Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

BF_3•OEt_2-mediated one pot synthesis of 10-indolyldibenzo[*b,f*]azepine derivatives via tandem ring expansion and C-C bond formation

Trimurtulu Kotipalli, Donala Janreddy, Veerababurao Kavala, Chun-Wei Kuo, Ting-Shen Kuo, Mei-Ling Chen, Chiu-Hui He and Ching-Fa Yao *

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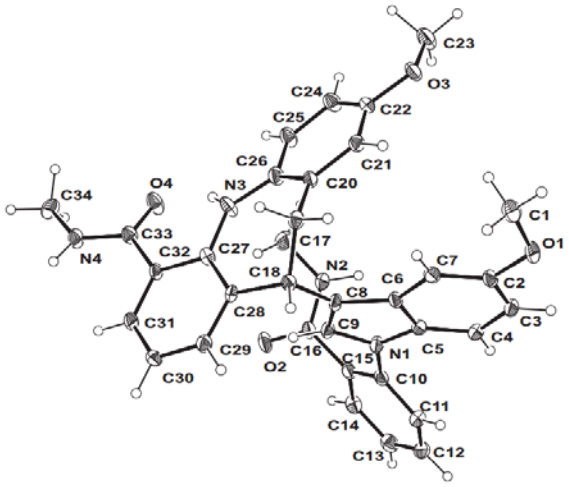
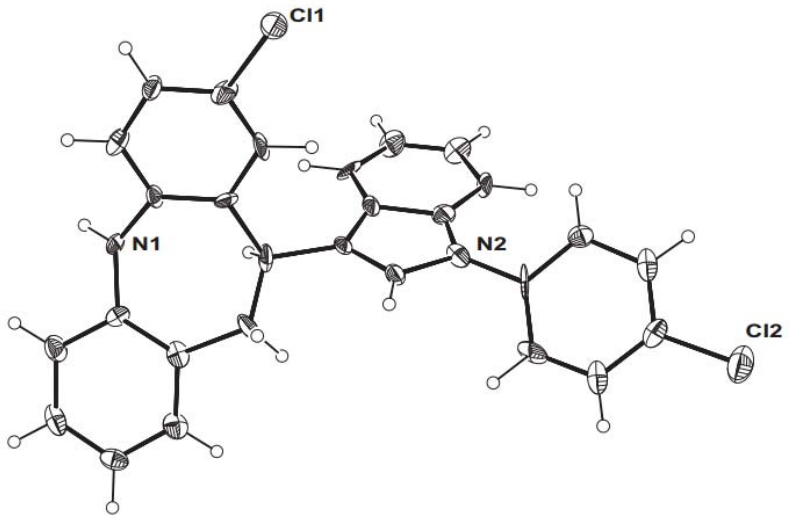
Crystal structure and data of compound 18b



Identification code		ch15119
Empirical formula	C_{34} H_{32} N_4 O_4	
Formula weight	560.64	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 10.786(3) Å	α= 67.852(4)°.
	b = 11.071(3) Å	β= 80.937(4)°.
	c = 12.689(3) Å	γ = 81.886(5)°.
Volume	1380.4(6) $Å^3$	
Z	2	
Density (calculated)	1.349 Mg/m^3	
Absorption coefficient	0.090 mm^{-1}	
F(000)	592	
Crystal size	0.24 x 0.13 x 0.03 mm^3	
Theta range for data collection	1.74 to 25.00°.	
Index ranges	-12<=h<=12, -13<=k<=13, -15<=l<=15	
Reflections collected	10954	
Independent reflections	4790 [R(int) = 0.0561]	
Completeness to theta = 25.00°	98.7 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.9973 and 0.9788	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4790 / 0 / 379
Goodness-of-fit on F^2	1.012
Final R indices [I>2sigma(I)]	R1 = 0.0592, wR2 = 0.1432
R indices (all data)	R1 = 0.1140, wR2 = 0.1950
Largest diff. peak and hole	0.298 and -0.303 e.Å^{-3}

Crystal structure and data of compound 23b

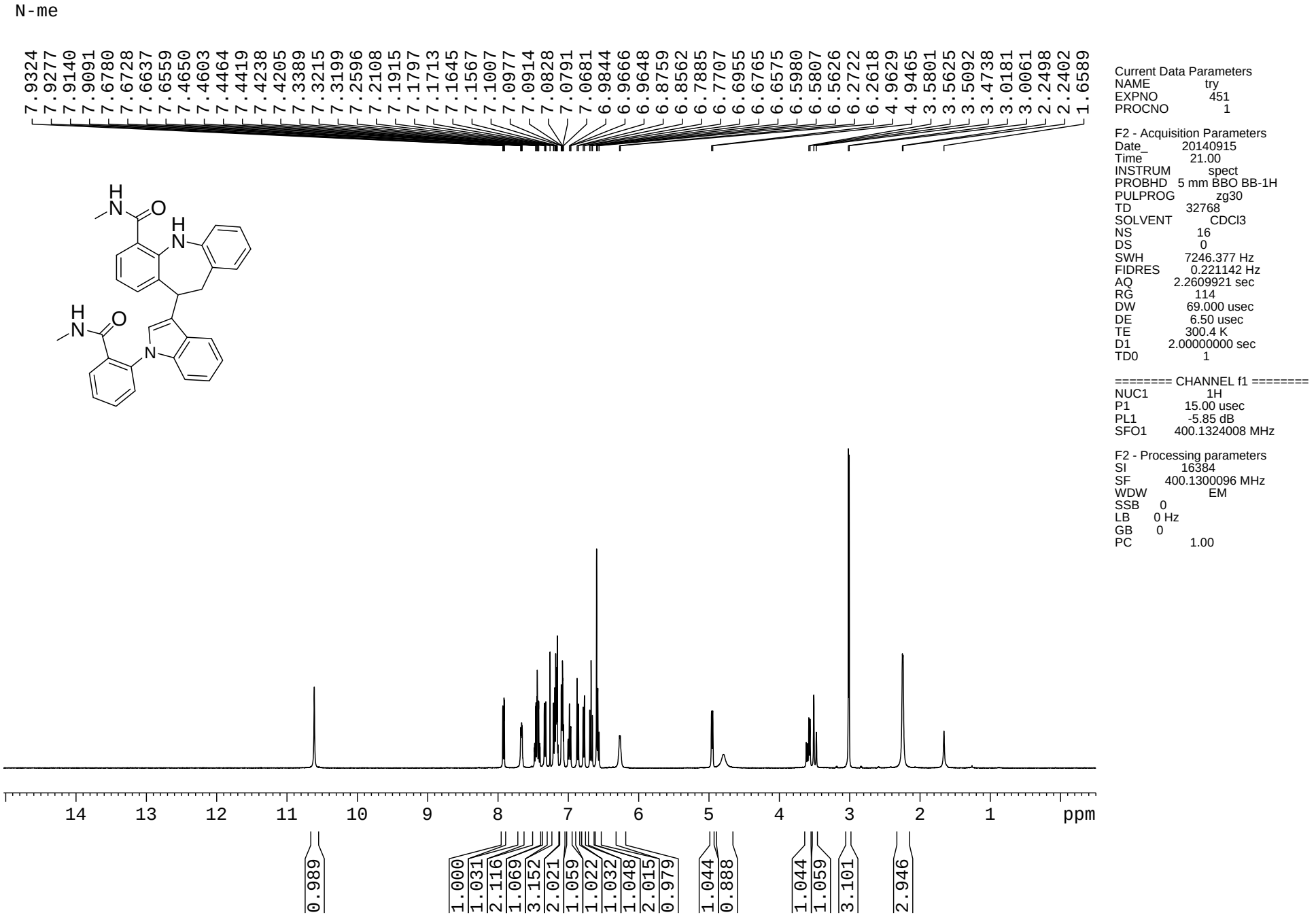


Identification code	a16134	
Empirical formula	C28 H20 Cl2 N2	
Formula weight	455.36	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 7.242(6) Å	α= 90°.
	b = 21.438(12) Å	β= 96.92(3)°.
	c = 14.019(9) Å	γ = 90°.
Volume	2161(2) Å^3	
Z	4	
Density (calculated)	1.400 Mg/m^3	
Absorption coefficient	0.320 mm^{-1}	
F(000)	944	

Crystal size	0.51 x 0.03 x 0.02 mm^3
Theta range for data collection	1.74 to 25.30°.
Index ranges	-8<=h<=3, -25<=k<=24, -14<=l<=16
Reflections collected	10614
Independent reflections	3907 [R(int) = 0.2401]
Completeness to theta = 25.30°	99.2 %
Absorption correction	multi-scan
Max. and min. transmission	0.9936 and 0.8537
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3907 / 0 / 283
Goodness-of-fit on F^2	0.950
Final R indices [I>2sigma(I)]	R1 = 0.1027, wR2 = 0.1930
R indices (all data)	R1 = 0.3364, wR2 = 0.2902
Largest diff. peak and hole	0.461 and -0.441 e.$Å^{-3}$

^{1}H NMR and ^{13}C NMR Spectra copies

1H NMR of N-Methyl-11-(1-(2-(methylcarbamoyl)phenyl)-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (1b)



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EXPNO 451
PROCNO 1

F2 - Acquisition Parameters
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Time 21.00
INSTRUM spect
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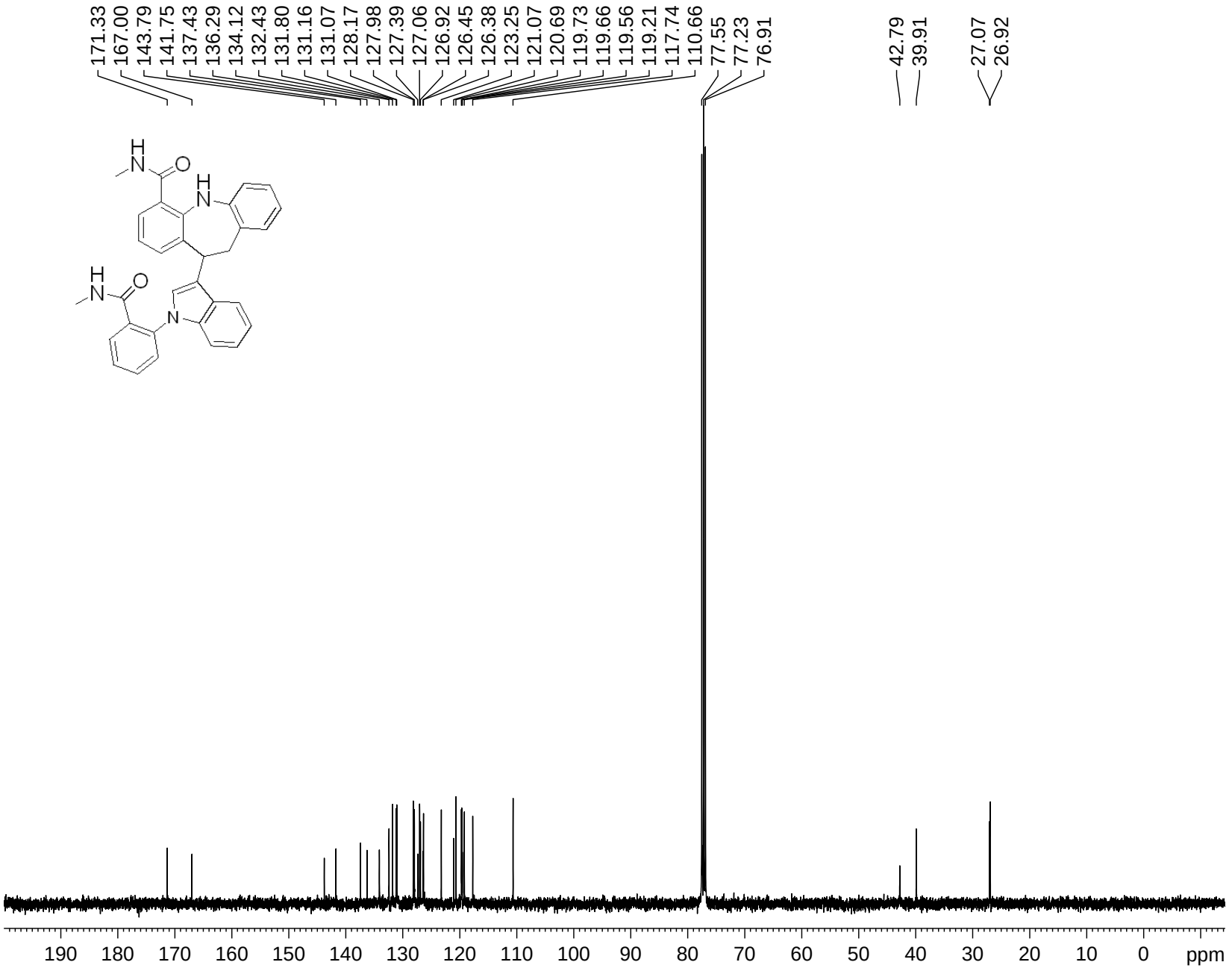
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 114
DW 69.000 usec
DE 6.50 usec
TE 300.4 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

13C NMR of N-Methyl-11-(1-(2-(methylcarbamoyl)phenyl)-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (1b)

13c of N-ch3



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PROCNO 1

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Time 22.54
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PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 375
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 300.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

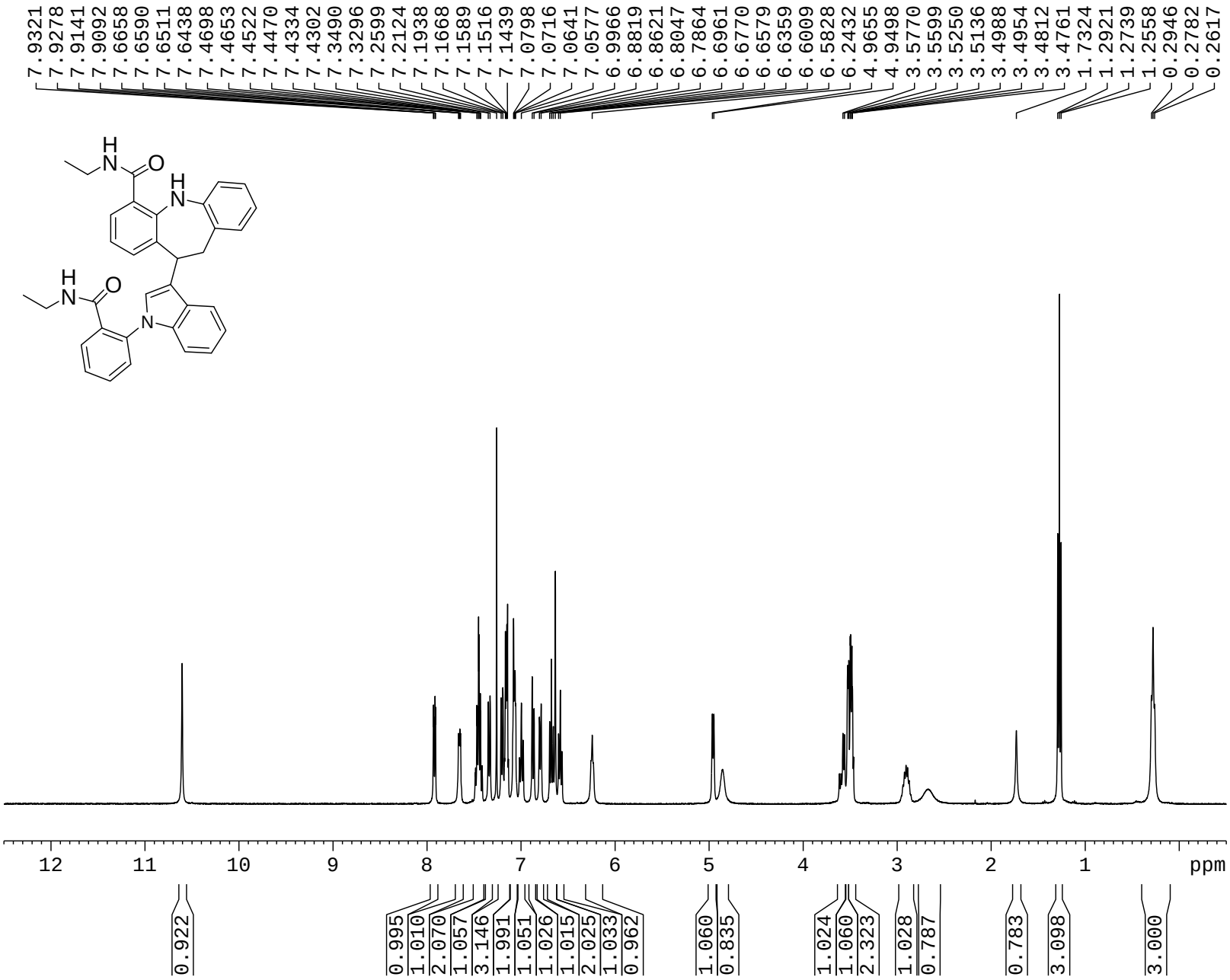
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 13.95 dB
PL13 17.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127499 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1H NMR of N-Ethyl-11-(1-(2-(ethylcarbamoyl)phenyl)-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (2b)

1h of N-ethyl



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Time 20.44
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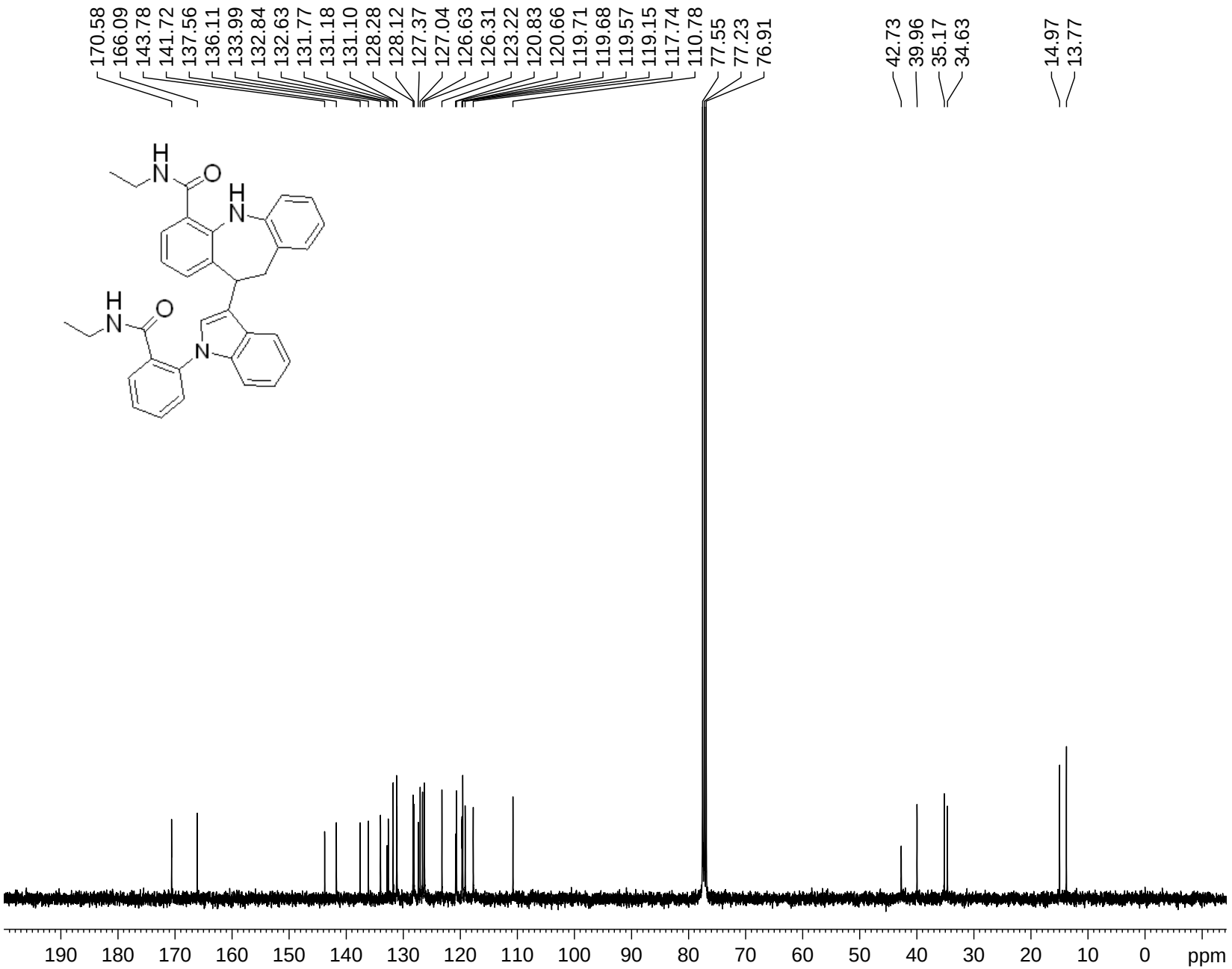
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 114
DW 69.000 usec
DE 6.50 usec
TE 295.2 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.90 usec
PL1 3.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

13C NMR of N-Ethyl-11-(1-(2-(ethylcarbamoyl)phenyl)-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (2b)

13c of N-ethyl



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PROCNO 1

F2 - Acquisition Parameters
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Time 20.46
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PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 476
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 295.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

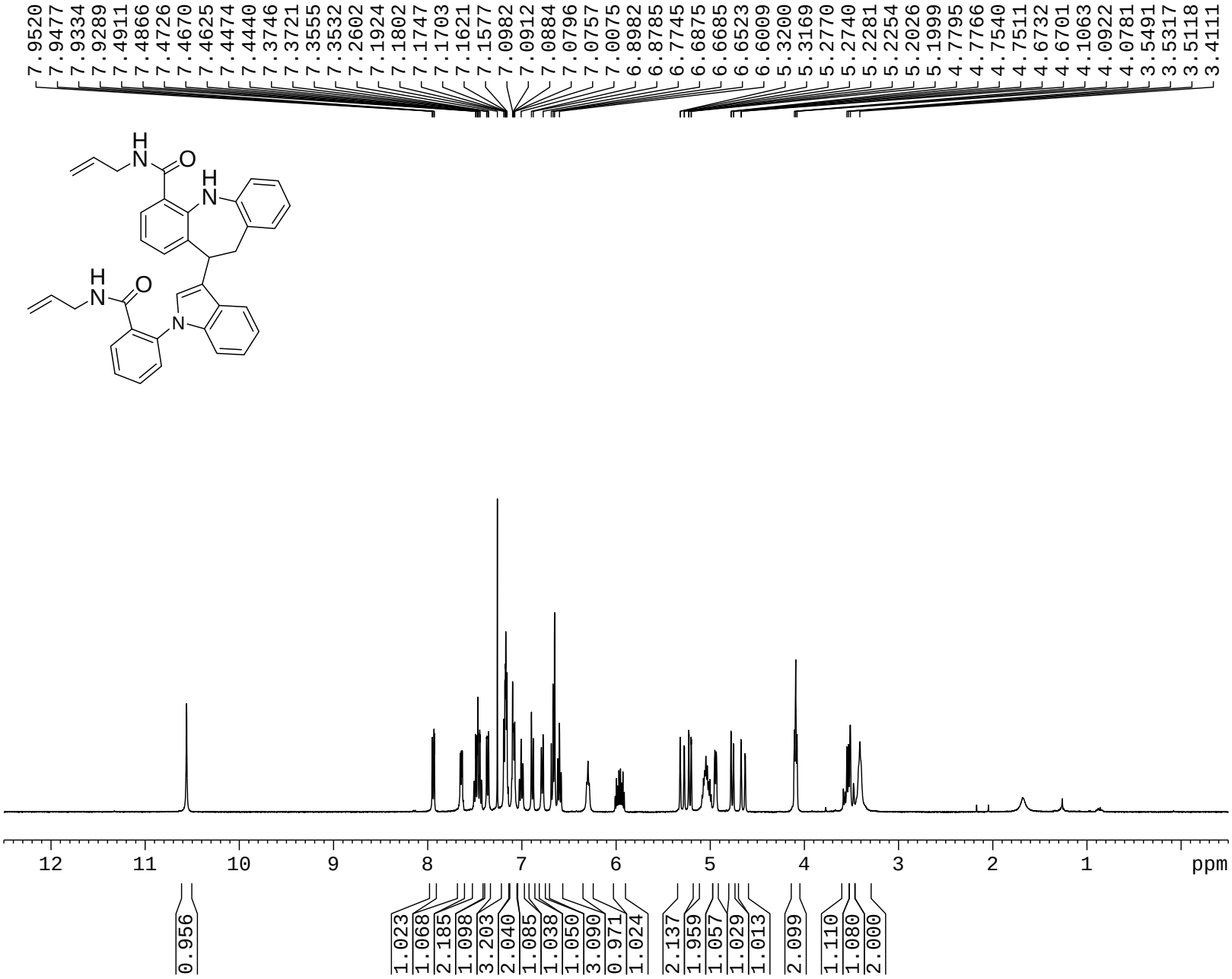
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.00 dB
PL12 20.70 dB
PL13 23.70 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127521 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1H NMR of N-allyl-11-(1-(2-(allylcarbamoyl)phenyl)-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (3b)

1h of N-allyl amide



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PROCNO 1

F2 - Acquisition Parameters
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Time 1.42
INSTRUM spect
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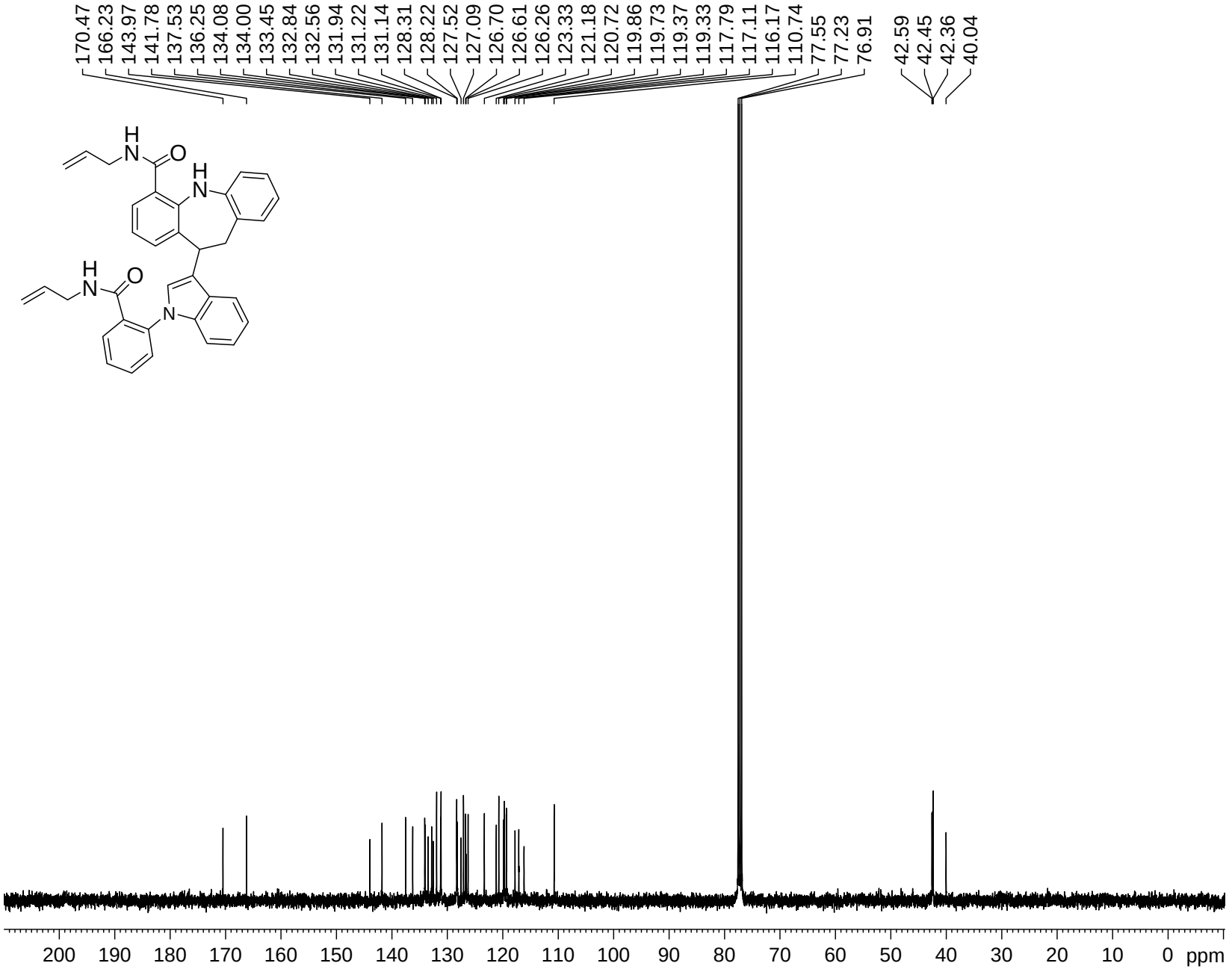
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 181
DW 69.000 usec
DE 6.50 usec
TE 295.8 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.90 usec
PL1 3.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

13C NMR of N-allyl-11-(1-(2-(allylcarbamoyl)phenyl)-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (3b)

13c of N-allyl amide



Current Data Parameters
NAME try
EXPNO 67
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140118
Time 1.44
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 524
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 295.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

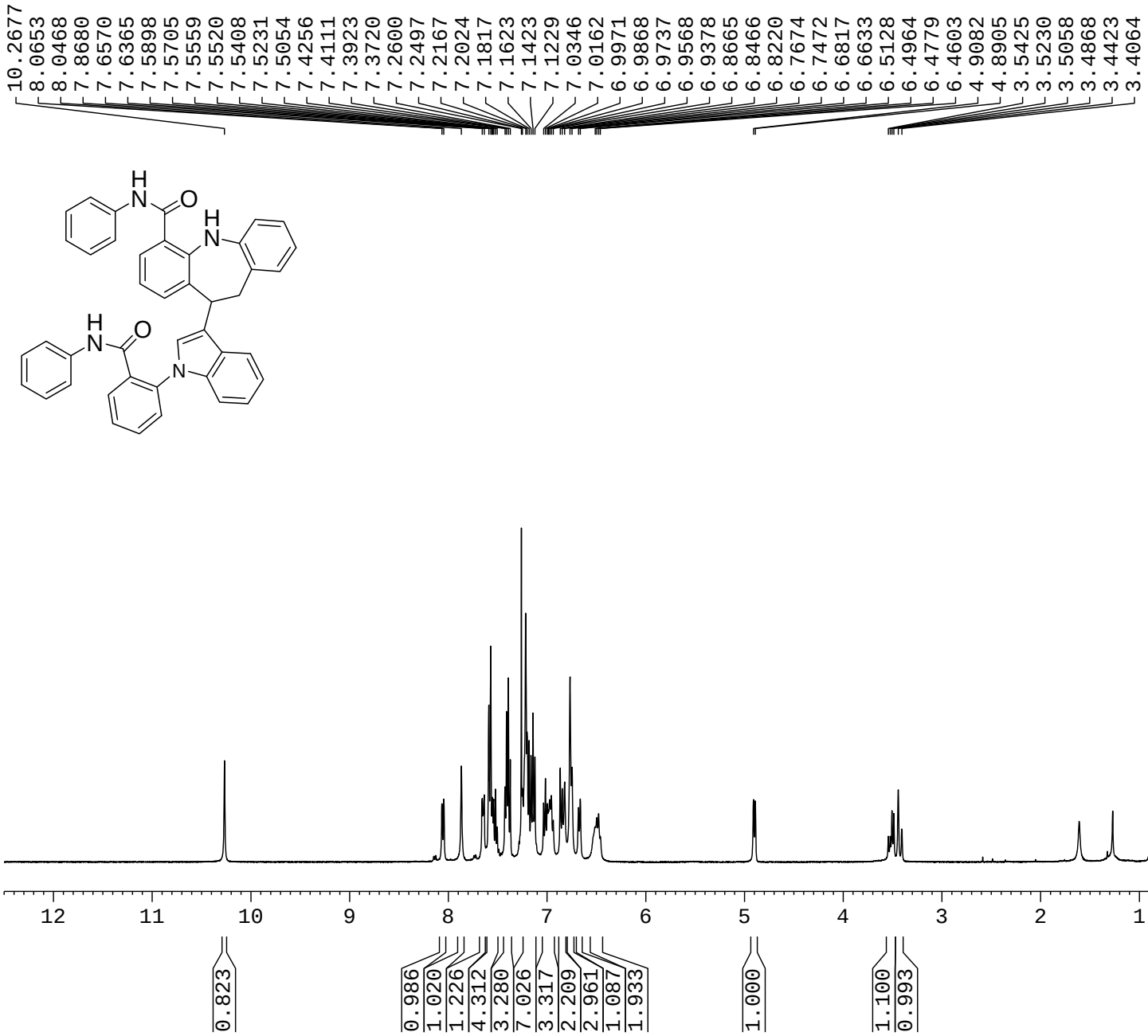
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.00 dB
PL12 20.70 dB
PL13 23.70 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127507 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1H NMR of N-phenyl-11-(1-(2-(phenylcarbamoyl)phenyl)-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (4b)

1H of N-Ph with bf3.oet



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NAME try
EXPNO 12
PROCNO 1

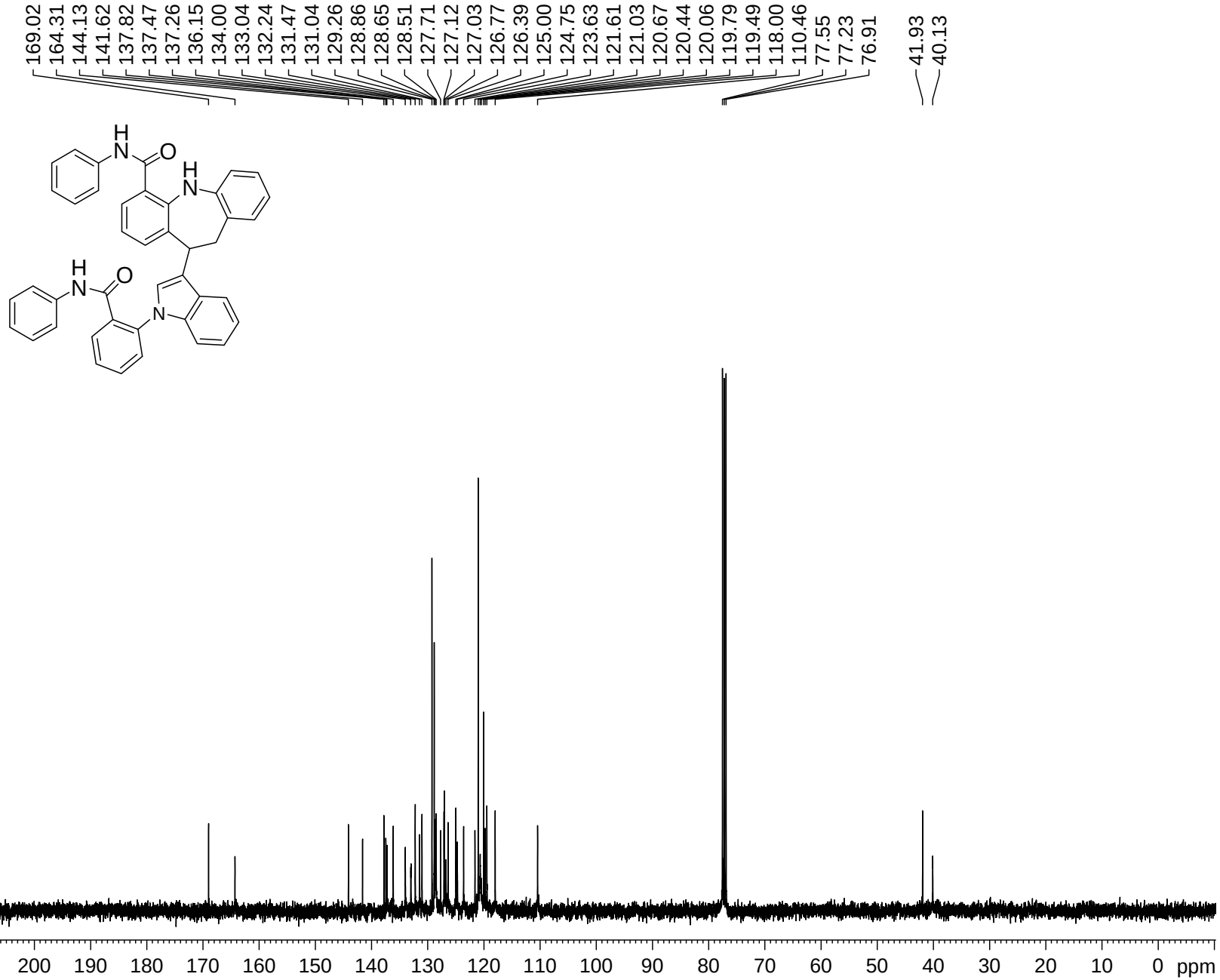
F2 - Acquisition Parameters
Date_ 20140106
Time 11.49
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 181
DW 69.000 usec
DE 6.50 usec
TE 296.8 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.90 usec
PL1 3.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

13C NMR of N-phenyl-11-(1-(2-(phenylcarbamoyl)phenyl)-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (4b)

13c of N-Ph with bf3.oet



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EXPNO 32
PROCNO 1

F2 - Acquisition Parameters
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Time 23.34
INSTRUM spect
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PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 190
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 295.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

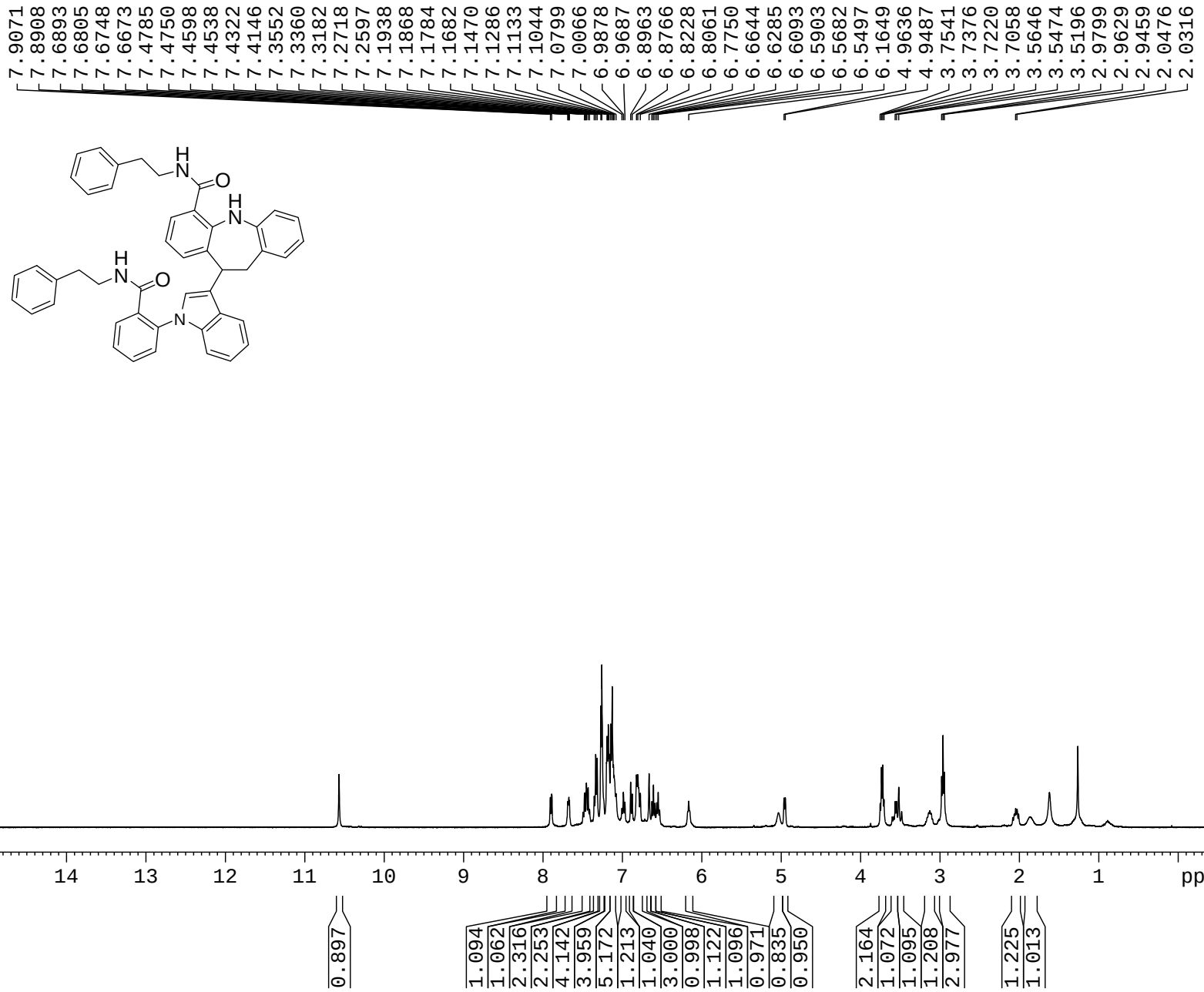
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.00 dB
PL12 20.70 dB
PL13 23.70 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127573 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1H NMR of N-phenethyl-11-(1-(2-(phenethylcarbamoyl)phenyl)-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (5b)

N-ethyl ph



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EXPNO 442
PROCNO 1

F2 - Acquisition Parameters
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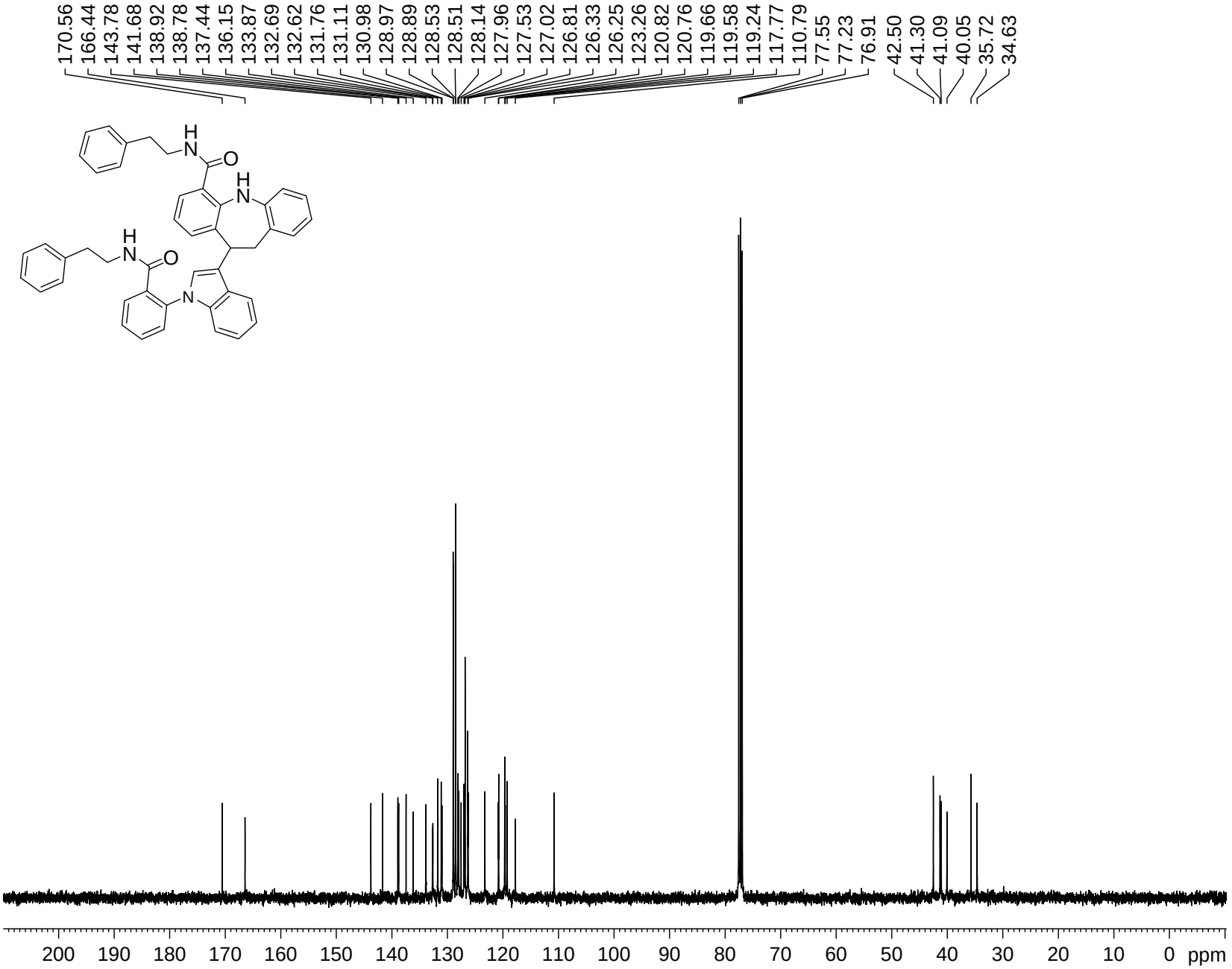
Time 11.44
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 114
DW 69.000 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

13C NMR of N-phenethyl-11-(1-(2-(phenethylcarbamoyl)phenyl)-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (5b)

13c of l N-ethyl-Ph amide with bf3.oet



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PROCNO 1

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Date_ 20140111
Time 0.17
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 379
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 295.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

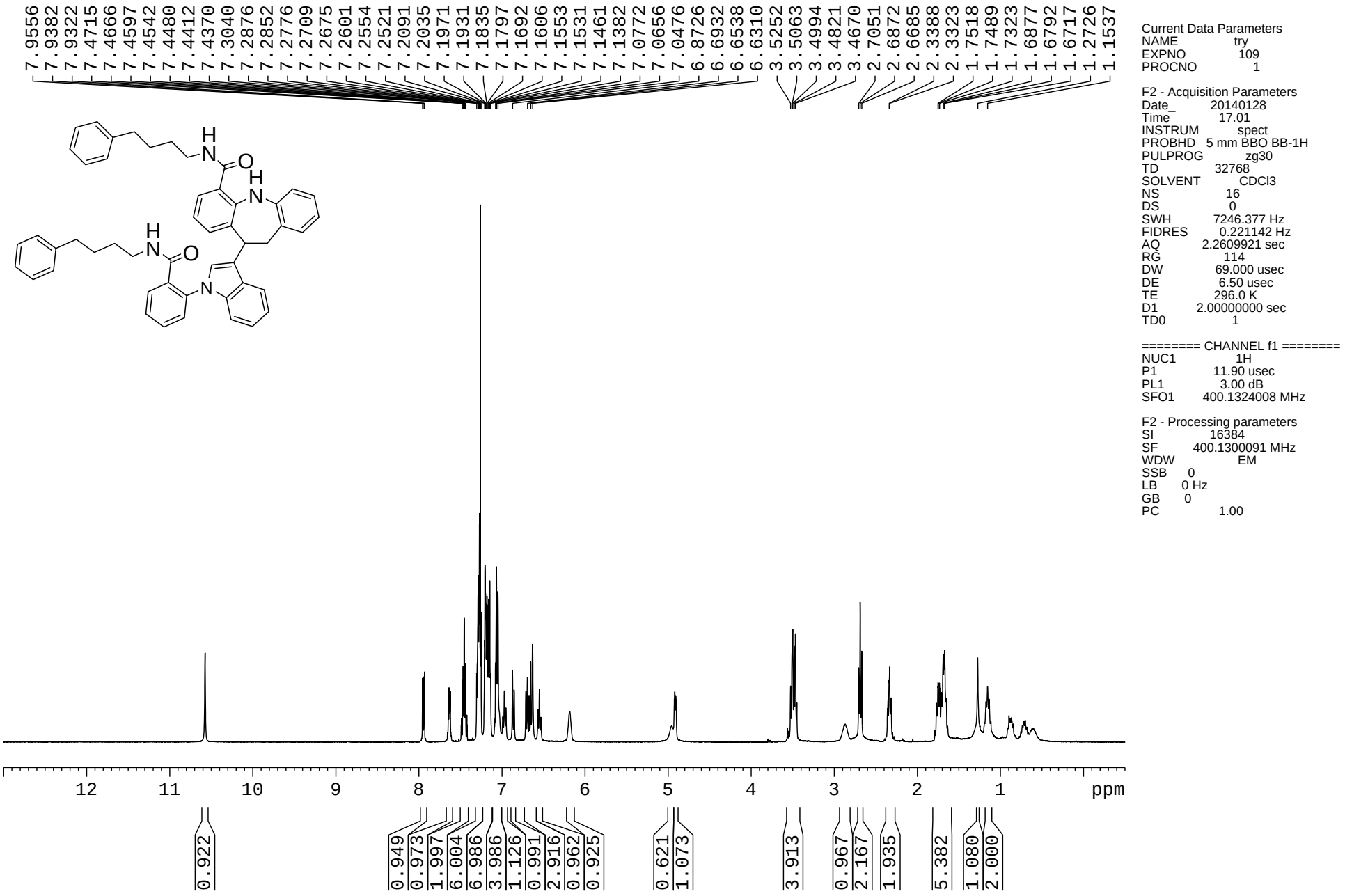
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.00 dB
PL12 20.70 dB
PL13 23.70 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127587 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1H NMR of N-(4-phenylbutyl)-11-(1-(2-(4-phenylbutylcarbamoyl)phenyl)-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (6b)

1h of n-butyl



Current Data Parameters
NAME try
EXPNO 109
PROCNO 1

F2 - Acquisition Parameters
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Time 17.01
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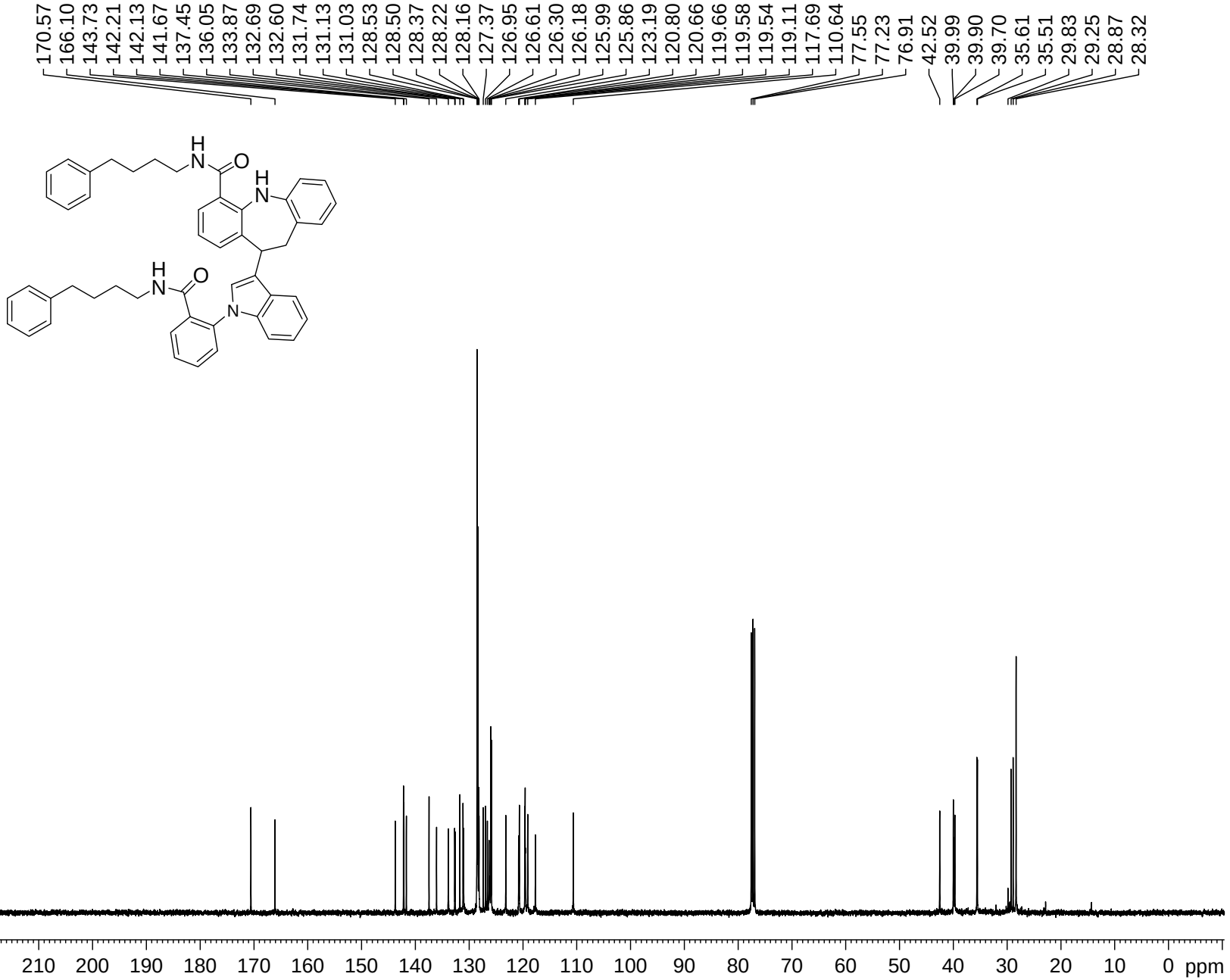
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 114
DW 69.000 usec
DE 6.50 usec
TE 296.0 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.90 usec
PL1 3.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

1H NMR of N-(4-phenylbutyl)-11-(1-(2-(4-phenylbutylcarbamoyl)phenyl)-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (6b)

13c of N-butyl ph amide



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PROCNO 1

F2 - Acquisition Parameters
Date_ 20140118
Time 0.59
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 820
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 295.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

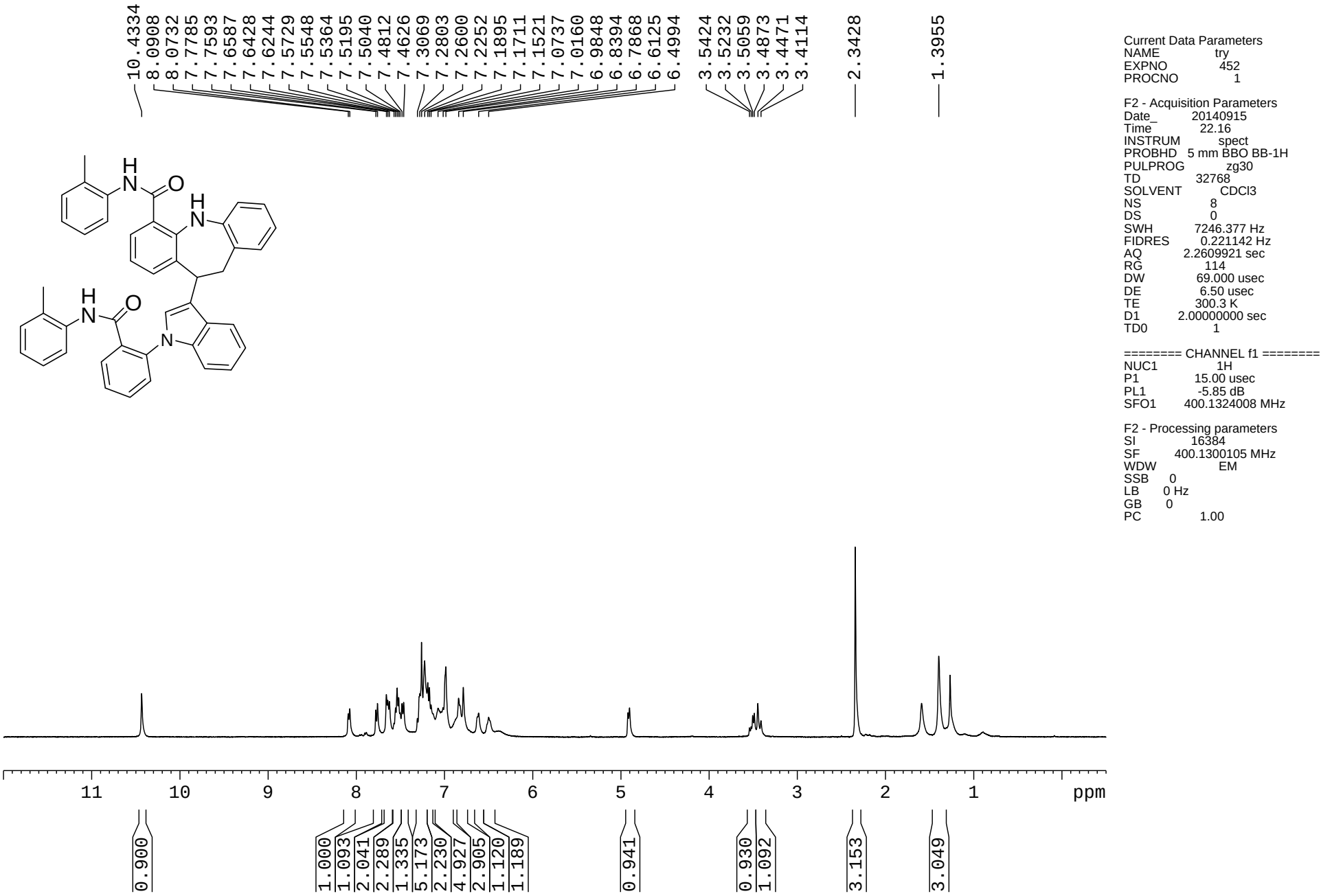
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.00 dB
PL12 20.70 dB
PL13 23.70 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127631 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1H NMR of N-o-Tolyl-11-(1-(2-(o-tolylcarbamoyl)phenyl)-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (7b)

o-me



Current Data Parameters
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F2 - Acquisition Parameters
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Time 22.16
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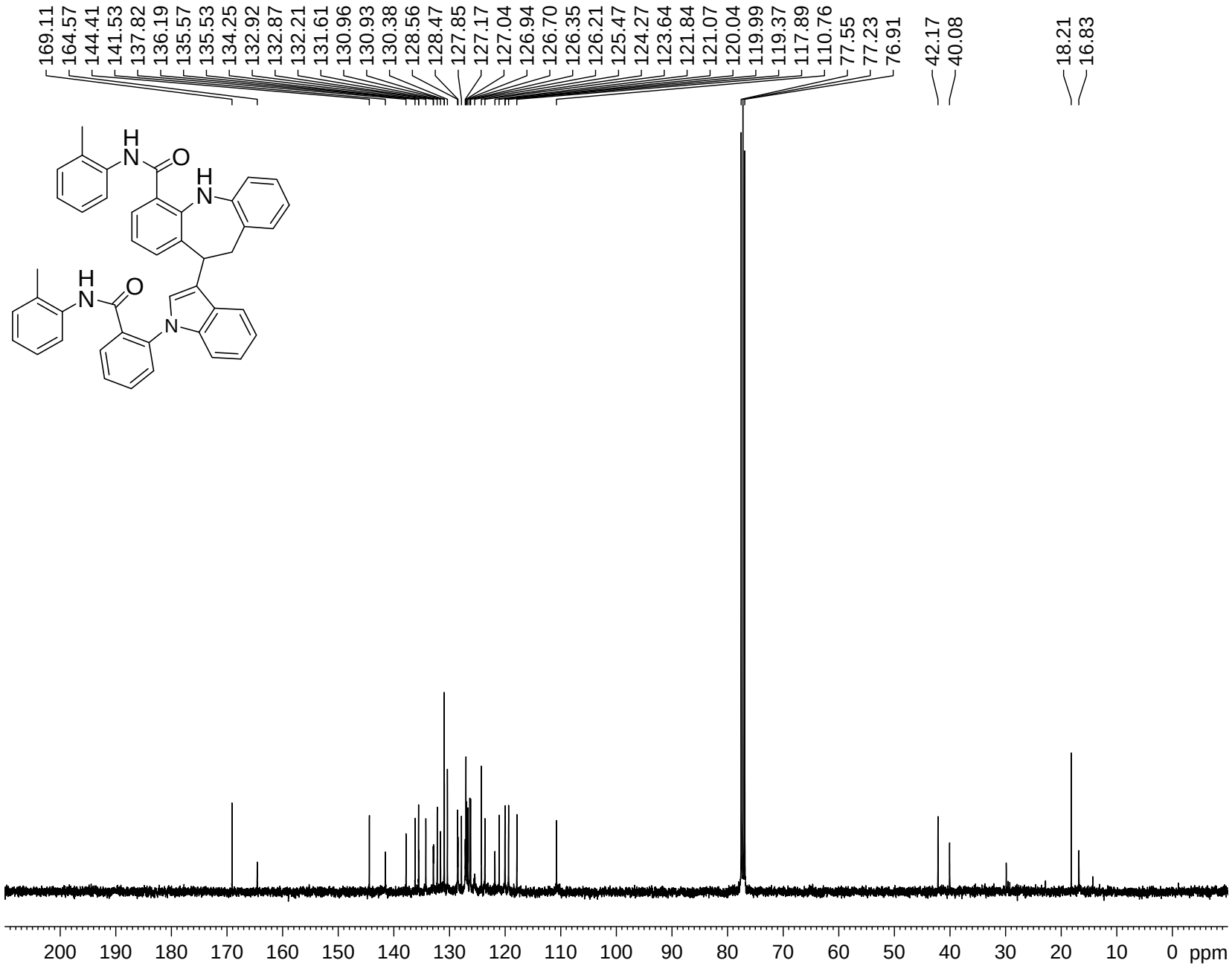
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 114
DW 69.000 usec
DE 6.50 usec
TE 300.3 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300105 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

13c NMR of N-o-Tolyl-11-(1-(2-(o-tolylcarbamoyl)phenyl)-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (7b)

13c of o-me N-ph amide



Current Data Parameters
NAME try
EXPNO 63
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140118
Time 0.27
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 542
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 295.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

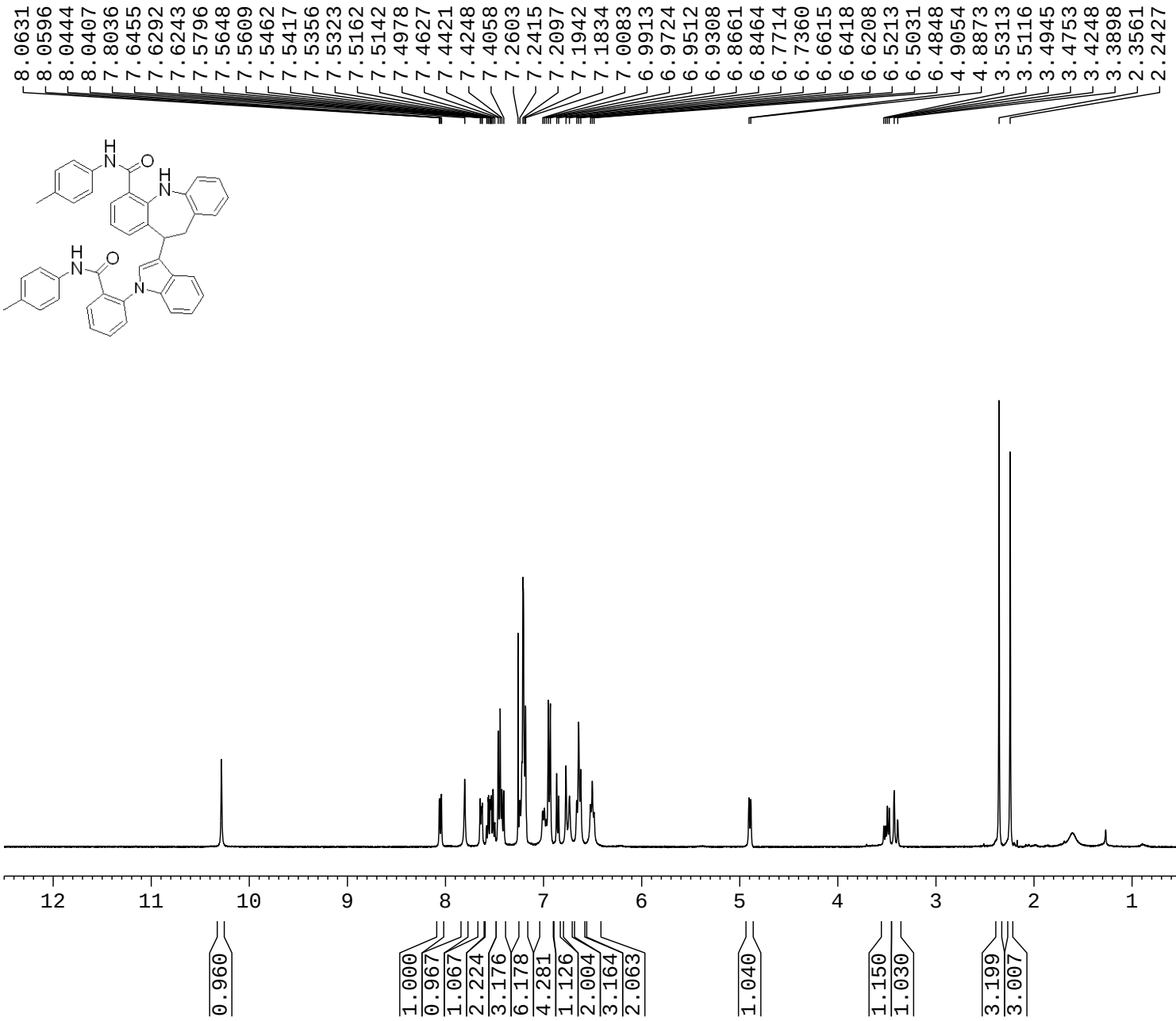
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.00 dB
PL12 20.70 dB
PL13 23.70 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127543 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1H NMR of N-p-Tolyl-11-(1-(2-(p-tolylcarbamoyl)phenyl)-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (8b)

1h of p-methyl



Current Data Parameters
NAME try
EXPNO 131
PROCNO 1

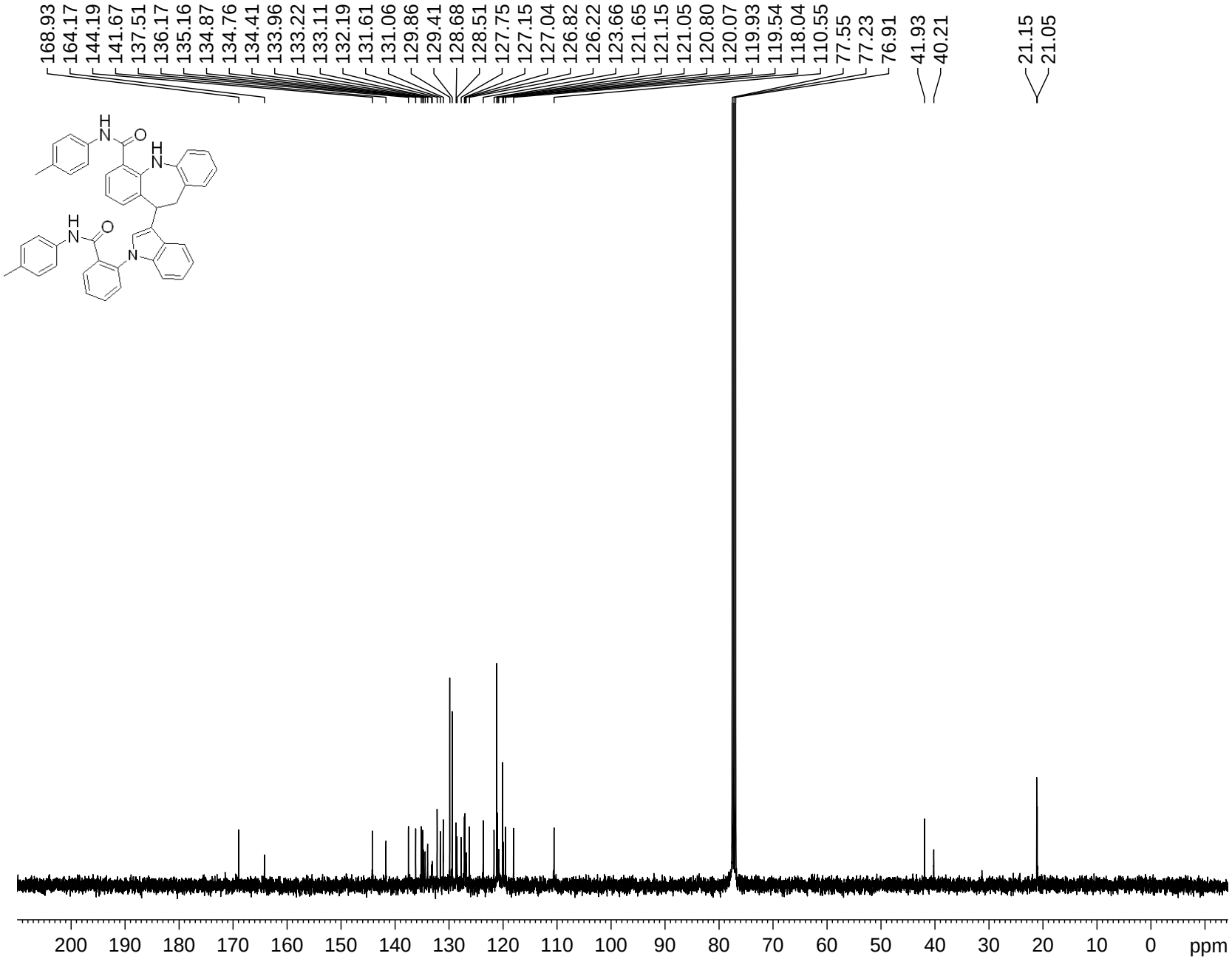
F2 - Acquisition Parameters
Date_ 20140131
Time 15.43
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 228.1
DW 69.000 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.90 usec
PL1 3.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

13C NMR of N-p-Tolyl-11-(1-(2-(p-tolylcarbamoyl)phenyl)-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (8b)

13c of N-P-Me with bf3.oet



Current Data Parameters
NAME try
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140110
Time 22.56
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 647
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 295.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

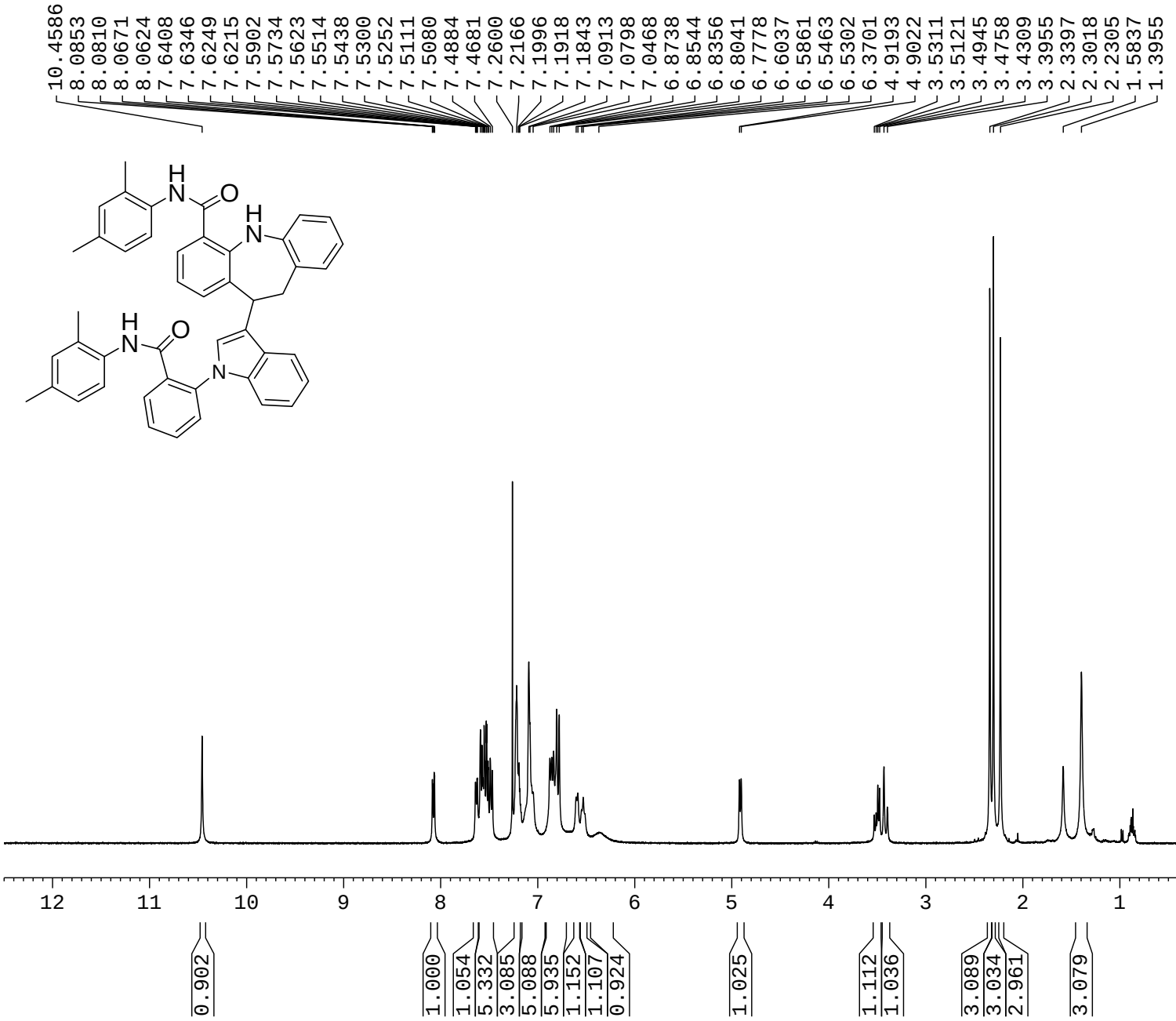
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.00 dB
PL12 20.70 dB
PL13 23.70 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127507 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1H NMR of N-(2,4-Dimethylphenyl)-11-(1-(2-(2,4-dimethylphenylcarbamoyl)phenyl)-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (9b)

1H of n-dimethyl with bf3.oet



Current Data Parameters
NAME try
EXPNO 8
PROCNO 1

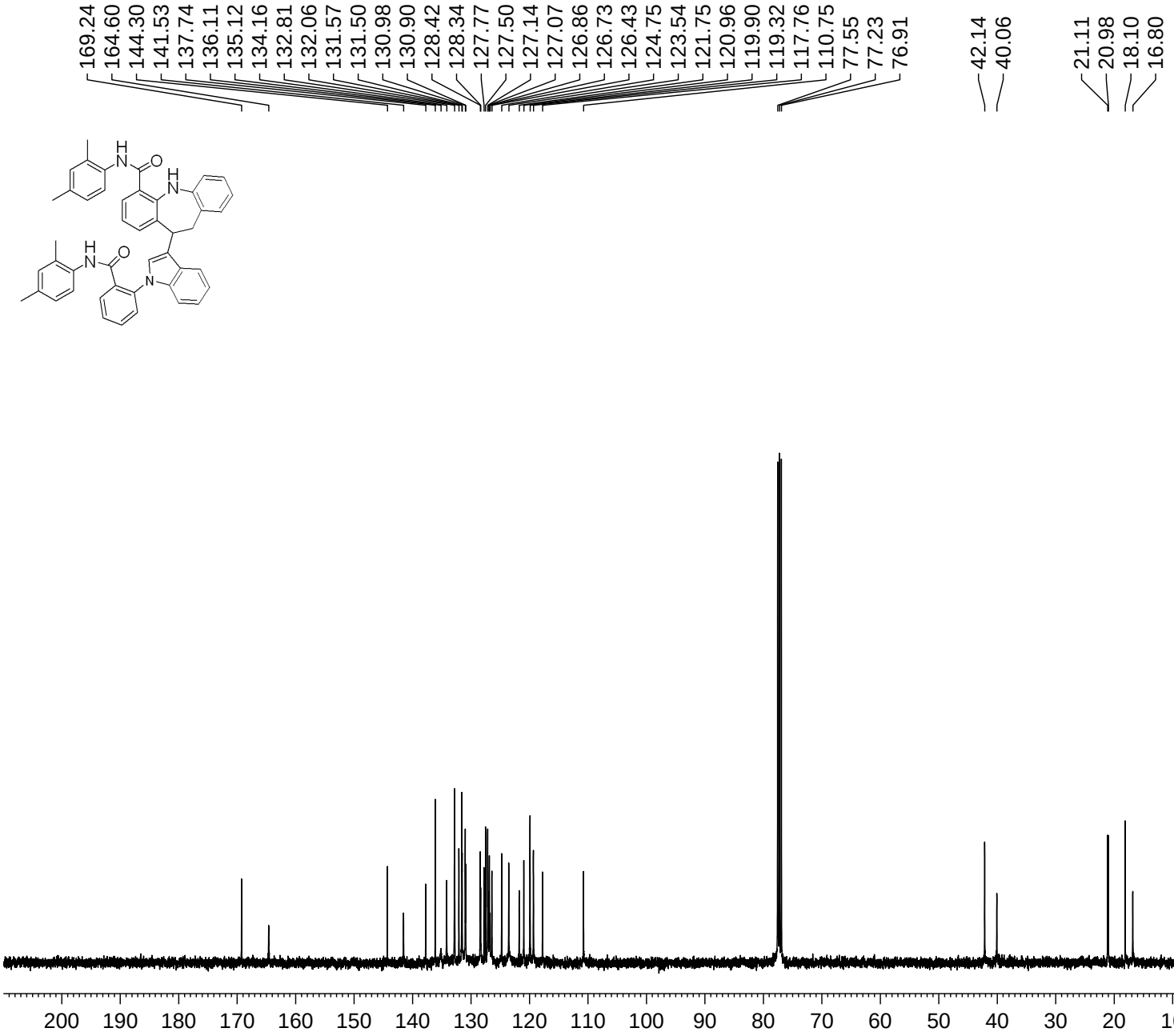
F2 - Acquisition Parameters
Date_ 20140104
Time 19.24
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 228.1
DW 69.000 usec
DE 6.50 usec
TE 297.8 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.90 usec
PL1 3.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

13C NMR of N-(2,4-Dimethylphenyl)-11-(1-(2-(2,4-dimethylphenylcarbamoyl)phenyl)-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (9b)

13c of di methyl N-Ph amide with bf3.oet



Current Data Parameters
NAME try
EXPNO 35
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140110
Time 23.50
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 385
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 295.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

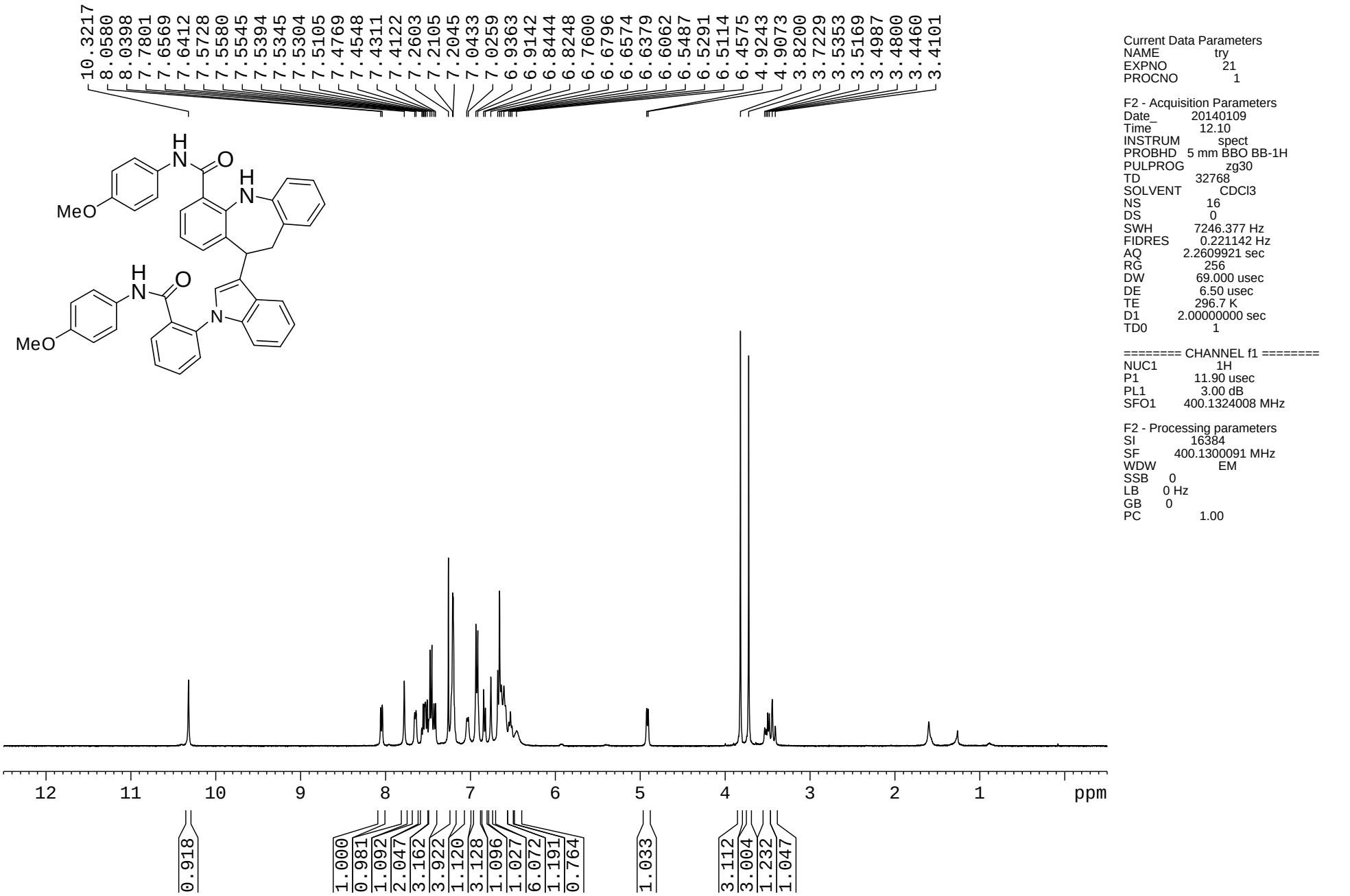
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.00 dB
PL12 20.70 dB
PL13 23.70 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127616 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1H NMR of N-(4-methoxyphenyl)-11-(1-(2-(4-methoxyphenylcarbamoyl)phenyl)-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (10b)

1H of 4-OMe N- Ph amide with bf3.oet



Current Data Parameters
NAME try
EXPNO 21
PROCNO 1

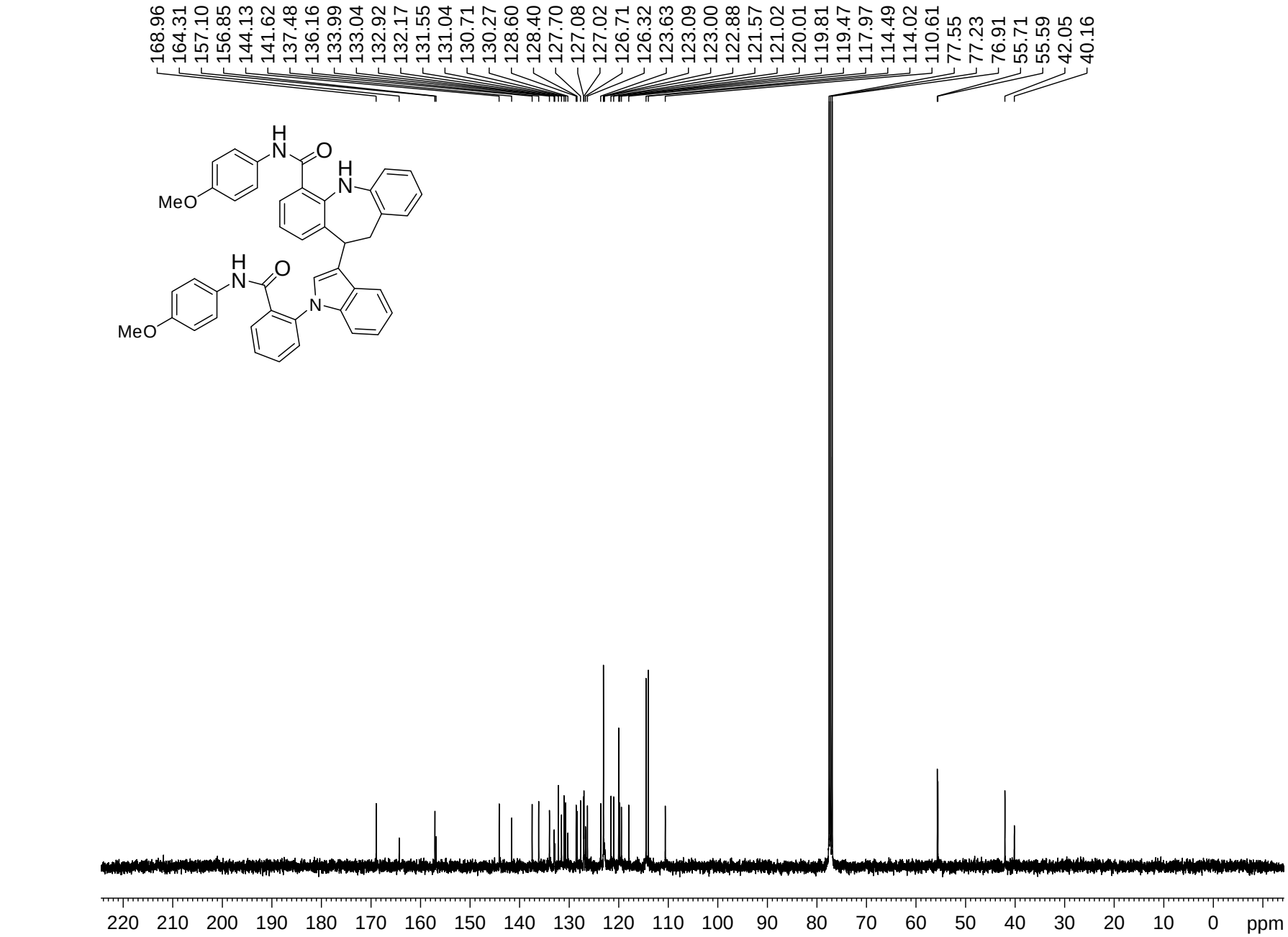
F2 - Acquisition Parameters
Date_ 20140109
Time 12.10
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 256
DW 69.000 usec
DE 6.50 usec
TE 296.7 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.90 usec
PL1 3.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

13C NMR of N-(4-methoxyphenyl)-11-(1-(2-(4-methoxyphenylcarbamoyl)phenyl)-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (10b)

13c of 4-OMe N-ph amide



Current Data Parameters
NAME try
EXPNO 59
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140117
Time 23.12
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 587
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 295.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

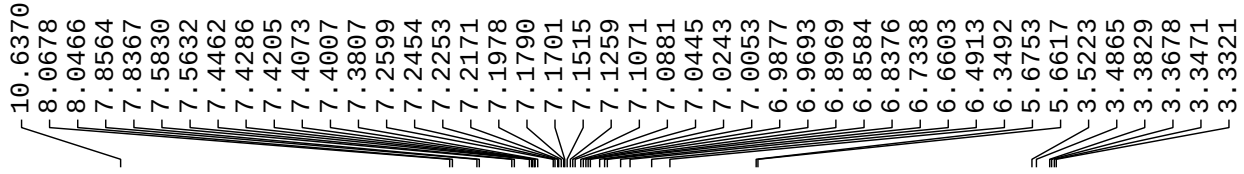
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

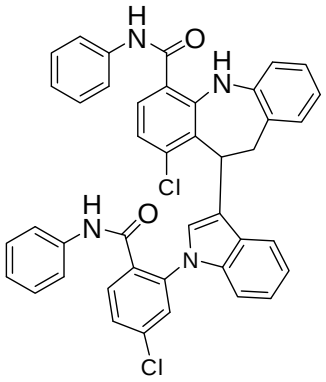
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.00 dB
PL12 20.70 dB
PL13 23.70 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127521 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1H NMR of 1-Chloro-11-(1-(5-chloro-2-(phenylcarbamoyl)phenyl)-1H-indol-3-yl)-N-phenyl-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (11b)

P-cl amide



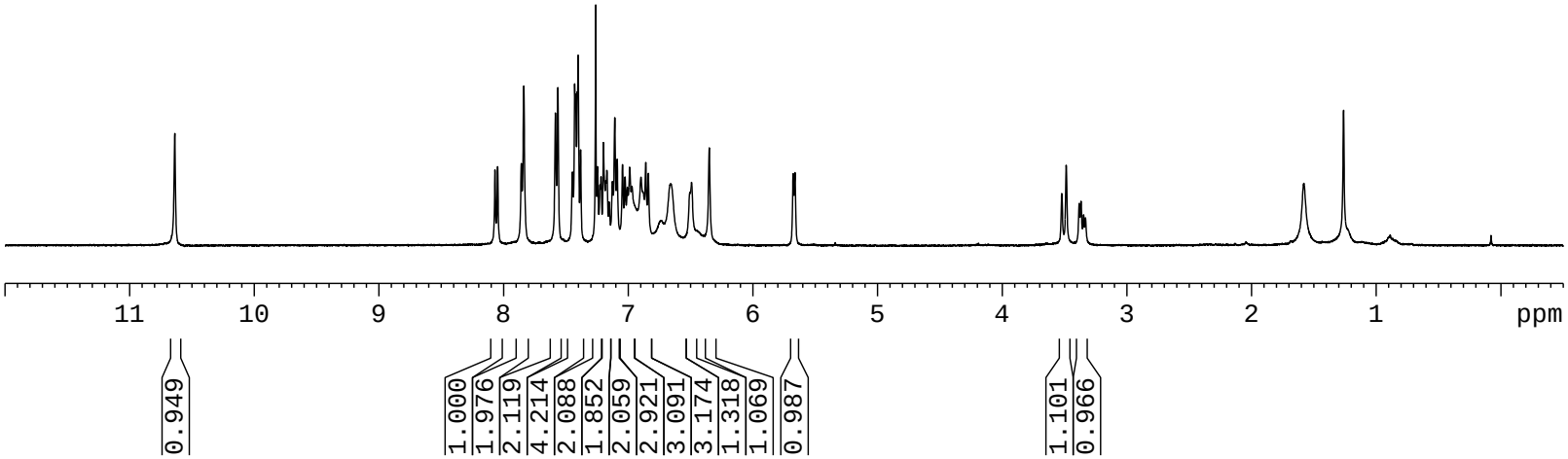


Current Data Parameters
NAME try
EXPNO 443
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140915
Time 11.59
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 181
DW 69.000 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
TD0 1

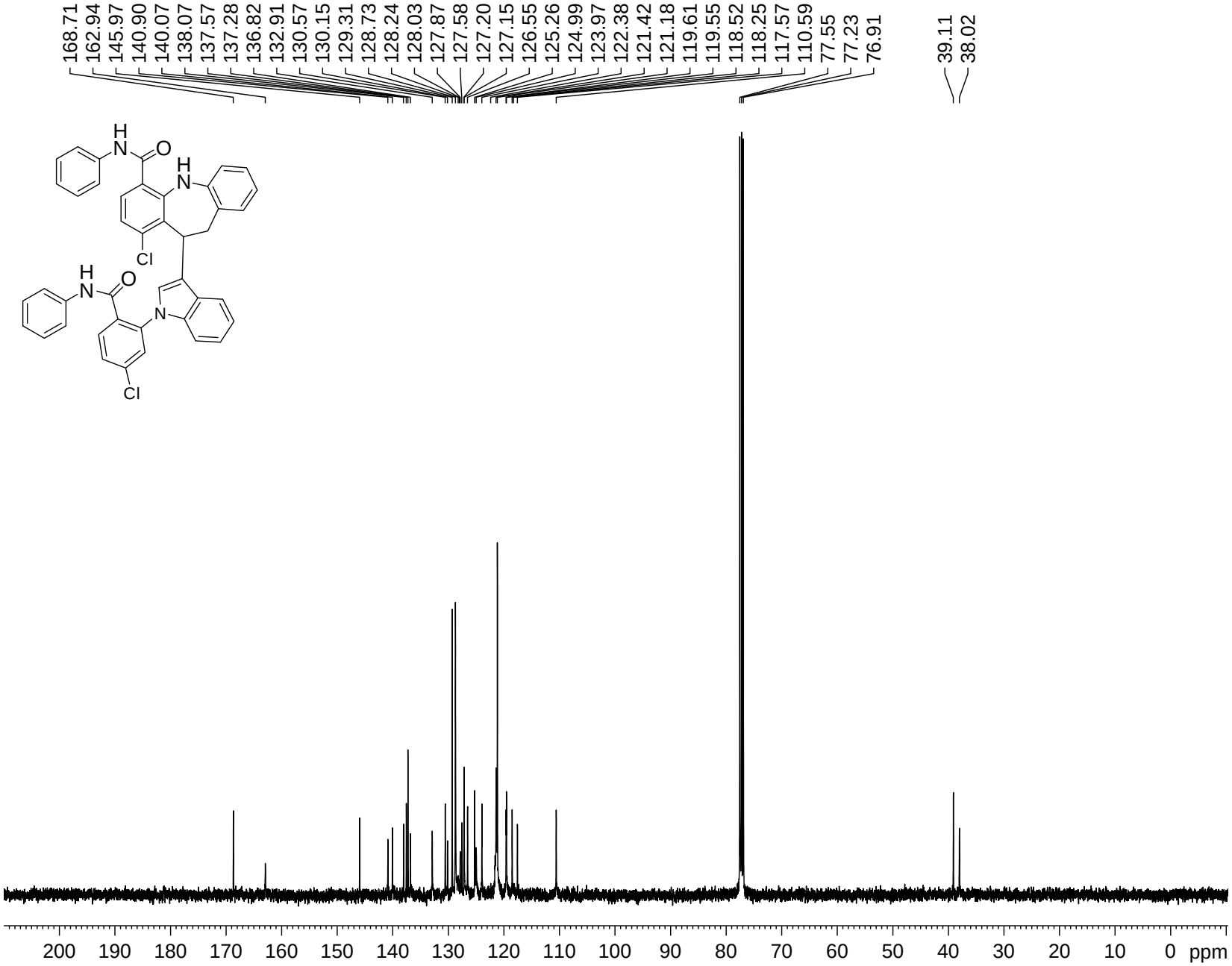
======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



13C NMR of 1-Chloro-11-(1-(5-chloro-2-(phenylcarbamoyl)phenyl)-1H-indol-3-yl)-N-phenyl-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (11b)

13 of P-cl



Current Data Parameters
NAME try
EXPNO 81
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140123
Time 18.13
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 696
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 295.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

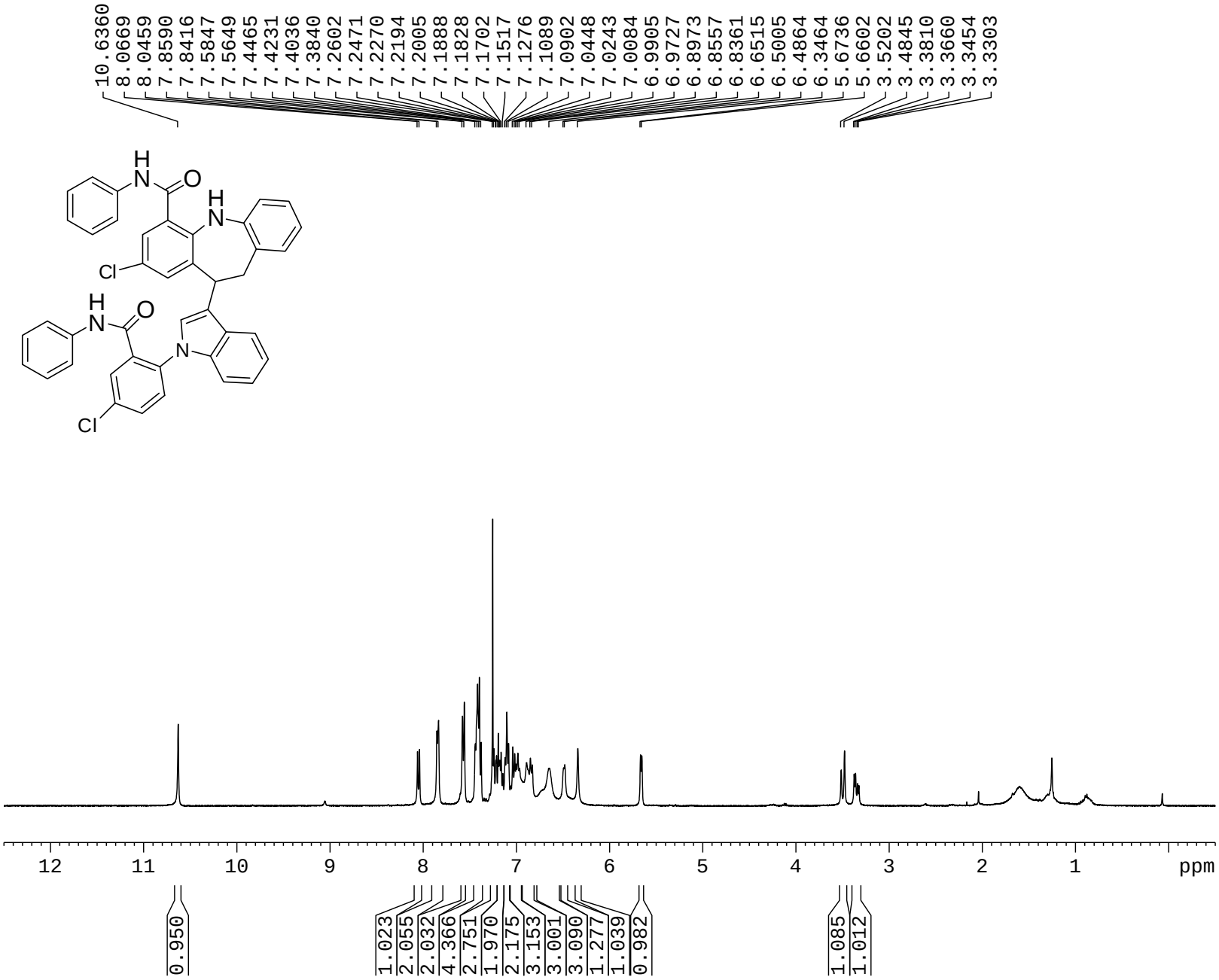
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.00 dB
PL12 20.70 dB
PL13 23.70 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127551 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1H NMR of 2-Chloro-11-(1-(4-chloro-2-(phenylcarbamoyl)phenyl)-1H-indol-3-yl)-N-phenyl-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (12b)

mcl



Current Data Parameters
NAME try
EXPNO 195
PROCNO 1

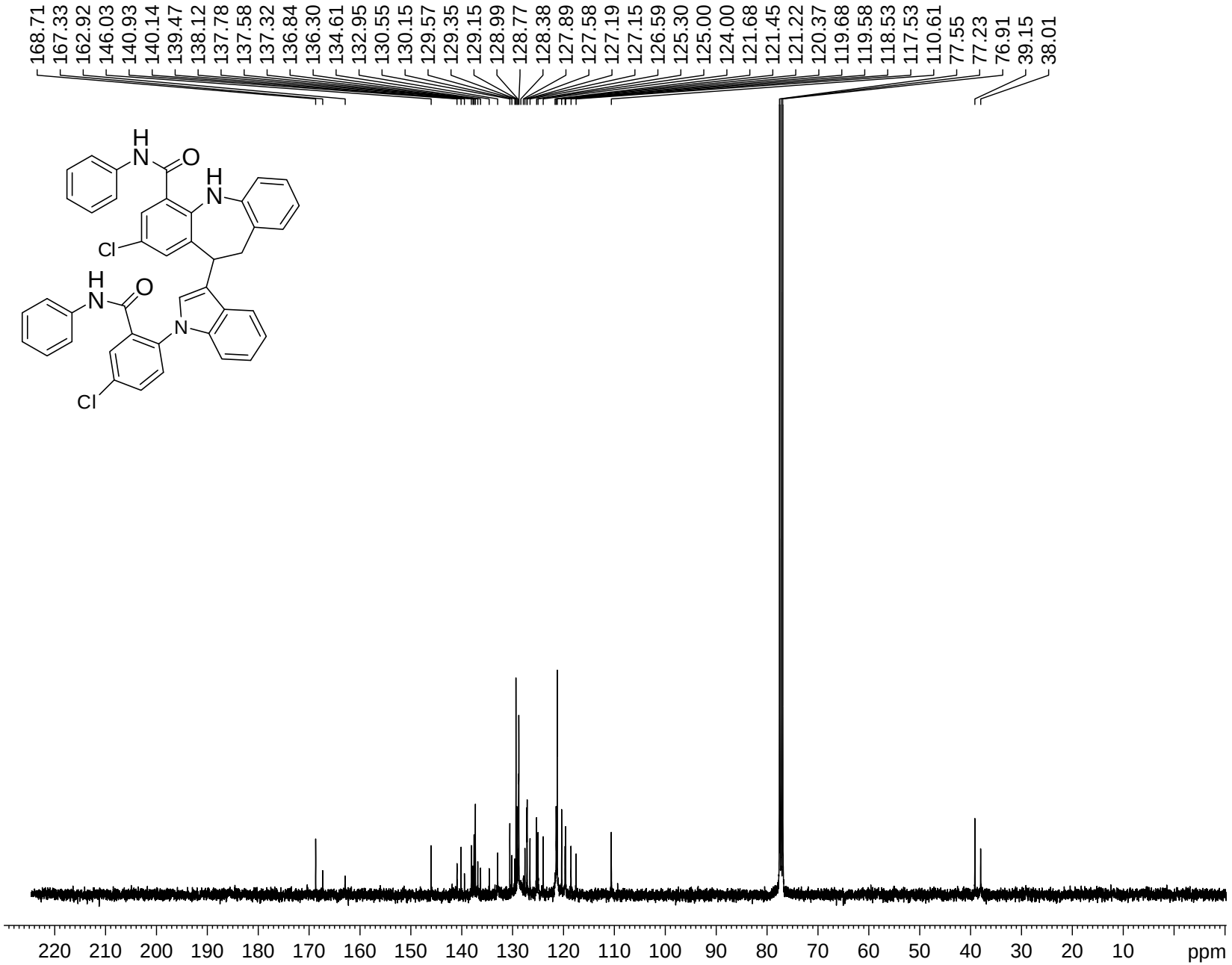
F2 - Acquisition Parameters
Date_ 20140308
Time 14.58
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 181
DW 69.000 usec
DE 6.50 usec
TE 295.3 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.35 usec
PL1 -2.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300118 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

13C NMR of 2-Chloro-11-(1-(4-chloro-2-(phenylcarbamoyl)phenyl)-1H-indol-3-yl)-N-phenyl-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (12b)

13 of M-Cl



Current Data Parameters
NAME try
EXPNO 69
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140118
Time 2.16
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 877
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 295.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

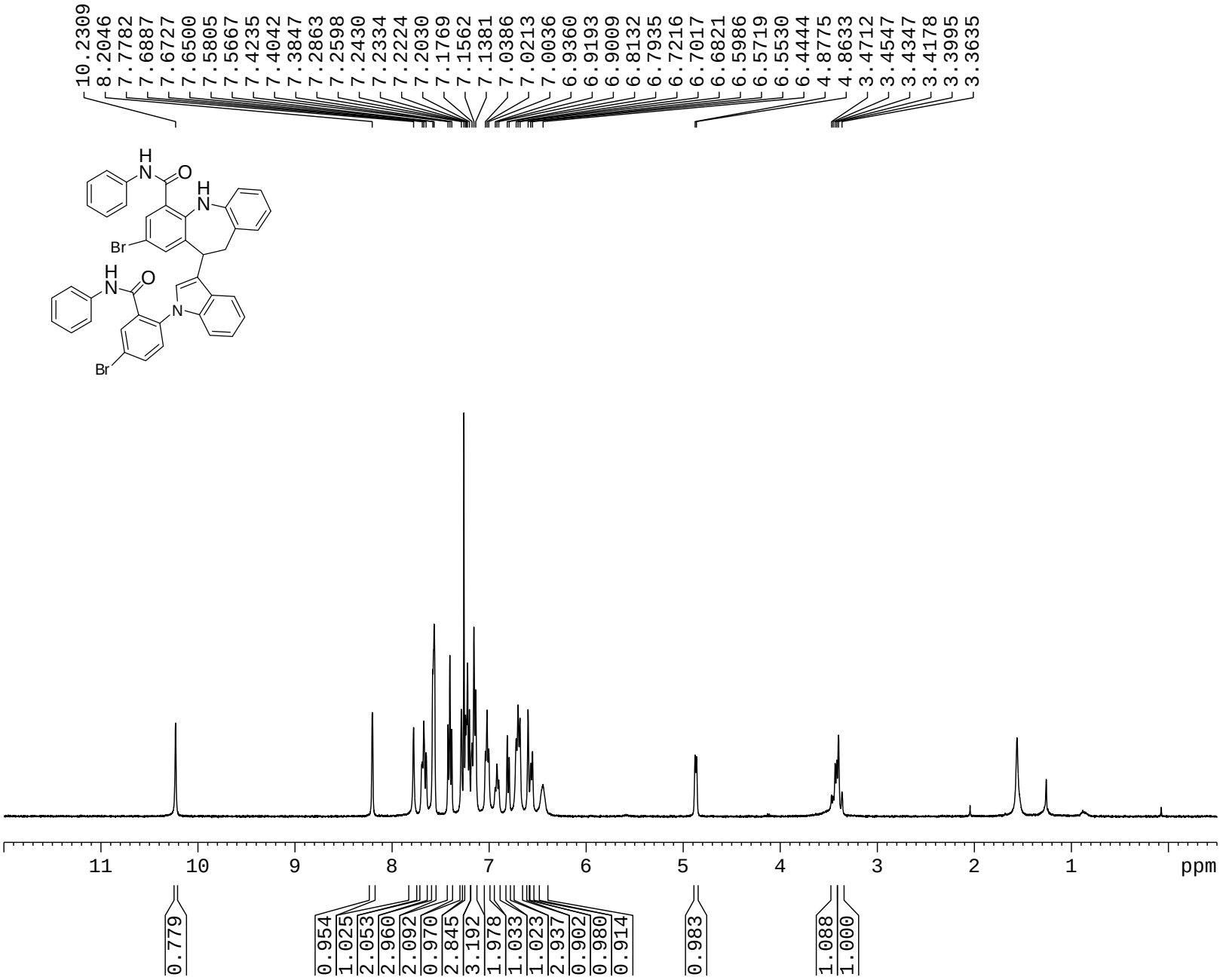
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.00 dB
PL12 20.70 dB
PL13 23.70 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127529 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1H NMR of 2-Bromo-11-(1-(4-bromo-2-(phenylcarbamoyl)phenyl)-1H-indol-3-yl)-N-phenyl-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (13b)

mbr



Current Data Parameters
NAME try
EXPNO 226
PROCNO 1

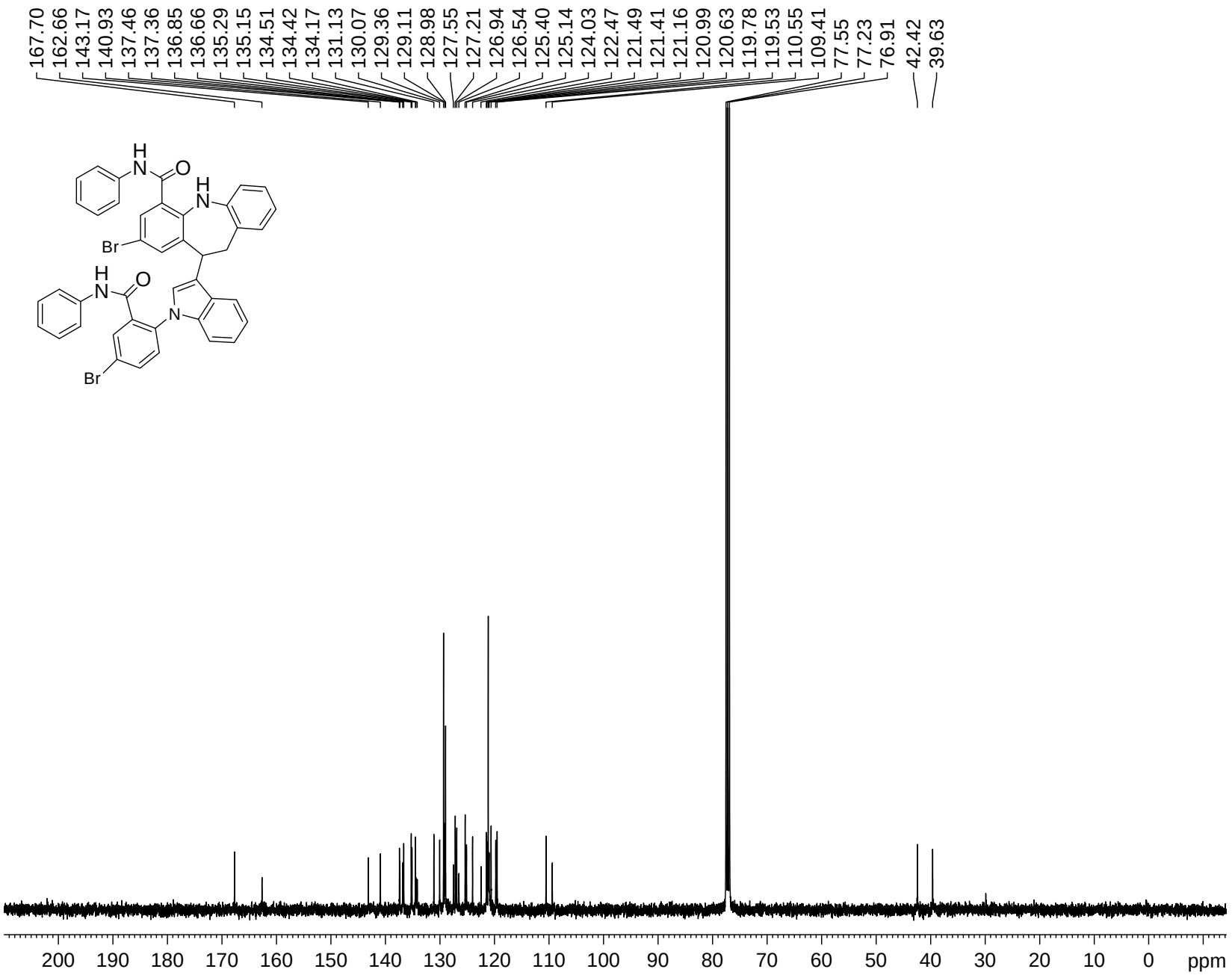
F2 - Acquisition Parameters
Date_ 20140401
Time 14.41
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 256
DW 69.000 usec
DE 6.50 usec
TE 299.6 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.35 usec
PL1 -2.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

13C NMR of 2-Bromo-11-(1-(4-bromo-2-(phenylcarbamoyl)phenyl)-1H-indol-3-yl)-N-phenyl-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (13b)

13c of mbr



Current Data Parameters
NAME try
EXPNO 246
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140411
Time 12.07
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 596
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 300.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

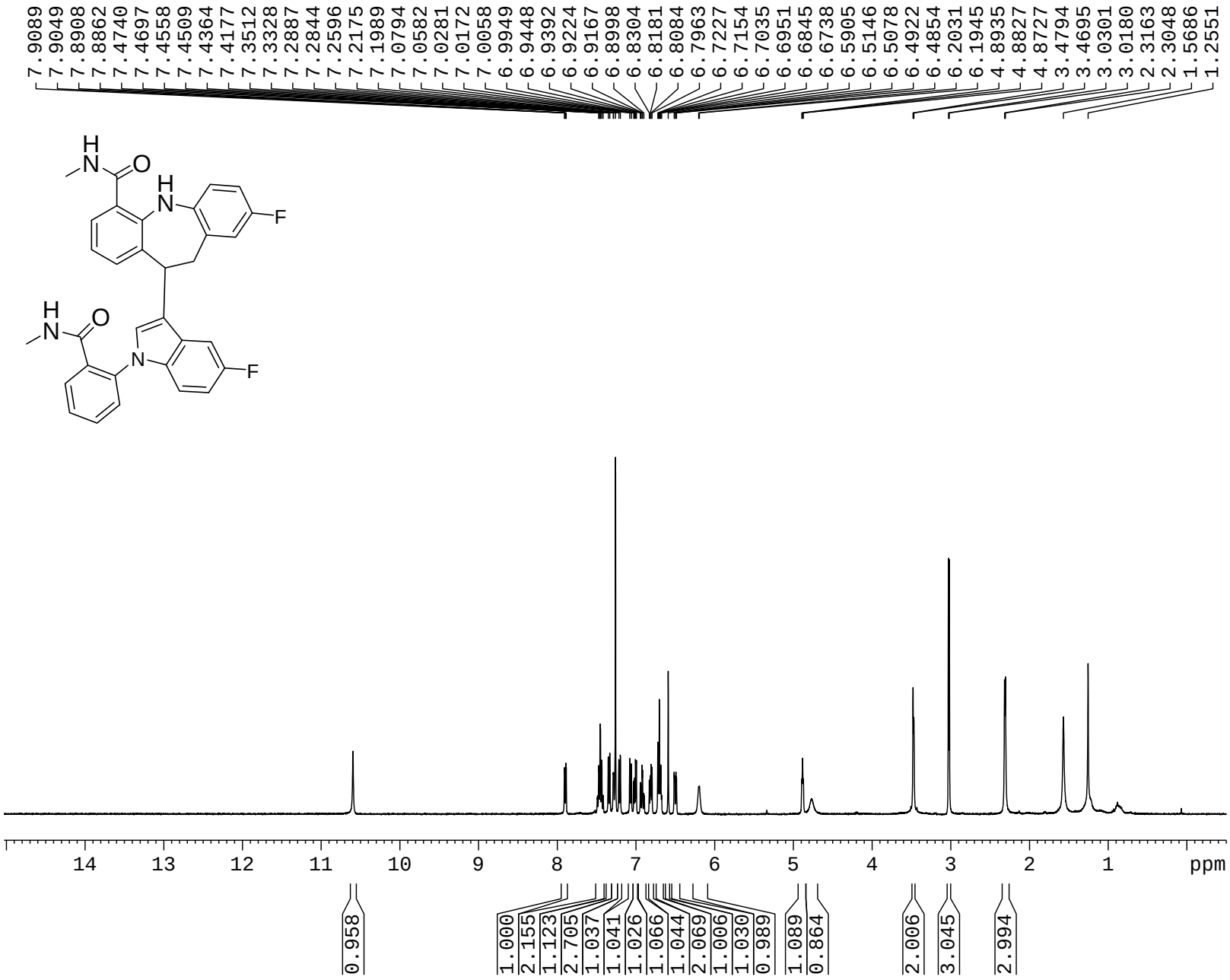
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 13.95 dB
PL13 17.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127514 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1H NMR of 8-Fluoro-11-(5-fluoro-1-(2-(methylcarbamoyl)phenyl)-1H-indol-3-yl)-N-methyl-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (14b)

5-F



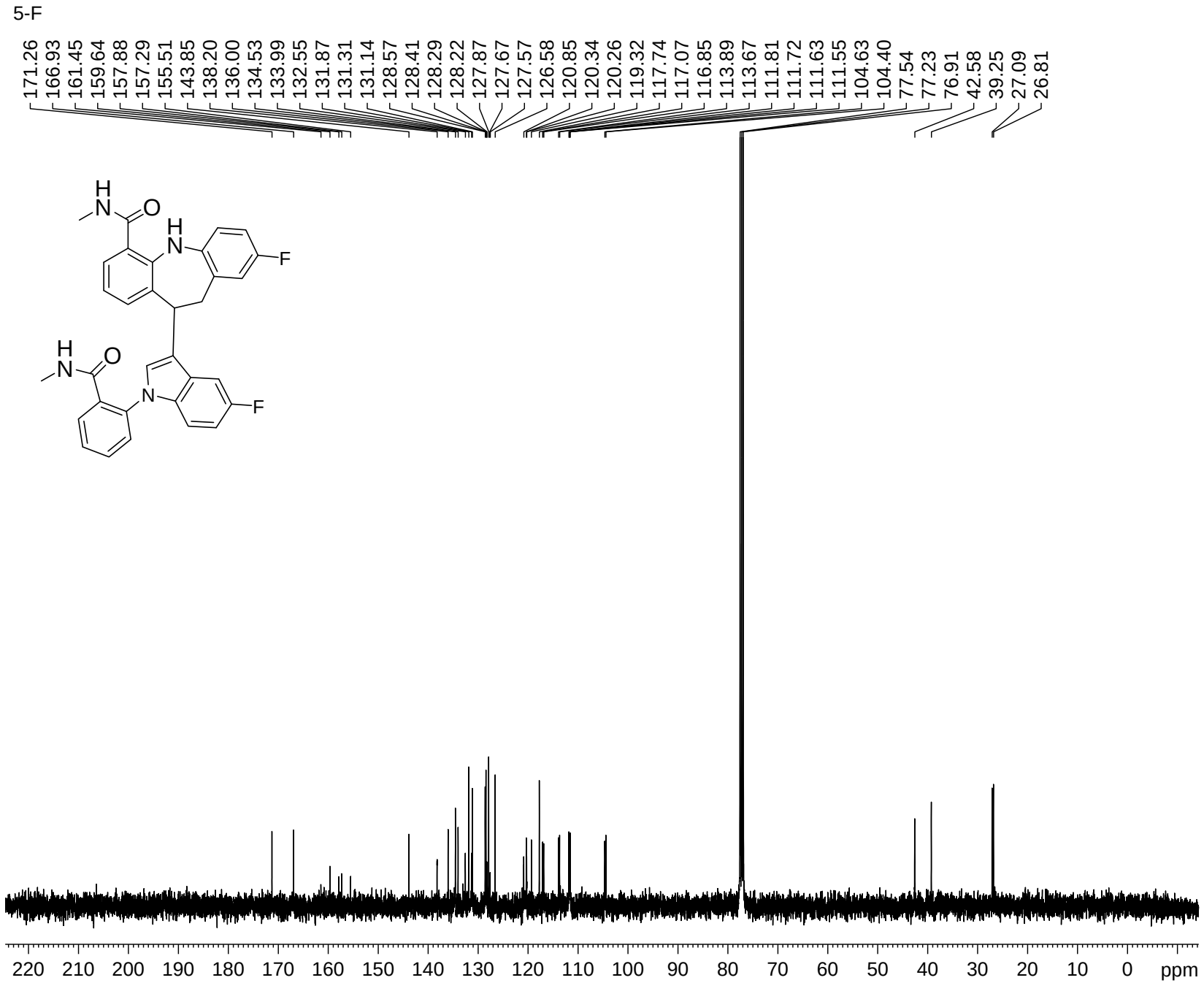
Current Data Parameters
NAME try
EXPNO 444
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140915
Time 14.45
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 256
DW 69.000 usec
DE 6.50 usec
TE 300.6 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

13C NMR of 8-Fluoro-11-(5-fluoro-1-(2-(methylcarbamoyl)phenyl)-1H-indol-3-yl)-N-methyl-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (14b)



Current Data Parameters
NAME try
EXPNO 322
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140514
Time 22.12
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 298.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

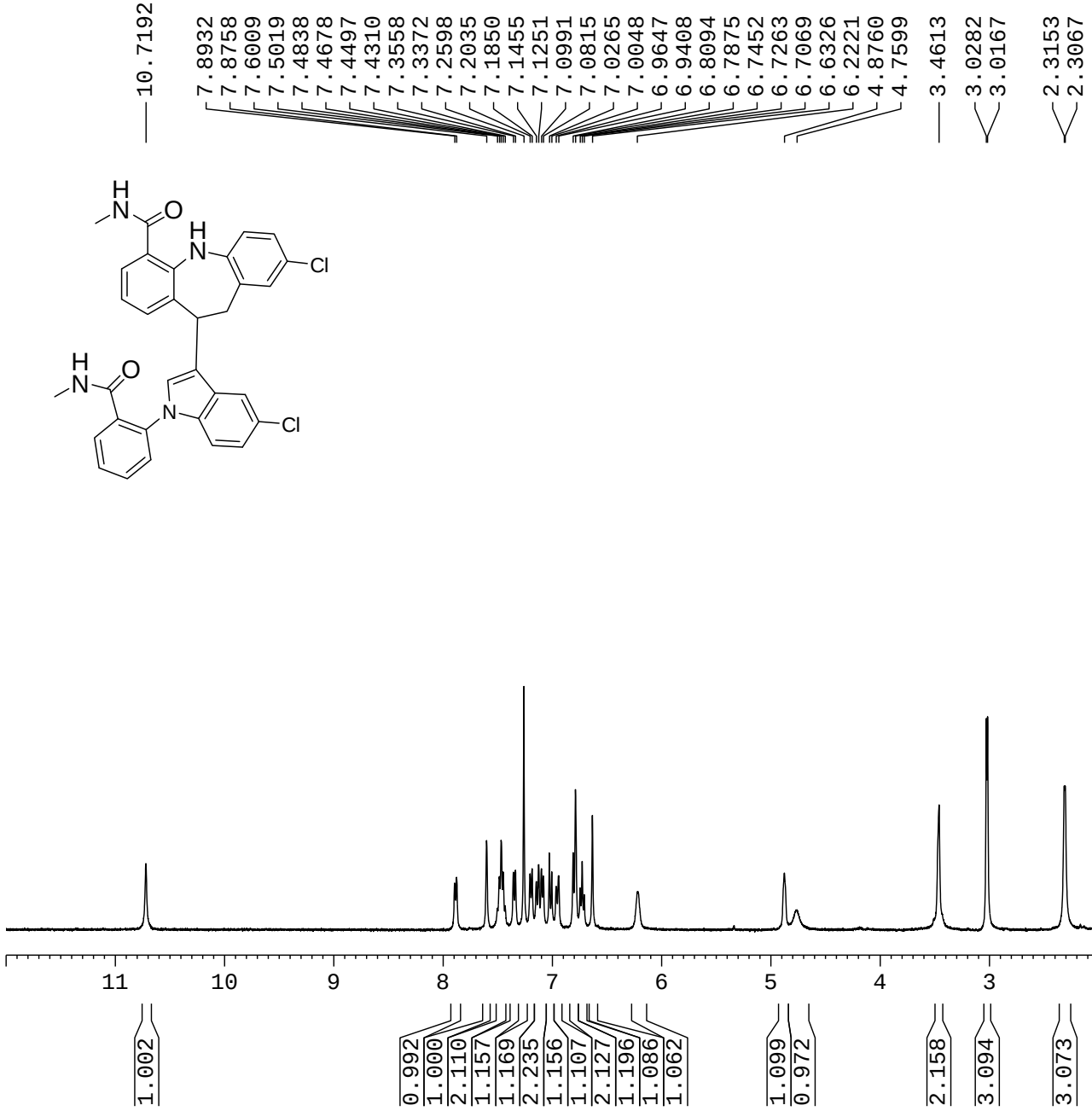
======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
PL1 7.30 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.20 dB
PL12 13.10 dB
PL13 16.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127467 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1H NMR of 8-Chloro-11-(5-chloro-1-(2-(methylcarbamoyl)phenyl)-1H-indol-3-yl)-N-methyl-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (15b)

5-cl



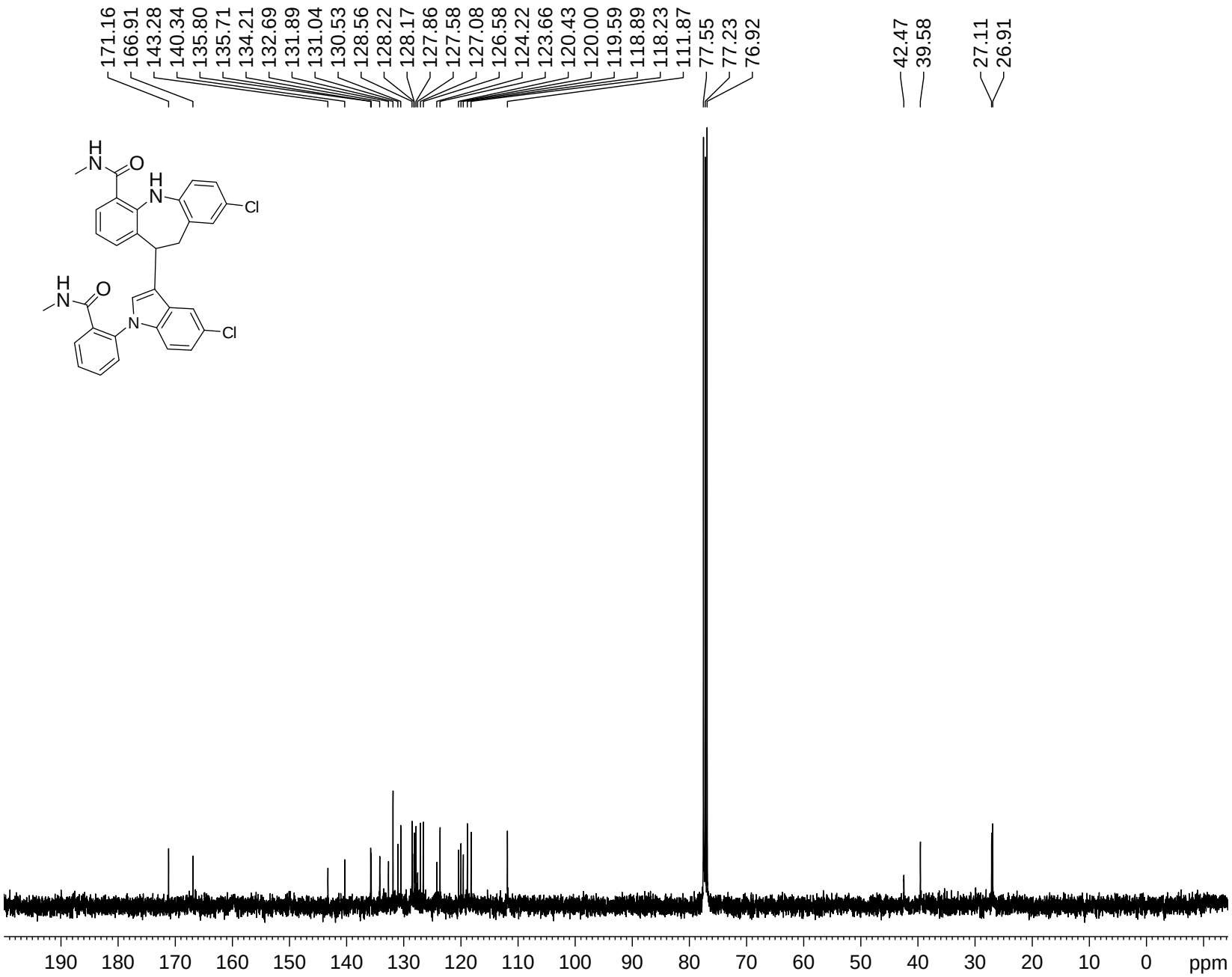
NAME	try
EXPNO	450
PROCNO	1
Date_	20140915
Time	20.50
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	7246.377 Hz
FIDRES	0.221142 Hz
AQ	2.2611110 sec
RG	256
DW	69.000 usec
DE	6.50 usec
TE	300.5 K
D1	2.00000000 sec
TD0	1

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

NUC1	1H
P1	15.00 usec
PL1	-5.85 dB
SFO1	400.1324008 MHz
SI	16384
SF	400.1300096 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

13C NMR of 8-Chloro-11-(5-chloro-1-(2-(methylcarbamoyl)phenyl)-1H-indol-3-yl)-N-methyl-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (15b)

13c of 5-cl indole with bf3.oet



Current Data Parameters
NAME try
EXPNO 45
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140111
Time 1.44
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 385
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 295.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

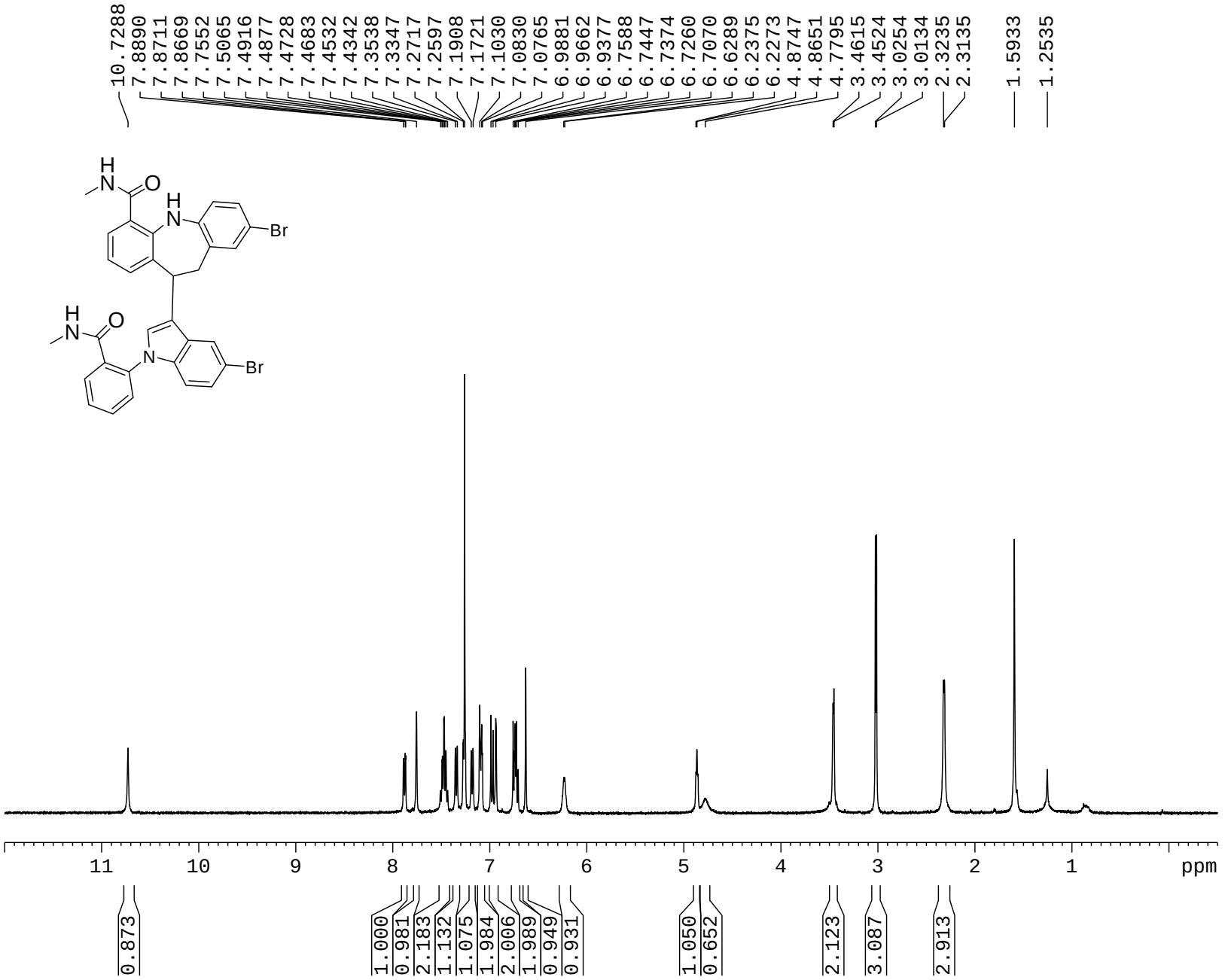
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.00 dB
PL12 20.70 dB
PL13 23.70 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127499 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1H NMR of 8-Bromo-11-(5-bromo-1-(2-(methylcarbamoyl)phenyl)-1H-indol-3-yl)-N-methyl-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (16b)

1H of 5-Bromo indole with bf3.oet



Current Data Parameters
NAME try
EXPNO 20
PROCNO 1

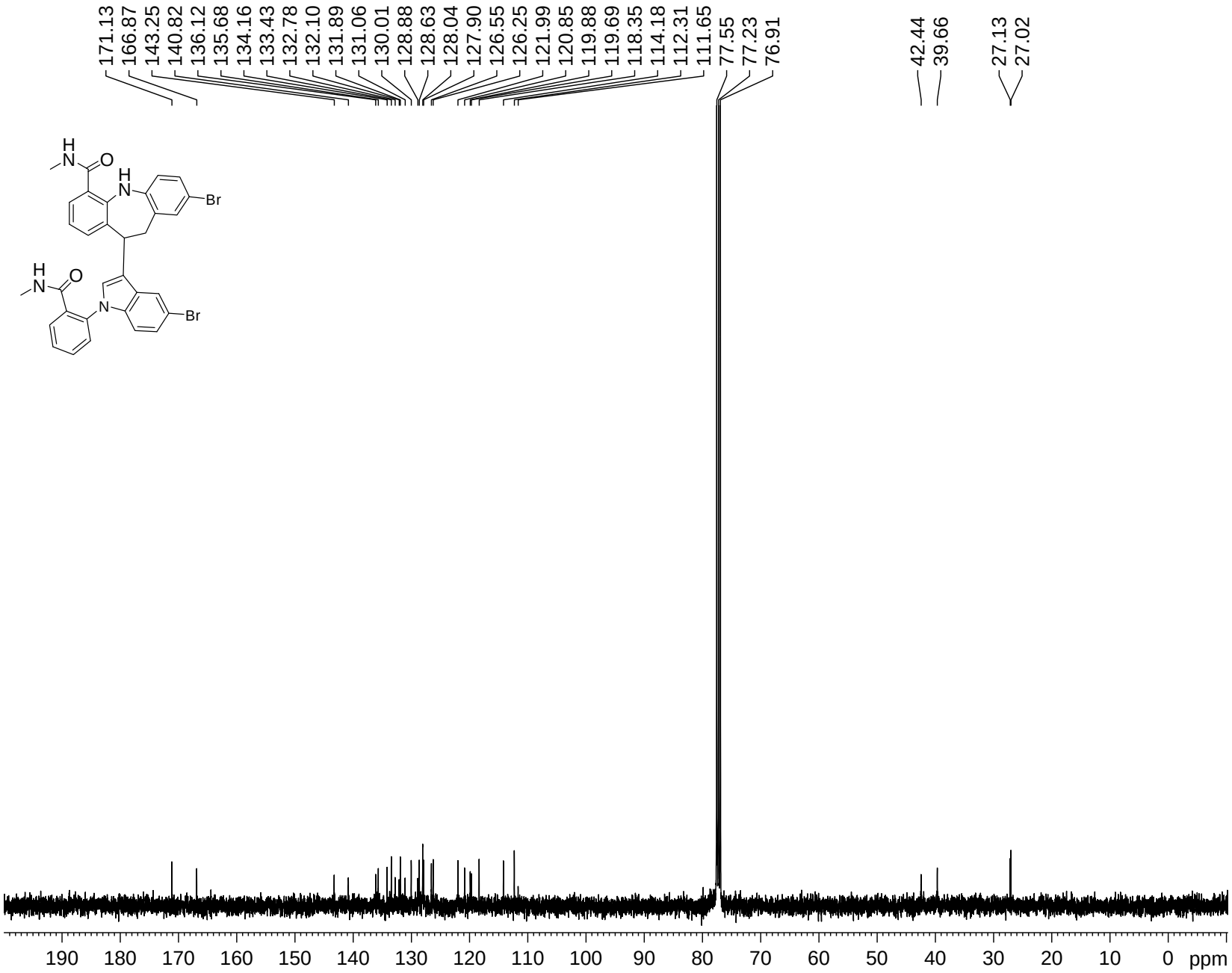
F2 - Acquisition Parameters
Date_ 20140108
Time 16.42
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 362
DW 69.000 usec
DE 6.50 usec
TE 297.1 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.90 usec
PL1 3.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

13C NMR of 8-Bromo-11-(5-bromo-1-(2-(methylcarbamoyl)phenyl)-1H-indol-3-yl)-N-methyl-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (16b)

13c of 5-Bromo indole with bf3.oet



Current Data Parameters
NAME try
EXPNO 24
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140109
Time 12.50
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 750
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 296.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

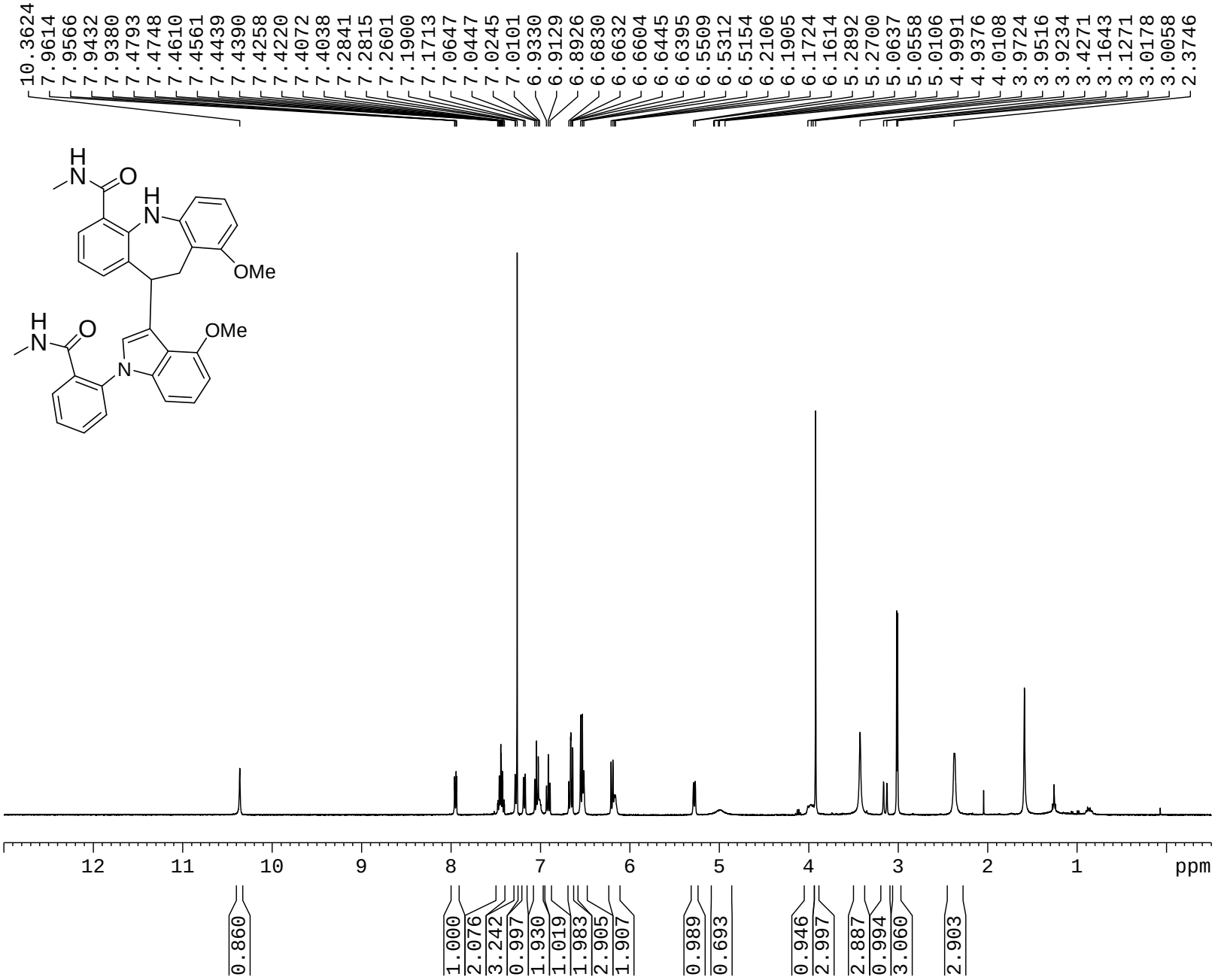
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.00 dB
PL12 20.70 dB
PL13 23.70 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1H NMR of 9-methoxy-11-(4-methoxy-1-(2-(methylcarbamoyl)phenyl)-1H-indol-3-yl)-N-methyl-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (17b)

4-ome



Current Data Parameters
NAME try
EXPNO 164
PROCNO 1

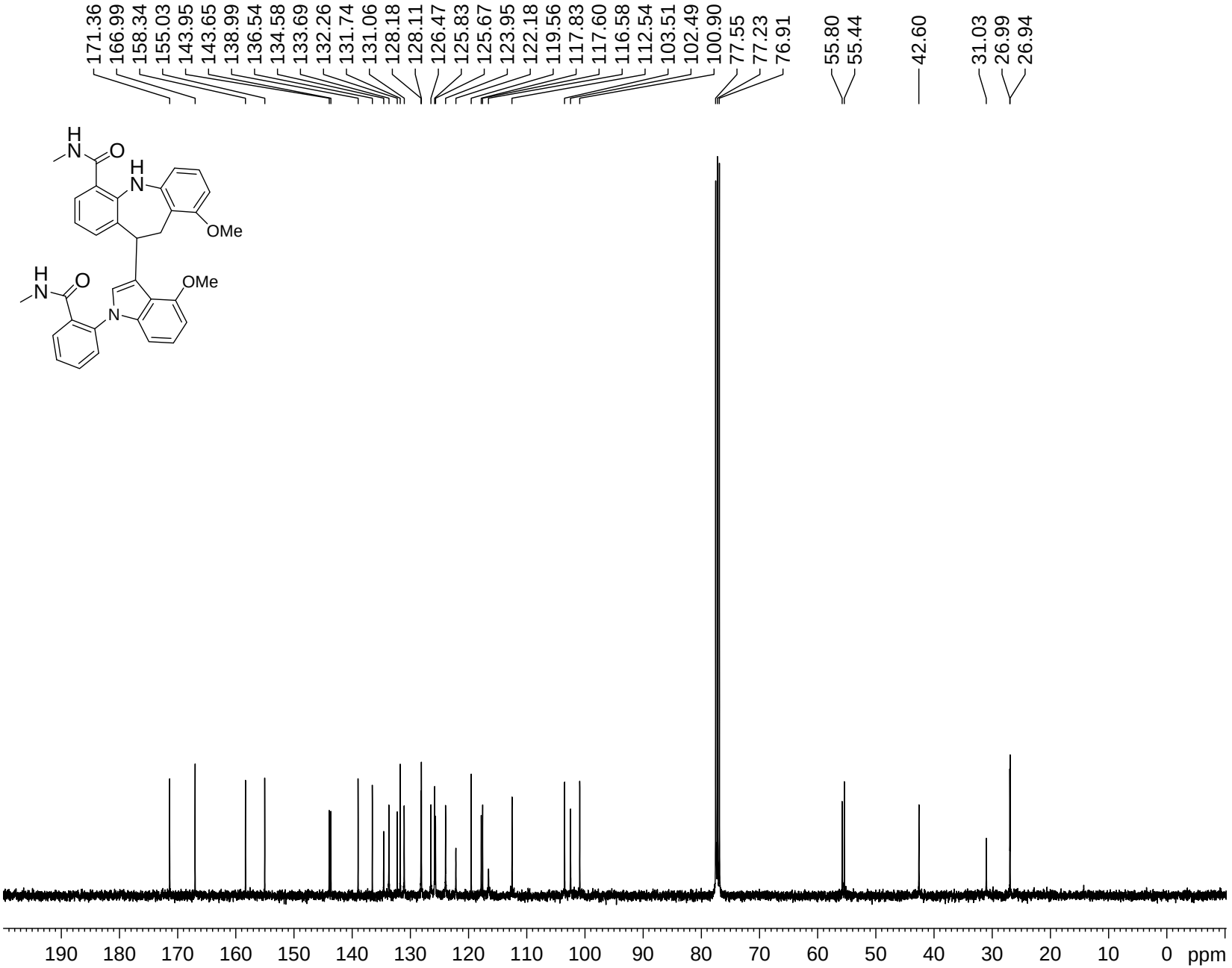
F2 - Acquisition Parameters
Date_ 20140220
Time 17.26
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 256
DW 69.000 usec
DE 6.50 usec
TE 297.3 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.35 usec
PL1 -2.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

13C NMR of 9-methoxy-11-(4-methoxy-1-(2-(methylcarbamoyl)phenyl)-1H-indol-3-yl)-N-methyl-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (17b)

13c of 4ome indole



Current Data Parameters
NAME try
EXPNO 139
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140131
Time 17.25
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 504
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 299.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

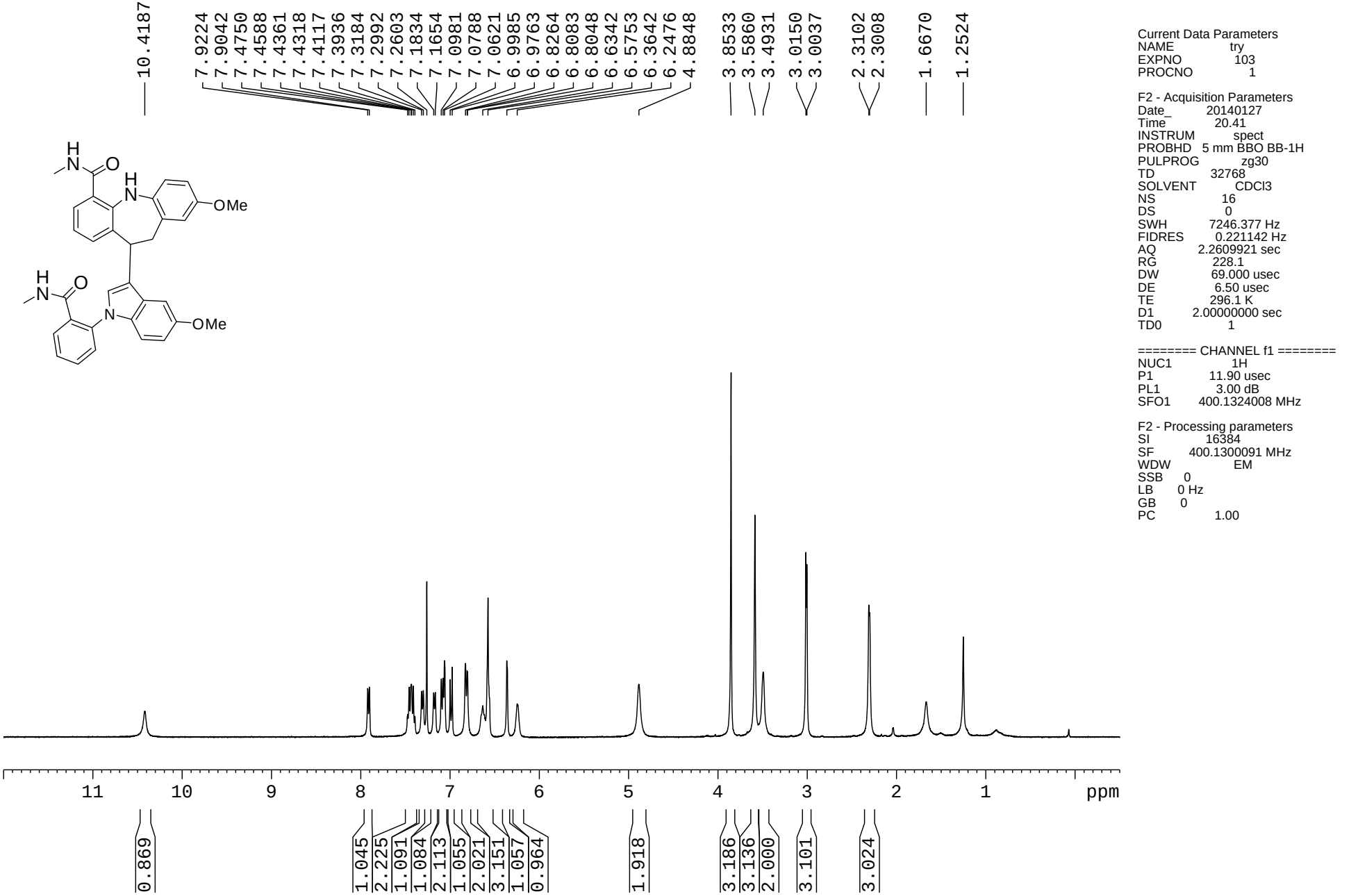
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.00 dB
PL12 20.70 dB
PL13 23.70 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127543 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1H NMR of 8-Methoxy-11-(5-methoxy-1-(2-(methylcarbamoyl)phenyl)-1H-indol-3-yl)-N-methyl-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (18b)

1h of 5methoxy indole



Current Data Parameters
NAME try
EXPNO 103
PROCNO 1

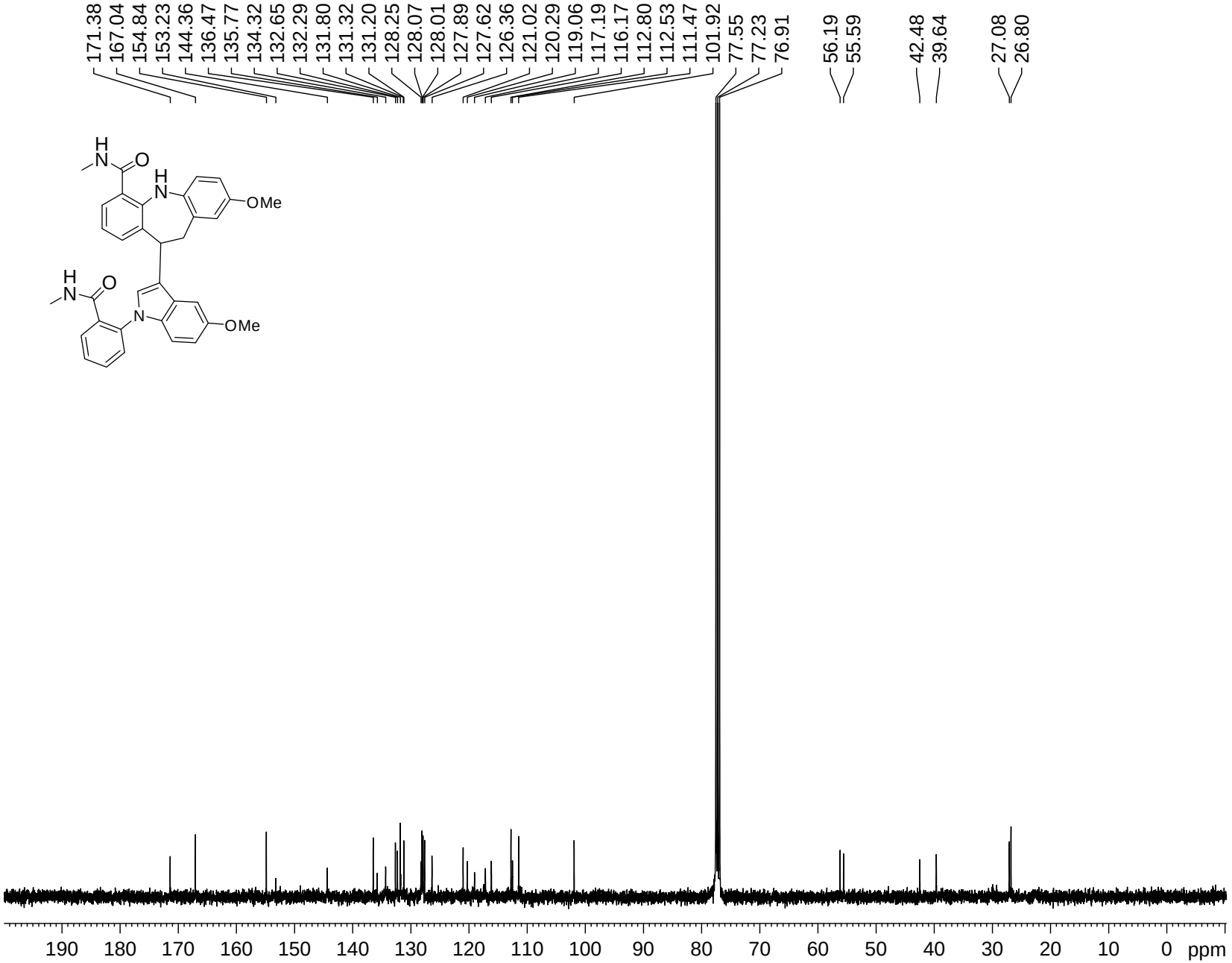
F2 - Acquisition Parameters
Date_ 20140127
Time 20.41
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 228.1
DW 69.000 usec
DE 6.50 usec
TE 296.1 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.90 usec
PL1 3.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

13C NMR of 8-Methoxy-11-(5-methoxy-1-(2-(methylcarbamoyl)phenyl)-1H-indol-3-yl)-N-methyl-10,11-dihydro-5H-dibenzo[b,f]azepine-4-carboxamide (18b)

13c of 5-ome indole



Current Data Parameters
NAME try
EXPNO 135
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140131
Time 16.07
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 298.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

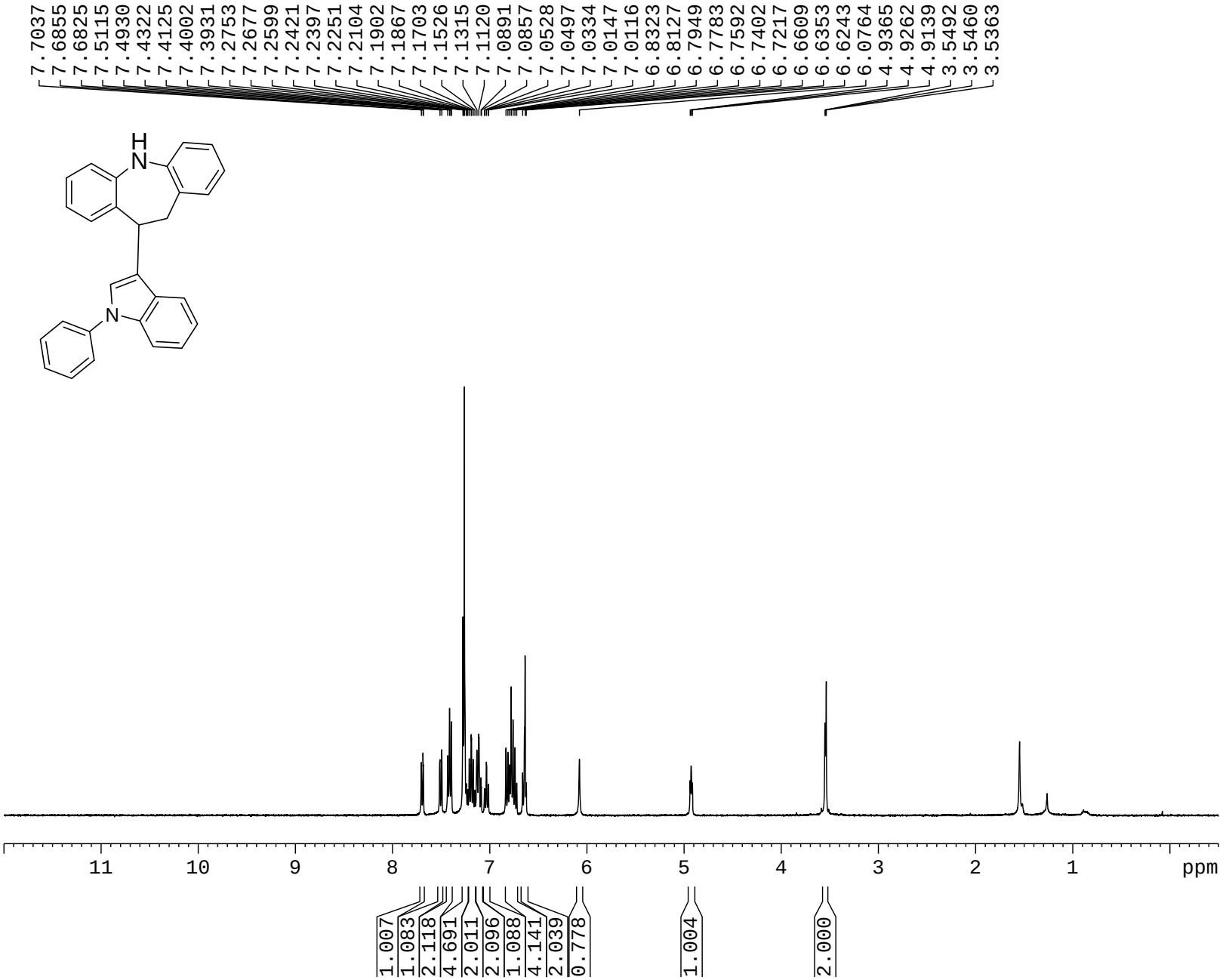
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.00 dB
PL12 20.70 dB
PL13 23.70 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1H NMR of 10-(1-Phenyl-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine (19b)

1H of N-phenyl indole with bf3.oet



Current Data Parameters
NAME try
EXPNO 15
PROCNO 1

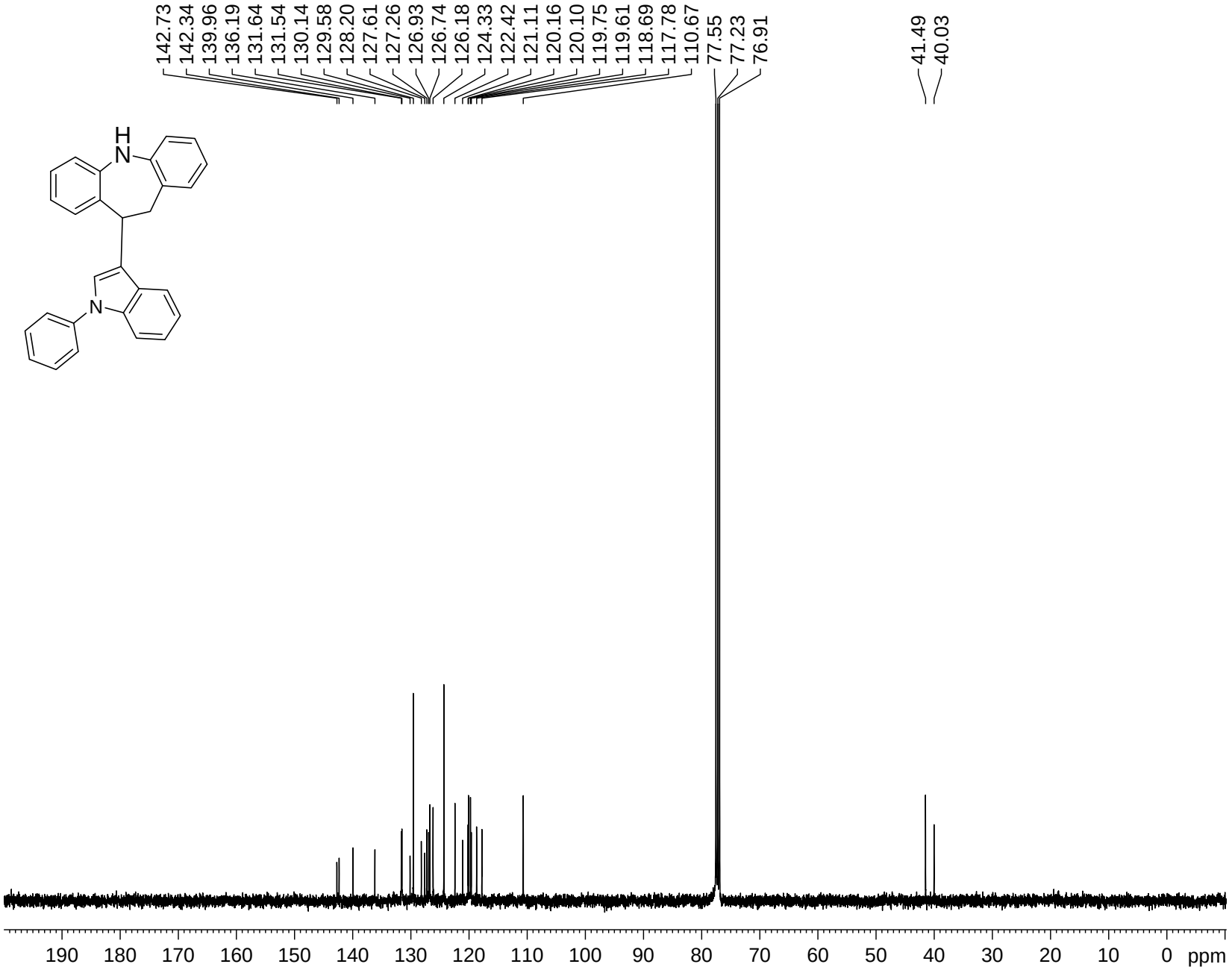
F2 - Acquisition Parameters
Date_ 20140106
Time 15.50
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 362
DW 69.000 usec
DE 6.50 usec
TE 296.6 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.90 usec
PL1 3.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

13C NMR of 10-(1-Phenyl-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine (19b)

13c of N-ph indole



Current Data Parameters
NAME try
EXPNO 72
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140118
Time 3.04
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 544
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 295.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

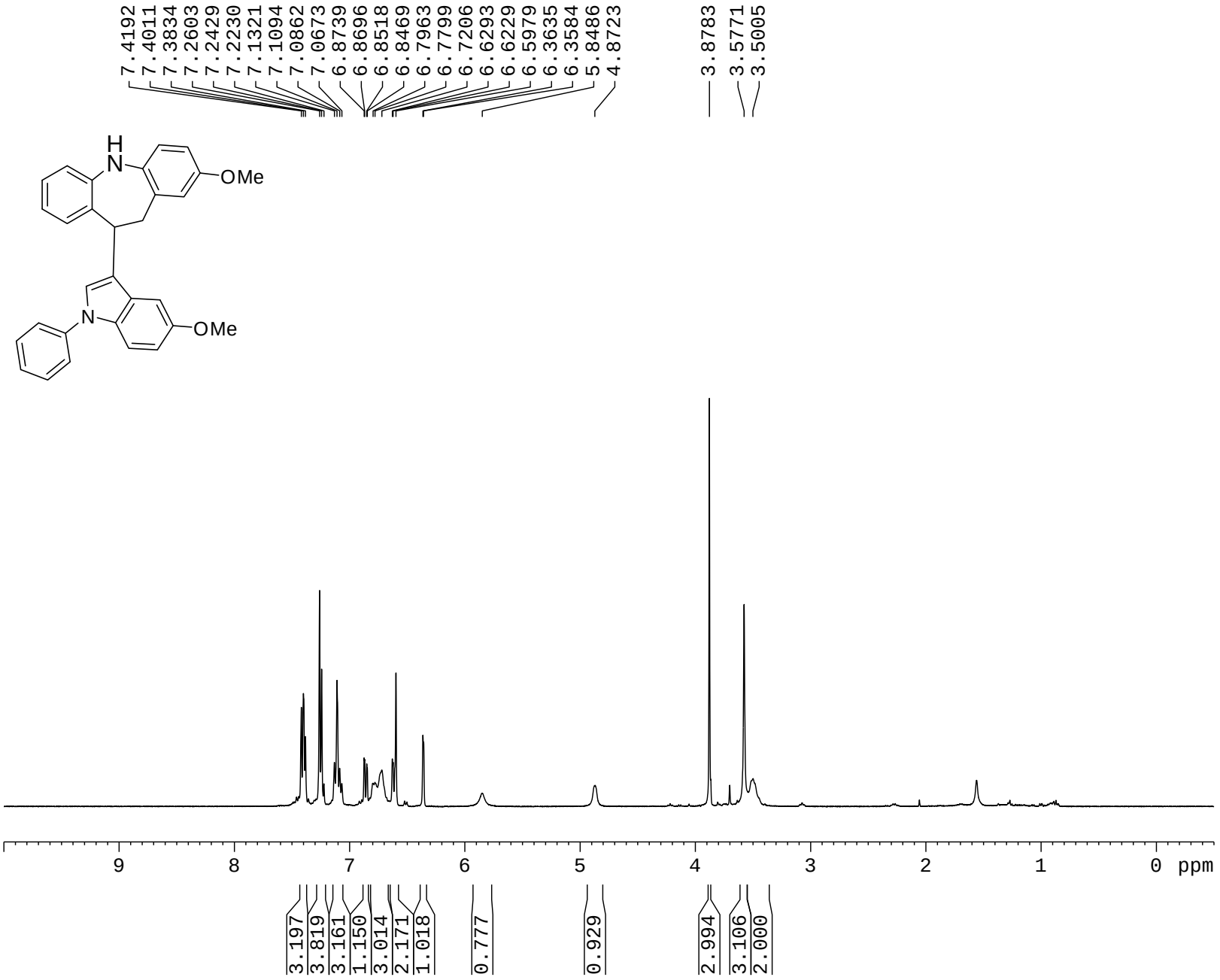
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.00 dB
PL12 20.70 dB
PL13 23.70 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127506 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1H NMR of 2-Methoxy-10-(5-methoxy-1-phenyl-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine (20b)

5-ome n-ph indole lowerr prod



Current Data Parameters
NAME try
EXPNO 250
PROCNO 1

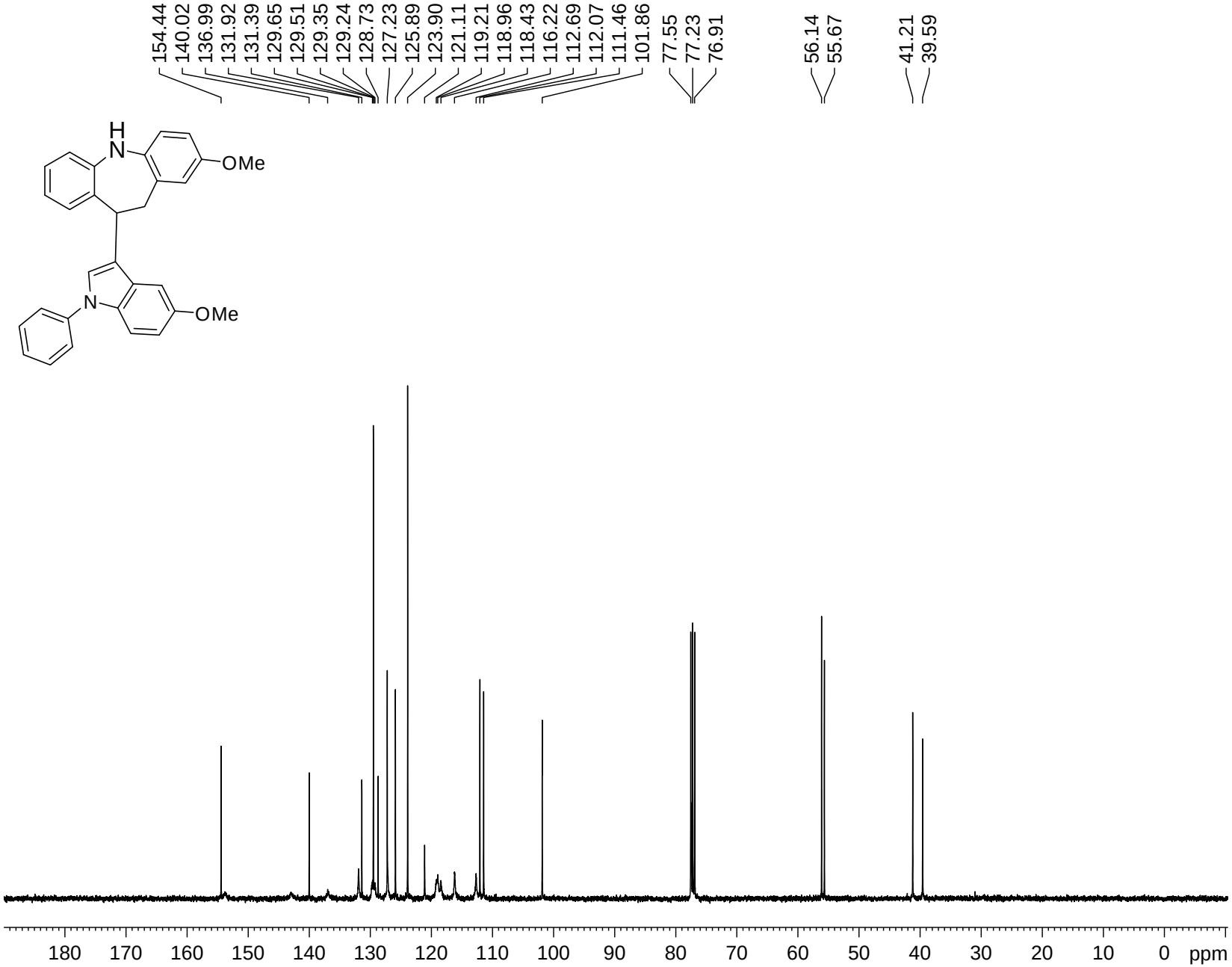
F2 - Acquisition Parameters
Date_ 20140411
Time 20.58
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 181
DW 69.000 usec
DE 6.50 usec
TE 300.2 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.35 usec
PL1 -2.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

13C NMR of 2-Methoxy-10-(5-methoxy-1-phenyl-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine (20b)

13c of 5-ome N-ph indole wt bf3 pure



Current Data Parameters
NAME try
EXPNO 277
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140419
Time 22.16
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1055
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

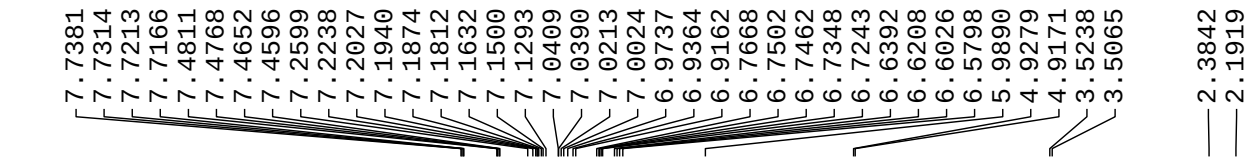
======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
PL1 7.30 dB
SFO1 100.6233325 MHz

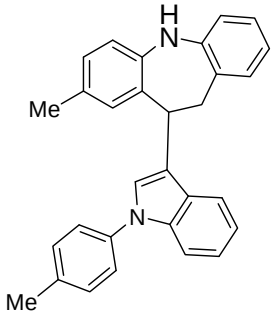
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.20 dB
PL12 13.10 dB
PL13 16.10 dB
SFO2 400.1316005 MHz

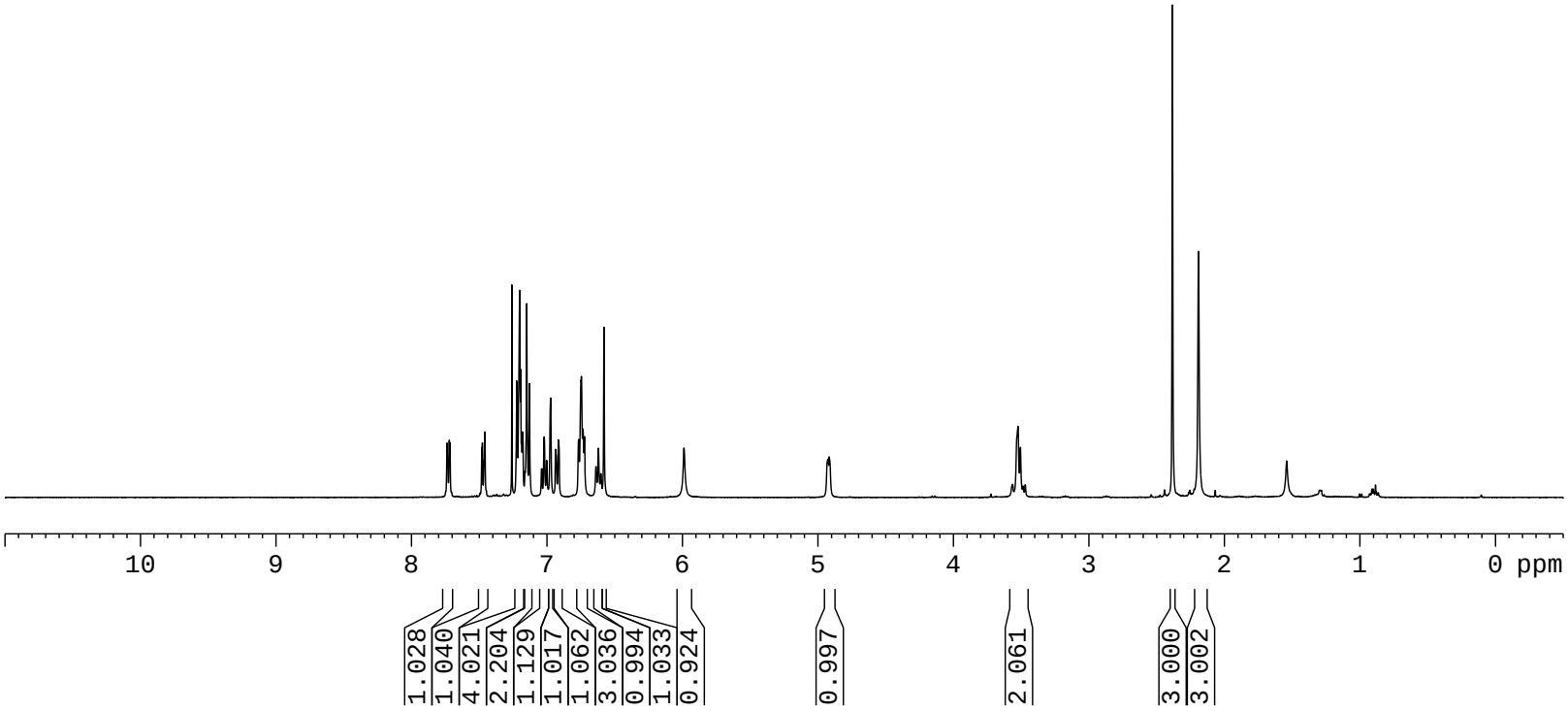
F2 - Processing parameters
SI 32768
SF 100.6127646 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1H NMR of 2-Methyl-11-(1-p-tolyl-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine (21b)

p-me N-ph indole wt bf3 pure







Current Data Parameters
NAME try
EXPNO 278
PROCNO 1

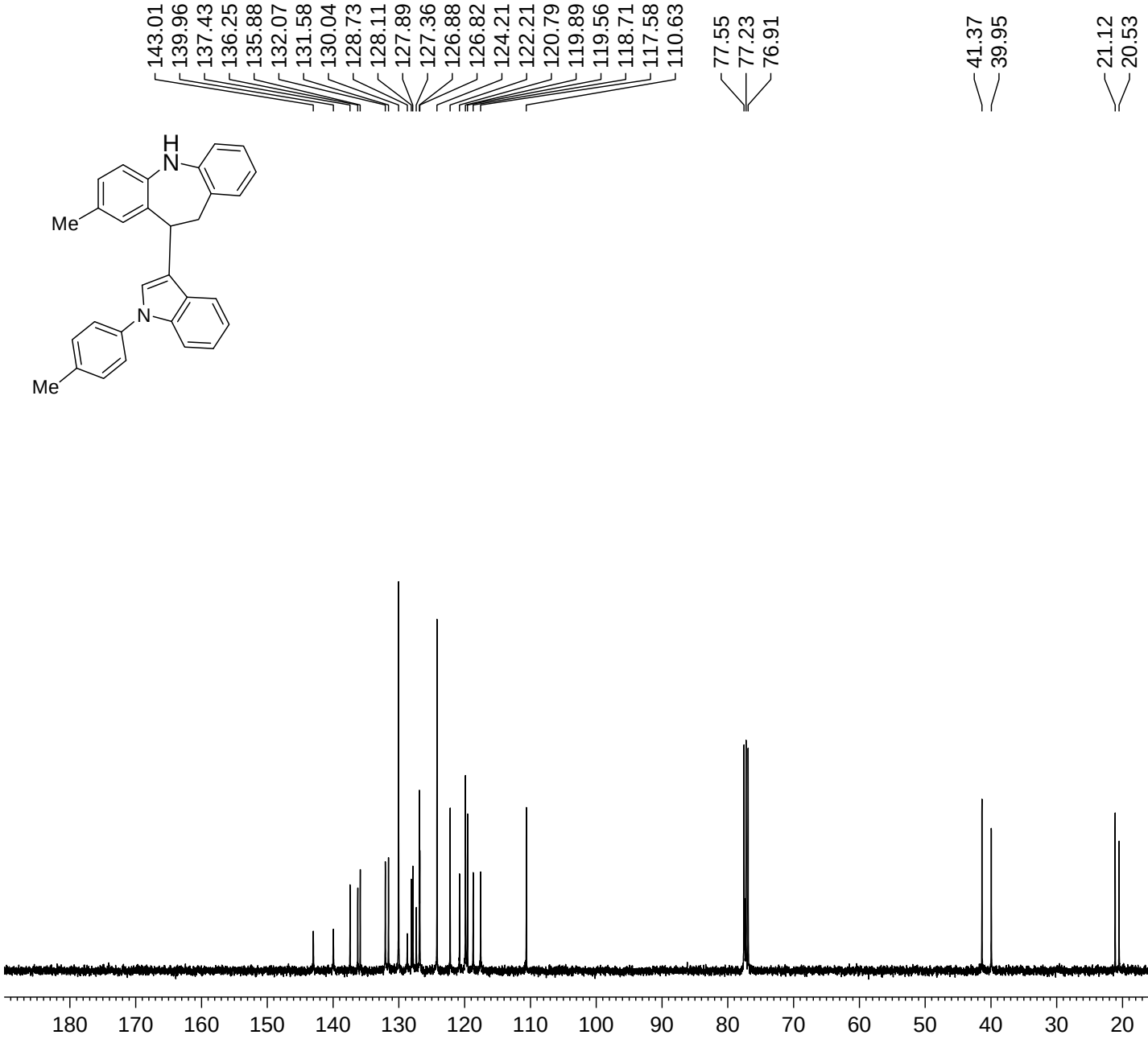
F2 - Acquisition Parameters
Date_ 20140419
Time 23.27
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 114
DW 69.000 usec
DE 6.50 usec
TE 299.9 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -4.20 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

13C NMR of 2-Methyl-11-(1-p-tolyl-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine (21b)

13c of p-me N-ph indole wt bf3 pure



Current Data Parameters
NAME try
EXPNO 273
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140419
Time 14.49
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 236
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

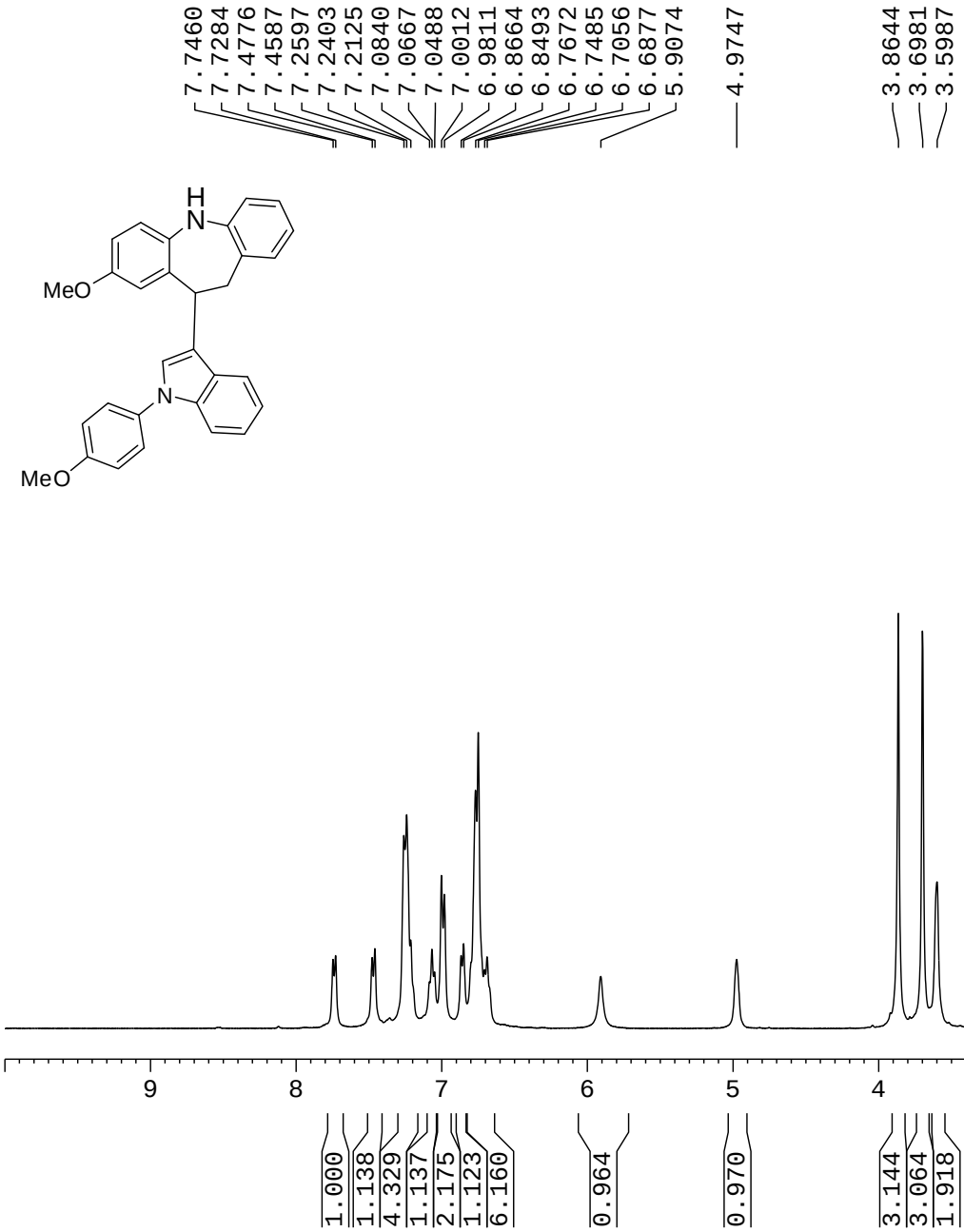
======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
PL1 7.30 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.20 dB
PL12 13.10 dB
PL13 16.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127661 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1H NMR of 2-Methoxy-11-(1-(4-methoxyphenyl)-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine (22b)

4-ome n-ph indole lower spot



Current Data Parameters
NAME try
EXPNO 252
PROCNO 1

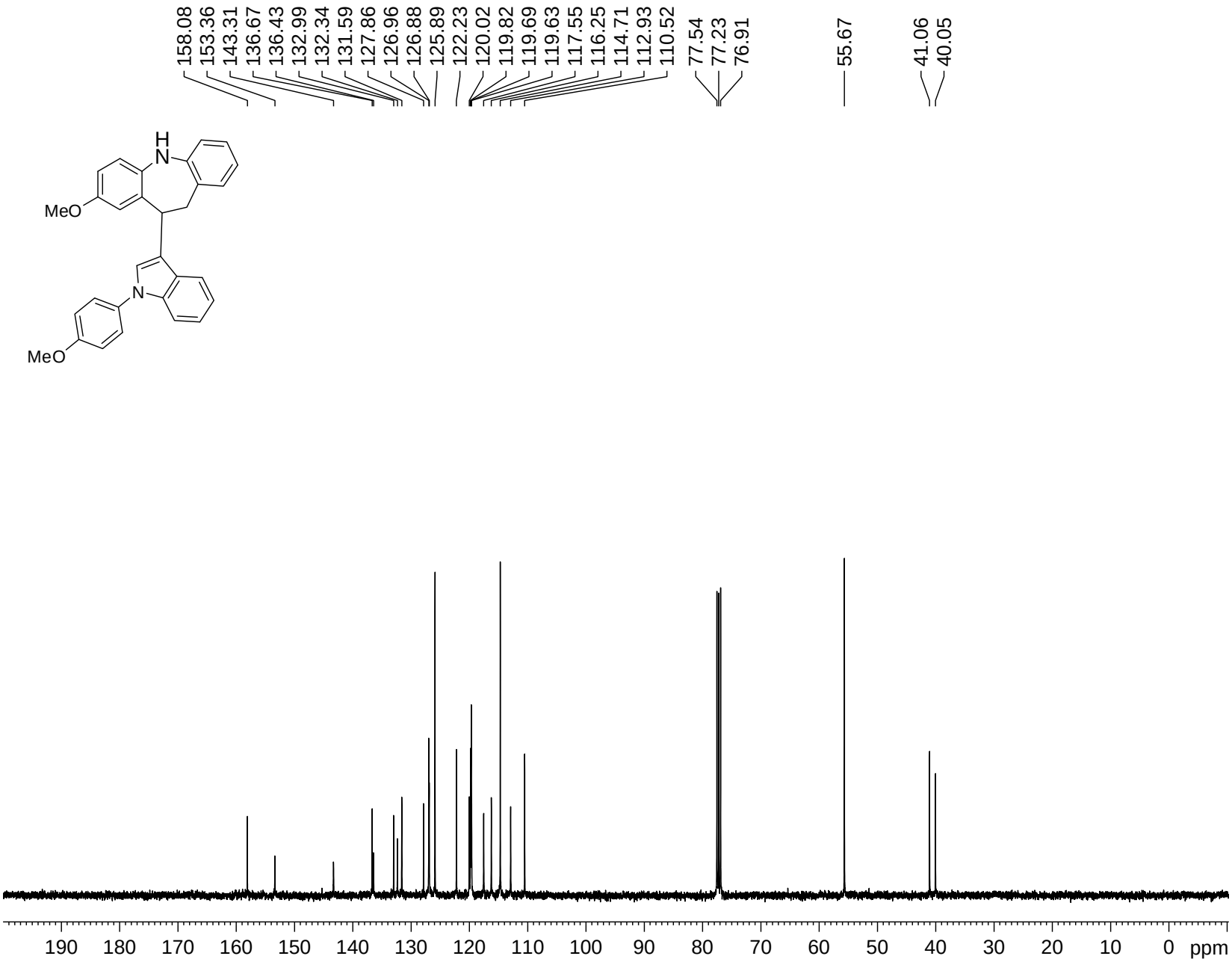
F2 - Acquisition Parameters
Date_ 20140411
Time 21.40
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 40.3
DW 69.000 usec
DE 6.50 usec
TE 300.3 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.35 usec
PL1 -2.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

13C NMR of 2-Methoxy-11-(1-(4-methoxyphenyl)-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine (22b)

13c of 4-ome n-ph indole



Current Data Parameters
NAME try
EXPNO 253
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140411
Time 21.42
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 235
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 300.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

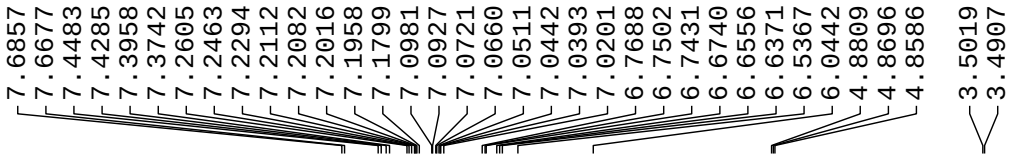
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

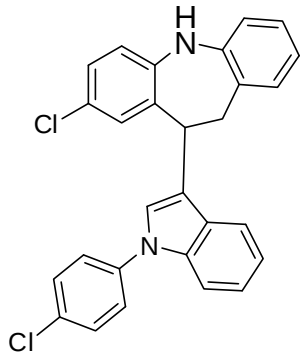
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 13.95 dB
PL13 17.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127617 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1H NMR of 2-Chloro-11-(1-(4-chlorophenyl)-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine (23b)

p-cl n-ph indole



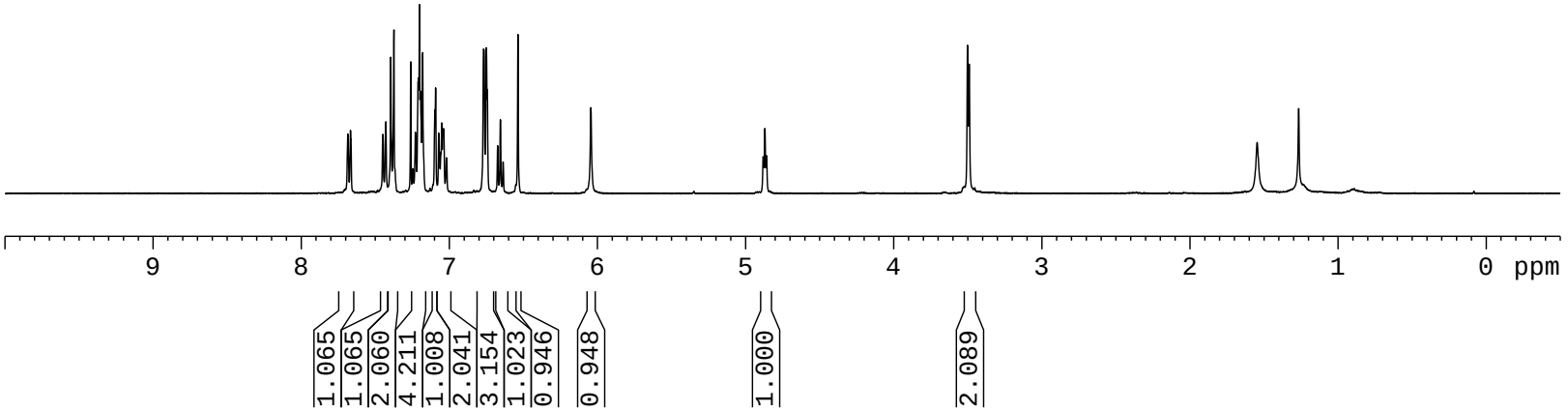


Current Data Parameters
NAME try
EXPNO 440
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140915
Time 11.19
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 181
DW 69.000 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

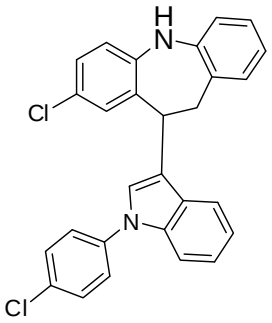
F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

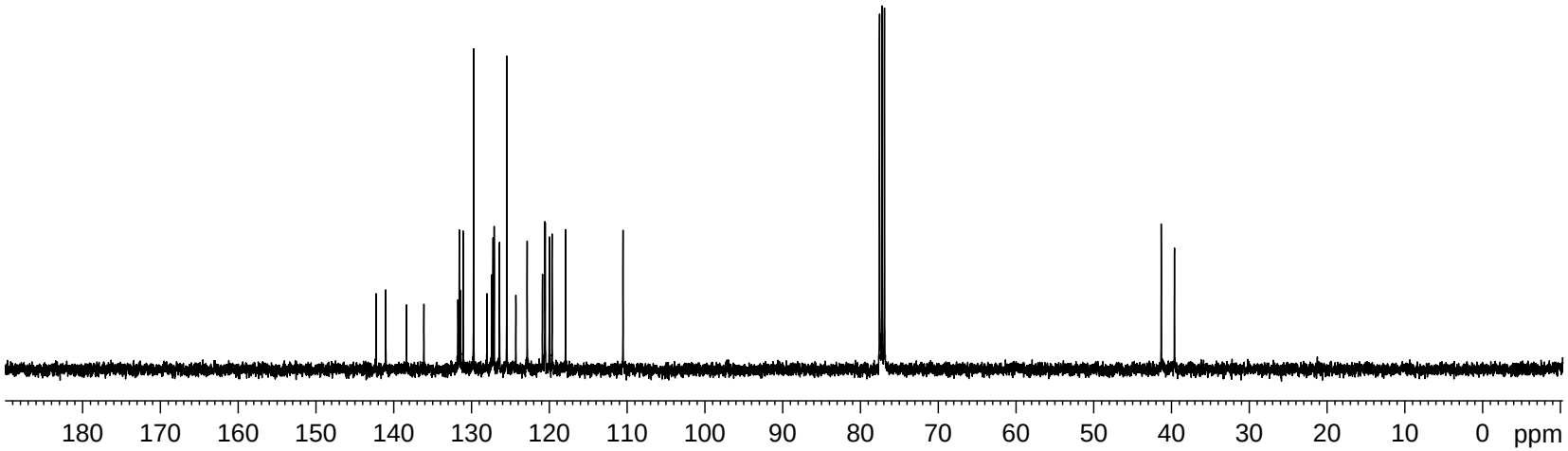


13C NMR of 2-Chloro-11-(1-(4-chlorophenyl)-1H-indol-3-yl)-10,11-dihydro-5H-dibenzo[b,f]azepine (23b)

13c of p-cl N-ph indloe wt bf3 pure

142.28 141.03 138.37 136.12 131.75 131.58 131.42 131.09 129.74 128.03 127.42 127.24 127.09 126.41 125.48 124.30 122.85 120.88 120.58 120.53 120.00 119.65 117.91 110.53 77.55 77.23 76.91 41.32 39.62





Current Data Parameters
NAME try
EXPNO 287
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140423
Time 20.45
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 227
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 299.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
PL1 7.30 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.20 dB
PL12 13.10 dB
PL13 16.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127543 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00