

Supplementary Information

Identification of synthetic impurities in a vape pen containing Δ^9 -tetrahydrocannabinol by GC-MS

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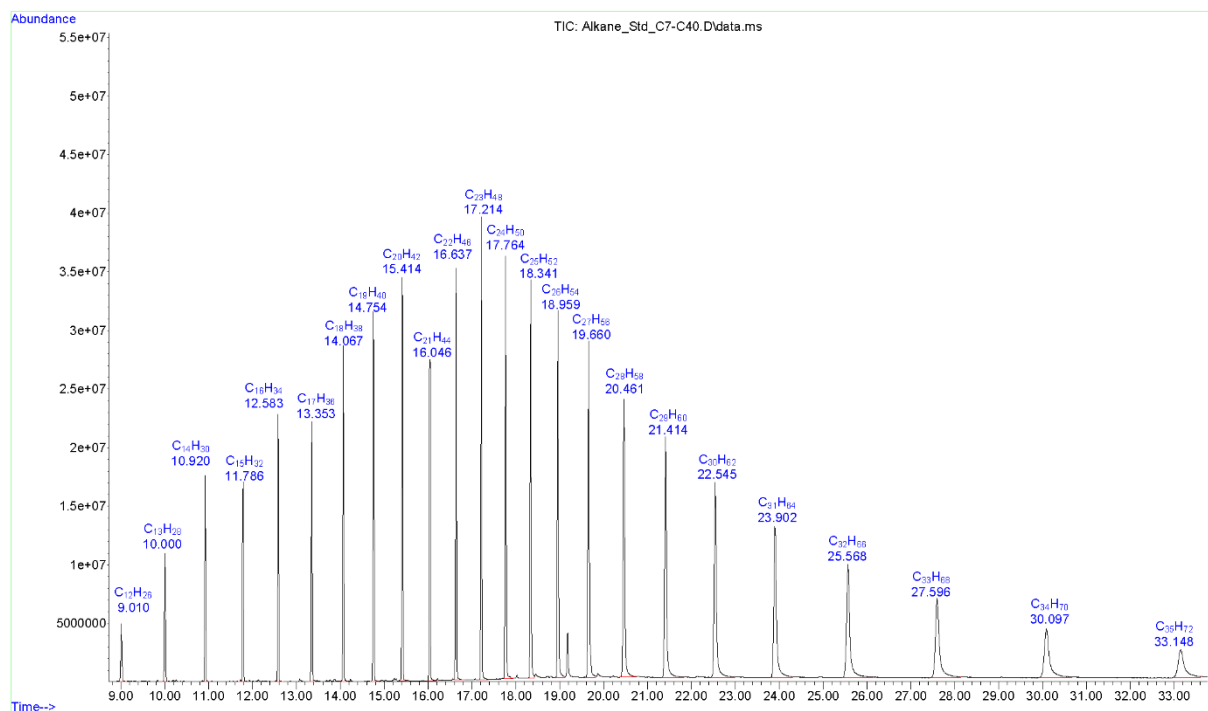
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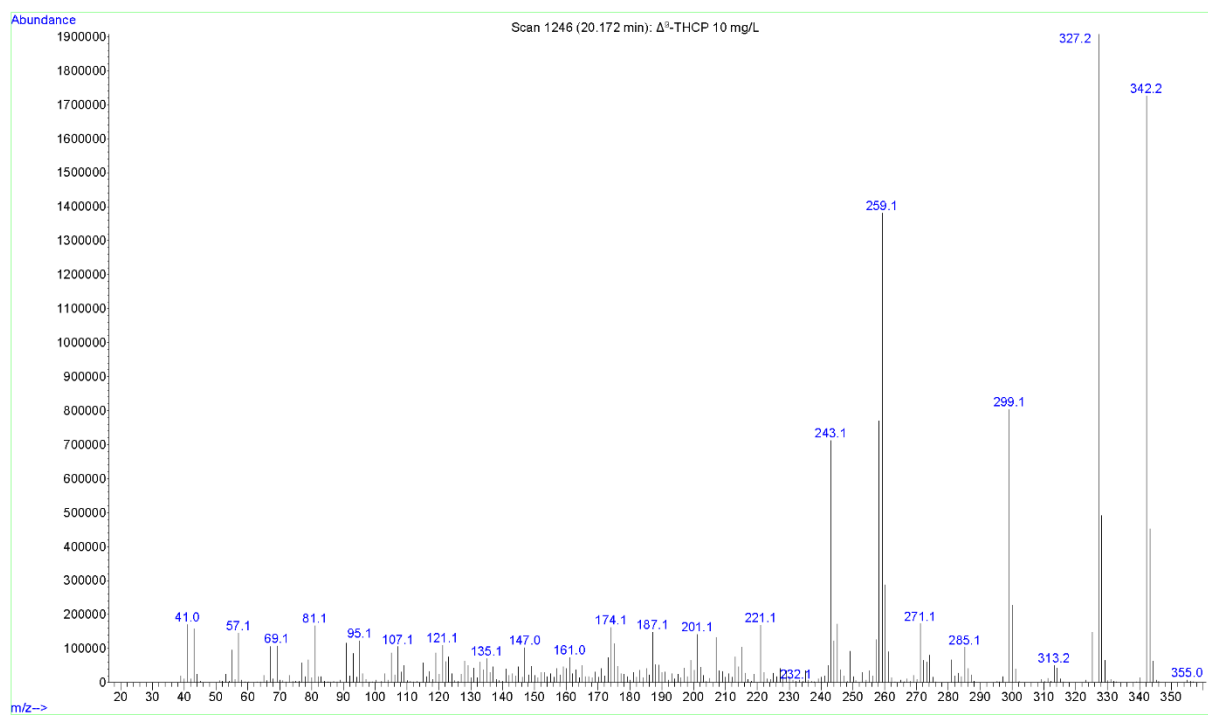
e-mail address: willi.schirmer@irm.unibe.ch

Table of contents

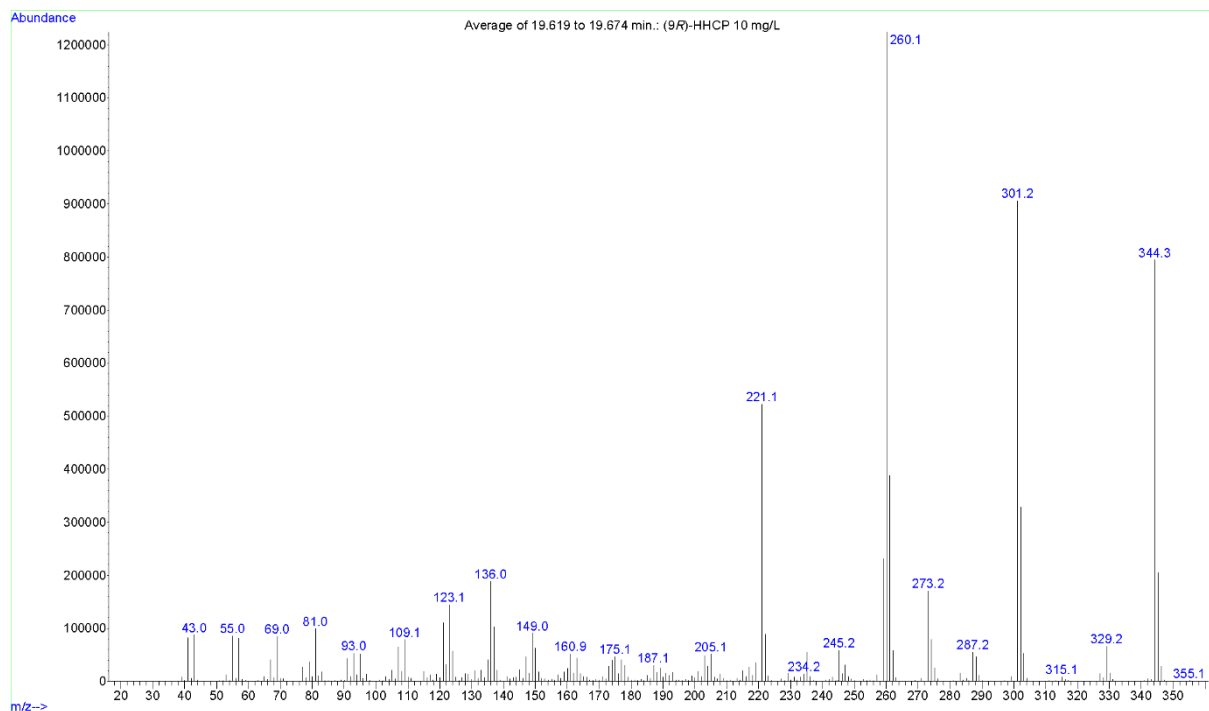
• TIC of <i>n</i> -Alkanes (Kováts-index)	S1
• EI reference mass spectra	S2-S8
○ Δ^9 -THCP, (9 <i>R</i>)-HHCP, (9 <i>S</i>)-HHCP, CBDP, CBP, 5-Heptylresorcinol, Δ^8 -THCP	
• EI mass spectra of identified terpenes in the sample.....	S9-S15
○ α -humulene, β -myrcene, β -pinene, caryophyllene, β -phellandrene, (<i>R</i>)-limonene, <i>m</i> -camphorene	
• EI mass spectra of identified cannabinoids in the sample	S16-S19
○ CBDP, CBP, Δ^8 -THCP, Δ^9 -THCP	
• EI mass spectra of THCP isomers and analogues	S20-S23
○ THCP impurities A-D	
• Chromatograms and mass spectra of high molecular mass fraction	
○ TIC of the fraction	S24
○ TIC of the fraction (detail)	S25
○ EI mass spectra of compounds with <i>m/z</i> 476	S26-29
• Chromatograms and mass spectra of Δ^9 -THCP Mosher esters	
○ (<i>S</i>)-Mosher ester of Δ^9 -THCP Reference	S30-S31
○ (<i>R</i>)-Mosher ester of Δ^9 -THCP Reference.....	S32-S33
○ (<i>S</i>)-Mosher ester of Δ^9 -THCP from vape pen	S34-S35
○ (<i>R</i>)-Mosher ester of Δ^9 -THCP from vape pen.....	S36-S37



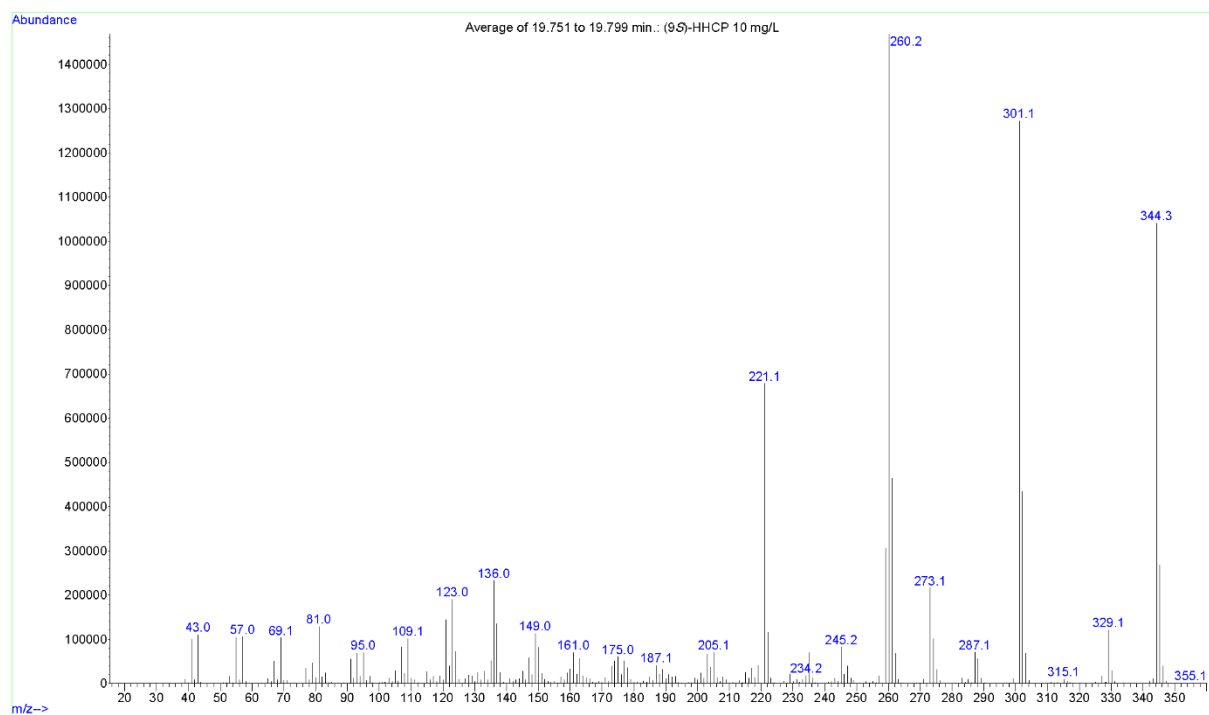
S1 TIC of an alkane standard (C7-C40) for the determination of Kováts indices.



S2: EI mass spectrum of Δ^9 -THCP (reference)



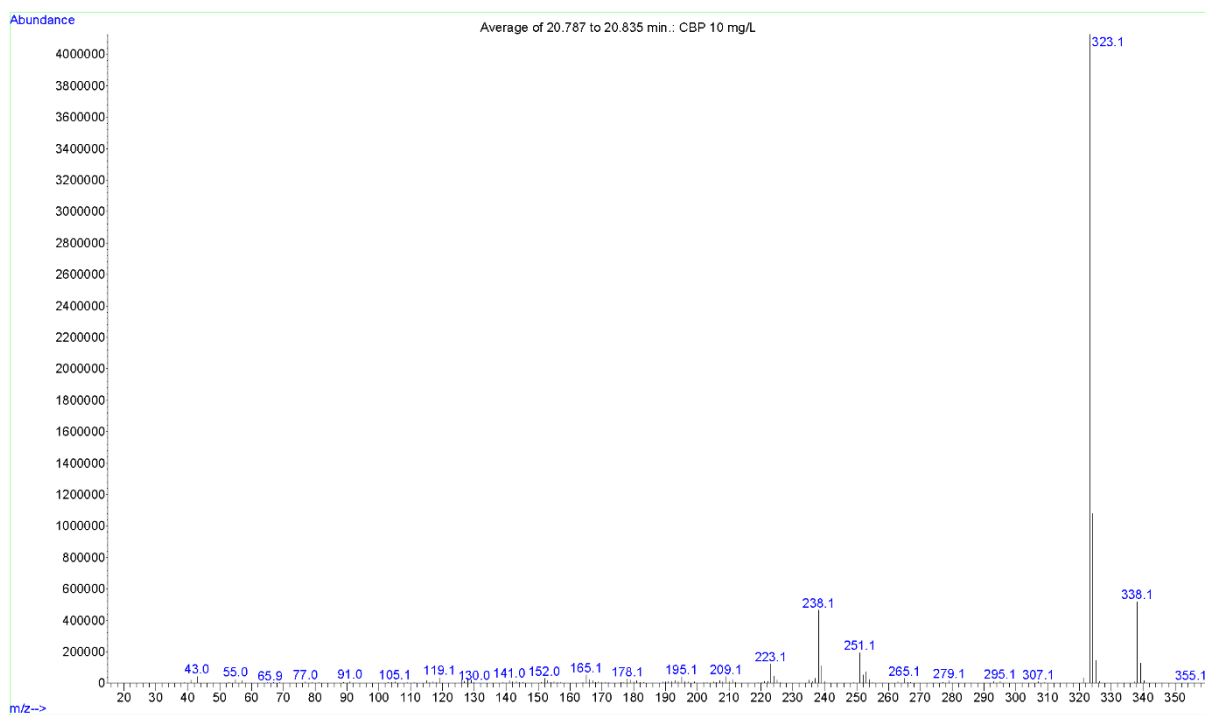
S3: EI mass spectrum of (9R)-HHCP (reference)



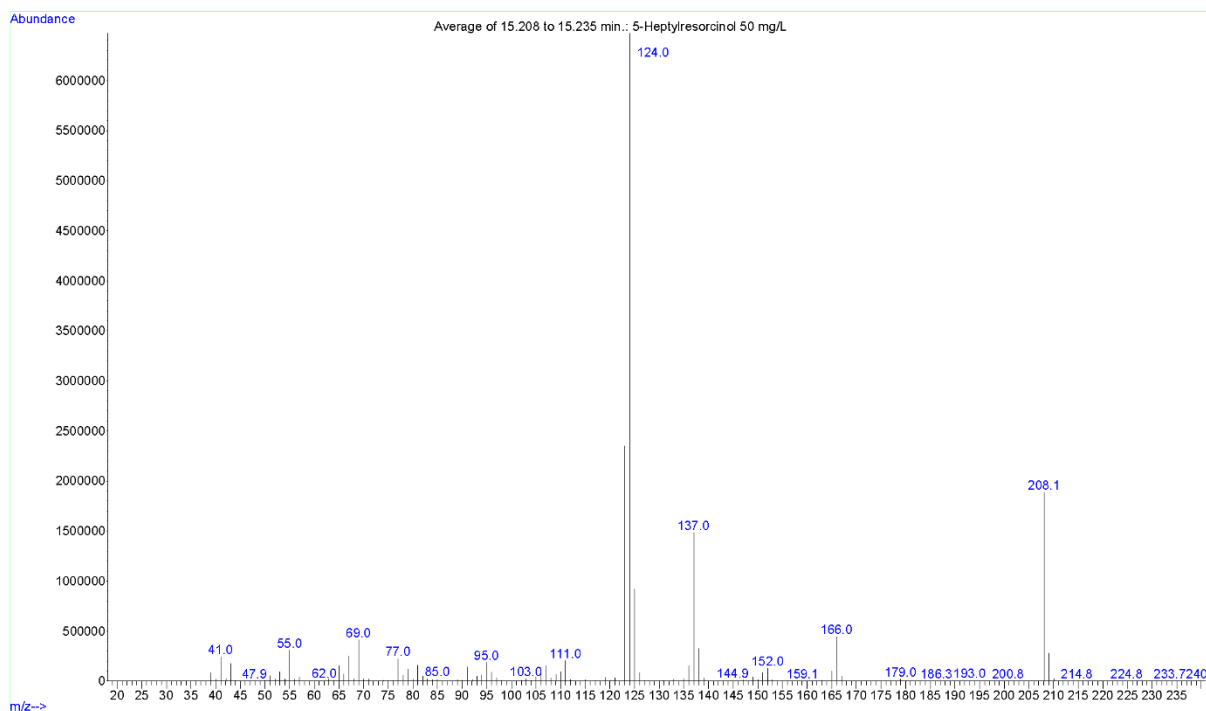
S4: EI mass spectrum of (9S)-HHCP (reference)



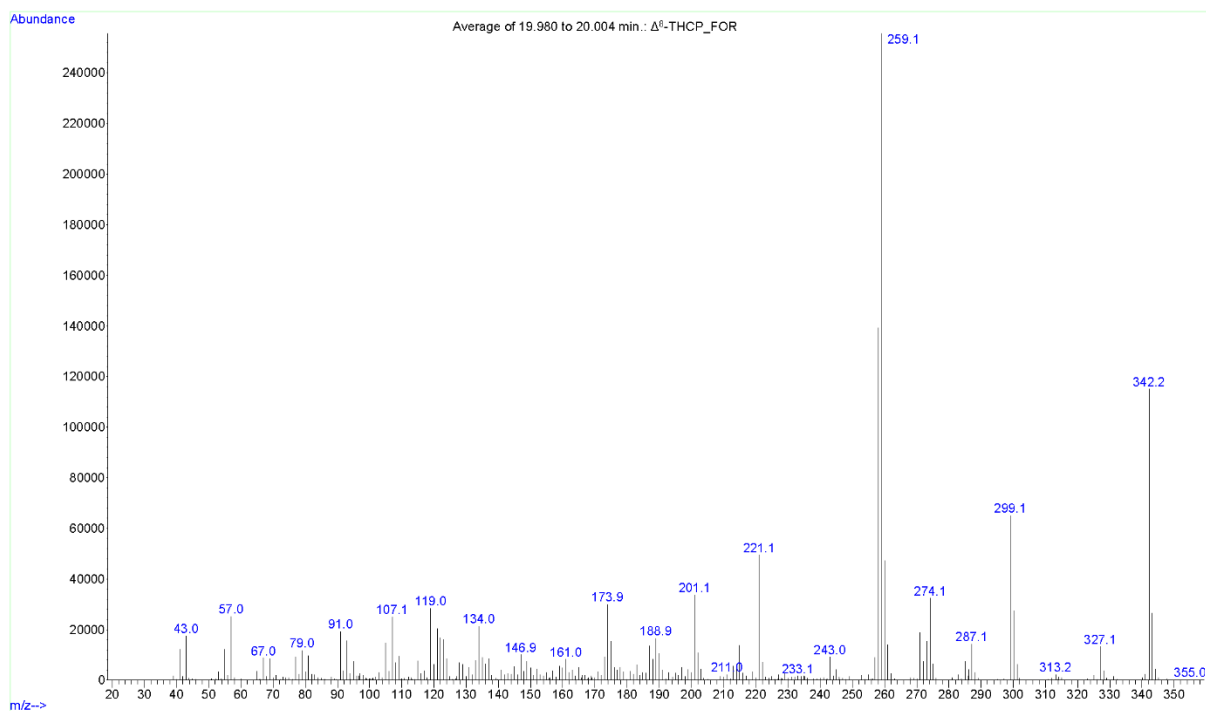
S5: EI mass spectrum of CDBP (reference)



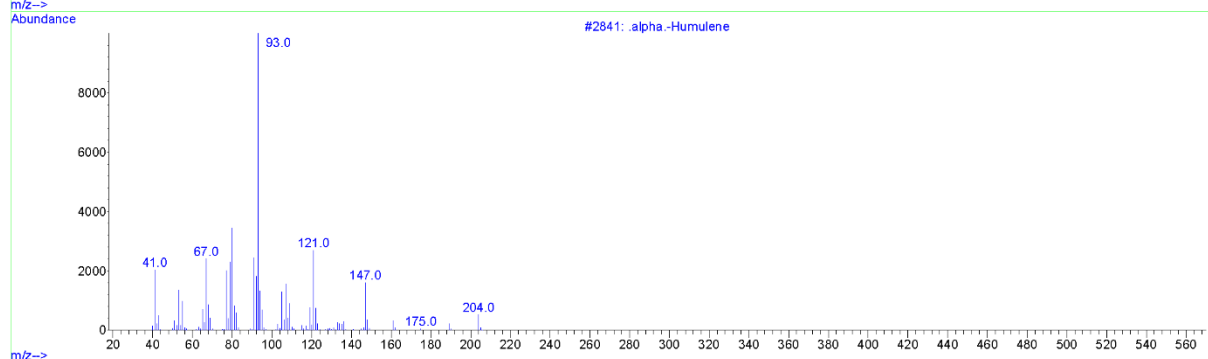
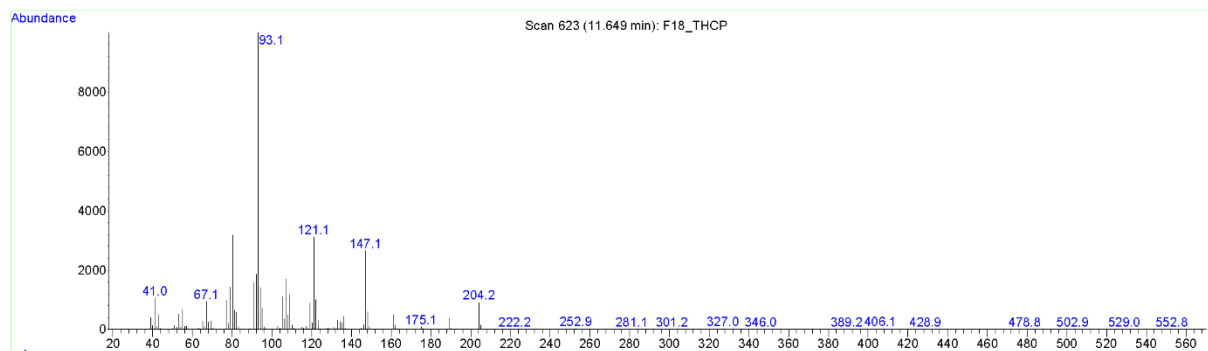
S6: EI mass spectrum of CBP (reference)



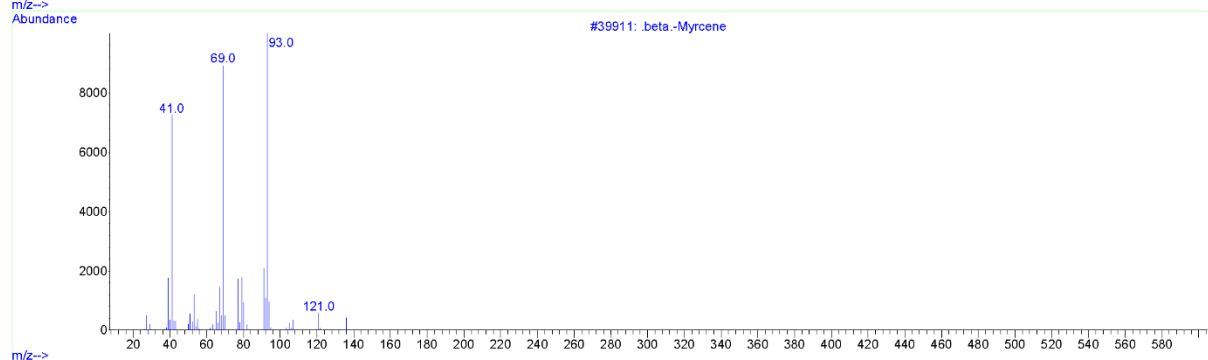
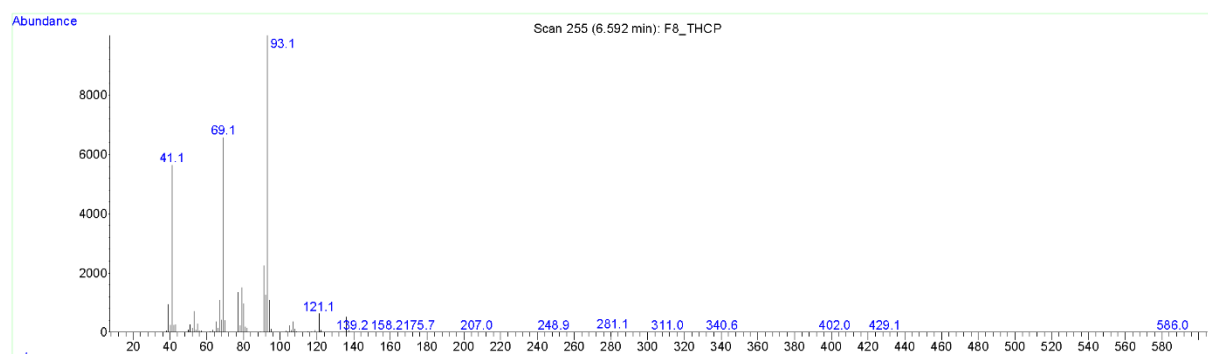
S7: EI mass spectrum of 5-heptylresorcinol (reference)



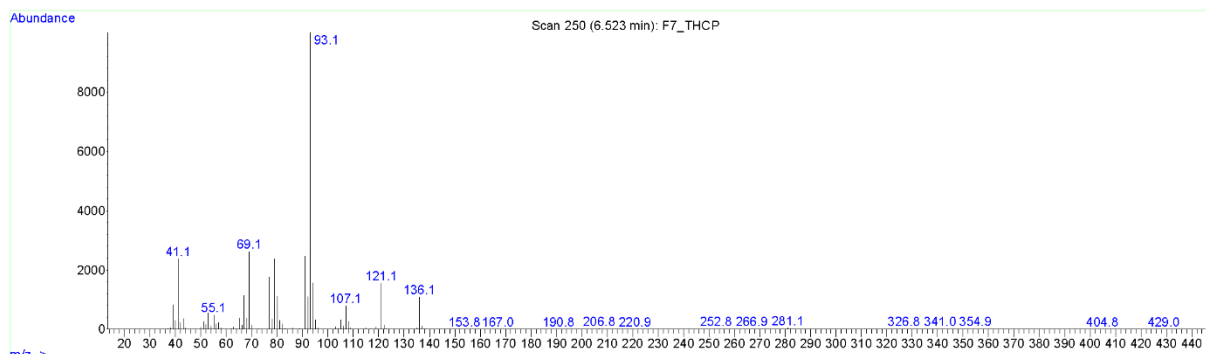
S8: EI mass spectrum of Δ^8 -THCP (reference)



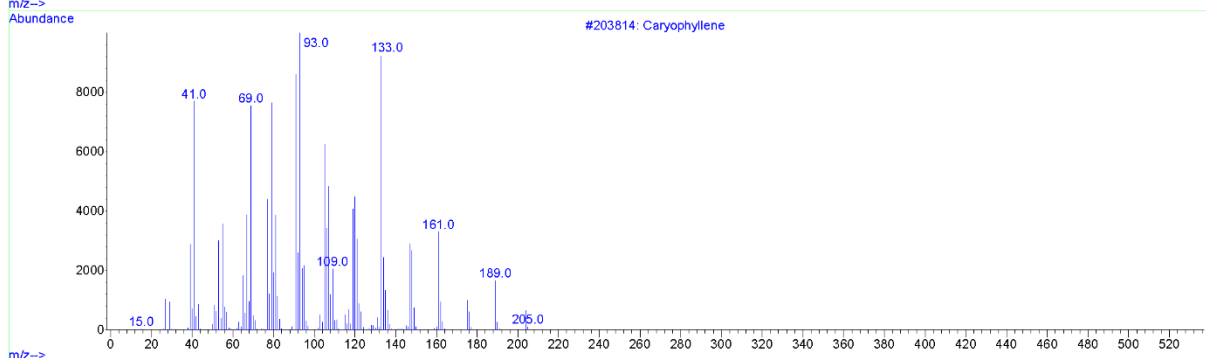
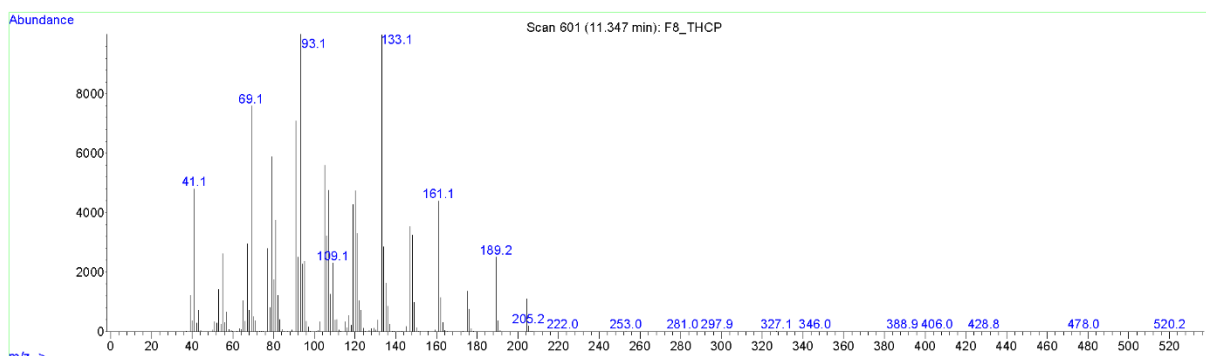
S9: α -Humulene found in a chromatographic fraction of the THCP vape pen liquid.



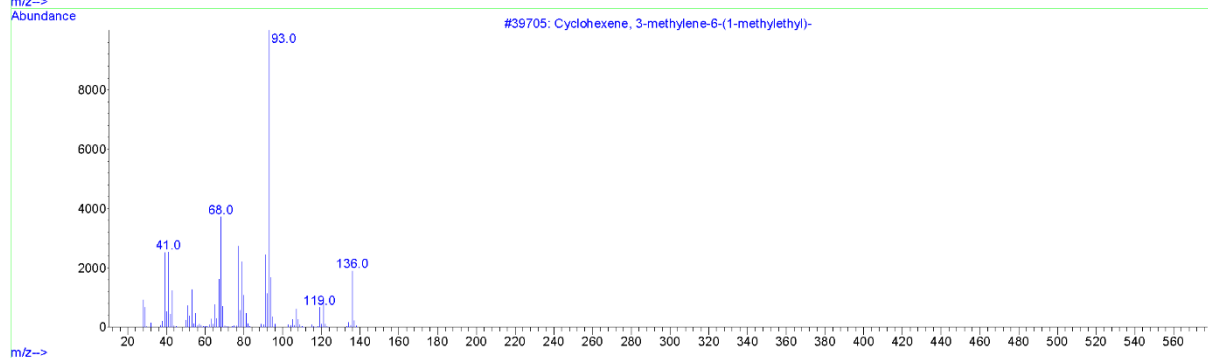
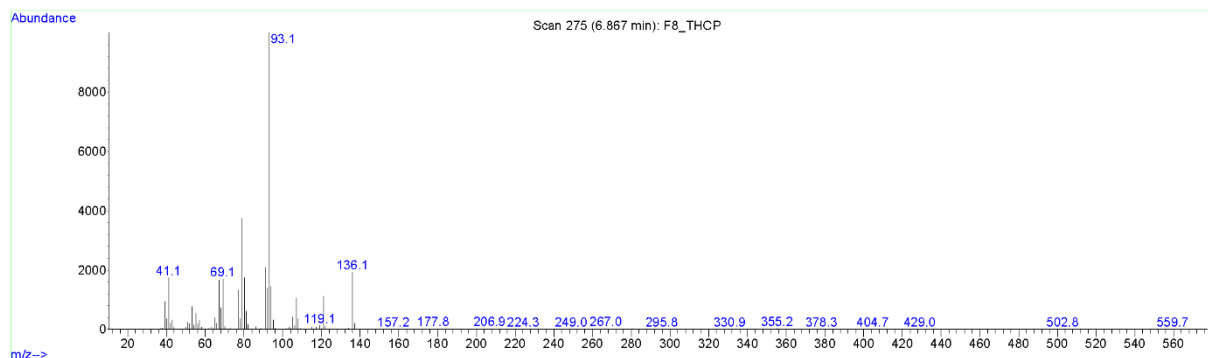
S10: β -Myrcene found in a chromatographic fraction of the THCP vape pen liquid.



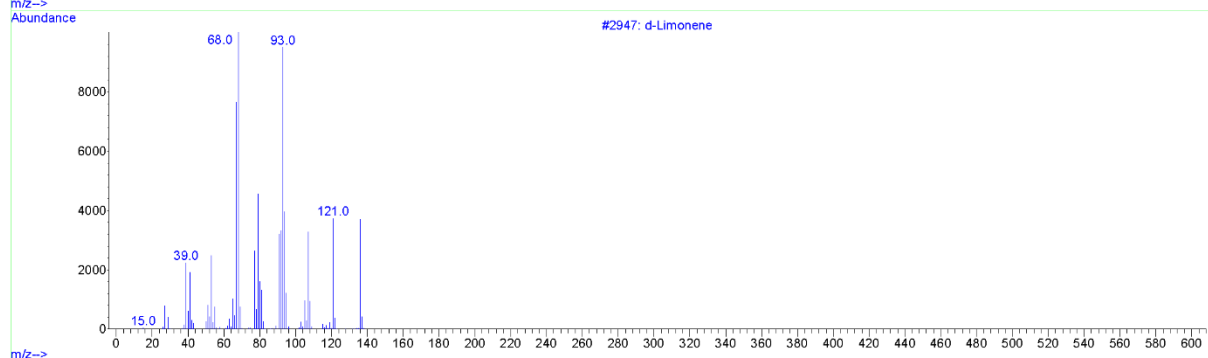
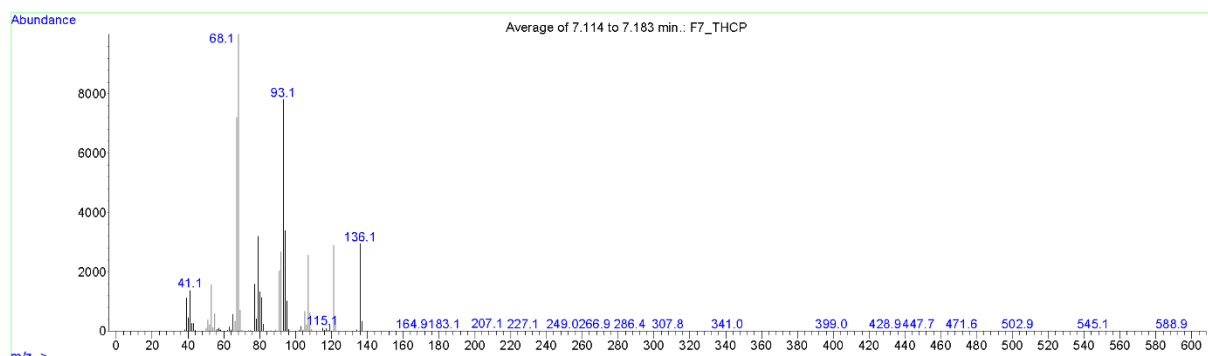
S11: β -Pinene found in a chromatographic fraction of the THCP vape pen liquid



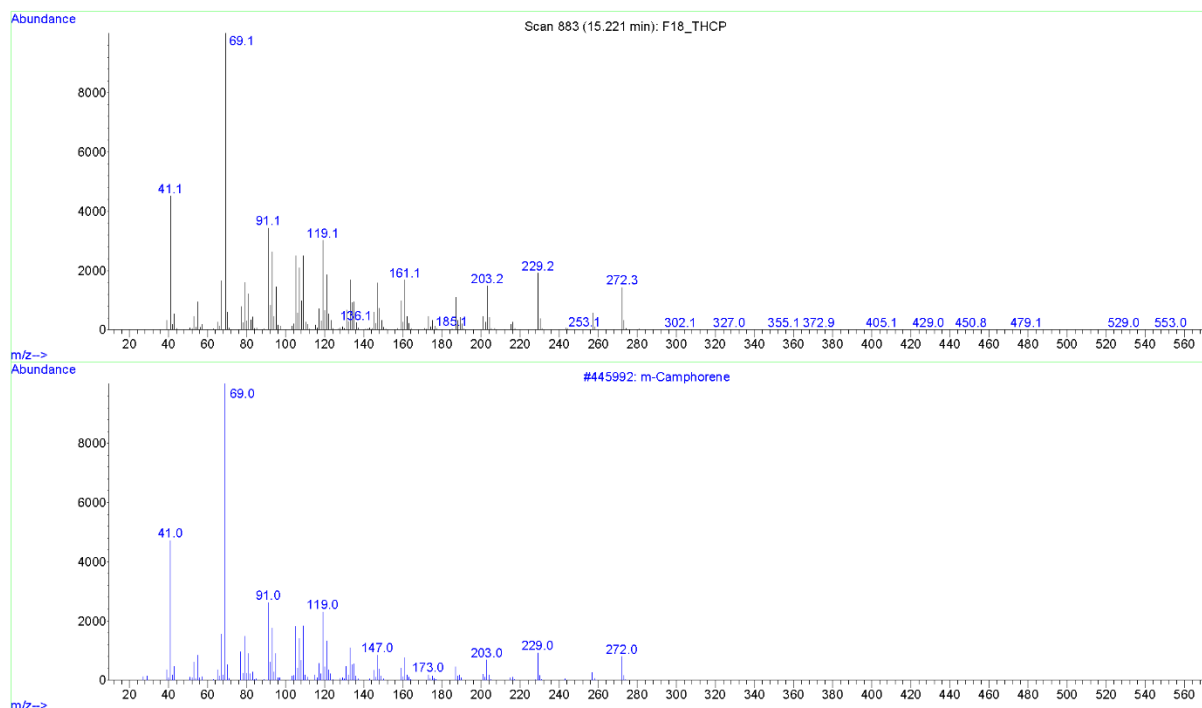
S12: Caryophyllene found in a chromatographic fraction of the THCP vape pen liquid



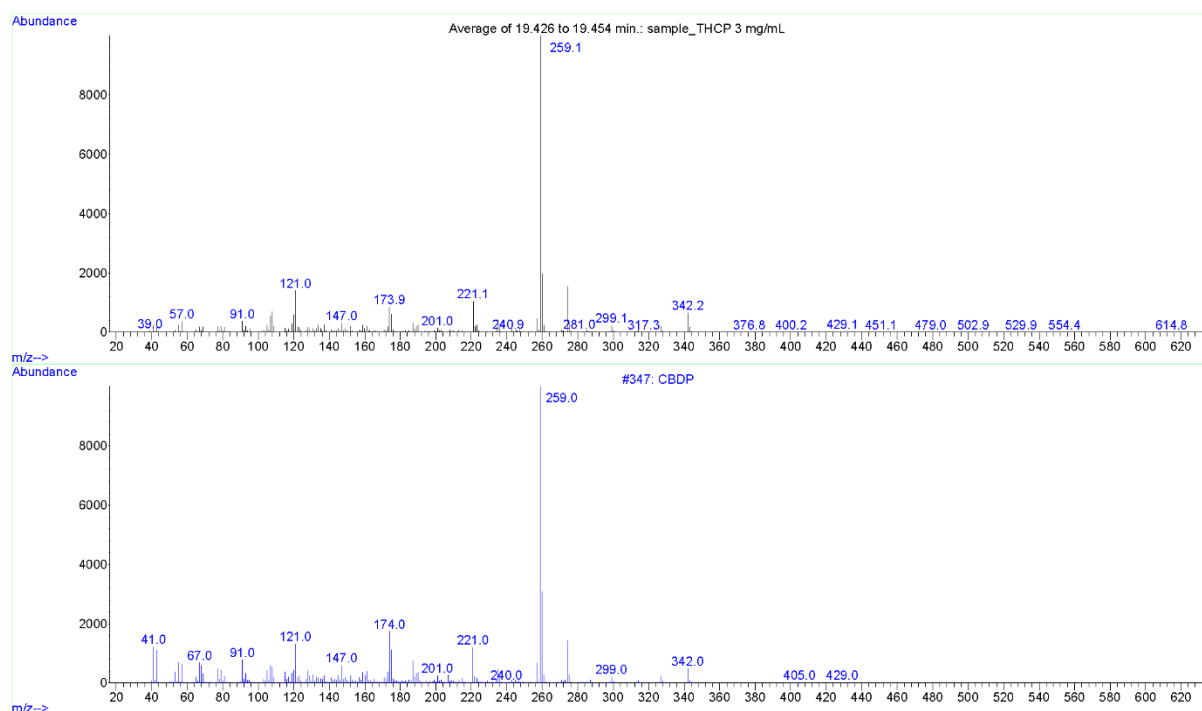
S13: β -Phellandrene found in a chromatographic fraction of the THCP vape pen liquid



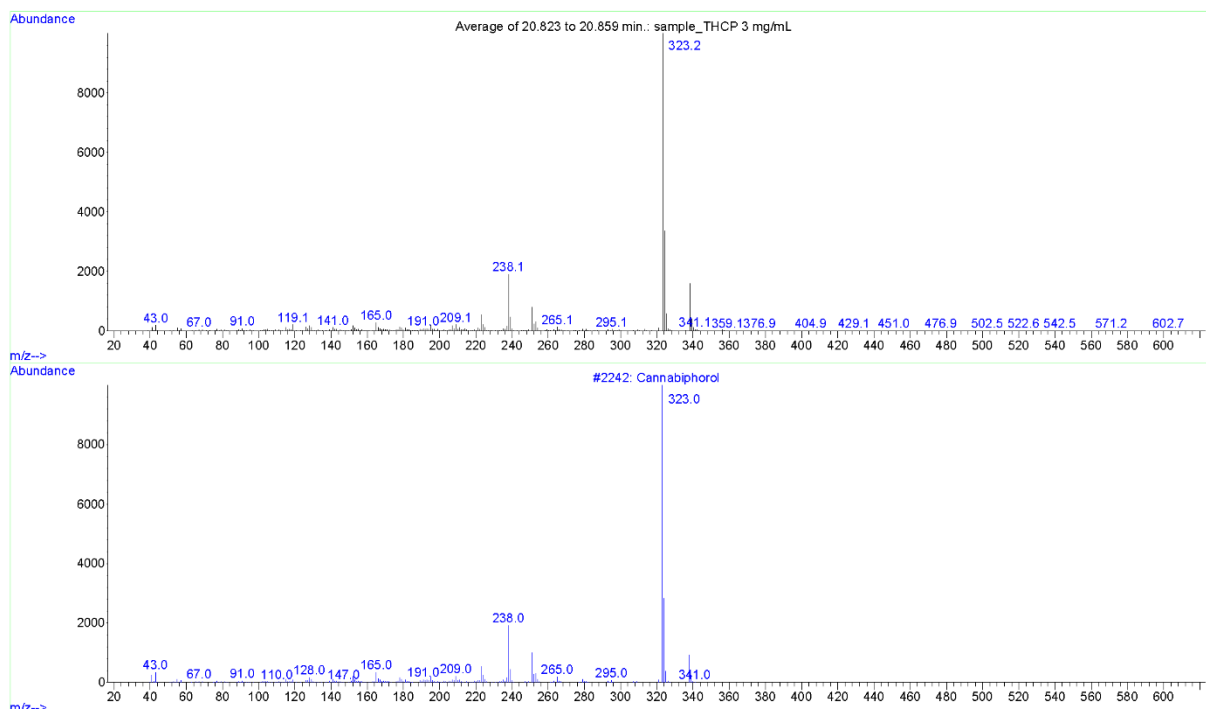
S14: (*R*)-Limonene found in a chromatographic fraction of the THCP vape pen liquid



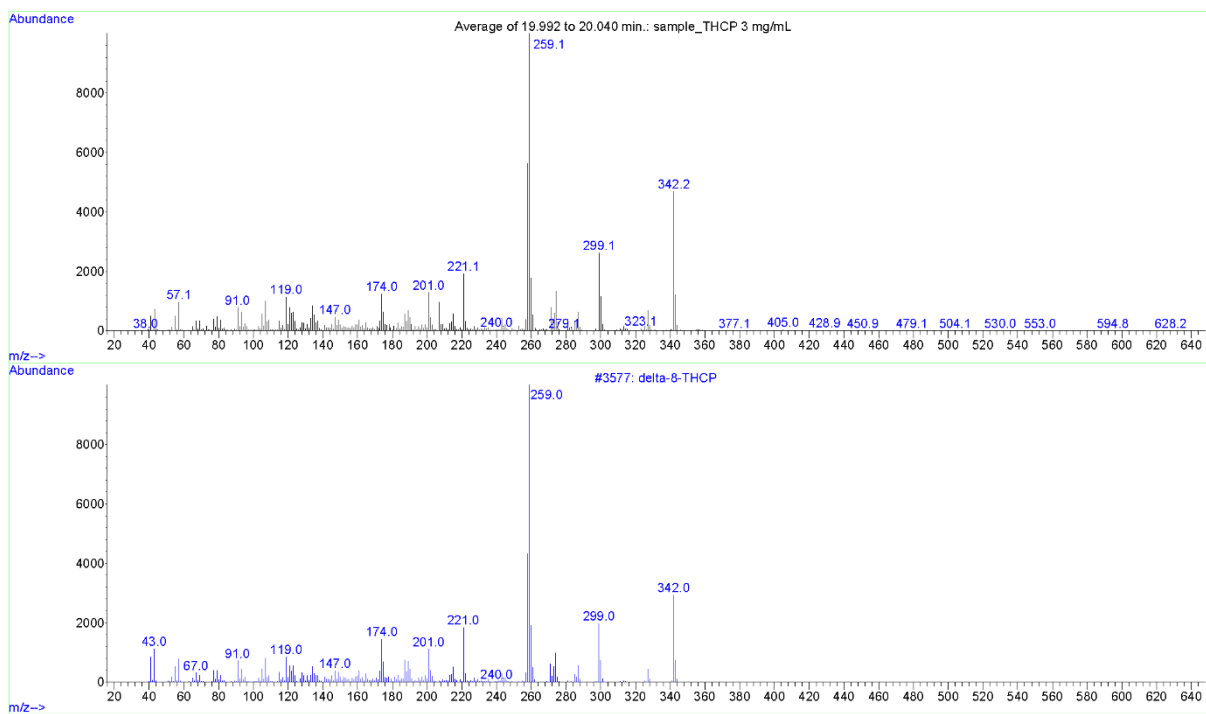
S15: *m*-Camphorene found in a chromatographic fraction of the THCP vape pen liquid



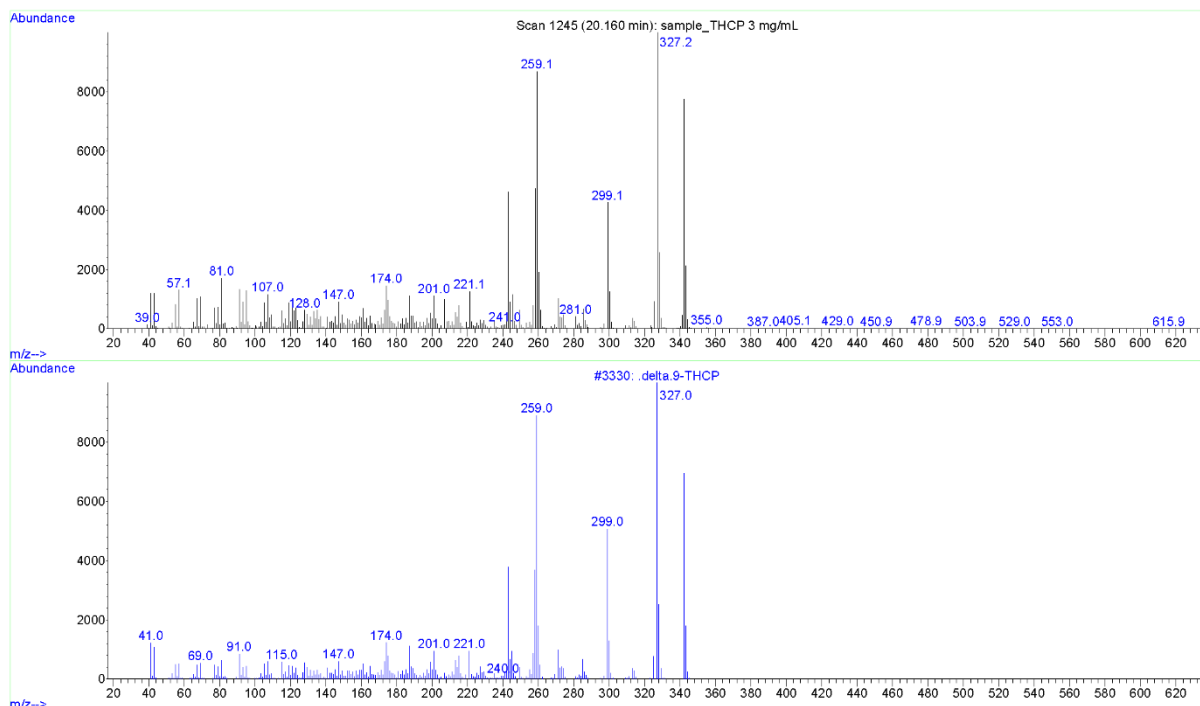
S16: CBDP found in the THCP vape pen liquid



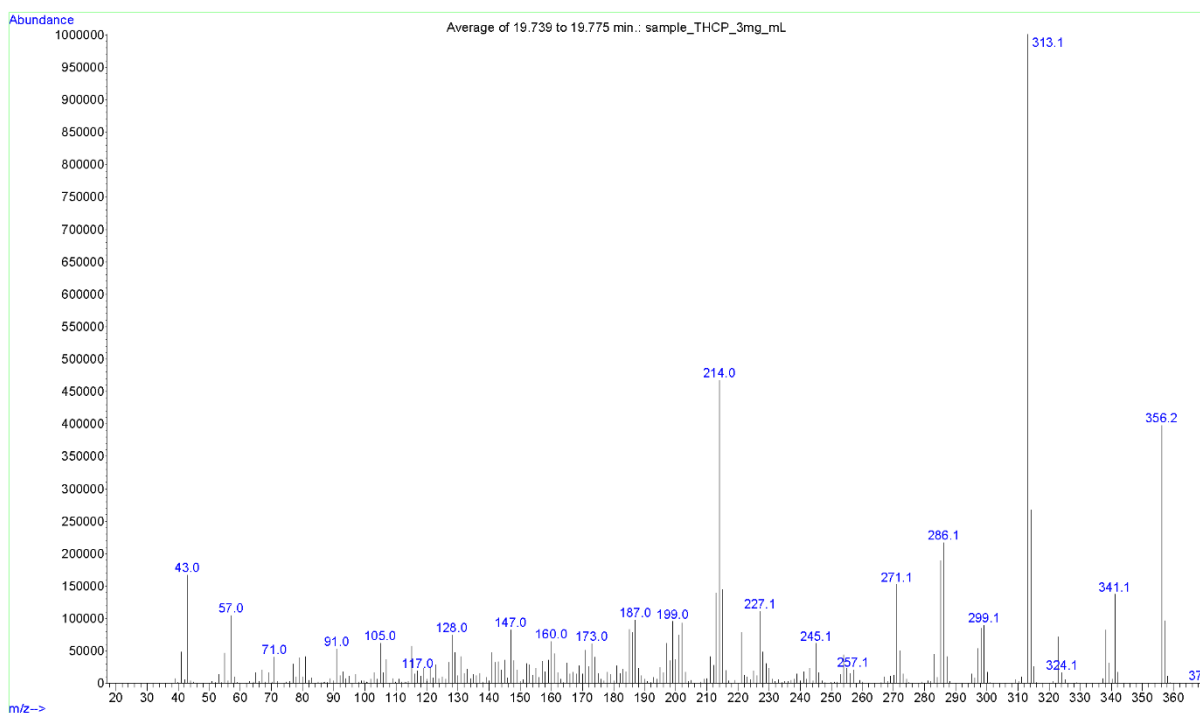
S17: CBP found in the THCP vape pen liquid



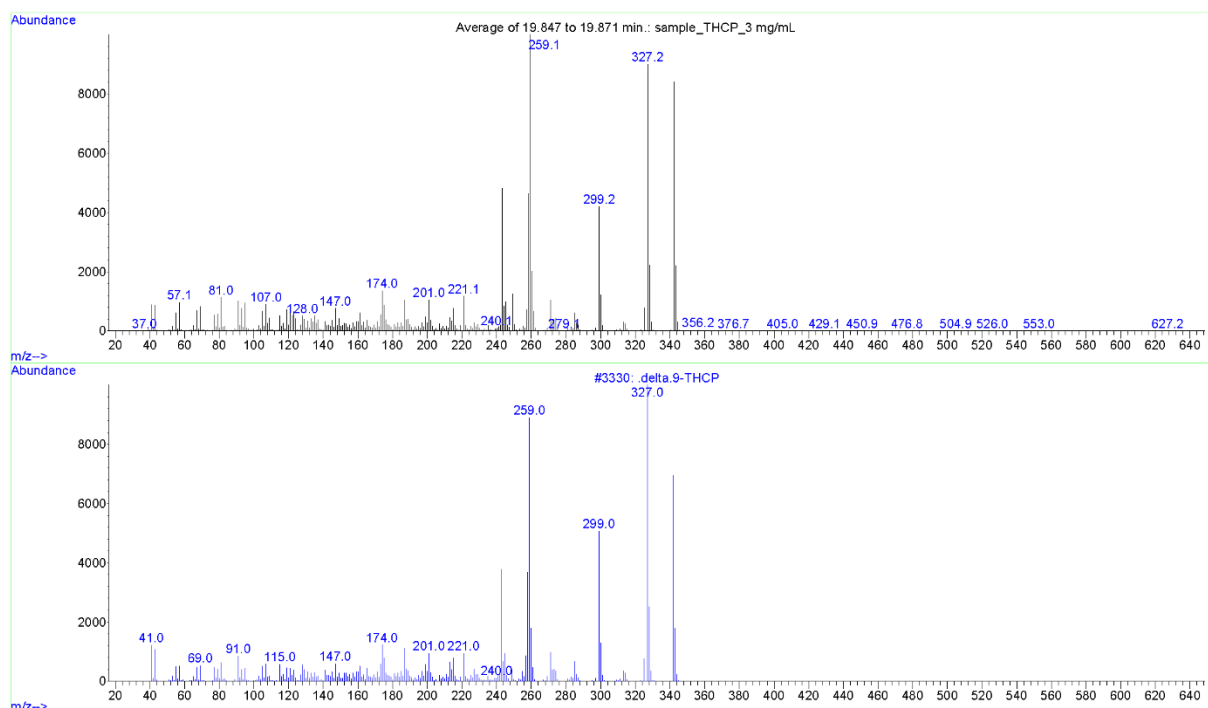
S18: Δ^8 -THCP found in the THCP vape pen liquid



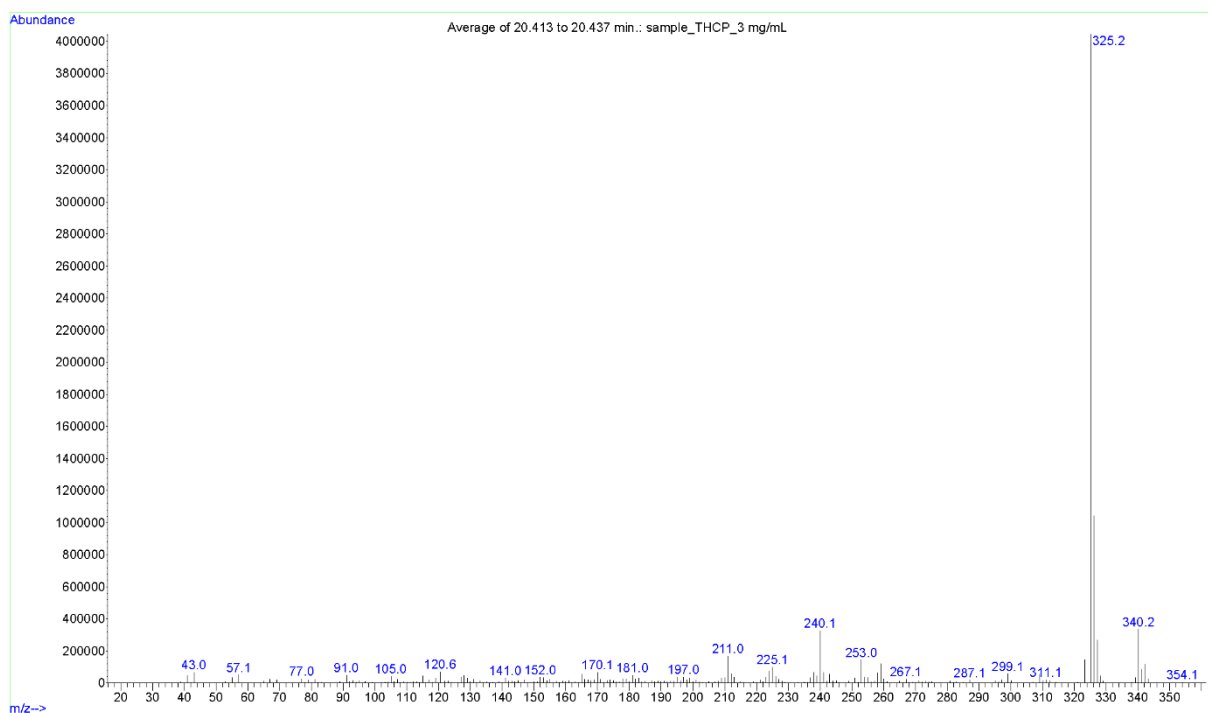
S19: Δ^9 -THCP found in the THCP vape pen liquid



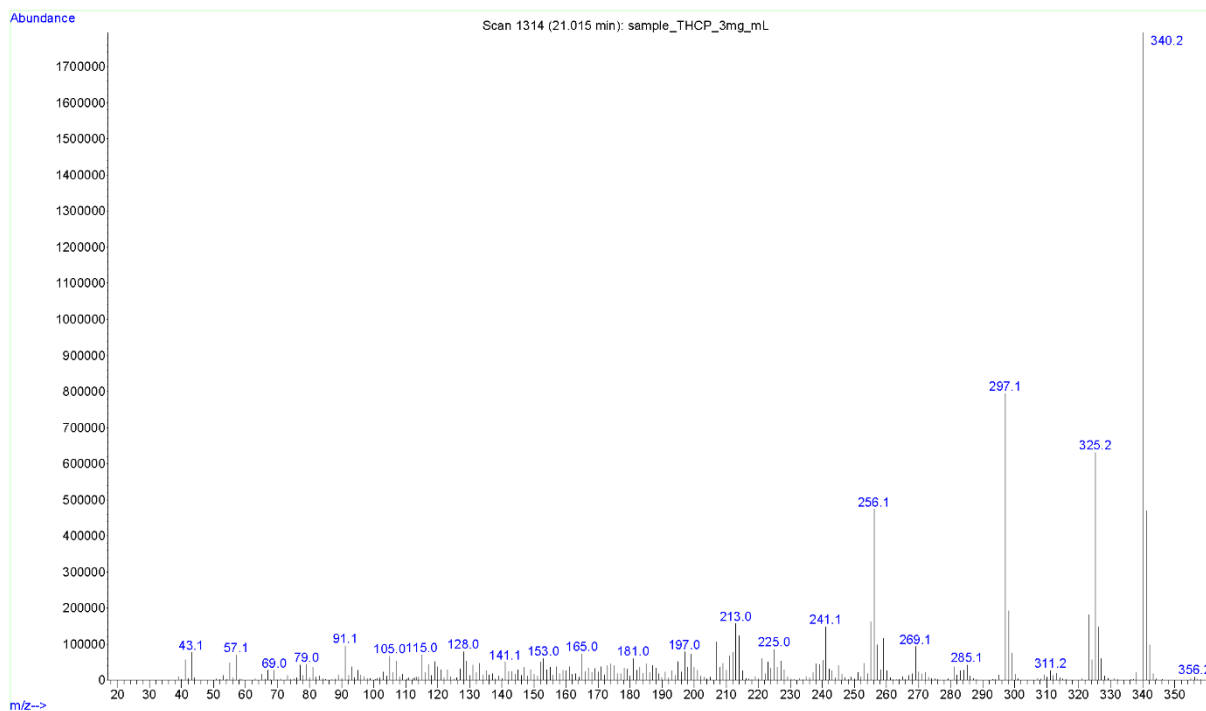
S20: Unknown THCP impurity found in the THCP vape pen liquid, potentially an oxo-THCP. (THCP impurity A)



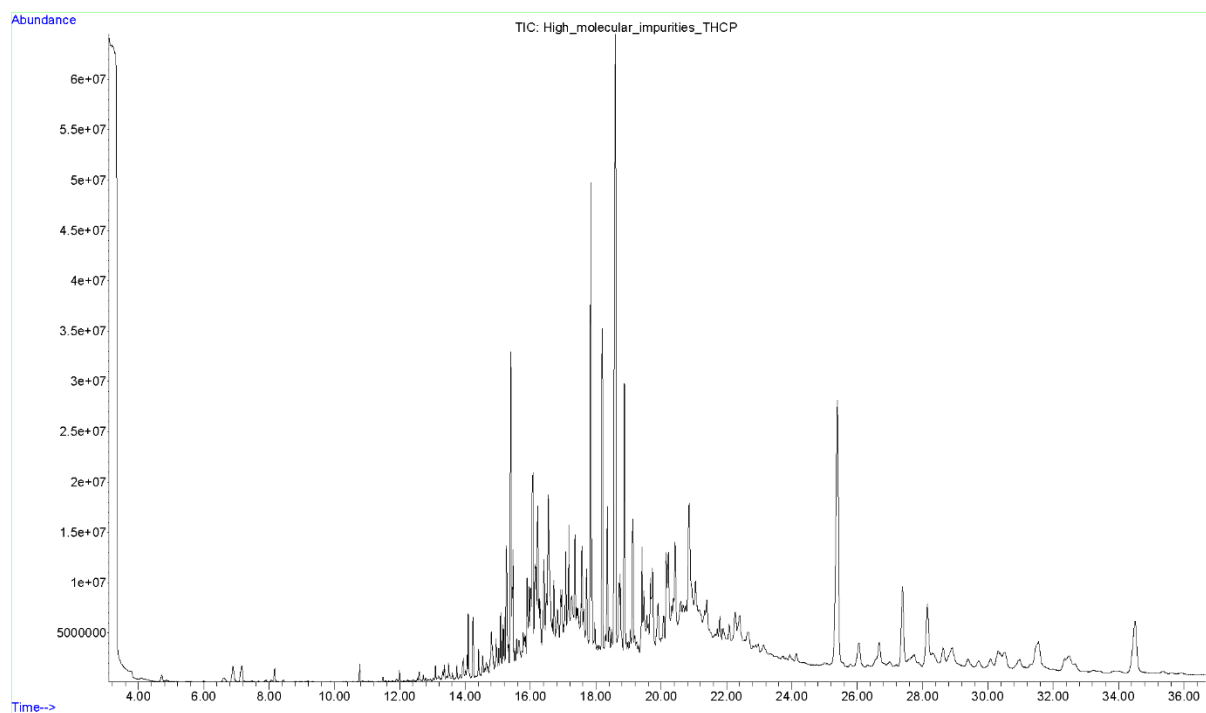
S21: THCP isomer found in the THCP vape pen liquid with a very similar fragmentation pattern as Δ^9 -THCP, potentially the *cis*-isomer *cis*- Δ^9 -THCP (THCP impurity B)



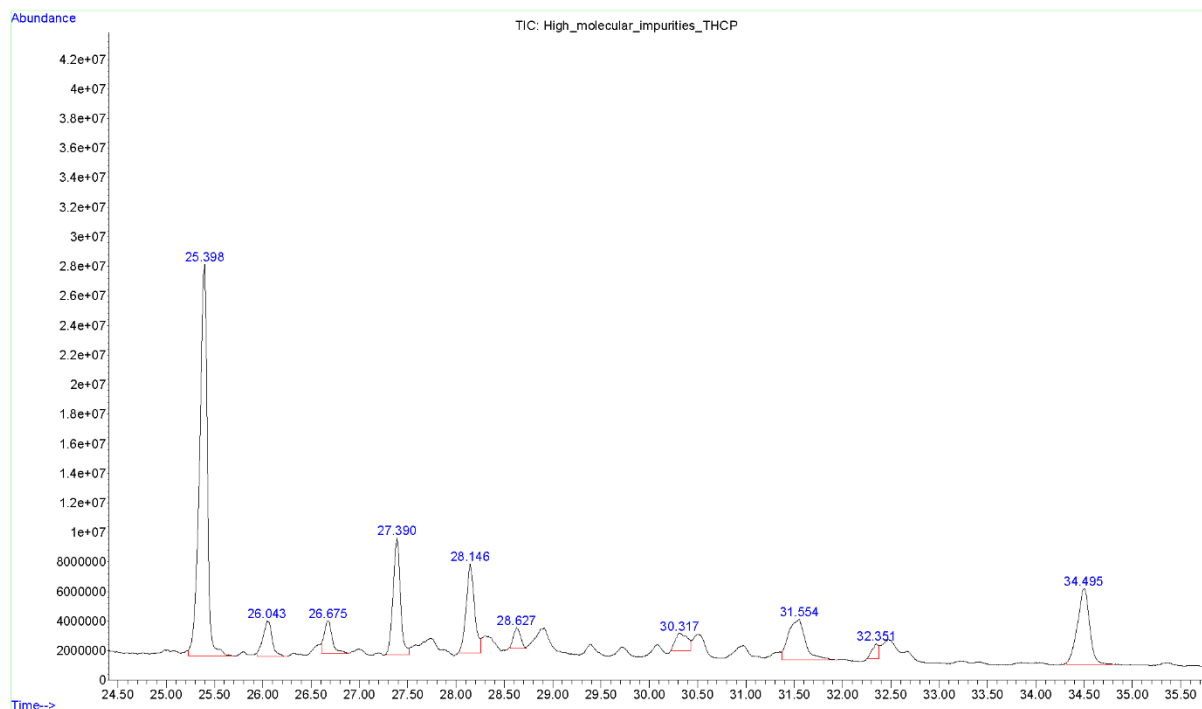
S22: Unknown impurity found in the THCP vape pen liquid, potentially a dihydrocannabiphorol (THCP impurity C)



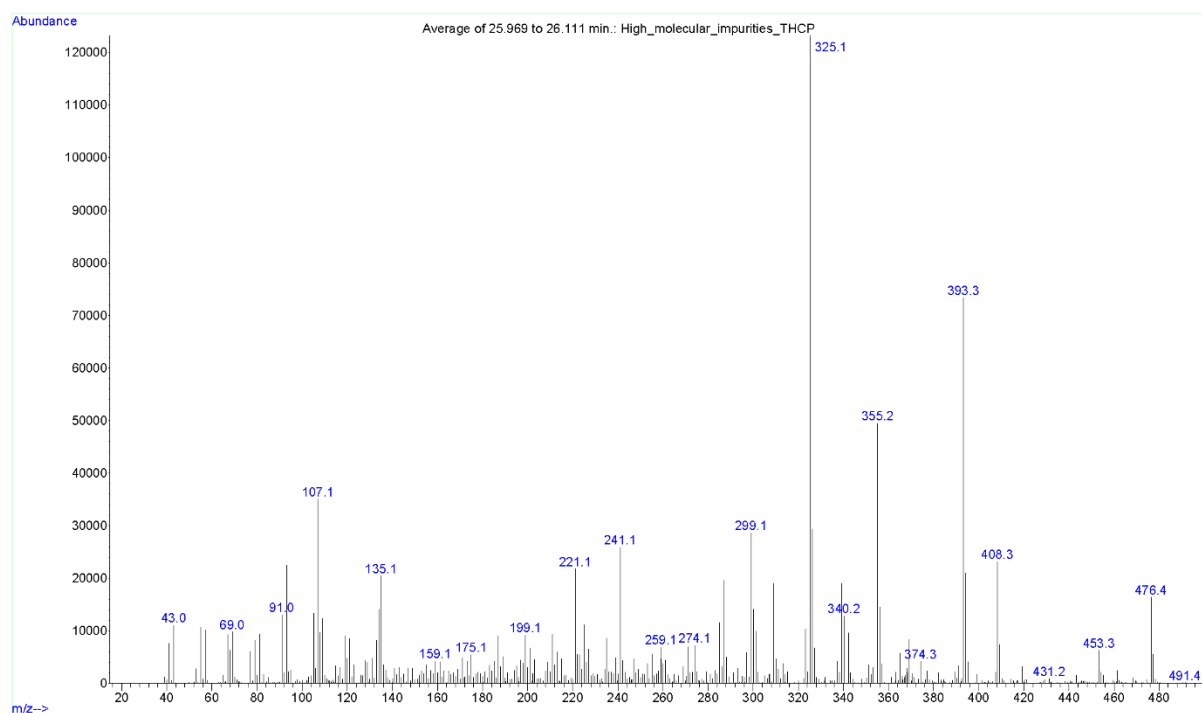
S23: Unknown impurity found in the THCP vape pen liquid, potentially a second dihydrocannabiphorol (THCP impurity D)



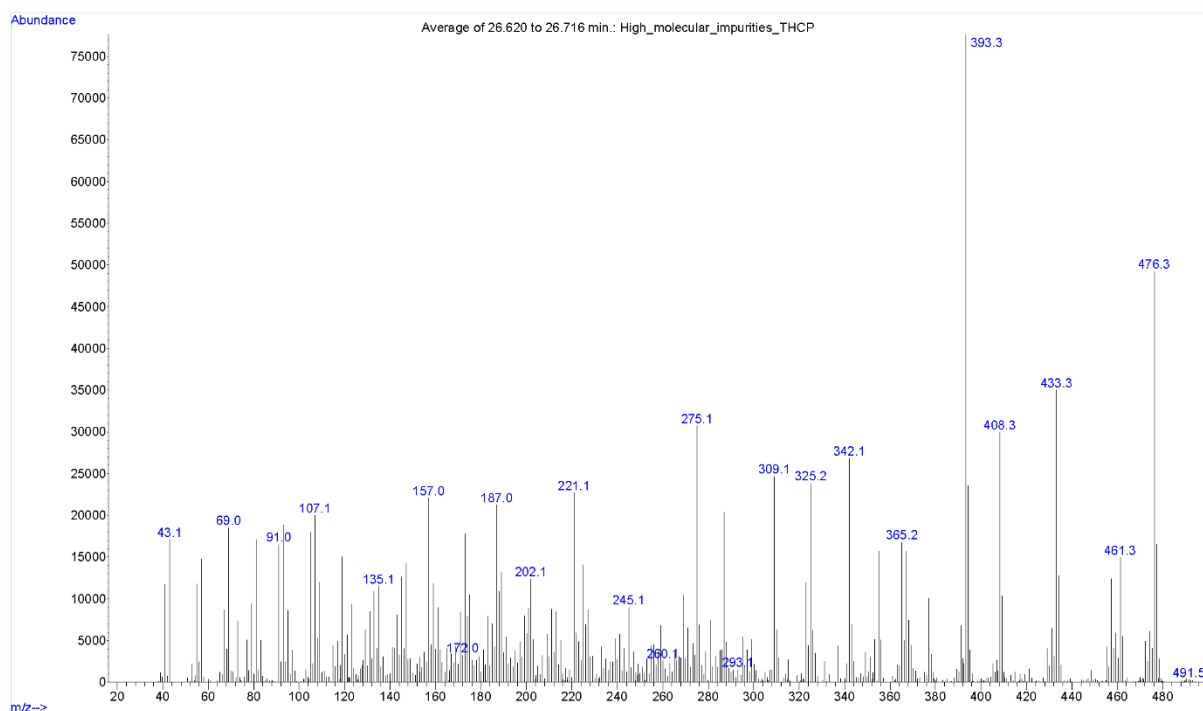
S24: TIC of a chromatographic fraction from the THCP vape pen liquid containing impurities with a high molecular mass. The impurities are found between 24 and 36 min.



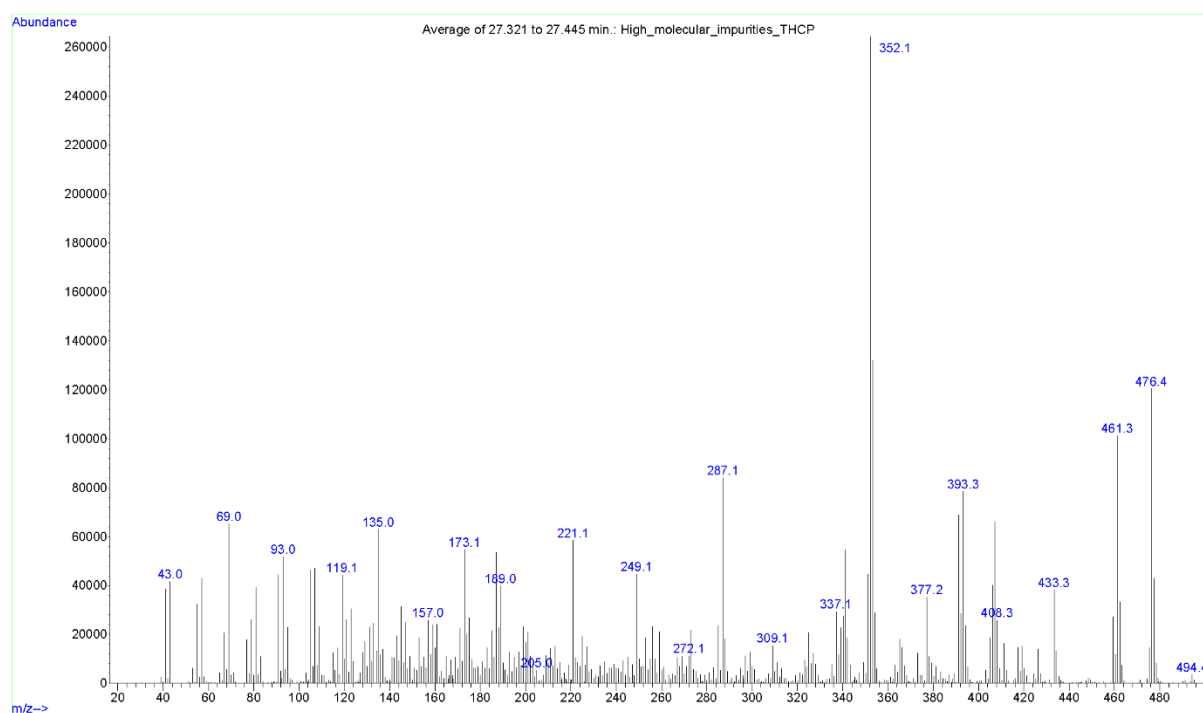
S25: TIC of a chromatographic fraction of the THCP vape pen liquid. Detail from S25.



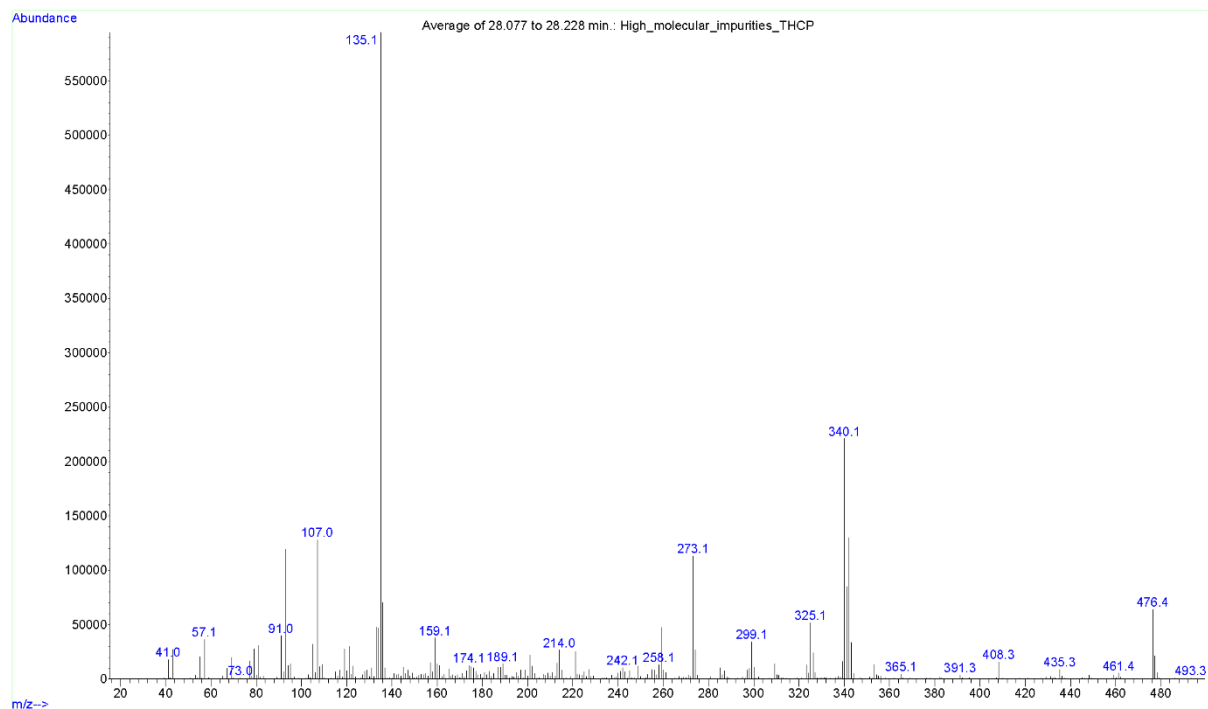
S26: EI mass spectrum of a bisalkylated cannabinoid



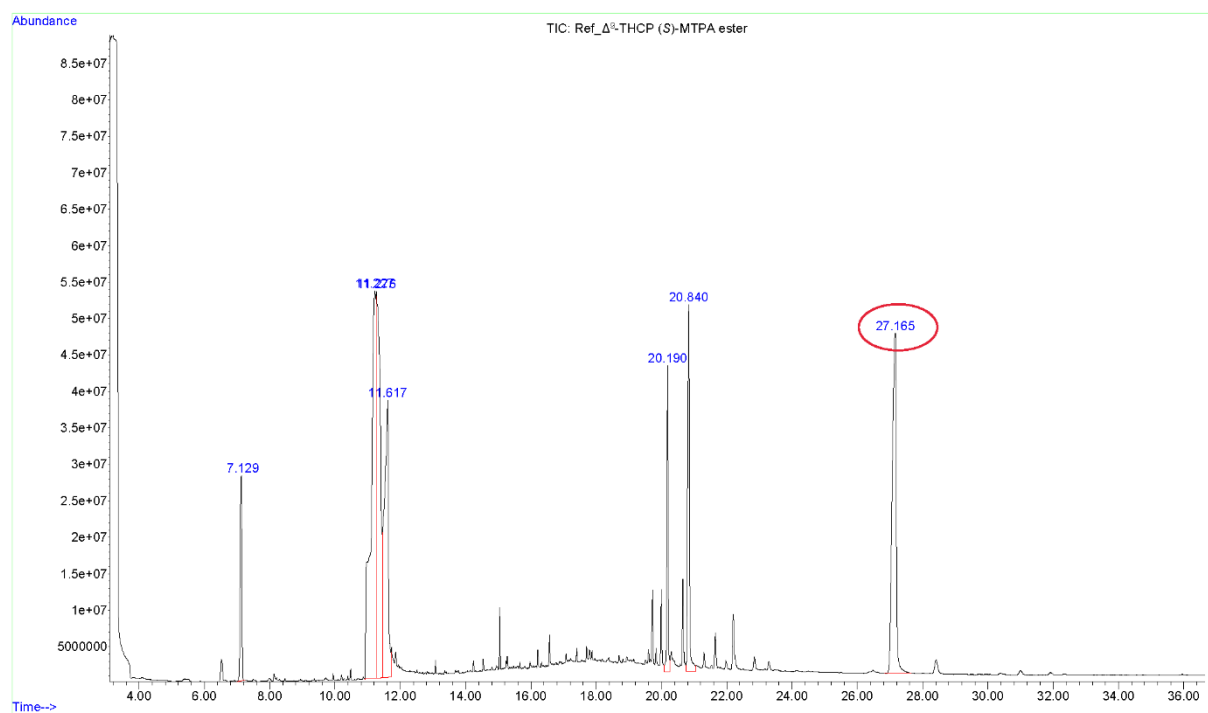
S27: EI mass spectrum of a bisalkylated cannabinoid



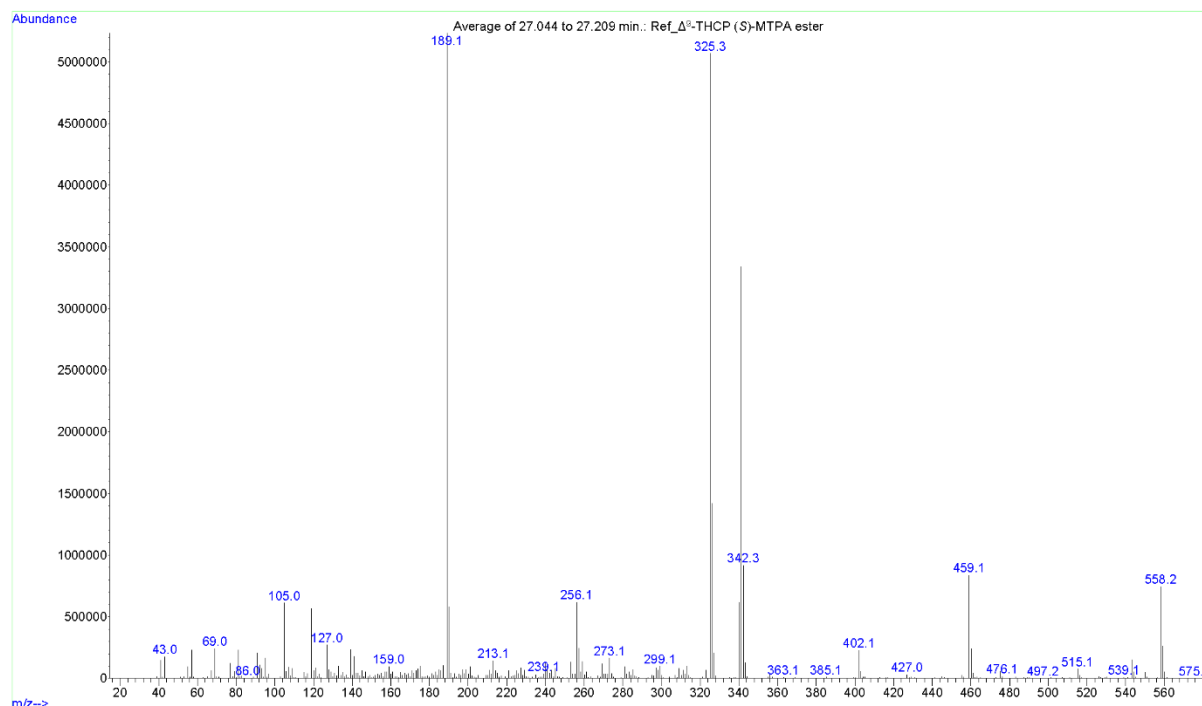
S28: EI mass spectrum of a bisalkylated cannabinoid



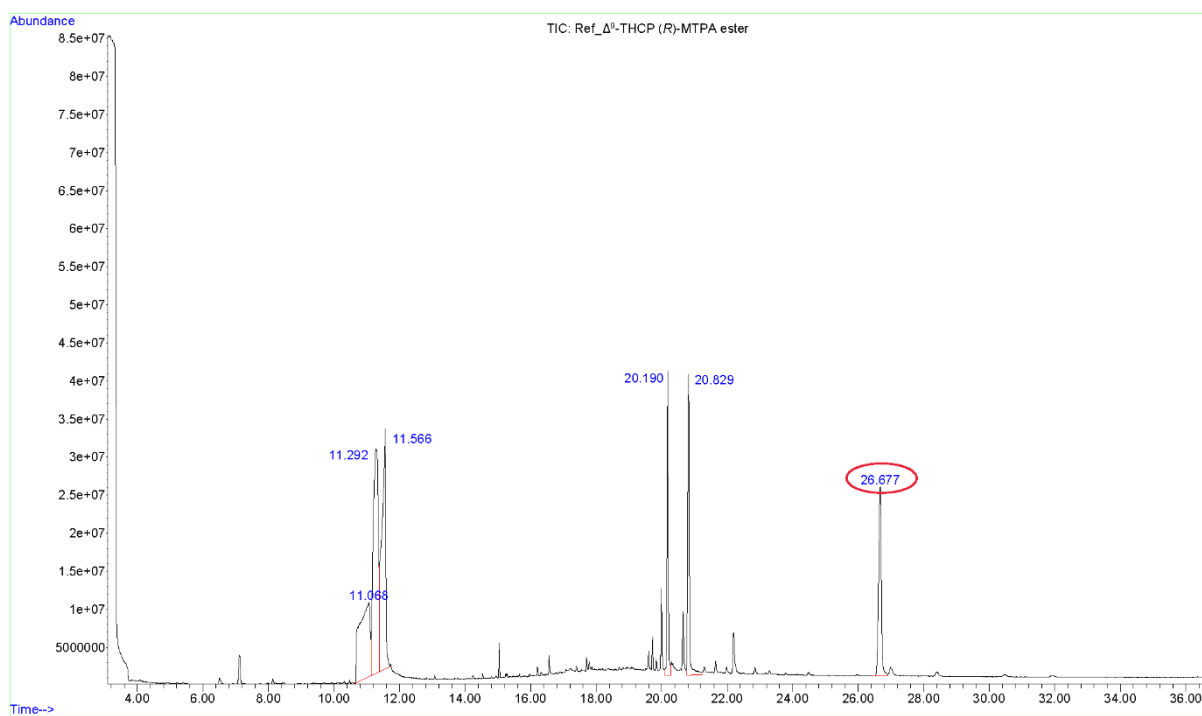
S29: EI mass spectrum of a bisalkylated cannabinoid



S30: TIC of the (S)-Mosher ester of Δ^9 -THCP.



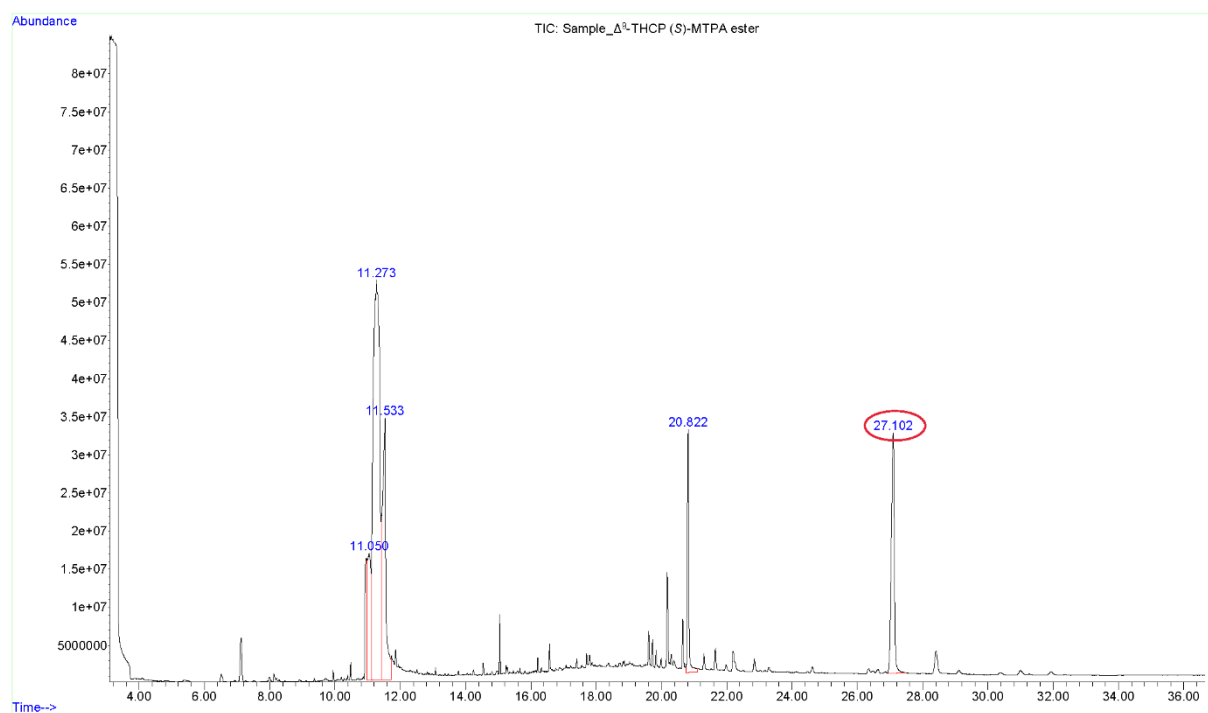
S31: EI mass spectrum of the (S)-Mosher ester of Δ⁹-THCP.



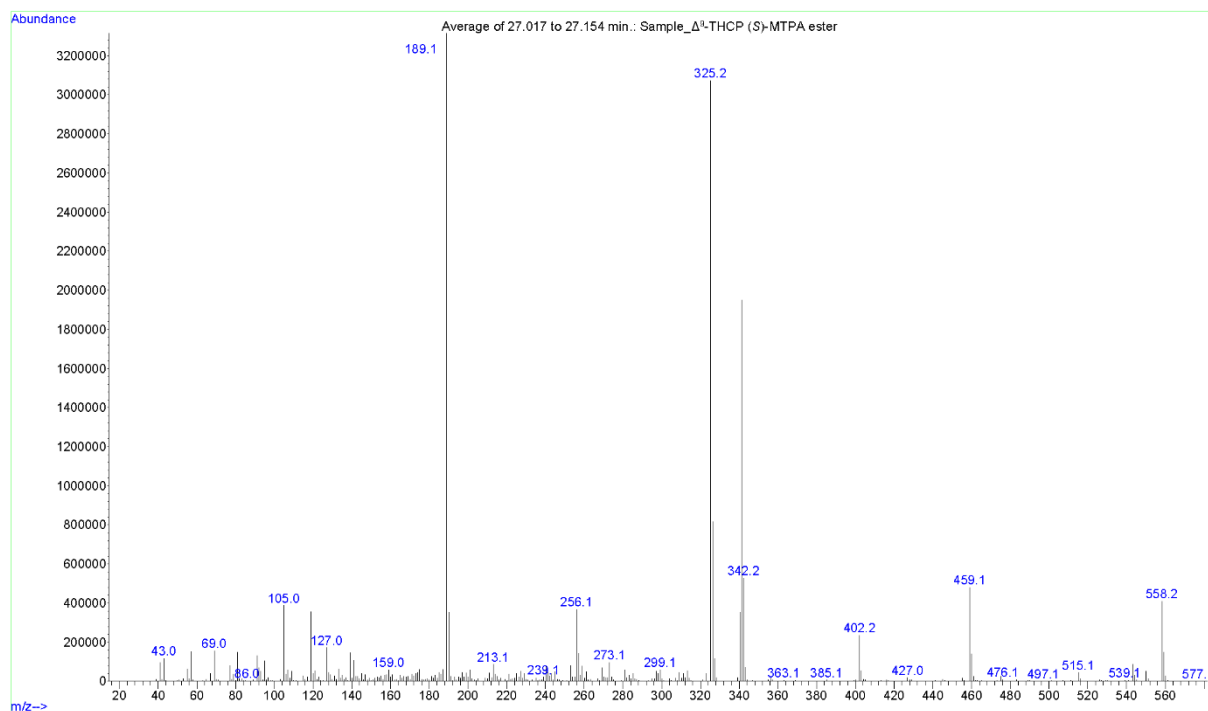
S32: TIC of the (R)-Mosher ester of Δ⁹-THCP.



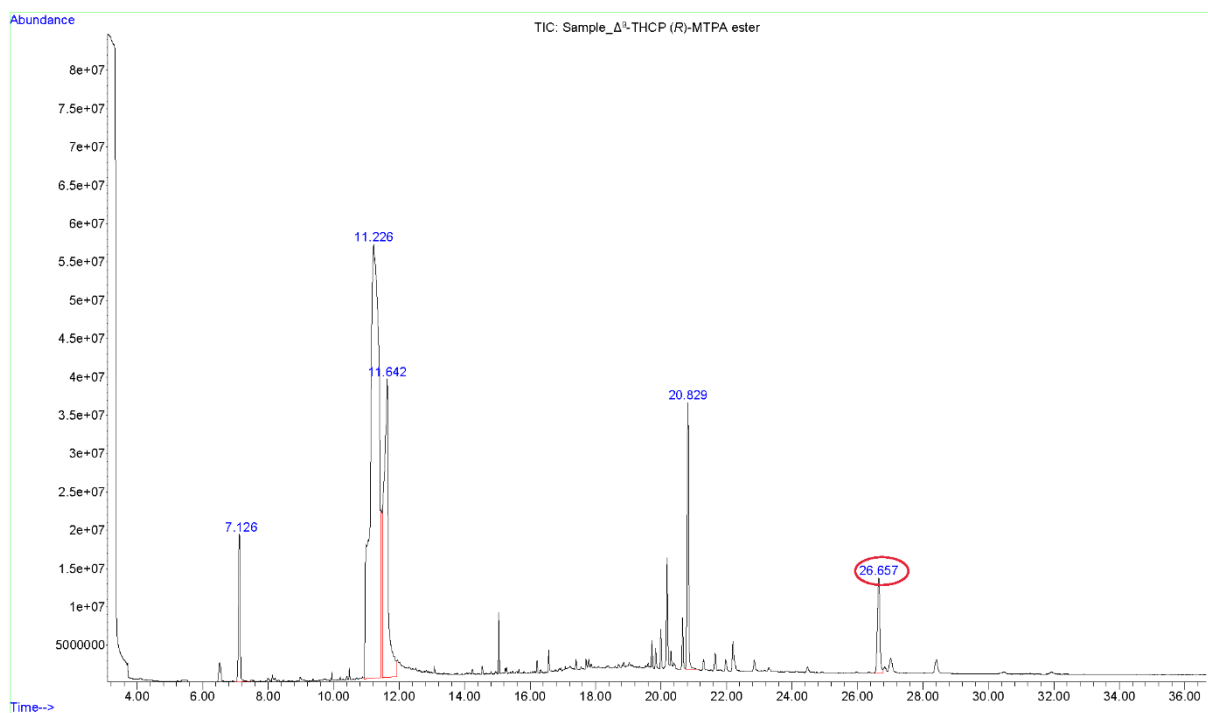
S33: EI mass spectrum of the (R)-Mosher ester of Δ⁹-THCP.



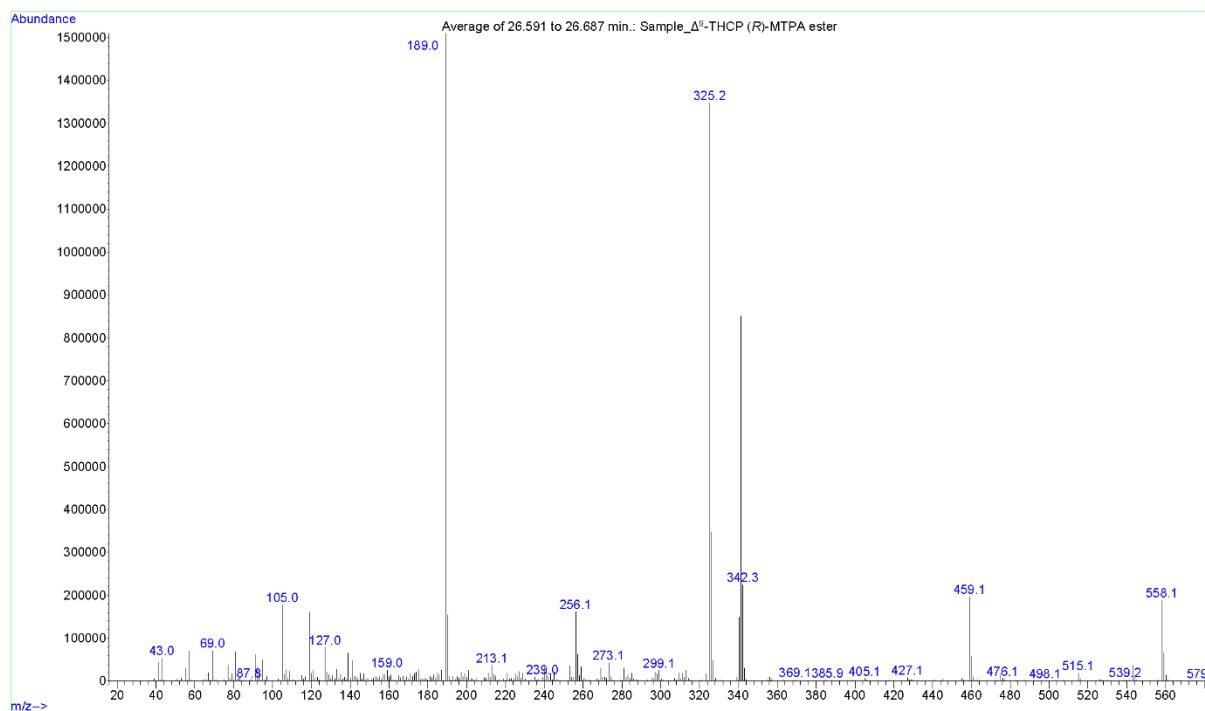
S34: TIC of the (S)-Mosher ester of the isolated Δ⁹-THCP.



S35: EI mass spectrum of the (S)-Mosher ester of the isolated Δ⁹-THCP.



S36: TIC of the (R)-Mosher ester of the isolated Δ⁹-THCP.



S37: EI mass spectrum of the (R)-Mosher ester of the isolated Δ^9 -THCP.