Supplementary Information

Table S1. Relative and free energies^a and equilibrium populations^b of low-energy conformers of **1** and **2** in MeOH.

Figure S1. Low-energy conformers of 1'*S*-isomer. Fragment from C-1 to C-4 was removed and replaced by hydrogen atoms in order to save computation time.

Figure S2. Low-energy conformers of 1'*R*-isomers. Fragment from C-1 to C-4 was removed and replaced by hydrogen atoms in order to save computation time.

Figure S3. ¹H NMR spectrum of Myrothecol G (1)

Figure S4. ¹³C NMR spectrum of Myrothecol G (1)

Figure S5. HSQC spectrum of Myrothecol G (1)

Figure S6. ¹H-¹H COSY spectrum of Myrothecol G (1)

Figure S7. HMBC spectrum of Myrothecol G (1)

Figure S8. NOESY spectrum of Myrothecol G (1)

Figure S9. HRESIMS spectrum of Myrothecol G (1)

Figure S10. ¹H NMR spectrum of Myrothecol H (2)

Figure S11. ¹³C NMR spectrum of Myrothecol H (2)

Figure S12. HSQC spectrum of Myrothecol H (2)

Figure S13. ¹H-¹H COSY spectrum of Myrothecol H (2)

Figure S14. HMBC spectrum of Myrothecol H (2)

Figure S15. NOESY spectrum of Myrothecol H (2)

Figure S16. HRESIMS spectrum of Myrothecol H (2)

Conformer	ΔE	ΔG	P (%)
1'S-isomers			
1a1	0.56	0.0	42.8
1a2	0.60	1.17	6.0
1a3	0.77	1.44	3.8
1b1	0.0	0.15	33.0
1b2	0.26	1.06	7.1
1b3	0.35	1.30	4.7
1c	0.92	1.65	2.6
1'R-isomers			
2a1	0.00	0.00	75.6
2a2	0.98	0.65	6.2
2a3	1.19	1.24	5.0
2b1	1.76	1.76	8.3
2b2	2.47	1.96	2.5
2b3	2.75	2.54	2.3

Table S1. Relative and free energies a and equilibrium populations b of low-energy conformers of 1 and 2 in MeOH.

^{*a*} At the B3LYP/def2-TZVP level, in kcal/mol; ^{*b*} From ΔG values at 298.15 K.



Figure S1. Low-energy conformers of 1'*S*-isomers. Fragment from C-1 to C-4 was removed and replaced by hydrogen atoms in order to save computation time.

1b3

1b2

1c



Figure S2. Low-energy conformers of 1'R-isomers. Fragment from C-1 to C-4 was removed and replaced by hydrogen atoms in order to save computation time.



Figure S3. ¹H NMR spectrum of Myrothecol G (1).



Figure S4. ¹³C NMR spectrum of Myrothecol G (1).



Figure S5. HSQC spectrum of Myrothecol G (1).



Figure S6. ¹H–¹H COSY spectrum of Myrothecol G (1).



Figure S7. HMBC spectrum of Myrothecol G (1).



Figure S8. NOESY spectrum of Myrothecol G (1)



Figure S9. HRESIMS spectrum of Myrothecol G (1).



Figure S10. ¹H NMR spectrum of Myrothecol H (2).



Figure S11. ¹³C NMR spectrum of Myrothecol H (2).







Figure S13. ¹H–¹H COSY spectrum of Myrothecol H (2).



Figure S14. HMBC spectrum of Myrothecol H (2).



Figure S15. NOESY spectrum of Myrothecol H (2).



Figure S16. HRESIMS spectrum of Myrothecol H (2).

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