Structure and Absolute Configuration of Cytotoxic Polyketide Pigments from the Fruiting Bodies of the Fungus *Cortinarius rufo-olivaceus* (Basidiomycetes)

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Supporting Information

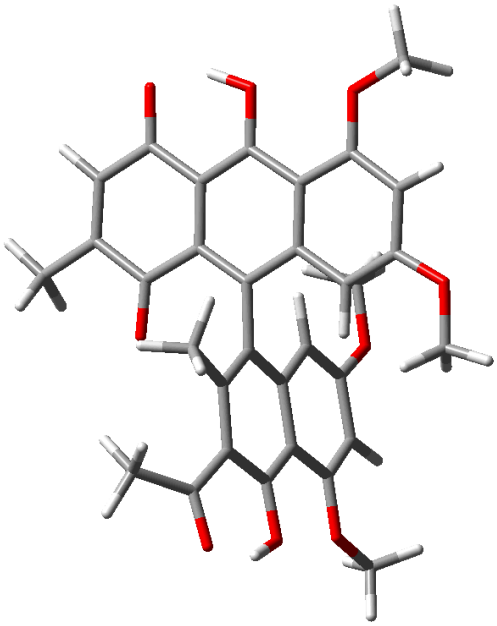
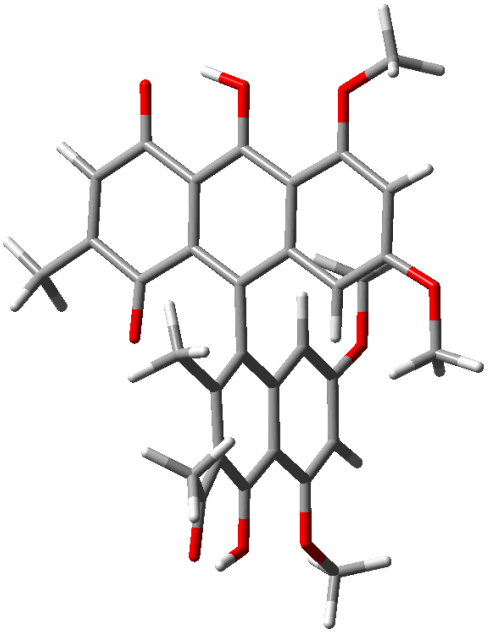
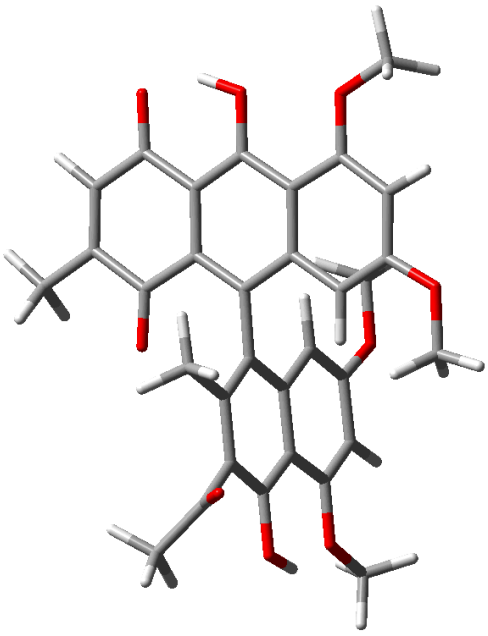
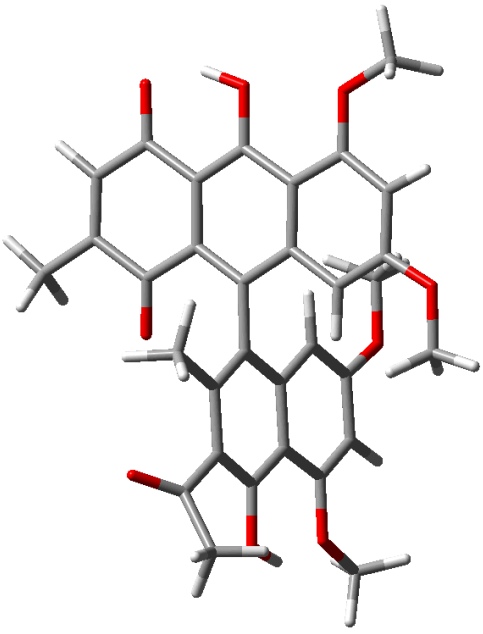
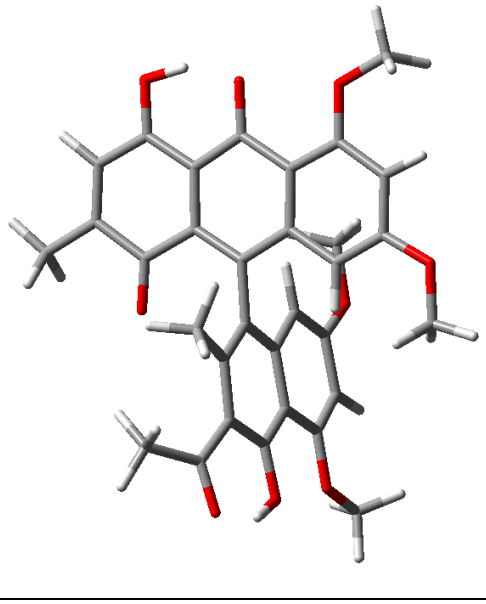
	
I 0 (43)	**II** +0.33 (25)
	
III +0.45 (20)	**IV$_{PQ}$** +0.84 (11)

Figure S1. DFT-calculated low-energy structures for compound (a*S*)-**1**, with relative energies in kcal/mol (and Boltzmann populations at 300K).



I_{ND}
+4.15 kcal/mol[(a)]

Figure S2. DFT-calculated lowest-energy structure for compound (a*S*)-**1** in the "ND" tautomeric form.

[(a)] Relatively to **I** shown in Figure S1.

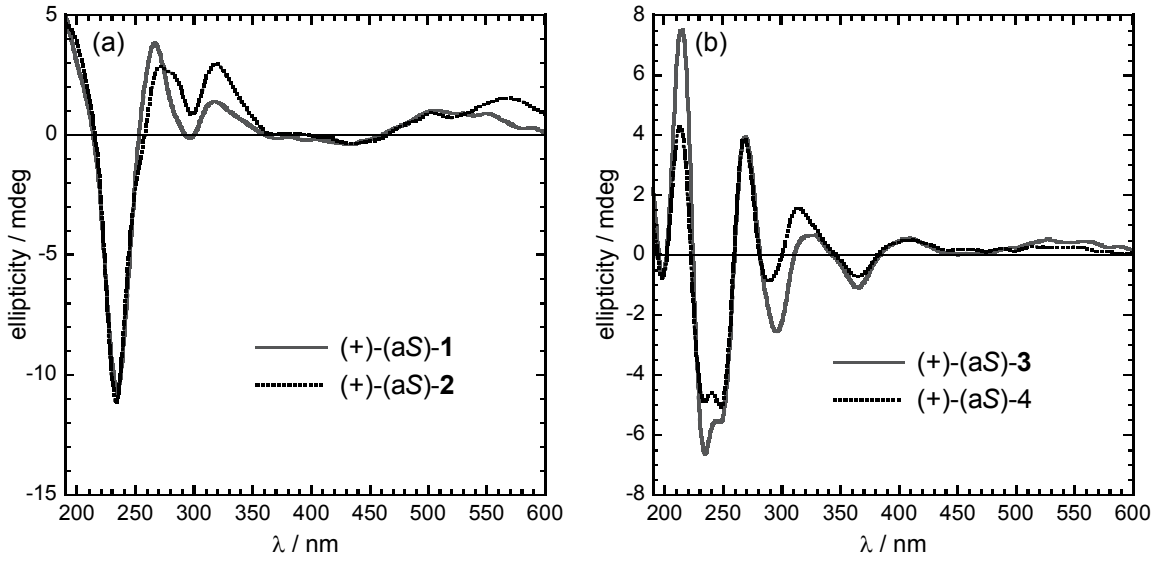


Figure S3. CD spectra of rufoolivacins **1-4** in acetonitrile. Concentrations 2-2.5 mM, 0.02 cm cell.

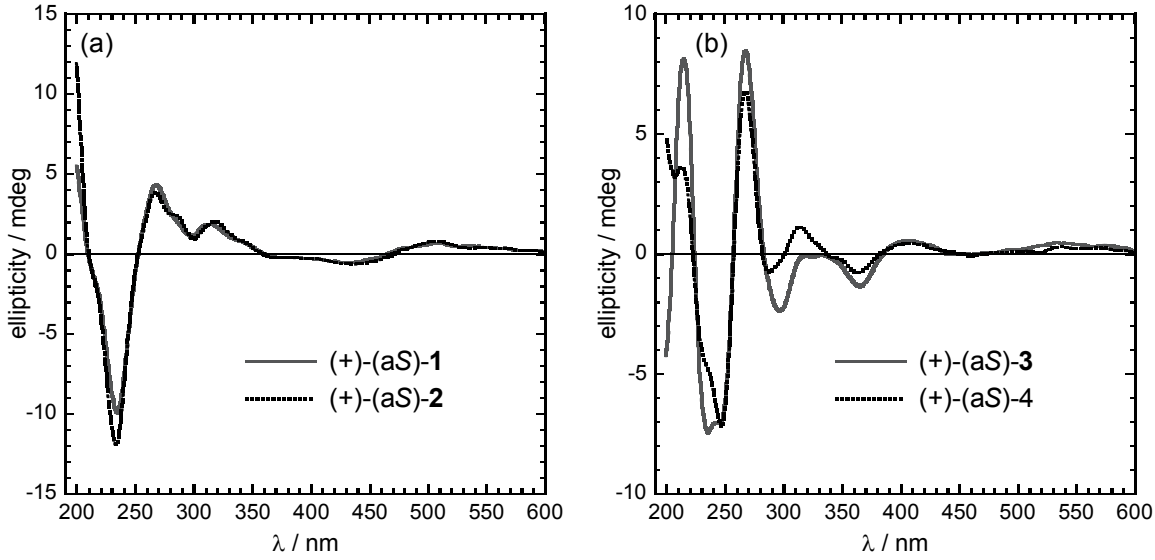


Figure S4. CD spectra of rufoolivacins **1-4** in THF. Concentrations 2-2.5 mM, 0.02 cm cell.

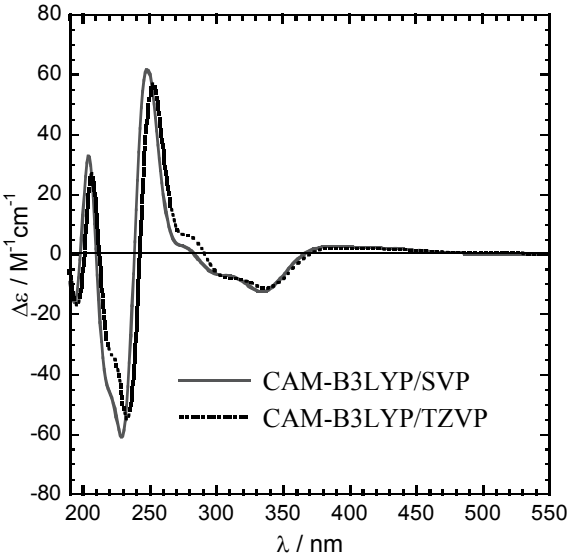


Figure S5. Comparison between CD spectra calculated with CAM-B3LYP/SVP and CAM-B3LYP/TZVP on the lowest-energy structure I optimized with B3LYP/6-31G(d) for (a*S*)-rufoolivacin (**1**).

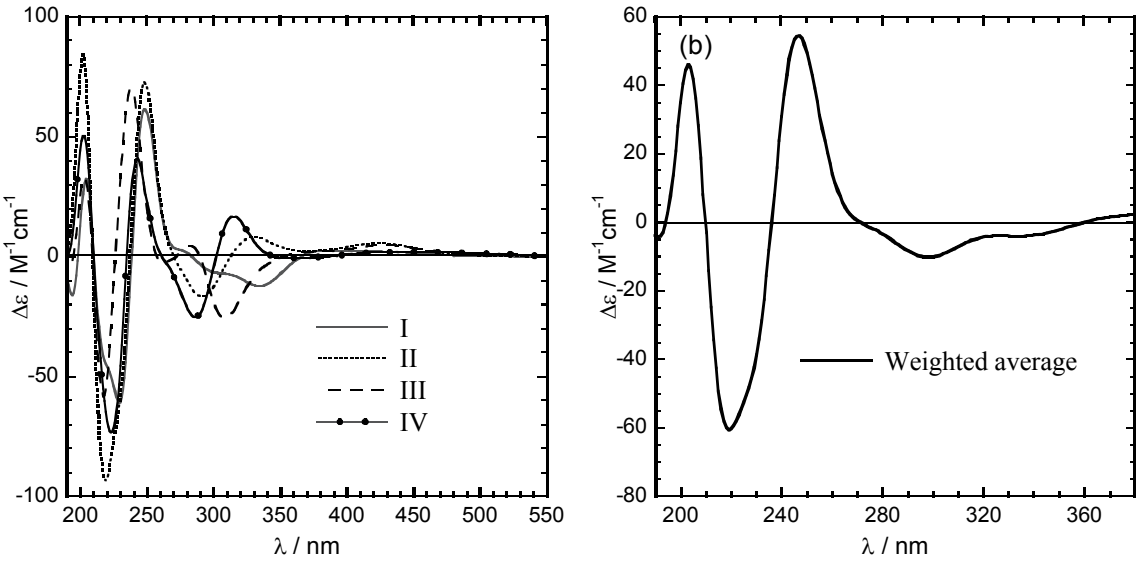


Figure S6. (a) CD spectra calculated with ZINDO/S-CI on the low-energy structures I-IV optimized with B3LYP/6-31G(d) for (a*S*)-rufoolivacin (**1**). (b) Expansion of the weighted average of the four spectra shown in (a).