

Supplementary Data

This supplementary data is a part of a paper entitled “The Cytotoxicity of Phenolic Sesquiterpenes from *Dysoxylum parasiticum* Leaves Against MCF-7 Human Breast Cancer Cells”.

Table S1. Energy analysis for conformers of **1a** at wB97XD/6-31G(d) level in MeOH

Conformation	G (Hartree)	G (kcal/mol)	ΔG (kcal/mol)	Boltzmann Pop.
1	-659.705909480	-413972.055257795	-4.096748608	0.000976987
2	-659.707806298	-413973.245530058	-2.906476345	0.007283900
3	-659.706024596	-413972.127494236	-4.024512167	0.001103670
4	-659.707172934	-413972.848087814	-3.303918589	0.003724230
5	-659.706669546	-413972.532206810	-3.619799593	0.002185220
6	-659.705688310	-413971.916471408	-4.235534995	0.000772962
7	-659.704913429	-413971.430225832	-4.721780571	0.000340203
8	-659.712438059	-413976.152006403	0	0.983613000

Table S2. ^1H , ^{13}C , ^1H - ^1H COSY, HMBC, and NOE NMR data for dysoxyphenol (**1**) in CDCl_3 ^a

Position ^b	δ_{C} , type	δ_{H} , mult. (<i>J</i> in Hz)	^1H - ^1H COSY	HMBC (H $\rightarrow$ C)	NOE
1	31.6, CH	2.72, sext (6.8)	H-2a,2b,11	C-2,3,8,9,10,11	H-3a,12
2	29.6, CH ₂	1.95, <i>m</i> 1.23, <i>m</i>	H-1,2b,3a,3b H-1,2a,3a,3b	C-1,9 C-3,4,9	
3	21.9, CH ₂	1.83, <i>m</i> 1.74, <i>m</i>	H-2a,2b,3b,4 H-2a,2b,3a,4	C-1,4,10 C-1,2,4,10	
4	40.9, CH	2.94, <i>td</i> (4.4, 6.7)	H-3a,3b,12	C-2,9,10,12,13,14	H-15
5	121.7, C				
6	151.9, C				
7	112.1, CH	6.62, <i>d</i> (8.3)	H-8	C-5,6,9	
8	124.2, CH	6.95, <i>d</i> (8.3)	H-7	C-1,6,10	
9	136.1, C				
10	141.3, C				
11	22.3, CH ₃	1.23, <i>d</i> (6,8)	H-1	C-1,2,9	
12	31.9, CH	1.95, <i>m</i>	H-4,13,14	C-4,13,14	
13	19.2, CH ₃	0.79, <i>d</i> (6,7)	H-12	C-4,12,14	H-1,3a,4,12
14	21.3, CH ₃	0.88, <i>d</i> (6,8)	H-12	C-4,12,13	H-3a,4,12
15	12.5, CH ₃	2.19, <i>s</i>	-	C-5,6,10	
6-OH		4.52, <i>s</i>		C-5,6,7	

^a 600 MHz for ^1H NMR and 150 MHz for ^{13}C NMR. ^b The number of attached protons was determined by analysis of DEPT135 and 2D NMR spectroscopic data

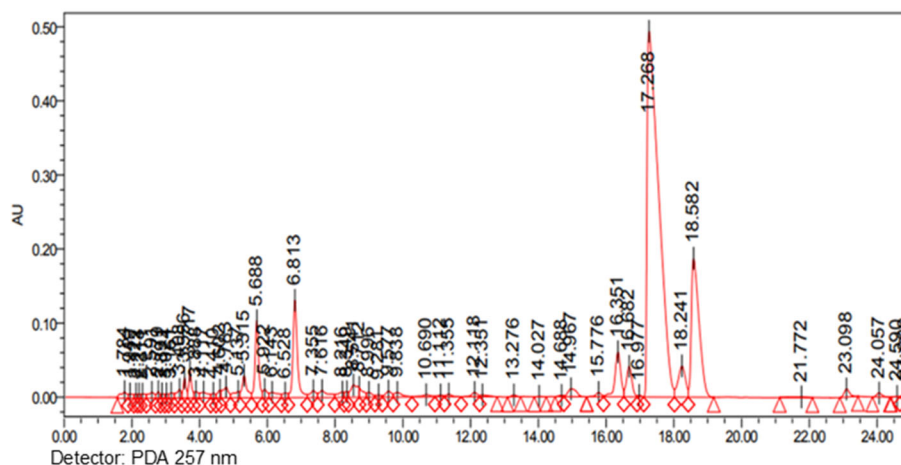
Table S3. ^1H , ^{13}C , ^1H - ^1H COSY, HMBC, and NOE NMR data for 7-hydroxycalamenene (**2**) in CDCl_3 ^a

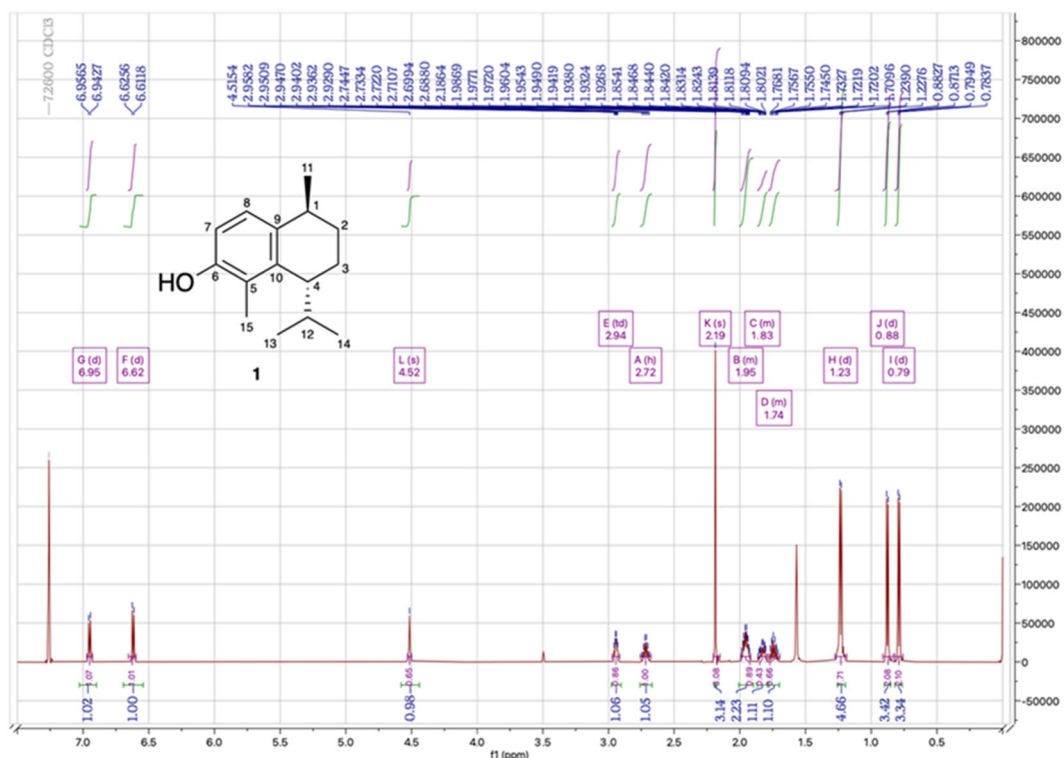
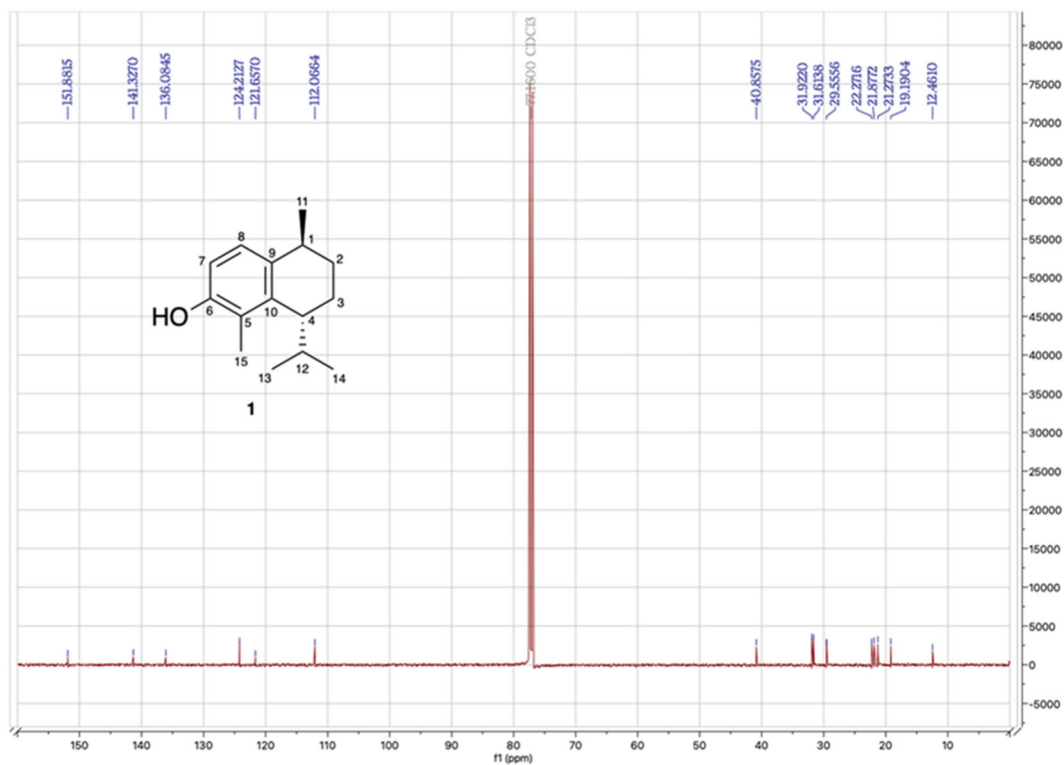
Position ^b	δ_{C} , type	δ_{H} , mult. (<i>J</i> in Hz)	^1H - ^1H COSY	HMBC (H $\rightarrow$ C)	NOE
1	32.7, CH	2.71, sext (6.8)	H-2a,2b,11	C-9,11	H-2a,12
2	30.9, CH ₂	1.93, <i>m</i>	H-1,2b,3a		
		1.31, <i>m</i>	H-1,2a,3b	C-3	
3	21.7, CH ₂	1.80, <i>m</i>	H-2a,3b,4	C-1,2	
		1.54, <i>m</i>	H-2b,3a,4	C-2	
4	43.2, CH	2.63, <i>q</i> (6.1)	H-3a,3b,12	C-9,10,12,13,14	H-3a,12,14
5	130.6, CH	6.94, <i>s</i>		C-4,7,9,15	
6	120.7, C				
7	151.5, C				
8	113.1, CH	6.65, <i>s</i>		C-1,6,7,10	
9	142.3, C				
10	132.4, C				
11	22.4, CH ₃	1.24, <i>d</i> (6.9)	H-1	C-1,2,9	H-1,2a,3a,8
12	32.0, CH	2.21, <i>m</i>	H-4,13,14	C-4,13,14	
13	17.3, CH ₃	0.70, <i>d</i> (6.8)	H-12	C-4,12,14	H-1,2a,4,12,14
14	21.3, CH ₃	0.99, <i>d</i> (6.8)	H-12	C-4,12,13	H-1,3a,4,5,12,13
15	15.7, CH ₃	2.21, <i>s</i>		C-5,6,7	
7-OH		4.47, <i>s</i>		C-6,7,8	

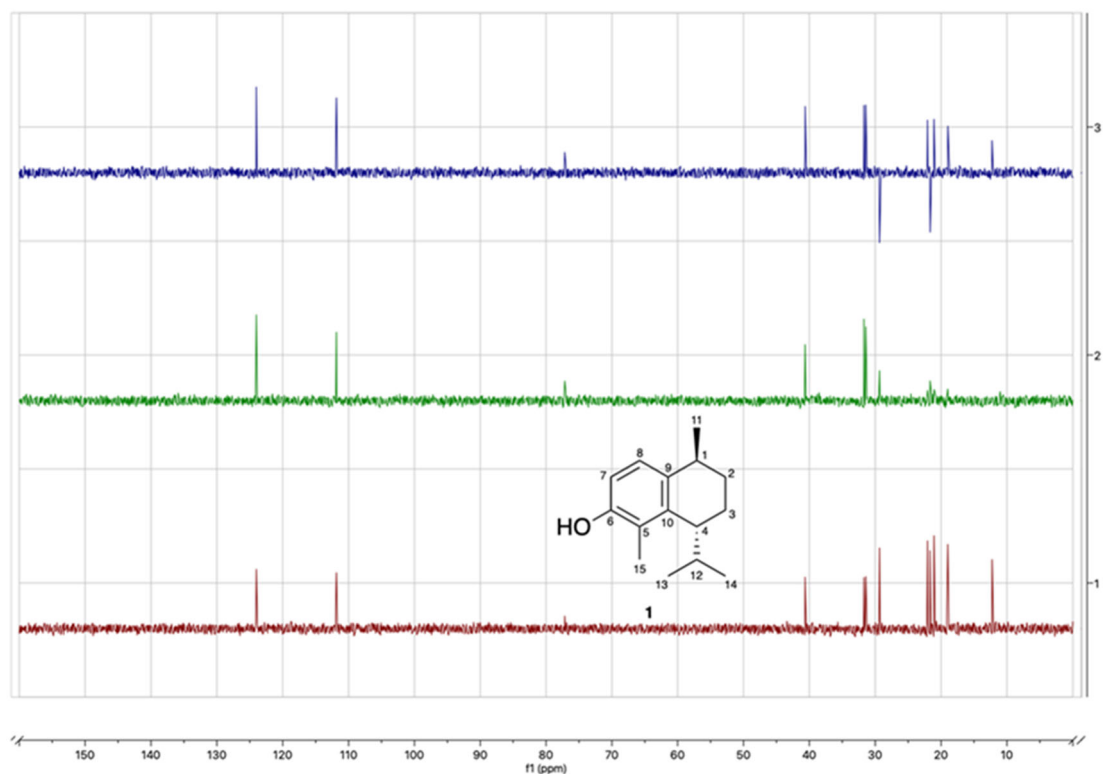
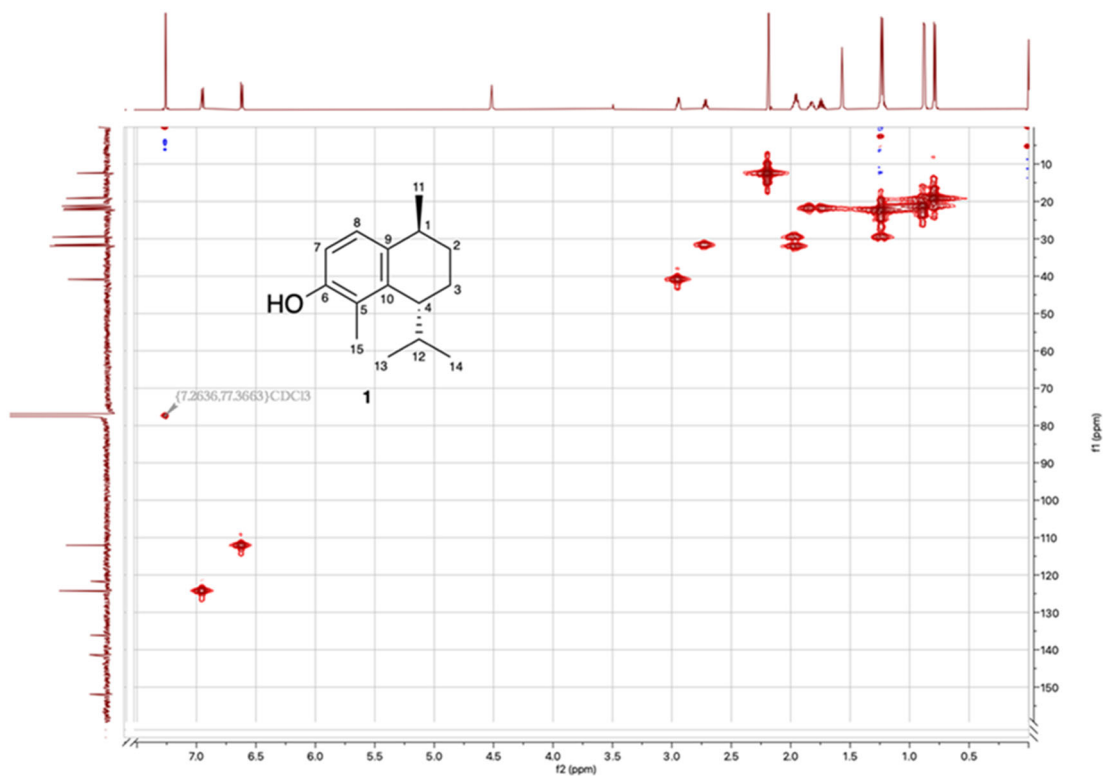
^a 600 MHz for ^1H -NMR and 150 MHz for ^{13}C -NMR. ^b The number of attached protons was determined by analysis of DEPT135 and 2D NMR spectroscopic data

Table S4. Grid parameters and RMSD value used for docking validation with protein target 3ERT

PDB ID	Grid box			Grid spacing	Grid center			RMSD (Å)
	X	Y	Z		X	Y	Z	
3ERT	40	40	40	0.375	30.162	-1.913	24.207	1.254

**Fig S1.** HPLC chromatogram for compounds **1** and **2**

Fig S2. ^1H -NMR spectrum (600 MHz) of dysoxyphenol (1) in CDCl_3 Fig S3. ^{13}C -NMR spectrum (150 MHz) of dysoxyphenol (1) in CDCl_3

Fig S4. DEPT135-NMR spectrum of dysoxyphenol (1) in CDCl₃Fig S5. HMQC spectrum (600 MHz) of dysoxyphenol (1) in CDCl₃

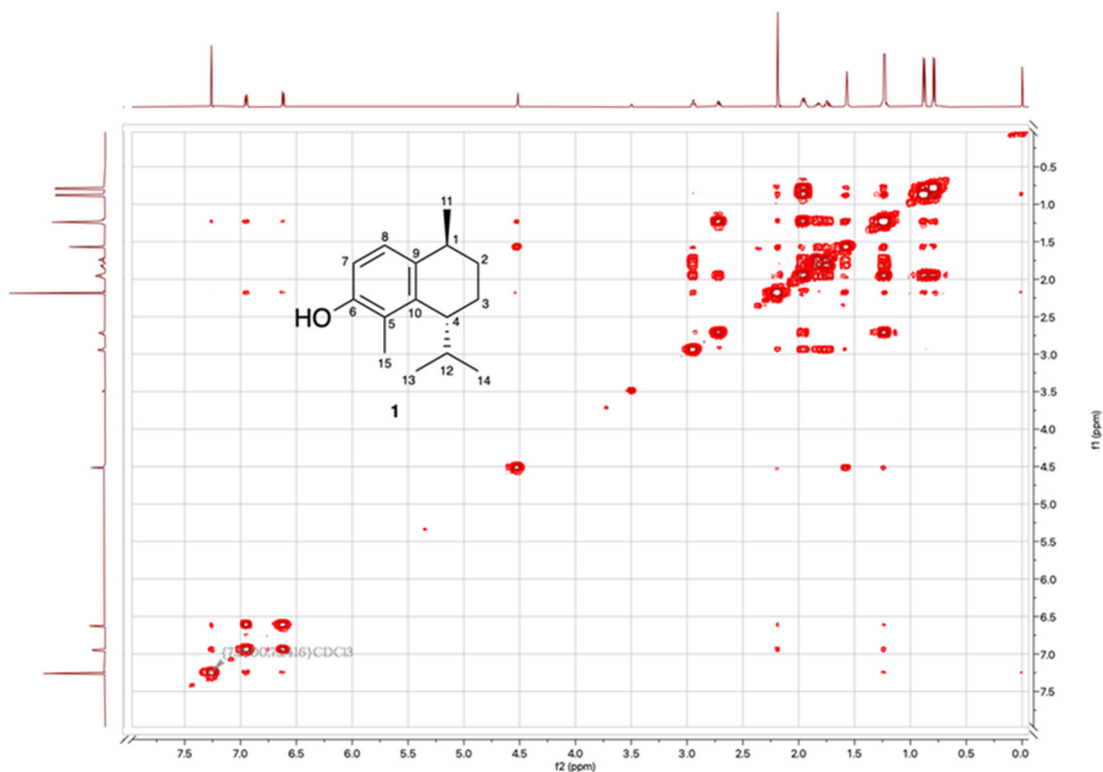


Fig S6. ^1H - ^1H COSY spectrum (600 MHz) of dysoxyphenol (1) in CDCl_3

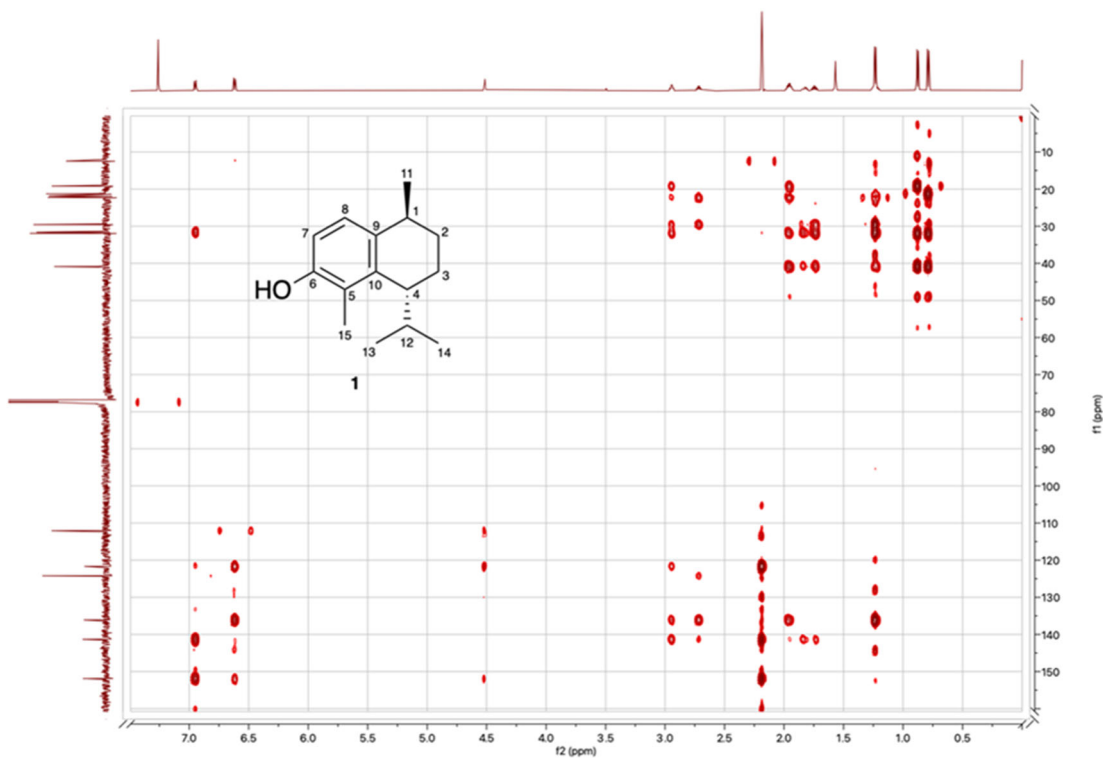


Fig S7. HMBC spectrum (600 MHz) of dysoxyphenol (1) in CDCl_3

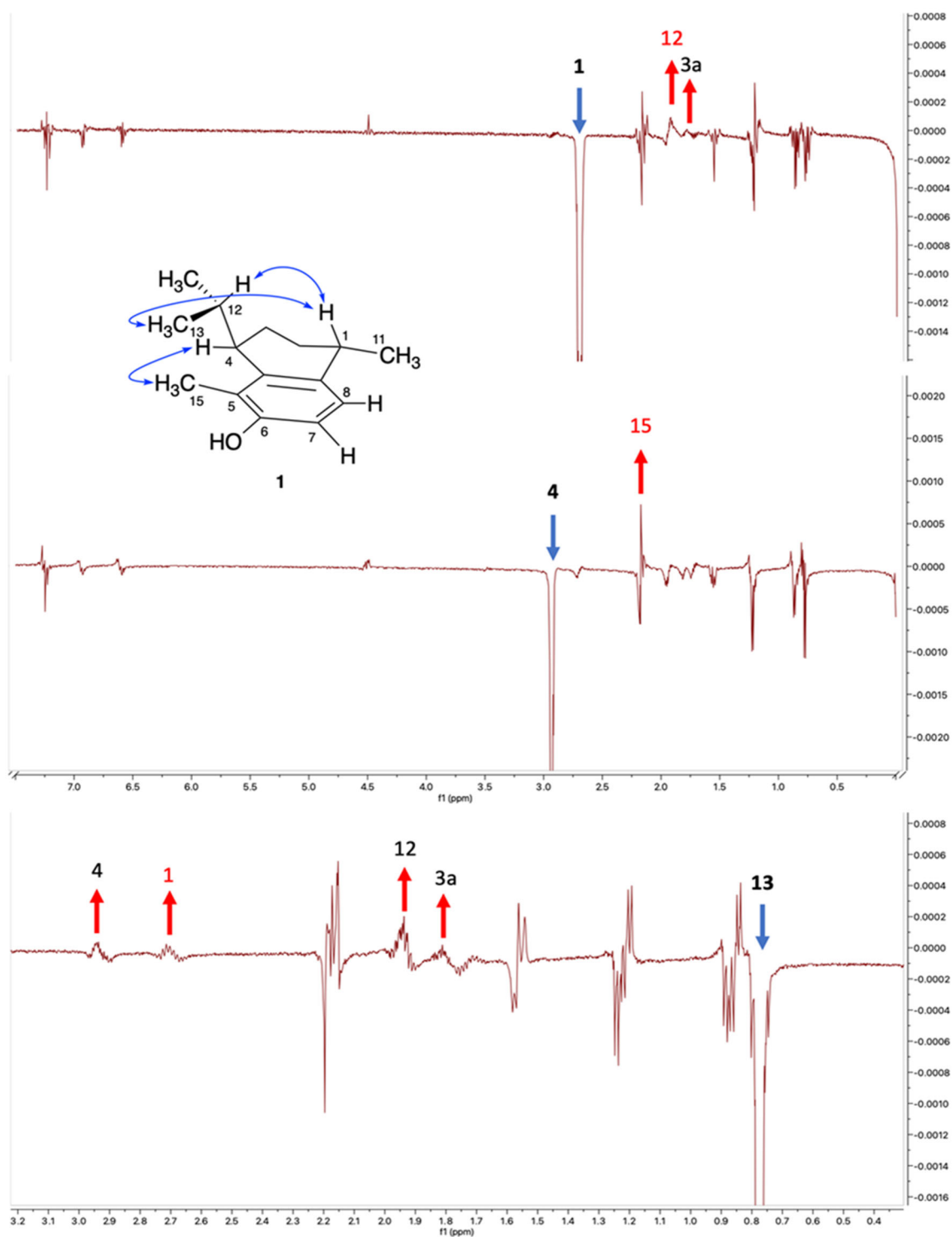


Fig S8. Selected NOE spectra of dysoxyphenol (**1**) in CDCl₃

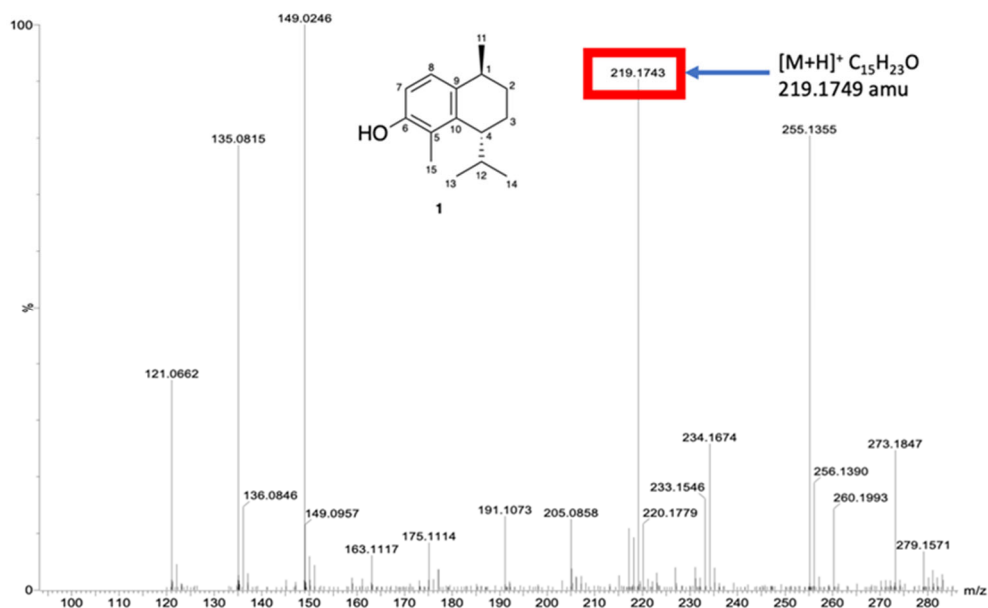


Fig S9. HR-ESI TOF-MS spectrum of dysoxyphenol (1)

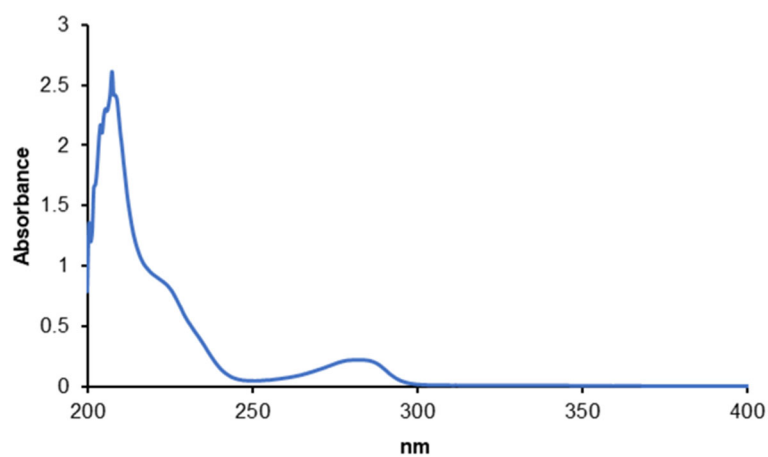


Fig S10. UV absorbance spectrum of dysoxyphenol (1)

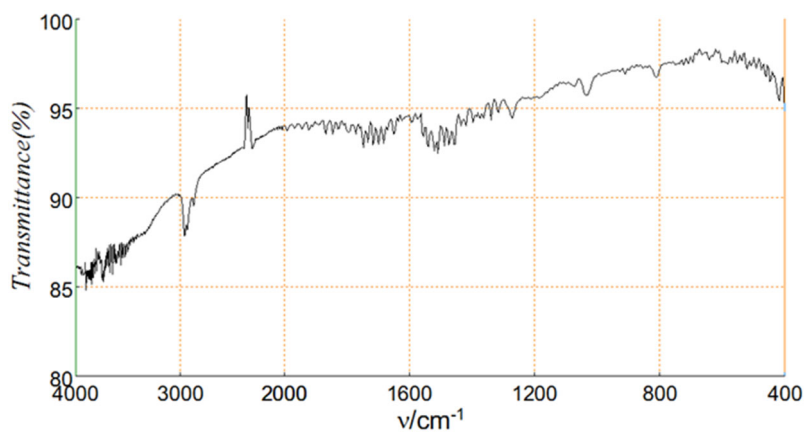


Fig S11. FTIR spectrum of dysoxyphenol (1)

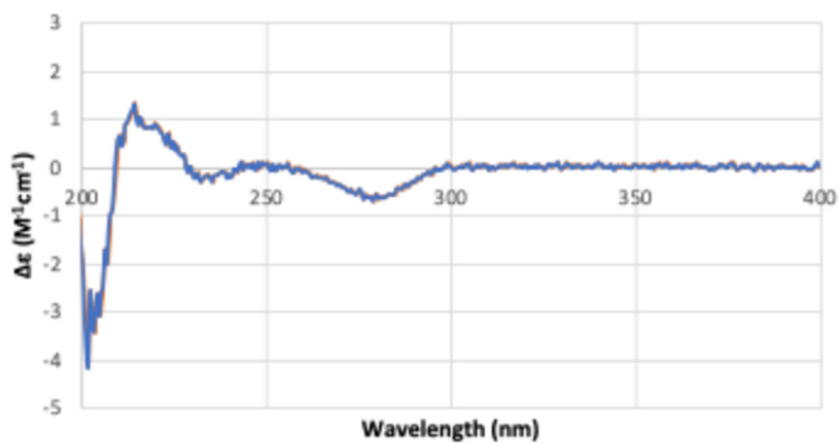
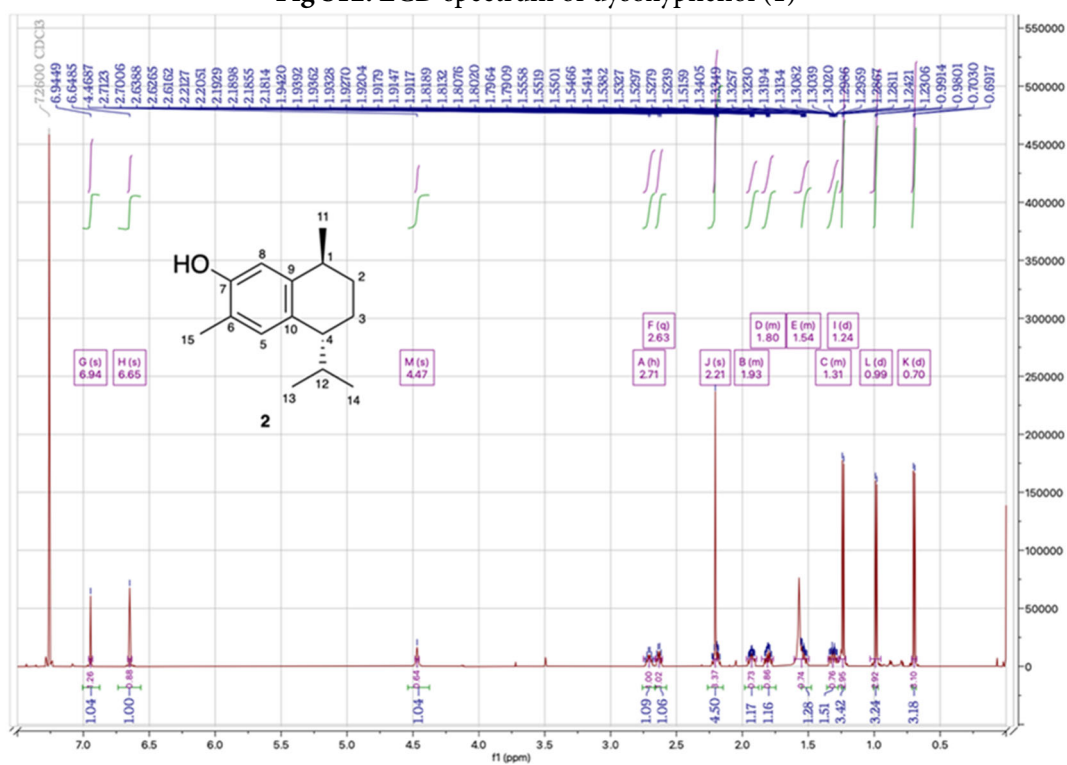


Fig S12. ECD spectrum of dysoxyphenol (1)

Fig S13. ^1H (600 MHz) NMR spectrum of 7-hydroxycalamenene (2) in CDCl_3

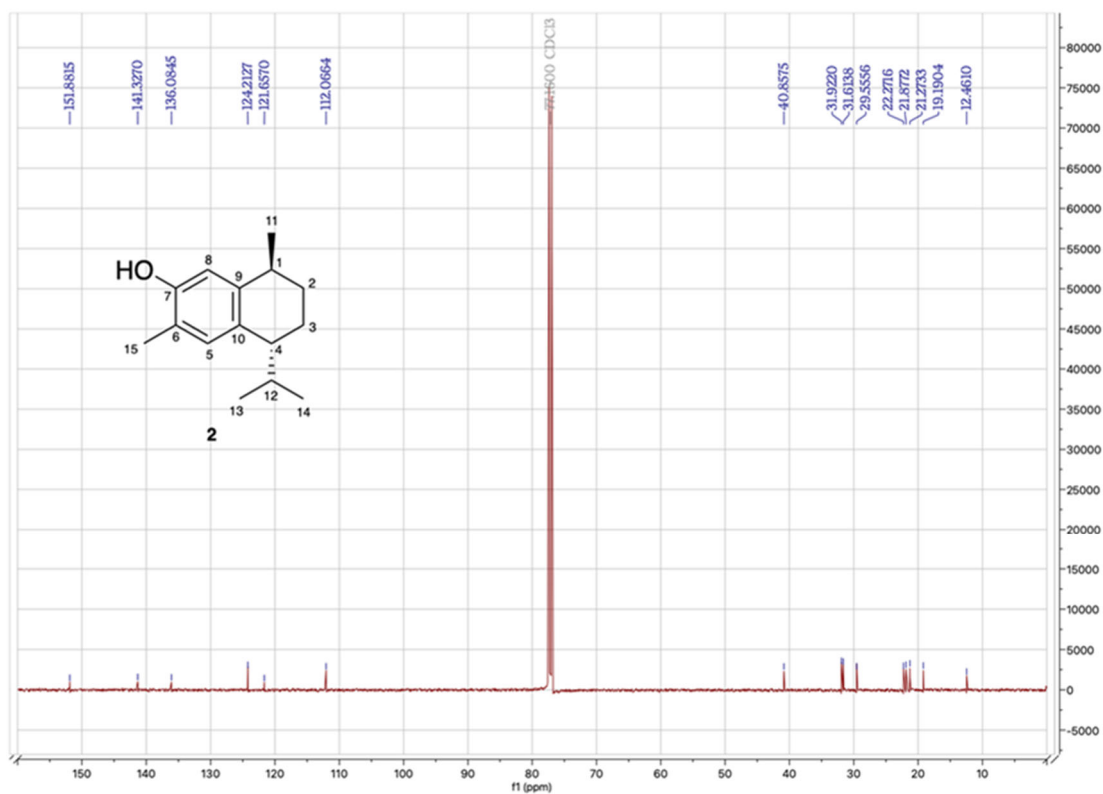


Fig S14. ^{13}C (150 MHz) NMR spectrum of 7-hydroxycalamenene (2) in CDCl_3

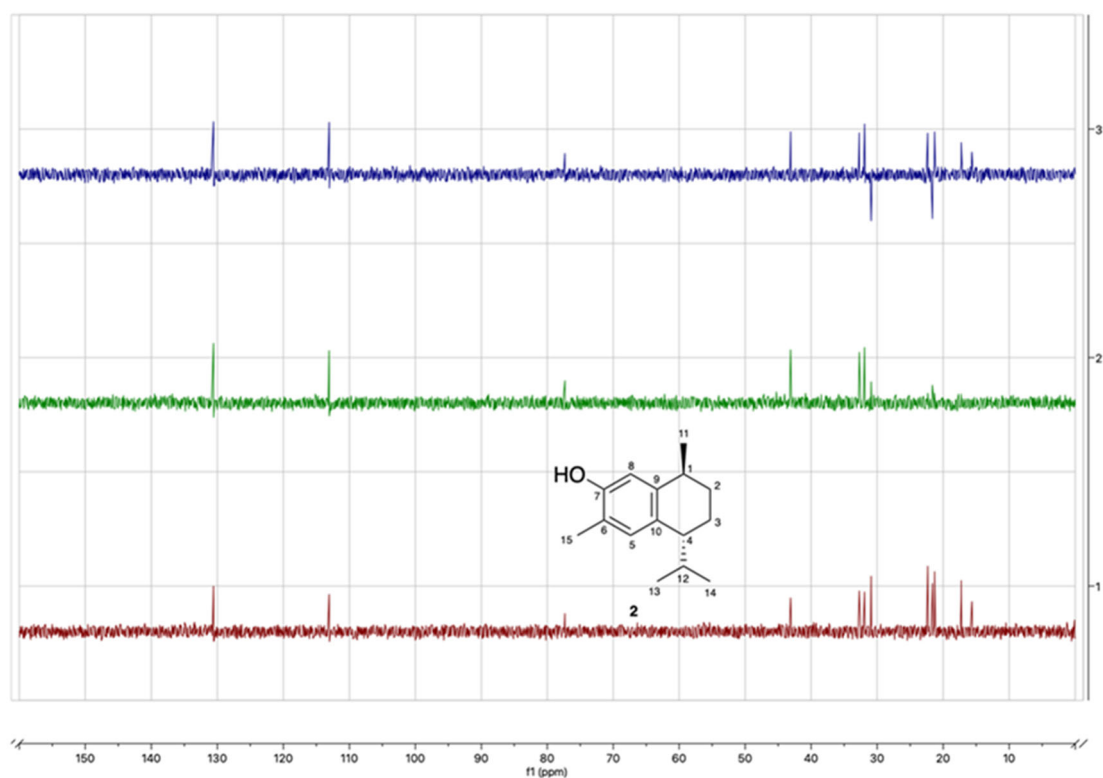


Fig S15. DEPT135 NMR spectrum of 7-hydroxycalamenene (2) in CDCl_3

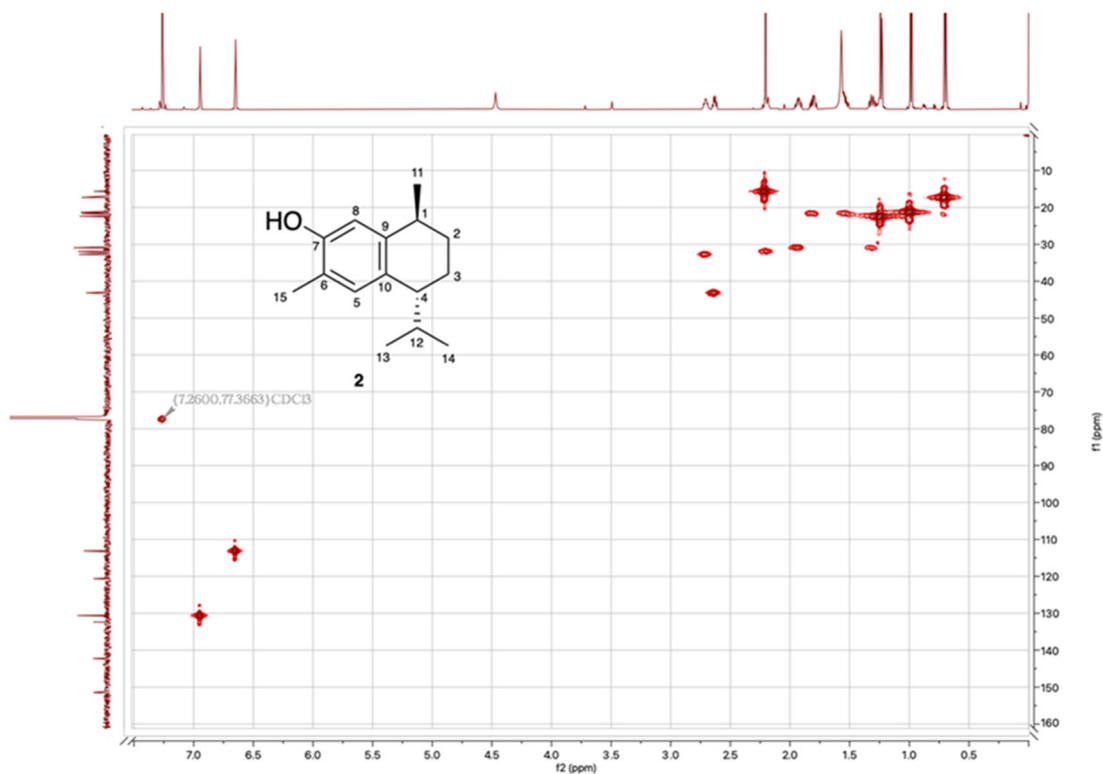


Fig S16. HMQC (600 MHz) spectrum of 7-hydroxycalamenene (2) in CDCl₃

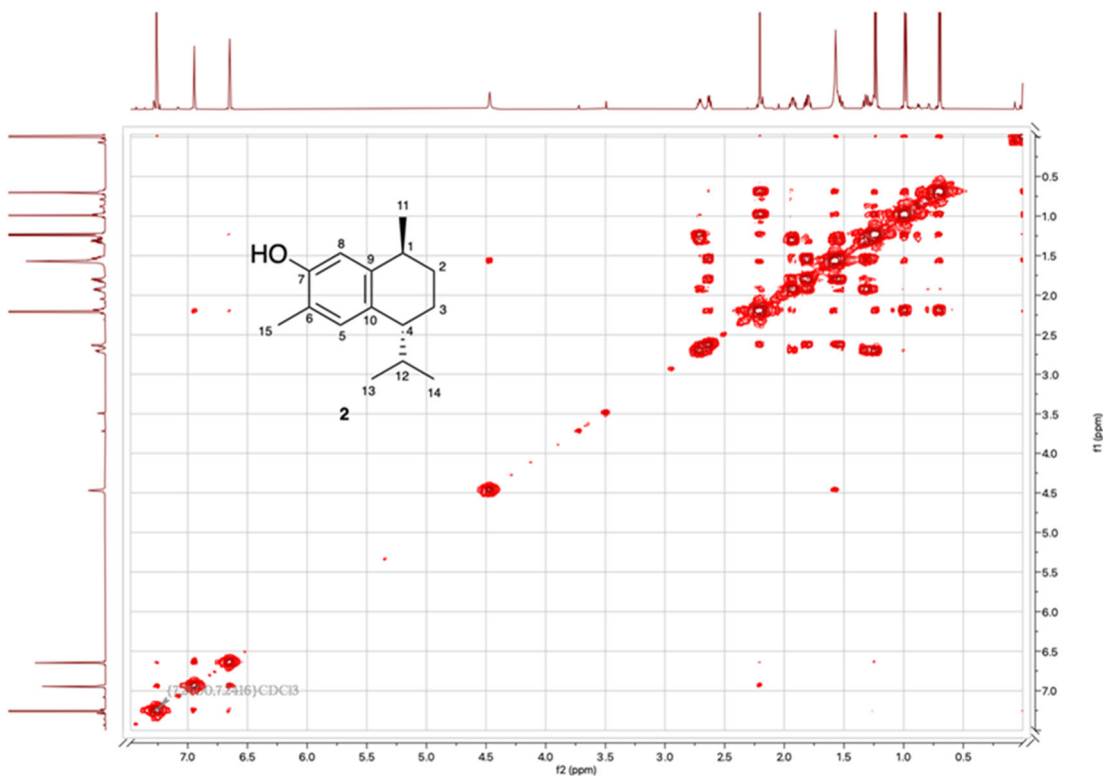


Fig S17. ¹H-¹H COSY (600 MHz) spectrum of 7-hydroxycalamenene (2) in CDCl₃

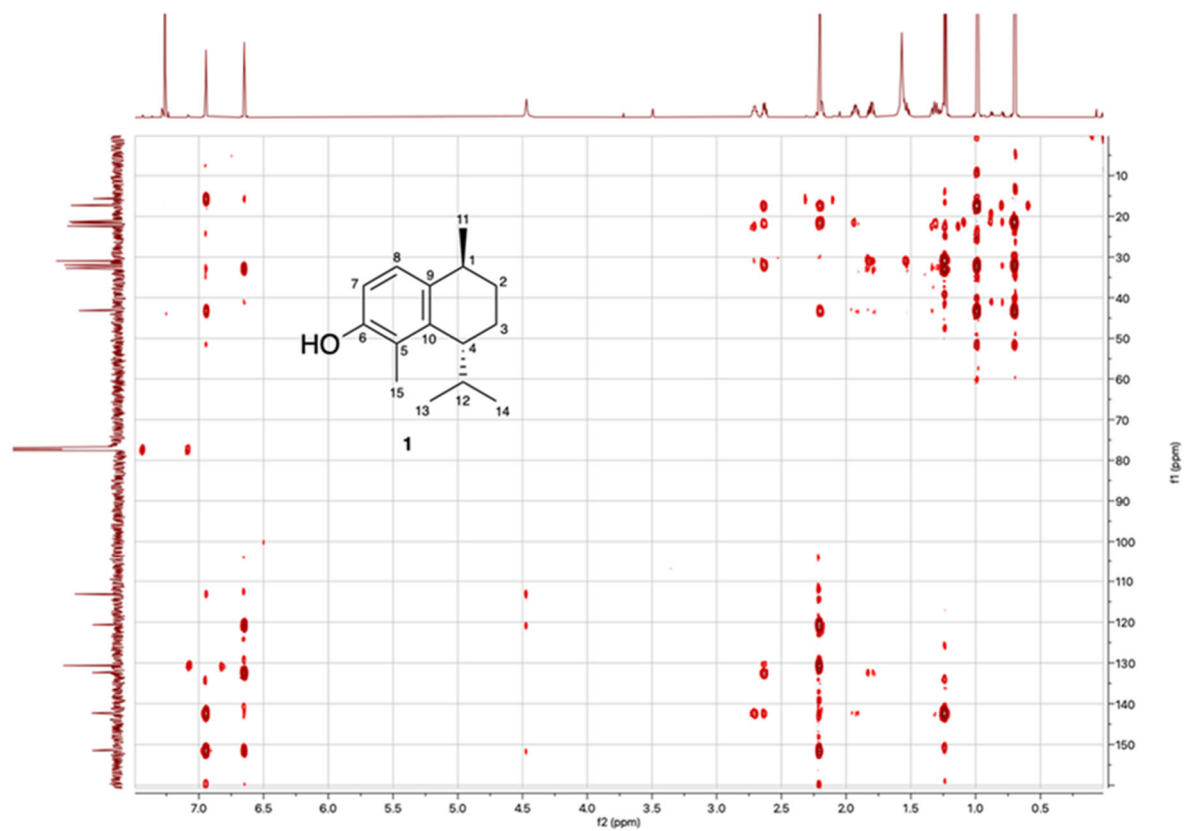


Fig S18. HMBC (600 MHz) spectrum of 7-hydroxycalamenene (2) in CDCl_3

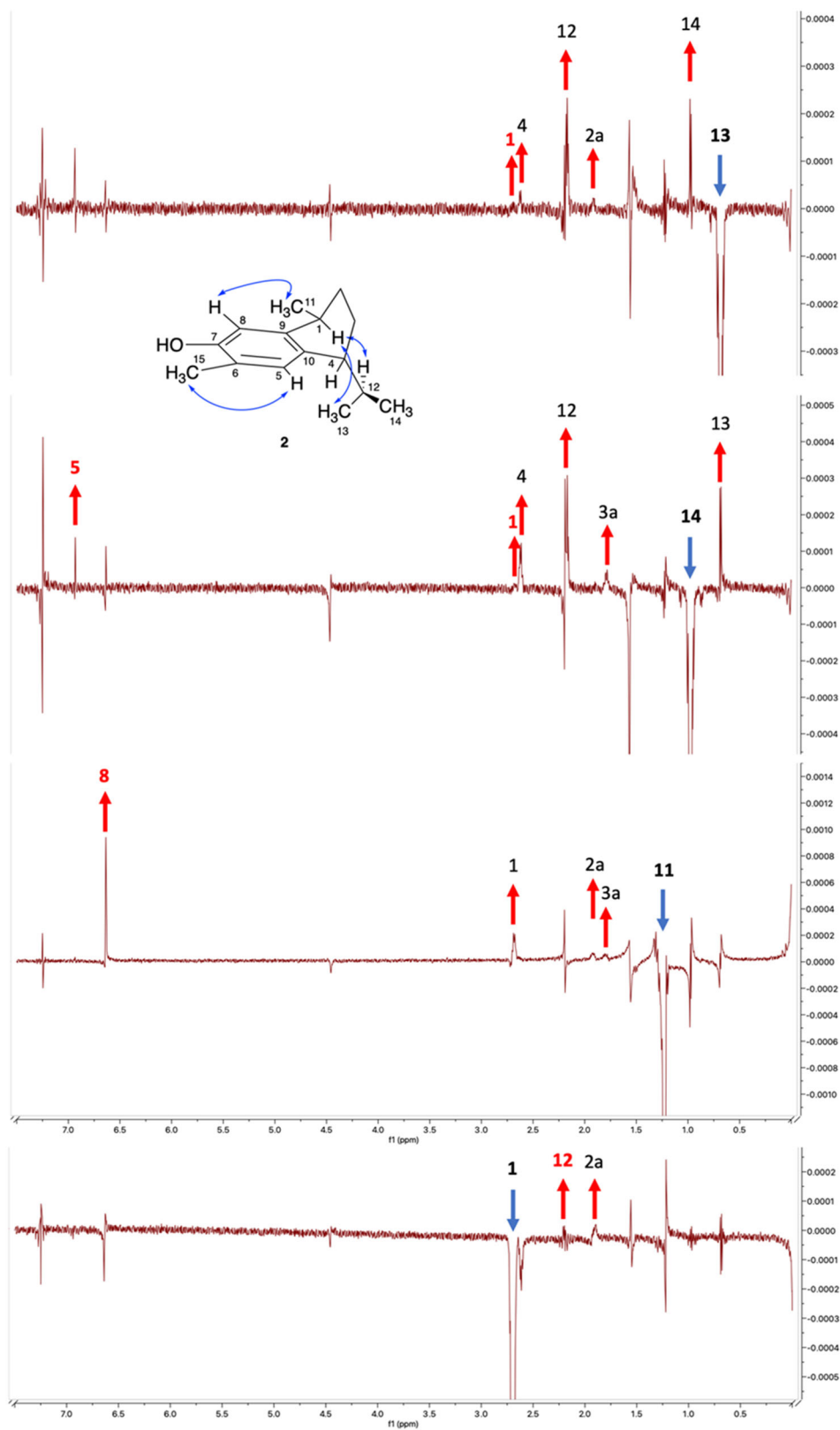
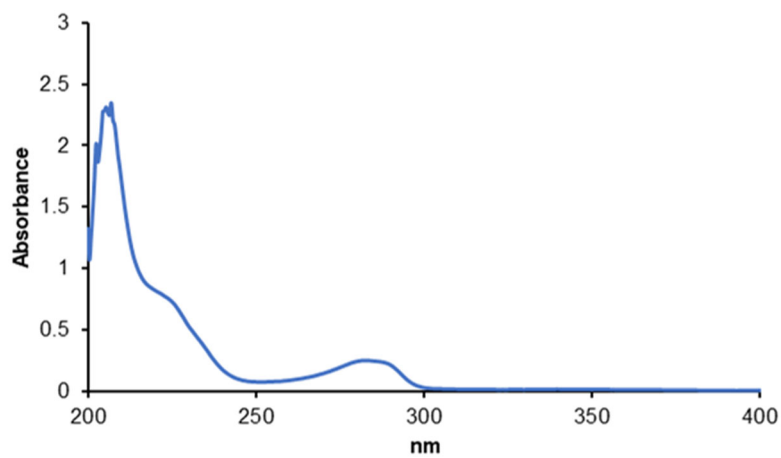
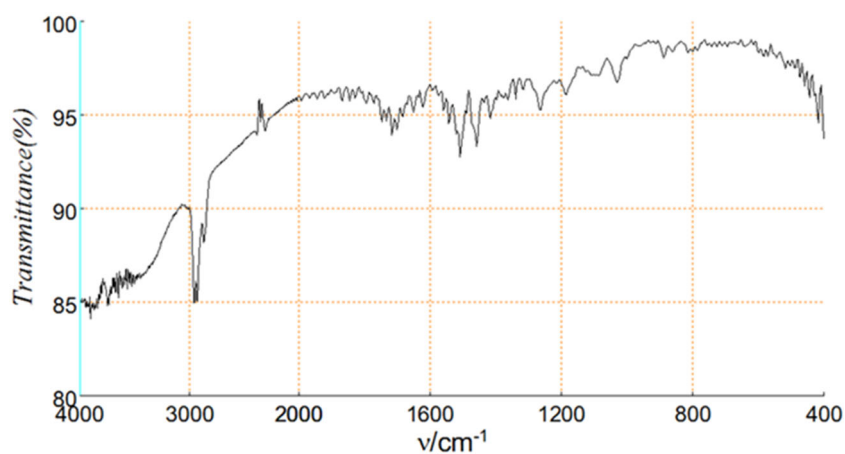
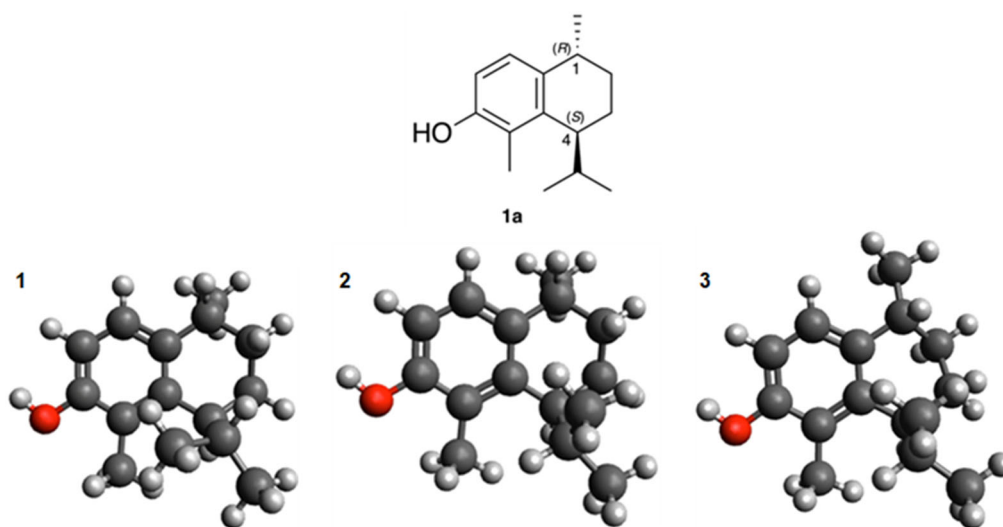


Fig S19. Selected NOE spectra of 7-hydroxycalamenene (2) in CDCl₃

**Fig S20.** UV absorbance spectrum of 7-hydroxycalamenene (2)**Fig S21.** FTIR spectrum of 7-hydroxycalamenene (2)

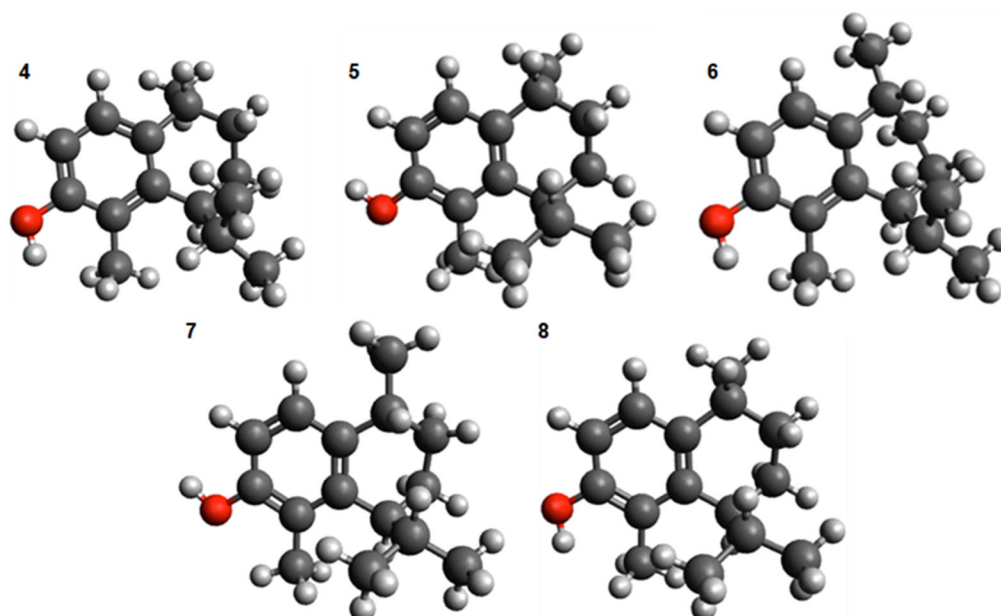


Fig S22. Minimized energy conformers of **1a** and their Boltzmann distribution in MeOH using DFT at WB97XD/6-31G(d) level

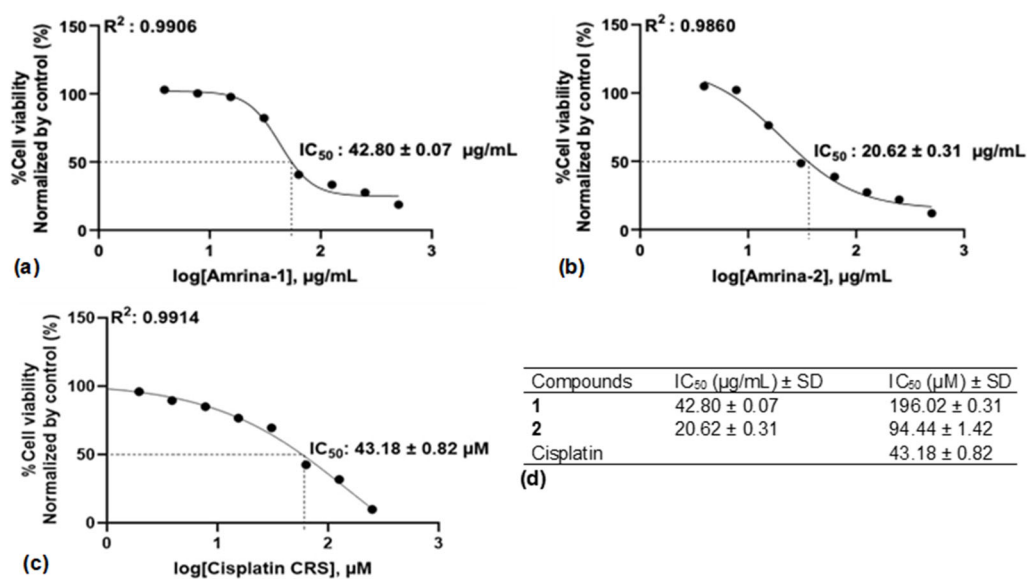


Fig S23. The curve of cytotoxic assay of compounds **1** (a), **2** (b), and cisplatin (c) against MCF-7 cells, and the LC₅₀ conversion values of compounds 1 and 2 from µg/mL to µM (d)

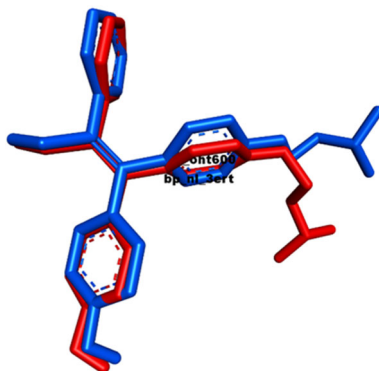


Fig S24. Overlay of the native ligand (4-hydroxytamoxifen, OHT) in the estrogen receptor alpha (PDB ID 3ERT) target. The 3D pose from the crystal structure is shown in **blue**, while the best redocked pose is shown in **red**. The native ligand, OHT, was extracted from the 3ERT crystal structure and redocked into the binding site using AutoDock 4.2. The result was compared with the original pose to check the accuracy of the docking method