Supporting Information

Antiprotozoal Activities of Heterocyclic Substituted Xanthones from the Marine-Derived Fungus *Chaetomium* sp.

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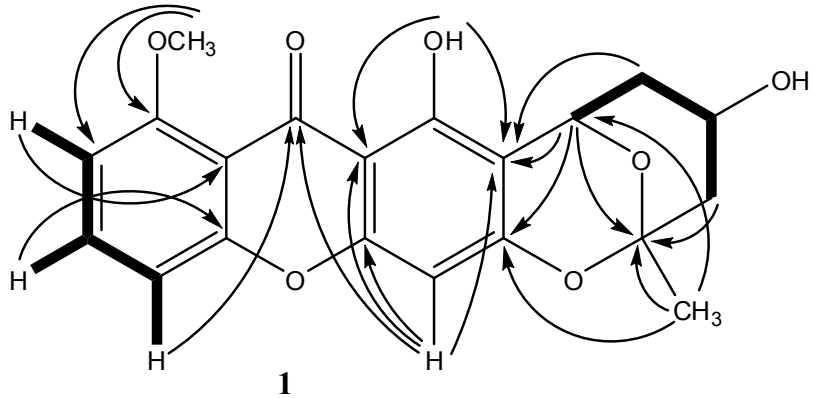
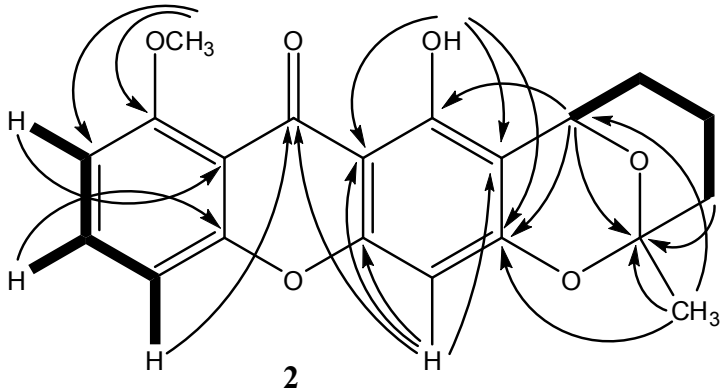
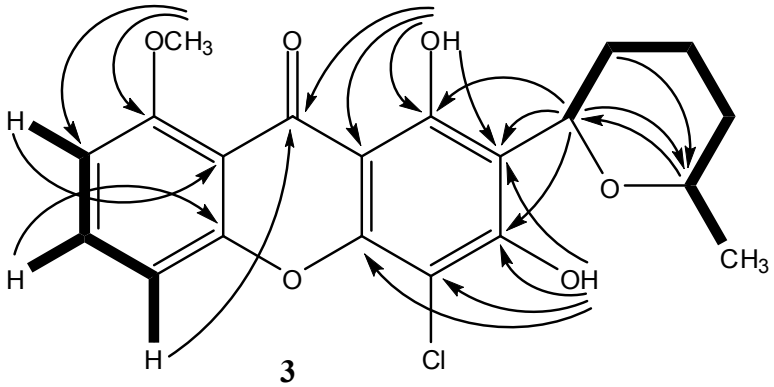
Figure S1. Important ^{1}H-^{1}H COSY and ^{1}H-^{13}C long range (HMBC) correlations of compounds 1, 2, 3.



1



2



3

COSY

HMBC

Figure S2. ^{1}H-^{1}H coupling constants measured for the protons of the tetrahydropyrane moiety (V) of **1** with calculated torsion angles (according to the Karplus equation)[15] between the protons depicted in Newman projections.

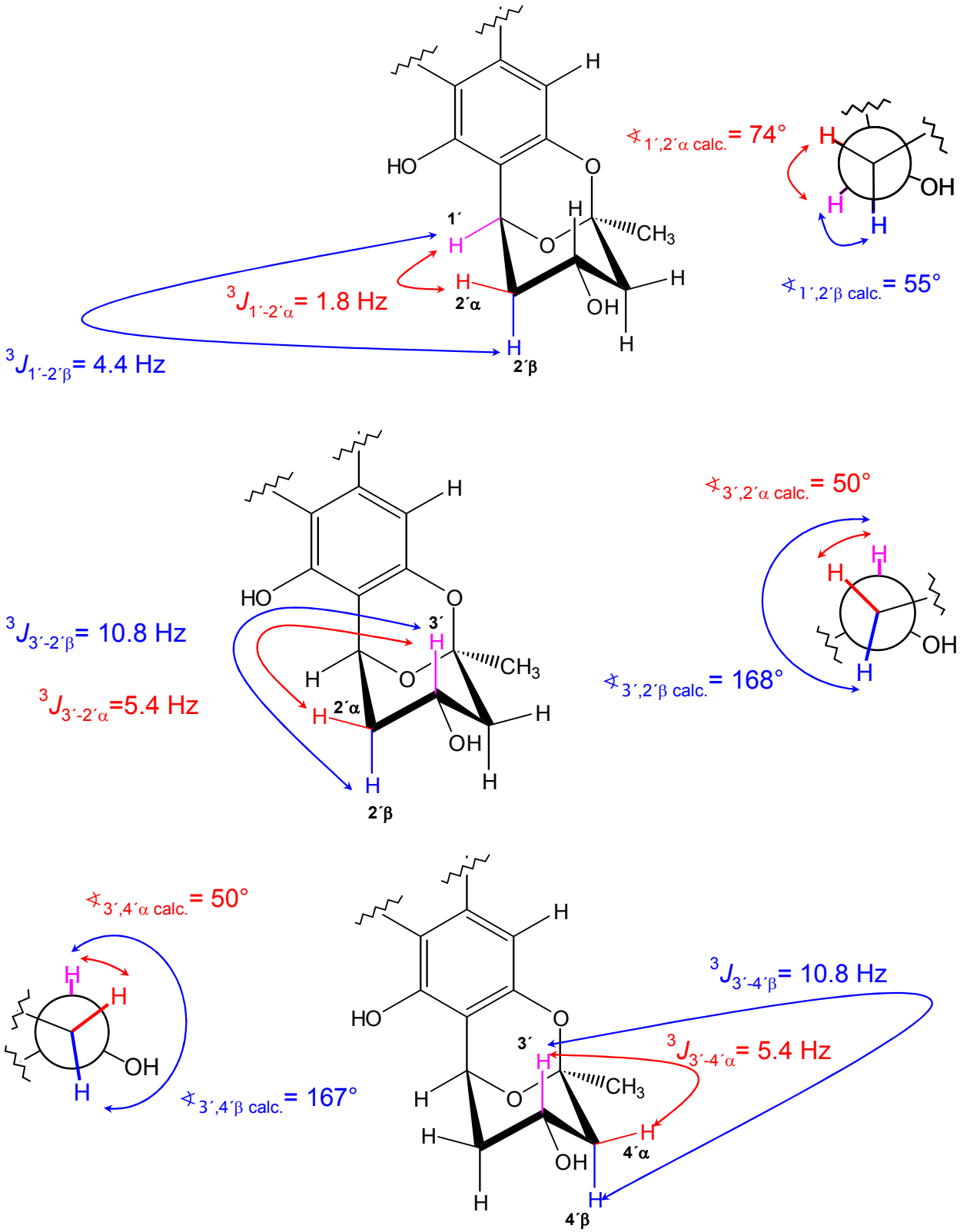
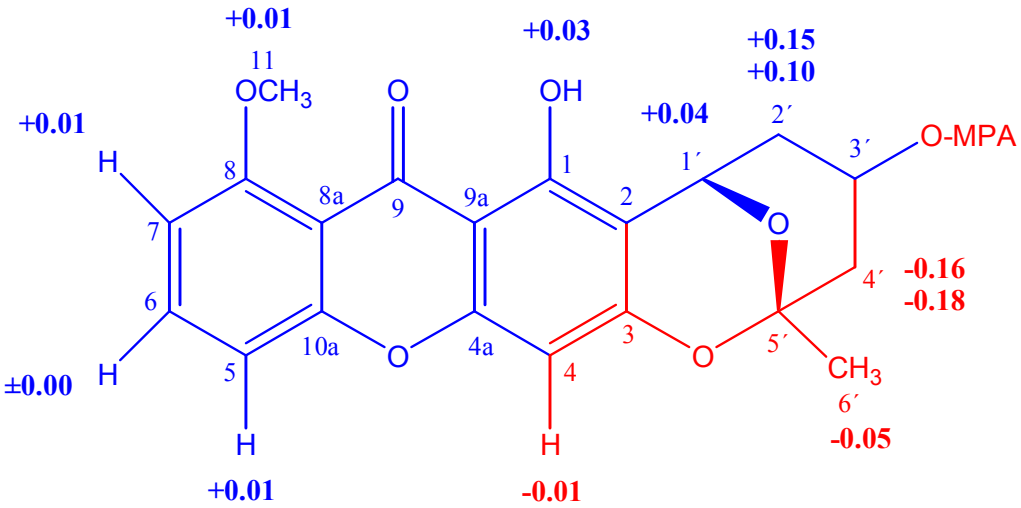


Figure S3. Deduction of the absolute configuration at C-3′ using modified Mosher's method with $\Delta\delta^{RS}$-values of MPA esters of compound **1**.[16]



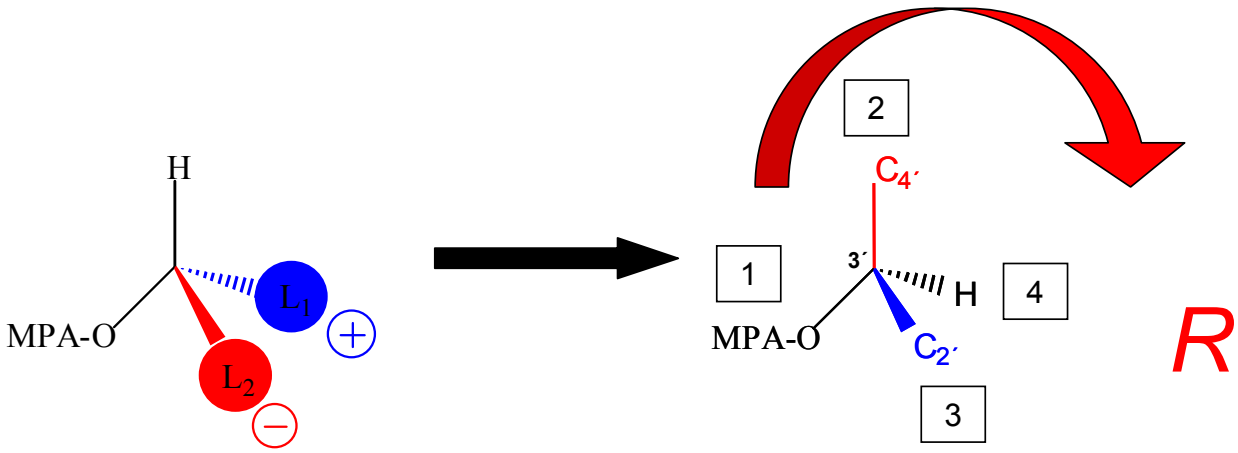


Figure S4. Minimum energy conformation of the 1′*R*, 3′*R*, 5′*R* isomer (*a*) and 1′*S*, 3′*R*, 5′*S* isomer (*b*) of **1**. Model *a* did not show the architecture deduced from ^{1}H,^{1}H coupling constant analysis.

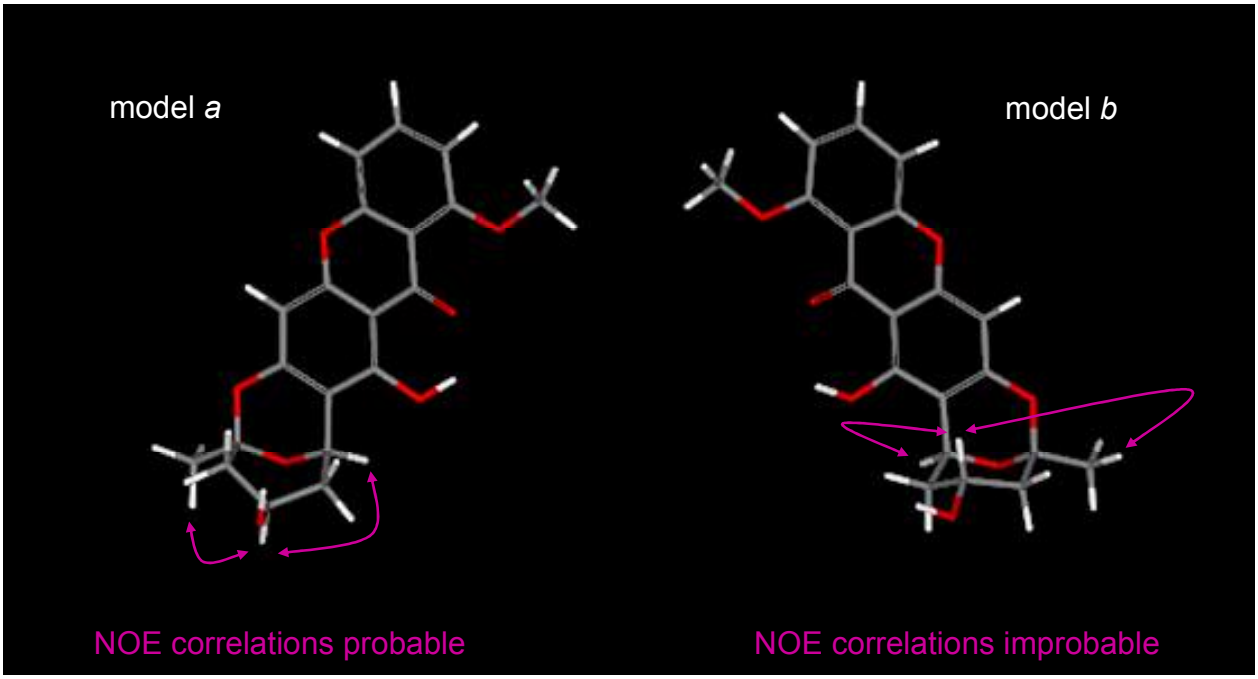


Figure S5. Important selective gradient NOEs (purple arrows) of **3** (A). Minimum energy conformation including NOE restraints with the boat conformation of ring IV within **3** (B).

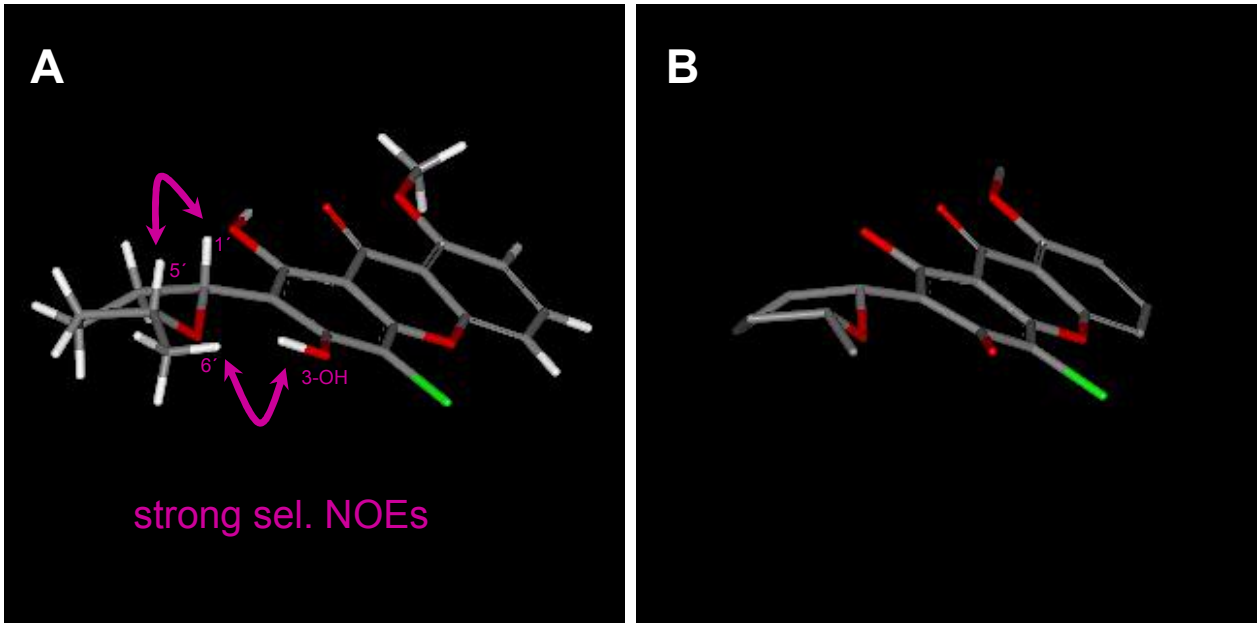


Figure S6. Proposed biogenesis for compounds **1 - 3**.

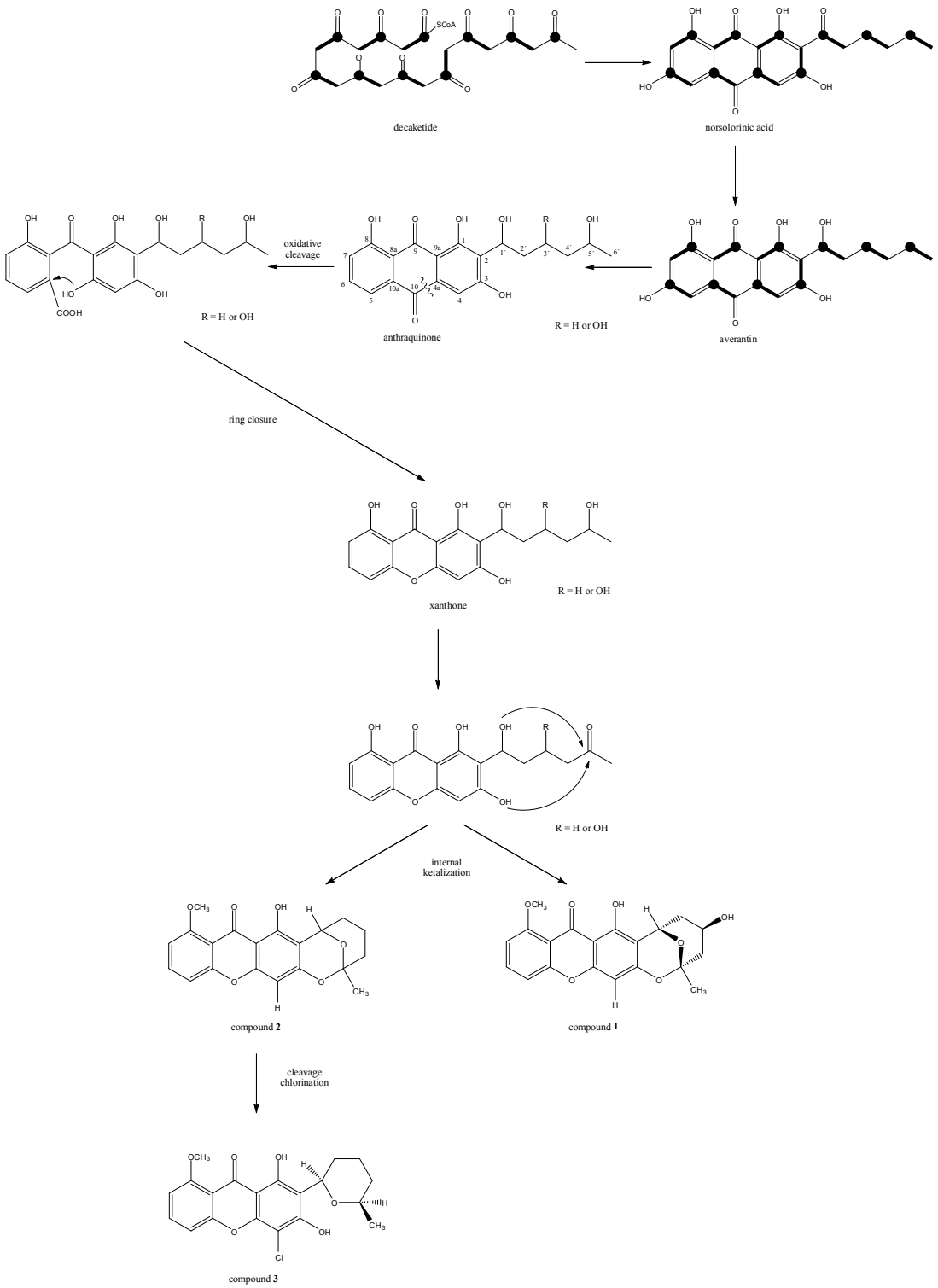
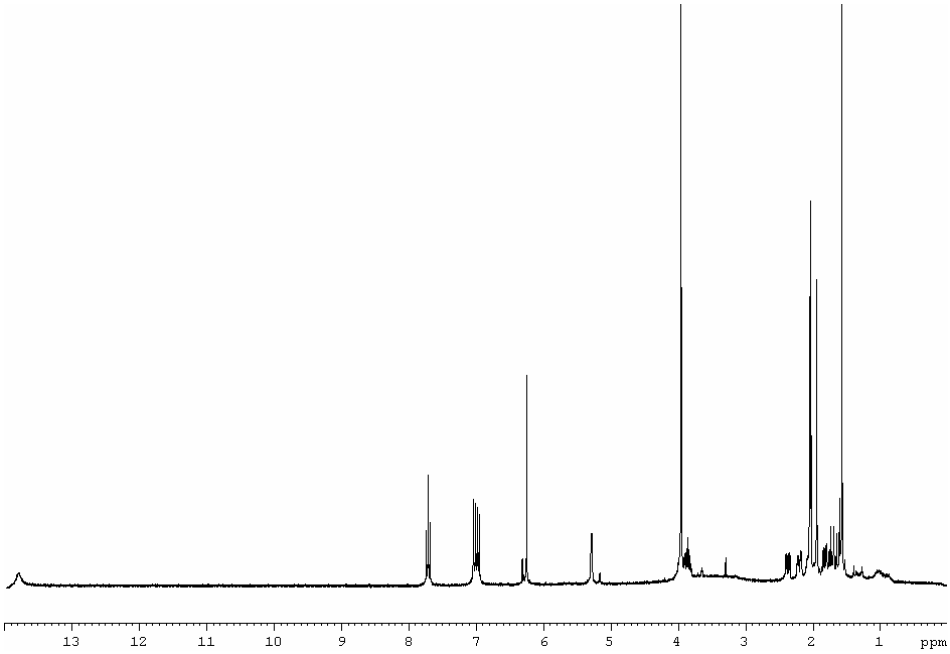


Figure S7. 1D NMR spectra of compound **1.**

^{1}H NMR spectrum (300 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**.

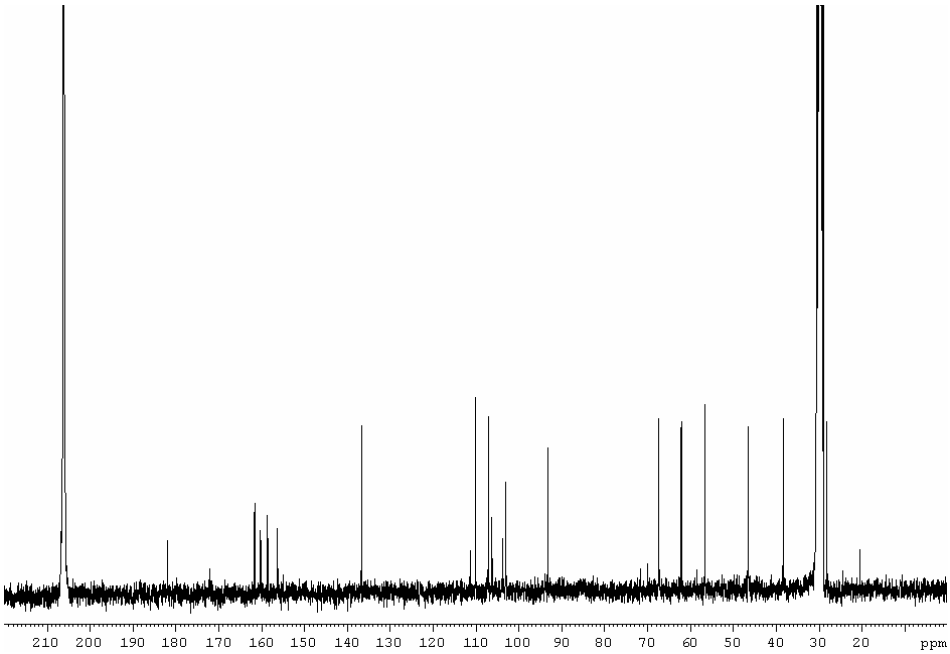
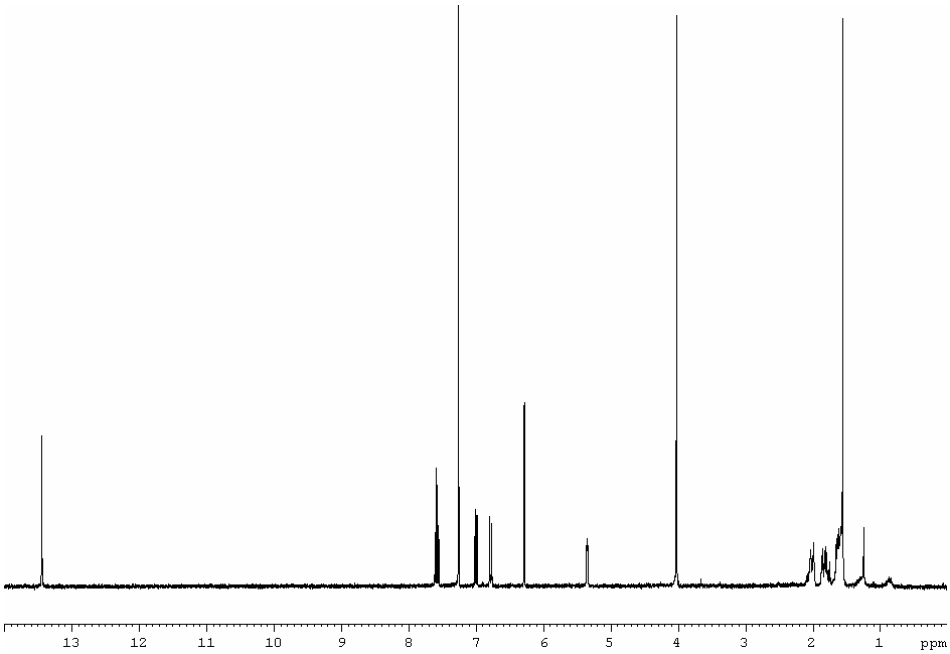


Figure S8. 1D NMR spectra of compound **2.**

^{1}H NMR spectrum (300 MHz in chloroform-d_1) of the new compound **2**.



^{13}C NMR spectrum (300 MHz in chloroform-d_1) of the new compound **2**.

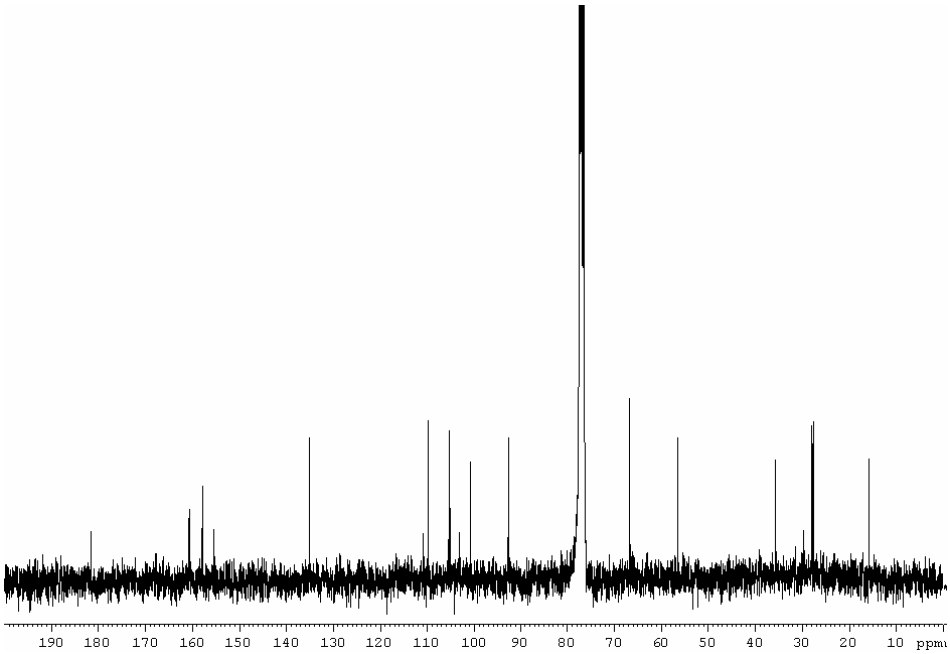
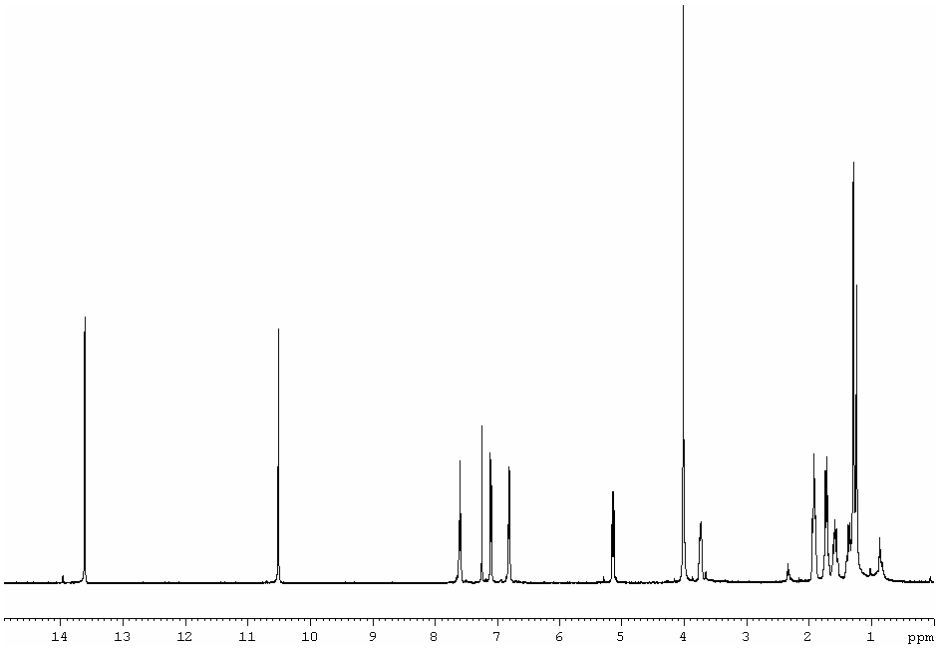


Figure S9. 1D NMR spectra of compound **3.**

^{1}H NMR spectrum (300 MHz in chloroform-d_1) of the new compound **3**.



^{13}C NMR spectrum (300 MHz in chloroform-d_1) of the new compound **3**.

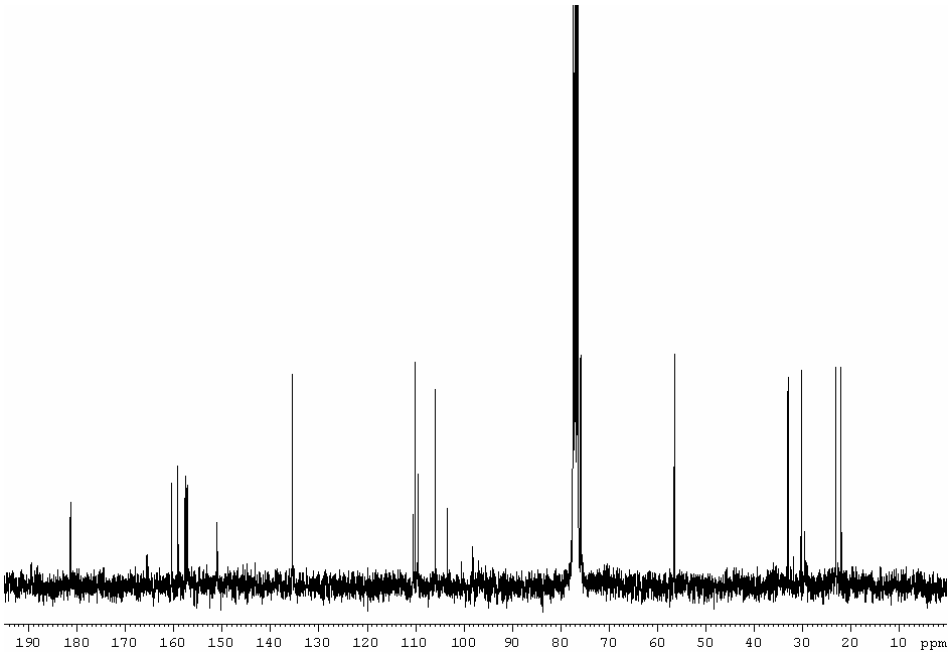
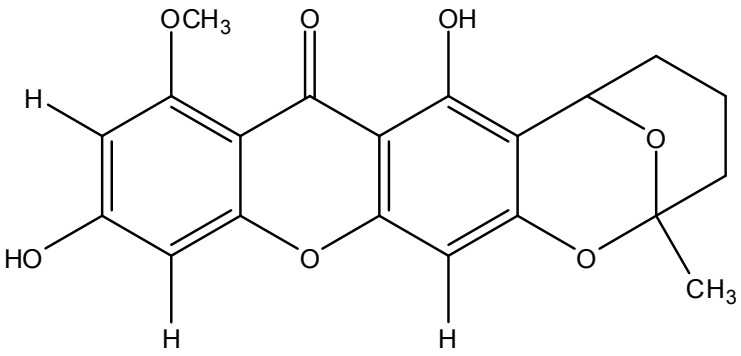
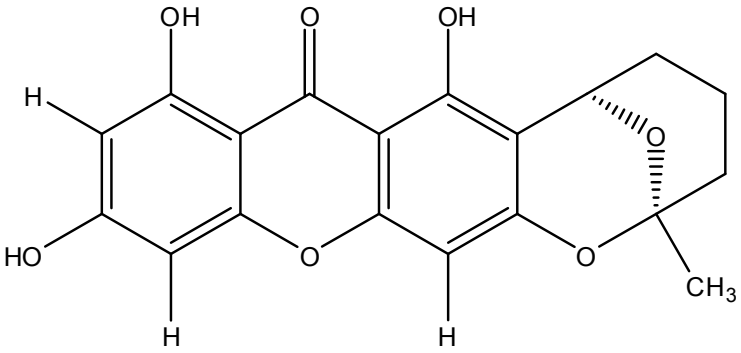


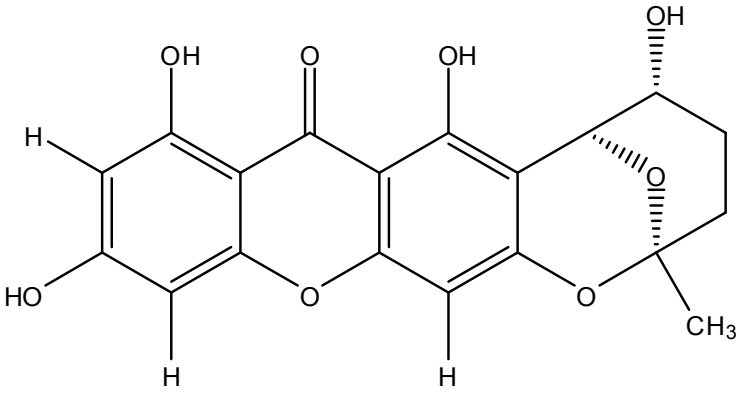
Figure S10. Selected structures of fungal metabolites related to **1**, **2**, **3**.



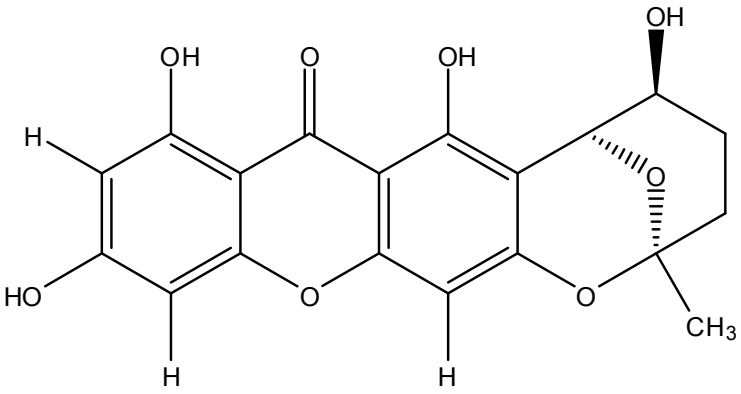
8-O-methyaverufin[17]



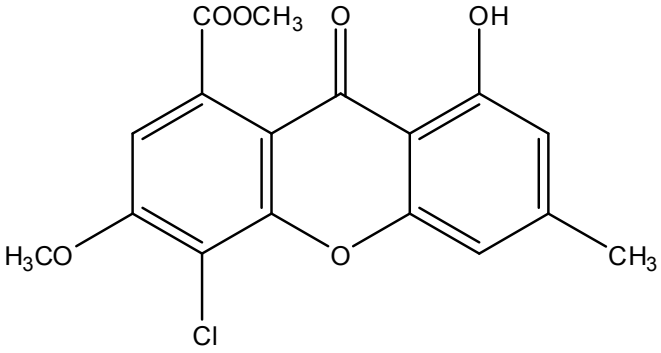
averufin[19]



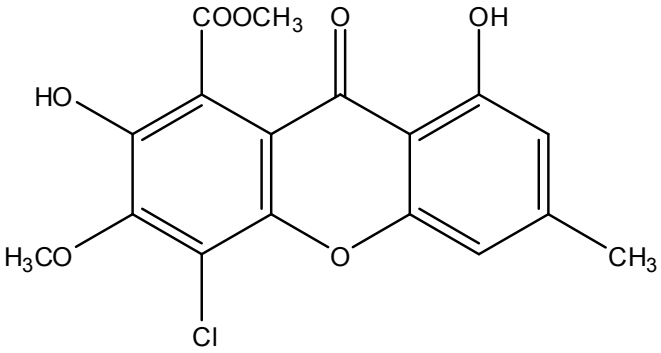
nidurufin[19]



2′-epi-nidurufin[19]



chloroisosulochrin dehydrate[23]



chloropinselin[24]

Table S1. ^{1}H NMR spectral data of (*R*)- and (*S*)-MPA products of **1** with calculated $\Delta\delta^{RS}$ values.

no.[a]	(*R*)-MPA product δ ^{1}H ppm (mult.)[b]	(*S*)-MPA product δ ^{1}H ppm (mult.)[b]	$\Delta\delta^{RS}$
1-OH	13.52 (s)	13.49 (s)	+0.03
6	7.59 (t)	7.59 (t)	±0.00
5	7.00 (d)	6.99 (d)	+0.01
7	6.79 (d)	6.78 (d)	+0.01
4	6.25 (s)	6.26 (s)	-0.01
1´	5.41 (m)	5.37 (m)	+0.04
3´	5.05 (m)	5.03 (m)	+0.02
11	4.03 (s)	4.02 (s)	+0.01
2´α	2.35 (m)	2.20 (m)	+0.15
2´β	2.01 (m)	1.91 (m)	+0.10
4´α	2.37 (m)	2.53 (m)	-0.16
4´β	1.61 (m)	1.79 (m)	-0.18
6´	1.56 (s)	1.61 (s)	-0.05

[a] Position of proton atom. [b] Chloroform-d_1, 300/75.5 MHz.