

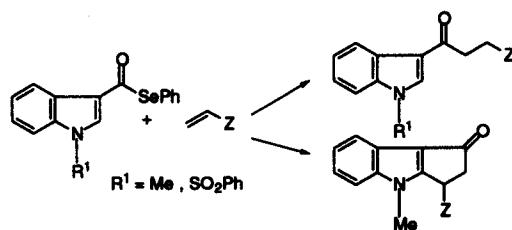
SUPPORTING INFORMATION

Supporting Information:

Generation and Intermolecular Reactions of 3-Indolylacyl Radicals

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General Procedure for the Preparation of Phenyl Selenoesters 2. A suspension of 1-methyl-¹ or 1-(phenylsulfonyl)-3-indolecarboxylic acid² (6 mmol) in anhydrous CH₂Cl₂ (15 mL) was treated with a solution of Et₃N (6 mmol) in CH₂Cl₂ (5 mL). After 10 min at rt, the mixture was concentrated under reduced pressure to give the corresponding triethylammonium salt.

Tributylphosphine (9 mmol) was added under Ar to a solution of PhSeCl (9 mmol) in anhydrous THF (20 mL). After 10 min at rt, a solution of the above triethylammonium salt in THF (15 mL) was added, and the mixture was stirred for 4 h. The reaction mixture was partitioned between Et₂O (50 mL) and H₂O (50 mL), and extracted with Et₂O (3 x 30 mL). The organic extracts were concentrated, and the resulting crude product was purified by flash chromatography (1:1 hexanes-AcOEt).

Se-Phenyl 1-Methyl-3-indolecarboselenoate (2a): 70%; mp 108-110 °C; ¹H NMR (200 MHz) δ 3.82 (s, 3H), 7.30 (m, 3H), 7.40 (m, 3H), 7.62 (m, 2H), 7.90 (s, 1H), 8.20 (m, 1H); ¹³C NMR (50.3 MHz) δ 33.8 (CH₃), 109.9 (CH), 116.9 (C), 121.9 (CH), 123.0 (CH), 123.7 (CH), 125.1 (C), 126.2 (C), 128.6 (CH), 129.2 (CH), 135.6 (CH), 136.4 (CH), 137.4 (C), 182.9 (C).

Se-Phenyl 1-(Phenylsulfonyl)-3-indolecarboselenoate (2b): 90%; ¹H NMR (200 MHz) δ 7.25-7.60 (m, 10H), 7.97 (m, 3H), 8.15 (m, 1H), 8.44 (s, 1H); ¹³C NMR (50.3 MHz) δ 113.2 (CH), 122.3 (CH), 122.6 (C), 125.1 (CH), 125.3 (C), 126.1 (CH), 126.3 (C), 127.2 (CH), 129.1 (CH), 129.4 (CH), 129.7 (CH), 131.7 (CH), 134.7 (CH), 134.8 (C), 136.3 (CH), 137.3(C), 185.1 (C).

4-(1-Methyl-3-indolyl)-4-oxobutanenitrile (4): 7:3 hexanes-AcOEt; mp 96-98 °C; ¹H NMR (200 MHz) δ 2.81 (t, *J* = 8 Hz, 2H), 3.26 (t, *J* = 8 Hz, 2H), 3.88 (s, 3H), 7.35 (m, 3H), 7.76 (s, 1H), 8.35 (m, 1H); ¹³C NMR (50.3 MHz) δ 12.0 (CH₂), 33.7 (CH₃), 34.8 (CH₂), 109.8 (CH), 115.3 (C), 119.7 (C), 122.3 (CH), 122.9 (CH), 123.6 (CH), 126.0 (C), 135.3 (CH), 137.4 (C), 189.7 (C); HRMS calcd for C₁₃H₁₂N₂O 212.0949, found 212.0942.

Dimethyl 2-(1-Methyl-3-indolylcarbonylmethyl)pentanedioate (6): 7:3 hexanes-AcOEt; ¹H NMR (200 MHz) δ 1.97 (m, 2H), 2.39 (m, 2H), 2.95 (dd, *J* = 5, 15.8 Hz, 1H), 3.16 (m, 1H), 3.33 (dd, *J* = 8.4, 15.9 Hz, 1H), 3.66 (s, 3H), 3.69 (s, 3H), 3.80 (s,

3H), 7.30 (m, 3H), 7.73 (s, 1H), 8.38 (m, 1H); HRMS calcd for C₁₈H₂₁NO₅ 331.1420, found 331.1428.

2-(1-Methyl-3-indolylcarbonylmethyl)pentanedinitrile (7): 3:7 hexanes-AcOEt; mp 144-146 °C; ¹H NMR (200 MHz) δ 2.12 (m, 2H), 2.65 (m, 2H), 3.21 (dd, J = 8.2, 16.5 Hz, 1H), 3.36 (dd, J = 5.6, 16.5 Hz, 1H), 3.52 (m, 1H), 3.89 (s, 3H), 7.37 (m, 3H), 7.76 (s, 1H), 8.32 (m, 1H); ¹³C NMR (50.3 MHz) δ 15.3 (CH₂), 26.0 (CH), 27.8 (CH₂), 33.7 (CH₃), 40.5 (CH₂), 109.9 (CH), 115.4 (C), 118.1 (C), 120.3 (C), 122.1 (CH), 123.1 (CH), 123.8 (CH), 125.9 (C), 135.9 (CH), 137.5 (C), 188.8 (C); HRMS calcd for C₁₆H₁₃N₃O 265.1215, found 265.1209.

Methyl 3-Methyl-4-(1-methyl-3-indolyl)-4-oxobutanoate (9): 1:1 hexanes-AcOEt; ¹H NMR (200 MHz) δ 1.28 (d, J = 7 Hz, 3H), 2.45 (dd, J = 6, 16.4 Hz, 1H), 2.98 (dd, J = 8.2, 16.4 Hz, 1H), 3.64 (s, 3H), 3.70 (m, 1H), 3.85 (s, 3H), 7.30 (m, 3H), 7.83 (s, 1H), 8.40 (m, 1H); ¹³C NMR (50.3 MHz) δ 18.9 (CH₃), 33.6 (CH₃), 37.4 (CH₂), 38.9 (CH), 51.7 (CH₃), 109.6 (CH), 114.9 (C), 122.5 (CH), 122.6 (CH), 123.3 (CH), 126.6 (C), 135.6 (CH), 137.5 (C), 173.1 (C), 197.5 (C); HRMS calcd for C₁₅H₁₇NO₃ 257.1208, found 257.1204.

Methyl 2-(1-Methyl-3-indolylcarbonyl)cyclohexanecarboxylate (10): 3:1 Mixture of cis/trans stereoisomers; 7:3 hexanes-AcOEt. Major *cis* isomer: ¹H NMR (200 MHz) δ 1.40-1.60 (m, 3H), 1.80-1.95 (m, 3H), 2.20-2.40 (m, 2H), 2.68 (ddd, J = 4.4, 4.6, 9.8 Hz, 1H, 1-Hax), 3.61 (s, 3H), 3.73 (q, J = 5.6 Hz, 1H, 2-Heq), 3.82 (s, 3H), 7.30 (m, 3H), 7.72 (s, 1H), 8.33 (m, 1H); ¹³C NMR (50.3 MHz) δ 22.8 (CH₂), 24.5 (CH₂), 25.8 (CH₂), 29.1 (CH₂), 33.4 (CH₃), 43.1 (CH), 45.8 (CH), 51.5 (CH₃), 109.6 (CH), 115.2 (C), 122.4 (CH), 122.6 (CH), 123.0 (CH), 126.5 (C), 135.0 (CH), 137.2 (C), 174.9 (C), 197.3 (C); HRMS calcd for C₁₈H₂₁NO₃ 299.1521, found 299.1509.

4-(1-Methyl-3-indolylcarbonyl)-1-(*p*-toluenesulfonyl)-2-piperidone (12): AcOEt; mp 168-170 °C; ¹H NMR (300 MHz) δ 2.20 (m, 2H), 2.44 (s, 3H), 2.55 (ddd, J = 1.2, 5.7, 17.4 Hz, 1H), 2.80 (dd, J = 9, 17.5 Hz, 1H), 3.56 (dd, J = 5.4, 5.6, 8.8, 9 Hz, 1H), 3.85 (s, 3H), 3.98 (m, 2H), 7.32 (m, 5H), 7.76 (s, 1H), 7.92 (d, J = 8.4 Hz, 2H), 8.32 (m, 1H); ¹³C NMR (75.4 MHz) δ 21.7 (CH₃), 27.3 (CH₂), 33.7 (CH₃), 36.5 (CH₂), 40.6

(CH), 45.0 (CH₂), 109.8 (CH), 114.3 (C), 122.3 (CH), 122.9 (CH), 123.7 (CH), 126.2 (C), 128.5 (CH), 129.3 (CH), 135.4 (CH), 135.8 (C), 137.5 (C), 144.7 (C), 169.6 (C), 193.7 (C). Anal. Calcd for C₂₂H₂₃N₂O₄·1/2H₂O: C, 62.84; H, 5.75; N, 6.66; S, 7.62. Found: C, 63.11; H, 5.40; N, 6.48; S, 7.31.

(1-Methyl-3-indolyl) (2-Phenylethyl) Ketone (15): 7:3 hexanes-AcOEt; ¹H NMR (200 MHz) δ 3.14 (m, 4H), 3.83 (s, 3H), 7.20-7.35 (m, 8H), 7.67 (s, 1H), 8.40 (m, 1H); ¹³C NMR (75.4 MHz) δ 30.7 (CH₂), 33.3 (CH₃), 41.5 (CH₂), 109.5 (CH), 116.1 (C), 122.4 (2CH), 123.1 (CH), 125.8 (CH), 126.1 (C), 128.2 (CH), 128.3 (CH), 135.2 (CH), 137.2 (C), 141.6 (C), 194.2 (C); HRMS calcd for C₁₈H₁₇NO 263.1310, found 263.1313.

1-Methyl-3-indolyl Octyl Ketone (16): 9:1 hexanes-AcOEt; ¹H NMR (300 MHz) δ 0.88 (t, *J* = 6.6 Hz, 3H), 1.27 (m, 10H), 1.77 (m, 2H), 2.83 (t, *J* = 6.6 Hz, 2H), 3.84 (s, 3H), 7.30 (m, 3H), 7.71 (s, 1H), 8.40 (m, 1H); ¹³C NMR (75.4 MHz) δ 14.1 (CH₃), 22.7 (CH₂), 25.3 (CH₂), 29.2 (CH₂), 29.5 (CH₂), 29.6 (CH₂), 31.9 (CH₂), 33.5 (CH₃), 41.0 (CH₂), 109.5 (CH), 116.6 (C), 122.4 (CH), 122.6 (CH), 123.2 (CH), 126.3 (C), 135.1 (CH), 137.4 (C), 196.0 (C).

3-(1-Methyl-3-indolyl)-3-oxopropyl Acetate (17): 1:1 hexanes-AcOEt; ¹H NMR (200 MHz) δ 2.03 (s, 3H), 3.19 (t, *J* = 6.6 Hz, 2H), 3.87 (s, 3H), 4.55 (t, *J* = 6.6 Hz, 2H), 7.35 (m, 3H), 7.77 (s, 1H), 8.40 (m, 1H); ¹³C NMR (100.6 MHz) δ 21.0 (CH₃), 33.6 (CH₃), 35.5 (CH₂), 60.4 (CH₃), 109.6 (CH), 116.6 (C), 122.6 (CH), 122.8 (CH), 123.6 (CH), 126.2 (C), 135.6 (CH), 137.5 (C), 171.2 (C), 191.7 (C).

Methyl 4-[(1-Phenylsulfonyl)-3-indolyl]-4-oxobutanoate (18): 8:2 hexanes-AcOEt; ¹H NMR (200 MHz) δ 2.79 (t, *J* = 6.6 Hz, 2H), 3.28 (t, *J* = 6.6 Hz, 2H), 3.71 (s, 3H), 7.35 (m, 2H), 7.50-7.60 (m, 3H), 7.95 (m, 3H), 8.30 (m, 1H), 8.31 (s, 1H); ¹³C NMR (50.3 MHz) δ 27.8 (CH₂), 34.6 (CH₂), 52.0 (CH₃), 113.0 (CH), 120.8 (C), 123.0 (CH), 124.9 (CH), 125.8 (CH), 127.0 (CH), 127.4 (C), 129.6 (CH), 131.8 (CH), 134.6 (CH), 134.7 (C), 137.3 (C), 173.3 (C), 193.6 (C); HRMS calcd for C₁₉H₁₇NO₅S 371.0827, found 371.0824.

3-[1-(Phenylsulfonyl)-3-indolylcarbonyl]cyclohexanone (19): 7:3 hexanes-AcOEt; mp 123-125 °C; ¹H NMR (300 MHz) δ 1.90 (m, 2H), 2.15 (m, 2H), 2.44 (m, 2H), 2.48 (dd, *J* = 4.2, 15.9 Hz, 1H), 2.78 (dd, *J* = 10.8, 14.7 Hz, 1H), 3.65 (m, 1H), 7.35 (m, 2H), 7.51 (m, 2H), 7.62 (m, 1H), 7.95 (m, 3H), 8.27 (s, 1H), 8.34 (d, *J* = 7.5 Hz, 1H); ¹³C NMR (75.4 MHz) δ 24.8 (CH₂), 28.9 (CH₂), 40.9 (CH₂), 43.1 (CH₂), 47.2 (CH), 112.9 (CH), 119.5 (C), 123.1 (CH), 125.0 (CH), 126.0 (CH), 127.0 (CH), 127.6 (C), 129.6 (CH), 131.5 (CH), 134.6 (CH), 134.9 (C), 137.2 (C), 196.1 (C), 210.1 (C). Anal. Calcd for C₂₁H₁₉NO₄S·1/2H₂O: C, 64.60; H, 5.16; N, 3.59; S, 8.21. Found: C, 64.56; H, 5.00; N, 3.88; S, 8.00.

Trans-1,3-bis(Benzoyloxycarbonyl)-4-[1-(phenylsulfonyl)-3-indolylcarbonyl]-2-piperidone (20): 7:3 hexanes-AcOEt; ¹H NMR (400 MHz) δ 2.03 (m, 1H), 2.32 (m, 1H), 3.73 (m, 1H), 4.05 (m, 1H), 4.09 (m, 1H), 4.18 (d, *J* = 10 Hz, 1H), 5.17 and 5.16 (2 d, *J* = 12.4 Hz, 2H), 5.32 (s, 2H), 7.20-7.60 (m, 15H), 7.96 (m, 3H), 8.26 (d, *J* = 7.2 Hz, 1H), 8.27 (s, 1H); ¹³C NMR (100.6 MHz) δ 26.2 (CH₂), 43.7 (CH), 43.8 (CH₂), 52.4 (CH), 67.5 (CH₂), 69.0 (CH₂), 113.1 (CH), 119.2 (C), 123.1 (CH), 125.2 (CH), 126.2 (CH), 127.2 (CH), 127.5 (C), 127.9-128.6 (6 CH), 129.7 (CH), 132.6 (CH), 134.7 (CH), 134.9 (C), 135.0 (C), 135.1 (C), 137.3 (C), 153.3 (C), 167.0 (C), 168.4 (C), 194.1 (C).

2,4-Dimethyl-1-oxocyclopenta[b]indole-3-carbonitrile (22): 1:1 mixture of stereoisomers; 1:1 hexanes-AcOEt. *Cis* isomer: ¹H NMR (200 MHz) δ 1.53 (d, *J* = 7.2 Hz, 3H), 3.36 (dd, *J* = 7.6 Hz, 1H), 3.92 (s, 3H), 4.52 (d, *J* = 7 Hz, 1H), 7.25-7.40 (m, 3H), 7.95 (d, *J* = 7.4 Hz, 1H). *Trans* isomer: ¹H NMR (200 MHz) δ 1.59 (d, *J* = 7.6 Hz, 3H), 3.41 (qd, *J* = 3.6, 6.5 Hz, 1H), 3.88 (m, 1H), 3.92 (s, 3H), 7.25-7.40 (m, 3H), 7.95 (d, *J* = 7.4 Hz, 1H).

3-Hexyl-4-methylcyclopenta[b]indol-1-one (23): 1:1 hexanes-AcOEt; ¹H NMR (200 MHz) δ 0.88 (t, *J* = 6.6 Hz, 3H), 1.28 (m, 8H), 1.60 (m, 1H), 1.95 (m, 1H), 2.65 (dd, *J* = 2, 17.6 Hz, 1H), 3.13 (dd, *J* = 6.6, 17.8 Hz, 1H), 3.41 (m, 1H), 3.78 (s, 3H), 7.25-7.30 (m, 3H), 7.94 (m, 1H); ¹³C NMR (75.4 MHz) δ 14.1 (CH₃), 22.6 (CH₂), 27.0 (CH₂), 29.3 (CH₂), 31.0 (CH₃), 31.6 (CH₂), 33.8 (CH₂), 34.0 (CH), 47.8 (CH₂), 109.8 (CH), 119.3 (C), 121.1 (CH), 121.2 (C), 122.3 (CH), 123.3 (CH), 143.1 (C), 170.1 (C), 194.7 (C).

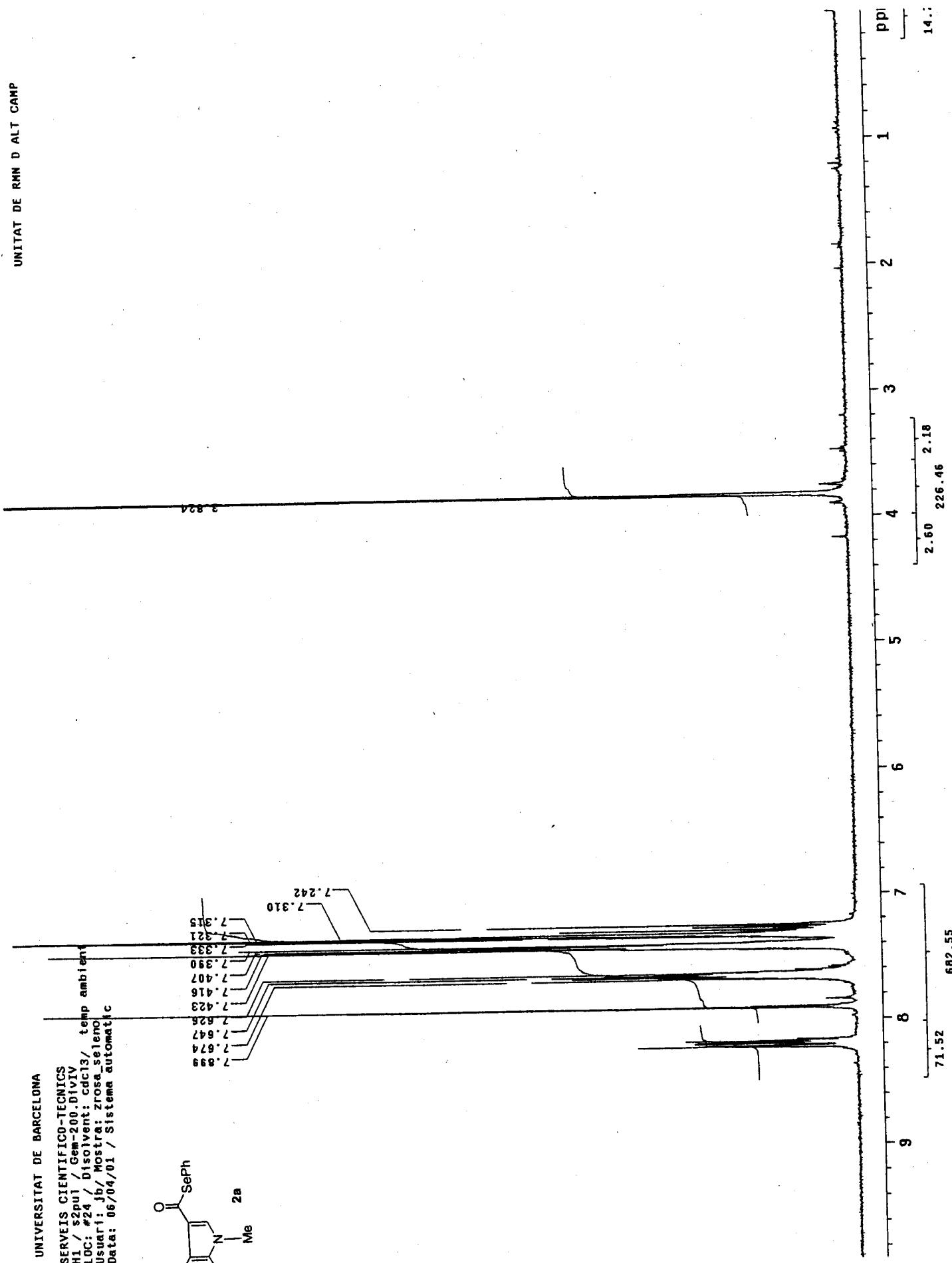
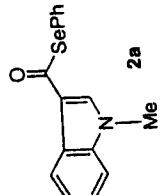
3-Acetoxy-4-methylcyclopenta[*b*]indol-1-one (24): 7:3 hexanes-AcOEt; ^1H NMR (400 MHz) δ 2.17 (s, 3H), 2.85 (dd, J = 1.8, 18 Hz, 1H), 3.51 (dd, J = 6.2, 18 Hz, 1H), 3.79 (s, 3H), 6.39 (dd, J = 1.8, 6.2 Hz, 1H), 7.35 (m, 1H), 7.40 (m, 2H), 7.97 (dt, J = 1.5, 7 Hz, 1H); ^{13}C NMR (100.6 MHz) δ 21.1 (CH₃), 31.2 (CH₃), 49.5 (CH₂), 64.9 (CH), 110.7 (CH), 120.9 (C), 121.9 (C), 122.0 (CH), 123.1 (CH), 124.9 (CH), 143.8 (C), 161.5 (C), 170.7 (C), 191.3 (C).

6,8-Diacetoxy-5-methylcyclohepta[*b*]indol-10-one (25). Major *trans* isomer: 7:3 hexanes-AcOEt; ^1H NMR (200 MHz) δ 2.05 (s, 3H), 2.17 (s, 3H), 2.34 (ddd, J = 2.4, 8.8, 15 Hz, 1H), 2.83 (dddd, J = 1.8, 3.7, 5.1, 15 Hz, 1H), 3.07 (dd, J = 9.4, 16.7 Hz, 1H), 3.39 (ddd, J = 1.6, 3.7, 16.5 Hz, 1H), 3.76 (s, 3H), 5.55 (tt, J = 3.6, 3.8, 9, 9.1 Hz, 1H), 6.42 (dd, J = 2.6, 5.2 Hz, 1H), 7.35 (m, 3H), 8.52 (m, 1H).

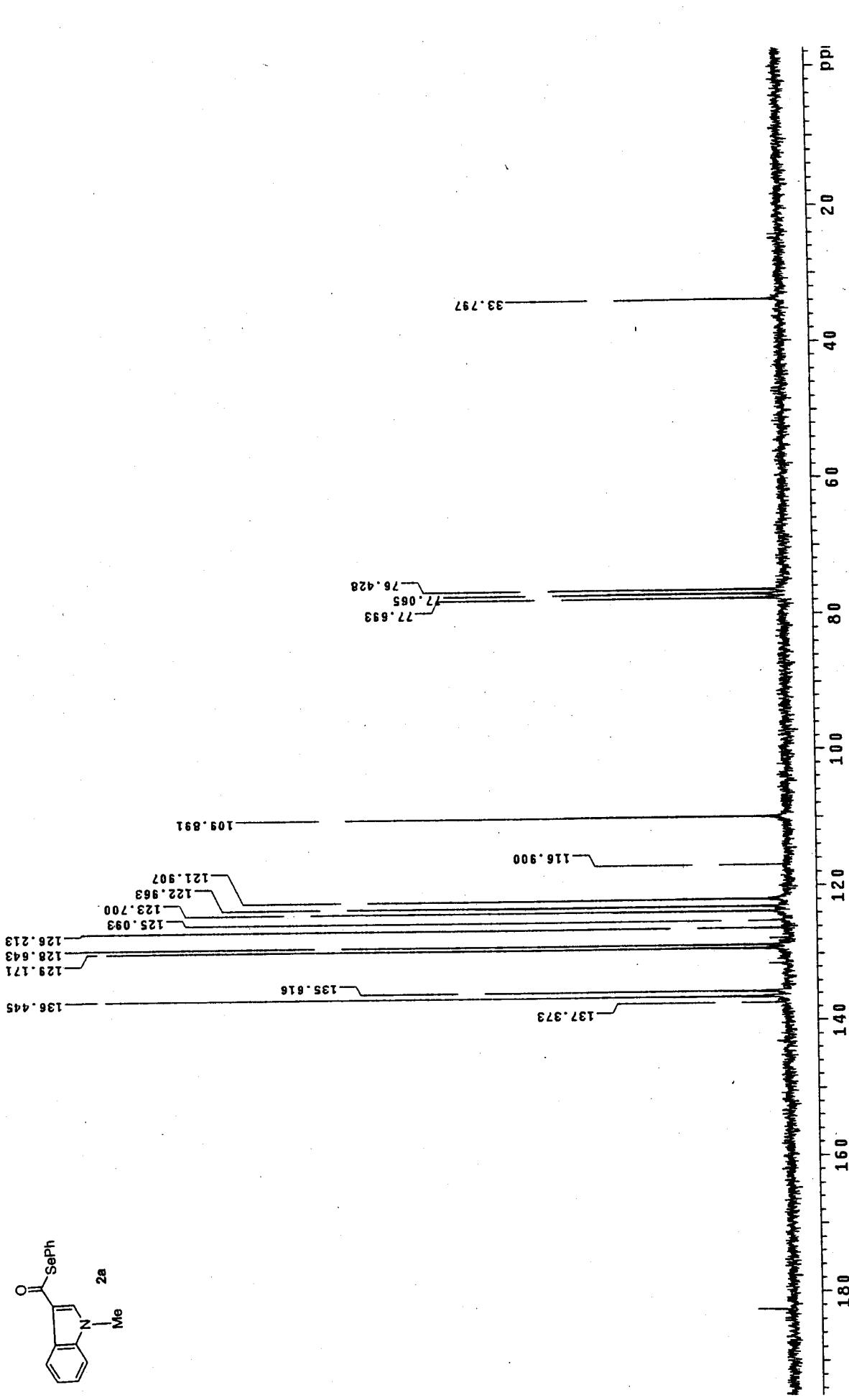
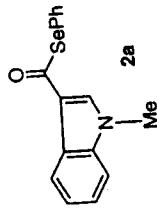
¹Hart, G.; Potts, K. T. *J. Org. Chem.* **1962**, *27*, 2940-2942.

²Mouaddib, A.; Joseph, B.; Hasnaoui, A.; Mérour, J.-Y. *Synthesis* **2000**, 549-556.

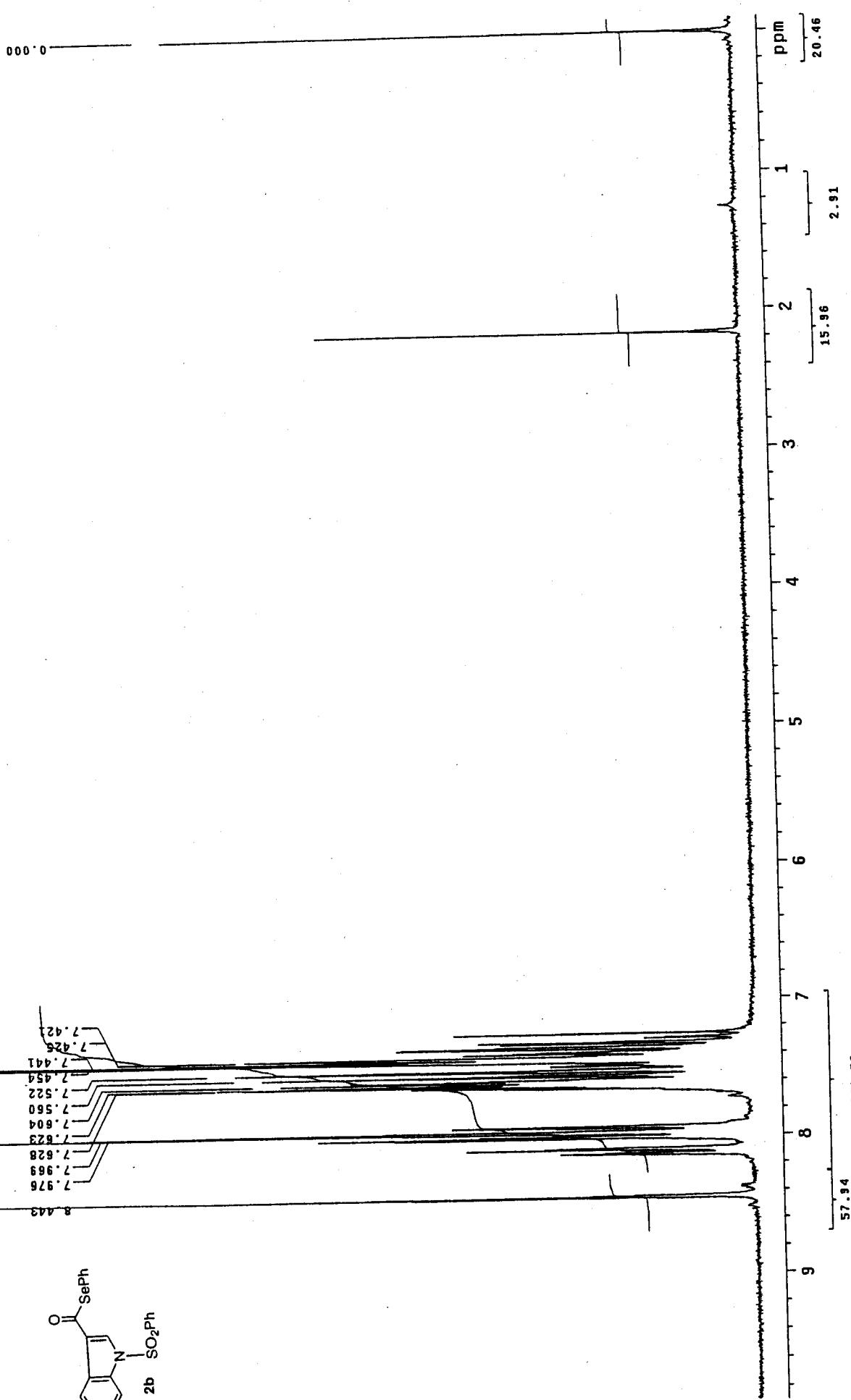
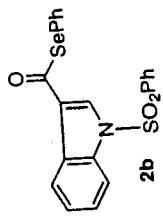
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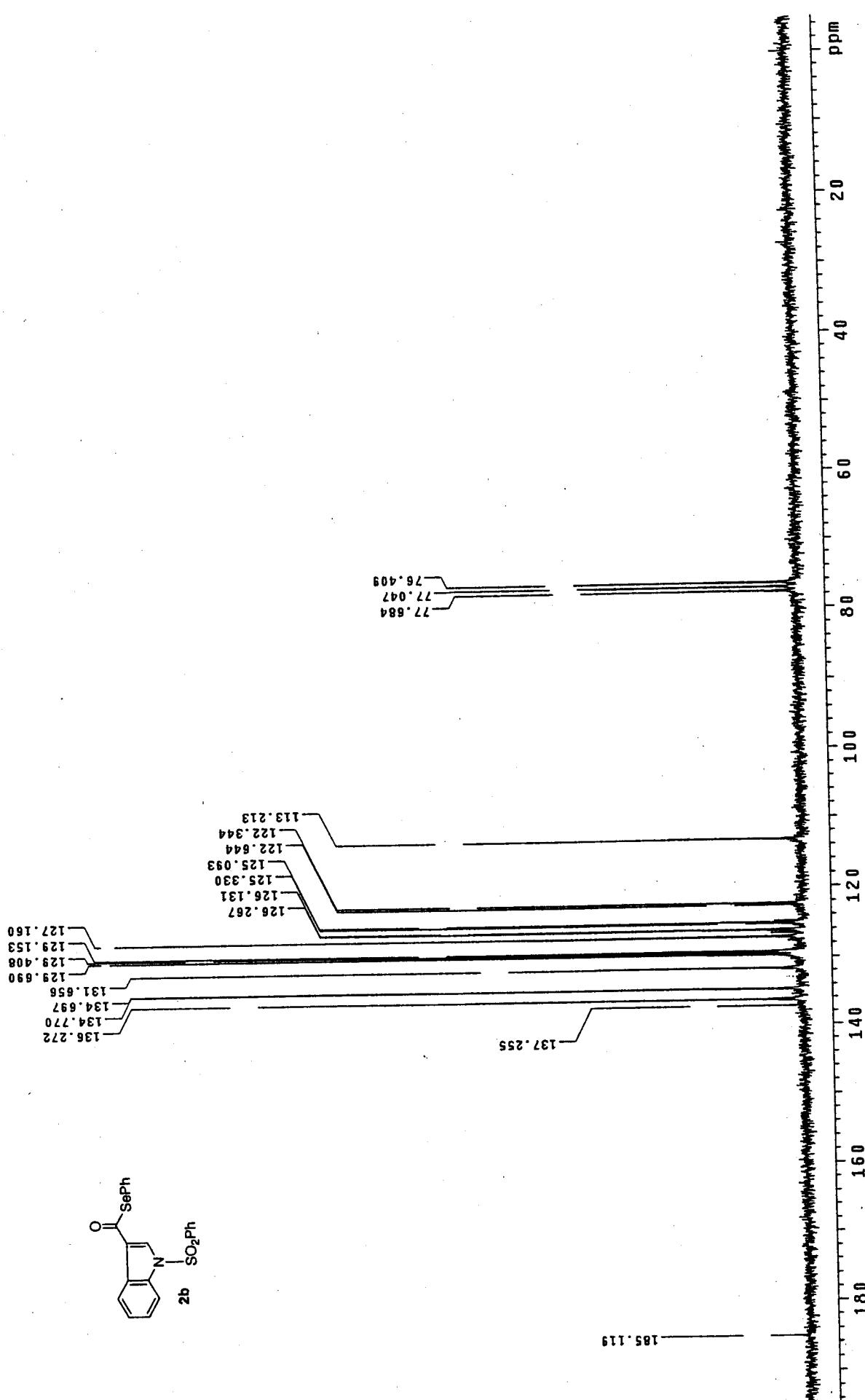
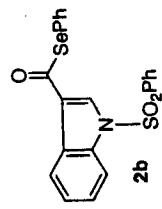
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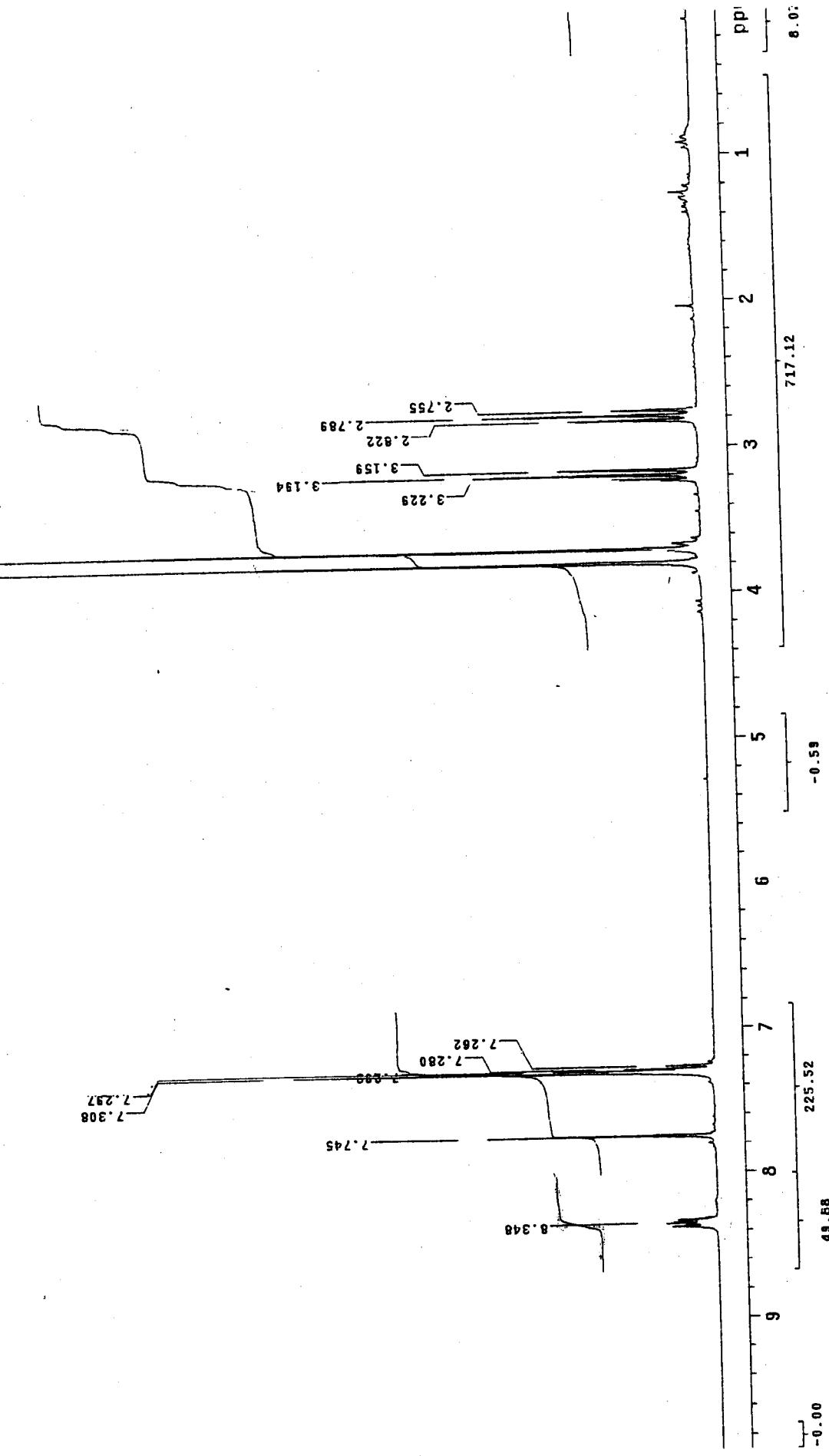
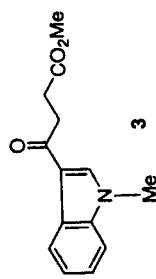


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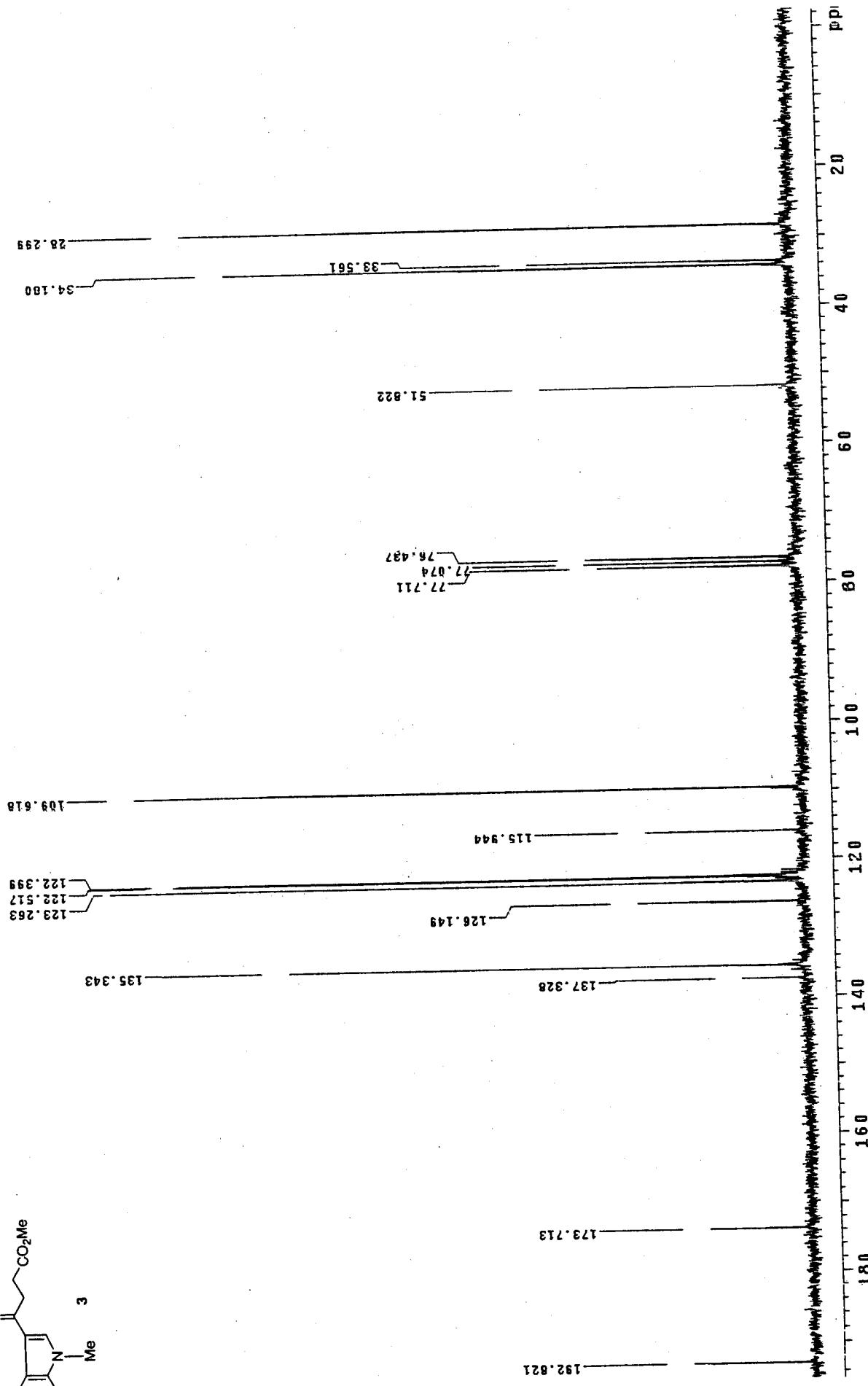
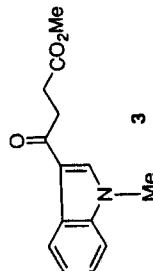


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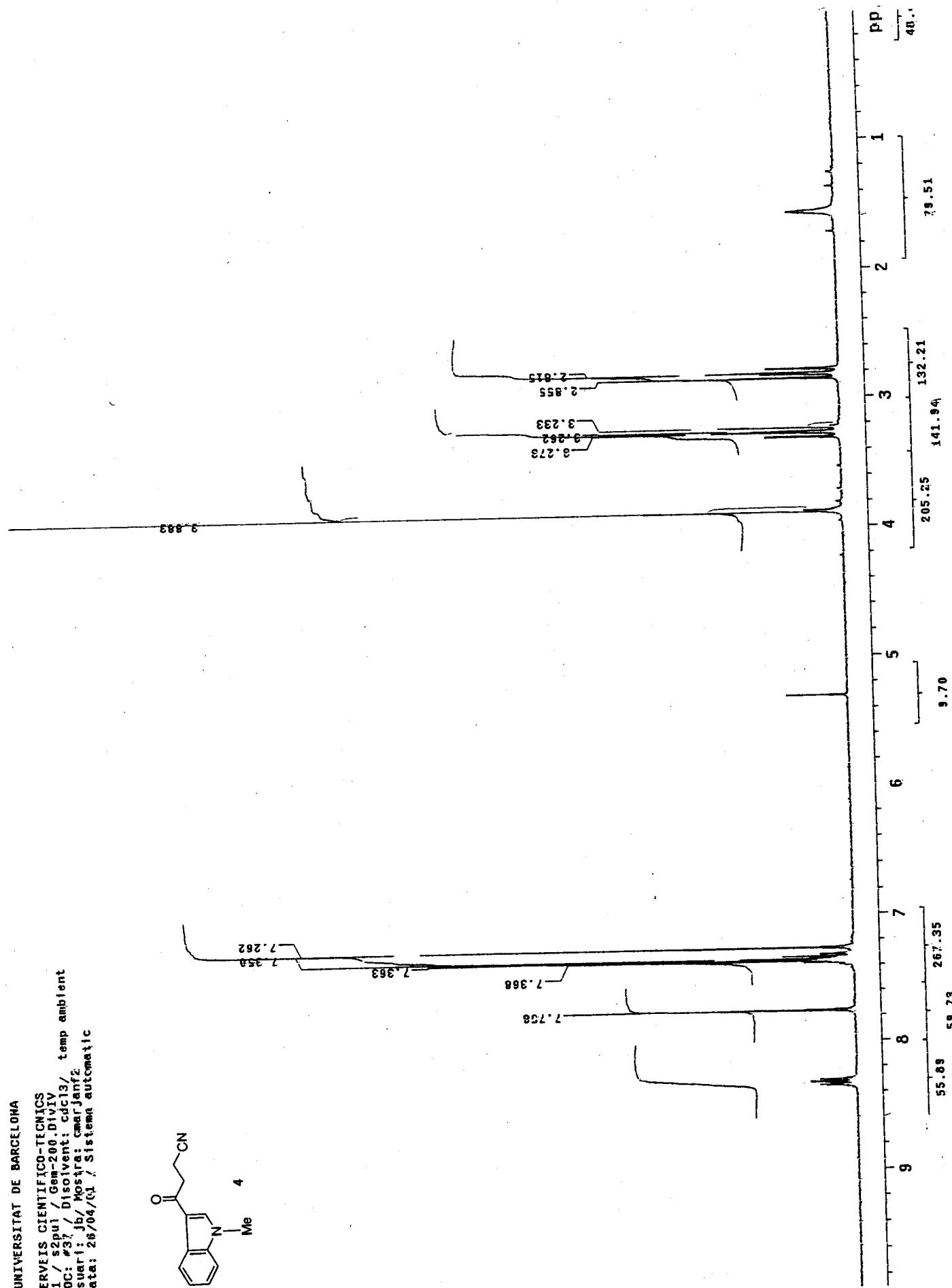
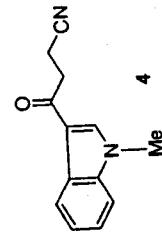
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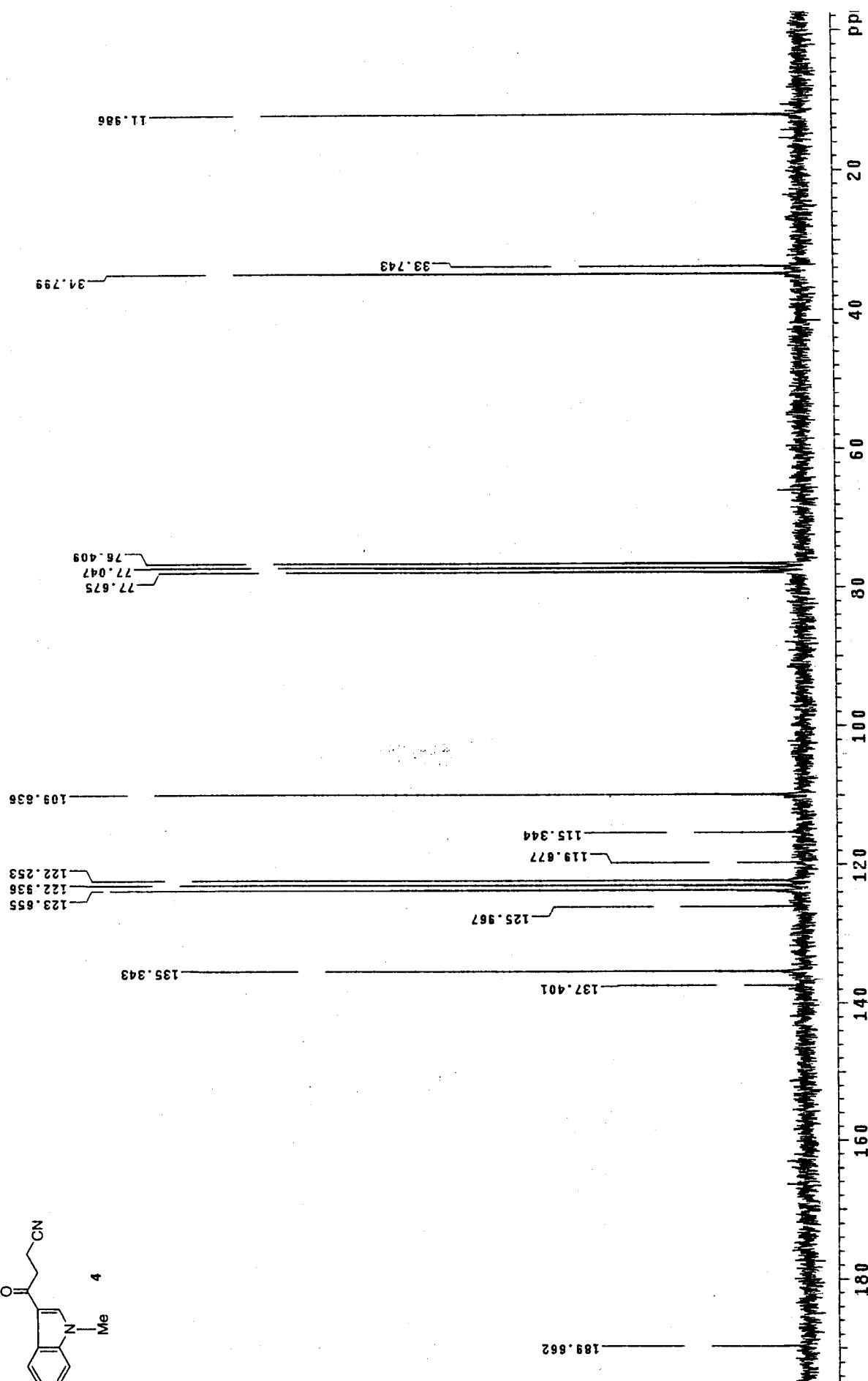
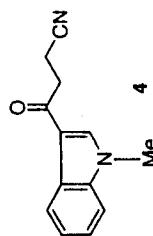
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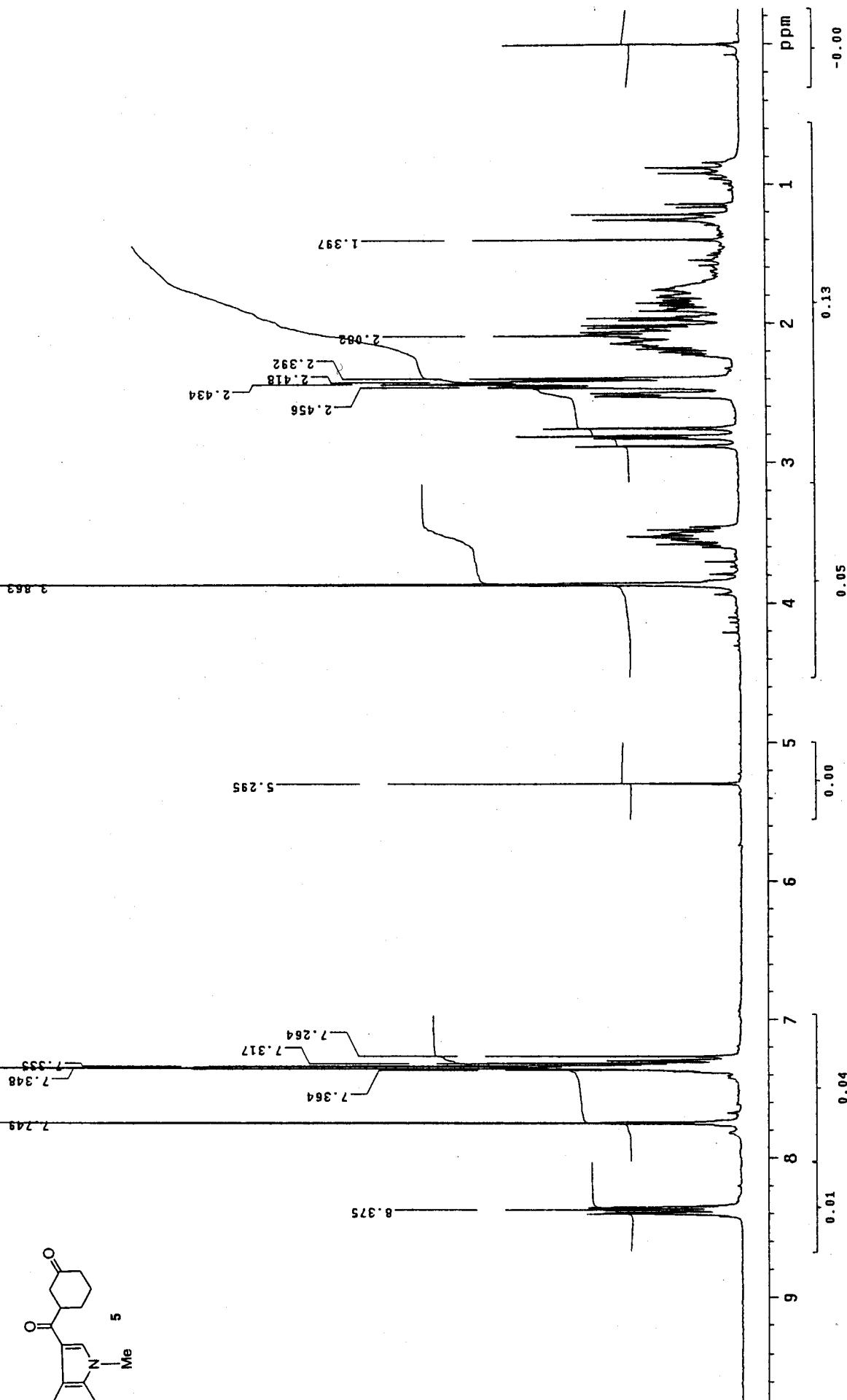
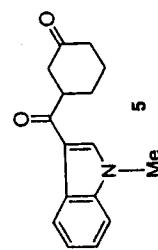
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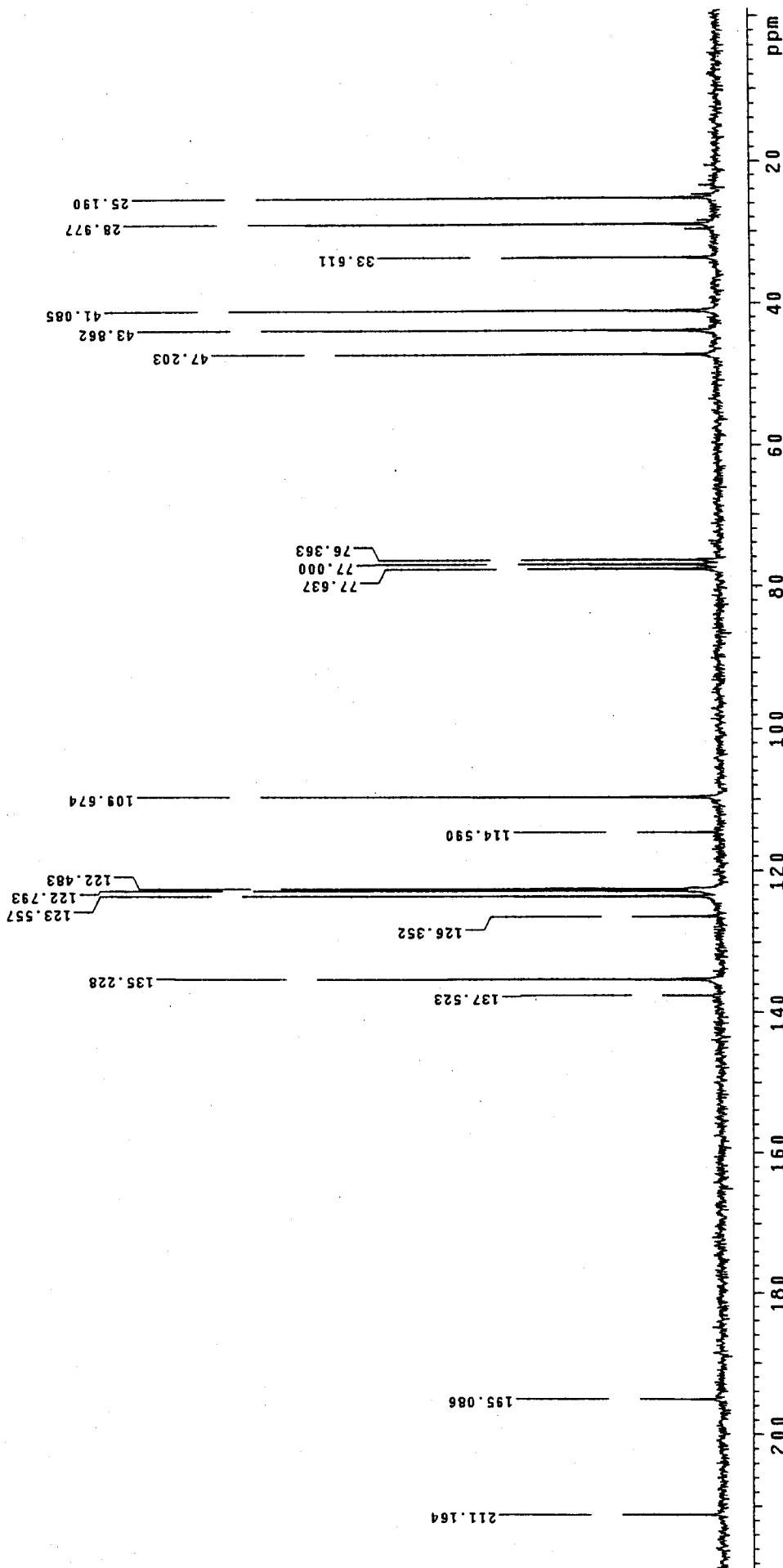
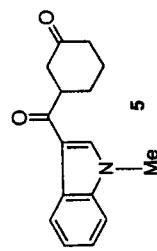
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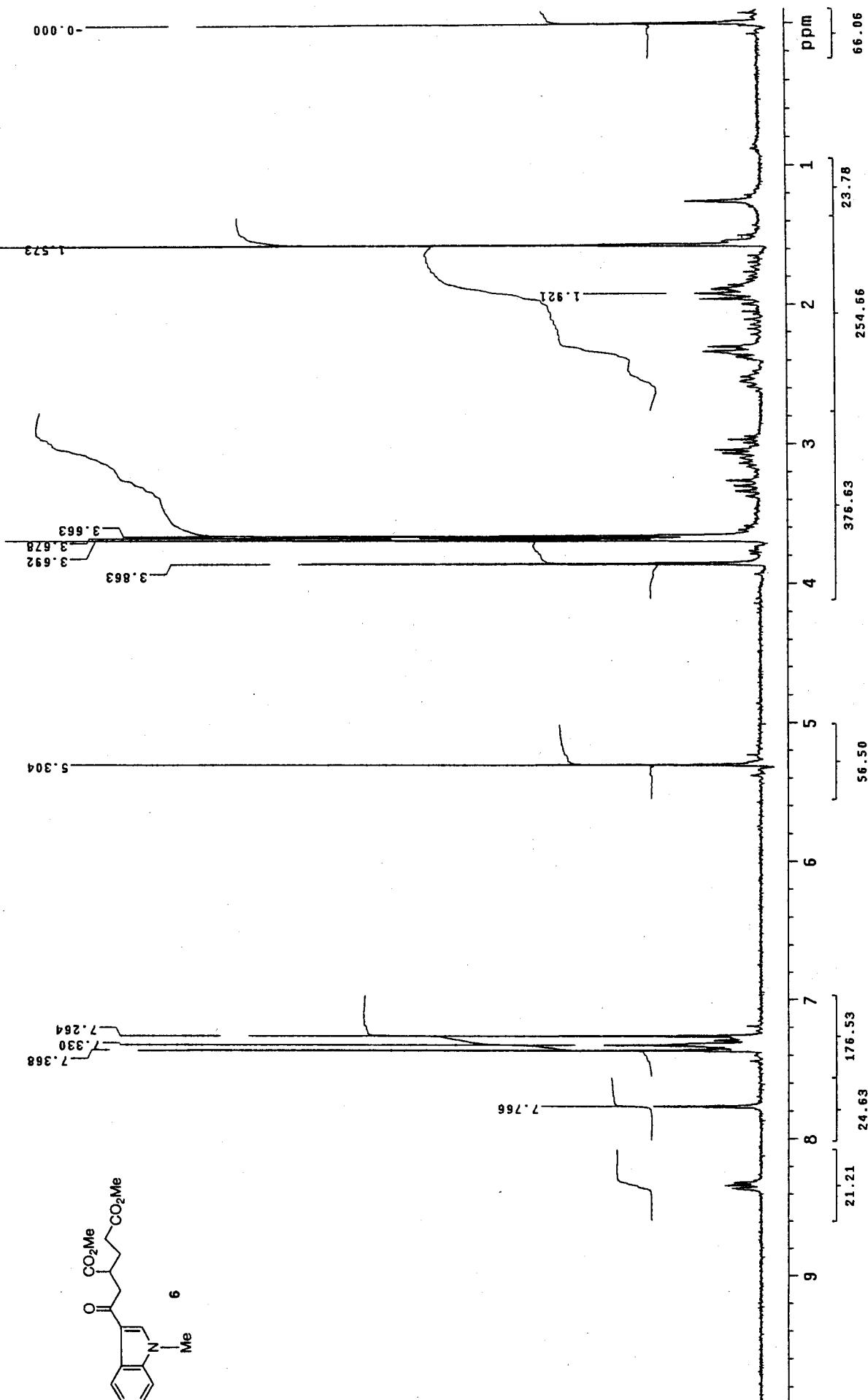
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Pulse Sequence: s2pul



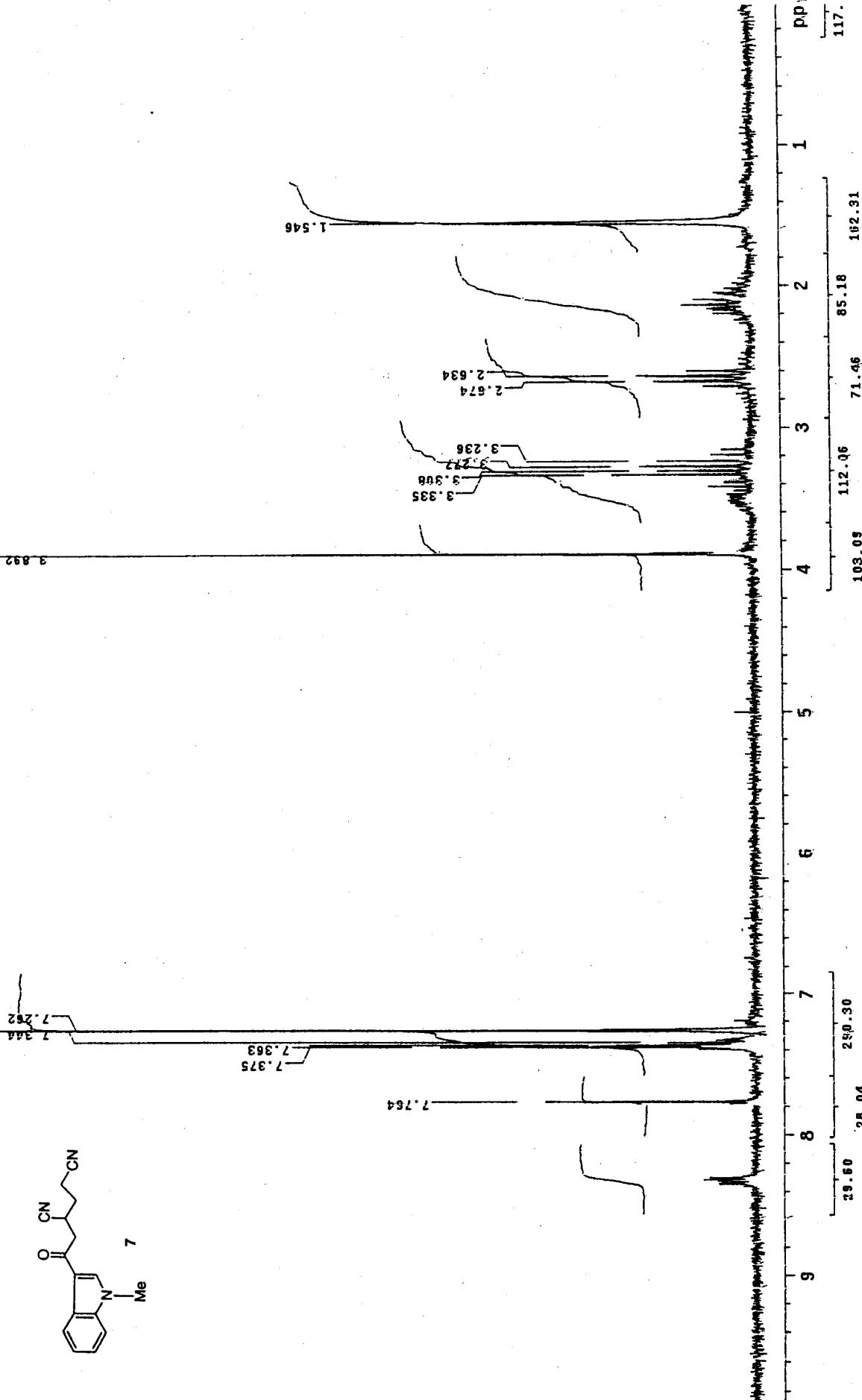
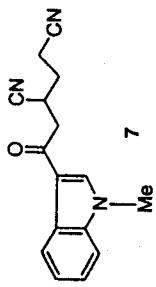
C13 / s2pu1 / Gem-200 DIVIV
LOC: #14 / Solvent: cdc13 / temp ambient
Usari: Jb/Mosra: cmarjanf3
Data: 09/05/01 / Sistema automatic
Pulse Sequence: s2pu1



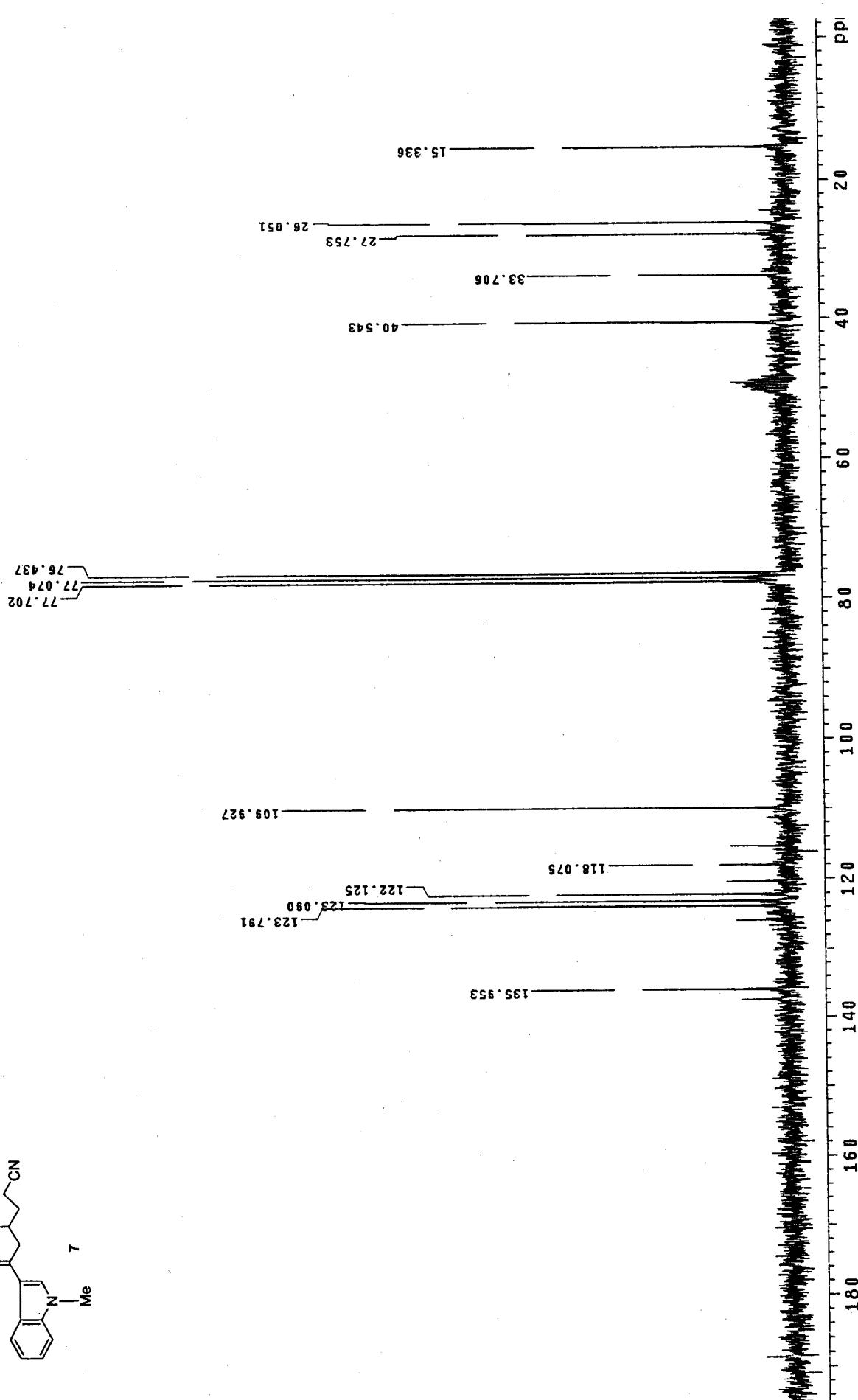
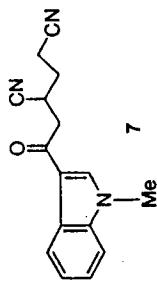
H1 / s2pul / Qem-200.D1\IV
LOC: # 5 / Disolvent: cdc13/ temp ambient
User: Jb/ Mostre: arosamar15rec
Data: 08/04/02 / Sistema automatic



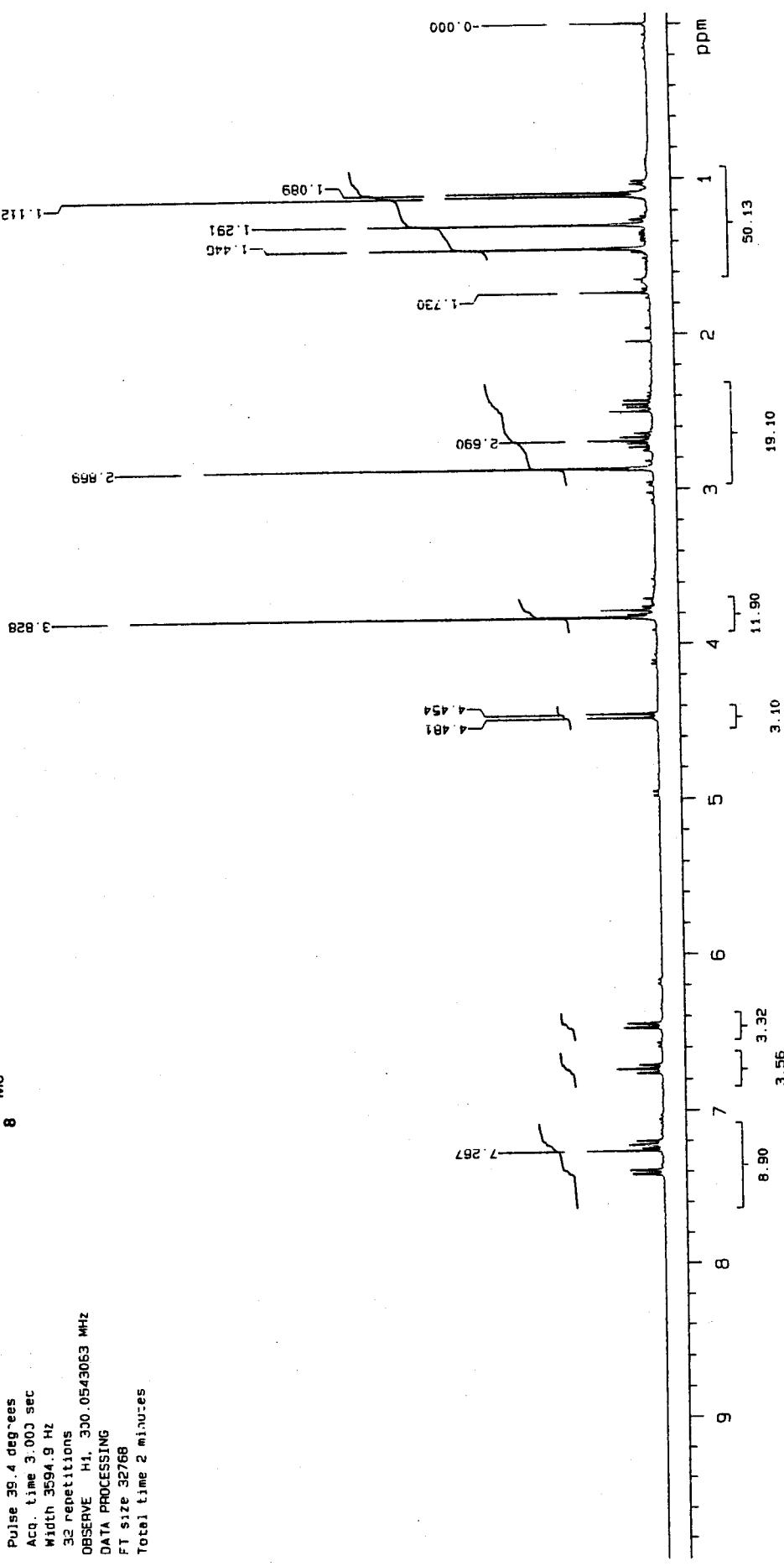
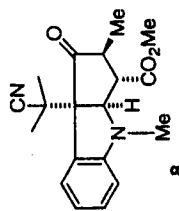
SERVEIS CIENTÍFICO-TÈCNICS
 H1 / s2pu1 / Gem-200 DIVIV
 LOC: #3b / Dissolvent: cdC13 / temp ambient
 Usuari: Jb / Mostra: dimarJanfS
 Data: 26/04/01 / Sistema automàtic



UNIVERSITAT DE BARCELONA
 SERVEIS CIENTÍFICO-TECNICS
 C13 / s2pu1 / Gem-200-DIV4V
 LOC: #30 / Dissolvent: cdcl3/
 Usuari: jb/ Mostre: dmarjanf3
 Data: 05/05/01 / Sistema automatic



H1 / SP2D1 / Gemini-300
 CDCl₃ / 29C / N reg: F0C32
 1b / RG49F1-2 / Rossa
 Date: 25/01/02 / Ope.: An8
 Solvent: CDCl₃
 Ambient temperature
 GEMINI-300 "29C"
 PULSE SEQUENCE
 Relax. delay 1.000 sec
 Pulse 39.4 degrees
 Acq. time 3.003 sec
 Width 3594.9 Hz
 32 repetitions
 OBSERVE H1, 330.0543063 MHz
 DATA PROCESSING
 FT size 32768
 Total time 2 minutes



13C / S2PUL / Gemini-30C
CDC13 / 29C / N reg: F0C32
Job / RG-S3F1-2 / Rosa
Date: 25/01/02 / Ope.: Ana

Solvent: CDCl₃

Ambient temperature
GEMINI-30 "zane"

PULSE SEQUENCE

Relax. delay 0.500 sec

Pulse 44.1 degrees

Acq. time 1.600 sec

Width 2000.0 Hz

1024 repetitions

OBSERVE C13, 75.4487066 MHz

DECOPPLE H1, 330.0556111 MHz

Power 30 dB

continuously

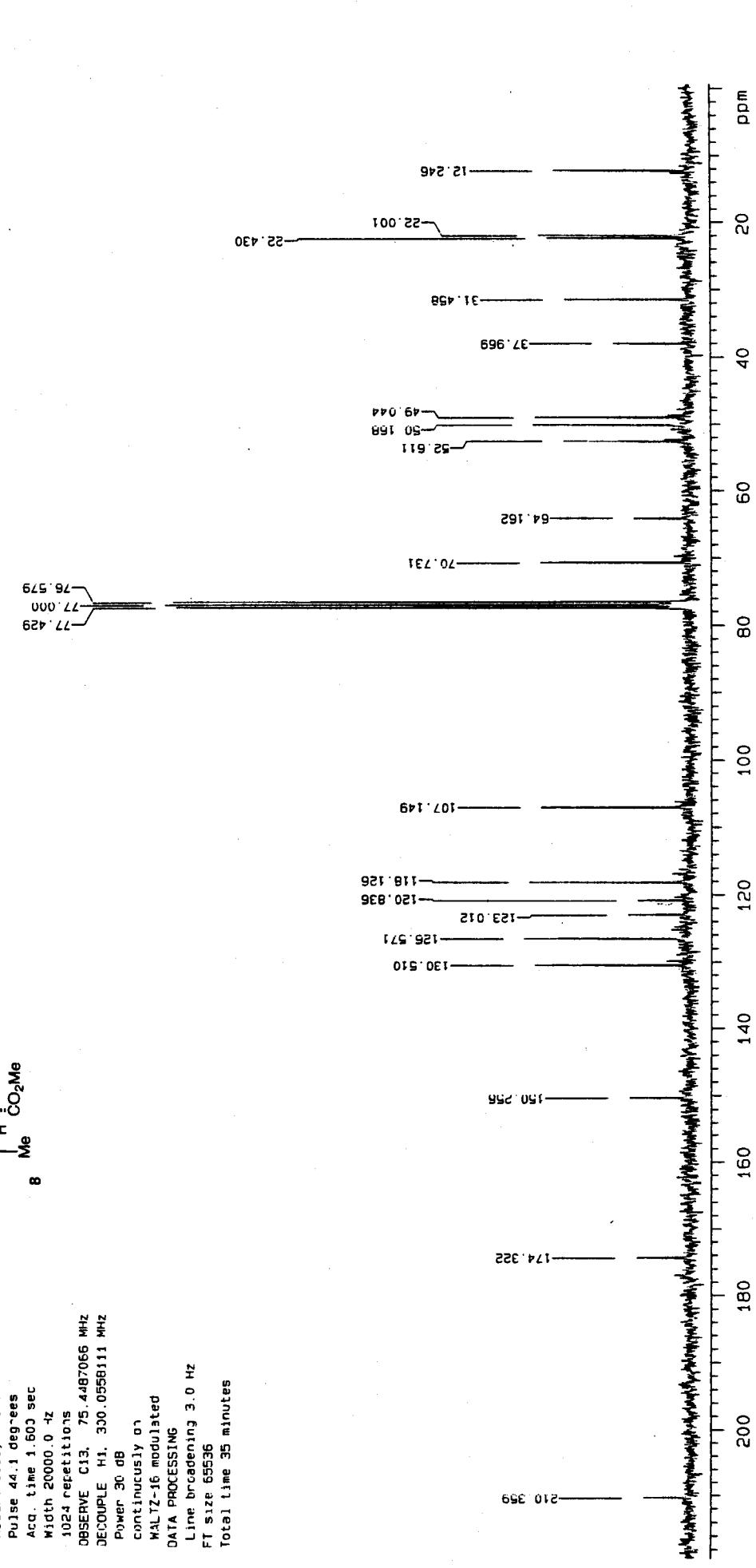
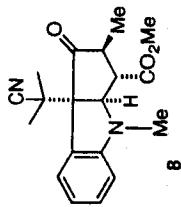
WALTZ-16 modulated

DATA PROCESSING

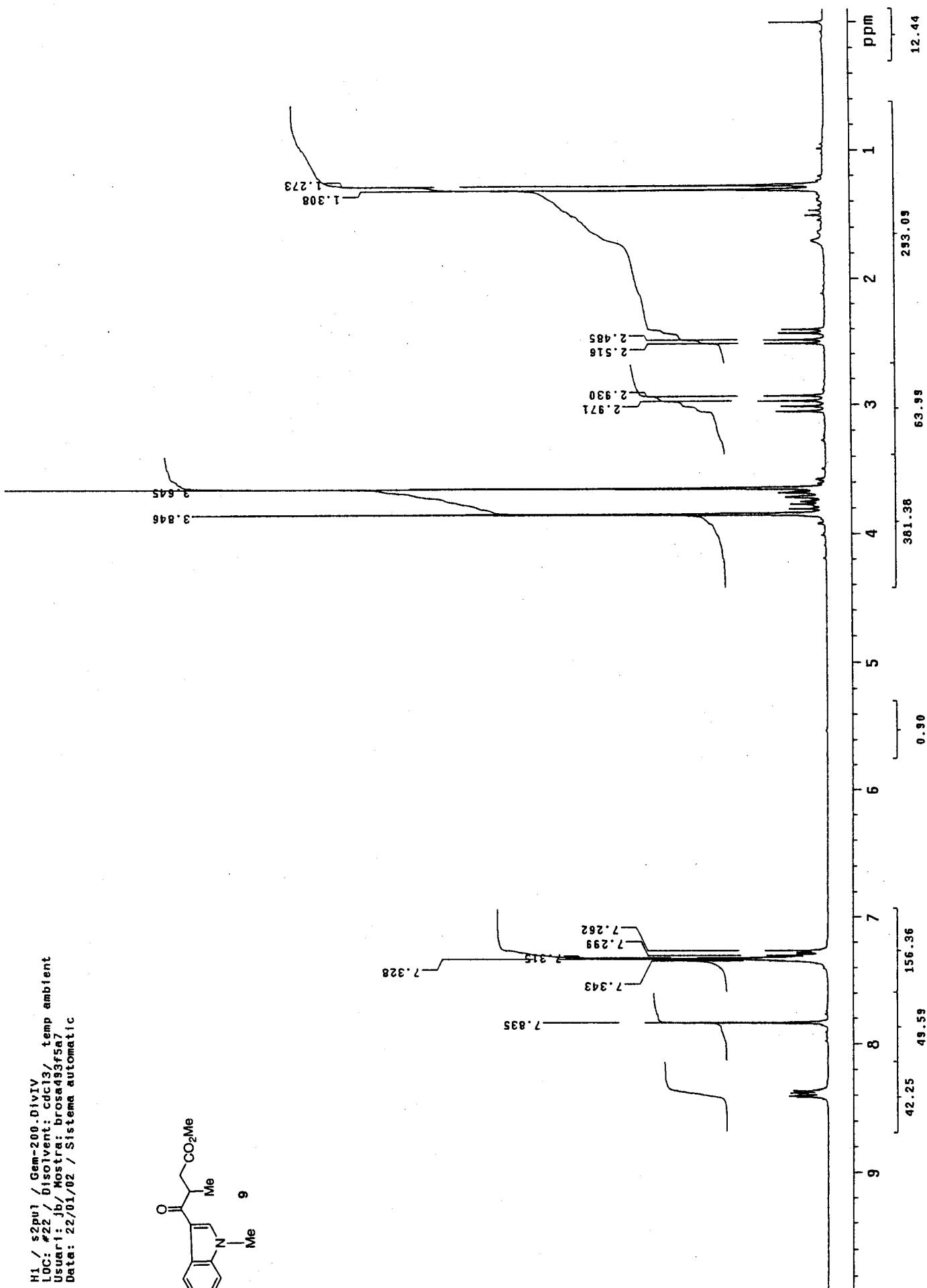
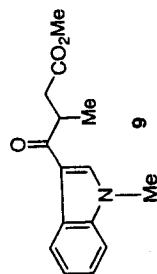
Line broadening 3.0 Hz

FT size 65536

Total time 35 minutes

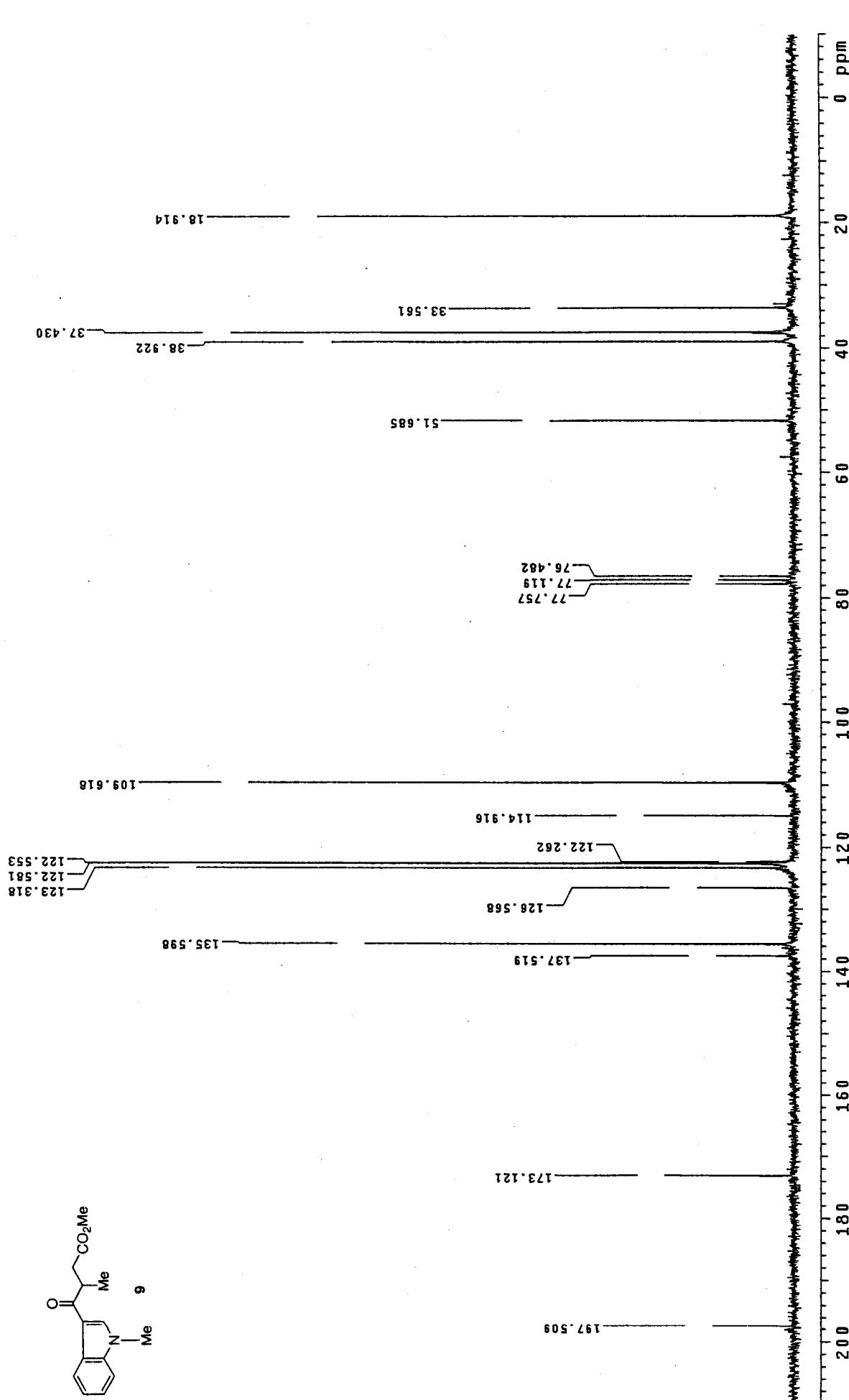
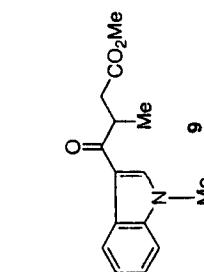


H1 / 52pu1 / Gem-200.DIVIV
LOC: #22 / Disolvent: cdc13 / temp ambient
User: jb / Mostra: brosa49ff5a7
Data: 22/01/02 / Sistema automatico

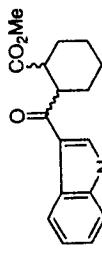


H1 / s2pu1 / Gem-200.DivIV
Loc: #32 / Dissolvent: cdcl3 / temp ambient
User1: Jb/ Mostra: rosat30
Data: 25/04/01 / Sistema automatic

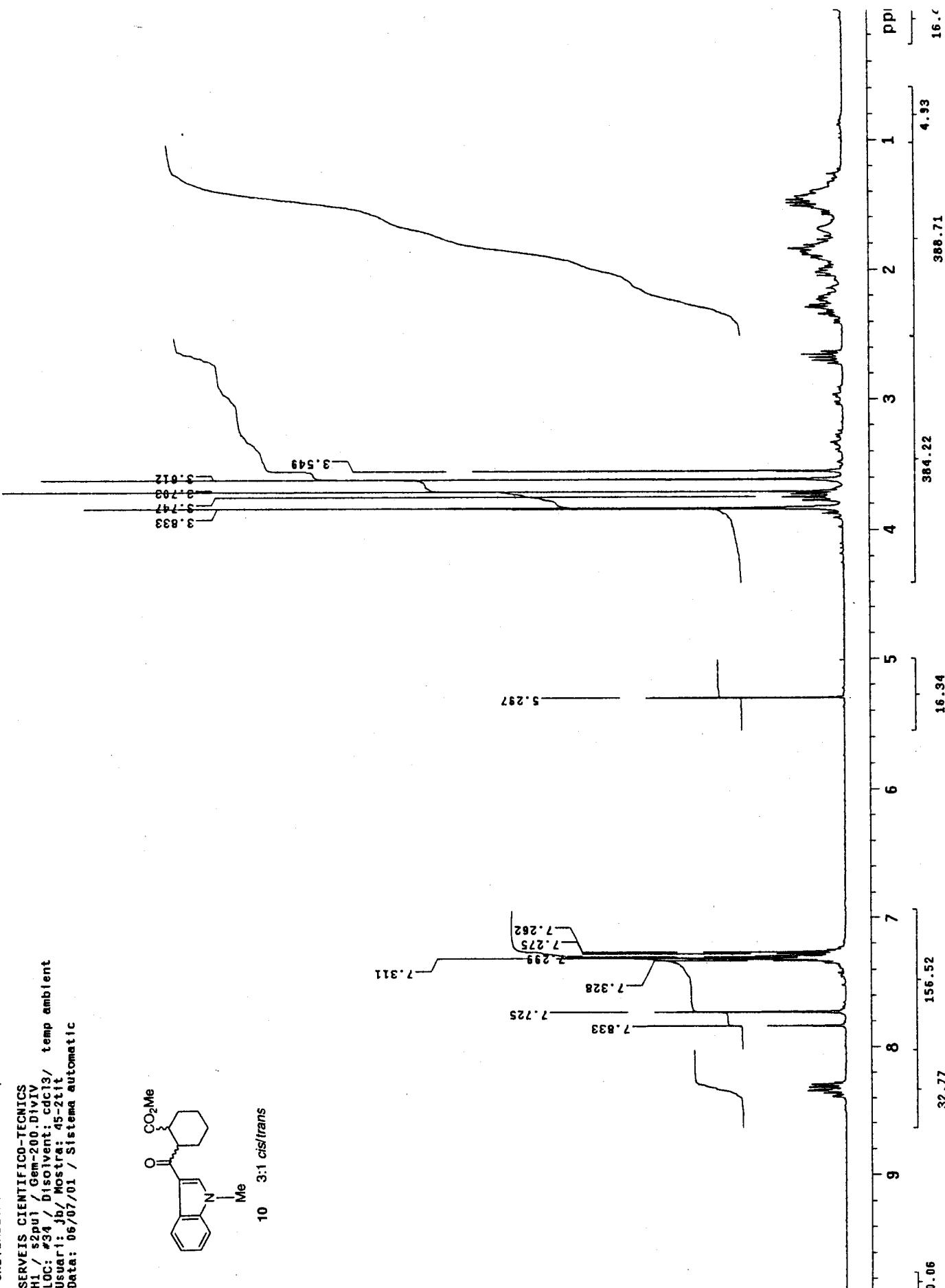
Pulse Sequence: s2pu1

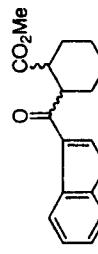


SERVEIS CIENTÍFICO-TECNICS
 H1 / s2pu1 / Gem-200-DivTV
 LOC: #34 / Disolvent: cdcl3 / temp ambient
 Usuari: jb / Mostre: 45-2tit
 Data: 06/07/01 / Sistema Automatic

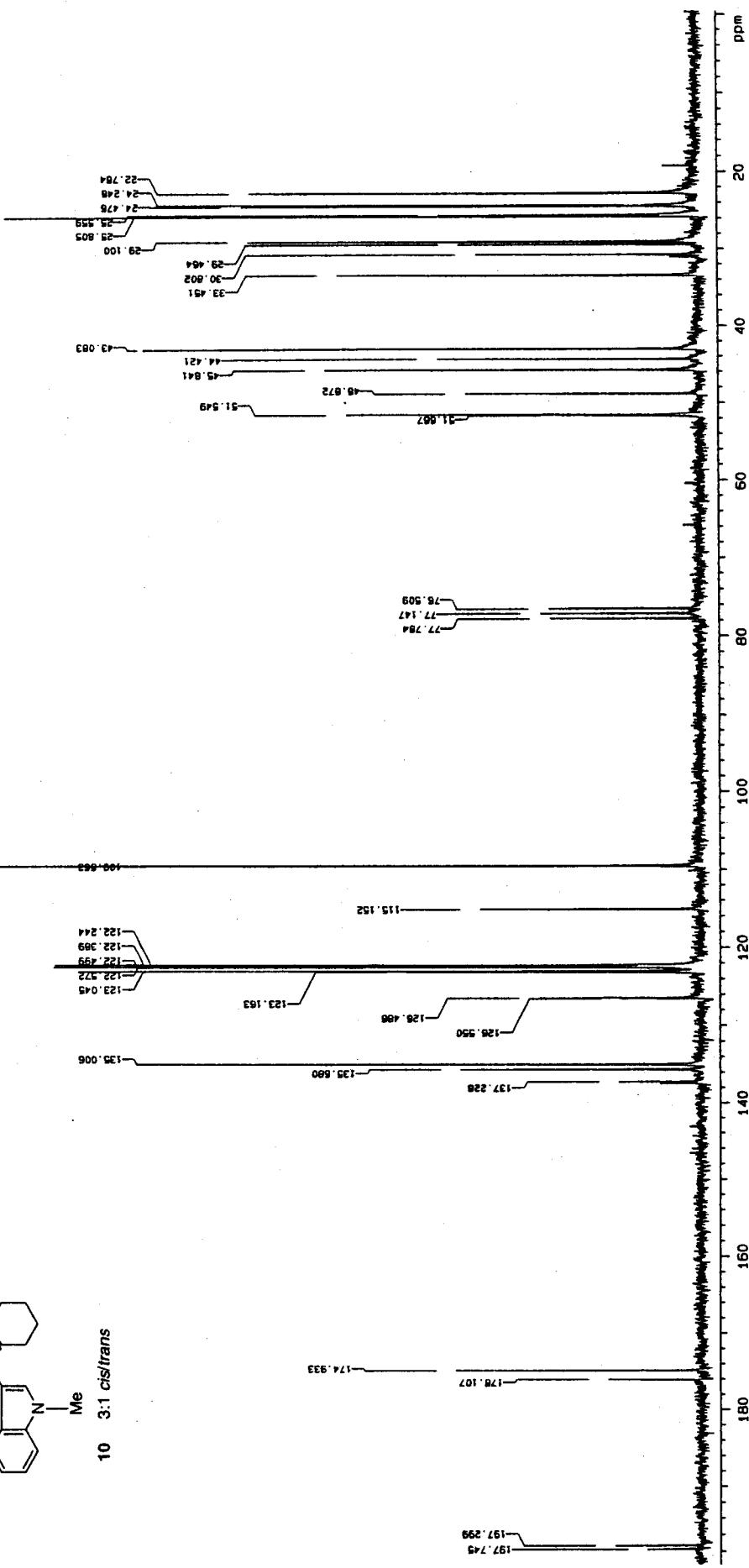


10 3:1 cis/trans





10 3:1 cis/trans



PULSE SEQUENCE	OBSERVE C13, 50.287655	DATA PROCESSING
	DECUPLE H1, 180.5072738	Line broadening 1.0 Hz
	Power 30 dB	FT size 65536
	continuously on	Total time 11 minutes
		WALTZ-16 modulated
		512 repetitions
Relax. delay 0.200 sec		
Pulse 64.6 degrees		
Acq. time 1.200 sec		
Width 15000.0 Hz		

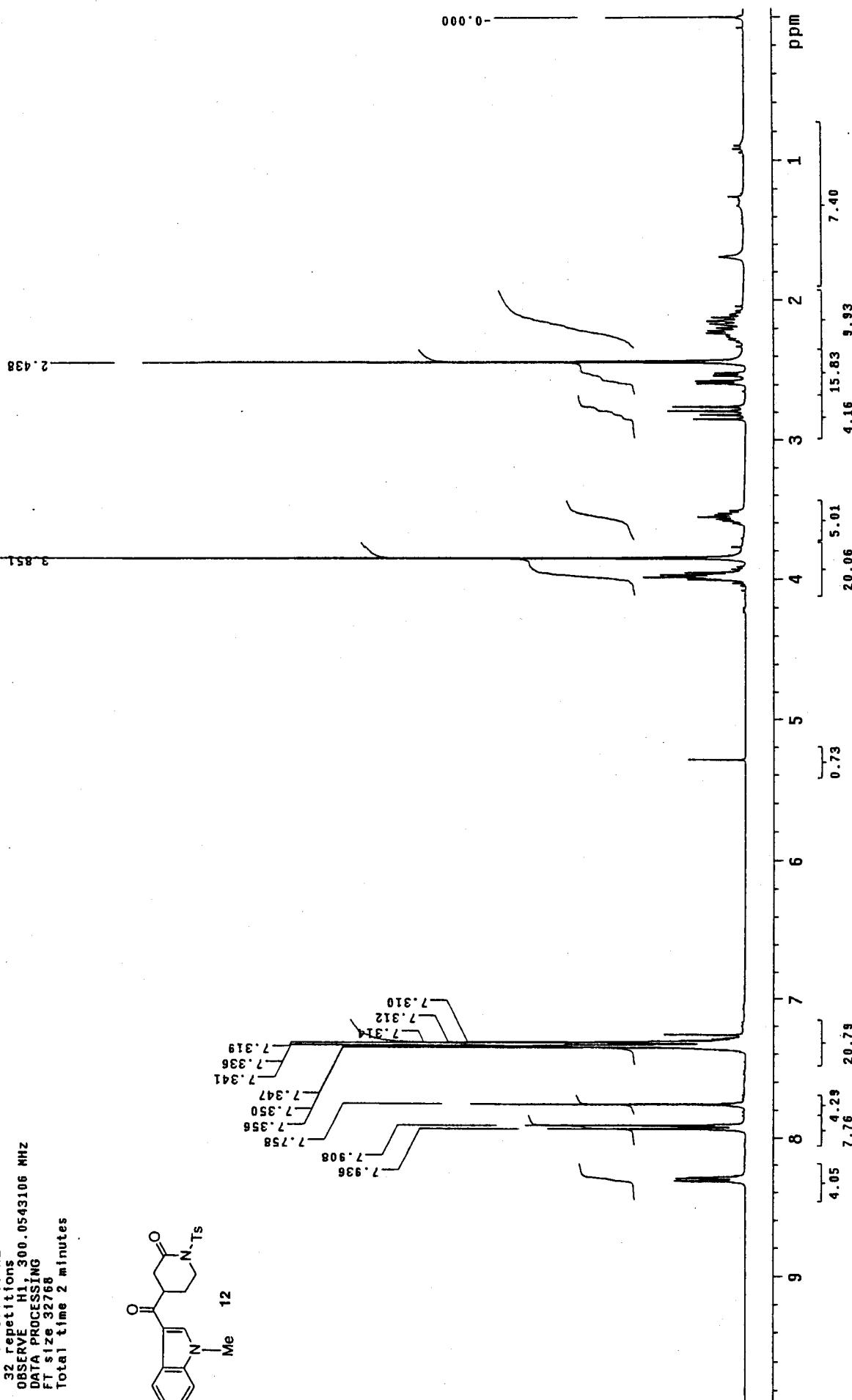
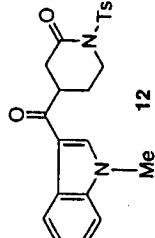
C13 / 8200J / Gem-200 Div IV
LOC: #22 / Dissolvent: cdc13/
temp: ambient
User: Jrb/ Month: m050-2
Date: 14/07/01 / Sistema
automatique
sobremesa@ub.edu.es

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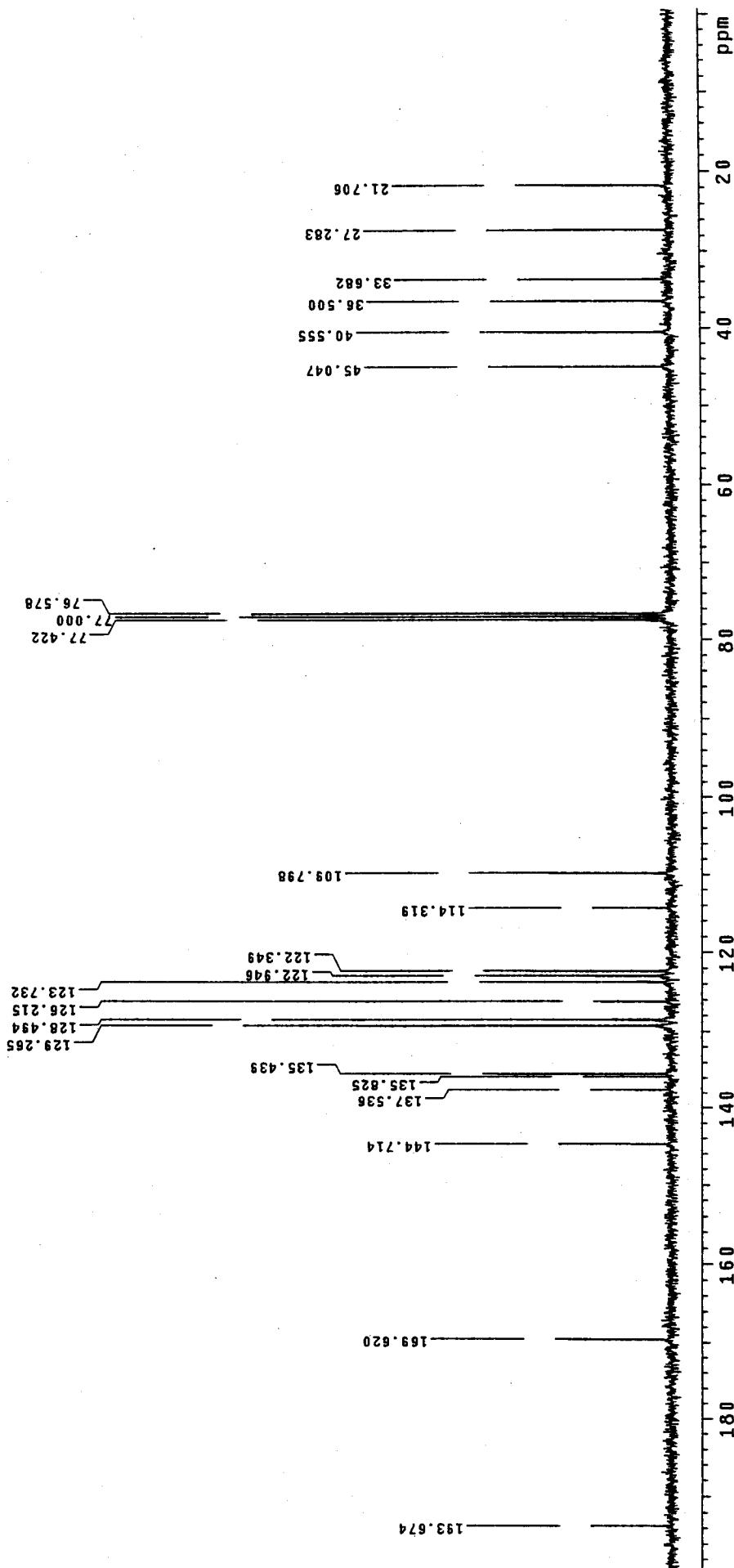
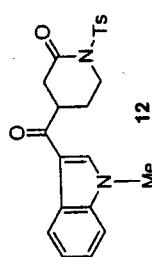
H1 / s2pul / Gemini-300
CDC13 / 29C / N reg: F0594
    / RG454 f41-46 / Rosa
Data: 22/10/01 / Ope.:Ana

Solvent: CDC13
Ambient temperature
GEMINI-300 "zape"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 38.4 degrees
Acq. time 3.000 sec
Width 3898.0 Hz
32 repetitions
OBSERVE H1, 300.0543106 MHz
DATA PROCESSING
FT size 32768
Total time 2 minutes

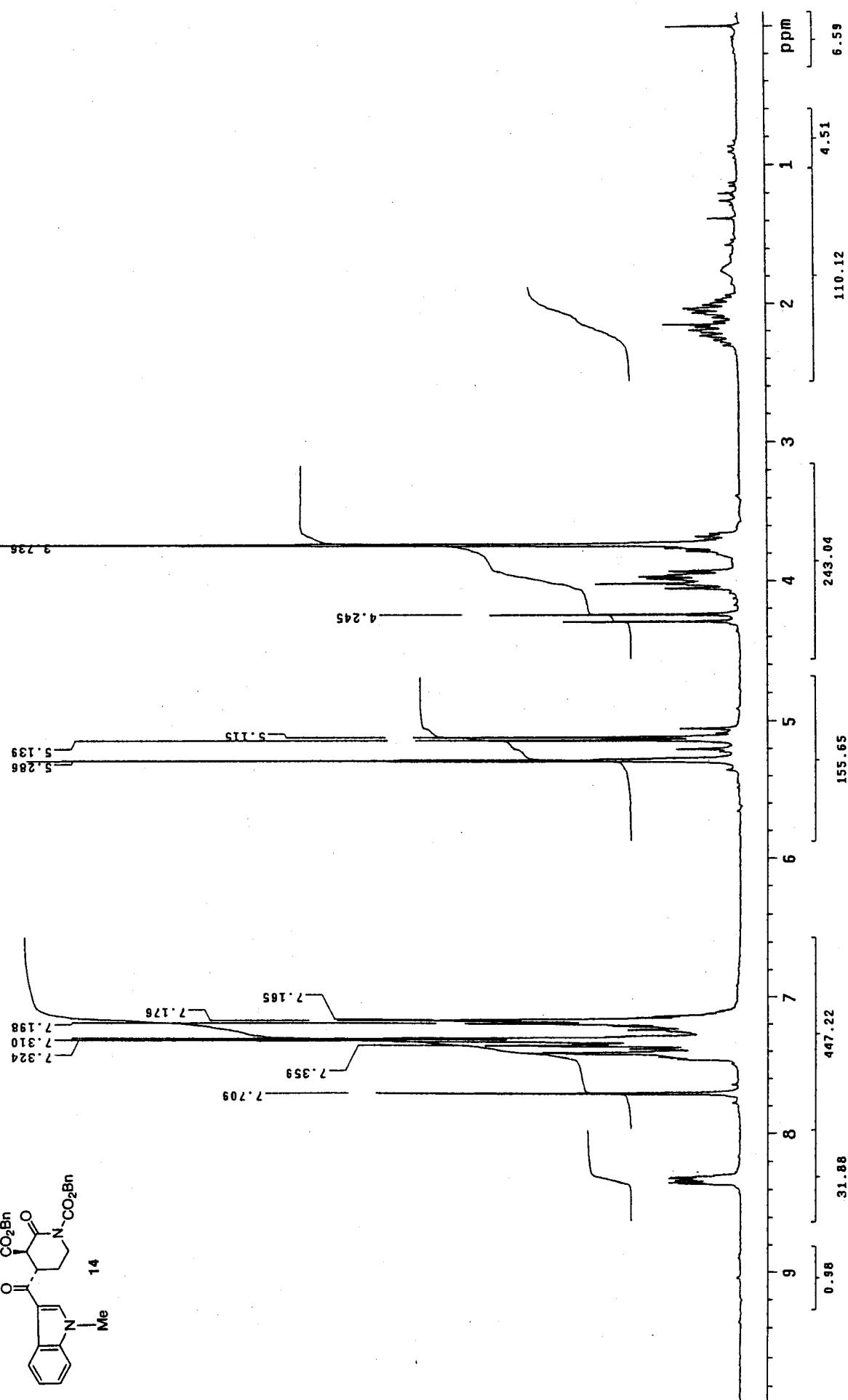
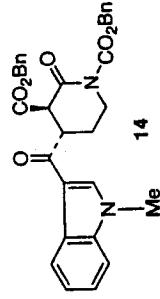
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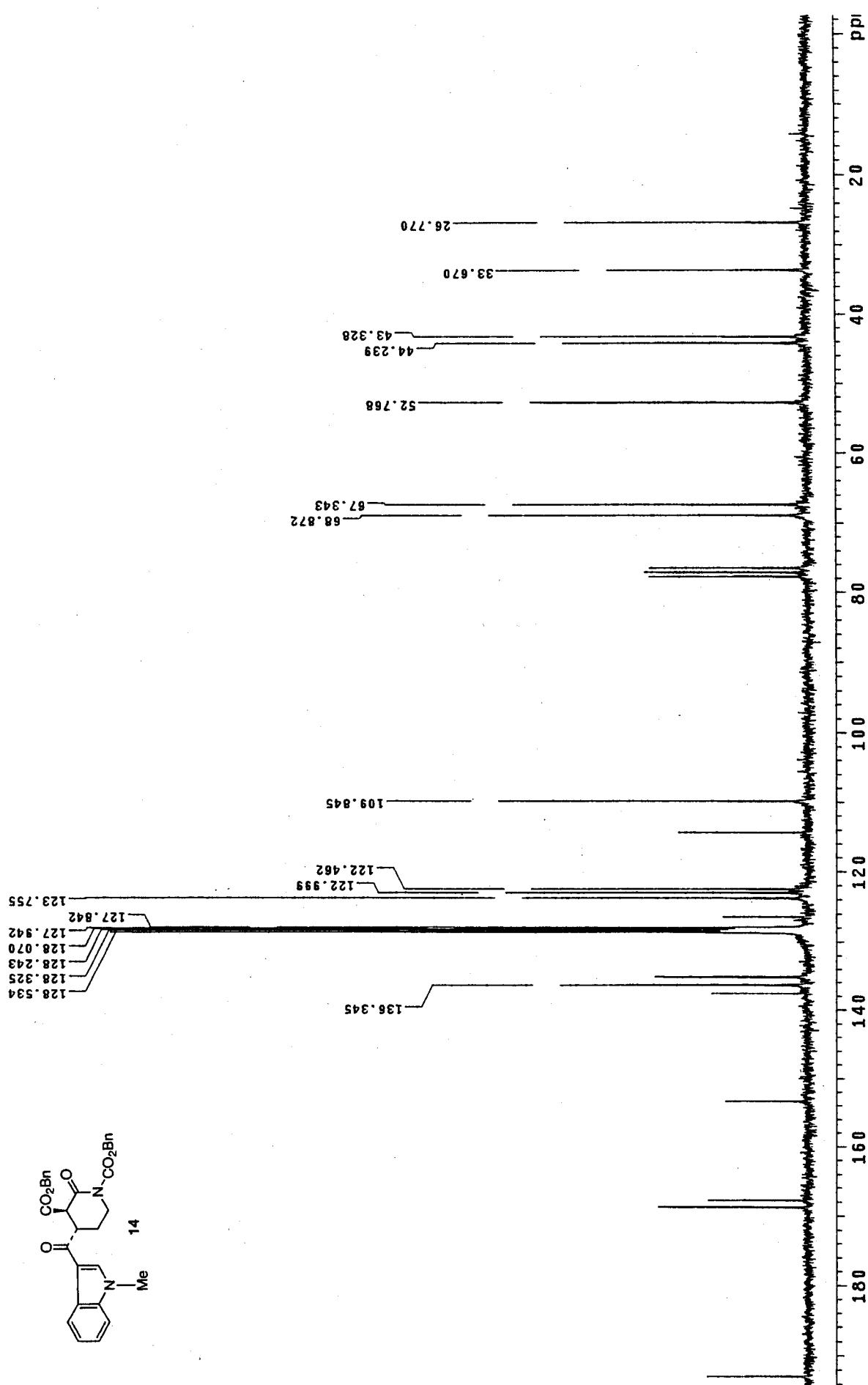
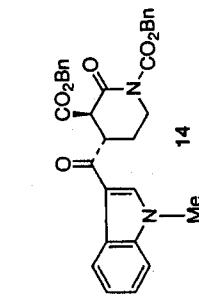
13C / s2pu1 / Gemini-300
 CDC13 / 29C / N reg; F0594
 Jb / RG454 f41-6 / Rosa
 Data:22/11/01 / Ope.:Ana
 Solvent: CDCl3
 Ambient temperature
 GEMINI-300 "zepe"
 PULSE SEQUENCE
 Relax . delay 0 . 500 sec
 Pulse 44.1 degrees
 Acc. time 1.705 sec
 Width 18000.0 Hz
 608 repetitions
 OBSERVE C13, 75.4487113 MHz
 DECOUPLE H1, 300.0558111 MHz
 Power 30 dB,
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.5 Hz
 FT size 65536
 Total time 22 minutes



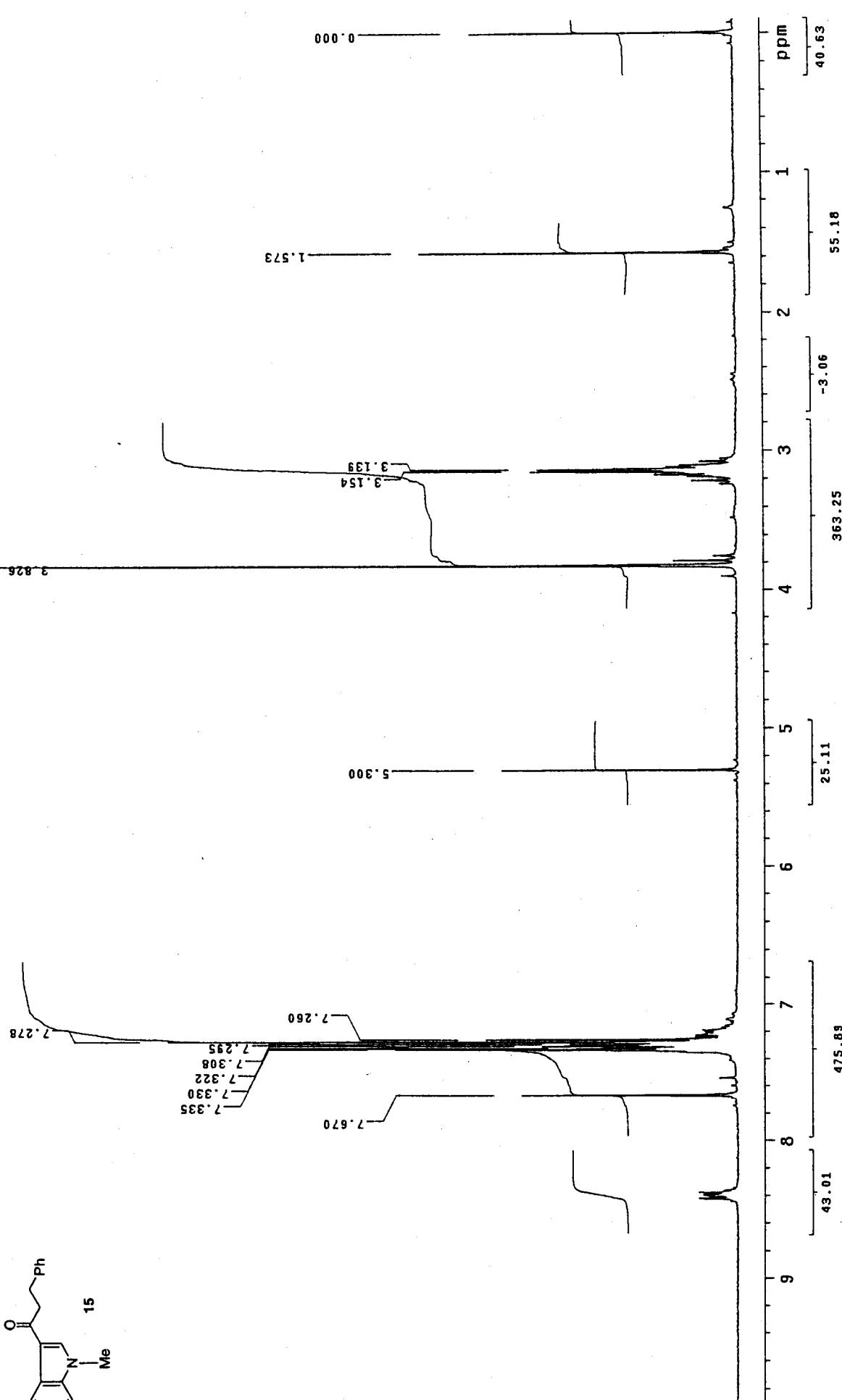
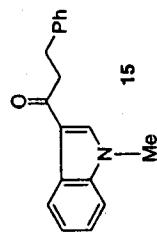
H1 / s2pul / Gem-200.DIV1V
LOC: #24 / Dissolvent: cdc13/ temp ambient
User1: jb/ Nostra: cross489rBa16
Data: 10/01/02 / Sistema automatic



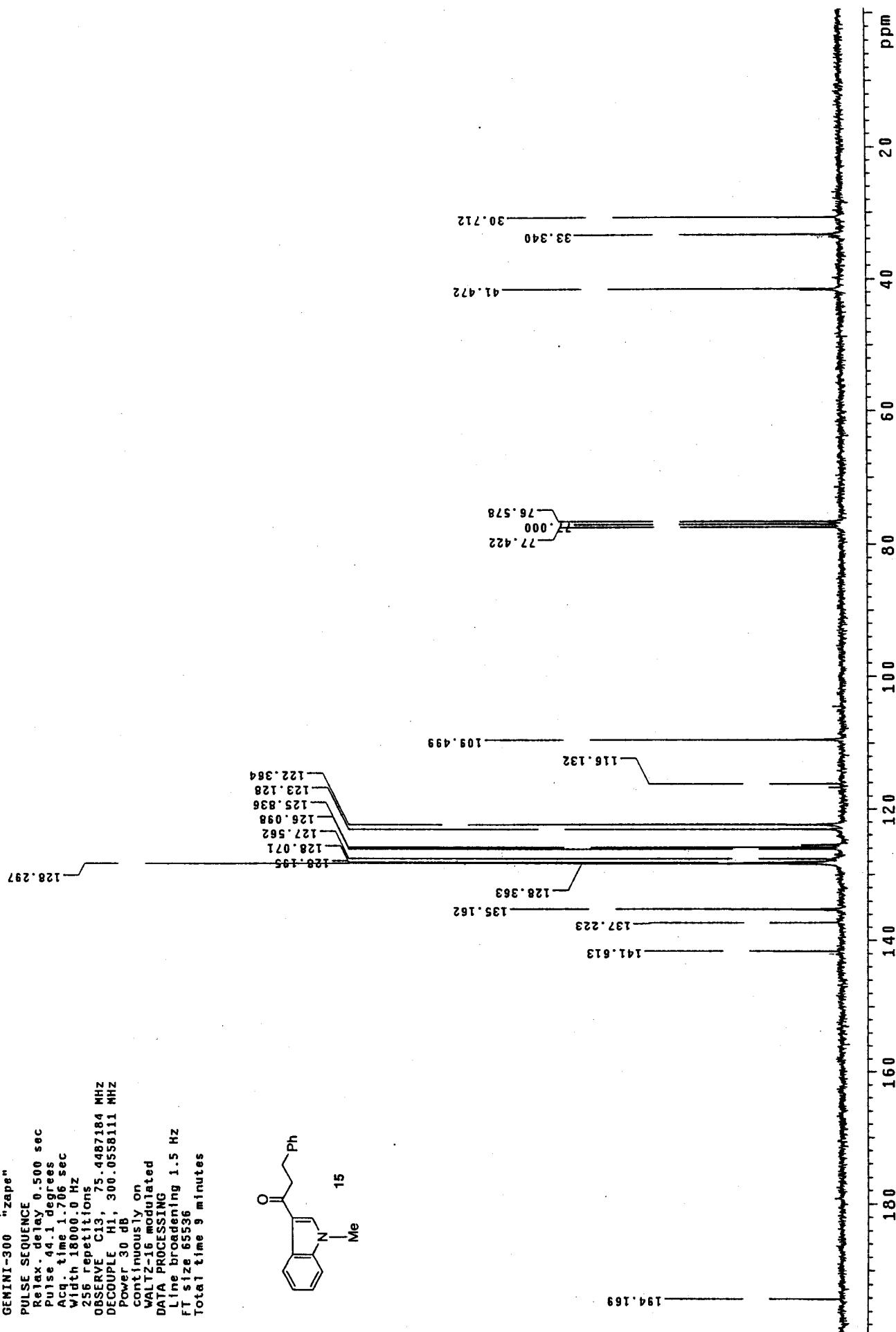
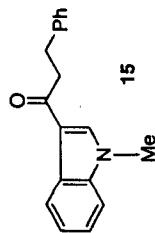
SERVEIS CIENTÍFICO-TECNICS
 C13 / s2pu1 / Gen-200 DivIV
 LOC: #35 / Dissolvent: cdc13/ temp ambient
 Usuari: Jb / Mostre: 263marJan
 Data: 24/05/01 / Sistema automatic

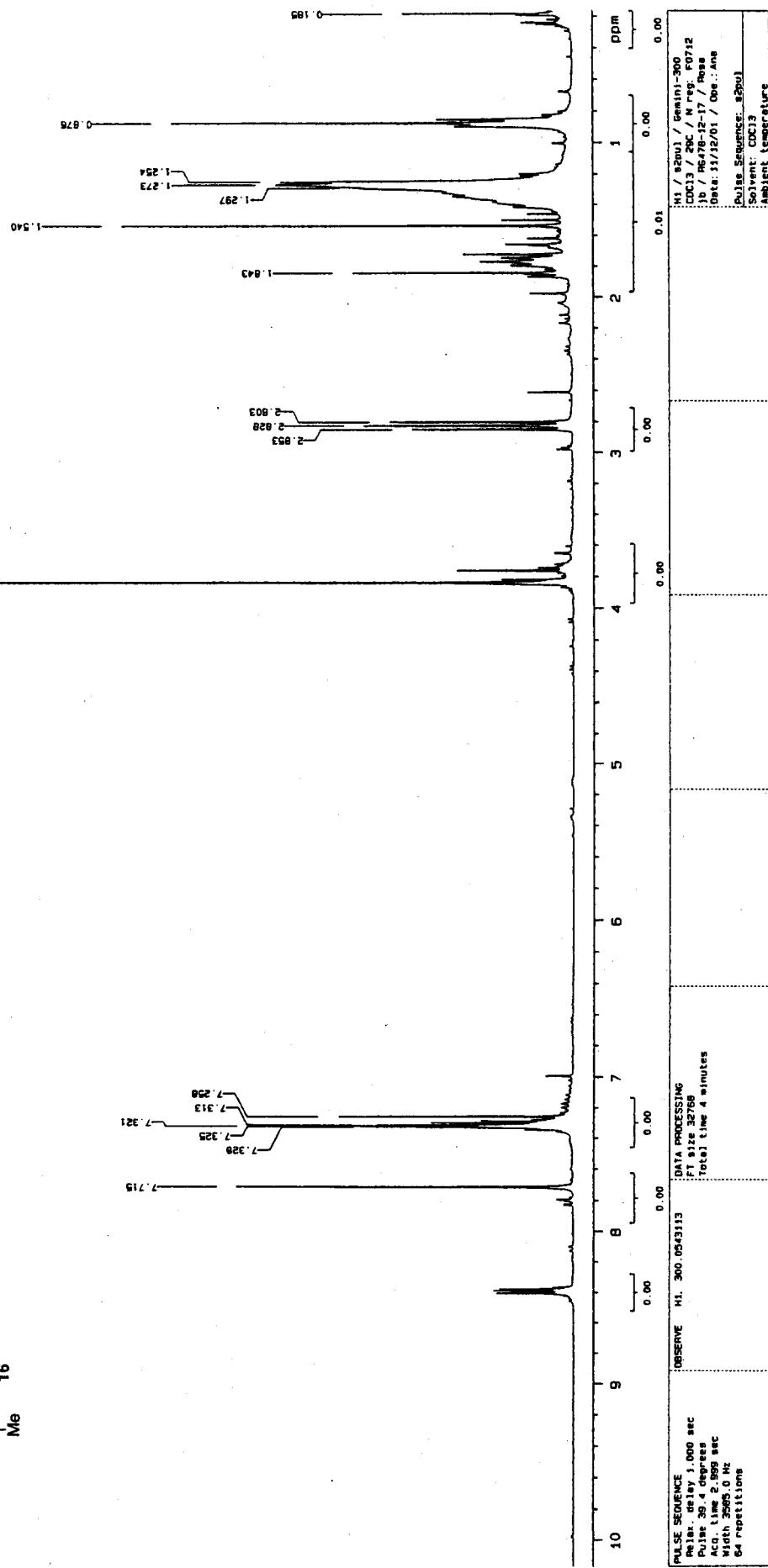
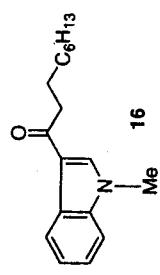


H1 / s2pu1 / Chem-200.Div1V
LOC: #34 / D solvent: cdcl3/ temp ambient
User1: Jb/ Mostra: arosetet43
Data: 05/04/02 / Sistema automatic



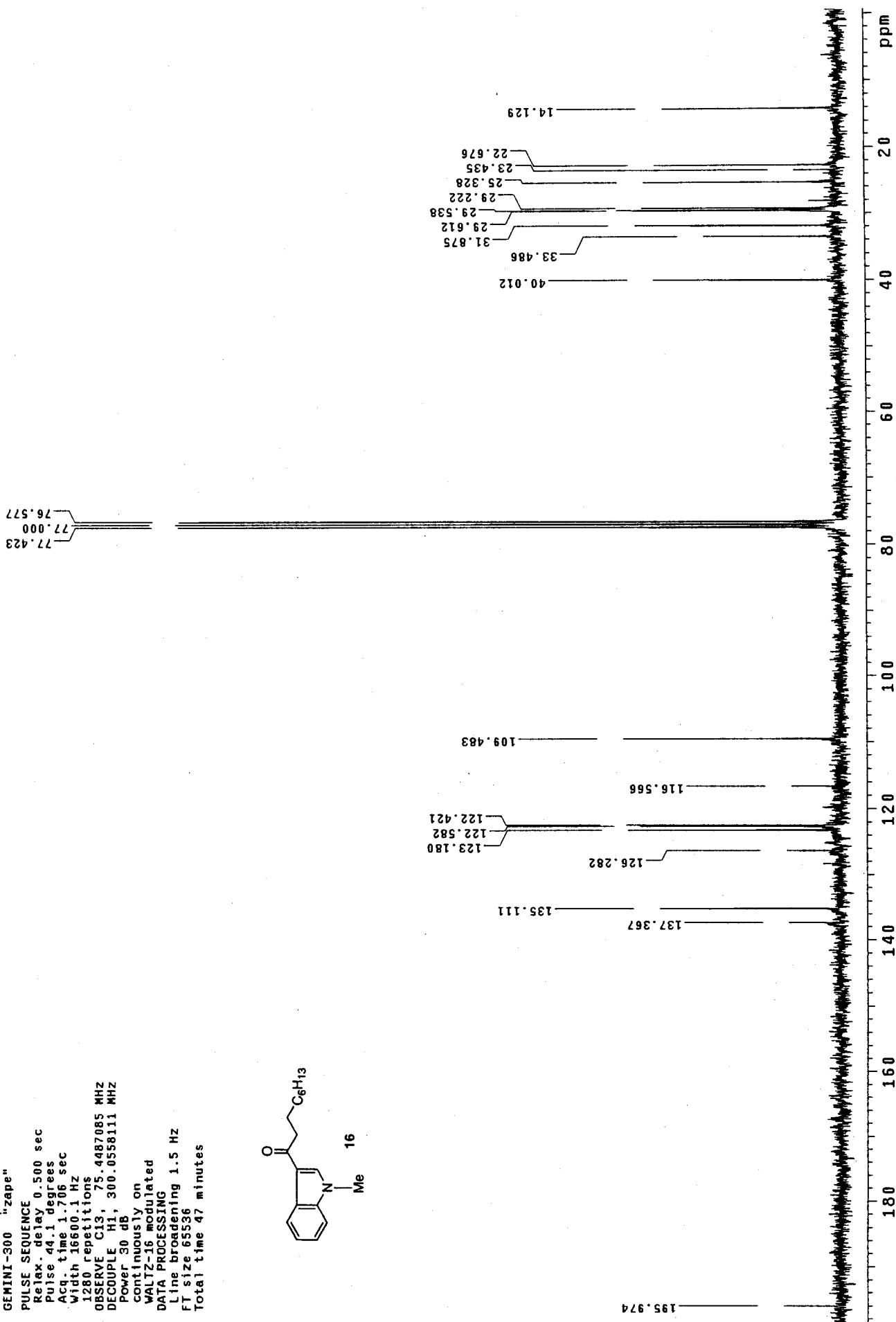
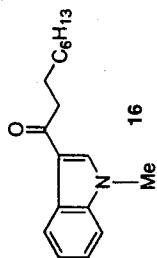
¹³C / s2pu1 / Gemini-300
 CDC13 / ²⁹Si / N reg: F0593
 Jb / RG453 fg-11 / Rosa
 Data: 22/10/01 / Ope.: Ana
 Solvent: CBC13
 Ambient temperature
 GEMINI-300 "Zape"
 PULSE SEQUENCE
 Relax. delay 0.500 sec
 Pulse 44.1 degrees
 Acq. time 1.706 sec
 Width 1800.0 Hz
 256 repetitions
 OBSERVE C13, 75.4487184 MHz
 DECOUPLE H1, 300.0550111 MHz
 Power 30 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.5 Hz
 FT size 55536
 Total time 9 minutes



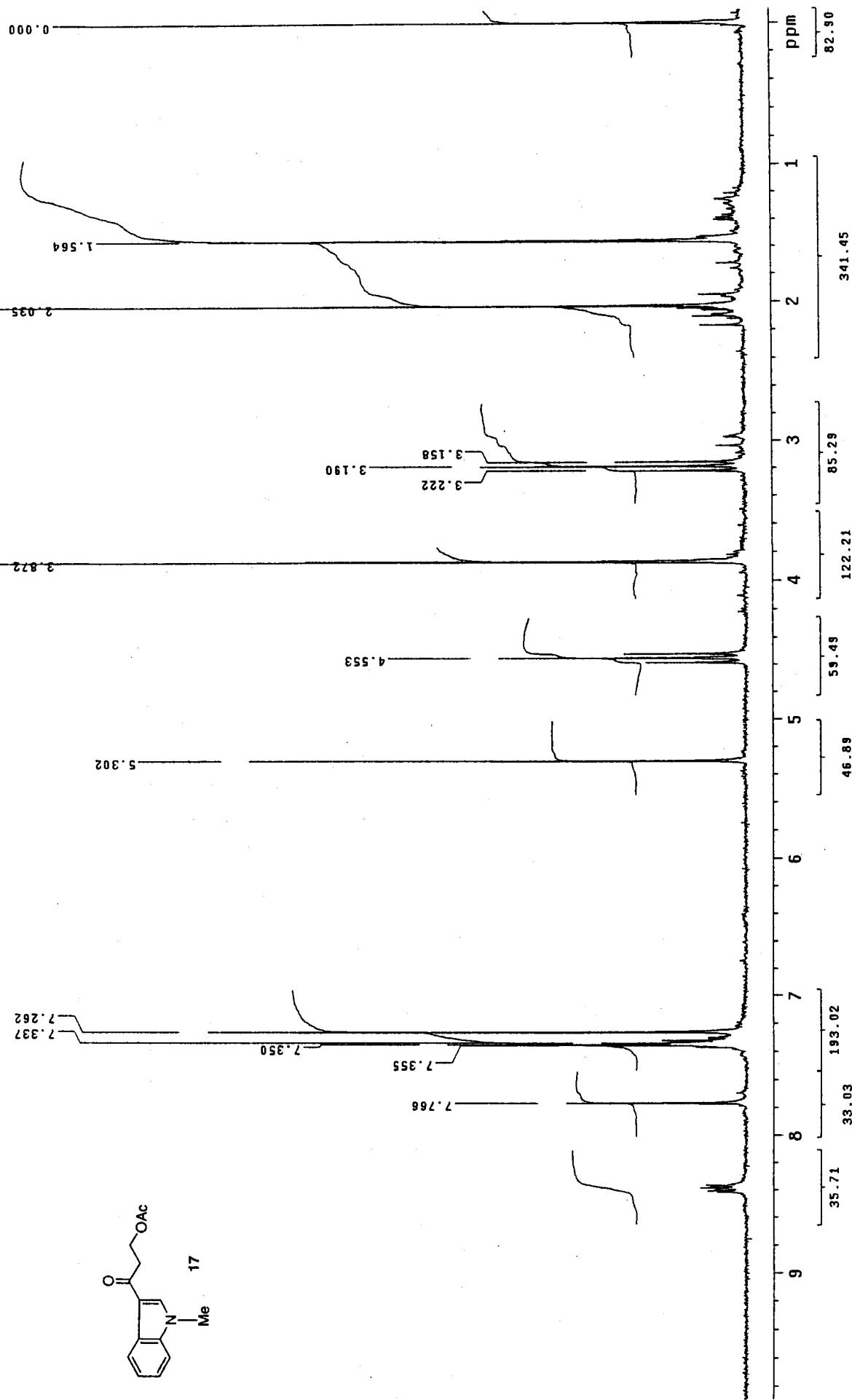


¹³C / s2pul / Gemini-300
 CDC13 / temp amb / N reg: F0712
 Jb / RG478-12-17 / Rosa
 Data: 11/12/01 / Ope.: Ana
 Solvent: CDCl₃
 Ambient temperature
 GEMINI-300 "zape"

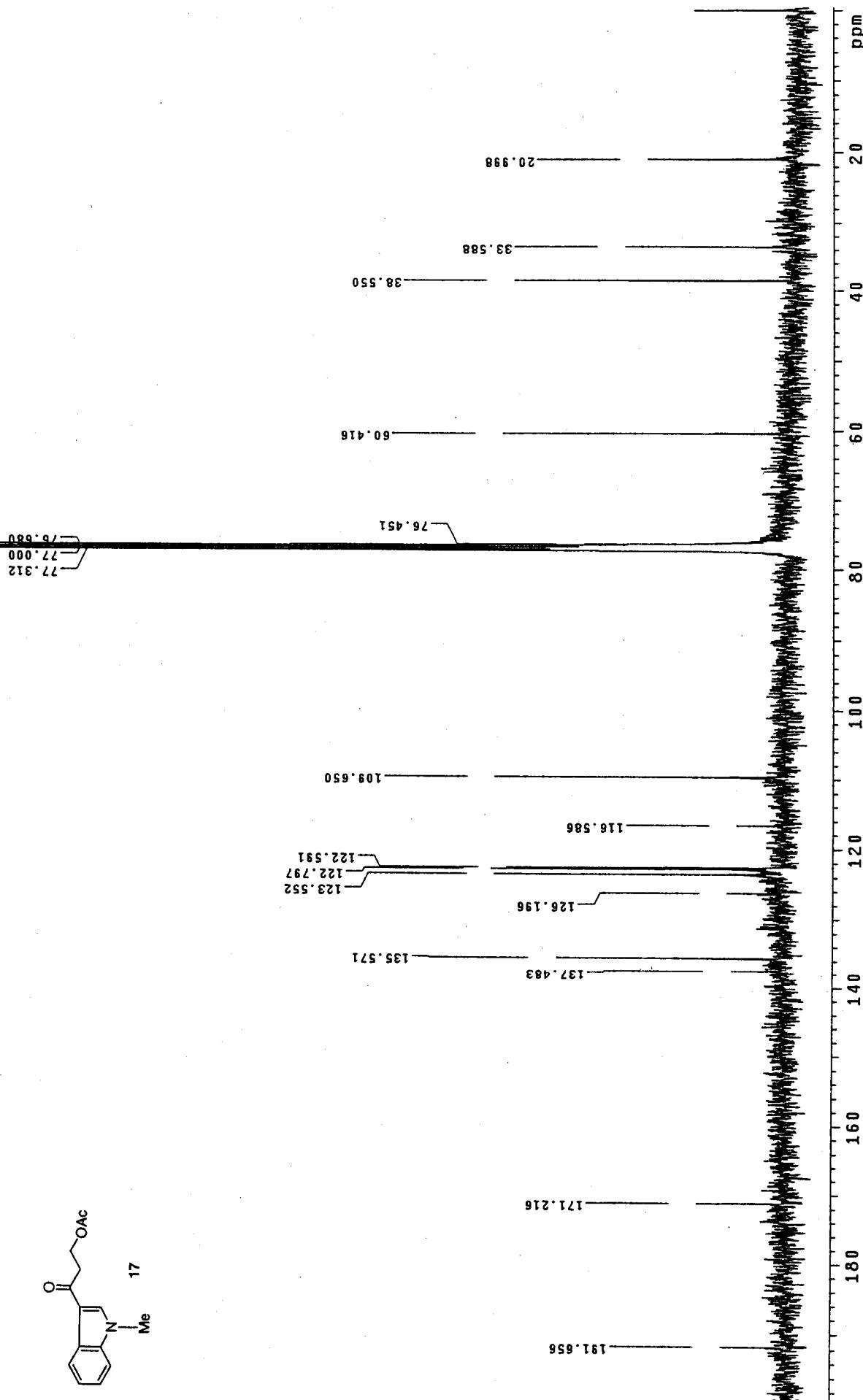
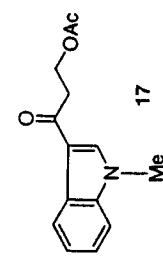
PULSE SEQUENCE
 Relax. delay 0.500 sec
 Pulse 44.1 degrees
 Acq. time 1.706 sec
 Width 16610.1 Hz
 1280 repetitions
 OBSERVE C13, 75.4487085 MHz
 DECOUPLE H1, 300.0556111 MHz
 Power 30 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.5 Hz
 FT size 65536
 Total time 47 minutes



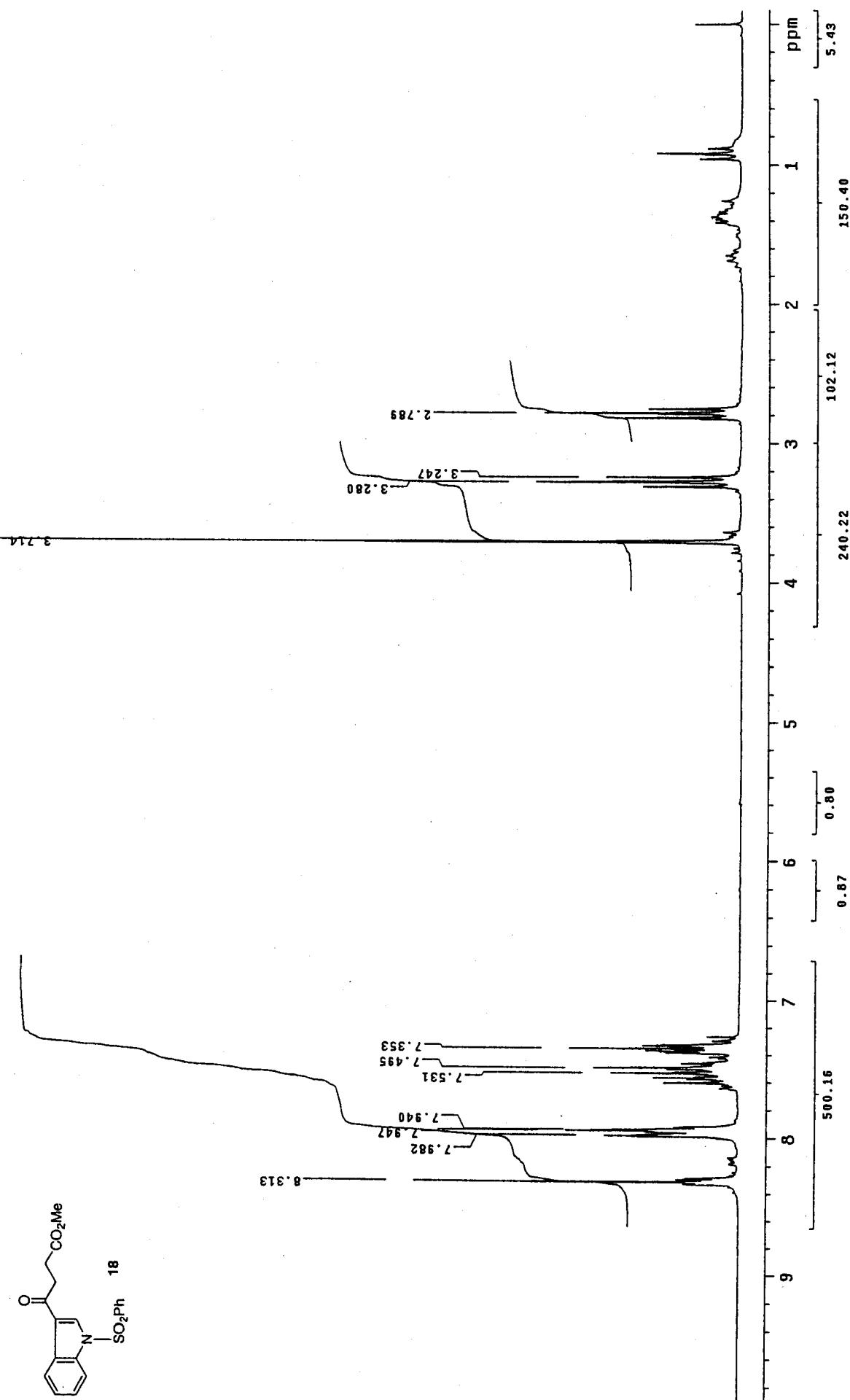
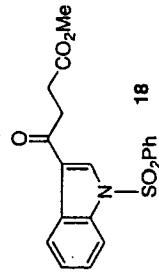
H1 / s2pu1 / Gem-200-DIVIV
LOC: #26 / Dissolvent: cdc13/ temp ambient
Usuar: Jb/ Mostra: brotsegregrec
Data: 22/11/01 / Sistema automatic



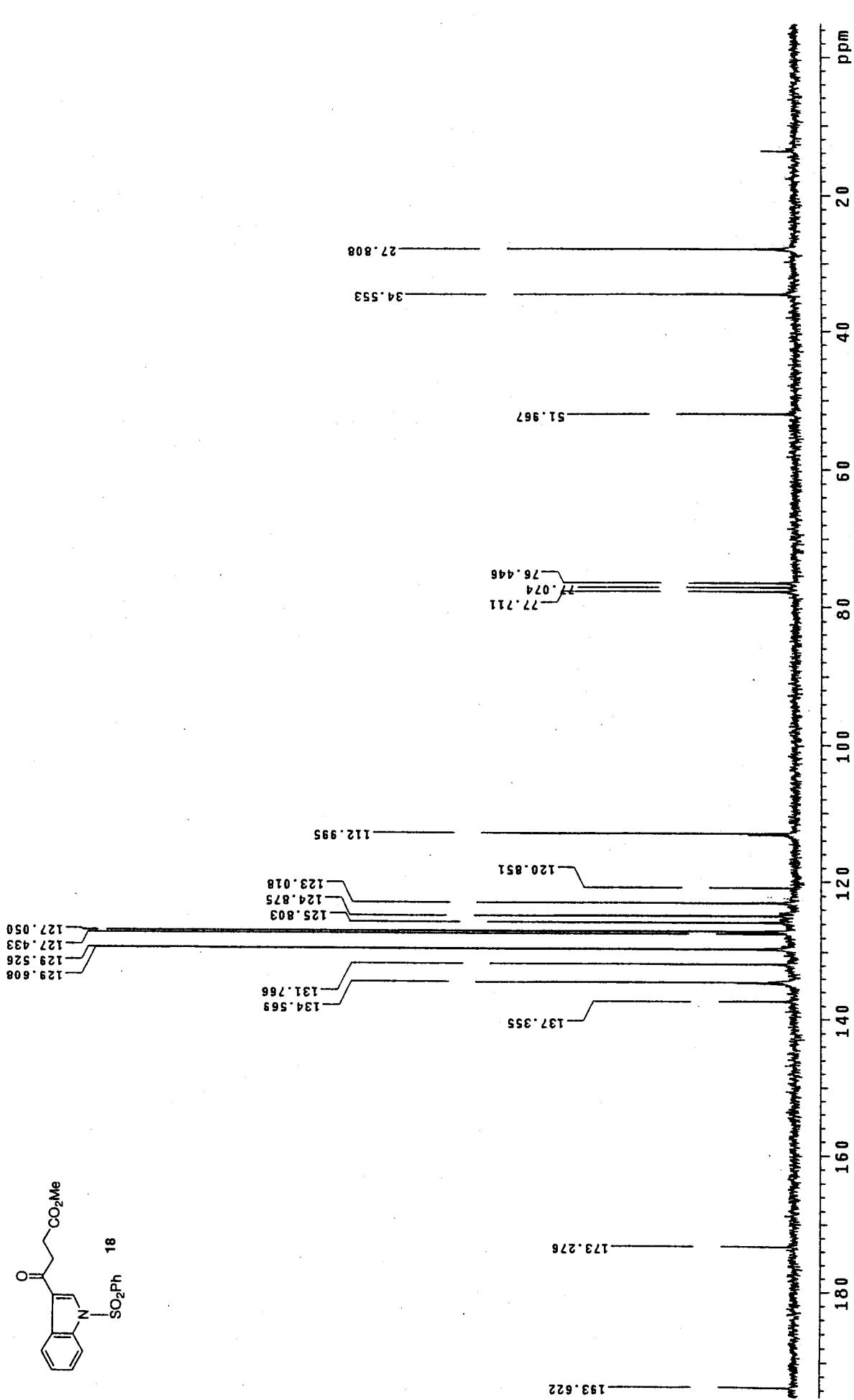
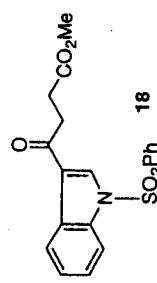
C13 / s2pu1 / Mercury-400
cdcl3 / temp: Ambient / N reg: pcb
User1 / jb / Mostra: rgf5rec2
Data: 21/11/01 / Sist automatic
Pulse Sequence: s2pu1



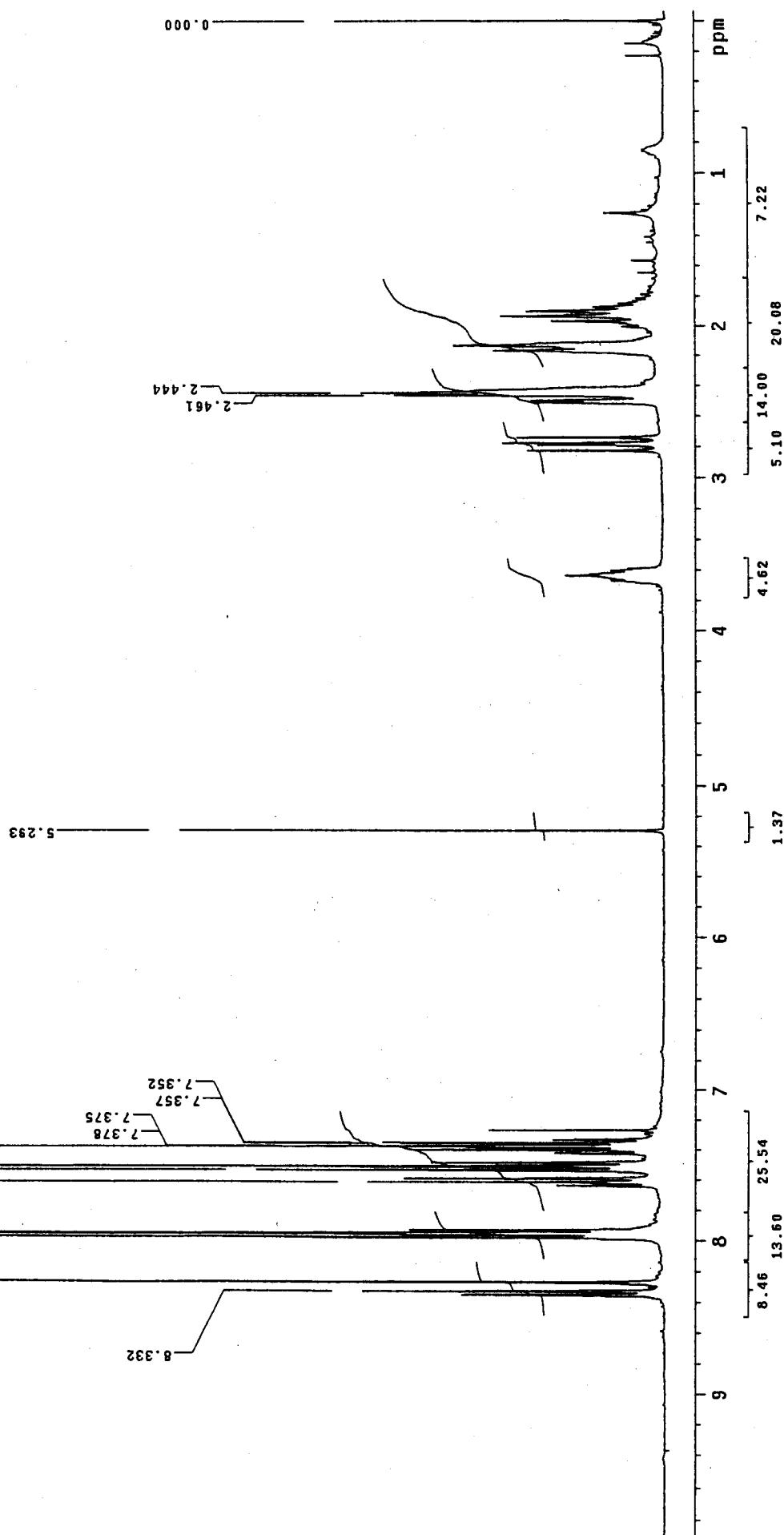
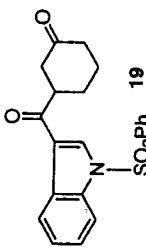
H1 / s2pu1 / Gem-200-DivIV
LOC: # 6 / Disolvent: ddc13/ temp ambient
Usuar: Jb/ Nostra: drosa446f20aa33
Data: 01/10/01 / Sistema automatic

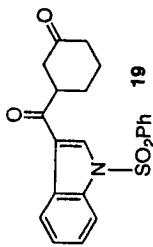


H1 / s2pul / Gem-200.DIVIV
LOC: #38 / Di solvent: cdc13 / temp ambient
User: Jb / Mostra: rg-444
Data: 03/10/01 / Sistema automatic

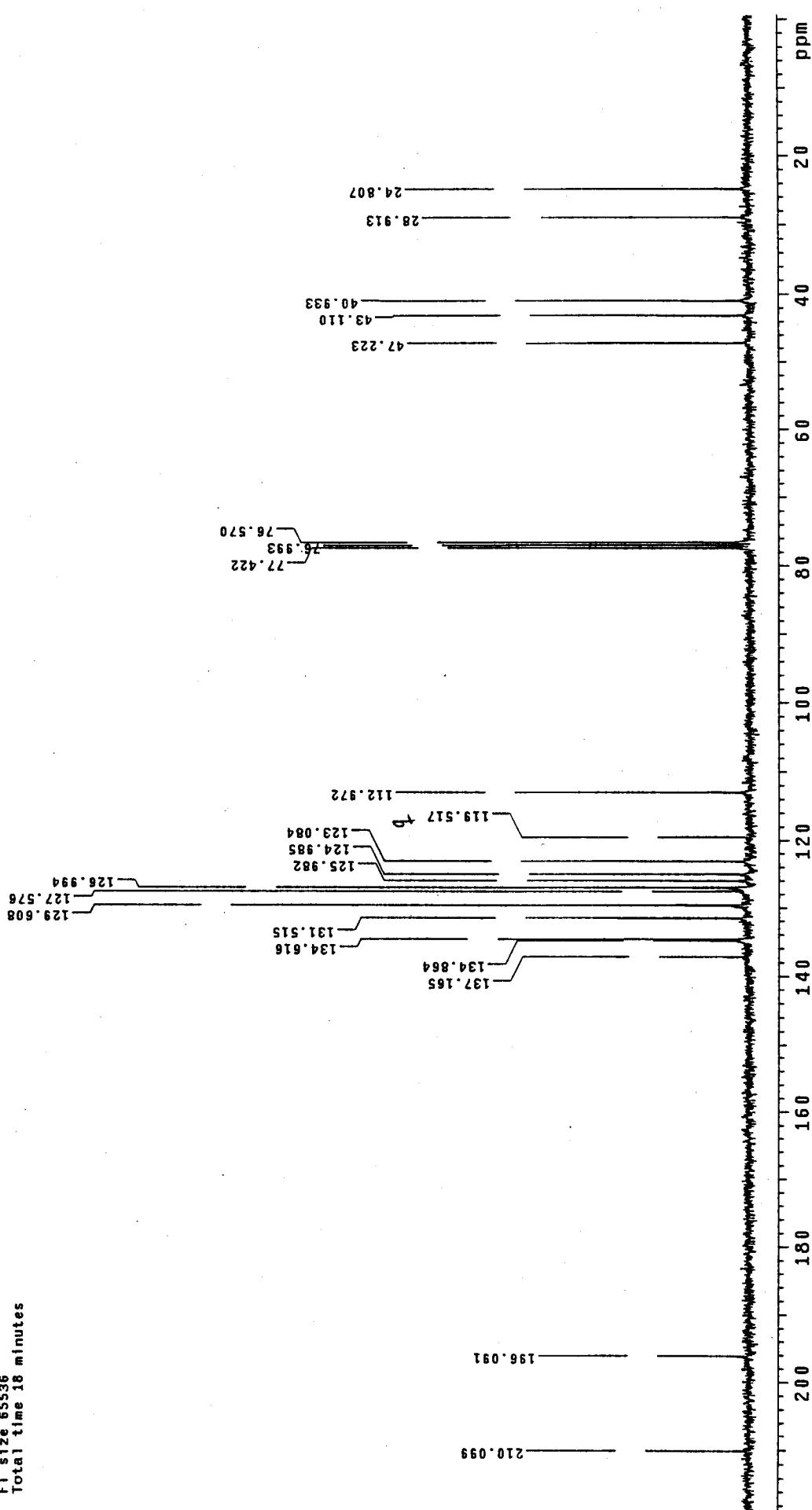


H1 / s2pu1 / Gemini-300
 CDPC13 / 29G / N reg: F0592
 Jb / RGA511B-22 / P0592
 Data: 19/10/01 / Op: C267
 Solvent: CDC13
 Ambient temperature: 23°C
 GEMINI-300 "zape"
 SPIN SEQUENCE
 Relax.: delay 1.000 sec
 Pulse time 39.4 degrees
 Acq. time 2.998 sec
 Width 3650.0 Hz
 32 repetitions
 OBSERVE H1, 300.0543079 MHz
 DATA PROCESSING
 FFT size 32768
 total time 2 minutes



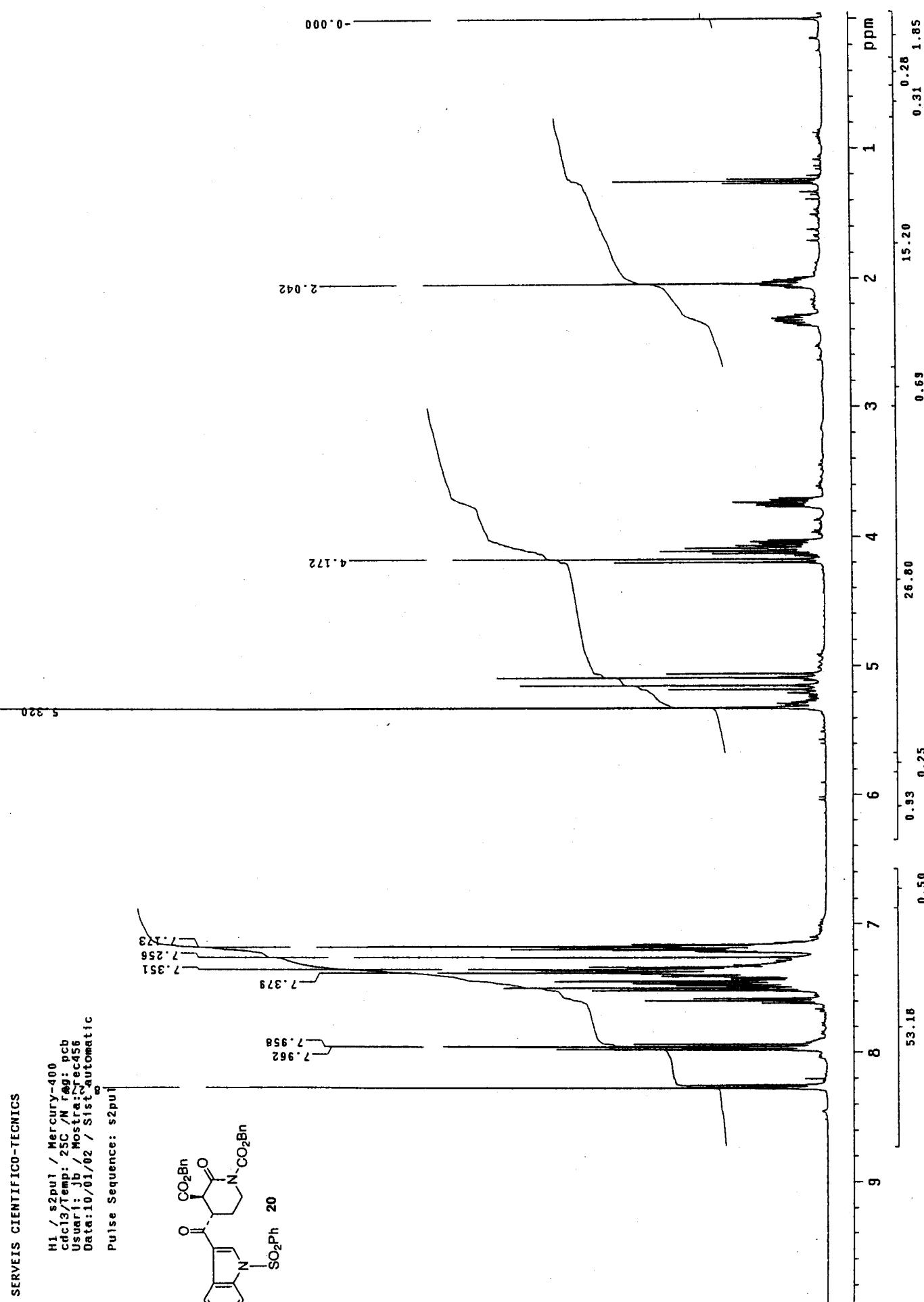
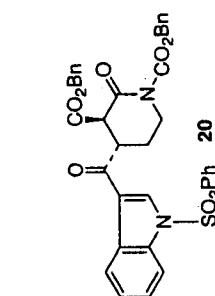


¹³C / s2pu1 / Gemini!-300
 CDCl₃ / 29C / N reg: F0592
 Jb / R0451916-22 / Rosa
 Data:11/10/01 / Ope.:Ana
 Solvent: CDCl₃
 Ambient temperature
 GEMINI-300 "zape"
 PULSE SEQUENCE
 Relax delay 0.500 sec
 Pulse 44.1 degrees
 Acq. time 1.706 sec
 Width 18000.0 Hz
 512 repetitions
 OBSERVE C13, 75.4487124 MHz
 DECOUPLE H1, 300.0558111 MHz
 Power 30 dB,
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.5 Hz
 FT size 65536
 Total time 18 minutes



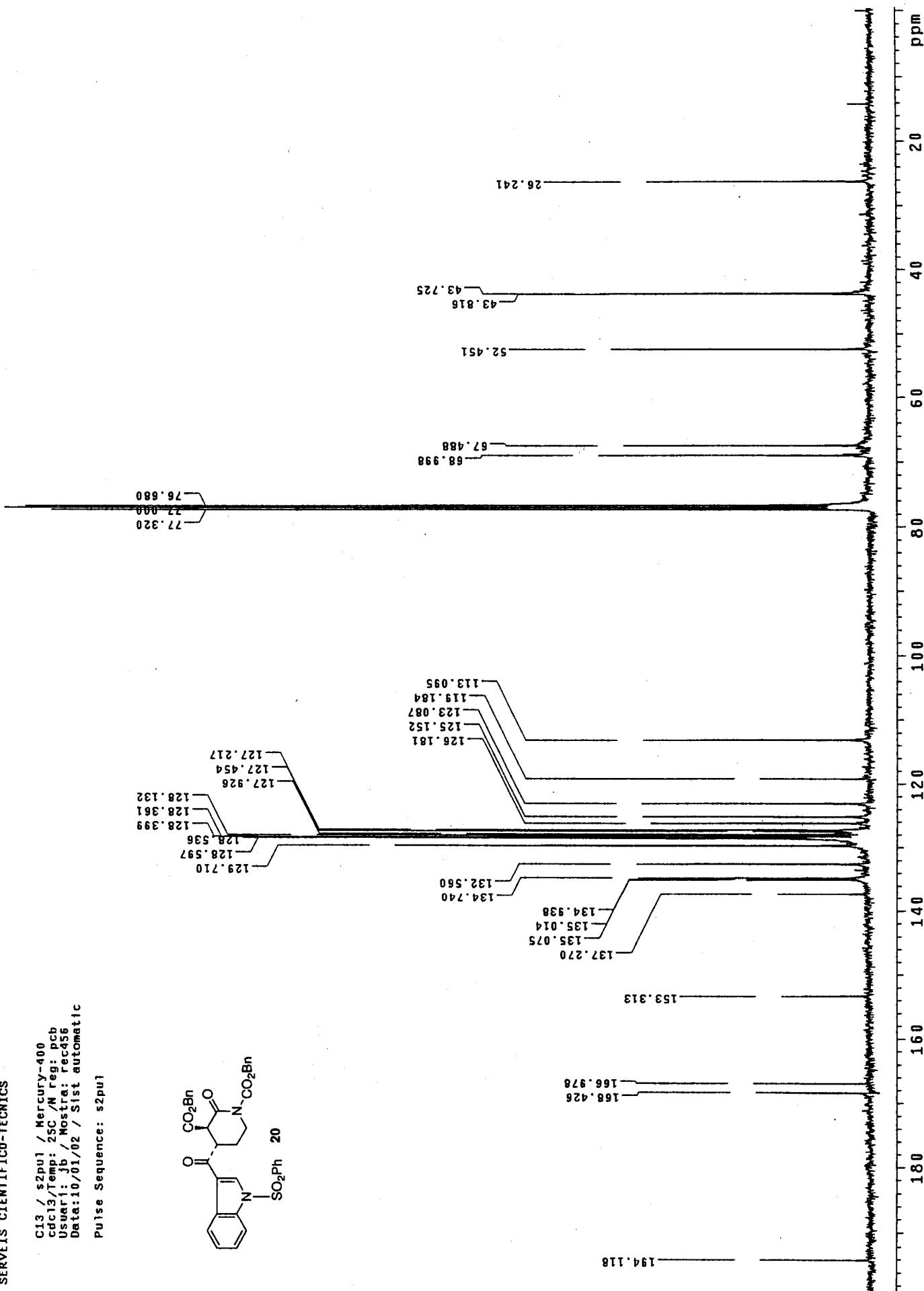
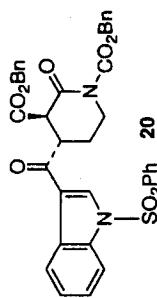
H1 / s2pul / Mercury-400
cdcl₃/Temp: 25C / N r_{avg}: pcb
User: Jb / Mostra: Tec456
Data: 10/01/02 / Sist: Automatic

Pulse Sequence: s2pul

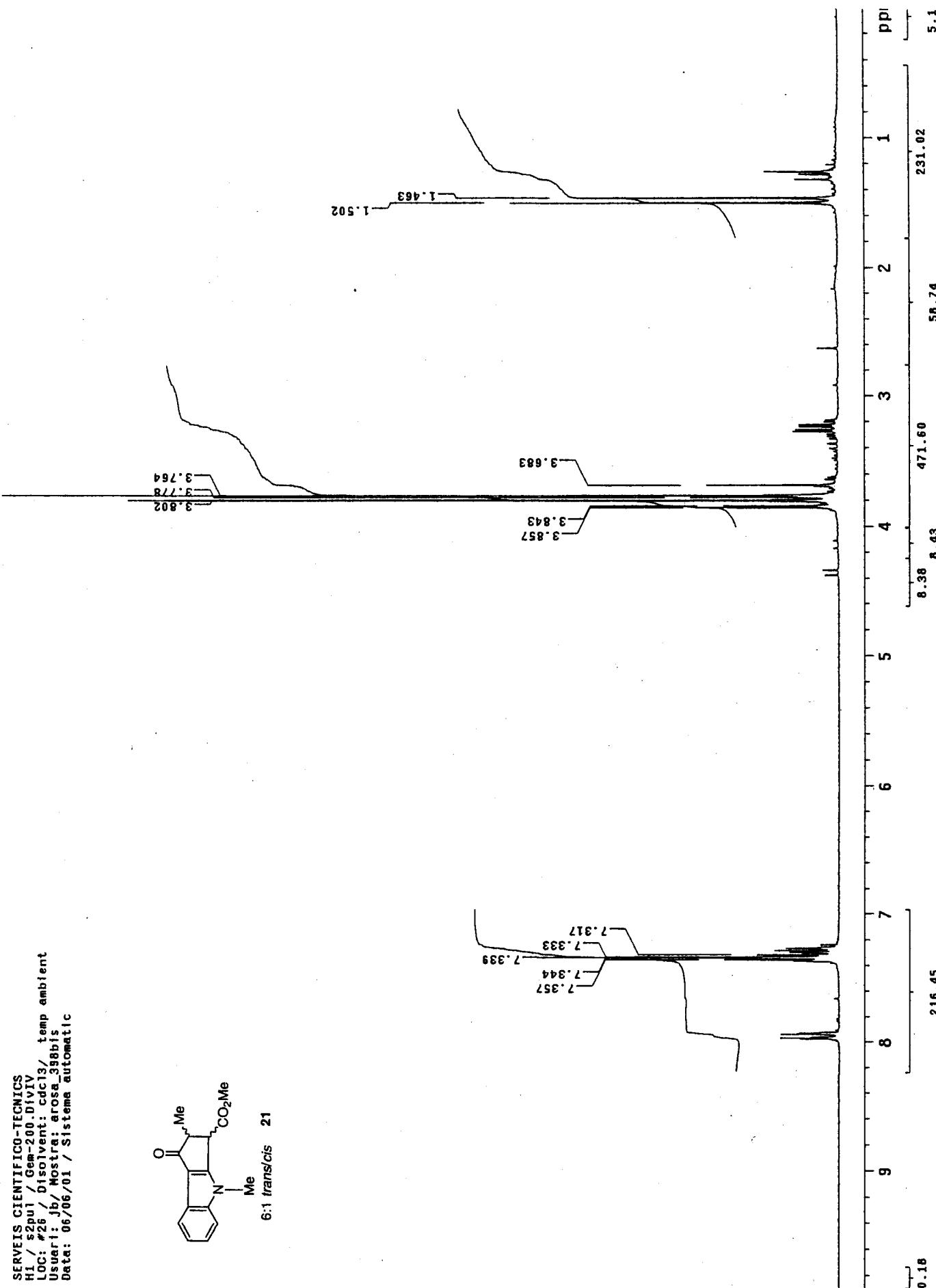
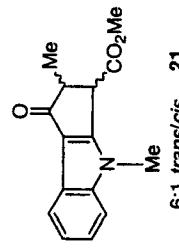


C113 / \$2pu1 / Mercury-400
ccdc13/Temp: 25C /N reg: pcb
Usuar1: jb / Mostra: rec456
Data:10/01/02 / Sist automatic

Pulse Sequence: s2pu1

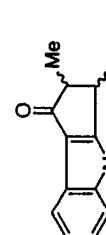


SERVEIS CIENTÍFICO-TECNICS
 H1 / s2pu1 / Gem-200 DIVIV
 LOC: #26 / Dissolvent: cdc13 / temp ambient
 Usuari: Jb / Mostra: arosa_398b1S
 Data: 06/06/01 / Sistema automatic

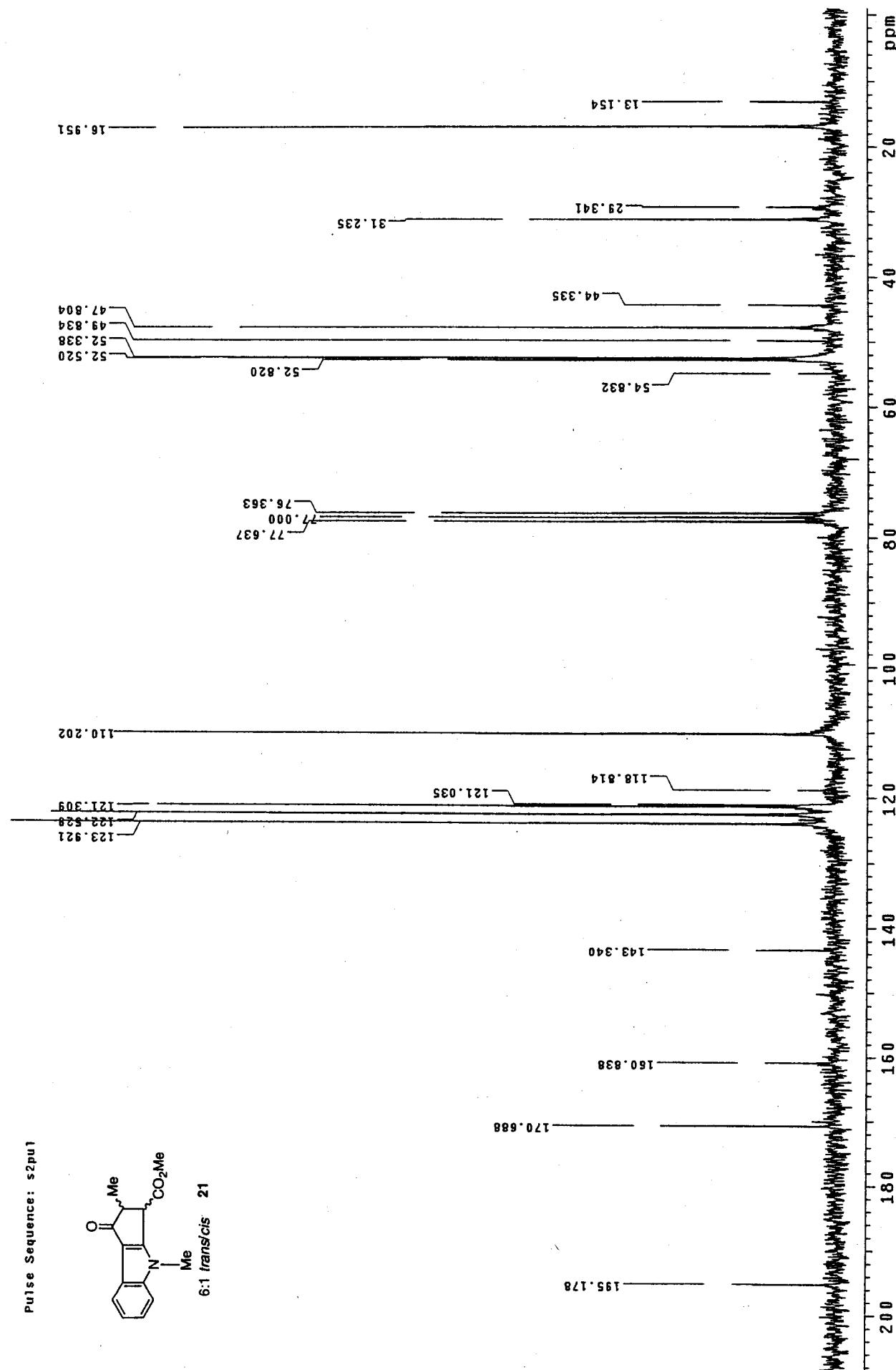


H1 / s2pu1 / Gem200.DIVIV
LOC: #26 / Dissolvent: cdc13/ temp ambient
User1: Jb / Mostre: arosa_398bis
Data: 06/06/01 / Sistema automatic

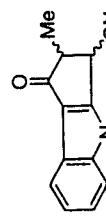
Pulse Sequence: s2pu1



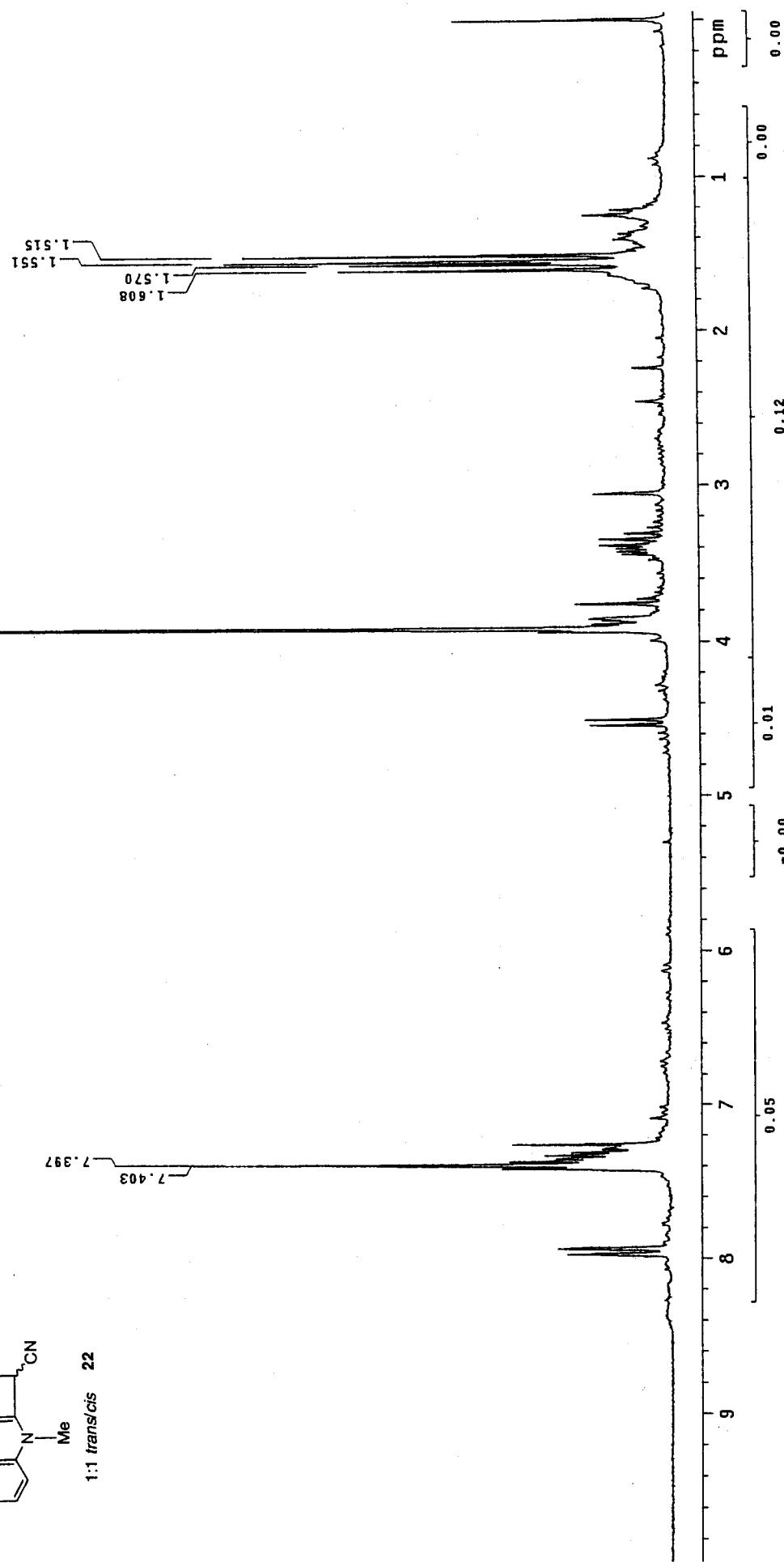
6:1 trans/cis: 21



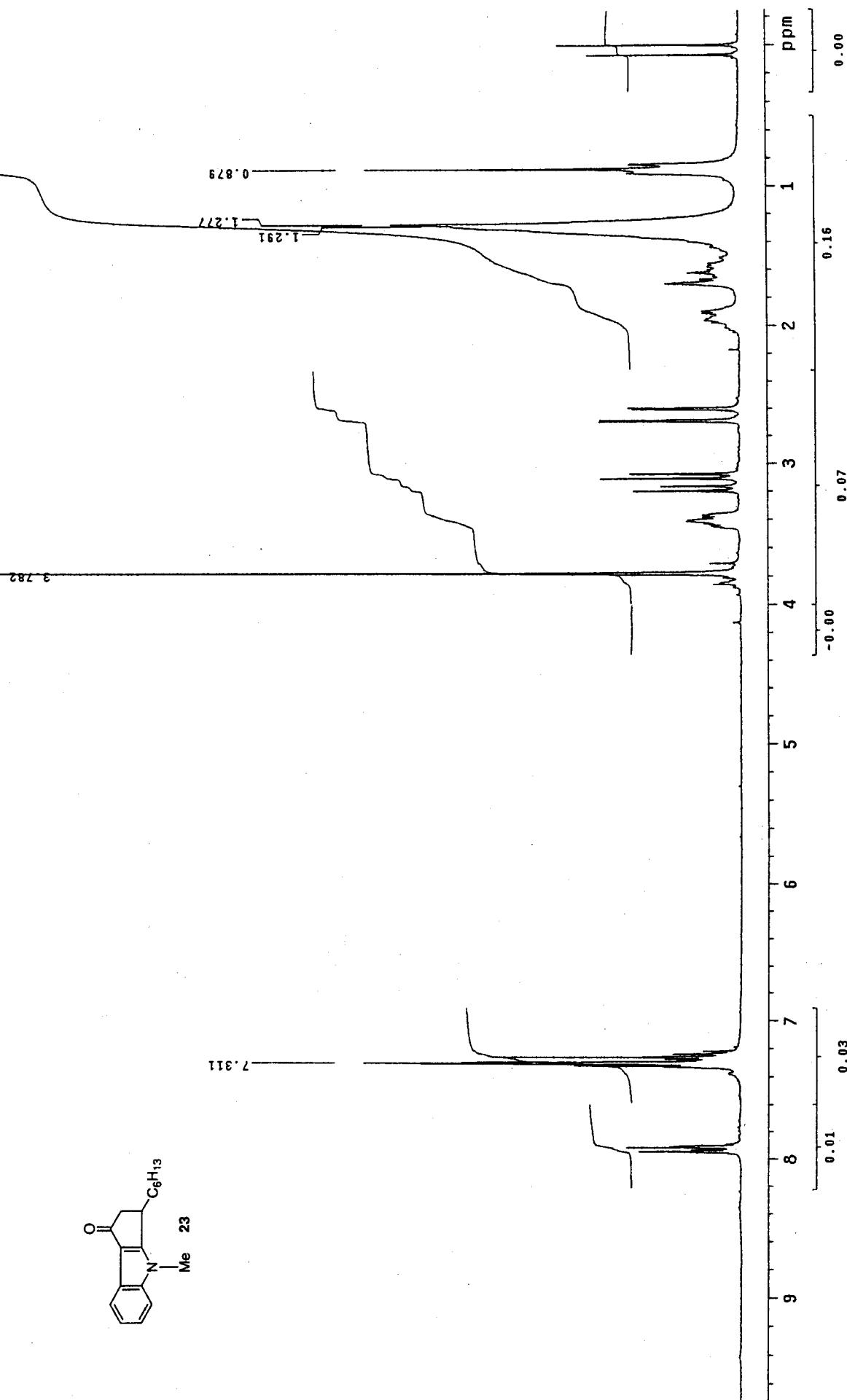
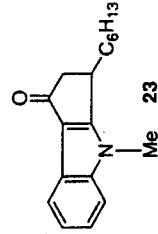
H1 / s2pu1 / Gem-200-DivIV
LOC: # 3 / Dissolvent: cdc13/ temp ambient
User1: jb/ Mostra: brosarecnf2
Data: 21/12/01 / Sistema automatic
Pulse Sequence: s2pu1



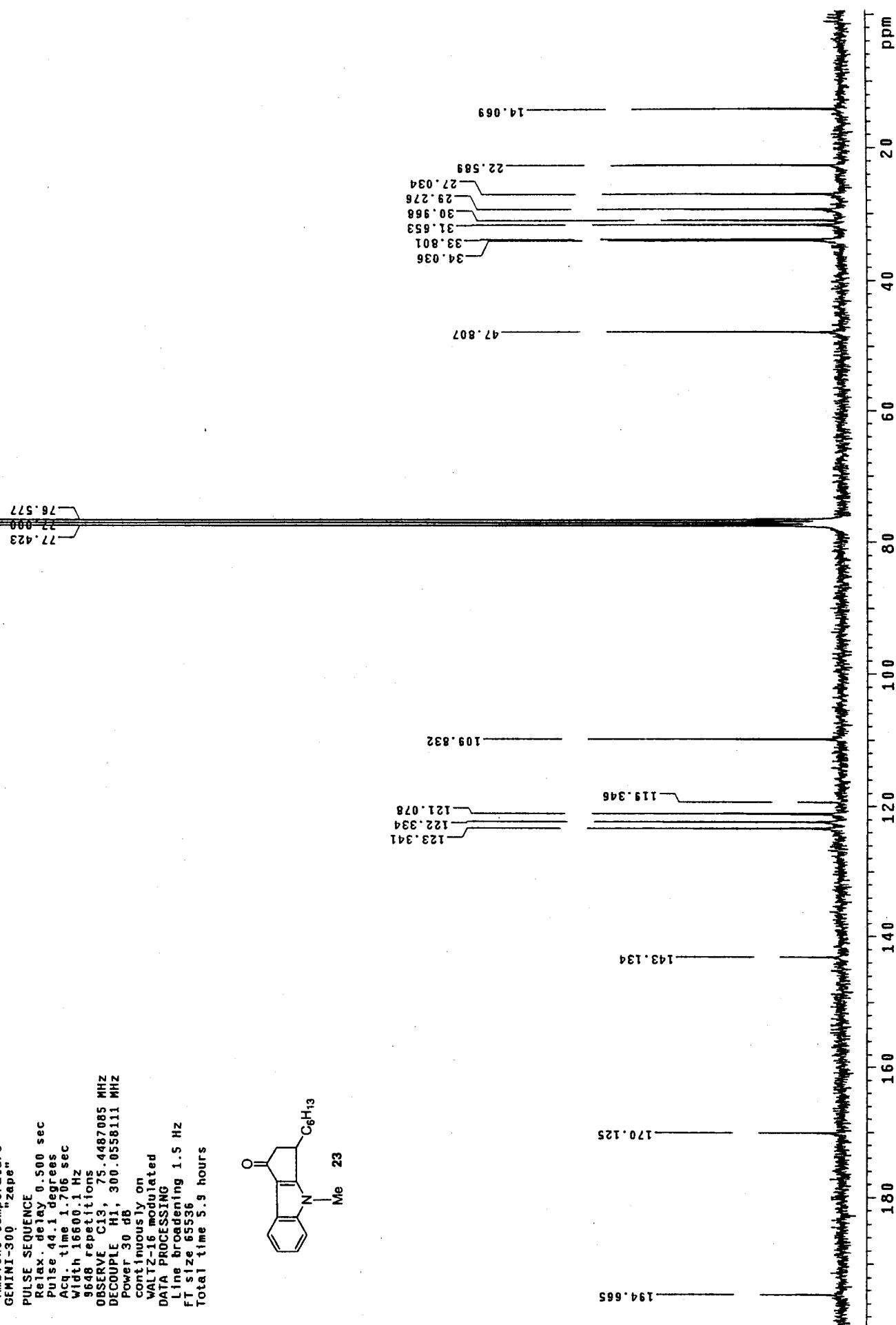
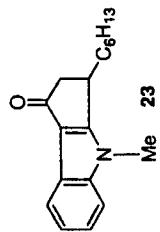
1:1 trans/cis 22



H1 / s2pu1 / Gem-200.DivIV
LOC: # 5 / Dissolvent: cdc13/ temp ambient
Usuar: Jb/ Mostre: arosa482.ec
Data: 20/12/01 / Sistema automatic
Pulse Sequence: s2pu1

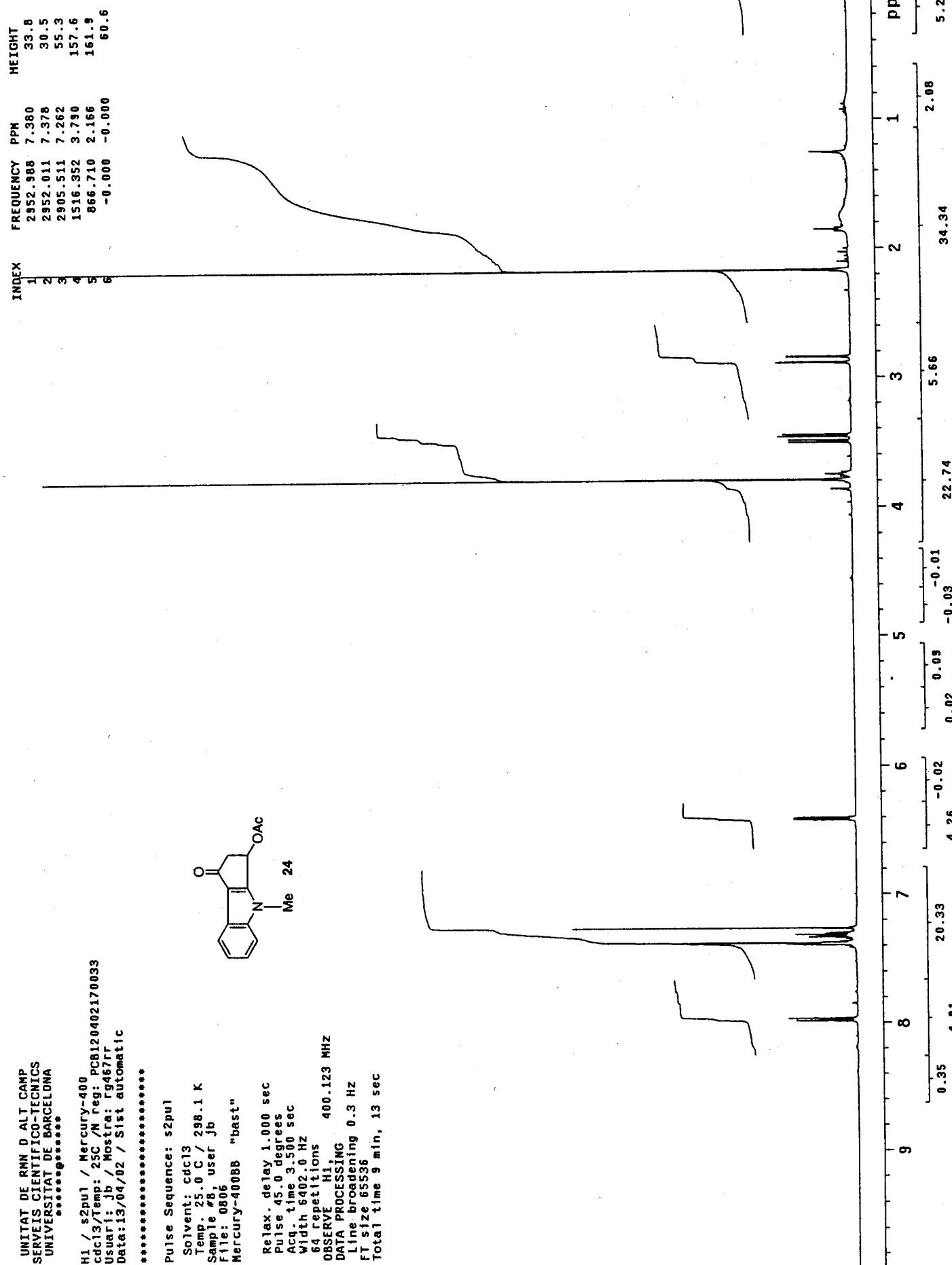
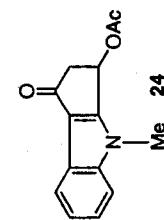


C13 / s2pu1 / Gemini-300
 CDCl₃ / 25C / N reg: F 0000
 Jb / rosa / Rosa
 Date 21/12/01 / qpe:r
 Solvent: CDCl₃
 Ambient temperature
 GEMINI-300 "Zap"
 PULSE SEQUENCE
 Relax. delay 0.500 sec
 Pulse 44.1 degrees
 Acq. time 1.706 sec
 Width 16600.1 Hz
 9648 repetitions
 OBSERVE C13, 75.4487085 MHz
 DECOUPLE H1, 300.0558111 MHz
 Power 30 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.5 Hz
 FT size 65536
 Total time 5.9 hours

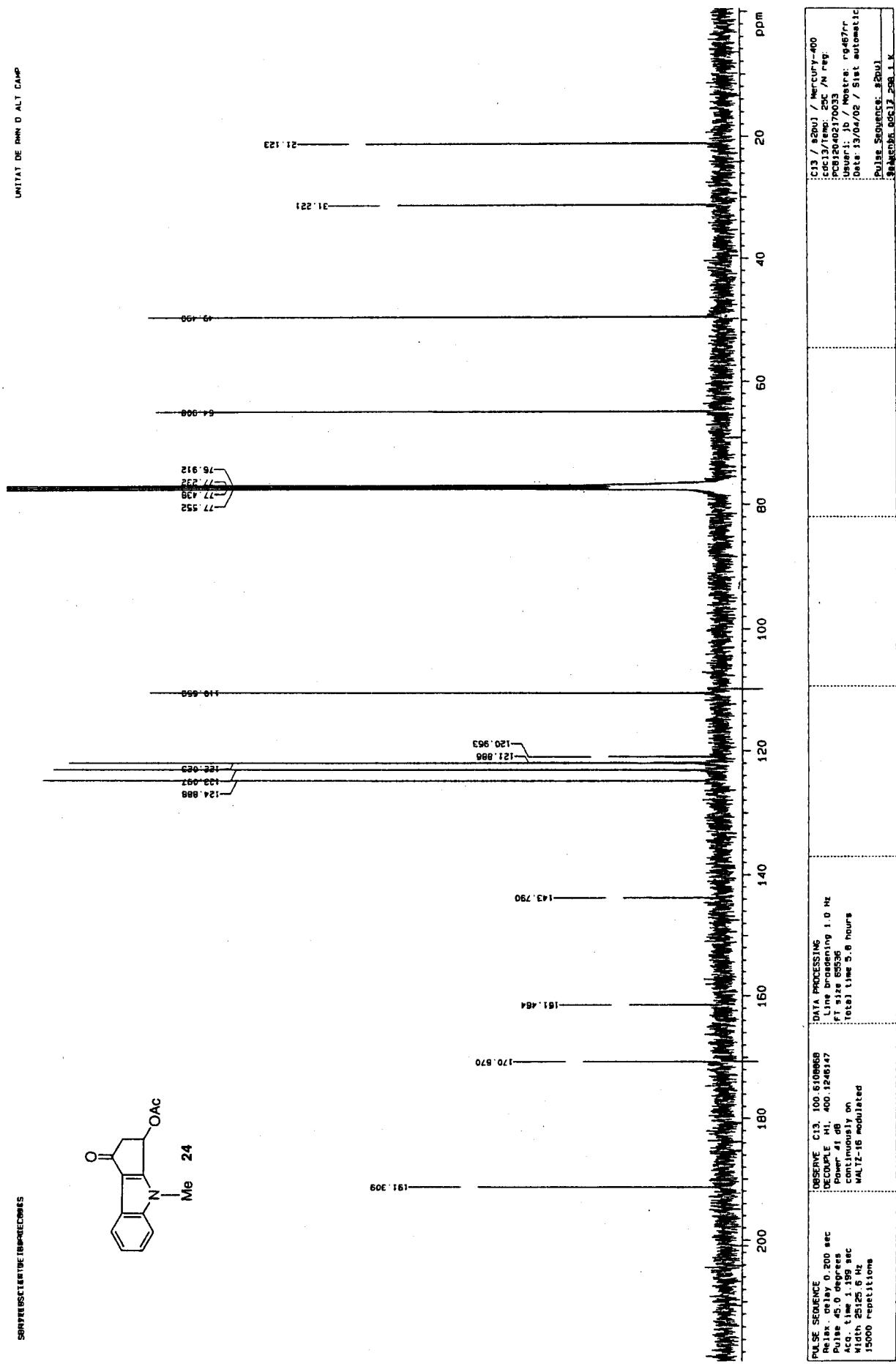
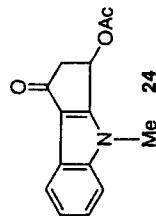


UNITAT DE RMN D ALT CAMP
 SECCIÓ CIENTÍFICO-TECNICS
 UNIVERSITAT DE BARCELONA
 *****@*****.es
 H1 / s2pu1 / Mercury-400
 cdc13/Temp: 25C / N reg: PCB120402170033
 User: jb / Hostra: rg467rf
 Data:13/04/02 / Sist: automatic

Pulse Sequence: s2pu1
 Solvent: cdc13
 Temp: 25.0 C / 298.1 K
 Sample #8, user jb
 File: 0806
 Mercury-400BB "bast"
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 3.500 sec
 Width 6402.0 Hz
 64 repetitions
 OBSERVE H1 400.123 MHz
 DATA PROCESSING
 Line broadening 0.3 Hz
 FT size 65536
 Total time 9 min, 13 sec



SOCIETY FOR SCIENCE IN MEDICINE



H1 / s2pu1 / Gem-200.DIVIV
LOC: # 3 / Dissolvent: cdc13/ temp ambient
User: jb/ Mostre: rg458720
Data: 22/10/01 / Sistema automatic
Pulse Sequence: s2pu1

