Supporting Information

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Diterpenoids from the Roots of Clerodendrum bungei

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No.	Conformer	Energy (hartree)	Energy (Kcal/mol)	Proportion (%)
1		-1151.8059374	-722769.743777874	52.57
2		-1151.8058152	-722769.667096152	46.18
3		-1151.8022875	-722767.453429125	1.10
4		-1151.7997953	-722765.889548703	0.08
5		-1151.7996883	-722765.822405133	0.07

 Table S1. Re-optimized conformers, energies and proportions for 1.





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Figure S8: The UV spectrum of 1.



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Figure S14: NOESY spectrum of 2 in CD₃OD.

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Figure S16: The UV spectrum of 2.



Figure S18: ¹³C and DEPT NMR spectra of 2 in CDCl₃.

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Figure S20: ¹H NMR spectrum of 2b in CDCl₃.





-13.73

Figure S22: ¹³C and DEPT NMR spectra of 3 in CDCl₃.

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Figure S24: HSQC spectrum of 3 in CDCl₃.





Figure S26: NOESY spectrum of 3 in CDCl₃.

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Figure S27: Linear correlation between the experimental ¹³C NMR data for **3** and the calculated data for (*Z*)- Δ^{15} (left) and (*E*)- Δ^{15} (right) isomers, respectively.

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Figure S28: SciFinder search report for compound 1.

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Figure S29: SciFinder search report for compound 2.



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Figure S37: ¹³C and DEPT NMR spectra of 7 in CDCl₃.

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Figure S49:¹³C and DEPT NMR spectra of 13 in CDCl₃.