Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

A Mechanistic Study on Hooker Oxidation: Synthesis of Novel Indane Carboxylic acid Derivatives from Lapachol

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General Considerations: All the solvents were distilled prior to use. Dry solvents were prepared according to the standard procedures. Reactions requiring inert atmosphere were carried out under argon atmosphere. Infrared (IR) spectra were recorded on a Shimadzu IR 470 spectrometer (or) THERMO NICOLET 6700 FT-IR spectrometer. ^{1}H NMR spectra were measured on Bruker ADVANCE 400 MHz spectrometers. Chemical shifts were reported in ppm using tetramethylsilane as an internal standard. ^{13}C NMR spectra were recorded on Bruker 100 MHz spectrometers with complete proton decoupling. Chemical shifts were reported in ppm from the residual solvent as an internal standard. The high-resolution mass spectra (HRMS) were performed on Micromass Q-TOF micro mass spectrometer equipped with a Harvard apparatus syringe pump. X-ray crystallographic data were recorded using Bruker-AXS Kappa CCD-Diffractometer with graphite-monochromator $Cu_{K\alpha}$ radiation (λ=1.5418 A). The structures were solved by direct methods (SHELXS-97) and refined by full-matrix least squares techniques against *F2* (SHELXL-97). Hydrogen atoms were inserted from geometry consideration using the HFIX option of the program. For thin layer chromatography (TLC) analysis throughout this work, E-merck precoated TLC plates (silica gel 60 F254 grade, 0.25 mm) were used. Acme (India) silica gel (100-200 mesh) was used for column chromatography.

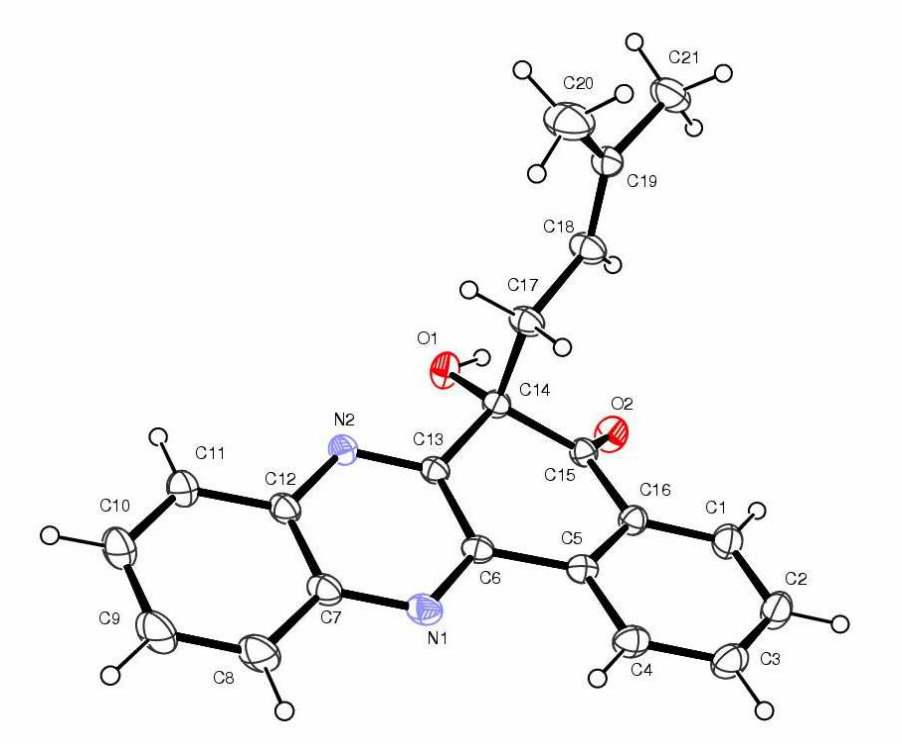
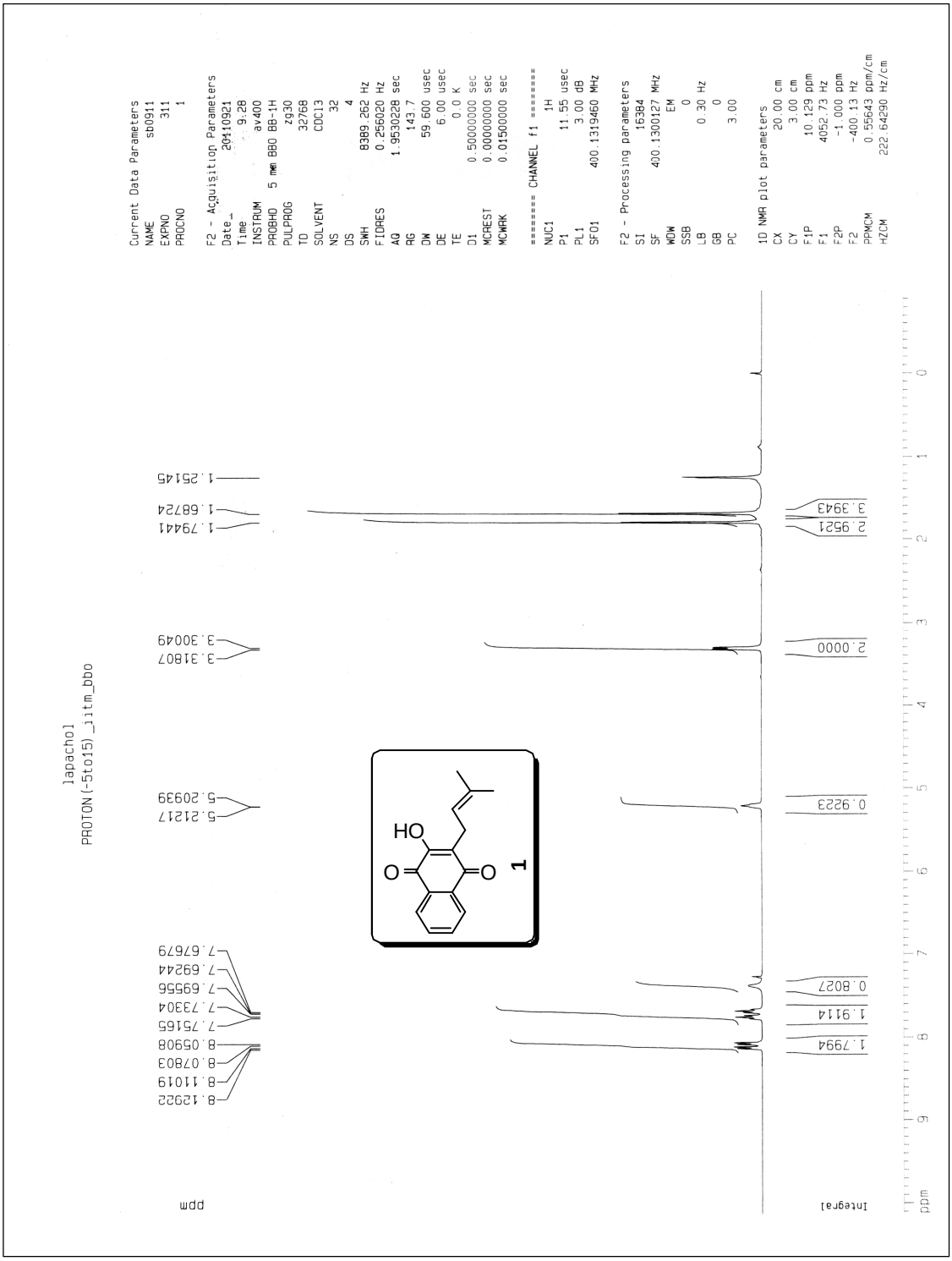


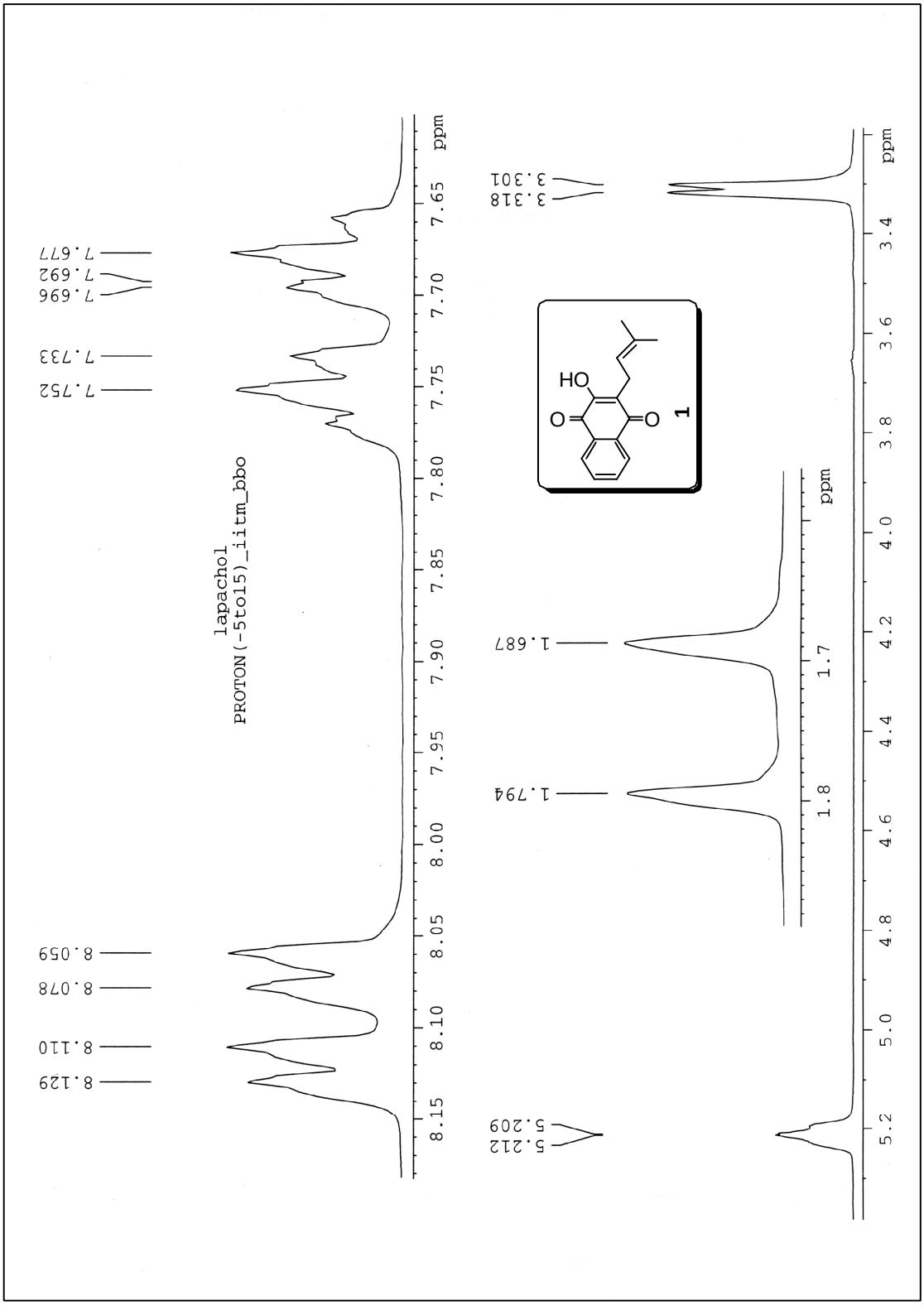
Table 1. Crystal data and structure refinement for new.

Identification code	new
Empirical formula	C21 H18 N2 O2
Formula weight	330.37
Temperature	298(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 11.3037(4) A alpha = 90 deg. b = 17.9419(6) A beta = 105.439(2) deg. c = 8.3981(3) A gamma = 90 deg.
Volume	1641.76(10) A^3
Z, Calculated density	4, 1.337 Mg/m^3
Absorption coefficient	0.087 mm^-1

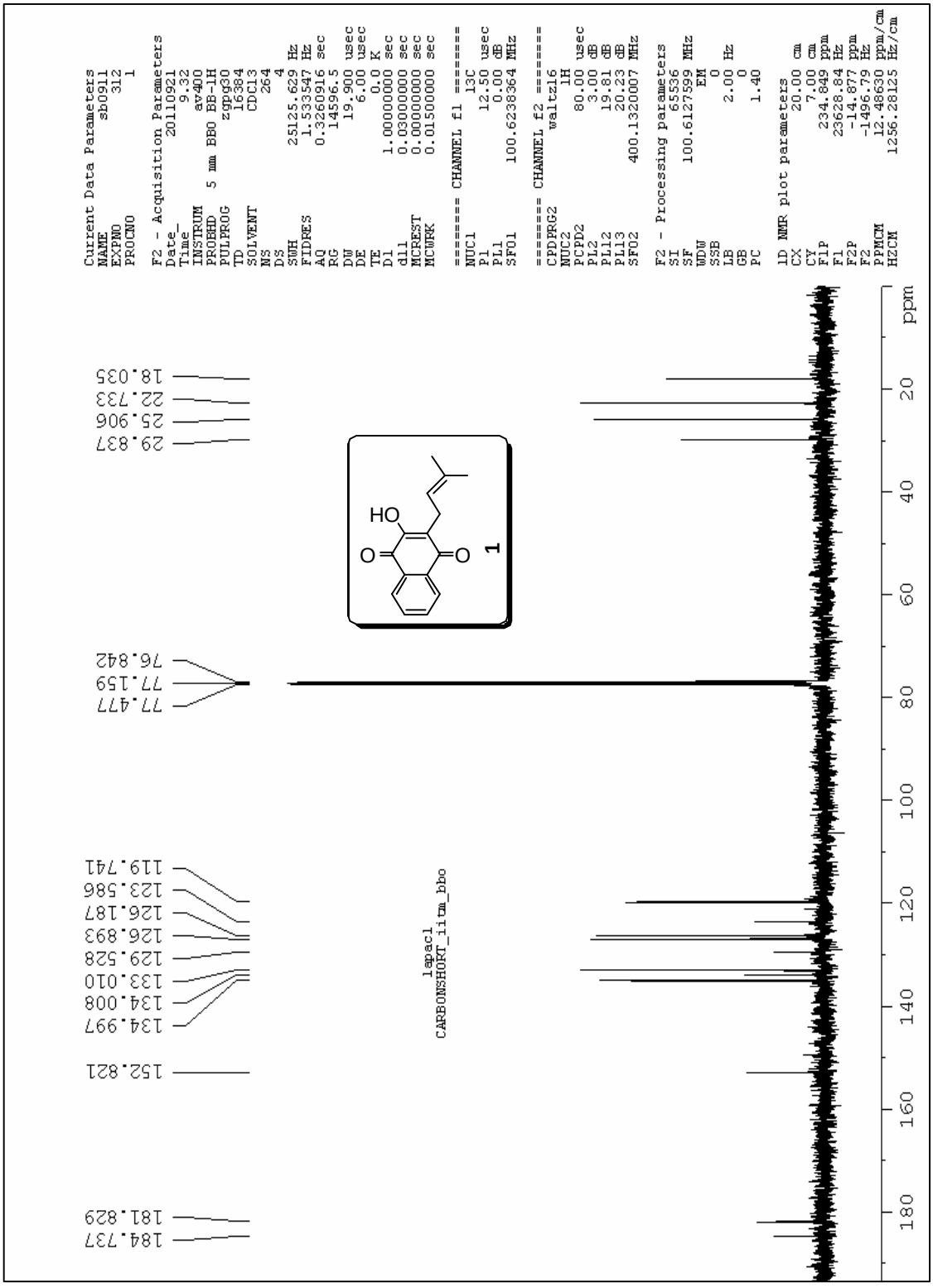
F(000)	696
Crystal size	0.48 x 0.35 x 0.28 mm
Theta range for data collection	1.87 to 34.28 deg.
Limiting indices	-13<=h<=17, -27<=k<=28, -13<=l<=12
Reflections collected / unique	20040 / 6204 [R(int) = 0.0216]
Completeness to theta = 25.00	96.7 %
Absorption correction	Multi-scan
Max. and min. transmission	0.9761 and 0.9594
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6204 / 0 / 232
Goodness-of-fit on F^2	1.039
Final R indices [I>2sigma(I)]	R1 = 0.0516, wR2 = 0.1406
R indices (all data)	R1 = 0.0776, wR2 = 0.1633
Largest diff. peak and hole	0.377 and -0.192 e.A^-3



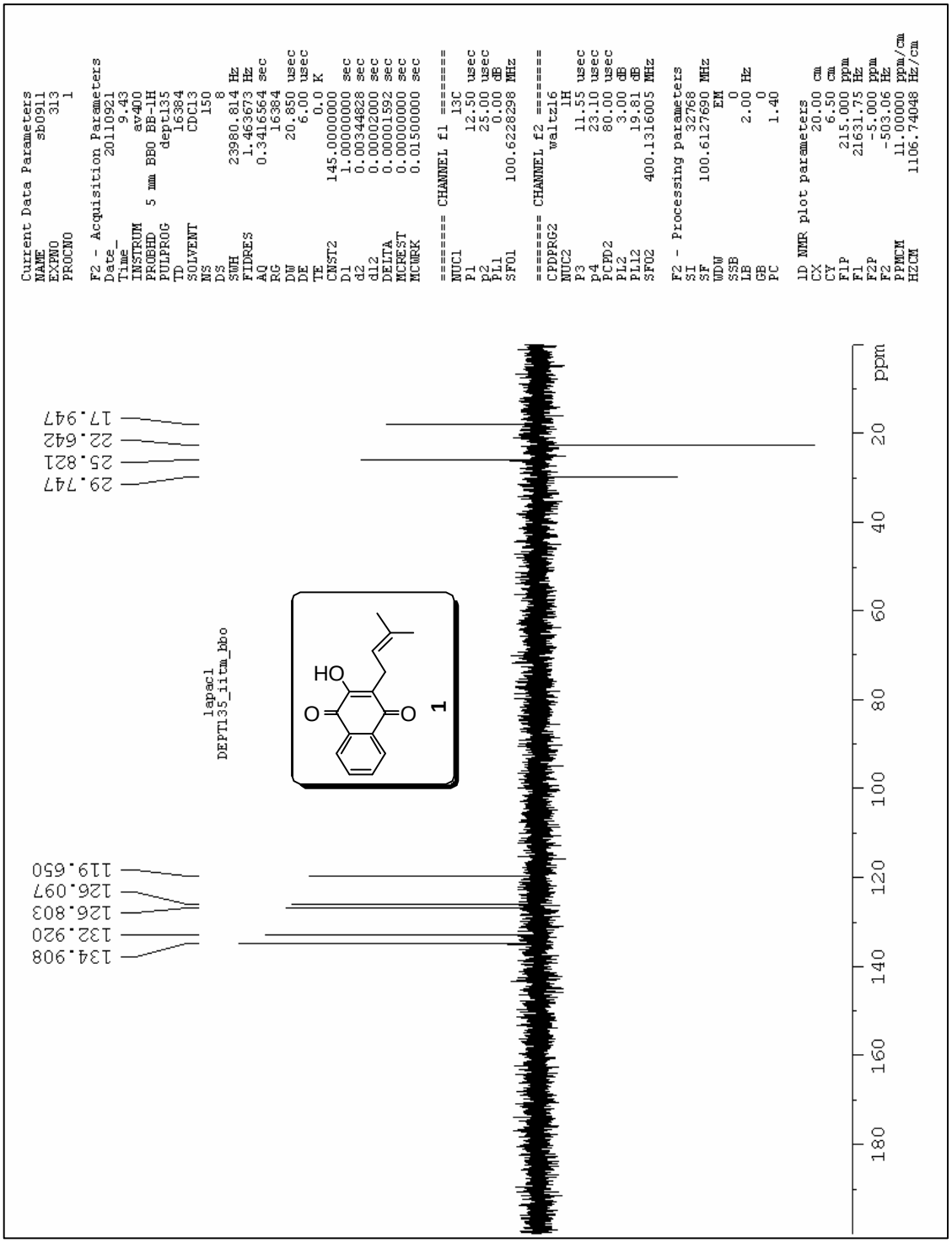
^{1}H NMR spectrum of compound **1**



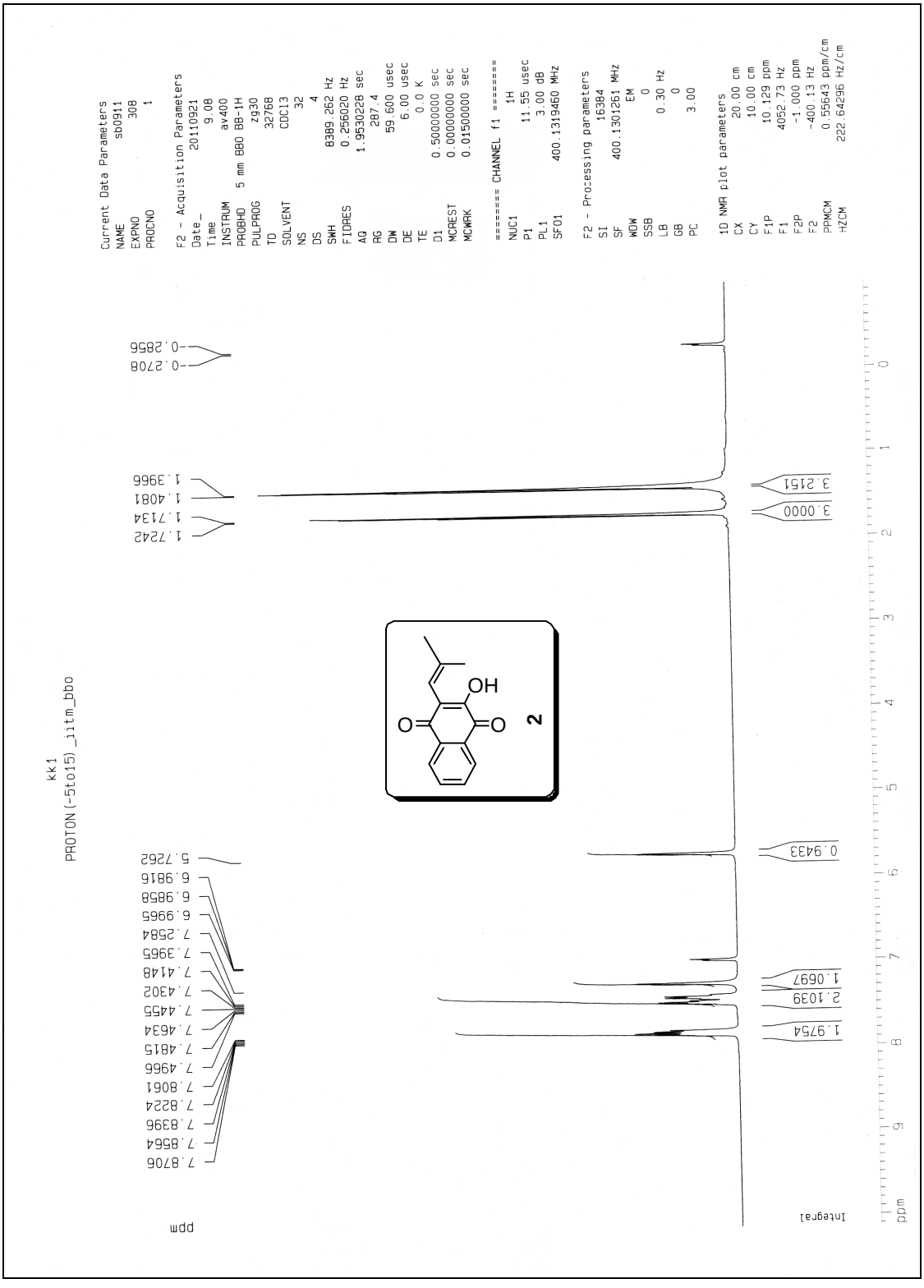
Expandeed ^{1}H NMR spectrum of compound **1**



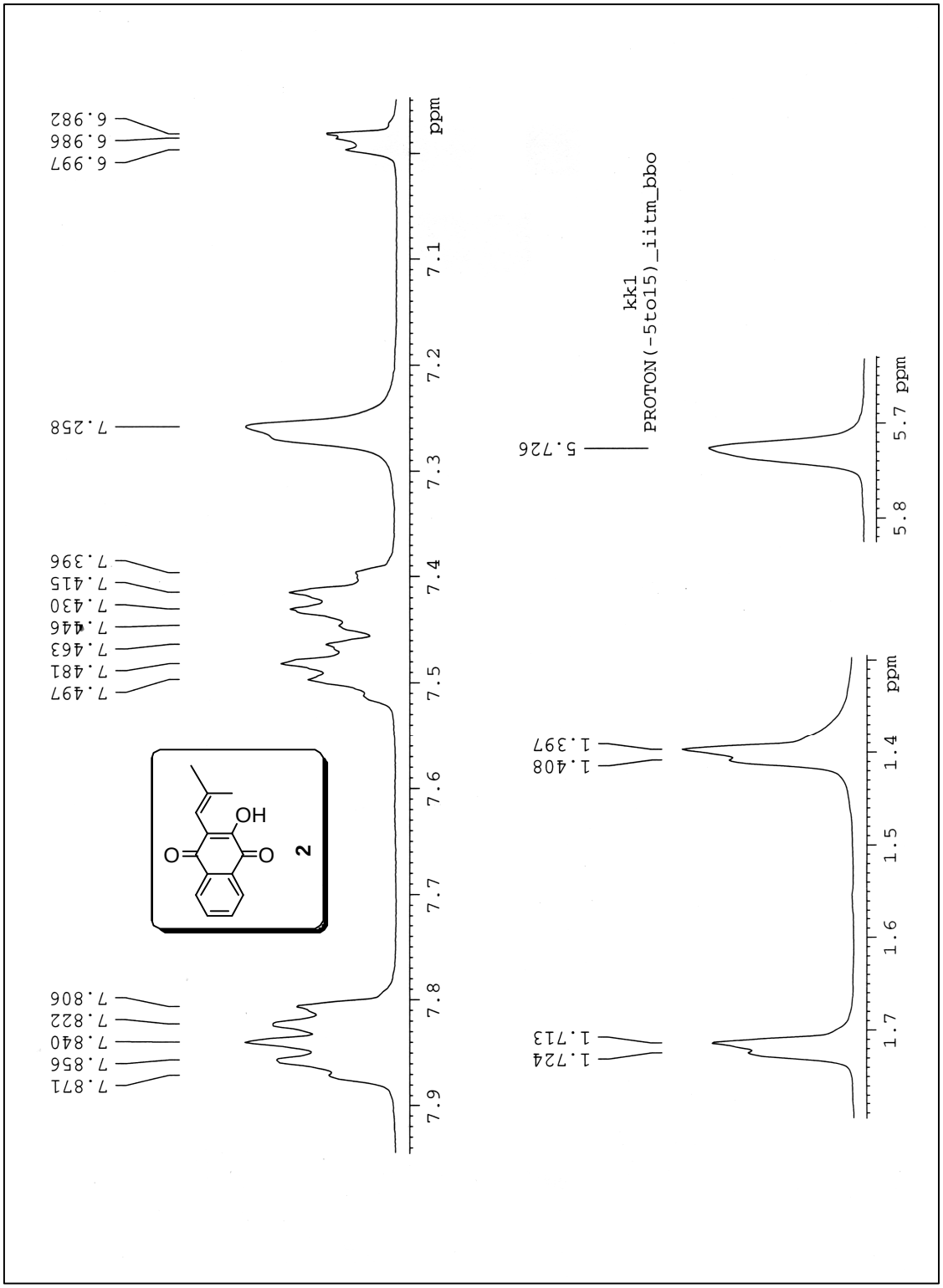
^{13}C NMR spectrum of compound **1**



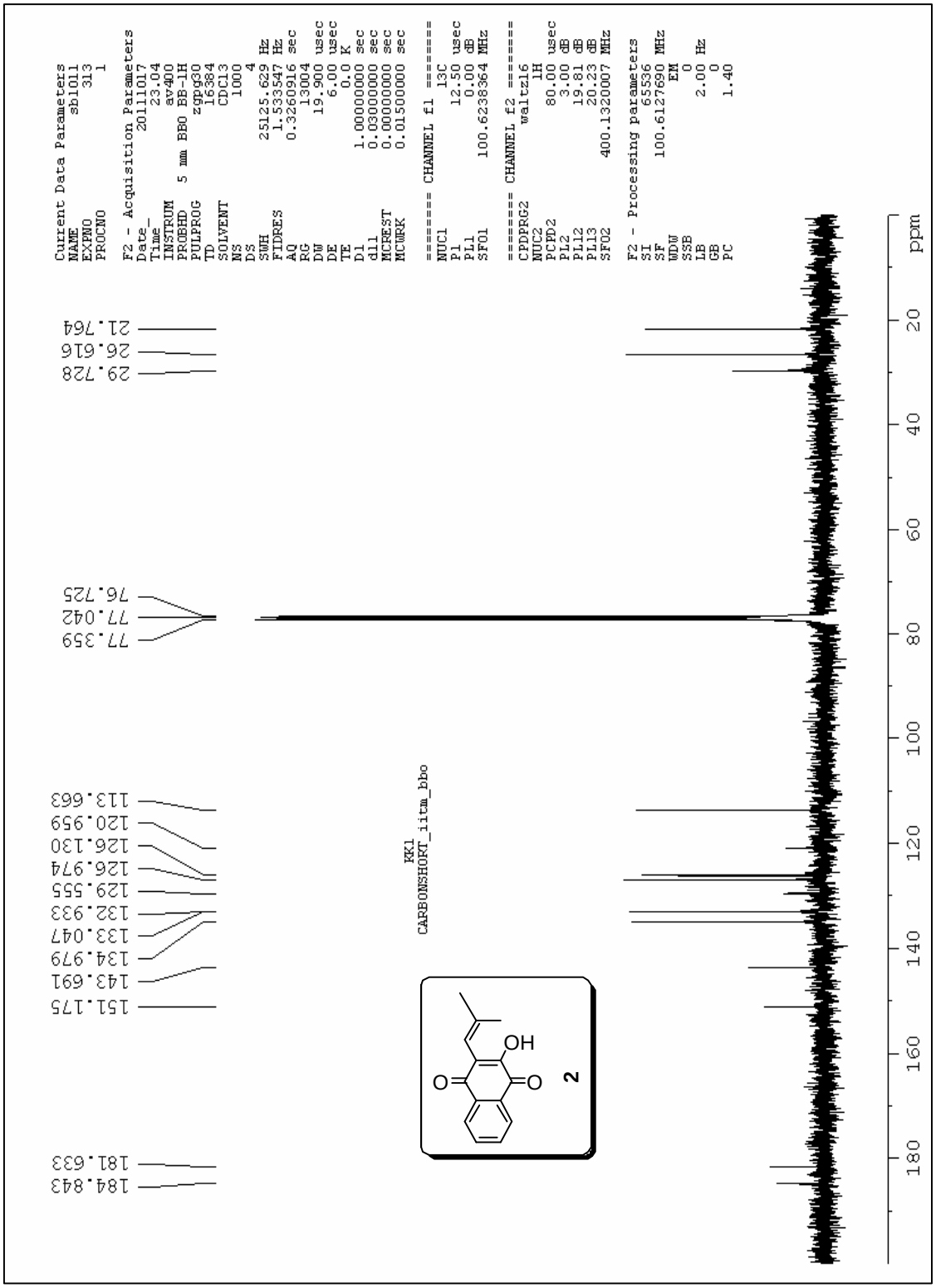
DEPT spectrum of compound **1**



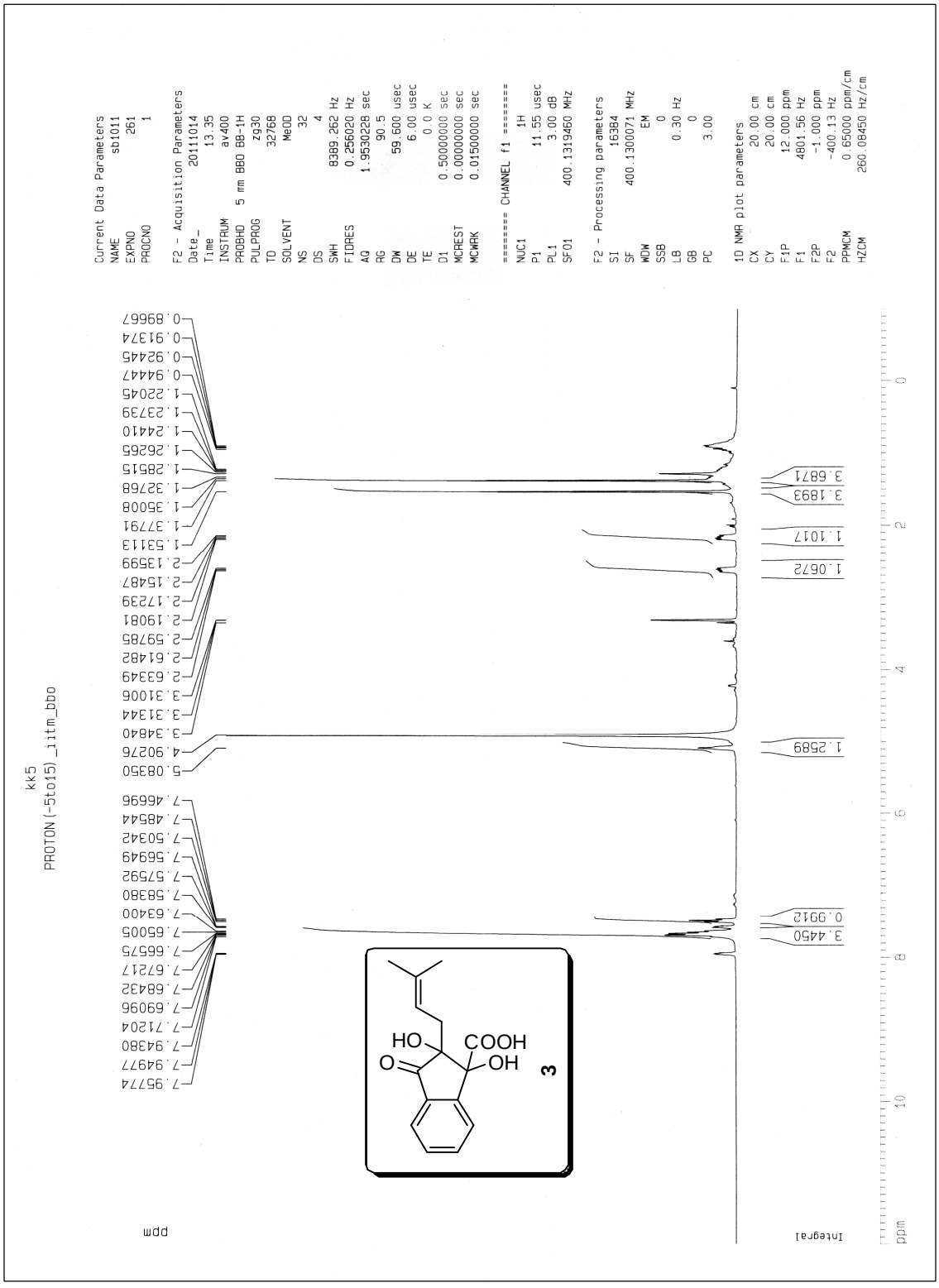
^{1}H NMR spectrum of compound **2**



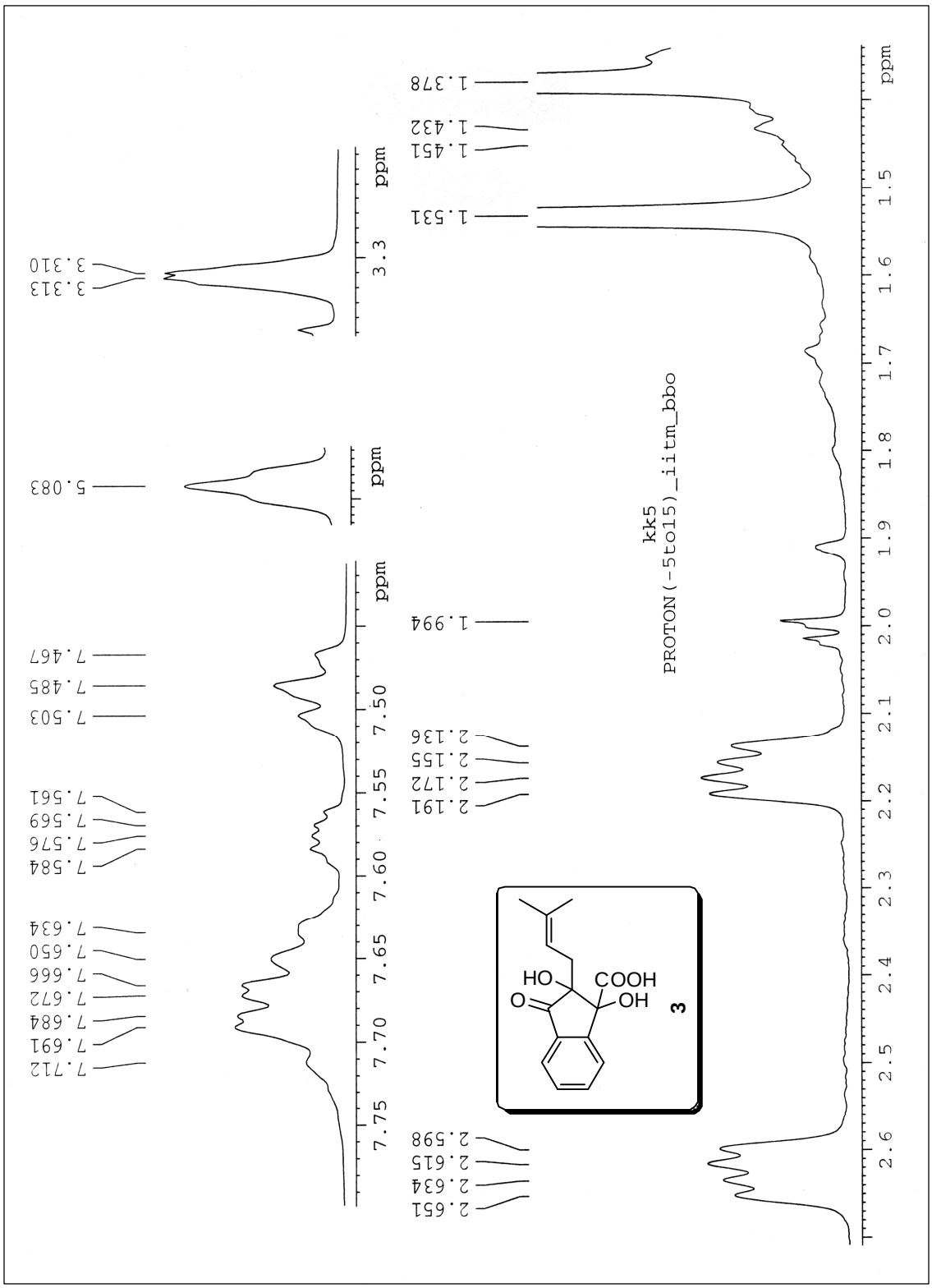
Expandeed ^{1}H NMR spectrum of compound **2**



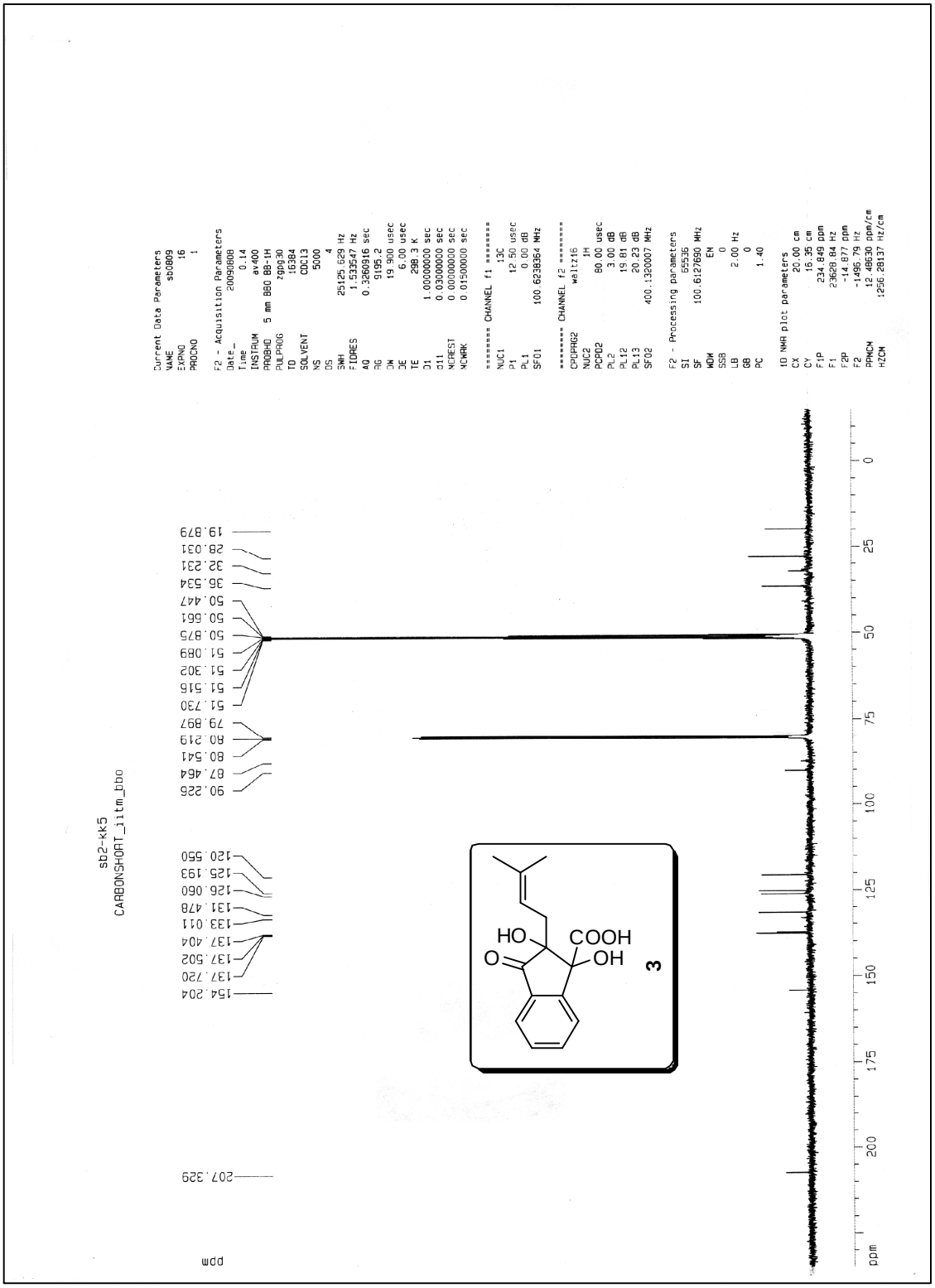
^{13}C NMR spectrum of compound **2**



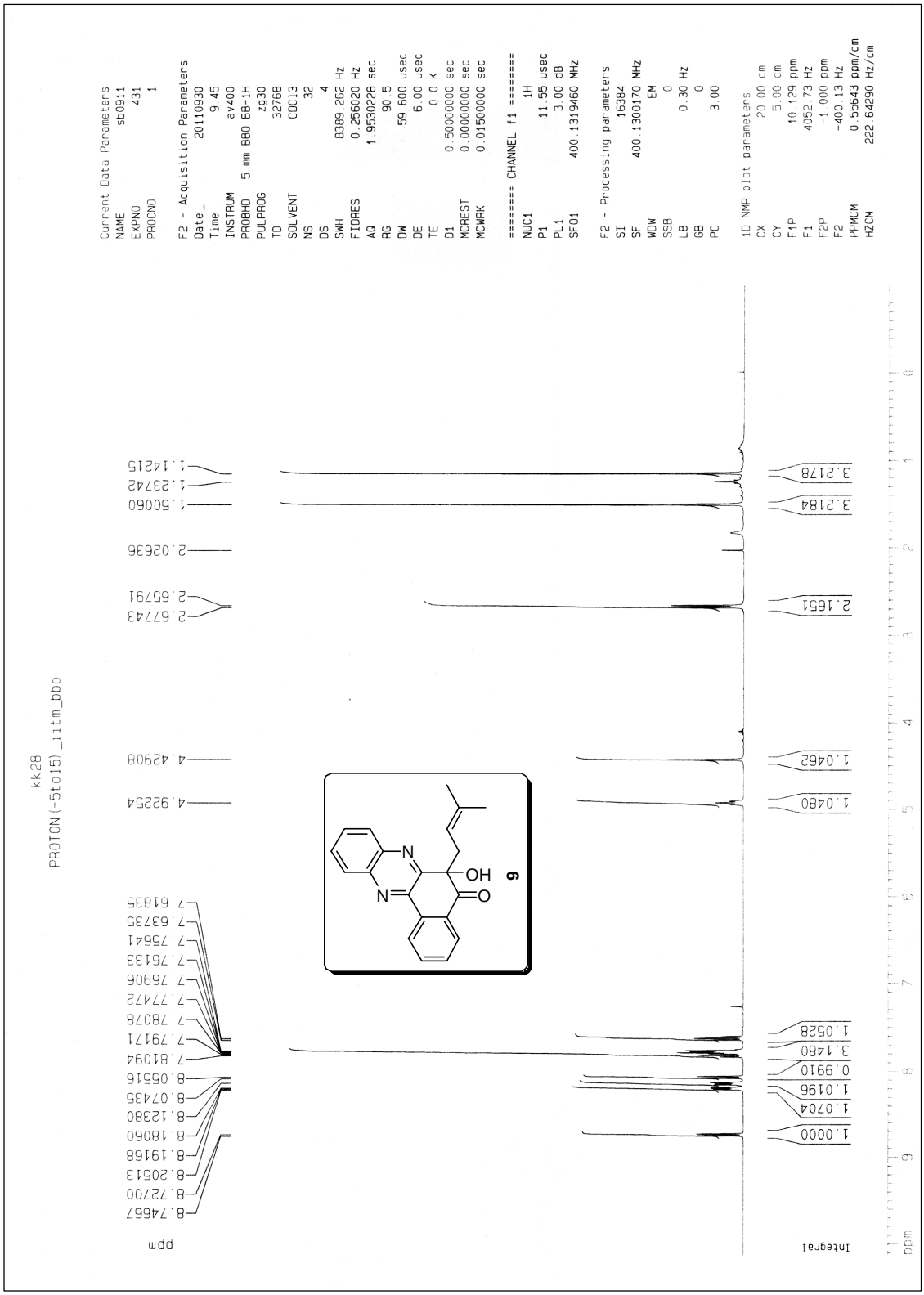
^{1}H NMR spectrum of compound **3**



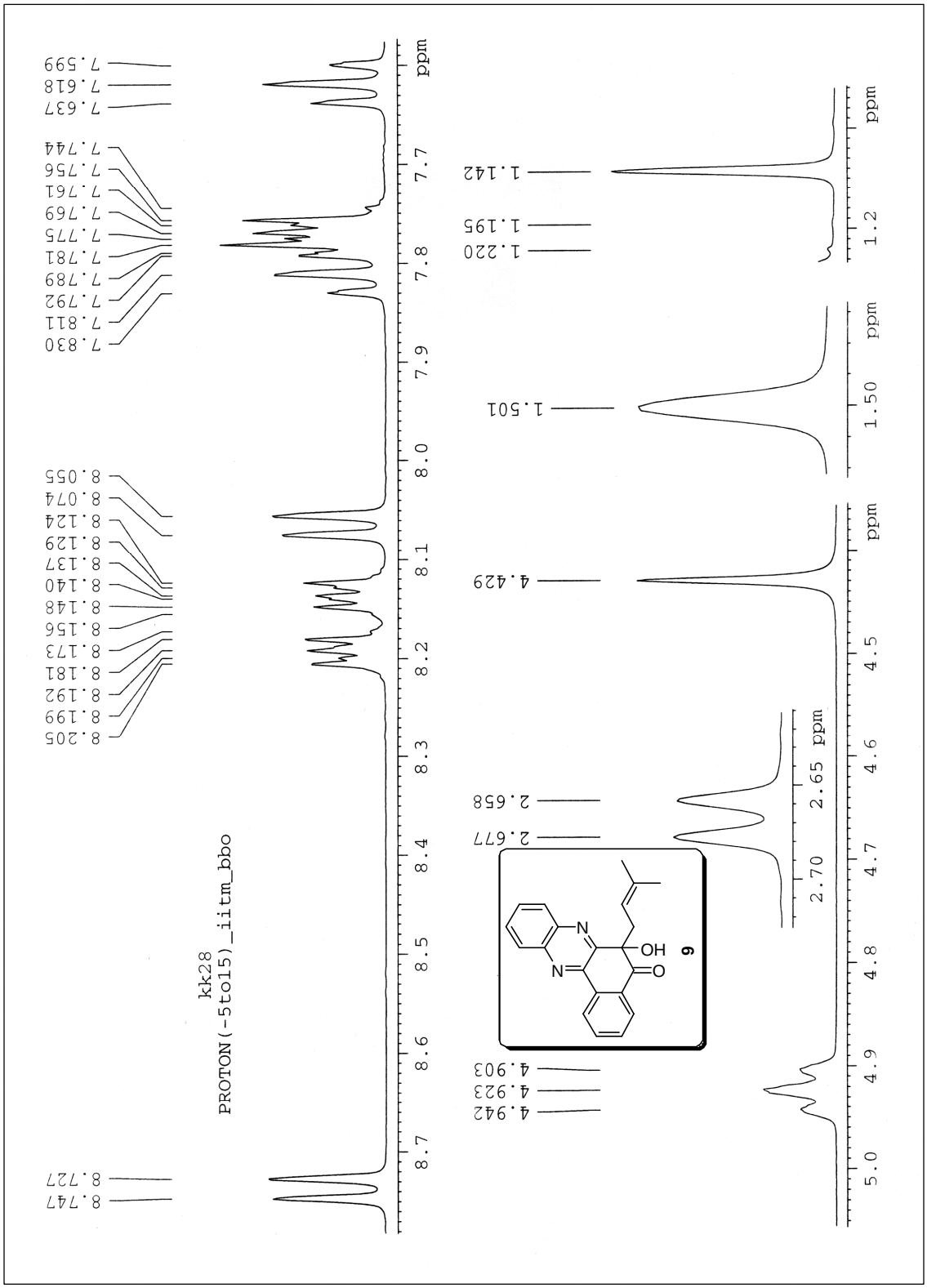
Expandeed ^{1}H NMR spectrum of compound **3**



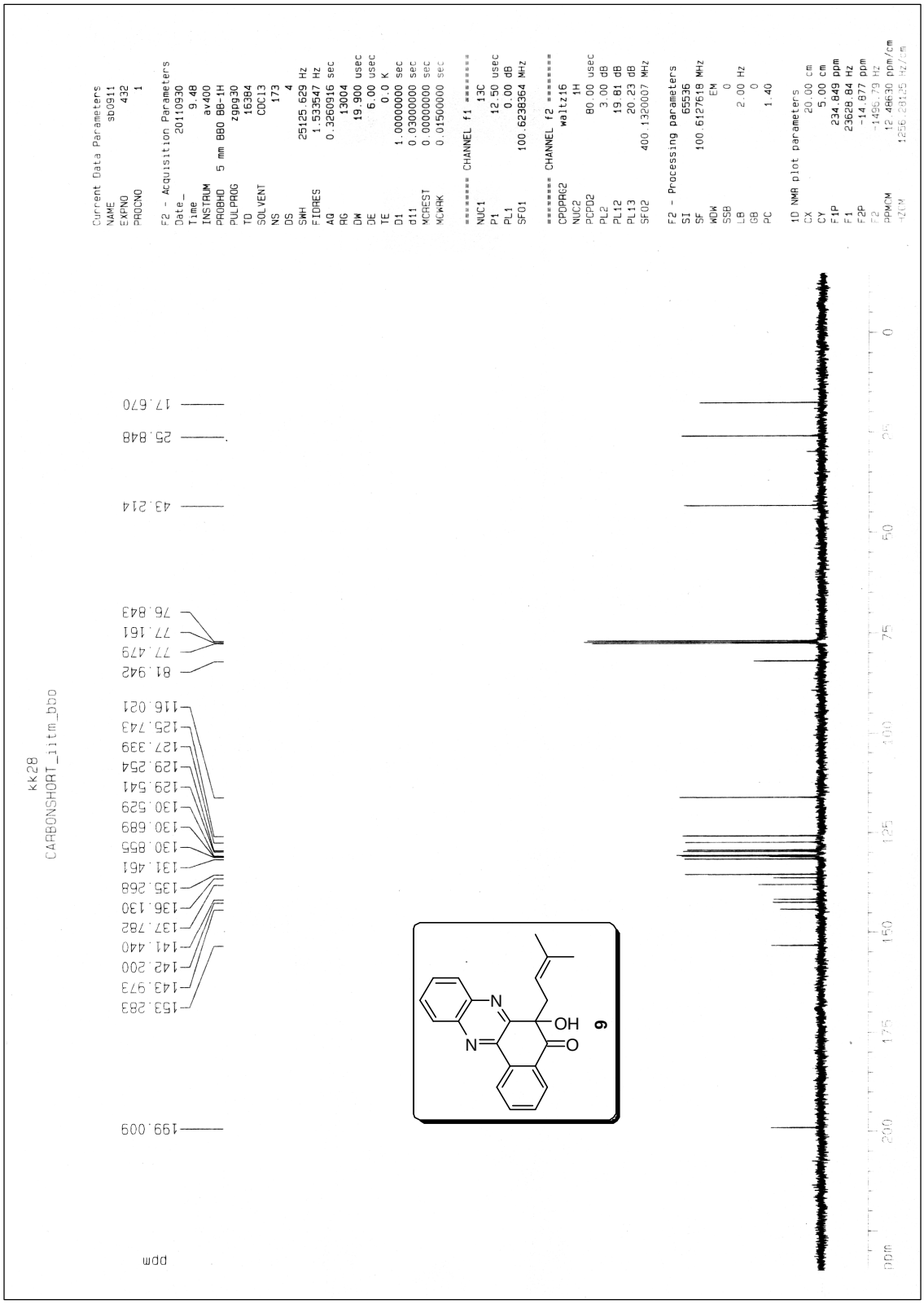
^{13}C NMR spectrum of compound **3**



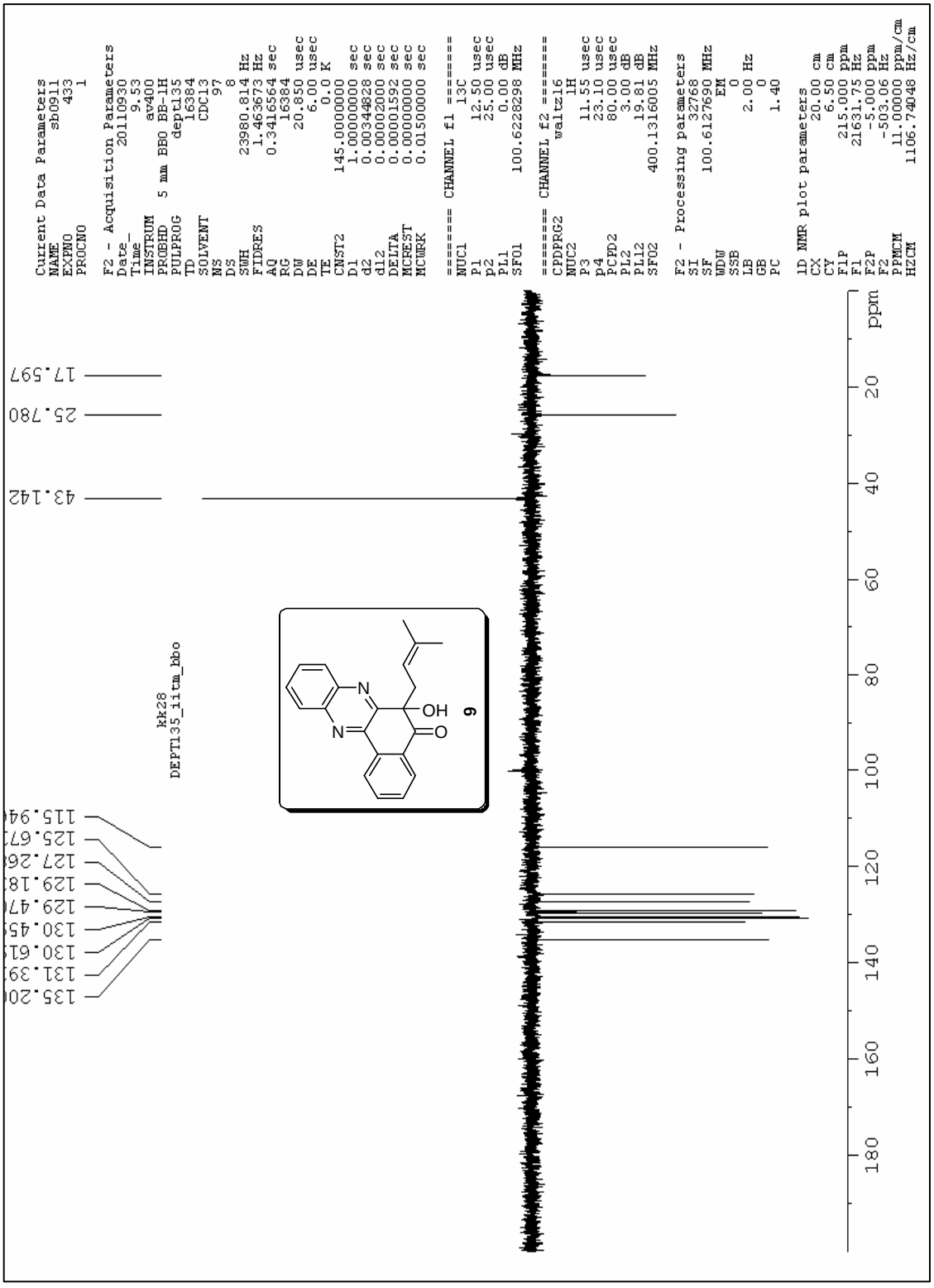
^{1}H NMR spectrum of compound **9**



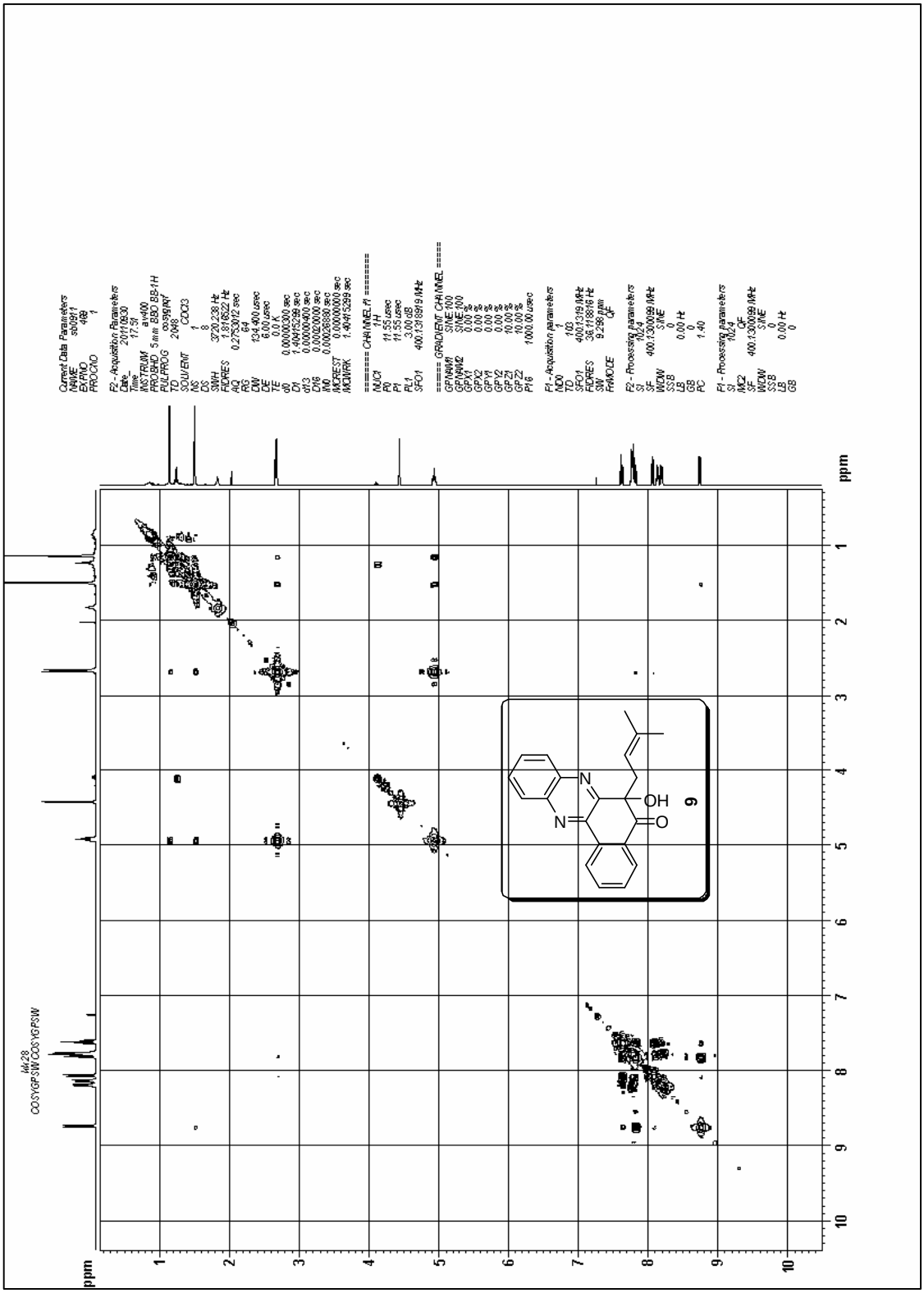
Expandeed ^{1}H NMR spectrum of compound **9**



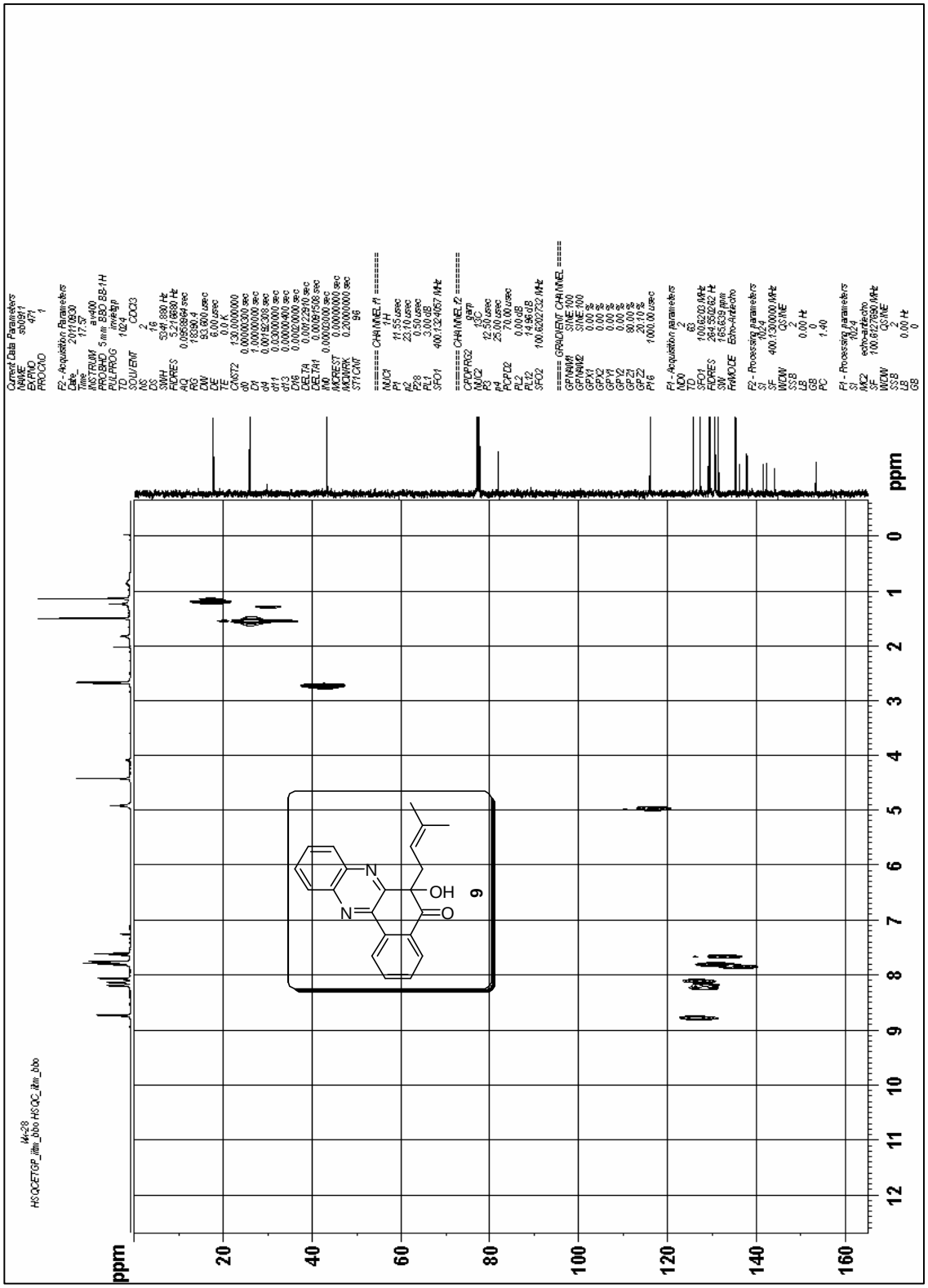
^{13}C NMR spectrum of compound **9**



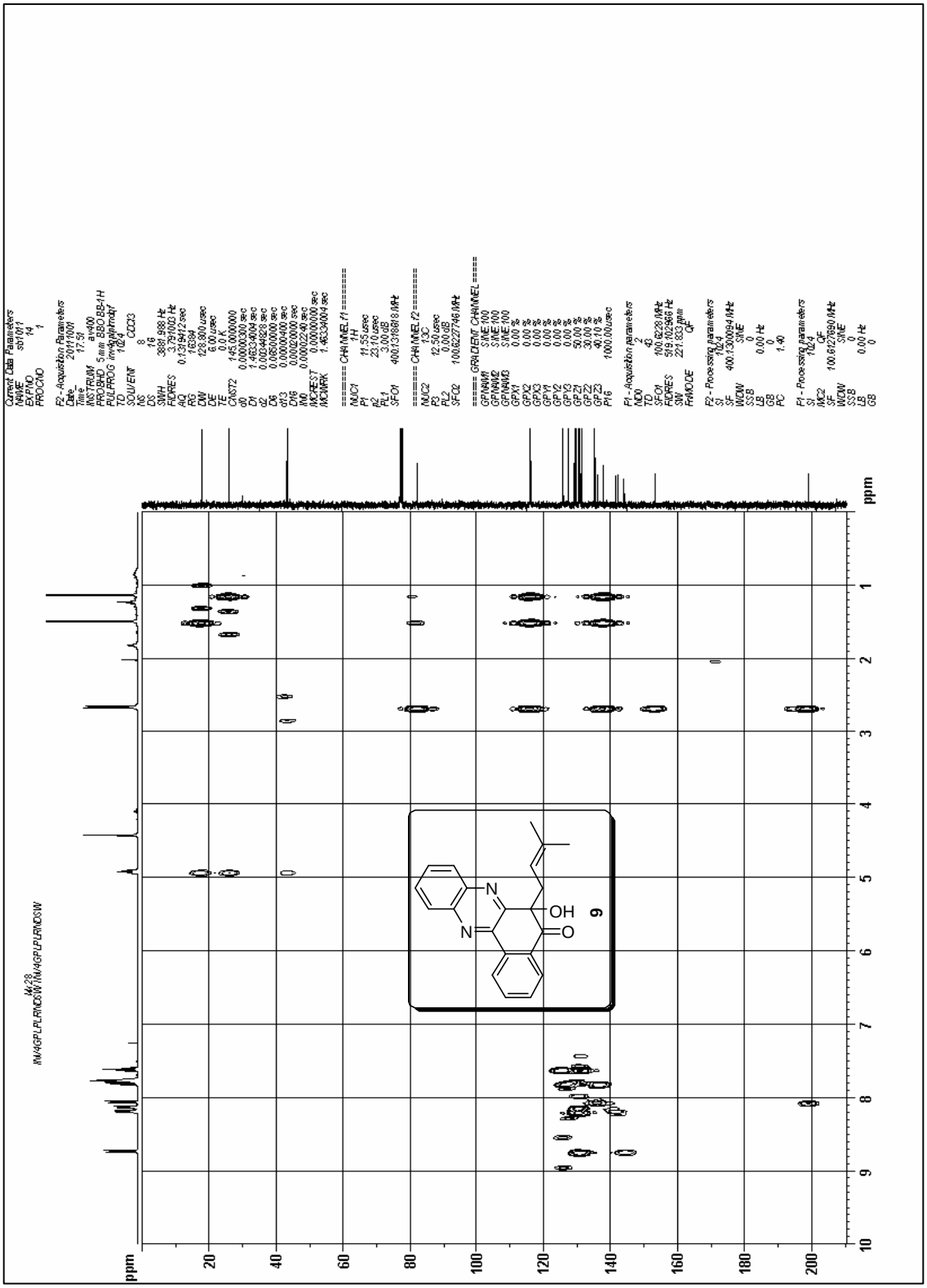
DEPT spectrum of compound **9**



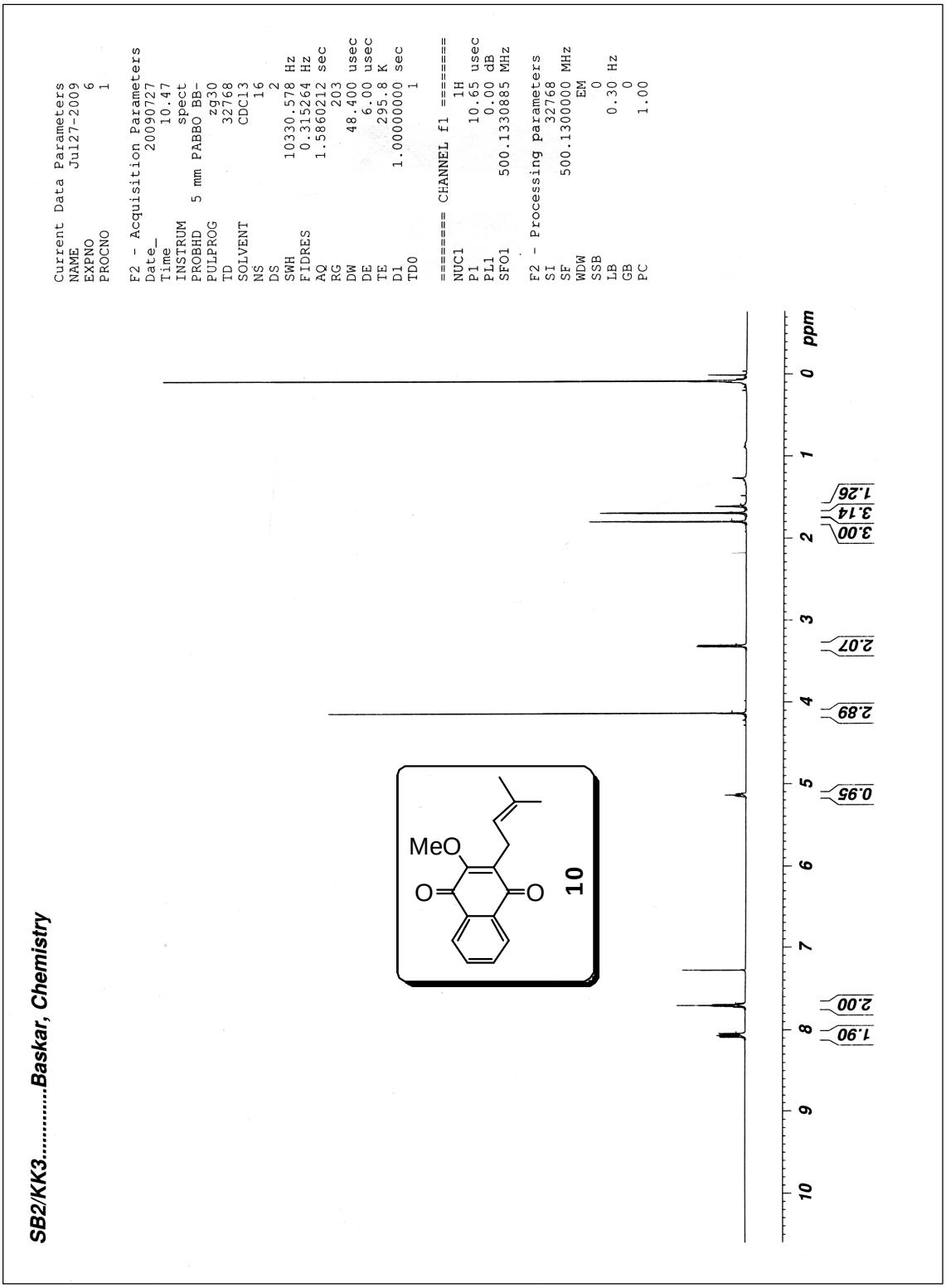
^{1}H-^{1}H COSY spectrum of compound **9**



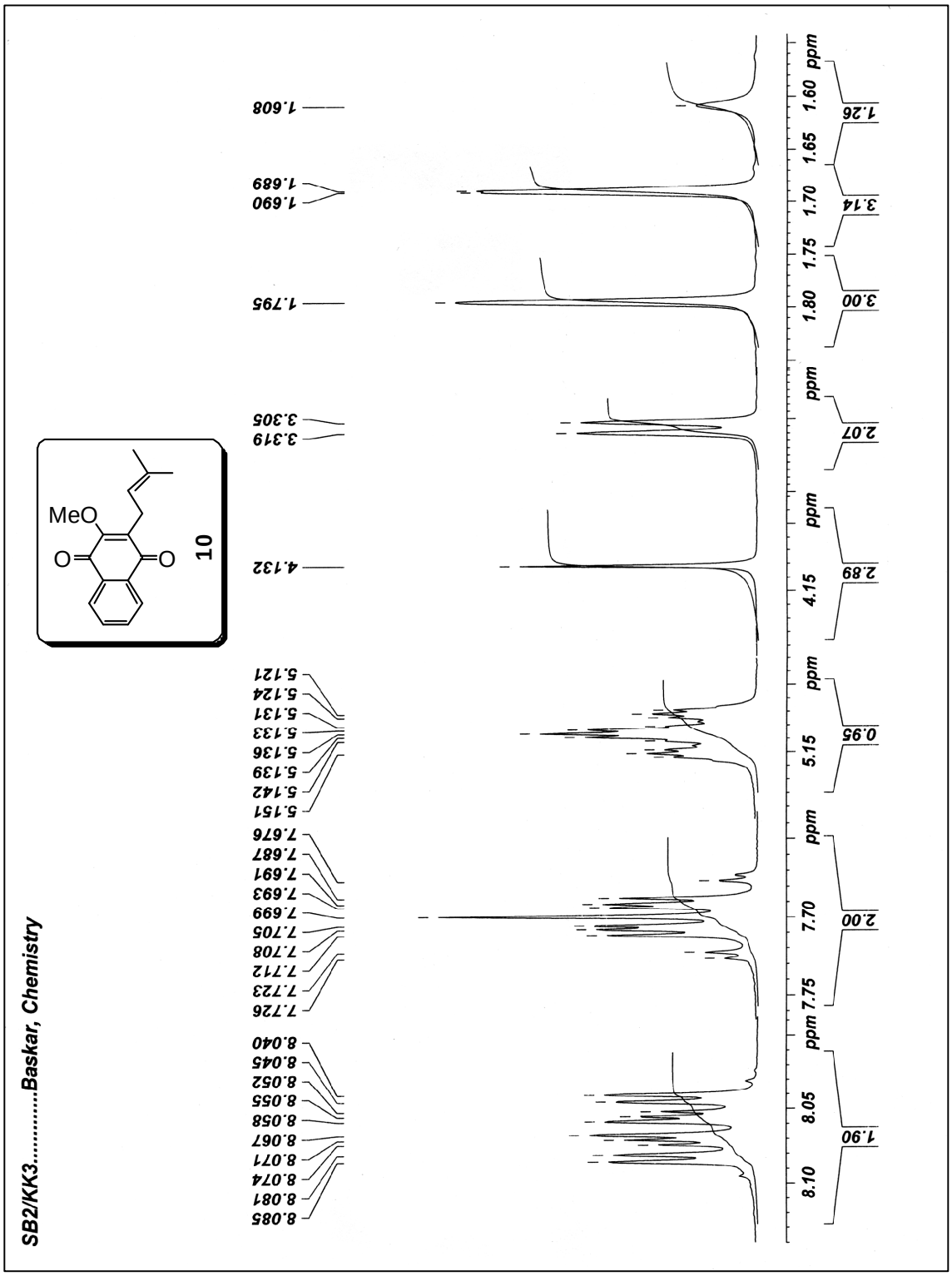
^{1}H-^{13}C COSY (HSQC) NMR spectrum of compound **9**



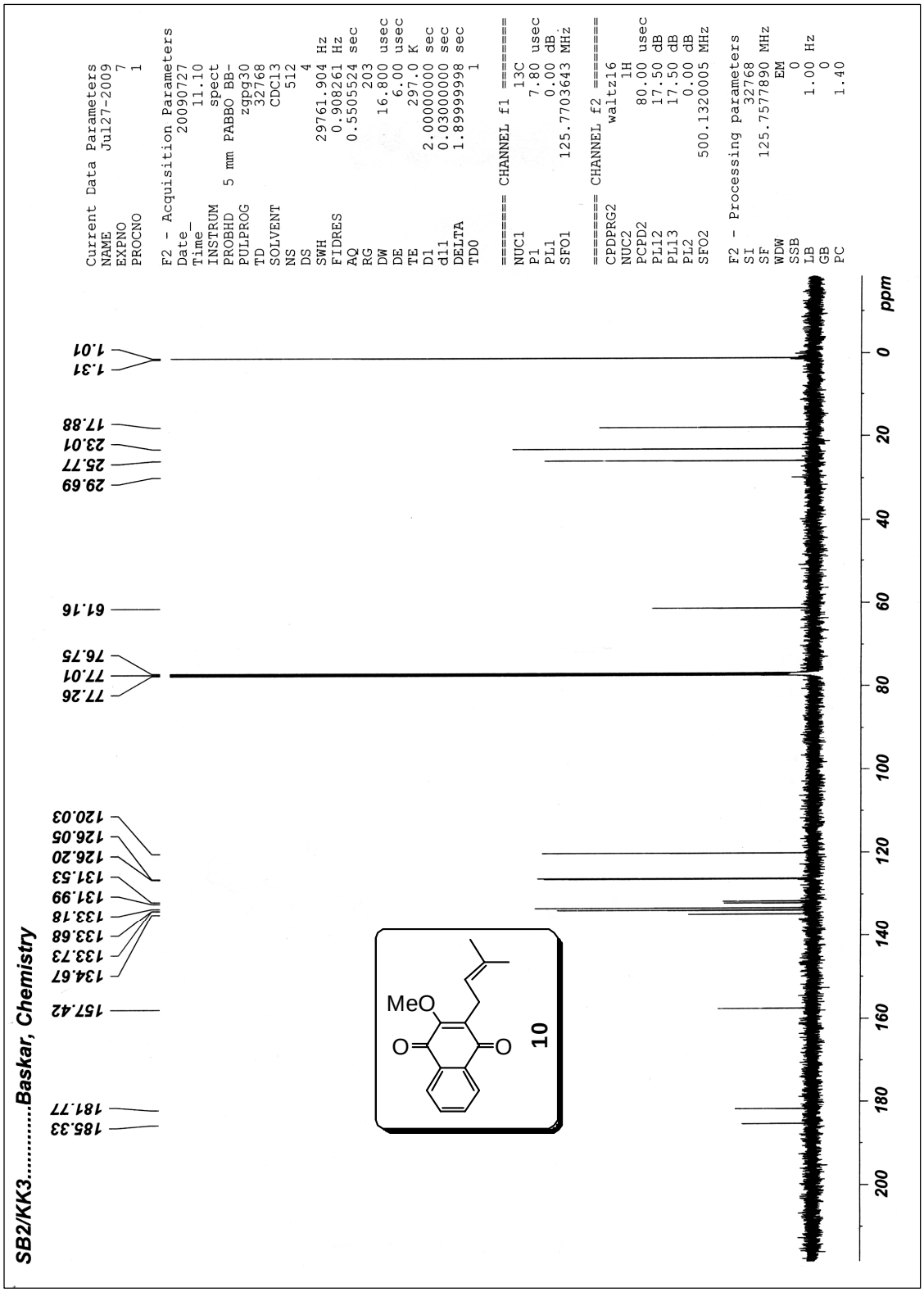
^{1}H-^{13}C COSY (HMBC) NMR spectrum of compound **9**



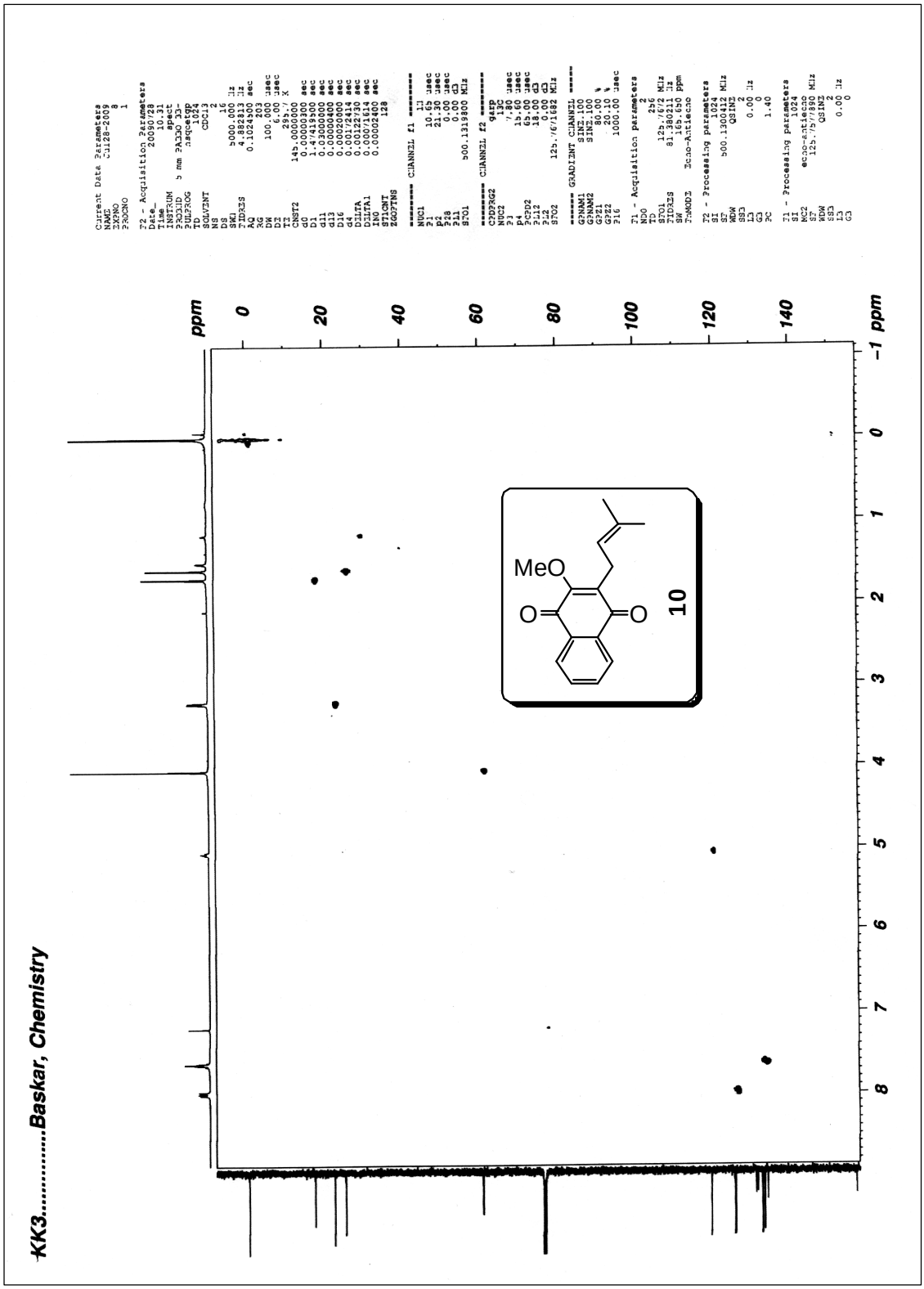
^{1}H NMR spectrum of compound **10**



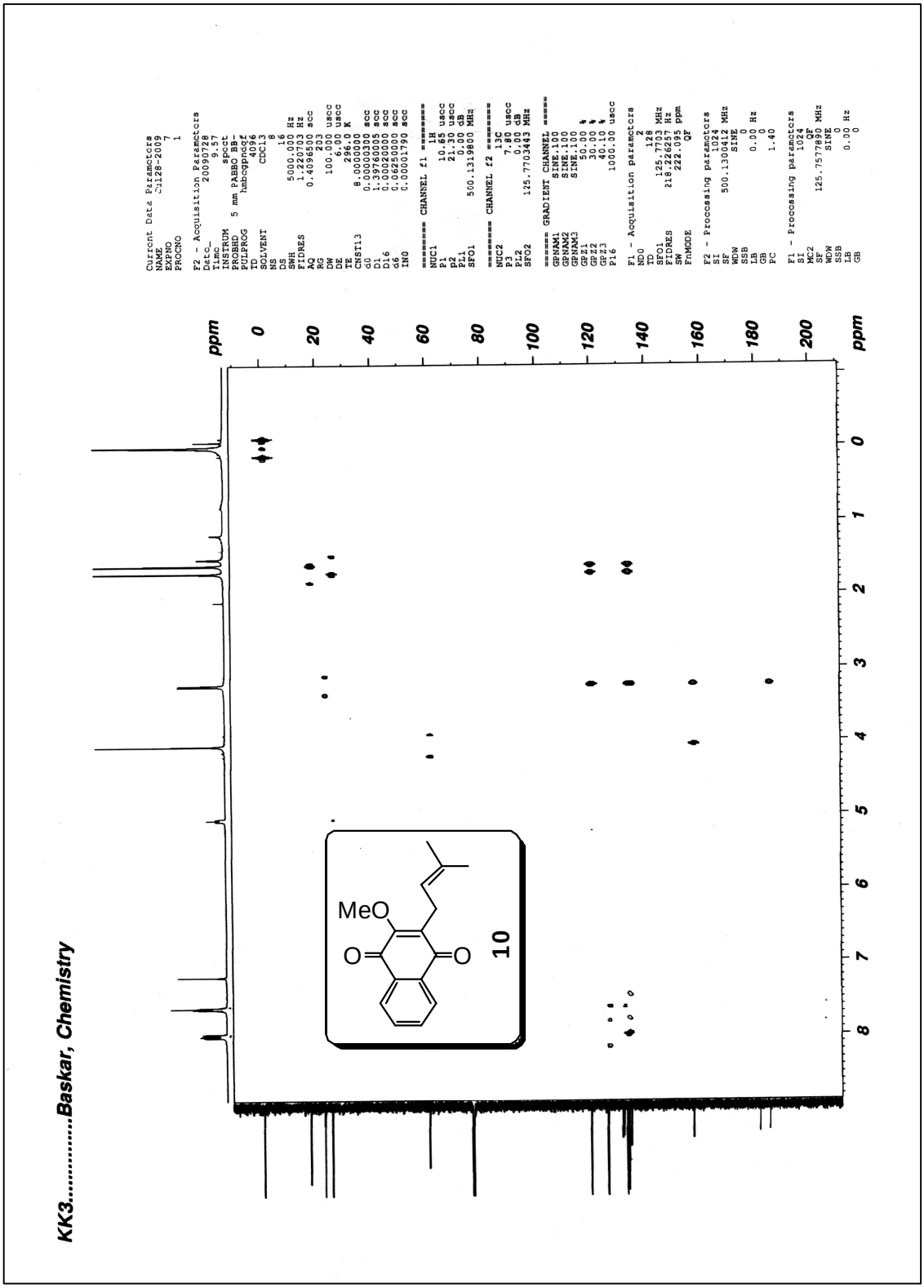
Expandeed ^{1}H NMR spectrum of compound **10**



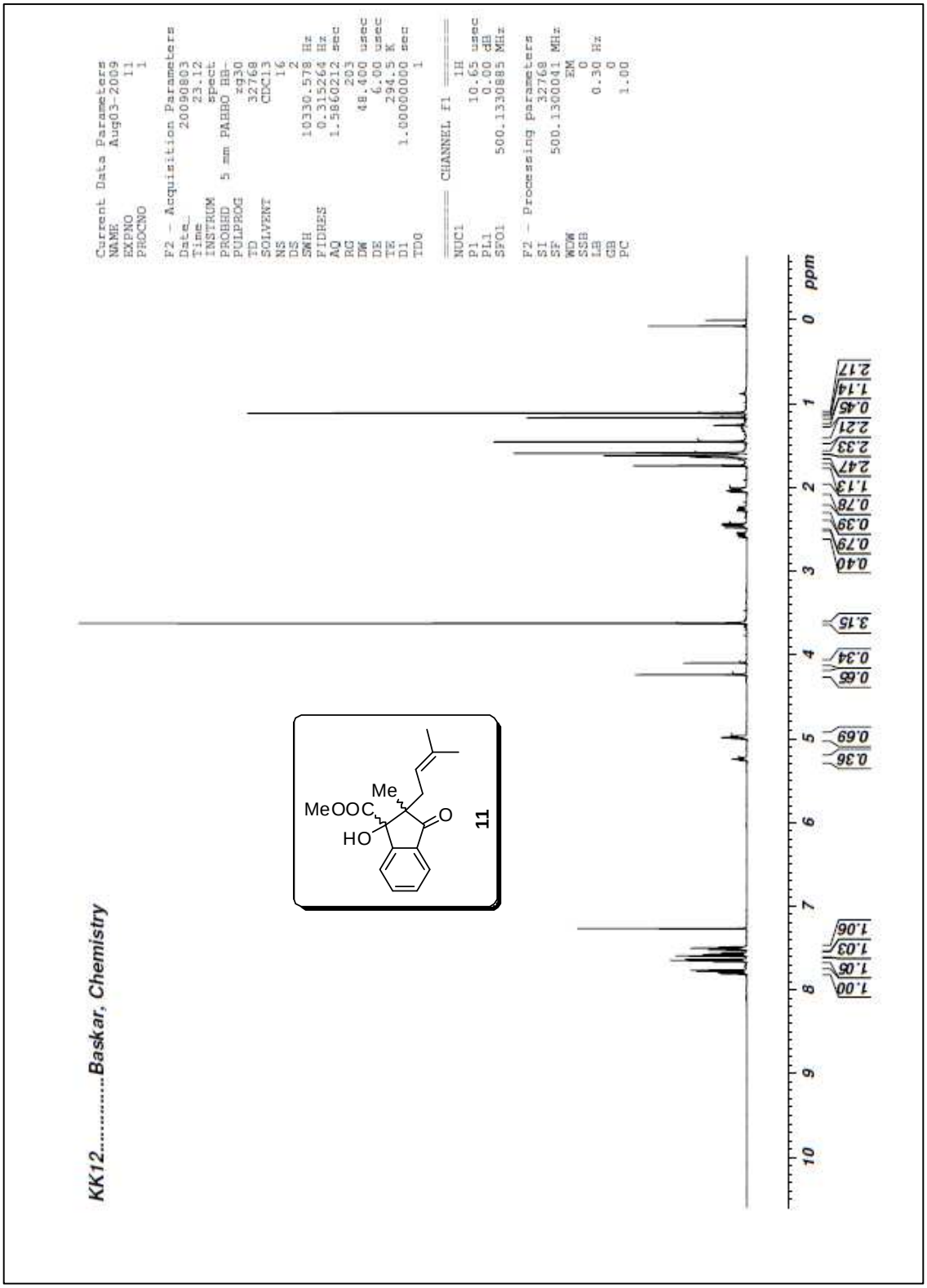
^{13}C NMR spectrum of compound **10**



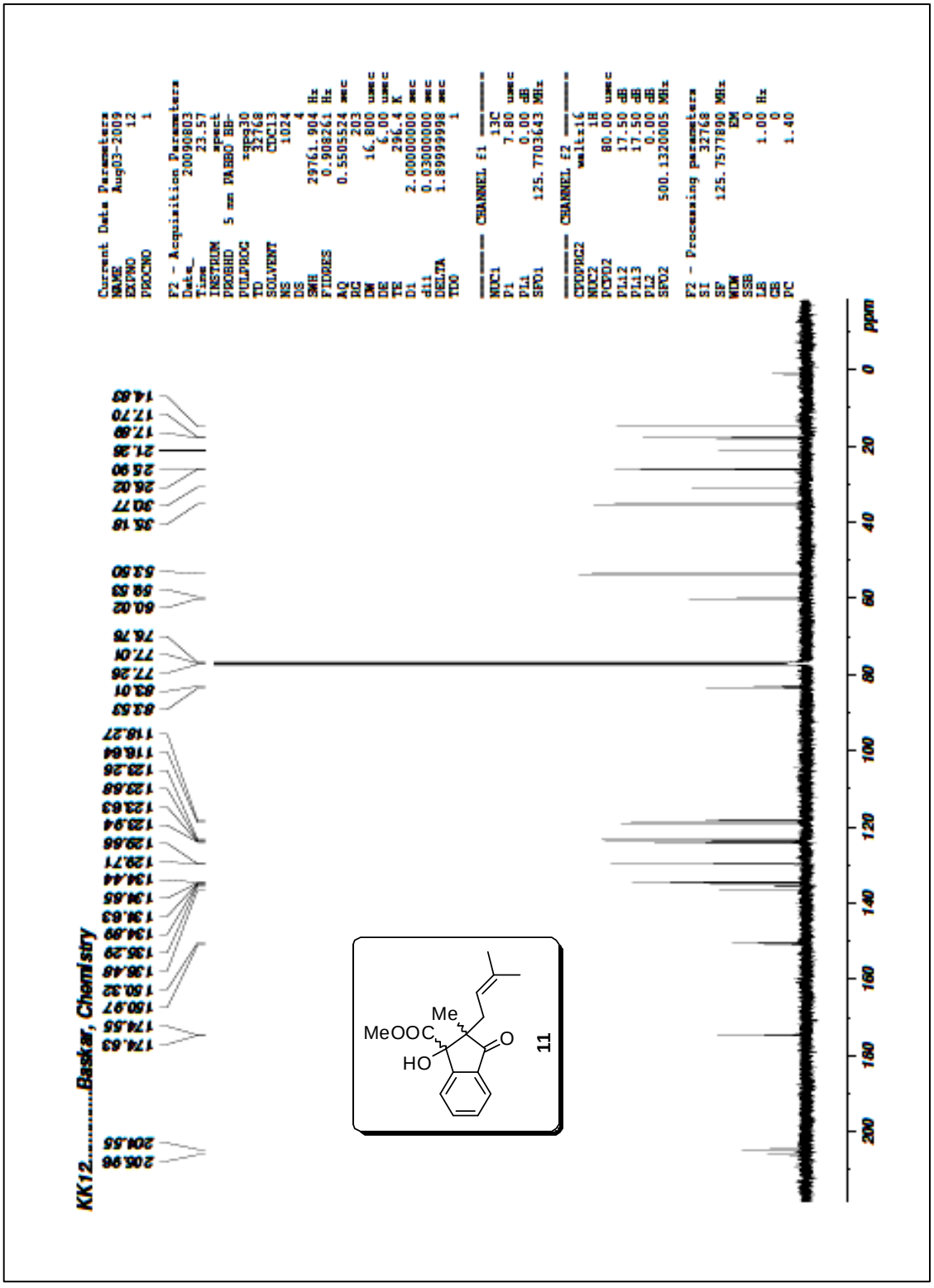
^{1}H-^{13}C COSY (HSQC) NMR spectrum of compound **10**



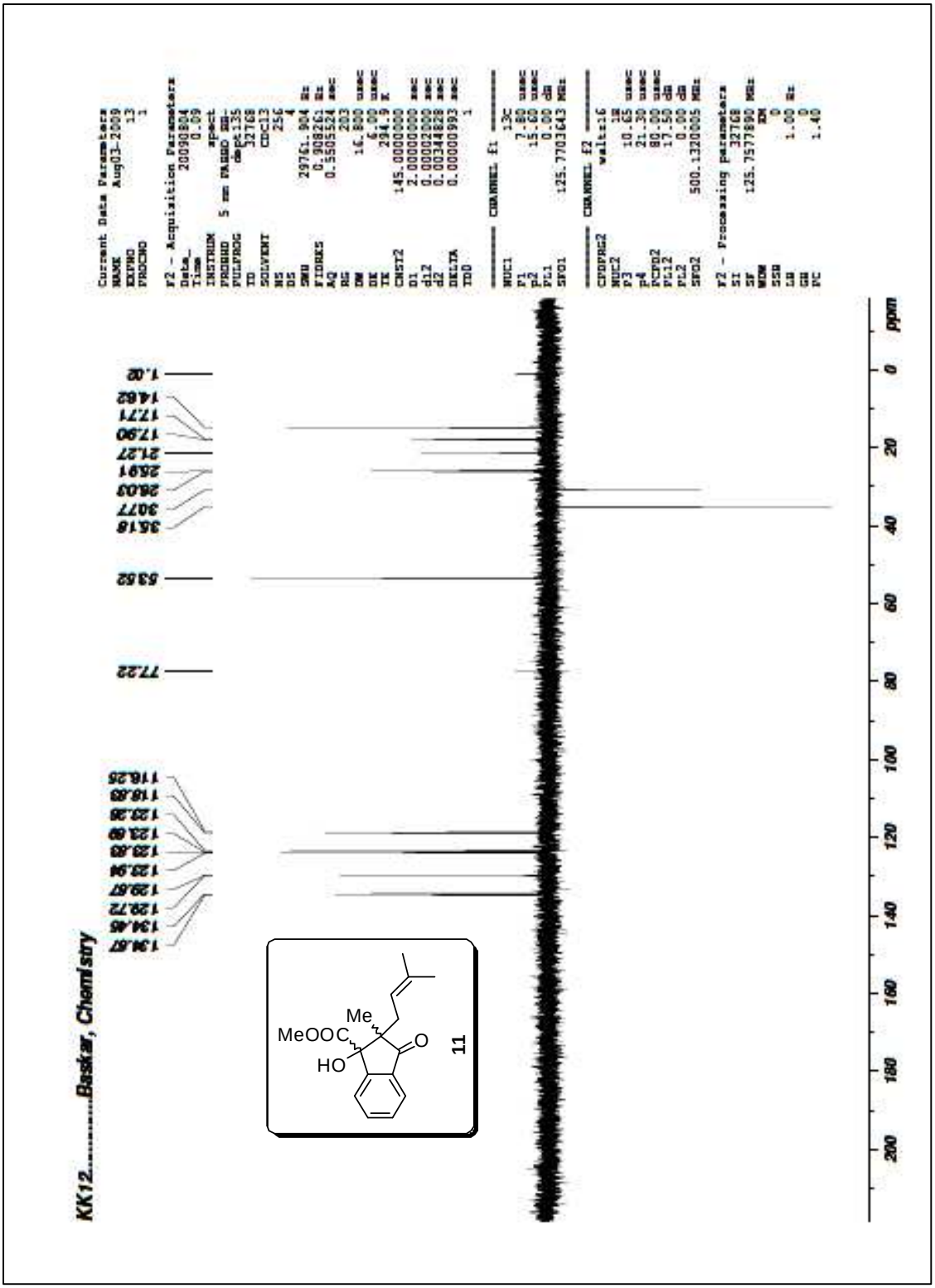
^{1}H-^{13}C COSY (HMBC) NMR spectrum of compound **10**



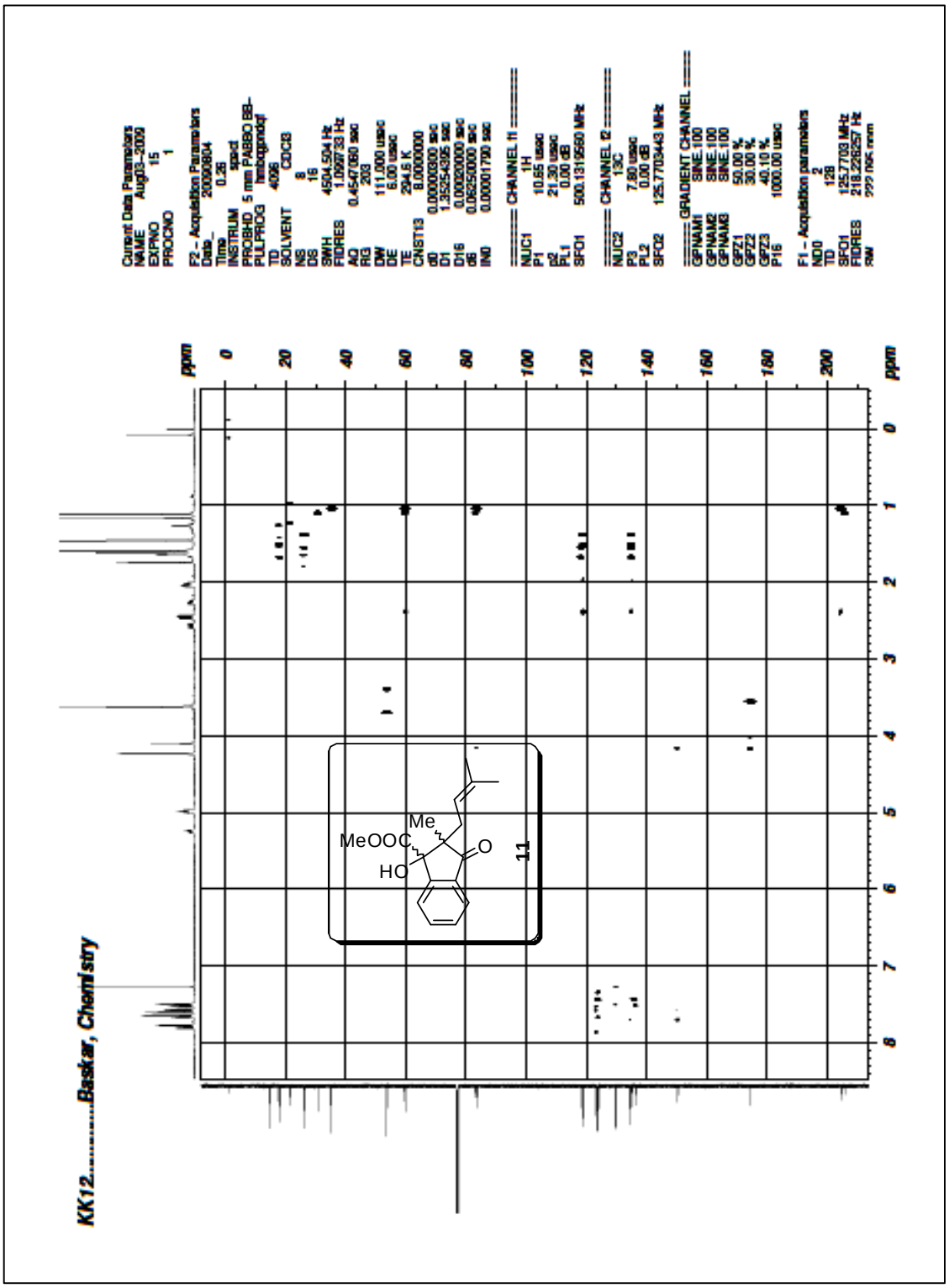
^{1}H NMR spectrum of compound **11**



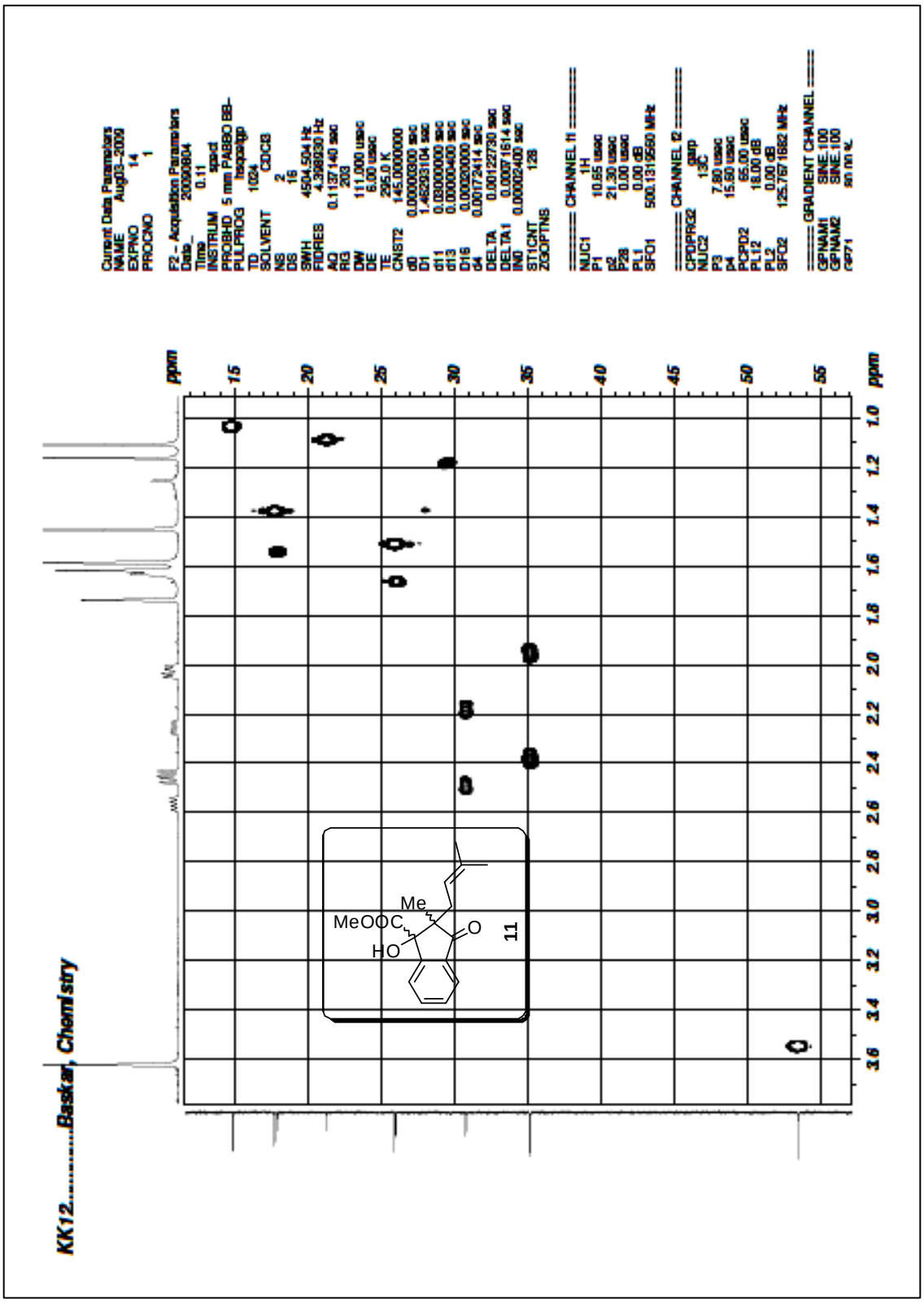
^{13}C NMR spectrum of compound **11**



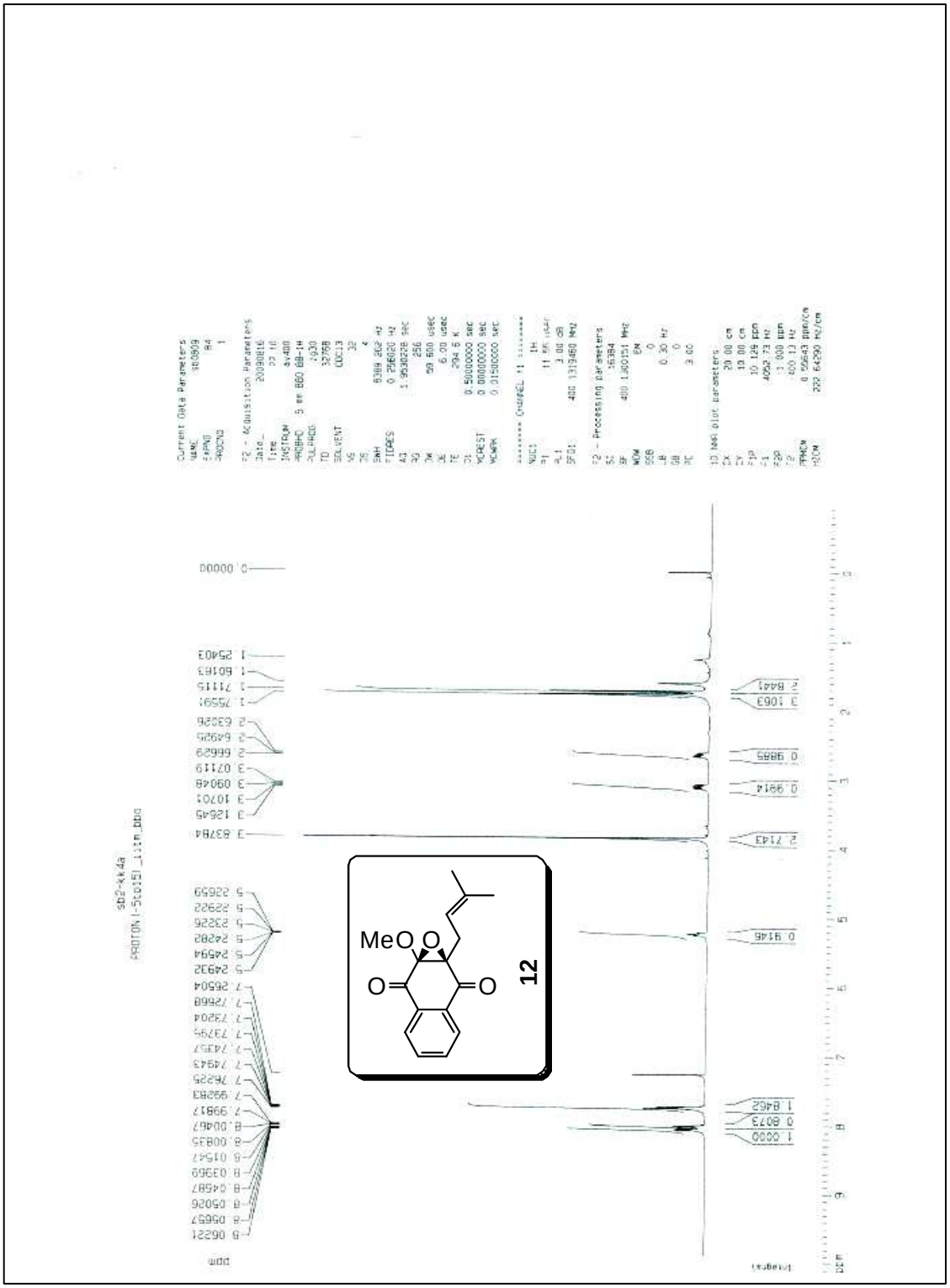
DEPT spectrum of compound **11**



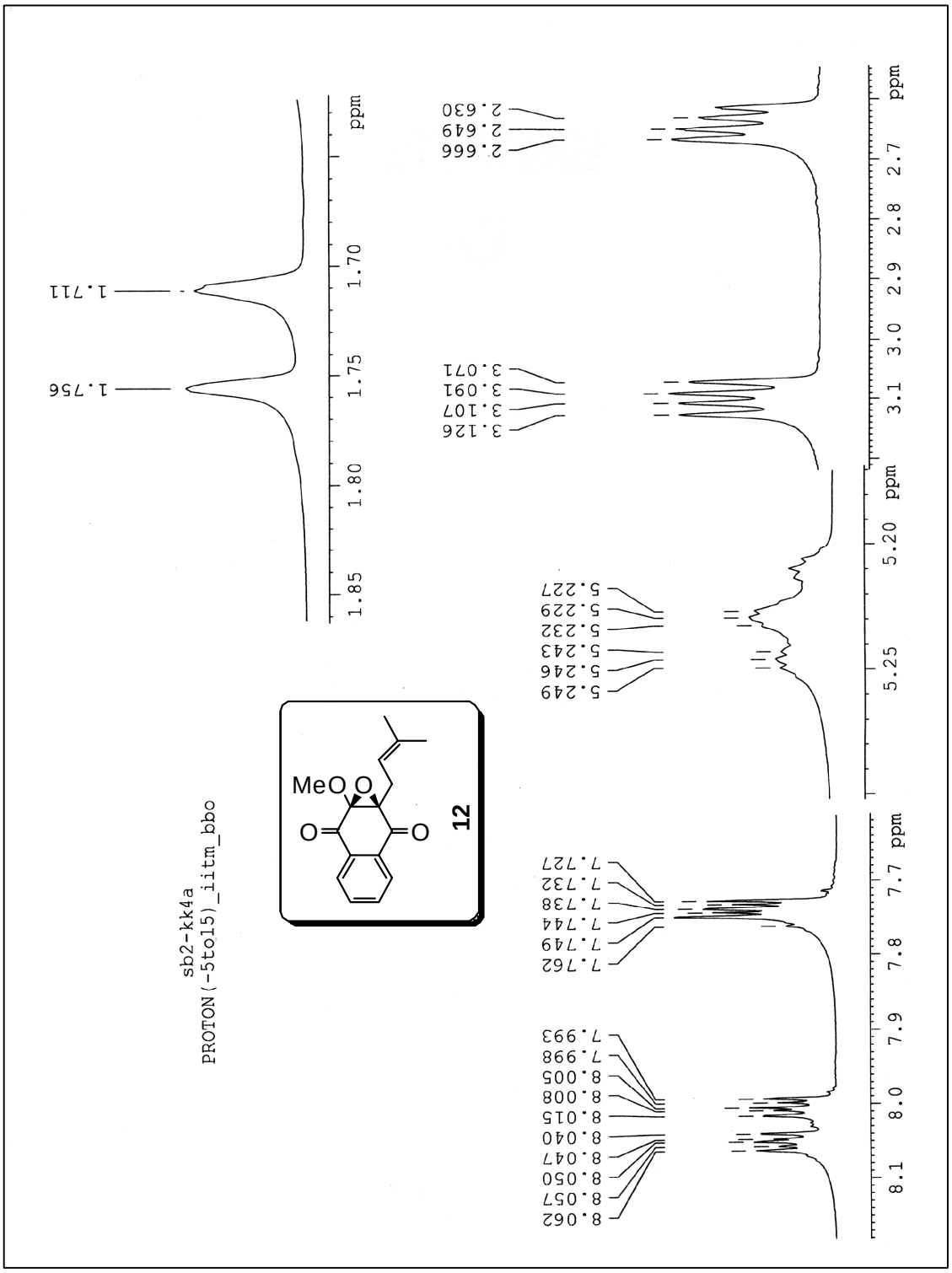
^{1}H-^{13}C COSY (HMBC) NMR spectrum of compound **11**



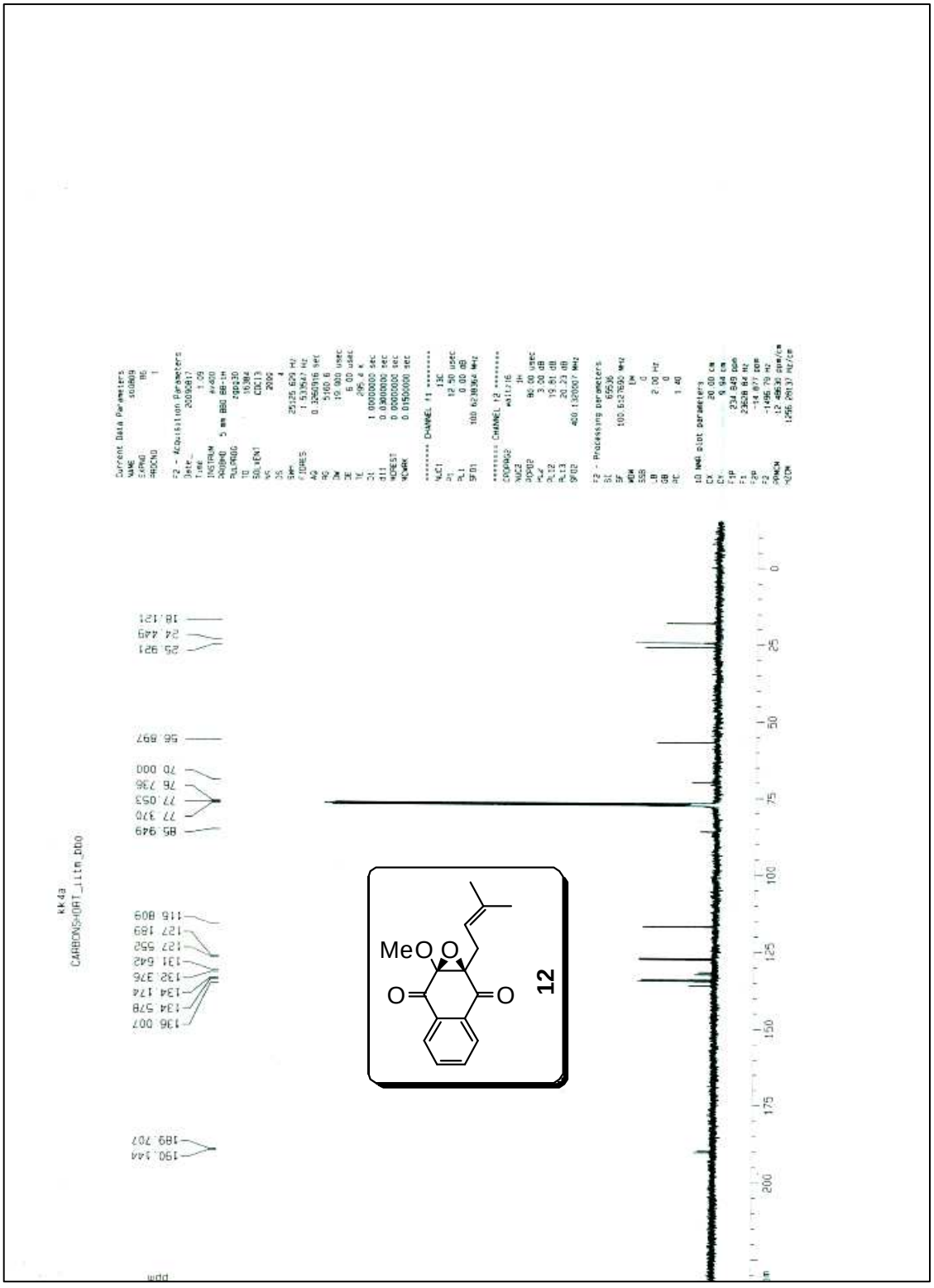
^{1}H-^{13}C COSY (HSQC) NMR spectrum of compound **11**



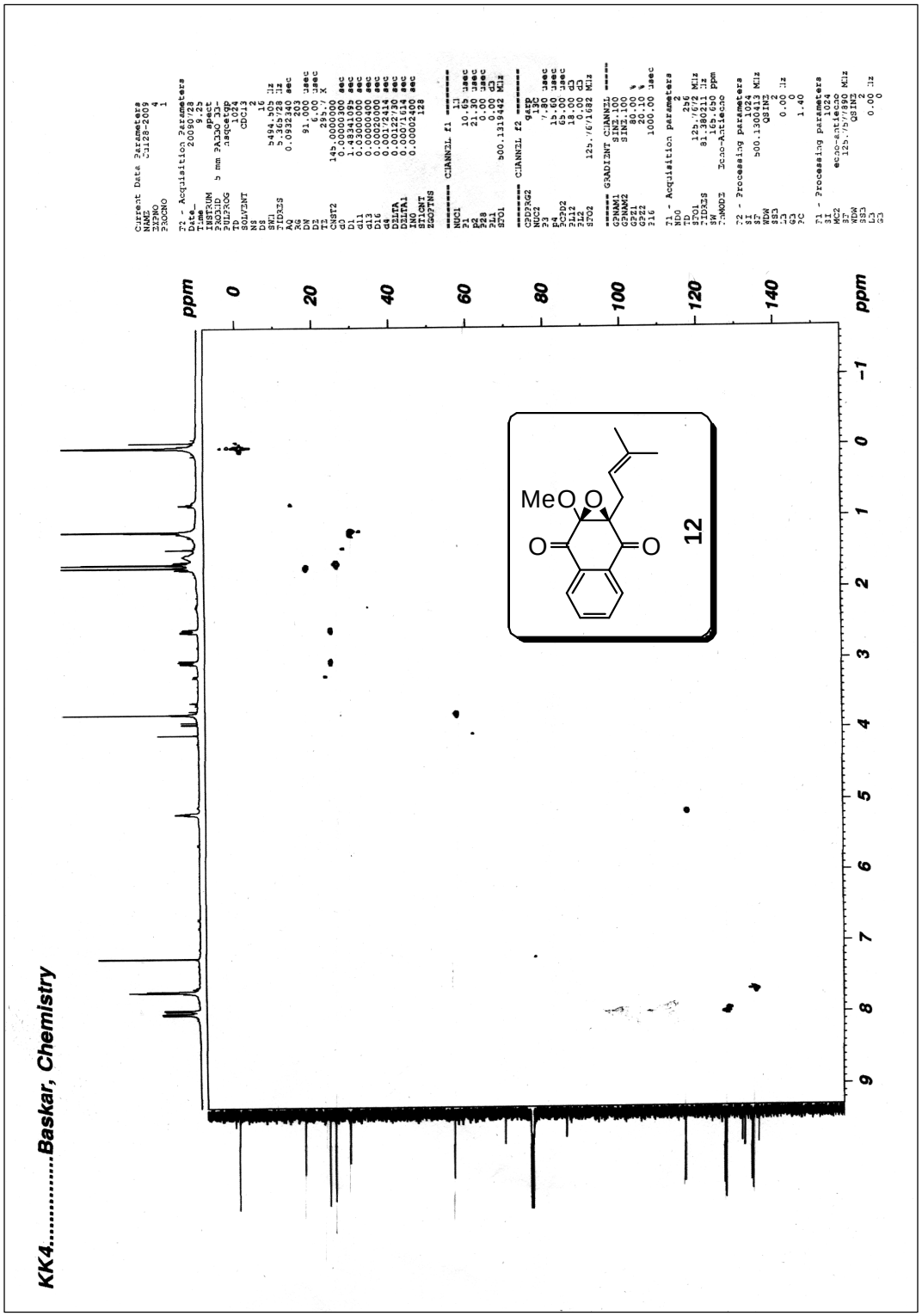
^{1}H NMR spectrum of compound **12**



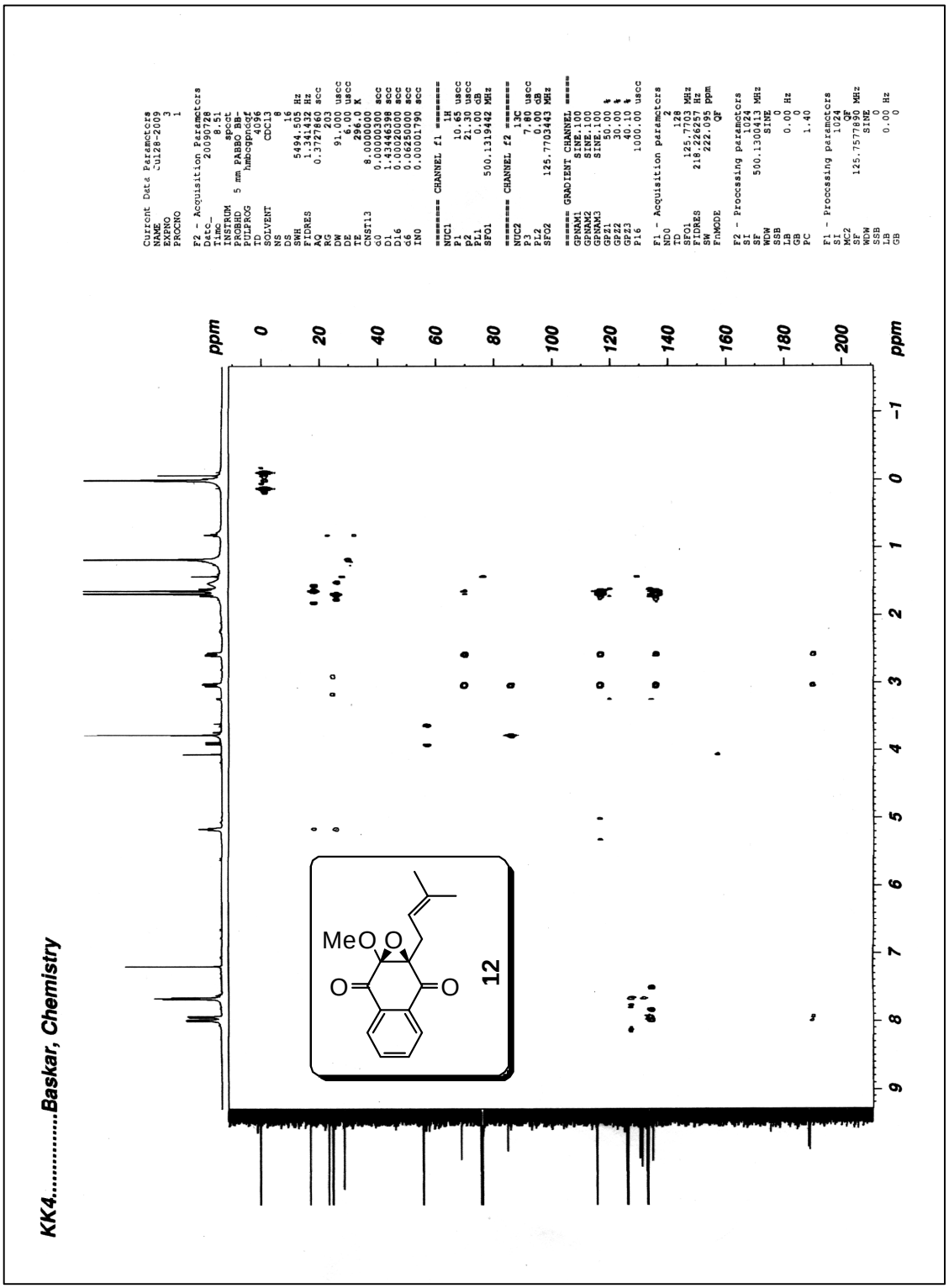
Expandeed ^{1}H NMR spectrum of compound **12**



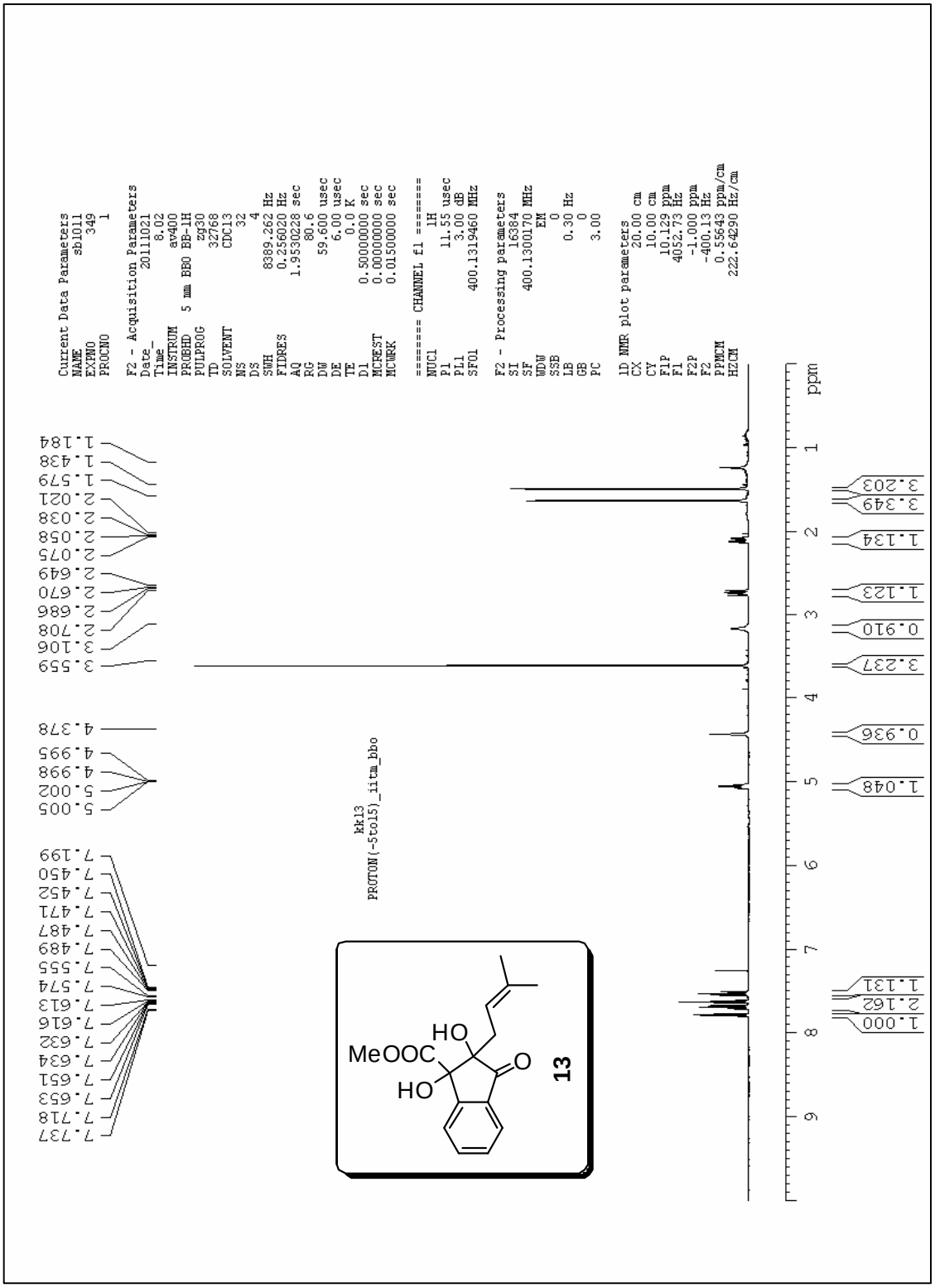
^{13}C NMR spectrum of compound **12**



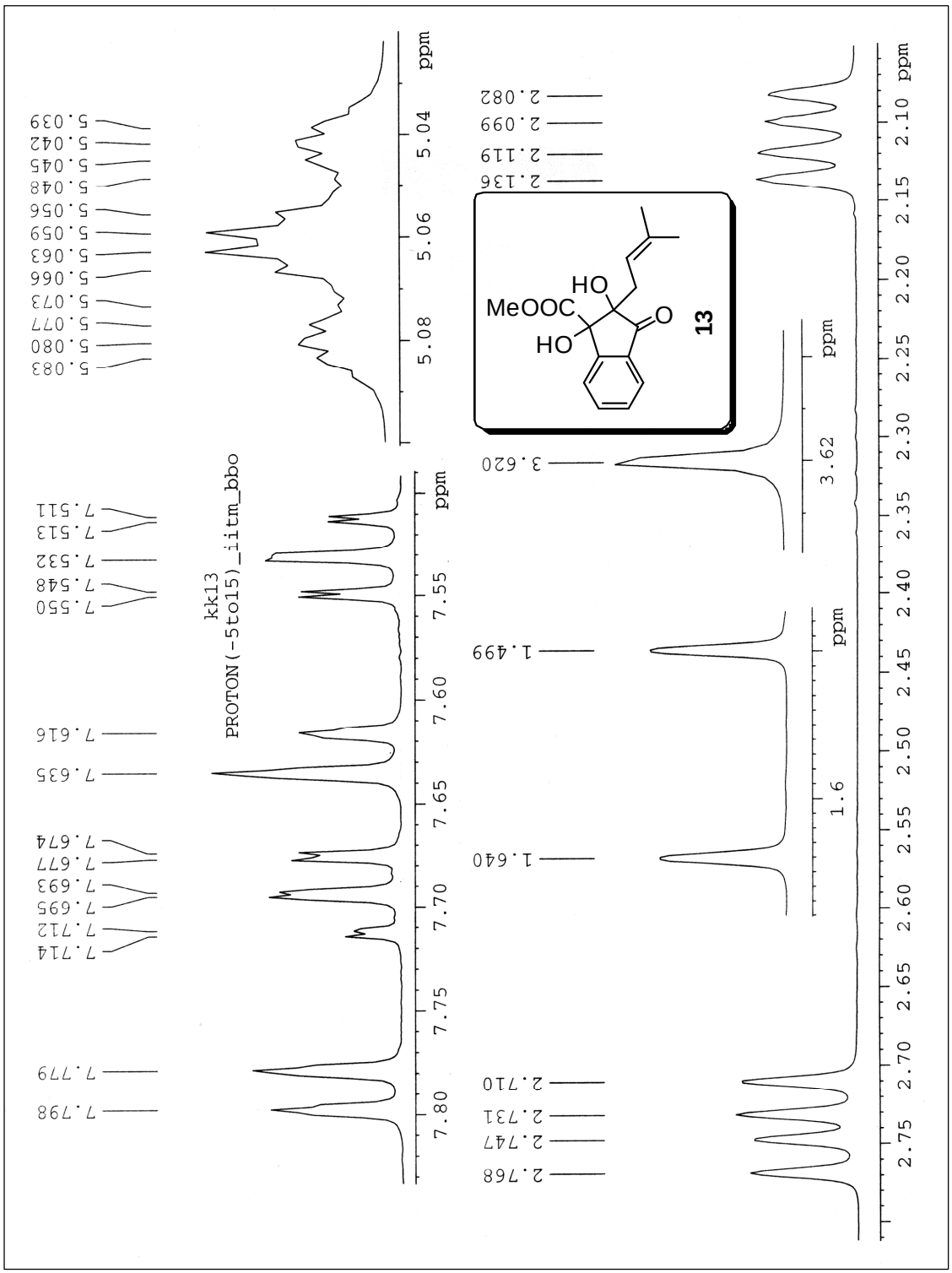
^{1}H-^{13}C COSY (HSQC) NMR spectrum of compound **12**



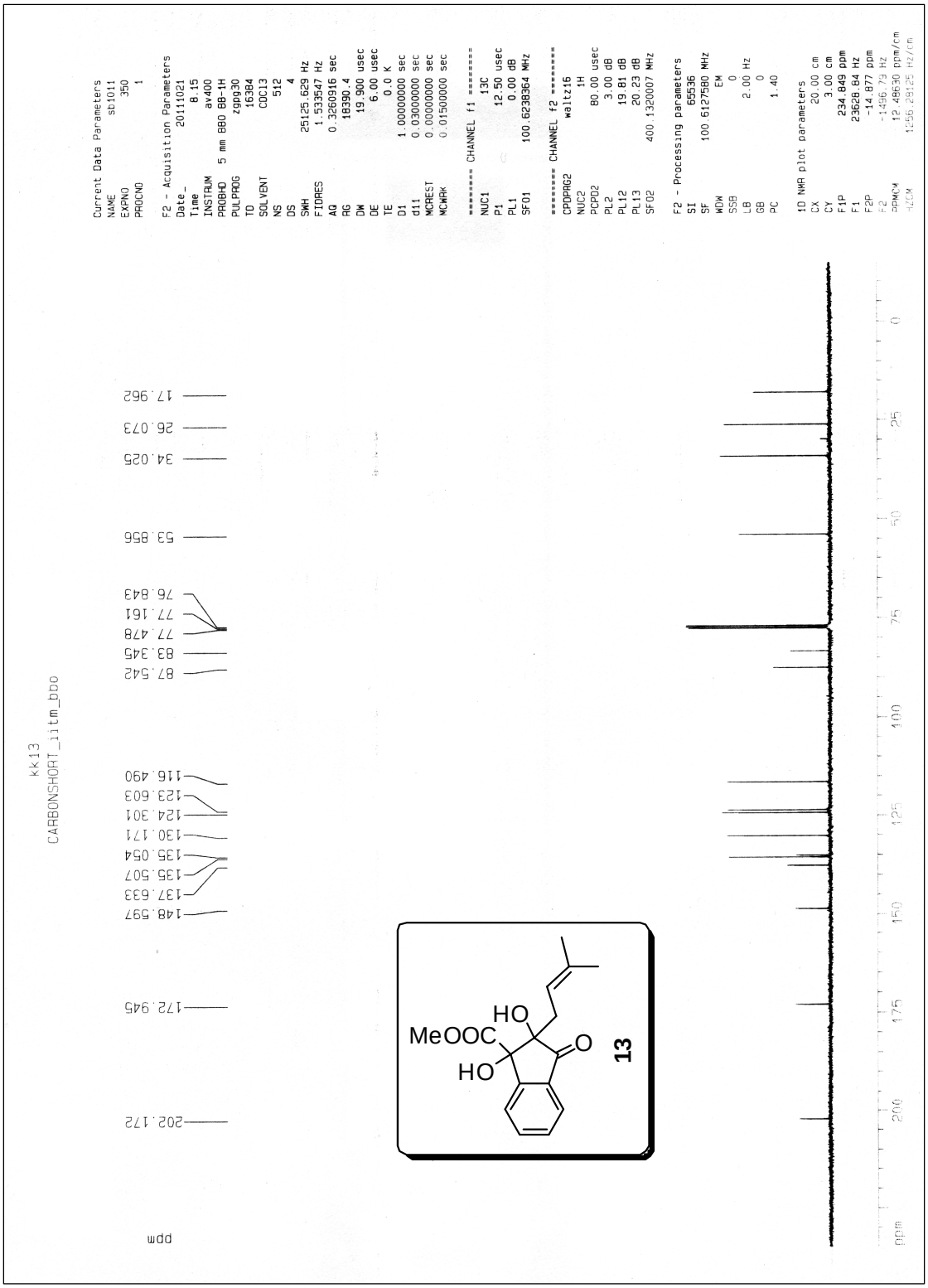
^{1}H-^{13}C COSY (HMBC) NMR spectrum of compound **12**



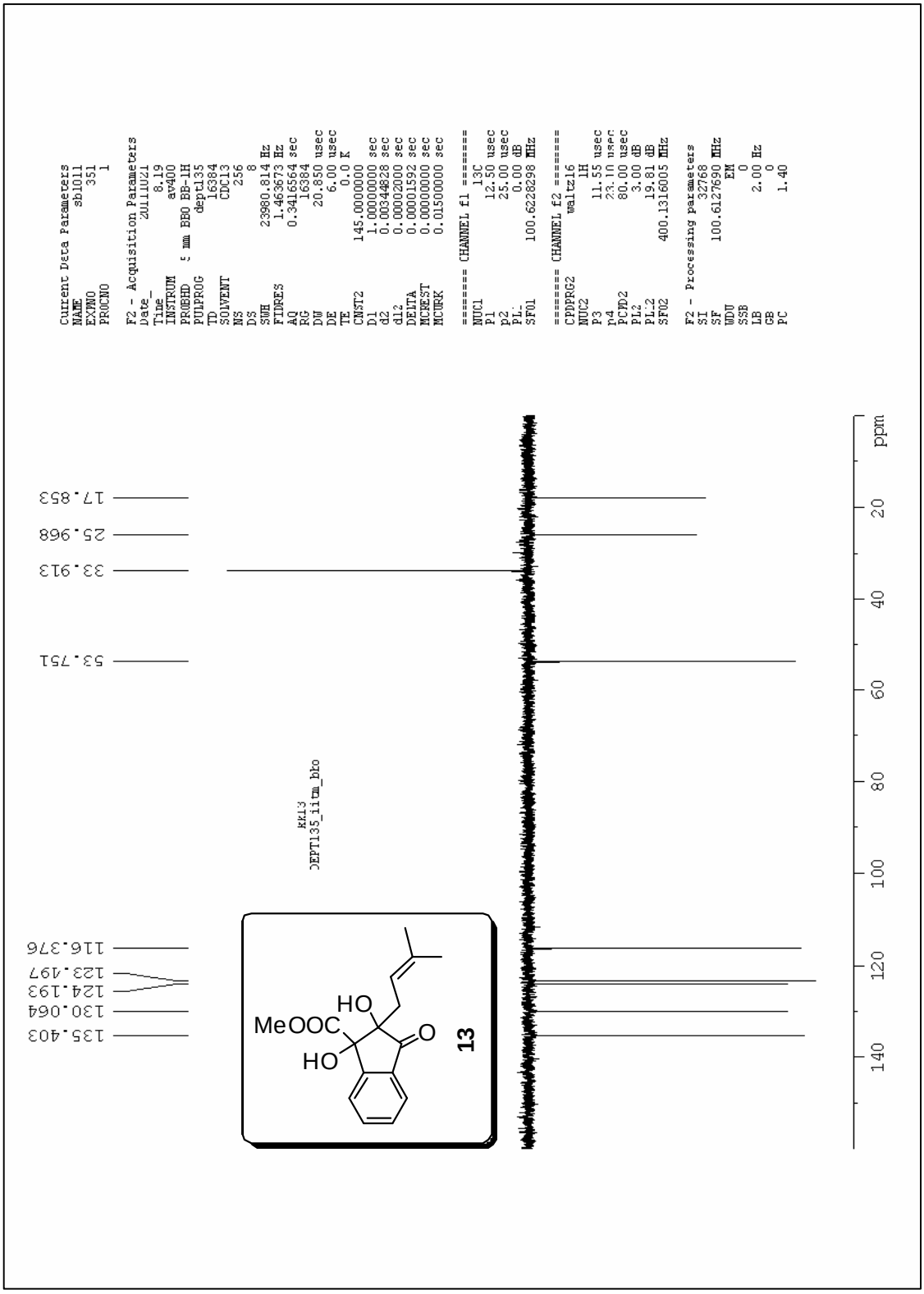
^{1}H NMR spectrum of compound **13**



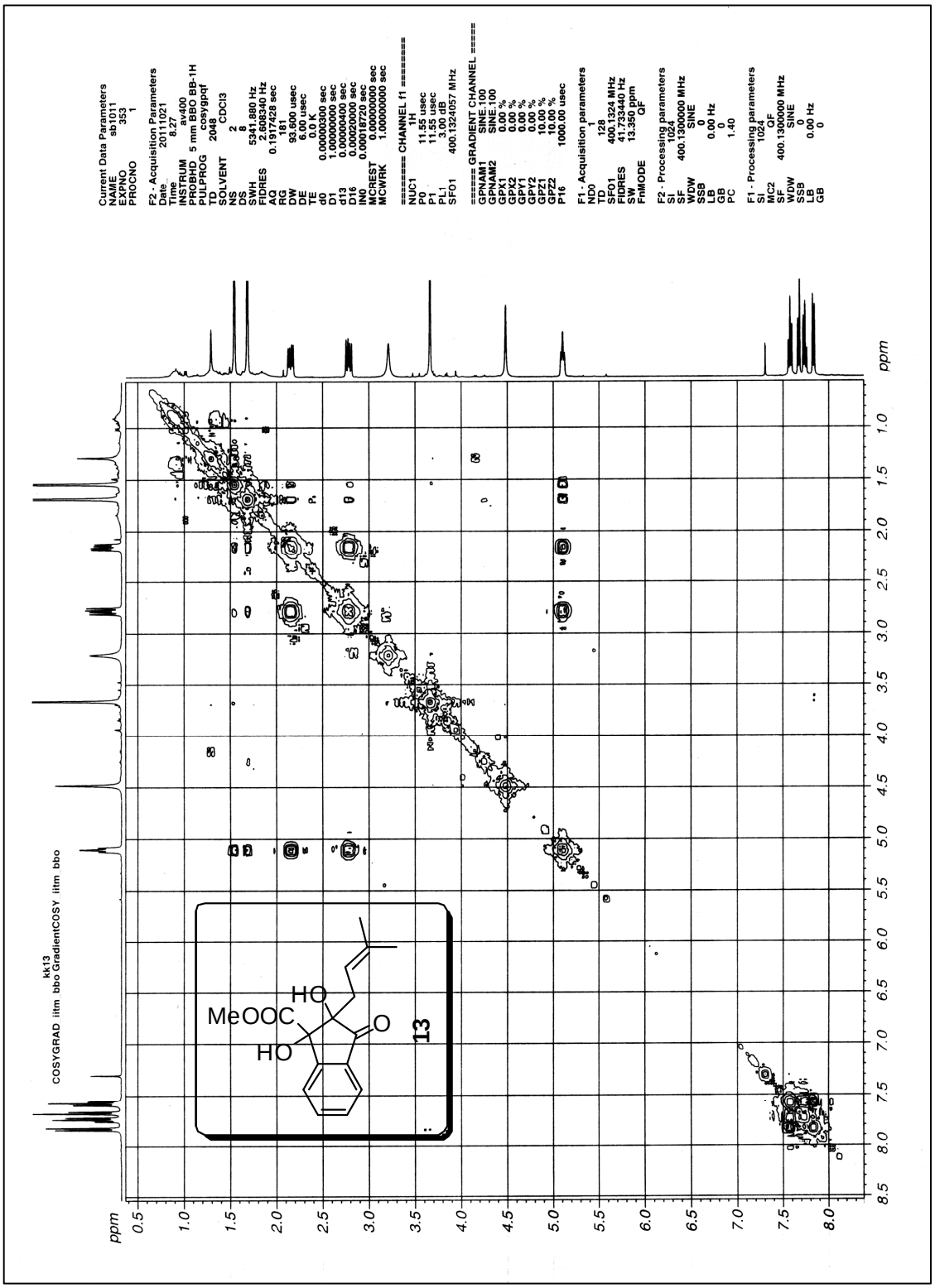
Expandeed ^{1}H NMR spectrum of compound **13**



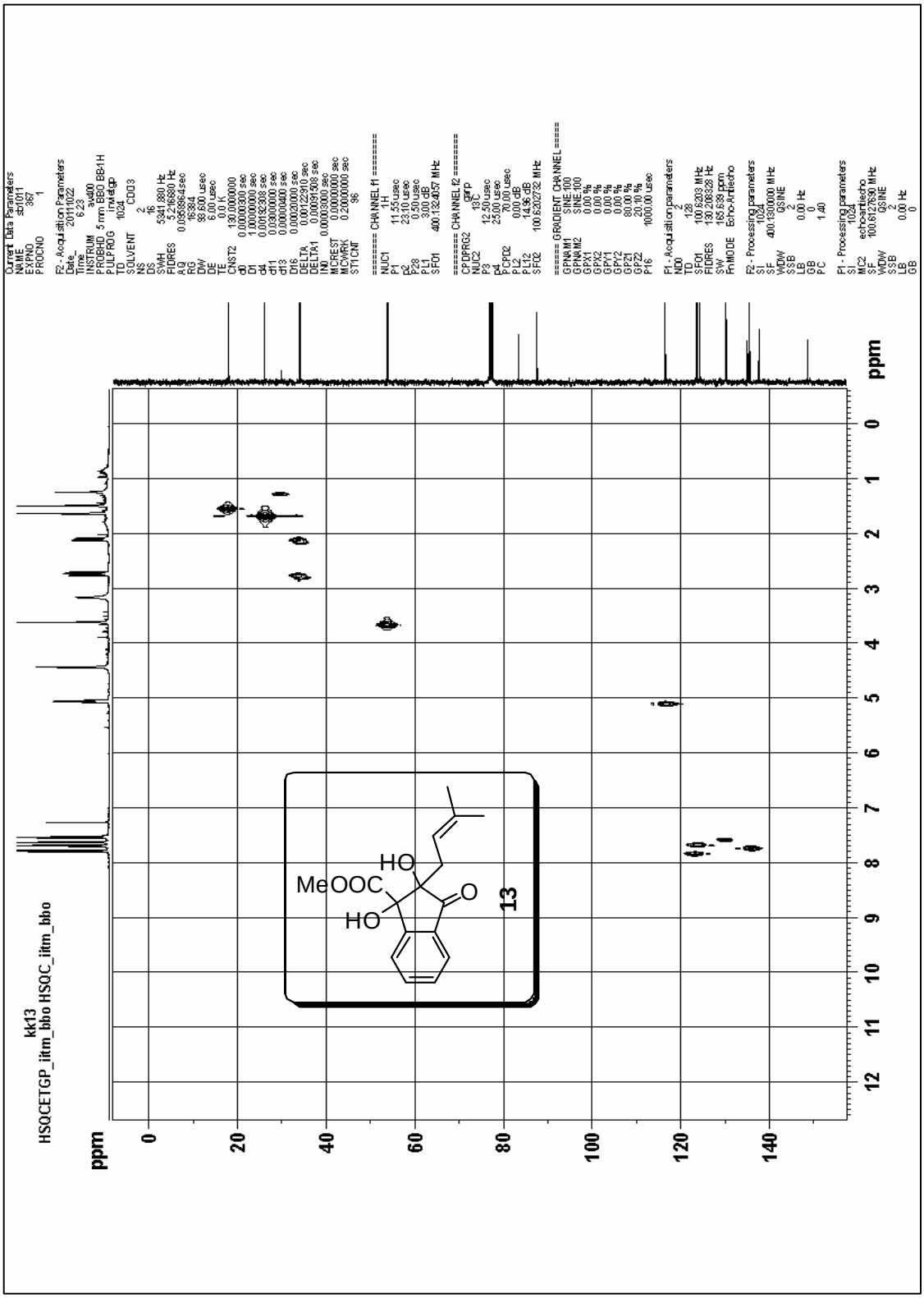
^{13}C NMR spectrum of compound **13**



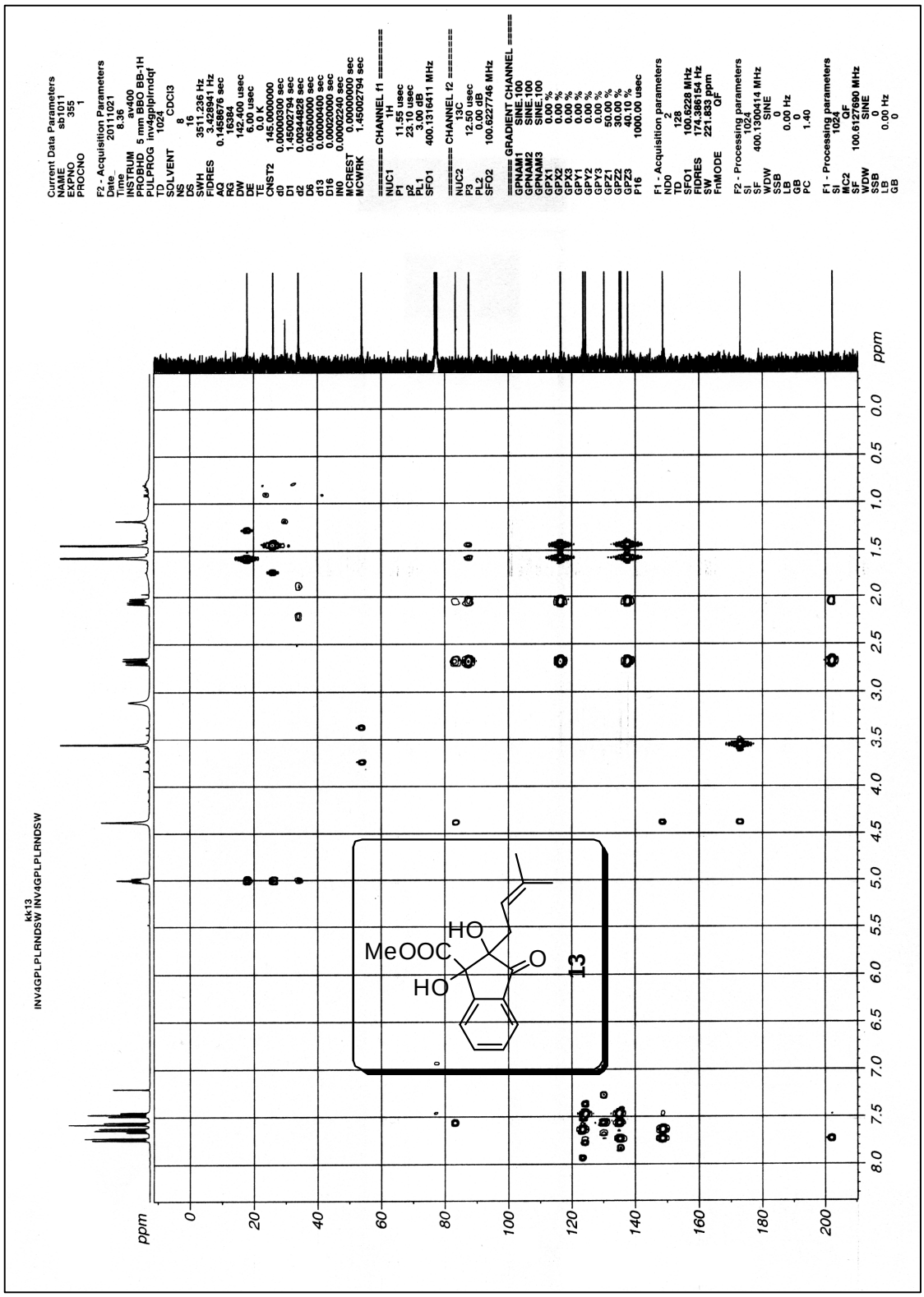
DEPT spectrum of compound **13**



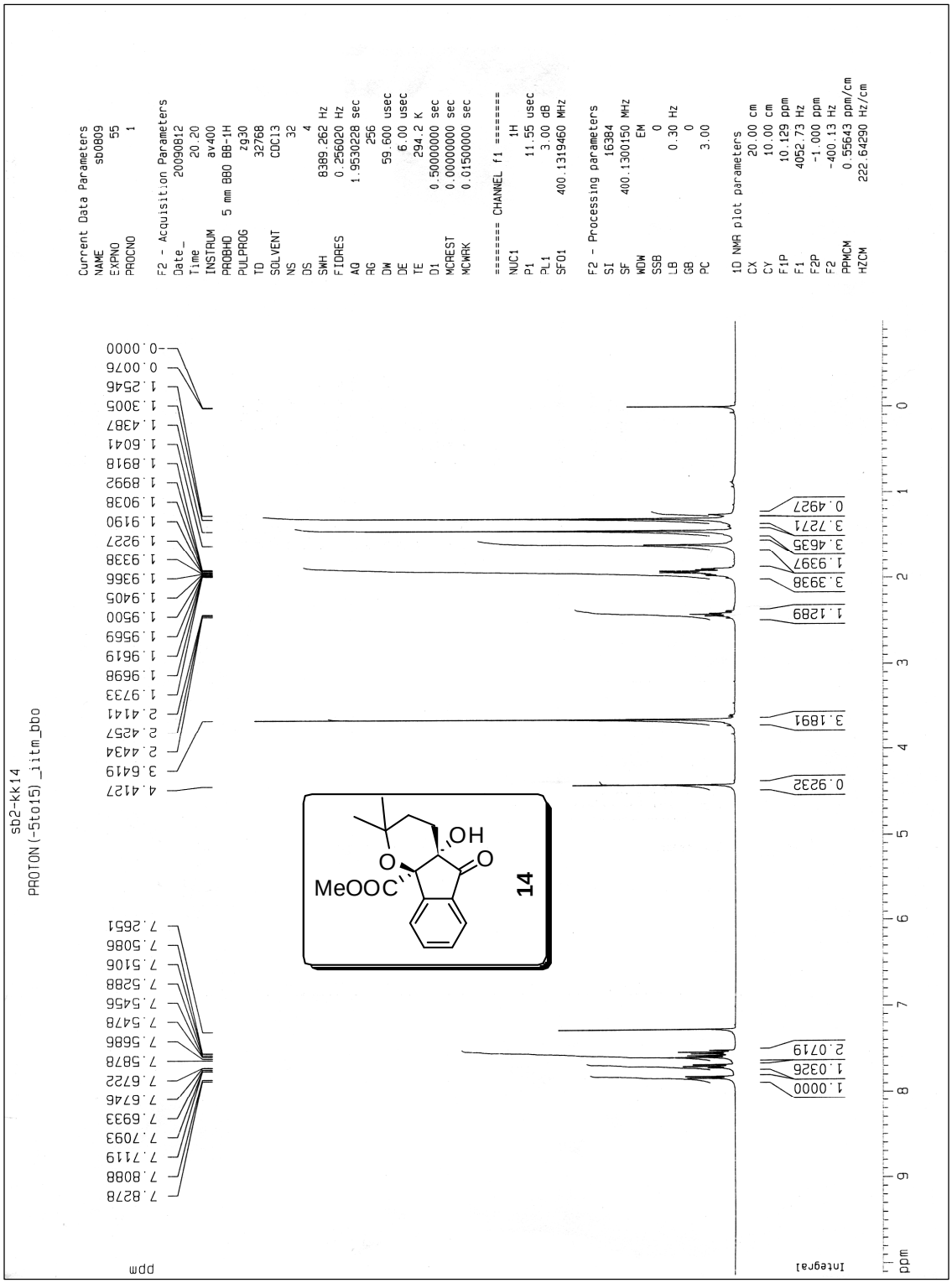
^{1}H-^{1}H COSY spectrum of compound **13**



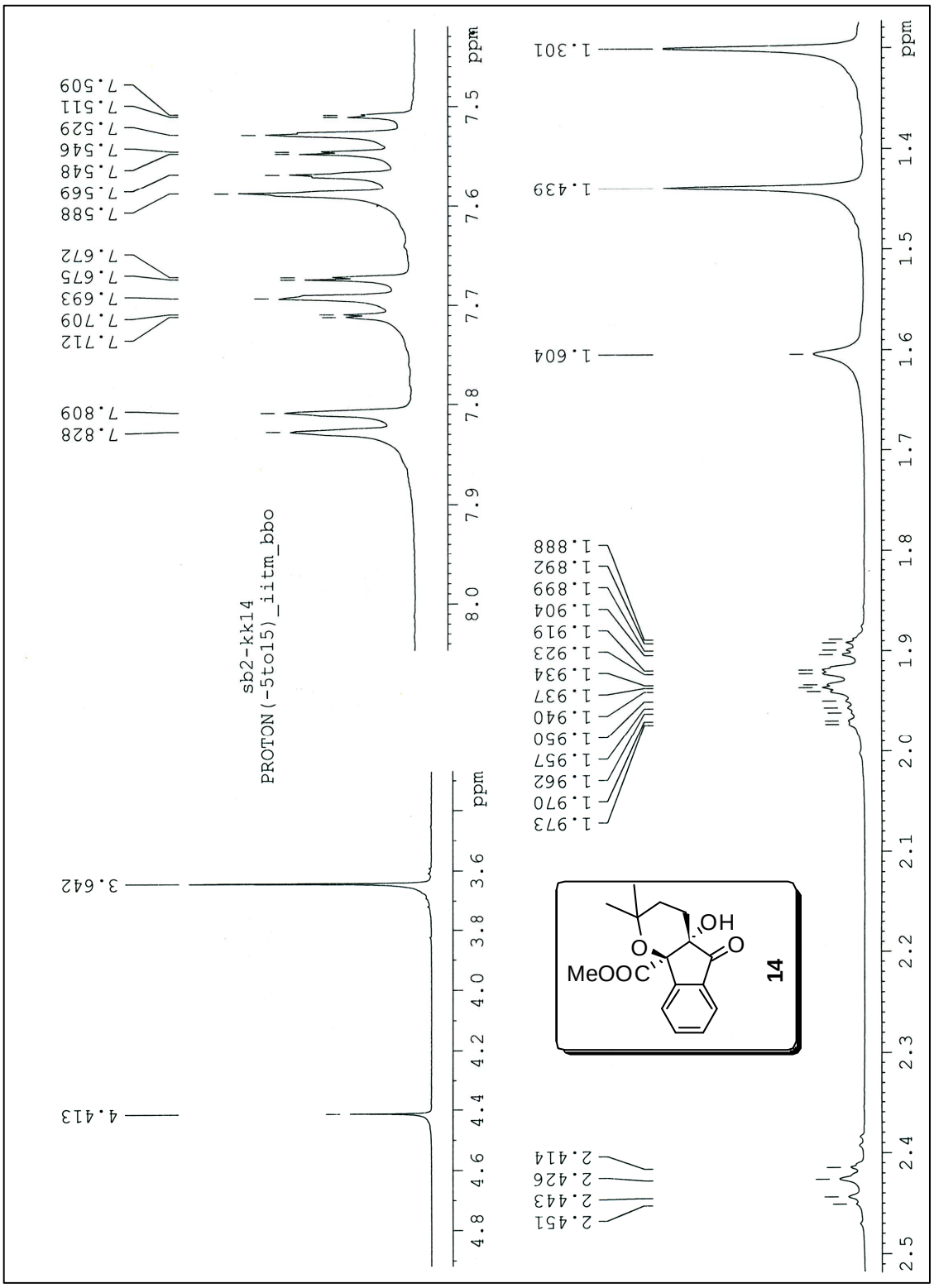
^{1}H-^{13}C COSY (HSQC) NMR spectrum of compound **13**



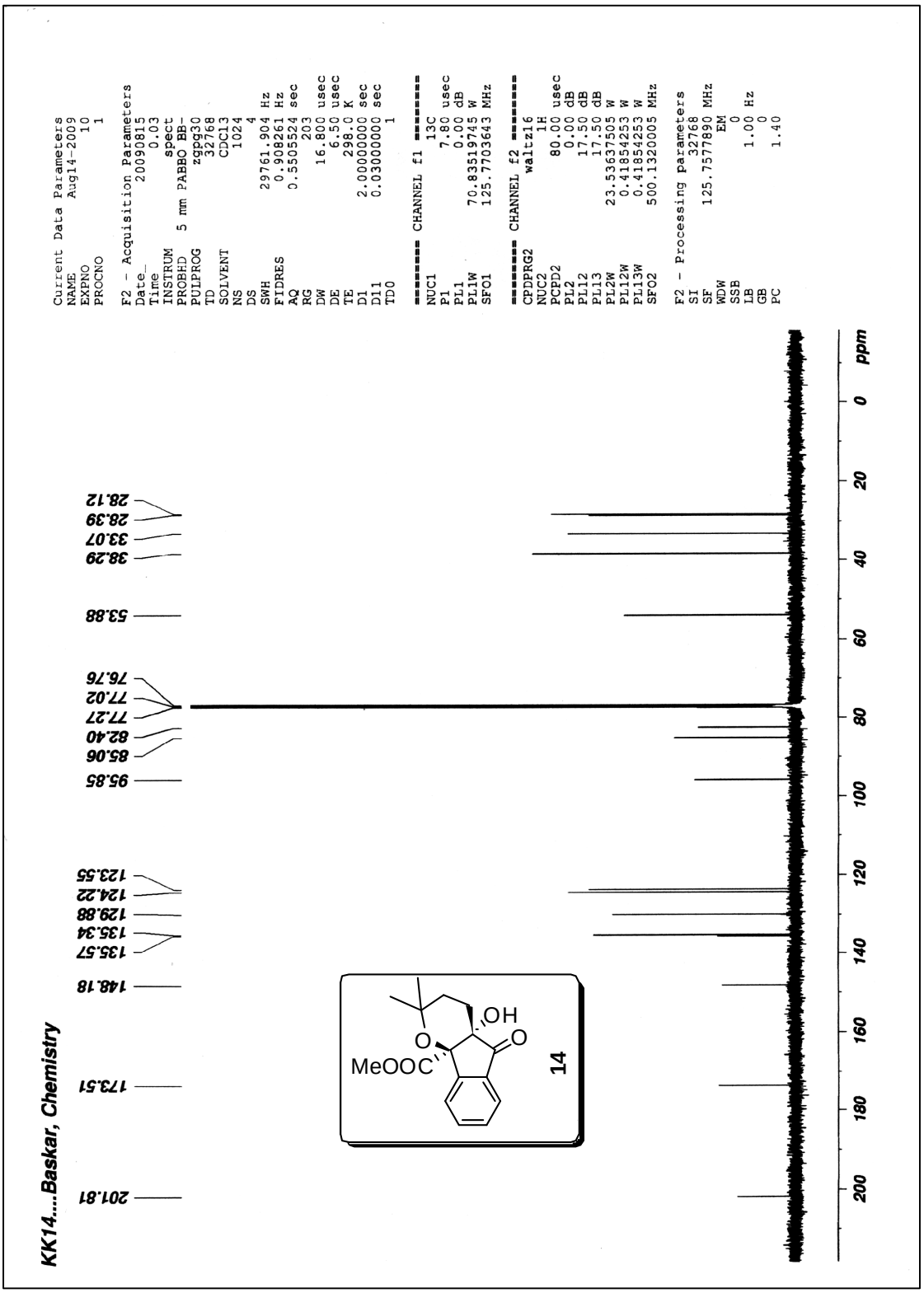
^{1}H-^{13}C COSY (HMBC) NMR spectrum of compound **13**



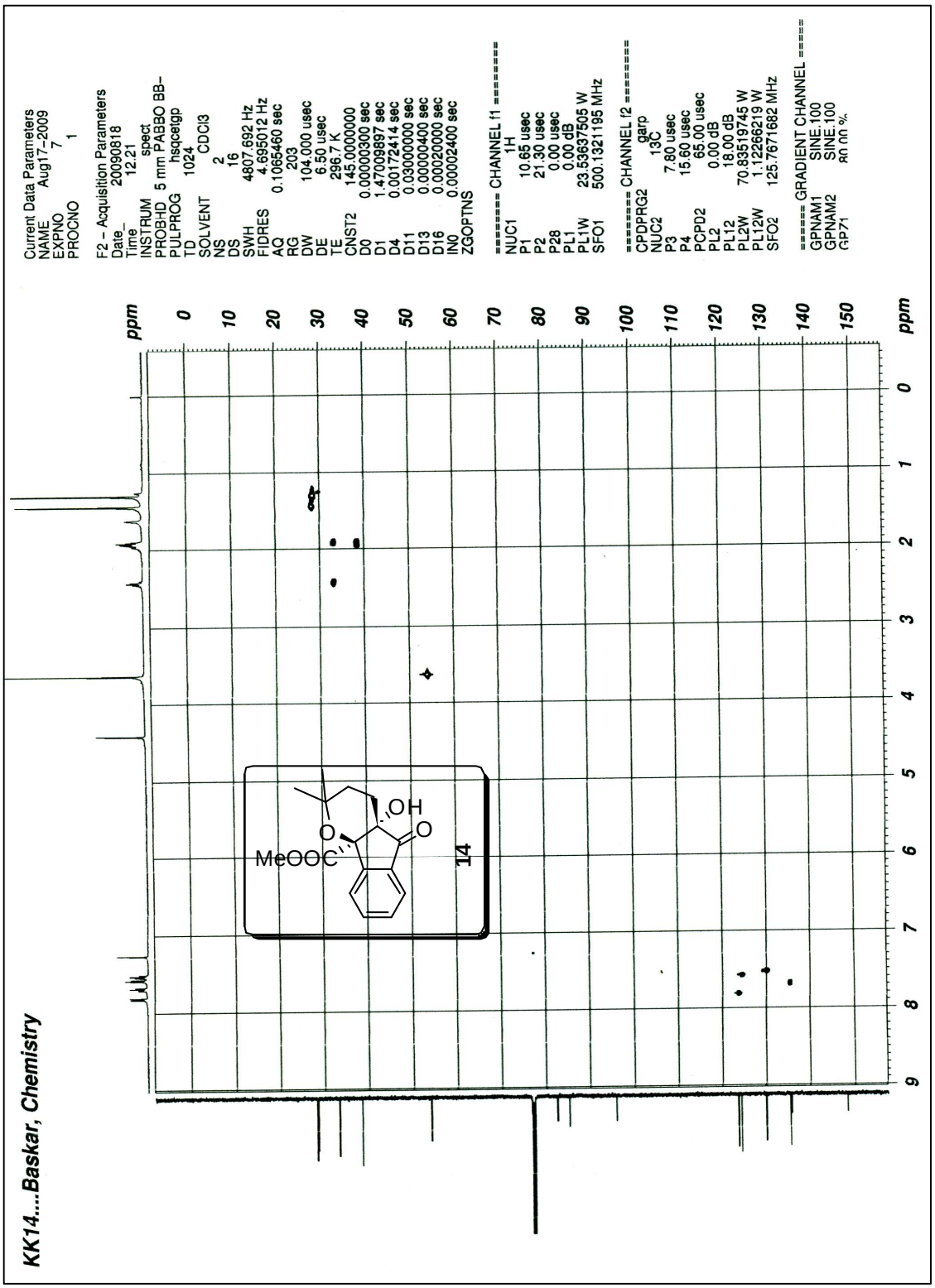
^{1}H NMR spectrum of compound **14**



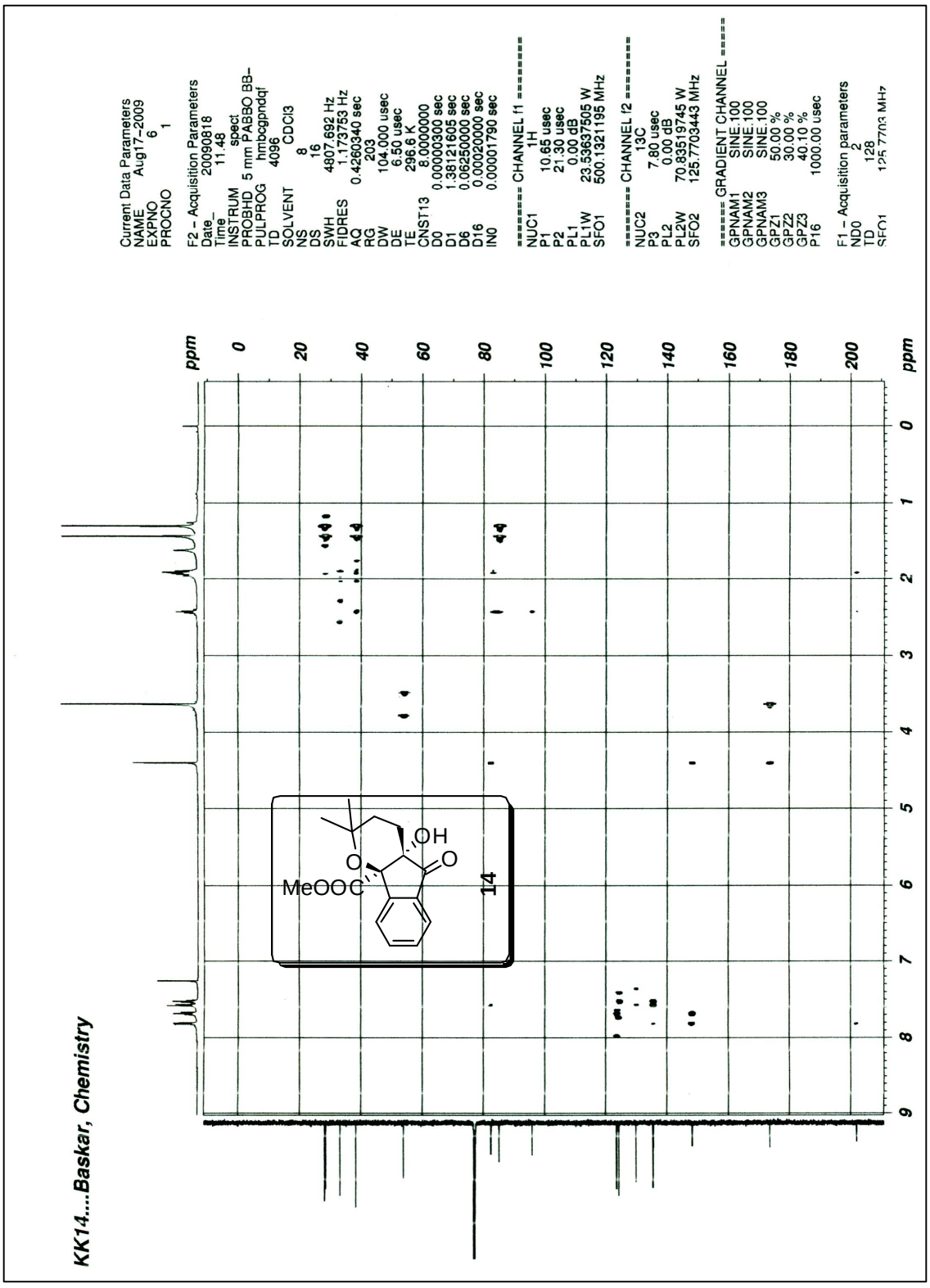
Expandeed ^{1}H NMR spectrum of compound **14**



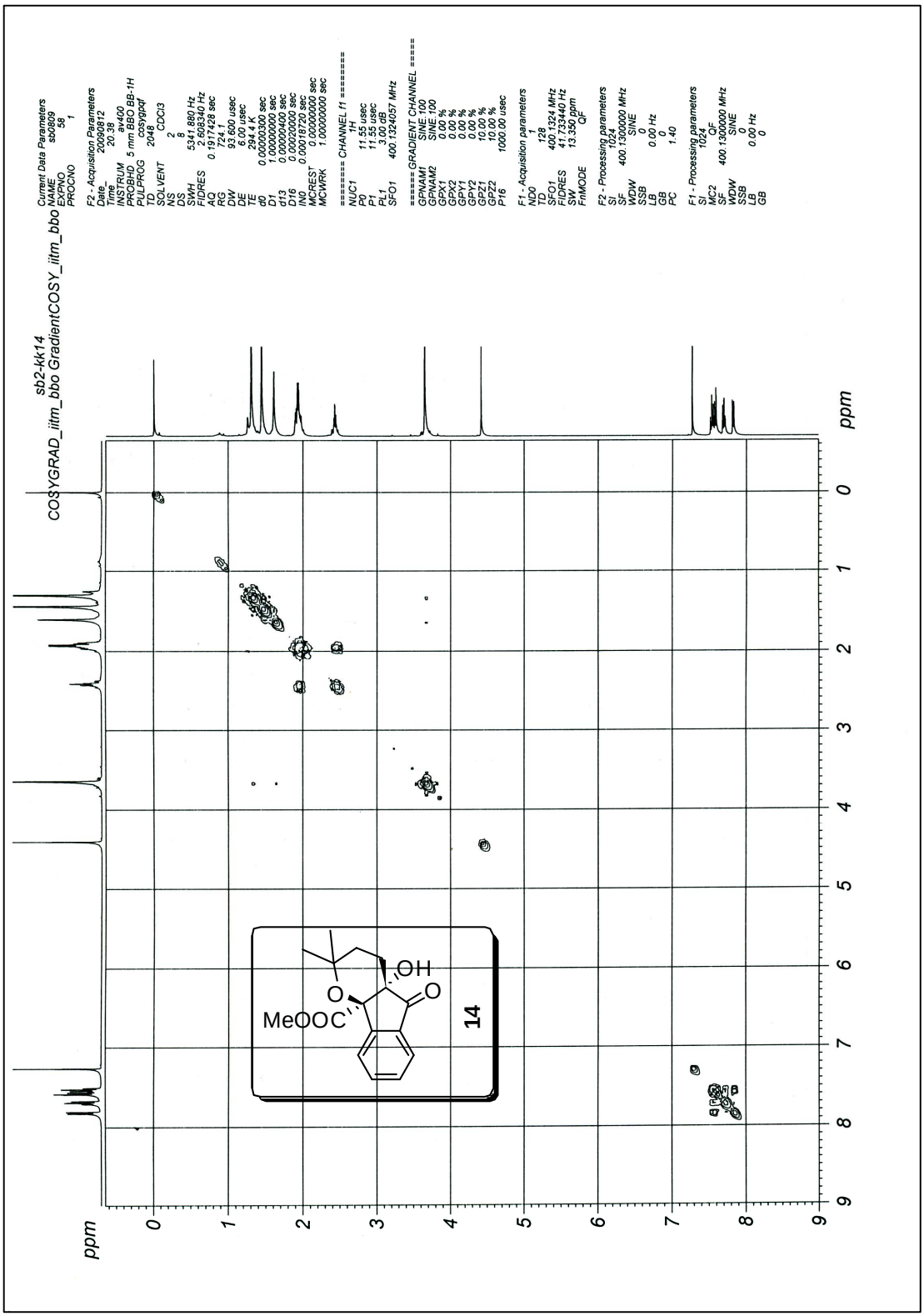
^{13}C NMR spectrum of compound **14**



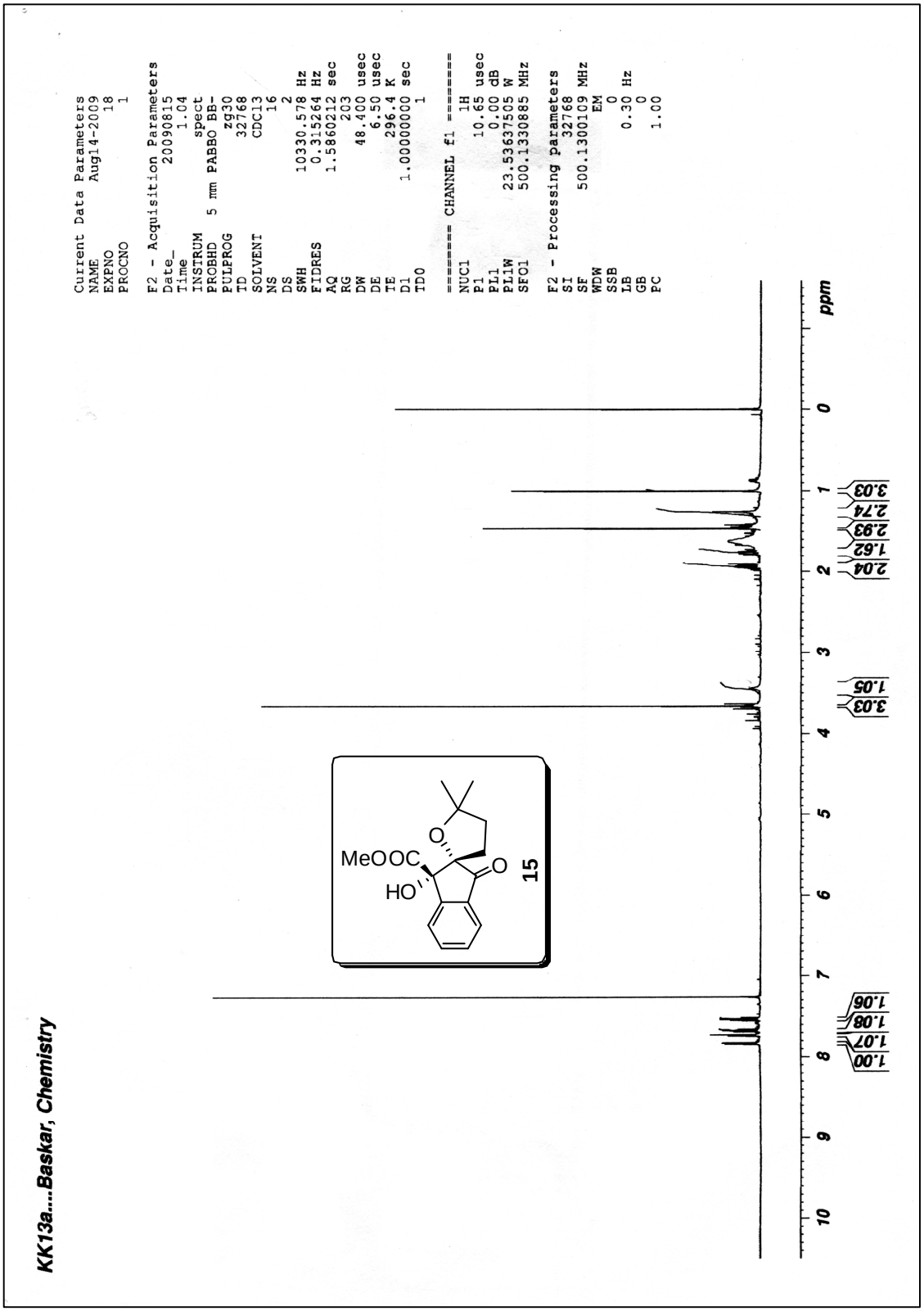
^{1}H-^{13}C COSY (HSQC) NMR spectrum of compound **14**



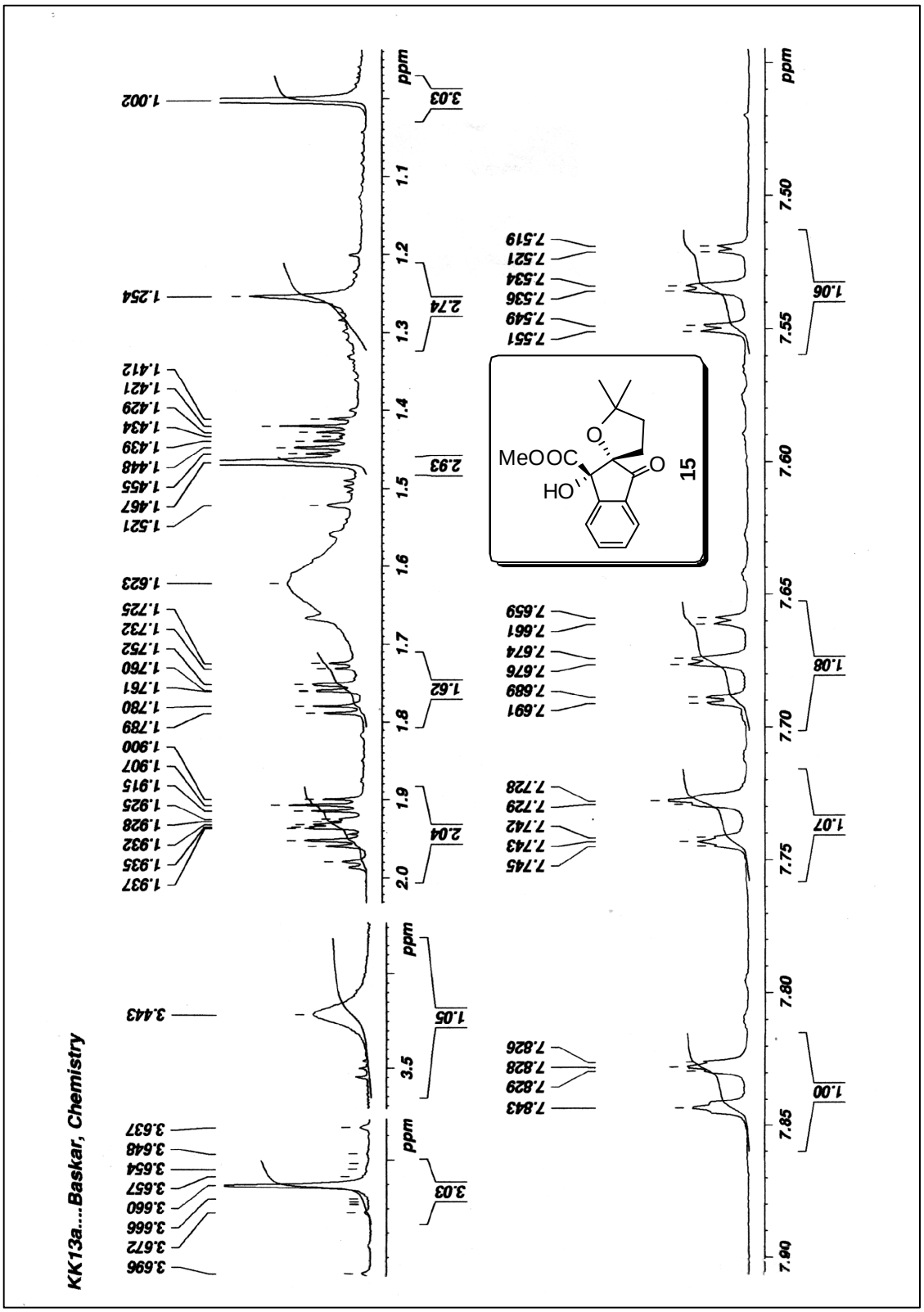
^{1}H-^{13}C COSY (HMBC) NMR spectrum of compound **14**



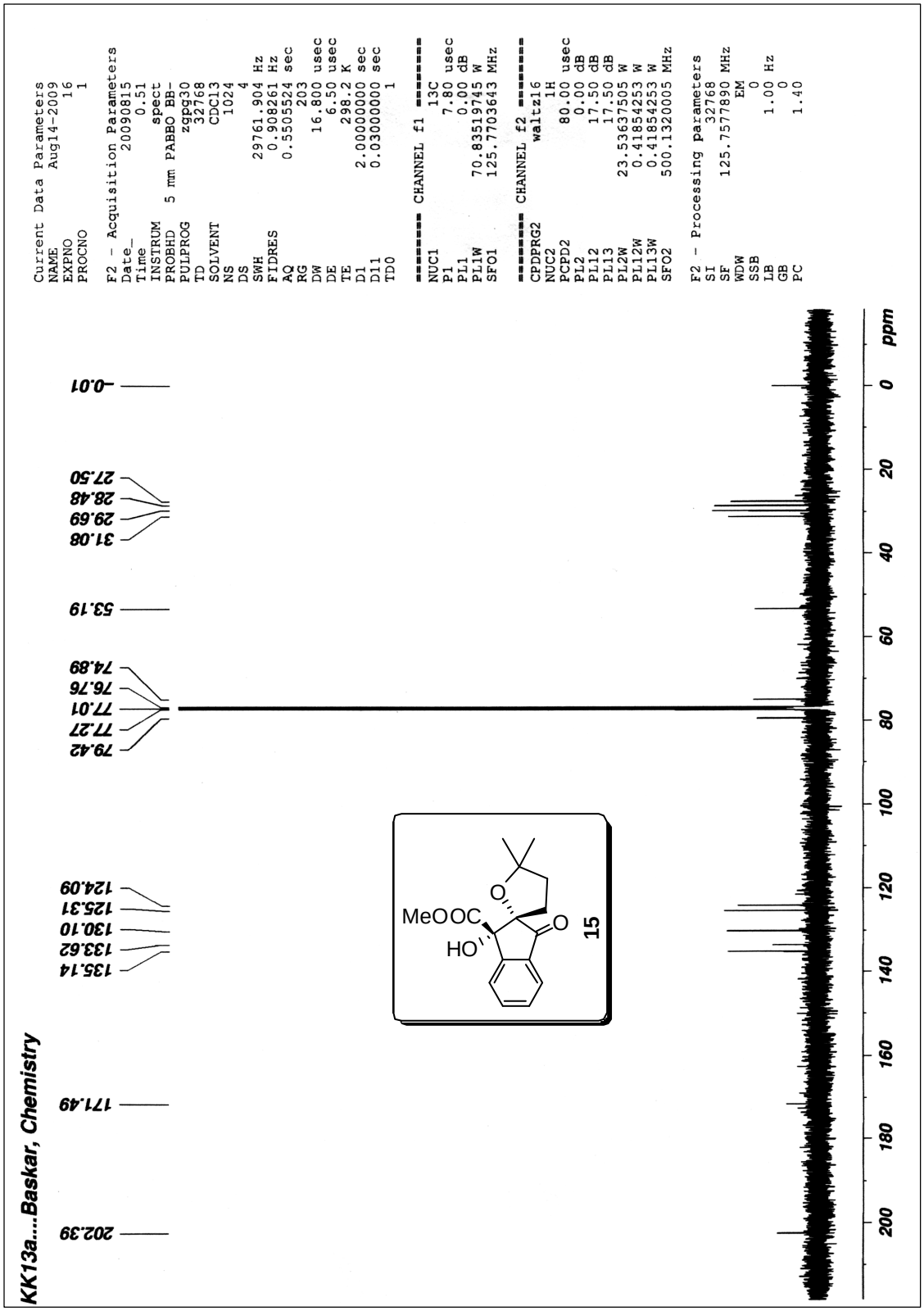
^{1}H-^{1}H COSY spectrum of compound **14**



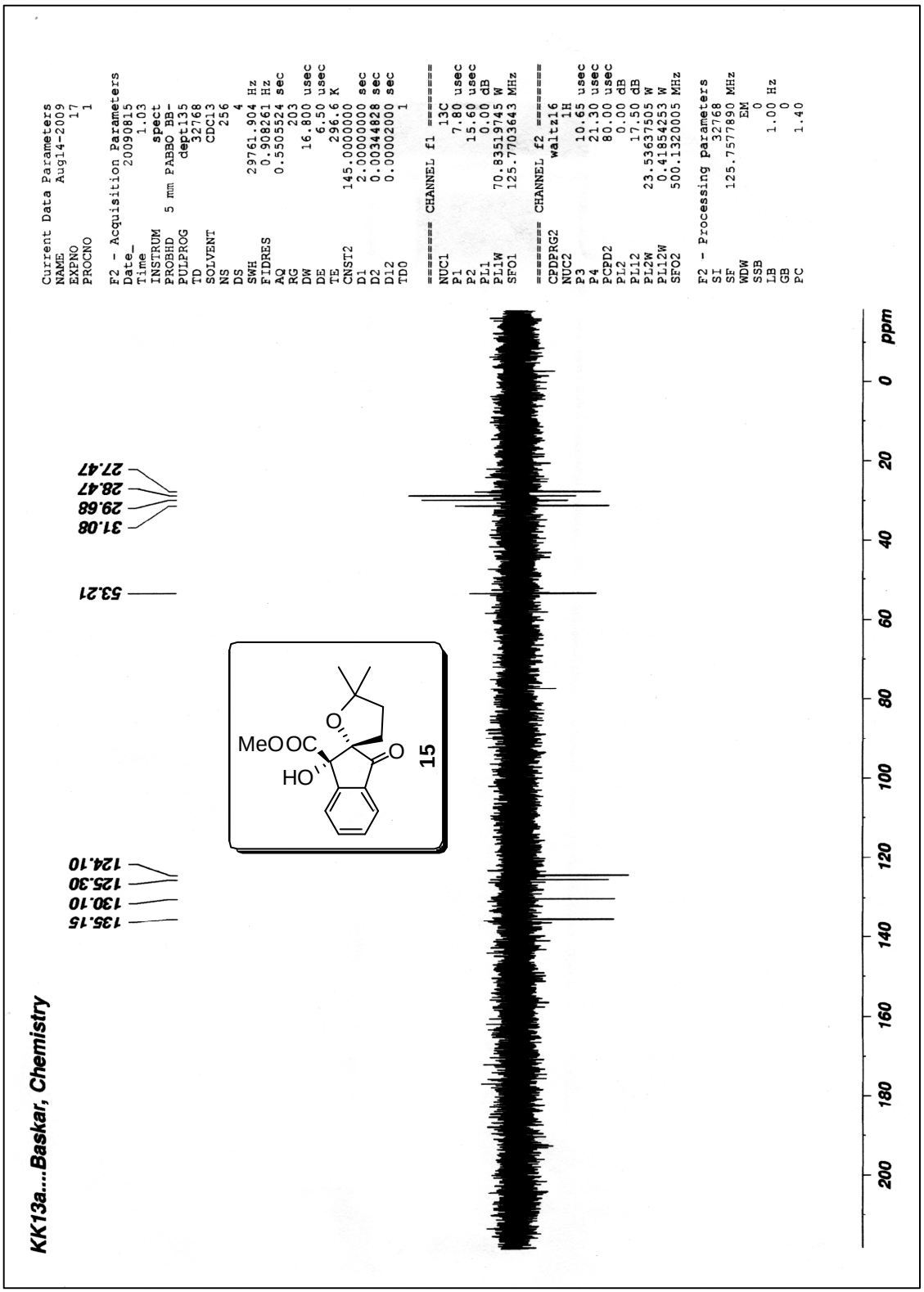
^{1}H NMR spectrum ofcompound **15**



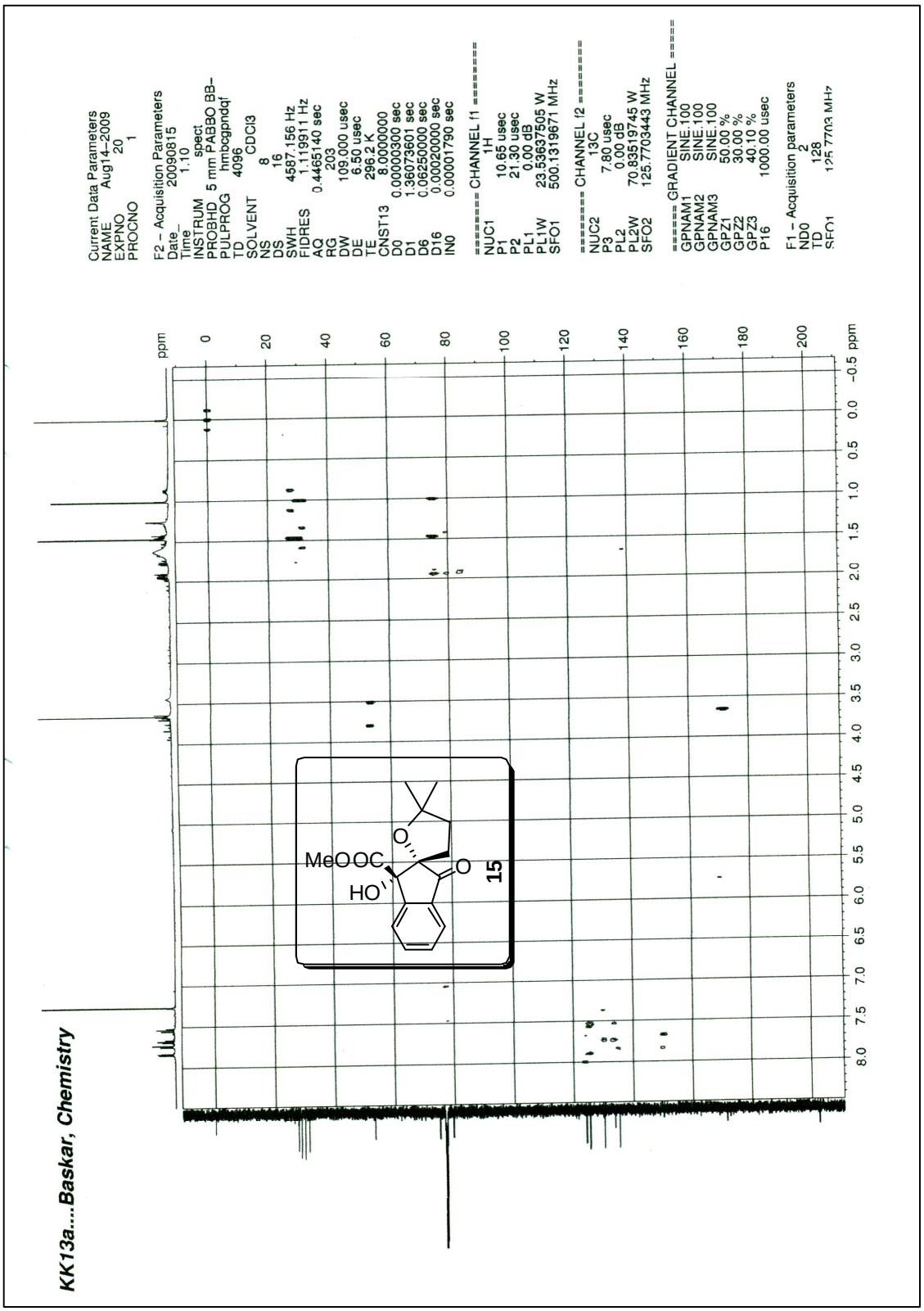
Expandeed ^{1}H NMR spectrum of compound **15**



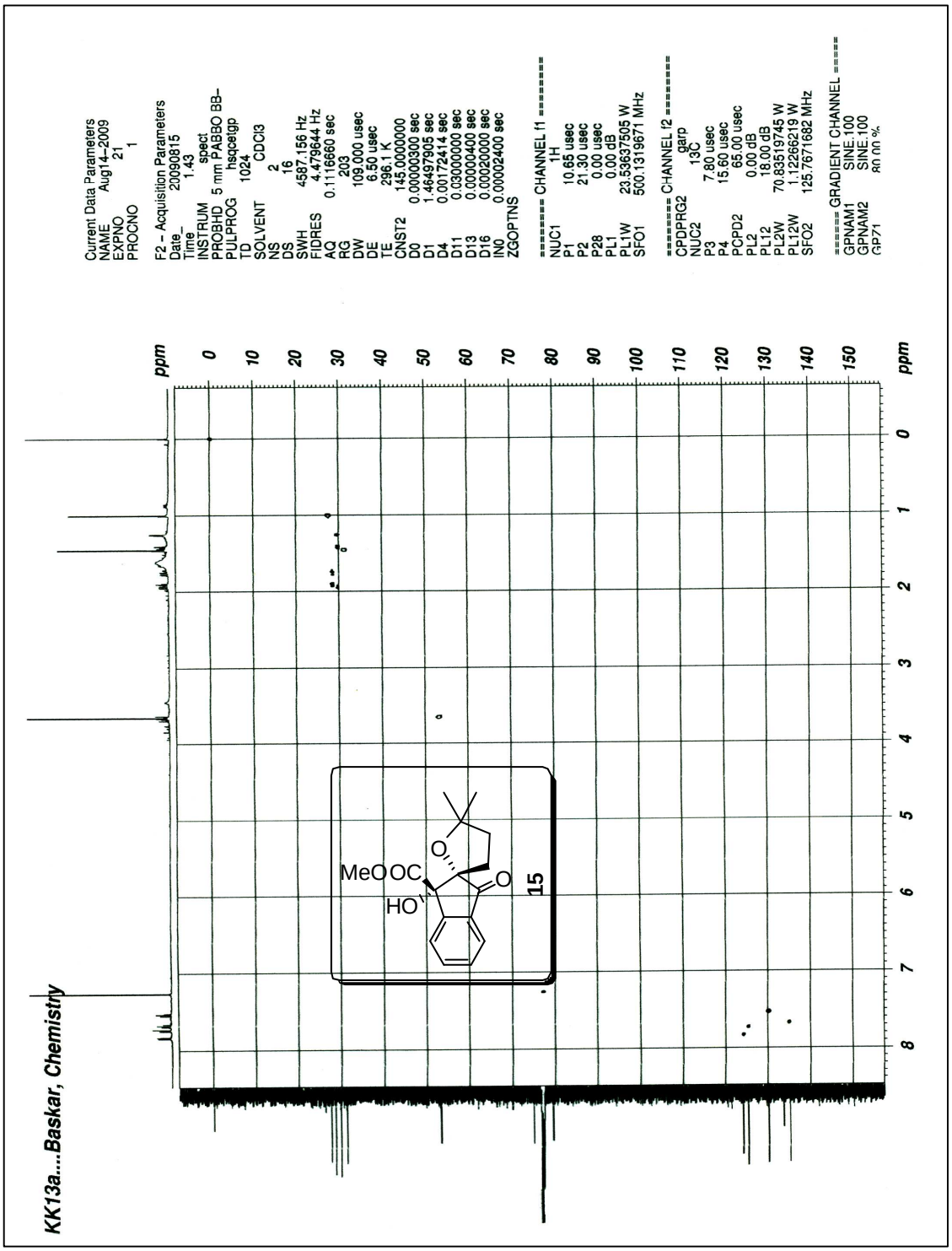
^{13}C NMR spectrum of compound **15**



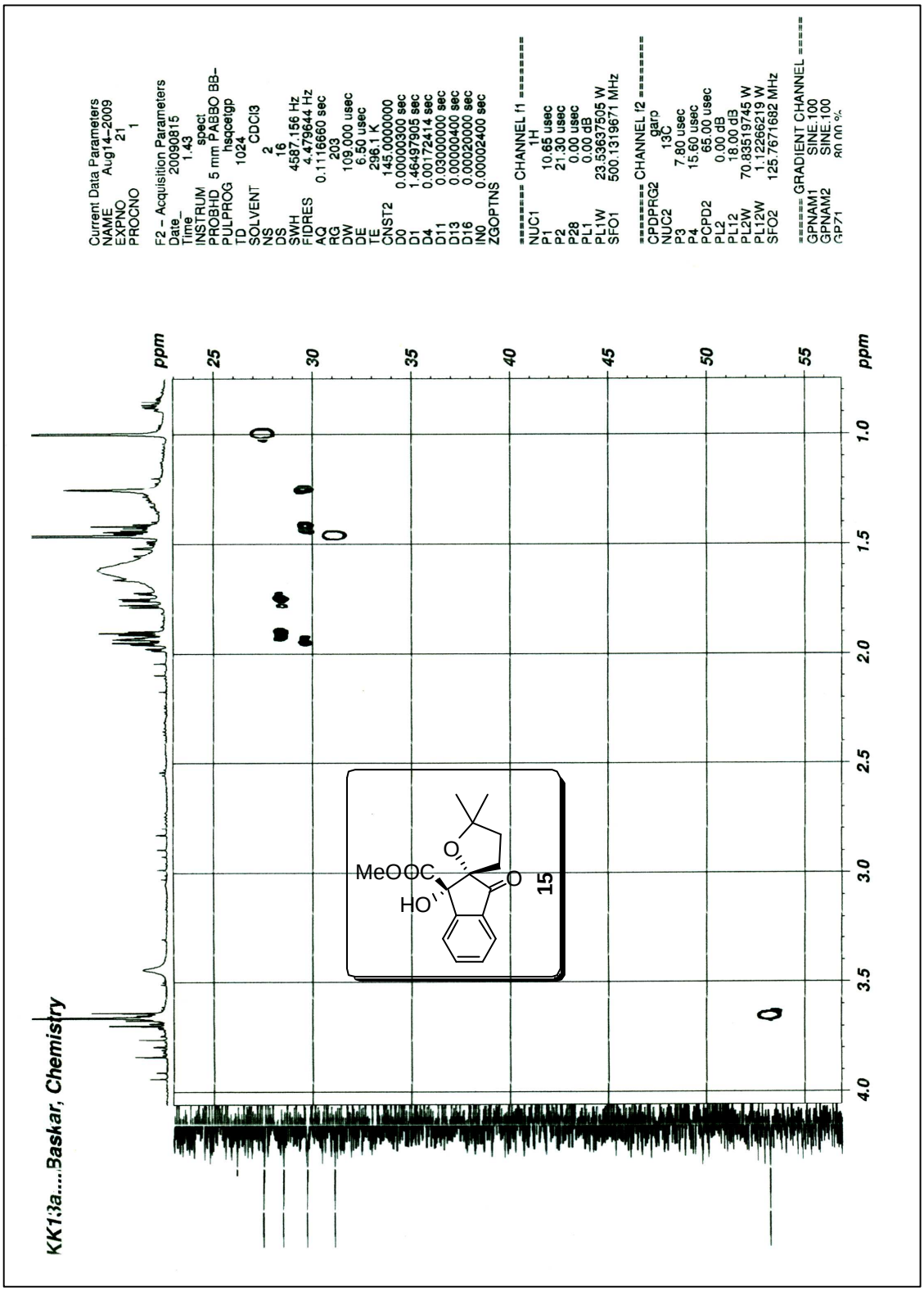
DEPT spectrum of compound **15**



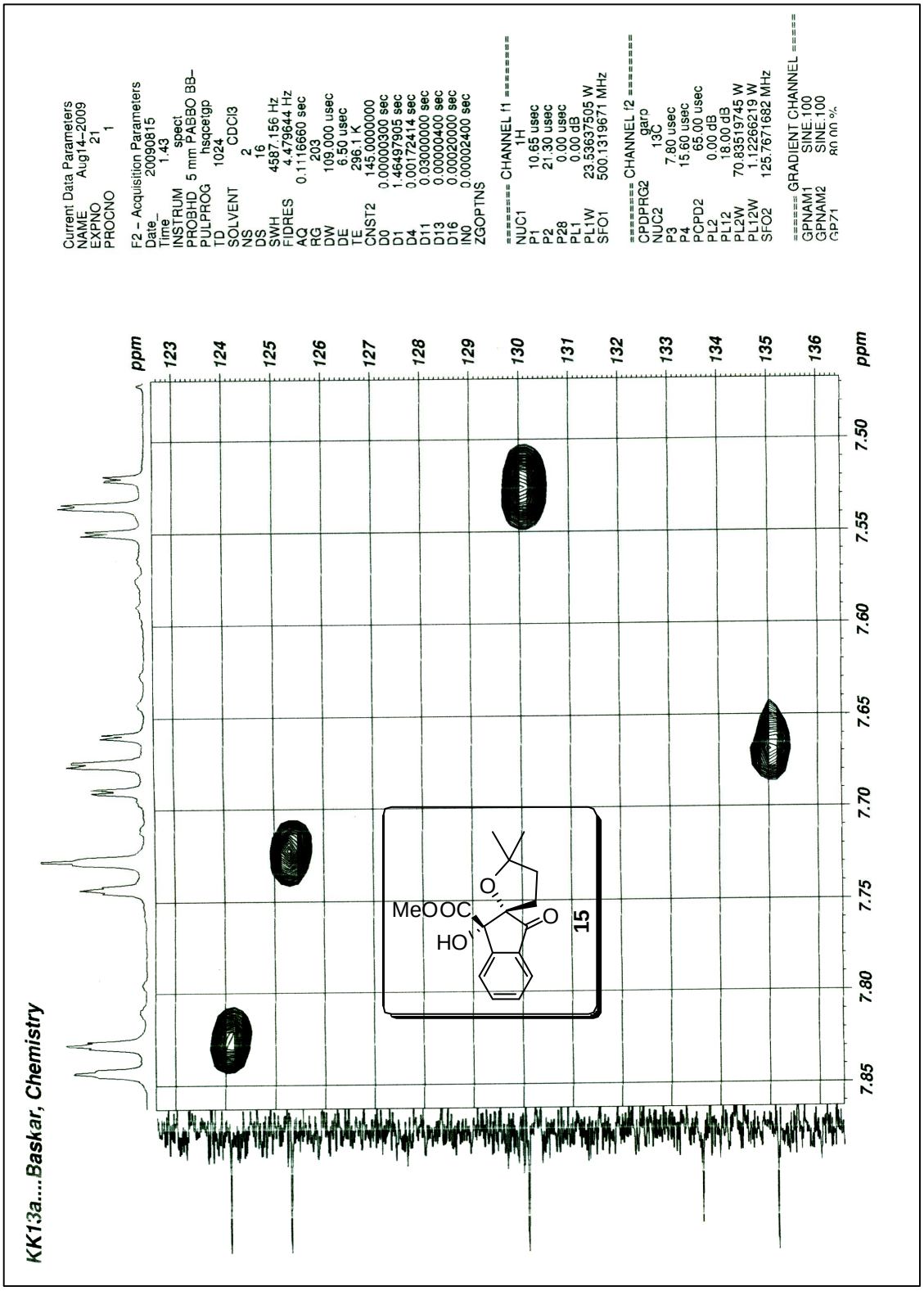
^{1}H-^{13}C COSY (HMBC) NMR spectrum of compound **15**



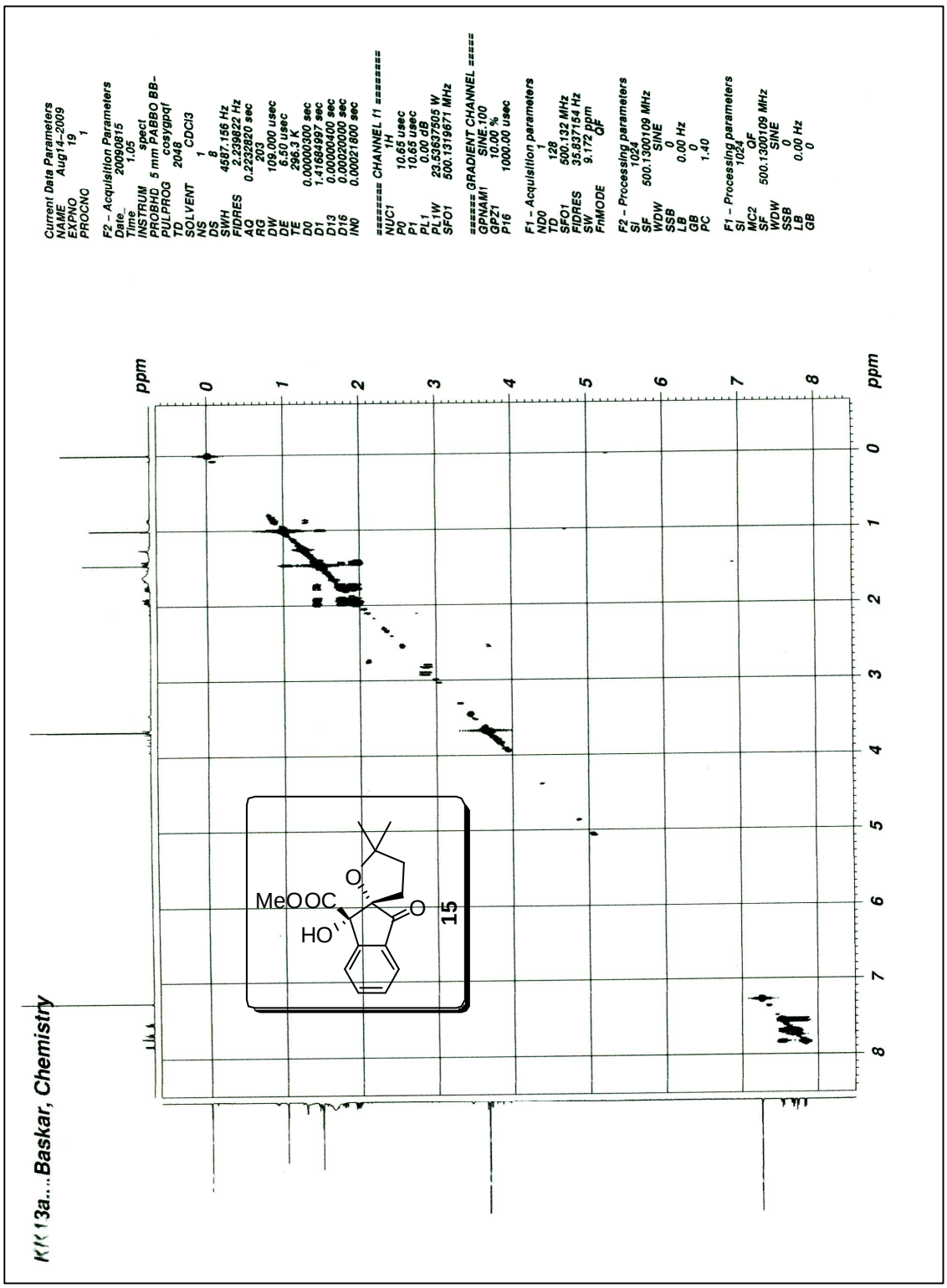
^{1}H-^{13}C COSY (HSQC) NMR spectrum of compound **15**



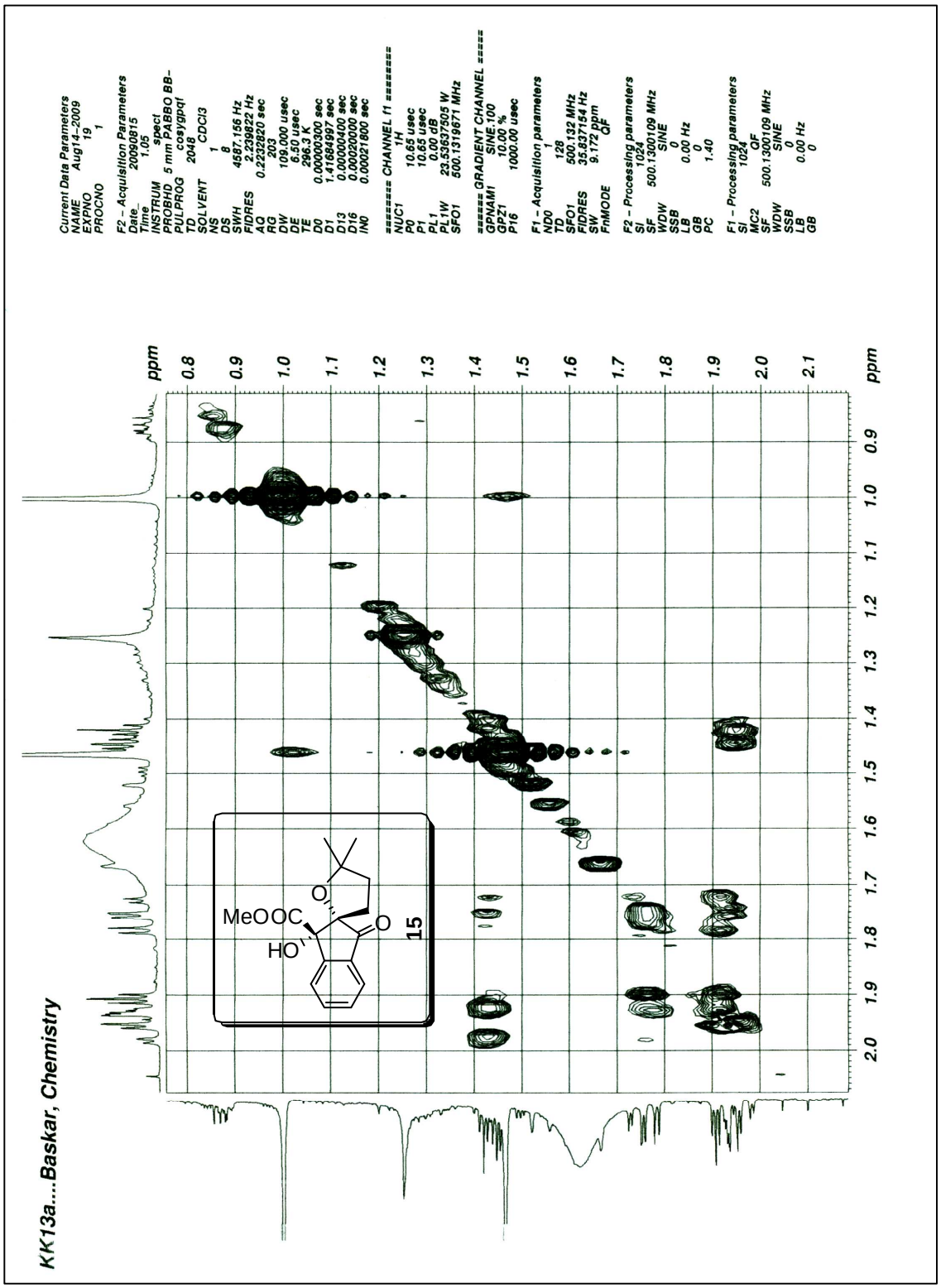
Expanded ^{1}H-^{13}C COSY (HSQC) NMR spectrum of compound **15**



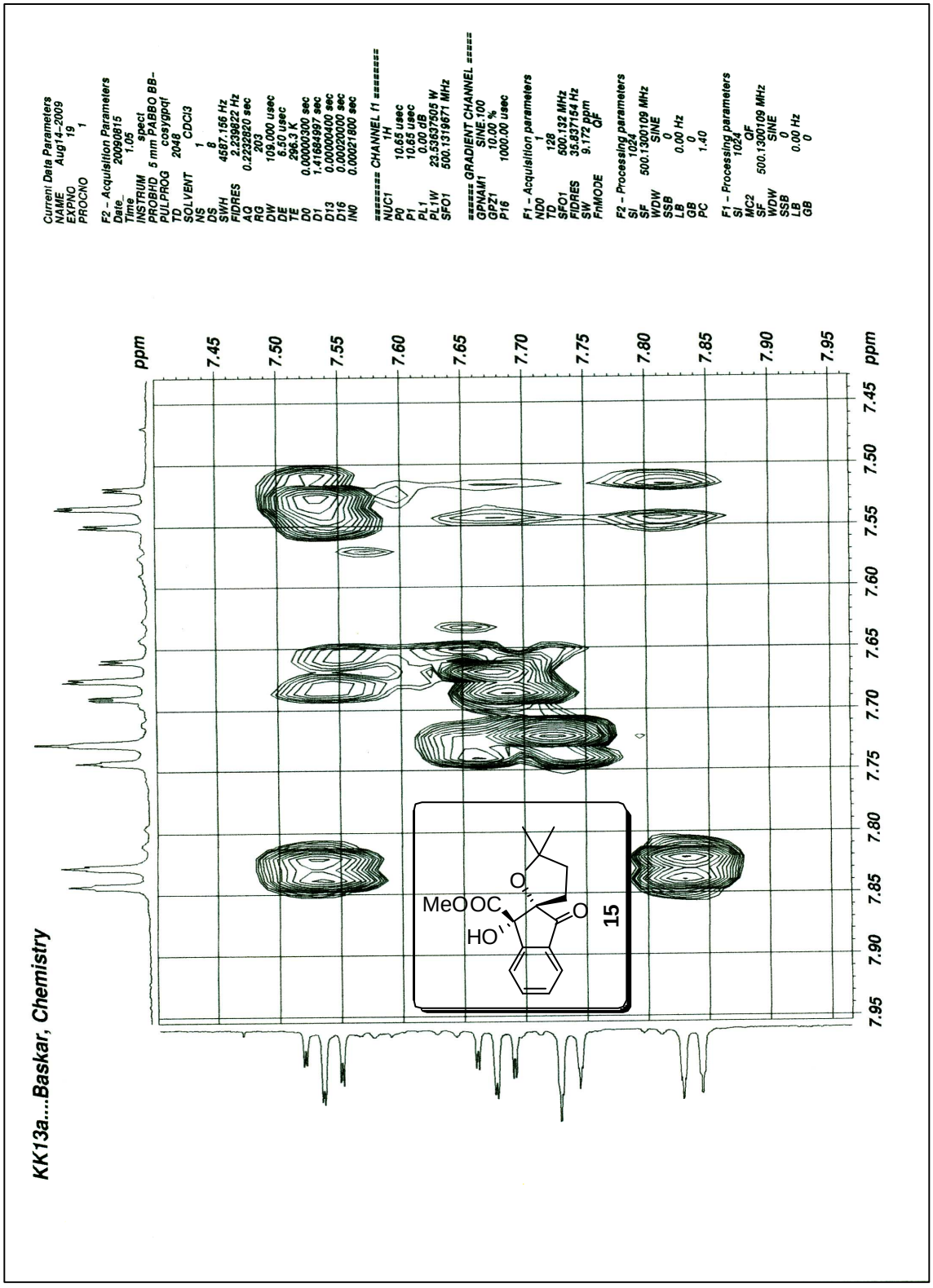
Expanded ^{1}H-^{13}C COSY (HSQC) NMR spectrum of compound **15**



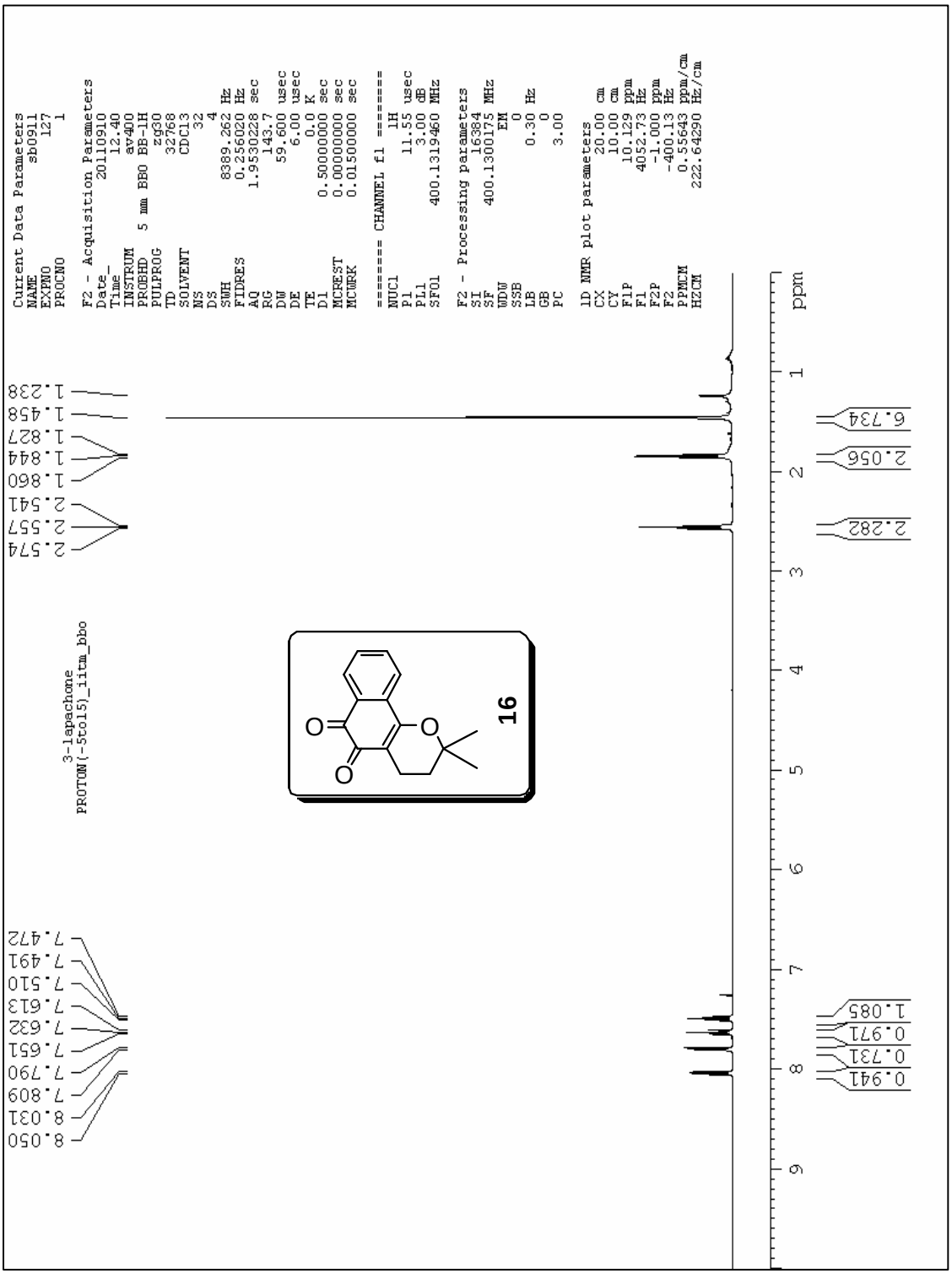
^{1}H-^{1}H COSY spectrum of compound **15**



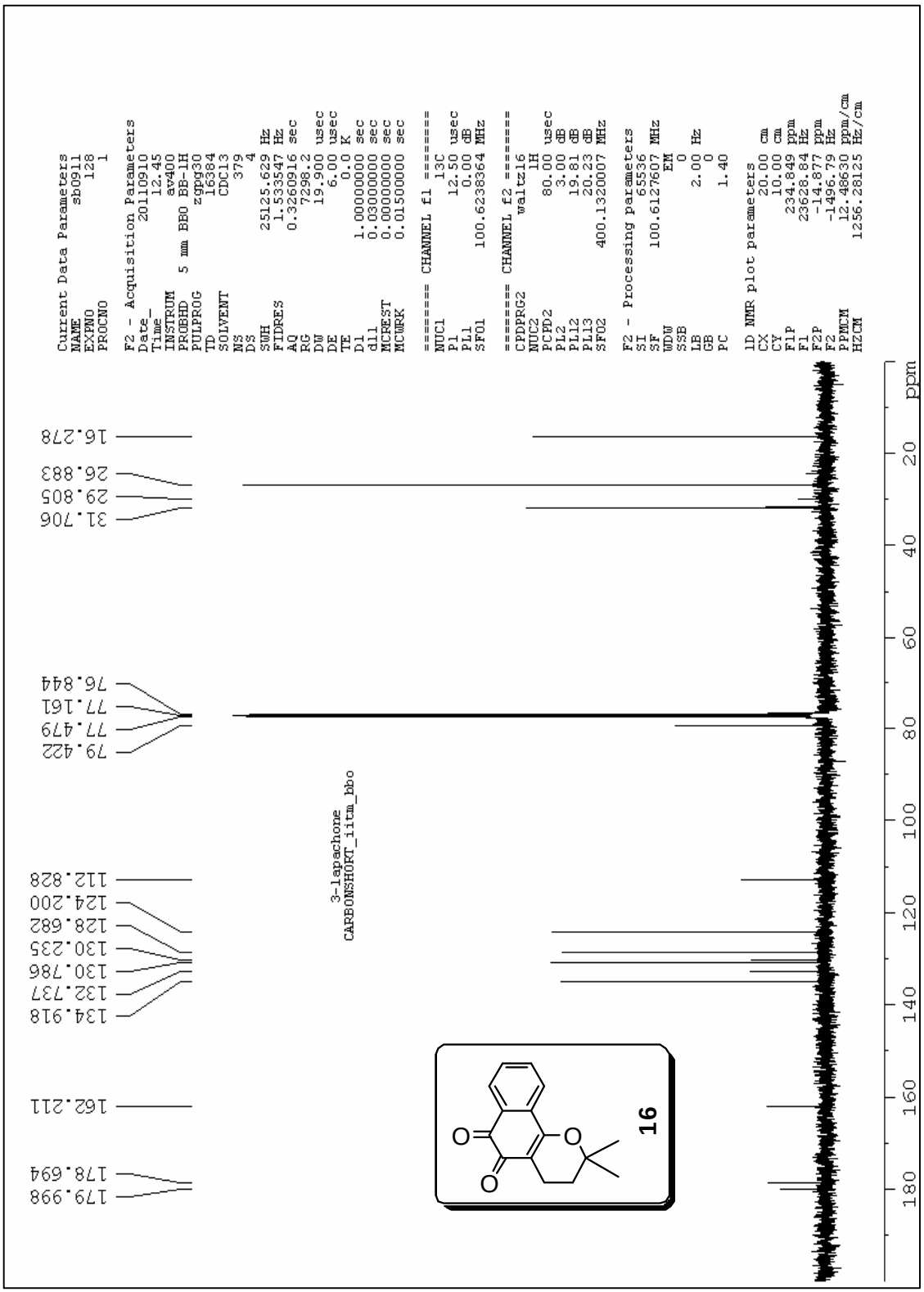
Expanded ^{1}H-^{1}H COSY spectrum of compound **15**



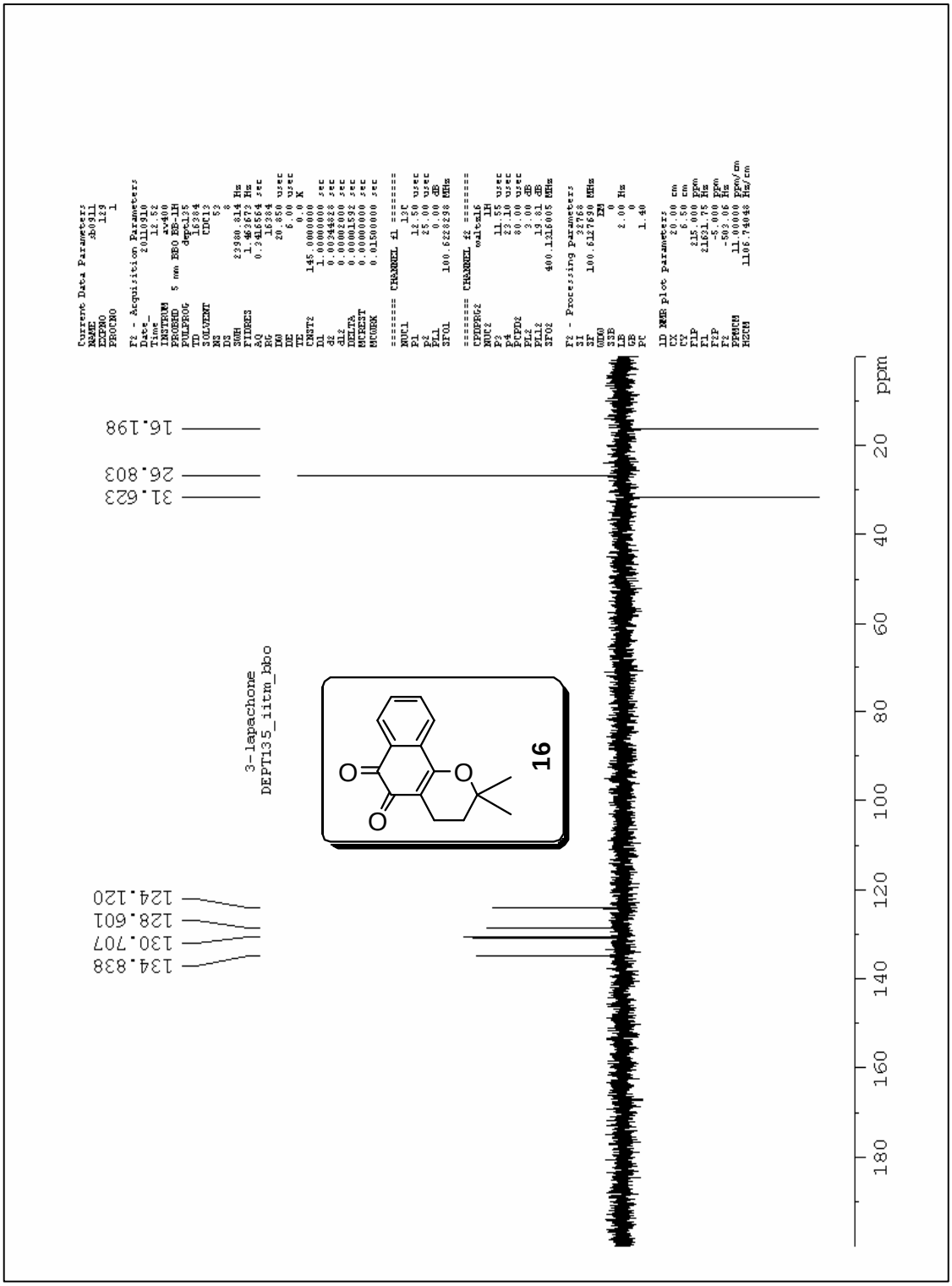
Expanded ^{1}H-^{1}H COSY spectrum of compound **15**



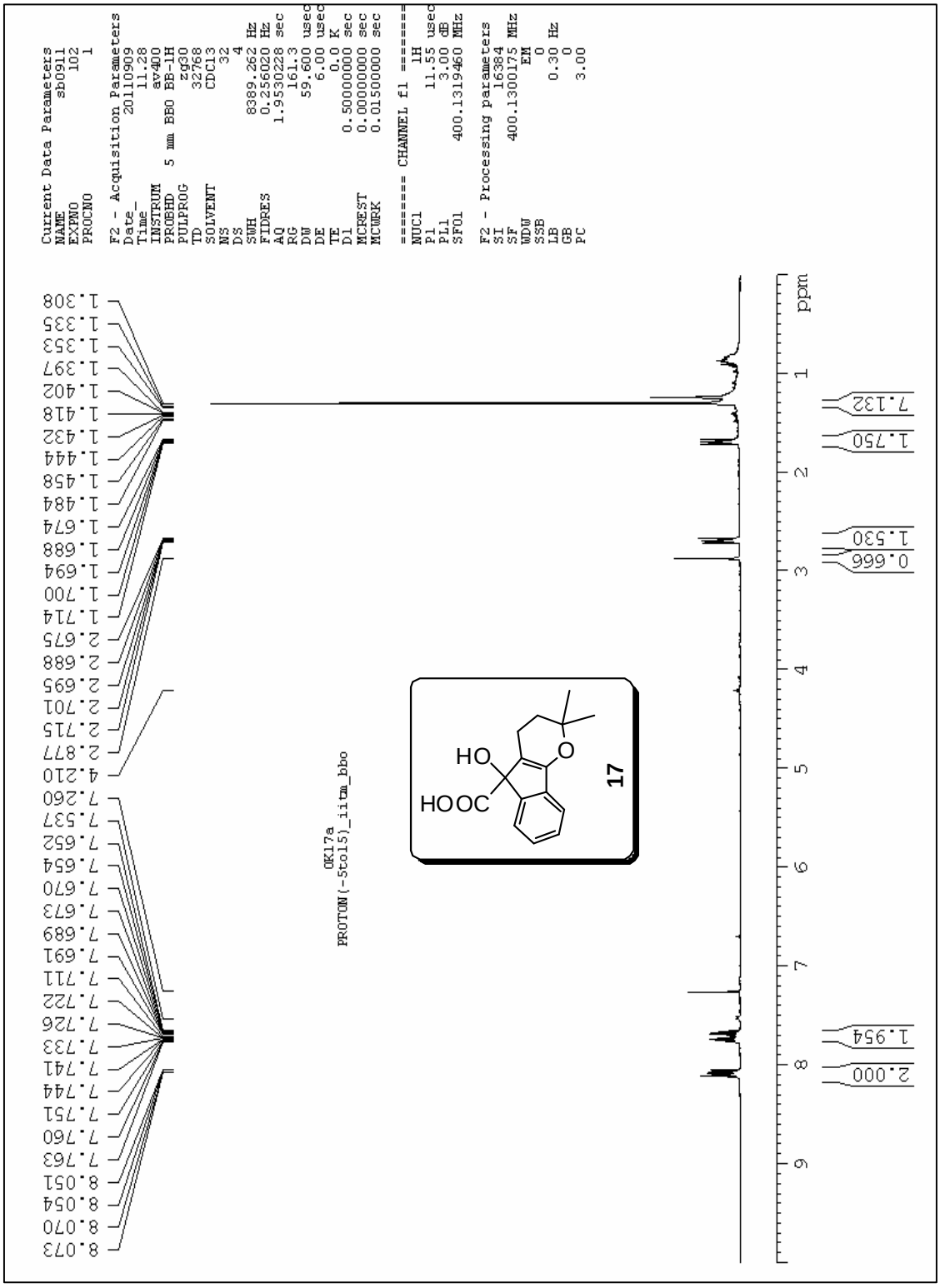
^{1}H NMR spectrum of compound **16**



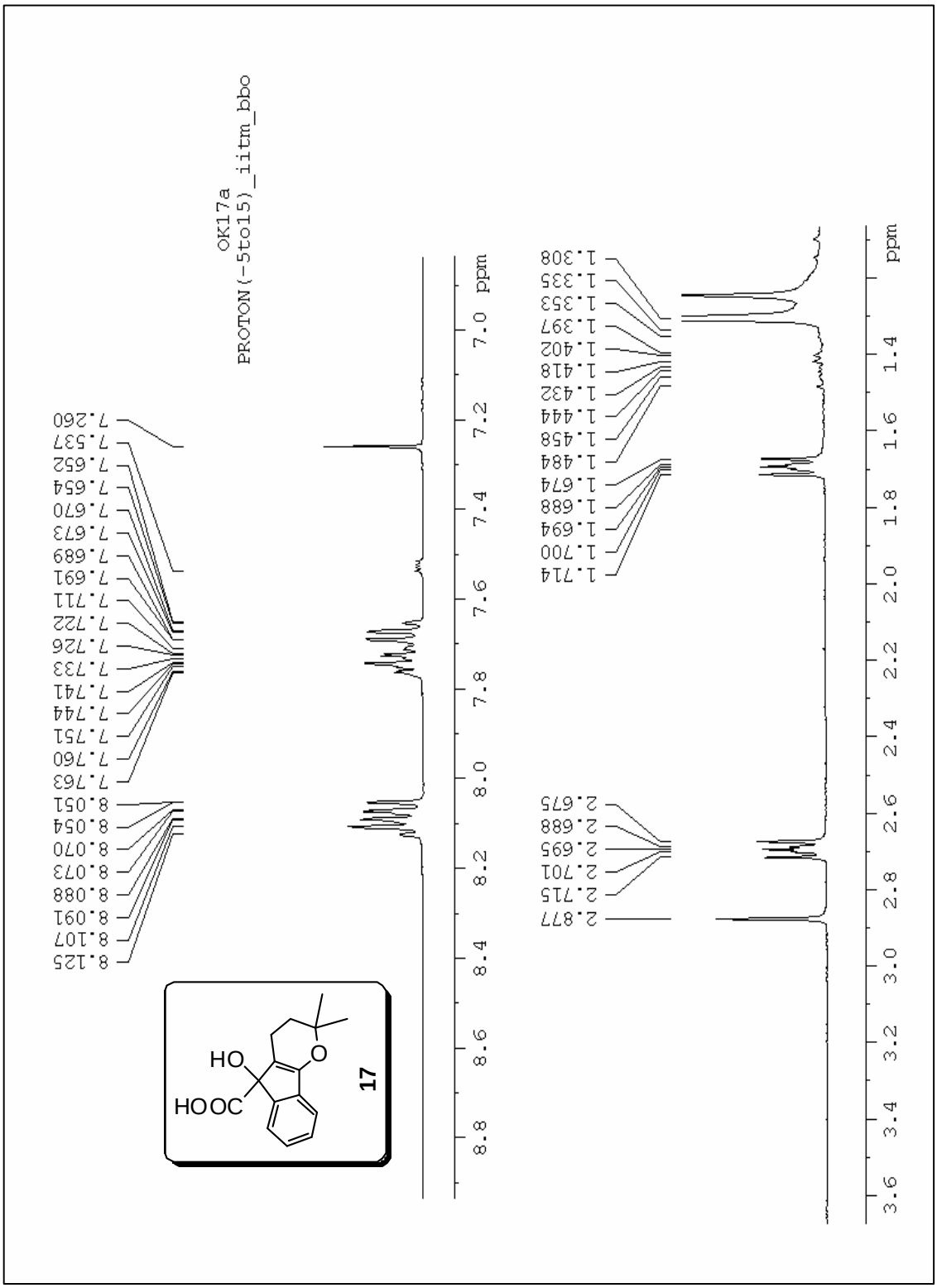
^{13}C NMR spectrum of compound **16**



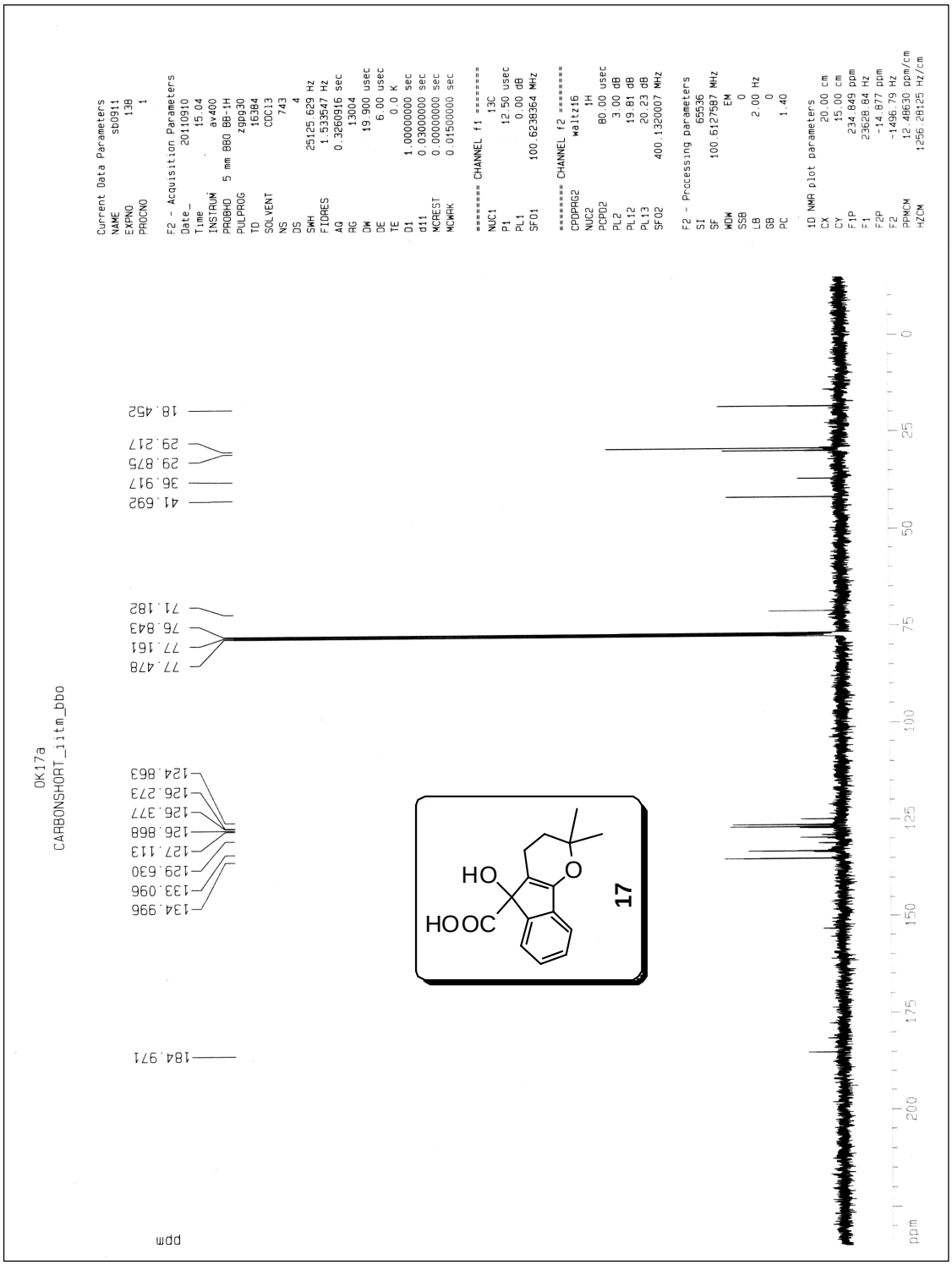
DEPT spectrum of compound **16**



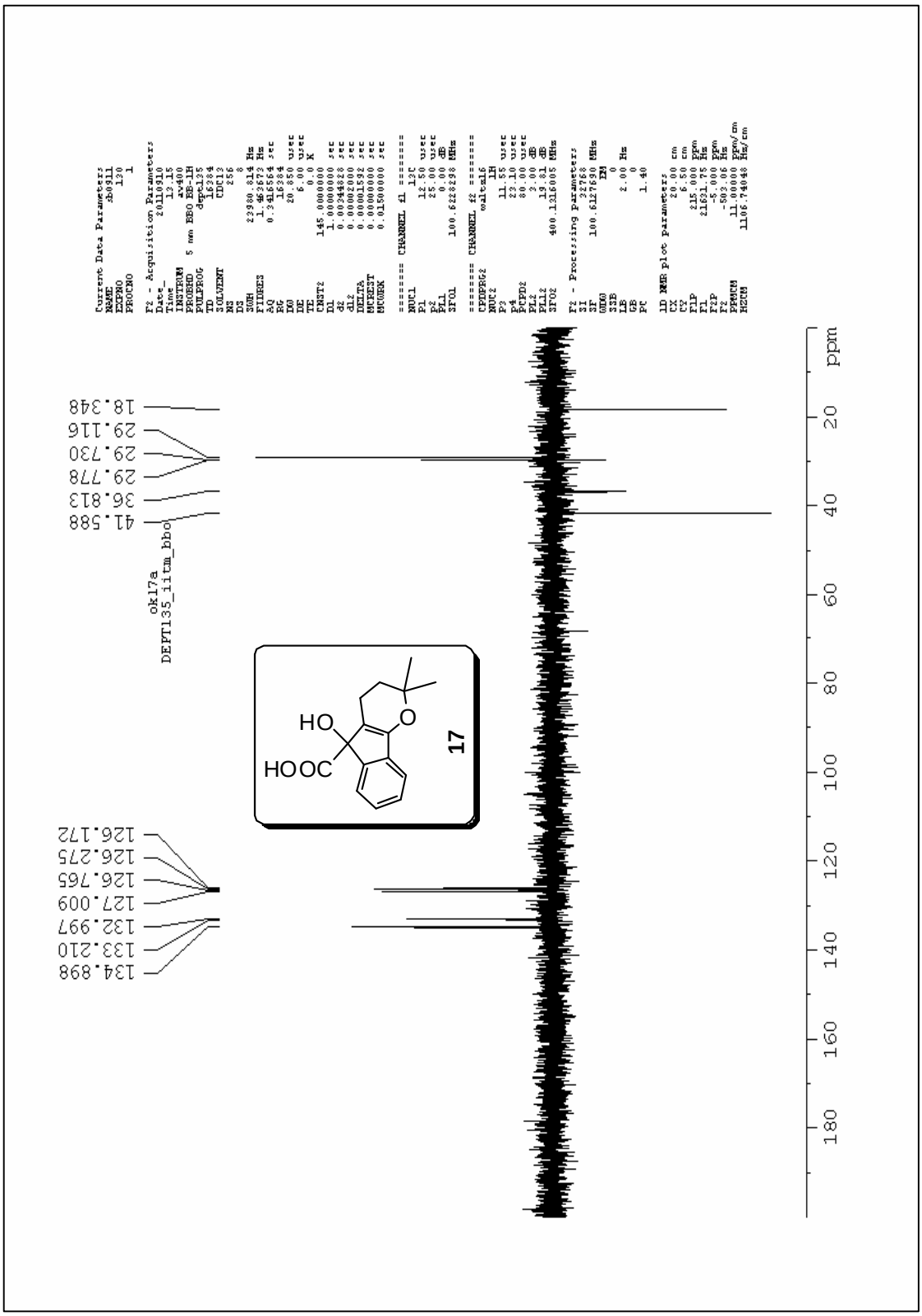
^{1}H NMR spectrum of compound **17**



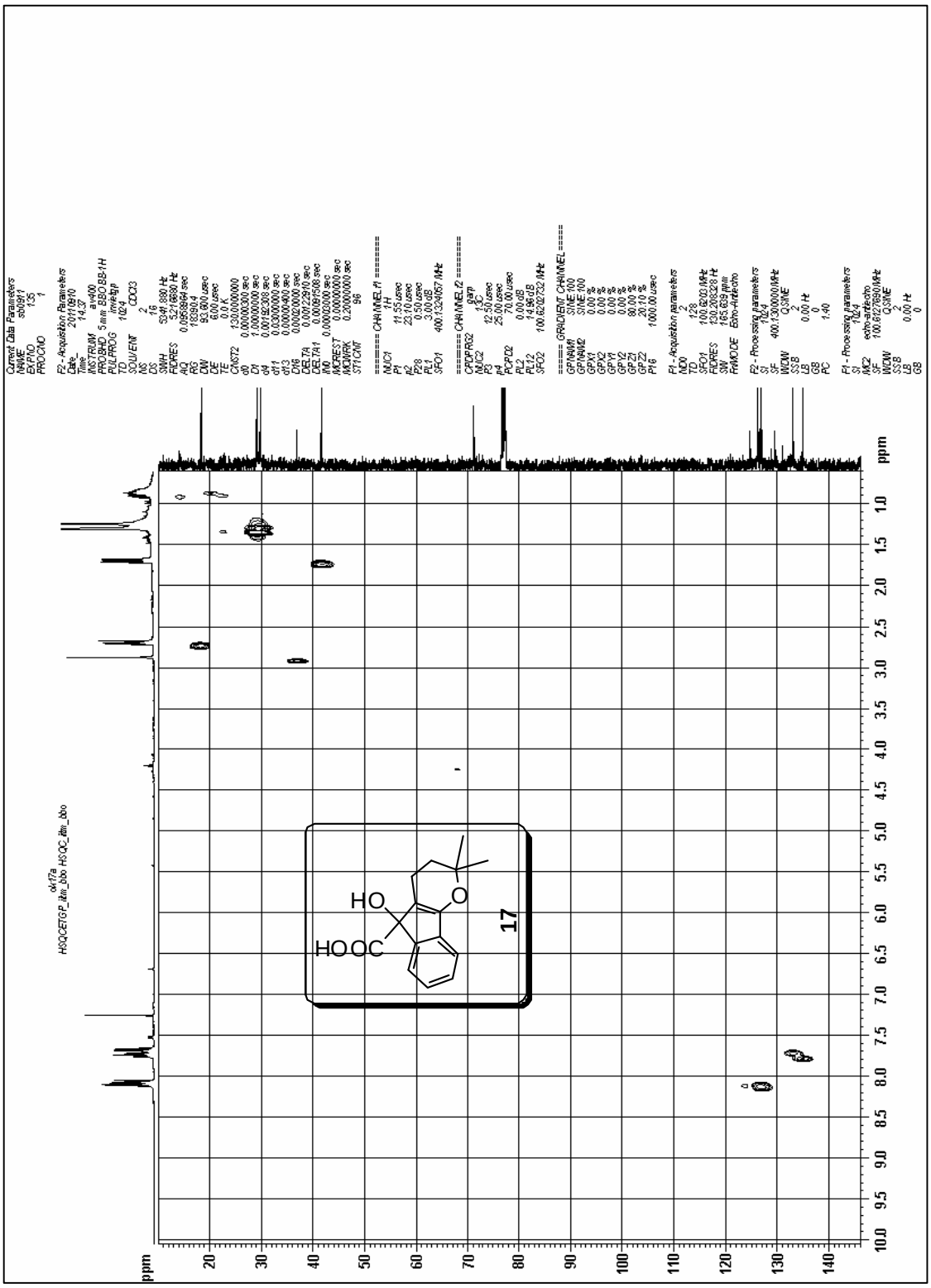
Expandeed ^{1}H NMR spectrum of compound **17**



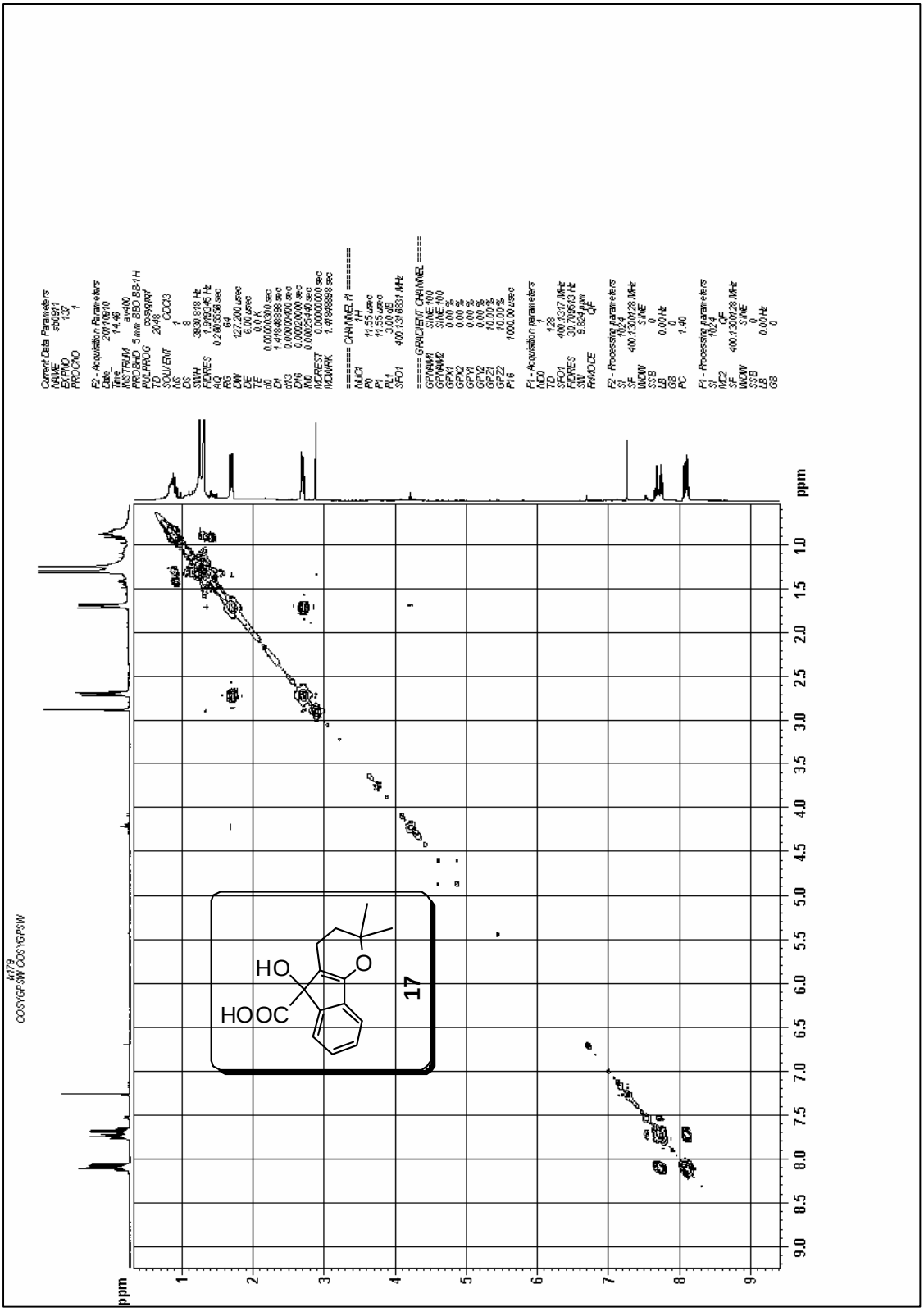
^{13}C NMR spectrum of compound **17**



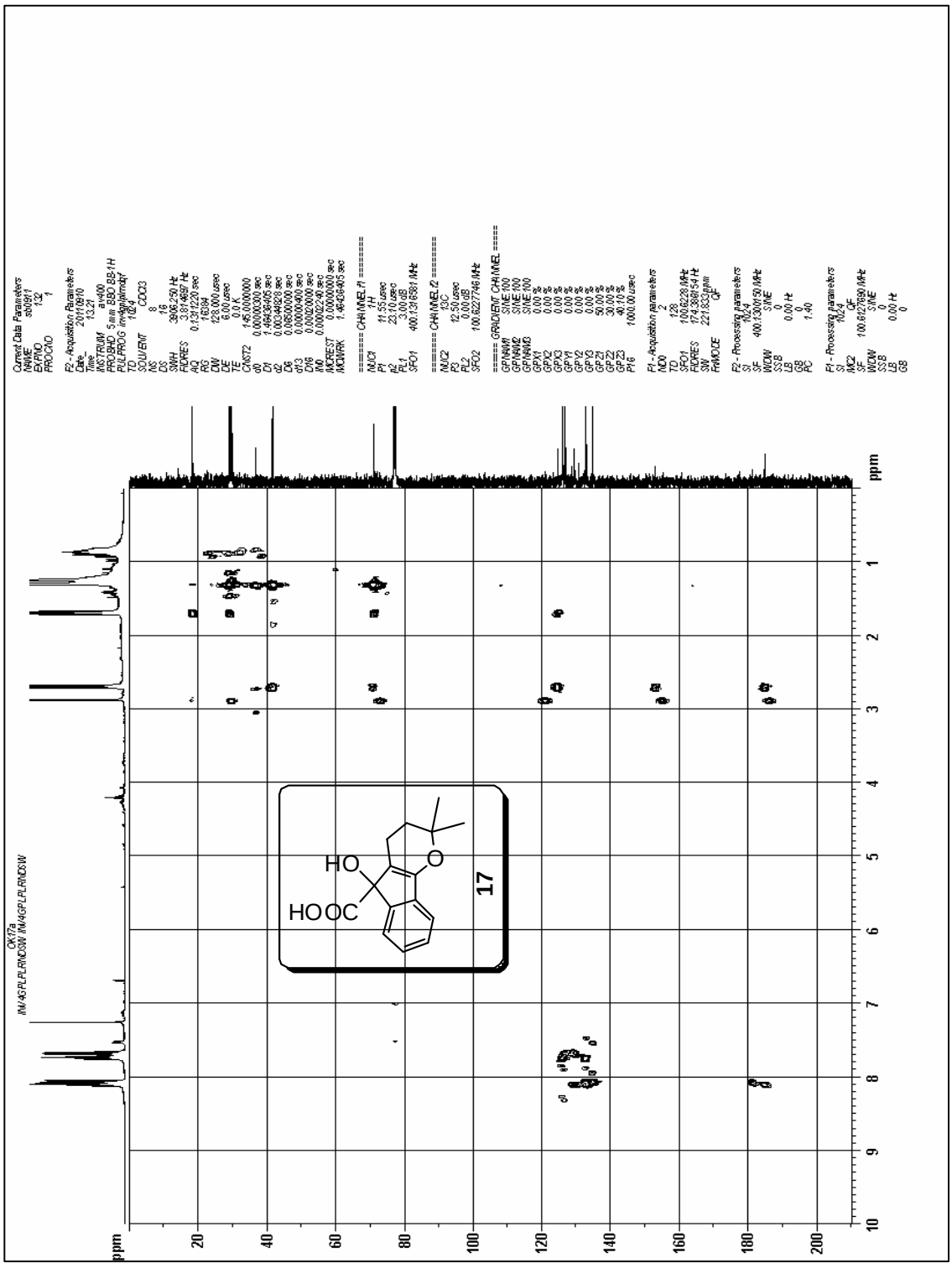
DEPT spectrum of compound **17**



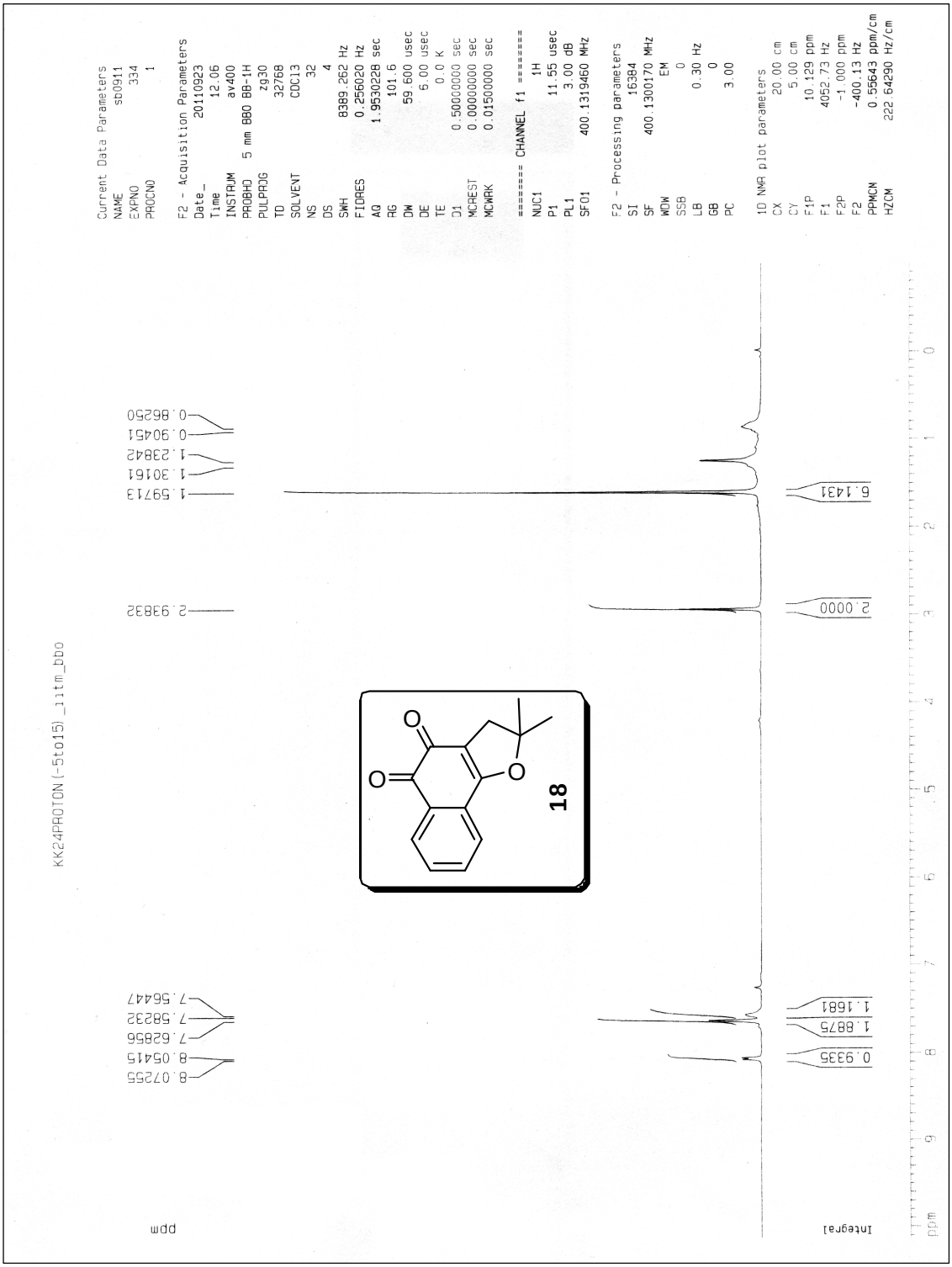
^{1}H-^{13}C COSY (HSQC) NMR spectrum of compound **17**



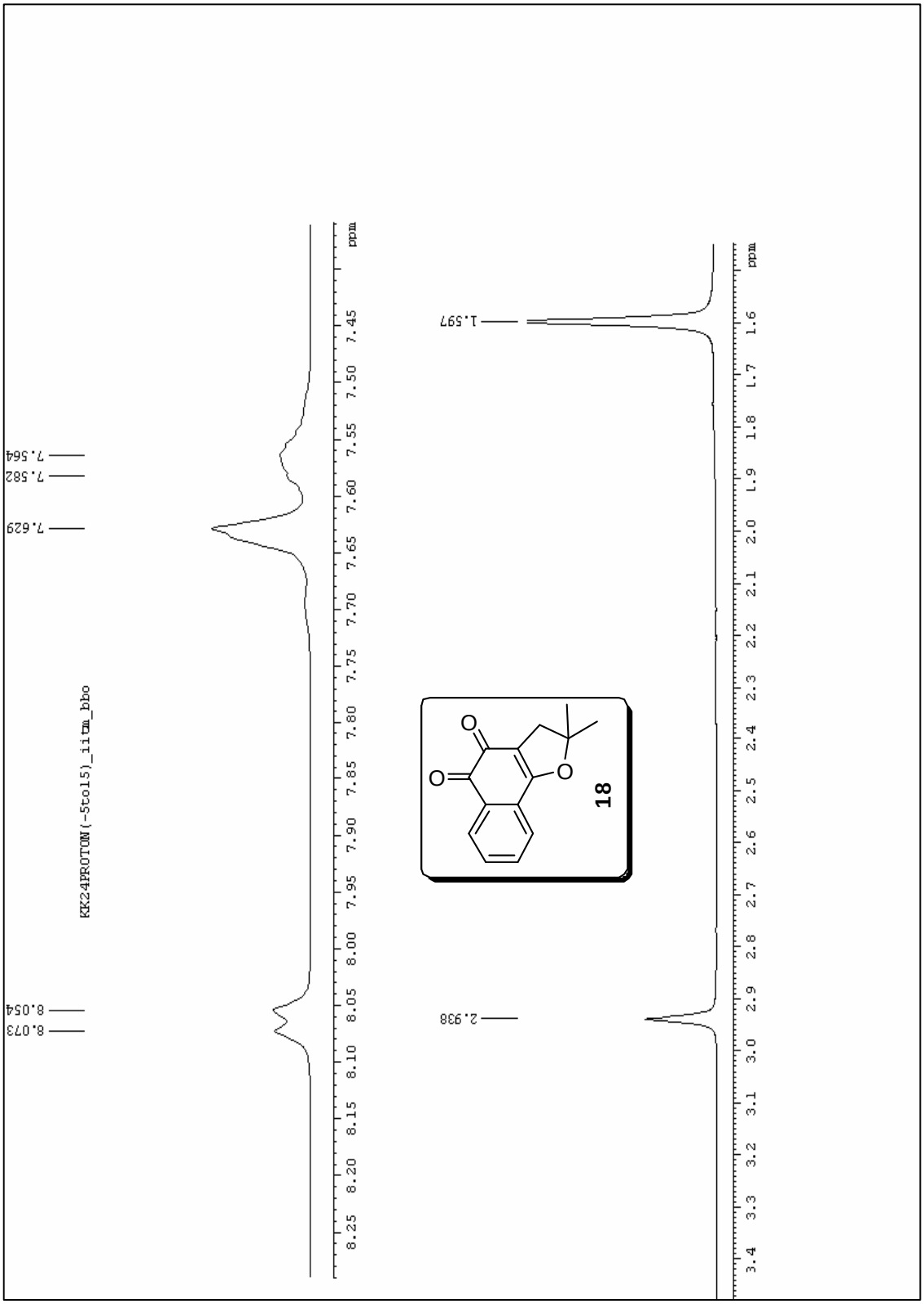
^{1}H-^{1}H COSY spectrum of compound **17**



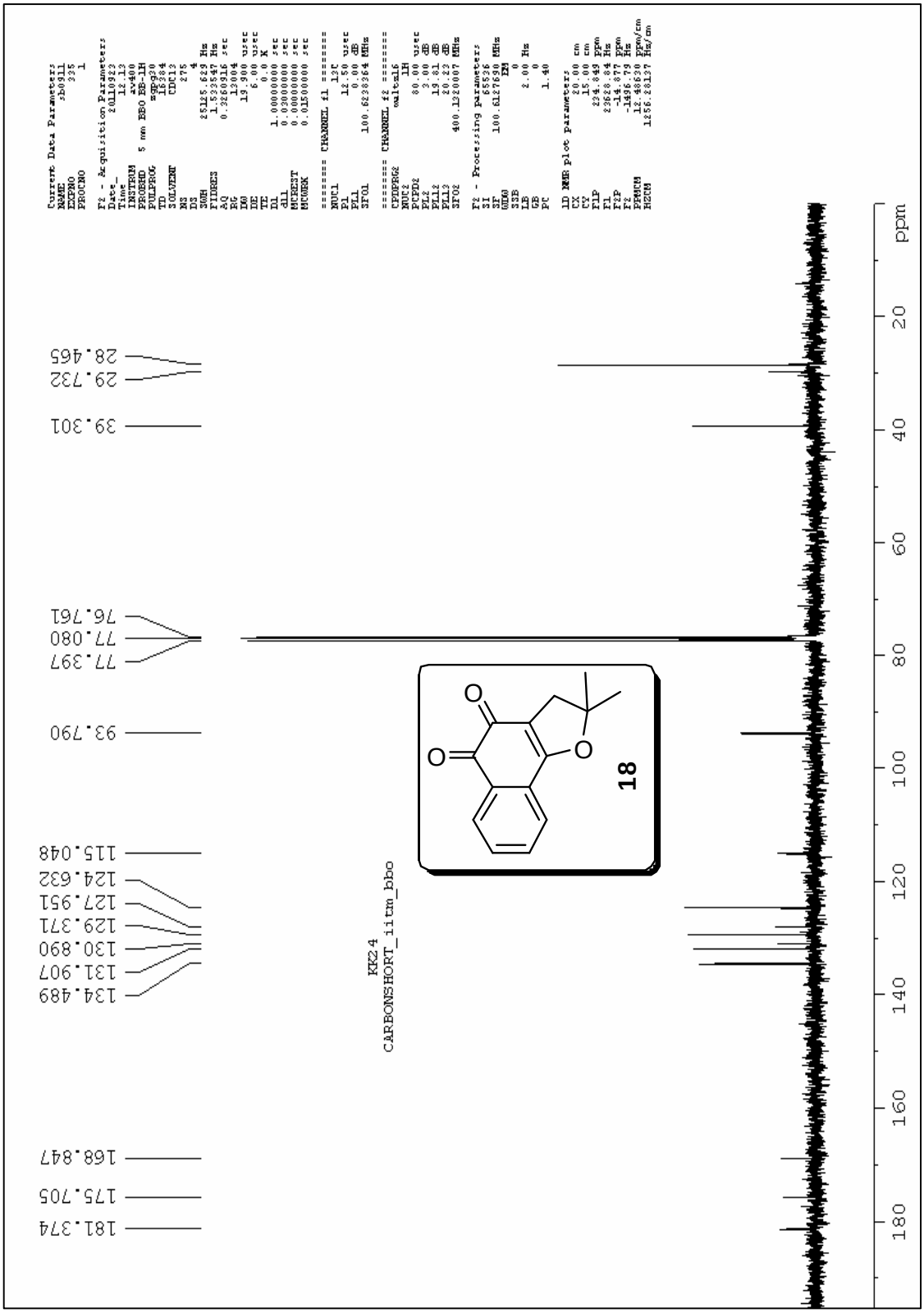
^{1}H-^{13}C COSY (HMBC) NMR spectrum of compound **17**



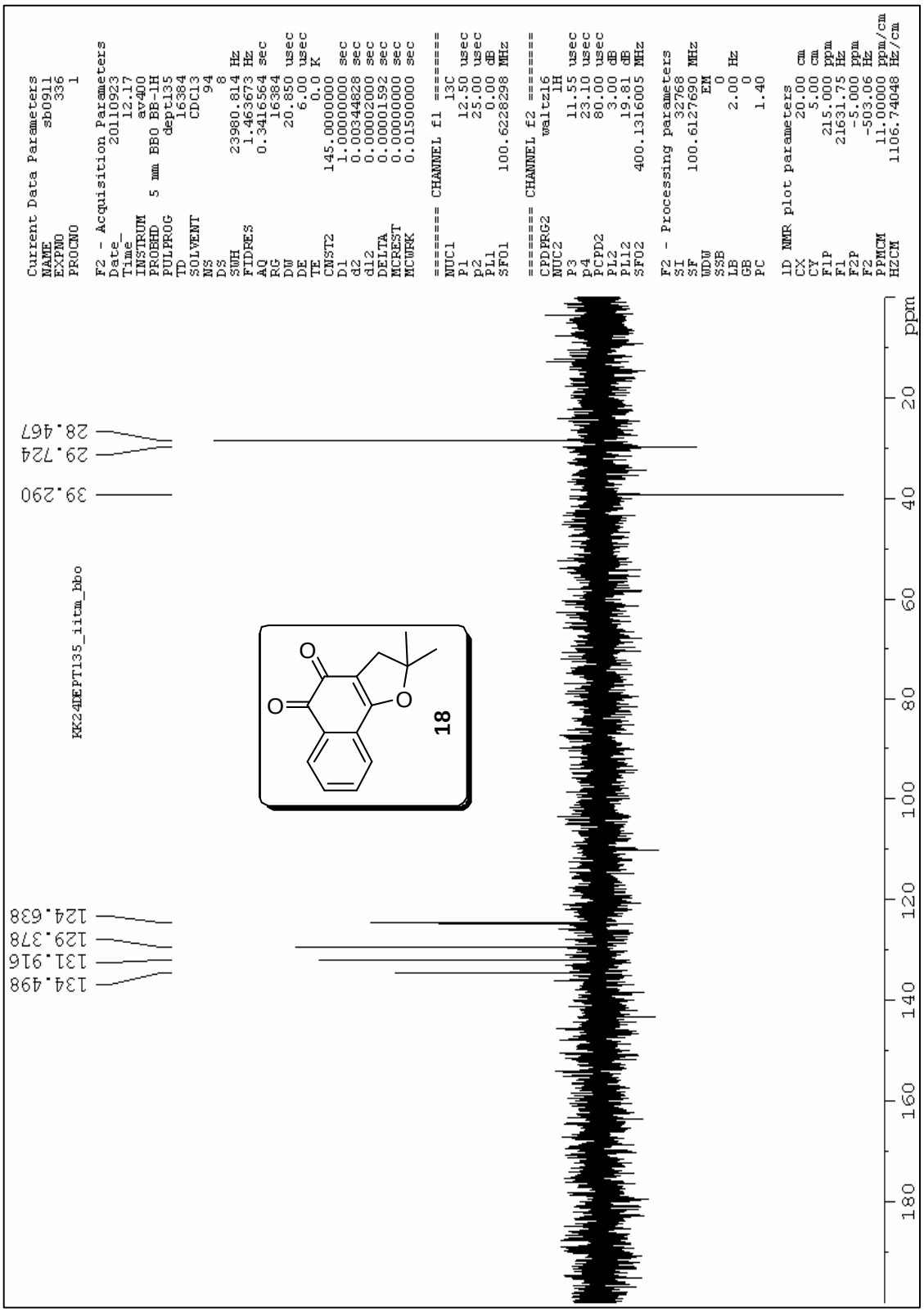
^{1}H NMR spectrum of compound **18**



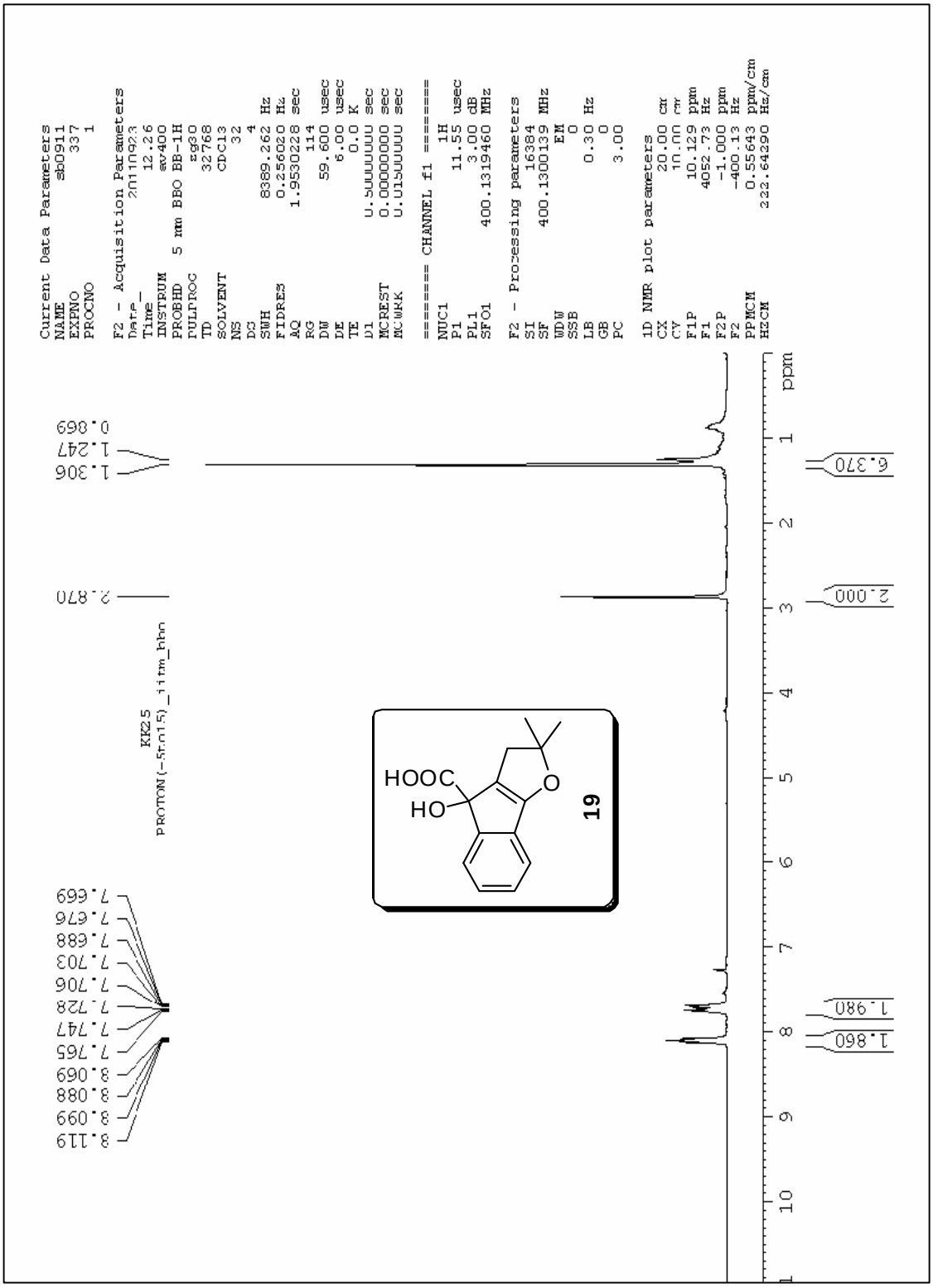
Expandeed ^{1}H NMR spectrum of compound **18**



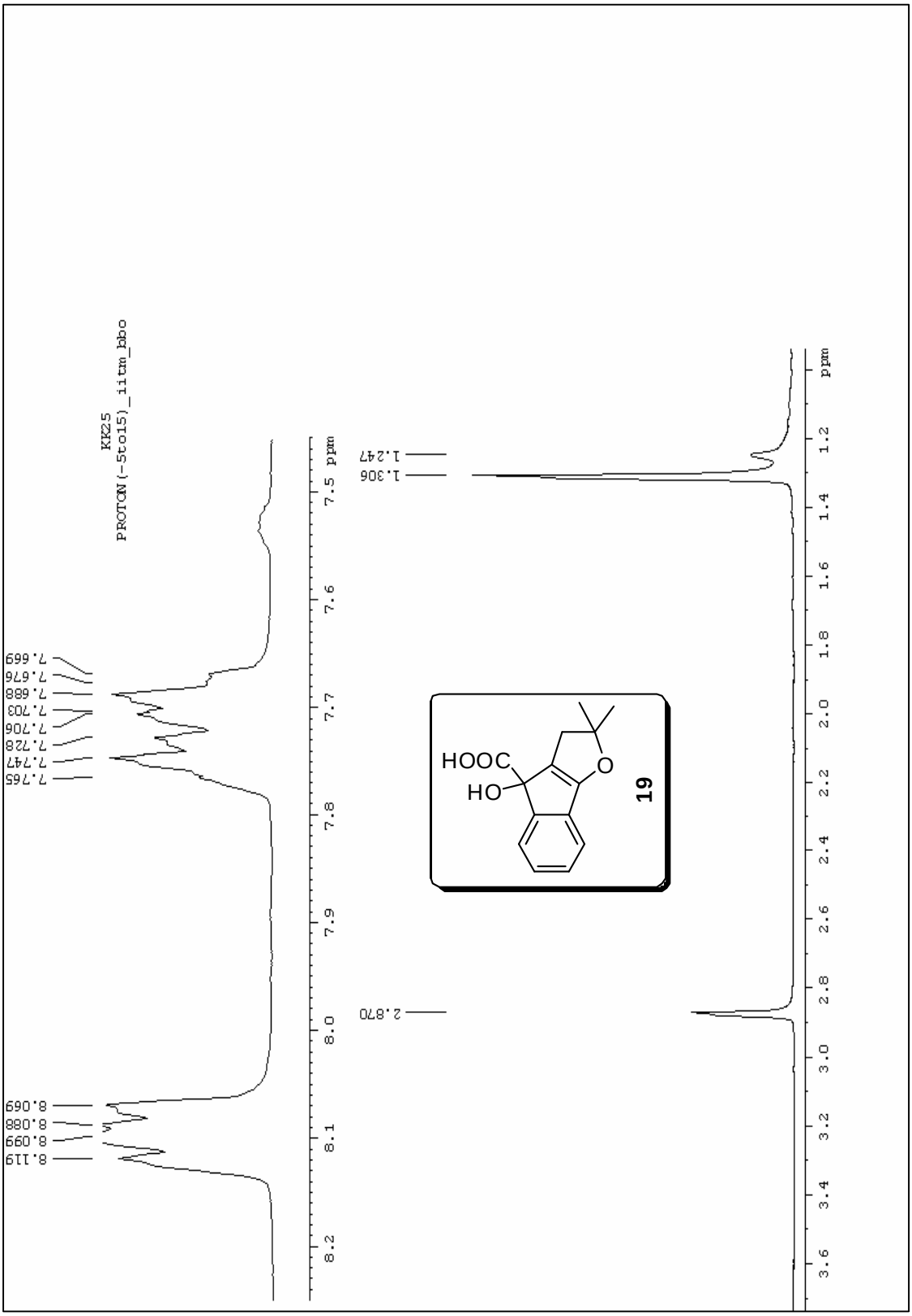
^{13}C NMR spectrum of compound **18**



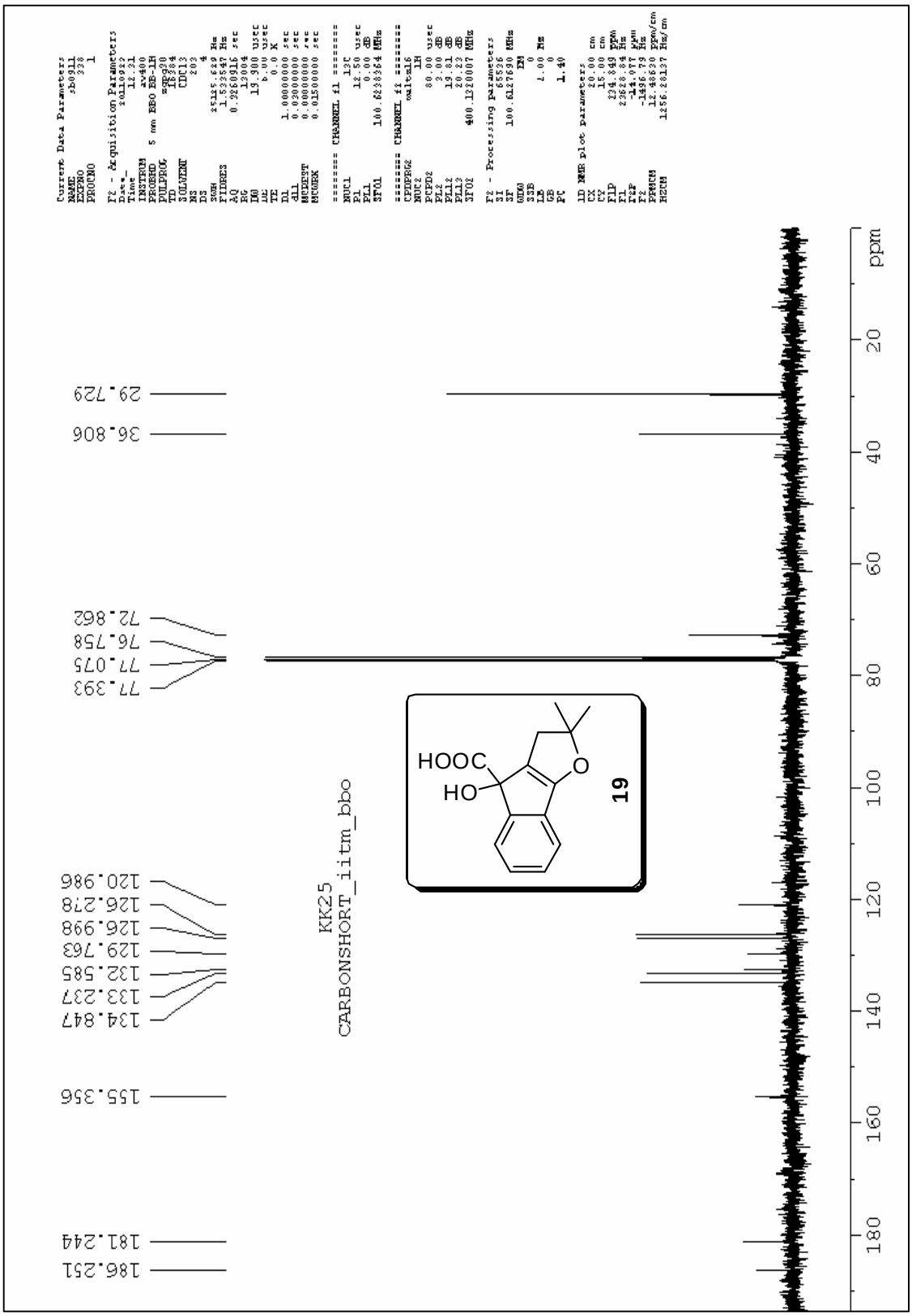
DEPT spectrum of compound **18**



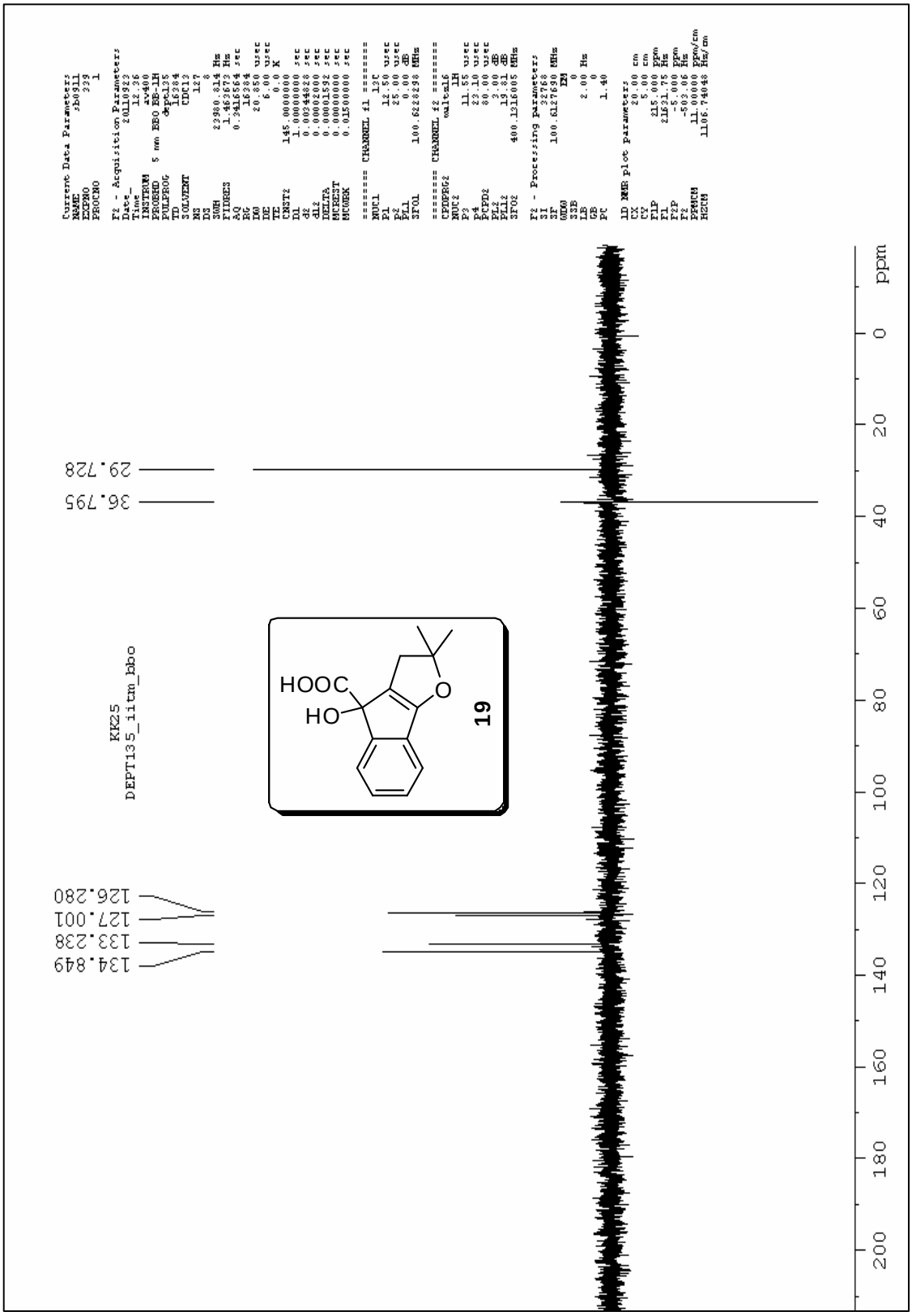
^{1}H NMR spectrum of compound **19**



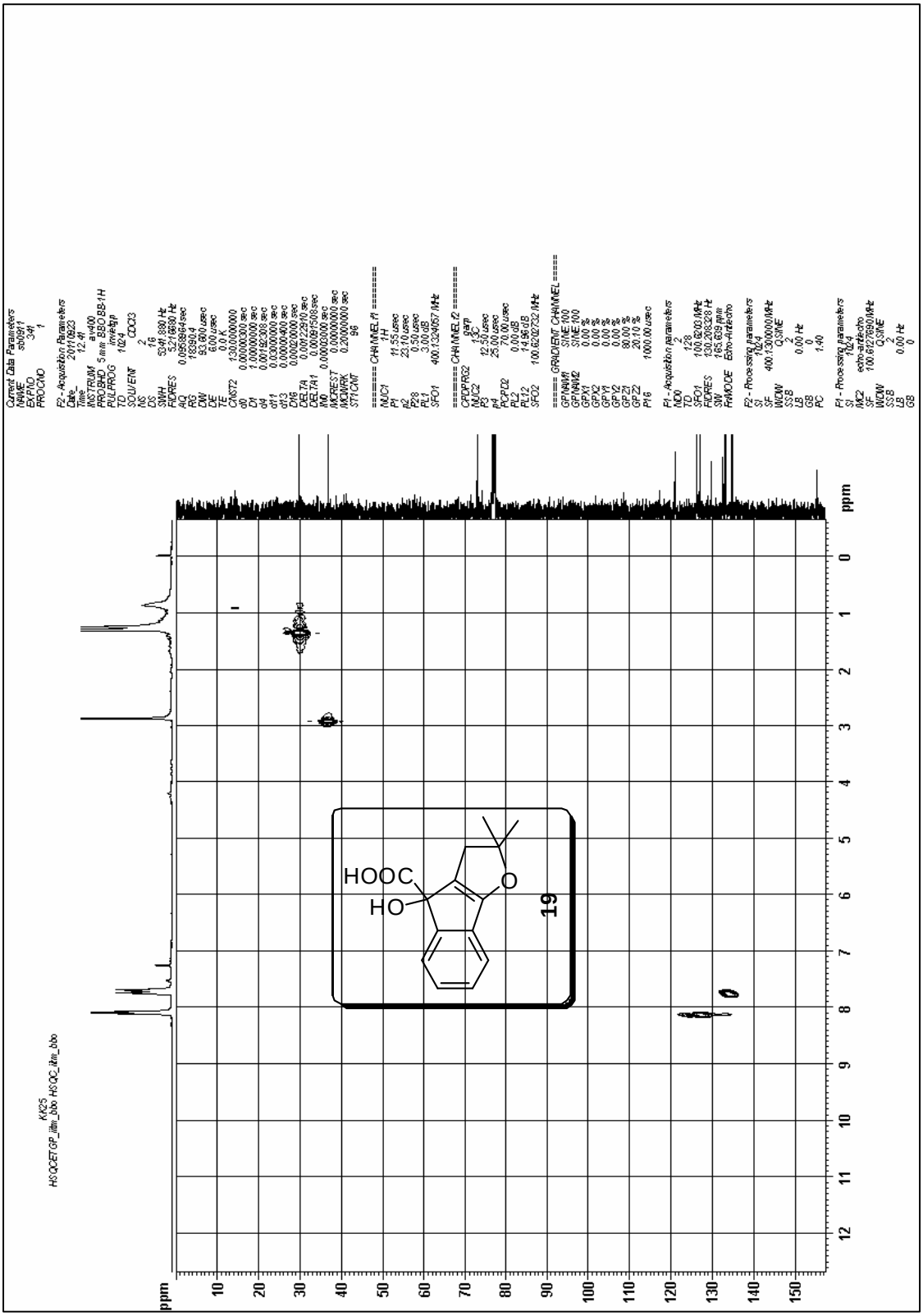
Expandeed ^{1}H NMR spectrum of compound **19**



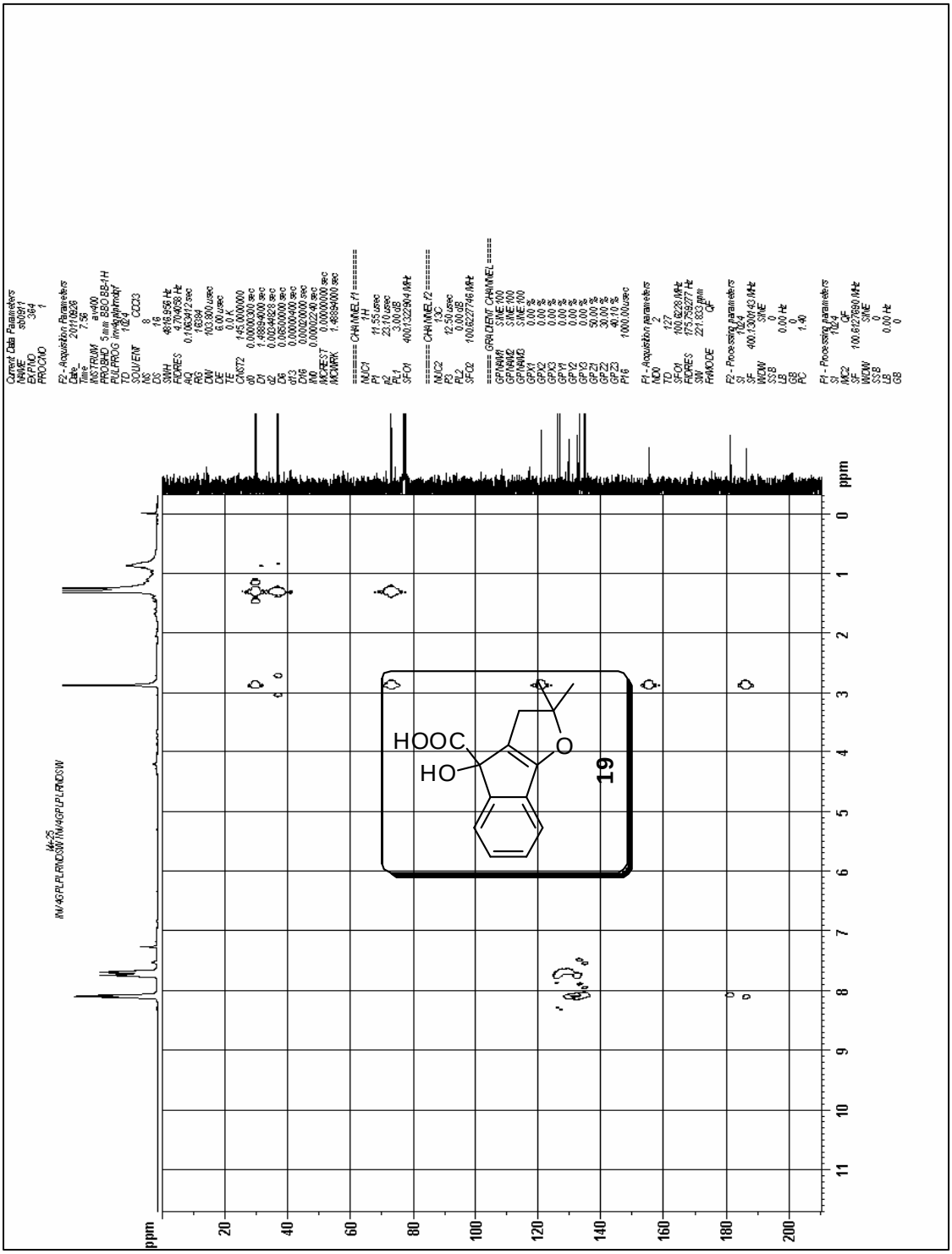
^{13}C NMR spectrum of compound **19**



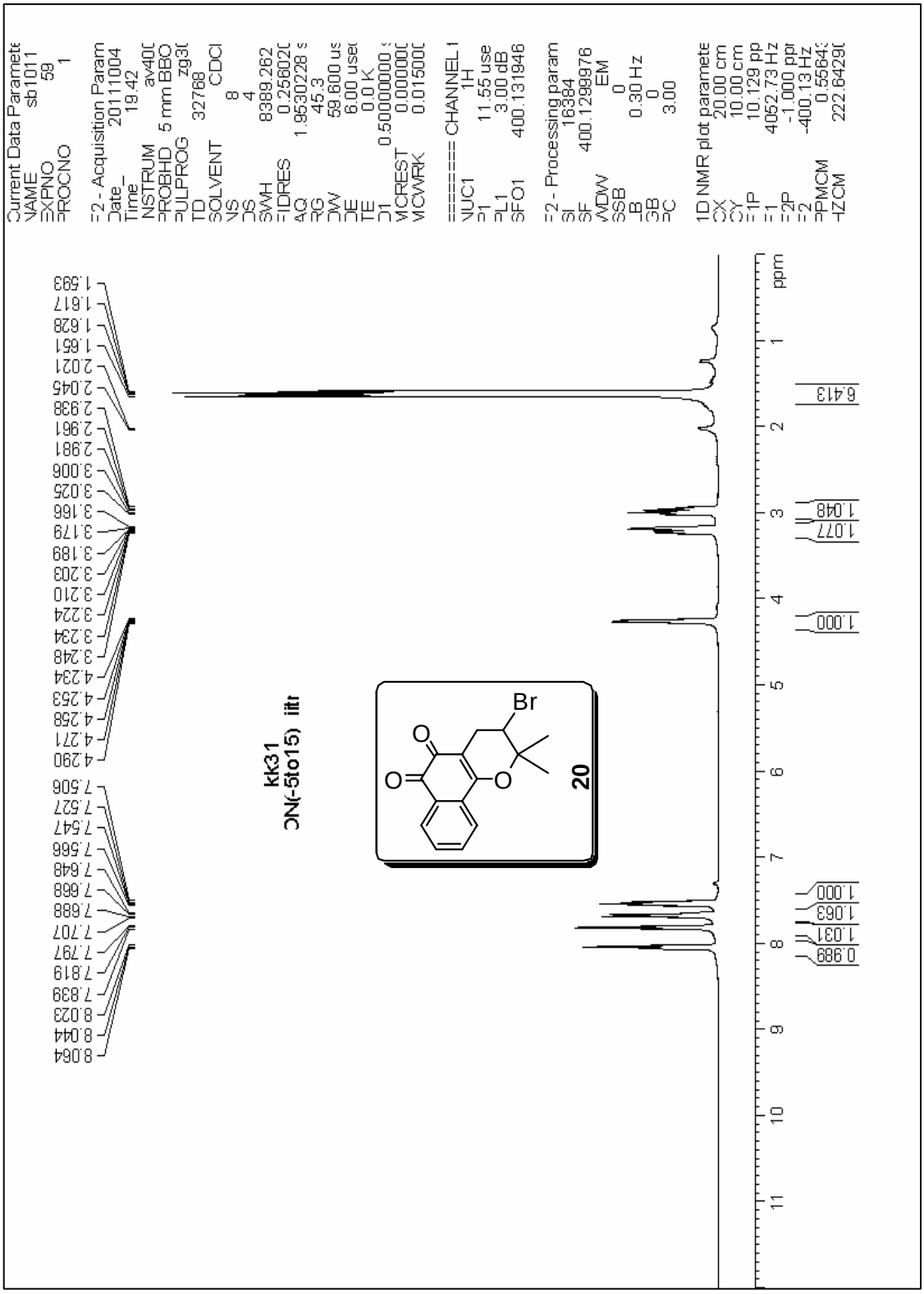
DEPT spectrum of compound **19**



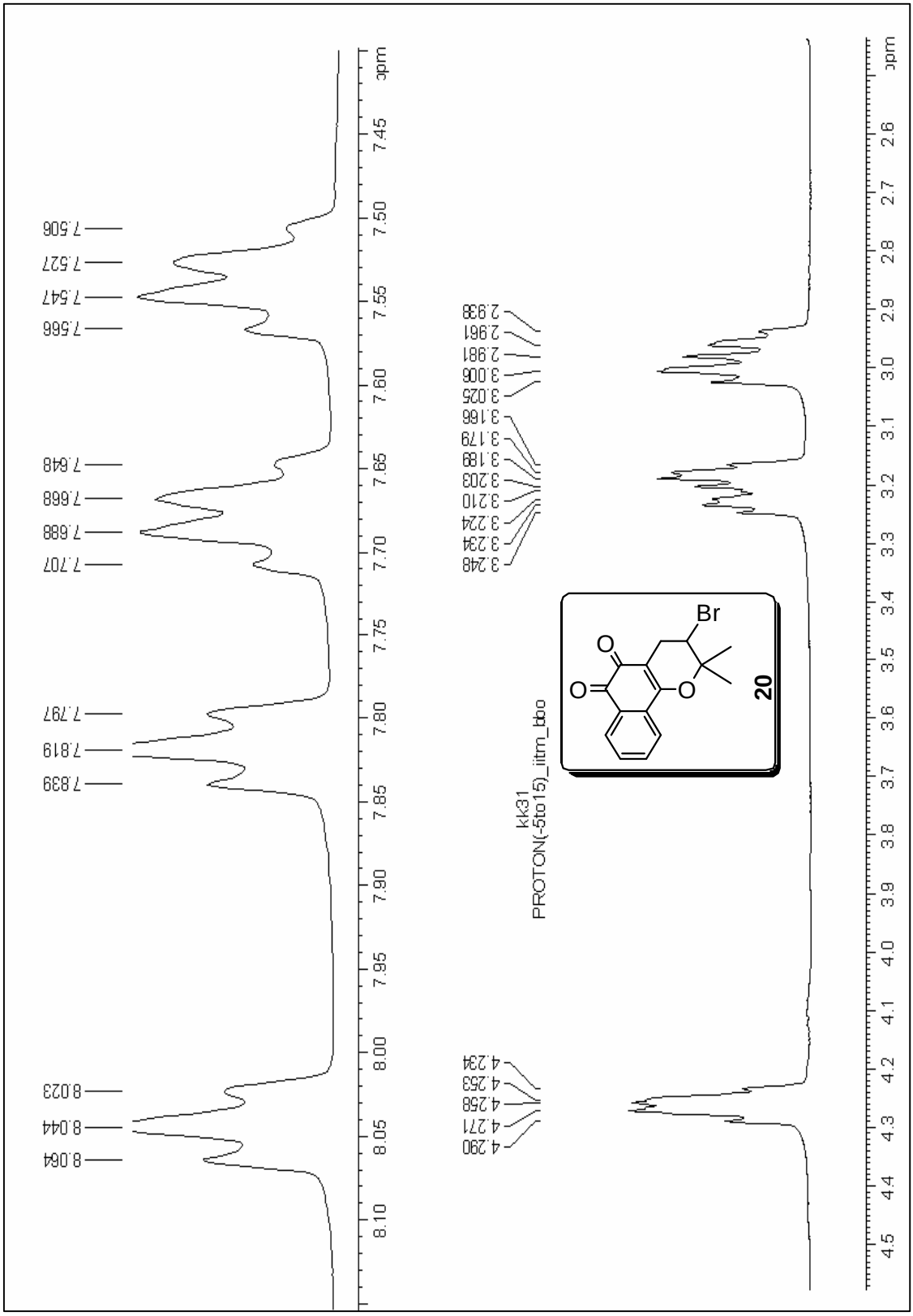
^{1}H-^{13}C COSY (HSQC) NMR spectrum of compound **19**



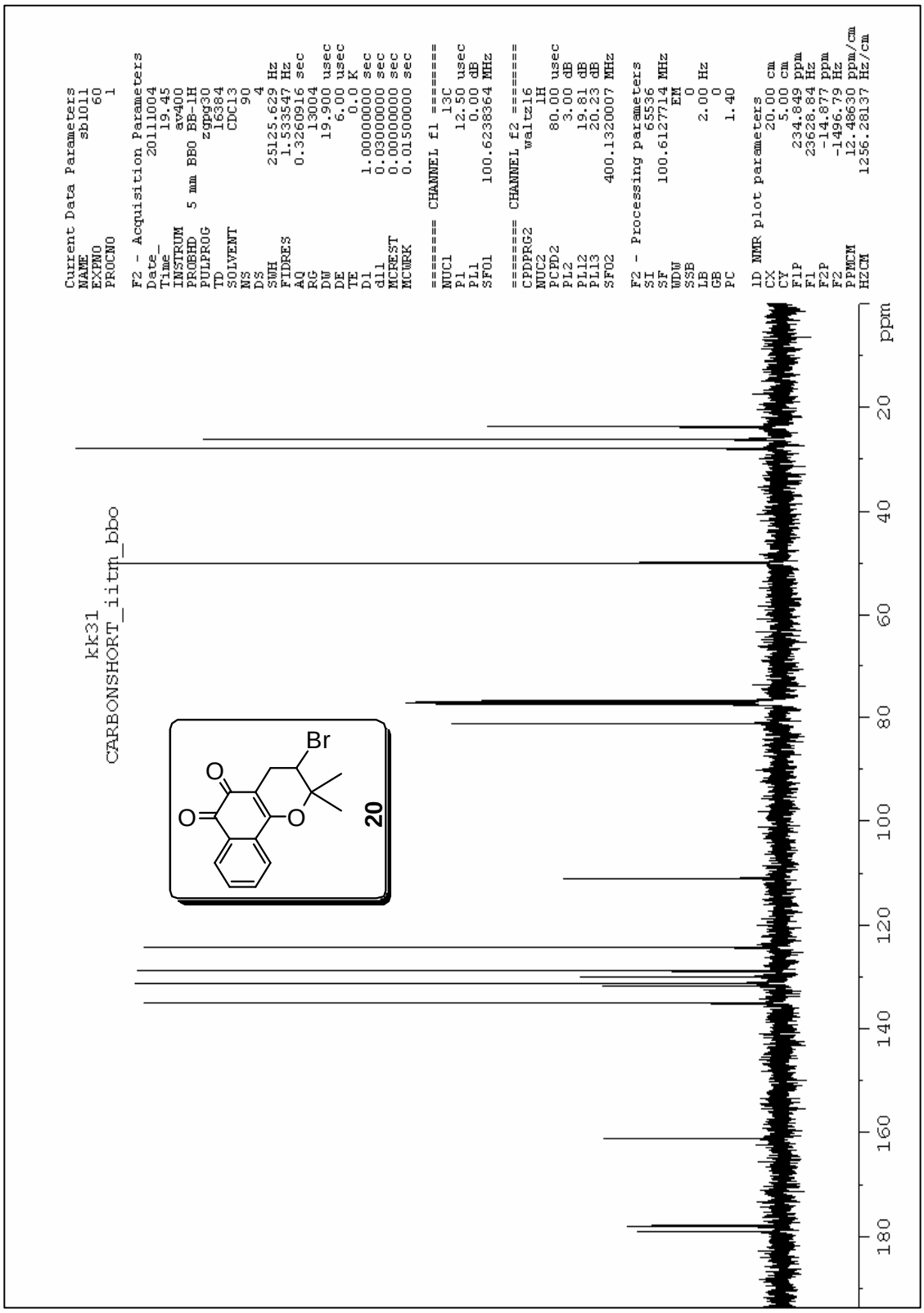
^{1}H-^{13}C COSY (HMBC) NMR spectrum of compound **19**



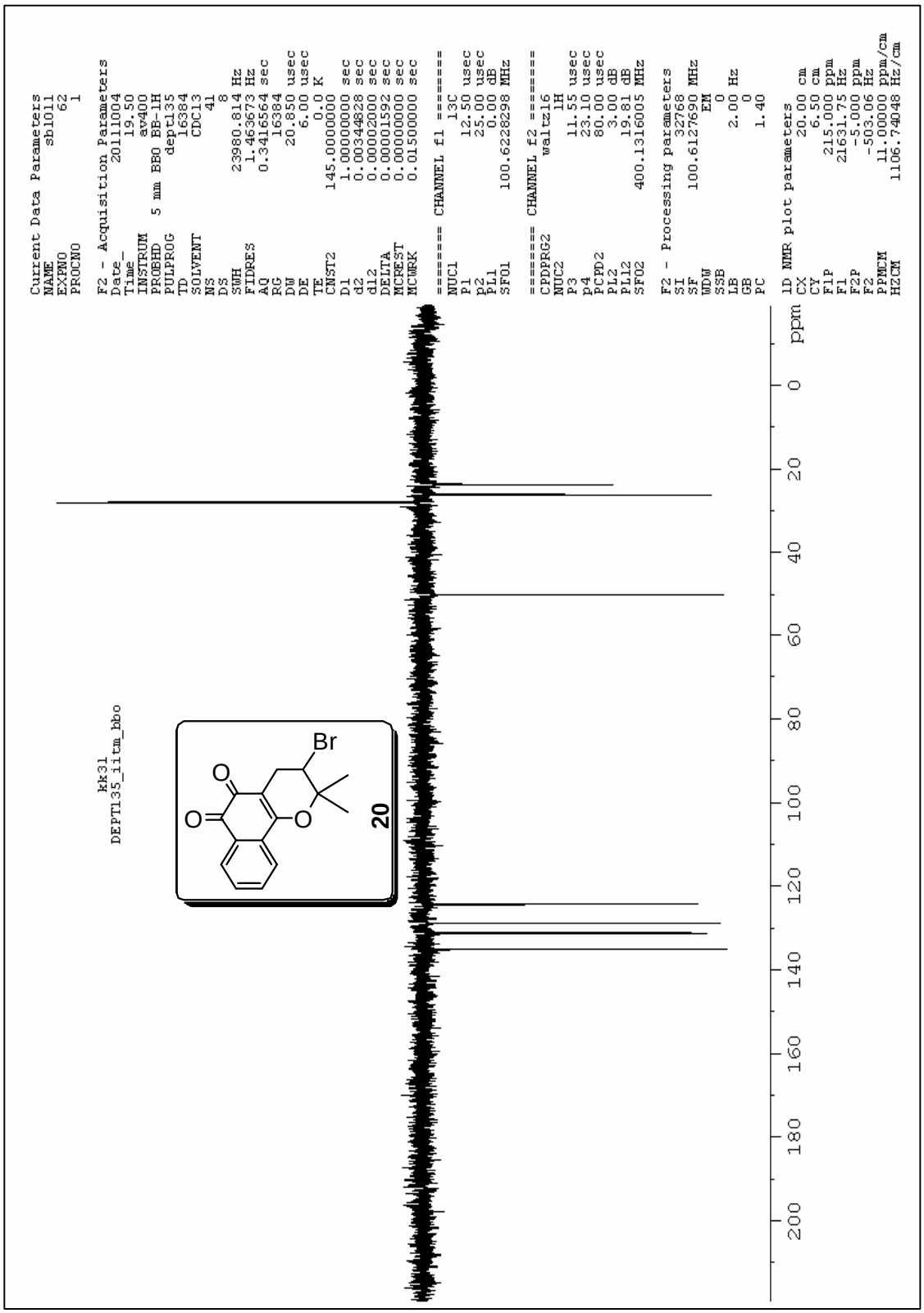
^{1}H NMR spectrum of compound **20**



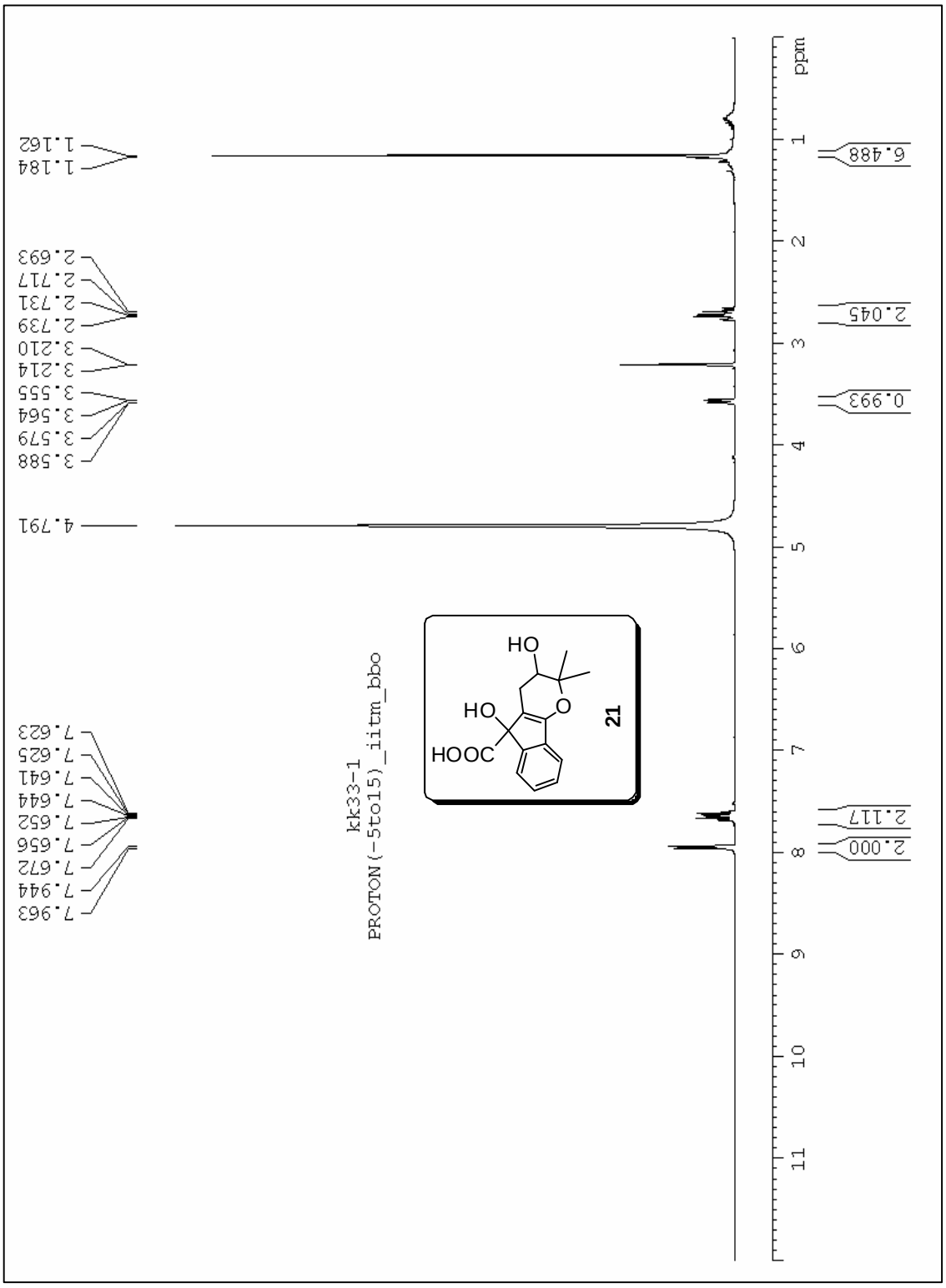
Expandeed ^{1}H NMR spectrum of compound **20**



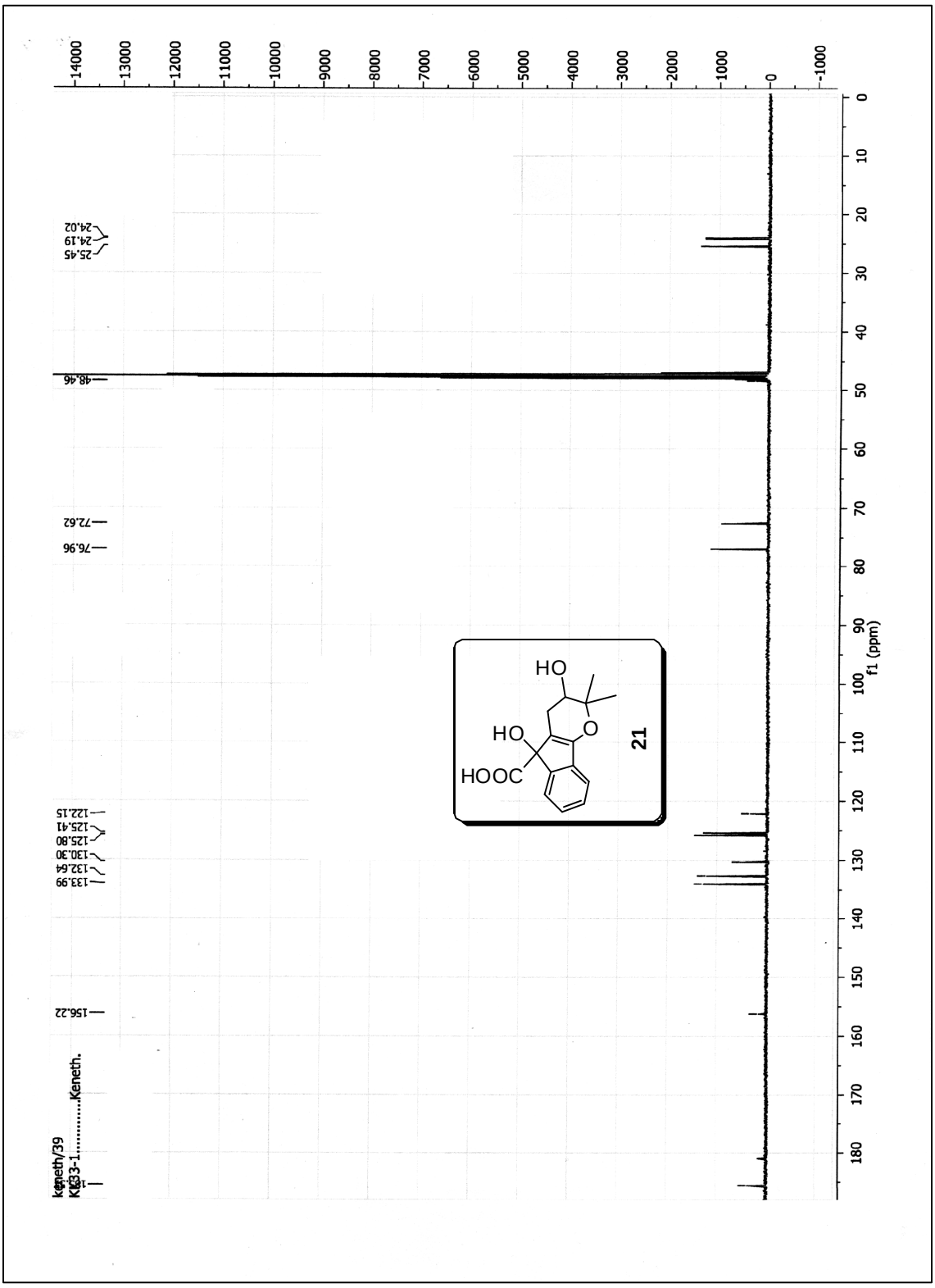
^{13}C NMR spectrum of compound **20**



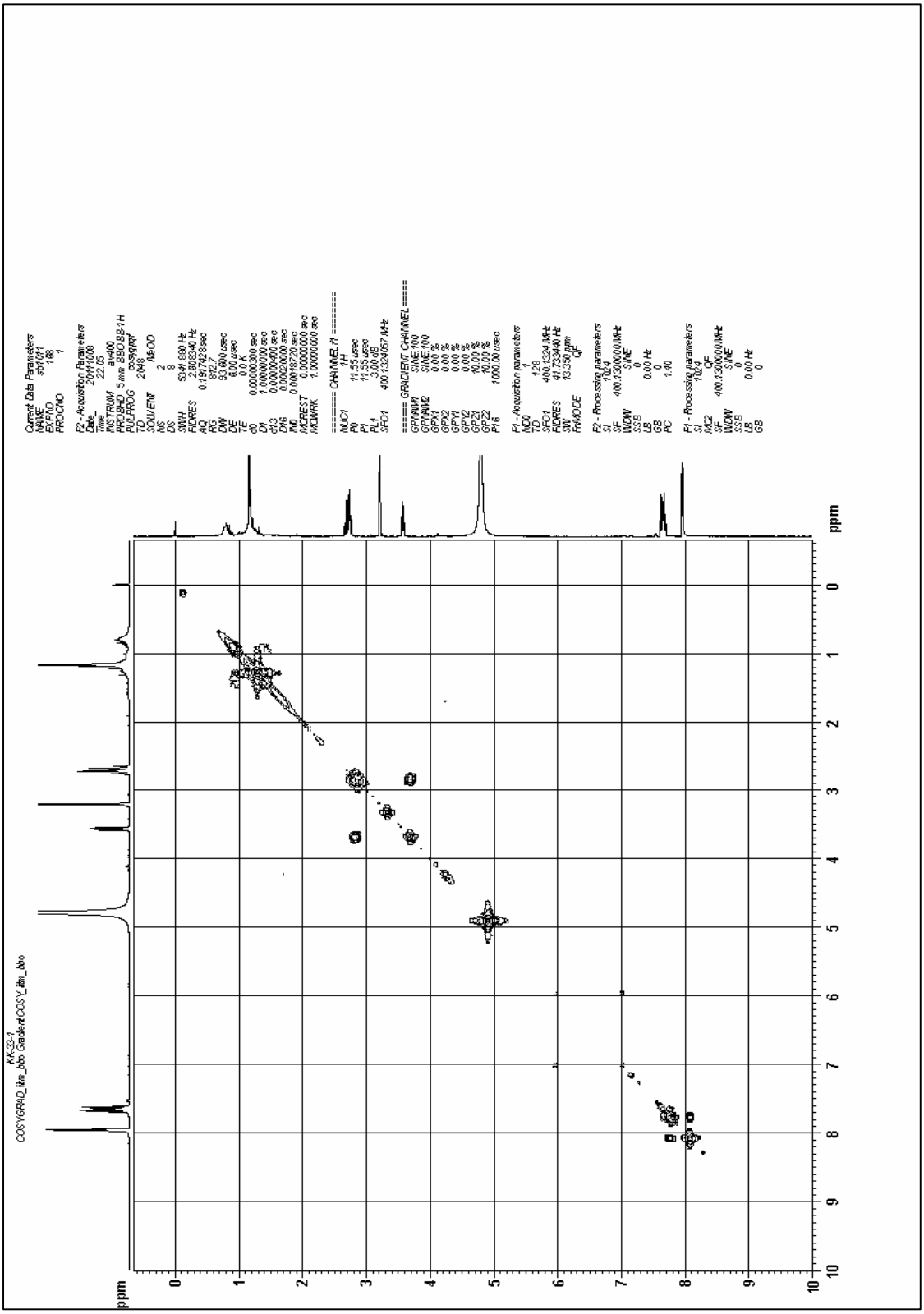
DEPT spectrum of compound **20**



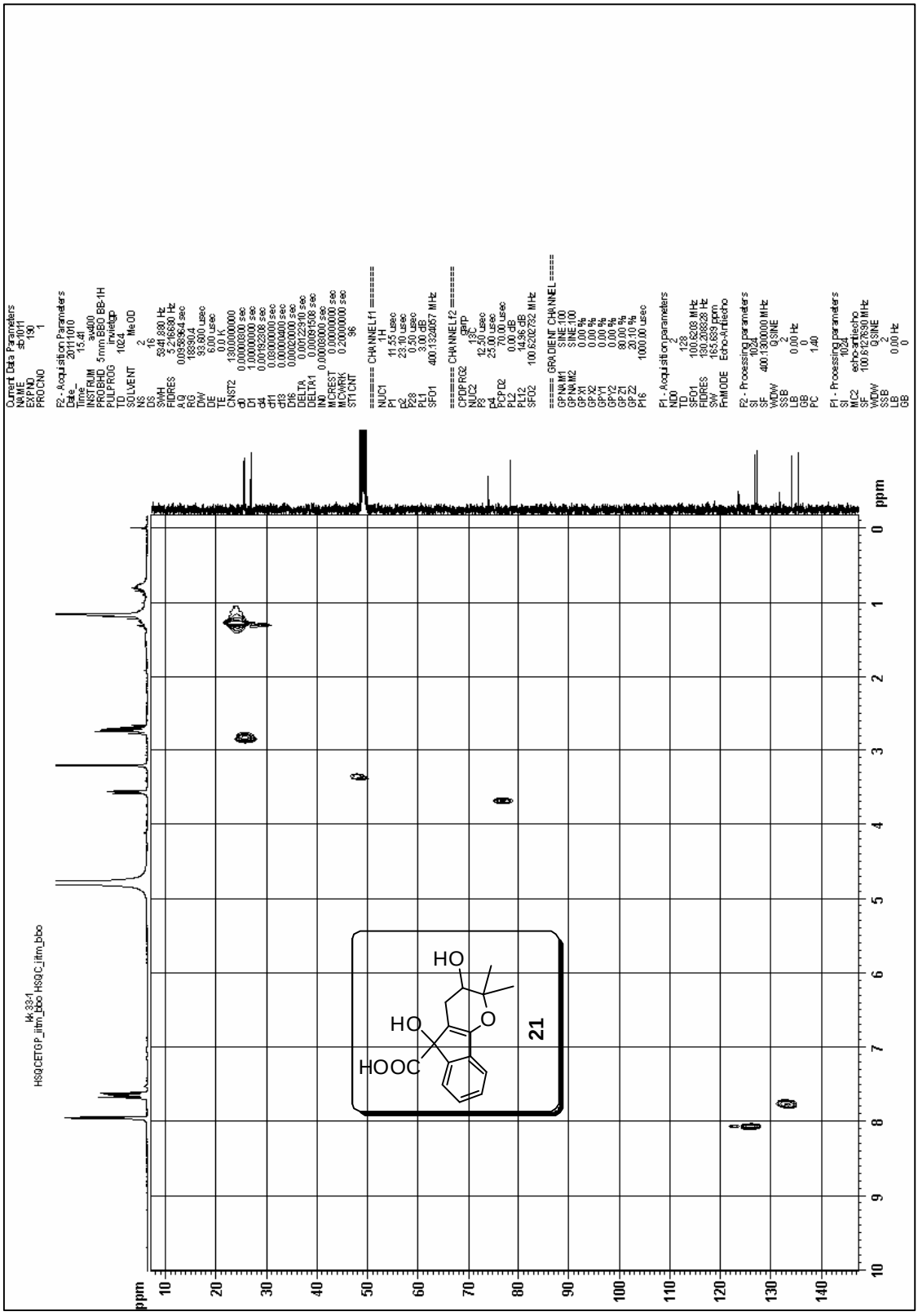
^{1}H NMR spectrum of compound **21**



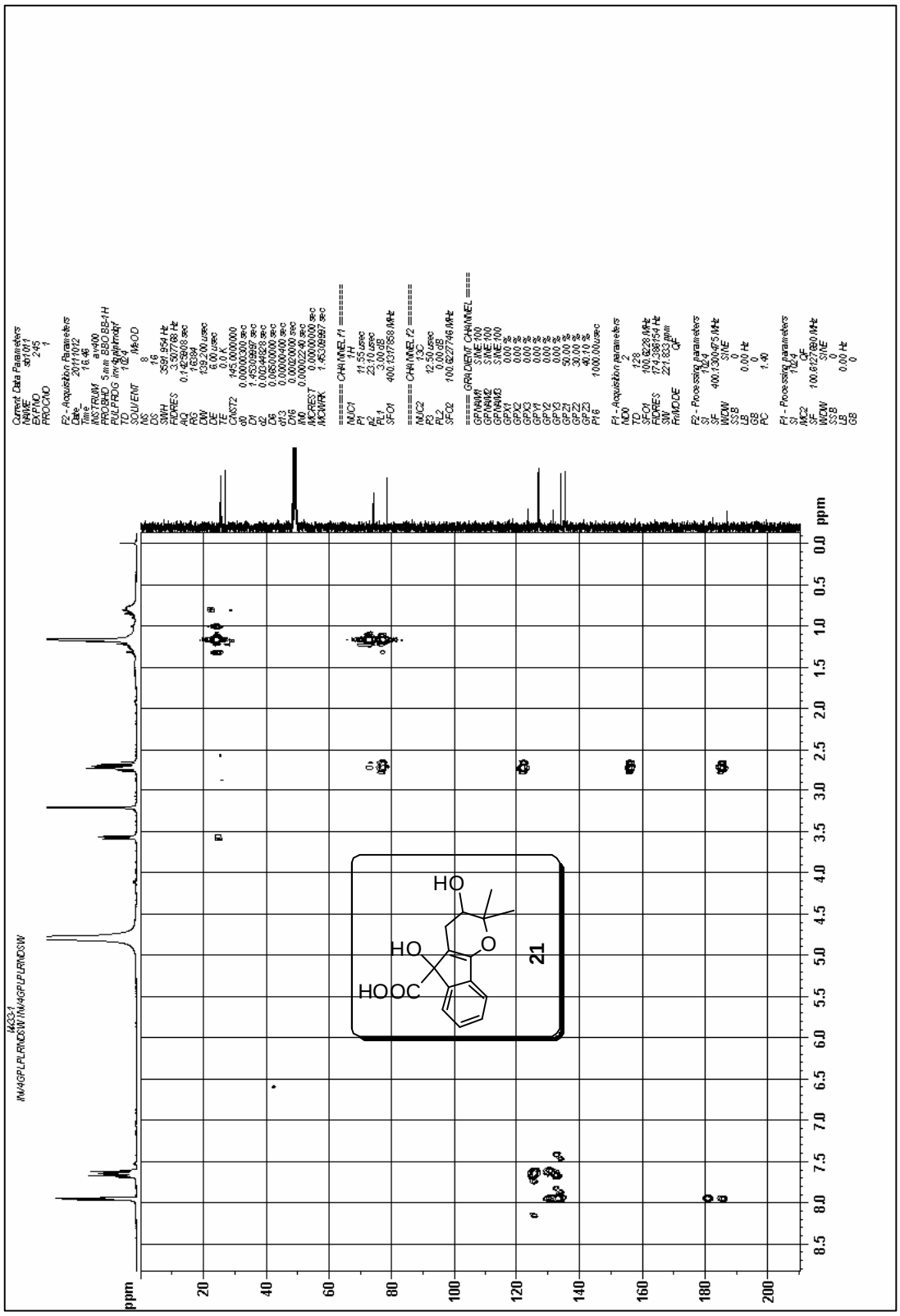
^{13}C NMR spectrum of compound **21**



^{1}H-^{1}H COSY spectrum of compound **21**



^{1}H-^{13}C COSY (HSQC) NMR spectrum of compound **21**



^{1}H-^{13}C COSY (HMBC) NMR spectrum of compound **21**