Supporting Information

The First Total Synthesis of (±)-Scopadulin, an Antiviral Aphidicolane Diterpene

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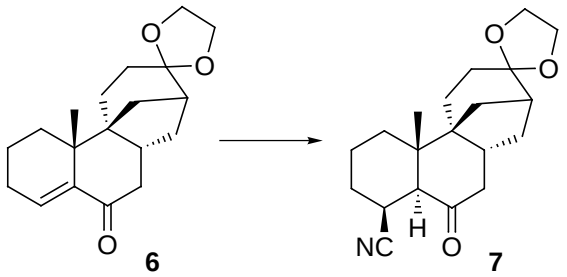
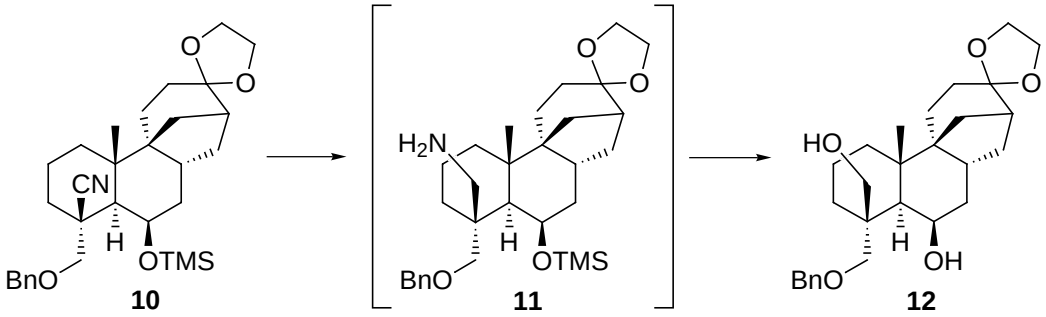
General Methods. Melting points are uncorrected. Nominal (LRMS) and exact mass (HRMS) spectra were recorded on a JEOL JMS-01SG-2 or JMS-HX/HX 110A mass spectrometer. ^{1}H- and ^{13}C-NMR spectra were recorded in $CDCl_3$. Chemical shifts are reported in parts per million downfield from internal Me_4Si (s = singlet, d = doublet, dd = double doublet, ddd = doublet of double doublet, t = triplet, m = multiplet).



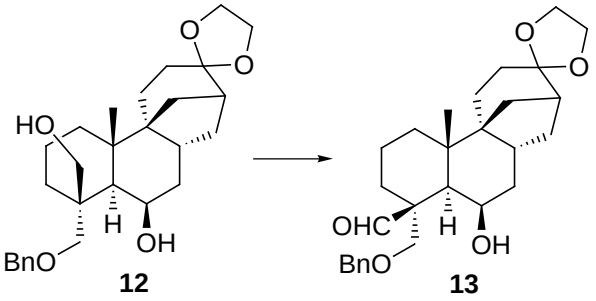
(1*S,2*S**,6*S**,7*S**,10*R**,12*R**)-2-Methyl-8,13-dioxotetracyclo[10.3.1.0^{1,10}.0^{2,7}]hexadecan-6-carbonitrile 13,13-Ethylene Acetal (7).** A solution of the enone **6** (145 mg, 0.48 mmol) in benzene (1.4 mL) was added dropwise to a stirring solution of Et_2AlCN (1.0 M in toluene, 1.4 mL) at 0 °C. After being stirred for 1.5 h at 0 °C, a viscous solution of Et_3N (0.625 mL, 4.50 mmol) and TMSCl (0.295 mL, 2.34 mmol) in benzene (0.4 mL) was added using a canula. The resulting mixture was warmed to rt, and Et_2O (20 mL) and saturated aqueous $NaHCO_3$ (9 mL) were added carefully. The organic layer was separated and the aqueous layer was extracted with CH_2Cl_2. The combined organic layers were washed with saturated aqueous $NaHCO_3$, dried (K_2CO_3), filtered and concentrated to give the crude silyl enol ether. The concentrate was then dissolved in MeOH-benzene (10:1; 4 mL), and K_2CO_3 (130 mg) was added. The mixture was stirred for 10 min at 0 °C, dried (Na_2SO_4), filtered, and concentrated. Purification of the residue by column chromatography (1:1 hexane/EtOAc) gave 128 mg (81%) of **7** as a colorless solid. Recrystallization (*n*-hexane/CH_2Cl_2) provided analytically pure coarse powder: Mp 124-126 °C. IR (KBr) cm^{-1}: 2227, 1708. ^{1}H-NMR ($CDCl_3$, 500 MHz) δ: 1.22 (s, 3H), 1.37-1.46 (m, 3H), 1.59-1.75 (m, 6H), 1.86-1.97 (m, 4H), 2.13-2.15 (m, 1H), 2.26 (t, *J* = 7.0 Hz, 1H), 2.34 (t, *J* = 14.5 Hz, 1H), 2.46-2.54 (m, 1H), 2.57 (dd, *J* = 13.5, 3.5 Hz, 1H), 2.66 (d, *J* = 3.5 Hz, 1H), 3.10 (br s, 1H), 3.84-4.01 (m, 4H). ^{13}C-

NMR ($CDCl_3$, 125 MHz) δ: 15.7, 18.7, 23.8, 25.6, 29.2, 29.8, 29.9, 32.7, 34.0, 39.9, 42.5, 42.8, 43.5, 47.6, 52.7, 64.0, 64.6, 111.2, 122.0, 207.1. MS (EI) *m/z* (%): 329 (M^+, 4.3), 99 (100). HRMS (EI) Calcd for $C_{20}H_{27}NO_3$: 329.1993. Found: 329.1991. *Anal.* Calcd for $C_{20}H_{27}NO_3$: C, 72.92; H, 8.26; N, 4.25. Found: C, 72.63; H, 8.14; N, 4.10.

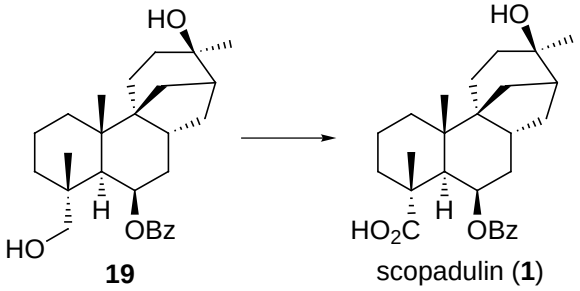


(1*S,2*S**,6*R**,7*R**,8*R**,10*R**,12*R**)-6-[(Benzyloxy)methyl]-8-hydroxy-6-hydroxymethyl-2-methyltetracyclo[10.3.1.0^{1,10}.0^{2,7}]hexadecan-13-one 13,13-Ethylene Acetal (12).** To a solution of the nitrile **10** (21 mg, 0.040 mmol) in THF (1.4 mL) was added $LiAlH_4$ (1.0 M in ether, 0.65 mL) at 0 °C, and the resulting mixture was warmed to rt and then refluxed at 75 °C for 4 h. The solution was cooled to 0 °C, quenched by successive addition of H_2O (55 μL), 2 M NaOH (55 μL), and H_2O (170 μL). The resulting heterogeneous mixture was stirred at rt for 2 h, filtered, and the solid was washed with EtOAc. The combined filtrate was concentrated to give the amine **11**.[1] The crude amine **11**, KOH (110 mg, 1.93 mmol) and a degassed diethylene glycol (0.9 mL) were placed under N_2 in a round-bottom flask equipped with a refluxing condenser. The mixture was heated at 210 °C for 4 h. The black solution was then cooled to rt, Et_2O (3 mL) and H_2O (2 mL) were added. The organic phase was separated and the aqueous layer was extracted with Et_2O (5 × 6 mL). The combined organic layers were washed with brine, dried ($MgSO_4$), filtered and concentrated. Purification of the residue by column chromatography (5:1 hexane/EtOAc) gave 11.5 mg (63%, two steps) of the diol **12** as a solid mass. Crystallization from benzene provided a pure white solid: mp >300 °C. IR (KBr) cm^{-1}: 3267 (br), 1115. ^{1}H-NMR ($CDCl_3$, 500 MHz) δ: 1.16 (d, *J* = 10.5 Hz, 1H), 1.25-1.29 (m, 4H), 1.31 (s, 3H), 1.39-1.72 (m, 10H), 1.77-1.93 (m, 4H), 2.14 (m, 1H), 2.66 (m, 1H), 3.41 (d, *J* = 9.0 Hz, 1H), 3.47 (d, *J* = 9.0 Hz, 1H), 3.53 (d, *J* = 12.0 Hz, 1H), 3.82-4.00 (m, 4H), 4.23 (m, 1H), 4.32 (d, *J* = 12.0 Hz, 1H), 4.47 (d, *J* = 12.5 Hz, 1H), 4.53 (d, *J* = 12.5 Hz, 1H), 7.28-7.37 (m, 5H). ^{13}C-NMR ($CDCl_3$, 125 MHz) δ: 18.5, 18.7, 26.4, 29.7, 30.5, 33.5, 34.9, 35.4, 35.8, 35.9, 40.8, 43.0, 43.1, 46.8, 48.5, 63.9, 64.5, 67.6, 67.7, 73.4, 79.0, 111.9, 127.5 (2C), 127.7, 128.5 (2C), 138.2. MS (FAB) *m/z* (%): 457 (MH^+, 10.8), 212 (100), 91 (84). HRMS (FAB) Calcd for $C_{28}H_{41}O_5$ (MH^+): 457.2954. Found: 457.2954.

(1) Rahman, S. M. A.; Ohno, H.; Maezaki, N.; Iwata, C.; Tanaka, T. *Org. Lett.* **2000**, *2*, 2893.

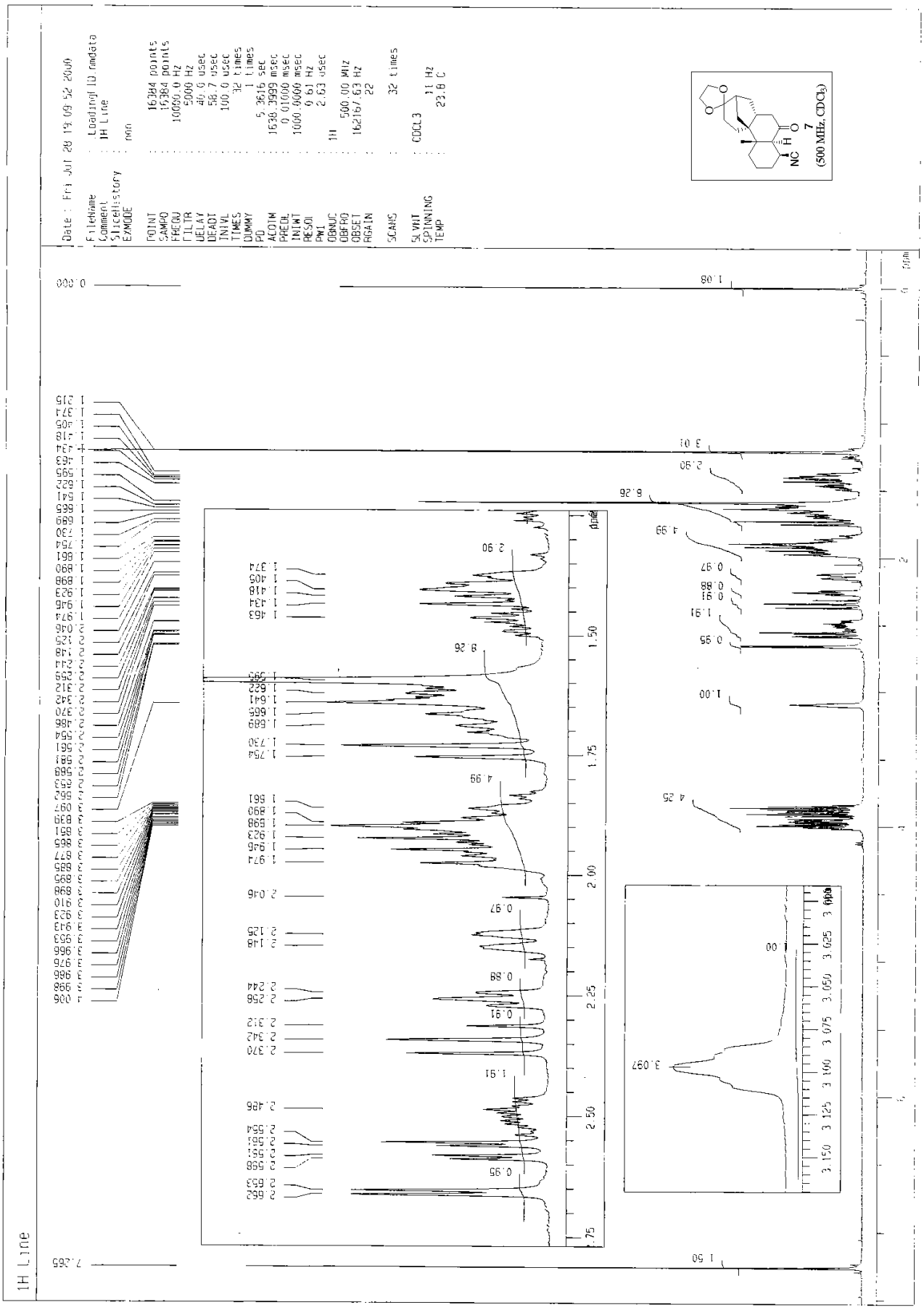


(1*S,2*S**,6*S**,7*R**,8*R**,10*R**,12*R**)-6-[(Benzyloxy)methyl]-8-hydroxy-2-methyl-13-oxotetracyclo[10.3.1.0^{1,10}.0^{2,7}]hexadecan-6-carboaldehyde 13,13-Ethylene Acetal (13).** $RuCl_2(PPh_3)_3$ (30 mg, 0.031 mmol) was added to a solution of the diol **12** (14 mg, 0.0307 mmol) in benzene (0.7 mL), and the resulting mixture was stirred in the presence of air at rt for 24 h. The dark solution obtained was passed through a short silica gel column eluting with EtOAc. The eluate was then concentrated and the residue was chromatographed on silica gel (3:1 hexane/EtOAc) to afford **13** (10 mg, 72%) as a colorless oil, together with 3.0 mg (21%) of the recovered diol **12**. Compound **13**: IR (KBr) cm^{-1}: 3493, 1705, 1115. ^{1}H-NMR ($CDCl_3$, 500 MHz) δ: 1.00 (s, 3H), 1.16-1.29 (m, 4H), 1.56-1.68 (m, 8H), 1.76-1.83 (m, 2H), 1.88-1.94 (m, 2H), 2.14 (t, *J* = 7.0 Hz, 1H), 2.32 (d, *J* = 13.0 Hz, 1H), 2.57-2.65 (m, 1H), 3.35 (s, 1H), 3.44 (d, *J* = 8.5 Hz, 1H), 3.55 (d, *J* = 8.5 Hz, 1H), 3.81-3.99 (m, 4H), 4.28 (br s, 1H), 4.42 (d, *J* = 12.0 Hz, 1H), 4.47 (d, *J* = 12.0 Hz, 1H), 7.25-7.36 (m, 5H), 10.19 (s, 1H). ^{13}C-NMR ($CDCl_3$, 125 MHz) δ: 18.8 19.0, 26.2, 29.6, 30.4, 32.7, 33.3, 34.7, 34.8, 35.1, 35.7, 40.6, 43.2, 43.5, 48.7, 63.9, 64.5, 67.9, 73.6, 76.3, 111.7, 127.5 (2C), 127.7, 128.4 (2C), 137.6, 211.1. MS (FAB) *m/z* (%): 477 (MNa^+, 16), 176 (100). HRMS (FAB) Calcd for $C_{28}H_{38}NaO_5$ (MNa^+): 477.2617. Found: 477.2602.



(±)-Scopadulin (1). $NaIO_4$ (45 mg, 0.21 mmol) was added to a solution of **19** (4.0 mg, 0.0094 mmol) in a mixed solvent of CCl_4–CH_3CN–H_2O (1:1:1.5; 0.35 ml) in a micro-reactor, and the mixture was stirred at rt for 20 min. $RuCl_3{\cdot}3H_2O$ (about 0.5 mg) was added and the mixture was stirred overnight at rt. After 15 h, the reaction mixture was filtered through a plug of celite, and the filter cake was washed with EtOAc. The filtrate was dried ($MgSO_4$), filtered, concentrated, and the residue was purified by column chromatography (1:2 hexane/EtOAc → EtOAc → 7:3 EtOAc/MeOH) to give (±)-scopadulin **1** (12.6 mg, 63%) as a white solid. Recrystallization from EtOAc provided an analytically pure colorless solid. Mp 238–240 °C (EtOAc). IR (KBr) cm^{-1}: 3436 (br), 1716, 1701, 1603. ^{1}H-NMR (C_5D_5N, 500 MHz) δ: 1.06 (dd, *J* = 13.0, 8.0 Hz, 1H), 1.27-1.30 (m, 2H), 1.29 (s, 3H), 1.50-1.61 (m, 4H), 1.59 (s, 3H), 1.74 (s, 3H), 1.78-1.89 (m, 7H), 2.11-

2.24 (m, 4H), 2.43 (d, *J* = 11.0 Hz, 1H), 2.62-2.68 (m, 1H), 3.03 (d, *J* = 2.0 Hz, 1H), 6.03 (d, *J* = 2.0 Hz, 1H), 7.50-7.57 (m, 3H), 8.34 (d, *J* = 8.0 Hz, 2H). ^{13}C-NMR (C_5D_5N, 125 MHz) δ: 18.7, 19.0, 20.2, 25.7, 28.6, 31.6, 33.2, 33.5, 33.9, 35.3, 36.0, 40.6, 41.1, 44.5, 47.6, 48.1, 48.6, 71.4, 75.2, 129.1 (2C), 130.0 (2C), 131.7, 133.3, 166.2, 182.8. MS (FAB) *m/z* (%): 441 (MH^+, 29), 185 (100). HRMS (FAB) Calcd for $C_{27}H_{37}O_5$ (MH^+): 441.2641. Found: 441.2631.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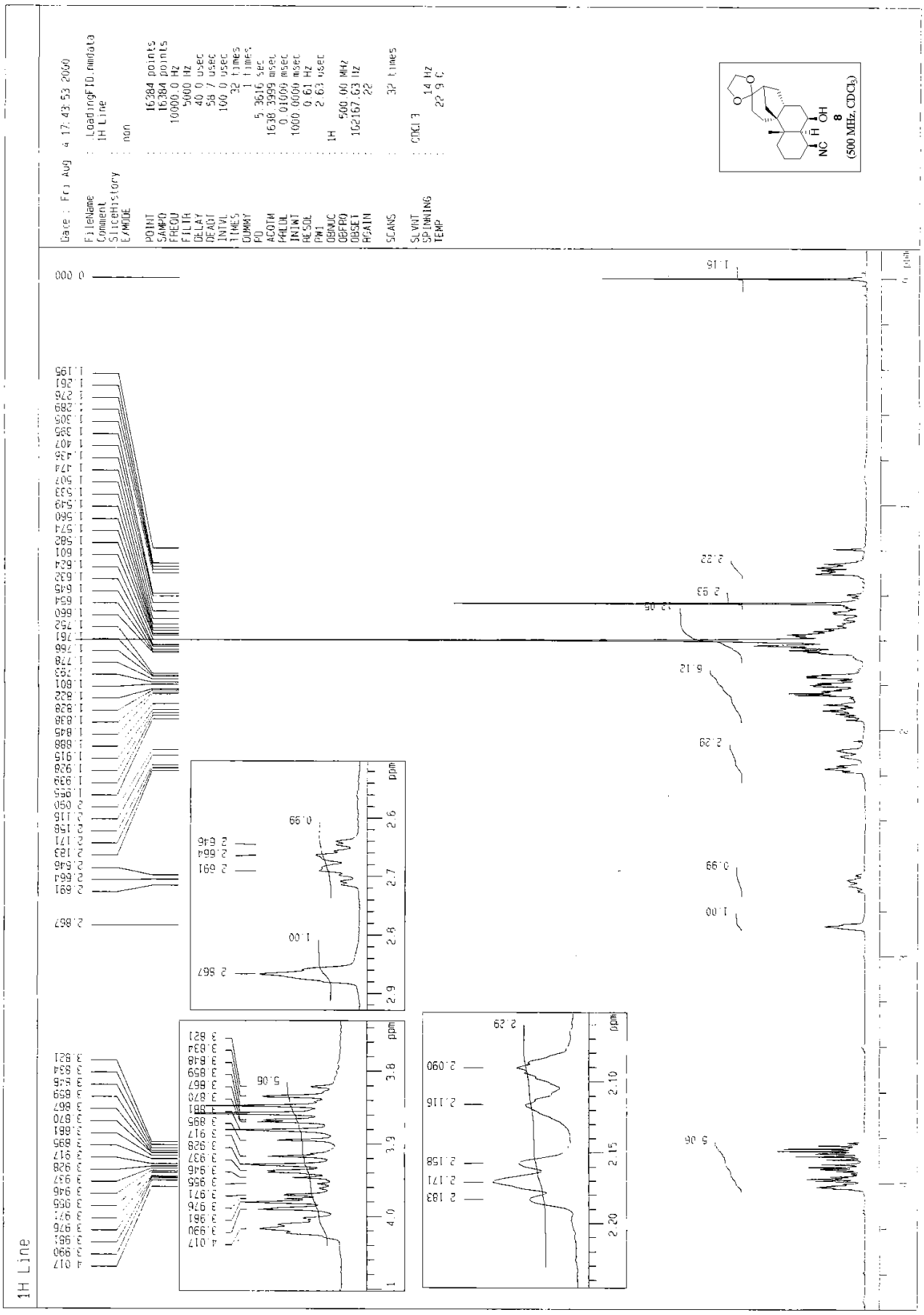
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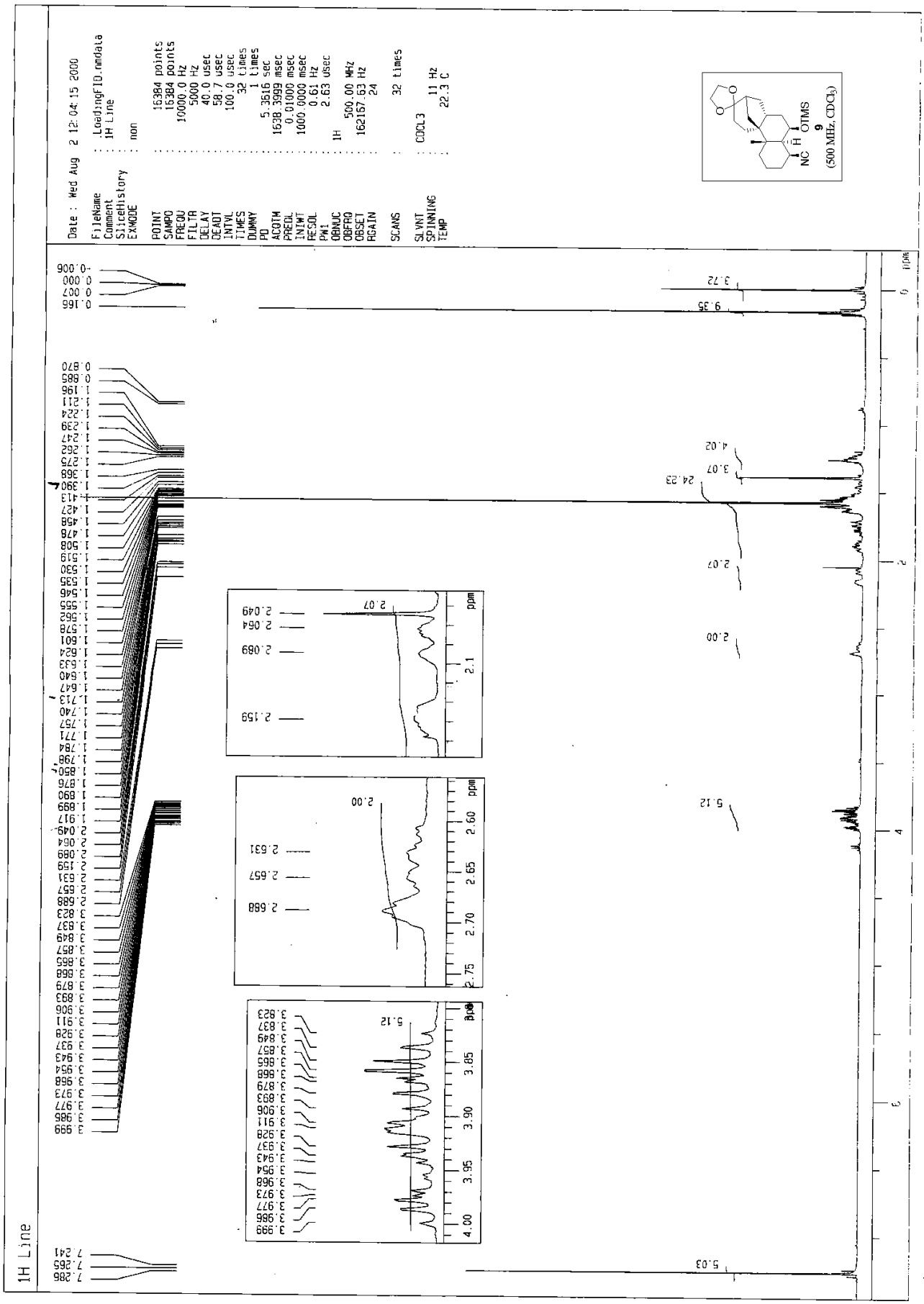
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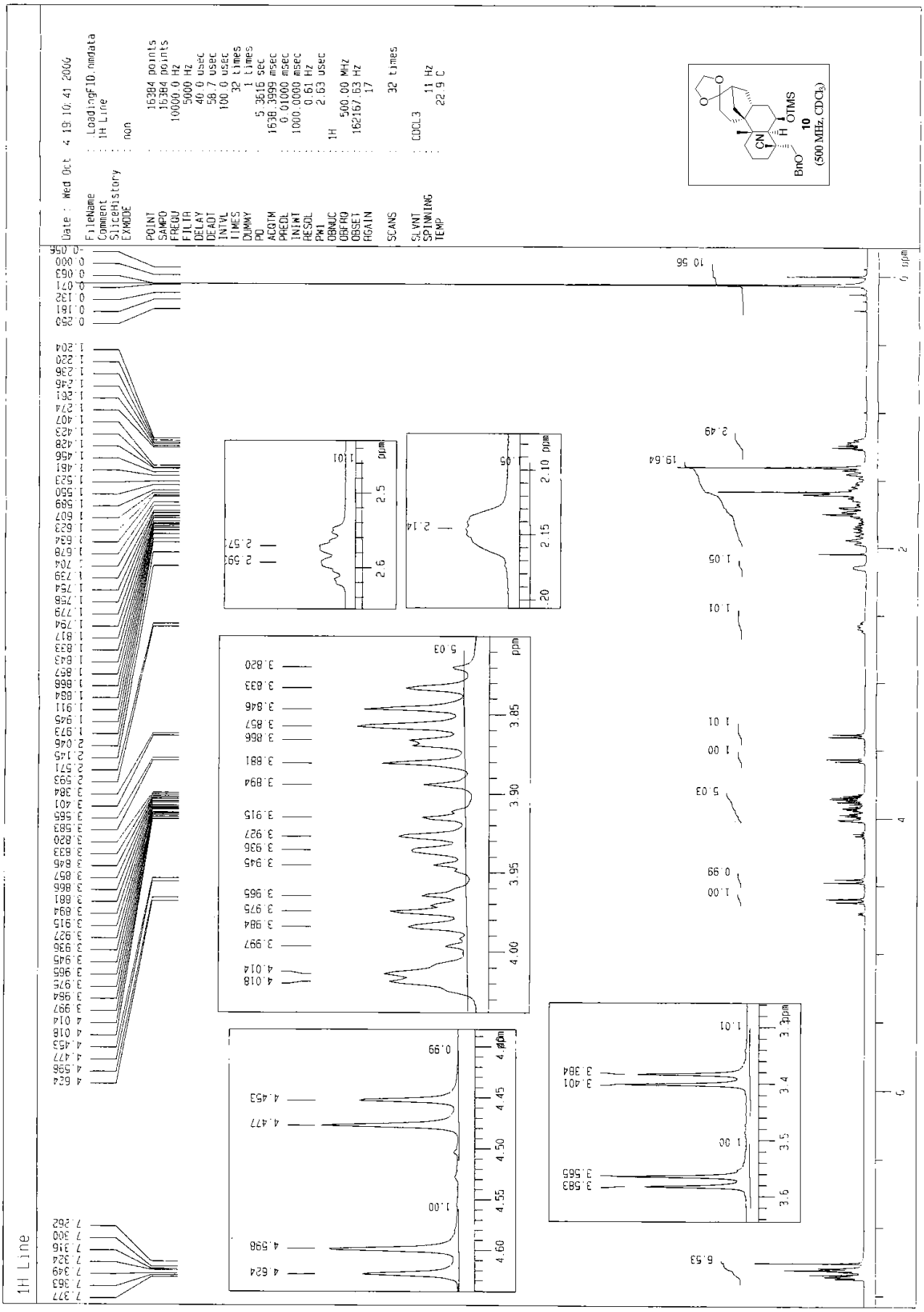
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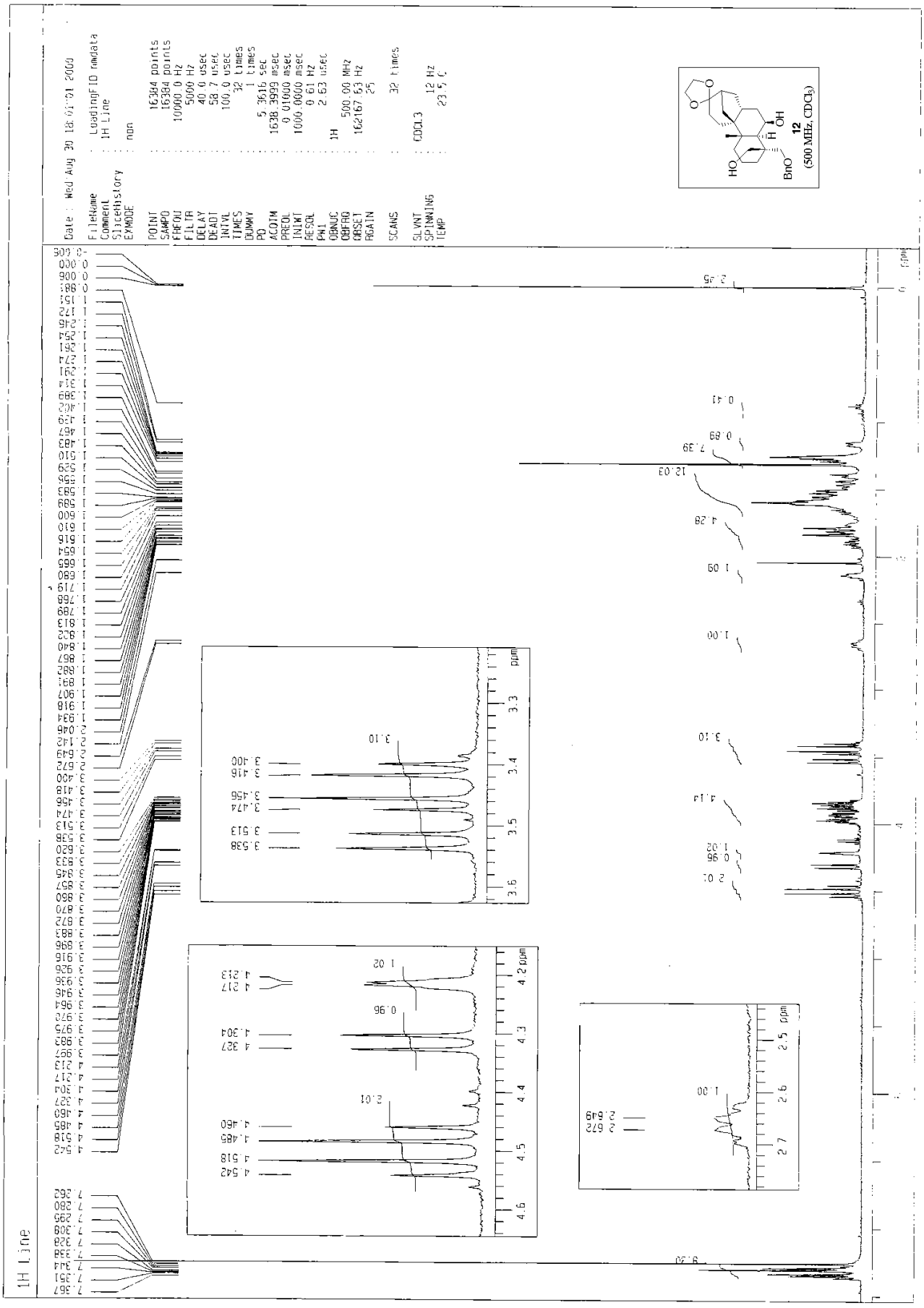
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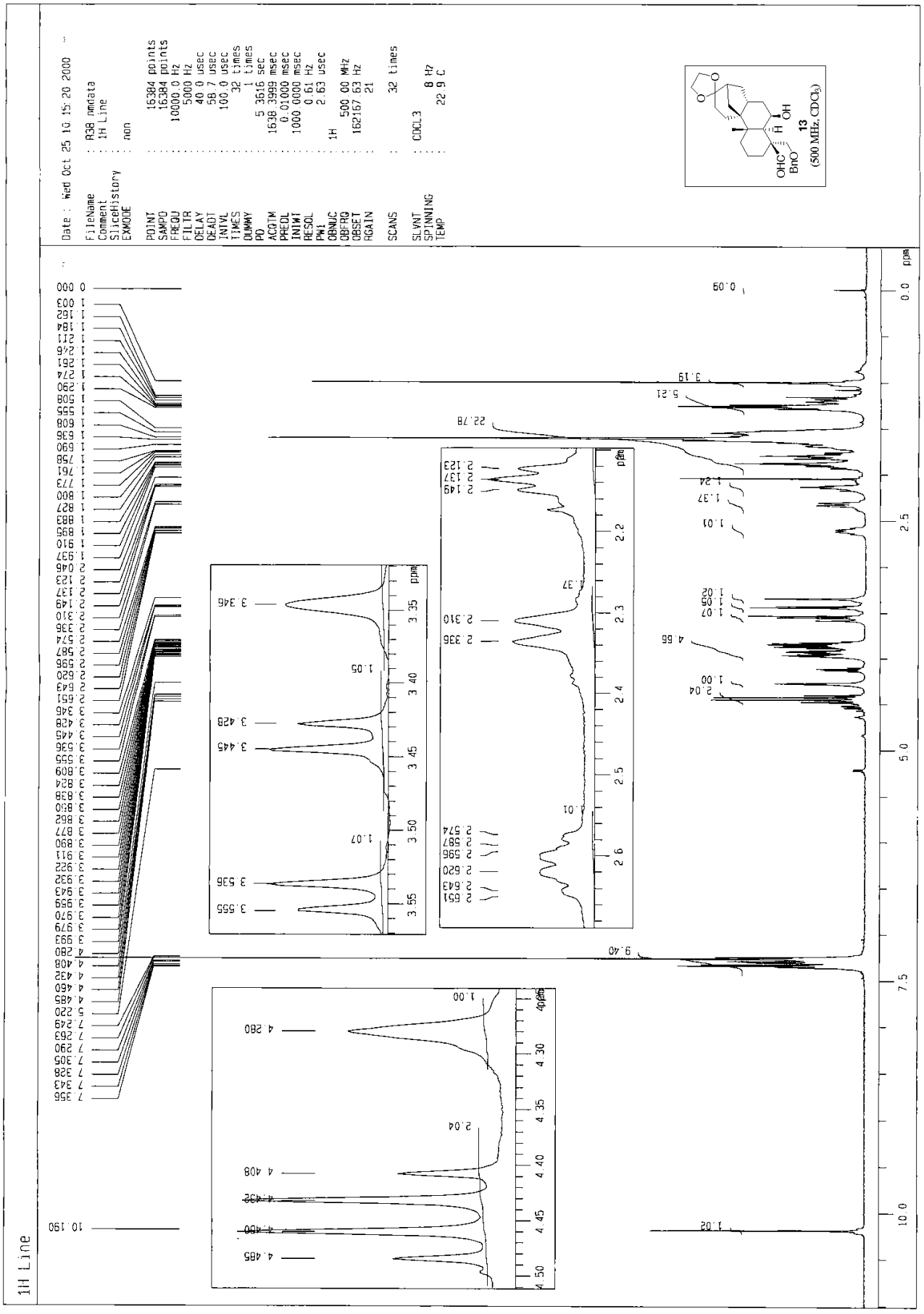
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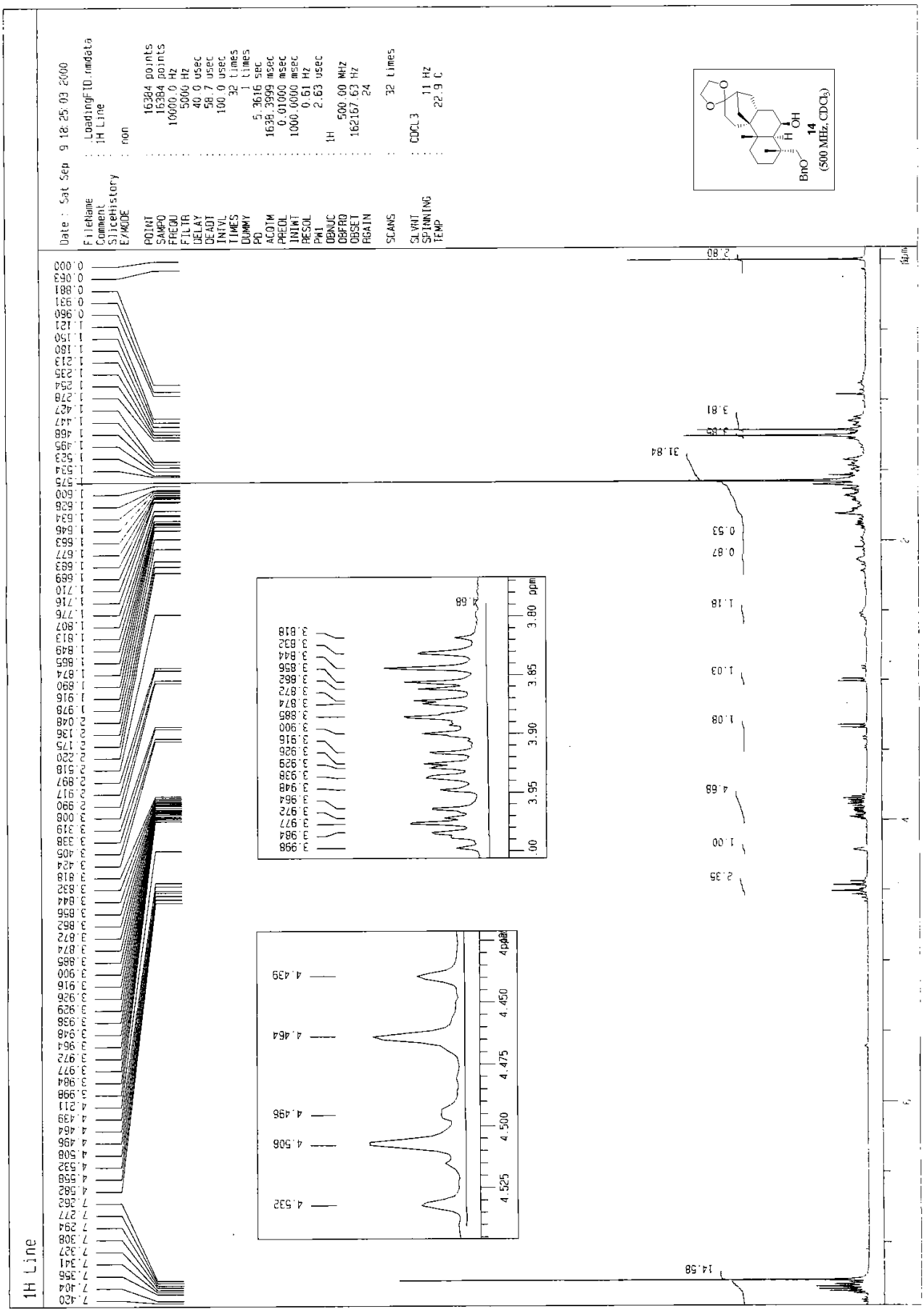
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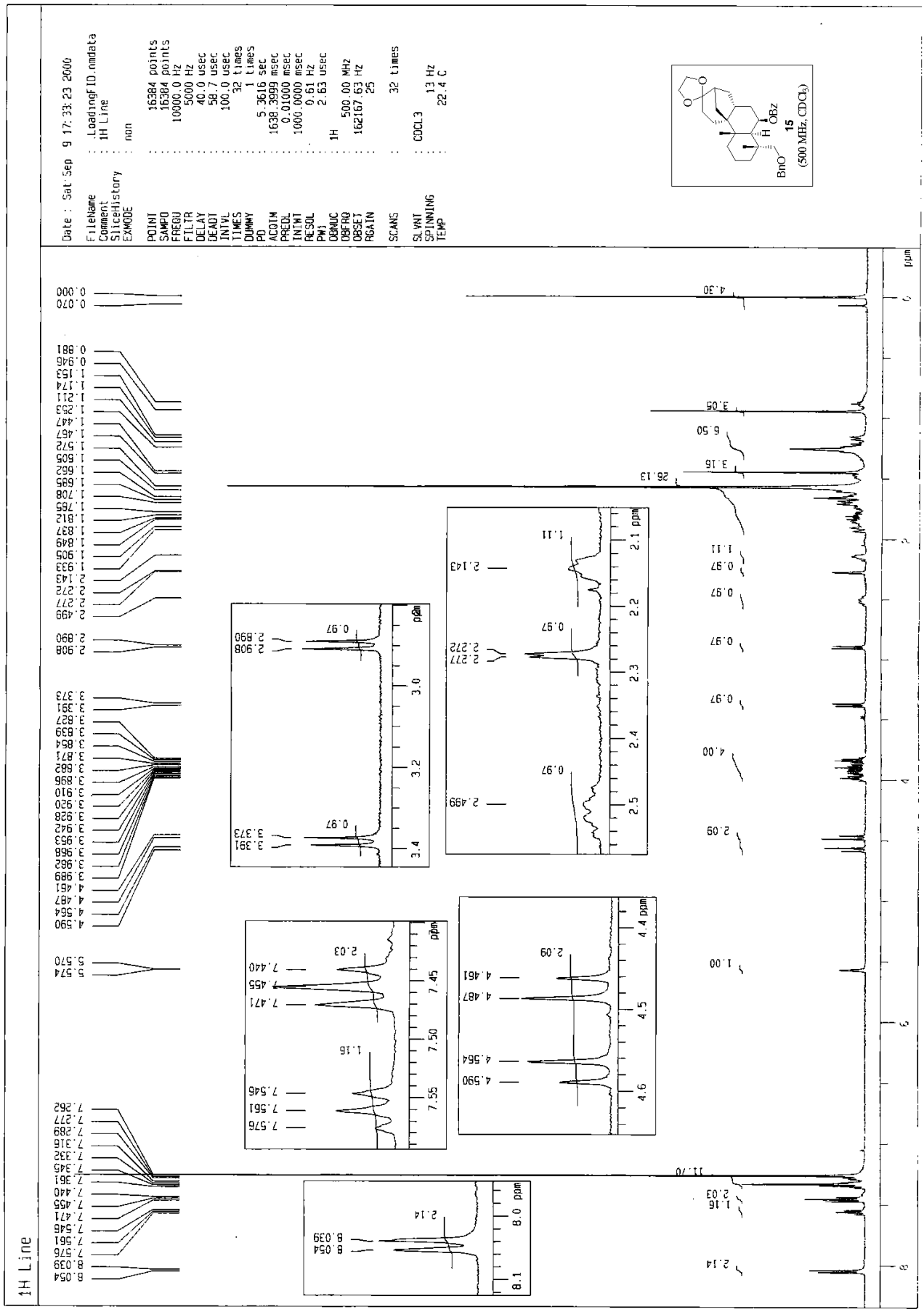
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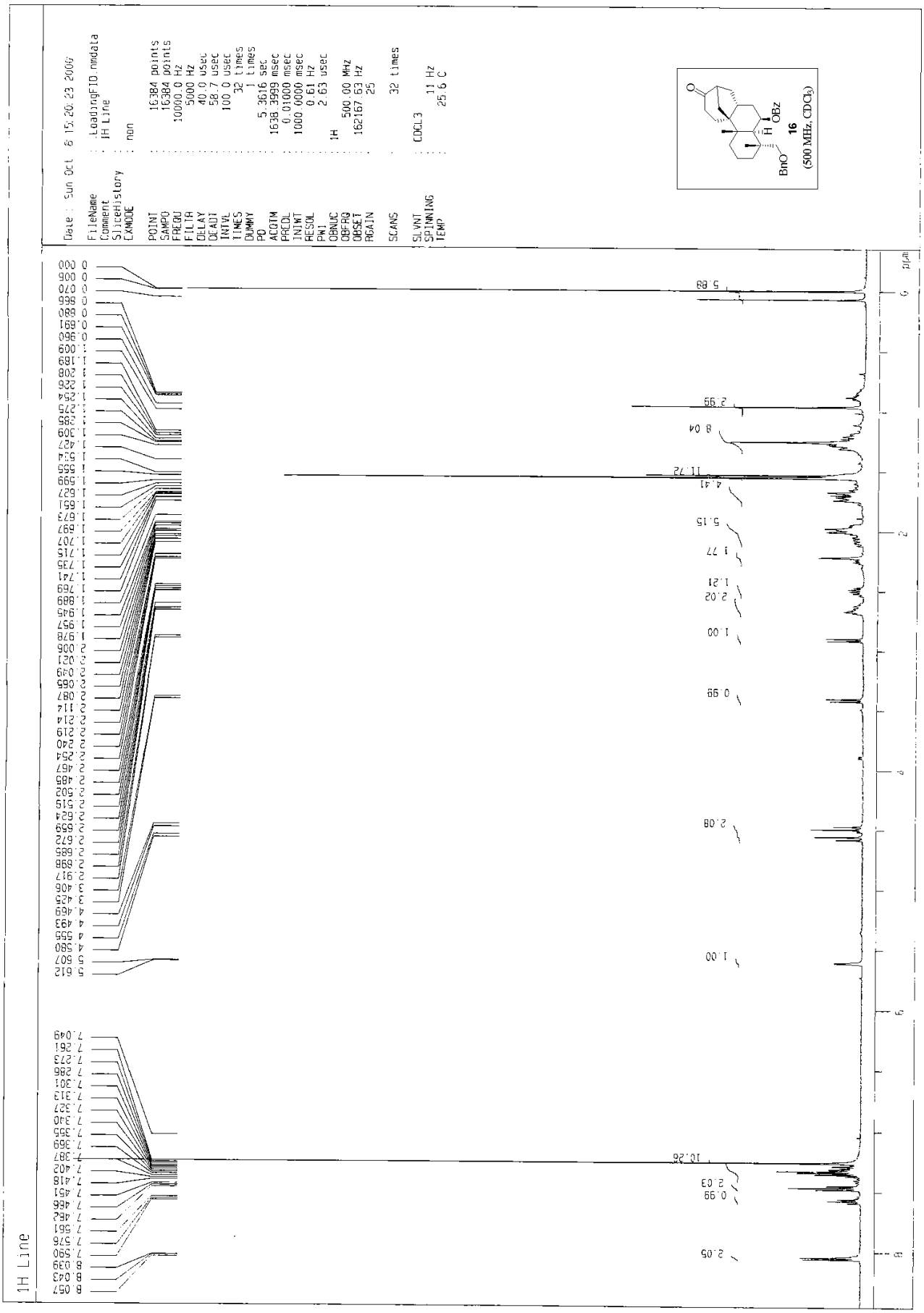
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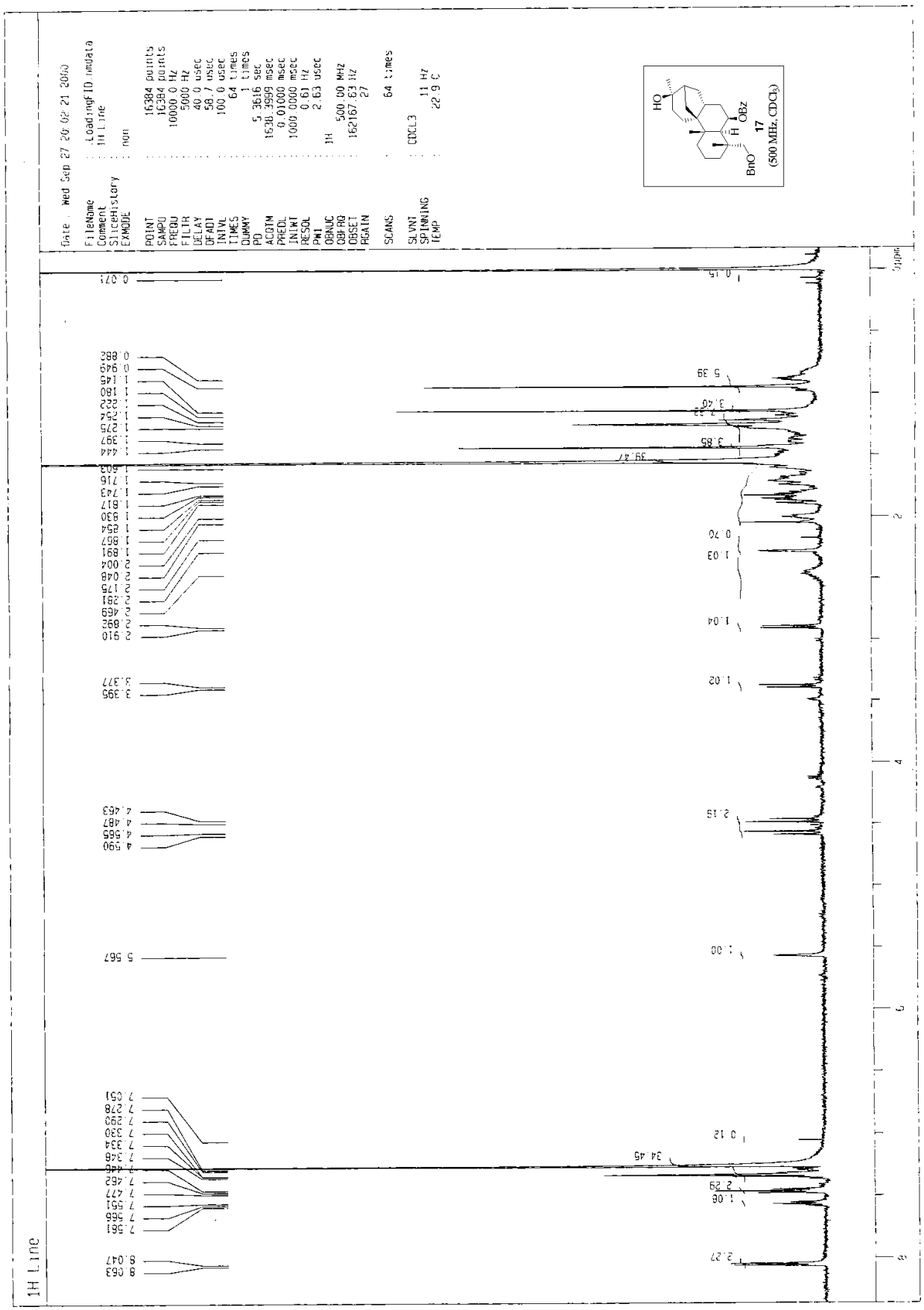
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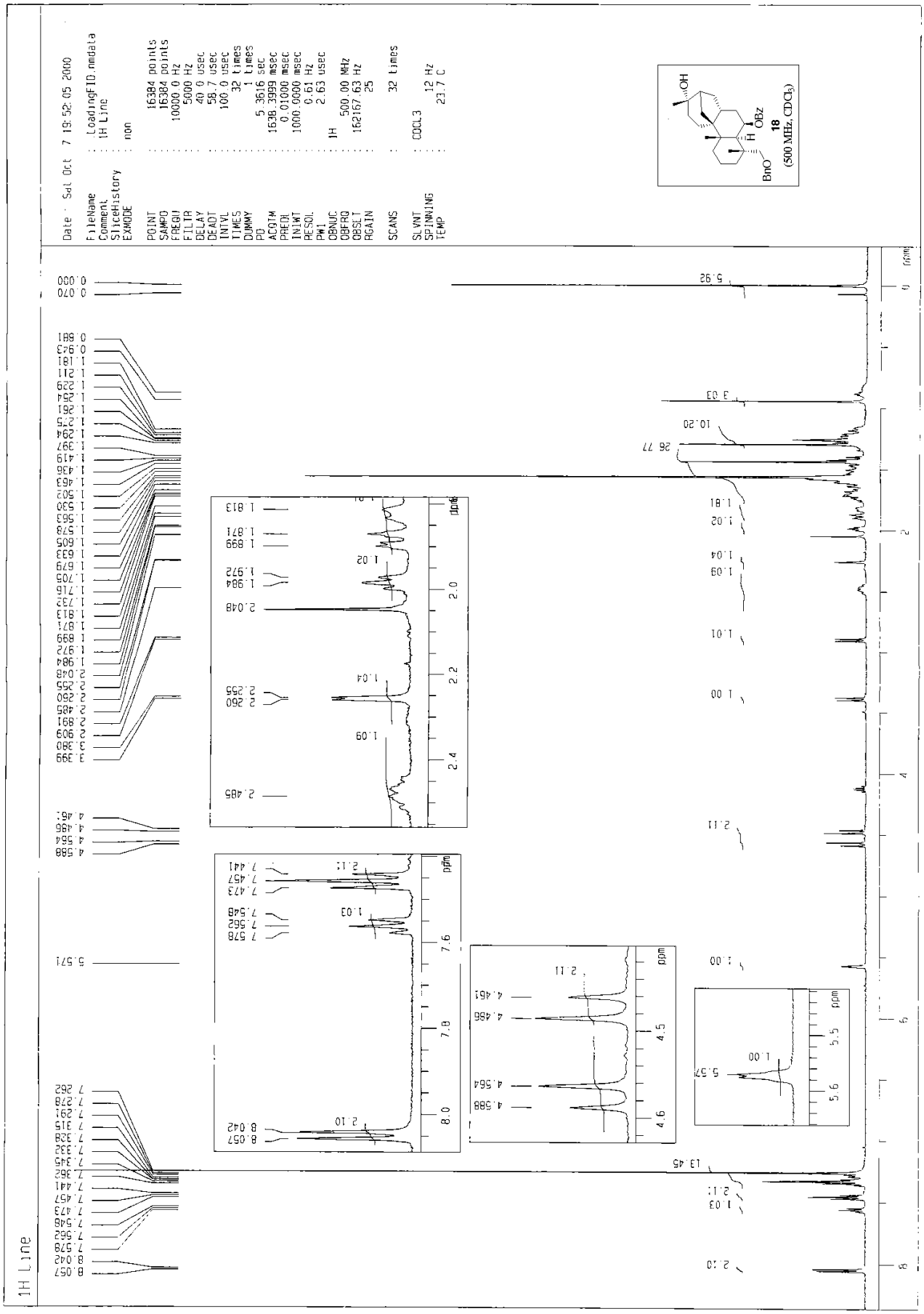
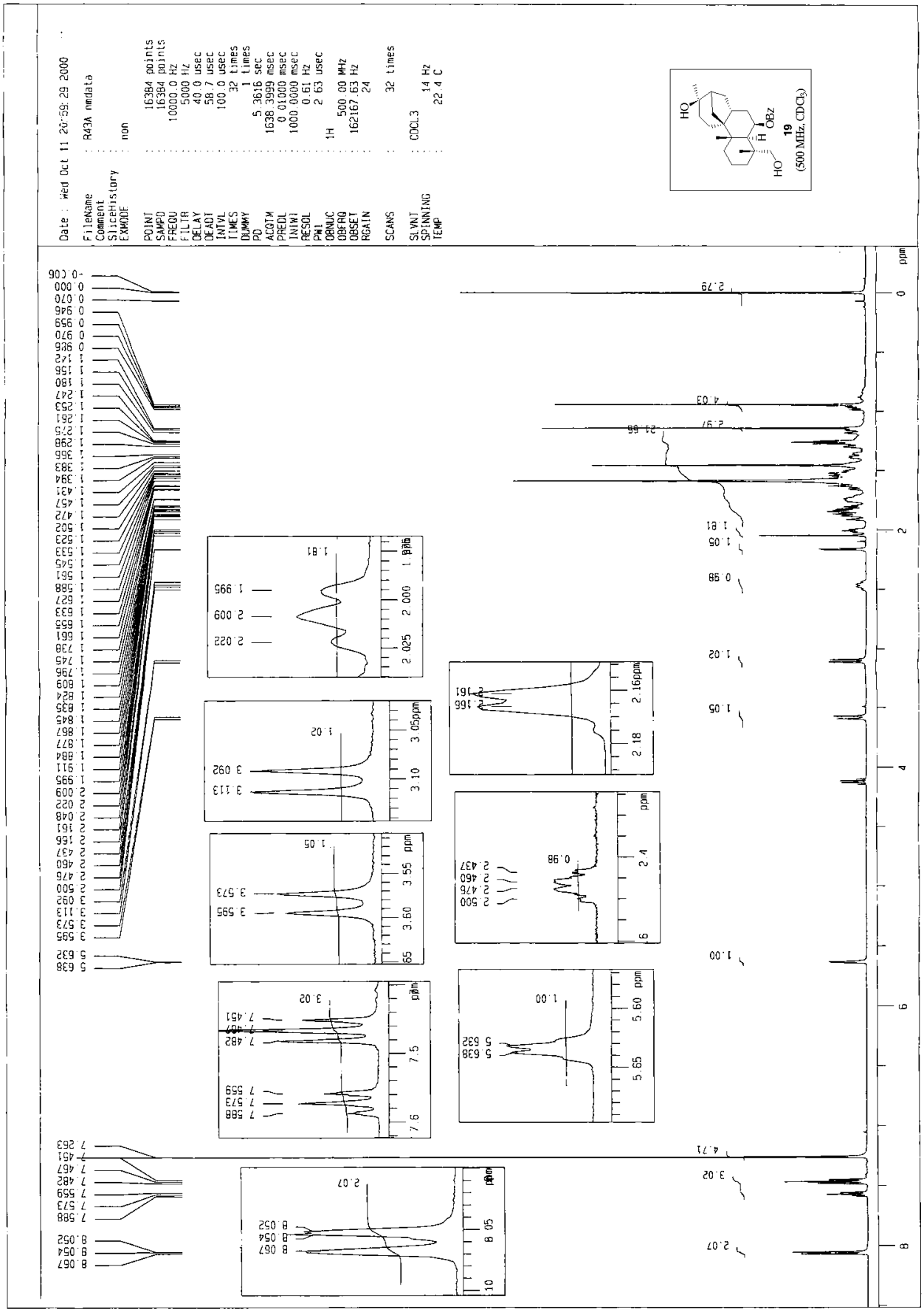
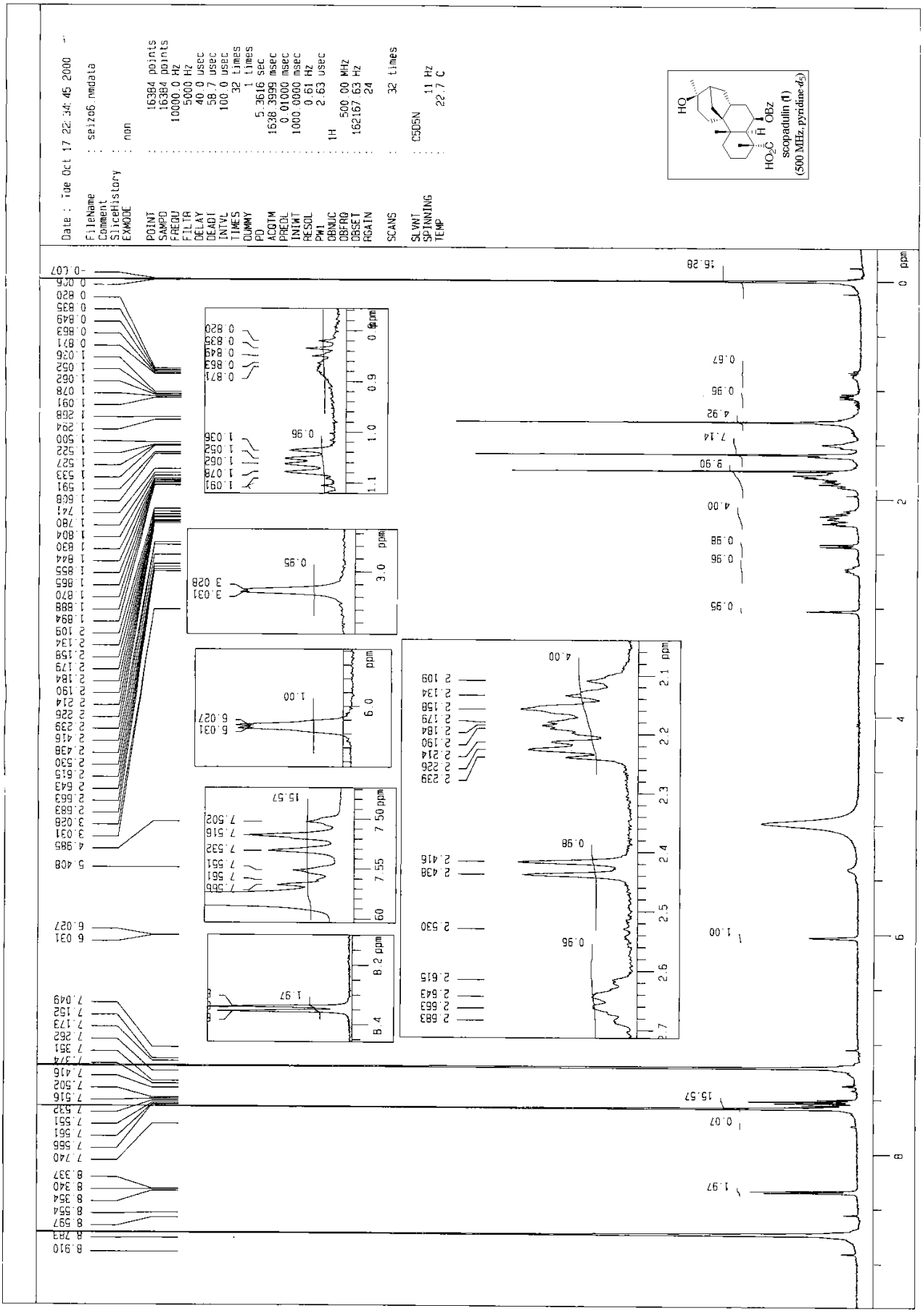
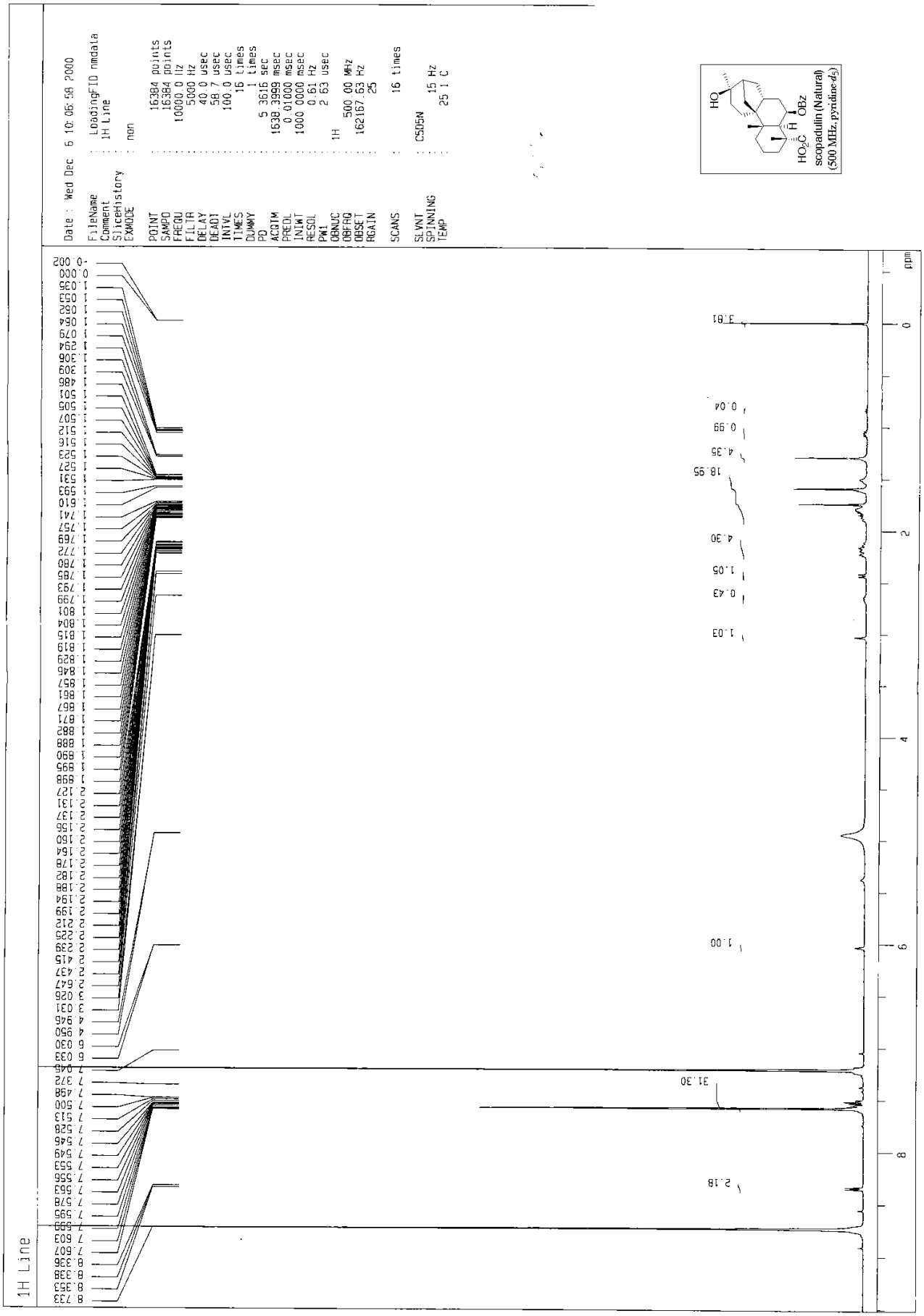
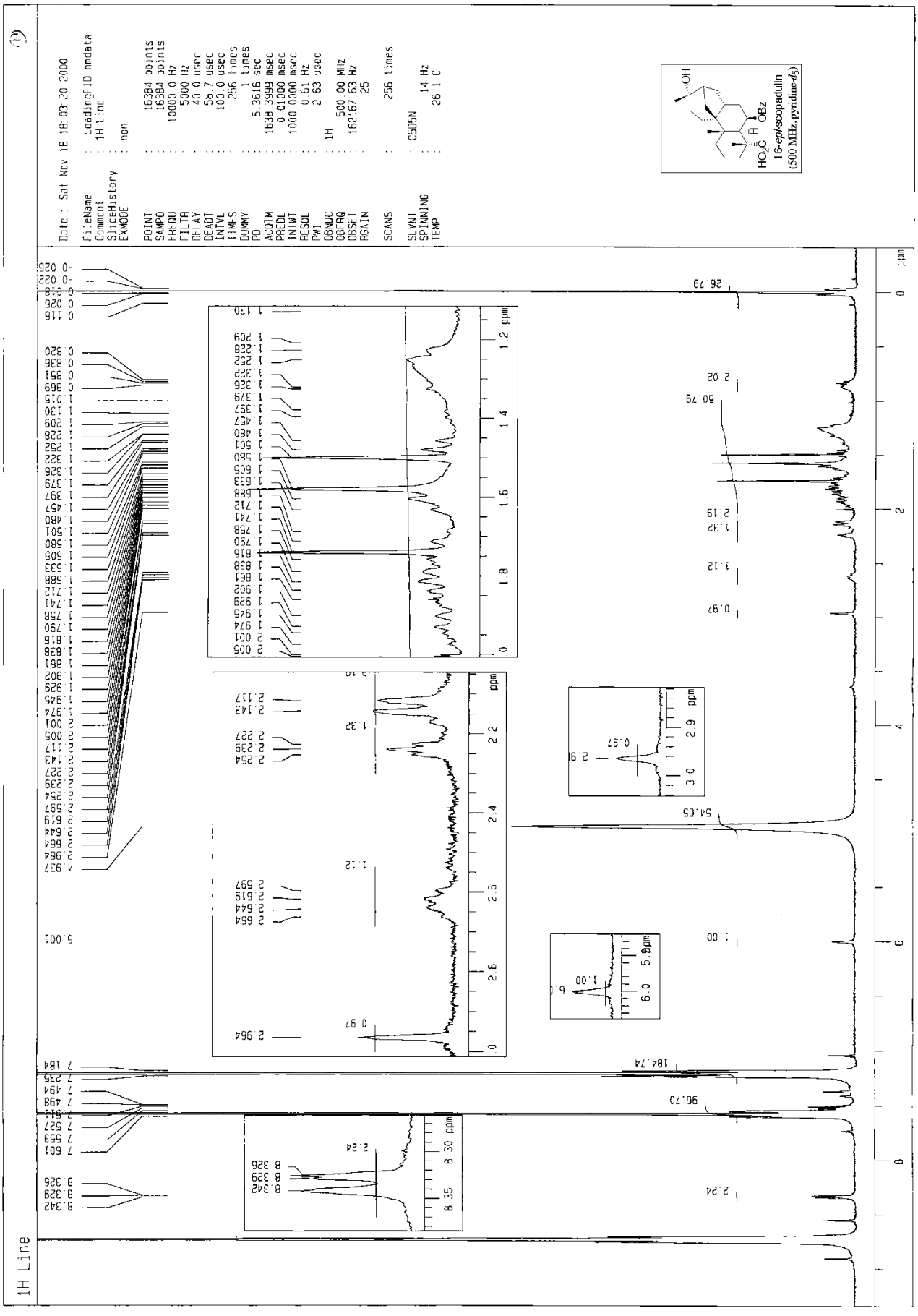
(500 MHz, CDCl3)
1H Line


Date · Sat Oct 7 19:52:05 2000
FileName : LoadingFID.nmrdata
Comment : 1H Line
SliceHistory :
EXMODE : non
POINT : 16384 points
SAMPO : 16384 points
FREQU : 10000.0 Hz
FILTR : 5000 Hz
DELAY : 40.0 usec
DEADT : 58.7 usec
INTVL : 100.0 usec
TIMES : 32 times
DUMMY : 1 times
PD : 5.3616 sec
ACQTM : 1638.3999 msec
PREDL : 0.01000 msec
INIWT : 1000.0000 msec
RESOL : 0.61 Hz
PW1 : 2.63 usec
OBNUC : 1H
OBFRQ : 500.00 MHz
OBSLT : 16216?.63 Hz
RGAIN : 25
SCANS : 32 times
SLVNT : CDCL3
SPINNING : 12 Hz
TEMP : 23.7 C
OH
OBz
BnO
18
(500 MHz, CDCl3)
1H Line
ppm


Date : Wed Oct 11 20:59:29 2000
FileName : R43A nmdata
Comment :
SliceHistory :
EXMODE : non
POINT : 16384 points
SAMPD : 16384 points
FREQU : 10000.0 Hz
FILTR : 5000 Hz
DELAY : 40.0 usec
DEADT : 58.7 usec
INTVL : 100.0 usec
TIMES : 32 times
DUMMY : 1 times
PD : 5.3616 sec
ACQTM : 1638.3999 msec
PREDL : 0.01000 msec
IN1W1 : 1000.0000 msec
RESOL : 0.61 Hz
PW1 : 2.63 usec
ORNUC : 1H 500.00 MHz
OBFRQ : 162167.63 Hz
OBSET : 24
RGAIN :
SCANS : 32 times
SLVNT : CDCL3 14 Hz
SPINNING : 22.4 C
TEMP :
HO
H
OBz
HO
19
(500 MHz, CDCl3)


Date : Tue Oct 17 22:34:45 2000
FileName : seizo6.nmdata
Comment :
SliceHistory :
EXMODE : non
POINT : 16384 points
SAMPO : 16384 points
FREQU : 10000.0 Hz
FILTR : 5000 Hz
DELAY : 40.0 usec
DEAD1 : 58.7 usec
INTVL : 100.0 usec
TIMES : 32 times
DUMMY : 1 times
PD : 5.3616 sec
ACQTM : 1638.3999 msec
PREDL : 0.01000 msec
INIWT : 1000.0000 msec
RESOL : 0.61 Hz
PW1 : 2.63 usec
OBNUC : 1H 500.00 MHz
OBFRQ : 162167.63 Hz
OBSET : 24
AGAIN :
SCANS : 32 times
SLVNT : C5D5N
SPINNING : 11 Hz
TEMP : 22.7 C
HO
H
OBz
HO2C
scopadulin (1)
(500 MHz, pyridine-d5)
ppm


Date : Wed Dec 6 10:06:58 2000
FileName : LoadingFID nmrdata
Comment : 1H Line
SliceHistory :
EXMODE : non
POINT : 16384 points
SAMPO : 16384 points
FREQU : 10000.0 Hz
FILTR : 5000 Hz
DELAY : 40.0 usec
DEADI : 58.7 usec
INTVL : 100.0 usec
TIMES : 16 times
DUMMY : 1 times
PD : 5.3616 sec
ACQTM : 1638.3999 msec
PREDL : 0.01000 msec
INIWT : 1000.0000 msec
RESOL : 0.61 Hz
PW1 : 2.63 usec
OBNUC : 1H 500.00 MHz
OBFRQ : 162167.63 Hz
OBSET : 25
RGAIN :
SCANS : 16 times
SLVNT : C5D5N
SPINNING : 15 Hz
TEMP : 25.1 C
HO
HO2C
H
OBz
scopadulin (Natural)
(500 MHz, pyridine-d5)
1H Line
ppm
31.30
18.95
3.81
2.18
1.00
1.03
0.43
1.05
4.30
4.35
0.99
0.04


1H Line
Date : Sat Nov 18 18:03:20 2000
FileName : Loading\1D nmrdata
Comment : 1H Line
SliceHistory :
EXMODE : non
POINT : 16384 points
SAMPO : 16384 points
FREQU : 10000.0 Hz
FILTR : 5000 Hz
DELAY : 40.0 usec
DEADT : 58.7 usec
INTVL : 100.0 usec
TIMES : 256 times
DUMMY : 1 times
PD : 5.3616 sec
ACQTM : 1638.3999 msec
PREDL : 0.01000 msec
INIWT : 1000.0000 msec
RESOL : 0.61 Hz
PW1 : 2.63 usec
OBNUC : 1H 500.00 MHz
OBFRQ : 162167.63 Hz
OBSET : 25
RGAIN :
SCANS : 256 times
SLVNT : C5D5N 14 Hz
SPINNING : 26.1 C
TEMP :
HO2C H OBz
OH
16-epi-scopadulin
(500 MHz, pyridine-d5)
ppm