Xanthoquinodins from an Endolichenic Fungal Strain *Chaetomium elatum*

Guo-Dong Chen,[†, ⊥, ‖] Ying Chen,[†, ‖] Hao Gao,[†, *] Li-Qing Shen,[†] Yang Wu,[†] Xiao-Xia Li,[†] Yan Li,[‡] Liang-Dong Guo,[§] Ying-Zhou Cen,[⊥] Xin-Sheng Yao[†, *]

Affiliation

Institute of Traditional Chinese Medicine and Natural Products, College of Pharmacy, Jinan University, Guangzhou 510632, People's Republic of China, State Key Laboratory of Photochemistry and Plant Resources in West China, Kunming Institute of Botany, Chinese Academy of Sciences, Kunming 650204, People's Republic of China, State Key Laboratory of Mycology, Institute of Microbiology, Chinese Academy of Sciences, Beijing 100190, People's Republic of China, and Department of Chemistry, Jinan University, Guangzhou 510632, People's Republic of China

* To whom correspondence should be addressed. Telephone: +86-20-85221559. Fax: +86-20-85221559. E-mail: (H.G.) tghao@jnu.edu.cn; (X.Y.) tyaoxs@jnu.edu.cn

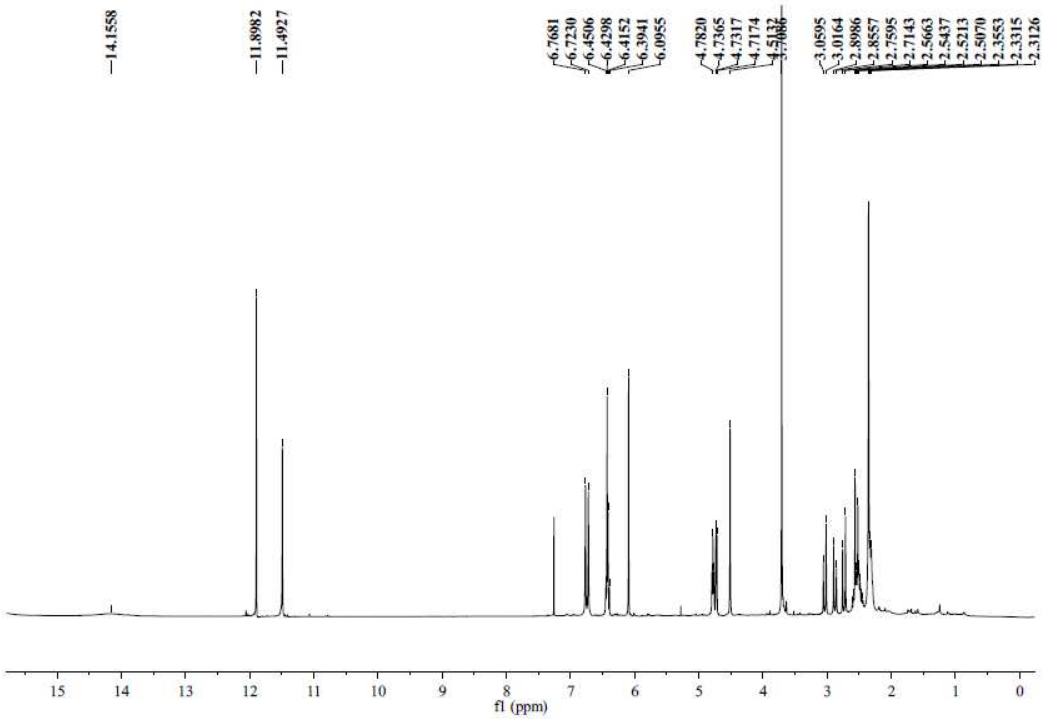
[†] College of Pharmacy, Jinan University.

[‡] Kunming Institute of Botany, Chinese Academy of Sciences.

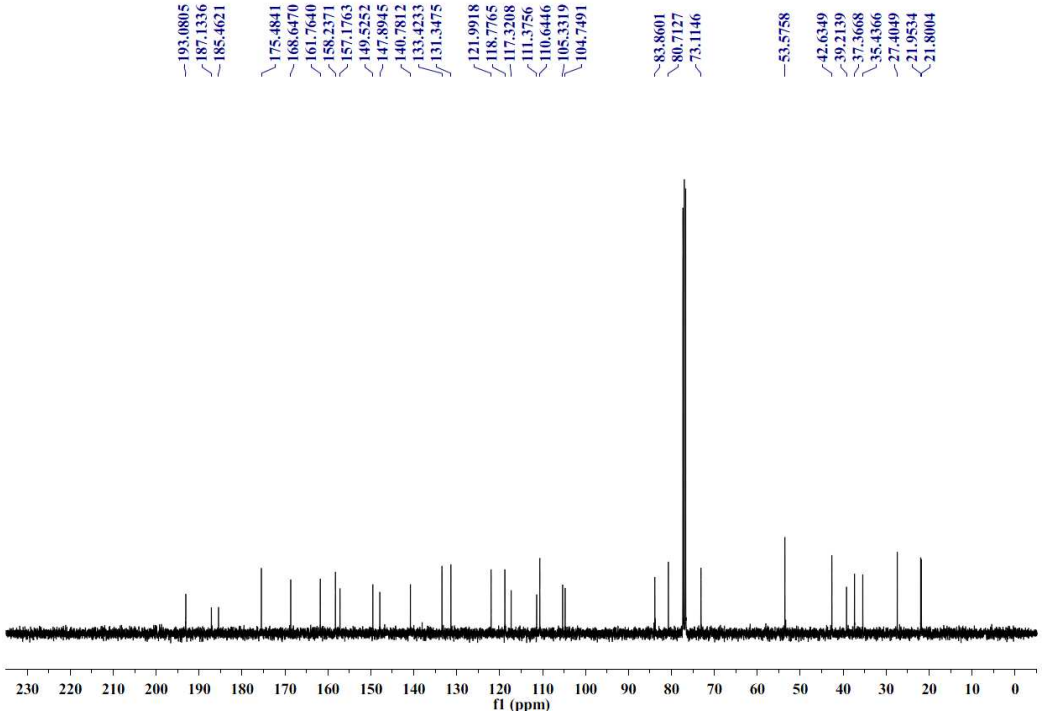
[§] Institute of Microbiology, Chinese Academy of Sciences.

[⊥] Department of Chemisitry, Jinan University

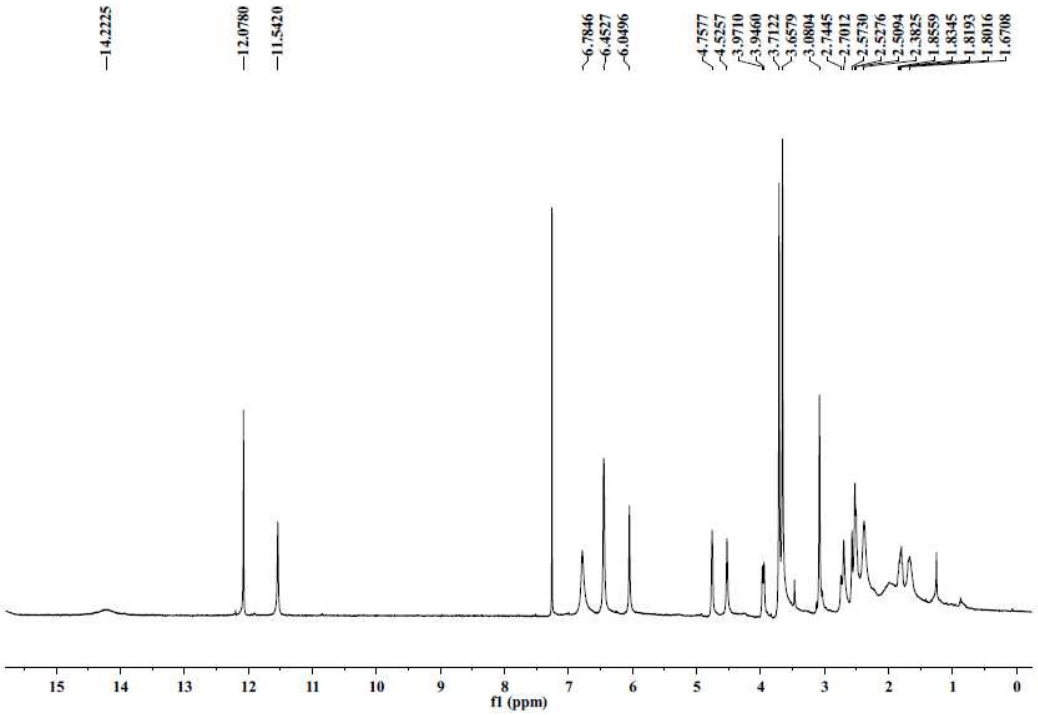
[‖] Contributed equally to this work.



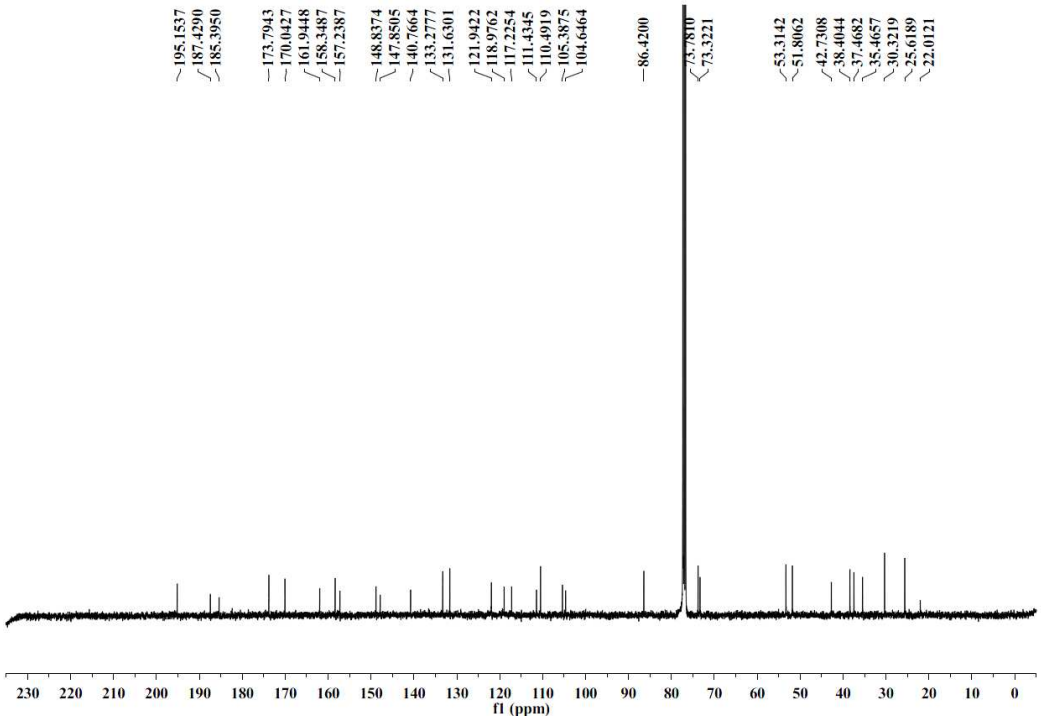
S1 ^{1}H NMR spectrum for xanthoquinodin A4 (400 MHz, in $CDCl_3$)



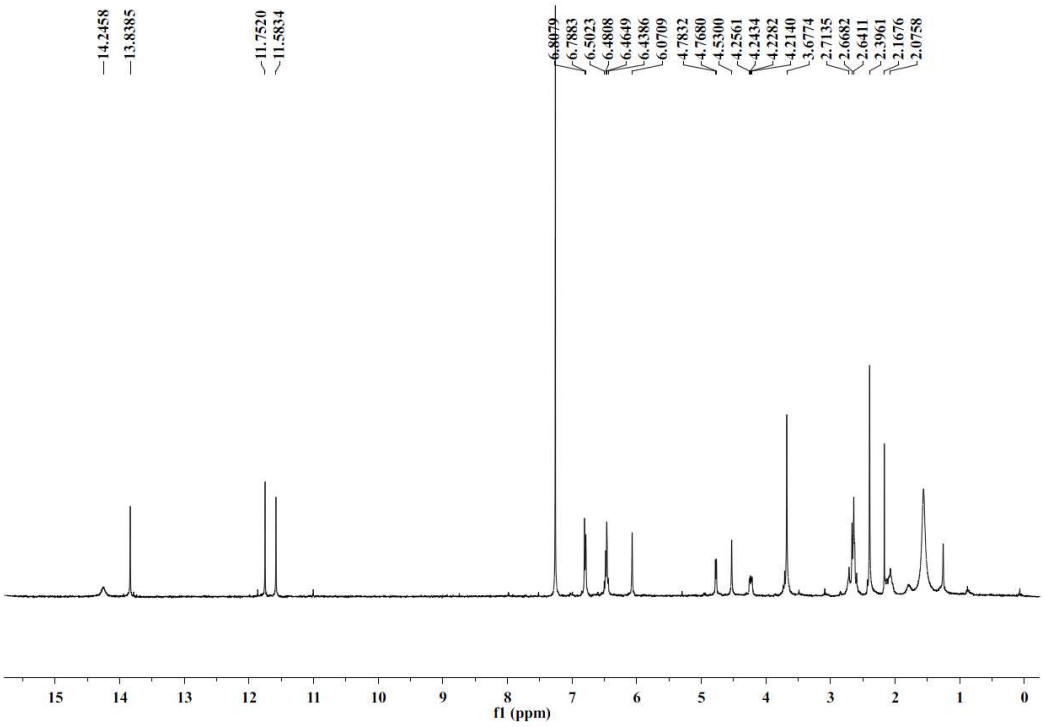
S2 ^{13}C NMR spectrum for xanthoquinodin A4 (100 MHz, in $CDCl_3$)



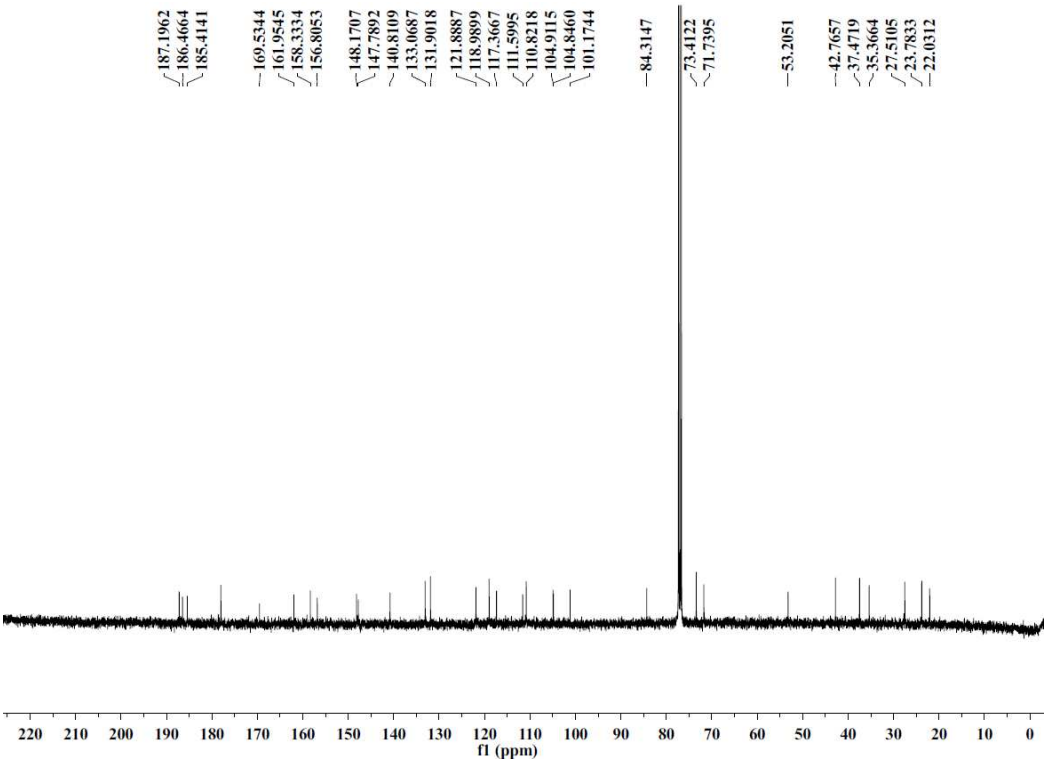
S3 ^{1}H NMR spectrum for xanthoquinodin A5 (400 MHz, in $CDCl_3$)



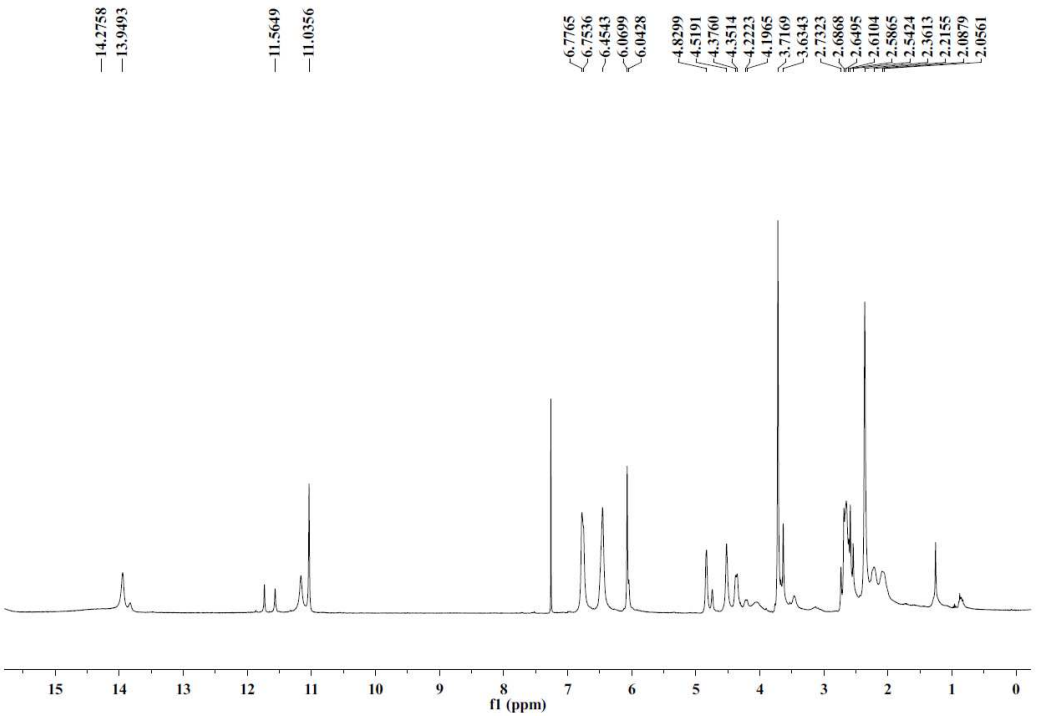
S4 ^{13}C NMR spectrum for xanthoquinodin A5 (100 MHz, in $CDCl_3$)



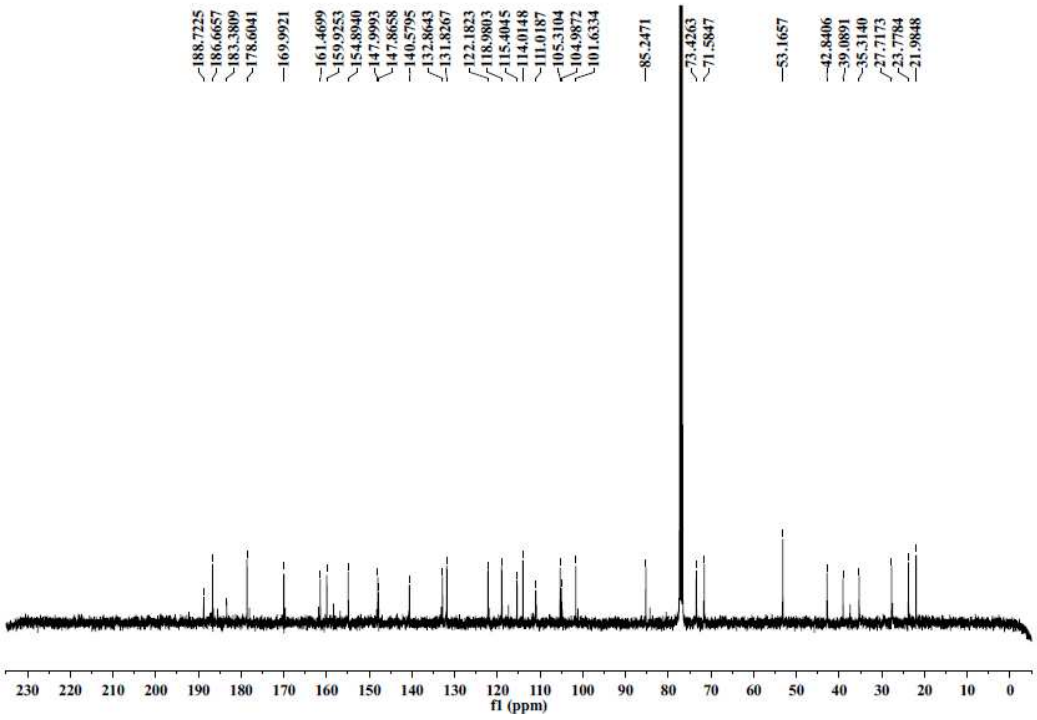
S5 ^{1}H NMR spectrum for xanthoquinodin A6 (400 MHz, in $CDCl_3$)



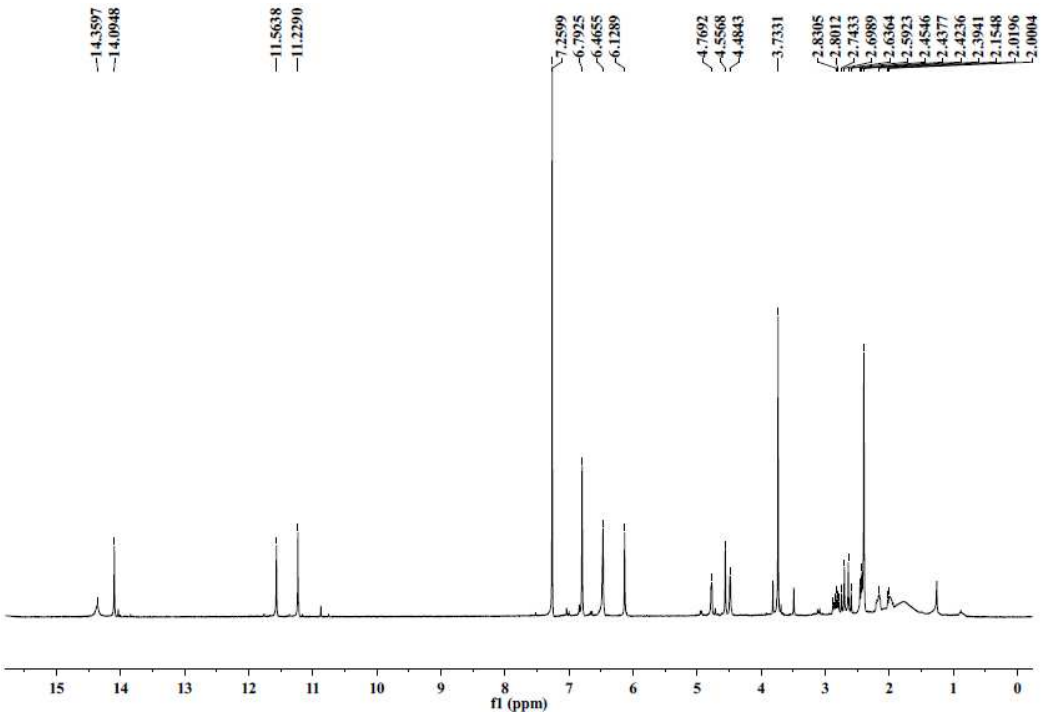
S6 ^{13}C NMR spectrum for xanthoquinodin A6 (100 MHz, in $CDCl_3$)



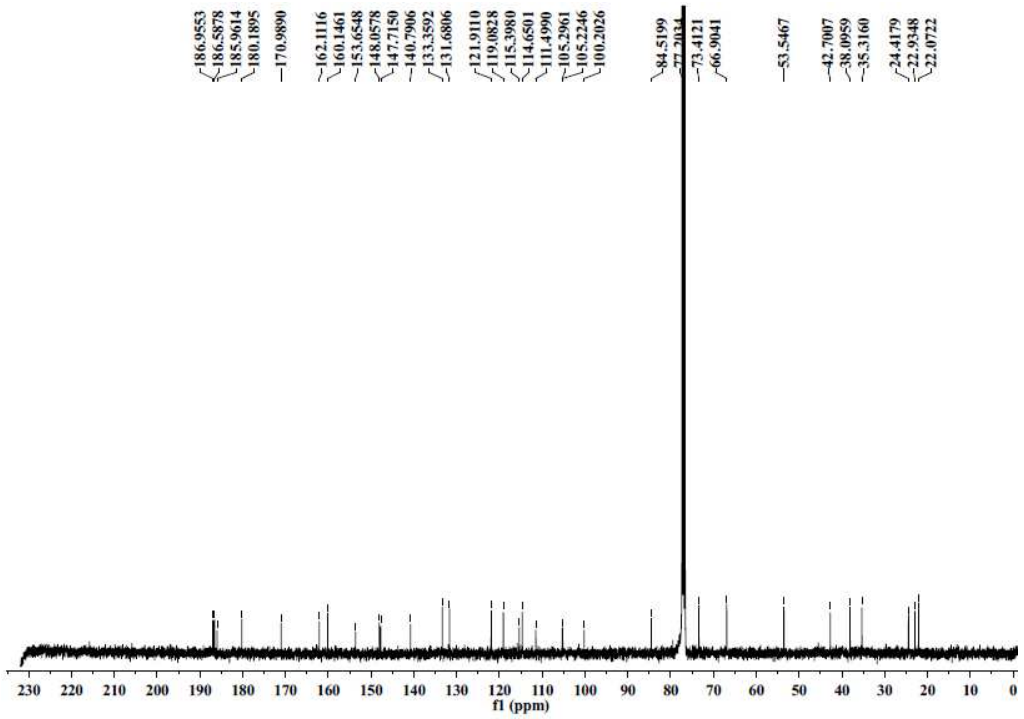
S7 ^{1}H NMR spectrum for xanthoquinodin B4 (400 MHz, in $CDCl_3$)



S8 ^{13}C NMR spectrum for xanthoquinodin B4 (100 MHz, in $CDCl_3$)



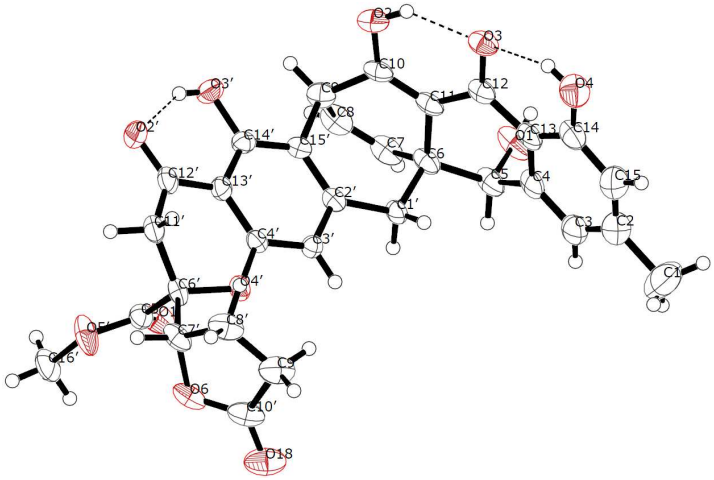
S9 ^{1}H NMR spectrum for xanthoquinodin B5 (400 MHz, in $CDCl_3$)



S10 ^{13}C NMR spectrum for xanthoquinodin B5 (100 MHz, in $CDCl_3$)

S11 X-ray Crystallographic Analysis of xanthoquinodin A4 (1).

Upon crystallization from CH_2Cl_2:MeOH 2:1 using the vapor diffusion method, needles of xanthoquinodin A4 were obtained. Data were collected using a Sapphire CCD with a graphite monochromated Cu Kα radiation, λ = 1.54184 Å at 173.0 (3) K. Crystal data: $C_{31}H_{26}O_{11}$, H_2O, CH_3OH, M = 624.58, monoclinic, space group $C2$; unit cell dimensions were determined to be a = 19.3701(7) Å, b = 11.4826(4) Å, c = 12.6416(4) Å, α = 90.00 °, β = 95.310(3) °, γ = 90.00 °, V = 2799.65(17) Å^3, Z = 4, Dx = 1.482 g/cm^3, F (000) = 1312, μ (Cu K_α) = 0.979 mm^{-1}. 20967 reflections were collected until θ_{max} = 60.86°, in which independent unique 3929 reflections were observed [$F^2 > 4\sigma$ (F^2)]. The structure was solved by direct methods using the SHELXS-97 program, and refined by the SHELXL-97 program and full-matrix least-squares calculations[1]. In the structure refinements, nonhydrogen atoms were placed on the geometrically ideal positions by the "ride on" method. Hydrogen atoms bonded to oxygen were located by the structure factors with isotropic temperature factors. The final refinement gave R = 0.0600, R_W = 0.1625, S = 1.049, and Flack = –0.1(3).



S12 The calculated ECD spectra of 1, 3–5.

The X-ray conformation was assigned as the preliminary conformation of **1** for calculation. The initial conformations of **3–5** were optimized using MMFF94 method in MarvinSketch 5.8.1. The corresponding minimum geometries were further fully optimized by using HF/6-31G(d) method as implemented in the Gaussian

09 program package. The stable conformers obtained were submitted to ECD calculation by TDDFT [B3P86/6-311++G(2d, p)] method[2]. The solvent effects were taken into account by the polarizable-conductor calculation model (CPCM, methanol as the solvent).

Reference:

(1) Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. *J. Appl. Cryst.* **2009**, *42*, 339-341.

(2) Frisch, M.J.; Trucks, G.W.; Schlegel, H.B.; Scuseria, G.E.; Robb, M.A.; Cheeseman, J.R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G.A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H.P.; Izmaylov, A.F.; Bloino, J.; Zheng, G.; Sonnenberg, J.L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J.A.; Jr.; Peralta, J.E.; Ogliaro, F.; Bearpark, M.; Heyd, J.J.; Brothers, E.; Kudin, K.N.; Staroverov, V.N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J.C.; Iyengar, S.S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J.M.; Klene, M.; Knox, J.E.; Cross, J.B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R.E.; Yazyev, O.; Austin, A.J.; Cammi, R.; Pomelli, C.; Ochterski, J.W.; Martin, R.L.; Morokuma, K.; Zakrzewski, V.G.; Voth, G.A.; Salvador, P.; Dannenberg, J.J.; Dapprich, S.; Daniels, A.D.; Farkas, O.; Foresman, J.B.; Ortiz, J.V.; Cioslowski, J.; Fox, D.J. Gaussian, Inc., Wallingford CT, **2010**.