

Supplementary Information

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

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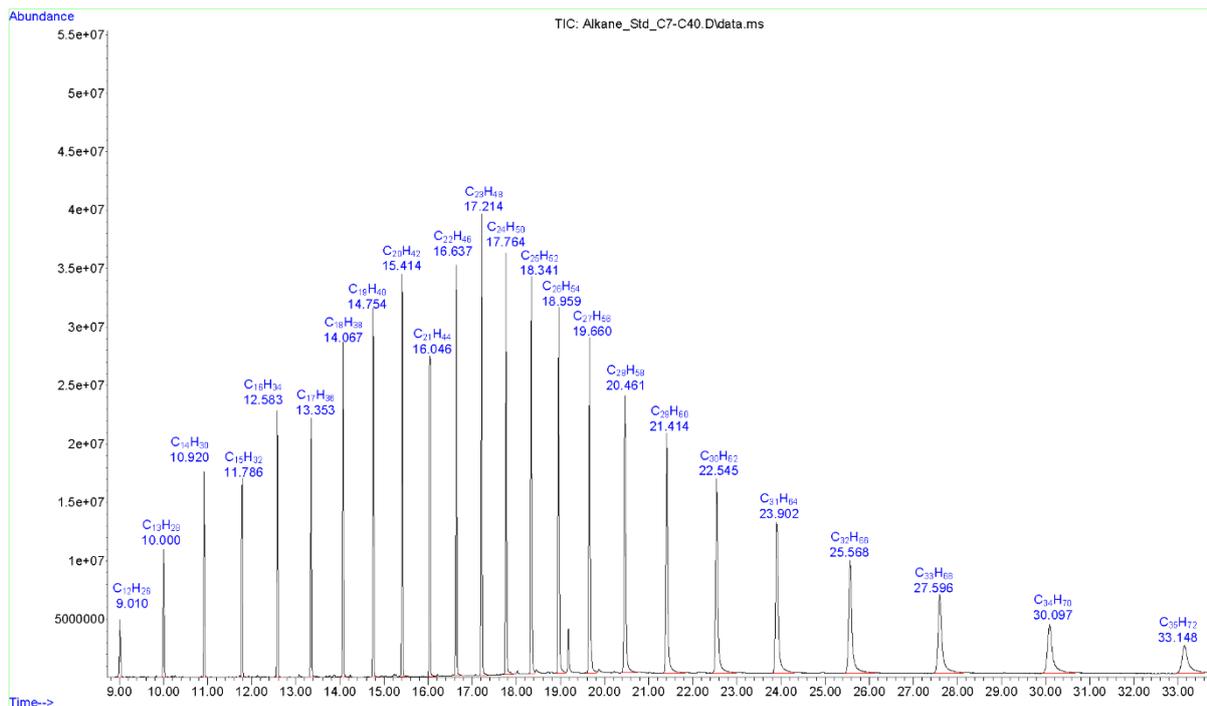
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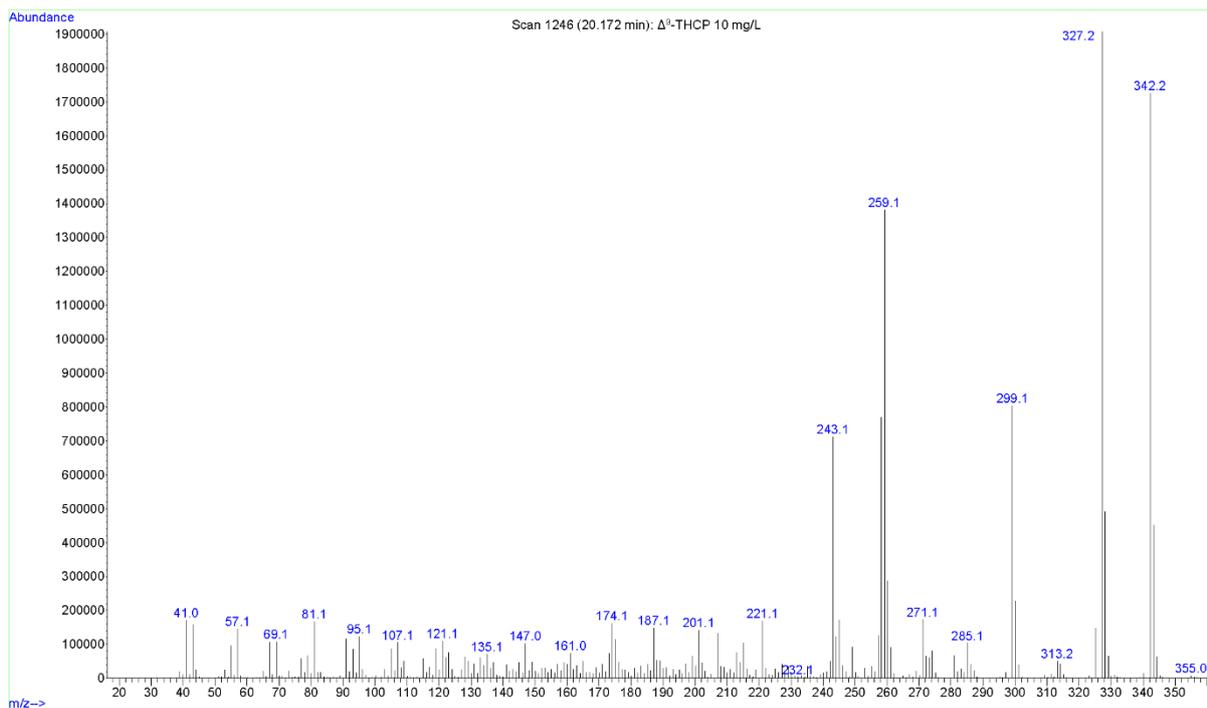
e-mail address: willi.schirmer@irm.unibe.ch

Table of contents

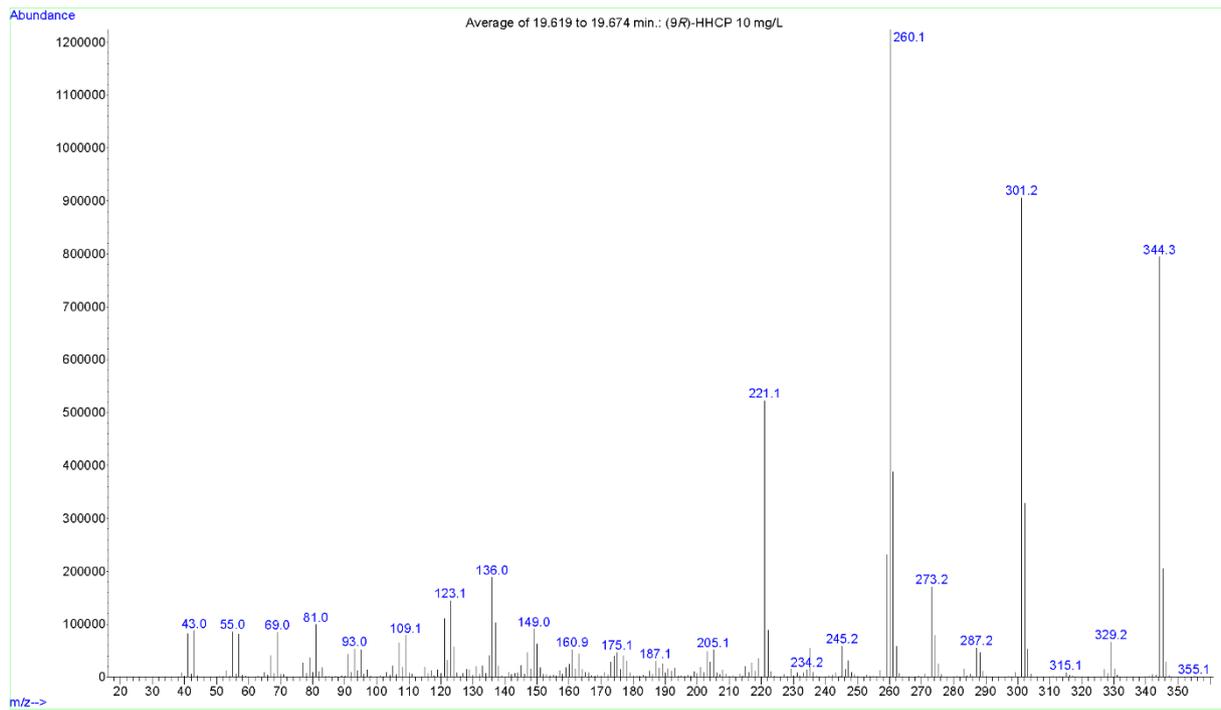
- TIC of *n*-Alkanes (Kovàts-index) **S1**
- EI reference mass spectra **S2-S8**
 - Δ^9 -THCP, (9*R*)-HHCP, (9*S*)-HHCP, CBDP, CBP, 5-Heptylresorcinol, Δ^8 -THCP
- EI mass spectra of identified terpenes in the sample..... **S9-S15**
 - α -humulene, β -myrcene, β -pinene, caryophyllene, β -phellandrene, (*R*)-limonene, *m*-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 *m/z* 476 **S26-29**
- Chromatograms and mass spectra of Δ^9 -THCP Mosher esters
 - (*S*)-Mosher ester of Δ^9 -THCP Reference **S30-S31**
 - (*R*)-Mosher ester of Δ^9 -THCP Reference..... **S32-S33**
 - (*S*)-Mosher ester of Δ^9 -THCP from vape pen **S34-S35**
 - (*R*)-Mosher ester of Δ^9 -THCP from vape pen..... **S36-S37**



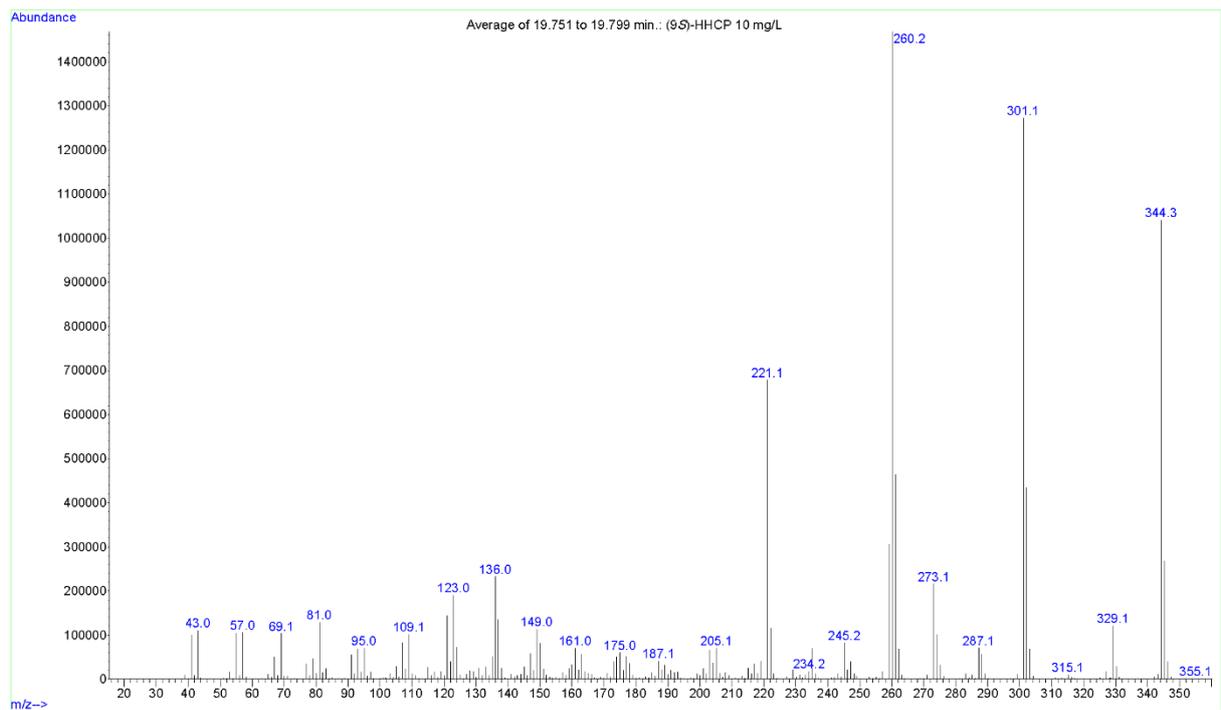
S1 TIC of an alkane standard (C7-C40) for the determination of Kováts indices.



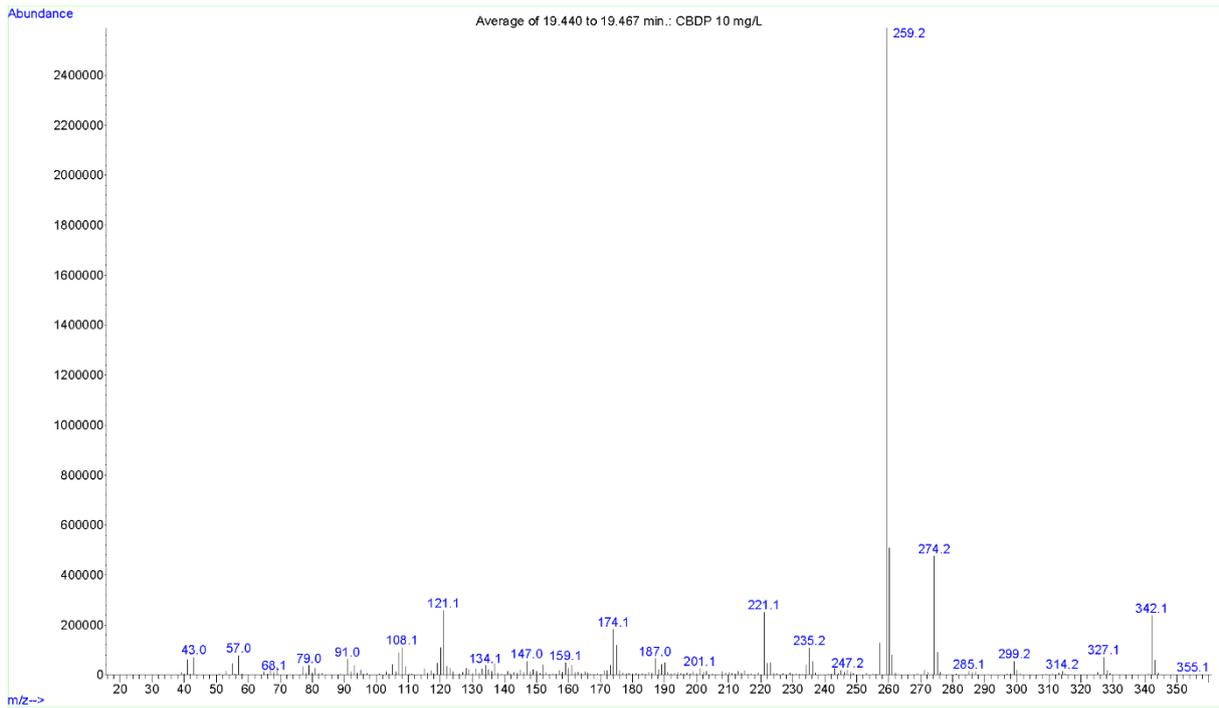
S2: EI mass spectrum of Δ⁹-THCP (reference)



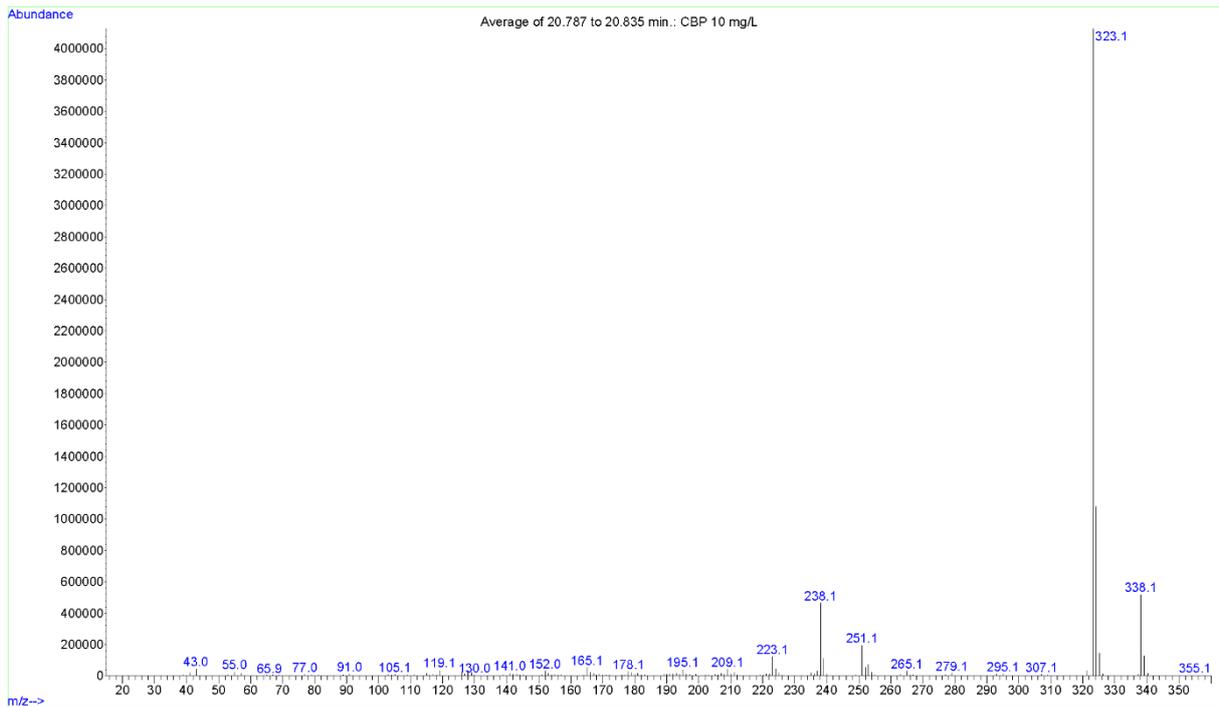
S3: EI mass spectrum of (9R)-HHCP (reference)



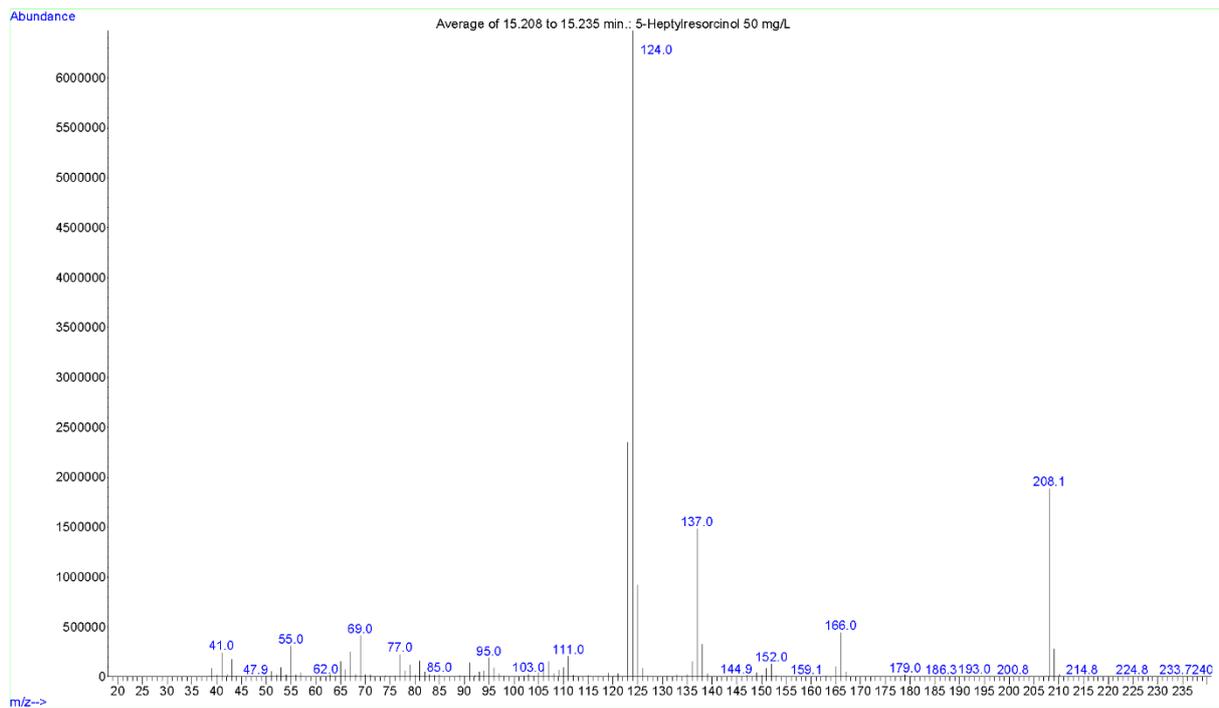
S4: EI mass spectrum of (9S)-HHCP (reference)



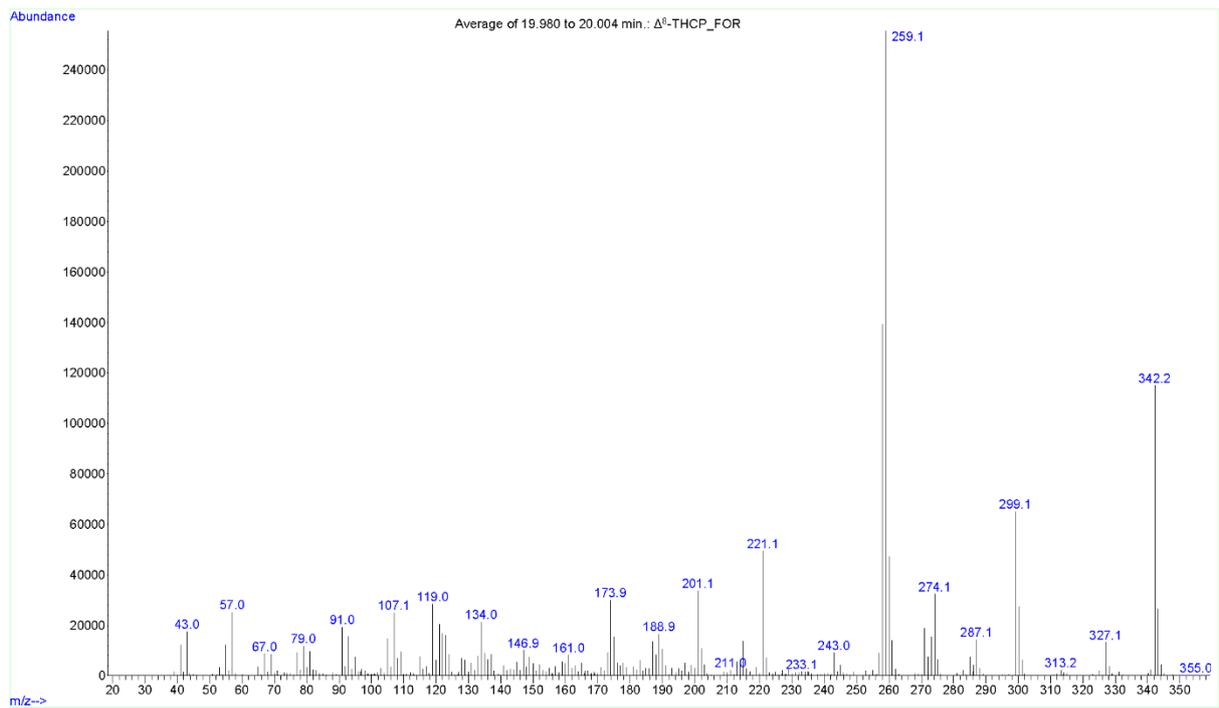
S5: EI mass spectrum of CDBP (reference)



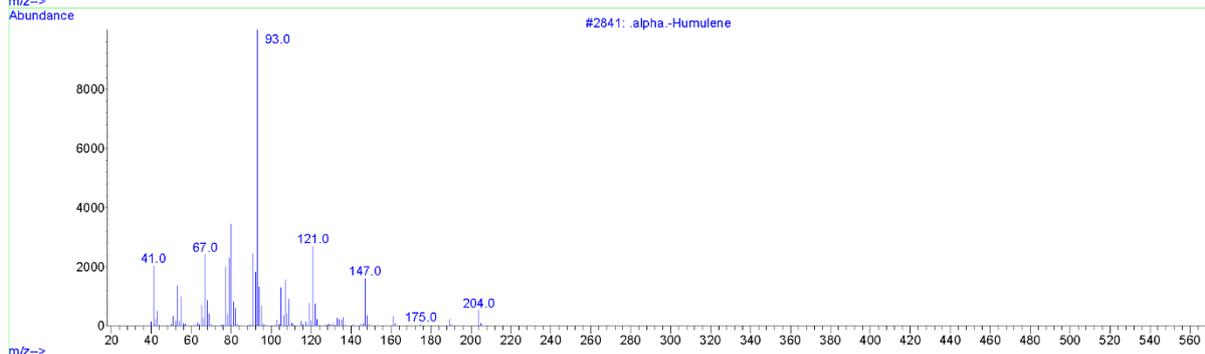
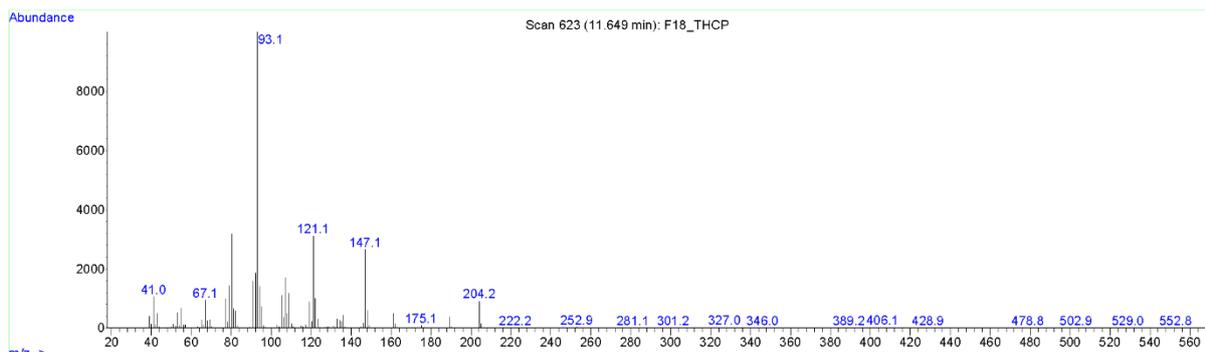
S6: EI mass spectrum of CBP (reference)



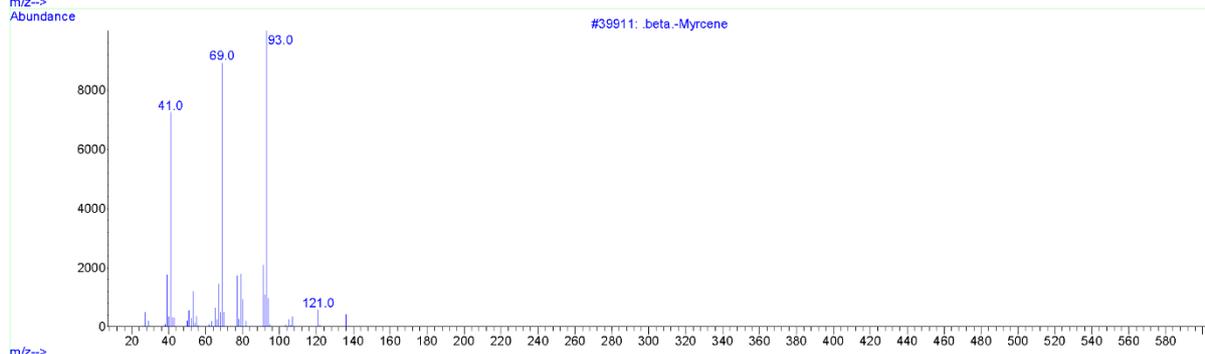
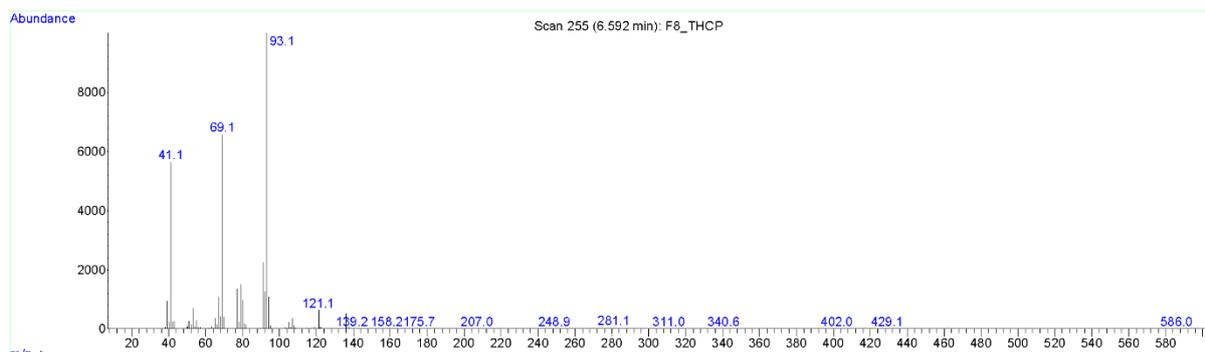
S7: EI mass spectrum of 5-heptylresorcinol (reference)



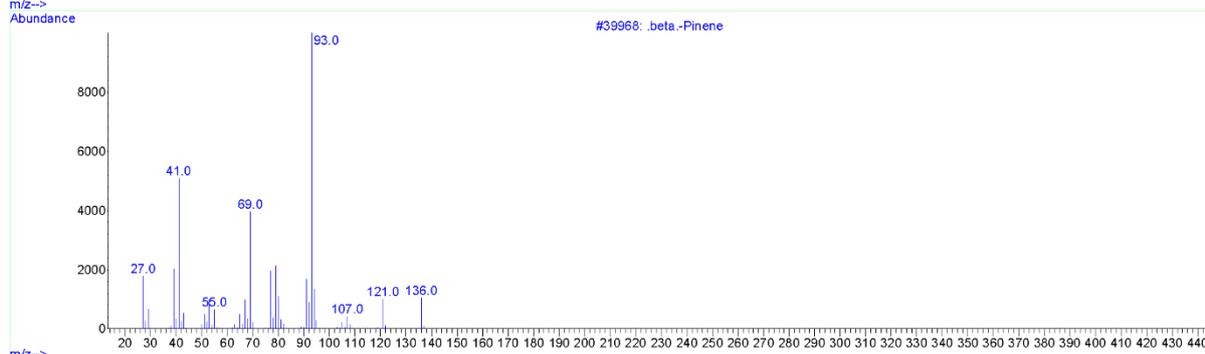
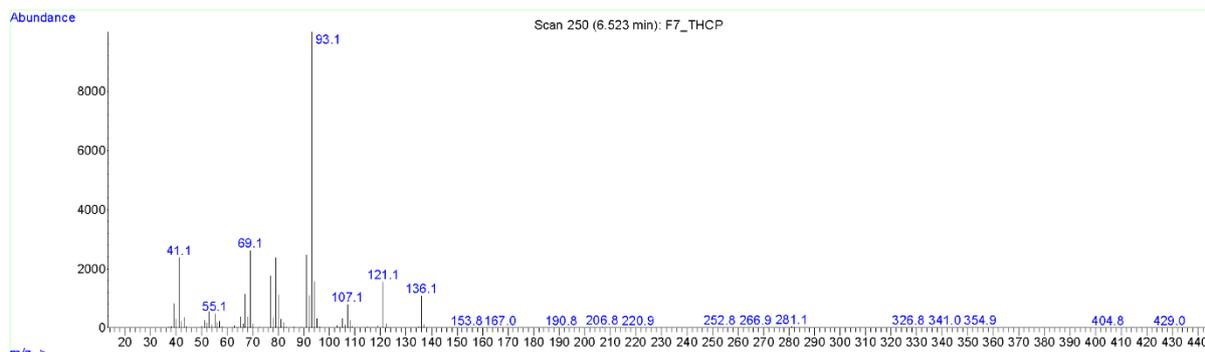
S8: EI mass spectrum of Δ^8 -THCP (reference)



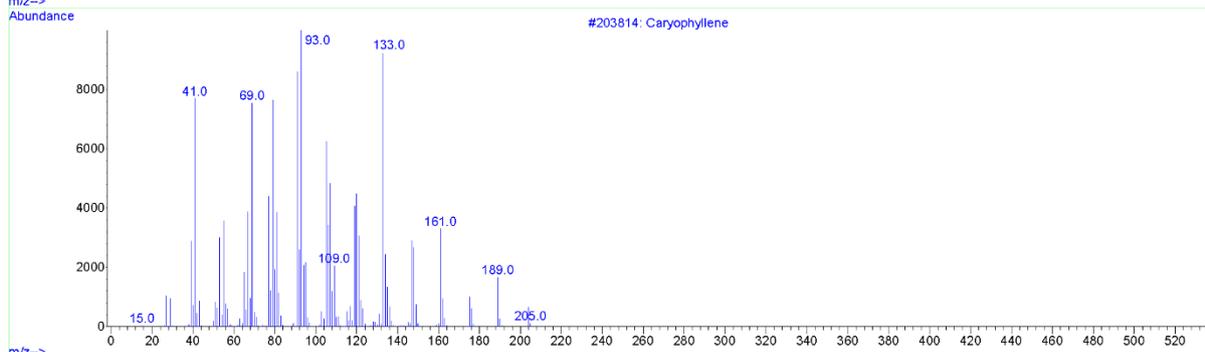
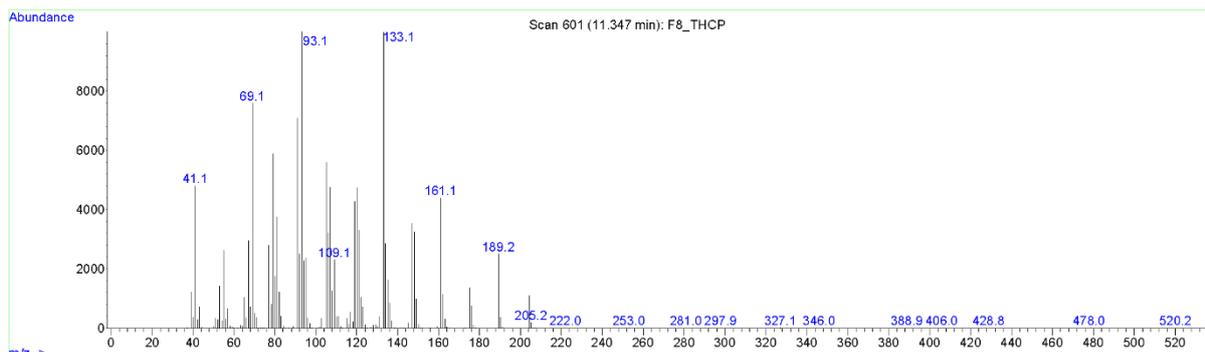
S9: α -Humulene found in a chromatographic fraction of the THCP vape pen liquid.



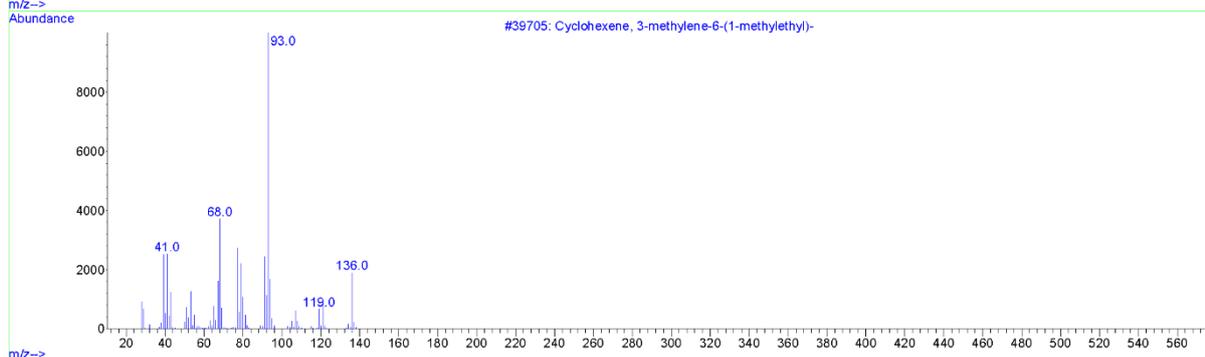
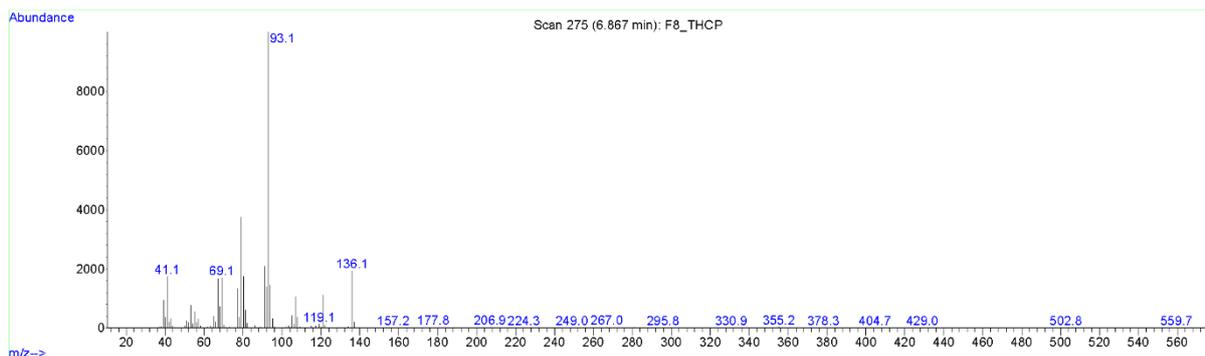
S10: β -Myrcene found in a chromatographic fraction of the THCP vape pen liquid.



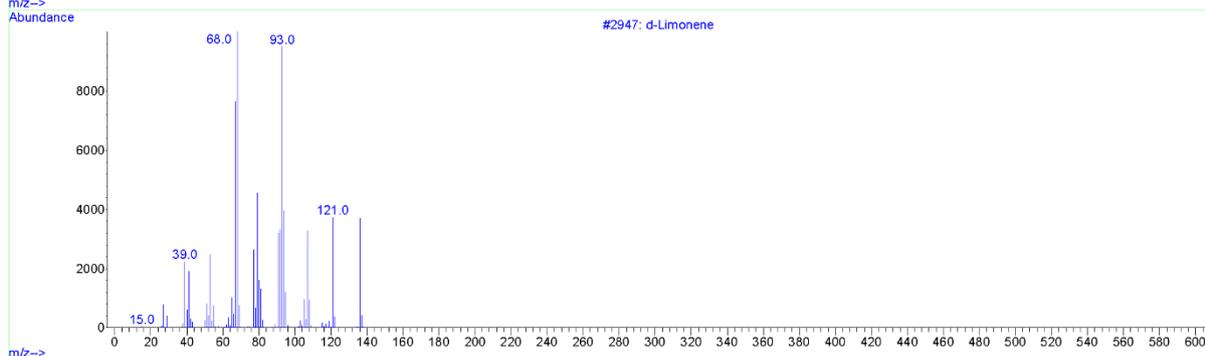
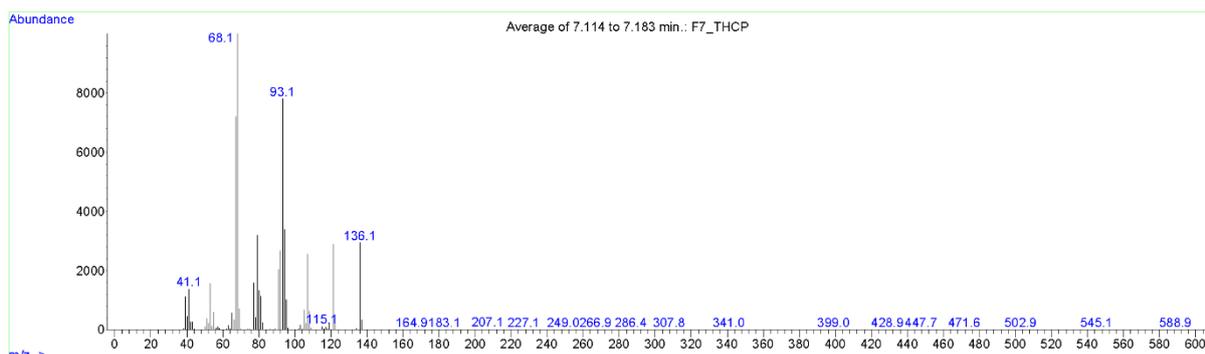
S11: β -Pinene found in a chromatographic fraction of the THCP vape pen liquid



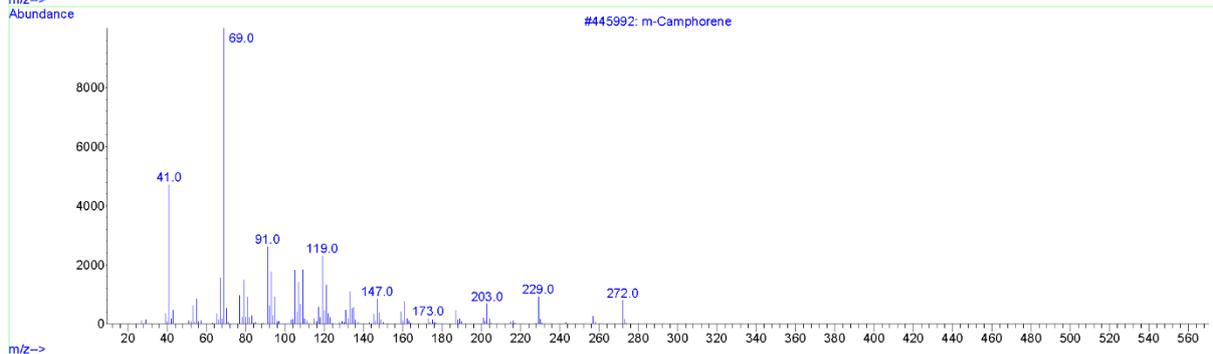
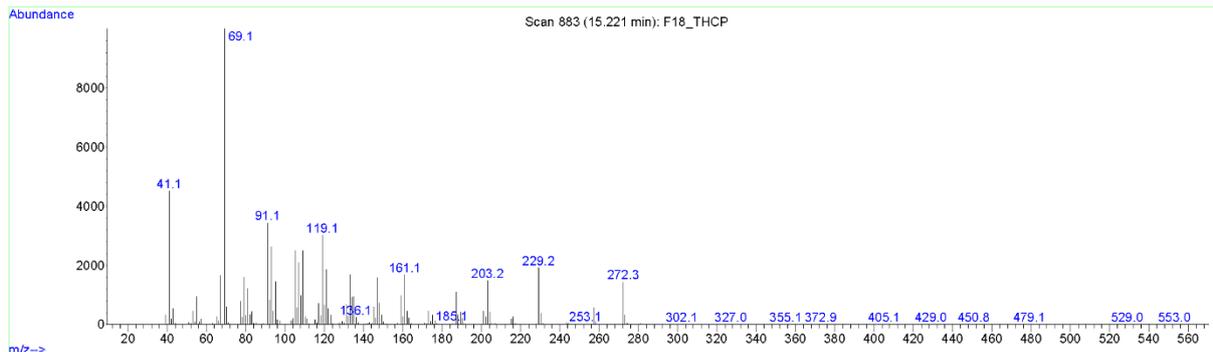
S12: Caryophyllene found in a chromatographic fraction of the THCP vape pen liquid



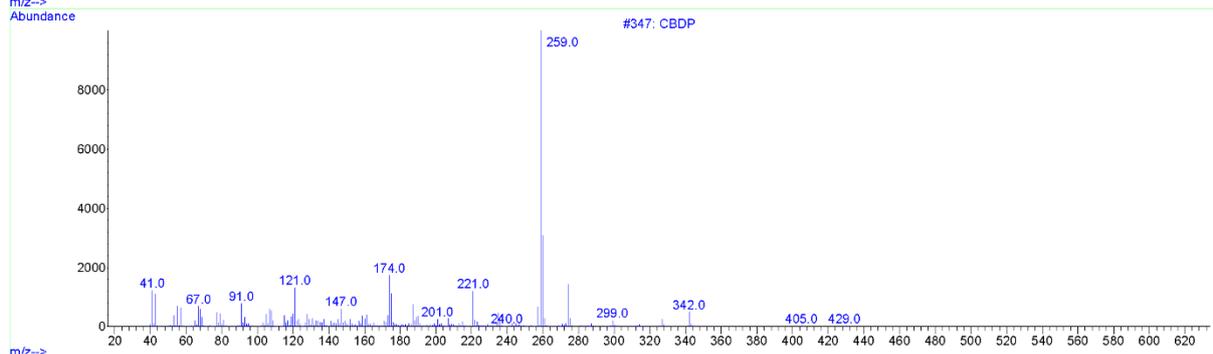
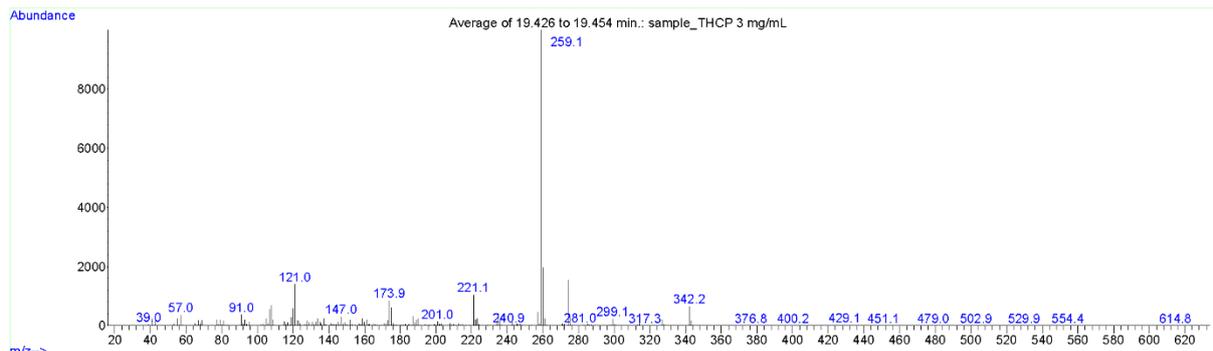
S13: β -Phellandrene found in a chromatographic fraction of the THCP vape pen liquid



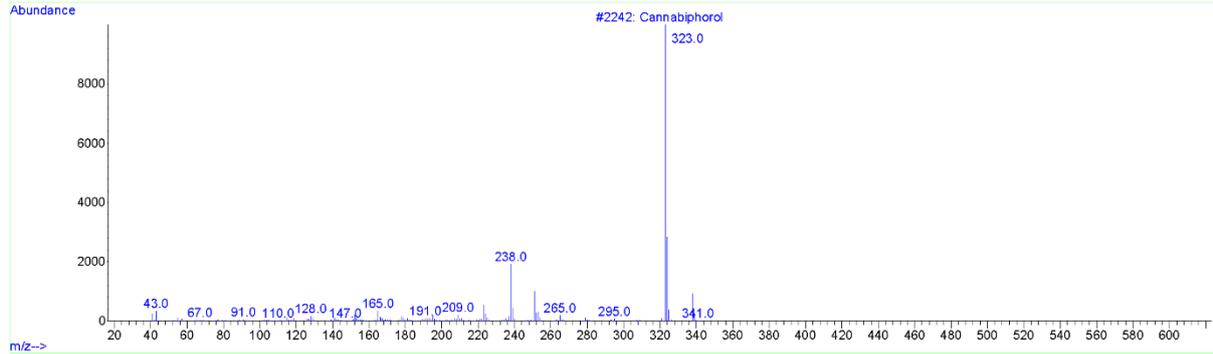
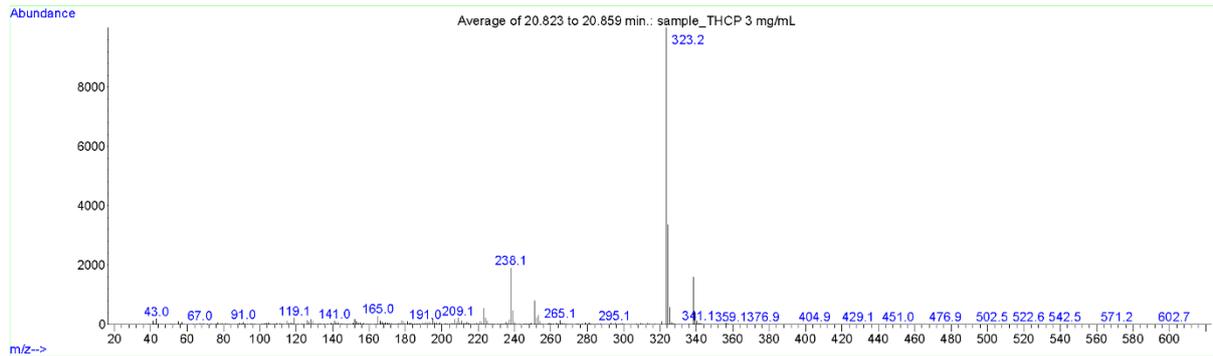
S14: (*R*)-Limonene found in a chromatographic fraction of the THCP vape pen liquid



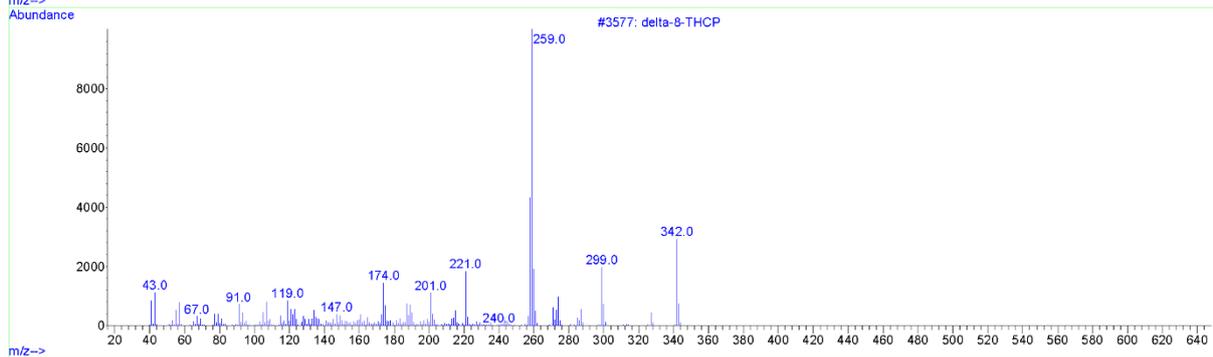
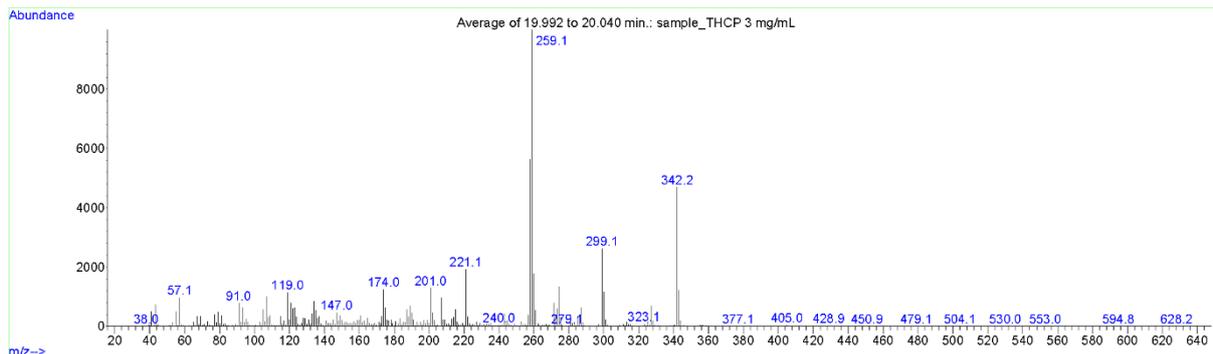
S15: *m*-Camphorene found in a chromatographic fraction of the THCP vape pen liquid



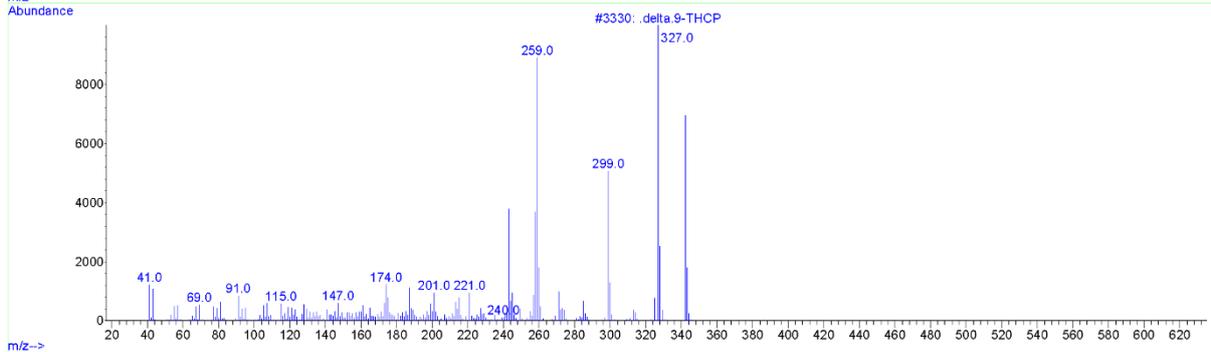
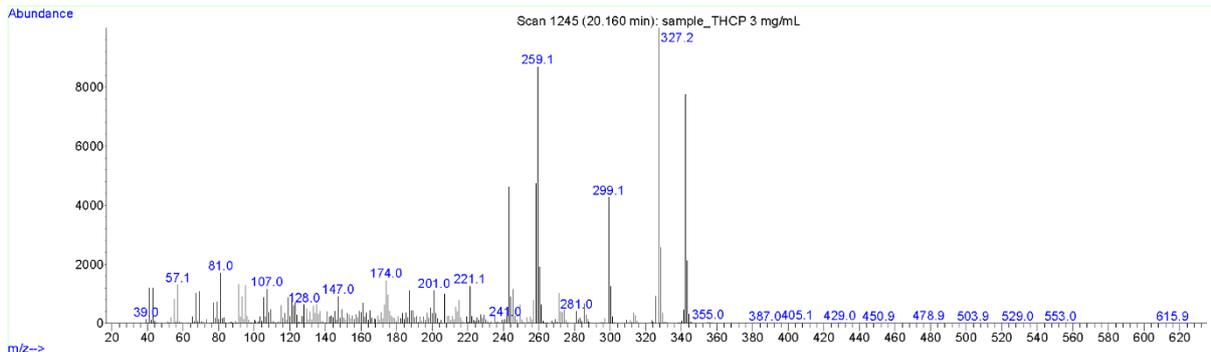
S16: CBDP found in the THCP vape pen liquid



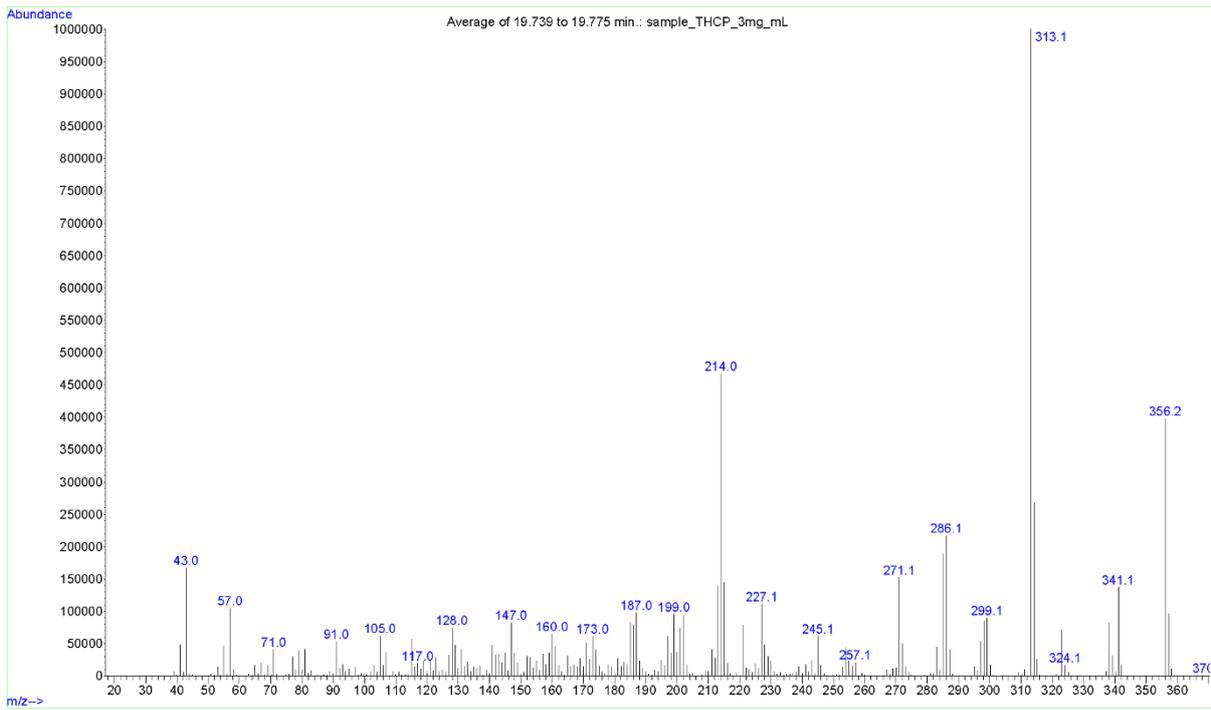
S17: CBP found in the THCP vape pen liquid



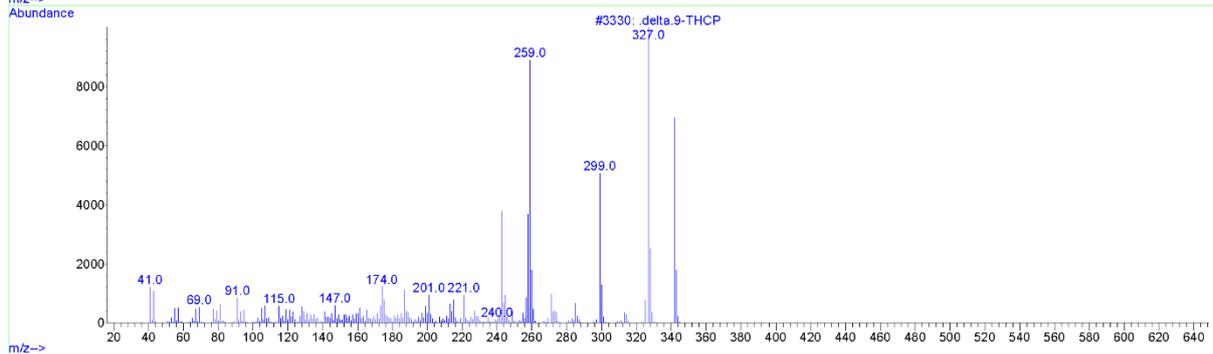
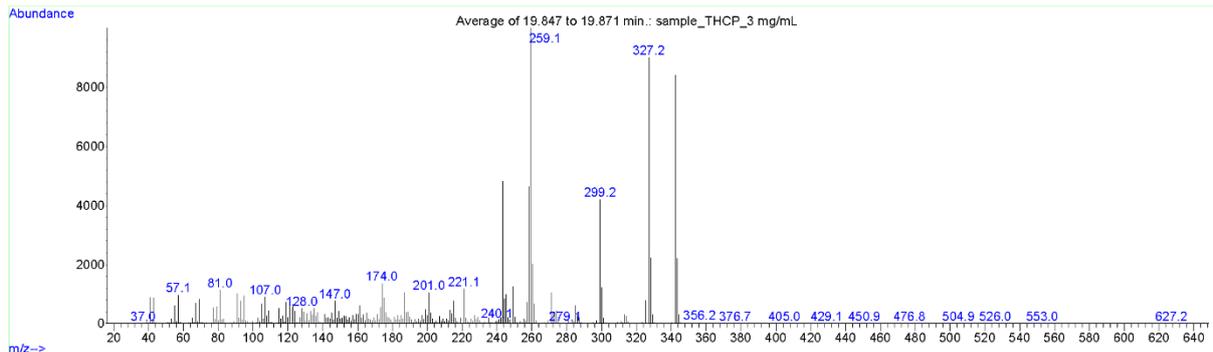
S18: Δ^8 -THCP found in the THCP vape pen liquid



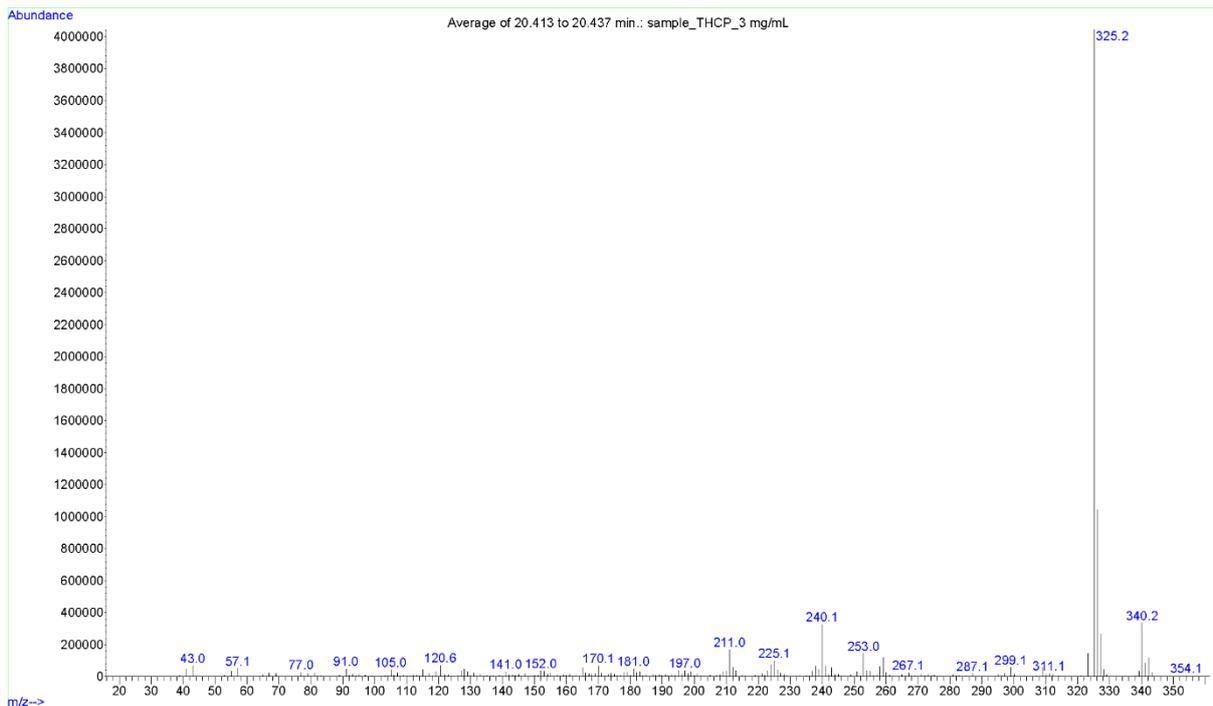
S19: Δ^9 -THCP found in the THCP vape pen liquid



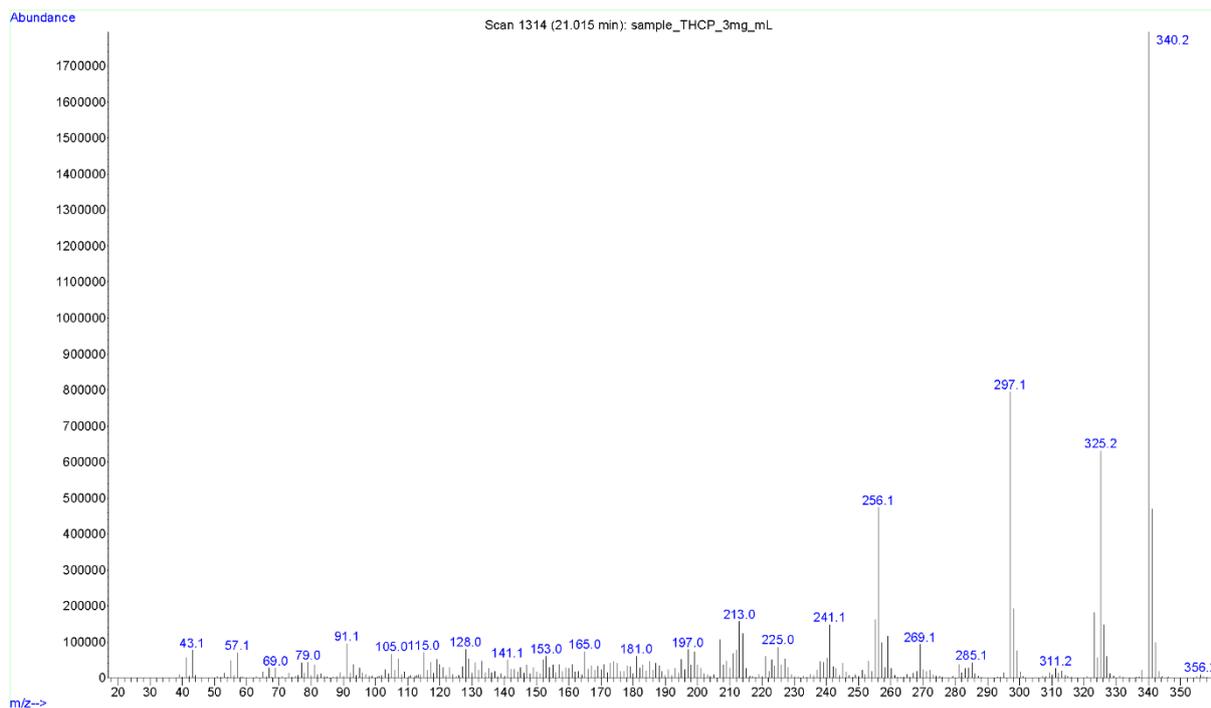
S20: Unknown THCP impurity found in the THCP vape pen liquid, potentially an oxo-THCP. (THCP impurity A)



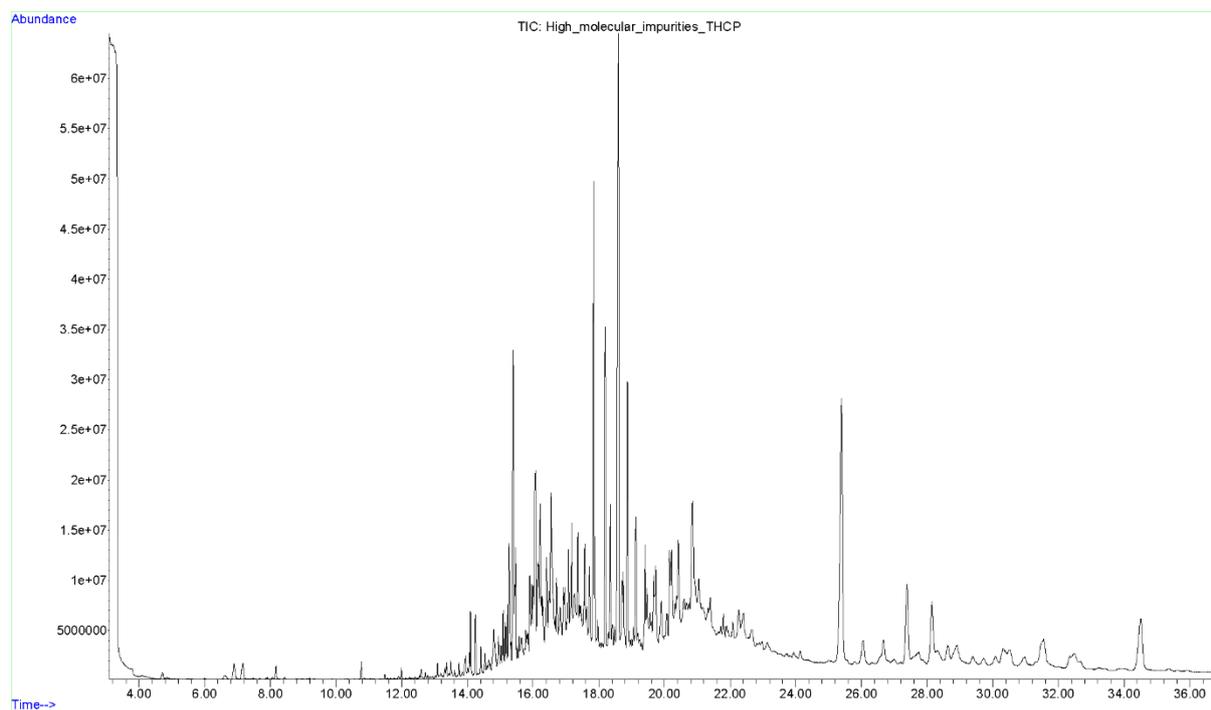
S21: THCP isomer found in the THCP vape pen liquid with a very similar fragmentation pattern as Δ^9 -THCP, potentially the *cis*-isomer *cis*- Δ^9 -THCP (THCP impurity B)



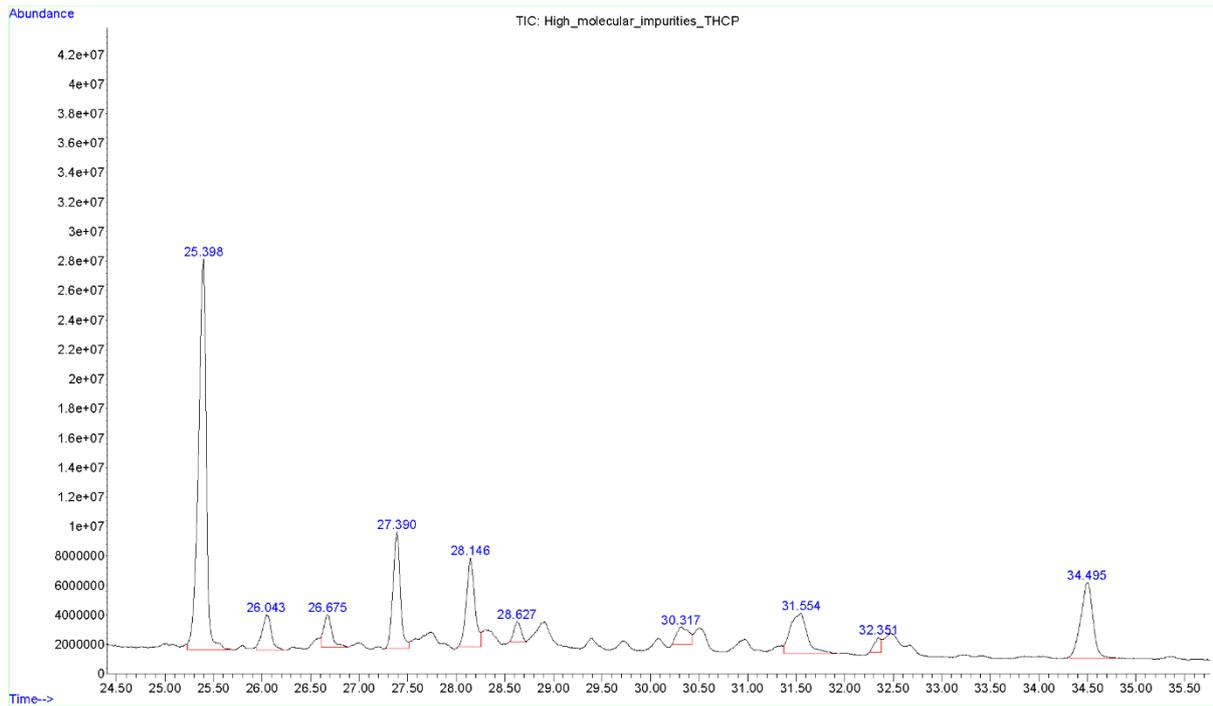
S22: Unknown impurity found in the THCP vape pen liquid, potentially a dihydrocannabiphorol (THCP impurity C)



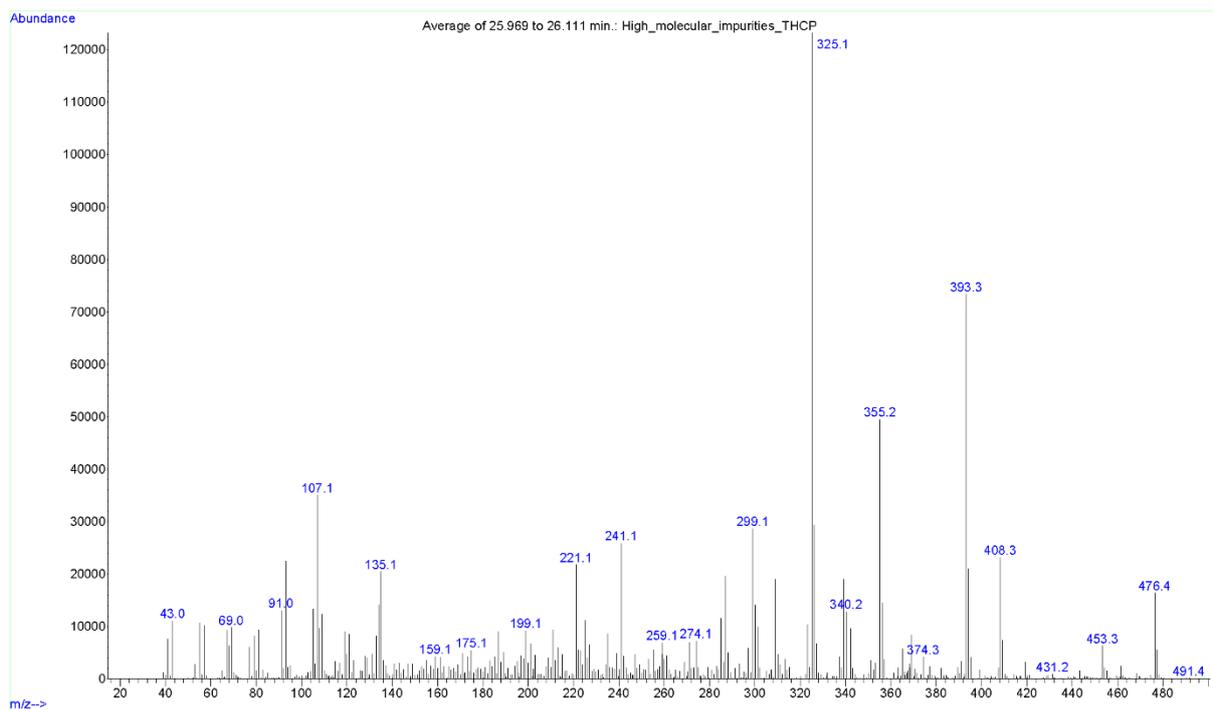
S23: Unknown impurity found in the THCP vape pen liquid, potentially a second dihydrocannabiphorol (THCP impurity D)



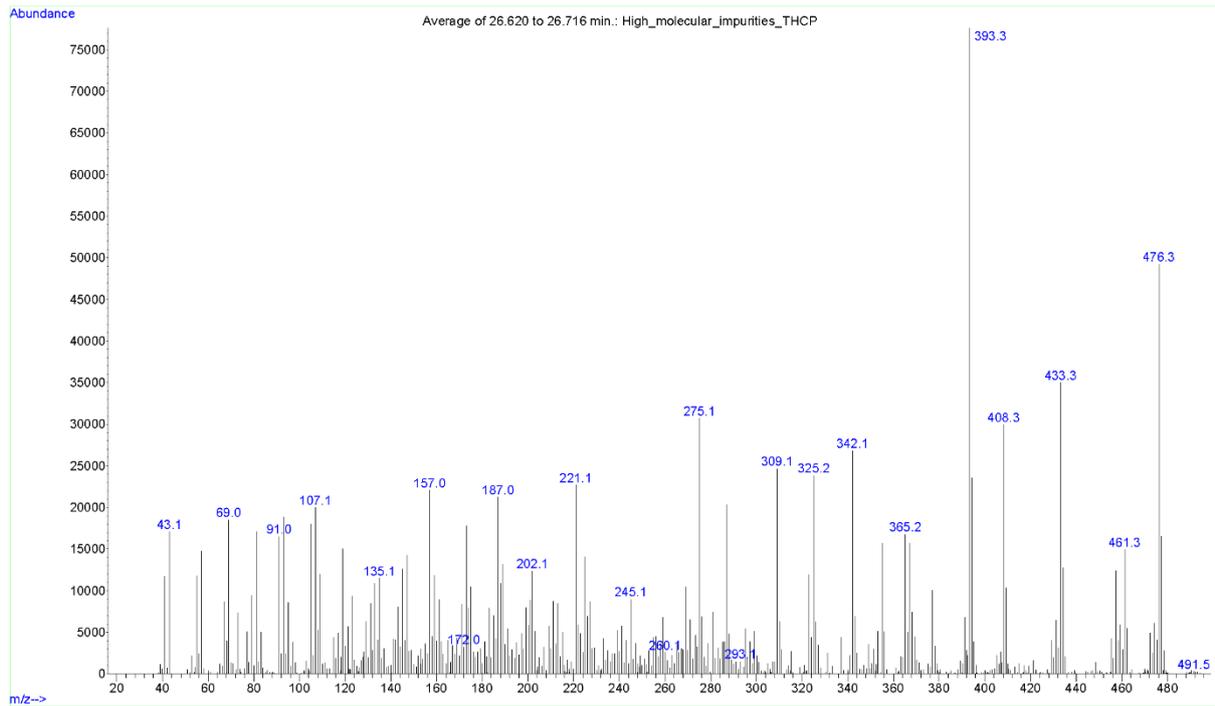
S24: TIC of a chromatographic fraction from the THCP vape pen liquid containing impurities with a high molecular mass. The impurities are found between 24 and 36 min.



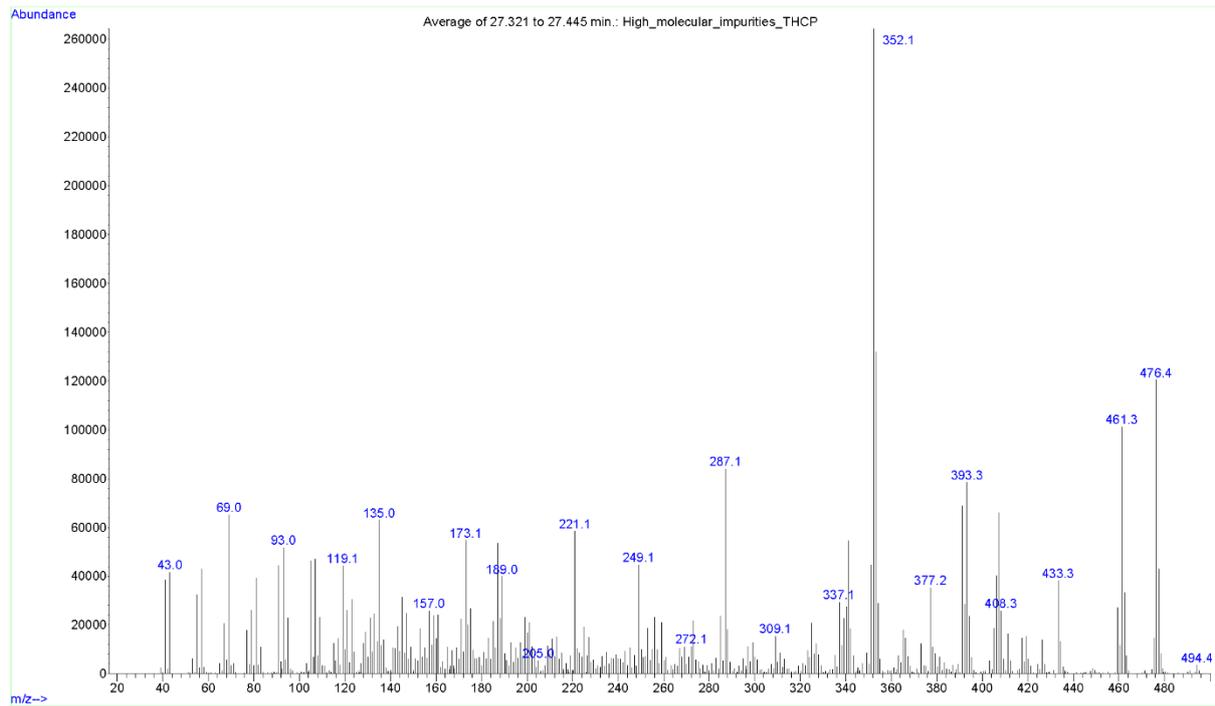
S25: TIC of a chromatographic fraction of the THCP vape pen liquid. Detail from S25.



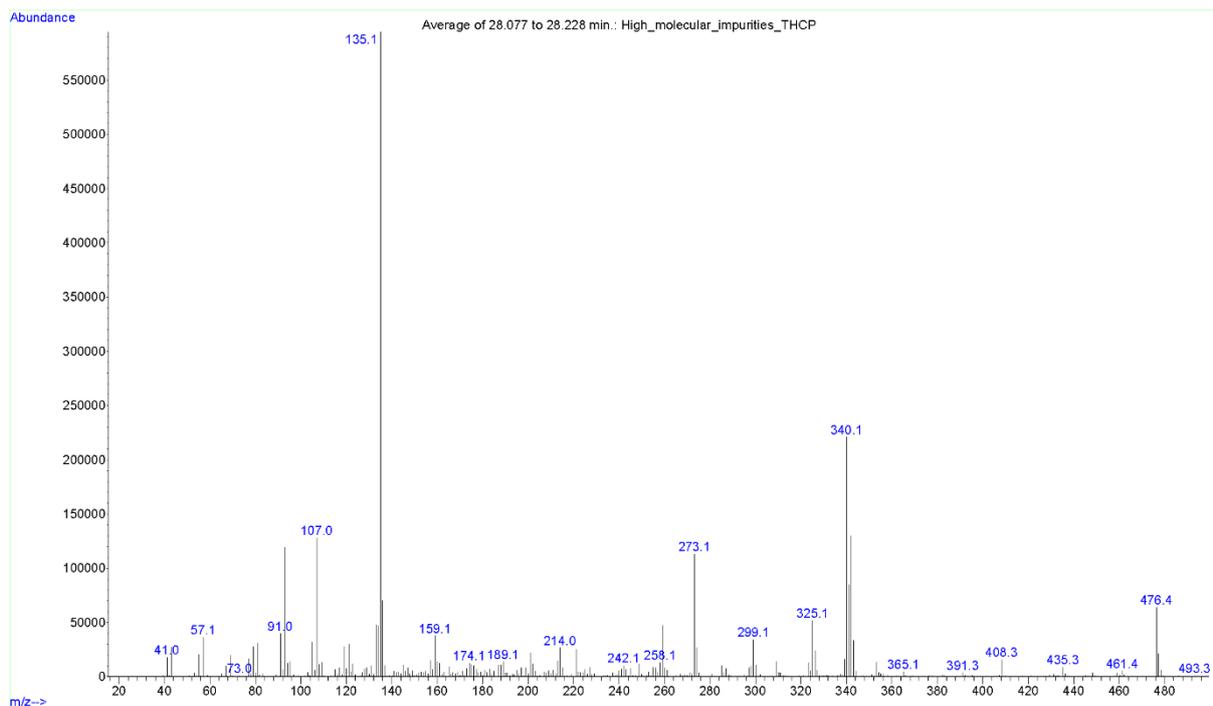
S26: EI mass spectrum of a bisalkylated cannabinoid



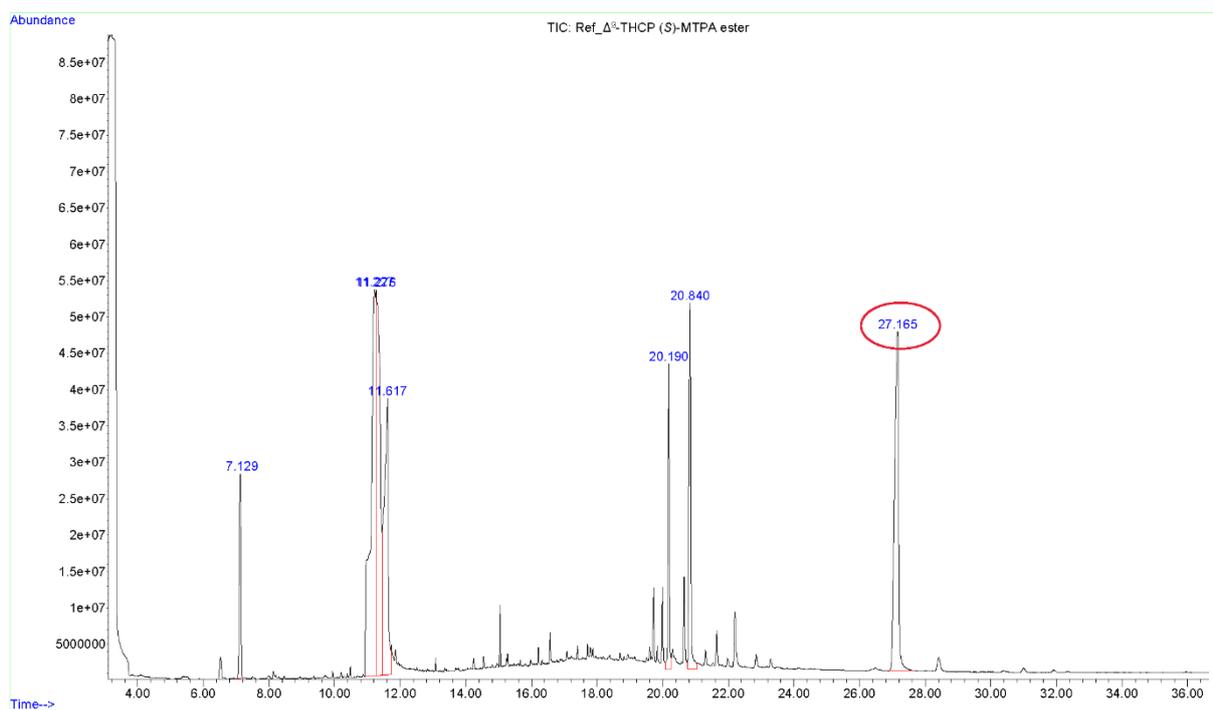
S27: EI mass spectrum of a bisalkylated cannabinoid



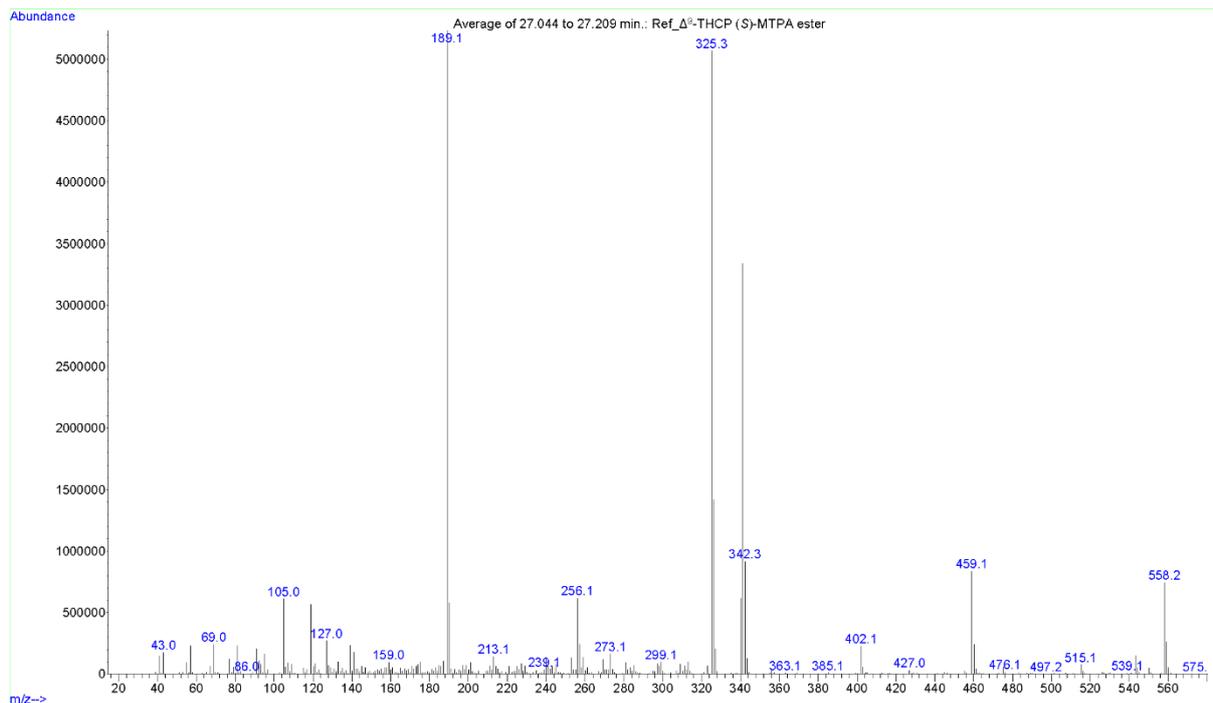
S28: EI mass spectrum of a bisalkylated cannabinoid



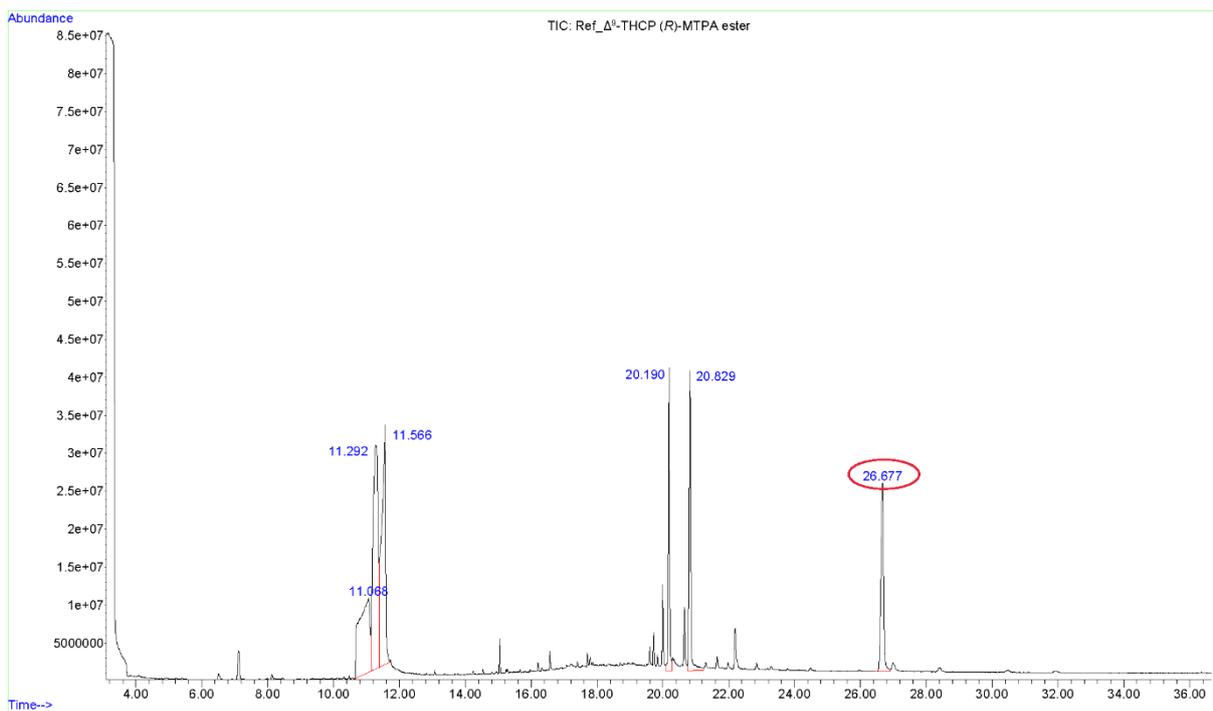
S29: EI mass spectrum of a bisalkylated cannabinoid



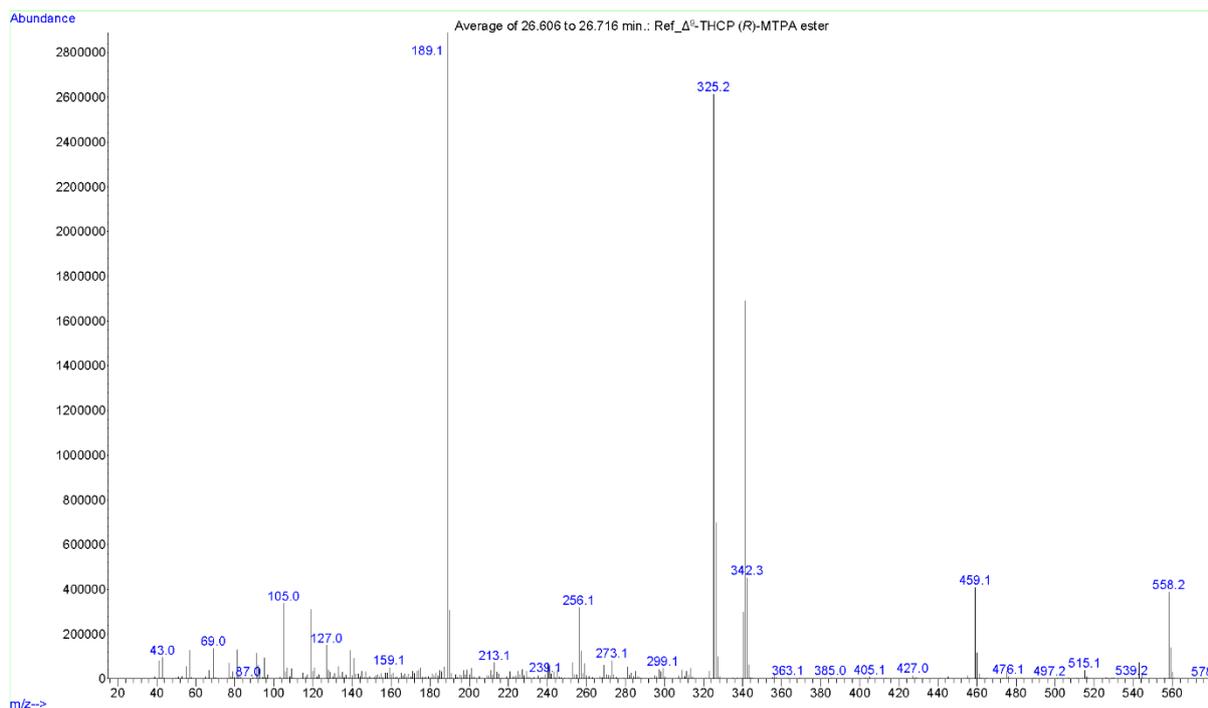
S30: TIC of the (S)-Mosher ester of Δ⁹-THCP.



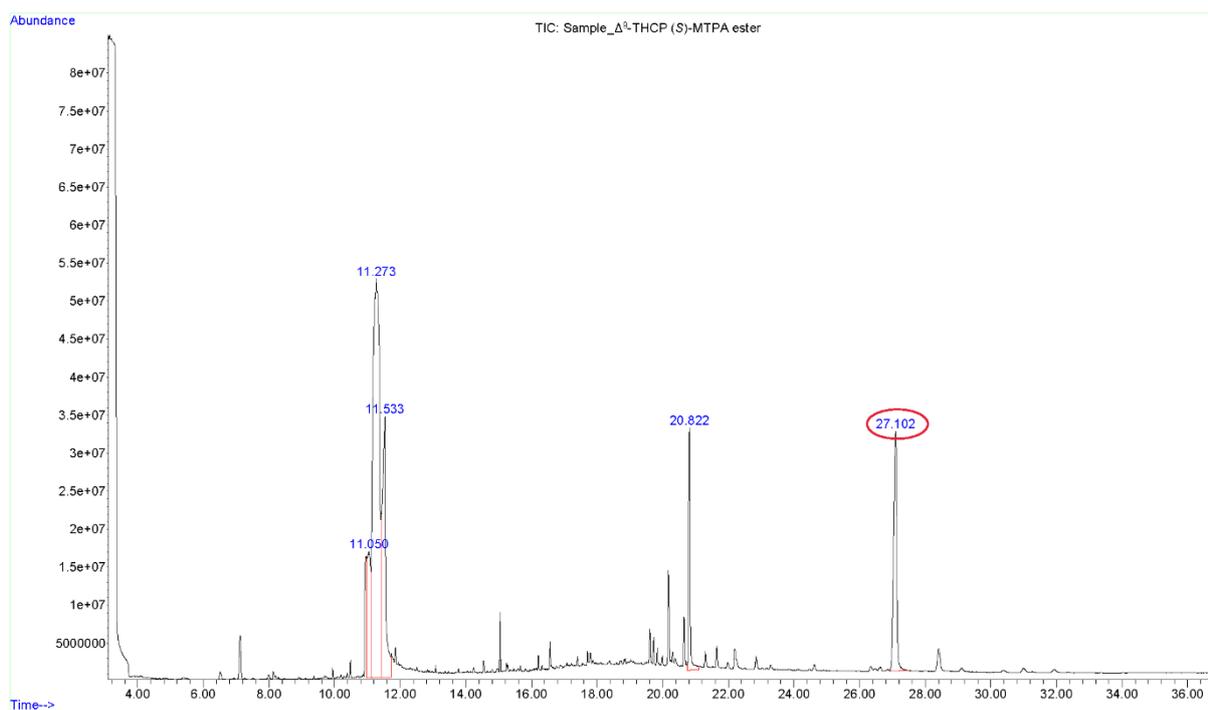
S31: EI mass spectrum of the (S)-Mosher ester of Δ^9 -THCP.



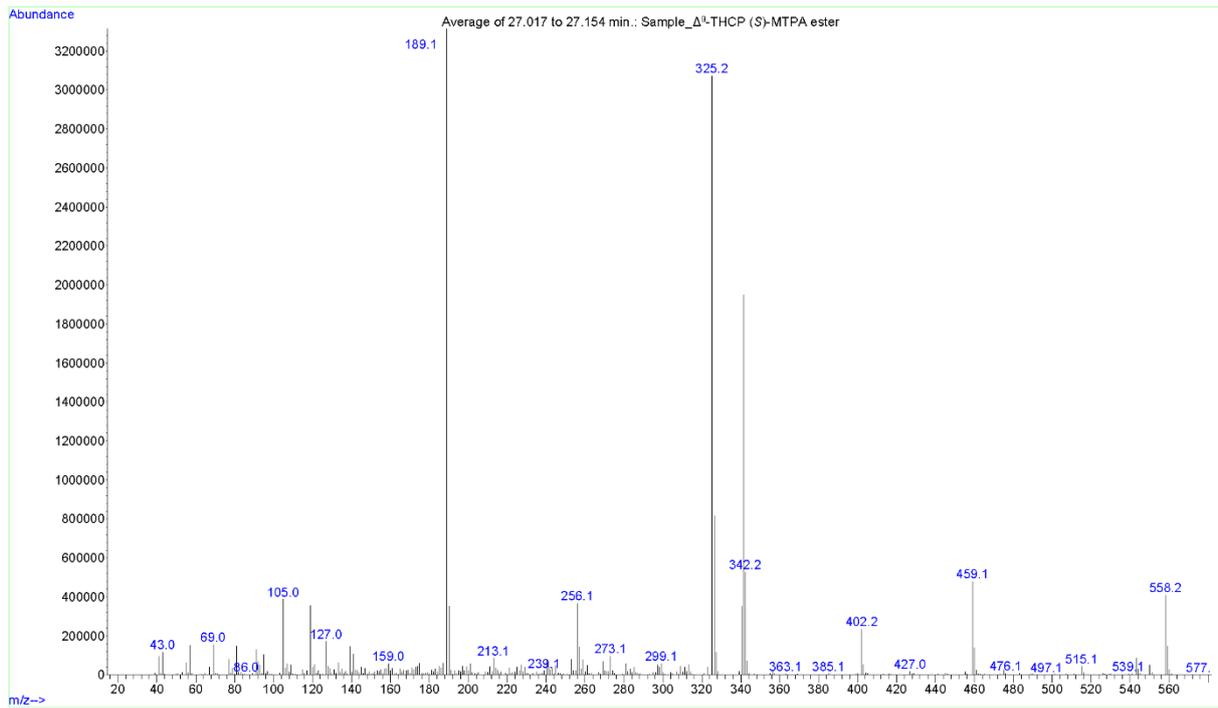
S32: TIC of the (R)-Mosher ester of Δ^9 -THCP.



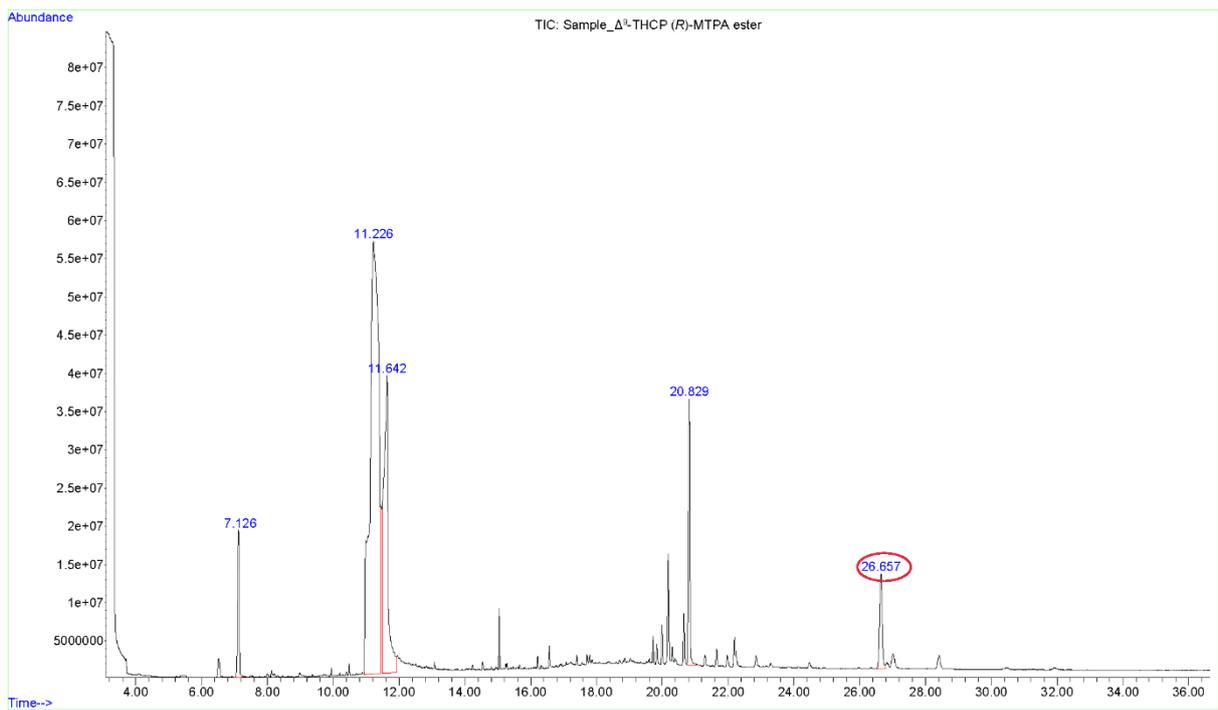
S33: EI mass spectrum of the (R)-Mosher ester of Δ⁹-THCP.



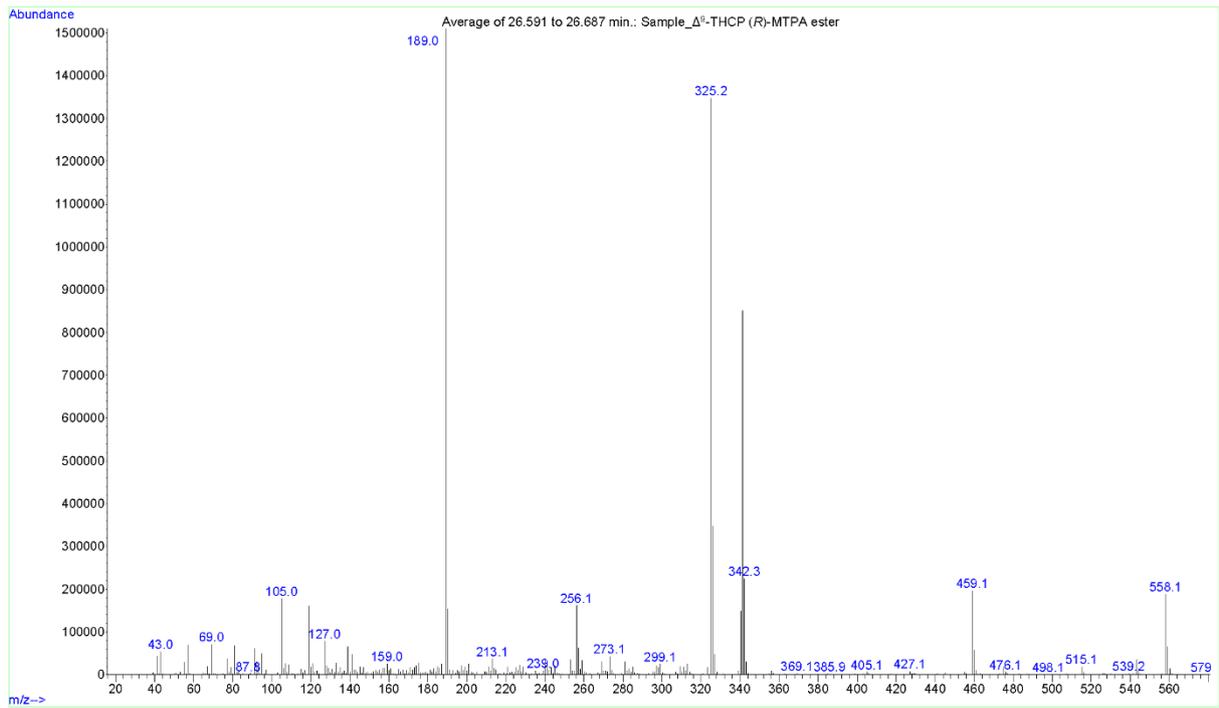
S34: TIC of the (S)-Mosher ester of the isolated Δ⁹-THCP.



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.