

**Total Synthesis and Evaluation of C26-Hydroxyepothilone D Derivatives
for Photoaffinity Labeling of β -Tubulin**

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Supporting Information

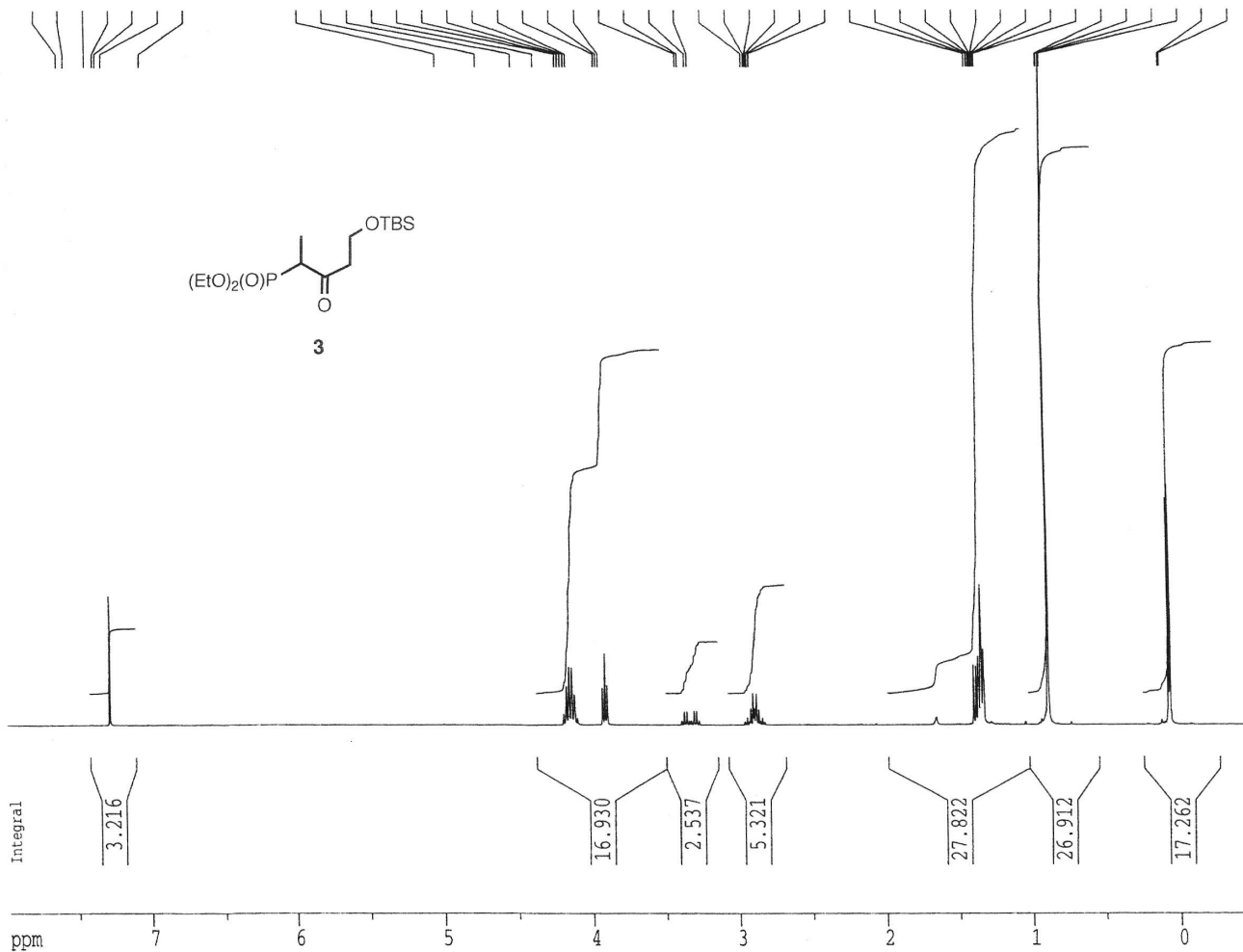
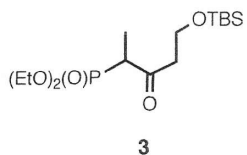
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¹ H NMR spectrum of 14	S11
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¹ H NMR spectrum of 15	S13
¹³ C NMR spectrum of 15	S14
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General Methods. All NMR spectra were acquired using either a 400 MHz (100 MHz) NMR or a 500 MHz (125 MHz) instrument and samples were dissolved in CDCl₃. All of the compounds prepared were oils unless specifically mentioned in the text. Infrared spectra were obtained using the oils on NaCl plates on a FT-IR. Optical rotations were obtained on a Polarimeter at 20 °C. Chemical ionization mass spectra were obtained on a quadrupole GC/MS system. Fast atom bombardment mass spectra were obtained on a mass spectrometer using a Xenon gun. Exact mass experiments were carried out on this instrument at 1:10,000 resolution using linear voltage scans. A HPLC system was used with a Chiracel OD-H column to determine the enantiomeric excess for the catalytic asymmetric reductions for **5** and **10**. All reagents were purchased and used without further purification unless mentioned specifically. THF and Et₂O were distilled from sodium benzophenone ketyl and CH₂Cl₂ from calcium hydride. All moisture sensitive reactions were conducted under a positive argon or nitrogen pressure. Column chromatography was carried out on silica gel 60 with a 0.040-0.063 particle size (230-400 mesh). TLCs were recorded on silica gel 60 F254 aluminum plates. Preparative chromatography was done on 1000 micron silica gel GF plates with UV 254.

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7.5418
7.3974
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7.3234
7.2831
7.0192

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4.4882
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4.1535
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3.2847
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2.8907
2.8820
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2.8606
1.3945
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1.3635
1.3593
1.3495
1.3460
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Current Data Parameters
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PROCNO 1

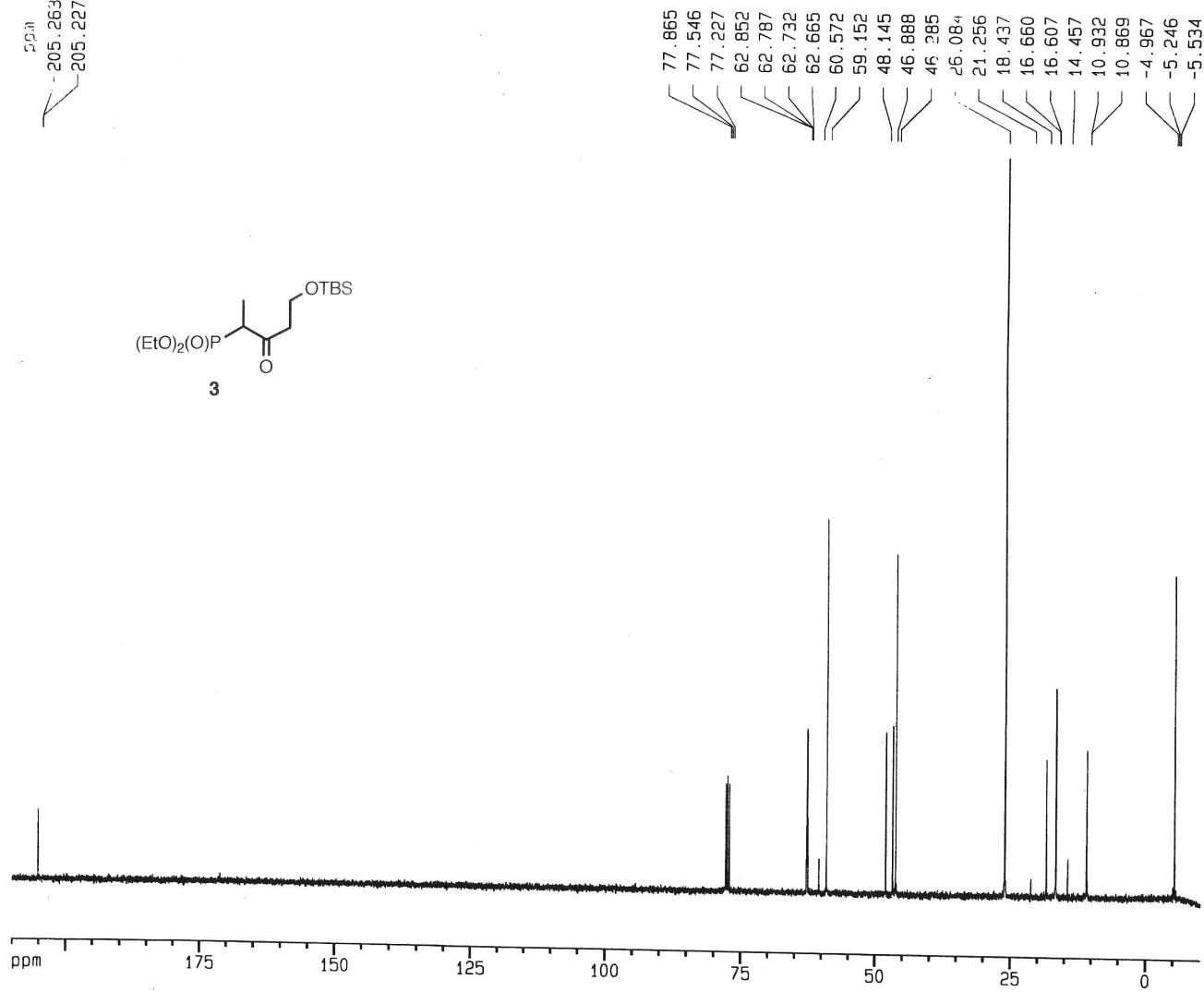
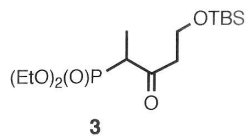
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TE 300.0 K
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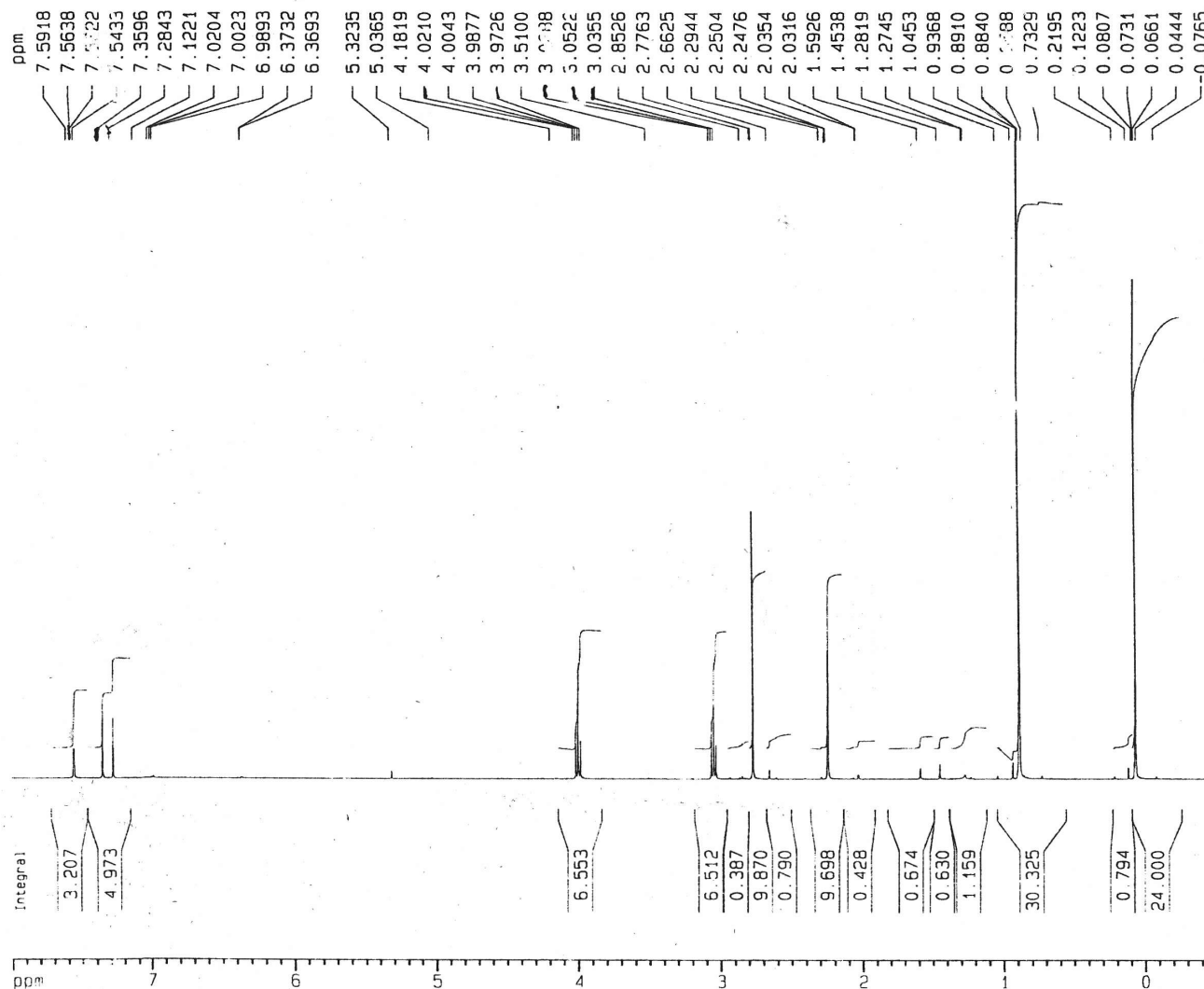
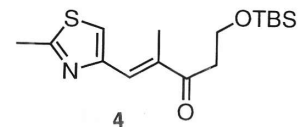


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NUC2 1H
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PROCNO 1

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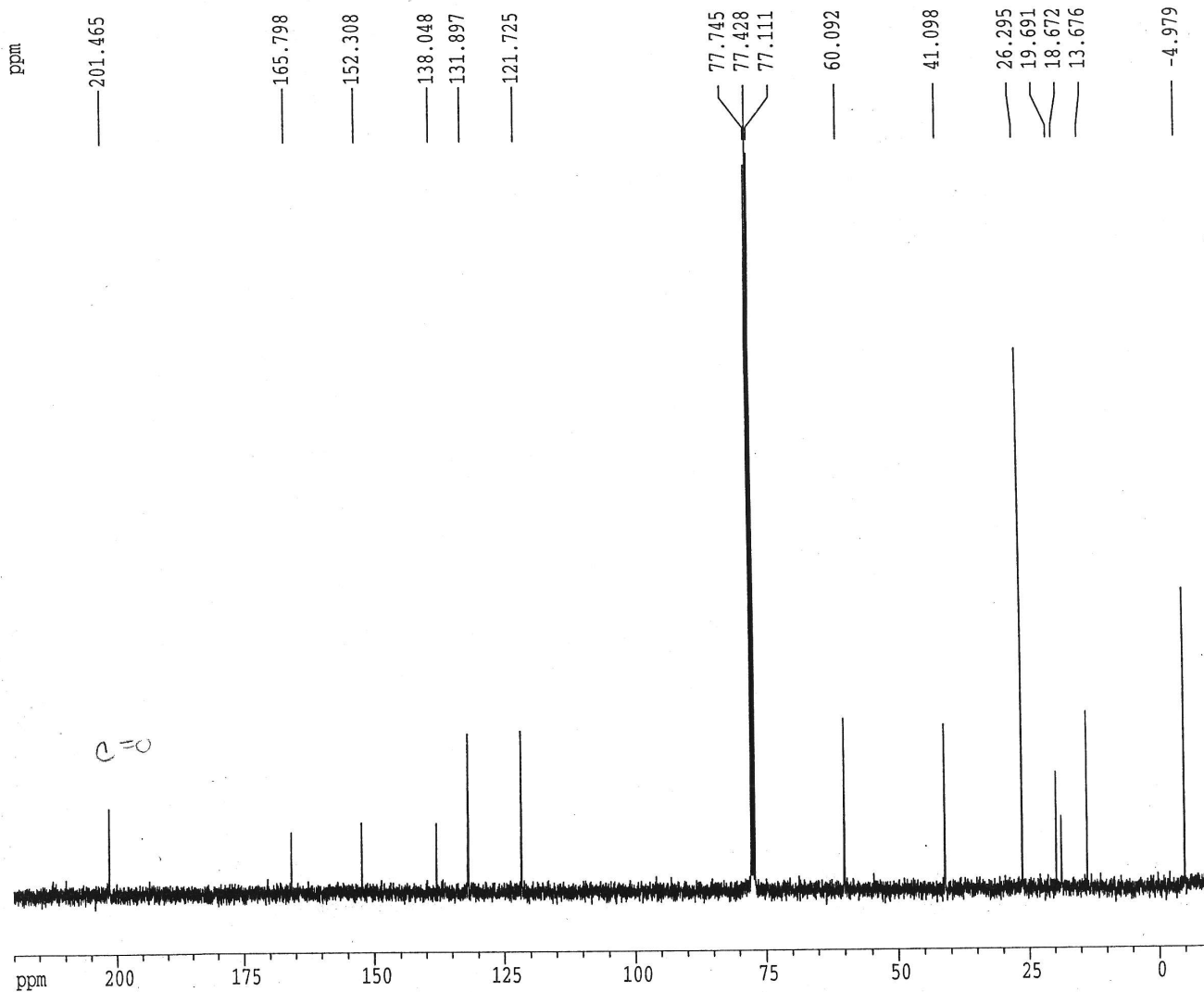
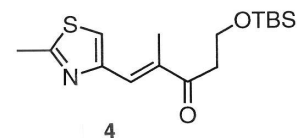
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DE 4.50 usec
TE 300.2 K
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DE 4.50 usec
SF01 400.1320007 MHz
NUC1 1H
PL1 -6.00 dB

F2 - Processing parameters

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SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters

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F1P 8.000 ppm
F1 3201.04 Hz
F2P -0.500 ppm
F2 -200.07 Hz
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HZCM 170.05525 Hz/cm



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 SOLVENT CDCl3
 NS 793
 DS 2
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 FIDRES 0.353213 Hz
 AQ 1.4156276 sec
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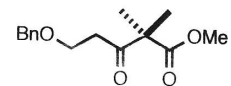
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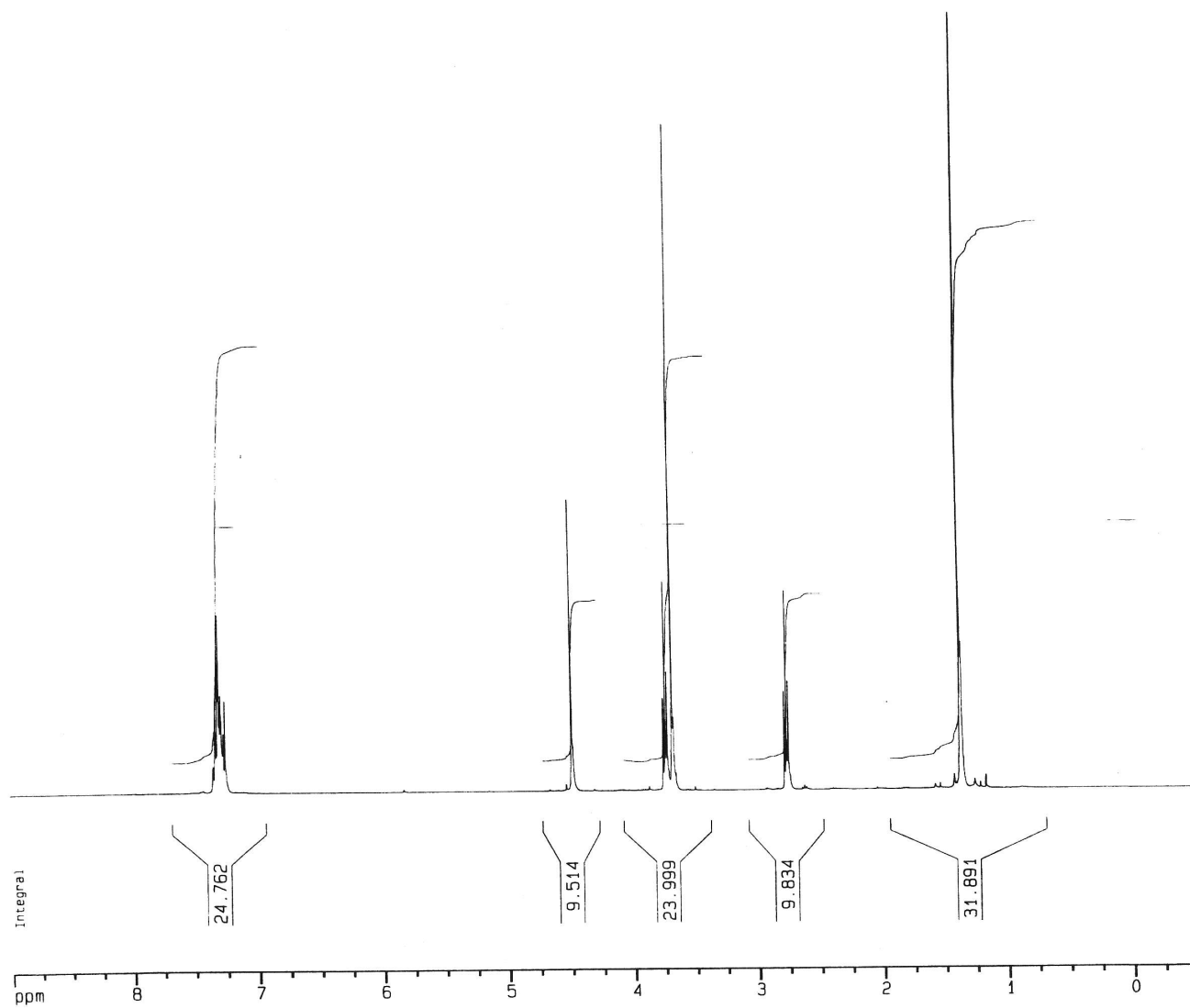
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ii-ear-154
fractions
187 mg b-keto ester



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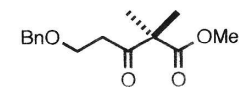
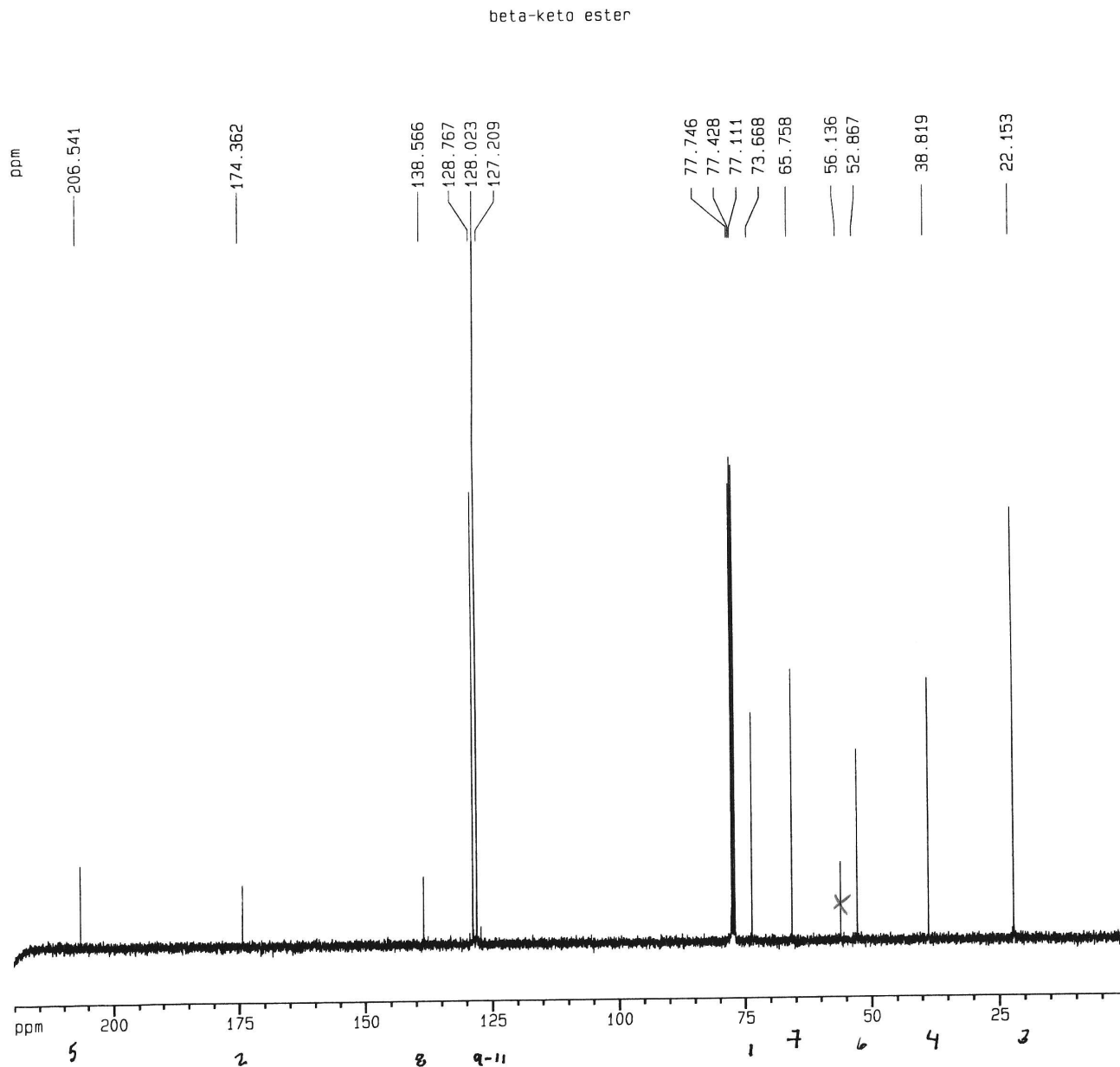


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DE 4.50 usec
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NUC1 1H
PL1 -6.00 dB

F2 - Processing parameters
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LB 0.30 Hz
GB 0
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1D NMR plot parameters
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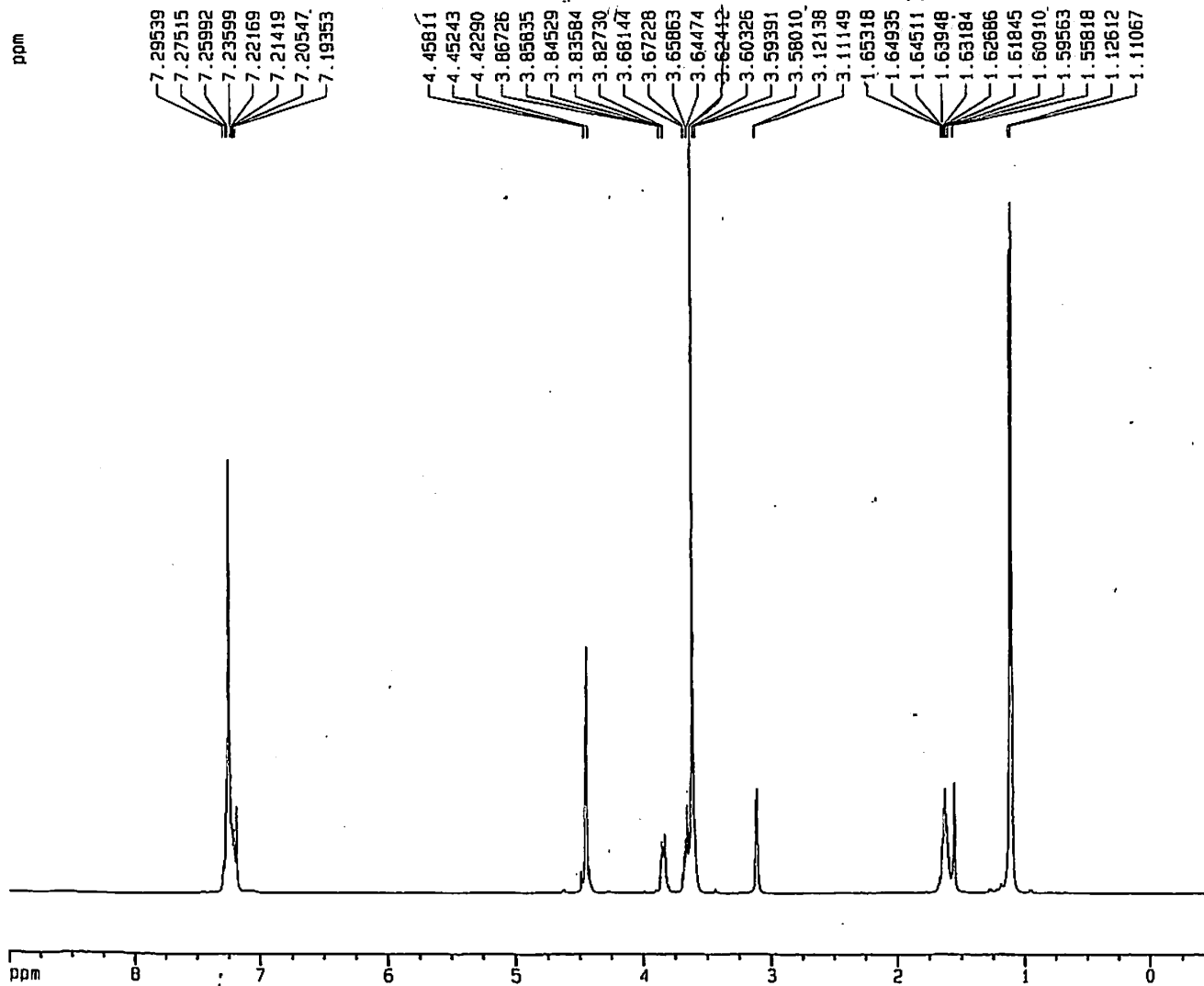
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 SF02 400.1316005 MHz
 NUC2 1H
 PL2 -6.00 dB
 PL12 18.00 dB
 P1 6.90 usec
 DE 4.50 usec
 SF01 100.6232933 MHz
 NUC1 13C
 PL1 -6.00 dB

F2 - Processing parameters
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1D NMR plot parameters
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 F2P 0.000 ppm
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ppm



Current Data Parameters

NAME ear2.197
EXPNO 1
PROCNO 1

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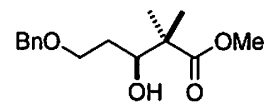
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PL1 -6.00 dB

F2 - Processing parameters

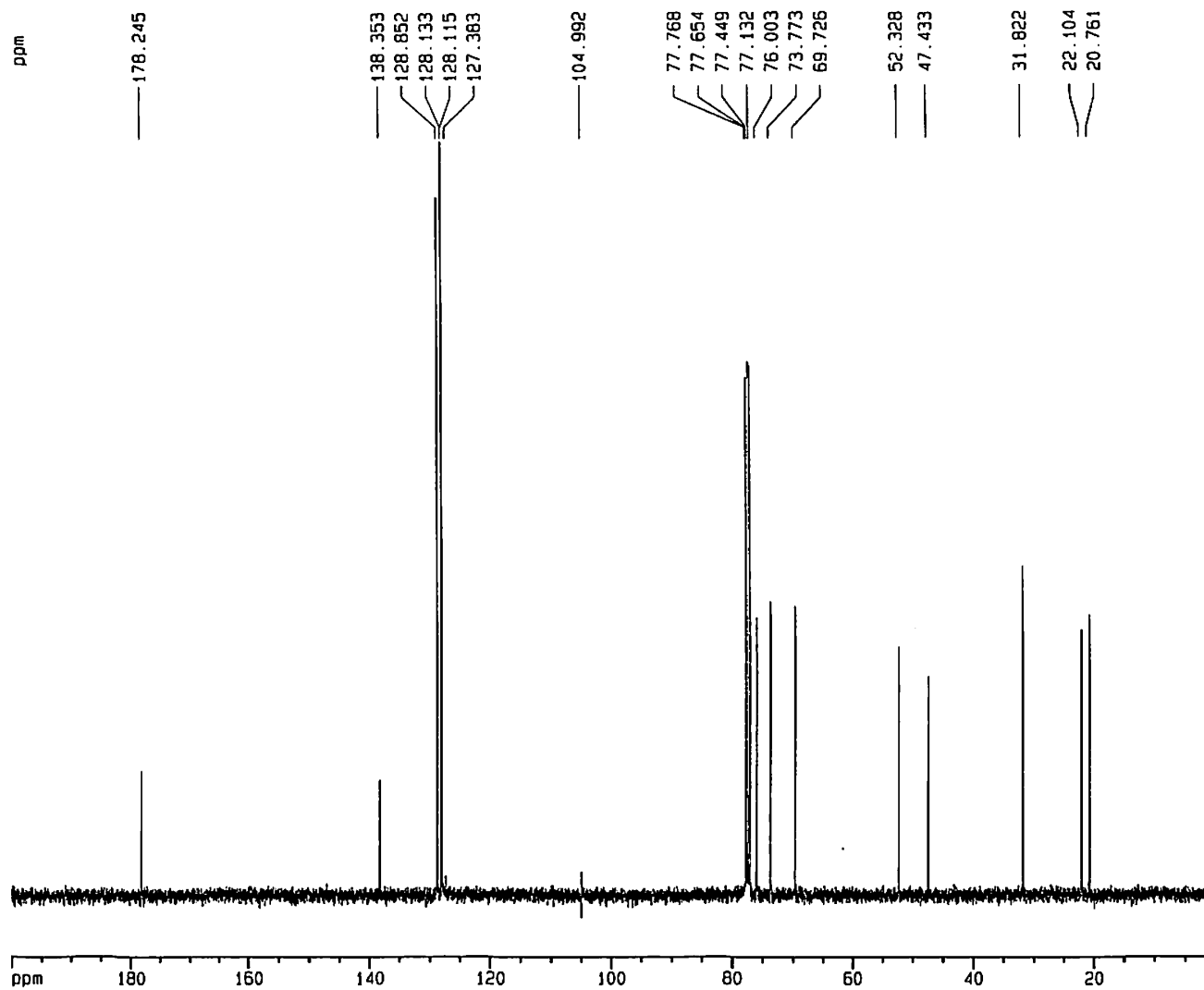
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1D NMR plot parameters

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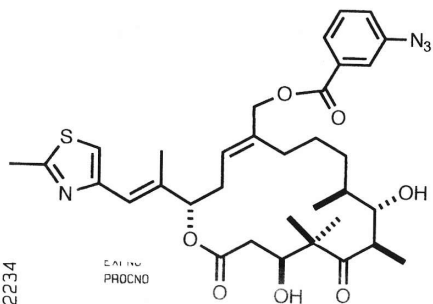
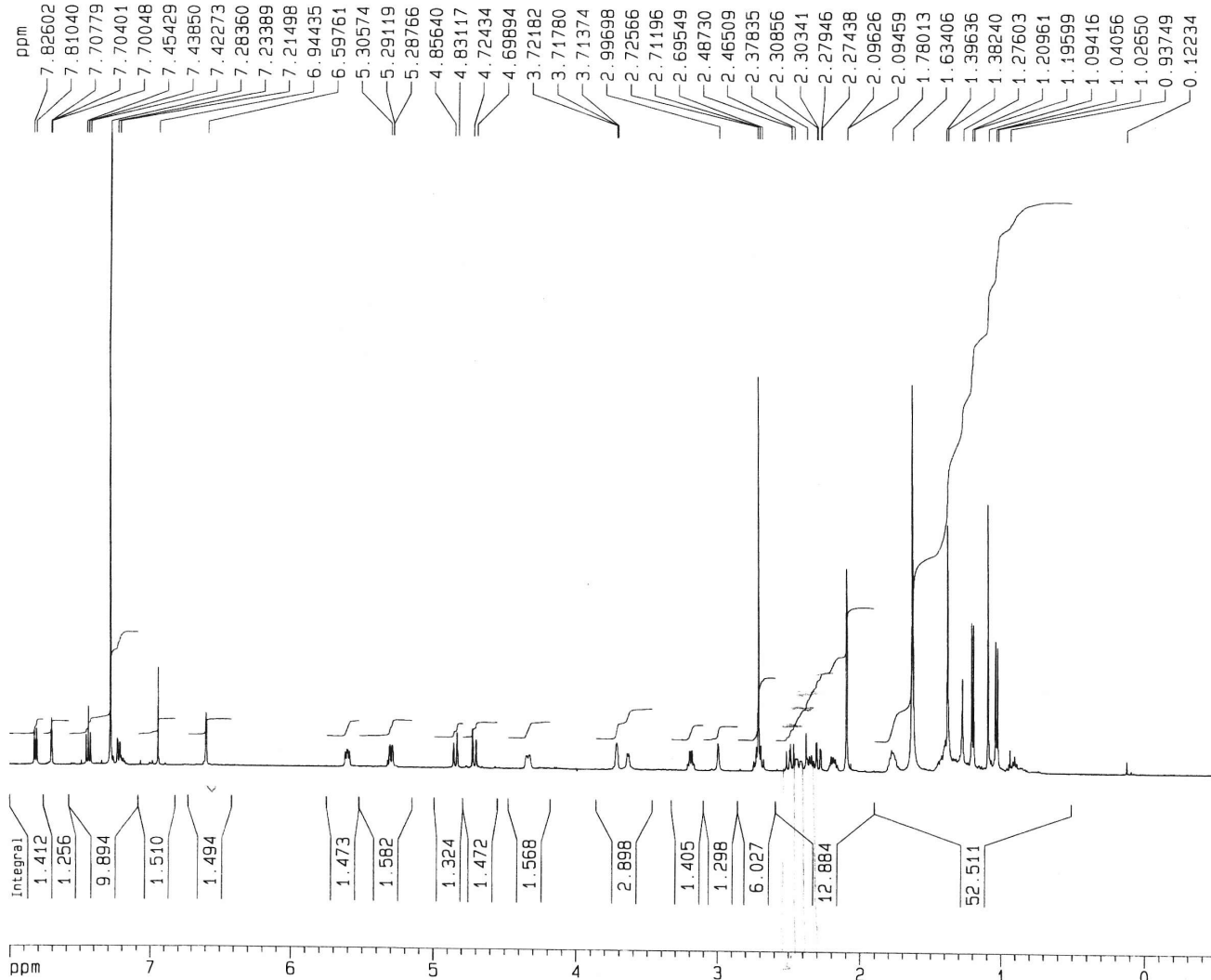


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 PROCNO 1

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 SOLVENT COC13
 NS 945
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 FIDRES 0.353213 Hz
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 DE 4.50 usec
 TE 300.0 K
 d11 0.0300000 sec
 d12 0.0000200 sec
 PL13 18.00 dB
 O1 0.05000000 sec
 CPOPRG2 waltz16
 PCPD2 100.00 usec
 SF02 400.1316005 MHz
 NUC2 1H
 PL2 -6.00 dB
 PL12 18.00 dB
 P1 6.90 usec
 DE 4.50 usec
 SF01 100.6232933 MHz
 NUC1 13C
 PL1 -6.00 dB

F2 - Processing parameters
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 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
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 F1 20122.55 Hz
 F2P 0.000 ppm
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 HZCM 1006.12732 Hz/cm



```

NAME
PROCNO

F2 - Acquisition
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Time
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SOLVENT CDC13
NS 65
DS 2
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RG 1149.4
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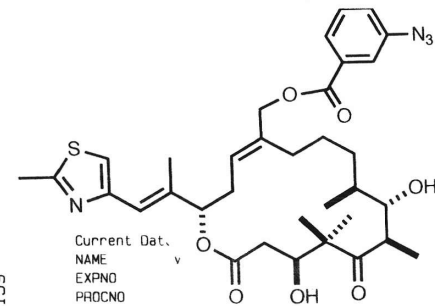
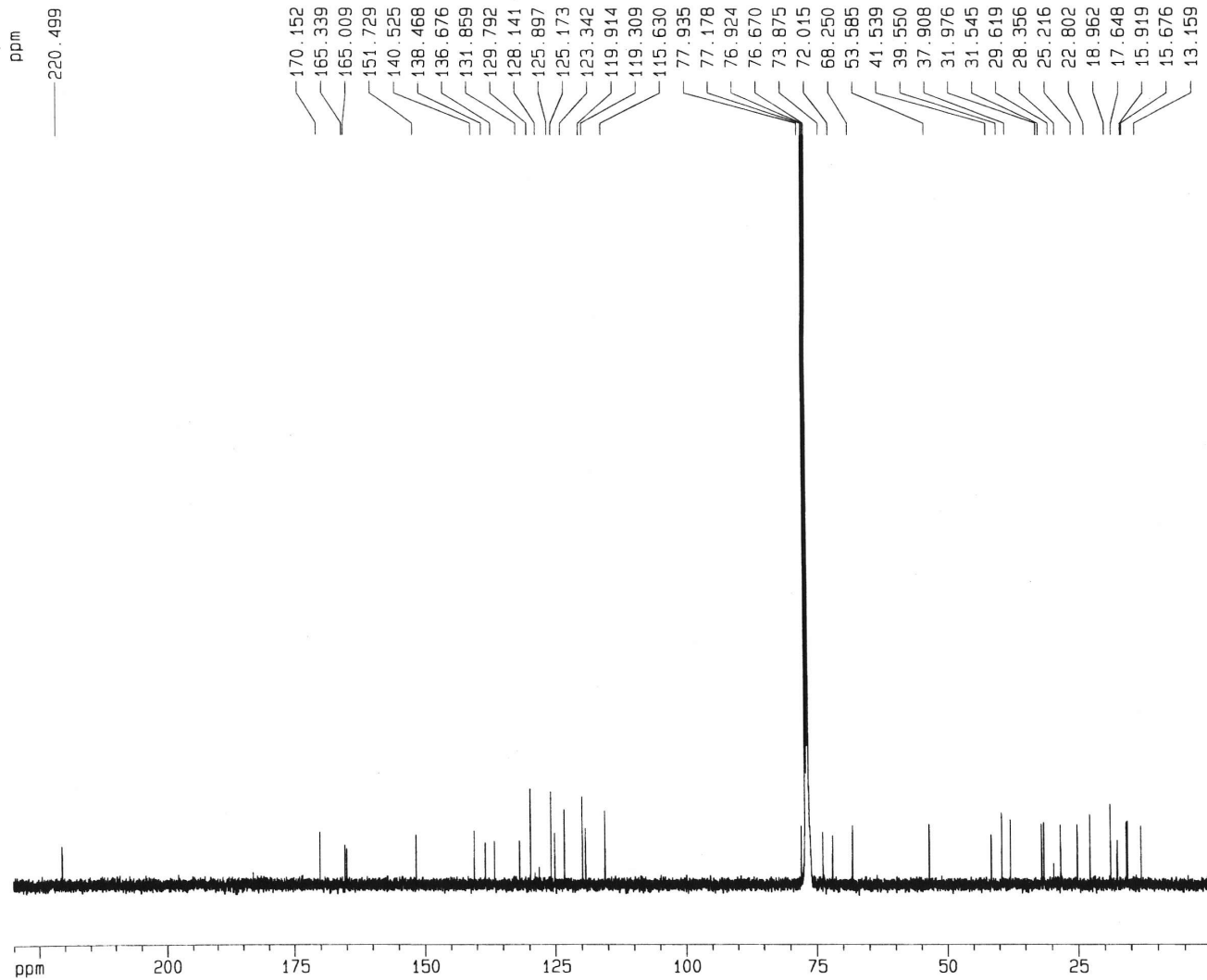
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LB 0.30 Hz
GB 0
PC 1.00

F1 - Processing parameters
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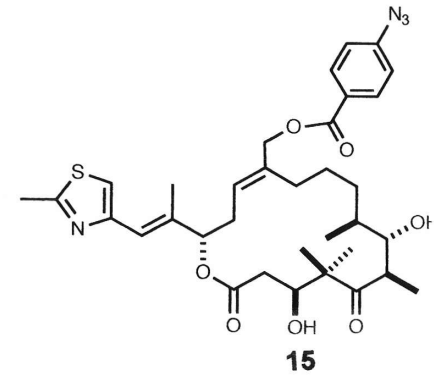
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PL13 30.00 dB
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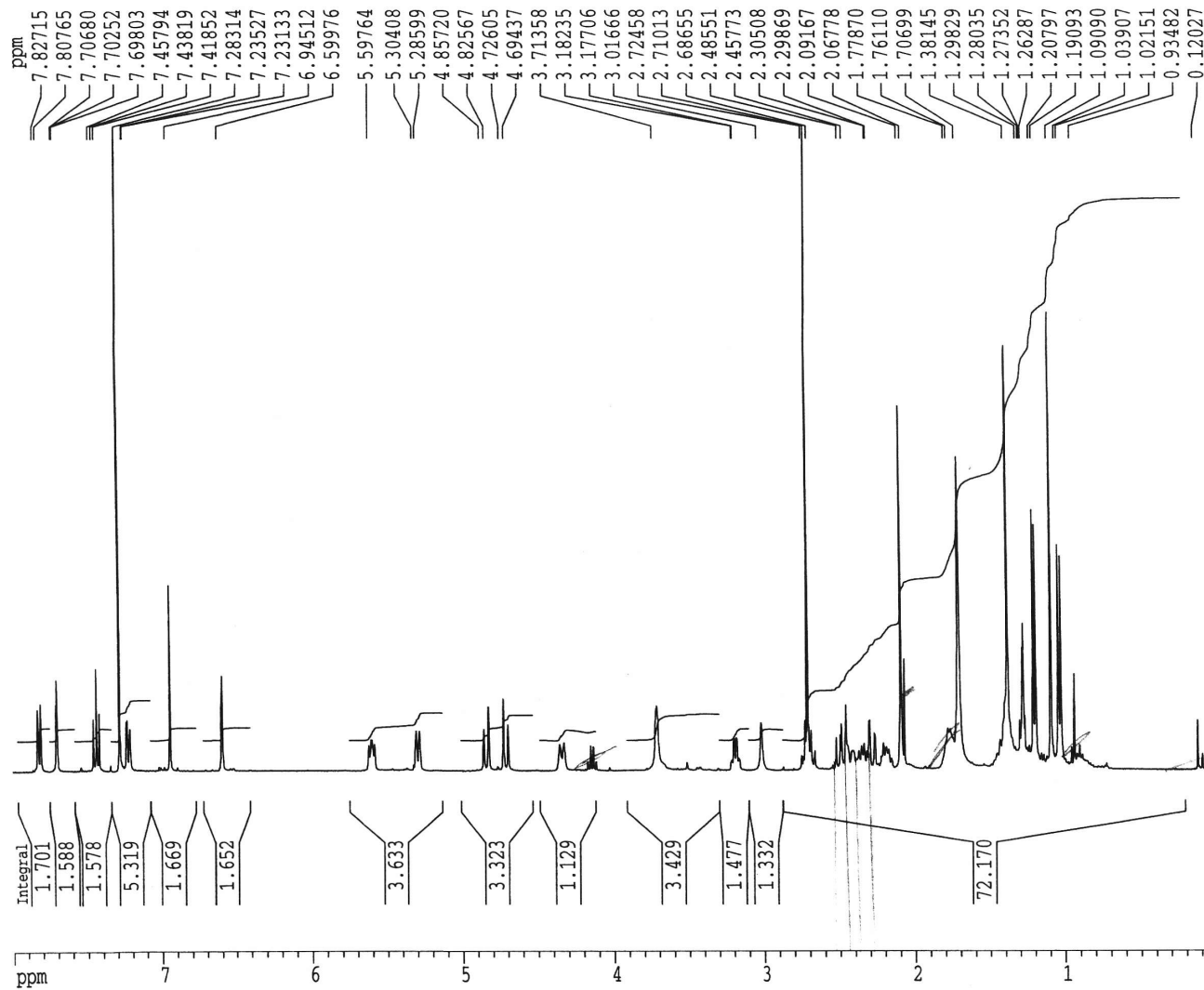


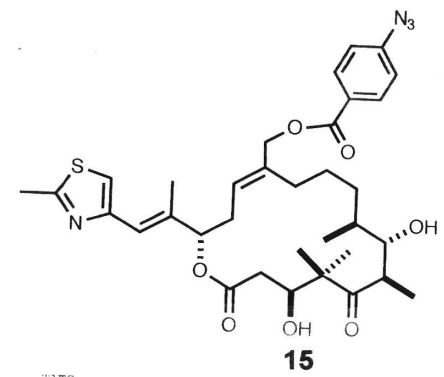
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1D NMR plot parameters
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 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 0.40000 ppm/cm
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```

time 1.00
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TE 300.0 K
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d11 0.03000000 sec
d12 0.00002000 sec

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PL1 2.00 dB
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PL12 18.00 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

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F2 - Processing parameters
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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1D NMR plot parameters
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HZCM 1131.89319 Hz/cm

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