

Supplementary file

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

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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-Dimethylaniline	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 ($p < 0.05$)

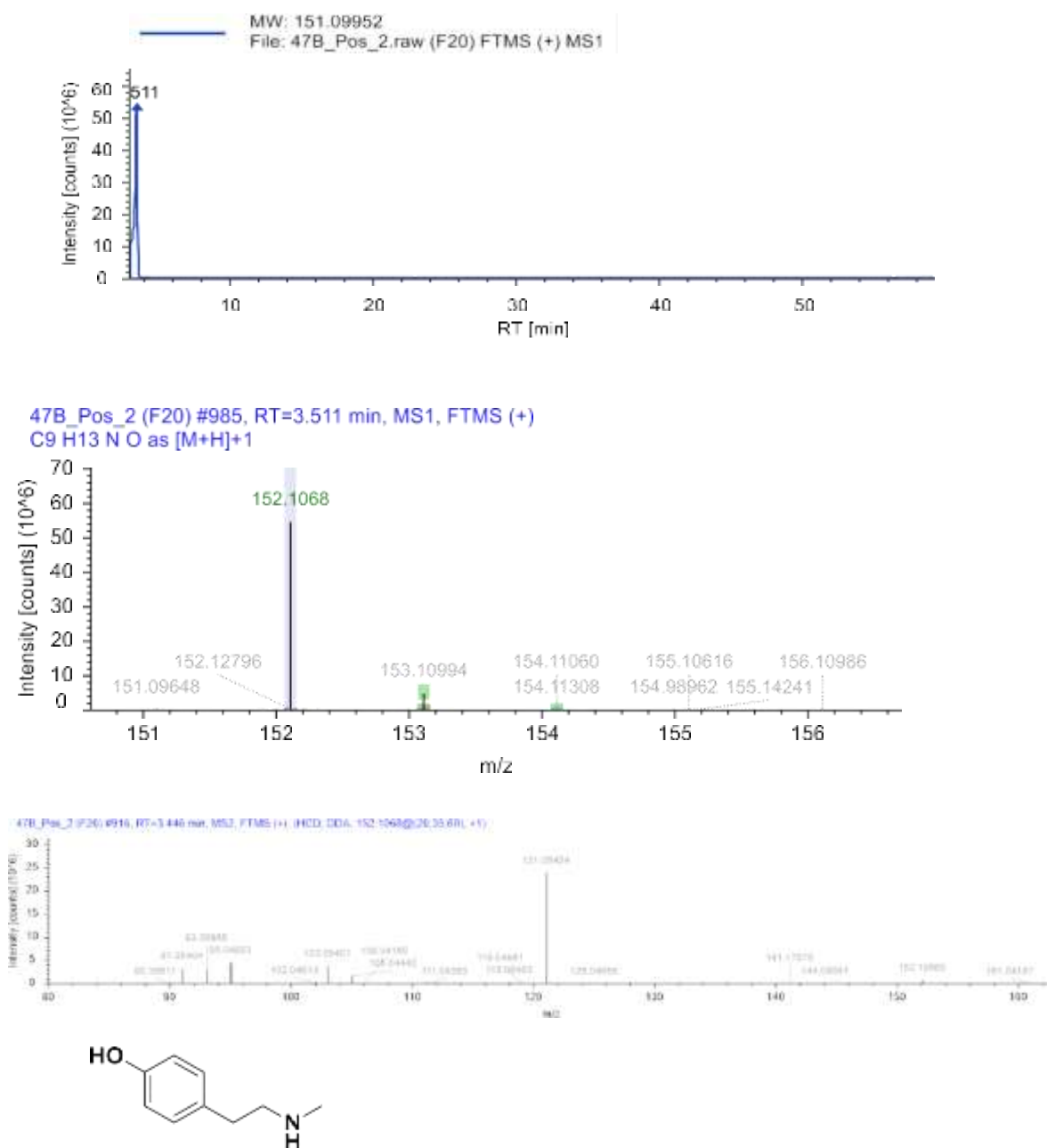


Figure S1: Retention time peak, fragmentation pattern and chemical structure of N-Methyltyramine

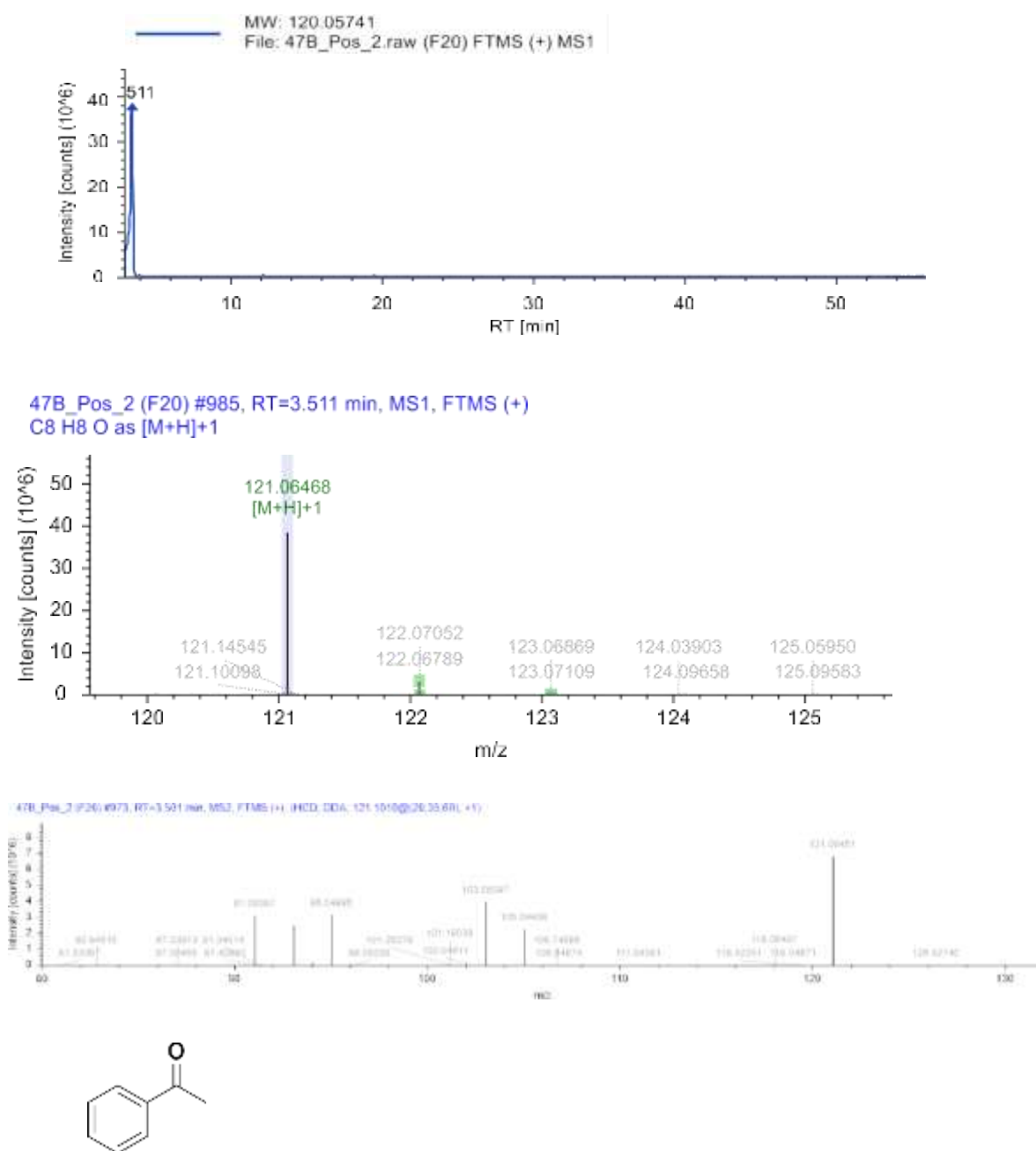


Figure S2: Retention time peak, fragmentation pattern and chemical structure of Acetophenone

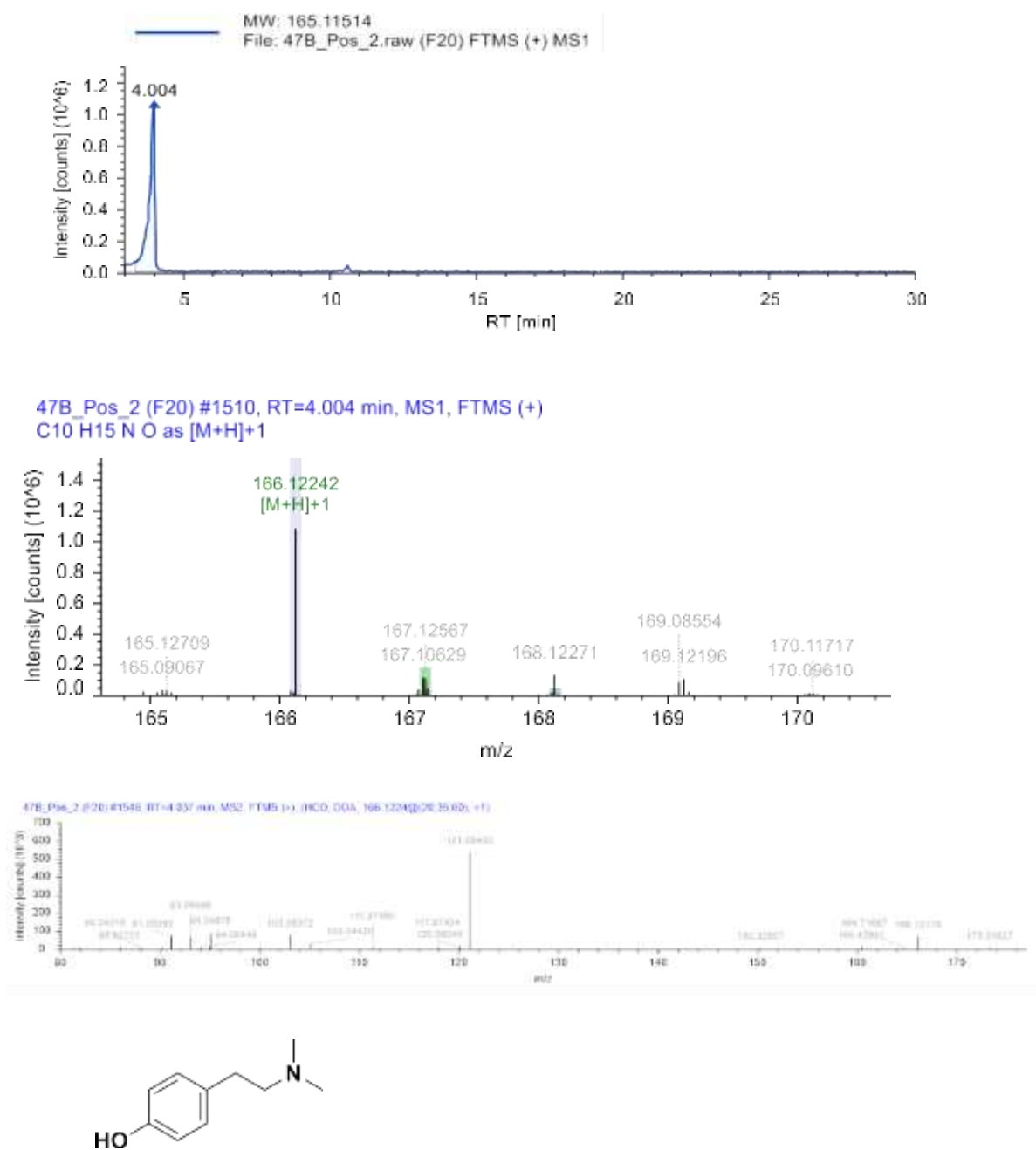


Figure S3: Retention time peak, fragmentation pattern and chemical structure of Hordenine

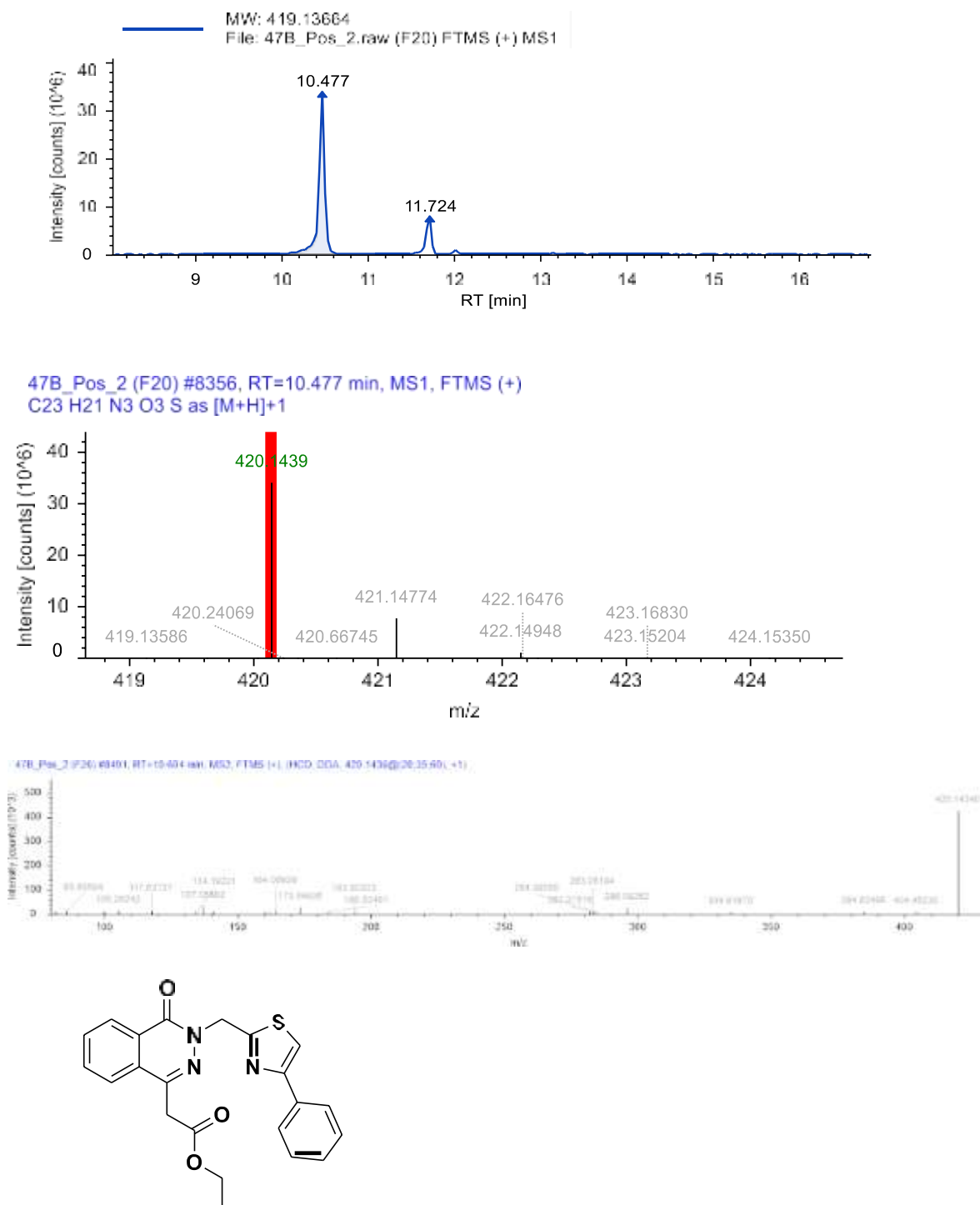


Figure S4: Retention time peak, fragmentation pattern and chemical structure of Ethyl 2-(3-([4-(4-methylphenyl)-1,3-thiazol-2-yl]methyl)-4-oxo-3,4-dihydrophthalazin-1-yl)acetate

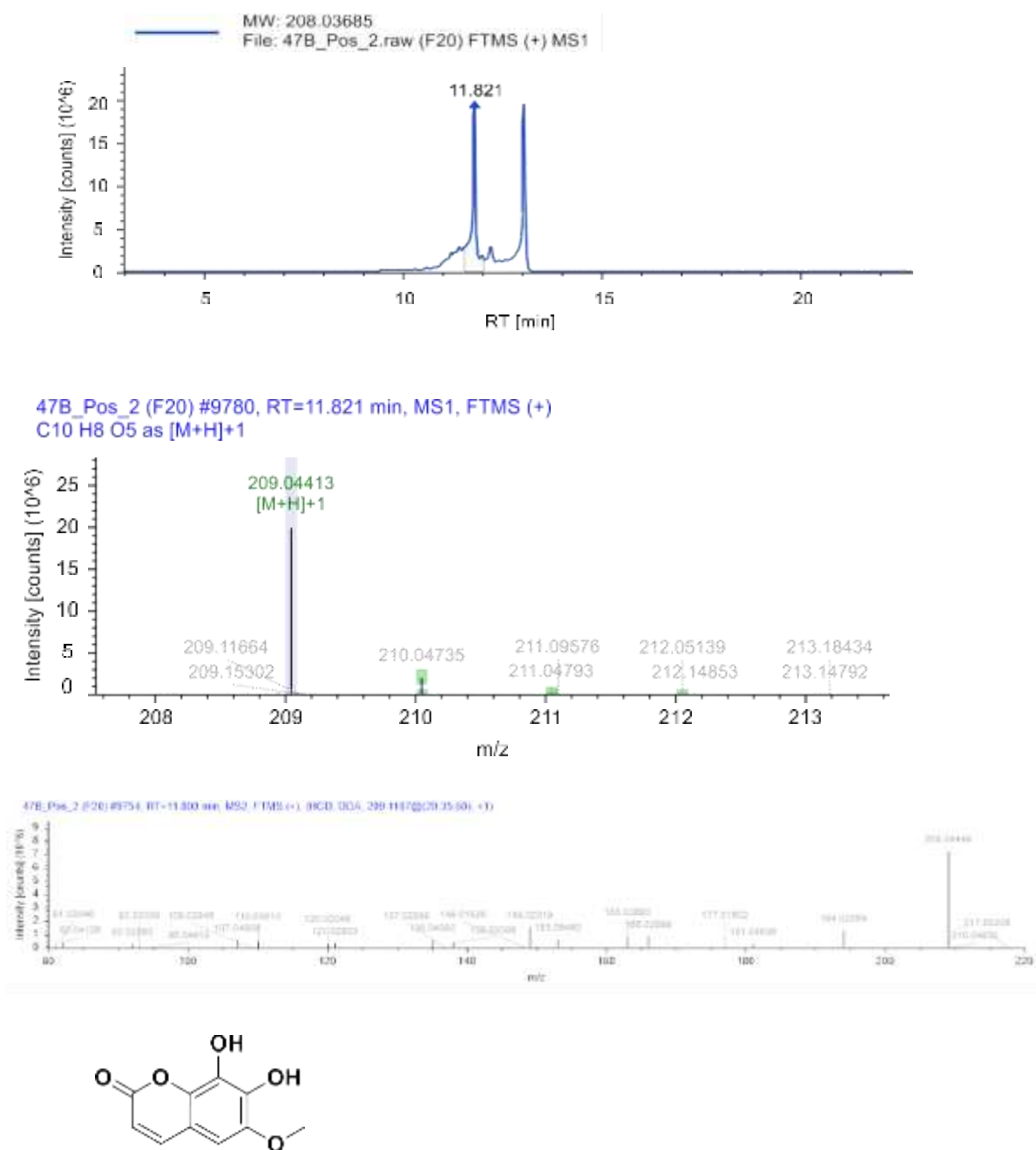


Figure S5: Retention time peak, fragmentation pattern and chemical structure of Fraxetin

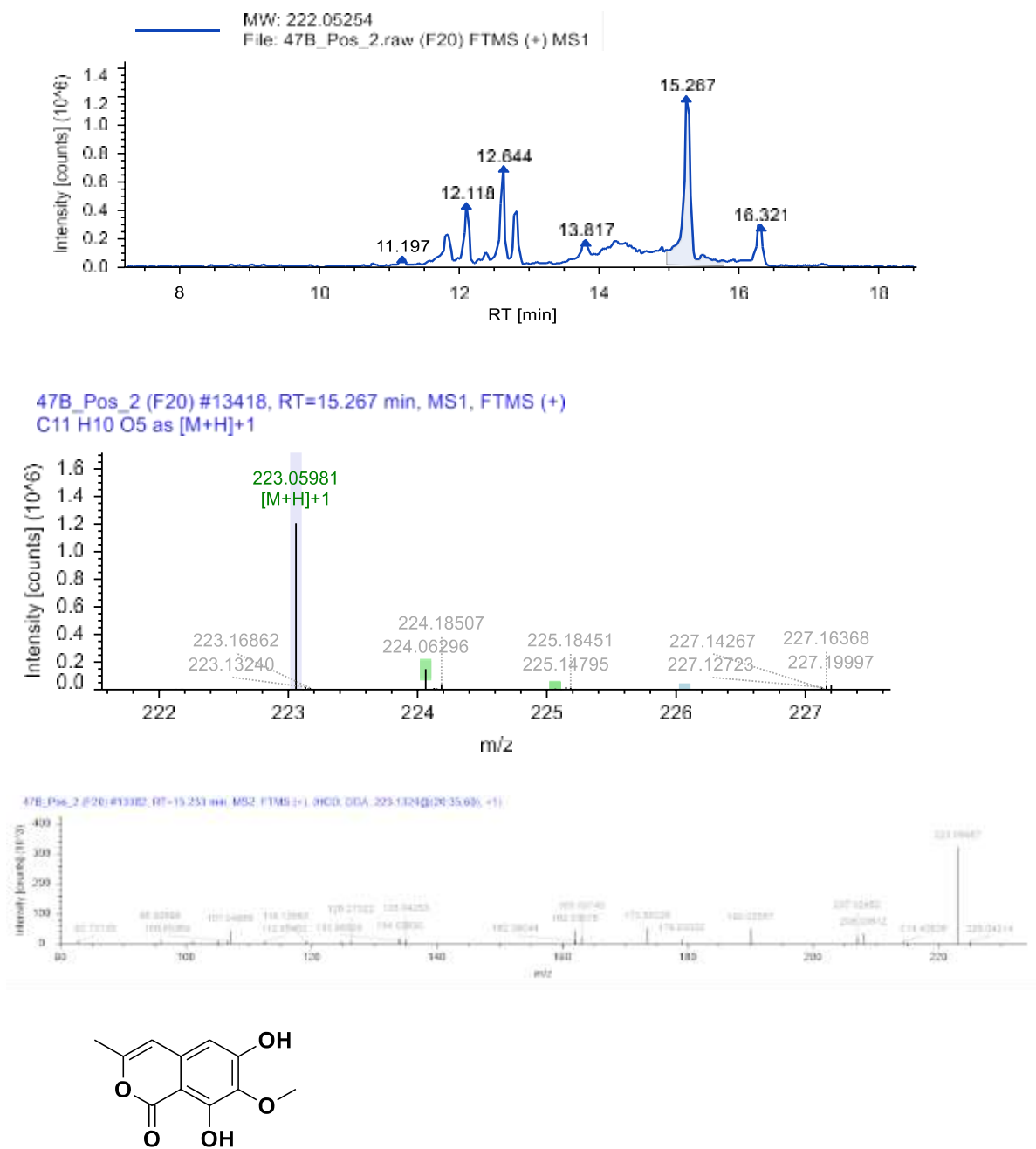


Figure S6: Retention time peak, fragmentation pattern and chemical structure of 6,8-dihydroxy-7-methoxy-3-methyl-1H-isochromen-1-one

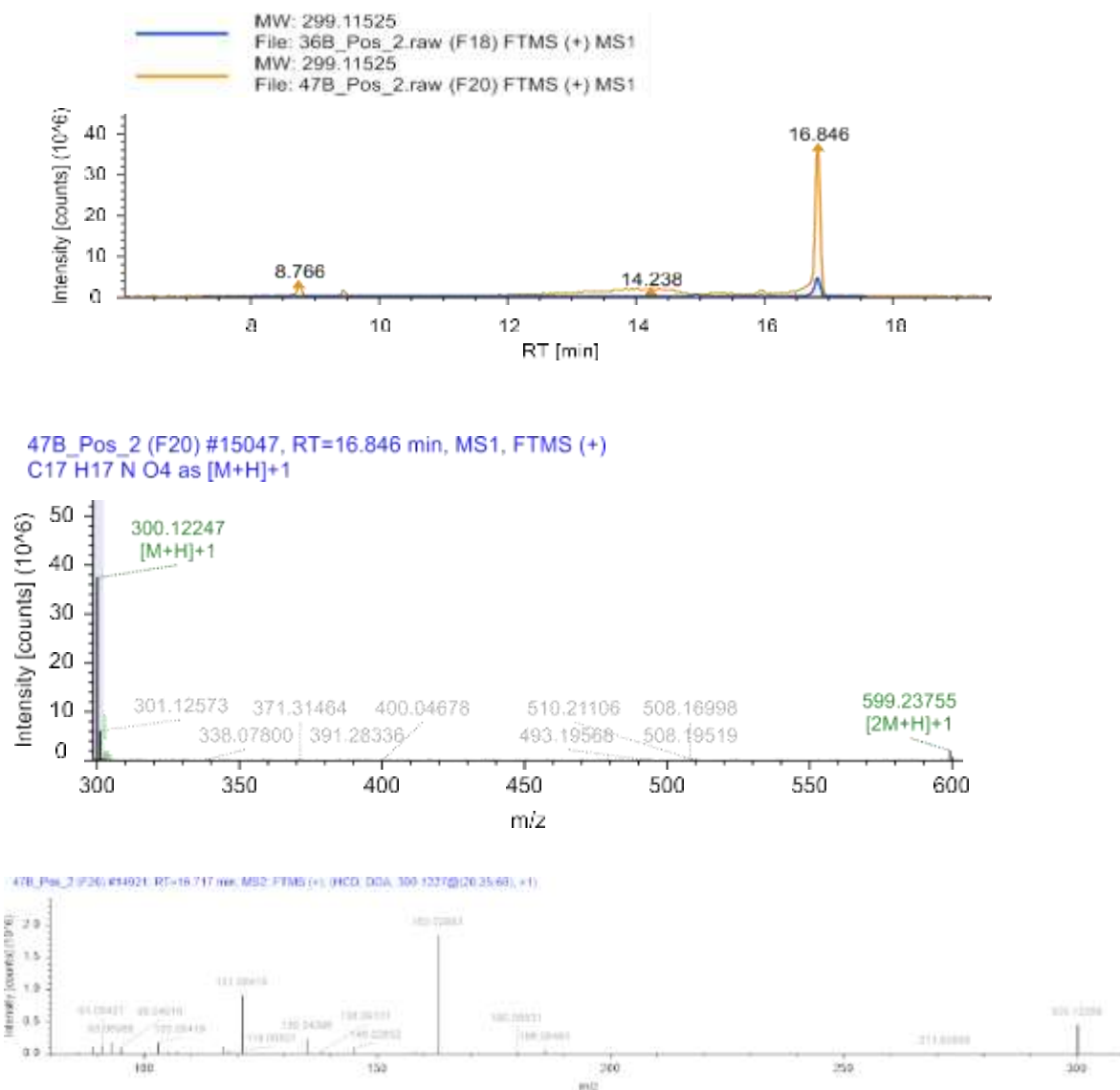
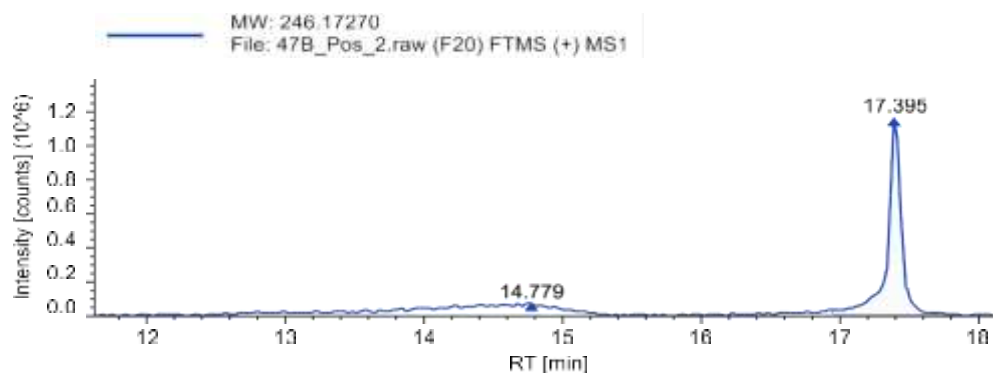


Figure S7: Retention time peak, and fragmentation pattern of Unknown compound (not identified with library)



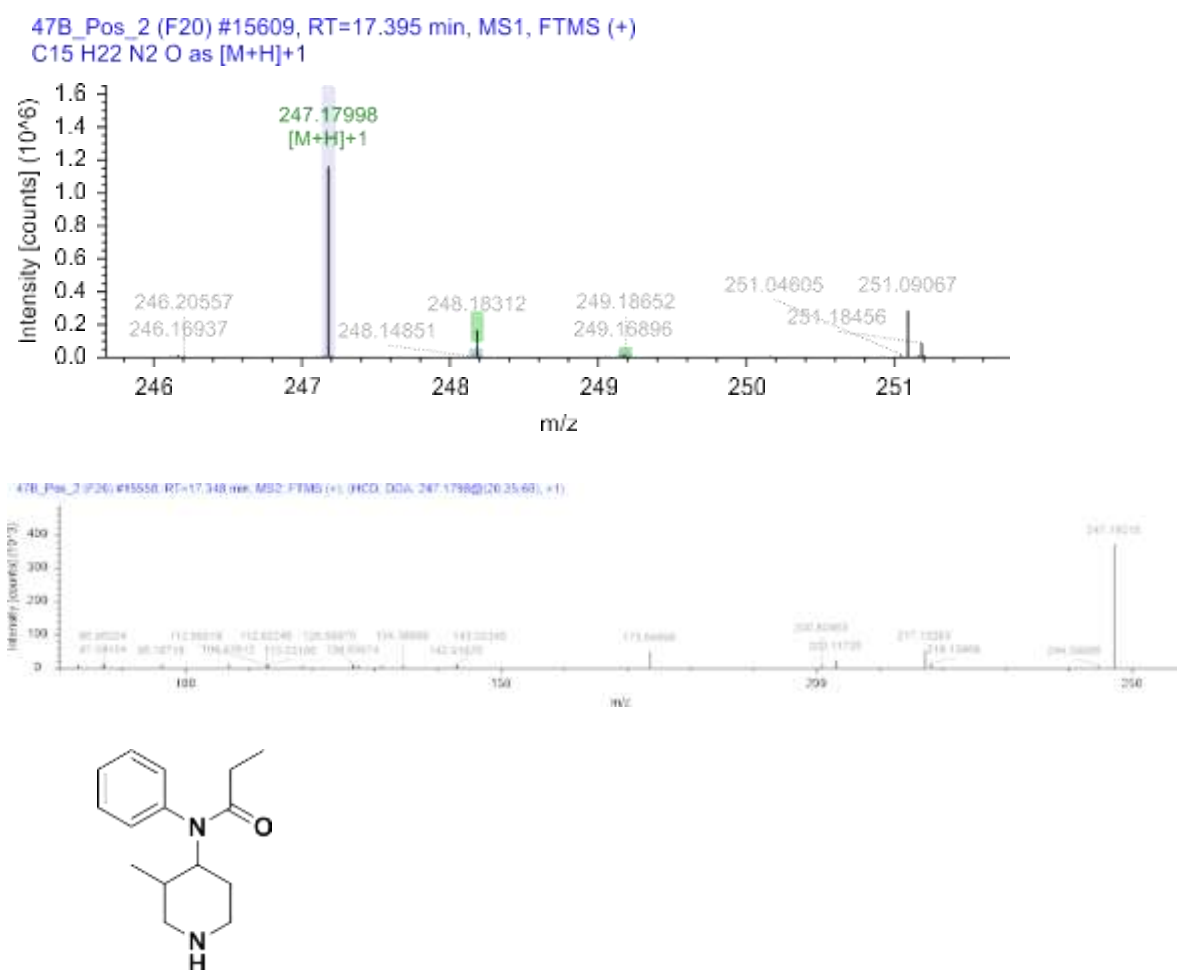
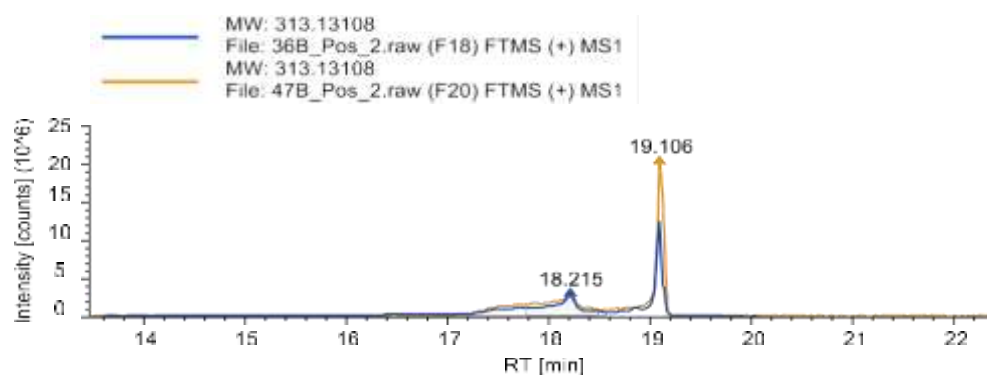


Figure S8: Retention time peak, fragmentation pattern and chemical structure of nor -3-methylfentanyl



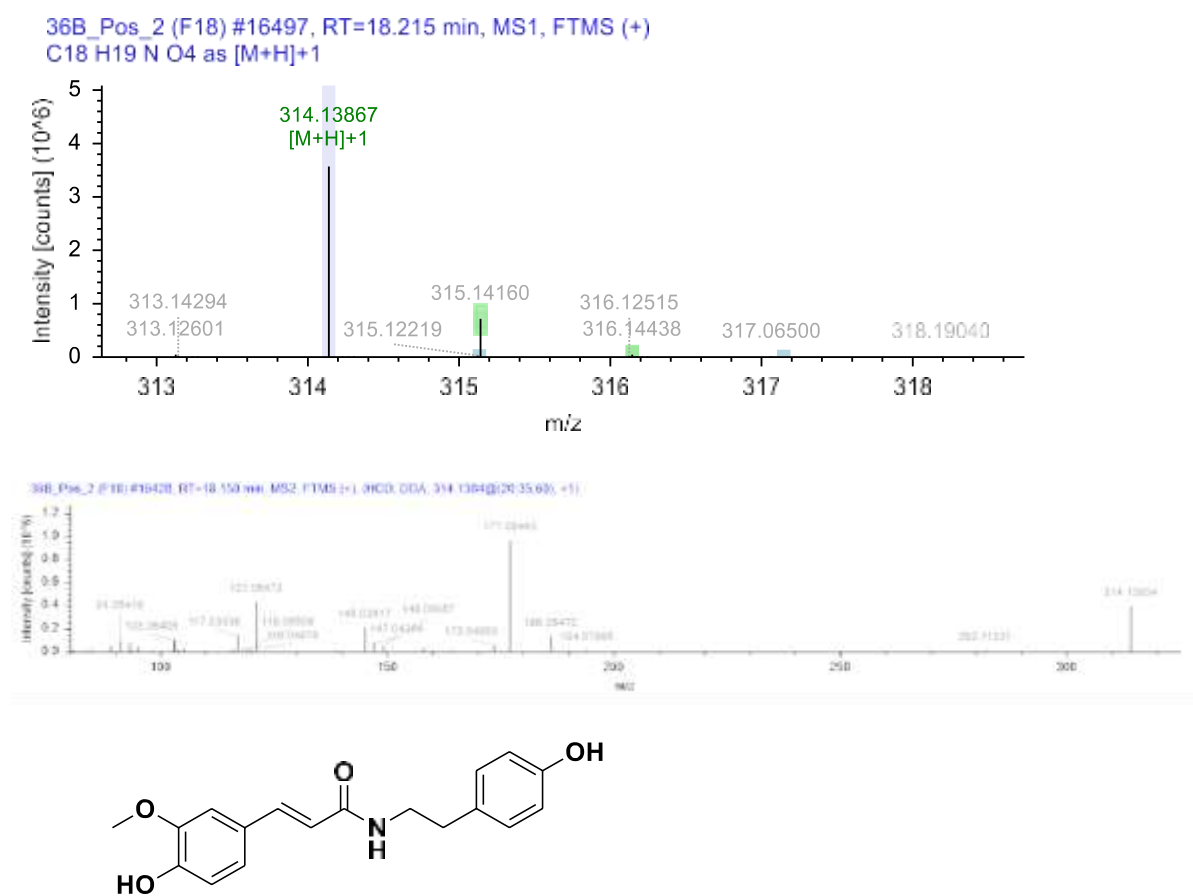
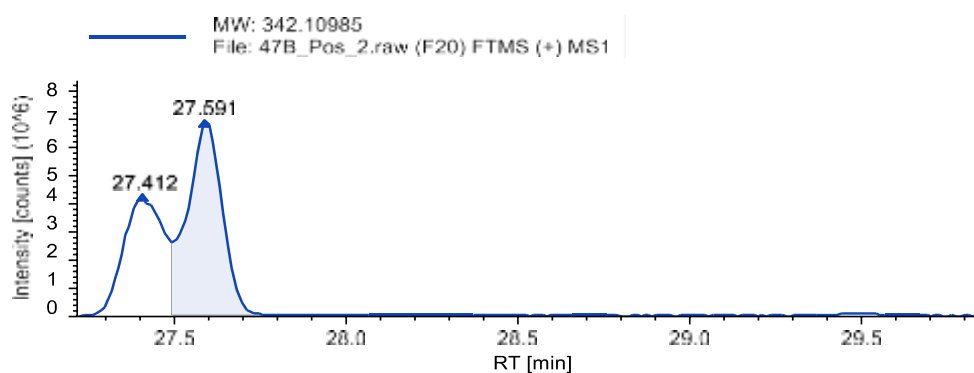
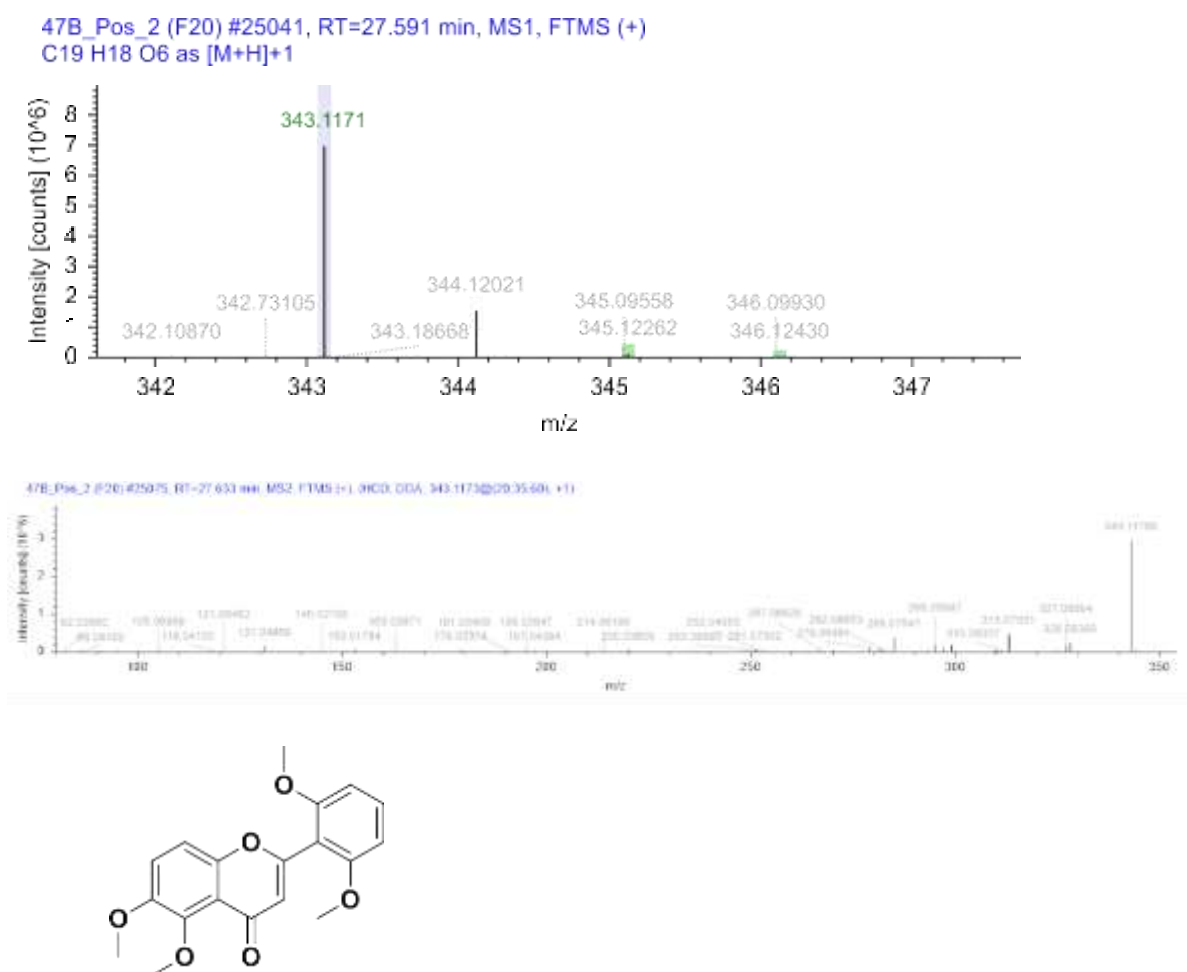
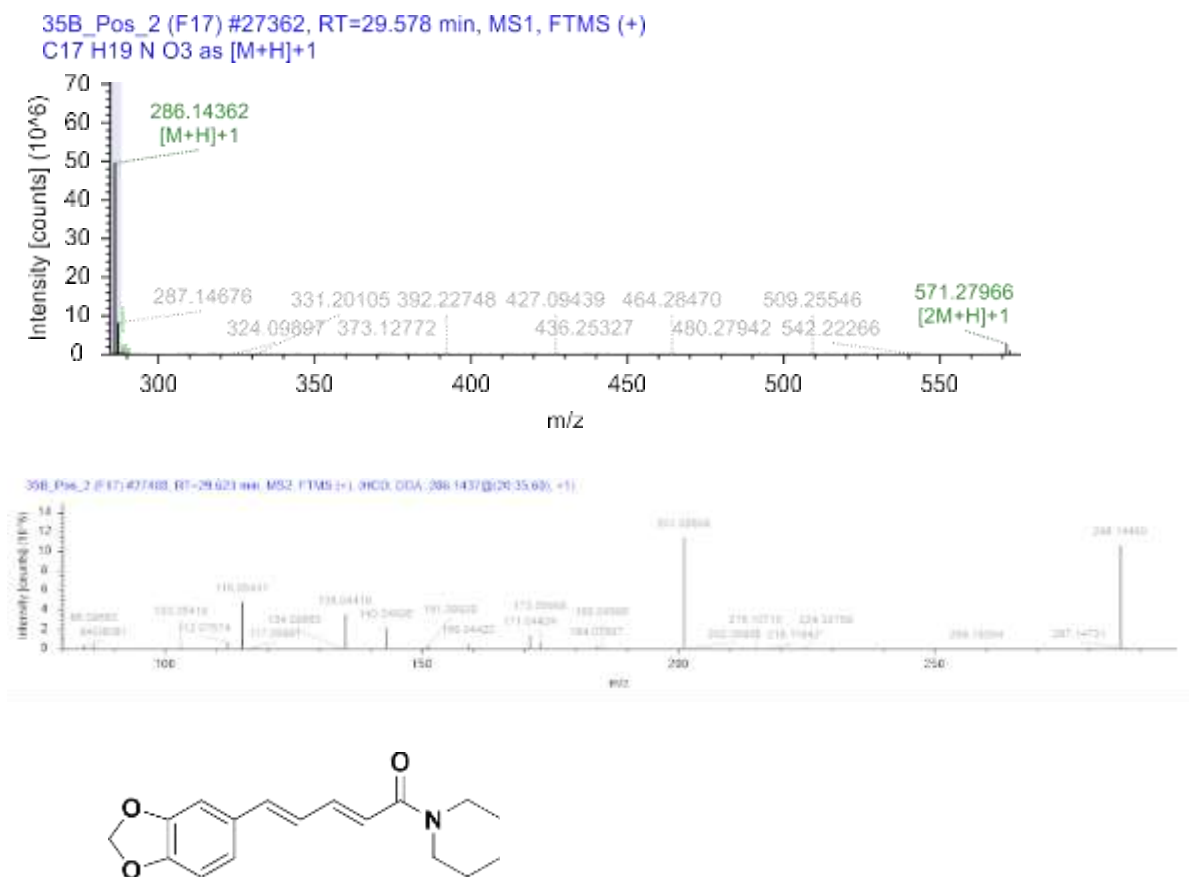


Figure S9: Retention time peak, fragmentation pattern and chemical structure of Moupinamide







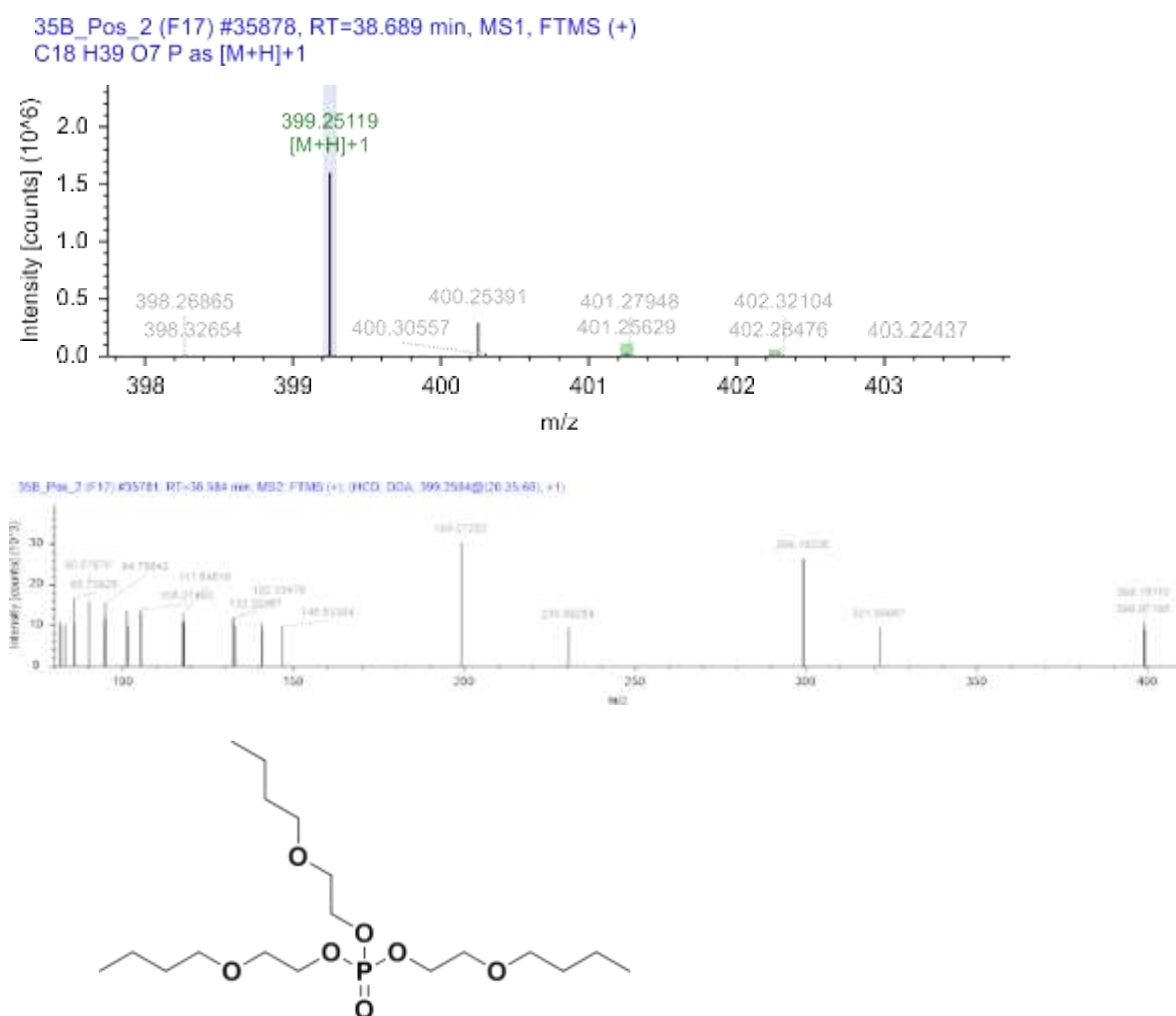
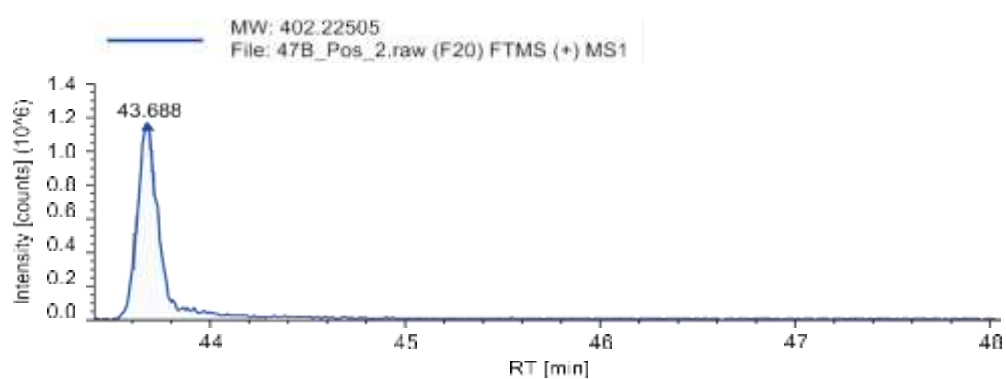


Figure S12: Retention time peak, fragmentation pattern and chemical structure of tris(2-Butoxyethyl) phosphate



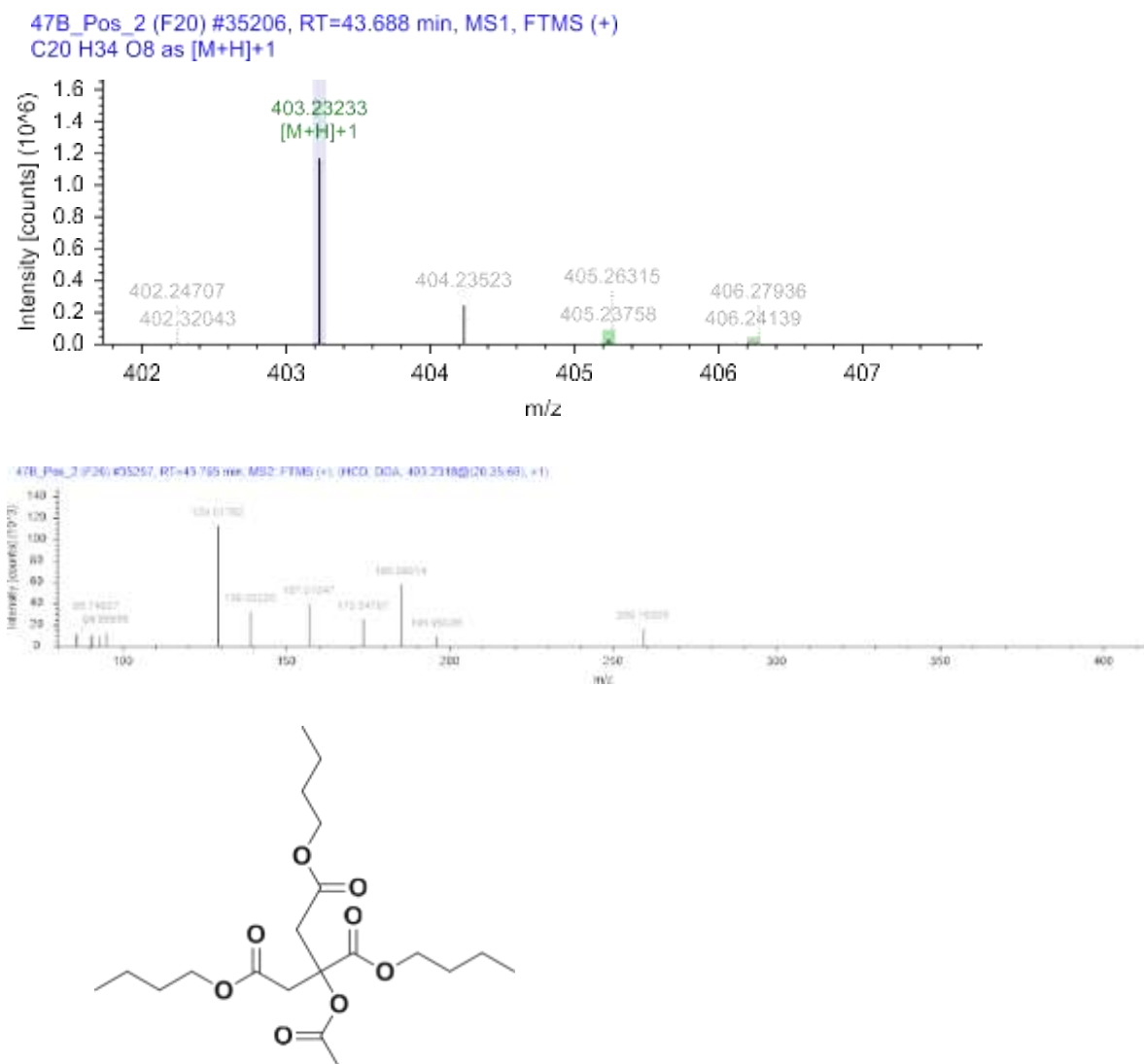
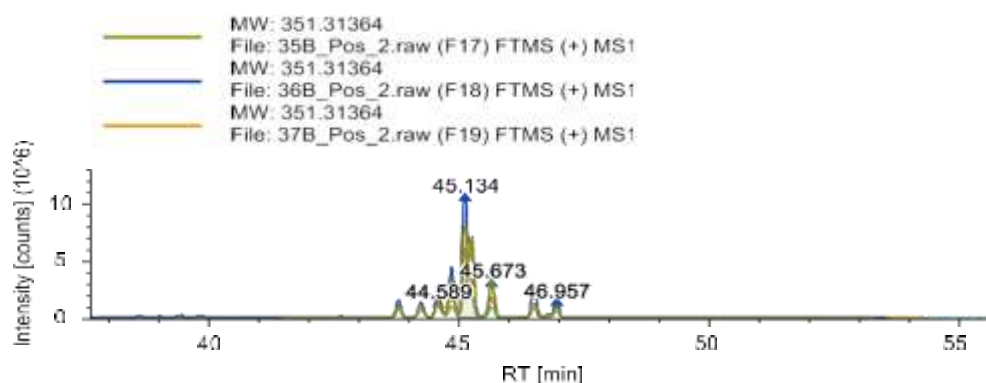


Figure S13: Retention time peak, fragmentation pattern and chemical structure of Acetyl tributyl citrate



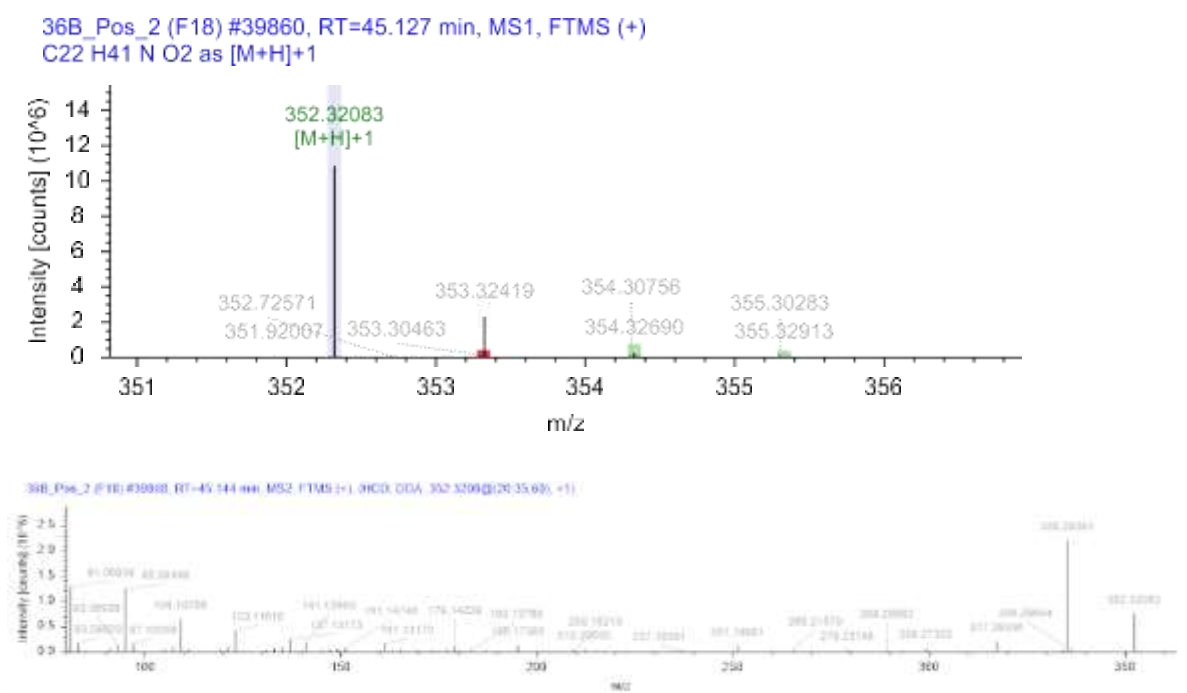
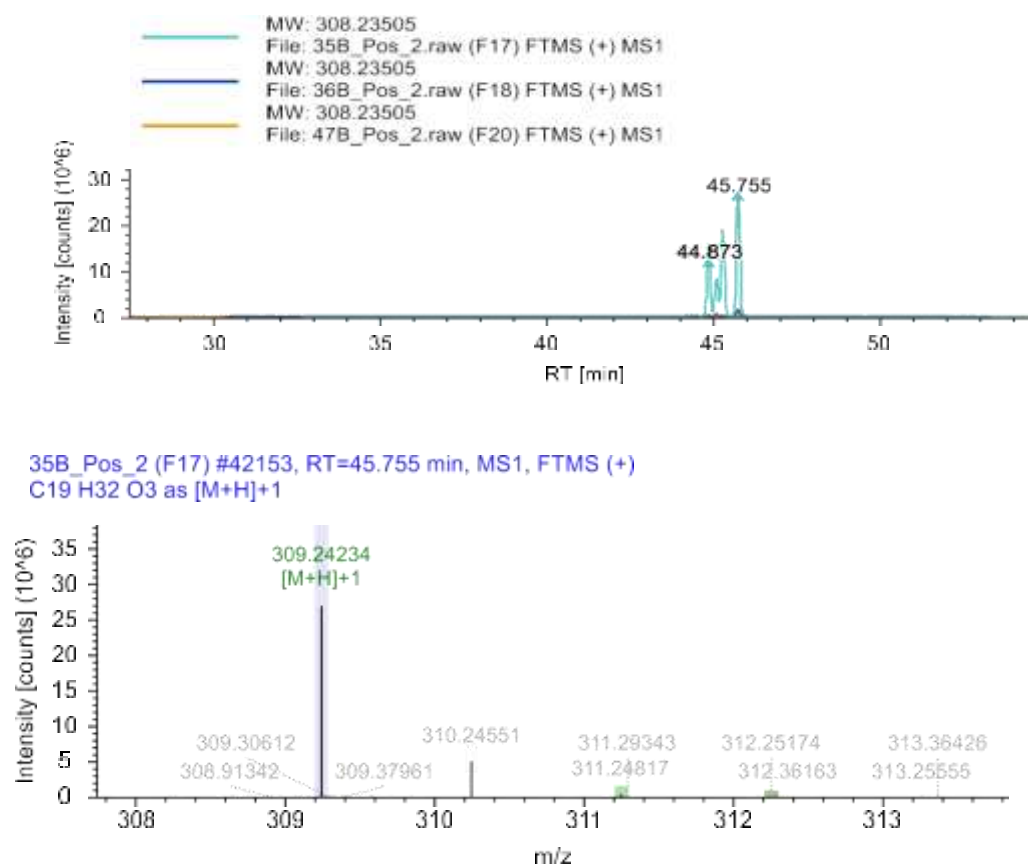


Figure S14: Retention time peak, and fragmentation pattern of Unknown compound (not identified with library)



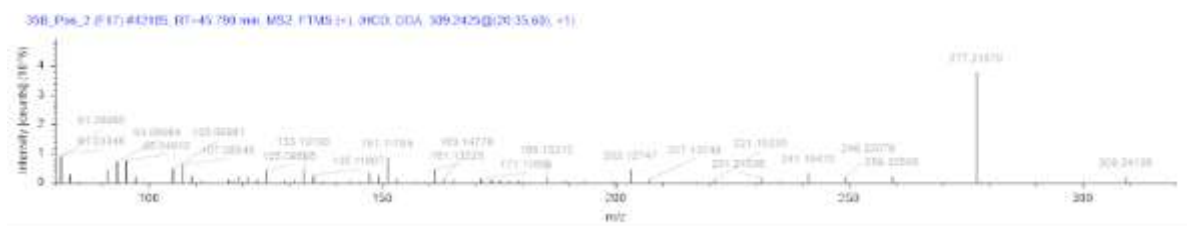
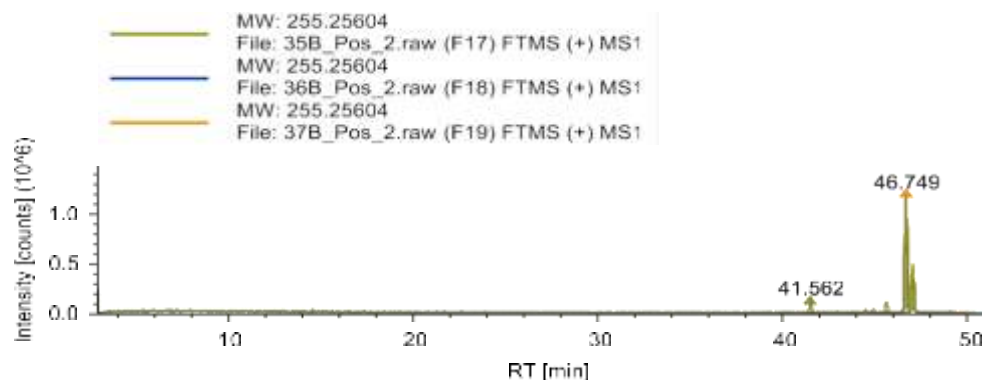


Figure S15: Retention time peak, and fragmentation pattern of Unknown compound (not identified with library)



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

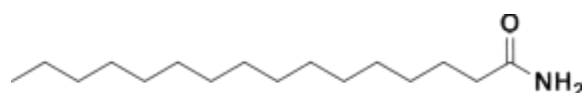
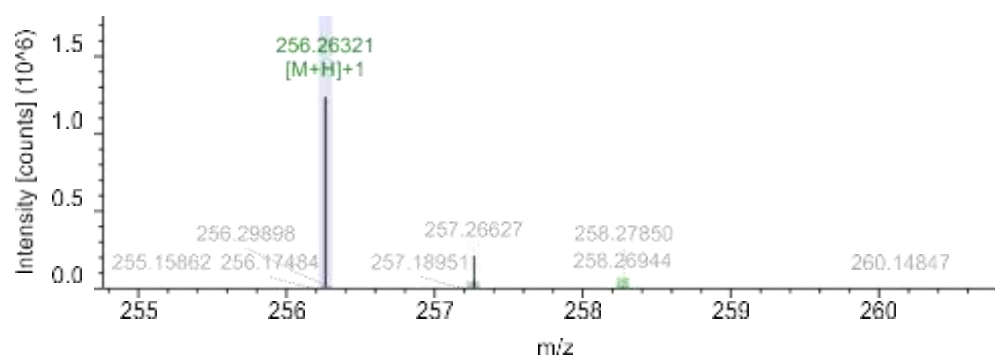


Figure S16: Retention time peak, fragmentation pattern and chemical structure of Hexadecanamide

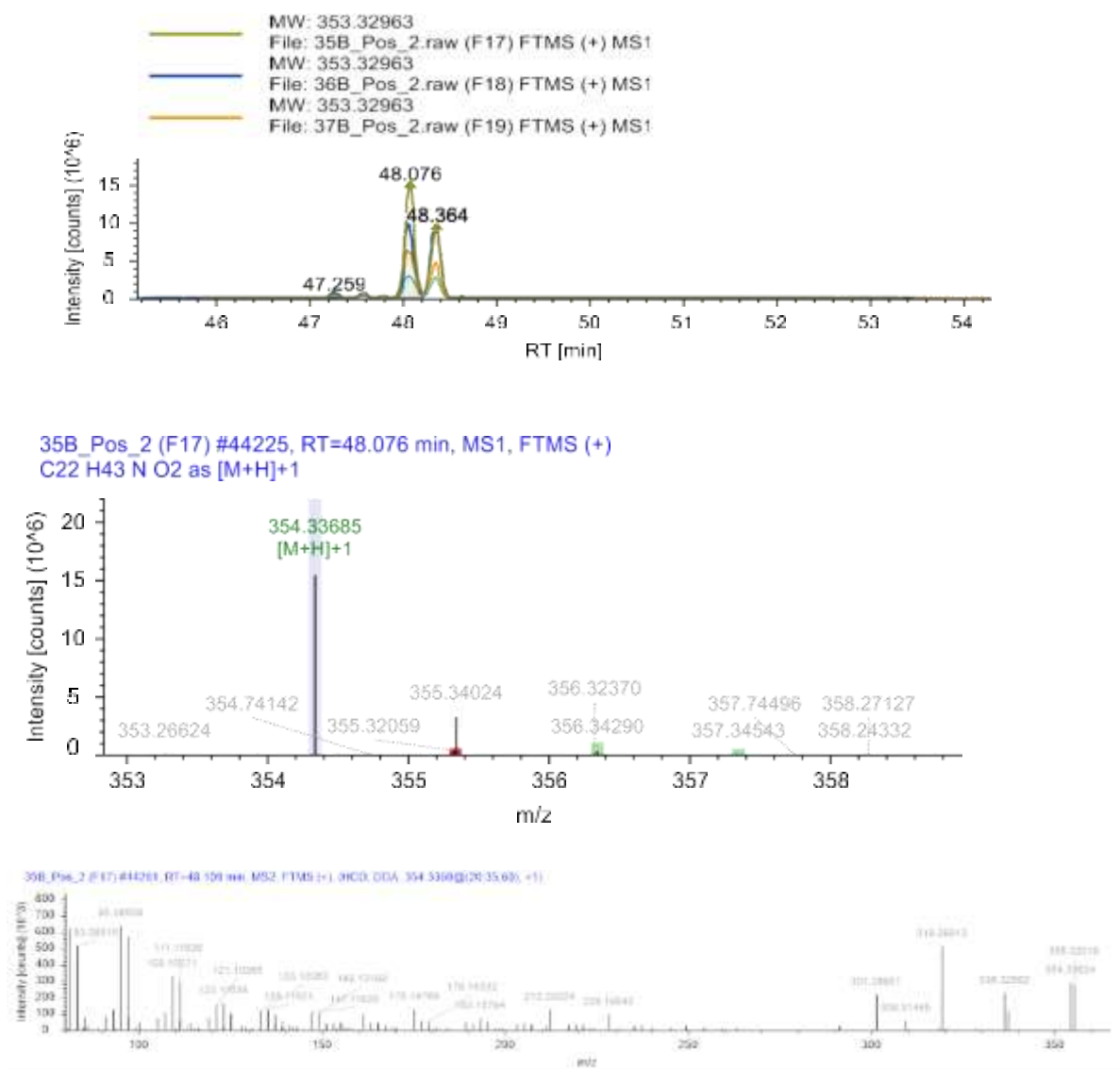
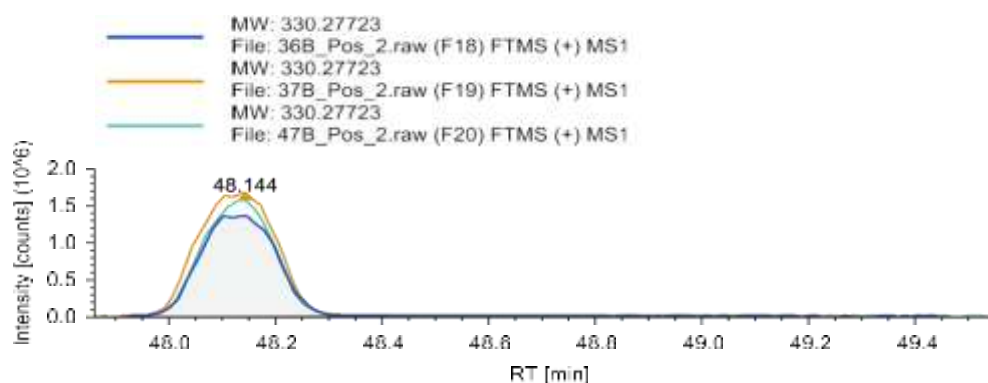


Figure S17: Retention time peak, fragmentation pattern and chemical structure of Unknown compound (not identified with library)



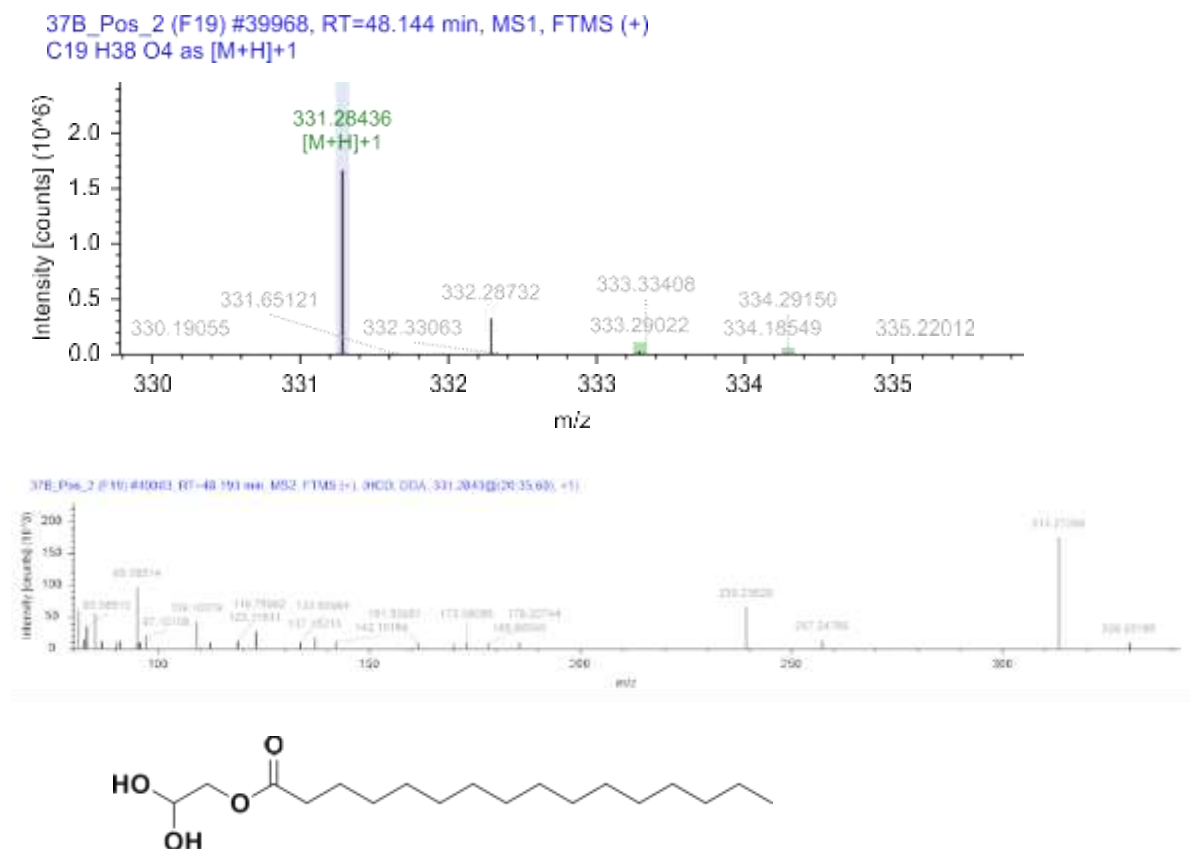
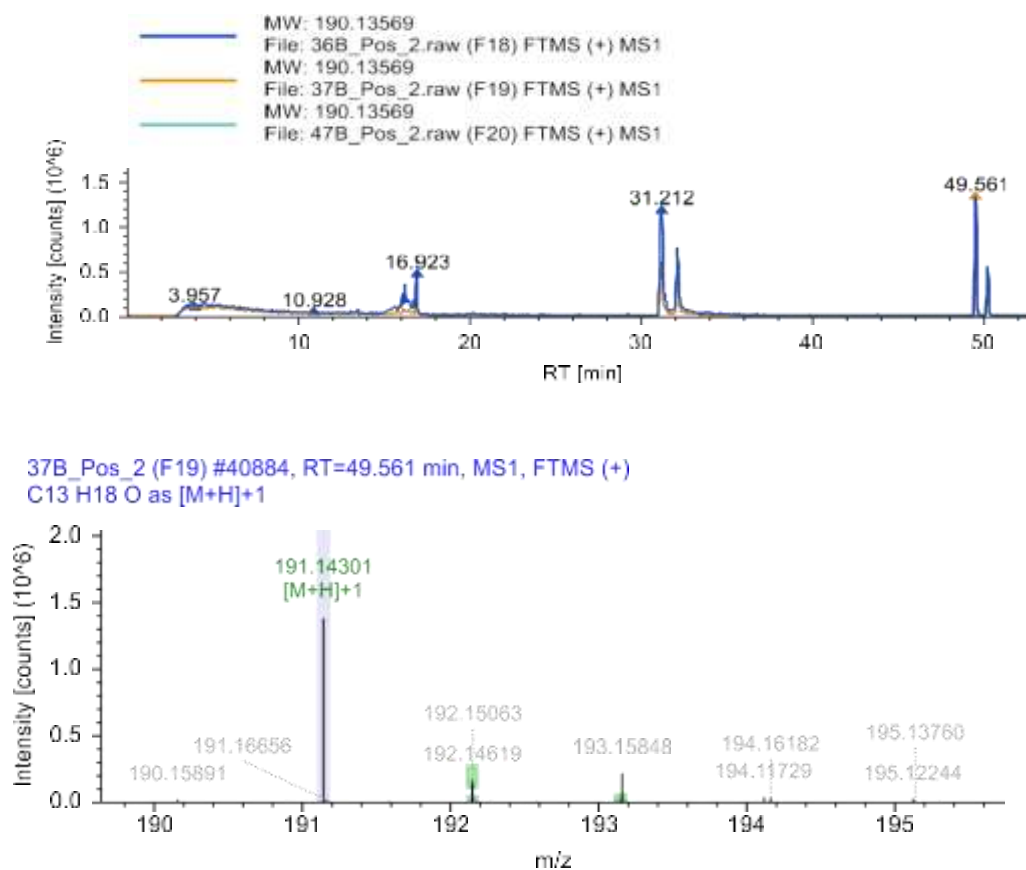


Figure S18: Retention time peak, fragmentation pattern and chemical structure of 1-Palmitoylglycerol



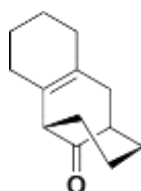
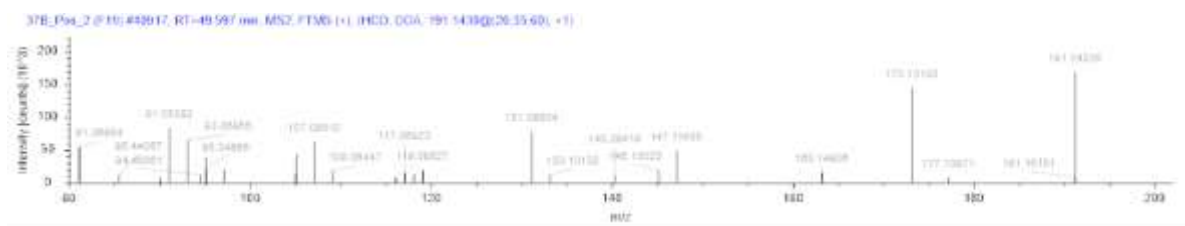
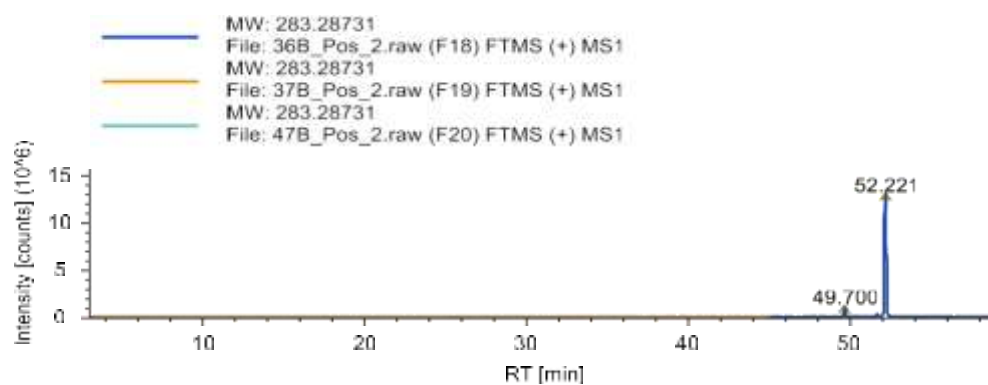
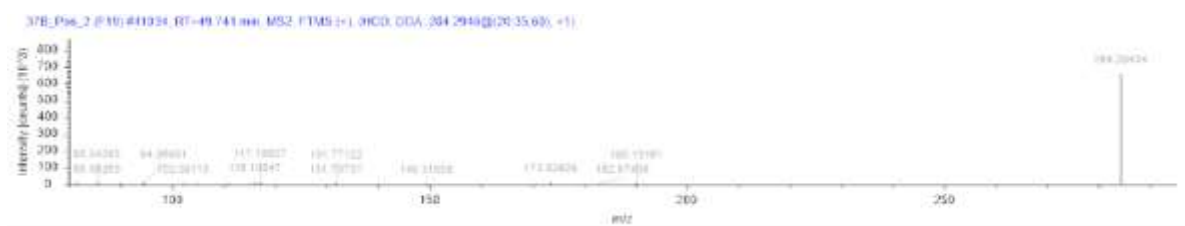
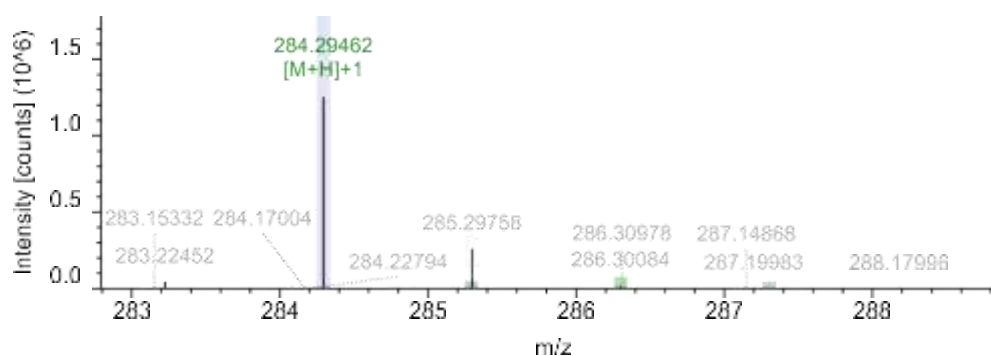


Figure S19: Retention time peak, fragmentation pattern and chemical structure of (1S)-Tricyclo[7.3.1.0~2,7~]tridec-2(7)-en-13-one



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



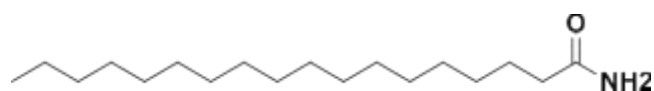
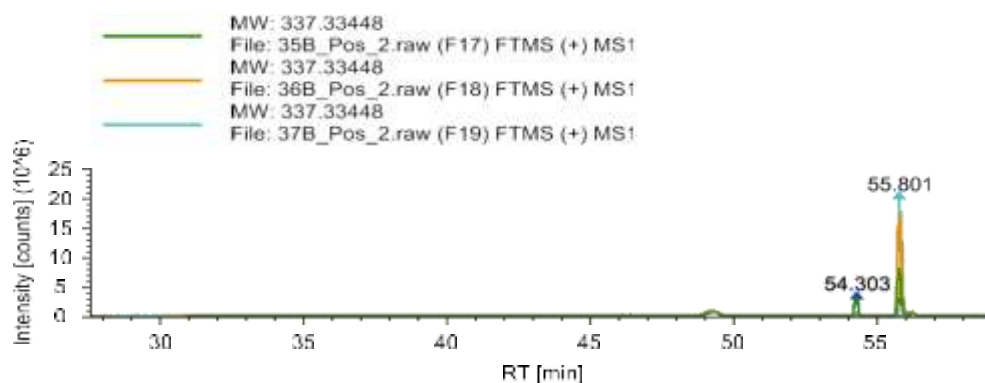


Figure S20: Retention time peak, fragmentation pattern and chemical structure of Stearamide



37B_Pos_2 (F19) #44952, RT=55.801 min, MS1, FTMS (+)
C₂₂H₄₃N O as [M+H]⁺1

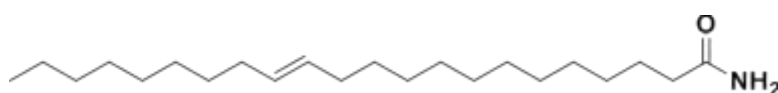
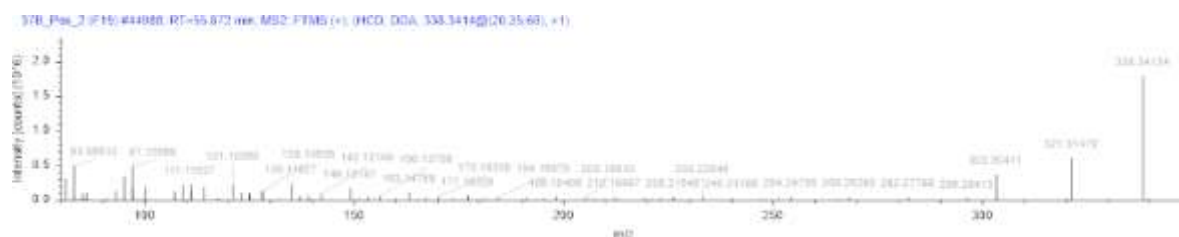
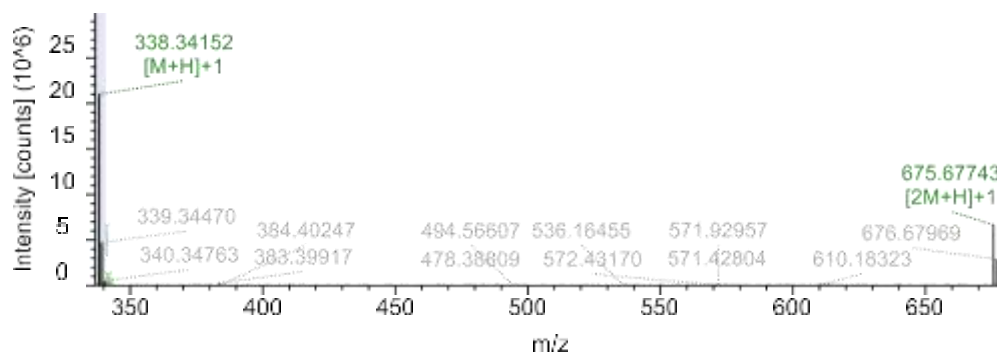
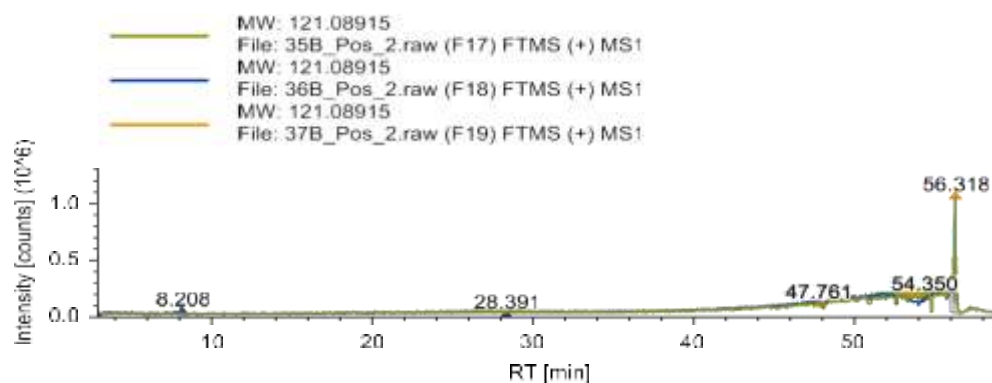


Figure S21: Retention time peak, fragmentation pattern and chemical structure of Erucamide



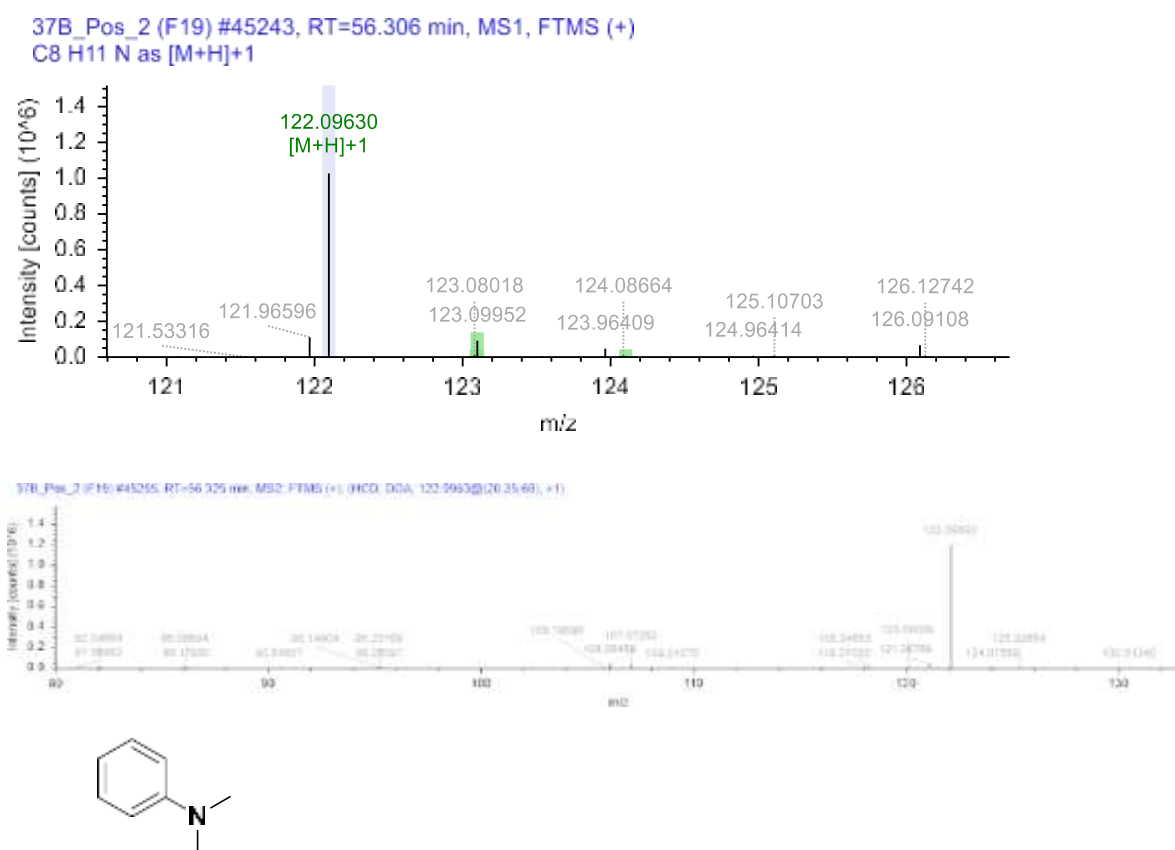


Figure S23: Retention time peak, fragmentation pattern and chemical structure of N,N-Dimethylaniline