

# Selective Preparation and High Dynamic-Range Analysis of Cannabinoids in “CBD Oil” and Other *Cannabis sativa* Preparations

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## ■ SUPPORTING INFORMATION

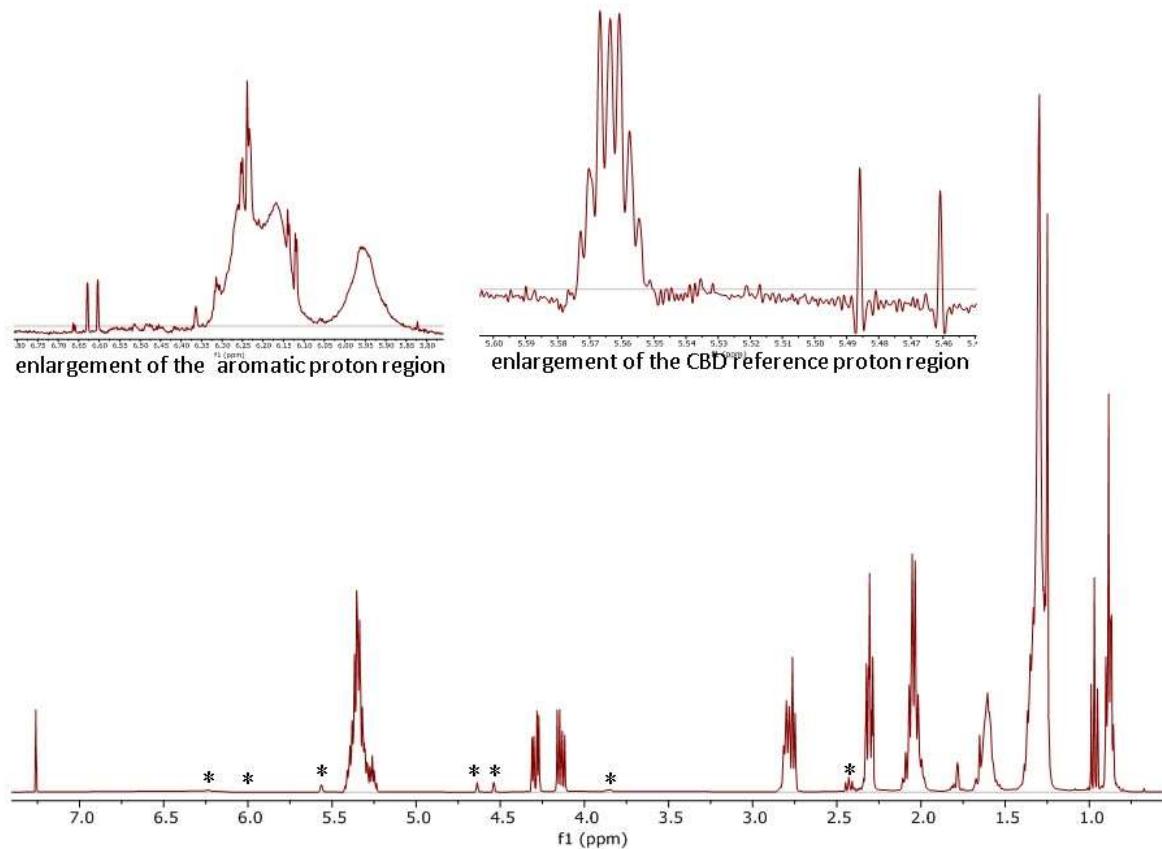
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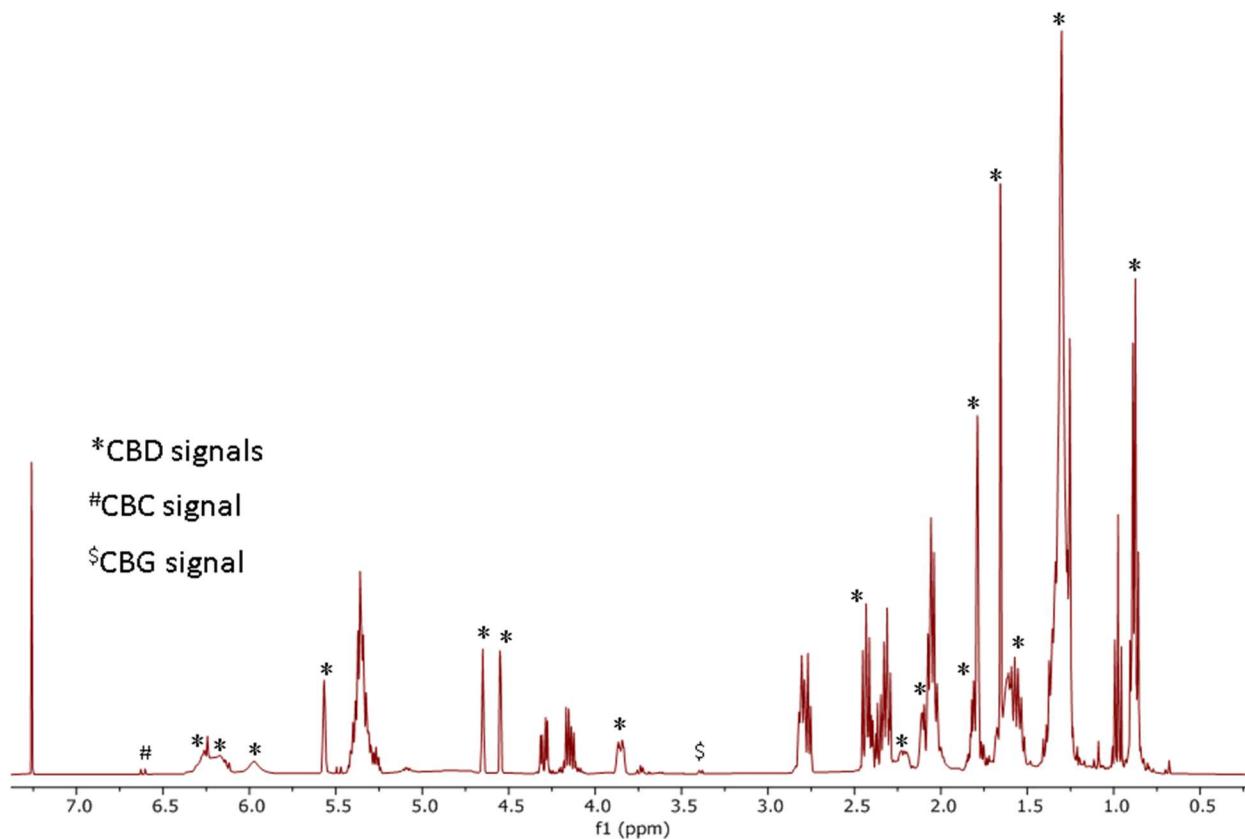
**Figure S1.**  $^1\text{H}$  NMR of CBD (**1**) and related cannabinoids in “CBD Oil” (400 MHz,  $\text{CDCl}_3$ ).

## $^1\text{H}$ NMR of CBD oil



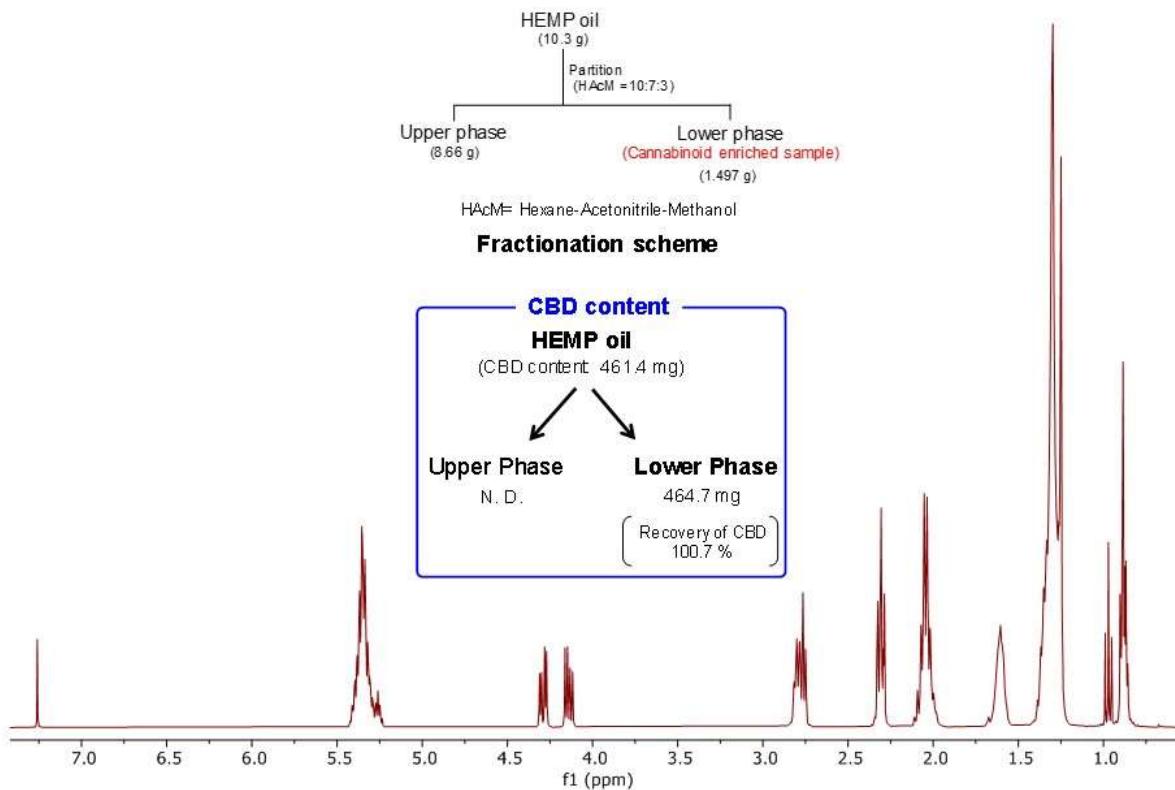
**Figure S2.**  $^1\text{H}$  NMR of the Lower Phase (HAcM extractions) (400 MHz,  $\text{CDCl}_3$ ).

### $^1\text{H}$ NMR of Lower Phase (HAcM extraction)

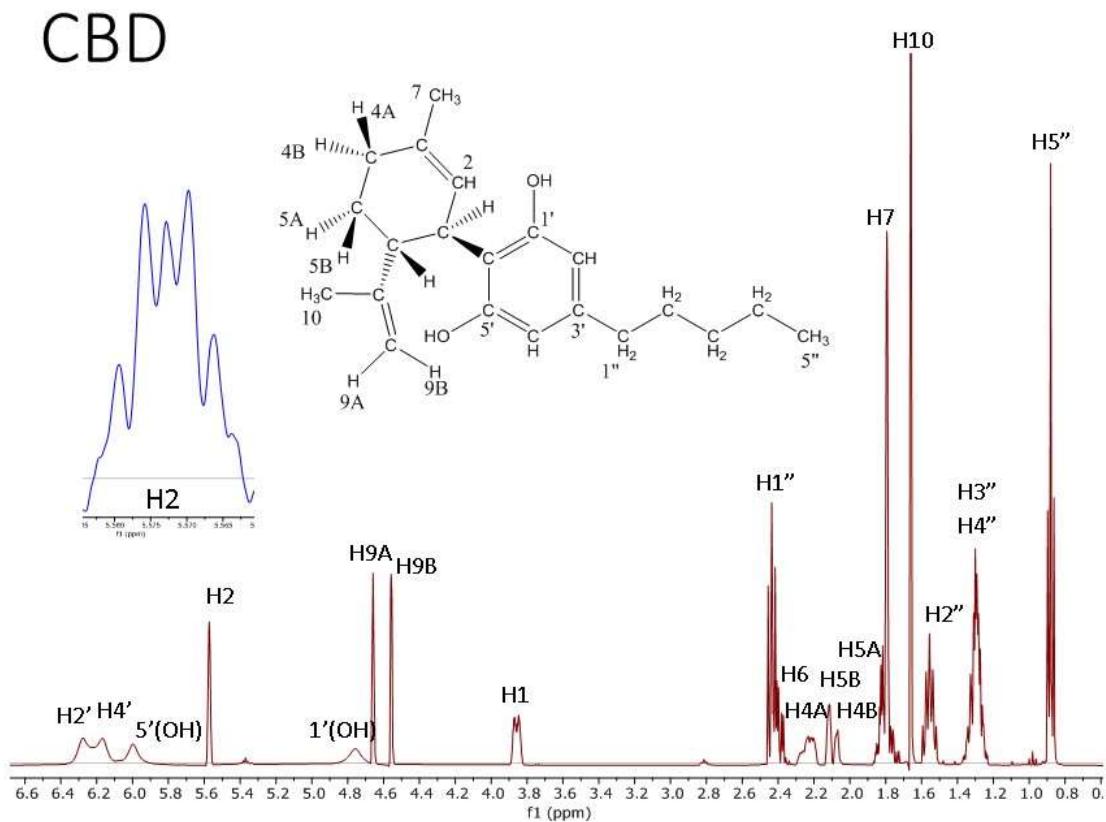


**Figure S3.**  $^1\text{H}$  NMR of the Upper Phase (HAcM extractions) (400 MHz,  $\text{CDCl}_3$ ).

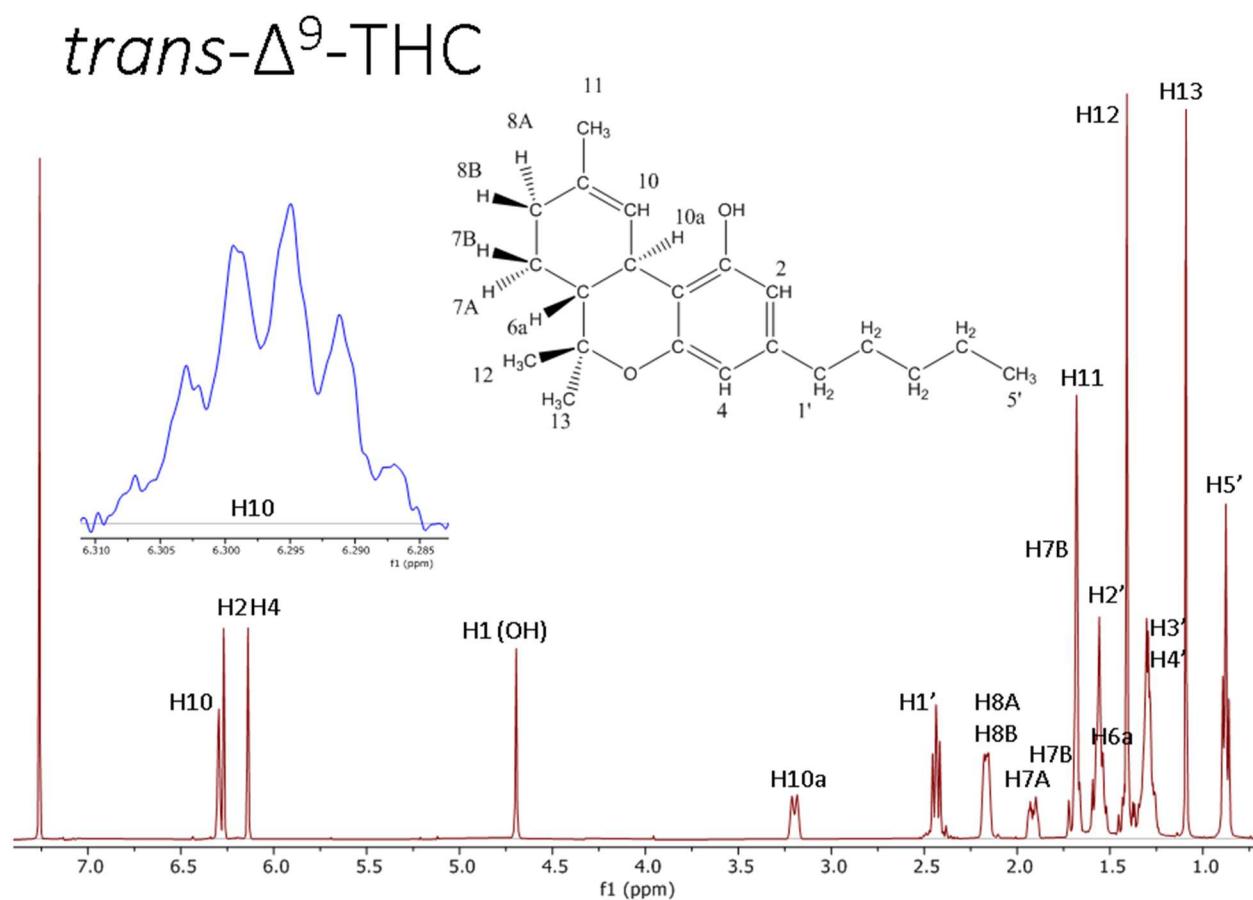
## $^1\text{H}$ NMR of Upper Phase (HAcM extraction)



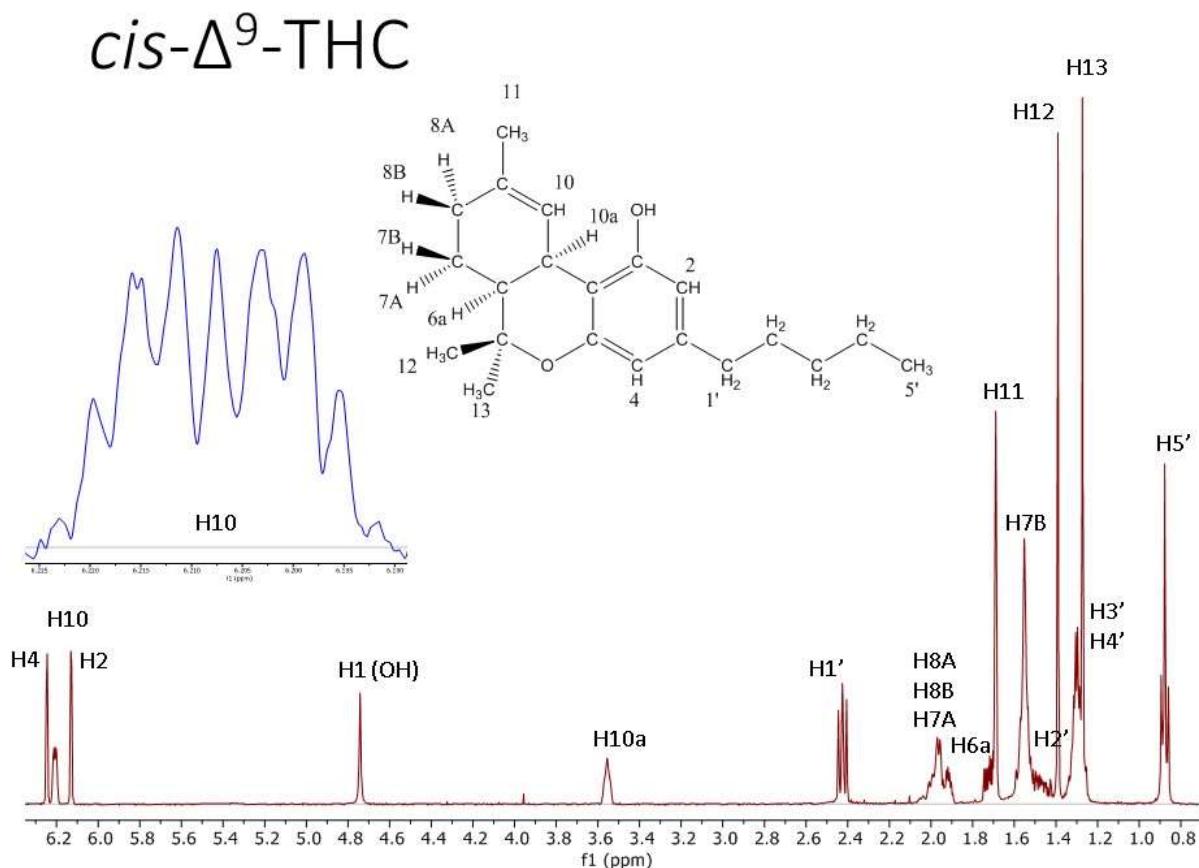
**Figure S4.**  $^1\text{H}$  NMR Spectrum of CBD (**1**) (400 MHz,  $\text{CDCl}_3$ ).



**Figure S5.**  $^1\text{H}$  NMR Spectrum of *trans*- $\Delta^9$ -THC (**2b**) (400 MHz,  $\text{CDCl}_3$ ).

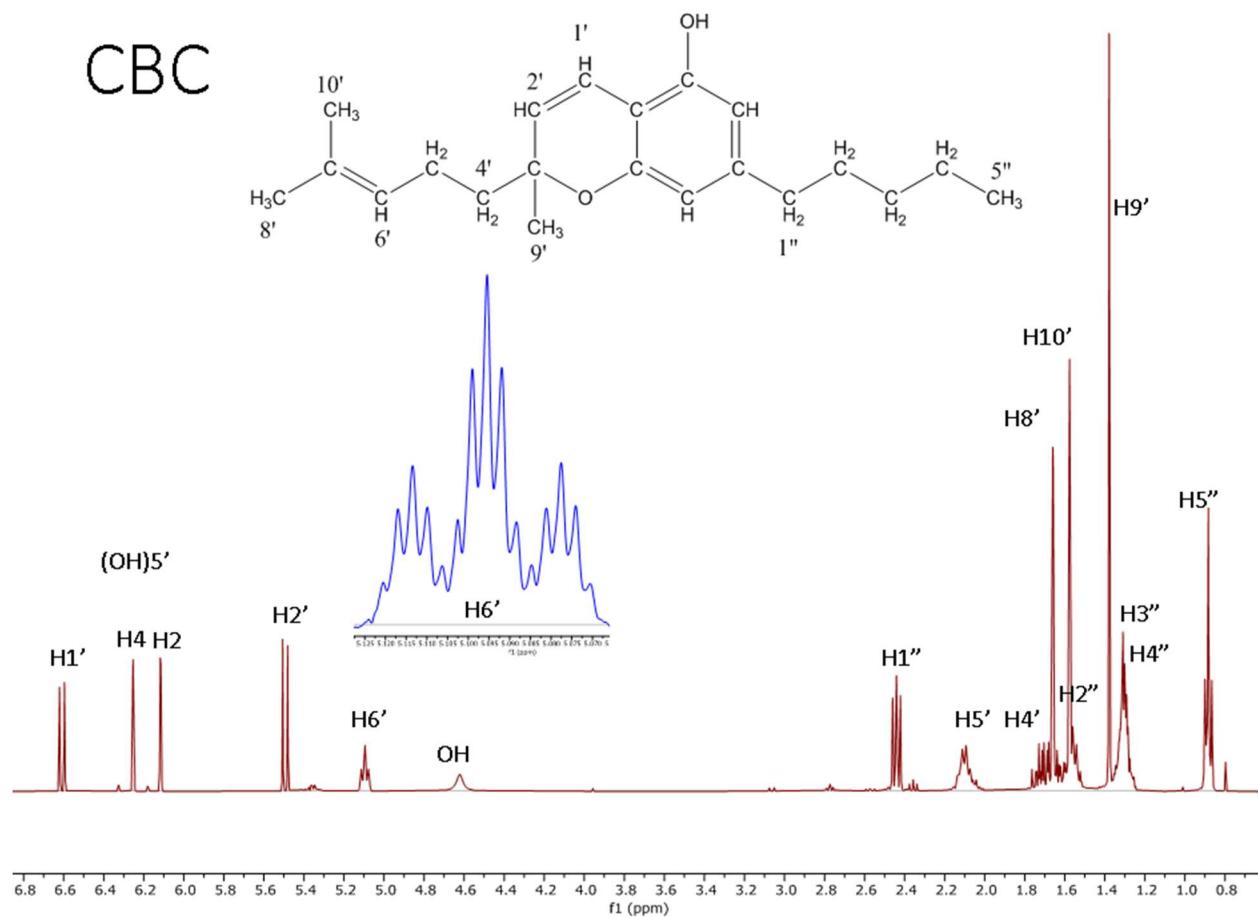


**Figure S6.**  $^1\text{H}$  NMR Spectrum of *cis*- $\Delta^9$ -THC (**2a**) (400 MHz,  $\text{CDCl}_3$ ).

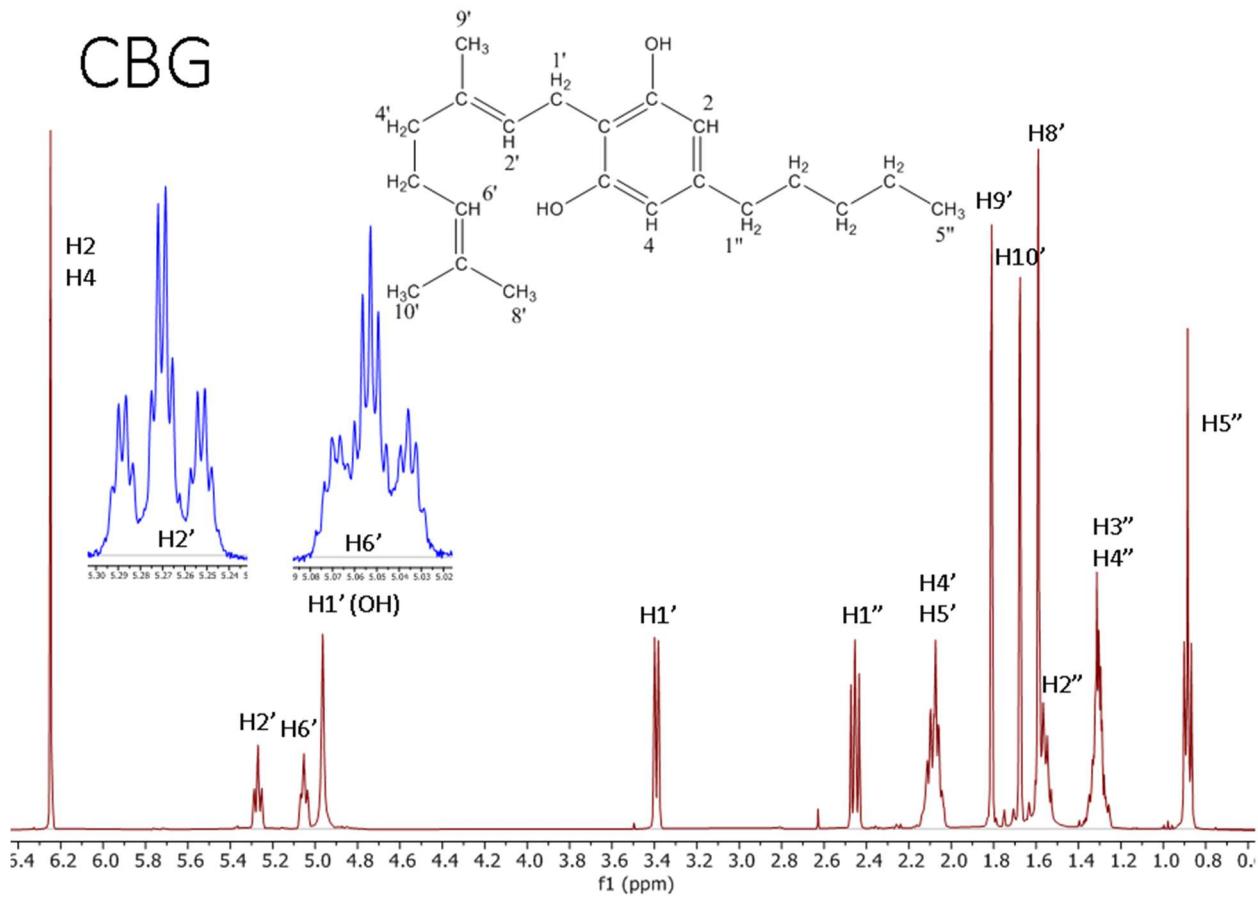


**Figure S7.**  $^1\text{H}$  NMR Spectrum of CBC (**3**) (400 MHz,  $\text{CDCl}_3$ ).

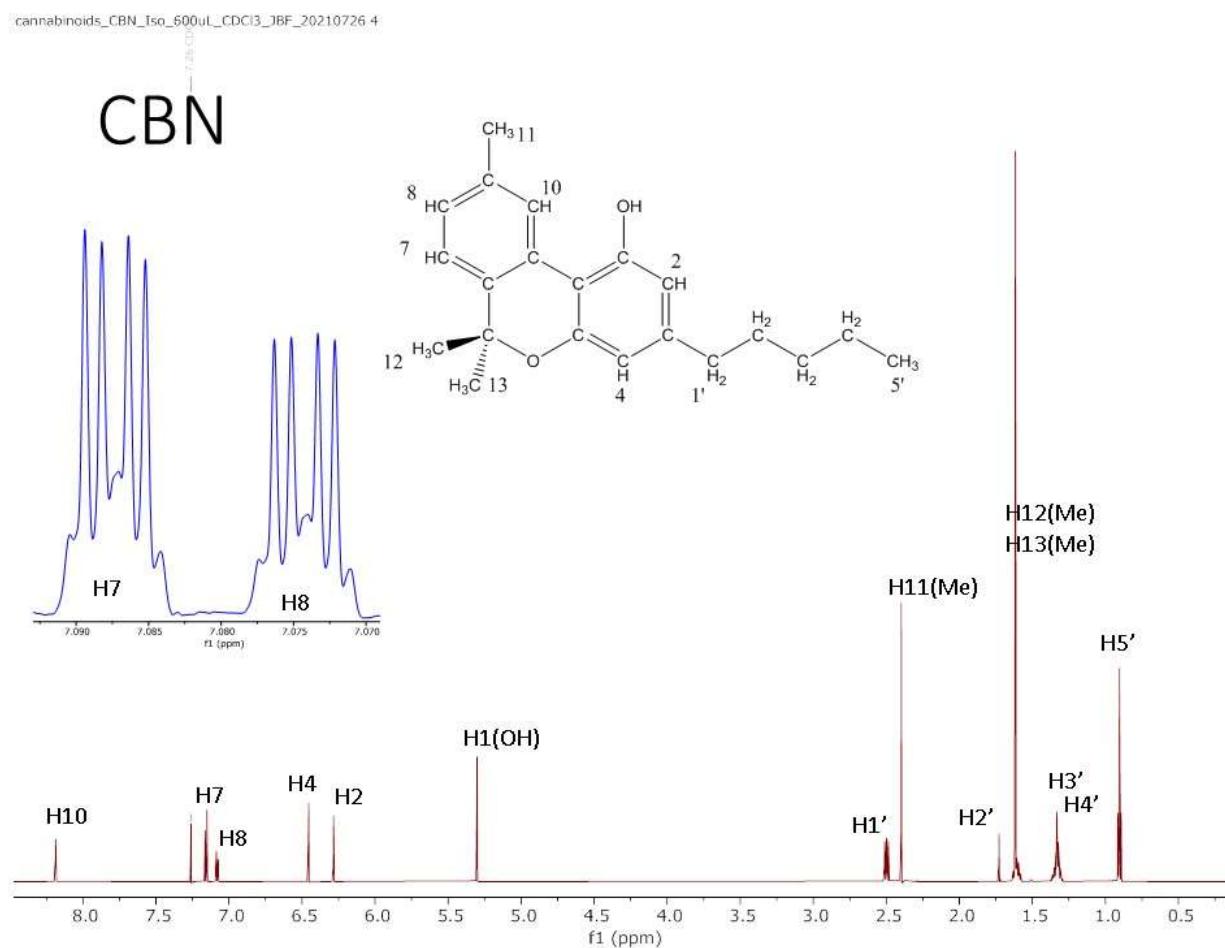
191111-Fr14-18-5\_4600ug600uL\_CDCl3\_Takashi\_191120



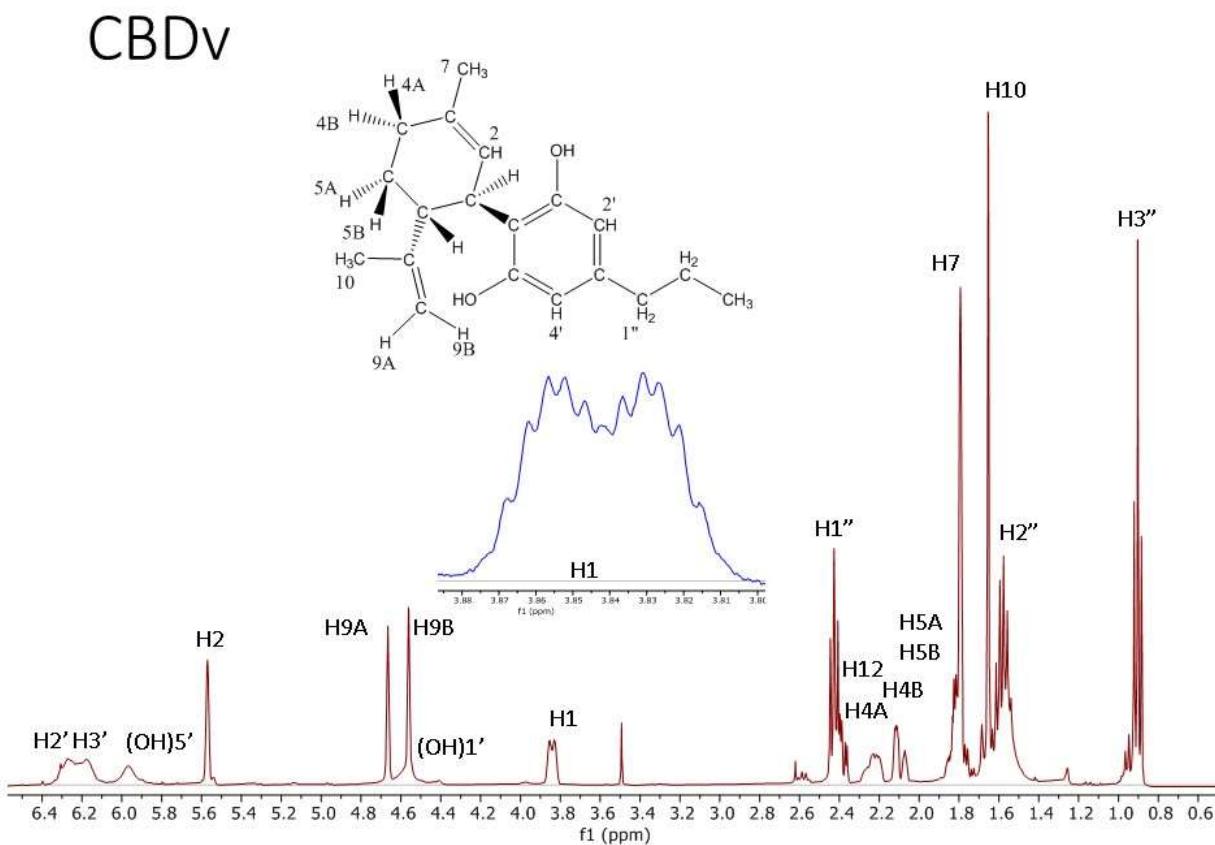
**Figure S8.**  $^1\text{H}$  NMR Spectrum of CBG (**4**) (400 MHz,  $\text{CDCl}_3$ ).



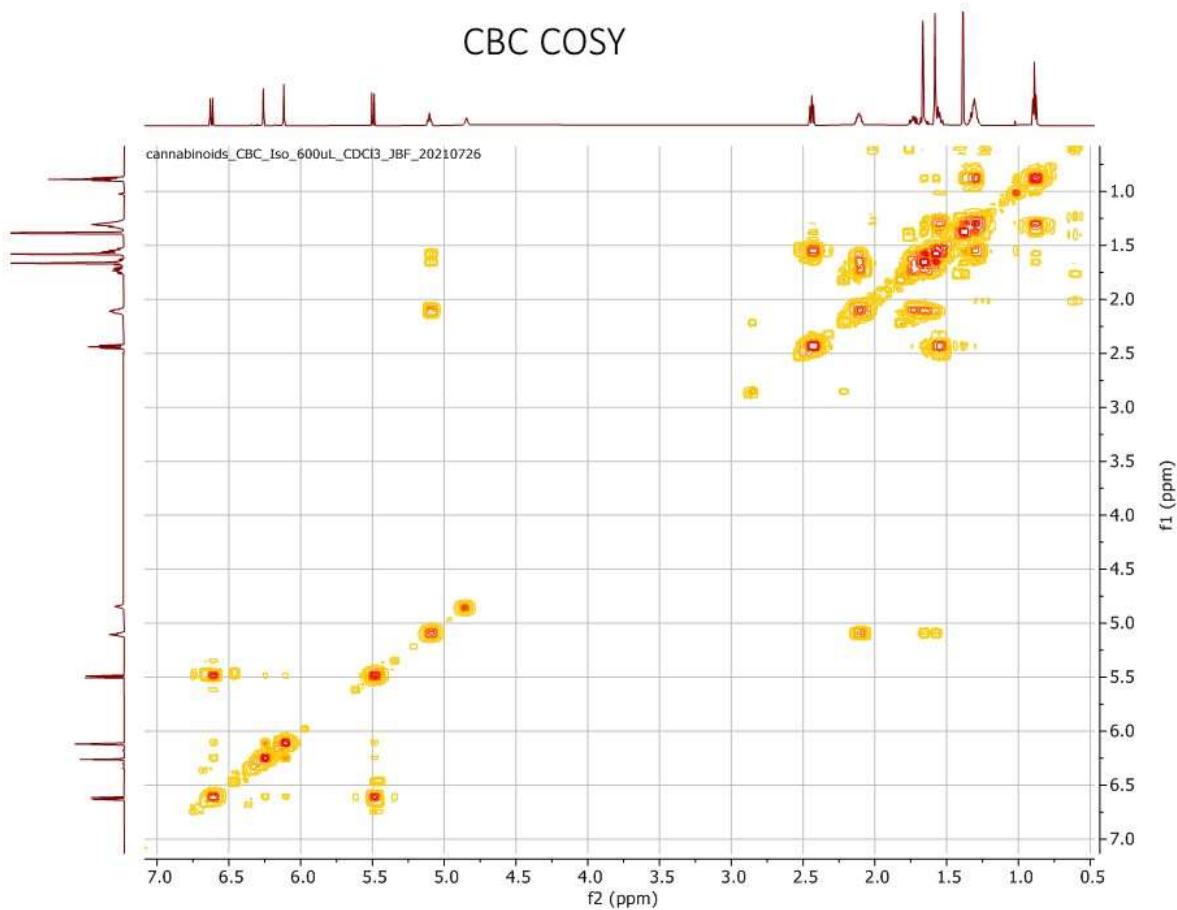
**Figure S9.**  $^1\text{H}$  NMR Spectrum of CBN (**5**) (400 MHz,  $\text{CDCl}_3$ ).



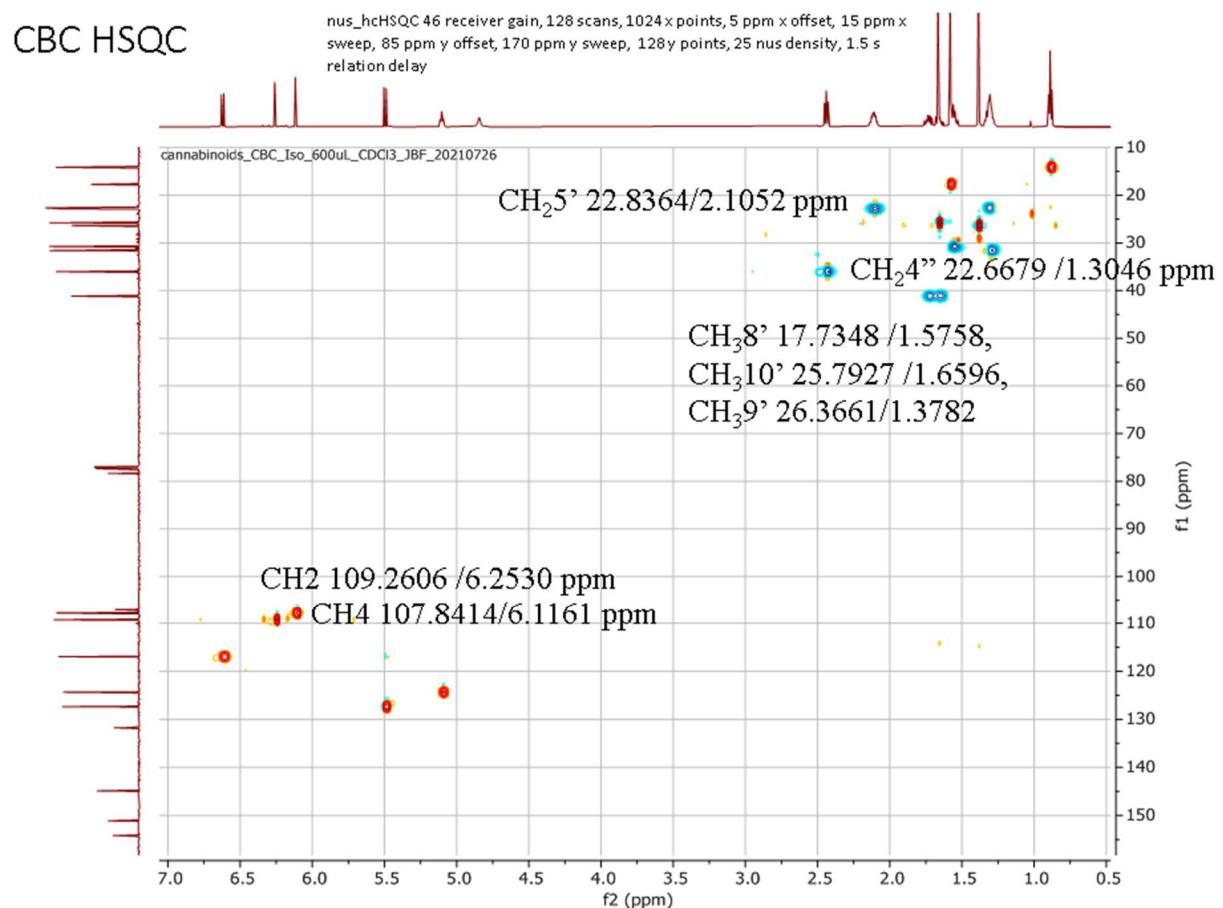
**Figure S10.**  $^1\text{H}$  NMR Spectrum of CBDV (**6**) (400 MHz,  $\text{CDCl}_3$ ).



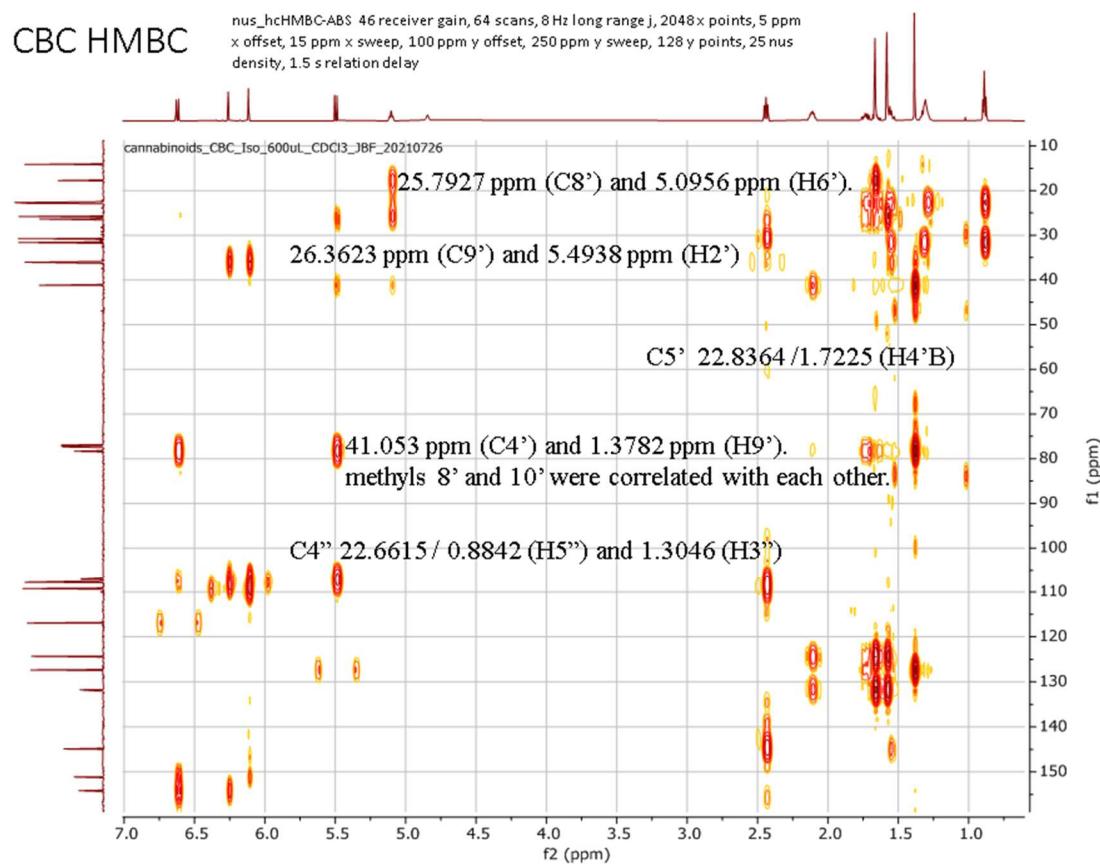
**Figure S11.**  $^1\text{H}$  NMR COSY Spectrum of CBC (**3**) (400 MHz,  $\text{CDCl}_3$ ).



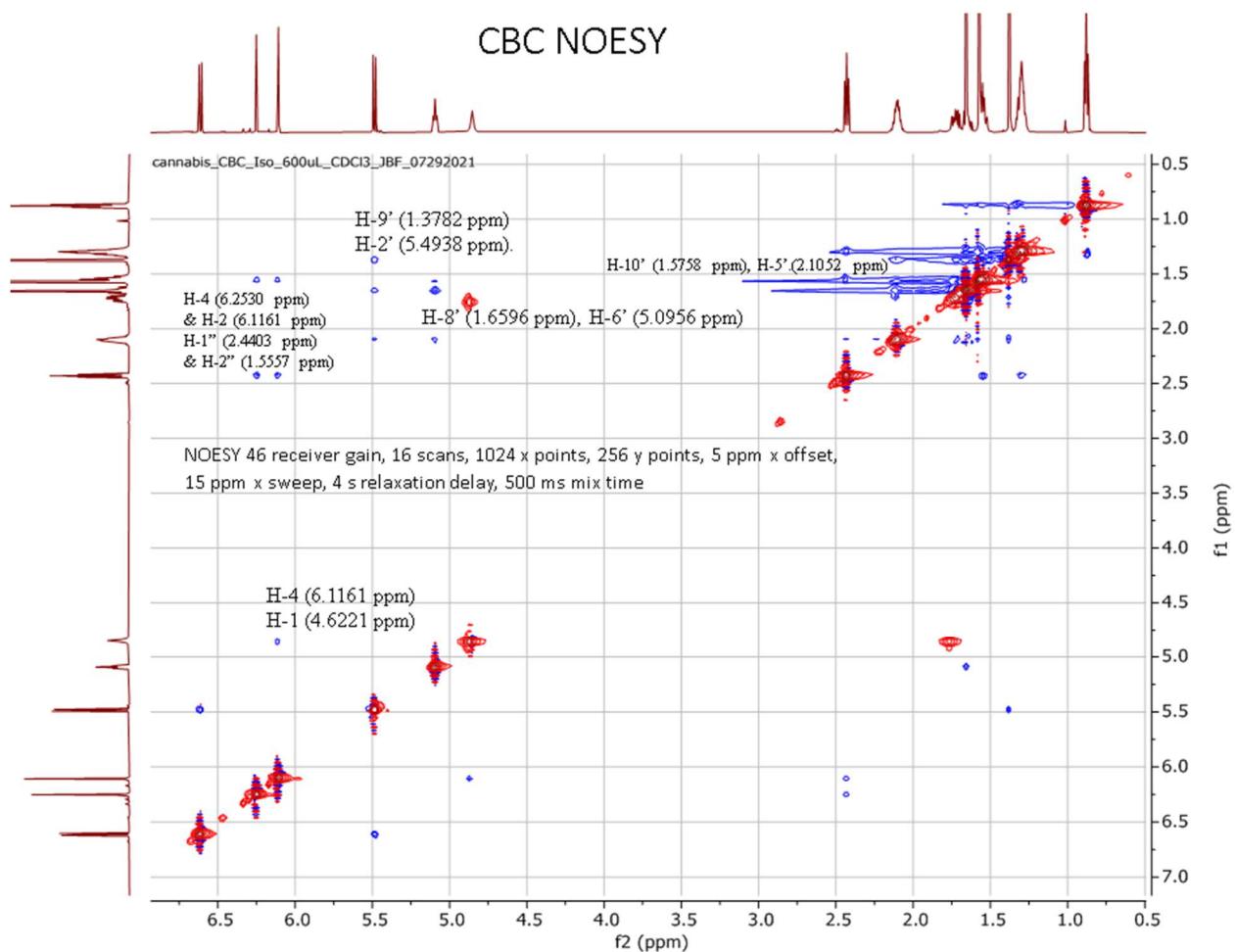
**Figure S12.**  $^1\text{H}/^{13}\text{C}$  NMR HSQC Spectrum of CBC (**3**) (400/100 MHz,  $\text{CDCl}_3$ ).



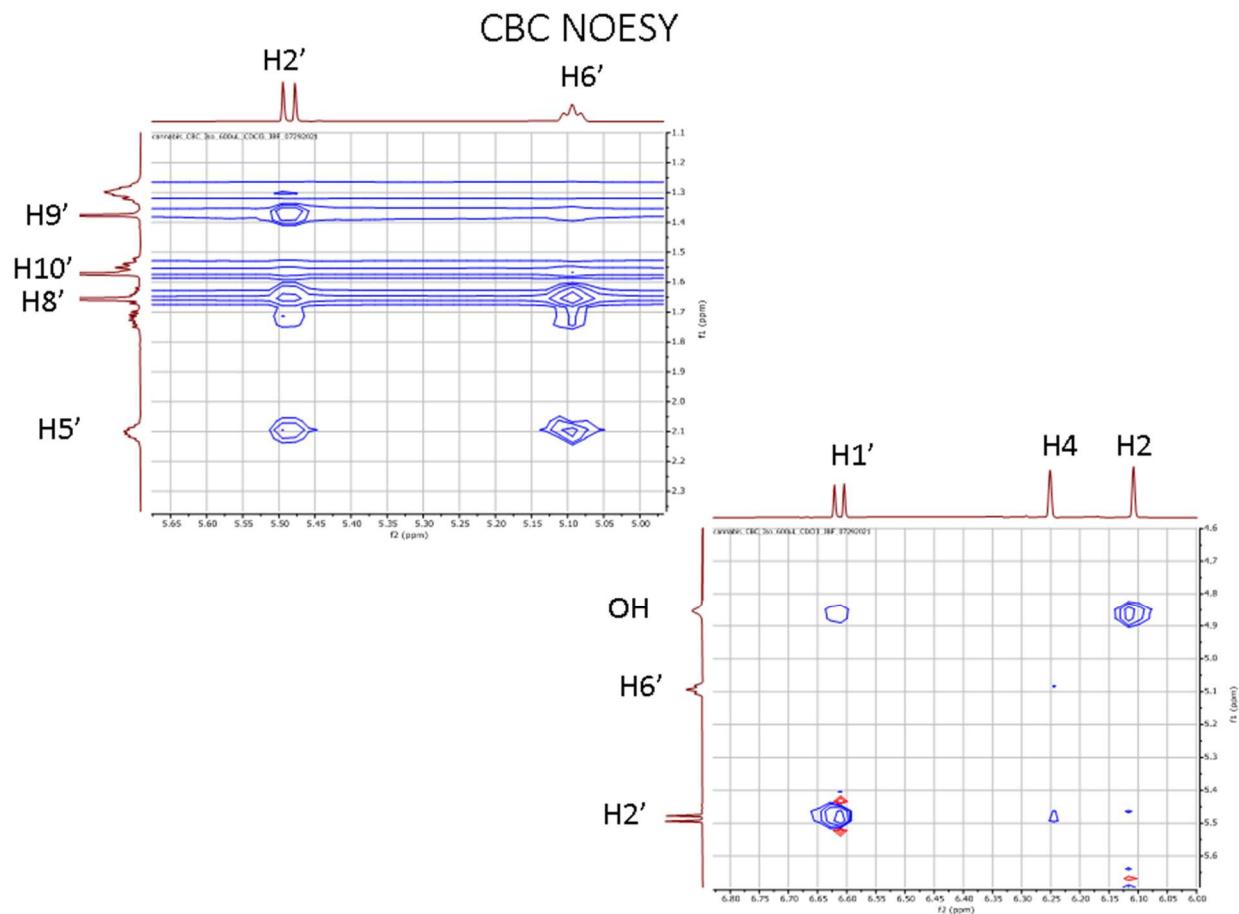
**Figure S13.**  $^1\text{H}/^{13}\text{C}$  NMR HMBC Spectrum of CBC (**3**) (400/100 MHz,  $\text{CDCl}_3$ ).



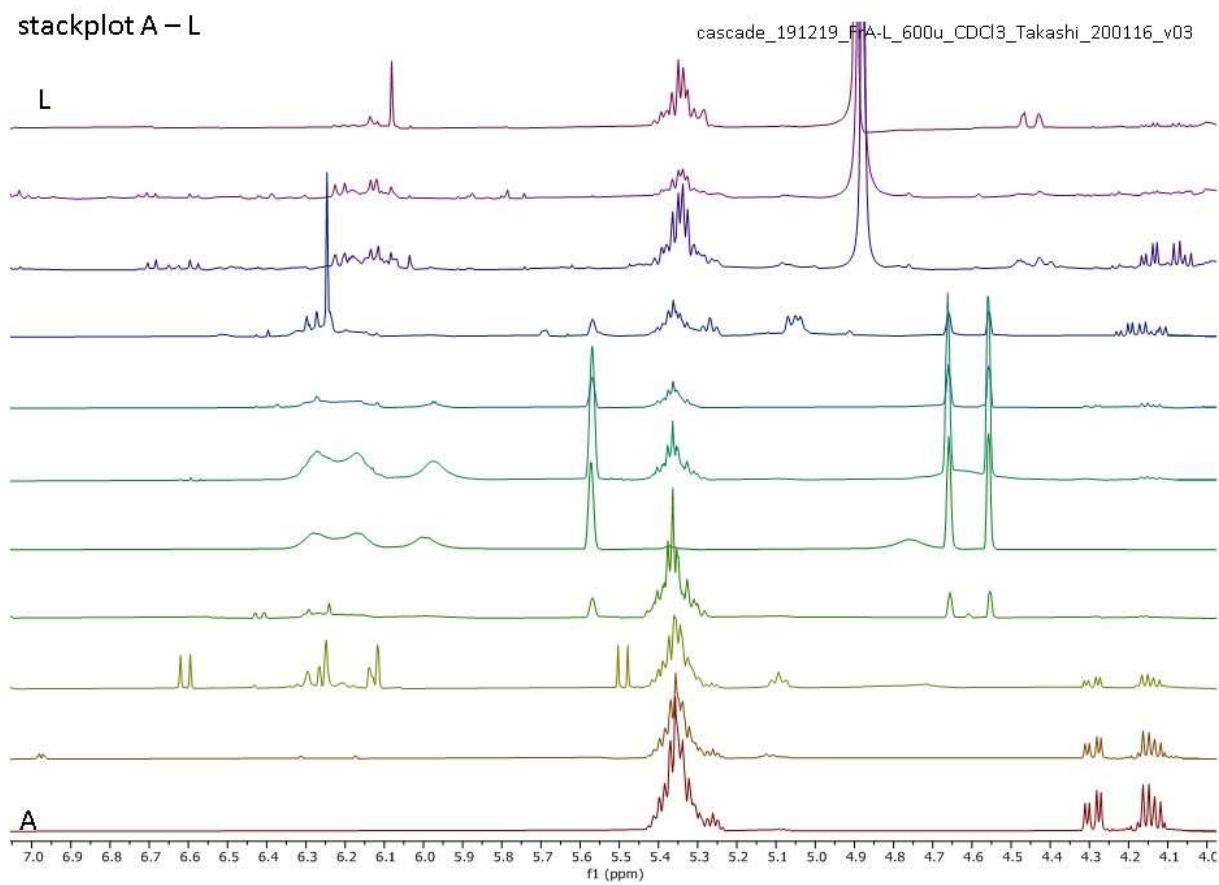
**Figure S14.**  $^1\text{H}$  NMR NOESY Spectrum of CBC (**3**) (400 MHz,  $\text{CDCl}_3$ ).



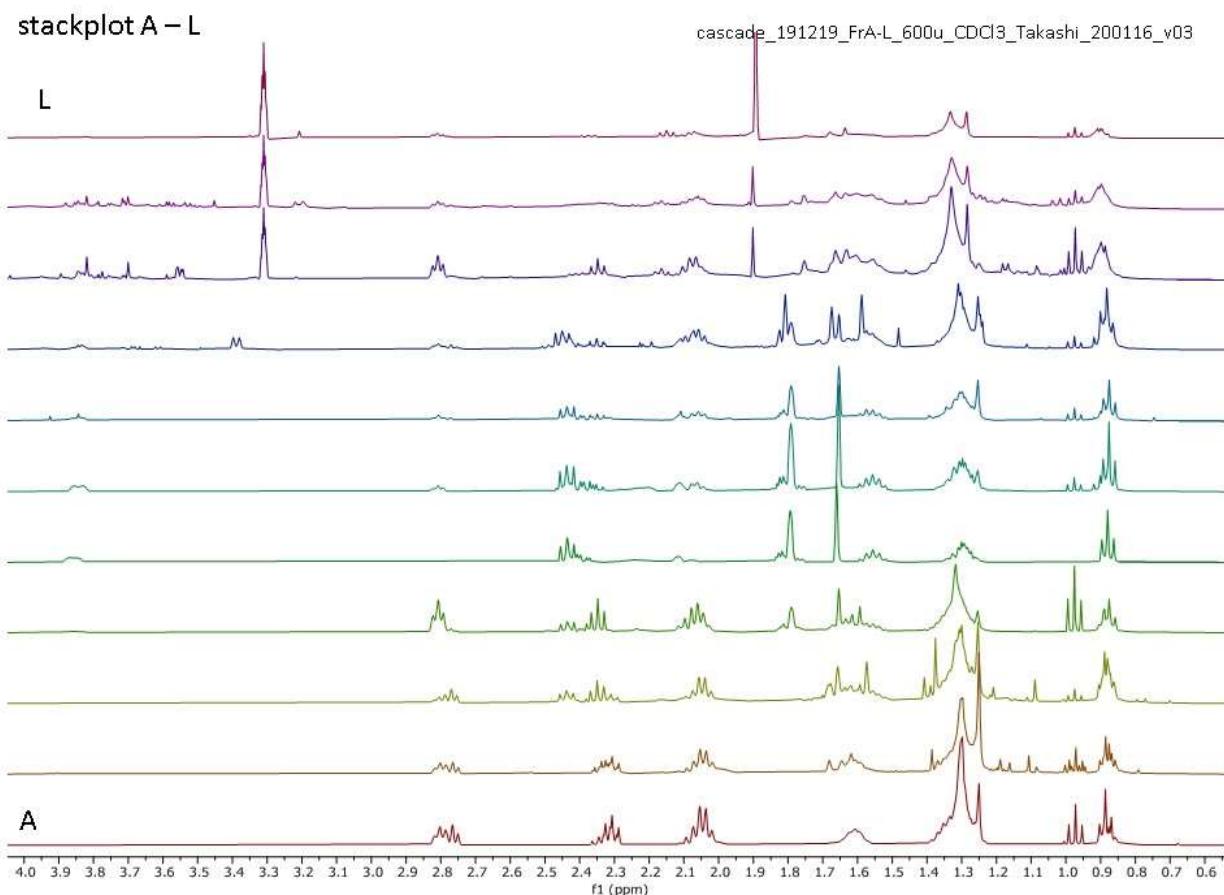
**Figure S15.**  $^1\text{H}$  NMR NOESY Spectrum of CBC (**3**) (400 MHz,  $\text{CDCl}_3$ ).



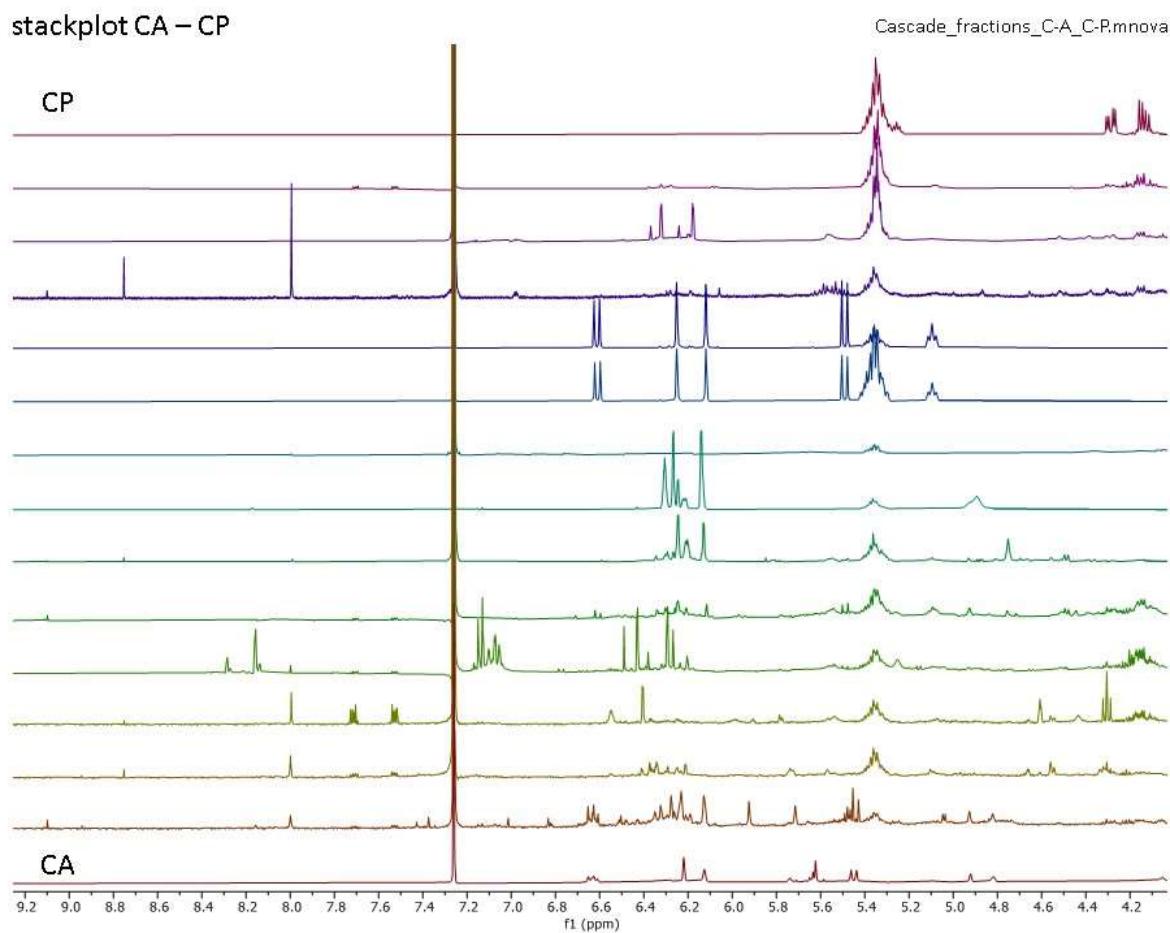
**Figure S16.** High-frequency region stacked plot of  $^1\text{H}$  NMR spectra (400 MHz,  $\text{CDCl}_3$ ).



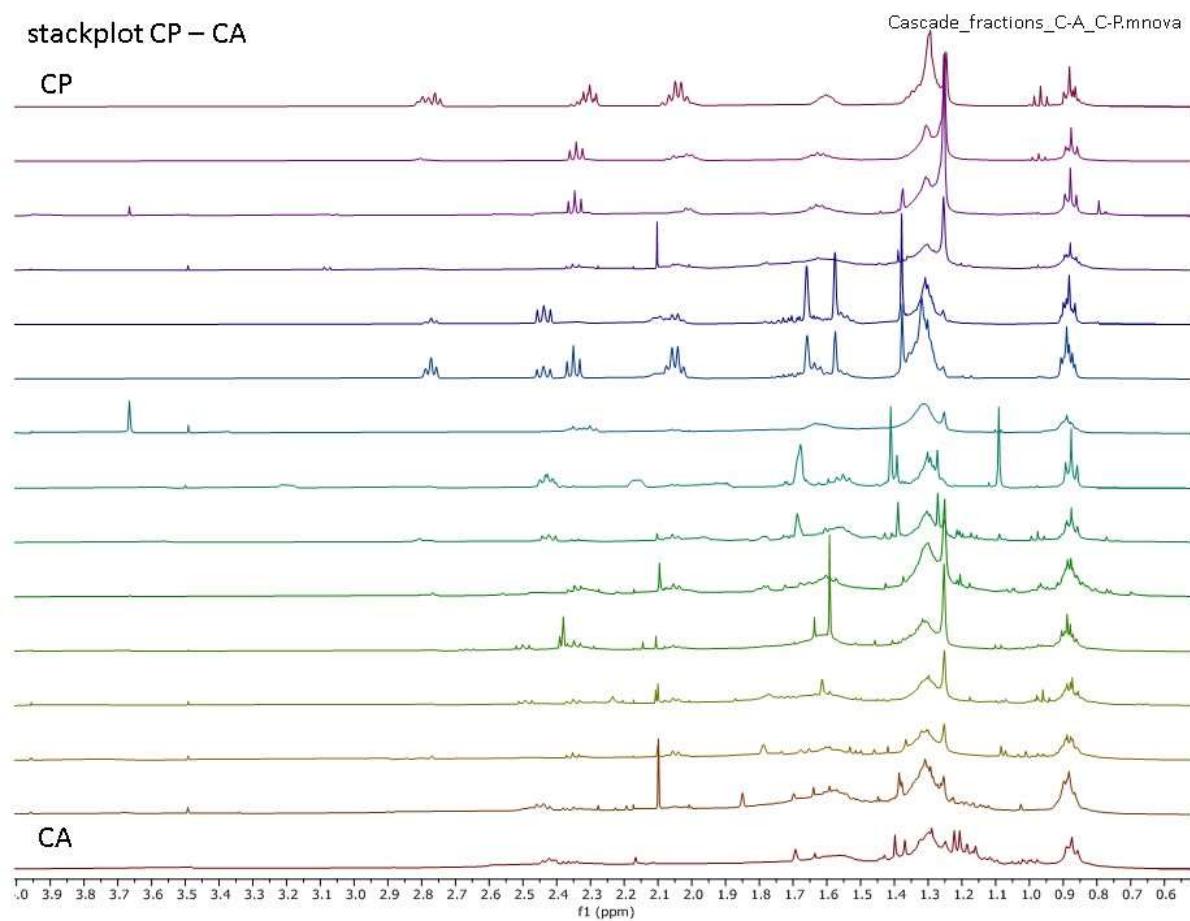
**Figure S17.** Low-frequency region stacked plot of  $^1\text{H}$  NMR spectra (400 MHz,  $\text{CDCl}_3$ ).



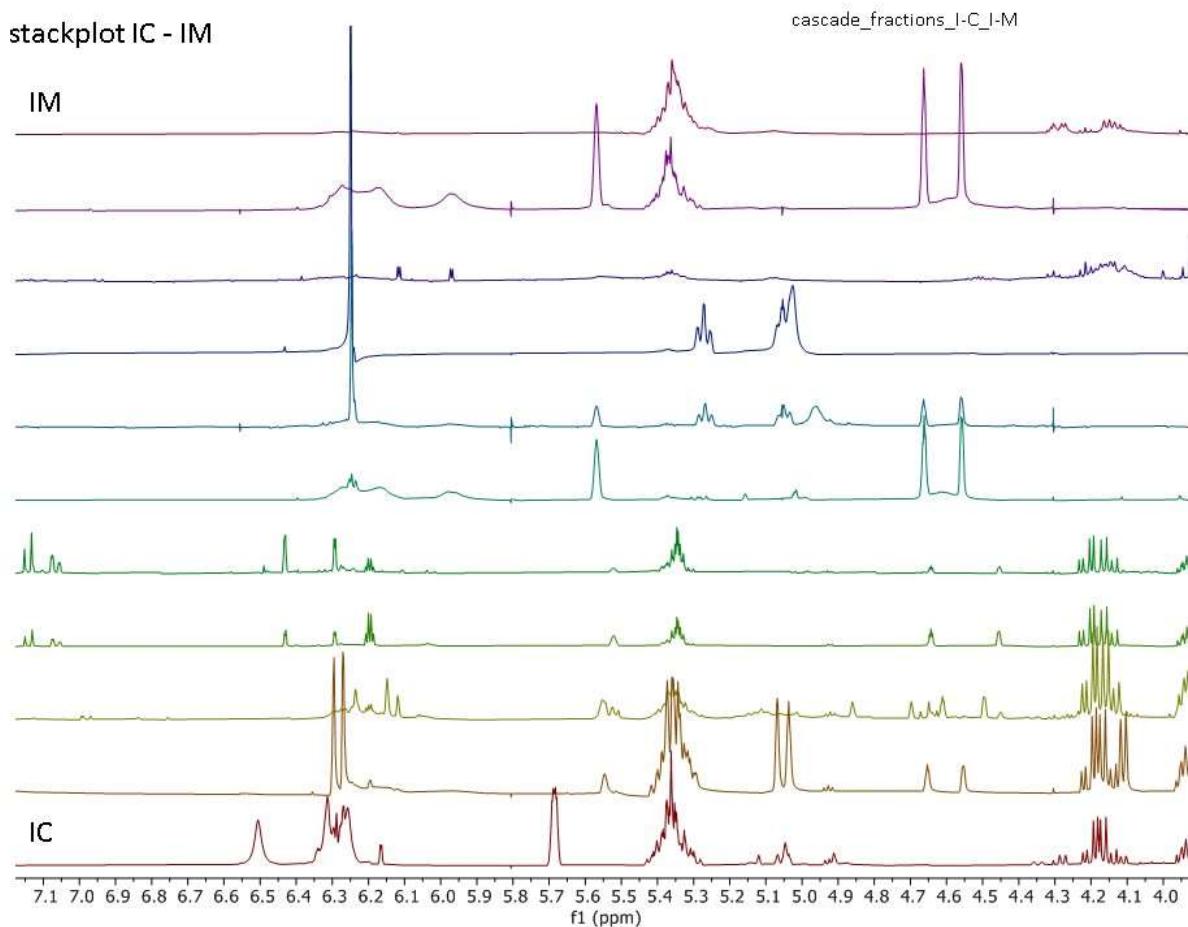
**Figure S18.** High-frequency region stacked plot of  $^1\text{H}$  NMR spectra (400 MHz,  $\text{CDCl}_3$ ).



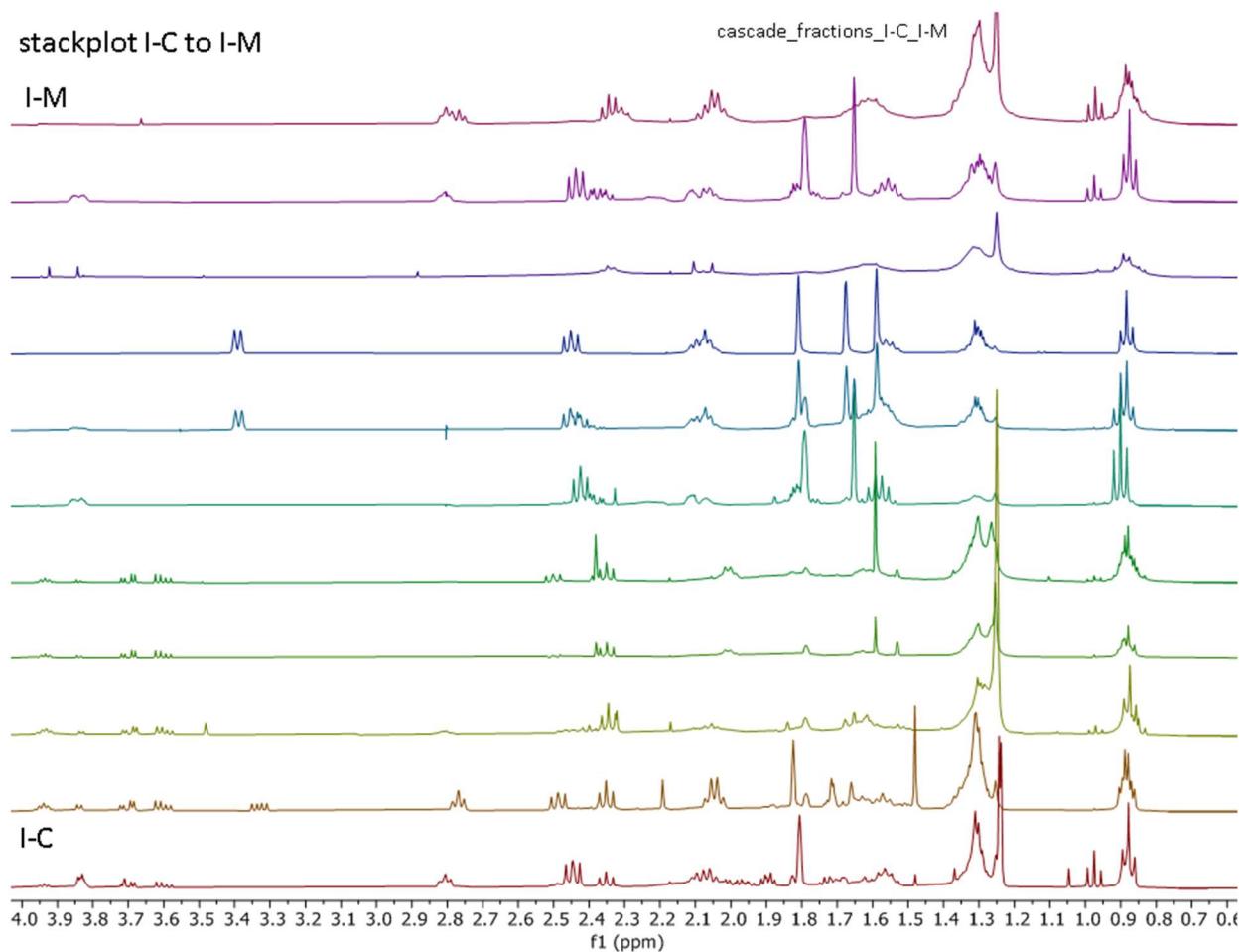
**Figure S19.** Low-frequency region stacked plot of  $^1\text{H}$  NMR spectra (400 MHz,  $\text{CDCl}_3$ ).



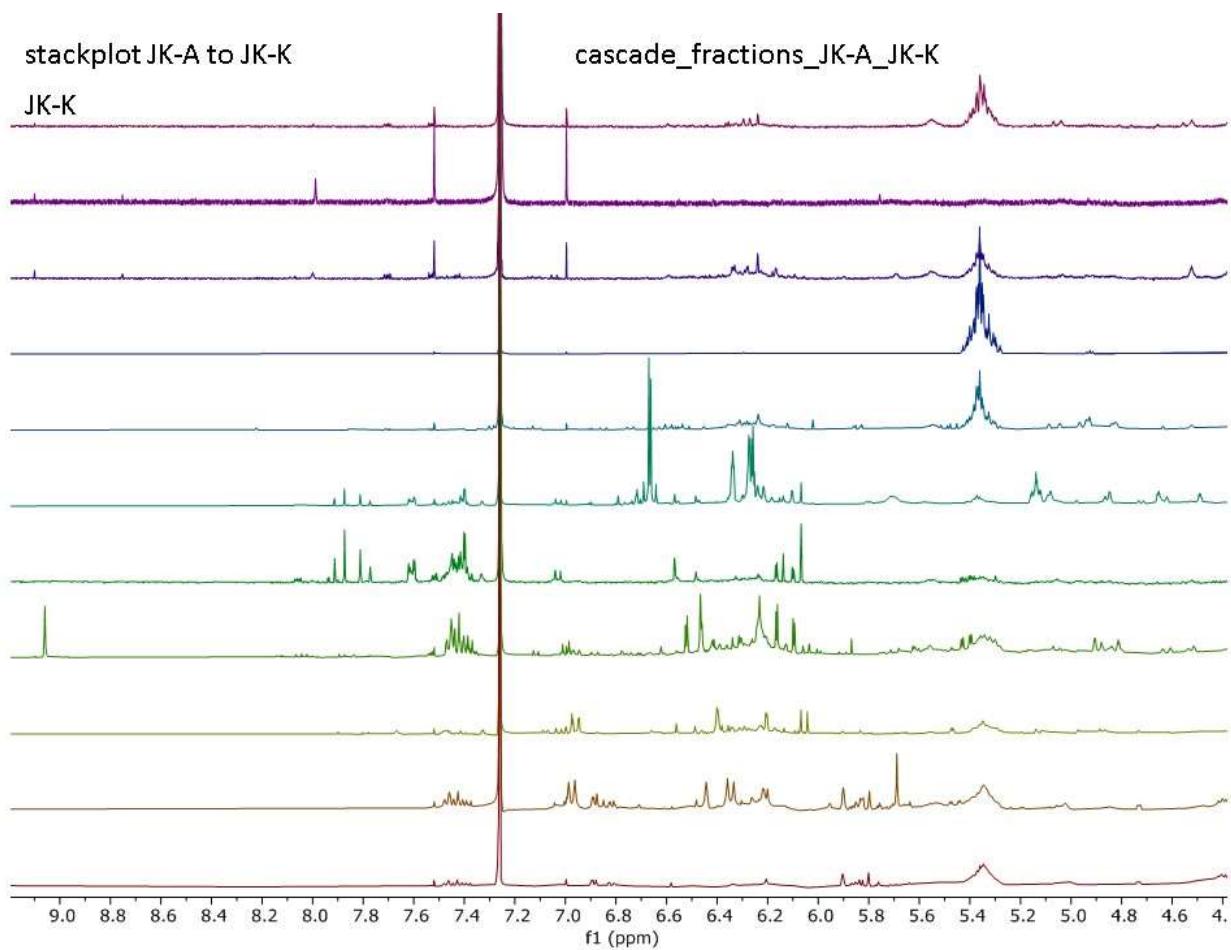
**Figure S20.** High-frequency region stacked plot of  $^1\text{H}$  NMR spectra (400 MHz,  $\text{CDCl}_3$ ).



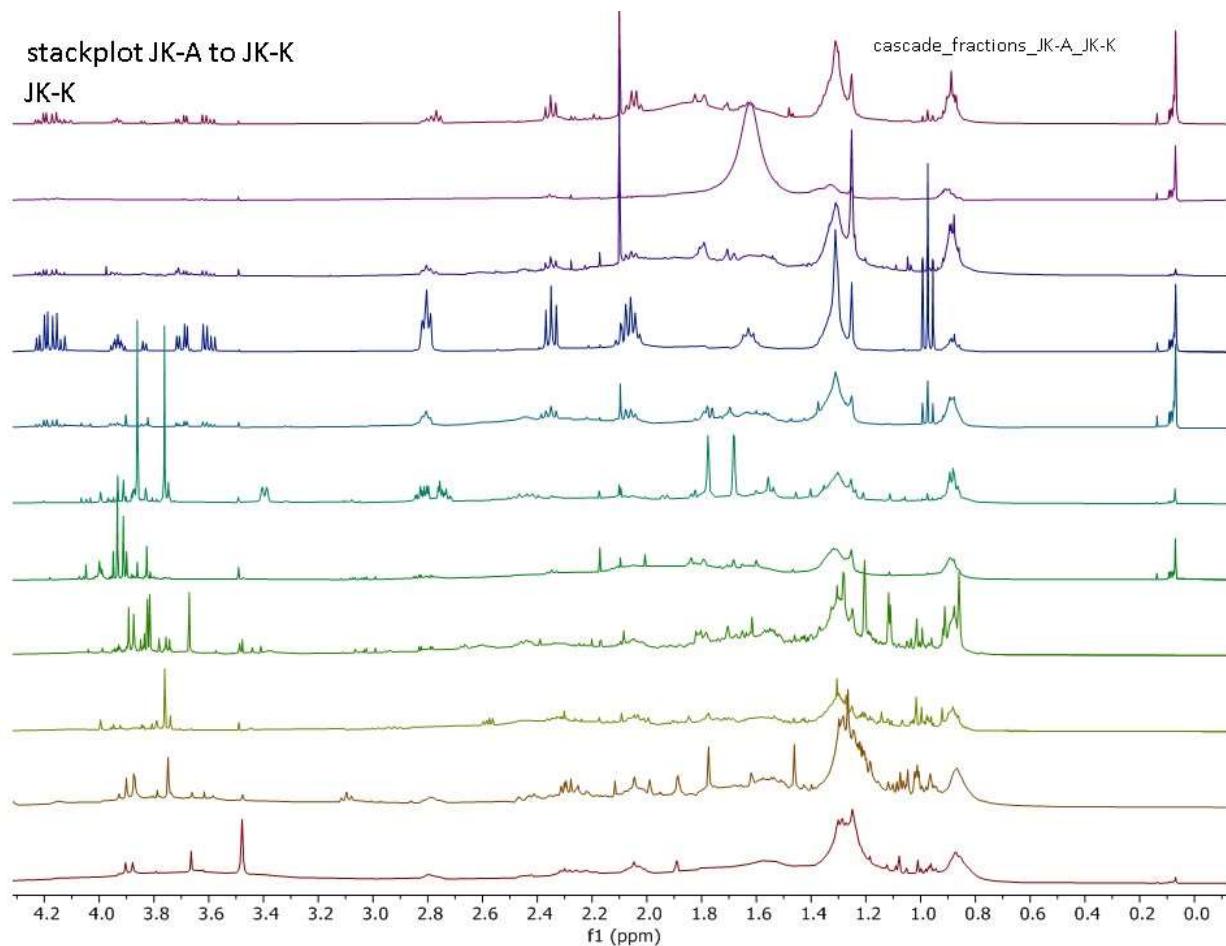
**Figure S21.** Low-frequency region stacked plot of  $^1\text{H}$  NMR spectra (400 MHz,  $\text{CDCl}_3$ ).



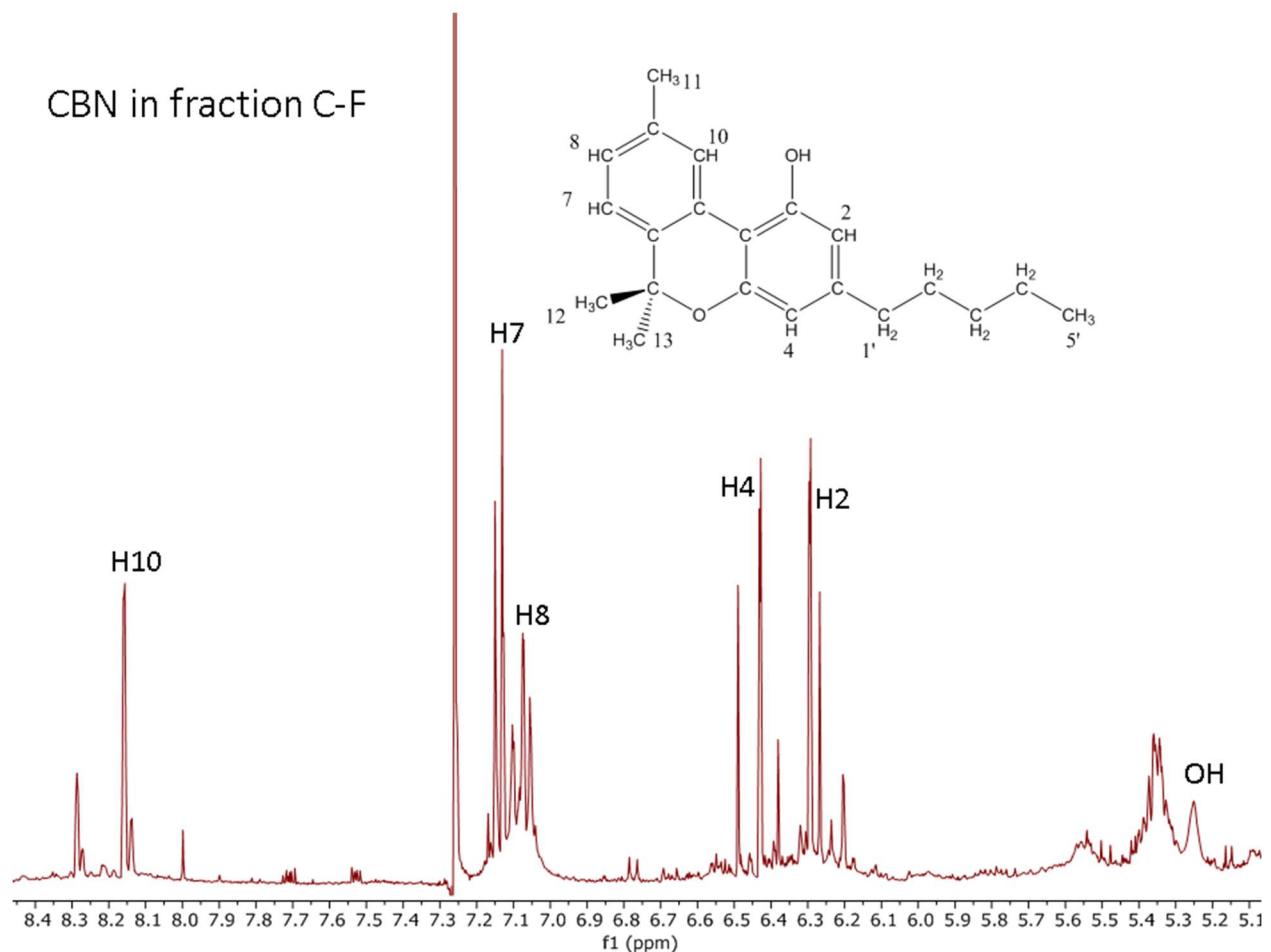
**Figure S22.** High-frequency region stacked plot of  $^1\text{H}$  NMR spectra (400 MHz,  $\text{CDCl}_3$ ).



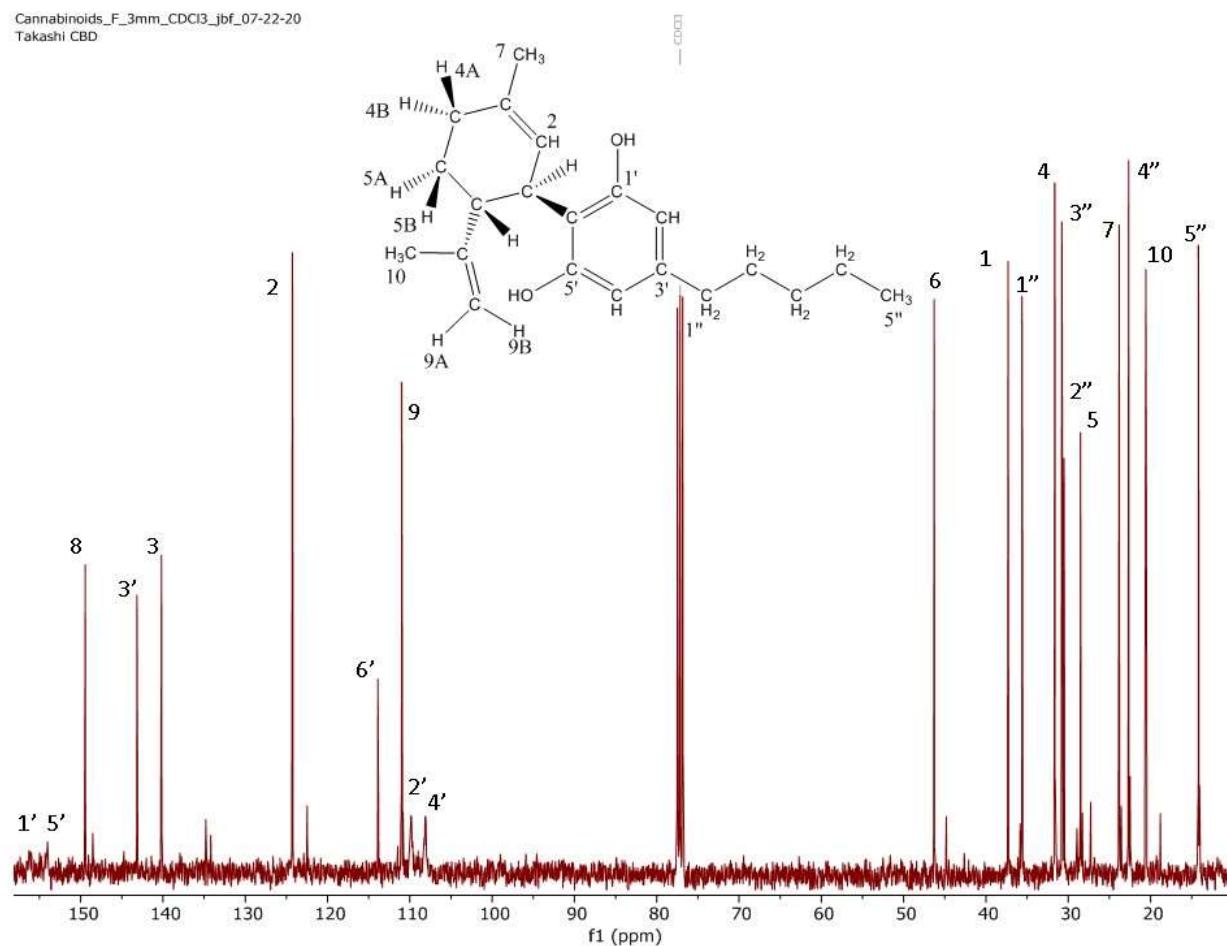
**Figure S23.** Low-frequency region stacked plot of  $^1\text{H}$  NMR spectra (400 MHz,  $\text{CDCl}_3$ ).



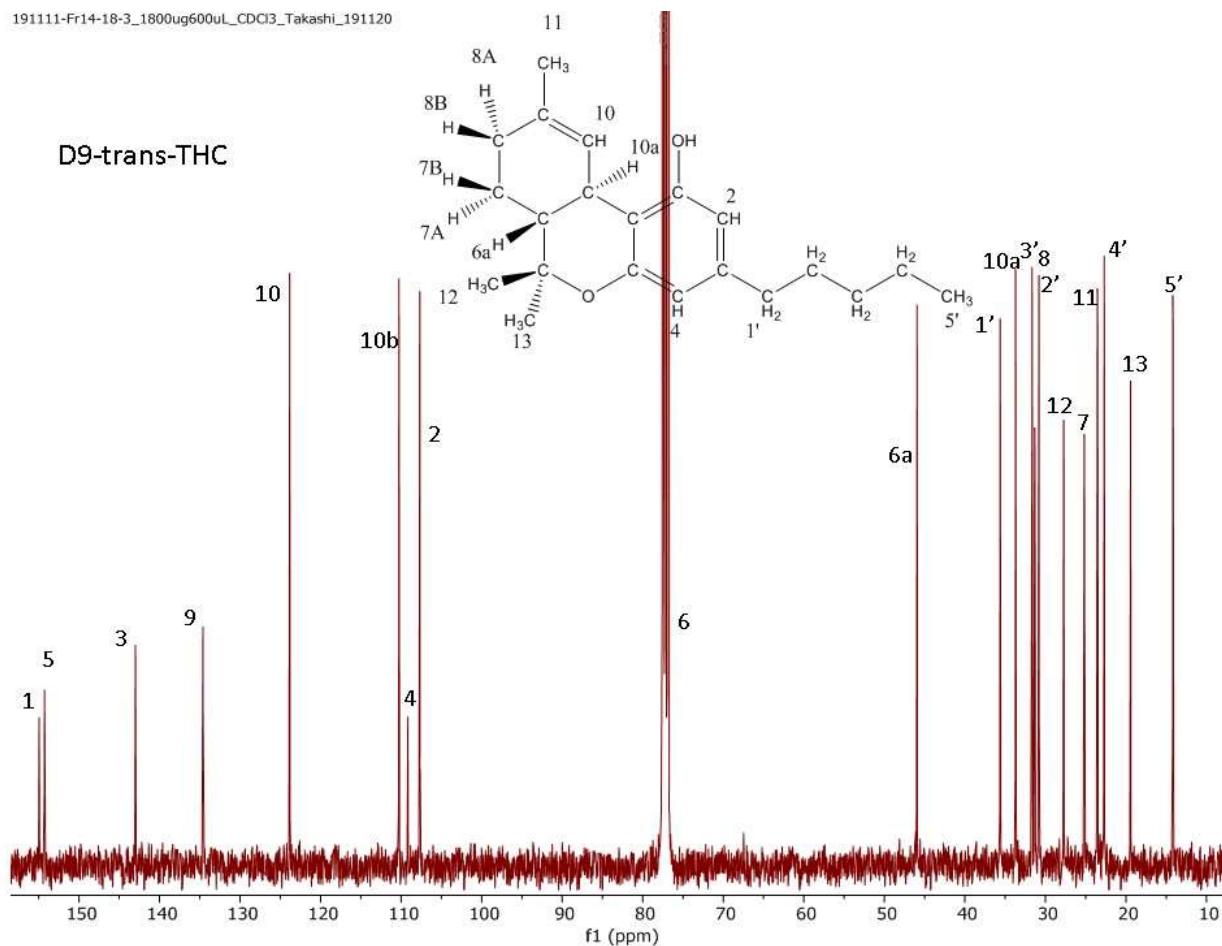
**Figure S24.**  $^1\text{H}$  NMR Spectrum of CBN (**5**) in fraction C-F (400 MHz,  $\text{CDCl}_3$ ).



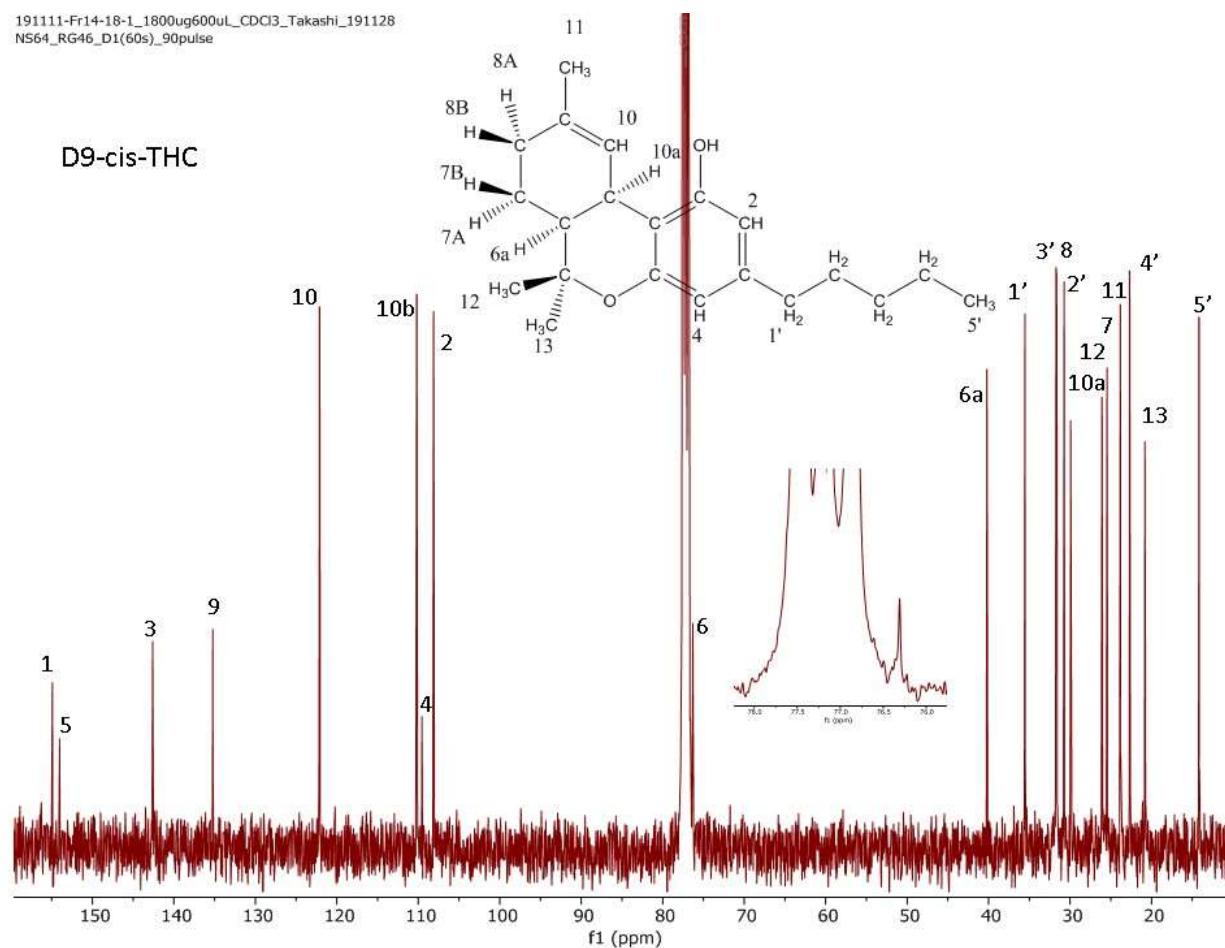
**Figure S25.**  $^{13}\text{C}$  NMR Spectrum of CBD (**1**) (100 MHz,  $\text{CDCl}_3$ ).



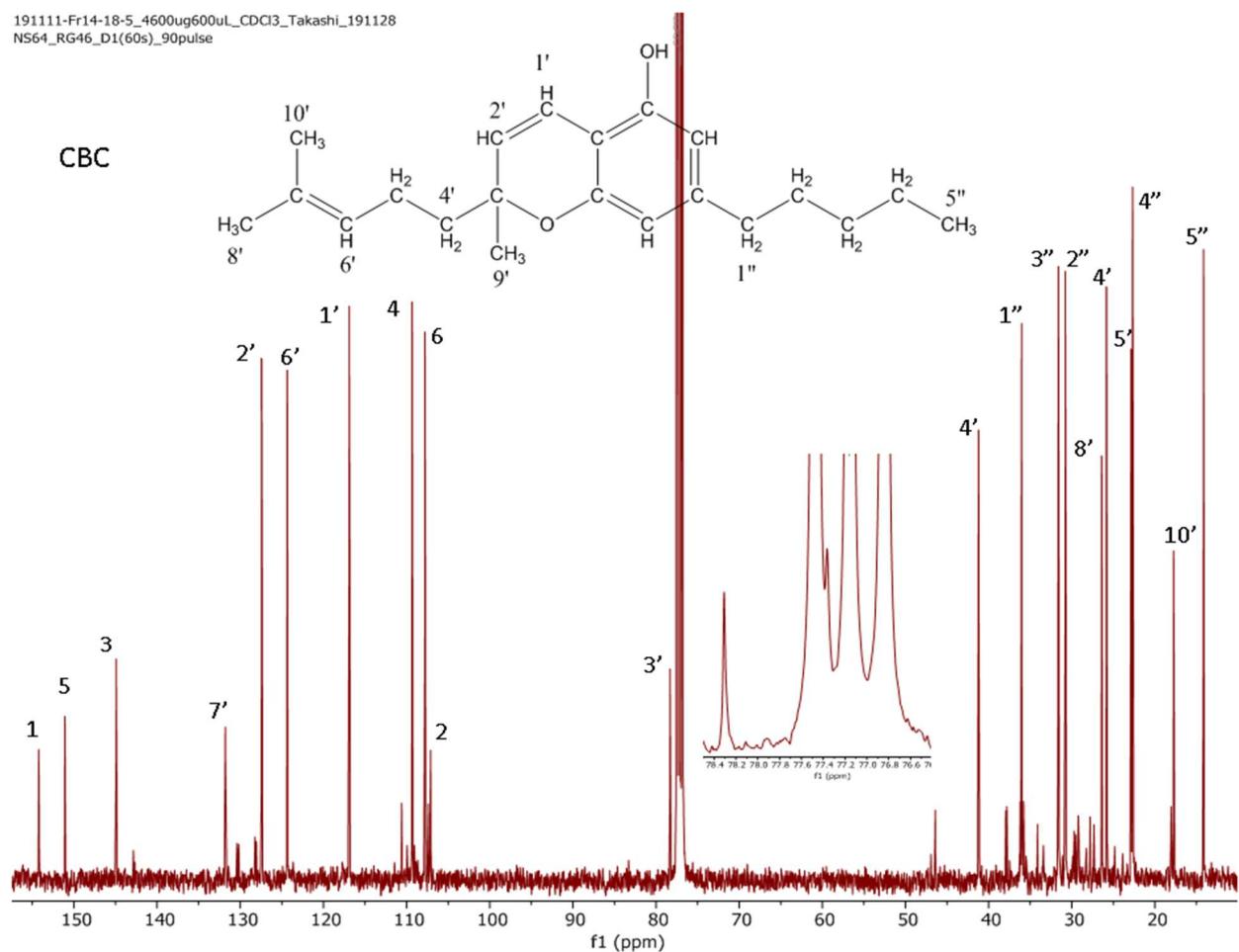
**Figure S26.**  $^{13}\text{C}$  NMR Spectrum of *trans*- $\Delta^9$ -THC (**2a**) (100 MHz,  $\text{CDCl}_3$ ).



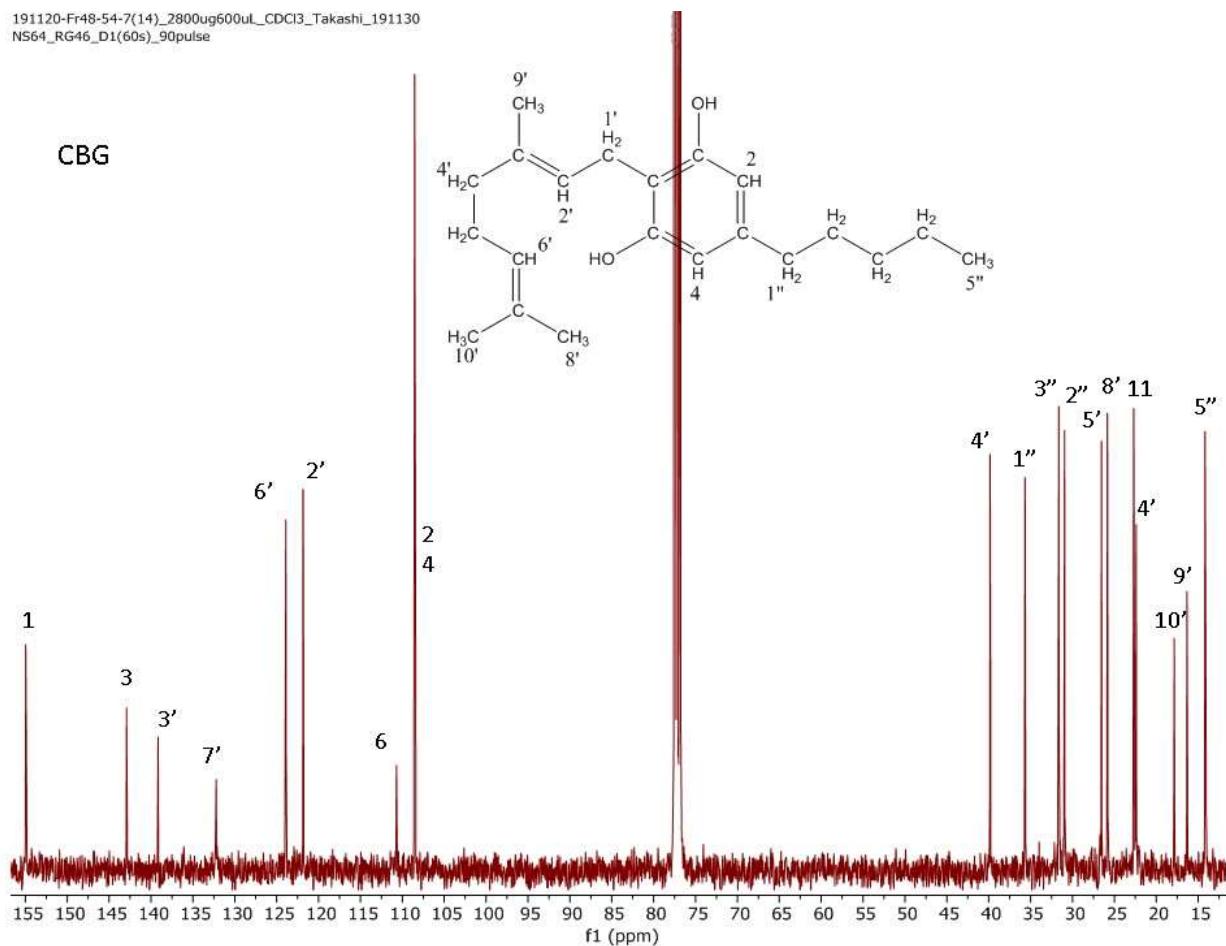
**Figure S27.**  $^{13}\text{C}$  NMR Spectrum of *cis*- $\Delta^9$ -THC (**2b**) (100 MHz,  $\text{CDCl}_3$ ).



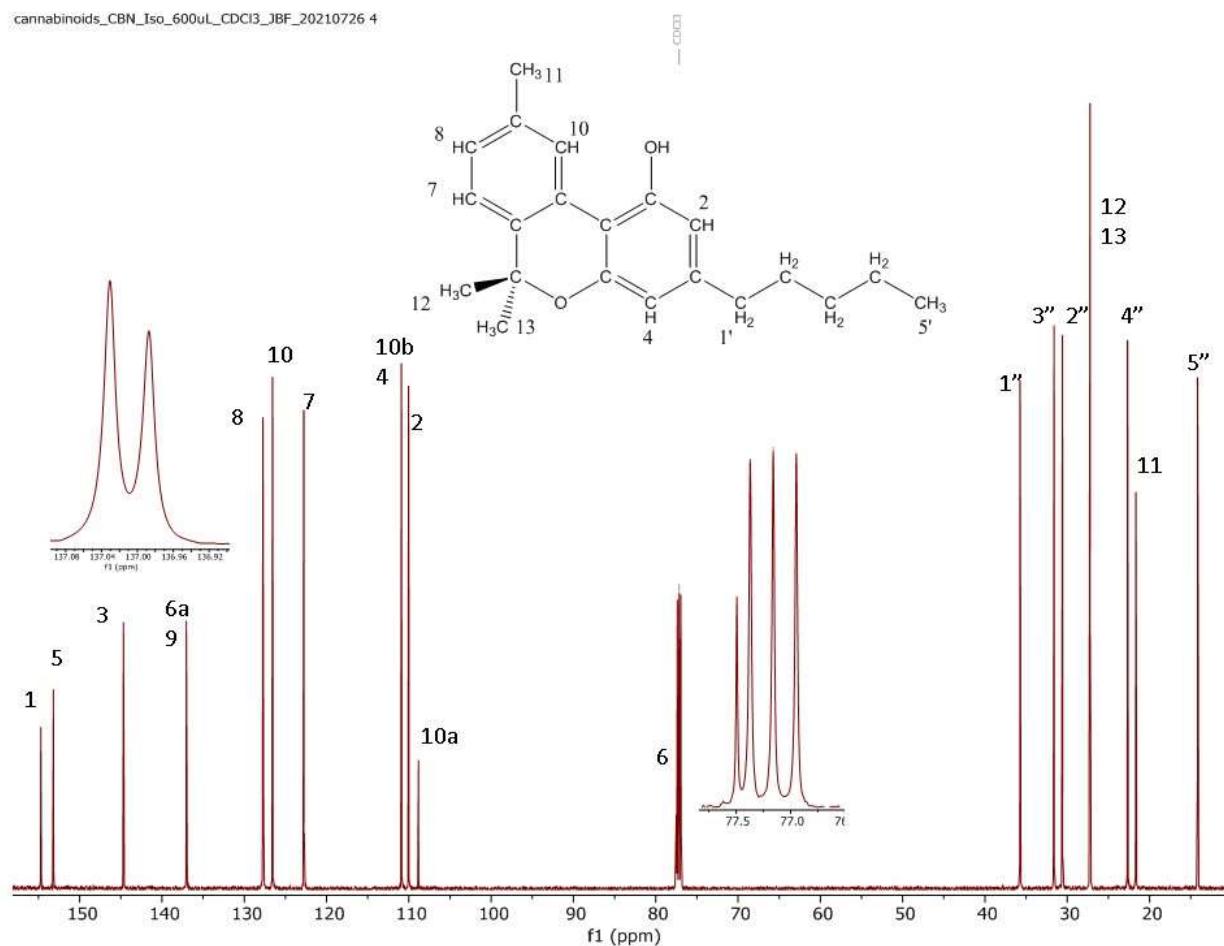
**Figure S28.**  $^{13}\text{C}$  NMR Spectrum of CBC (**3**) (100 MHz,  $\text{CDCl}_3$ ).



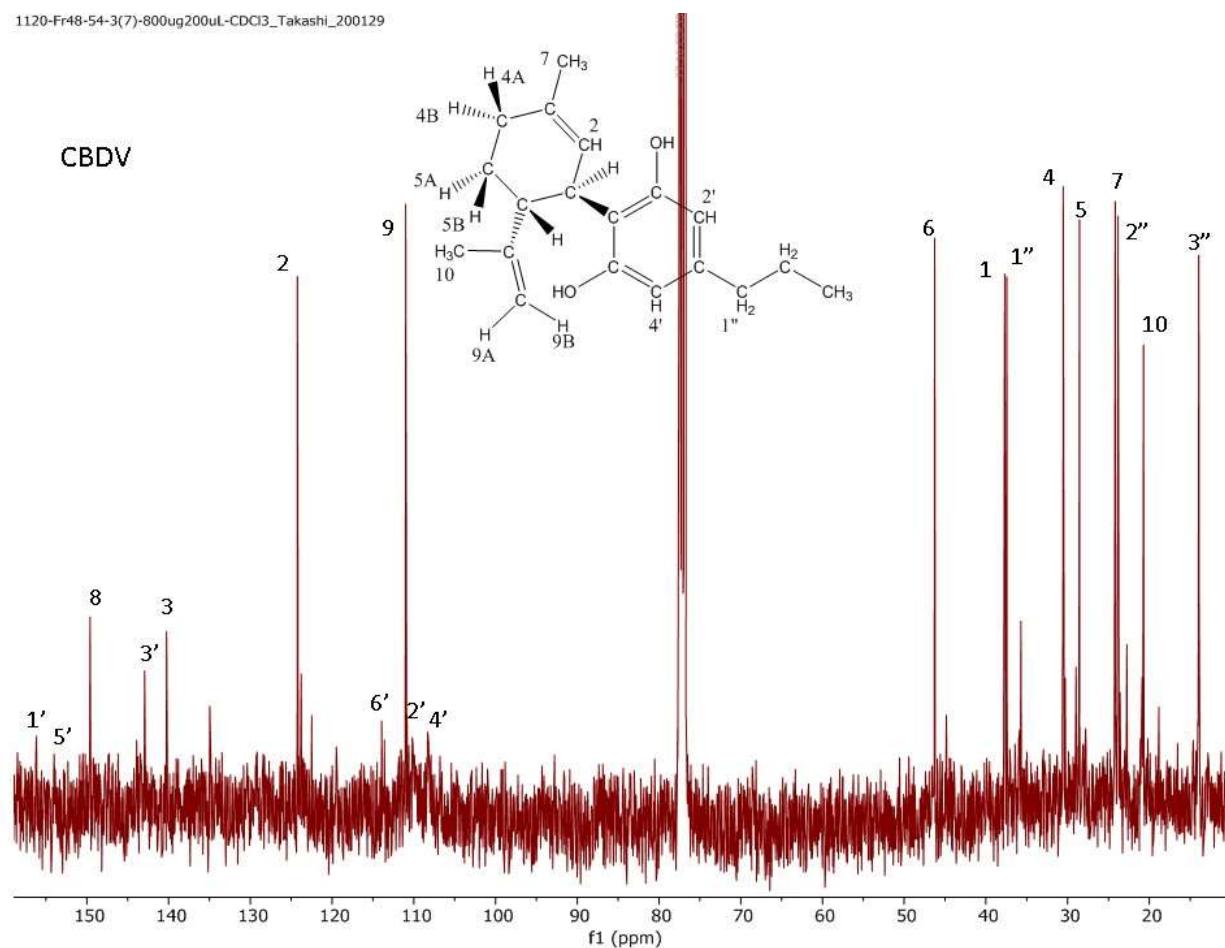
**Figure S29.**  $^{13}\text{C}$  NMR Spectrum of CBG (**4**) (100 MHz,  $\text{CDCl}_3$ ).



**Figure S30.**  $^{13}\text{C}$  NMR Spectrum of CBN (**5**) (100 MHz,  $\text{CDCl}_3$ ).

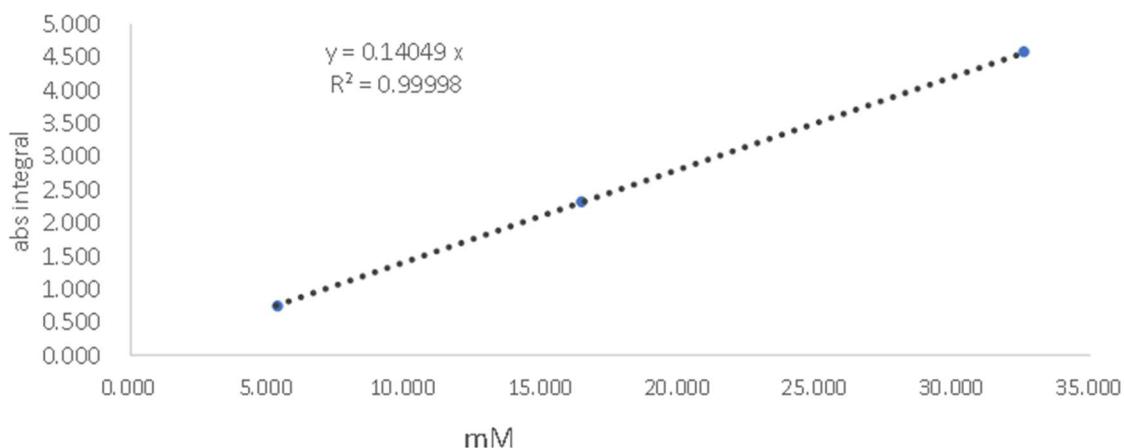


**Figure S31.**  $^{13}\text{C}$  NMR Spectrum of CBDV (**6**) (100 MHz,  $\text{CDCl}_3$ )



**Figure S32.** Calibration Curve for EC DMSO<sub>2</sub>.

Solvent	Class	Tube	File Name	mM	absolute integral value	90pw
	EC1		DMSO2_C_5mm_1659u3300uL	5.335	0.741	7.298
CDCI3	EC2	5mm	DMSO2_C_5mm_1701u1100uL	16.412	2.315	7.262
	EC3		DMSO2_C_5mm_3683u1200uL	32.573	4.573	7.278



**Table S33.** The  $^1\text{H}$  iterative full spin analysis (HiFSA) profiles of CBD (**1**),

Name:	CBD	CHEMICAL SHIFTS (ppm)							COUPLING CONSTANTS (Hz)								
Syssystem	1H	ppm	Syssystem	Name	Shift	Shift	Hz	Syssystem	Name	Shift	Shift	Hz	Syssystem	Name	Shift	Shift	Hz
CBD	1'OH	4.7593	CBD	H1'A,H1'B-H2'A,H2'B	H1'A,H1'B	H2'A,H2'B	8.65										
CBD	5'OH	5.9969	CBD	H1'A,H1'B-H2'A,H2'B	H1'A,H1'B	H2'A,H2'B	6.85										
CBD	H1	3.8582	CBD	H1-H2	H1	H2	2.85										
CBD	H1'A,H1'B	2.4358	CBD	H1-H6	H1	H6	10.28										
CBD	H10	1.6603	CBD	H1-H7	H1	H7	2.49										
CBD	H2	5.5724	CBD	H10-H9A	H10	H9A	-1.37										
CBD	H2'A,H2'B	1.5561	CBD	H10-H9B	H10	H9B	-0.63										
CBD	H2'	6.2730	CBD	H2'A,H2'B-H3'A,H3'B	H3'A,H3'B	H2'A,H2'B	6.01										
CBD	H3'A,H3'B	1.2782	CBD	H2'A,H2'B-H3'A,H3'B	H3'A,H3'B	H2'A,H2'B	9.23										
CBD	H4'A,H4'B	1.3146	CBD	H2'-H1	H1	H2'	1.00										
CBD	H4'	6.1729	CBD	H2'-H4'	H4'	H2'	3.03										
CBD	H4A	2.2345	CBD	H2-H4A	H2	H4A	-1.45										
CBD	H4B	2.0987	CBD	H2-H4B	H2	H4B	1.35										
CBD	H5'	0.8799	CBD	H2-H7	H2	H7	-1.12										
CBD	H5A	1.7848	CBD	H3'A,H3'B-H4'A,H4'B	H4'A,H4'B	H3'A,H3'B	9.53										
CBD	H5B	1.8291	CBD	H3'A,H3'B-H4'A,H4'B	H4'A,H4'B	H3'A,H3'B	6.06										
CBD	H6	2.4026	CBD	H4'A,H4'B-H5'	H5'	H4'A,H4'B	7.34										
CBD	H7	1.7936	CBD	H4'-H1	H1	H4'	1.00										
CBD	H9A	4.6589	CBD	H4A-H5A	H4A	H5A	11.36										
CBD	H9B	4.5573	CBD	H4A-H5B	H4A	H5B	5.21										
H2O	H2O	1.7274	CBD	H4A-H7	H4A	H7	-1.84										
			CBD	H4B-H4A	H4B	H4A	-17.75										
	13C	ppm	CBD	H4B-H5A	H4B	H5A	4.94										
CBD	1'	156.1906	CBD	H4B-H5B	H4B	H5B	2.12										
CBD	5'	154.1038	CBD	H4B-H7	H4B	H7	-1.25										
CBD	8	149.8283	CBD	H5A-H5B	H5A	H5B	-12.88										
CBD	3'	143.1579	CBD	H6-H10	H6	H10	0.00										
CBD	3	140.1739	CBD	H6-H2	H6	H2	0.00										
CBD	2	124.2599	CBD	H6-H5A	H6	H5A	12.35										
CBD	6'	113.8857	CBD	H6-H5B	H6	H5B	2.79										
CBD	9	110.9821	CBD	H6-H9A	H6	H9A	-0.04										
CBD	2'	109.7716	CBD	H6-H9B	H6	H9B	-0.70										
CBD	4'	108.0558	CBD	H9A-H9B	H9A	H9B	2.13										
CBD	6	46.2884															
CBD	1	37.2992															
CBD	1'	35.6023															
CBD	4	31.5024															
CBD	3'	30.7663															
CBD	2'	30.5776															
CBD	5	29.5077															
CBD	7	29.8064															
CBD	4'	22.6625															
CBD	10	20.5676															
CBD	5'	14.1657															

**Table 34.** The  $^1\text{H}$  iterative full spin analysis (HiFSA) profiles of *trans*- $\Delta^9$ -THC (**2b**).

Name: <i>trans</i> -9D-THC							
CHEMICALSHIFTS (ppm)				COUPLING CONSTANTS (Hz)			
Spinsystem	Name	ppm	Spinsystem	Name	Shift	Shift	Hz
t-D9-THC	1(OH)	4.6954	t-D9-THC	H1'A,H1'B-H2'A,H2'B	H2'A,H2'B	H1'A,H1'B	7.81
t-D9-THC	H1'A,H1'B	2.4345	t-D9-THC	H10-H10a	H10	H10a	2.63
t-D9-THC	H10	6.2963	t-D9-THC	H10-H11(Me)	H10	H11(Me)	-1.40
t-D9-THC	H10a	3.1976	t-D9-THC	H10-H6a	H10	H6a	0.60
t-D9-THC	H11(Me)	1.6794	t-D9-THC	H10-H8A	H10	H8A	-0.36
t-D9-THC	H12(Me)	1.4095	t-D9-THC	H10-H8B	H10	H8B	0.38
t-D9-THC	H13(Me)	1.0908	t-D9-THC	H10a-H11(Me)	H10a	H11(Me)	2.21
t-D9-THC	H2	6.1383	t-D9-THC	H2'A,H2'B-H3'A,H3'B	H3'A,H3'B	H2'A,H2'B	7.39
t-D9-THC	H2'A,H2'B	1.5567	t-D9-THC	H2-H10a	H2	H10a	0.31
t-D9-THC	H3'A,H3'B	1.3004	t-D9-THC	H2-H4	H2	H4	0.65
t-D9-THC	H4	6.2687	t-D9-THC	H2-H6a	H2	H6a	-1.19
t-D9-THC	H4'A,H4'B	1.2980	t-D9-THC	H22A-H22B	H4'A,H4'B	H4'A,H4'B	-12.84
t-D9-THC	H5'	0.8777	t-D9-THC	H3'A,H3'B-H4'A,H4'B	H4'A,H4'B	H3'A,H3'B	8.04
t-D9-THC	H6a	1.6904	t-D9-THC	H3'A,H3'B-H5'	H5'	H3'A,H3'B	-0.67
t-D9-THC	H7A	1.9140	t-D9-THC	H4-H10a	H4	H10a	0.32
t-D9-THC	H7B	1.4051	t-D9-THC	H4-H6a	H4	H6a	-1.16
t-D9-THC	H8A	2.1624	t-D9-THC	H5'-H22A	H5'	H4'A,H4'B	7.47
t-D9-THC	H8B	2.1677	t-D9-THC	H6a-H10a	H6a	H10a	10.99
			t-D9-THC	H6a-H12(Me)	H6a	H12(Me)	-0.24
	$^{13}\text{C}$	ppm	t-D9-THC	H6a-H13(Me)	H6a	H13(Me)	-0.14
t-D9-THC	1	154.9373	t-D9-THC	H6a-H7A	H6a	H7A	2.12
t-D9-THC	5	154.2775	t-D9-THC	H6a-H7B	H6a	H7B	12.49
t-D9-THC	3	142.9864	t-D9-THC	H7A-H7B	H7A	H7B	-12.72
t-D9-THC	9	134.6058	t-D9-THC	H7A-H8A	H7A	H8A	3.96
t-D9-THC	10	123.833	t-D9-THC	H7A-H8B	H7A	H8B	3.87
t-D9-THC	10b	110.2634	t-D9-THC	H7B-H8A	H7B	H8A	12.11
t-D9-THC	4	109.1607	t-D9-THC	H7B-H8B	H7B	H8B	5.70
t-D9-THC	2	107.6692	t-D9-THC	H8A-H10a	H8A	H10a	2.43
t-D9-THC	6	76.5461	t-D9-THC	H8A-H11(Me)	H8A	H11(Me)	-0.04
t-D9-THC	6a	45.9371	t-D9-THC	H8A-H8B	H8A	H8B	-14.53
t-D9-THC	1'	35.6163	t-D9-THC	H8B-H10a	H8B	H10a	2.68
t-D9-THC	10a	33.7	t-D9-THC	H8B-H11(Me)	H8B	H11(Me)	-1.04
t-D9-THC	3'	31.6534					
t-D9-THC	8	31.3063					
t-D9-THC	2'	30.7966					
t-D9-THC	12	27.7188					
t-D9-THC	7	25.1574					
t-D9-THC	11	23.5184					
t-D9-THC	4'	22.6904					
t-D9-THC	13	19.4168					
t-D9-THC	5'	14.1605					

**Table S35.** The  $^1\text{H}$  iterative full spin analysis (HiFSA) profiles of *cis*- $\Delta^9$ -THC (**2a**).

Name:	cis-D9-THC			CHEMICALSHIFTS (ppm)				COUPLING CONSTANTS (Hz)			
Spinsystem	Name	ppm		Spinsystem	Name	Shift	Shift	Hz			
cis-D9-THC	H1'A,H1'B	2.4249		cis-D9-THC	H1'A,H1'B-H2'A,H2'B	H1'A,H1'B	H2'A,H2'B	7.86			
cis-D9-THC	H10	6.2074		cis-D9-THC	H10-H10a	H10	H10a	4.91			
cis-D9-THC	H10a	3.5552		cis-D9-THC	H10-H6a	H10	H6a	1.60			
cis-D9-THC	H11(Me)	1.6894		cis-D9-THC	H10-H8A	H10	H8B	-1.56			
cis-D9-THC	H12(Me)	1.3902		cis-D9-THC	H11(Me)-H10	H10	H11(Me)	-1.23			
cis-D9-THC	H13(Me)	1.2725		cis-D9-THC	H11(Me)-H10a	H11(Me)	H10a	1.75			
cis-D9-THC	H2	6.1298		cis-D9-THC	H12(Me)-H6a	H12(Me)	H6a	-0.01			
cis-D9-THC	H2'A,H2'B	1.5612		cis-D9-THC	H13(Me)-H6a	H13(Me)	H6a	0.00			
cis-D9-THC	H3'A,H3'B	1.3421		cis-D9-THC	H2'A,H2'B-H3'A,H3'B	H2'A,H2'B	H3'A,H3'B	12.17			
cis-D9-THC	H4	6.2463		cis-D9-THC	H2-H10a	H2	H10a	0.01			
cis-D9-THC	H4'A,H4'B	1.2888		cis-D9-THC	H2-H4	H2	H4	1.62			
cis-D9-THC	H5'(Me)	0.8779		cis-D9-THC	H3'A,H3'B-H4'A,H4'B	H3'A,H3'B	H4'A,H4'B	10.29			
cis-D9-THC	H6a	1.7238		cis-D9-THC	H4'A,H4'B-H5'(Me)	H5'(Me)	H4'A,H4'B	6.89			
cis-D9-THC	H7B	1.9287		cis-D9-THC	H4-H10a	H4	H10a	0.01			
cis-D9-THC	H7A	1.5201		cis-D9-THC	H6a-H10a	H6a	H10a	5.62			
cis-D9-THC	H8B	1.9943		cis-D9-THC	H7B-H10a	H7B	H10a	1.18			
cis-D9-THC	H8A	1.9786		cis-D9-THC	H7B-H6a	H7B	H6a	2.59			
cis-D9-THC	OH	4.7421		cis-D9-THC	H7A-H7B	H7B	H7A	-13.89			
				cis-D9-THC	H7A-H6a	H7A	H6a	10.56			
				cis-D9-THC	H8B-H11(Me)	H8B	H11(Me)	0.00			
cis-D9-THC	1	154.911		cis-D9-THC	H8B-H7B	H8B	H7B	6.88			
cis-D9-THC	5	154.0197		cis-D9-THC	H8B-H7A	H8B	H7A	17.13			
cis-D9-THC	3	142.6079		cis-D9-THC	H8A-H8B	H8A	H8B	-14.35			
cis-D9-THC	9	135.2224		cis-D9-THC	H8A-H11(Me)	H8A	H11(Me)	-1.47			
cis-D9-THC	10	122.1876		cis-D9-THC	H8A-H7B	H8A	H7B	3.22			
cis-D9-THC	4	110.1727		cis-D9-THC	H8A-H7A	H8A	H7A	3.63			
cis-D9-THC	10b	109.5531									
cis-D9-THC	2	108.1195									
cis-D9-THC	6	76.3101									
cis-D9-THC	6a	40.1938									
cis-D9-THC	1'	35.5383									
cis-D9-THC	3'	31.7179									
cis-D9-THC	8	31.64									
cis-D9-THC	2'	30.7187									
cis-D9-THC	10a	29.9233									
cis-D9-THC	12	26.0725									
cis-D9-THC	7	25.4625									
cis-D9-THC	11	23.8238									
cis-D9-THC	4'	22.6875									
cis-D9-THC	13	20.8053									
cis-D9-THC	5'	14.1596									

**Table S36.** The  $^1\text{H}$  iterative full spin analysis (HiFSA) profiles of CBC (**3**).

Name:	CBC						
CHEMICAL SHIFTS			COUPLING CONSTANTS (Hz)				
Spin system	$\delta$	ppm	Spin system	Name	Shift	Shift	Coupling (Hz)
CBC	1(OH)	4.6221	CBC	H1'A,H1'B-H2'A,H2'B	H2'A,H2'B	H1'A,H1'B	7.75
CBC	H1'A,H1'B	2.4403	CBC	H1'-H2'	H1'	H2'	9.99
CBC	H1'	6.6060	CBC	H8'(Me)-H6'	H8'(Me)	H6'	-0.93
CBC	H8'(Me)	1.6596	CBC	H2'A,H2'B-H3'A	H3'A	H2'A,H2'B	10.86
CBC	H2	6.1161	CBC	H2'A,H2'B-H3'B	H3'B	H2'A,H2'B	5.43
CBC	H2'A,H2'B	1.5557	CBC	H2'-H4'A	H2'	H4'A	-0.01
CBC	H2'	5.4938	CBC	H2'-H4'B	H2'	H4'B	-0.08
CBC	H3'A	13.278	CBC	H2'-H9'(Me)	H2'	H9'(Me)	-0.04
CBC	H3'B	13.046	CBC	H2'-H1'	H2	H1'	0.61
CBC	H4	6.2530	CBC	H2'-H2'	H2	H2'	-0.01
CBC	H4'A,H4'B	1.2985	CBC	H22A-H22B	H4'A,H4'B	H4'A,H4'B	-11.44
CBC	H4'A	1.6462	CBC	H22A-H5'(Me)	H4'A,H4'B	H5'(Me)	7.28
CBC	H4'B	1.7225	CBC	H3'A-H22A	H3'A	H4'A,H4'B	8.49
CBC	H5'(Me)	0.8842	CBC	H3'A-H22B	H3'A	H4'A,H4'B	6.42
CBC	H5'A	2.1052	CBC	H3'A-H3'B	H3'A	H3'B	-10.97
CBC	H5'B	2.0993	CBC	H3'A-H5'(Me)	H3'A	H5'(Me)	-0.08
CBC	H6'	5.0956	CBC	H3'B-H22A	H3'B	H4'A,H4'B	6.24
CBC	H10'(Me)	1.5758	CBC	H3'B-H22B	H3'B	H4'A,H4'B	11.94
CBC	H9'(Me)	1.3782	CBC	H3'B-H5'(Me)	H3'B	H5'(Me)	0.04
H2O	H2O	15.600	CBC	H4'A-H4'B	H4'A	H4'B	-14.12
			CBC	H4'A-H5'A	H4'A	H5'A	11.77
			13C				
			CBC	H4'A-H5'B	H4'A	H5'B	5.20
CBC	1	134.1387	CBC	H4'A-H6'	H4'A	H6'	-0.30
CBC	5	151.1303	CBC	H4'B-H5'A	H4'B	H5'A	3.91
CBC	3	144.8956	CBC	H4'B-H5'B	H4'B	H5'B	13.21
CBC	7'	131.7643	CBC	H4'B-H6'	H4'B	H6'	-0.21
CBC	2'	127.3652	CBC	H4'-H1'	H4	H1'	0.19
CBC	6'	124.3348	CBC	H4-H2	H4	H2	151
CBC	1'	116.9369	CBC	H4-H2'	H4	H2'	-0.02
CBC	4	108.2606	CBC	H5'A-H8'(Me)	H5'A	H8'(Me)	0.68
CBC	2	107.8414	CBC	H5'A-H5'B	H5'A	H5'B	-14.18
CBC	6	107.1392	CBC	H5'A-H6'	H5'A	H6'	6.91
CBC	3'	78.3383	CBC	H5'A-H10'(Me)	H5'A	H10'(Me)	0.36
CBC	4'	41.17	CBC	H5'B-H8'(Me)	H5'B	H8'(Me)	0.87
CBC	1'	36.0274	CBC	H5'B-H6'	H5'B	H6'	7.38
CBC	3'	31.6007	CBC	H5'B-H10'(Me)	H5'B	H10'(Me)	0.38
CBC	2'	30.7567	CBC	H8'(Me)-H10'(Me)	H8'(Me)	H10'(Me)	0.00
CBC	9'	26.3623	CBC	H10'(Me)-H6'	H10'(Me)	H6'	-0.27
CBC	8'	25.7927					
CBC	5'	22.8364					
CBC	4'	22.6615					
CBC	10'	17.7348					
CBC	5'	14.1383					

**Table S37.** The  $^1\text{H}$  iterative full spin analysis (HiFSA) profiles of CBG (4).

Name:	CBG					
CHEMICAL SHIFTS (ppm)			COUPLING CONSTANTS (Hz)			
Spinsystem	Name	ppm	Spinsystem	Shift	Shift	Hz
CBG	H1'A,H1"B	2.4536	CBG	H4,H2	H4,H2	1.80
CBG	H1'A,H1'B	3.3903	CBG	H1"A,H1"B	H1"A,H1"B	-13.28
CBG	H1,H5	4.9645	CBG	H1'A,H1"B	H2'A,H2"B	9.36
CBG	H10'(Me)	1.5897	CBG	H1"A,H1"B	H2'A,H2"B	6.17
CBG	H2"A,H2"B	1.5837	CBG	H2'	H4'A,H4"B	-1.44
CBG	H2'	5.2701	CBG	H2'	H1'A,H1"B	7.10
CBG	H3"A,H3"B	1.3210	CBG	H2'	H9'(Me)	-1.10
CBG	H4"A,H4"B	1.2974	CBG	H2"A,H2"B	H2"A,H2"B	-12.28
CBG	H4'A,H4'B	2.0602	CBG	H2"A,H2"B	H3'A,H3"B	7.93
CBG	H4,H2	6.2478	CBG	H2'A,H2"B	H3'A,H3"B	7.51
CBG	H5"(Me)	0.8853	CBG	H3'A,H3"B	H3'A,H3"B	-13.03
CBG	H5'A,H5'B	2.1035	CBG	H3'A,H3"B	H4'A,H4"B	9.64
CBG	H6'	5.0528	CBG	H3"A,H3"B	H4"A,H4"B	4.78
CBG	H8'(Me)	1.6760	CBG	H4"A,H4"B	H4'A,H4"B	-12.38
CBG	H9'(Me)	1.8100	CBG	H4"A,H4"B	H5'(Me)	7.14
H2O	H2O	1.5579	CBG	H5'A,H5'B	H10'(Me)	0.49
			CBG	H5'A,H5'B	H5'A,H5'B	-13.44
	13C	PPM	CBG	H5'A,H5'B	H6'	6.53
1		154.9569	CBG	H5'A,H5'B	H8'(Me)	1.00
5		154.9569	CBG	H4'A,H4'B	H5'A,H5'B	5.63
3		142.9181	CBG	H4'A,H4'B	H5'A,H5'B	8.93
3'		139.1569	CBG	H4'A,H4'B	H4'A,H4'B	-13.16
7'		132.2154	CBG	H4'A,H4'B	H9'(Me)	-0.17
6'		123.8989	CBG	H4'A,H4'B	H6'	0.00
2'		121.8321	CBG	H6'	H10'(Me)	-1.39
6		110.6944	CBG	H6'	H8'(Me)	-1.44
2		108.5095	CBG	H8'(Me)	H10'(Me)	-0.01
4		108.4281	CBG	H1'A,H1'B	H1'A,H1'B	-18.32
4'		39.8402	CBG	H9'(Me)	H1'A,H1'B	1.02
1''		35.6523				
3''		31.632				
2''		30.938				
5'		26.7293				
8'		25.8206				
1'		22.6897				
4''		22.3993				
10'		17.8447				
9'		16.3366				
5''		14.1678				

**Table S38.** The  $^1\text{H}$  iterative full spin analysis (HiFSA) profiles of CBN (**5**).

Name:	CBN	CHEMICALSHIFTS (ppm)			COUPLING CONSTANTS (Hz)		
Spinsystem	Name	ppm	Spinsystem	Name	Shift	Shift	Hz
CBN	1(OH)	5.3012	CBN	H1'A,H1'B	H1'A,H1'B	H1'A,H1'B	-13.12
CBN	H1'A,H1'B	2.4986	CBN	H1'A-H2'A	H1'A,H1'B	H2'A,H2'B	9.27
CBN	H10	8.1857	CBN	H1'A-H2'B	H1'A,H1'B	H2'A,H2'B	6.23
CBN	H11(Me)	2.3968	CBN	H10-H8	H10	H8	1.81
CBN	H12(Me),H13(Me)	1.6151	CBN	H11(Me)-H10	H11(Me)	H10	-0.65
CBN	H2	6.2831	CBN	H11(Me)-H7	H11(Me)	H7	0.03
CBN	H2'A,H2'B	1.5998	CBN	H11(Me)-H8	H11(Me)	H8	-0.69
CBN	H3'A,H3'B	1.3221	CBN	H2'A-H2'B	H2'A,H2'B	H2'A,H2'B	-13.27
CBN	H4	6.4552	CBN	H2'A-H3'A	H2'A,H2'B	H3'A,H3'B	7.40
CBN	H4'A,H4'B	1.3400	CBN	H2'A-H3'B	H2'A,H2'B	H3'A,H3'B	0.00
CBN	H5'(Me)	0.9036	CBN	H3'A-H3'B	H3'A,H3'B	H3'A,H3'B	-14.60
CBN	H7	7.1563	CBN	H3'A-H4'A	H3'A,H3'B	H4'A,H4'B	4.93
CBN	H8	7.0813	CBN	H3'A-H4'B	H3'A,H3'B	H4'A,H4'B	5.44
H2O	H2O	1.7282	CBN	H3'A-H5'(Me)	H3'A,H3'B	H5'(Me)	0.00
			CBN	H4'A-H4'B	H4'A,H4'B	H4'A,H4'B	-11.78
	13C	ppm	CBN	H4'A-H5'(Me)	H4'A,H4'B	H5'(Me)	7.14
CBN	1	154.7159	CBN	H4-H2	H4	H2	1.63
CBN	5	153.1846	CBN	H7-H10	H7	H10	0.22
CBN	3	144.6768	CBN	H7-H8	H7	H8	7.84
CBN	6a	137.0308					
CBN	9	136.9873					
CBN	8	127.6644					
CBN	10	126.5514					
CBN	7	122.7475					
CBN	10b, 4	110.8925					
CBN	10b, 4	110.8925					
CBN	2	110.0289					
CBN	10a	108.8335					
CBN	6	77.4942					
CBN	1"	35.7244					
CBN	3"	31.5991					
CBN	2"	30.5759					
CBN	12, 13	27.2232					
CBN	12, 13	27.2232					
CBN	4"	22.6611					
CBN	11	21.6534					
CBN	5"	14.1522					

**Table S39.** The  $^1\text{H}$  iterative full spin analysis (HiFSA) profiles of CBDV (**6**).

Name:	CBDV	CHEMICALSHIFTS (ppm)						COUPLING CONSTANTS (Hz)					
Spiystem	Name	ppm	Spiystem	Name	Shift	Shift	Hz						
CBDV	H1	3.8420	CBDV	H1"A,H1"B-H2"A,H2"B	H1"A,H1"B	H2"A,H2"B	7.60						
CBDV	H1"A,H1"B	2.4265	CBDV	H1"A,H1"B-H3"(Me)	H3"(Me)	H1"A,H1"B	0.01						
CBDV	H1'(OH)	5.9652	CBDV	H1-H2'	H1	H2'	0.43						
CBDV	H10(Me)	1.6534	CBDV	H1-H4'	H1	H4'	0.43						
CBDV	H2	5.5702	CBDV	H10(Me)-H9A	H10(Me)	H9A	-1.42						
CBDV	H2"A,H2"B	1.5856	CBDV	H10(Me)-H9B	H10(Me)	H9B	-0.40						
CBDV	H2'	6.2683	CBDV	H2"A,H2"B-H3"(Me)	H3"(Me)	H2"A,H2"B	7.35						
CBDV	H3"(Me)	0.9032	CBDV	H2'-H6	H6	H2'	-0.88						
CBDV	H4'	6.1786	CBDV	H2-H1	H2	H1	1.55						
CBDV	H4A	2.2329	CBDV	H2-H4A	H2	H4A	-0.38						
CBDV	H4B	2.0974	CBDV	H2-H4B	H2	H4B	0.39						
CBDV	H5'(OH)	4.5878	CBDV	H2-H7(Me)	H2	H7(Me)	-0.56						
CBDV	H5A	1.7810	CBDV	H4'-H6	H6	H4'	-0.37						
CBDV	H5B	1.8367	CBDV	H4A-H1	H4A	H1	3.38						
CBDV	H6	2.3938	CBDV	H4A-H5A	H4A	H5A	11.71						
CBDV	H7(Me)	1.7933	CBDV	H4A-H5B	H4A	H5B	5.85						
CBDV	H9A	4.6650	CBDV	H4A-H7(Me)	H4A	H7(Me)	-0.61						
CBDV	H9B	4.5610	CBDV	H4B-H1	H4B	H1	2.67						
H2O	H2O	1.6857	CBDV	H4B-H4A	H4B	H4A	-17.95						
			CBDV	H4B-H5A	H4B	H5A	5.18						
			$^{13}\text{C}$	ppm	CBDV	H4B-H5B	H4B	H5B	2.16				
CBDV	1'	156.0116	CBDV	H4B-H7(Me)	H4B	H7(Me)	-0.30						
CBDV	5'	153.7236	CBDV	H5A-H5B	H5A	H5B	-14.31						
CBDV	8	149.6006	CBDV	H6-H1	H6	H1	10.47						
CBDV	3'	142.9353	CBDV	H6-H10(Me)	H6	H10(Me)	-0.07						
CBDV	3	140.2473	CBDV	H6-H2	H6	H2	0.24						
CBDV	2	124.2339	CBDV	H6-H5A	H6	H5A	12.34						
CBDV	6'	113.921	CBDV	H6-H5B	H6	H5B	2.98						
CBDV	9	110.9781	CBDV	H6-H9A	H6	H9A	-0.46						
CBDV	2'	110.2509	CBDV	H6-H9B	H6	H9B	-0.11						
CBDV	4'	108.1496	CBDV	H7(Me)-H1	H7(Me)	H1	1.32						
CBDV	6	46.2713	CBDV	H9A-H9B	H9A	H9B	0.95						
CBDV	1	37.7068											
CBDV	1"	37.4399											
CBDV	4	30.4463											
CBDV	5	28.5451											
CBDV	7	24.1685											
CBDV	2"	23.5891											
CBDV	10	20.7092											
CBDV	3"	13.873											