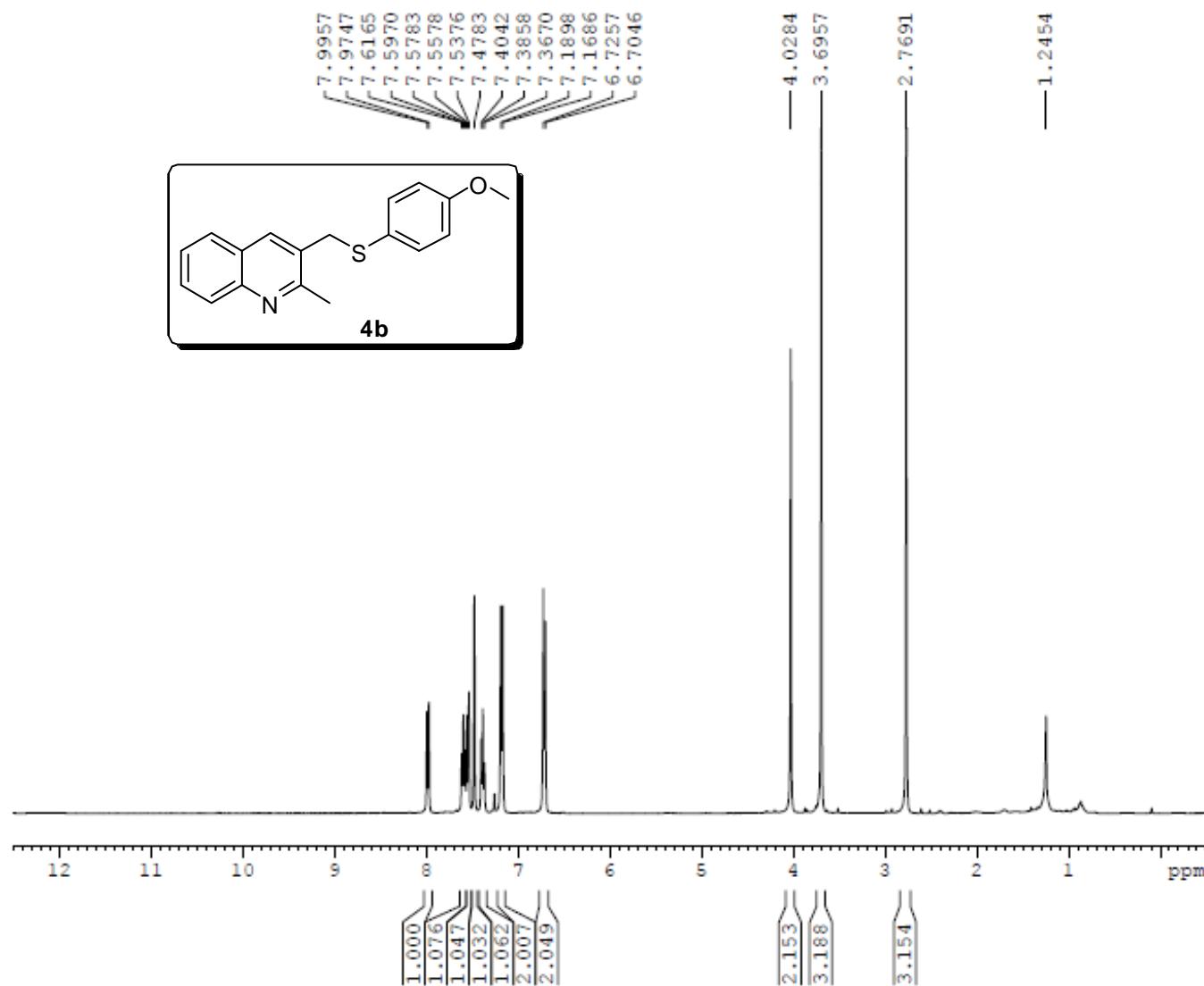


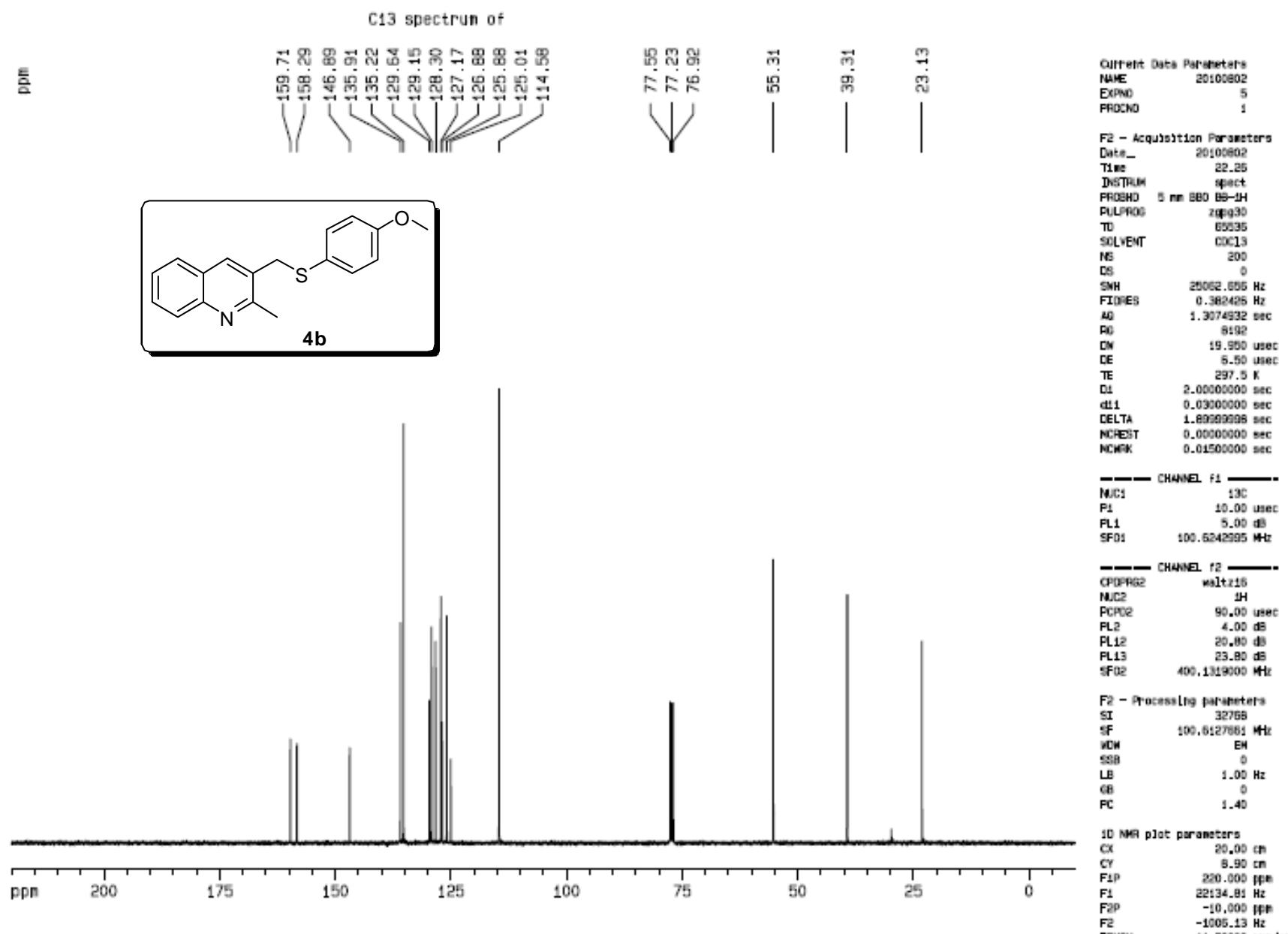
¹H spectrum of

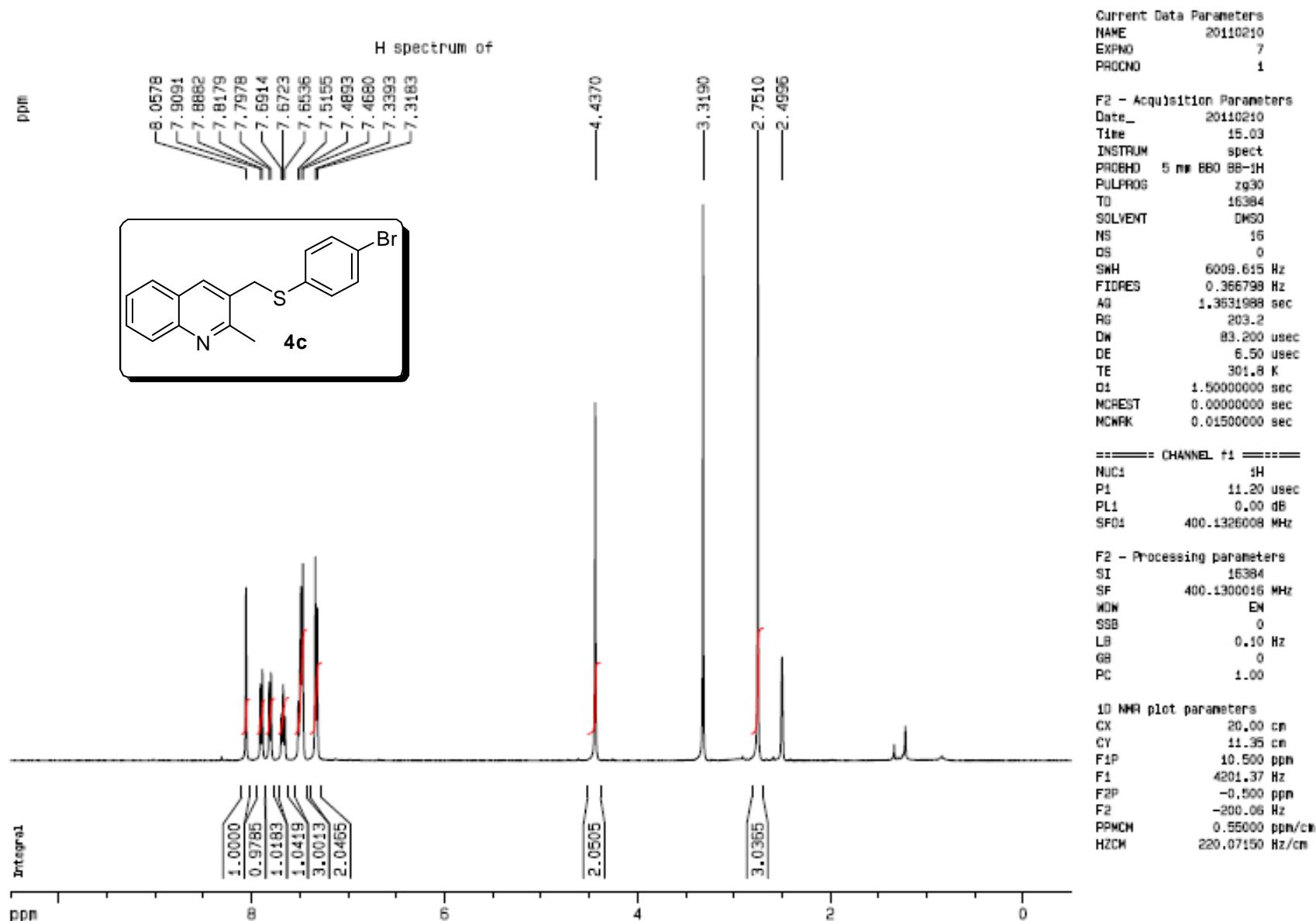
Current Data Parameters
NAME 20100725
EXPNO 2
PROCNO 1

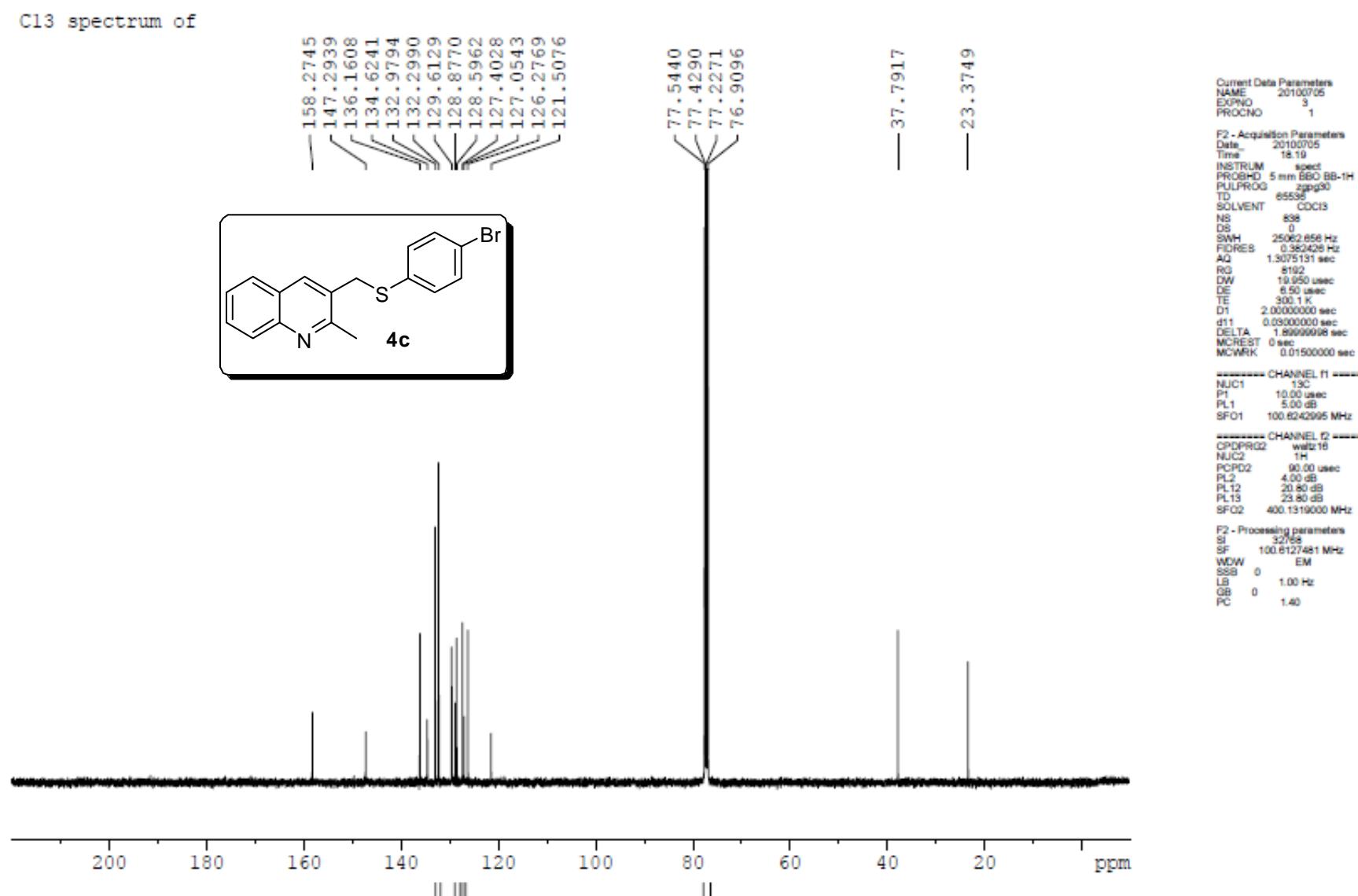
F2 - Acquisition Parameters
Date 20100725
Time 23.17
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl₃
NS 16
DS 0
SWH 6009.615 Hz
FIDRES 0.366798 Hz
AQ 1.3632820 sec
RG 28.5
DW 83.200 usec
DE 6.50 usec
TE 298.4 K
D1 1.5000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec

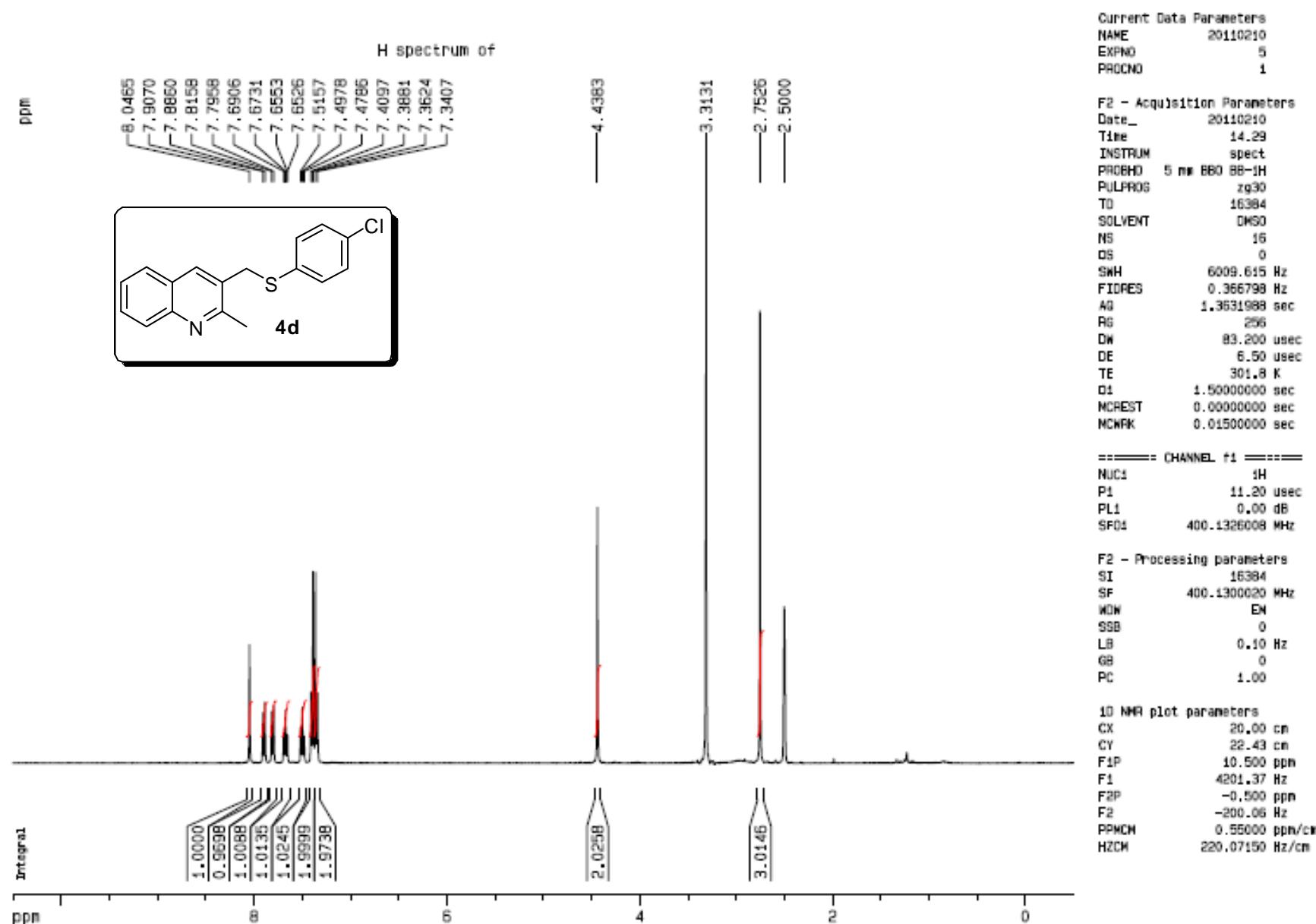
CHANNEL 11
NUC1 ¹H
P1 14.50 usec
PL1 5.20 dB
SFO1 400.1326008 MHz

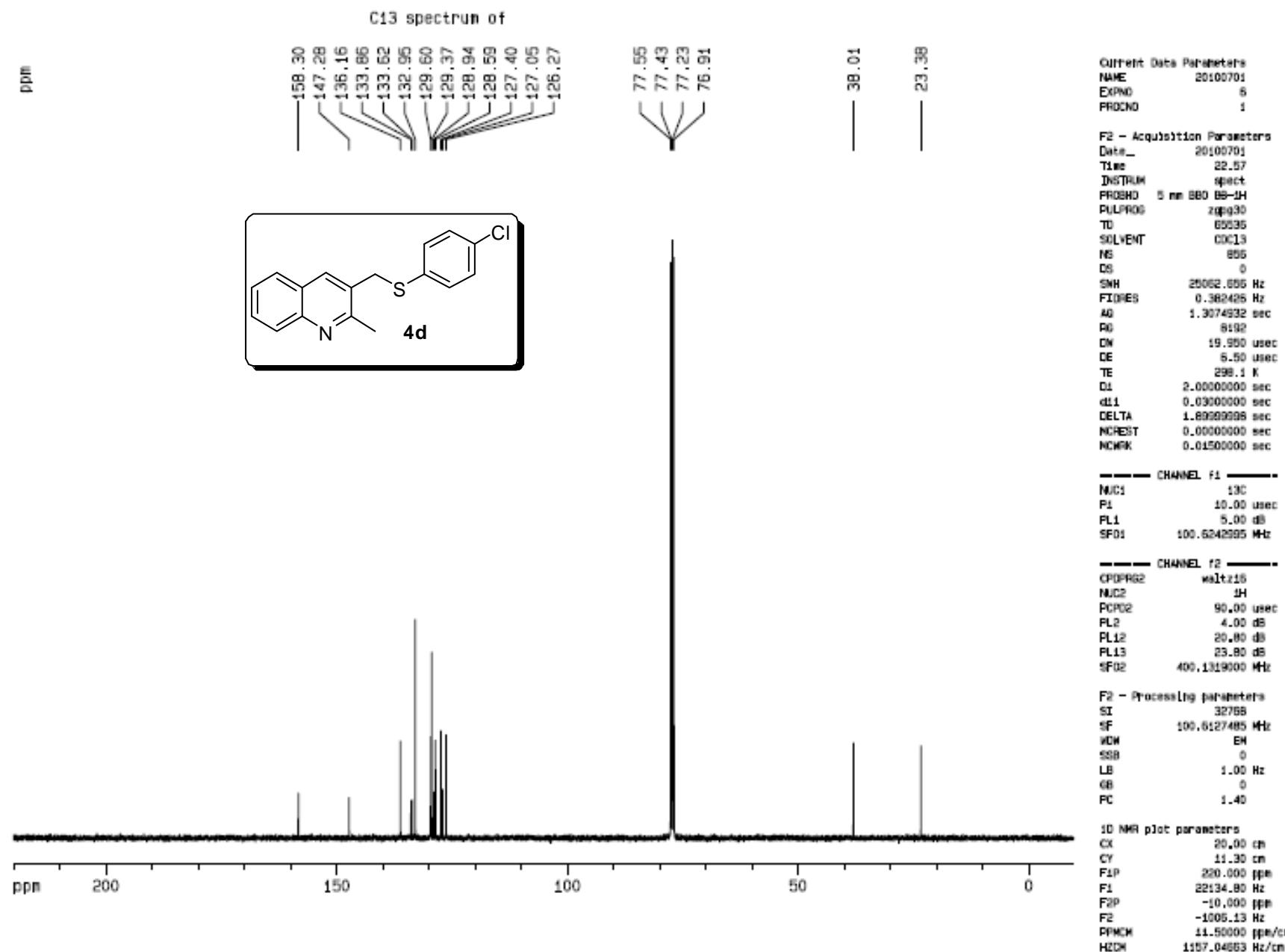
F2 - Processing parameters
SI 16384
SF 400.1300080 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

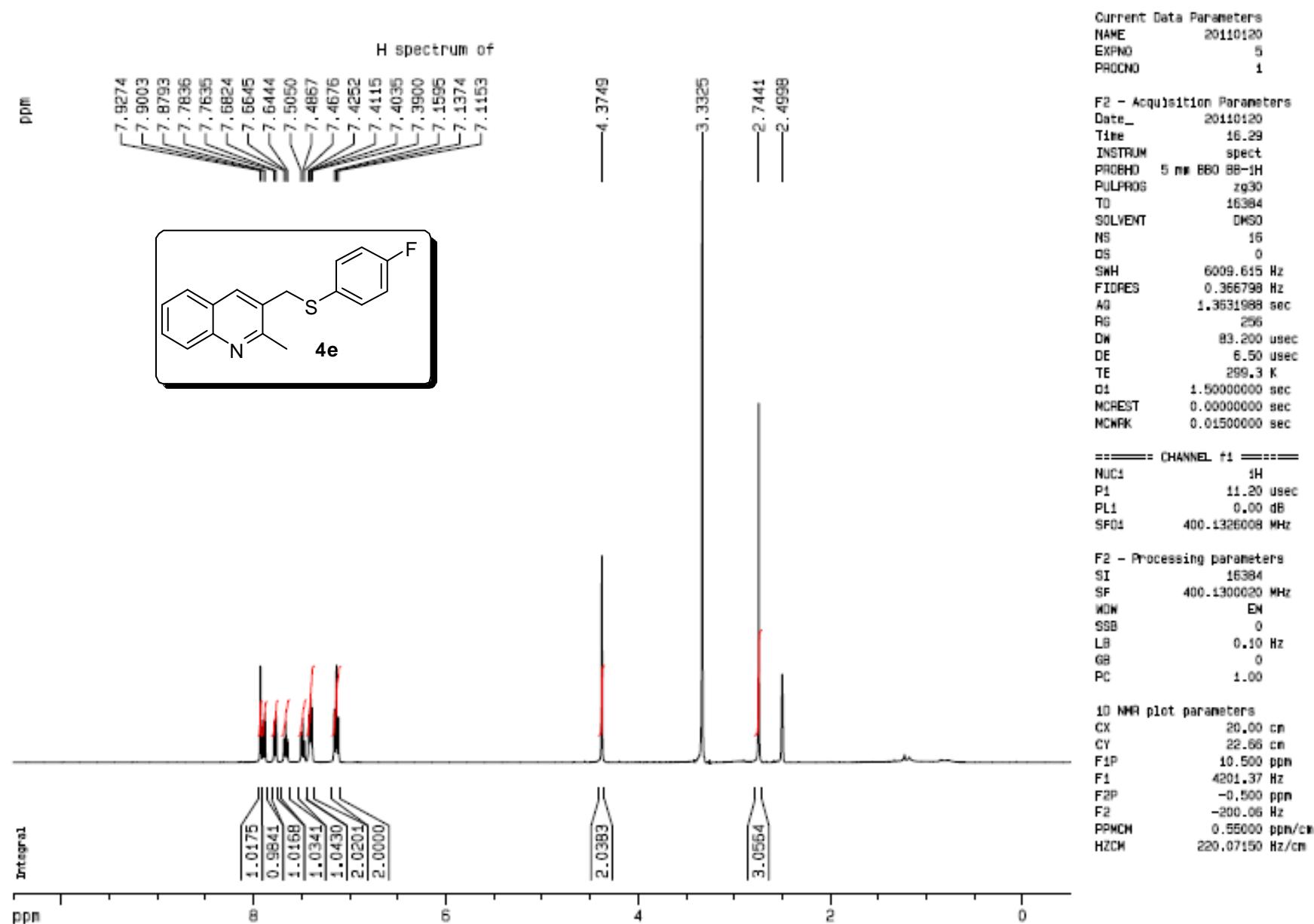


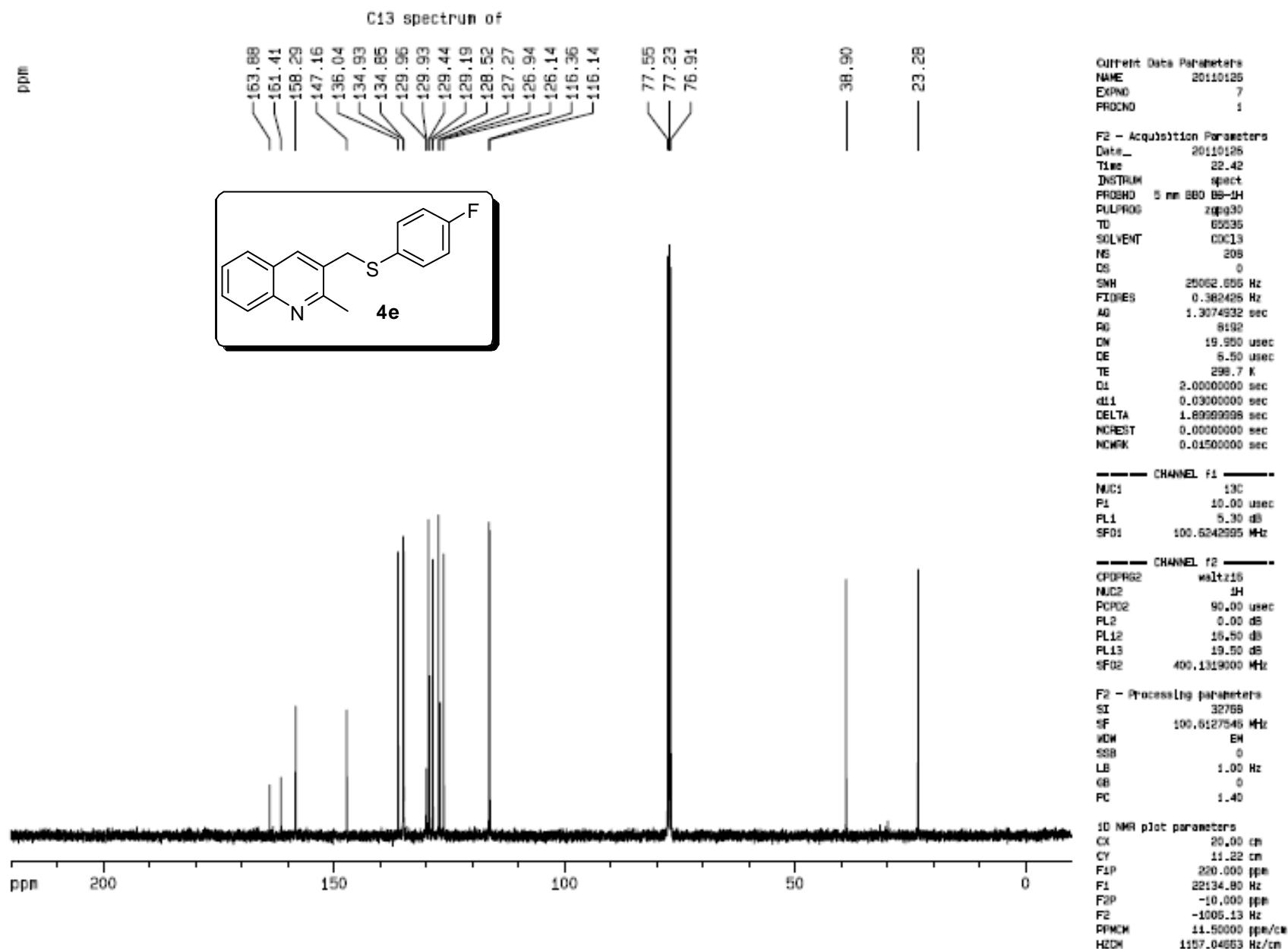


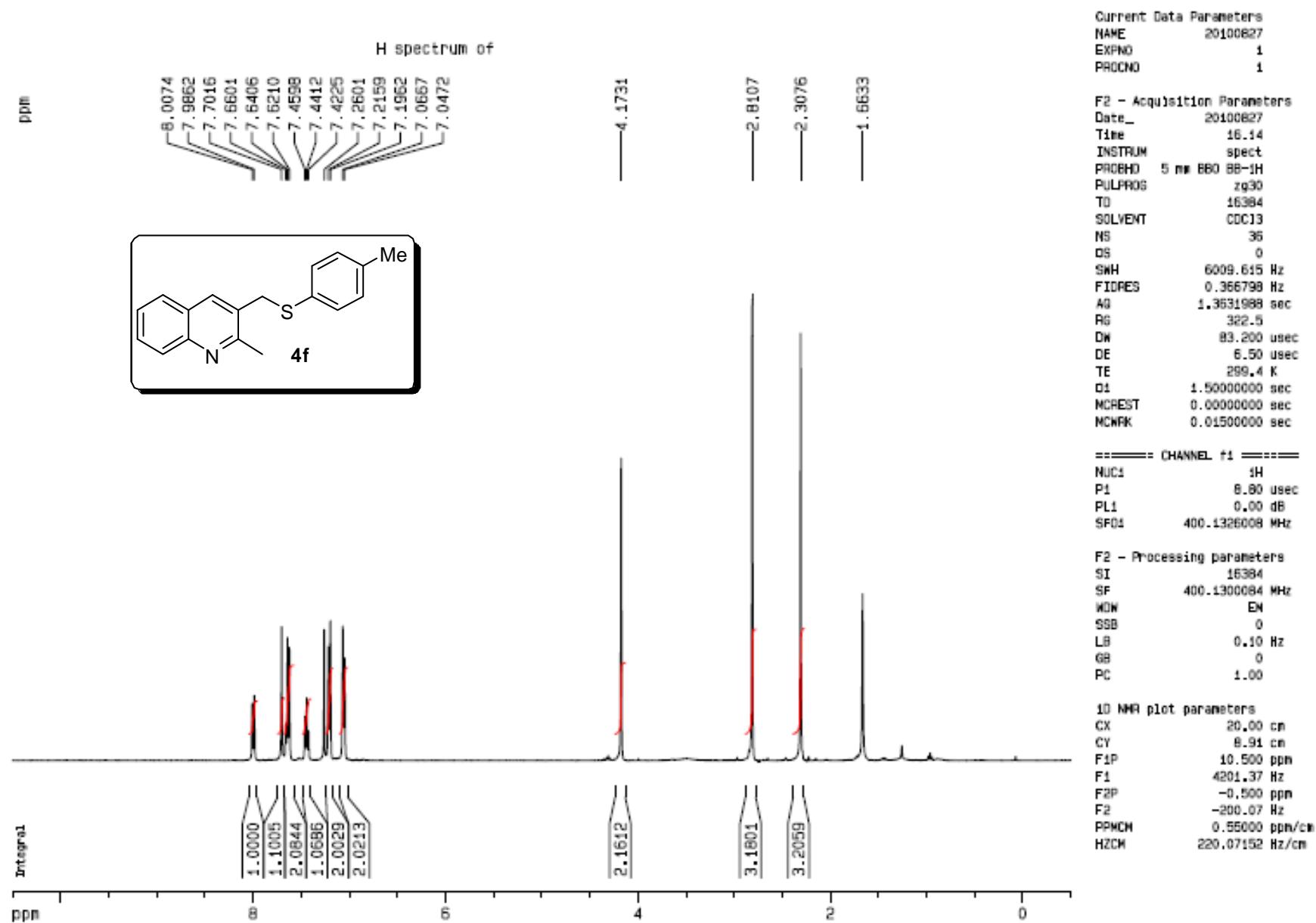


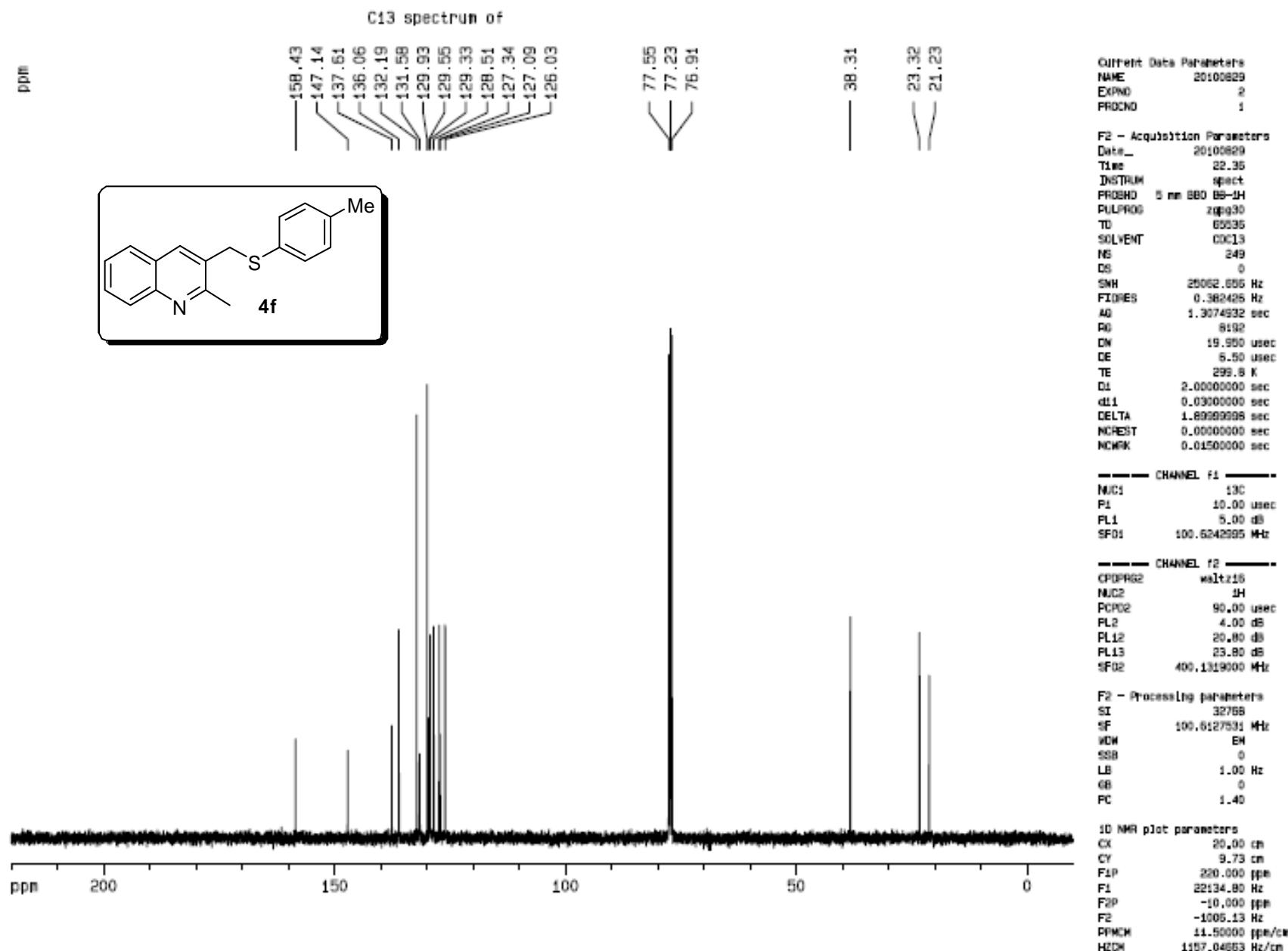


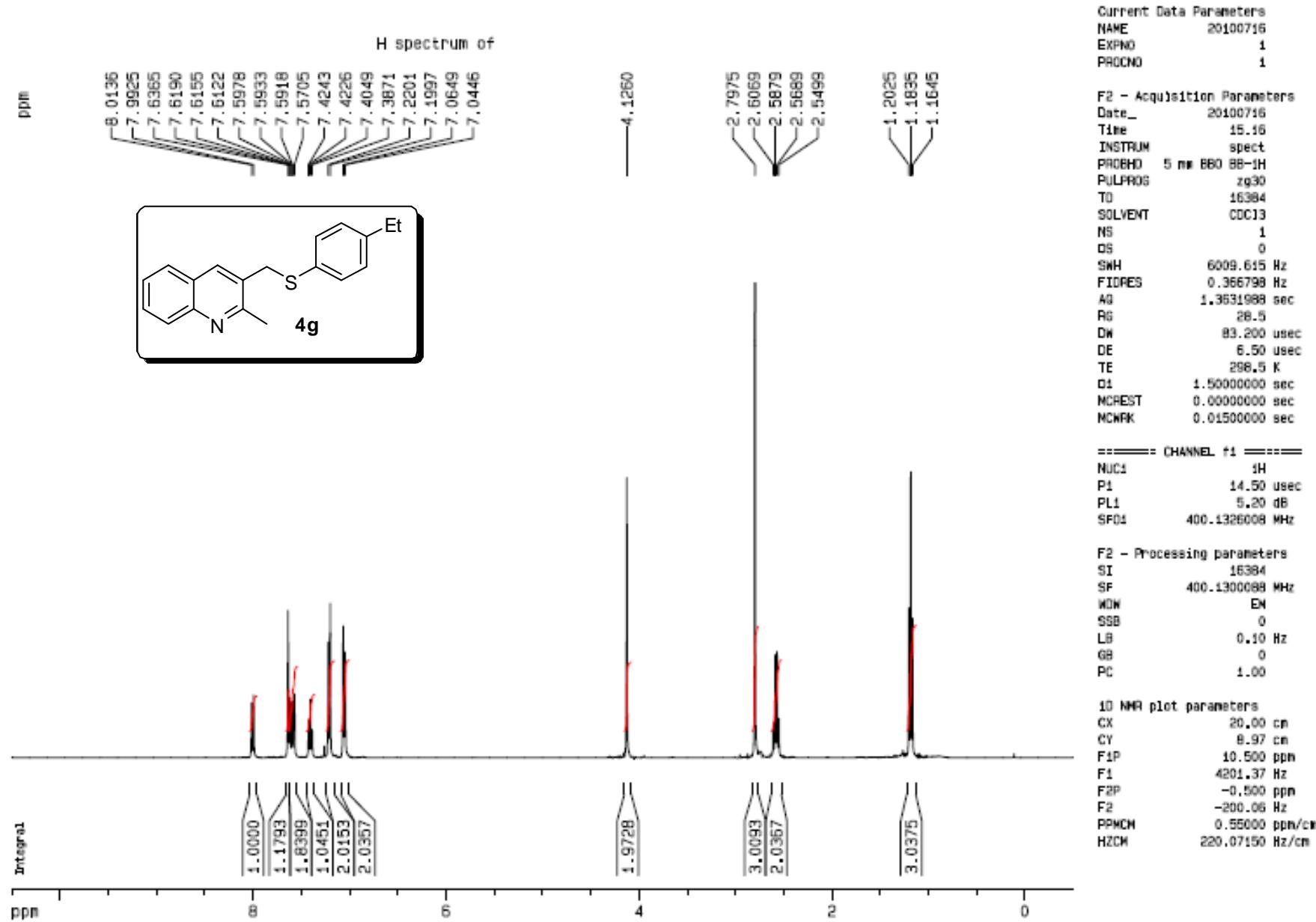


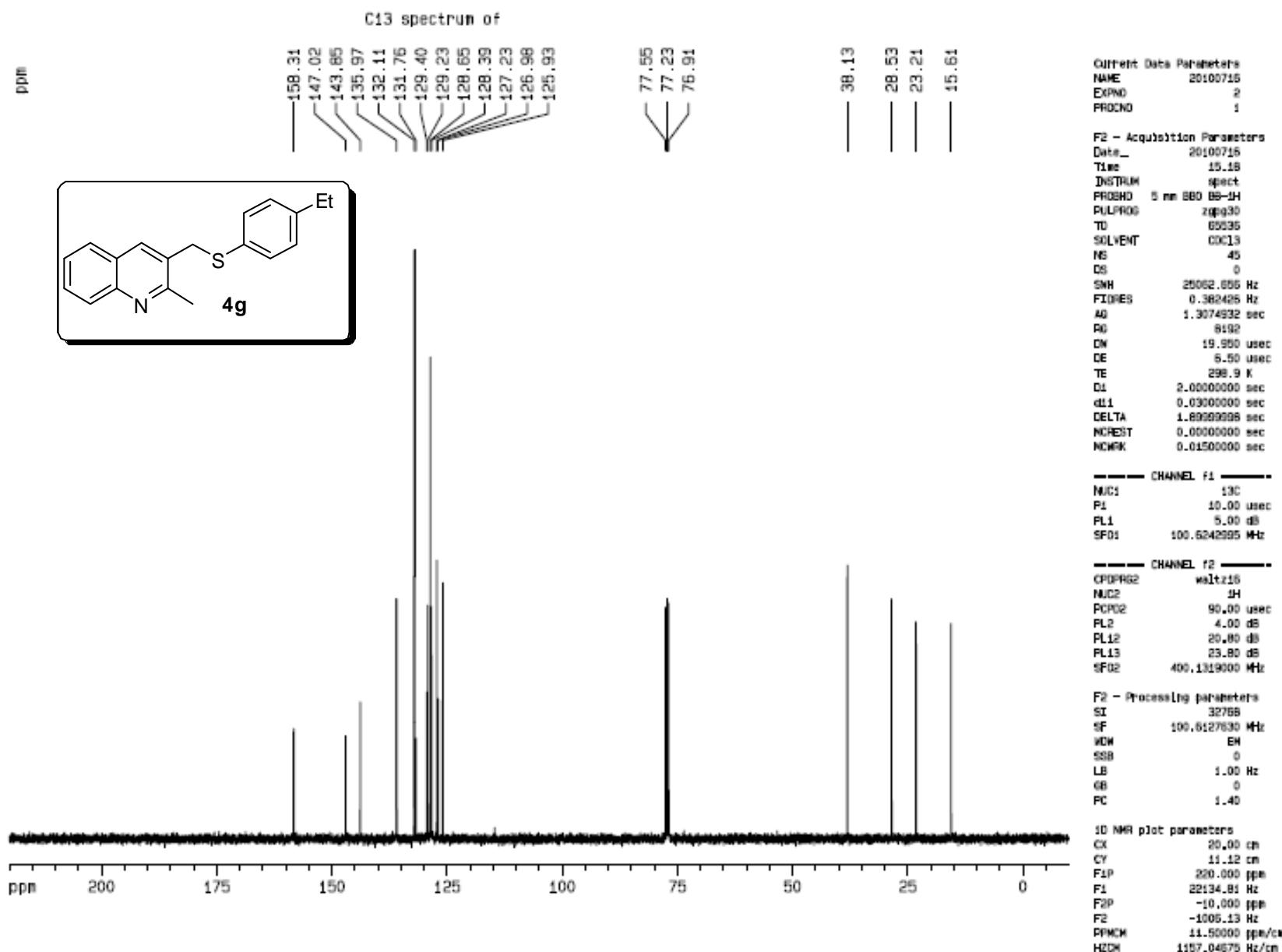


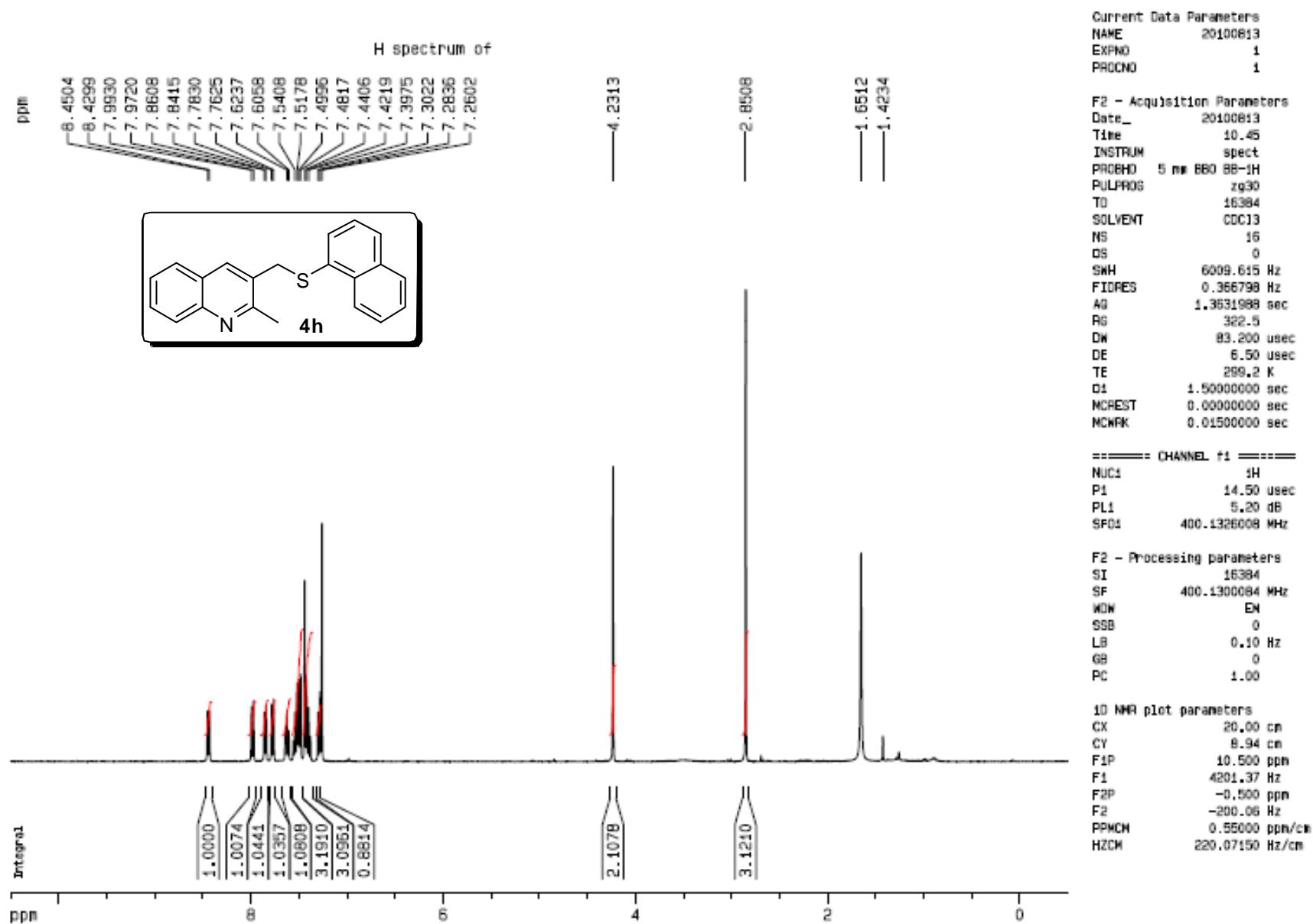


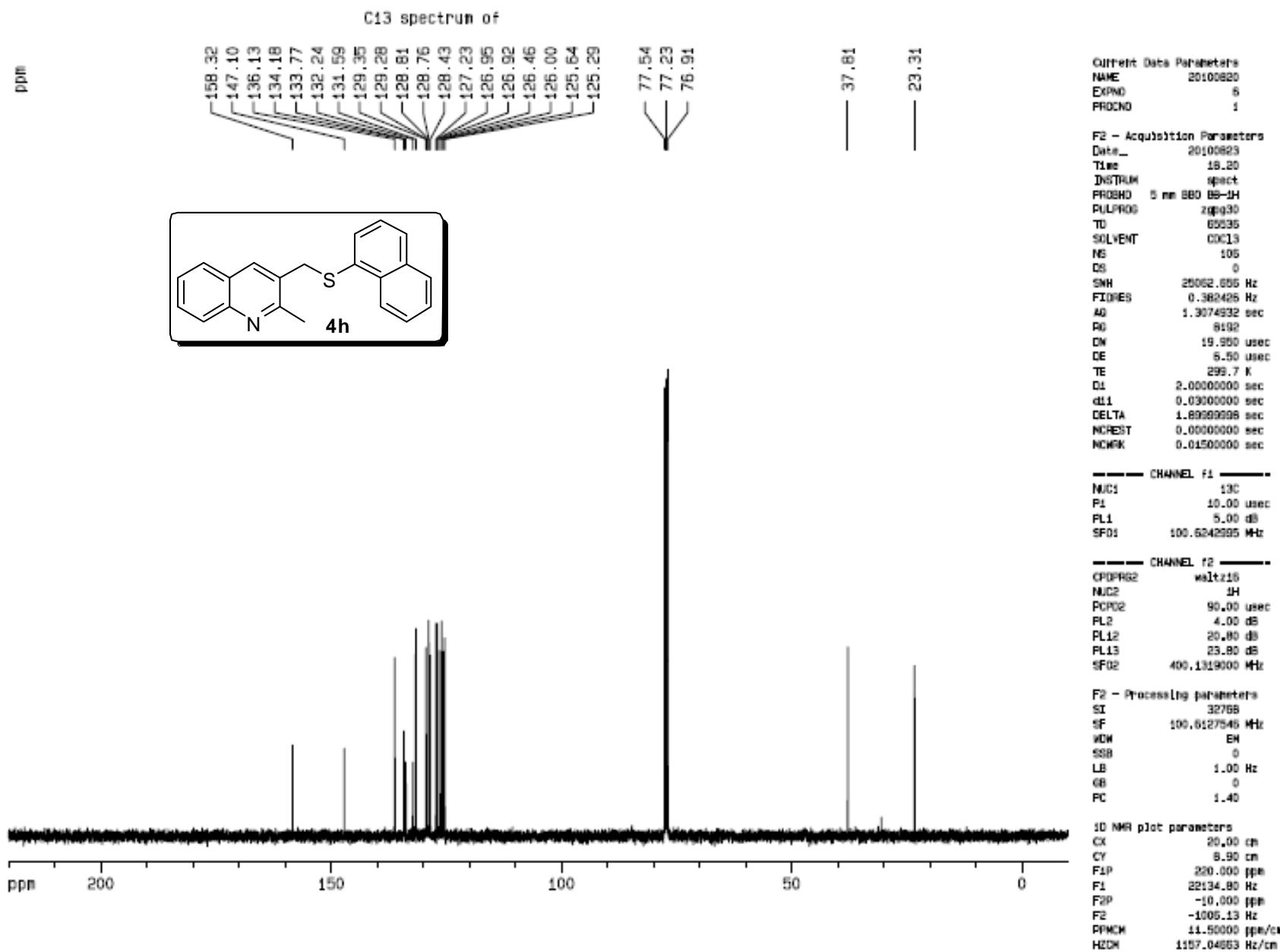


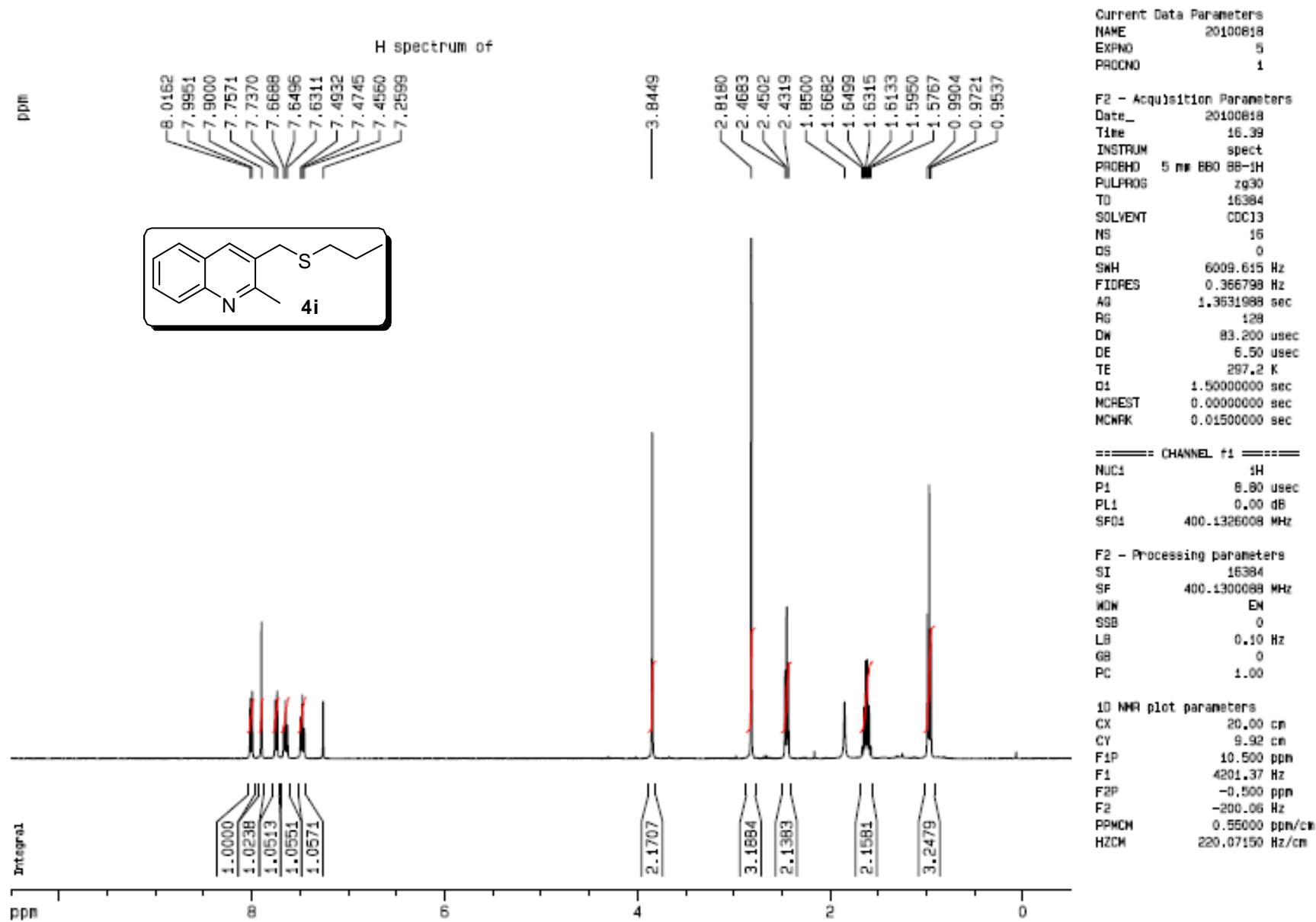


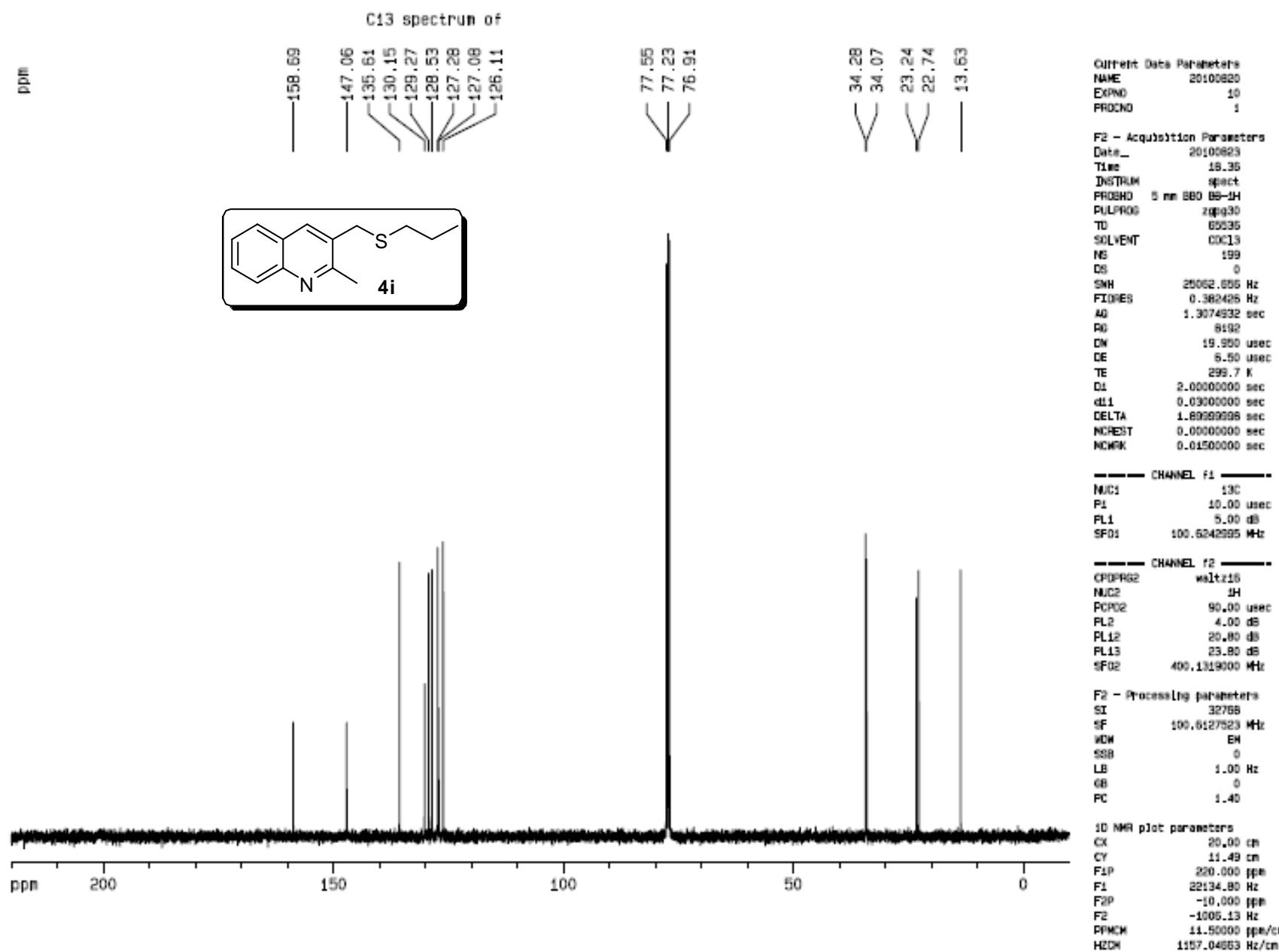


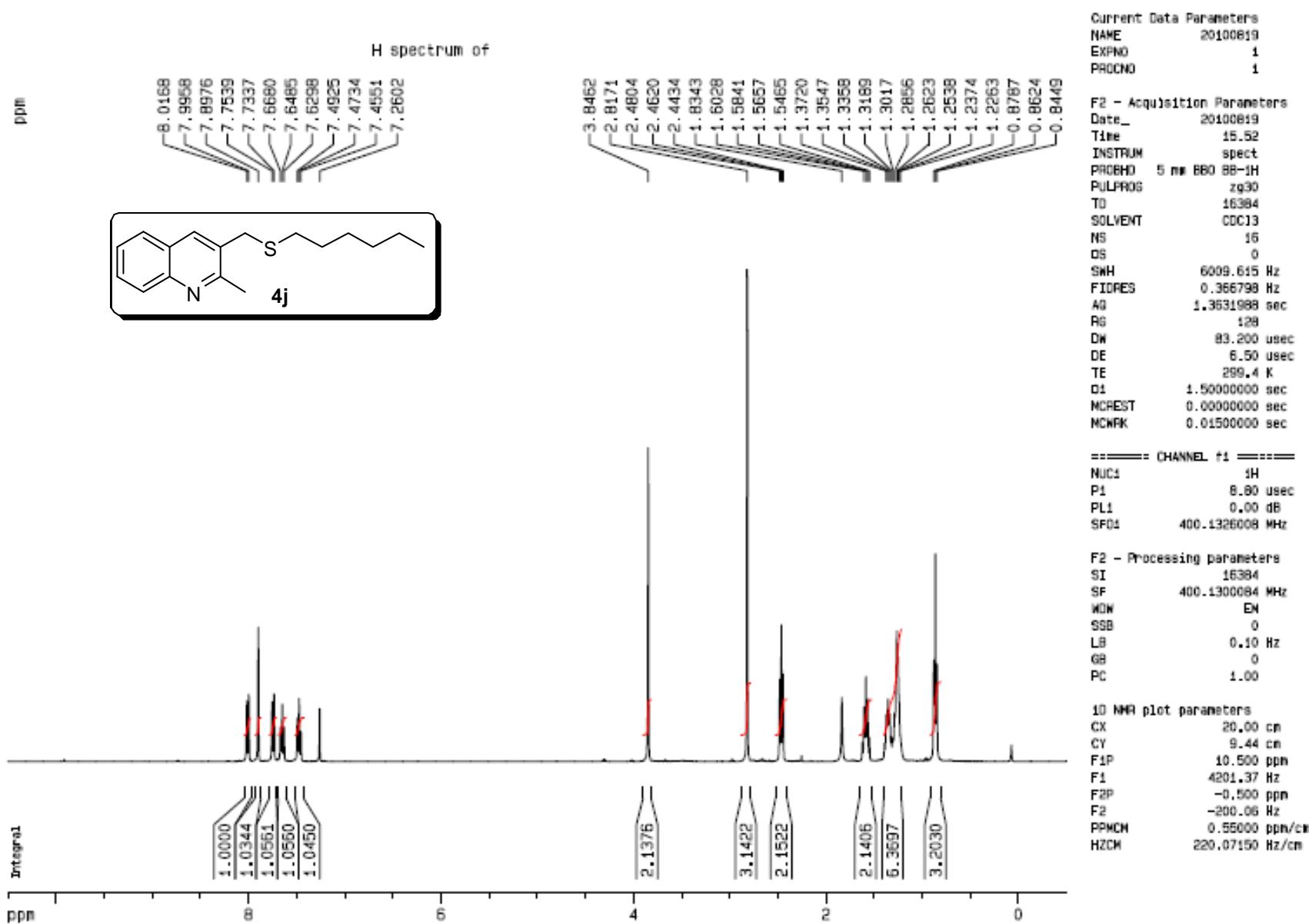


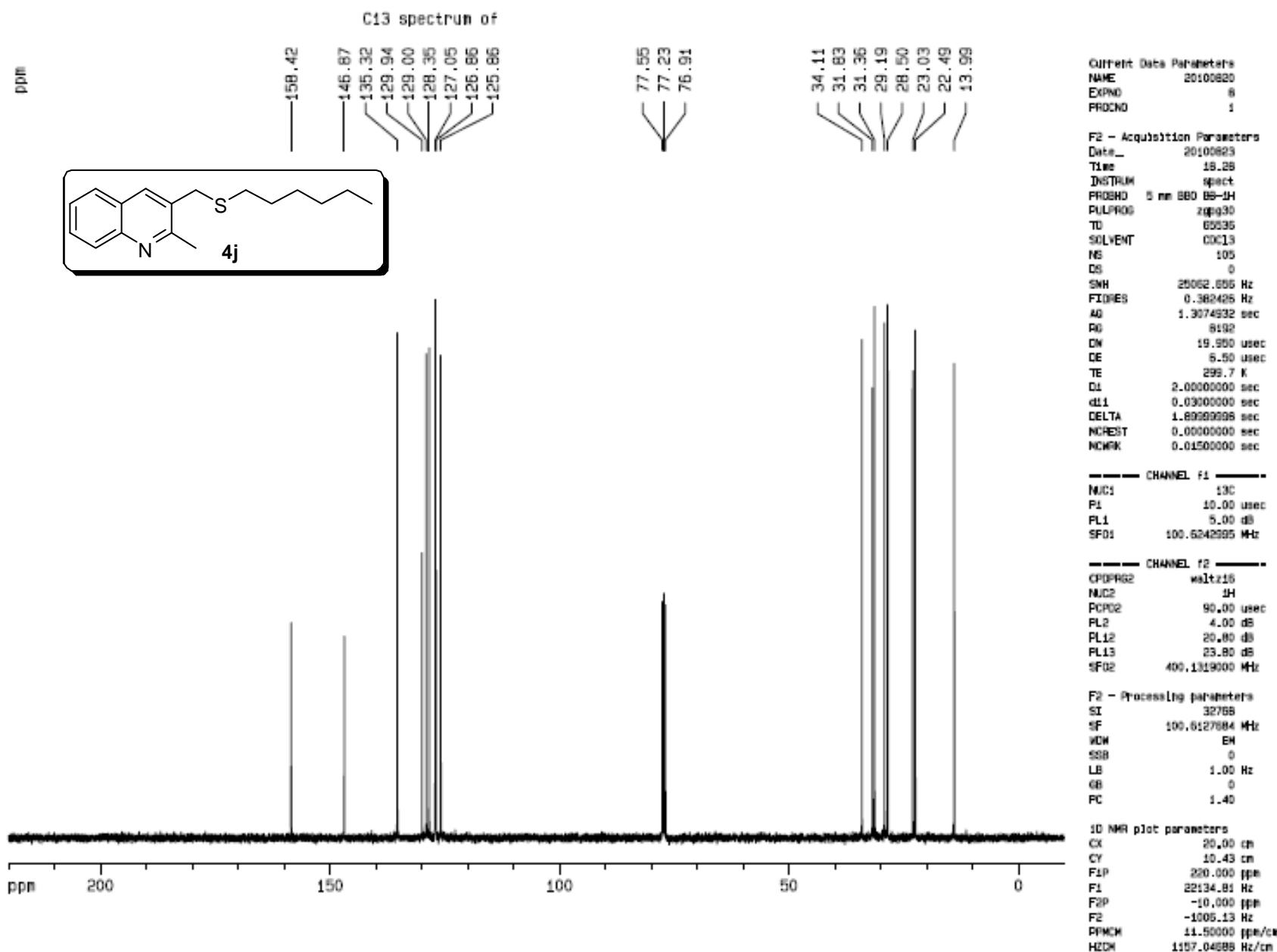


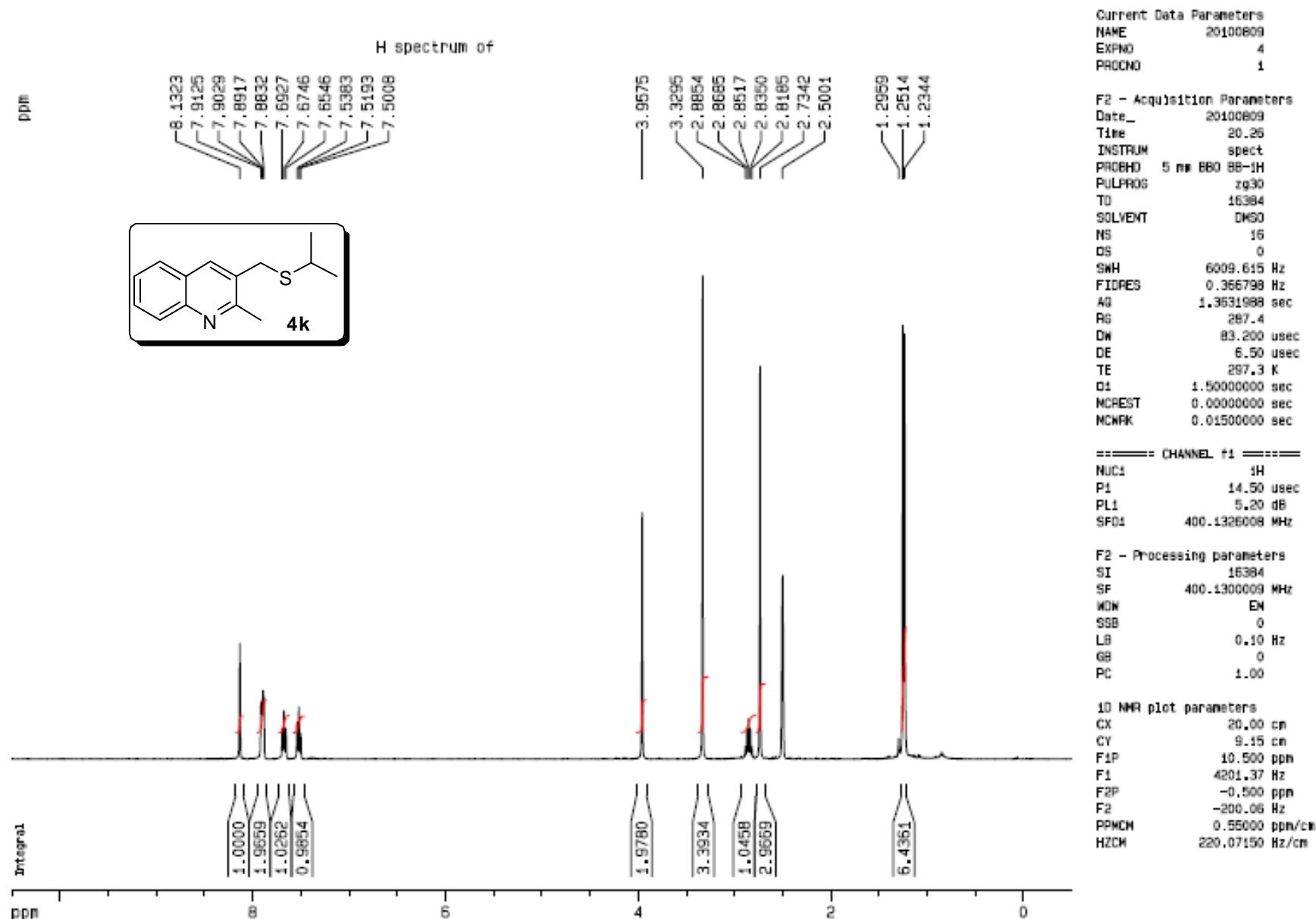


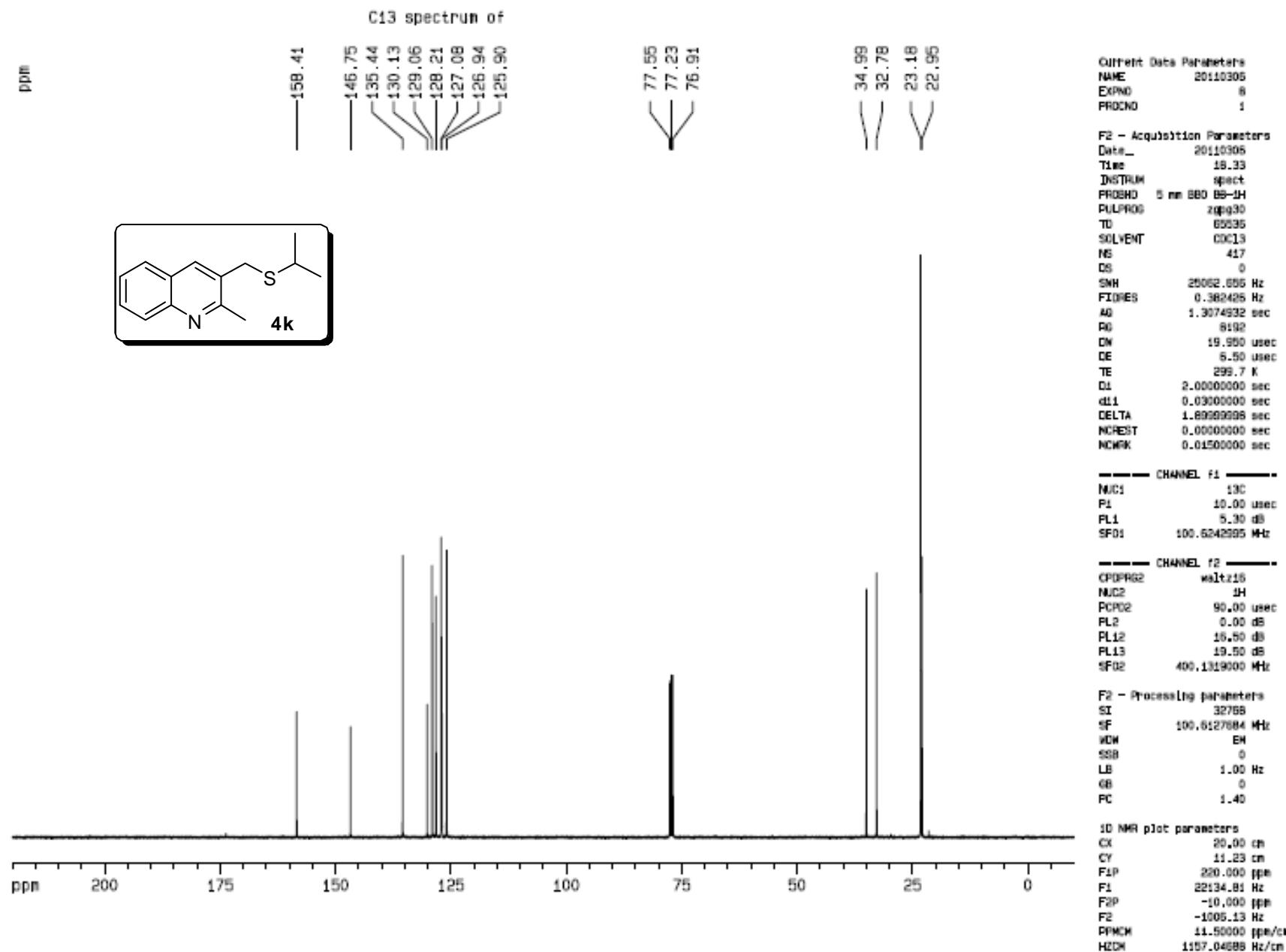


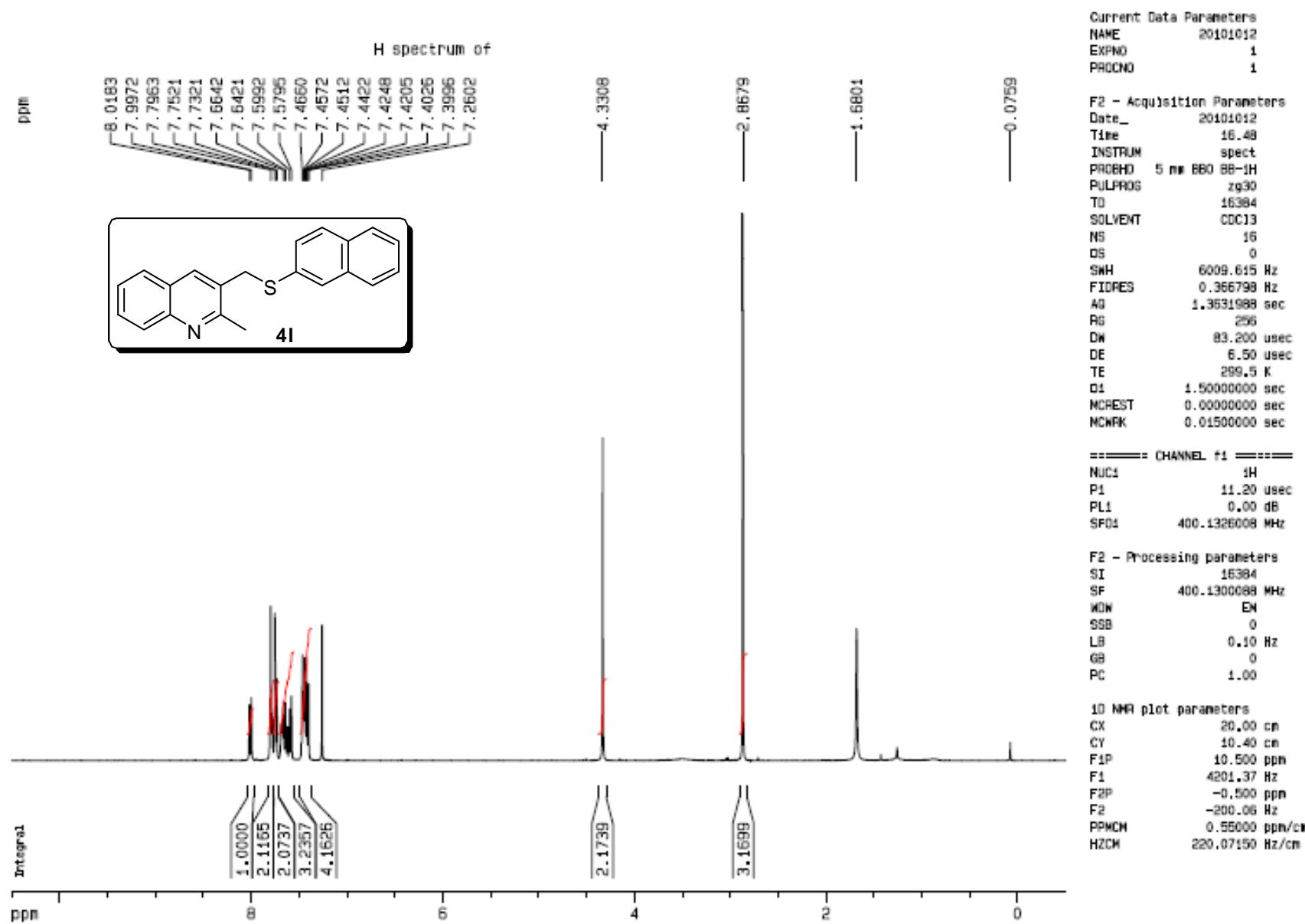


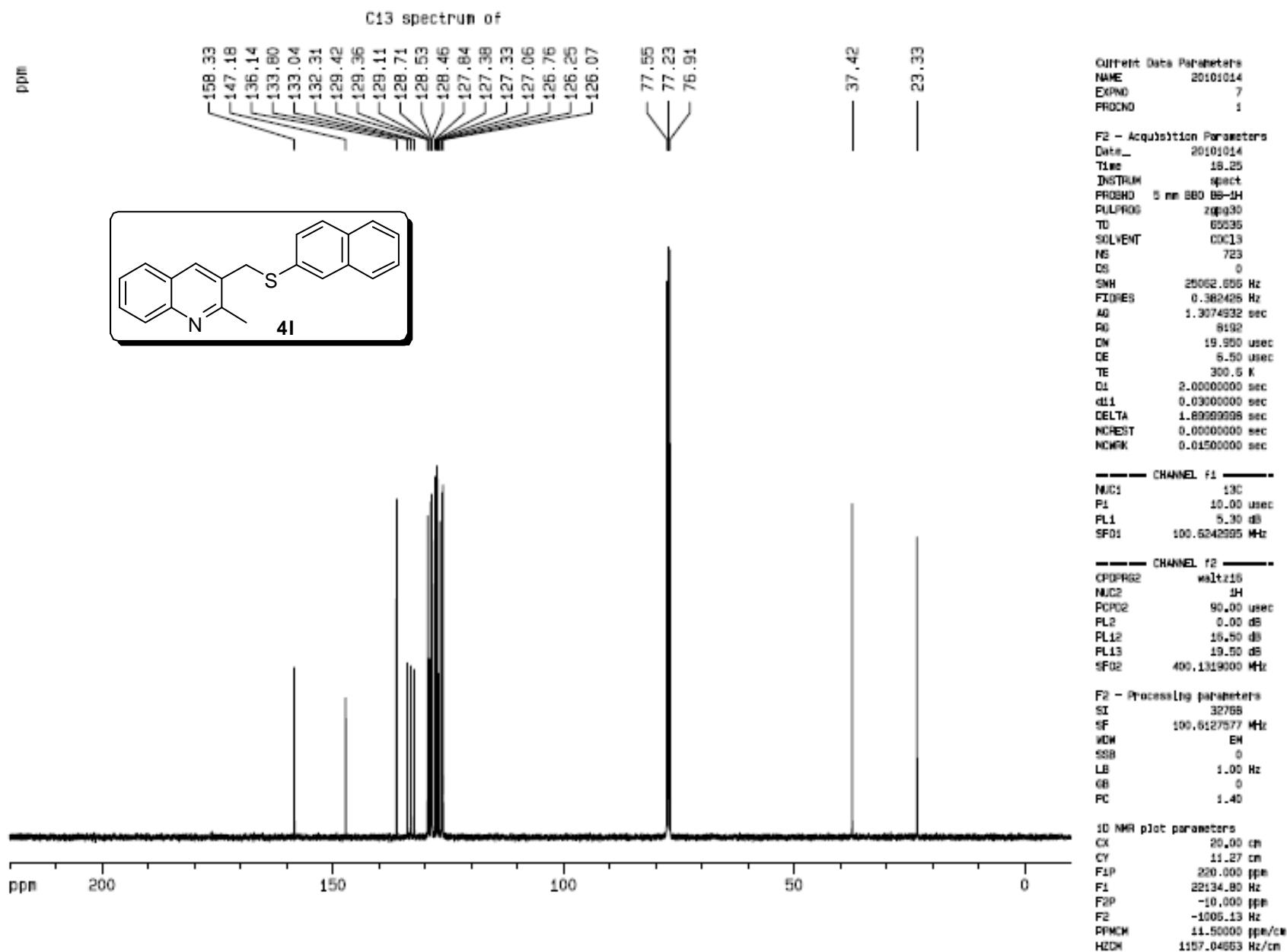


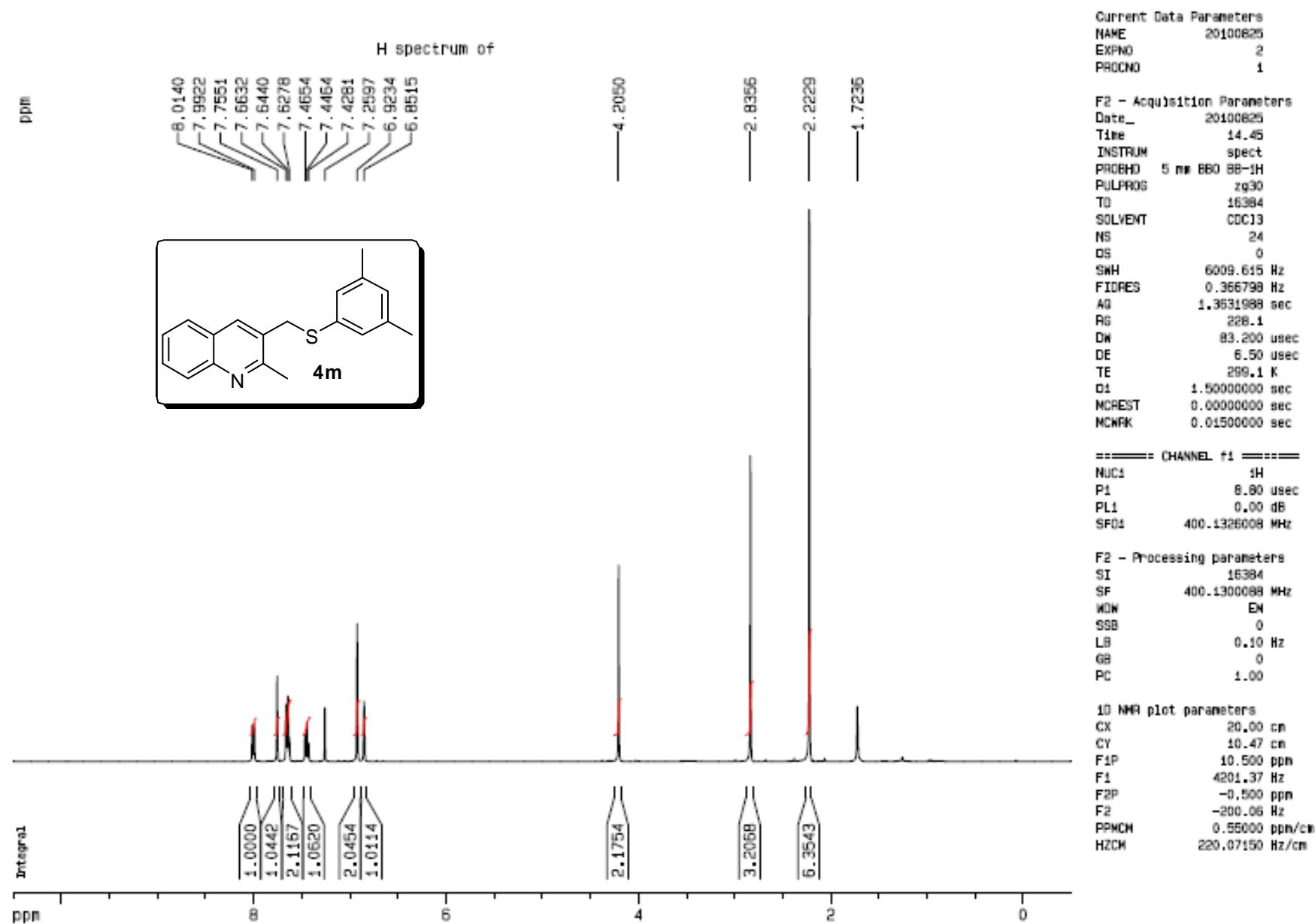


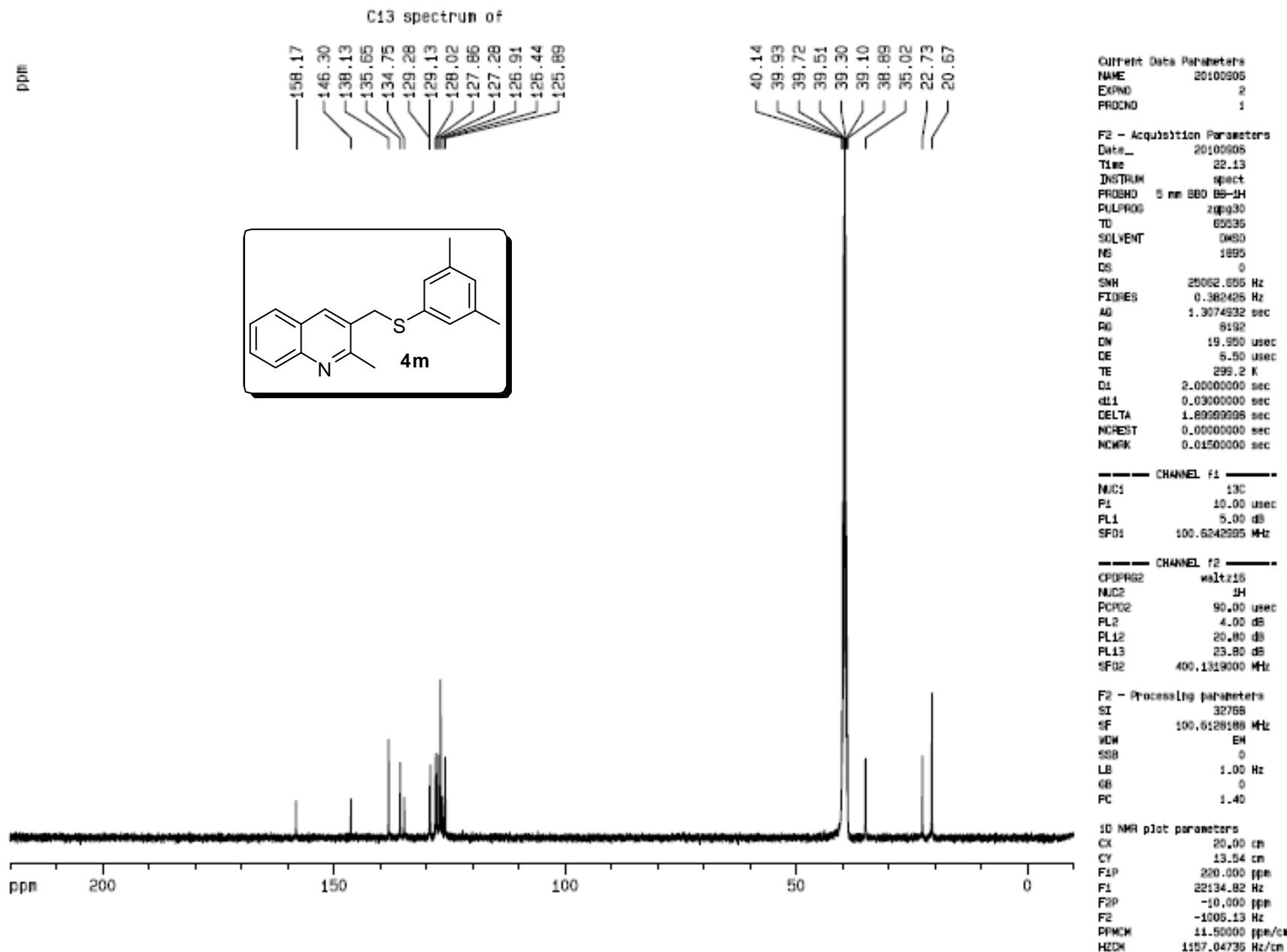


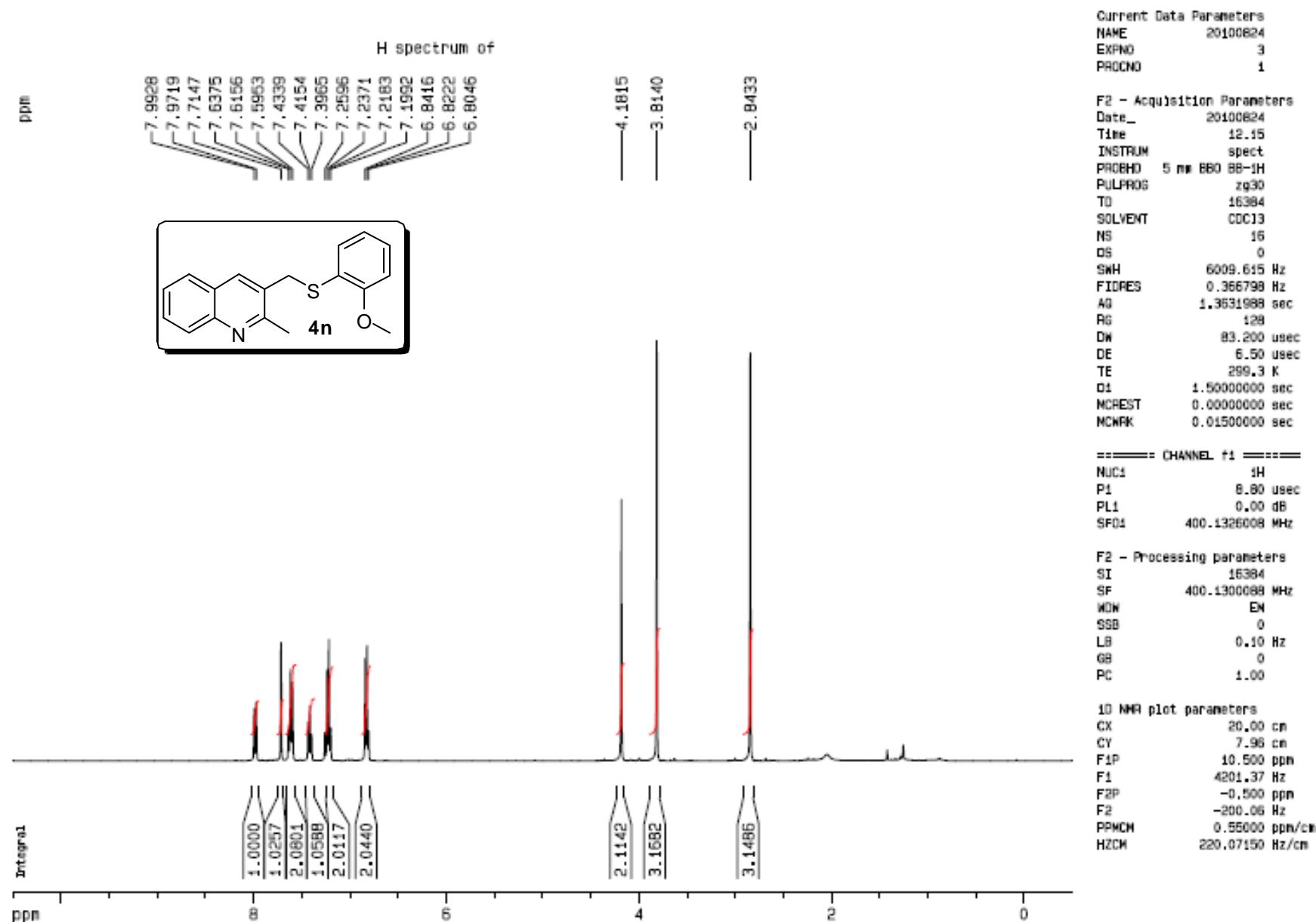


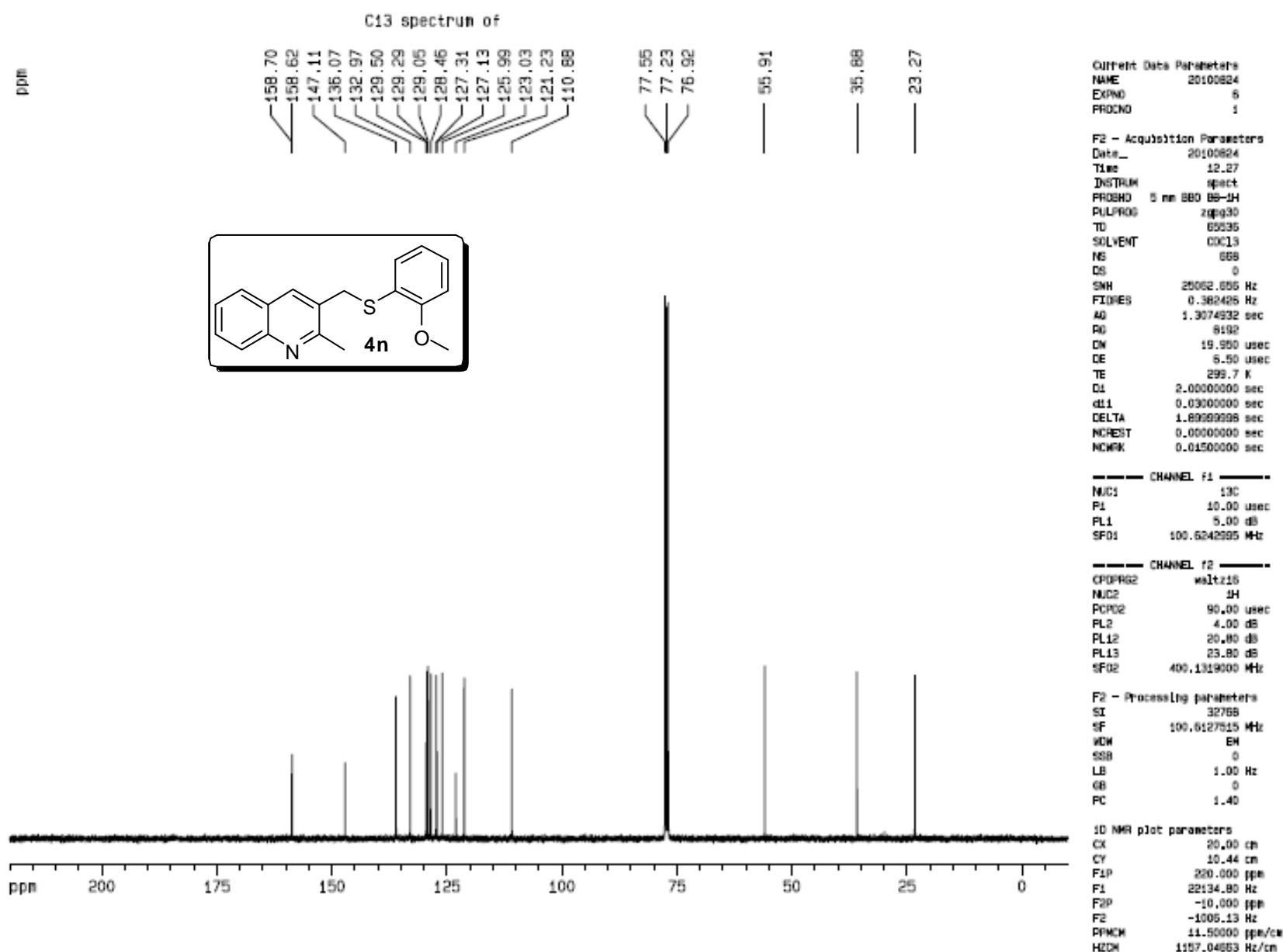


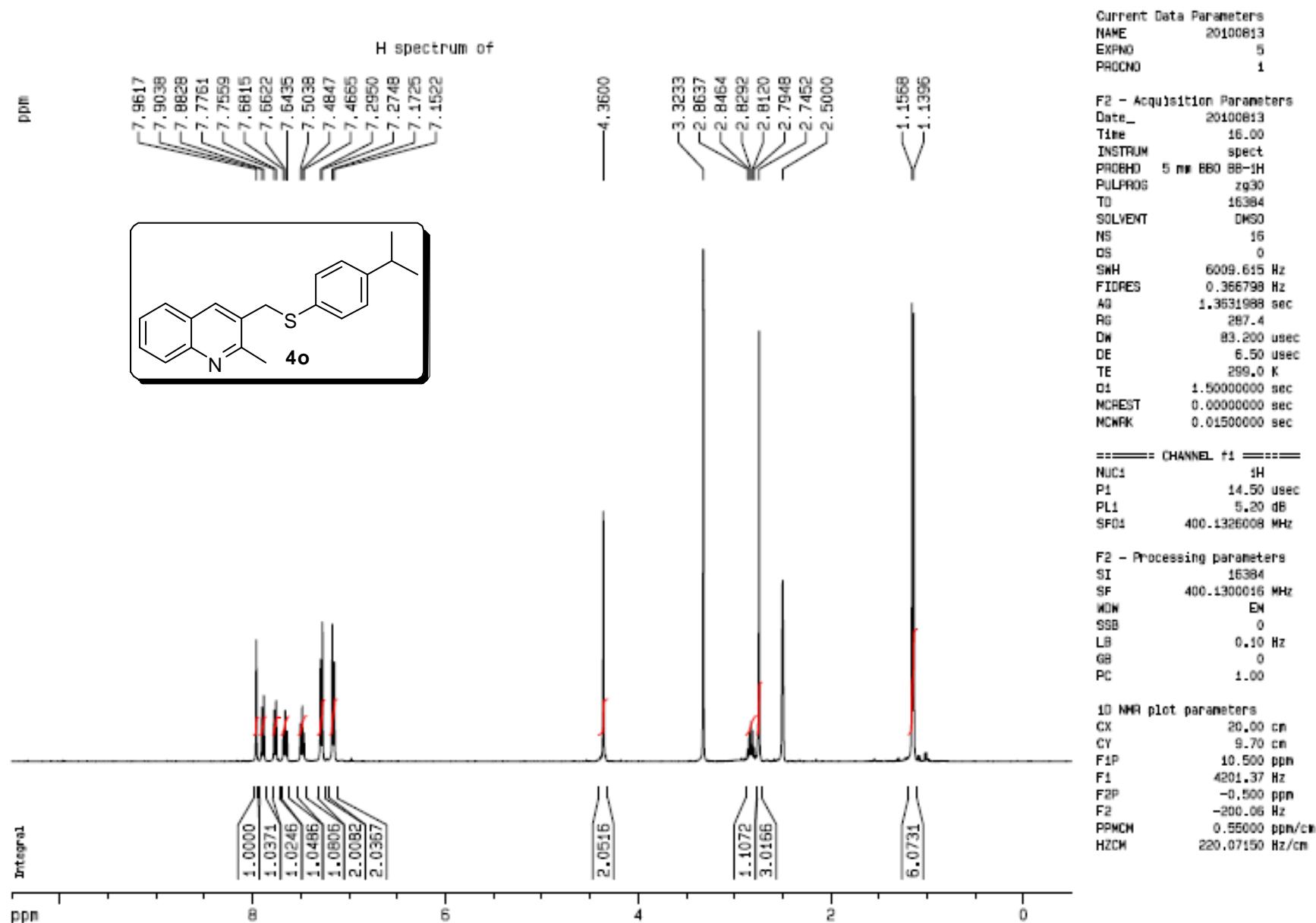


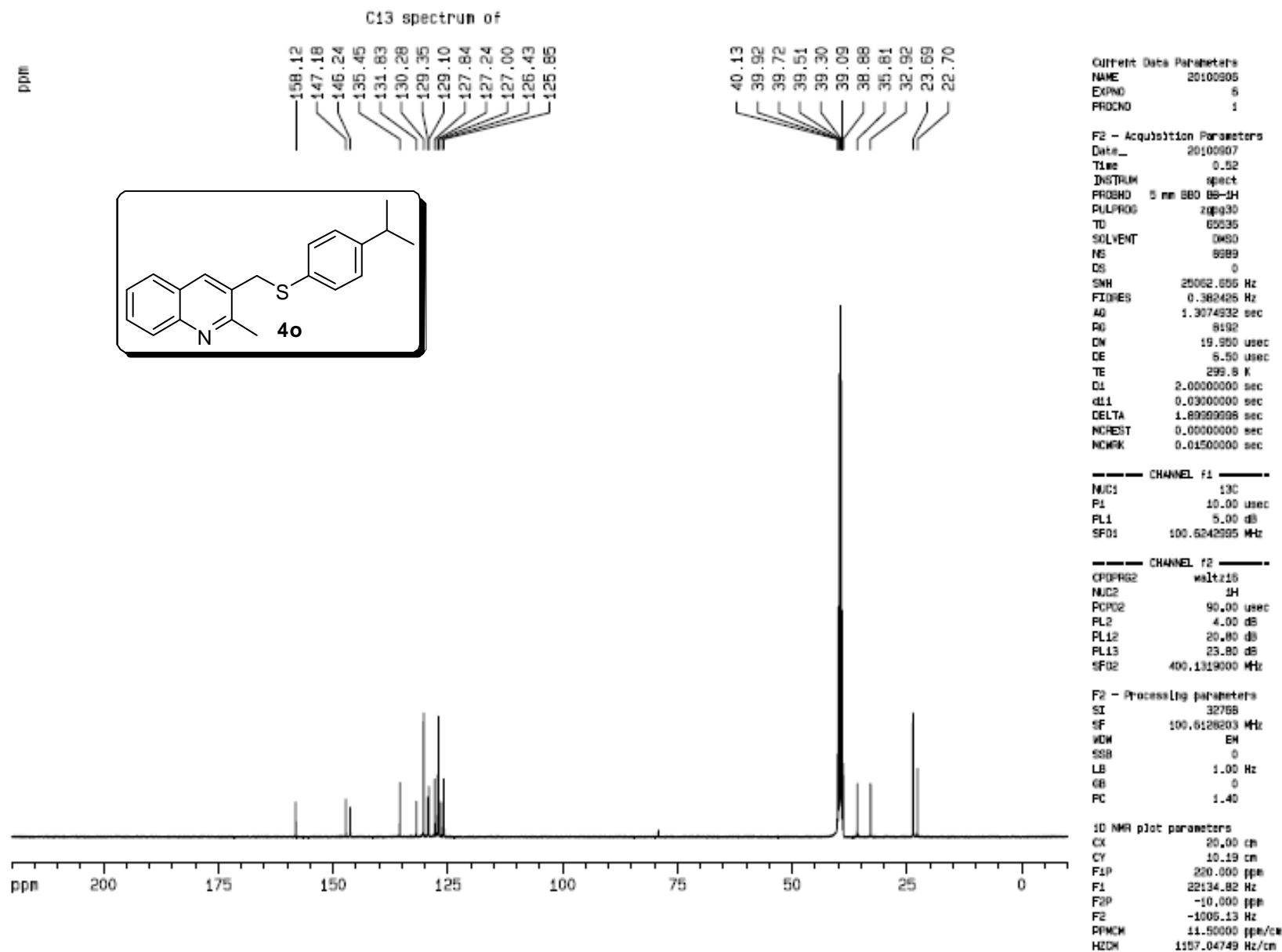


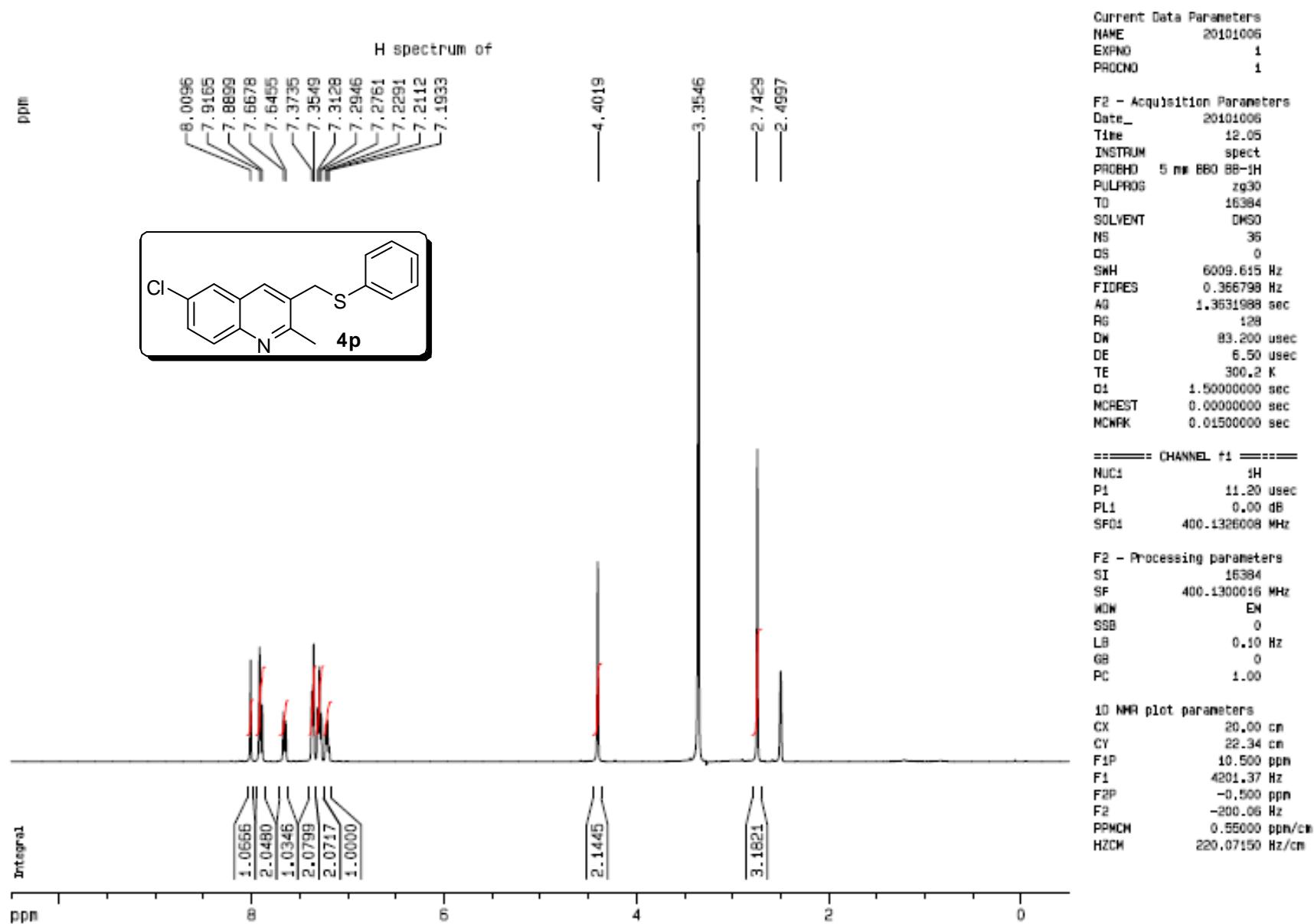


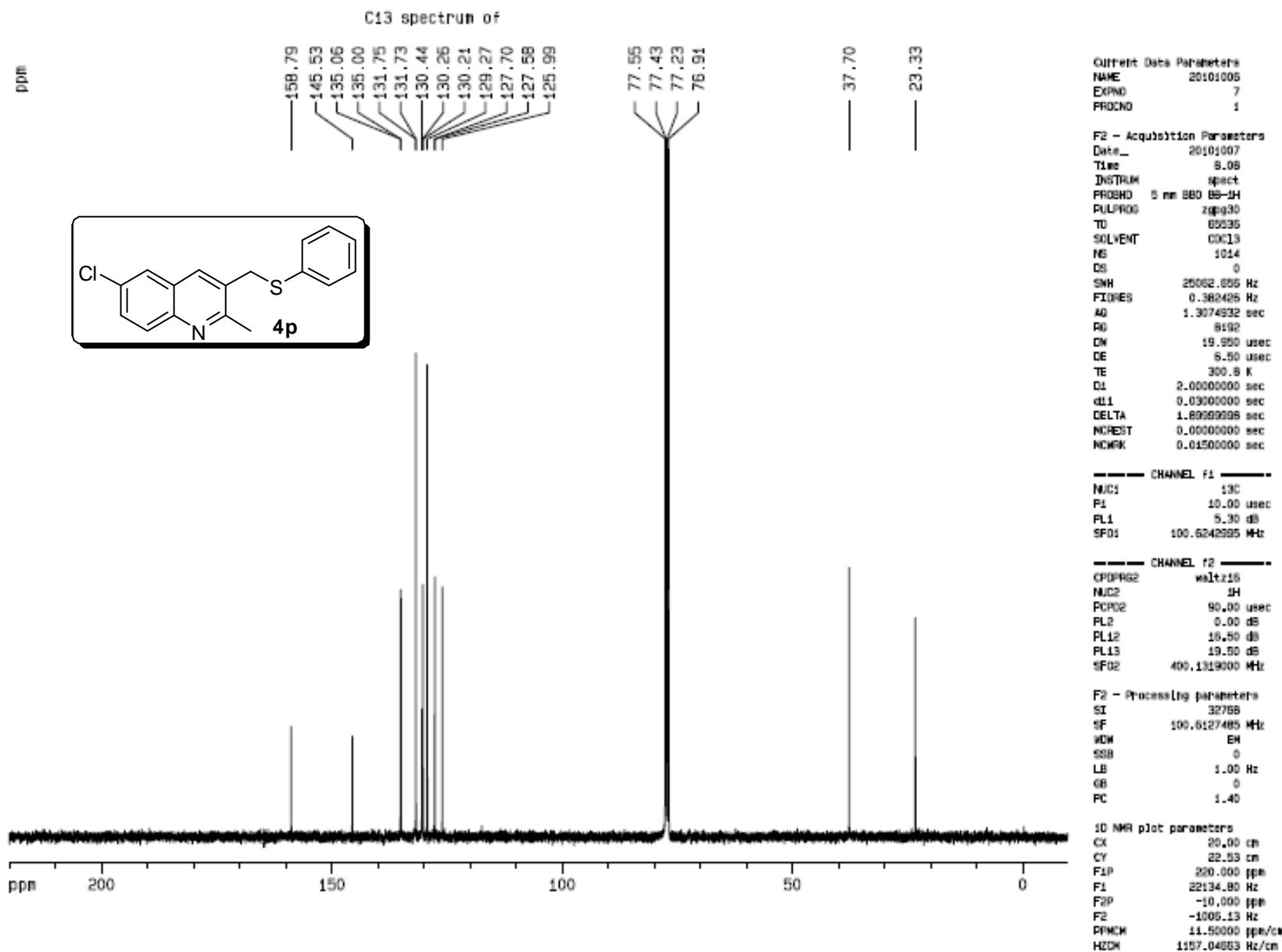


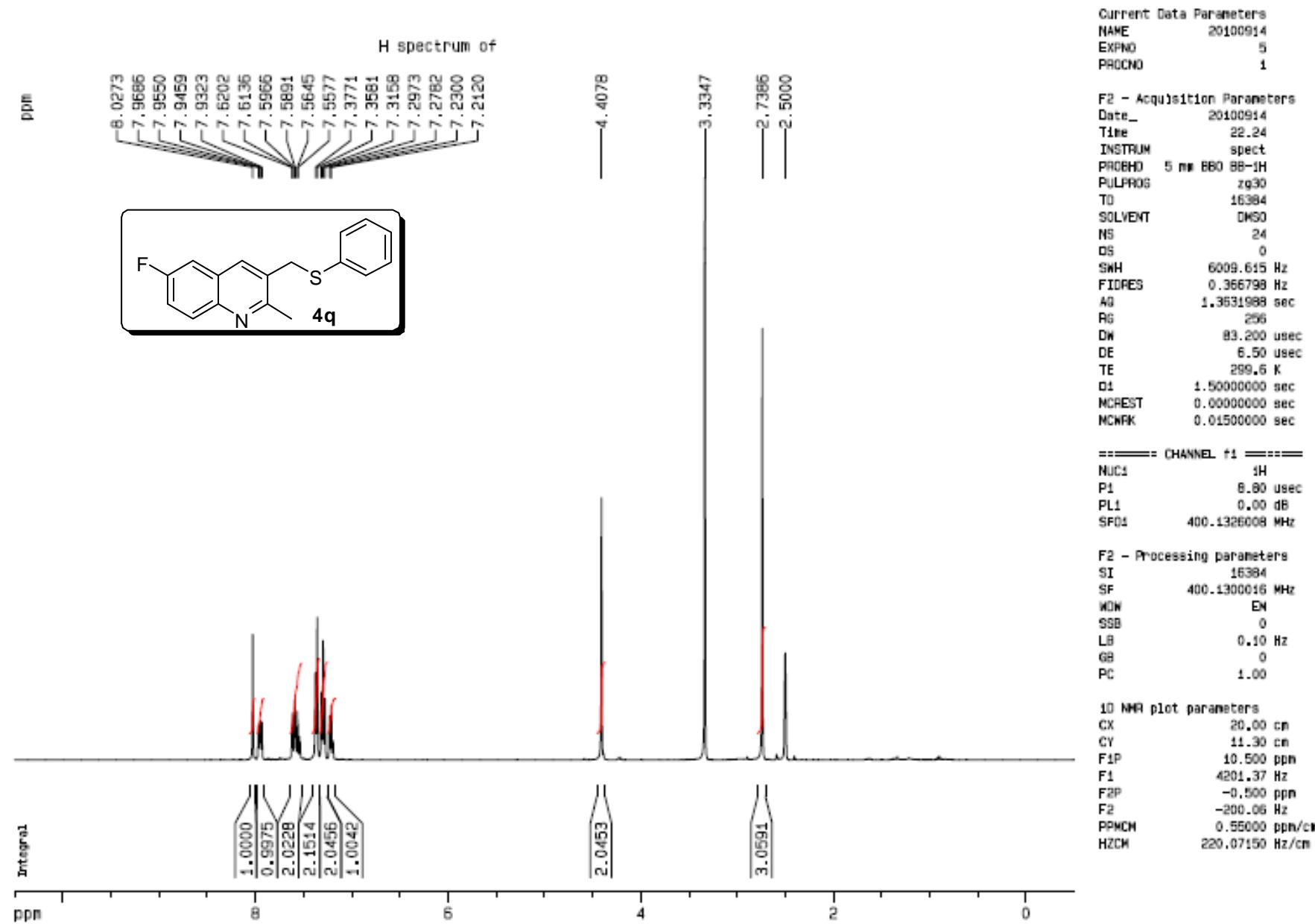


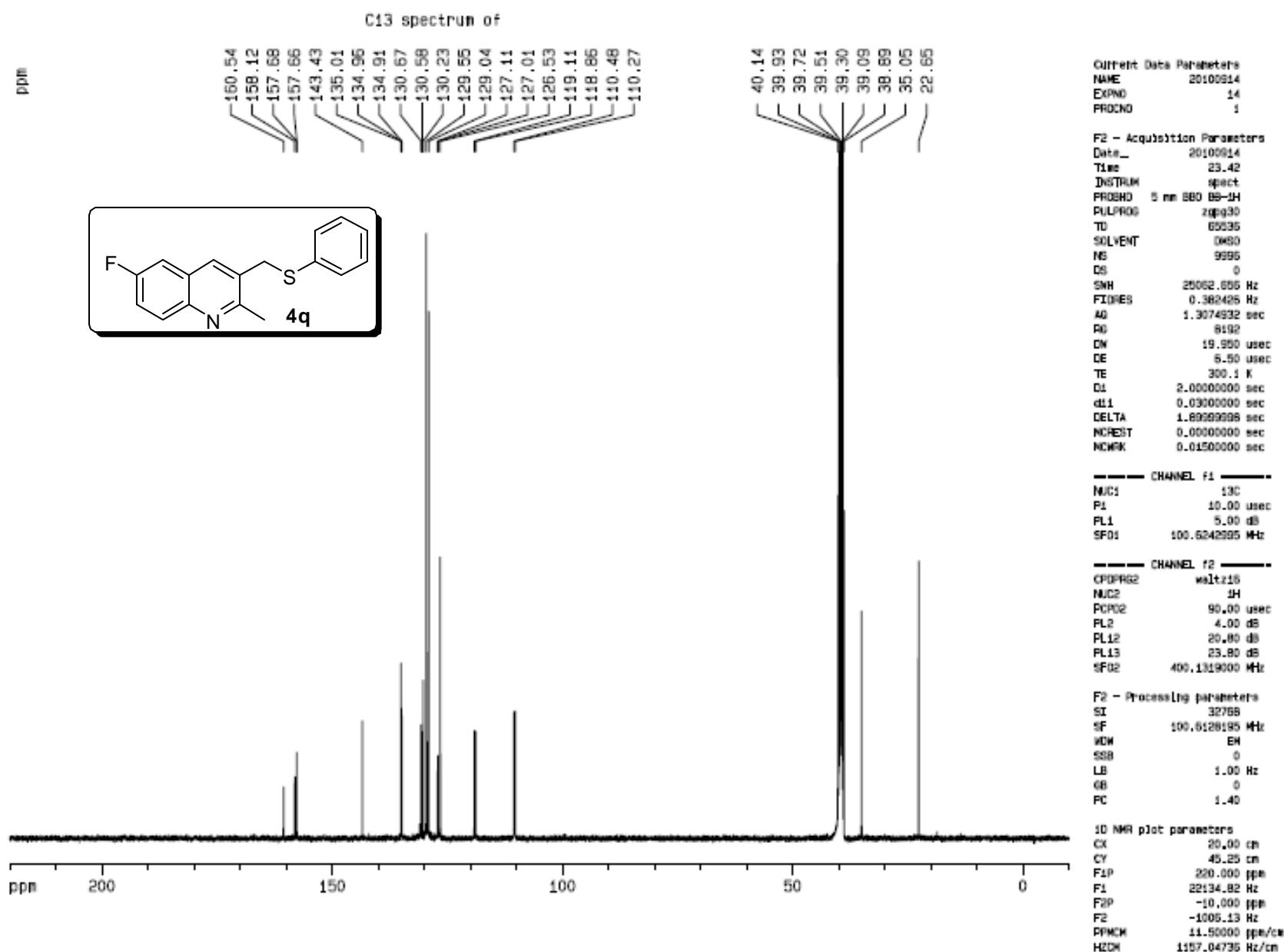


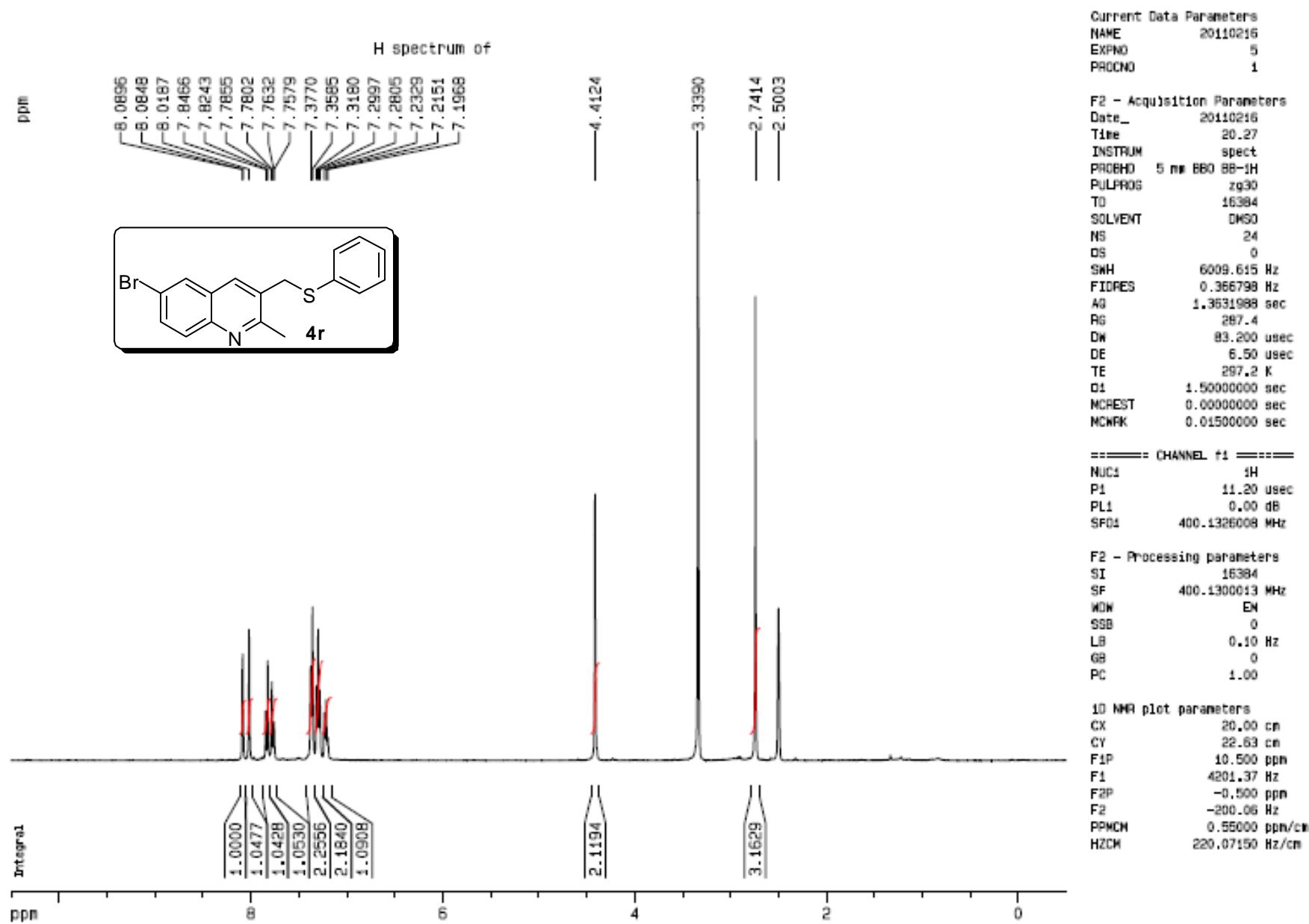


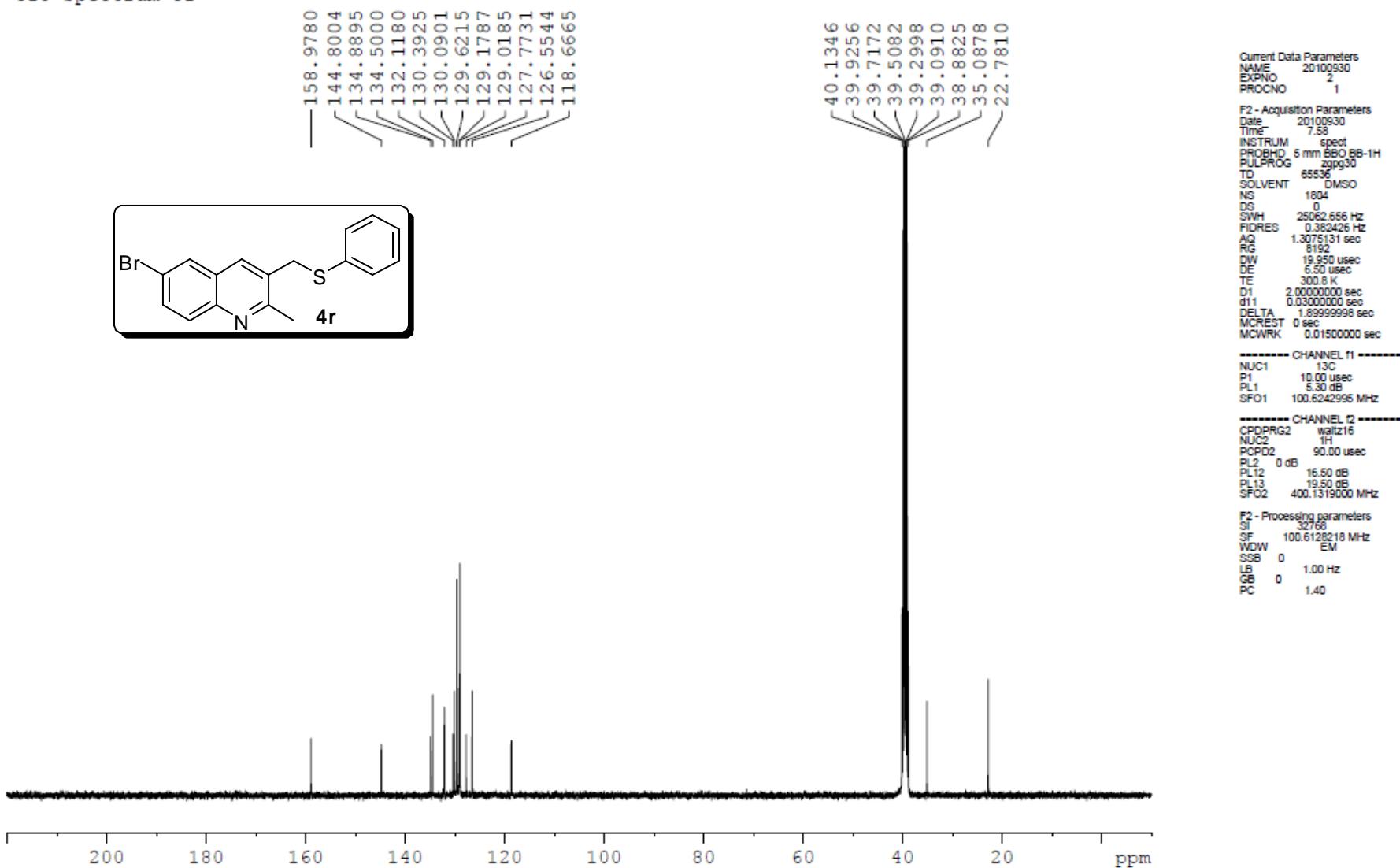


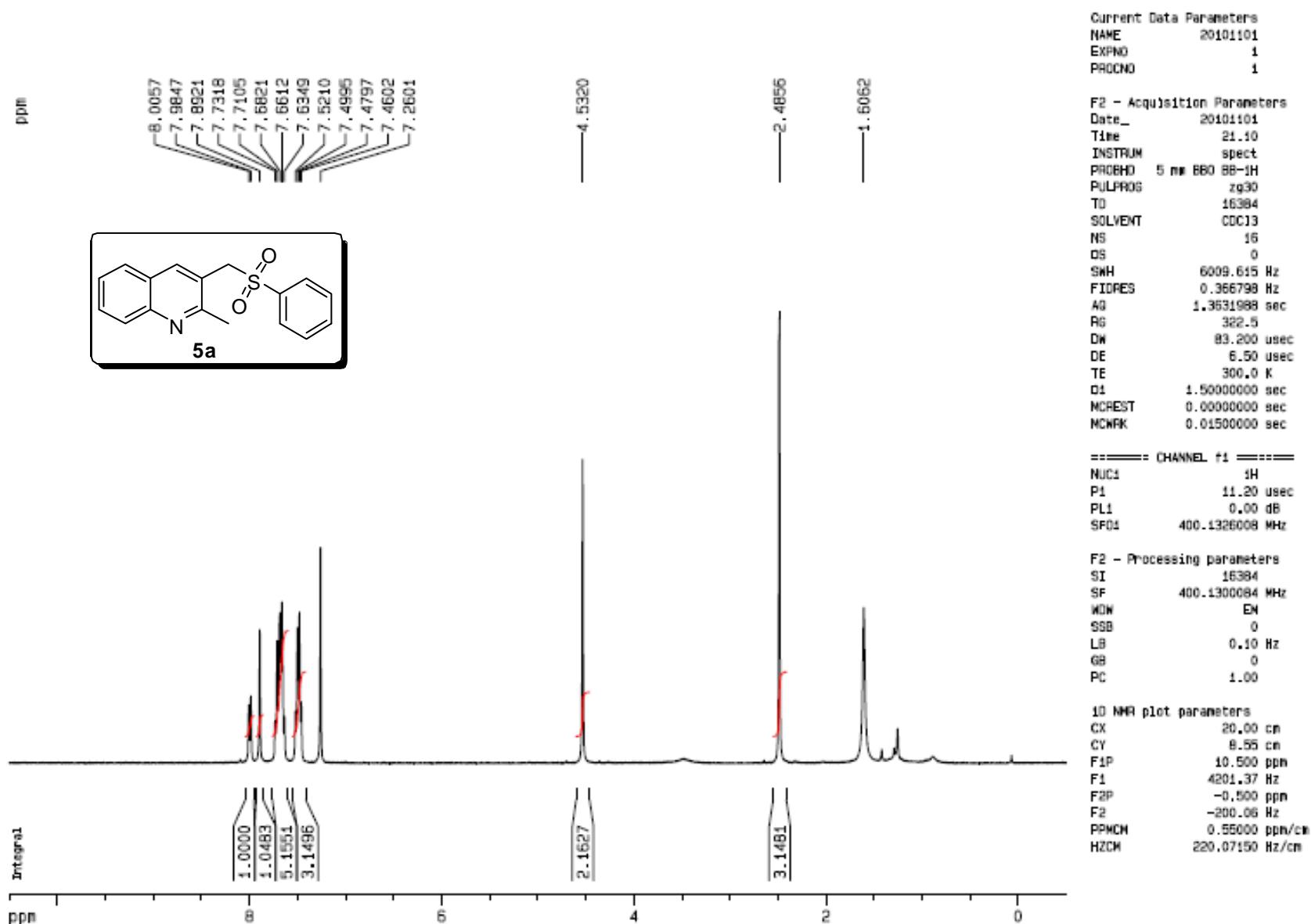


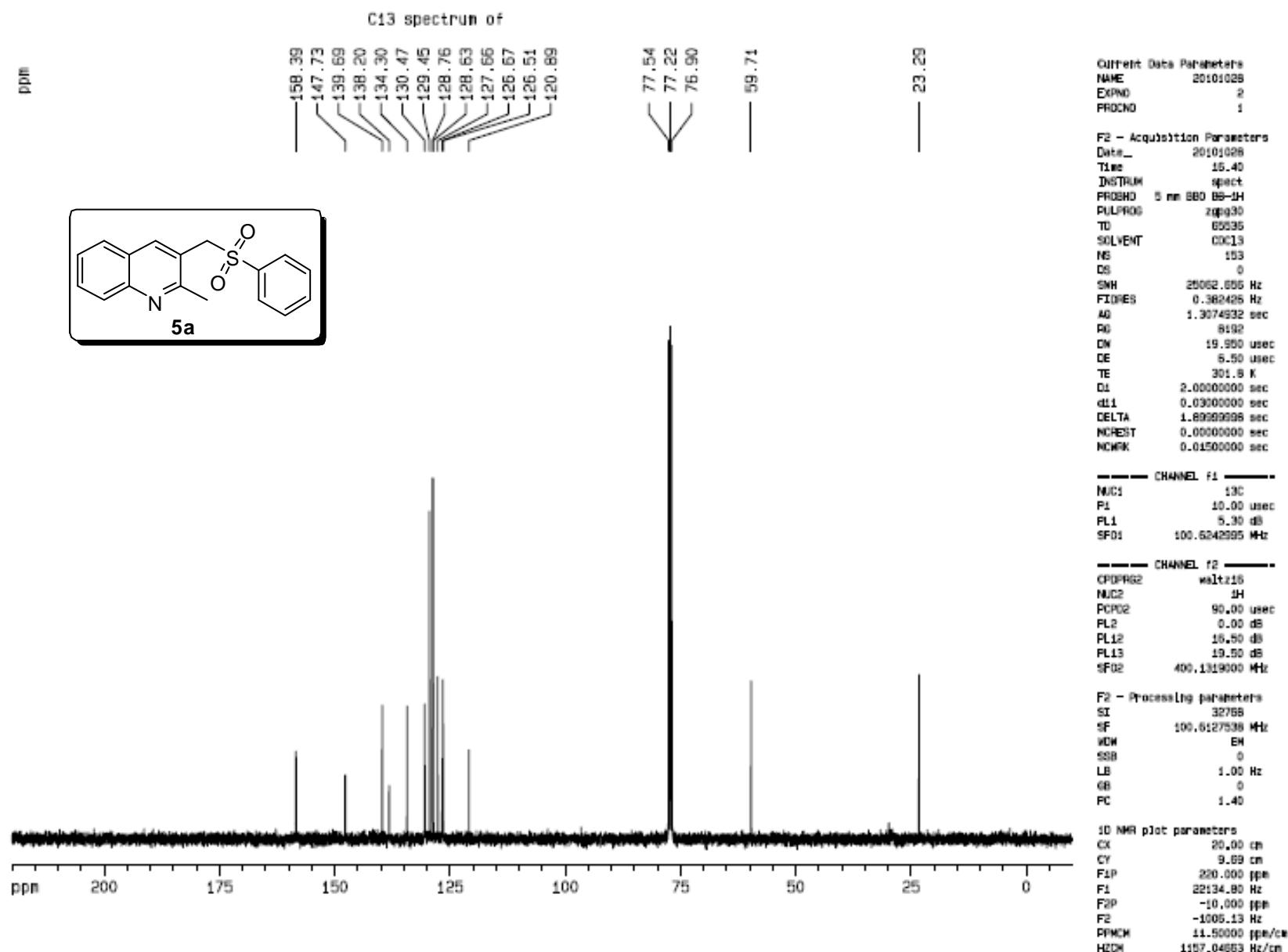


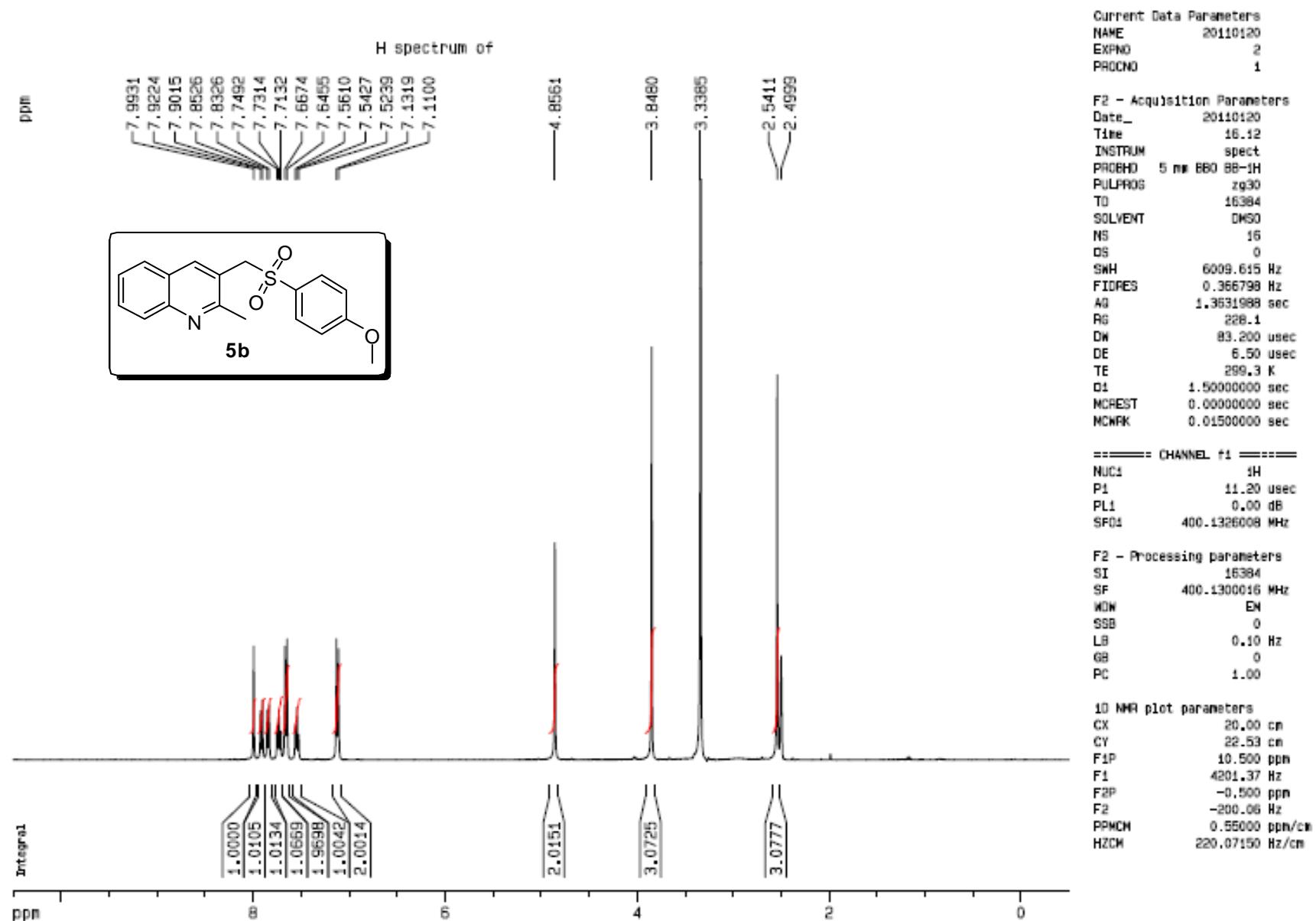


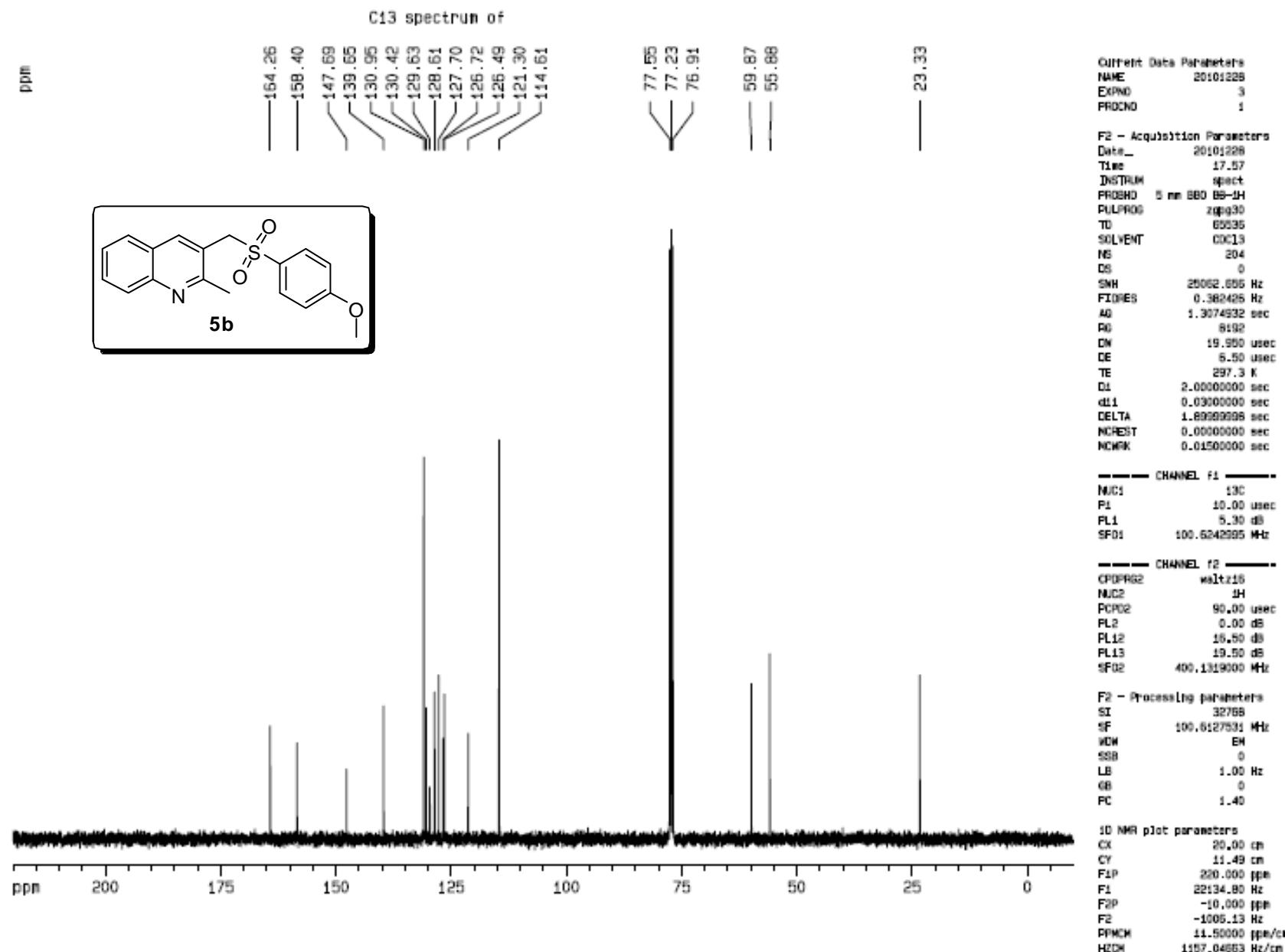


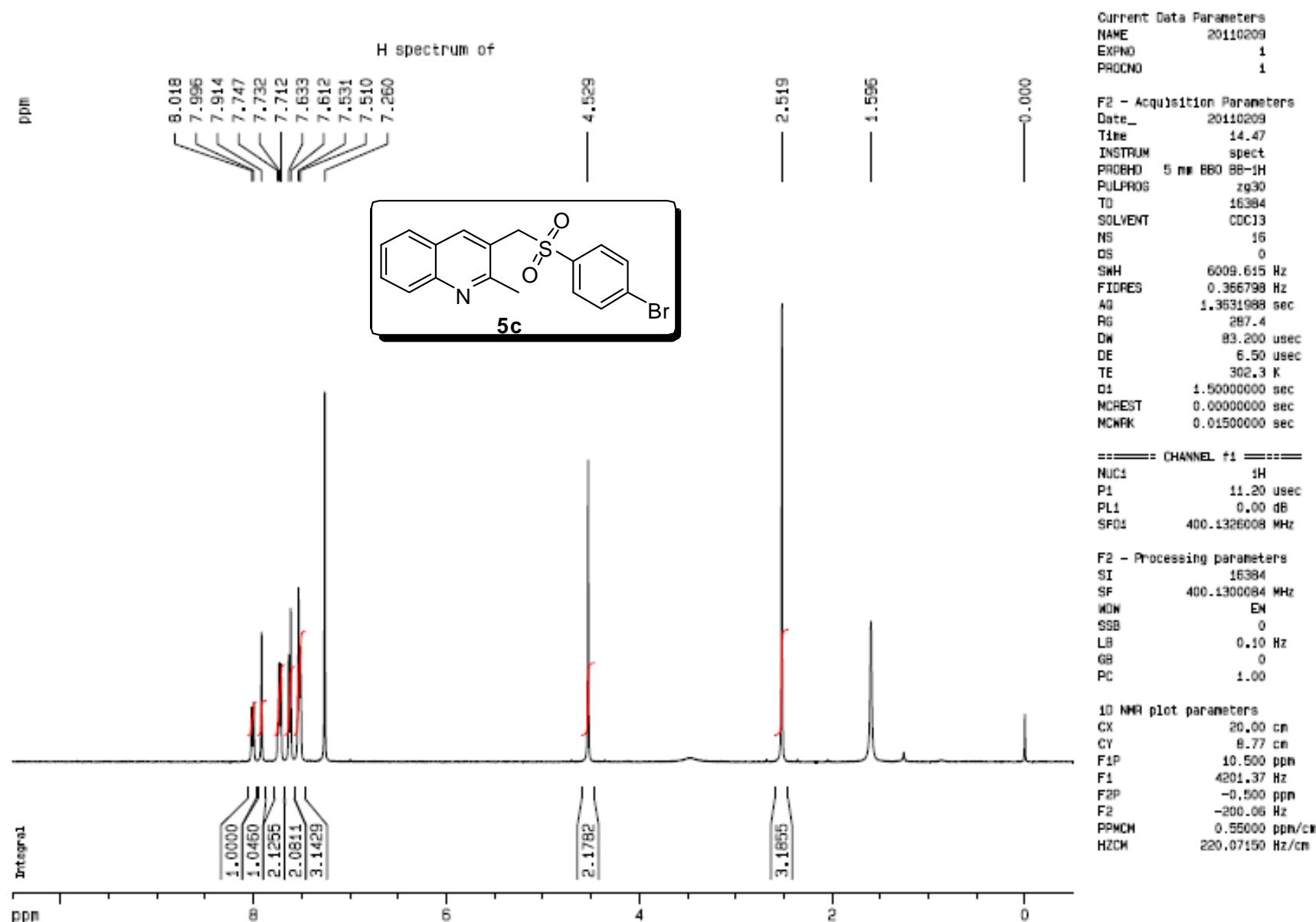
C₁₃ spectrum of

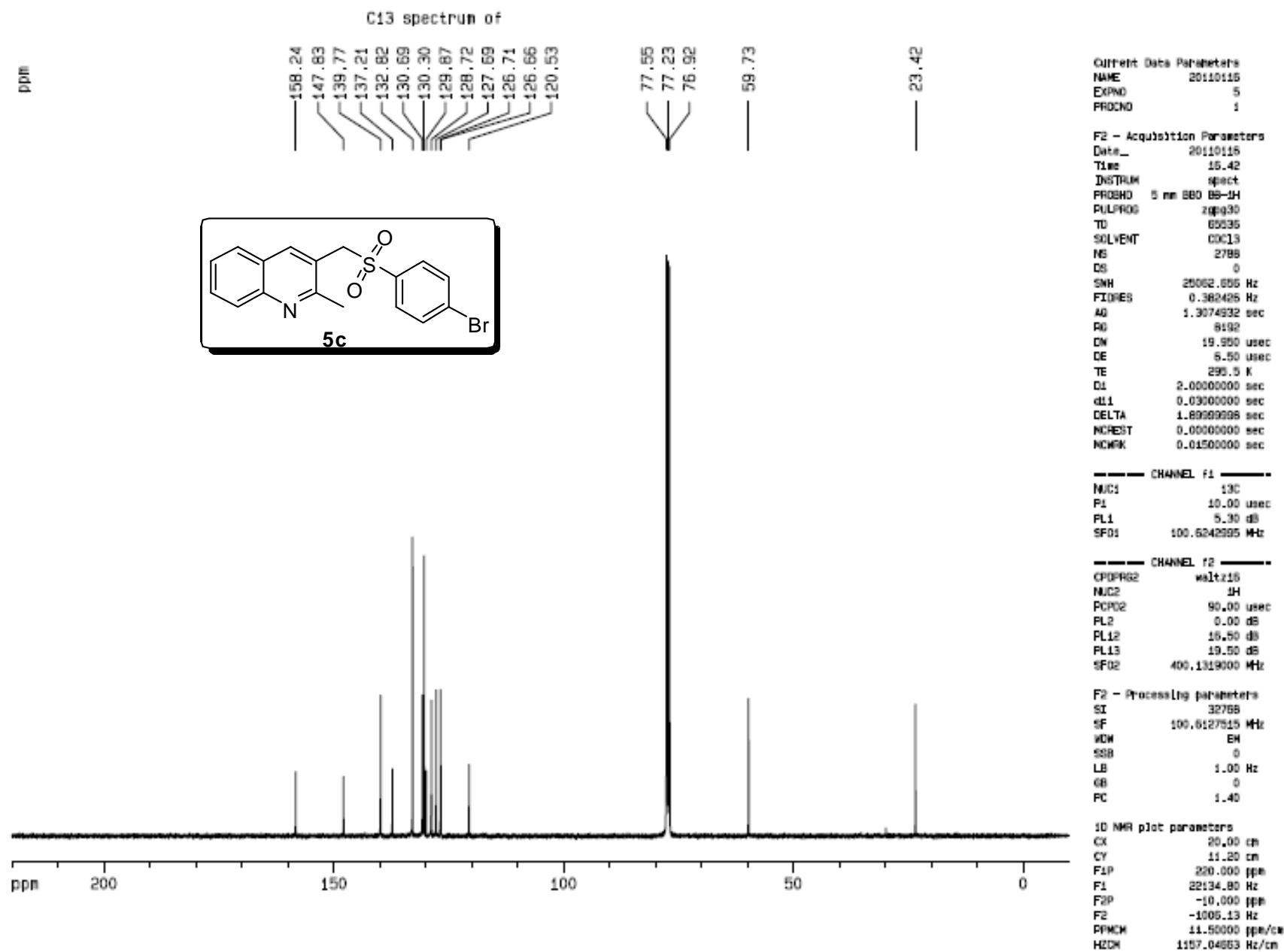


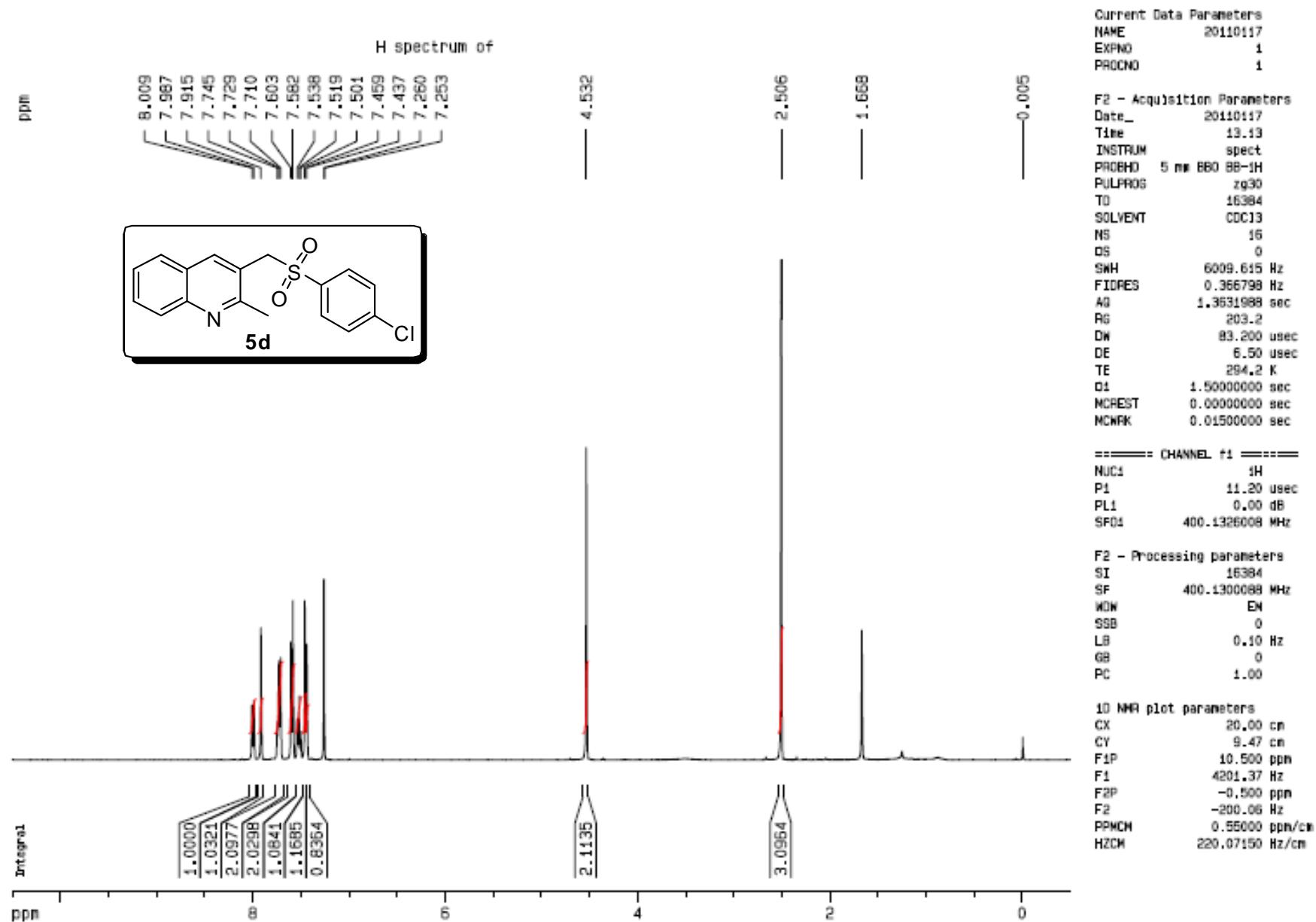


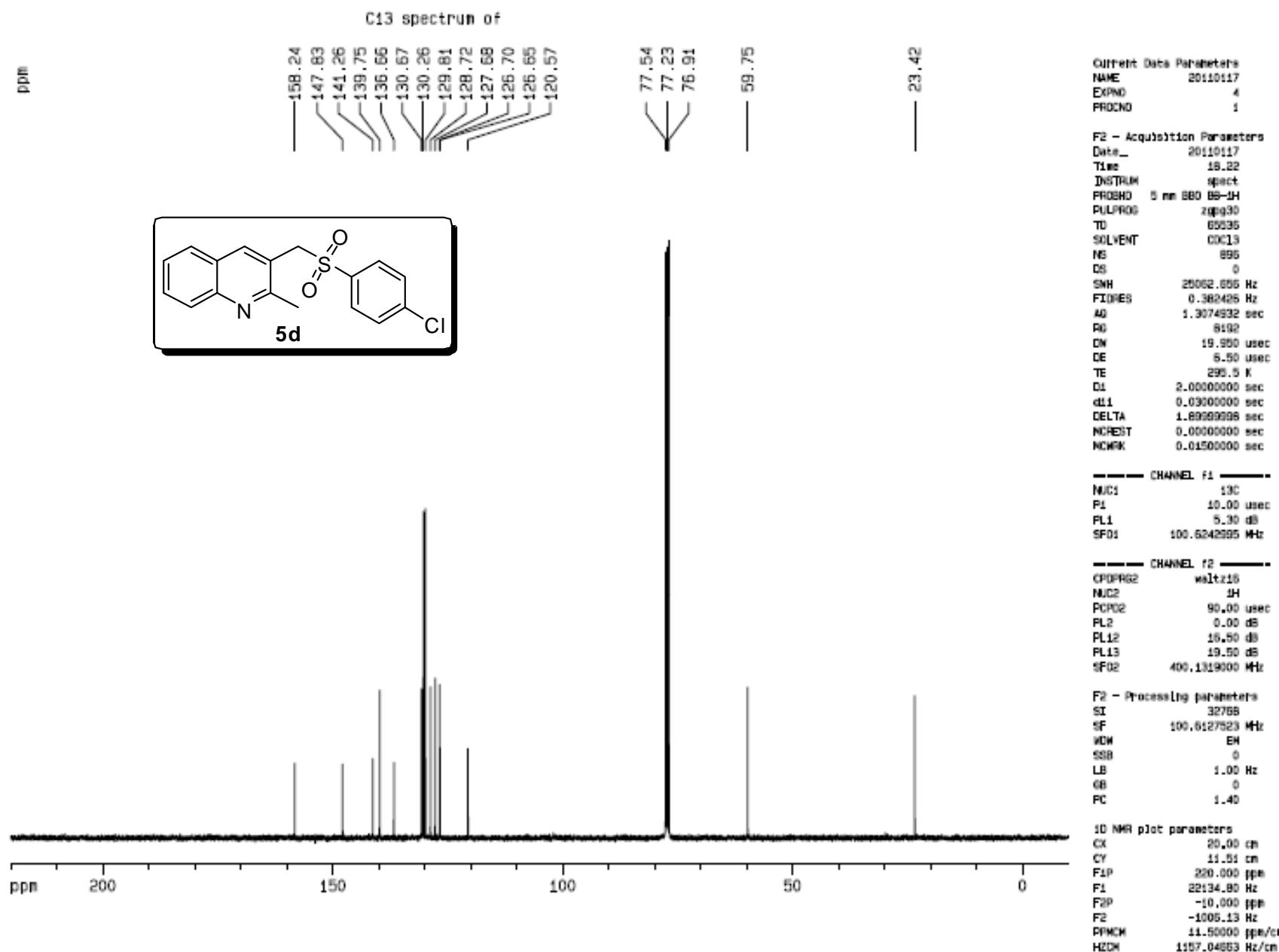


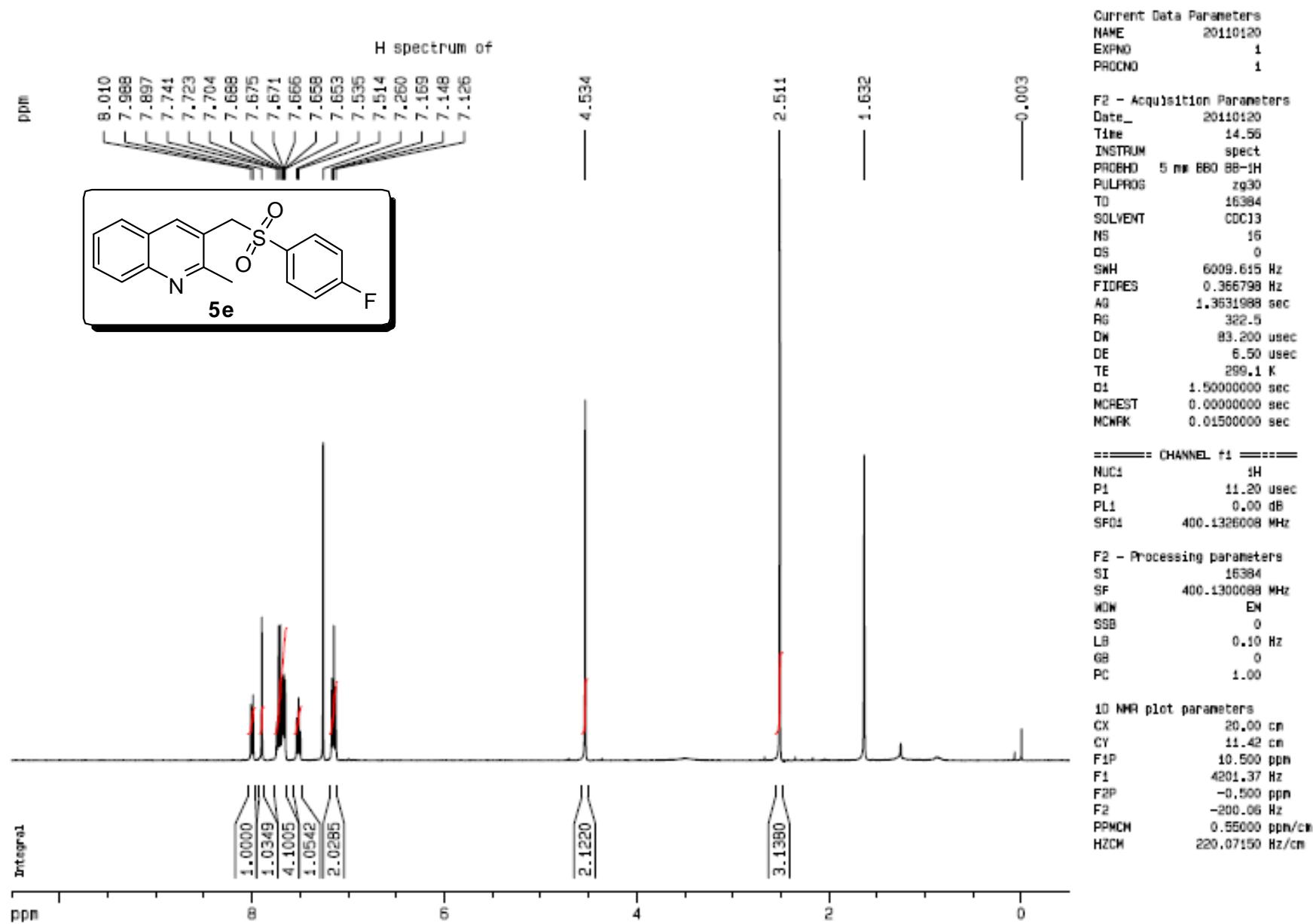


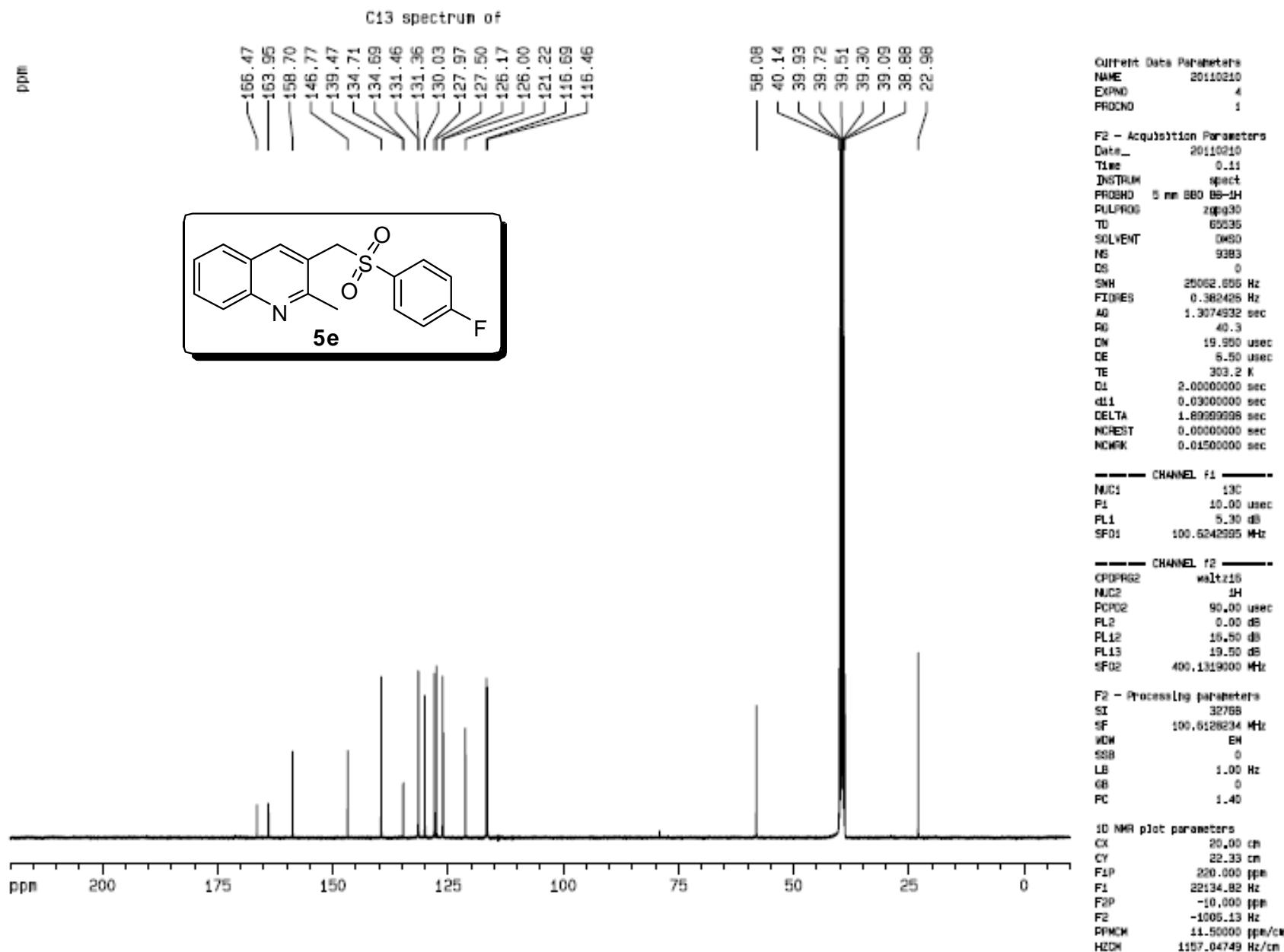


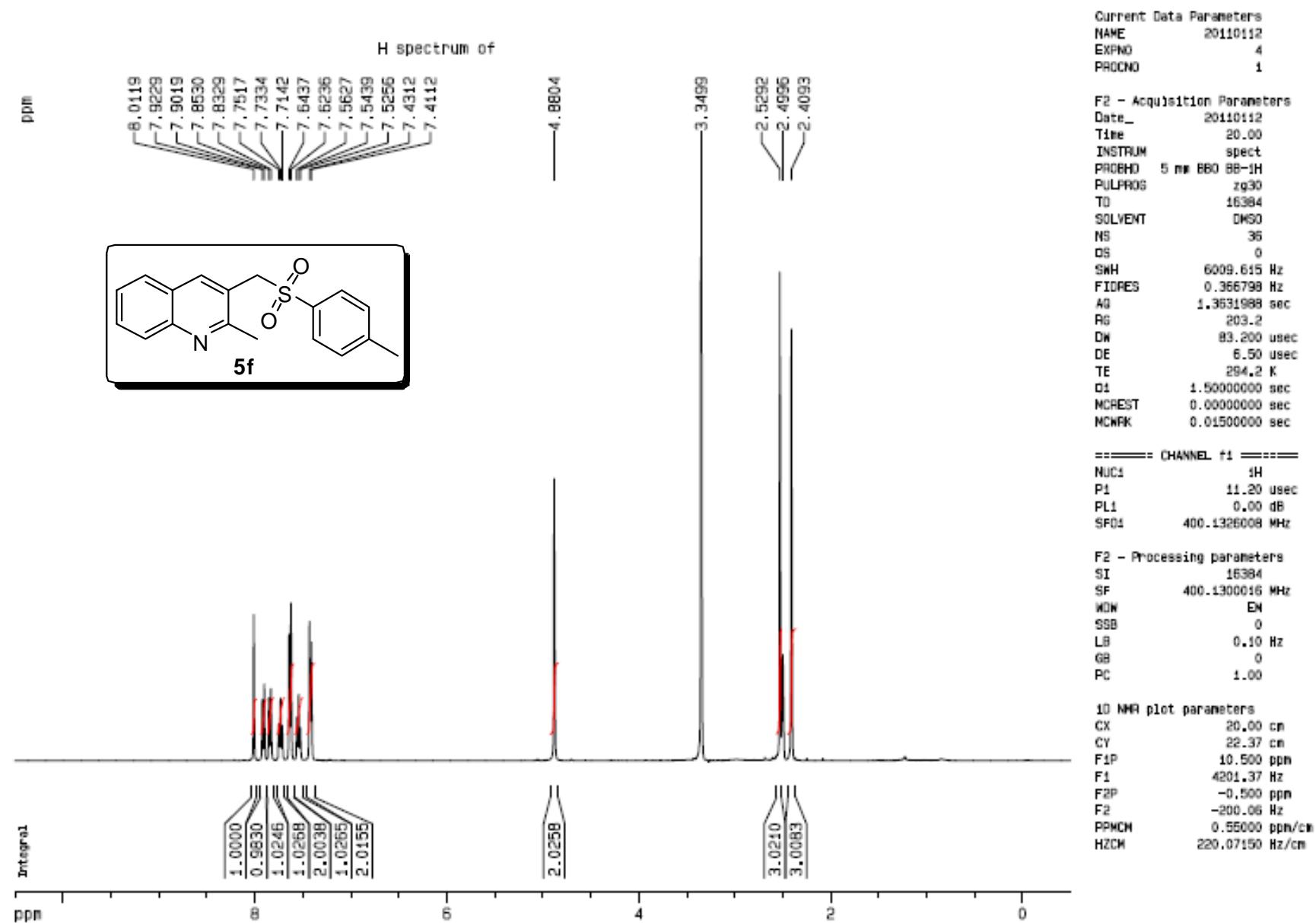


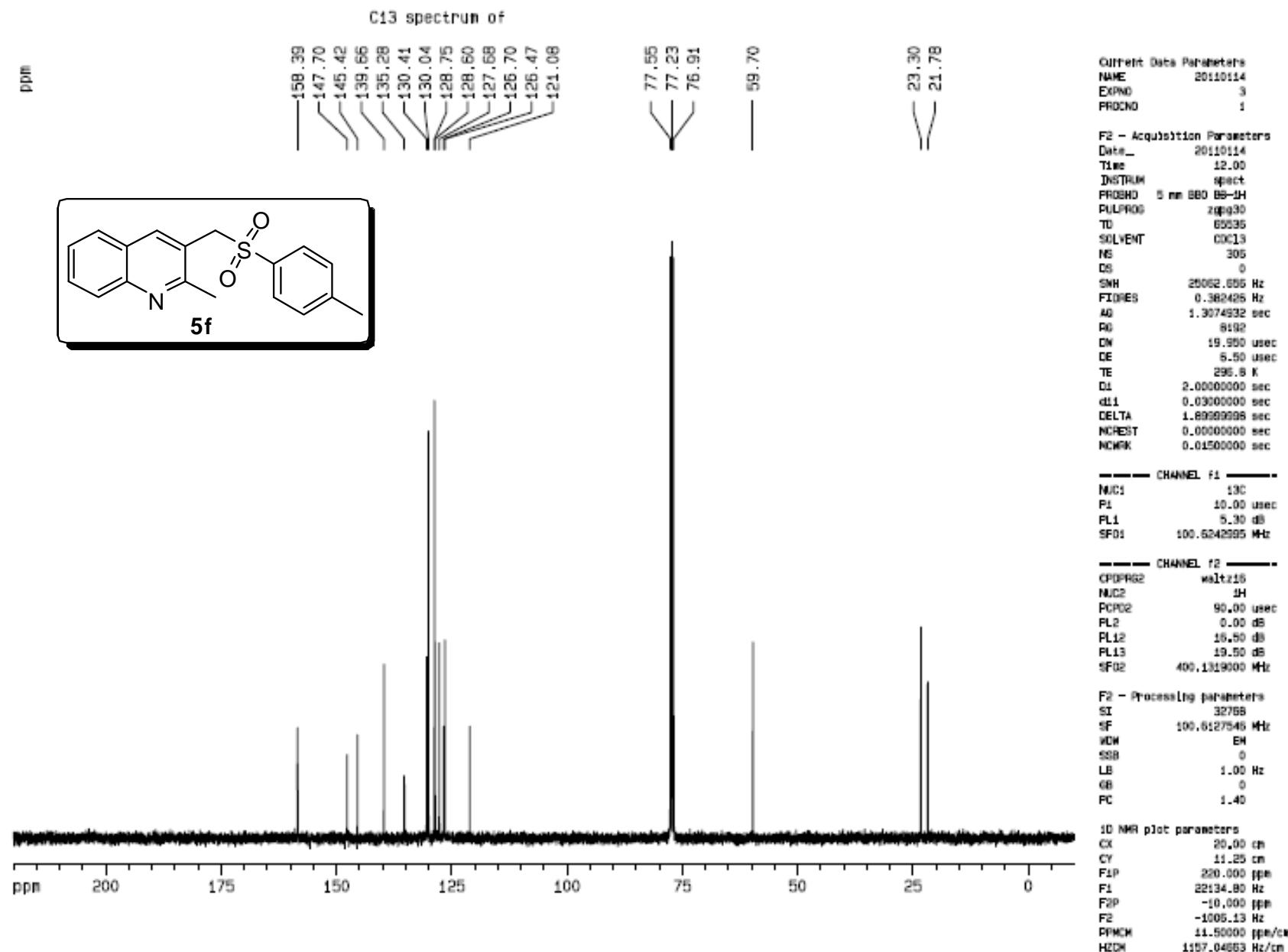


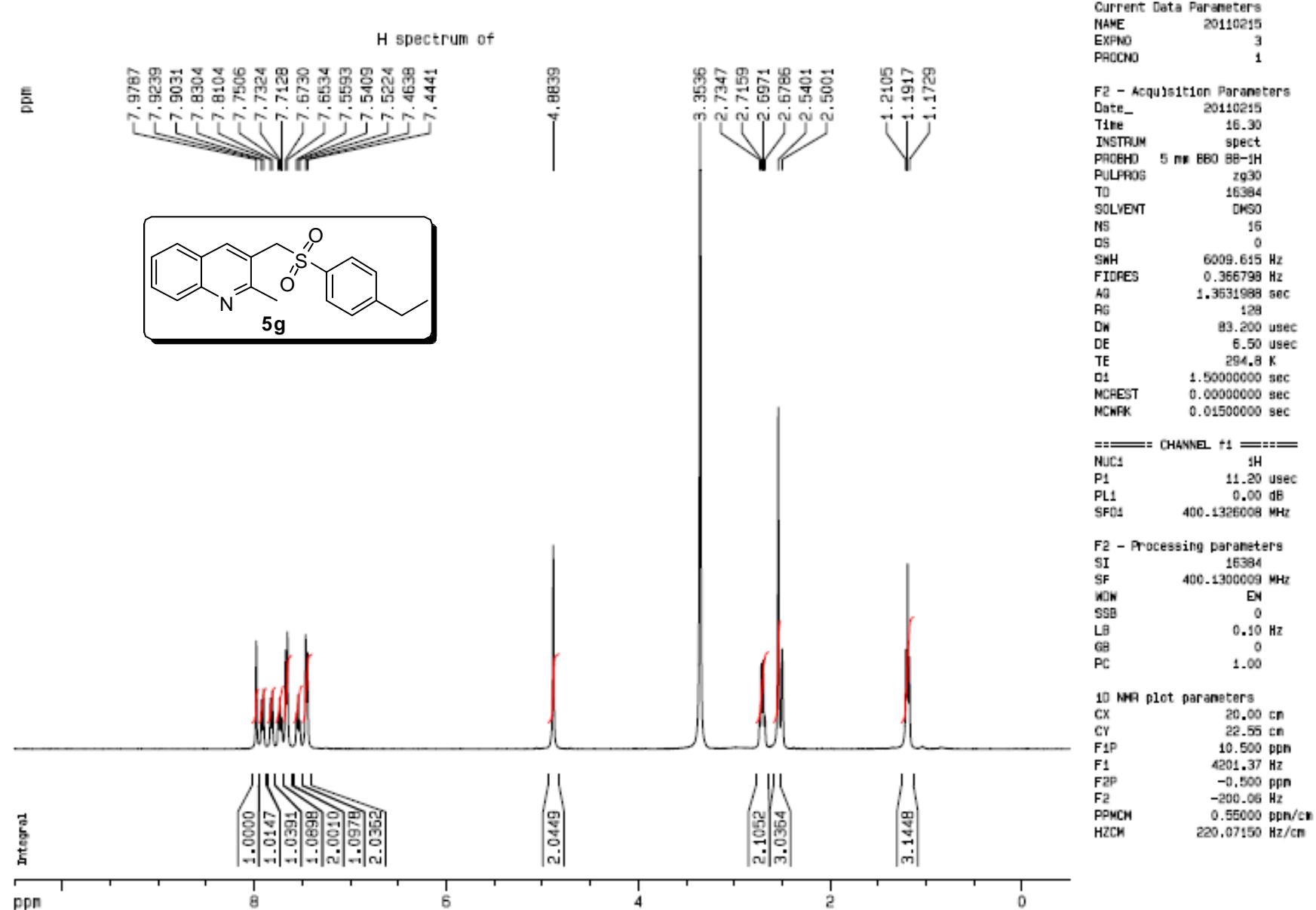


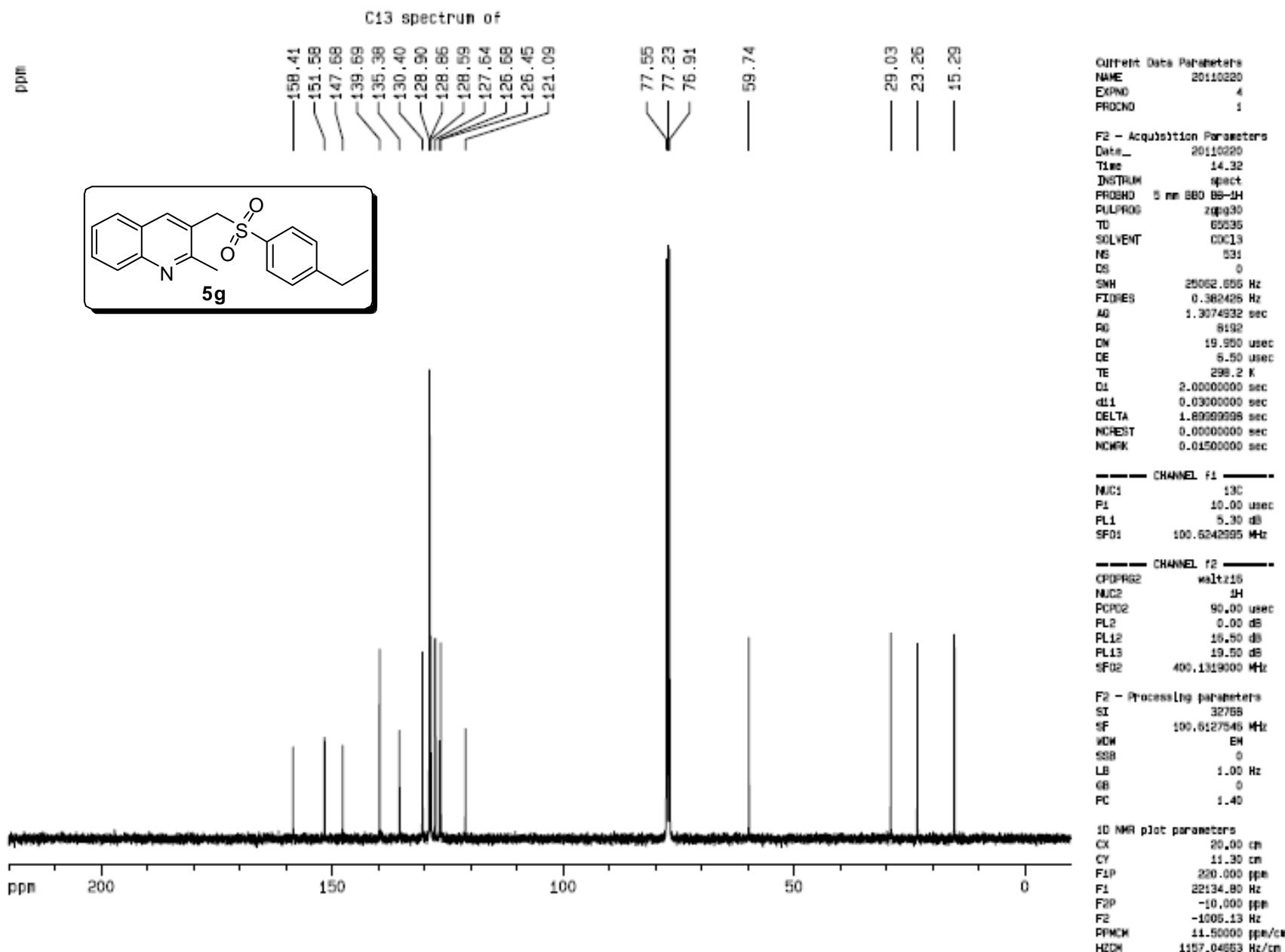


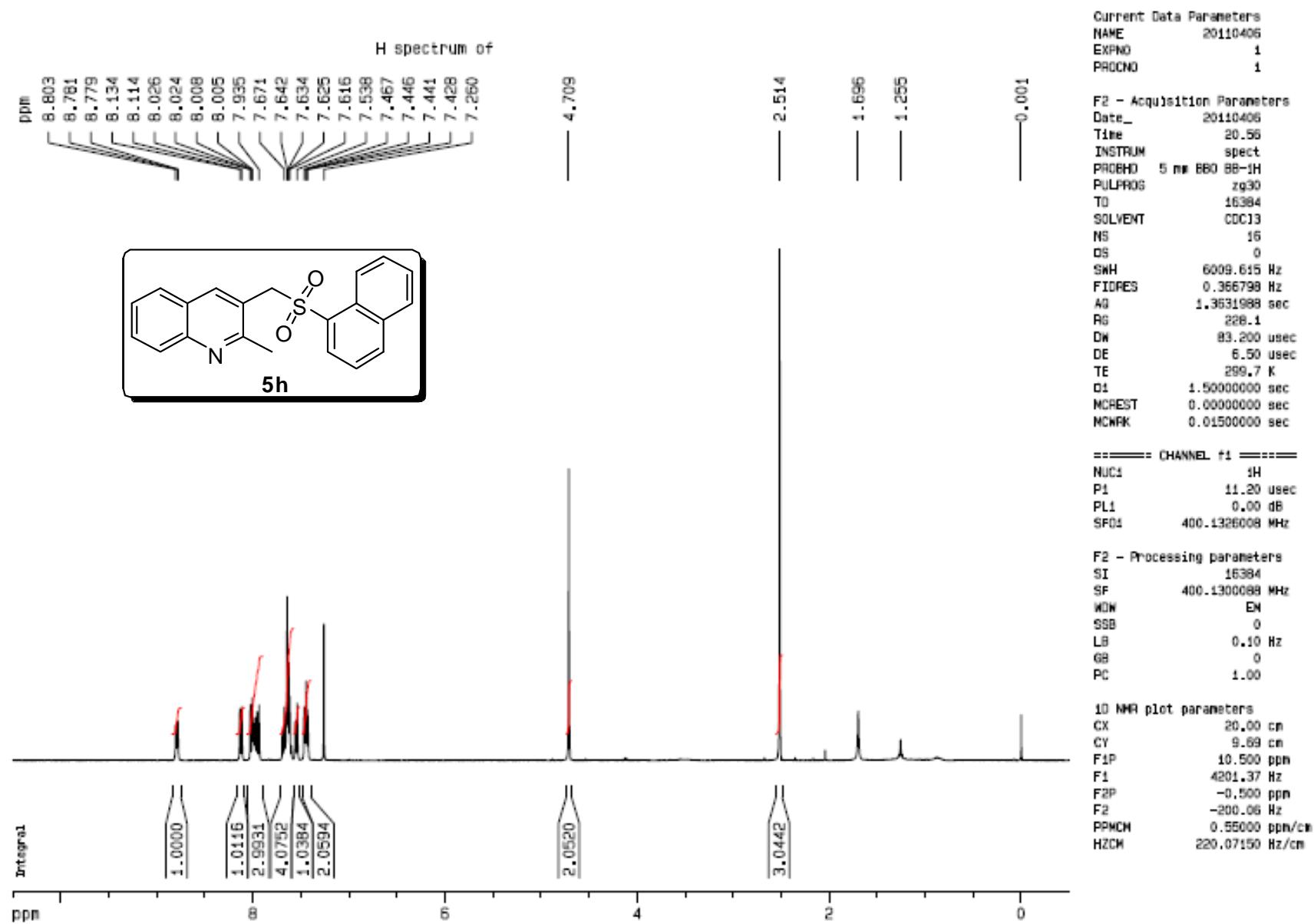


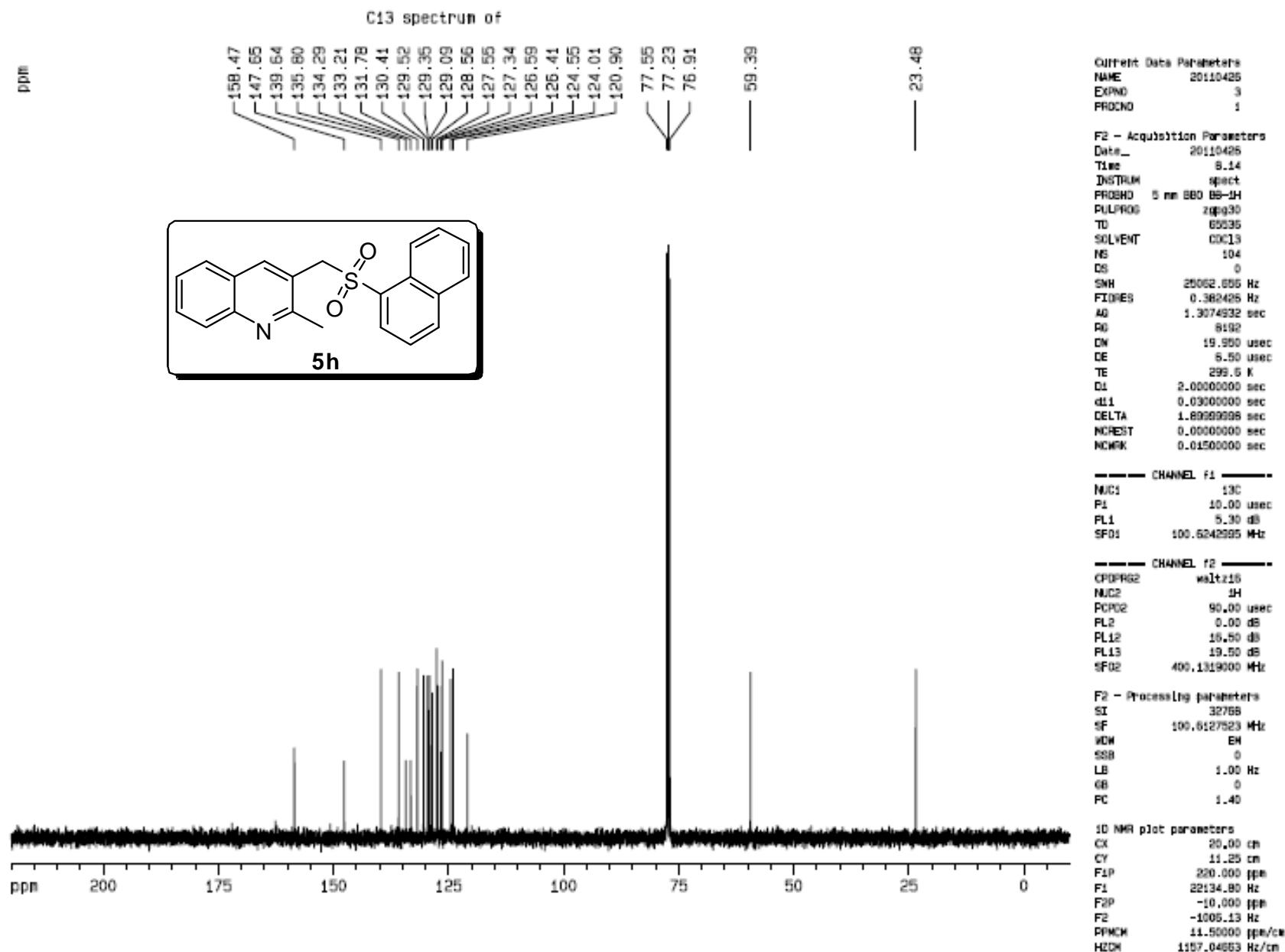


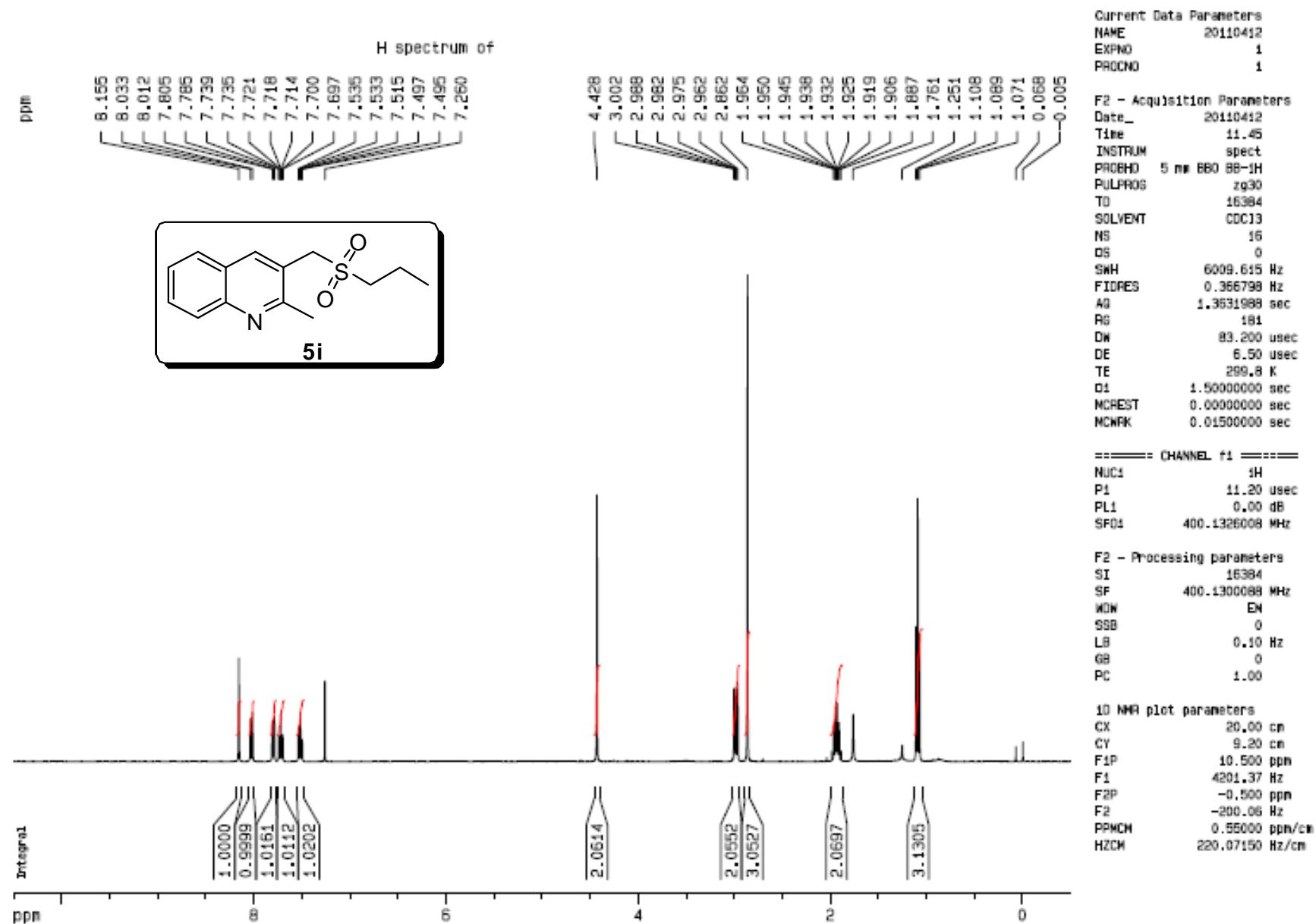


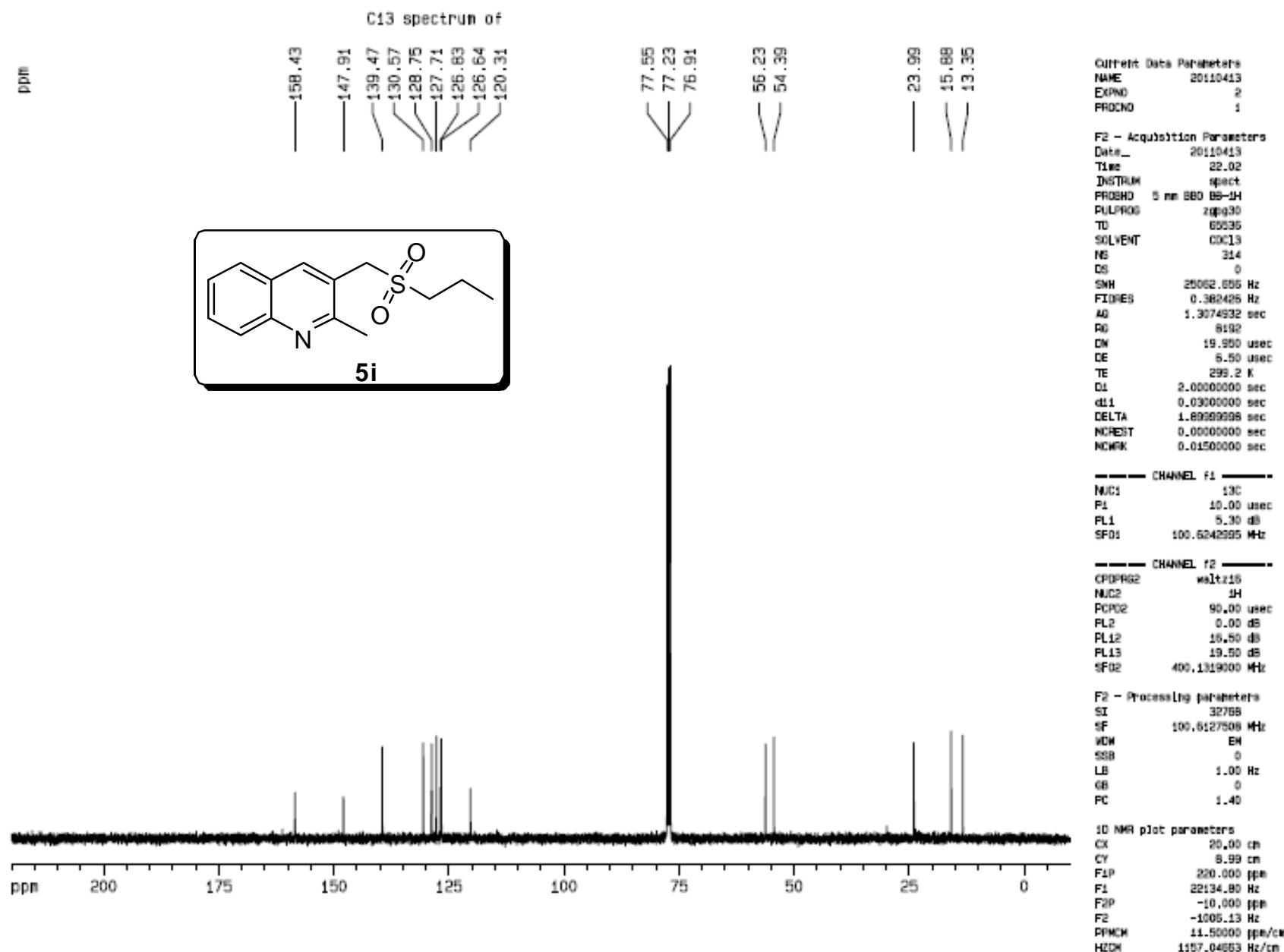


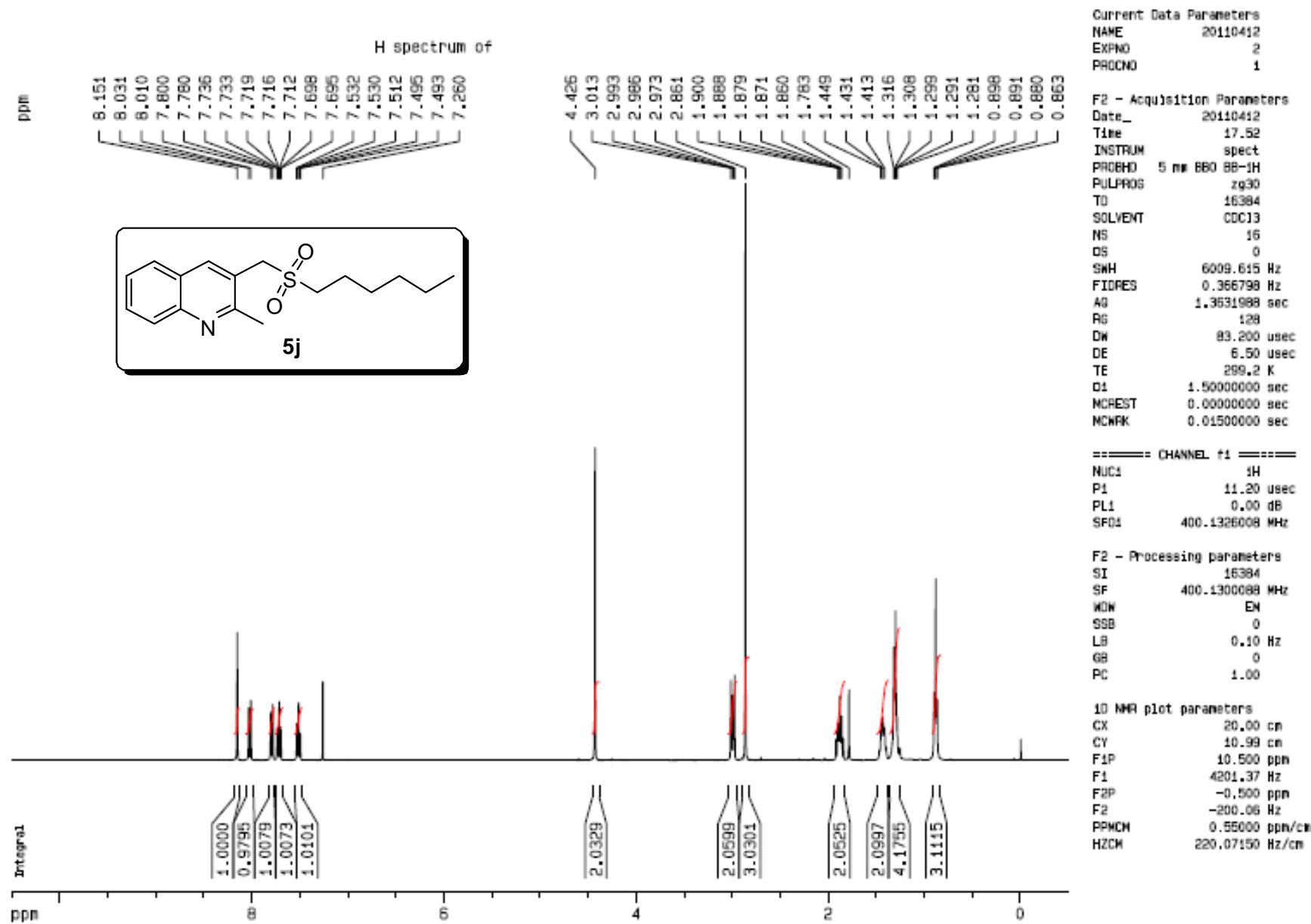


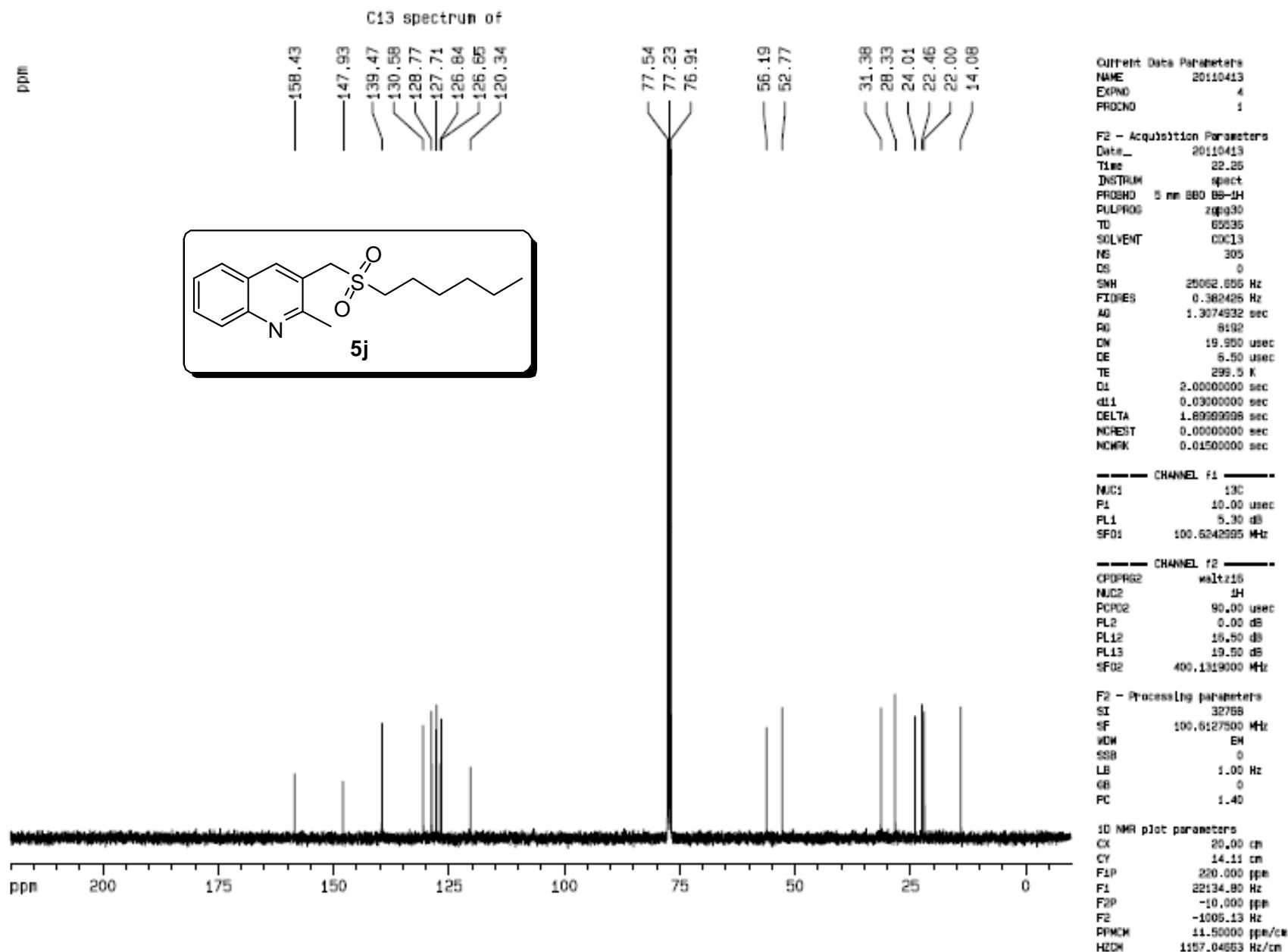


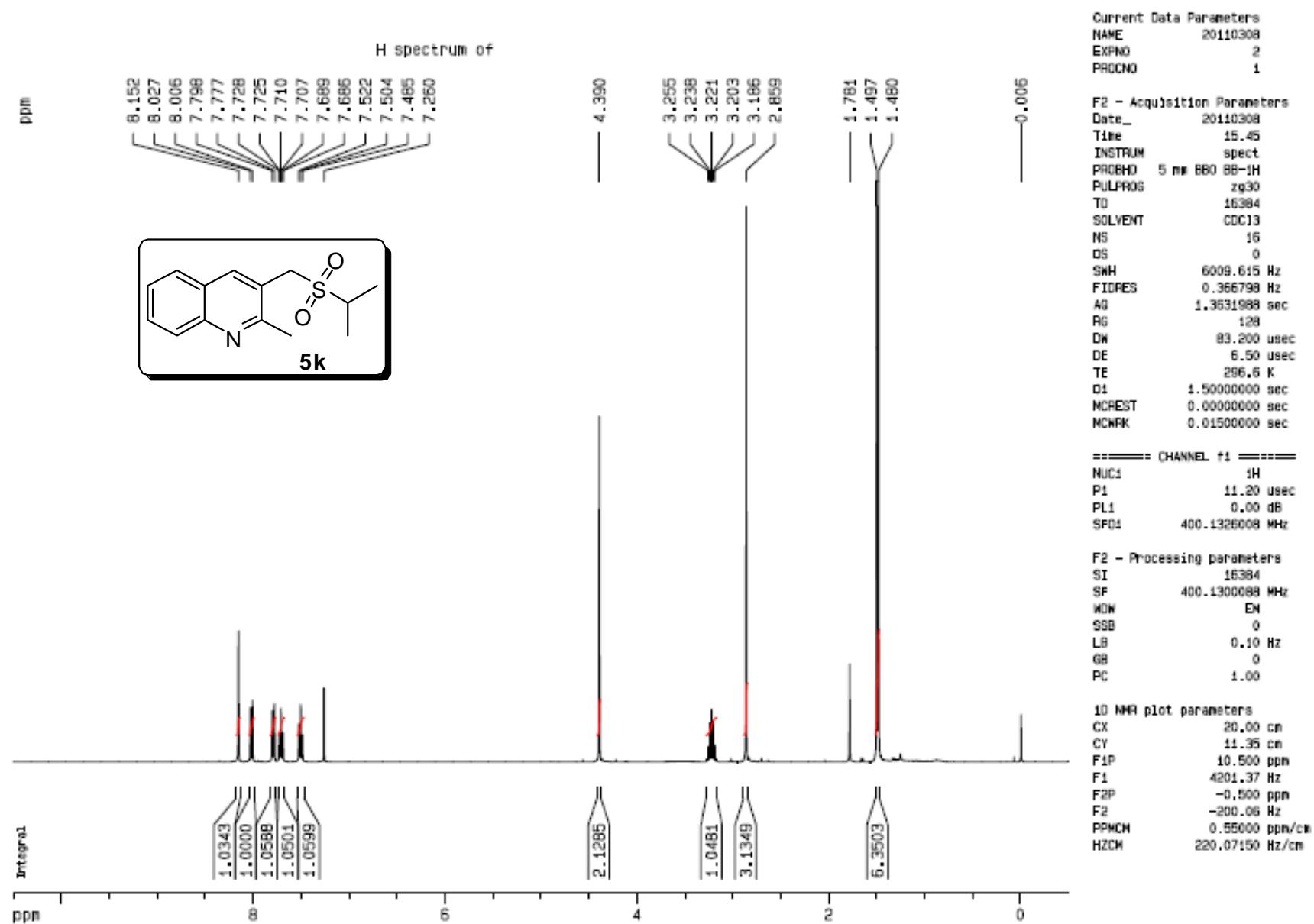


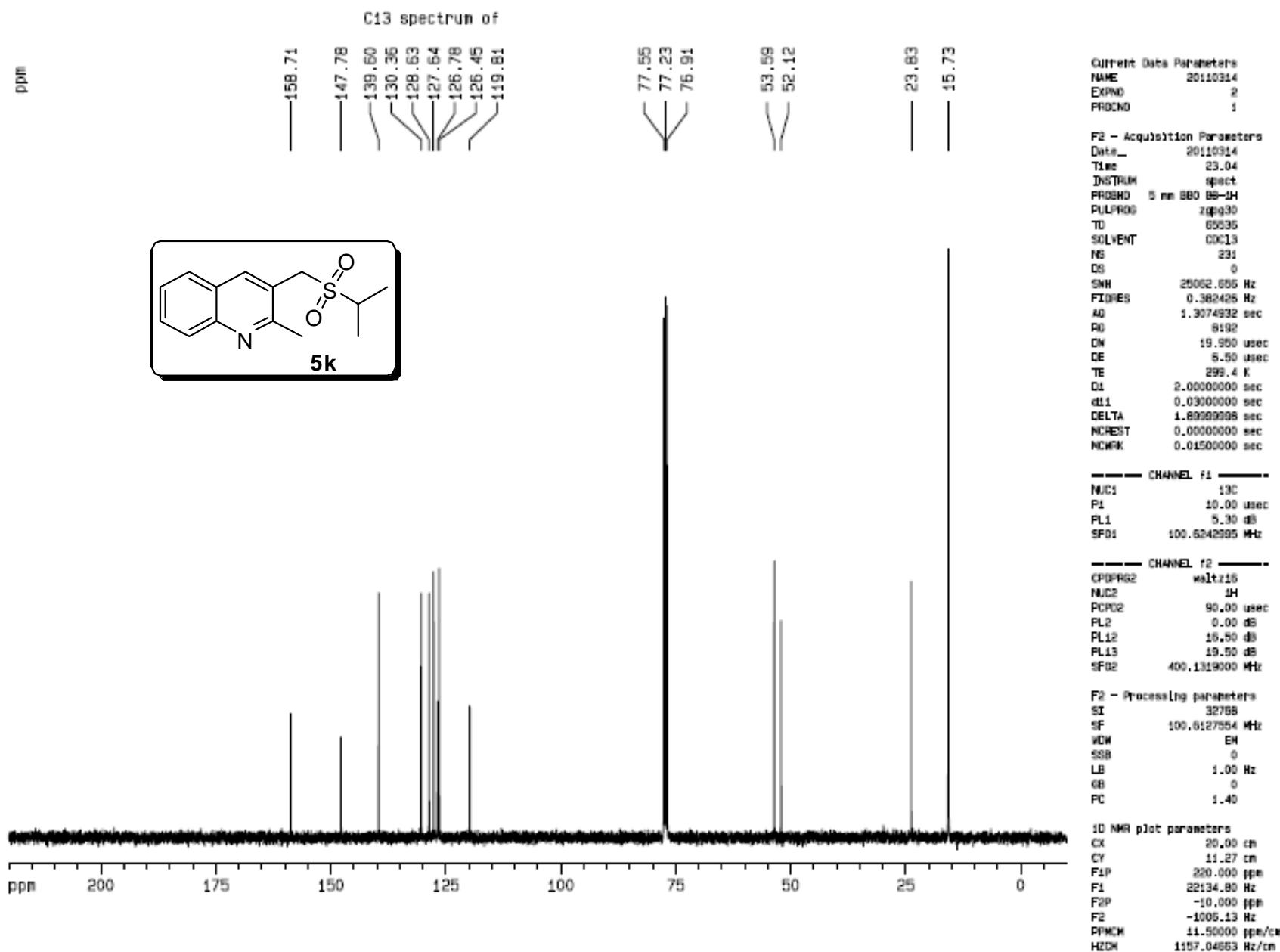


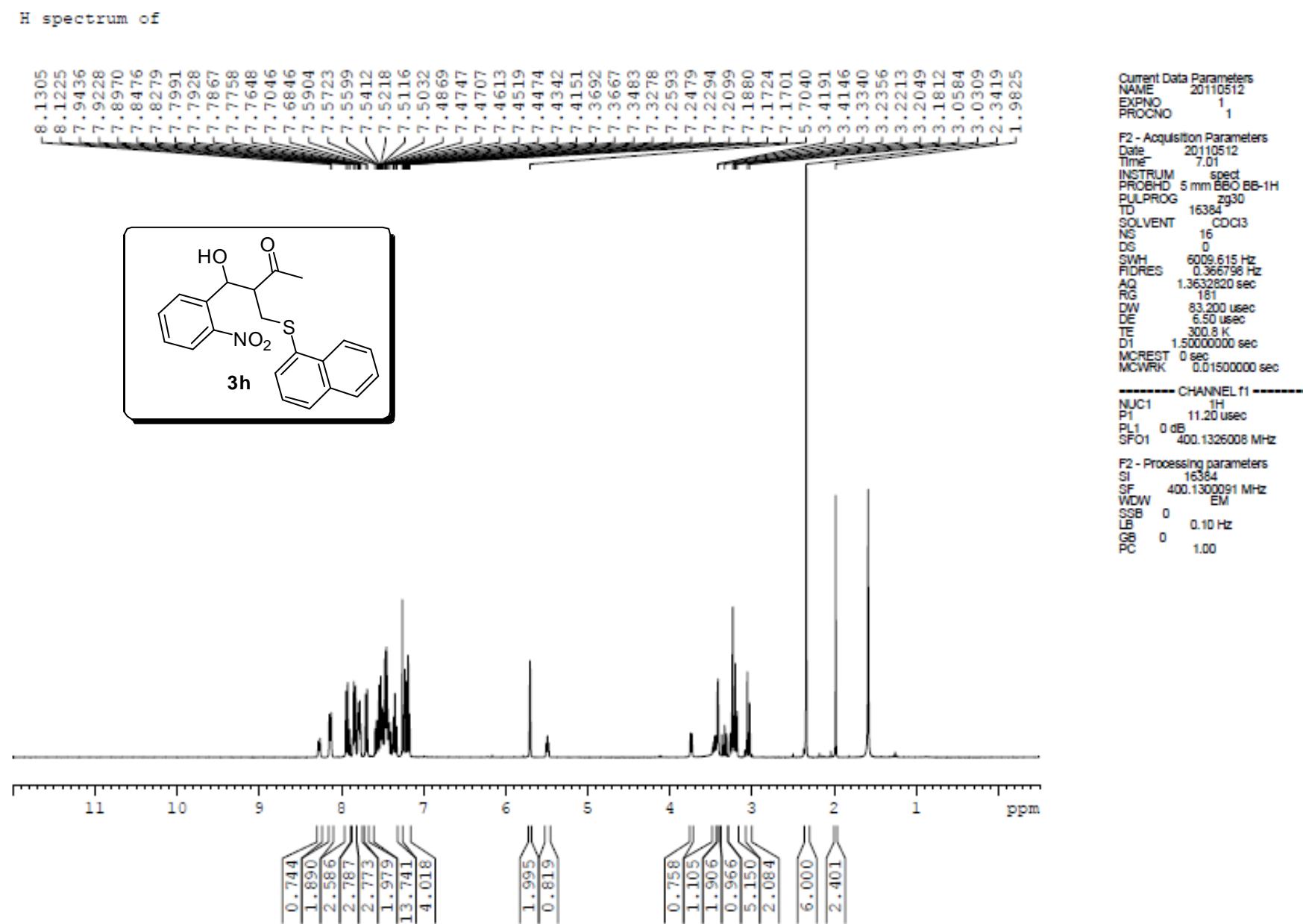


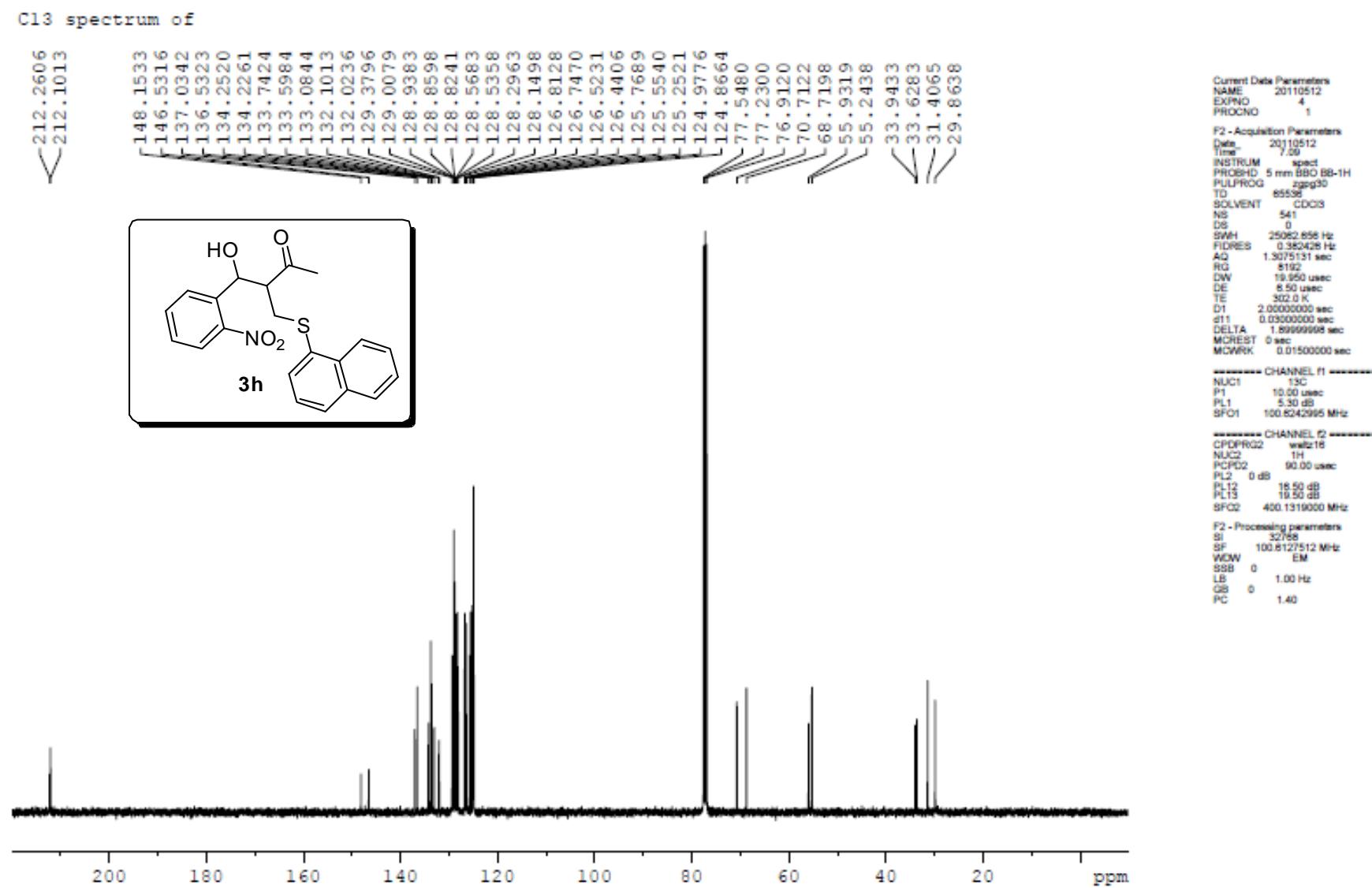












Crystallographic description of 3h:

Identification code	a12327
Empirical formula	C ₂₁ H ₁₉ N O ₄ S
Formula weight	381.43
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 21/c
Unit cell dimensions	a = 32.290(4) Å α = 90°. b = 7.4466(9) Å β = 103.742(6)° c = 15.7324(16) Å γ = 90°.
Volume	3674.6(7) Å ³
Z	8
Density (calculated)	1.379 Mg/m ³
Absorption coefficient	0.204 mm ⁻¹
F(000)	1600
Crystal size	0.44 × 0.32 × 0.08 mm ³
Theta range for data collection	1.30 to 25.02°.
Index ranges	-29 ≤ h ≤ 38, -7 ≤ k ≤ 8, -16 ≤ l ≤ 18
Reflections collected	13232
Independent reflections	6139 [R(int) = 0.0734]
Completeness to theta = 25.02°	94.4%
Absorption correction	multi-scan
Max. and min. transmission	0.9839 and 0.9158
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6139 / 0 / 277
Goodness-of-fit on F ²	1.183
Final R indices [I>2sigma(I)]	R1 = 0.2457, wR2 = 0.4913
R indices (all data)	R1 = 0.2811, wR2 = 0.5062
Largest diff. peak and hole	1.222 and -0.713 e.Å ⁻³