

Supporting Information

Asymmetric Cyanation of Nitroalkenes Catalyzed by A Salen-Titanium Catalyst

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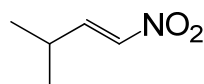
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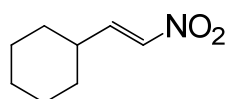
General methods:

All reactions were monitored by thin layer chromatography (TLC), column chromatography purifications were carried out using silica gel. All of the alkyl nitroolefins were prepared according to the literature. ¹H NMR and ¹³C NMR spectra were recorded on a 300M Bruker[®] instrument (300 MHz and 75 MHz, respectively) using tetramethylsilane as internal reference. Data for ¹H NMR are recorded as follows: chemical shift (δ, ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet, q = quartet or unresolved, coupling constant(s) in Hz, integration). Data for ¹³C NMR are reported in terms of chemical shift (δ, ppm). Optical rotations were reported as follows: [α]_D²⁰ (c: g/100 mL, in solvent). HR-MS was measured with an APEX II 47e mass spectrometer. The e.r. value determination was carried out using chiral HPLC with Daicel Chiracel AD-H/OD-H/OJ column on Waters[®] with a 996 UV-detector, flow rate = 1.0 mL/min.

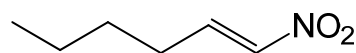
NMR datas for the starting materials 1:



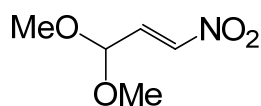
(E)-3-methyl-1-nitrobut-1-ene (1a): ^1H NMR (300 MHz, CDCl_3) δ 7.33 – 7.19 (m, 1H), 6.95 (d, J = 13.5 Hz, 1H), 2.59 (dq, J = 13.5, 6.7 Hz, 1H), 1.15 (d, J = 6.8 Hz, 7H). ^{13}C NMR (75 MHz, CDCl_3) δ 148.5, 138.1, 28.3, 21.0.



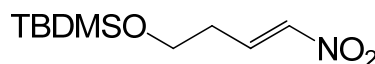
(E)-(2-nitrovinyl) cyclohexane (1b): ^1H NMR (300 MHz, CDCl_3) δ 7.23 (dd, J = 13.9, 7.6 Hz, 1H), 6.93 (dd, J = 13.5, 0.9 Hz, 1H), 2.25 (dd, J = 10.8, 6.9 Hz, 1H), 1.91 – 1.62 (m, 5H), 1.45 – 1.09 (m, 5H). ^{13}C NMR (75 MHz, CDCl_3) δ 147.3, 138.3, 37.6, 31.4, 25.6, 25.4.



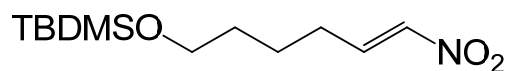
(E)-1-nitrohex-1-ene (1c): ^1H NMR (300 MHz, CDCl_3) δ 7.43 – 7.17 (m, 1H), 6.99 (d, J = 13.4 Hz, 1H), 2.29 (q, J = 7.3 Hz, 2H), 1.62 – 1.25 (m, 4H), 0.94 (t, J = 7.1 Hz, 3H). ^{13}C NMR (75 MHz, CDCl_3) δ 142.8, 139.5, 29.7, 28.1, 22.1, 13.6.



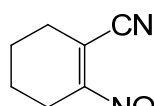
(E)-3,3-dimethoxy-1-nitroprop-1-ene (1d): ^1H NMR (300 MHz, CDCl_3) δ 7.21 (dd, J = 13.4, 1.0 Hz, 1H), 7.04 (dd, J = 13.4, 3.3 Hz, 1H), 5.14 (dd, J = 3.2, 1.1 Hz, 1H), 3.37 (s, 6H). ^{13}C NMR (75 MHz, CDCl_3) δ 142.5, 136.4, 97.9, 52.9.



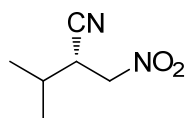
(E)-tert-butyldimethyl((4-nitrobut-3-en-1-yl)oxy) silane (1f): ^1H NMR (300 MHz, CDCl_3) δ 7.38 – 7.24 (m, 1H), 7.05 (d, J = 13.5 Hz, 1H), 3.78 (t, J = 5.9 Hz, 2H), 2.47 (ddd, J = 13.3, 6.0, 1.5 Hz, 2H), 0.89 (s, 9H), 0.06 (s, 6H). ^{13}C NMR (75 MHz, CDCl_3) δ 140.6, 139.8, 60.6, 31.8, 25.8, 18.2, -5.5.



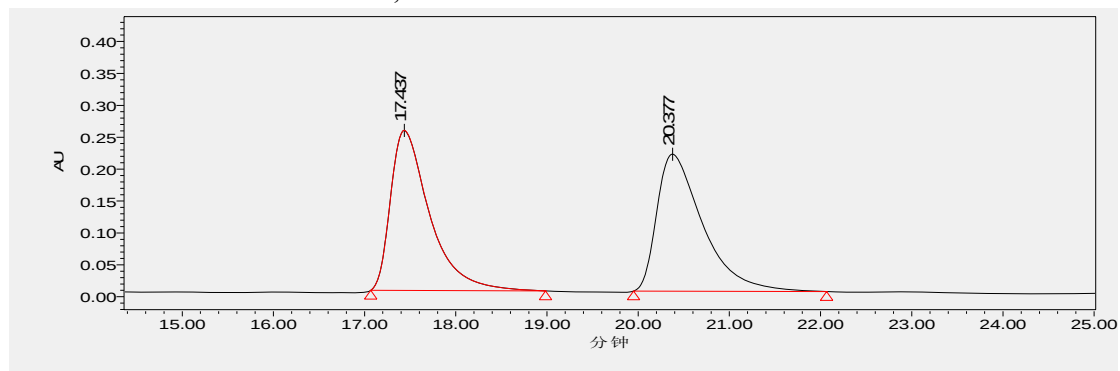
(E)-tert-butyldimethyl((6-nitrohex-5-en-1-yl)oxy) silane (1e): ^1H NMR (300 MHz, CDCl_3) δ 7.32 (dt, J = 13.6, 7.4 Hz, 1H), 7.00 (d, J = 13.4 Hz, 1H), 3.66 (t, J = 5.9 Hz, 2H), 2.38 (qd, J = 7.5, 1.4 Hz, 2H), 1.79 – 1.67 (m, 2H), 0.89 (s, 9H), 0.05 (s, 6H). ^{13}C NMR (75 MHz, CDCl_3) δ 142.7, 139.6, 61.7, 30.7, 25.9, 25.2, 18.2, -5.4.



2-nitrocyclohex-1-enecarbonitrile (1g): ^1H NMR (300 MHz, CDCl_3) δ 7.37 – 7.29 (m, 1H), 2.57 (ddd, J = 6.2, 5.2, 2.1 Hz, 2H), 2.42 – 2.25 (m, 2H), 1.84 – 1.71 (m, 2H), 1.71 – 1.57 (m, 2H). ^{13}C NMR (75 MHz, CDCl_3) δ 149.6, 134.3, 24.7, 23.9, 21.7, 20.6.

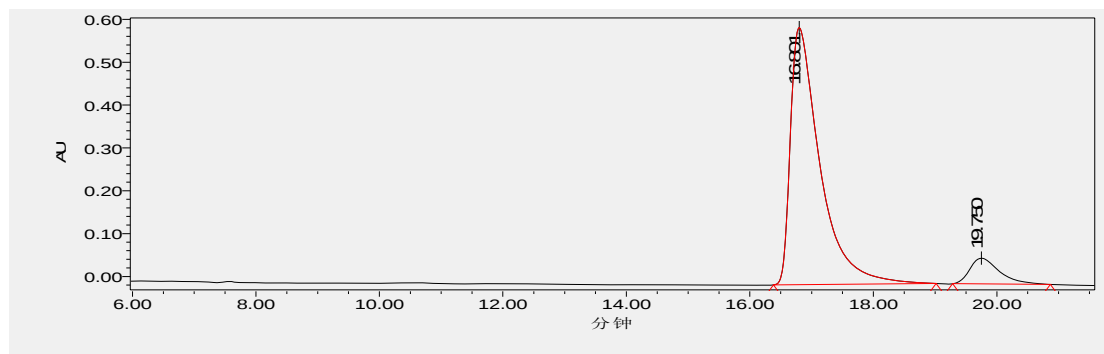


3a: OD-H column, Hexane/iPrOH = 90/10



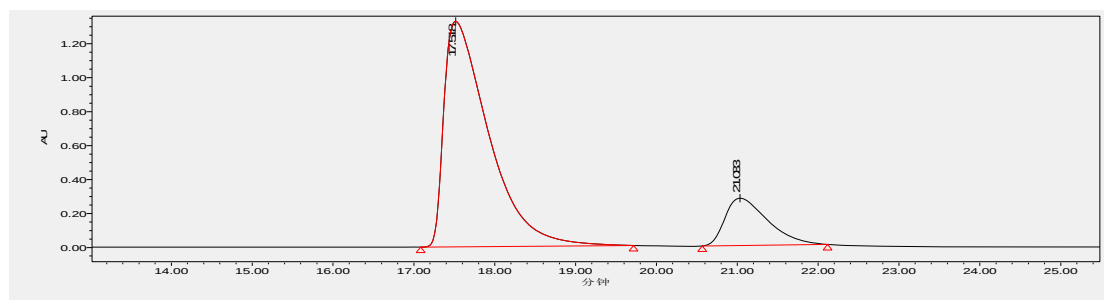
Racemic

	Retention Time	Area	% Area	Height	Int Type	Amount	Units	Peak Type	Peak Codes
1	17.437	7473643	49.92	251089	bb			Unknown	
2	20.377	7496770	50.08	214600	bb			Unknown	



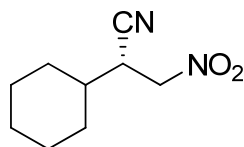
-40°C to -15°C

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1	16.801	19965740	90.94	599972	bb			Unknown	
2	19.750	1989442	9.06	60091	bb			Unknown	

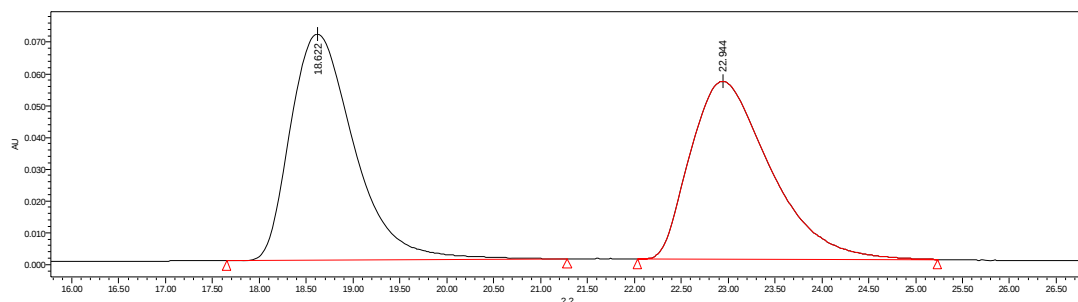


Room temperature

	Retention Time	Area	% Area	Height	Int Type	Amount	Units	Peak Type	Peak Codes
1	17.518	51088190	83.37	1328076	bb			Unknown	
2	21.033	10192285	16.63	278989	bb			Unknown	

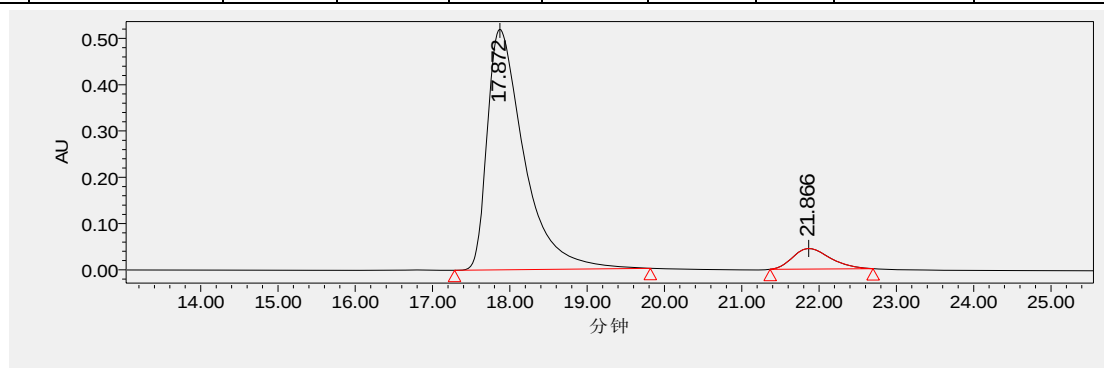


3b: OD-H column, Hexane/ iPrOH = 90/10



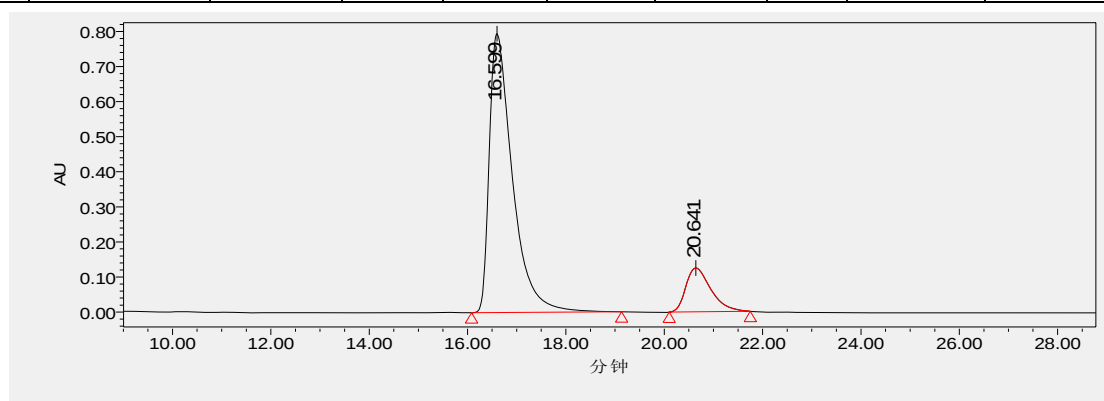
Racemic

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1	18.622	3350459	50.33	71141	bb			Unknown	
2	22.944	3307002	49.67	56033	bb			Unknown	



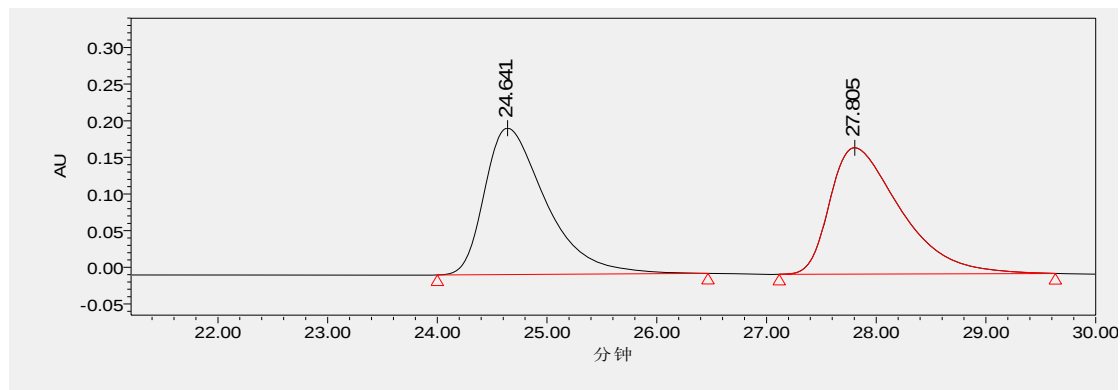
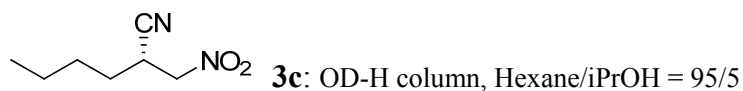
-40°C to -15°C

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1	17.872	17181742	91.98	519855	bb			Unknown	
2	21.866	1498525	8.02	44405	bb			Unknown	



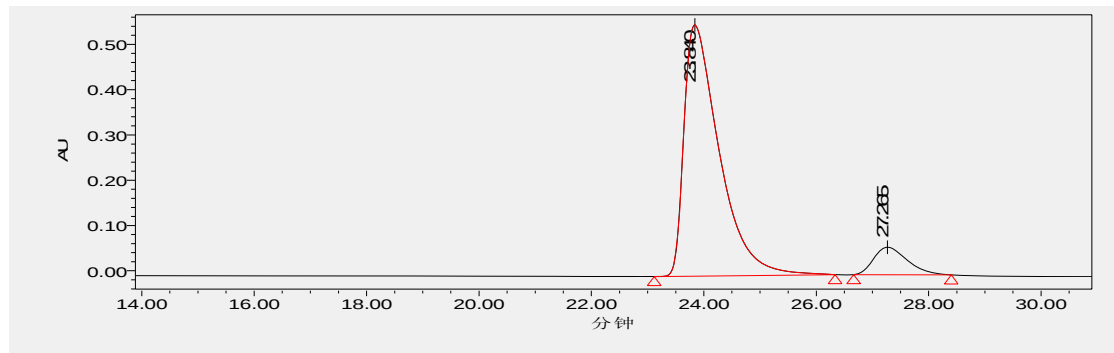
Room temperature

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1	16.599	25874578	85.42	794482	bb			Unknown	
2	20.641	4415118	14.58	124883	bb			Unknown	



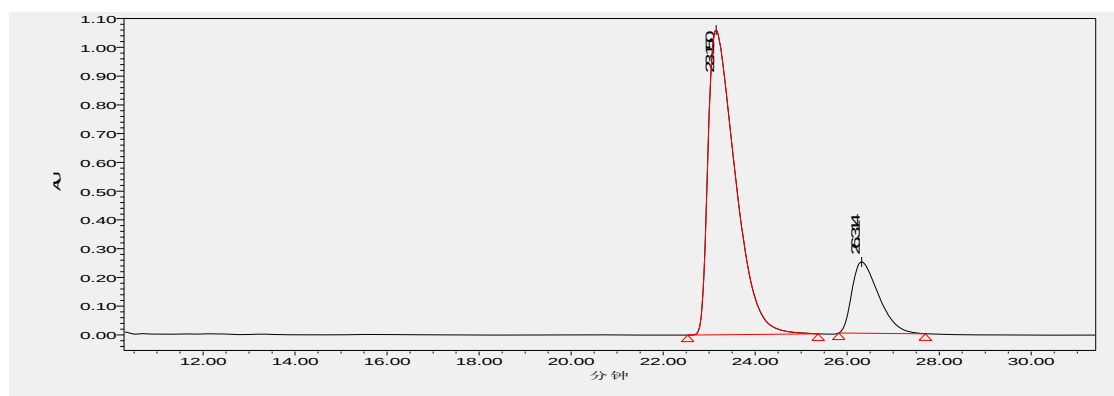
Racemic

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1	24.641	7754181	50.11	199836	bb			Unknown	
2	27.805	7720631	49.89	172494	bb			Unknown	



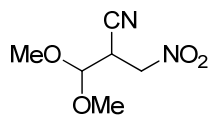
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1	23.840	24164632	90.55	555016	bb			Unknown	
2	27.265	2522937	9.45	60694	bb			Unknown	

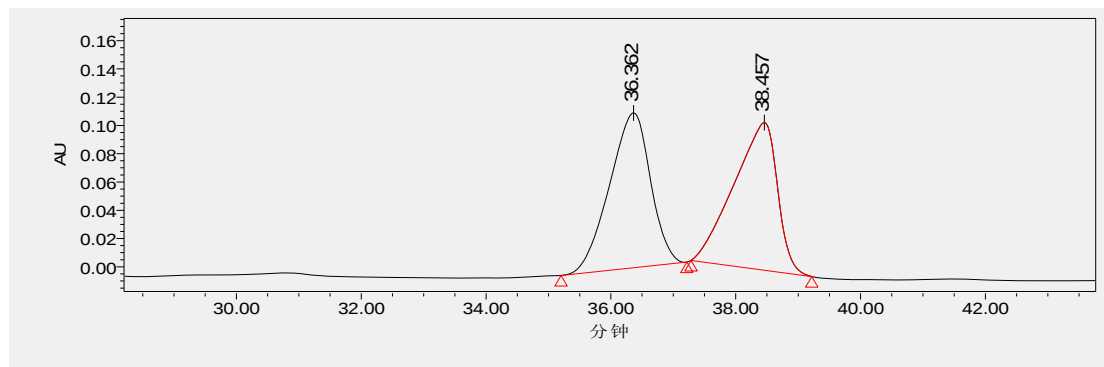


Room temperature

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2	26.314	9988235	18.65	247955	bb			Unknown	

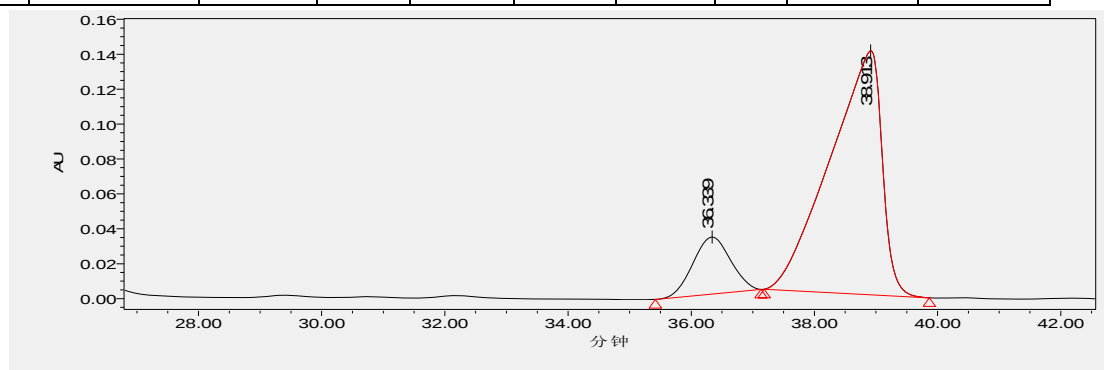


3d: AD-H column, Hexane/iPrOH = 97/3



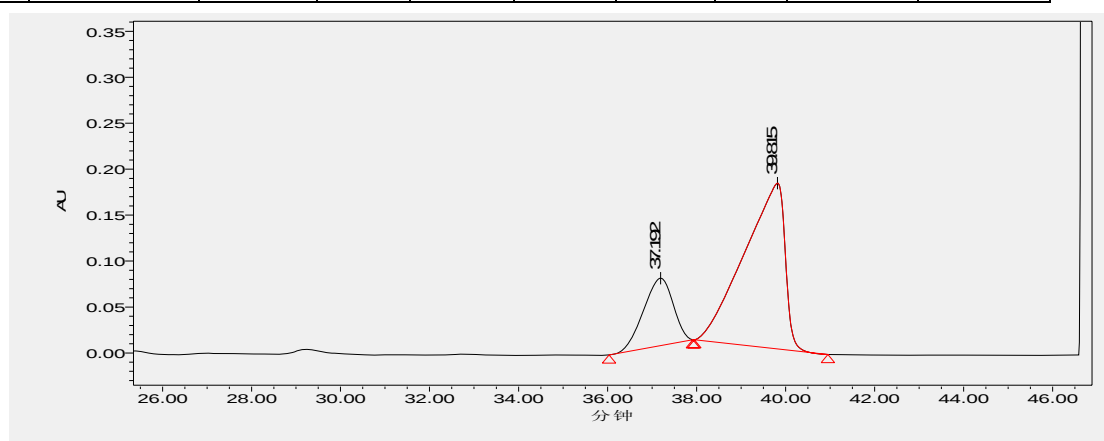
Racemic

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1	36.362	5001160	49.70	109575	bb			Unknown	
2	38.457	5060614	50.30	104427	bb			Unknown	



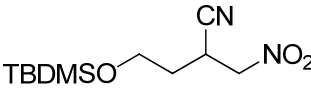
-40°C to -15°C

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1	36.339	1388251	14.50	32696	bb			Unknown	
2	38.913	8186778	85.50	139790	bb			Unknown	

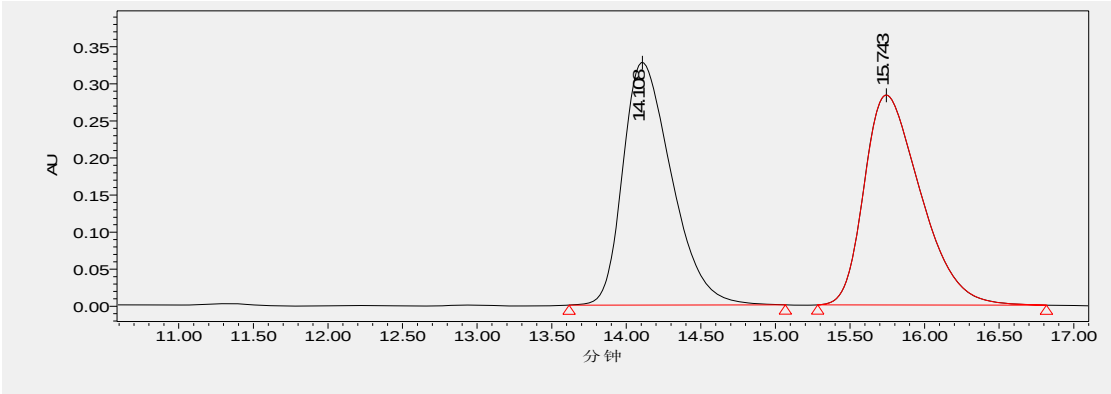


Room temperature

	Retention Time	Area	% Area	Height	Int Type	Amount	Units	Peak Type	Peak Codes
1	37.192	3398078	73298	22.92	bb			Unknown	
2	39.815	11428418	180301	77.08	bb			Unknown	

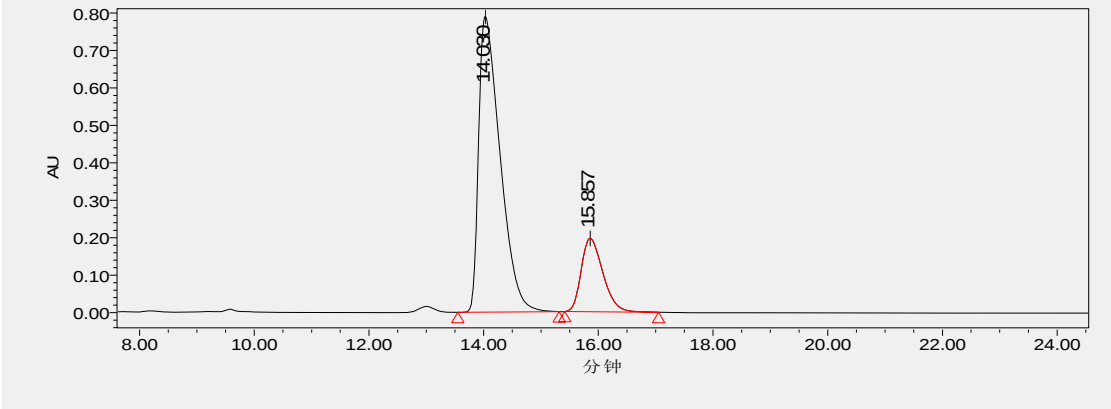


3e: OD-H column, Hexane/iPrOH = 95/5



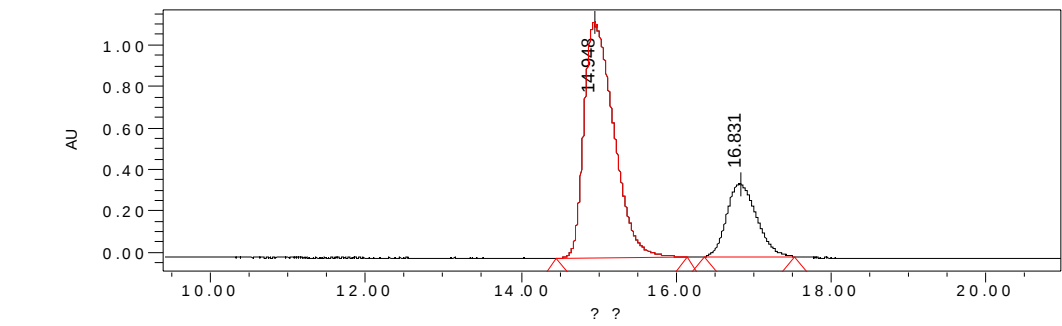
Racemic

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1	14.108	7446553	49.94	327339	bb			Unknown	
2	15.743	7463283	50.06	282904	bb			Unknown	



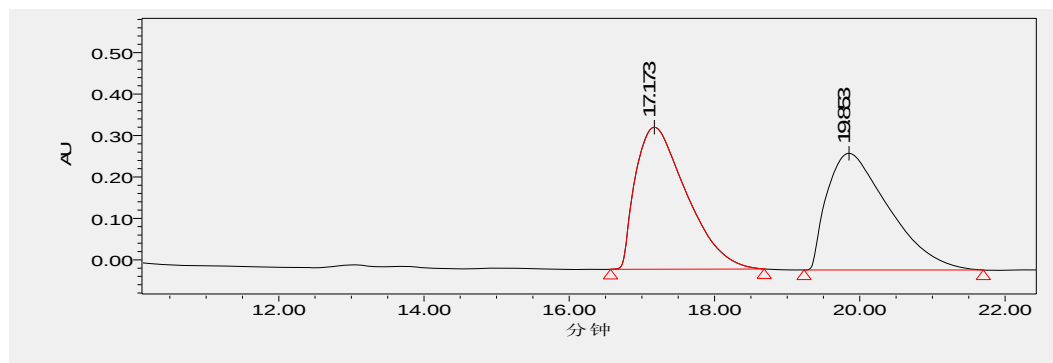
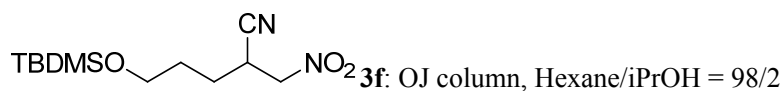
-40°C to -15°C

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1	14.030	20497763	79.96	789889	bb			Unknown	
2	15.857	5136557	20.04	195967	bb			Unknown	



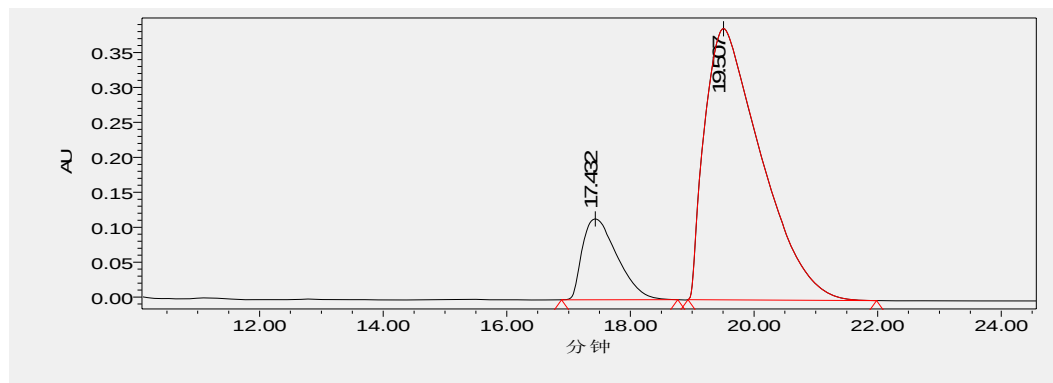
Room temperature

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1	14.948	30393736	76.55	1137246	bb			Unknown	
2	16.831	9311408	23.45	350047	bb			Unknown	



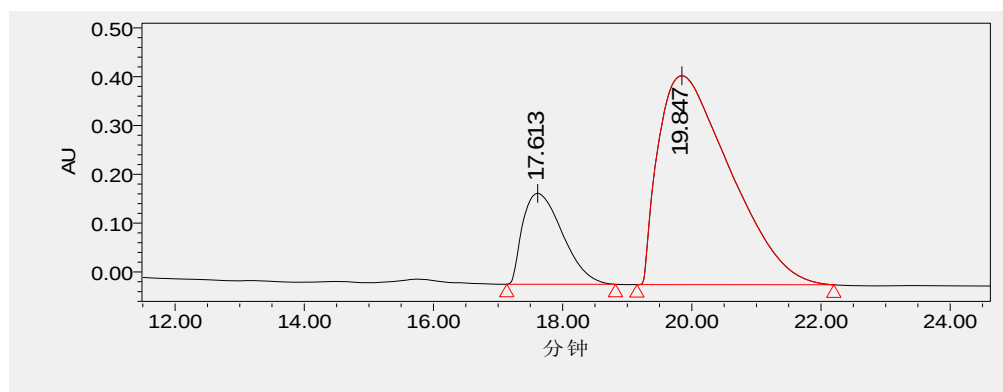
Racemic

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1	17.173	16718402	50.11	342710	bb			Unknown	
2	19.853	16648326	49.89	281685	bb			Unknown	



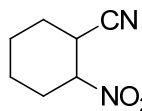
-40°C to -15°C

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1	17.432	4505437	15.49	115361	bb			Unknown	
2	19.507	24580487	84.51	387953	bb			Unknown	

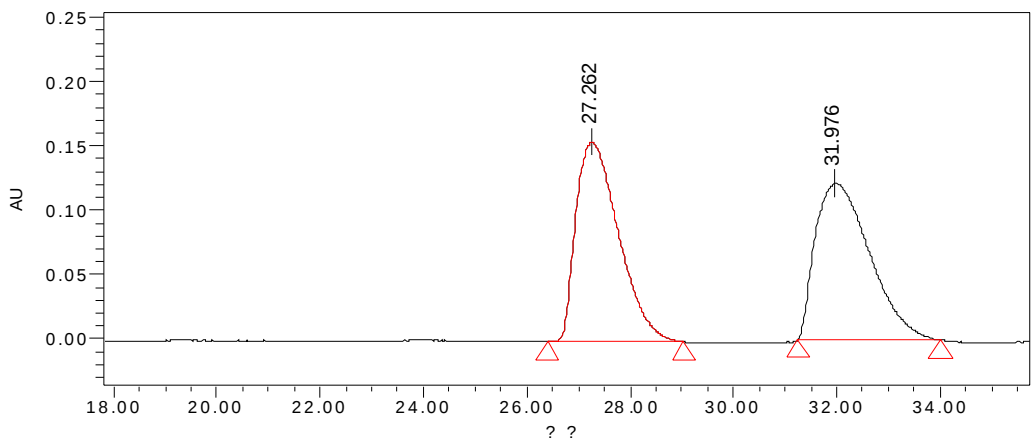


Room temperature

	Retention Time	Area	% Area	Height	Int Type	Amount	Units	Peak Type	Peak Codes
1	17.613	7988462	19.46	186148	bb			Unknown	
2	19.847	33060237	80.54	427969	bb			Unknown	

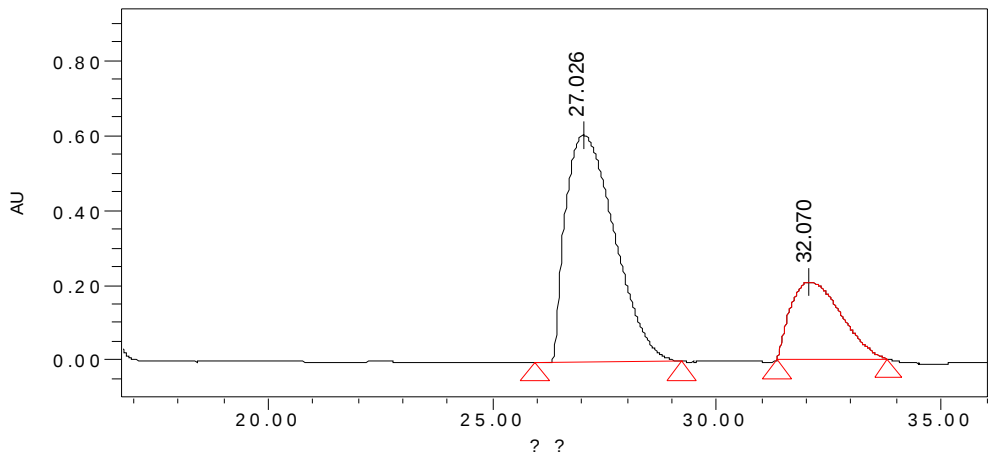


anti-3g: OJ column, Hexane/ iPrOH = 85/15



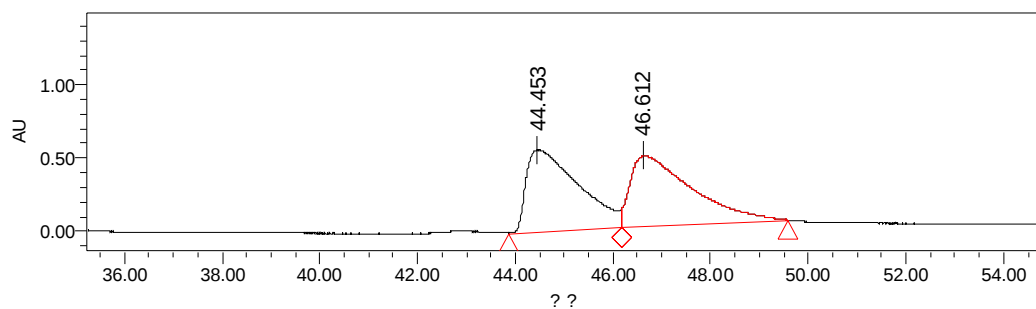
Racemic

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1	27.262	8917022	50.11	155405	bb			Unknown	
2	31.976	8876286	49.89	121600	bb			Unknown	



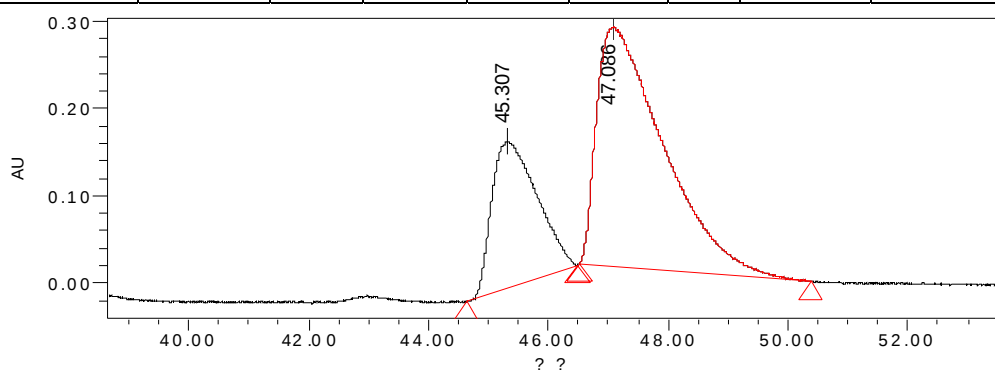
-40°C to -15°C

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1	27.026	46119465	73.91	606924	bb			Unknown	
2	32.070	16283083	26.09	207155	bb			Unknown	



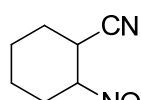
Racemic (OD-H column, Hexane/ iPrOH = 98/2, 0.8ml/min)

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1	44.453	41608703	49.52	560479	bb			Unknown	
2	46.612	42419198	50.48	484915	bb			Unknown	

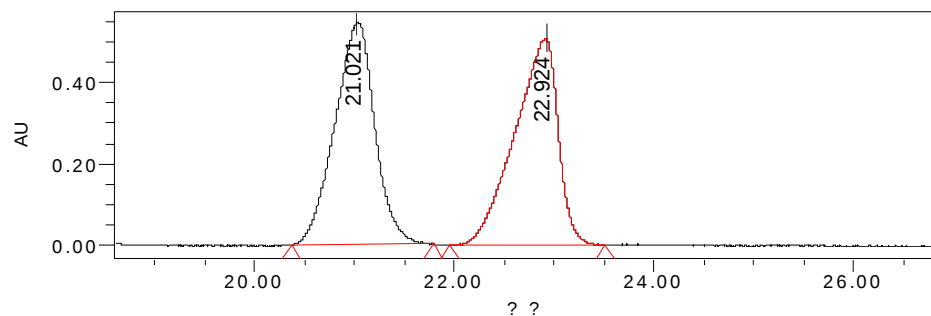


Room temperature (OD-H column, Hexane/ iPrOH = 98/2, 0.8ml/min)

	Retention Time	Area	% Area	Height	Int Type	Amount	Units	Peak Type	Peak Codes
1	45.307	8745591	29.08	168188	bb			Unknown	
2	47.086	21330141	70.92	275186	bb			Unknown	

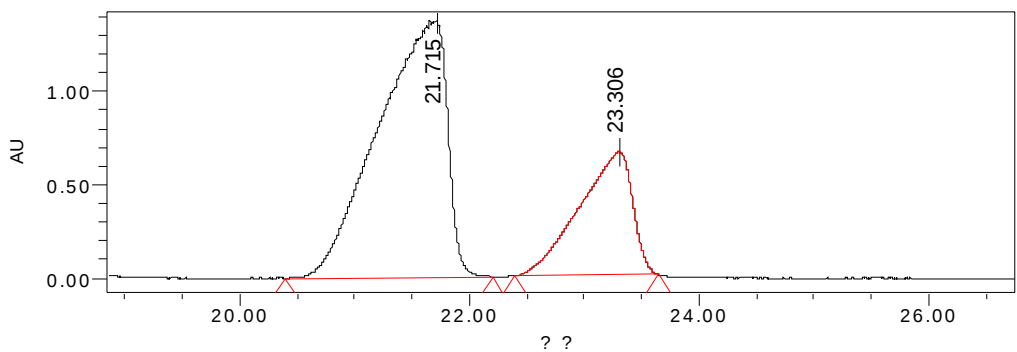


syn-3g: AD-H column, Hexane/ iPrOH = 95/5



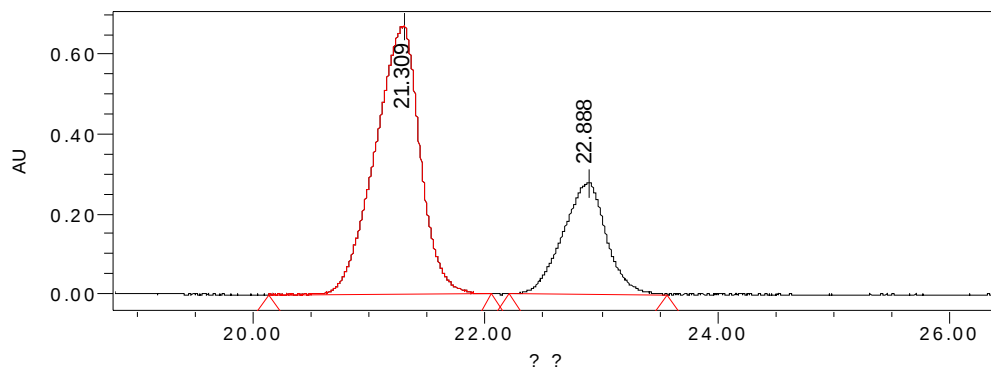
Racemic

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1	21.021	15305401	49.96	550046	bb			Unknown	
2	22.924	15327086	50.04	510486	bb			Unknown	



-40°C to -15°C

	Retention Time	Area	% Area	Height	Int Type	Amount	Units	Peak Type	Peak Codes
1	21.715	57378444	72.89	1375870	bb			Unknown	
2	23.306	21335588	27.11	661097	bb			Unknown	

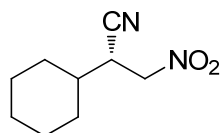


Room temperature

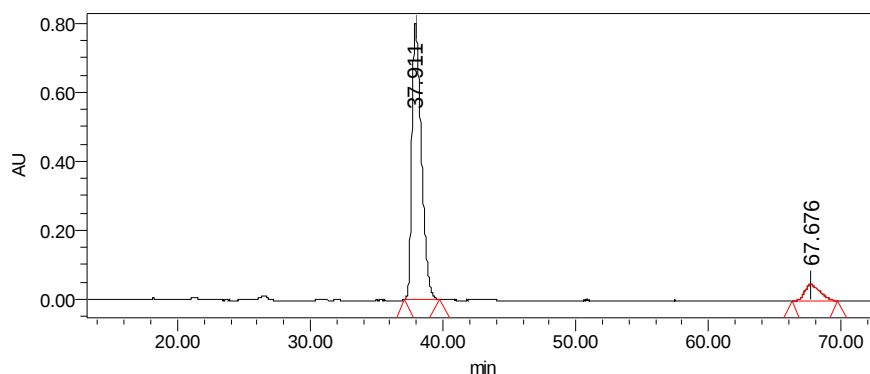
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1	21.309	18265500	71.58	674877	bb			Unknown	
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Additional HPLC Spectras for the Products **3b** and **3c**:

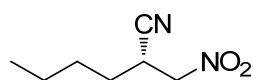
In order to confirm the absolute configuration of **3b** and **3c**, re-determining the e.r. value of **3b** and **3c** was carried out under the following conditions which were used in ref. 8c: Daicel Chiracel AD-H column, on Waters® with a 996 UV-detector, flow rate = 1.0 mL/min, Hexane/iPrOH = 98/2.



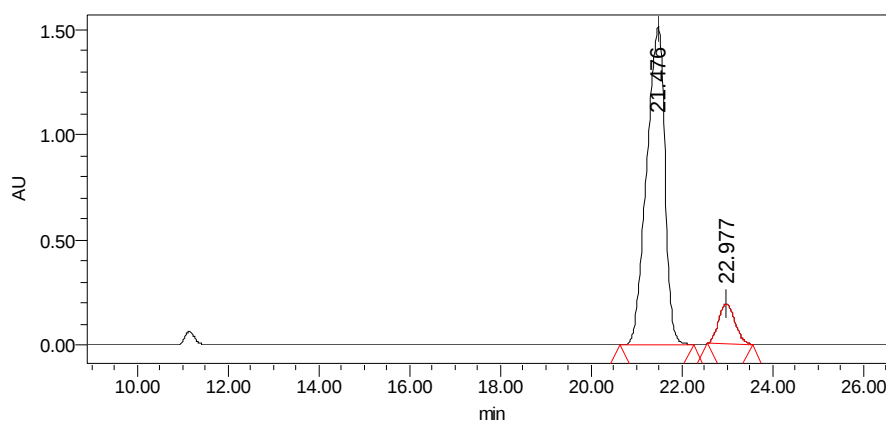
3b: AD-H column, Hexane/ iPrOH = 98/2,



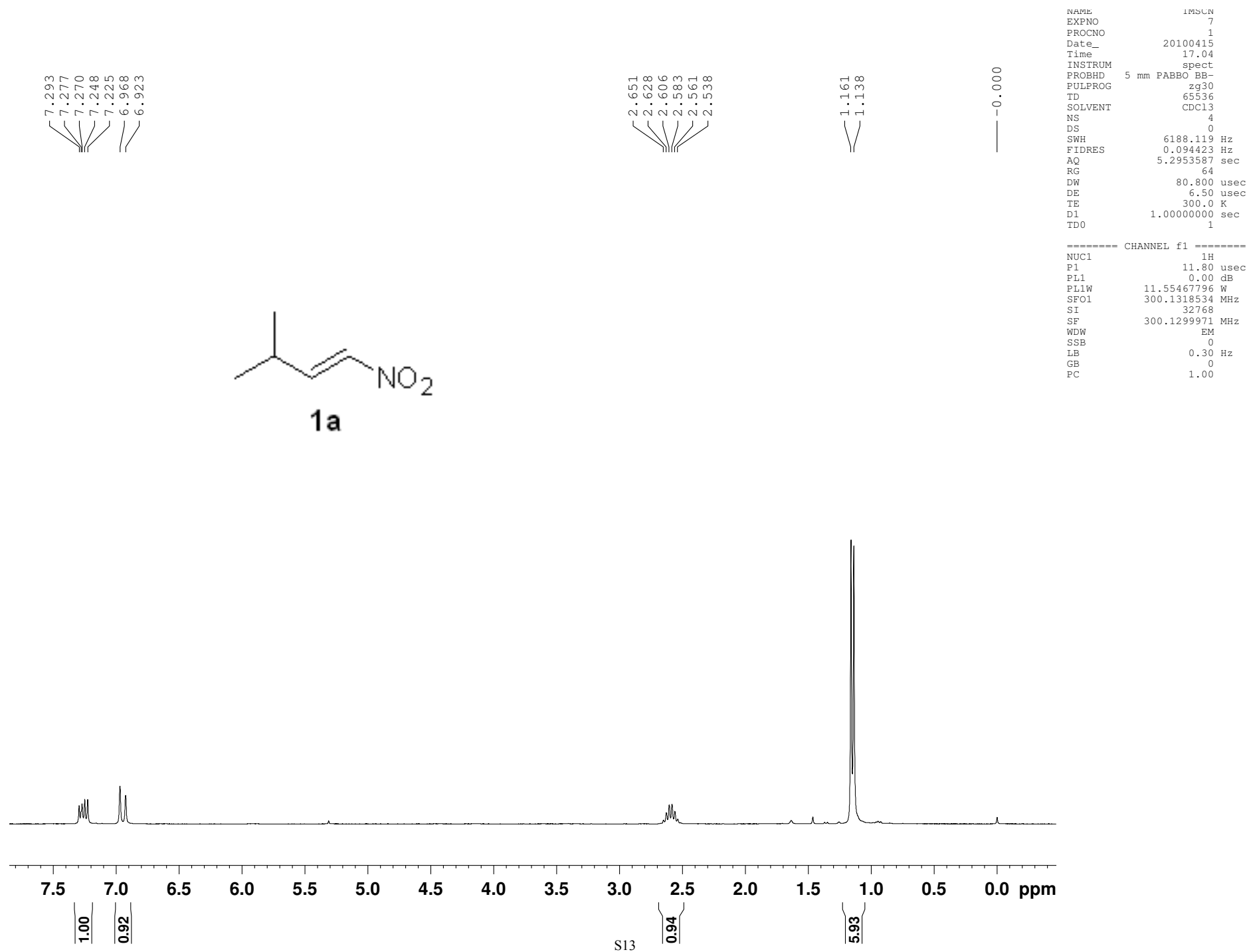
	Retention Time	Area	% Area	Height	Int Type	Amount	Units	Peak Type	Peak Codes
1	37.911	39499752	91.12	797325	bb			Unknown	
2	67.676	3851186	8.88	46937	bb			Unknown	

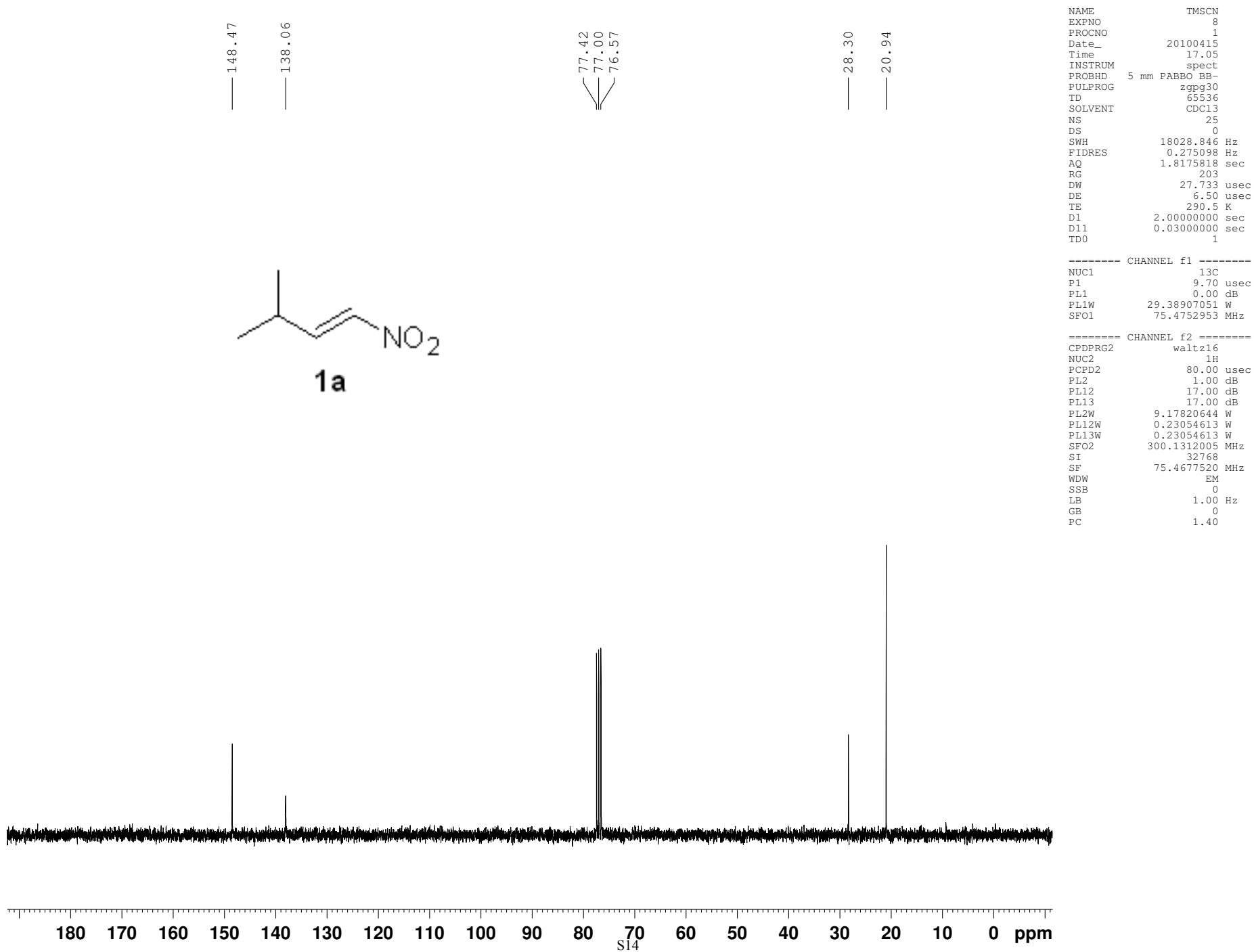


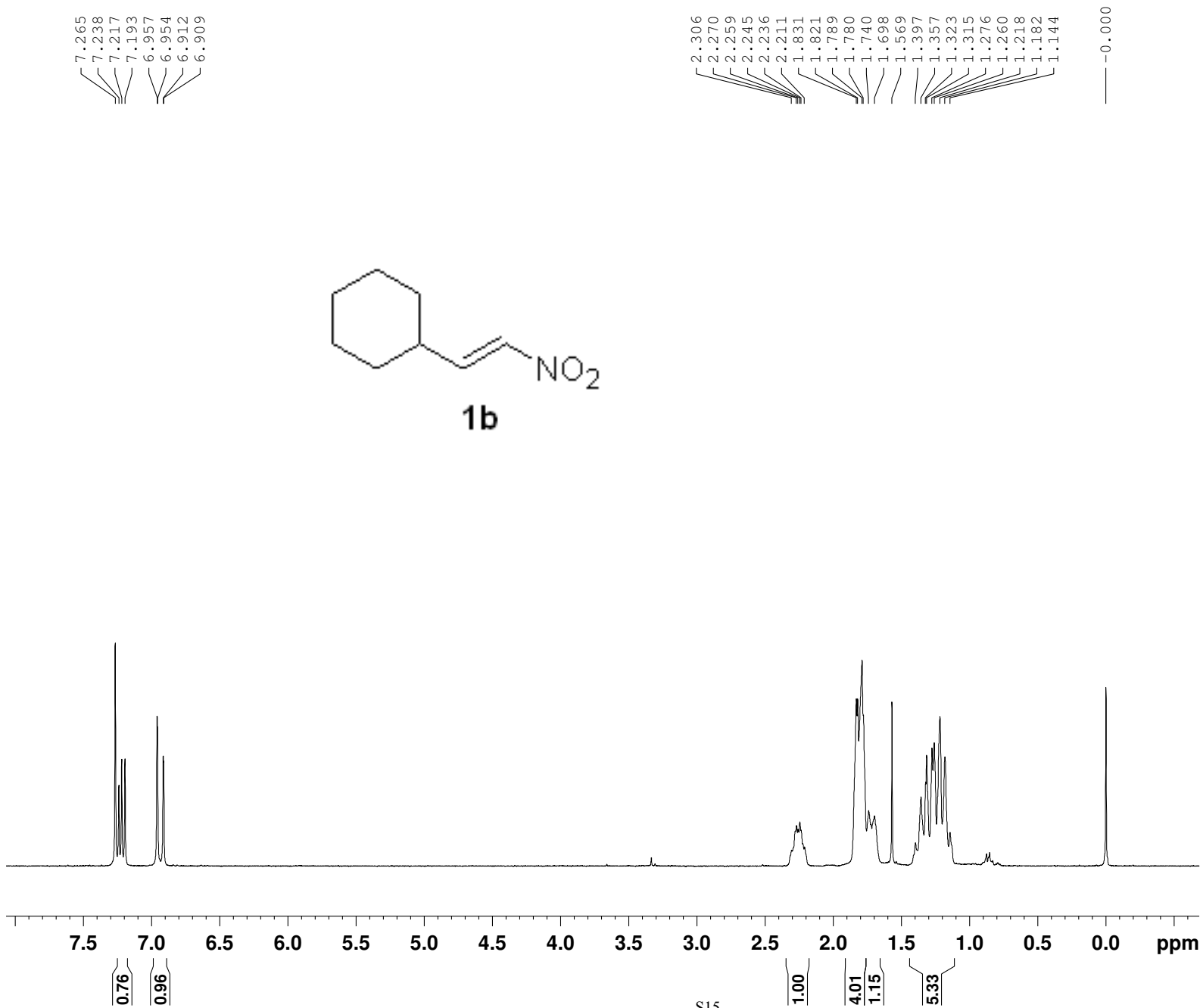
3c: AD-H column, Hexane/iPrOH = 98/2



	Retention Time	Area	% Area	Height	Int Type	Amount	Units	Peak Type	Peak Codes
1	21.476	42162766	89.93	1506730	bb			Unknown	
2	22.977	4718649	10.07	188938	bb			Unknown	

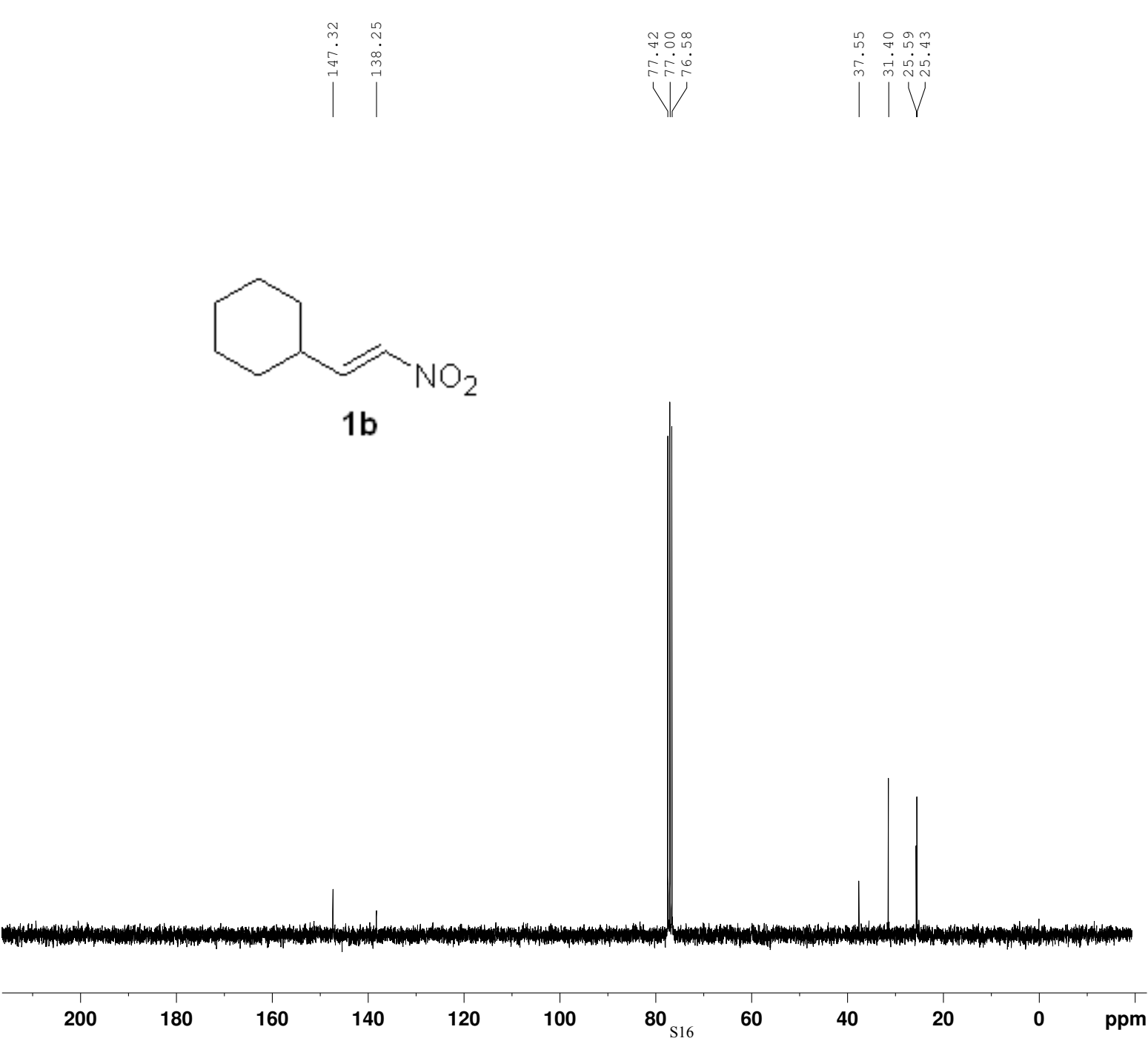






NAME 1MSUN
EXPNO 16
PROCNO 1
Date_ 20100415
Time 17.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 203
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

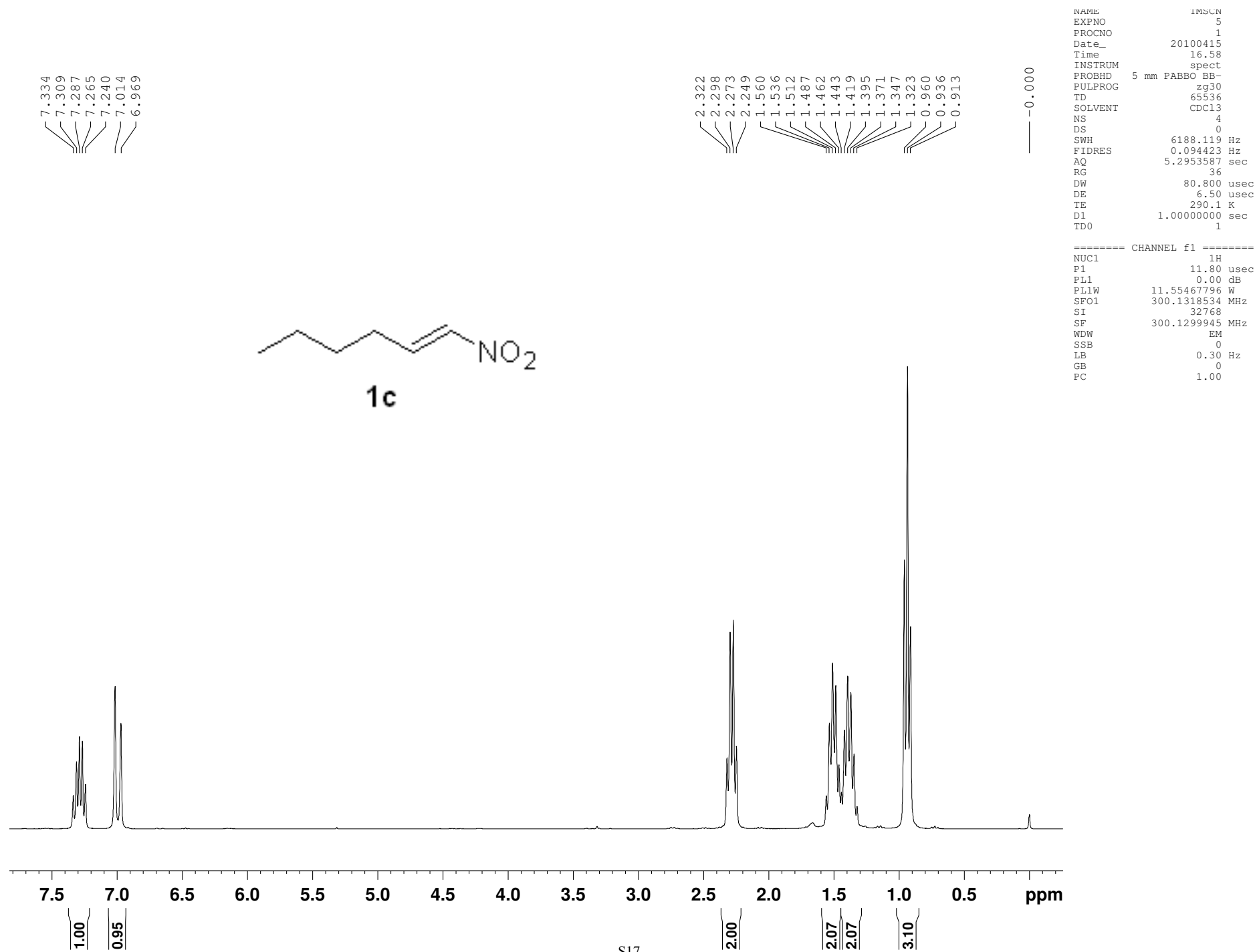
===== CHANNEL f1 =====
NUC1 1H
P1 11.80 usec
PL1 0.00 dB
PL1W 11.55467796 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300009 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

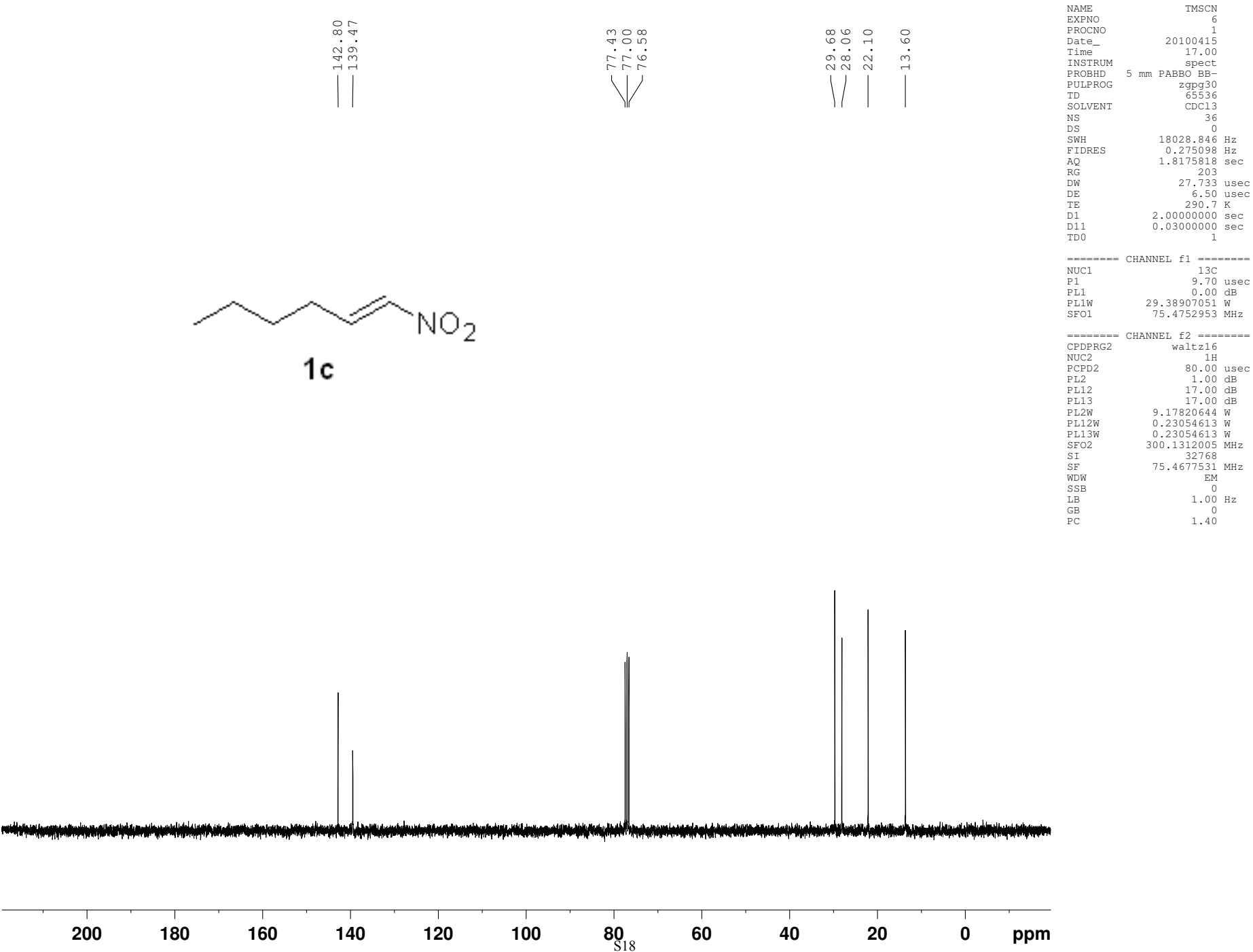


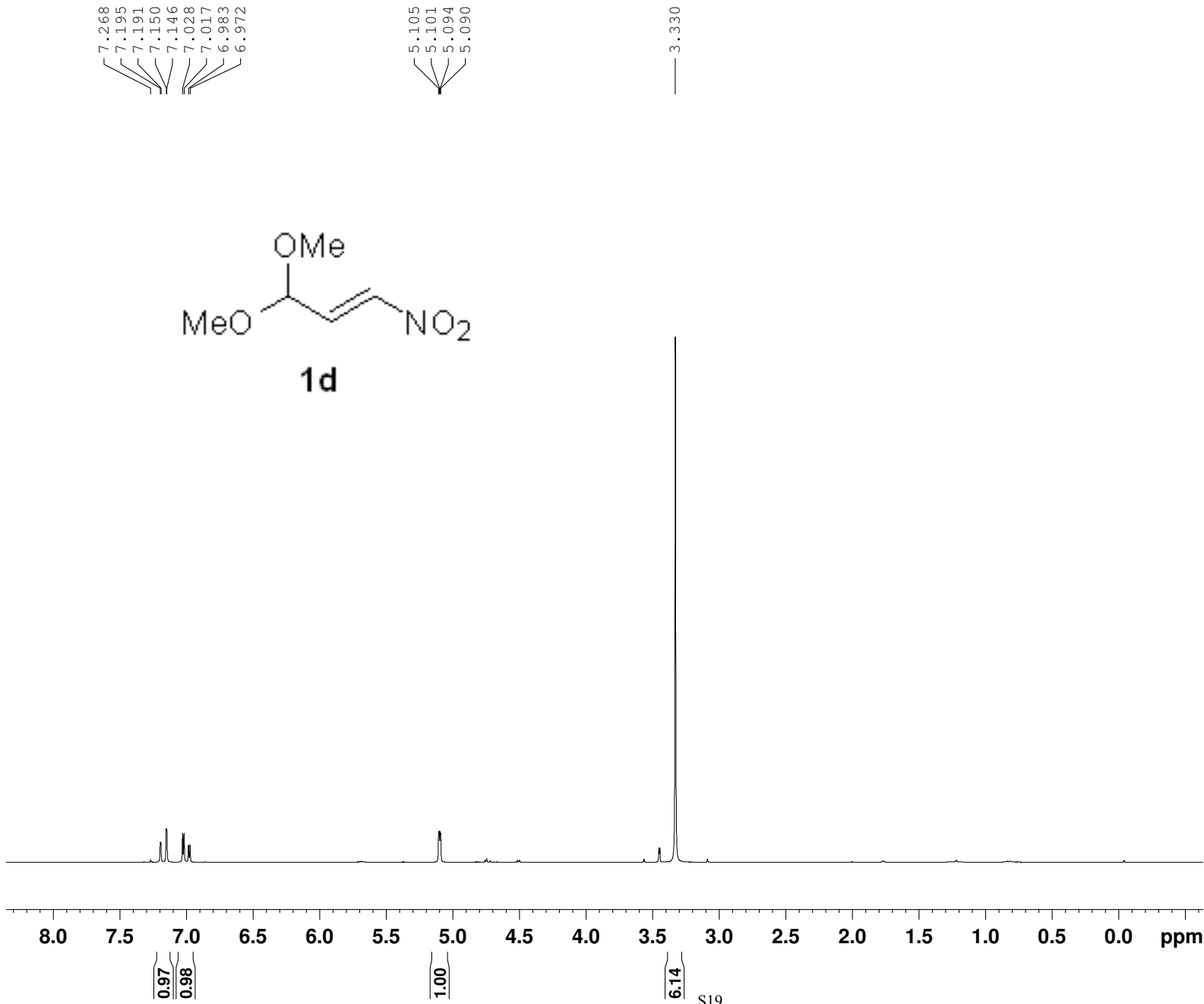
NAME TMS
EXPNO 17
PROCNO 1
Date_ 20100415
Time 17.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 86
DS 0
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 291.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.70 usec
PL1 0.00 dB
PL1W 29.38907051 W
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 9.17820644 W
PL12W 0.23054613 W
PL13W 0.23054613 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677498 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

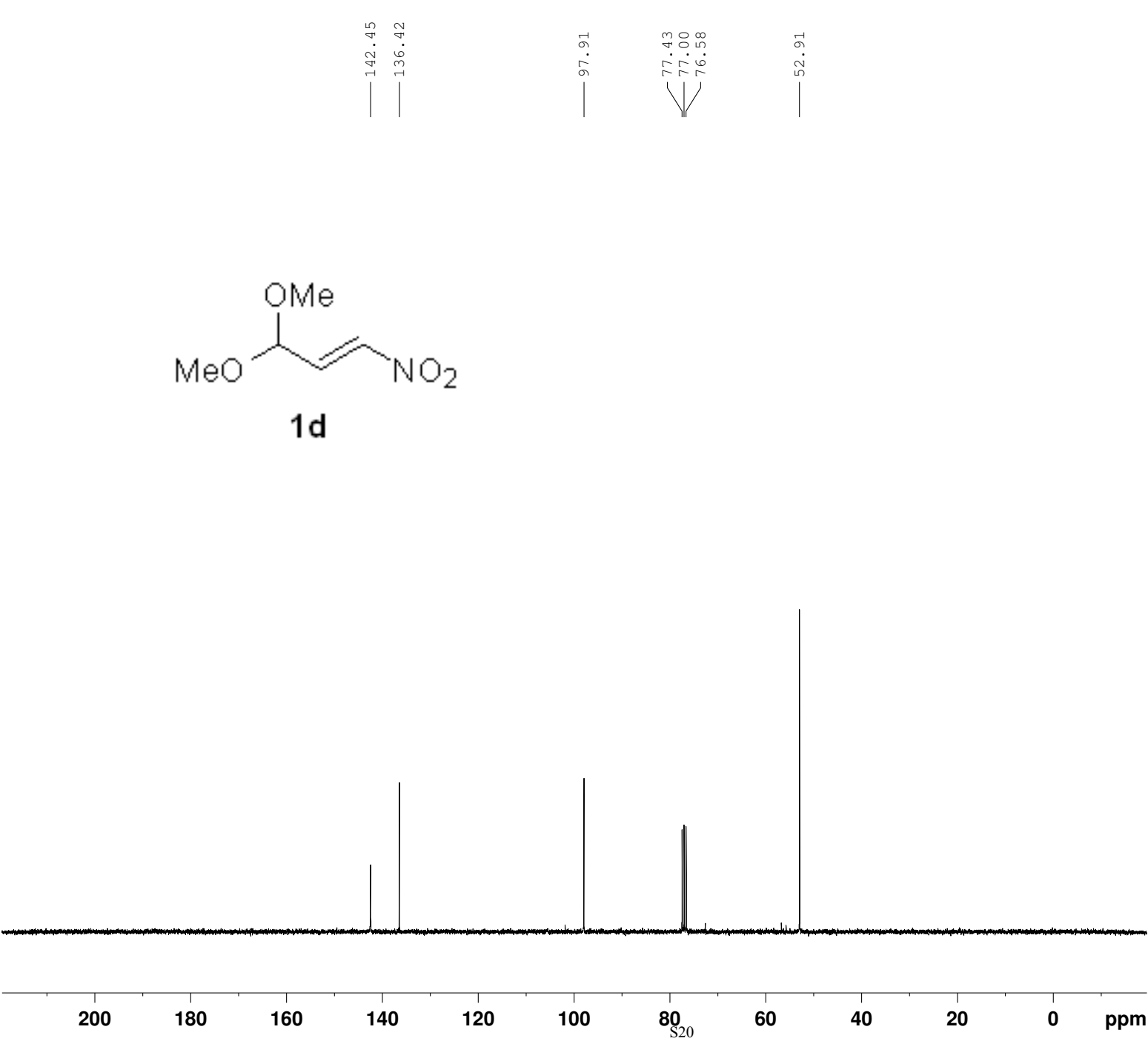
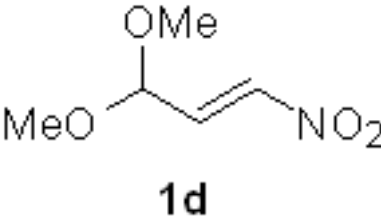






NAME 11nwl00428
EXPNO 3
PROCNO 1
Date_ 20100429
Time 9.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 25.4
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

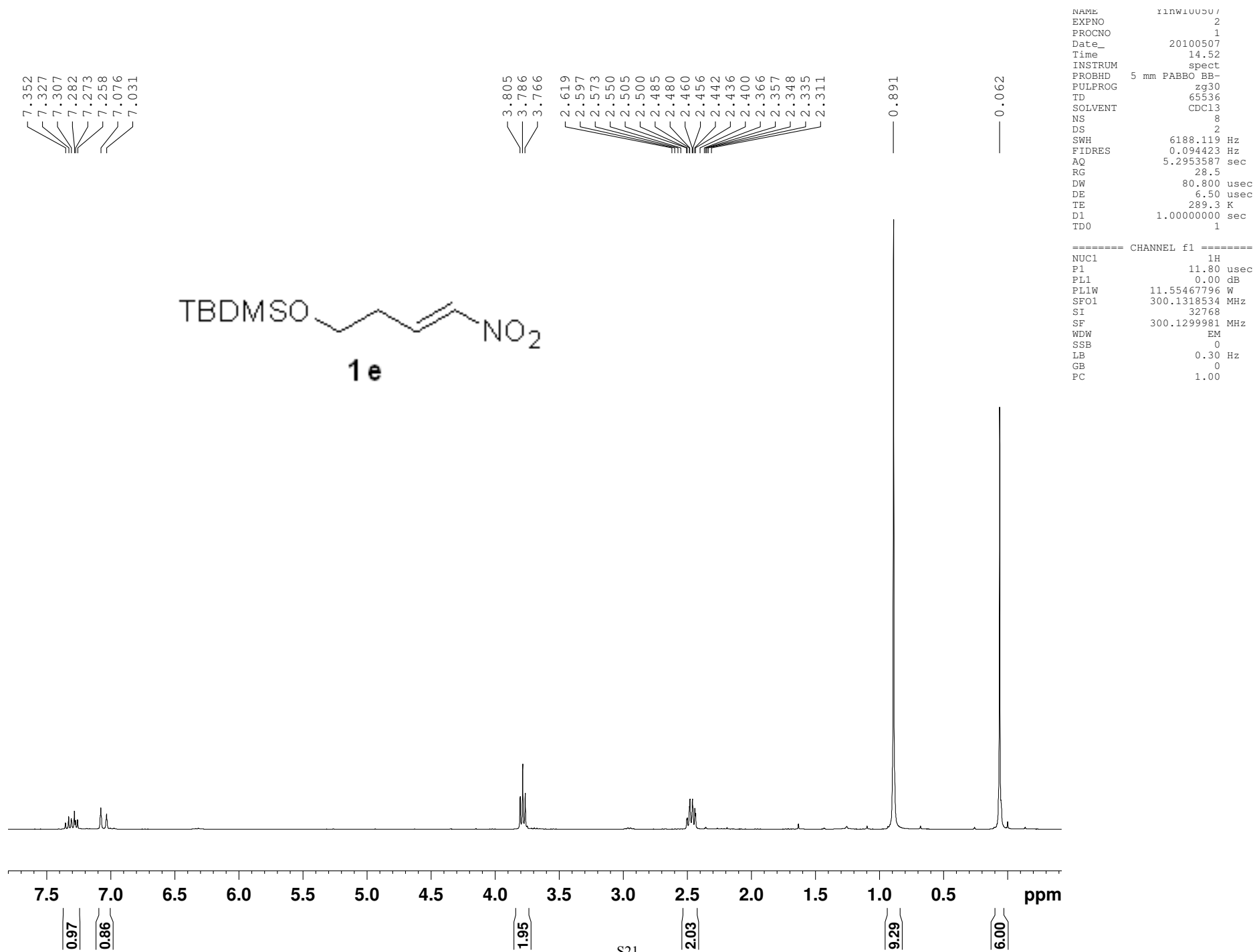
===== CHANNEL f1 =====
NUC1 1H
P1 11.80 usec
PL1 0.00 dB
PL1W 11.55467796 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

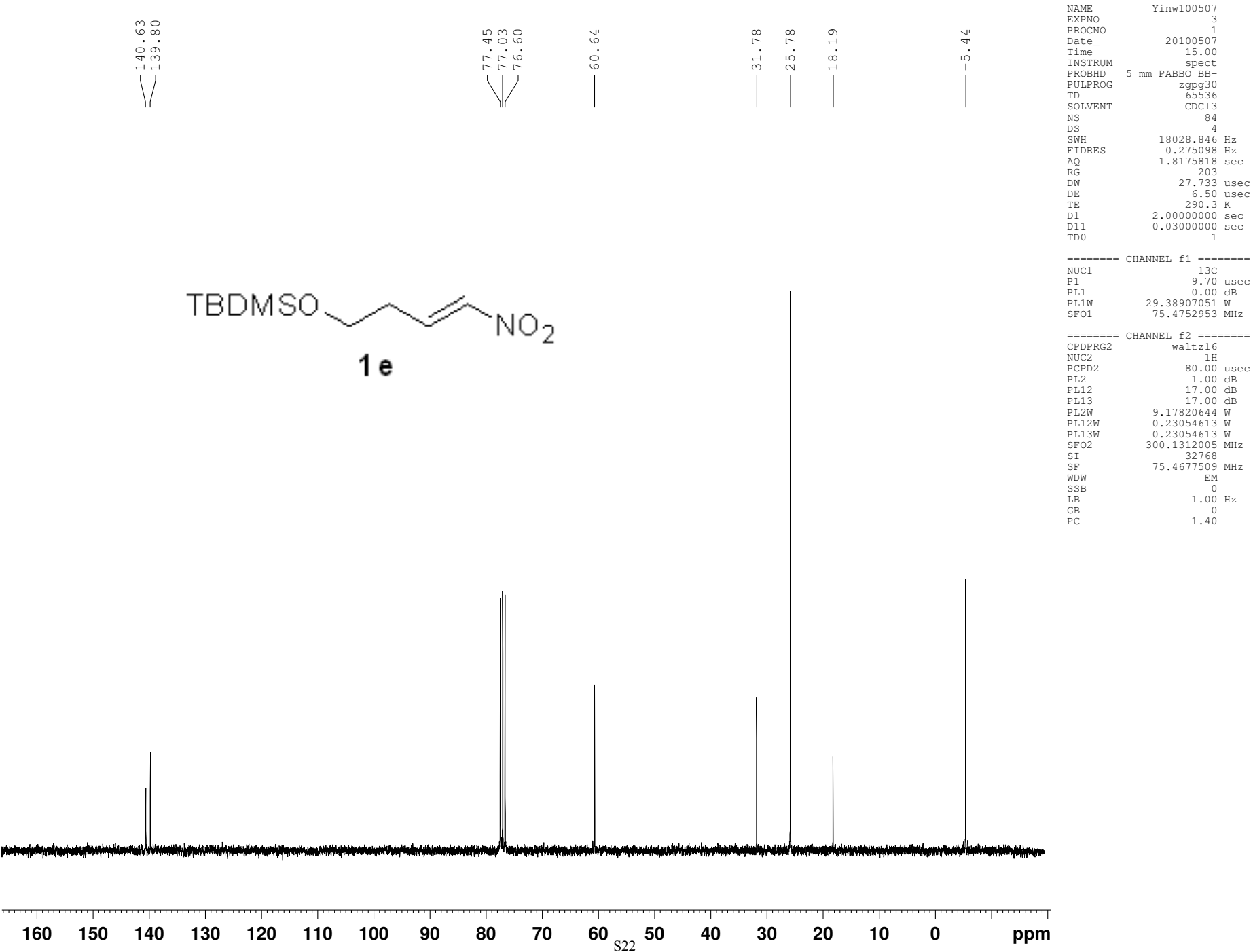


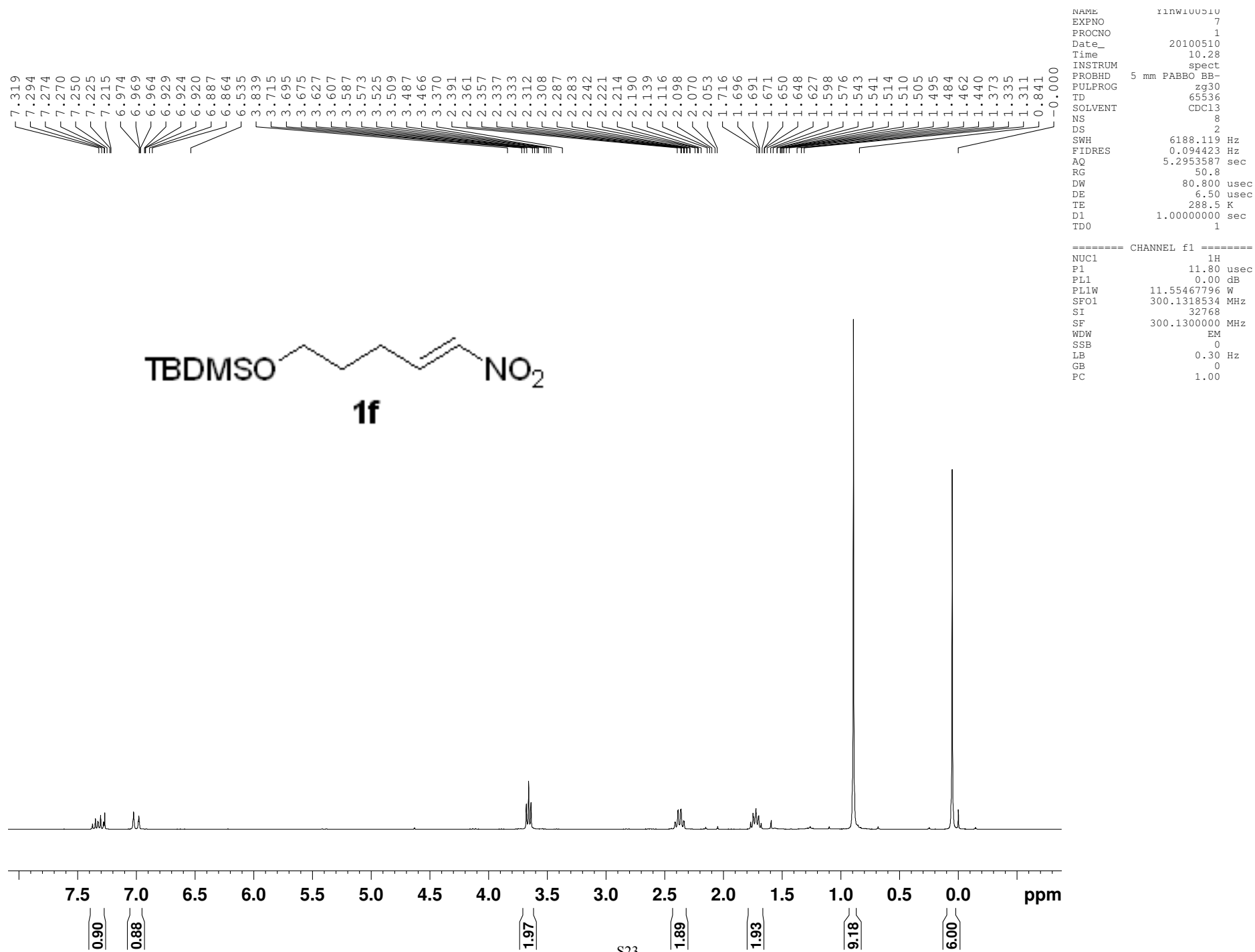
NAME Yinwl00428
EXPNO 4
PROCNO 1
Date_ 20100429
Time_ 9.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 38
DS 0
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 291.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

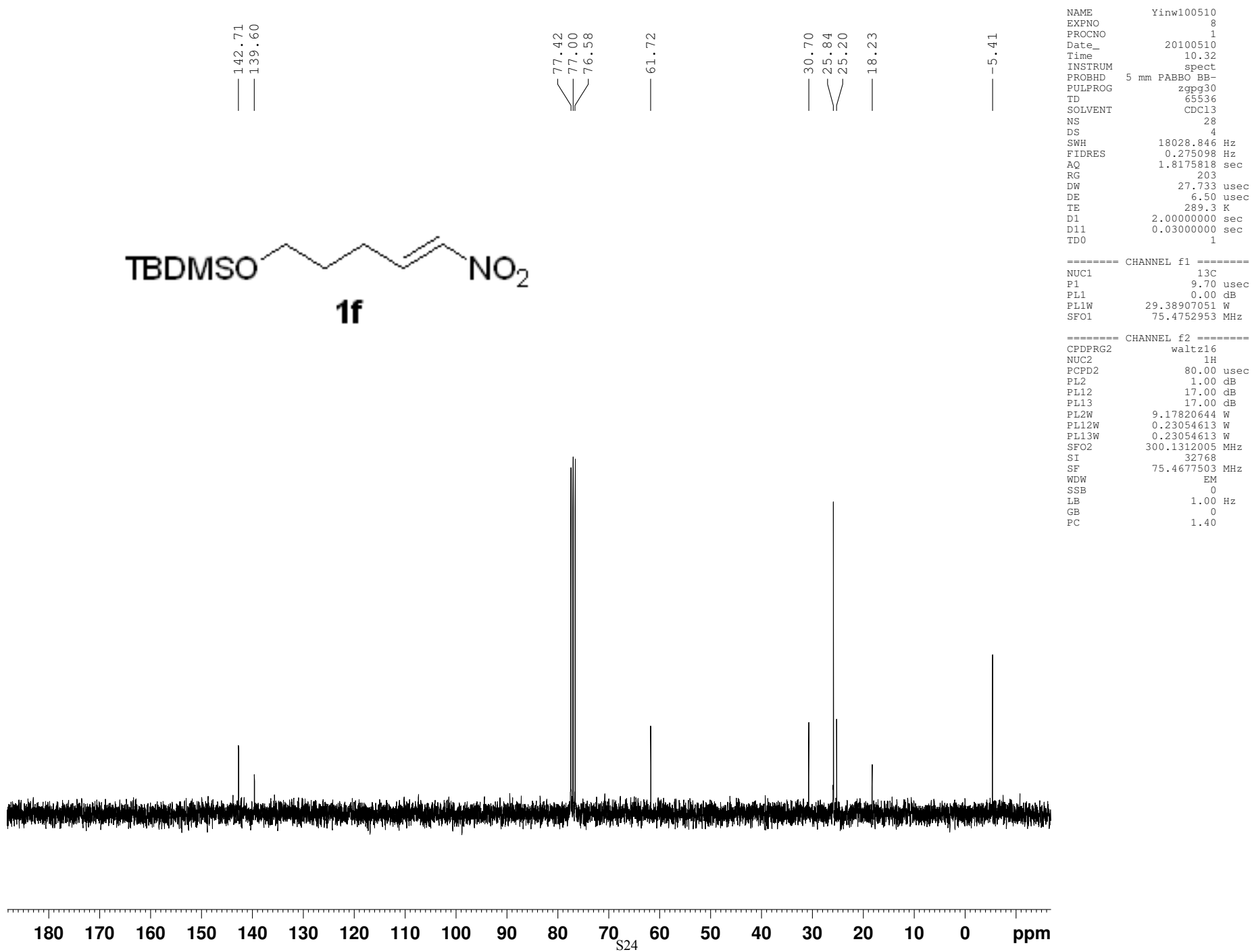
===== CHANNEL f1 =====
NUC1 13C
P1 9.70 usec
PL1 0.00 dB
PL1W 29.38907051 W
SFO1 75.4752953 MHz

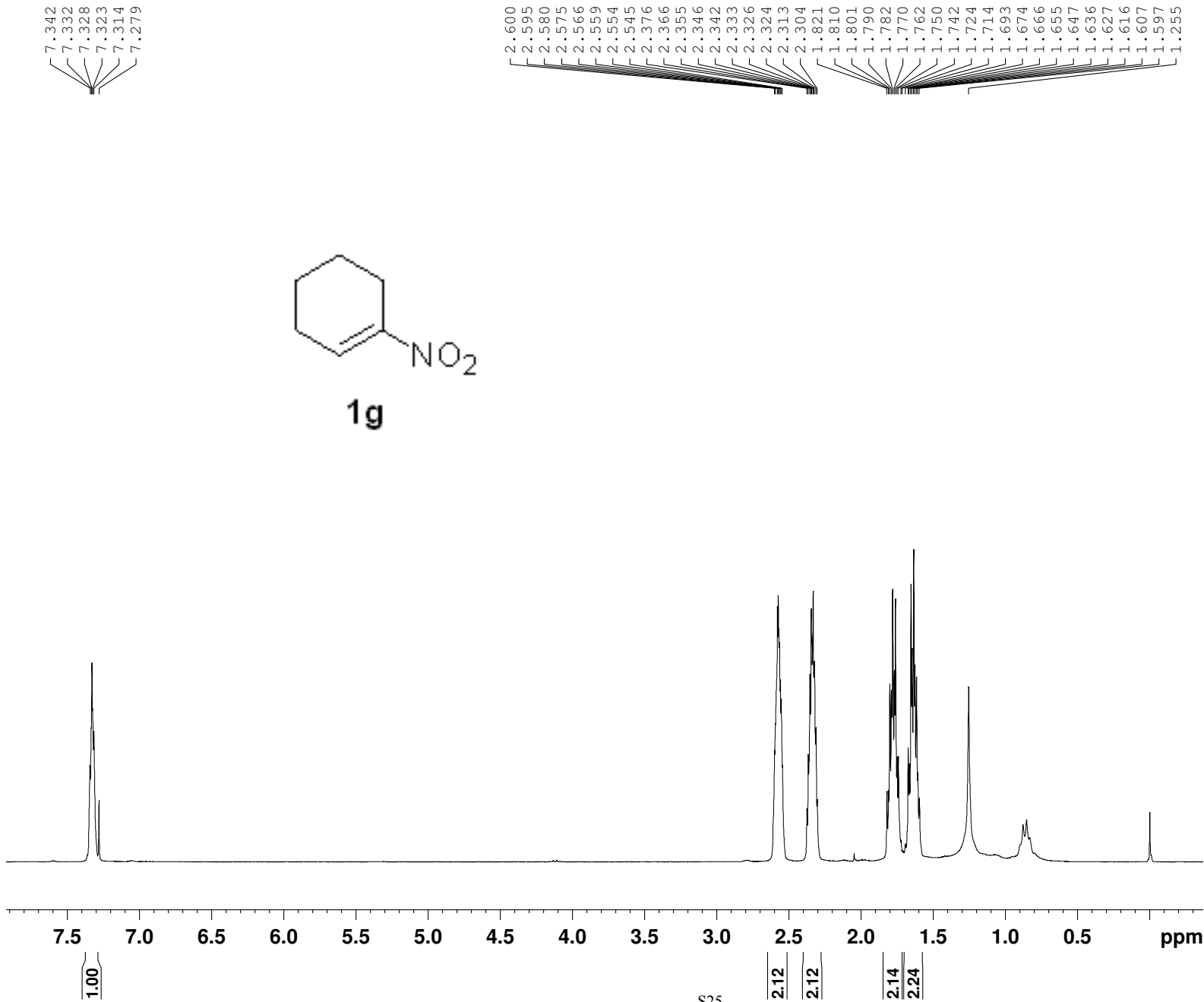
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 9.17820644 W
PL12W 0.23054613 W
PL13W 0.23054613 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677548 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





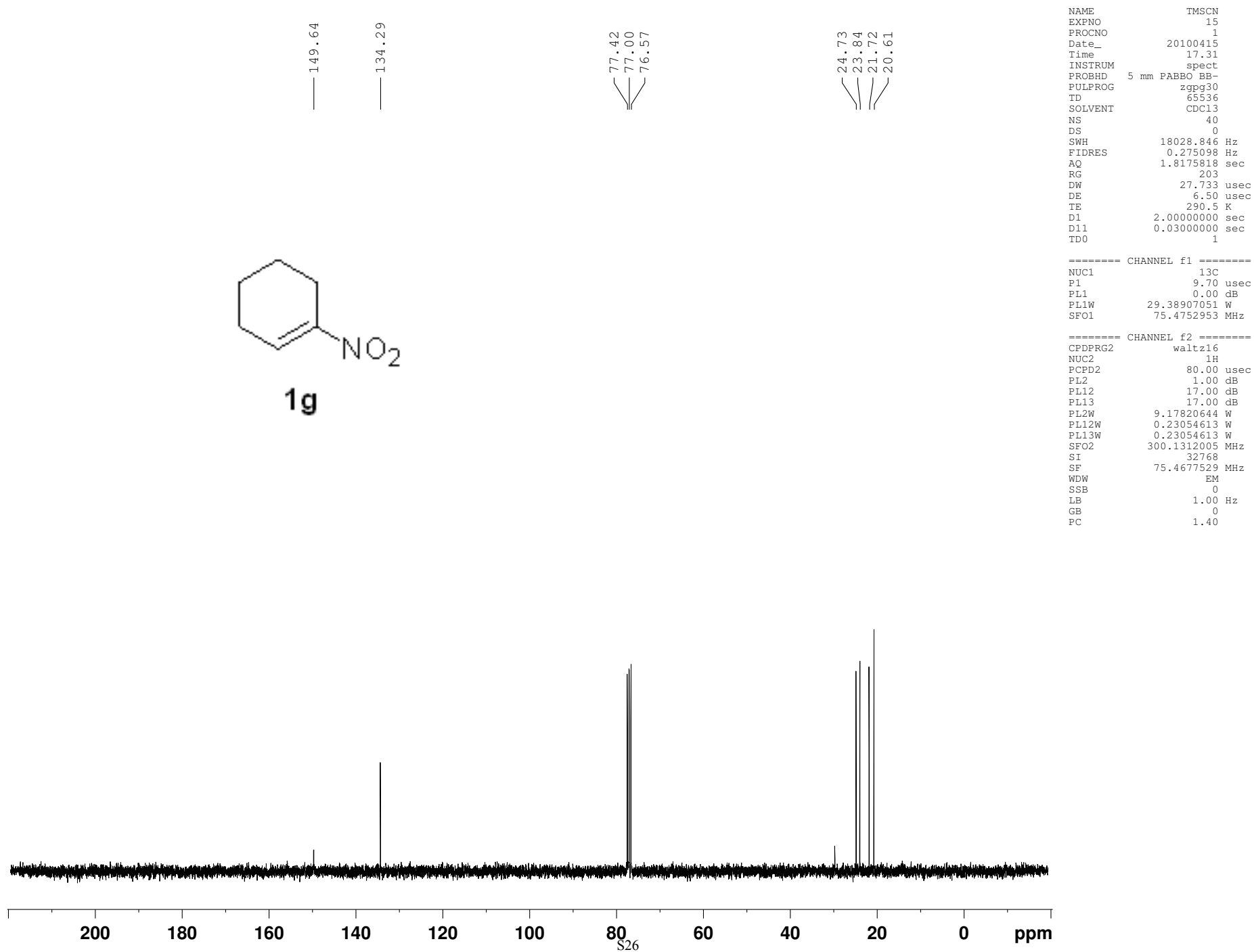


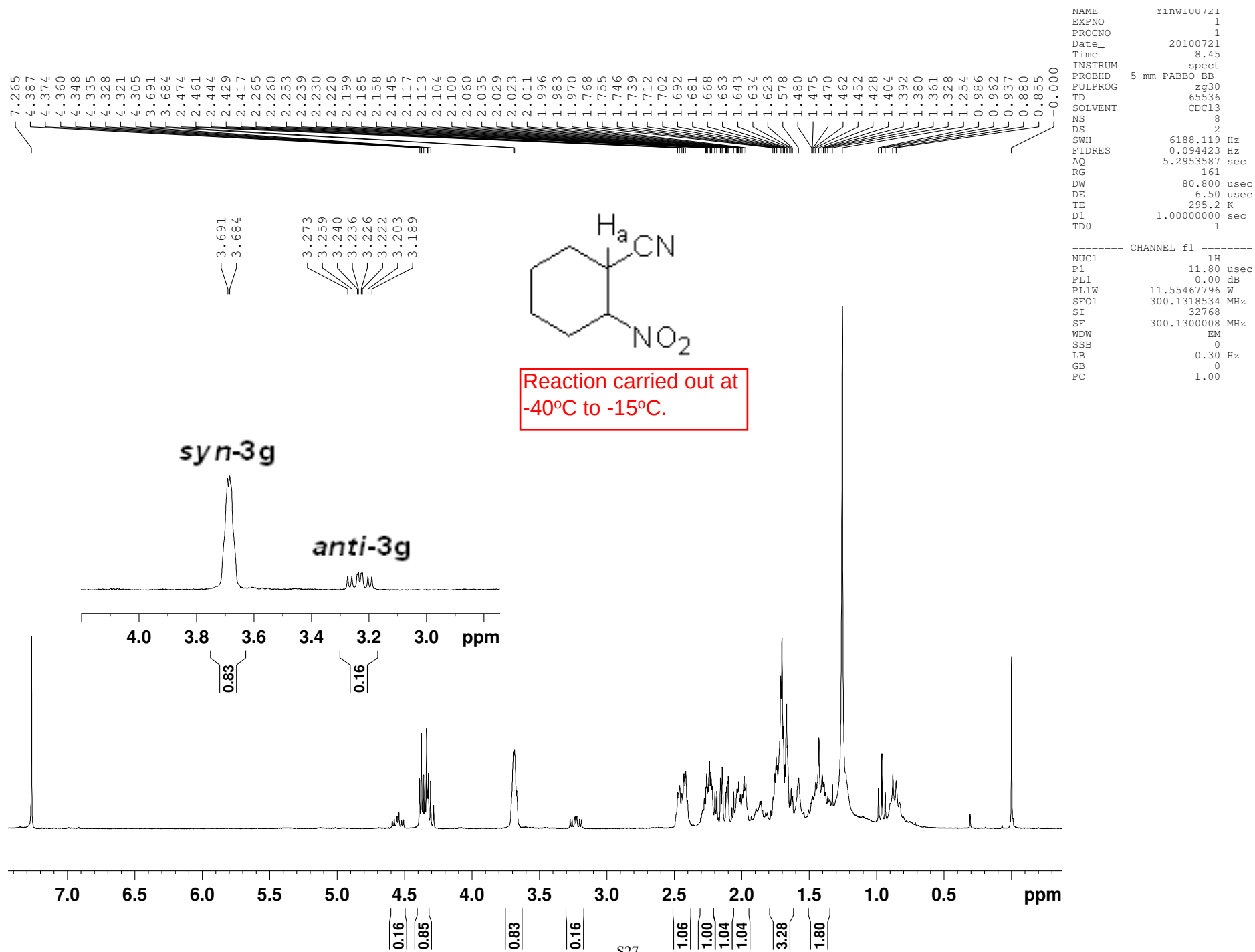


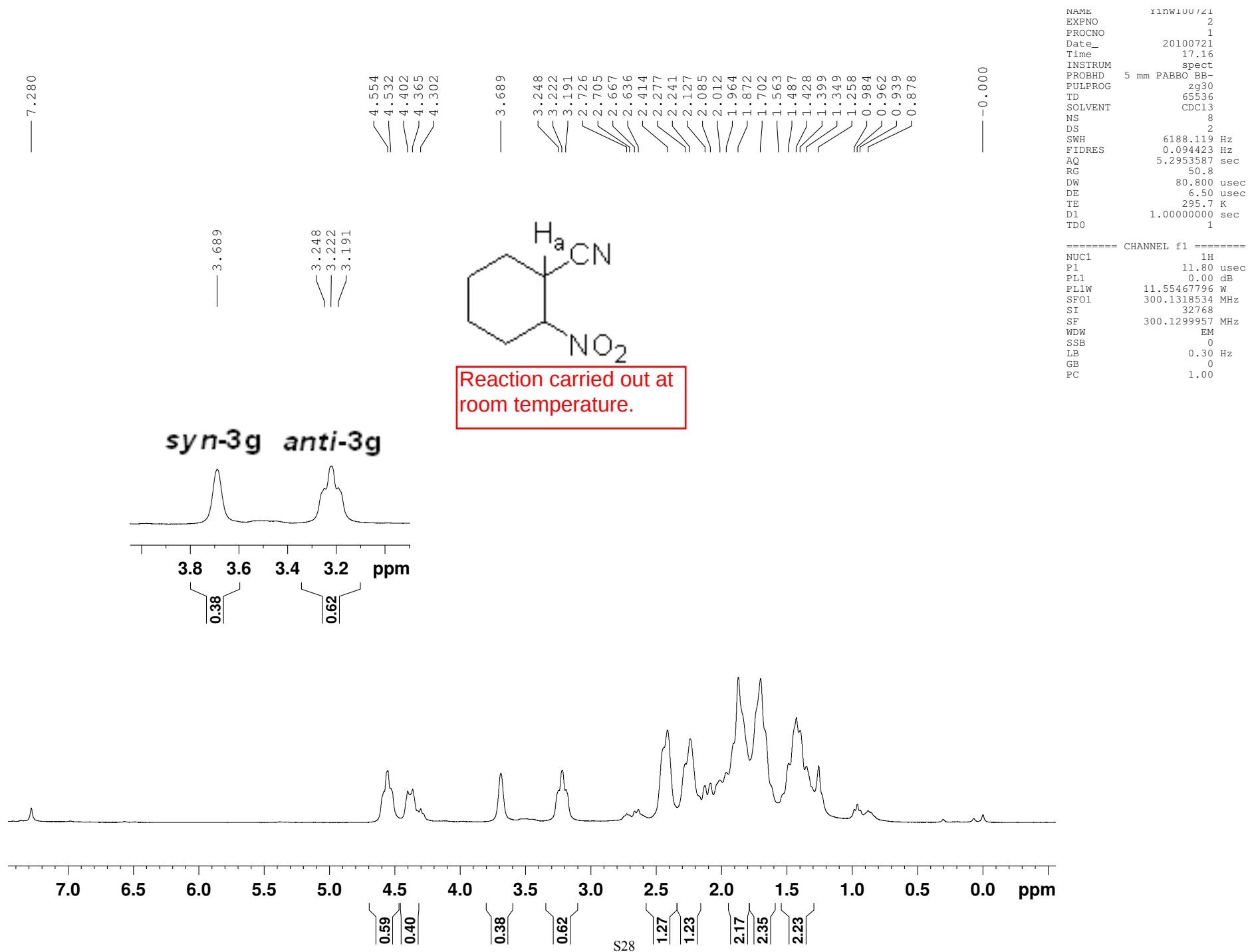


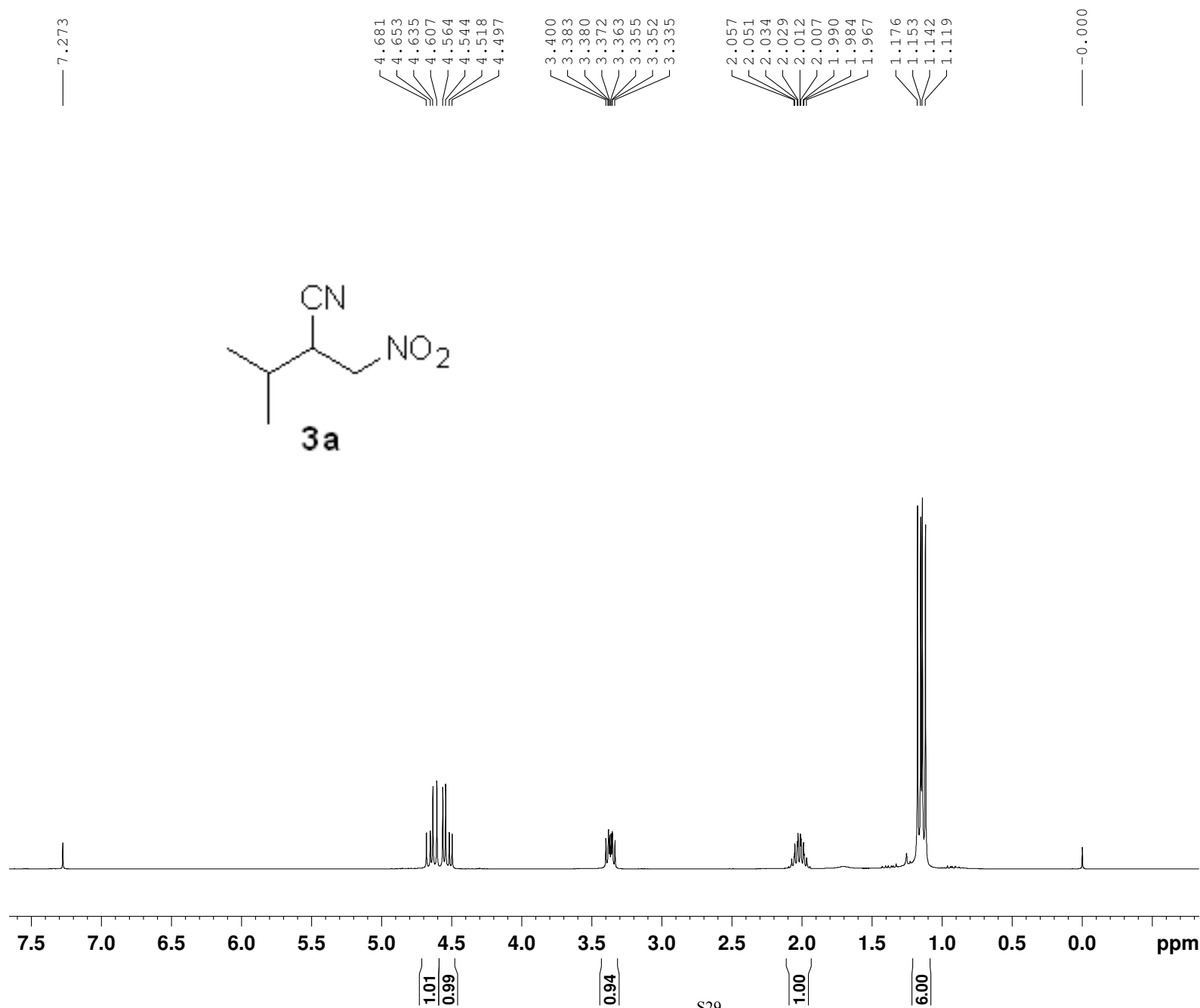
NAME 1P50N
EXPNO 14
PROCNO 1
Date_ 20100415
Time 17.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 45.2
DW 80.800 usec
DE 6.50 usec
TE 290.3 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.80 usec
PL1 0.00 dB
PL1W 11.55467796 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1299968 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



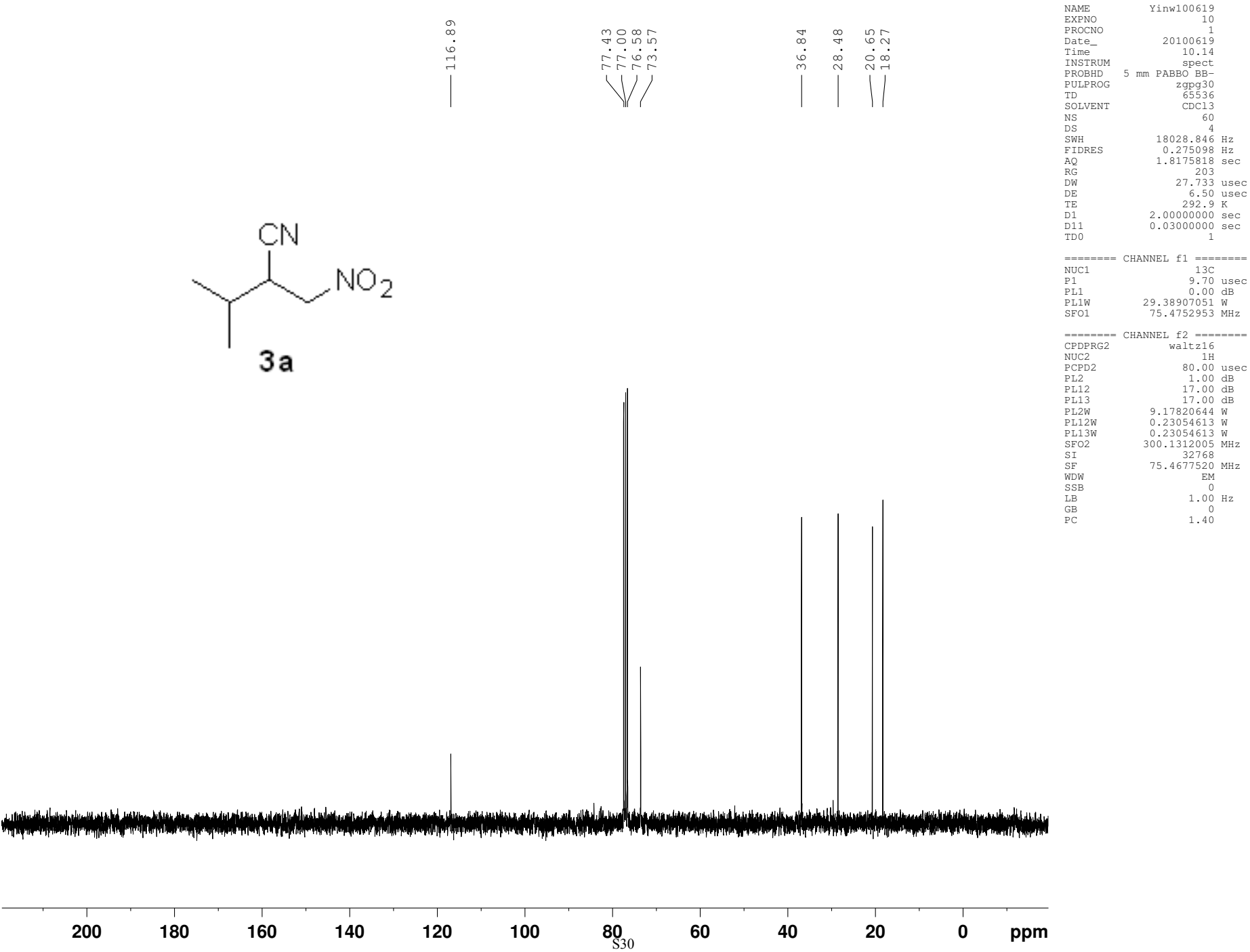


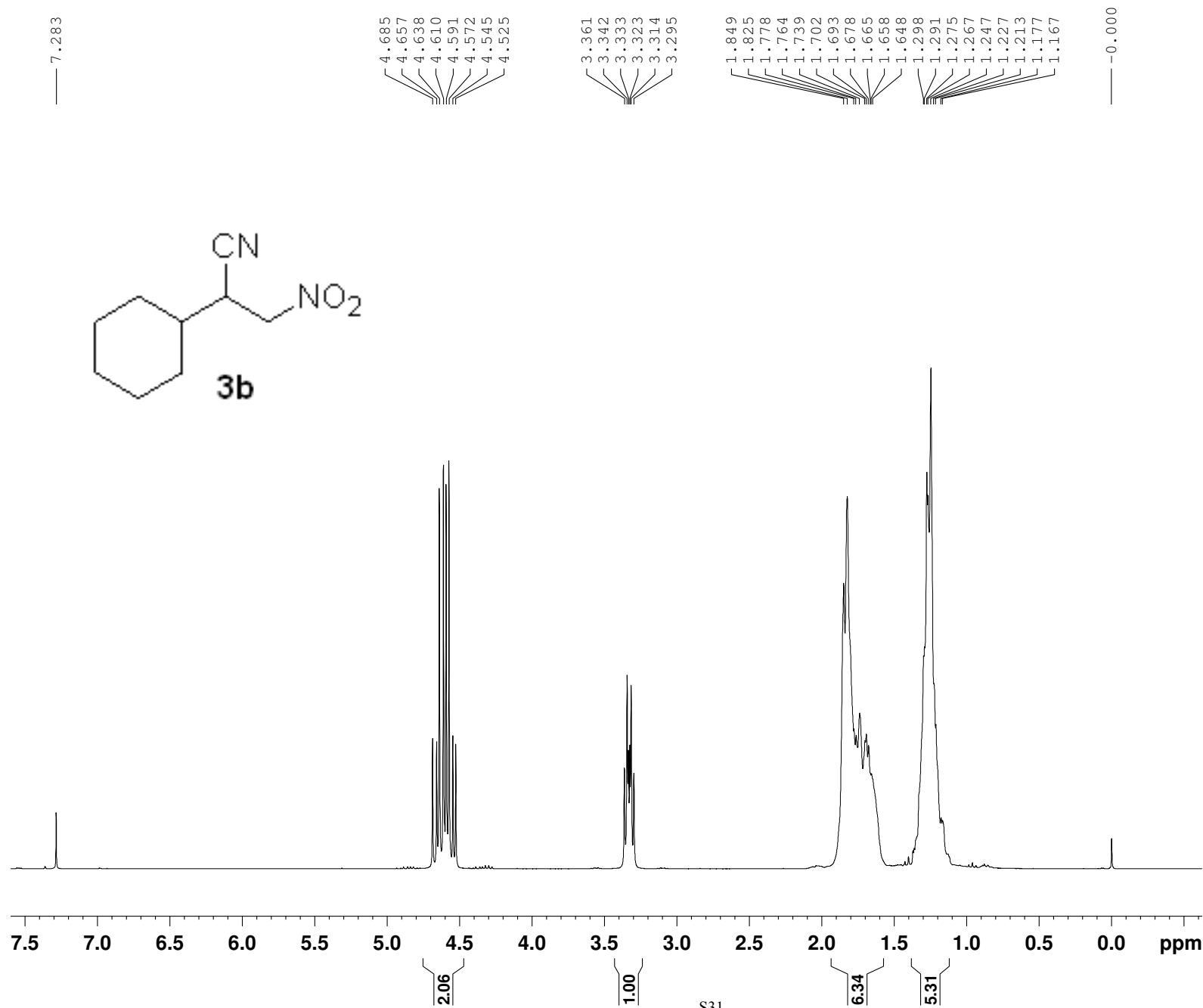




NAME 11nwl00019
EXPNO 8
PROCNO 1
Date_ 20100619
Time 9.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 50.8
DW 80.800 usec
DE 6.50 usec
TE 292.0 K
D1 1.00000000 sec
TD0 1

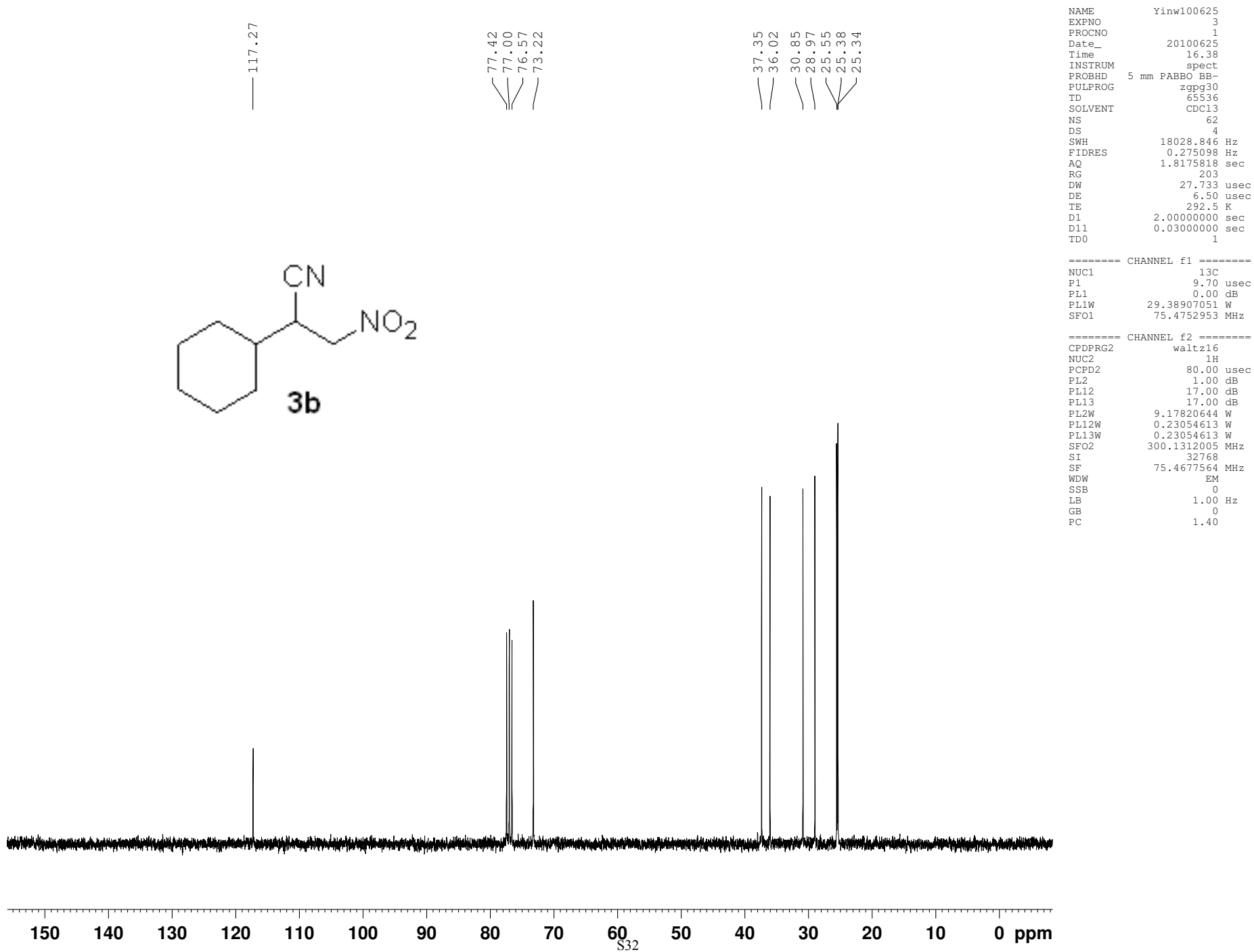
===== CHANNEL f1 =====
NUC1 1H
P1 11.80 usec
PL1 0.00 dB
PL1W 11.55467796 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1299983 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

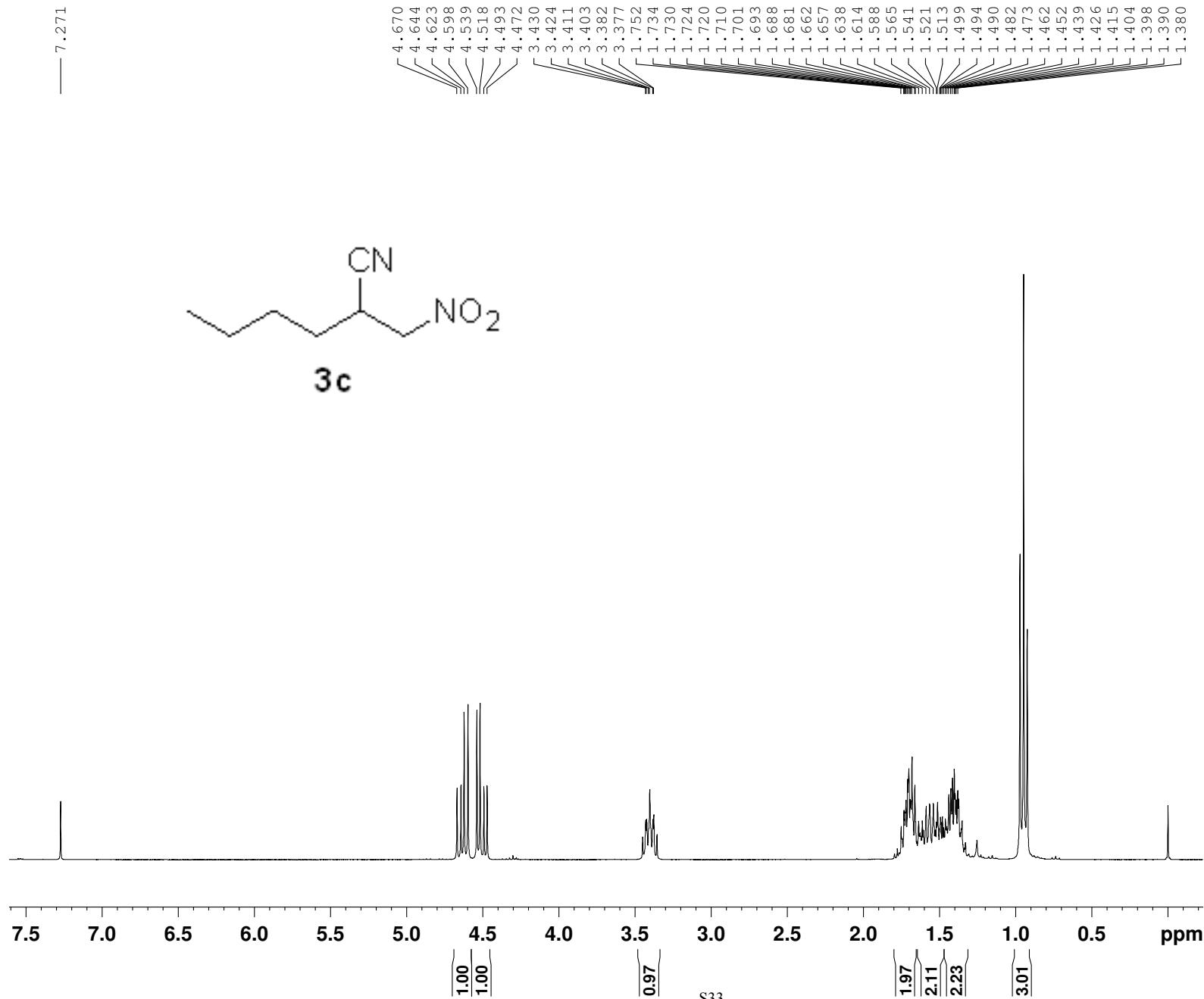




NAME 11NW100625
EXPNO 2
PROCNO 1
Date_ 20100625
Time 16.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 25.4
DW 80.800 usec
DE 6.50 usec
TE 292.1 K
D1 1.00000000 sec
TD0 1

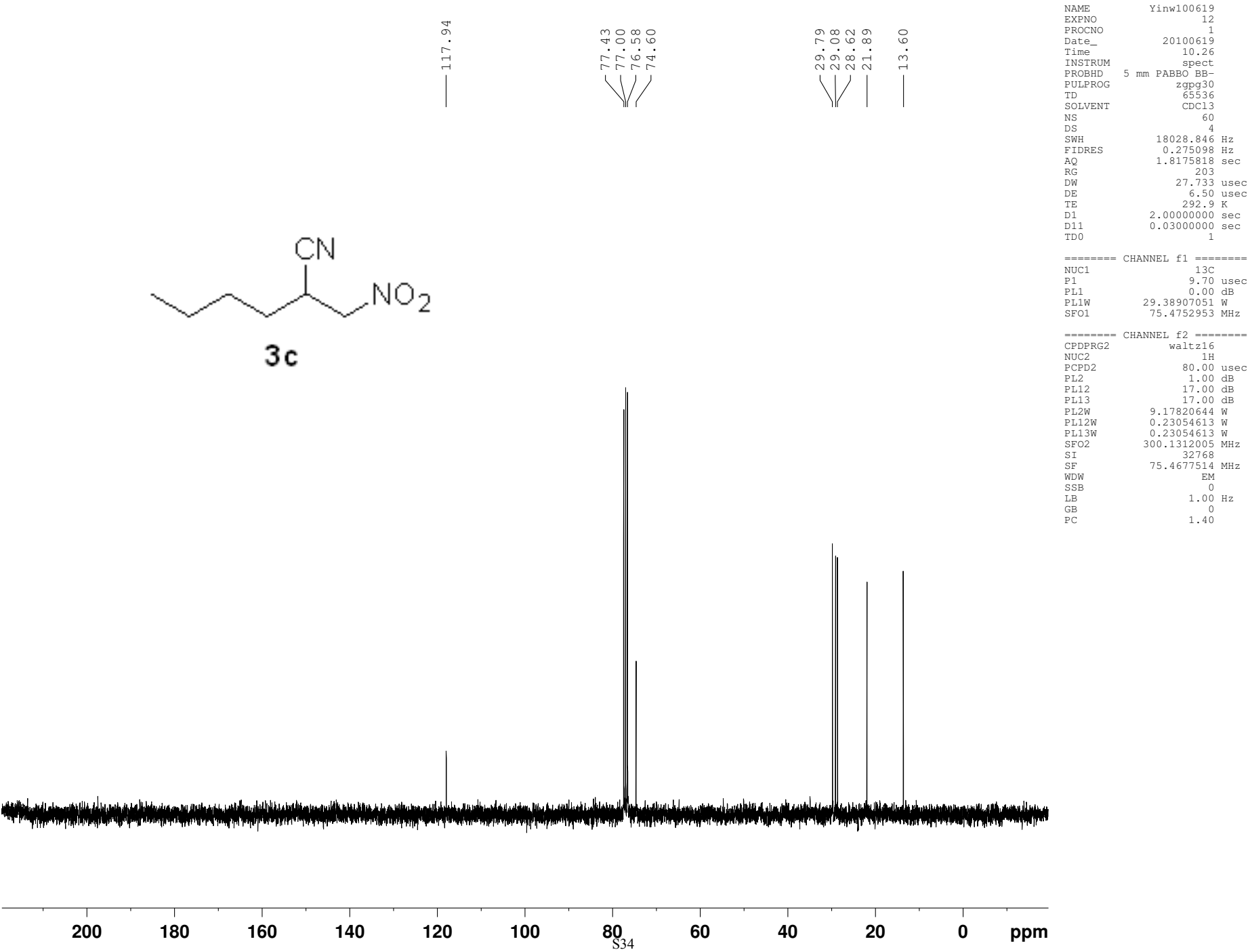
===== CHANNEL f1 =====
NUC1 1H
P1 11.80 usec
PL1 0.00 dB
PL1W 11.55467796 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1299952 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

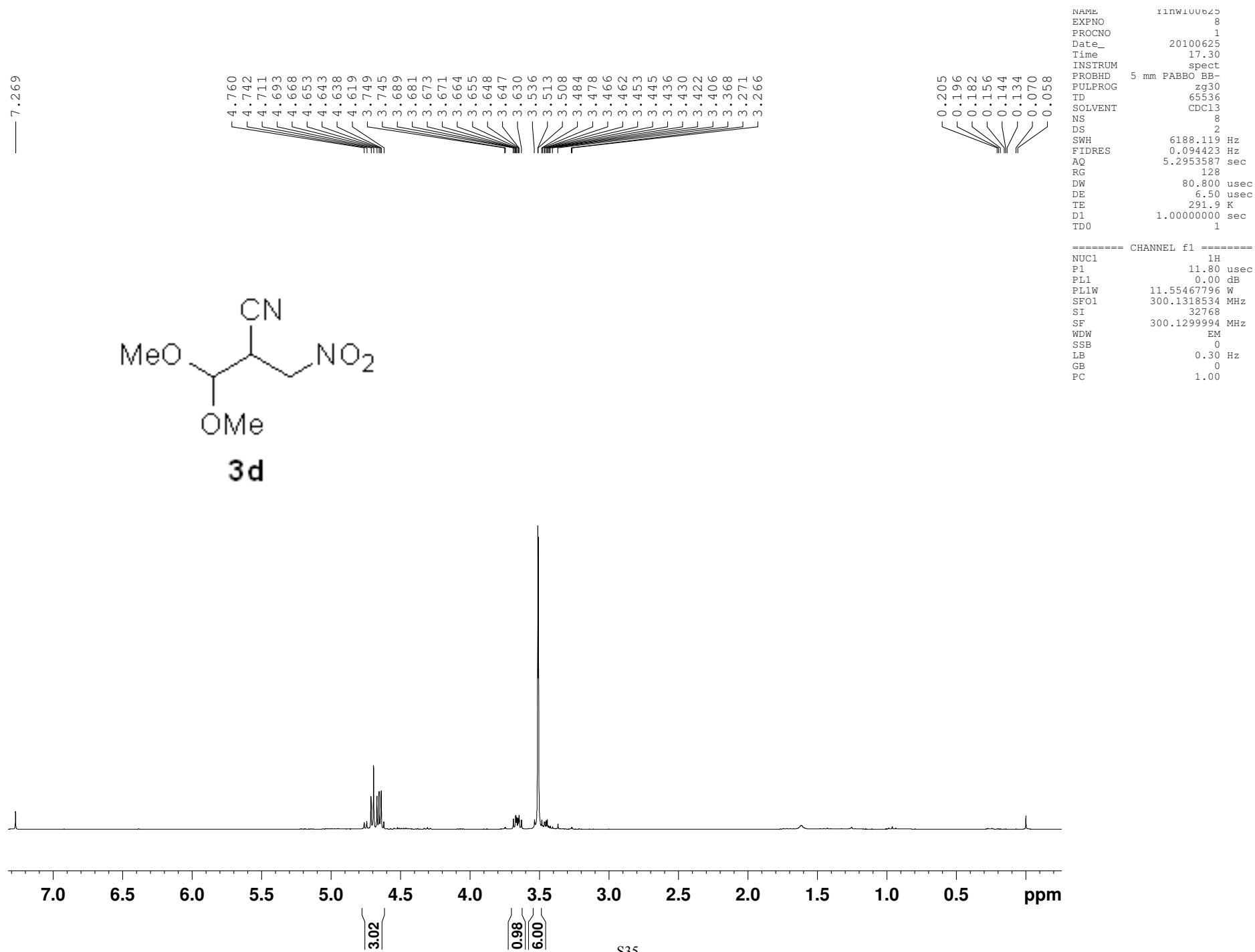


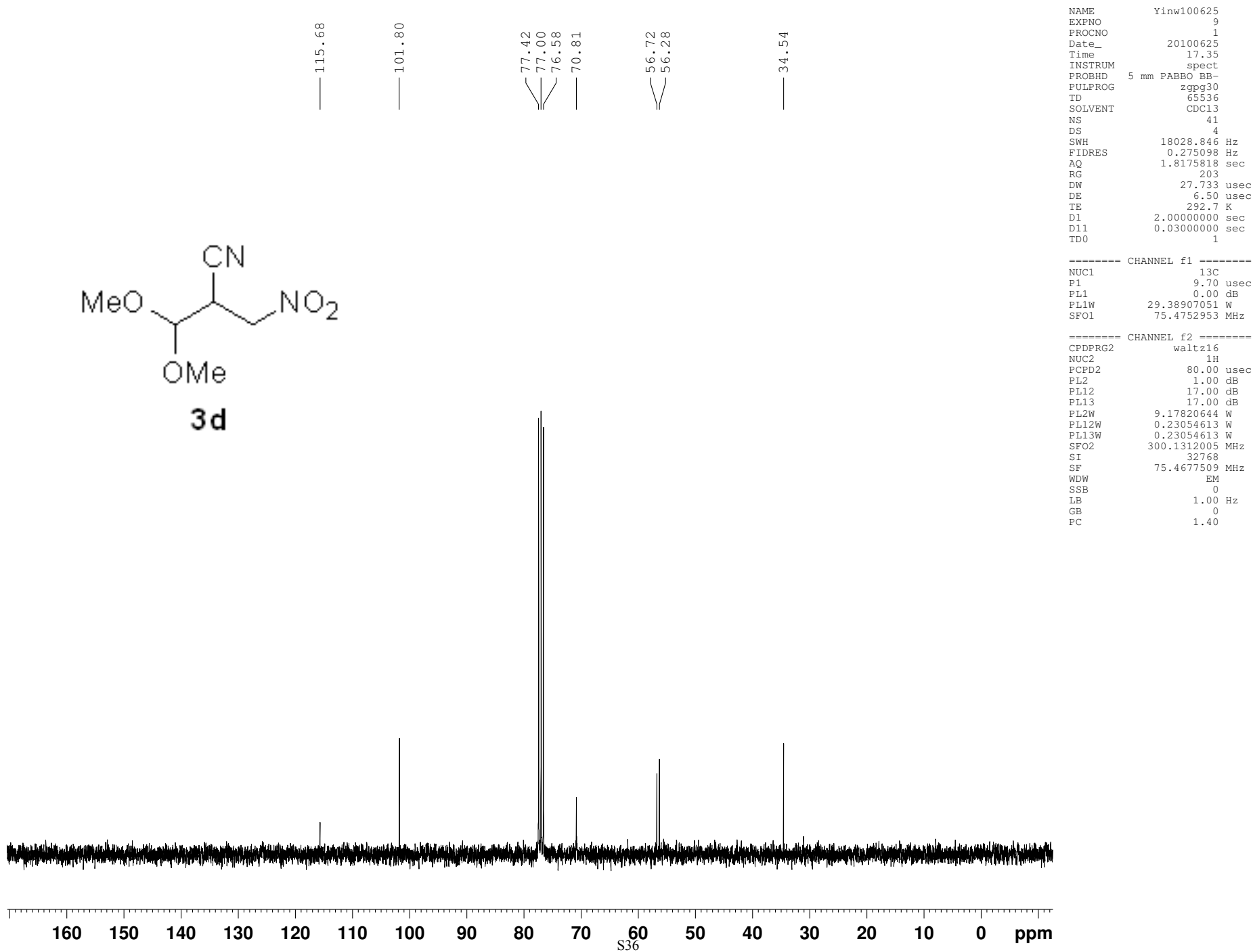


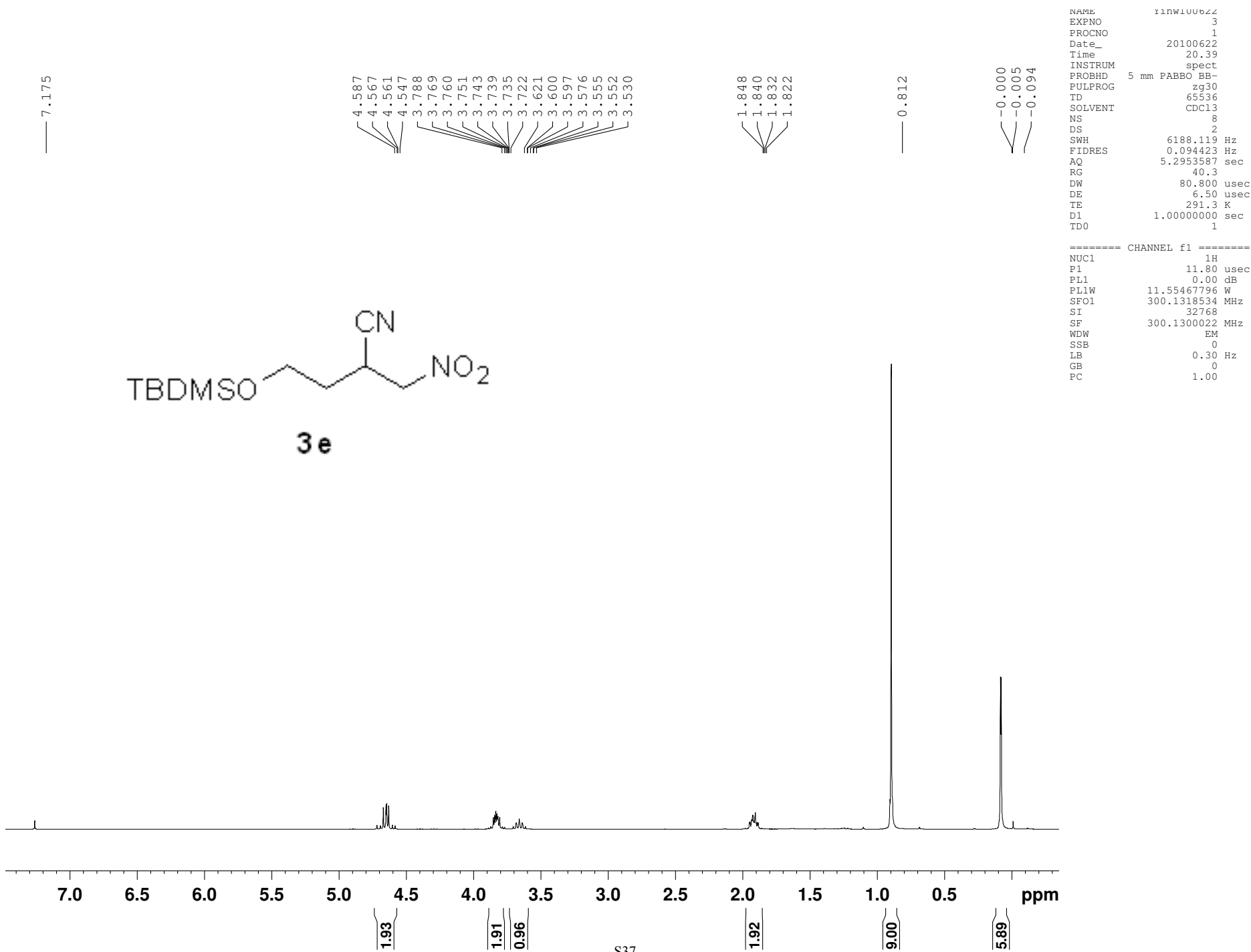
NAME 11nw100619
EXPNO 11
PROCNO 1
Date_ 20100619
Time 10.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 57
DW 80.800 usec
DE 6.50 usec
TE 292.3 K
D1 1.00000000 sec
TD0 1

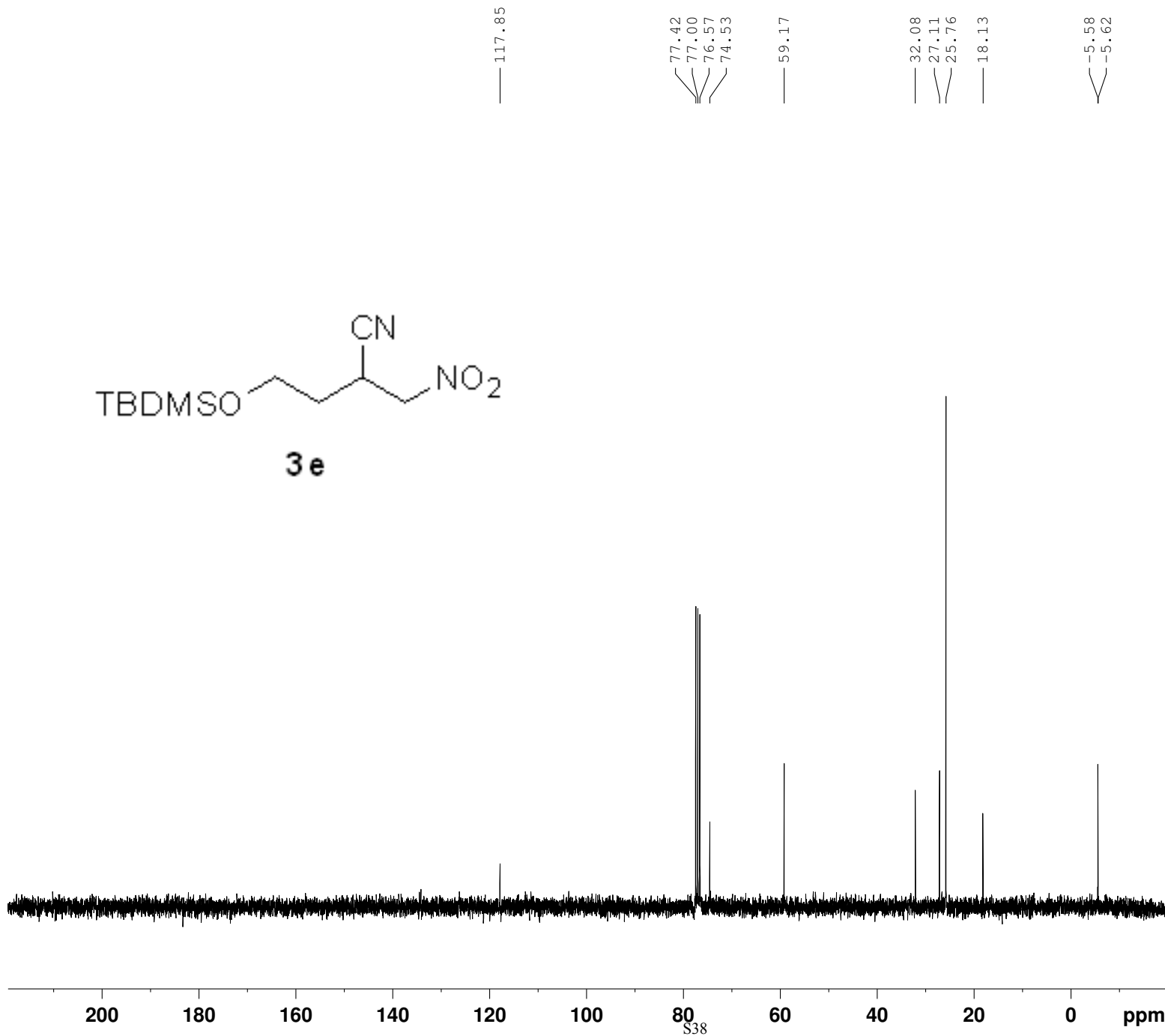
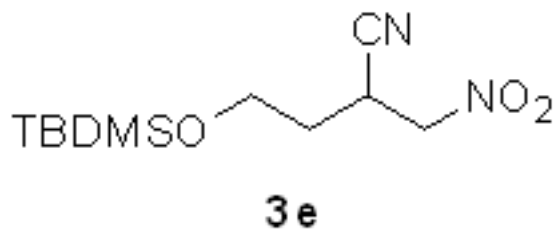
===== CHANNEL f1 =====
NUC1 1H
P1 11.80 usec
PL1 0.00 dB
PL1W 11.55467796 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1299990 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00







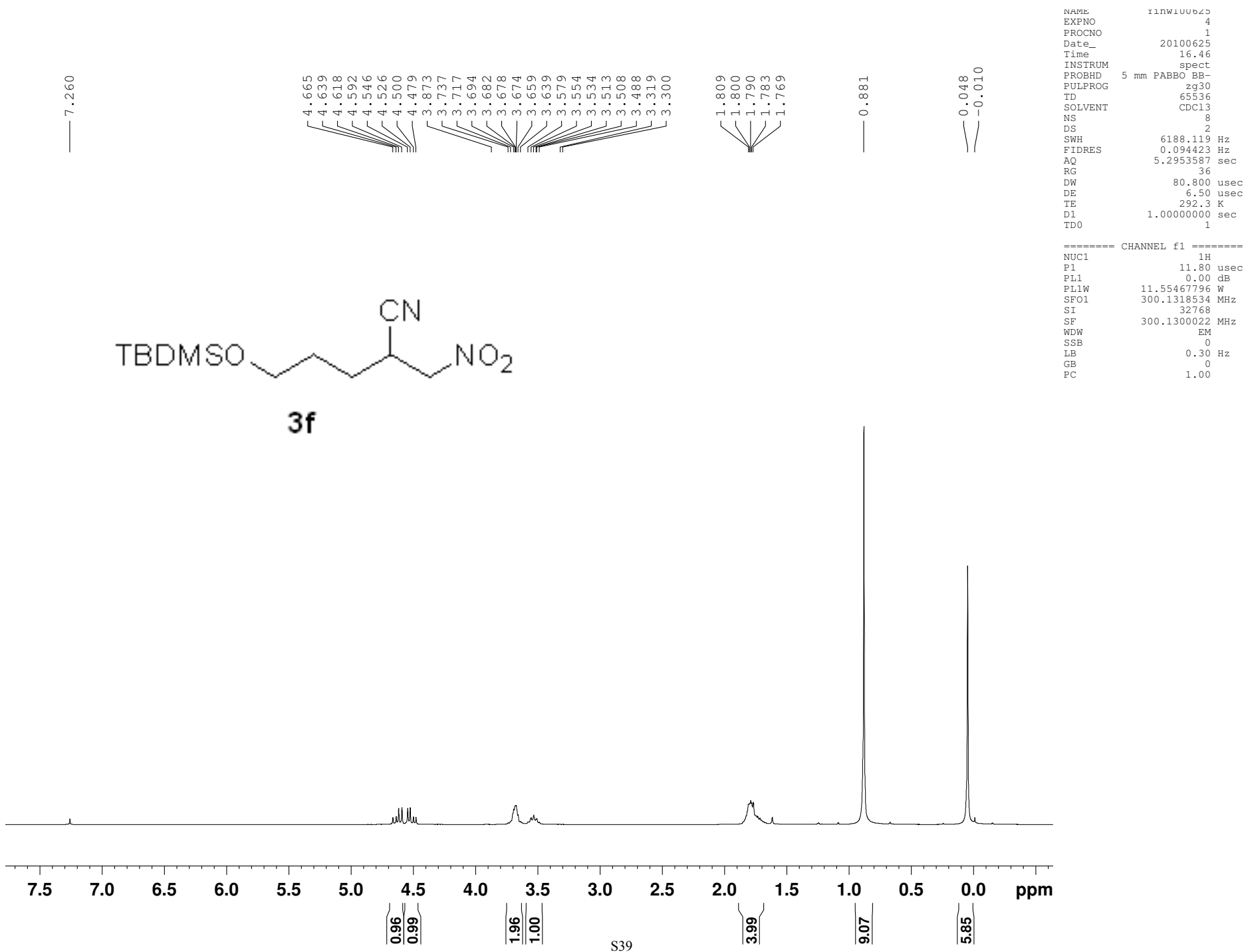


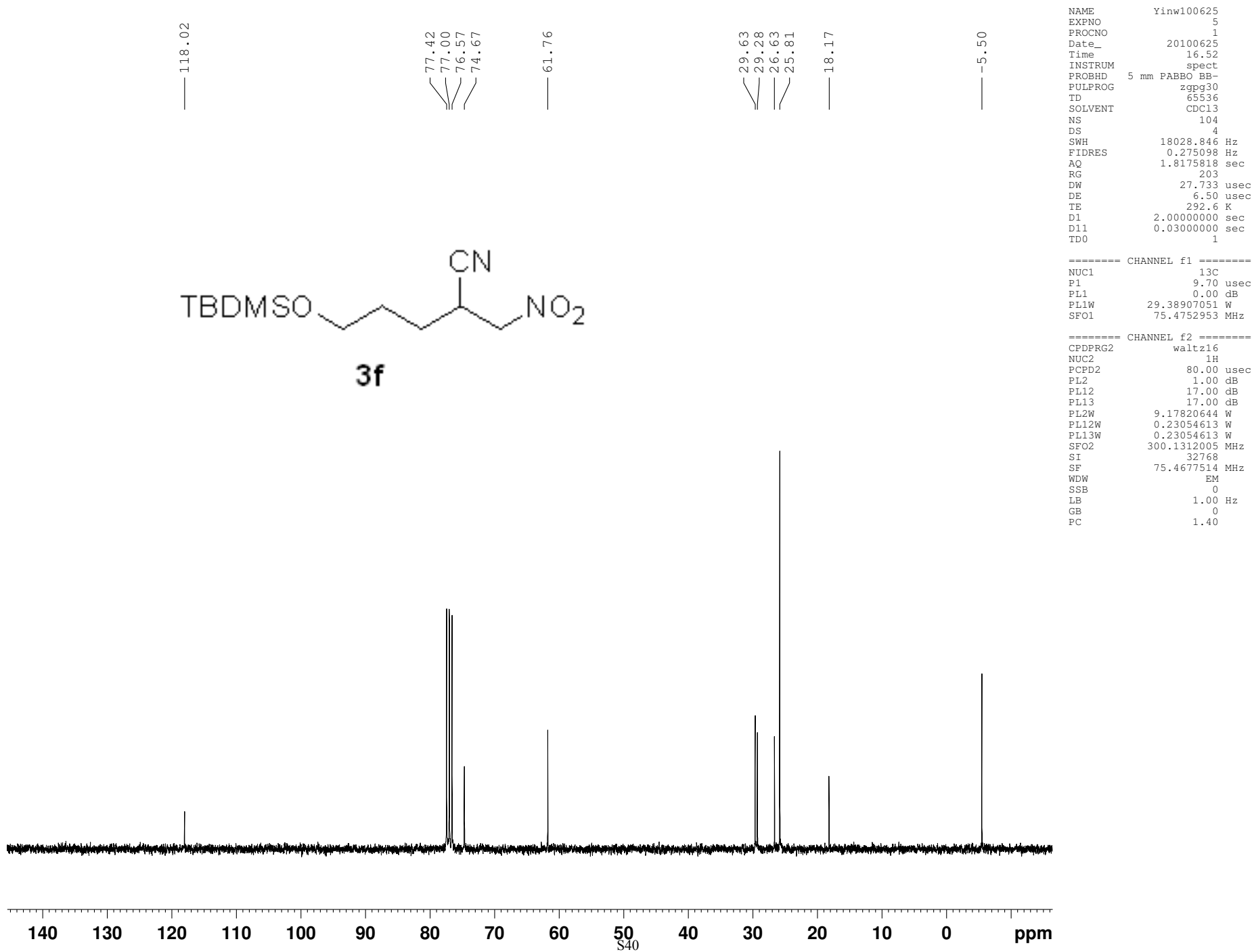


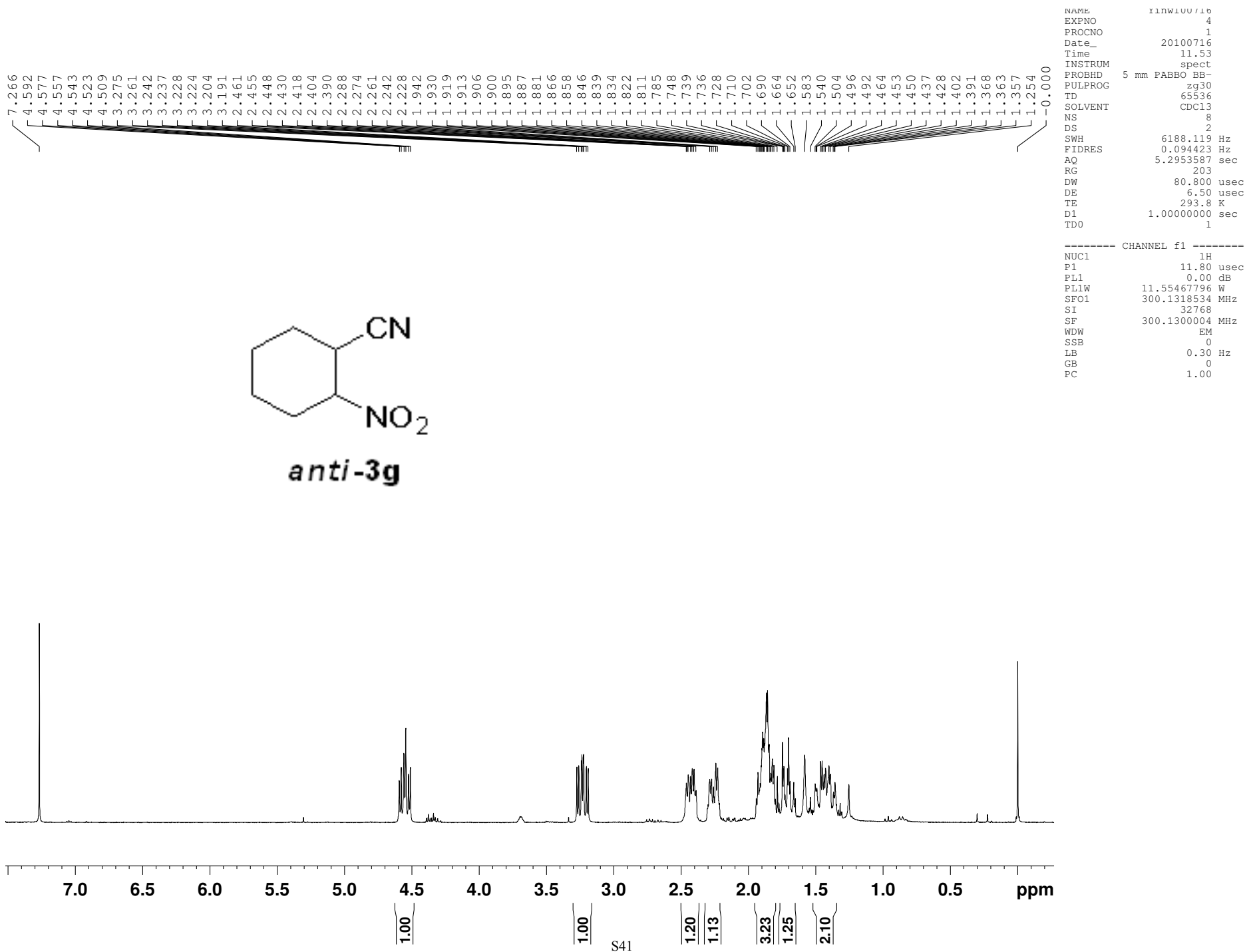
```
NAME Yinw100622
EXPNO 4
PROCNO 1
Date_ 20100622
Time 20.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 40
DS 4
SWH 18028.846 Hz
FIDRES 0.275998 Hz
AQ 1.817581 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 292.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

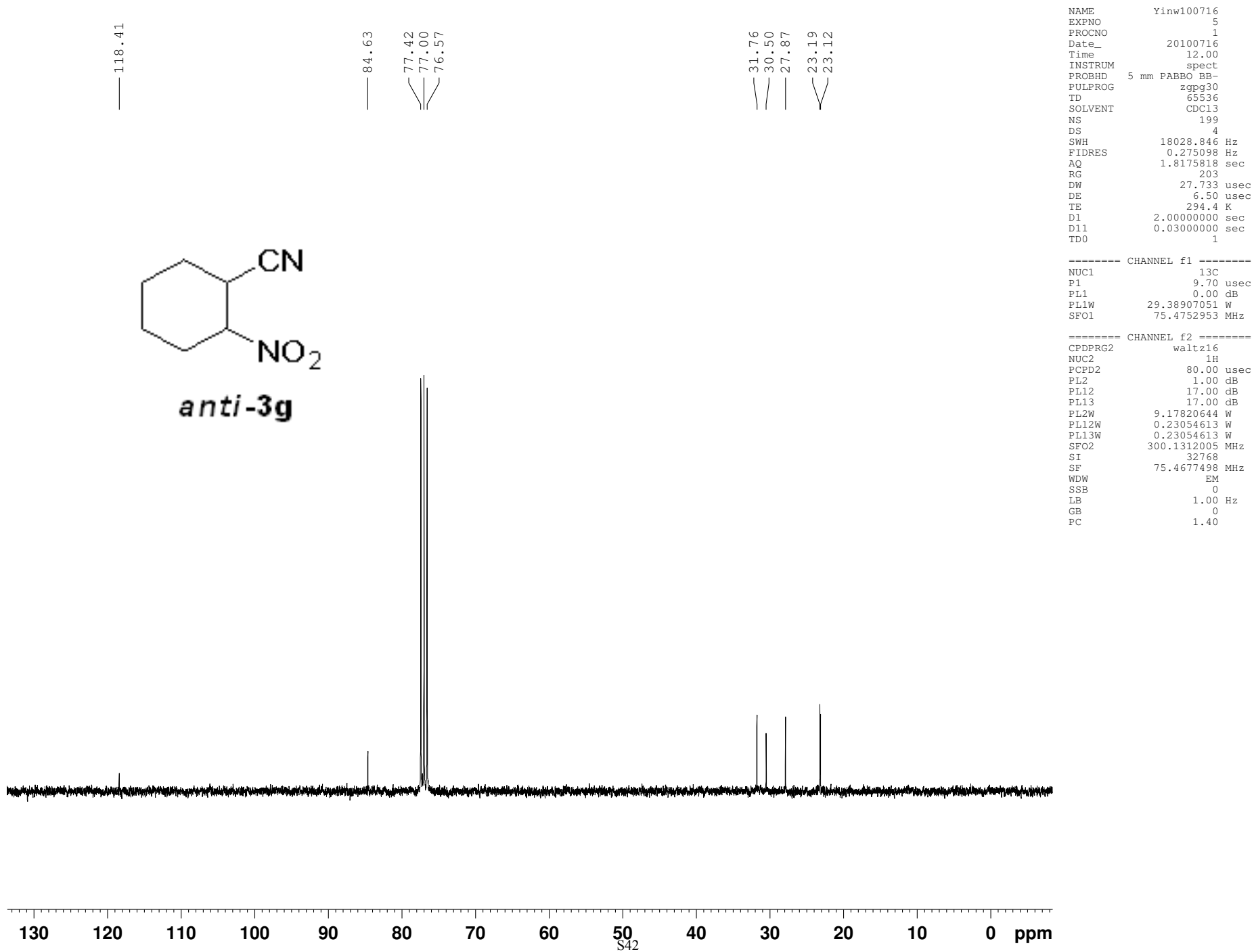
===== CHANNEL f1 =====
NUC1 13C
P1 9.70 usec
PL1 0.00 dB
PL1W 29.38907051 W
SFO1 75.4752953 MHz

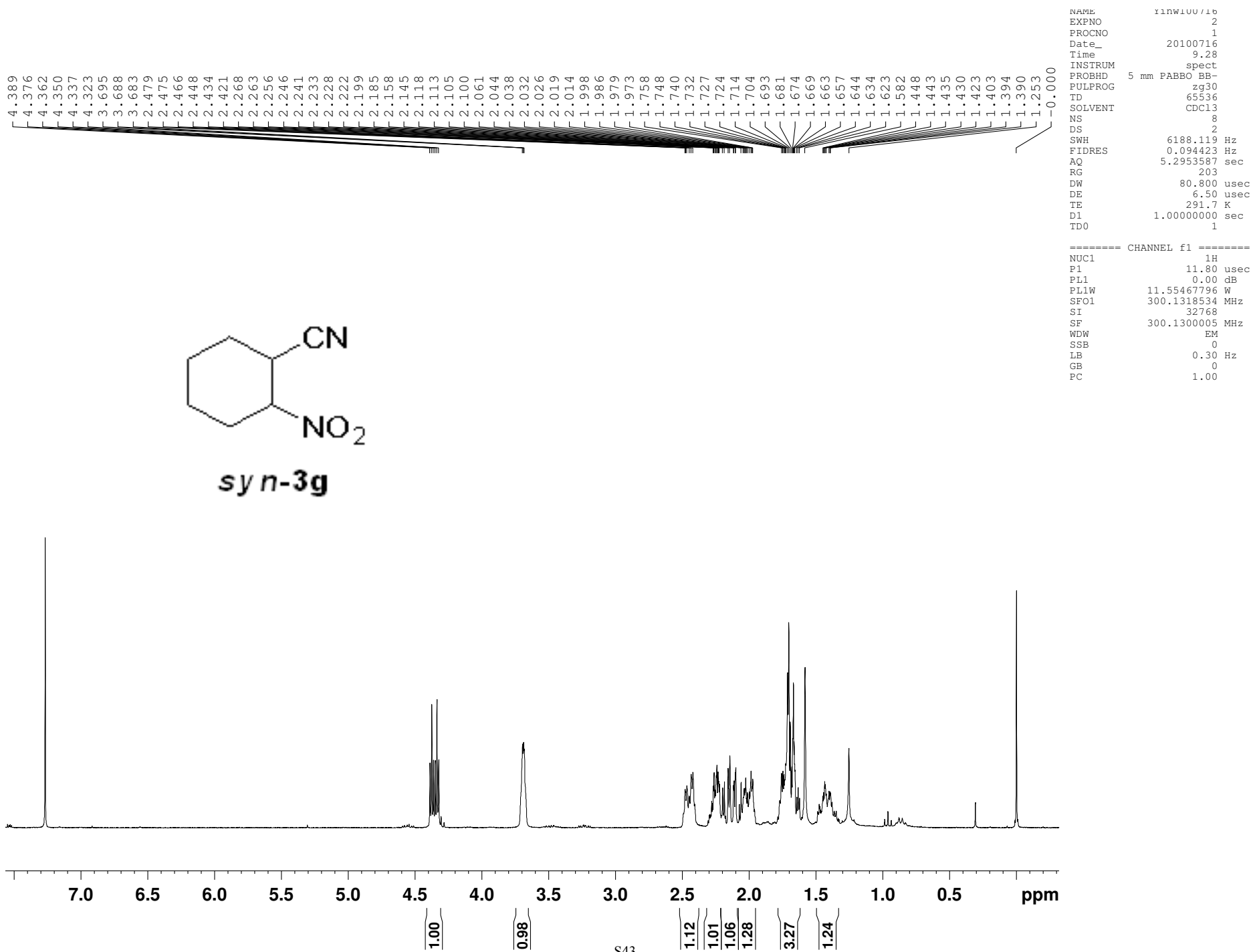
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 9.17820644 W
PL12W 0.23054613 W
PL13W 0.23054613 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677514 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```

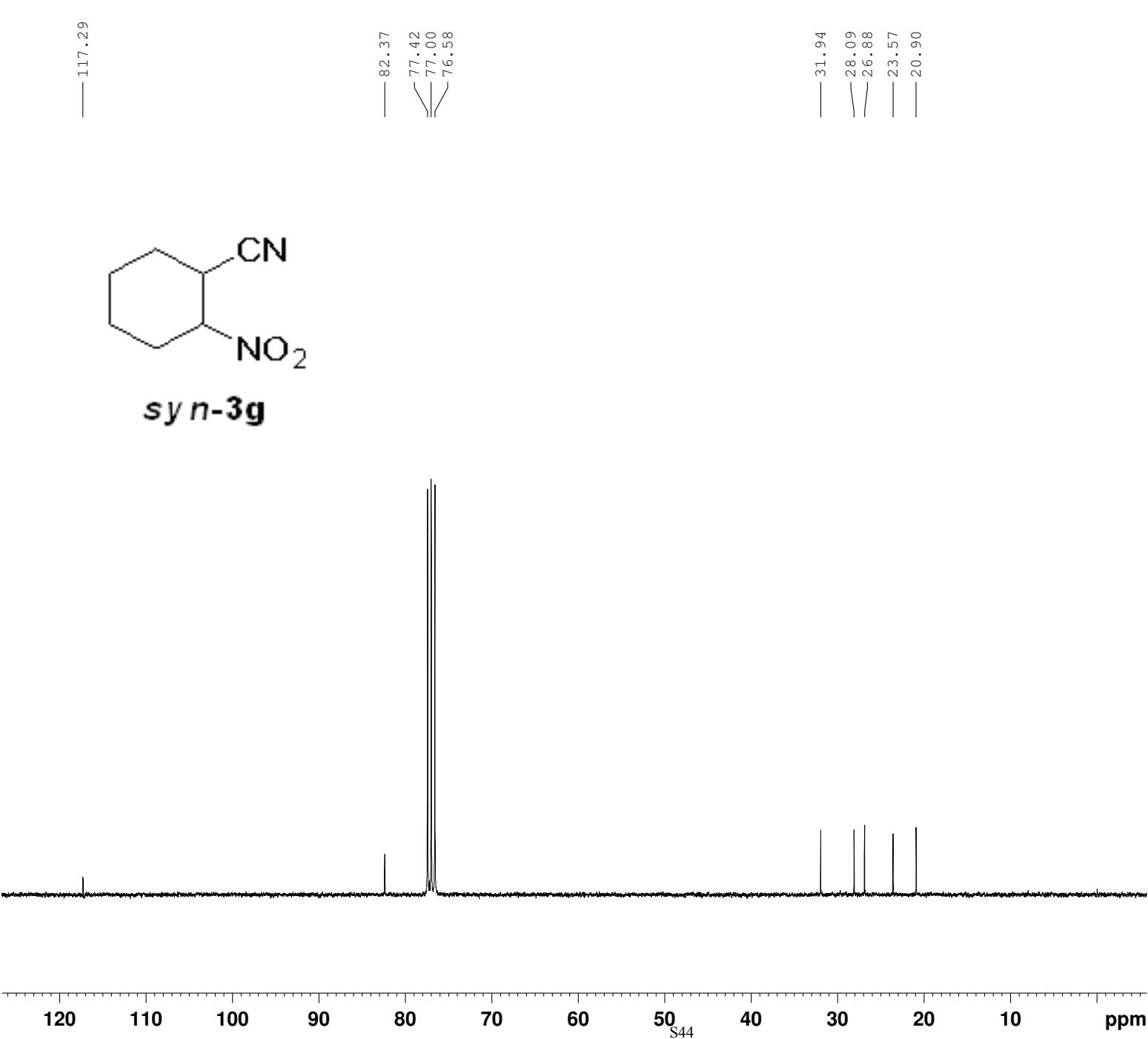


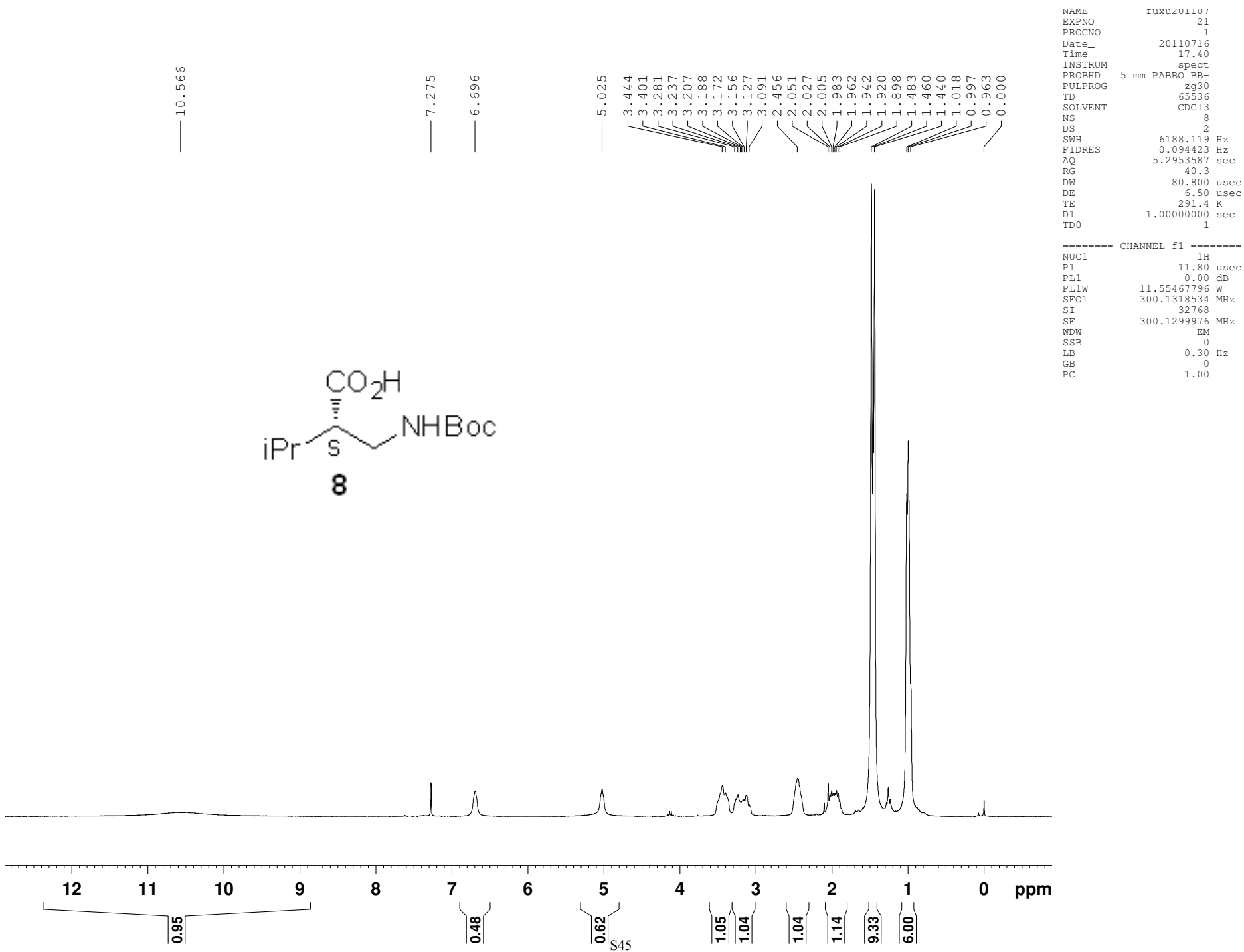












yan sheng

179.77
178.29

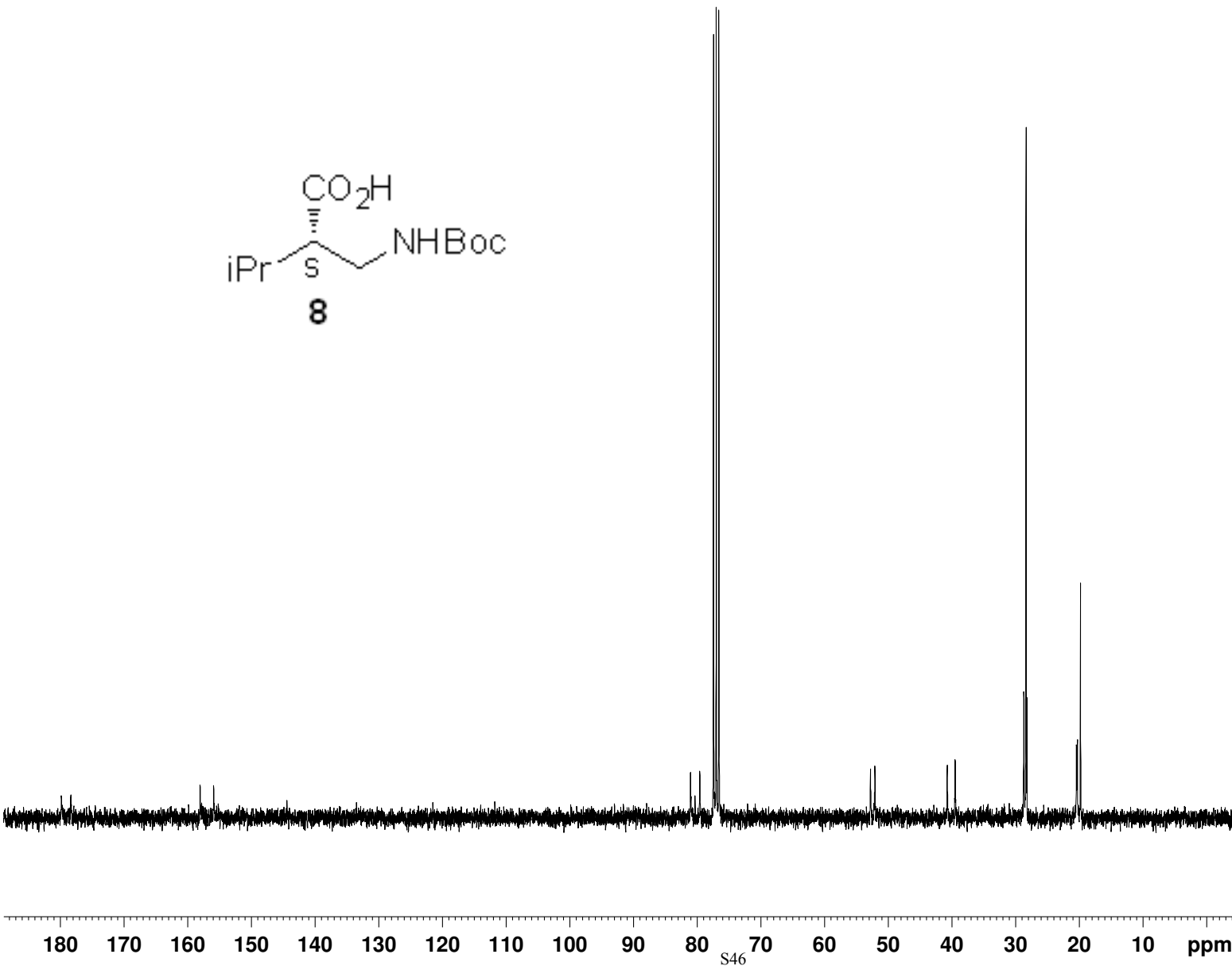
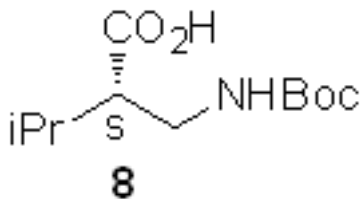
158.05
155.93

81.03
79.58
77.43
77.00
76.58

52.76
52.08

40.71
39.47

28.68
28.33
28.21
20.42
20.27
19.78



NAME fuxu201107
EXPNO 22
PROCNO 1
Date_ 20110716
Time_ 17.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 305
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 292.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 13C
P1 9.70 usec
PL1 0.00 dB
PL1W 29.38907051 W
SFO1 75.4752953 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 17.00 dB
PL13 17.00 dB
PL2W 9.17820644 W
PL12W 0.23054613 W
PL13W 0.23054613 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677492 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40