

Supplementary Information

Antimicrobial Diterpene from the Brazilian Termite *Nasutitermes macrocephalus* (Isoptera: Termitidae: Natutitermitinae)

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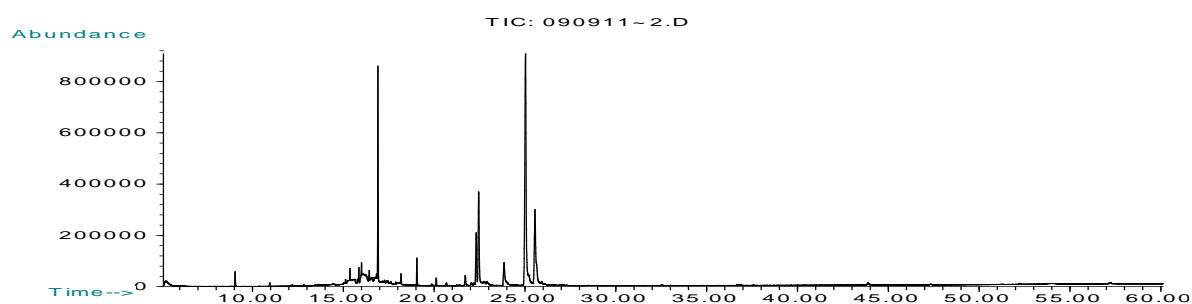


Figure S1. Chromatogram of sample *Nasutitermes microcephalus* extract obtained by GC-MS.

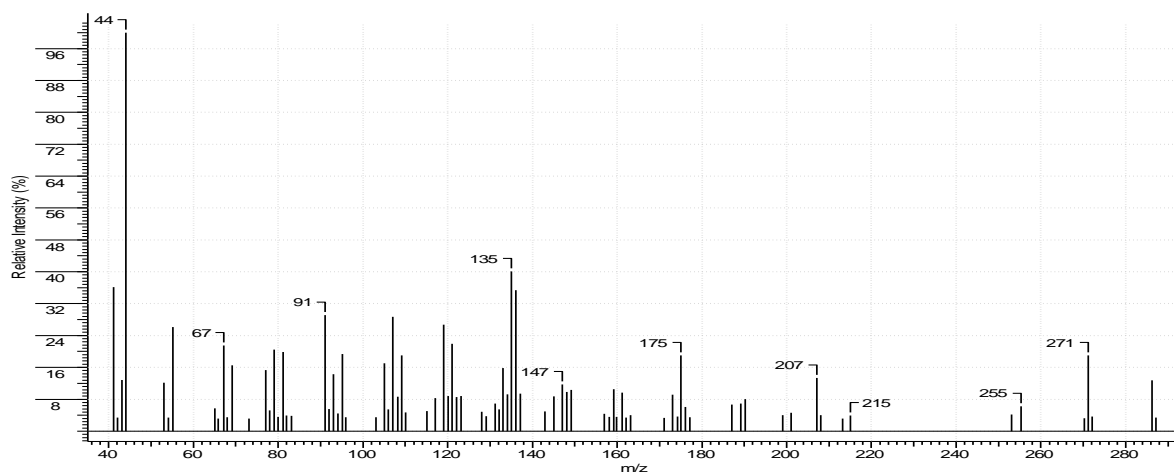


Figure S2. Mass spectrum of compound 2 β ,3 α -dihydroxy-trinervita-1(15),11-diene.

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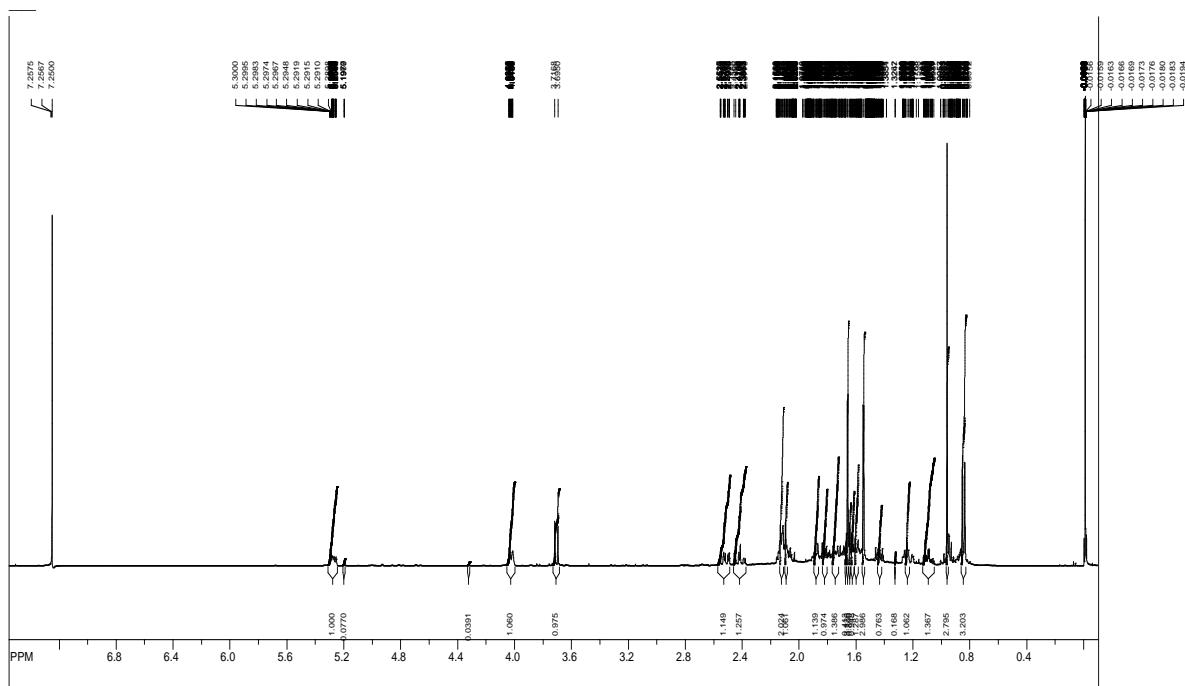


Figure S3. ¹H NMR spectrum (400 MHz, CDCl₃) of compound 2β,3α-dihydroxy-trinervita-1(15),11-diene.

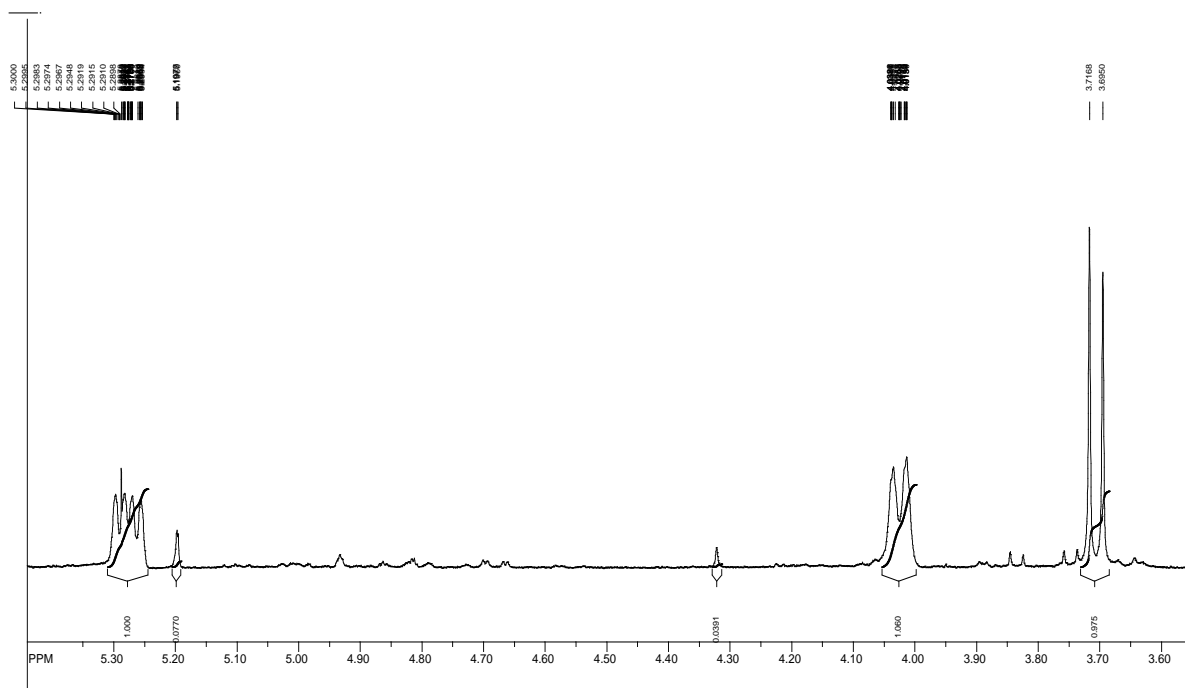


Figure S4. Expanded ¹H NMR spectrum (400 MHz, CDCl₃) of compound 2β,3α-dihydroxy-trinervita-1(15),11-diene.

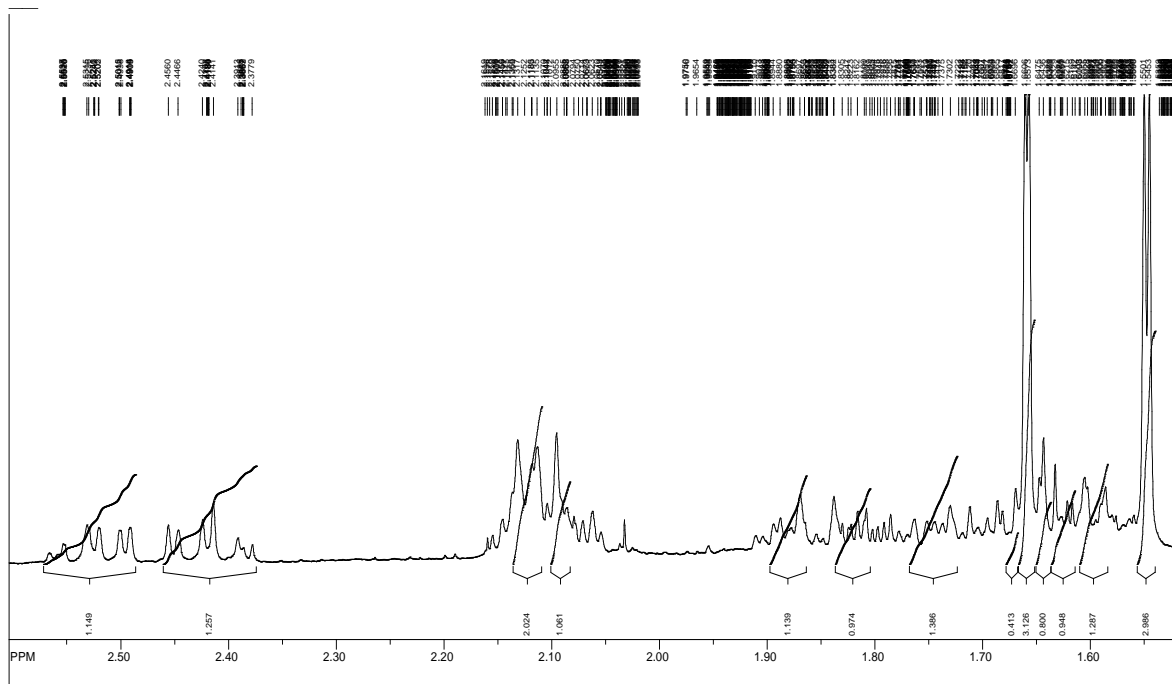


Figure S5. Expanded ^1H NMR spectrum (400 MHz, CDCl_3) of compound 2 β ,3 α -dihydroxy-trinervita-1(15),11-diene.

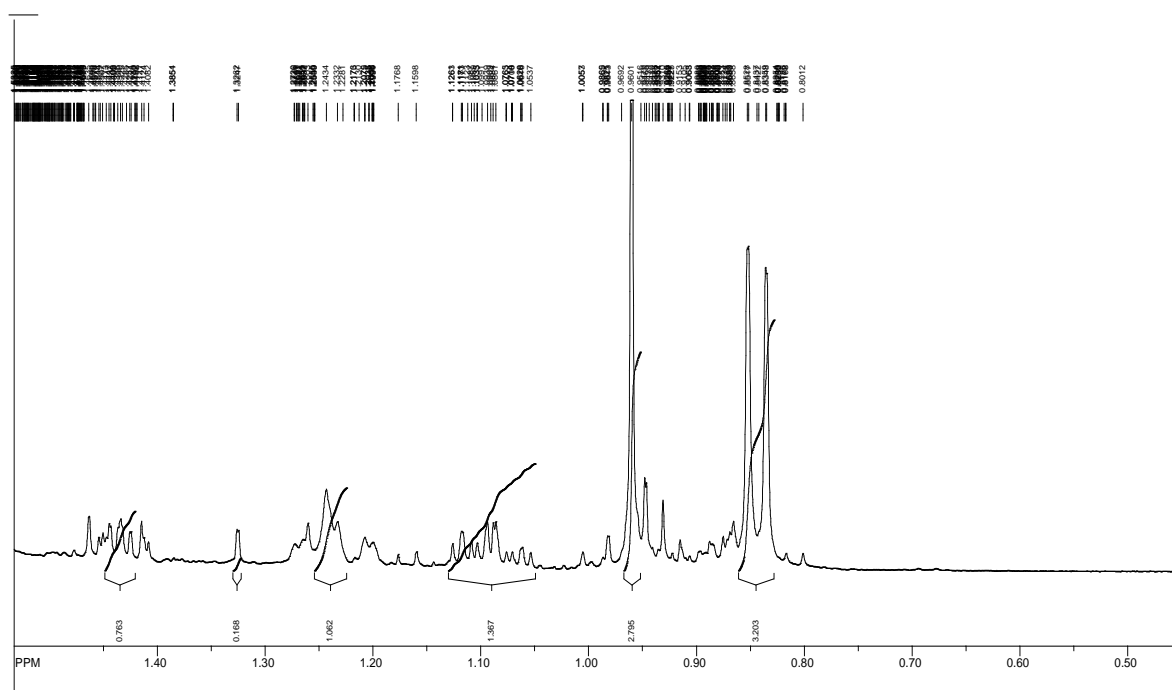


Figure S6. Expanded ^1H NMR spectrum (400 MHz, CDCl_3) of compound 2 β ,3 α -dihydroxy-trinervita-1(15),11-diene.

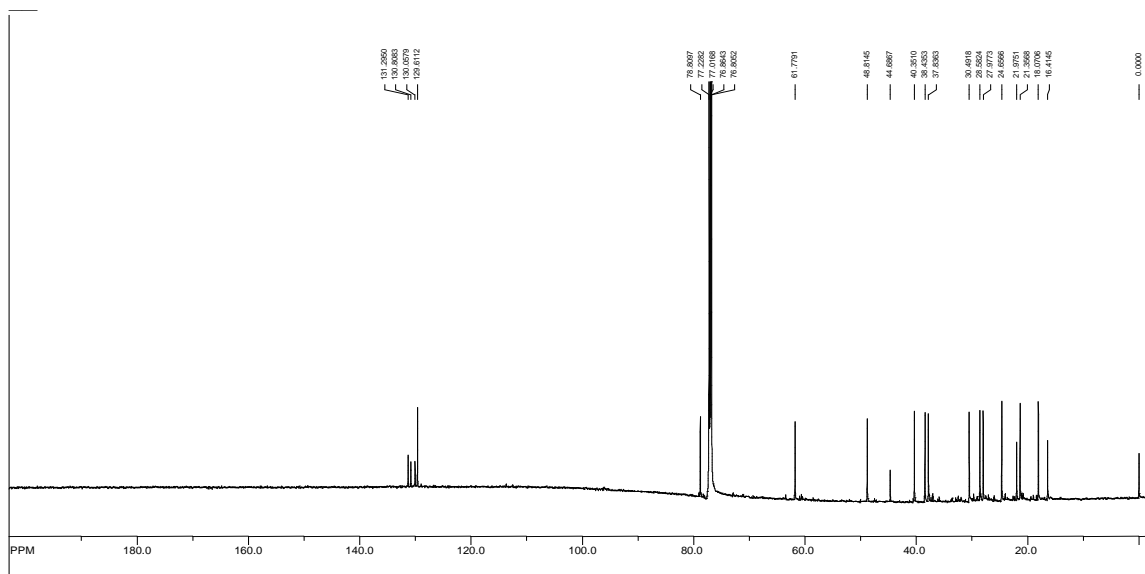


Figure S7. ¹³C NMR spectrum (150 MHz, CDCl₃) of compound 2β,3α-dihydroxy-trinervita-1(15),11-diene.

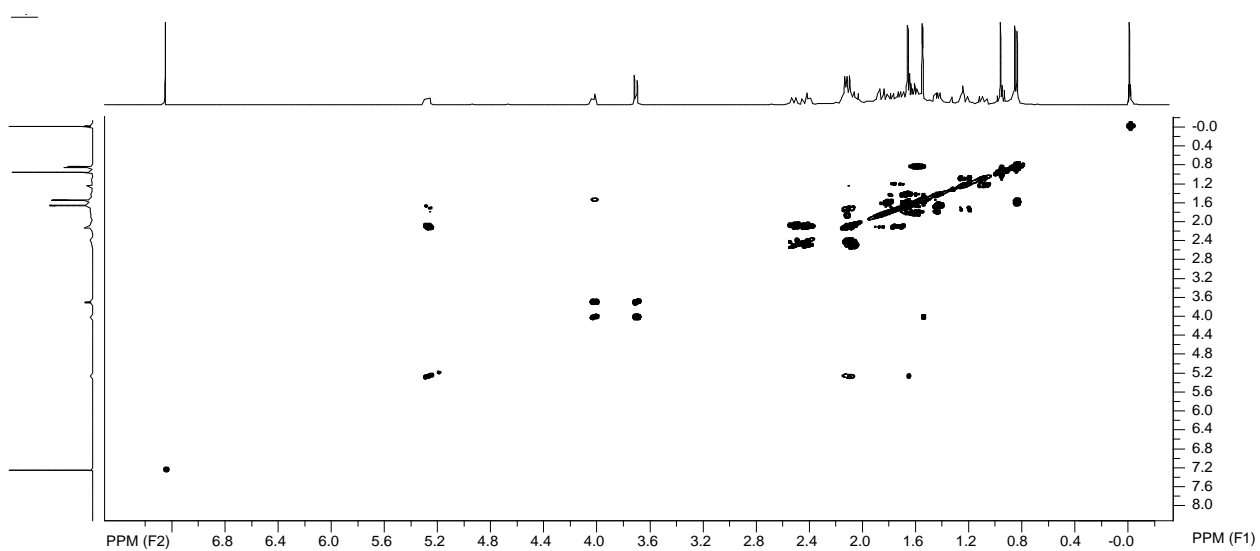


Figure S8. COSY correlation map (400 × 400 MHz, CDCl₃) of compound 2β,3α-dihydroxy-trinervita-1(15),11-diene.

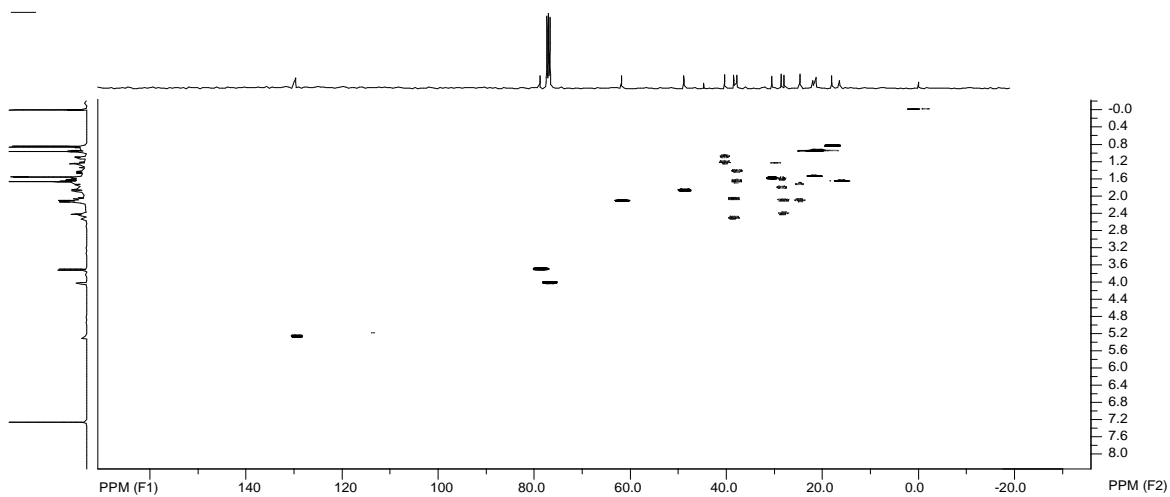


Figure S9. HSQC correlation map (400×100 MHz, CDCl_3) of compound $2\beta,3\alpha$ -dihydroxy-trinervita-1(15),11-diene.

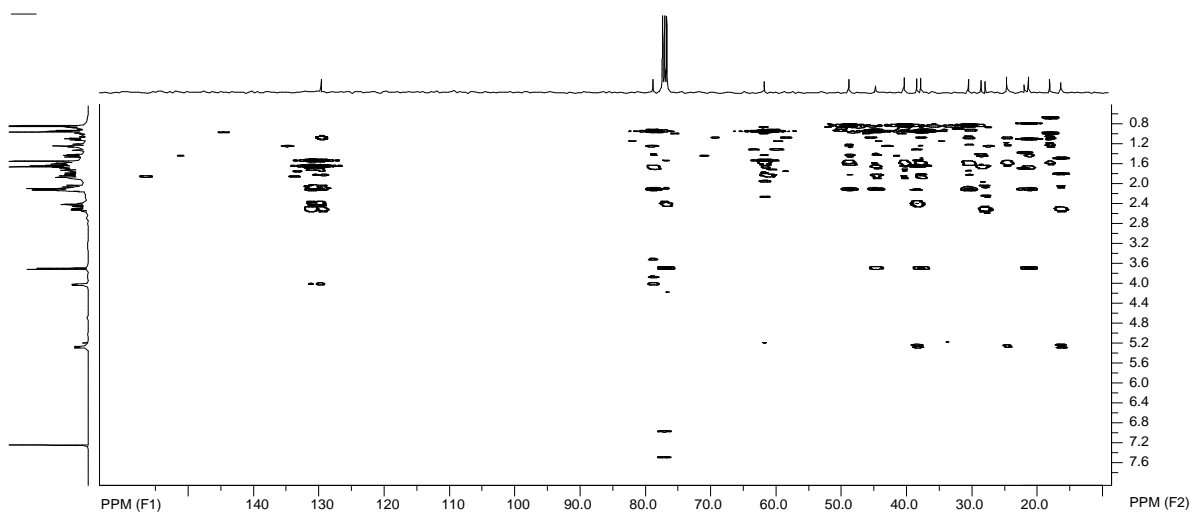


Figure S10. HMBC correlation map (400×100 MHz, CDCl_3) of compound $2\beta,3\alpha$ -dihydroxy-trinervita-1(15),11-diene.

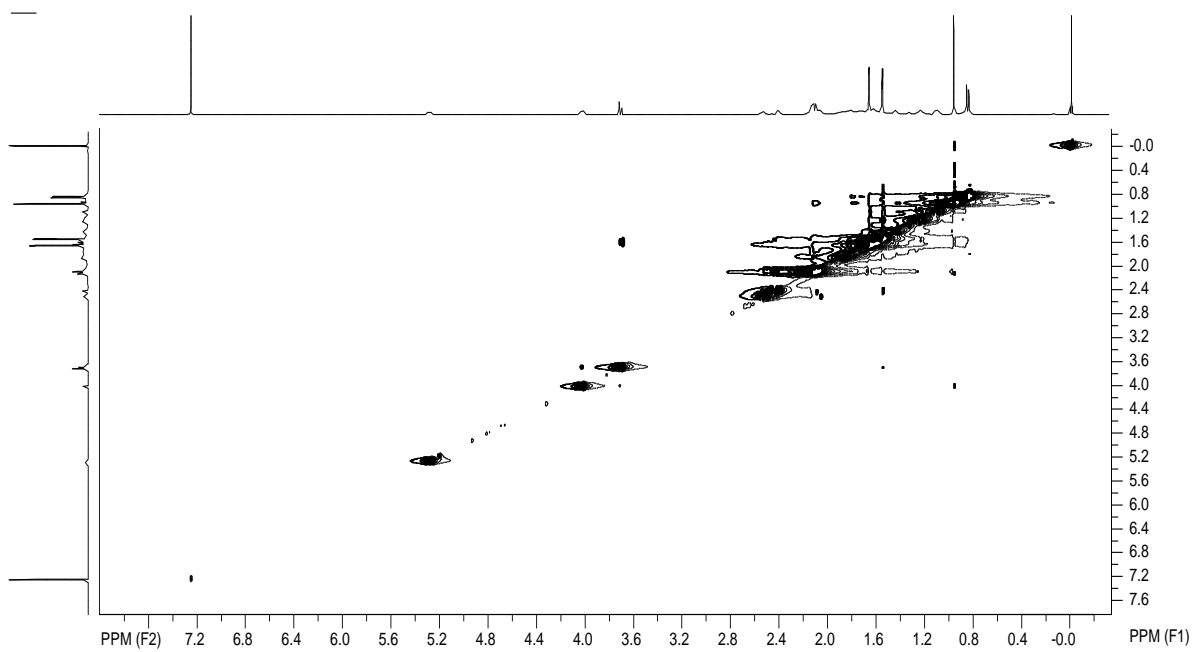


Figure S11. NOESY correlation map (400 × 400 MHz, CDCl₃) of compound 2β,3α-dihydroxy-trinervita-1(15),11-diene.

Table S1. Results of the conformational search subsequently carried out for the isolated compound through molecular mechanics, semiempirical and density functional theory calculations, using the software Open3Dalign, Mopac and Orca, respectively

Frame	Open3Dalign (MMFF94)		MOPAC (PM7)			ORCA (B3LYP/Def2-TZVP/RIJCOSX)		
	E / (kcal mol ⁻¹)	ΔE / (kcal mol ⁻¹)	E / eV	ΔE (kcal/mol ⁻¹)	Boltzmann / %	E / Eh	ΔE / Eh	Boltzmann / %
1	75.9222	0.0000	-3480.51497	0.00000000000	50.12	-931.547247278	0.0000000	99.58
2	77.3044	1.3822	-3480.42993	1.96106901809	1.82	-931.540170650	0.0070766	0.05
3	81.0454	5.1232	-3480.44584	1.59417569638	3.39	-931.541953150	0.0052941	0.36
4	81.8480	5.9258	-3480.12140	9.07593995114	0.00	–	–	–
5	81.8913	5.9691	-3480.19998	7.26384207438	0.00	–	–	–
6	82.2621	6.3399	-3480.51194	0.06987346102	44.54	-931.530274334	0.0169729	0.00
7	83.3870	7.4648	-3480.36132	3.54325322940	0.13	–	–	–
8	84.7268	8.8046	-3479.98662	12.18404063619	0.00	–	–	–

Similar results were obtained when the optimization was carried out at the B3LYP/6-311G-2d2p level of theory.