

Supplementary file

Chemical Characterisation, Antidiabetic, Antibacterial, and In silico Studies for Different Extracts of *Haloxylon stocksii* (Boiss.) Benth: A Promising Halophyte

Syed Nabil Raza Rizvi ¹, Samina Afzal ^{1,*}, Kashif-ur-Rehman Khan ^{2,*}, Hanan Y. Aati ³, Huma Rao ², Bilal Ahmad Ghalloo ^{2,4}, Muhammad Nadeem Shahzad ², Duraiz Ahmed Khan ², Tuba Esatbeyoglu ^{5,*} and Sameh A. Korma ^{6,7}

¹ Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Bahauddin Zakariya University, Multan 60000, Pakistan

² Department of Pharmaceutical Chemistry, Faculty of Pharmacy, The Islamia University of Bahawalpur, Bahawalpur 63100, Pakistan;

³ Department of Pharmacognosy, College of Pharmacy, King Saud University, Riyadh 11495, Saudi Arabia

⁴ Department of Medicinal Chemistry, College of Pharmacy, University of Minnesota, Minneapolis, MN 55454, USA

⁵ Department of Food Development and Food Quality, Institute of Food Science and Human Nutrition, Gottfried Wilhelm Leibniz University Hannover, Am Kleinen Felde 30, 30167 Hannover, Germany

⁶ Department of Food Science, Faculty of Agriculture, Zagazig University, Zagazig 44519, Egypt

⁷ School of Food Science and Engineering, South China University of Technology, Guangzhou 510641, China

* Correspondence: samina.afzal@bzu.edu.pk (S.A.); esatbeyoglu@lw.uni-hannover.de (T.E.)

Table S1: Safety Profile of LC-MS identified compound

Compound Name	Toxicity profile
N-Methyltyramine	LD ₅₀ = 780 mg/kg (Intraperitoneal) LD ₅₀ = 275 mg/kg (Intravenous)
Acetophenone	Safe, Hypnosis occur at 0.4 to 0.5 g/kg (Intravenous)
Hordenine	Harmful if swallowed, skin sensitization
Fraxetin	NA
6,8-dihydroxy-7-methoxy-3-methyl-1H-isochromen-1-one	NA
Nor-3-methylfentanyl	NA
Moupinamide	Very toxic to aquatic life
2-(2,6-dimethoxyphenyl)-5,6-dimethoxy-4H-chromen-4-one	NA
Piperine	LD ₅₀ = 34 mg/kg (Rats, Intraperitoneal) LD ₅₀ = 71 mg/kg (Mice, Intravenous)
Tris(2-butoxyethyl) phosphate	No skin sensitization
Acetyl tributyl citrate	No skin sensitization
Hexadecanamide	May cause irritation
1-Palmitoylglycerol	May cause irritation
(1S)-Tricyclo[7.3.1.0~2,7~]tridec-2(7)-en-13-one	NA
Stearamide	Cough and redness to the skin
Erucamide	Myocardial granulomas, necrosis, and lesions
N,N-Dimethyllaniline	LD ₅₀ = 50 mg/kg (Oral)

"NA" No toxicity data is available in <https://pubchem.ncbi.nlm.nih.gov/> database.

Table S2: α -amylase inhibition and α -glucosidase inhibition of *Haloxylon stocksii*

Sample Name	α -amylase inhibition	α -glucosidase inhibition
AMHS	65.78±3.19 ^b	59.91±4.16 ^b
ADHS	42.64±1.62 ^d	38.03±2.25 ^d
RMHS	58.82±2.92 ^c	53.41±5.64 ^c
RDHS	44.47±1.22 ^d	32.50±0.85 ^e
Acarbose	79.58±4.28 ^a	74.27±6.66 ^a

"AMHS" aerial parts methanolic *H. stocksii* extract, "ADHS" Aerial parts dichloromethane *H. stocksii* extract, "RMHS" roots methanolic *H. stocksii* extract, and "RDHS" roots dichloromethane *H. stocksii* extract; the superscripts a, b, c, d, and e represent significant difference ($p<0.05$)

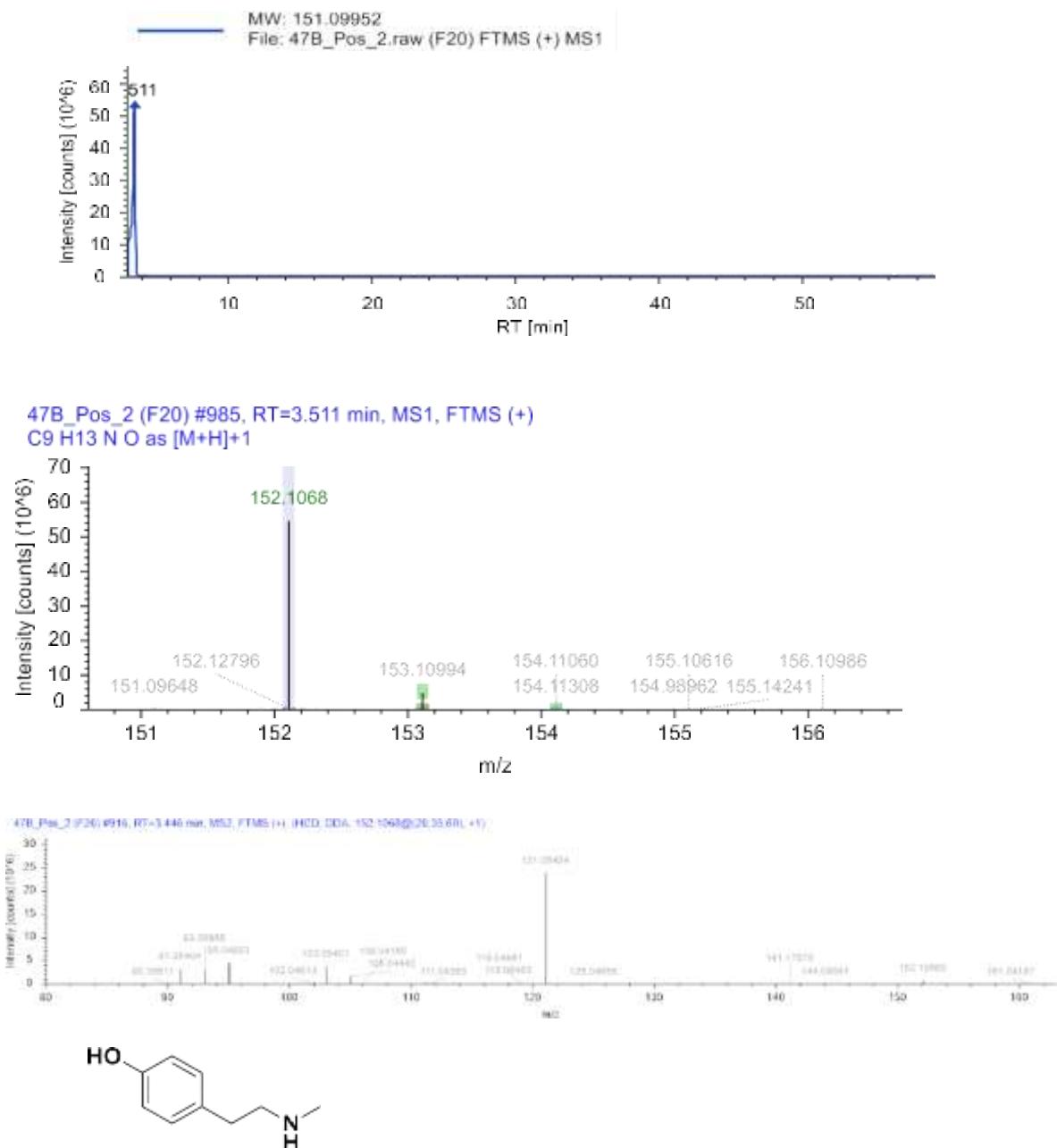


Figure S1: Retention time peak, fragmentation pattern and chemical structure of N-Methyltyramine

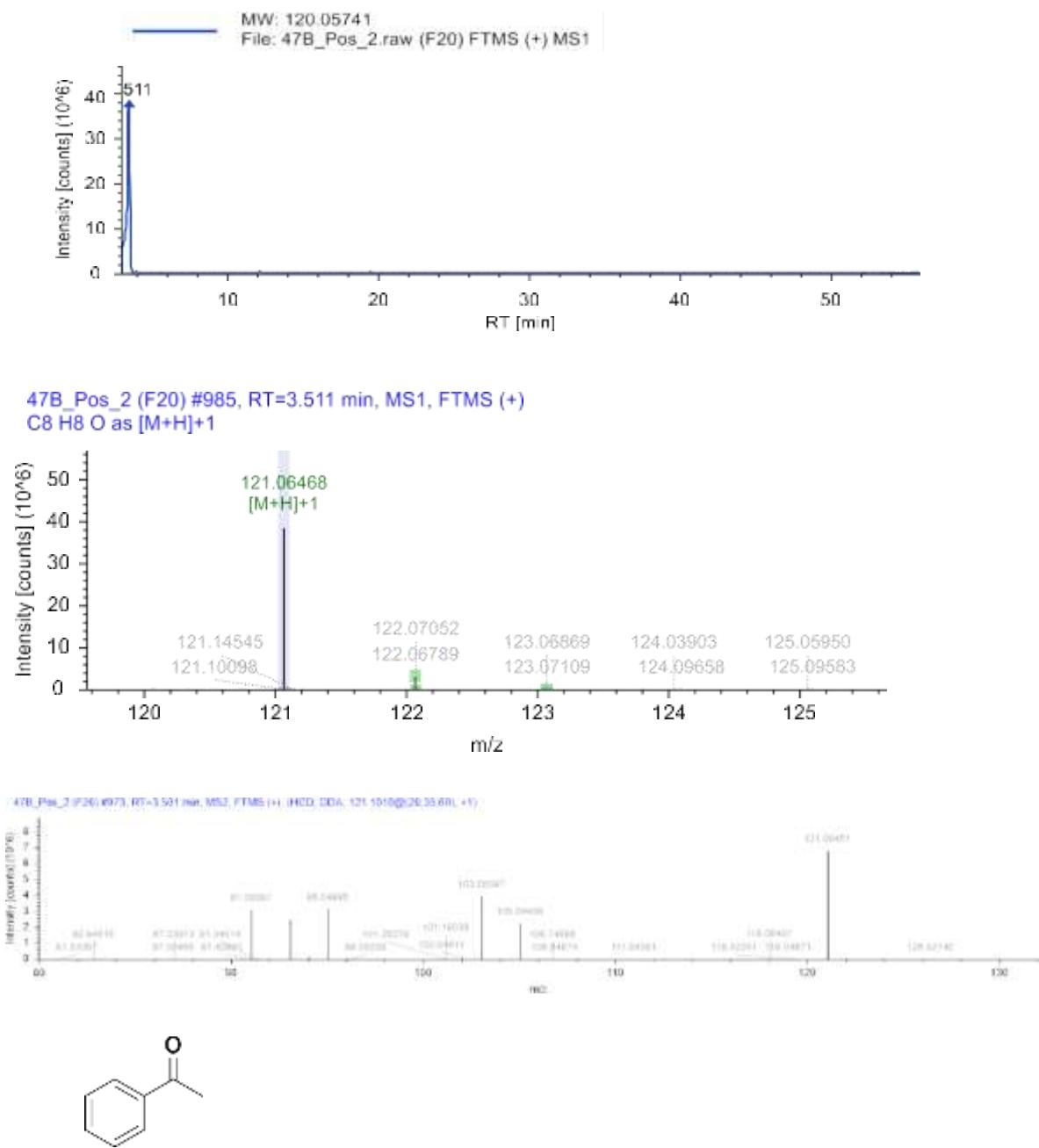


Figure S2: Retention time peak, fragmentation pattern and chemical structure of Acetophenone

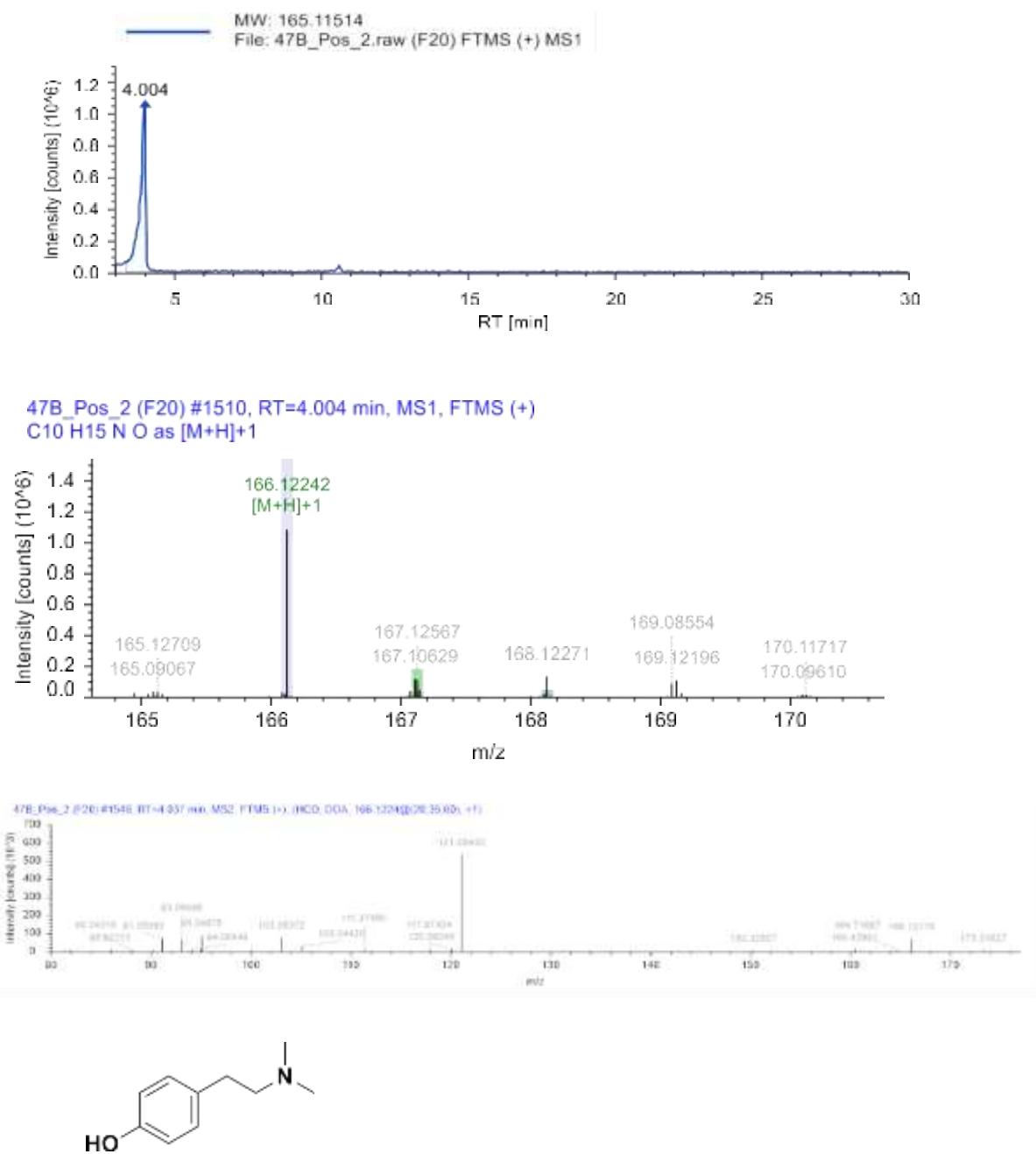


Figure S3: Retention time peak, fragmentation pattern and chemical structure of Hordenine

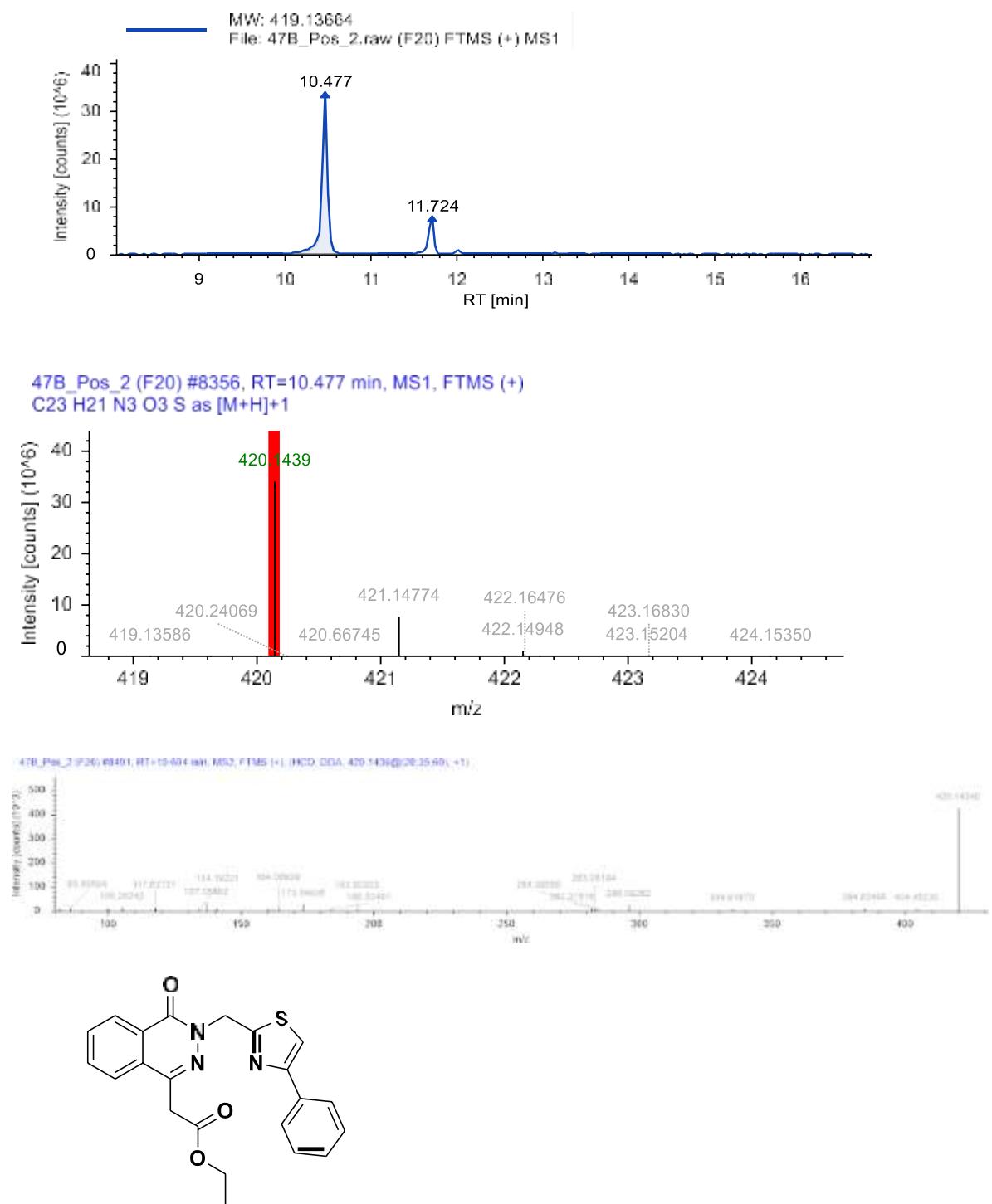


Figure S4: Retention time peak, fragmentation pattern and chemical structure of Ethyl 2-(3-[(4-methylphenyl)-1,3-thiazol-2-yl]methyl]-4-oxo-3,4-dihydrophthalazin-1-yl)acetate

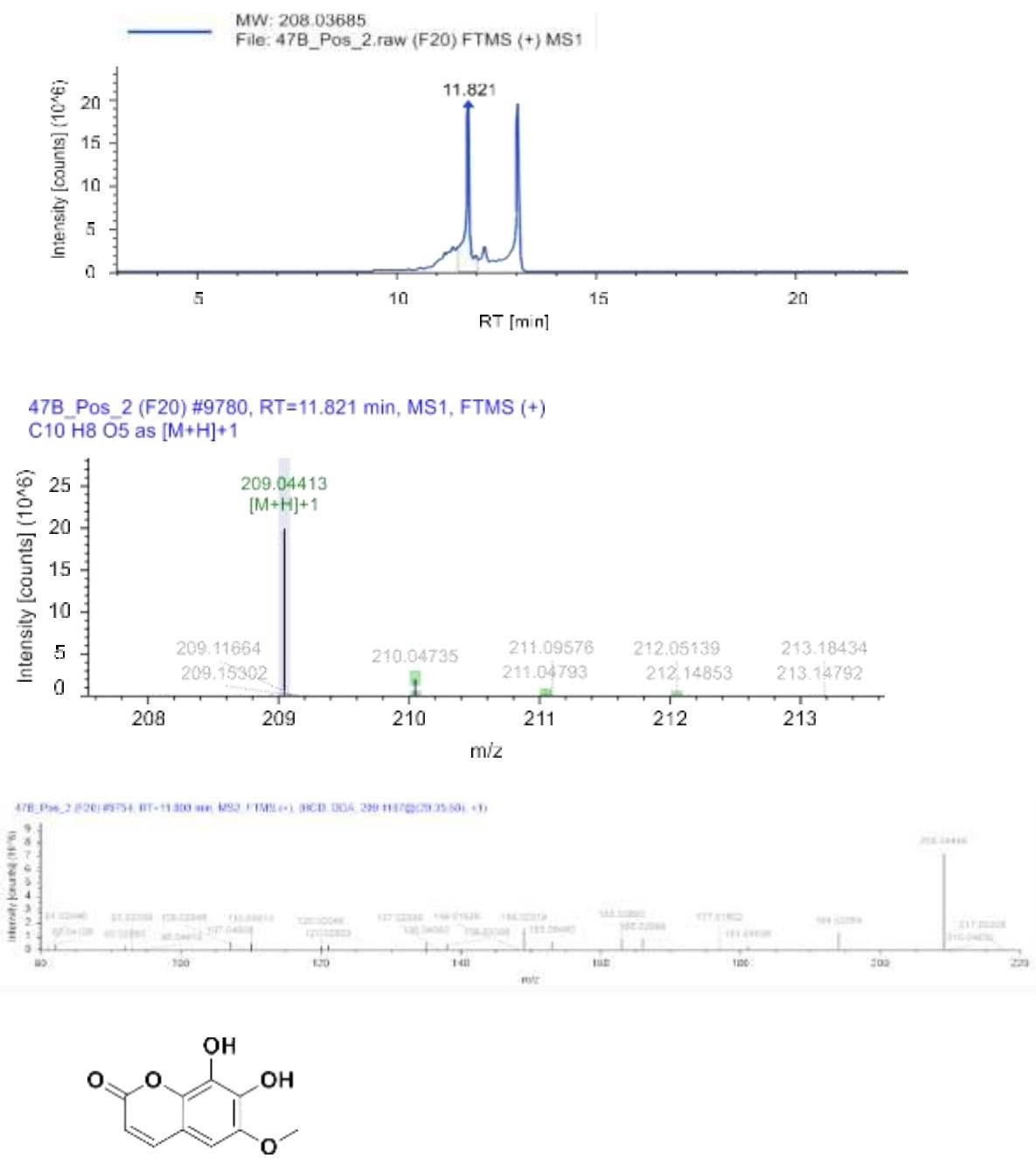
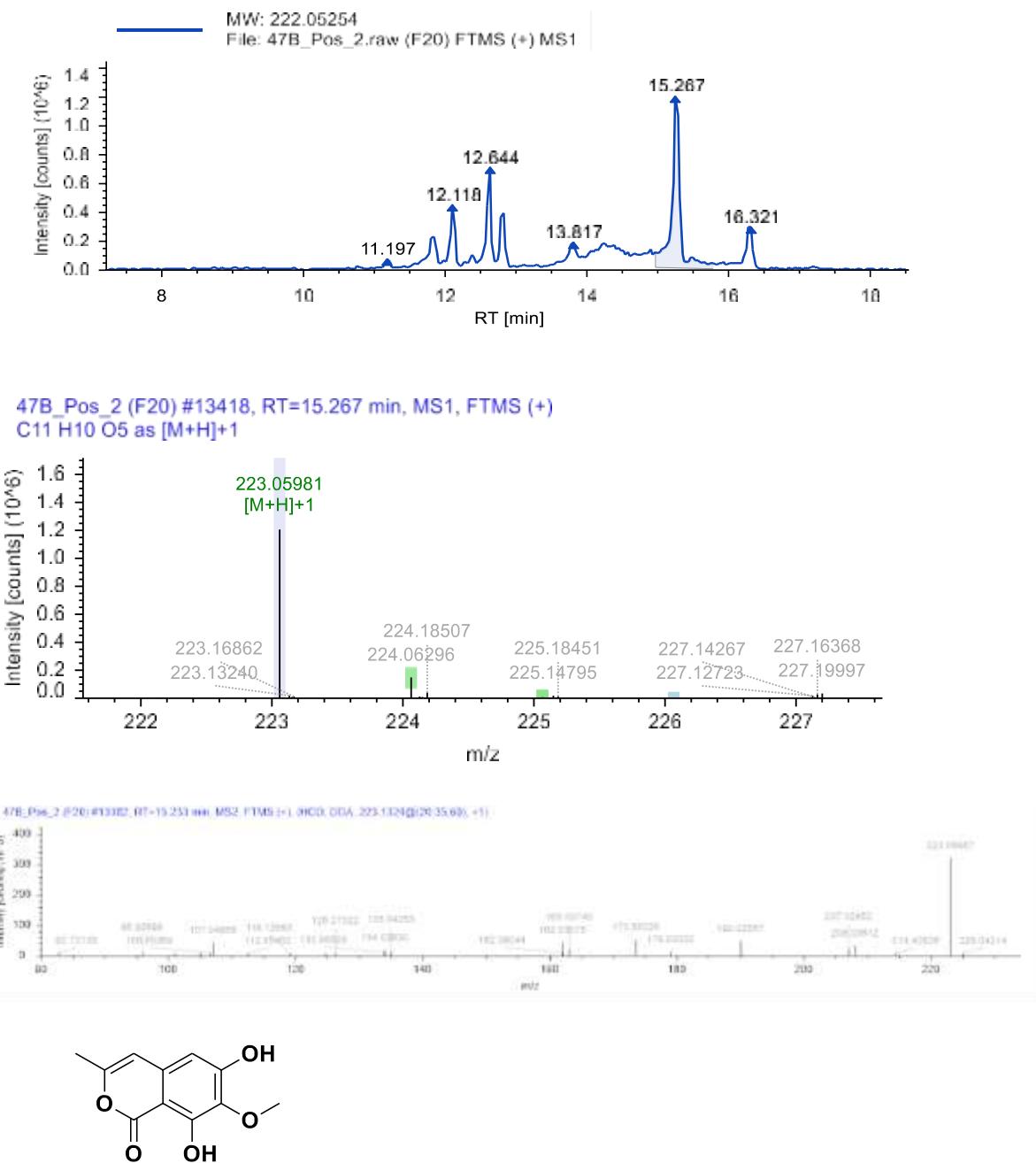


Figure S5: Retention time peak, fragmentation pattern and chemical structure of Fraxetin



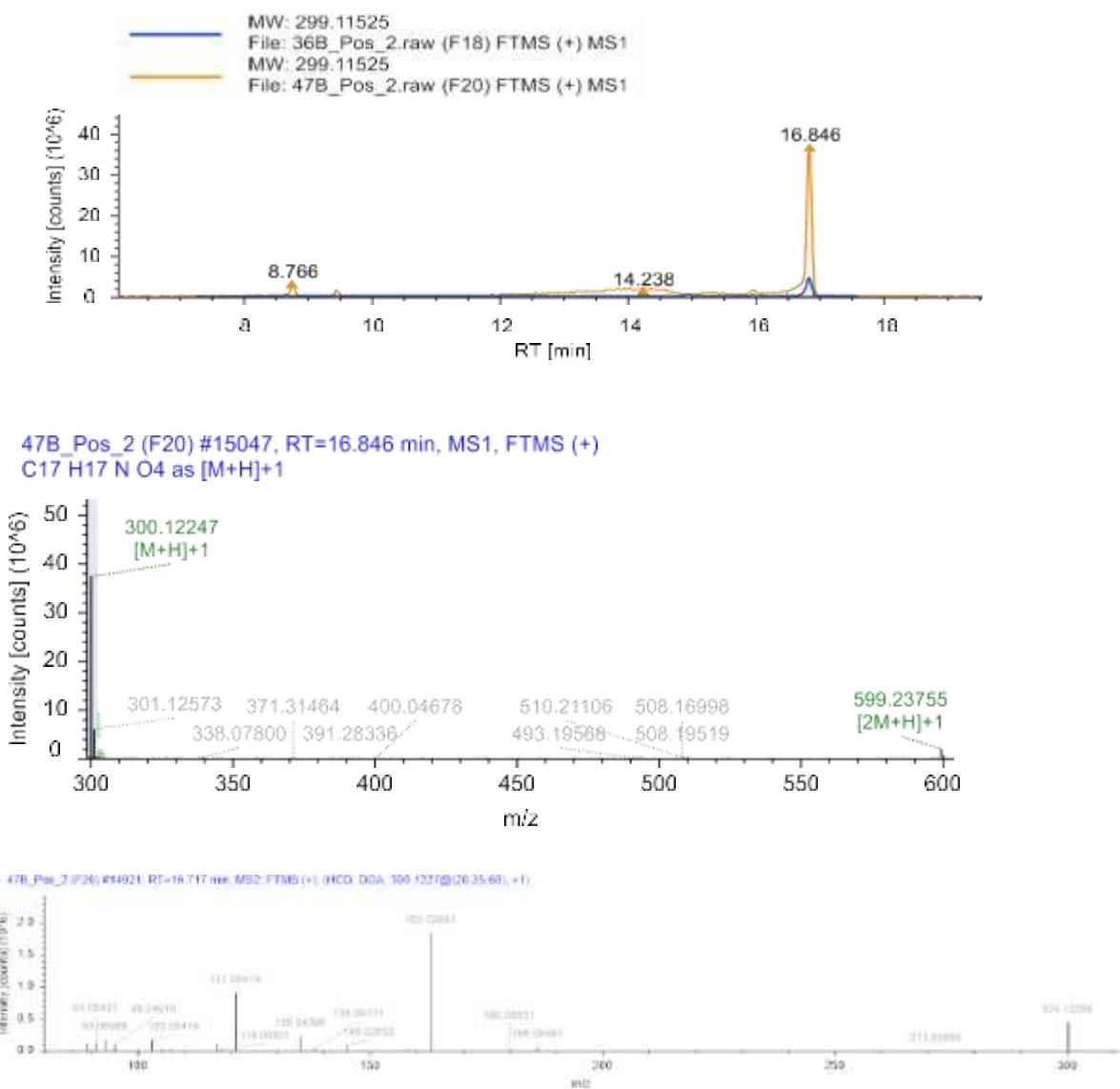
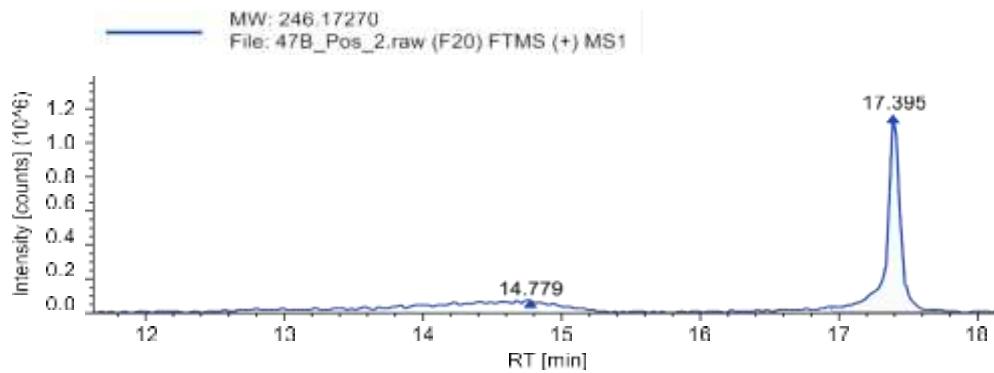
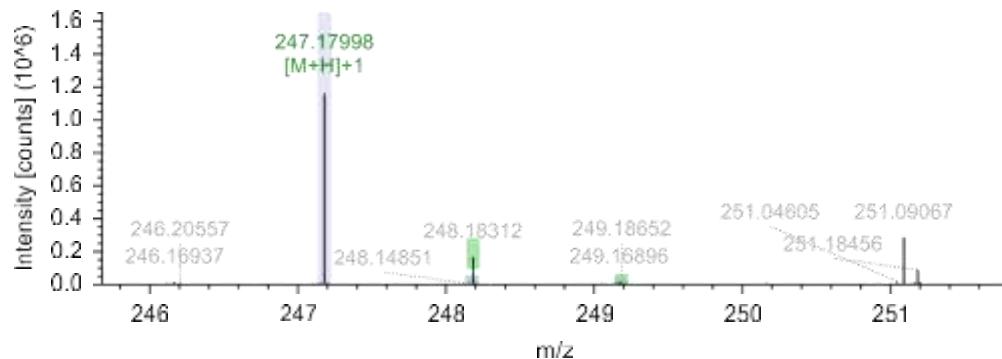


Figure S7: Retention time peak, and fragmentation pattern of Unknown compound (not identified with library)



47B_Pos_2 (F20) #15609, RT=17.395 min, MS1, FTMS (+)
C15 H22 N2 O as [M+H]+1



47B_Pos_2 (F20) #15550, RT=17.348 min, MS2, FTMS (+) (HCD, DDA, 247.17998(20.35.60), +1)

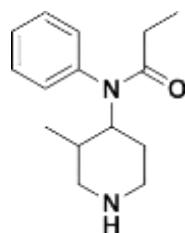
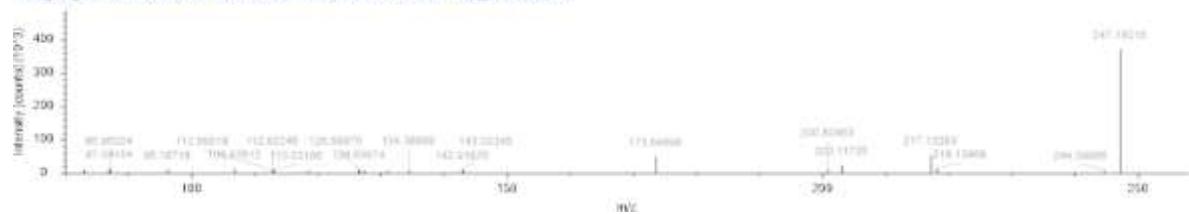
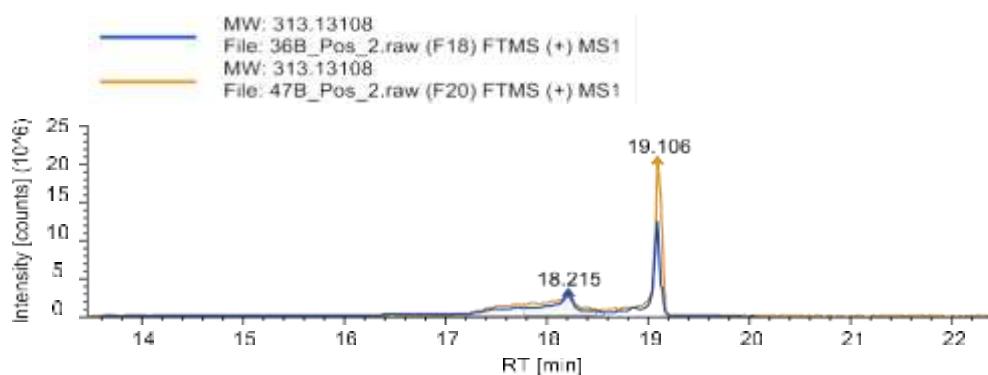
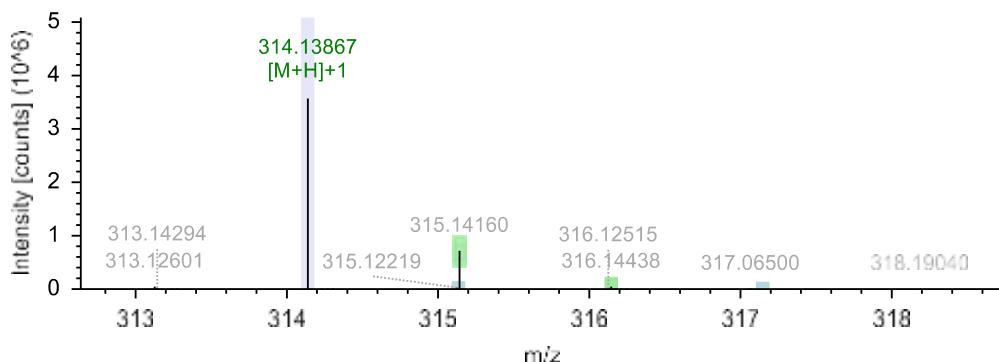


Figure S8: Retention time peak, fragmentation pattern and chemical structure of nor -3-methylfentanyl



36B_Pos_2 (F18) #16497, RT=18.215 min, MS1, FTMS (+)
C18 H19 N O4 as [M+H]+1



36B_Pos_2 (F18) #16497, RT=18.215 min, MS2, FTMS (+), (HCD; DDA, 314.13867(20:35.60), +1)

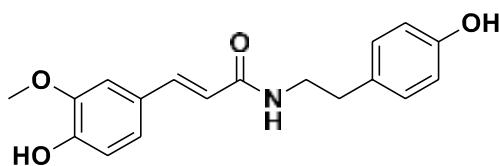
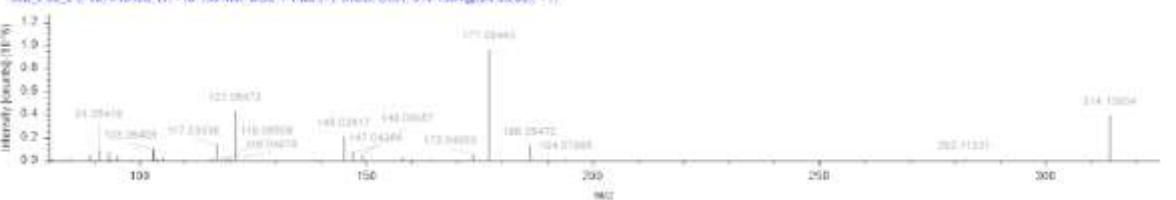
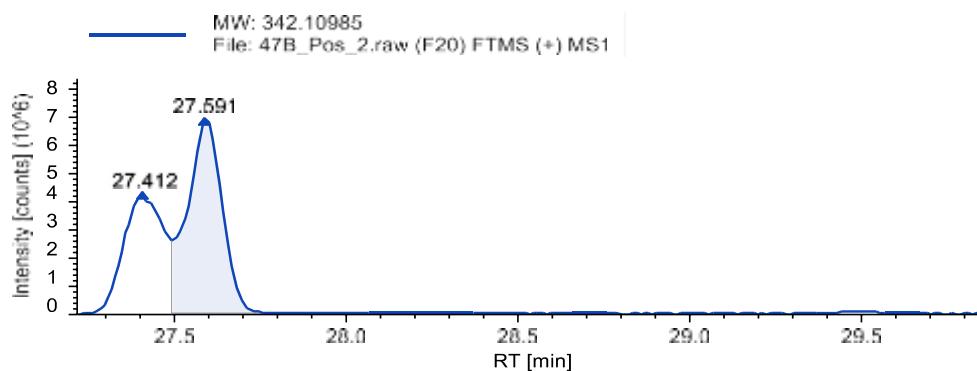
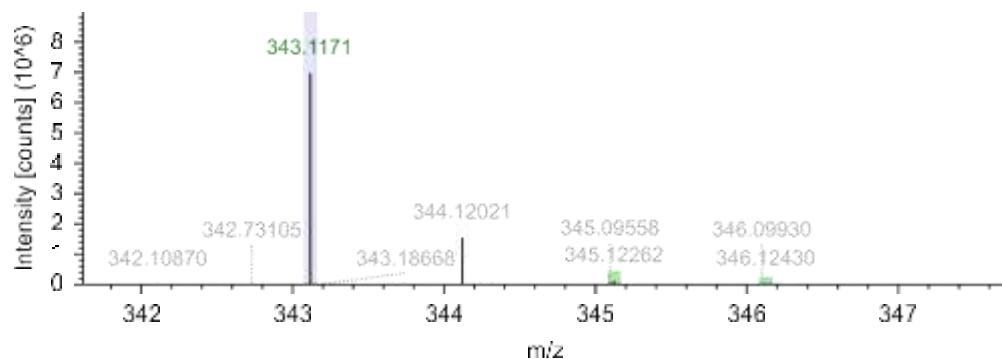


Figure S9: Retention time peak, fragmentation pattern and chemical structure of Moupinamide



47B_Pos_2 (F20) #25041, RT=27.591 min, MS1, FTMS (+)
C19 H18 O6 as [M+H]+1



47B_Pos_2 (F20) #25041, RT=27.633 min, MS2, FTMS (+), (HCD; DDA, 343.1171@0.05:60, +1)

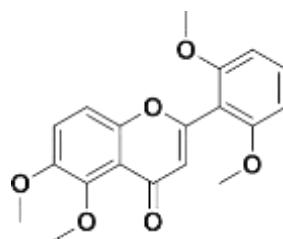
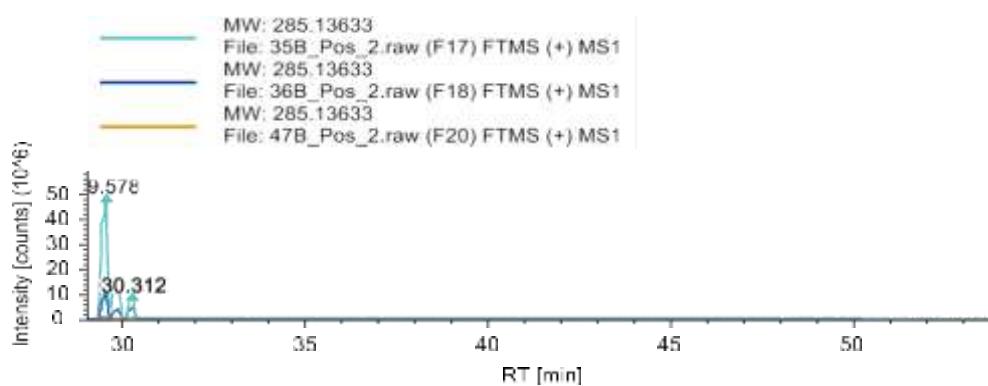
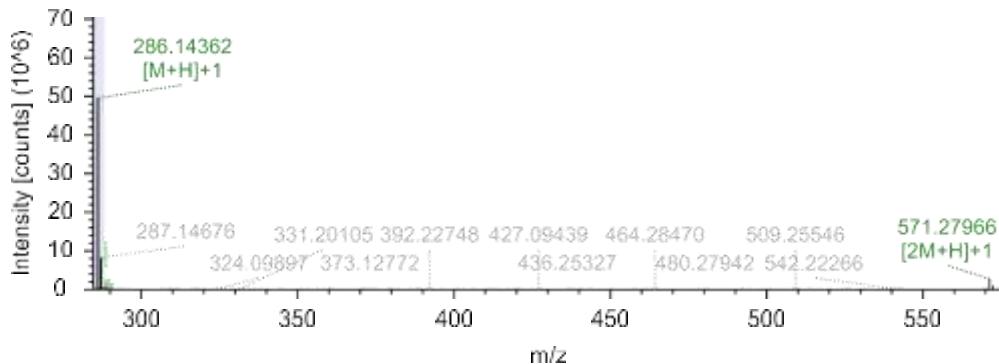


Figure S10: Retention time peak, fragmentation pattern and chemical structure of 2-(2,6-dimethoxyphenyl)-5,6-dimethoxy-4H-chromen-4-one



35B_Pos_2 (F17) #27362, RT=29.578 min, MS1, FTMS (+)
C₁₇H₁₉N O₃ as [M+H]₊₁



36B_Pos_2 (F18) #27408, RT=29.623 min, MS2, FTMS (+), (ICD: DDA, /286.1437@29.35.60, +1)

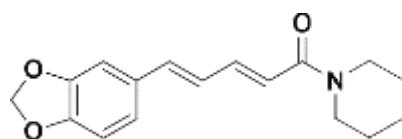
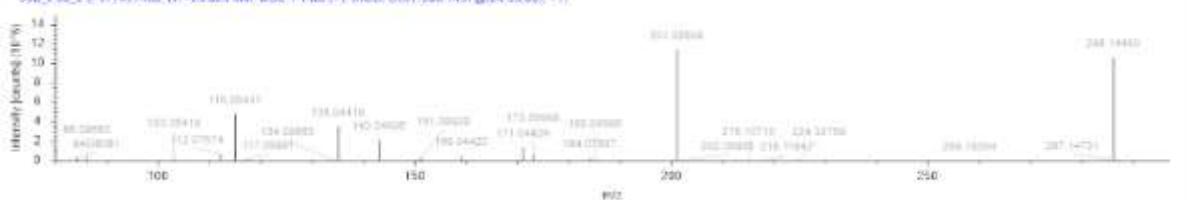
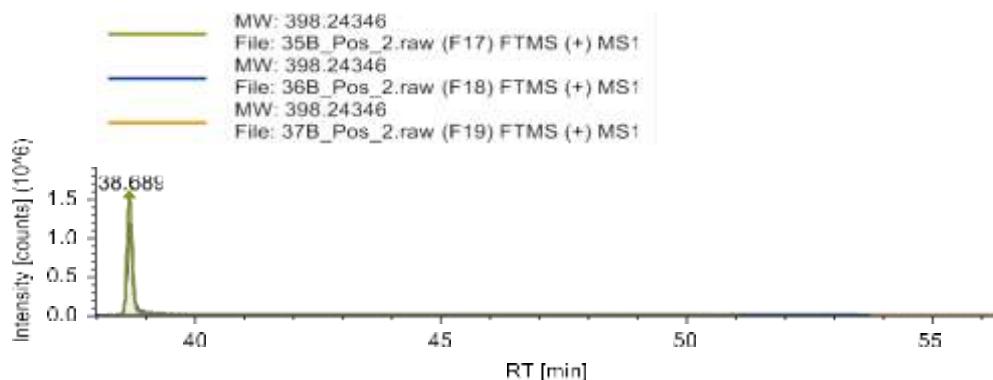
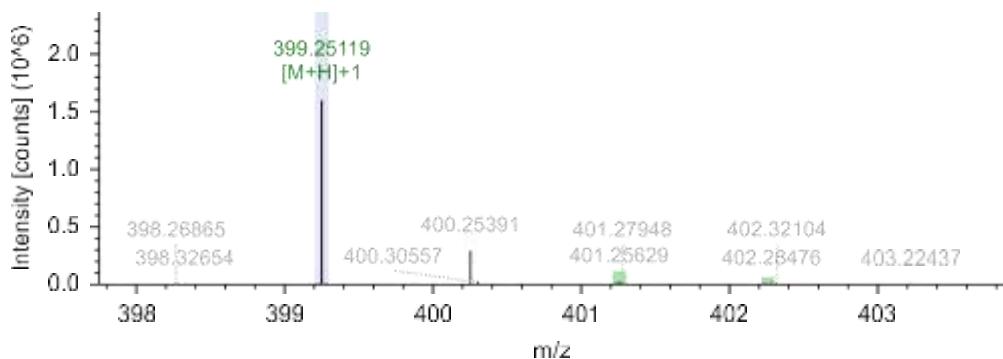


Figure S11: Retention time peak, fragmentation pattern and chemical structure of Piperine



35B_Pos_2 (F17) #35878, RT=38.689 min, MS1, FTMS (+)
C18 H39 O7 P as [M+H]+1



35B_Pos_2 (F17) #35878, RT=38.689 min, MS2, FTMS (+) (HCD, DDA, 399.25119@20.35.60), +1

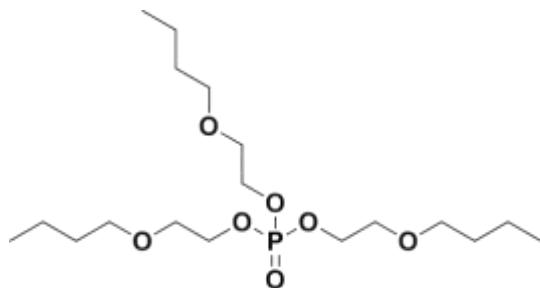
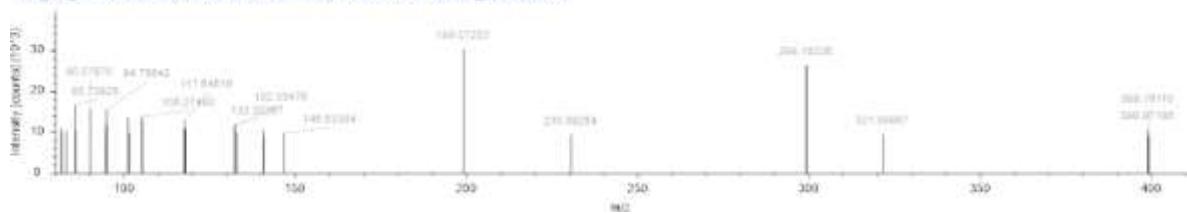
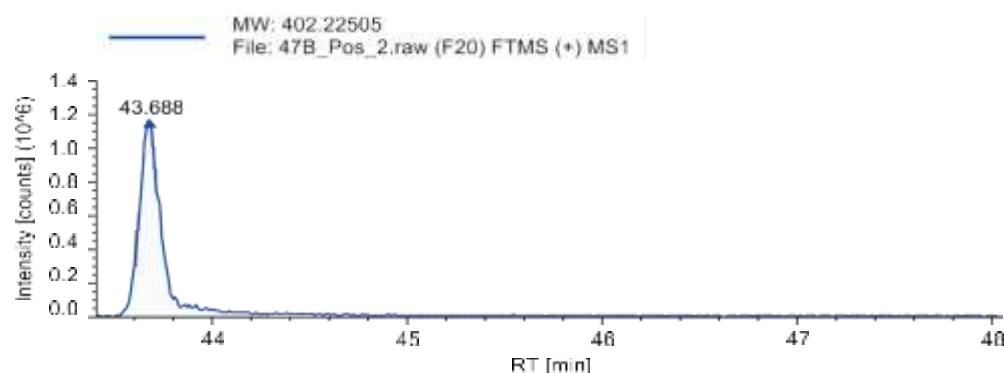


Figure S12: Retention time peak, fragmentation pattern and chemical structure of tris(2-Butoxyethyl) phosphate



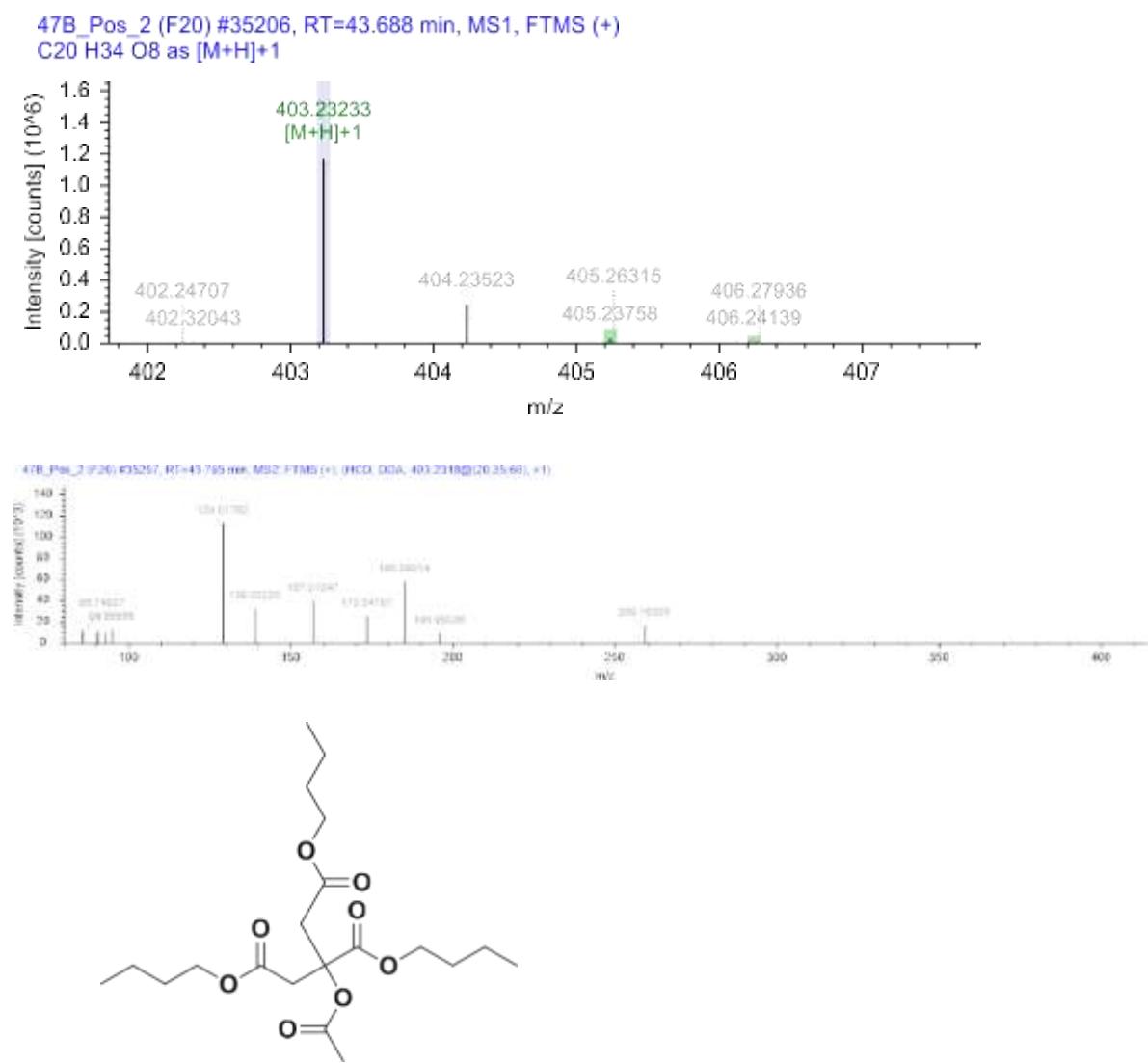
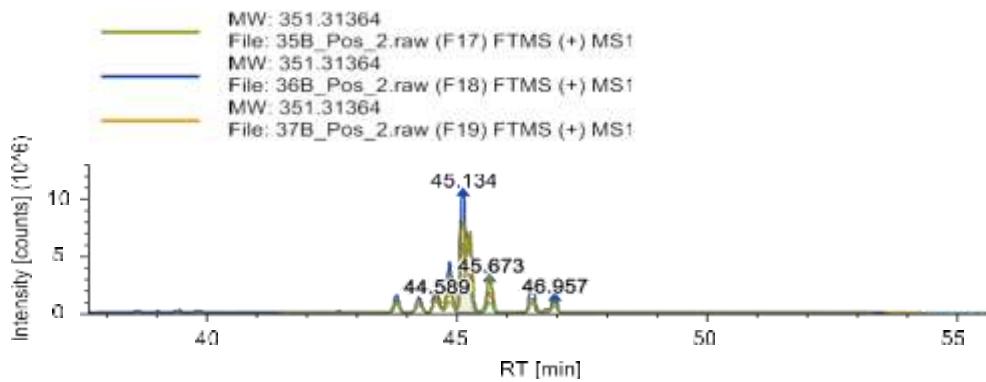


Figure S13: Retention time peak, fragmentation pattern and chemical structure of Acetyl tributyl citrate



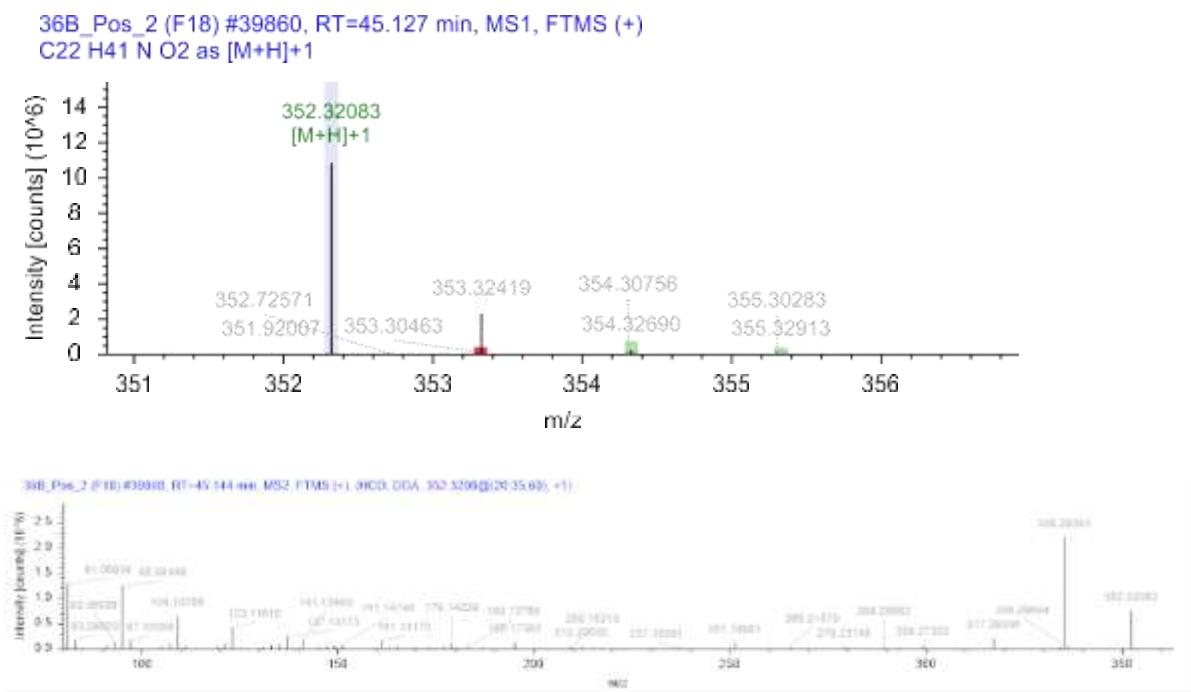
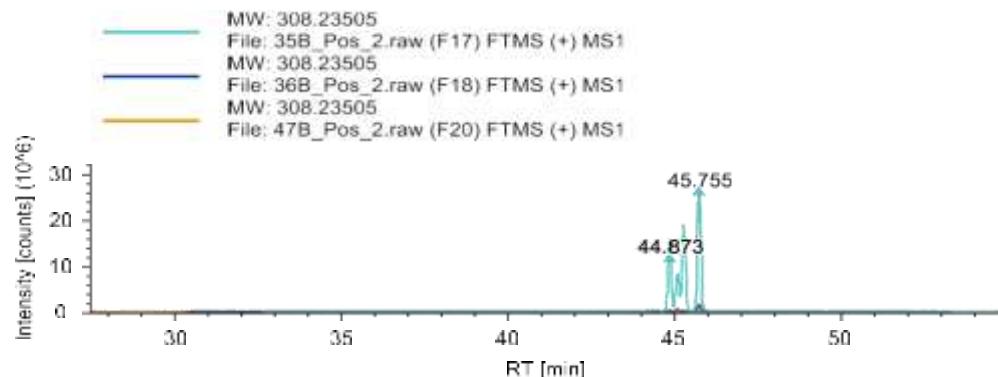
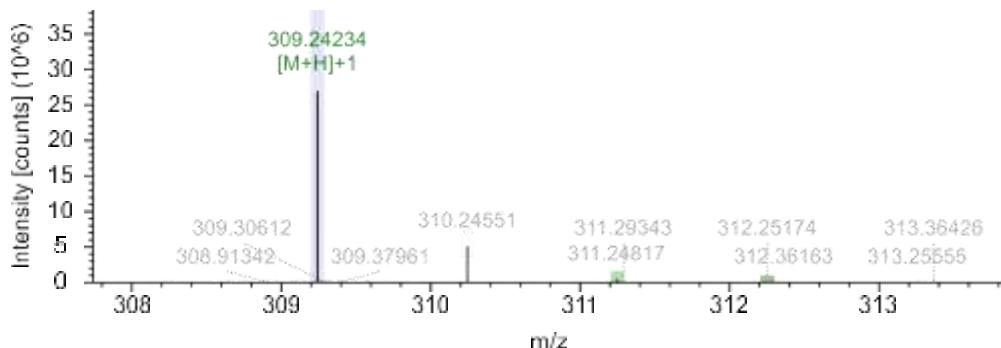


Figure S14: Retention time peak, and fragmentation pattern of Unknown compound (not identified with library)



35B_Pos_2 (F17) #42153, RT=45.755 min, MS1, FTMS (+)
C19 H32 O3 as [M+H]⁺



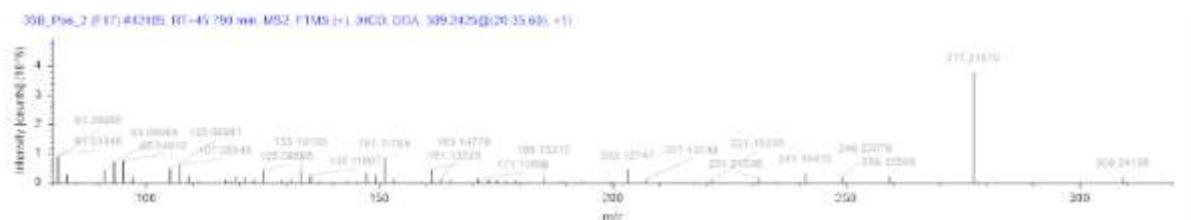
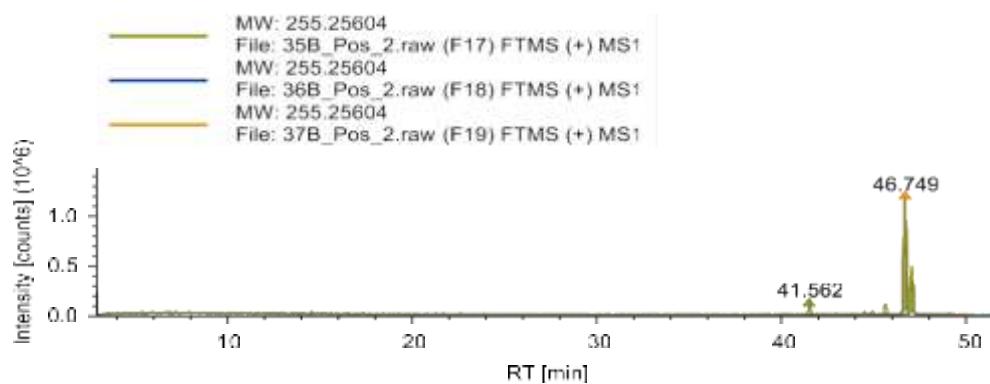
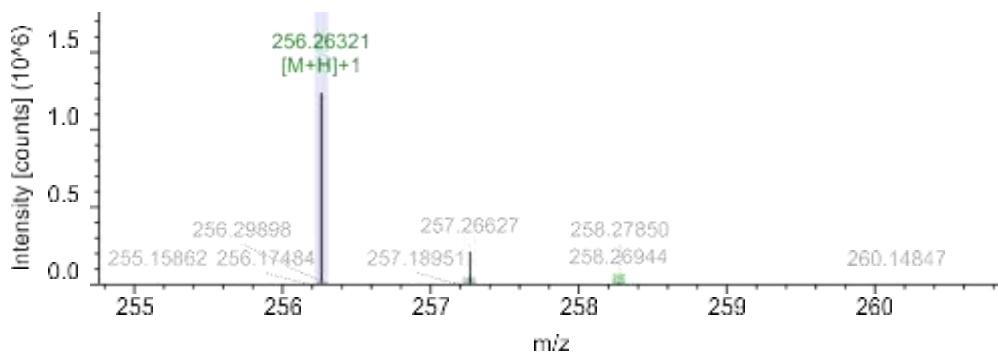


Figure S15: Retention time peak, and fragmentation pattern of Unknown compound (not identified with library)



37B_Pos_2 (F19) #39144, RT=46.749 min, MS1, FTMS (+)
C16 H33 N O as [M+H]⁺1



378_PeakList.mzML; RT=46.750 min; MS2_FTMS (+); FID; DDA; 256.26330(20.35.68); +1

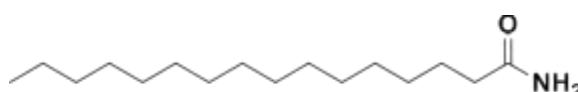
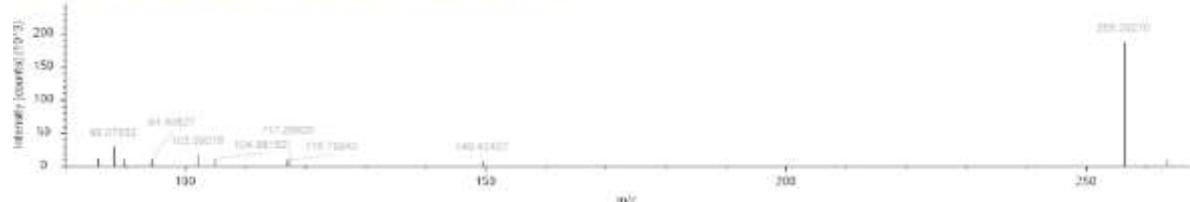


Figure S16: Retention time peak, fragmentation pattern and chemical structure of Hexadecanamide

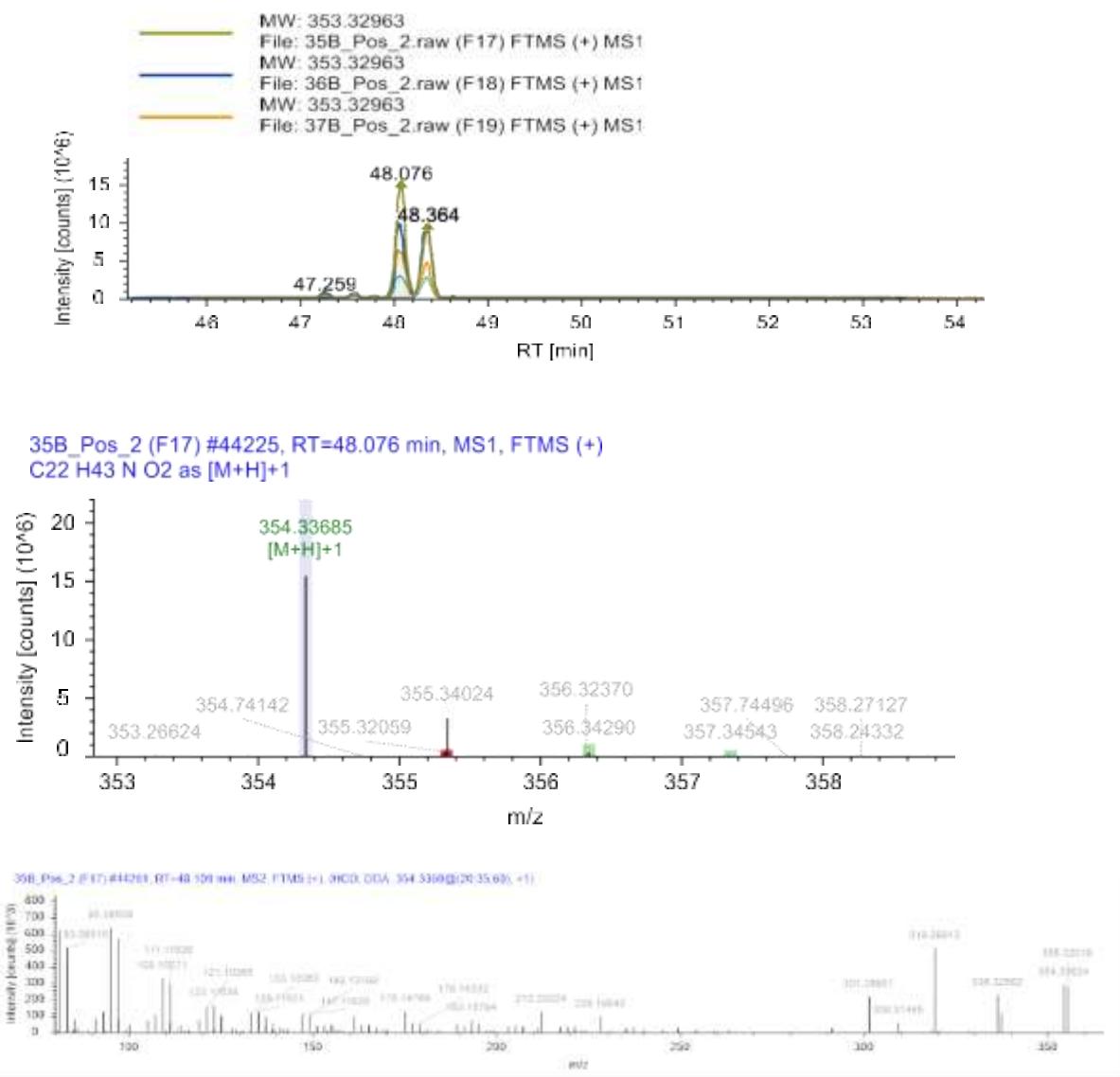
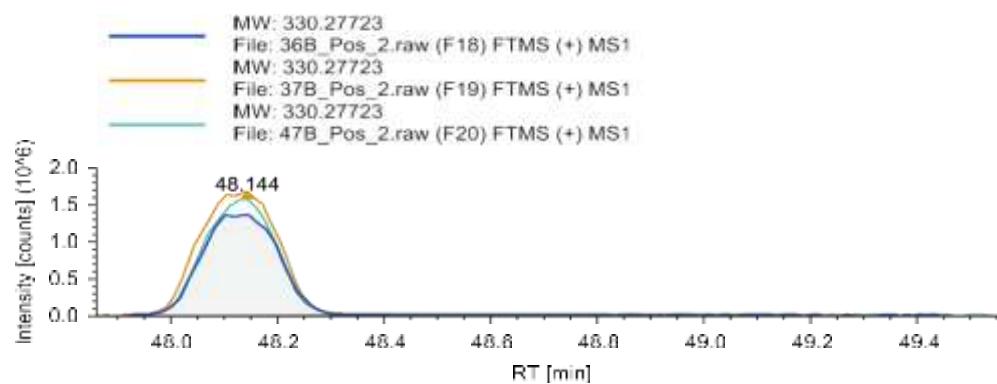


Figure S17: Retention time peak, fragmentation pattern and chemical structure of Unknown compound (not identified with library)



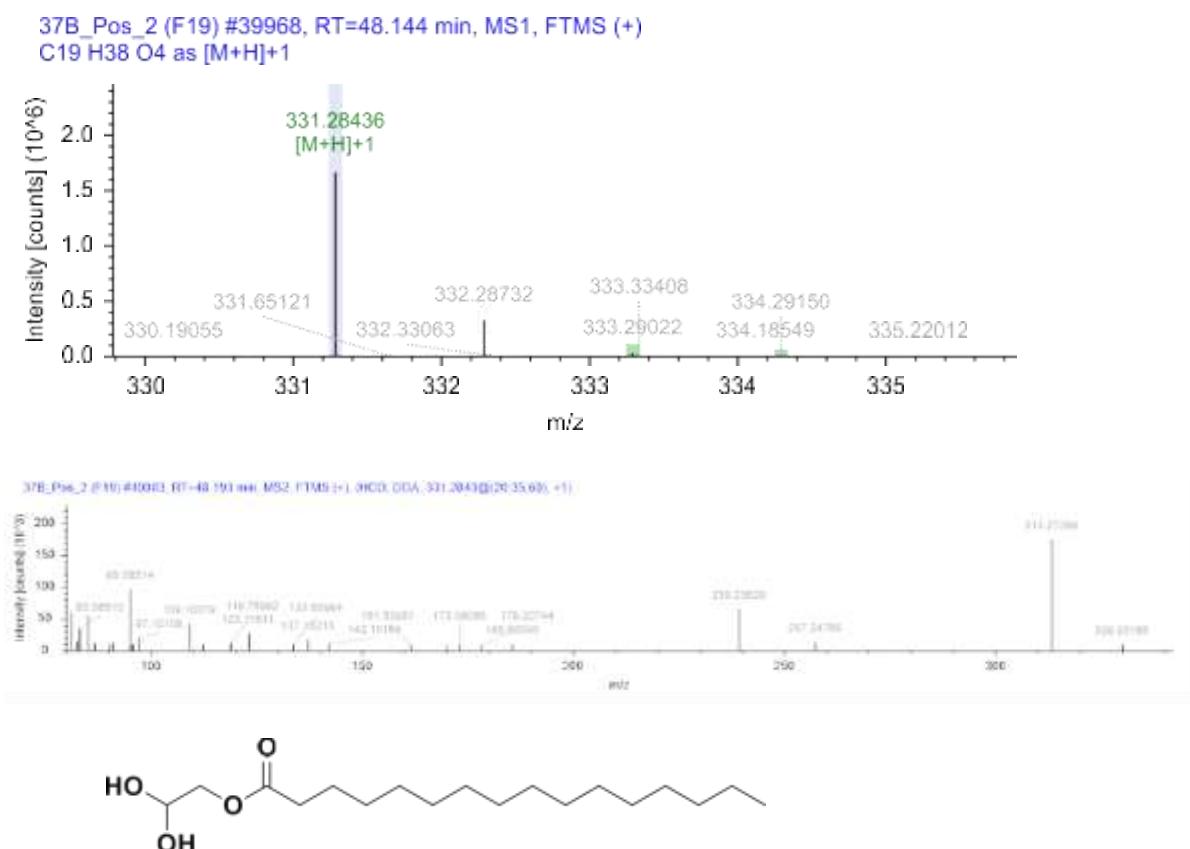
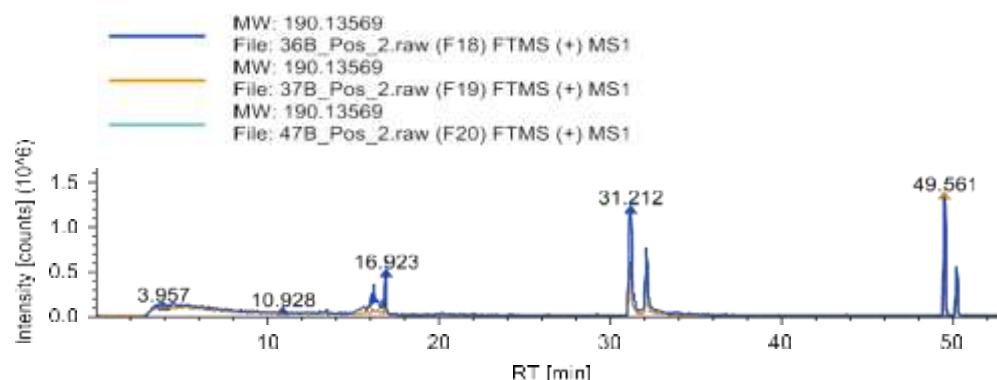
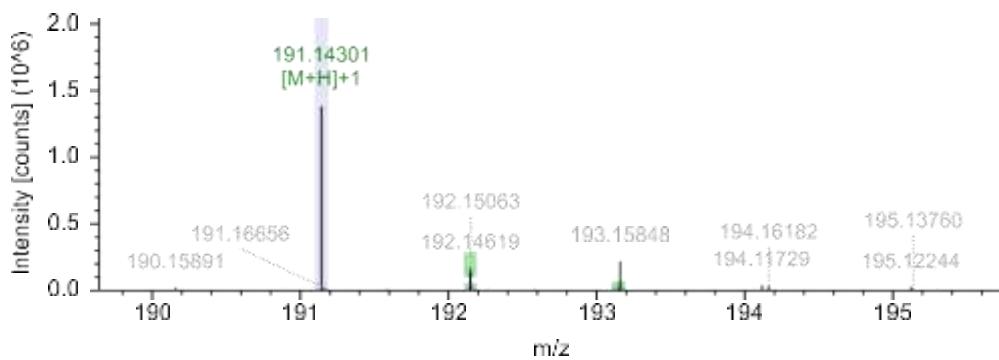


Figure S18: Retention time peak, fragmentation pattern and chemical structure of 1-Palmitoylglycerol



37B_Pos_2 (F19) #40884, RT=49.561 min, MS1, FTMS (+)
C13 H18 O as [M+H]⁺1



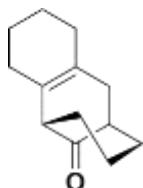
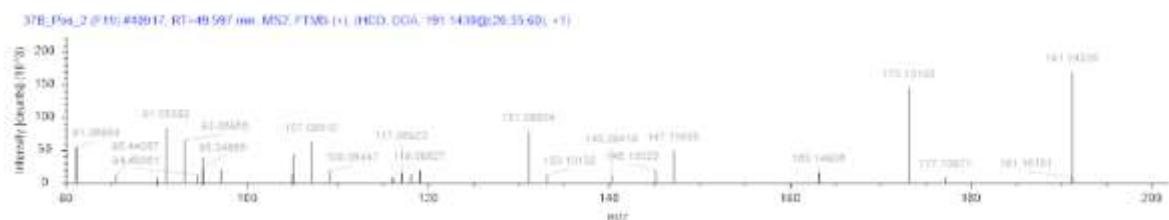
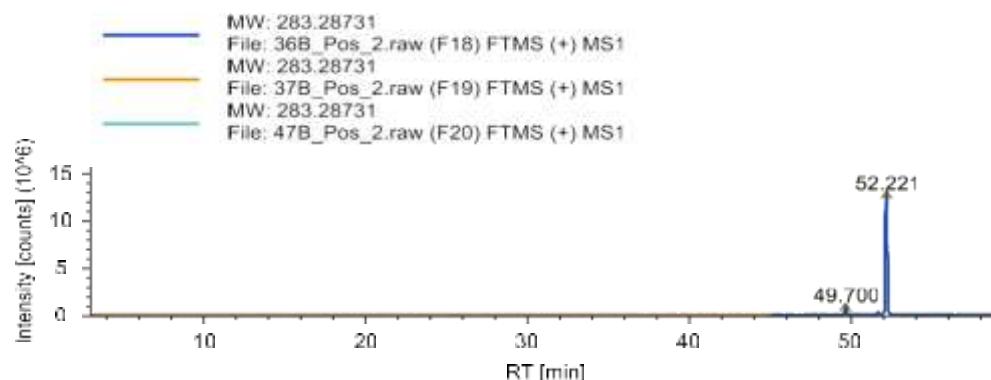
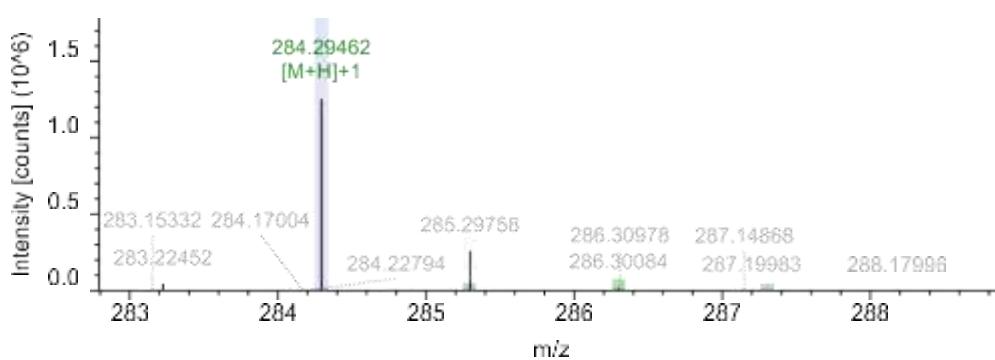


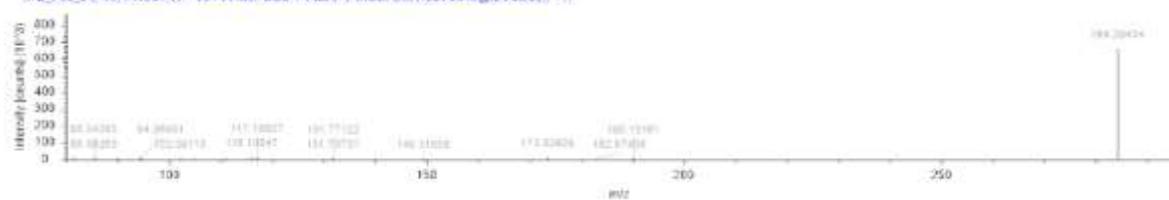
Figure S19: Retention time peak, fragmentation pattern and chemical structure of (1S)-Tricyclo[7.3.1.0~2,7~]tridec-2(7)-en-13-one



37B_Pos_2 (F19) #41008, RT=49.700 min, MS1, FTMS (+)
C18 H37 N O as [M+H]⁺¹



37B_Pos_2 (@ M) #41008, RT=49.741 min, MS2, FTMS (+), (HCD, DDA, 284.2946@26.35.60, +1)



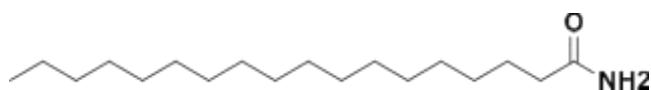
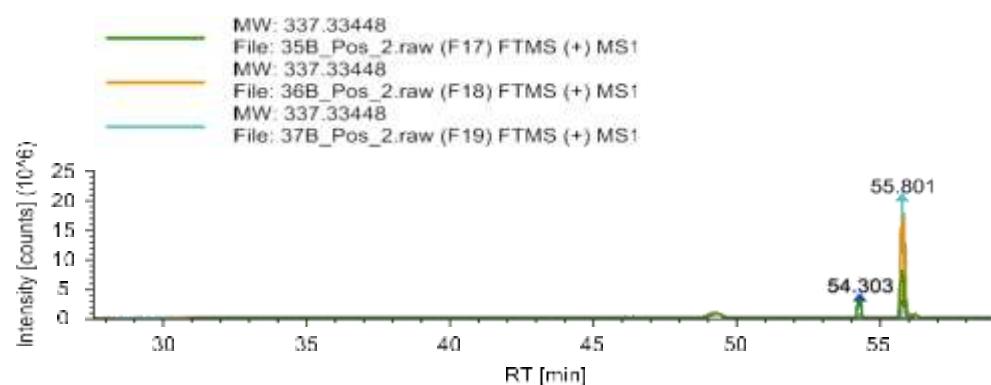


Figure S20: Retention time peak, fragmentation pattern and chemical structure of Stearamide



37B_Pos_2 (F19) #44952, RT=55.801 min, MS1, FTMS (+)
C₂₂H₄₃N O as $[\text{M}+\text{H}]^+$

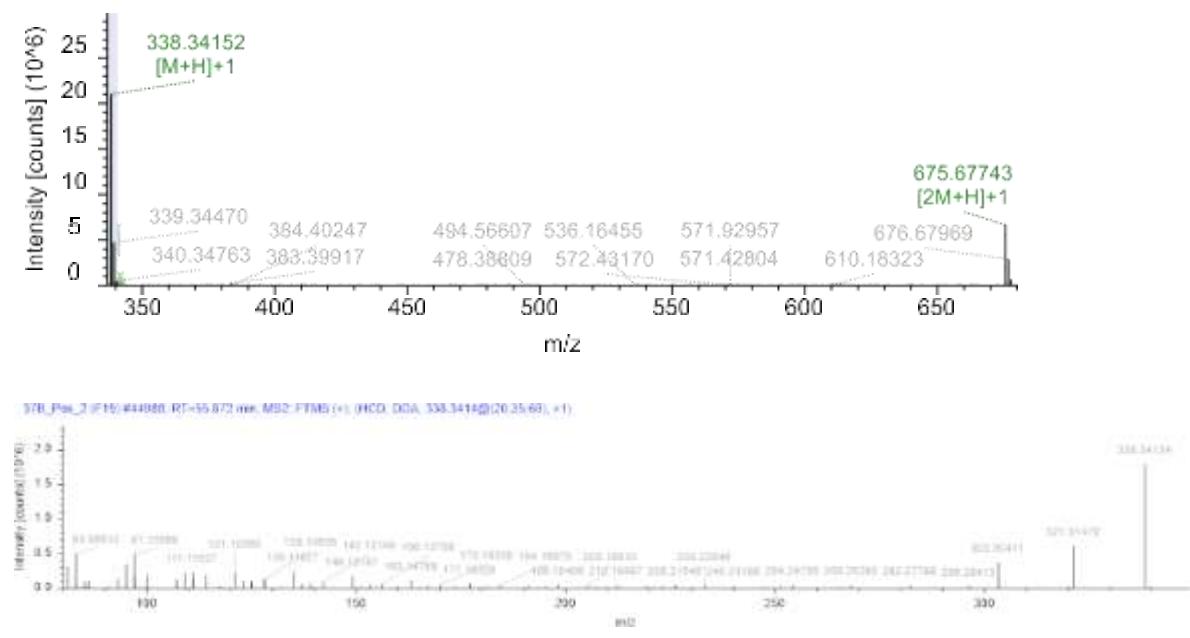
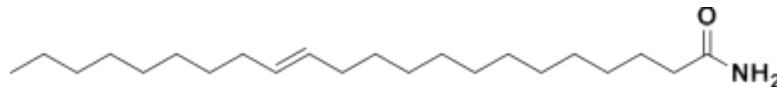


Figure S21: Retention time peak, fragmentation pattern and chemical structure of Erucamide



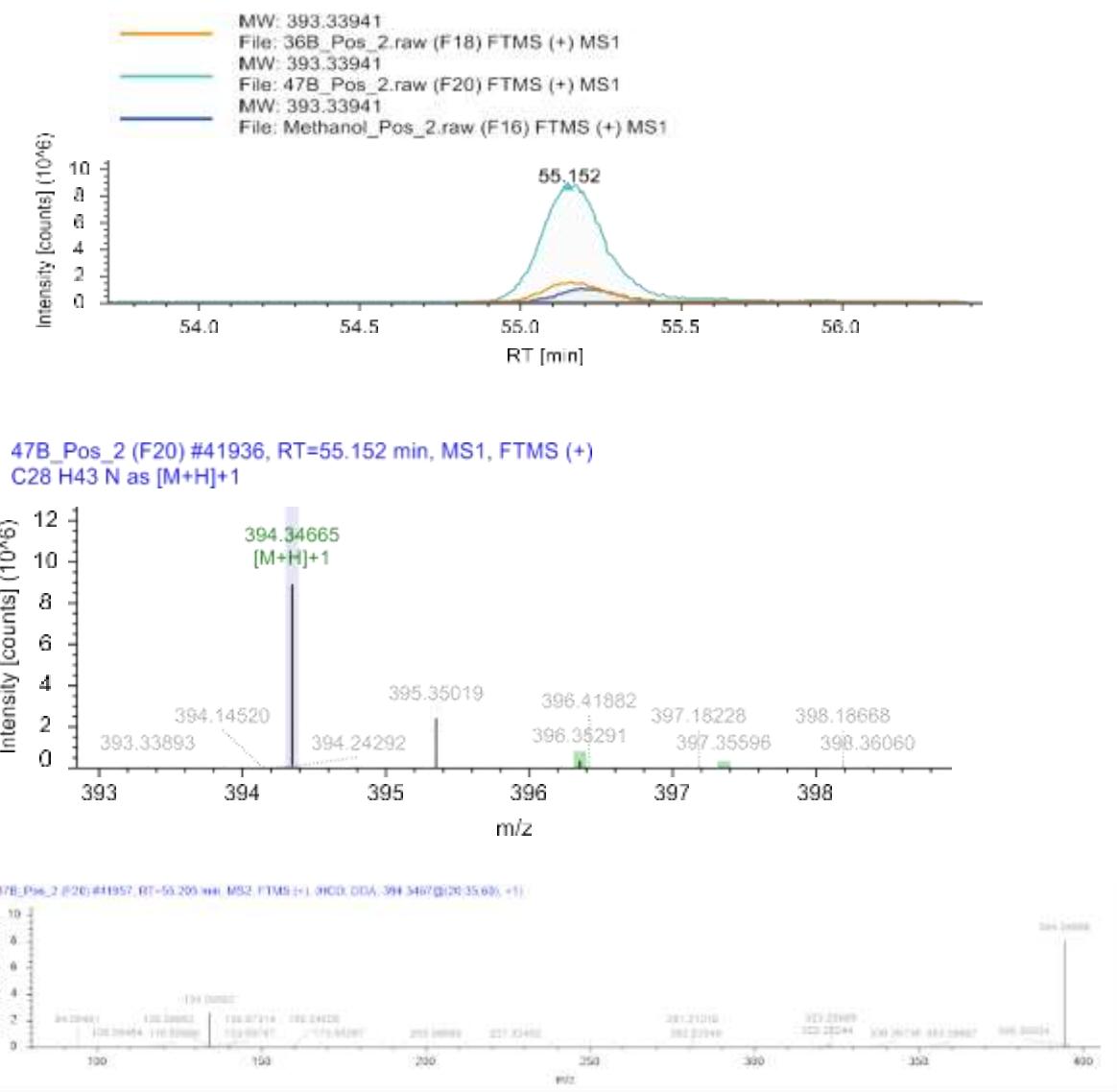
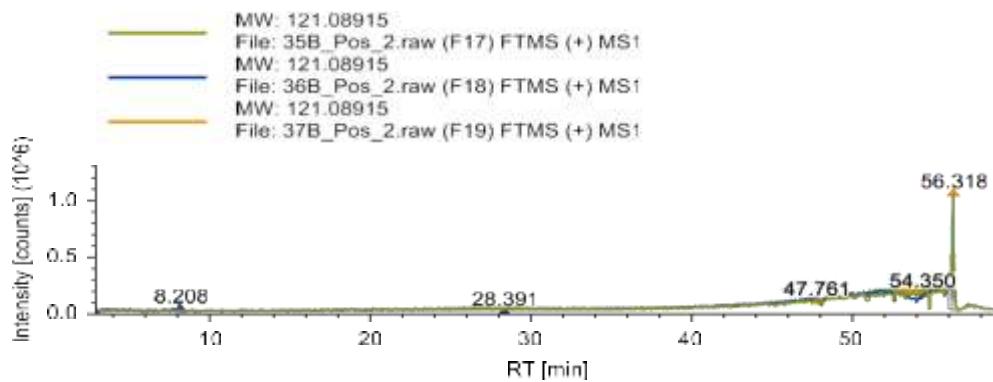
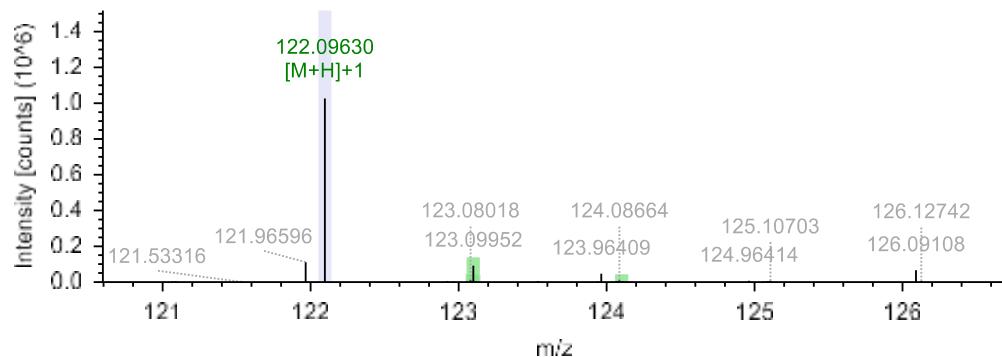


Figure S22: Retention time peak, fragmentation pattern and chemical structure of unknown compound (not identified with library)



37B_Pos_2 (F19) #45243, RT=56.306 min, MS1, FTMS (+)
C8 H11 N as [M+H]⁺



17B_Pas_2 (F15) #45295; RT=56.325 min; MS2-FTMS (+); (ICQ; DDA; 122.0953@ (20.3560), +1)

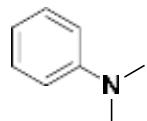
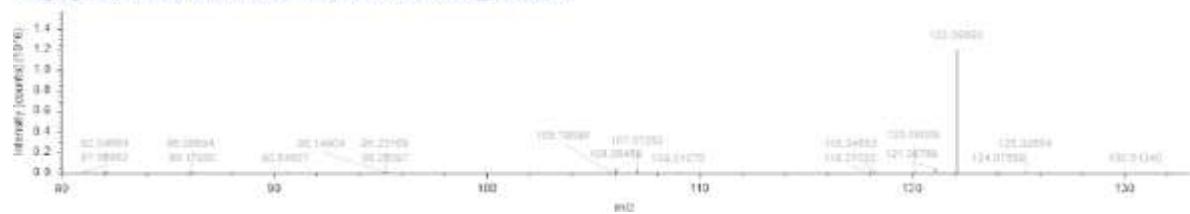


Figure S23: Retention time peak, fragmentation pattern and chemical structure of N,N-Dimethylaniline