A New example of Steroid-Amino Acid Hybrid: Construction of constrained nine membered D-ring steroids

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Supporting Information

Contents:

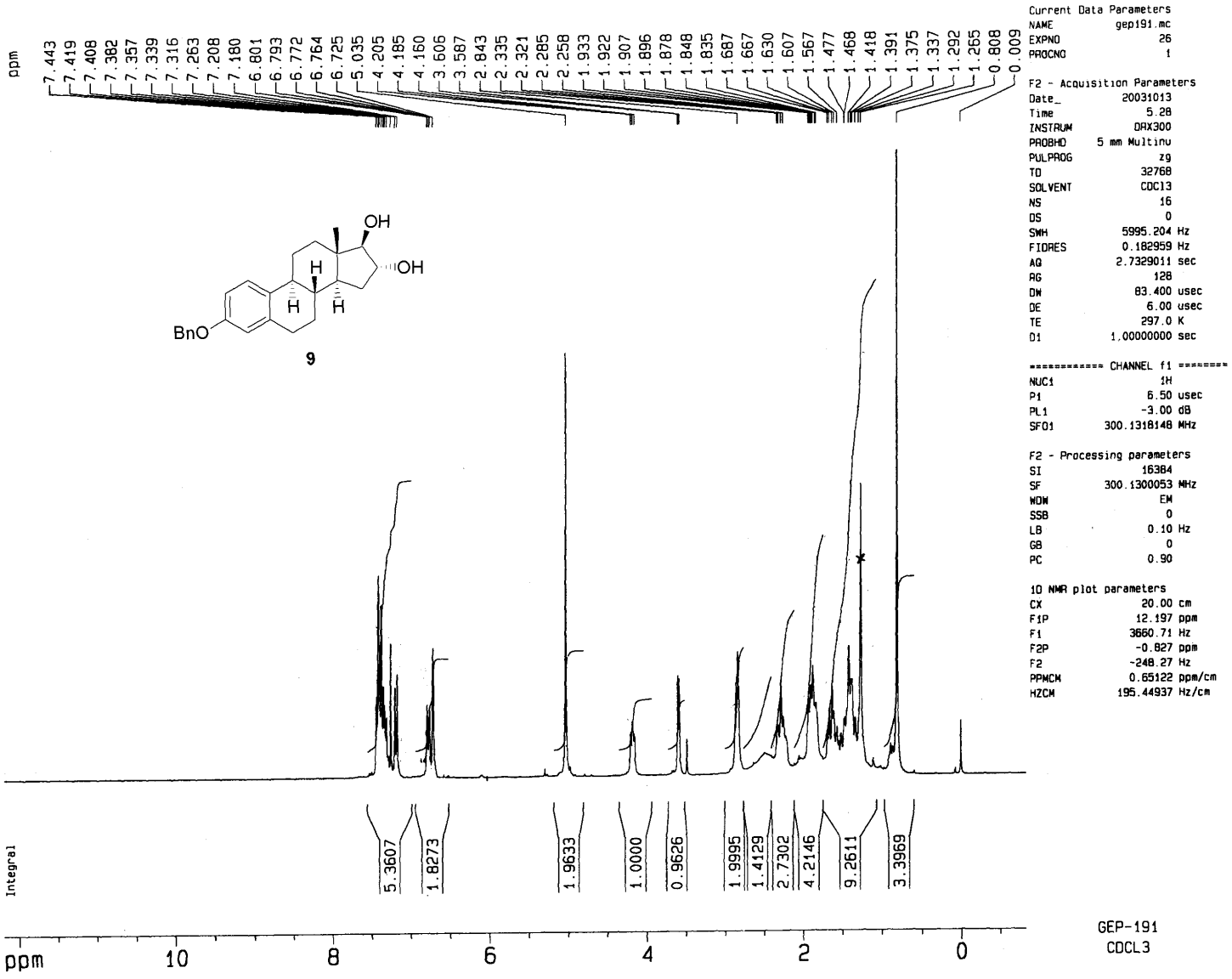


Fig. 1: ^{1}H NMR Spectrum of Benzylated Estriol **9**

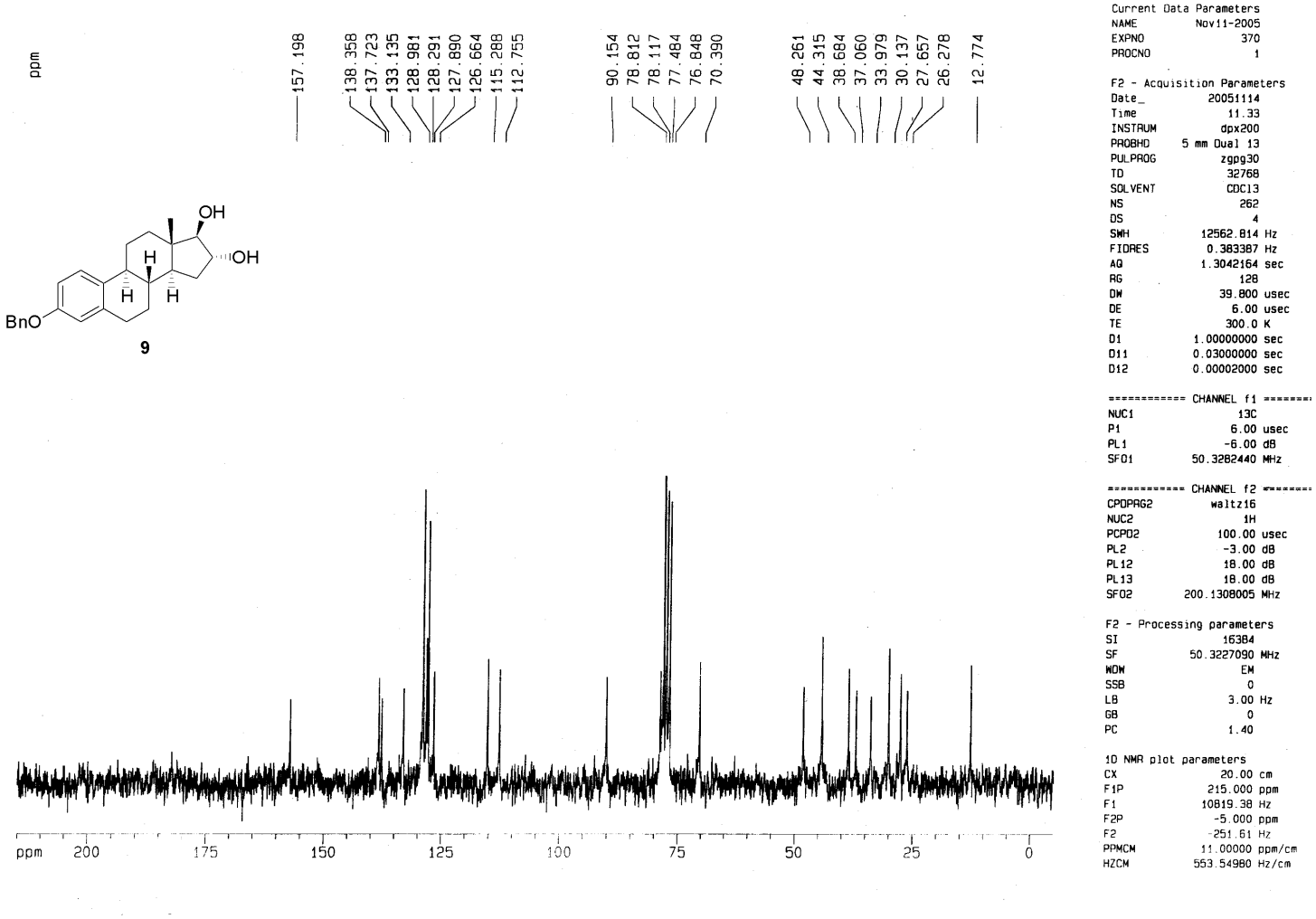


Fig. 2: ^{13}C NMR Spectrum of Benzylated Estriol **9**

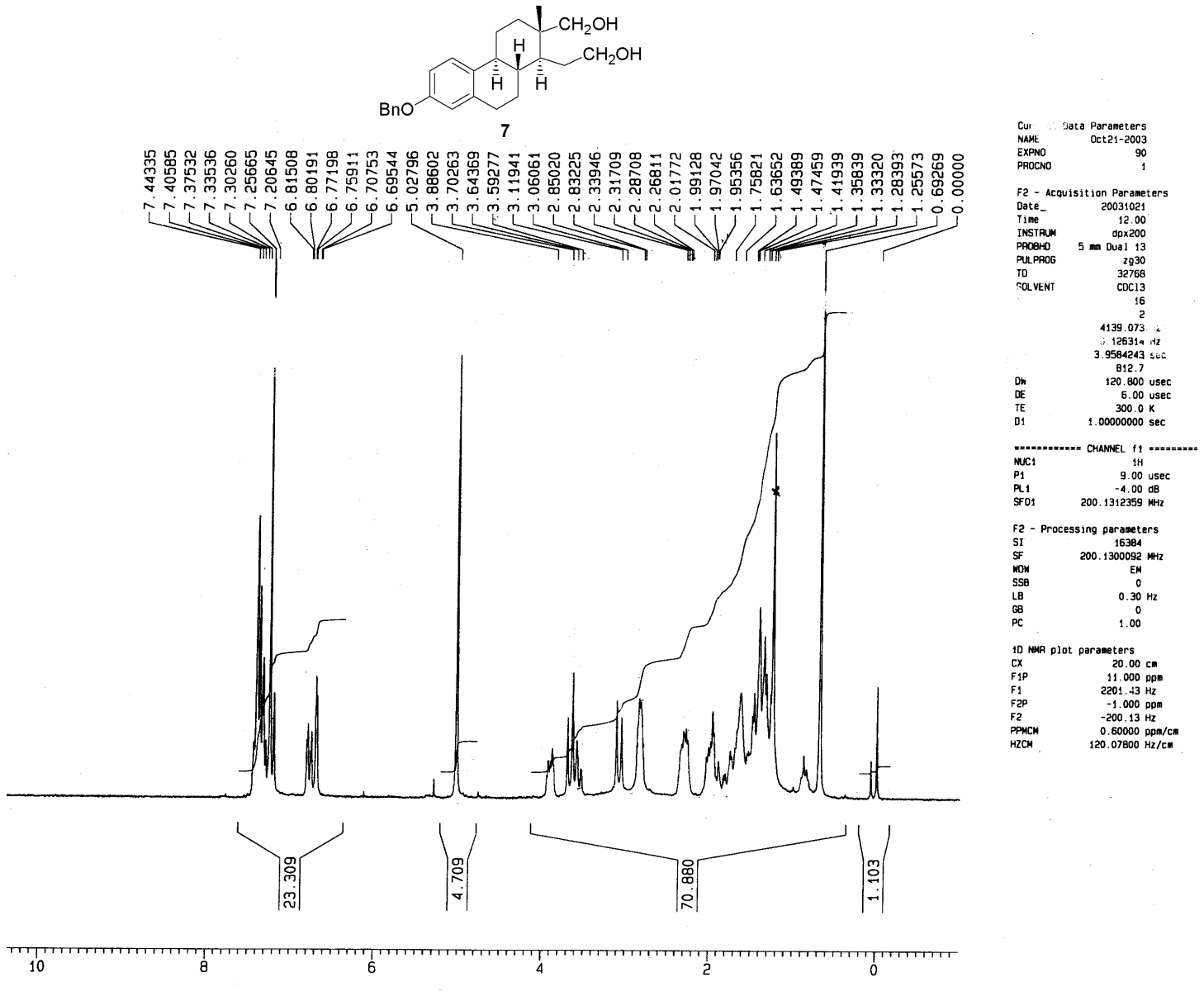


Fig. 3: ^{1}H NMR Spectrum of Diol **7**

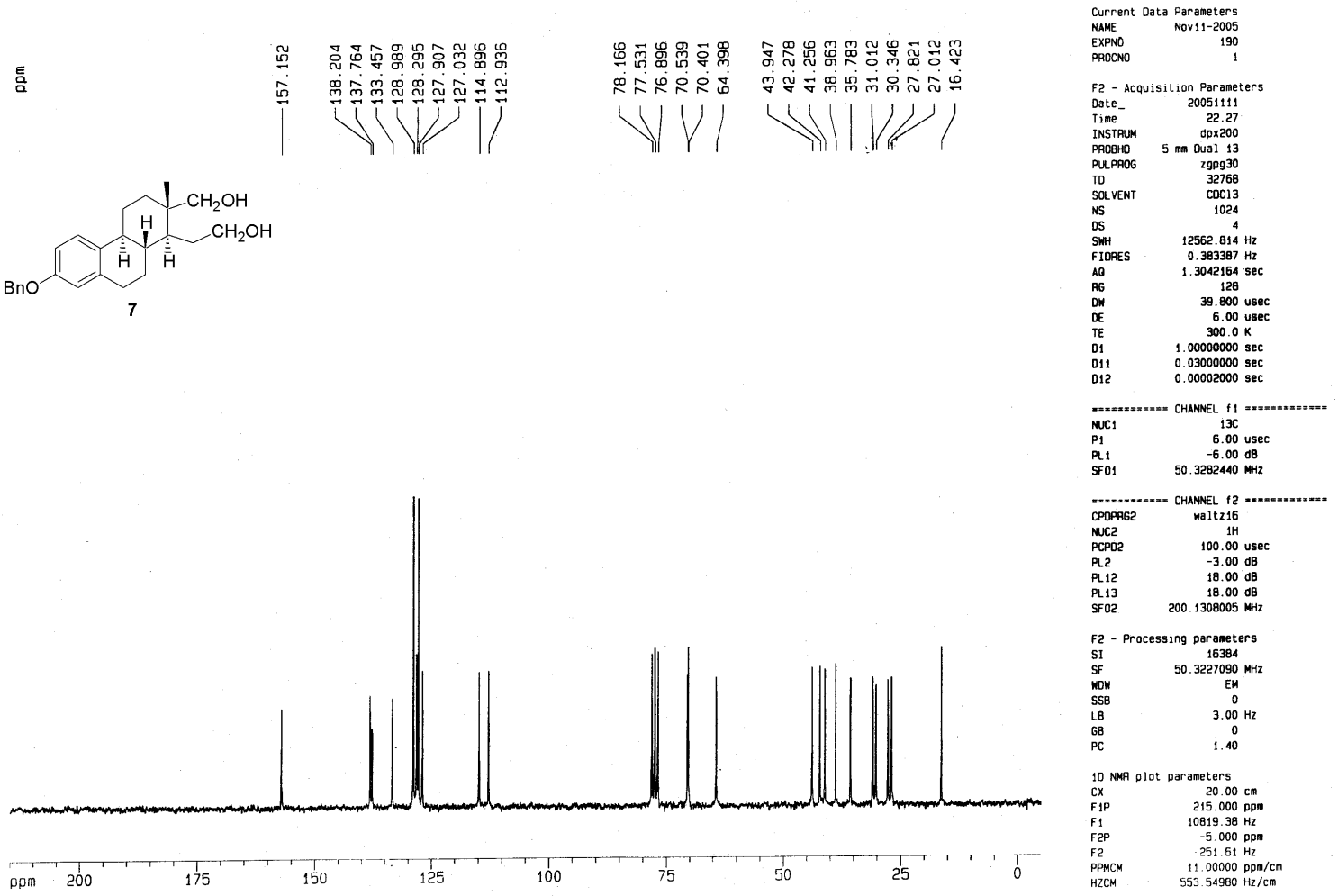


Fig. 4: ^{13}C NMR Spectrum of Diol **7**

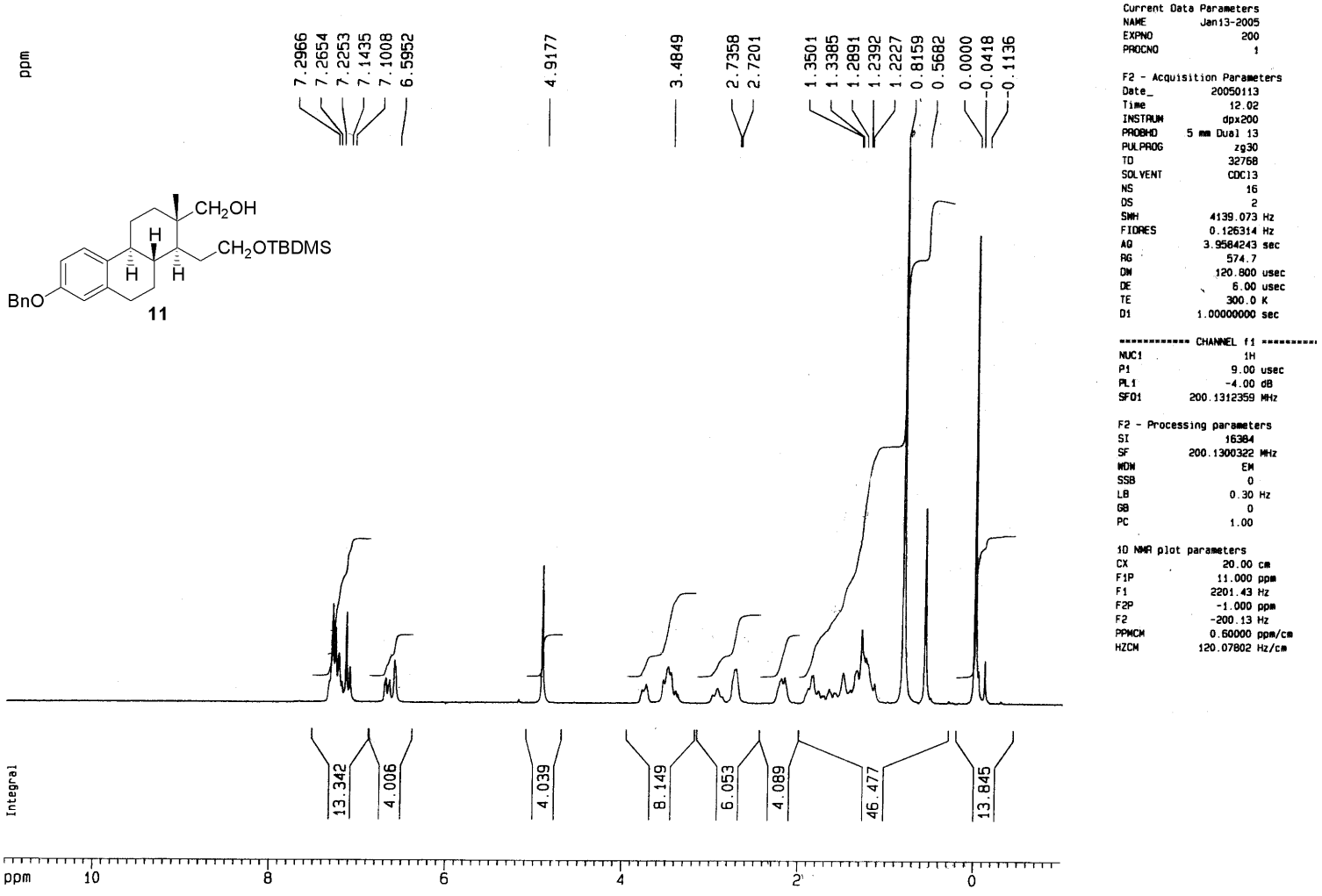


Fig. 5: ^{1}H NMR Spectrum of TBDMS Derivative **11**

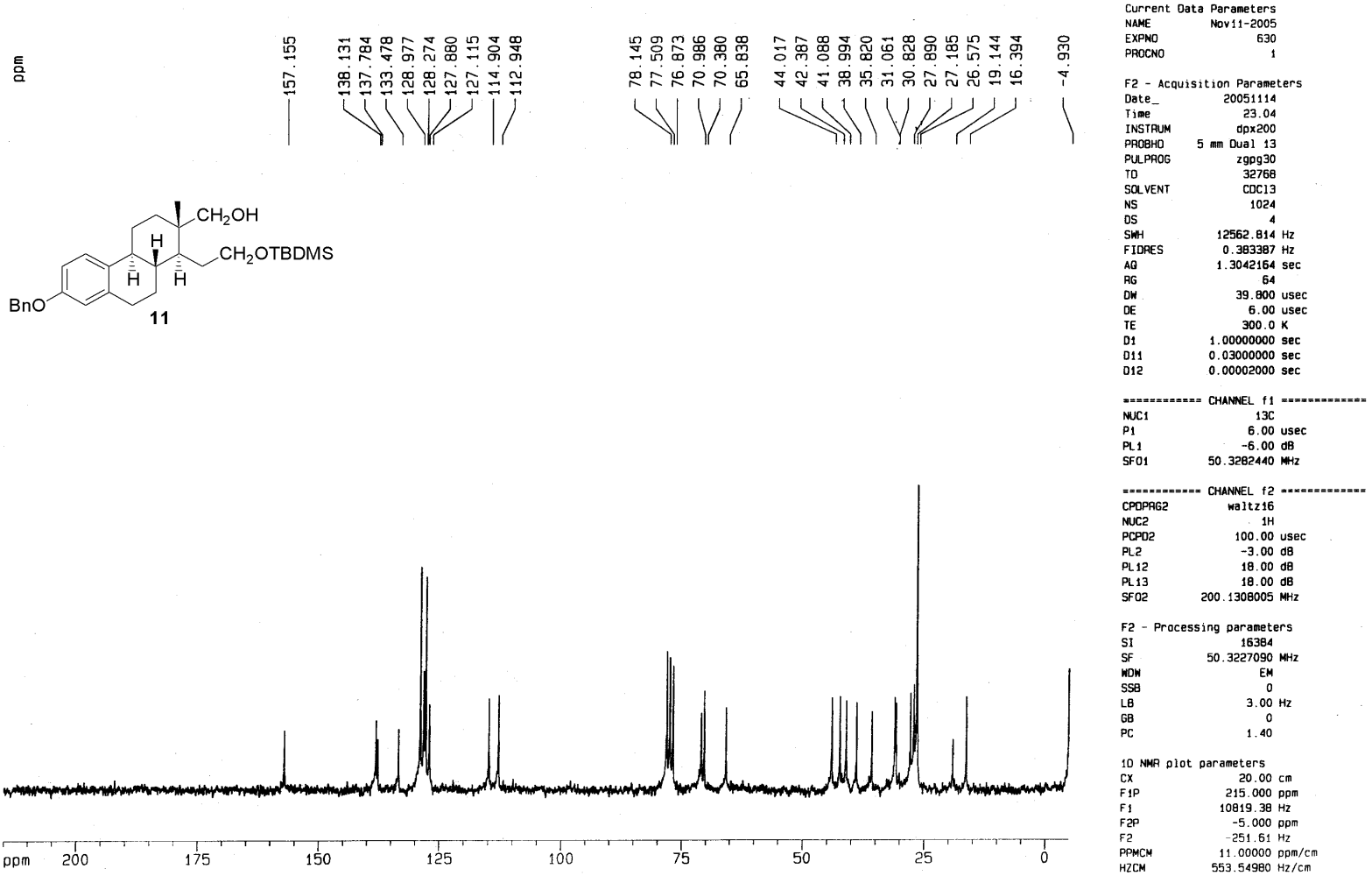


Fig. 6: ^{13}C NMR Spectrum of TBDMS Derivative **11**

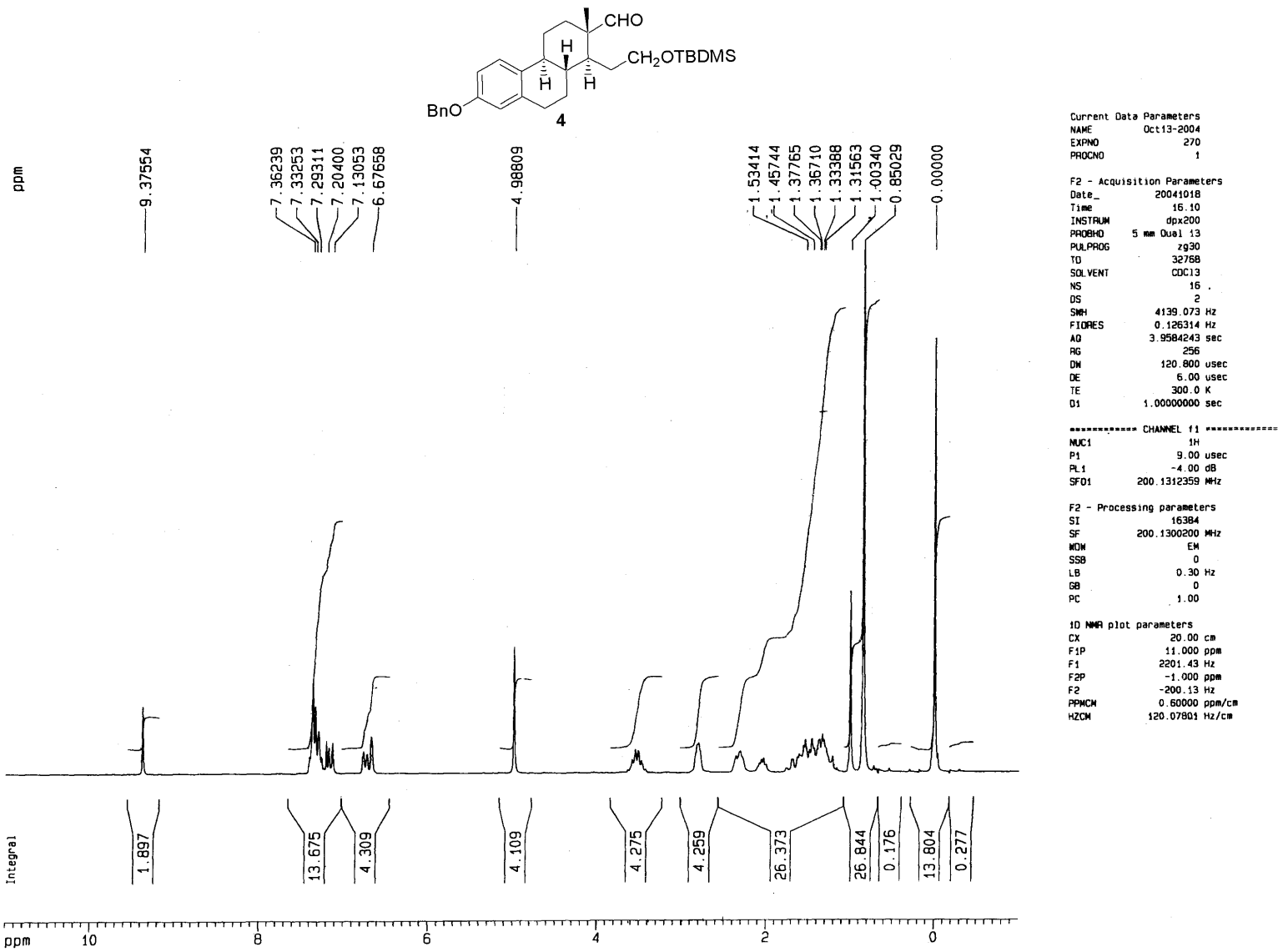


Fig. 7: ^{1}H NMR Spectrum of Aldehyde **4**

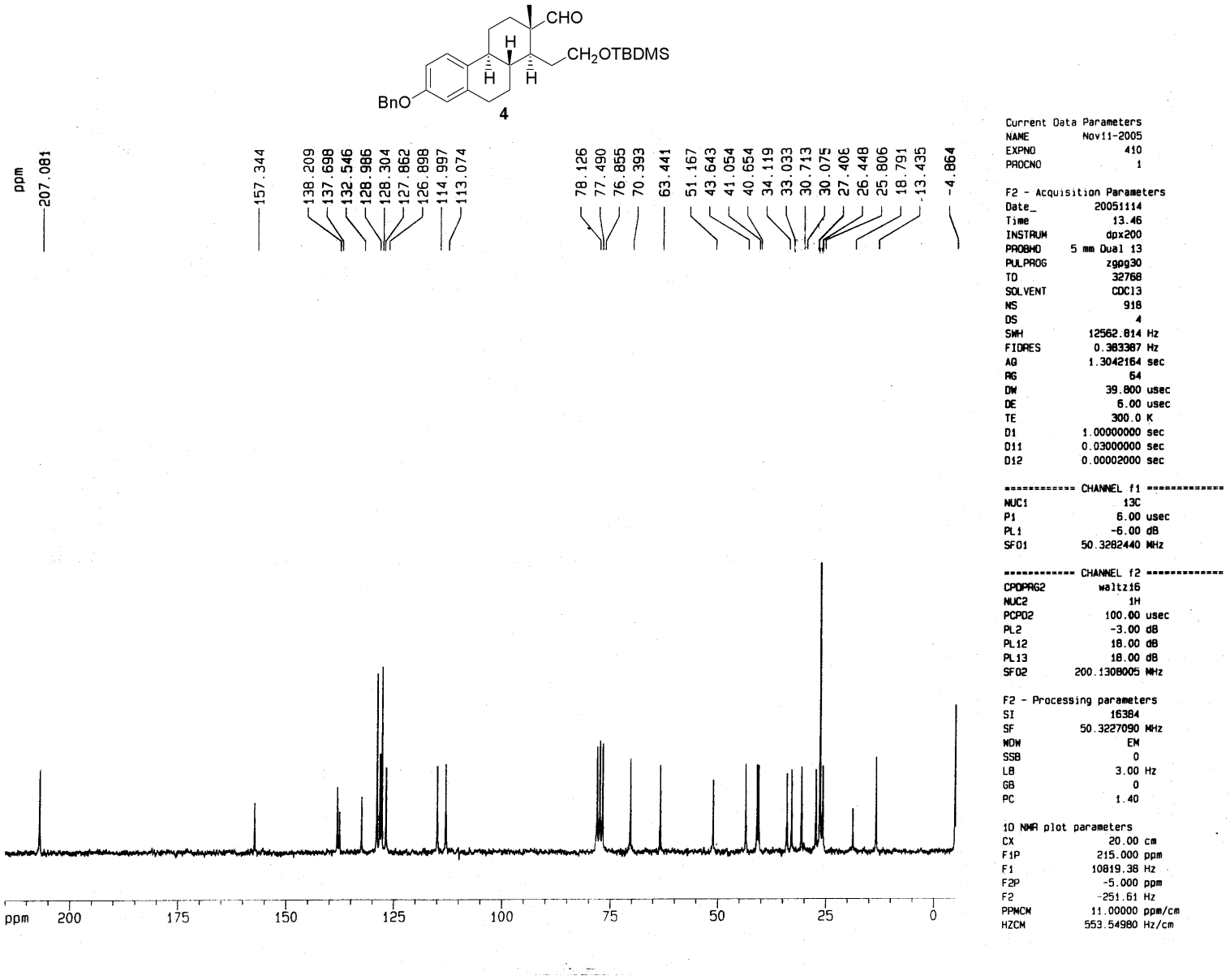


Fig. 8: ^{13}C NMR Spectrum of Aldehyde **4**

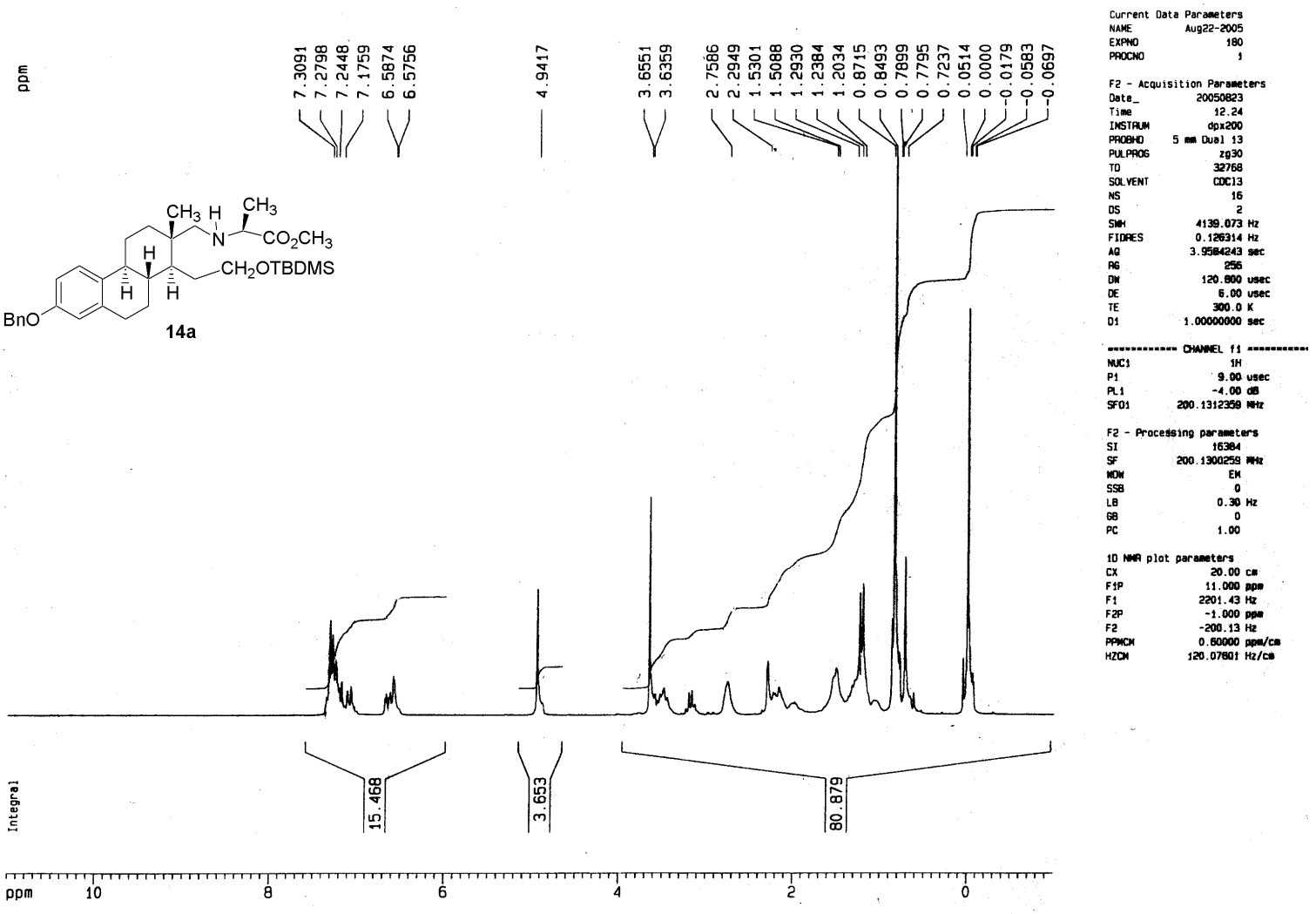


Fig. 9: ^{1}H NMR Spectrum of Amine **14a**

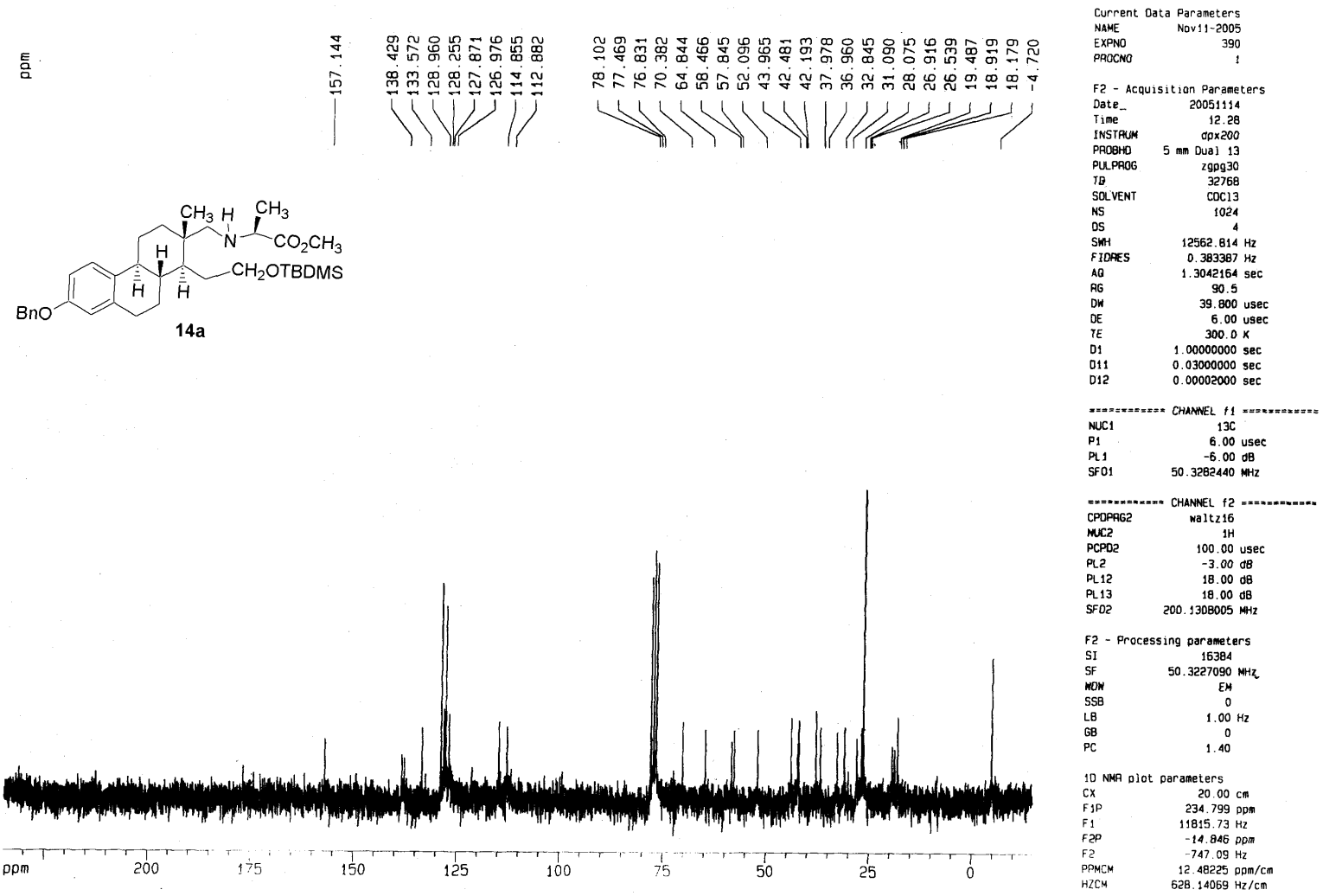


Fig. 10: ^{13}C NMR Spectra of Amine **14a**

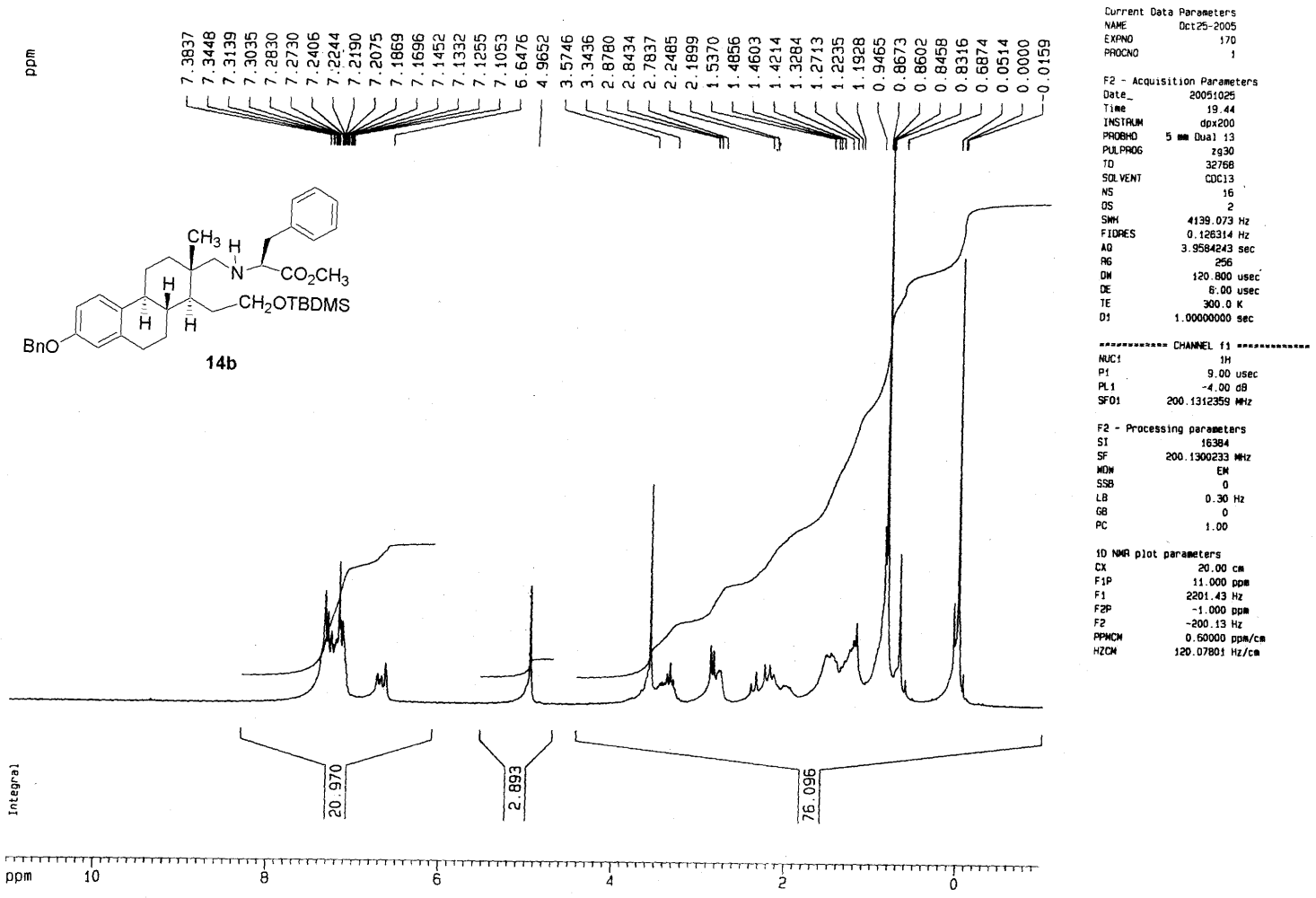
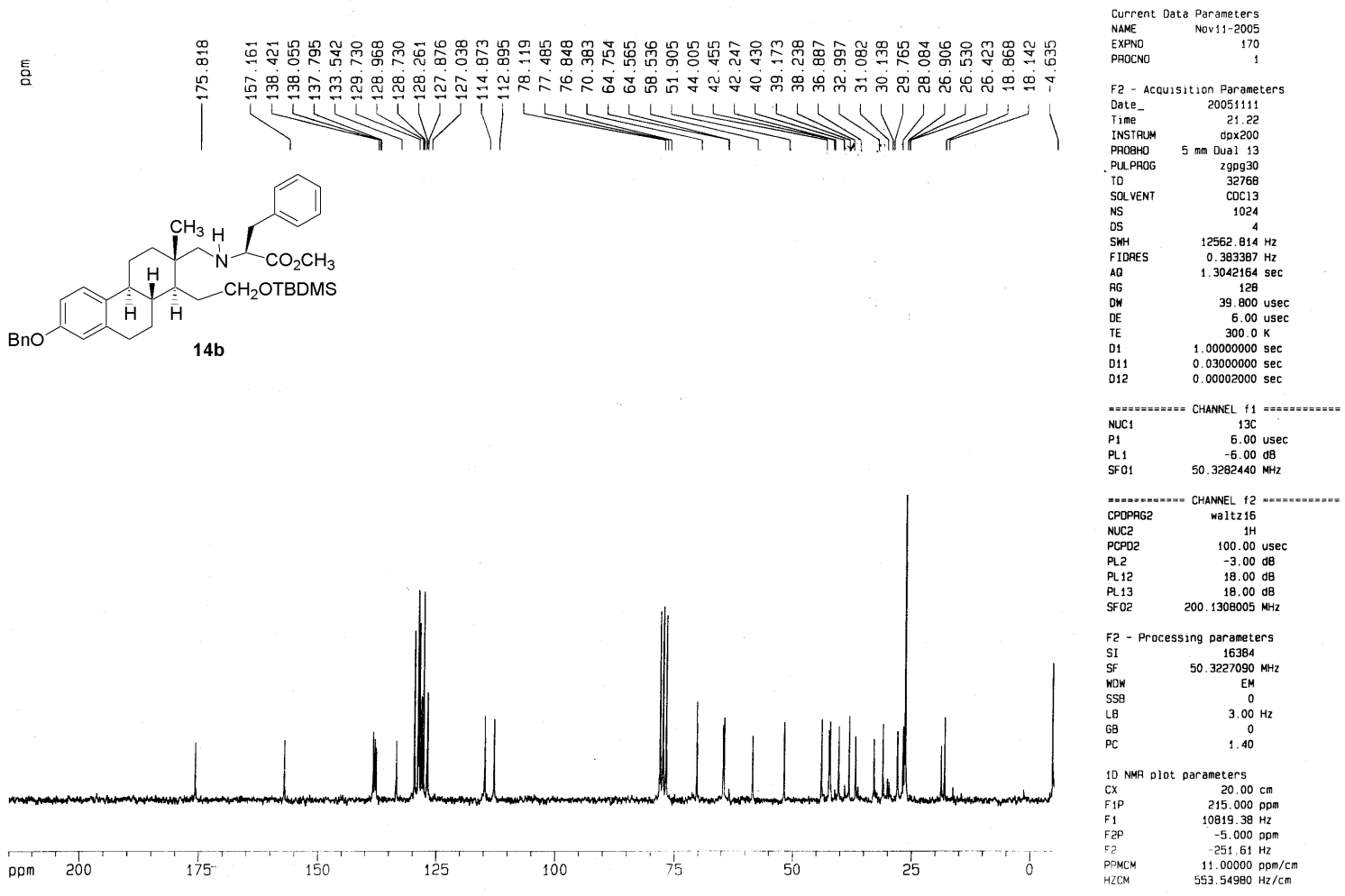


Fig. 11: ^{1}H NMR Spectrum of Amine **14b**

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PCPD2                   100.00 usec
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1D NMR plot parameters
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F1                    10819.38 Hz
F2P                      -5.000 ppm
F2                     -251.61 Hz
PPMCM                 11.00000 ppm/cm
HZCM                 553.54980 Hz/cm
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Fig. 12: ^{13}C NMR Spectrum of Amine **14b**

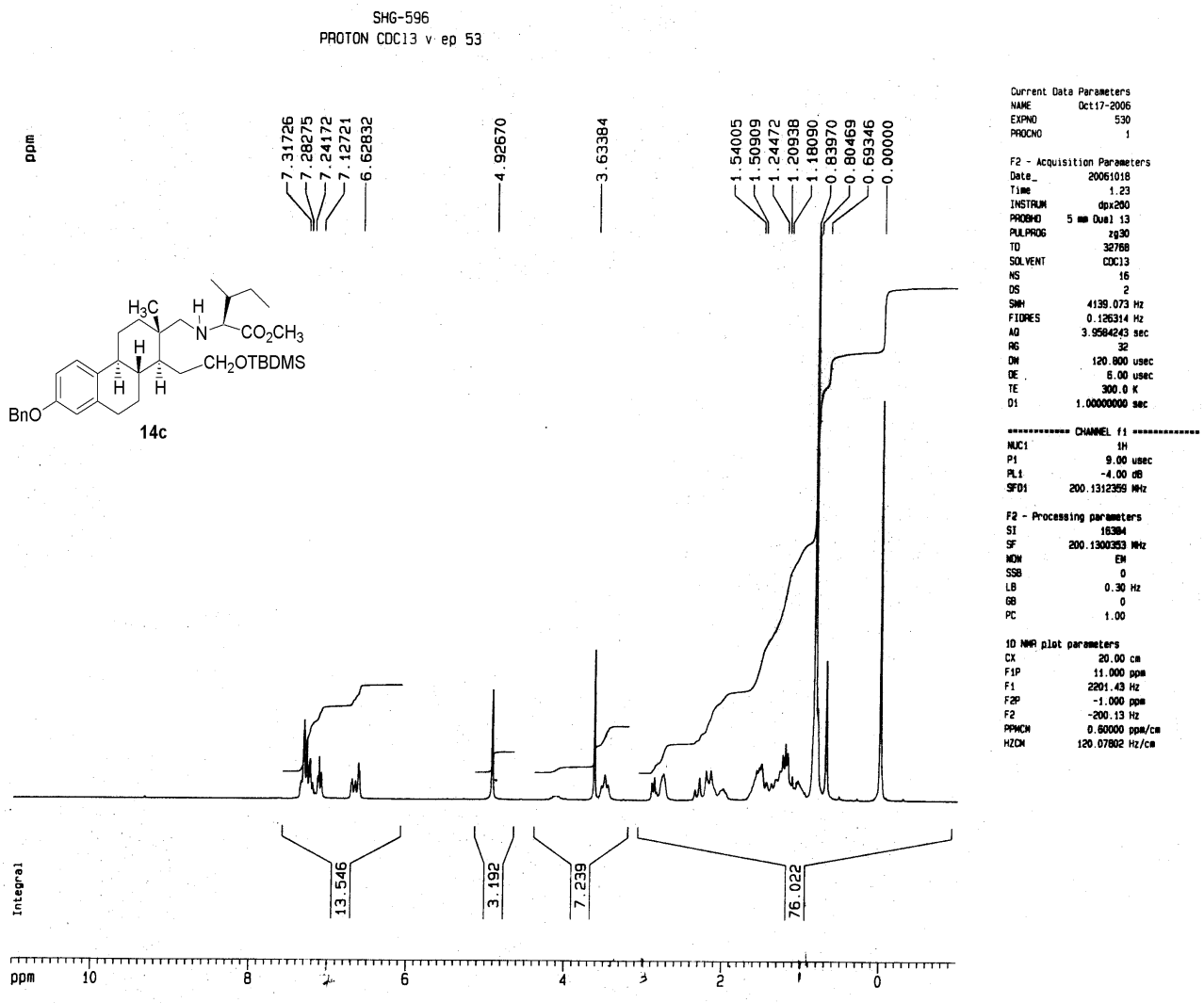


Fig. 13: ^{1}H NMR Spectrum of Amine **14c**

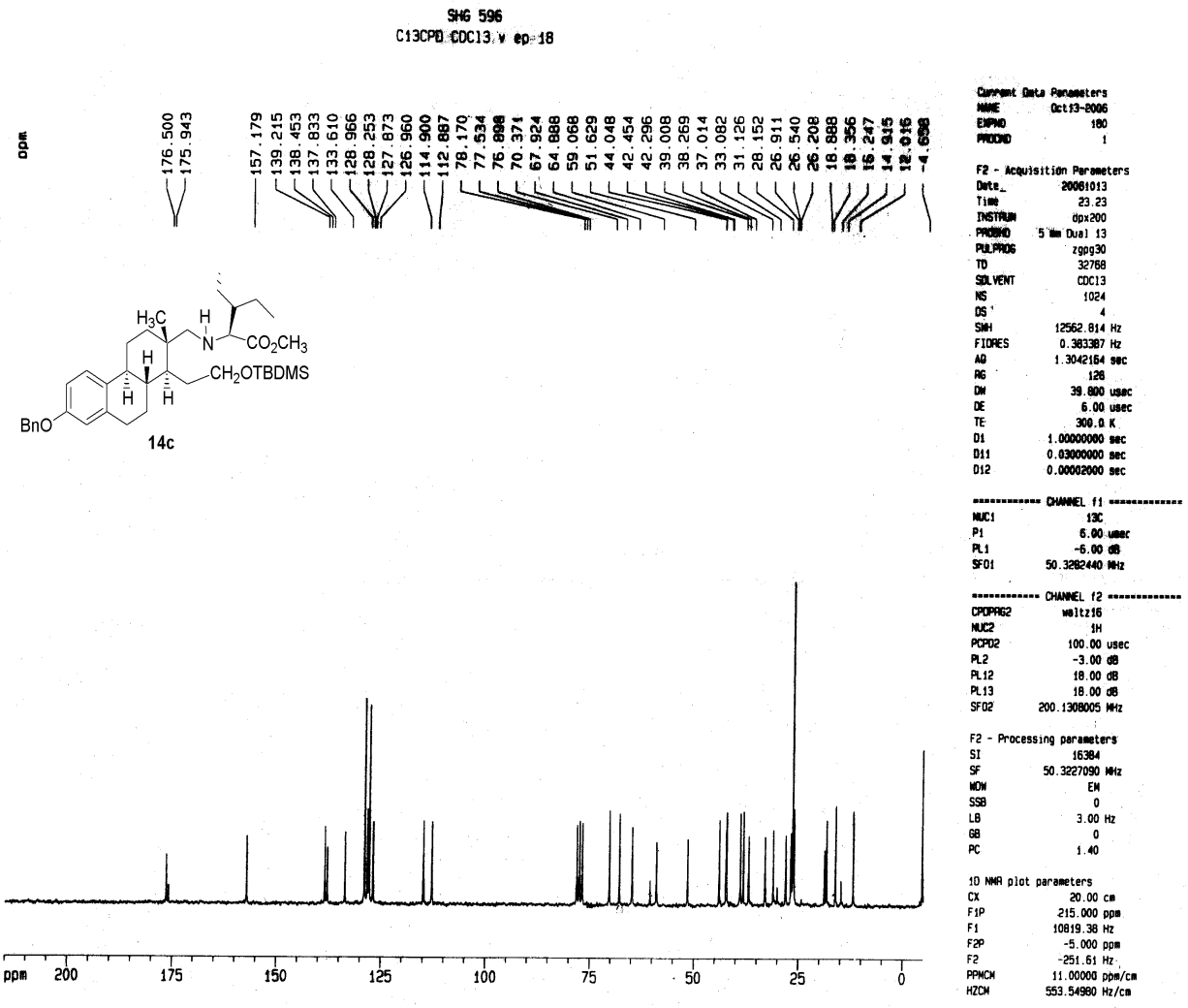


Fig. 14: ^{13}C NMR Spectrum of Amine **14c**

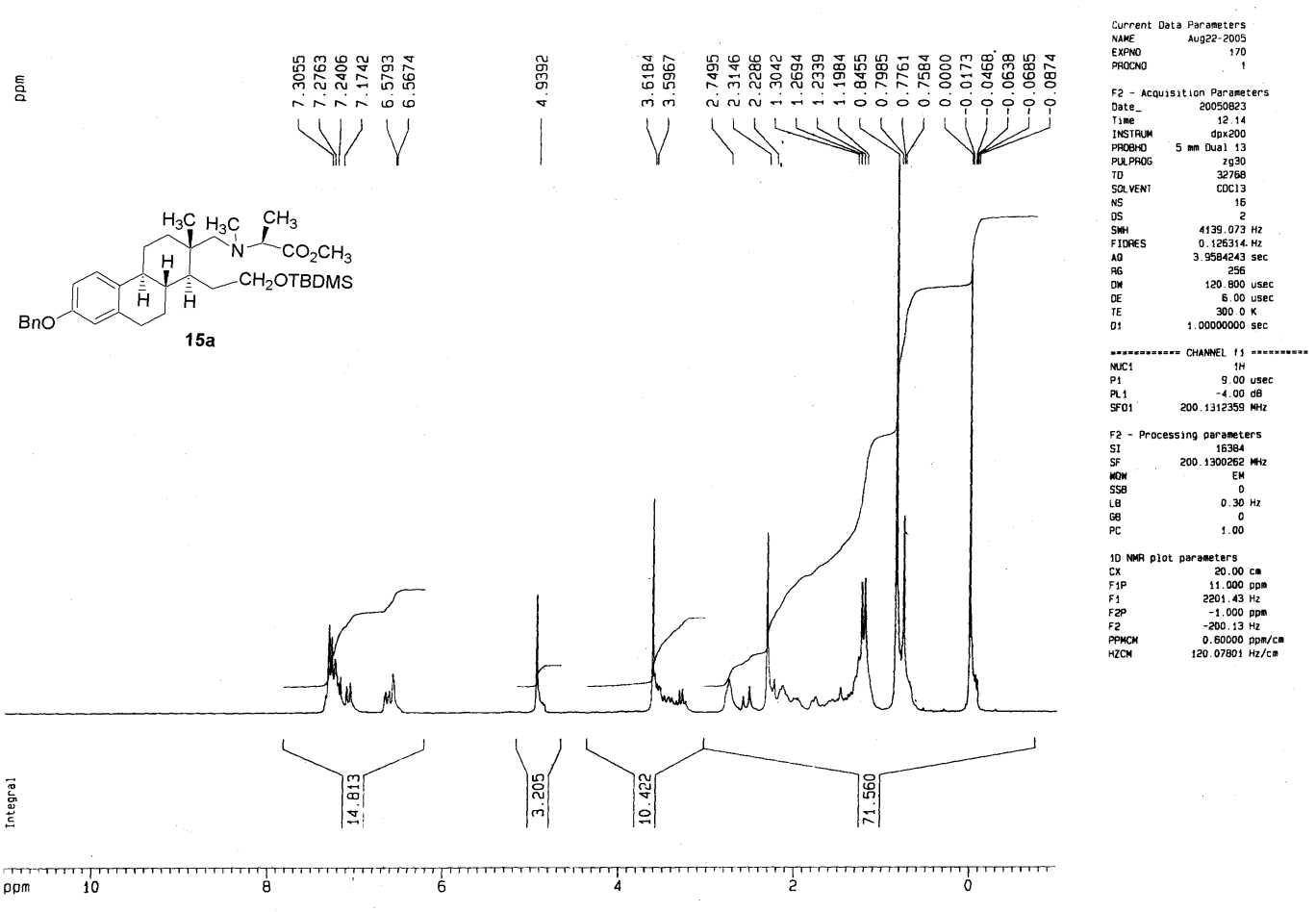


Fig. 15: ^{1}H NMR Spectrum of *N*-Methyl Amine Derivative **15a**

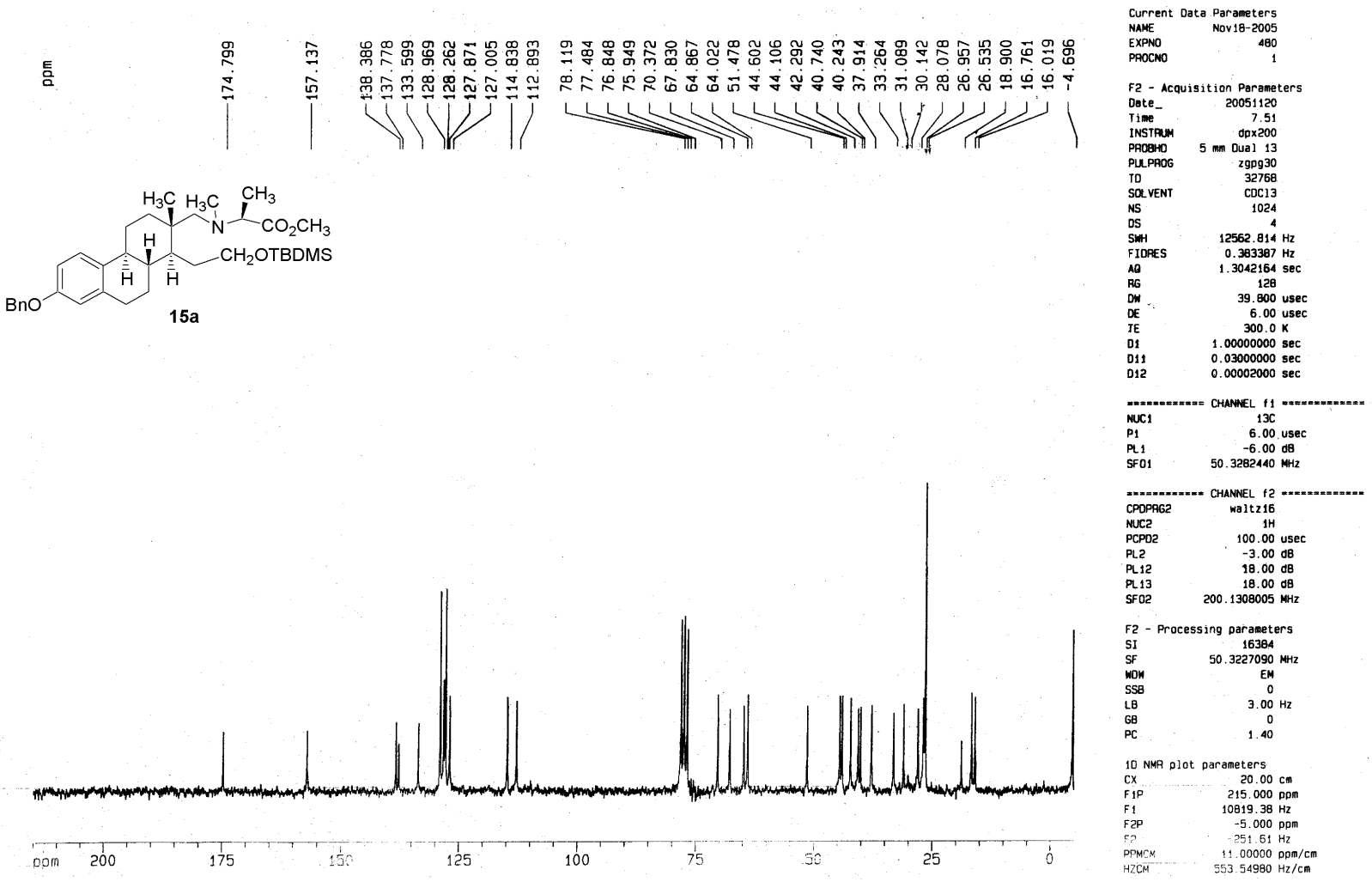
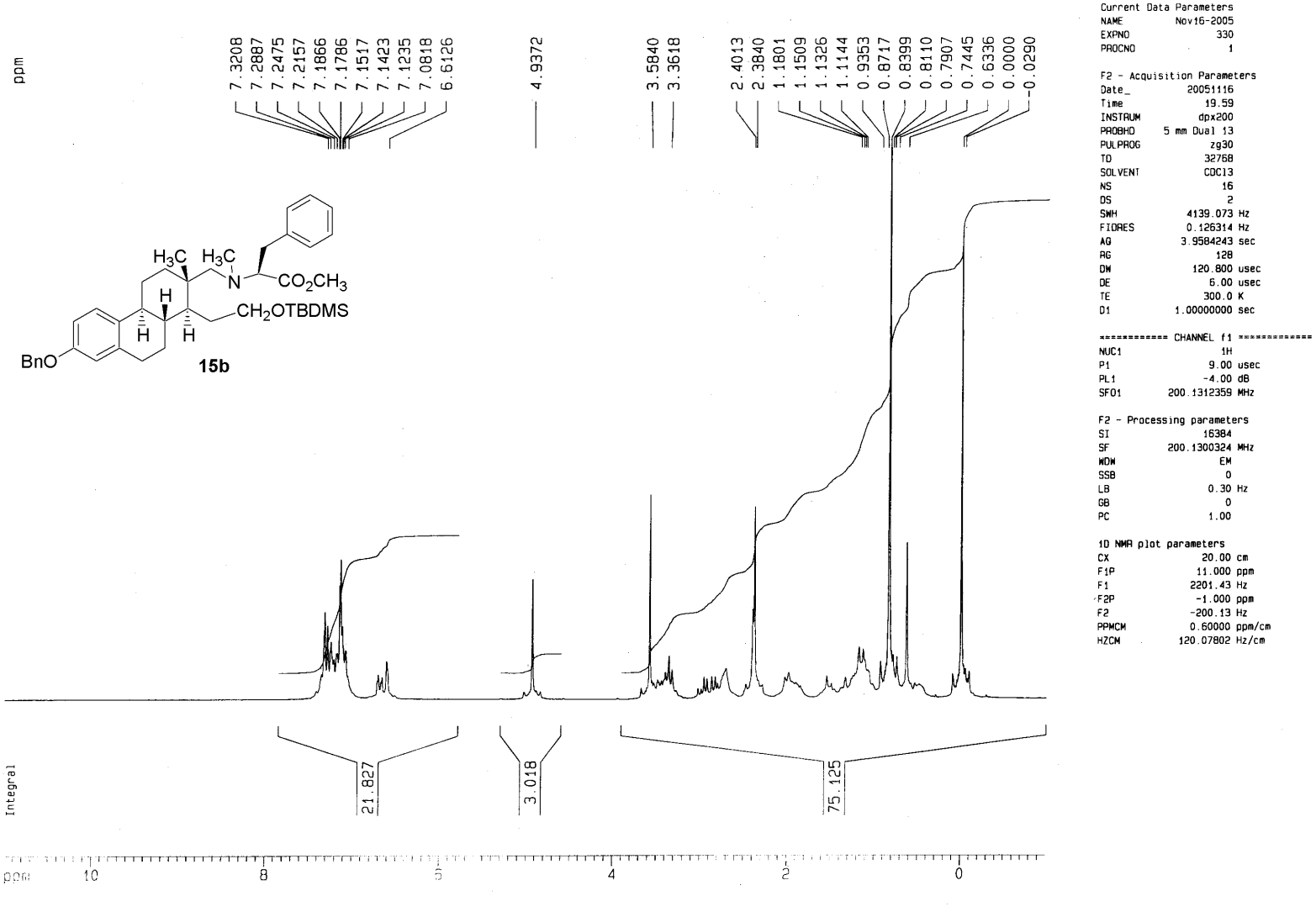


Fig. 16: ^{13}C NMR Spectrum of *N*-Methyl Amine Derivative **15a**

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RG                   128
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DE                  6.00 usec
TE                 300.0 K
D1              1.00000000 sec

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PL1               -4.00 dB
SFO1          200.1312359 MHz

F2 - Processing parameters
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SSB                    0
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1D NMR plot parameters
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F2              -200.13 Hz
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Fig. 17: ^{1}H NMR Spectrum of *N*-Methyl Amine Derivative **15b**

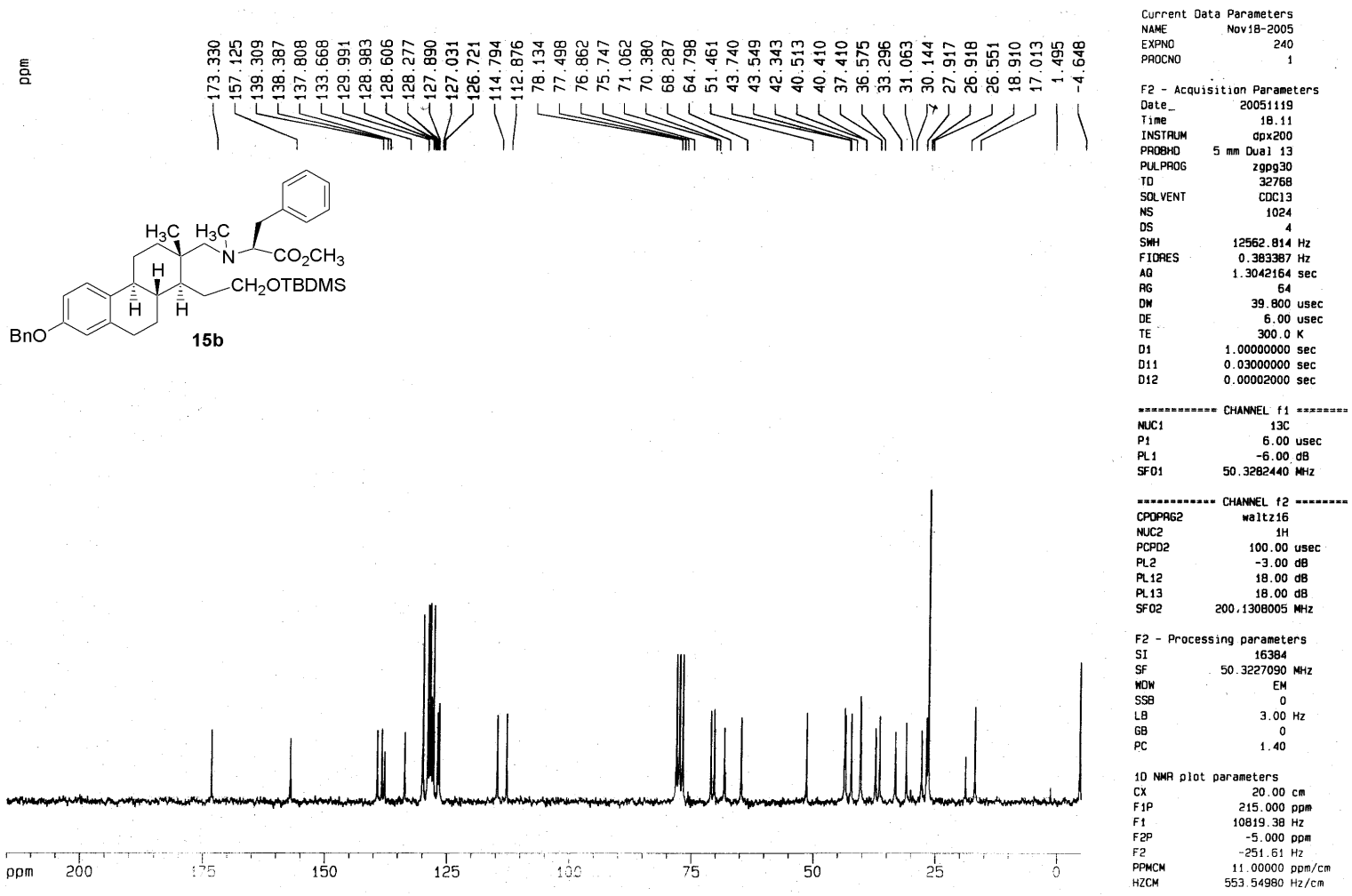


Fig. 18: ^{13}C NMR Spectrum of *N*-Methyl Amine Derivative **15b**

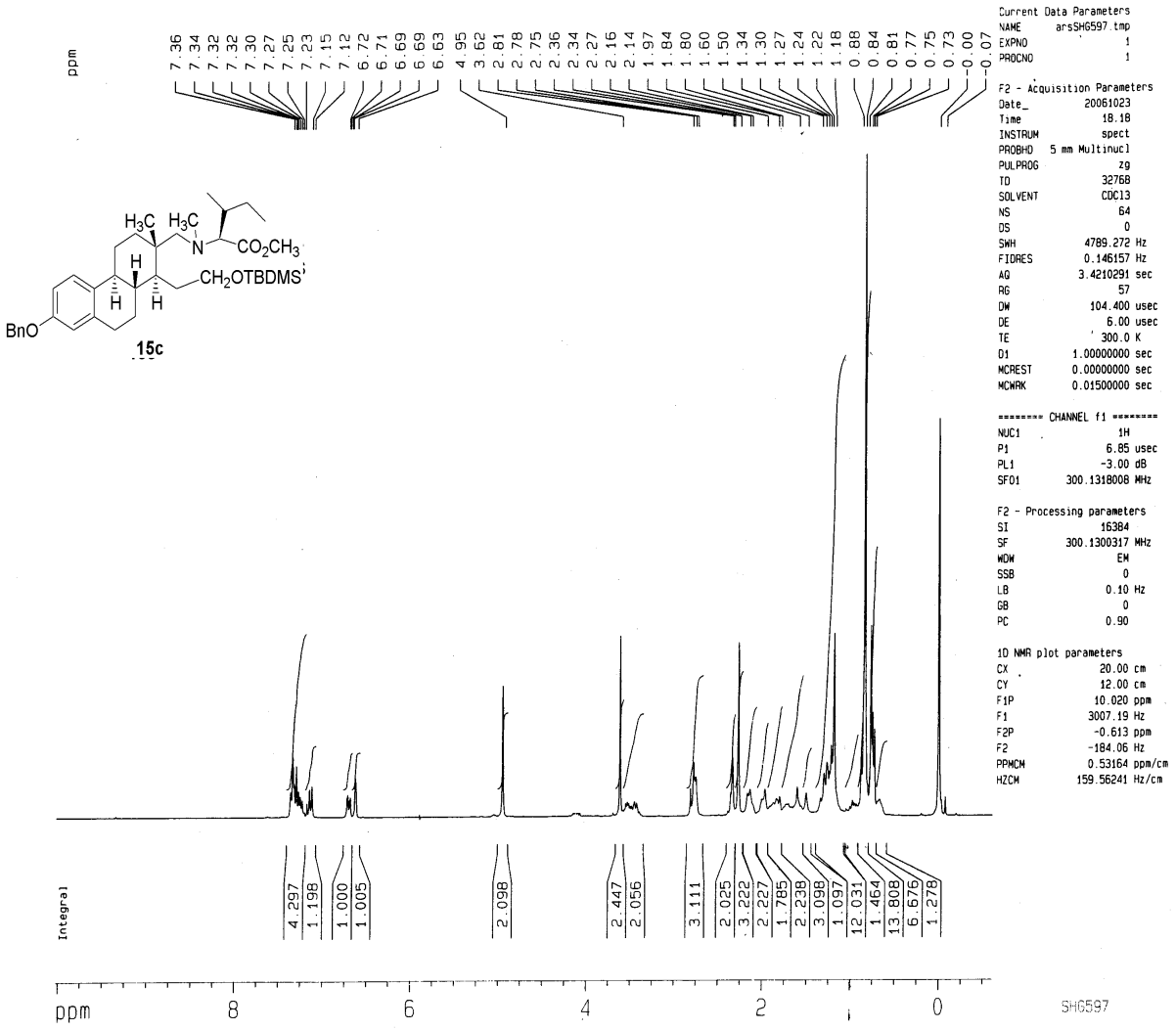


Fig. 19: ^{1}H NMR Spectrum of *N*-Methyl Amine Derivative **15c**

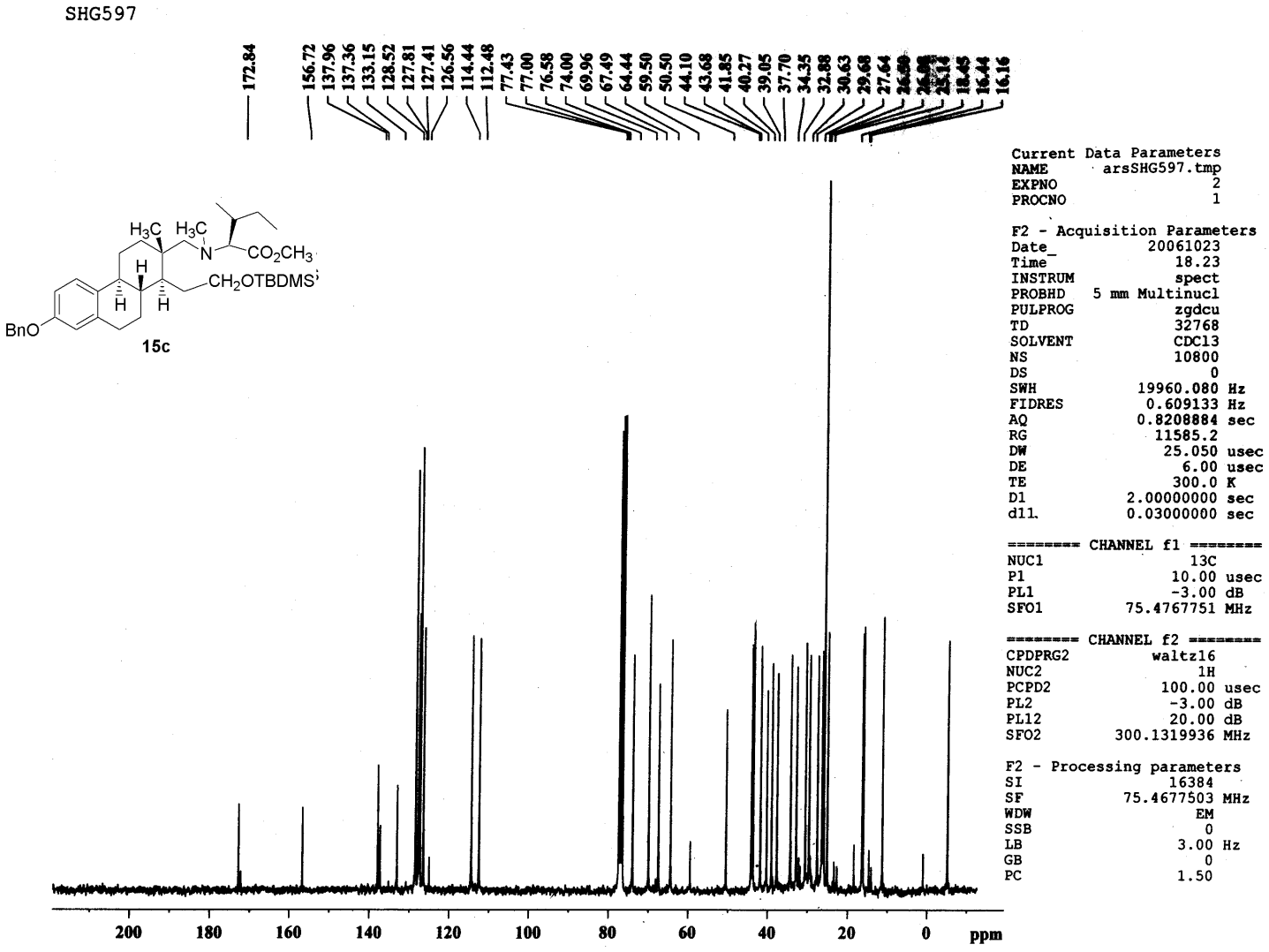


Fig. 20: ^{13}C NMR Spectrum of *N*-Methyl Amine Derivative **15c**

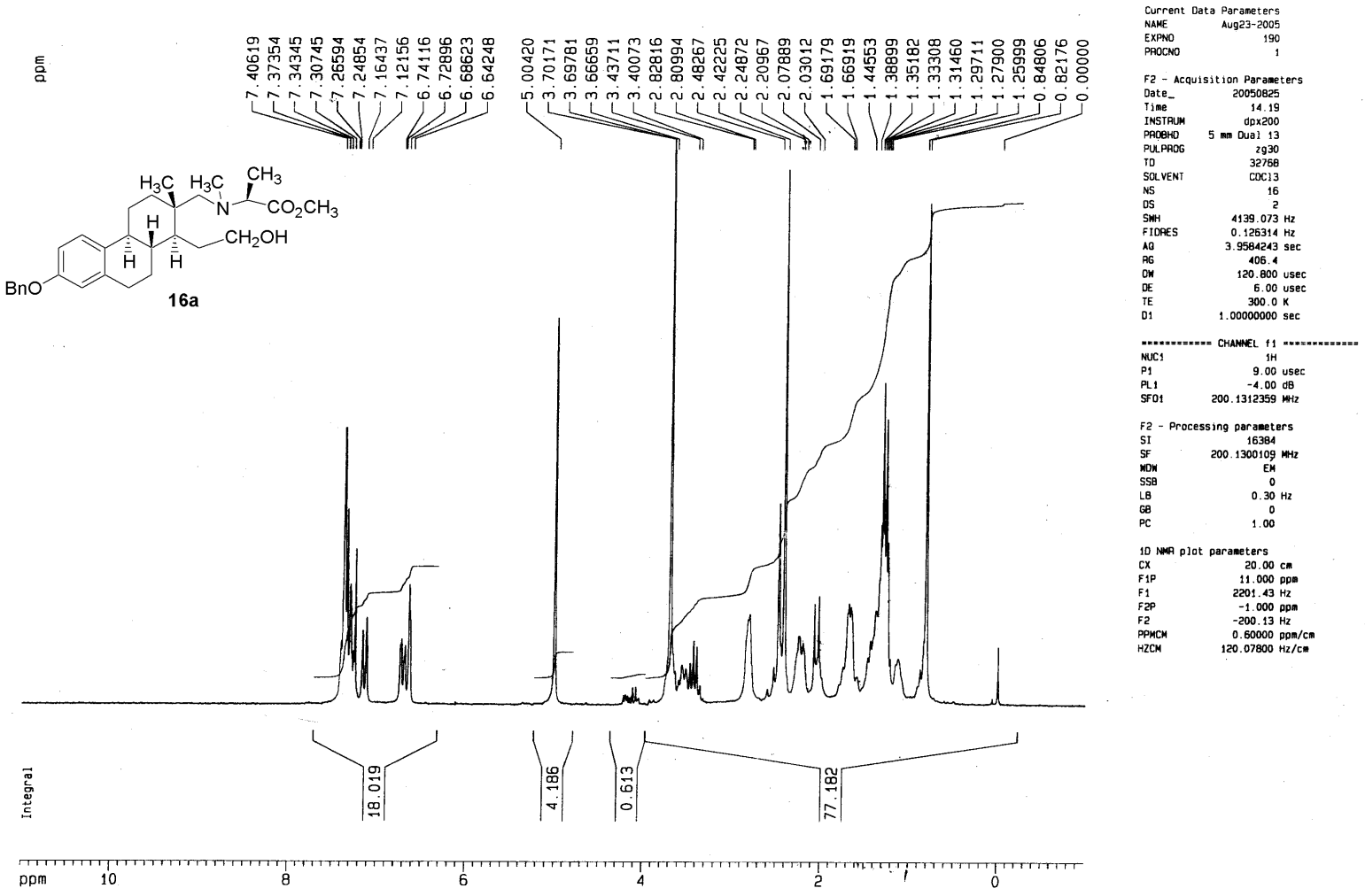


Fig. 21: ^{1}H NMR Spectrum of Alcohol **16a**

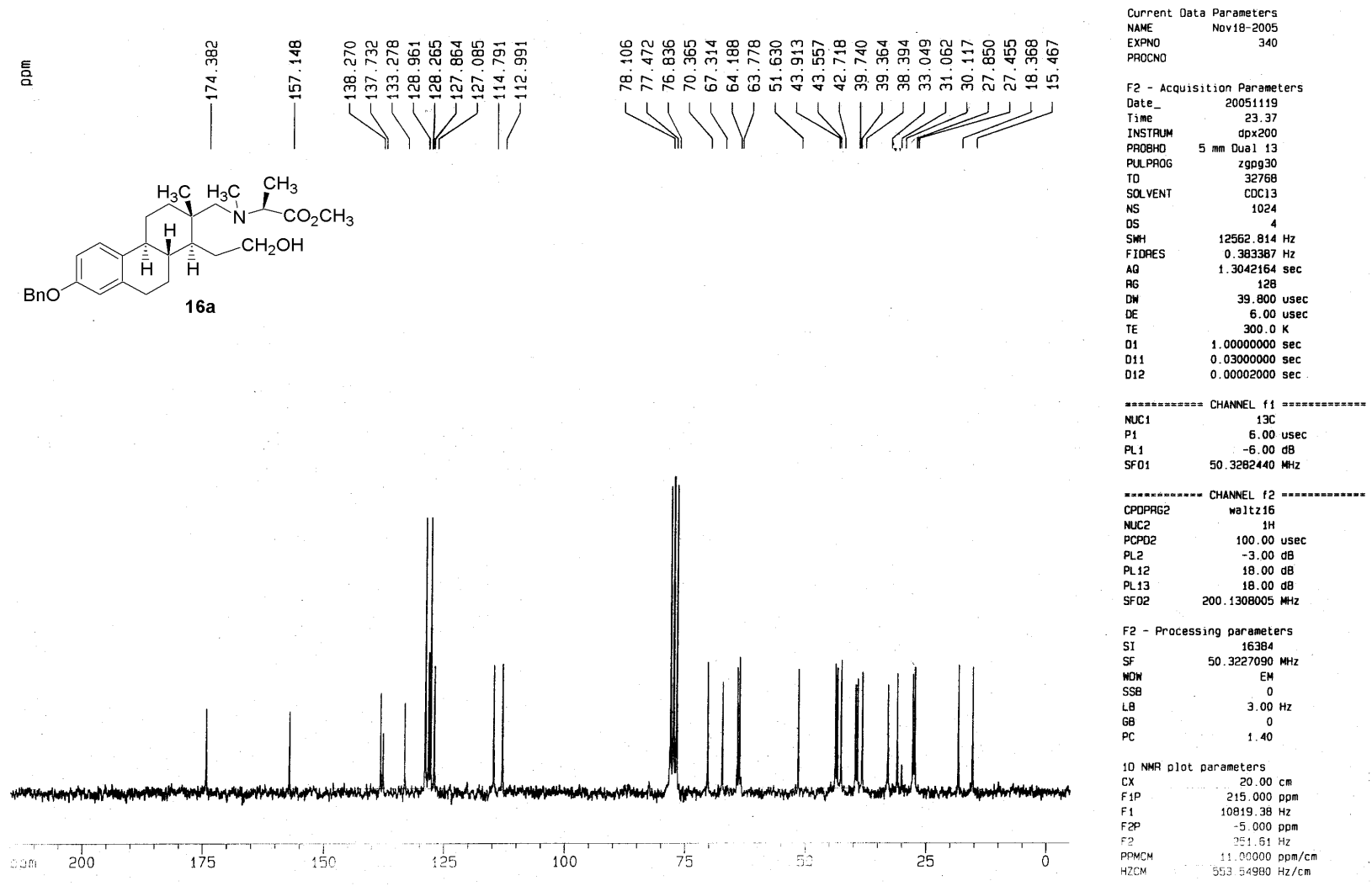
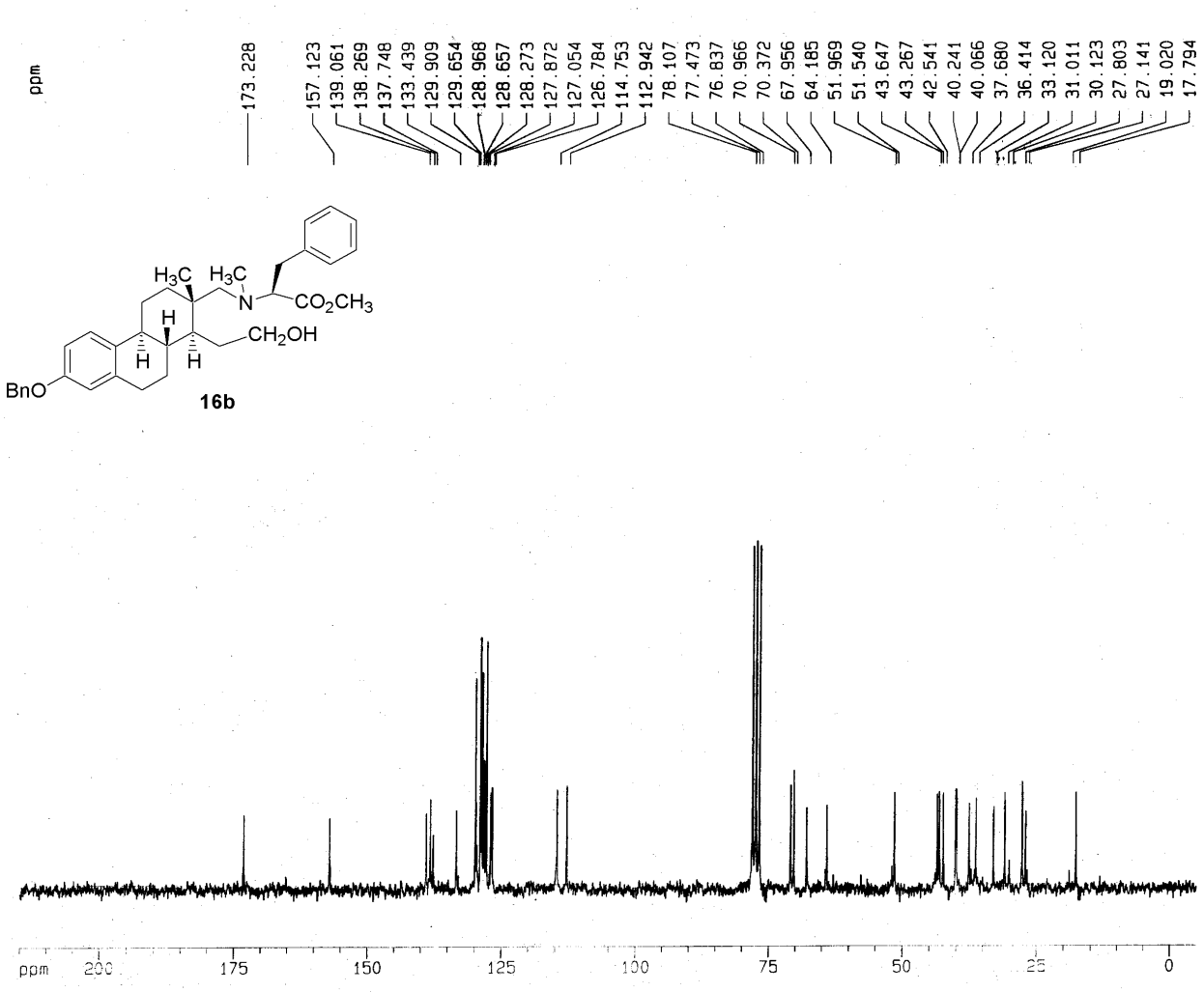


Fig. 22: ^{13}C NMR Spectrum of Alcohol **16a**



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RG	64
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TE	300.0 K
D1	1.00000000 sec
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D12	0.00002000 sec

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NUC1	13C
P1	6.00 usec
PL1	-6.00 dB
SFO1	50.3282440 MHz

========== CHANNEL f2 ==========

CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	-3.00 dB
PL12	18.00 dB
PL13	18.00 dB
SFO2	200.1308005 MHz

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1D NMR plot parameters

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F1P	215.000 ppm
F1	10819.38 Hz
F2P	-5.000 ppm
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HZCM	553.54980 Hz/

Fig. 23: ^{13}C NMR Spectrum of Alcohol **16b**

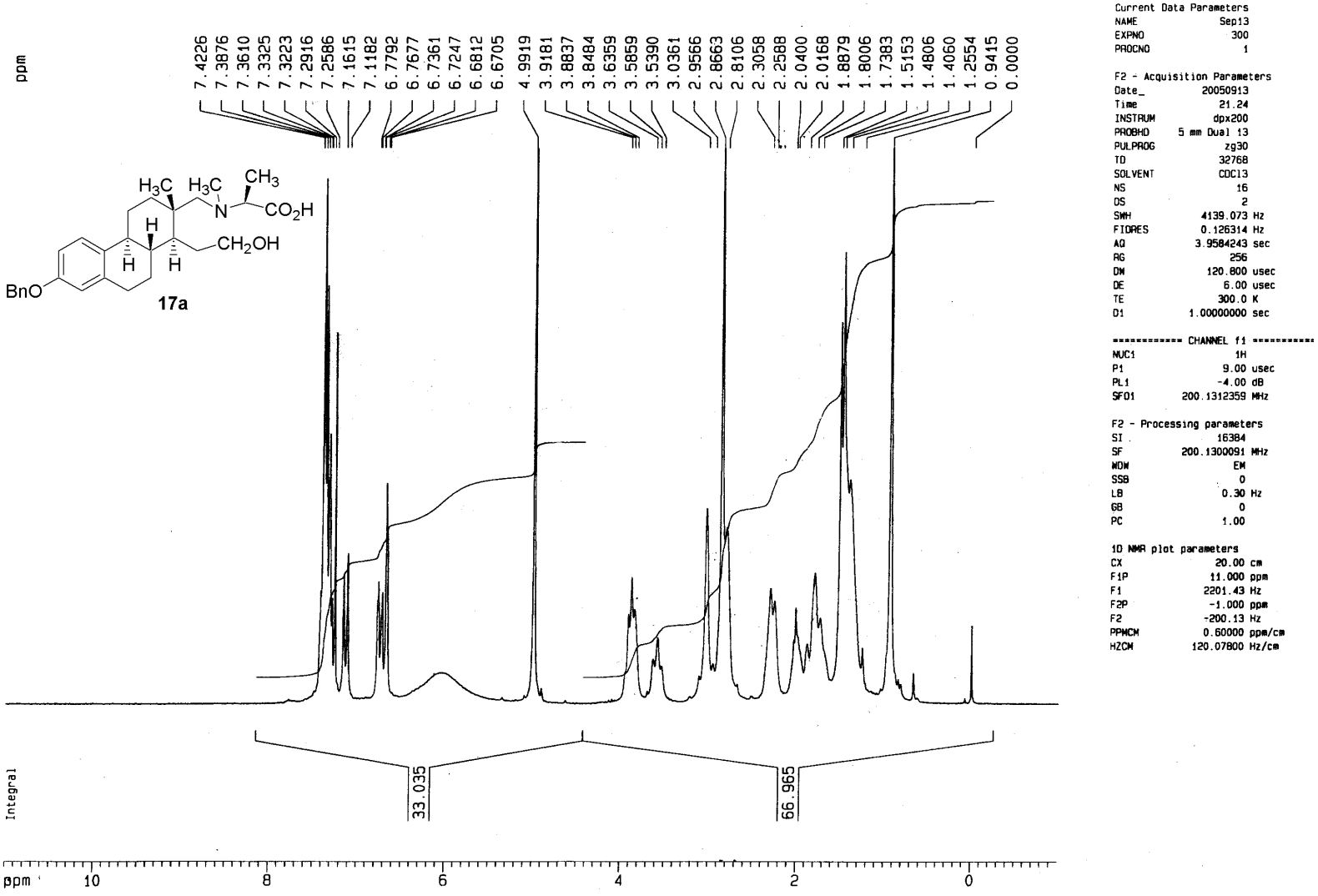


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Fig. 24: ^{1}H NMR Spectrum of Hydroxy Acid **17a**

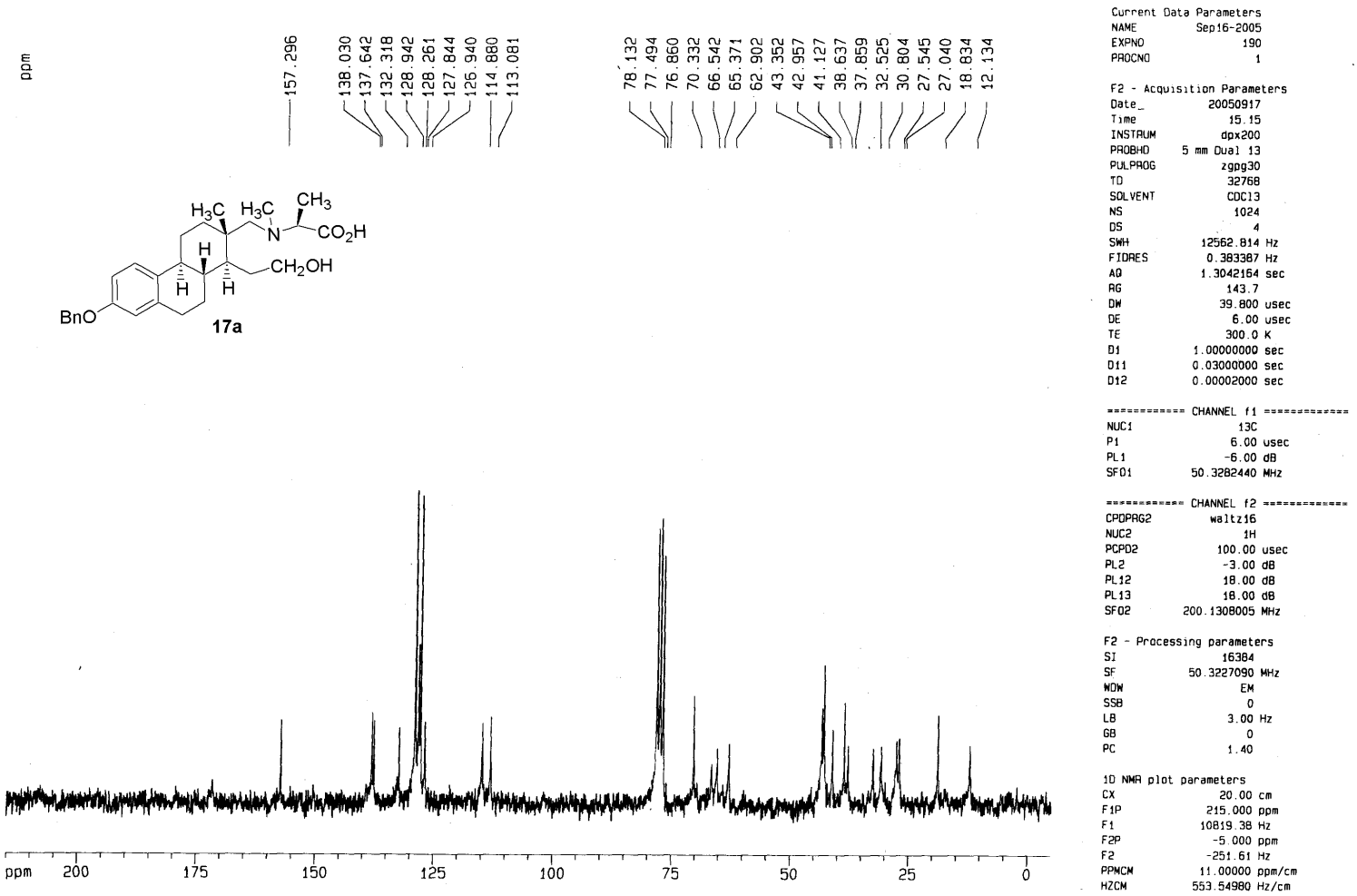

Fig. 25: ^{13}C NMR Spectrum of Hydroxy Acid **17a**

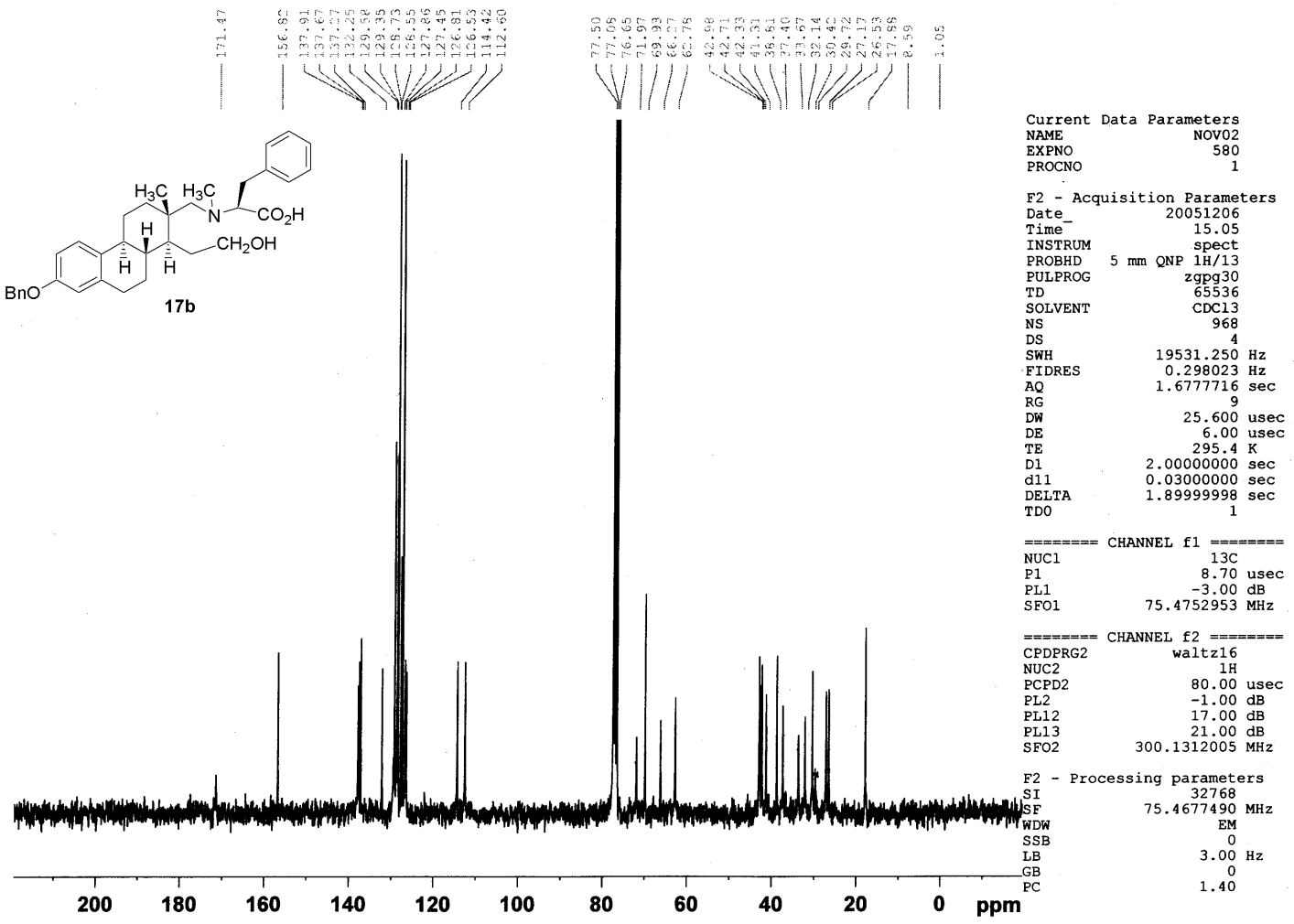

Fig. 26: ^{13}C NMR Spectrum of Hydroxy Acid **17b**

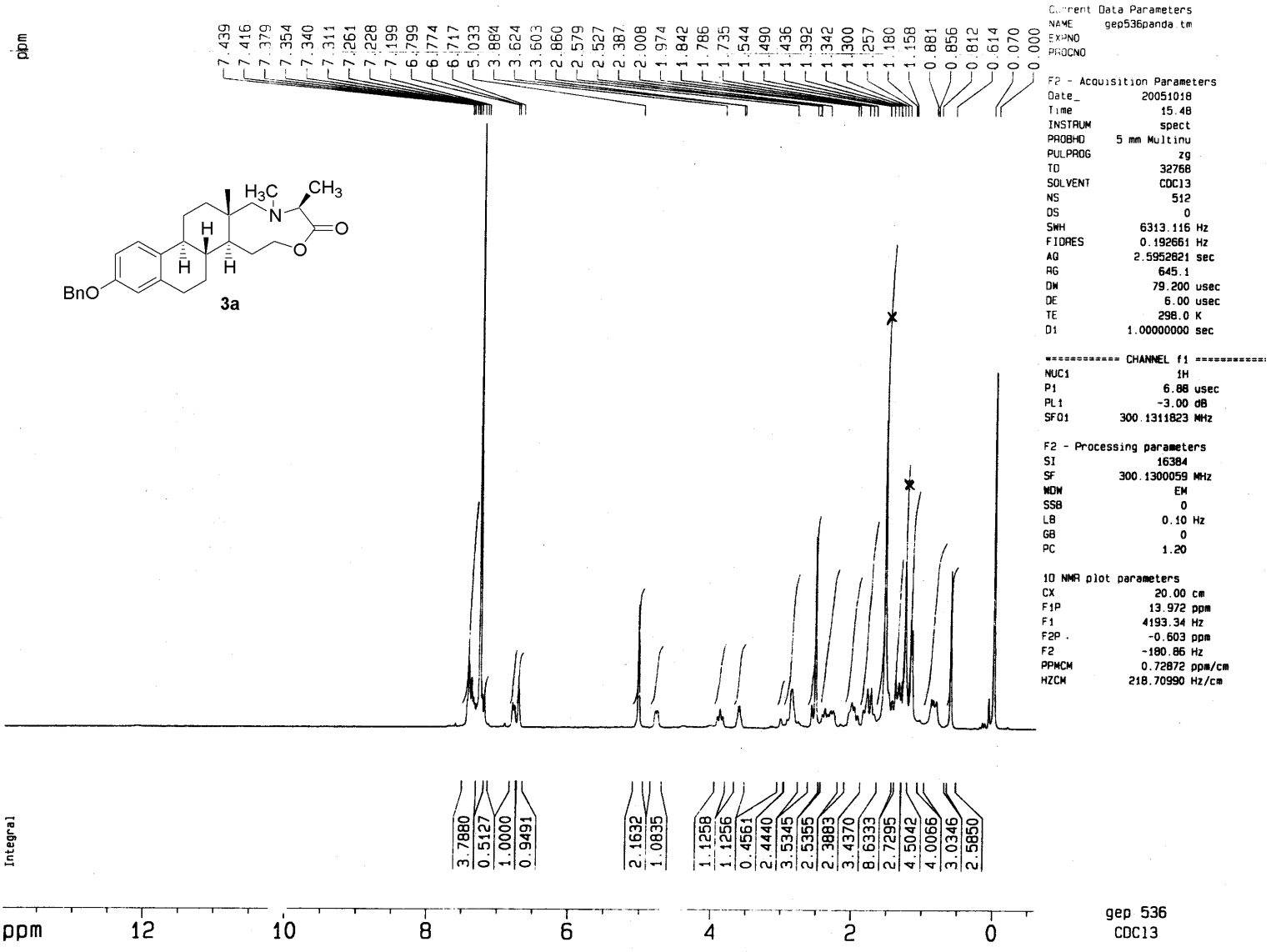

Fig. 27: ^{1}H NMR Spectrum of Lactone **3a**

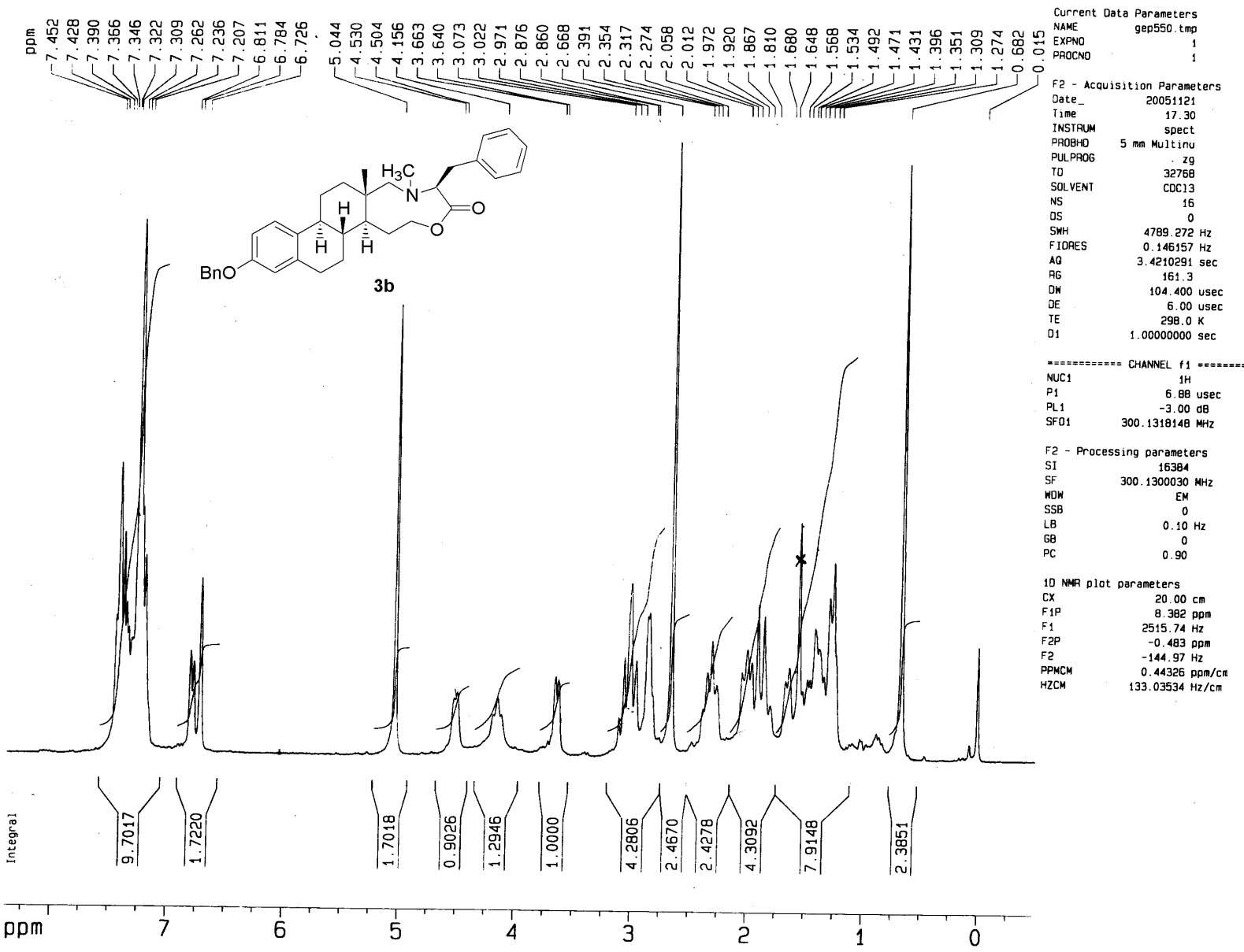

Fig. 28: ^{1}H NMR Spectrum of Lactone **3b**

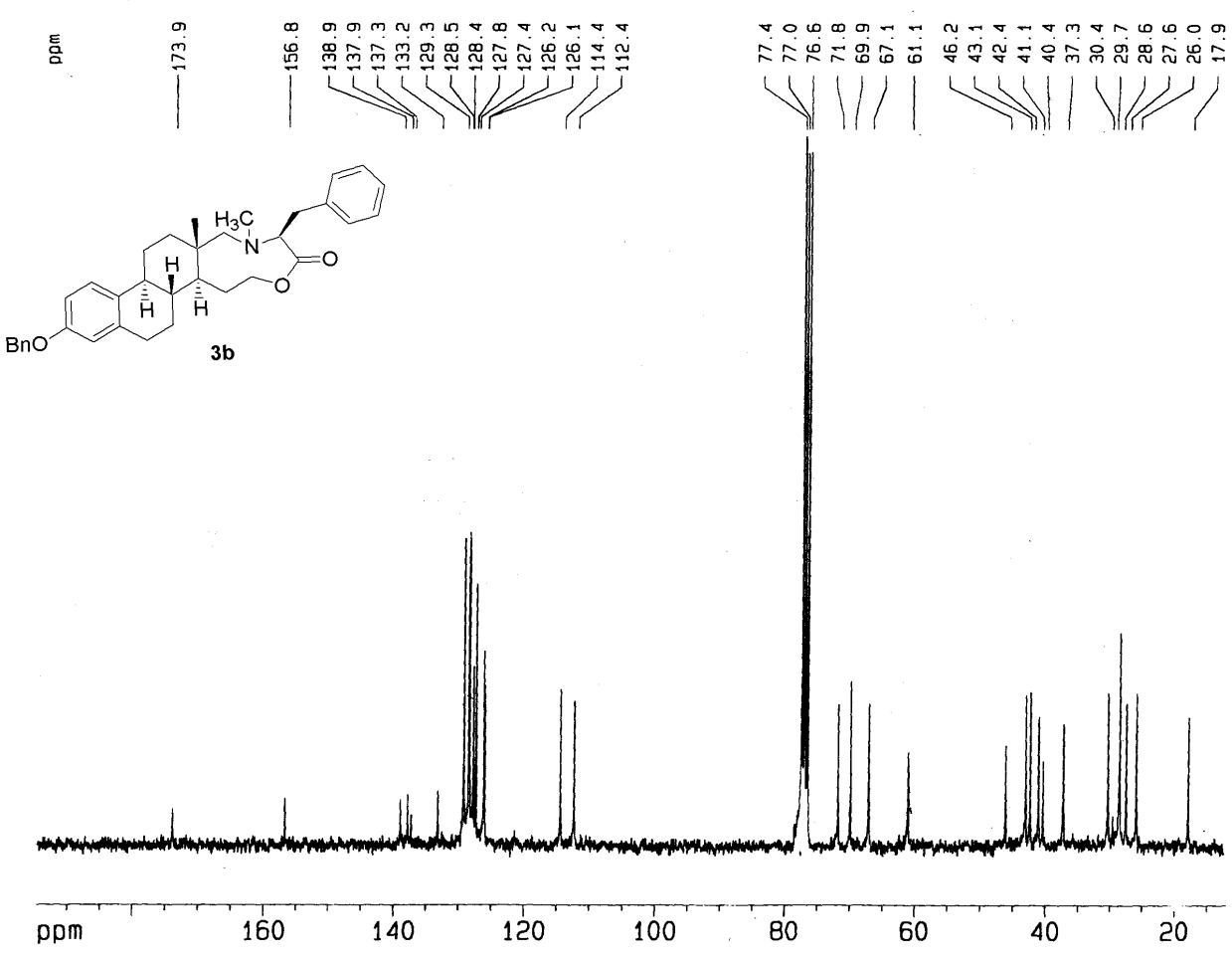

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Fig. 29: ^{13}C NMR Spectrum of Lactone **3b**

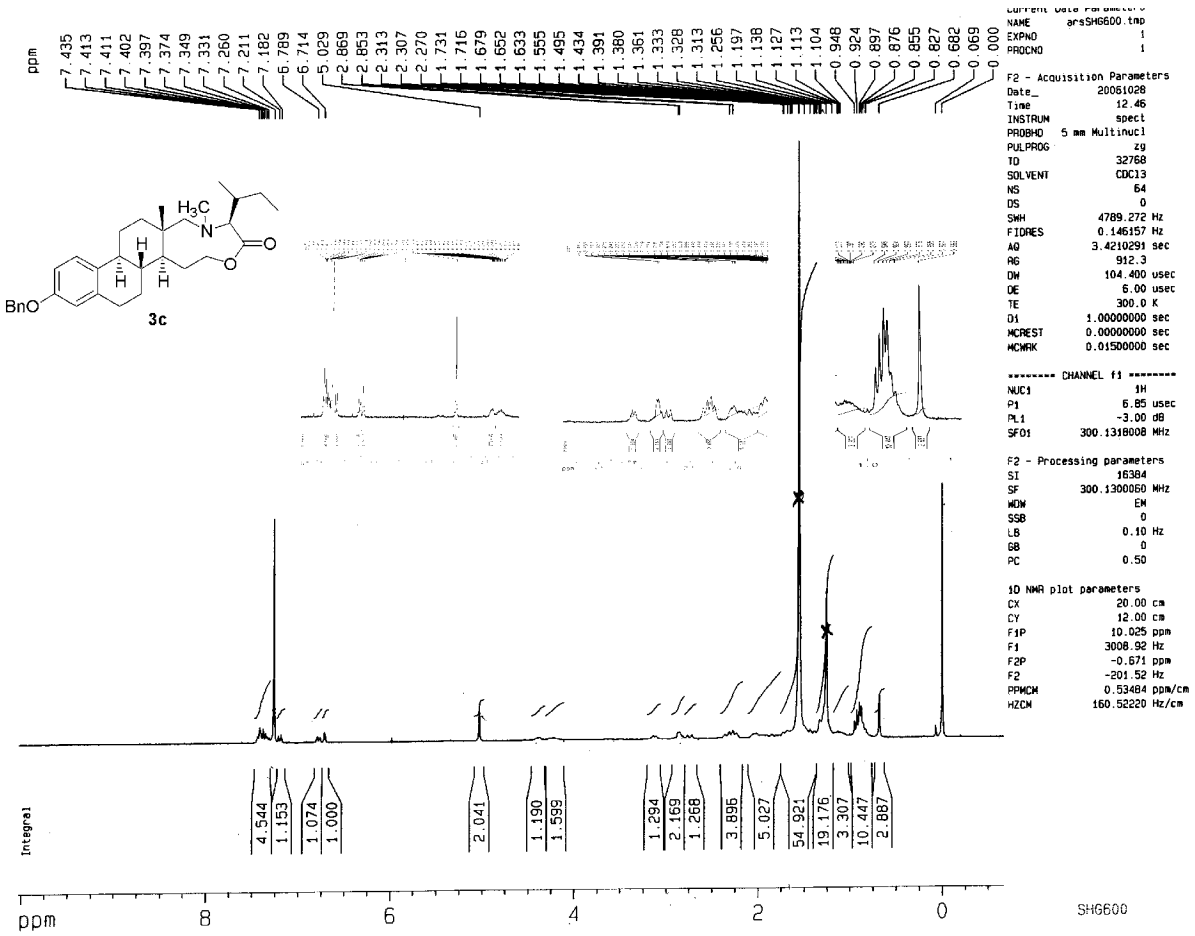

Fig. 33: ^{1}H NMR Spectrum of Lactone **3c**

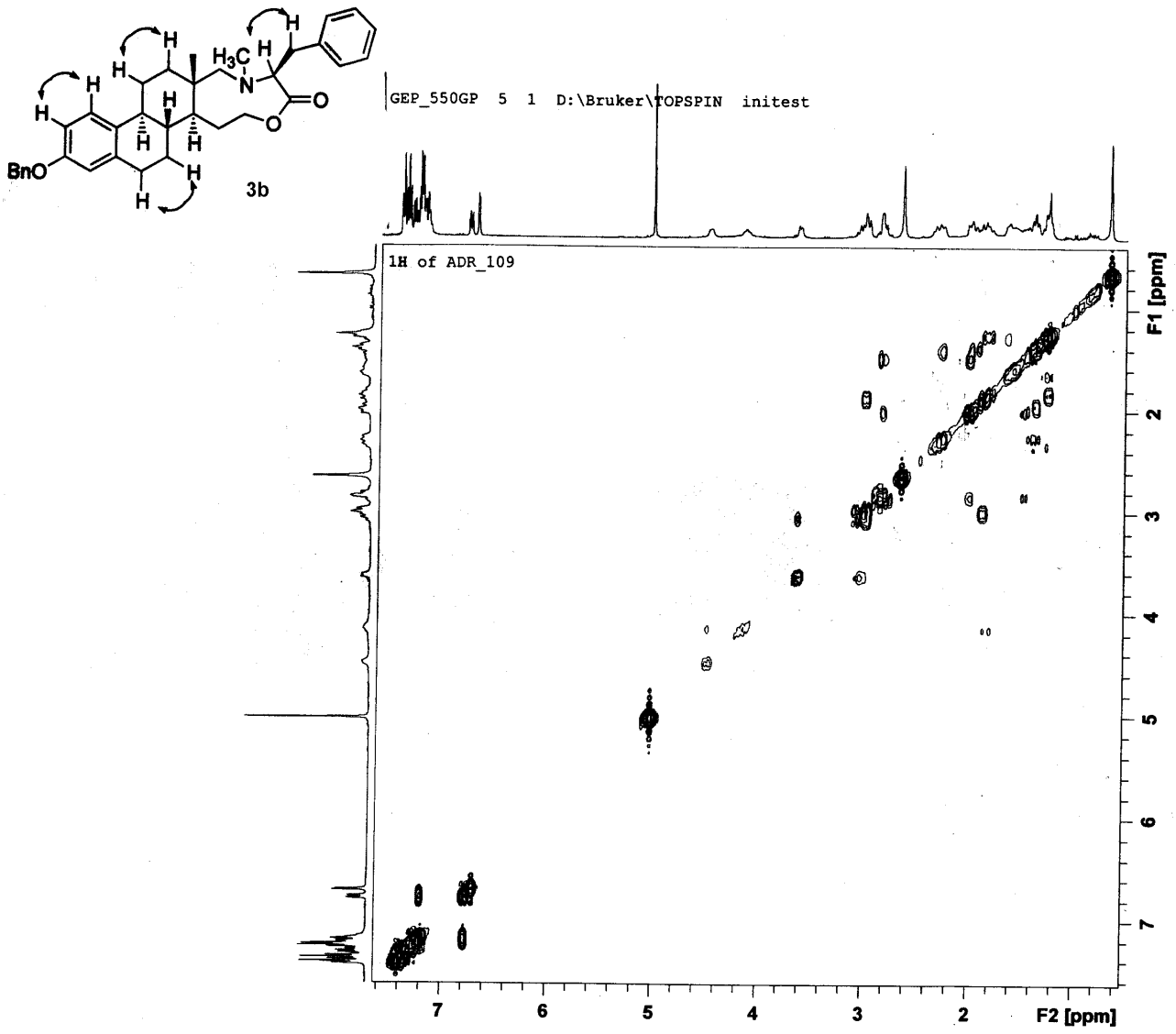

Fig. 30: ^{1}H-^{1}H COSY Spectrum of Lactone **3b**

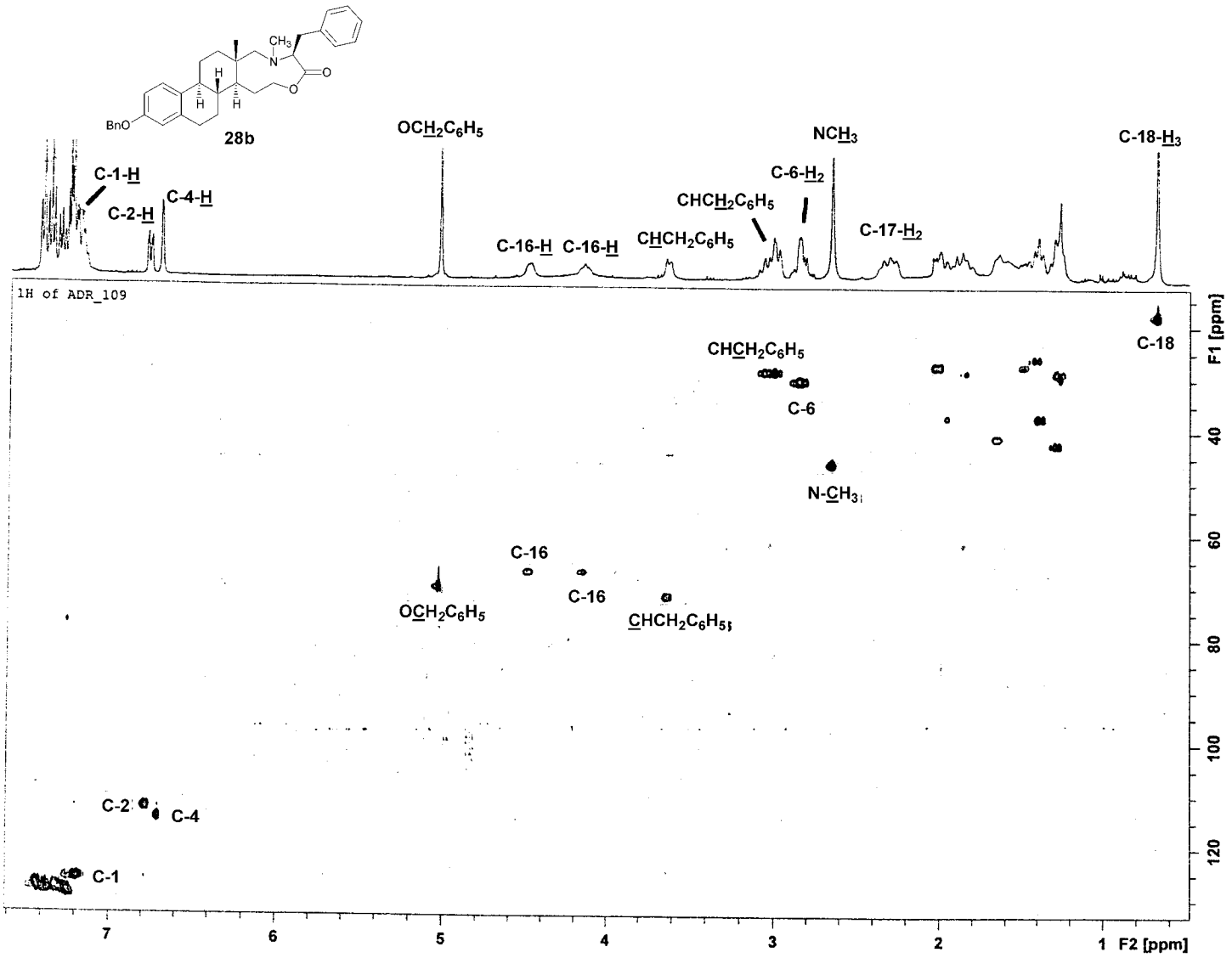

Fig. 31: 2-D HSQC Spectrum of Lactone **3b**

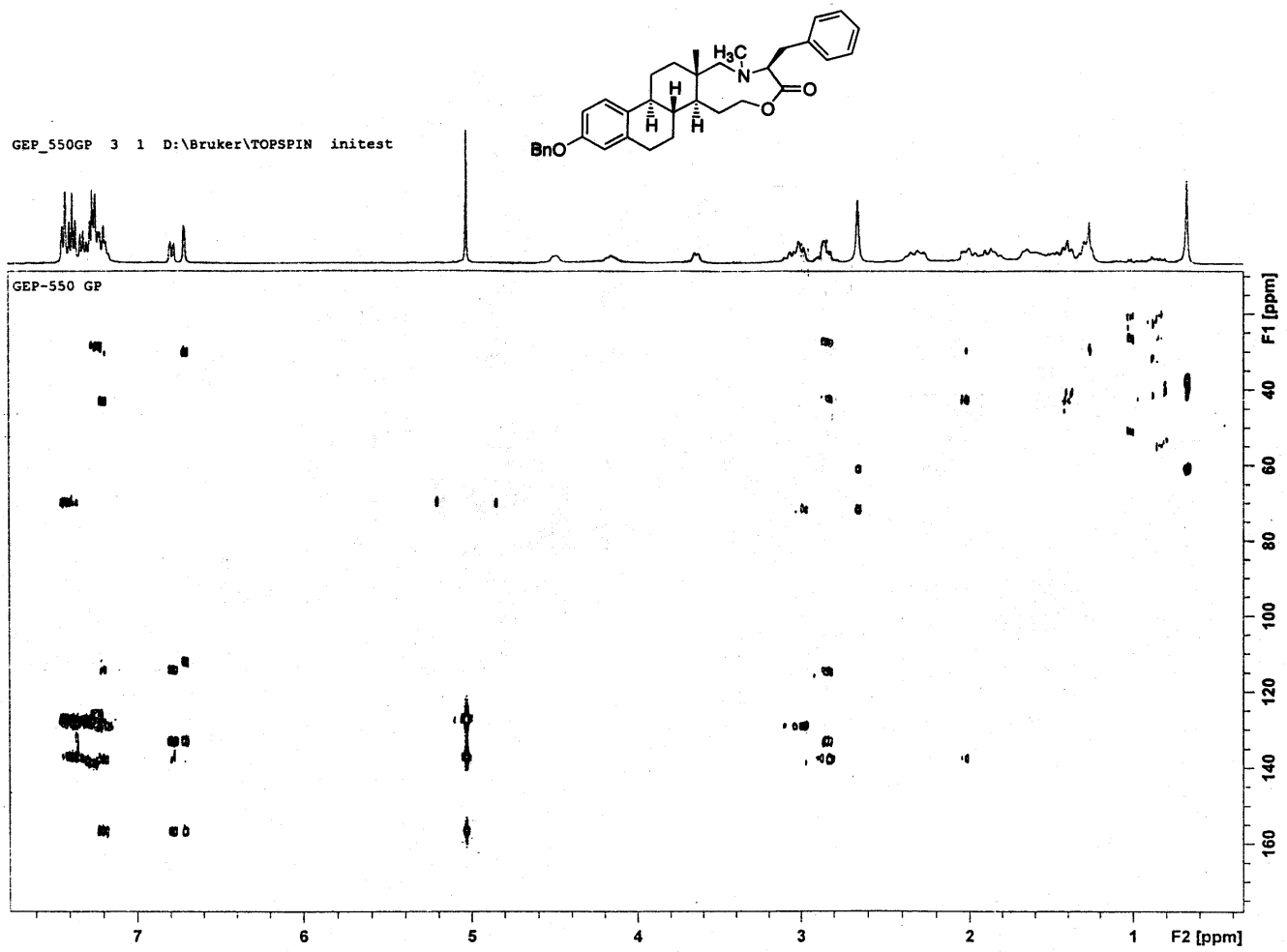

Fig. 32: 2-D HMBC Spectrum of Lactone **3b**