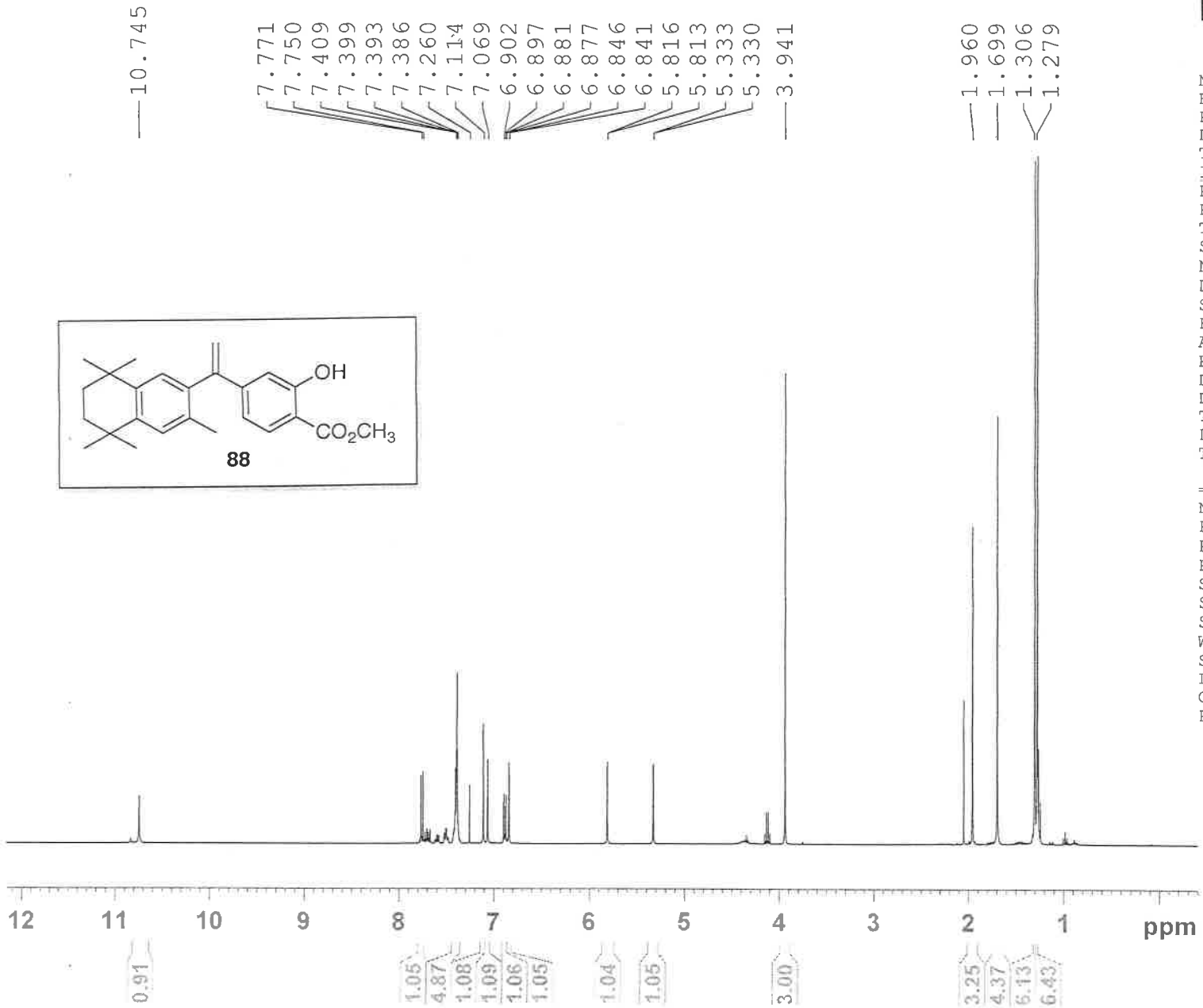
CWVI-069 f5-9



BRUKER

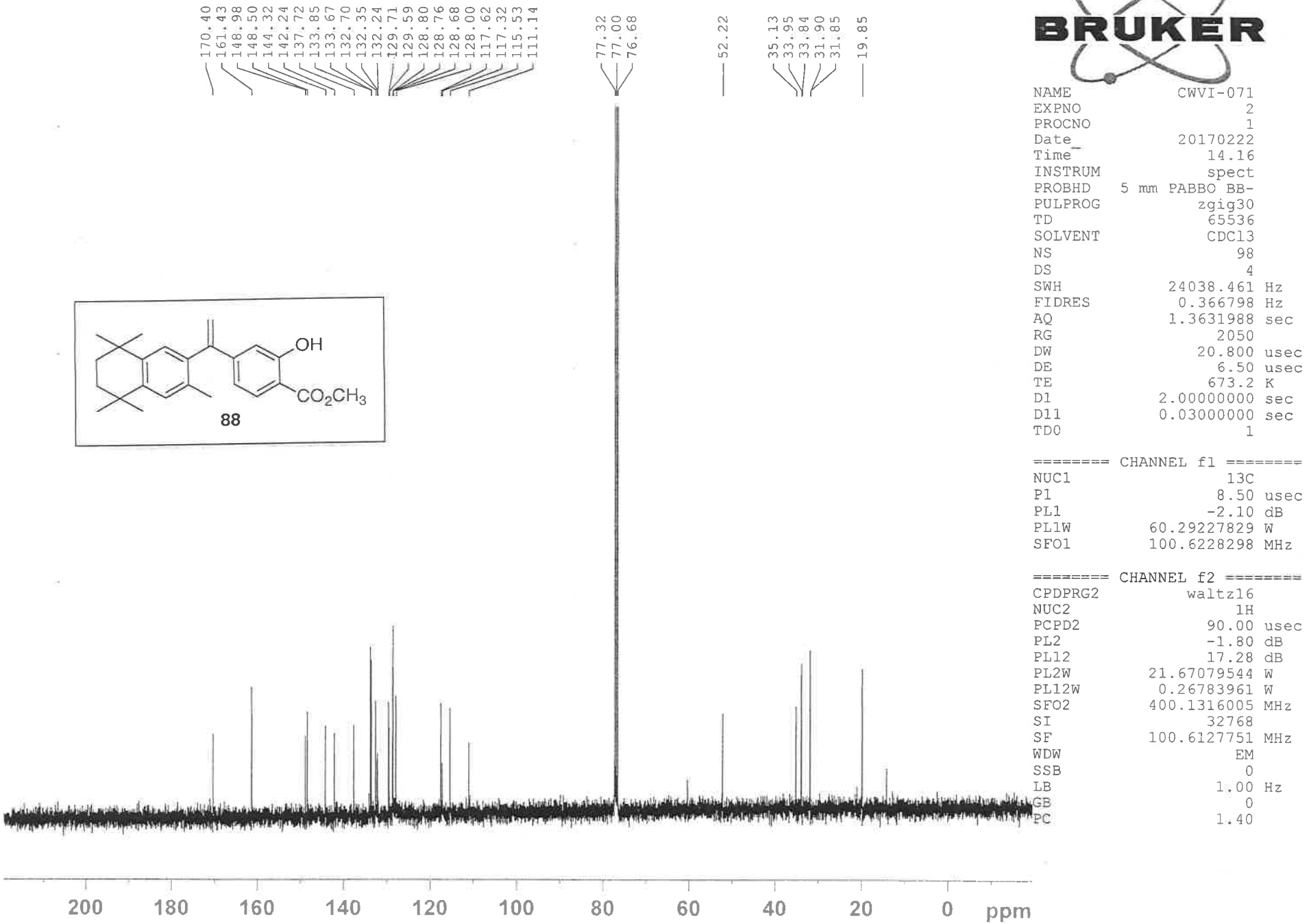
NAME	CWVI-069
EXPNO	2
PROCNO	1
Date_	20170210
Time	16.46
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	79
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	673.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127729 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

CWVI-071 f6B



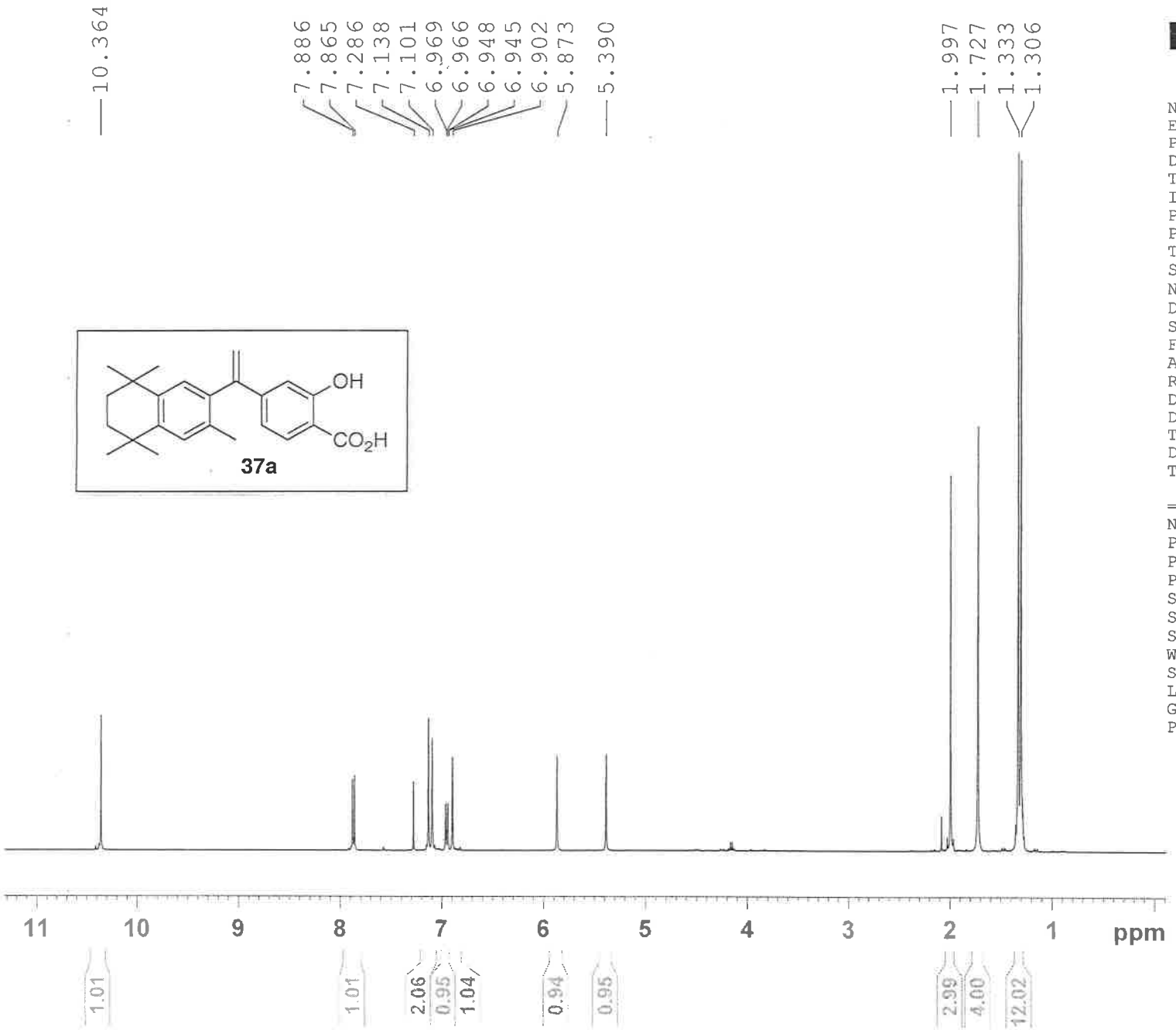
NAME	CWVI-071	
EXPNO	1	
PROCNO	1	
Date_	20170222	
Time	14.04	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	8223.685	Hz
FIDRES	0.125483	Hz
AQ	3.9846387	sec
RG	4	
DW	60.800	usec
DE	6.50	usec
TE	673.2	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	14.50	usec
PL1	0.50	dB
PL1W	12.76071072	W
SFO1	400.1324710	MHz
SI	32768	
SF	400.1300104	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

CWVI-071 f6B



NAME	CWVI-071
EXPNO	2
PROCNO	1
Date_	20170222
Time	14.16
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	98
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	673.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127751 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

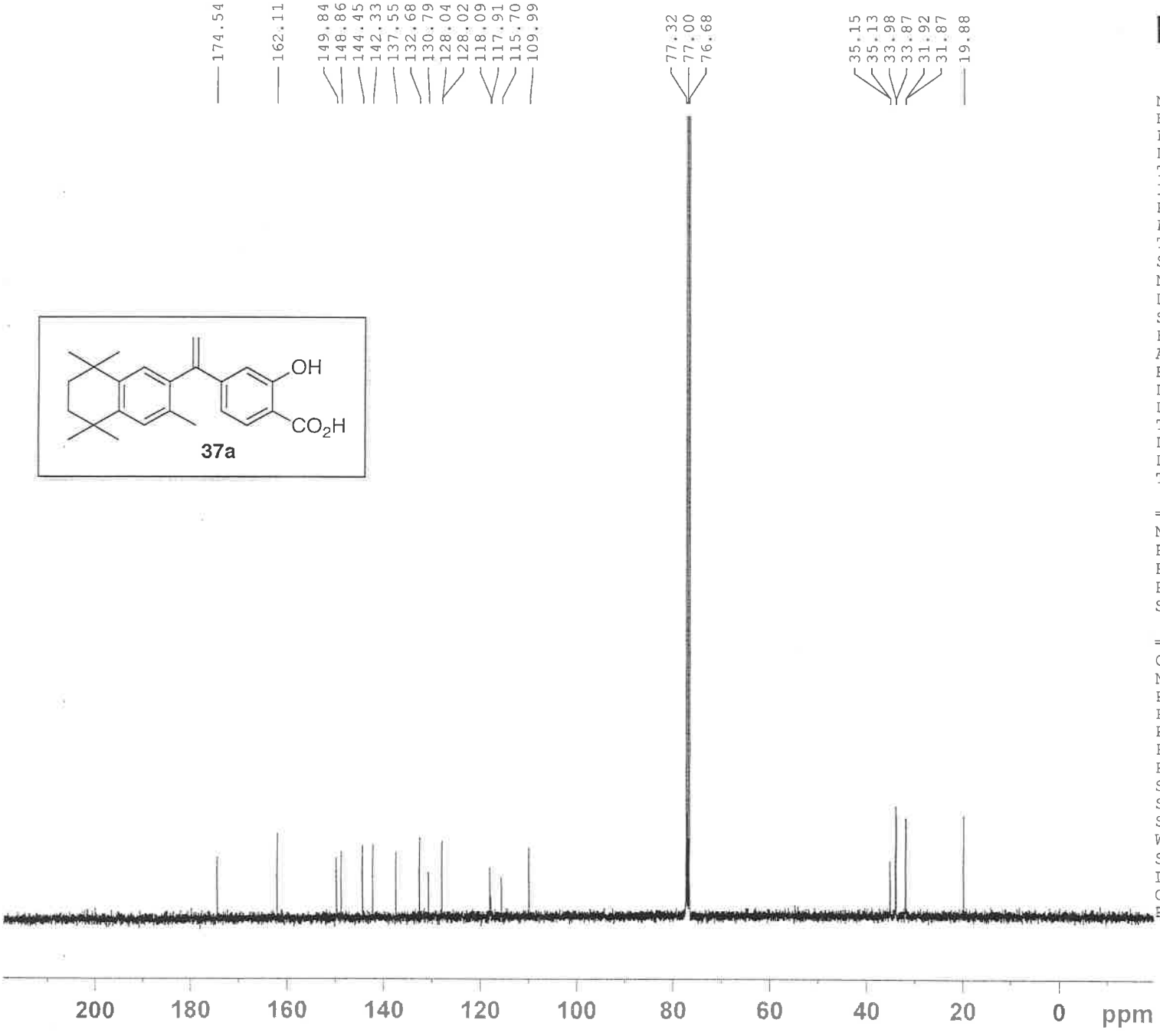
CWVI-073



BRUKER

NAME	CWVI-073
EXPNO	3
PROCNO	1
Date_	20170227
Time	14.28
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	298.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.75 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

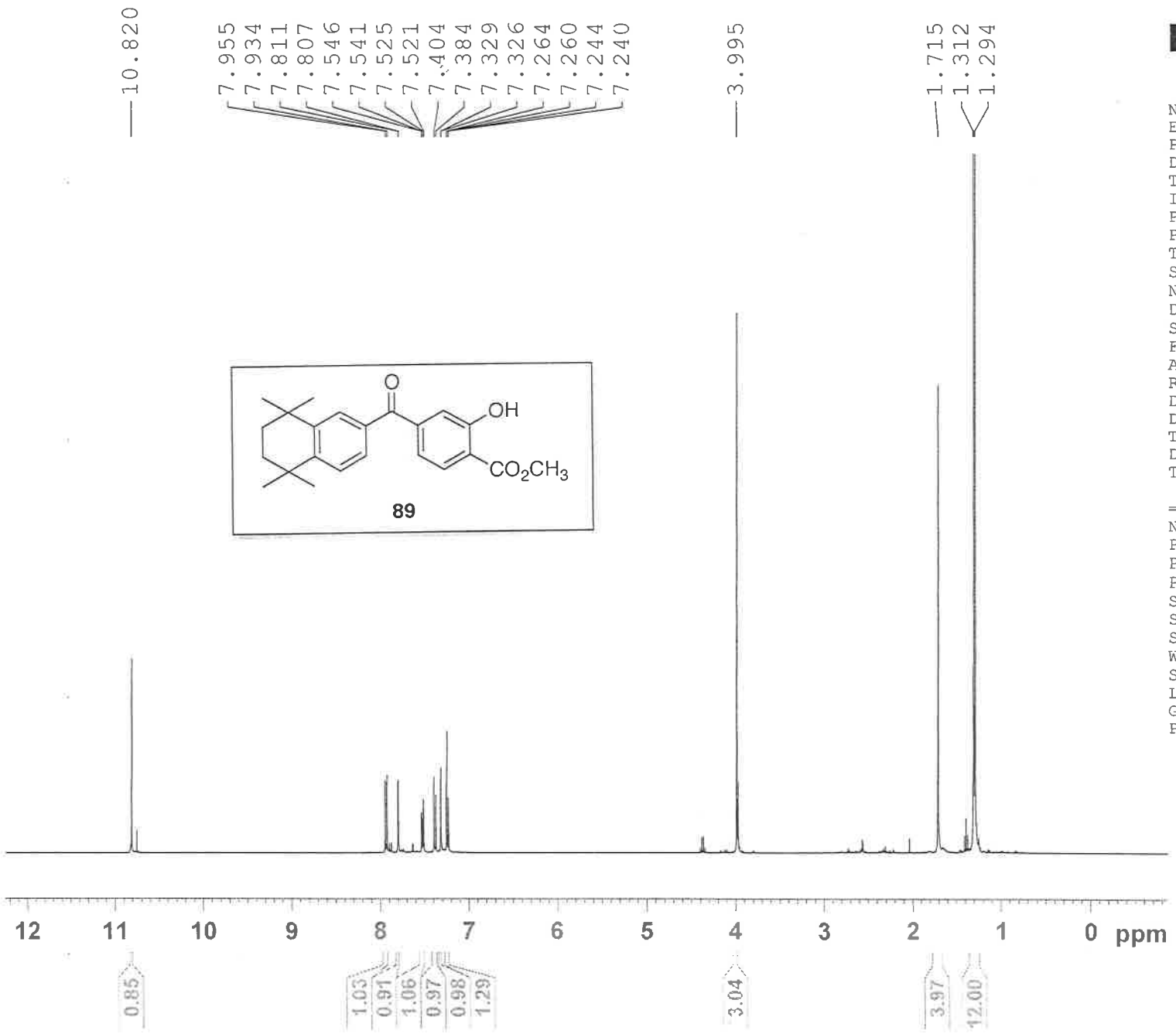
CWVI-073



BRUKER

NAME	CWVI-073
EXPNO	2
PROCNO	1
Date_	20170227
Time	9.58
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	500
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	673.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-1.80 dB
PL12	17.28 dB
PL2W	21.67079544 W
PL12W	0.26783961 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127729 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

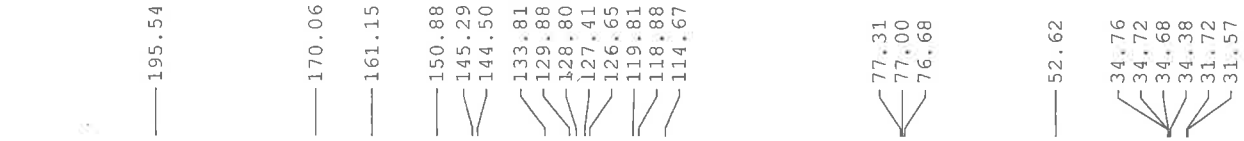
CWVI-099

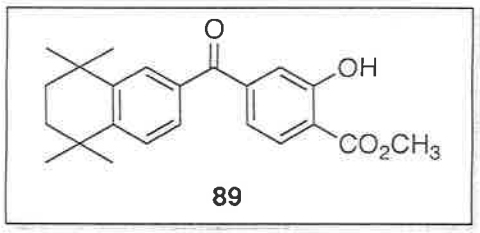


BRUKER

NAME	CWVI-099
EXPNO	1
PROCNO	1
Date_	20180305
Time	10.58
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	291.8 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.75 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300101 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWVI-099

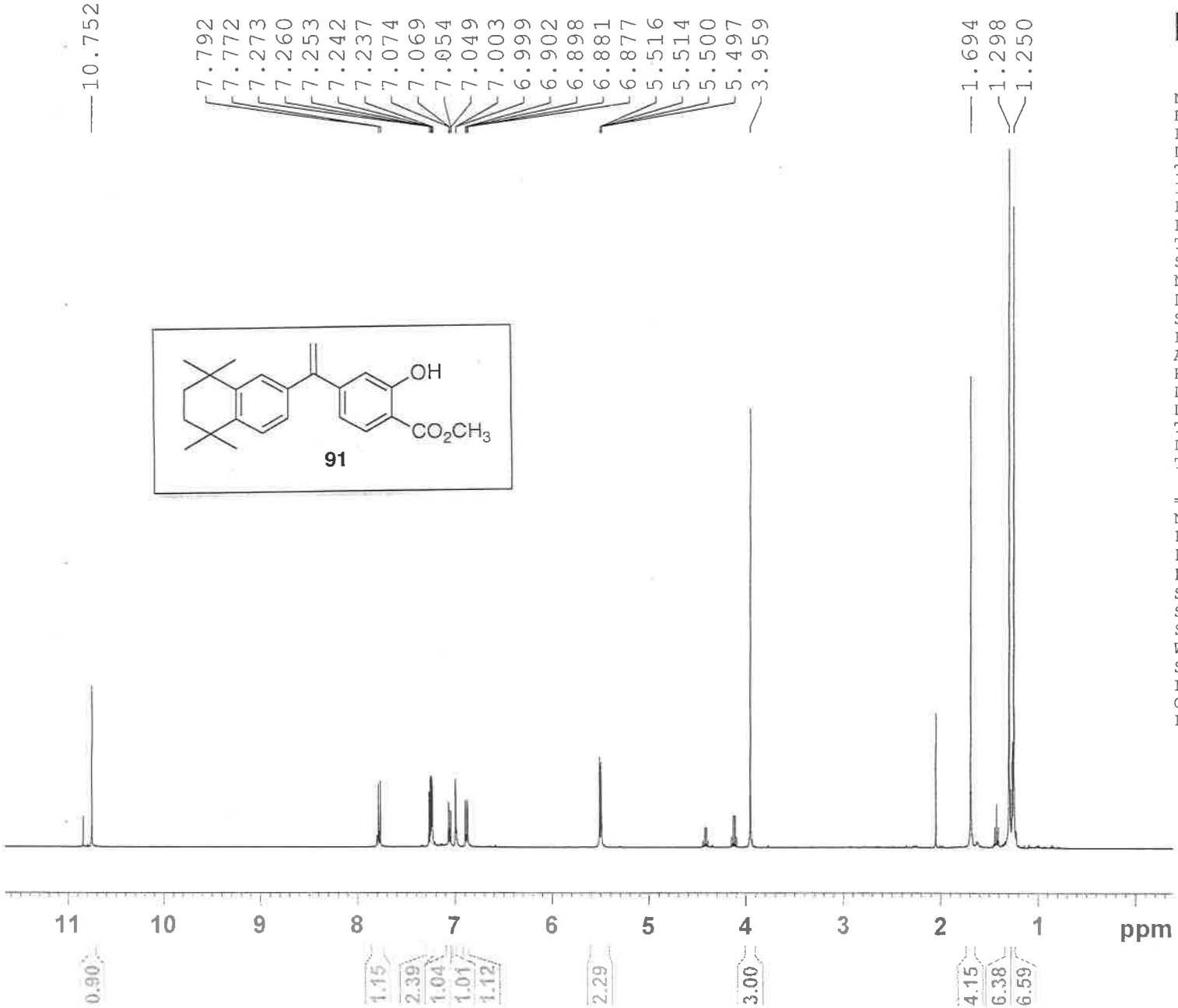




89

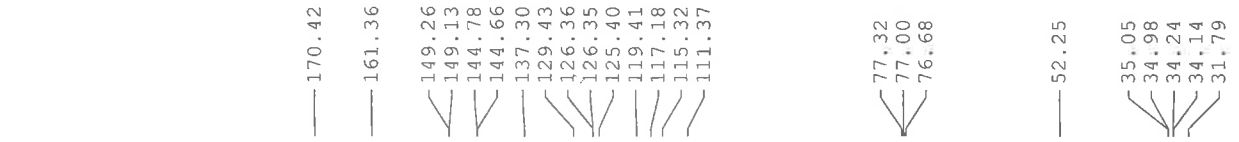
NAME	CWVI-099
EXPNO	2
PROCNO	1
Date_	20180305
Time	11.05
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	121
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	292.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	0.50 dB
PL12	16.21 dB
PL2W	12.76071072 W
PL12W	0.34266910 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127744 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

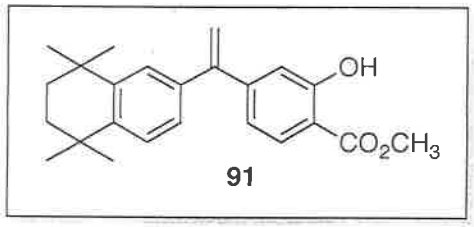
CWVI-101



NAME	CWVI-101
EXPNO	1
PROCNO	1
Date_	20180305
Time	11.12
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	291.9 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.75 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300104 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWVI-101

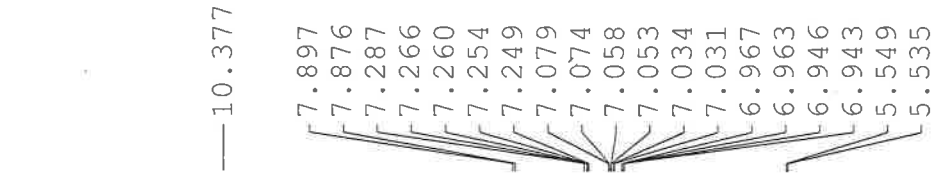


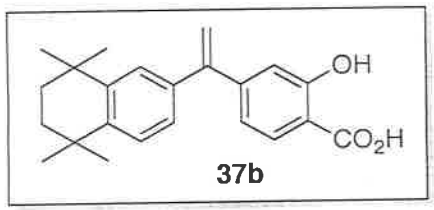


91

NAME	CWVI-101
EXPNO	2
PROCNO	1
Date_	20180305
Time	11.20
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	115
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	292.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	0.50 dB
PL12	16.21 dB
PL2W	12.76071072 W
PL12W	0.34266910 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127736 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

CWVI-103

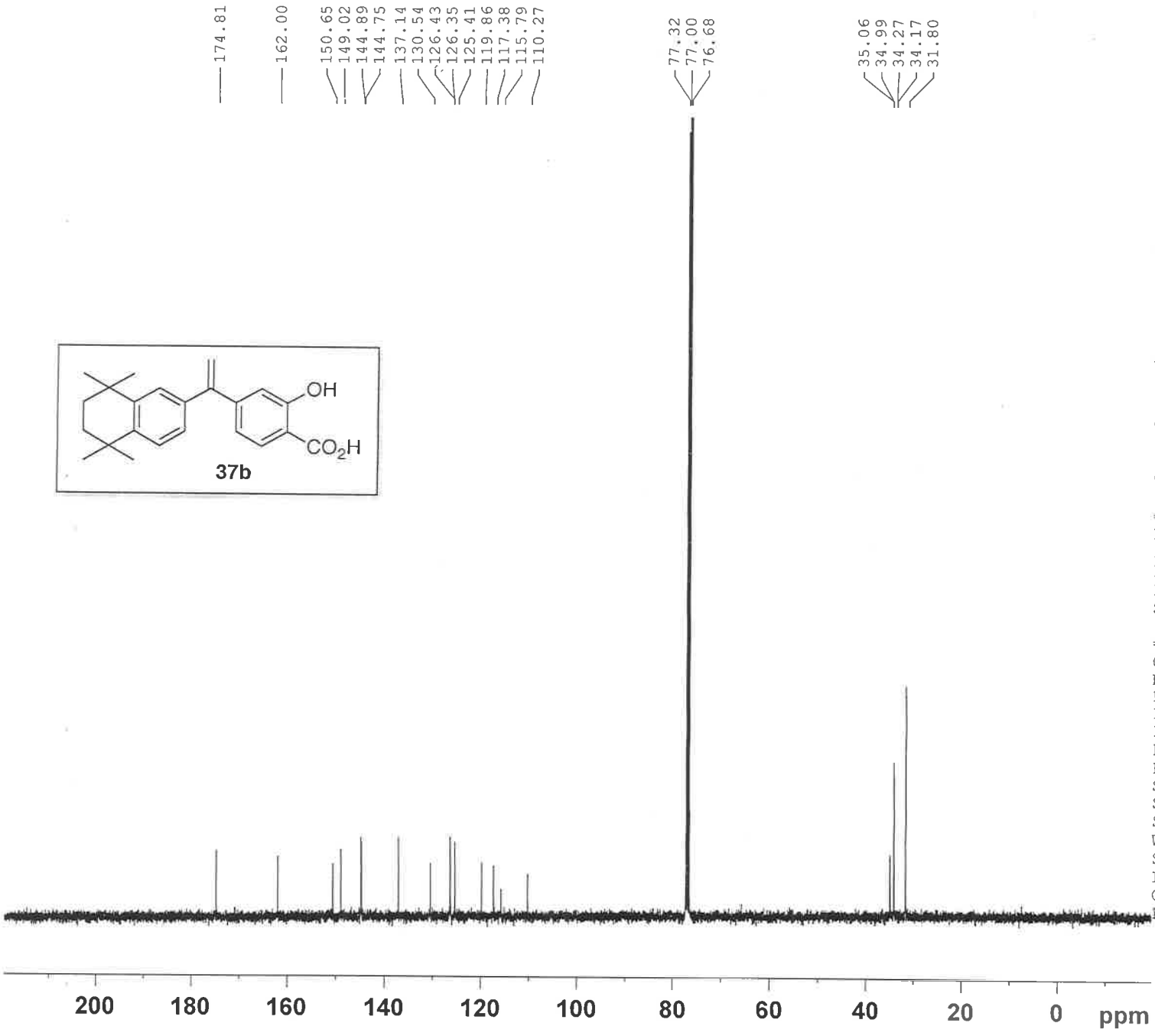




37b

NAME	CWVI-103
EXPNO	3
PROCNO	1
Date_	20181025
Time	13.57
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	4
DW	60.800 usec
DE	6.50 usec
TE	292.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.75 usec
PL1	0.50 dB
PL1W	12.76071072 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300099 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

CWVI-103



BRUKER

NAME	CWVI-103
EXPNO	4
PROCNO	1
Date_	20181025
Time	14.03
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgig30
TD	65536
SOLVENT	CDCl3
NS	541
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	292.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.25 usec
PL1	-2.10 dB
PL1W	60.29227829 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	0.50 dB
PL12	16.21 dB
PL2W	12.76071072 W
PL12W	0.34266910 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127729 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Acquisition Experiment Report
File: c:\masslynx\july 21.pro\data\210826_cw-vi-003.raw

Header
Acquired File Name: 210826_CW-VI-003
Acquired Date: 26-Aug-2021
Acquired Time: 09:54:58
Job Code: July21
Task Code:
User Name:
Laboratory Name:
Instrument: ACQ-QDA#KAD3226
Conditions:
Submitter:
SampleID:
Bottle Number: 2:1
Description:

Instrument Calibration:
Calibration File: C:\MassLynx\IntelliStart.pro\AcquDB\AutoCal.cal
Parameters
MS1 Static:
Mass: 30 Da to 1250 Da.
Resolution: -0.1/-0.0
Ion Energy: -0.3
Reference File: Internal
Acquisition File:
MS1 Scanning:
Mass: 30 Da to 1250 Da.
Resolution: -0.1/-0.0
Ion Energy: -0.3
Reference File: Internal
Acquisition File:
MS1 Scan Speed Compensation:
Scan: 40 to 10000 amu/sec.
Resolution: -0.1/-0.0
Ion Energy: -0.3
Reference File: Internal
Acquisition File:
Calibration Time: 10:54
Calibration Date: 09/13/17
Coefficients
MS1 Static: -0.000000000000*x^4 + 0.000000000656*x^3 +
-0.000001077025*x^2 + 1.000599988917*x +-0.085640798905
Function 1: -0.000000000000*x^4 + 0.000000000433*x^3 +
-0.000000811760*x^2 + 1.000482155999*x +-0.071926097790
Function 2: None

Parameters for C:\MassLynx\July

21.PRO\ACQUDB\NEG_100-500_C_2Hz_5min.EXP

Prescan Statistics:

Initial Average Intensity	379.7862	
Initial Average Std Dev		1.1247
Bunch Zero Level	0.0000	
Bunch Std Dev		0.0000
Bunch Threshold		0.0000
Spike Removal Std Dev		1.1245
Ion Count Threshold:		25.0000

Data Processing:

Targeted Sampling Frequency	2
Actual Sampling Frequency	2.000
SIR Chromatogram Spike Removal	ON
SIR Smoothing	ON
Smoothing window size (scans)	3
Number of smooths	2

Method Events:

Initial Stop Flow:	No Change
Initial Switch 1:	No Change

Timed Events Enabled

Event	Time(Sec)	Name	Action

Instrument Parameters - Function 1:

Polarity	ES-	
Calibration		Dynamic 2
Capillary (kV)		0.80
Cone (V)		5.00
Source Temperature (∞C)		120
Probe Temperature (∞C)		350
Calibration Temperature (∞C)		0

Engineers Settings:

LM 1 Resolution	-0.12
HM 1 Resolution	-0.02
Low Mass Ion Energy 1	-0.26
High Mass Ion Energy 1	-0.12
Low Mass Position	0.69
High Mass Position	-1.81
Low Mass Setup	0.63
High Mass Setup	-6.13
Detector Gain Positive	1.0
Detector Gain Negative	1.0
Nominal Rod Polarity	Negative

Dynamic Offset Positive Settings:

Dynamic Offset Low Mass Resolution	0.00
Dynamic Offset High Mass Resolution	0.00
Dynamic Offset Low Mass Ion Energy	0.00
Dynamic Offset High Mass Ion Energy	-0.02

Dynamic Offset Negative Settings:

Dynamic Offset Low Mass Resolution	-0.01
Dynamic Offset High Mass Resolution	0.21
Dynamic Offset Low Mass Ion Energy	0.00
Dynamic Offset High Mass Ion Energy	0.19

Dynamic Offset Settings:

Dynamic Offset Low Mass Position	-0.71
Dynamic Offset High Mass Position	-0.46
Dynamic Offset Low Mass Setup	0.55
Dynamic Offset High Mass Setup	-0.04
Dynamic Offset Linearity Gain	4.80

Set Detector Gain 1.0

Instrument Readbacks

Capillary (kV)		0.80
Cone (V)		-9.32
Source Temperature (∞C)		120
Multiplier	355	
Probe Temperature (∞C)		350
Calibration Temperature (∞C)		28

Inter-scan delays:
Automatic Mode
MS Delay Table

	R	delay
<=	16.000	0.005
>	16.000	0.006

Health Check Failures:
All Health Checks Passed

Health Checks all enabled unless shown below:
Resolution Setup Required
Recalibration Required
Service Due

ACE Experimental Record

Inlet Method File: c:\masslynx\july
21.pro\acqudb\col4_pfp_fa_acn_5mins

---------- Run method parameters ----------

-- PUMP --

Waters ACQUITY QSM
 Solvent A Name: Water
 Solvent B Name: Methanol
 Solvent C Name: 0.1% FA
 Solvent D Name: Acetonitrile
 Low Pressure Limit: 0 psi
 High Pressure Limit: 15000 psi
 Seal Wash Period: 5.00 min
 [Gradient Table]
  Time(min) Flow Rate(mL/min) %A %B %C %D Curve
 1. Initial 0.500 0.0 0.0 95.0 5.0 Initial
 2. 2.00 0.500 0.0 0.0 5.0 95.0 6
 3. 3.50 0.500 0.0 0.0 95.0 5.0 11
 4. 5.00 0.500 0.0 0.0 95.0 5.0 11
 Comment:
 Flow Ramp Rate: 0.45 min
 D Solvent Selection (if supported): No Change
 System Pressure Data Channel: No
 Flow Rate Data Channel: No
 %A Data Channel: No
 %B Data Channel: No
 %C Data Channel: No
 %D Data Channel: No
 Primary Data Channel: No
 Accumulator Data Channel: No
 Degasser Data Channel: No
 Gradient Start: At Injection
 Gradient Start Volume: 0 uL
 Gradient Start Time: 0.00 min
 Participate in pre-analysis: No

-- END PUMP --

-- DETECTOR --

Waters Acquity CM

 Target Column Temperature: 50.0 C
 Temperature Alarm Band: 5.0 C
 : No

Column Valve Position: Column 4
Equilibration Time: 0.1 min
External Valve 1: No Change
External Valve 2: No Change
External Valve 3: No Change
Comment:
Column Temperature Data Channel: No
Preheater Temperature Data Channel: No

-- END DETECTOR --

-- DETECTOR --

Waters Acquity PDA

Run Time: 5.00 min
PDA Detector Type: UPLC LG 500 nm
Lamp: On
Sampling Rate: 20 points/sec
Filter Time Constant: 0.2000 sec
Exposure Time: Auto msec
Interpolate 2nd order filter Region: No
Use UV Blocking Filter: Yes
3D Channel...
Range: 210 - 499
Resolution: 2.4 nm
Channel 1...
Data Mode: Absorbance at 214
Resolution: 2.4 nm
Channel 2...
Data Mode: Absorbance at 380
Resolution: 2.4 nm
Initial Switch 1: No Change
Initial Switch 2: No Change

-- END DETECTOR --

-- AUTOSAMPLER --

Waters ACQUITY FTN AutoSampler
Run Time: 5.00 min
Comment:
Load Ahead: Disabled
Loop Offline: Automatic min
Wash Solvent Name: Weak Wash
Pre-Inject Wash Time: 0.0 sec
Post-Inject Wash Time: 6.0 sec
Purge Solvent Name: Strong Wash

Maximum System Pressure: 5734.0 psi

Average System Pressure: 4515.0 psi

---------- oOo ----------

---------- Waters ACQUITY FTN Postrun Report ----------

Software Version: 1.60.1774

Firmware Version: 1.60.364 (Sep 20 2013)

Checksum: 0x35d5392b

Serial Number: D17SDI835G

Sample Syringe Size: 100.0

Extension Loop Size: 0.0

Needle Size: 30.0

Minimum Sample Temperature: 10.0

Maximum Sample Temperature: 10.2

Average Sample Temperature: 10.1

Minimum Column Temperature: -0.2

Maximum Column Temperature: 0.0

Average Column Temperature: -0.2

---------- oOo ----------

---------- Waters Acquity CM Postrun Report ----------

Software Version: 1.60.2072

Firmware Version: 1.65.142 (Apr 02 2015)

Checksum: 0x18bfb4ea

Serial Number: D17CMP604G

Valve Position: 4

Minimum Column Temperature: 50.0

Maximum Column Temperature: 50.0

Average Column Temperature: 50.0

---------- oOo ----------

---------- Active eCord Data ----------

Valve Current Position: 4
Failed to retrive Active eCord ColumnData Data

---------- oOo ----------

---------- Generic Instrument Postrun Report ----------

Software Version: 1.60.1390

Firmware Version: 1.60.6169 (Aug 13 2013)

Checksum: 0xdcfe9340

Serial Number: B17UPD132A

Lamp On/Off Event: No

Lamp Life: 3223.00 hours

Lamp Serial Number: 000133684

Exposure Time: 50.000 msec

Lambda1: 187.360

Lambda512: 502.647

Flow Cell Type: Analytical LG

Flow Cell Path Length: 10.000 mm

Flow Cell Volume: 0.500 microliters

Flow Cell Serial Number: PDA10-15625

Flow Cell Part Number: 205015017

Optics Temperature Stabilzation Setting: Normal Temperature

---------- oOo ----------

----------Failed to get IECordHost2 Interface ---------

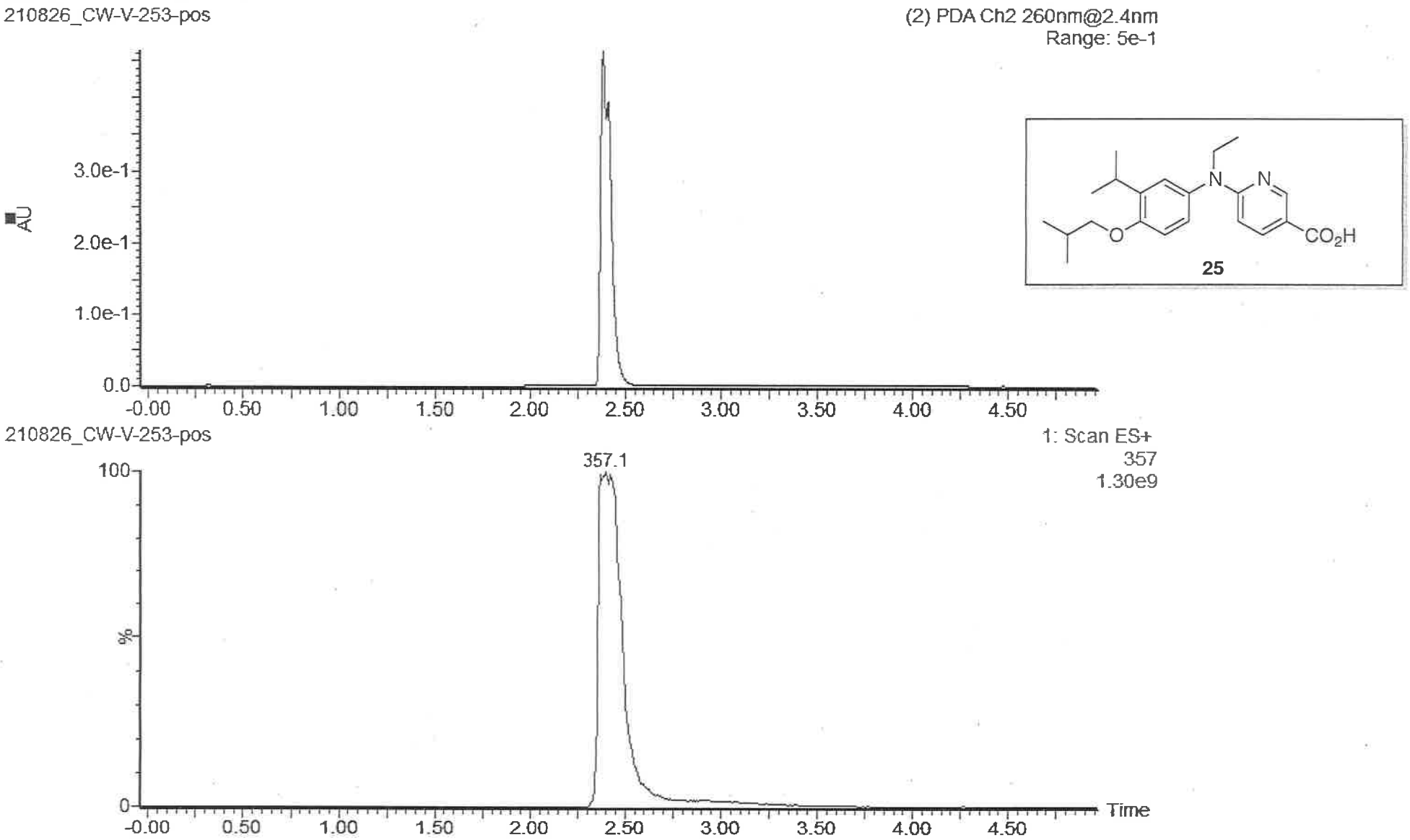
Function 1

Scans in function:	601
Cycle time (secs):	Automatic
Scan duration (secs):	0.495
Inter Scan Delay (secs):	Automatic
Start and End Time(mins):	0.000 to 5.000
Ionization mode:	ES-
Data type:	Accurate Mass
Function type:	Scan
Mass range:	100 to 500

Function 2

Scans in function:	6001
Function type:	Diode Array
Wavelength range (nm):	210 to 499

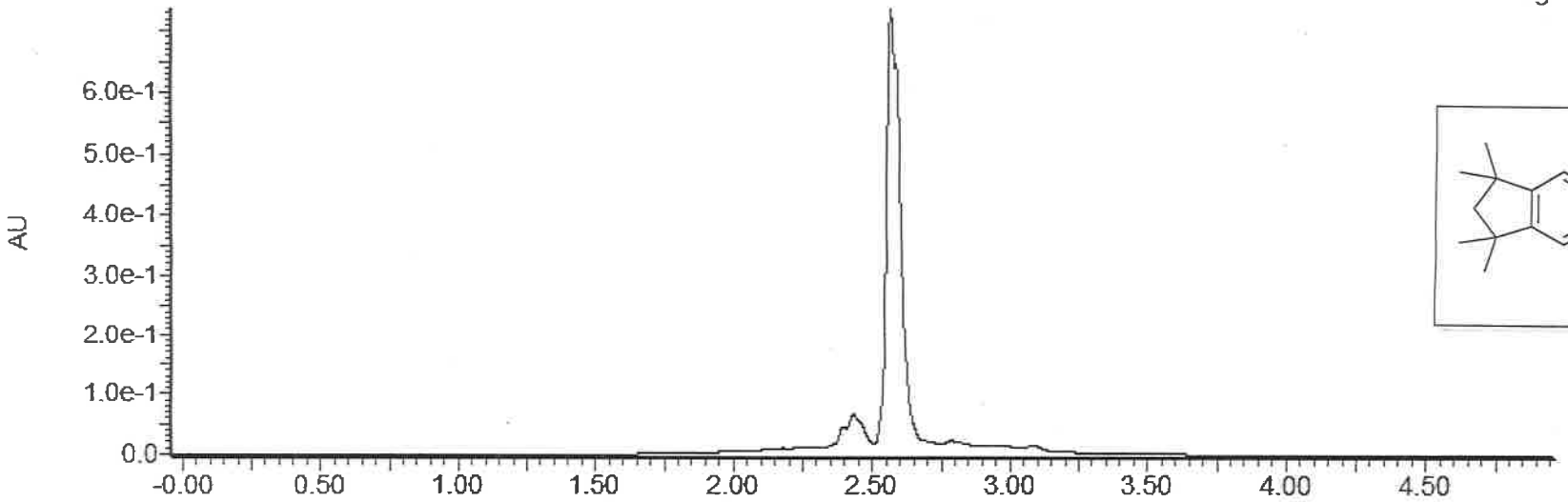
mz not observed; see 426

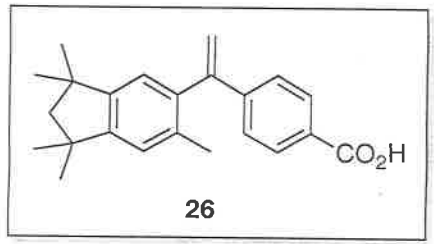


mz not observed

210826_CW-VI-035_pos

(2) PDA Ch2 260nm@2.4nm
Range: 7e-1

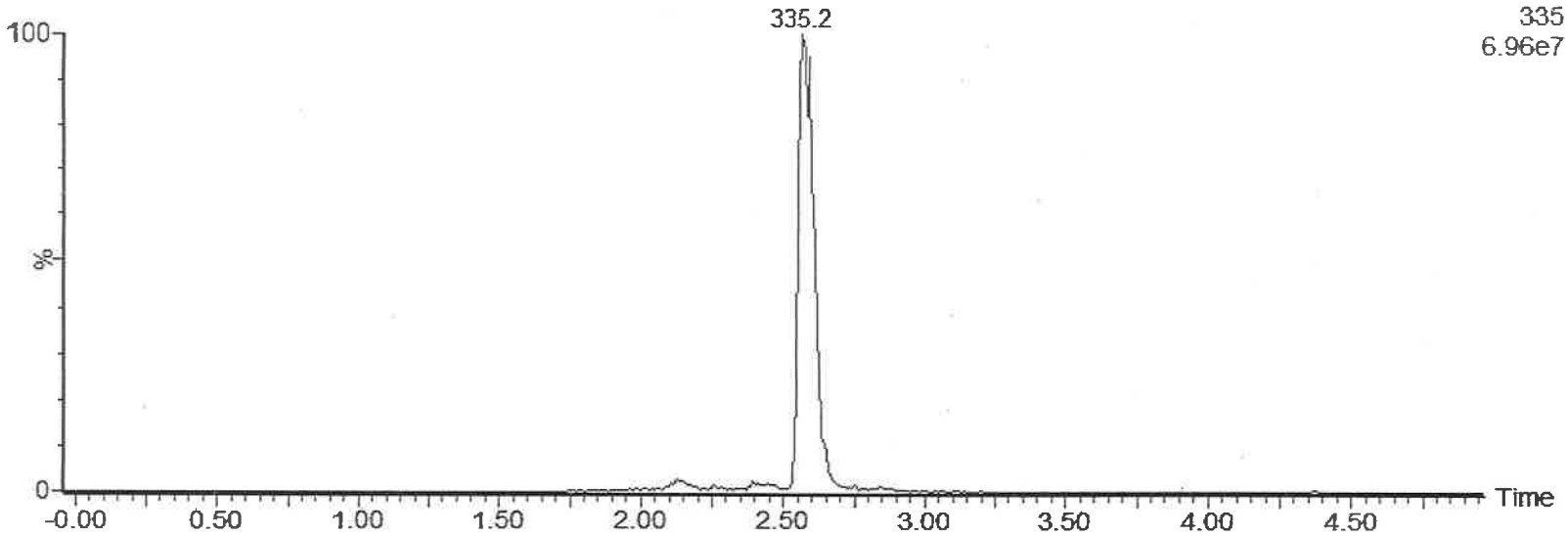




26

210826_CW-VI-035_pos

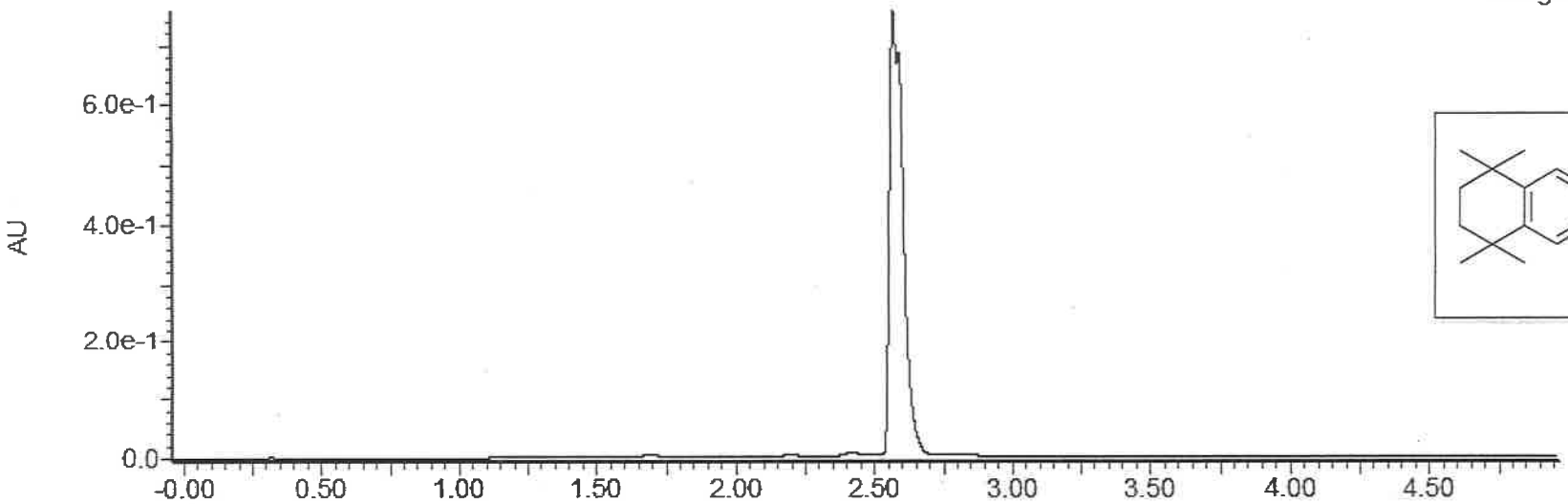
1: Scan ES+
335
6.96e7

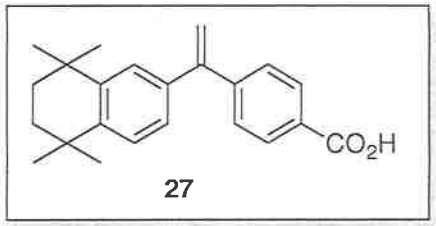


mz not observed

210826_CW-VI-025_pos

(2) PDA Ch2 260nm@2.4nm
Range: 8e-1

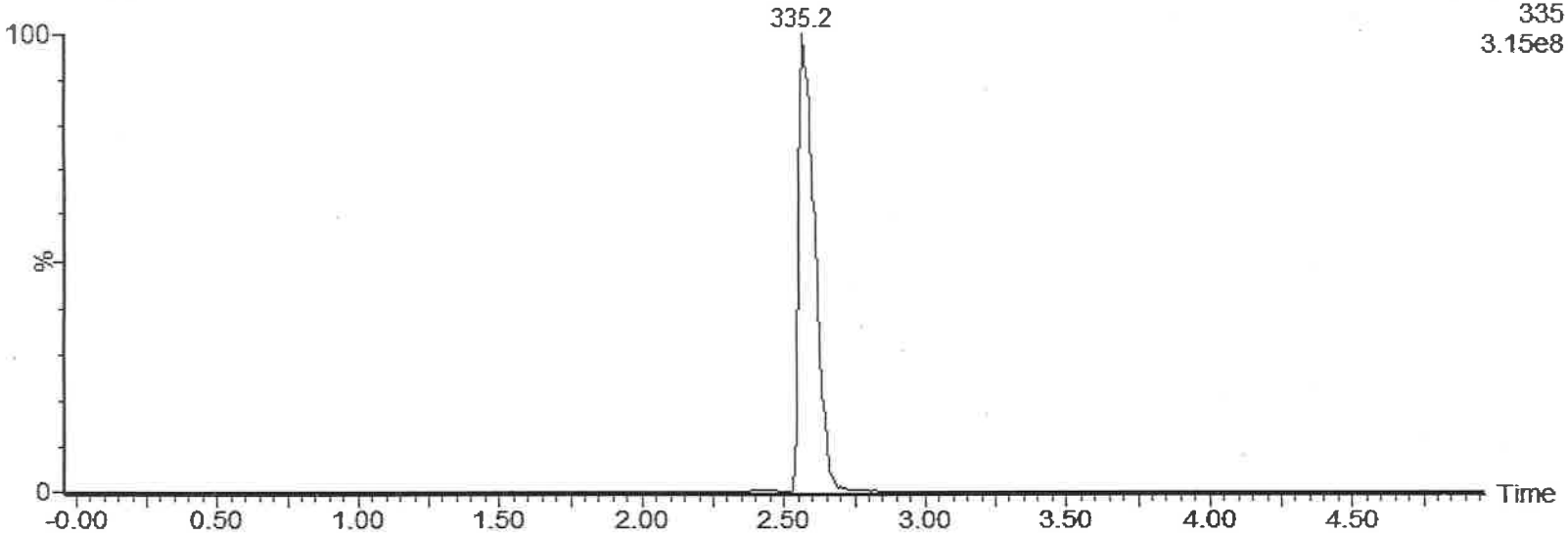




27

210826_CW-VI-025_pos

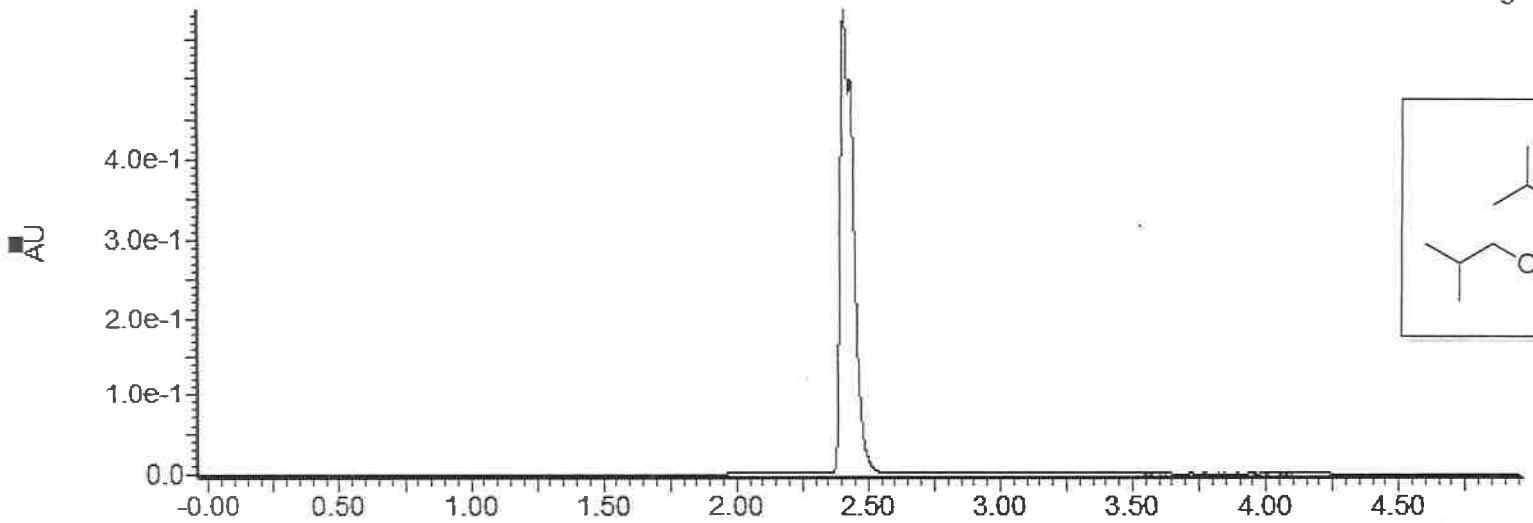
1: Scan ES+
335
3.15e8

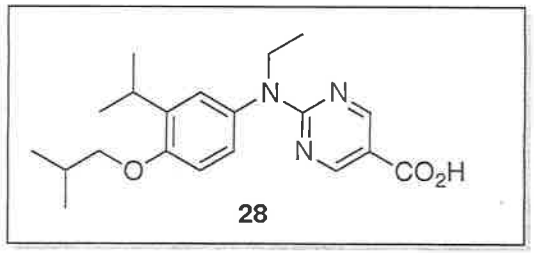


Label - CW-V-259; weak; see 402

210826_CW-V-257-pos

(2) PDA Ch2 260nm@2.4nm
Range: 6e-1

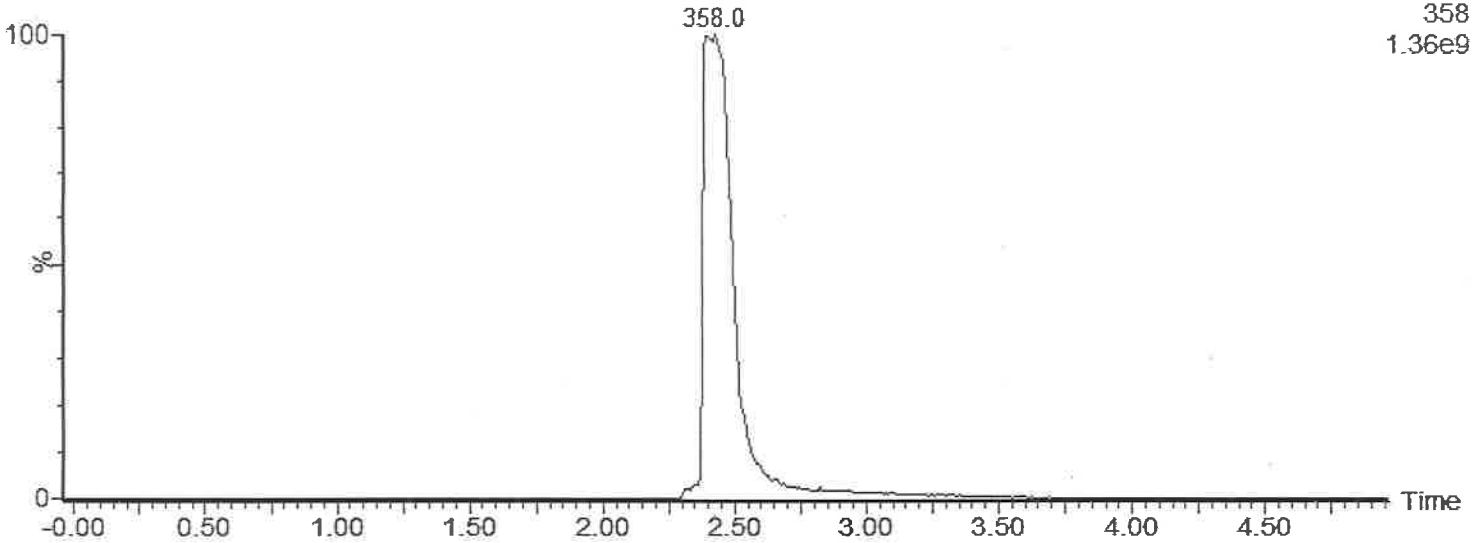




28

210826_CW-V-257-pos

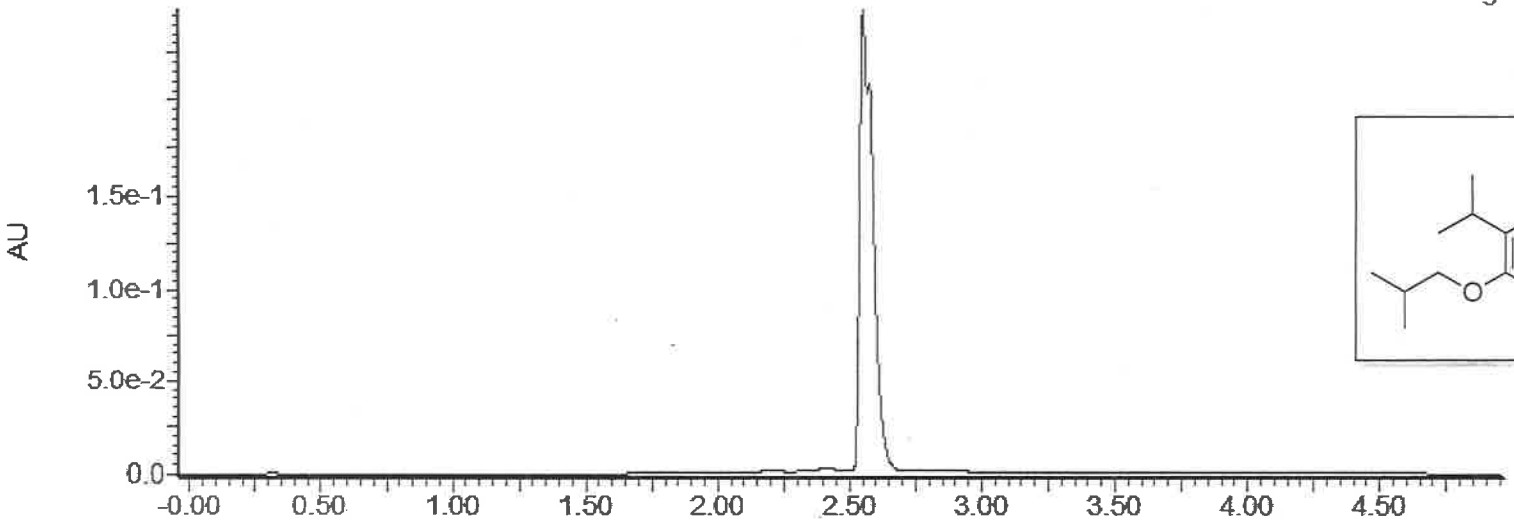
1: Scan ES+
358
1.36e9

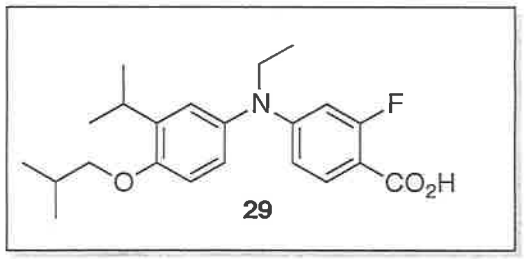


mz not observed

210826_CW-V-265-pos

(2) PDA Ch2 260nm@2.4nm
Range: 2e-1

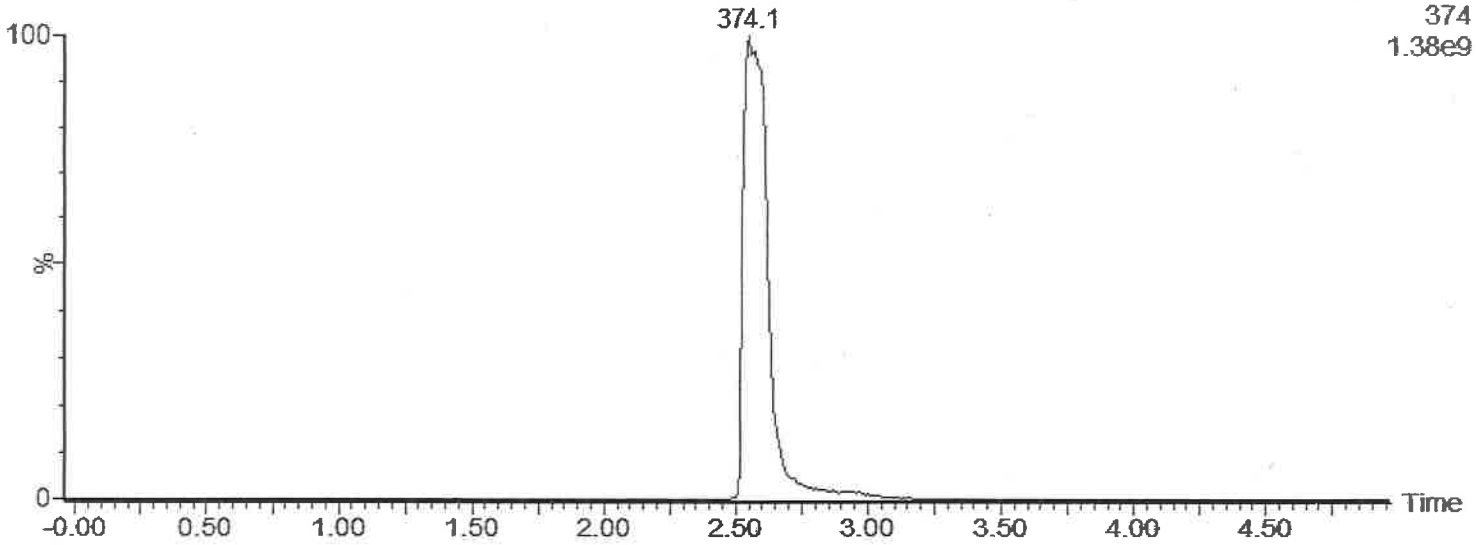




29

210826_CW-V-265-pos

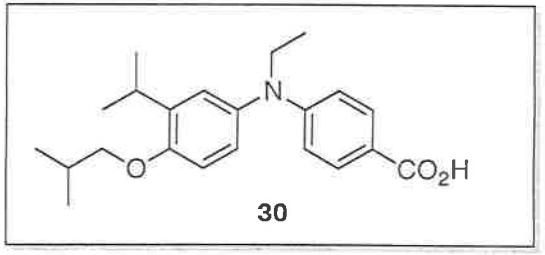
1: Scan ES+
374
1.38e9



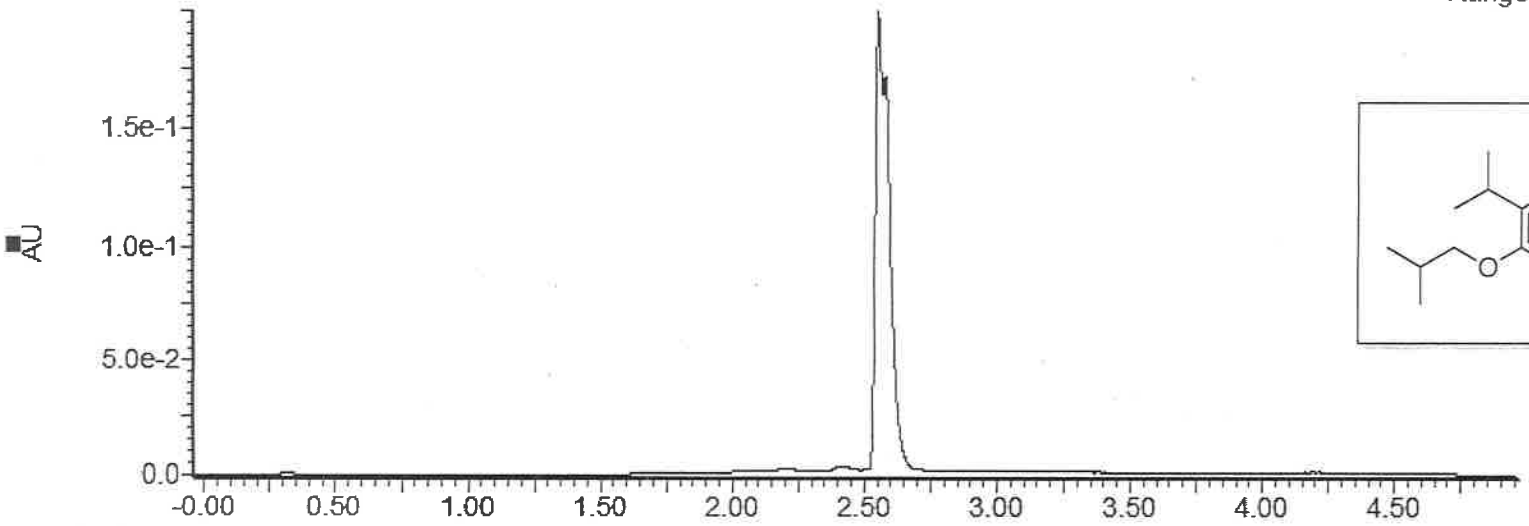
mz not observed

210826_CW-V-263-pos

(2) PDA Ch2 260nm@2.4nm
Range: 2e-1

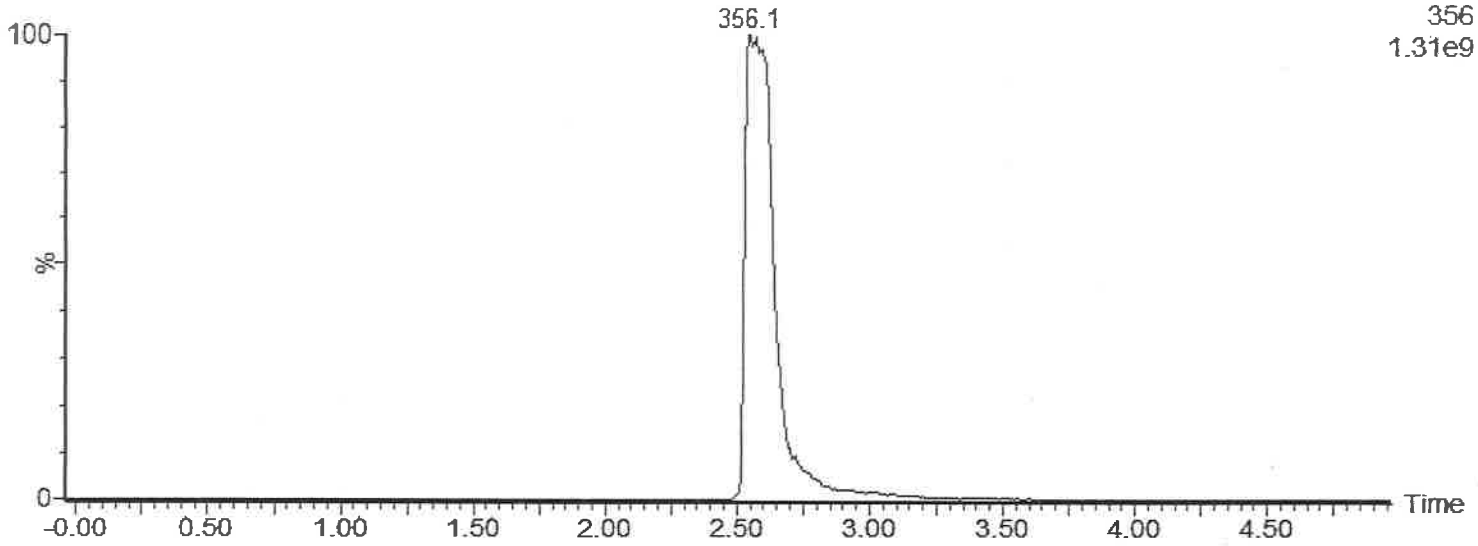


30

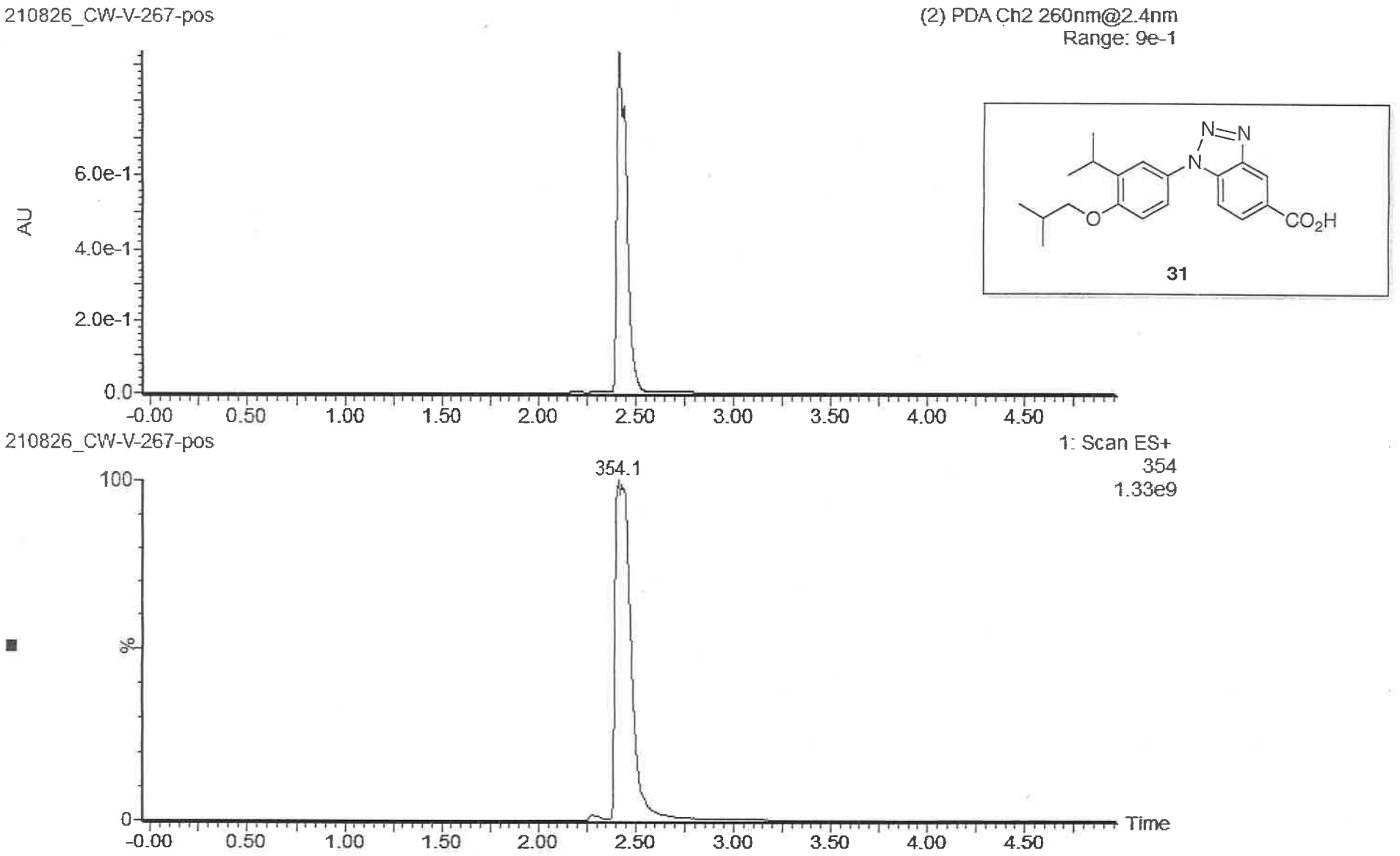


210826_CW-V-263-pos

1: Scan ES+
356
1.31e9

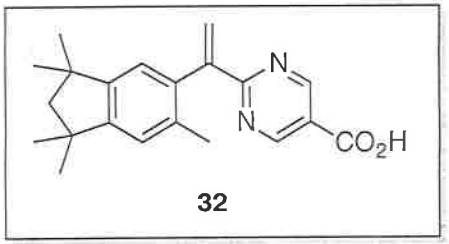


mz weak; see 398

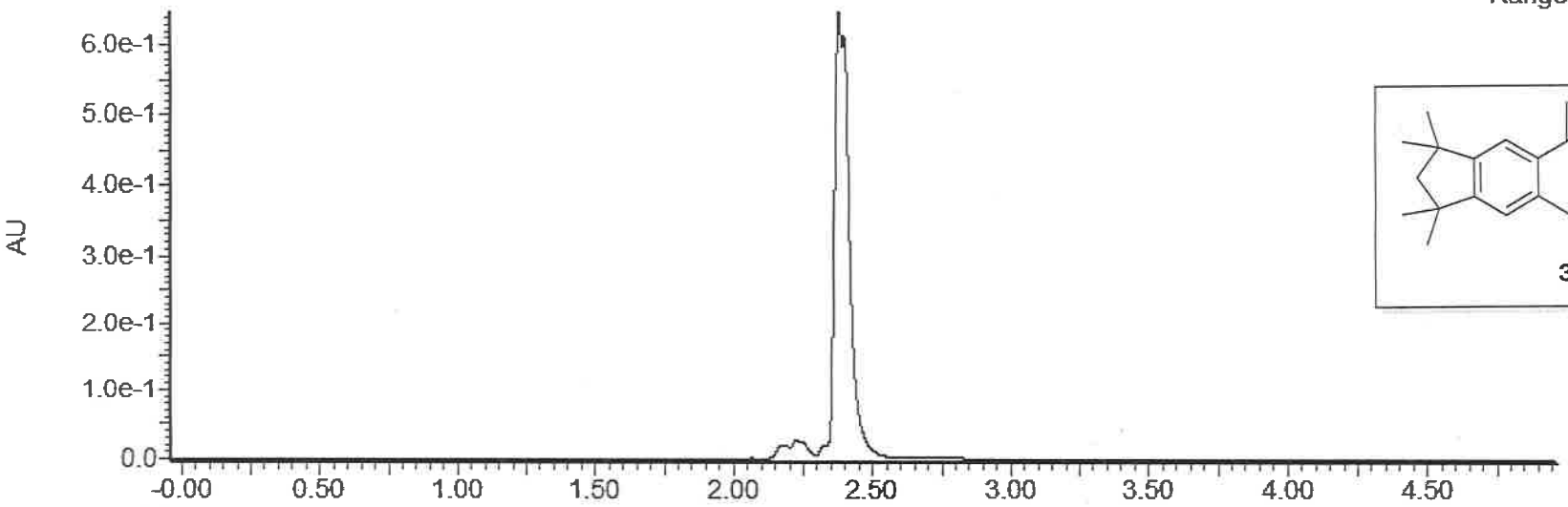


210826_CW-VI-007

(2) PDA Ch2 260nm@2.4nm
Range: 7e-1

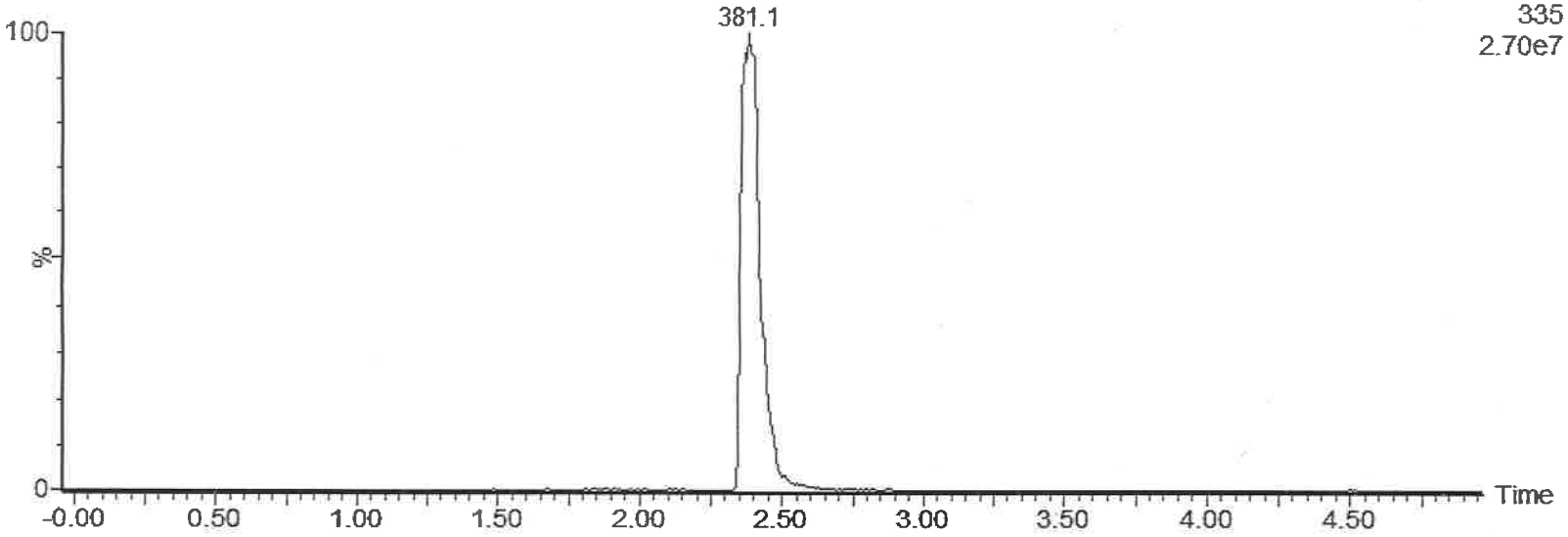


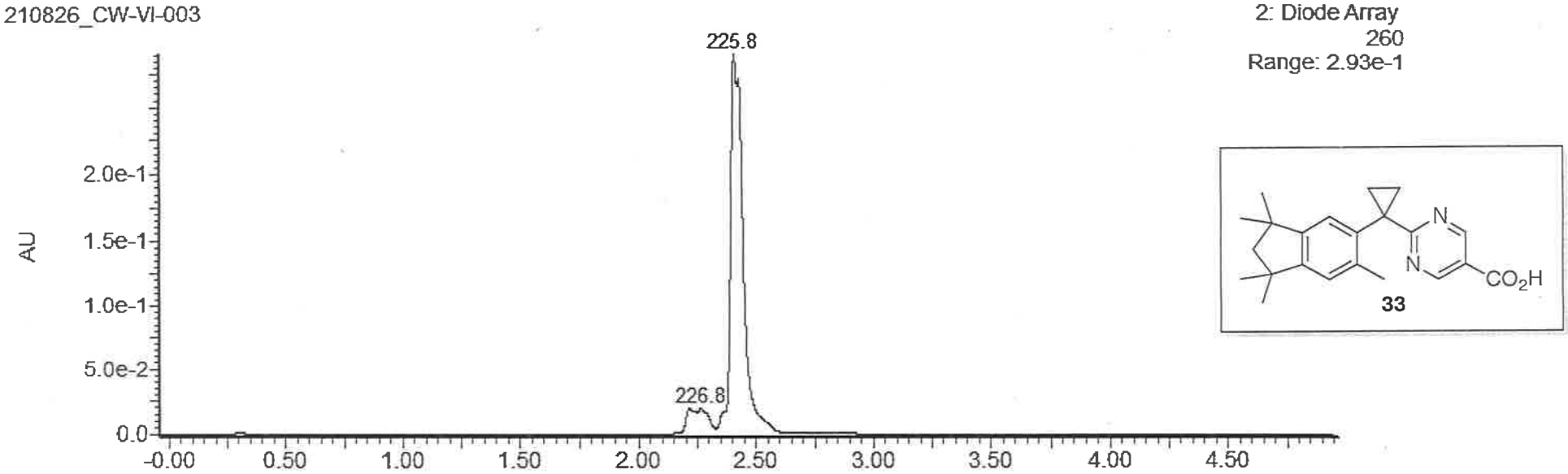
32

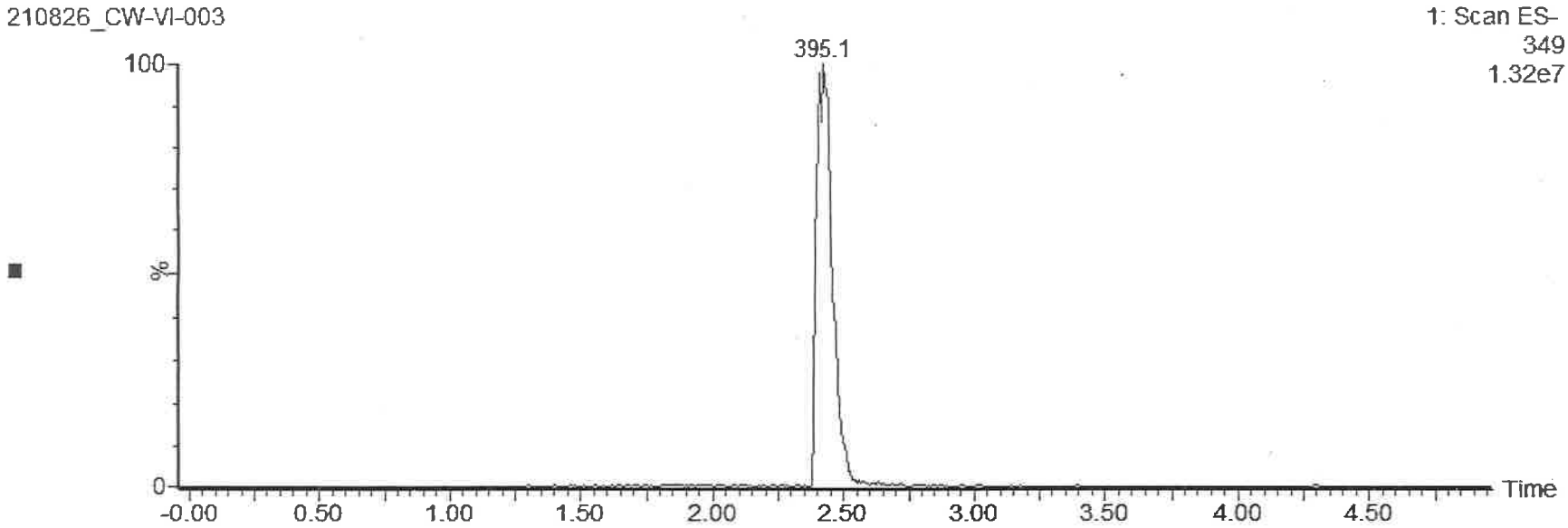


210826_CW-VI-007

1: Scan ES-
335
2.70e7

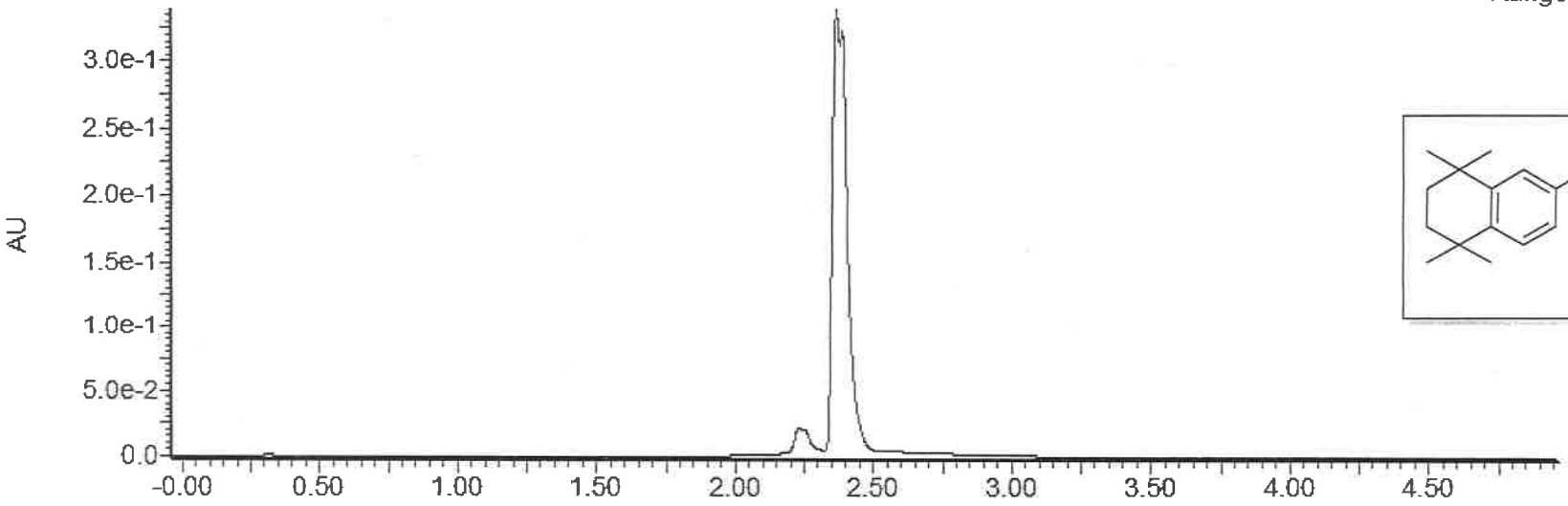


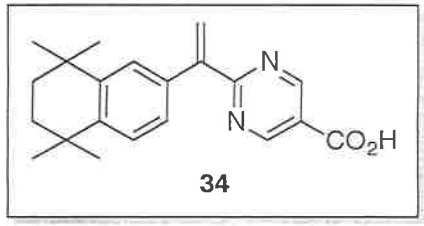

210826_CW-VI-003
2: Diode Array
260
Range: 2.93e-1
225.8
226.8
AU
2.0e-1
1.5e-1
1.0e-1
5.0e-2
0.0
-0.00
0.50
1.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
N
N
CO2H
33


210826_CW-VI-003
1: Scan ES-
349
1.32e7
395.1
100
%
0
-0.00
0.50
1.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
Time

210826_CW-VI-009

(2) PDA Ch2 260nm@2.4nm
Range: 3e-1

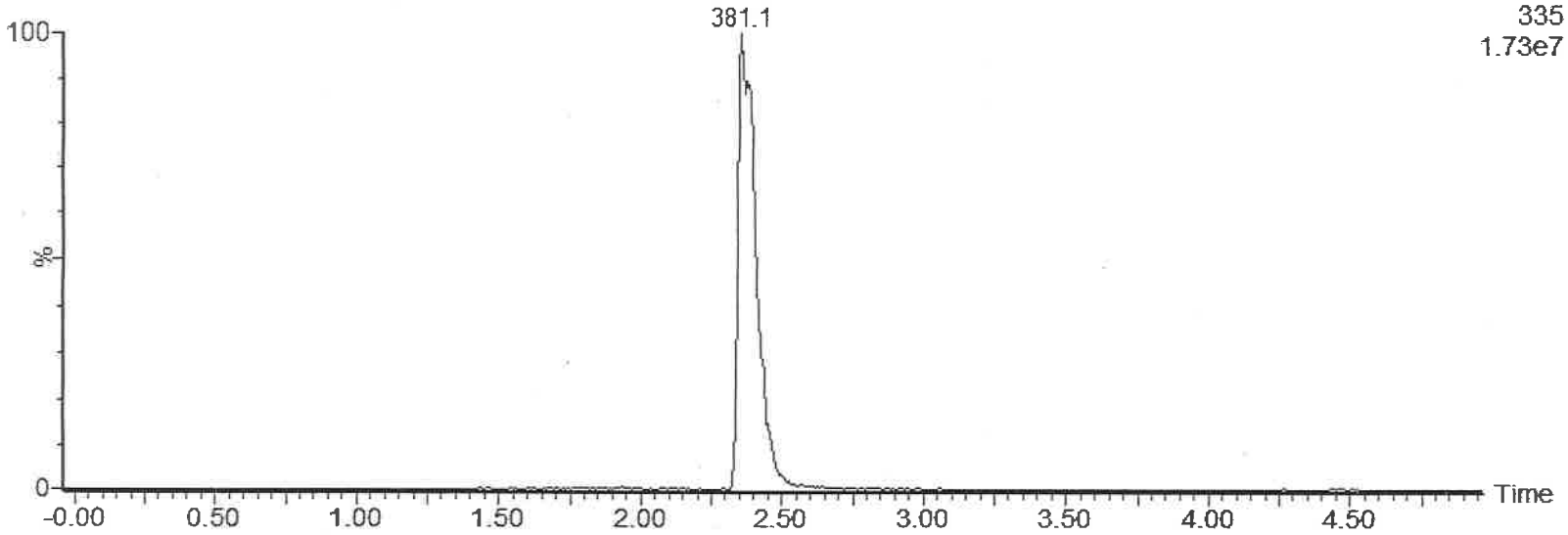


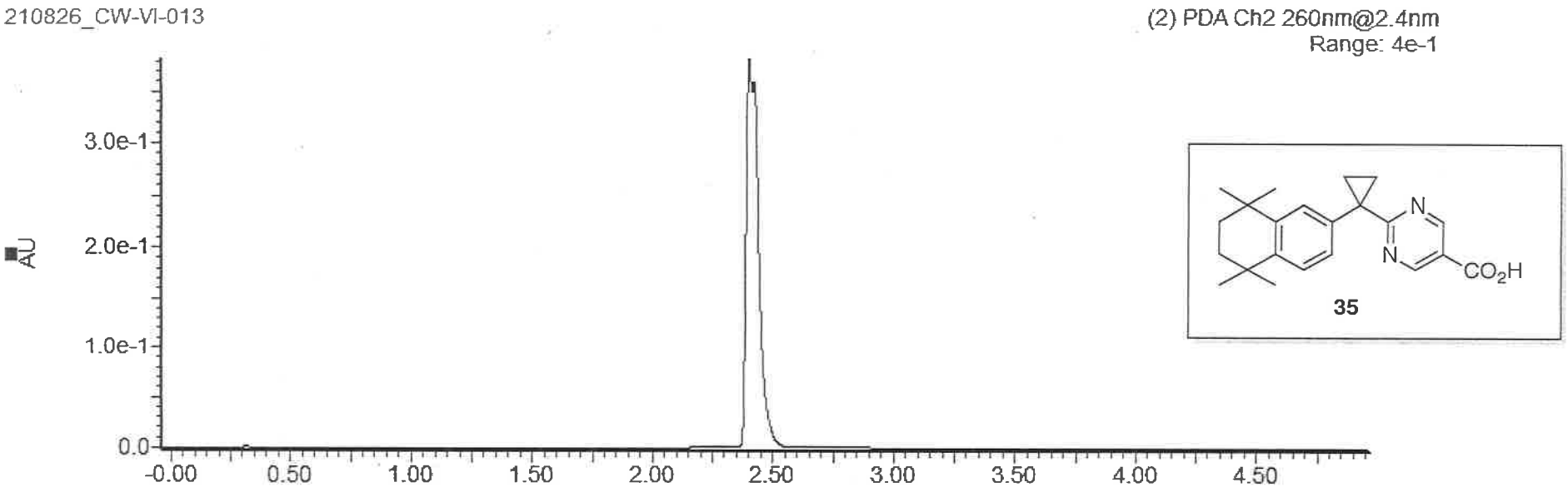


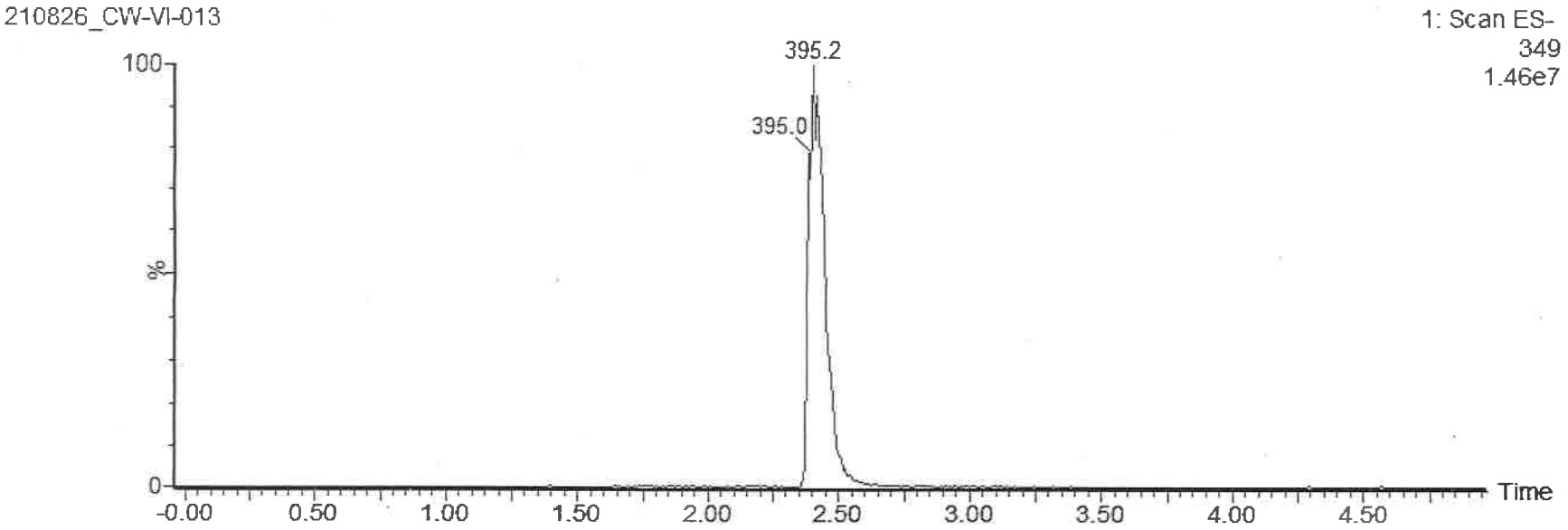
34

210826_CW-VI-009

1: Scan ES-
335
1.73e7



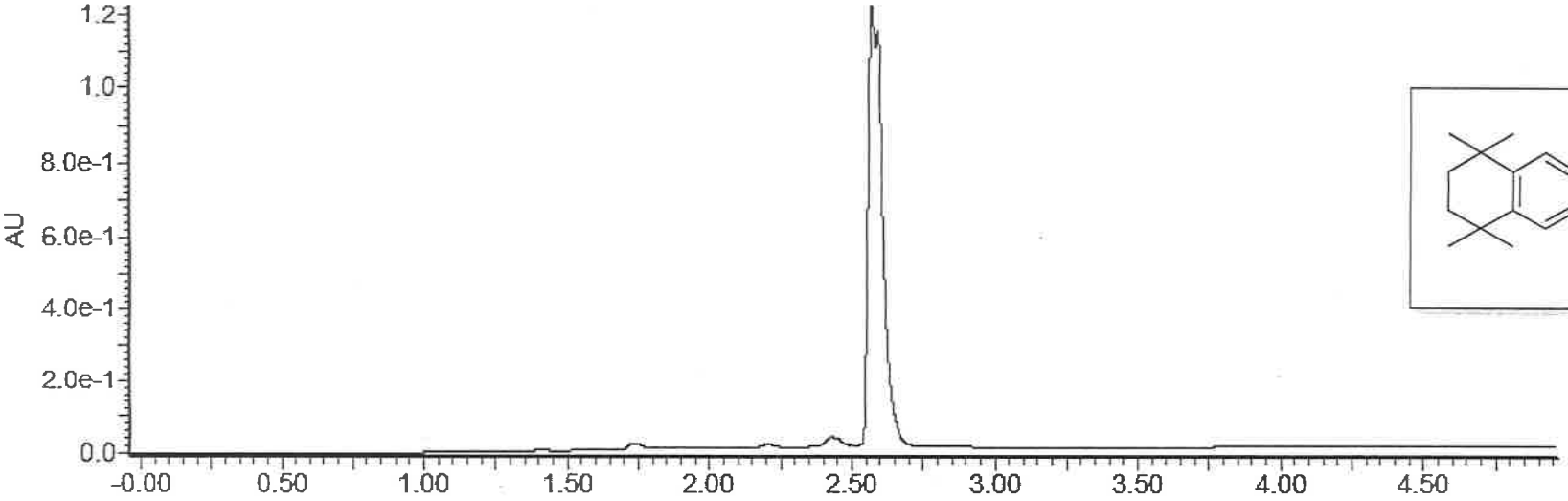

210826_CW-VI-013
(2) PDA Ch2 260nm@2.4nm
Range: 4e-1
AU
3.0e-1
2.0e-1
1.0e-1
0.0
-0.00
0.50
1.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
N
N
CO2H
35

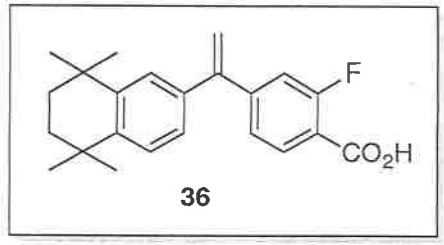

210826_CW-VI-013
1: Scan ES-
349
1.46e7
395.2
395.0
100
%
0
-0.00
0.50
1.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
Time

weak

210826_CW-VI-023_pos

(2) PDA Ch2 260nm@2.4nm
Range: 1

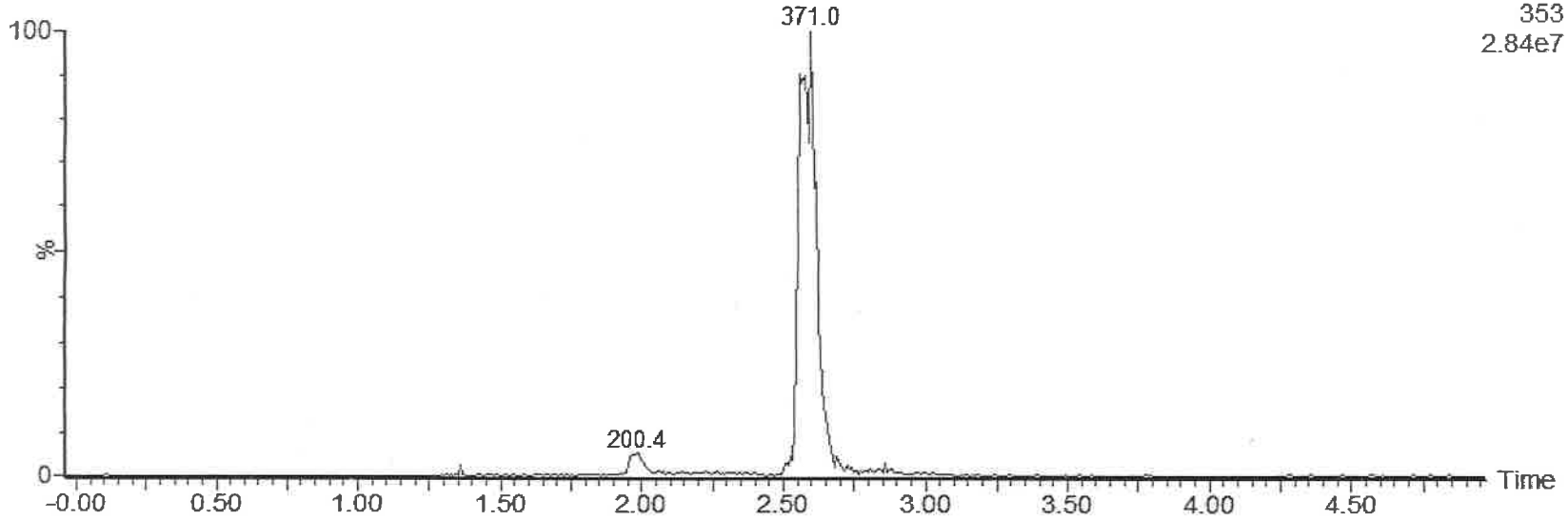




36

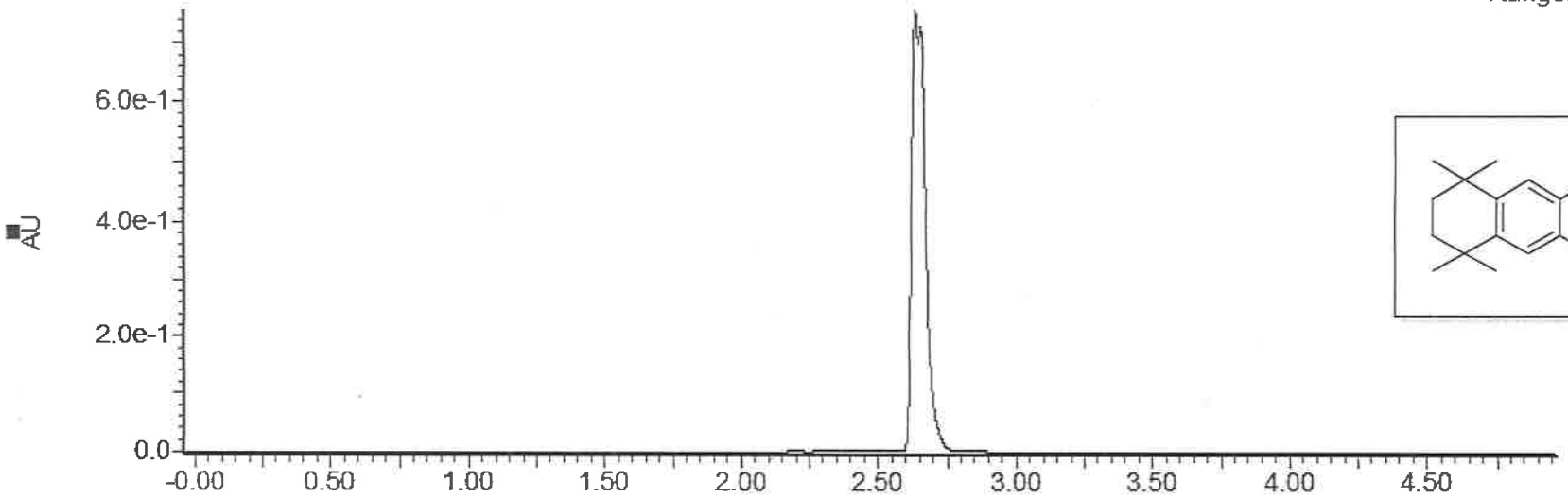
210826_CW-VI-023_pos

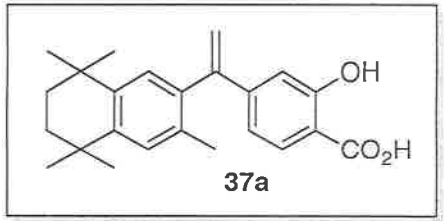
1: Scan ES+
353
2.84e7



210826_CW-VI-073

(2) PDA Ch2 260nm@2.4nm
Range: 8e-1

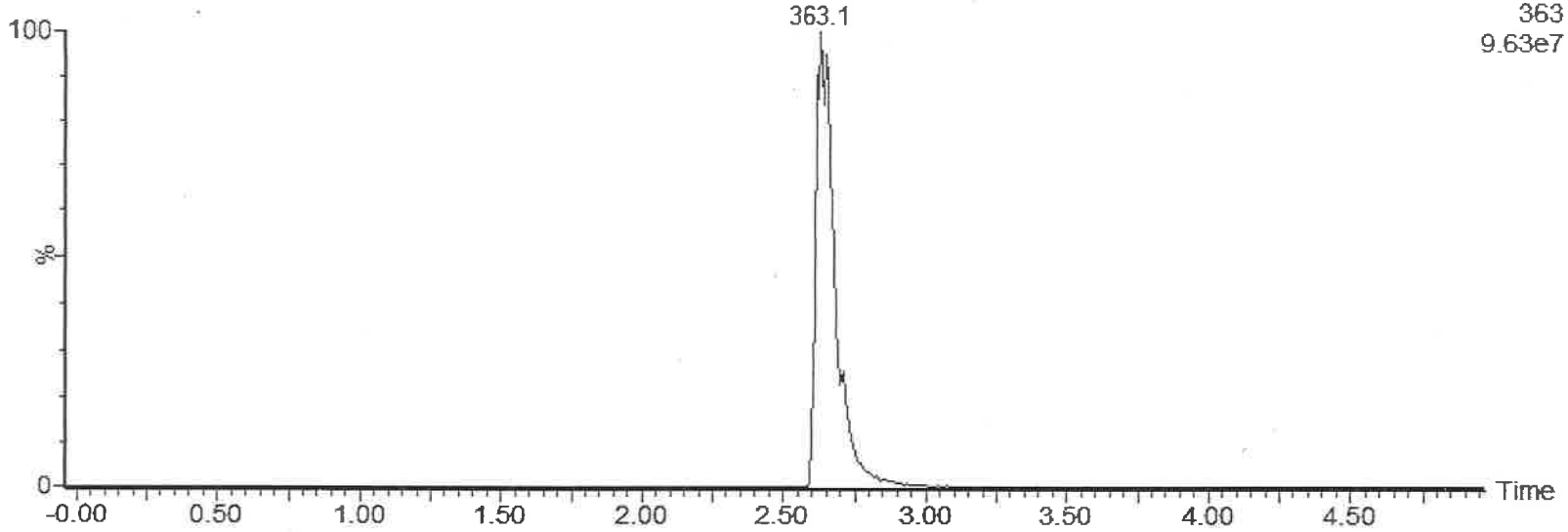


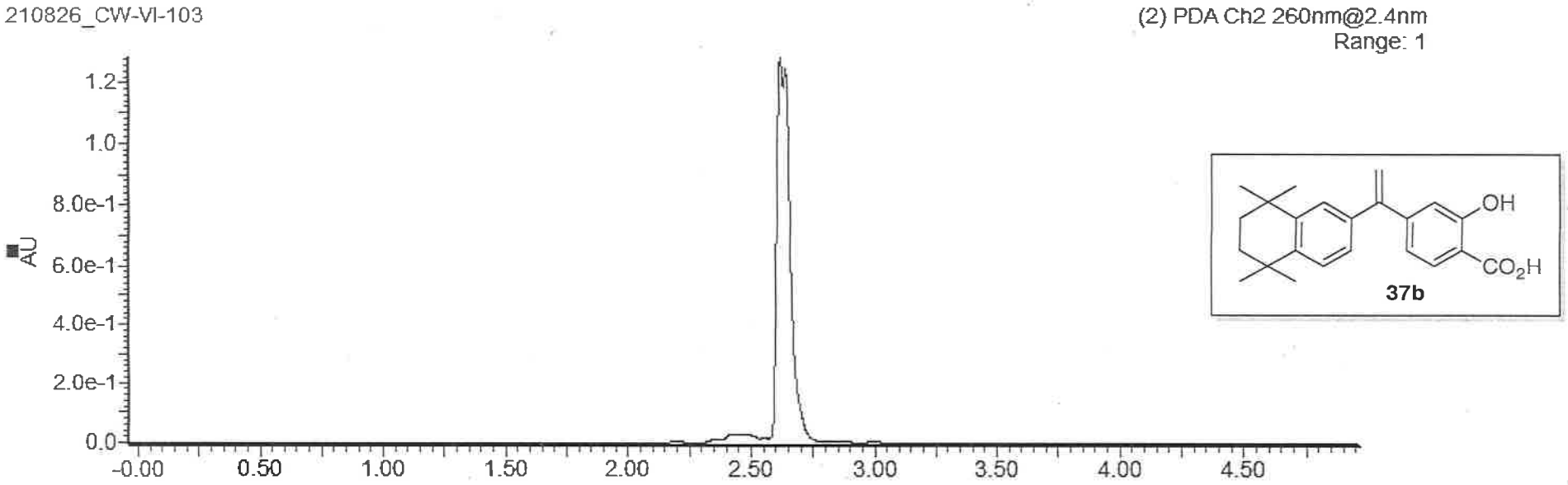


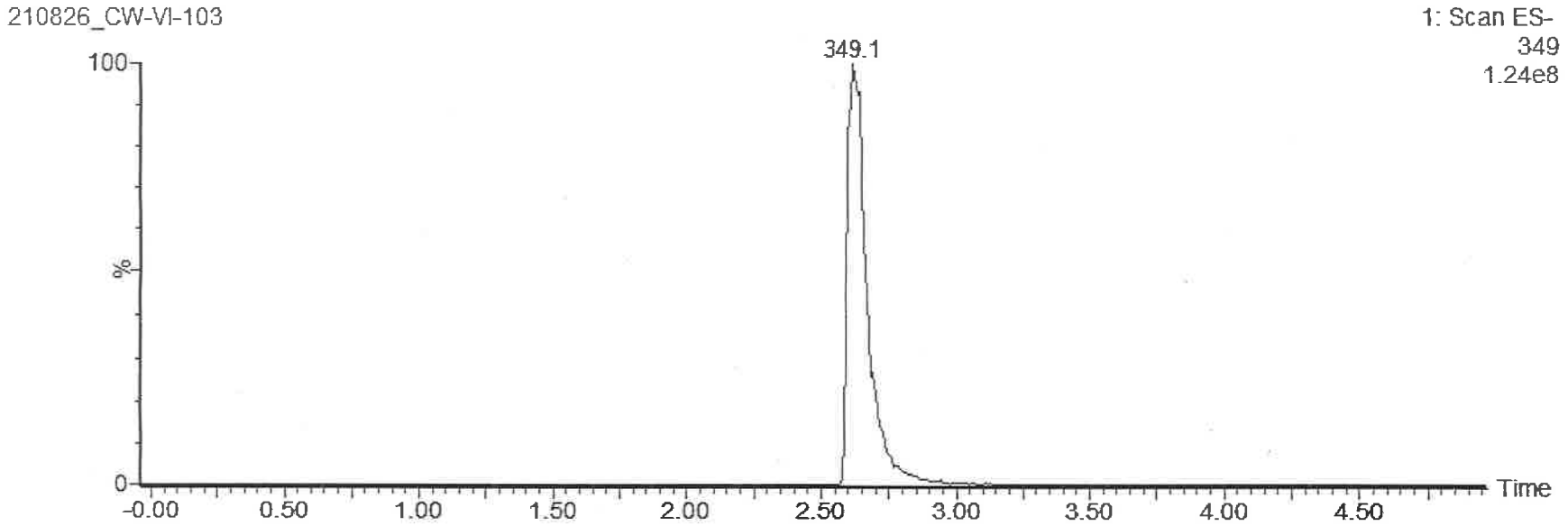
37a

210826_CW-VI-073

1: Scan ES-
363
9.63e7




210826_CW-VI-103
(2) PDA Ch2 260nm@2.4nm
Range: 1
AU
1.2
1.0
8.0e-1
6.0e-1
4.0e-1
2.0e-1
0.0
-0.00
0.50
1.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
OH
CO2H
37b


210826_CW-VI-103
1: Scan ES-
349
1.24e8
349.1
100
%
0
-0.00
0.50
1.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
Time