

# Demethylcalabaxanthone from *Garcinia mangostana* Exerts Antioxidant Effects through the Activation of the Nrf2 Pathway as Assessed via Molecular Docking and Biological Evaluation

Simona De Vita <sup>1</sup>, Milena Masullo <sup>1</sup>, Sabrina Grambone <sup>1</sup>, Paloma Bermejo Bescós <sup>2</sup>, Sonia Piacente <sup>1,\*</sup> and Giuseppe Bifulco <sup>1,\*</sup>

<sup>1</sup> Department of Pharmacy, University of Salerno, Via Giovanni Paolo II 134, 84084 Fisciano, Italy; sdevita@unisa.it (S.D.V.); mmasullo@unisa.it (M.M.) s.grambone@studenti.unisa.it (S.G.)

<sup>2</sup> Departamento de Farmacología, Farmacognosia y Botánica, Universidad Complutense de Madrid, 28040 Madrid, Spain; bescos@ucm.es

\* Correspondence: piacente@unisa.it (S.P.); bifulco@unisa.it (G.B.); Tel.: +39-089-969763 (S.P.); +39-089-969741 (G.B.)

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COMP. 4 #5 RT: 0.44 AV: 1 NL: 2.45E6  
T: FTMS - c ESI Full ms [200.00-800.00]

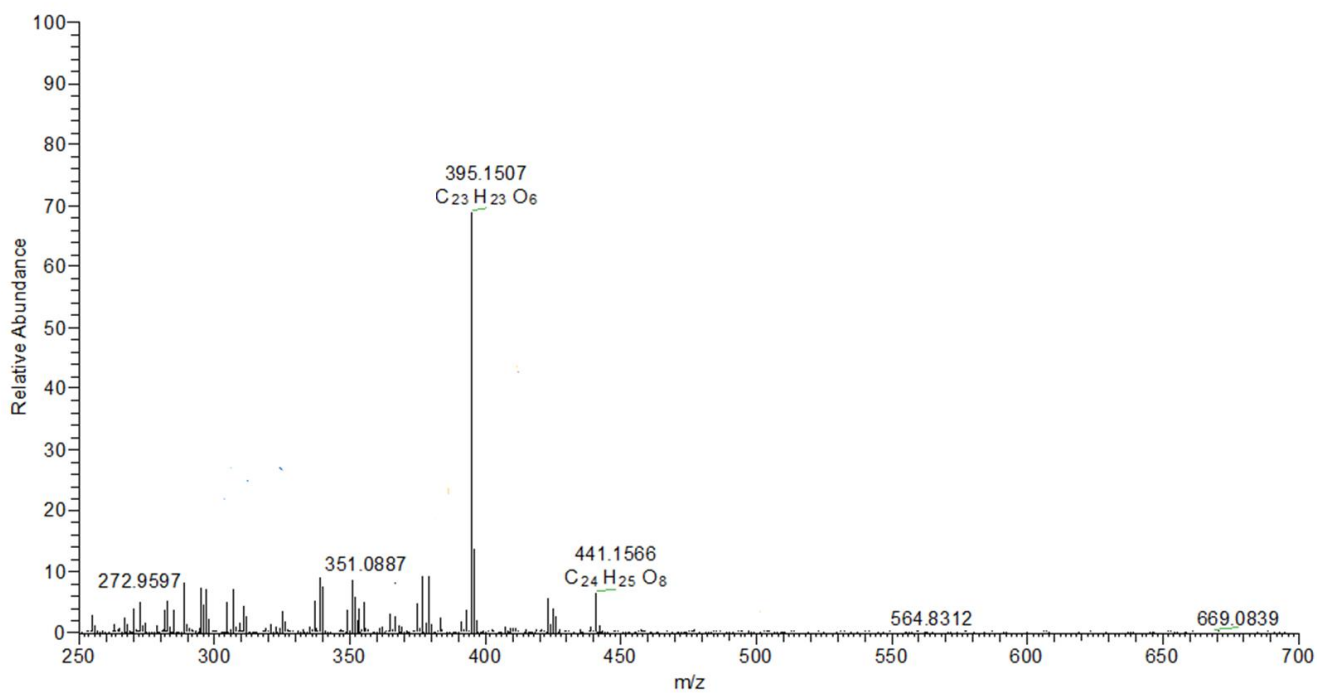


Figure S1. ESI/LTQ Orbitrap spectrum of  $\gamma$ -mangostin (1), in negative ion mode

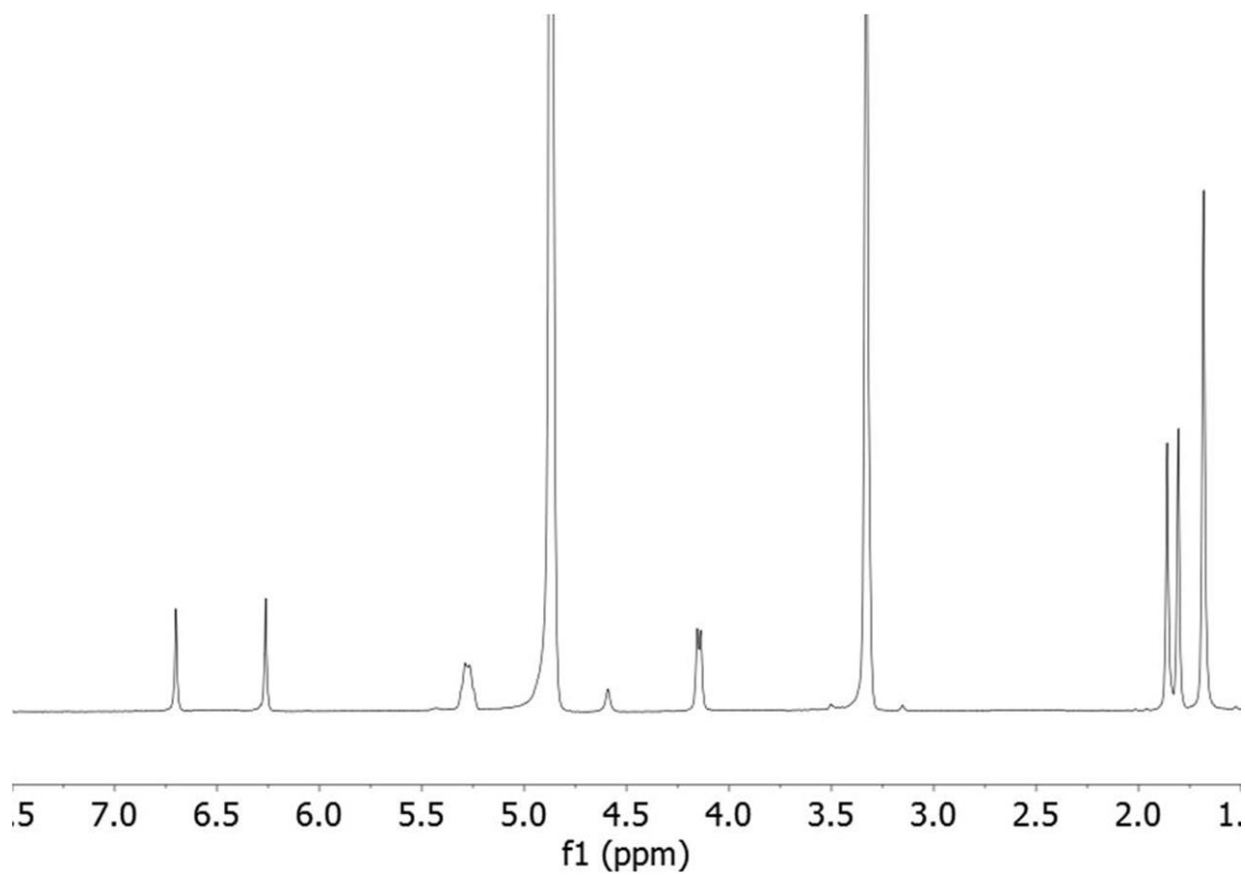
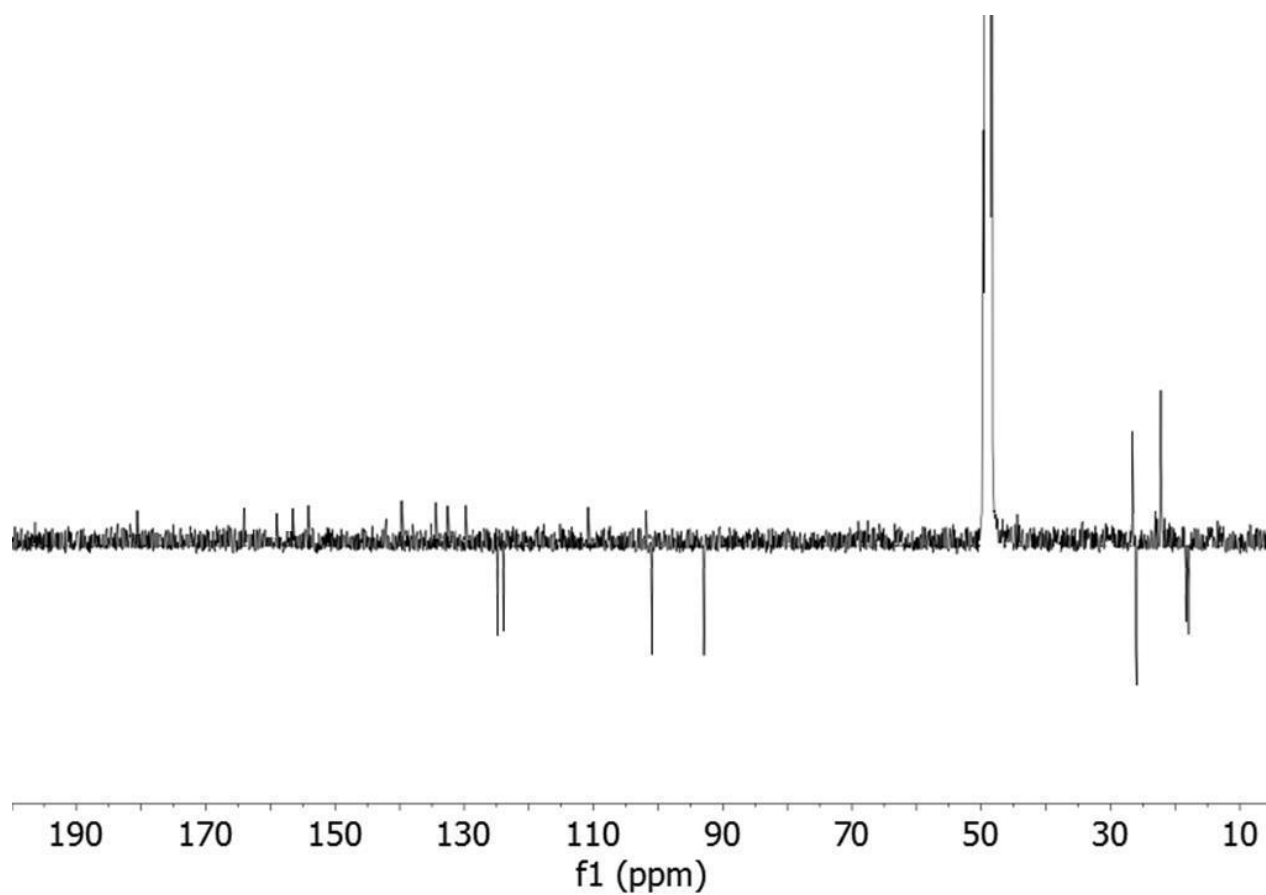
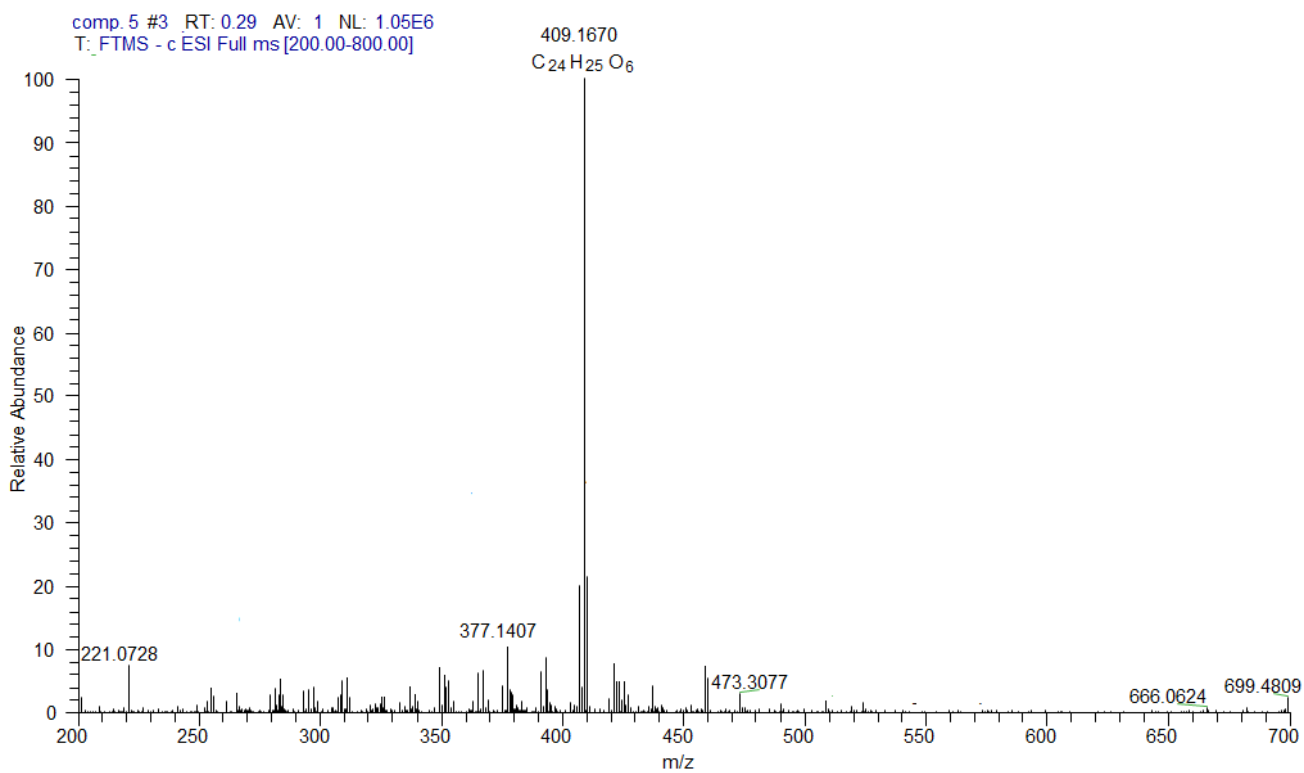


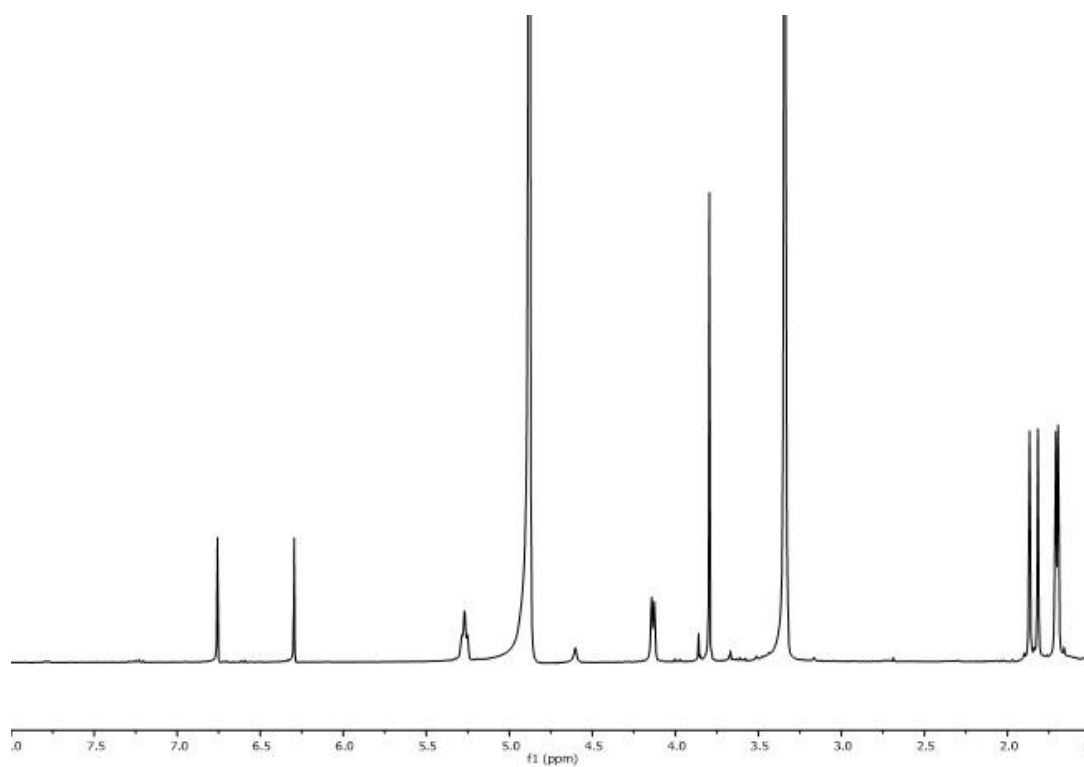
Figure S2.  $^1H$  NMR spectrum (600 MHz,  $CD_3OD$ ) of  $\gamma$ -mangostin (1)



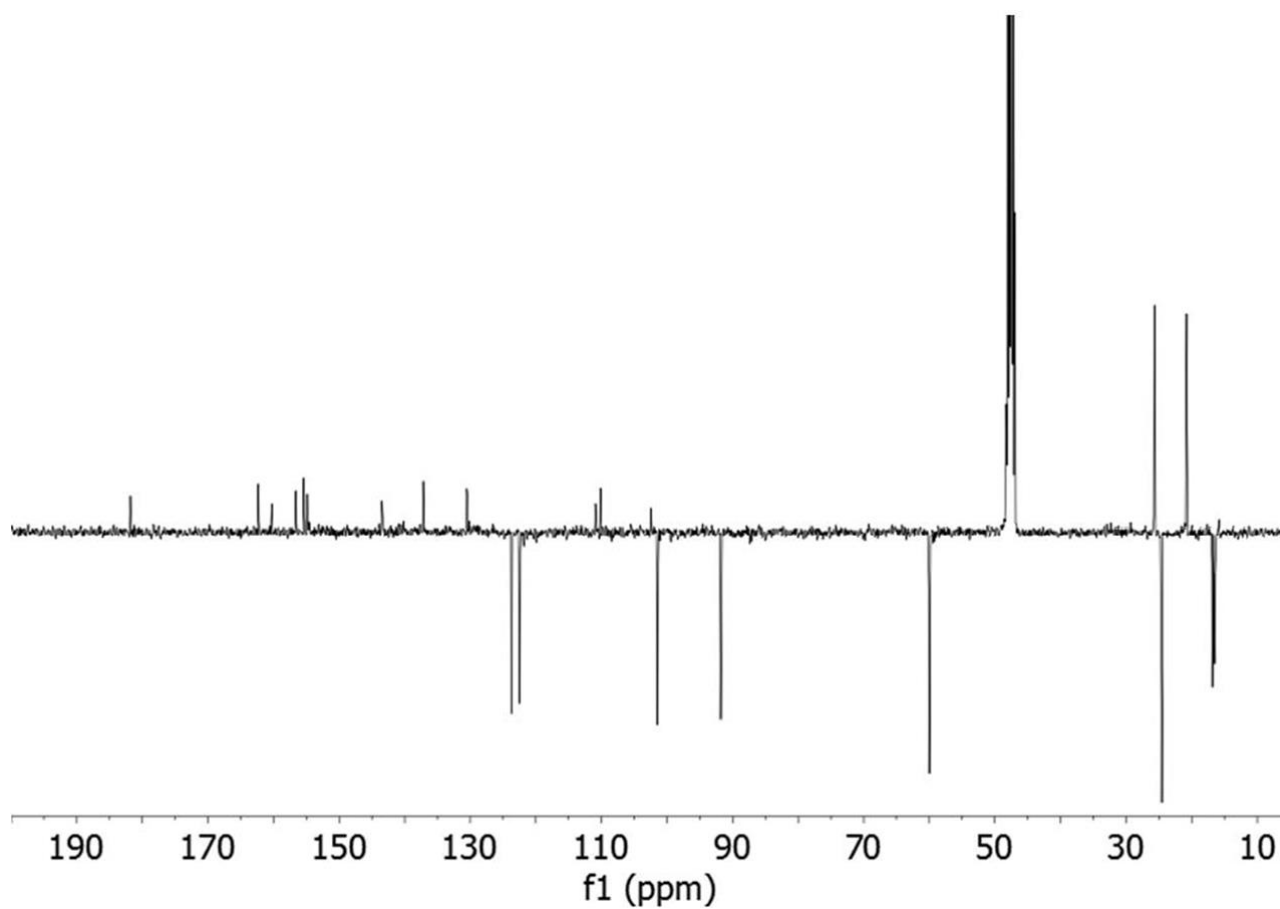
**Figure S3.**  $^{13}\text{C}$  NMR spectrum (100 MHz,  $\text{CD}_3\text{OD}$ ) of  $\gamma$ -mangostin (1)



**Figure S4.** ESI/LTQOrbitrap spectrum of  $\alpha$ -mangostin (2), in negative ion mode



**Figure S5.** <sup>1</sup>H NMR spectrum (600 MHz, CD<sub>3</sub>OD) of  $\alpha$ -mangostin (**2**)



**Figure S6.** <sup>13</sup>C NMR spectrum (100 MHz, CD<sub>3</sub>OD) of  $\alpha$ -mangostin (**2**)

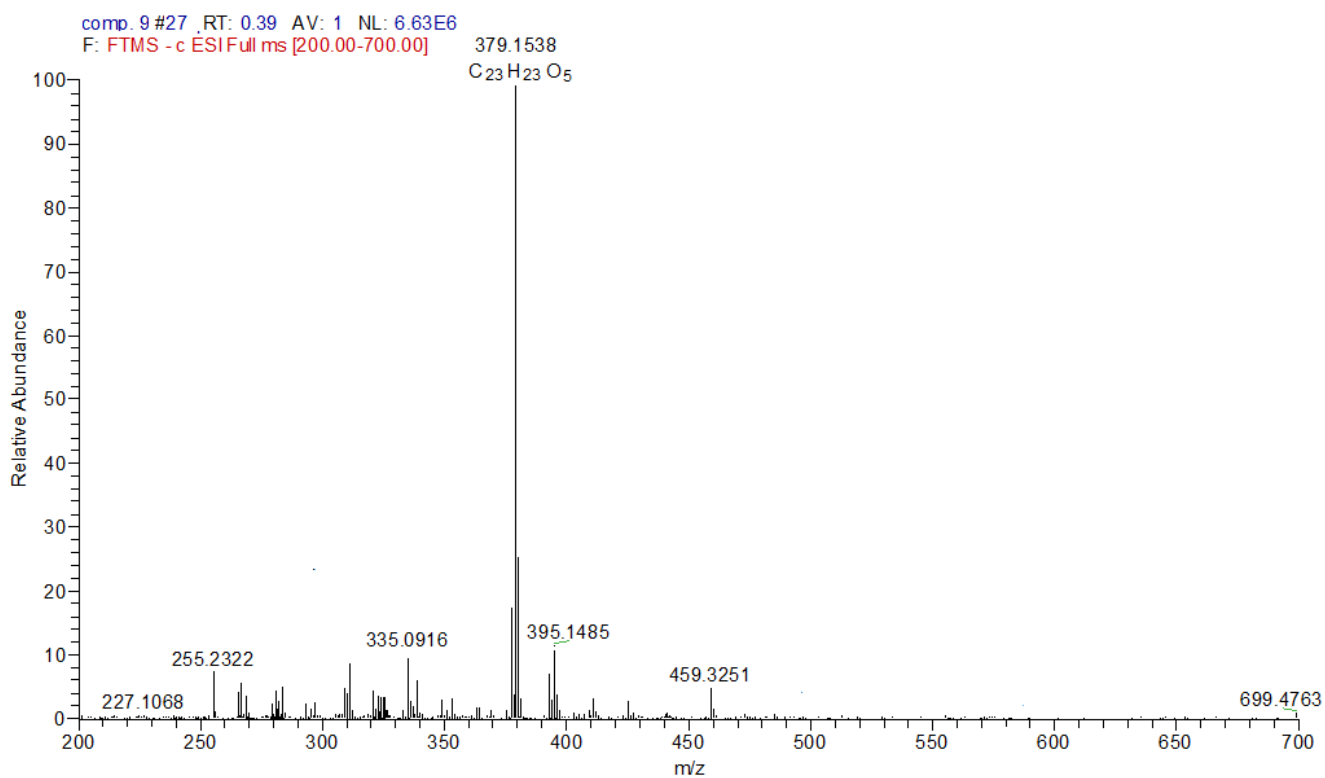


Figure S7. ESI/LTQOrbitrap spectrum of 8-deoxygartanin (3), in negative ion mode

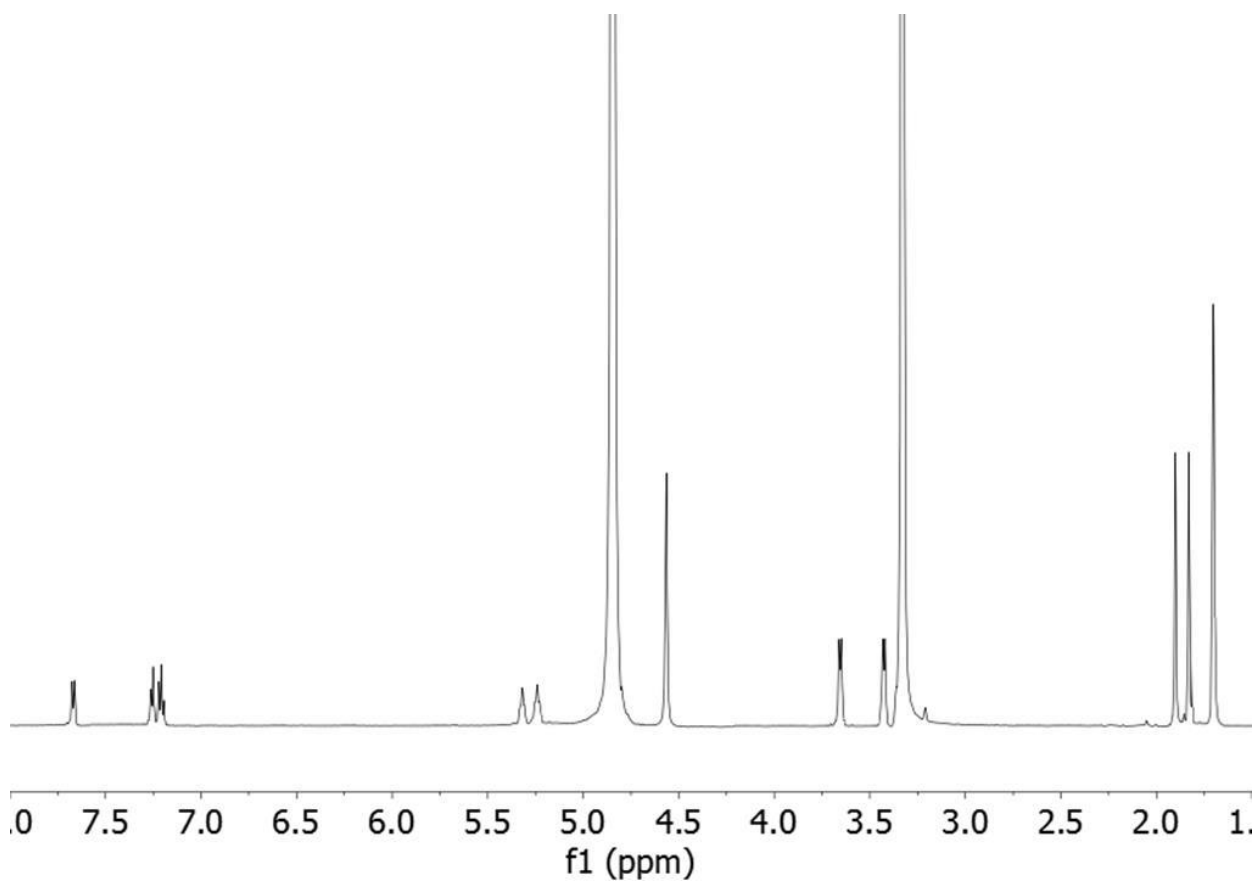
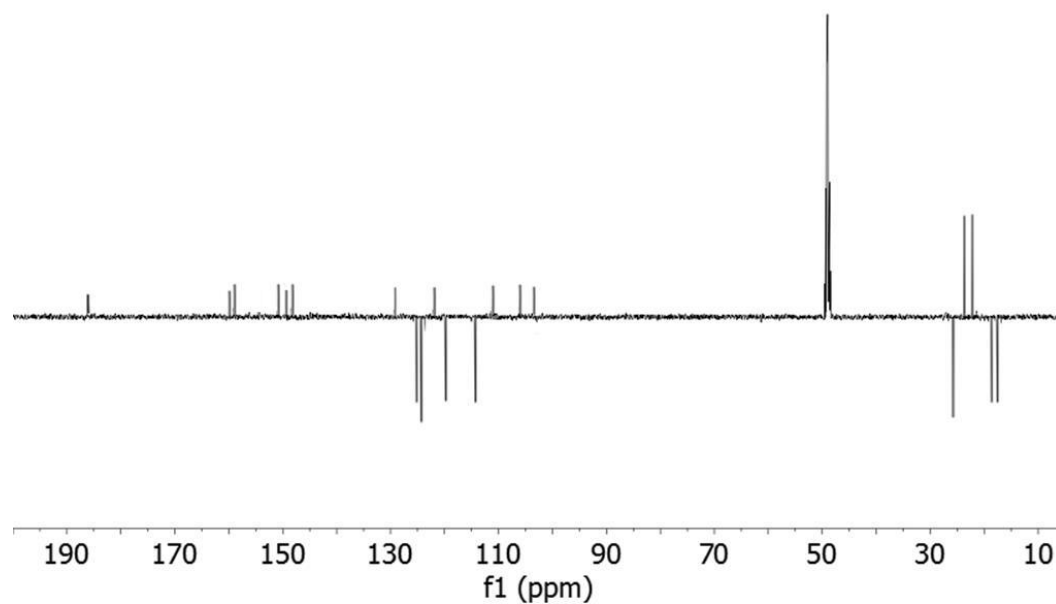
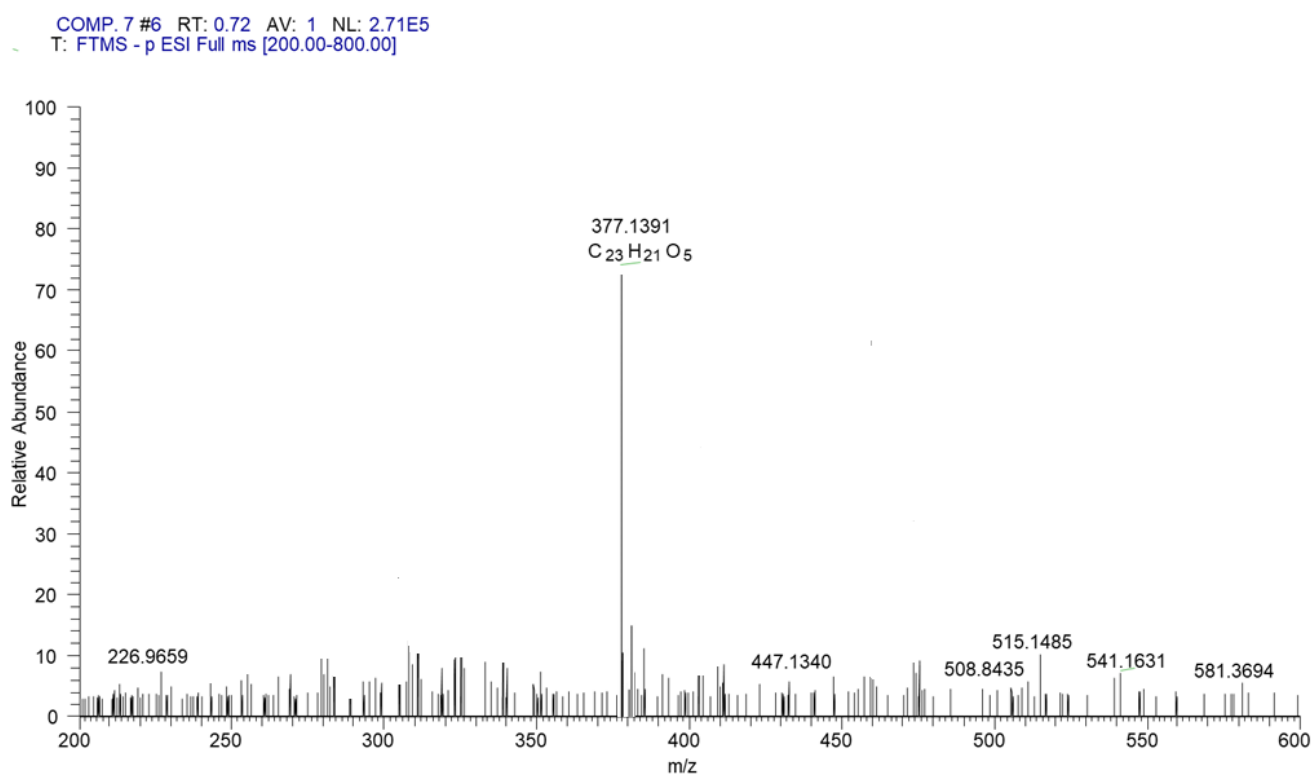


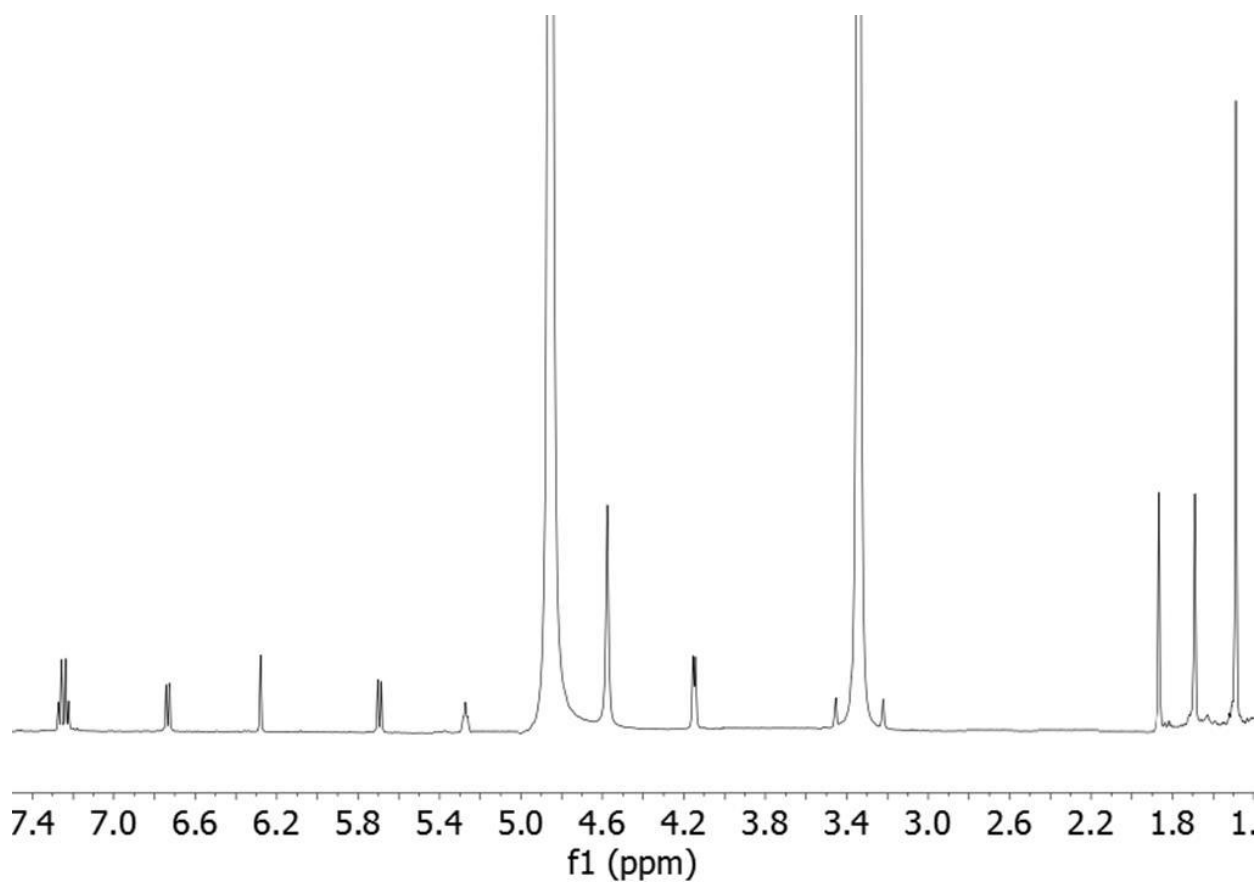
Figure S8.  $^1H$  NMR spectrum (600 MHz,  $CD_3OD$ ) of 8-deoxygartanin (3)



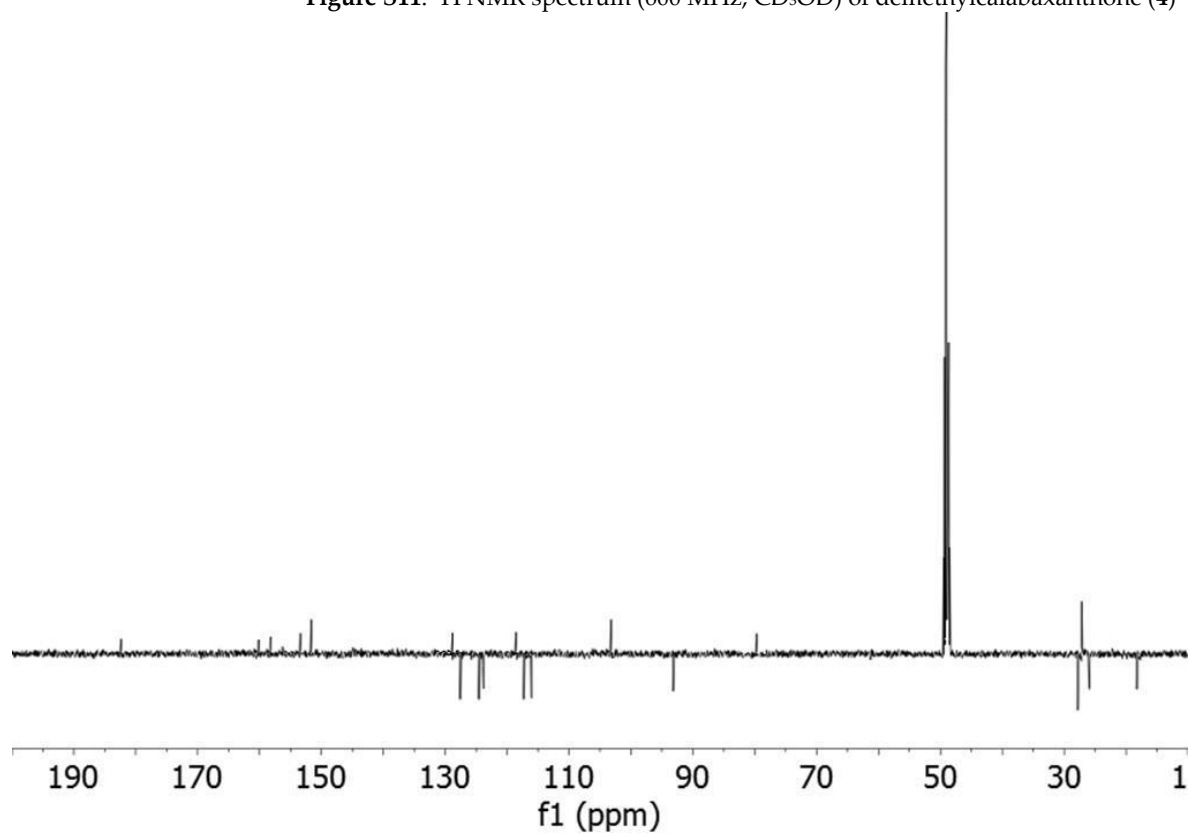
**Figure S9.**  $^{13}\text{C}$  NMR spectrum (100 MHz,  $\text{CD}_3\text{OD}$ ) of 8-deoxygartanin (**3**)



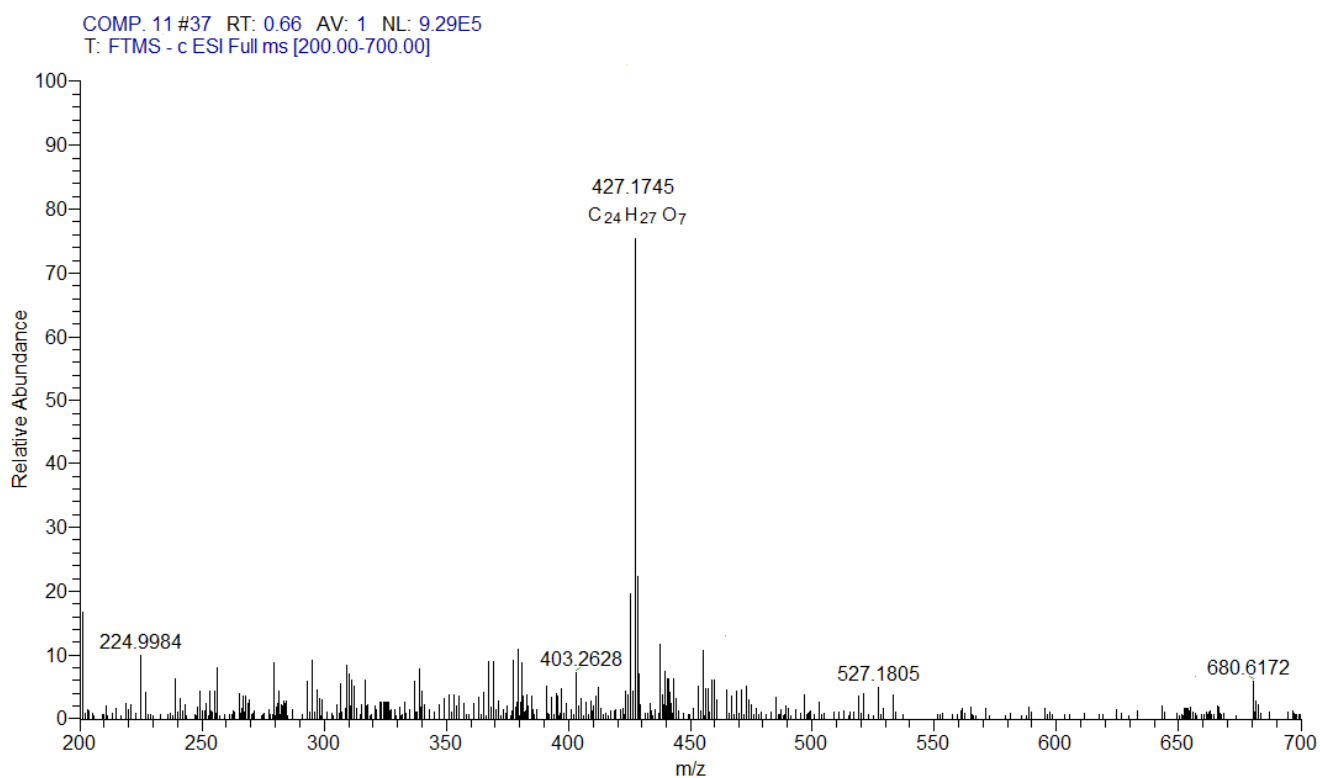
**Figure S10.** ESI/LTQOrbitrap spectrum of demethylcalabaxanthone (**4**), in negative ion mode



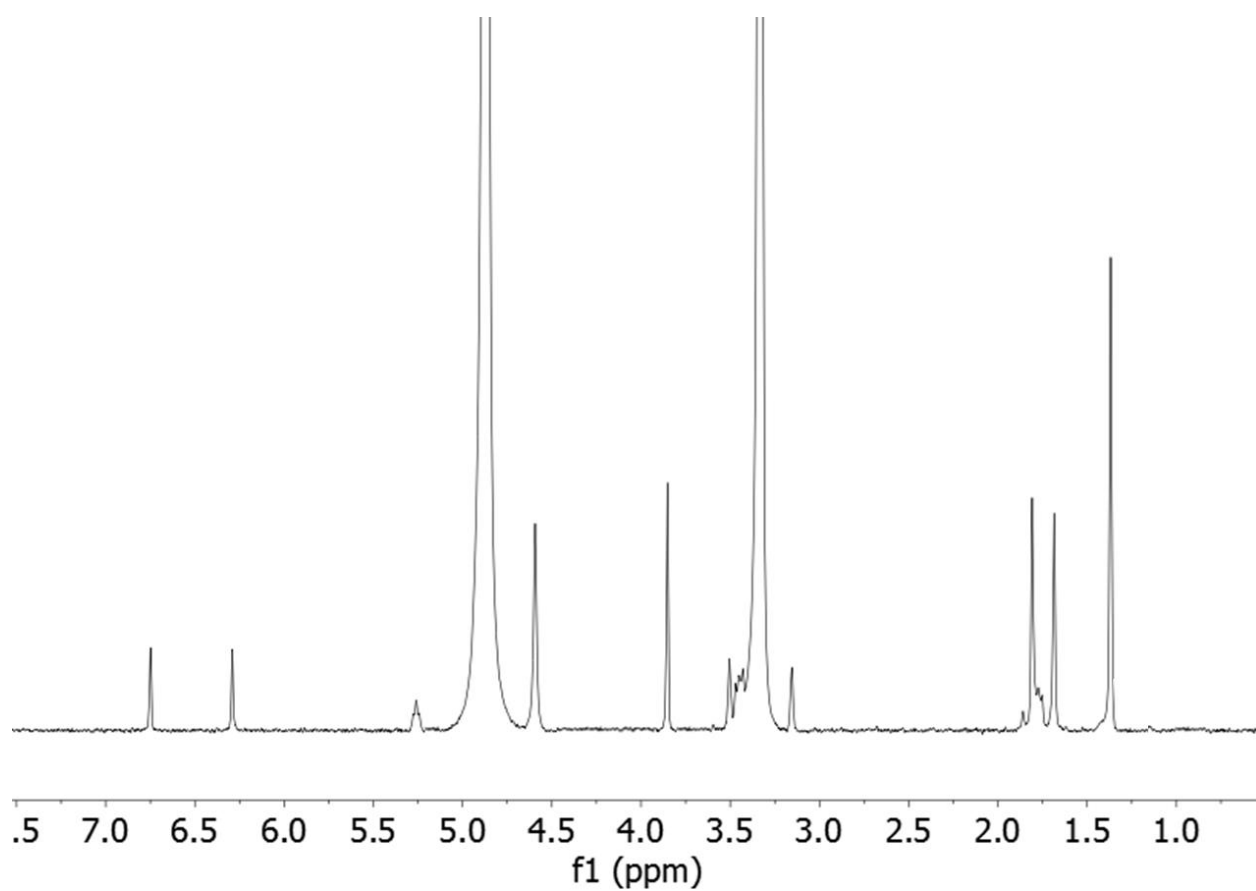
**Figure S11.**  $^1\text{H}$  NMR spectrum (600 MHz,  $\text{CD}_3\text{OD}$ ) of demethylcalabaxanthone (**4**)



**Figure S12.**  $^{13}\text{C}$  NMR (100 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of demethylcalabaxanthone (**4**)

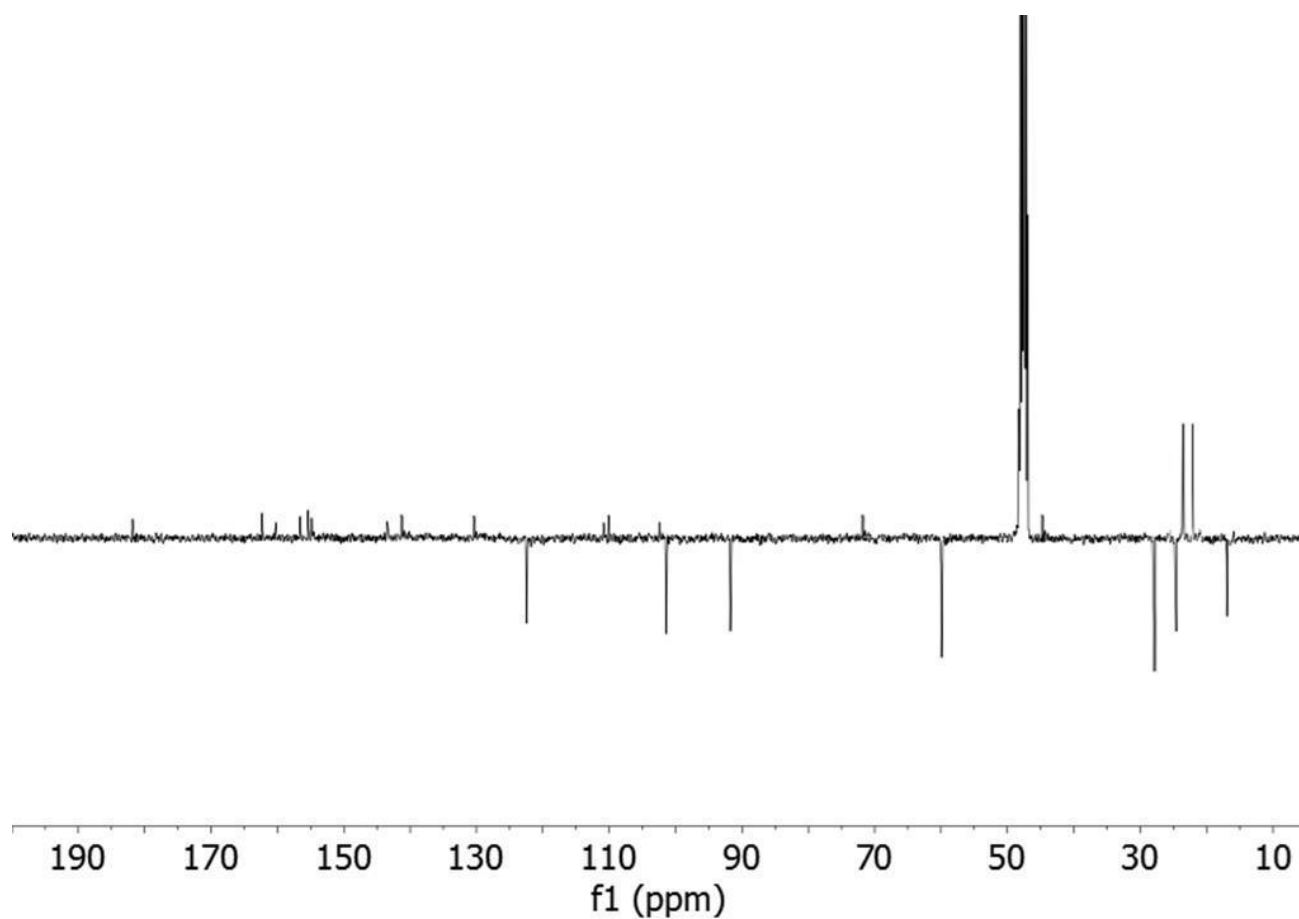


**Figure S13.** ESI/LTQ Orbitrap spectrum of garcinone D (5), in negative ion mode

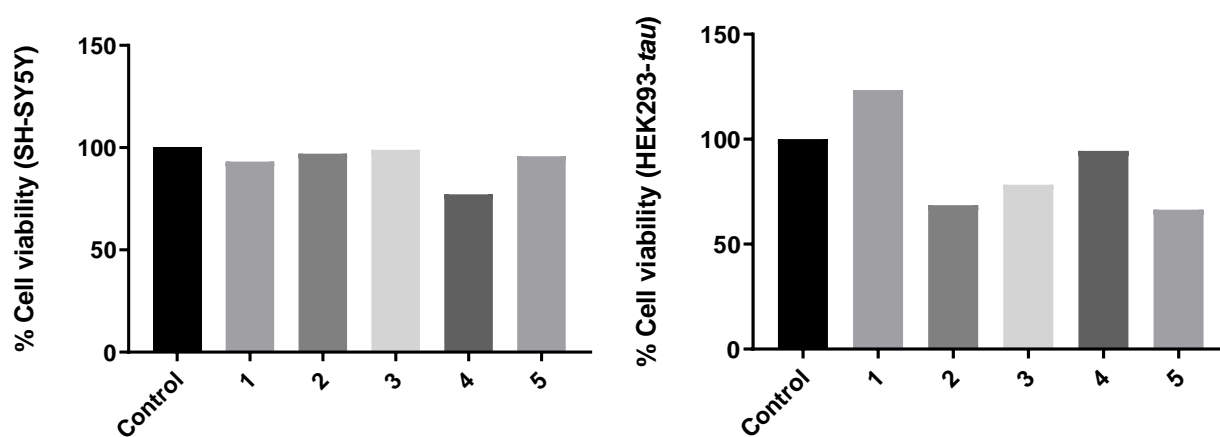


**Figure S14.**  $^1H$  NMR spectrum (600 MHz,  $CD_3OD$ ) of garcinone D (5)





**Figure S15.**  $^{13}\text{C}$  NMR (100 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of garcinone D (5)



**Figure S16.** Results of the cytotoxicity test of compounds 1, 2, 3, 4, and 5 on SH-SY5Y and HEK293-*tau*, expressed as the percentage of viability compared to the control (100%).