

Supporting Information

The one-step conversion of 2-amino-*N'*-arylbenzamidines into 3-aryl-4-imino-3,4-dihydroquinazoline-2-carbonitriles using 4,5-dichloro-1,2,3-dithiazolium chloride

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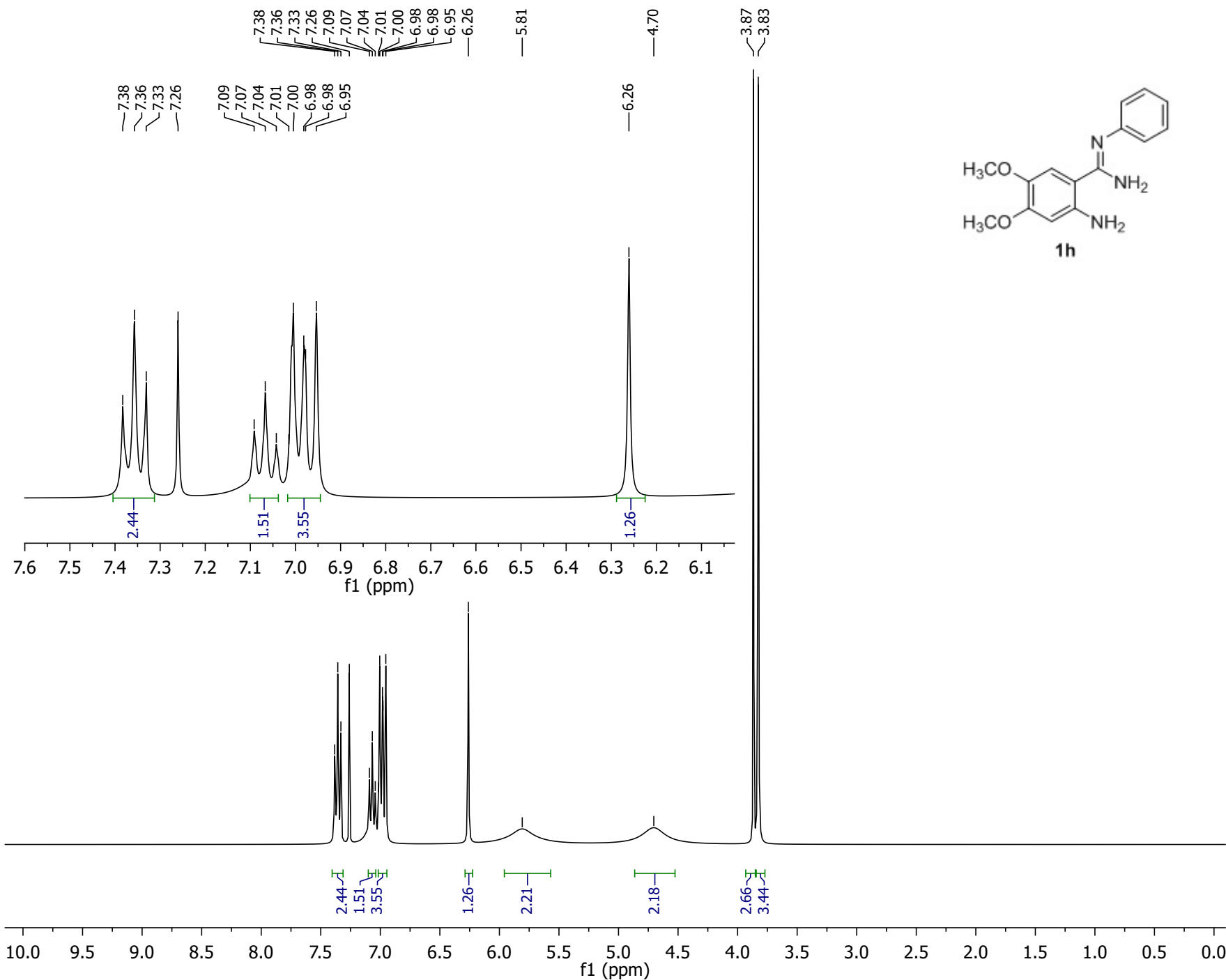
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Supporting Information

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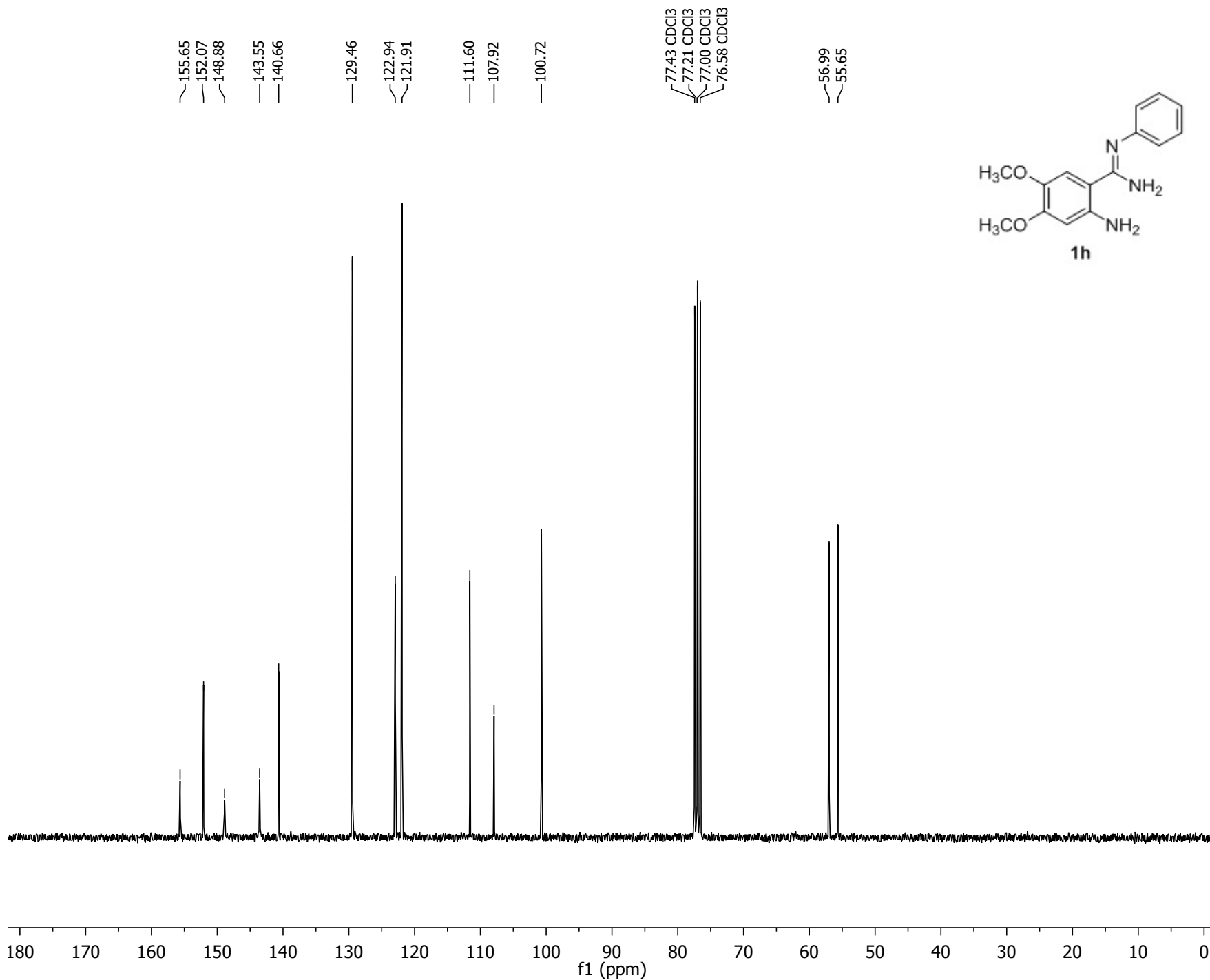
(Z)-2-Amino-4,5-dimethoxy-*N'*-phenylbenzamidine (**1h**)



Current Data Parameters

NAME	Styliana
EXPNO	92
PROCNO	1
F2 - Acquisition Parameters	
Date_	20101010
Time	14.00
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	6172.839 Hz
FIDRES	0.094190 Hz
AQ	5.3084660 sec
RG	406.4
DW	81.000 usec
DE	9.00 usec
TE	296.2 K
D1	1.00000000 sec
TD0	1
CHANNEL f1 =====	
NUC1	1H
P1	9.40 usec
PL1	0.00 dB
SFO1	300.1318534 MHz
F1 - Acquisition parameters	
ND0	2
TD	256
SFO1	300.1314 MHz
FIDRES	12.056327 Hz
SW	10.284 ppm
FnMODE	undefined
F2 - Processing parameters	
SI	32768
SF	300.1300063 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00
F1 - Processing parameters	
SI	1024
MC2	QF
SF	300.1300000 MHz
WDW	SINE
SSB	0
LB	0.30 Hz
GB	0.1

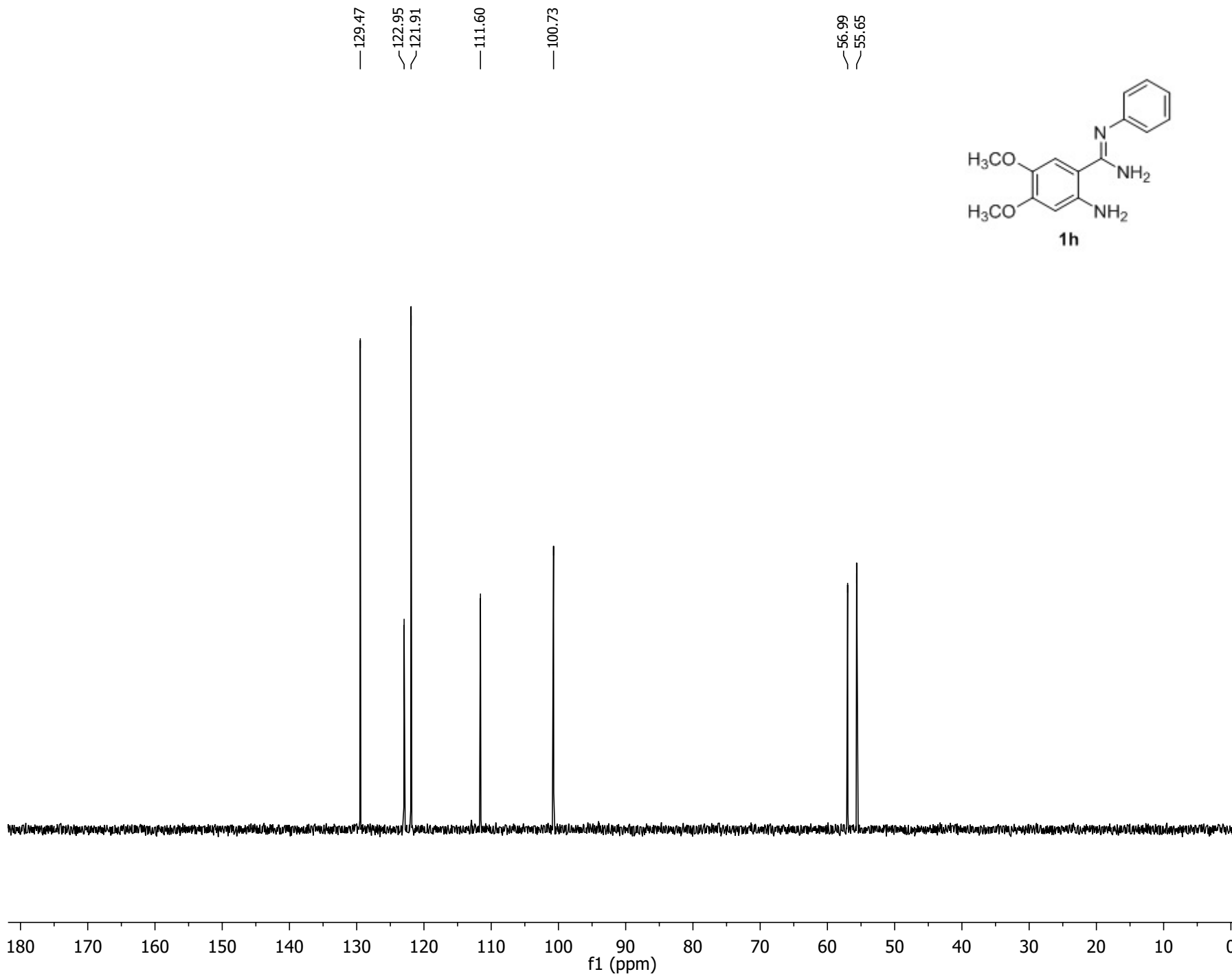
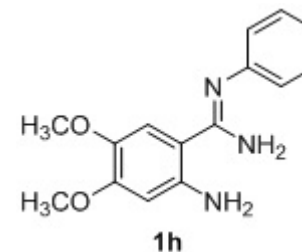
(Z)-2-Amino-4,5-dimethoxy-N'-phenylbenzamidine (**1h**)



LOCurrent Data Parameters
NAME Styliana
EXPNO 101
PROCNO 1
LOF2 - Acquisition Parameters
Date_ 20101010
Time 18.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 992
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 20642.5
DW 27.800 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
CHANNEL f1 =====
NUC1 13C
P1 7.95 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz
CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 110.00 usec
PL2 0.00 dB
PL12 22.00 dB
PL13 24.00 dB
SFO2 300.1312005 MHz
LOF2 - Processing parameters
SI 32768
SF 75.4677561 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

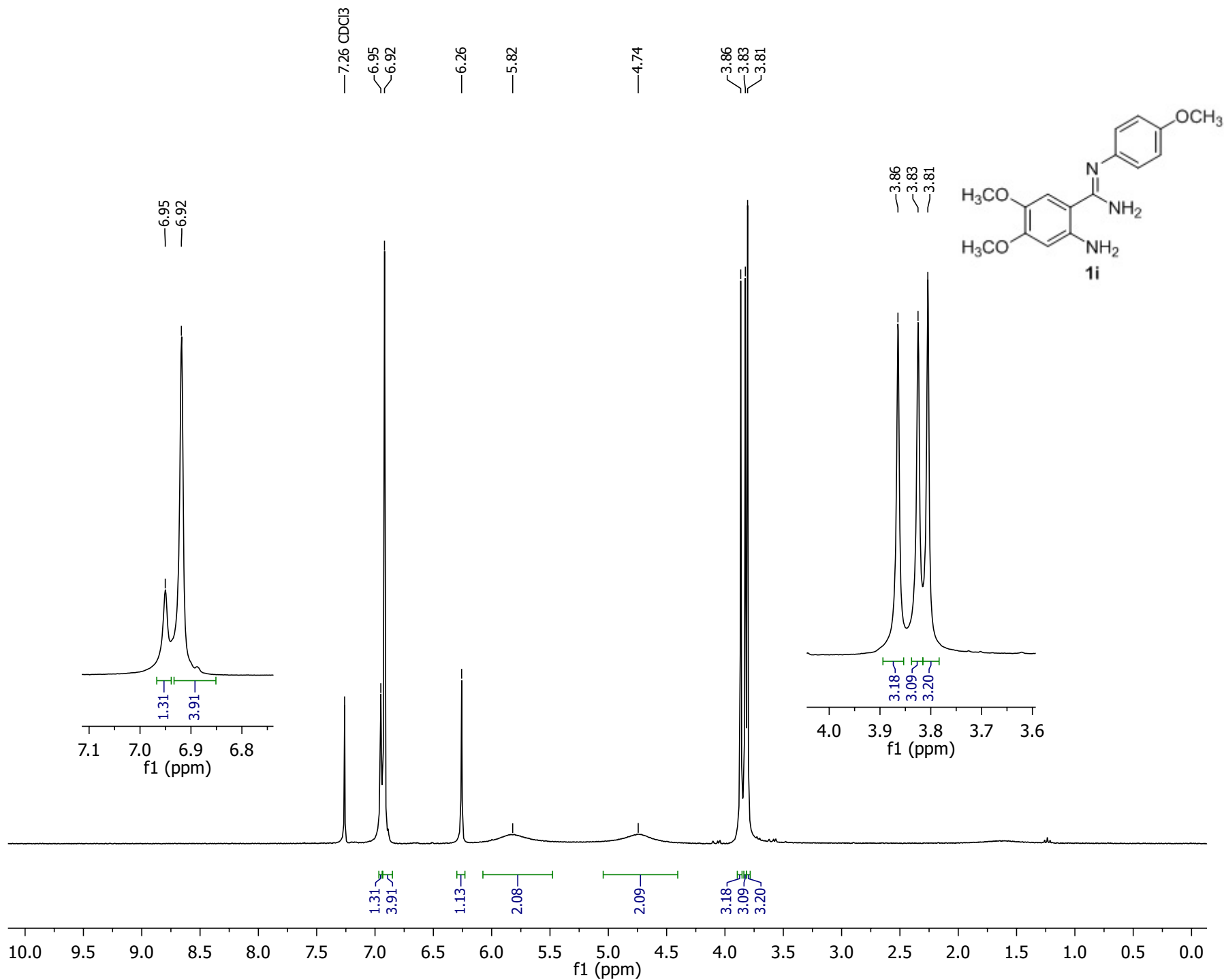
(Z)-2-Amino-4,5-dimethoxy-N'-phenylbenzamidine (**1h**)

D E P T 1 3 5



Current Data Parameters
NAME Styliana
EXPNO 100
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101010
Time 18.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 124
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 6.00 usec
TE 296.2 K
CNST2 145.000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001012 sec
TD0 1
CHANNEL f1 =====
NUC1 13C
P1 7.95 usec
p2 15.90 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz
CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 9.40 usec
p4 18.80 usec
PCPD2 110.00 usec
PL2 0.00 dB
PL12 22.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

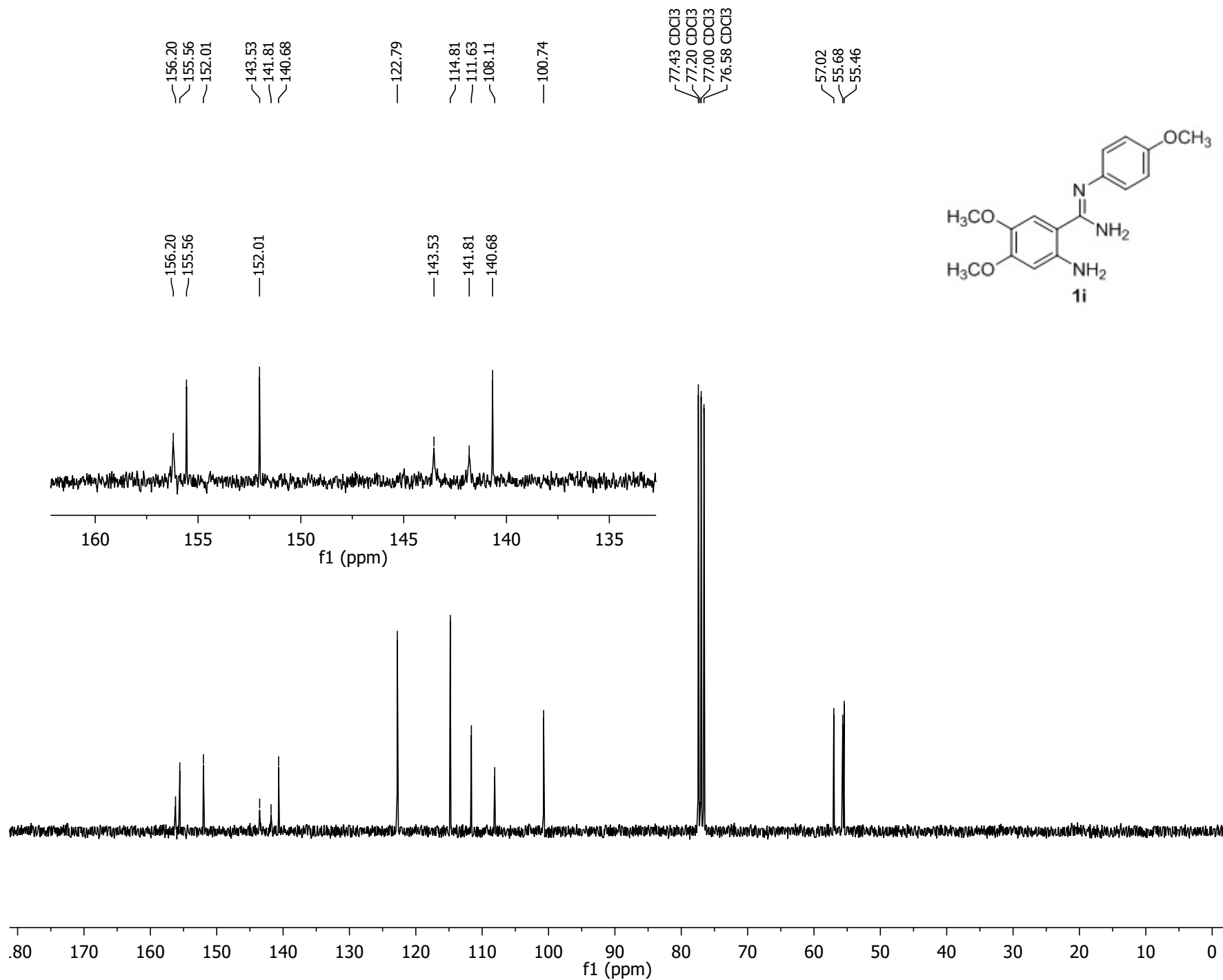
(Z)-2-Amino-4,5-dimethoxy-*N'*-(4-methoxyphenyl)benzamidine (**1i**)



Current Data Parameters

NAME	Styliana
EXPNO	88
PROCNO	1
F2 - Acquisition Parameters	
Date_	20101010
Time	13.05
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl ₃
NS	16
DS	2
SWH	6172.839 Hz
FIDRES	0.094190 Hz
AQ	5.3084660 sec
RG	456.1
DW	81.000 usec
DE	9.00 usec
TE	296.2 K
D1	1.00000000 sec
TD0	1
F1 - Acquisition parameters	
ICCHANNEL f1	=====
NUC1	¹ H
P1	9.40 usec
PL1	0.00 dB
SFO1	300.1318534 MHz
F2 - Processing parameters	
SI	32768
SF	300.1300061 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00
F1 - Processing parameters	
SI	1024
MC2	QF
SF	300.1300000 MHz
WDW	SINE
SSB	0
LB	0.30 Hz
GB	0.1

(Z)-2-Amino-4,5-dimethoxy-*N'*-(4-methoxyphenyl)benzamidine (**1i**)



Current Data Parameters

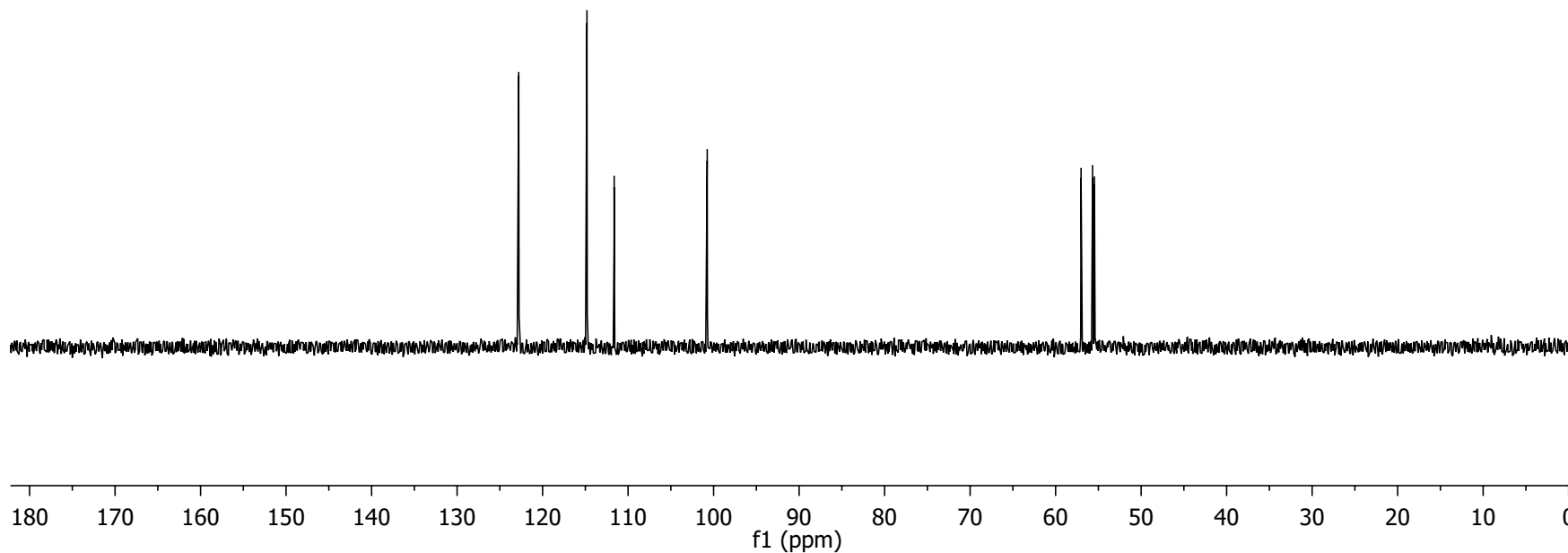
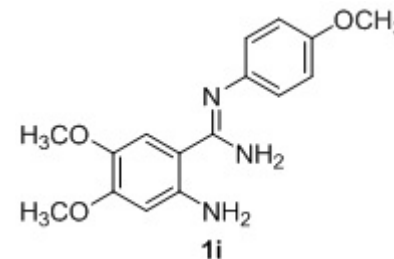
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EXPNO	103
PROCNO	1
F2 - Acquisition Parameters	
Date_	20101010
Time	20.01
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl ₃
NS	215
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	13004
DW	27.800 usec
DE	6.00 usec
TE	296.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
CHANNEL f1 =====	
NUC1	¹³ C
P1	7.95 usec
PL1	-2.00 dB
SFO1	75.4752953 MHz
CHANNEL f2 =====	
CPDPRG2	waltz16
NUC2	¹ H
PCPD2	110.00 usec
PL2	0.00 dB
PL12	22.00 dB
PL13	24.00 dB
SFO2	300.1312005 MHz
F2 - Processing parameters	
SI	32768
SF	75.4677540 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

(Z)-2-Amino-4,5-dimethoxy-*N'*-(4-methoxyphenyl)benzamidine (**1i**)

D E P T 1 3 5

—122.80
—114.81
—111.63
—100.75

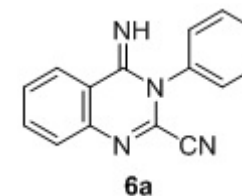
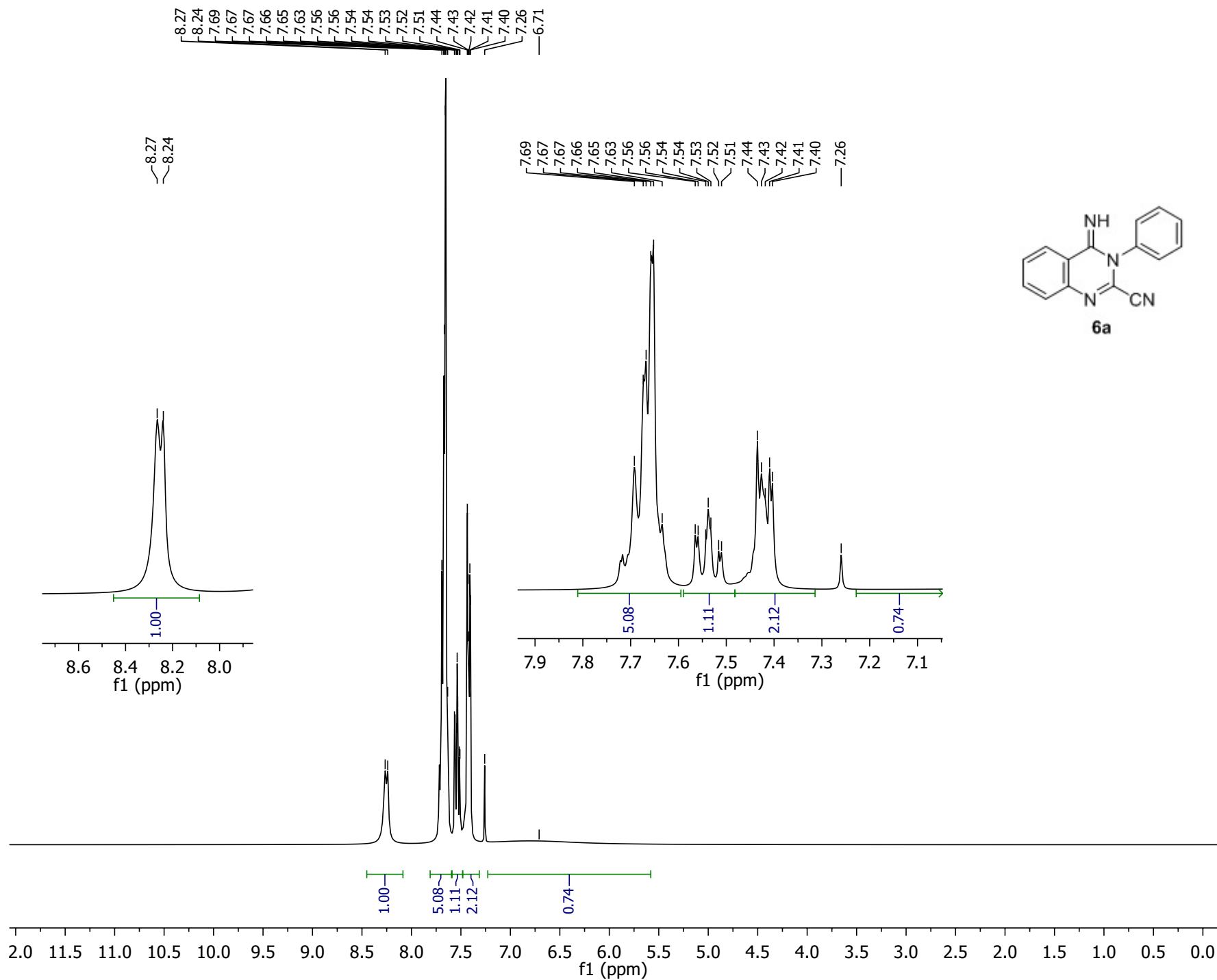
57.02
55.68
55.46



Current Data Parameters

NAME Stylina
EXPNO 102
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101010
Time 19.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 98
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 6.00 usec
TE 296.2 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.0001012 sec
TD0 1
CHANNEL f1 =====
NUC1 13C
P1 7.95 usec
p2 15.90 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz
CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 9.40 usec
p4 18.80 usec
PCPD2 110.00 usec
PL2 0.00 dB
PL12 22.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677535 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

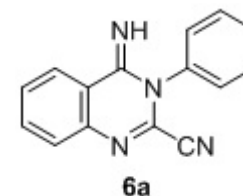
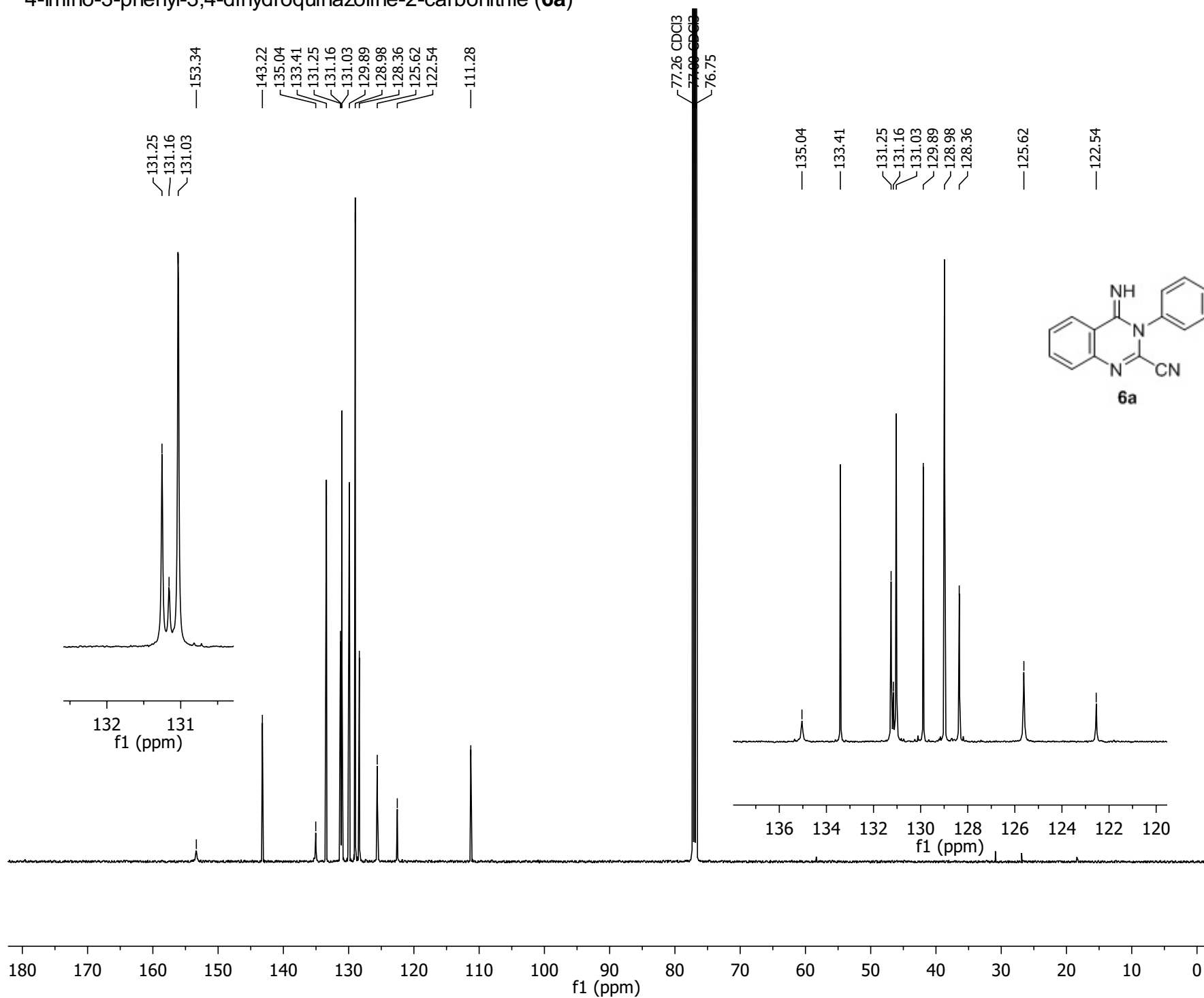
4-Imino-3-phenyl-3,4-dihydroquinazoline-2-carbonitrile (**6a**)



Current Data Parameters

NAME	Styiana
EXPNO	66
PROCNO	1
F2 - Acquisition Parameters	
Date_	20100823
Time	10.55
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl ₃
NS	16
DS	2
SWH	6172.839 Hz
FIDRES	0.094190 Hz
AQ	5.3084660 sec
RG	203.2
DW	81.000 usec
DE	9.00 usec
TE	294.2 K
D1	1.00000000 sec
TD0	1
CHANNEL f1 =====	
NUC1	¹ H
P1	9.40 usec
PL1	0.00 dB
SFO1	300.1318534 MHz
F1 - Acquisition parameters	
ND0	2
TD	256
SFO1	300.1314 MHz
FIDRES	12.056327 Hz
SW	10.284 ppm
FnMODE	undefined
F2 - Processing parameters	
SI	32768
SF	300.1300065 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00
F1 - Processing parameters	
SI	1024
MC2	QF
SF	300.1300000 MHz
WDW	SINE
SSB	0
LB	0.30 Hz
GB	0.1

4-Imino-3-phenyl-3,4-dihydroquinazoline-2-carbonitrile (**6a**)



Current Data Parameters

NAME	Styliana
EXPNO	14
PROCNO	1
F2 - Acquisition Parameters	
Date_	20110206
Time	15.36
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl ₃
NS	8765
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	2050
DW	16.800 usec
DE	6.50 usec
TE	298.4 K
D1	6.00000000 sec
D11	0.03000000 sec
CHANNEL f1	=====
NUC1	¹³ C
P1	8.00 usec
PLW1	138.00000000 W
SFO1	125.7459776 MHz
CHANNEL f2	=====
CPDPRG2	waltz16
NUC2	¹ H
PCPD2	80.00 usec
PLW2	13.00000000 W
PLW12	0.31738001 W
PLW13	0.20313001 W
SFO2	500.0350280 MHz
F2 - Processing parameters	
SI	32768
SF	125.7334120 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

4-Imino-3-phenyl-3,4-dihydroquinazoline-2-carbonitrile (**6a**)

D E P T 1 3 5

133.42
131.26
131.04
129.89
128.99
128.36
125.62

—133.42

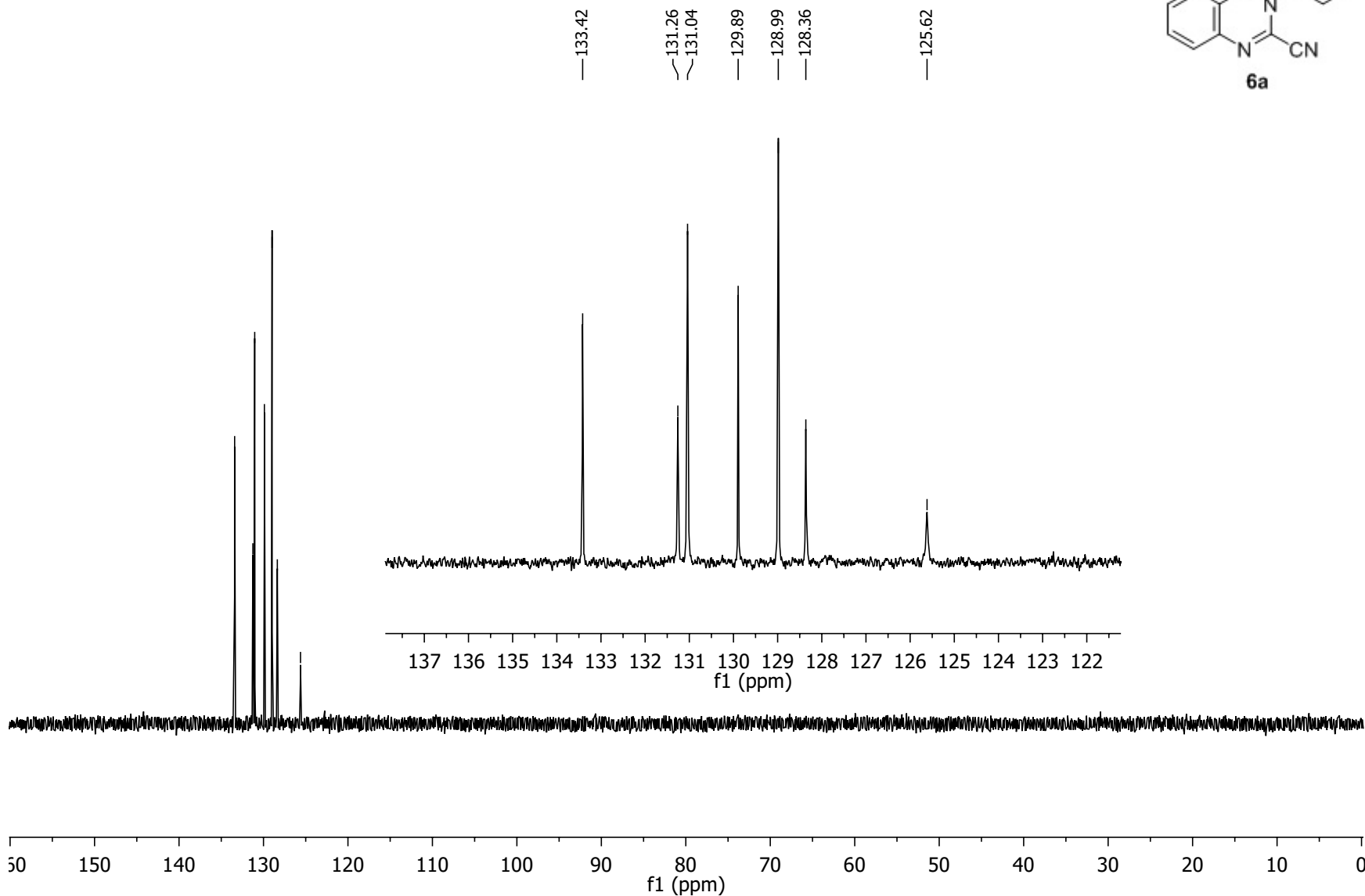
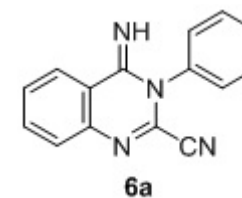
—131.26
—131.04

—129.89

—128.99

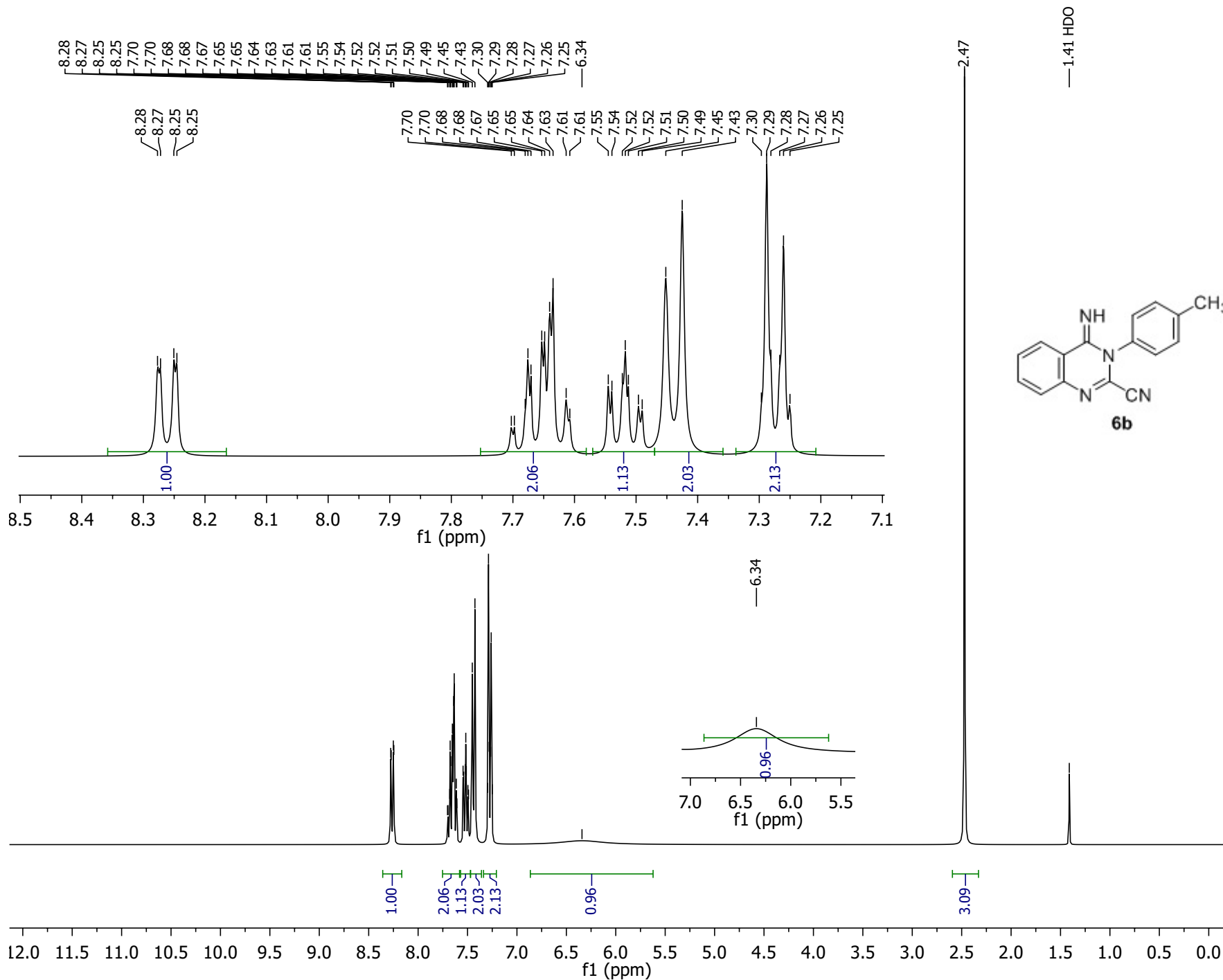
—128.36

—125.62



Current Data Parameters
NAME Styliana
EXPNO 15
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110207
Time 9.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG depts135
TD 65536
SOLVENT CDCl3
NS 75
DS 4
SWH 20161.291 Hz
FIDRES 0.307637 Hz
AQ 1.6253428 sec
RG 2050
DW 24.800 usec
DE 6.50 usec
TE 297.2 K
CNST2 145.0000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
CHANNEL f1 =====
NUC1 13C
P1 8.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 138.0000000 W
SFO1 125.7434630 MHz
SPNAM5 Crp60comp.4
SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 13.49400043 W
CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 12.50 usec
P4 25.00 usec
PCPD2 80.00 usec
PLW2 13.00000000 W
PLW12 0.31738001 W
SFO2 500.0346271 MHz
F2 - Processing parameters
SI 32768
SF 125.7334116 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

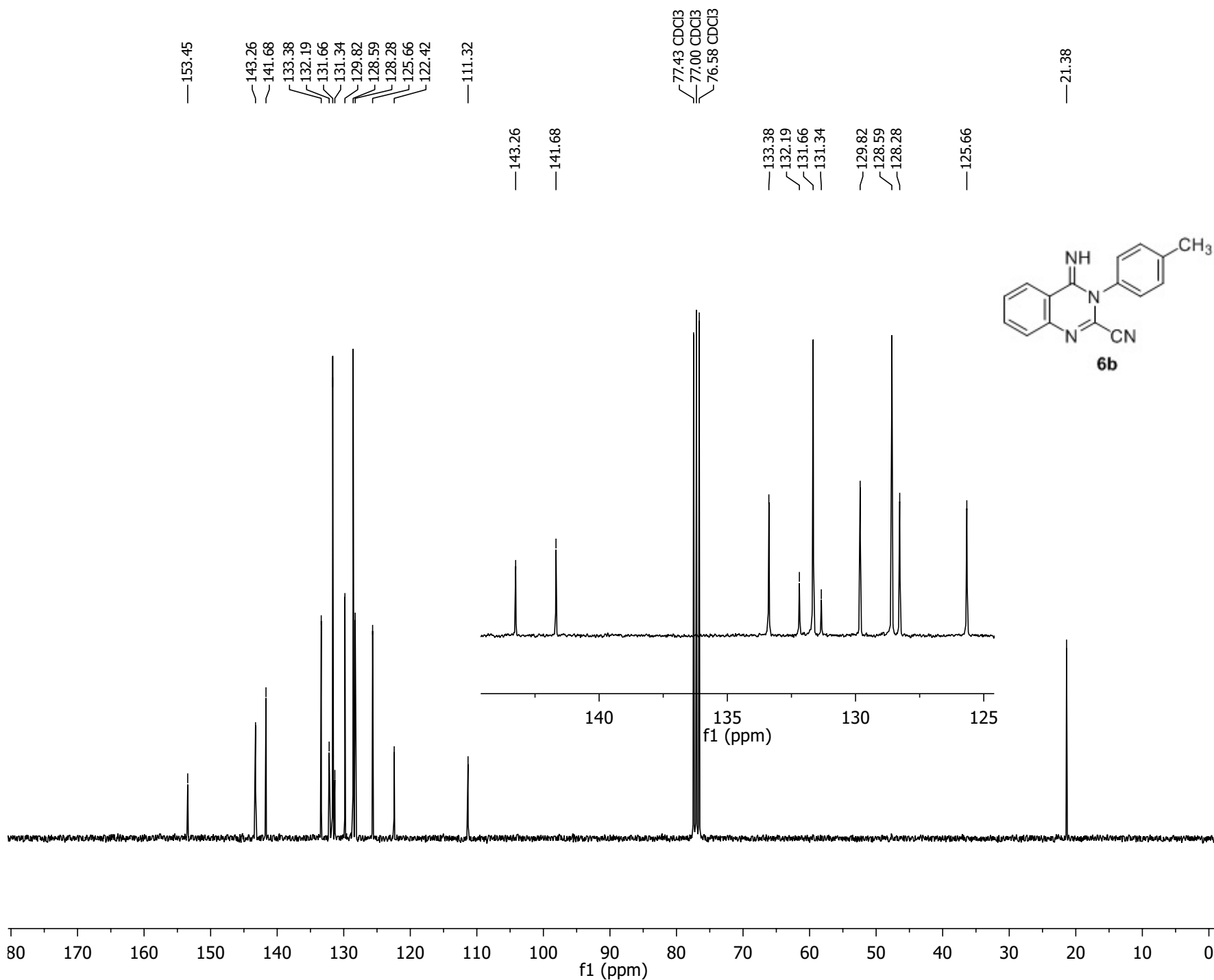
4-Imino-3-p-tolyl-3,4-dihydroquinazoline-2-carbonitrile (**6b**)



Current Data Parameters

NAME	Styliana
EXPNO	14
PROCNO	1
F2 - Acquisition Parameters	
Date_	20100313
Time	16.44
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	6172.839 Hz
FIDRES	0.094190 Hz
AQ	5.3084660 sec
RG	161.3
DW	81.000 usec
DE	9.00 usec
TE	298.2 K
D1	1.00000000 sec
TD0	1
CHANNEL f1	=====
NUC1	1H
P1	9.40 usec
PL1	0.00 dB
SFO1	300.1318534 MHz
F1 - Acquisition parameters	
ND0	2
TD	256
SFO1	300.1314 MHz
FIDRES	12.056327 Hz
SW	10.284 ppm
FnMODE	undefined
F2 - Processing parameters	
SI	32768
SF	300.1300094 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00
F1 - Processing parameters	
SI	1024
MC2	QF
SF	300.1300000 MHz
WDW	SINE
SSB	0
LB	0.30 Hz
GB	0.1

4-Imino-3-*p*-tolyl-3,4-dihydroquinazoline-2-carbonitrile (**6b**)



Current Data Parameters

NAME	Stylina
EXPNO	16
PROCNO	1
F2 - Acquisition Parameters	
Date_	20100313
Time	18.16
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl ₃
NS	1024
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	18390.4
DW	27.800 usec
DE	6.00 usec
TE	299.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
CHANNEL f1	=====
NUC1	¹³ C
P1	7.95 usec
PL1	-2.00 dB
SFO1	75.4752953 MHz
CHANNEL f2	=====
CPDPRG2	waltz16
NUC2	¹ H
PCPD2	110.00 usec
PL2	0.00 dB
PL12	22.00 dB
PL13	24.00 dB
SFO2	300.1312005 MHz
F2 - Processing parameters	
SI	32768
SF	75.4677545 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

4-Imino-3-*p*-tolyl-3,4-dihydroquinazoline-2-carbonitrile (**6b**)

D E P T 1 3 5

133.38
131.66
129.82
128.59
128.28
125.66

133.38

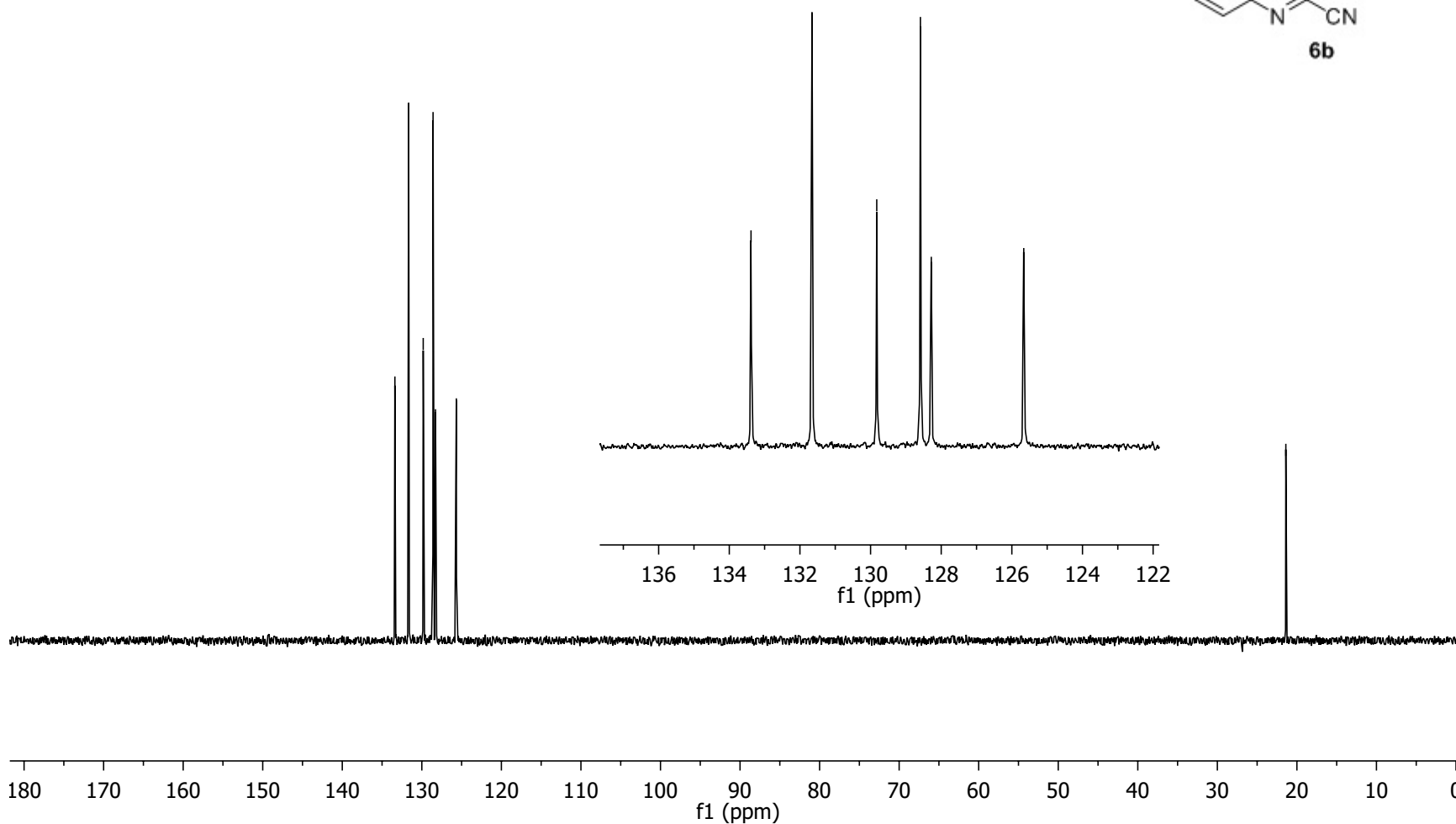
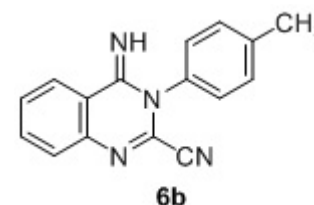
131.66

129.82

128.59
128.28

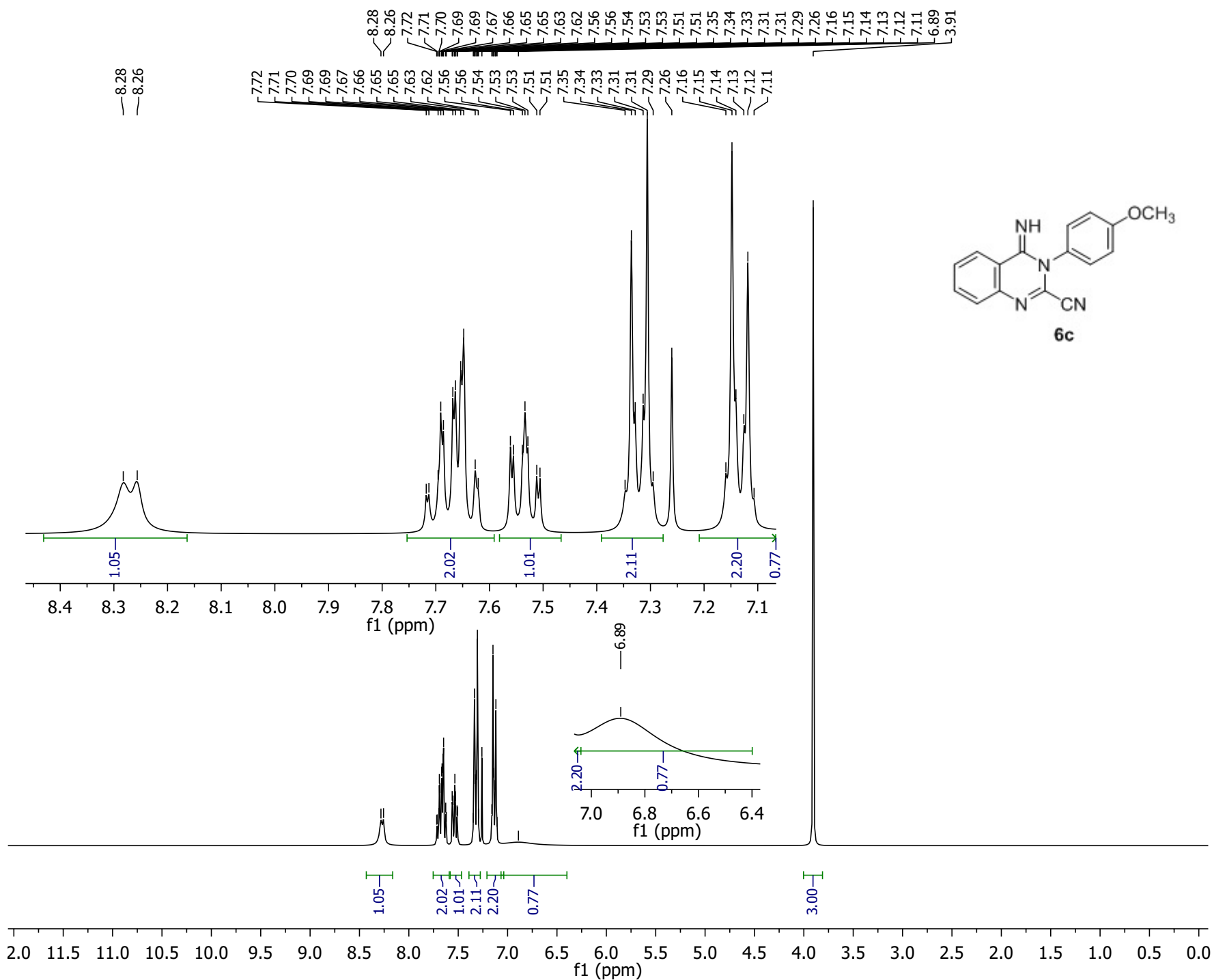
125.66

21.39



Current Data Parameters
NAME Styliana
EXPNO 15
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100313
Time 17.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 6.00 usec
TE 298.2 K
CNST2 145.000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001012 sec
TD0 1
CHANNEL f1 =====
NUC1 13C
P1 7.95 usec
p2 15.90 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz
CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 9.40 usec
p4 18.80 usec
PCPD2 110.00 usec
PL2 0.00 dB
PL12 22.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677541 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

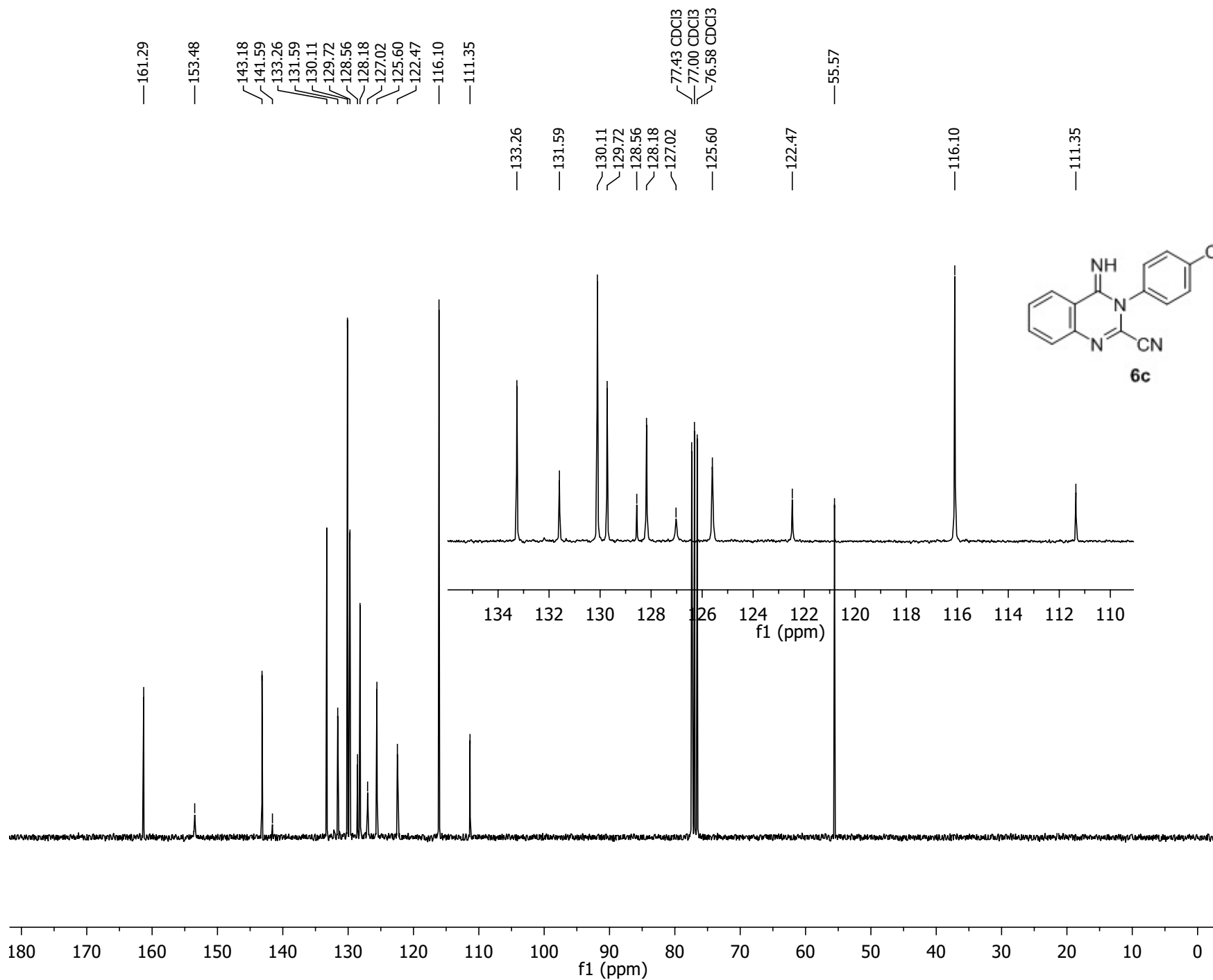
4-Imino-3-(4-methoxyphenyl)-3,4-dihydroquinazoline-2-carbonitrile (**6c**)



Current Data Parameters

NAME	Styliana
EXPNO	104
PROCNO	1
F2 - Acquisition Parameters	
Date_	20101018
Time	14.38
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	6172.839 Hz
FIDRES	0.094190 Hz
AQ	5.3084660 sec
RG	362
DW	81.000 usec
DE	9.00 usec
TE	295.2 K
D1	1.00000000 sec
TD0	1
CHANNEL f1	=====
NUC1	1H
P1	9.40 usec
PL1	0.00 dB
SFO1	300.1318534 MHz
F1 - Acquisition parameters	
ND0	2
TD	256
SFO1	300.1314 MHz
FIDRES	12.056327 Hz
SW	10.284 ppm
FnMODE	undefined
F2 - Processing parameters	
SI	32768
SF	300.1300063 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00
F1 - Processing parameters	
SI	1024
MC2	QF
SF	300.1300000 MHz
WDW	SINE
SSB	0
LB	0.30 Hz
GB	0.1

4-Imino-3-(4-methoxyphenyl)-3,4-dihydroquinazoline-2-carbonitrile (**6c**)



Current Data Parameters

NAME	Stylana
EXPNO	95
PROCNO	1
F2 - Acquisition Parameters	
Date_	20101010
Time	15.58
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	795
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	18390.4
DW	27.800 usec
DE	6.00 usec
TE	296.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
CHANNEL f1	=====
NUC1	13C
P1	7.95 usec
PL1	-2.00 dB
SFO1	75.4752953 MHz
CHANNEL f2	=====
CPDPRG2	waltz16
NUC2	1H
PCPD2	110.00 usec
PL2	0.00 dB
PL12	22.00 dB
PL13	24.00 dB
SFO2	300.1312005 MHz
F2 - Processing parameters	
SI	32768
SF	75.4677578 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

4-Imino-3-(4-methoxyphenyl)-3,4-dihydroquinazoline-2-carbonitrile (**6c**)

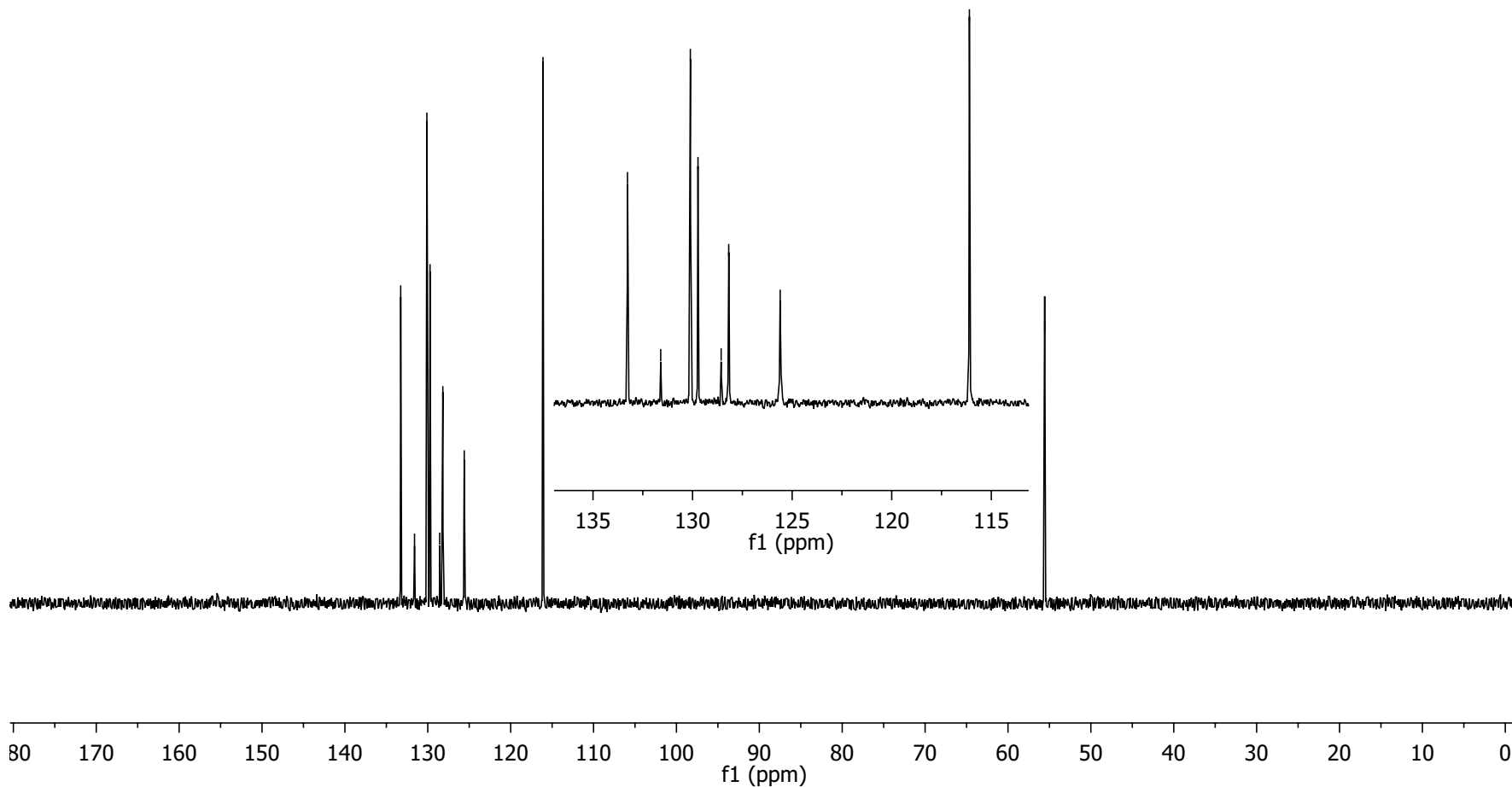
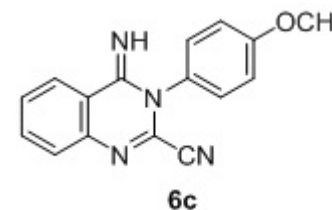
DEPT 135

133.27
131.60
130.11
129.73
128.57
128.19
125.60
— 116.10

133.27
131.60
130.11
129.73
128.57
128.19
— 125.60

— 116.10

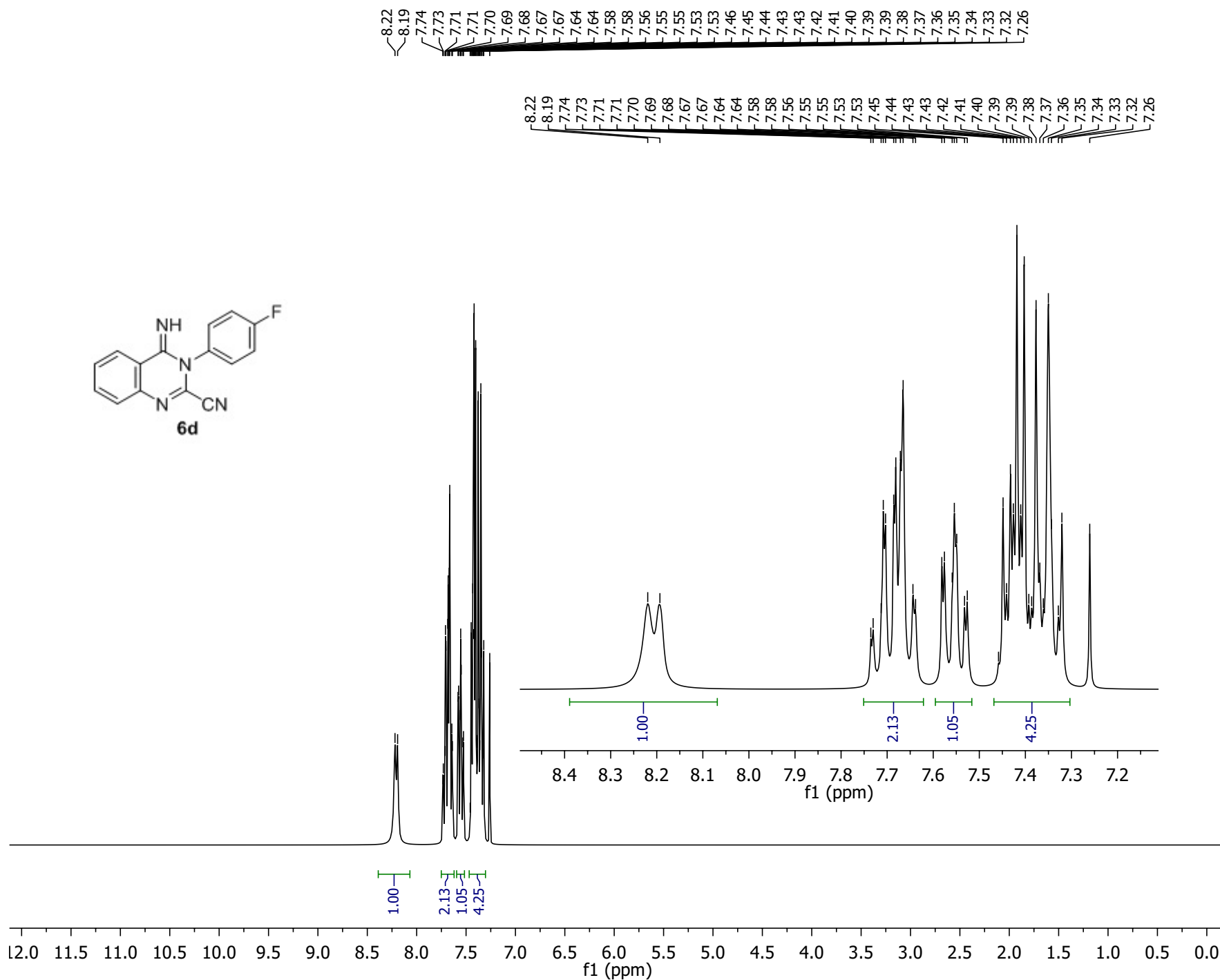
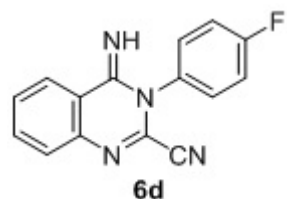
— 55.57



Current Data Parameters

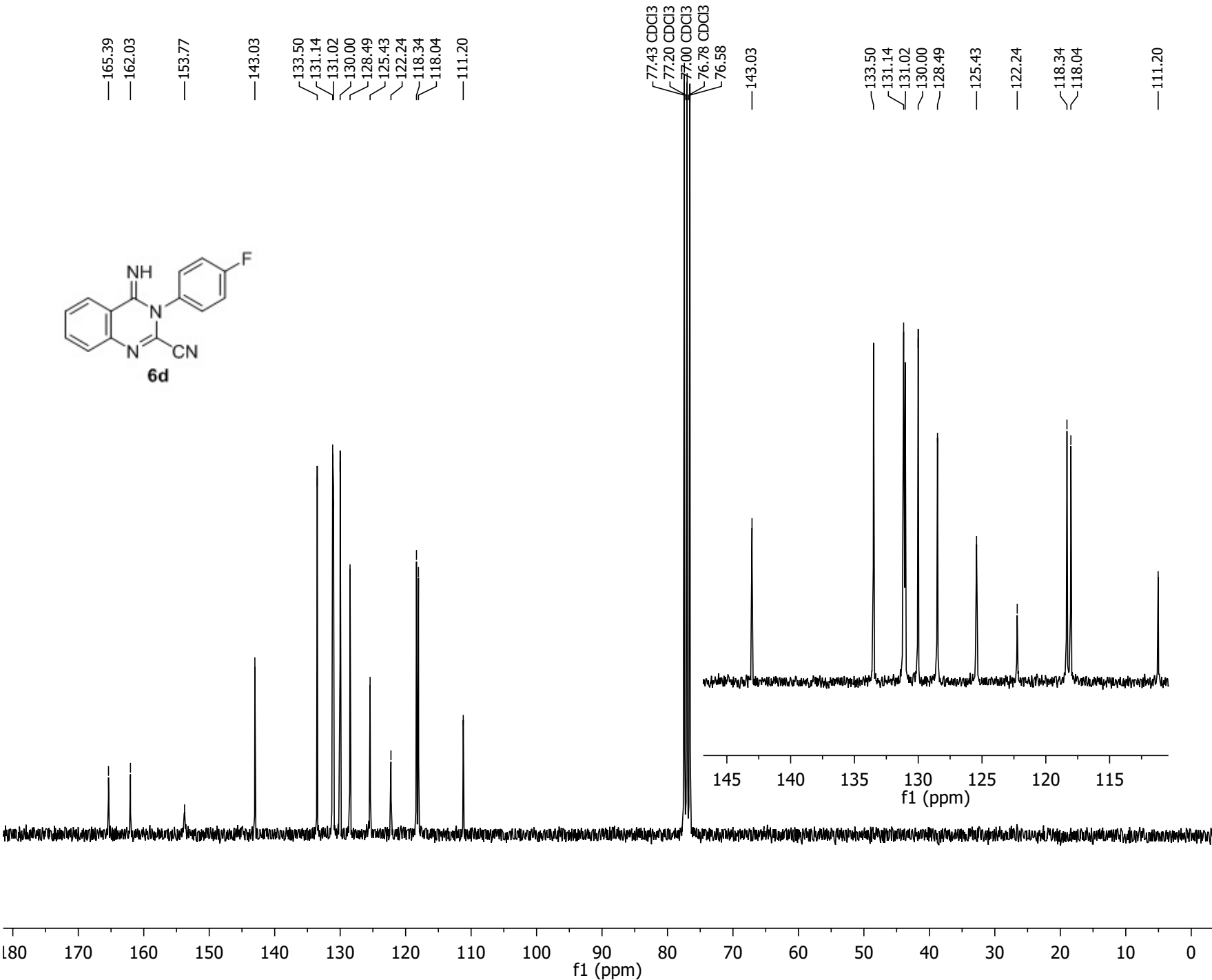
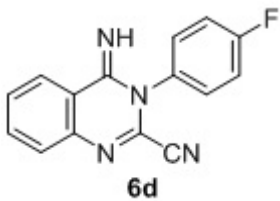
NAME	Stylia
EXPNO	97
PROCNO	1
F2 - Acquisition Parameters	
Date_	20101010
Time	16.51
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	dept135
TD	65536
SOLVENT	CDCl3
NS	61
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	16384
DW	27.800 usec
DE	6.00 usec
TE	296.2 K
CNST2	145.0000000
D1	2.00000000 sec
d2	0.00344828 sec
d12	0.00002000 sec
DELTA	0.00001012 sec
TD0	1
CHANNEL f1 =====	
NUC1	13C
P1	7.95 usec
p2	15.90 usec
PL1	-2.00 dB
SFO1	75.4752953 MHz
CHANNEL f2 =====	
CPDPRG2	waltz16
NUC2	1H
P3	9.40 usec
p4	18.80 usec
PCPD2	110.00 usec
PL2	0.00 dB
PL12	22.00 dB
SFO2	300.1312005 MHz
F2 - Processing parameters	
SI	32768
SF	75.4677575 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

3-(4-Fluorophenyl)-4-imino-3,4-dihydroquinazoline-2-carbonitrile (**6d**)



Current Data Parameters
NAME Styliana
EXPNO 37
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100712
Time 18.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 322.5
DW 81.000 usec
DE 9.00 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1
CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1318534 MHz
F1 - Acquisition parameters
ND0 2
TD 256
SFO1 300.1314 MHz
FIDRES 12.056327 Hz
SW 10.284 ppm
FnMODE undefined
F2 - Processing parameters
SI 32768
SF 300.1300063 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
F1 - Processing parameters
SI 1024
MC2 QF
SF 300.1300000 MHz
WDW SINE
SSB 0
LB 0.30 Hz
GB 0.1

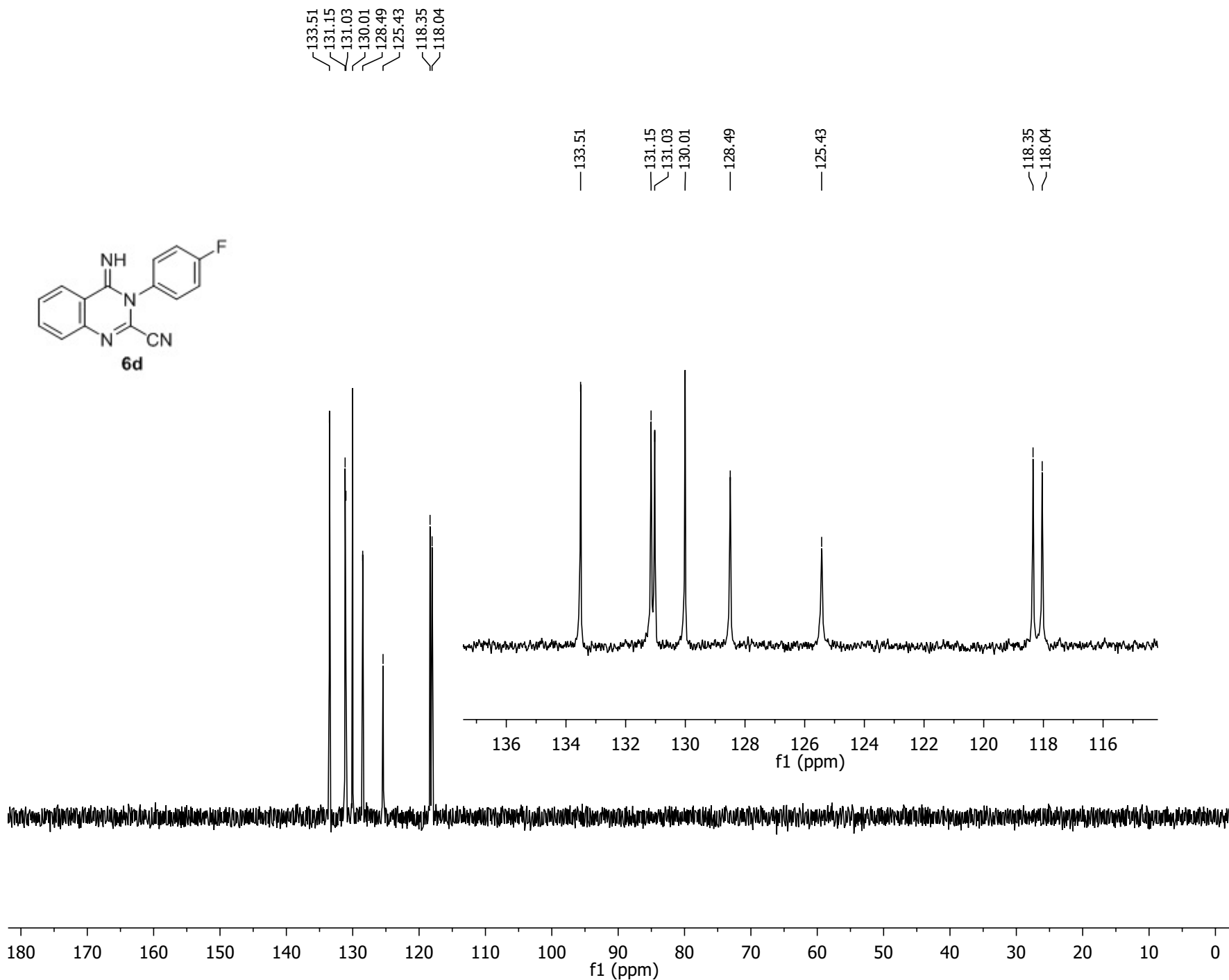
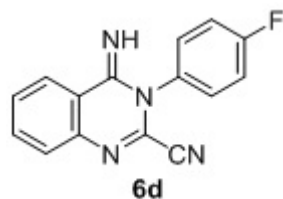
3-(4-Fluorophenyl)-4-imino-3,4-dihydroquinazoline-2-carbonitrile (**6d**)



Current Data Parameters
NAME Styliana
EXPNO 93
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101010
Time 14.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 11585.2
DW 27.800 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
CHANNEL f1 =====
NUC1 13C
P1 7.95 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz
CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 110.00 usec
PL2 0.00 dB
PL12 22.00 dB
PL13 24.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677545 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3-(4-Fluorophenyl)-4-imino-3,4-dihydroquinazoline-2-carbonitrile (**6d**)

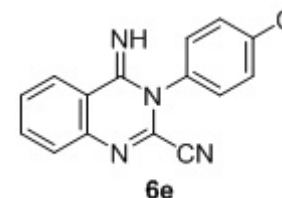
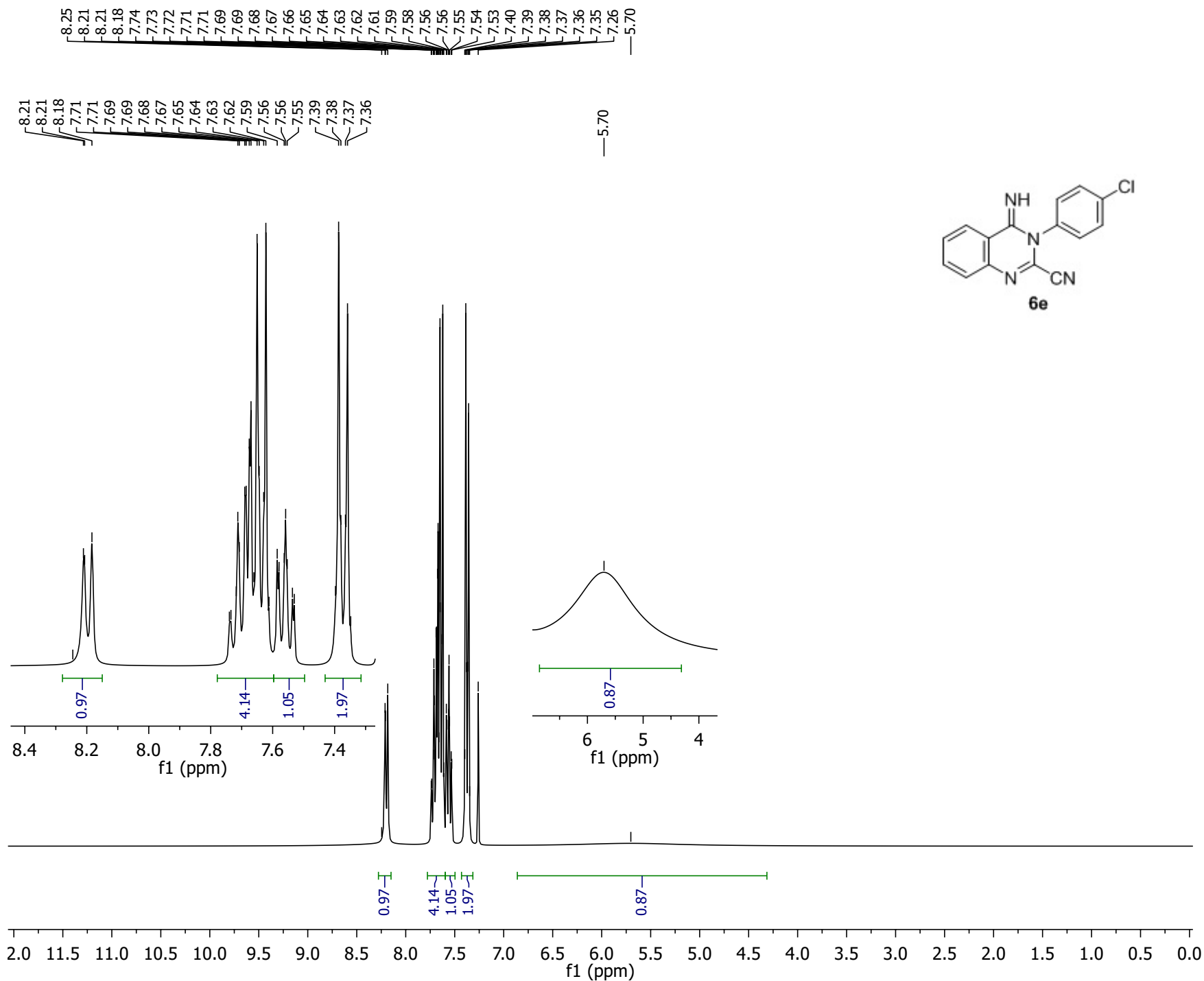
D E P T 1 3 5



Current Data Parameters

NAME	Styliana
EXPNO	94
PROCNO	1
F2 - Acquisition Parameters	
Date_	20101010
Time	15.34
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	dept135
TD	65536
SOLVENT	CDCl3
NS	203
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	16384
DW	27.800 usec
DE	6.00 usec
TE	296.2 K
CNST2	145.0000000
D1	2.00000000 sec
d2	0.00344828 sec
d12	0.00002000 sec
DELTA	0.00001012 sec
TD0	1
CHANNEL f1 =====	
NUC1	13C
P1	7.95 usec
p2	15.90 usec
PL1	-2.00 dB
SFO1	75.4752953 MHz
CHANNEL f2 =====	
CPDPRG2	waltz16
NUC2	1H
P3	9.40 usec
p4	18.80 usec
PCPD2	110.00 usec
PL2	0.00 dB
PL12	22.00 dB
SFO2	300.1312005 MHz
F2 - Processing parameters	
SI	32768
SF	75.4677542 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

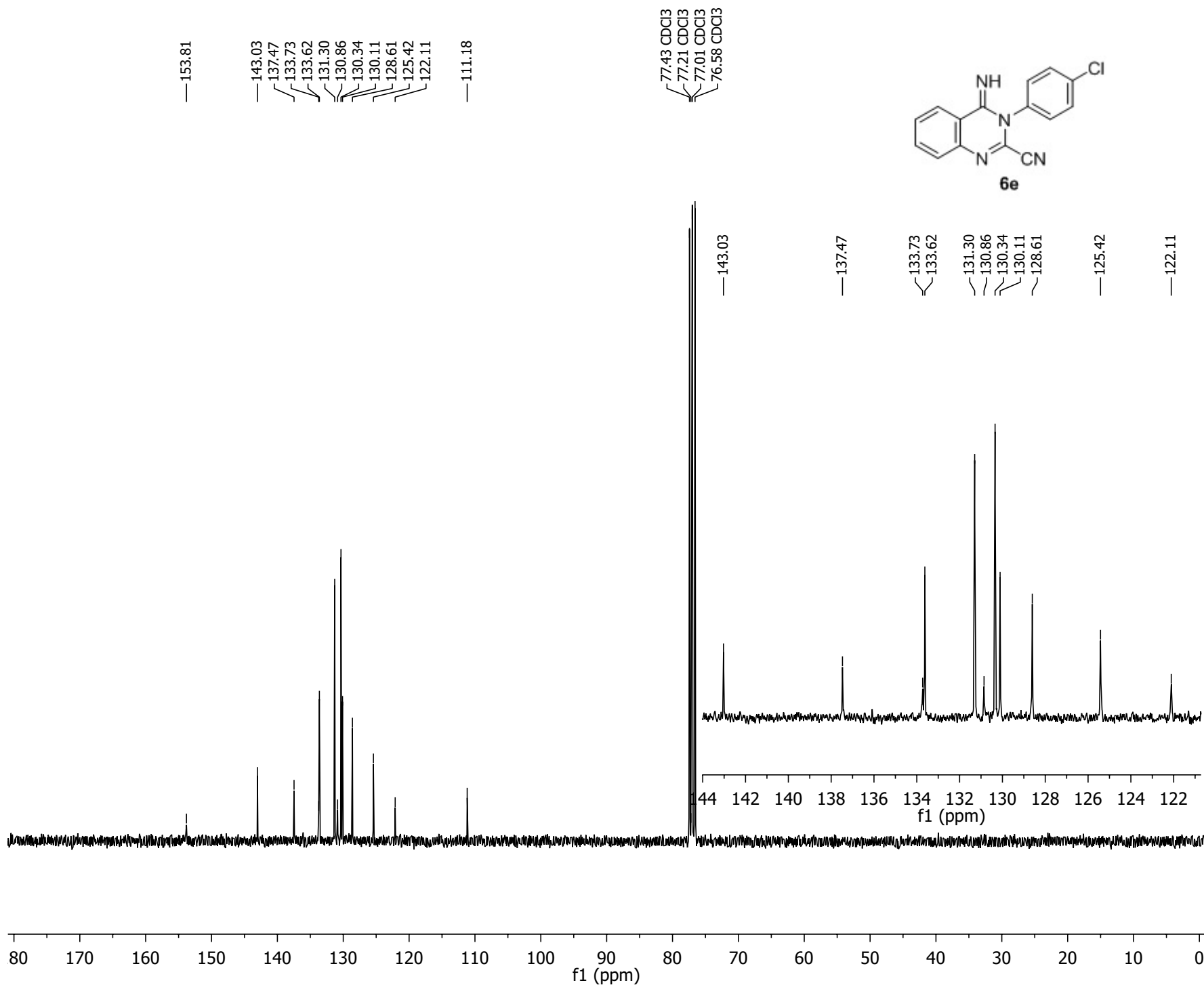
3-(4-Chlorophenyl)-4-imino-3,4-dihydroquinazoline-2-carbonitrile (**6e**)



Current Data Parameters

NAME	Styliana
EXPNO	46
PROCNO	1
F2 - Acquisition Parameters	
Date_	20100817
Time	13.12
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl ₃
NS	16
DS	2
SWH	6172.839 Hz
FIDRES	0.094190 Hz
AQ	5.3084660 sec
RG	322.5
DW	81.000 usec
DE	9.00 usec
TE	295.2 K
D1	1.00000000 sec
TD0	1
CHANNEL f1	=====
NUC1	¹ H
P1	9.40 usec
PL1	0.00 dB
SFO1	300.1318534 MHz
F1 - Acquisition parameters	
ND0	2
TD	256
SFO1	300.1314 MHz
FIDRES	12.056327 Hz
SW	10.284 ppm
FnMODE	undefined
F2 - Processing parameters	
SI	32768
SF	300.1300063 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00
F1 - Processing parameters	
SI	1024
MC2	QF
SF	300.1300000 MHz
WDW	SINE
SSB	0
LB	0.30 Hz
GB	0.1

3-(4-Chlorophenyl)-4-imino-3,4-dihydroquinazoline-2-carbonitrile (**6e**)

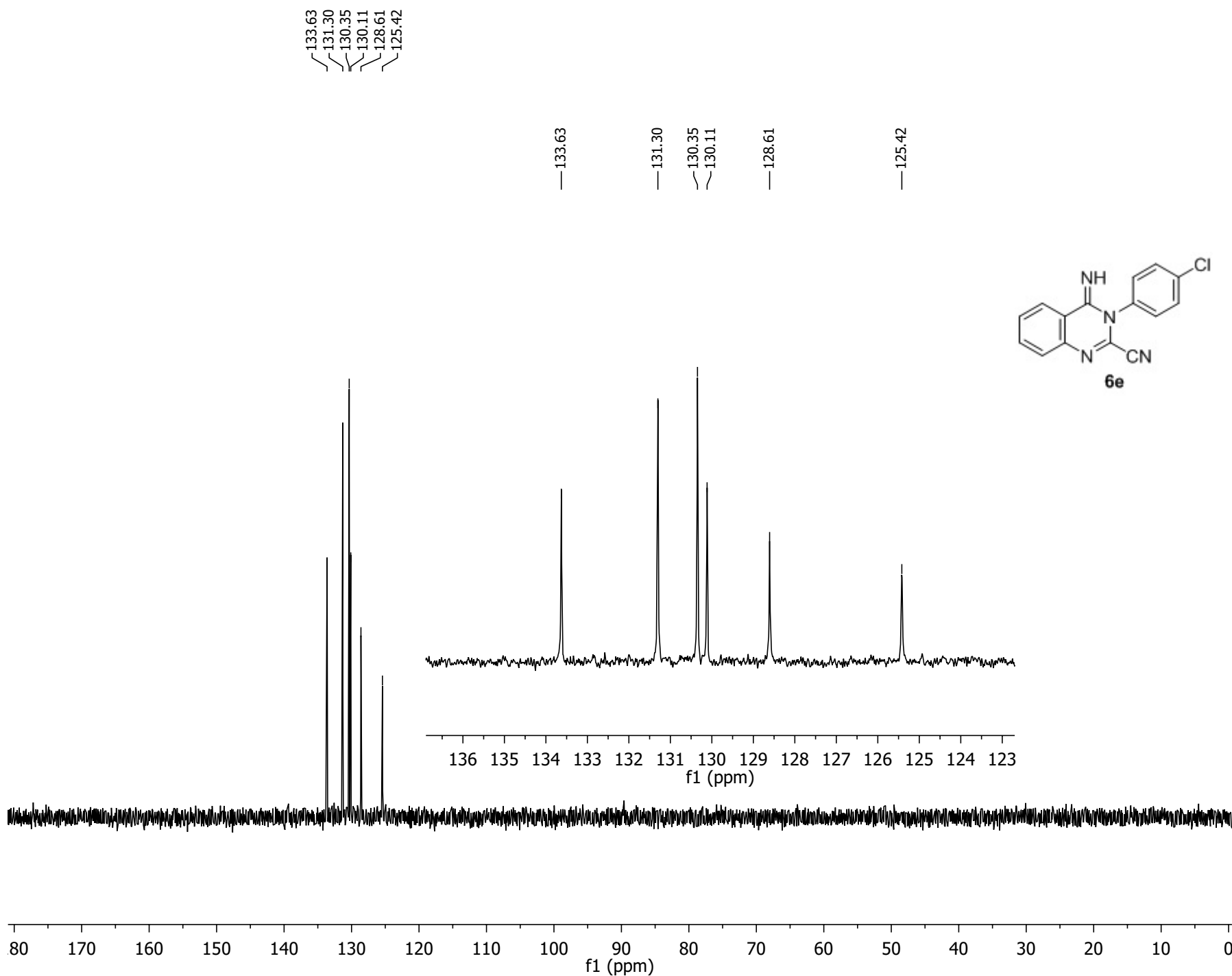


Current Data Parameters

NAME	Stylia
EXPNO	48
PROCNO	1
F2 - Acquisition Parameters	
Date_	20100817
Time	13.30
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl ₃
NS	491
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	8192
DW	27.800 usec
DE	6.00 usec
TE	296.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
CHANNEL f1	=====
NUC1	¹³ C
P1	7.95 usec
PL1	-2.00 dB
SFO1	75.4752953 MHz
CHANNEL f2	=====
CPDPRG2	waltz16
NUC2	¹ H
PCPD2	110.00 usec
PL2	0.00 dB
PL12	22.00 dB
PL13	24.00 dB
SFO2	300.1312005 MHz
F2 - Processing parameters	
SI	32768
SF	75.4677523 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

3-(4-Chlorophenyl)-4-imino-3,4-dihydroquinazoline-2-carbonitrile (**6e**)

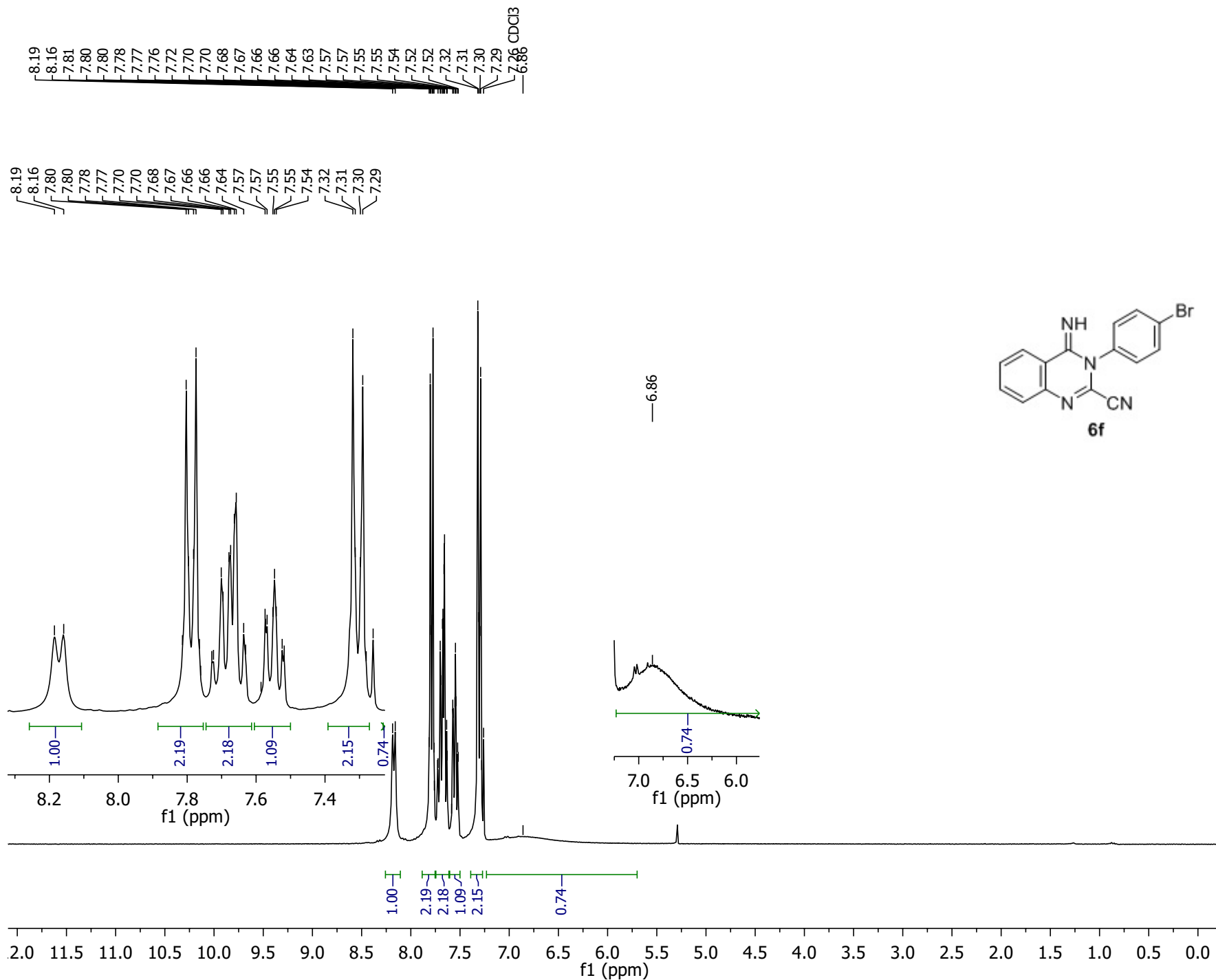
DEPT 135



Current Data Parameters

NAME	Stylia
EXPNO	47
PROCNO	1
F2 - Acquisition Parameters	
Date_	20100817
Time	13.26
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	dept135
TD	65536
SOLVENT	CDCl3
NS	199
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	16384
DW	27.800 usec
DE	6.00 usec
TE	296.2 K
CNST2	145.0000000
D1	2.00000000 sec
d2	0.00344828 sec
d12	0.00002000 sec
DELTA	0.00001012 sec
TD0	1
CHANNEL f1	=====
NUC1	13C
P1	7.95 usec
p2	15.90 usec
PL1	-2.00 dB
SFO1	75.4752953 MHz
CHANNEL f2	=====
CPDPRG2	waltz16
NUC2	1H
P3	9.40 usec
p4	18.80 usec
PCPD2	110.00 usec
PL2	0.00 dB
PL12	22.00 dB
SFO2	300.1312005 MHz
F2 - Processing parameters	
SI	32768
SF	75.4677521 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

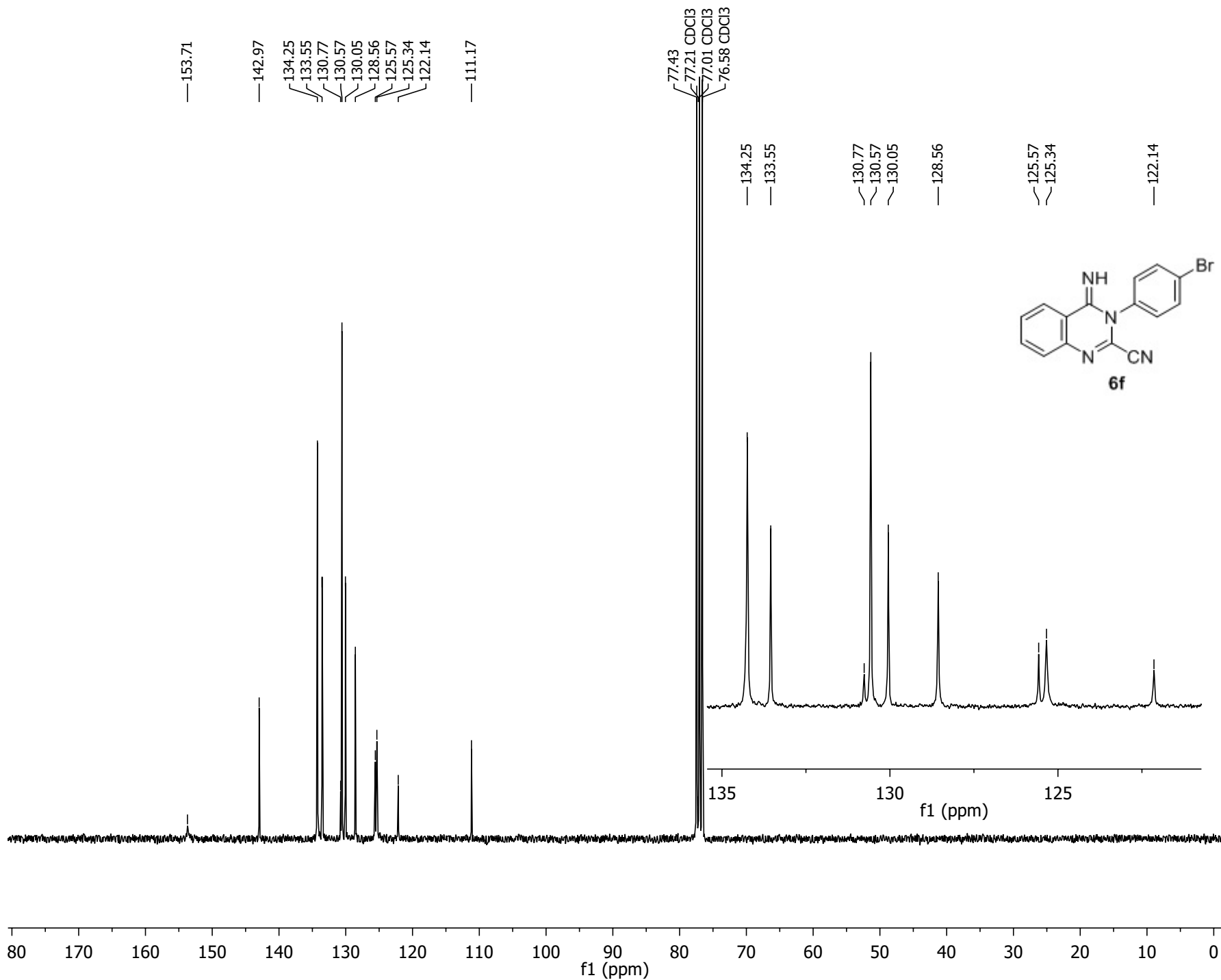
3-(4-Bromophenyl)-4-imino-3,4-dihydroquinazoline-2-carbonitrile (**6f**)



Current Data Parameters

NAME	Styliana
EXPNO	105
PROCNO	1
F2 - Acquisition Parameters	
Date_	20101018
Time	15.09
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	6172.839 Hz
FIDRES	0.094190 Hz
AQ	5.3084660 sec
RG	228.1
DW	81.000 usec
DE	9.00 usec
TE	295.2 K
D1	1.00000000 sec
TD0	1
CHANNEL f1 =====	
NUC1	1H
P1	9.40 usec
PL1	0.00 dB
SFO1	300.1318534 MHz
F1 - Acquisition parameters	
ND0	2
TD	256
SFO1	300.1314 MHz
FIDRES	12.056327 Hz
SW	10.284 ppm
FnMODE	undefined
F2 - Processing parameters	
SI	32768
SF	300.1300063 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00
F1 - Processing parameters	
SI	1024
MC2	QF
SF	300.1300000 MHz
WDW	SINE
SSB	0
LB	0.30 Hz
GB	0.1

3-(4-Bromophenyl)-4-imino-3,4-dihydroquinazoline-2-carbonitrile (**6f**)

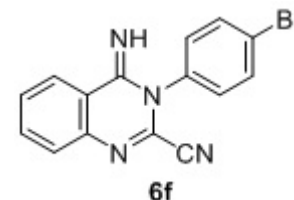
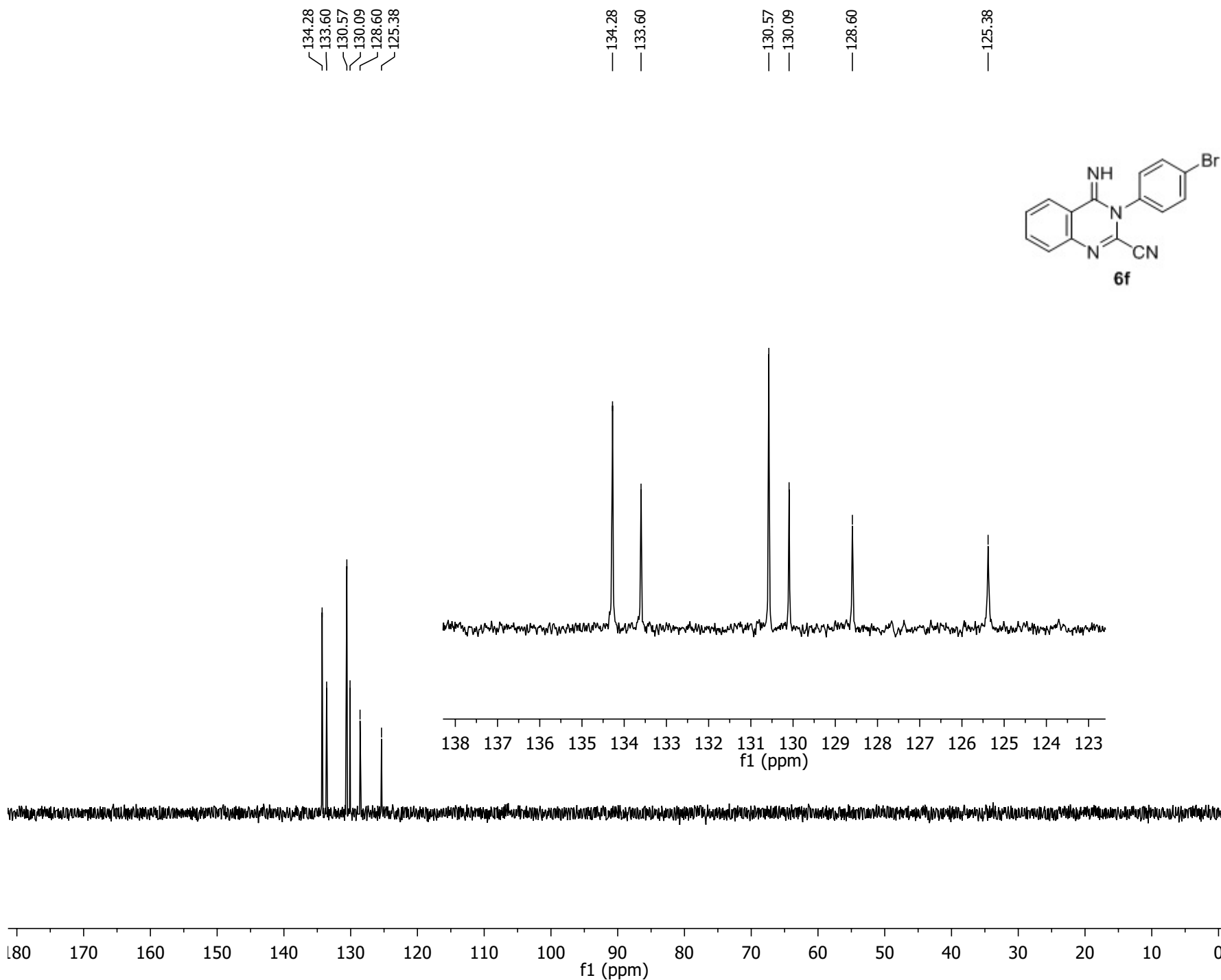


Current Data Parameters

NAME	Styliana
EXPNO	107
PROCNO	1
F2 - Acquisition Parameters	
Date_	20101018
Time	15.24
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl ₃
NS	1647
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	5160.6
DW	27.800 usec
DE	6.00 usec
TE	295.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
CHANNEL f1	=====
NUC1	¹³ C
P1	7.95 usec
PL1	-2.00 dB
SFO1	75.4752953 MHz
CHANNEL f2	=====
CPDPRG2	waltz16
NUC2	¹ H
PCPD2	110.00 usec
PL2	0.00 dB
PL12	22.00 dB
PL13	24.00 dB
SFO2	300.1312005 MHz
F2 - Processing parameters	
SI	32768
SF	75.4677545 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

3-(4-Bromophenyl)-4-imino-3,4-dihydroquinazoline-2-carbonitrile (**6f**)

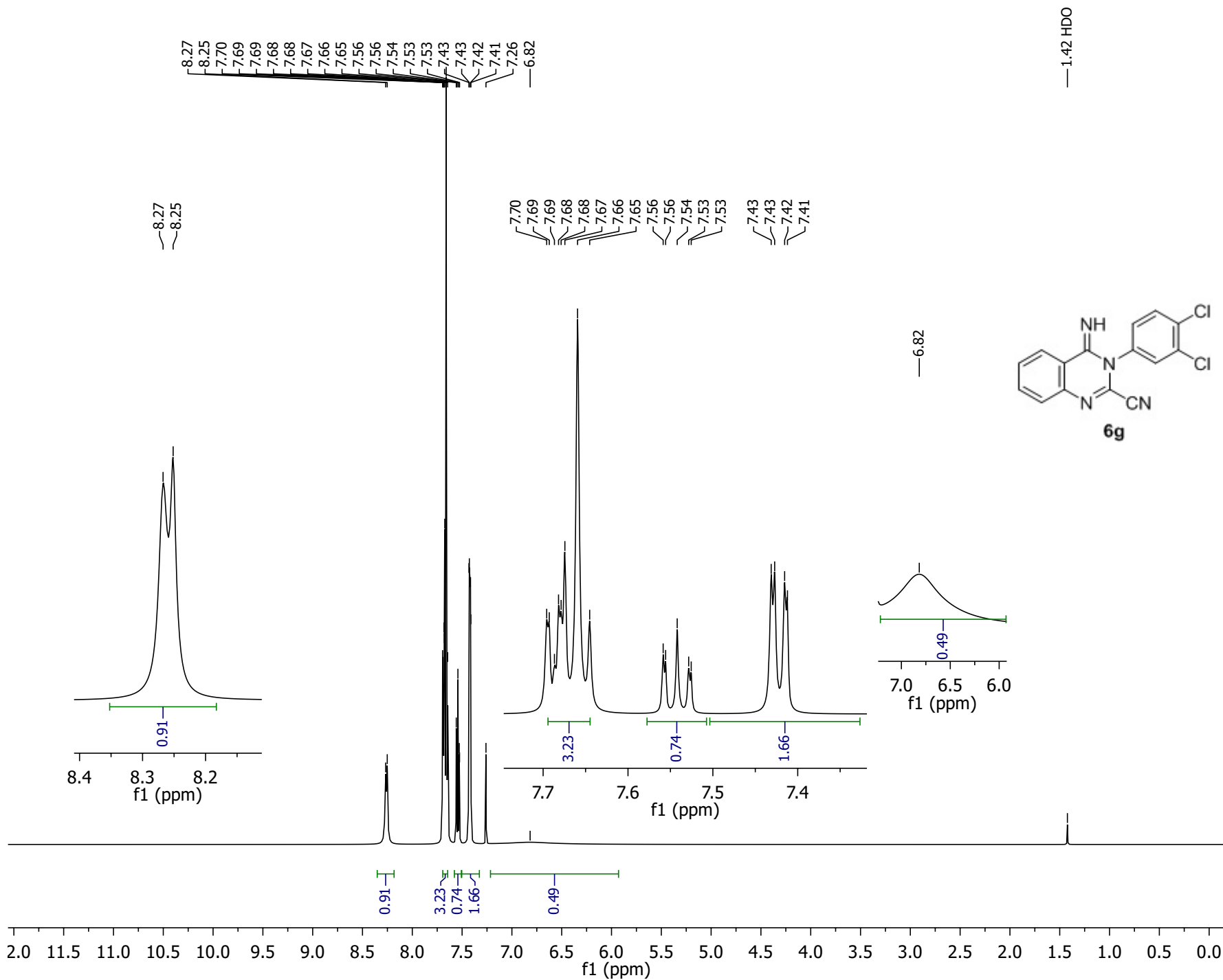
DEPT 135



Current Data Parameters

NAME	Styliana
EXPNO	23
PROCNO	1
F2 - Acquisition Parameters	
Date_	20100409
Time	16.50
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	dept135
TD	65536
SOLVENT	CDCl3
NS	139
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	16384
DW	27.800 usec
DE	6.00 usec
TE	296.2 K
CNST2	145.0000000
D1	2.00000000 sec
d2	0.00344828 sec
d12	0.00002000 sec
DELTA	0.00001012 sec
TD0	1
CHANNEL f1	=====
NUC1	13C
P1	7.95 usec
p2	15.90 usec
PL1	-2.00 dB
SFO1	75.4752953 MHz
CHANNEL f2	=====
CPDPRG2	waltz16
NUC2	1H
P3	9.40 usec
p4	18.80 usec
PCPD2	110.00 usec
PL2	0.00 dB
PL12	22.00 dB
SFO2	300.1312005 MHz
F2 - Processing parameters	
SI	32768
SF	75.4677531 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

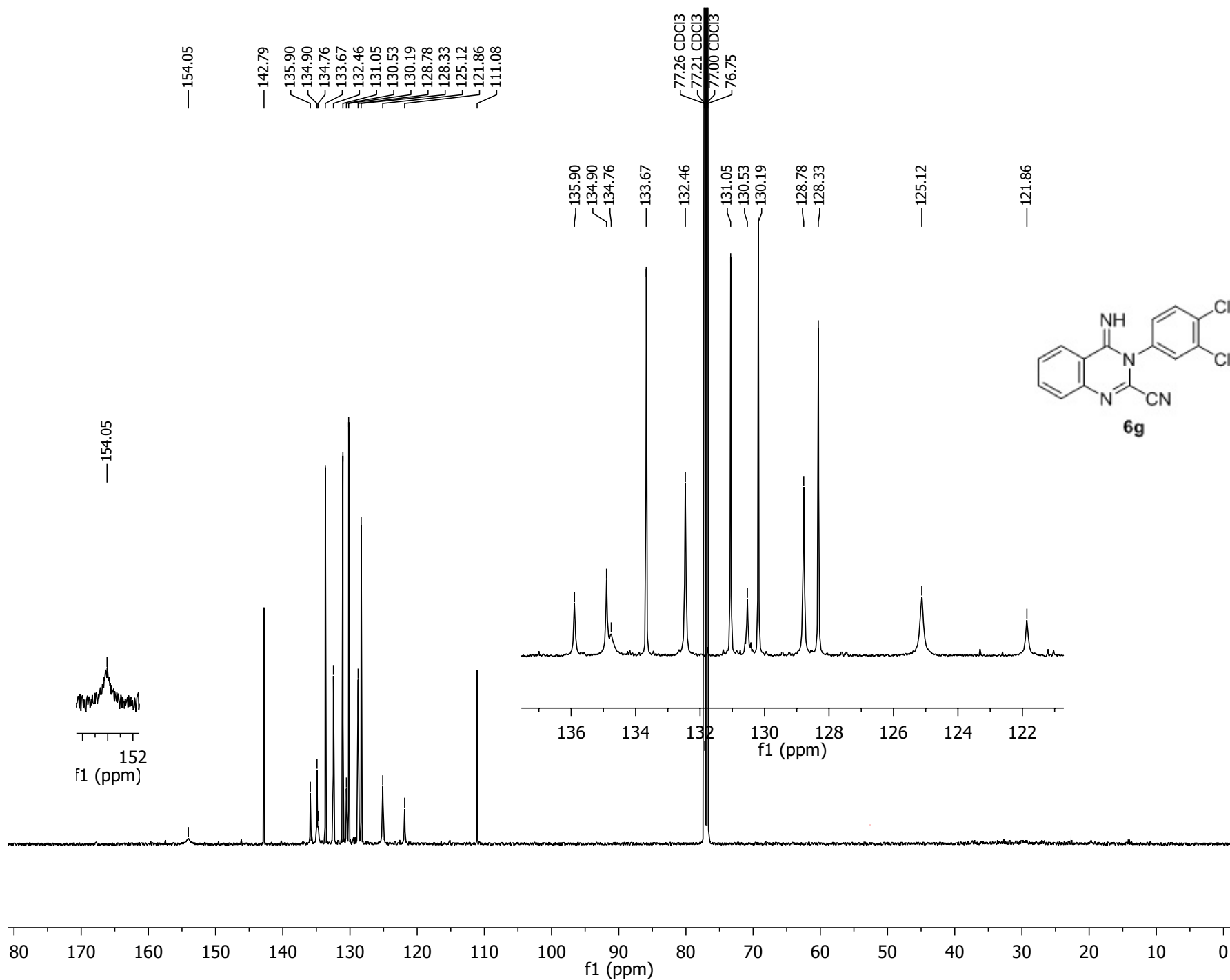
3-(3,4-Dichlorophenyl)-4-imino-3,4-dihydroquinazoline-2-carbonitrile (**6g**)



Current Data Parameters

NAME	Styliana
EXPNO	16
PROCNO	1
F2 - Acquisition Parameters	
Date_	20110207
Time	9.13
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	101
DW	48.400 usec
DE	6.50 usec
TE	297.1 K
D1	1.00000000 sec
CHANNEL f1	=====
NUC1	1H
P1	11.00 usec
PLW1	15.41699982 W
SFO1	500.0361158 MHz
F2 - Processing parameters	
SI	65536
SF	500.0330400 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

3-(3,4-Dichlorophenyl)-4-imino-3,4-dihydroquinazoline-2-carbonitrile (**6g**)



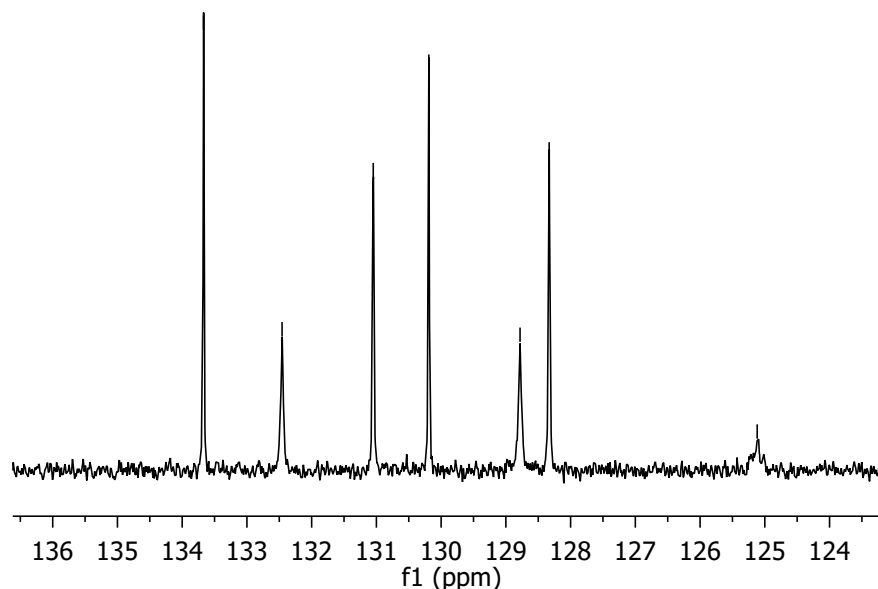
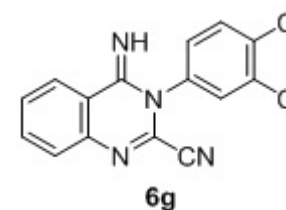
Current Data Parameters

NAME	Styliana
EXPNO	17
PROCNO	1
F2 - Acquisition Parameters	
Date_	20110207
Time	19.37
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl ₃
NS	7351
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	2050
DW	16.800 usec
DE	6.50 usec
TE	298.2 K
D1	6.00000000 sec
D11	0.03000000 sec
CHANNEL f1 =====	
NUC1	¹³ C
P1	8.00 usec
PLW1	138.00000000 W
SFO1	125.7459776 MHz
CHANNEL f2 =====	
CPDPRG2	waltz16
NUC2	¹ H
PCPD2	80.00 usec
PLW2	13.00000000 W
PLW12	0.31738001 W
PLW13	0.20313001 W
SFO2	500.0350280 MHz
F2 - Processing parameters	
SI	32768
SF	125.7334138 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

3-(3,4-Dichlorophenyl)-4-imino-3,4-dihydroquinazoline-2-carbonitrile (**6g**)

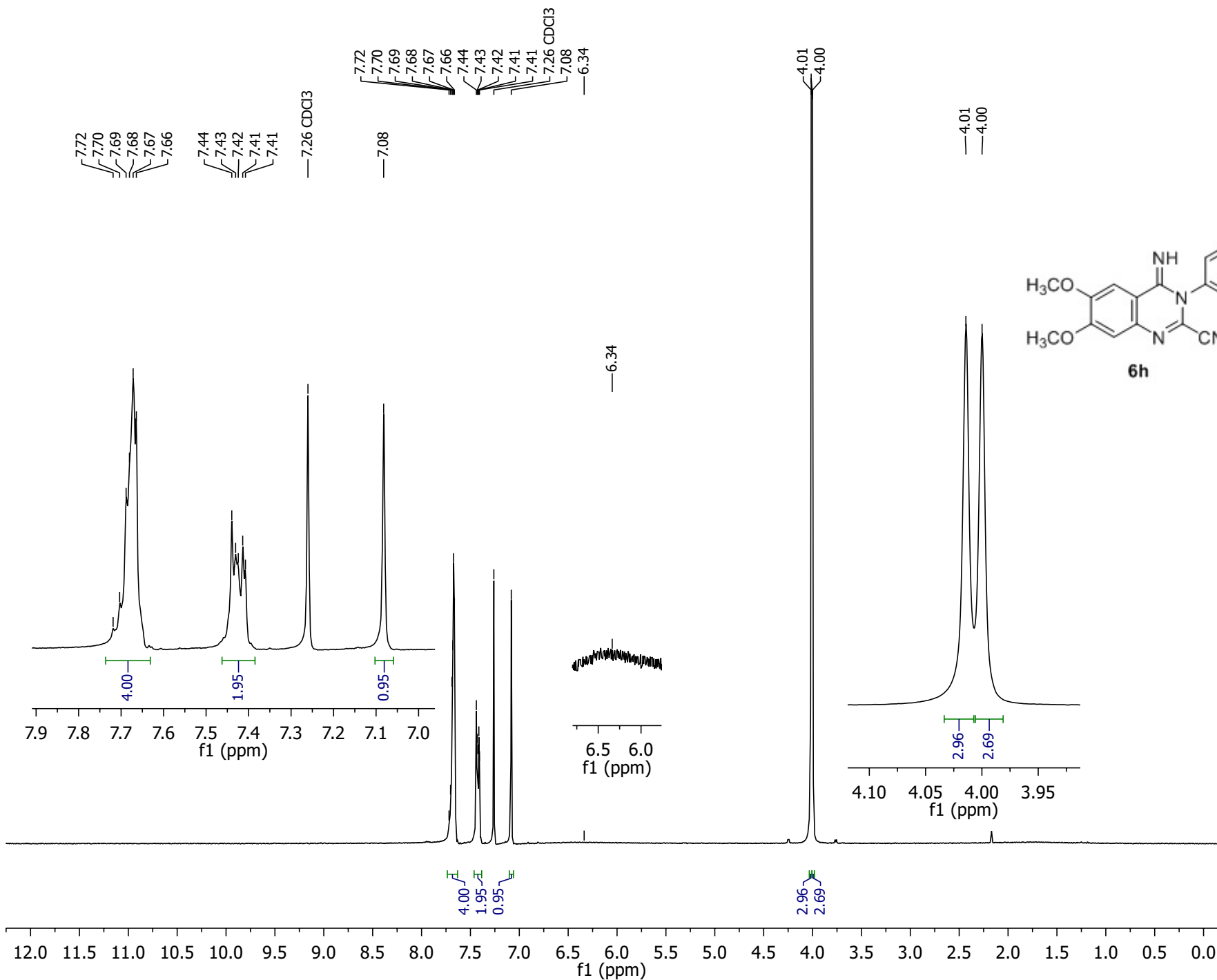
133.67
132.46
131.05
130.19
128.78
128.33
125.12

133.67
132.46
131.05
130.19
128.78
128.33
125.12



Current Data Parameters
NAME Styliana
EXPNO 18
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110208
Time 10.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG deptsp135
TD 65536
SOLVENT CDCl3
NS 54
DS 4
SWH 20161.291 Hz
FIDRES 0.307637 Hz
AQ 1.6253428 sec
RG 2050
DW 24.800 usec
DE 6.50 usec
TE 298.1 K
CNST2 145.000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
CHANNEL f1 =====
NUC1 13C
P1 8.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 138.0000000 W
SFO1 125.7434630 MHz
SPNAM5 Crp60comp.4
SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 13.49400043 W
CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 12.50 usec
P4 25.00 usec
PCPD2 80.00 usec
PLW2 13.0000000 W
PLW12 0.31738001 W
SFO2 500.0346271 MHz
F2 - Processing parameters
SI 32768
SF 125.7334139 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

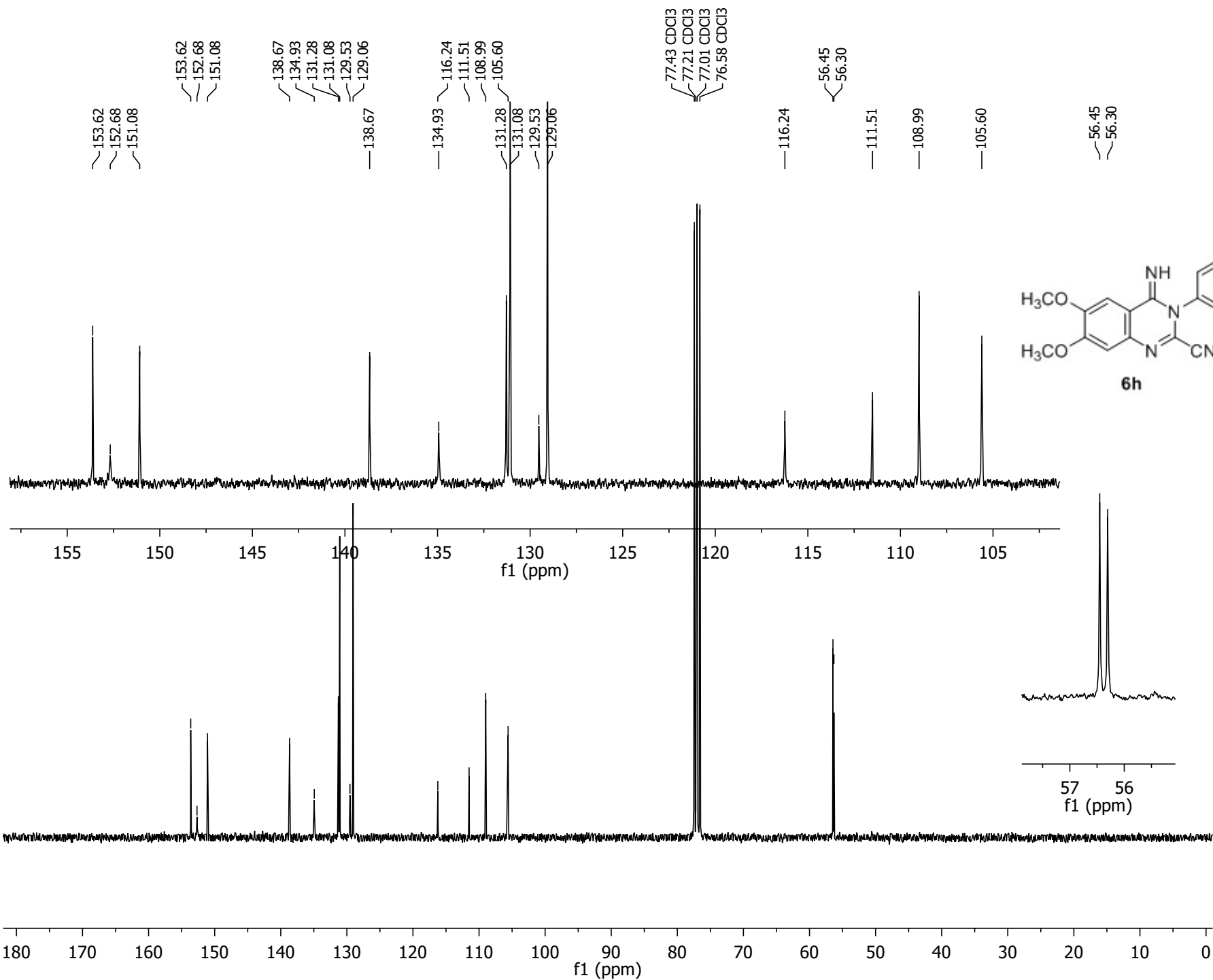
4-Imino-6,7-dimethoxy-3-phenyl-3,4-dihydroquinazoline-2-carbonitrile (**6h**)



Current Data Parameters

NAME	Styliana
EXPNO	91
PROCNO	1
F2 - Acquisition Parameters	
Date_	20101010
Time	13.43
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl ₃
NS	16
DS	2
SWH	6172.839 Hz
FIDRES	0.094190 Hz
AQ	5.3084660 sec
RG	574.7
DW	81.000 usec
DE	9.00 usec
TE	296.2 K
D1	1.00000000 sec
TD0	1
CHANNEL f1	=====
NUC1	1H
P1	9.40 usec
PL1	0.00 dB
SFO1	300.1318534 MHz
F1 - Acquisition parameters	
NDO	2
TD	256
SFO1	300.1314 MHz
FIDRES	12.056327 Hz
SW	10.284 ppm
FnMODE	undefined
F2 - Processing parameters	
SI	32768
SF	300.130063 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00
F1 - Processing parameters	
SI	1024
MC2	QF
SF	300.1300000 MHz
WDW	SINE
SSB	0
LB	0.30 Hz
GB	0.1

4-Imino-6,7-dimethoxy-3-phenyl-3,4-dihydroquinazoline-2-carbonitrile (**6h**)

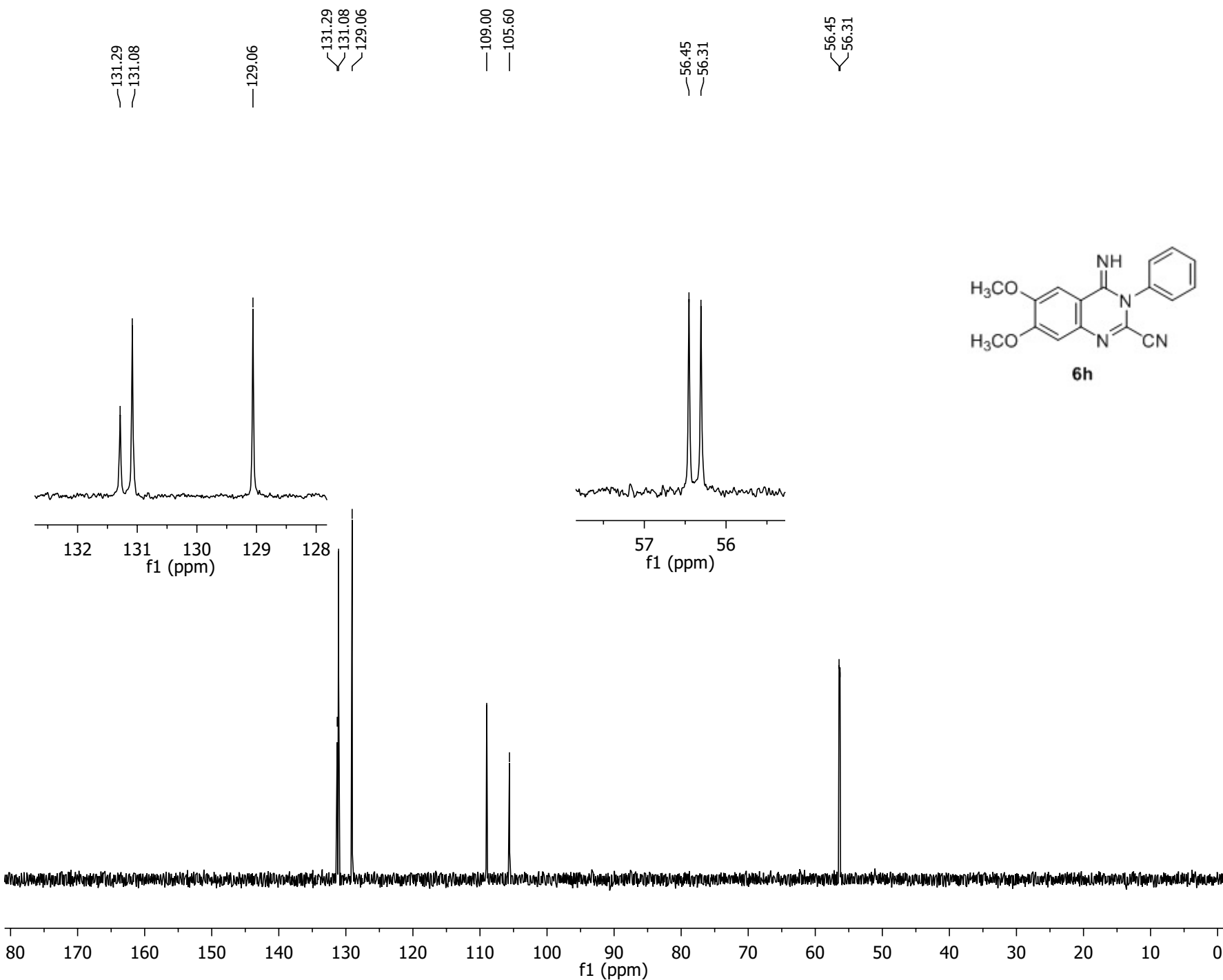


Current Data Parameters

NAME	Stylia
EXPNO	98
PROCNO	1
F2 - Acquisition Parameters	
Date_	20101010
Time	17.06
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl ₃
NS	1105
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	11585.2
DW	27.800 usec
DE	6.00 usec
TE	296.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
CHANNEL f1	=====
NUC1	¹³ C
P1	7.95 usec
PL1	-2.00 dB
SFO1	75.4752953 MHz
CHANNEL f2	=====
CPDPRG2	waltz16
NUC2	¹ H
PCPD2	110.00 usec
PL2	0.00 dB
PL12	22.00 dB
PL13	24.00 dB
SFO2	300.1312005 MHz
F2 - Processing parameters	
SI	32768
SF	75.4677528 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

4-Imino-6,7-dimethoxy-3-phenyl-3,4-dihydroquinazoline-2-carbonitrile (**6h**)

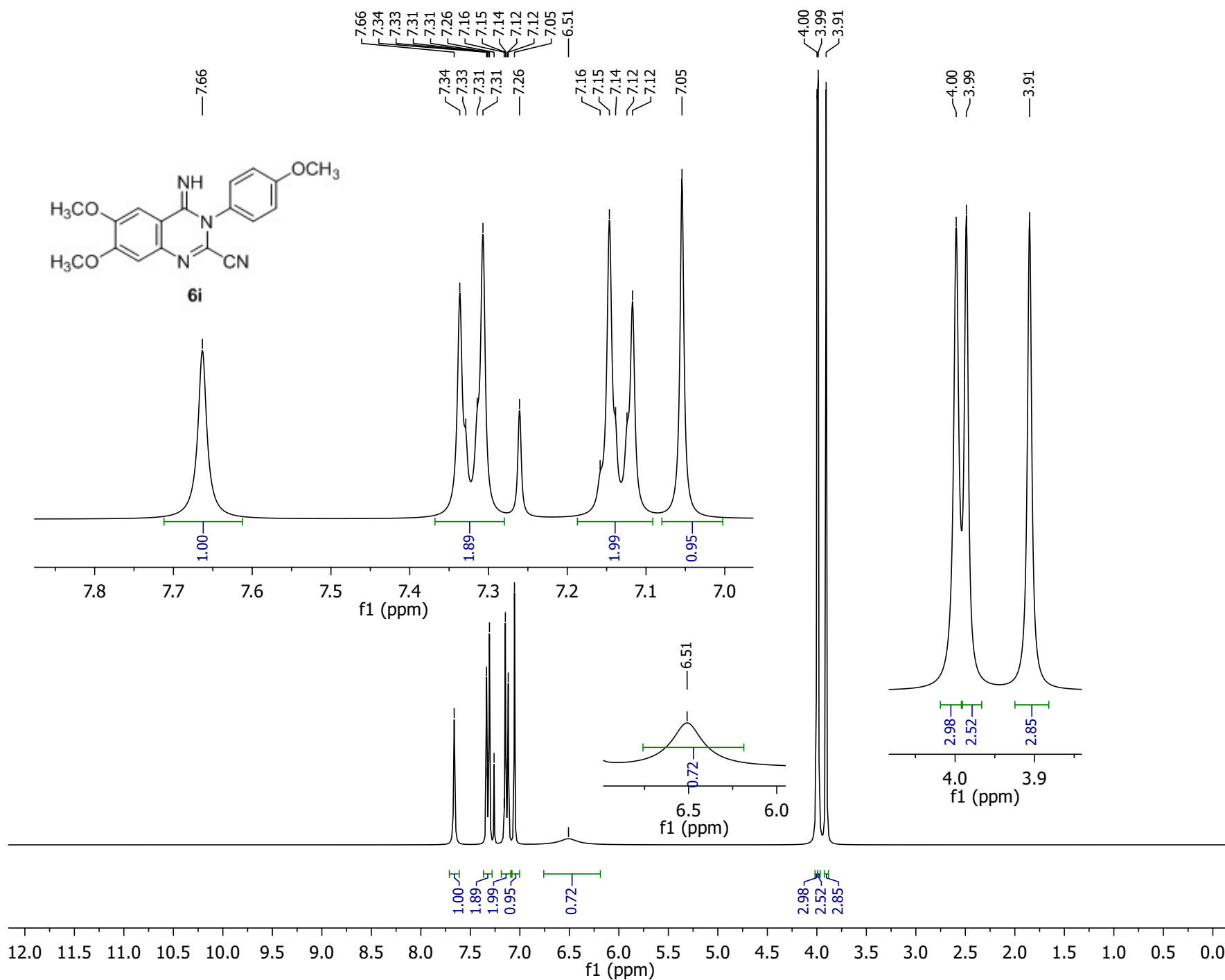
D E P T 1 3 5



Current Data Parameters

NAME	Styliana
EXPNO	99
PROCNO	1
F2 - Acquisition Parameters	
Date_	20101010
Time	18.14
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	dept135
TD	65536
SOLVENT	CDCl3
NS	164
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	16384
DW	27.800 usec
DE	6.00 usec
TE	296.2 K
CNST2	145.0000000
D1	2.00000000 sec
d2	0.00344828 sec
d12	0.00002000 sec
DELTA	0.00001012 sec
TD0	1
CHANNEL f1	=====
NUC1	13C
P1	7.95 usec
p2	15.90 usec
PL1	-2.00 dB
SFO1	75.4752953 MHz
CHANNEL f2	=====
CPDPRG2	waltz16
NUC2	1H
P3	9.40 usec
p4	18.80 usec
PCPD2	110.00 usec
PL2	0.00 dB
PL12	22.00 dB
SFO2	300.1312005 MHz
F2 - Processing parameters	
SI	32768
SF	75.4677526 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

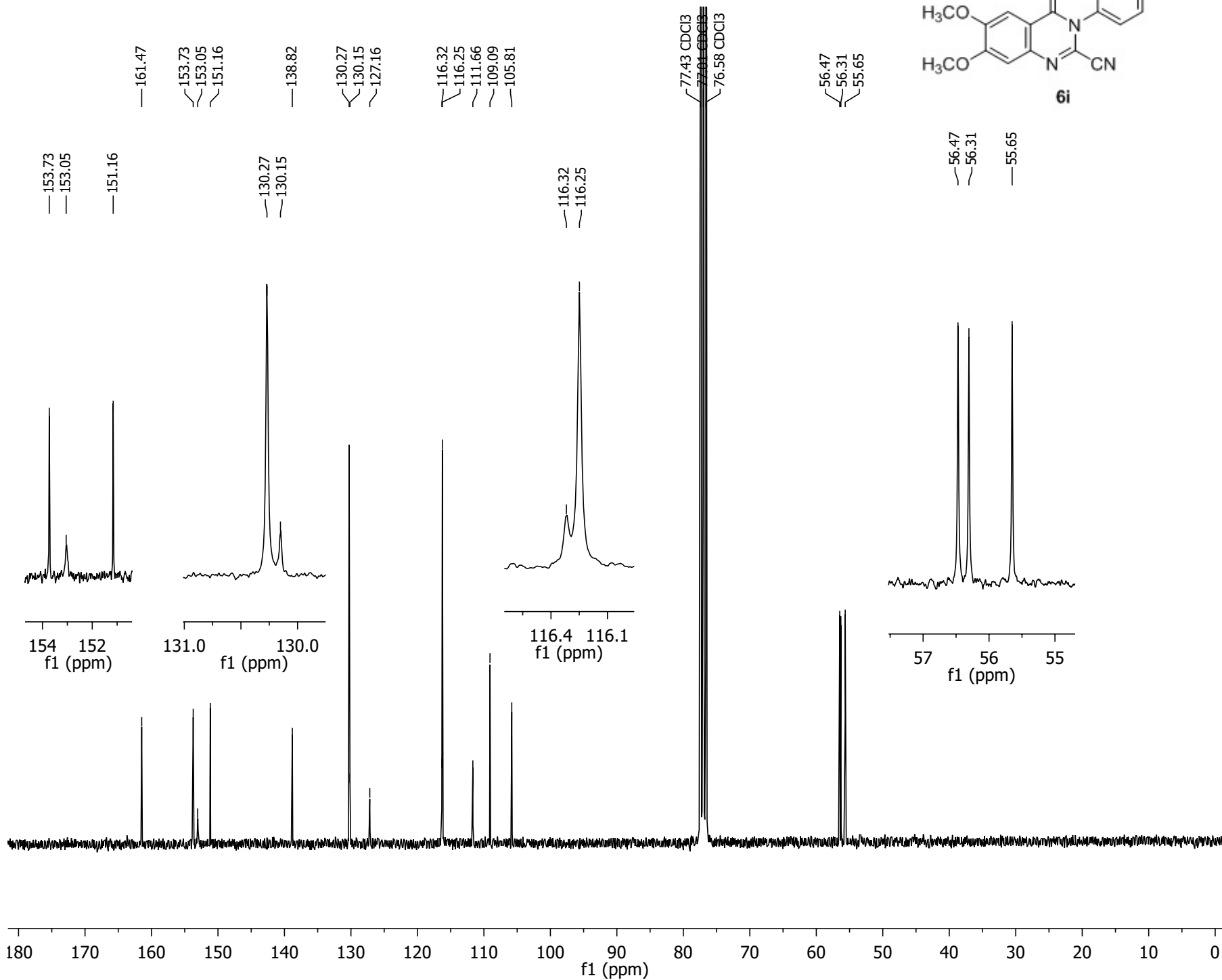
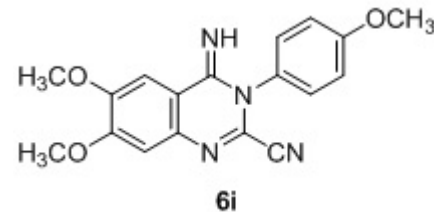
4-Imino-6,7-dimethoxy-3-(4-methoxyphenyl)-3,4-dihydroquinazoline-2-carbonitrile (**6i**)



Current Data Parameters

NAME	Styliana
EXPNO	123
PROCNO	1
F2 - Acquisition Parameters	
Date_	20110208
Time	19.38
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl ₃
NS	16
DS	2
SWH	6172.839 Hz
FIDRES	0.094190 Hz
AQ	5.3084660 sec
RG	287.4
DW	81.000 usec
DE	9.00 usec
TE	308.2 K
D1	1.00000000 sec
TD0	1
CHANNEL f1 =====	
NUC1	¹ H
P1	9.00 usec
PL1	0.00 dB
SFO1	300.1318534 MHz
F1 - Acquisition parameters	
ND0	2
TD	256
SFO1	300.1314 MHz
FIDRES	12.056327 Hz
SW	10.284 ppm
FnMODE	undefined
F2 - Processing parameters	
SI	32768
SF	300.1300059 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00
F1 - Processing parameters	
SI	1024
MC2	QF
SF	300.1300000 MHz
WDW	SINE
SSB	0
LB	0.30 Hz
GB	0.1

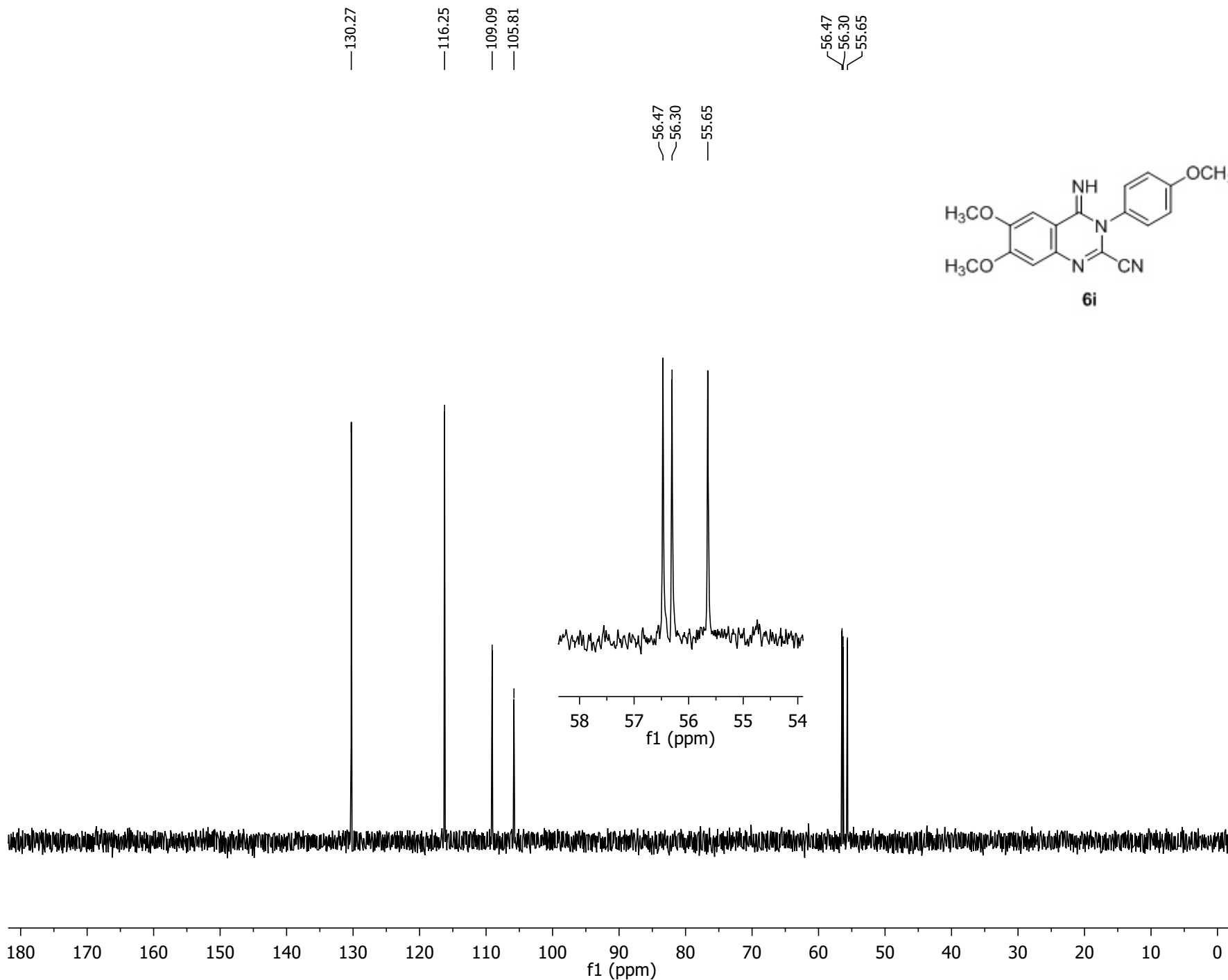
4-Imino-6,7-dimethoxy-3-(4-methoxyphenyl)-3,4-dihydroquinazoline-2-carbonitrile (**6i**)



Current Data Parameters	
NAME	Styliana
EXPNO	125
PROCNO	1
F2 - Acquisition Parameters	
Date_	20110208
Time	20.00
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl ₃
NS	3418
DS	4
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	16384
DW	27.800 usec
DE	6.00 usec
TE	308.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
CHANNEL f1 =====	
NUC1	¹³ C
P1	7.00 usec
PL1	-2.00 dB
SFO1	75.4752953 MHz
CHANNEL f2 =====	
CPDPRG2	waltz16
NUC2	¹ H
PCPD2	110.00 usec
PL2	0.00 dB
PL12	22.00 dB
PL13	24.00 dB
SFO2	300.1312005 MHz
F2 - Processing parameters	
SI	32768
SF	75.4677484 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

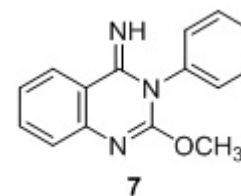
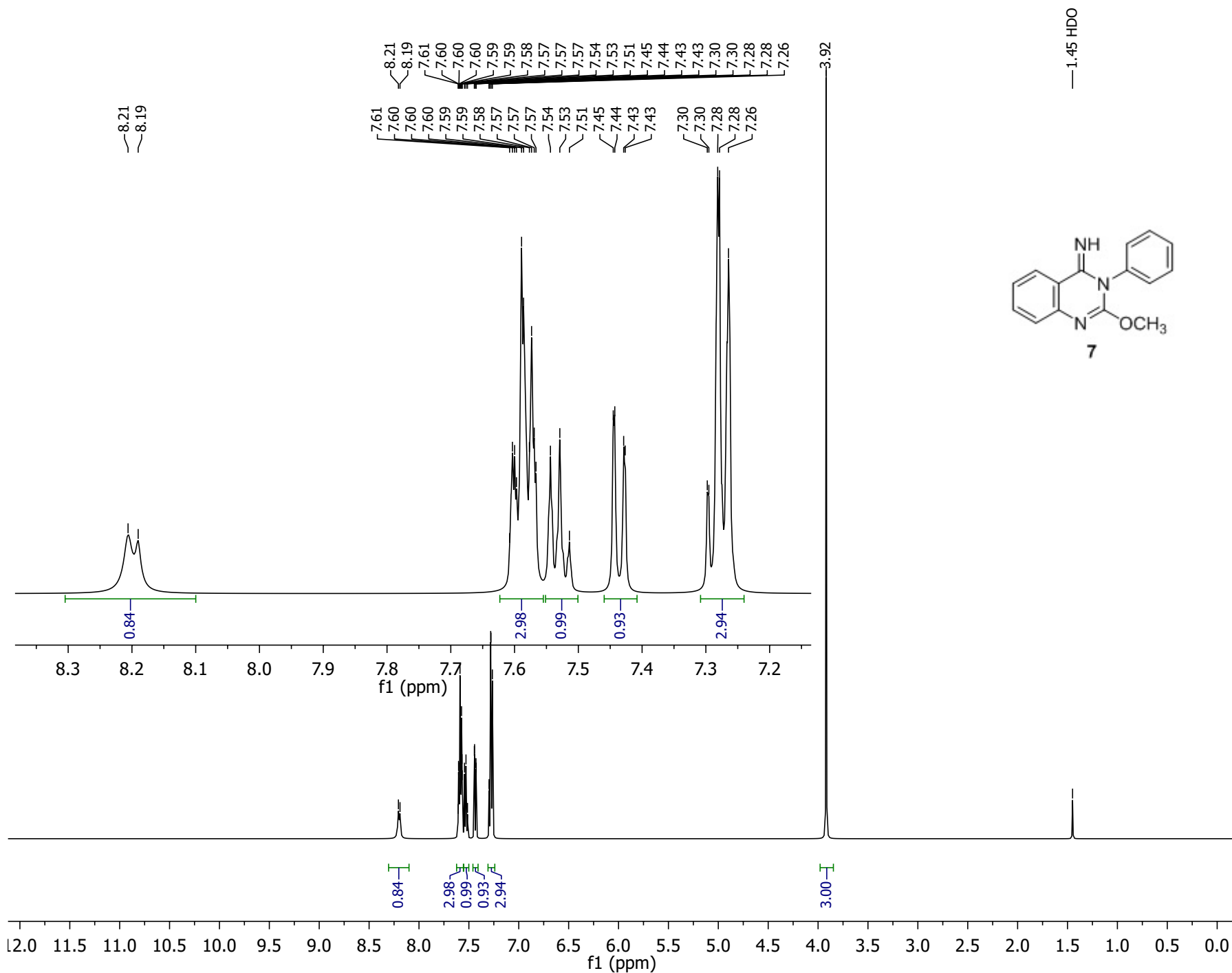
4-Imino-6,7-dimethoxy-3-(4-methoxyphenyl)-3,4-dihydroquinazoline-2-carbonitrile (**6i**)

DEPT 135



Current Data Parameters
NAME Styliana
EXPNO 124
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110208
Time 19.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 6.00 usec
TE 308.2 K
CNST2 145.000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00000891 sec
TD0 1
CHANNEL f1 =====
NUC1 13C
P1 7.00 usec
p2 14.00 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz
CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 9.40 usec
p4 18.80 usec
PCPD2 110.00 usec
PL2 0.00 dB
PL12 22.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677484 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

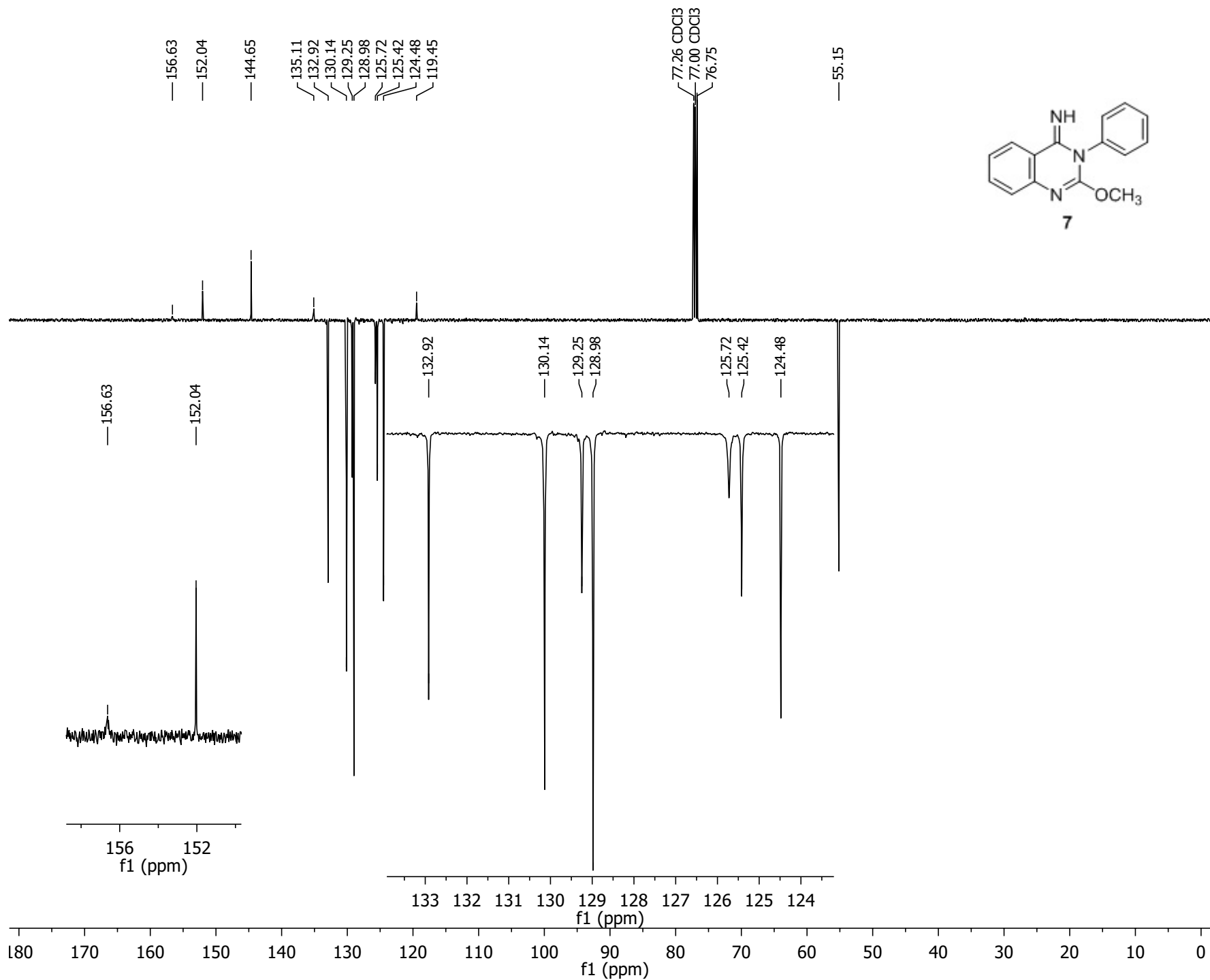
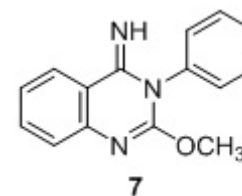
2-Methoxy-3-phenylquinazolin-4(3H)-imine (**7**)



Current Data Parameters

NAME	Stylana
EXPNO	204
PROCNO	1
F2 - Acquisition Parameters	
Date_	20110907
Time	14.18
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl ₃
NS	24
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	90.5
DW	48.400 usec
DE	6.50 usec
TE	296.1 K
D1	1.00000000 sec
CHANNEL f1 =====	
NUC1	¹ H
P1	11.00 usec
PLW1	15.41699982 W
SFO1	500.0361158 MHz
F2 - Processing parameters	
SI	65536
SF	500.0330280 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

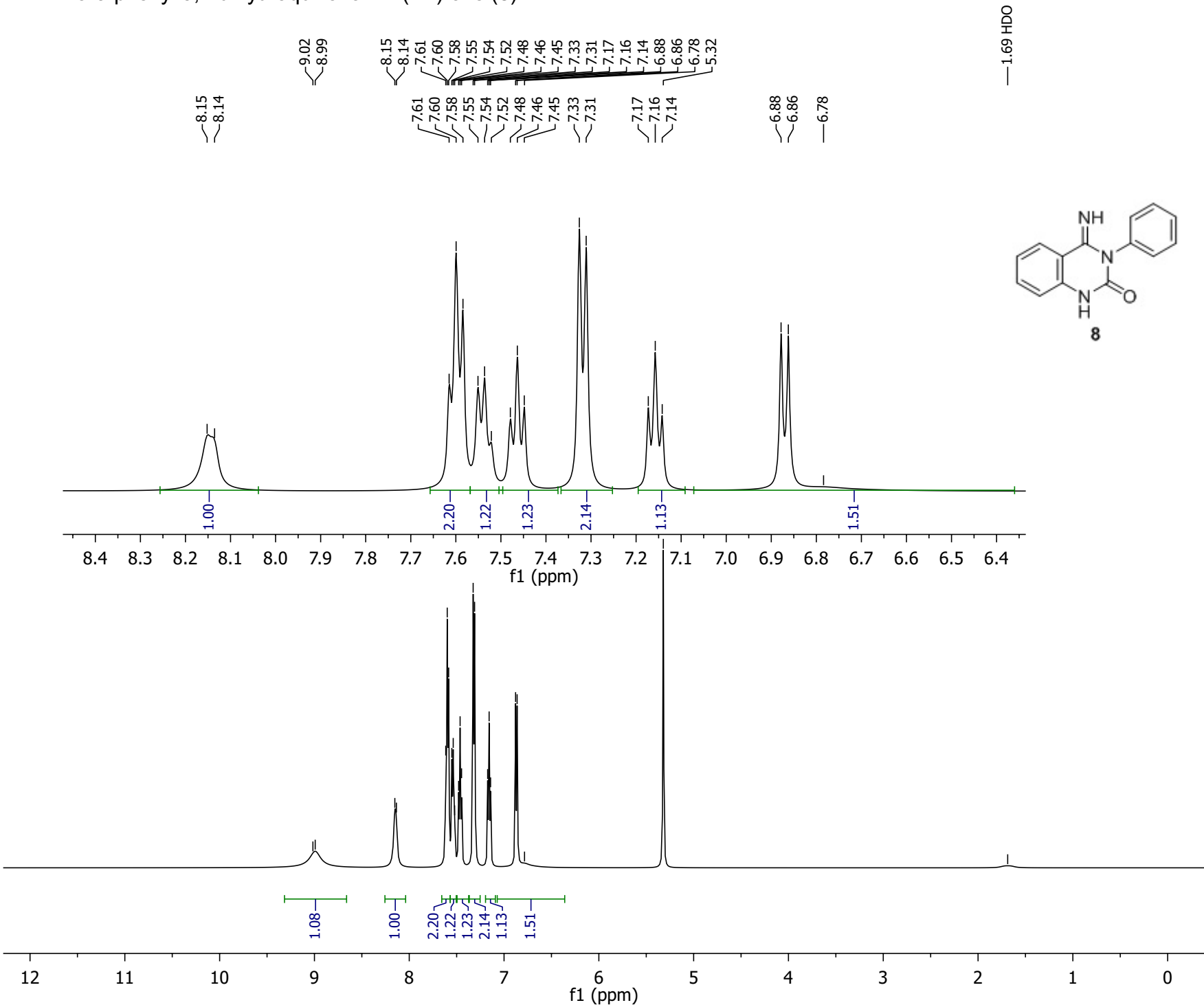
2-Methoxy-3-phenylquinazolin-4(3H)-imine (**7**)



Current Data Parameters

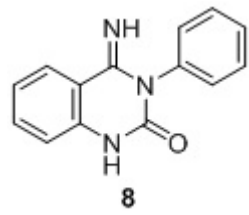
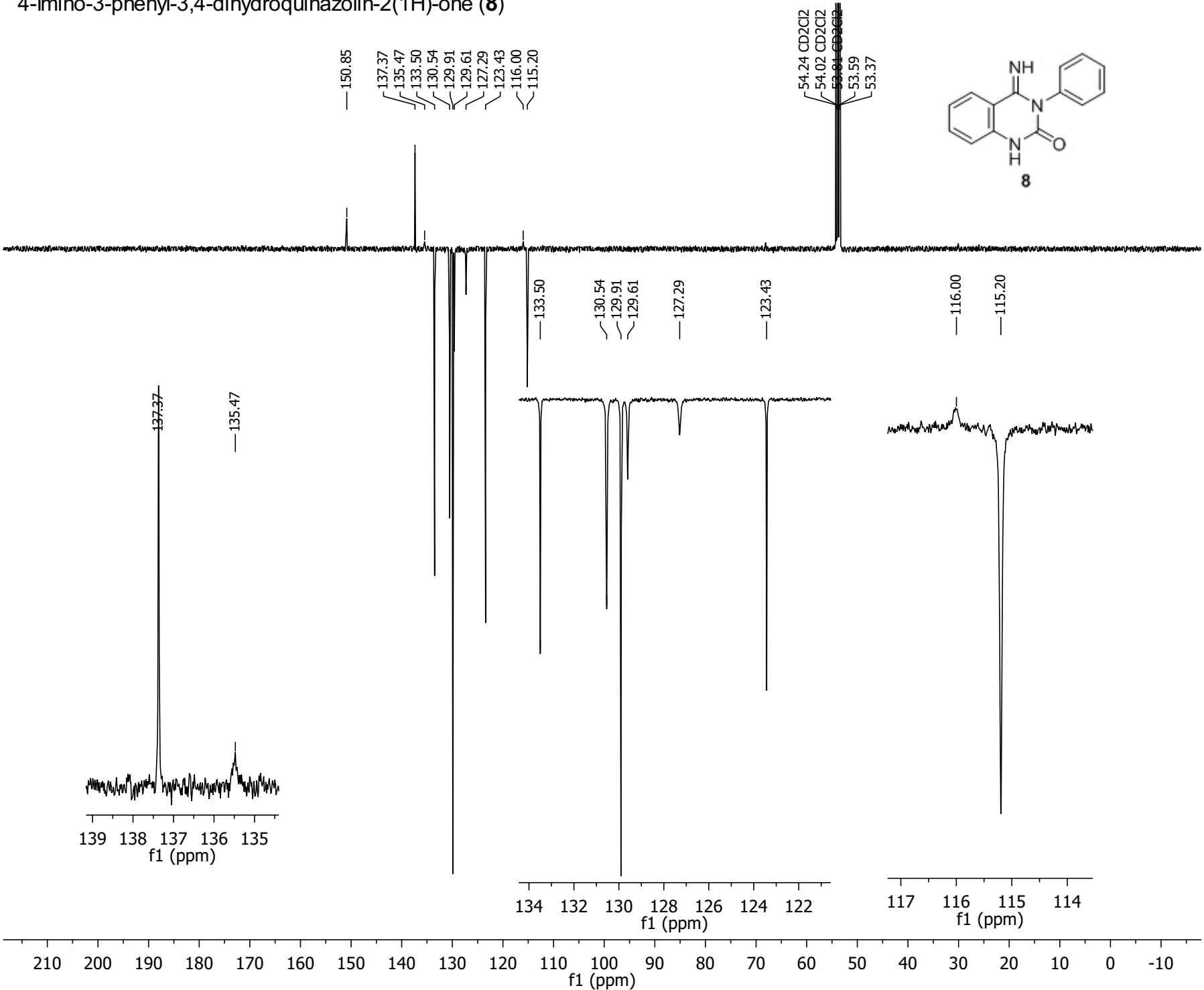
NAME	Stylia
EXPNO	203
PROCNO	1
F2 - Acquisition Parameters	
Date_	20110907
Time	13.51
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	jmod
TD	65536
SOLVENT	CDCl ₃
NS	1254
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	2050
DW	16.800 usec
DE	6.50 usec
TE	297.1 K
CNST2	145.0000000
CNST11	1.0000000
D1	6.00000000 sec
D20	0.00689655 sec
CHANNEL f1	=====
NUC1	¹³ C
P1	8.00 usec
P2	16.00 usec
PLW1	138.00000000 W
SFO1	125.7459782 MHz
CHANNEL f2	=====
CPDPRG2	waltz16
NUC2	¹ H
PCPD2	80.00 usec
PLW2	13.00000000 W
PLW12	0.31738001 W
SFO2	500.0350280 MHz
F2 - Processing parameters	
SI	32768
SF	125.7334112 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

4-Imino-3-phenyl-3,4-dihydroquinazolin-2(1H)-one (8)



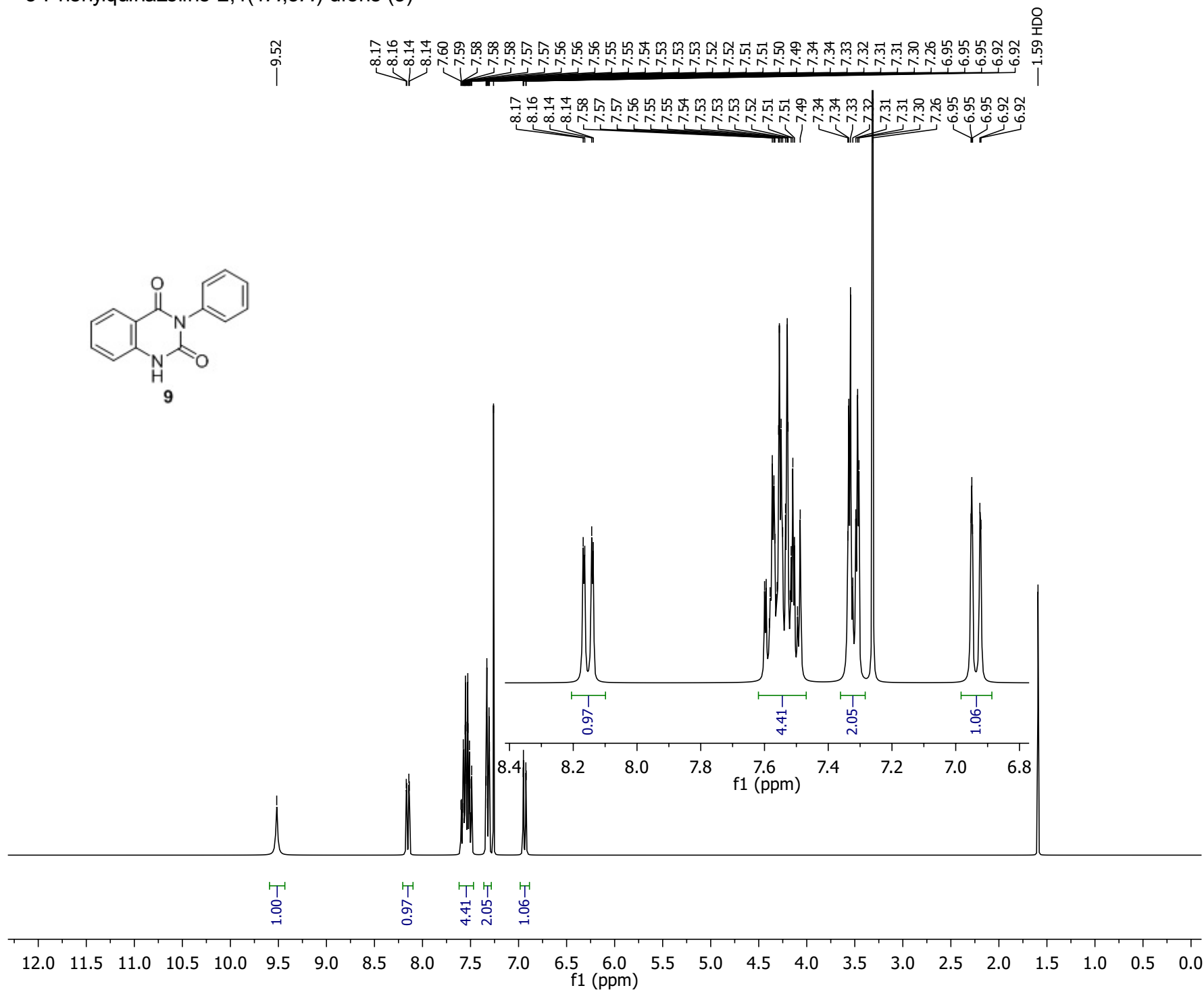
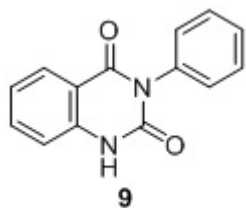
Current Data Parameters	
NAME	Styliana
EXPNO	181
PROCNO	1
F2 - Acquisition Parameters	
Date_	20110821
Time	18.10
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CD2Cl2
NS	25
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	144
DW	48.400 usec
DE	6.50 usec
TE	299.5 K
D1	1.00000000 sec
CHANNEL f1 =====	
NUC1	1H
P1	11.00 usec
PLW1	15.41699982 W
SFO1	500.0361158 MHz
F2 - Processing parameters	
SI	65536
SF	500.0330474 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

4-Imino-3-phenyl-3,4-dihydroquinazolin-2(1H)-one (8)



Current Data Parameters	
NAME	Styliana
EXPNO	182
PROCNO	1
F2 - Acquisition Parameters	
Date_	20110821
Time	18.29
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	jmod
TD	65536
SOLVENT	CD2Cl2
NS	7426
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	2050
DW	16.800 usec
DE	6.50 usec
TE	299.9 K
CNST2	145.0000000
CNST11	1.0000000
D1	6.00000000 sec
D20	0.00689655 sec
CHANNEL f1 =====	
NUC1	13C
P1	8.00 usec
P2	16.00 usec
PLW1	138.00000000 W
SFO1	125.7459782 MHz
CHANNEL f2 =====	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PLW2	13.00000000 W
PLW12	0.31738001 W
SFO2	500.0350280 MHz
F2 - Processing parameters	
SI	32768
SF	125.7333568 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

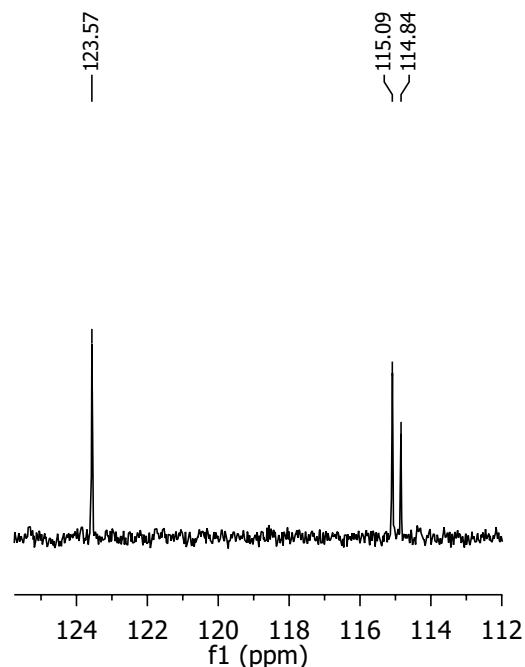
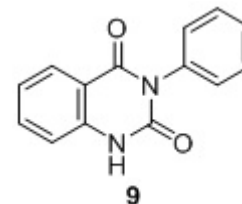
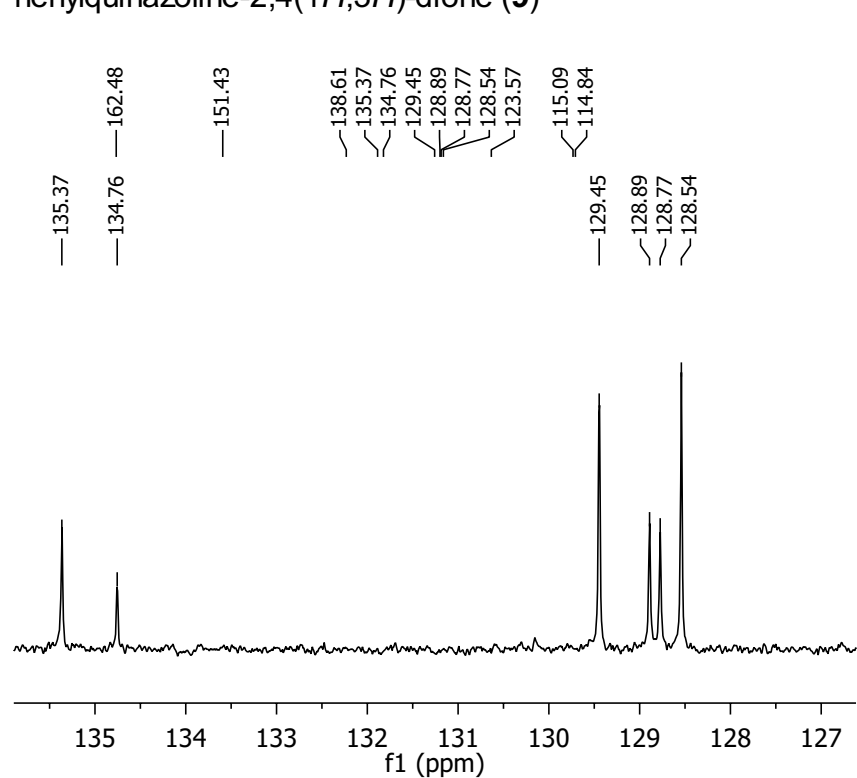
3-Phenylquinazoline-2,4(1*H*,3*H*)-dione (**9**)



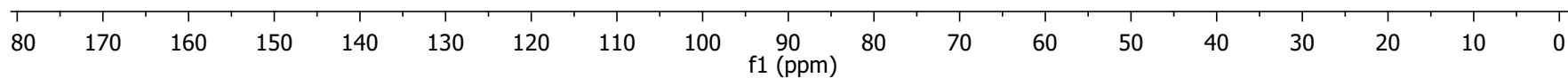
Current Data Parameters

NAME	Styliana
EXPNO	133
PROCNO	1
F2 - Acquisition Parameters	
Date_	20110403
Time	21.34
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl ₃
NS	16
DS	2
SWH	6172.839 Hz
FIDRES	0.094190 Hz
AQ	5.3084660 sec
RG	456.1
DW	81.000 usec
DE	9.00 usec
TE	297.2 K
D1	1.00000000 sec
TD0	1
CHANNEL f1	=====
NUC1	¹ H
P1	9.00 usec
PL1	0.00 dB
SFO1	300.1318534 MHz
F1 - Acquisition parameters	
ND0	2
TD	256
SFO1	300.1314 MHz
FIDRES	12.056327 Hz
SW	10.284 ppm
FnMODE	undefined
F2 - Processing parameters	
SI	32768
SF	300.1300061 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00
F1 - Processing parameters	
SI	1024
MC2	QF
SF	300.1300000 MHz
WDW	SINE
SSB	0
LB	0.30 Hz
GB	0.1

3-Phenylquinazoline-2,4(1*H*,3*H*)-dione (**9**)



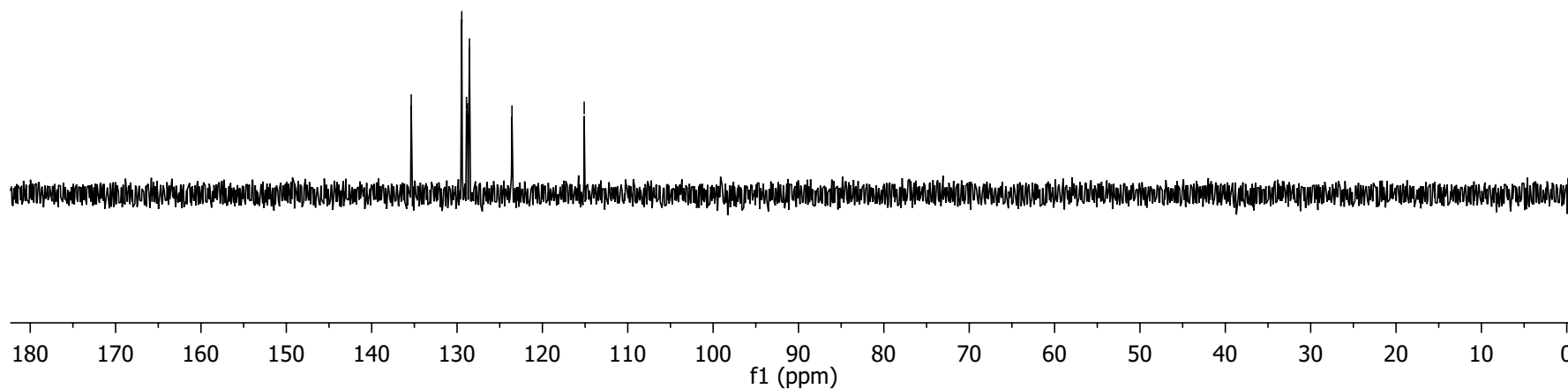
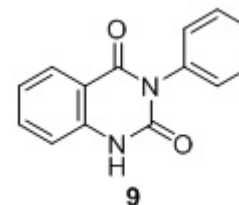
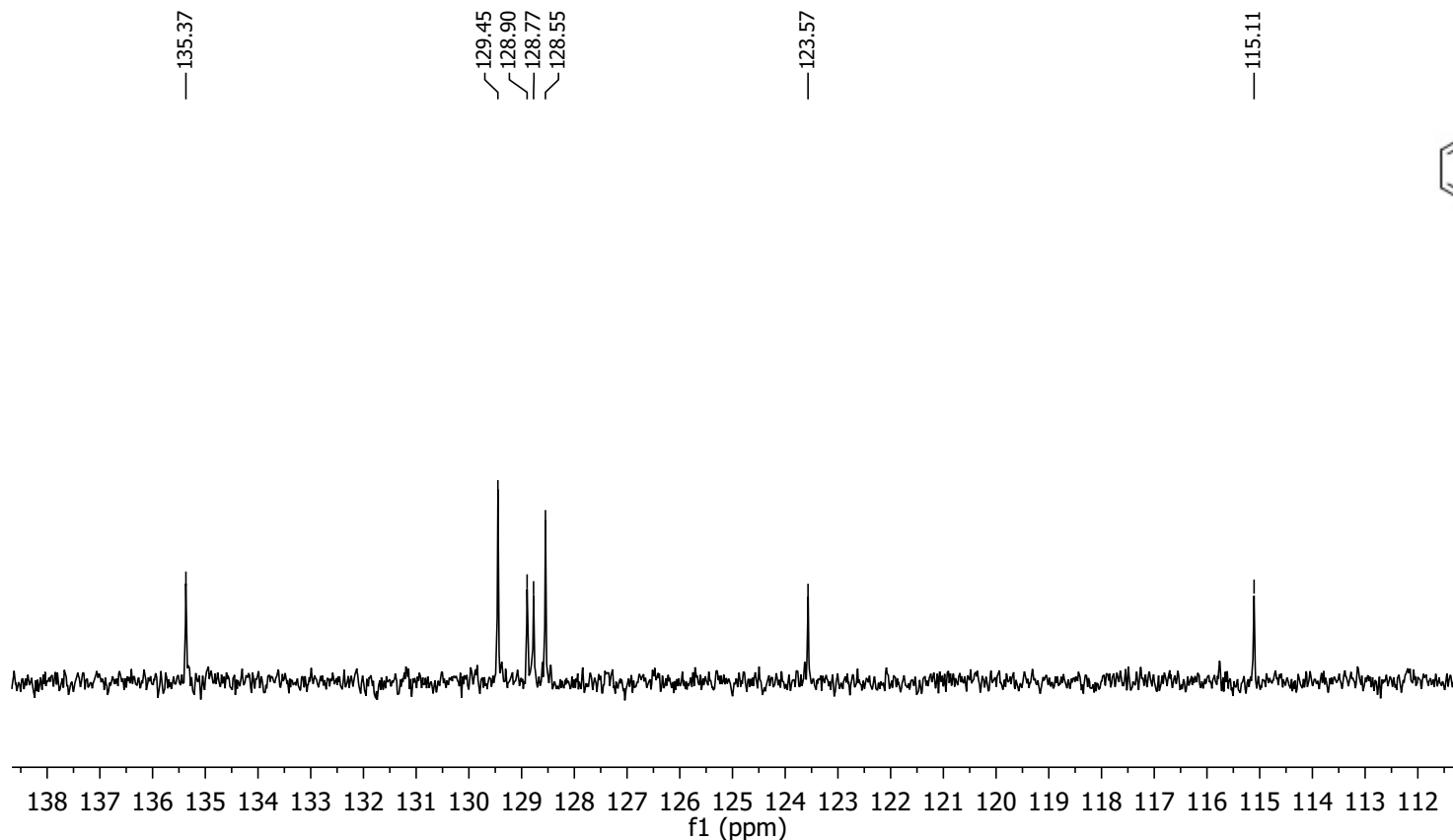
Current Data Parameters
NAME Styliana
EXPNO 135
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110403
Time 21.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 12821
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 6.00 usec
TE 297.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
CHANNEL f1 =====
NUC1 13C
P1 7.00 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz
CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 110.00 usec
PL2 0.00 dB
PL12 22.00 dB
PL13 24.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677501 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



3-Phenylquinazoline-2,4(1*H*,3*H*)-dione (**9**)

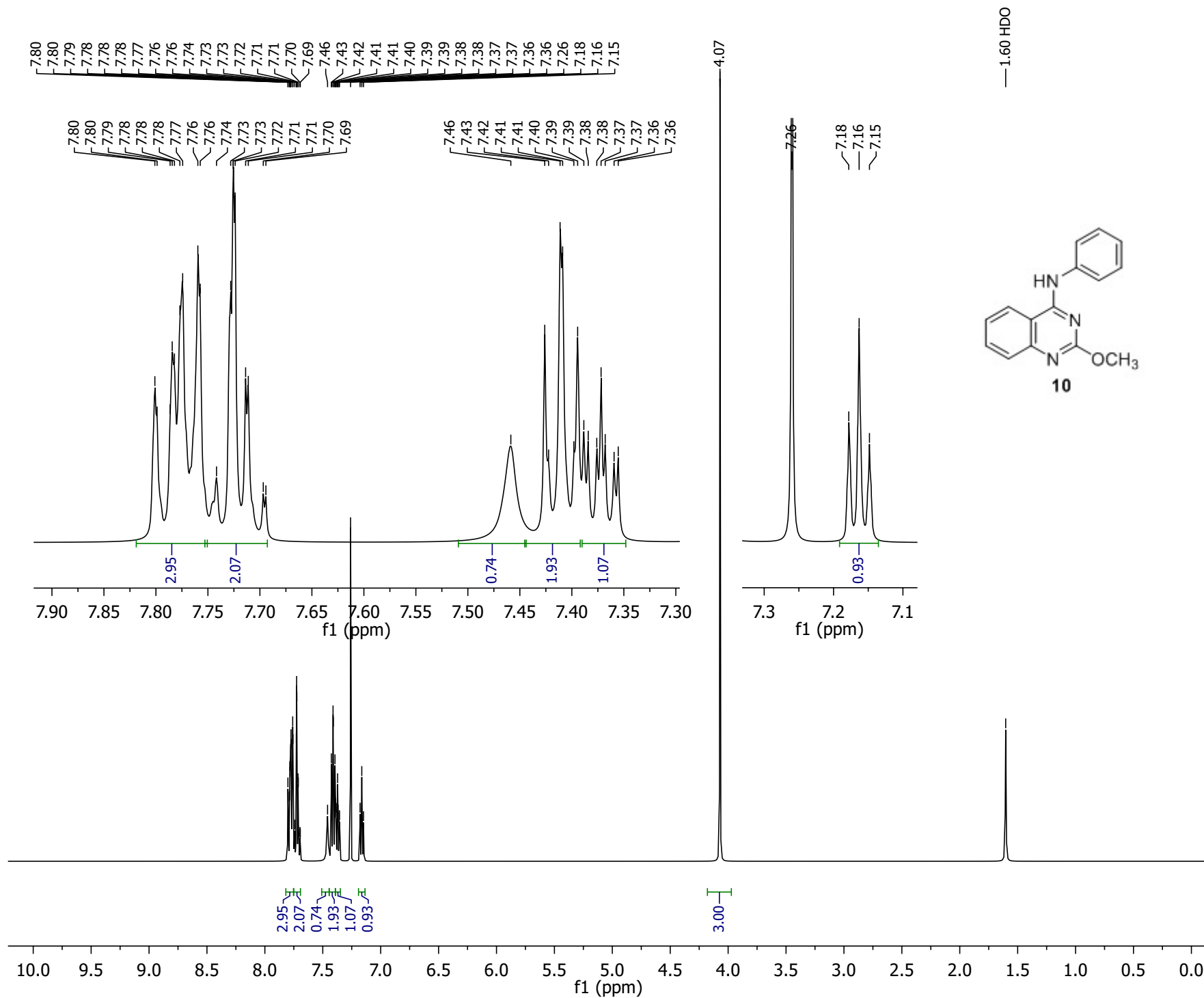
DEPT 135

135.37
129.45
128.90
128.77
128.55
123.57
115.11



Current Data Parameters
NAME Styliana
EXPNO 134
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110403
Time 21.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 300
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 6.00 usec
TE 297.2 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00000891 sec
TD0 1
CHANNEL f1 =====
NUC1 13C
P1 7.00 usec
p2 14.00 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz
CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 9.40 usec
p4 18.80 usec
PCPD2 110.00 usec
PL2 0.00 dB
PL12 22.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677496 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

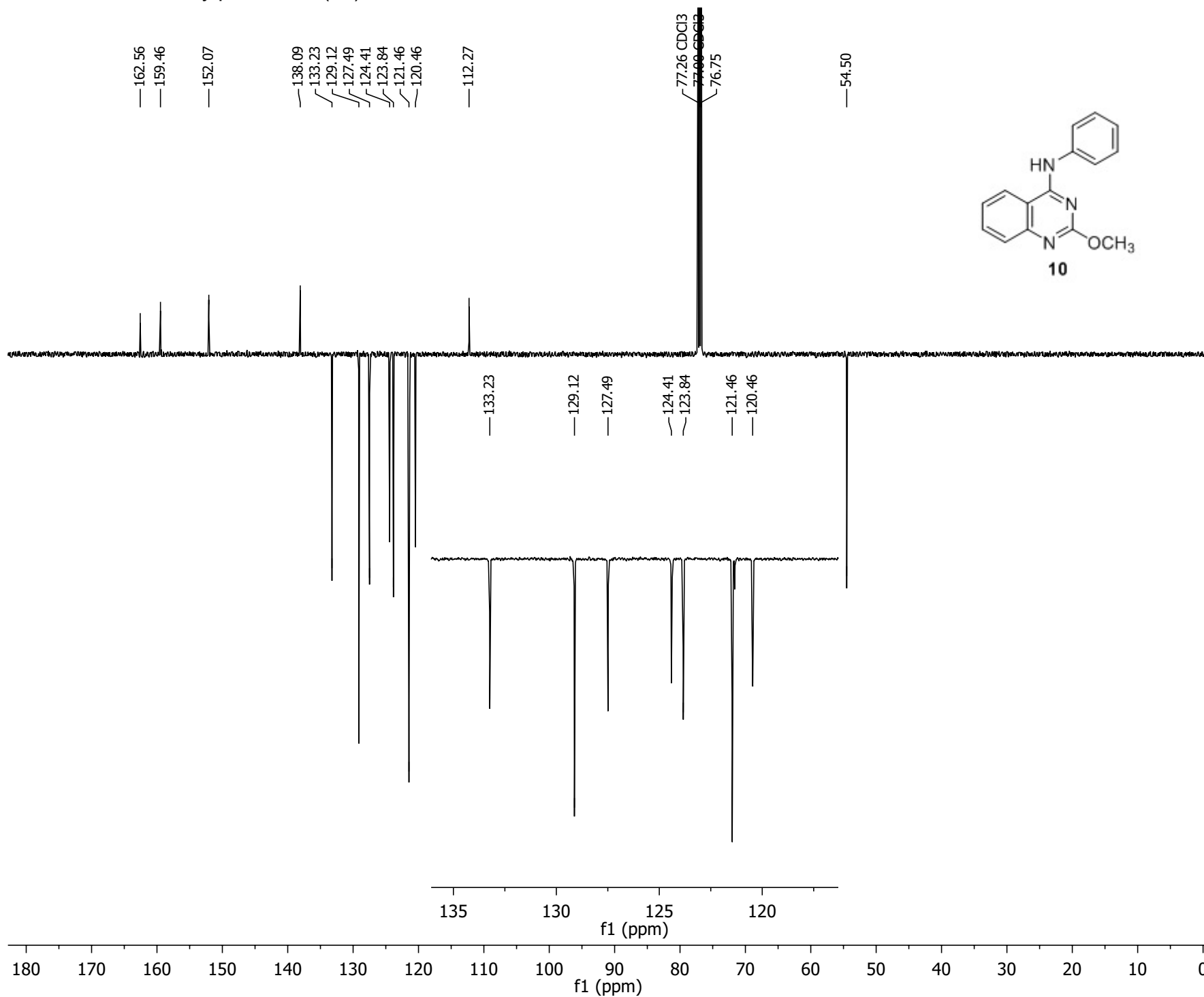
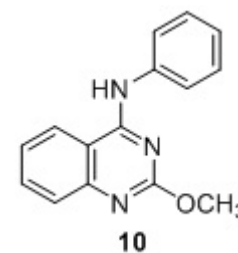
4-Anilino-2-methoxyquinazoline (**10**)



Current Data Parameters

NAME	Stylina
EXPNO	219
PROCNO	1
F2 - Acquisition Parameters	
Date_	20111018
Time	22.24
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	24
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	161
DW	48.400 usec
DE	6.50 usec
TE	296.8 K
D1	1.00000000 sec
CHANNEL f1	=====
NUC1	1H
P1	11.00 usec
PLW1	15.4169982 W
SFO1	500.0361158 MHz
F2 - Processing parameters	
SI	65536
SF	500.0330407 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

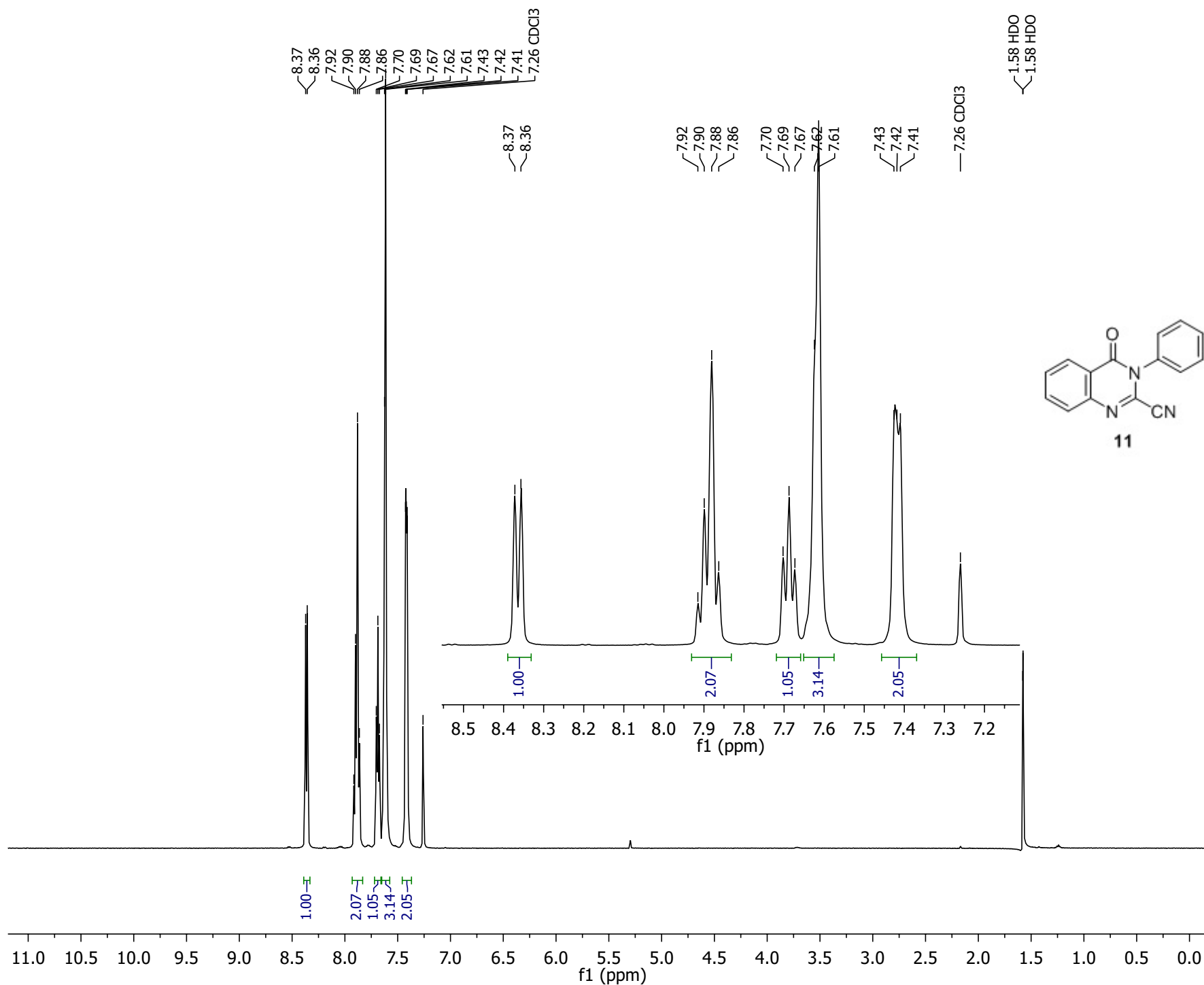
4-Anilino-2-methoxyquinazoline (**10**)



Current Data Parameters

NAME	Styliana
EXPNO	220
PROCNO	1
F2 - Acquisition Parameters	
Date_	20111019
Time	6.52
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	jmod
TD	65536
SOLVENT	CDCl3
NS	4250
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	2050
DW	16.800 usec
DE	6.50 usec
TE	297.6 K
CNST2	145.0000000
CNST11	1.0000000
D1	6.00000000 sec
D20	0.00689655 sec
CHANNEL f1	=====
NUC1	13C
P1	8.00 usec
P2	16.00 usec
PLW1	138.00000000 W
SFO1	125.7459782 MHz
CHANNEL f2	=====
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PLW2	13.00000000 W
PLW12	0.31738001 W
SFO2	500.0350280 MHz
F2 - Processing parameters	
SI	32768
SF	125.7334071 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

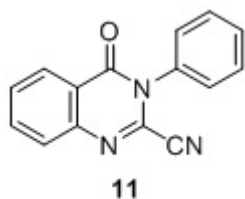
4-Oxo-3-phenyl-3,4-dihydroquinazoline-2-carbonitrile (**11**)



Current Data Parameters

NAME	Stylia
EXPNO	62
PROCNO	1
F2 - Acquisition Parameters	
Date_	20110329
Time	18.10
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	144
DW	48.400 usec
DE	6.50 usec
TE	297.0 K
D1	1.00000000 sec
CHANNEL f1	=====
NUC1	1H
P1	11.00 usec
PLW1	15.41699982 W
SFO1	500.0361158 MHz
F2 - Processing parameters	
SI	65536
SF	500.0330401 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

4-Oxo-3-phenyl-3,4-dihydroquinazoline-2-carbonitrile (**11**)



— 160.05
— 146.48
135.37
135.19
131.47
130.74
130.26
130.14
128.69
128.20
127.46
122.97
— 111.03

135.37
135.19

77.25 CDCl₃
77.20 CDCl₃
77.00
76.75

— 131.47

— 130.74

130.26
130.14

— 128.69

— 128.20

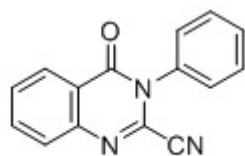
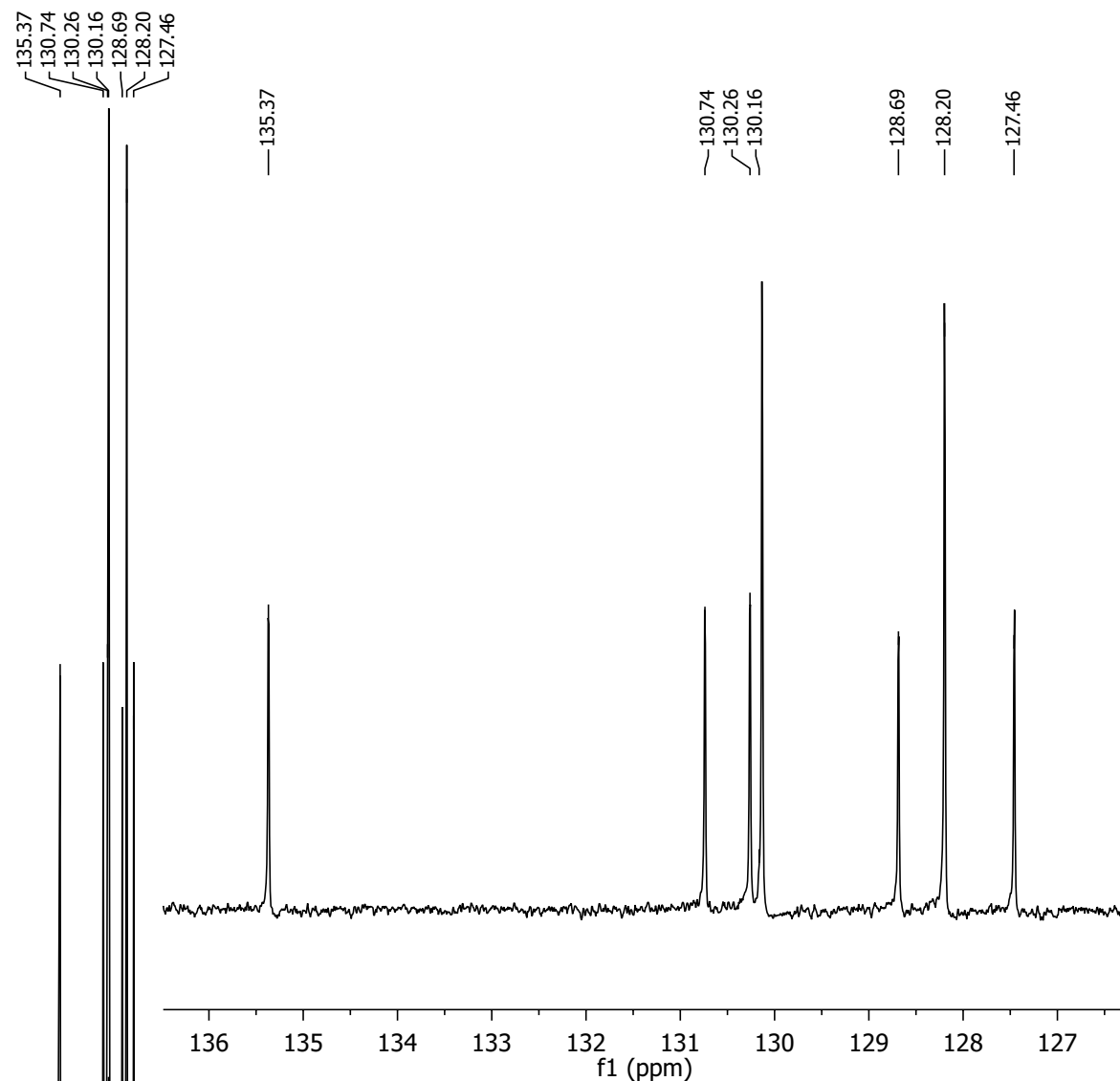
— 127.46

137 136 135 134 133 132 131 130 129 128 127
f1 (ppm)

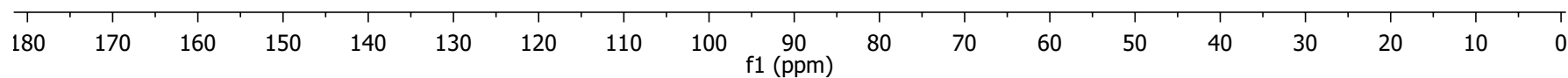
Current Data Parameters
NAME Styliana
EXPNO 63
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110329
Time 19.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
CHANNEL f1 =====
NUC1 ¹³C
P1 8.00 usec
PLW1 138.00000000 W
SFO1 125.7459776 MHz
CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 ¹H
PCPD2 80.00 usec
PLW2 13.00000000 W
PLW12 0.31738001 W
PLW13 0.20313001 W
SFO2 500.0350280 MHz
F2 - Processing parameters
SI 32768
SF 125.7334101 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

4-Oxo-3-phenyl-3,4-dihydroquinazoline-2-carbonitrile (**11**)

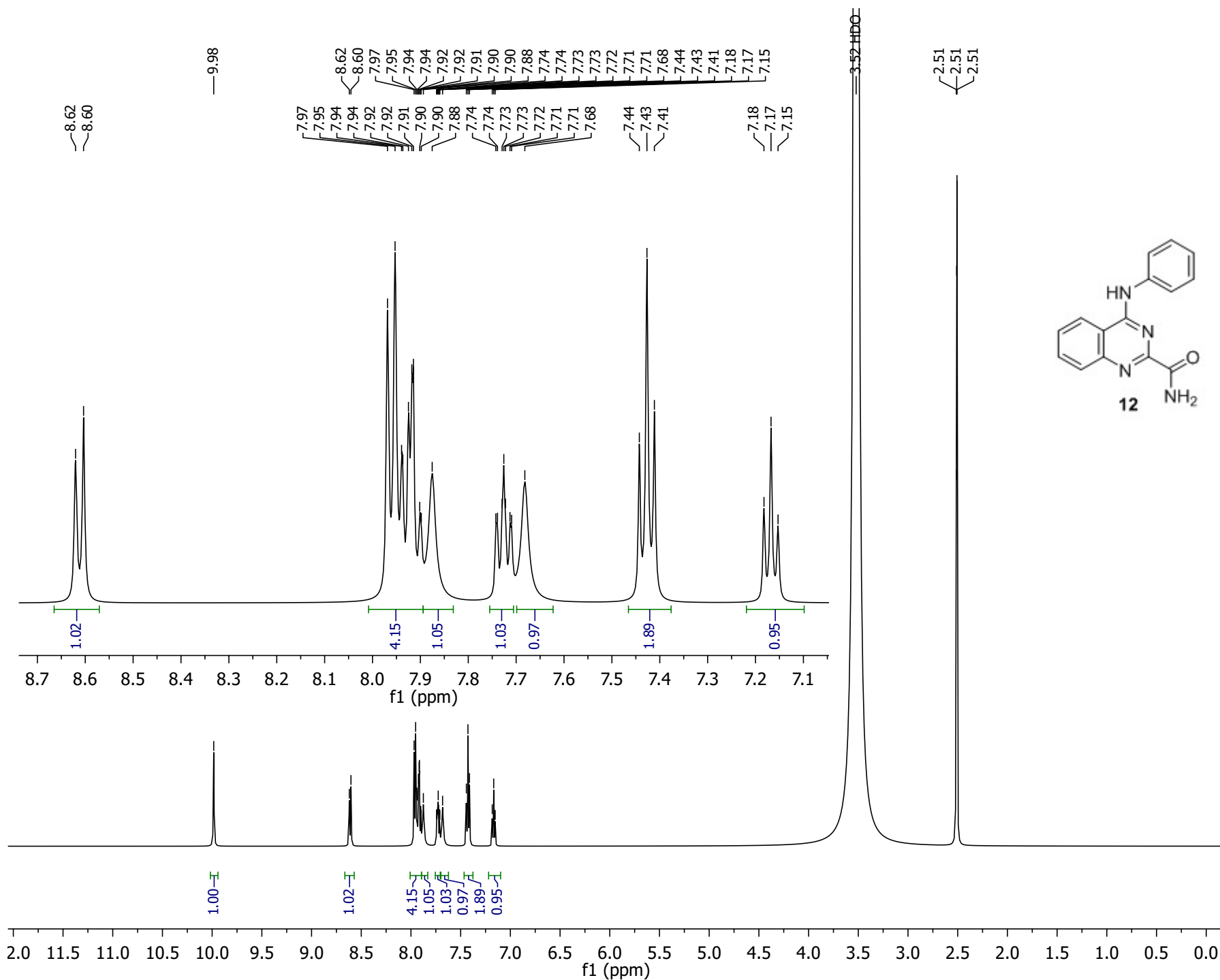
D E P T 1 3 5

**11**

Current Data Parameters
NAME Styliana
EXPNO 64
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110329
Time 19.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 297.6 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
CHANNEL f1 =====
NUC1 13C
P1 8.00 usec
P2 16.00 usec
PLW1 138.00000000 W
SFO1 125.7459776 MHz
CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 12.50 usec
P4 25.00 usec
PCPD2 80.00 usec
PLW2 13.00000000 W
PLW12 0.31738001 W
SFO2 500.0350280 MHz
F2 - Processing parameters
SI 32768
SF 125.7334110 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



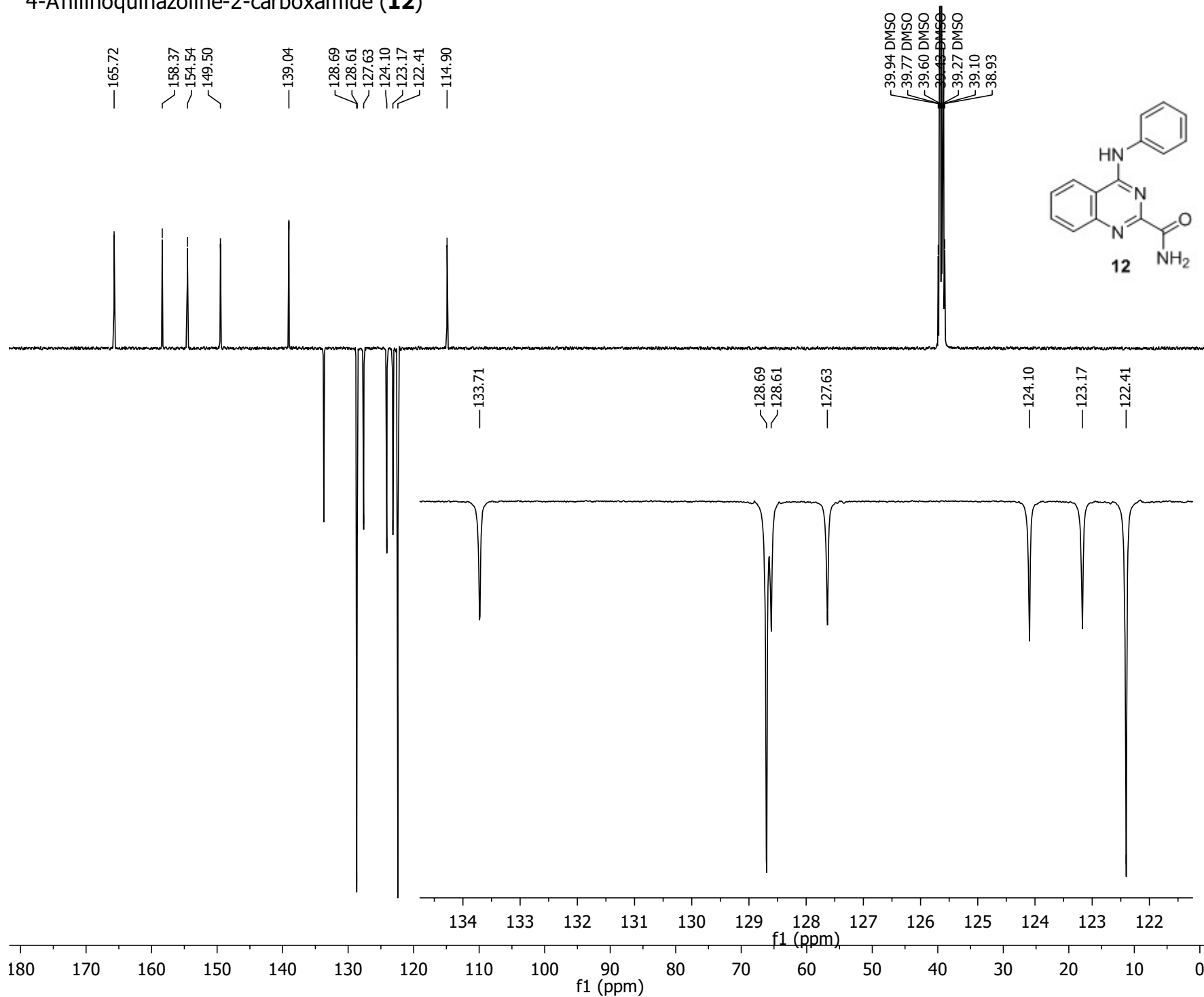
4-Anilinoquinazoline-2-carboxamide (**12**)



Current Data Parameters

NAME	Stylia
EXPNO	961
PROCNO	1
F2 - Acquisition Parameters	
Date_	20130724
Time	15.16
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	264
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719425 sec
RG	32
DW	48.400 usec
DE	6.50 usec
TE	295.7 K
D1	1.00000000 sec
TD0	1
CHANNEL f1	=====
SFO1	500.0361158 MHz
NUC1	1H
P1	11.75 usec
PLW1	15.41699982 W
F2 - Processing parameters	
SI	65536
SF	500.0330280 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

4-Anilinoquinazoline-2-carboxamide (**12**)



Current Data Parameters

NAME	Styliana
EXPNO	957
PROCNO	1
F2 - Acquisition Parameters	
Date_	20130723
Time	9.57
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	jmod
TD	65536
SOLVENT	DMSO
NS	18432
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010048 sec
RG	1820
DW	16.800 usec
DE	6.50 usec
TE	296.3 K
CNST2	145.0000000
CNST11	1.0000000
D1	2.00000000 sec
D20	0.00689655 sec
TD0	1
CHANNEL f1	=====
SFO1	125.7459782 MHz
NUC1	13C
P1	8.70 usec
P2	17.40 usec
PLW1	138.0000000 W
CHANNEL f2	=====
SFO2	500.0350280 MHz
NUC2	1H
CPDPRG[2]	waltz16
PCPD2	80.00 usec
PLW2	15.41699982 W
PLW12	0.33258000 W
F2 - Processing parameters	
SI	32768
SF	125.7334507 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Figure S1. Ellipsoid (probability level of 50%) representation of the crystal structure of 4-imino-3-phenyl-3,4-dihydroquinazoline-2-carbonitrile (**6a**) with atom labelling. The dihedral angle between the plane of the quinazoline and that of the phenyl ring is $68.94(4)^\circ$. Hydrogen atoms were omitted for clarity.

