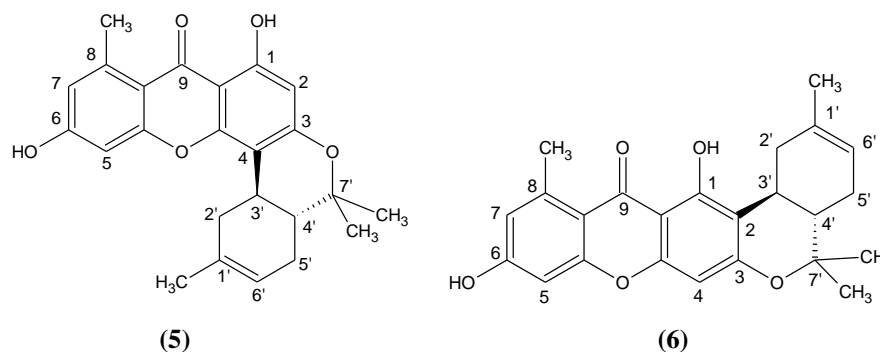


Design, Synthesis and in vitro Antimicrobial Activity Evaluation of Novel Hybrids of Lichexantone-THC Derivatives

Supplementary Material

Table 1. Chemical shifts (δ in ppm) for compounds **5** and **6**, en CDCl_3



C	Compound 5				Compound 6			
	H	^1H NMR (300MHz)	C-H long range correlations*	^{13}C NMR (75MHz)	H	^1H NMR (300MHz)	C-H long range correlations*	^{13}C NMR (75MHz)
C1	OH, s	13.29	99.8; 161.3	160.8				163.5
C2	1H, s	6.17	104.0; 161.3	99.8				104.0
C3				161.3				166.2

C4				103.8	1H, s	6.33	101.2; 110.7; 154.5; 166.2	95.5
C5	1H, bs	6.67		100.8	1H, bs	6.68	108.0	101.2
C6				160.8				163.5
C7	1H, bs	6.59		115.7	1H, bs	6.68	23.8; 101.2	117.6
C8				144.2				144.7
C9				182.5				182.1
C4a				155.0				154.5
C8a				113.0				108.0
C9a				104.0				110.7
C10a				160.0				160.5
C8-CH ₃	3H, s	2.82	113.0; 115.4; 144.2	23.4	3H, s,	2.79	108.0; 117.6; 144.7	23.8
C1'				134.2				134.9
C1'-CH ₃	3H, bs	1.75	36.8; 119.5; 134.2	23.6	3H, bs	1.66	34.9; 118.6; 134.9	23.5
C2'a	1H, bd, <i>J</i> =16Hz	3.15 – 3.18		36.8	1H, bd, <i>J</i> =15Hz	3.41 – 3.47		34.9
C2'b	1H, m	1.81 – 1.87			1H, m	1.71-1.83		
C3'	1H, m	2.86		30.9	1H, m	2.84 – 2.88	118.6	30.9
C4'	1H, m	1.81 – 1.87		44.4	1H, m	1.71-1.83		44.0
C5'a	1H, m	2.15 - 2.20		27.7	1H, m	2.15 – 2.20		27.6
C5'b	1H, m	1.81 – 1.87			1H, m	1.71-1.83		
C6'	1H, bs	5.47		119.5	1H, bs	5.41		118.6

C7'				78.5				80.5
C7'-CH ₃	3H, bs	1.13	27.4; 44.4; 78.5	18.7	3H, bs	1.15	27.4; 44.0; 80.5	19.2
C7'-CH ₃	3H, bs	1.40	18.7; 44.4; 78.5	27.4	3H, bs	1.45	19.2; 44.0; 80.5	27.3

*From gHMBC experiment.

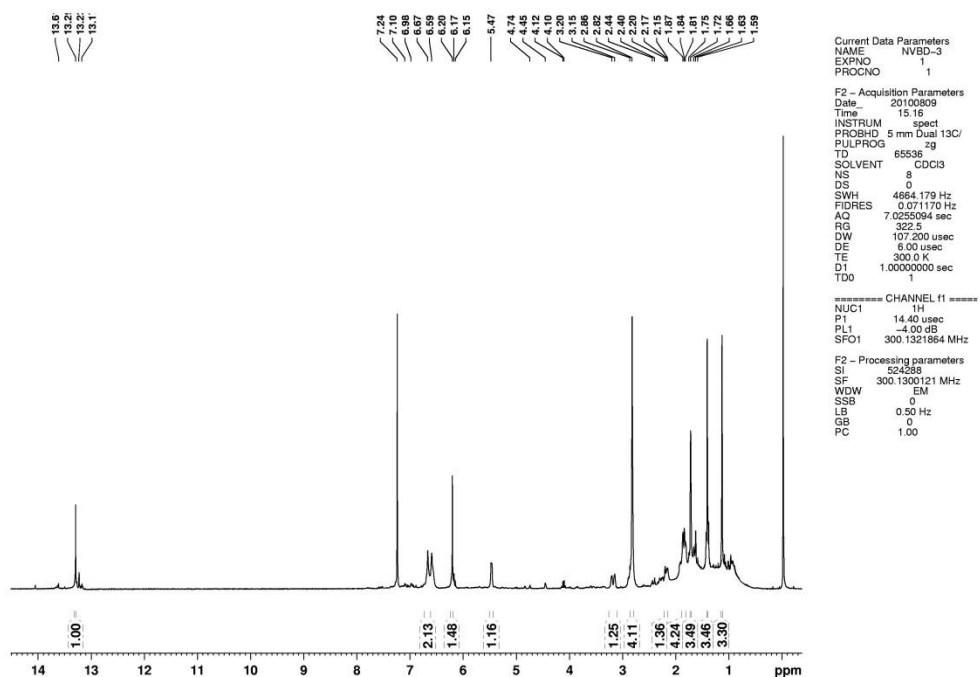


Figure 1S. ¹H NMR spectra of compound 5.

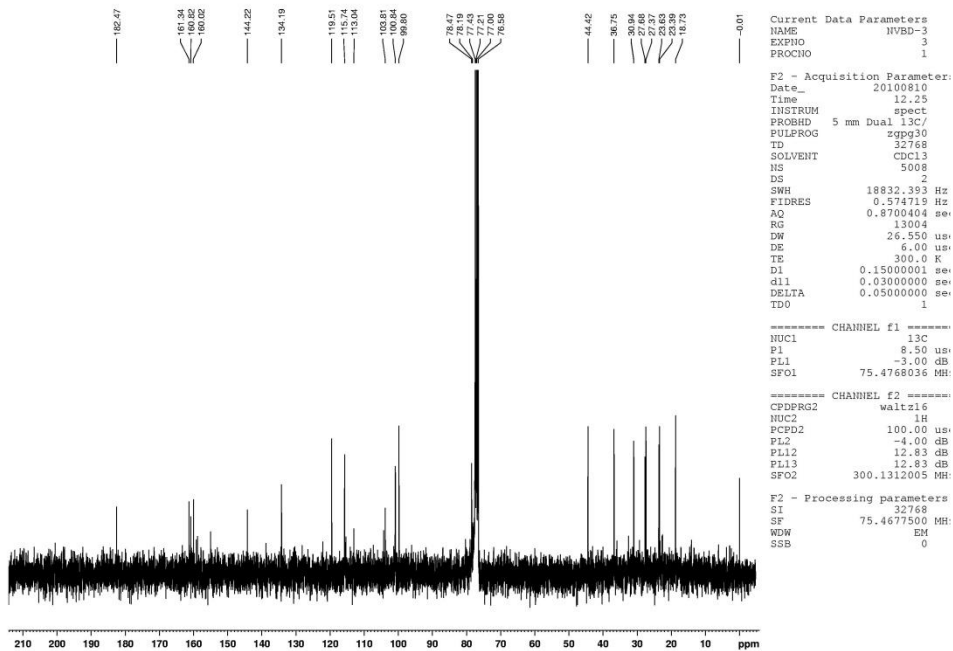


Figure 2S. ¹³C NMR spectra of compound 5.

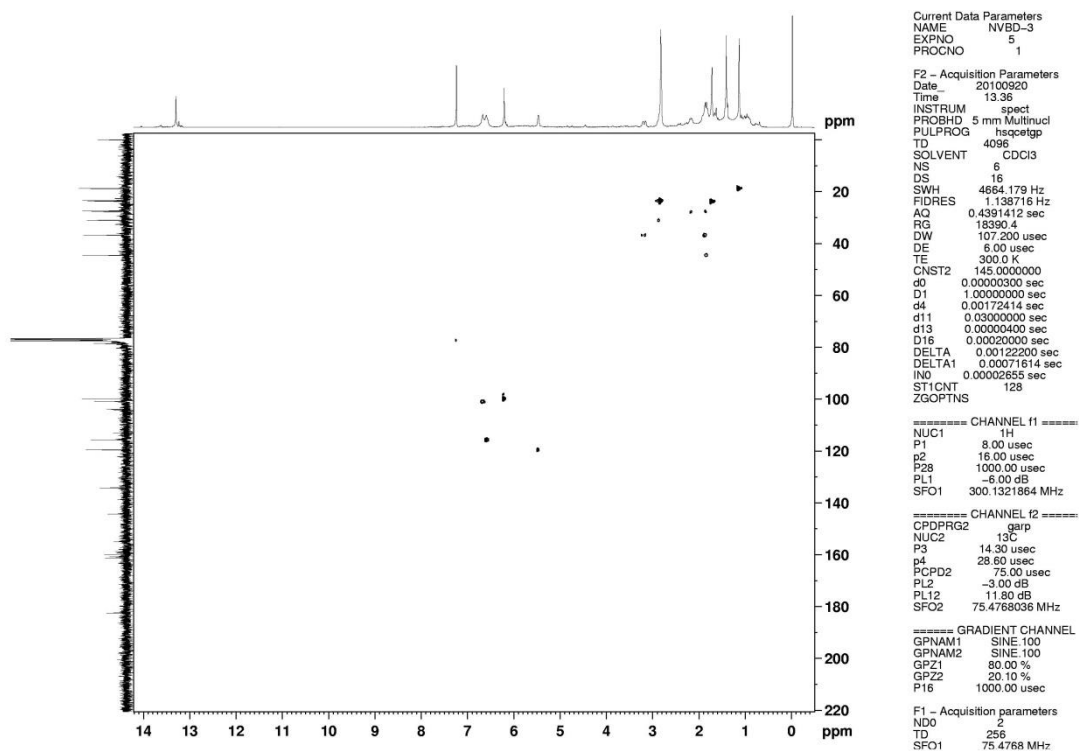


Figure 3S. Correlations from gHSQC experiment of compound 5.

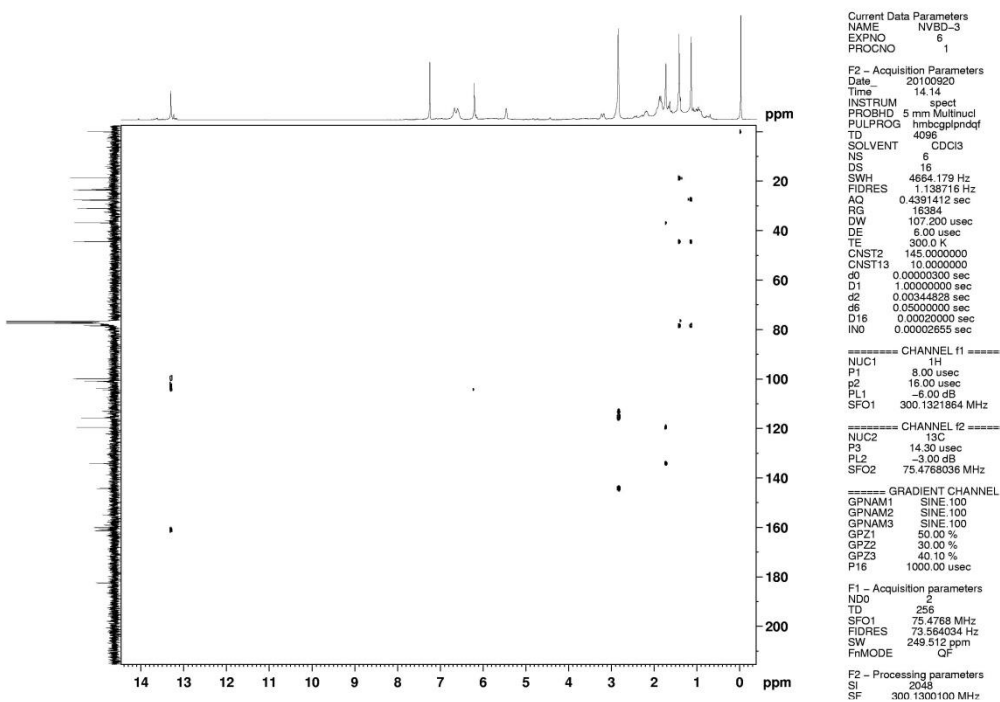


Figure 4S. Correlations from gHMBC experiment of compound 5.

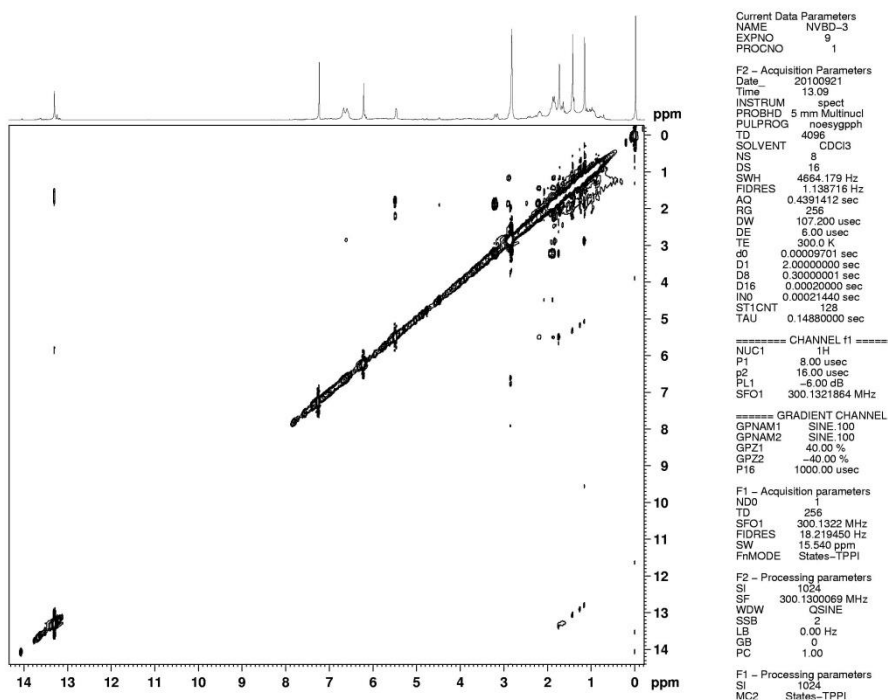


Figure 5S. H-H spatial interactions from NOESY experiment of compound 5.

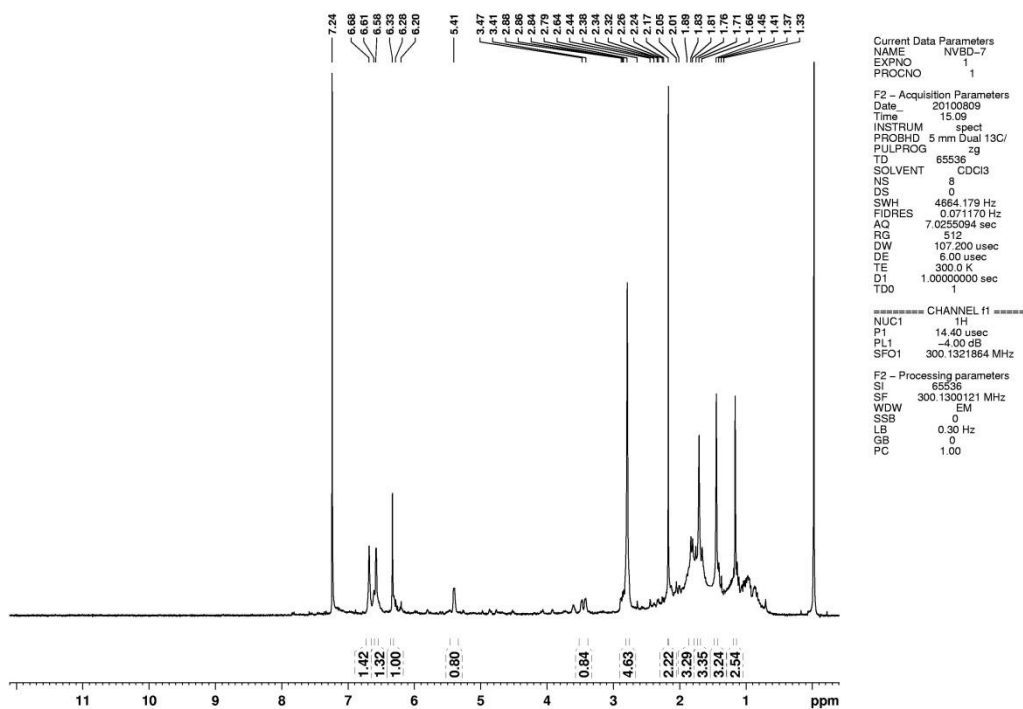


Figure 6S. ¹H NMR spectra of compound 6.

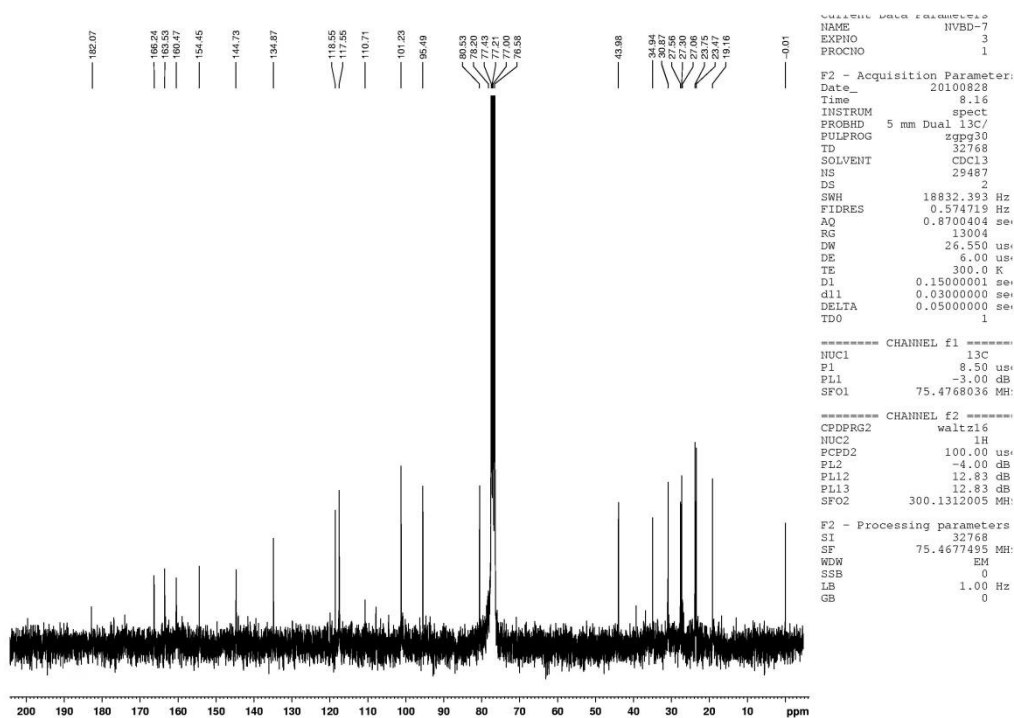


Figure 7S. ¹³C NMR spectra of compound 6.

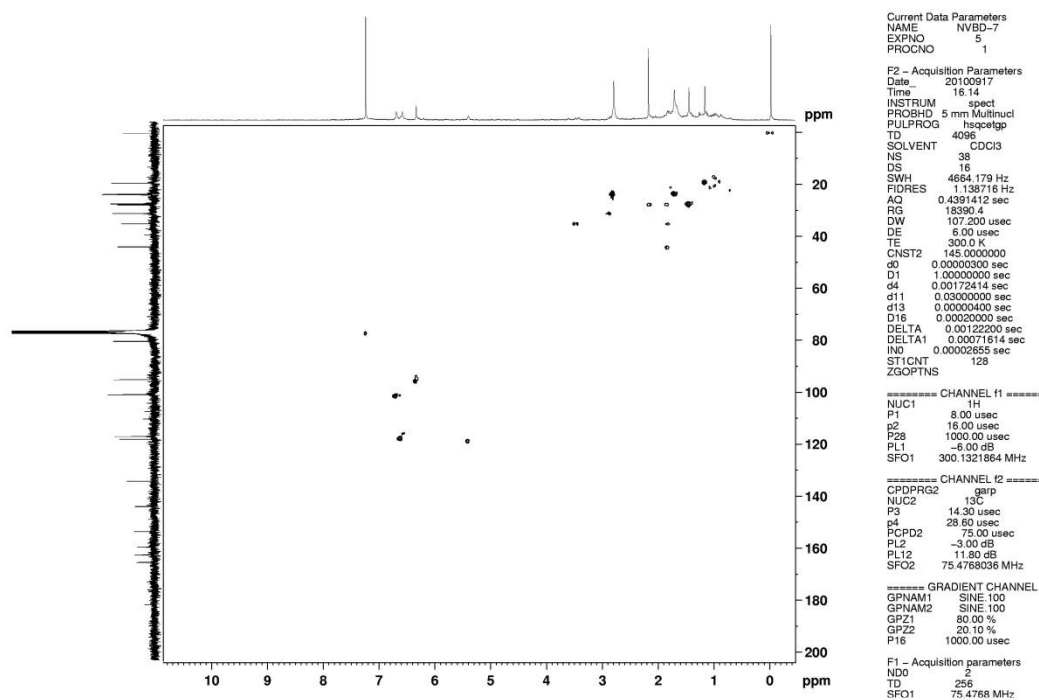


Figure 8S. Correlations from gHSQC experiment of compound 6.

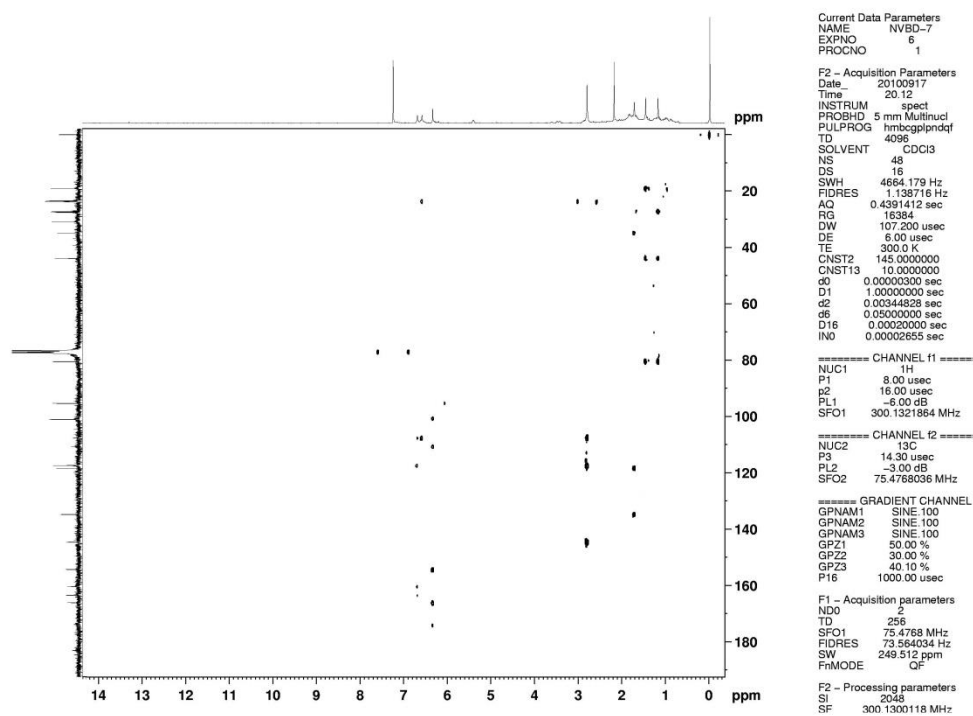


Figure 9S. Correlations from gHMBC experiment of compound 6.