

Supporting Information

Monodictyochrome A and B, Dimeric Xanthone Derivatives from the Marine Algicolous Fungus *Monodictys putredinis*

Alexander Pontius,[†] Anja Krick,[†] Ronak Mesry,[†] Stefan Kehraus,[†] Silke E. Foegen,[‡] Michael Müller,[‡] Karin Klimo,[§] Clarissa Gerhäuser,[§] and Gabriele M. König^{*,†}

Institute for Pharmaceutical Biology, University of Bonn, Nussallee 6, 53115 Bonn, Germany, Institute of Pharmaceutical Sciences, Albert-Ludwigs-University Freiburg, Albertstraße 25, 79104 Freiburg, Germany, and Department of Toxicology and Cancer Risk Factors, DKFZ-German Cancer Research Center, Im Neuenheimer Feld 280, D-69120 Heidelberg, Germany

Table of contents:

Figure S1. Important 1H-1H COSY and 1H-13C long range (HMBC) correlations of compound 1 and 2 .	2
Figure S2. Proposed biosynthesis for compound 1 and 2 .	3
Figure S3. 1D and 2D NMR spectra of compound 1 .	4-5
Figure S4. 1D and 2D NMR spectra of compound 2 .	6-7
Figure S5. Structures of fungal metabolites related to 1 and 2 .	8-10
Figure S6. Dose-dependent inhibition of aromatase activity by compounds 1 and 2 .	11

Figure S1. Important ^1H - ^1H COSY and ^1H - ^{13}C long range (HMBC) correlations of compound **1** and **2**.

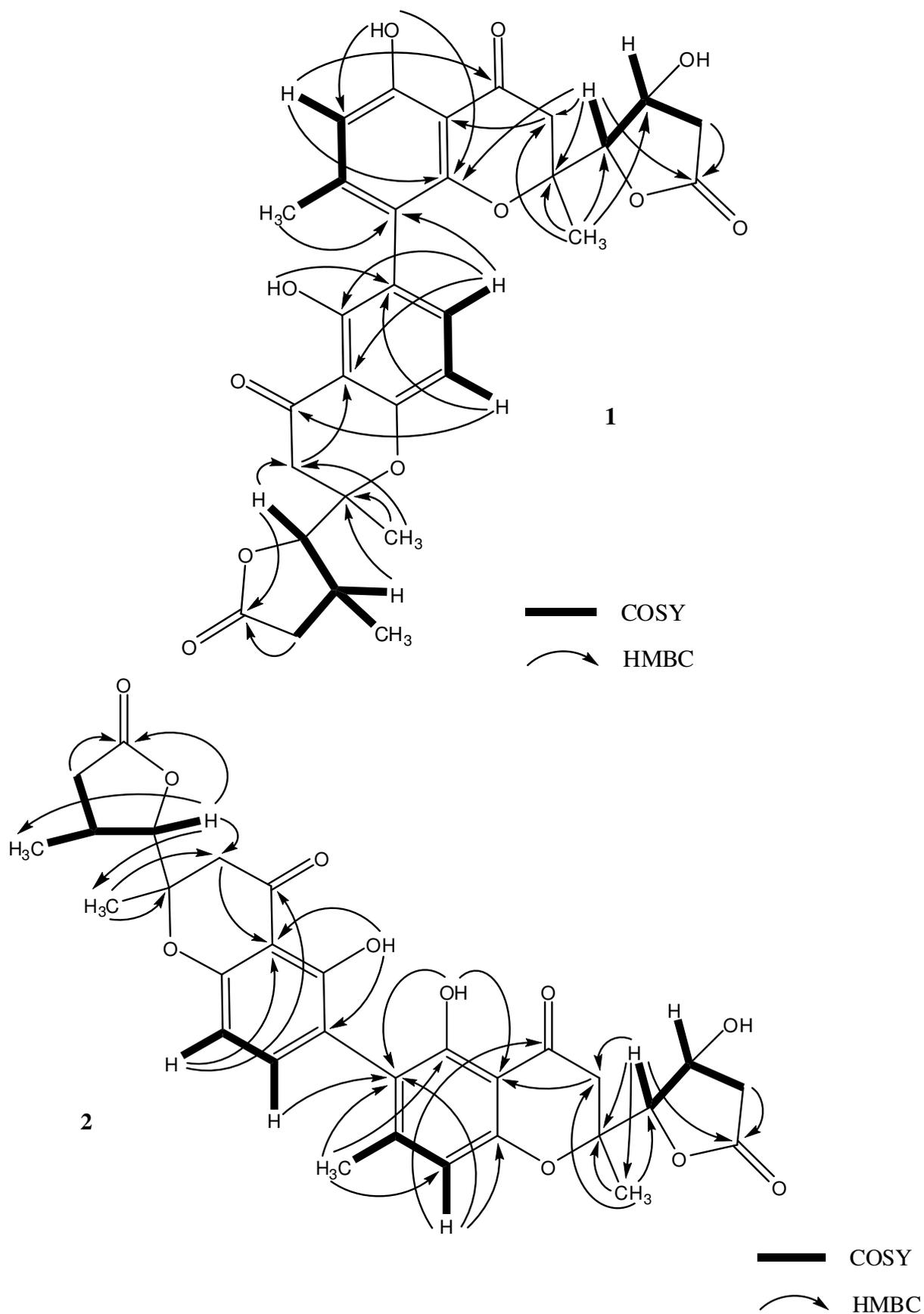


Figure S2. Proposed biosynthesis for compound **1** and **2**.

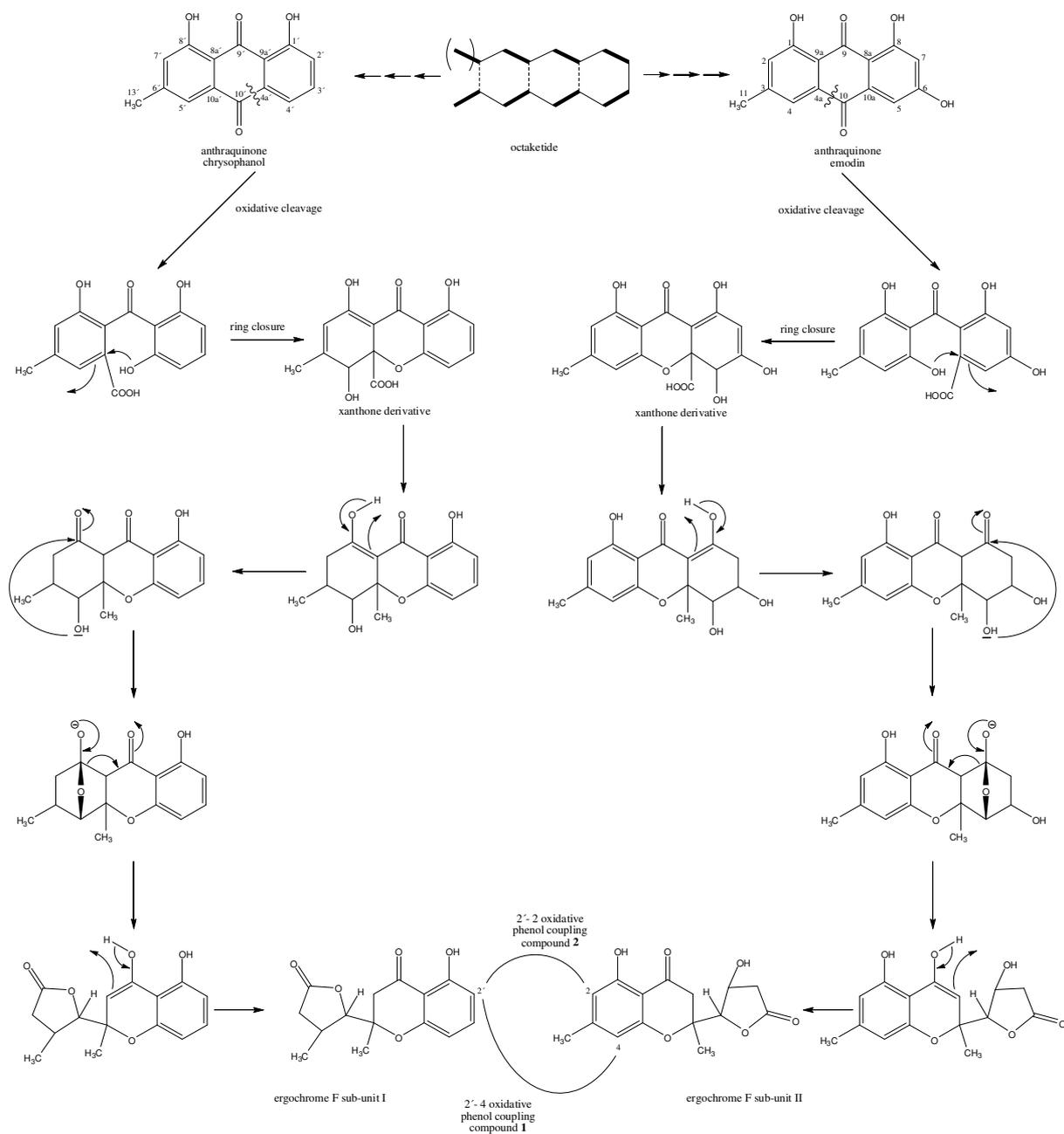
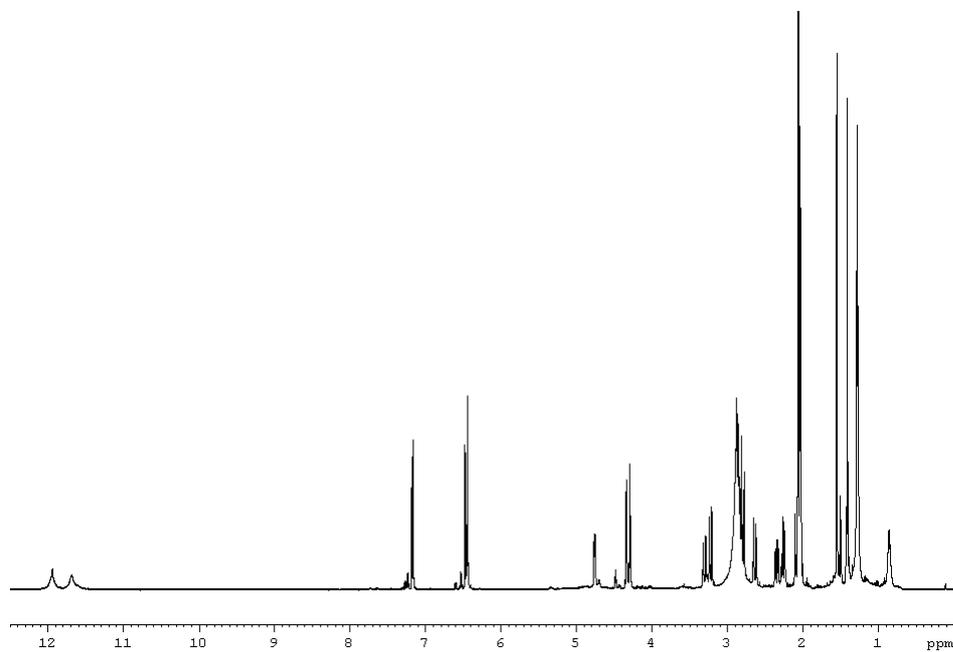
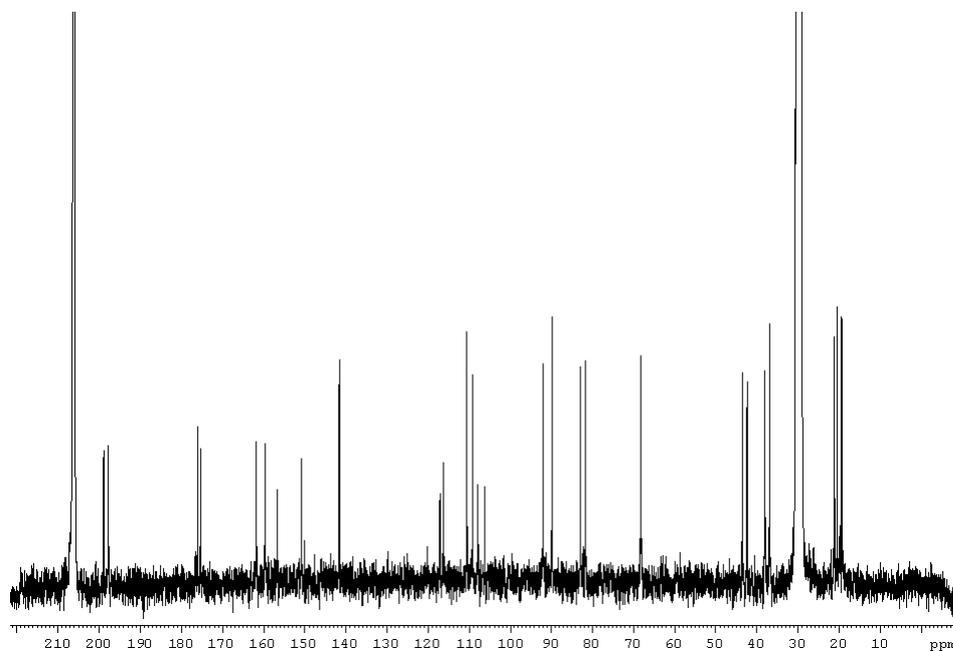


Figure S3. 1D and 2D NMR spectra of compound **1**.

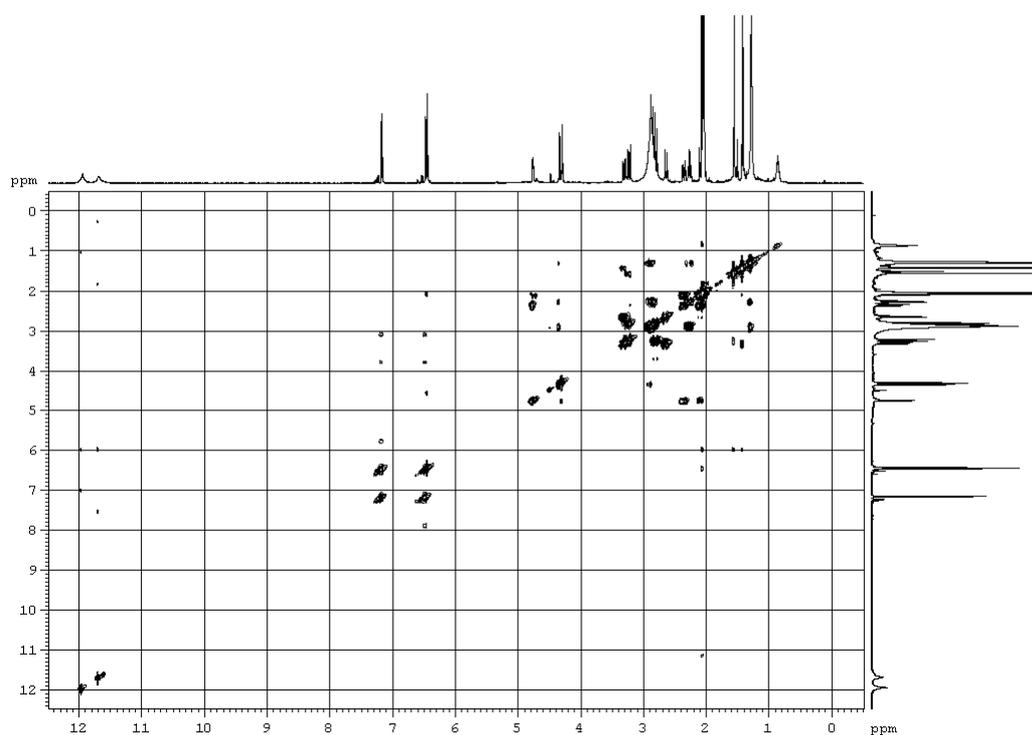
^1H NMR spectrum (500 MHz in acetone- d_6) of the new compound **1**.



^{13}C NMR spectrum (300 MHz in acetone- d_6) of the new compound **1**.



^1H , ^1H -COSY spectrum (300 MHz in acetone- d_6) of the new compound **1**.



^1H , ^{13}C -HMBC spectrum (300 MHz in acetone- d_6) of the new compound **1**.

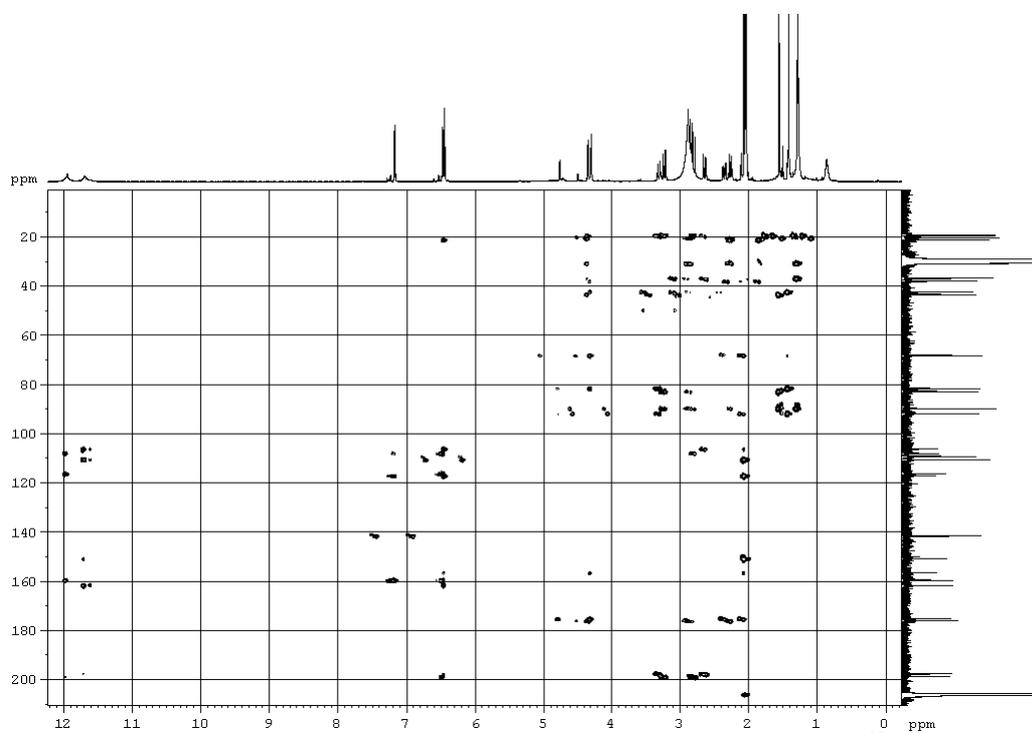
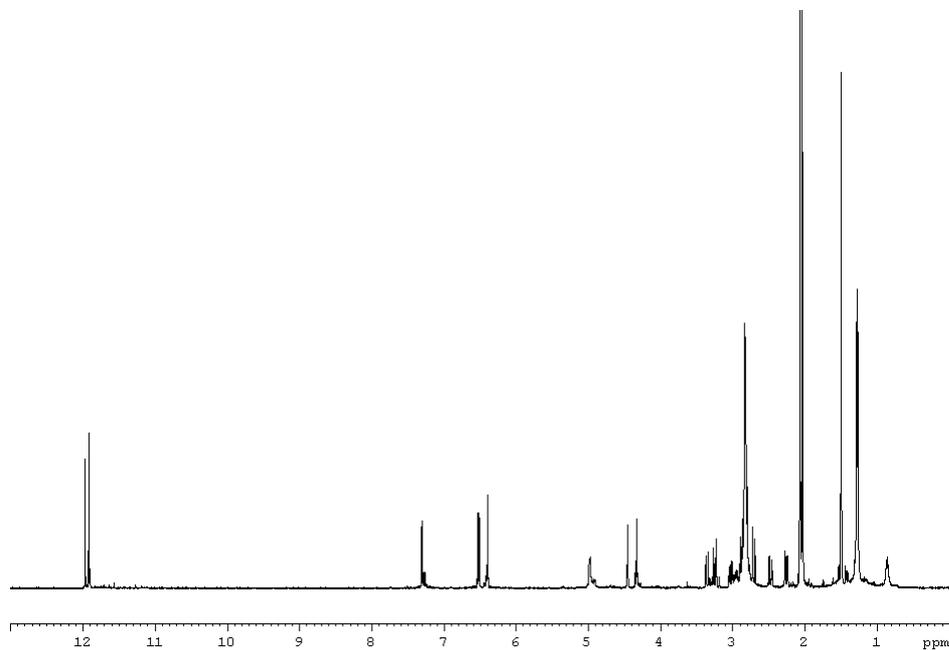
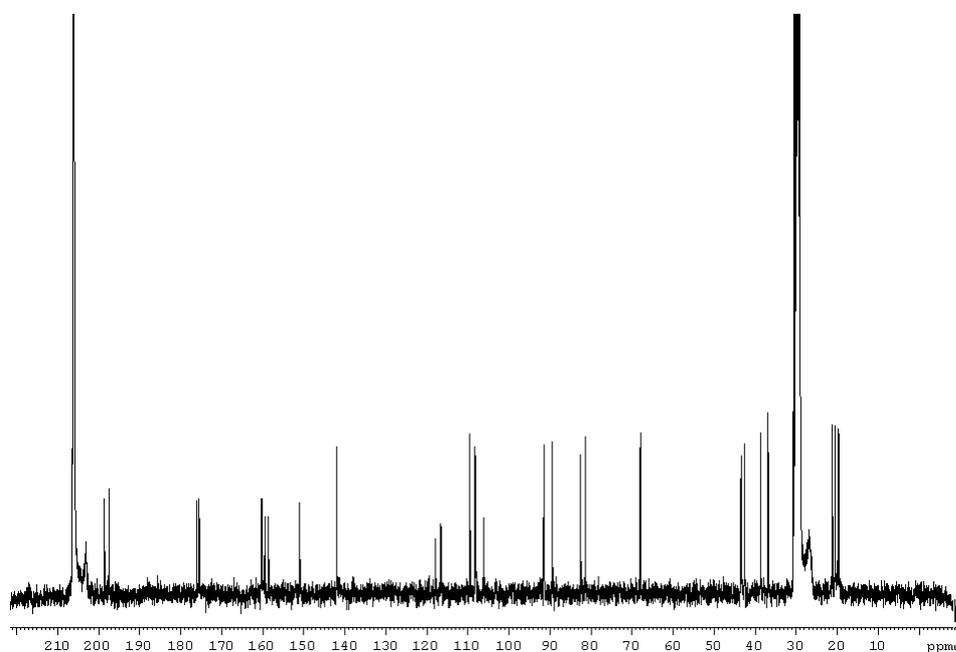


Figure S4. 1D and 2D NMR spectra of compound **2**.

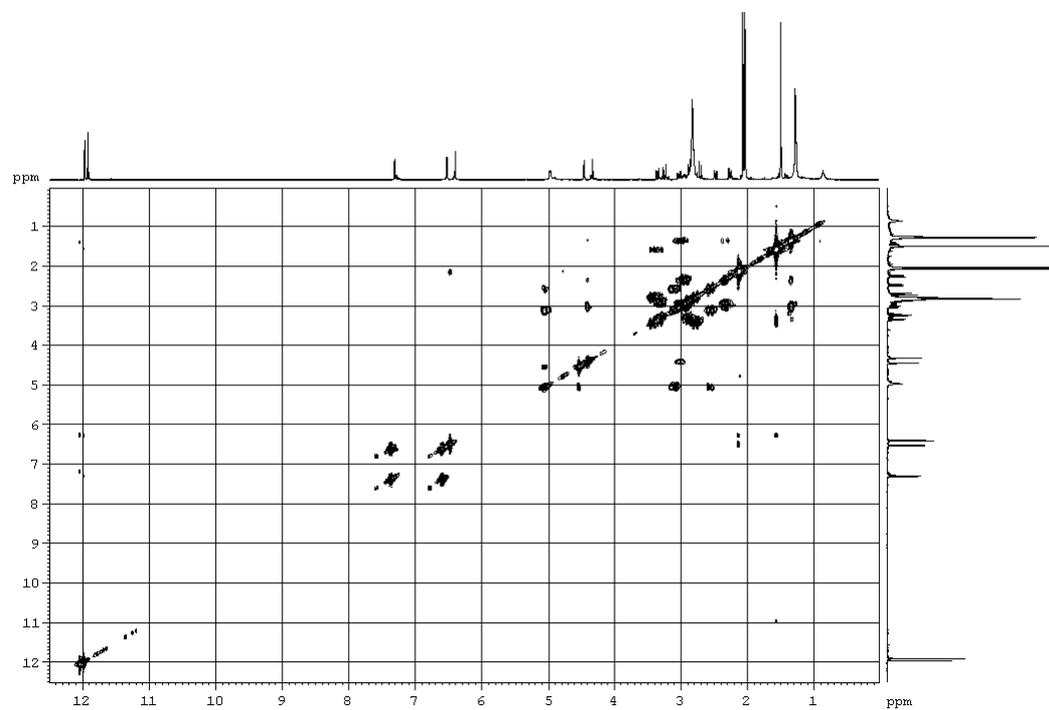
^1H NMR spectrum (500 MHz in acetone- d_6) of the new compound **2**.



^{13}C NMR spectrum (300 MHz in acetone- d_6) of the new compound **2**.



^1H , ^1H -COSY spectrum (300 MHz in acetone- d_6) of the new compound **2**.



^1H , ^{13}C -HMBC spectrum (300 MHz in acetone- d_6) of the new compound **2**.

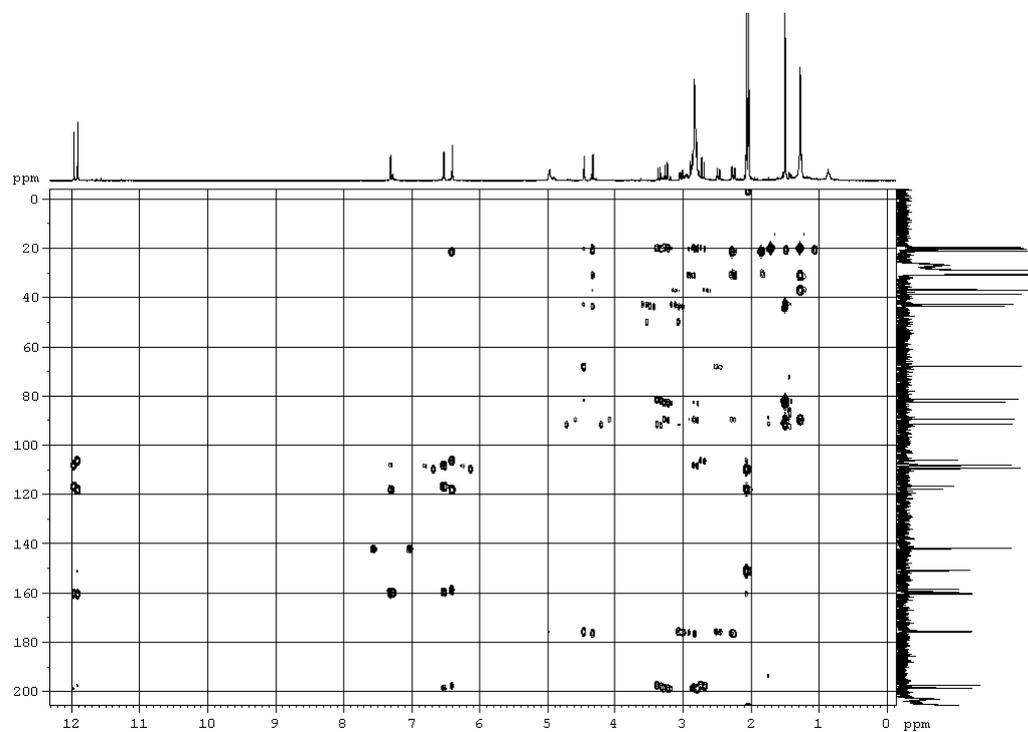
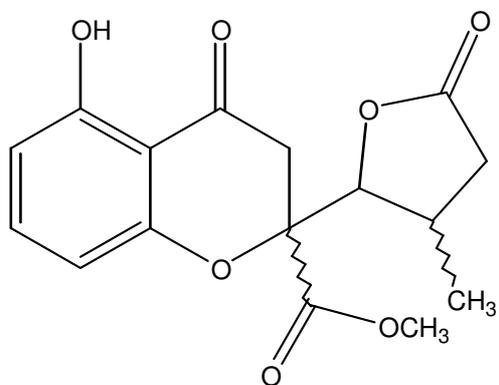
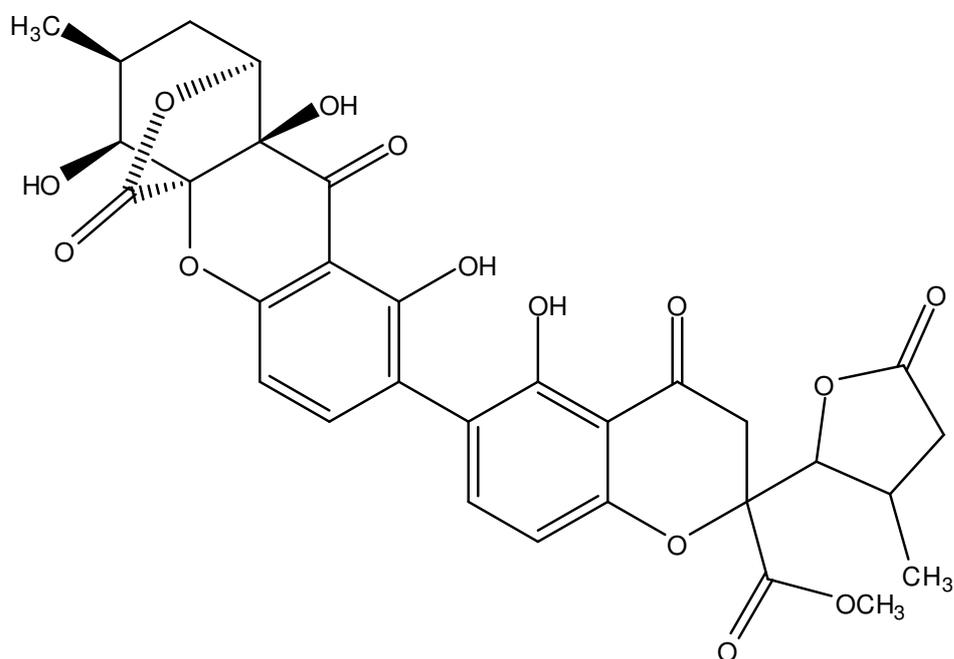


Figure S5. Structures of fungal metabolites related to **1** and **2**.

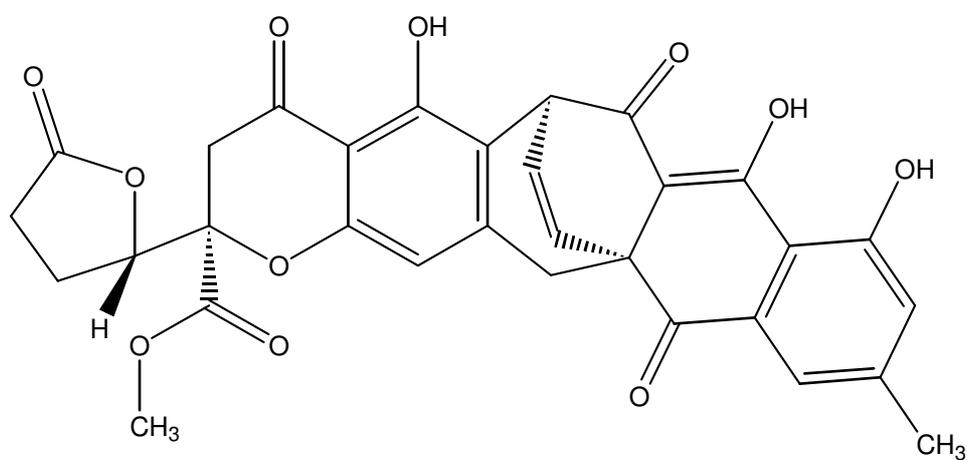
ergochrome F unit ¹⁵:



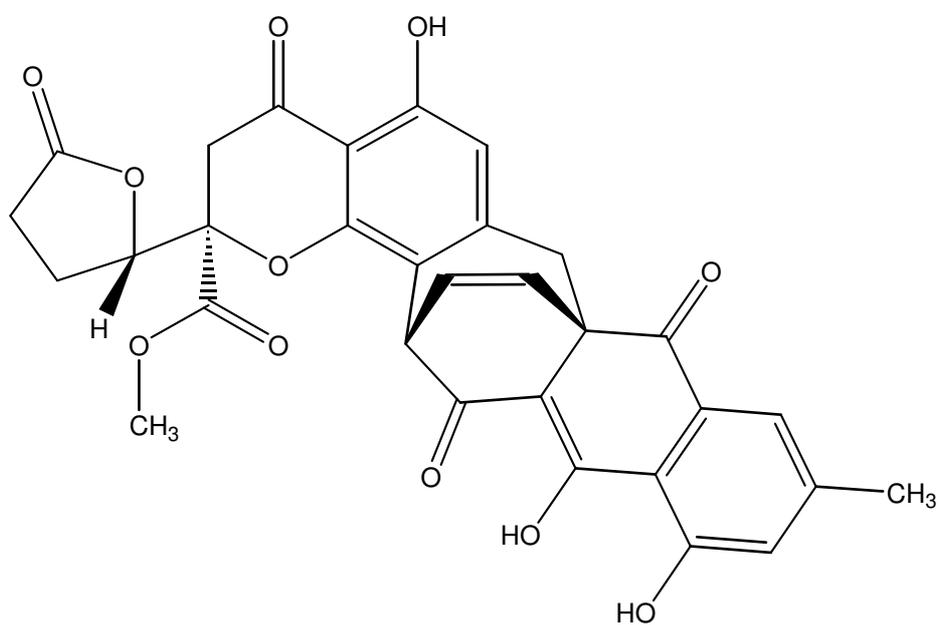
ergoxanthin ¹⁵:



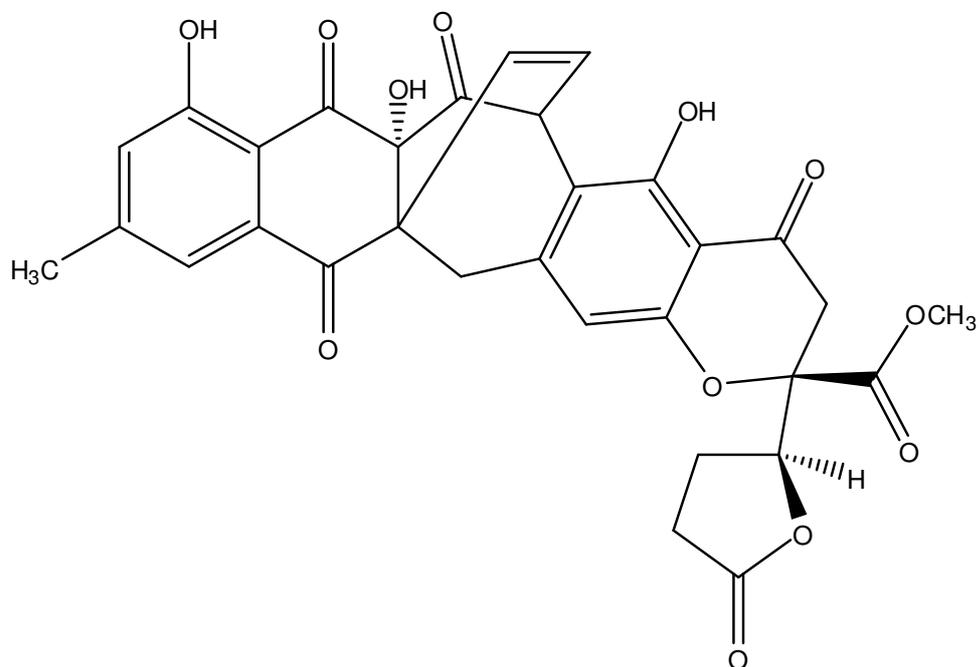
xanthoquinodin A3 ¹⁶:



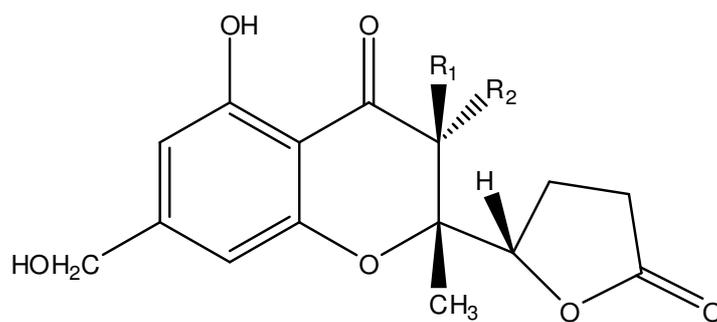
xanthoquinodin B3 ¹⁶:



chaetomanone ¹⁷:



lachnone 3, 4 and 5 ¹⁸:



3: R₁ = R₂ = H

4: R₁ = OH; R₂ = H

5: R₁ = -CH₂COCH₃; R₂ = OH

Figure S6. Dose-dependent inhibition of aromatase activity by compounds **1** and **2**. Ketokonazole was used as a positive control substance with an IC_{50} value of $0.8 \pm 0.3 \mu\text{M}$. Aromatase activity was measured using human recombinant aromatase (human CYP 19 + P450 reductase supersomes) and *O*-benzylfluorescein benzyl ester as a substrate.

