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Article

NMR Spectroscopy Applied to the Metabolic Analysis of Natural Extracts of *Cannabis sativa*

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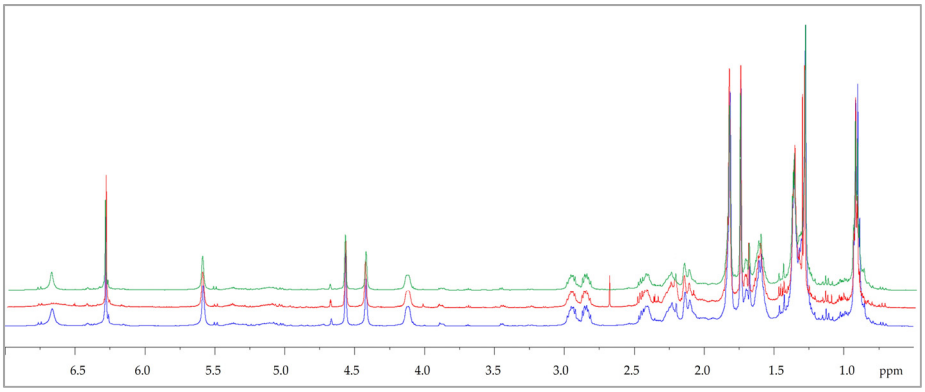

Figure S1. Comparison between ^{1}H NMR spectra of ethanol (blue), acetone (red) and hexane (green) extracts for *Tiborszallasi* variety.

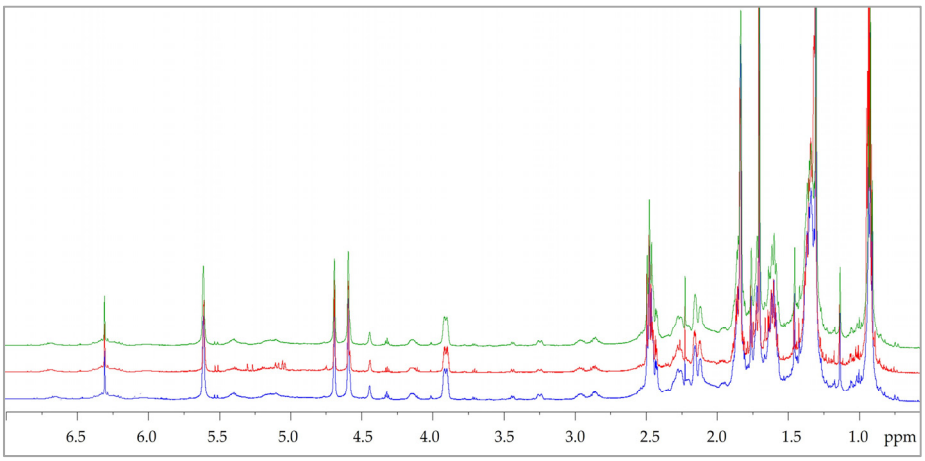

Figure S2. Comparison between ^{1}H NMR spectra of ethanol (blue), hexane (red) and acetone (green) extracts for *Kompolti* variety.

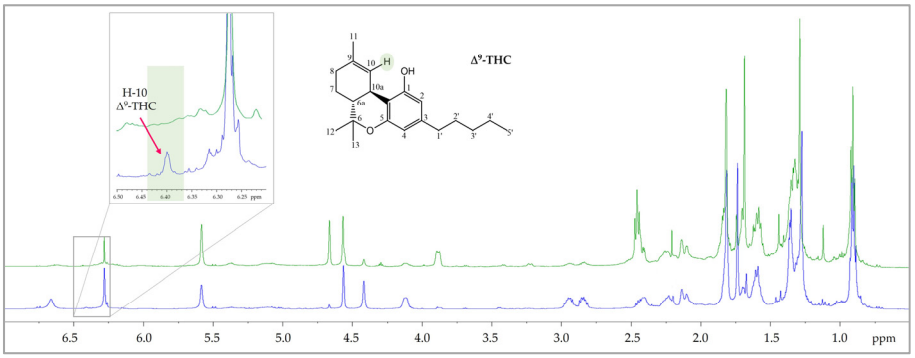

Figure S3. Comparison between the enlarged region [6.25 ppm - 6.5ppm] of the ^{1}H NMR spectra from hexane extract of *Tiborszallasi* (blue) and *Kompolti* (purple) variety. A broad peak isolated at 6.40 ppm corresponding to the proton H-10 of Δ^{9}-THC appears in the proton spectra of *Tiborszallasi* while this signal was undetectable in the ^{1}H NMR spectrum acquired for *Kompolti.*

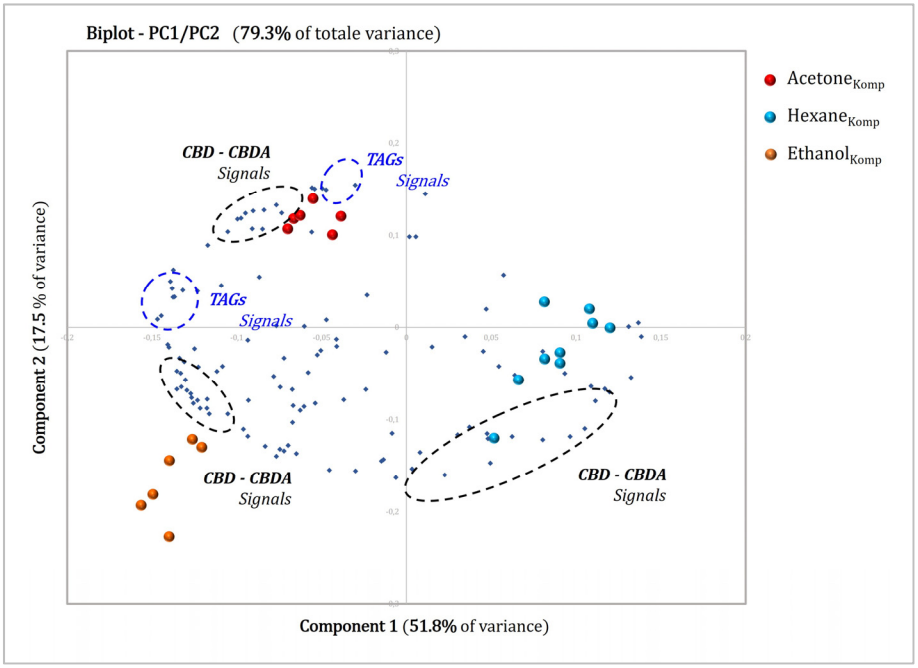

Figure S4. Biplot of PCA carried out on NMR spectra of acetone (red dots), hexane (blue dots) and ethanol (orange dots) extracts of *Kompolti* variety of hemp. The scores plot showing the first two PCs (PC1 and PC2) with their respective variation. R2X(PC1) = 51.8%, R2X(PC2) = 17.5%. .

Table S1. The ^{1}H NMR data of main cannabinoids in *Kompolti* inflorescences.

Compound	qNMR on Flowers UAE Extracts			
	qNMR IS	Hexane	Acetone	Ethanol
CBDA content*	Anthracene	0.4 ± 0.3	0.4 ± 0.2	0.5 ± 0.2
	Benzoic acid	0.6 ±0.2	0.5 ± 0.1	0.4± 0.1
	TMSP-d_4	0.4 ± 0.3	0.4 ± 0.3	0.5 ± 0.3
CBD content*	Anthracene	5.7 ±0.2	5.4 ± 0.3	5.2 ± 0.2
	Benzoic acid	5.9±0.2	5.2 ± 0.2	5.3 ± 0.1
	TMSP-d_4	5.9±0.2	5.6 ± 0.3	5.3 ± 0.3
Δ^{9}-THC content*	Anthracene Benzoic acid TMSP-d_4	<LOD	<LOD	< LOD

*% on dry weight.