Enantioselective and Rapid Rh-catalyzed Arylation of *N*-Tosyl and *N*-Nosyl Aldimines in Methanol

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Supporting Information:

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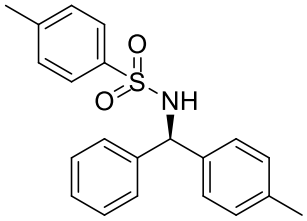
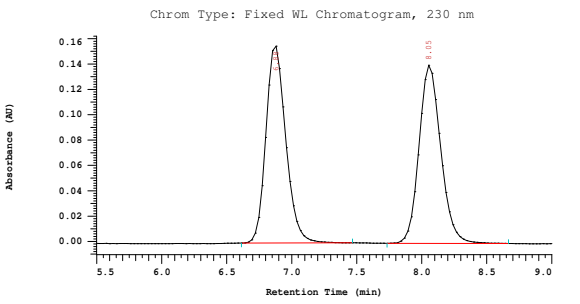
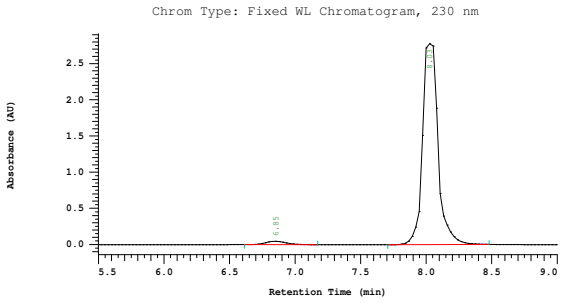


(*R*)-4-methyl-*N*-(phenyl(*p*-tolyl)methyl)benzenesulfonamide (5aa)[1]



No.	RT	Area	Conc 1	BC
1	6.88	825440	50.258	MC
2	8.05	816960	49.742	MC
		1642400	100.000	



No.	RT	Area	Conc 1	BC
1	6.85	256520	2.188	BB
2	8.03	11468100	97.812	BB
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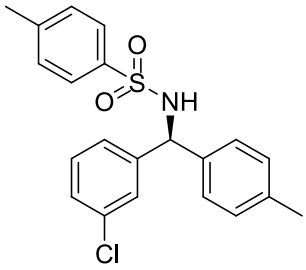
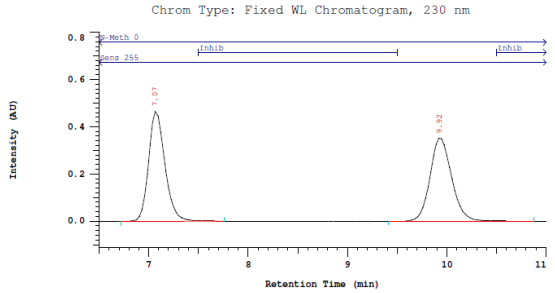


(*S*)-*N*-((3-chlorophenyl)(*p*-tolyl)methyl)-4-methylbenzenesulfonamide (5ba)



No.	RT	Area	Conc 1	BC
1	7.07	2669540	50.100	MC
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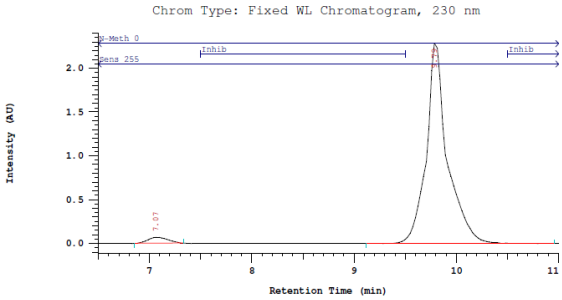
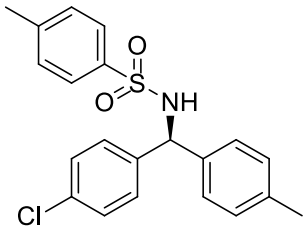
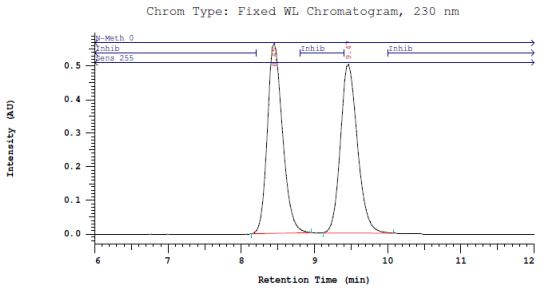
		5328460	100.000	



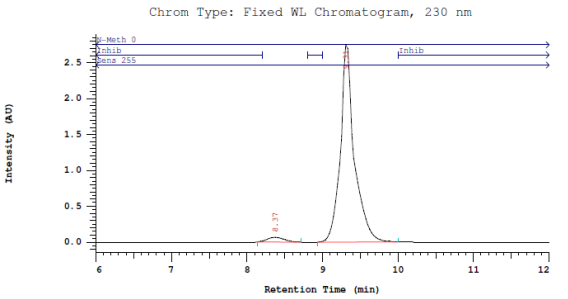
No.	RT	Area	Conc 1	BC
1	7.07	460080	2.738	MC
2	9.79	16341480	97.262	MC
		16801560	100.000	



(*S*)-*N*-((4-chlorophenyl)(*p*-tolyl)methyl)-4-methylbenzenesulfonamide (5ca)[2]



No.	RT	Area	Conc 1	BC
1	8.45	4088080	50.060	MC
2	9.47	4078200	49.940	MC
		8166280	100.000	



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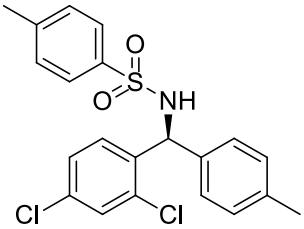
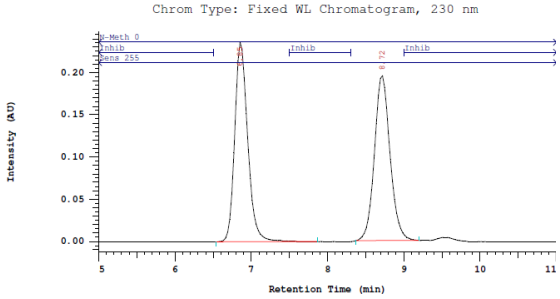
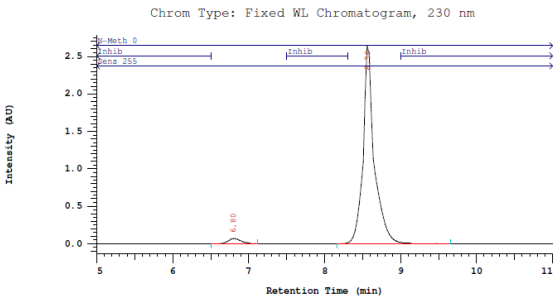
2	9.31	17584320	97.105	MC
		18108520	100.000	



(*S*)-*N*-((2,4-dichlorophenyl)(*p*-tolyl)methyl)-4-methylbenzenesulfonamide (5da)



No.	RT	Area	Conc 1	B
1	6.85	1387040	49.964	M
2	8.72	1389020	50.036	M
		2776060	100.000	



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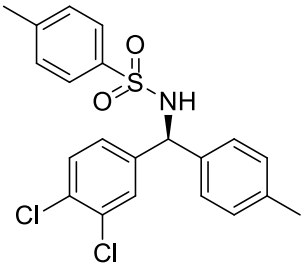
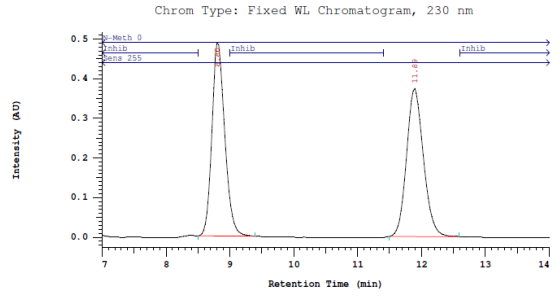
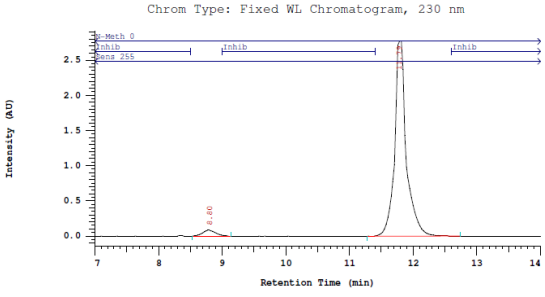
		14114020	100.000	



(*S*)-*N*-((3,4-dichlorophenyl)(*p*-tolyl)methyl)-4-methylbenzenesulfonamide (5ea)



No.	RT	Area	Conc 1	BC
1	8.80	3426960	49.903	MC
2	11.89	3440240	50.097	MC
		6867200	100.000	



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1	8.80	578360	3.158	MC
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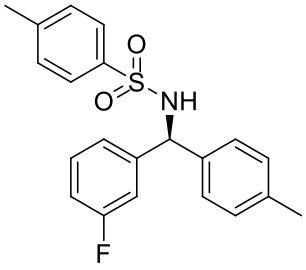
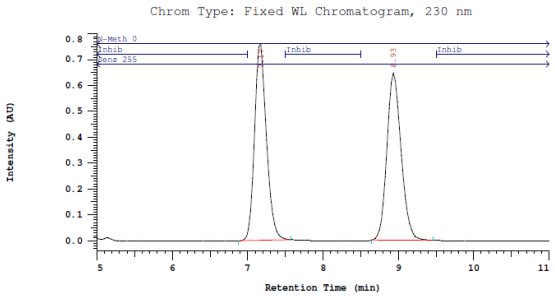
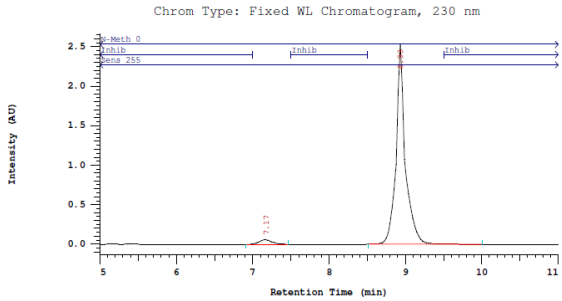
		18312539	100.000	



(*S*)-*N*-((3-fluorophenyl)(*p*-tolyl)methyl)-4-methylbenzenesulfonamide (5fa)



No.	RT	Area	Conc 1	BC
1	7.17	4189080	49.923	MC
2	8.93	4201940	50.077	MC
		8391020	100.000	



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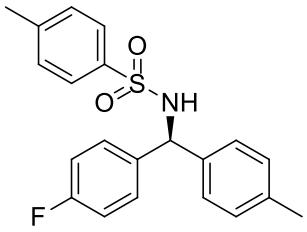
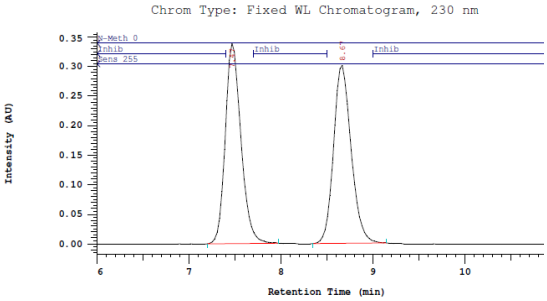
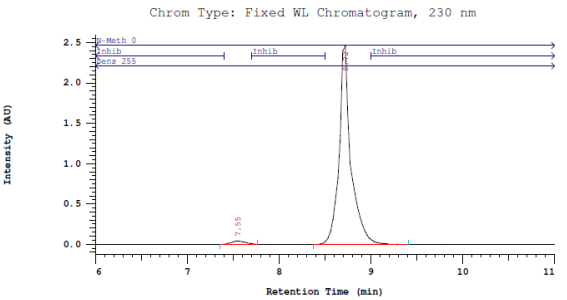
1	7.17	321580	2.955	MC
2	8.93	10561640	97.045	MC
		10883220	100.000	



(*S*)-*N*-((4-fluorophenyl)(*p*-tolyl)methyl)-4-methylbenzenesulfonamide (5ga)[2]



No.	RT	Area	Conc 1
1	7.47	1994220	50.008
2	8.67	1993600	49.992
		3987820	100.000



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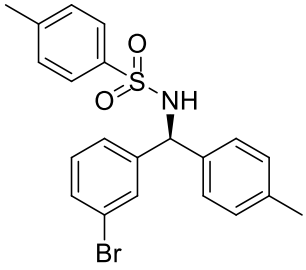
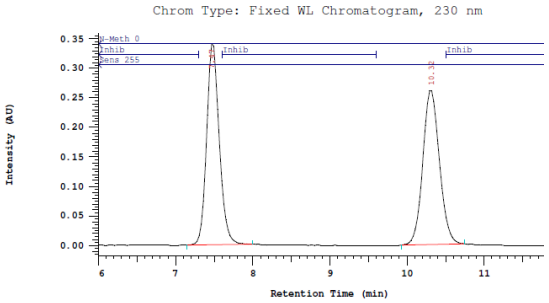
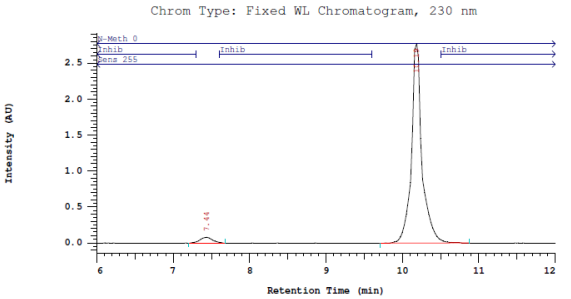
2	8.72	11006080	98.086	MC
		11220840	100.000	



(*S*)-*N*-((3-bromophenyl)(*p*-tolyl)methyl)-4-methylbenzenesulfonamide (5ha)



No.	RT	Area	Conc 1	B
1	7.47	1946160	49.983	M
2	10.32	1947500	50.017	M
		3893660	100.000	



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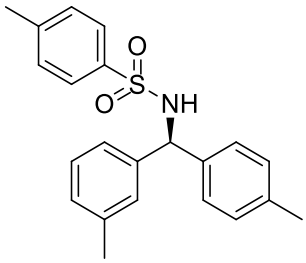
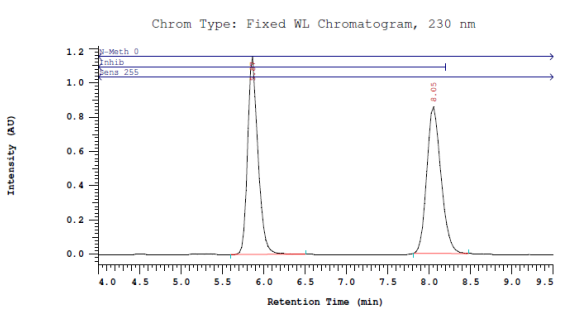
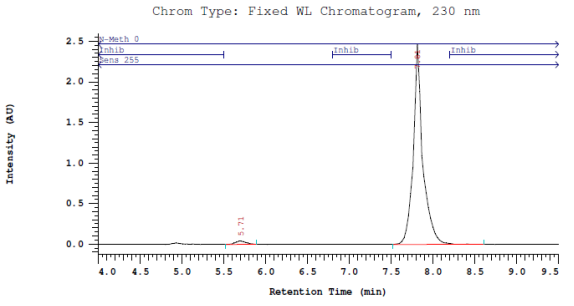
2	10.19	13516960	96.855	MC
		13955800	100.000	



(*S*)-4-methyl-*N*-(*m*-tolyl(*p*-tolyl)methyl)benzenesulfonamide (5ia)



No.	RT	Area	Conc 1	BC
1	5.87	4969200	49.279	MC
2	8.05	5114600	50.721	MC
		10083800	100.000	



No.	RT	Area	Conc 1	BC
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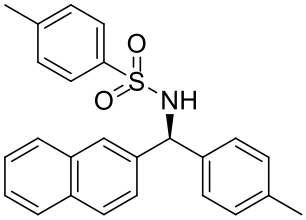
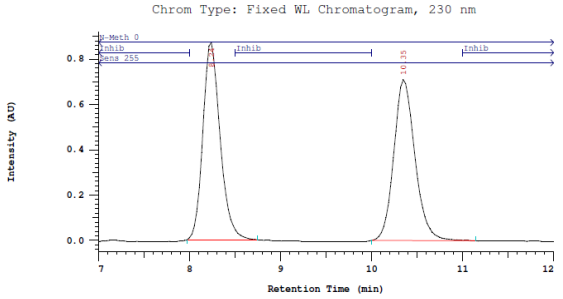
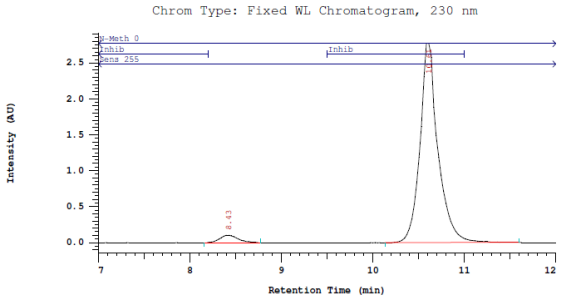
		9982660	100.000	



(*S*)-4-methyl-N-(naphthalen-2-yl(*p*-tolyl)methyl)benzenesulfonamide (5ja)



No.	RT	Area	Conc 1	BC
1	8.24	5746140	49.989	MC
2	10.35	5748720	50.011	MC
		11494860	100.000	



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1	8.43	689740	3.504	MC
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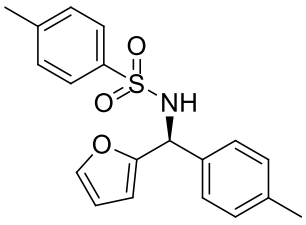
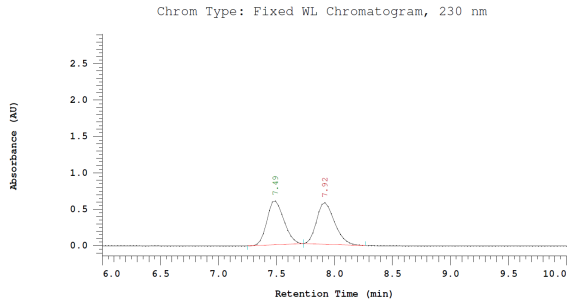


(*S*)-*N*-(furan-2-yl(*p*-tolyl)methyl)-4-methylbenzenesulfonamide (5ka)



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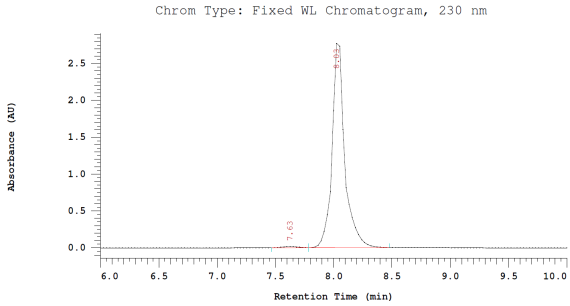

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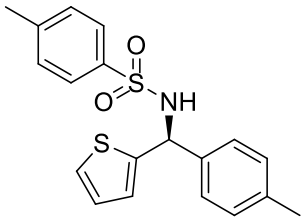
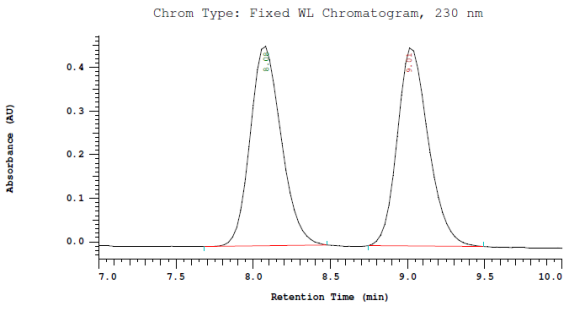
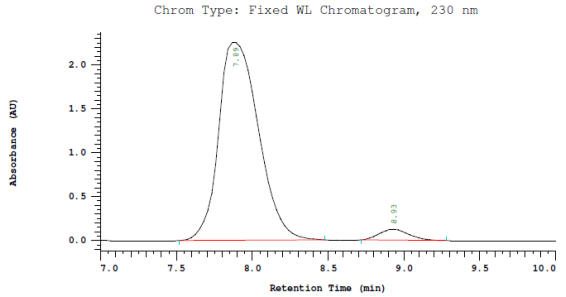


(*S*)-4-methyl-*N*-(thiophen-2-yl(*p*-tolyl)methyl)benzenesulfonamide (5la)



No.	RT	Area	Conc 1	BC
1	8.08	3199026	50.062	BB
2	9.01	3191084	49.938	MC
		6390110	100.000	



No.	RT	Area	Conc 1	BC
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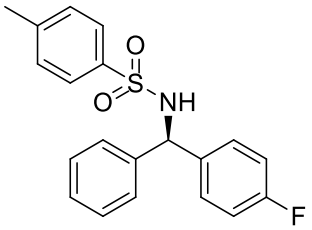
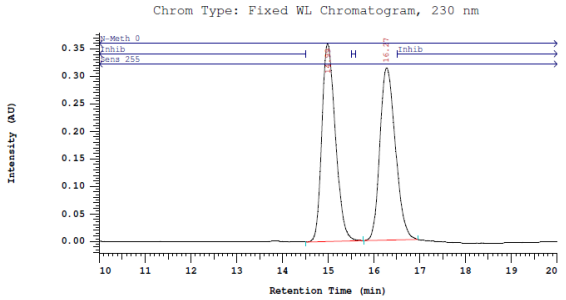
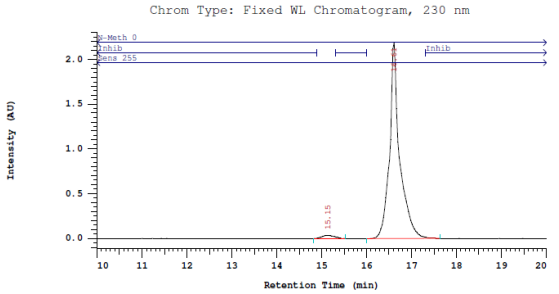
2	8.93	840754	3.921	BB
		21443352	100.000	



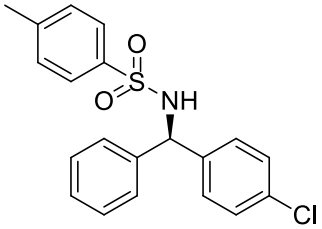
(*R*)-*N*-((4-fluorophenyl)(phenyl)methyl)-4-methylbenzenesulfonamide (5ab)[2]



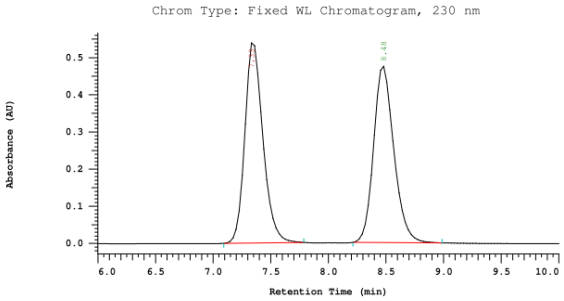
No.	RT	Area	Conc 1	BC
1	14.99	3688060	50.089	MC
2	16.27	3674920	49.911	MC
		7362980	100.000	



No.	RT	Area	Conc 1	BC
1	15.15	337160	1.918	MC
2	16.61	17244240	98.082	MC
		17581400	100.000	



(*R*)-*N*-((4-chlorophenyl)(phenyl)methyl)-4-methylbenzenesulfonamide (5ac)[3]



No.	RT	Area	Conc 1	BC
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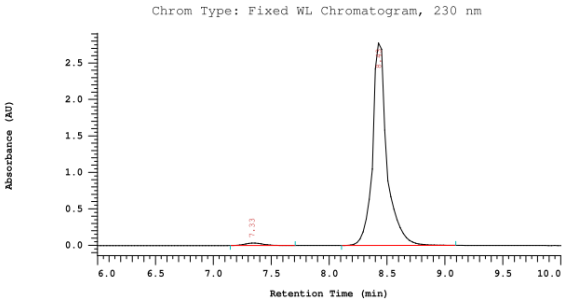
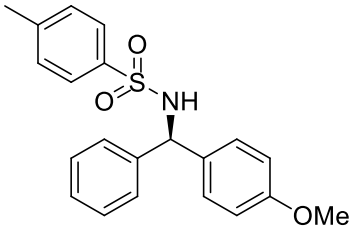
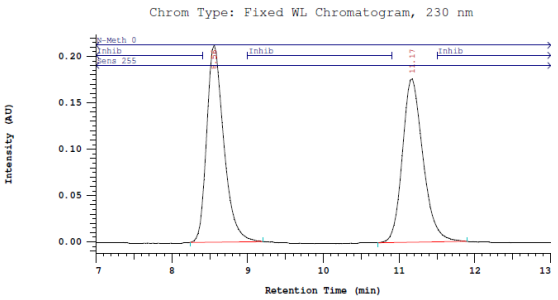
2	8.48	2892200	49.540	BB
		5838120	100.000	



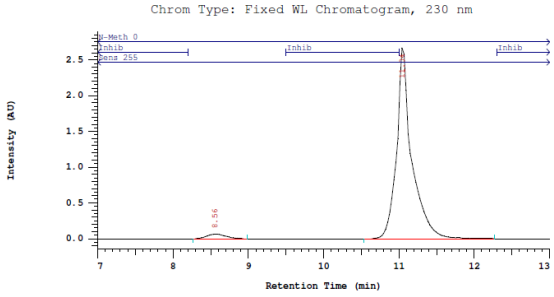
No.	RT	Area	Conc 1	BC
1	7.33	190040	1.561	MC
2	8.43	11981260	98.439	MC
		12171300	100.000	



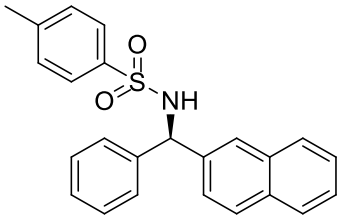
(*R*)-*N*-((4-methoxyphenyl)(phenyl)methyl)-4-methylbenzenesulfonamide (5ad)[3]



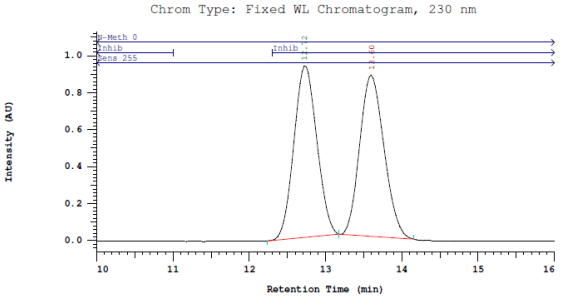
No.	RT	Area	Conc 1	BC
1	8.56	1665800	49.989	MC
2	11.17	1666520	50.011	MC
		3332320	100.000	



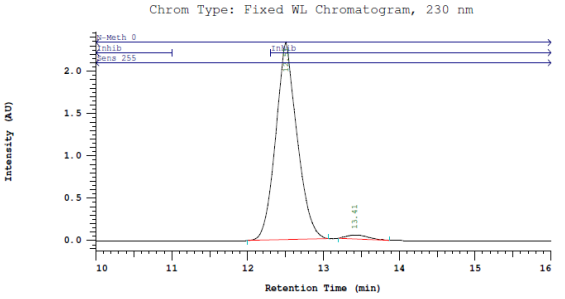
No.	RT	Area	Conc 1	BC
1	8.56	573260	2.993	MC
2	11.04	18579779	97.007	MC
		19153039	100.000	



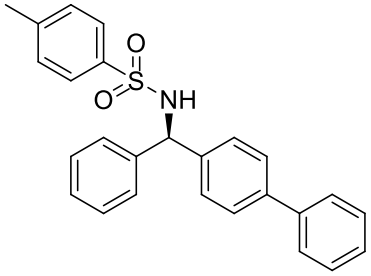
(*R*)-4-methyl-*N*-(naphthalen-2-yl(phenyl)methyl)benzenesulfonamide (5ae)[4]



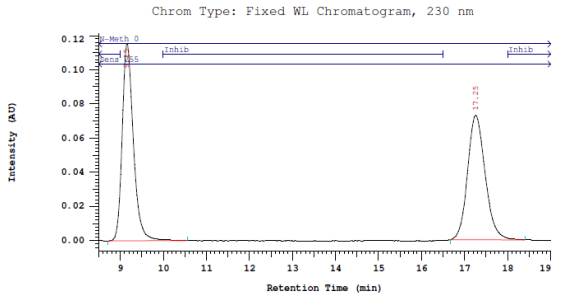
No.	RT	Area	Conc 1	BC
1	12.72	9677760	49.952	BB
2	13.60	9696200	50.048	MC
		19373960	100.000	



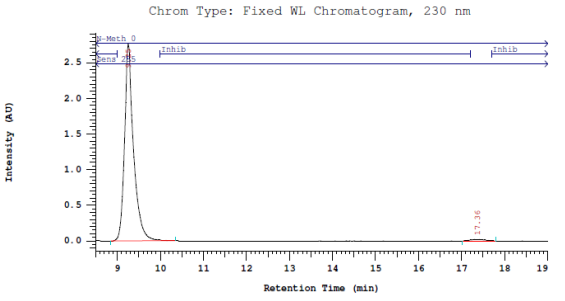
No.	RT	Area	Conc 1	BC
1	12.51	22699680	98.032	BB
2	13.41	455800	1.968	BB
		23155480	100.000	



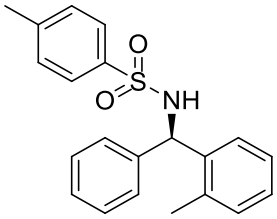
(*R*)-*N*-([1,1'-biphenyl]-4-yl(phenyl)methyl)-4-methylbenzenesulfonamide (5af)[1]



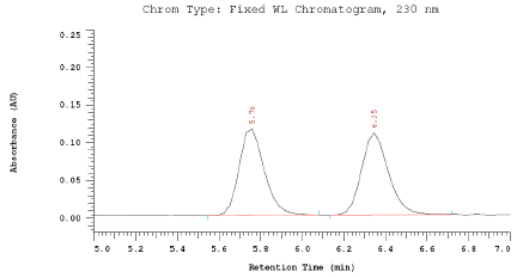
No.	RT	Area	Conc 1	BC
1	9.15	1027760	49.972	MC
2	17.25	1028920	50.028	MC
		2056680	100.000	



No.	RT	Area	Conc 1	BC
1	9.25	19804400	98.866	MC
2	17.36	227200	1.134	MC
		20031600	100.000	

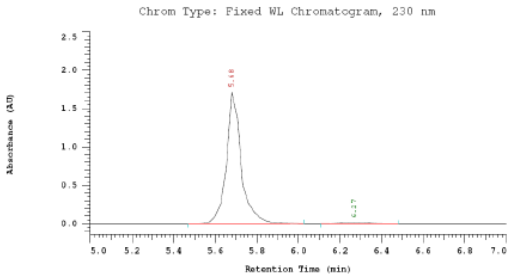


(*R*)-4-methyl-*N*-(phenyl(*o*-tolyl)methyl)benzenesulfonamide(5ag)



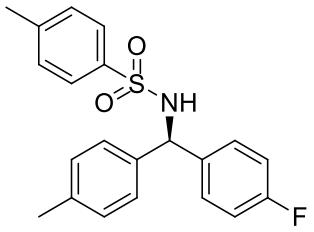
Peak Quantitation: AREA Calculation Method: AREA%

No.	RT	Area	Conc 1	BC
1	5.76	479960	49.938	MC
2	6.35	481160	50.062	MC
		961120	100.000	

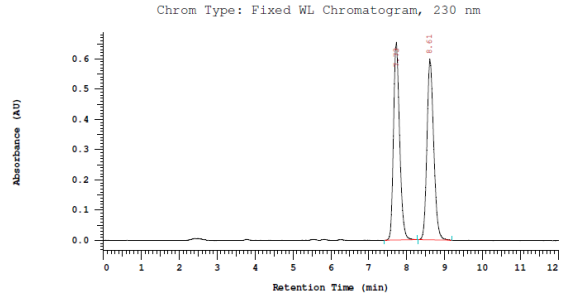


Peak Quantitation: AREA Calculation Method: AREA%

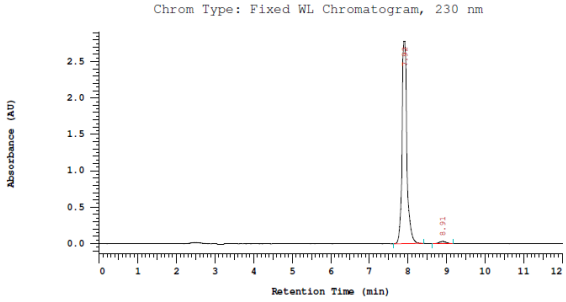
No.	RT	Area	Conc 1	BC
1	5.68	4247520	98.620	MC
2	6.27	59440	1.380	BB
		4306960	100.000	



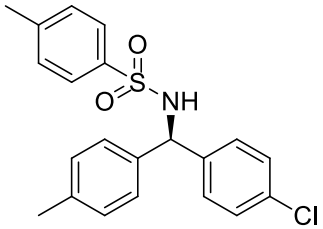
(*R*)-*N*-((4-fluorophenyl)(*p*-tolyl)methyl)-4-methylbenzenesulfonamide (*ent*-5ga)



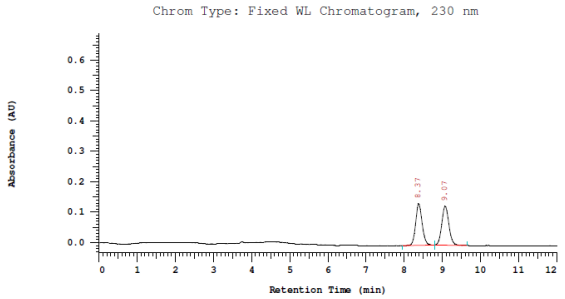
No.	RT	Area	Conc 1	BC
1	7.73	3612840	49.695	MC
2	8.61	3657200	50.305	MC
		7270040	100.000	



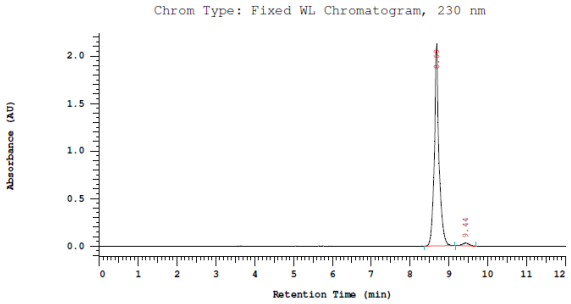
No.	RT	Area	Conc 1	BC
1	7.92	12183180	98.509	MC
2	8.91	184440	1.491	MC
		12367620	100.000	



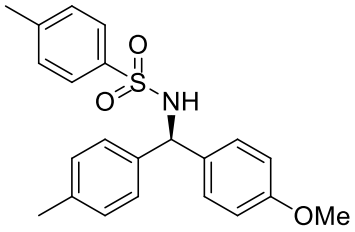
(*R*)-*N*-((4-chlorophenyl)(*p*-tolyl)methyl)-4-methylbenzenesulfonamide (*ent*-5ca)[2]



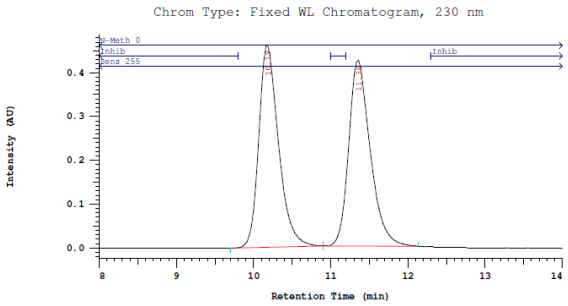
No.	RT	Area	Conc 1	BC
1	8.37	828960	49.999	MC
2	9.07	829000	50.001	MC
		1657960	100.000	



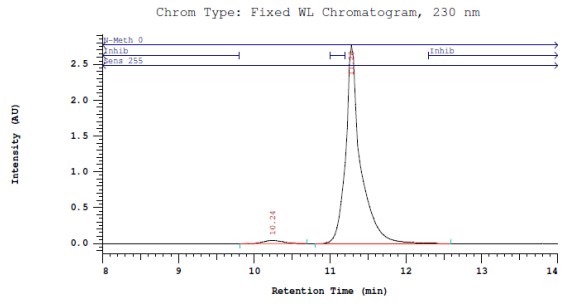
No.	RT	Area	Conc 1	BC
1	8.69	8733600	97.922	MC
2	9.44	185320	2.078	MC
		8918920	100.000	



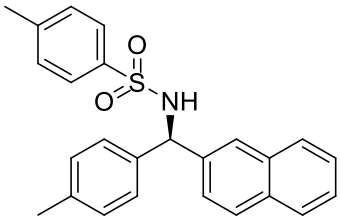
(*R*)-*N*-((4-methoxyphenyl)(*p*-tolyl)methyl)-4-methylbenzenesulfonamide (5md)[5]



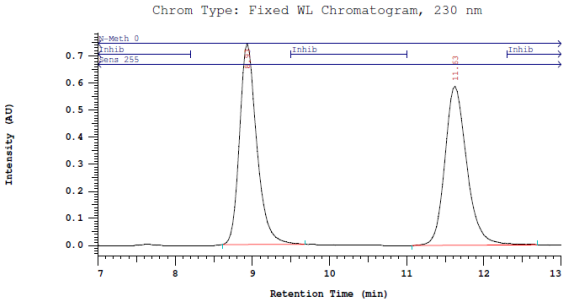
No.	RT	Area	Conc 1	BC
1	10.19	4112740	49.971	MC
2	11.36	4117440	50.029	MC
		8230180	100.000	



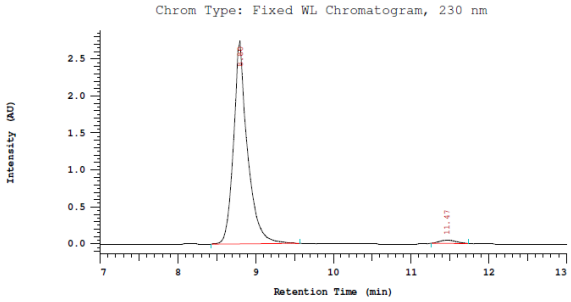
No.	RT	Area	Conc 1	BC
1	10.24	395560	2.065	MC
2	11.28	18762739	97.935	MC
		19158299	100.000	



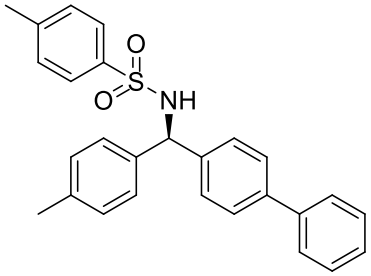
(*R*)-4-methyl-*N*-(naphthalen-2-yl(*p*-tolyl)methyl)benzenesulfonamide (*ent*-5ja)



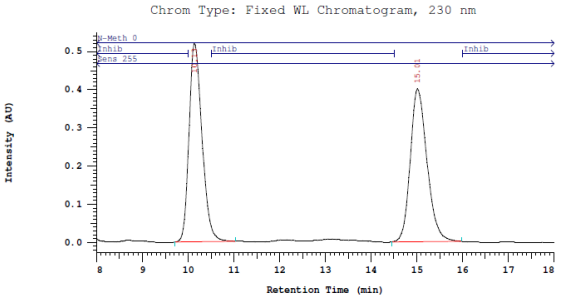
No.	RT	Area	Conc 1	BC
1	8.93	5772160	50.071	MC
2	11.63	5755820	49.929	MC
		11527980	100.000	



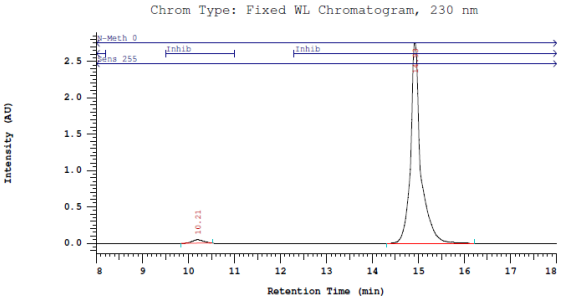
No.	RT	Area	Conc 1	BC
1	8.80	16857160	98.123	MC
2	11.47	322400	1.877	MC
		17179560	100.000	



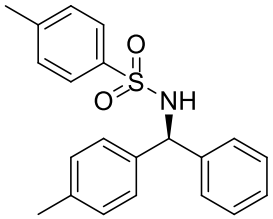
(*R*)-*N*-([1,1'-biphenyl]-4-yl(*p*-tolyl)methyl)-4-methylbenzenesulfonamide (5mf)[1]



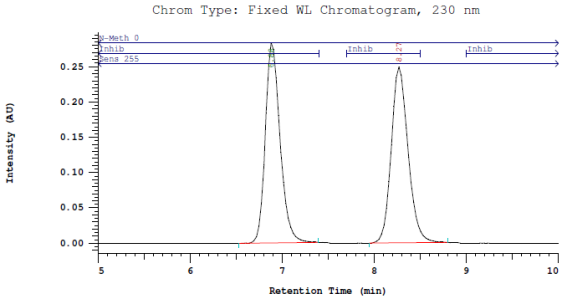
No.	RT	Area	Conc 1	BC
1	10.13	5119440	50.009	MC
2	15.01	5117640	49.991	MC
		10237080	100.000	



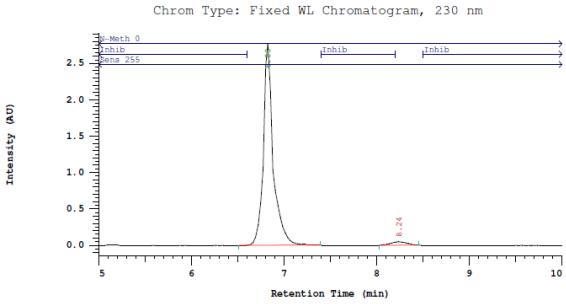
No.	RT	Area	Conc 1	BC
1	10.21	395640	1.820	MC
2	14.93	21336979	98.180	MC
		21732619	100.000	



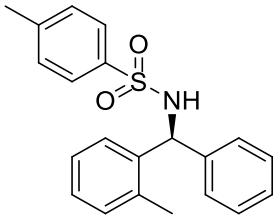
(*S*)-4-methyl-*N*-(phenyl(*p*-tolyl)methyl)benzenesulfonamide (*ent*-5aa)[1]



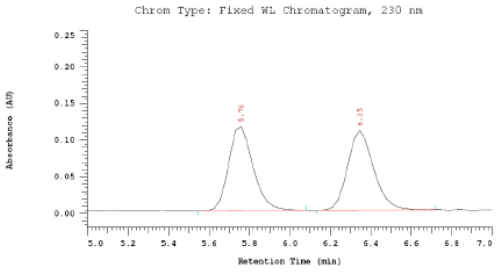
No.	RT	Area	Conc 1	BC
1	6.88	1580360	50.091	BB
2	8.27	1574600	49.909	MC
		3154960	100.000	



No.	RT	Area	Conc 1	BC
1	6.83	10316600	97.351	BB
2	8.24	280680	2.649	MC
		10597280	100.000	

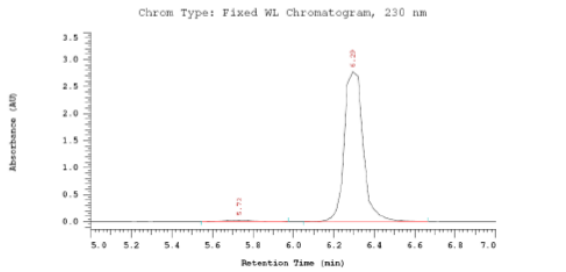


(*S*)-4-methyl-*N*-(phenyl(*o*-tolyl)methyl)benzenesulfonamide(*ent*-5ag)



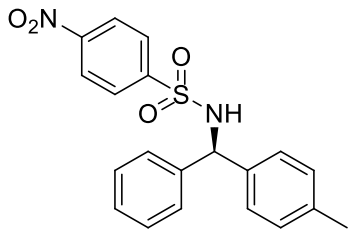
Peak Quantitation: AREA Calculation Method: AREA%

No.	RT	Area	Conc 1	BC
1	5.76	479960	49.938	MC
2	6.35	481160	50.062	MC
		961120	100.000	

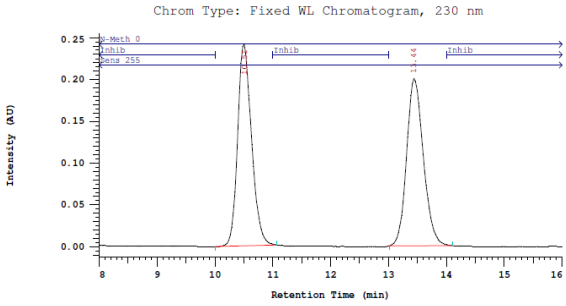


Peak Quantitation: AREA Calculation Method: AREA%

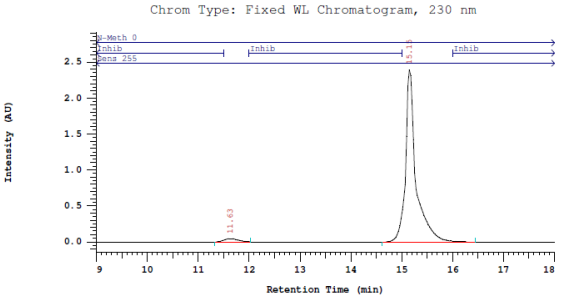
No.	RT	Area	Conc 1	BC
1	5.73	96760	1.073	MC
2	6.29	8918840	98.927	MC
		9015600	100.000	



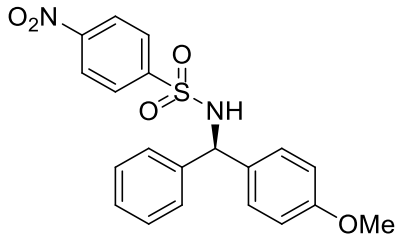
(*R*)-4-nitro-*N*-(phenyl(*p*-tolyl)methyl)benzenesulfonamide (10aa)



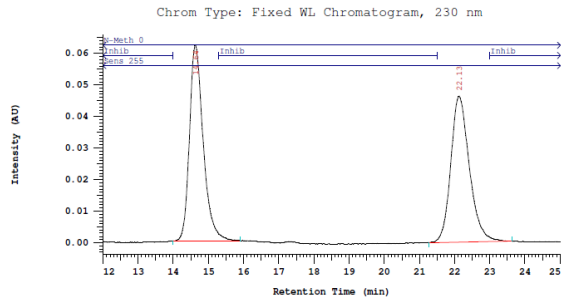
No.	RT	Area	Conc 1	BC
1	10.51	2007040	49.964	MC
2	13.44	2009960	50.036	MC
		4017000	100.000	



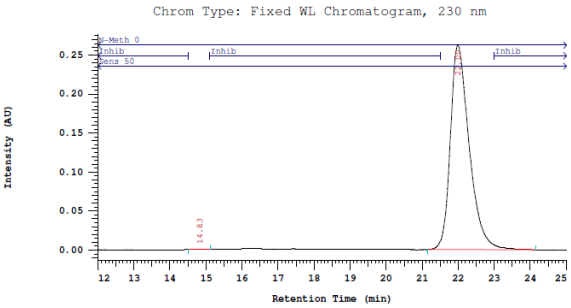
No.	RT	Area	Conc 1	BC
1	11.63	415120	2.374	MC
2	15.15	17070560	97.626	MC
		17485680	100.000	



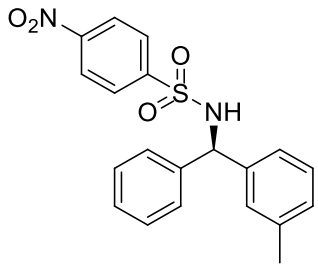
(*R*)-*N*-((4-methoxyphenyl)(phenyl)methyl)-4-nitrobenzenesulfonamide (10ad)[6]



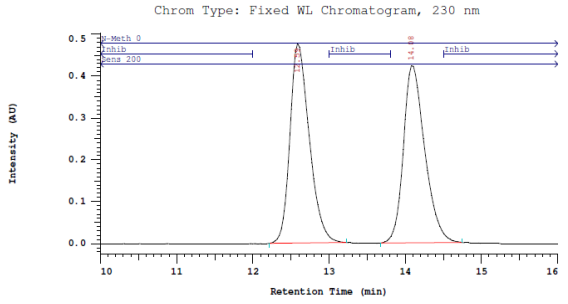
No.	RT	Area	Conc 1	BC
1	14.64	839020	49.853	MC
2	22.13	843960	50.147	MC
		1682980	100.000	



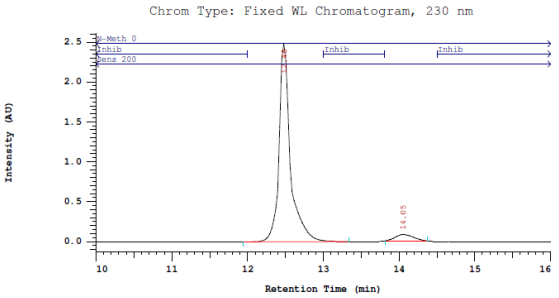
No.	RT	Area	Conc 1	BC
1	14.83	4900	0.103	MC
2	22.00	4771120	99.897	MC
		4776020	100.000	



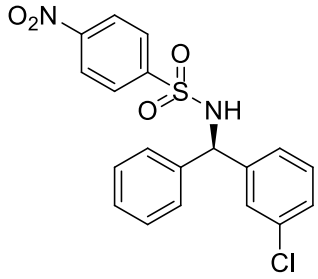
(*R*)-4-nitro-*N*-(phenyl(*m*-tolyl)methyl)benzenesulfonamide (10ai)



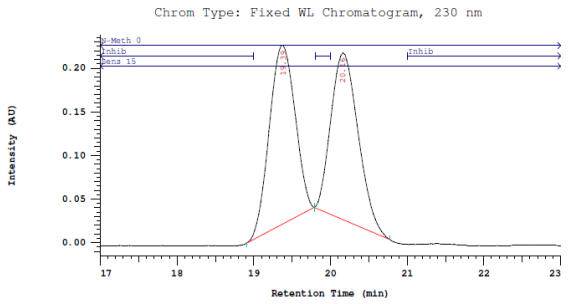
No.	RT	Area	Conc 1	BC
1	12.59	4172880	50.188	MC
2	14.08	4141680	49.812	MC
		8314560	100.000	



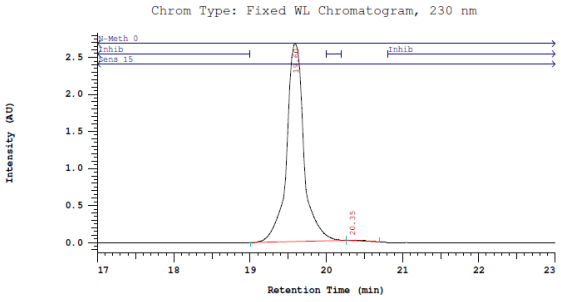
No.	RT	Area	Conc 1	BC
1	12.48	12888920	95.103	MC
2	14.05	663680	4.897	MC
		13552600	100.000	



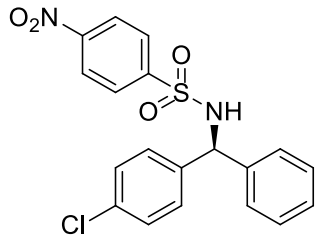
(*R*)-*N*-((3-chlorophenyl)(phenyl)methyl)-4-nitrobenzenesulfonamide (10aj)



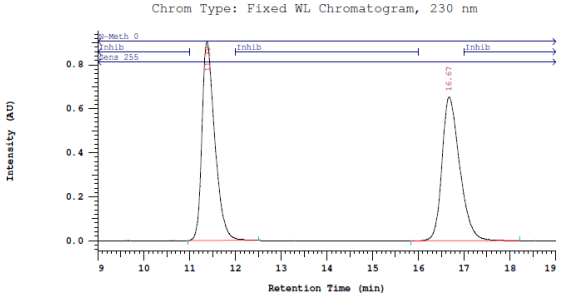
No.	RT	Area	Conc 1	BC
1	19.39	2361900	49.898	MC
2	20.16	2371600	50.102	MC
		4733500	100.000	



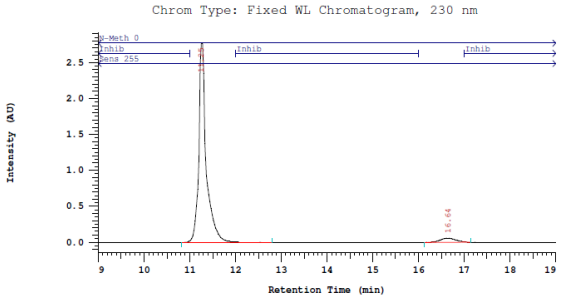
No.	RT	Area	Conc 1	BC
1	19.60	21063340	99.715	MC
2	20.35	60280	0.285	MC
		21123620	100.000	



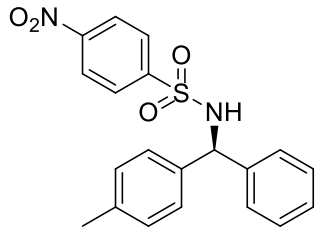
(*S*)-*N*-((4-chlorophenyl)(phenyl)methyl)-4-nitrobenzenesulfonamide (10bh)[5]



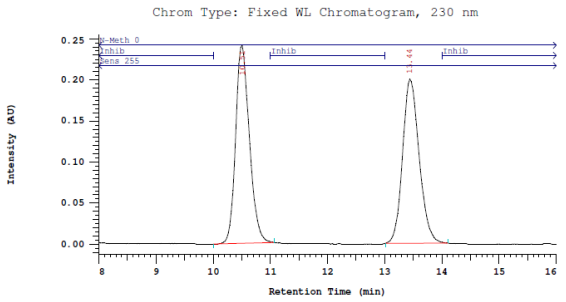
No.	RT	Area	Conc 1	BC
1	11.39	8868480	50.250	MC
2	16.67	8780400	49.750	MC
		17648880	100.000	



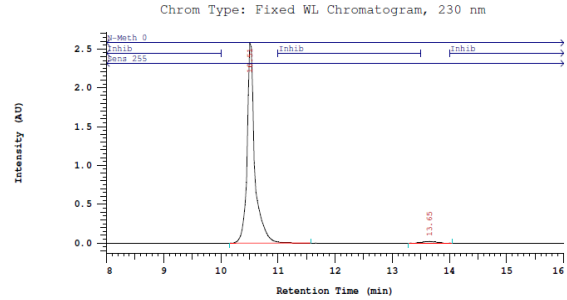
No.	RT	Area	Conc 1	BC
1	11.25	16087000	95.807	MC
2	16.64	704040	4.193	MC
		16791040	100.000	



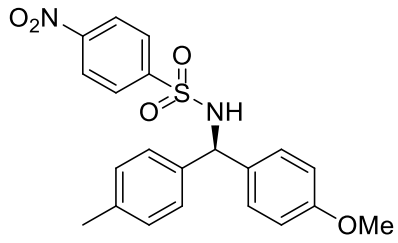
(*S*)-4-nitro-*N*-(phenyl(*p*-tolyl)methyl)benzenesulfonamide (*ent*-10aa)



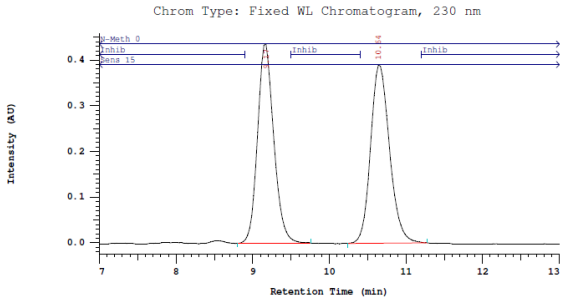
No.	RT	Area	Conc 1	BC
1	10.51	2007040	49.964	MC
2	13.44	2009960	50.036	MC
		4017000	100.000	



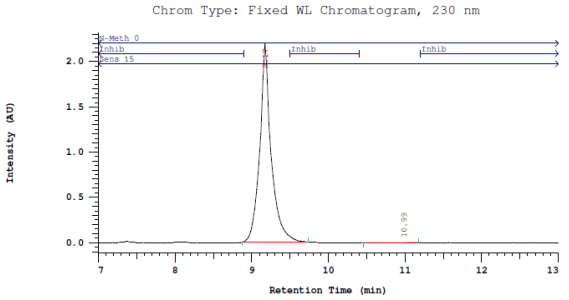
No.	RT	Area	Conc 1	BC
1	10.51	12119480	98.457	MC
2	13.65	189880	1.543	MC
		12309360	100.000	



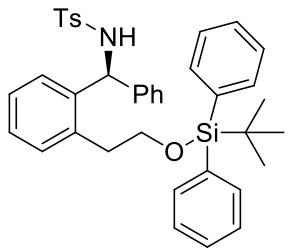
(*R*)-*N*-((4-methoxyphenyl)(*p*-tolyl)methyl)-4-nitrobenzenesulfonamide (10cd)[7]



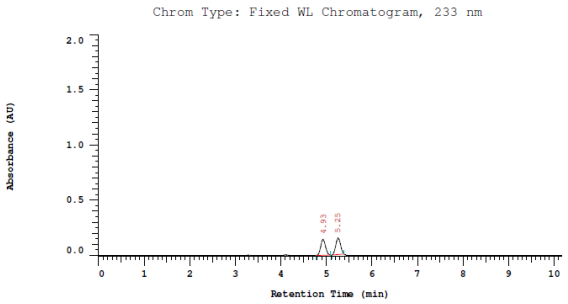
No.	RT	Area	Conc 1	BC
1	9.17	3220800	49.023	MC
2	10.64	3349200	50.977	MC
		6570000	100.000	



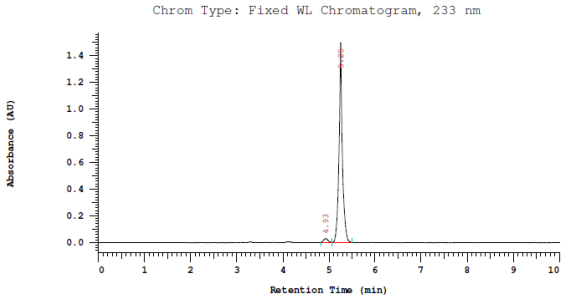
No.	RT	Area	Conc 1	BC
1	9.17	11426120	99.899	MC
2	10.99	11500	0.101	BB
		11437620	100.000	



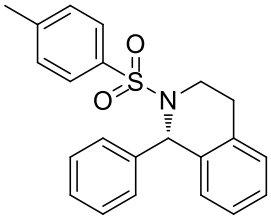
(*S*)-*N*-((2-(2-((tert-butyldiphenylsilyl)oxy)ethyl)phenyl)(phenyl)methyl)-4-methyl benzenesulfonamide (12)



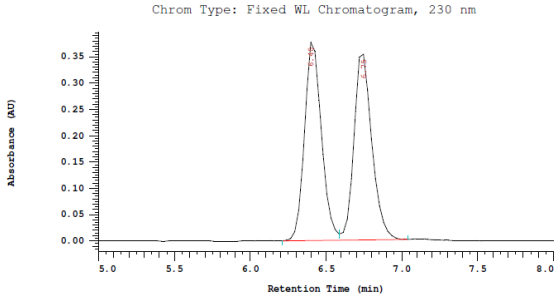
No.	RT	Area	Conc 1	BC
1	4.93	530400	49.468	MC
2	5.25	541800	50.532	MC
		1072200	100.000	



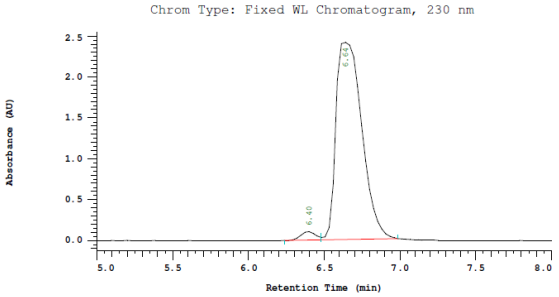
No.	RT	Area	Conc 1	BC
1	4.93	94740	2.491	MC
2	5.25	3707960	97.509	MC
		3802700	100.000	



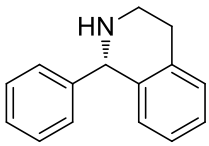
(*S*)-1-phenyl-2-tosyl-1,2,3,4-tetrahydroisoquinoline (A1)[8]



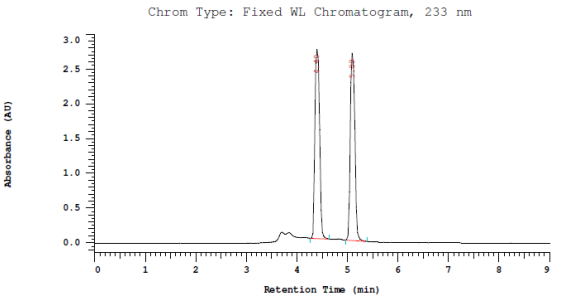
No.	RT	Area	Conc 1	BC
1	6.40	1470163	49.882	MC
2	6.75	1477120	50.118	MC
		2947283	100.000	



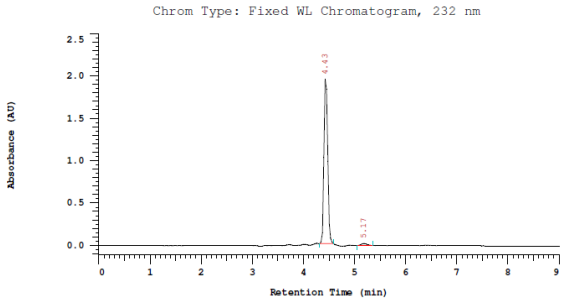
No.	RT	Area	Conc 1	BC
1	6.40	345350	2.358	BV
2	6.64	14302208	97.642	VB
		14647558	100.000	



(*S*)-1-phenyl-1,2,3,4-tetrahydroisoquinoline (14)[9]



No.	RT	Area	Conc 1	BC
1	4.40	8790960	50.967	MC
2	5.09	8457240	49.033	MC
		17248200	100.000	



No.	RT	Area	Conc 1	BC
1	4.43	4962160	98.150	MC
2	5.17	93520	1.850	MC
		5055680	100.000	

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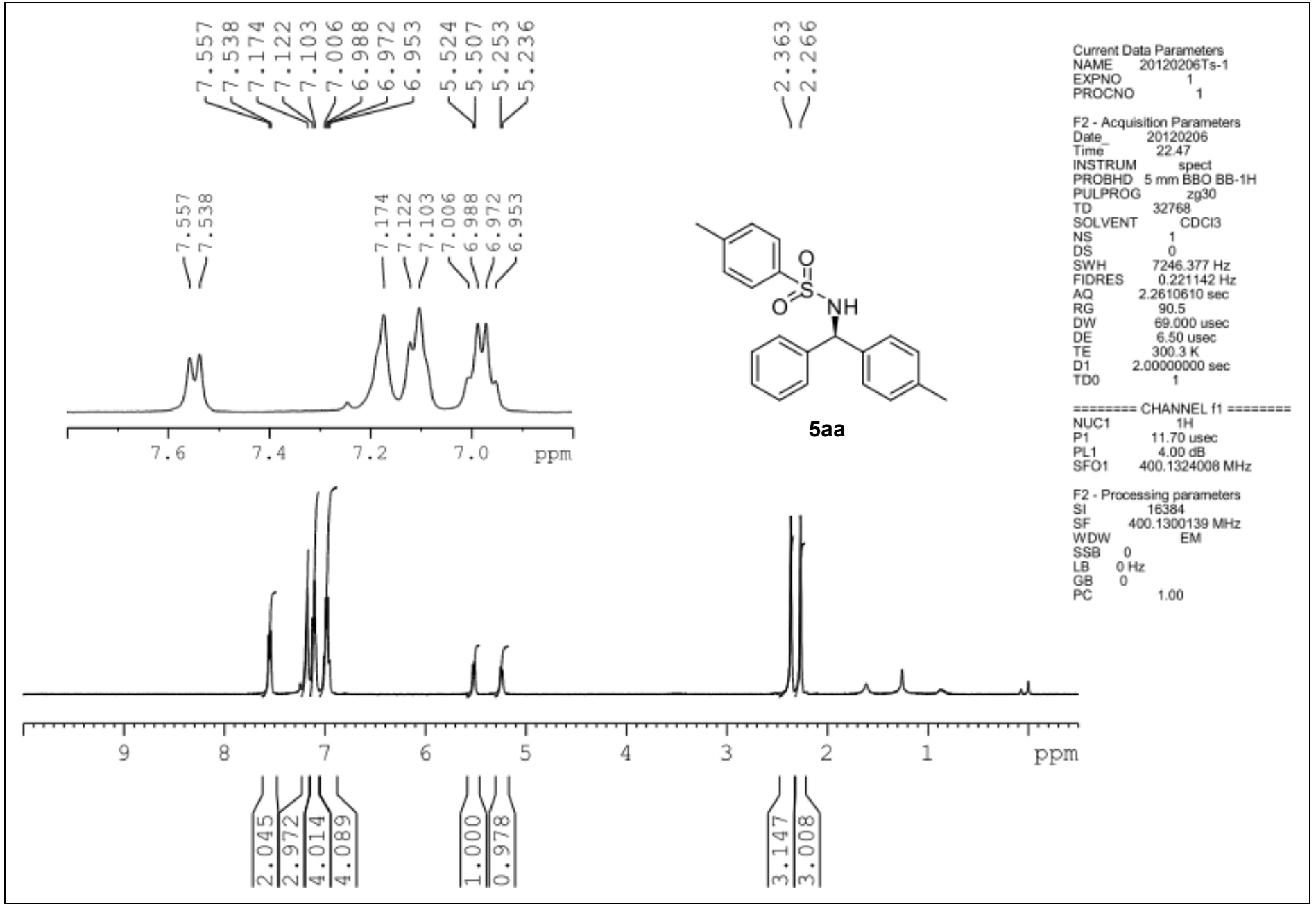
9. Pedrosa, R.; Andres, C.; Iglesias, J. M. *J. Org. Chem.* **2001,** *66,* 243.



Current Data Parameters
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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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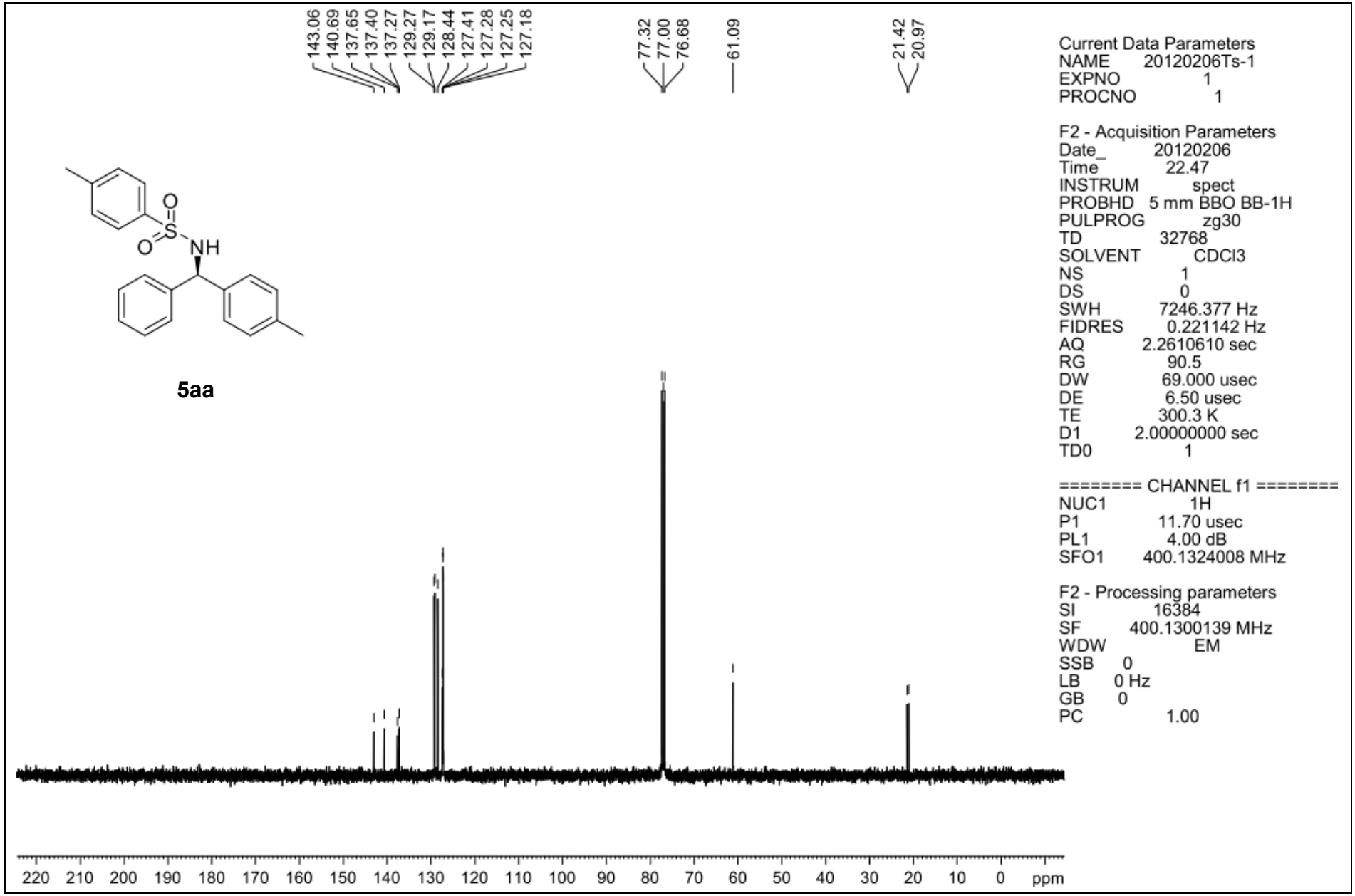
Time 22.47
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 1
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2610610 sec
RG 90.5
DW 69.000 usec
DE 6.50 usec
TE 300.3 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.70 usec
PL1 4.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300139 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00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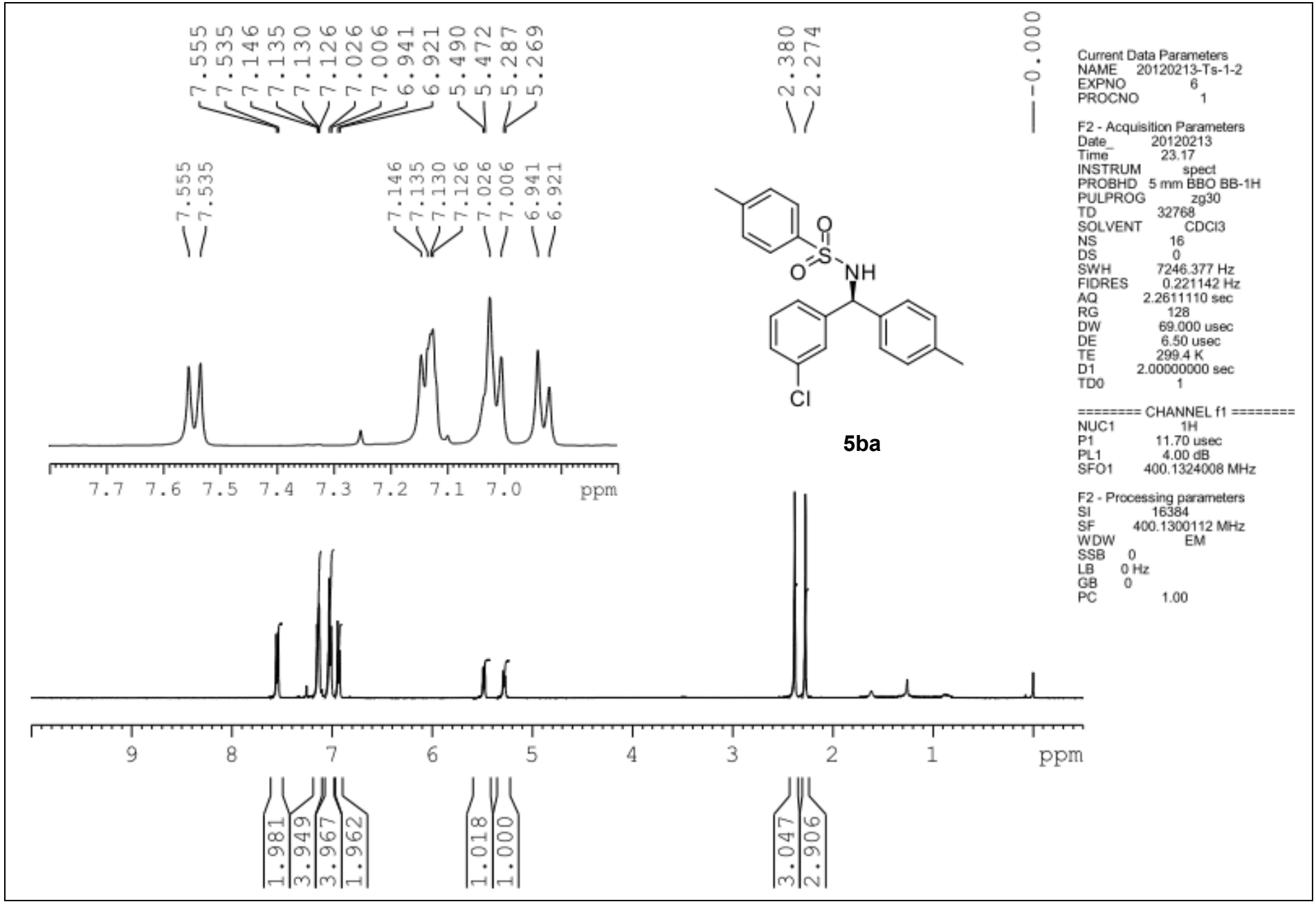
129.27
129.17
128.44
127.41
127.28
127.25
127.18
77.32
77.00
76.68
61.09
21.42
20.97
O
S
O
NH
5aa
Current Data Parameters
NAME 20120206Ts-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120206
Time 22.47
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 1
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2610610 sec
RG 90.5
DW 69.000 usec
DE 6.50 usec
TE 300.3 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.70 usec
PL1 4.00 dB
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300139 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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7.146
7.135
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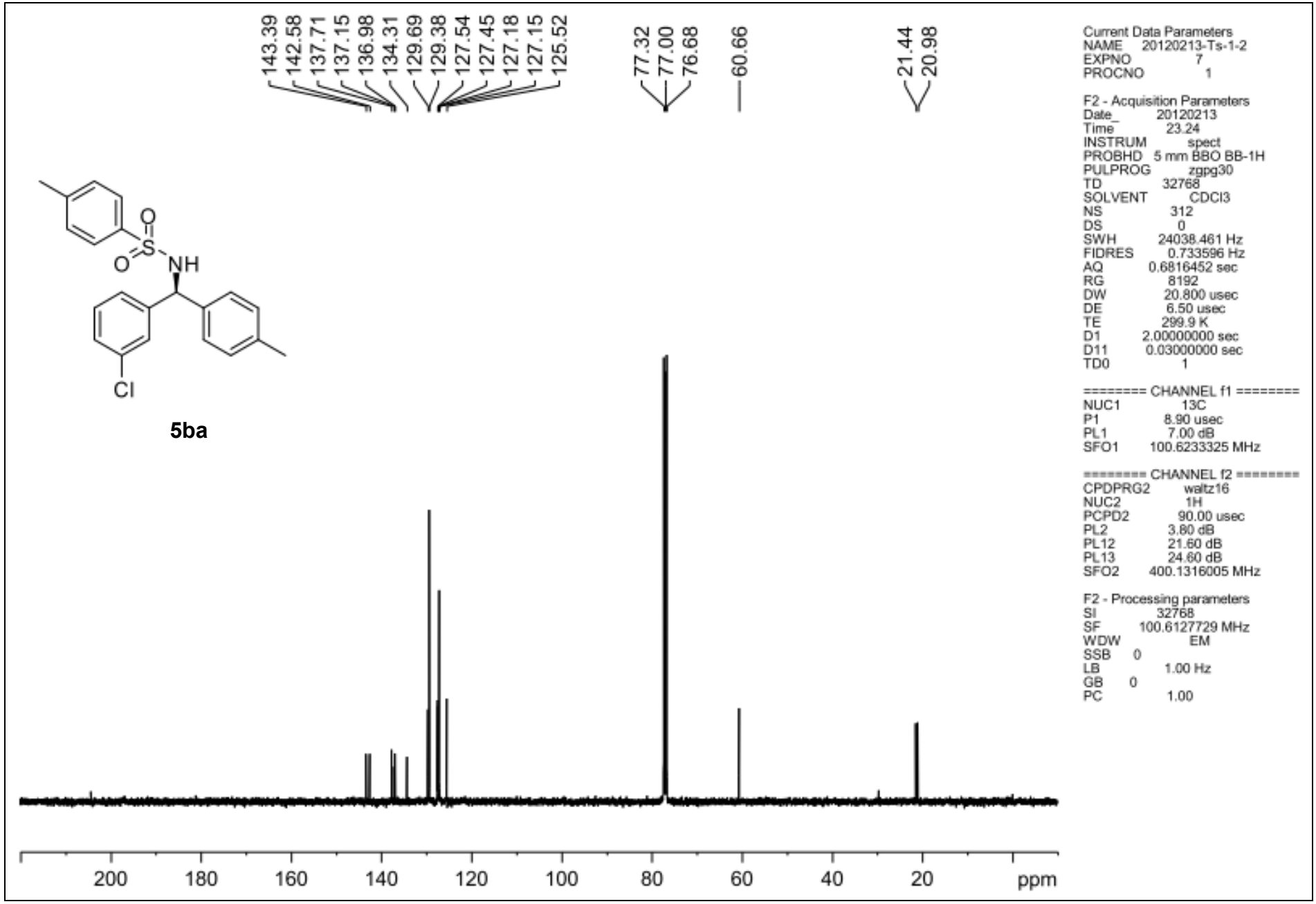
7.006
6.941
6.921
5.490
5.472
5.287
5.269
2.380
2.274
0.000
O
S
O
NH
Cl
5ba
Current Data Parameters
NAME 20120213-Ts-1-2
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120213
Time 23.17
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2611110 sec
RG 128
DW 69.000 usec
DE 6.50 usec
TE 299.4 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.70 usec
PL1 4.00 dB
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300112 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 ppm
9 8 7 6 5 4 3 2 1 ppm
1.981
3.949
3.967
1.962
1.018
1.000
3.047
2.906


143.39
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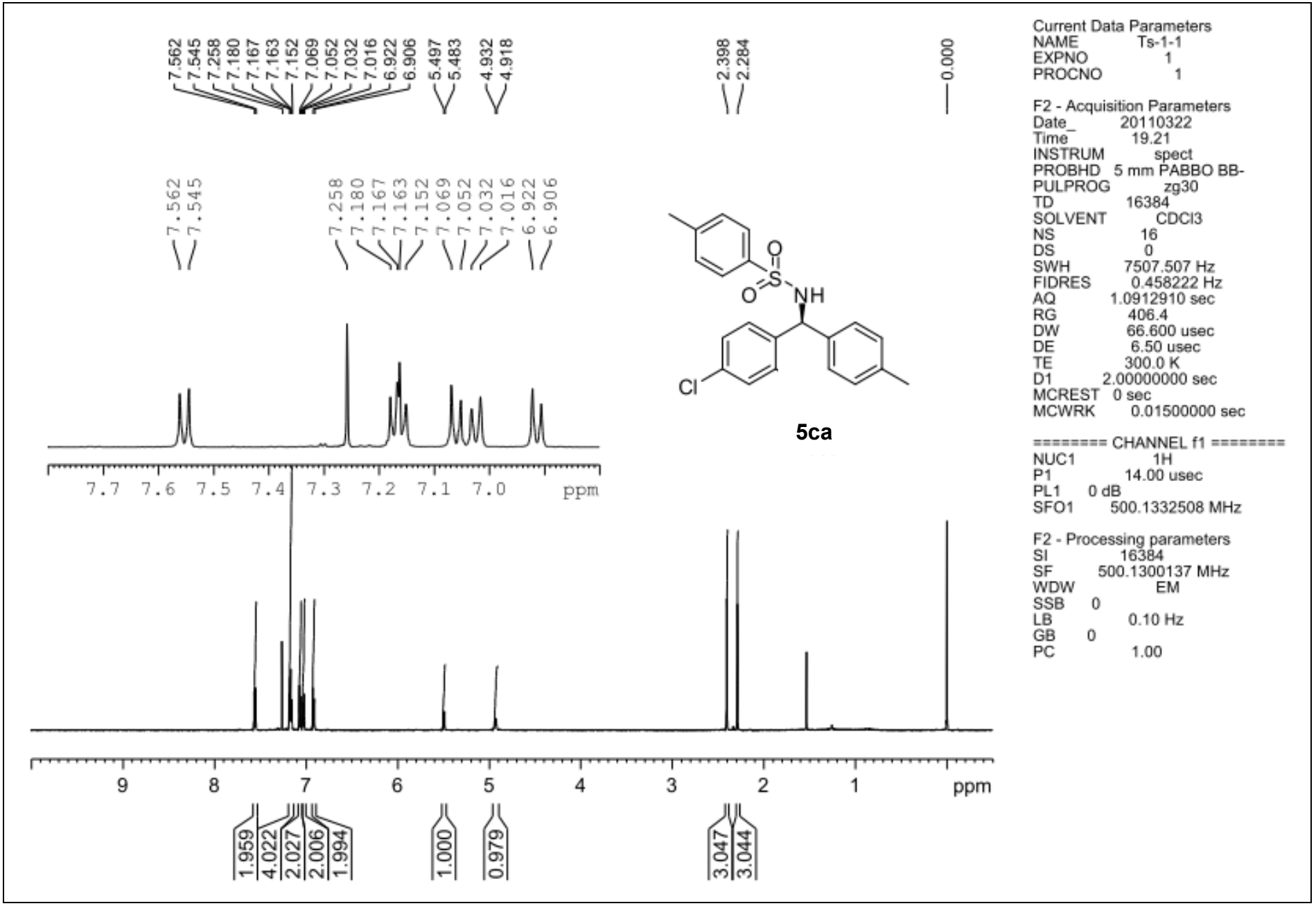
129.38
127.54
127.45
127.18
127.15
125.52
77.32
77.00
76.68
60.66
21.44
20.98
O
S
O
NH
Cl
5ba
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME 20120213-Ts-1-2
EXPNO 7
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120213
Time 23.24
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 312
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816452 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 299.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PL1 7.00 dB
SFO1 100.6233325 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.80 dB
PL12 21.60 dB
PL13 24.60 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127729 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

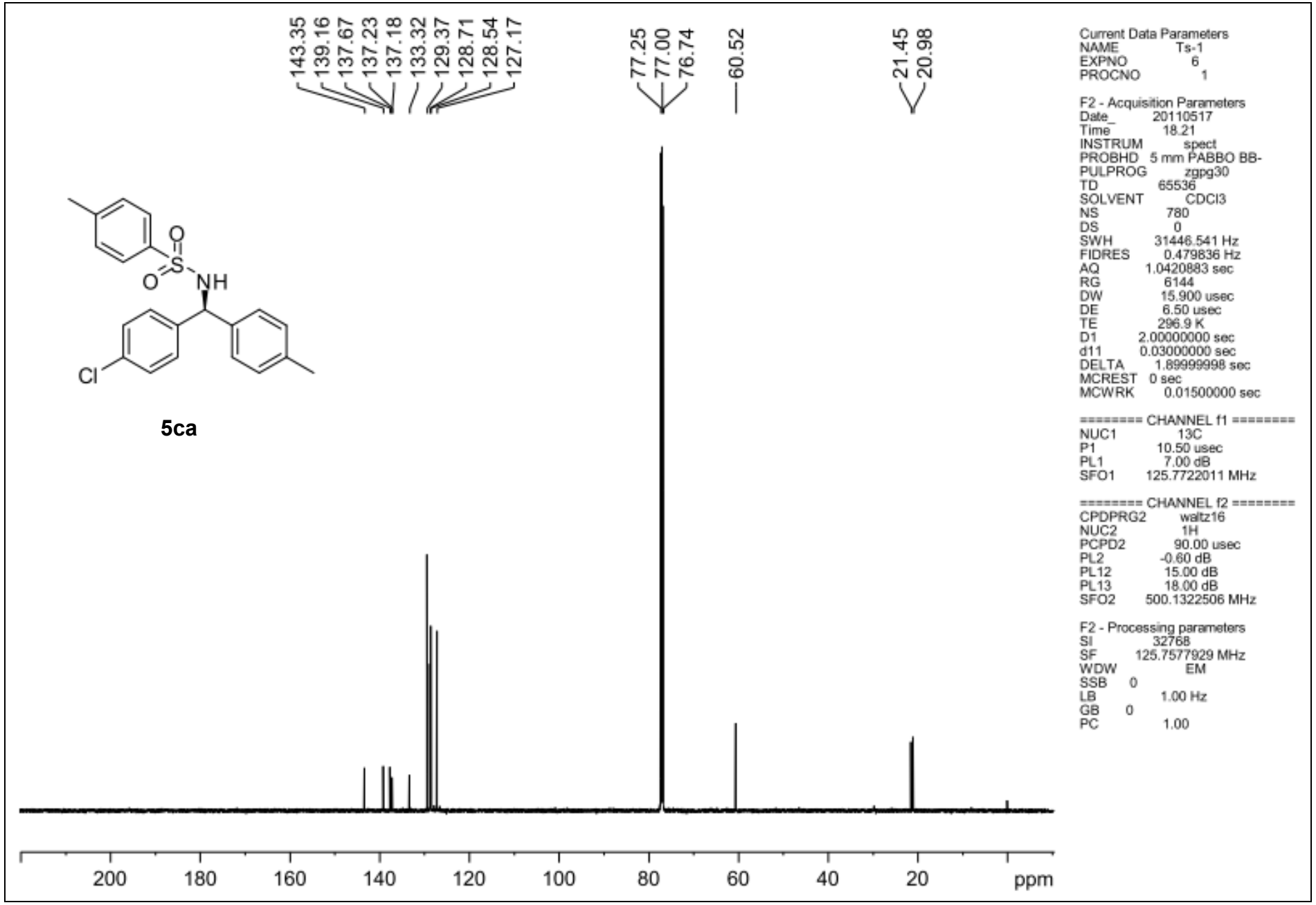


Current Data Parameters
NAME Ts-1-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110322
Time 19.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 7507.507 Hz
FIDRES 0.458222 Hz
AQ 1.0912910 sec
RG 406.4
DW 66.600 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0 dB
SFO1 500.1332508 MHz

F2 - Processing parameters
SI 16384
SF 500.1300137 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00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127.17
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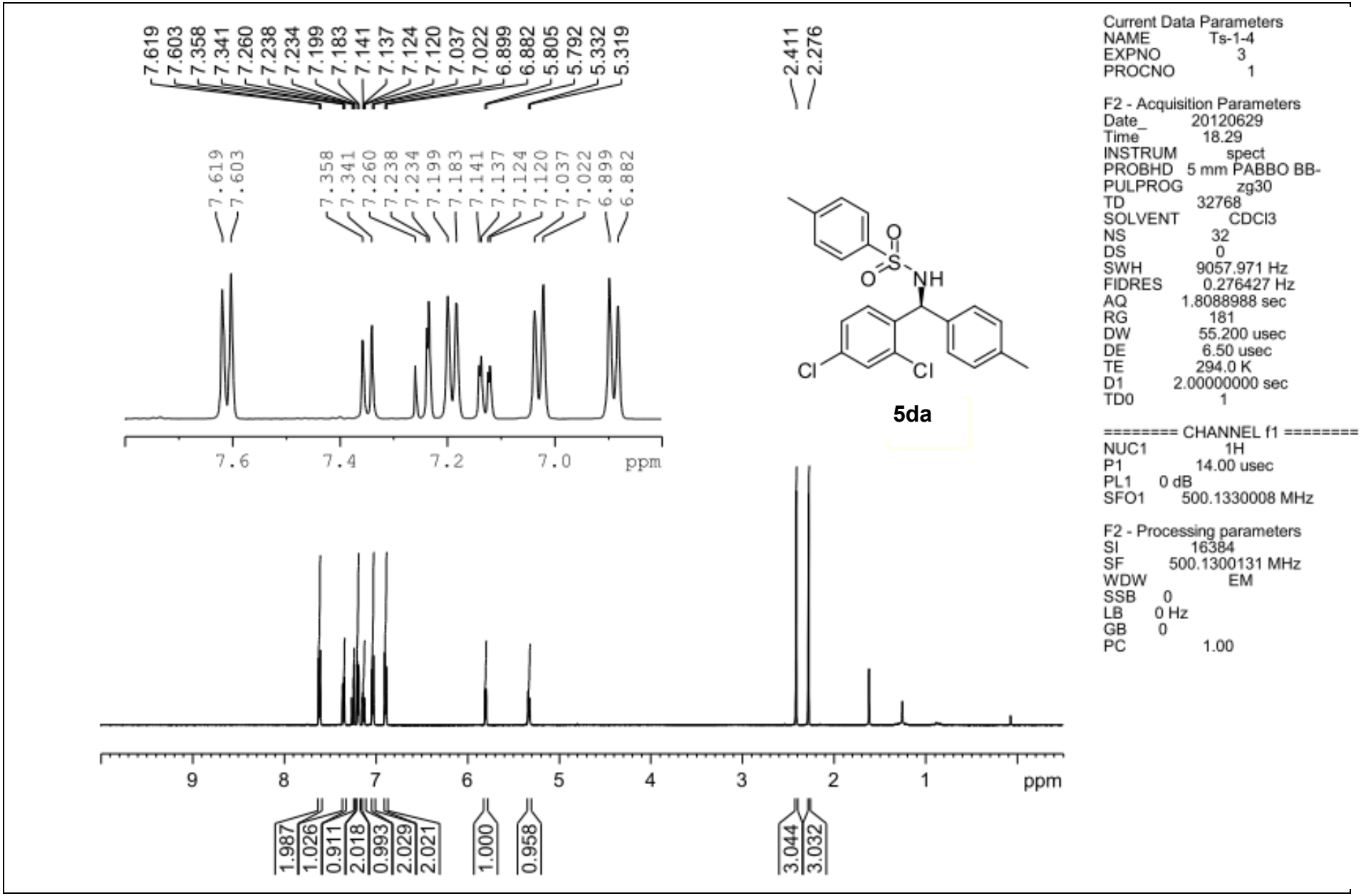
60.52
21.45
20.98
O
S
O
NH
Cl
5ca
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME Ts-1
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110517
Time 18.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 780
DS 0
SWH 31446.541 Hz
FIDRES 0.479836 Hz
AQ 1.0420883 sec
RG 6144
DW 15.900 usec
DE 6.50 usec
TE 296.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 125.7722011 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1322506 MHz
F2 - Processing parameters
SI 32768
SF 125.7577929 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

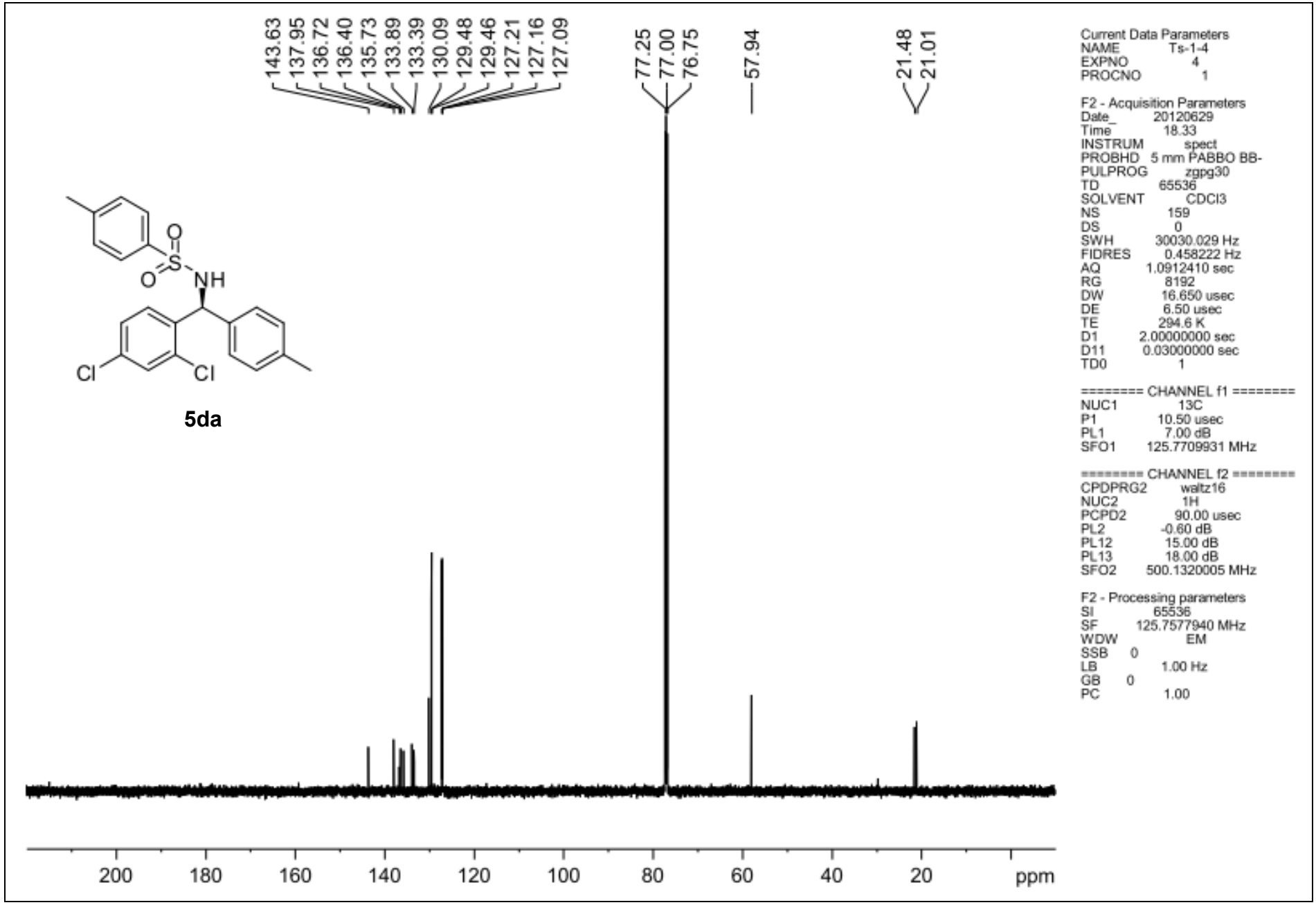


Current Data Parameters
NAME Ts-1-4
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120629
Time 18.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9057.971 Hz
FIDRES 0.276427 Hz
AQ 1.8088988 sec
RG 181
DW 55.200 usec
DE 6.50 usec
TE 294.0 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0 dB
SFO1 500.1330008 MHz

F2 - Processing parameters
SI 16384
SF 500.1300131 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00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127.09
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77.00
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57.94
21.48
21.01
O
S
O
NH
Cl
Cl
5da
200
180
160
140
120
100
80
60
40
20
ppm
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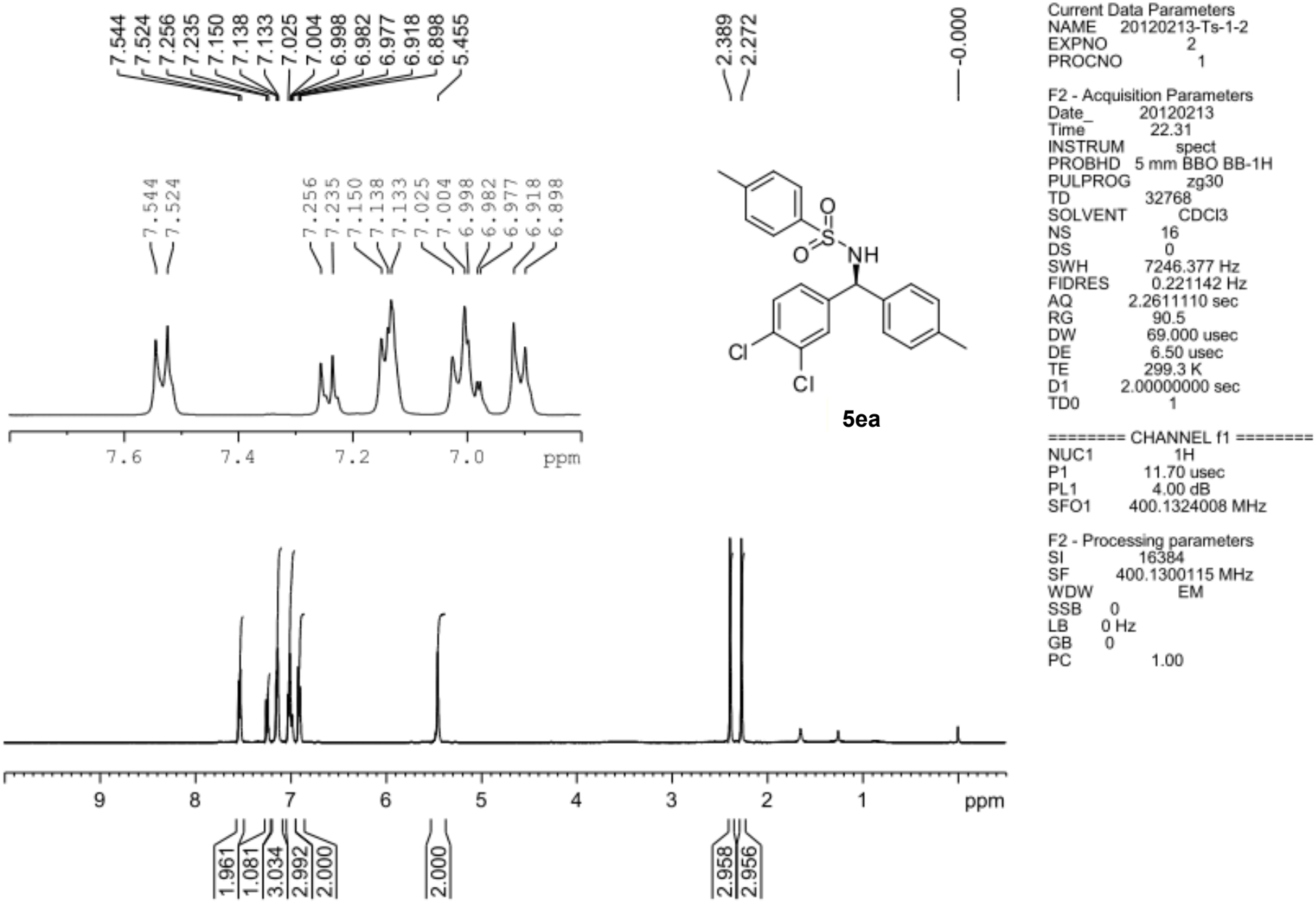
NAME Ts-1-4
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120629
Time 18.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 159
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 8192
DW 16.650 usec
DE 6.50 usec
TE 294.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 125.7709931 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 65536
SF 125.7577940 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

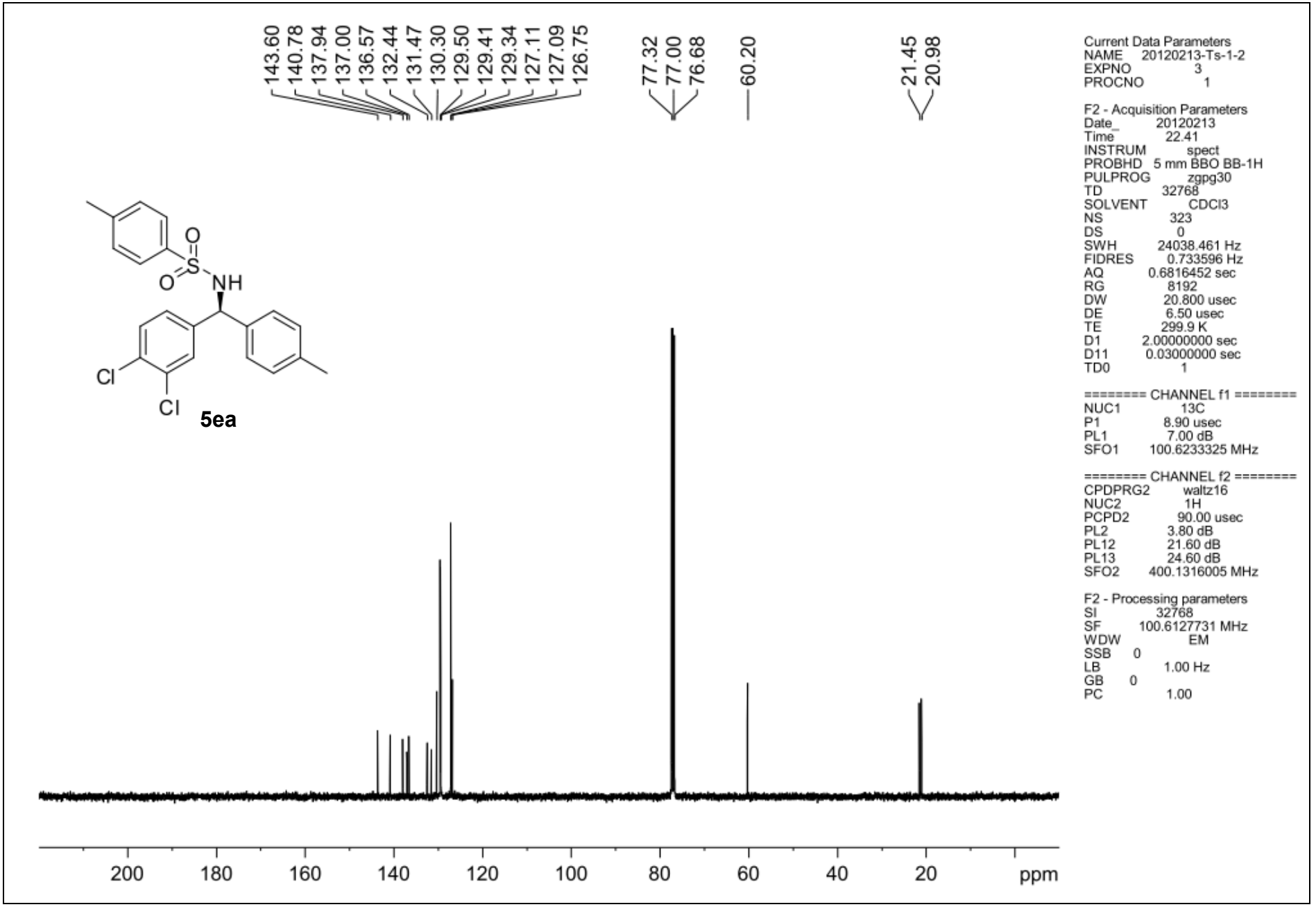


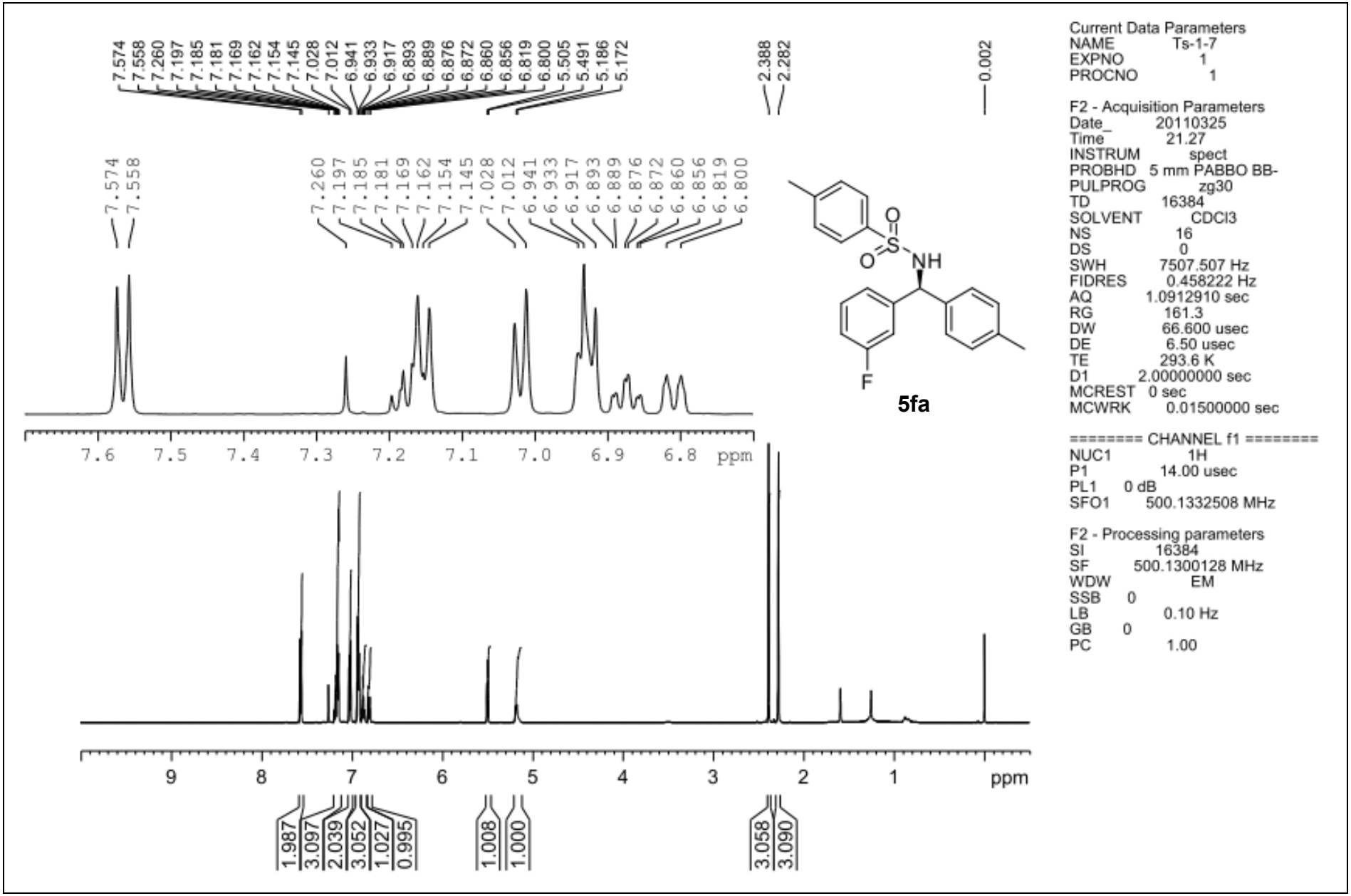
Current Data Parameters
NAME 20120213-Ts-1-2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120213
Time 22.31
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 90.5
DW 69.000 usec
DE 6.50 usec
TE 299.3 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.70 usec
PL1 4.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300115 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00


143.60
140.78
137.94
137.00
136.57
132.44
131.47
130.30
129.50
129.41
129.34
127.11
127.09
126.75
77.32
77.00
76.68
60.20
21.45
20.98
O
S
O
NH
Cl
Cl
5ea
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME 20120213-Ts-1-2
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120213
Time 22.41
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 323
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816452 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 299.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PL1 7.00 dB
SFO1 100.6233325 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.80 dB
PL12 21.60 dB
PL13 24.60 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127731 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

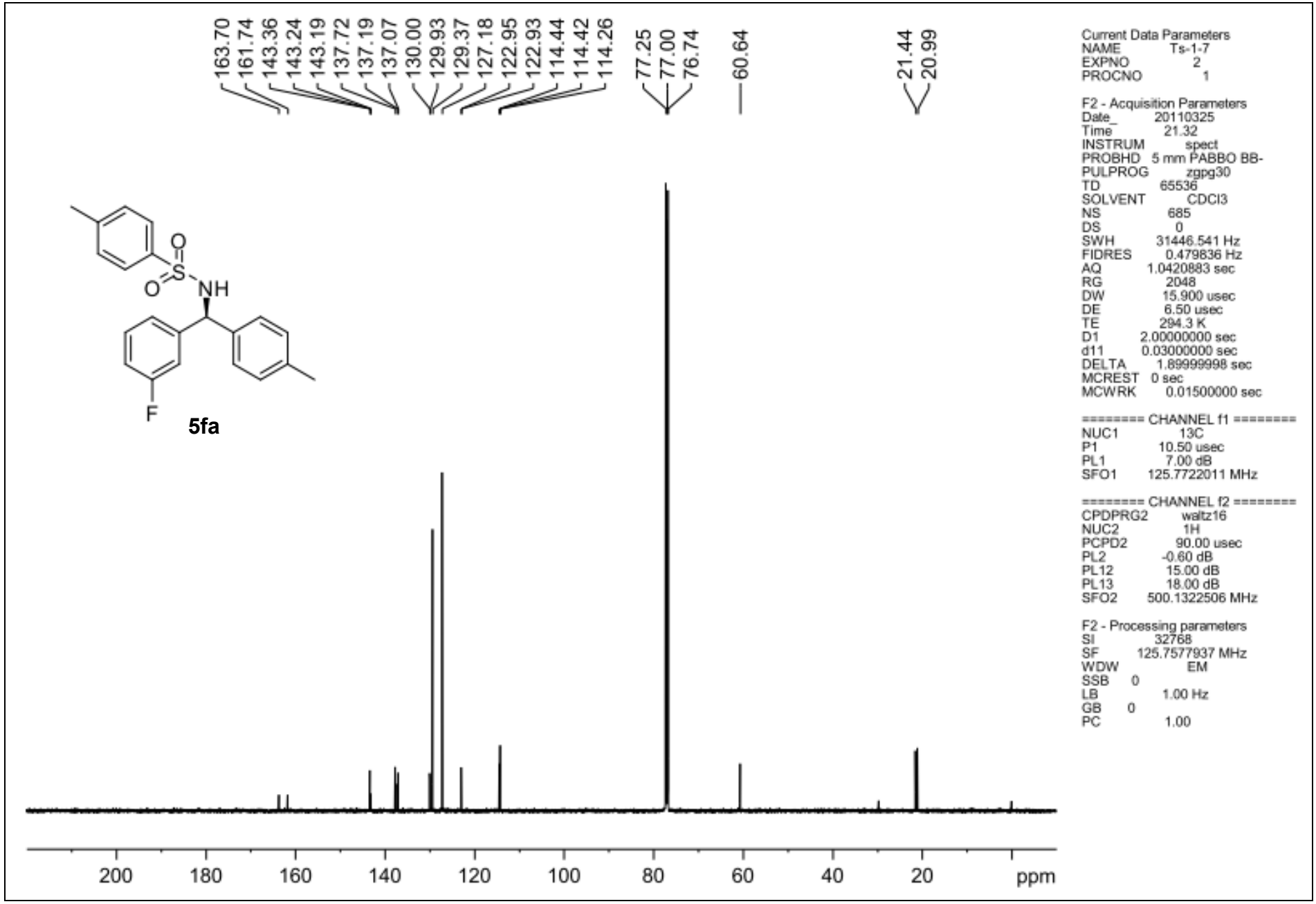


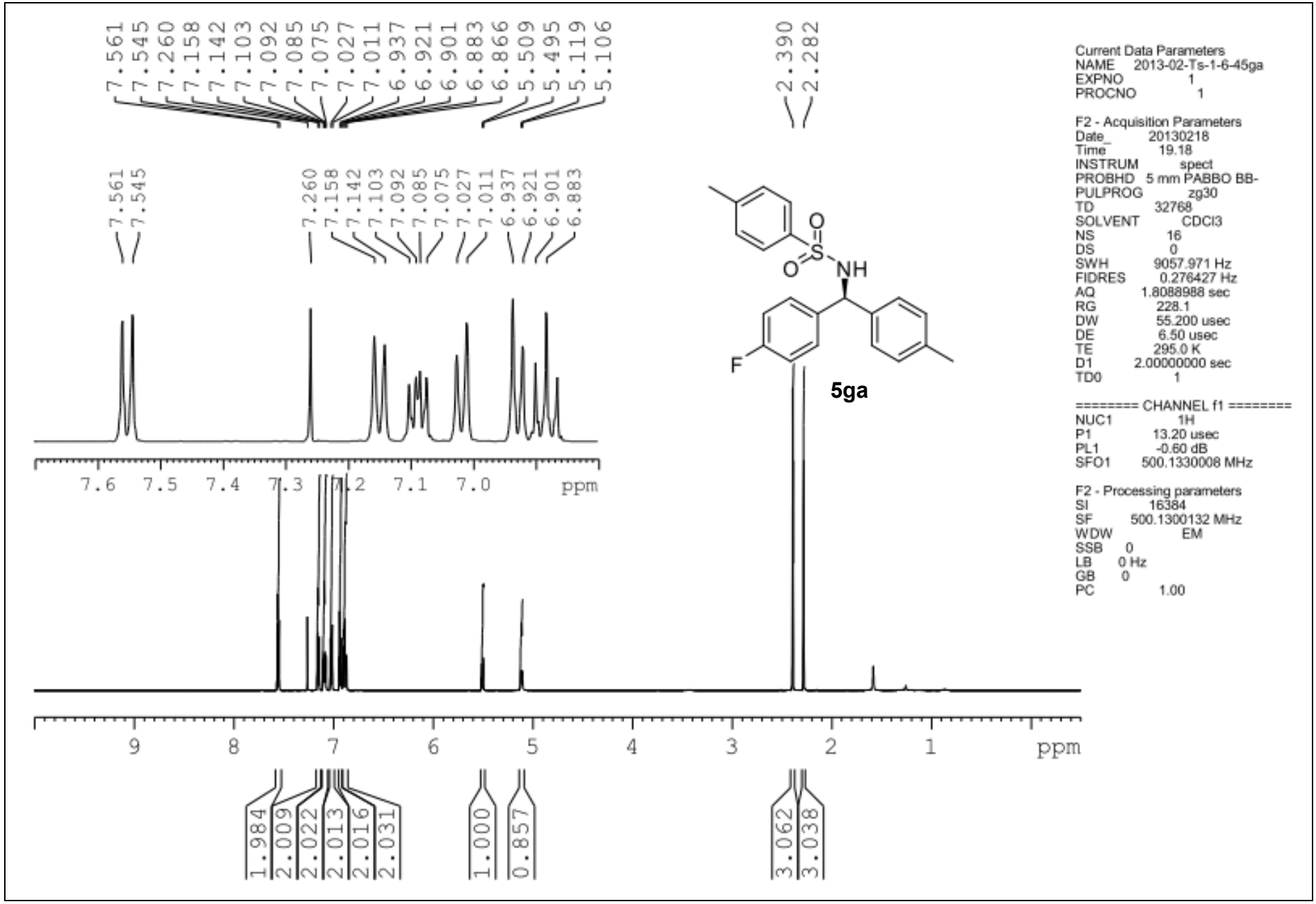
Current Data Parameters
NAME Ts-1-7
EXPNO 1
PROCNO 1

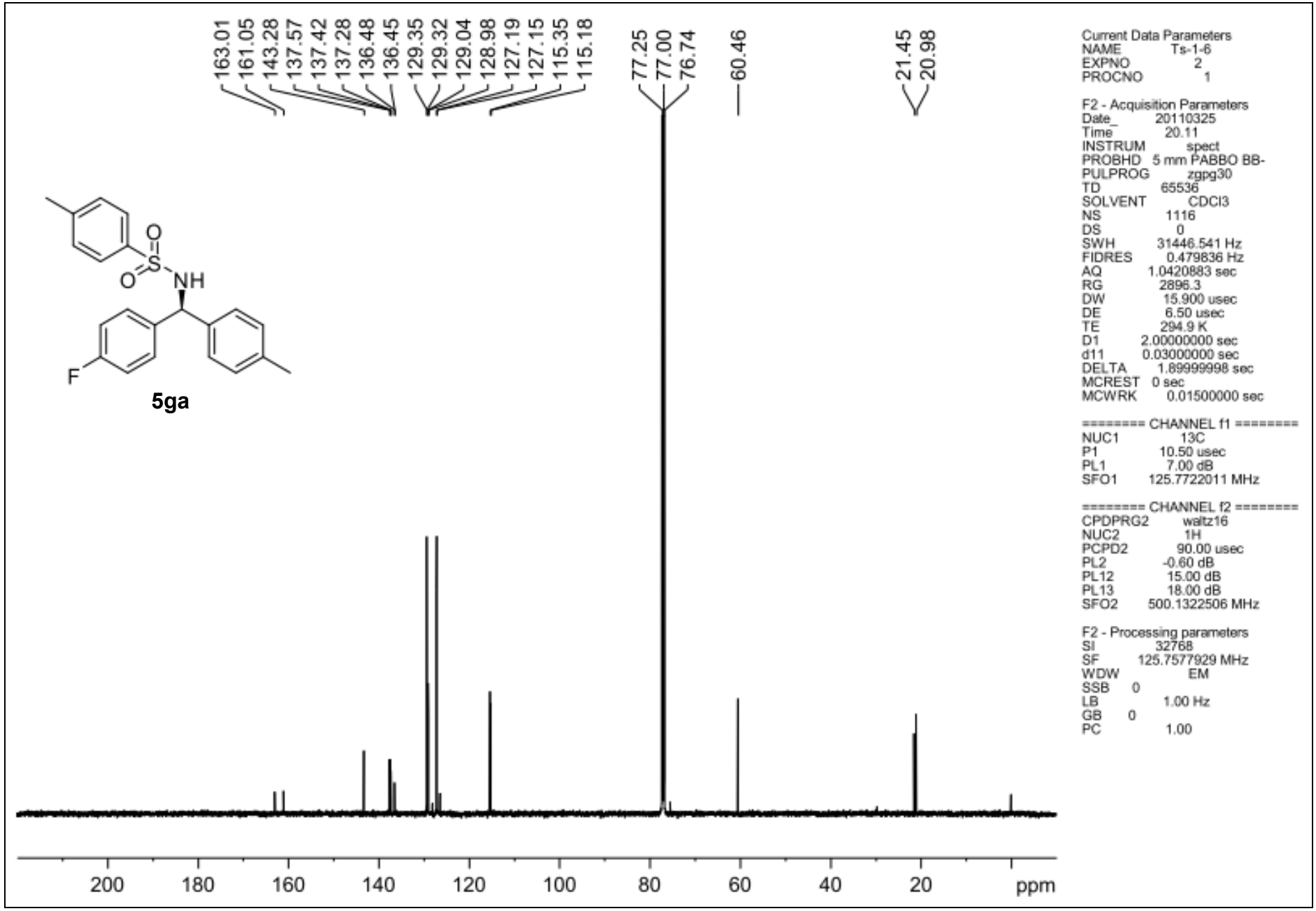
F2 - Acquisition Parameters
Date_ 20110325
Time 21.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 7507.507 Hz
FIDRES 0.458222 Hz
AQ 1.0912910 sec
RG 161.3
DW 66.600 usec
DE 6.50 usec
TE 293.6 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec

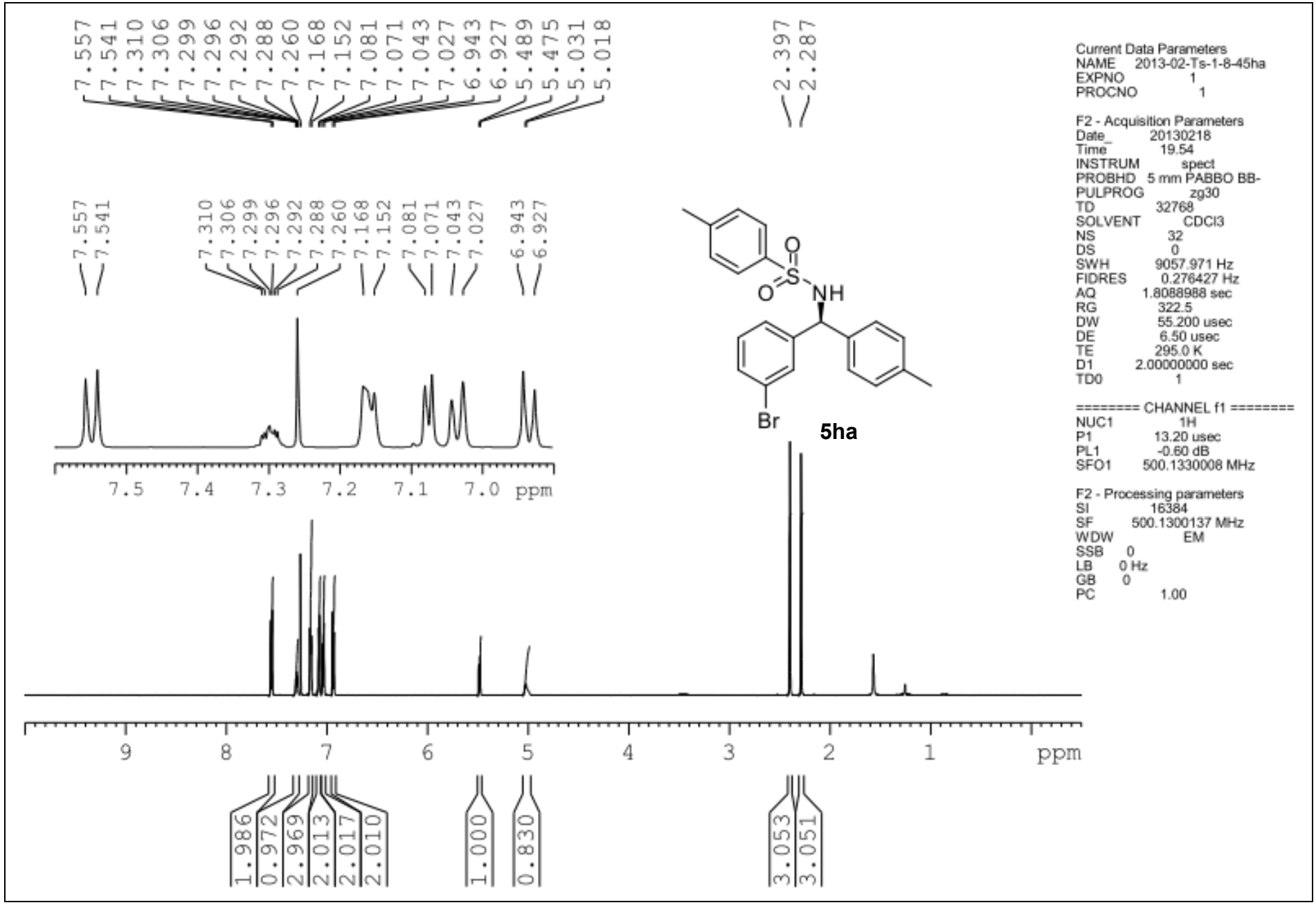
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0 dB
SFO1 500.1332508 MHz

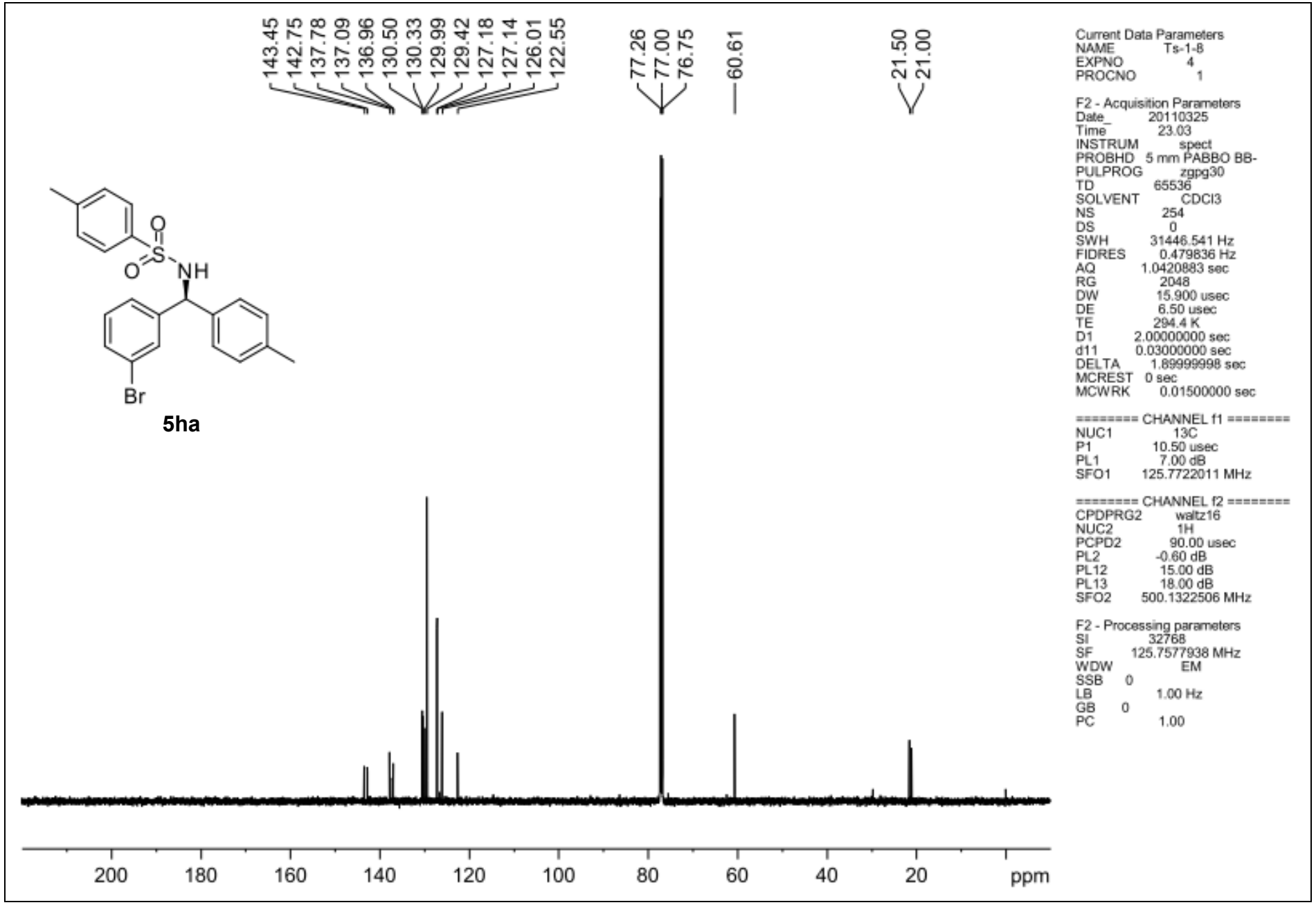
F2 - Processing parameters
SI 16384
SF 500.1300128 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

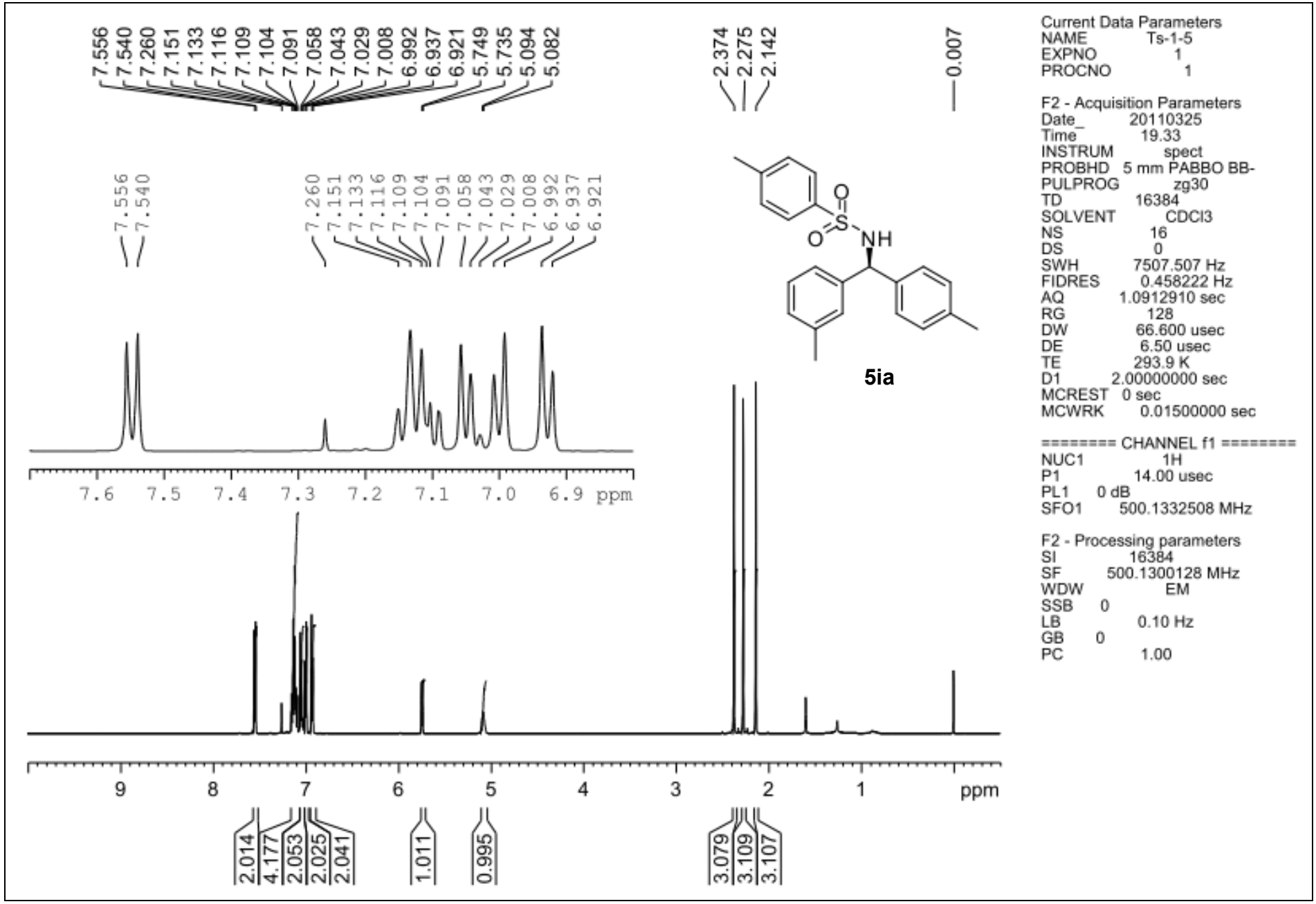

163.70
161.74
143.36
143.24
143.19
137.72
137.19
137.07
130.00
129.93
129.37
127.18
122.95
122.93
114.44
114.42
114.26
77.25
77.00
76.74
60.64
21.44
20.99
O
S
O
NH
F
5fa
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME Ts-1-7
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110325
Time 21.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 685
DS 0
SWH 31446.541 Hz
FIDRES 0.479836 Hz
AQ 1.0420883 sec
RG 2048
DW 15.900 usec
DE 6.50 usec
TE 294.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 125.7722011 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1322506 MHz
F2 - Processing parameters
SI 32768
SF 125.7577937 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00


7.561
7.545
7.260
7.158
7.142
7.103
7.092
7.085
7.075
7.027
7.011
6.937
6.921
6.901
6.883
6.866
5.509
5.495
5.119
5.106
2.390
2.282
7.6 7.5 7.4 7.3 7.2 7.1 7.0 ppm
9 8 7 6 5 4 3 2 1 ppm
1.984
2.009
2.022
2.013
2.016
2.031
1.000
0.857
3.062
3.038
5ga
Current Data Parameters
NAME 2013-02-Ts-1-6-45ga
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130218
Time 19.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 9057.971 Hz
FIDRES 0.276427 Hz
AQ 1.8088988 sec
RG 228.1
DW 55.200 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.20 usec
PL1 -0.60 dB
SFO1 500.1330008 MHz
F2 - Processing parameters
SI 16384
SF 500.1300132 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00


163.01
161.05
143.28
137.57
137.42
137.28
136.48
136.45
129.35
129.32
129.04
128.98
127.19
127.15
115.35
115.18
77.25
77.00
76.74
60.46
21.45
20.98
O
S
O
NH
F
5ga
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME Ts-1-6
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110325
Time 20.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1116
DS 0
SWH 31446.541 Hz
FIDRES 0.479836 Hz
AQ 1.0420883 sec
RG 2896.3
DW 15.900 usec
DE 6.50 usec
TE 294.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 125.7722011 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1322506 MHz
F2 - Processing parameters
SI 32768
SF 125.7577929 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00


7.557
7.541
7.310
7.306
7.299
7.296
7.292
7.288
7.260
7.168
7.152
7.081
7.071
7.043
7.027
6.943
6.927
5.489
5.475
5.031
5.018
2.397
2.287
O
S
O
NH
Br
5ha
7.5
7.4
7.3
7.2
7.1
7.0
ppm
9
8
7
6
5
4
3
2
1
ppm
1.986
0.972
2.969
2.013
2.017
2.010
1.000
0.830
3.053
3.051
Current Data Parameters
NAME 2013-02-Ts-1-8-45ha
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130218
Time 19.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9057.971 Hz
FIDRES 0.276427 Hz
AQ 1.8088988 sec
RG 322.5
DW 55.200 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.20 usec
PL1 -0.60 dB
SFO1 500.1330008 MHz
F2 - Processing parameters
SI 16384
SF 500.1300137 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00


143.45
142.75
137.78
137.09
136.96
130.50
130.33
129.99
129.42
127.18
127.14
126.01
122.55
77.26
77.00
76.75
60.61
21.50
21.00
O
S
O
NH
Br
5ha
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME Ts-1-8
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110325
Time 23.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 254
DS 0
SWH 31446.541 Hz
FIDRES 0.479836 Hz
AQ 1.0420883 sec
RG 2048
DW 15.900 usec
DE 6.50 usec
TE 294.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 125.7722011 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1322506 MHz
F2 - Processing parameters
SI 32768
SF 125.7577938 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

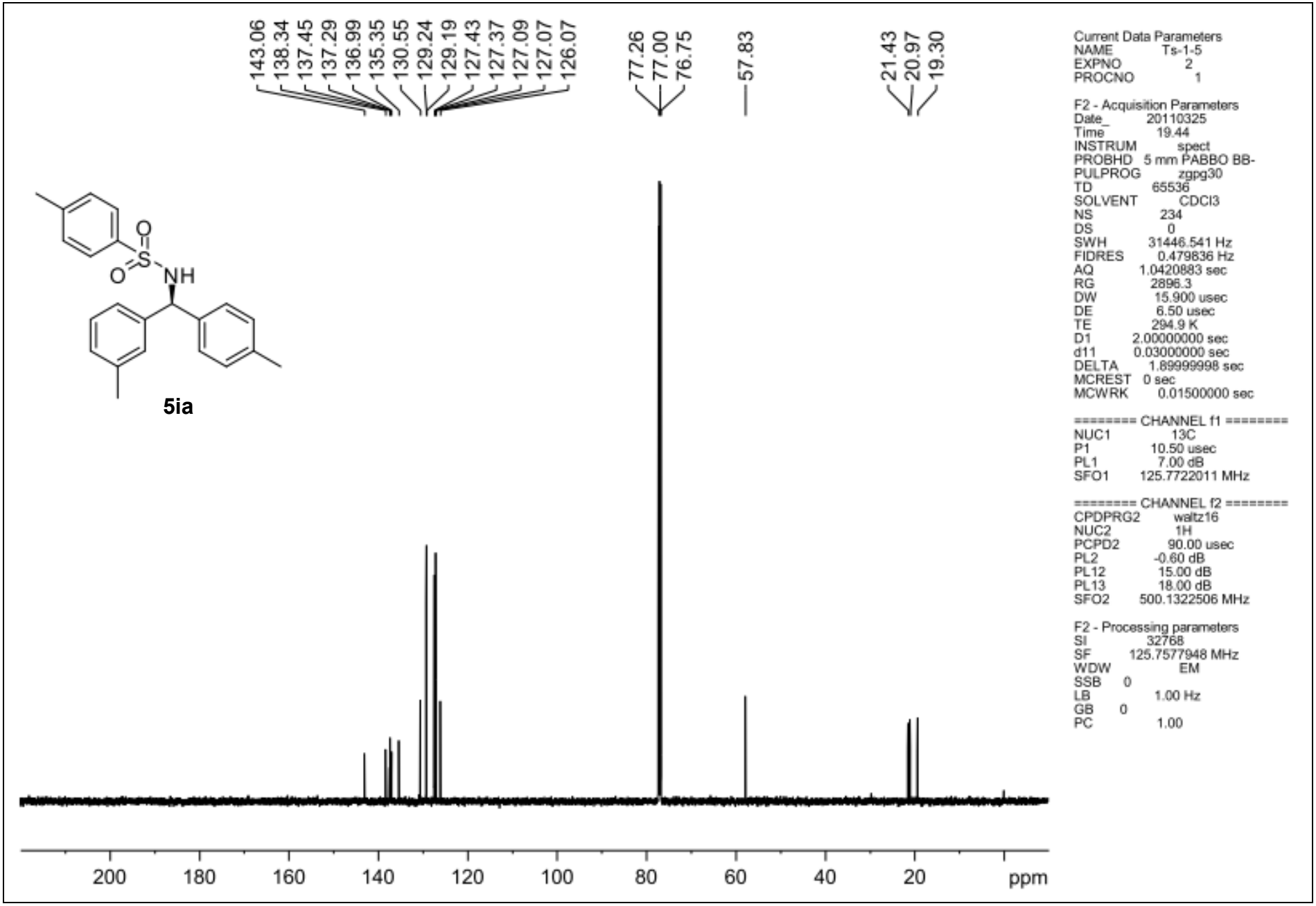


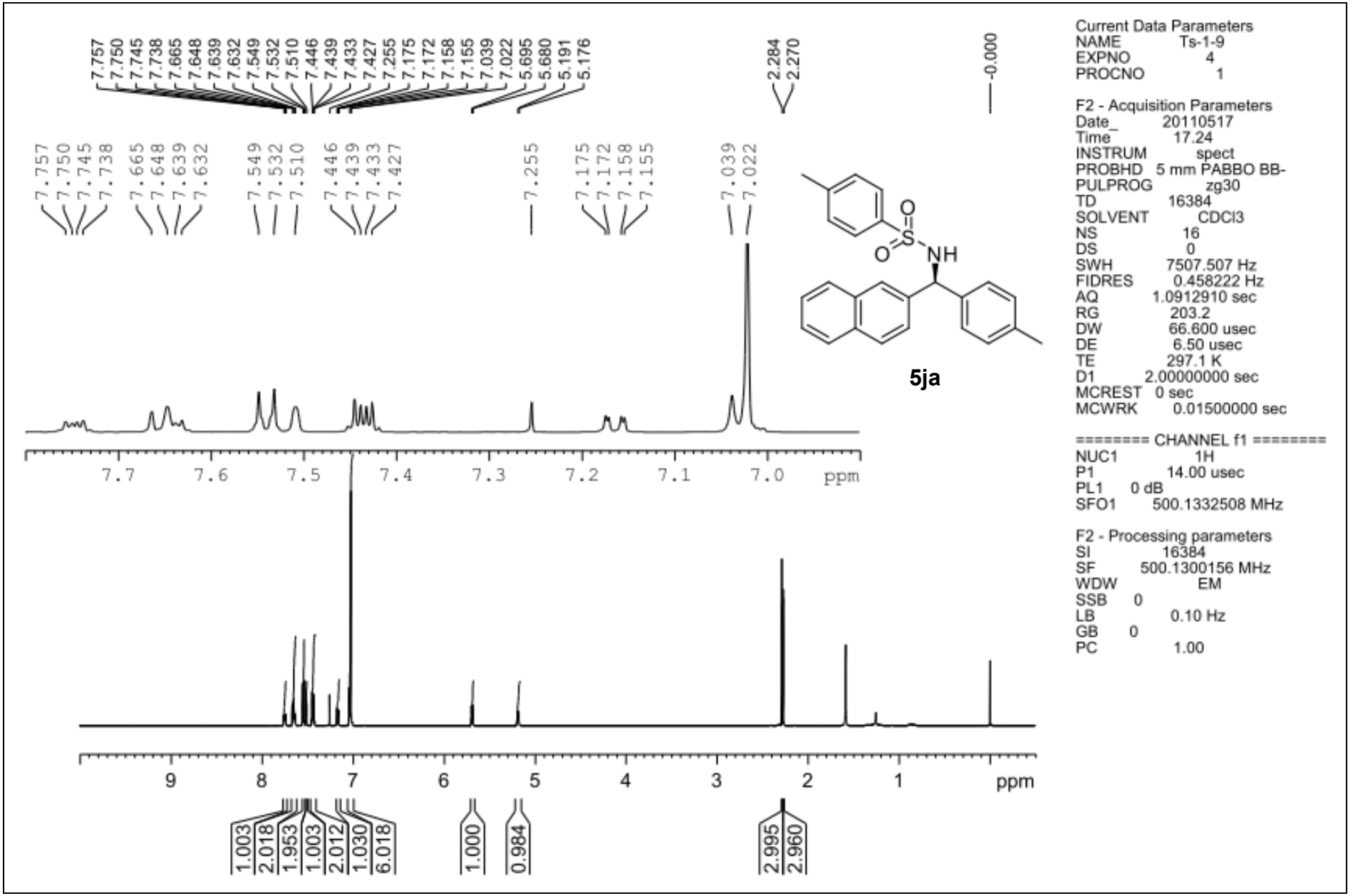
Current Data Parameters
NAME Ts-1-5
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110325
Time 19.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 7507.507 Hz
FIDRES 0.458222 Hz
AQ 1.0912910 sec
RG 128
DW 66.600 usec
DE 6.50 usec
TE 293.9 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0 dB
SFO1 500.1332508 MHz

F2 - Processing parameters
SI 16384
SF 500.1300128 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00


143.06
138.34
137.45
137.29
136.99
135.35
130.55
129.24
129.19
127.43
127.37
127.09
127.07
126.07
77.26
77.00
76.75
57.83
21.43
20.97
19.30
O
S
O
NH
5ia
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME Ts-1-5
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110325
Time 19.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 234
DS 0
SWH 31446.541 Hz
FIDRES 0.479836 Hz
AQ 1.0420883 sec
RG 2896.3
DW 15.900 usec
DE 6.50 usec
TE 294.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 125.7722011 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1322506 MHz
F2 - Processing parameters
SI 32768
SF 125.7577948 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

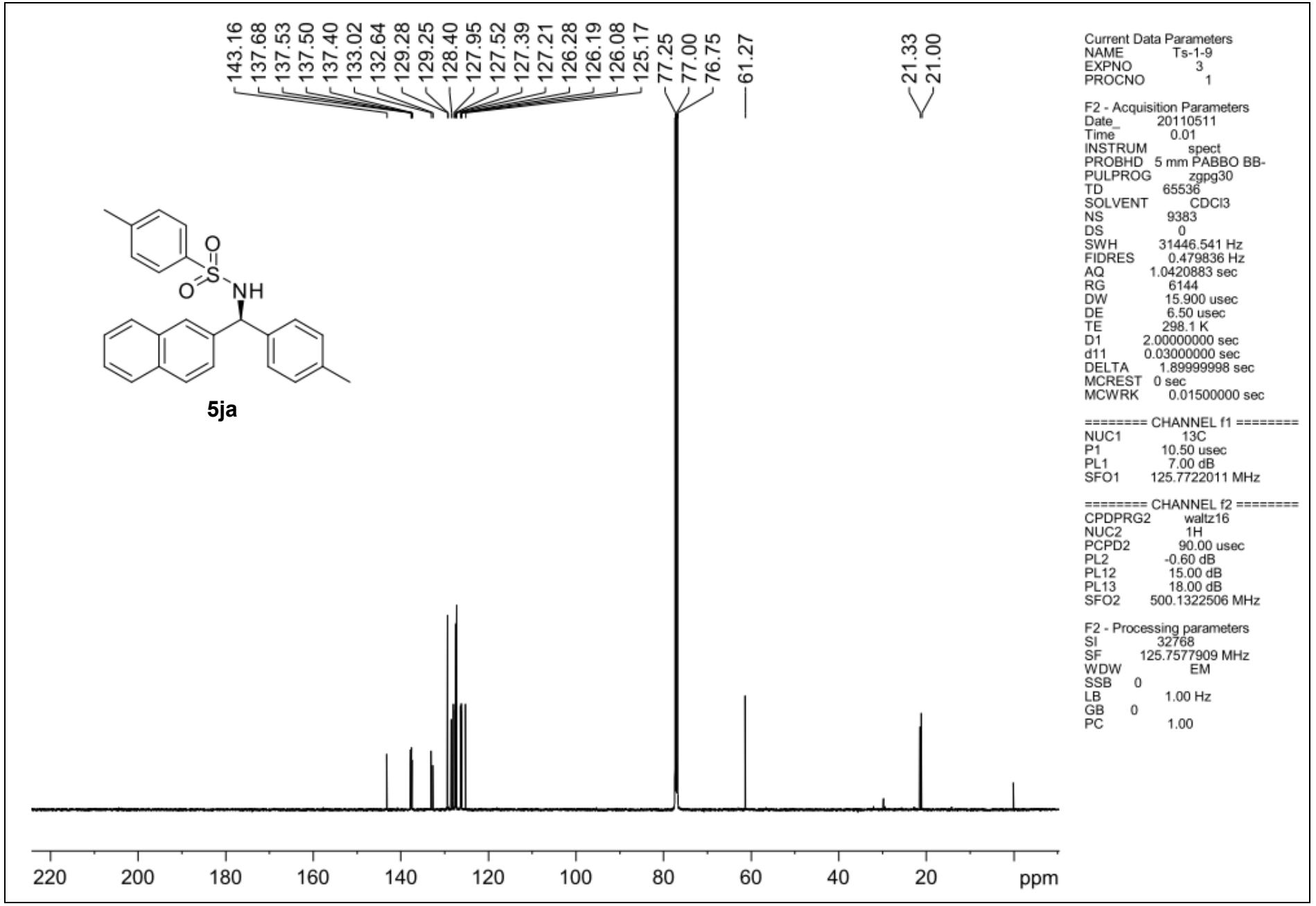


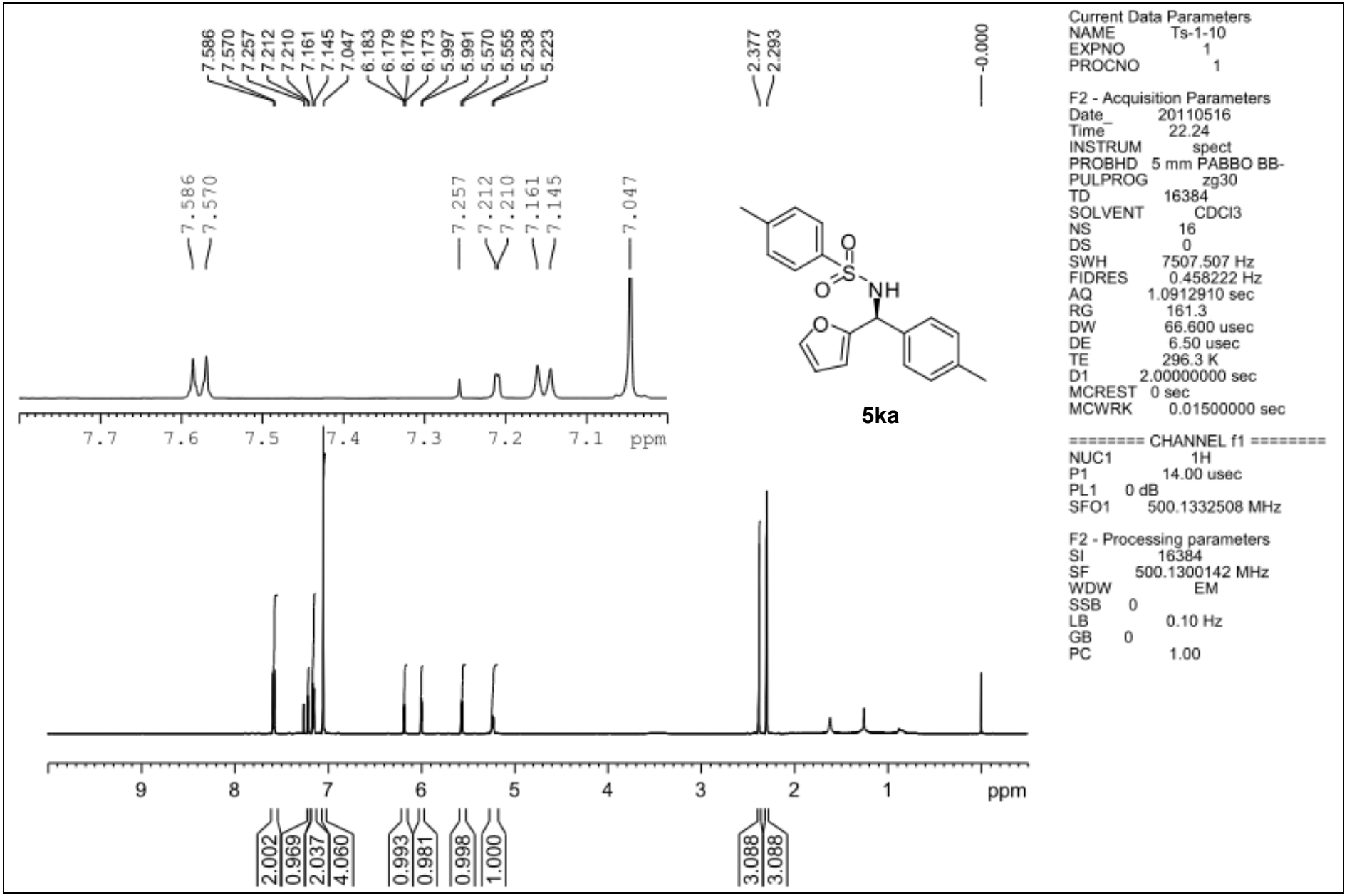
Current Data Parameters
NAME Ts-1-9
EXPNO 4
PROCNO 1

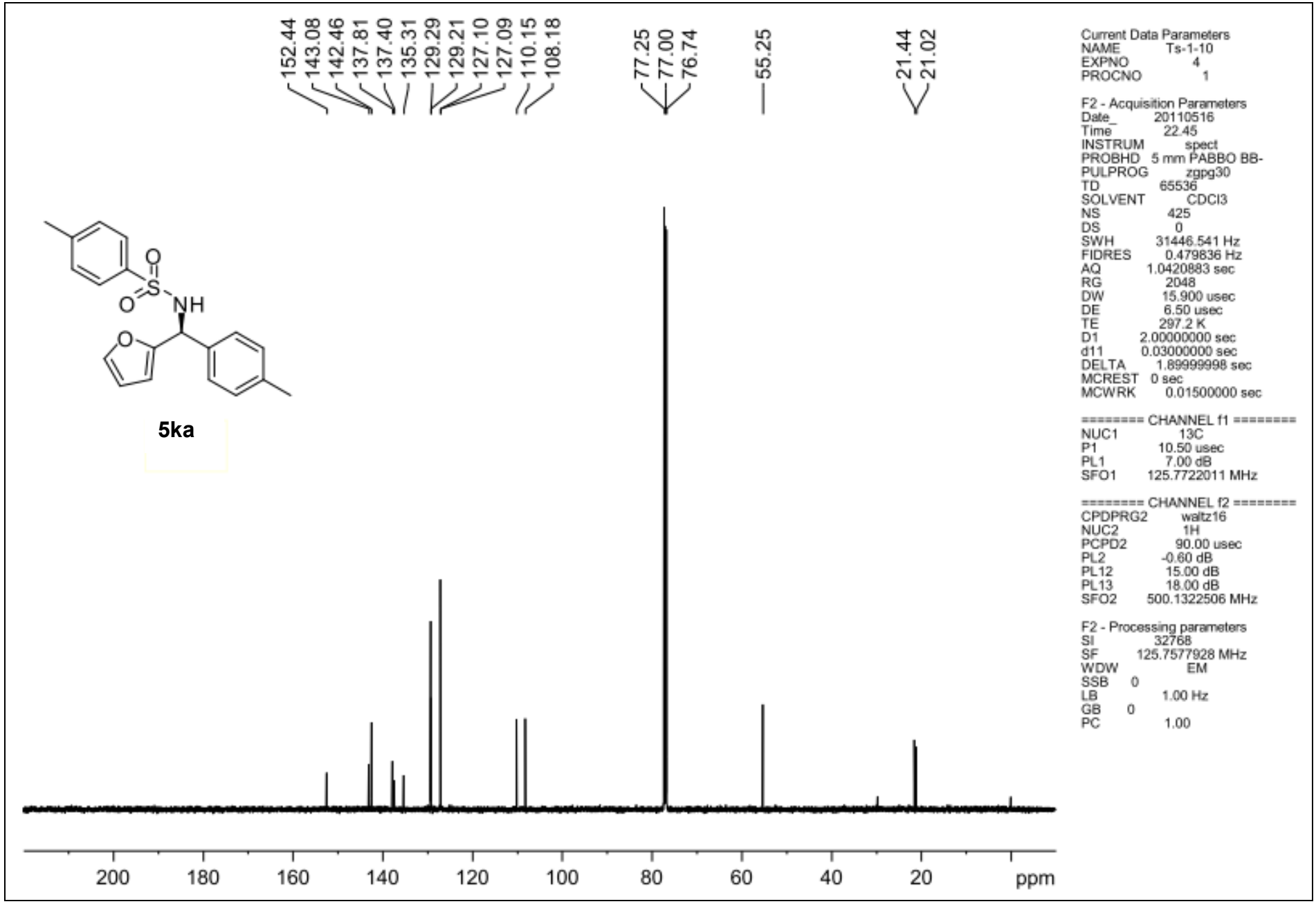
F2 - Acquisition Parameters
Date_ 20110517
Time 17.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 7507.507 Hz
FIDRES 0.458222 Hz
AQ 1.0912910 sec
RG 203.2
DW 66.600 usec
DE 6.50 usec
TE 297.1 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec

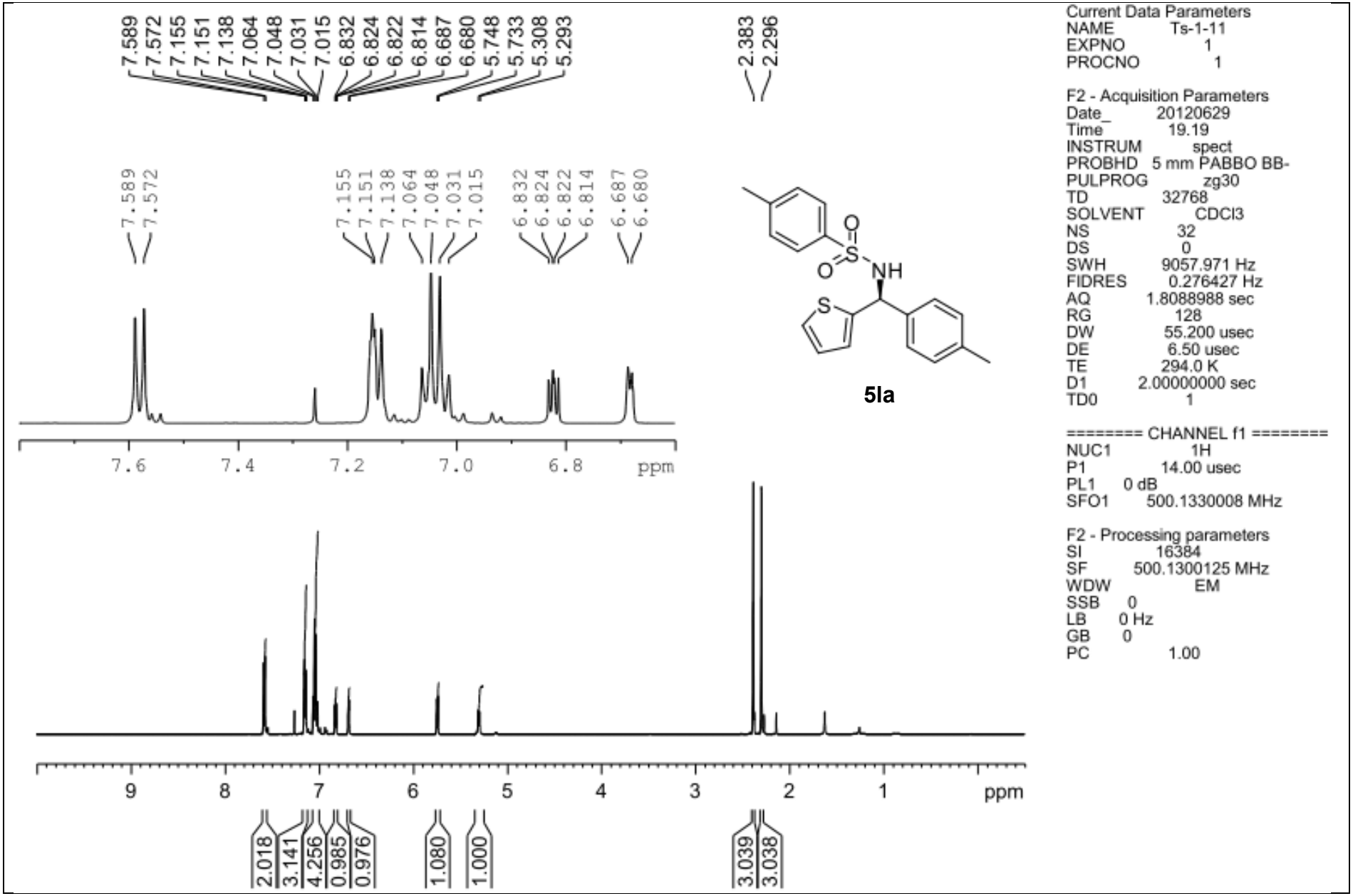
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0 dB
SFO1 500.1332508 MHz

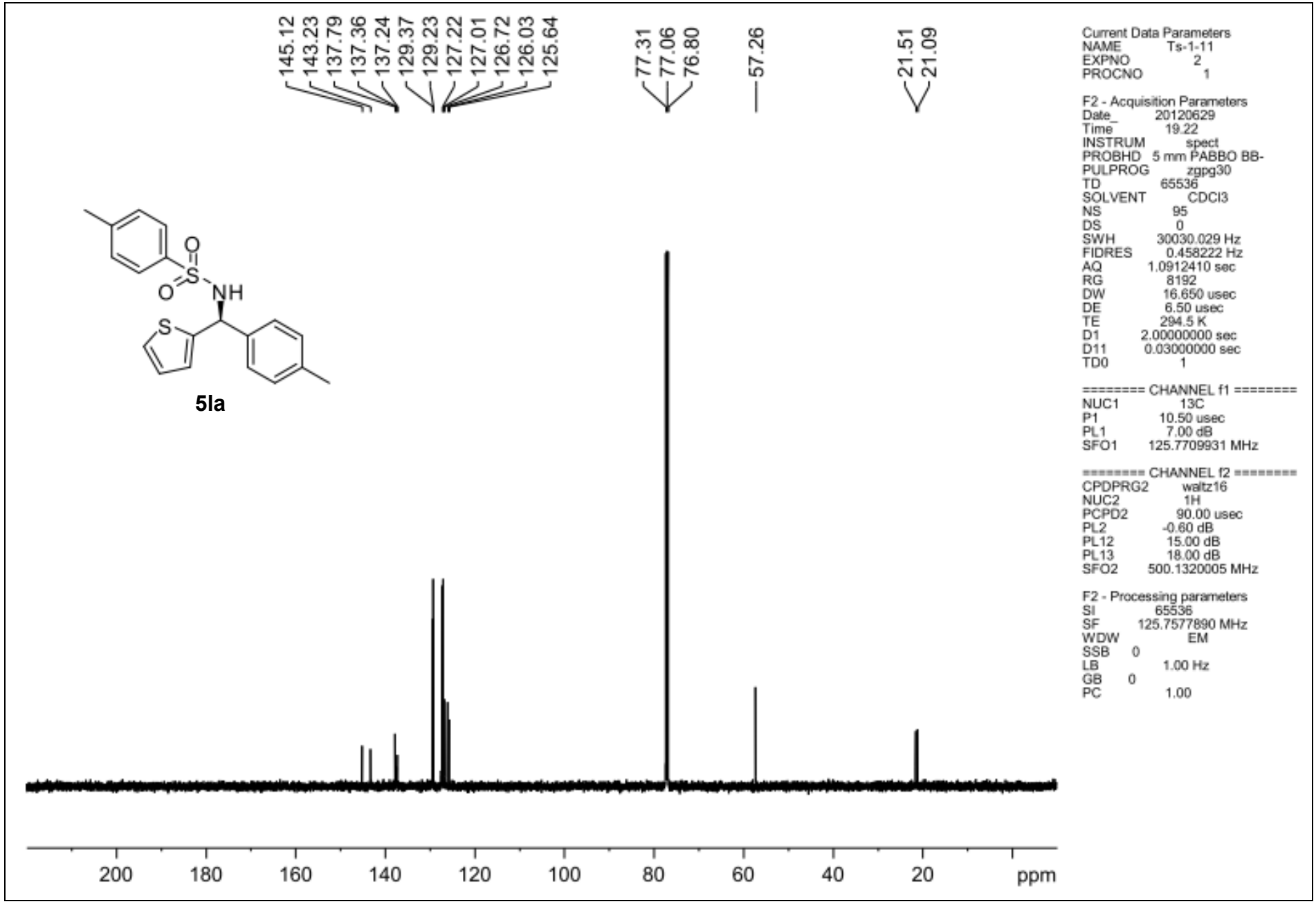
F2 - Processing parameters
SI 16384
SF 500.1300156 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

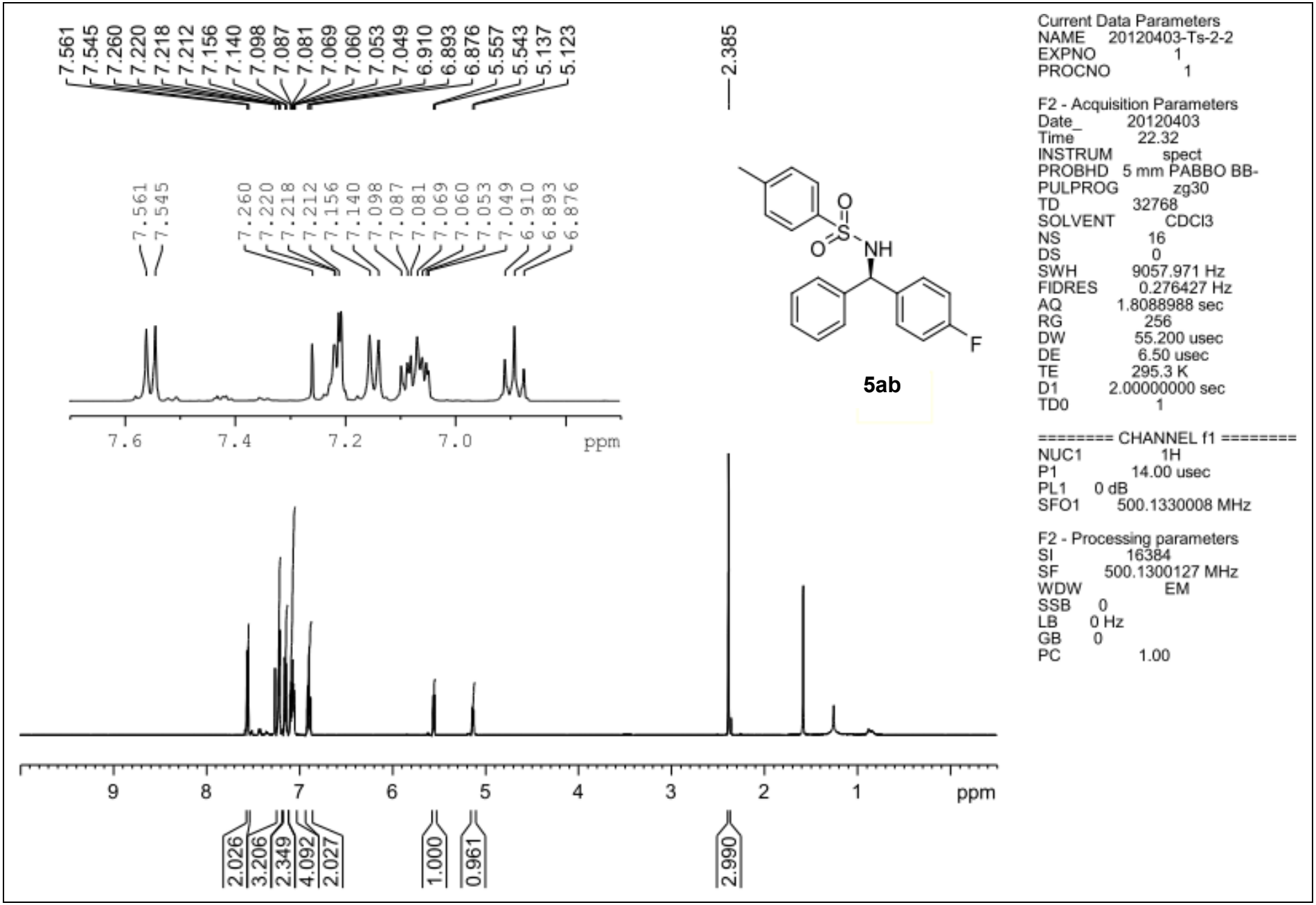

143.16
137.68
137.53
137.50
137.40
133.02
132.64
129.28
129.25
128.40
127.95
127.52
127.39
127.21
126.28
126.19
126.08
125.17
77.25
77.00
76.75
61.27
21.33
21.00
O
S
O
NH
5ja
220
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME Ts-1-9
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110511
Time 0.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 9383
DS 0
SWH 31446.541 Hz
FIDRES 0.479836 Hz
AQ 1.0420883 sec
RG 6144
DW 15.900 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 125.7722011 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1322506 MHz
F2 - Processing parameters
SI 32768
SF 125.7577909 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00


7.586
7.570
7.257
7.212
7.210
7.161
7.145
7.047
6.183
6.179
6.176
6.173
5.997
5.991
5.570
5.555
5.238
5.223
2.377
2.293
-0.000
7.7
7.6
7.5
7.4
7.3
7.2
7.1
ppm
9
8
7
6
5
4
3
2
1
ppm
2.002
0.969
2.037
4.060
0.993
0.981
0.998
1.000
3.088
3.088
5ka
Current Data Parameters
NAME Ts-1-10
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110516
Time 22.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 7507.507 Hz
FIDRES 0.458222 Hz
AQ 1.0912910 sec
RG 161.3
DW 66.600 usec
DE 6.50 usec
TE 296.3 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0 dB
SFO1 500.1332508 MHz
F2 - Processing parameters
SI 16384
SF 500.1300142 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00


152.44
143.08
142.46
137.81
137.40
135.31
129.29
129.21
127.10
127.09
110.15
108.18
77.25
77.00
76.74
55.25
21.44
21.02
O
S
O
NH
O
5ka
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME Ts-1-10
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110516
Time 22.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 425
DS 0
SWH 31446.541 Hz
FIDRES 0.479836 Hz
AQ 1.0420883 sec
RG 2048
DW 15.900 usec
DE 6.50 usec
TE 297.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 125.7722011 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1322506 MHz
F2 - Processing parameters
SI 32768
SF 125.7577928 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00


7.589
7.572
7.155
7.151
7.138
7.064
7.048
7.031
7.015
6.832
6.824
6.822
6.814
6.687
6.680
5.748
5.733
5.308
5.293
2.383
2.296
7.6
7.4
7.2
7.0
6.8
ppm
9
8
7
6
5
4
3
2
1
ppm
2.018
3.141
4.256
0.985
0.976
1.080
1.000
3.039
3.038
O
S
NH
O
S
5la
Current Data Parameters
NAME Ts-1-11
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120629
Time 19.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9057.971 Hz
FIDRES 0.276427 Hz
AQ 1.8088988 sec
RG 128
DW 55.200 usec
DE 6.50 usec
TE 294.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0 dB
SFO1 500.1330008 MHz
F2 - Processing parameters
SI 16384
SF 500.1300125 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00


145.12
143.23
137.79
137.36
137.24
129.37
129.23
127.22
127.01
126.72
126.03
125.64
77.31
77.06
76.80
57.26
21.51
21.09
O
S
O
NH
S
5la
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME Ts-1-11
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120629
Time 19.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 95
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 8192
DW 16.650 usec
DE 6.50 usec
TE 294.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 125.7709931 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 65536
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

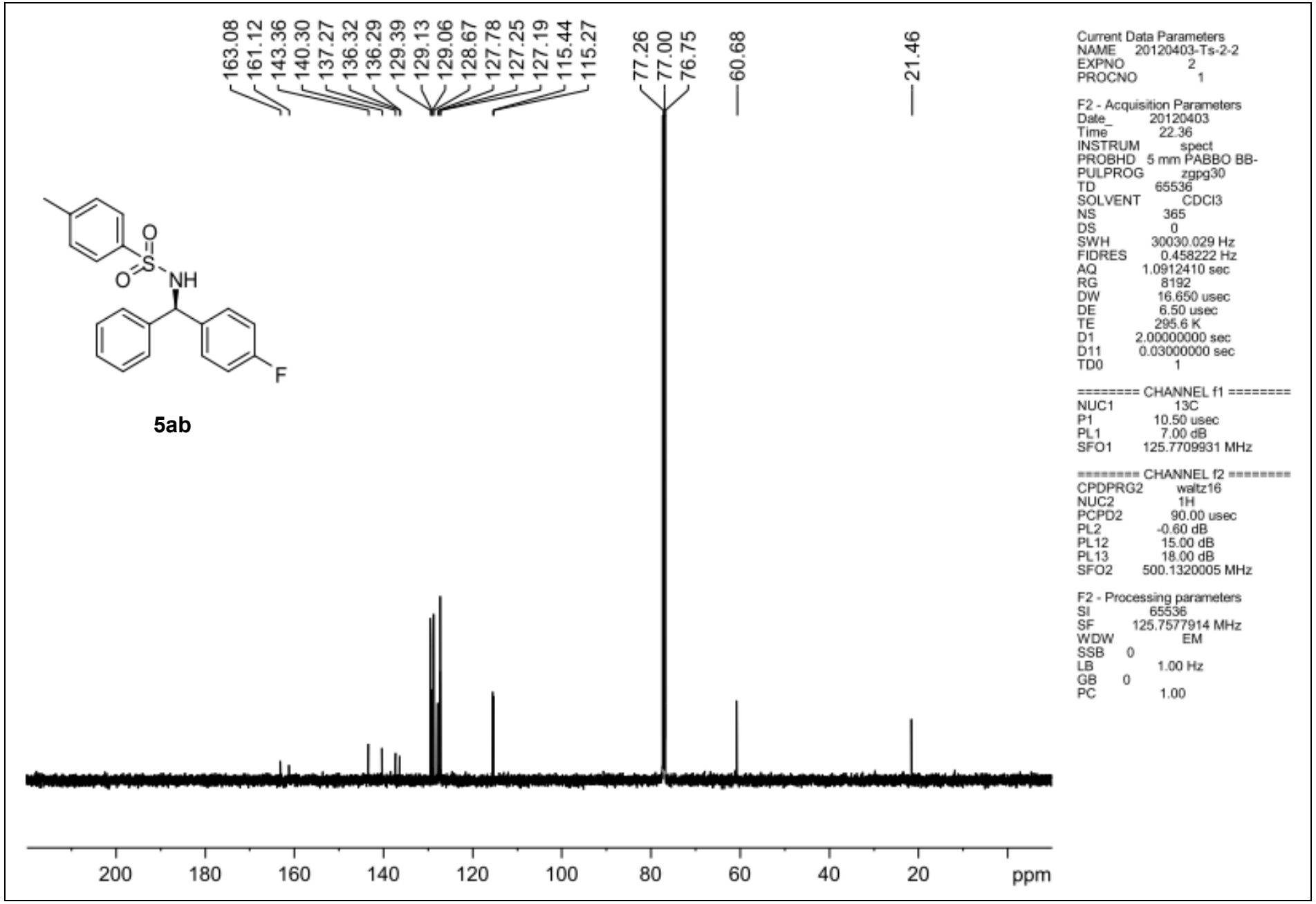


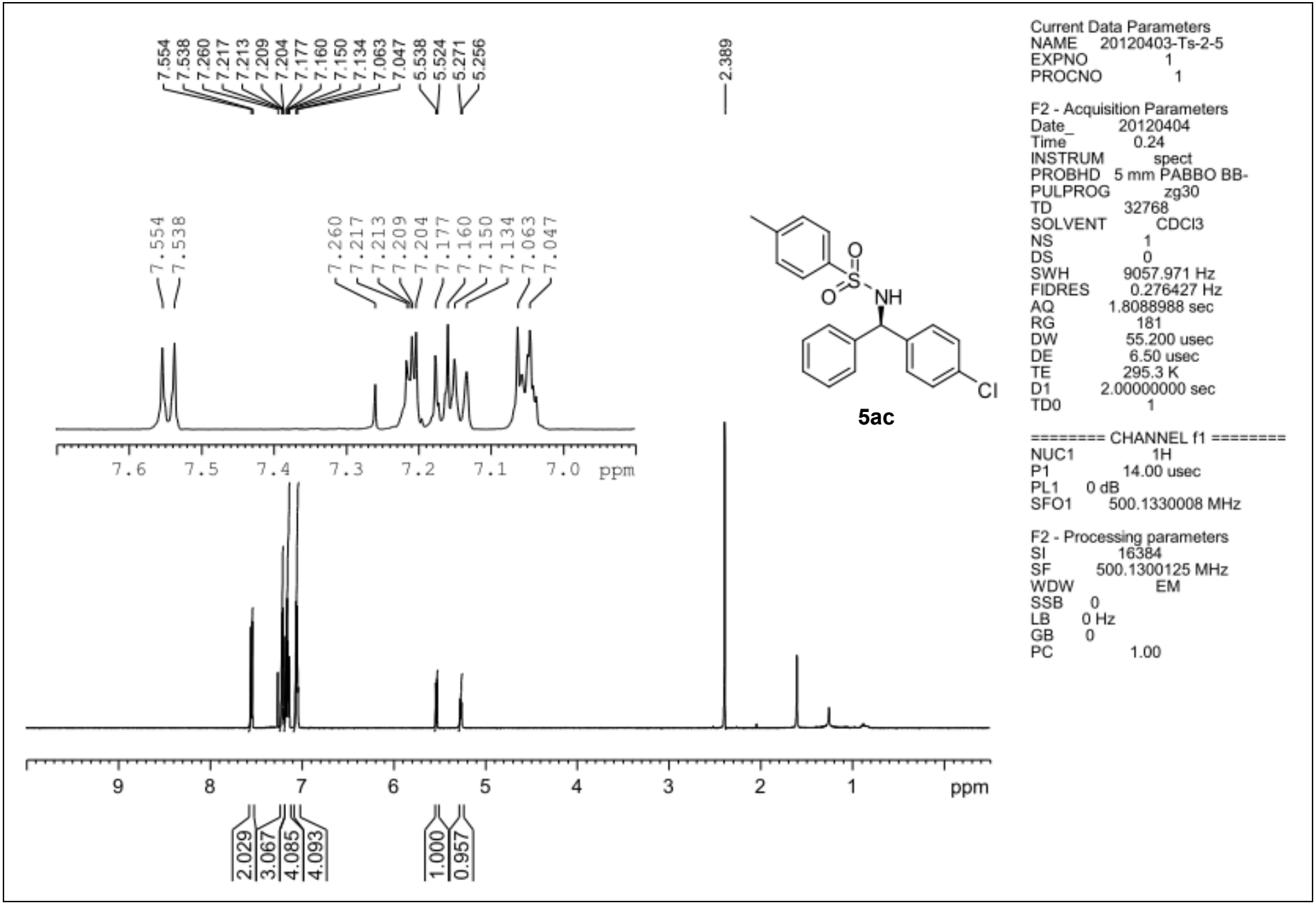
Current Data Parameters
NAME 20120403-Ts-2-2
EXPNO 1
PROCNO 1

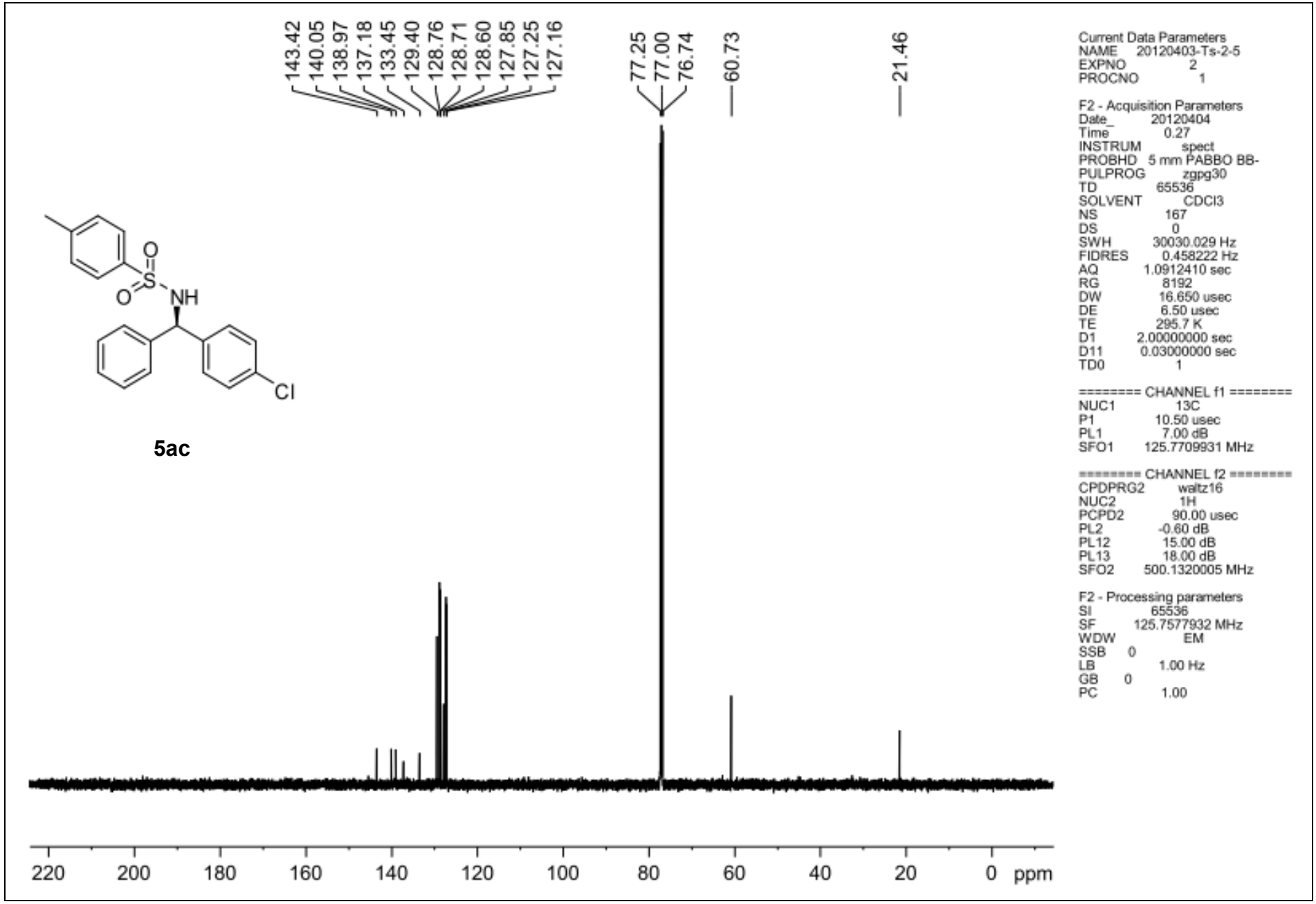
F2 - Acquisition Parameters
Date_ 20120403
Time 22.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 9057.971 Hz
FIDRES 0.276427 Hz
AQ 1.8088988 sec
RG 256
DW 55.200 usec
DE 6.50 usec
TE 295.3 K
D1 2.00000000 sec
TD0 1

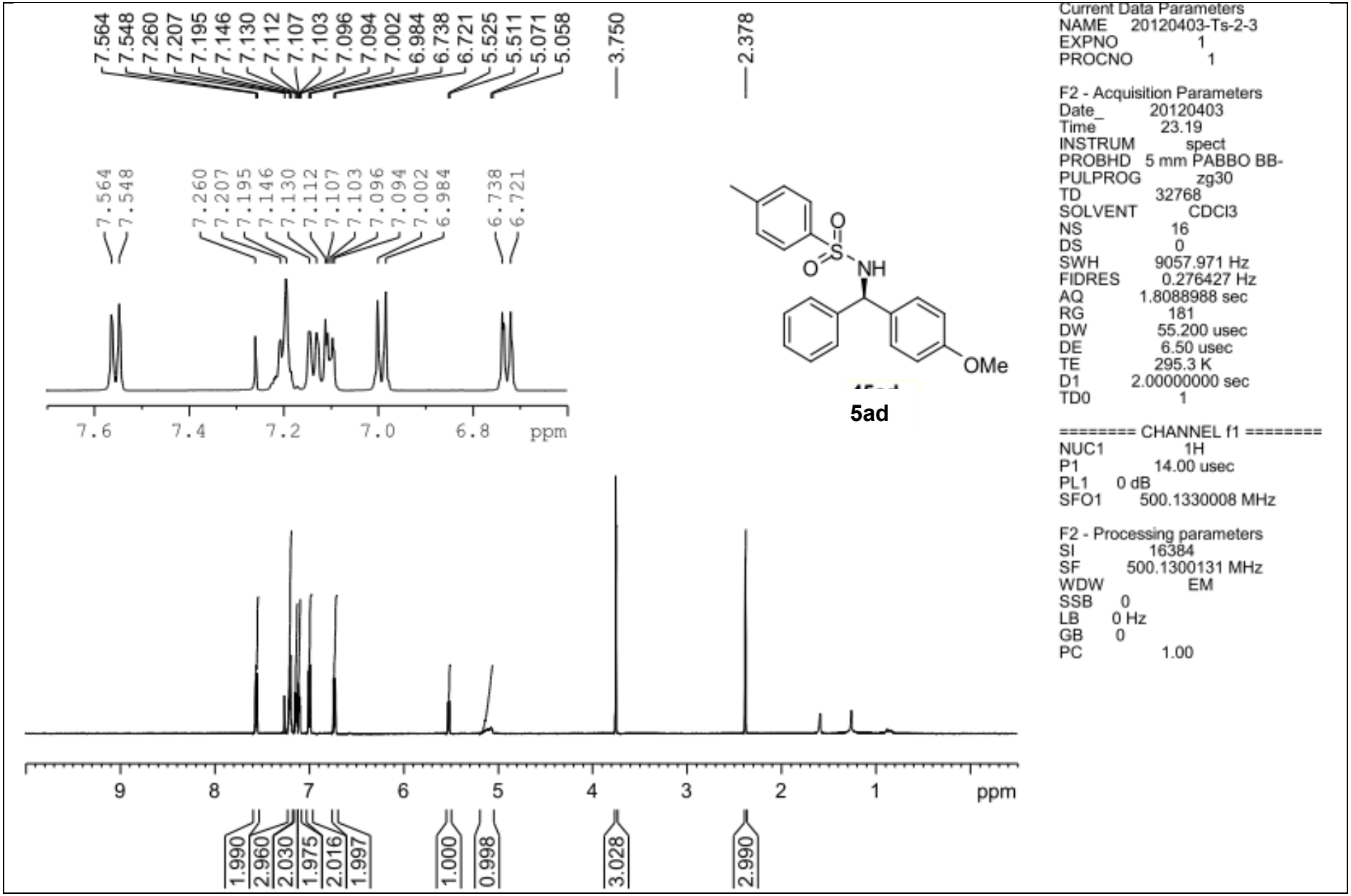
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0 dB
SFO1 500.1330008 MHz

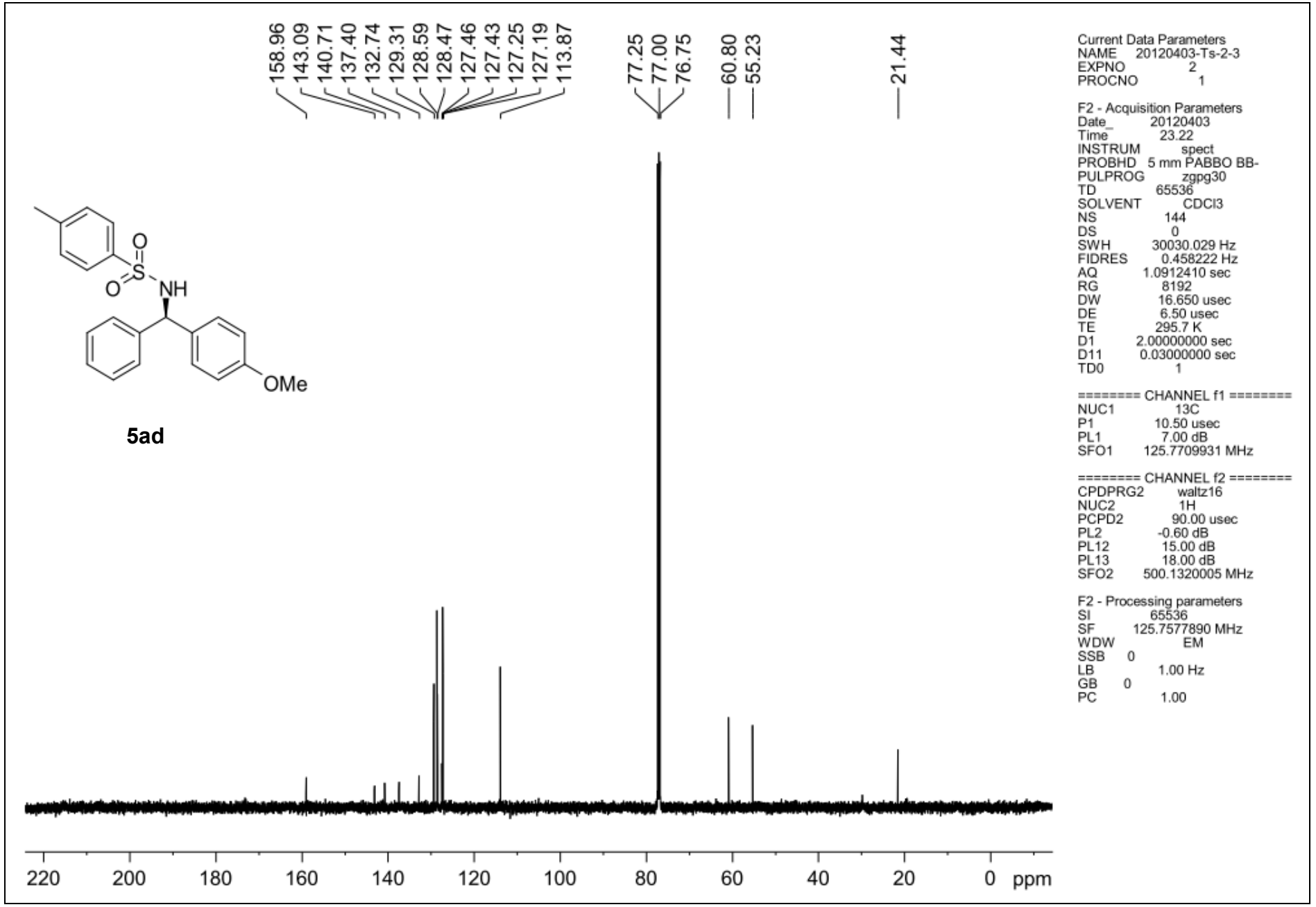
F2 - Processing parameters
SI 16384
SF 500.1300127 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

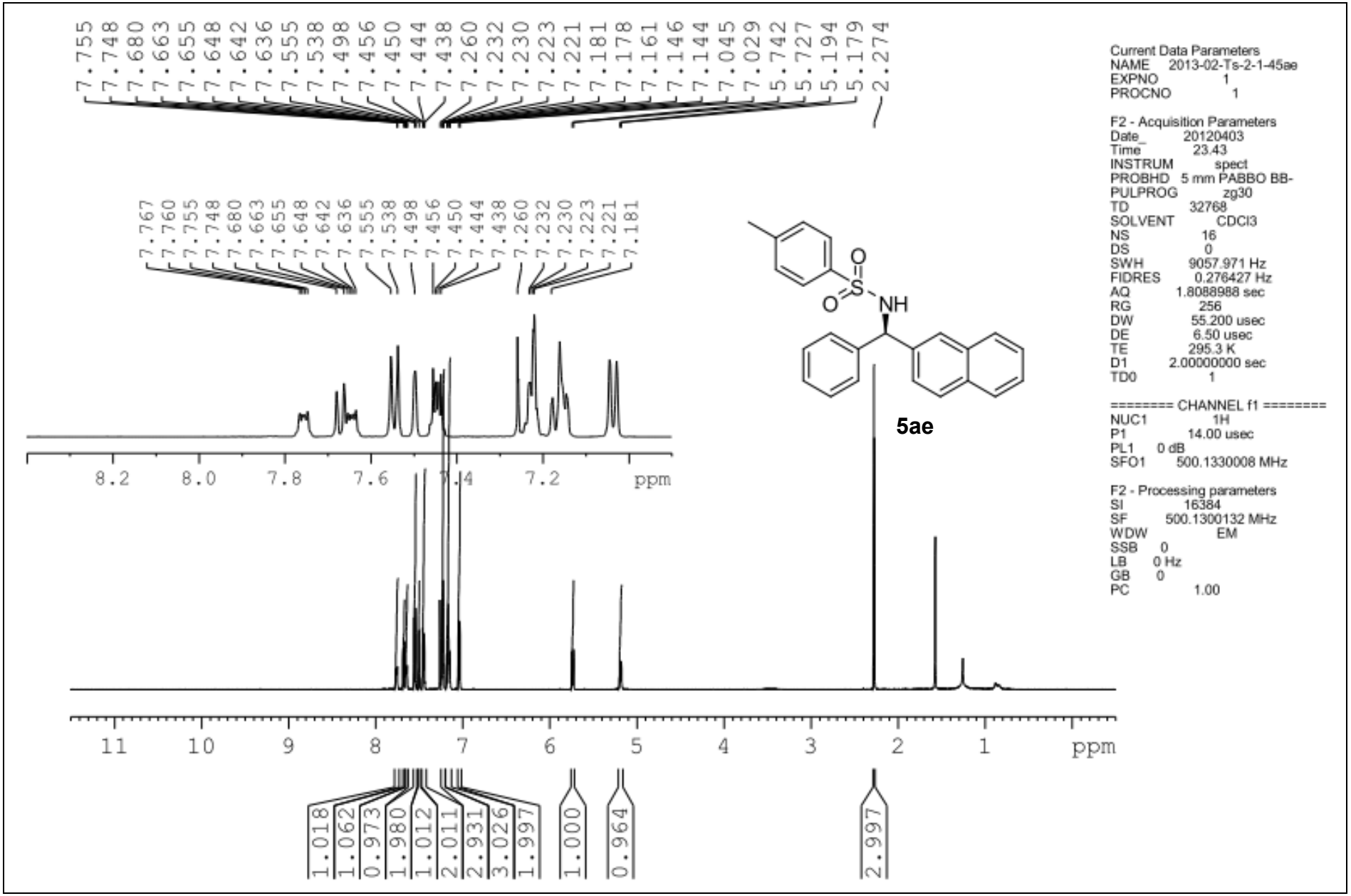

163.08
161.12
143.36
140.30
137.27
136.32
136.29
129.39
129.13
129.06
128.67
127.78
127.25
127.19
115.44
115.27
77.26
77.00
76.75
60.68
21.46
O
S
O
NH
F
5ab
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME 20120403-Ts-2-2
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120403
Time 22.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 365
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 8192
DW 16.650 usec
DE 6.50 usec
TE 295.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 125.7709931 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 65536
SF 125.7577914 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

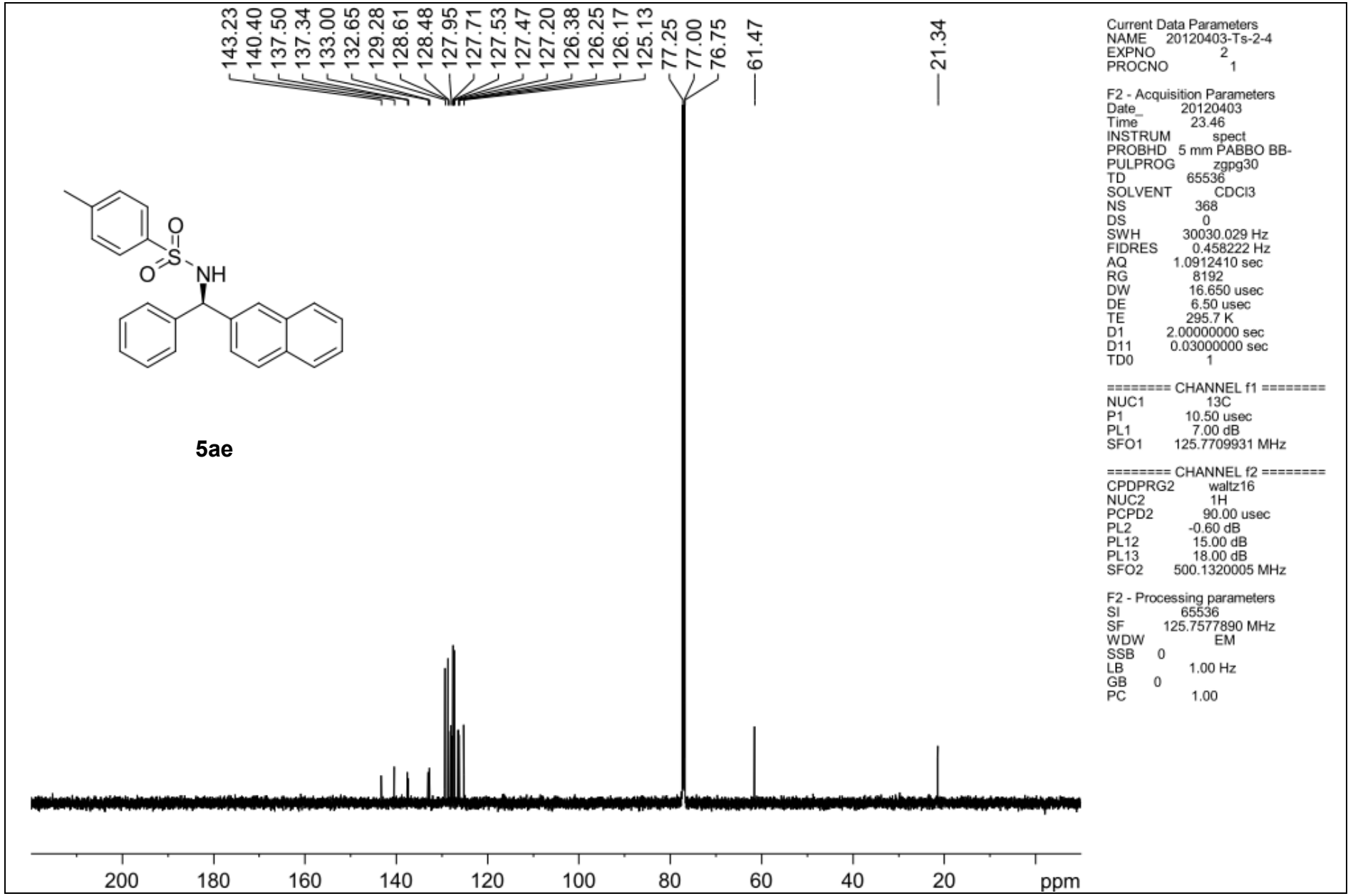

7.554
7.538
7.260
7.217
7.213
7.209
7.204
7.177
7.160
7.150
7.134
7.063
7.047
5.538
5.524
5.271
5.256
2.389
7.6
7.5
7.4
7.3
7.2
7.1
7.0
ppm
9
8
7
6
5
4
3
2
1
ppm
2.029
3.067
4.085
4.093
1.000
0.957
O
S
O
NH
Cl
5ac
Current Data Parameters
NAME 20120403-Ts-2-5
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120404
Time 0.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 1
DS 0
SWH 9057.971 Hz
FIDRES 0.276427 Hz
AQ 1.8088988 sec
RG 181
DW 55.200 usec
DE 6.50 usec
TE 295.3 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0 dB
SFO1 500.1330008 MHz
F2 - Processing parameters
SI 16384
SF 500.1300125 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00


143.42
140.05
138.97
137.18
133.45
129.40
128.76
128.71
128.60
127.85
127.25
127.16
77.25
77.00
76.74
60.73
21.46
O
S
O
NH
Cl
5ac
220
200
180
160
140
120
100
80
60
40
20
0
ppm
Current Data Parameters
NAME 20120403-Ts-2-5
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120404
Time 0.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 167
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 8192
DW 16.650 usec
DE 6.50 usec
TE 295.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 125.7709931 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 65536
SF 125.7577932 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

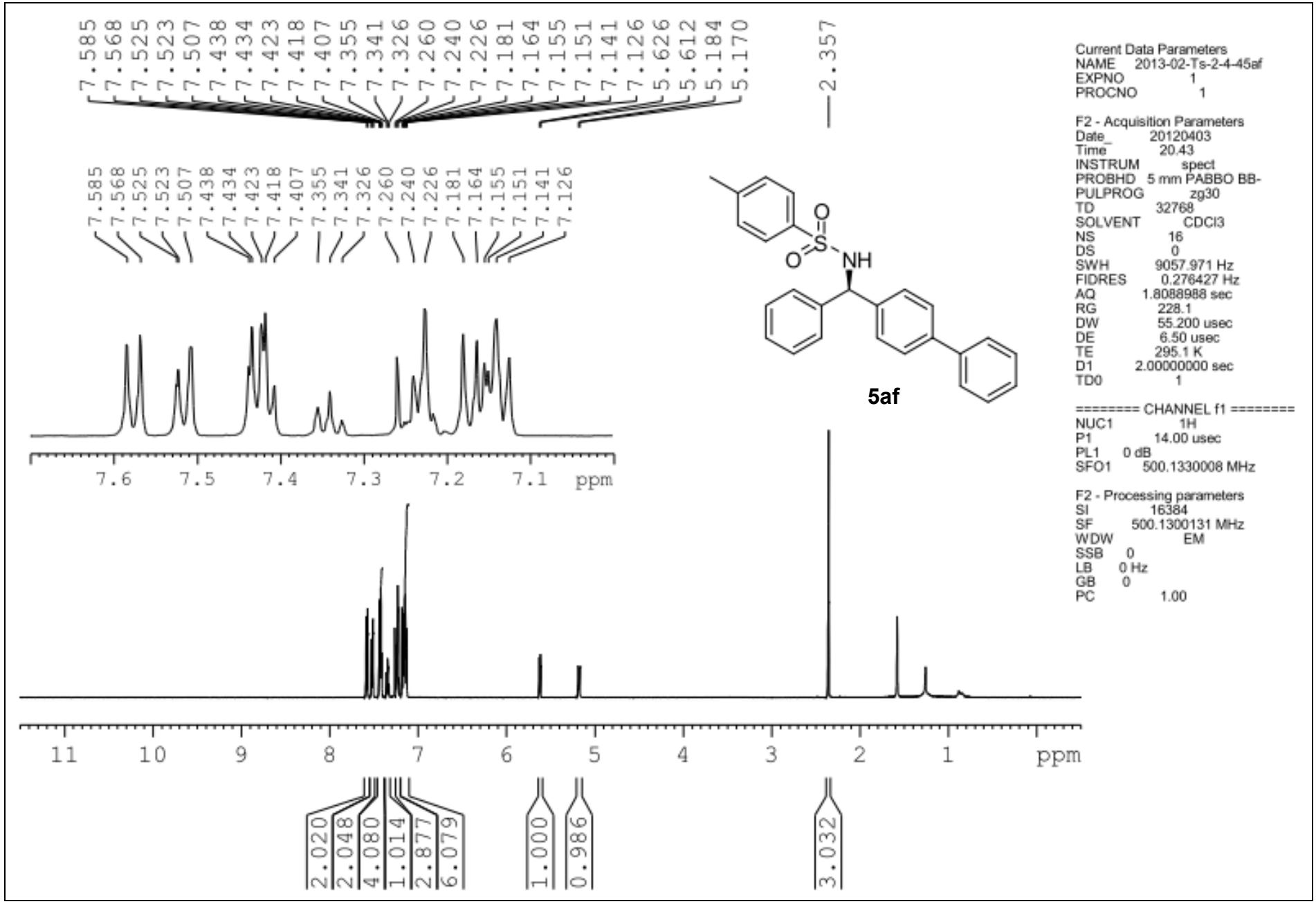

7.564
7.548
7.260
7.207
7.195
7.146
7.130
7.112
7.107
7.103
7.096
7.094
7.002
6.984
6.738
6.721
5.525
5.511
5.071
5.058
3.750
2.378
7.6
7.4
7.2
7.0
6.8
ppm
NH
OMe
5ad
9
8
7
6
5
4
3
2
1
ppm
1.990
2.960
2.030
1.975
2.016
1.997
1.000
0.998
3.028
2.990
Current Data Parameters
NAME 20120403-Ts-2-3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120403
Time 23.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 9057.971 Hz
FIDRES 0.276427 Hz
AQ 1.8088988 sec
RG 181
DW 55.200 usec
DE 6.50 usec
TE 295.3 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0 dB
SFO1 500.1330008 MHz
F2 - Processing parameters
SI 16384
SF 500.1300131 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

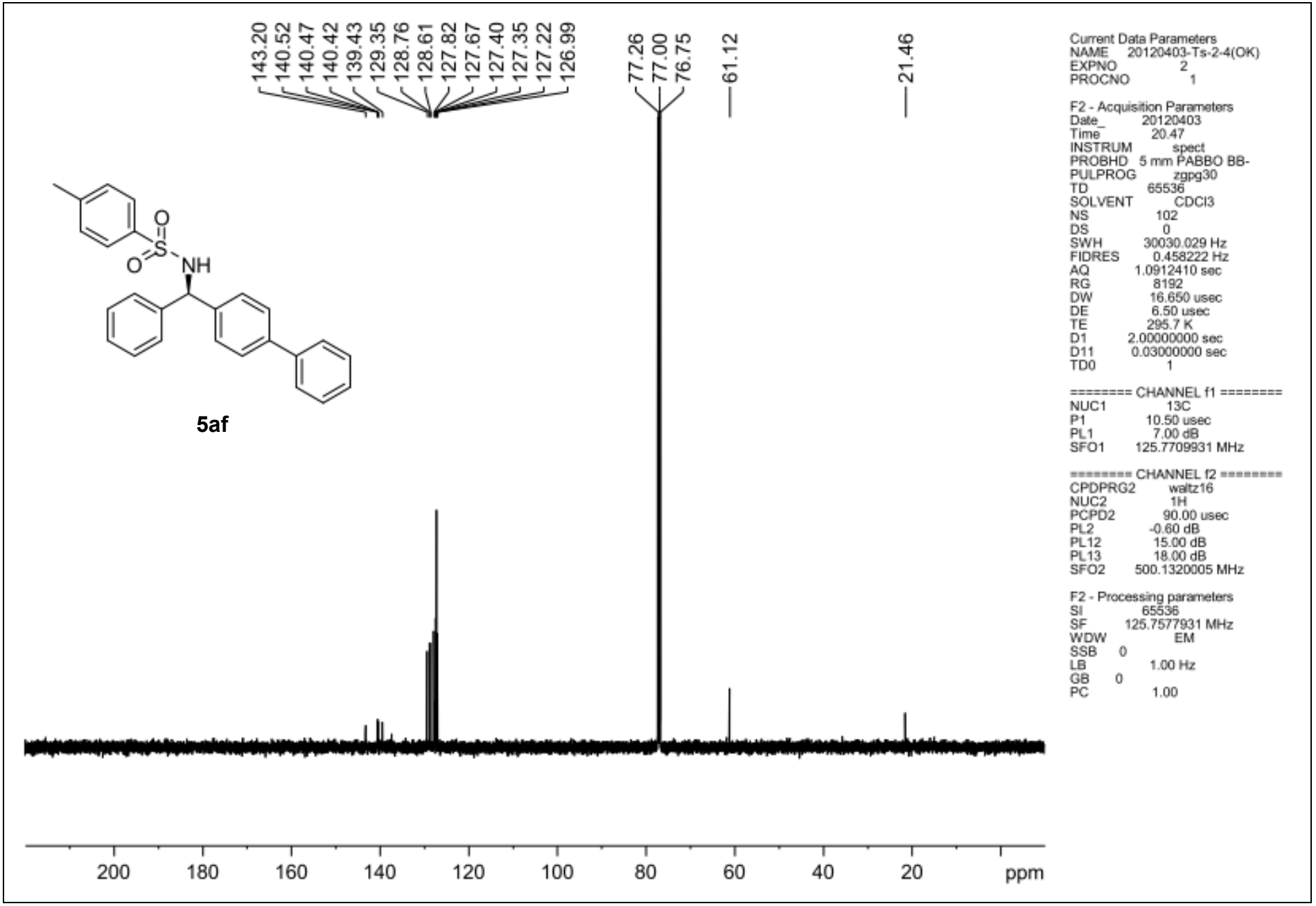

158.96
143.09
140.71
137.40
132.74
129.31
128.59
128.47
127.46
127.43
127.25
127.19
113.87
77.25
77.00
76.75
60.80
55.23
21.44
O
S
O
NH
OMe
5ad
220
200
180
160
140
120
100
80
60
40
20
0 ppm
Current Data Parameters
NAME 20120403-Ts-2-3
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120403
Time 23.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 144
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 8192
DW 16.650 usec
DE 6.50 usec
TE 295.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 125.7709931 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 65536
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

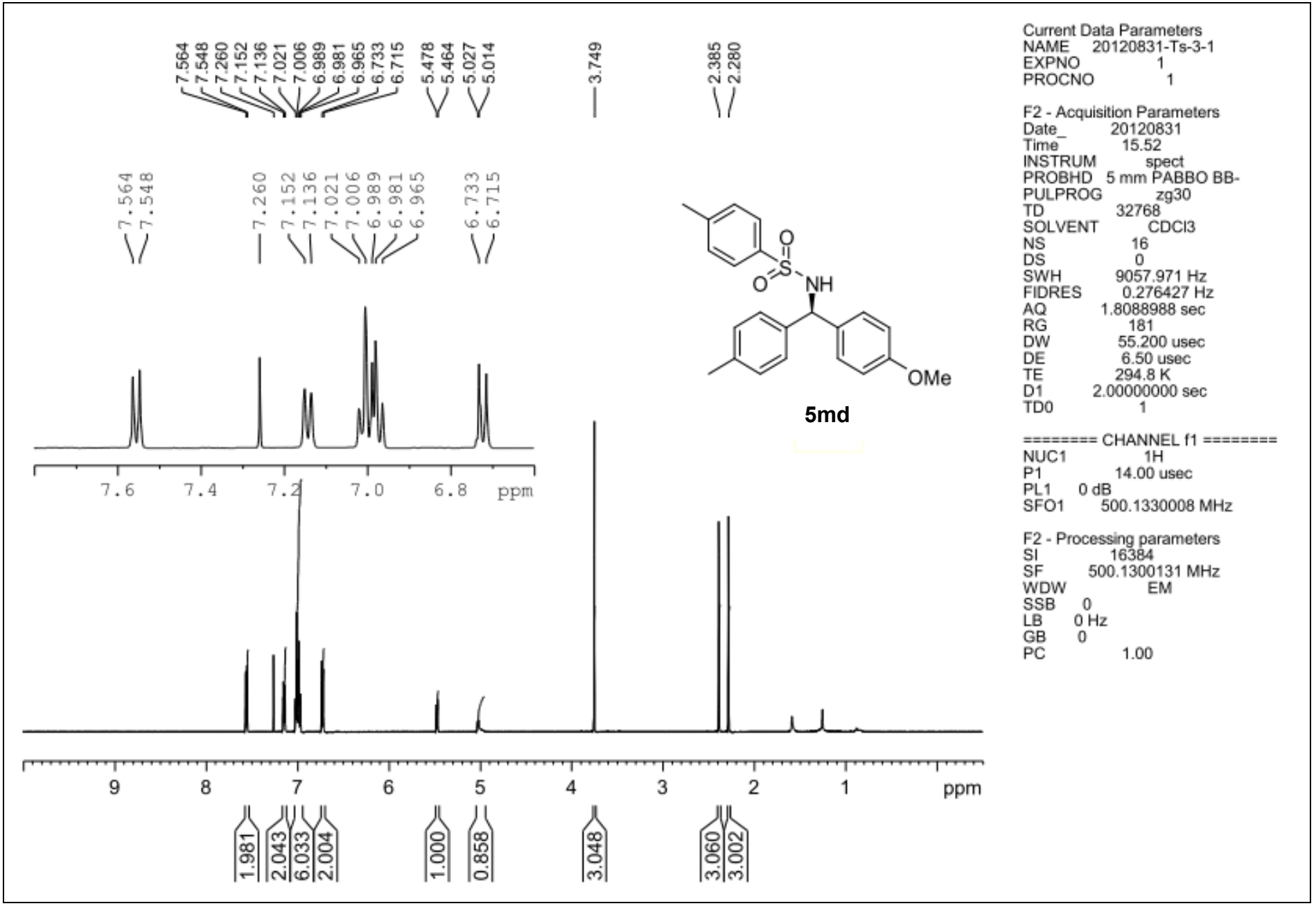

7.755
7.748
7.680
7.663
7.655
7.648
7.642
7.636
7.555
7.538
7.498
7.456
7.450
7.444
7.438
7.260
7.232
7.230
7.223
7.221
7.181
7.178
7.161
7.146
7.144
7.045
7.029
5.742
5.727
5.194
5.179
2.274
7.767
7.760
7.755
7.748
7.680
7.663
7.655
7.648
7.642
7.636
7.555
7.538
7.498
7.456
7.450
7.444
7.438
7.260
7.232
7.230
7.223
7.221
7.181
8.2
8.0
7.8
7.6
7.4
7.2
ppm
O
S
O
NH
5ae
11
10
9
8
7
6
5
4
3
2
1
ppm
1.018
1.062
0.973
1.980
1.012
2.011
2.931
3.026
1.997
1.000
0.964
2.997
Current Data Parameters
NAME 2013-02-Ts-2-1-45ae
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120403
Time 23.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 9057.971 Hz
FIDRES 0.276427 Hz
AQ 1.8088988 sec
RG 256
DW 55.200 usec
DE 6.50 usec
TE 295.3 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0 dB
SFO1 500.1330008 MHz
F2 - Processing parameters
SI 16384
SF 500.1300132 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00


143.23
140.40
137.50
137.34
133.00
132.65
129.28
128.61
128.48
127.95
127.71
127.53
127.47
127.20
126.38
126.25
126.17
125.13
77.25
77.00
76.75
61.47
21.34
O
S
O
NH
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME 20120403-Ts-2-4
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120403
Time 23.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 368
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 8192
DW 16.650 usec
DE 6.50 usec
TE 295.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 125.7709931 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 65536
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

5ae


7.585
7.568
7.525
7.523
7.507
7.438
7.434
7.423
7.418
7.407
7.355
7.341
7.326
7.260
7.240
7.226
7.181
7.164
7.155
7.151
7.141
7.126
5.626
5.612
5.184
5.170
2.357
5af
7.6
7.5
7.4
7.3
7.2
7.1
ppm
11
10
9
8
7
6
5
4
3
2
1
ppm
2.020
2.048
4.080
1.014
2.877
6.079
1.000
0.986
3.032
Current Data Parameters
NAME 2013-02-Ts-2-4-45af
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120403
Time 20.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 9057.971 Hz
FIDRES 0.276427 Hz
AQ 1.8088988 sec
RG 228.1
DW 55.200 usec
DE 6.50 usec
TE 295.1 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0 dB
SFO1 500.1330008 MHz
F2 - Processing parameters
SI 16384
SF 500.1300131 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00


143.20
140.52
140.47
140.42
139.43
129.35
128.76
128.61
127.82
127.67
127.40
127.35
127.22
126.99
77.26
77.00
76.75
61.12
21.46
O
S
O
NH
5af
Current Data Parameters
NAME 20120403-Ts-2-4(OK)
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120403
Time 20.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 102
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 8192
DW 16.650 usec
DE 6.50 usec
TE 295.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 125.7709931 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 65536
SF 125.7577931 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
200
180
160
140
120
100
80
60
40
20
ppm

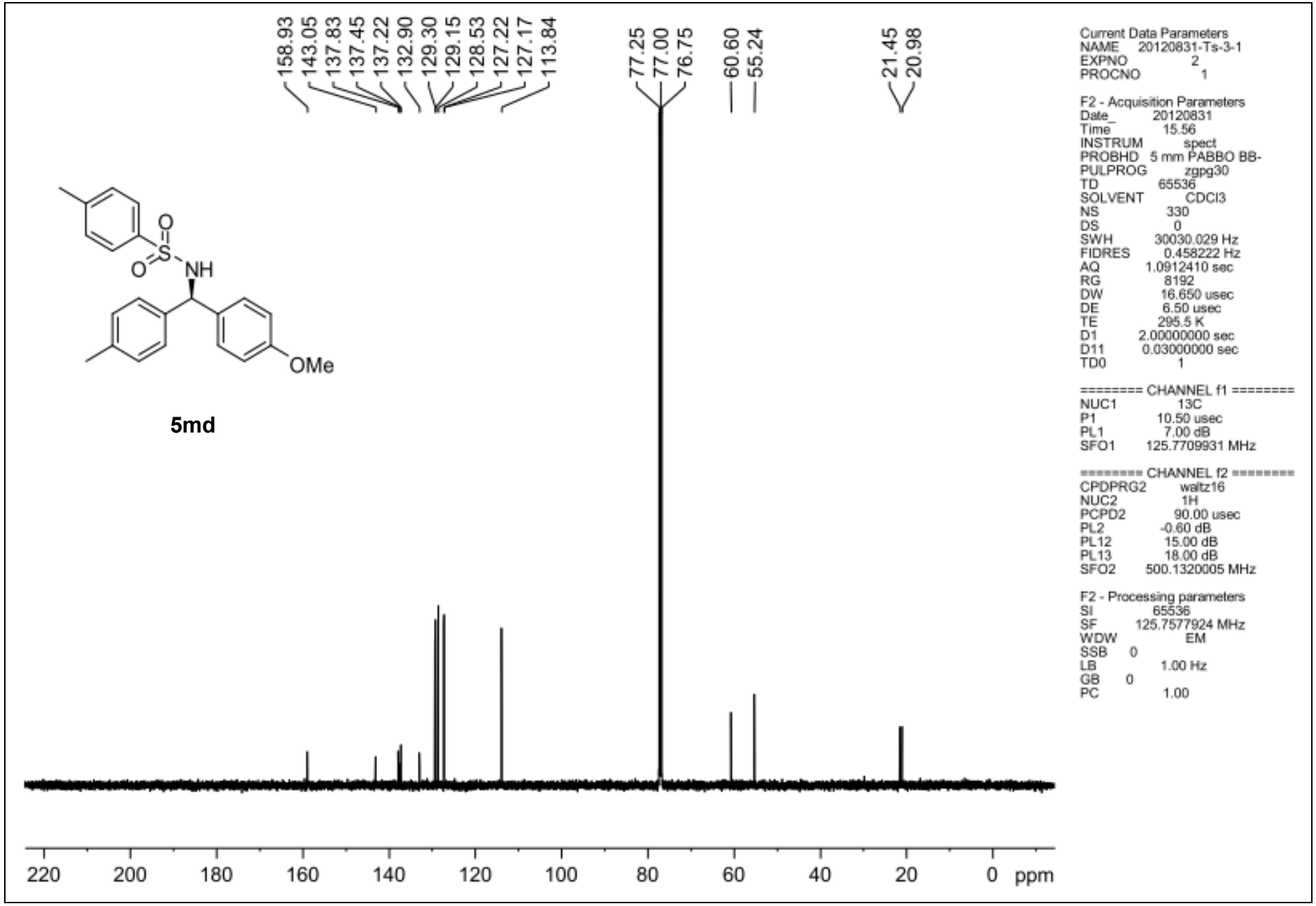


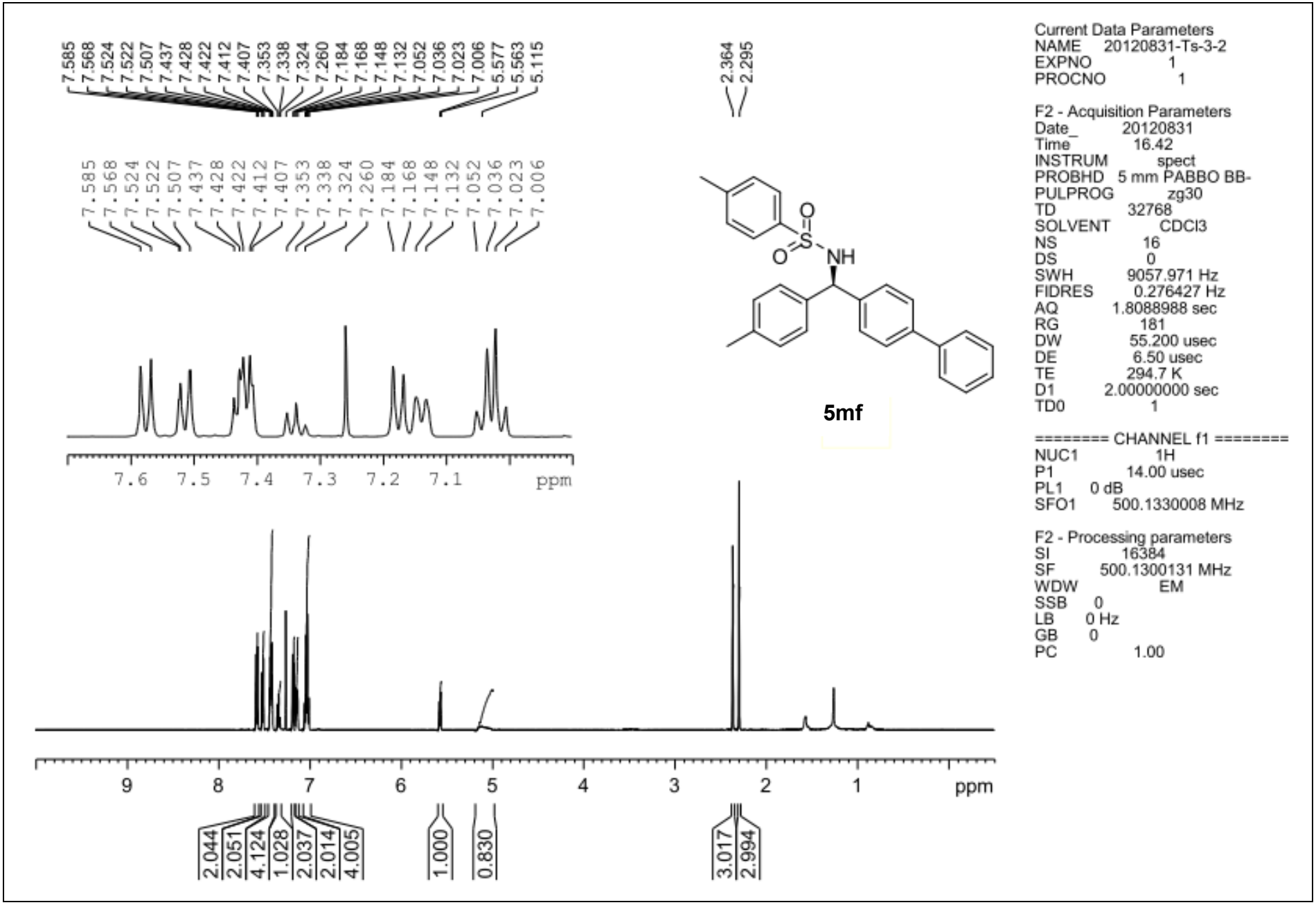
Current Data Parameters
NAME 20120831-Ts-3-1
EXPNO 1
PROCNO 1

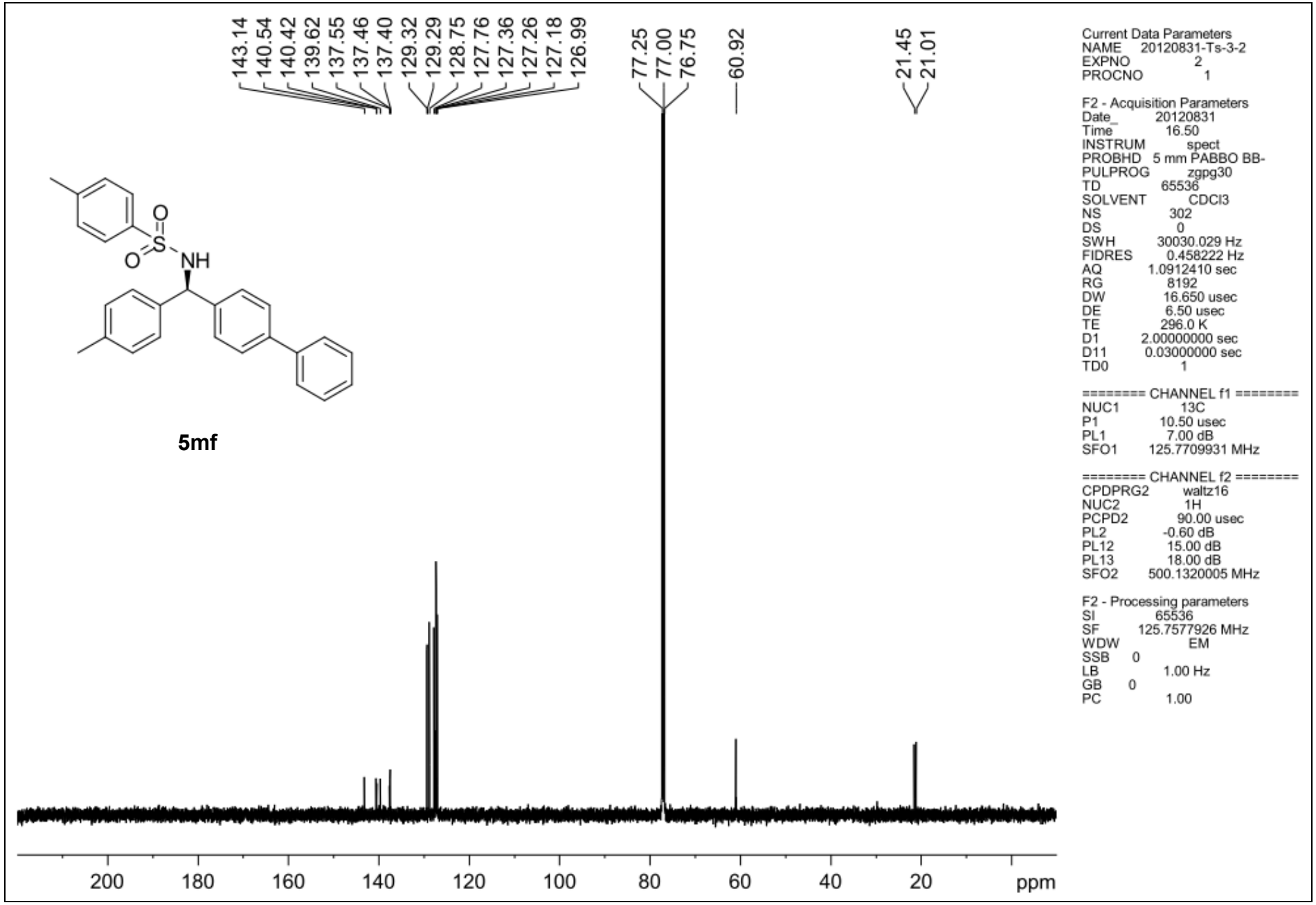
F2 - Acquisition Parameters
Date_ 20120831
Time 15.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 9057.971 Hz
FIDRES 0.276427 Hz
AQ 1.8088988 sec
RG 181
DW 55.200 usec
DE 6.50 usec
TE 294.8 K
D1 2.00000000 sec
TD0 1

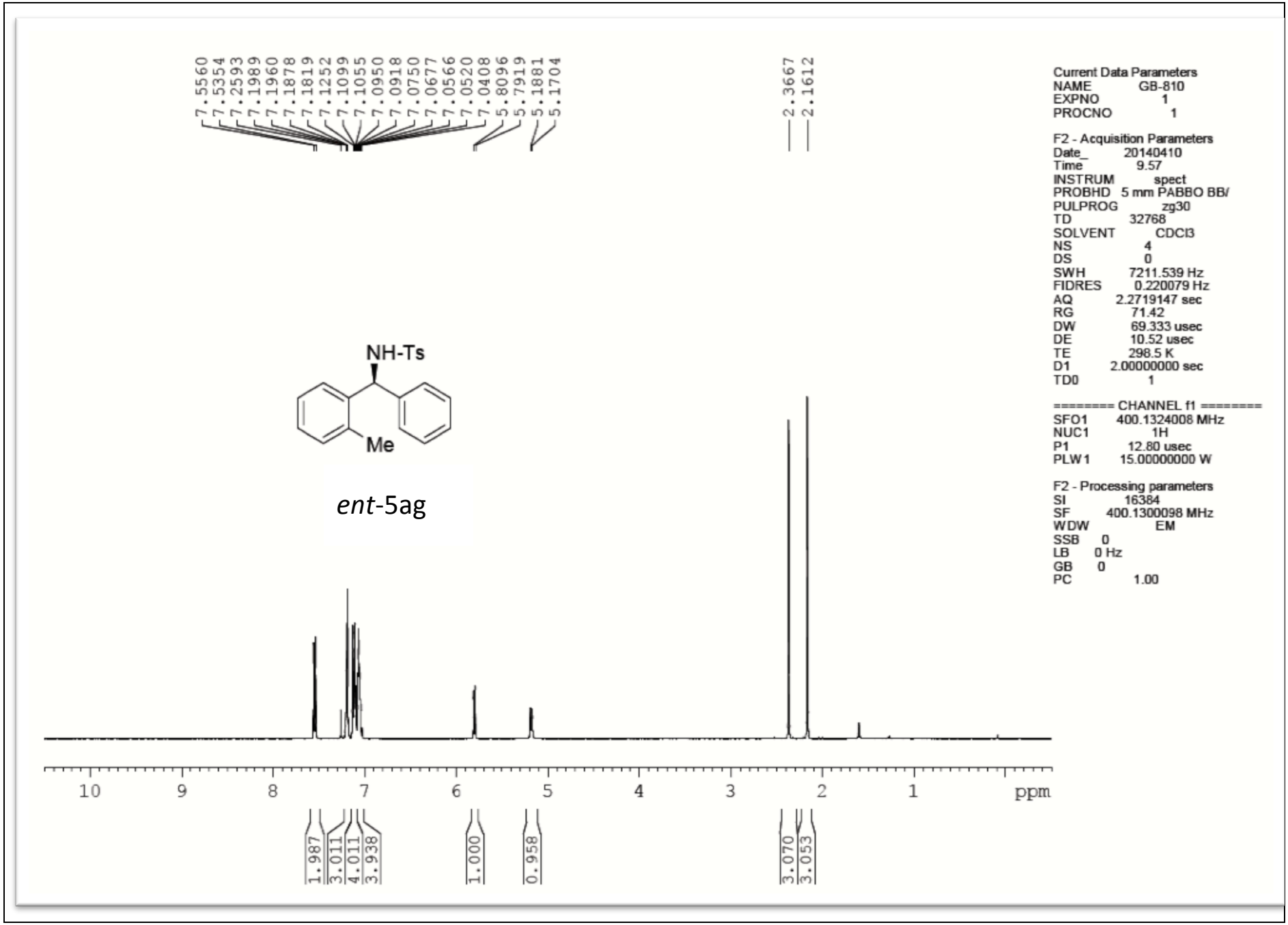
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0 dB
SFO1 500.1330008 MHz

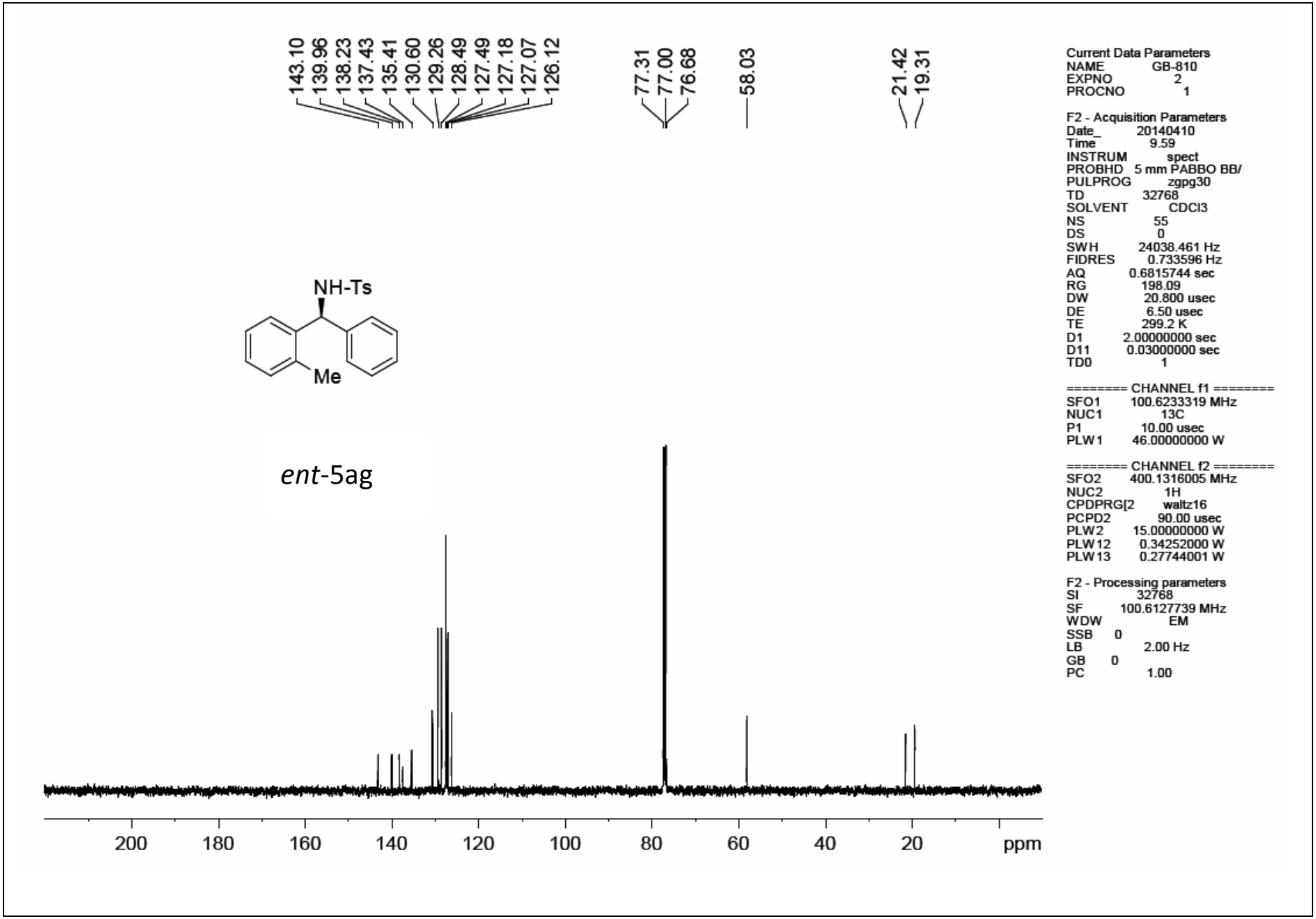
F2 - Processing parameters
SI 16384
SF 500.1300131 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

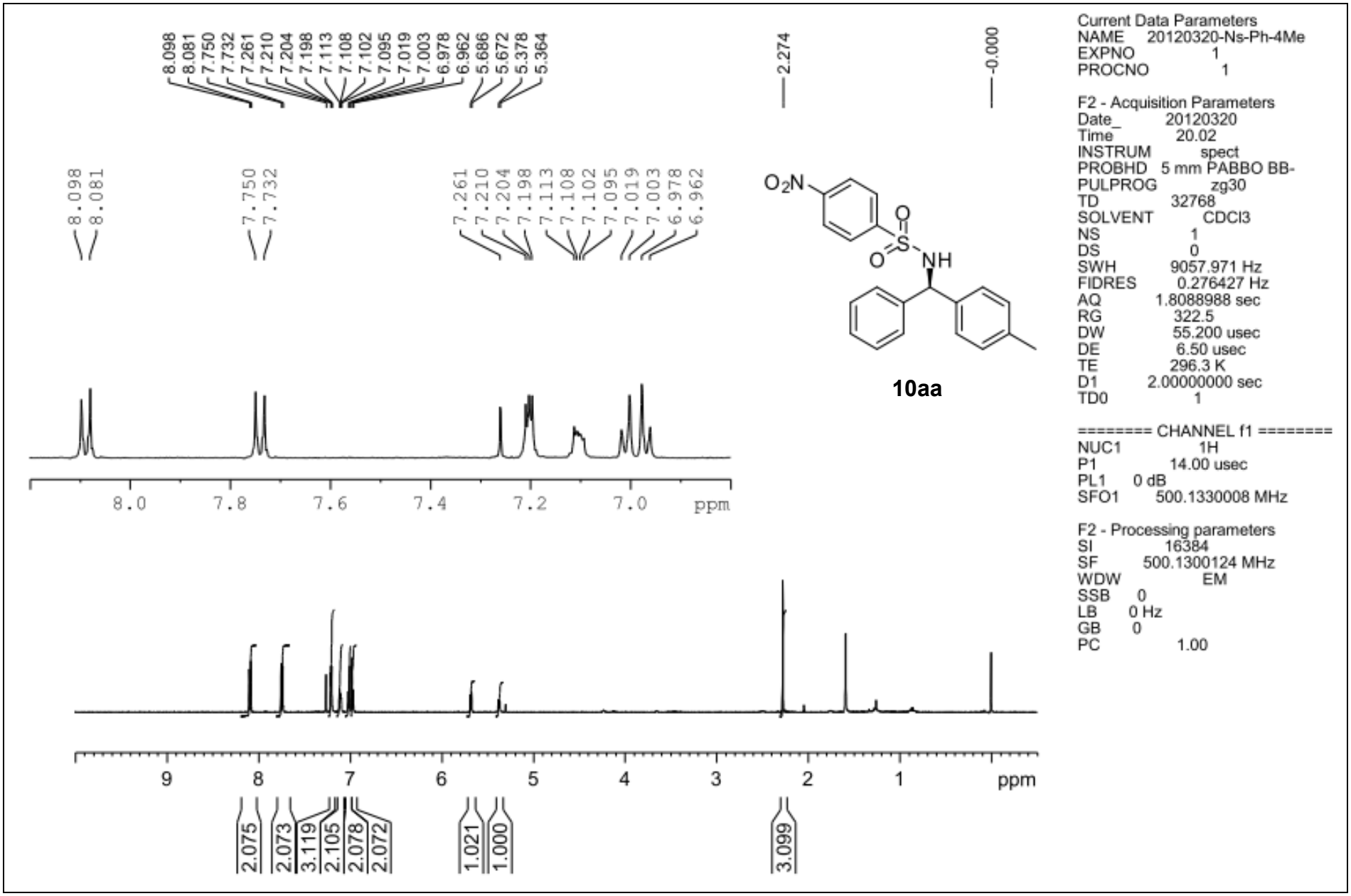

158.93
143.05
137.83
137.45
137.22
132.90
129.30
129.15
128.53
127.22
127.17
113.84
77.25
77.00
76.75
60.60
55.24
21.45
20.98
O
S
O
NH
OMe
5md
220
200
180
160
140
120
100
80
60
40
20
0
ppm
Current Data Parameters
NAME 20120831-Ts-3-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120831
Time 15.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 330
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 8192
DW 16.650 usec
DE 6.50 usec
TE 295.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 125.7709931 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 65536
SF 125.7577924 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00


7.585
7.568
7.524
7.522
7.507
7.437
7.428
7.422
7.412
7.407
7.353
7.338
7.324
7.260
7.184
7.168
7.148
7.132
7.052
7.036
7.023
7.006
5.577
5.563
5.115
2.364
2.295
O
S
O
NH
5mf
7.6
7.5
7.4
7.3
7.2
7.1
ppm
9
8
7
6
5
4
3
2
1
ppm
2.044
2.051
4.124
1.028
2.037
2.014
4.005
1.000
0.830
3.017
2.994
Current Data Parameters
NAME 20120831-Ts-3-2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120831
Time 16.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 9057.971 Hz
FIDRES 0.276427 Hz
AQ 1.8088988 sec
RG 181
DW 55.200 usec
DE 6.50 usec
TE 294.7 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0 dB
SFO1 500.1330008 MHz
F2 - Processing parameters
SI 16384
SF 500.1300131 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00


143.14
140.54
140.42
139.62
137.55
137.46
137.40
129.32
129.29
128.75
127.76
127.36
127.26
127.18
126.99
77.25
77.00
76.75
60.92
21.45
21.01
O
S
O
NH
5mf
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME 20120831-Ts-3-2
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120831
Time 16.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 302
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 8192
DW 16.650 usec
DE 6.50 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 125.7709931 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 65536
SF 125.7577926 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00


7.5560
7.5354
7.2593
7.1989
7.1960
7.1878
7.1819
7.1252
7.1099
7.1055
7.0950
7.0918
7.0750
7.0677
7.0566
7.0520
7.0408
5.8096
5.7919
5.1881
5.1704
2.3667
2.1612
NH-Ts
Me
ent-5ag
Current Data Parameters
NAME GB-810
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140410
Time 9.57
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 71.42
DW 69.333 usec
DE 10.52 usec
TE 298.5 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W
F2 - Processing parameters
SI 16384
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
1.987
3.011
4.011
3.938
1.000
0.958
3.070
3.053


143.10
139.96
138.23
137.43
135.41
130.60
129.26
128.49
127.49
127.18
127.07
126.12
77.31
77.00
76.68
58.03
21.42
19.31
NH-Ts
Me
ent-5ag
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME GB-810
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140410
Time 9.59
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 55
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W
F2 - Processing parameters
SI 32768
SF 100.6127739 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

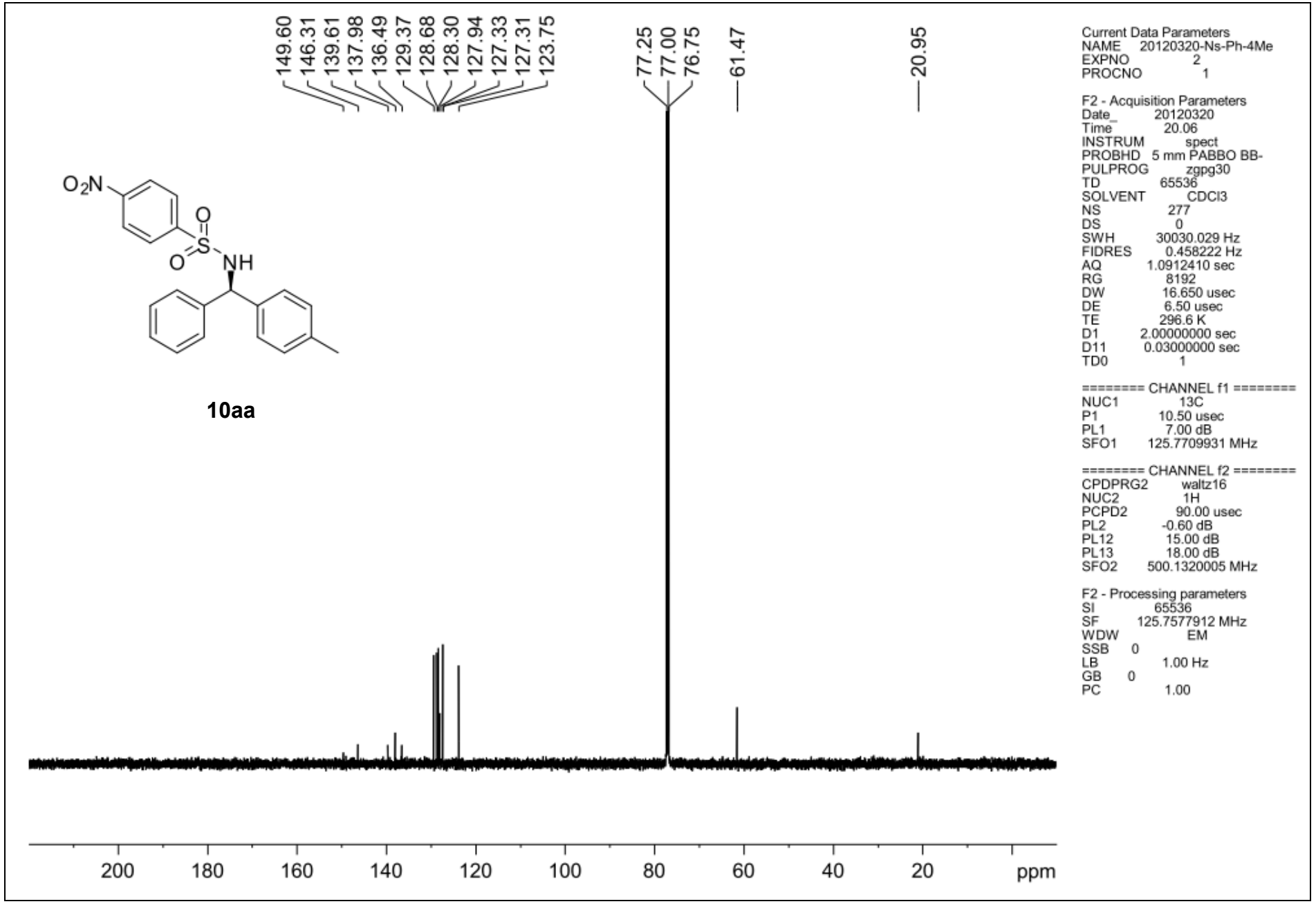


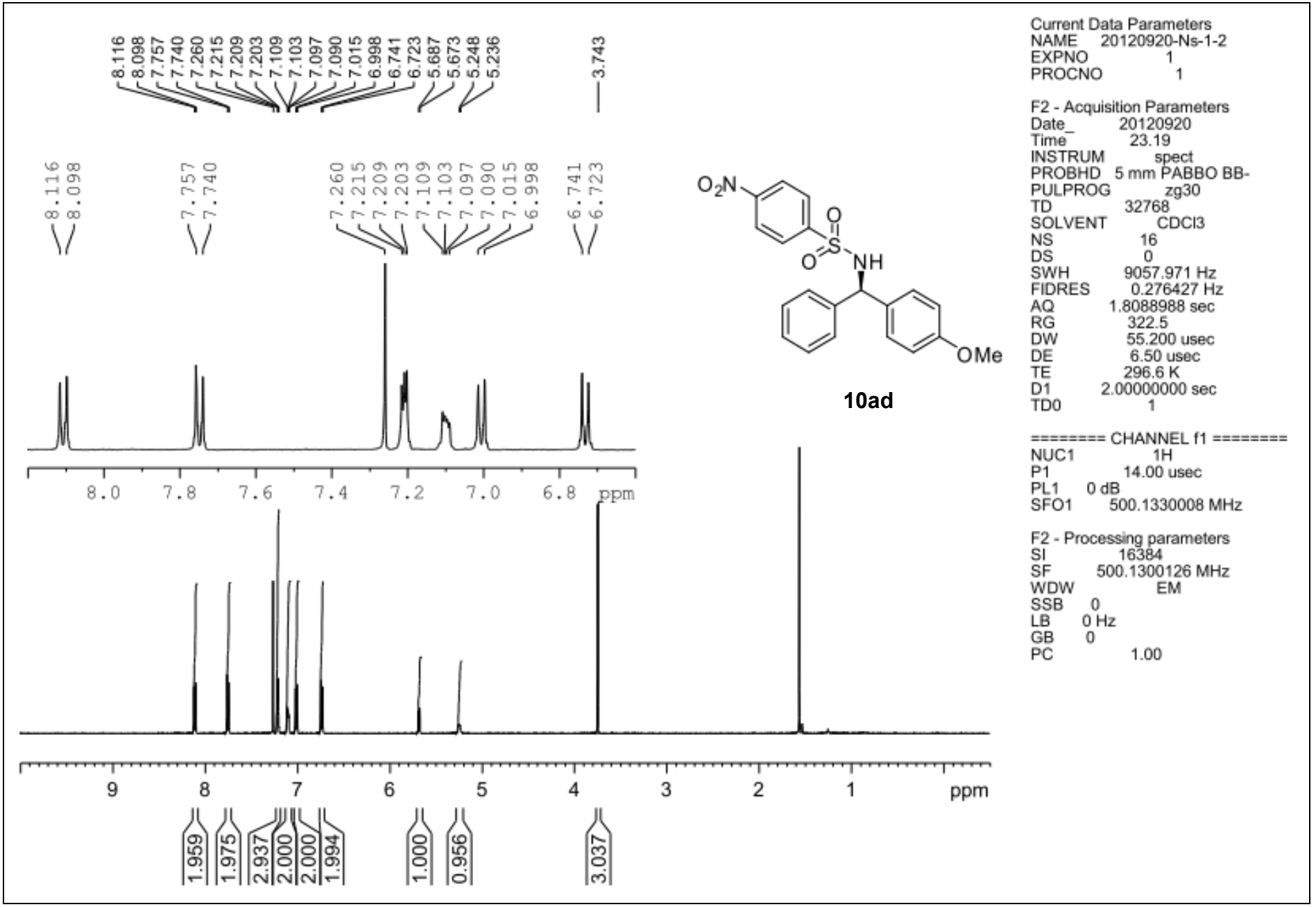
Current Data Parameters
NAME 20120320-Ns-Ph-4Me
EXPNO 1
PROCNO 1

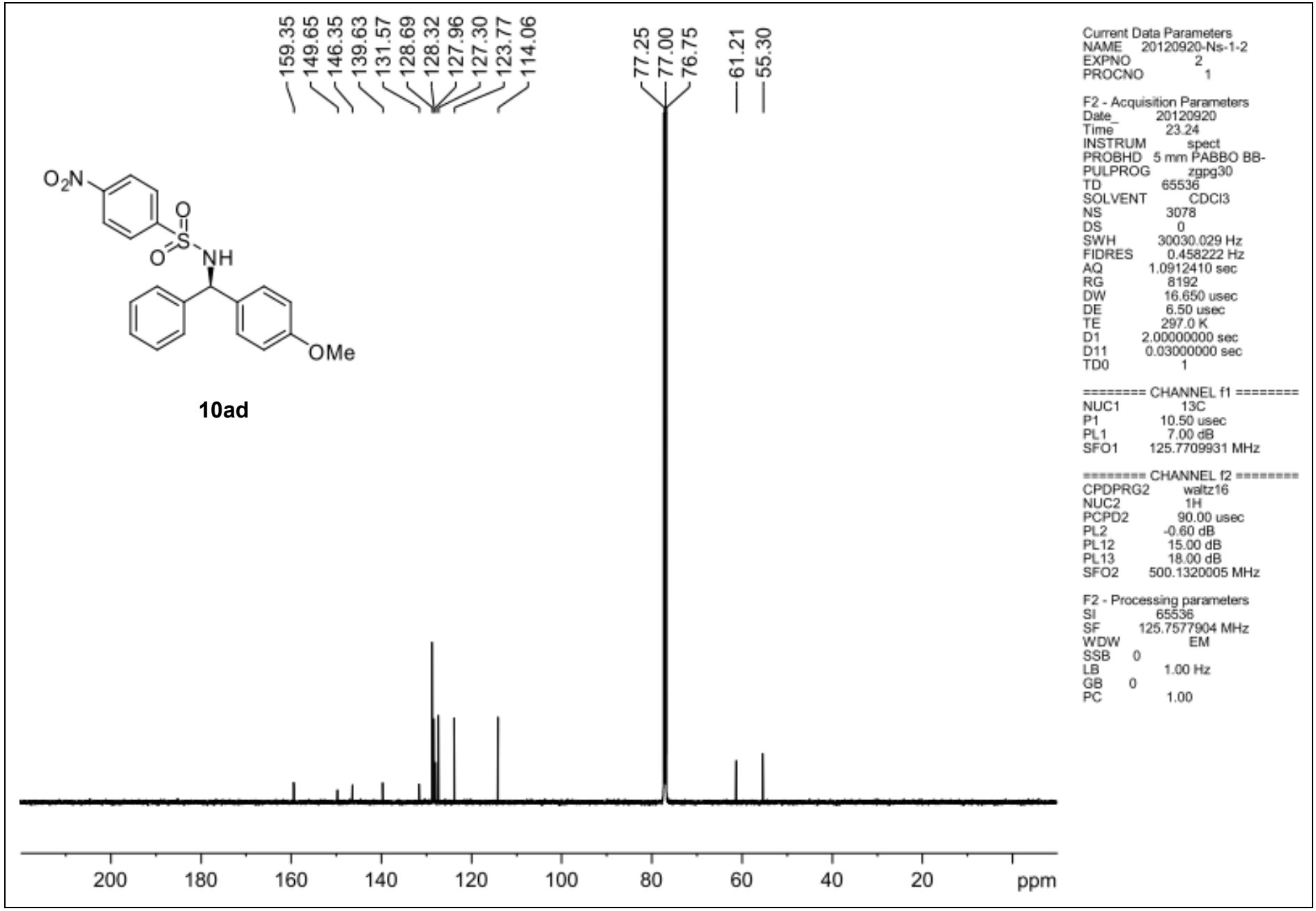
F2 - Acquisition Parameters
Date_ 20120320
Time 20.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 1
DS 0
SWH 9057.971 Hz
FIDRES 0.276427 Hz
AQ 1.8088988 sec
RG 322.5
DW 55.200 usec
DE 6.50 usec
TE 296.3 K
D1 2.00000000 sec
TD0 1

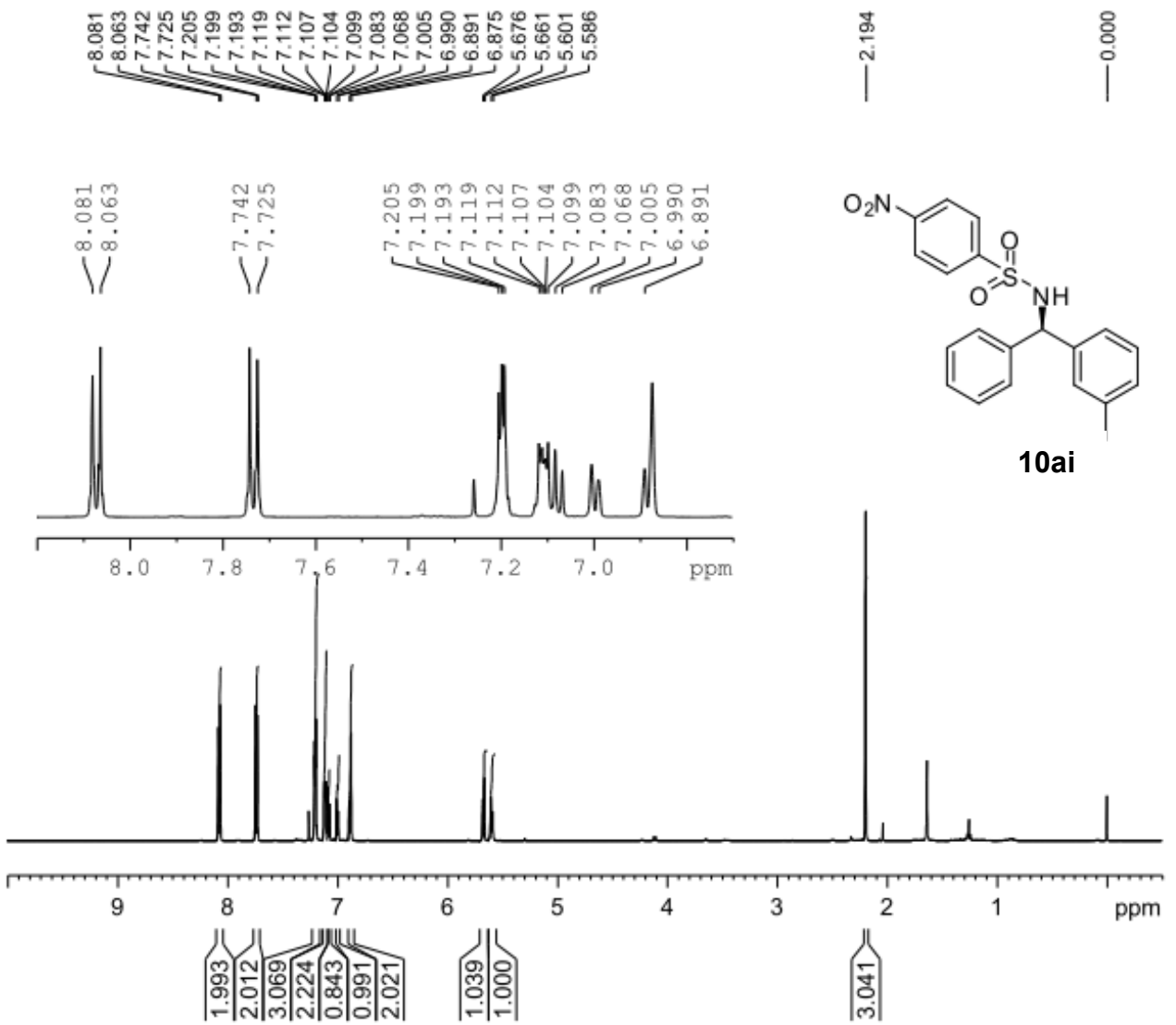
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0 dB
SFO1 500.1330008 MHz

F2 - Processing parameters
SI 16384
SF 500.1300124 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00


149.60
146.31
139.61
137.98
136.49
129.37
128.68
128.30
127.94
127.33
127.31
123.75
77.25
77.00
76.75
61.47
20.95
O2N
O
S
O
NH
10aa
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME 20120320-Ns-Ph-4Me
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120320
Time 20.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 277
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 8192
DW 16.650 usec
DE 6.50 usec
TE 296.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 125.7709931 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 65536
SF 125.7577912 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00


8.116
8.098
7.757
7.740
7.260
7.215
7.209
7.203
7.109
7.103
7.097
7.090
7.015
6.998
6.741
6.723
5.687
5.673
5.248
5.236
3.743
8.0
7.8
7.6
7.4
7.2
7.0
6.8
ppm
9
8
7
6
5
4
3
2
1
ppm
1.959
1.975
2.937
2.000
2.000
1.994
1.000
0.956
3.037
O2N
O
S
O
NH
OMe
10ad
Current Data Parameters
NAME 20120920-Ns-1-2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120920
Time 23.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 9057.971 Hz
FIDRES 0.276427 Hz
AQ 1.8088988 sec
RG 322.5
DW 55.200 usec
DE 6.50 usec
TE 296.6 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0 dB
SFO1 500.1330008 MHz
F2 - Processing parameters
SI 16384
SF 500.1300126 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00


159.35
149.65
146.35
139.63
131.57
128.69
128.32
127.96
127.30
123.77
114.06
77.25
77.00
76.75
61.21
55.30
O2N
O
S
O
NH
OMe
10ad
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME 20120920-Ns-1-2
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120920
Time 23.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3078
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 8192
DW 16.650 usec
DE 6.50 usec
TE 297.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 125.7709931 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 65536
SF 125.7577904 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

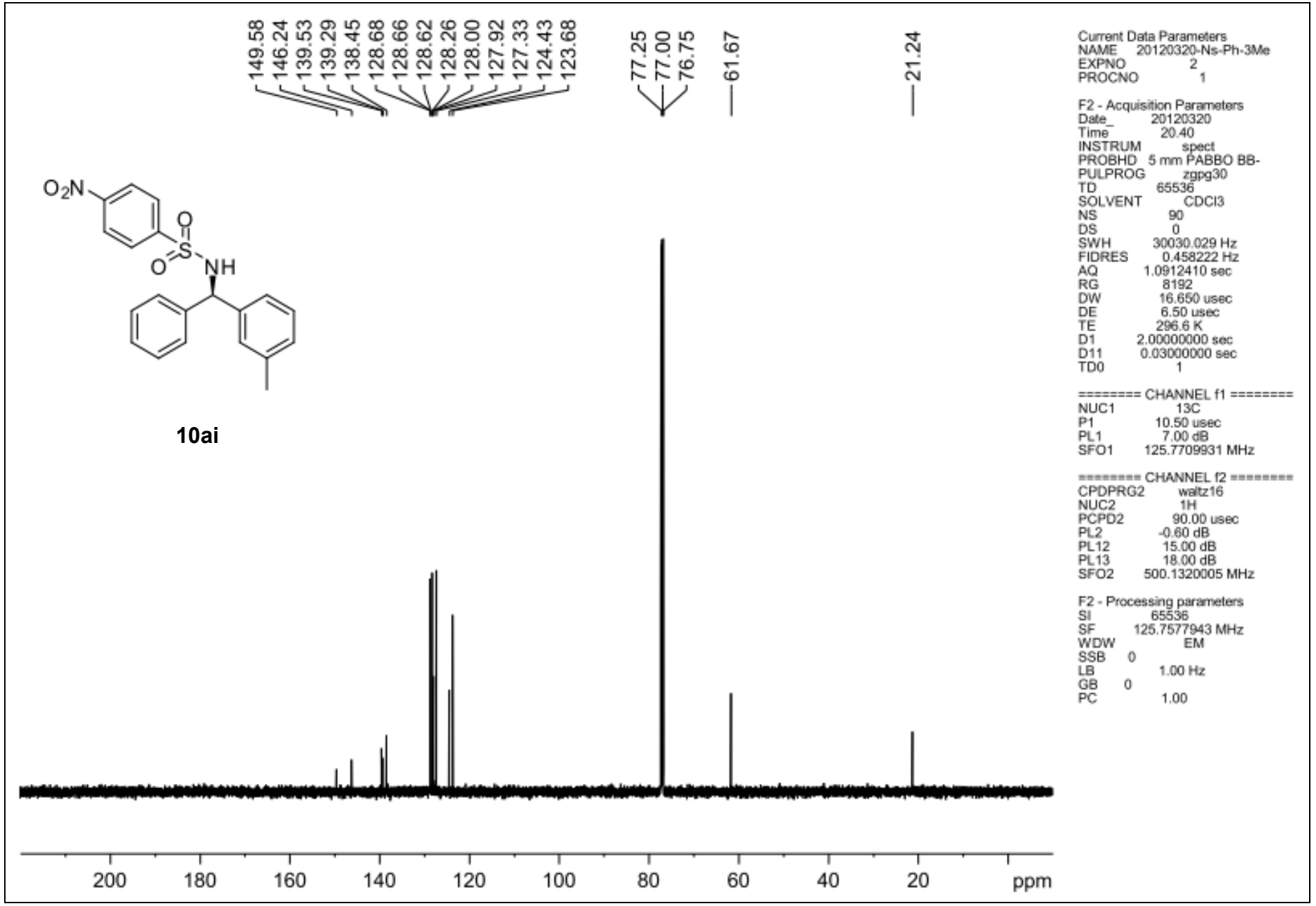


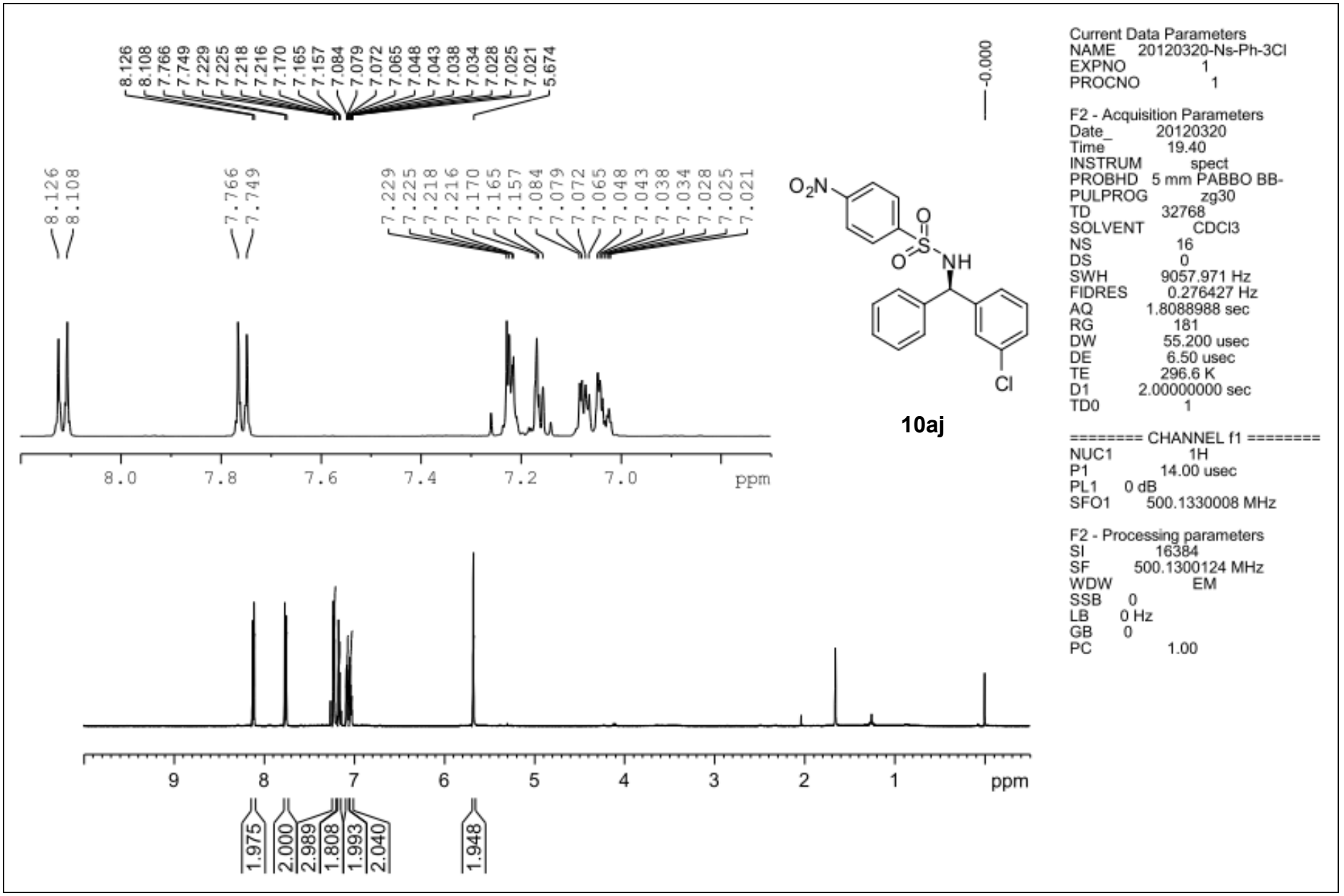
Current Data Parameters
NAME 20120320-Ns-Ph-3Me
EXPNO 1
PROCNO 1

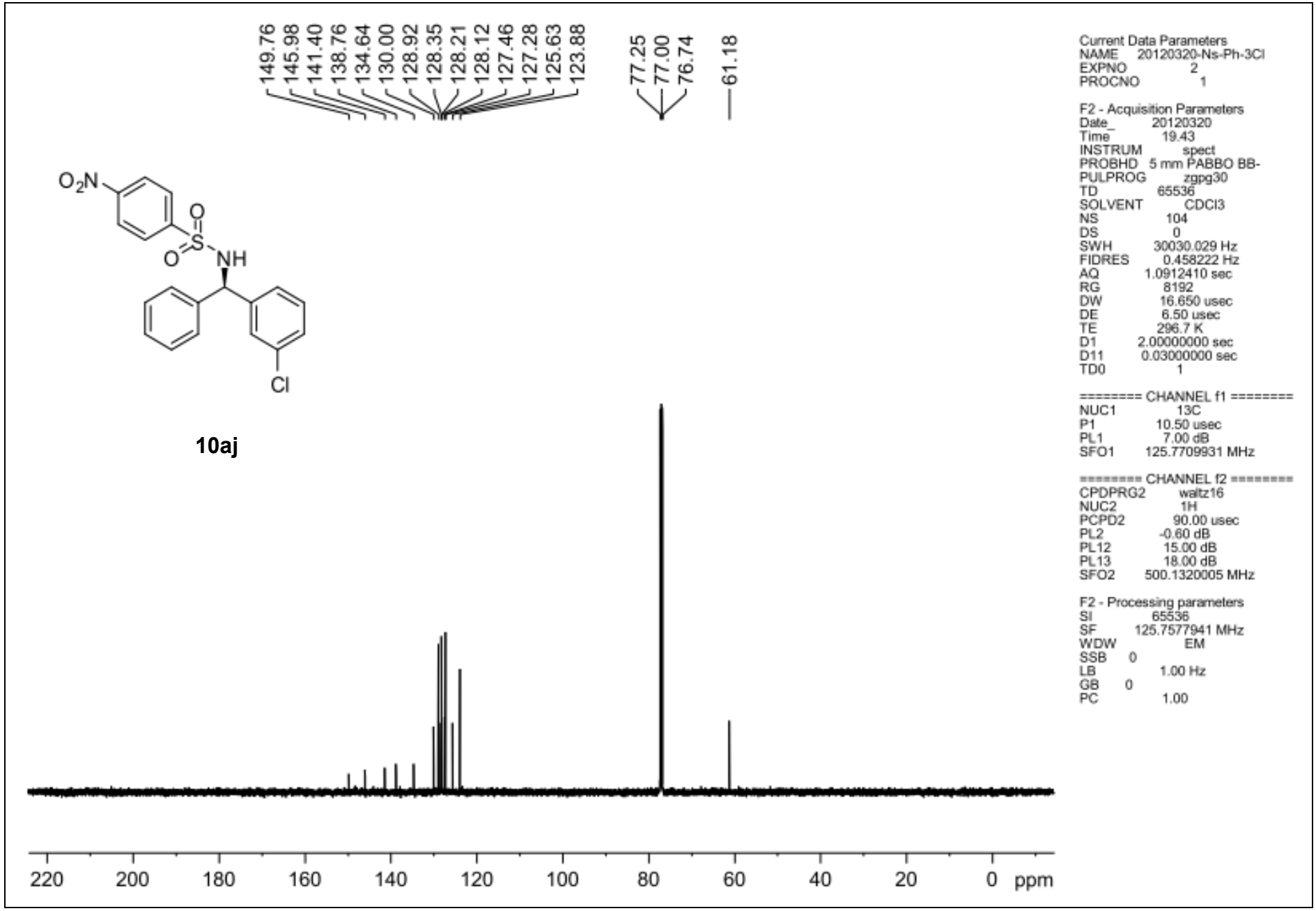
F2 - Acquisition Parameters
Date_ 20120320
Time 20.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 9057.971 Hz
FIDRES 0.276427 Hz
AQ 1.8088988 sec
RG 161.3
DW 55.200 usec
DE 6.50 usec
TE 296.1 K
D1 2.00000000 sec
TD0 1

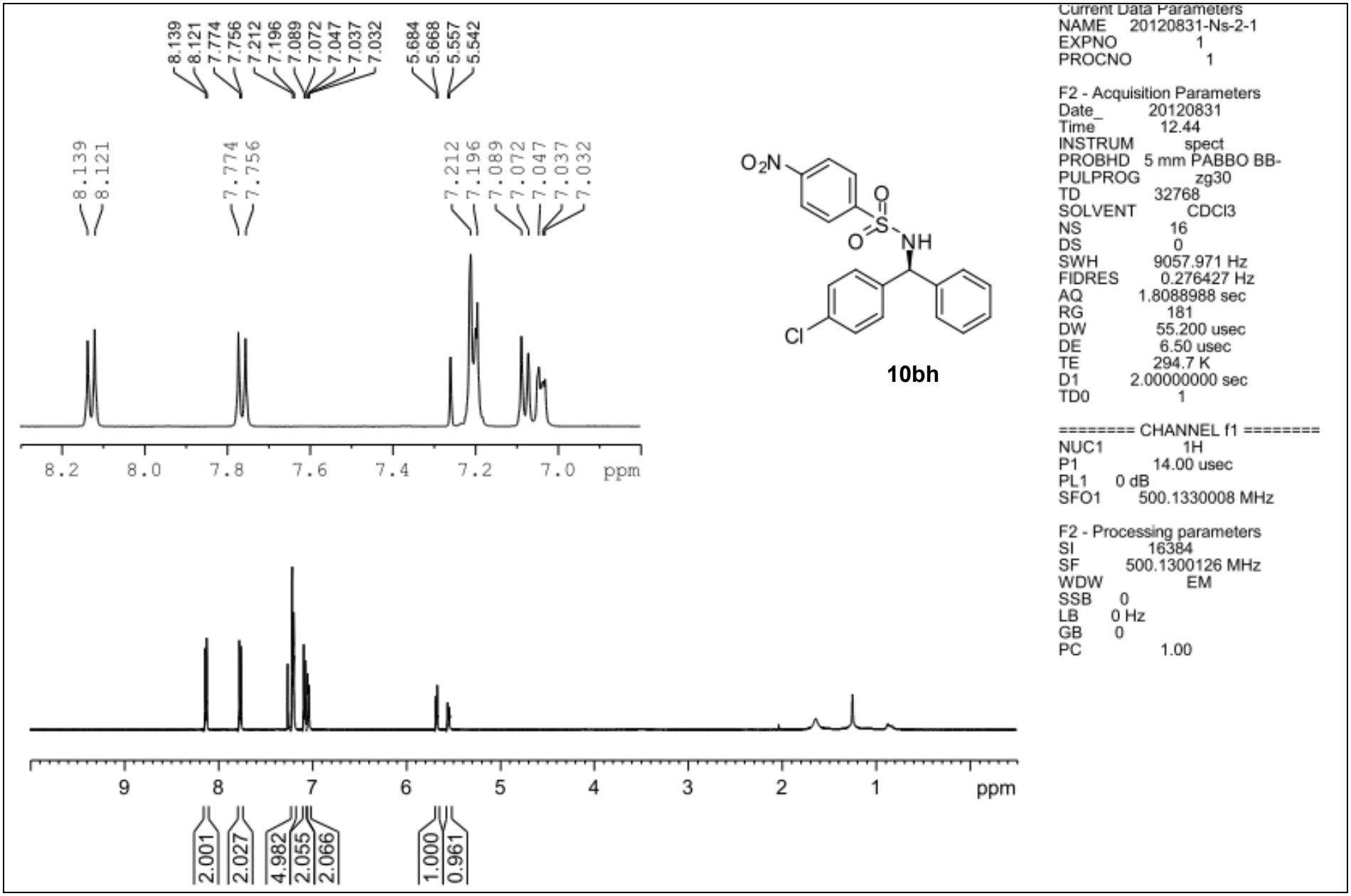
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0 dB
SFO1 500.1330008 MHz

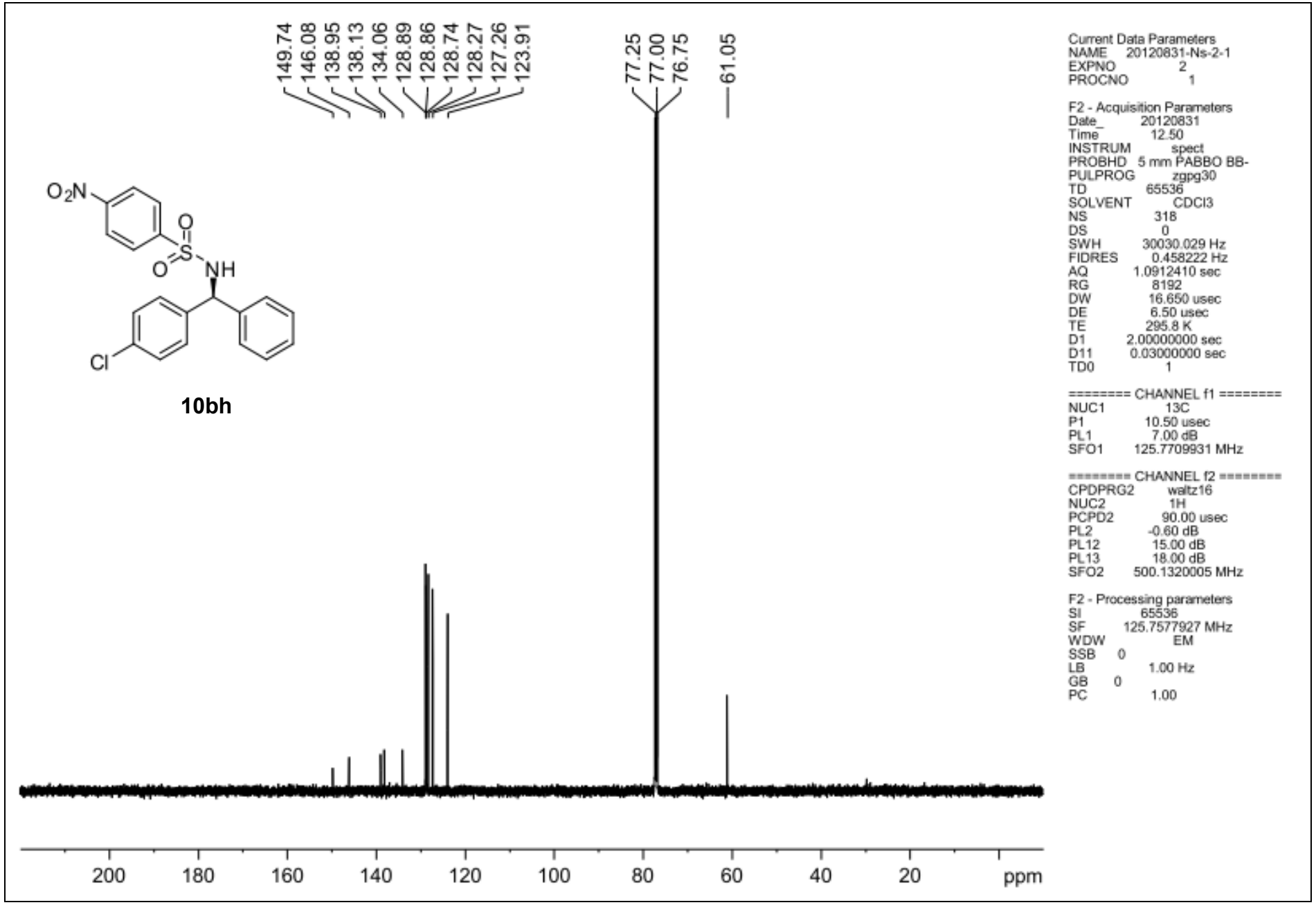
F2 - Processing parameters
SI 16384
SF 500.1300135 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

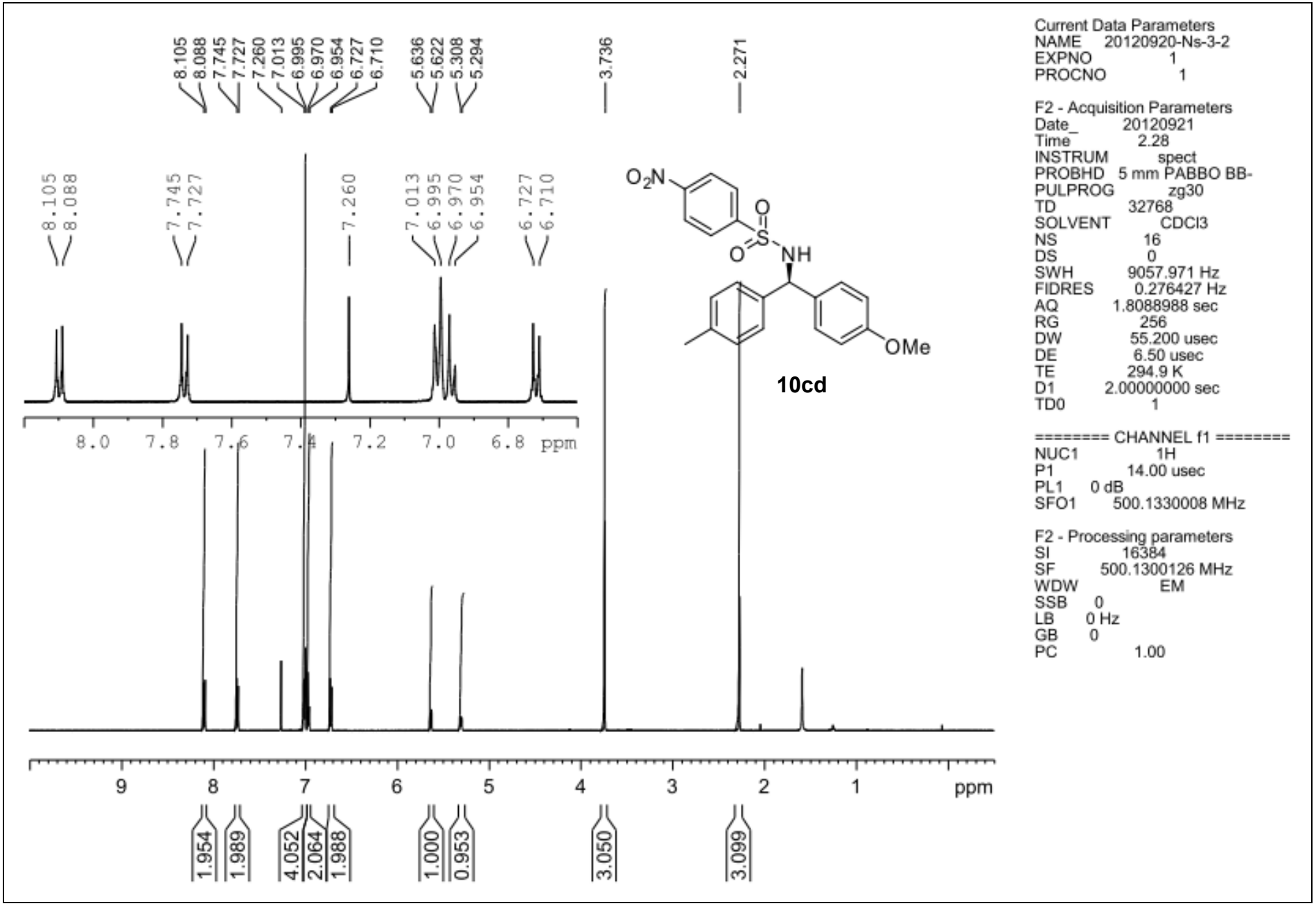

149.58
146.24
139.53
139.29
138.45
128.68
128.66
128.62
128.26
128.00
127.92
127.33
124.43
123.68
77.25
77.00
76.75
61.67
21.24
O2N
O
S
O
NH
10ai
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME 20120320-Ns-Ph-3Me
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120320
Time 20.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 90
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 8192
DW 16.650 usec
DE 6.50 usec
TE 296.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 125.7709931 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 65536
SF 125.7577943 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00


8.126
8.108
7.766
7.749
7.229
7.225
7.218
7.216
7.170
7.165
7.157
7.084
7.079
7.072
7.065
7.048
7.043
7.038
7.034
7.028
7.025
7.021
5.674
-0.000
8.0
7.8
7.6
7.4
7.2
7.0
ppm
9
8
7
6
5
4
3
2
1
ppm
1.975
2.000
2.989
1.808
1.993
2.040
1.948
O2N
O
S
O
NH
Cl
10aj
Current Data Parameters
NAME 20120320-Ns-Ph-3Cl
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120320
Time 19.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 9057.971 Hz
FIDRES 0.276427 Hz
AQ 1.8088988 sec
RG 181
DW 55.200 usec
DE 6.50 usec
TE 296.6 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0 dB
SFO1 500.1330008 MHz
F2 - Processing parameters
SI 16384
SF 500.1300124 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00


149.76
145.98
141.40
138.76
134.64
130.00
128.92
128.35
128.21
128.12
127.46
127.28
125.63
123.88
77.25
77.00
76.74
61.18
O2N
O
S
O
NH
Cl
10aj
220
200
180
160
140
120
100
80
60
40
20
0
ppm
Current Data Parameters
NAME 20120320-Ns-Ph-3Cl
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120320
Time 19.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 104
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 8192
DW 16.650 usec
DE 6.50 usec
TE 296.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 125.7709931 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 65536
SF 125.7577941 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00


8.139
8.121
7.774
7.756
7.212
7.196
7.089
7.072
7.047
7.037
7.032
5.684
5.668
5.557
5.542
8.2
8.0
7.8
7.6
7.4
7.2
7.0
ppm
9
8
7
6
5
4
3
2
1
ppm
2.001
2.027
4.982
2.055
2.066
1.000
0.961
O2N
S
O
NH
Cl
10bh
Current Data Parameters
NAME 20120831-Ns-2-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120831
Time 12.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 9057.971 Hz
FIDRES 0.276427 Hz
AQ 1.8088988 sec
RG 181
DW 55.200 usec
DE 6.50 usec
TE 294.7 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0 dB
SFO1 500.1330008 MHz
F2 - Processing parameters
SI 16384
SF 500.1300126 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00


149.74
146.08
138.95
138.13
134.06
128.89
128.86
128.74
128.27
127.26
123.91
77.25
77.00
76.75
61.05
O2N
O
S
O
NH
Cl
10bh
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME 20120831-Ns-2-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120831
Time 12.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 318
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 8192
DW 16.650 usec
DE 6.50 usec
TE 295.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 125.7709931 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 65536
SF 125.7577927 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

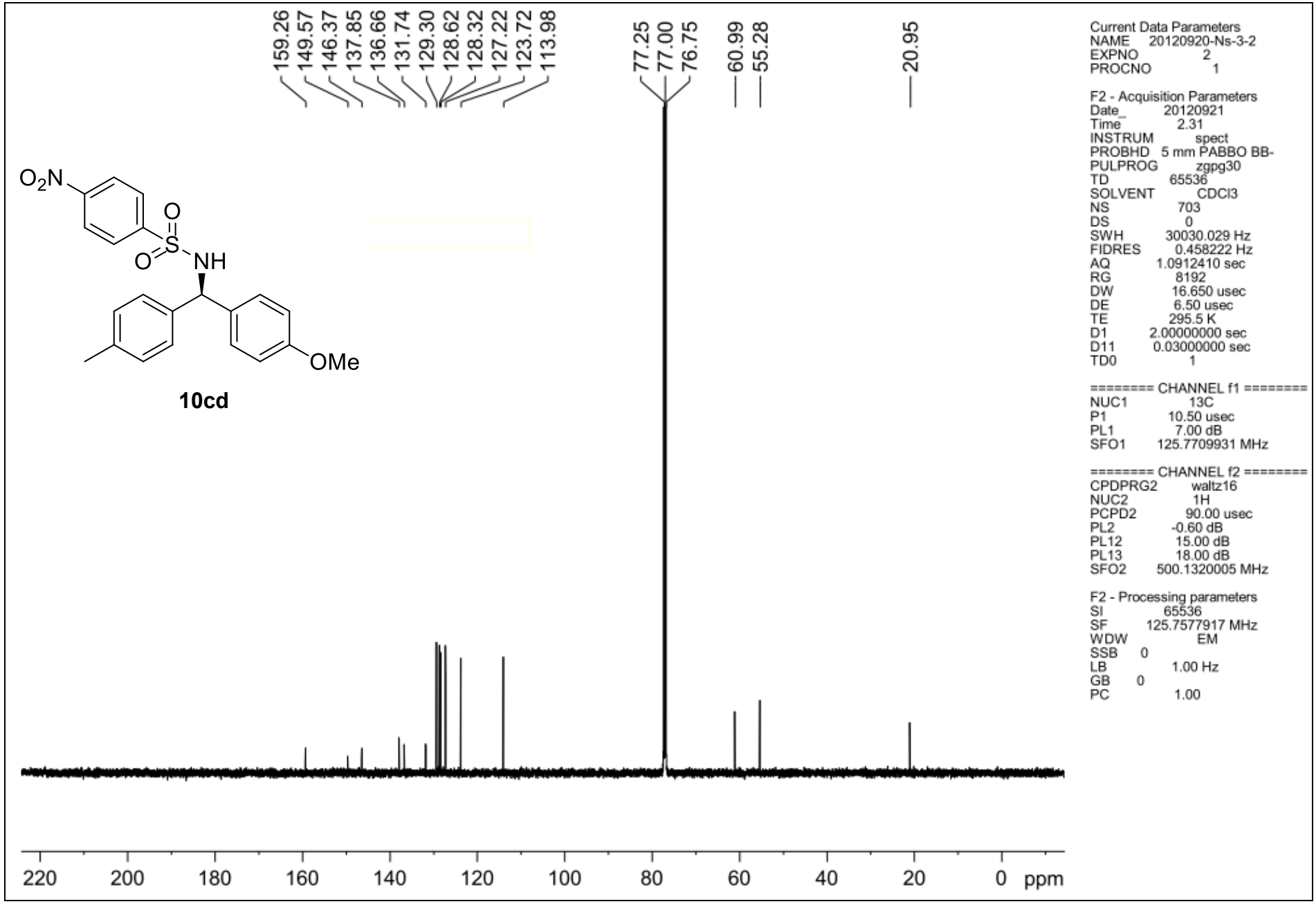


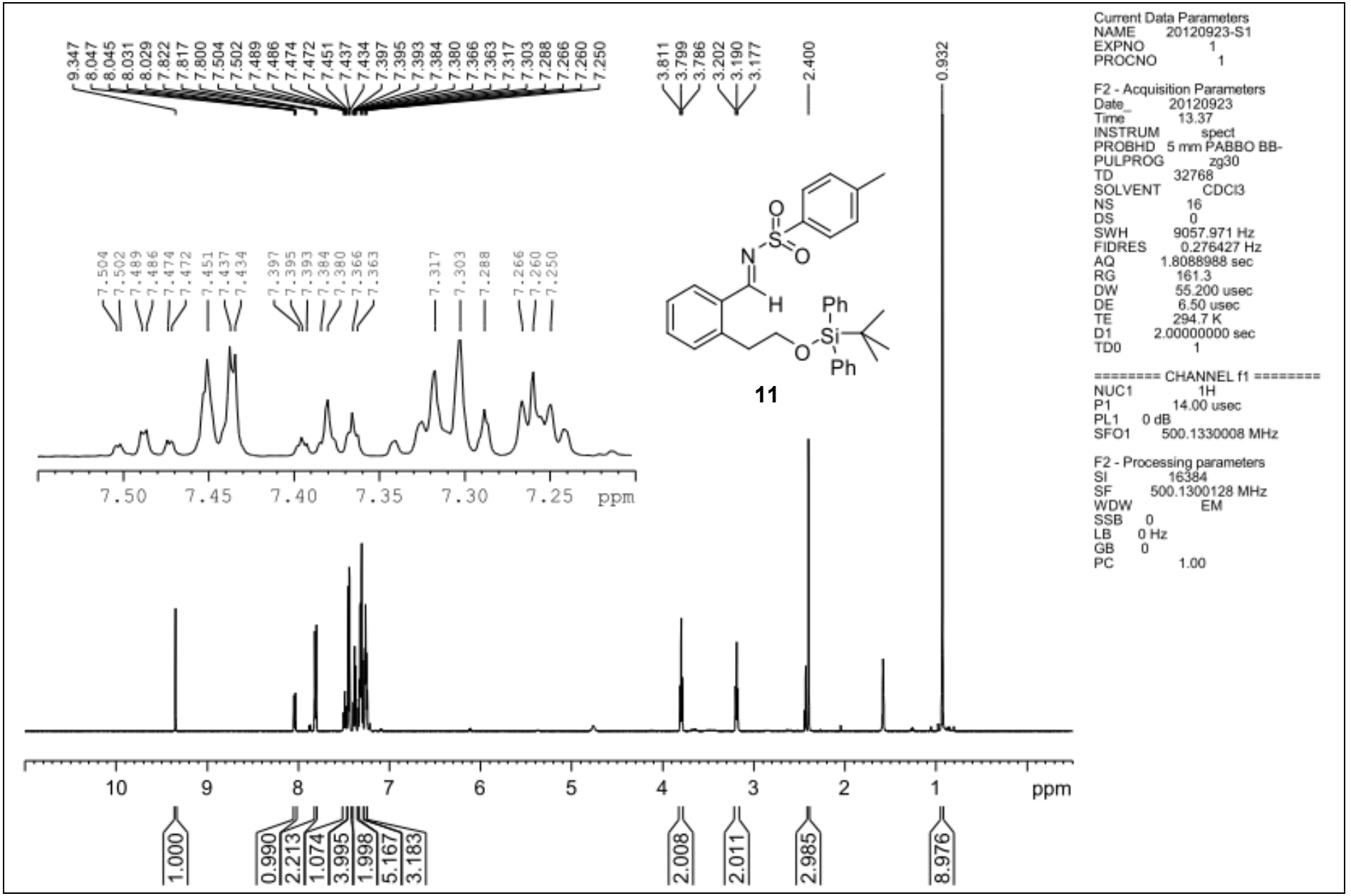
Current Data Parameters
NAME 20120920-Ns-3-2
EXPNO 1
PROCNO 1

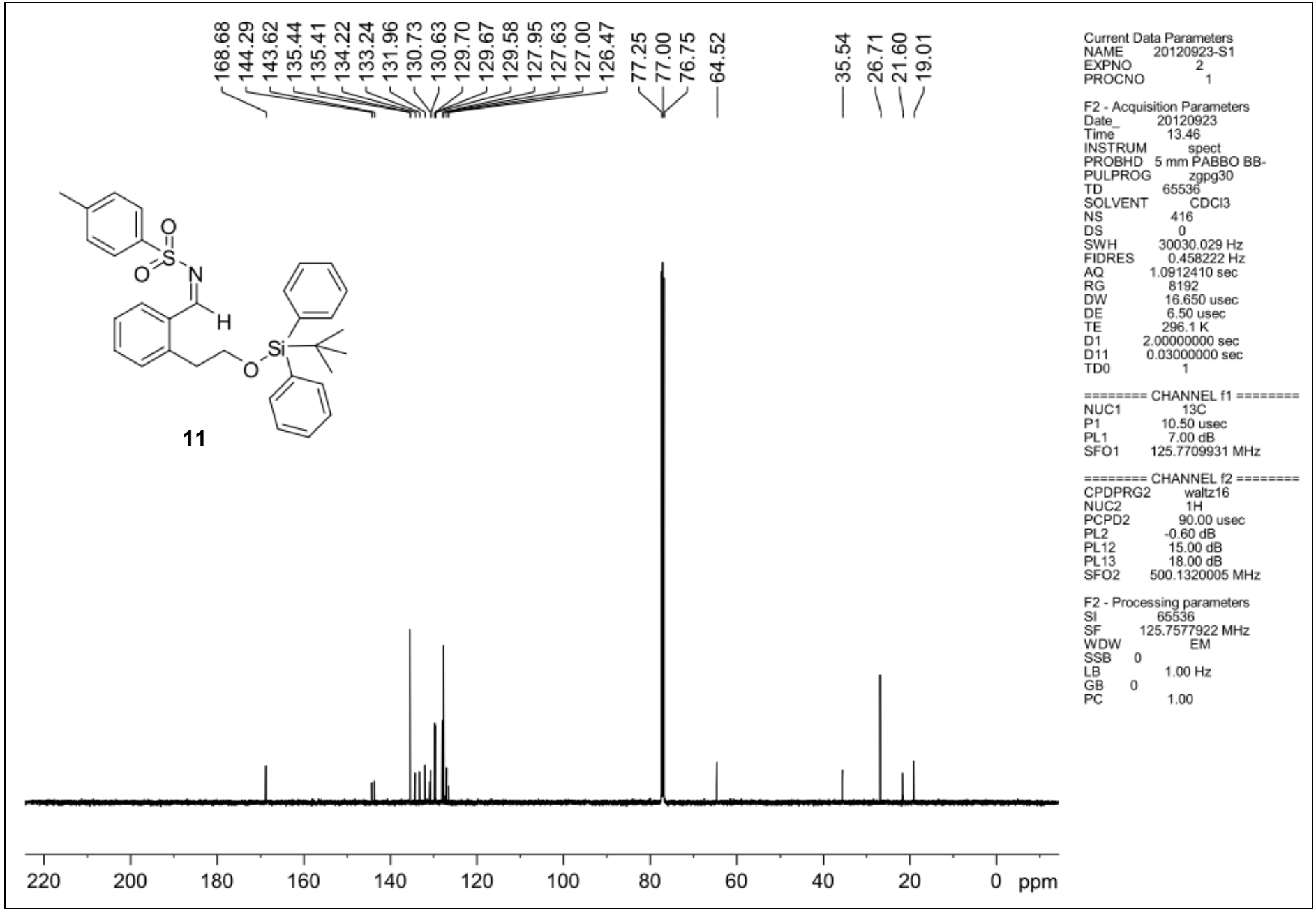
F2 - Acquisition Parameters
Date_ 20120921
Time 2.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 9057.971 Hz
FIDRES 0.276427 Hz
AQ 1.8088988 sec
RG 256
DW 55.200 usec
DE 6.50 usec
TE 294.9 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0 dB
SFO1 500.1330008 MHz

F2 - Processing parameters
SI 16384
SF 500.1300126 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00


159.26
149.57
146.37
137.85
136.66
131.74
129.30
128.62
128.32
127.22
123.72
113.98
77.25
77.00
76.75
60.99
55.28
20.95
O2N
O
S
O
NH
OMe
10cd
Current Data Parameters
NAME 20120920-Ns-3-2
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120921
Time 2.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 703
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 8192
DW 16.650 usec
DE 6.50 usec
TE 295.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 125.7709931 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 65536
SF 125.7577917 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
220
200
180
160
140
120
100
80
60
40
20
0
ppm


9.347
8.047
8.045
8.031
8.029
7.822
7.817
7.800
7.504
7.502
7.489
7.486
7.474
7.472
7.451
7.437
7.434
7.397
7.395
7.393
7.384
7.380
7.366
7.363
7.317
7.303
7.288
7.266
7.260
7.250
3.811
3.799
3.786
3.202
3.190
3.177
2.400
0.932
11
7.50
7.45
7.40
7.35
7.30
7.25
ppm
10
9
8
7
6
5
4
3
2
1
ppm
1.000
0.990
2.213
1.074
3.995
1.998
5.167
3.183
2.008
2.011
2.985
8.976
Current Data Parameters
NAME 20120923-S1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120923
Time 13.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 9057.971 Hz
FIDRES 0.276427 Hz
AQ 1.8088988 sec
RG 161.3
DW 55.200 usec
DE 6.50 usec
TE 294.7 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0 dB
SFO1 500.1330008 MHz
F2 - Processing parameters
SI 16384
SF 500.1300128 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



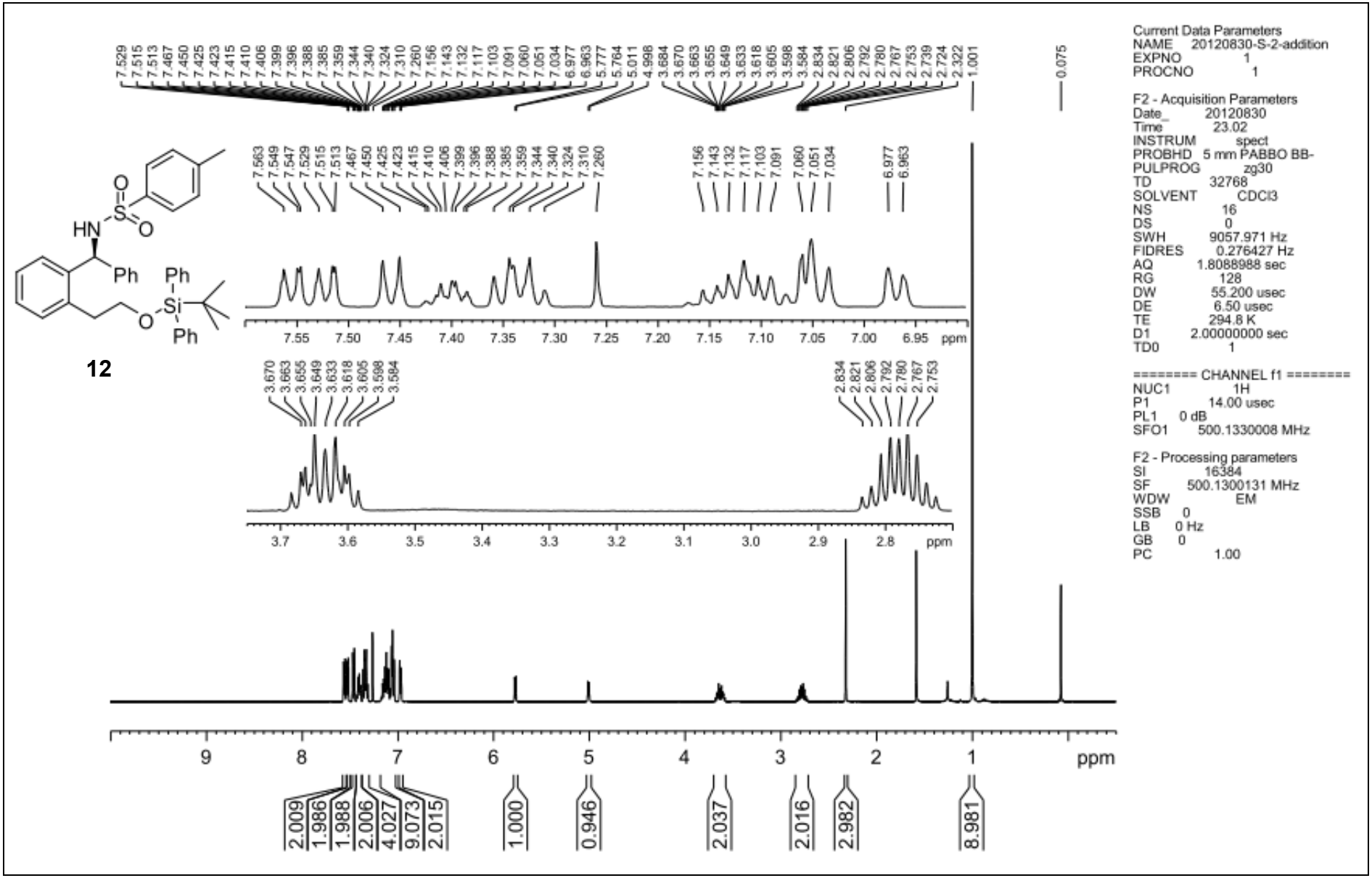
Current Data Parameters
NAME 20120923-S1
EXPNO 2
PROCNO 1

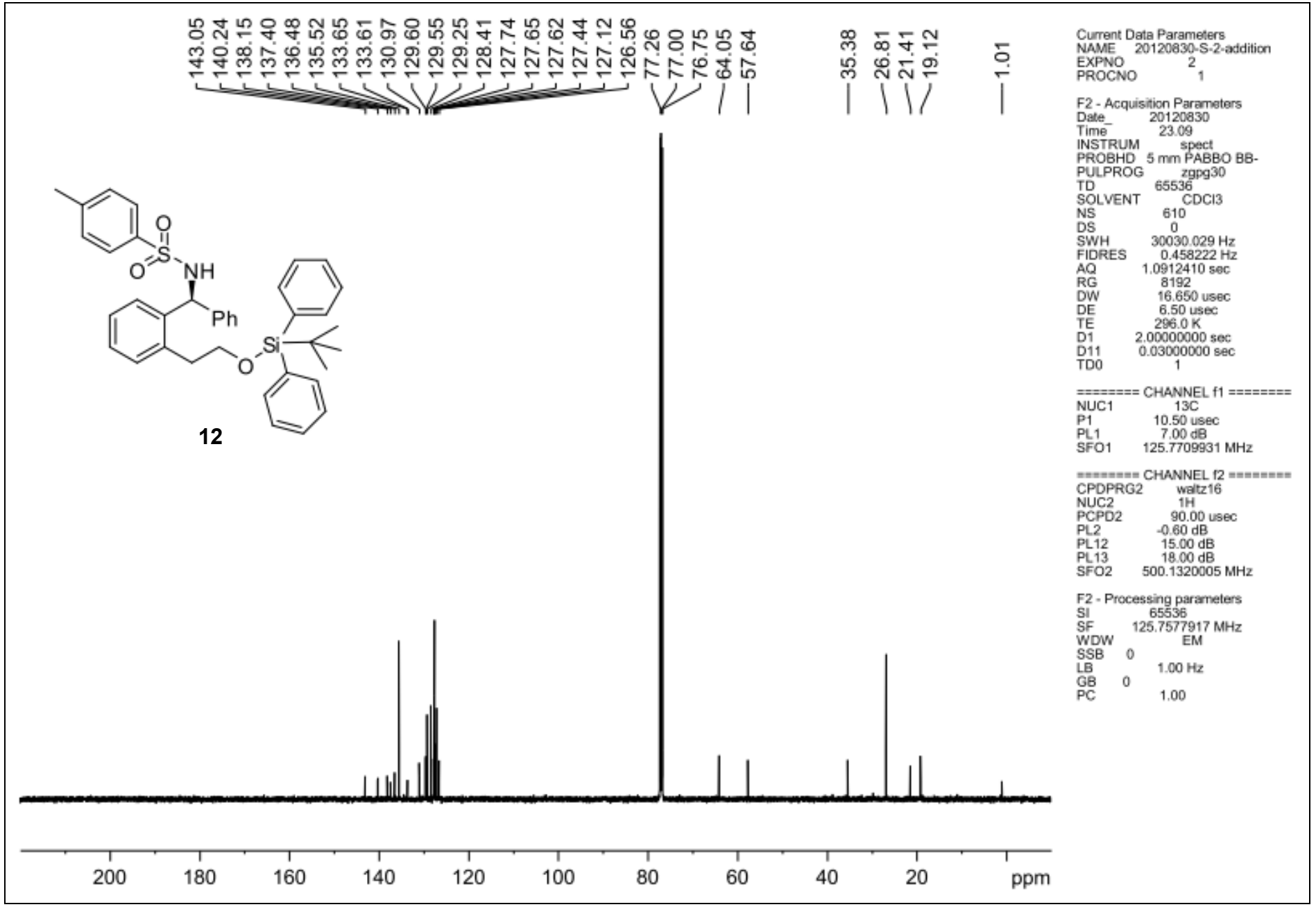
F2 - Acquisition Parameters
Date_ 20120923
Time 13.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 416
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 8192
DW 16.650 usec
DE 6.50 usec
TE 296.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

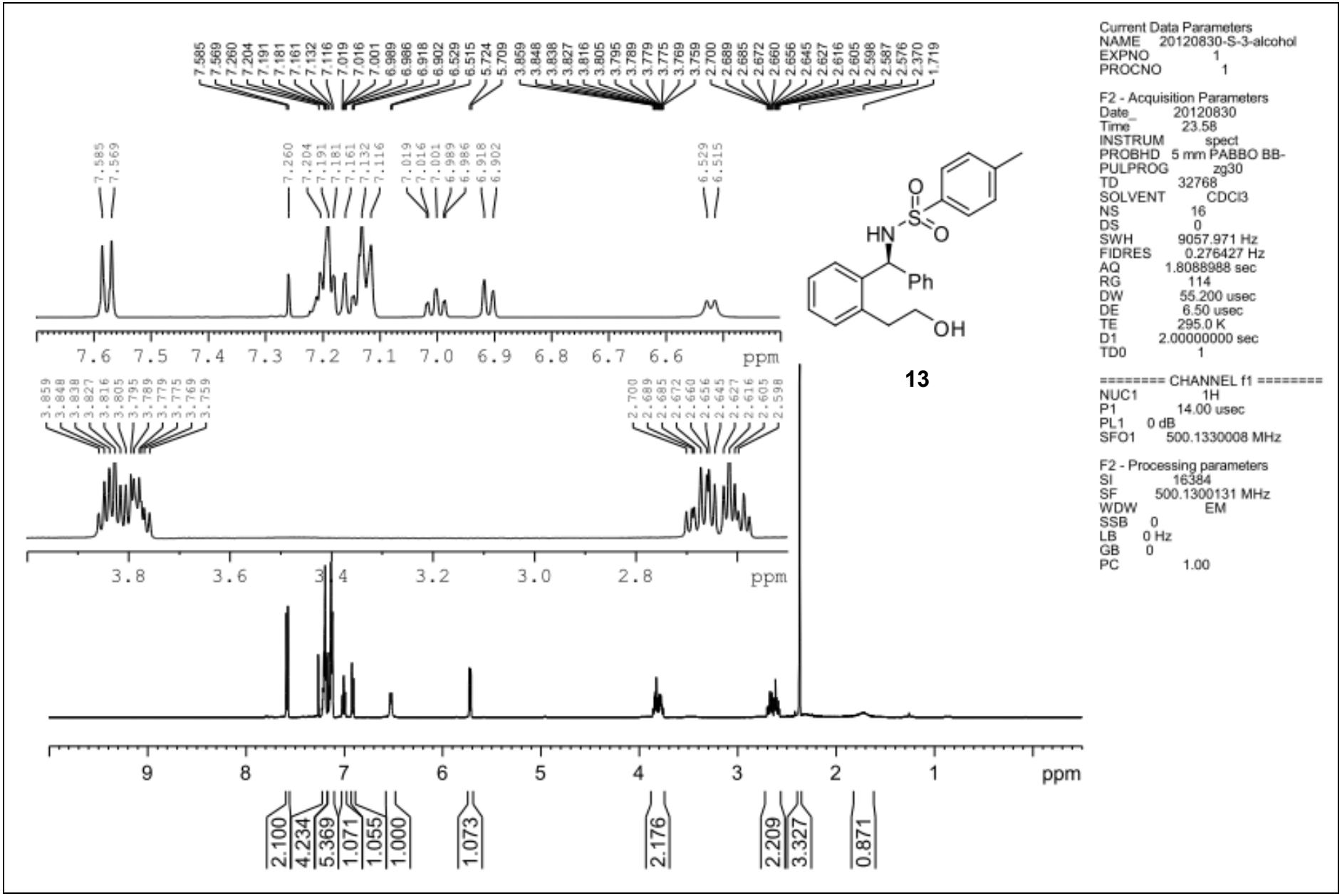
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 125.7709931 MHz

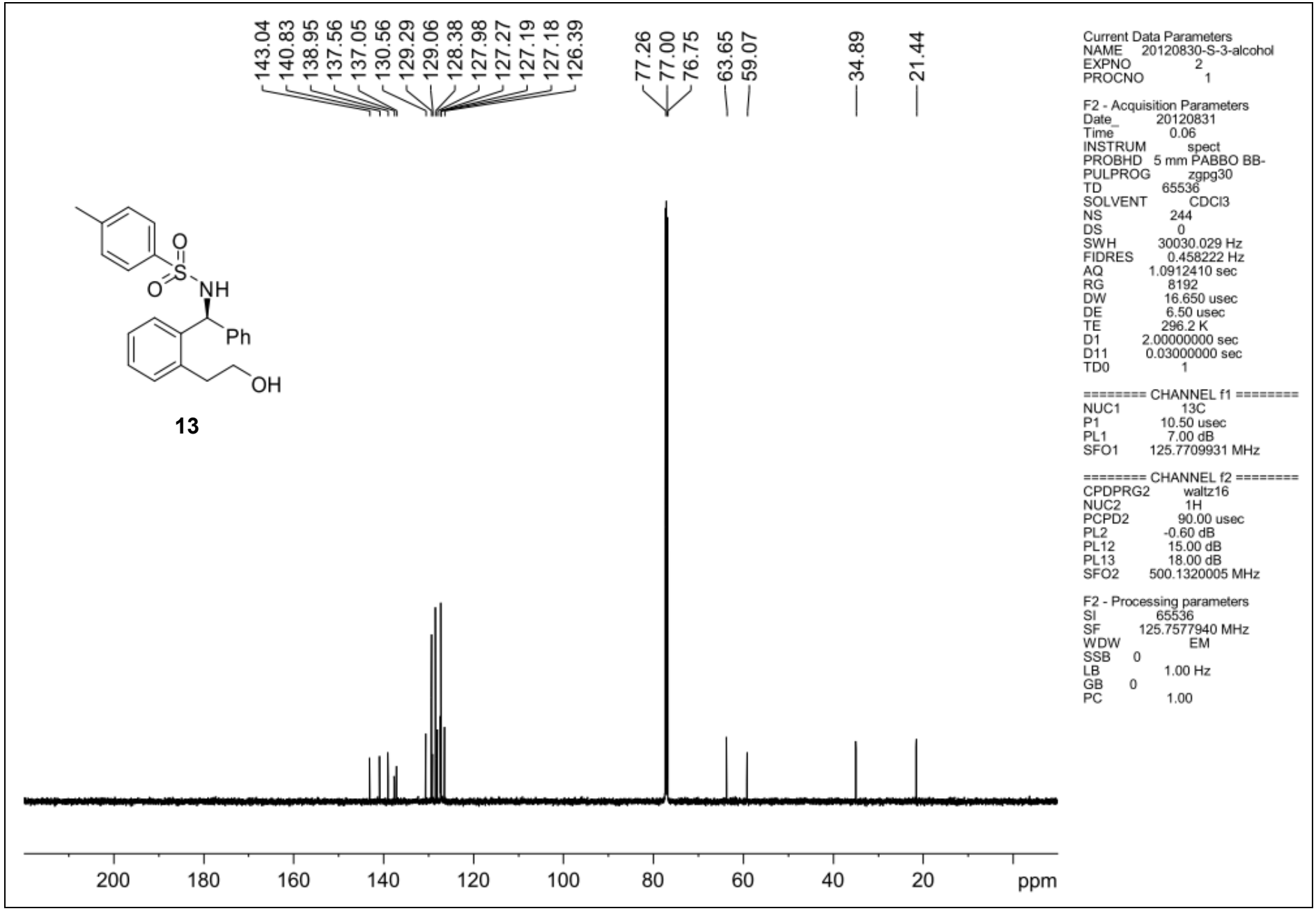
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1320005 MHz

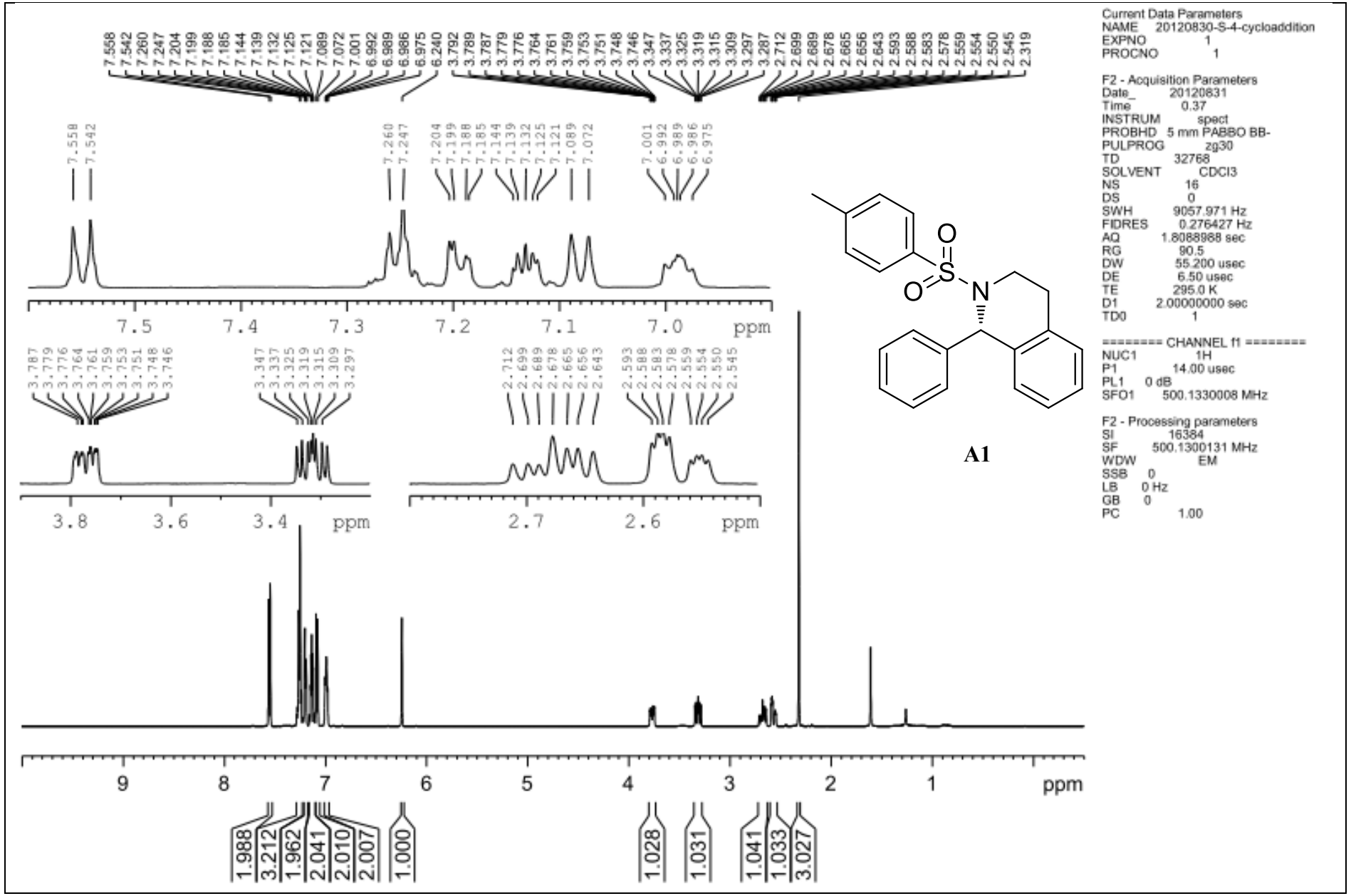
F2 - Processing parameters
SI 65536
SF 125.7577922 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

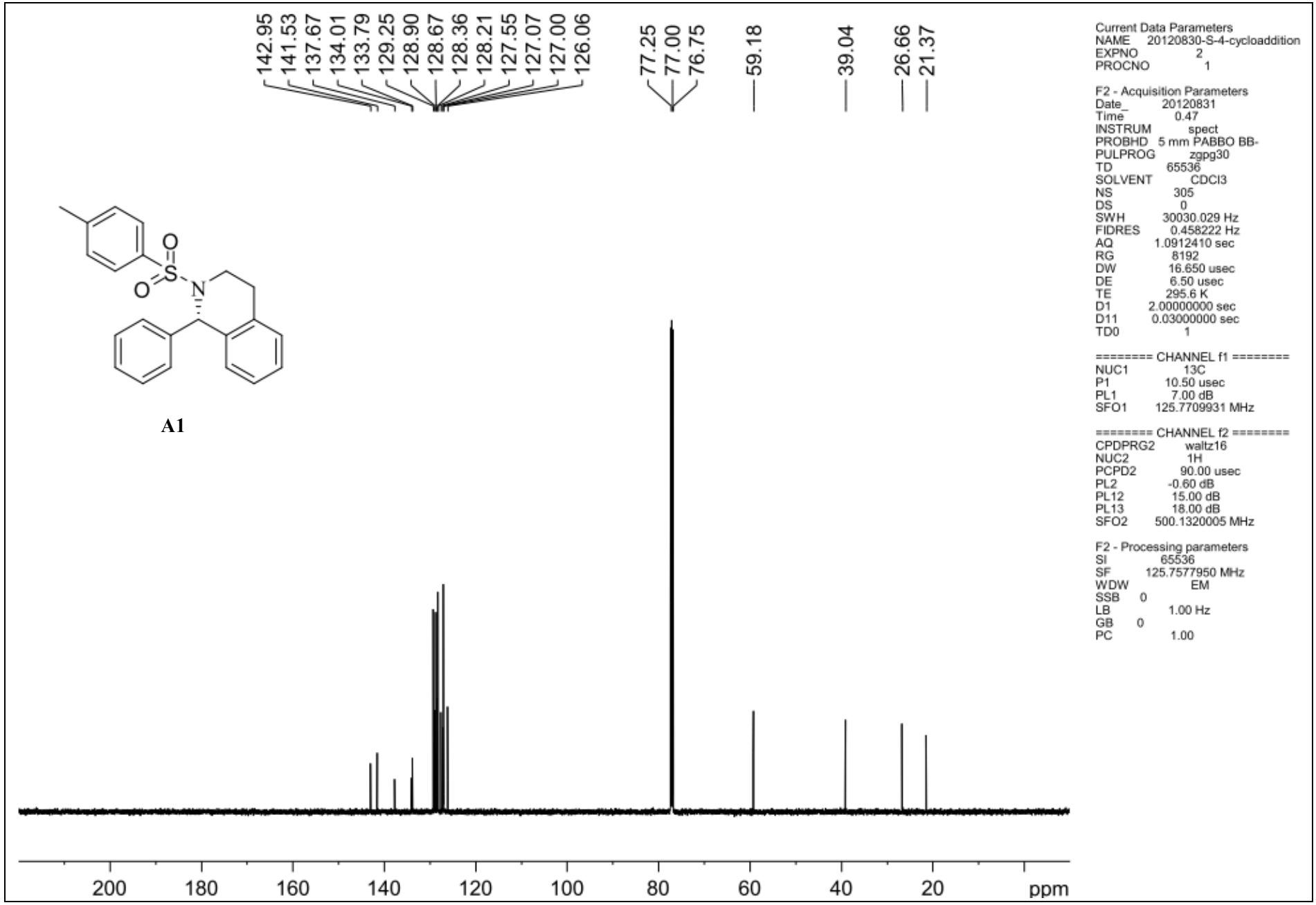

12
Current Data Parameters
NAME 20120830-S-2-addition
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120830
Time 23.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 9057.971 Hz
FIDRES 0.276427 Hz
AQ 1.8088988 sec
RG 128
DW 55.200 usec
DE 6.50 usec
TE 294.8 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0 dB
SFO1 500.1330008 MHz
F2 - Processing parameters
SI 16384
SF 500.1300131 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
ppm
2.009
1.986
1.988
2.006
4.027
9.073
2.015
1.000
0.946
2.037
2.016
2.982
8.981

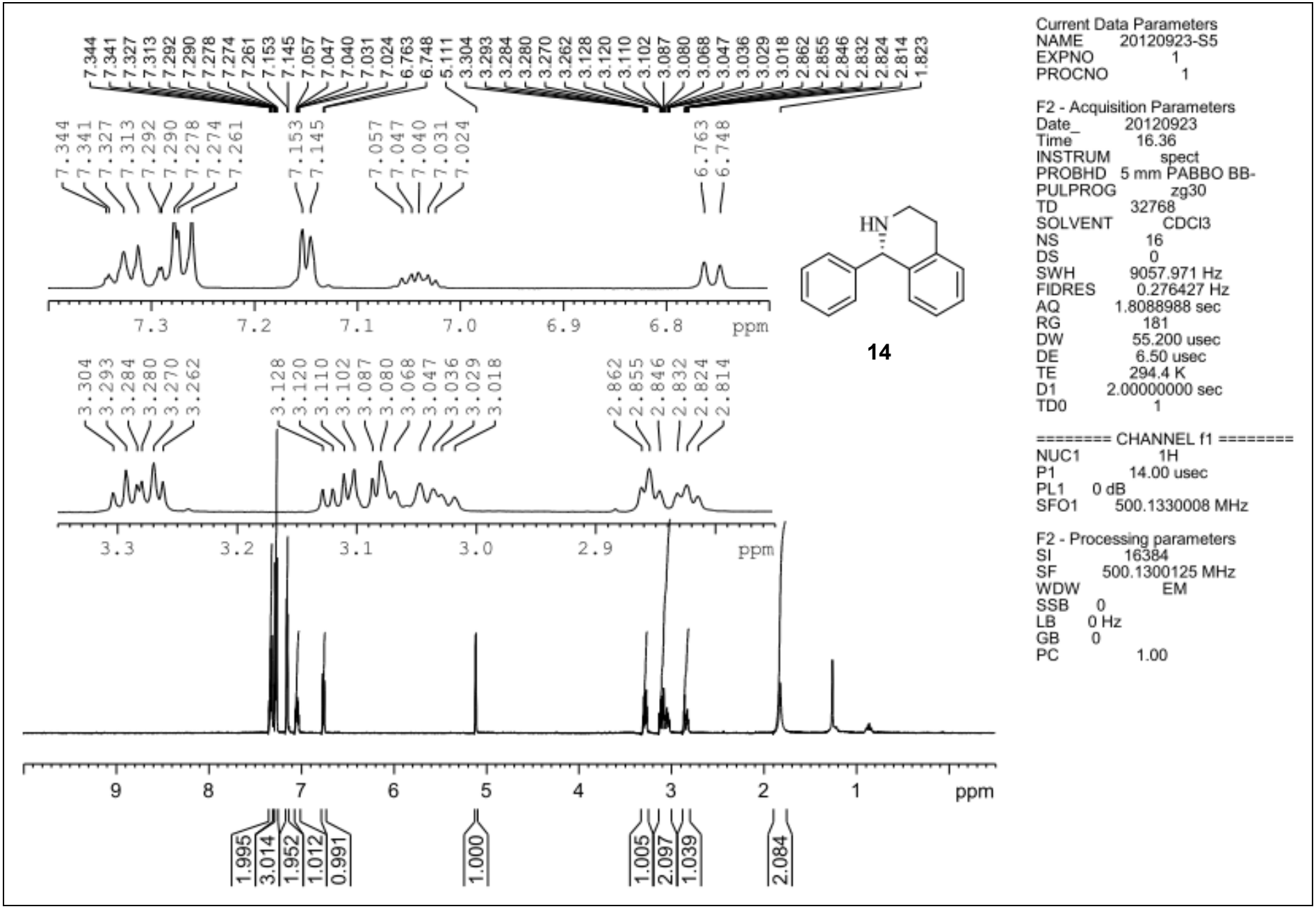

143.05
140.24
138.15
137.40
136.48
135.52
133.65
133.61
130.97
129.60
129.55
129.25
128.41
127.74
127.65
127.62
127.44
127.12
126.56
77.26
77.00
76.75
64.05
57.64
35.38
26.81
21.41
19.12
1.01
O
S
O
NH
Ph
Si
O
12
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME 20120830-S-2-addition
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120830
Time 23.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 610
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 8192
DW 16.650 usec
DE 6.50 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 125.7709931 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 65536
SF 125.7577917 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00


7.585 7.569 7.260 7.204 7.191 7.181 7.161 7.132 7.116 7.019 7.016 7.001 6.989 6.986 6.918 6.902 6.529 6.515 5.724 5.709
3.859 3.848 3.838 3.827 3.816 3.805 3.795 3.789 3.779 3.775 3.769 3.759
2.700 2.689 2.685 2.672 2.660 2.656 2.645 2.627 2.616 2.605 2.598 2.587 2.576 2.370 1.719
7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 ppm
3.8 3.6 3.4 3.2 3.0 2.8 ppm
9 8 7 6 5 4 3 2 1 ppm
2.100 4.234 5.369 1.071 1.055 1.000 1.073 2.176 2.209 3.327 0.871
HN S O O Ph OH
13
Current Data Parameters
NAME 20120830-S-3-alcohol
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120830
Time 23.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 9057.971 Hz
FIDRES 0.276427 Hz
AQ 1.8088988 sec
RG 114
DW 55.200 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0 dB
SFO1 500.1330008 MHz
F2 - Processing parameters
SI 16384
SF 500.1300131 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00


143.04
140.83
138.95
137.56
137.05
130.56
129.29
129.06
128.38
127.98
127.27
127.19
127.18
126.39
77.26
77.00
76.75
63.65
59.07
34.89
21.44
O
S
O
NH
Ph
OH
13
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME 20120830-S-3-alcohol
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120831
Time 0.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 244
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 8192
DW 16.650 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 125.7709931 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 65536
SF 125.7577940 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00


7.558 7.542 7.260 7.247 7.204 7.199 7.188 7.185 7.144 7.139 7.132 7.125 7.121 7.089 7.072 7.001 6.992 6.989 6.986 6.975 6.240 3.792 3.789 3.787 3.779 3.776 3.764 3.761 3.759 3.753 3.751 3.748 3.746 3.347 3.337 3.325 3.319 3.315 3.309 3.297 3.287 2.712 2.699 2.689 2.678 2.665 2.656 2.643 2.593 2.588 2.583 2.578 2.559 2.554 2.550 2.545 2.319
7.5 7.4 7.3 7.2 7.1 7.0 ppm
3.8 3.6 3.4 ppm
2.7 2.6 ppm
9 8 7 6 5 4 3 2 1 ppm
1.988 3.212 1.962 2.041 2.010 2.007 1.000 1.028 1.031 1.041 1.033 3.027
A1
Current Data Parameters
NAME 20120830-S-4-cycloaddition
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120831
Time 0.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 9057.971 Hz
FIDRES 0.276427 Hz
AQ 1.8088988 sec
RG 90.5
DW 55.200 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0 dB
SFO1 500.1330008 MHz
F2 - Processing parameters
SI 16384
SF 500.1300131 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00


142.95
141.53
137.67
134.01
133.79
129.25
128.90
128.67
128.36
128.21
127.55
127.07
127.00
126.06
77.25
77.00
76.75
59.18
39.04
26.66
21.37
A1
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME 20120830-S-4-cycloaddition
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120831
Time 0.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 305
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 8192
DW 16.650 usec
DE 6.50 usec
TE 295.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 125.7709931 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 65536
SF 125.7577950 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

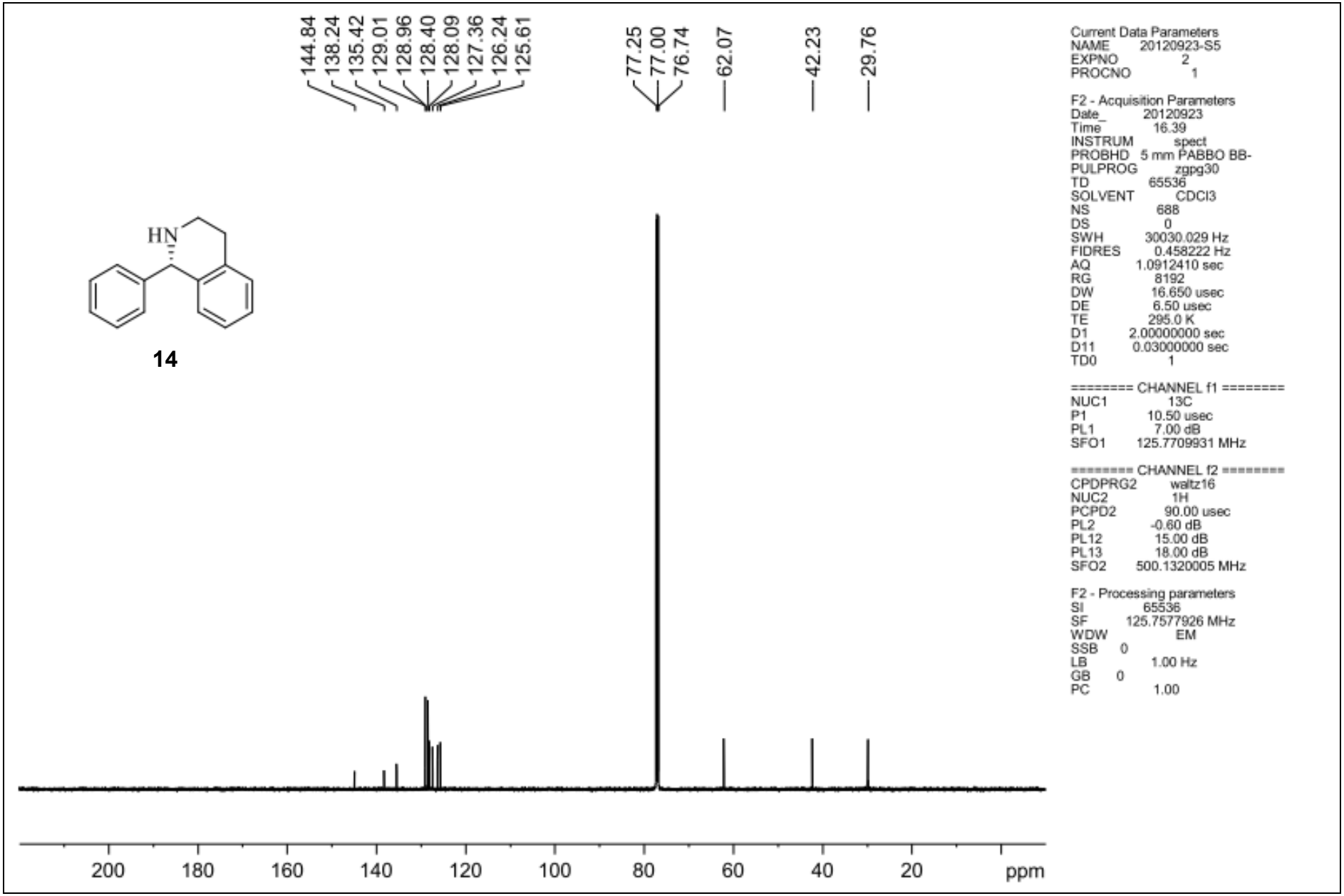


Current Data Parameters
NAME 20120923-S5
EXPNO 1
PROCNO 1

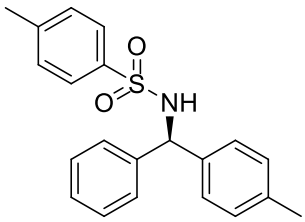
F2 - Acquisition Parameters
Date_ 20120923
Time 16.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 9057.971 Hz
FIDRES 0.276427 Hz
AQ 1.8088988 sec
RG 181
DW 55.200 usec
DE 6.50 usec
TE 294.4 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0 dB
SFO1 500.1330008 MHz

F2 - Processing parameters
SI 16384
SF 500.1300125 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00


144.84
138.24
135.42
129.01
128.96
128.40
128.09
127.36
126.24
125.61
77.25
77.00
76.74
62.07
42.23
29.76
HN
14
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME 20120923-S5
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120923
Time 16.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 688
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 8192
DW 16.650 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 125.7709931 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 65536
SF 125.7577926 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

X-ray ORTEP Illustration of (*R*)-4-methyl-*N*-(phenyl(*p*-tolyl)methyl) benzenesulfonamide (**5aa**)



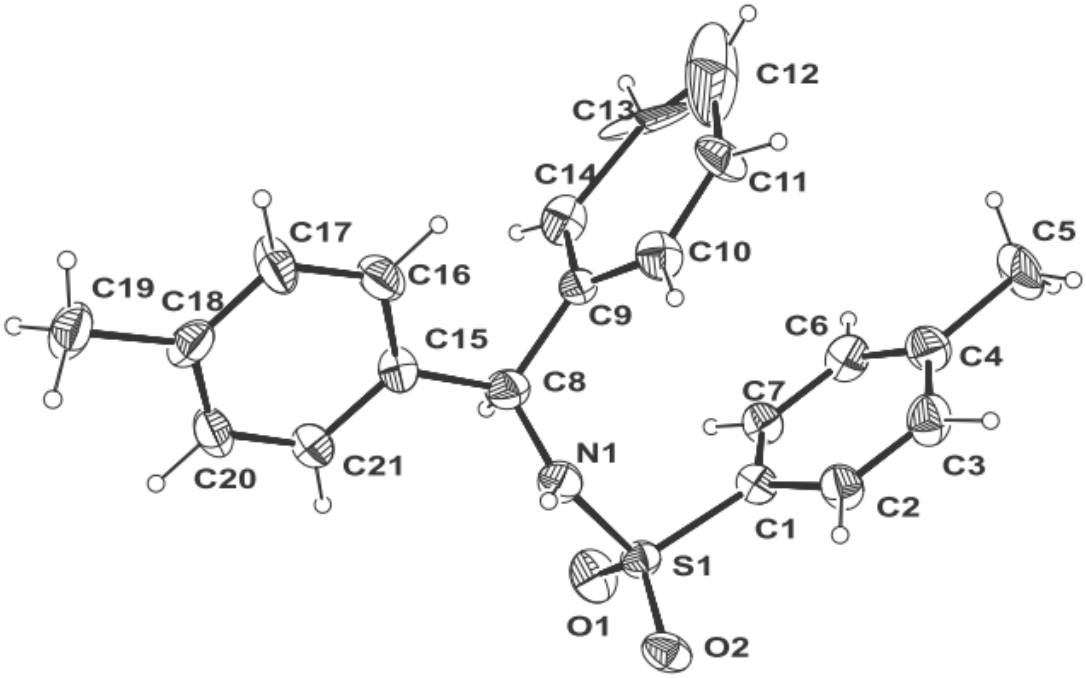


Table 1. Crystal data and structure refinement for ch14725.

Identification code	ch14725	
Empirical formula	C42.50 H43 Cl N2 O4 S2	
Formula weight	745.36	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 9.6551(6) Å	α= 90°.
	b = 18.2180(10) Å	β= 105.377(3)°.
	c = 12.0682(6) Å	γ = 90°.
Volume	2046.8(2) $Å^3$	
Z	2	
Density (calculated)	1.209 Mg/m^3	
Absorption coefficient	0.237 mm^{-1}	
F(000)	786	
Crystal size	0.28 x 0.21 x 0.12 mm^3	
Theta range for data collection	2.08 to 25.13°.	
Index ranges	-11<=h<=11, -20<=k<=21, -14<=l<=12	
Reflections collected	12645	
Independent reflections	6788 [R(int) = 0.0606]	
Completeness to theta = 25.13°	99.2 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.9721 and 0.9366	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6788 / 3 / 471	
Goodness-of-fit on F^2	1.006	
Final R indices [I>2sigma(I)]	R1 = 0.0919, wR2 = 0.2472	
R indices (all data)	R1 = 0.1719, wR2 = 0.3111	
Absolute structure parameter	0.2(2)	
Largest diff. peak and hole	0.956 and -0.535 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for ch14725. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	2322(9)	564(15)	7450(8)	53(2)
C(2)	3551(11)	150(15)	7518(9)	71(3)
C(3)	3452(13)	-502(16)	6970(11)	85(4)
C(4)	2048(16)	-766(16)	6306(11)	86(4)
C(5)	2062(17)	-1472(16)	5605(13)	120(6)
C(6)	913(12)	-363(15)	6270(10)	73(3)
C(7)	1020(11)	298(15)	6852(8)	63(3)
C(8)	1831(12)	2186(15)	6021(7)	70(3)
C(9)	1506(11)	1597(15)	5066(7)	58(3)
C(10)	2556(12)	1147(15)	4874(8)	69(3)
C(11)	2173(14)	625(15)	3994(9)	84(4)
C(12)	838(18)	537(16)	3323(11)	101(4)
C(13)	-181(17)	995(16)	3538(10)	106(5)
C(14)	101(11)	1515(15)	4373(8)	73(3)
C(15)	2198(10)	2942(15)	5660(8)	56(3)
C(16)	2706(14)	3034(16)	4657(11)	90(4)
C(17)	3076(15)	3732(16)	4361(13)	98(5)
C(18)	3000(11)	4323(16)	5063(10)	76(3)
C(19)	3427(14)	5078(16)	4710(12)	105(5)
C(20)	2468(12)	4230(16)	5988(10)	73(3)
C(21)	2083(11)	3559(16)	6272(8)	64(3)
C(22)	2578(10)	7937(15)	2450(7)	52(2)
C(23)	3812(12)	8357(16)	2555(10)	80(3)
C(24)	3608(14)	9034(16)	1955(13)	92(4)
C(25)	2258(14)	9286(16)	1315(10)	75(3)
C(26)	2101(16)	9988(17)	625(13)	126(6)
C(27)	1101(12)	8862(16)	1296(10)	77(3)
C(28)	1243(11)	8204(16)	1842(10)	75(3)
C(29)	2640(9)	6395(15)	1077(6)	51(2)
C(30)	1939(11)	6891(15)	58(8)	65(3)
C(31)	2759(13)	7430(16)	-291(11)	82(4)

C(32)	2140(20)	7910(17)	-1194(13)	107(5)
C(33)	720(19)	7848(17)	-1677(11)	99(5)
C(34)	-140(15)	7330(16)	-1395(10)	94(4)
C(35)	475(13)	6827(15)	-497(9)	80(3)
C(36)	2597(8)	5588(15)	718(7)	50(2)
C(37)	2221(13)	5036(16)	1330(10)	75(3)
C(38)	2321(14)	4290(16)	1000(11)	87(4)
C(39)	2767(12)	4114(16)	97(10)	75(3)
C(40)	2871(16)	3297(16)	-275(13)	116(5)
C(41)	3131(14)	4678(17)	-510(11)	89(4)
C(42)	3070(13)	5395(16)	-200(10)	80(3)
C(43)	5443	1815	3217	114(9)
N(1)	2825(8)	1993(15)	7049(6)	67(2)
N(2)	1952(7)	6491(15)	2032(5)	51(2)
O(1)	1198(7)	1642(15)	8250(6)	84(2)
O(2)	3790(6)	1476(14)	8951(5)	68(2)
O(3)	4241(6)	6884(15)	3464(5)	65(2)
O(4)	1858(7)	7027(15)	3861(5)	76(2)
S(1)	2507(2)	1445(14)	8041(2)	54(1)
S(2)	2723(2)	7058(14)	3063(2)	56(1)
Cl(1)	4606(7)	2505(14)	2561(6)	92(2)
Cl(2)	5366(8)	991(14)	2527(5)	97(2)

Table 3. Bond lengths [Å] and angles [°] for ch14725.

C(1)-C(7)	1.362(12)
C(1)-C(2)	1.390(14)
C(1)-S(1)	1.747(11)
C(2)-C(3)	1.350(16)
C(2)-H(2)	0.9300
C(3)-C(4)	1.462(17)
C(3)-H(3)	0.9300
C(4)-C(6)	1.310(17)
C(4)-C(5)	1.542(18)
C(5)-H(5A)	0.9600
C(5)-H(5B)	0.9600
C(5)-H(5C)	0.9600
C(6)-C(7)	1.384(15)
C(6)-H(6)	0.9300
C(7)-H(7)	0.9300
C(8)-N(1)	1.397(11)
C(8)-C(15)	1.514(16)
C(8)-C(9)	1.544(14)
C(8)-H(8)	0.9800
C(9)-C(10)	1.370(13)
C(9)-C(14)	1.401(13)
C(10)-C(11)	1.401(15)
C(10)-H(10)	0.9300
C(11)-C(12)	1.338(17)
C(11)-H(11)	0.9300
C(12)-C(13)	1.37(2)
C(12)-H(12)	0.9300
C(13)-C(14)	1.355(17)
C(13)-H(13)	0.9300
C(14)-H(14)	0.9300
C(15)-C(21)	1.364(15)
C(15)-C(16)	1.431(14)
C(16)-C(17)	1.394(19)
C(16)-H(16)	0.9300

C(17)-C(18)	1.384(17)
C(17)-H(17)	0.9300
C(18)-C(20)	1.357(16)
C(18)-C(19)	1.529(17)
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
C(20)-C(21)	1.349(17)
C(20)-H(20)	0.9300
C(21)-H(21)	0.9300
C(22)-C(28)	1.390(13)
C(22)-C(23)	1.394(14)
C(22)-S(2)	1.754(11)
C(23)-C(24)	1.417(17)
C(23)-H(23)	0.9300
C(24)-C(25)	1.404(16)
C(24)-H(24)	0.9300
C(25)-C(27)	1.354(16)
C(25)-C(26)	1.511(19)
C(26)-H(26A)	0.9600
C(26)-H(26B)	0.9600
C(26)-H(26C)	0.9600
C(27)-C(28)	1.357(16)
C(27)-H(27)	0.9300
C(28)-H(28)	0.9300
C(29)-N(2)	1.486(10)
C(29)-C(30)	1.531(13)
C(29)-C(36)	1.530(15)
C(29)-H(29)	0.9800
C(30)-C(35)	1.400(14)
C(30)-C(31)	1.394(15)
C(31)-C(32)	1.402(18)
C(31)-H(31)	0.9300
C(32)-C(33)	1.344(19)
C(32)-H(32)	0.9300
C(33)-C(34)	1.357(19)

C(33)-H(33)	0.9300
C(34)-C(35)	1.423(16)
C(34)-H(34)	0.9300
C(35)-H(35)	0.9300
C(36)-C(42)	1.352(13)
C(36)-C(37)	1.354(15)
C(37)-C(38)	1.428(17)
C(37)-H(37)	0.9300
C(38)-C(39)	1.312(15)
C(38)-H(38)	0.9300
C(39)-C(41)	1.360(19)
C(39)-C(40)	1.566(18)
C(40)-H(40A)	0.9600
C(40)-H(40B)	0.9600
C(40)-H(40C)	0.9600
C(41)-C(42)	1.364(19)
C(41)-H(41)	0.9300
C(42)-H(42)	0.9300
C(43)-Cl(1)	1.59(2)
C(43)-Cl(2)	1.71(2)
C(43)-H(43A)	0.9700
C(43)-H(43B)	0.9700
N(1)-S(1)	1.649(8)
N(1)-H(1)	0.8600
N(2)-S(2)	1.636(7)
N(2)-H(2A)	0.8600
O(1)-S(1)	1.399(6)
O(2)-S(1)	1.422(5)
O(3)-S(2)	1.452(6)
O(4)-S(2)	1.434(6)

C(7)-C(1)-C(2)	119.5(11)
C(7)-C(1)-S(1)	121.6(8)
C(2)-C(1)-S(1)	118.8(8)
C(3)-C(2)-C(1)	120.0(11)
C(3)-C(2)-H(2)	120.0

C(1)-C(2)-H(2)	120.0
C(2)-C(3)-C(4)	119.5(12)
C(2)-C(3)-H(3)	120.2
C(4)-C(3)-H(3)	120.2
C(6)-C(4)-C(3)	118.7(13)
C(6)-C(4)-C(5)	125.4(13)
C(3)-C(4)-C(5)	115.7(13)
C(4)-C(5)-H(5A)	109.5
C(4)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(4)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
C(4)-C(6)-C(7)	121.4(11)
C(4)-C(6)-H(6)	119.3
C(7)-C(6)-H(6)	119.3
C(1)-C(7)-C(6)	120.8(10)
C(1)-C(7)-H(7)	119.6
C(6)-C(7)-H(7)	119.6
N(1)-C(8)-C(15)	109.0(9)
N(1)-C(8)-C(9)	116.3(9)
C(15)-C(8)-C(9)	115.7(7)
N(1)-C(8)-H(8)	104.8
C(15)-C(8)-H(8)	104.8
C(9)-C(8)-H(8)	104.8
C(10)-C(9)-C(14)	118.5(10)
C(10)-C(9)-C(8)	121.9(10)
C(14)-C(9)-C(8)	119.6(9)
C(9)-C(10)-C(11)	118.5(11)
C(9)-C(10)-H(10)	120.8
C(11)-C(10)-H(10)	120.8
C(12)-C(11)-C(10)	123.9(12)
C(12)-C(11)-H(11)	118.0
C(10)-C(11)-H(11)	118.0
C(11)-C(12)-C(13)	116.0(13)
C(11)-C(12)-H(12)	122.0

C(13)-C(12)-H(12)	122.0
C(12)-C(13)-C(14)	123.7(13)
C(12)-C(13)-H(13)	118.2
C(14)-C(13)-H(13)	118.2
C(13)-C(14)-C(9)	119.4(12)
C(13)-C(14)-H(14)	120.3
C(9)-C(14)-H(14)	120.3
C(21)-C(15)-C(16)	117.2(11)
C(21)-C(15)-C(8)	122.3(9)
C(16)-C(15)-C(8)	120.5(10)
C(17)-C(16)-C(15)	119.5(12)
C(17)-C(16)-H(16)	120.3
C(15)-C(16)-H(16)	120.3
C(18)-C(17)-C(16)	119.6(12)
C(18)-C(17)-H(17)	120.2
C(16)-C(17)-H(17)	120.2
C(20)-C(18)-C(17)	120.0(11)
C(20)-C(18)-C(19)	122.0(13)
C(17)-C(18)-C(19)	117.8(12)
C(18)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(21)-C(20)-C(18)	120.7(11)
C(21)-C(20)-H(20)	119.6
C(18)-C(20)-H(20)	119.6
C(20)-C(21)-C(15)	122.8(11)
C(20)-C(21)-H(21)	118.6
C(15)-C(21)-H(21)	118.6
C(28)-C(22)-C(23)	120.5(11)
C(28)-C(22)-S(2)	120.0(8)
C(23)-C(22)-S(2)	119.5(8)
C(22)-C(23)-C(24)	115.5(11)
C(22)-C(23)-H(23)	122.2

C(24)-C(23)-H(23)	122.2
C(25)-C(24)-C(23)	123.3(11)
C(25)-C(24)-H(24)	118.4
C(23)-C(24)-H(24)	118.4
C(27)-C(25)-C(24)	117.7(12)
C(27)-C(25)-C(26)	120.8(12)
C(24)-C(25)-C(26)	121.5(12)
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(25)-C(27)-C(28)	121.3(12)
C(25)-C(27)-H(27)	119.4
C(28)-C(27)-H(27)	119.4
C(27)-C(28)-C(22)	121.7(11)
C(27)-C(28)-H(28)	119.2
C(22)-C(28)-H(28)	119.2
N(2)-C(29)-C(30)	111.1(7)
N(2)-C(29)-C(36)	110.4(8)
C(30)-C(29)-C(36)	111.5(8)
N(2)-C(29)-H(29)	107.9
C(30)-C(29)-H(29)	107.9
C(36)-C(29)-H(29)	107.9
C(35)-C(30)-C(31)	119.7(11)
C(35)-C(30)-C(29)	120.7(10)
C(31)-C(30)-C(29)	119.5(10)
C(32)-C(31)-C(30)	121.0(13)
C(32)-C(31)-H(31)	119.5
C(30)-C(31)-H(31)	119.5
C(33)-C(32)-C(31)	117.4(14)
C(33)-C(32)-H(32)	121.3
C(31)-C(32)-H(32)	121.3
C(32)-C(33)-C(34)	124.8(13)
C(32)-C(33)-H(33)	117.6

C(34)-C(33)-H(33)	117.6
C(33)-C(34)-C(35)	118.6(13)
C(33)-C(34)-H(34)	120.7
C(35)-C(34)-H(34)	120.7
C(30)-C(35)-C(34)	118.4(12)
C(30)-C(35)-H(35)	120.8
C(34)-C(35)-H(35)	120.8
C(42)-C(36)-C(37)	116.9(11)
C(42)-C(36)-C(29)	119.5(10)
C(37)-C(36)-C(29)	123.4(8)
C(36)-C(37)-C(38)	120.4(11)
C(36)-C(37)-H(37)	119.8
C(38)-C(37)-H(37)	119.8
C(39)-C(38)-C(37)	121.7(13)
C(39)-C(38)-H(38)	119.1
C(37)-C(38)-H(38)	119.1
C(38)-C(39)-C(41)	116.9(12)
C(38)-C(39)-C(40)	122.0(14)
C(41)-C(39)-C(40)	121.2(12)
C(39)-C(40)-H(40A)	109.5
C(39)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(39)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(39)-C(41)-C(42)	122.6(12)
C(39)-C(41)-H(41)	118.7
C(42)-C(41)-H(41)	118.7
C(36)-C(42)-C(41)	121.5(12)
C(36)-C(42)-H(42)	119.2
C(41)-C(42)-H(42)	119.2
Cl(1)-C(43)-Cl(2)	120.1(4)
Cl(1)-C(43)-H(43A)	107.3
Cl(2)-C(43)-H(43A)	107.3
Cl(1)-C(43)-H(43B)	107.3
Cl(2)-C(43)-H(43B)	107.3

H(43A)-C(43)-H(43B)	106.9
C(8)-N(1)-S(1)	125.5(7)
C(8)-N(1)-H(1)	117.3
S(1)-N(1)-H(1)	117.2
C(29)-N(2)-S(2)	117.2(6)
C(29)-N(2)-H(2A)	121.4
S(2)-N(2)-H(2A)	121.4
O(1)-S(1)-O(2)	119.6(4)
O(1)-S(1)-N(1)	109.1(5)
O(2)-S(1)-N(1)	104.2(4)
O(1)-S(1)-C(1)	108.0(5)
O(2)-S(1)-C(1)	109.0(5)
N(1)-S(1)-C(1)	106.2(4)
O(4)-S(2)-O(3)	118.9(4)
O(4)-S(2)-N(2)	104.9(4)
O(3)-S(2)-N(2)	109.4(4)
O(4)-S(2)-C(22)	108.9(5)
O(3)-S(2)-C(22)	107.5(4)
N(2)-S(2)-C(22)	106.7(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for ch14725. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	40(5)	56(7)	65(6)	1(5)	19(4)	-8(5)
C(2)	53(6)	60(8)	89(7)	-12(6)	2(5)	-6(6)
C(3)	63(7)	78(11)	103(9)	0(8)	4(6)	9(7)
C(4)	104(10)	65(10)	89(9)	-5(7)	24(8)	-25(8)
C(5)	143(13)	41(9)	156(13)	-42(9)	8(10)	-19(8)
C(6)	58(7)	62(9)	93(8)	6(7)	9(6)	-12(6)
C(7)	57(6)	58(8)	75(7)	-4(6)	22(5)	-7(5)
C(8)	83(7)	76(8)	51(5)	3(5)	18(5)	-3(6)
C(9)	78(7)	50(7)	48(5)	6(5)	23(5)	2(6)
C(10)	68(7)	72(9)	74(6)	-1(6)	33(5)	-3(6)
C(11)	84(8)	92(11)	80(7)	-43(7)	29(7)	6(7)
C(12)	127(12)	100(12)	87(8)	-20(8)	47(9)	-4(10)
C(13)	114(11)	127(14)	62(7)	3(8)	-4(7)	-37(10)
C(14)	77(7)	75(8)	72(6)	-10(7)	26(5)	-3(7)
C(15)	51(5)	58(7)	65(6)	-3(5)	25(5)	-1(5)
C(16)	124(10)	75(10)	84(8)	-15(7)	54(8)	-16(8)
C(17)	141(12)	56(9)	129(11)	-16(8)	91(10)	-17(8)
C(18)	72(7)	63(9)	86(8)	22(7)	11(6)	-18(6)
C(19)	92(9)	79(10)	127(10)	44(8)	-2(8)	-15(8)
C(20)	80(8)	56(9)	74(7)	-14(7)	5(6)	-1(7)
C(21)	68(7)	74(10)	52(6)	-5(6)	17(5)	3(6)
C(22)	51(6)	52(7)	52(5)	-3(5)	13(4)	-7(5)
C(23)	59(7)	68(9)	109(9)	17(7)	14(6)	-8(6)
C(24)	77(8)	64(10)	142(11)	17(9)	41(8)	-16(7)
C(25)	92(9)	64(9)	66(7)	10(6)	18(6)	-6(7)
C(26)	121(12)	113(16)	138(12)	42(11)	22(10)	-7(11)
C(27)	65(7)	73(10)	85(8)	8(7)	6(6)	2(7)
C(28)	63(7)	67(9)	90(8)	0(7)	14(6)	-10(6)
C(29)	46(5)	60(6)	48(4)	-1(5)	13(4)	3(5)
C(30)	64(6)	66(8)	73(6)	3(5)	34(5)	6(6)
C(31)	65(7)	83(9)	105(9)	9(7)	38(7)	-3(7)

C(32)	130(13)	101(13)	100(10)	32(9)	46(9)	16(11)
C(33)	144(13)	84(11)	81(8)	45(7)	49(9)	49(10)
C(34)	99(9)	110(12)	64(7)	6(7)	7(6)	-3(8)
C(35)	87(8)	81(9)	69(6)	-13(6)	14(6)	-3(7)
C(36)	34(4)	62(7)	51(5)	-7(5)	6(4)	1(5)
C(37)	103(9)	49(8)	82(8)	-12(6)	42(7)	0(6)
C(38)	117(11)	63(10)	87(8)	-12(7)	39(8)	-5(8)
C(39)	79(8)	68(9)	65(7)	-10(6)	-2(6)	15(7)
C(40)	133(12)	78(11)	124(11)	-24(9)	13(9)	28(9)
C(41)	108(10)	87(11)	79(8)	-23(8)	39(7)	-5(8)
C(42)	106(9)	58(8)	93(8)	-6(7)	56(7)	4(7)
N(1)	55(5)	67(6)	72(5)	-5(4)	5(4)	-17(5)
N(2)	48(4)	50(5)	62(4)	-18(4)	25(3)	-4(4)
O(1)	63(4)	93(6)	107(5)	-7(5)	42(4)	16(4)
O(2)	50(3)	85(5)	62(3)	-20(4)	4(3)	-4(4)
O(3)	41(3)	71(5)	78(4)	4(3)	6(3)	9(3)
O(4)	86(5)	82(5)	75(4)	-12(4)	47(4)	-15(5)
S(1)	50(1)	61(2)	52(1)	-1(1)	13(1)	0(1)
S(2)	59(1)	56(2)	57(1)	1(1)	21(1)	-2(1)
Cl(1)	89(4)	80(5)	112(5)	3(4)	33(4)	18(4)
Cl(2)	122(5)	86(5)	101(4)	-4(4)	58(4)	17(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for ch14725.

	x	y	z	U(eq)
H(2)	4441	322	7941	85
H(3)	4272	-780	7014	102
H(5A)	3024	-1660	5768	179
H(5B)	1722	-1364	4800	179
H(5C)	1448	-1833	5810	179
H(6)	16	-524	5845	88
H(7)	192	564	6835	75
H(8)	923	2252	6227	84
H(10)	3500	1187	5318	83
H(11)	2891	321	3867	101
H(12)	616	185	2745	121
H(13)	-1121	948	3087	127
H(14)	-632	1813	4484	88
H(16)	2788	2630	4207	107
H(17)	3372	3801	3695	118
H(19A)	3748	5031	4025	158
H(19B)	4188	5276	5317	158
H(19C)	2613	5401	4565	158
H(20)	2368	4634	6432	87
H(21)	1725	3514	6912	77
H(23)	4711	8204	2990	96
H(24)	4407	9327	1988	110
H(26A)	3026	10213	732	189
H(26B)	1473	10318	878	189
H(26C)	1703	9878	-175	189
H(27)	190	9024	902	92
H(28)	427	7924	1809	90
H(29)	3650	6540	1359	62
H(31)	3731	7471	80	98
H(32)	2688	8259	-1448	128

H(33)	296	8184	-2246	119
H(34)	-1110	7305	-1781	112
H(35)	-83	6465	-285	96
H(37)	1894	5144	1971	90
H(38)	2065	3918	1435	104
H(40A)	2567	2978	248	174
H(40B)	3846	3186	-264	174
H(40C)	2263	3226	-1038	174
H(41)	3434	4570	-1162	107
H(42)	3360	5759	-630	96
H(43A)	5101	1735	3894	137
H(43B)	6448	1951	3486	137
H(1)	3674	2176	7175	80
H(2A)	1181	6259	2043	62