

# First Multi-gram Preparation of SCP-123, A Novel Water Soluble Analgesic

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## **Supporting Information (6 pages)**

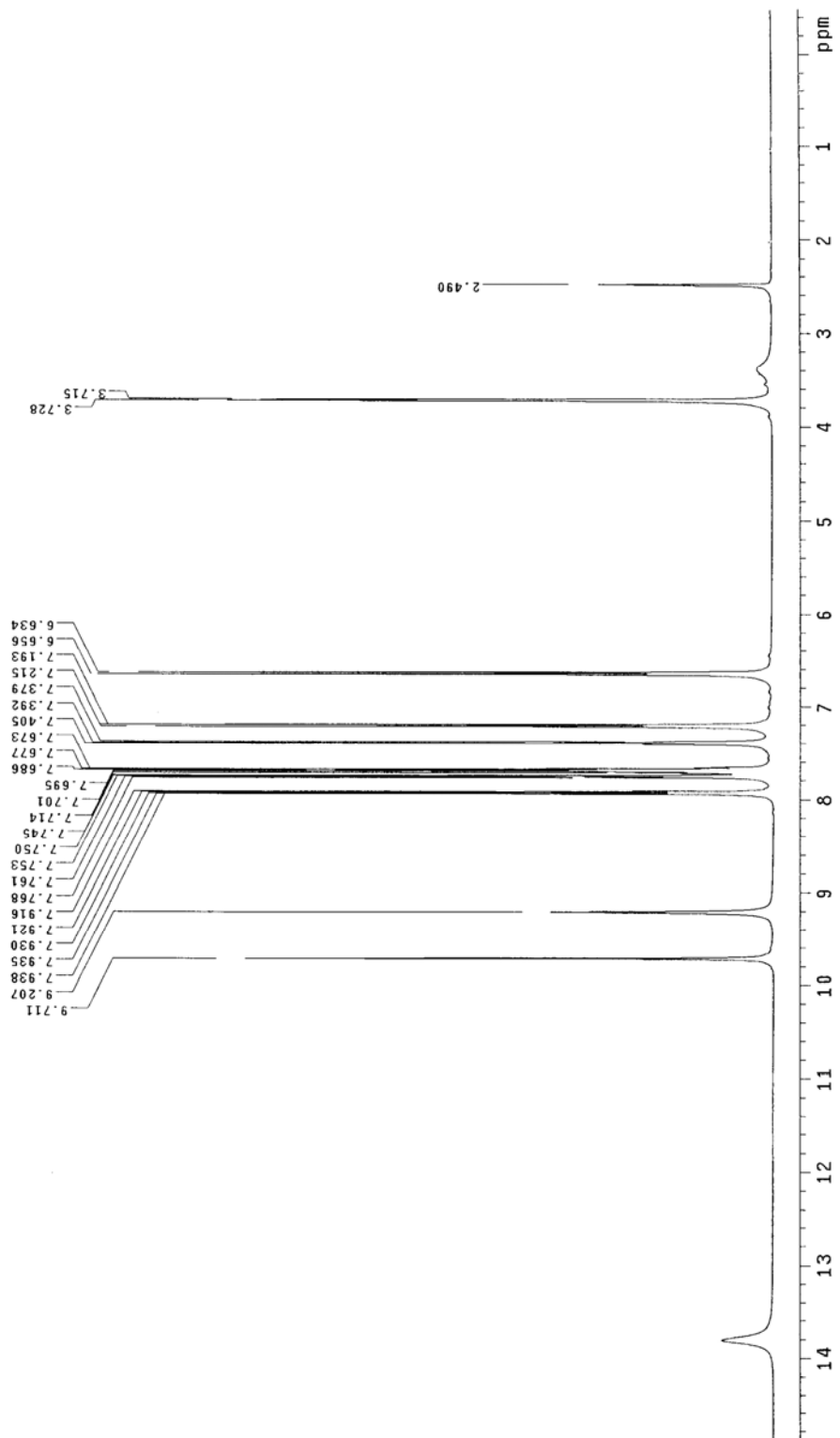
<sup>1</sup>H NMR **4**, **5** and **12**

HPLC Conditions

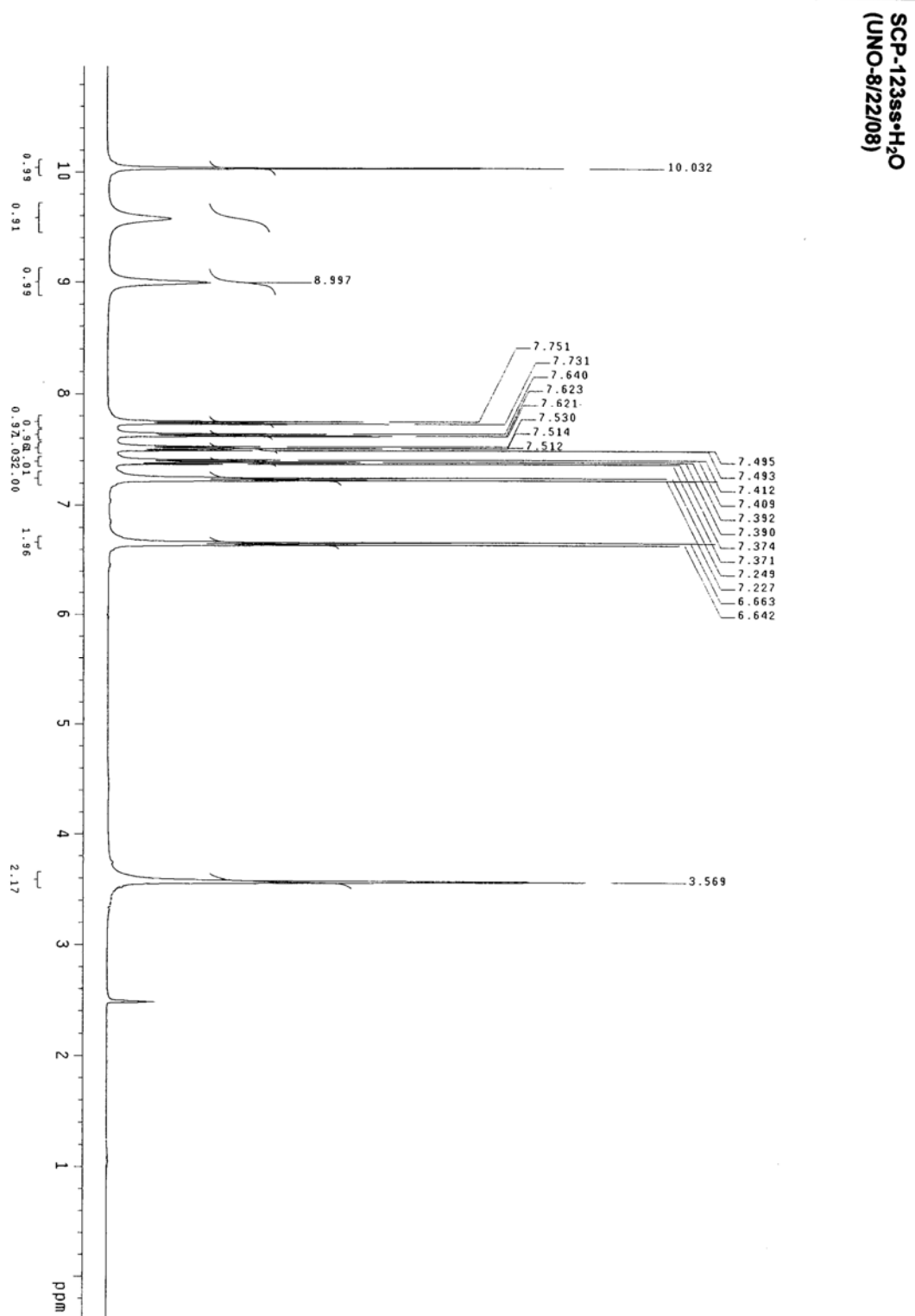
LC-ESI-MS spectrum of **12**.

<sup>1</sup>H NMR Spectrum of SCP-123 (4) in DMSO-d<sub>6</sub>.

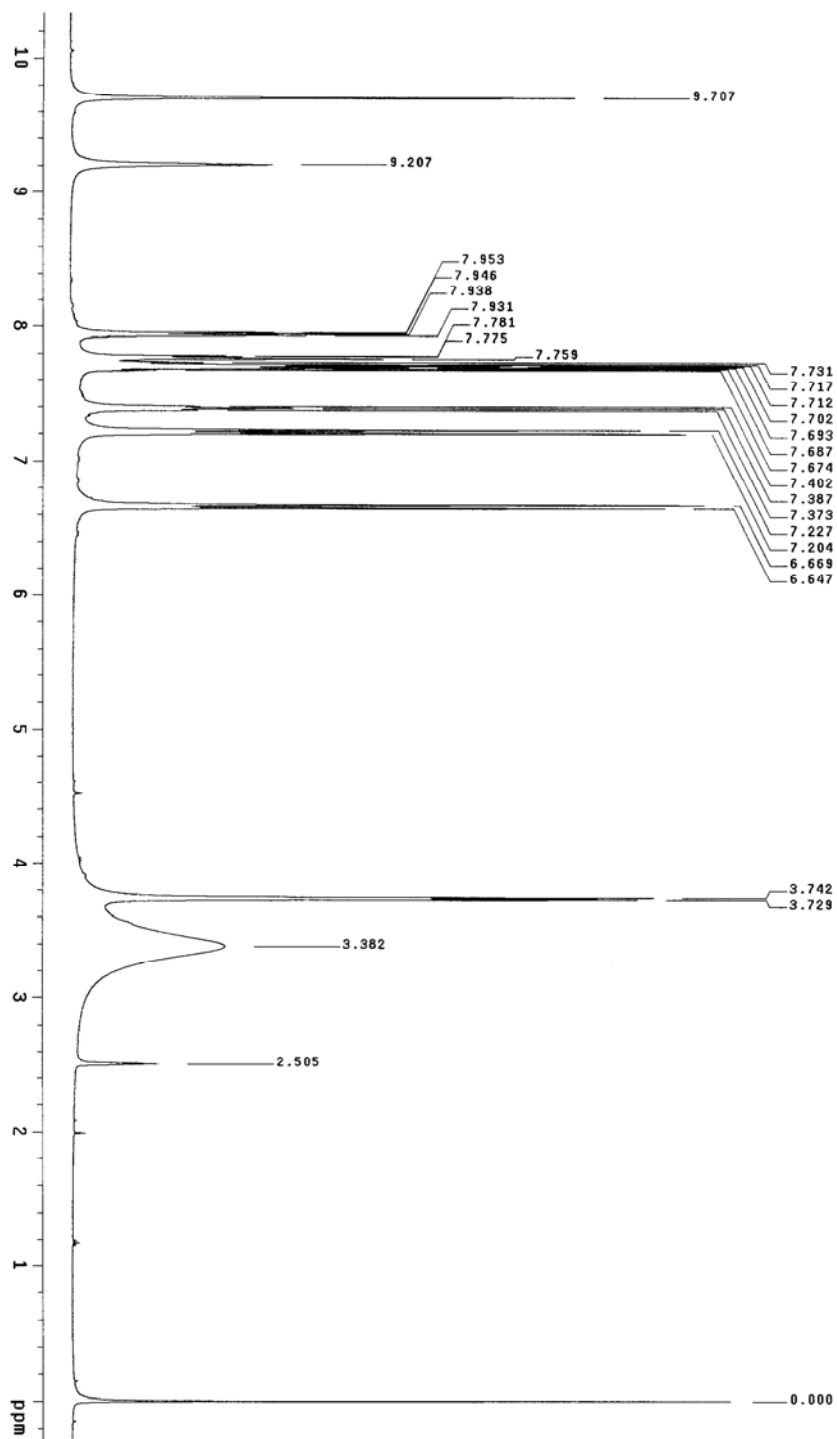
SCP-123  
(UNO-5/29/08)



$^1\text{H}$  NMR Spectrum of SCP-123ss (5) in DMSO- $d_6$ .



$^1\text{H}$  NMR Spectrum of **12** in  $\text{DMSO-d}_6$ .



## **HPLC ANALYSIS**

### **1. REAGENTS AND INSTRUMENTATION**

- Trifluoroacetic acid, HPLC Grade Aldrich.
- Acetonitrile HPLC grade EM Science.
- HPLC Waters 501/486 Tunable Detector
- Column: Waters Nova-Pak C18 (3.9 x 150 mm) Steel Analytical.

### **2. CROMATOGRAPHIC CONDITIONS**

- Flow: 1.0 ml/min
- Column Temperature 25<sup>0</sup>C
- Volume injection: 5 µl
- Detector: Ultraviolet absorption- wavelength 254 nm.

Mobile phase: Gradient, **Table 1.**

A. TFA 0.1 % in acetonitrile

B. TFA 0.1% in water.

**Table 1: Gradient.**

Time (min)	%A	%B
0	0	100
5	0	100
30	100	0
32	100	0
33	0	100
45	0	100

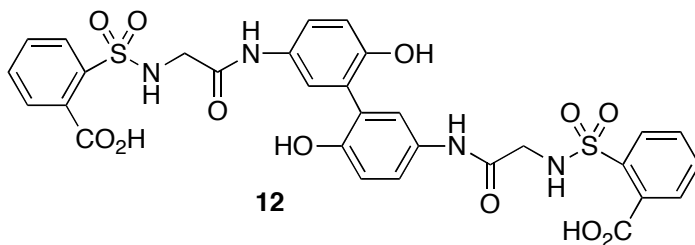
### **3. RETENTION TIME**

Compound	t <sub>R</sub> (min)*
<b>3</b>	3.1
<b>4</b>	15.8
<b>12</b>	17.0

\*Average of three runs.

## LC-ESI-MS IDENTIFICATION OF DIMER 12

LC-TSQ Quantum Instrument (Thermo-Finnigan) coupled to Surveyor, equipped with electro-spray ionization (ESI)



Chemical Formula:  $C_{30}H_{26}N_4O_{12}S_2$   
MW: 698.68

### Q1 Full Scan

JMM-1-28 Mark-2 13Feb04 #43 RT: 0.64 AV: 1 NL: 1.24E7  
T: - p sld=10.00 Q1MS [00.00-1000.00]

