

Supporting Information

Rec. Nat. Prod. **9:2** (2015) 184-189

Isolation, Structure Determination, In Vivo/Vitro Assay and Docking Study of a Xanthone with antitumor activity from Fungus *Penicillium oxalicum*.

Gang Chen^{1,2}, Jiao Bai^{1,2}, Haifeng Wang^{1,2}, Shuling Zhang³
and Yuehu Pei^{1,2*}

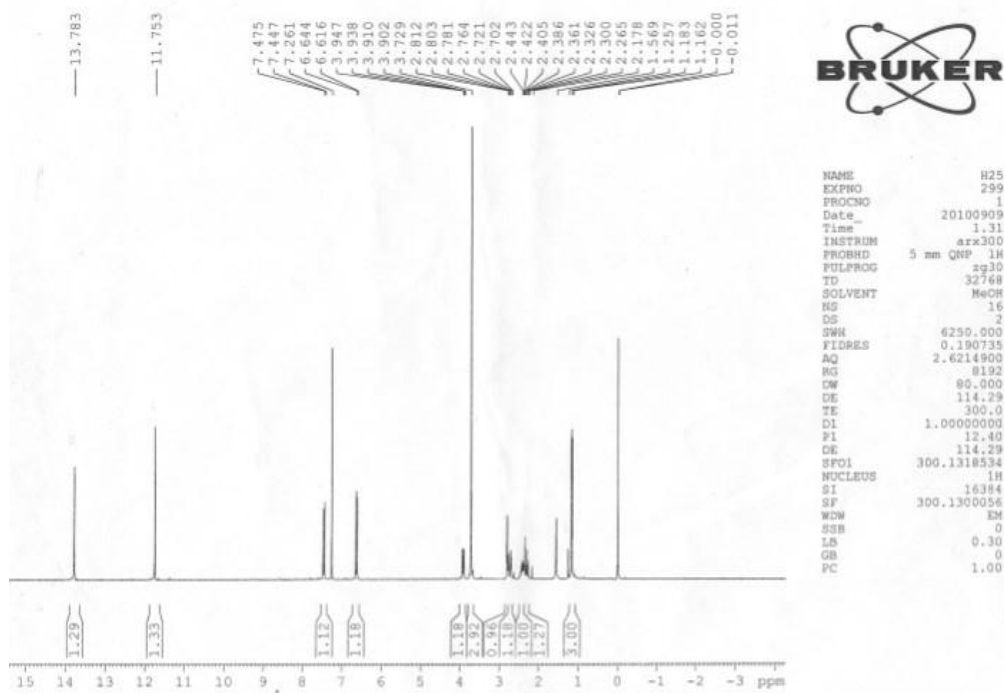
¹ School of Traditional Chinese Materia Medica, Shenyang Pharmaceutical University, Shenyang 110016, China

² Key Laboratory of Structure-Based Drug Design & Discovery Ministry of Education, Shenyang Pharmaceutical University, Shenyang 110016, China

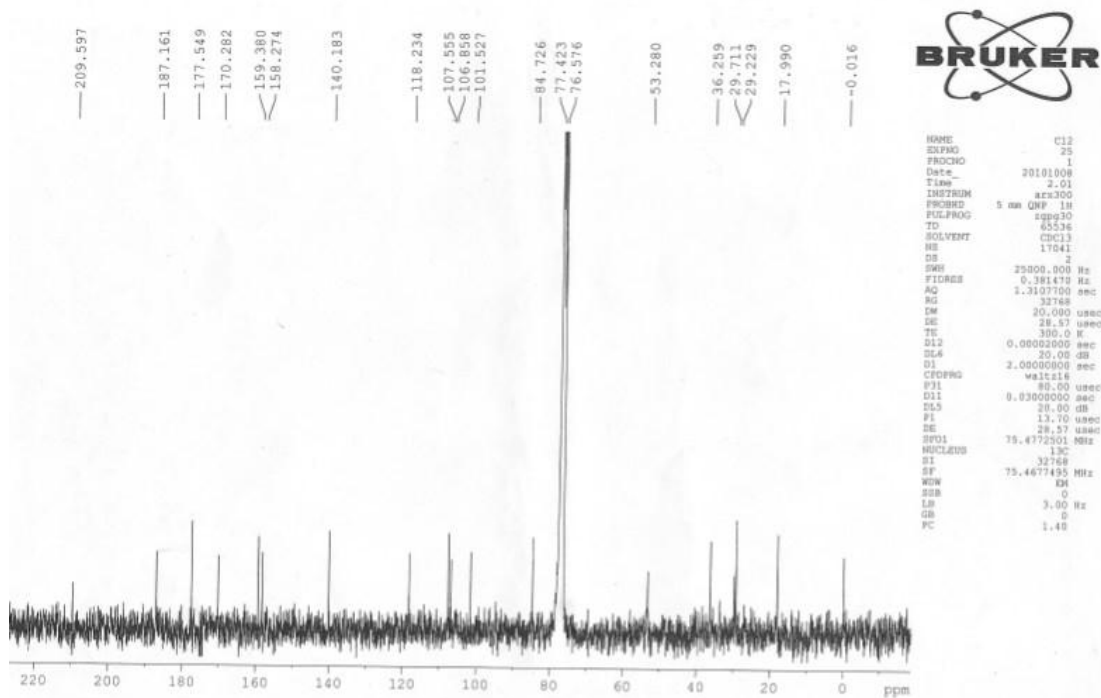
³ Division of Oncology, Shengjing Hospital of China Medical University, Shenyang, 110004, China

Table of Contents	Page
S1: The ¹ H NMR spectrum of compound 1	2
S2: The ¹³ C NMR spectrum of compound 1	2
S3: The ESIMS spectrum of compound 1	3
S4: The HSQC spectrum of compound 1	3
S5: The HMBC spectrum of compound 1	4

* Corresponding author: E-Mail: peiyuehu@vip.163.com ; Phone:086-024-23986485



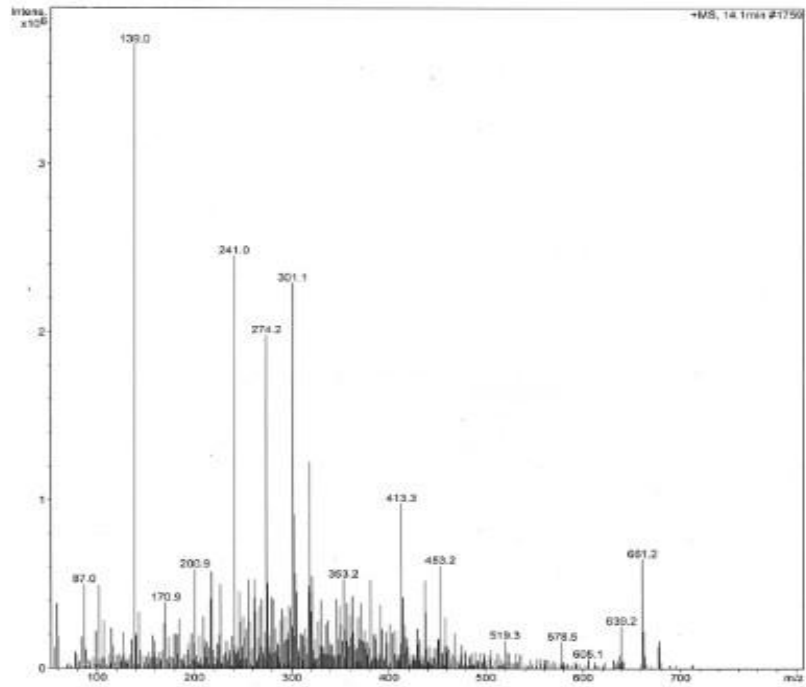
S1 : The ^1H NMR spectrum of compound 1



S2 :The ^{13}C NMR spectrum of compound 1

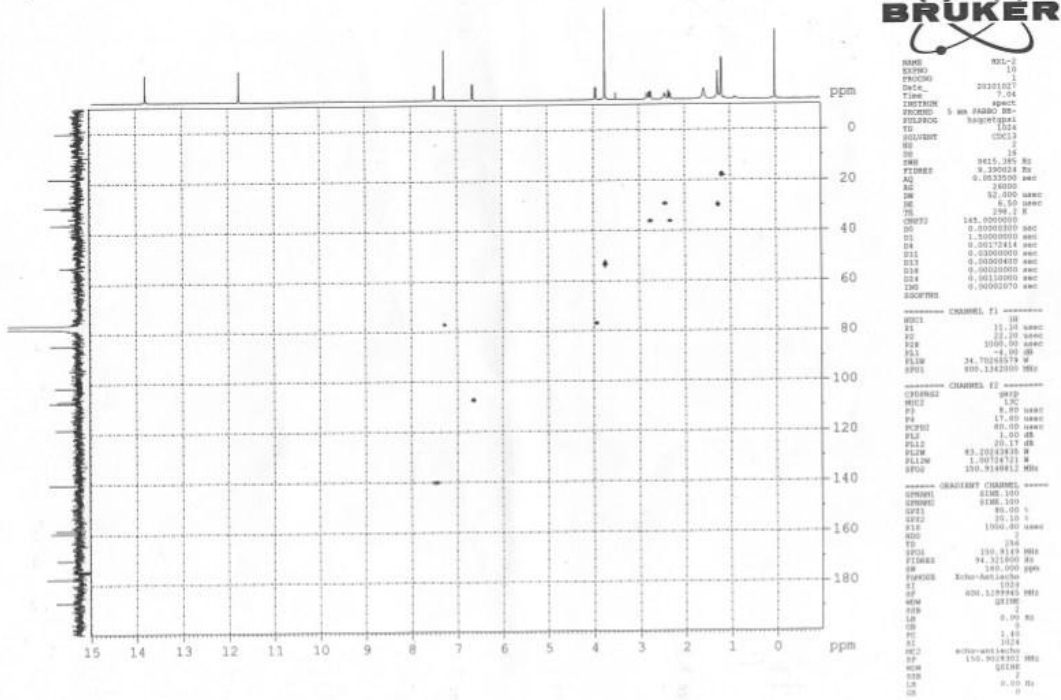
Direct Mass Spectrometry Analysis

Analysis Name: 10113002.d **Instrument:** LC-MSD-Trip-SL **Print Date:** 11/30/2010 6:36:59 PM
Sample Name: HDL-2 **Operator:** admin **Acq. Date:** 11/30/2010 6:18:50 PM

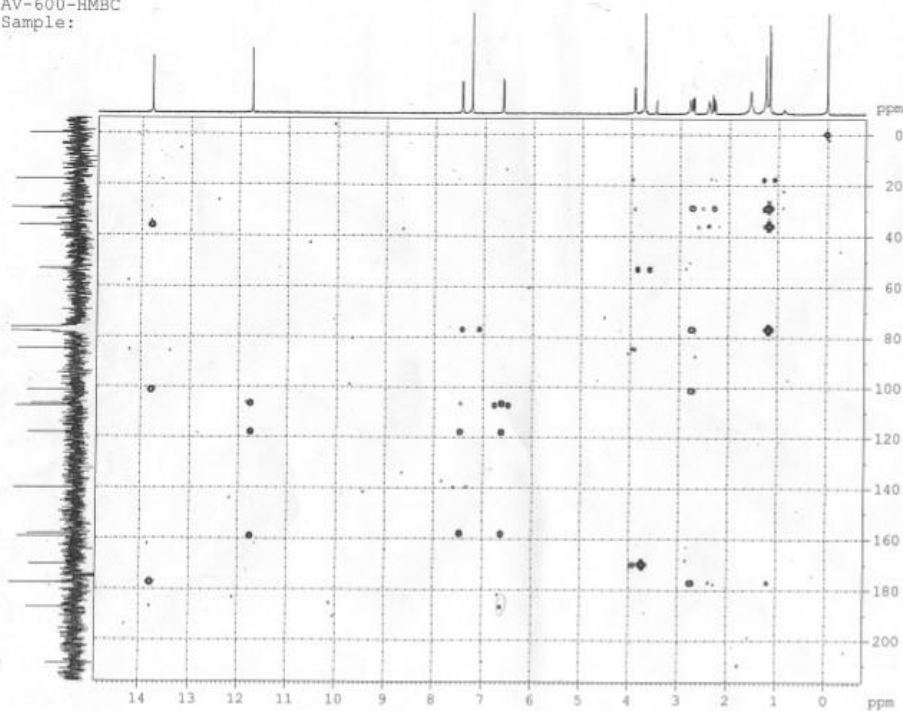


S3 : The ESIMS spectrum of compound 1

AV-600-HSQC
Sample:



AV-600-HMBC
Sample:



```

NAME          HXZ-2
EXPNO         1
PROCNO        1
DATE_         20101026
TIME          18.16
INSTRUM       spect
PROBHD        5 mm PABBO DD-
PULPROG       hmcq1600d4
TD            1024
SOLVENT       CDCl3
NS            198
DS            16
SWH           5615.369 Hz
FIDRES        9.790274 Hz
AQ            0.0233560 sec
RG            39180
WDW           92.000 usec
SS            6.50 usec
TE            298.2 K
CHFT2         143.000000
CHFT3         5.0000000
DE            0.0000000 sec
DI            1.0000000 sec
DU            0.0034838 sec
DC            0.1000000 sec
DLE           0.0000000 sec
LWD           0.00001388 sec

----- CHANNEL f1 -----
NUC1          1H
P1            11.10 usec
PD            22.20 usec
PL1           -8.00 dB
PL12          31.30245578 W
NUC2          13C
P2            8.00 usec
PD2           1.00 dB
PL2           82.20243825 W
NUC3          13C
P3            8.00 usec
PD3           1.00 dB
PL3           82.20243825 W

----- GRADIENT CHANNEL -----
GPMAG1        SINE.100
GPMAG2        SINE.100
GPMAG3        SINE.100
GPI1          50.00 %
GPI2          20.00 %
GPI3          40.10 %
PIG           1000.00 usec
NSG           1
TD            256
SFO1          150.924 MHz
SFO2          141.488647 Hz
SF           240.000 MHz
ST            1024
SF           800.1300336 MHz
SFO          0
SR            0
LX            0.00 Hz
UR            0
PC            1.40
ZG            1024
SFO          0
SF           150.9024524 MHz
SFO          0
SR            0
LX            0.00 Hz
UR            0
  
```

S5 : The HMBC spectrum of compound 1