

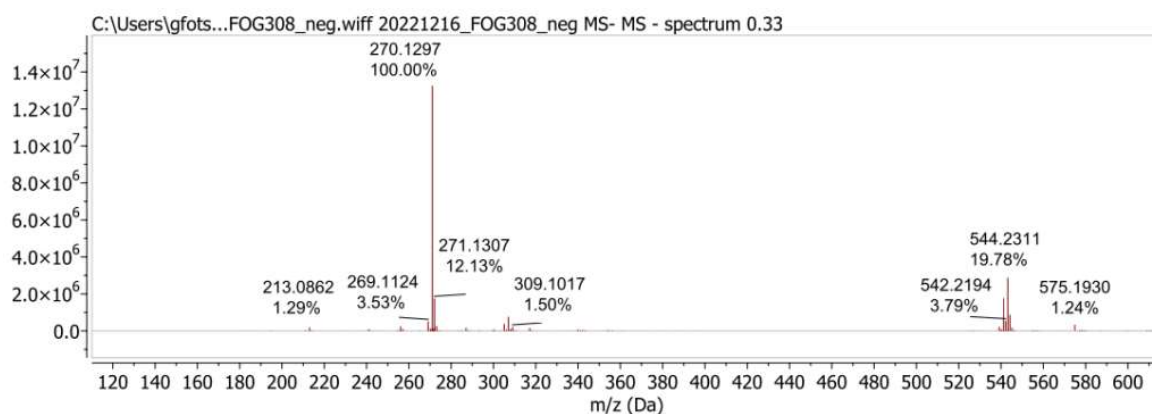


Figure S1: HR-ESI-MS (-) spectrum of compound **1**

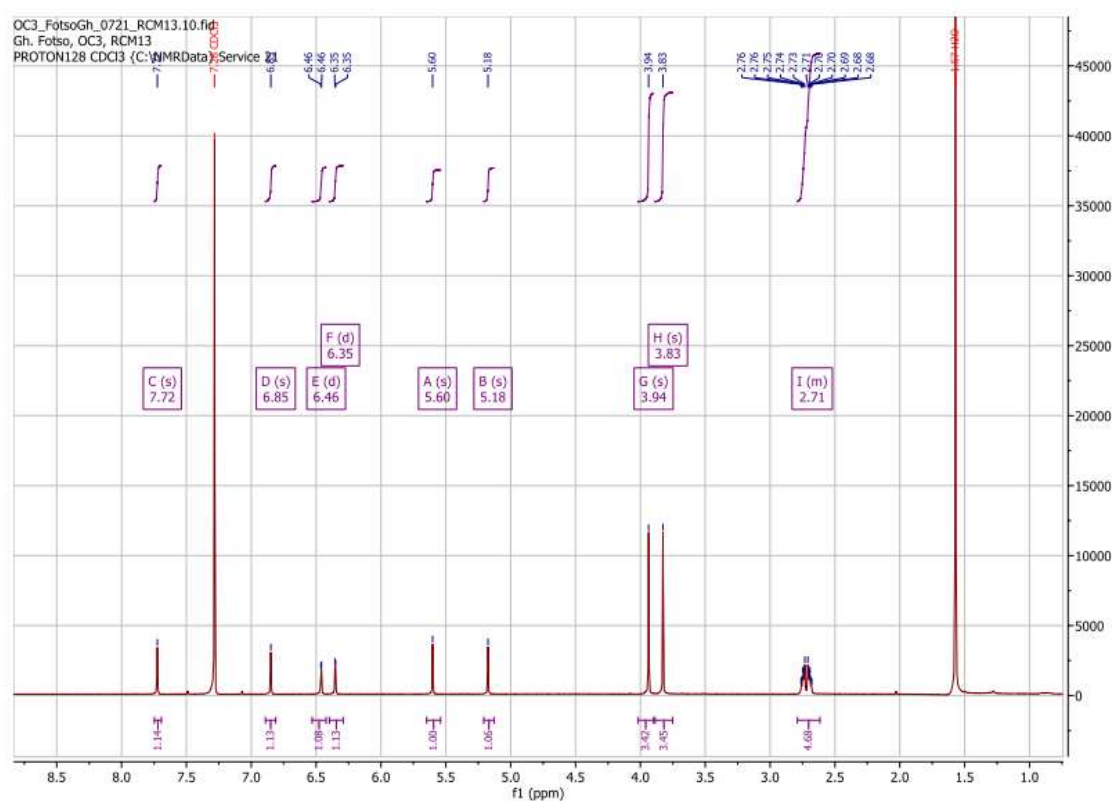


Figure S2: ^1H NMR spectrum of compound **1**

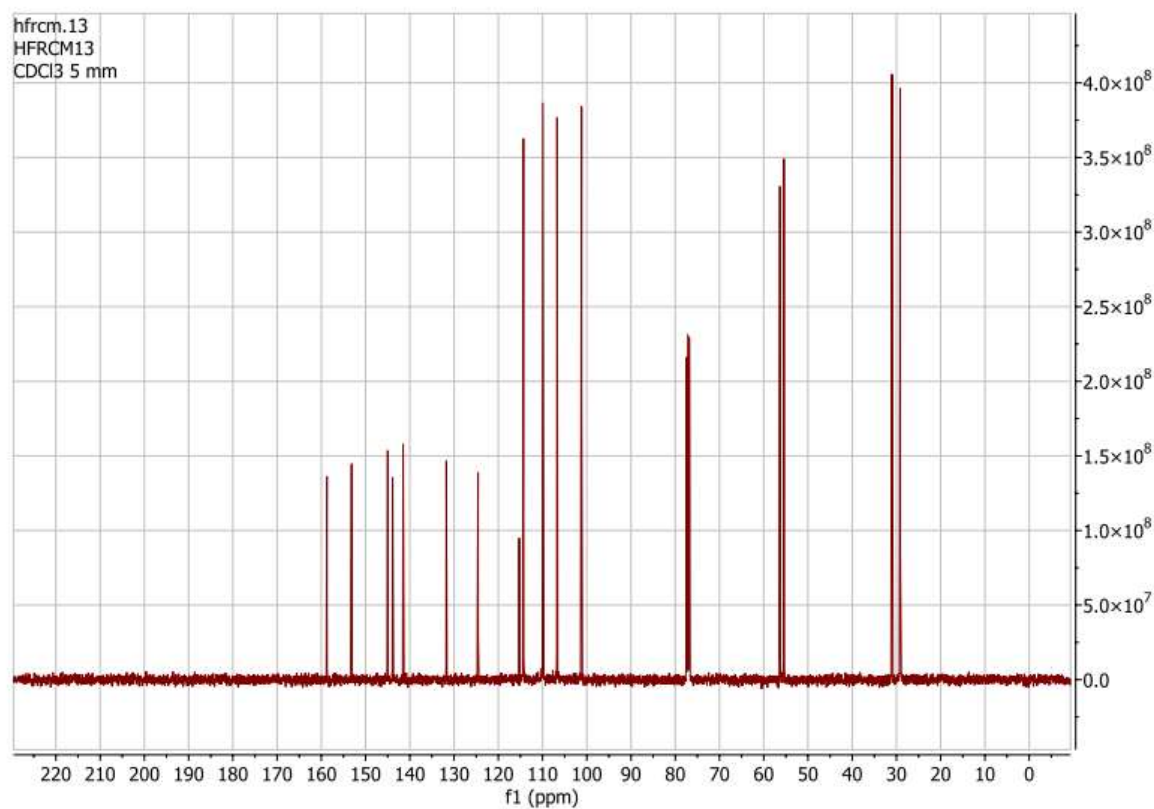


Figure S3: ¹³C NMR spectrum of compound 1

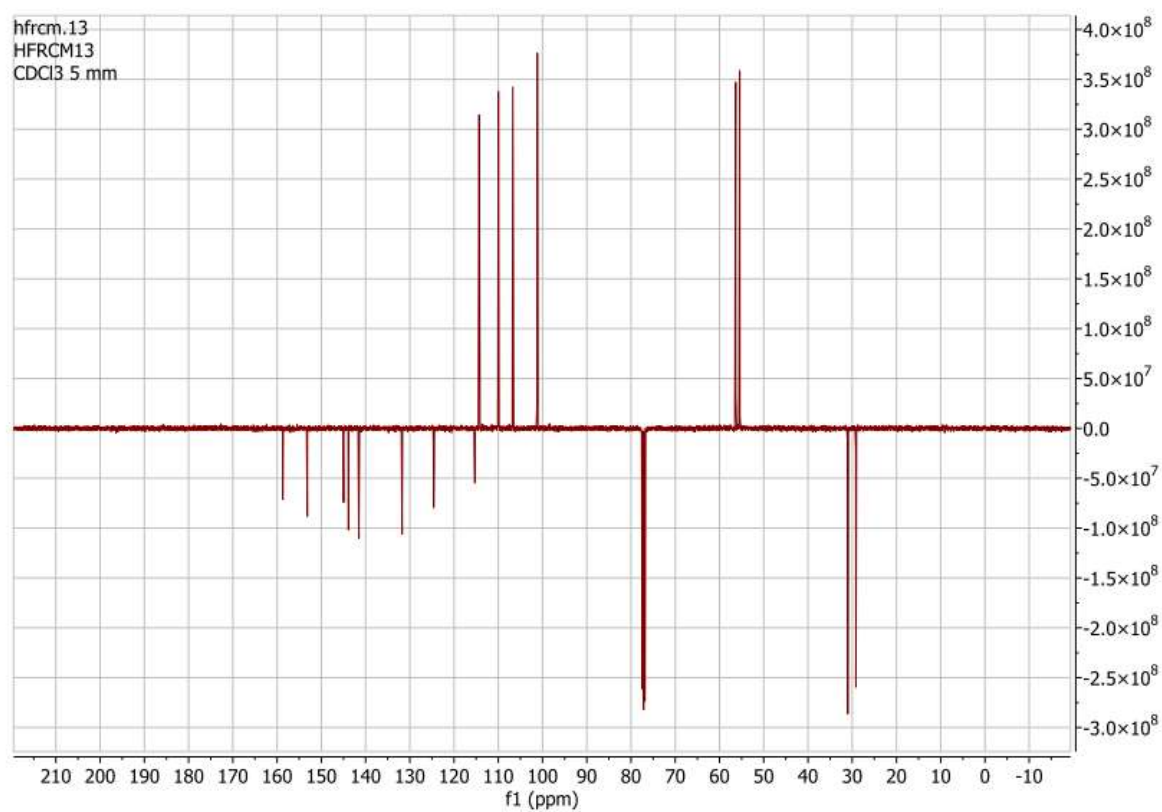


Figure S4: APT NMR spectrum of compound 1

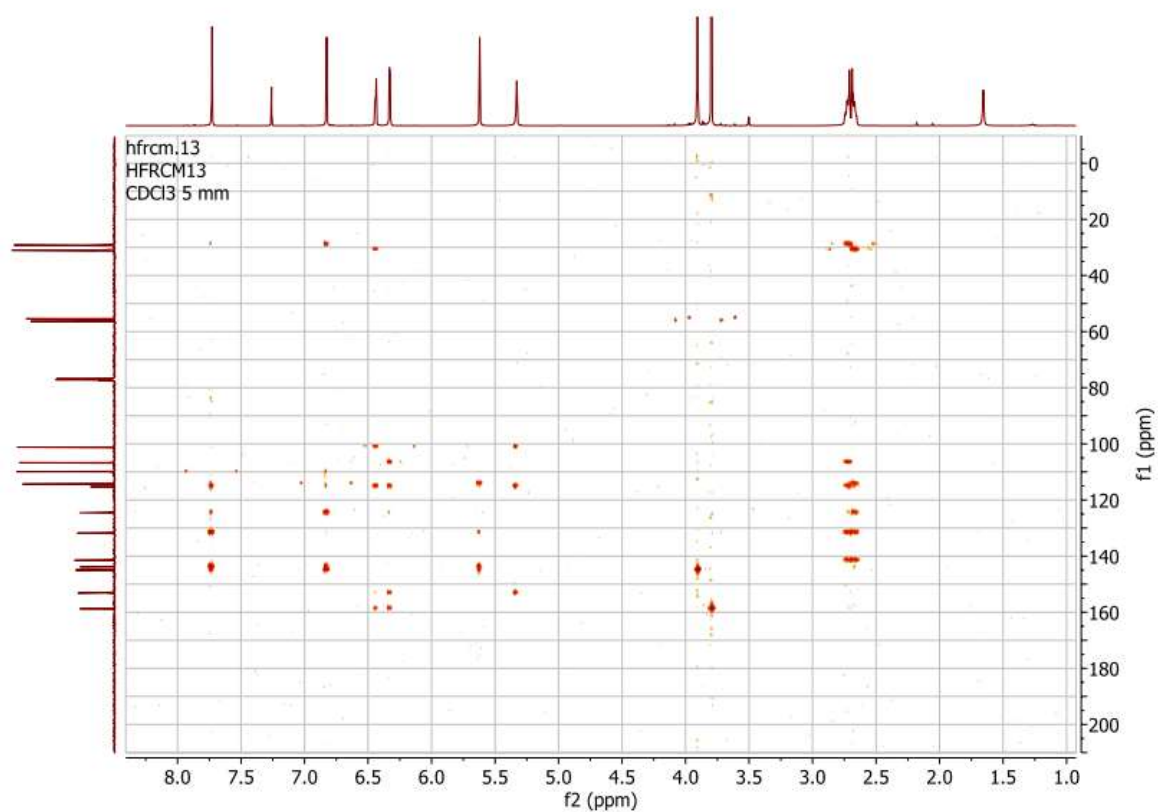


Figure S5: HMBC spectrum of compound **1**

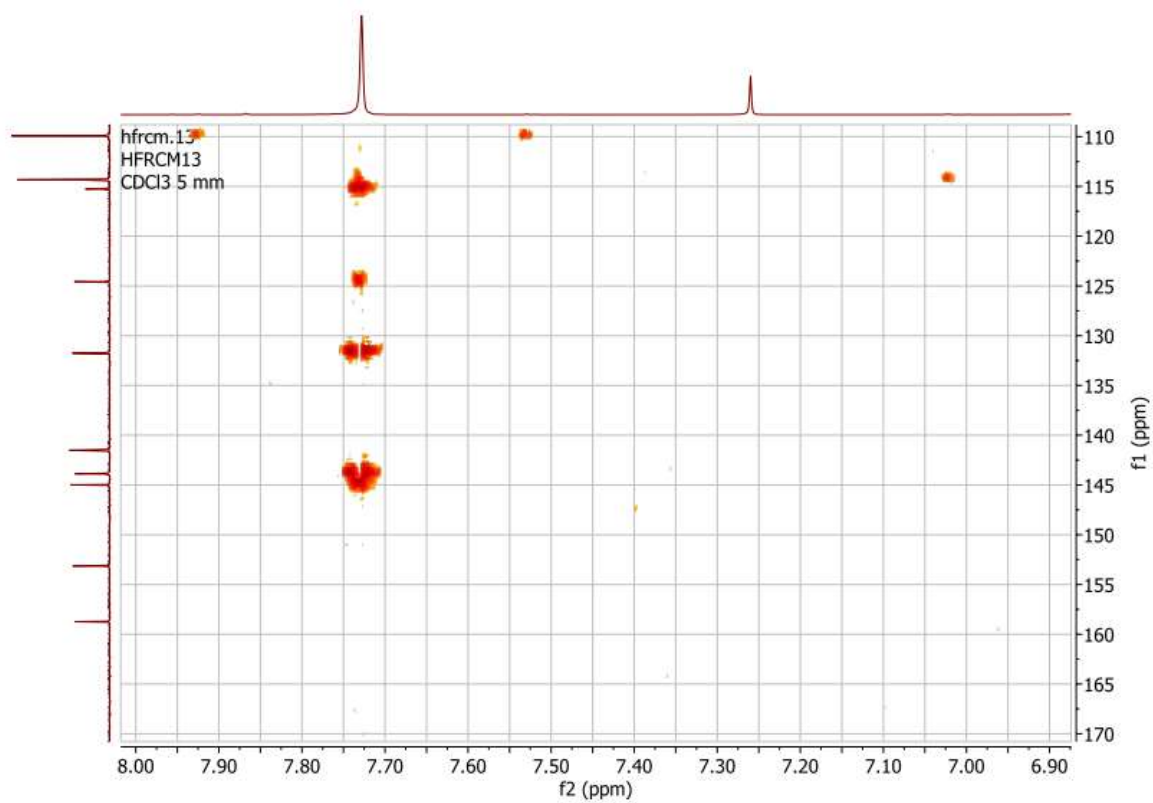
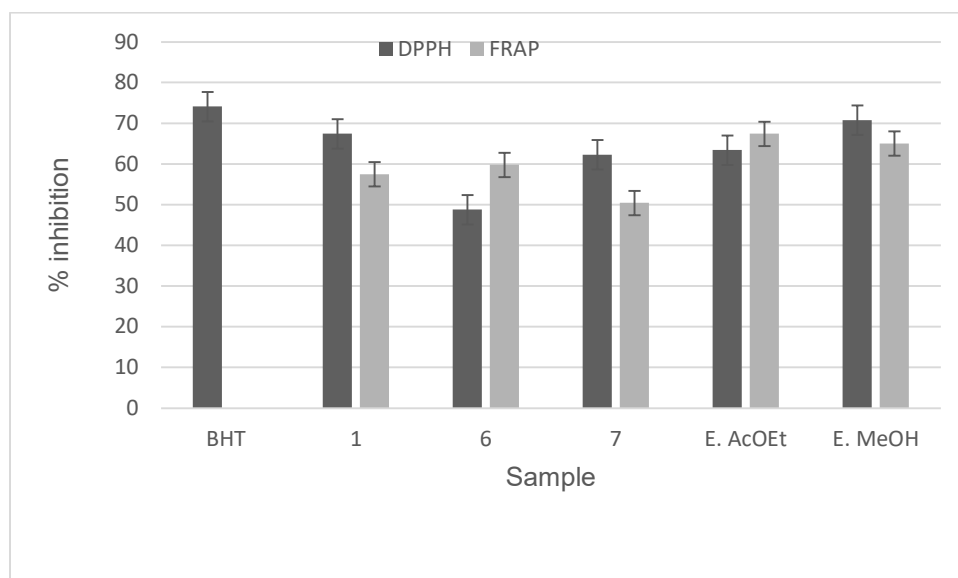


Figure S6: HMBC spectrum of compound **1** showing 5J correlation

Table S1. ^1H , ^{13}C NMR Data and correlation HMBC of Compounds **1** (CDCl_3 , 500 MHz) δ in ppm

Position	1		
	δ_c	δ_H	HMBC
1/12'	144.9	-	-
2/13'	143.8	-	-
3/14'	114.3	6.83 (s, 2H)	C-1, C-2, C-4, C-7/C-12', C-13', C-9'
4/9'	124.6	-	-
5/10'	131.7	-	-
6/11'	109.9	7.73 (s, 2H)	C-1, C-2, C-4, C-5, C-4'/C-12', C-13', C-9', C-10', C-9
7/7'	29.2	2.70 (m, 4H)	C-3, C-4, C-5, C-8/C-8', C-3'
8/8'	31.0	2.72 (m, 4H)	C-7, C-9, C-14/C-10', C-7', C-4'
9/4'	115.2	-	-
10/5'	101.2	6.33 (d, 2H, $J=2.5\text{Hz}$)	C-8, C-9, C-11, C-12/C-4', C-6', C-1', C-7'
11/6'	158.7	-	-
12/1'	106.7	6.44 (d, 2H, $J=2.5\text{Hz}$)	C-10, C-11, C-13/C-5', C-6', C-2'
13/2'	153.1	-	-
14/3'	141.5	-	-
11/6'-OCH ₃	55.4	3.80 (s, 6H)	C-11/C-6'
1/12'-OCH ₃	56.3	3.91 (s, 6H)	C-1/ C-12'
2/13'-OH	-	5.62 (s, 2H)	C-1, C-3/ C-12', C-13'
13/2'-OH	-	5.33 (s, 2H)	C-13/C-2'

**Figure S7.** Diagrams determining inhibition percentage of antioxidant activities of extracts and isolated compounds according to DPPH and FRAP test

Highlight

- First chemical and pharmacological investigation of the twigs of *Combretum molle*
- Isolation and characterizations of a new macrocyclic bisbibenzyl from *C. molle*
- Potent antioxidant activities of extract and pure isolated compounds
- Results are in agreement with the traditional health uses of the plant