Supporting Information

Novel synthesis of C-methylated phytocannabinoids bearing anti-inflammatory properties

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Figure S19 GCMS and purity reports of **(15)**

Figure S20 GCMS and purity reports of **(16)**

Compound	Code name	SMILES
1	**HUM-216**	OC1=C(C)C(CCCCC)=CC(O)=C1[C@@H]2C=C(C)CC[C@H]2C(C)=C
2	**HUM-217**	OC1=C(C)C(CCCCC)=CC(O)=C1[C@@H]2C=C(C)CC[C@H]2C(C)C
3		OC(C=C1CCCCC)=CC(O)=C1[R]
4		CC1=C(C=C(C=C1CCCCC)O)O
5		OC(C(C)=C1CCCCC)=CC(O)=C1C=O
6		OC1=C(C=O)C(O)=CC(CCCCC)=C1C
7		CC1=C(C=C(C(C)=C1CCCCC)O)O
8		OC1=C(C)C(O)=CC(CCCCC)=C1C
9	**HUM-229**	CC1=C[C@@H](C2=C(O)C=C(O)C(C)=C2CCCCC)[C@H](C(C)=C)CC1
10	**HUM-236**	OC1=C(C)C(CCCCC)=C(C)C(O)=C1[C@@H]2C=C(C)CC[C@H]2C(C)=C
11	**HUM-218**	OC1=C(C)C(CCCCC)=CC(O)=C1C/C=C(C)/CC/C=C(C)\C
12		CC(C(CCCCC)=C(C/C=C(C)/CC/C=C(C)\C)C(O)=C1)=C1O
13	**HUM-237**	C/C(C)=C/CCC1(C)OC2=CC(CCCCC)=C(C)C(O)=C2C=C1
14	**HUM-238**	C/C(C)=C/CCC1(C)OC2=C(C)C(CCCCC)=CC(O)=C2C=C1
15	**HUM-219**	CC(CC[C@H]1C(C)=C)=C[C@H]1C2=C(OC)C=C(CCCCC)C(C)=C2OC
16	**HUM-235**	C/C(CC/C=C(C)/C)=C\CC1=C(OC)C=C(CCCCC)C(C)=C1OC

Table S1. Code names and SMILES for compounds.

2D NMR spectra of compounds 13 and 14

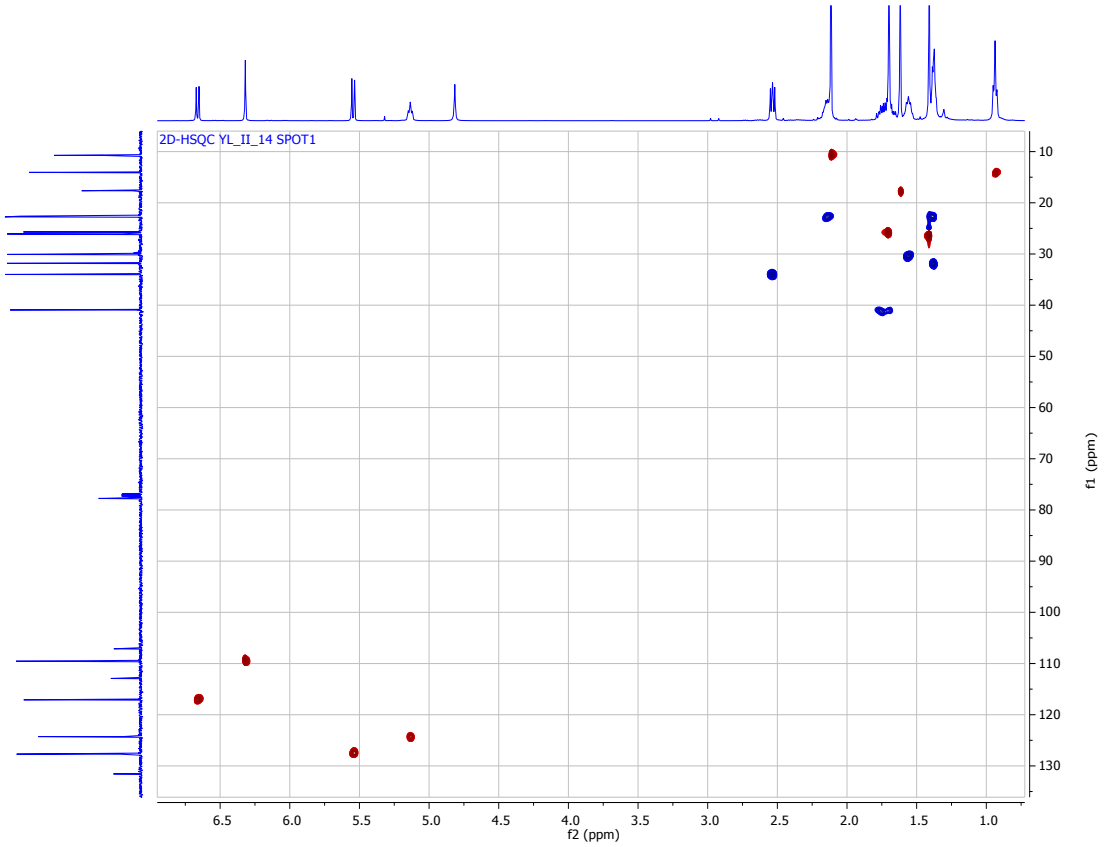


Figure S1. HSQC experiment of (13). Odd protons in red and even numbers in blue.

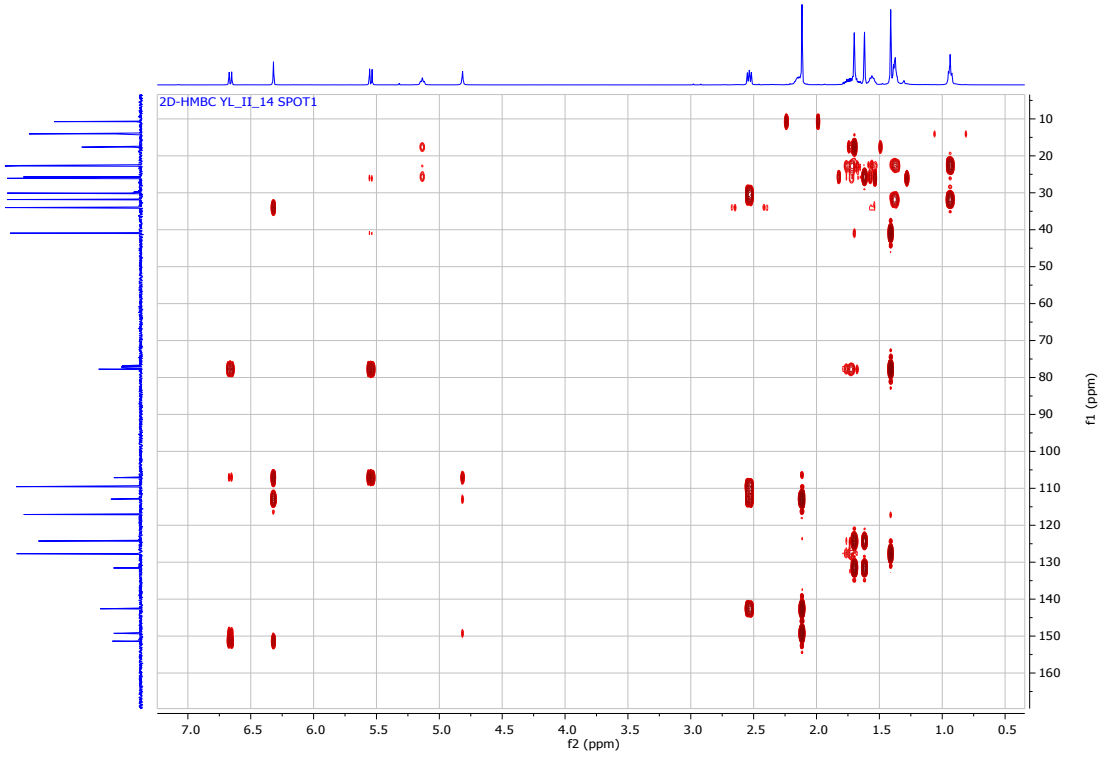


Figure S2. HMBC experiment of (13)

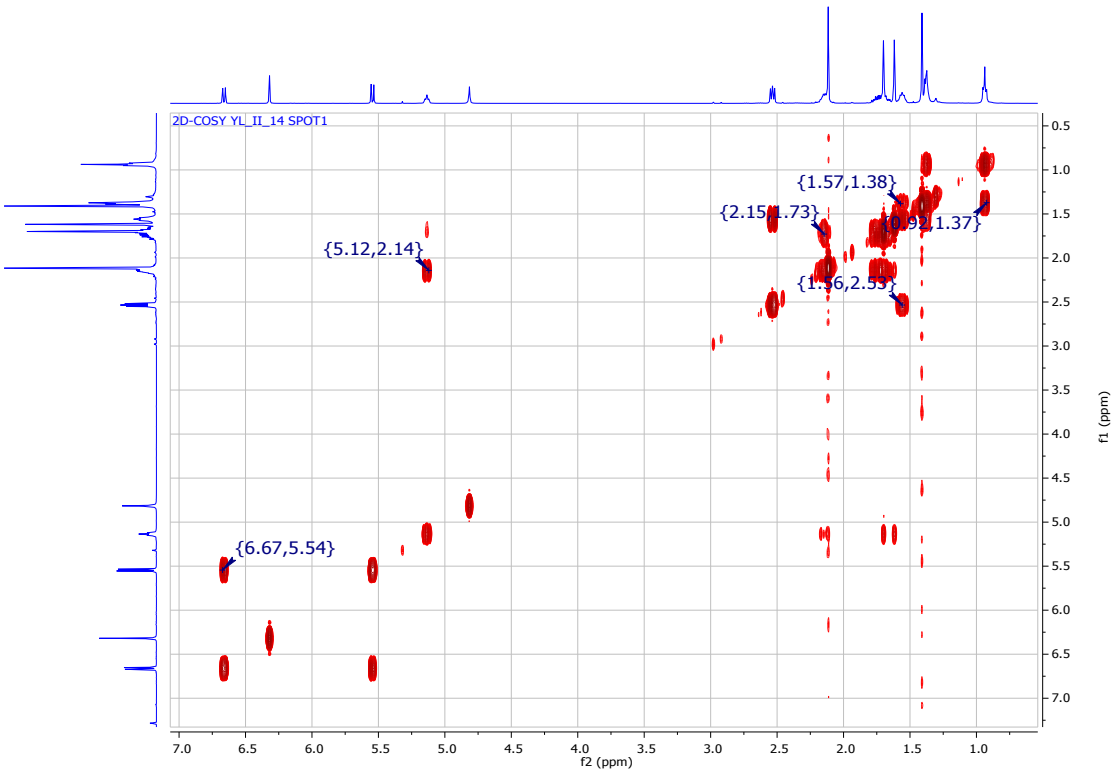


Figure S3. 2D-COSY of (13)

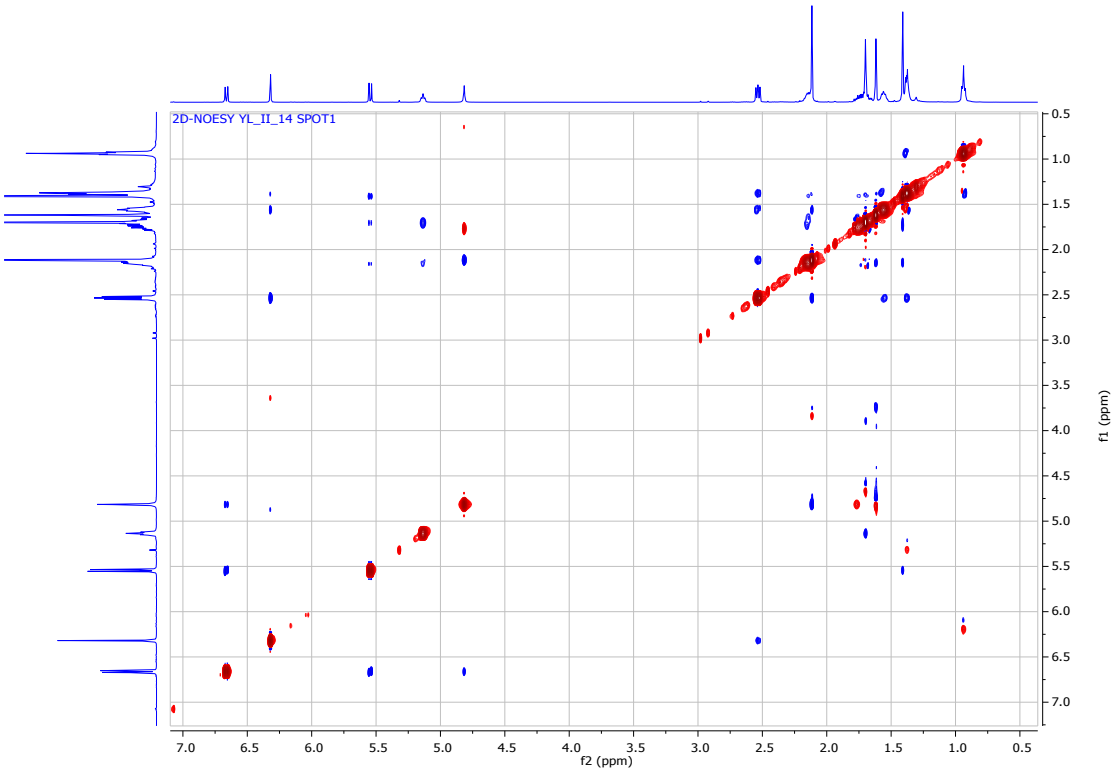


Figure S4. 2D-NOSEY of (13)

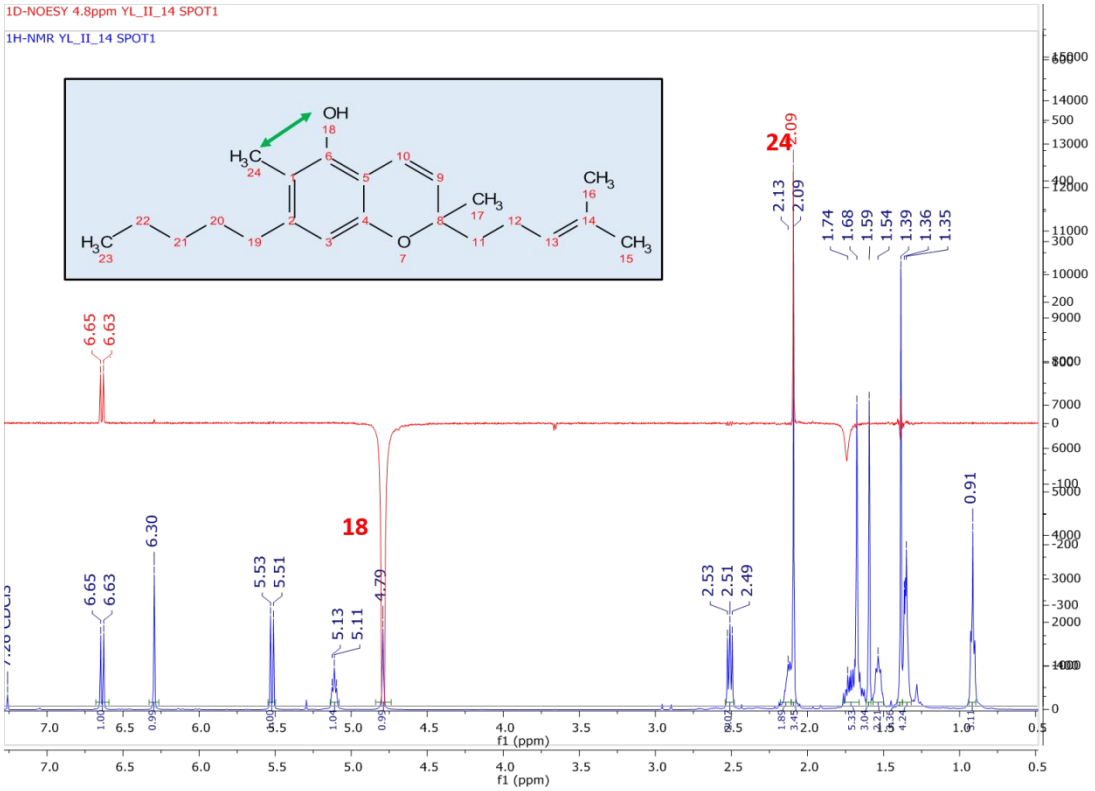


Figure S5. 1D-NOSEY of (13) in Red and ^{1}H NMR in Blue. The focus is on the phenolic proton (pick is turning downwards). The highlighted protons after the pulse are turning upwards. The conclusion is illustrated on the structure as shown in the green arrow.

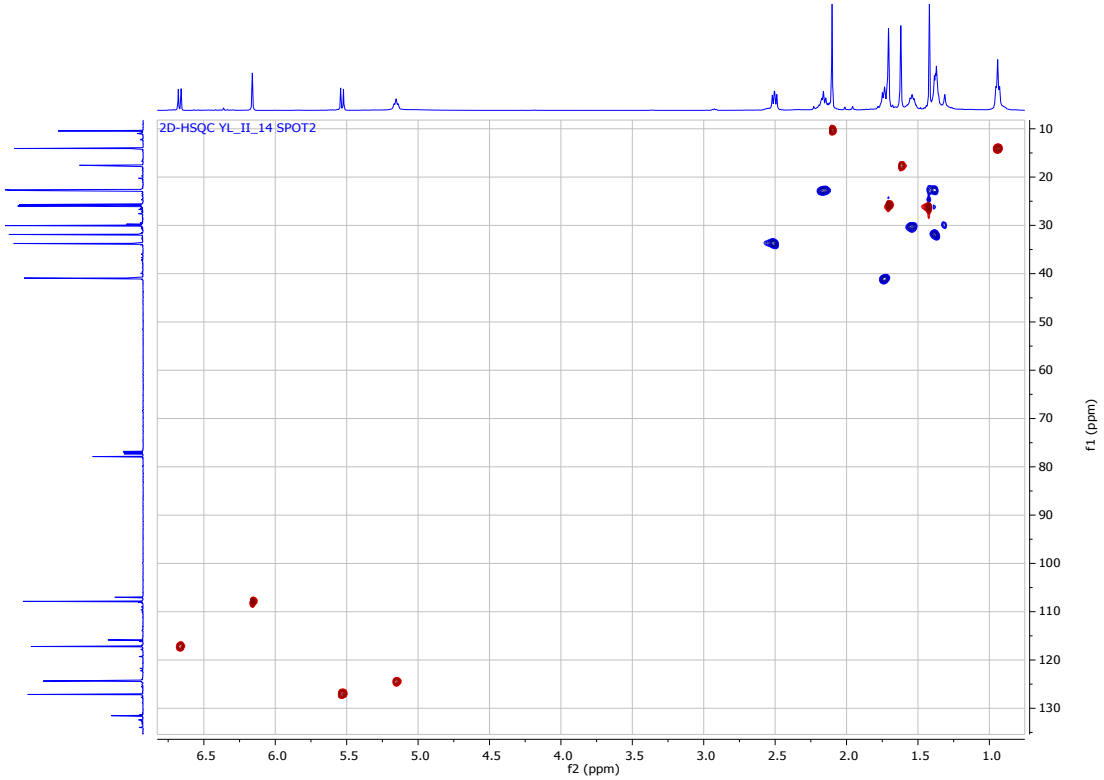


Figure S6. HSQC experiment for (14). Odd numbered nuclei in Red and even number nuclei in Blue.

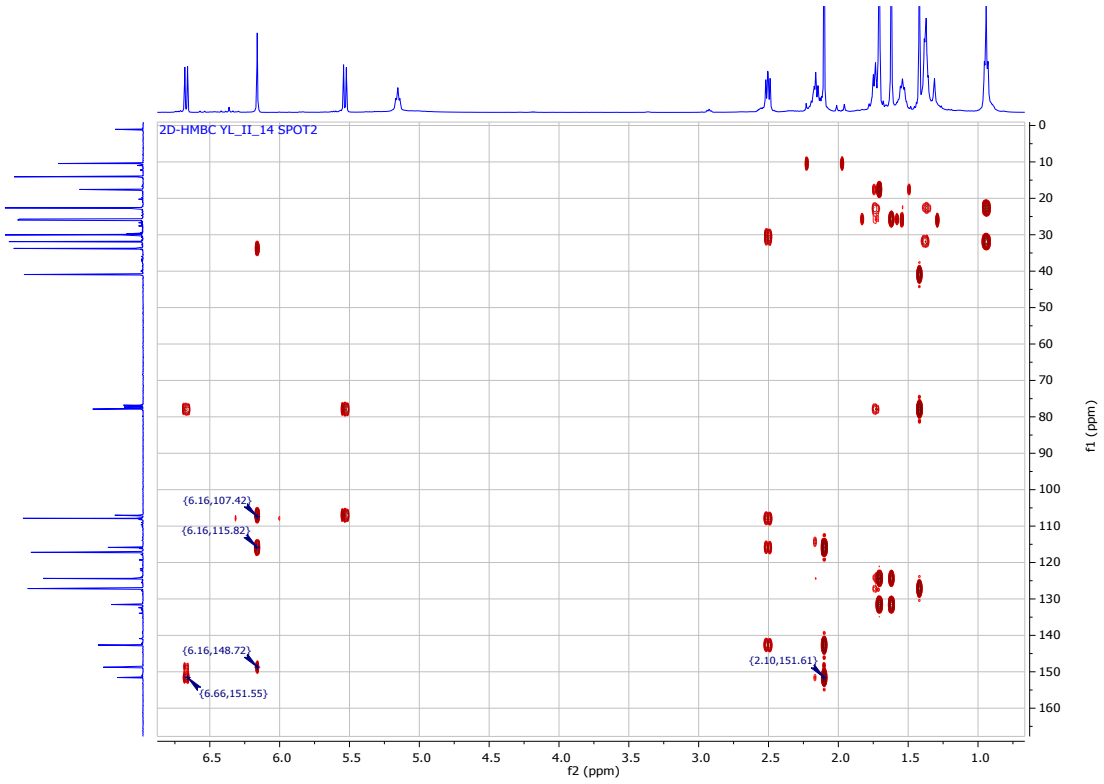


Figure S7. HMBC experiment of (14)

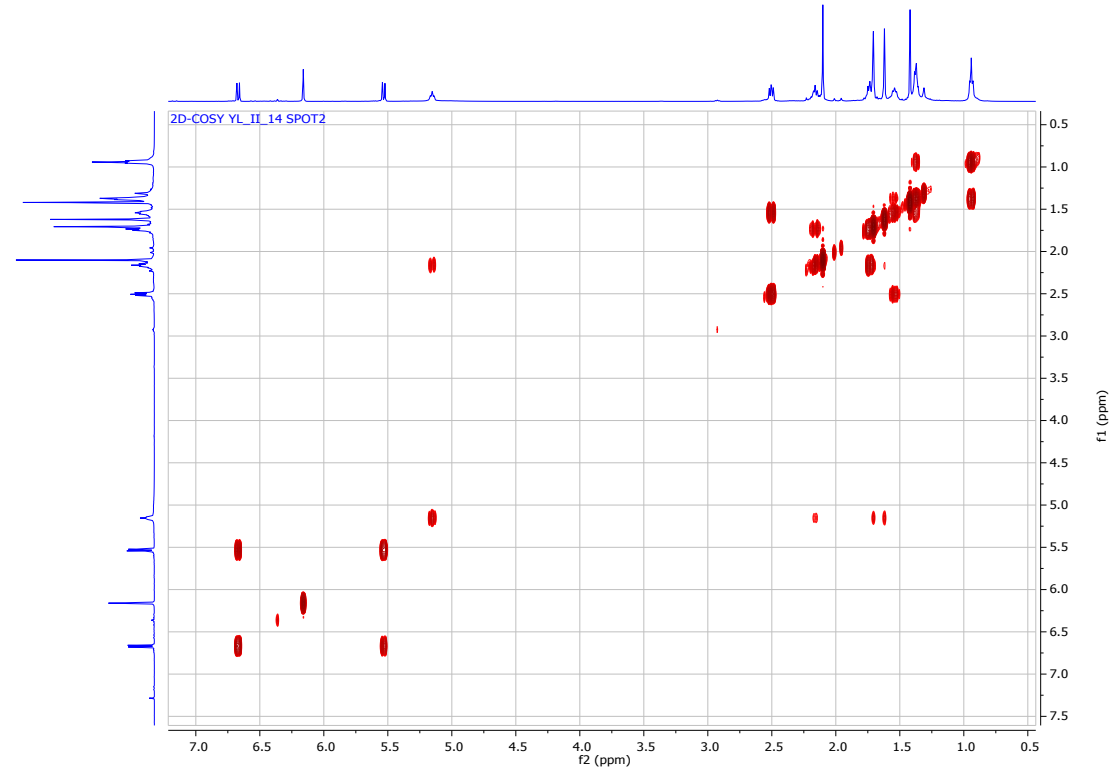


Figure S8. 2D-COSY of (14)

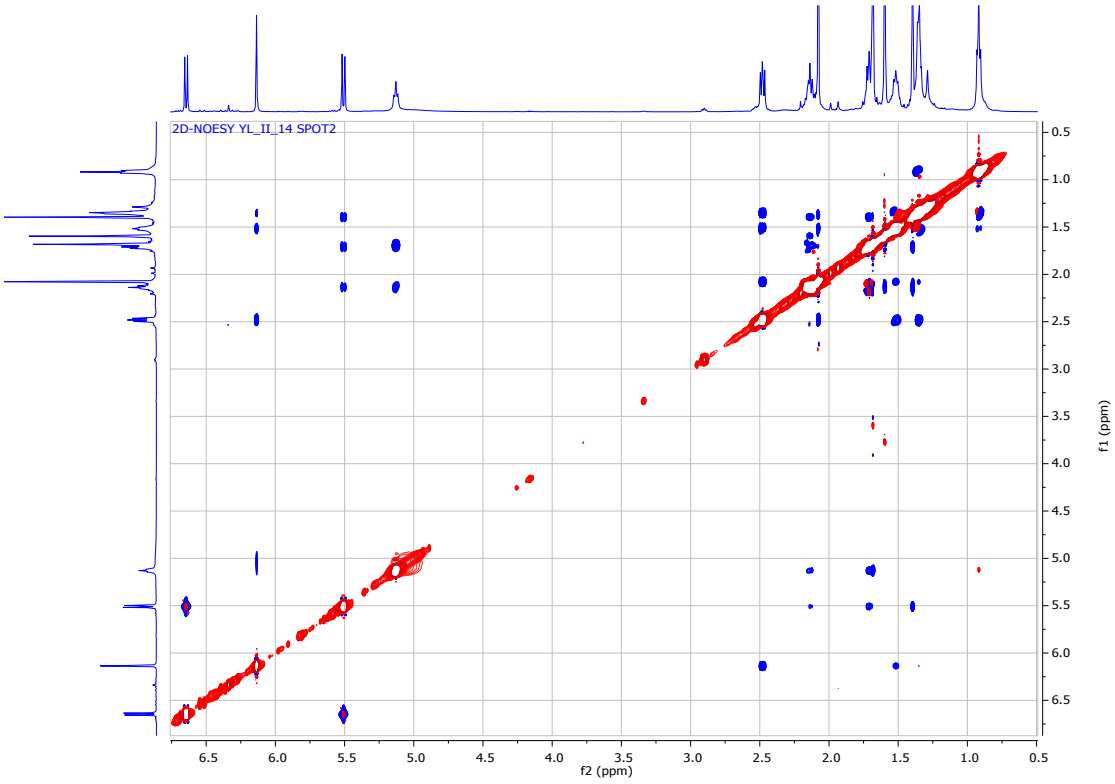


Figure S9. 2D-NOESY of (14)

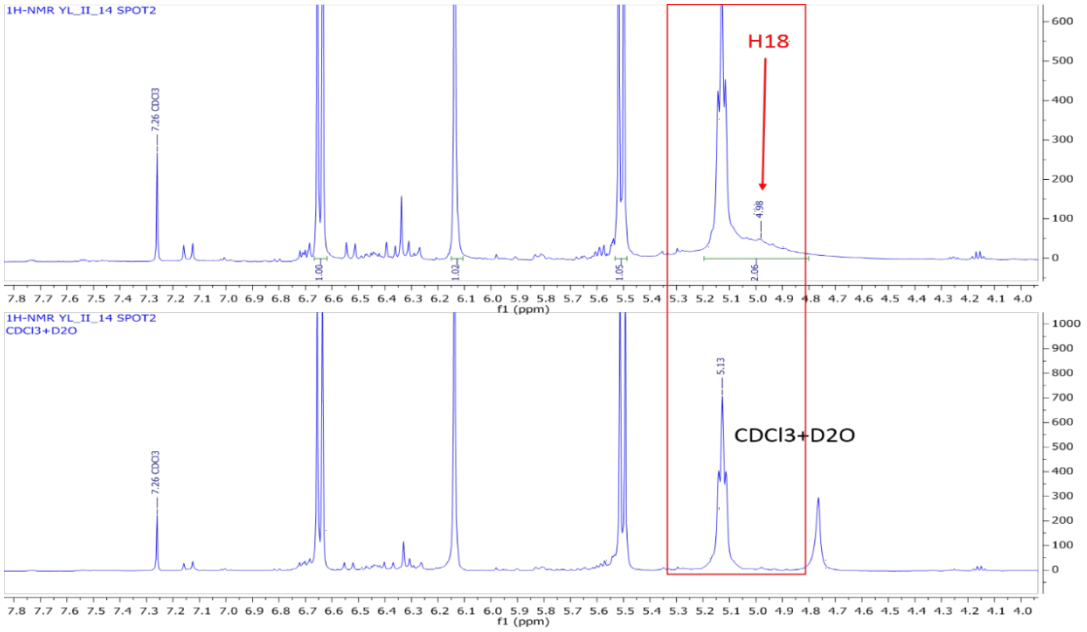


Figure S10. ^{1}H NMR of (14) with focus between 4.0 and 7.5 ppm. The upper spectrum is with $CDCl_3$ as solvent and the lower spectrum is with an addition of a small quantity of D_2O. Highlighted in the red rectangle is the phenolic proton.

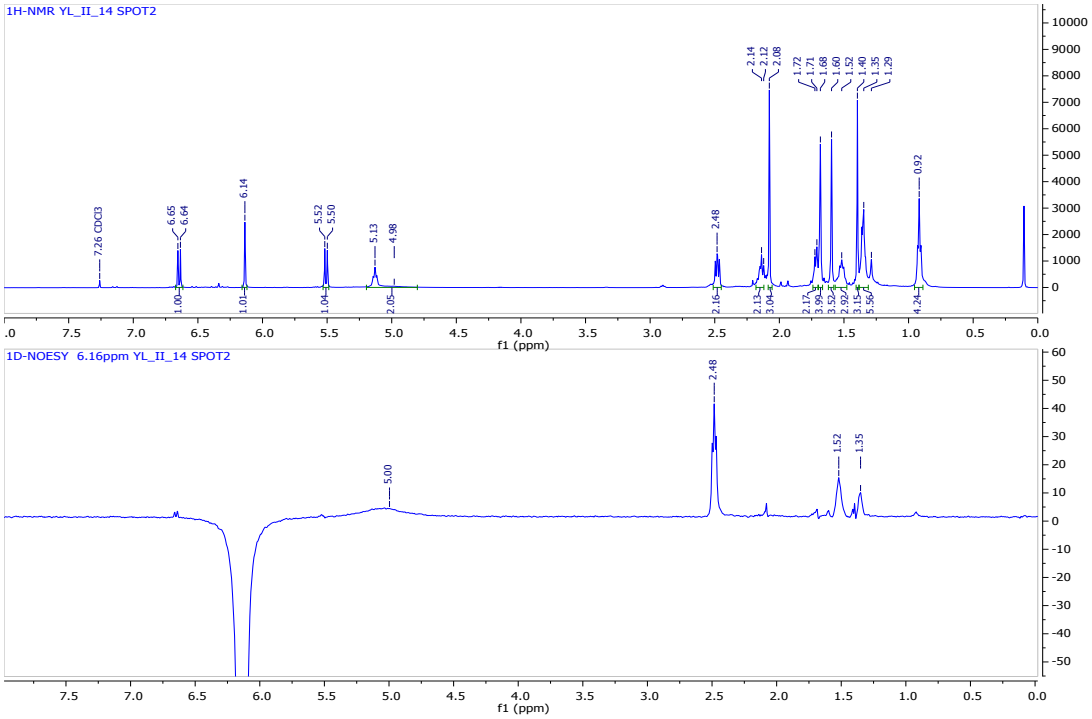


Figure S11. 1D-NOSEY of (14) coupled to ^{1}H NMR of the compound. The focus is on the aromatic proton (turning downwards)

GCMS and purity reports of phytocannabinoid derivatives

Compound (1)

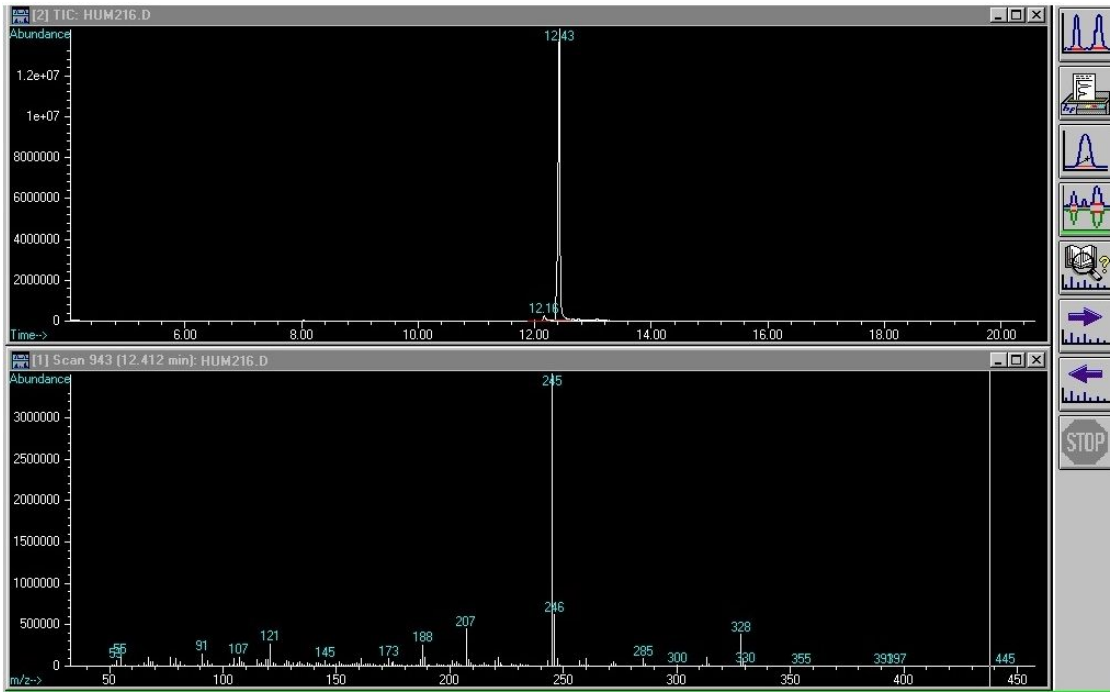


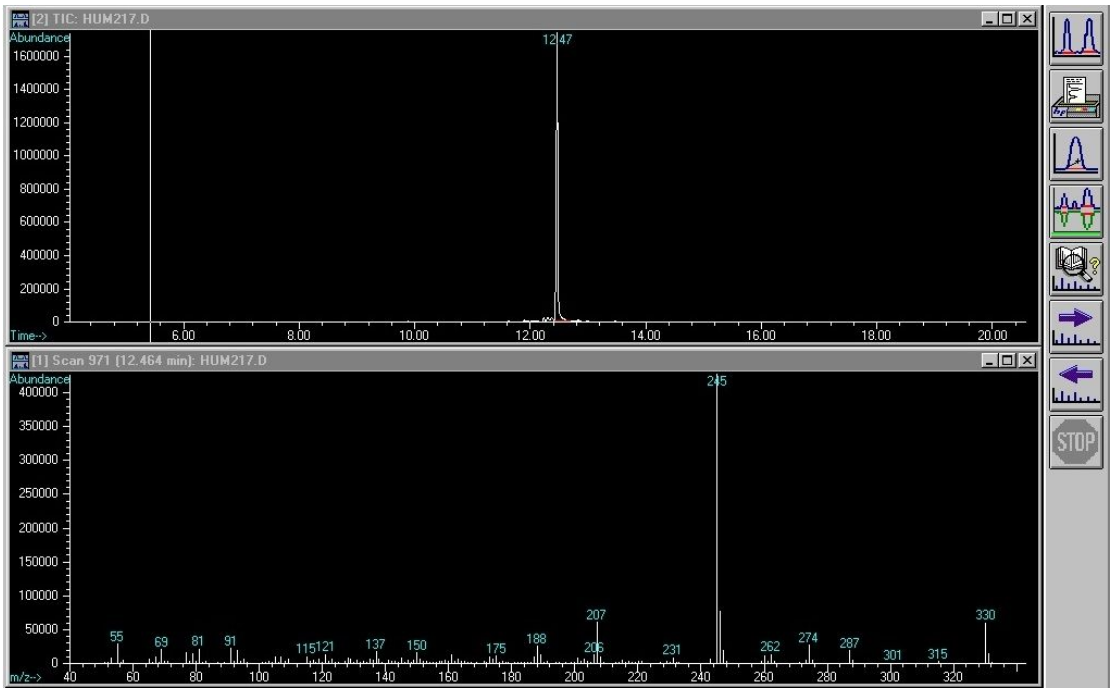
Figure S12. GCMS chromatogram and purity report for Compound 1

Area Percent Report -- Sorted by Signal

Retention Time	Area	Area %	Ratio %	Type	Width
Total Ion Chromatogram					
12.164	6385283	1.685	1.714	BV	0.041
12.428	372497825	98.315	100.000	PV	0.043

Figure S12. GCMS chromatogram and purity report for Compound 1

Compound (2)

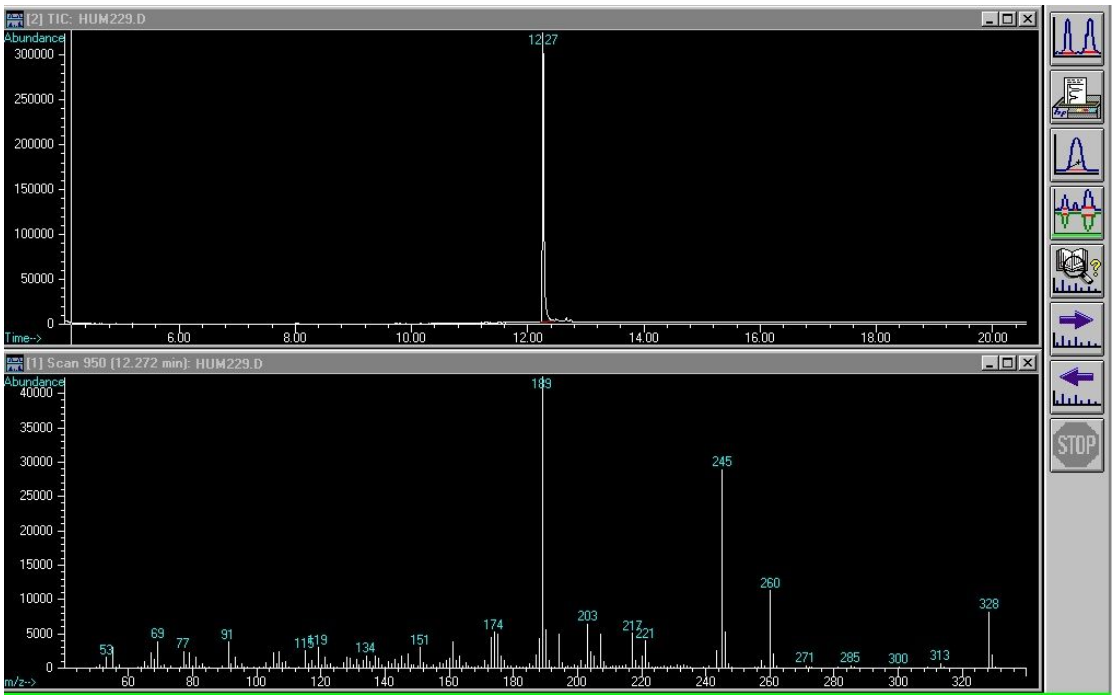


Area Percent Report -- Sorted by Signal

Retention Time	Area	Area %	Ratio %	Type	Width
Total Ion Chromatogram					
12.473	29927363	100.000	100.000	VB	0.049

Figure S13. GCMS chromatogram and purity report for Compound 2

Compound (9)



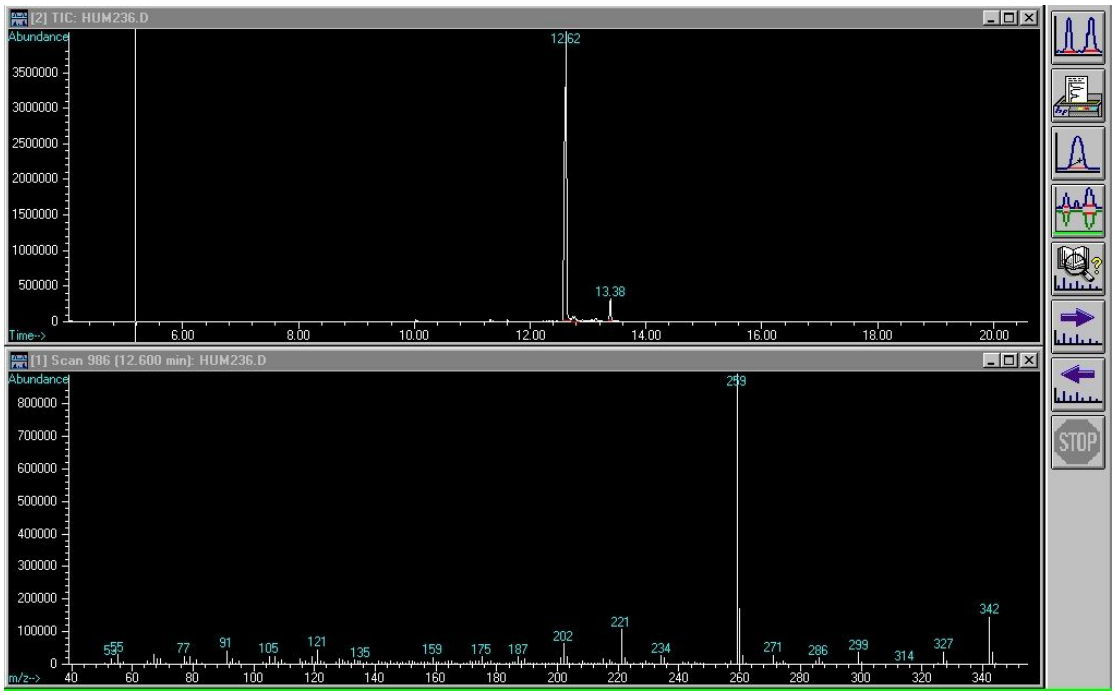
Area Percent Report -- Sorted by Signal

Retention Time	Area	Area %	Ratio %	Type	Width
12.270	5766795	100.000	100.000	BV	0.029

Total Ion Chromatogram

Figure S14. GCMS chromatogram and purity report for Compound 9

Compound (10)



Area Percent Report -- Sorted by Signal

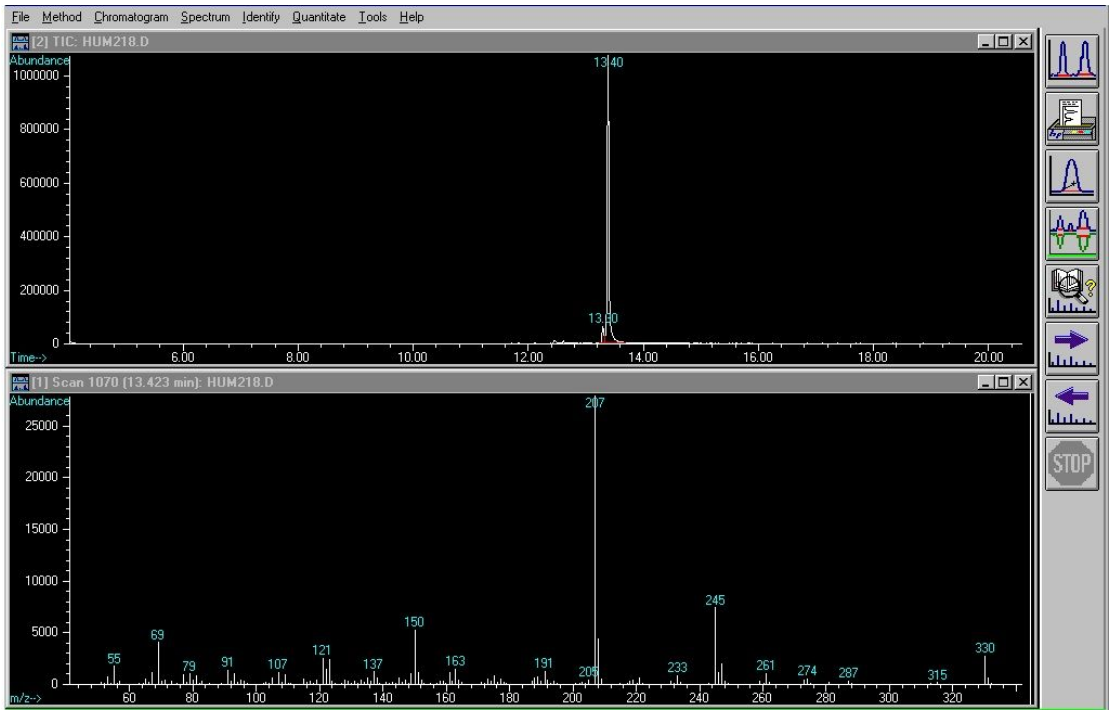
Retention Time	Area	Area %	Ratio %	Type	Width

Total Ion Chromatogram

12.618	105032454	95.233	100.000	M	0.043
13.382	5257217	4.767	5.005	M	0.029

Figure S15. GCMS chromatogram and purity report for Compound 10

Compound (11)



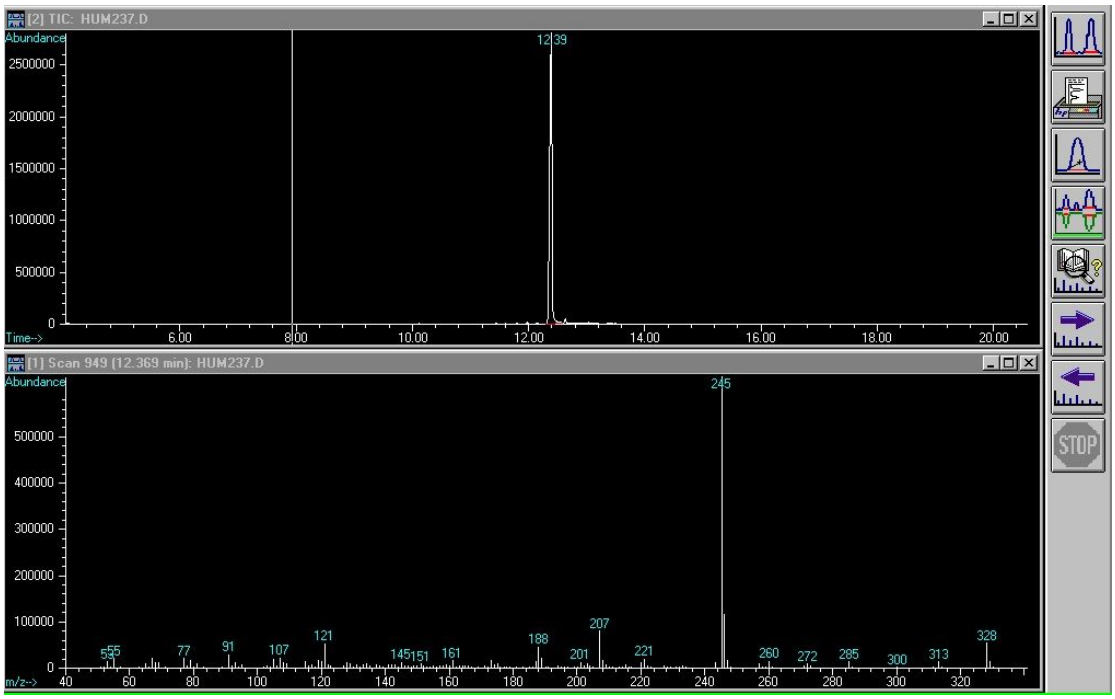
Area Percent Report -- Sorted by Signal

Retention Time	Area	Area %	Ratio %	Type	Width
13.298	704229	3.022	3.116	M	0.027
13.393	22597523	96.978	100.000	M	0.035

Total Ion Chromatogram

Figure S16. GCMS chromatogram and purity report for Compound 11

Compound (13)



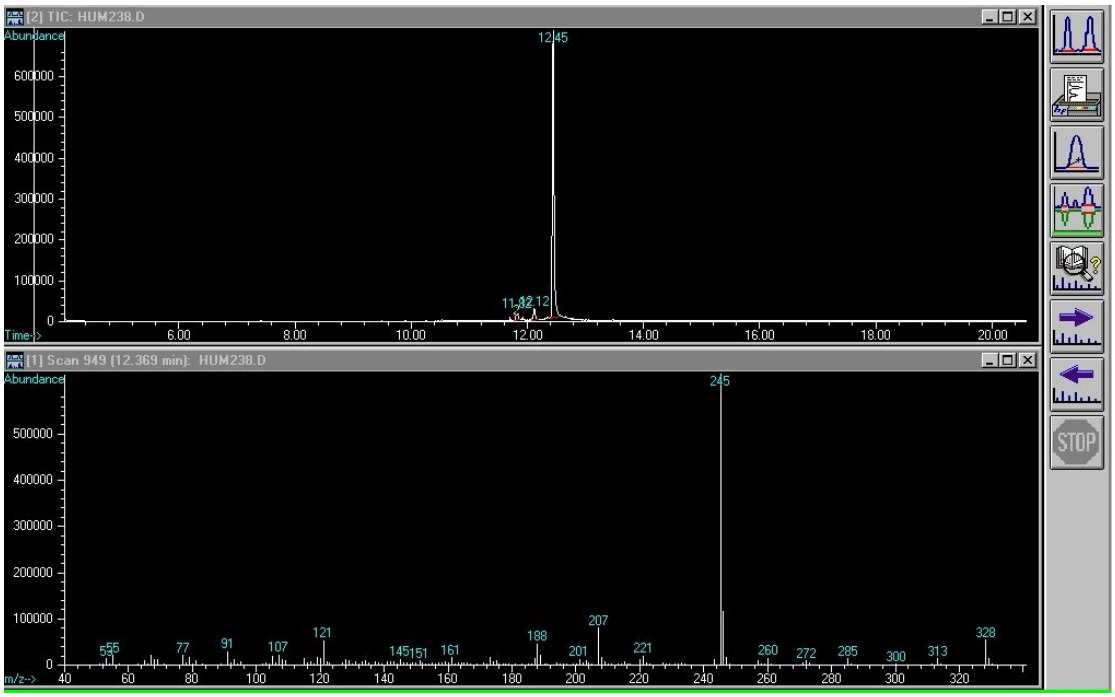
Area Percent Report -- Sorted by Signal

Retention Time	Area	Area %	Ratio %	Type	Width
12.394	74981490	100.000	100.000	BV	0.045

Total Ion Chromatogram

Figure S17. GCMS chromatogram and purity report for Compound 13

Compound (14)



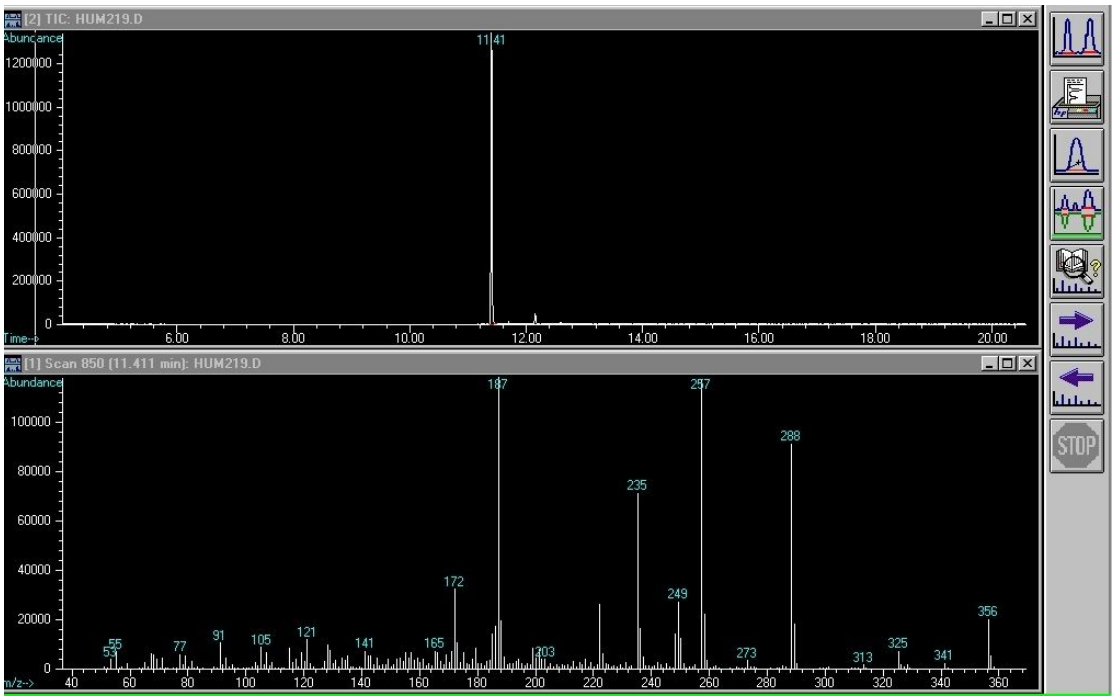
Area Percent Report -- Sorted by Signal

Retention Time	Area	Area %	Ratio %	Type	Width
11.820	154692	1.061	1.111	BV	0.036
12.123	543096	3.795	3.973	BB	0.026
12.448	13881993	95.521	100.000	BV	0.031

Total Ion Chromatogram

Figure S18. GCMS chromatogram and purity report for Compound 14

Compound (15)



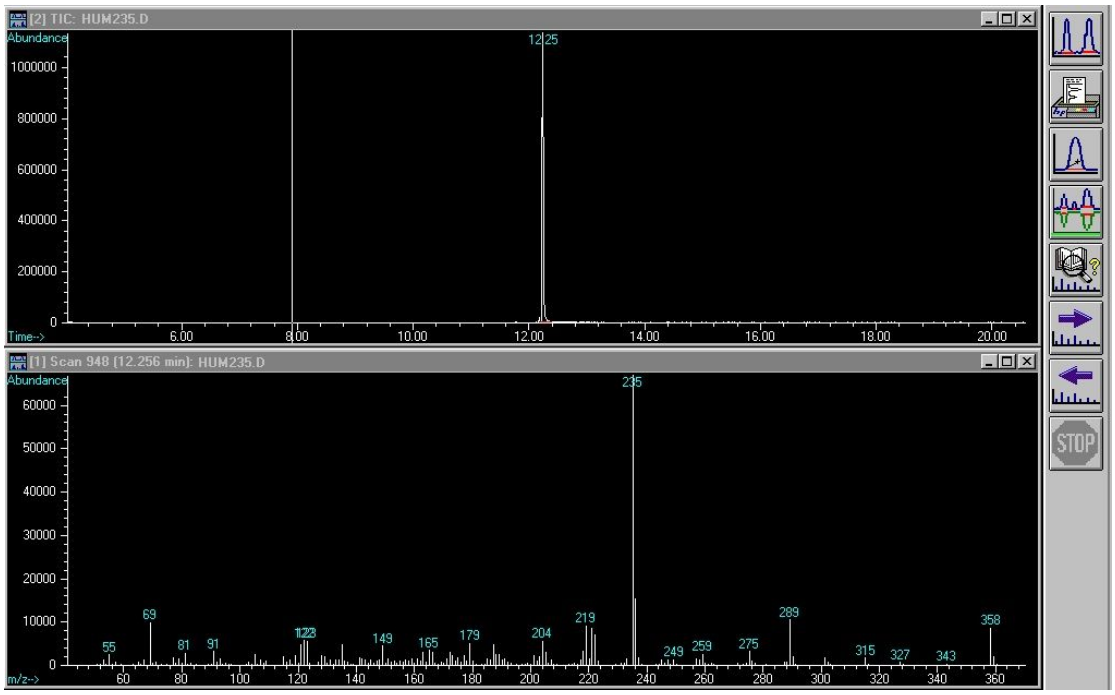
Area Percent Report -- Sorted by Signal

Retention Time	Area	Area %	Ratio %	Type	Width
11.409	17137770	100.000	100.000	BB	0.022

Total Ion Chromatogram

Figure S19. GCMS chromatogram and purity report for Compound 15

Compound (16)



Area Percent Report -- Sorted by Signal

Retention Time	Area	Area %	Ratio %	Type	Width

Total Ion Chromatogram

12.246	18034182	100.000	100.000	VB	0.026

Figure S20. GCMS chromatogram and purity report for Compound 16