

Supporting Information

Ultrafast, Selective and Highly Sensitive Non-Chromatographic Analysis of Fourteen Cannabinoids in Cannabis Extracts, Δ^8 -Tetrahydrocannabinol Synthetic Mixtures and Edibles by Cyclic Ion Mobility Spectrometry-Mass Spectrometry

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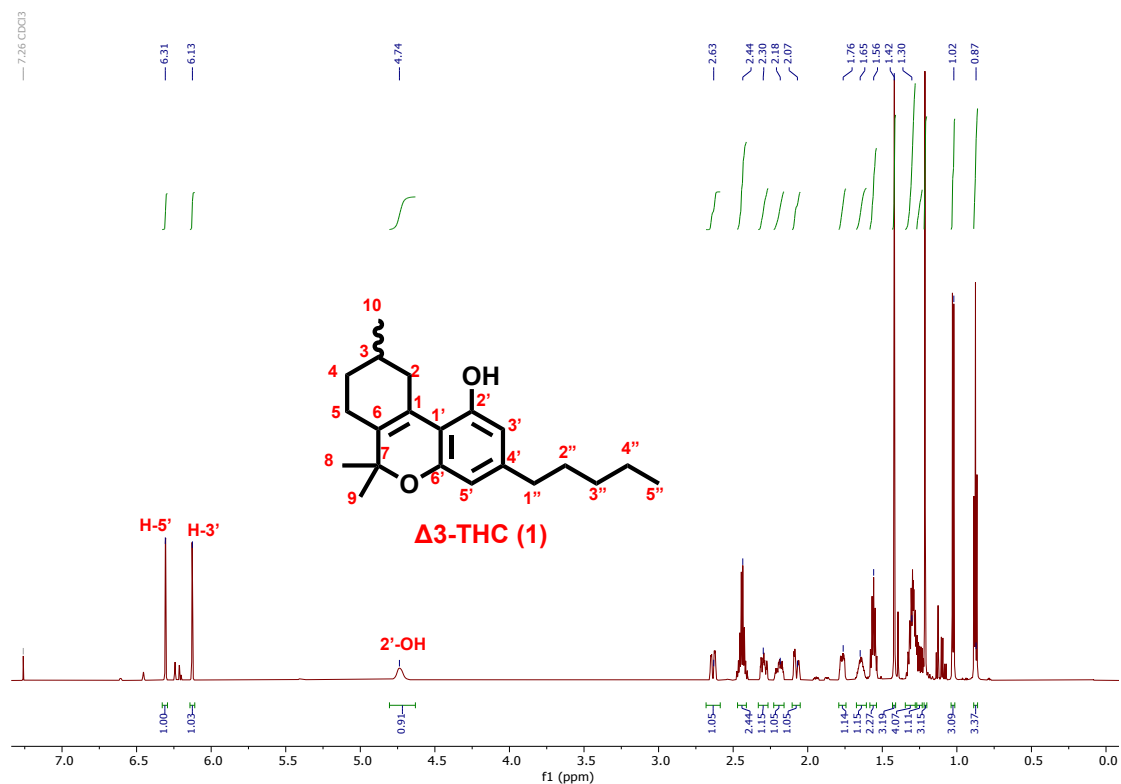
Table S1. Preparation of acid-treated CBD mixtures.

#	Acid	Solvent	Temperature (°C)	Time (h)
1	pTSA 10% (mole ratio of acid/CBD=0.1)	Toluene	Room temperature	39
2	pTSA 200% (mole ratio of acid/CBD=2)	Toluene	Room temperature	39
3	pTSA 200% (mole ratio of acid/CBD=1)	DCM	Room temperature	43
4	pTSA 200% (mole ratio of acid/CBD=1)	Hexane	Room temperature	43
5	BF ₃ ·OEt ₂ (mole ratio of acid/CBD=1)	ACN	−10	6
6	H ₂ SO ₄ (mole ratio of acid/CBD=1)	EtOH	70	39
7	acetic acid (mole ratio of acid/CBD=1)	EtOH	70	39
8	HCl (mole ratio of acid/CBD=1)	EtOH	70	39

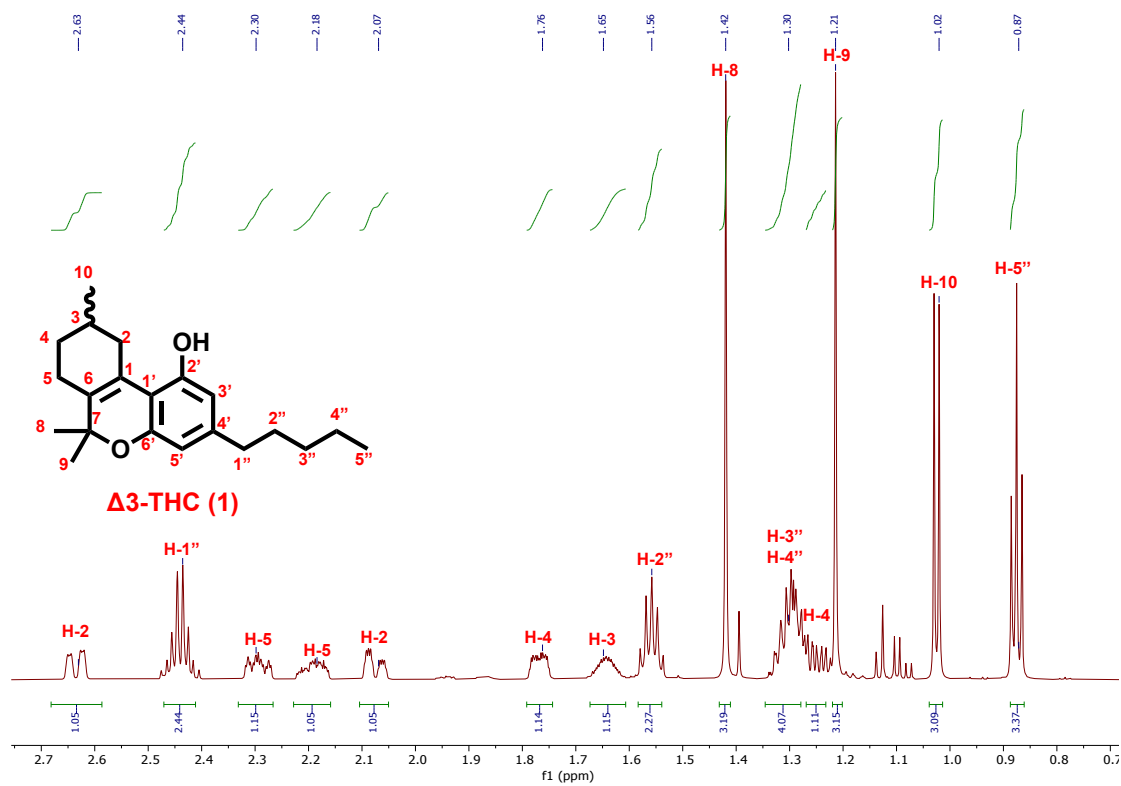
Data are from our previous paper.^[1]

Table S2. Cannabinoid composition information of Cannabis and $\Delta 8$ -THC gummies provided by merchants.

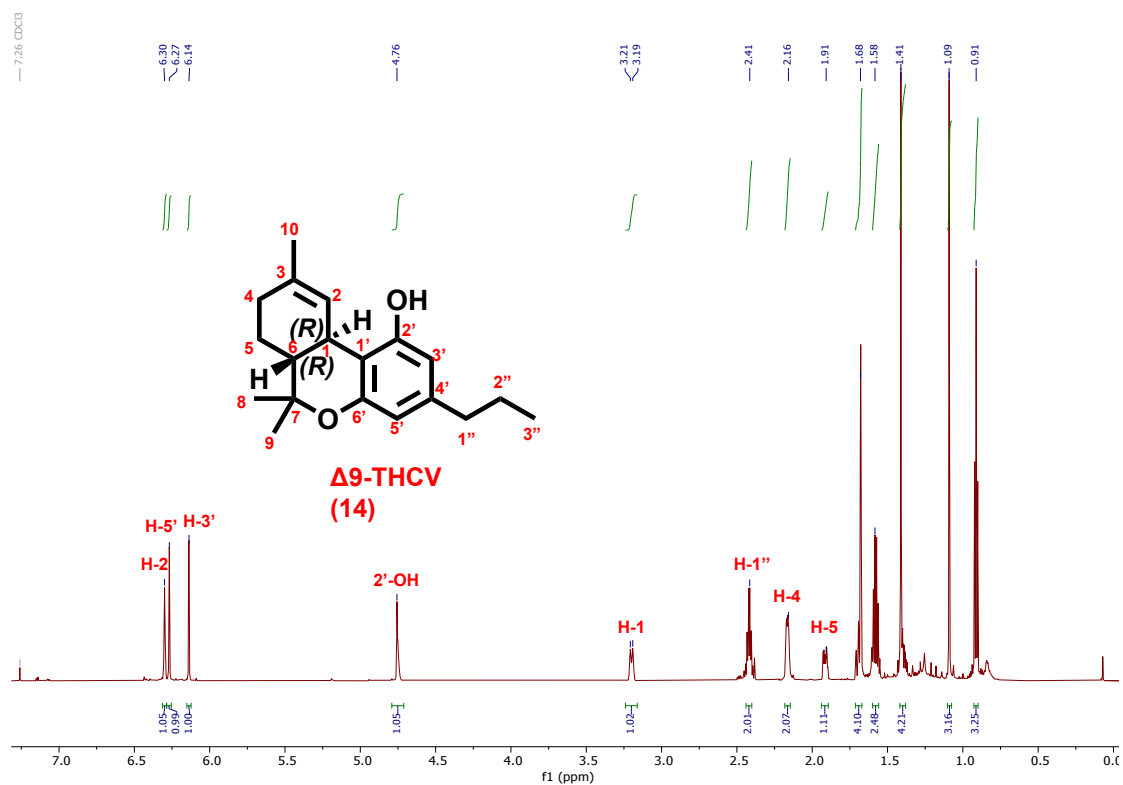
Products	Cannabinoid composition information
C#1	Not available
C#2	THC 24.55%, CBD 7.72%; CBG 1.46%; THCA 6.17%; CBDA 2.43%; CBC 0.33%; THCV 2.31%; CBN 0.57%; CBL 0.
C#3	THC 1.05%; CBD 0; CBG 1.19%; THCA 19.31%; CBDA 0.02%; CBC 0.11%; THCV 0.63%; CBN 0.09%; CBL 0.
G#1	$\Delta 8$ -THC 1 g; $\Delta 9$ -THC<0.3%; CBD<0.3%
G#2	$\Delta 8$ -THC 1.25%; $\Delta 9$ -THC<0.3%



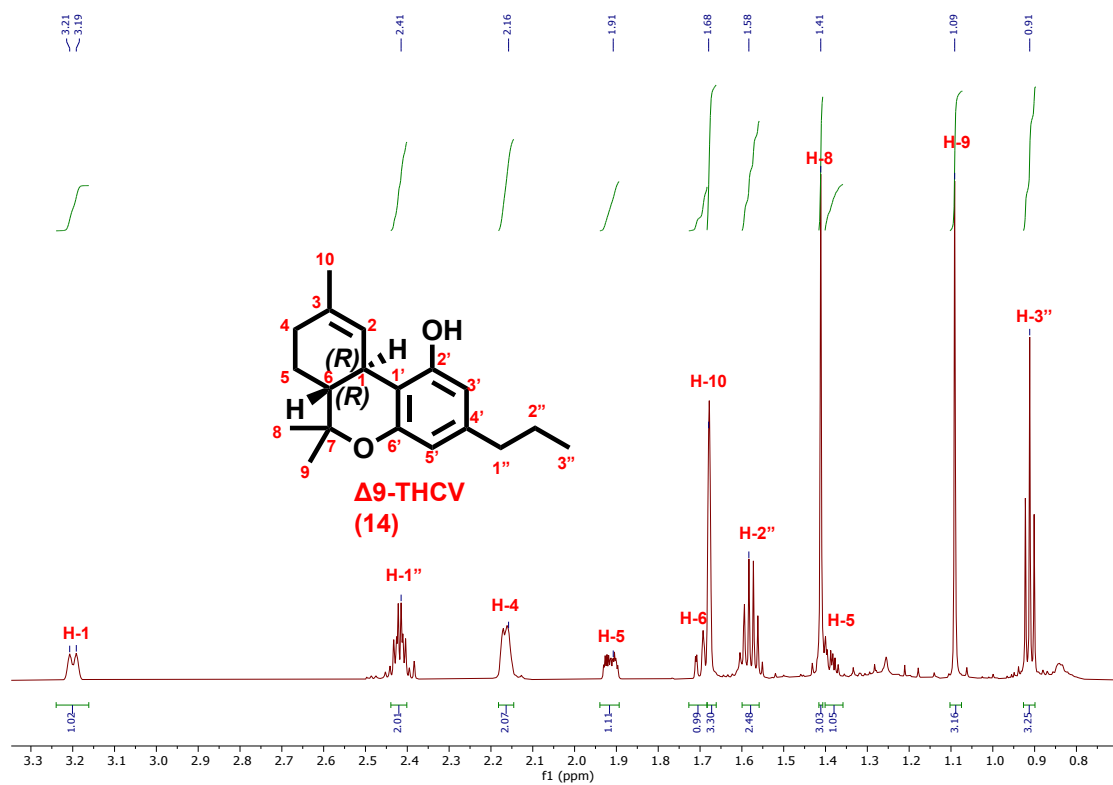
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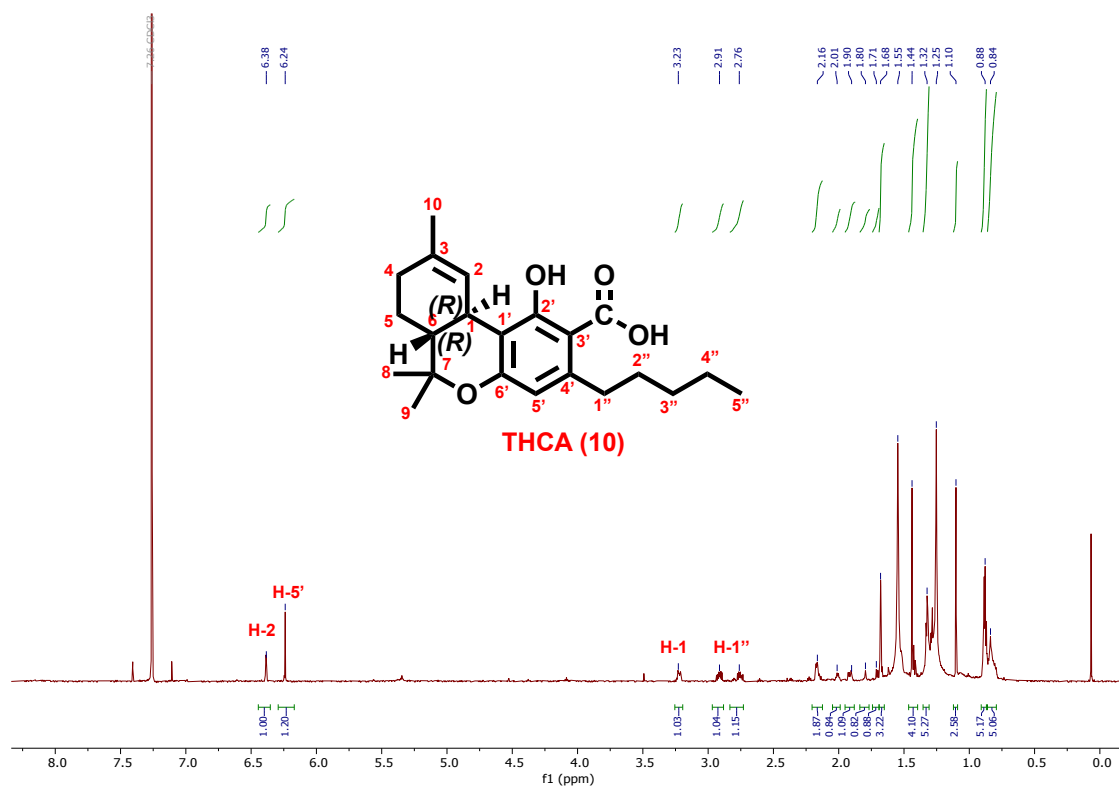
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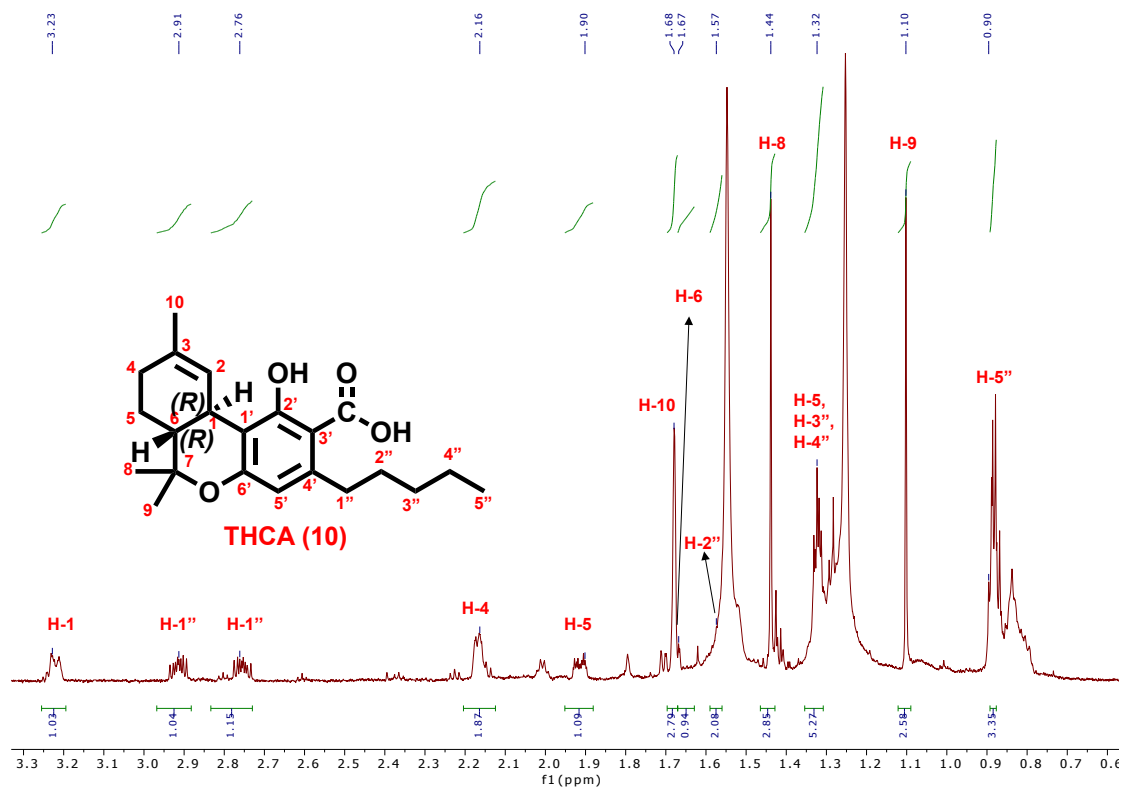
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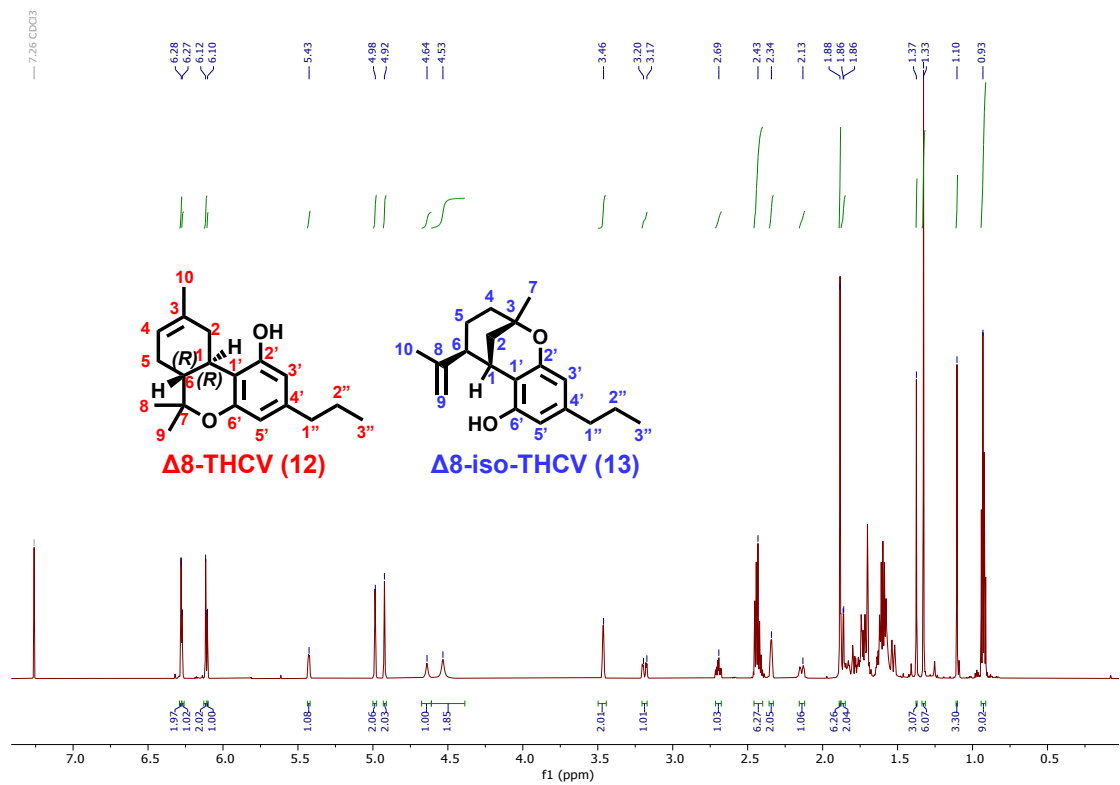
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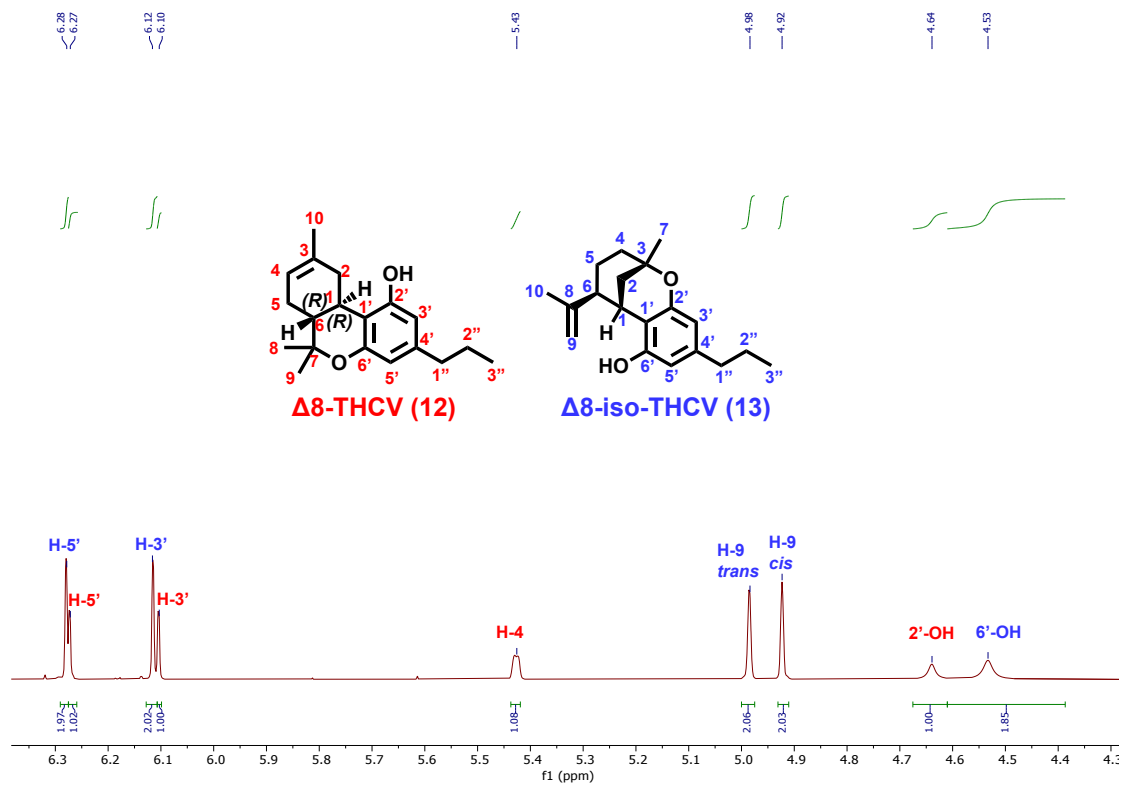
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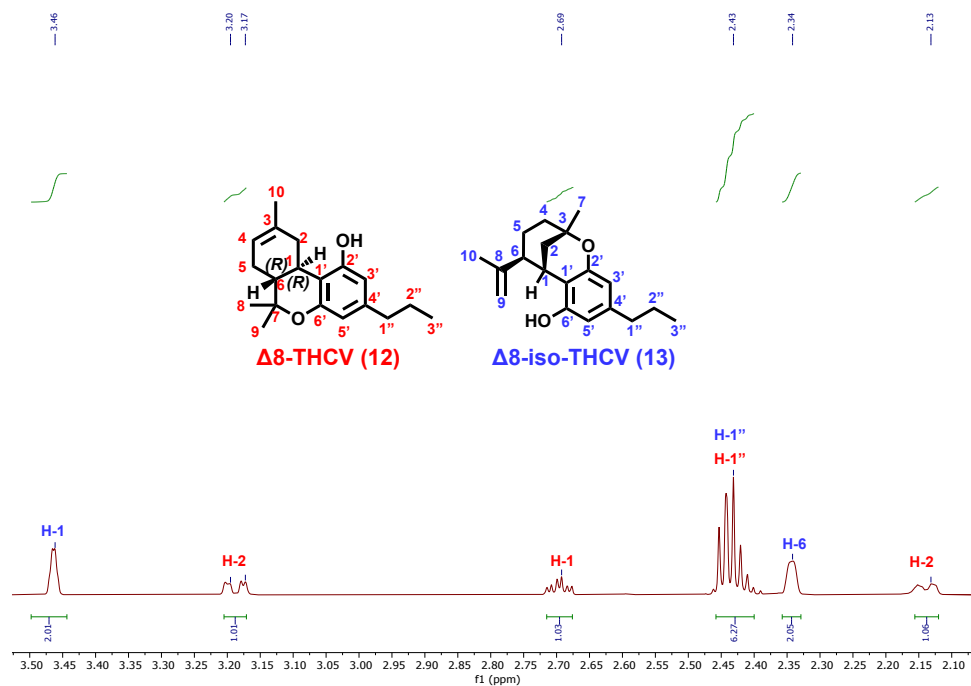
d)



Zoom in



Zoom in



Zoom in

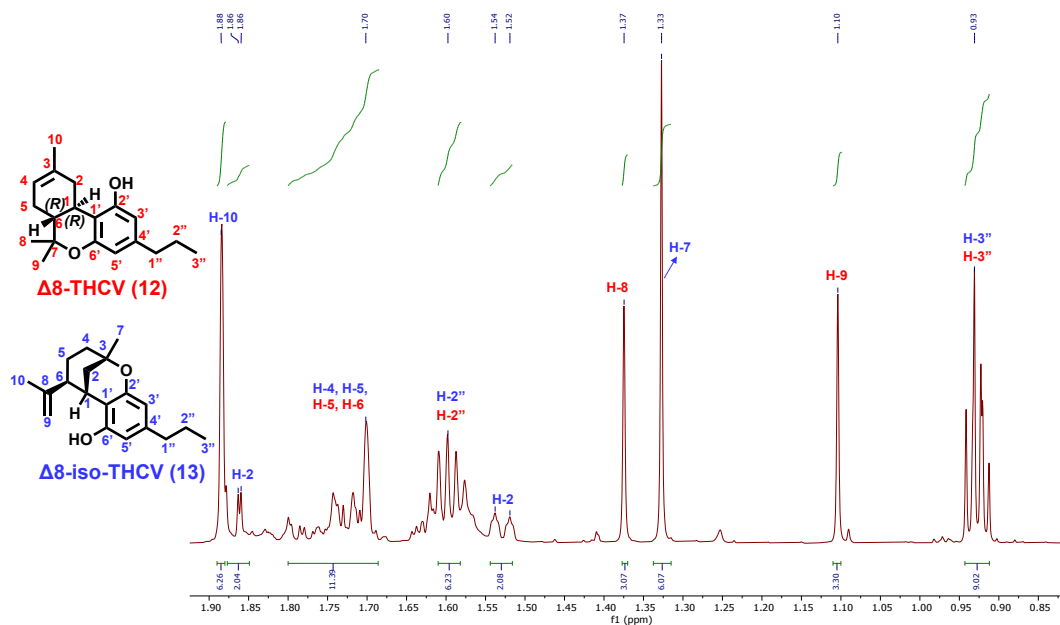


Figure S1. ^1H NMR spectra of a) Δ^3 -THC, b) Δ^9 -THCV, c) THCA, and d) a mixture of Δ^8 -THCV and Δ^8 -iso-THCV.

5 mg of Δ^3 -THC (**1**), Δ^9 -THCV (**14**), THCA (**10**), or a mixture of Δ^8 -THCV and Δ^8 -iso-THCV (**12**, **13**) were dissolved in CDCl_3 , and ^1H NMR spectra were recorded on a Bruker Avance 700 MHz spectrometer at 298 K. The assignments are based on data by Cheng et al.,^[2] Srebnik et al.,^[3] Dadiotis et al.,^[4] Radwan et al.^[5]

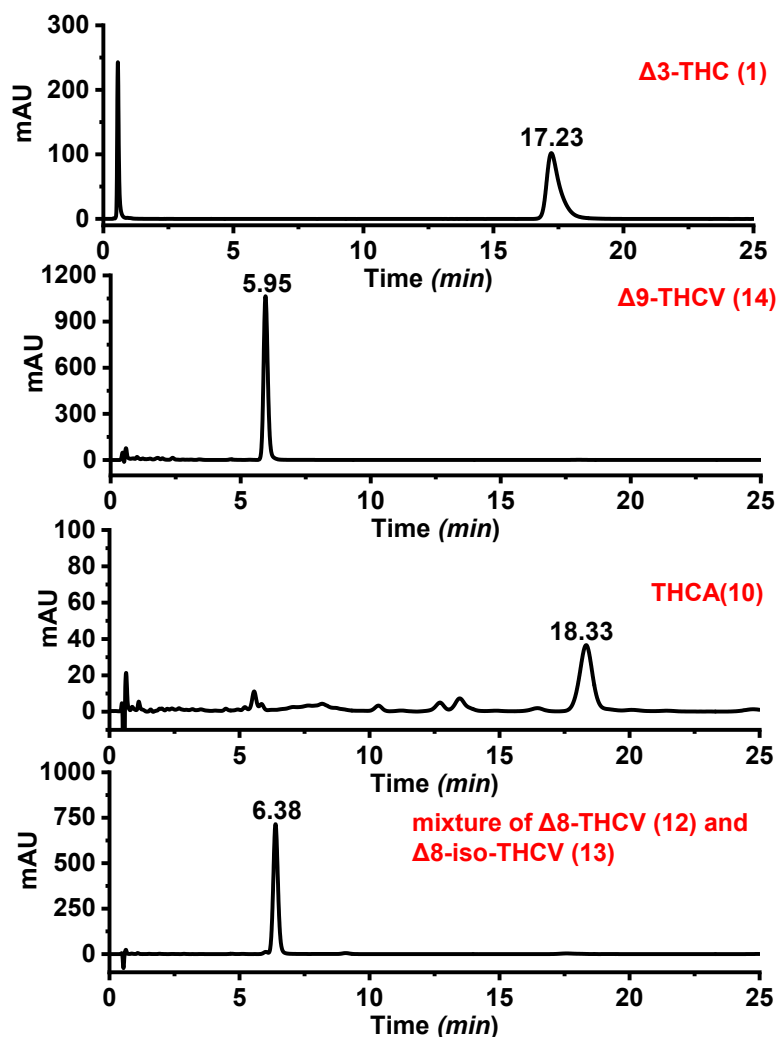
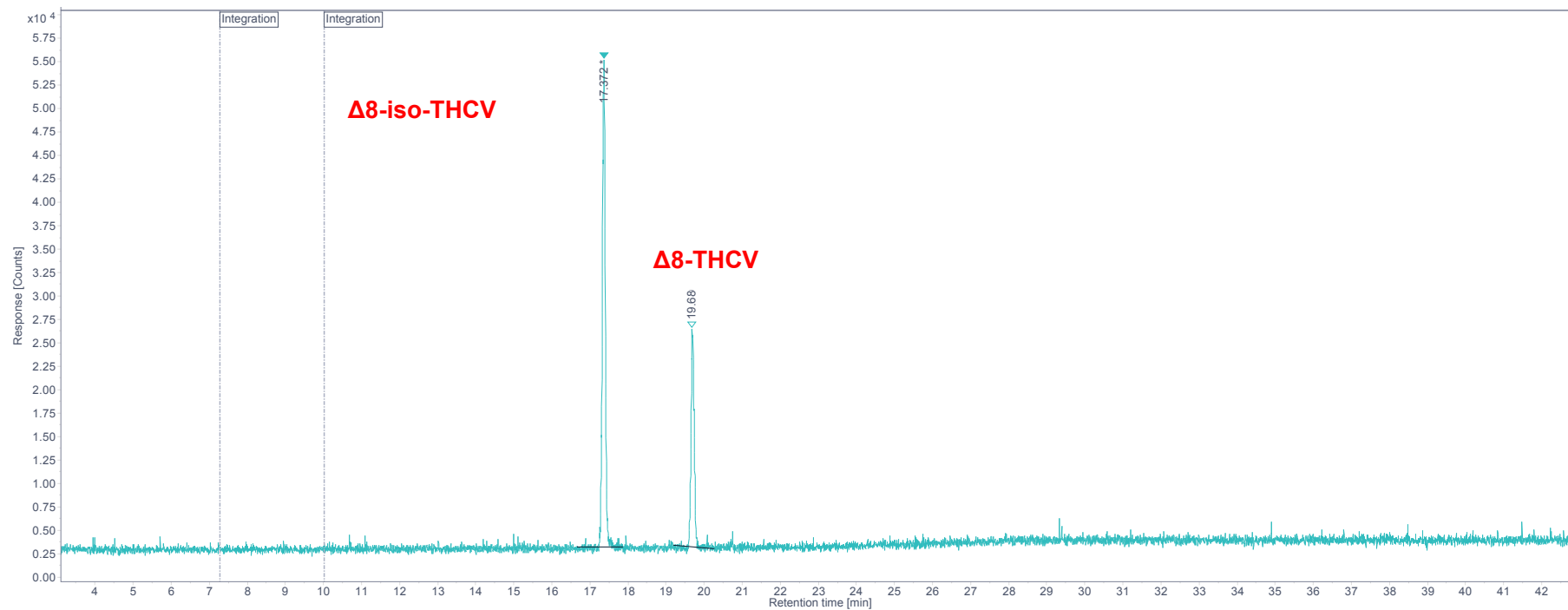
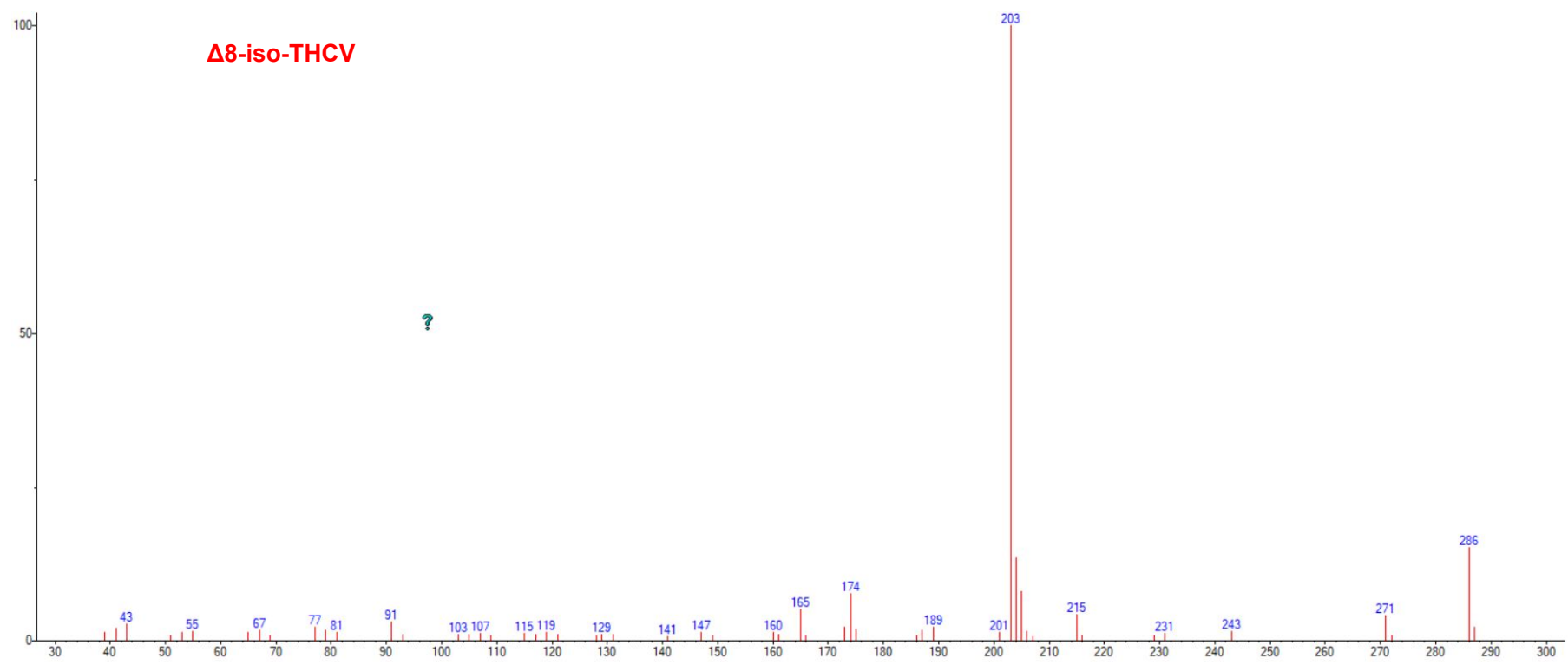


Figure S2. RP-UHPLC-UV (215nm) chromatograms of Δ^3 -THC, Δ^9 -THCV, THCA, and mixture of Δ^8 -THCV and Δ^8 -iso-THCV.

A Zorbax Eclipse Plus C18 chromatographic column (2.1 mm $\times$ 100 mm, particle size: 1.8 μ m; Agilent Technologies, Santa Clara, CA, USA) was integrated with a 1290 Infinity ultra-performance liquid chromatography (UHPLC) system (Agilent Technologies, Santa Clara, United States) employing Diode Array Detection (DAD) as the detection method. The mobile phase employed was a solution comprising 5 mM formic acid in water (mobile phase A) and acetonitrile (mobile phase B). Isocratic elution was achieved by maintaining a constant ratio of 58% mobile phase B at a flow rate of 0.50 mL $\cdot$ min⁻¹. An aliquot of purified Δ^3 -THC (**1**), Δ^9 -THCV (**14**), THCA (**10**), and a mixture of Δ^8 -THCV (**12**) and Δ^8 -iso-THCV (**13**) was sampled with the tip of a spatula and dissolved in MeOH. Subsequently, 8 μ L of each sample was injected for the analysis.





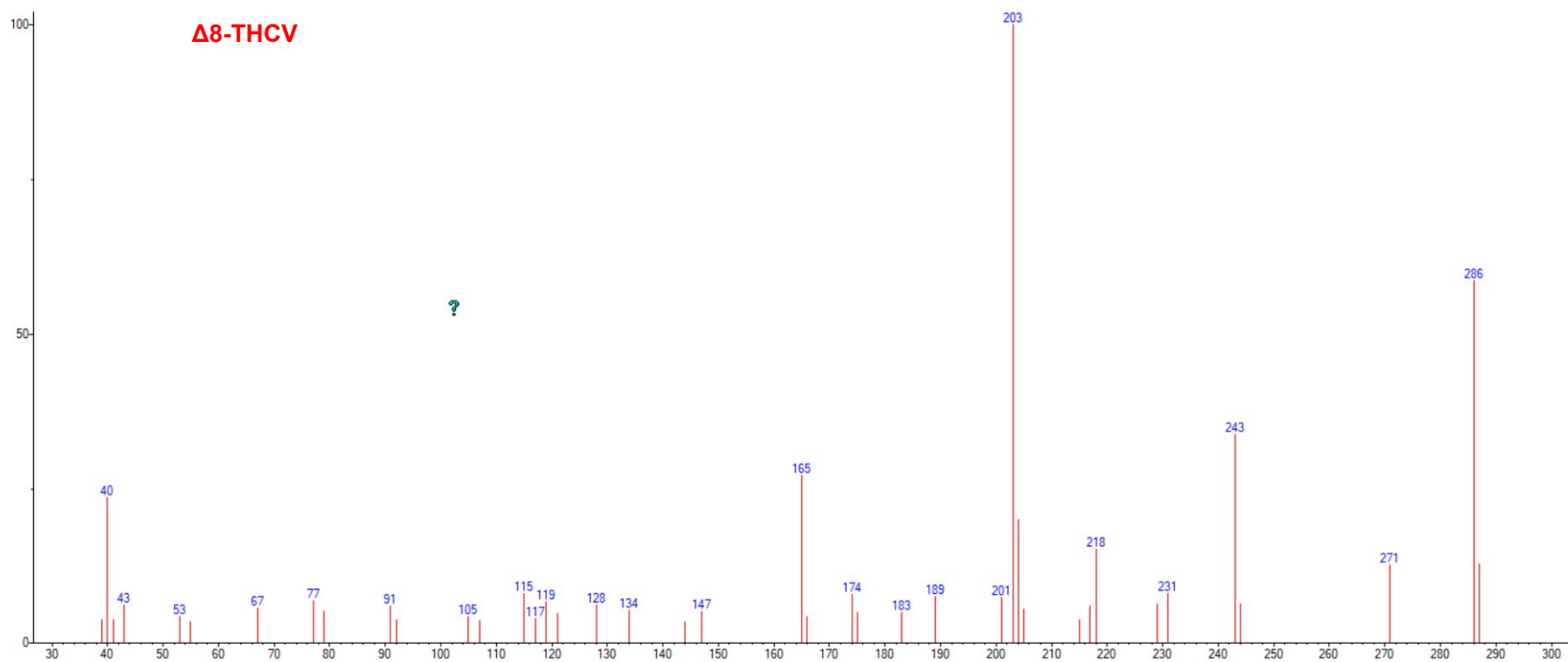


Figure S3. GC-FID profile of the mixture of $\Delta 8$ -THCV and $\Delta 8$ -iso-THCV, and EI-MS spectra of $\Delta 8$ -THCV and $\Delta 8$ -iso-THCV.

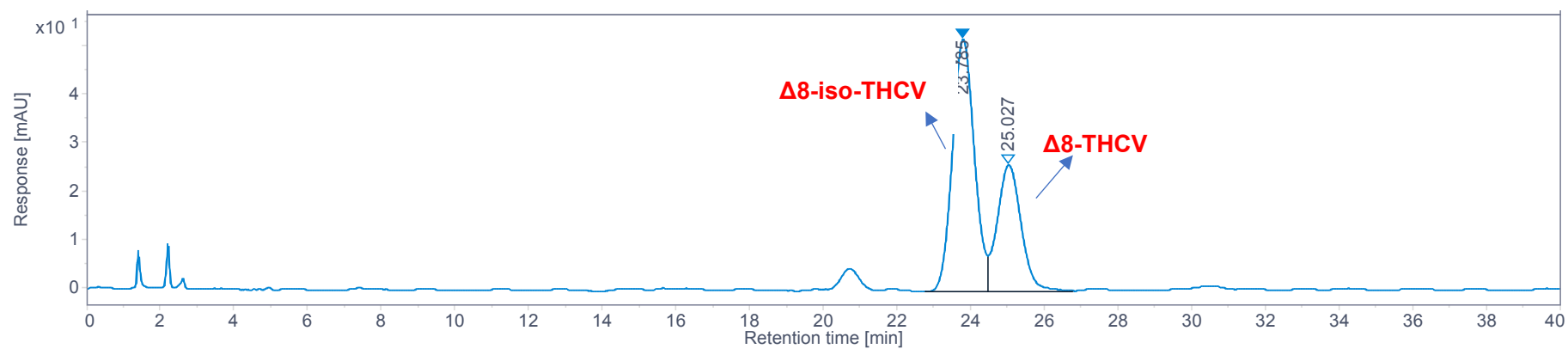


Figure S4. Silica-Ag(I) HPLC-DAD (215 nm) profile of the mixture $\Delta 8$ -THCV and $\Delta 8$ -iso-THCV.

Table S3. Calibrants used for multi-pass CCS calibrations.

Major mix calibrant	Positive ionization mode	
	m/z	CCS ($\text{\AA}^2$)
Sulphaguanidine	215.5970	146.8
Sulfadimethoxine	311.0809	168.4
Val-Tyr-Val	380.2180	191.7
Verapamil	455.2904	208.8
Terfenadine	472.3210	228.7
Reserpine	609.2807	252.3

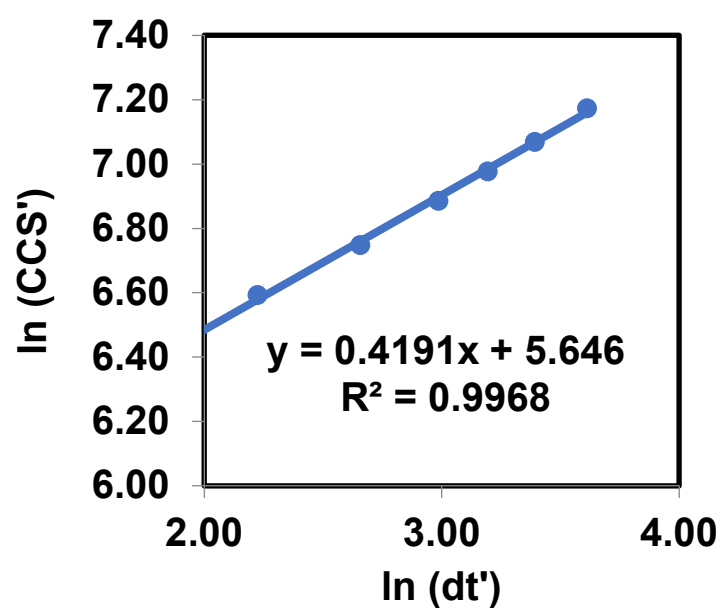


Figure S5. The logarithmic fit calibration curve between drift time and CCS values.

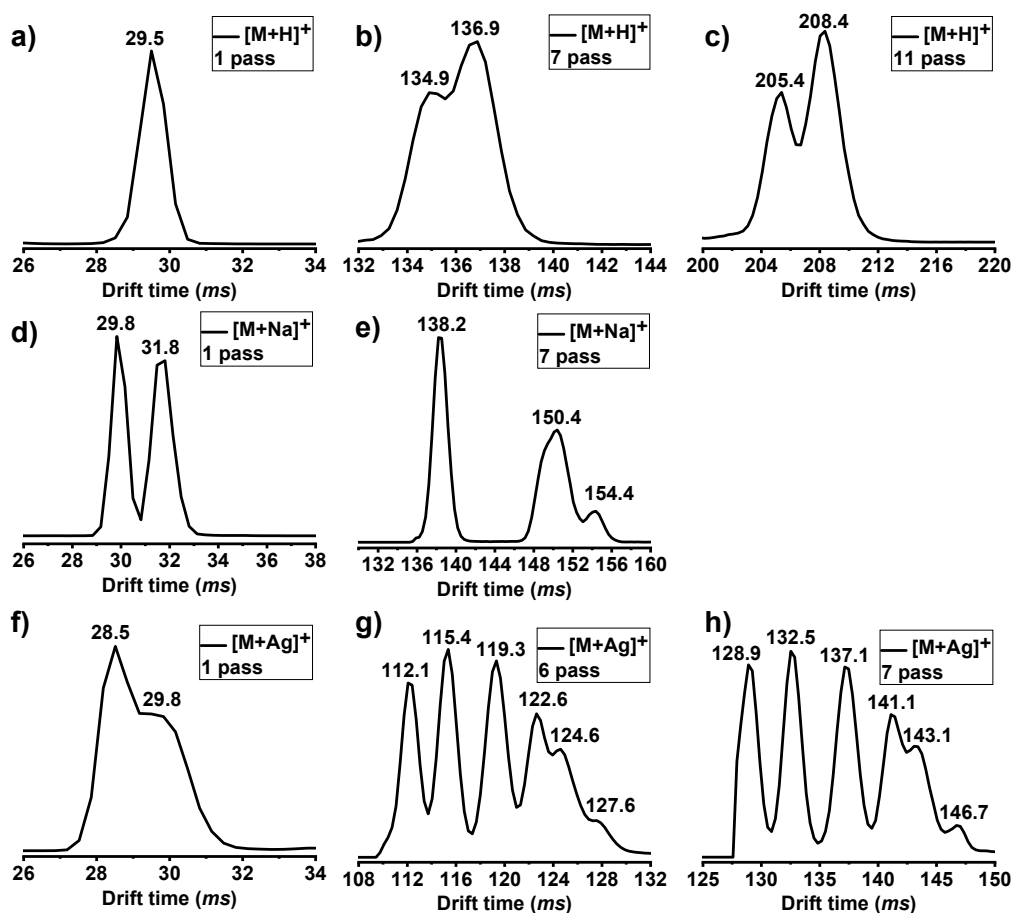
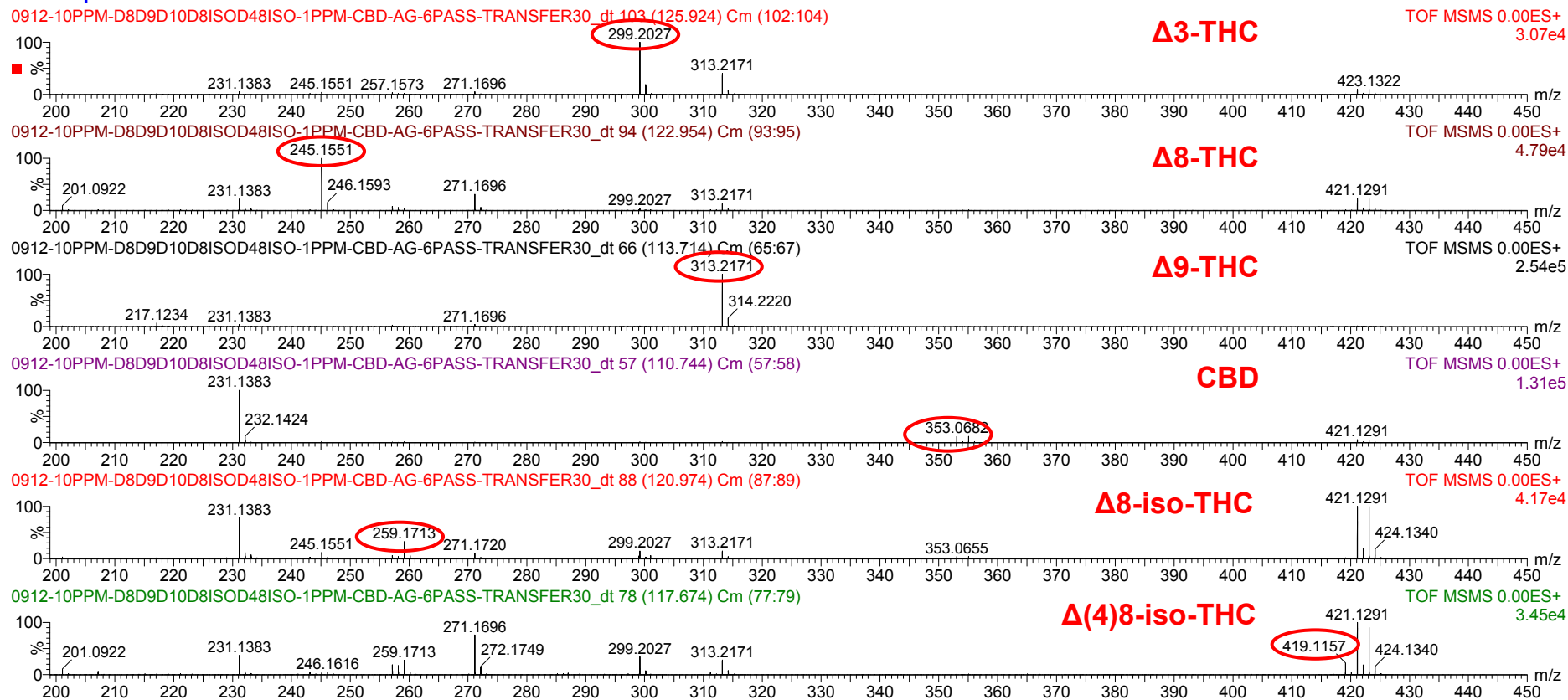
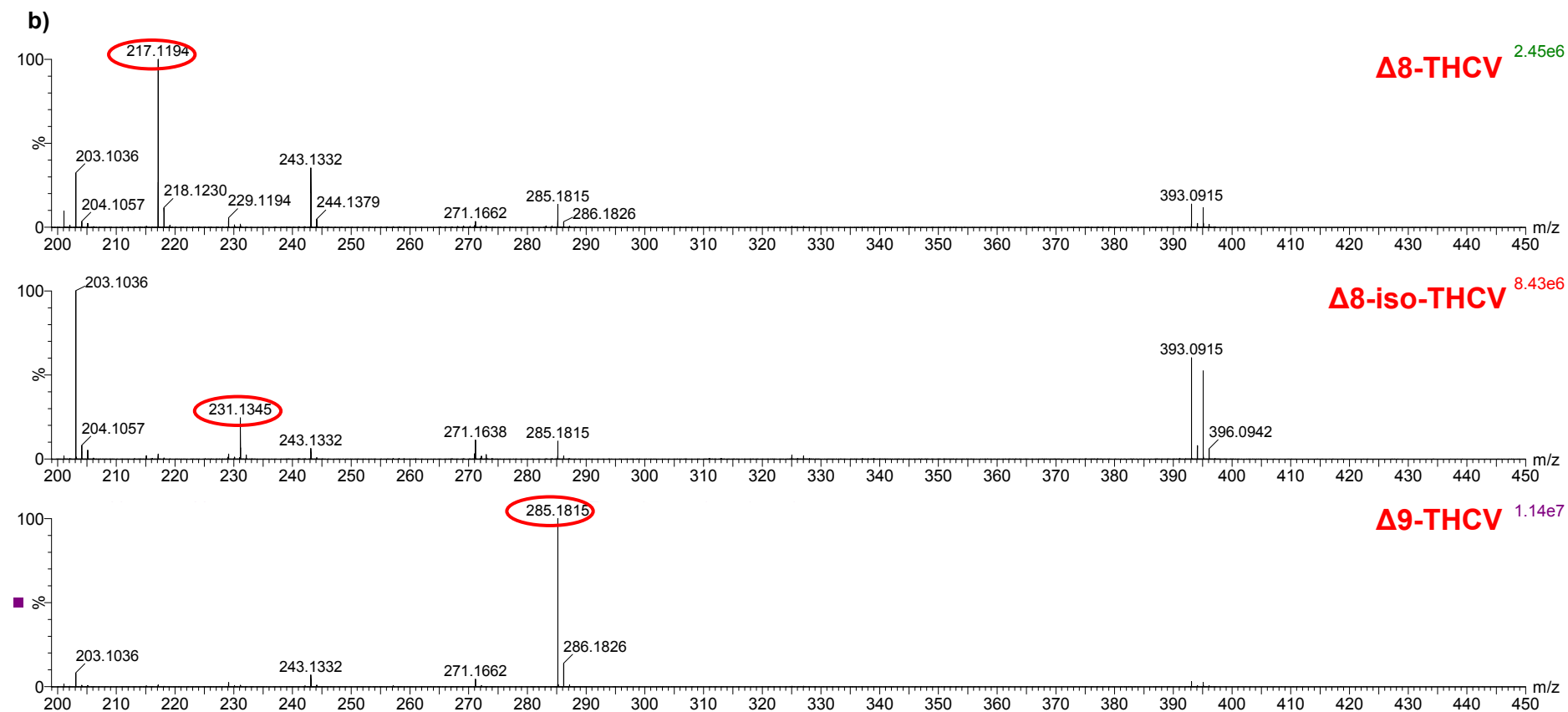


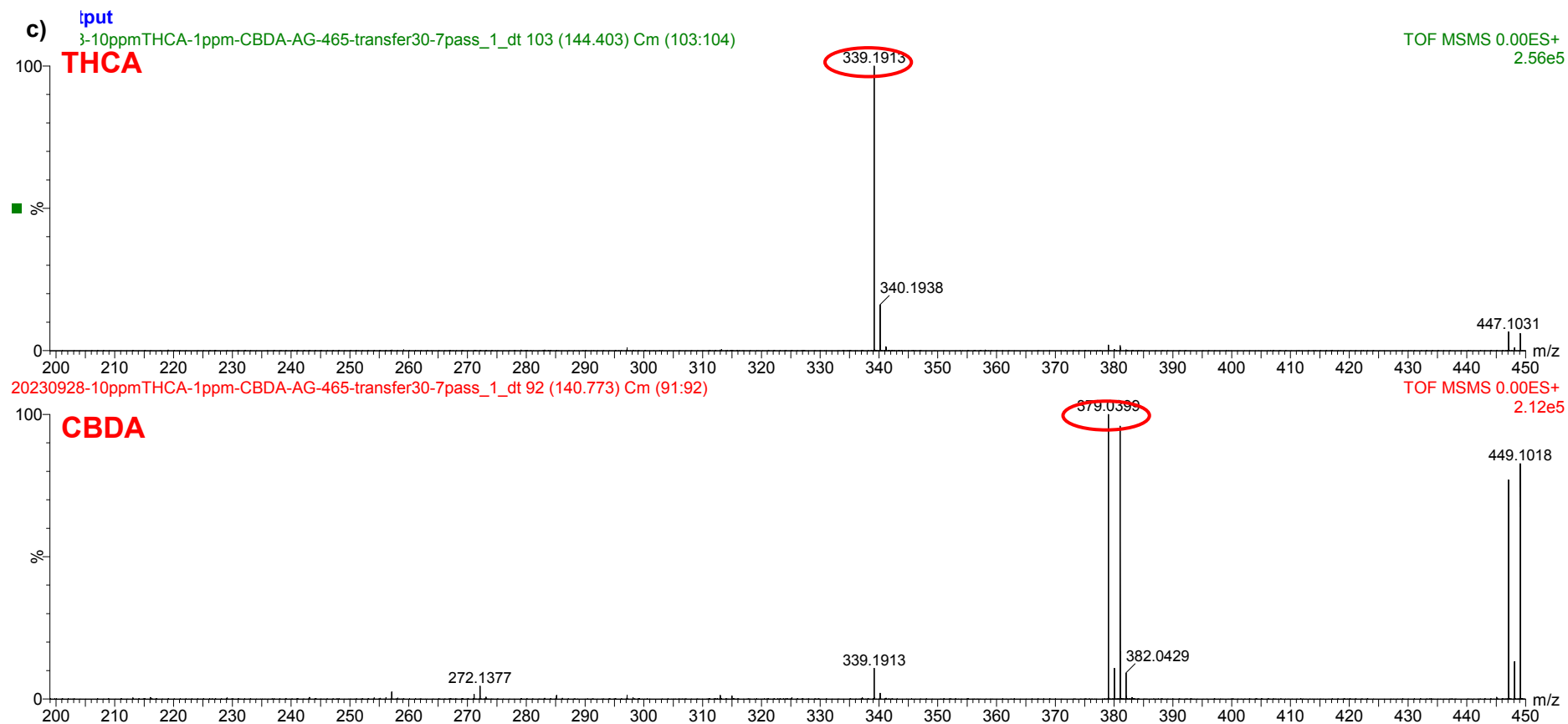
Figure S6. Mobiligrams of charged adducts of the mixture of Δ^3 -THC, Δ^8 -THC, Δ^9 -THC, CBD, Δ^8 -iso-THC and $\Delta(4)8$ -iso-THC. Protonated species (extracting $[M+H]^+$ signal at m/z 315) after a) 1 pass, b) 7 passes and c) 11 passes. Sodiated species (extracting $[M+Na]^+$ signal at m/z 337) after d) 1 pass and e) 7 passes. Argentated species (extracting $[M+Ag]^+$ signal at m/z 421) after f) 1 pass, g) 6 passes and h) 7 passes.

a)

raw output







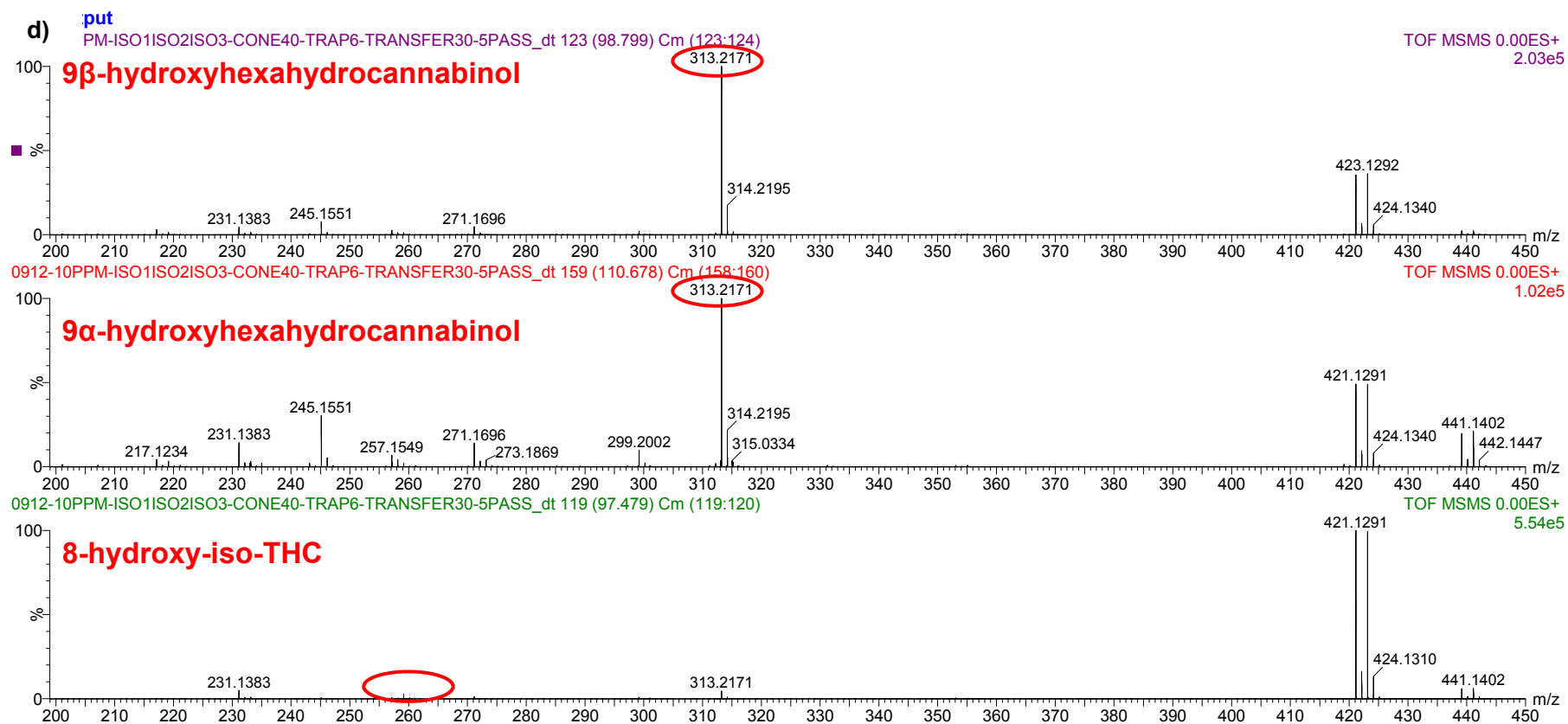


Figure S7. Characteristic fragments of a) Δ 8-THC, Δ 9-THC, Δ 3-THC, CBD, Δ 8-iso-THC and Δ (4)8-iso-THC; b) Δ 8-THCV, Δ 8-iso-THCV and Δ 9-THCV; c) THCA and CBDA; d) 9 α -hydroxyhexahydrocannabinol, 9 β -hydroxyhexahydrocannabinol and 8-hydroxy-iso-THC in the presence of Ag(I) at trap energy of 30 V.

**8-hydroxy-iso-tetrahydrocannabinol,
9 β -hydroxyhexahydrocannabinol**

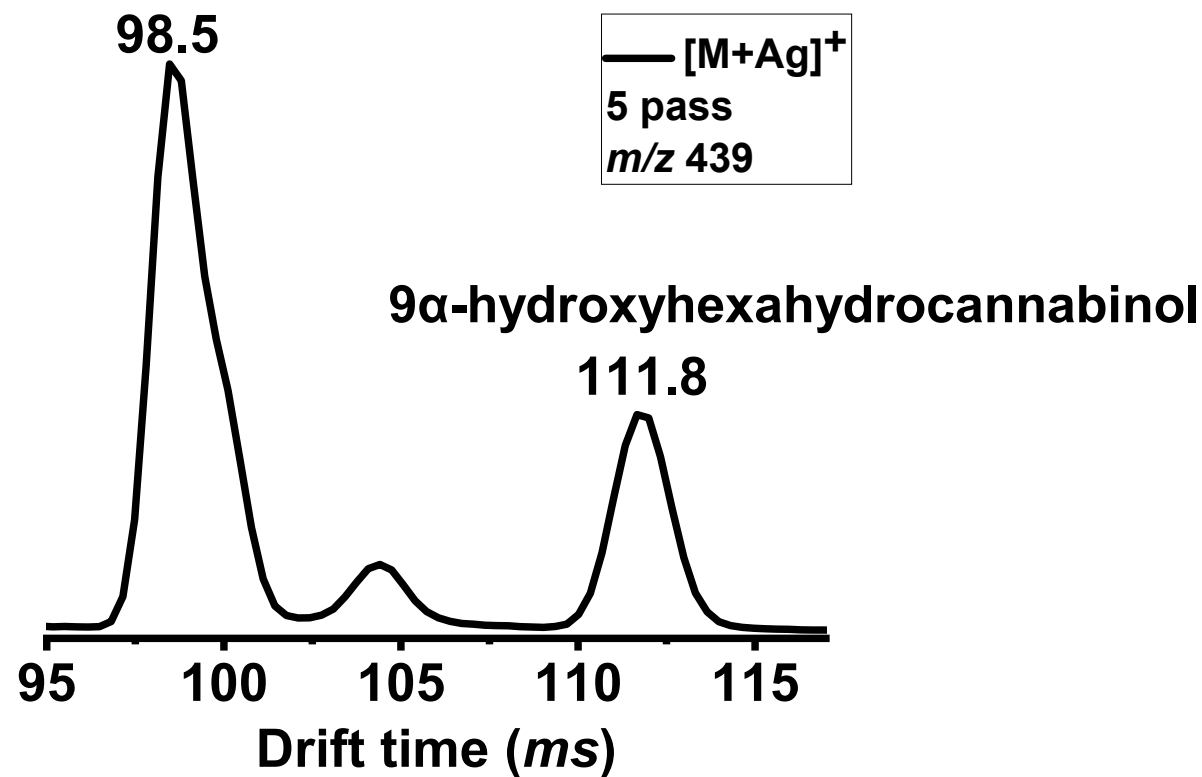


Figure S8. Mobiligram of the mixture consisting of 8-hydroxy-iso-THC, 9 α -hydroxyhexahydrocannabinol, and 9 β -hydroxyhexahydrocannabinol in the form of Ag(I) species.

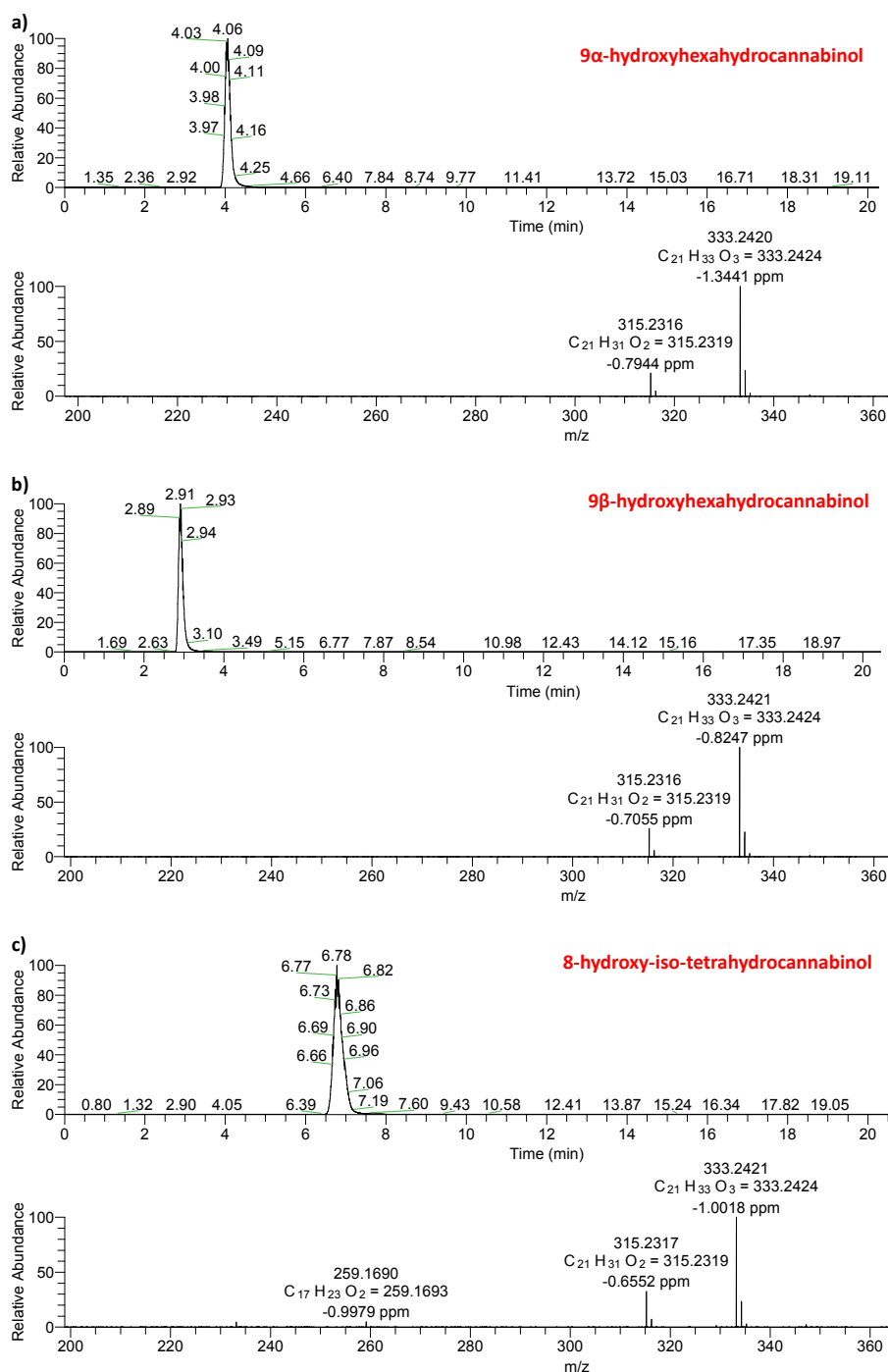


Figure S9. Reversed-phase UHPLC-ESI-Orbitrap mass spectra of a) 9 α -hydroxyhexahydrocannabinol, b) 9 β -hydroxyhexahydrocannabinol, and c) 8-hydroxy-iso-THC.

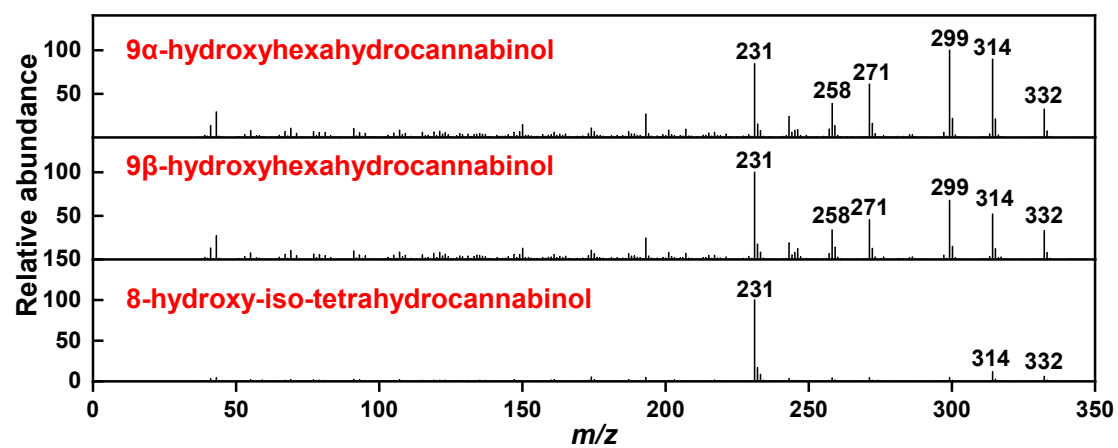


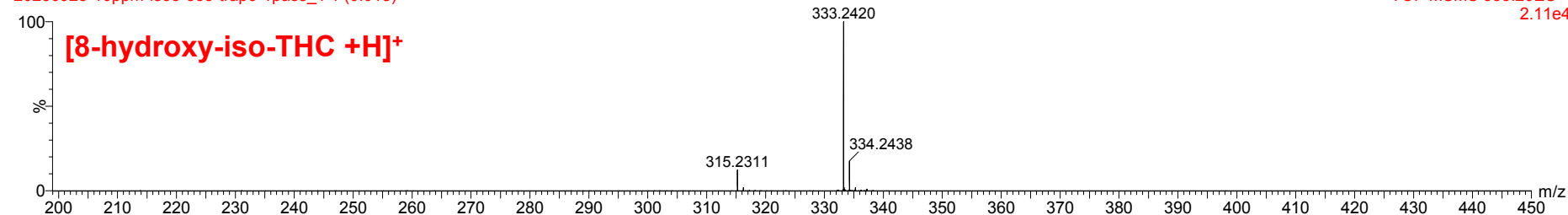
Figure S10. EI-MS spectra obtained after GC separation of 9 α -hydroxyhexahydrocannabinol, 9 β -hydroxyhexahydrocannabinol, and 8-hydroxy-iso-THC.

a)

Raw output

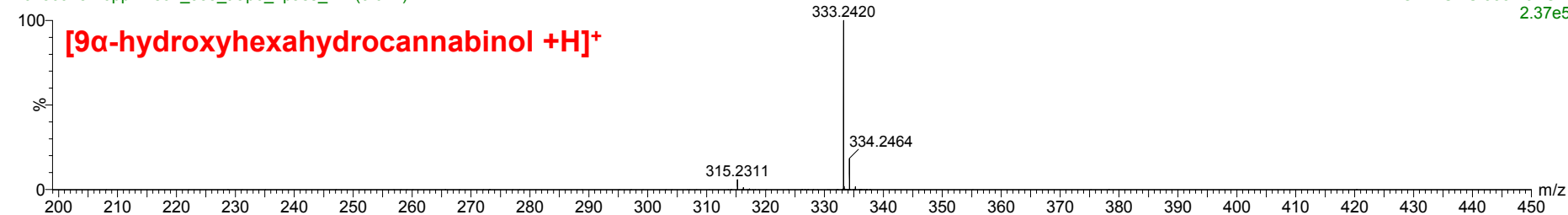
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2.11e4



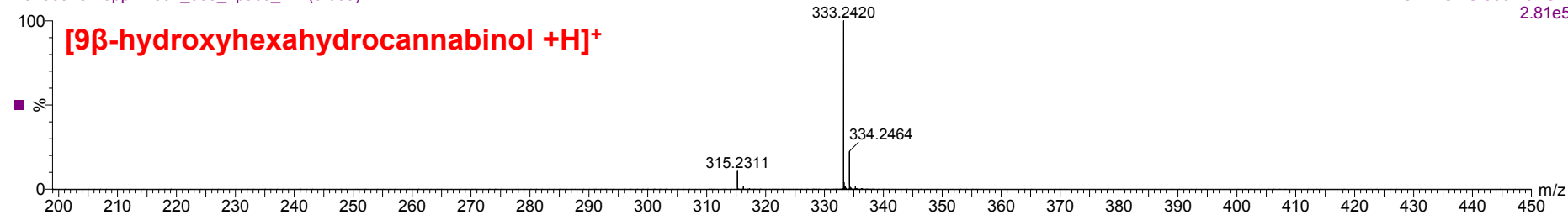
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2.37e5



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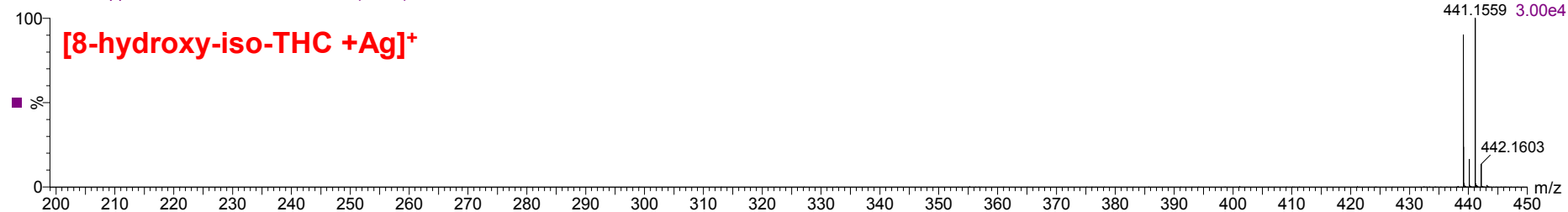
TOF MSMS 333.20ES+
2.81e5



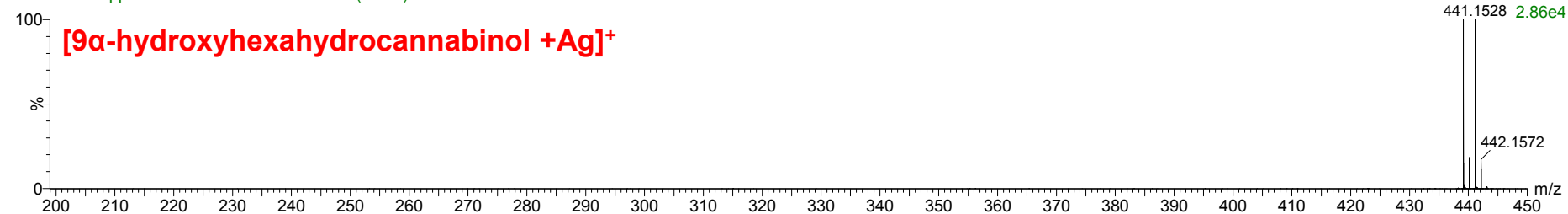
b)

Raw output

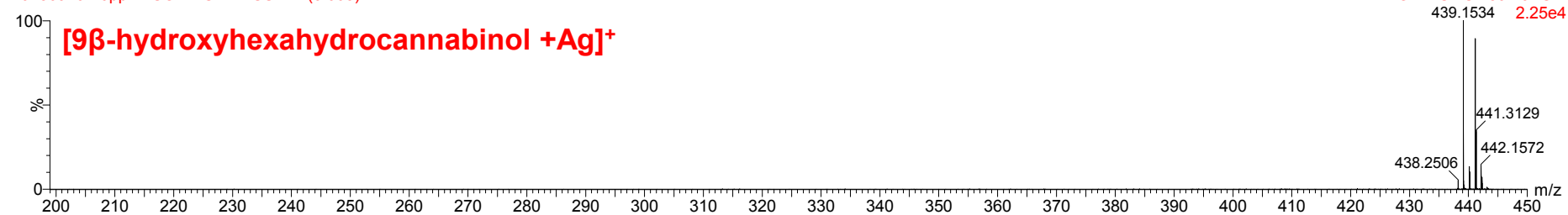
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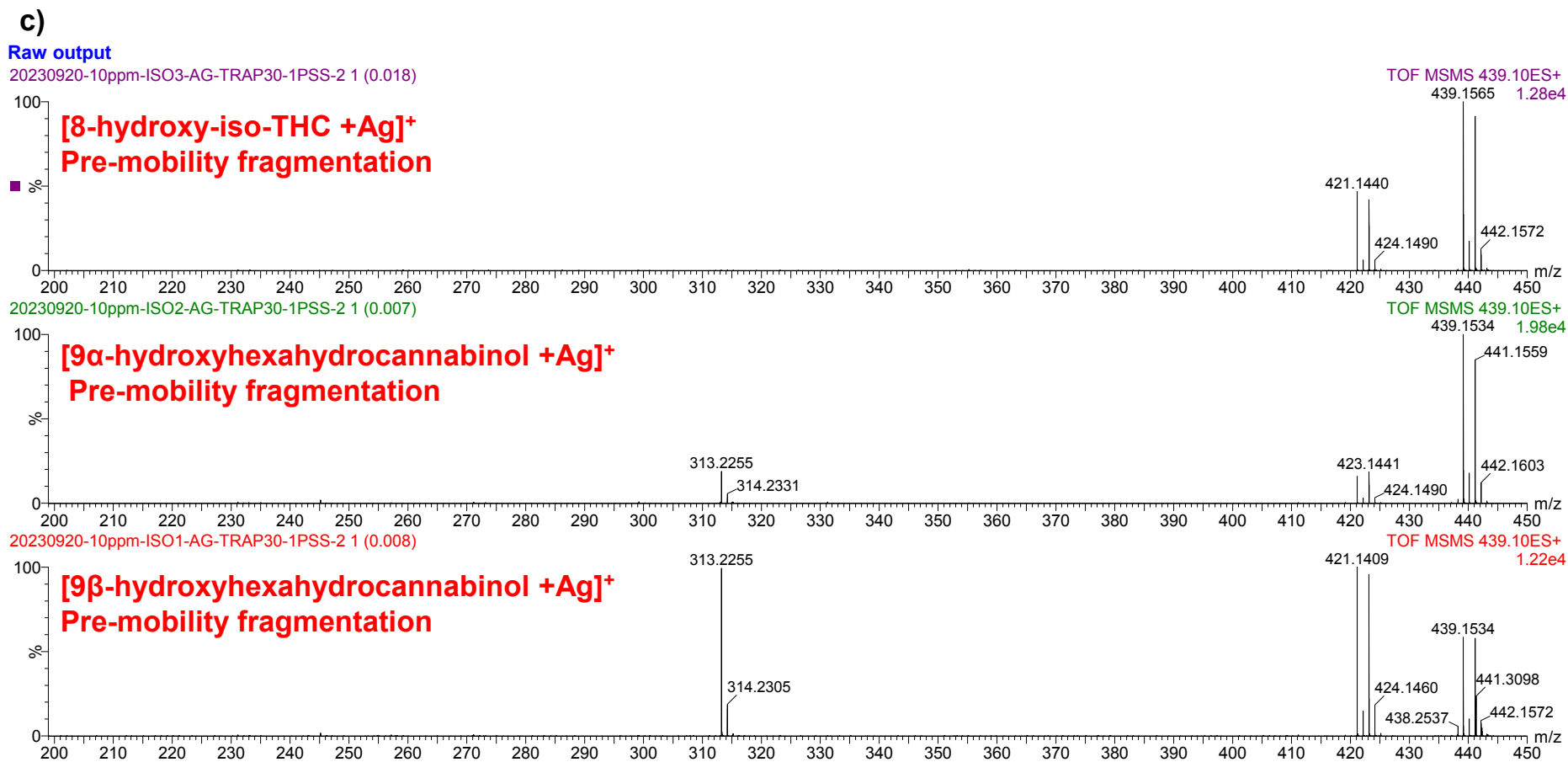


Figure S11. Mass spectra of a) protonated 8-hydroxy-iso-tetrahydrocannabinol, 9 α -hydroxyhexahydrocannabinol, and 9 β -hydroxyhexahydrocannabinol b) Ag(I) species of 8-hydroxy-iso-THC, 9 α -hydroxyhexahydrocannabinol, and 9 β -hydroxyhexahydrocannabinol, c) pre-mobility fragmentation of 8-hydroxy-iso-THC, 9 α -hydroxyhexahydrocannabinol, and 9 β -hydroxyhexahydrocannabinol in the presence of Ag(I) with trap energy of 30 V.

Table S4. Comparison of predicted CCS values by AllCCS, CCS values from literature and experimental CCS values obtained by cIMS of cannabinoids as protonated species and sodiated species.

Compounds	$[M+H]^+$ (m/z 315) ($\text{\AA}^2$)				$[M+Na]^+$ (m/z 337) ($\text{\AA}^2$)	
	Experimental $^{TW}CCS_{N_2}$	Predicted CCS	Literature ^[6] $^{DT}CCS_{N_2}$	Literature ^[7] $^{TI}CCS_{N_2}$	Experimental $^{TW}CCS_{N_2}$	Predicted CCS
Δ^3 -THC	188.4±0.01	186.5 (−1.0%)			197.9±0.03	203.5 (2.8%)
Δ^8 -THC	187.8±0.05	187.5 (−0.2%)			196.4±0.04	203.4 (3.6%)
Δ^9 -THC	187.8±0.03	187.5 (−0.2%)	187.4 (−0.2%)	183.9 (−2.1%)	194.8±0.01	203.5 (4.5%)
CBD	187.8±0.01	183.8 (−2.1%)	185.3 (−1.3%)	183.9 (−2.1%)	188.5±0.02	198.3 (5.2%)
Δ^8 -iso-THC	186.5±0.03	183.3 (−1.7%)			195.7±0.01	198.8 (1.6%)
$\Delta(4)8$ -iso-THC	186.6±0.04	185.1 (−0.8%)			195.8±0.01	202.3 (3.3%)
9 α -hydroxyhexahydrocannabinol	191.2±0.02	190.7 (−0.3%)			201.7±0.02	205.8 (2.0%)
9 β -hydroxyhexahydrocannabinol	191.6±0.2	190.6 (−0.5%)			193.0±0.01	205.6 (6.5%)
8-hydroxy-iso-THC	187.9±0.01	183.7 (−2.2%)			200.8±0.02	196.9 (−1.9%)
THCA	194.0±0.2	196.8 (1.4%)			212.2±0.01	210.8 (−0.7%)
CBDA	193.6±0.03	195.0 (0.7%)			206.7±0.01	208.3 (0.8%)
Δ^8 -THCV	174.9±0.01	172.5 (−1.4%)			188.0±0.02	191.5 (1.9%)
Δ^8 -iso-THCV	173.5±0.01	174.9 (0.8%)			183.8±0.01	194.4 (5.8%)
Δ^9 -THCV	174.7±0.01	175.0 (0.2%)			185.9±0.01	194.4 (4.6%)

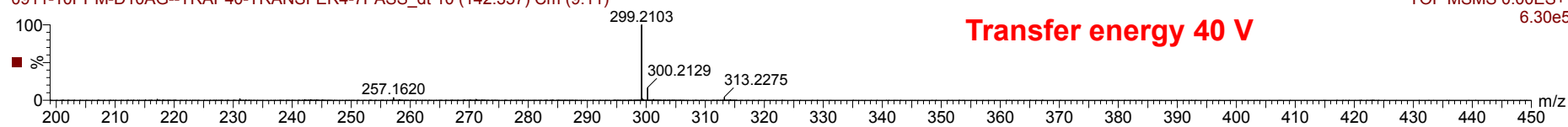
*Values in brackets represent relative deviations from experimental CCS value

a) Δ^3 -THC

Raw output

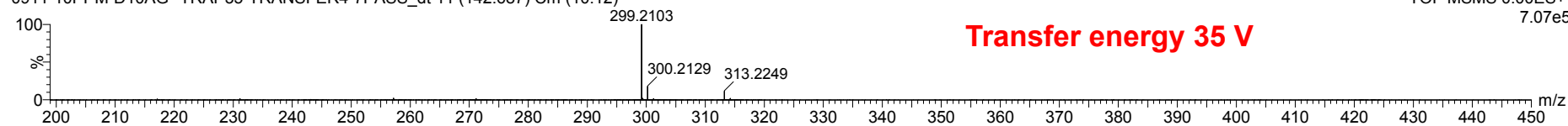
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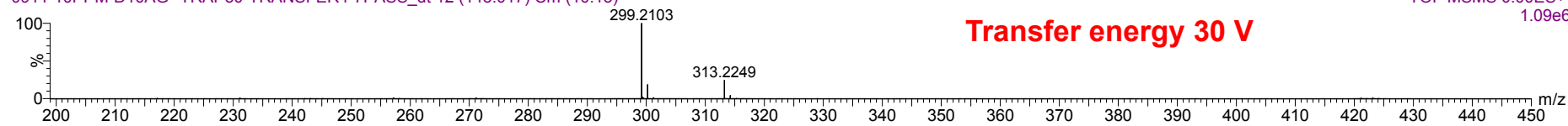
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7.07e5



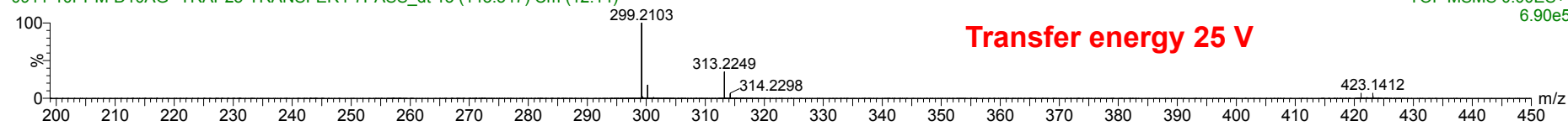
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1.09e6



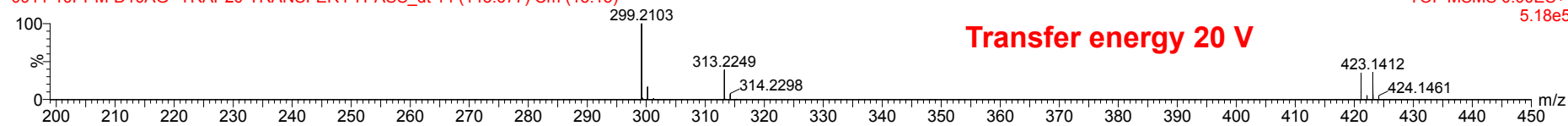
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TOF MSMS 0.00ES+
6.90e5



0911-10PPM-D10AG--TRAP20-TRANSFER4-7PASS_dt 14 (143.677) Cm (13:15)

TOF MSMS 0.00ES+
5.18e5

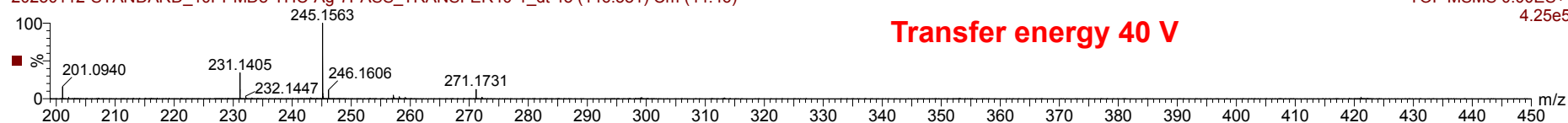


b) $\Delta 8$ -THC

Raw output

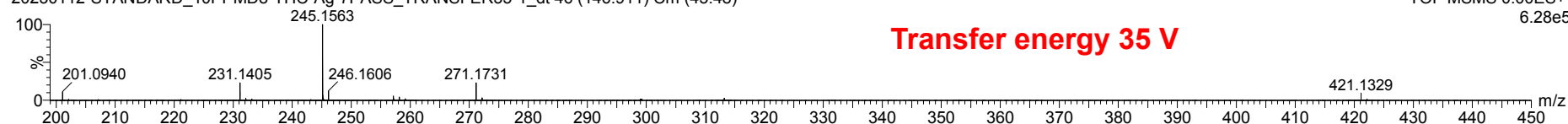
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TOF MSMS 0.00ES+
4.25e5



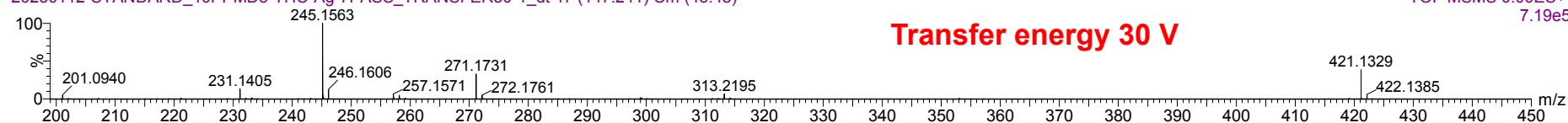
20230112-STANDARD_10PPMD8-THC-Ag-7PASS_TRANSFER35-1_dt 46 (146.911) Cm (45:48)

TOF MSMS 0.00ES+
6.28e5



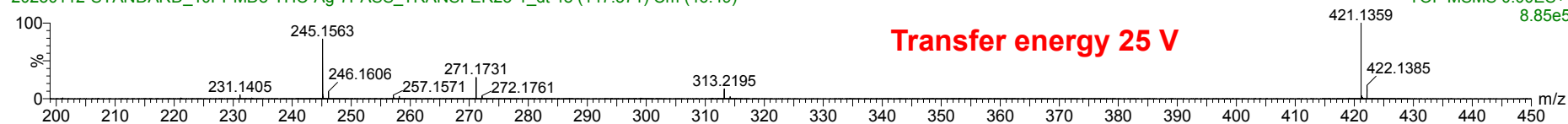
20230112-STANDARD_10PPMD8-THC-Ag-7PASS_TRANSFER30-1_dt 47 (147.241) Cm (45:48)

TOF MSMS 0.00ES+
7.19e5



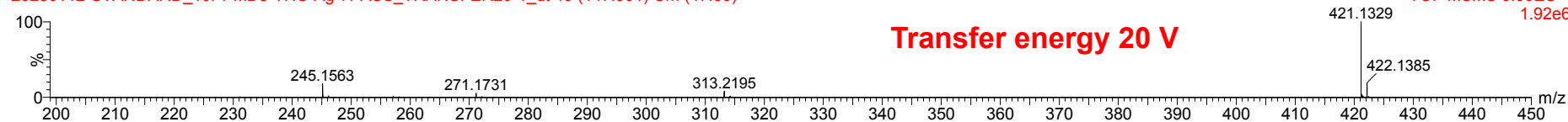
20230112-STANDARD_10PPMD8-THC-Ag-7PASS_TRANSFER25-1_dt 48 (147.571) Cm (46:49)

TOF MSMS 0.00ES+
8.85e5



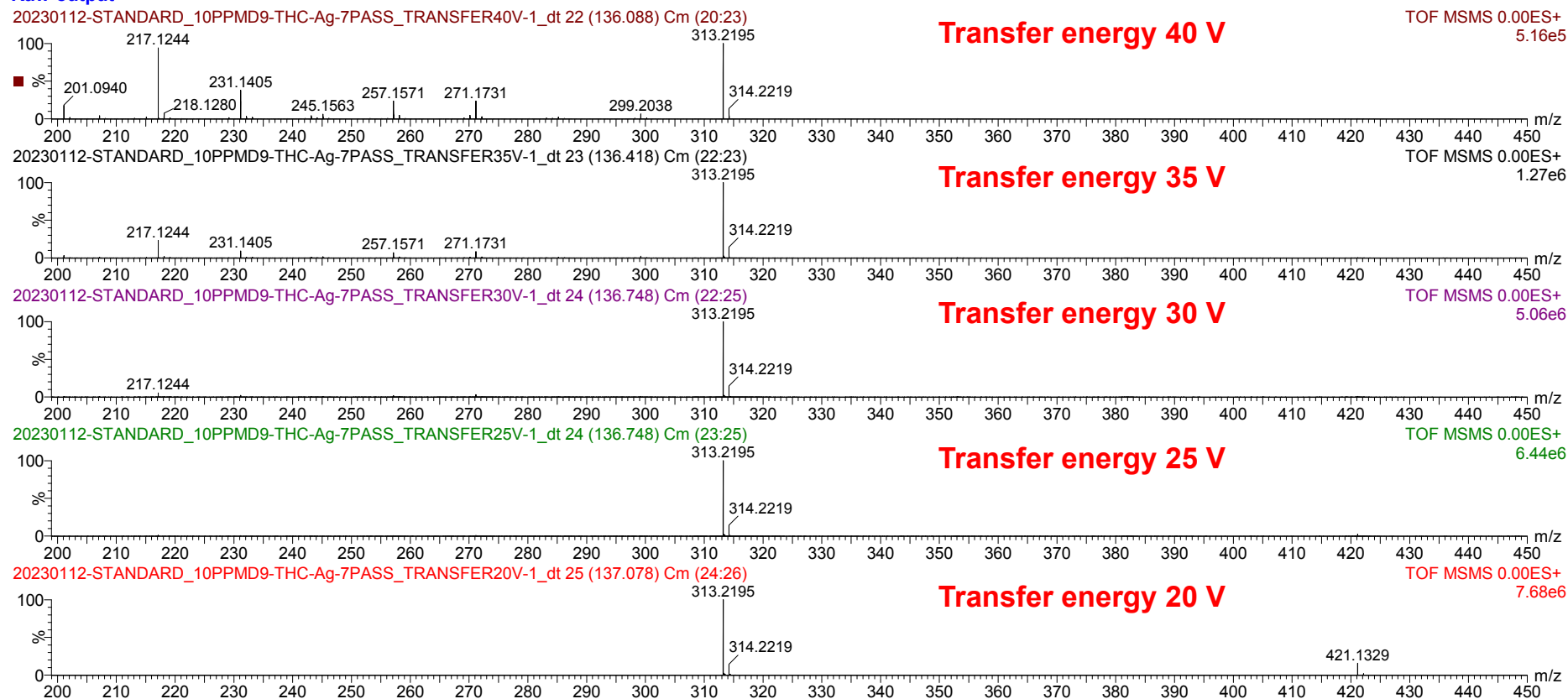
20230112-STANDARD_10PPMD8-THC-Ag-7PASS_TRANSFER20-1_dt 49 (147.901) Cm (47:50)

TOF MSMS 0.00ES+
1.92e6



c) Δ9-THC

Raw output

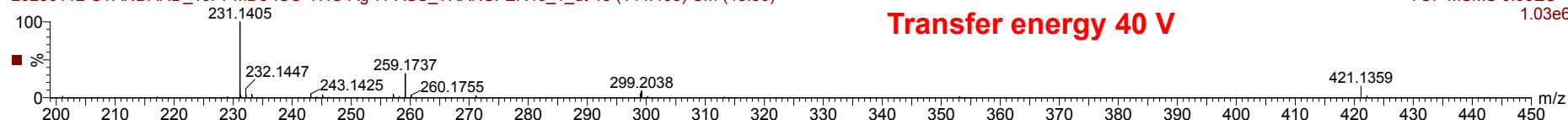


d) $\Delta 8$ -iso-THC

Raw output

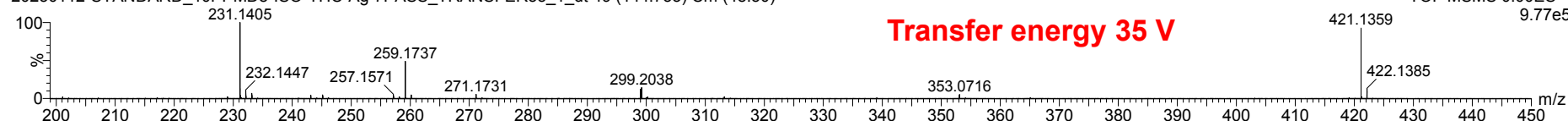
20230112-STANDARD_10PPMD8-ISO-THC-Ag-7PASS_TRANSFER40_1_dt 48 (144.403) Cm (48:50)

TOF MSMS 0.00ES+
1.03e6



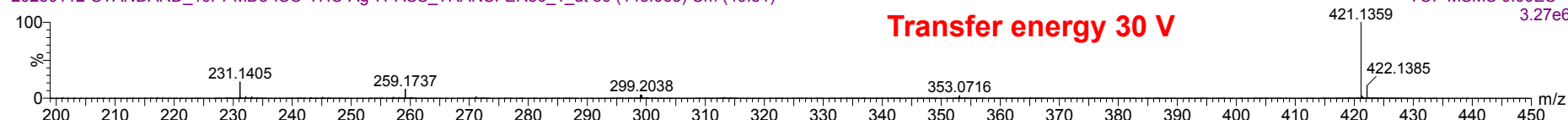
20230112-STANDARD_10PPMD8-ISO-THC-Ag-7PASS_TRANSFER35_1_dt 49 (144.733) Cm (48:50)

TOF MSMS 0.00ES+
9.77e5



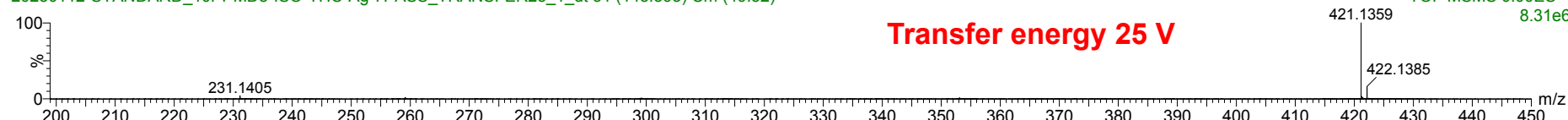
20230112-STANDARD_10PPMD8-ISO-THC-Ag-7PASS_TRANSFER30_1_dt 50 (145.063) Cm (49:51)

TOF MSMS 0.00ES+
3.27e6



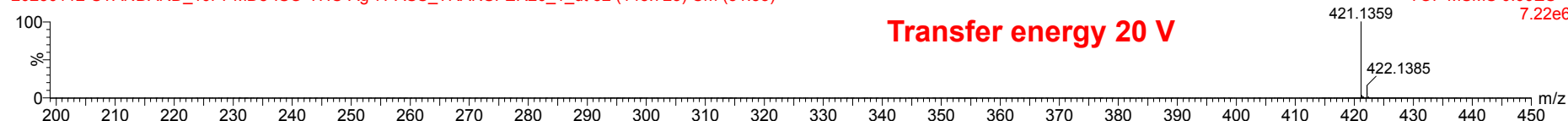
20230112-STANDARD_10PPMD8-ISO-THC-Ag-7PASS_TRANSFER25_1_dt 51 (145.393) Cm (49:52)

TOF MSMS 0.00ES+
8.31e6



20230112-STANDARD_10PPMD8-ISO-THC-Ag-7PASS_TRANSFER20_1_dt 52 (145.723) Cm (51:53)

TOF MSMS 0.00ES+
7.22e6

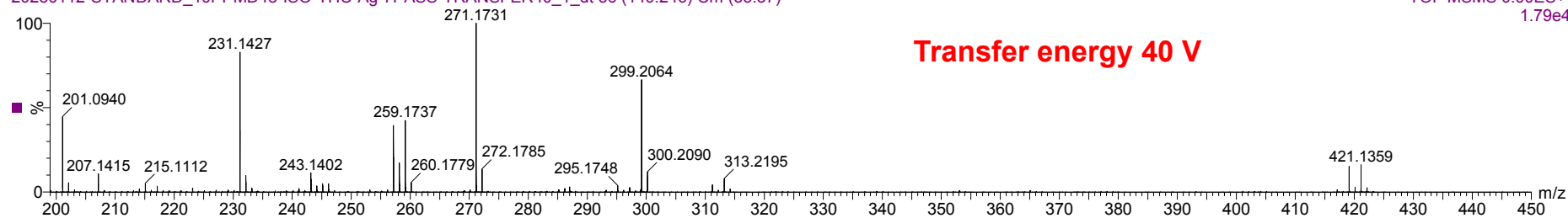


e) $\Delta(4)$ 8-iso-THC

Raw output

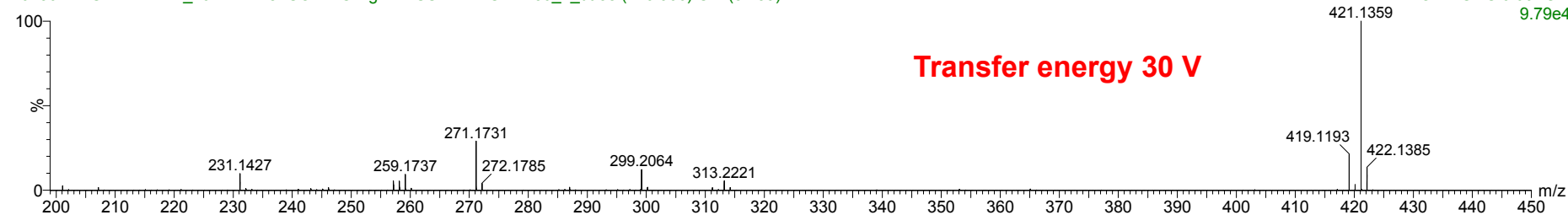
20230112-STANDARD_10PPMD48-ISO-THC-Ag-7PASS-TRANSFER40_1_dt 36 (140.246) Cm (35:37)

TOF MSMS 0.00ES+
1.79e4



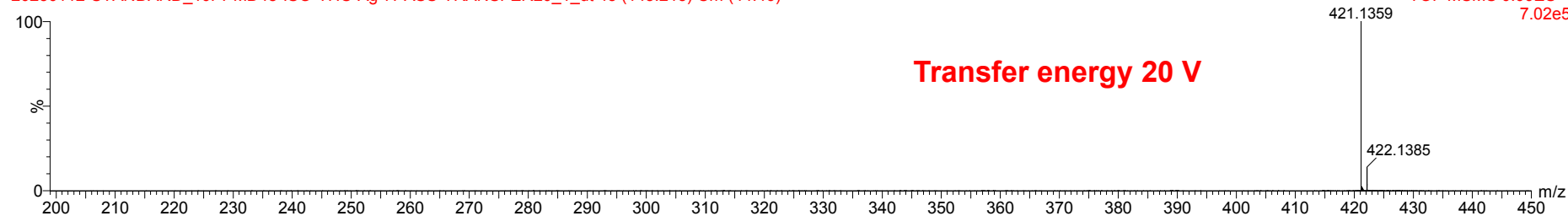
20230112-STANDARD_10PPMD48-ISO-THC-Ag-7PASS-TRANSFER30_1_dt 38 (140.906) Cm (37:39)

TOF MSMS 0.00ES+
9.79e4



20230112-STANDARD_10PPMD48-ISO-THC-Ag-7PASS-TRANSFER20_1_dt 45 (143.215) Cm (44:46)

TOF MSMS 0.00ES+
7.02e5



f) CBD

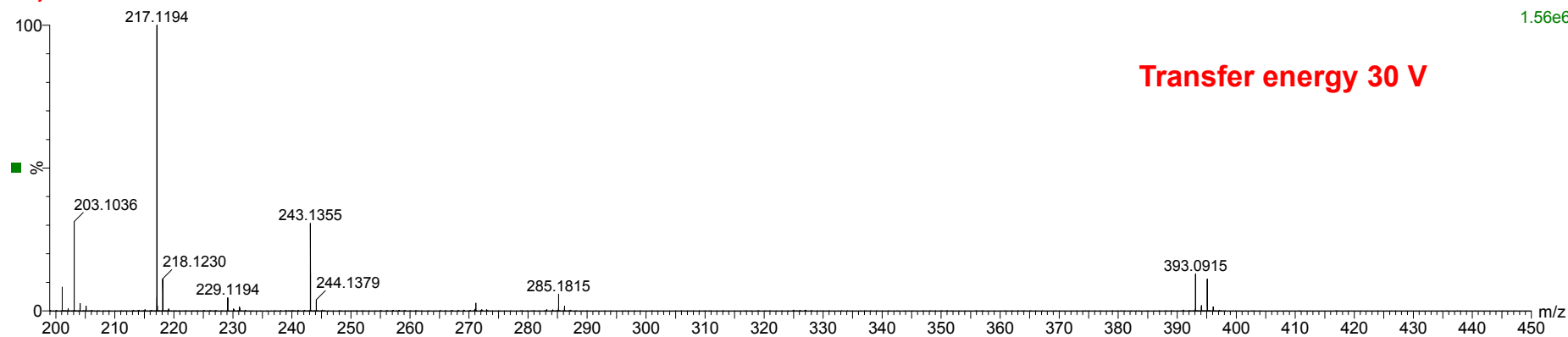
Raw output



Figure S12-1. Post-mobility fragmentation of a) Δ^3 -THC ($10 \mu\text{g}\cdot\text{mL}^{-1}$), b) Δ^8 -THC ($10 \mu\text{g}\cdot\text{mL}^{-1}$), c) Δ^9 -THC ($10 \mu\text{g}\cdot\text{mL}^{-1}$), d) Δ^8 -iso-THC ($10 \mu\text{g}\cdot\text{mL}^{-1}$), e) Δ^4 (8)-iso-THC ($10 \mu\text{g}\cdot\text{mL}^{-1}$), and f) CBD ($1.0 \mu\text{g}\cdot\text{mL}^{-1}$), in the presence of Ag(I) after 7-pass separation under different transfer energies. (selecting $[\text{M}+\text{Ag}]^+$ precursor at m/z 421 for cIMS separation, followed by fragmentation).

a) Δ^8 -THCV

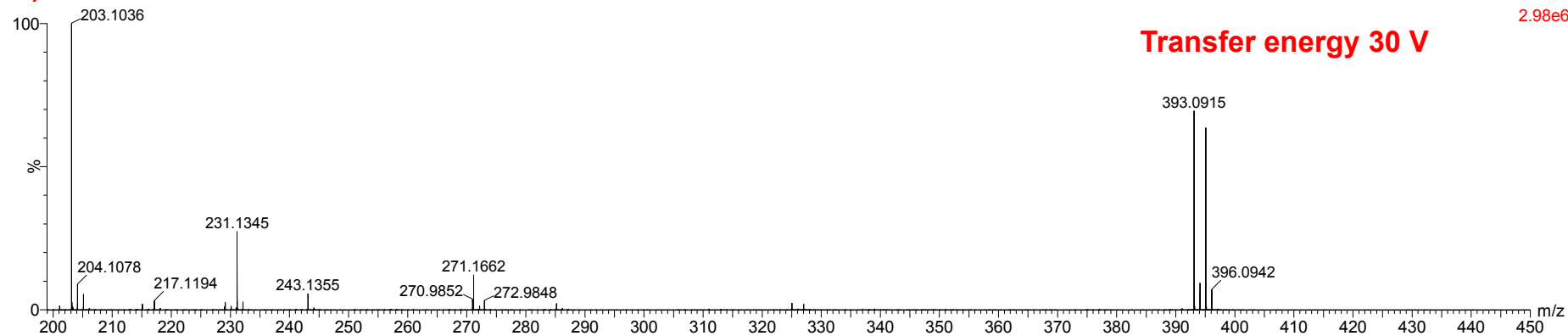
1.56e6



Transfer energy 30 V

b) Δ^8 -iso-THCV

2.98e6



Transfer energy 30 V

c) Δ^9 -THCV

Raw output

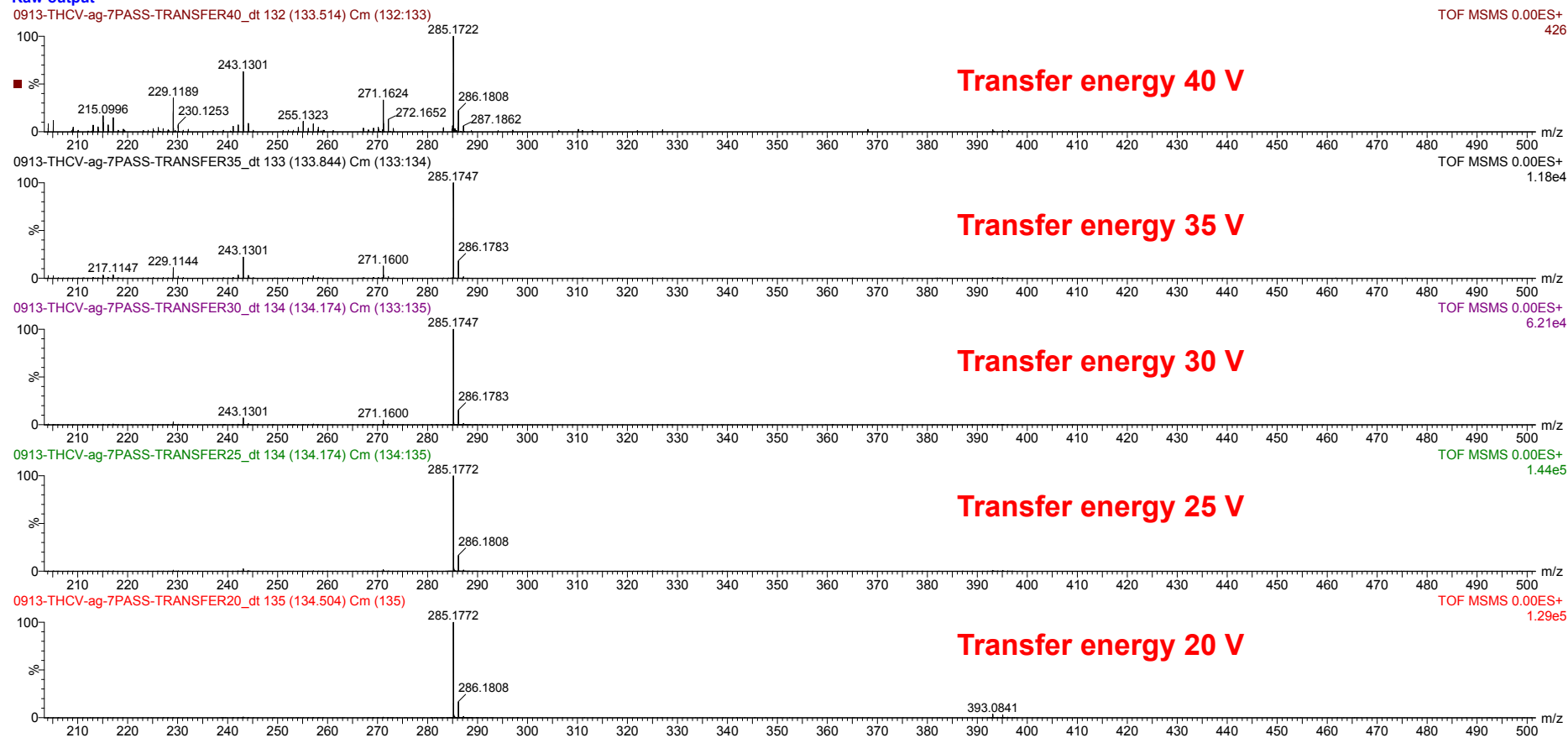


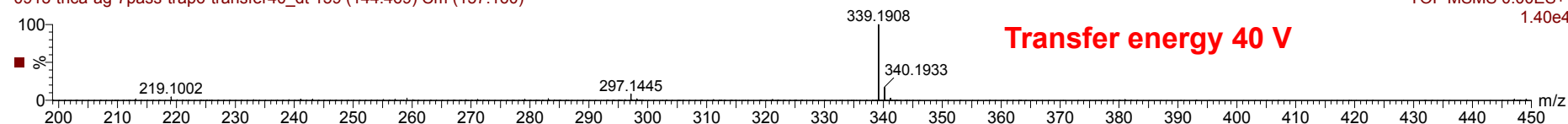
Figure S12-2. Post-mobility fragmentation of a) Δ^8 -THCV ($1.0 \mu\text{g} \cdot \text{mL}^{-1}$), b) Δ^8 -iso-THCV ($1.0 \mu\text{g} \cdot \text{mL}^{-1}$) and c) Δ^9 -THCV ($10 \mu\text{g} \cdot \text{mL}^{-1}$) in the presence of Ag(I) after 7-pass separation under different transfer energies (selecting $[M+\text{Ag}]^+$ precursor at m/z 393 for cIMS separation, followed by fragmentation).

a) THCA

Raw output

0913-thca-ag-7pass-trap6-transfer40_dt 159 (144.469) Cm (157:160)

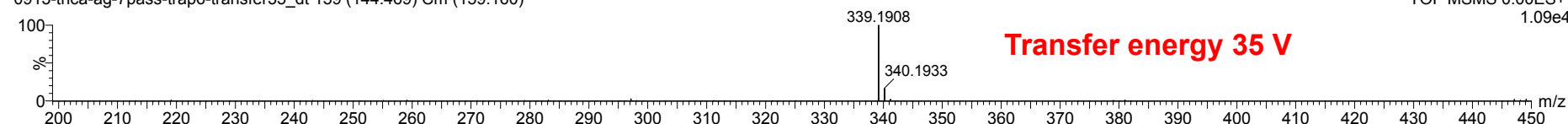
TOF MSMS 0.00ES+
1.40e4



Transfer energy 40 V

0913-thca-ag-7pass-trap6-transfer35_dt 159 (144.469) Cm (159:160)

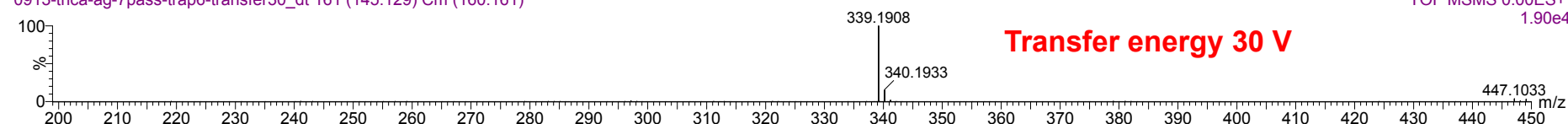
TOF MSMS 0.00ES+
1.09e4



Transfer energy 35 V

0913-thca-ag-7pass-trap6-transfer30_dt 161 (145.129) Cm (160:161)

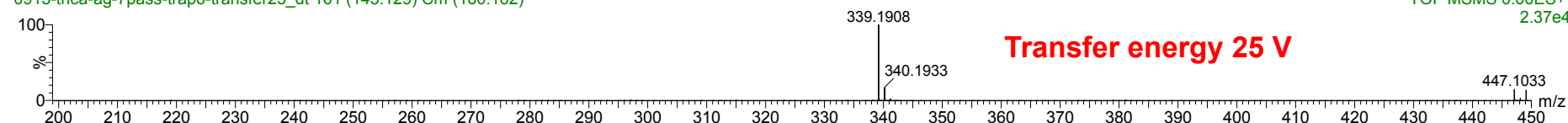
TOF MSMS 0.00ES+
1.90e4



Transfer energy 30 V

0913-thca-ag-7pass-trap6-transfer25_dt 161 (145.129) Cm (160:162)

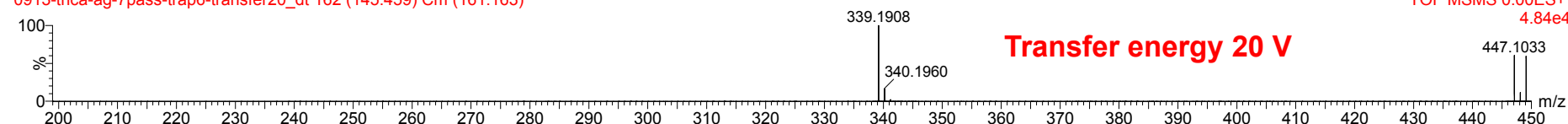
TOF MSMS 0.00ES+
2.37e4



Transfer energy 25 V

0913-thca-ag-7pass-trap6-transfer20_dt 162 (145.459) Cm (161:163)

TOF MSMS 0.00ES+
4.84e4



Transfer energy 20 V

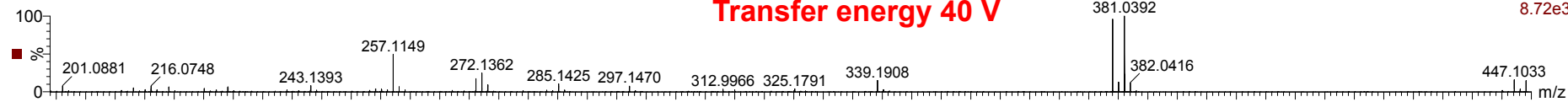
b) CBDA

Raw output

0913-cbda-ag-7pass-trap6-transfer40_dt 145 (139.718) Cm (144:146)

TOF MSMS 0.00ES+
8.72e3

Transfer energy 40 V



0913-cbda-ag-7pass-trap6-transfer35_dt 146 (140.048) Cm (145:148)

TOF MSMS 0.00ES+
2.64e4

Transfer energy 35 V



0913-cbda-ag-7pass-trap6-transfer30_dt 147 (140.378) Cm (146:148)

TOF MSMS 0.00ES+
3.62e4

Transfer energy 30 V



0913-cbda-ag-7pass-trap6-transfer25_dt 148 (140.708) Cm (147:148)

TOF MSMS 0.00ES+
4.24e4

Transfer energy 25 V



0913-cbda-ag-7pass-trap6-transfer20_dt 149 (141.037) Cm (147:150)

TOF MSMS 0.00ES+
1.43e5

Transfer energy 20 V

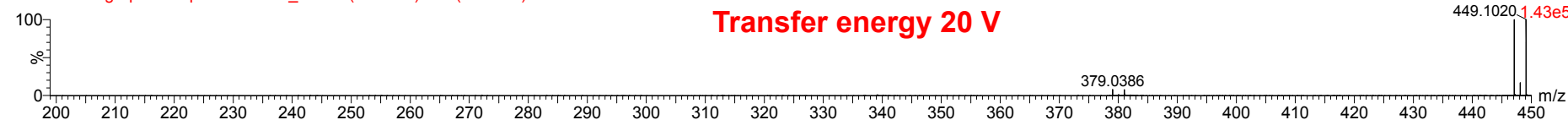


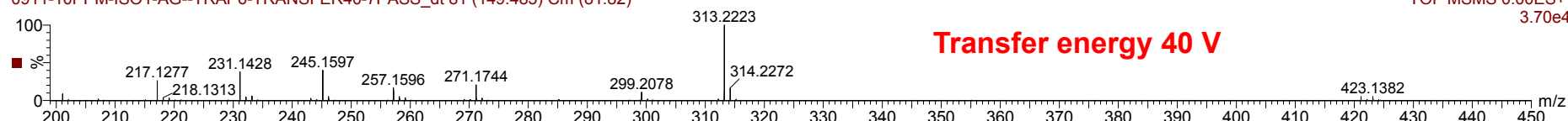
Figure S12-3. Post-mobility fragmentation of a) THCA ($10 \mu\text{g}\cdot\text{mL}^{-1}$) and b) CBDA ($10 \mu\text{g}\cdot\text{mL}^{-1}$) in the presence of Ag(I) after 7-pass separation under different transfer energies (selecting $[\text{M}+\text{Ag}]^+$ precursor at m/z 465 for cIMS separation, followed by fragmentation).

a) 9 β -hydroxyhexahydrocannabinol

Raw output

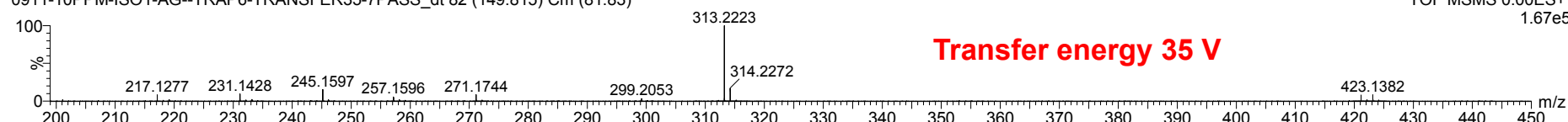
0911-10PPM-ISO1-AG--TRAP6-TRANSFER40-7PASS_dt 81 (149.485) Cm (81:82)

TOF MSMS 0.00ES+
3.70e4



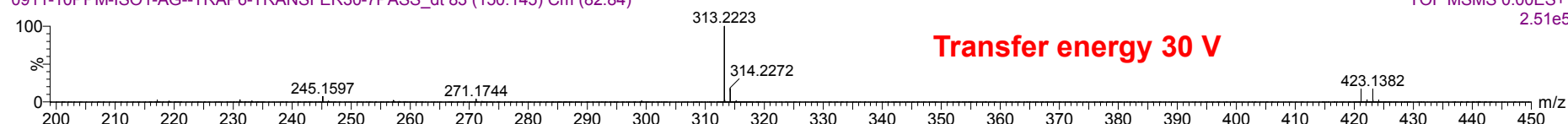
0911-10PPM-ISO1-AG--TRAP6-TRANSFER35-7PASS_dt 82 (149.815) Cm (81:83)

TOF MSMS 0.00ES+
1.67e5



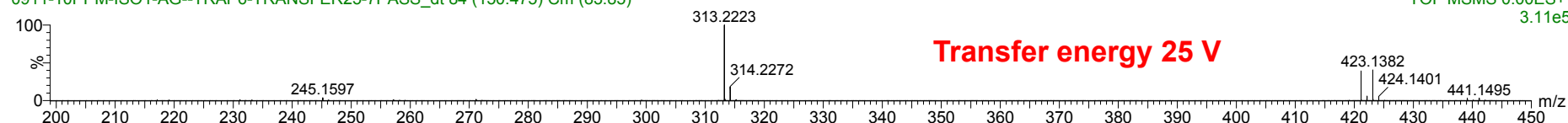
0911-10PPM-ISO1-AG--TRAP6-TRANSFER30-7PASS_dt 83 (150.145) Cm (82:84)

TOF MSMS 0.00ES+
2.51e5



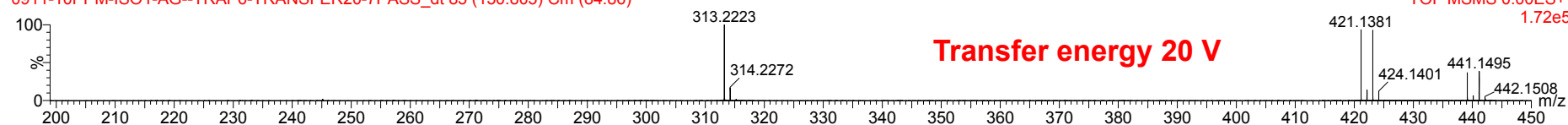
0911-10PPM-ISO1-AG--TRAP6-TRANSFER25-7PASS_dt 84 (150.475) Cm (83:85)

TOF MSMS 0.00ES+
3.11e5



0911-10PPM-ISO1-AG--TRAP6-TRANSFER20-7PASS_dt 85 (150.805) Cm (84:86)

TOF MSMS 0.00ES+
1.72e5

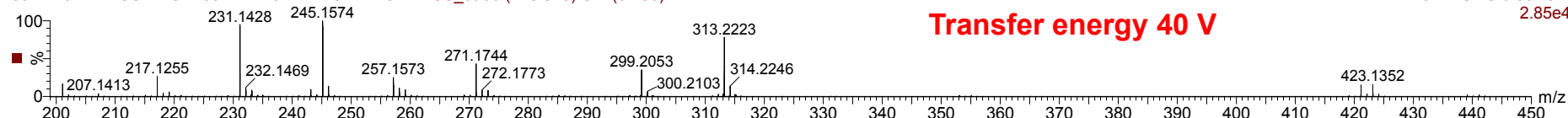


b) 9 α -hydroxyhexahydrocannabinol

Raw output

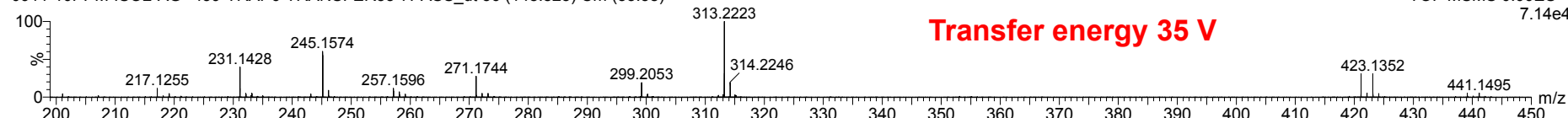
0911-10PPM-ISO2-AG--439-TRAP6-TRANSFER40-7PASS_dt 36 (148.825) Cm (34:36)

TOF MSMS 0.00ES+
2.85e4



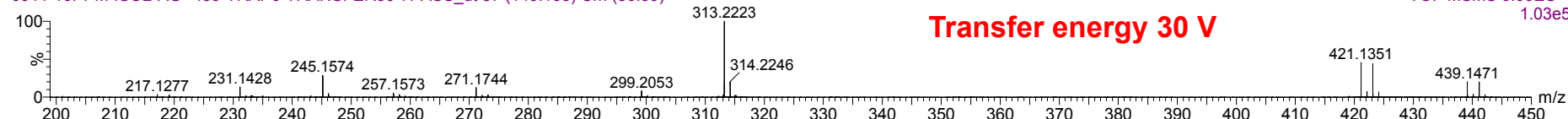
0911-10PPM-ISO2-AG--439-TRAP6-TRANSFER35-7PASS_dt 36 (148.825) Cm (35:38)

TOF MSMS 0.00ES+
7.14e4



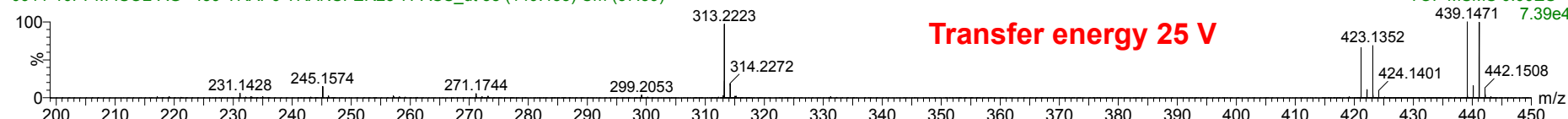
0911-10PPM-ISO2-AG--439-TRAP6-TRANSFER30-7PASS_dt 37 (149.155) Cm (36:39)

TOF MSMS 0.00ES+
1.03e5



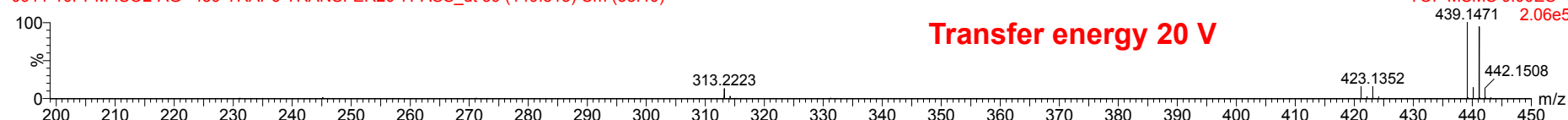
0911-10PPM-ISO2-AG--439-TRAP6-TRANSFER25-7PASS_dt 38 (149.485) Cm (37:39)

TOF MSMS 0.00ES+
7.39e4



0911-10PPM-ISO2-AG--439-TRAP6-TRANSFER20-7PASS_dt 39 (149.815) Cm (38:40)

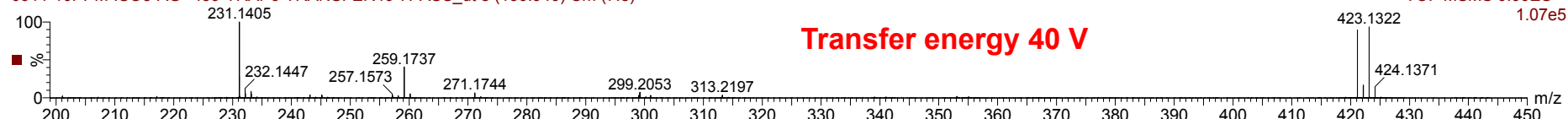
TOF MSMS 0.00ES+
2.06e5



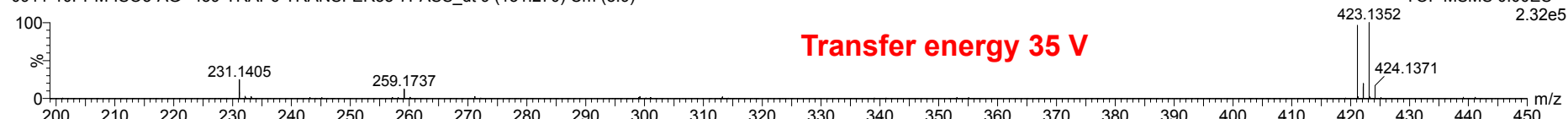
c) 8-hydroxy-iso-THC

Raw output

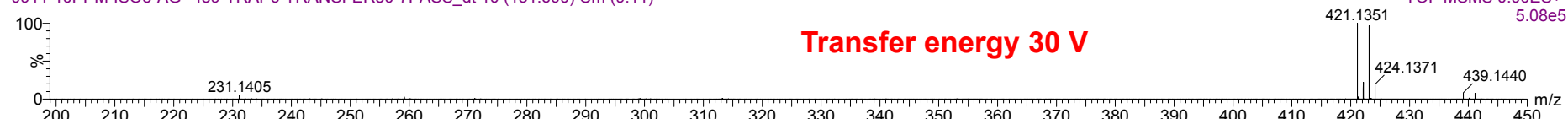
0911-10PPM-ISO3-AG--439-TRAP6-TRANSFER40-7PASS_dt 8 (130.940) Cm (7:8)



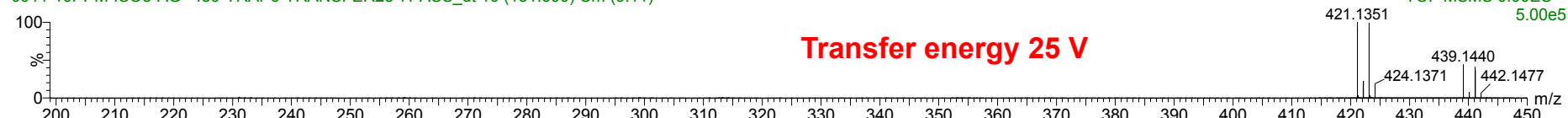
0911-10PPM-ISO3-AG--439-TRAP6-TRANSFER35-7PASS_dt 9 (131.270) Cm (8:9)



0911-10PPM-ISO3-AG--439-TRAP6-TRANSFER30-7PASS_dt 10 (131.600) Cm (9:11)



0911-10PPM-ISO3-AG--439-TRAP6-TRANSFER25-7PASS_dt 10 (131.600) Cm (9:11)



0911-10PPM-ISO3-AG--439-TRAP6-TRANSFER20-7PASS_dt 11 (131.930) Cm (10:12)

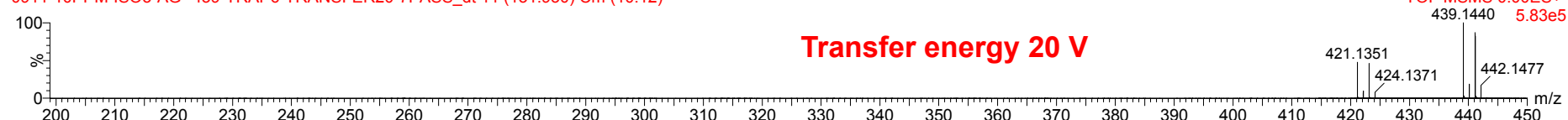
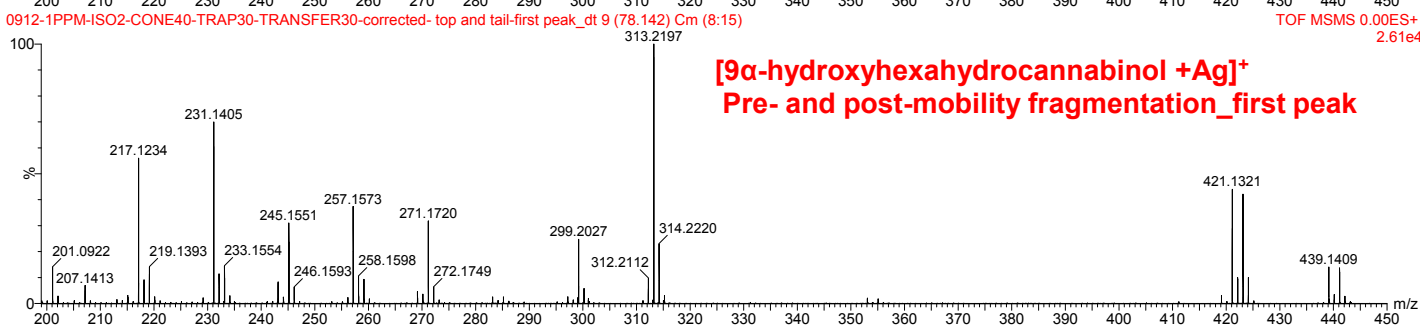
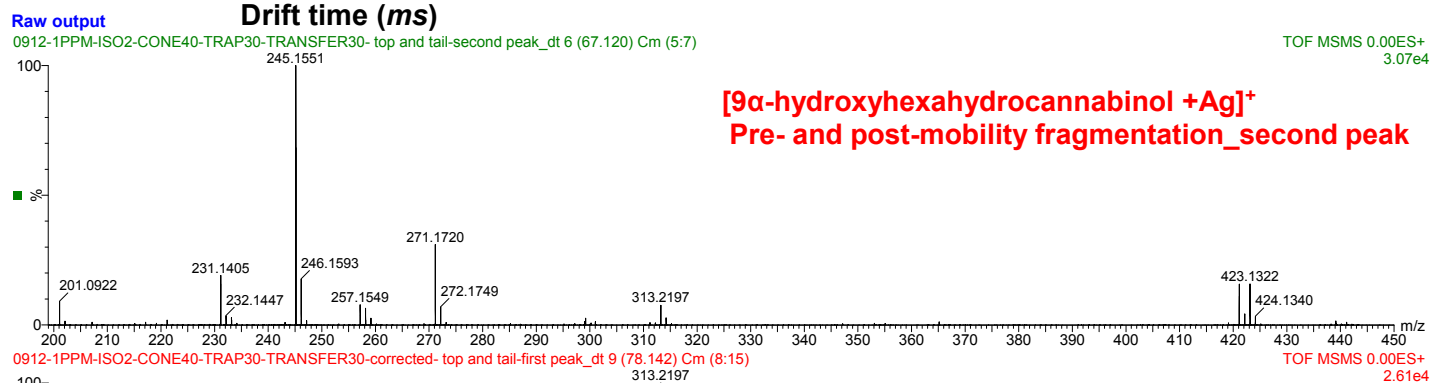
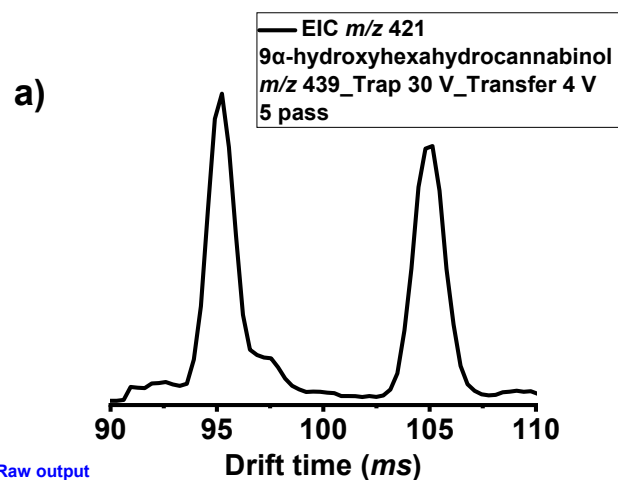
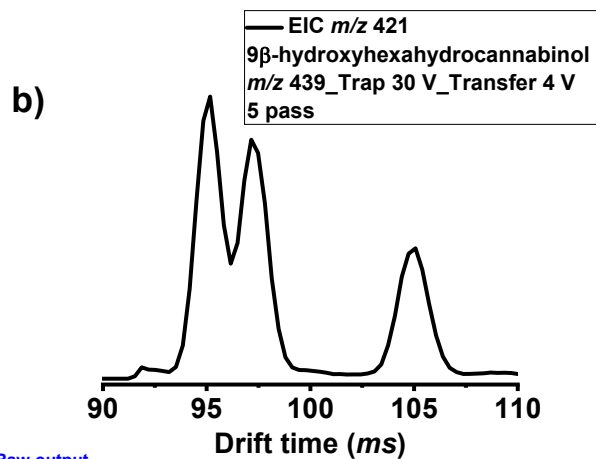


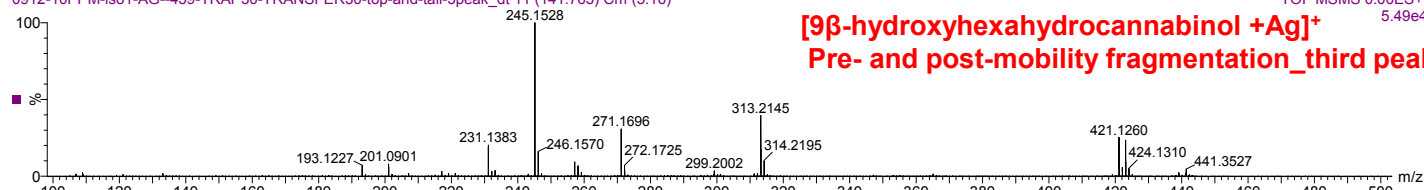
Figure S12-4. Post-mobility fragmentation of a) 9 β -hydroxyhexahydrocannabinol ($10\ \mu\text{g}\cdot\text{mL}^{-1}$), b) 9 α -hydroxyhexahydrocannabinol ($10\ \mu\text{g}\cdot\text{mL}^{-1}$) and c) 8-hydroxy-iso-tetrahydrocannabinol ($10\ \mu\text{g}\cdot\text{mL}^{-1}$) in the presence of Ag(I) after 7-pass separation under different transfer energies (selecting $[\text{M}+\text{Ag}]^+$ precursor at m/z 439 for cIMS separation, followed by fragmentation).



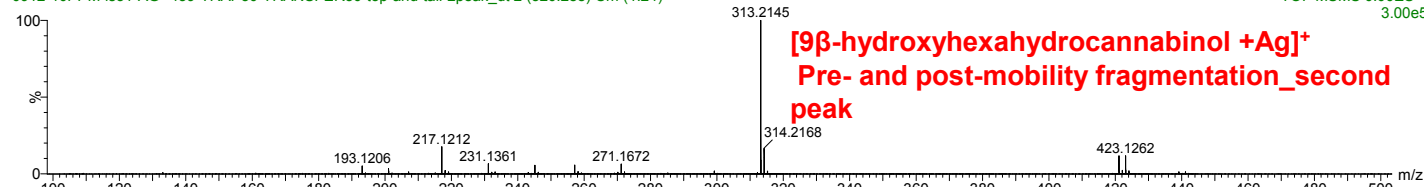


Raw output

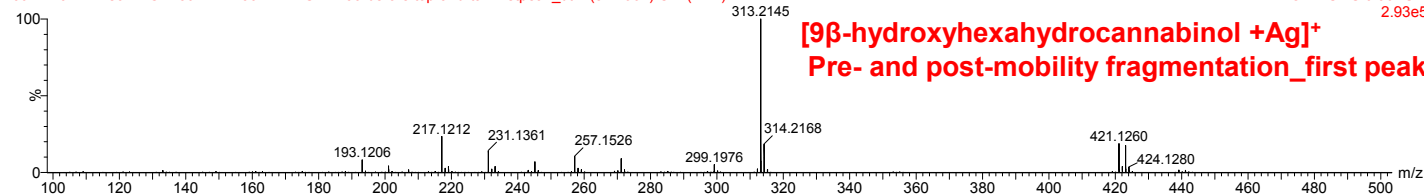
0912-10PPM-iso1-AG--439-TRAP30-TRANSFER30-top-and-tail-3peak_dt 11 (141.763) Cm (5:16)



0912-10PPM-iso1-AG--439-TRAP30-TRANSFER30-top-and-tail-2peak_dt 2 (320.288) Cm (1:24)



0912-10PPM-iso1-AG--439-TRAP30-TRANSFER30-before top-and-tail-firstpeak_dt 4 (312.962) Cm (4:27)



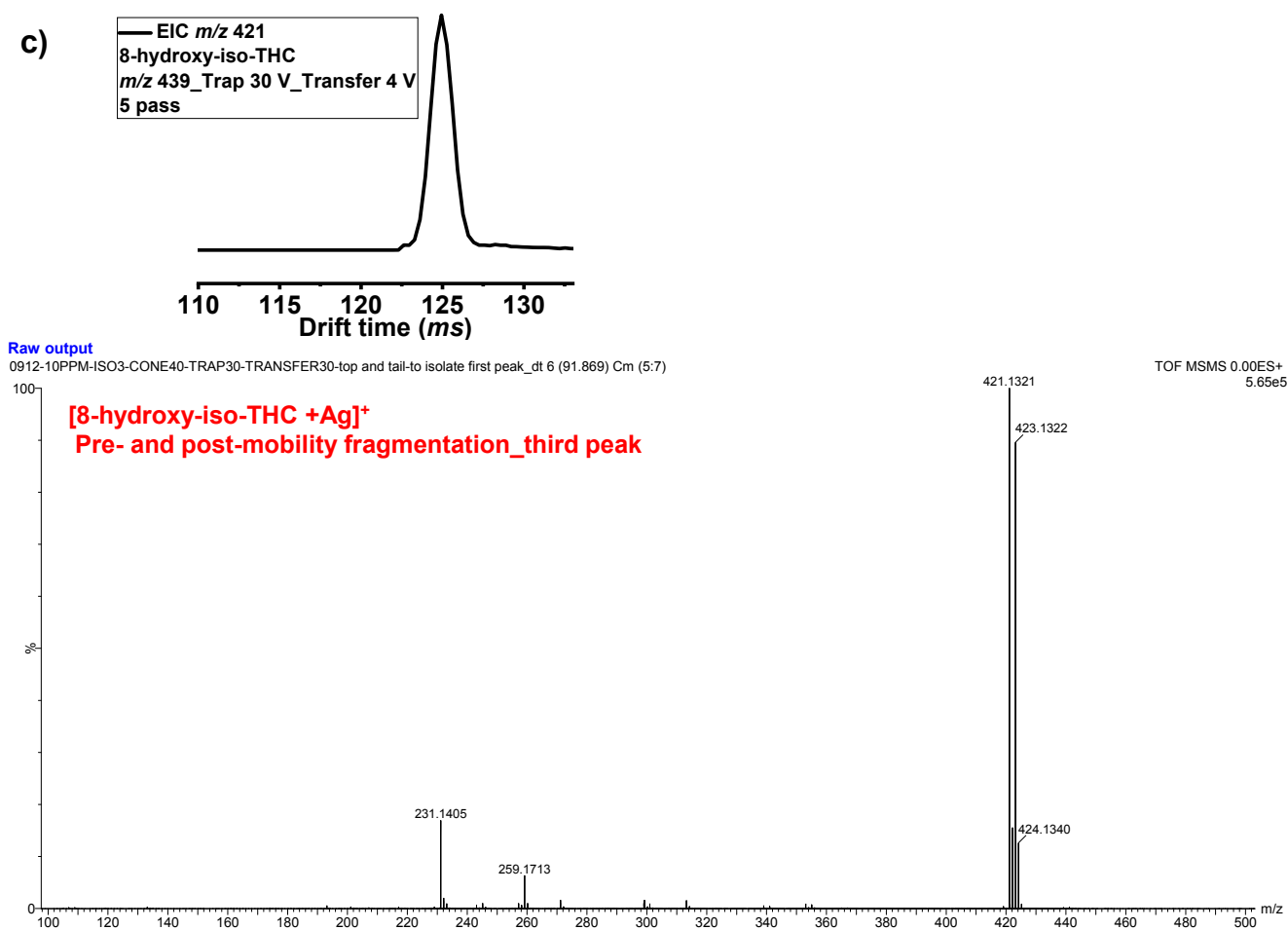


Figure S13. Pre- and post-mobility fragmentation of a) 9 α -hydroxyhexahydrocannabinol, b) 9 β -hydroxyhexahydrocannabinol, and c) 8-hydroxy-iso-THC in the presence of Ag(I) with trap energy of 30 V and transfer energy of 30 V.

Table S5. CCS of 9 α -hydroxyhexahydrocannabinol, 9 β -hydroxyhexahydrocannabinol, and 8-hydroxy-iso-THC as well as their dehydrated species in the presence of Ag(I).

	$[M+Ag]^+$ $^{TW}CCS_{N_2}(\text{\AA}^2)$
9 α -hydroxyhexahydrocannabinol	195.6 $\pm$ 0.01
Dehydrated	182.0 $\pm$ 0.01
9 α -hydroxyhexahydrocannabinol	190.6 $\pm$ 0.02
	(−0.2% to Δ 8-THC)
9 β -hydroxyhexahydrocannabinol	185.9 $\pm$ 0.01
Dehydrated	181.9 $\pm$ 0.01
9 β -hydroxyhexahydrocannabinol	183.9 $\pm$ 0.01
	190.6 $\pm$ 0.01
	(−0.2% to Δ 8-THC)
8-hydroxy-iso-THC	184.6 $\pm$ 0.02
Dehydrated	179.7 $\pm$ 0.01
8-hydroxy-iso-THC	

Table S6. Intra-day, inter-day, and inter-pass relative standard deviation of [Δ^8 -THC+Ag]⁺ CCS.

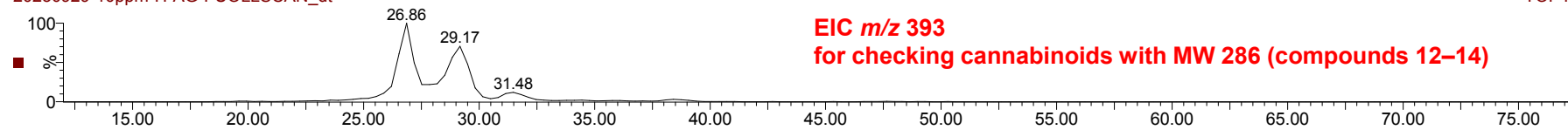
Measured date and separation passes	[Δ^8 -THC+Ag] ⁺ eCCS	Intra-day RSD (%)	Inter-day RSD (%)	Inter-pass RSD (%)
11 th November 2022_7 passes	190.7	0		
	190.7			
	190.7			
12 th January 2023_7 passes	190.9	0.03	0.04	
	190.9			
	190.8			
20 th September 2023_7 passes	190.7	0		0.3
	190.7			
	190.7			
28 th September 2023_7 passes	190.7	0		
	190.7			
	190.7			
12 th January 2023_1 pass	190.3	0.03	0.2	
	190.3			
	190.2			
20 th September 2023_1 pass	189.3	0.1		
	189.6			
	189.7			

C#1_full scan_for checking Ag(I) adducts

Raw output

20230929-10ppm-H-AG-FUOLLSCAN_dt

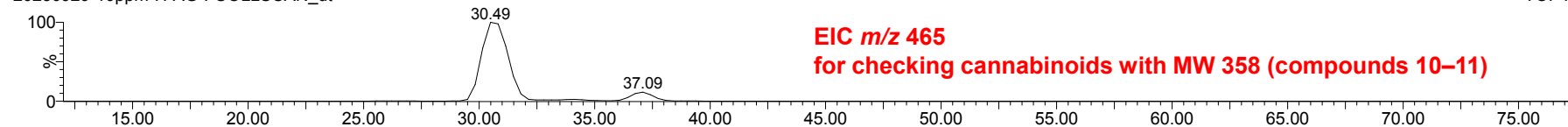
TOF MS ES+
393
2.61e4



EIC m/z 393
for checking cannabinoids with MW 286 (compounds 12–14)

20230929-10ppm-H-AG-FUOLLSCAN_dt

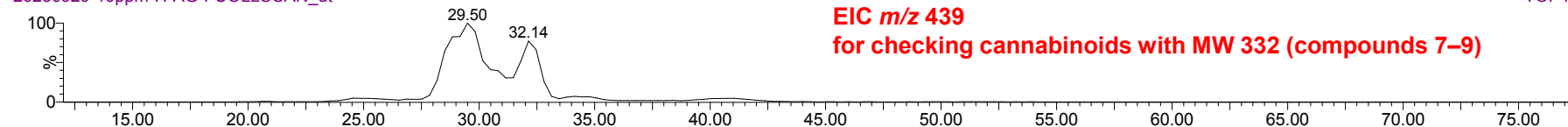
TOF MS ES+
465
8.05e5



EIC m/z 465
for checking cannabinoids with MW 358 (compounds 10–11)

20230929-10ppm-H-AG-FUOLLSCAN_dt

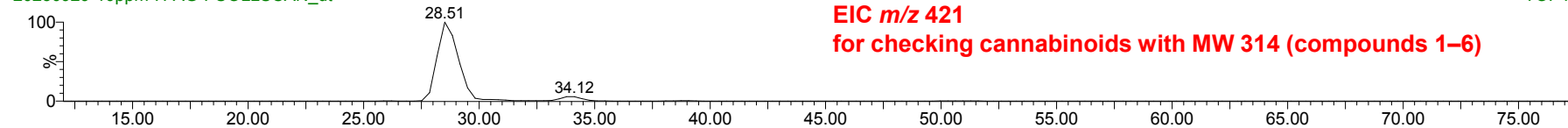
TOF MS ES+
439
3.71e4



EIC m/z 439
for checking cannabinoids with MW 332 (compounds 7–9)

20230929-10ppm-H-AG-FUOLLSCAN_dt

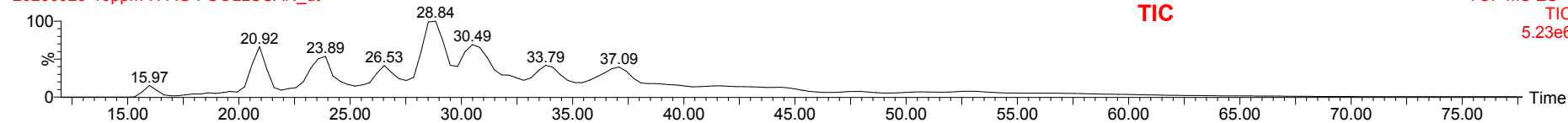
TOF MS ES+
421
1.53e6



EIC m/z 421
for checking cannabinoids with MW 314 (compounds 1–6)

20230929-10ppm-H-AG-FUOLLSCAN_dt

TOF MS ES+
TIC
5.23e6



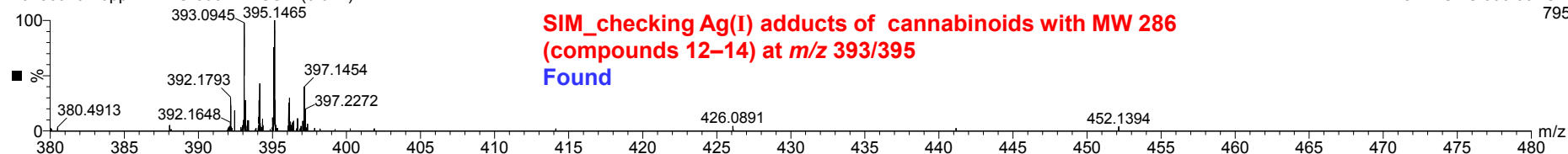
TIC

C#1 _SIM_for checking Ag(I) adducts

Raw output

20230929-10ppm-H-AG-393-1PASS 1 (0.017)

TOF MSMS 393.00ES+
795

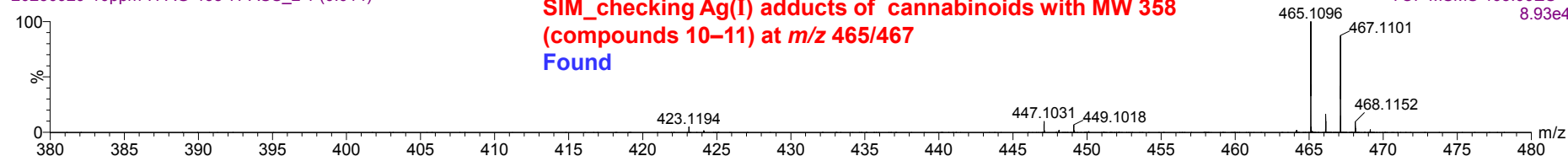


**SIM_checking Ag(I) adducts of cannabinoids with MW 286
(compounds 12–14) at m/z 393/395**

Found

20230929-10ppm-H-AG-465-7PASS_2 1 (0.014)

TOF MSMS 465.00ES+
8.93e4

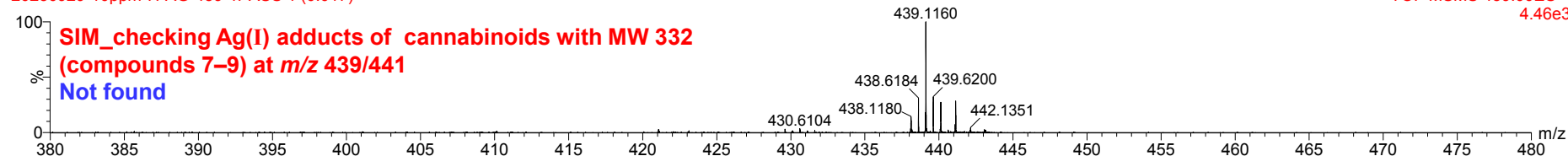


**SIM_checking Ag(I) adducts of cannabinoids with MW 358
(compounds 10–11) at m/z 465/467**

Found

20230929-10ppm-H-AG-439-1PASS 1 (0.017)

TOF MSMS 439.00ES+
4.46e3

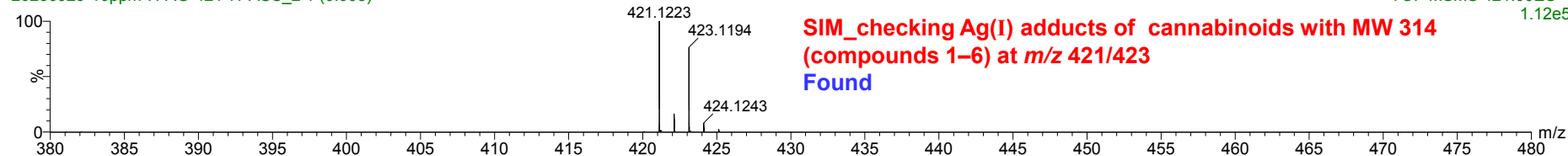


**SIM_checking Ag(I) adducts of cannabinoids with MW 332
(compounds 7–9) at m/z 439/441**

Not found

20230929-10ppm-H-AG-421-7PASS_2 1 (0.008)

TOF MSMS 421.00ES+
1.12e5



**SIM_checking Ag(I) adducts of cannabinoids with MW 314
(compounds 1–6) at m/z 421/423**

Found

C#1 _mobility separation_for checking CCS

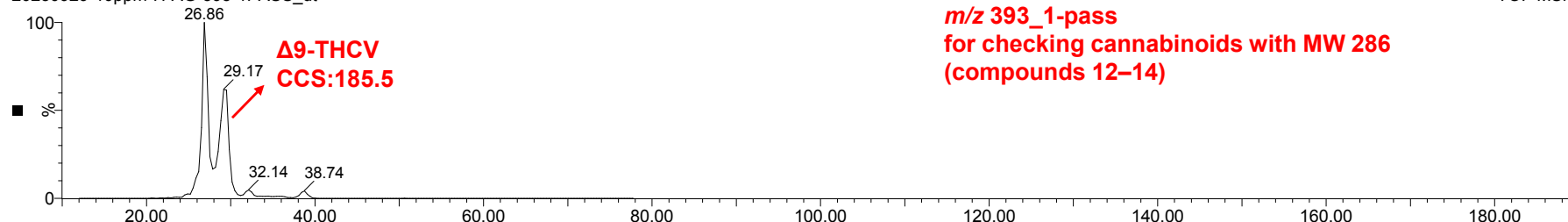
Raw output

20230929-10ppm-H-AG-393-1PASS_dt

TOF MSMS ES+

393

3.41e4



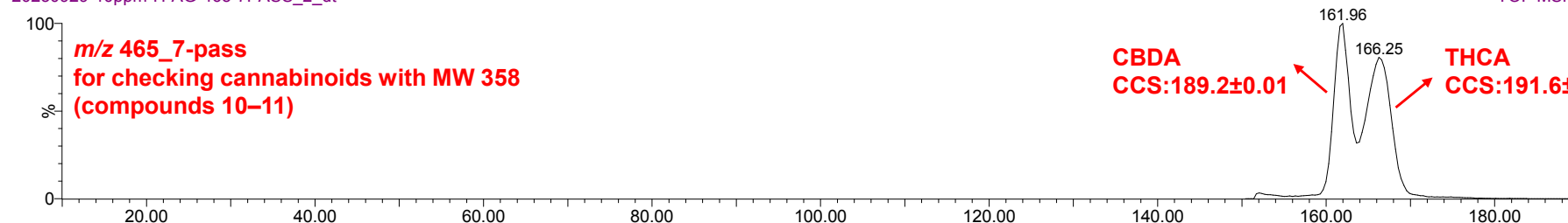
m/z 393_1-pass
for checking cannabinoids with MW 286
(compounds 12–14)

20230929-10ppm-H-AG-465-7PASS_2_dt

TOF MSMS ES+

465

3.55e5



m/z 465_7-pass
for checking cannabinoids with MW 358
(compounds 10–11)

CBDA
CCS:189.2±0.01

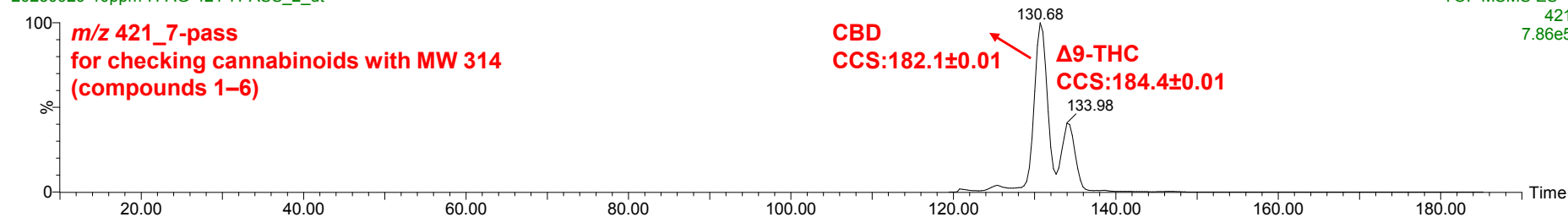
THCA
CCS:191.6±0.03

20230929-10ppm-H-AG-421-7PASS_2_dt

TOF MSMS ES+

421

7.86e5



m/z 421_7-pass
for checking cannabinoids with MW 314
(compounds 1–6)

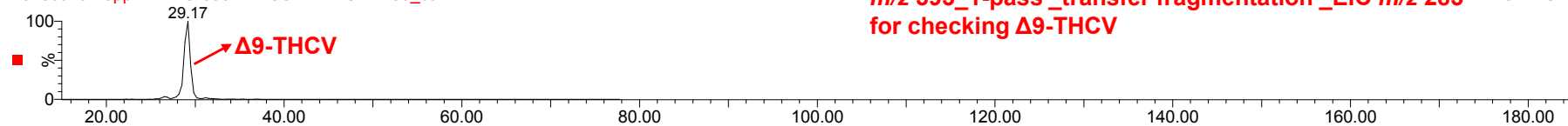
CBD
CCS:182.1±0.01

Δ9-THC
CCS:184.4±0.01

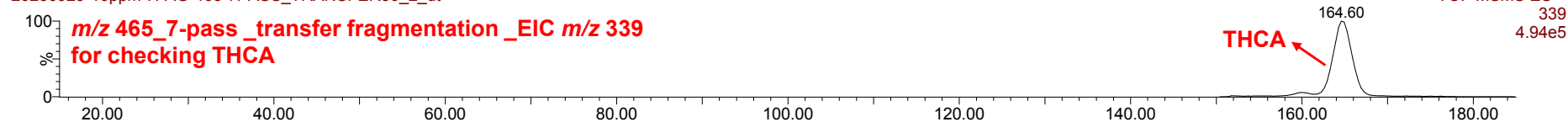
C#1_mobility separation+transfer fragmentation_for checking fragments

Raw output

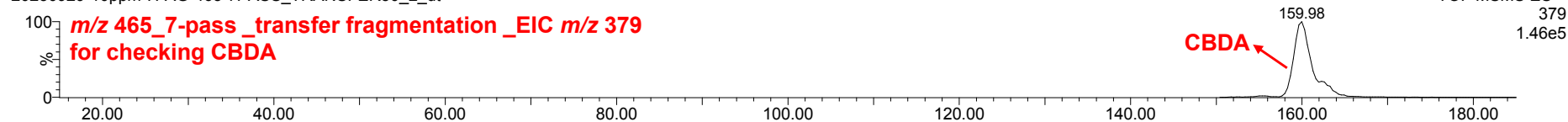
20230929-10ppm-H-AG-393-1PASS-TRANSFER30_dt



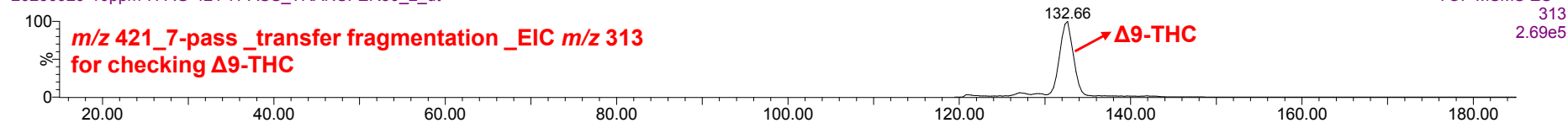
20230929-10ppm-H-AG-465-7PASS-TRANSFER30_2_dt



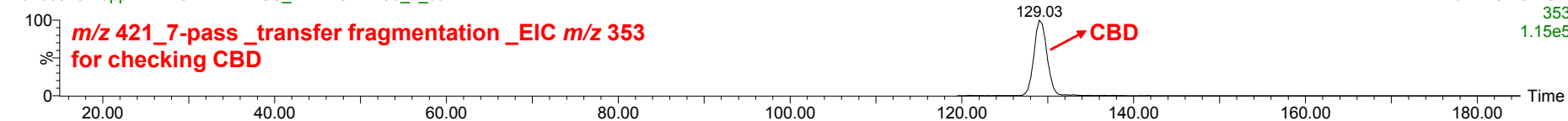
20230929-10ppm-H-AG-465-7PASS-TRANSFER30_2_dt



20230929-10ppm-H-AG-421-7PASS-TRANSFER30_2_dt



20230929-10ppm-H-AG-421-7PASS-TRANSFER30_2_dt

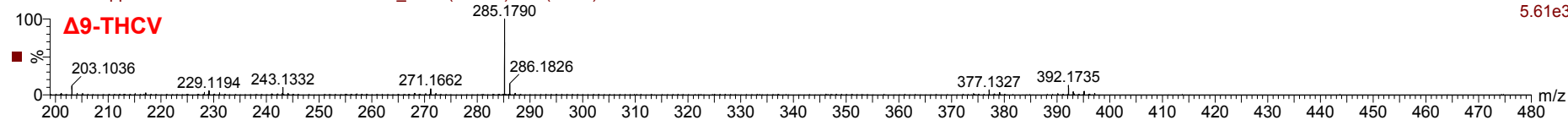


C#1_mobility separation+transfer fragmentation_for checking fragments

Raw output

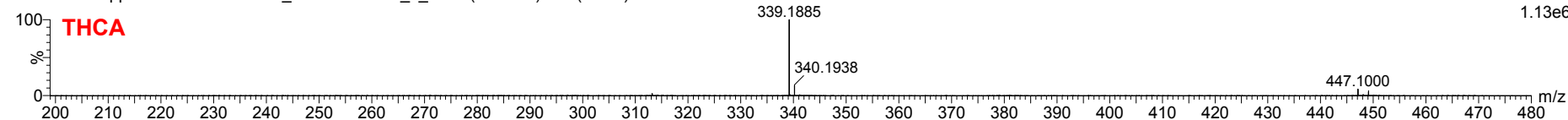
20230929-10ppm-H-AG-393-1PASS-TRANSFER30_dt 52 (28.841) Cm (51:55)

TOF MSMS 0.00ES+
5.61e3



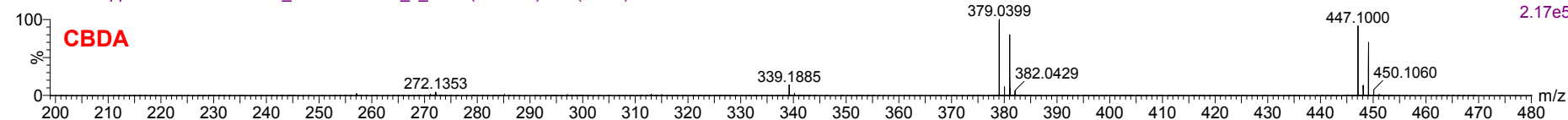
20230929-10ppm-H-AG-465-7PASS_TRANSFER30_2_dt 44 (164.599) Cm (42:47)

TOF MSMS 0.00ES+
1.13e6



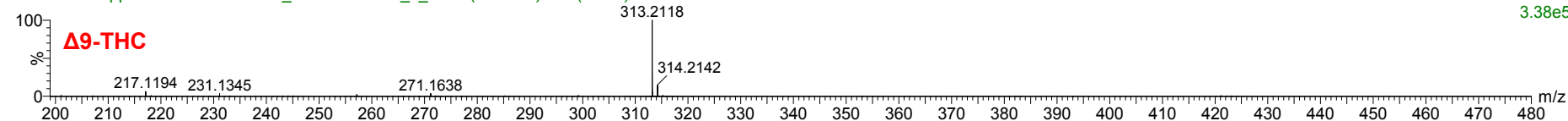
20230929-10ppm-H-AG-465-7PASS_TRANSFER30_2_dt 30 (159.979) Cm (27:32)

TOF MSMS 0.00ES+
2.17e5



20230929-10ppm-H-AG-421-7PASS_TRANSFER30_2_dt 41 (132.656) Cm (39:42)

TOF MSMS 0.00ES+
3.38e5



20230929-10ppm-H-AG-421-7PASS_TRANSFER30_2_dt 30 (129.026) Cm (28:33)

TOF MSMS 0.00ES+
1.03e6

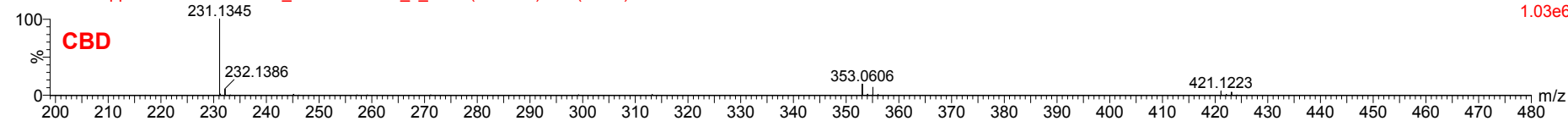
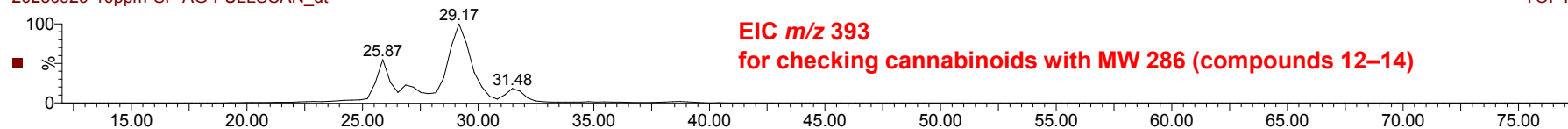


Figure S14-1. Mobiligram and mass spectra of cannabinoids in sample C#1.

C#2_full scan_for checking Ag(I) adducts

Raw output

20230929-10ppm-SP-AG-FULLSCAN_dt

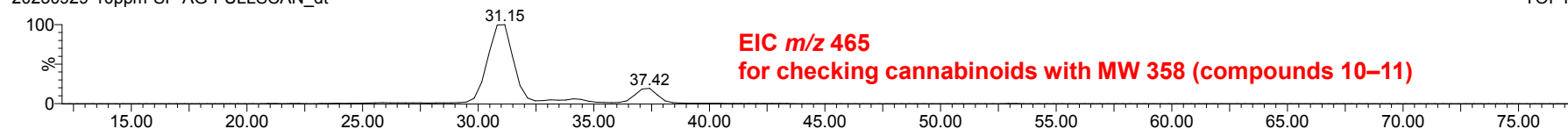


EIC m/z 393

for checking cannabinoids with MW 286 (compounds 12–14)

TOF MS ES+
393
6.24e4

20230929-10ppm-SP-AG-FULLSCAN_dt

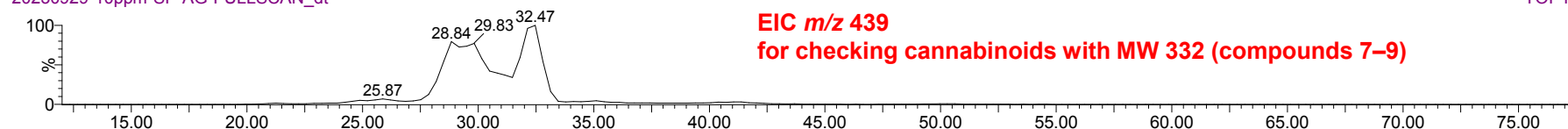


EIC m/z 465

for checking cannabinoids with MW 358 (compounds 10–11)

TOF MS ES+
465
1.74e5

20230929-10ppm-SP-AG-FULLSCAN_dt

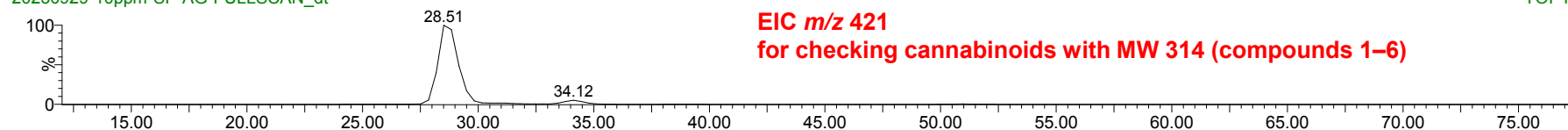


EIC m/z 439

for checking cannabinoids with MW 332 (compounds 7–9)

TOF MS ES+
439
4.38e4

20230929-10ppm-SP-AG-FULLSCAN_dt

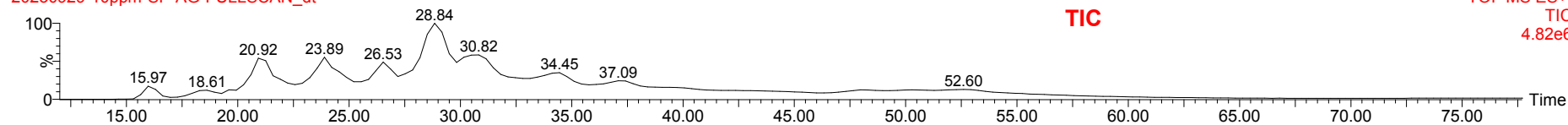


EIC m/z 421

for checking cannabinoids with MW 314 (compounds 1–6)

TOF MS ES+
421
8.21e5

20230929-10ppm-SP-AG-FULLSCAN_dt



TIC

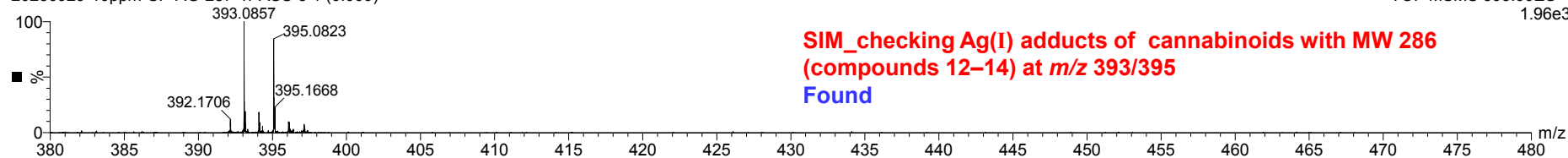
TOF MS ES+
TIC
4.82e6

C#2_SIM for checking Ag(I) adducts

Raw output

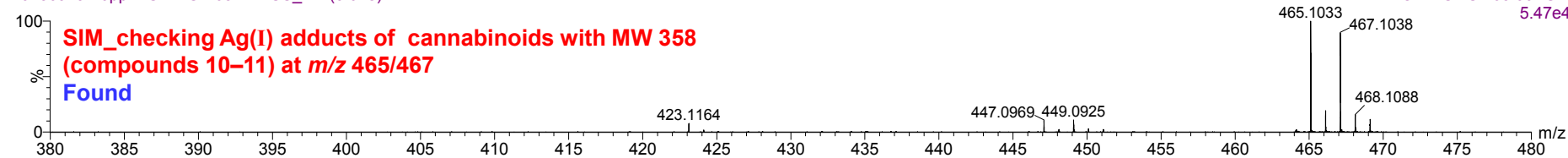
20230929-10ppm-SP-AG-287-1PASS-3 1 (0.009)

TOF MSMS 393.00ES+
1.96e3



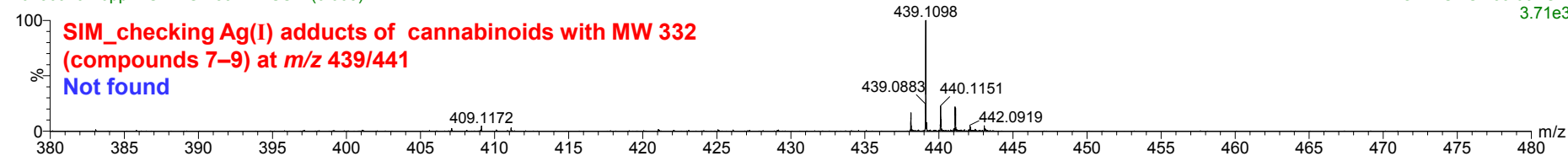
20230929-10ppm-SP-AG-465-7PASS_2 1 (0.018)

TOF MSMS 465.00ES+
5.47e4



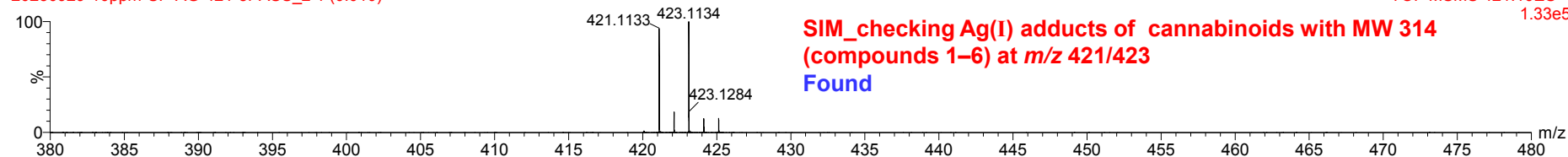
20230929-10ppm-SP-AG-439-1PASS 1 (0.003)

TOF MSMS 439.00ES+
3.71e3



20230929-10ppm-SP-AG-421-5PASS_2 1 (0.010)

TOF MSMS 421.10ES+
1.33e5

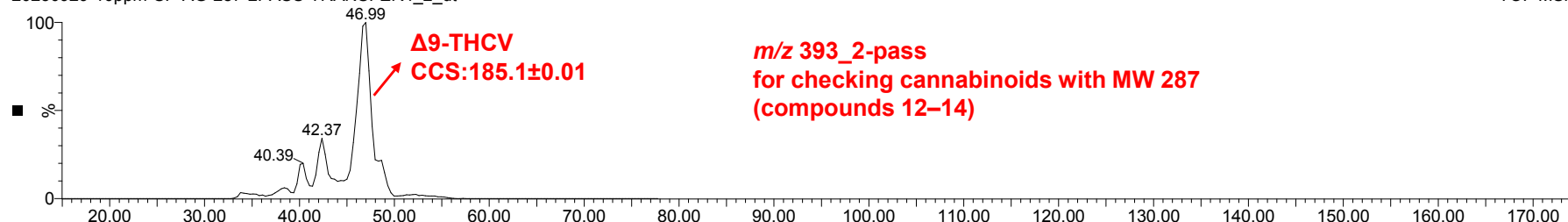


C#2 _mobility separation_for checking CCS

Raw output

20230929-10ppm-SP-AG-287-2PASS-TRANSFER4_2_dt

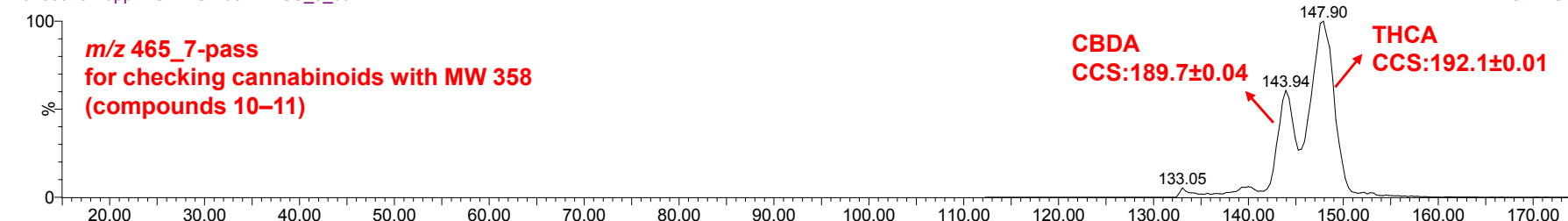
TOF MSMS ES+
393
5.27e4



m/z 393_2-pass
for checking cannabinoids with MW 287
(compounds 12–14)

20230929-10ppm-SP-AG-465-7PASS_3_dt

TOF MSMS ES+
465
2.82e5

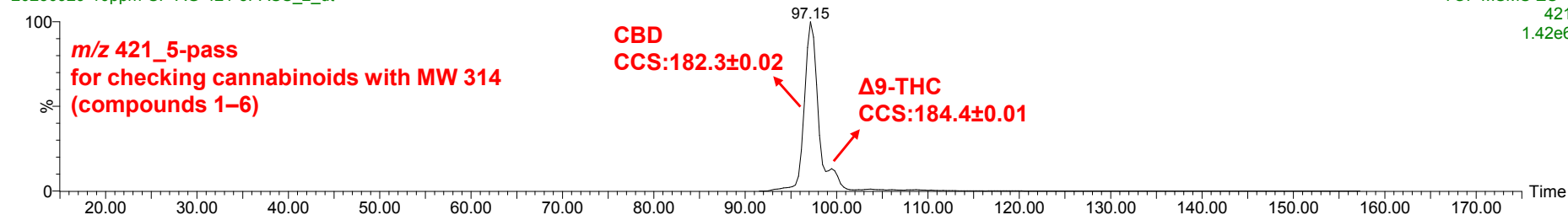


m/z 465_7-pass
for checking cannabinoids with MW 358
(compounds 10–11)

CBDA
CCS:189.7 $\pm$ 0.04
THCA
CCS:192.1 $\pm$ 0.01

20230929-10ppm-SP-AG-421-5PASS_2_dt

TOF MSMS ES+
421
1.42e6



m/z 421_5-pass
for checking cannabinoids with MW 314
(compounds 1–6)

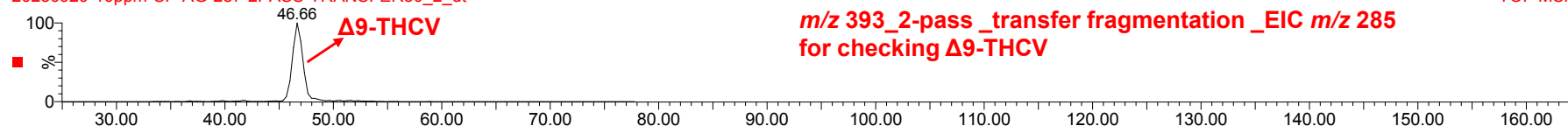
CBD
CCS:182.3 $\pm$ 0.02
 $\Delta 9$ -THC
CCS:184.4 $\pm$ 0.01

C#2_mobility separation+transfer fragmentation_for checking fragments

Raw output

20230929-10ppm-SP-AG-287-2PASS-TRANSFER30_2_dt

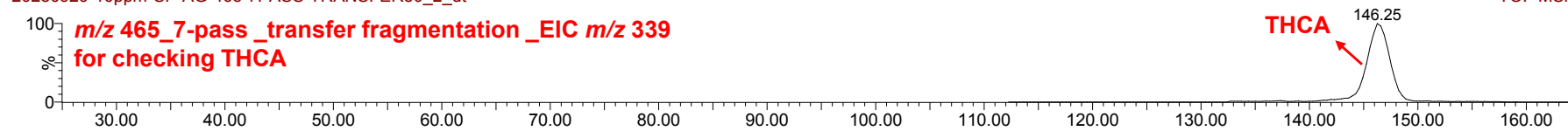
TOF MSMS ES+
285
1.35e4



m/z 393_2-pass_transfer fragmentation_EIC m/z 285
for checking $\Delta 9$ -THCV

20230929-10ppm-SP-AG-465-7PASS-TRANSFER30_2_dt

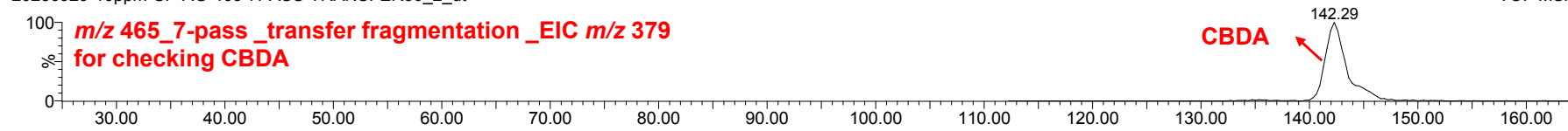
TOF MSMS ES+
339
4.06e5



m/z 465_7-pass_transfer fragmentation_EIC m/z 339
for checking THCA

20230929-10ppm-SP-AG-465-7PASS-TRANSFER30_2_dt

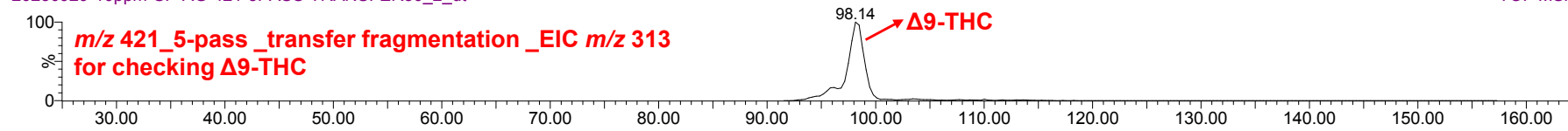
TOF MSMS ES+
379
5.88e4



m/z 465_7-pass_transfer fragmentation_EIC m/z 379
for checking CBDA

20230929-10ppm-SP-AG-421-5PASS-TRANSFER30_2_dt

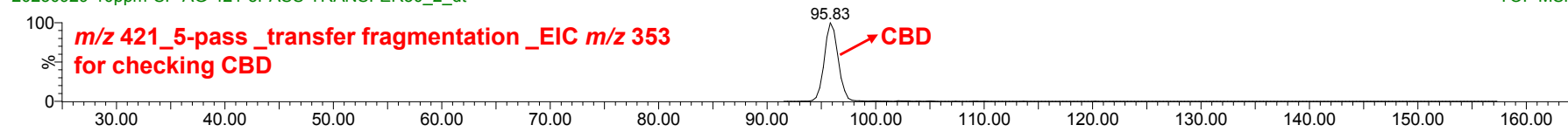
TOF MSMS ES+
313
1.90e5



m/z 421_5-pass_transfer fragmentation_EIC m/z 313
for checking $\Delta 9$ -THC

20230929-10ppm-SP-AG-421-5PASS-TRANSFER30_2_dt

TOF MSMS ES+
353
1.78e5



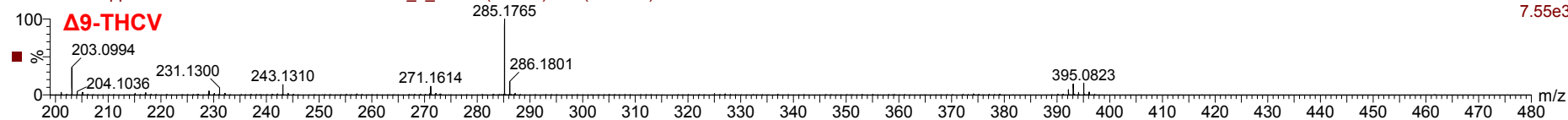
m/z 421_5-pass_transfer fragmentation_EIC m/z 353
for checking CBD

C#2_mobility separation+transfer fragmentation_for checking fragments

Raw output

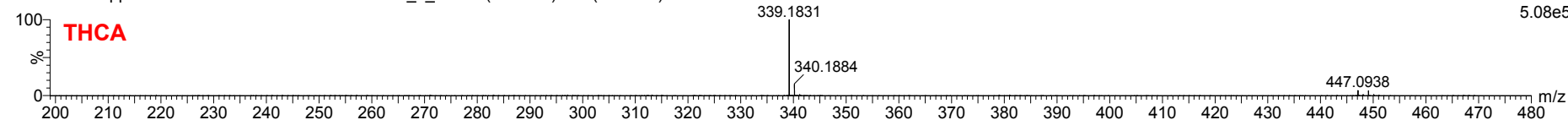
20230929-10ppm-SP-AG-287-2PASS-TRANSFER30_2_dt 105 (46.331) Cm (105:107)

TOF MSMS 0.00ES+
7.55e3



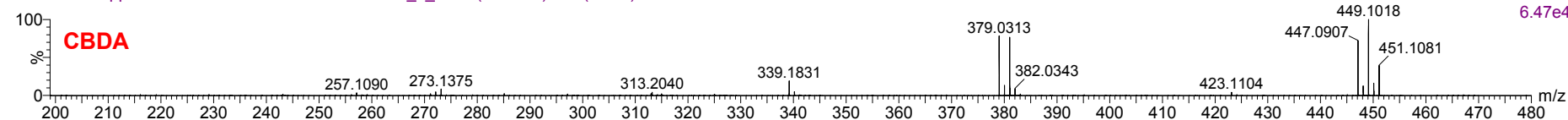
20230929-10ppm-SP-AG-465-7PASS-TRANSFER30_2_dt 104 (146.251) Cm (103:106)

TOF MSMS 0.00ES+
5.08e5



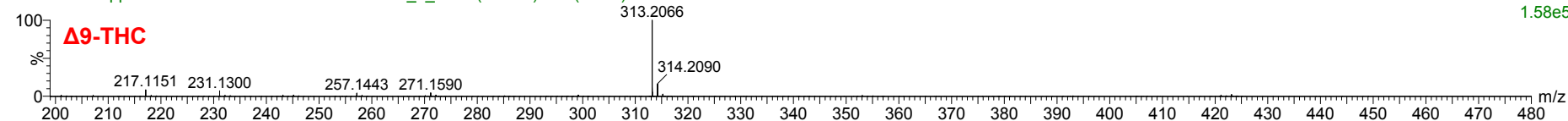
20230929-10ppm-SP-AG-465-7PASS-TRANSFER30_2_dt 91 (141.961) Cm (90:94)

TOF MSMS 0.00ES+
6.47e4



20230929-10ppm-SP-AG-421-5PASS-TRANSFER30_2_dt 21 (98.139) Cm (20:23)

TOF MSMS 0.00ES+
1.58e5



20230929-10ppm-SP-AG-421-5PASS-TRANSFER30_2_dt 14 (95.829) Cm (11:18)

TOF MSMS 0.00ES+
1.47e6

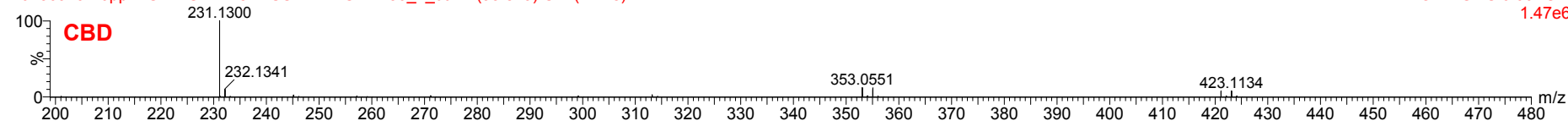
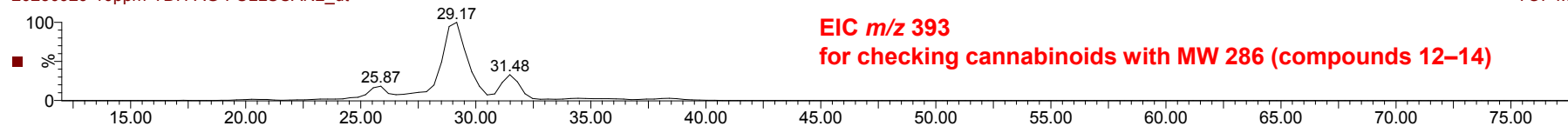


Figure S14-2. Mobiligram and mass spectra of cannabinoids in sample C#2.

C#3_full scan_for checking Ag(I) adducts

Raw output

20230929-10ppm-TDH-AG-FULLSCAN2_dt

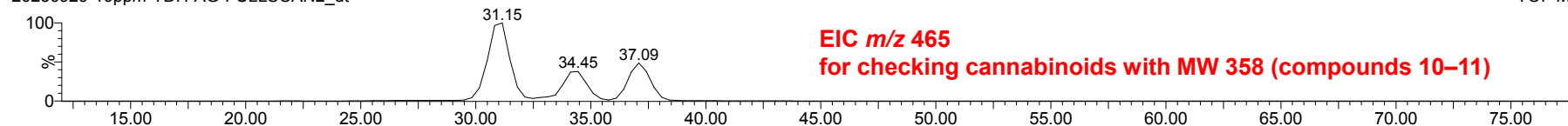


EIC m/z 393

for checking cannabinoids with MW 286 (compounds 12–14)

TOF MS ES+
393
4.23e4

20230929-10ppm-TDH-AG-FULLSCAN2_dt

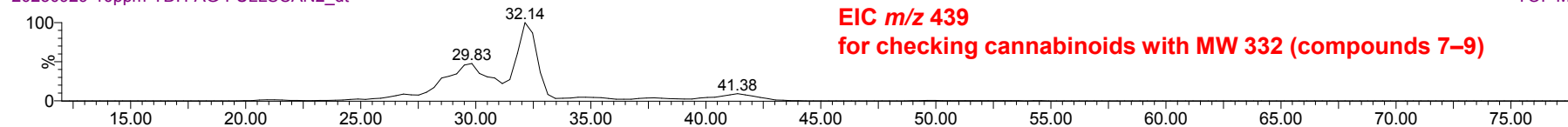


EIC m/z 465

for checking cannabinoids with MW 358 (compounds 10–11)

TOF MS ES+
465
2.29e5

20230929-10ppm-TDH-AG-FULLSCAN2_dt

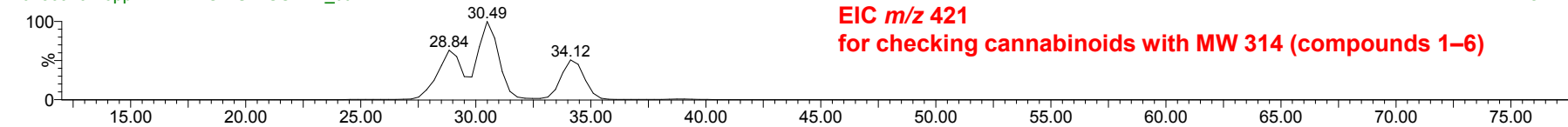


EIC m/z 439

for checking cannabinoids with MW 332 (compounds 7–9)

TOF MS ES+
439
5.21e4

20230929-10ppm-TDH-AG-FULLSCAN2_dt

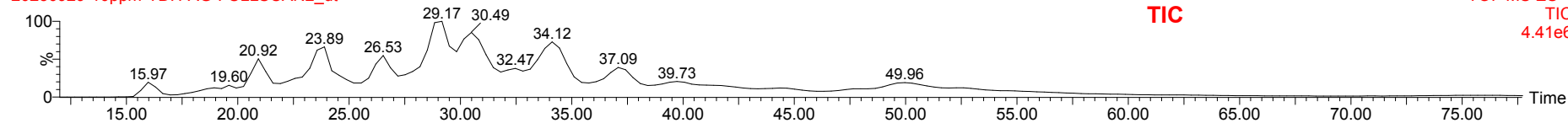


EIC m/z 421

for checking cannabinoids with MW 314 (compounds 1–6)

TOF MS ES+
421
7.47e5

20230929-10ppm-TDH-AG-FULLSCAN2_dt



TIC

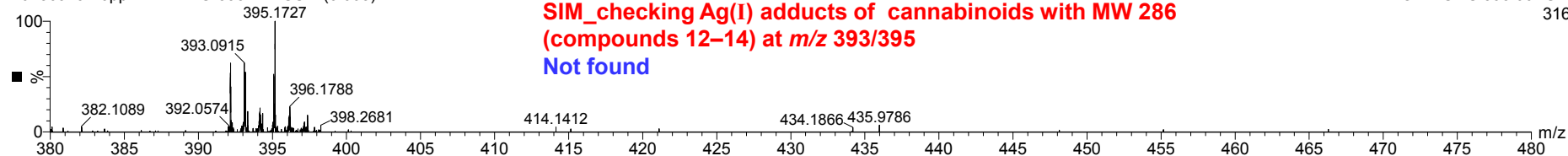
TOF MS ES+
TIC
4.41e6

C#3 _SIM_for checking Ag(I) adducts

Raw output

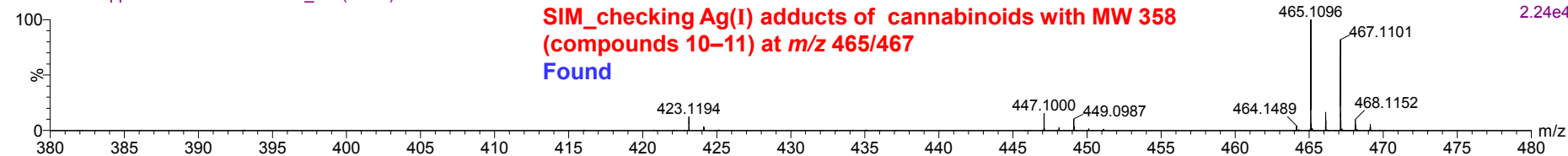
20230929-10ppm-TDH-AG-393-1PASS 1 (0.003)

TOF MSMS 393.00ES+
316



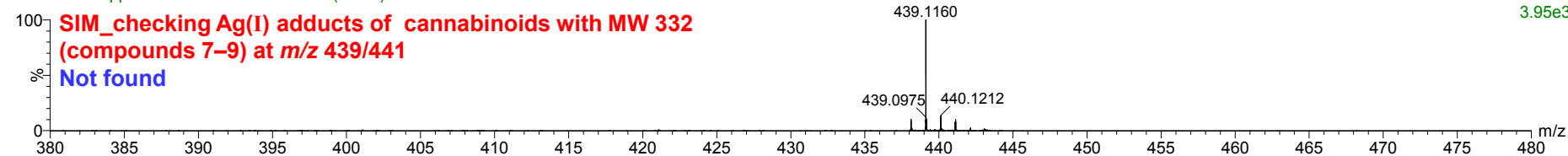
20230929-10ppm-TDH-AG-465-4PASS_2 1 (0.005)

TOF MSMS 465.00ES+
2.24e4



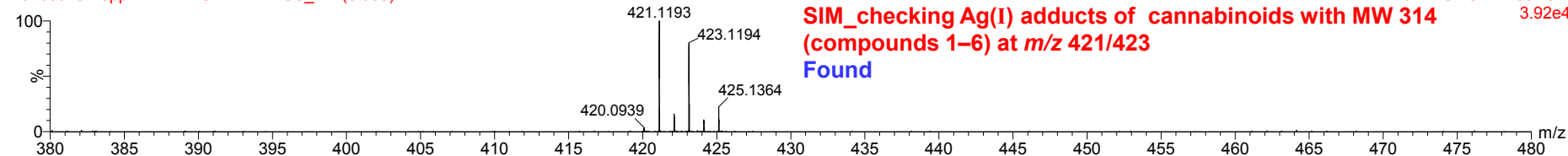
20230929-10ppm-TDH-AG-439-1PASS2 1 (0.012)

TOF MSMS 439.00ES+
3.95e3



20230929-10ppm-TDH-AG-421-7PASS_1 1 (0.008)

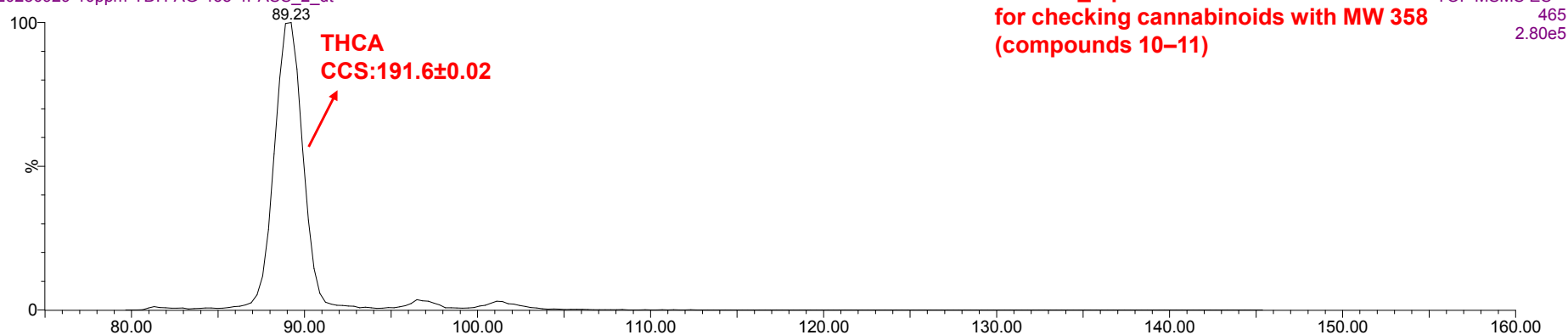
TOF MSMS 421.00ES+
3.92e4



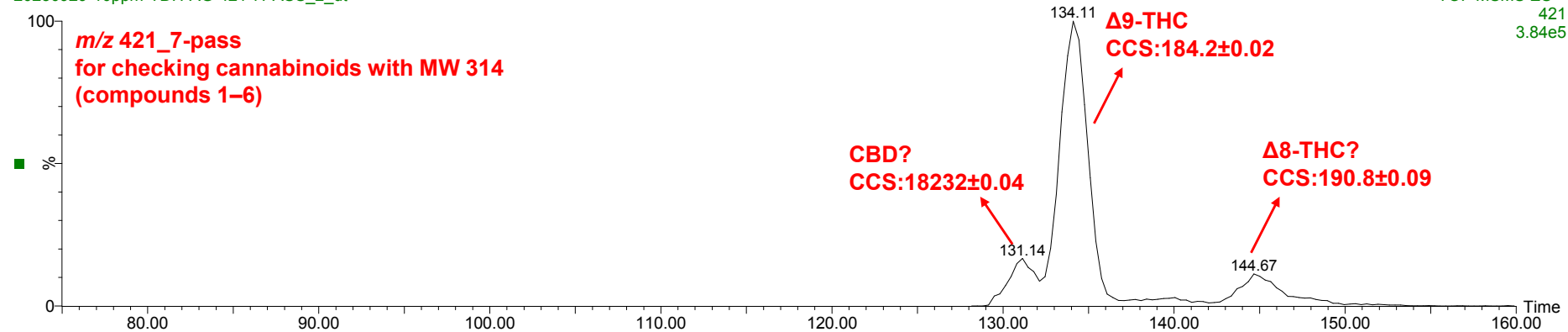
C#3_mobility separation_for checking CCS

Raw output

20230929-10ppm-TDH-AG-465-4PASS_2_dt



20230929-10ppm-TDH-AG-421-7PASS_2_dt

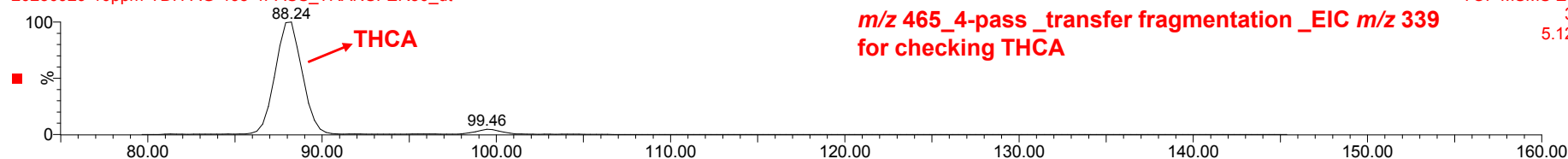


C#3_mobility separation+transfer fragmentation_for checking fragments

Raw output

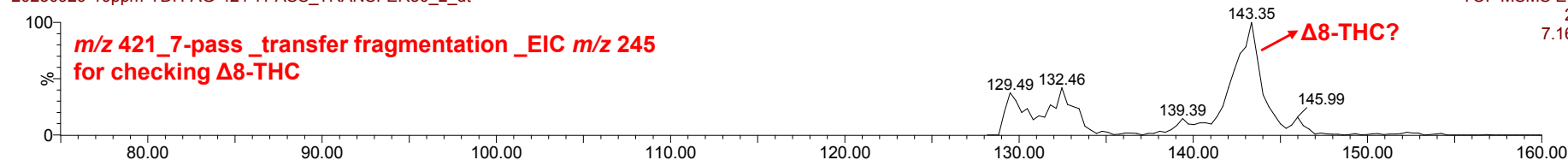
20230929-10ppm-TDH-AG-465-4PASS_TRANSFER30_dt

TOF MSMS ES+
339
5.12e5



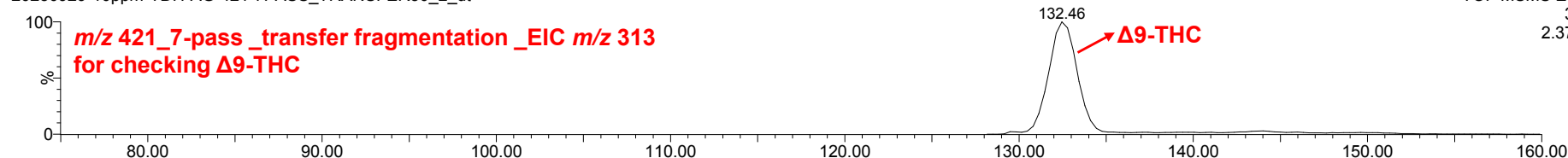
20230929-10ppm-TDH-AG-421-7PASS_TRANSFER30_2_dt

TOF MSMS ES+
245
7.16e3



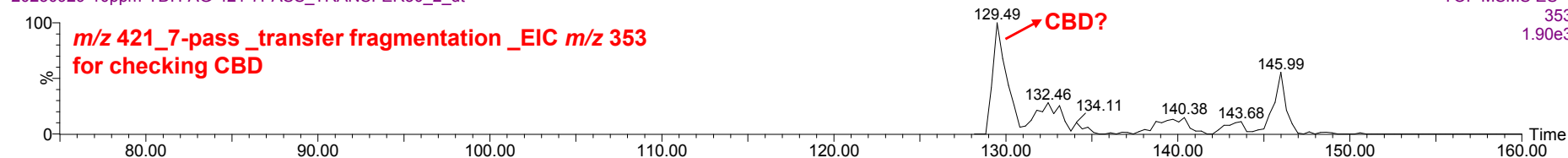
20230929-10ppm-TDH-AG-421-7PASS_TRANSFER30_2_dt

TOF MSMS ES+
313
2.37e5



20230929-10ppm-TDH-AG-421-7PASS_TRANSFER30_2_dt

TOF MSMS ES+
353
1.90e3

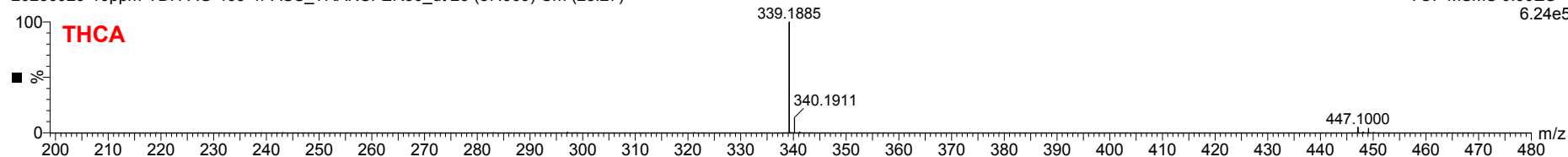


C#3_mobility separation+transfer fragmentation_for checking fragments

Raw output

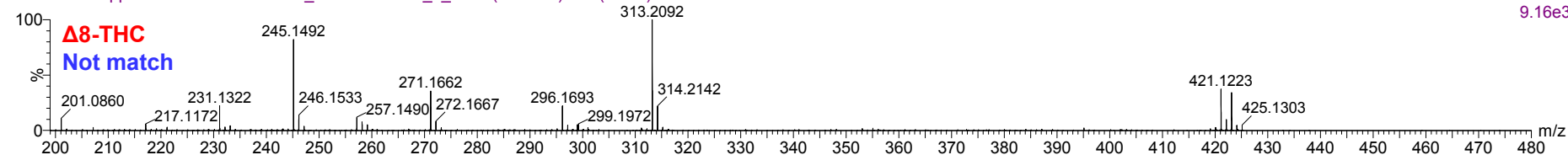
20230929-10ppm-TDH-AG-465-4PASS_TRANSFER30_dt 26 (87.909) Cm (25:27)

TOF MSMS 0.00ES+
6.24e5



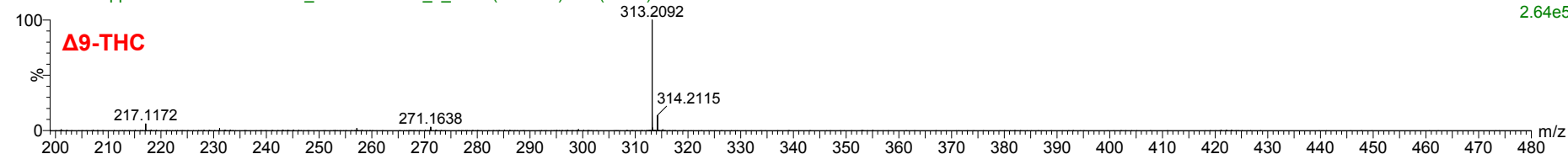
20230929-10ppm-TDH-AG-421-7PASS_TRANSFER30_2_dt 47 (143.347) Cm (42:50)

TOF MSMS 0.00ES+
9.16e3



20230929-10ppm-TDH-AG-421-7PASS_TRANSFER30_2_dt 14 (132.458) Cm (13:15)

TOF MSMS 0.00ES+
2.64e5



20230929-10ppm-TDH-AG-421-7PASS_TRANSFER30_2_dt 5 (129.488) Cm (4:8)

TOF MSMS 0.00ES+
1.07e4

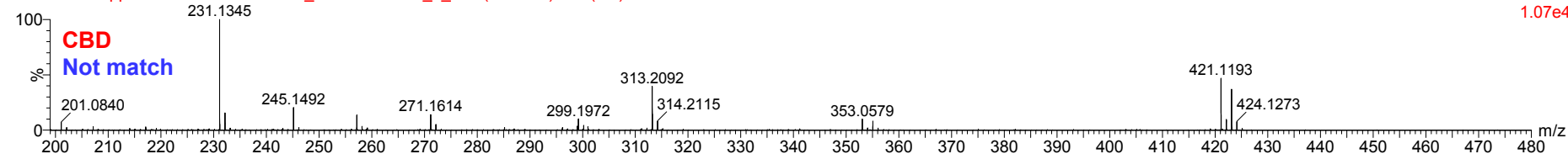


Figure S14-3. Mobiligram and mass spectra of cannabinoids in sample C#3.

G#1_full scan_for checking Ag(I) adducts

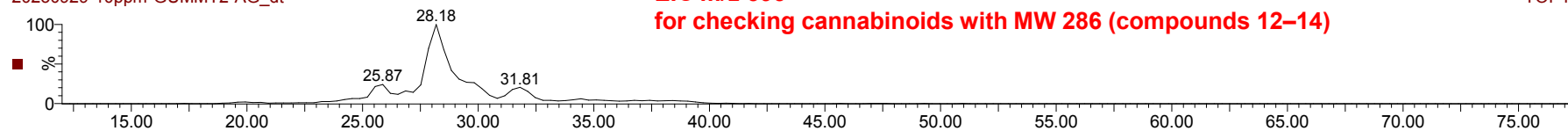
Raw output

20230929-10ppm-GUMMY2-AG_dt

EIC m/z 393

for checking cannabinoids with MW 286 (compounds 12–14)

TOF MS ES+
393
1.96e4

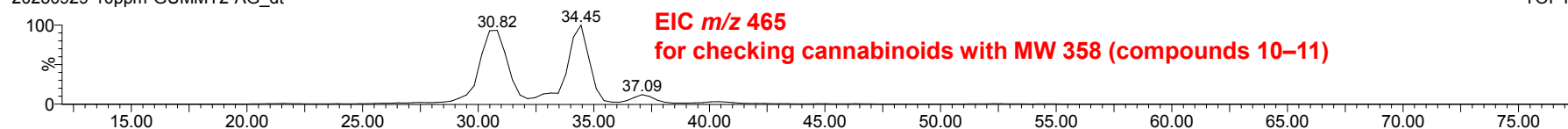


20230929-10ppm-GUMMY2-AG_dt

EIC m/z 465

for checking cannabinoids with MW 358 (compounds 10–11)

TOF MS ES+
465
4.38e4

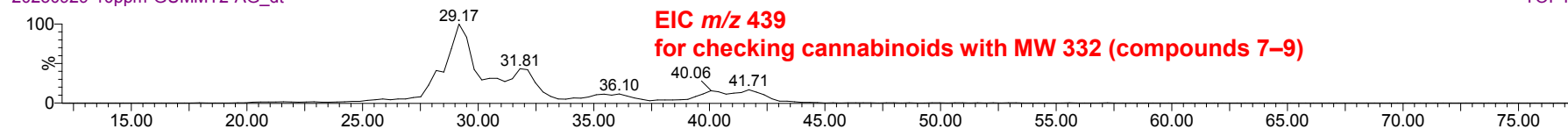


20230929-10ppm-GUMMY2-AG_dt

EIC m/z 439

for checking cannabinoids with MW 332 (compounds 7–9)

TOF MS ES+
439
2.02e4

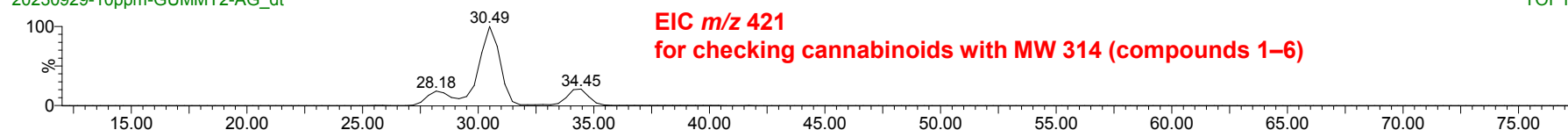


20230929-10ppm-GUMMY2-AG_dt

EIC m/z 421

for checking cannabinoids with MW 314 (compounds 1–6)

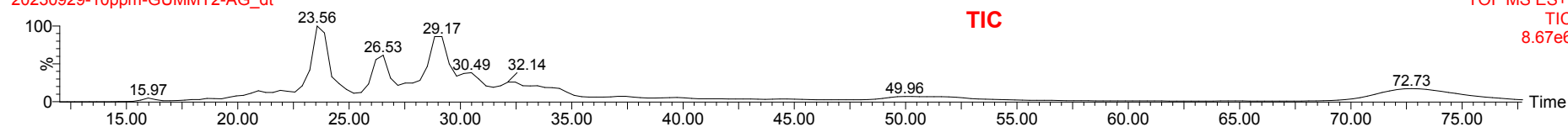
TOF MS ES+
421
8.21e5



20230929-10ppm-GUMMY2-AG_dt

TIC

TOF MS ES+
TIC
8.67e6

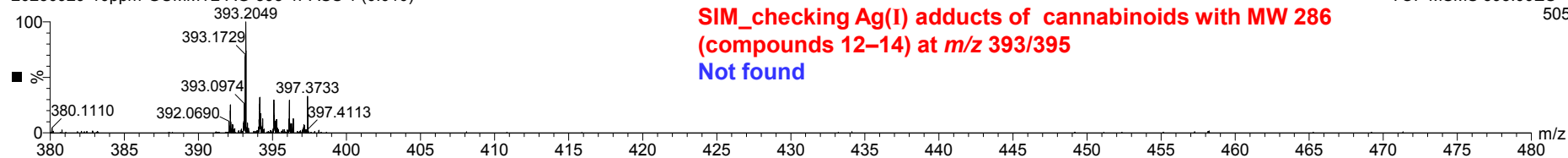


G#1_SIM_for checking Ag(I) adducts

Raw output

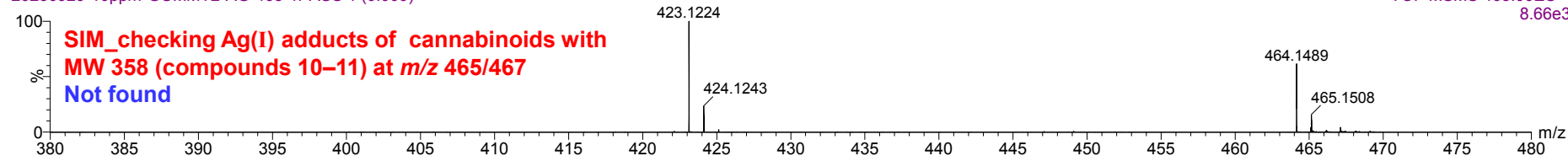
20230929-10ppm-GUMMY2-AG-393-1PASS 1 (0.010)

TOF MSMS 393.00ES+
505



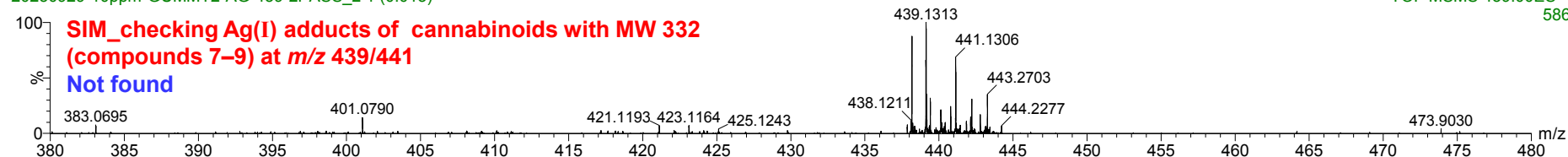
20230929-10ppm-GUMMY2-AG-465-1PASS 1 (0.009)

TOF MSMS 465.00ES+
8.66e3



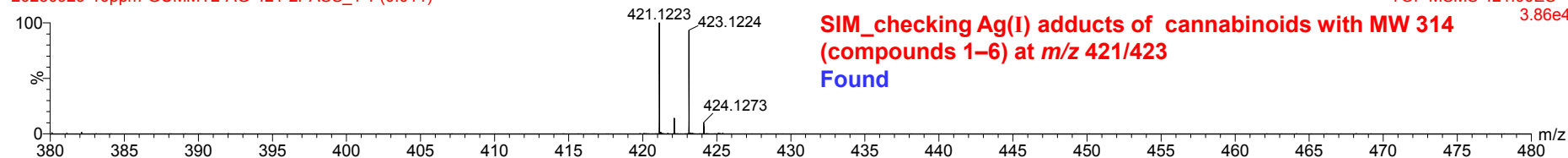
20230929-10ppm-GUMMY2-AG-439-2PASS_2 1 (0.013)

TOF MSMS 439.00ES+
586



20230929-10ppm-GUMMY2-AG-421-2PASS_1 1 (0.011)

TOF MSMS 421.00ES+
3.86e4

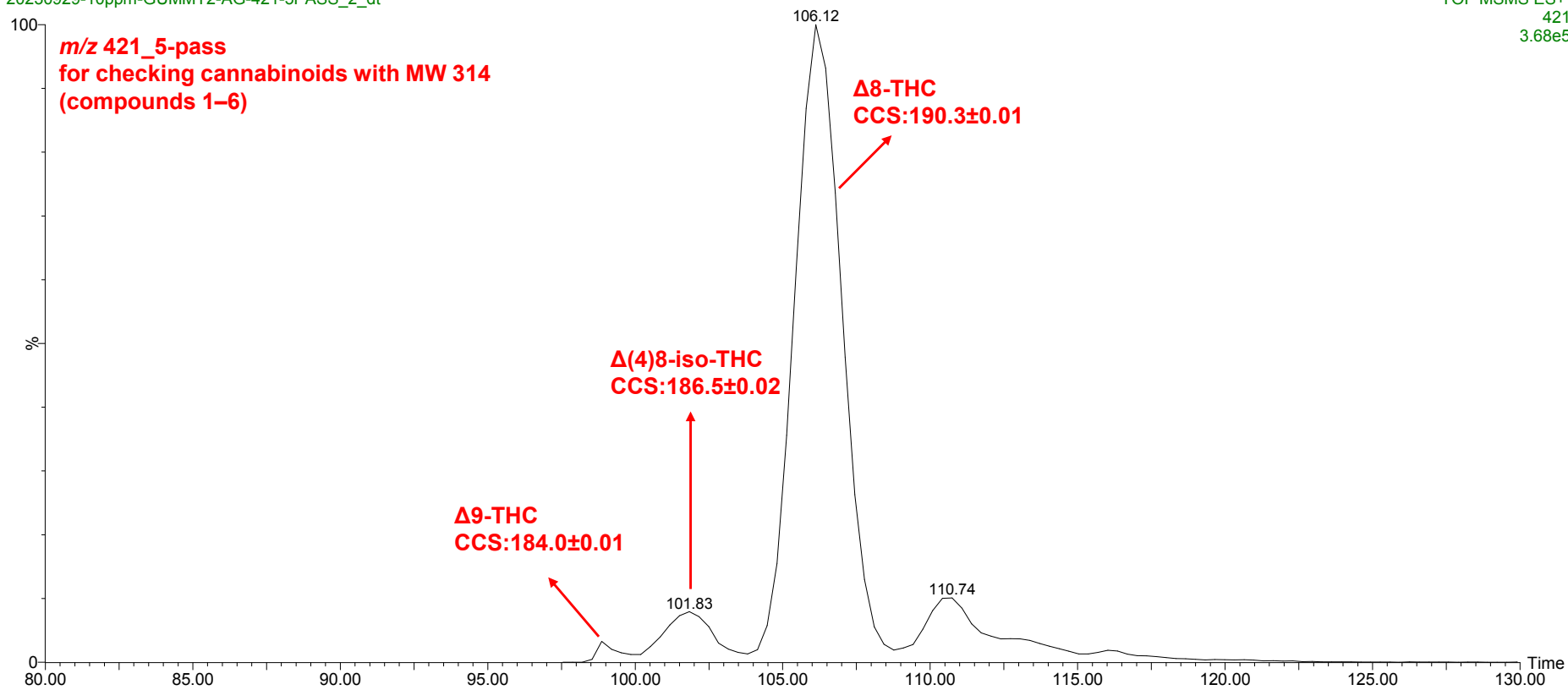


G#1 _mobility separation_for checking CCS

Raw output

20230929-10ppm-GUMMY2-AG-421-5PASS_2_dt

TOF MSMS ES+
421
3.68e5

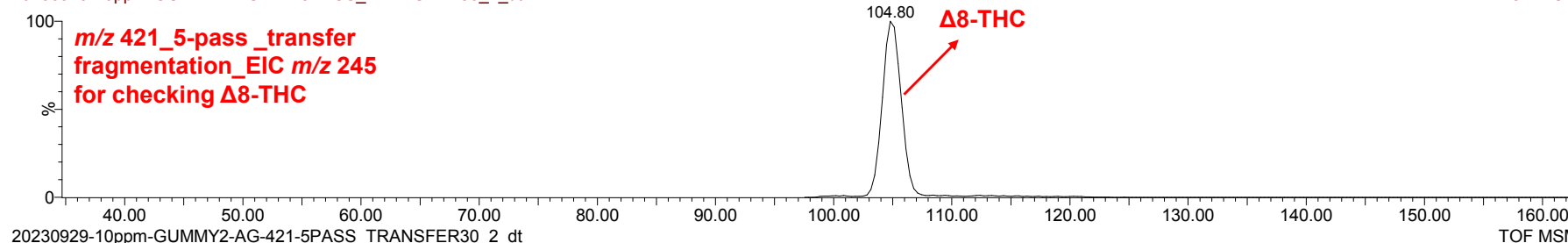


G#1_mobility separation+transfer fragmentation_for checking fragments

Raw output

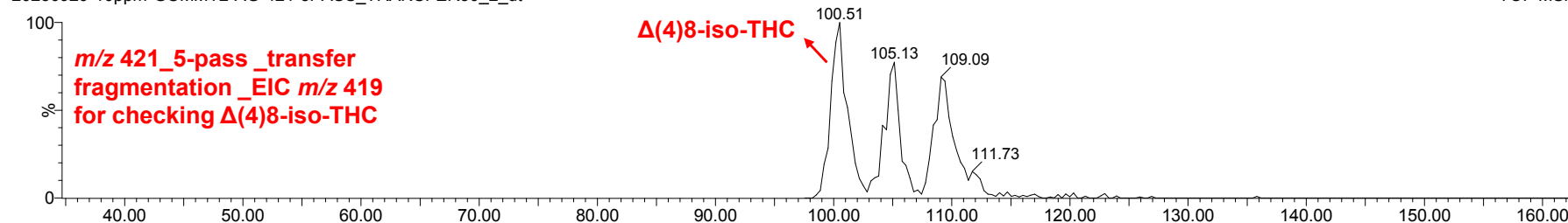
20230929-10ppm-GUMMY2-AG-421-5PASS_TRANSFER30_2_dt

TOF MSMS ES+
245
1.20e5



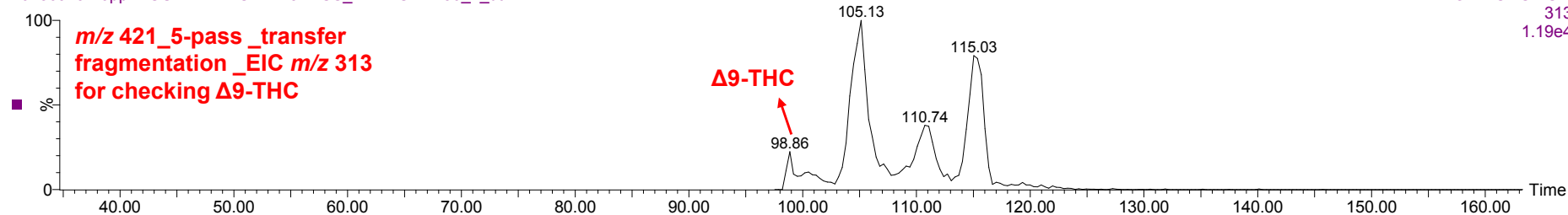
20230929-10ppm-GUMMY2-AG-421-5PASS_TRANSFER30_2_dt

TOF MSMS ES+
419
1.43e3



20230929-10ppm-GUMMY2-AG-421-5PASS_TRANSFER30_2_dt

TOF MSMS ES+
313
1.19e4

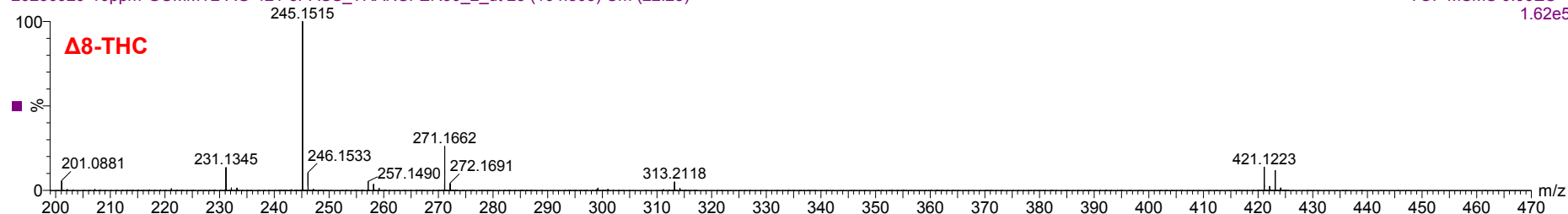


G#1_mobility separation+transfer fragmentation_for checking fragments

Raw output

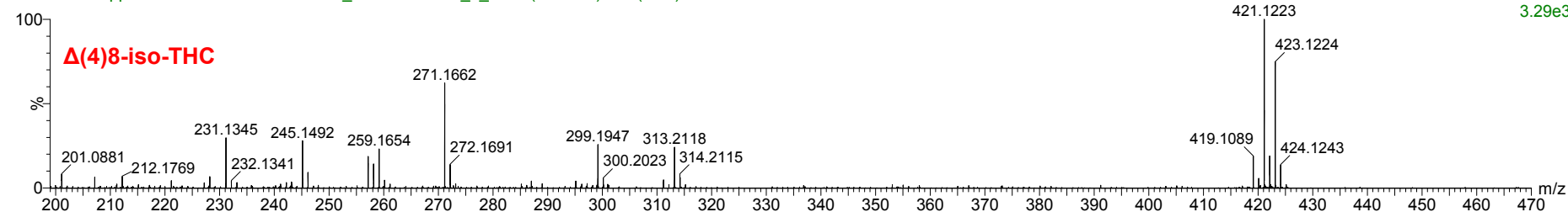
20230929-10ppm-GUMMY2-AG-421-5PASS_TRANSFER30_2_dt 23 (104.805) Cm (22:25)

TOF MSMS 0.00ES+
1.62e5



20230929-10ppm-GUMMY2-AG-421-5PASS_TRANSFER30_2_dt 10 (100.515) Cm (8:11)

TOF MSMS 0.00ES+
3.29e5



20230929-10ppm-GUMMY2-AG-421-5PASS_TRANSFER30_2_dt 5 (98.865) Cm (4:6)

TOF MSMS 0.00ES+
929

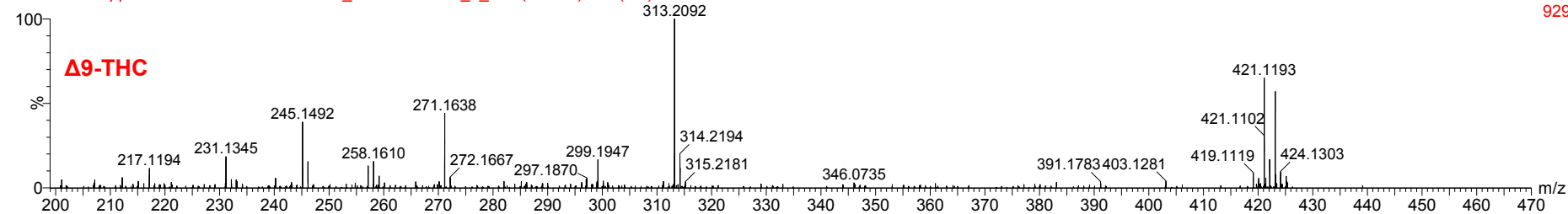
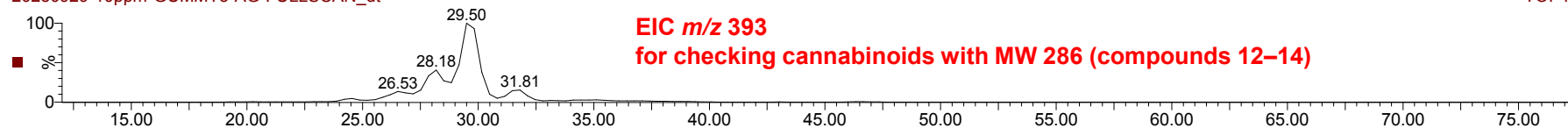


Figure S14-4. Mobiligram and mass spectra of cannabinoids in sample G#1.

G#2_full scan_for checking Ag(I) adducts

Raw output

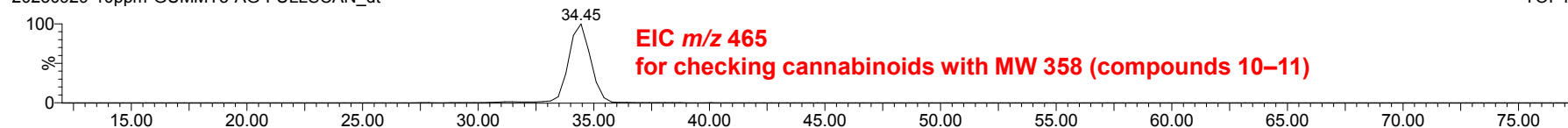
20230929-10ppm-GUMMY3-AG-FULLSCAN_dt



EIC m/z 393
for checking cannabinoids with MW 286 (compounds 12–14)

TOF MS ES+
393
2.37e4

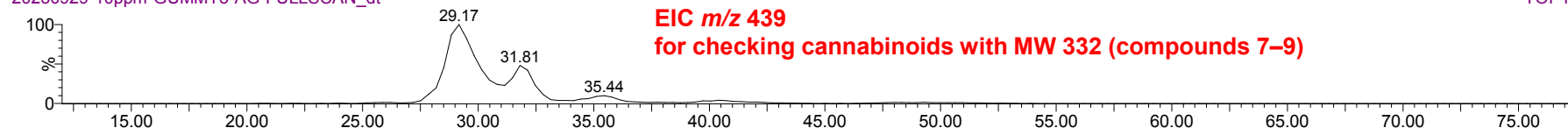
20230929-10ppm-GUMMY3-AG-FULLSCAN_dt



EIC m/z 465
for checking cannabinoids with MW 358 (compounds 10–11)

TOF MS ES+
465
2.23e5

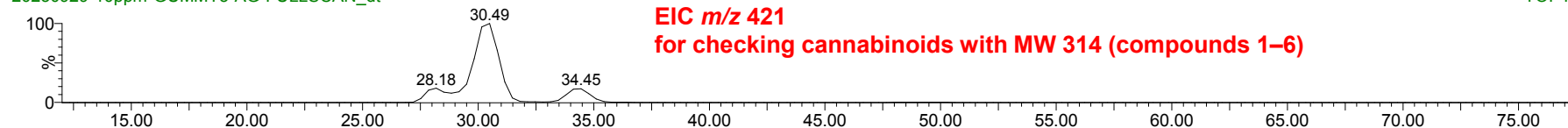
20230929-10ppm-GUMMY3-AG-FULLSCAN_dt



EIC m/z 439
for checking cannabinoids with MW 332 (compounds 7–9)

TOF MS ES+
439
2.65e4

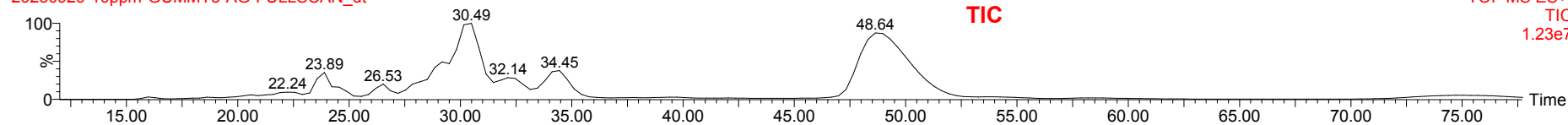
20230929-10ppm-GUMMY3-AG-FULLSCAN_dt



EIC m/z 421
for checking cannabinoids with MW 314 (compounds 1–6)

TOF MS ES+
421
4.50e6

20230929-10ppm-GUMMY3-AG-FULLSCAN_dt



TIC

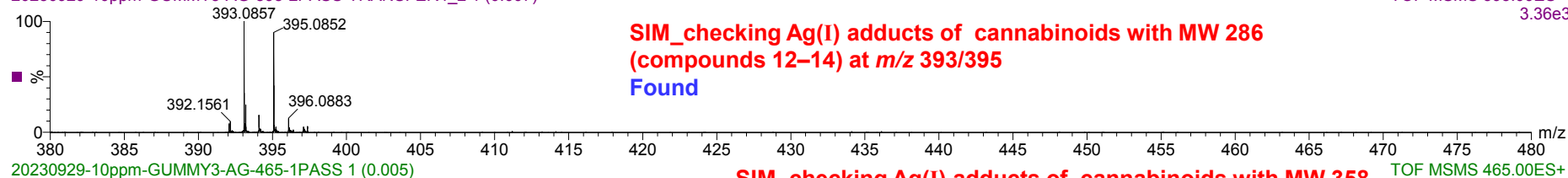
TOF MS ES+
TIC
1.23e7

G#2_SIM for checking Ag(I) adducts

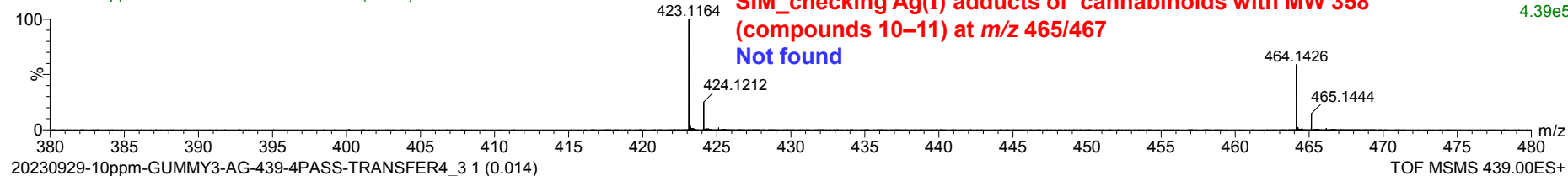
Raw output

20230929-10ppm-GUMMY3-AG-393-2PASS-TRANSFER4_2 1 (0.007)

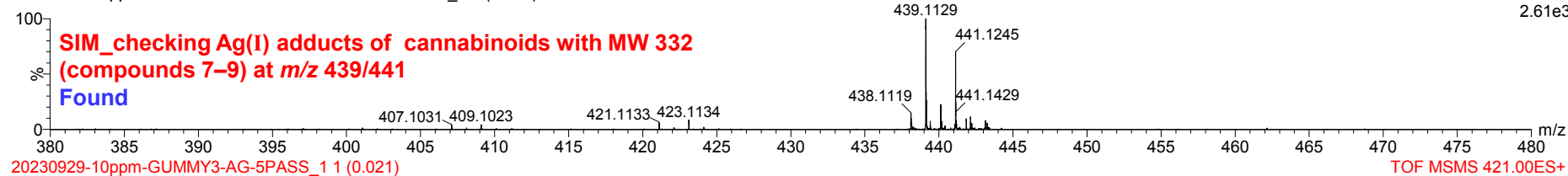
TOF MSMS 393.00ES+
3.36e3



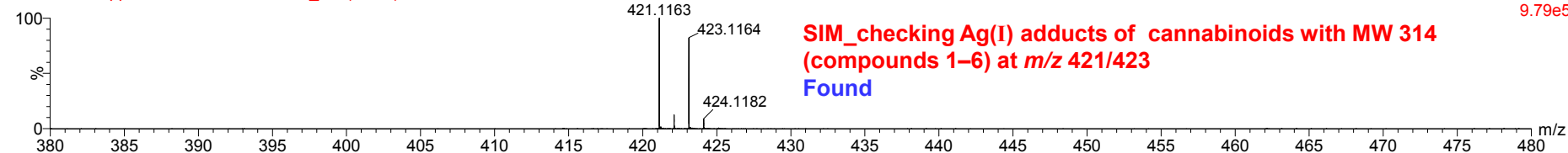
TOF MSMS 465.00ES+
4.39e5



TOF MSMS 439.00ES+
2.61e3



TOF MSMS 421.00ES+
9.79e5



G#2_mobility separation_for checking CCS

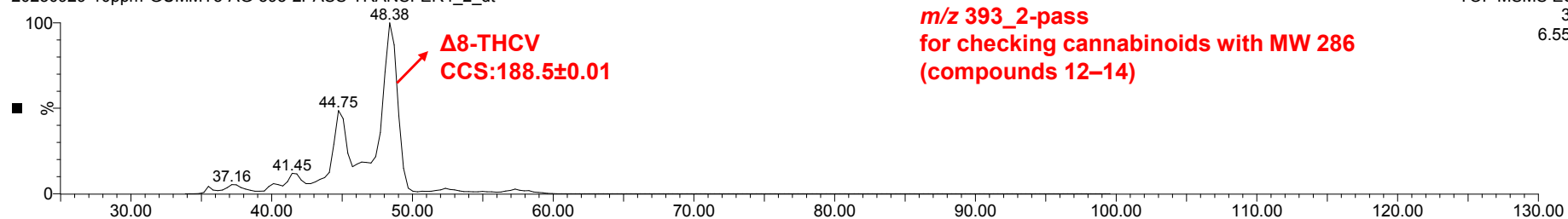
Raw output

20230929-10ppm-GUMMY3-AG-393-2PASS-TRANSFER4_2_dt

TOF MSMS ES+

393

6.55e4

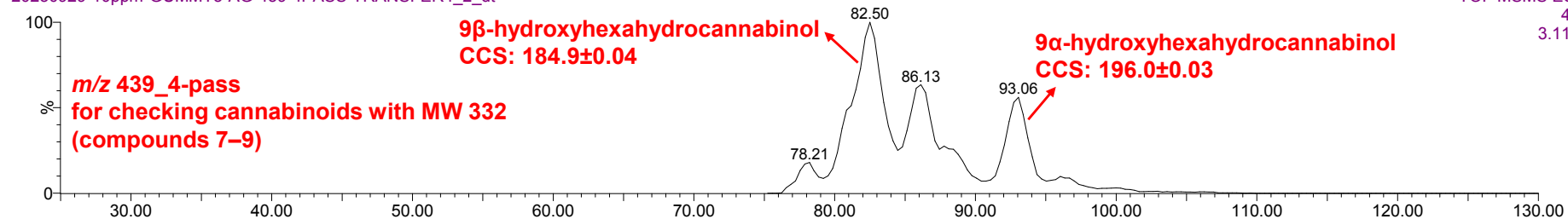


20230929-10ppm-GUMMY3-AG-439-4PASS-TRANSFER4_2_dt

TOF MSMS ES+

439

3.11e4

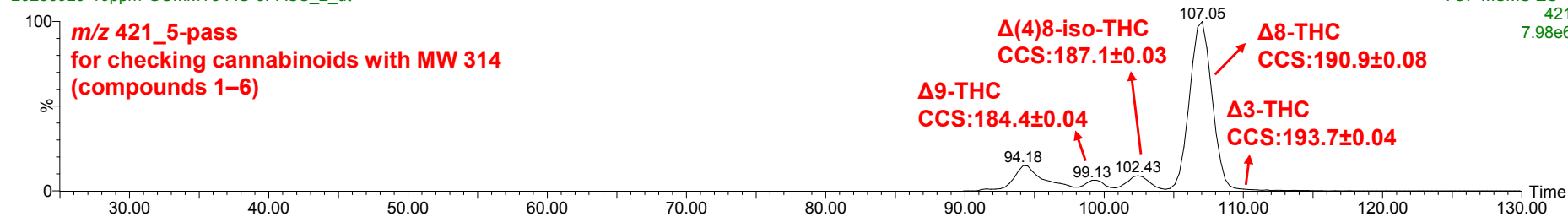


20230929-10ppm-GUMMY3-AG-5PASS_2_dt

TOF MSMS ES+

421

7.98e6

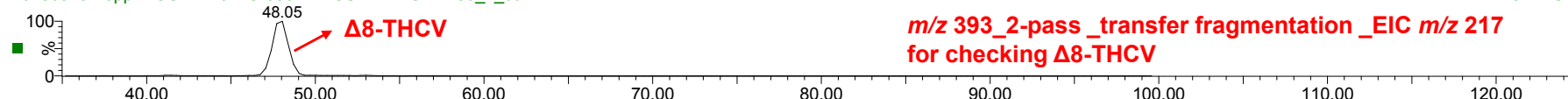


G#2_mobility separation+transfer fragmentation_for checking fragments

Raw output

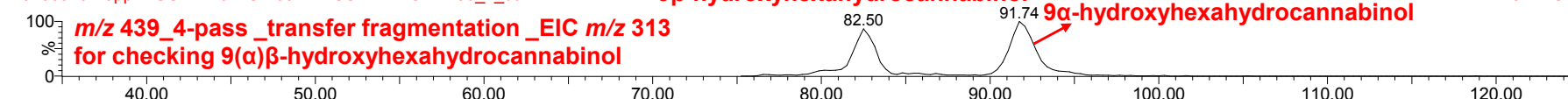
20230929-10ppm-GUMMY3-AG-393-2PASS-TRANSFER30_2_dt

TOF MSMS ES+
217
1.93e4



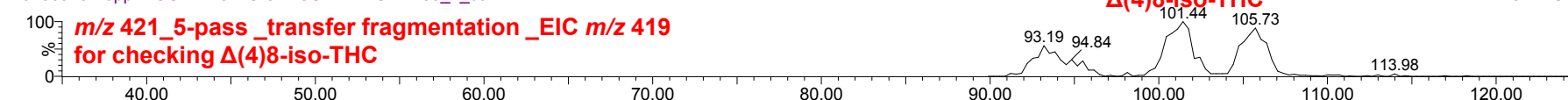
20230929-10ppm-GUMMY3-AG-439-4PASS-TRANSFER30_2_dt

TOF MSMS ES+
313
5.80e3



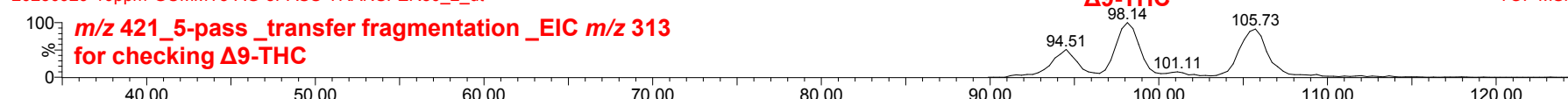
20230929-10ppm-GUMMY3-AG-5PASS-TRANSFER30_2_dt

TOF MSMS ES+
419
4.10e4



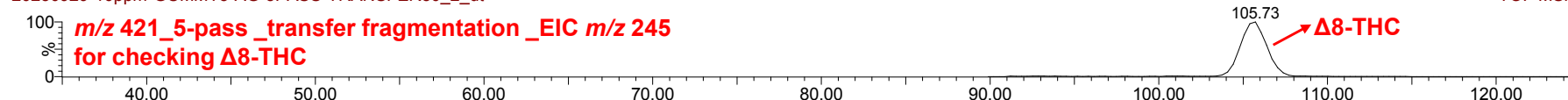
20230929-10ppm-GUMMY3-AG-5PASS-TRANSFER30_2_dt

TOF MSMS ES+
313
4.30e5



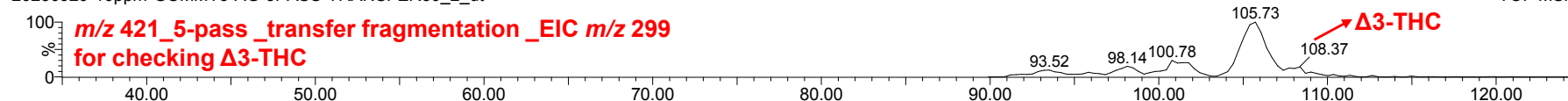
20230929-10ppm-GUMMY3-AG-5PASS-TRANSFER30_2_dt

TOF MSMS ES+
245
4.00e6



20230929-10ppm-GUMMY3-AG-5PASS-TRANSFER30_2_dt

TOF MSMS ES+
299
1.61e5



G#2_mobility separation+transfer fragmentation_for checking fragments

Raw output

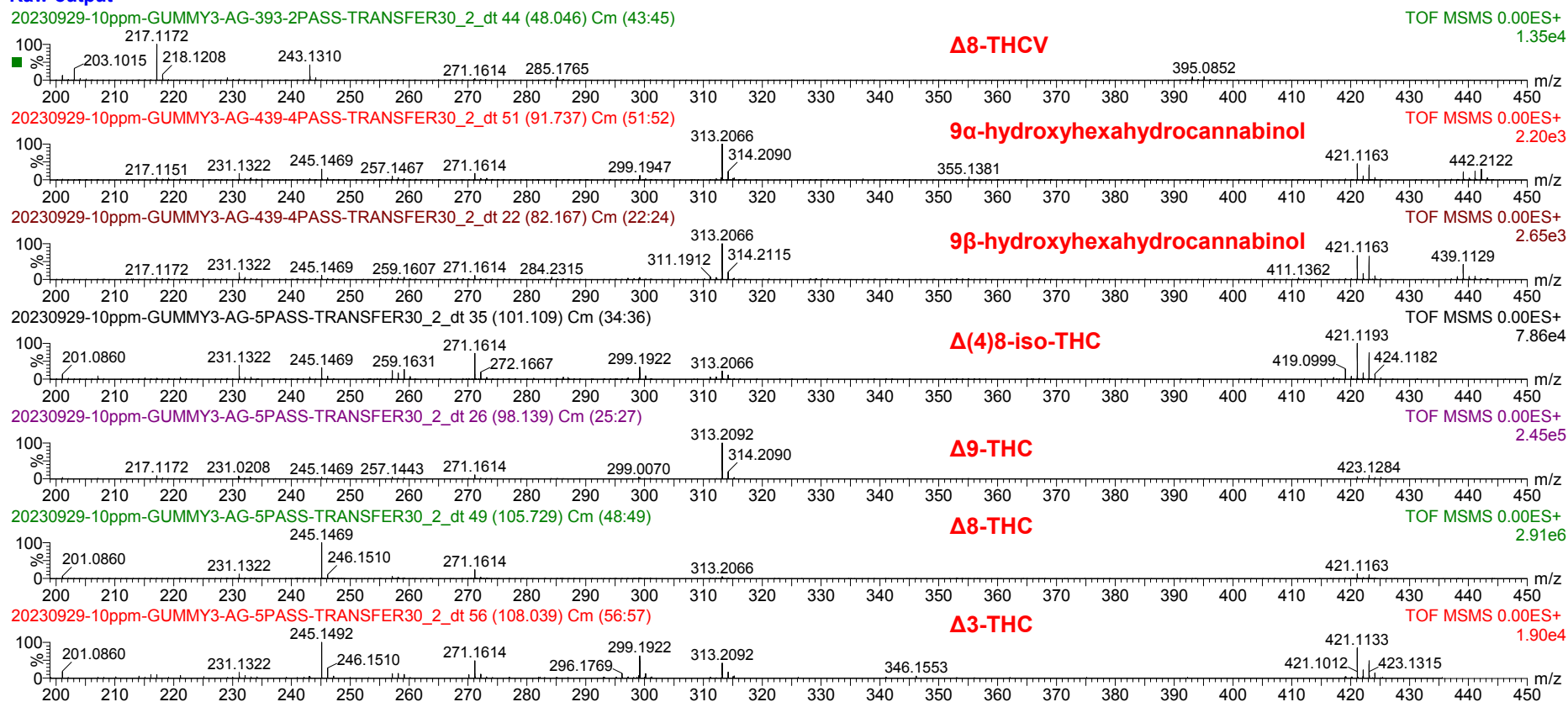


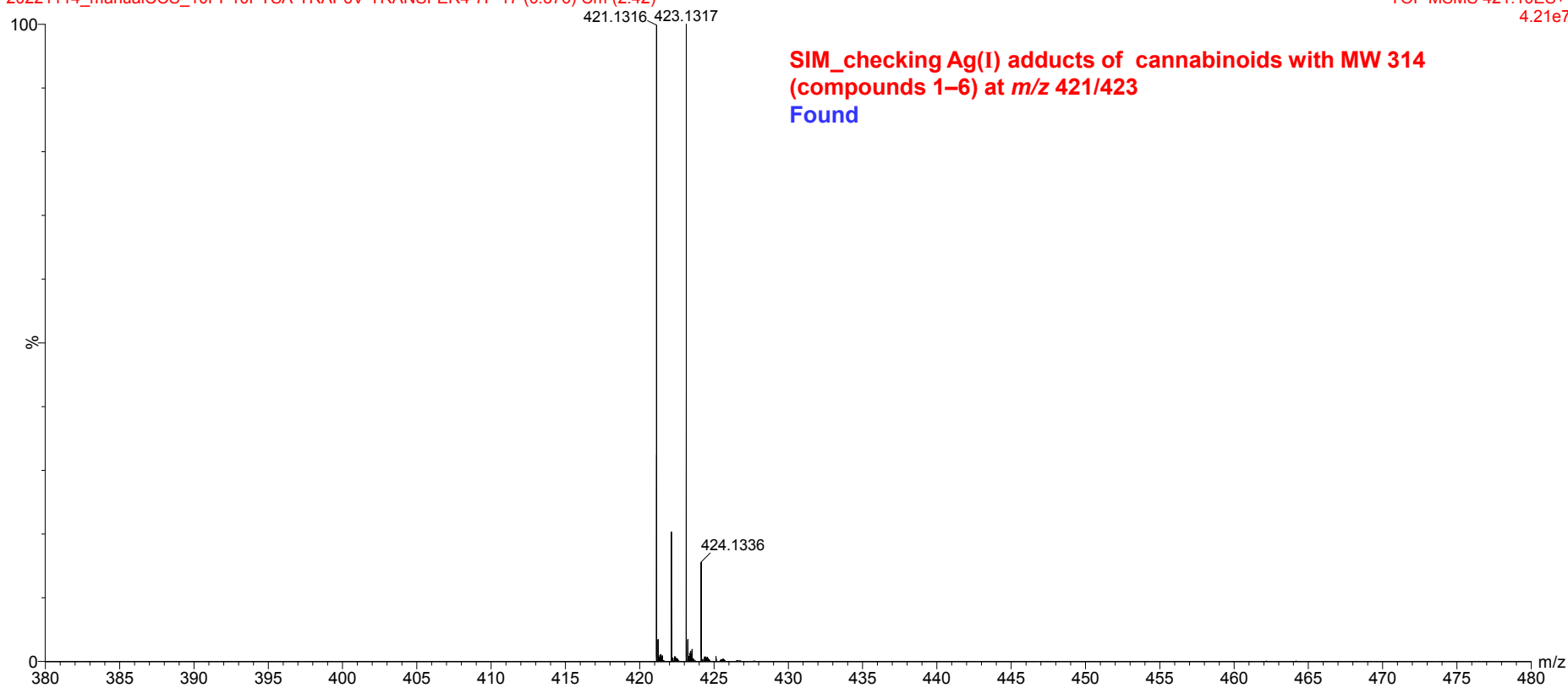
Figure S14-5. Mobiligram and mass spectra of cannabinoids in sample G#2.

R#1 _SIM_for checking Ag(I) adducts

Raw output

20221114_manualCCS_10PP10PTSA-TRAP6V-TRANSFER4-7P 17 (0.376) Cm (2:42)

TOF MSMS 421.10ES+
4.21e7



SIM_checking Ag(I) adducts of cannabinoids with MW 314
(compounds 1–6) at m/z 421/423

Found

R#1 _mobility separation_for checking CCS

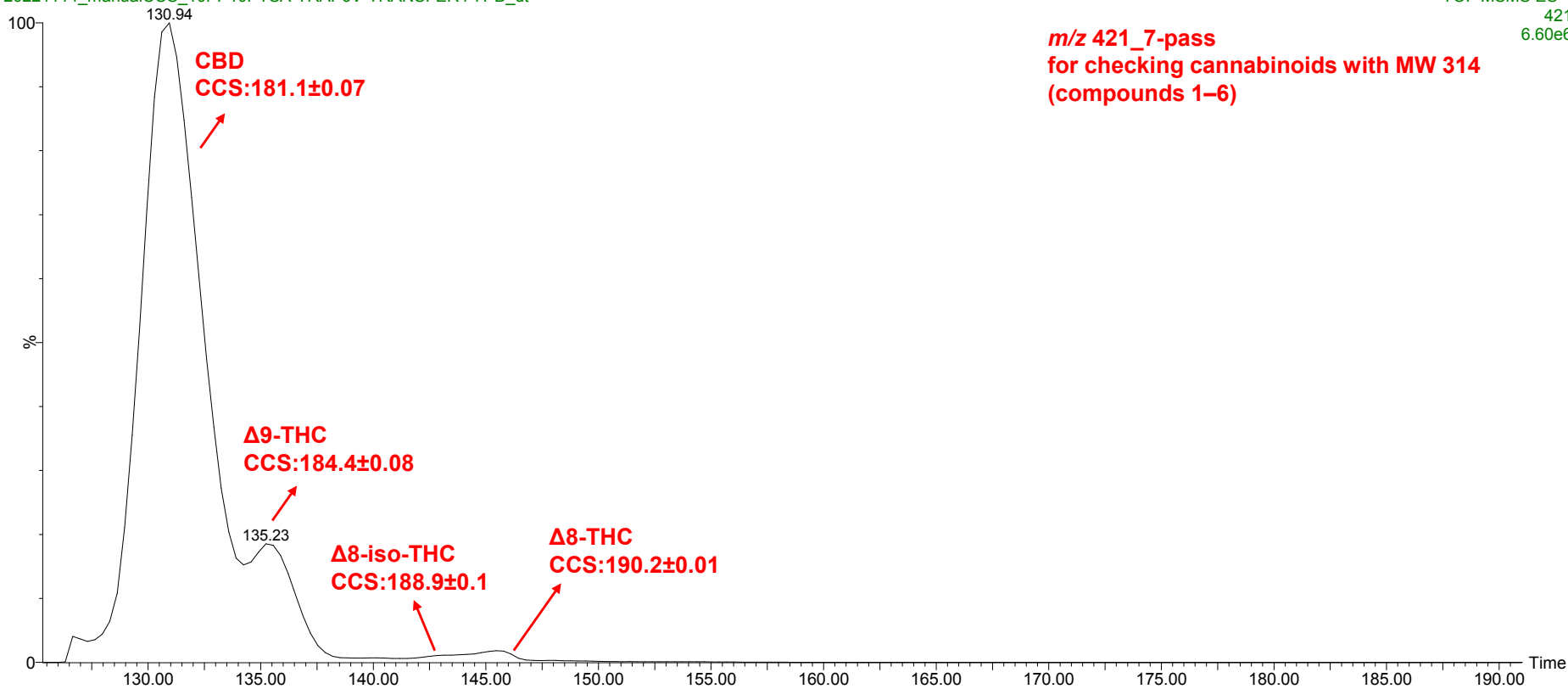
Raw output

20221114_manualCCS_10PP10PTSA-TRAP6V-TRANSFER4-7PB_dt

TOF MSMS ES+

421

6.60e6



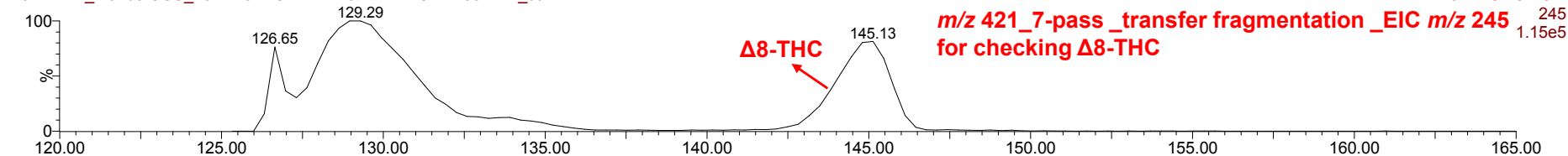
m/z 421_7-pass
for checking cannabinoids with MW 314
(compounds 1–6)

R#1_mobility separation+transfer fragmentation_for checking fragments

Raw output

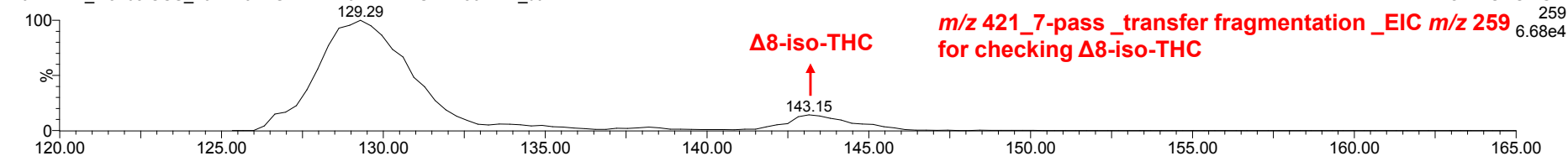
20221114_manualCCS_10PP10PTSA-TRAP6V-TRANSFER30-7PB_dt

TOF MSMS ES+



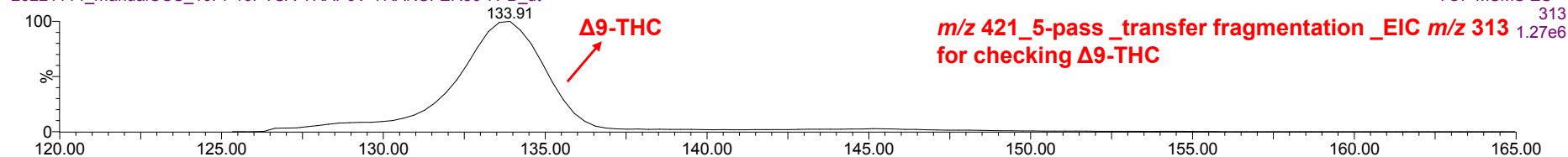
20221114_manualCCS_10PP10PTSA-TRAP6V-TRANSFER30-7PB_dt

TOF MSMS ES+



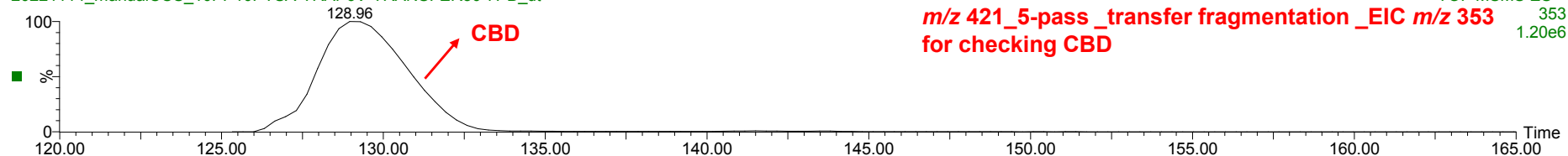
20221114_manualCCS_10PP10PTSA-TRAP6V-TRANSFER30-7PB_dt

TOF MSMS ES+



20221114_manualCCS_10PP10PTSA-TRAP6V-TRANSFER30-7PB_dt

TOF MSMS ES+

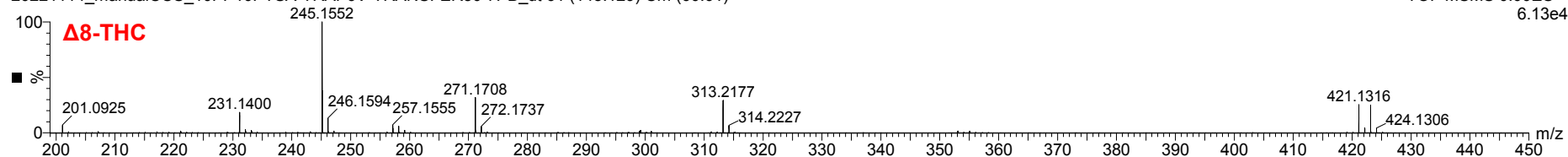


R#1_mobility separation+transfer fragmentation_for checking fragments

Raw output

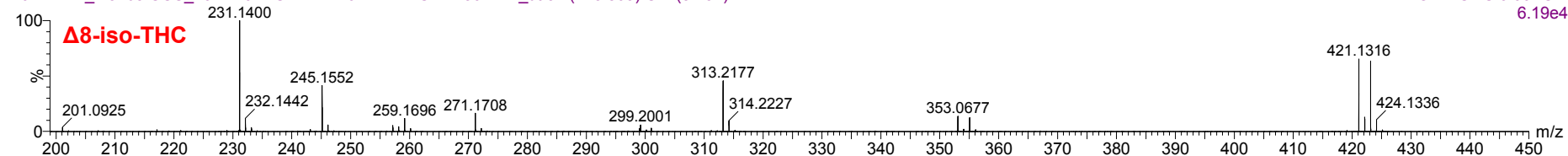
20221114_manualCCS_10PP10PTSA-TRAP6V-TRANSFER30-7PB_dt 61 (145.129) Cm (60:61)

TOF MSMS 0.00ES+
6.13e4



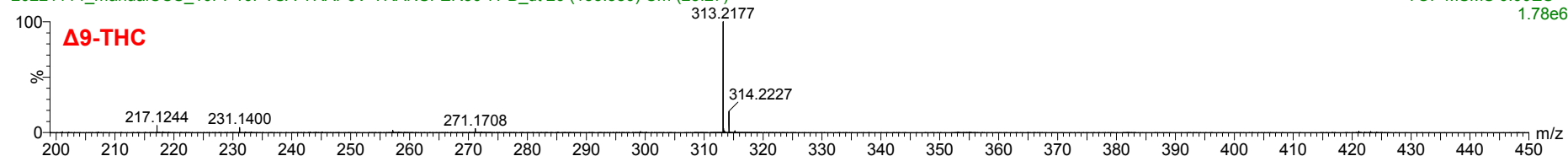
20221114_manualCCS_10PP10PTSA-TRAP6V-TRANSFER30-7PB_dt 57 (143.809) Cm (54:57)

TOF MSMS 0.00ES+
6.19e4



20221114_manualCCS_10PP10PTSA-TRAP6V-TRANSFER30-7PB_dt 26 (133.580) Cm (25:27)

TOF MSMS 0.00ES+
1.78e6



20221114_manualCCS_10PP10PTSA-TRAP6V-TRANSFER30-7PB_dt 12 (128.960) Cm (11:15)

TOF MSMS 0.00ES+
1.11e7

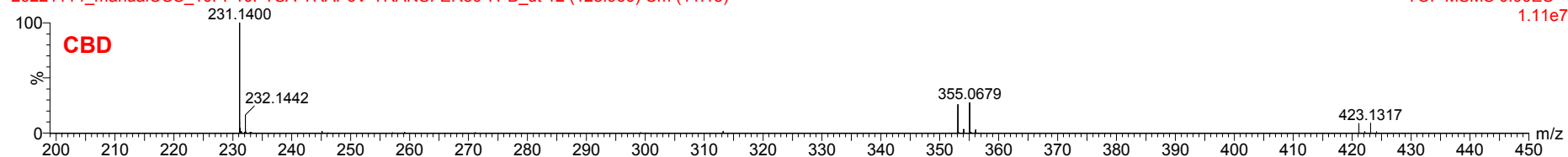


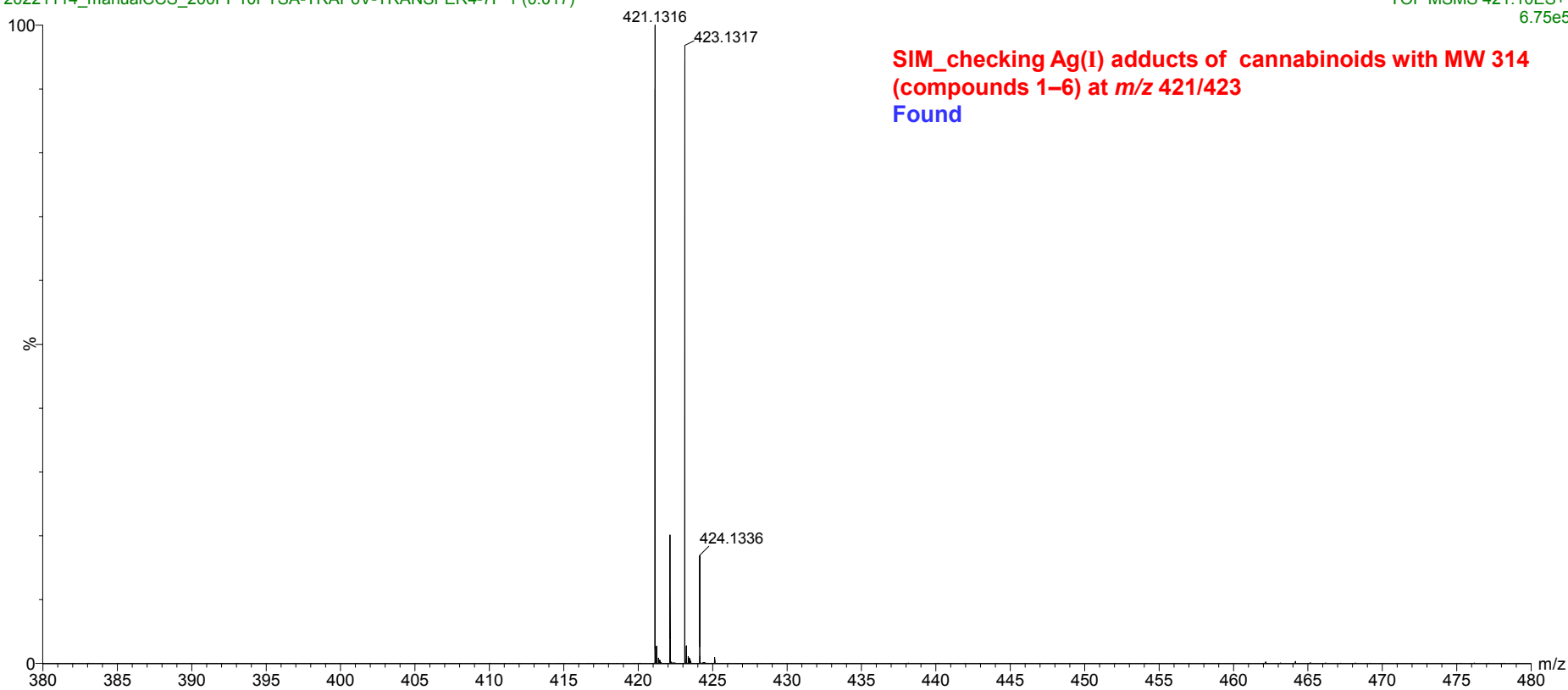
Figure S14-6. Mobiligram and mass spectra of cannabinoids in sample R#1.

R#2 _SIM_ for checking Ag(I) isotope pattern

ADC129.25-5PPB-SEP119.25

20221114_manualICCS_200PP10PTSA-TRAP6V-TRANSFER4-7P 1 (0.017)

TOF MSMS 421.10ES+
6.75e5



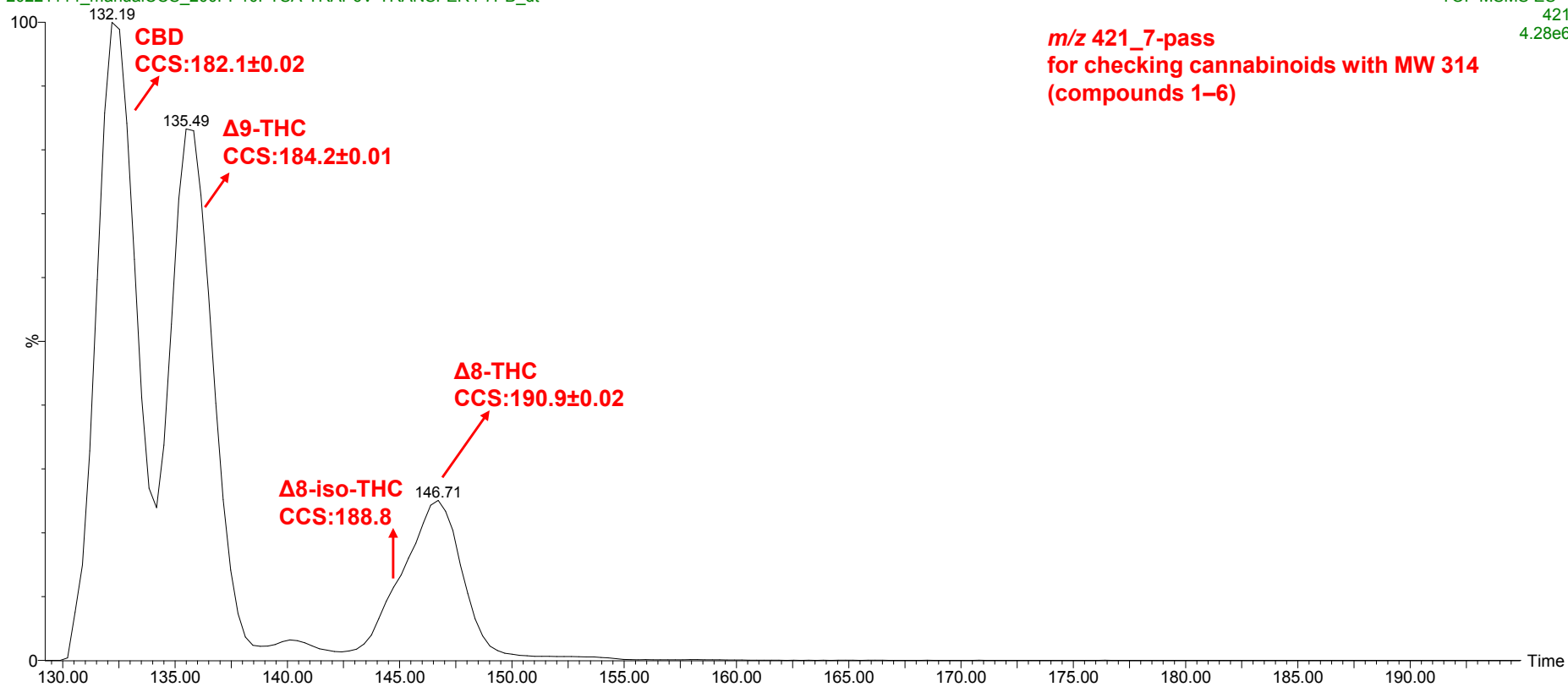
SIM_checking Ag(I) adducts of cannabinoids with MW 314
(compounds 1–6) at m/z 421/423
Found

R#2 _mobility separation_for checking CCS

Raw output

20221114_manualCCS_200PP10PTSA-TRAP6V-TRANSFER4-7PB_dt

TOF MSMS ES+
421
4.28e6

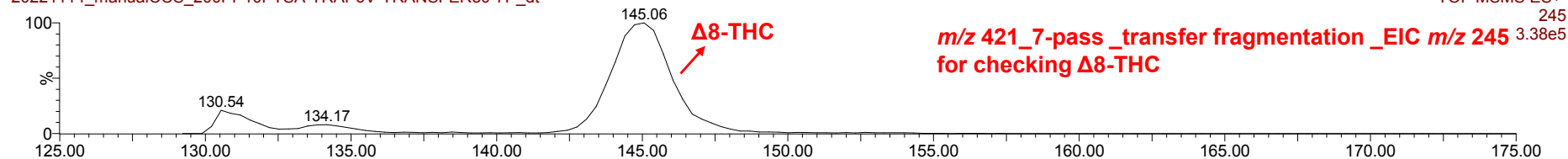


R#2_mobility separation+transfer fragmentation_for checking fragments

Raw output

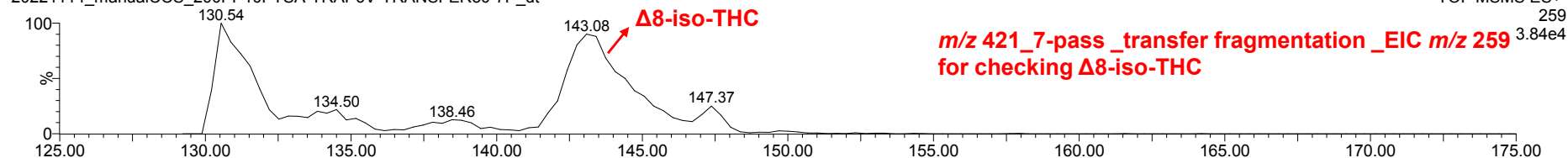
20221114_manualCCS_200PP10PTSA-TRAP6V-TRANSFER30-7P_dt

TOF MSMS ES+
245



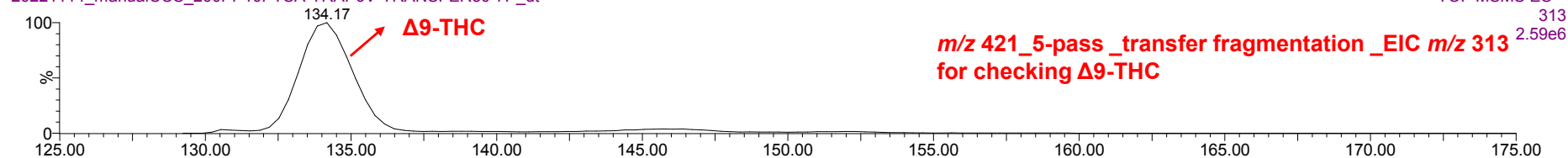
20221114_manualCCS_200PP10PTSA-TRAP6V-TRANSFER30-7P_dt

TOF MSMS ES+
259



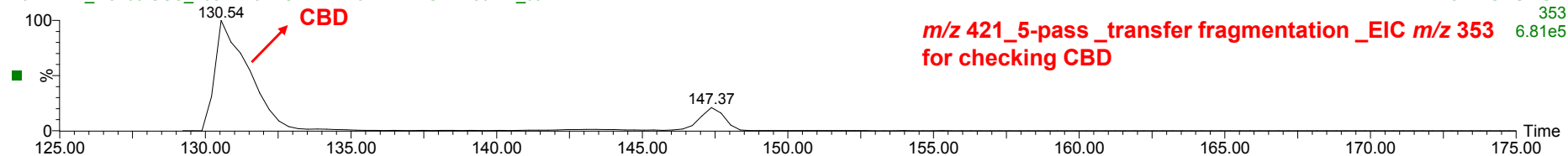
20221114_manualCCS_200PP10PTSA-TRAP6V-TRANSFER30-7P_dt

TOF MSMS ES+
313



20221114_manualCCS_200PP10PTSA-TRAP6V-TRANSFER30-7P_dt

TOF MSMS ES+
353

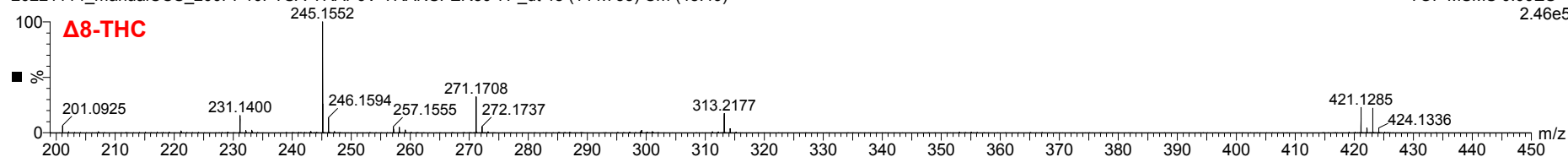


R#2_mobility separation+transfer fragmentation_for checking fragments

Raw output

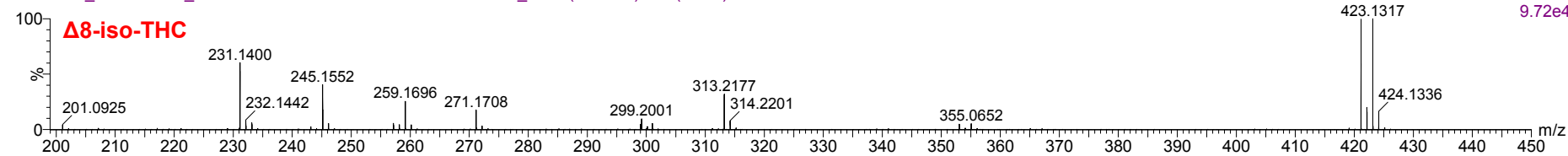
20221114_manualCCS_200PP10PTSA-TRAP6V-TRANSFER30-7P_dt 48 (144.733) Cm (48:49)

TOF MSMS 0.00ES+
2.46e5



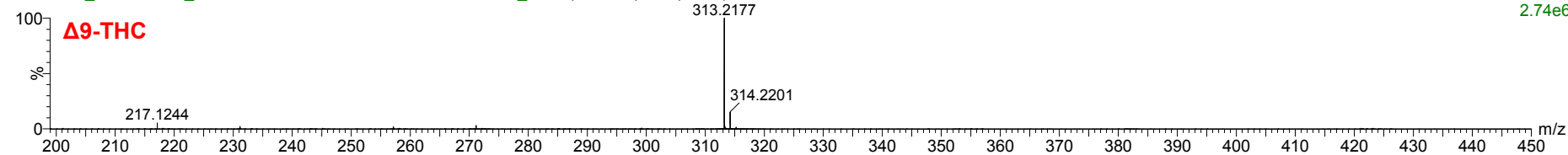
20221114_manualCCS_200PP10PTSA-TRAP6V-TRANSFER30-7P_dt 44 (143.413) Cm (42:44)

TOF MSMS 0.00ES+
9.72e4



20221114_manualCCS_200PP10PTSA-TRAP6V-TRANSFER30-7P_dt 16 (134.174) Cm (15:16)

TOF MSMS 0.00ES+
2.74e6



20221114_manualCCS_200PP10PTSA-TRAP6V-TRANSFER30-7P_dt 5 (130.544) Cm (4:8)

TOF MSMS 0.00ES+
4.63e6

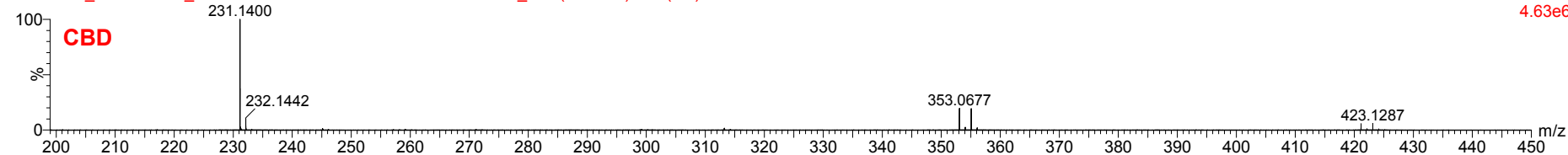


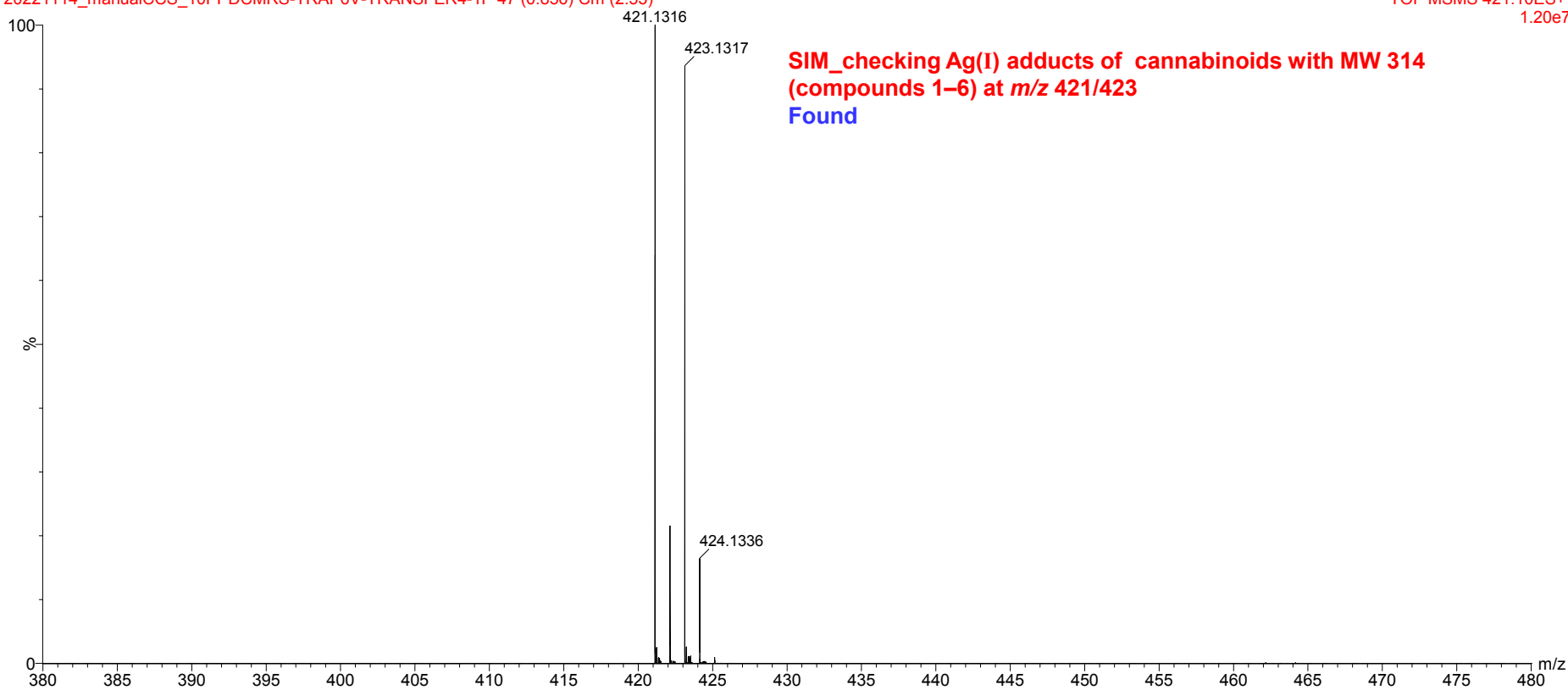
Figure S14-7. Mobiligram and mass spectra of cannabinoids in sample R#2.

R#3 _SIM_ for checking Ag(I) adducts

ADC12-5PPB-SEP2

20221114_manualCCS_10PPDCMRS-TRAP6V-TRANSFER4-1P 47 (0.856) Cm (2:53)

TOF MSMS 421.10ES+
1.20e7



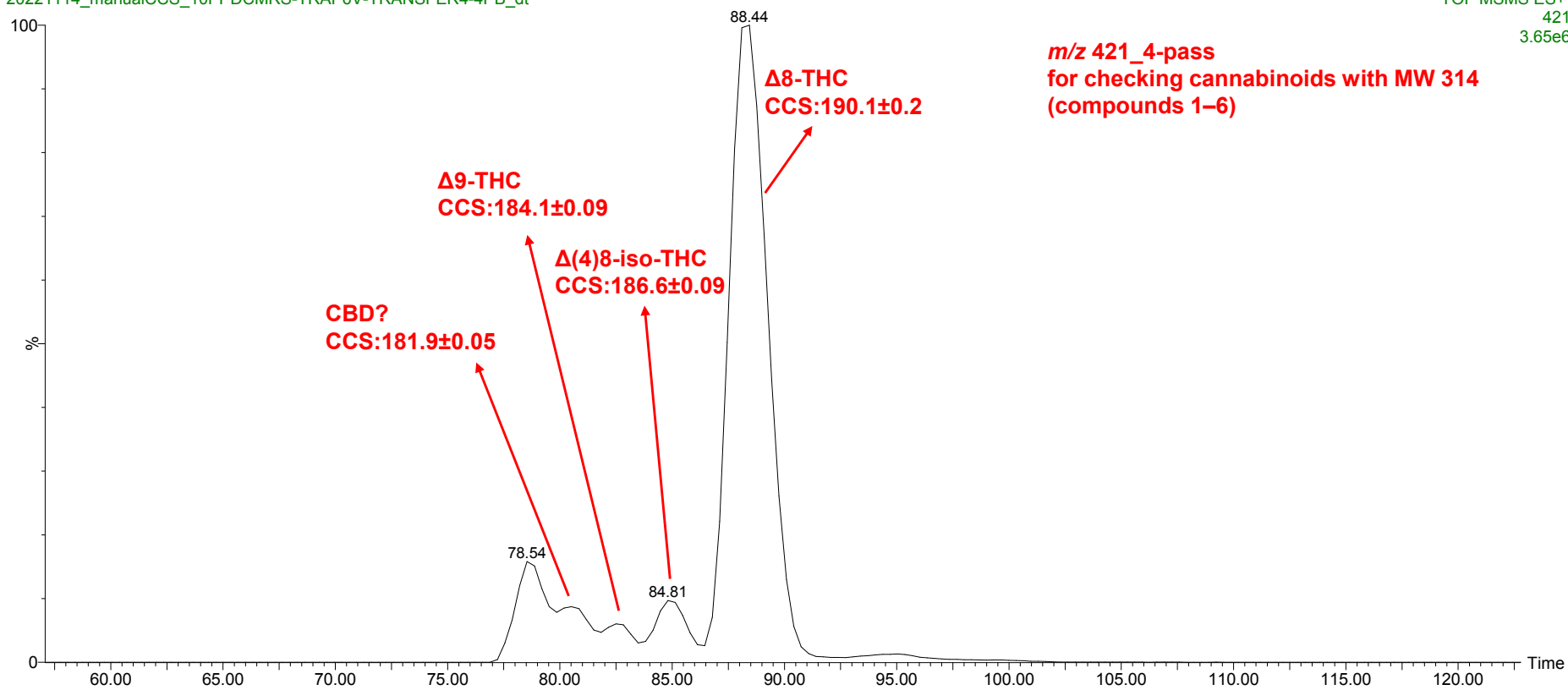
SIM_checking Ag(I) adducts of cannabinoids with MW 314
(compounds 1–6) at m/z 421/423
Found

R#3 _mobility separation_for checking CCS

Raw output

20221114_manualCCS_10PPDCMRS-TRAP6V-TRANSFER4-4PB_dt

TOF MSMS ES+
421
3.65e6

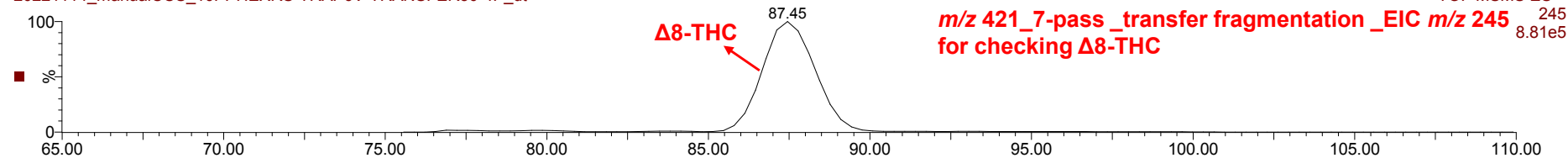


R#3_mobility separation+transfer fragmentation_for checking fragments

Raw output

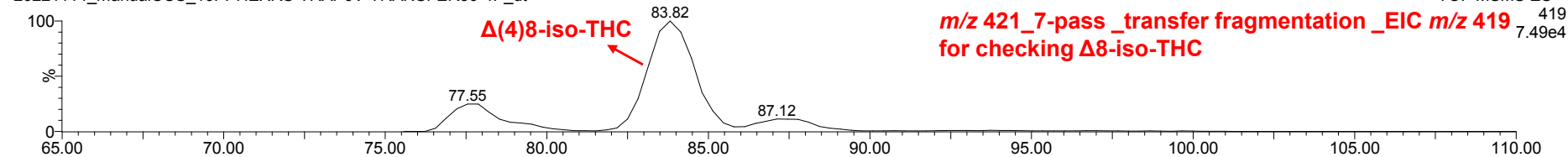
20221114_manualCCS_10PPHEXRS-TRAP6V-TRANSFER30-4P_dt

TOF MSMS ES+



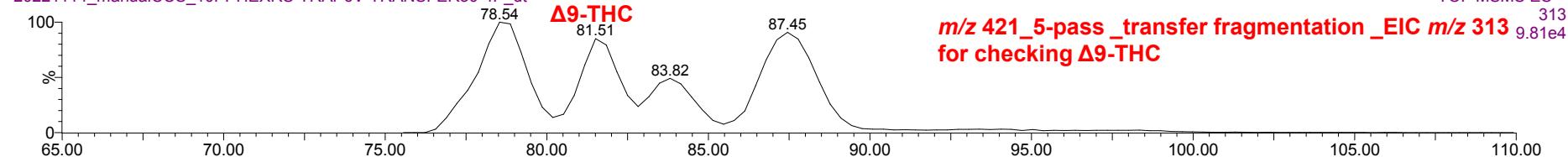
20221114_manualCCS_10PPHEXRS-TRAP6V-TRANSFER30-4P_dt

TOF MSMS ES+



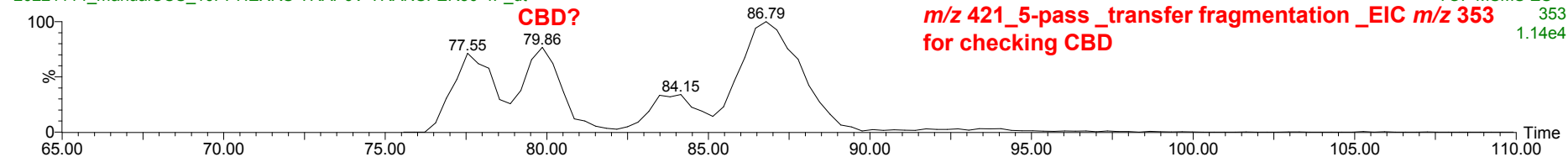
20221114_manualCCS_10PPHEXRS-TRAP6V-TRANSFER30-4P_dt

TOF MSMS ES+



20221114_manualCCS_10PPHEXRS-TRAP6V-TRANSFER30-4P_dt

TOF MSMS ES+

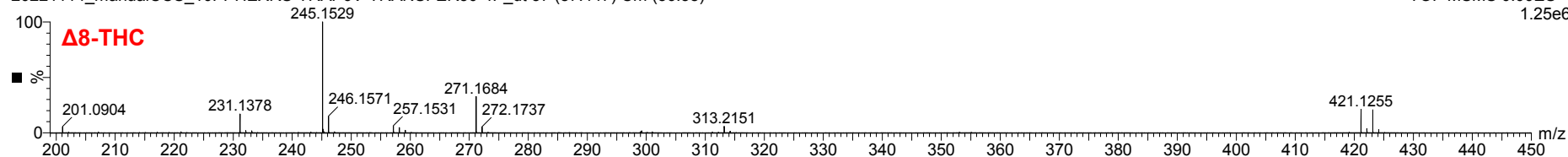


R#3_mobility separation+transfer fragmentation_for checking fragments

Raw output

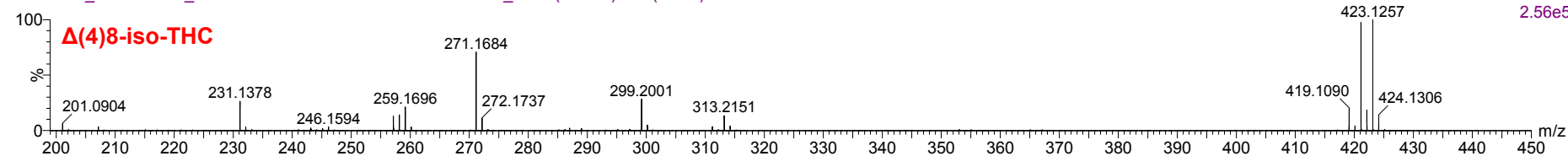
20221114_manualCCS_10PPHEXRS-TRAP6V-TRANSFER30-4P_dt 37 (87.447) Cm (36:38)

TOF MSMS 0.00ES+
1.25e6



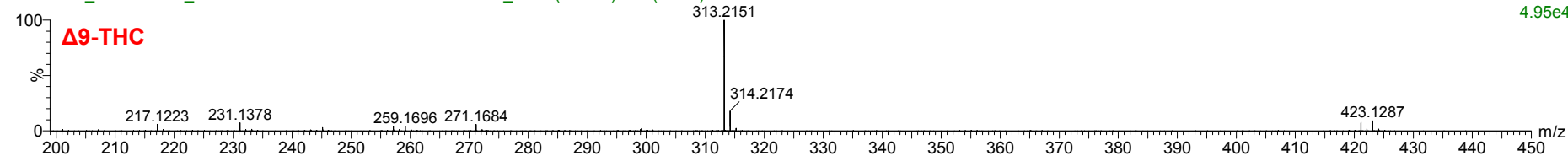
20221114_manualCCS_10PPHEXRS-TRAP6V-TRANSFER30-4P_dt 26 (83.817) Cm (25:27)

TOF MSMS 0.00ES+
2.56e5



20221114_manualCCS_10PPHEXRS-TRAP6V-TRANSFER30-4P_dt 19 (81.507) Cm (19:20)

TOF MSMS 0.00ES+
4.95e4



20221114_manualCCS_10PPHEXRS-TRAP6V-TRANSFER30-4P_dt 13 (79.527) Cm (13:14)

TOF MSMS 0.00ES+
2.57e4

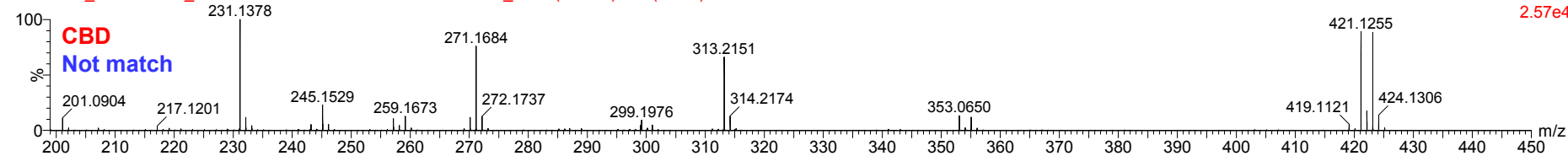


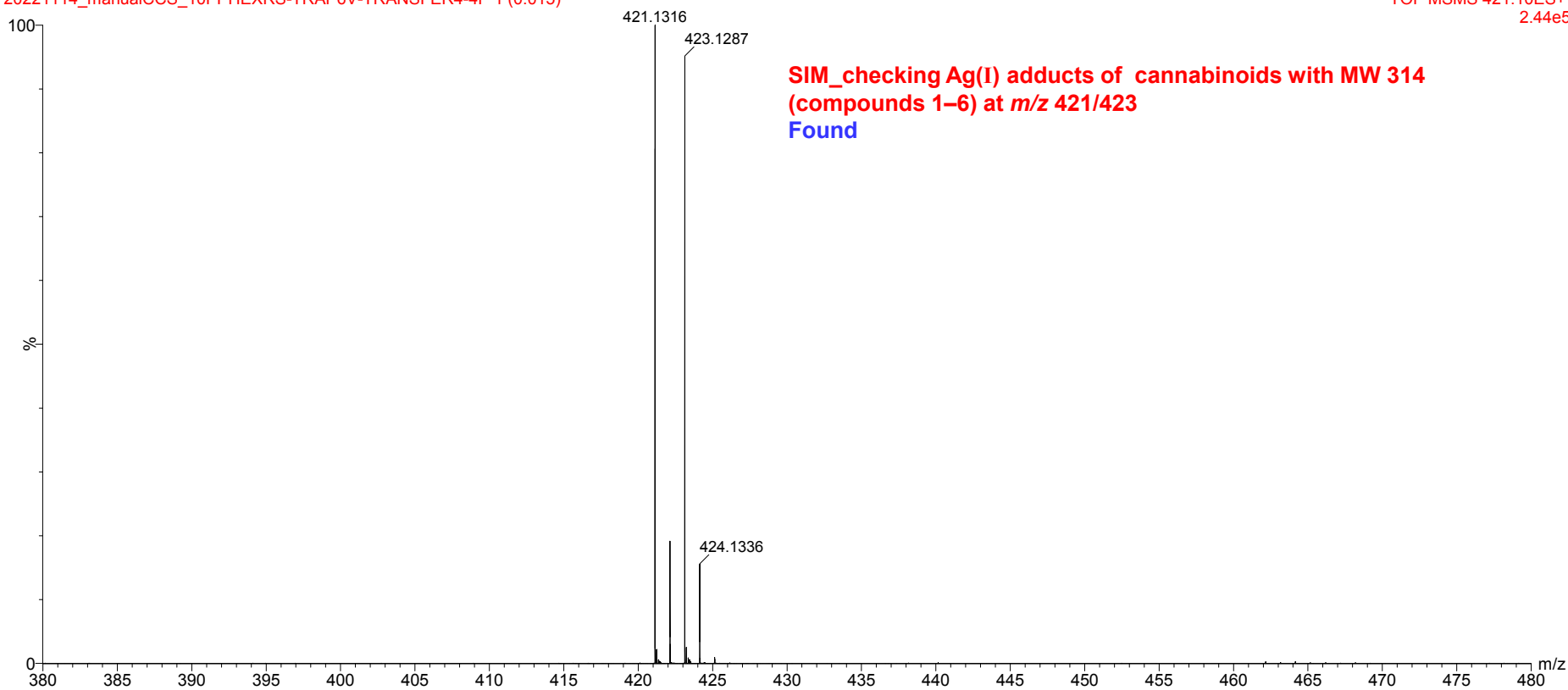
Figure S14-8. Mobiligram and mass spectra of cannabinoids in sample R#3.

R#4 _SIM_ for checking Ag(I) adducts

ADC75.57-5PPB-SEP65.57

20221114_manualCCS_10PPHEXRS-TRAP6V-TRANSFER4-4P 1 (0.015)

TOF MSMS 421.10ES+
2.44e5



R#4 _mobility separation_for checking CCS

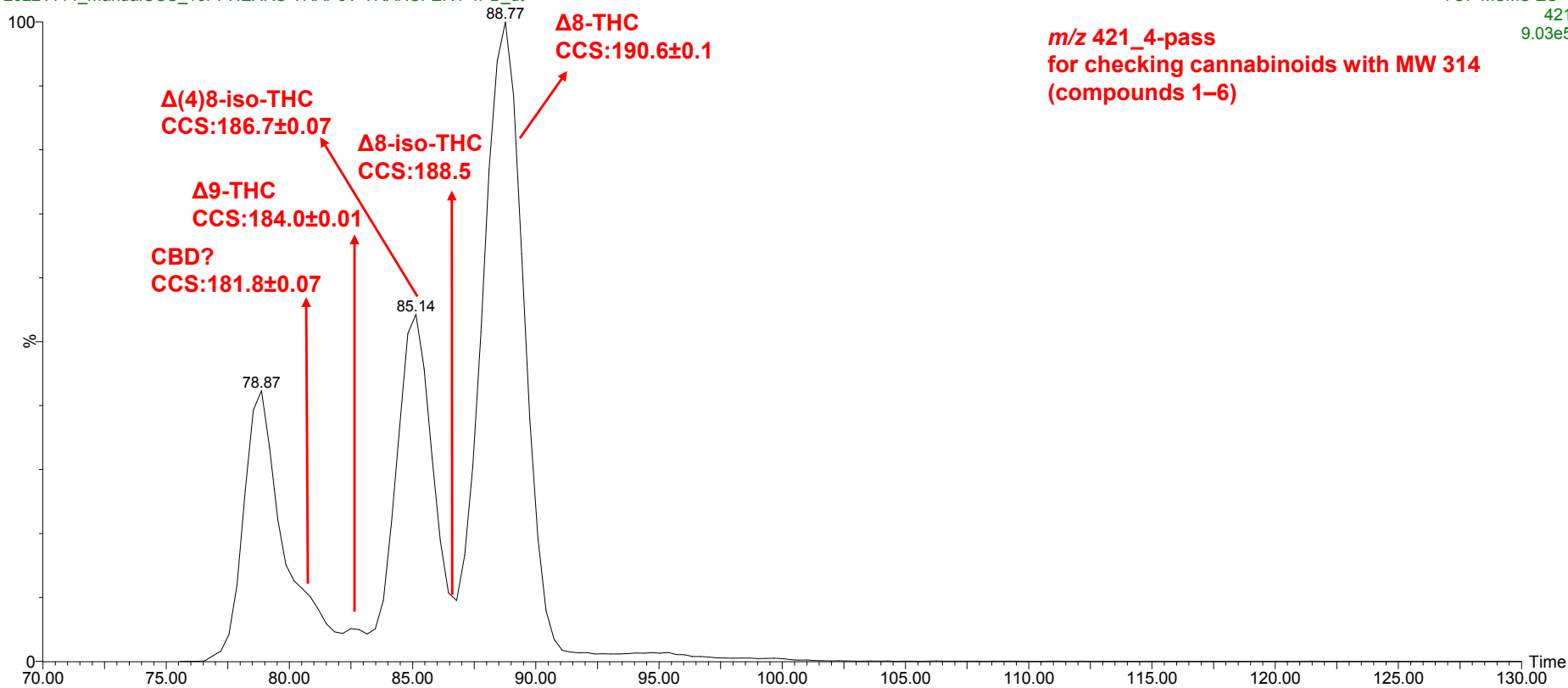
Raw output

20221114_manualCCS_10PPHEXRS-TRAP6V-TRANSFER4-4PB_dt

TOF MSMS ES+

421

9.03e5

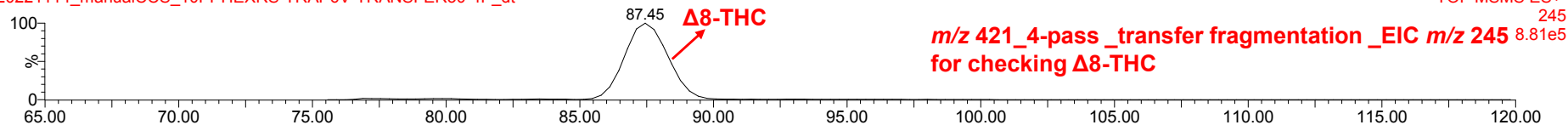


R#4_mobility separation+transfer fragmentation_for checking fragments

Raw output

20221114_manualCCS_10PPHEXRS-TRAP6V-TRANSFER30-4P_dt

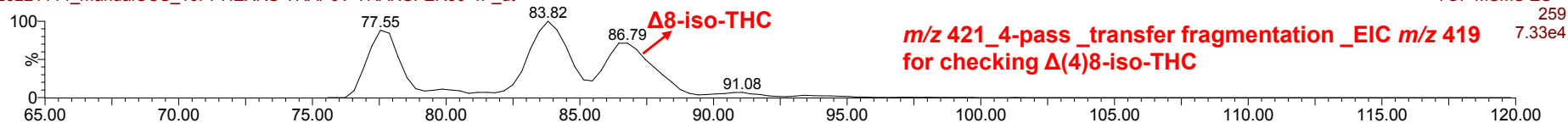
TOF MSMS ES+
245



m/z 421_4-pass_transfer fragmentation _EIC m/z 245
for checking Δ8-THC

20221114_manualCCS_10PPHEXRS-TRAP6V-TRANSFER30-4P_dt

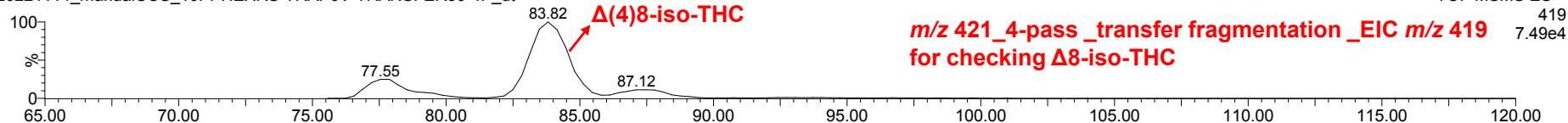
TOF MSMS ES+
259



m/z 421_4-pass_transfer fragmentation _EIC m/z 419
for checking Δ(4)8-iso-THC

20221114_manualCCS_10PPHEXRS-TRAP6V-TRANSFER30-4P_dt

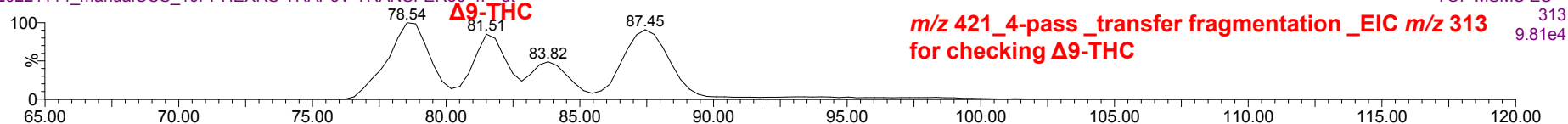
TOF MSMS ES+
419



m/z 421_4-pass_transfer fragmentation _EIC m/z 419
for checking Δ8-iso-THC

20221114_manualCCS_10PPHEXRS-TRAP6V-TRANSFER30-4P_dt

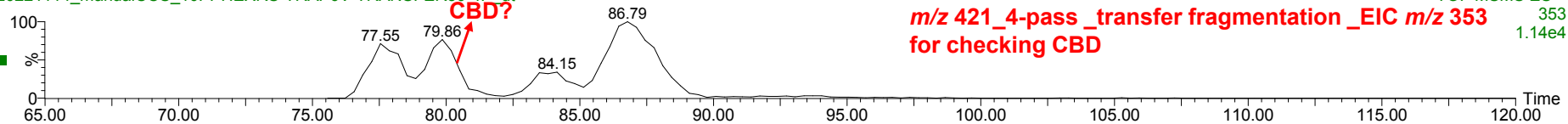
TOF MSMS ES+
313



m/z 421_4-pass_transfer fragmentation _EIC m/z 313
for checking Δ9-THC

20221114_manualCCS_10PPHEXRS-TRAP6V-TRANSFER30-4P_dt

TOF MSMS ES+
353



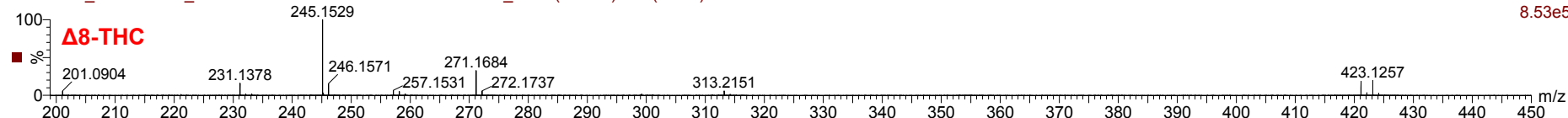
m/z 421_4-pass_transfer fragmentation _EIC m/z 353
for checking CBD

R#4_mobility separation+transfer fragmentation_for checking fragments

Raw output

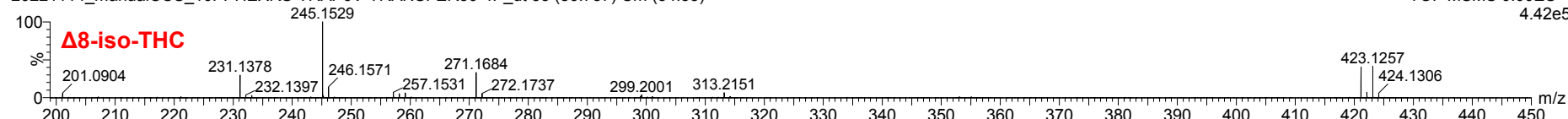
20221114_manualCCS_10PPHEXRS-TRAP6V-TRANSFER30-4P_dt 37 (87.447) Cm (37:38)

TOF MSMS 0.00ES+
8.53e5



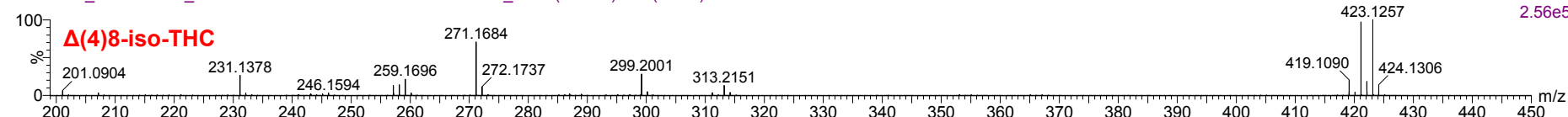
20221114_manualCCS_10PPHEXRS-TRAP6V-TRANSFER30-4P_dt 35 (86.787) Cm (34:35)

TOF MSMS 0.00ES+
4.42e5



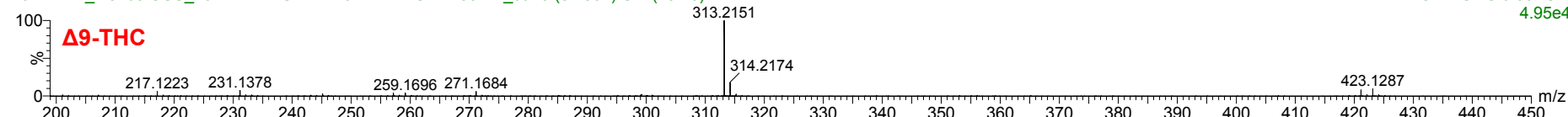
20221114_manualCCS_10PPHEXRS-TRAP6V-TRANSFER30-4P_dt 26 (83.817) Cm (25:27)

TOF MSMS 0.00ES+
2.56e5



20221114_manualCCS_10PPHEXRS-TRAP6V-TRANSFER30-4P_dt 19 (81.507) Cm (19:20)

TOF MSMS 0.00ES+
4.95e4



20221114_manualCCS_10PPHEXRS-TRAP6V-TRANSFER30-4P_dt 13 (79.527) Cm (13:15)

TOF MSMS 0.00ES+
3.94e4

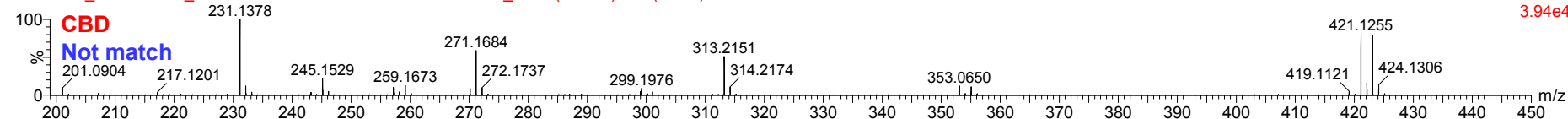


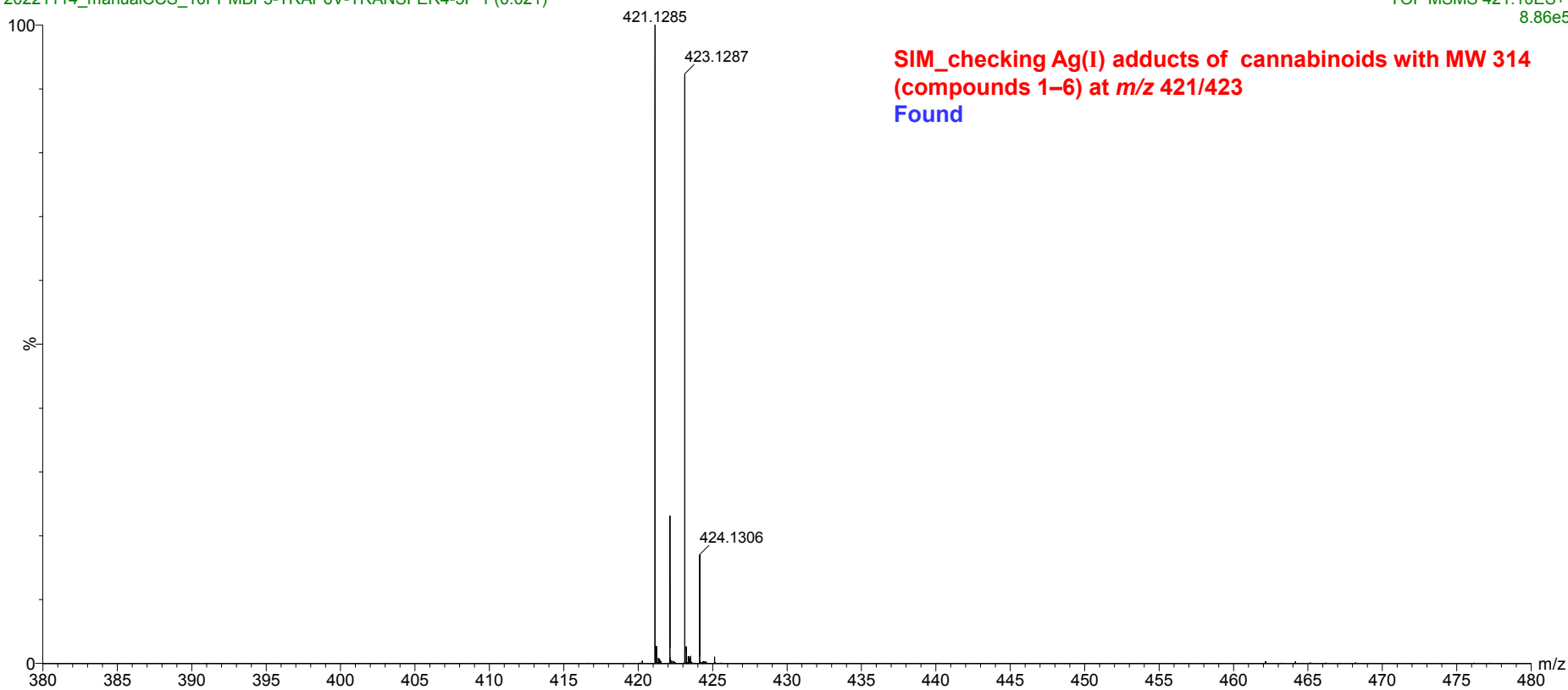
Figure S14-9. Mobiligram and mass spectra of cannabinoids in sample R#4.

R#5 _SIM_for checking Ag(I) adducts

ADC92.96-5PPB-SEP82.96

20221114_manualCCS_10PPMBF3-TRAP6V-TRANSFER4-5P 1 (0.021)

TOF MSMS 421.10ES+
8.86e5



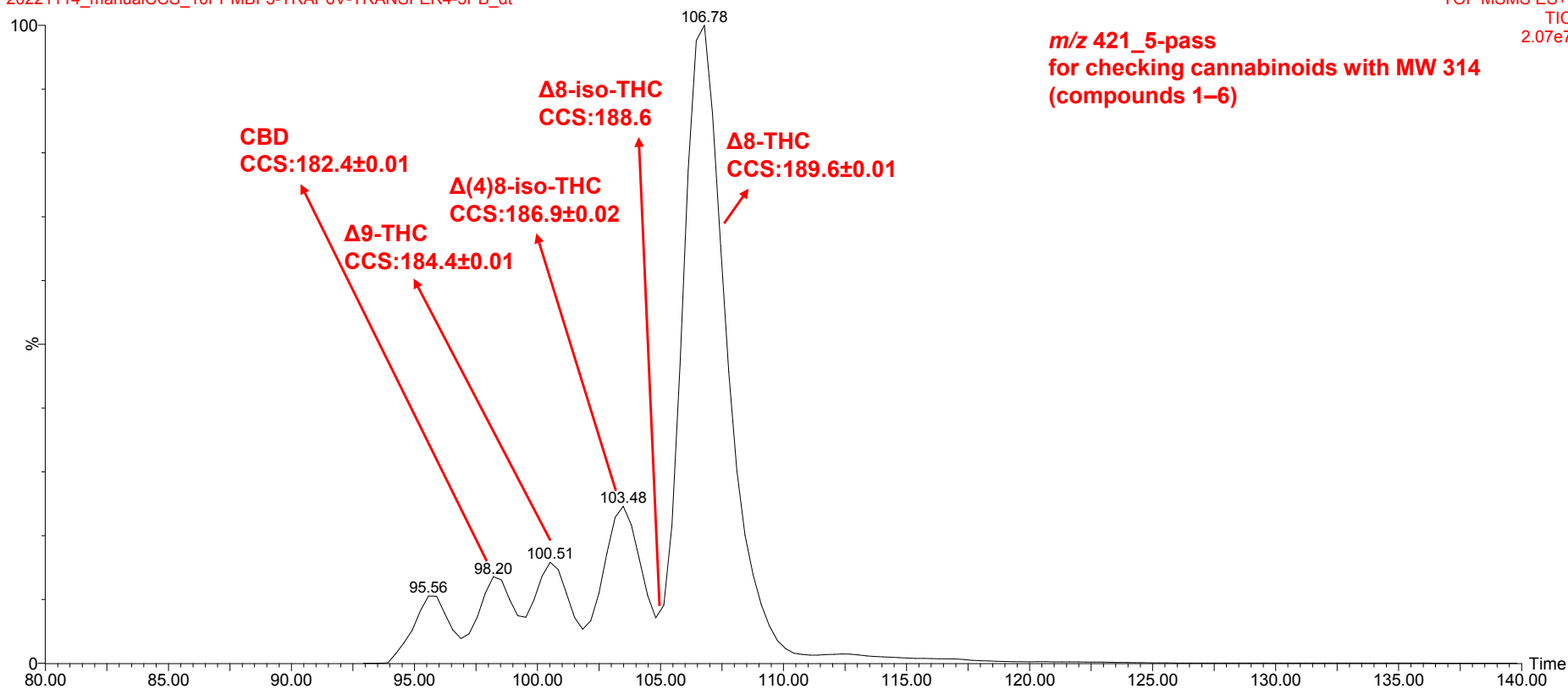
SIM_checking Ag(I) adducts of cannabinoids with MW 314
(compounds 1–6) at m/z 421/423
Found

R#5 _mobility separation_for checking CCS

Raw output

20221114_manualCCS_10PPMBF3-TRAP6V-TRANSFER4-5PB_dt

TOF MSMS ES+
TIC
2.07e7

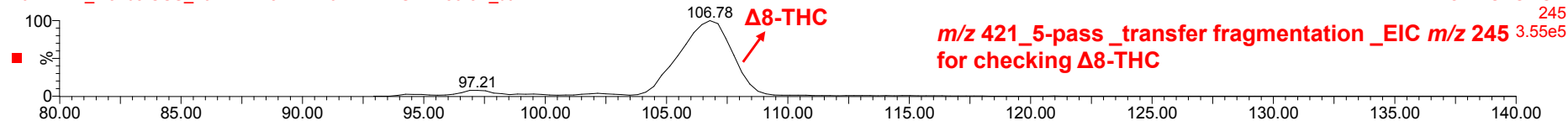


R#5_mobility separation+transfer fragmentation_for checking fragments

Raw output

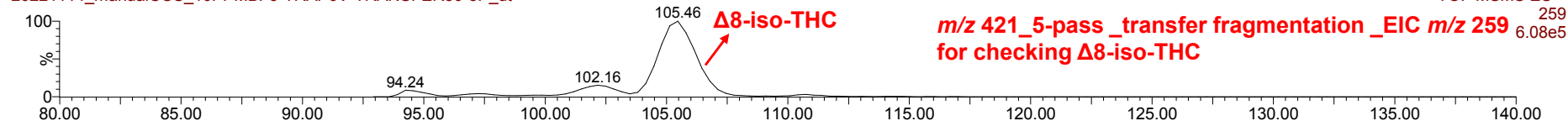
20221114_manualCCS_10PPMBF3-TRAP6V-TRANSFER30-5P_dt

TOF MSMS ES+
245



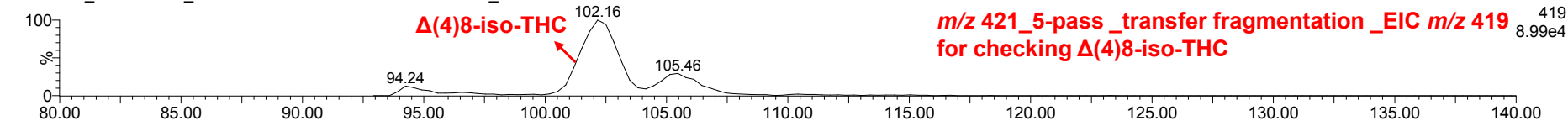
20221114_manualCCS_10PPMBF3-TRAP6V-TRANSFER30-5P_dt

TOF MSMS ES+
259



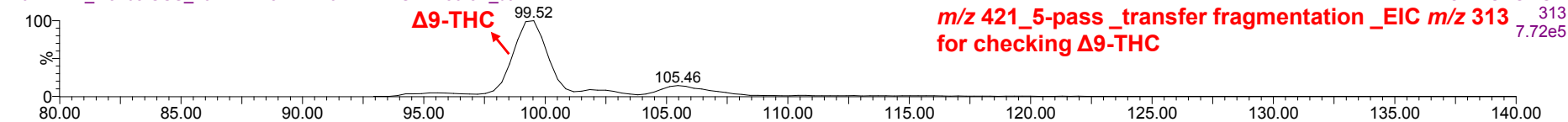
20221114_manualCCS_10PPMBF3-TRAP6V-TRANSFER30-5P_dt

TOF MSMS ES+
419



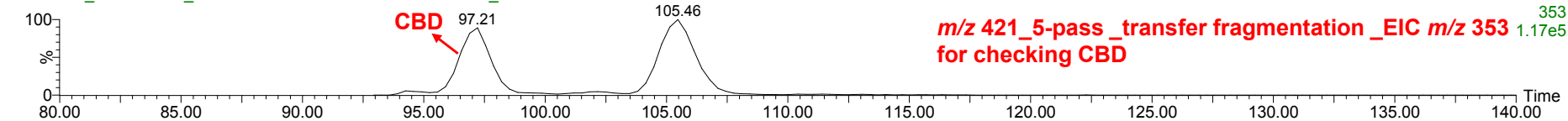
20221114_manualCCS_10PPMBF3-TRAP6V-TRANSFER30-5P_dt

TOF MSMS ES+
313



20221114_manualCCS_10PPMBF3-TRAP6V-TRANSFER30-5P_dt

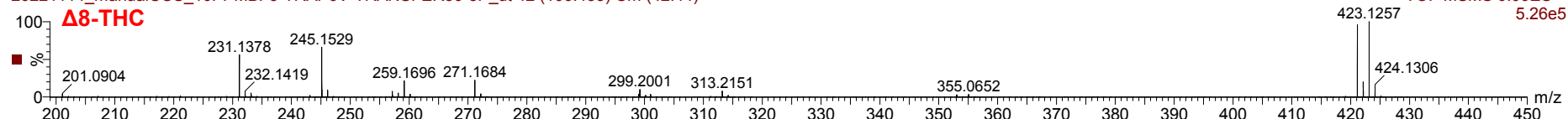
TOF MSMS ES+
353



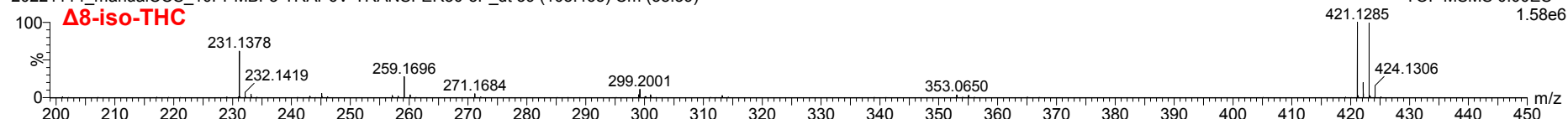
R#5_mobility separation+transfer fragmentation_for checking fragments

Raw output

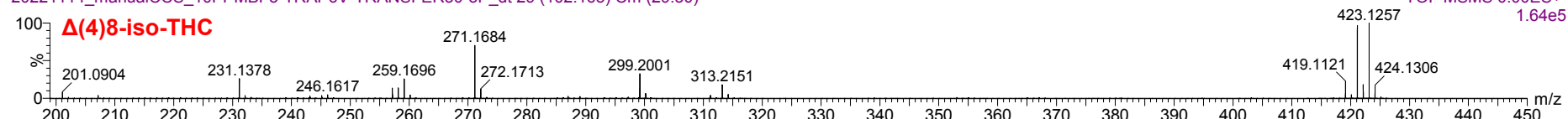
20221114_manualCCS_10PPMBF3-TRAP6V-TRANSFER30-5P_dt 42 (106.455) Cm (42:44)



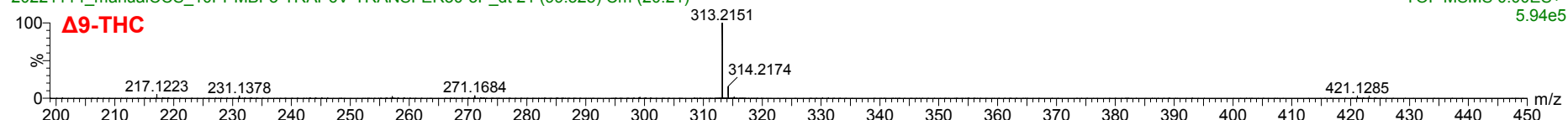
20221114_manualCCS_10PPMBF3-TRAP6V-TRANSFER30-5P_dt 39 (105.465) Cm (38:39)



20221114_manualCCS_10PPMBF3-TRAP6V-TRANSFER30-5P_dt 29 (102.165) Cm (29:30)



20221114_manualCCS_10PPMBF3-TRAP6V-TRANSFER30-5P_dt 21 (99.525) Cm (20:21)



20221114_manualCCS_10PPMBF3-TRAP6V-TRANSFER30-5P_dt 14 (97.215) Cm (12:15)

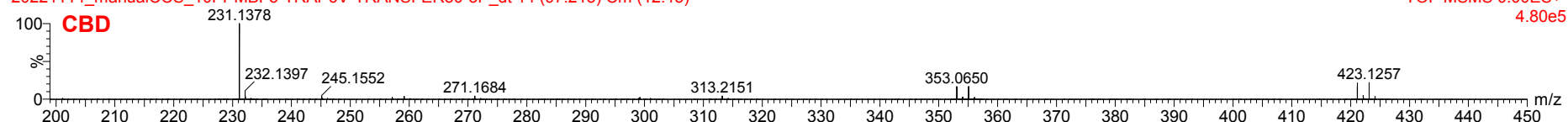


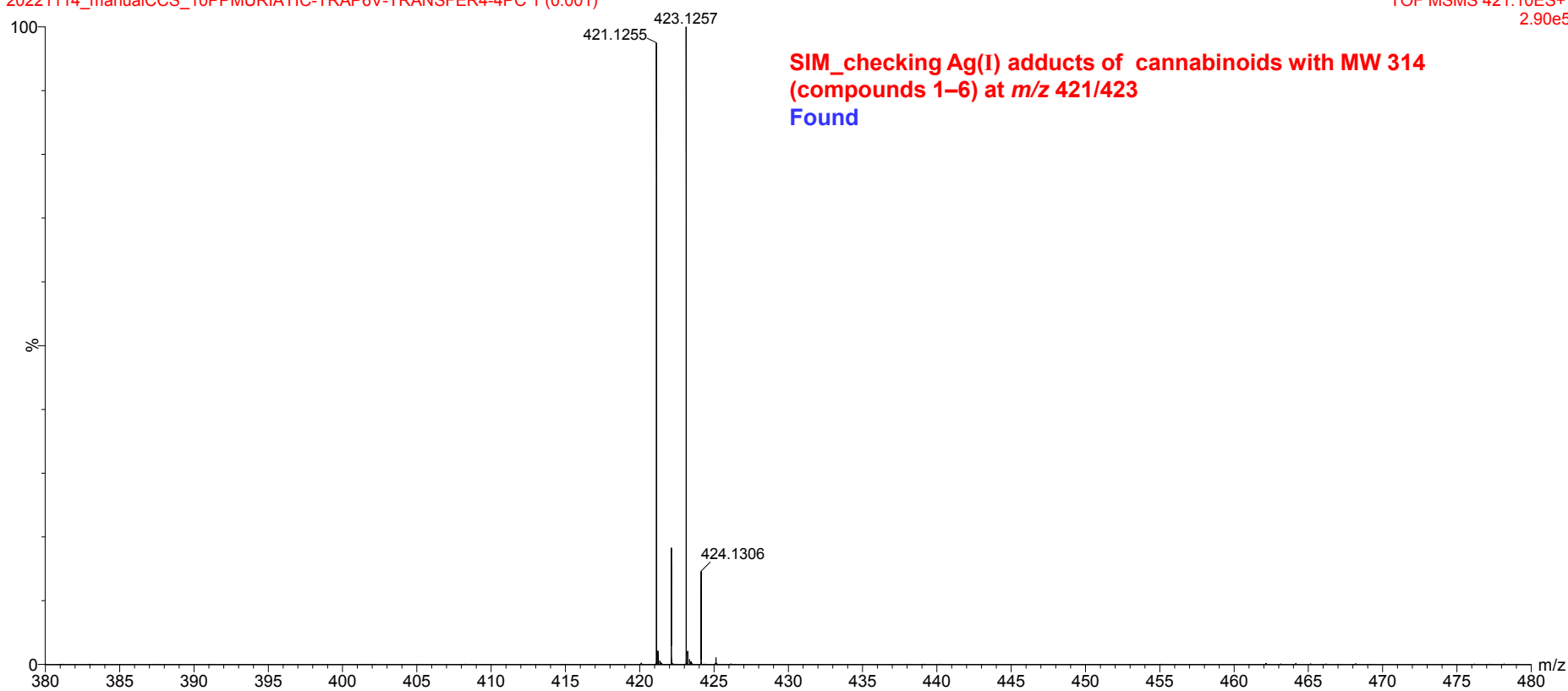
Figure S14-10. Mobiligram and mass spectra of cannabinoids in sample R#5.

R#6 _SIM_ for checking Ag(I) adducts

Raw output

20221114_manualCCS_10PPMURIATIC-TRAP6V-TRANSFER4-4PC 1 (0.001)

TOF MSMS 421.10ES+
2.90e5



SIM_checking Ag(I) adducts of cannabinoids with MW 314
(compounds 1–6) at m/z 421/423

Found

R#6 _mobility separation_for checking CCS

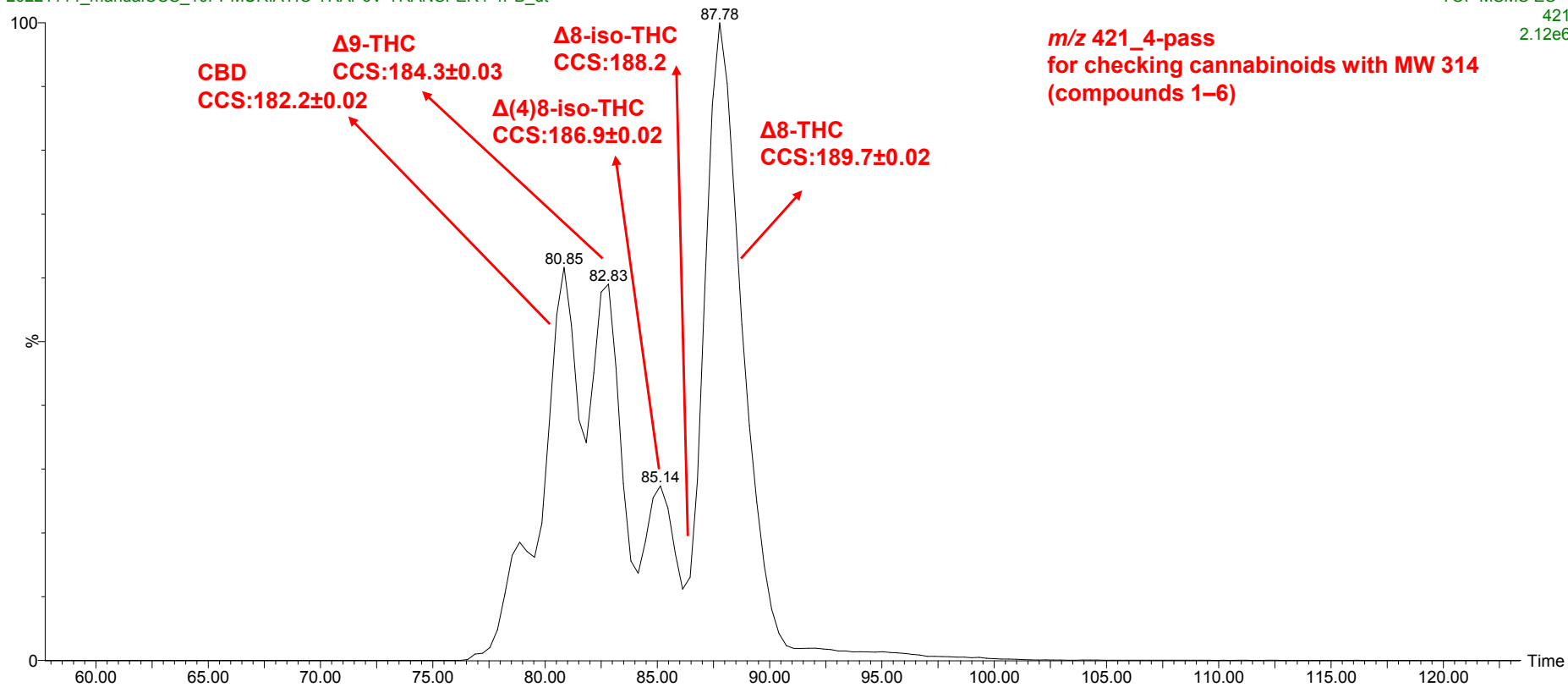
Raw output

20221114_manualCCS_10PPMURIATIC-TRAP6V-TRANSFER4-4PB_dt

TOF MSMS ES+

421

2.12e6

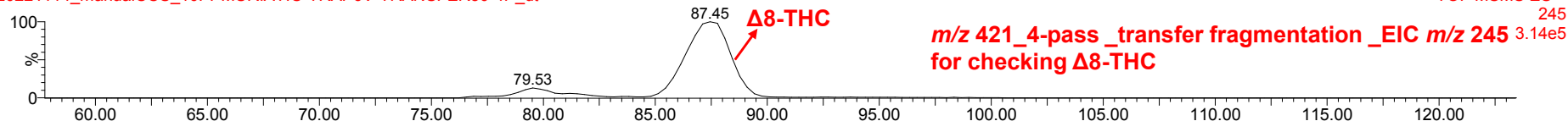


R#6_mobility separation+transfer fragmentation_for checking fragments

Raw output

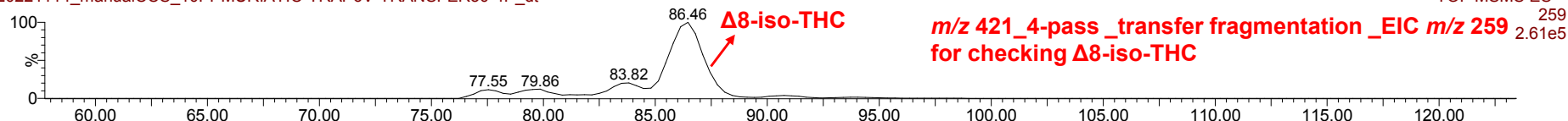
20221114_manualCCS_10PPMURIATIC-TRAP6V-TRANSFER30-4P_dt

TOF MSMS ES+
245



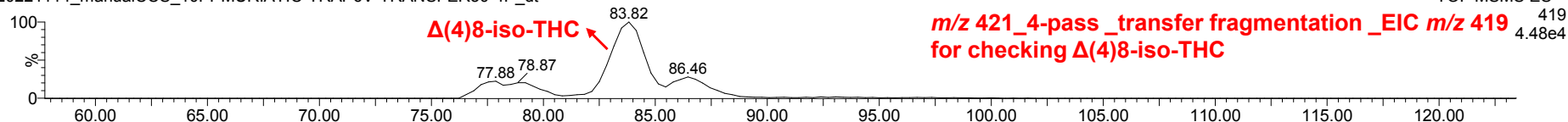
20221114_manualCCS_10PPMURIATIC-TRAP6V-TRANSFER30-4P_dt

TOF MSMS ES+
259



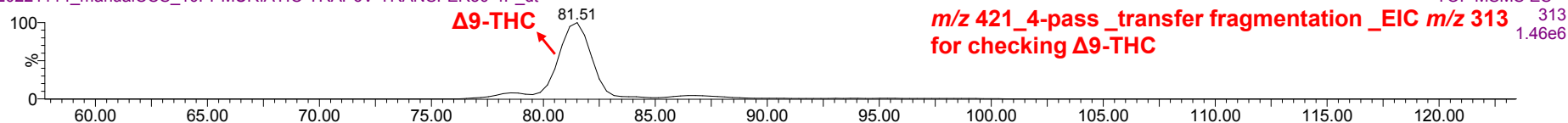
20221114_manualCCS_10PPMURIATIC-TRAP6V-TRANSFER30-4P_dt

TOF MSMS ES+
419



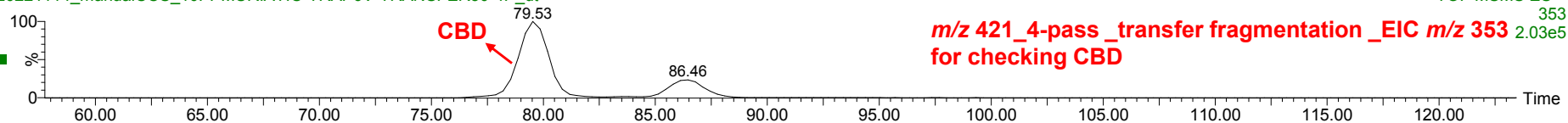
20221114_manualCCS_10PPMURIATIC-TRAP6V-TRANSFER30-4P_dt

TOF MSMS ES+
313



20221114_manualCCS_10PPMURIATIC-TRAP6V-TRANSFER30-4P_dt

TOF MSMS ES+
353

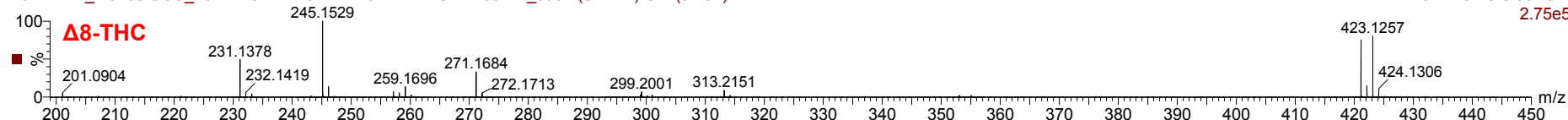


R#6_mobility separation+transfer fragmentation_for checking fragments

Raw output

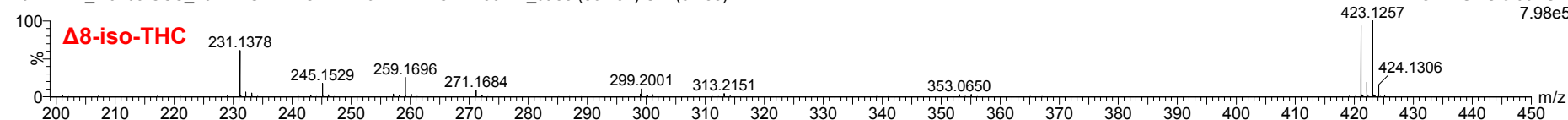
20221114_manualCCS_10PPMURIATIC-TRAP6V-TRANSFER30-4P_dt 91 (87.447) Cm (91:92)

TOF MSMS 0.00ES+
2.75e5



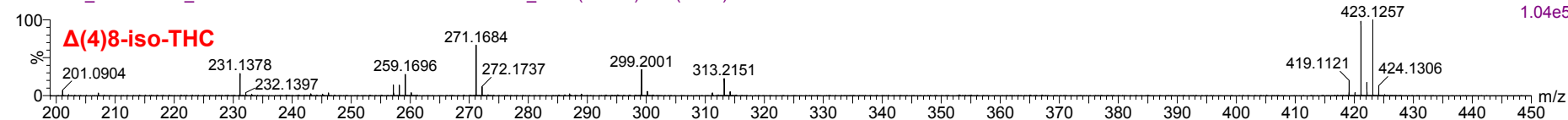
20221114_manualCCS_10PPMURIATIC-TRAP6V-TRANSFER30-4P_dt 88 (86.457) Cm (87:88)

TOF MSMS 0.00ES+
7.98e5



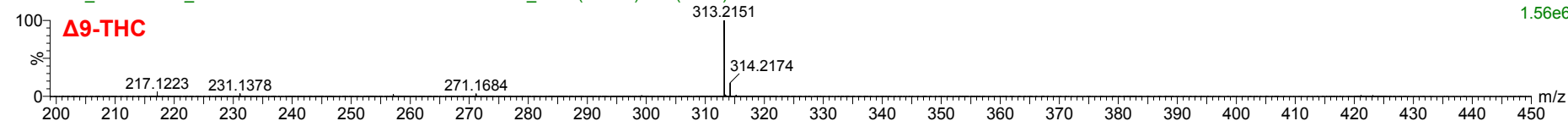
20221114_manualCCS_10PPMURIATIC-TRAP6V-TRANSFER30-4P_dt 80 (83.817) Cm (79:80)

TOF MSMS 0.00ES+
1.04e5



20221114_manualCCS_10PPMURIATIC-TRAP6V-TRANSFER30-4P_dt 73 (81.507) Cm (72:73)

TOF MSMS 0.00ES+
1.56e6



20221114_manualCCS_10PPMURIATIC-TRAP6V-TRANSFER30-4P_dt 67 (79.527) Cm (67)

TOF MSMS 0.00ES+
4.53e5

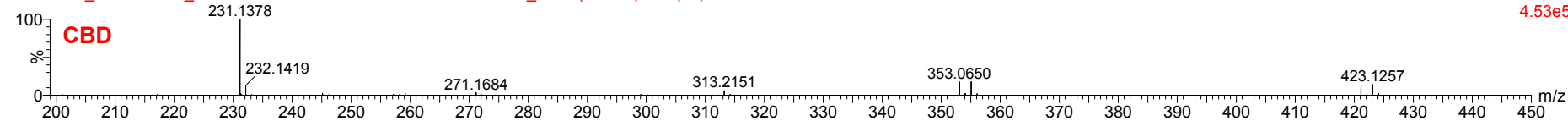


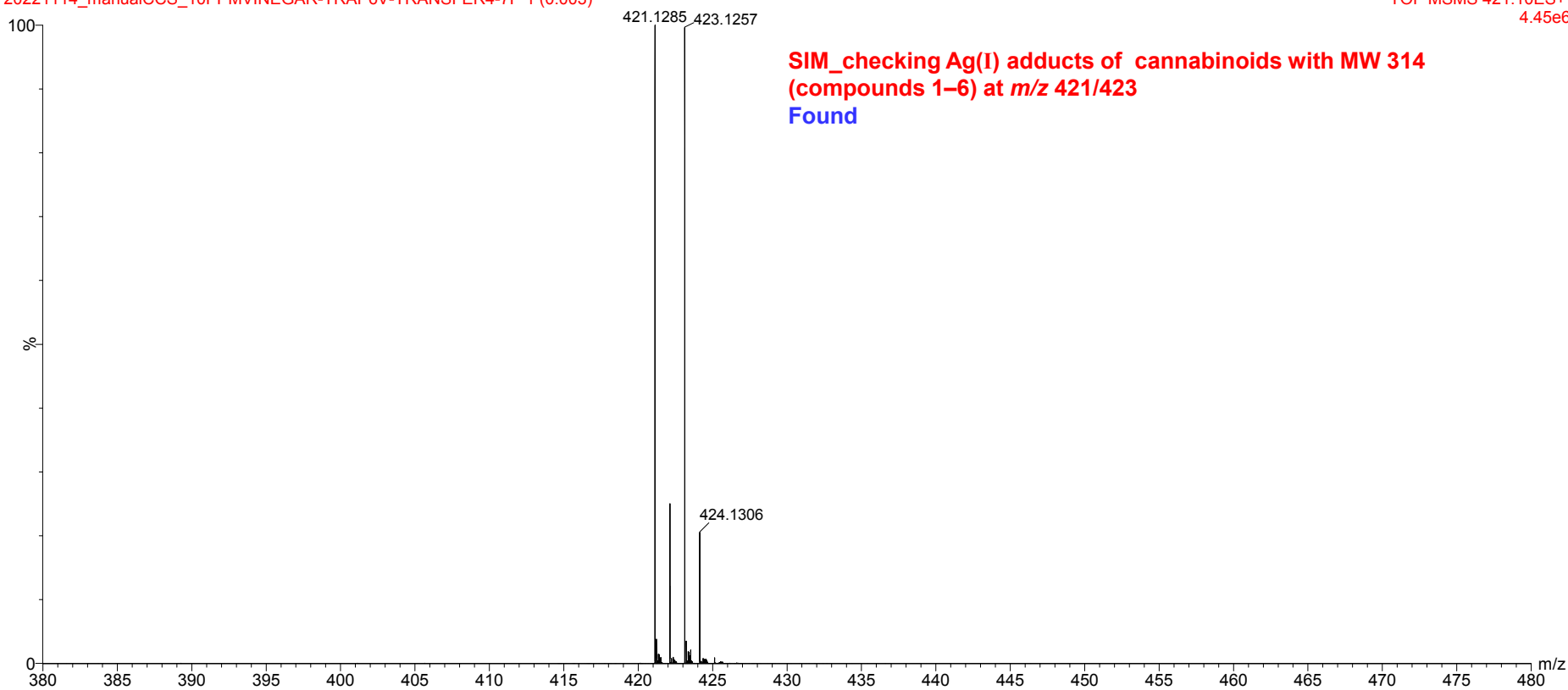
Figure S14-11. Mobiligram and mass spectra of cannabinoids in sample R#6.

R#7 _SIM_ for checking Ag(I) adducts

ADC120.83-5PPB-110.83

20221114_manualCCS_10PPMVINEGAR-TRAP6V-TRANSFER4-7P 1 (0.003)

TOF MSMS 421.10ES+
4.45e6



R#7 _mobility separation_for checking CCS

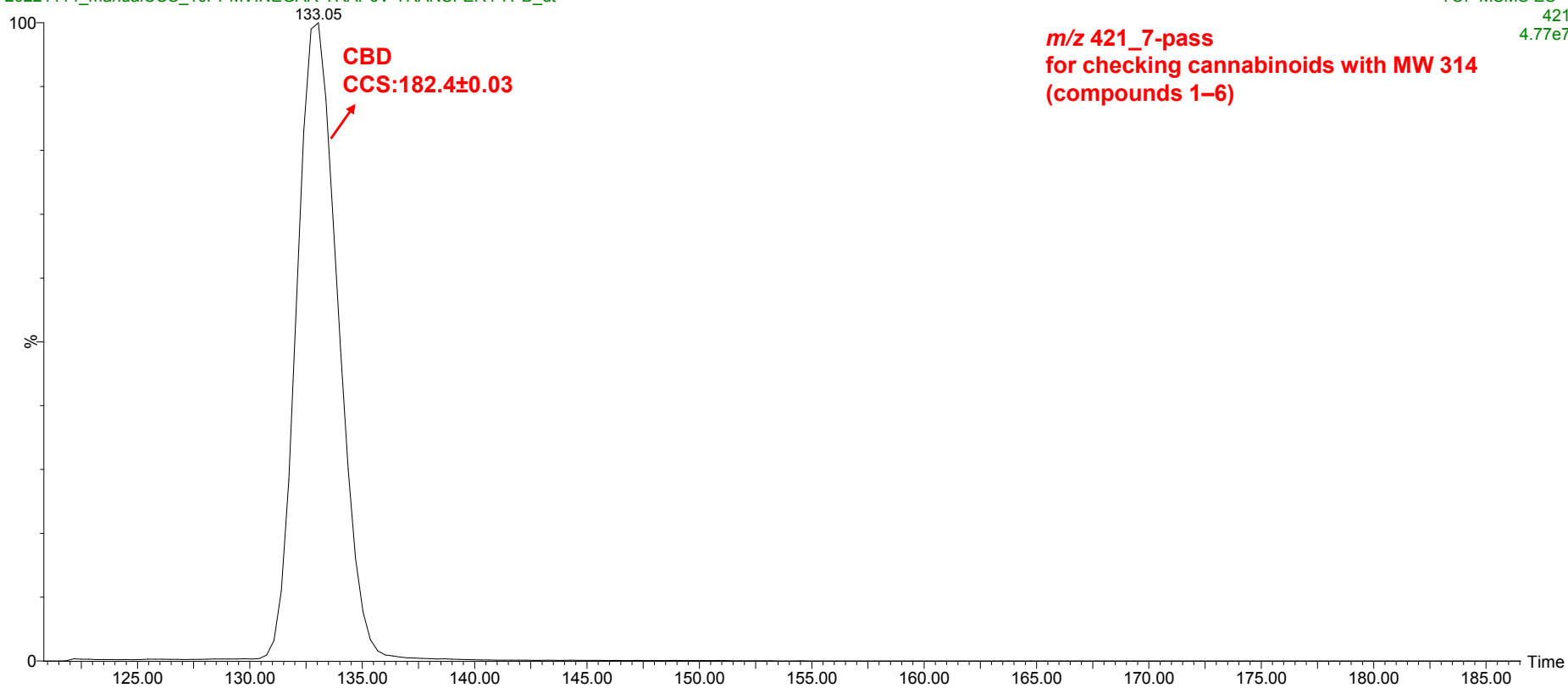
Raw output

20221114_manualCCS_10PPMVINEGAR-TRAP6V-TRANSFER4-7PB_dt

TOF MSMS ES+

421

4.77e7



m/z 421_7-pass
for checking cannabinoids with MW 314
(compounds 1–6)

R#7_mobility separation+transfer fragmentation_for checking fragments

Raw output

20221114_manualCCS_10PPMVINEGAR-TRAP6V-TRANSFER30-7PC_dt

TOF MSMS ES+

353

1.01e7



R#7_mobility separation+transfer fragmentation_for checking fragments

Raw output

20221114_manualCCS_10PPMVINEGAR-TRAP6V-TRANSFER30-7PC_dt 32 (131.072) Cm (31:33)

TOF MSMS 0.00ES+
5.82e7

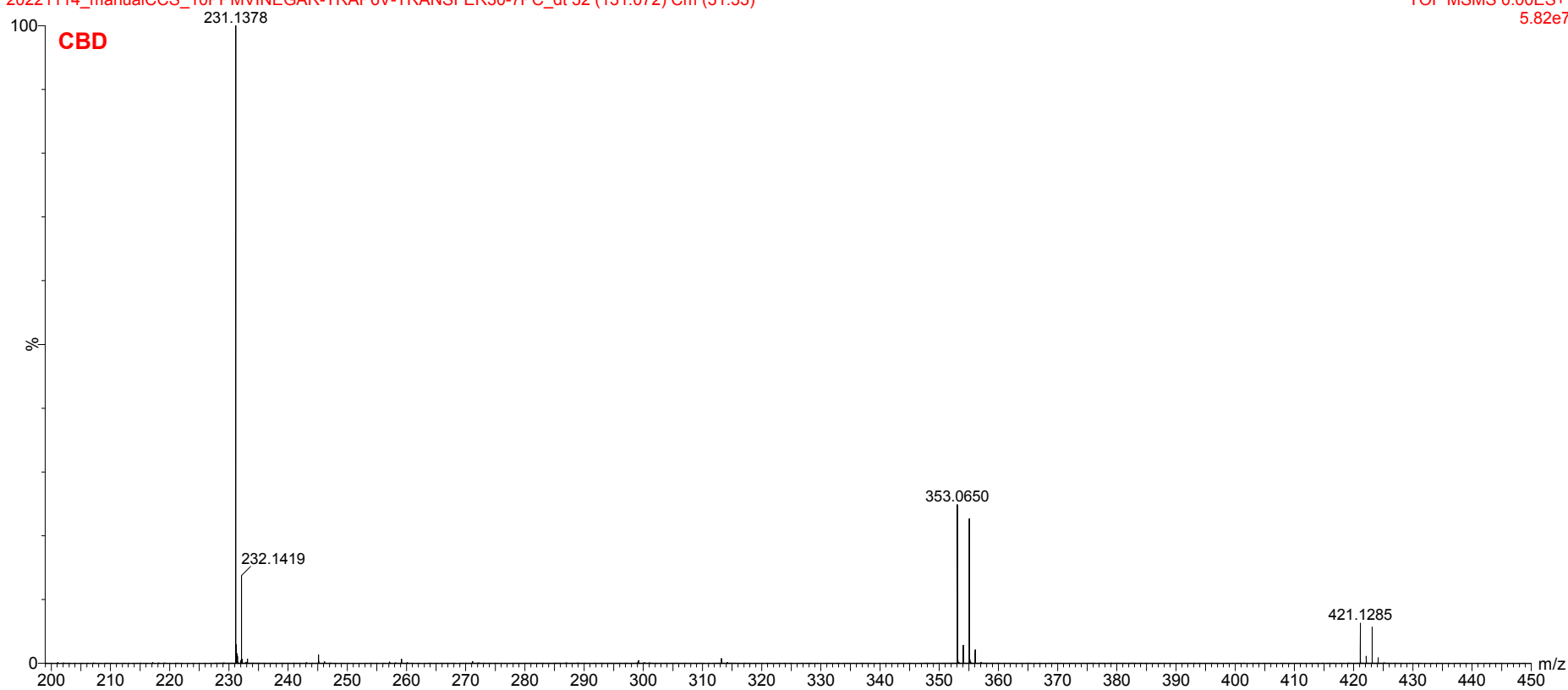


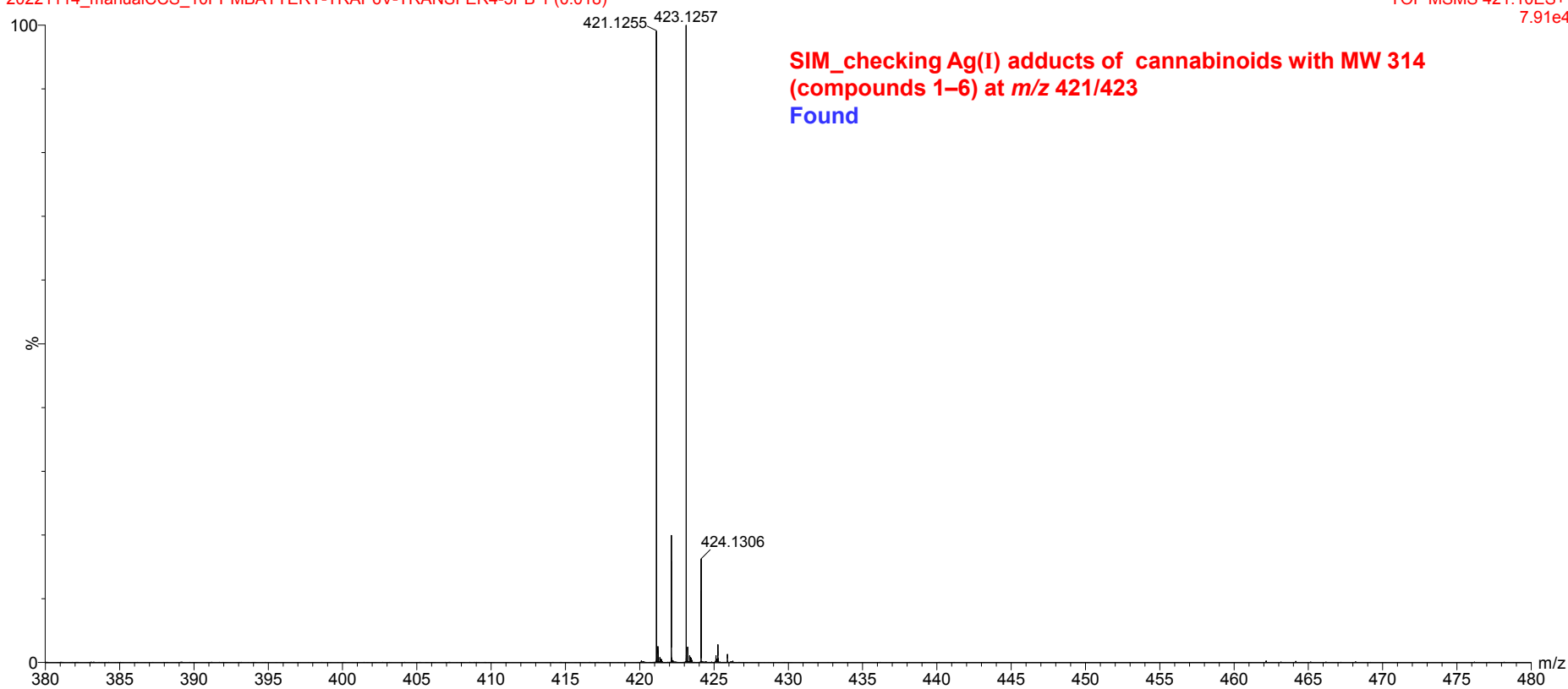
Figure S14-12. Mobiligram and mass spectra of cannabinoids in sample R#7.

R#8 _SIM_for checking Ag(I) adducts

Raw output

20221114_manualCCS_10PPMBATTERY-TRAP6V-TRANSFER4-5PB 1 (0.018)

TOF MSMS 421.10ES+
7.91e4



SIM_checking Ag(I) adducts of cannabinoids with MW 314
(compounds 1–6) at m/z 421/423
Found

R#8 _mobility separation_for checking CCS

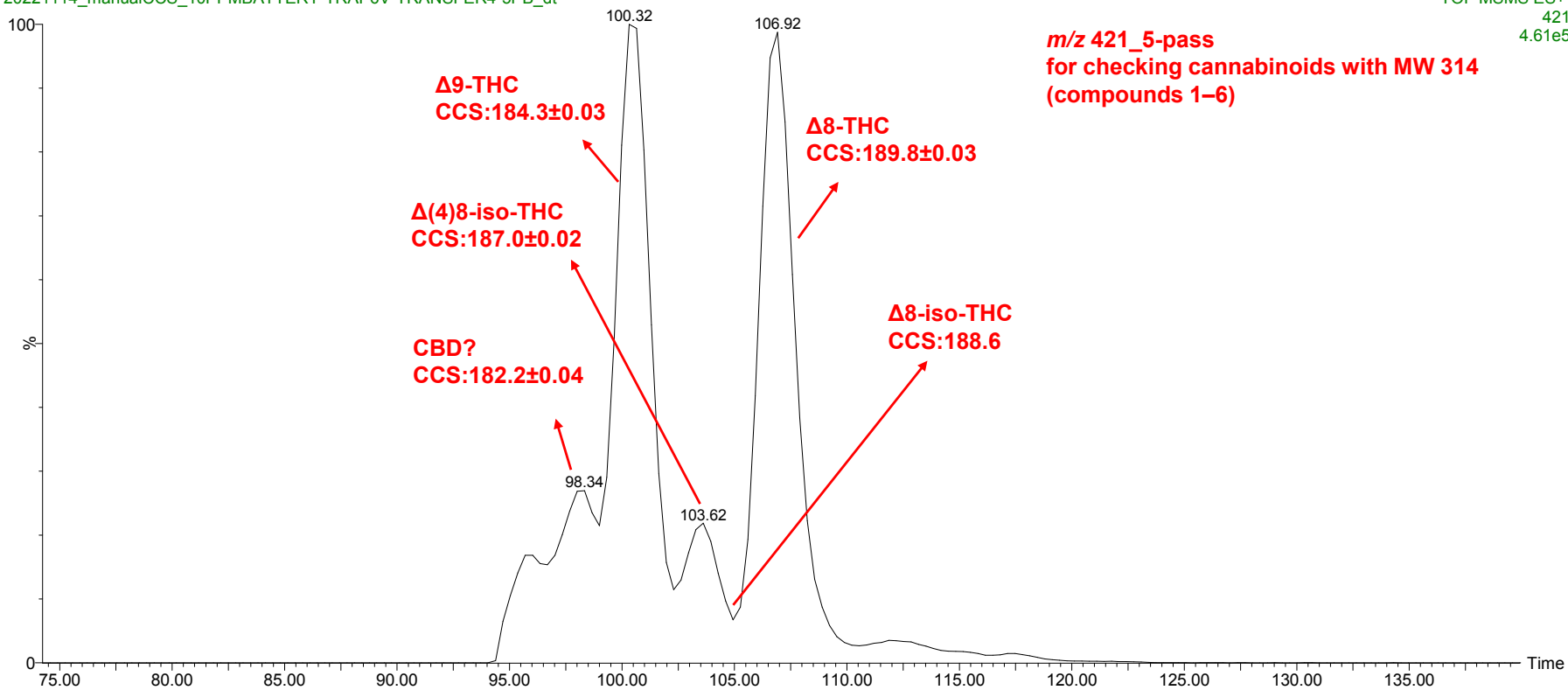
Raw output

20221114_manualCCS_10PPMBATTERY-TRAP6V-TRANSFER4-5PB_dt

TOF MSMS ES+

421

4.61e5

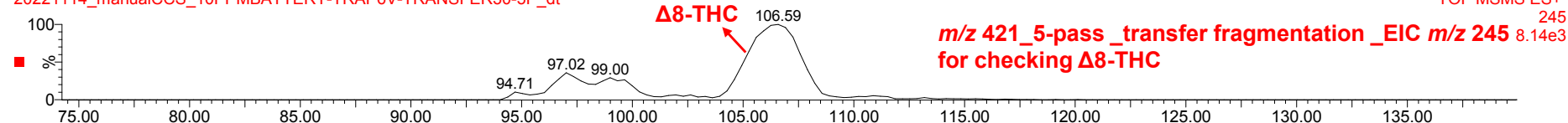


R#8_mobility separation+transfer fragmentation_for checking fragments

Raw output

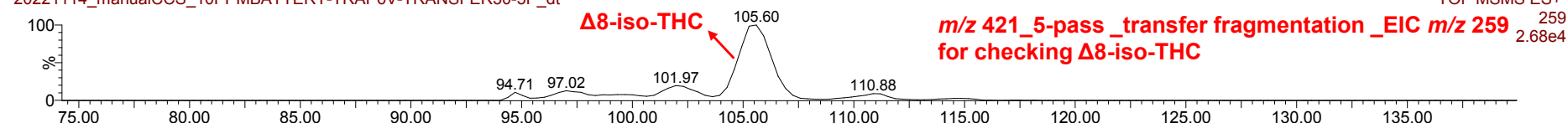
20221114_manualCCS_10PPMBATTERY-TRAP6V-TRANSFER30-5P_dt

TOF MSMS ES+



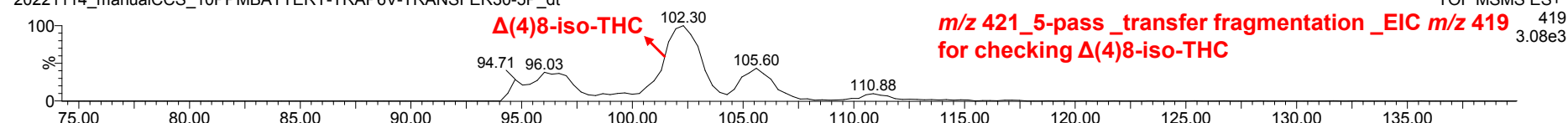
20221114_manualCCS_10PPMBATTERY-TRAP6V-TRANSFER30-5P_dt

TOF MSMS ES+



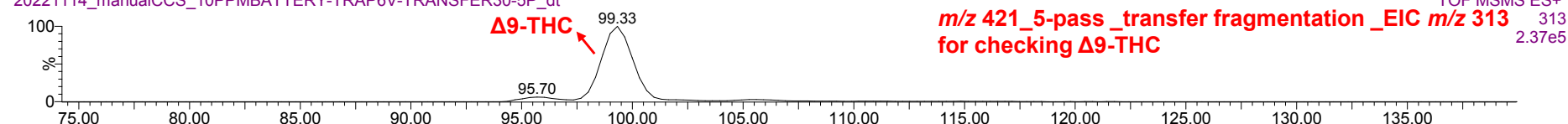
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TOF MSMS ES+



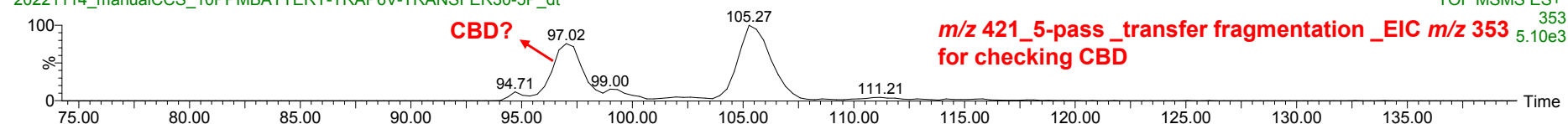
20221114_manualCCS_10PPMBATTERY-TRAP6V-TRANSFER30-5P_dt

TOF MSMS ES+



20221114_manualCCS_10PPMBATTERY-TRAP6V-TRANSFER30-5P_dt

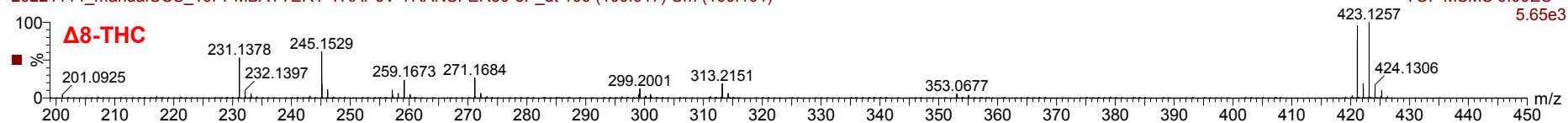
TOF MSMS ES+



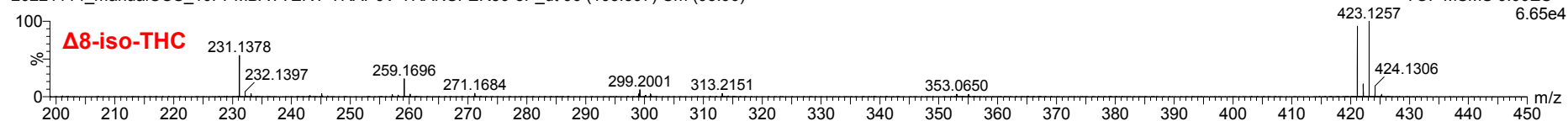
R#8_mobility separation+transfer fragmentation_for checking fragments

Raw output

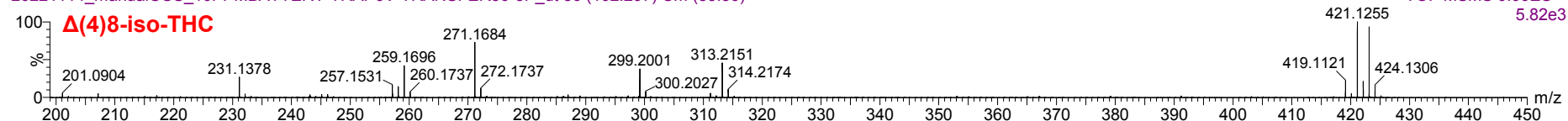
20221114_manualCCS_10PPMBATTERY-TRAP6V-TRANSFER30-5P_dt 100 (106.917) Cm (100:101)



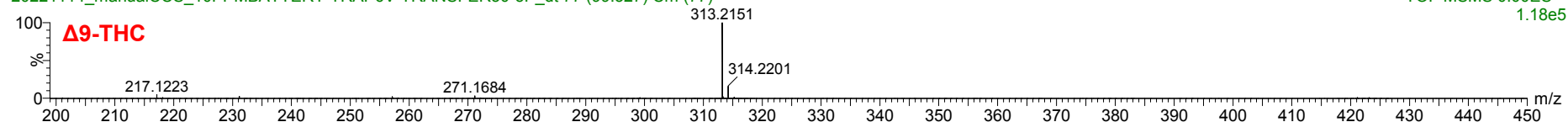
20221114_manualCCS_10PPMBATTERY-TRAP6V-TRANSFER30-5P_dt 96 (105.597) Cm (95:96)



20221114_manualCCS_10PPMBATTERY-TRAP6V-TRANSFER30-5P_dt 86 (102.297) Cm (85:86)



20221114_manualCCS_10PPMBATTERY-TRAP6V-TRANSFER30-5P_dt 77 (99.327) Cm (77)



20221114_manualCCS_10PPMBATTERY-TRAP6V-TRANSFER30-5P_dt 70 (97.017) Cm (69:71)

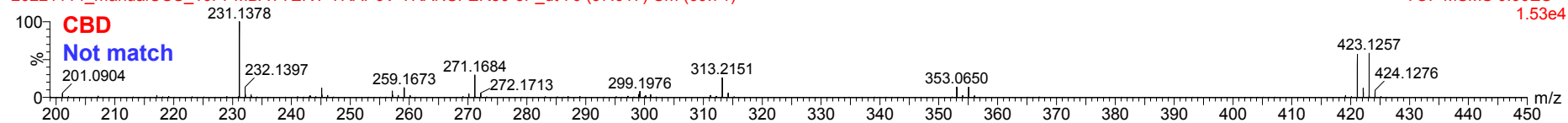


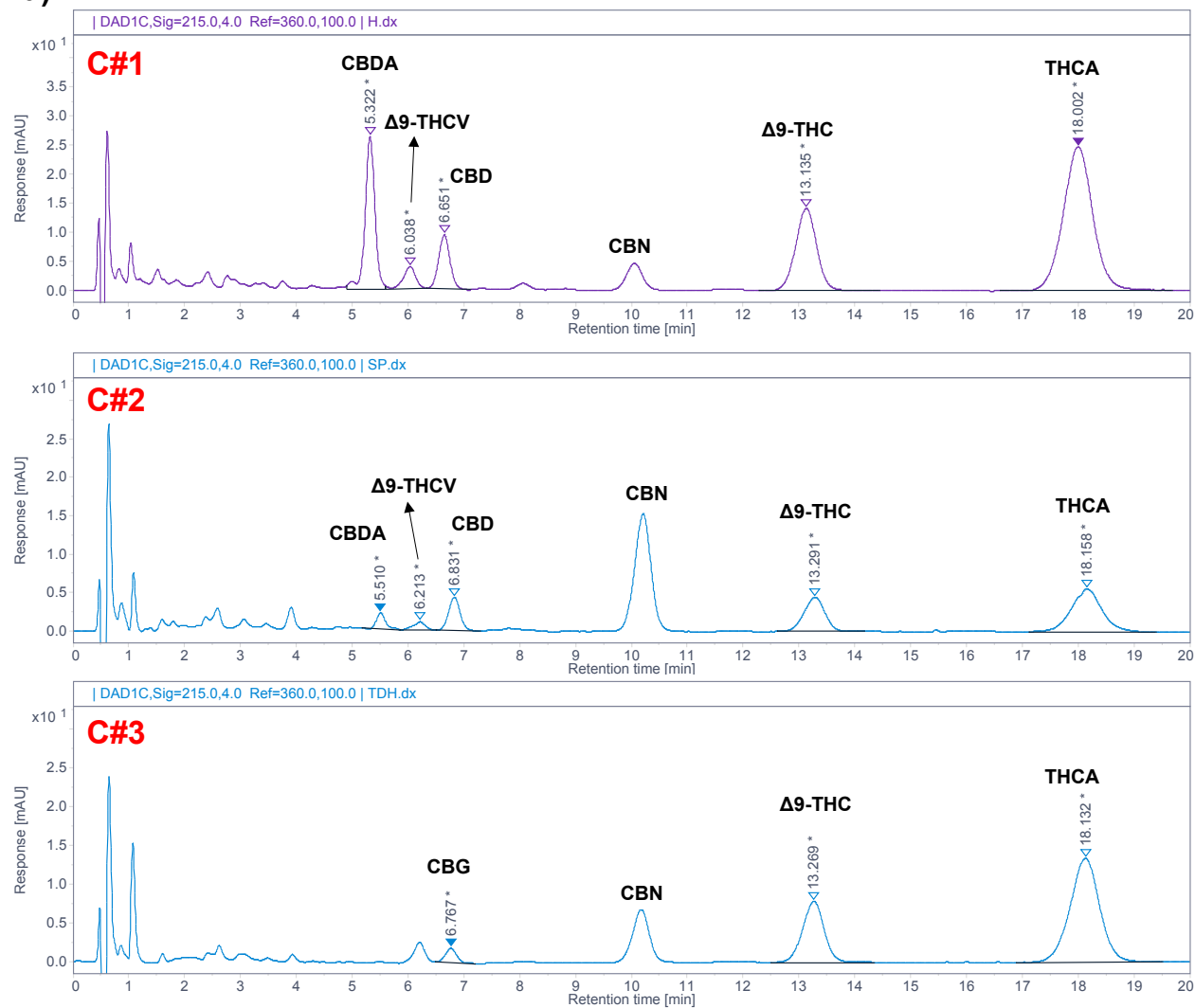
Figure S14-13. Mobiligram and mass spectra of cannabinoids in sample R#8.

Table S7. CCS values of detected cannabinoids in samples.

Sample	$\Delta 8$ -THC	$\Delta 9$ -THC	$\Delta 3$ -THC	CBD	$\Delta 8$ -iso-THC	$\Delta(4)8$ -iso-THC	THCA	CBDa	$\Delta 8$ -THCV and $\Delta 8$ -iso-THCV	$\Delta 9$ -THCV	9 α -hydroxyhexahydrocannabinol	9 β -hydroxyhexahydrocannabinol	8-hydroxy-iso-THC
C#1	/	184.2 $\pm$ 0.01 (0.2%)	/	182.1 $\pm$ 0.01 (0.2%)	/	/	191.6 $\pm$ 0.03 (0.4%)	189.2 $\pm$ 0.01 (0.3%)	/	185.5 (0.3%)	/	/	/
C#2	/	184.4 $\pm$ 0.01 (0.3%)	/	182.3 $\pm$ 0.02 (0.3%)	/	/	192.1 $\pm$ 0.01 (0.6%)	189.7 $\pm$ 0.04 (0.6%)	/	185.1 $\pm$ 0.01 (0.1%)	/	/	/
C#3	/	184.2 $\pm$ 0.02 (0.2%)	/	/	/	/	191.6 $\pm$ 0.02 (0.4%)	/	/	/	/	/	/
G#1	190.3 $\pm$ 0.01 (-0.3%)	184.0 $\pm$ 0.01 (0.05%)	/	/	/	186.5 $\pm$ 0.02 (-0.3%)	/	/	/	/	/	/	/
G#2	190.9 $\pm$ 0.08 (0)	184.4 $\pm$ 0.04 (0.3%)	193.7 $\pm$ 0.04 (0.4%)	/	/	187.1 $\pm$ 0.03 (0)	/	/	/	/	196.0 $\pm$ 0.03 (0.2%)	184.9 $\pm$ 0.04 (-0.5%)	/
R#1	190.2 $\pm$ 0.01 (-0.4%)	184.0 $\pm$ 0.08 (0.05%)	/	181.1 $\pm$ 0.07 (-0.4%)	188.9 $\pm$ 0.1 (-0.3%)	/	NA	NA	NA	NA	NA	NA	NA
R#2	190.9 $\pm$ 0.02 (0)	184.2 $\pm$ 0.01 (0.2%)	/	182.1 $\pm$ 0.02 (0.2%)	188.8* (-0.4%)	/	NA	NA	NA	NA	NA	NA	NA
R#3	190.1 $\pm$ 0.2 (-0.4%)	184.1 $\pm$ 0.09 (0.1%)	/	/	/	186.6 $\pm$ 0.09 (-0.3%)	NA	NA	NA	NA	NA	NA	NA
R#4	190.6 $\pm$ 0.1 (-0.2%)	184.0 $\pm$ 0.01 (0.05%)	/	/	188.5* (-0.5%)	186.7 $\pm$ 0.07 (-0.2%)	NA	NA	NA	NA	NA	NA	NA
R#5	189.6 $\pm$ 0.01 (-0.7%)	184.4 $\pm$ 0.01 (0.3%)	/	182.4 $\pm$ 0.01 (0.3%)	188.6* (-0.5%)	186.9 $\pm$ 0.02 (-0.1%)	NA	NA	NA	NA	NA	NA	NA
R#6	189.7 $\pm$ 0.02 (-0.6%)	184.3 $\pm$ 0.03 (0.2%)	/	182.2 $\pm$ 0.02 (0.2%)	188.2* (-0.7%)	186.9 $\pm$ 0.02 (-0.1%)	NA	NA	NA	N	NA	NA	NA
R#7	/	/	/	182.4 $\pm$ 0.03 (0.3%)	/	/	NA	NA	NA	NA	NA	NA	NA
R#8	189.8 $\pm$ 0.03 (-0.6%)	184.3 $\pm$ 0.03 (0.2%)	/	/	188.6* (-0.5%)	187.0 $\pm$ 0.02 (-0.05%)	NA	NA	NA	NA	NA	NA	NA

Values in brackets represent the relative deviation compared to the CCS values ($^{TW}CCS_{N_2}$ ($\text{\AA}^2$)) from standards; $\pm$ SD (n=3); NA represents “not analyzed”; * represents the drift time decided by characteristic fragment due to the overlap of precursor ions.

a)



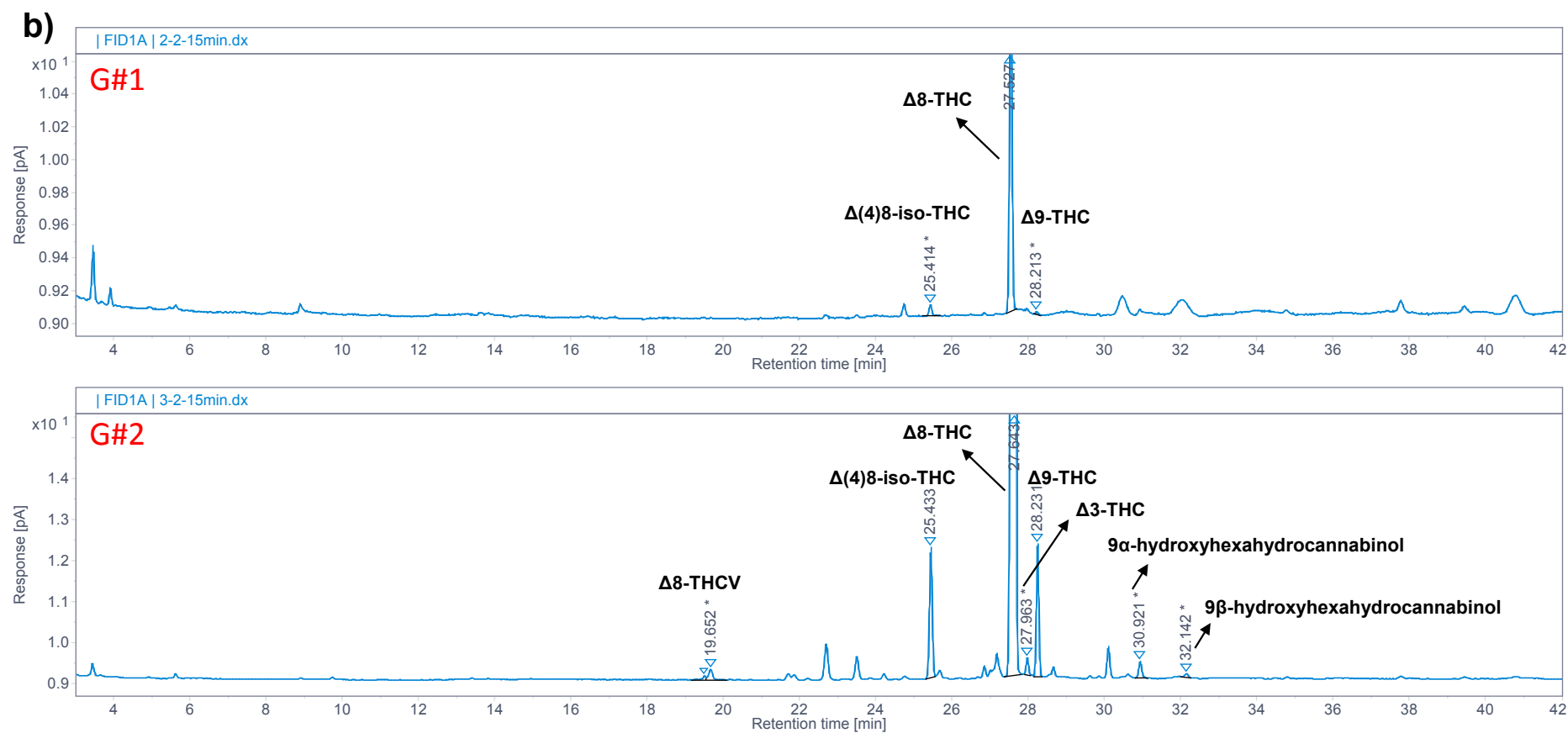


Figure S15. a) Reversed-phase UHPLC-UV (215 nm) profile of samples C#1, C#2, and C#3; b) GC-FID profile of samples G#1 and G#2.

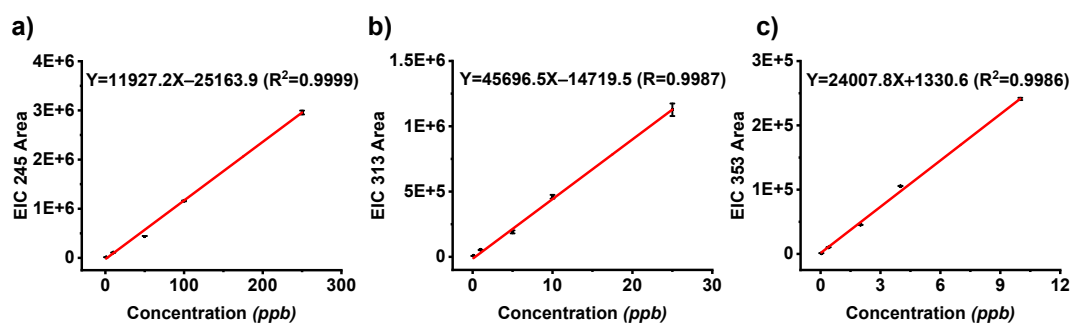


Figure S16. Calibration curves between the extracted ion chromatogram peak area of characteristic fragments and concentrations of a) $\Delta 8$ -THC, b) $\Delta 9$ -THC, and c) CBD. Error bars represent the standard deviation (n=3).

Table S8. Absolute weight percentages (w/w%, after solvent evaporation) of $\Delta 8$ -THC, $\Delta 9$ -THC, and CBD in acid-treated CBD mixtures by cIMS and GC-FID.

Sample	$\Delta 8$ -THC			$\Delta 9$ -THC			CBD		
	GC-FID	cIMS	Deviation	GC-FID	cIMS	Deviation	GC-FID	cIMS	Deviation
R#1	11 (2.6%)	15 (0.4%)	36%	49 (0.3%)	70 (0.4%)	43%	26 (2.0%)	36 (0.2%)	39%
R#2	26 (4.0%)	30 (3.2%)	15%	48 (0.1%)	61 (3.2%)	27%	6.9 (0.4%)	6.6 (3.1%)	-4%
R#3	78 (2.1%)	115 (0.9%)	47%	1.6 (1.1%)	2.4 (0.3%)	50%	ND ^[b]	ND ^[b]	/
R#4	70 (1.8%)	96 (1.3%)	37%	1.1 (5.6%)	2.9 (1.1%)	164%	ND ^[b]	ND ^[b]	/
R#5	14 (3.7%)	23 (1.1%)	64%	6.3 (5.2%)	11 (0.9%)	75%	ND	0.6 (2.2%)	/
R#6	8.1 (0.5%)	13 (0.7%)	61%	8.9 (1.2%)	14 (1.2%)	57%	4.2 (0.2%)	1.2 (1.8%)	-71%
R#7	ND	ND	/	ND	ND	/	48 (0.7%)	59 (0.5%)	23%
R#8	1.4 (1.1%)	3.1 (1.3%)	121%	5.0 (2.5%)	6.7 (1.0%)	34%	ND	ND	/

All values are average of triplicate experiments; ND: Not detected (<LOD).

Table S9. Ratio of $\Delta 9$ -THC/ $\Delta 8$ -THC in acid-treated CBD mixtures analyzed by cIMS and GC-FID.

Sample	$\Delta 8$ -THC		$\Delta 9$ -THC		$\Delta 9$ -THC/ $\Delta 8$ -THC ratio	
	GC-FID	cIMS	GC-FID	cIMS	GC-FID	cIMS
R #1	11 (2.6%)	15 (0.4%)	49 (0.3%)	70 (0.4%)	4.5	4.7
R #2	26 (4.0%)	30 (3.2%)	48 (0.1%)	61 (3.2%)	1.8	2.0
R #3	78 (2.1%)	115 (0.9%)	1.6 (1.1%)	2.4 (0.3%)	0.02	0.02
R #4	70 (1.8%)	96 (1.3%)	1.1 (5.6%)	2.9 (1.1%)	0.02	0.03
R #5	14 (3.7%)	23 (1.1%)	6.3 (5.2%)	11 (0.9%)	0.45	0.48
R #6	8.1 (0.5%)	13 (0.7%)	8.9 (1.2%)	14 (1.2%)	1.1	1.1
R #7	ND	ND	ND	ND	/	/
R #8	1.4 (1.1%)	3.1 (1.3%)	5.0 (2.5%)	6.7 (1.0%)	3.6	2.2

All values are average of triplicate experiments; ND: Not detected (<LOD).

Table S10. Comparison of LODs between the cIMS method and GC-FID method¹

	cIMS	GC-FID
Injection volume	5 μL	1 μL
split ratios	NA	Split ratio for injector 1:10, split ratio for detector 1:1.
LOD expressed as concentration	0.2 $\text{ng}\cdot\text{ml}^{-1}$ for $\Delta 8$ -THC, 0.04 $\text{ng}\cdot\text{ml}^{-1}$ for $\Delta 9$ -THC, and 0.008 $\text{ng}\cdot\text{ml}^{-1}$ for CBD.	0.3 $\mu\text{g}\cdot\text{ml}^{-1}$ for $\Delta 8$ -THC, 0.3 $\mu\text{g}\cdot\text{ml}^{-1}$ for $\Delta 9$ -THC, and 1.3 $\mu\text{g}\cdot\text{ml}^{-1}$ for CBD.
LOD expressed as absolute mass	1 pg for $\Delta 8$ -THC, 0.2 pg for $\Delta 9$ - THC, and 0.04 pg for CBD.	15 pg for $\Delta 8$ -THC, 15 pg for $\Delta 9$ - THC, and 65 pg for CBD.

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