Supporting Information

***Rec. Nat. Prod*. 13:5 (2019) 385-389**

New Xanthone from *Millettia pachyloba* Drake

Zhi Na , Qishi Song and Qingfei Fan

CAS Key Laboratory of Tropical Plant Resources and Sustainable Use, Xishuangbanna Tropical Botanical Garden, Chinese Academy of Sciences, Mengla, Yunnan, 666303, P. R. China

Table of Contents **Page**

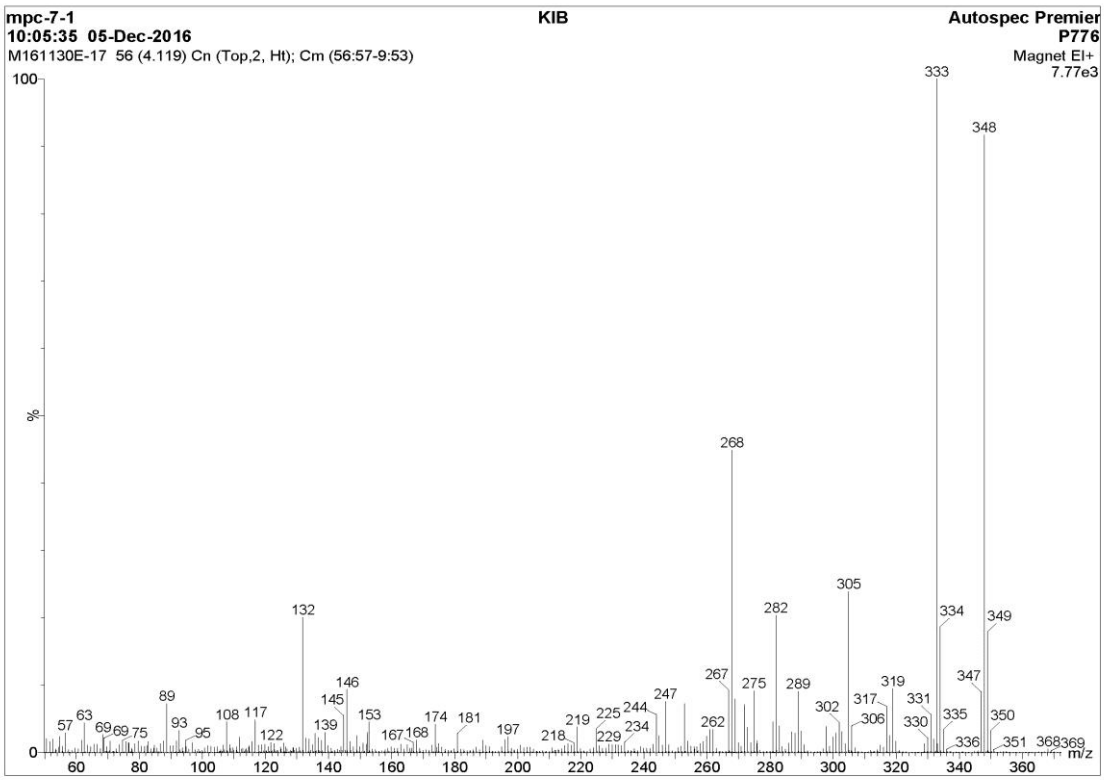
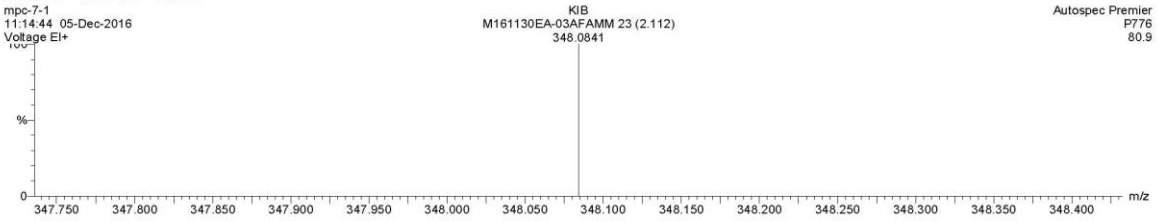


Figure S1: EI-MS spectrum of compound **1**

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -10.0, max = 120.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
15 formula(e) evaluated with 1 results within limits (up to 51 closest results for each mass)
Elements Used:
C: 0-200 H: 0-400 O: 7-9



Minimum:				-10.0		
Maximum:		200.0	10.0	120.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
348.0841	348.0845	-0.4	-1.1	10.0	5546052.0	C17 H16 O8

Figure S2: HREI-MS spectrum of compound **1**

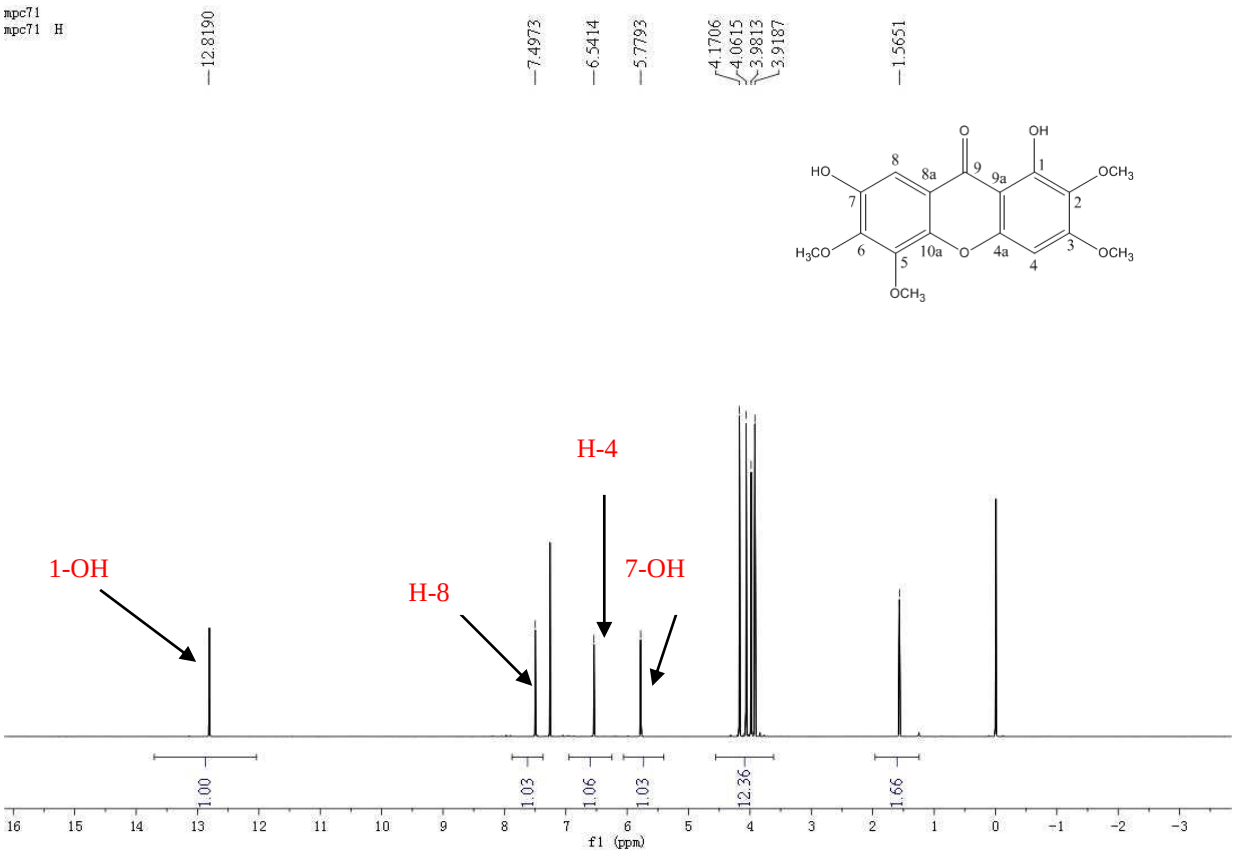


Figure S3: ^{1}H-NMR (500 MHz, $CDCl_3$) spectrum of compound **1**

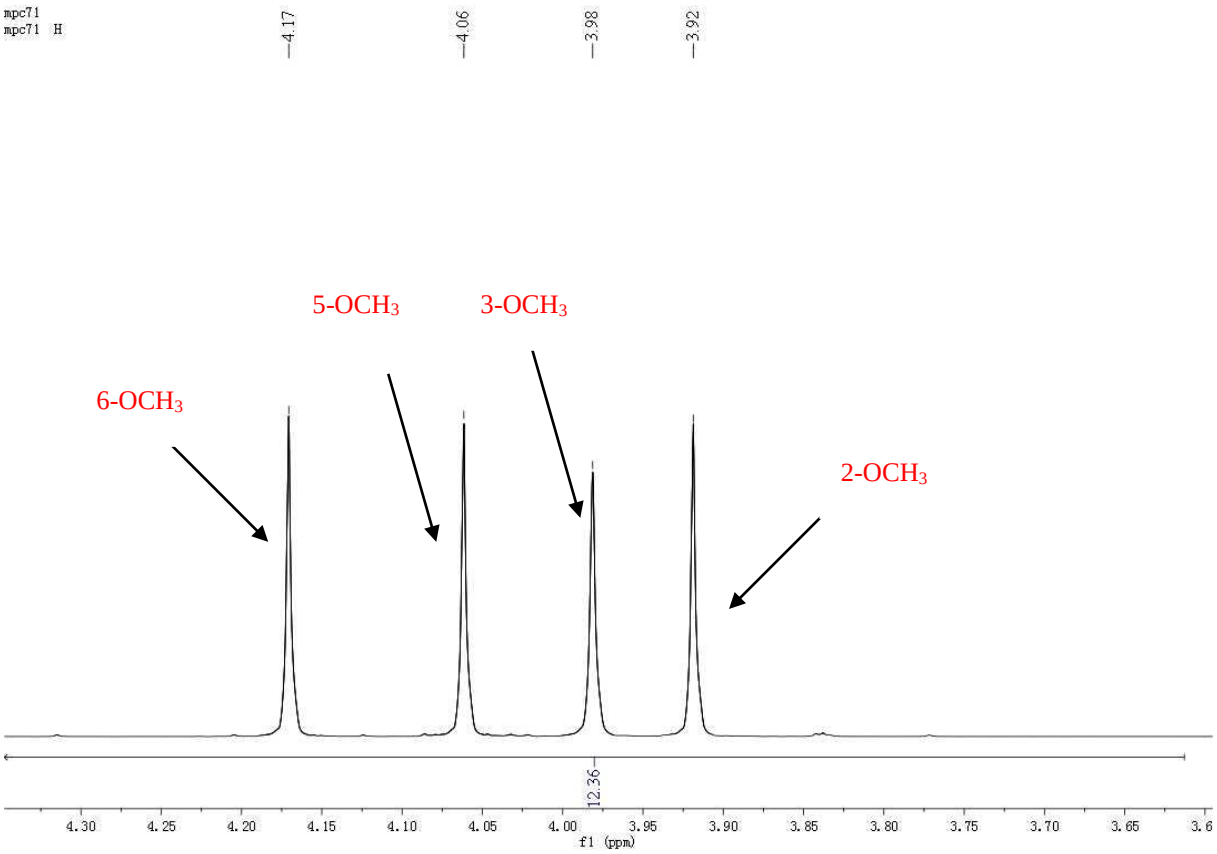


Figure S4: ^{1}H-NMR (500 MHz, $CDCl_3$) spectrum of compound **1** (From 3.6 to 4.3 ppm)

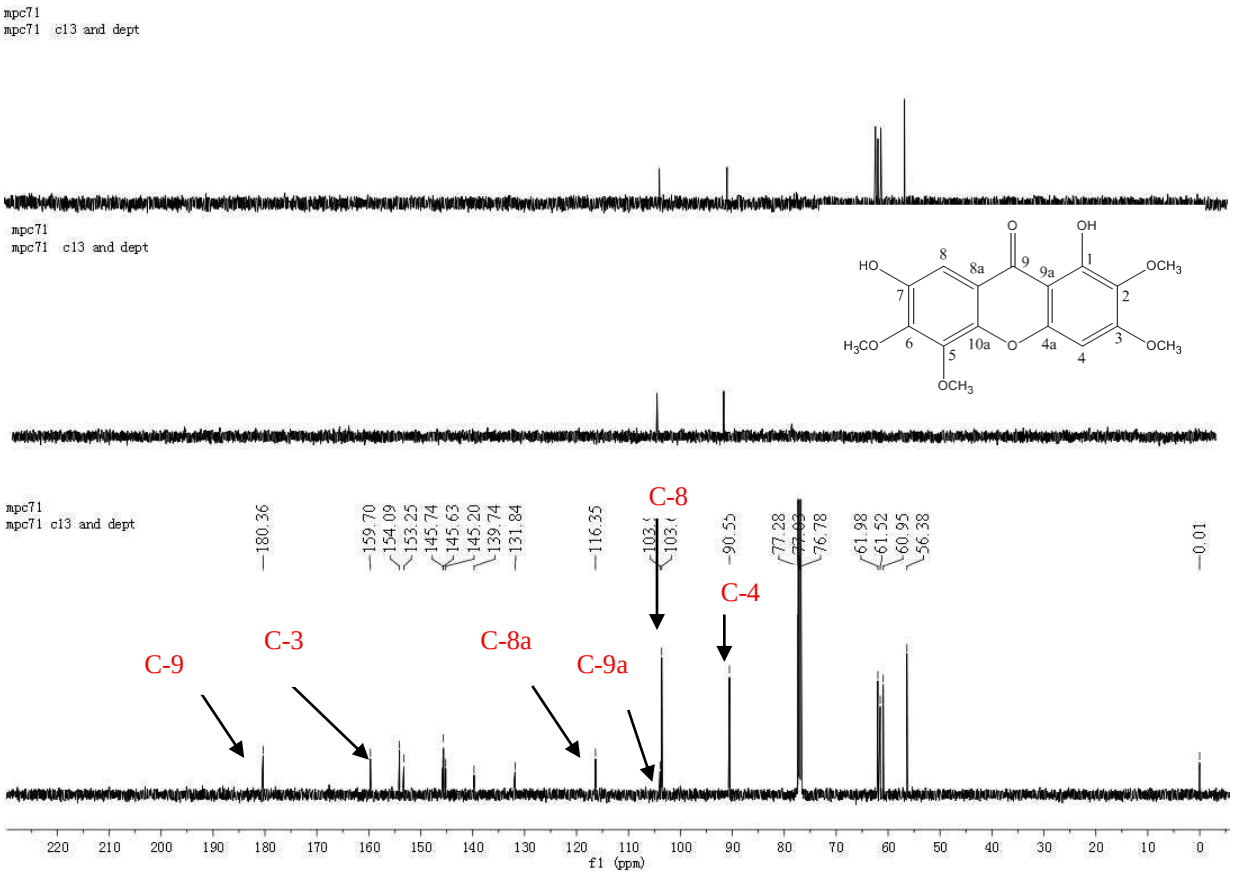


Figure S5: ^{13}C-NMR and DEPT (125 MHz, $CDCl_3$) spectrum of compound **1**

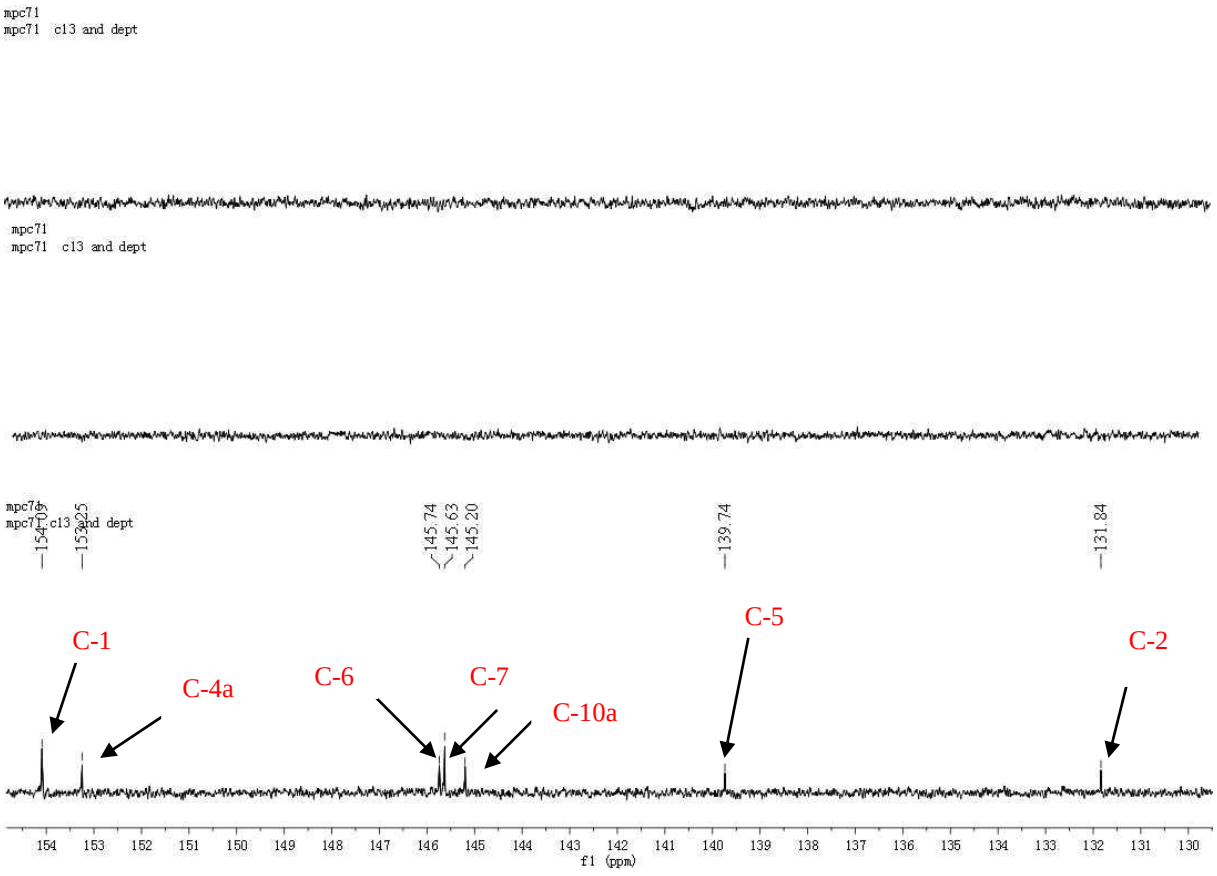


Figure S6: ^{13}C-NMR and DEPT (125 MHz, $CDCl_3$) spectrum of compound **1** (From 130 to 154 ppm)

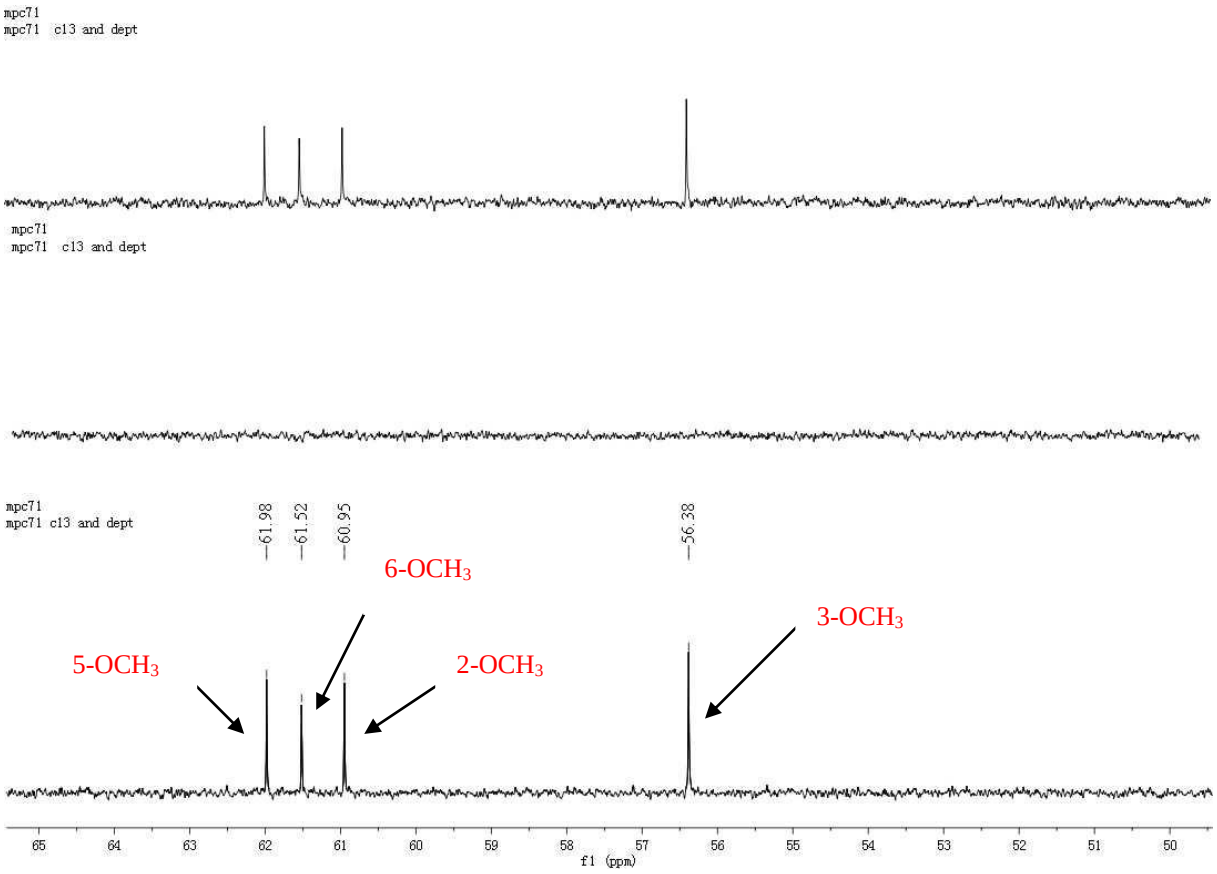


Figure S7: ^{13}C-NMR and DEPT (125 MHz, $CDCl_3$) spectrum of compound **1** (From 50 to 65 ppm)

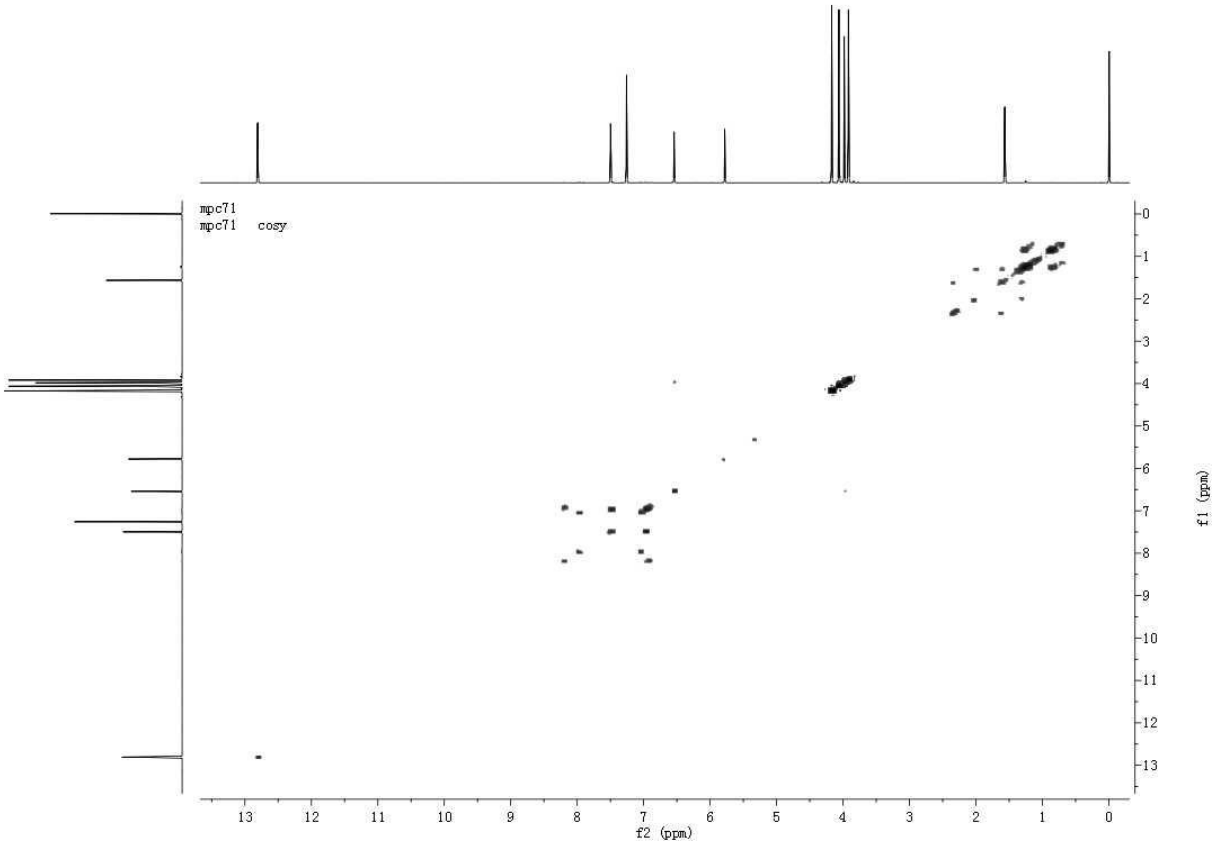


Figure S8: ^{1}H-^{1}H COSY spectrum of compound **1**

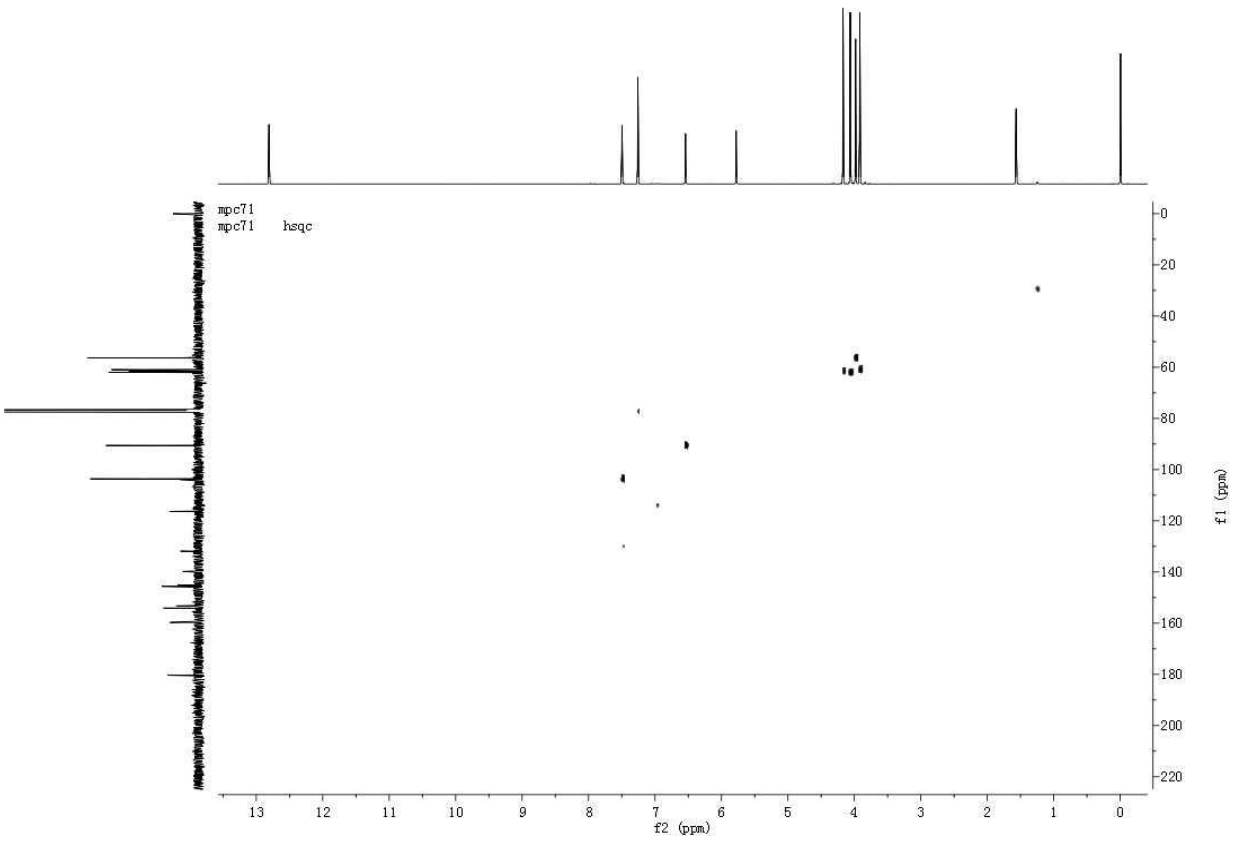


Figure S9: HSQC spectrum of compound **1**

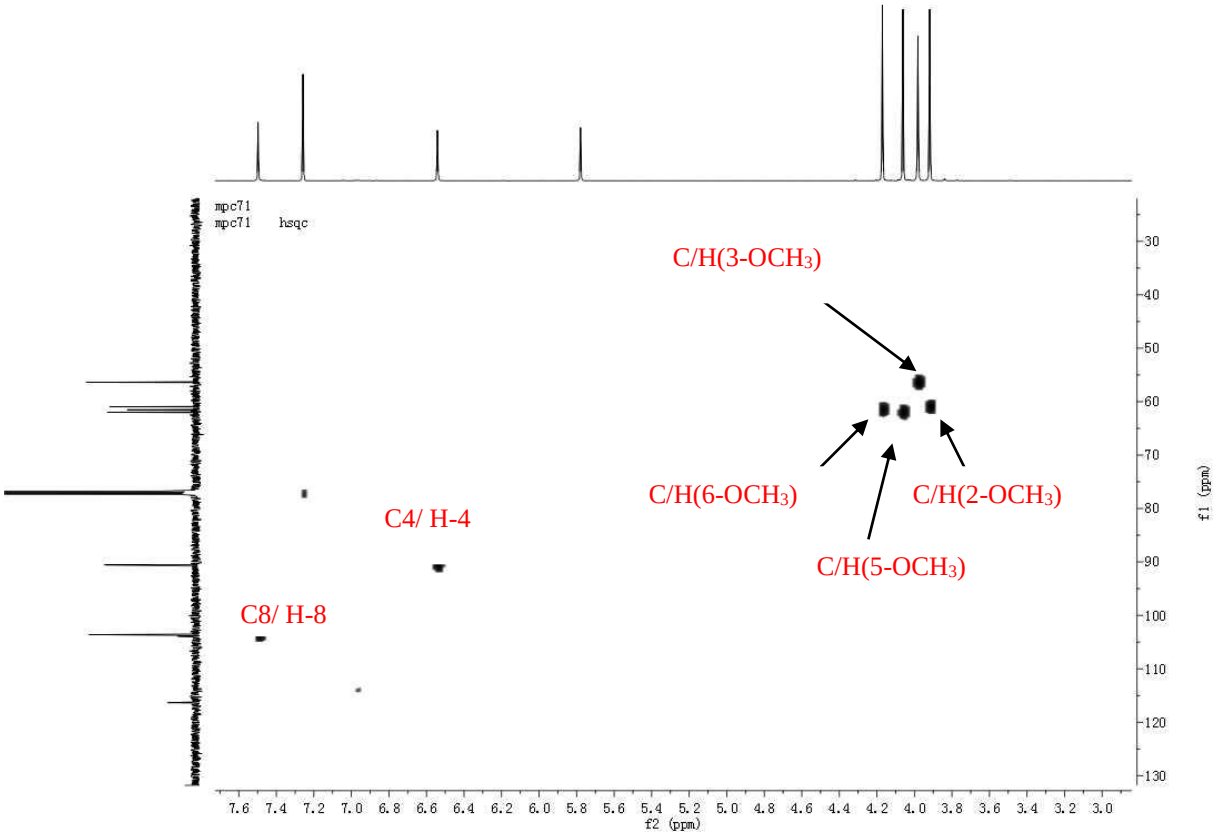


Figure S10: HSQC spectrum of compound **1** (From 30 to 130 ppm)

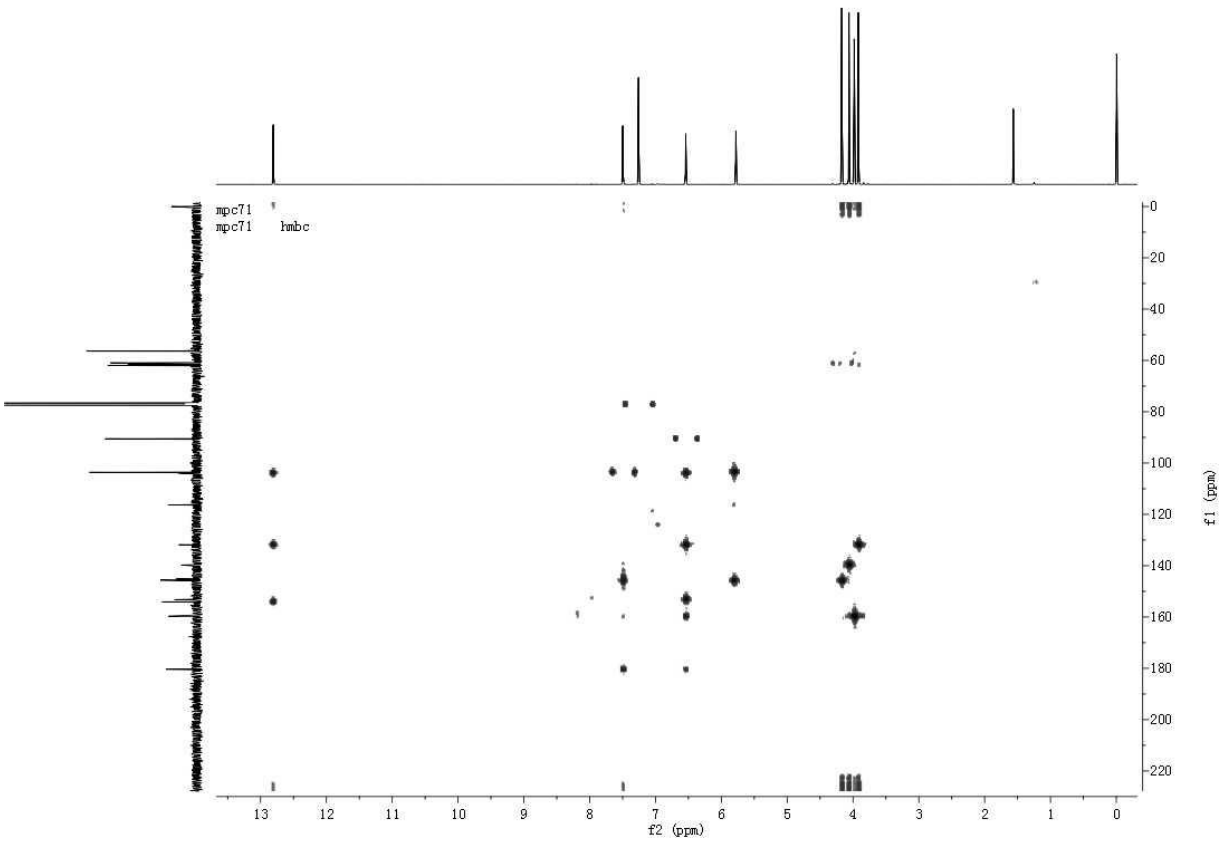


Figure S11: HMBC spectrum of compound **1**

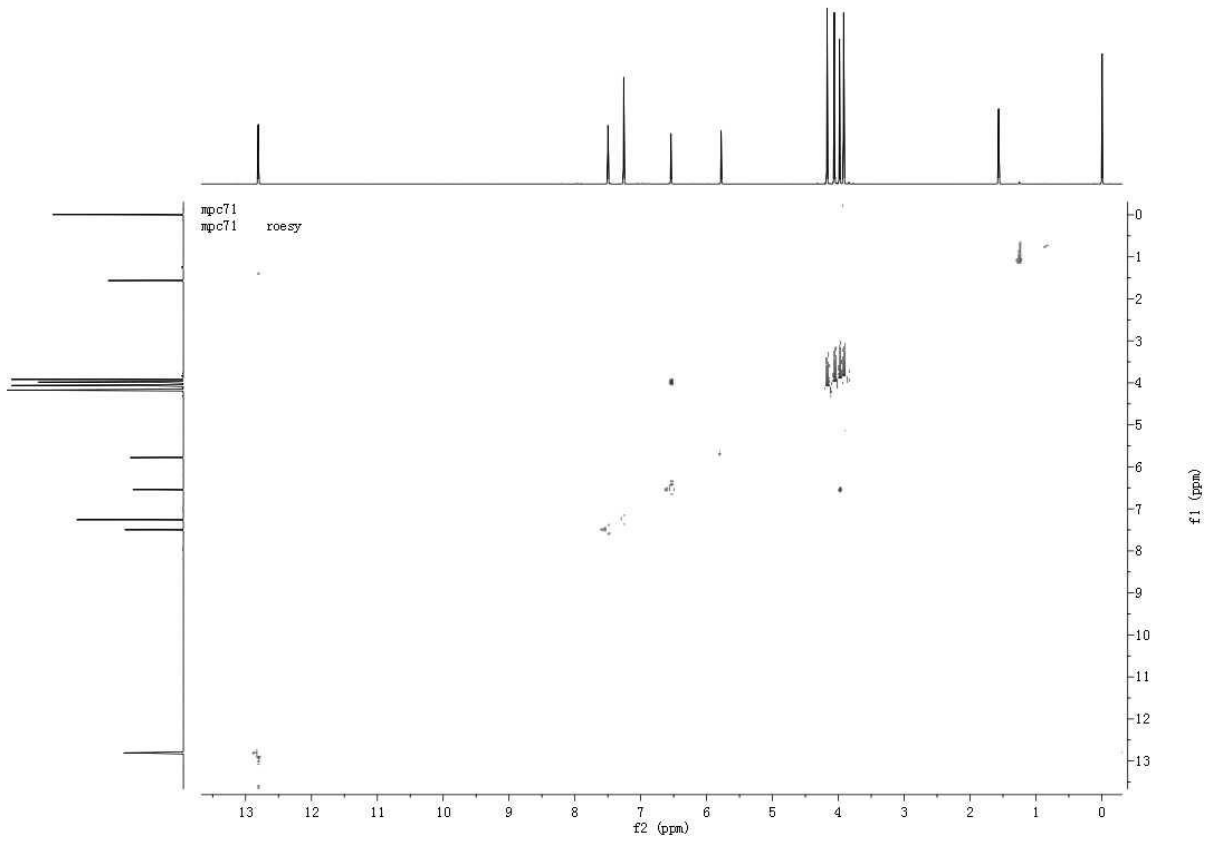


Figure S12: ROESY spectrum of compound **1**

Growth inhibition by the sample of tumour cells was measured by microculture tetrazolium (MTT) assay, with minor modification [1-3]. Briefly, adherent cells were seeded into 96-well microculture plates and allowed to adhere for 24 h before drug addition, while suspended cells were seeded just before drug addition. The cell densities were selected based on the results of preliminary tests, in order to maintain the control cells in an exponential phase of growth during the period of the experiment and to obtain a linear relationship between the optical density and the number of viable cells. Each tumour cell line was exposed to sample at 0.01, 0.1, 1.0, 10 and 100 μM concentrations for different periods (adherent cells 72 h, suspended cells 48 h) and each concentration was tested in triplicate. At the end of exposure, 20 μl of 5 g per l MTT was added to each well and the plates were incubated for 4 h at 37 °C. Then triplex solution (10% SDS–5% isobutanol–0.012 M HCl) was added and the plates were incubated for 12–20 h at 37 °C. The optical density (OD) was read on a plate reader at 570 nm. Media and DMSO control wells, in which sample was absent, were included in all the experiments, in order to eliminate the influence of DMSO. The inhibitory rate of cell proliferation was calculated by the following formula:

Growth inhibition (%)=($OD_{control}$ －$OD_{treated}$/$OD_{control}$) ×100%

The cytotoxicity of sample on tumour cells was expressed as IC_{50} values (the drug concentration reducing by 50% the absorbance in treated cells, with respect to untreated cells), which were calculated by LOGIT method.

Table 1: Cytotoxicity of compound **1**.

Compound	IC_{50} value (μM)				
/positive control	HL-60	SMMC-7721	A-549	MCF-7	SW480
1	＞40	＞40	＞40	＞40	＞40
cis-platinum (MW300)	1.05	4.46	6.57	13.13	11.07
taxol	<0.008	<0.008	<0.008	<0.008	<0.008

Reference

[1] T. Mosmann (1983). Rapid colorimetric assay for cellular growth and survival: Application to proliferation and cytotoxicity assays, *J. Immunol. Methods* **65**, 55-63.

[2] M. C. Alley, D. A.Scudiero, A. Monks, M. L. Hursey, M.J. Czerwinski, and D. L. Fine (1988). Feasibility of drug screening with panels of human tumor cell lines using a microculture tetrazolium assay, *Cancer Res*. **48**, 589–601.

[3] J. J. Zhou, X. F. Yue, J. X. Han, and W. Y. Yang (1993). Improved MTT assay for activity of antitumor agents, *Chin. J. Pharm.* **24**, 455−457.