

Supplementary Material

Characterization and quantification of phytochemical constituents and anti-inflammatory properties of *Lindera aggregata*

Song-Song Wen^{a,b}, Yong-Jun Liu^a, Yu-Lin Liu^c, Yan Zhao^b, Xiao-Xi Xu^d, Chang-Chuan Guo^b, Chong Niu^b, Wei-Jian Wang^b, Yu-Wen Xu^{b*}, and Na Zhang^{a*}

^aDepartment of Pharmaceutics, Key Laboratory of Chemical Biology (Ministry of Education), School of Pharmaceutical Sciences, Cheeloo College of Medicine, Shandong University, Jinan, 250012, China

^bNMPA Key Laboratory for Research and Evaluation of Generic Drugs, Shandong Research Center of Engineering and Technology for Consistency Evaluation of Generic Drugs, Shandong Institute for Food and Drug Control, Jinan, 250101, China

^cDepartment of Marine Pharmacology, College of Food Science and Technology, Shanghai Ocean University, Shanghai, 201306, China

^dBeijing Normal University, Beijing, 100875, China

*Corresponding author

Na Zhang, Department of Pharmaceutics, Key Laboratory of Chemical Biology (Ministry of Education), School of Pharmaceutical Sciences, Cheeloo College of Medicine, Shandong University, E-mail: zhangnancy9@sdu.edu.cn; Yu-Wen Xu, NMPA Key Laboratory for Research and Evaluation of Generic Drugs, Shandong Research Center of Engineering and Technology for Consistency Evaluation of Generic Drugs, Shandong Institute for Food and Drug Control, E-mail: 13553158409@163.com.

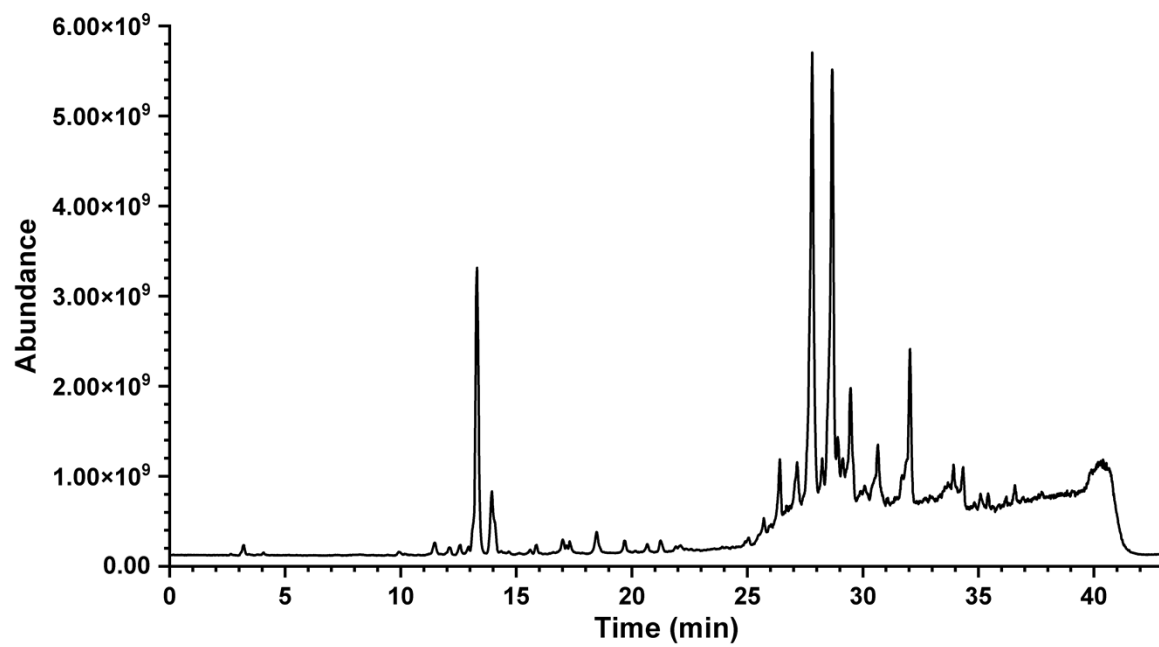
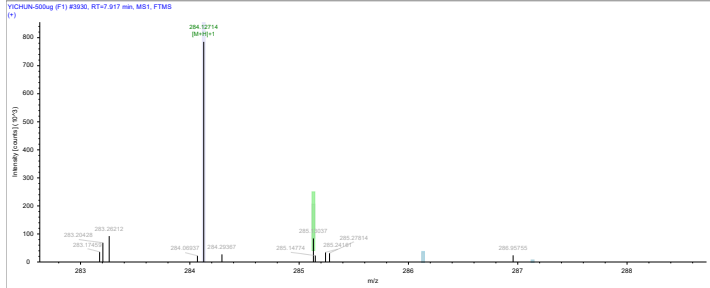


Figure S1. Total ion chromatogram (TIC) of LAE

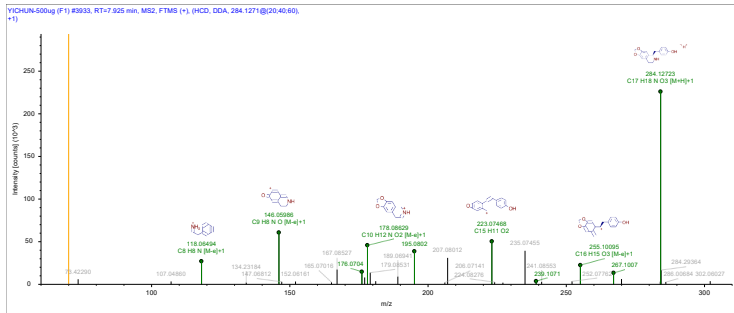
MS and MS/MS spectra of identified compounds

7.937 min Norcinnamolaurine

MS

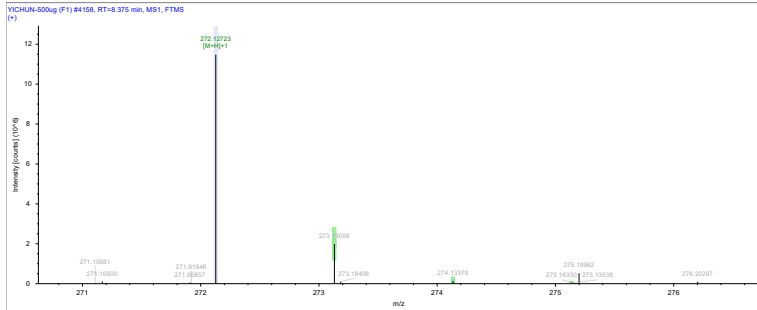


MS/MS

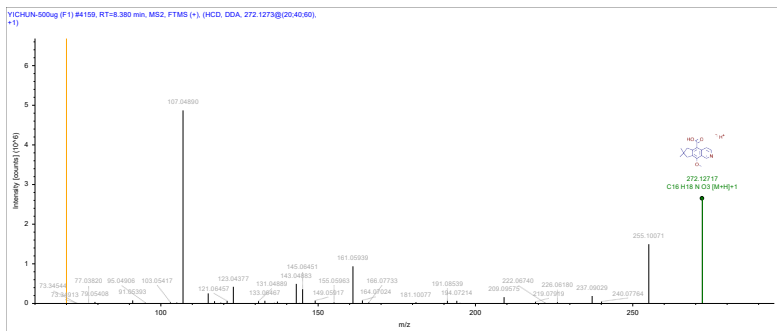


8.39 min Higenamine

MS

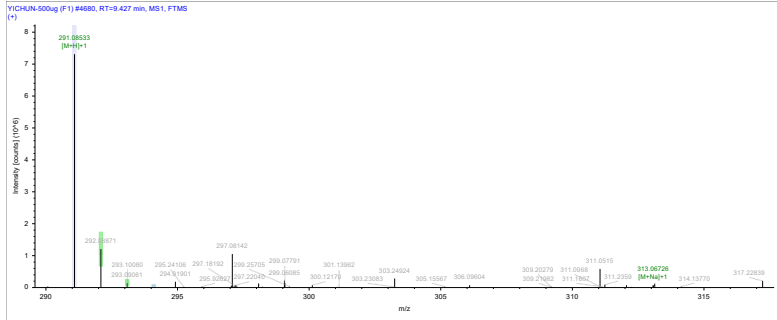


MS/MS

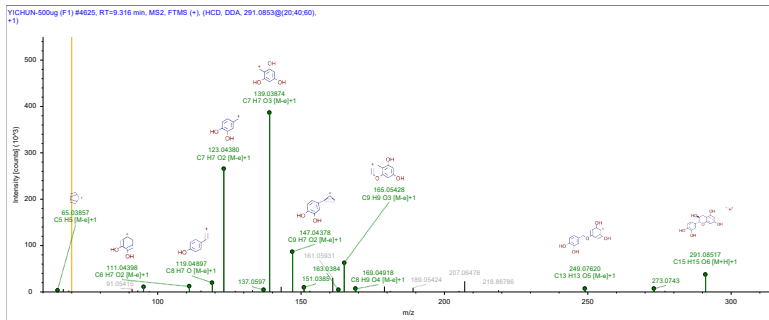


9.424 min Catechin

MS

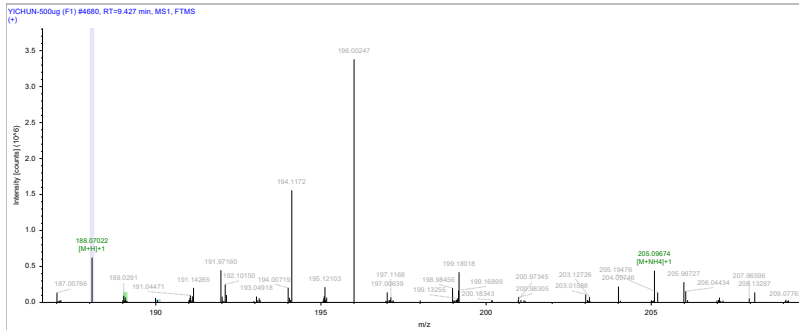


MS/MS

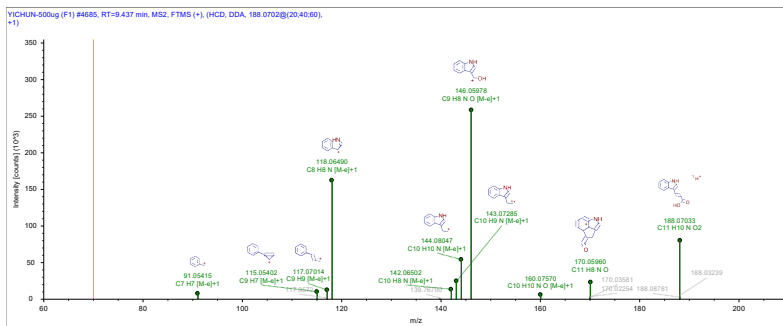


9.569 min Indole-3-acrylic acid

MS

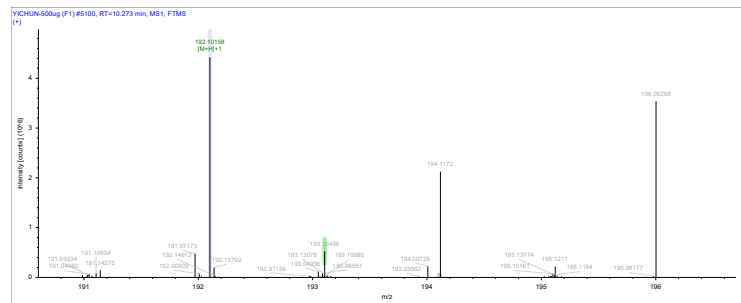


MS/MS

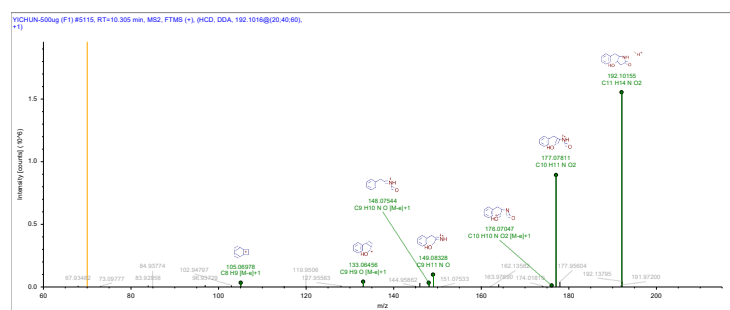


10.271 min Streptopyrrolidine

MS

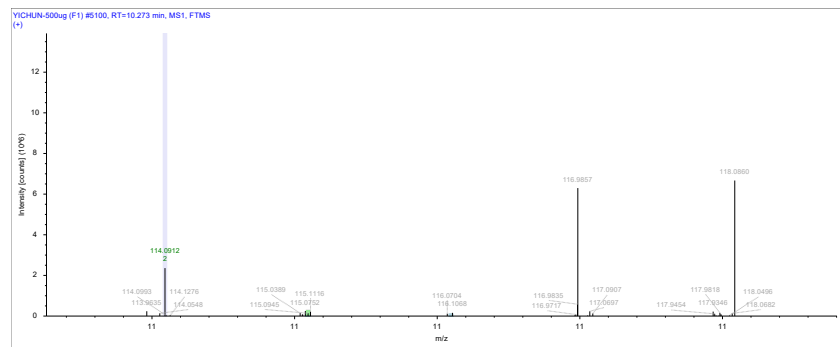


MS/MS

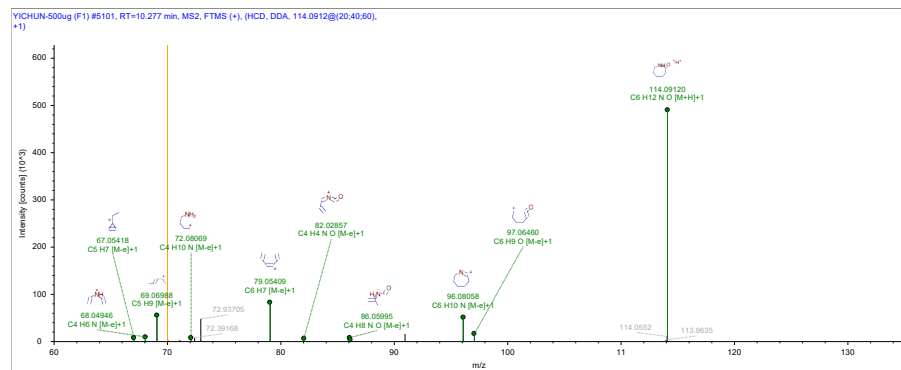


10.433 min Caprolactam

MS

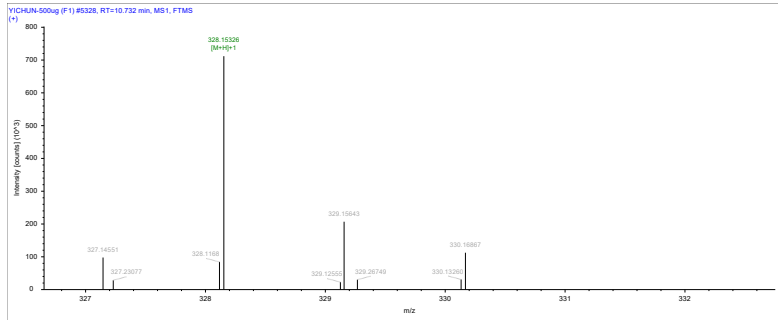


MS/MS

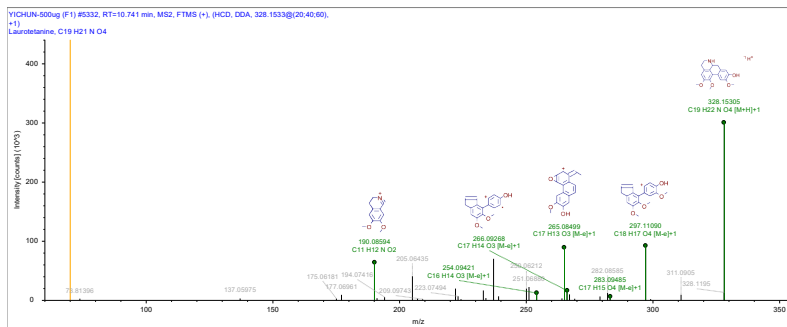


10.802 min Laurotetanine

MS

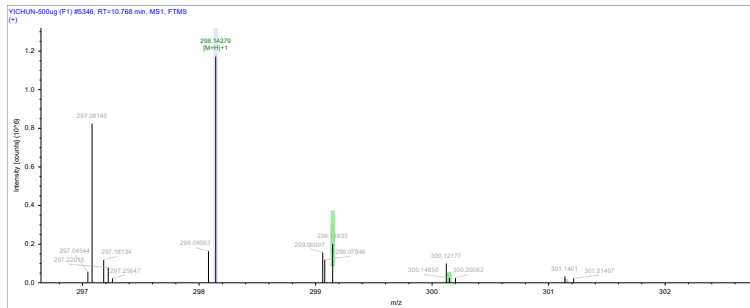


MS/MS

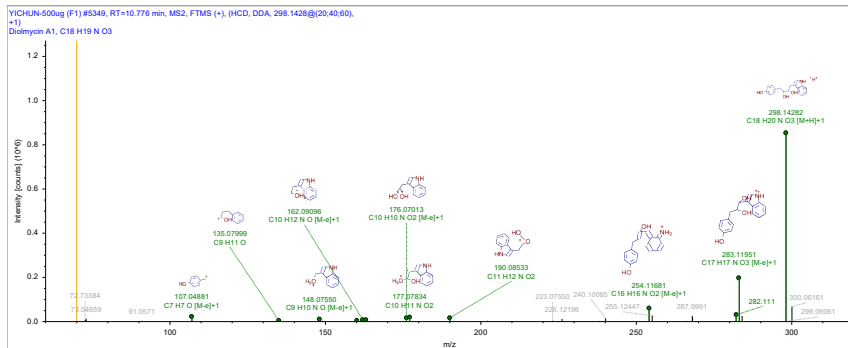


10.82 min Diolmycin A1

MS

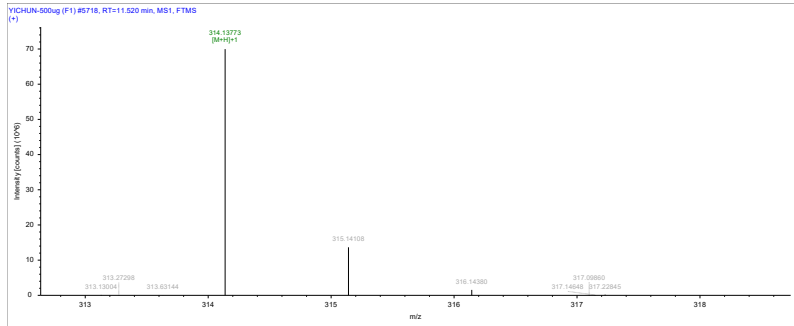


MS/MS

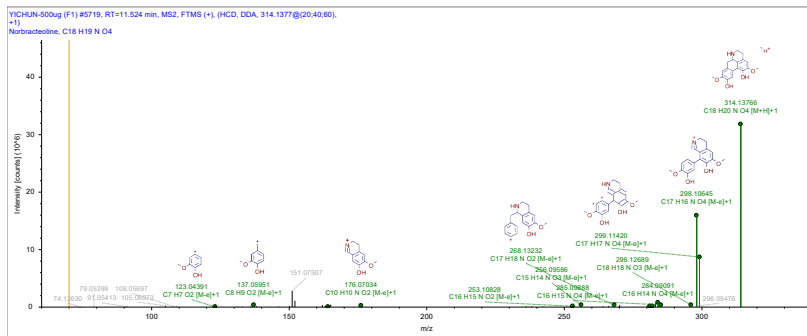


11.53 min Norbracteoline

MS

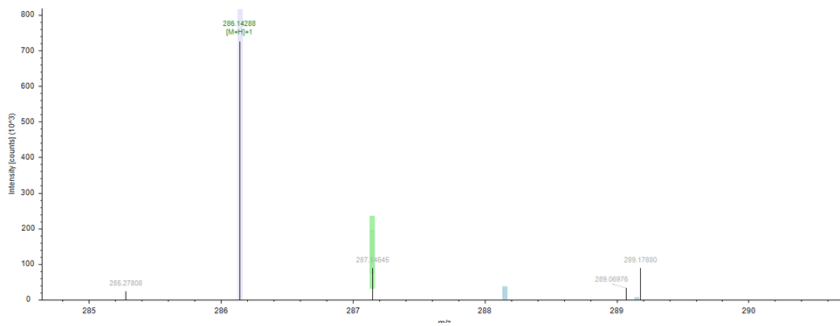


MS/MS

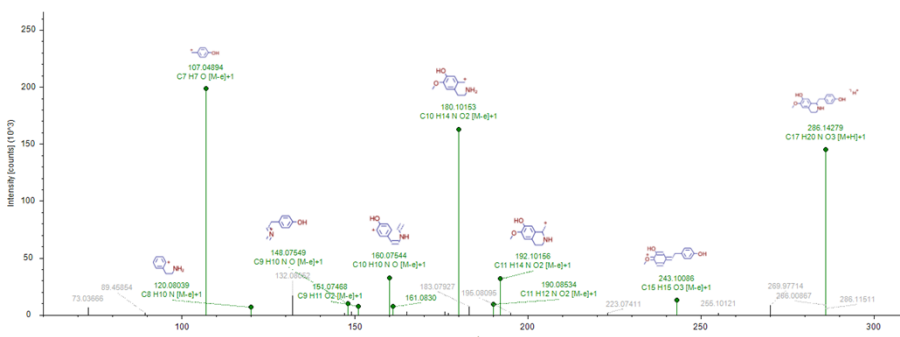


12.19 min Coclaurine

MS

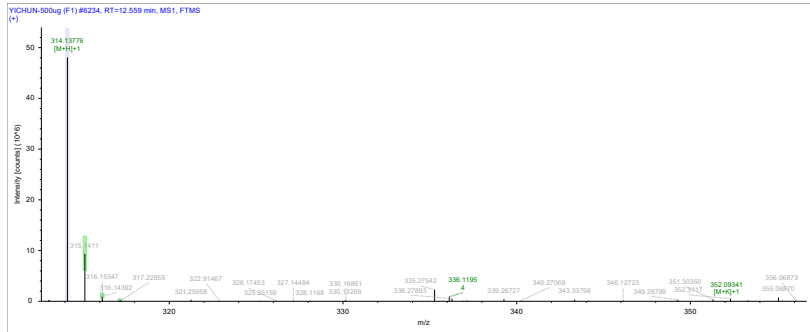


MS/MS

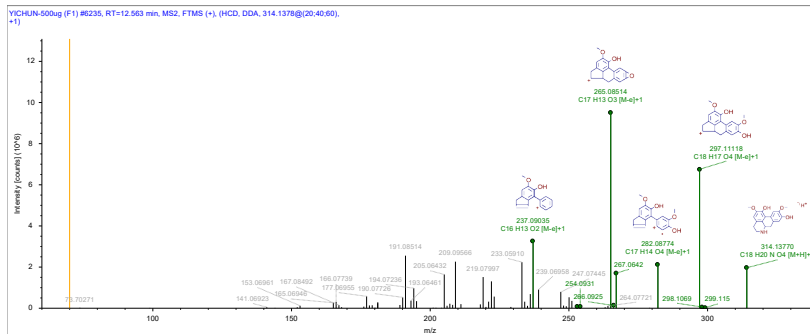


13.371 min Norisoboldine

MS

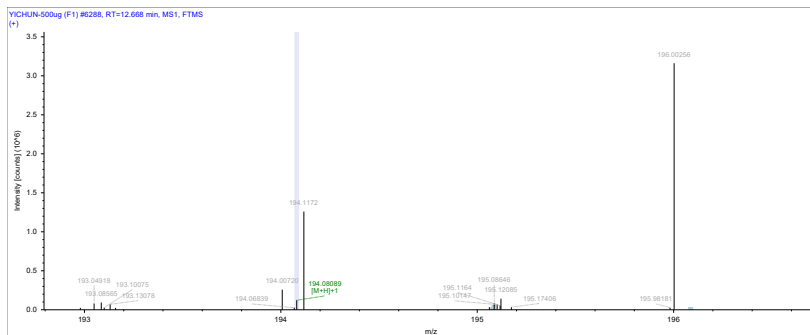


MS/MS

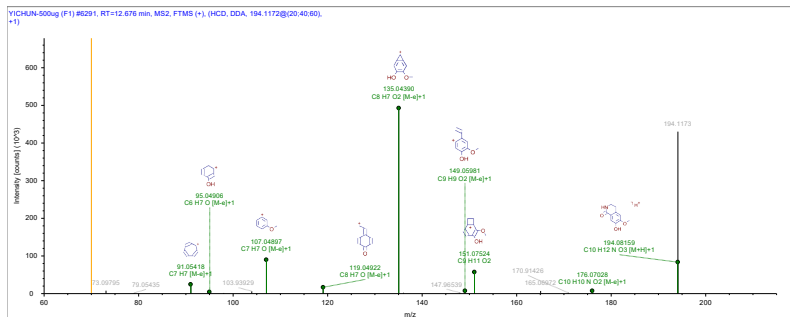


12.83 min Northalifoline

MS

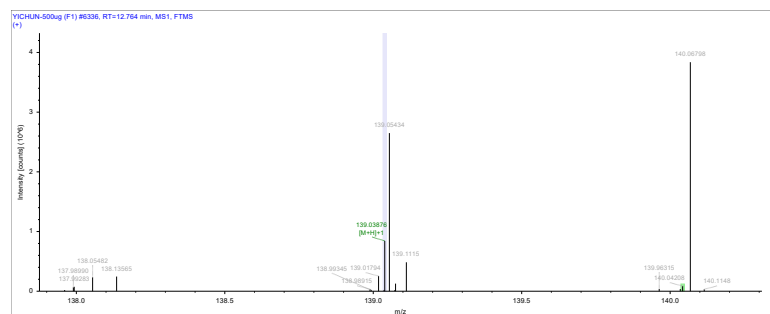


MS/MS

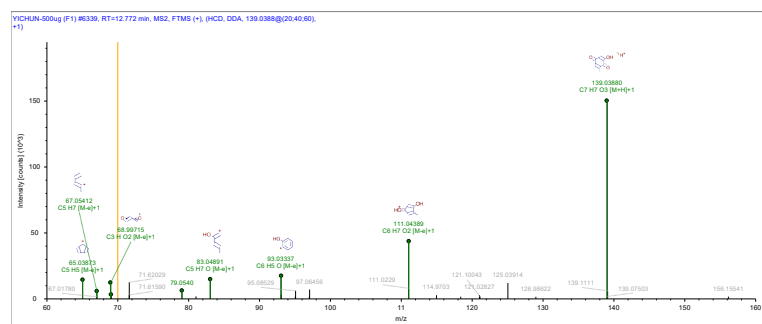


12.866 min 3-hydroxy-2,5-toluquinone

MS

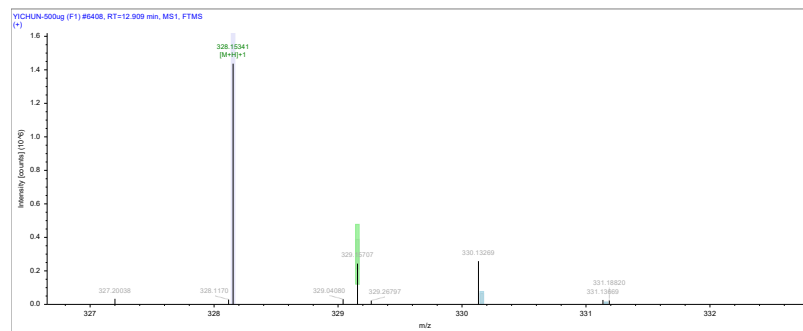


MS/MS

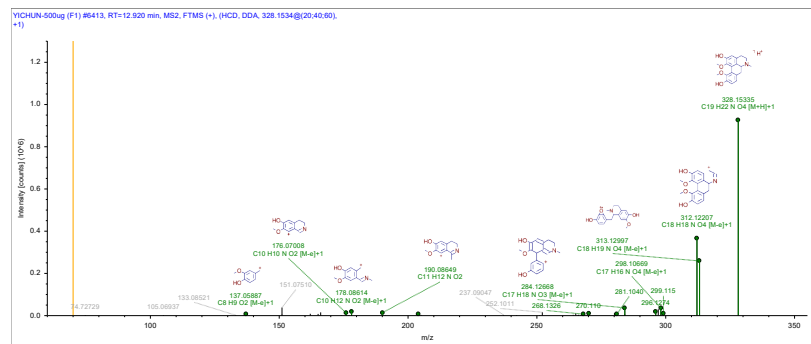


12.99 min N-Methylhernovine

MS

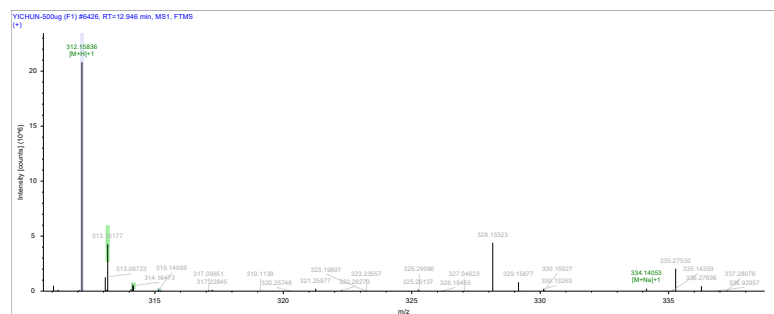


MS/MS

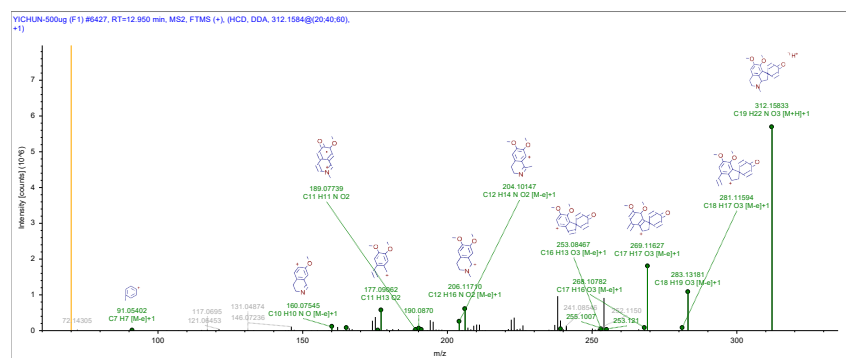


13.008 min Pronuciferine

MS

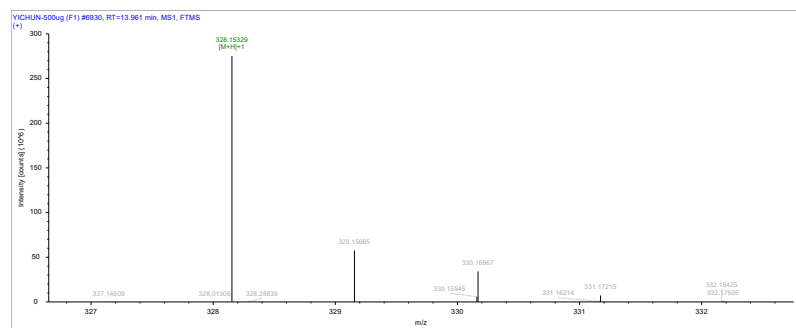


MS/MS

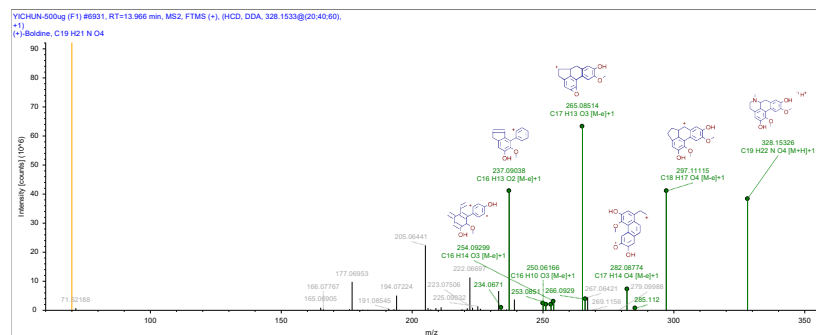


14 min Boldine

MS

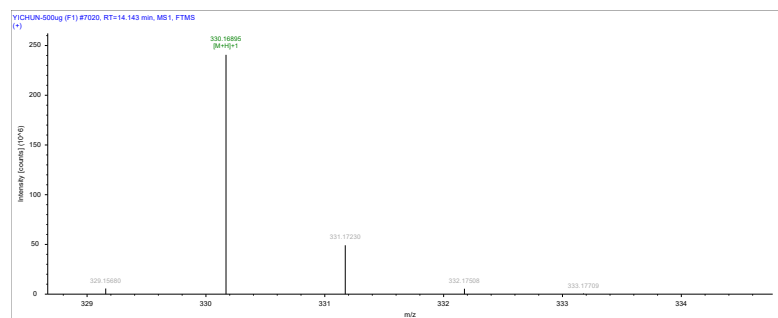


MS/MS

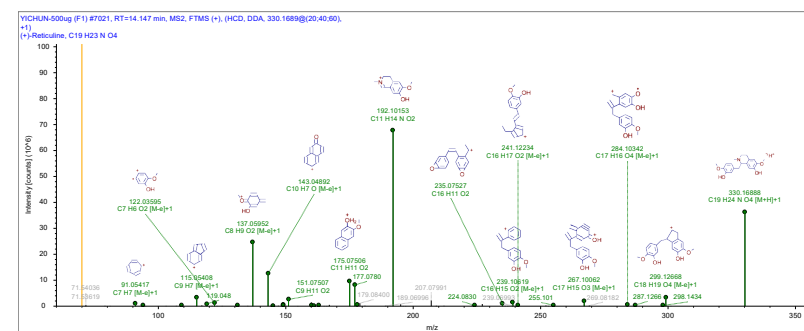


14.138 min Reticuline

MS

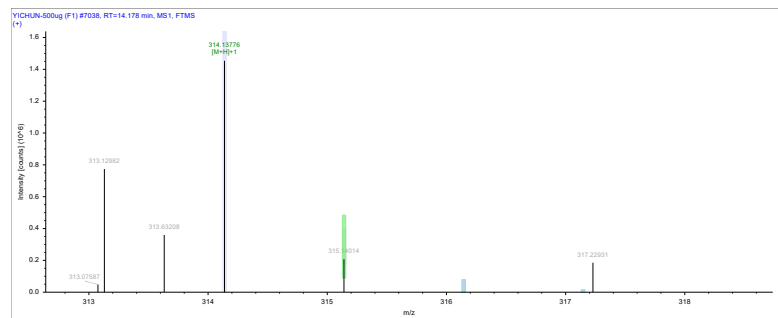


MS/MS

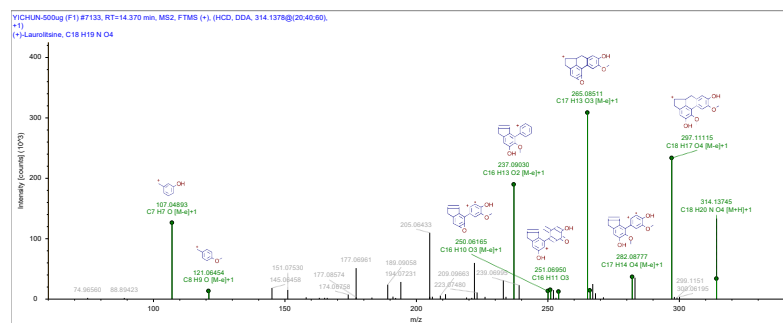


14.242 min Norboldine

MS

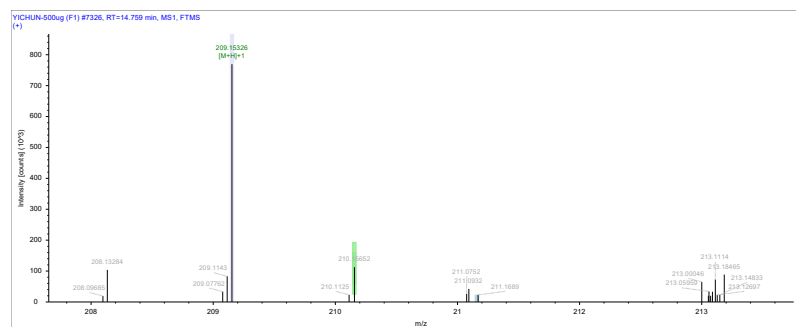


MS/MS

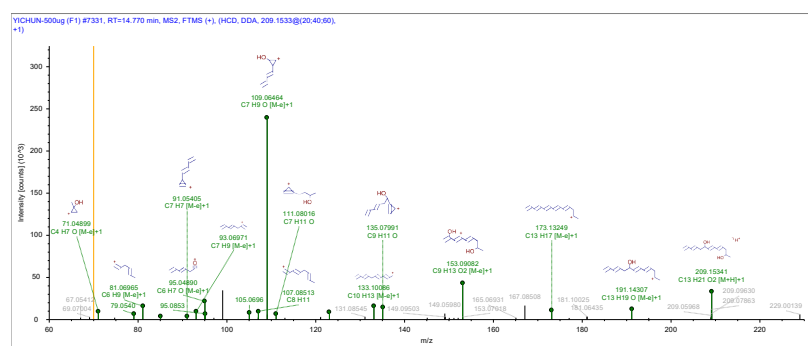


14.818 min 4,6,10,12-Tridecatetraene-2,8-diol

MS

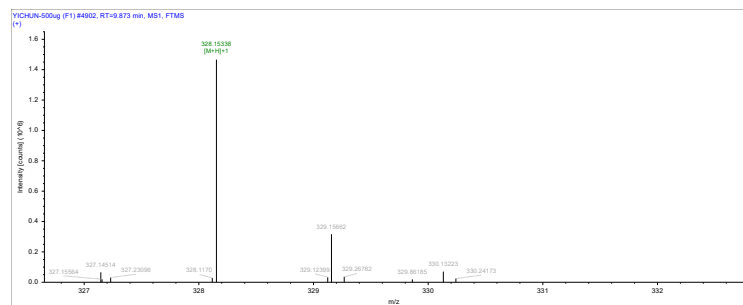


MS/MS

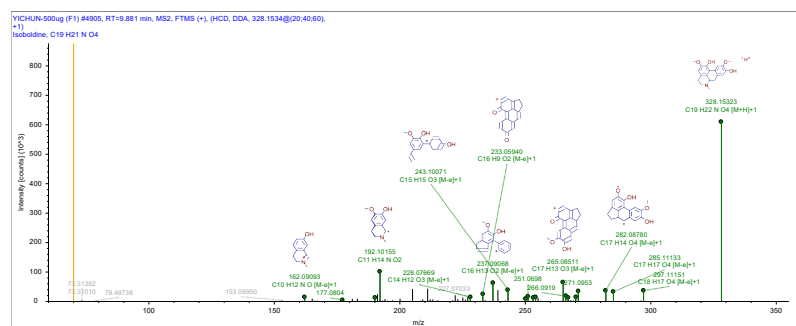


15.924 min Isoboldine

MS

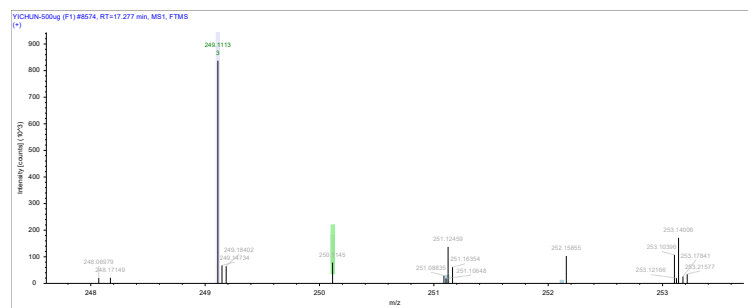


MS/MS

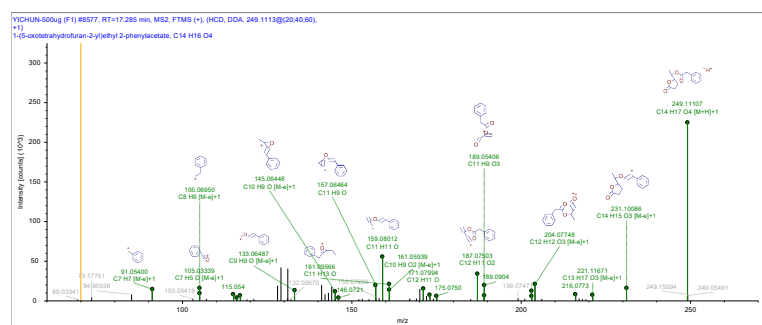


17.327 min 1-(5-oxotetrahydrofuran-2-yl)ethyl 2-phenylacetate

MS

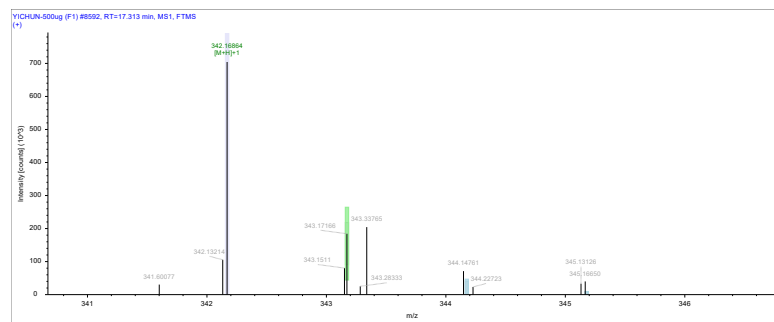


MS/MS

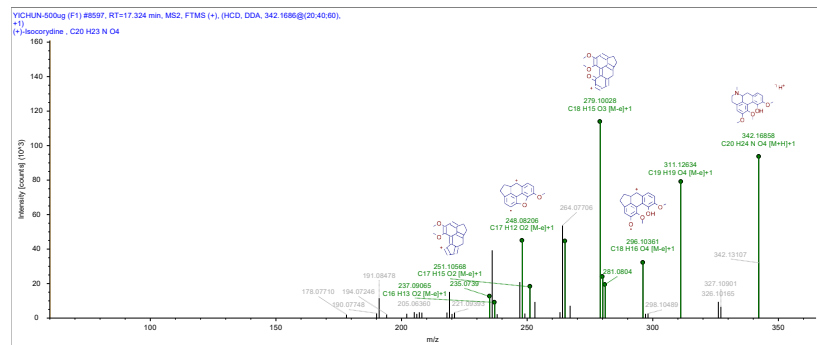


17.398 min Isocorydine

MS

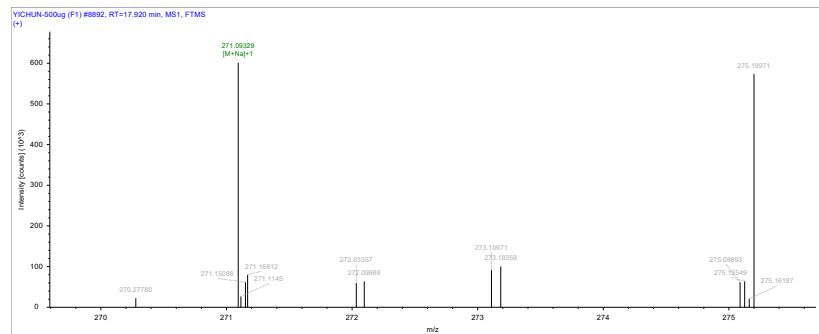


MS/MS

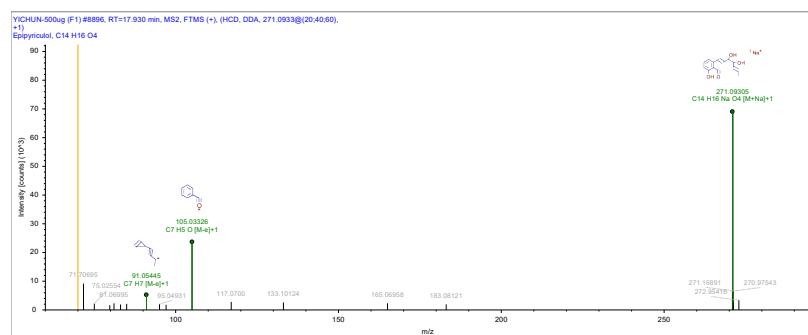


18.013 min Epipyrliculol

MS

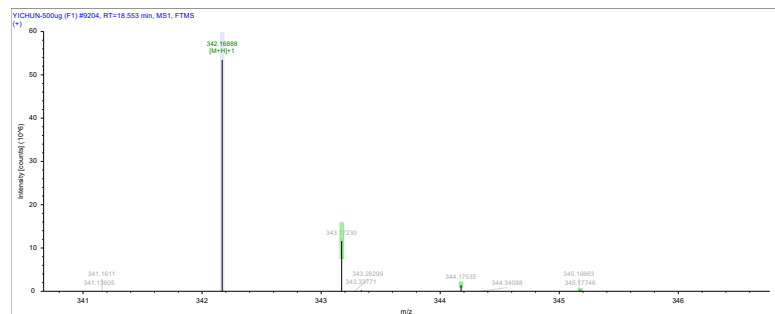


MS/MS

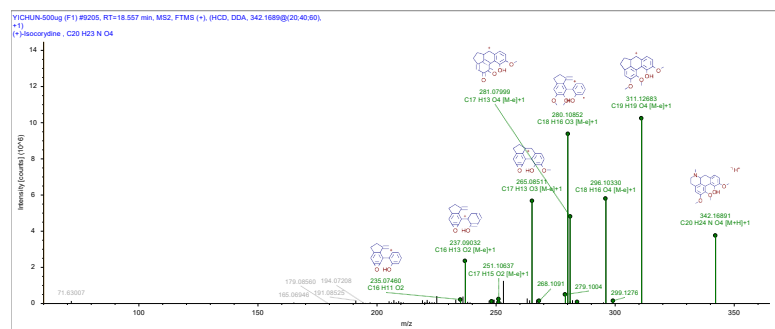


18.58 min N-Methyllaurotetanine

MS

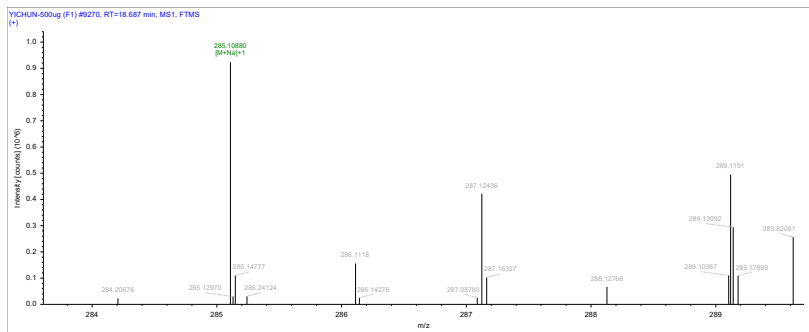


MS/MS

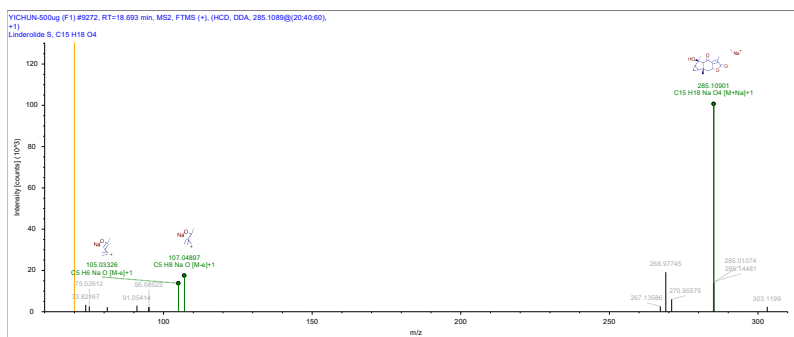


18.915 min Linderolide S

MS

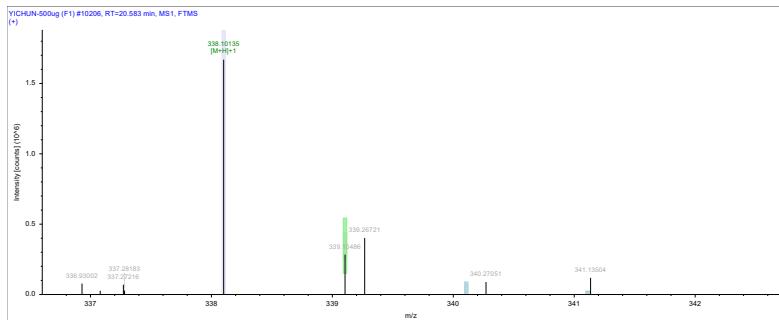


MS/MS

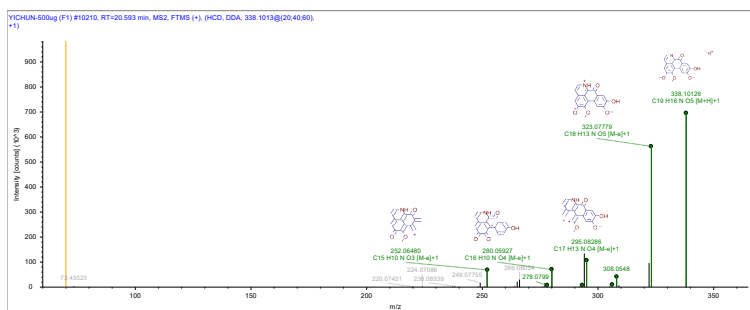


20.637 min 9-Hydroxy-1,2,10-trimethoxy-7H-dibenzo[de,g]quinolin-7-one

MS

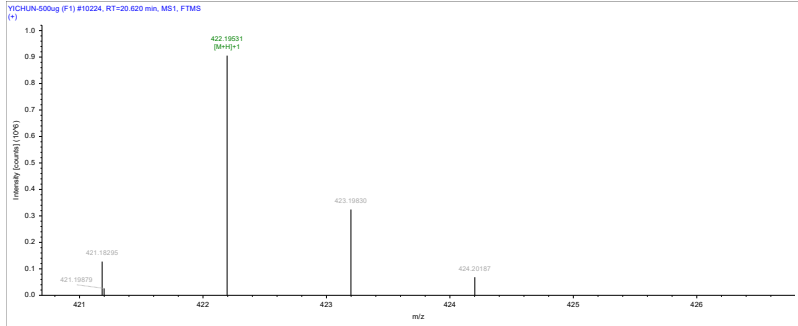


MS/MS

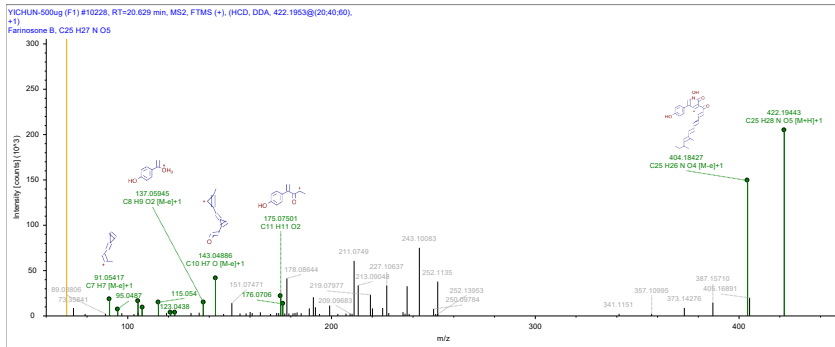


20.757 min Karakoramine

MS

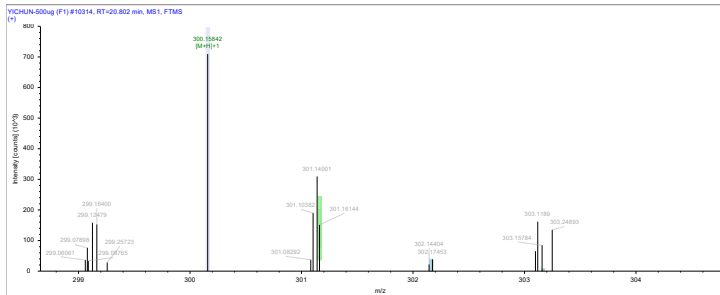


MS/MS

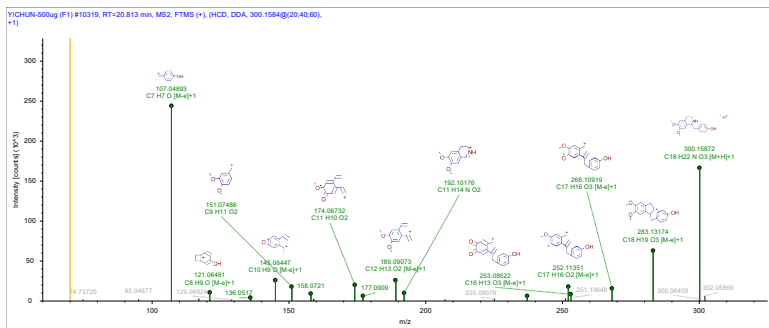


20.807 min Norarmepavine

MS

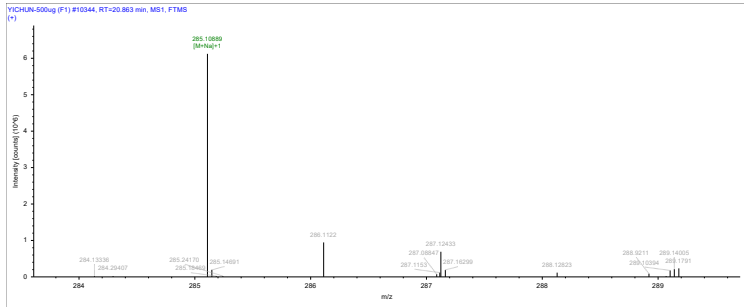


MS/MS

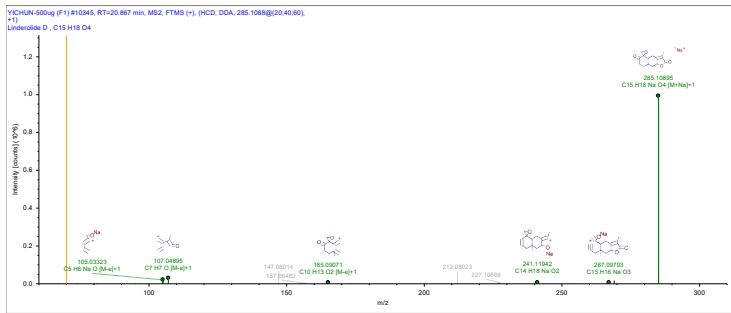


20.884 min Linderolide D

MS

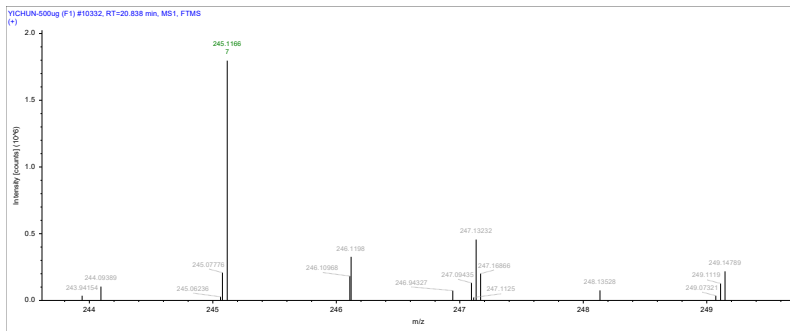


MS/MS

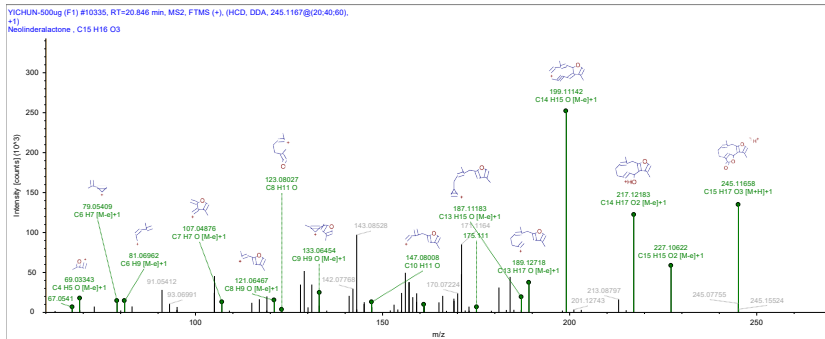


20.89 min Neolinderolactone

MS

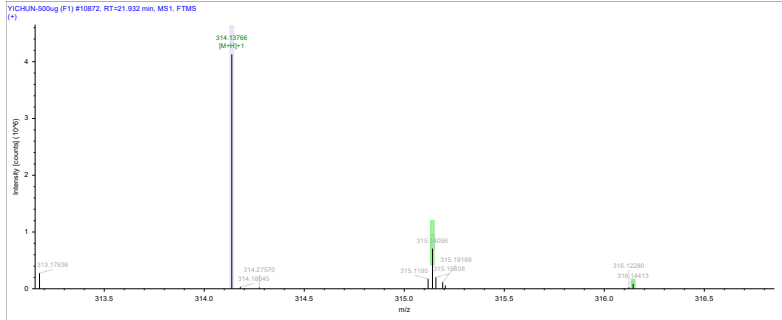


MS/MS

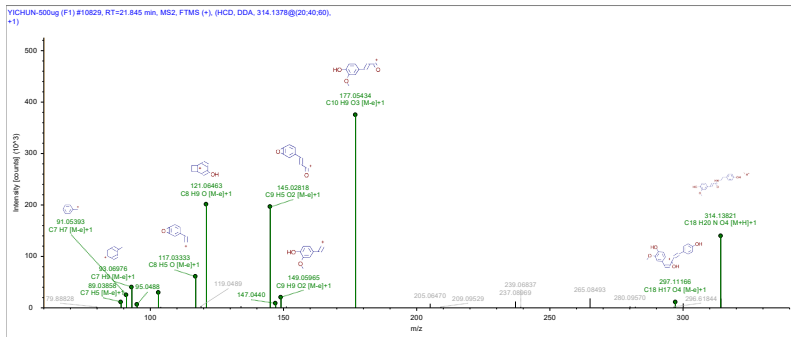


21.927 min *N*-Feruloyltyramine

MS

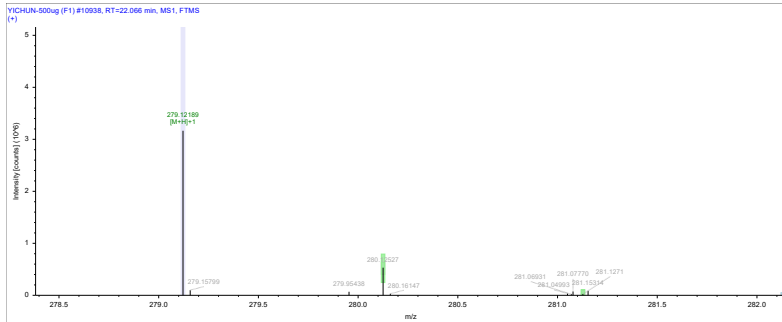


MS/MS

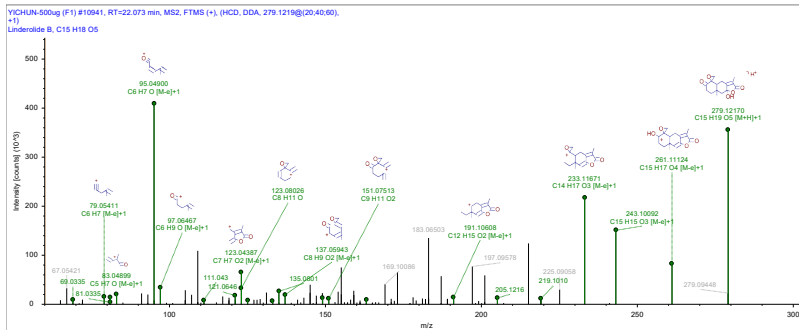


22.125 min Linderolide B

MS

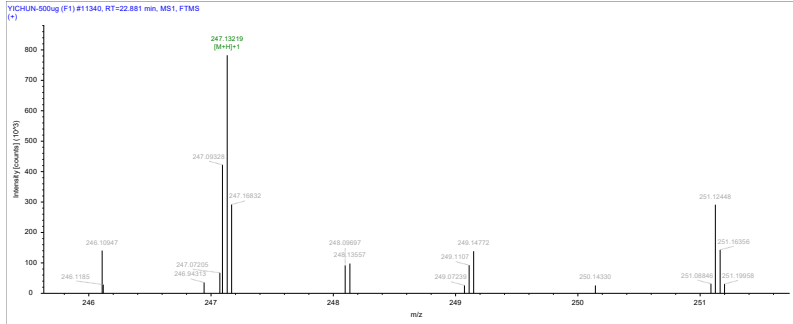


MS/MS

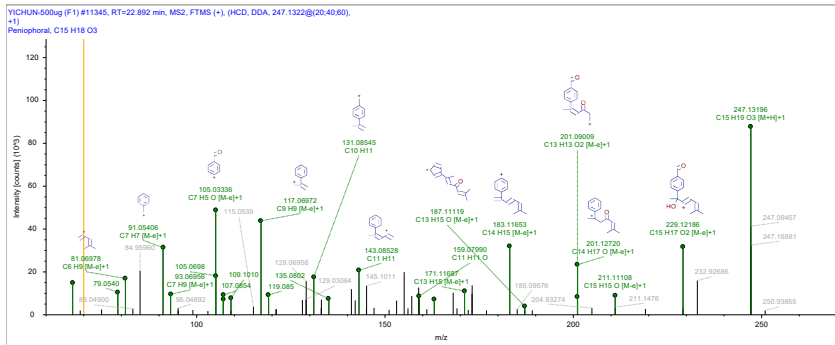


22.901 min Peniophoral

MS

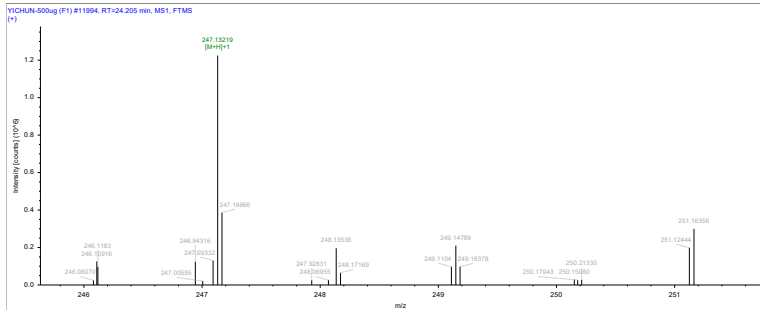


MS/MS

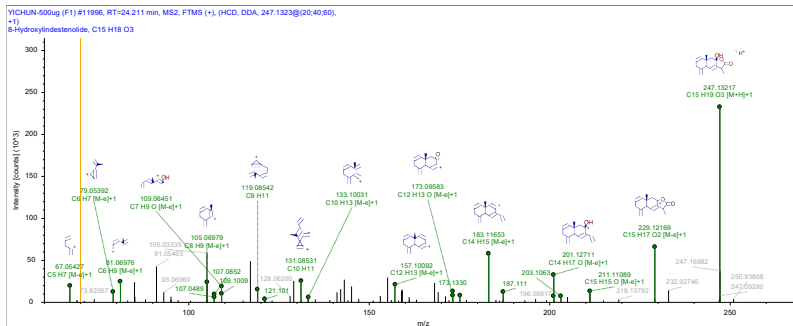


24.674 min 8-Hydroxyindestenolide

MS

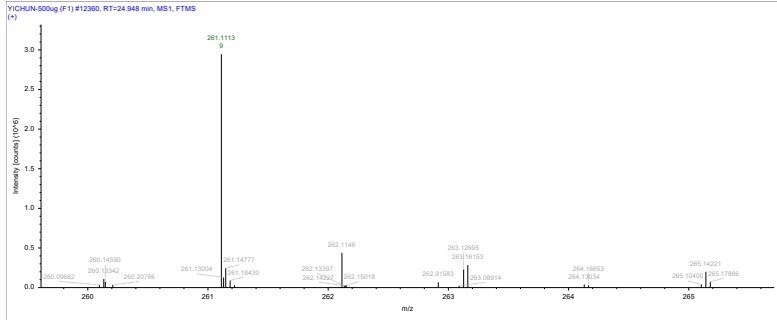


MS/MS

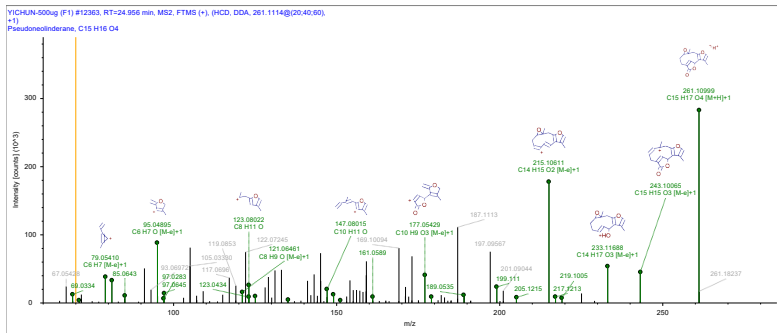


25.094 min Parvigemone

MS

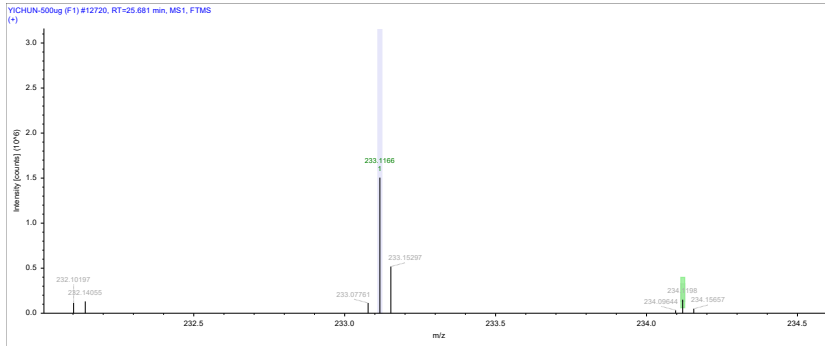


MS/MS

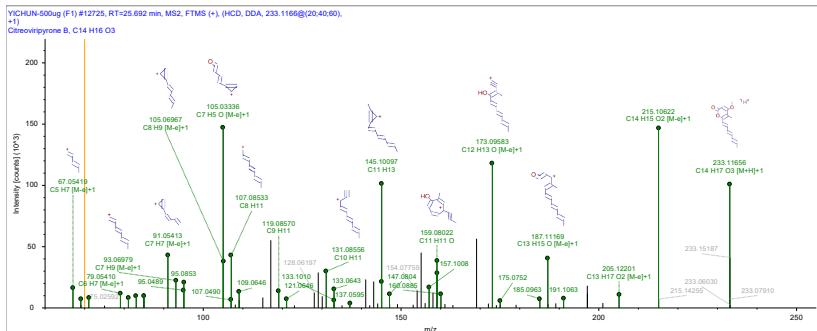


25.788 min Citroeviriprone B

MS

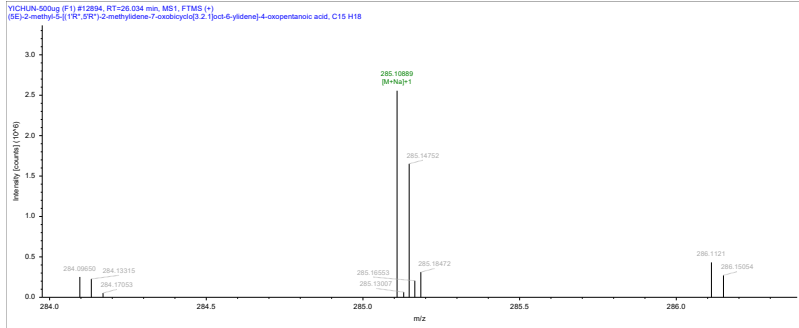


MS/MS

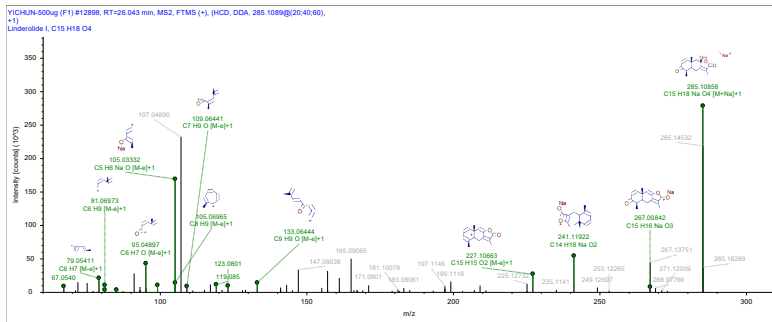


26.105 min Linderolide I

MS

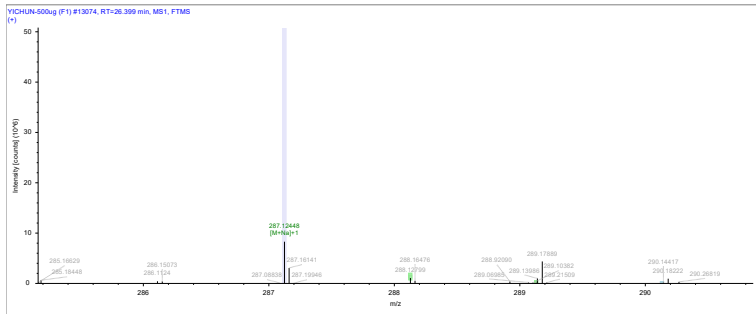


MS/MS

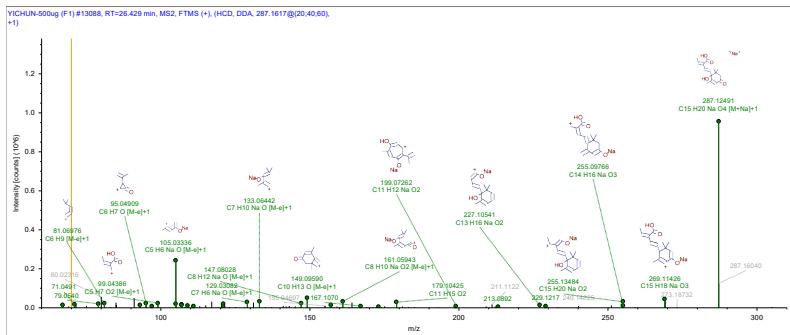


26.402 min 1-methylabscisic-6-acid

MS

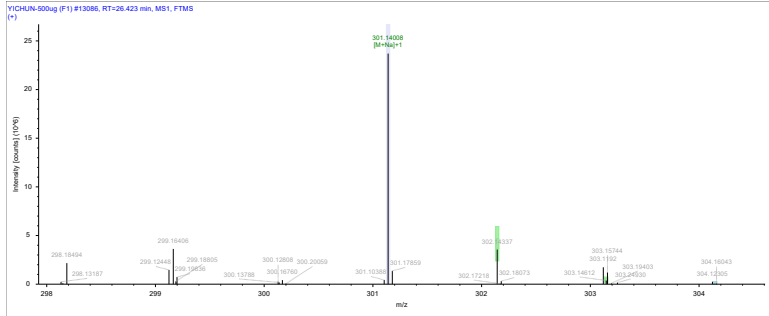


MS/MS

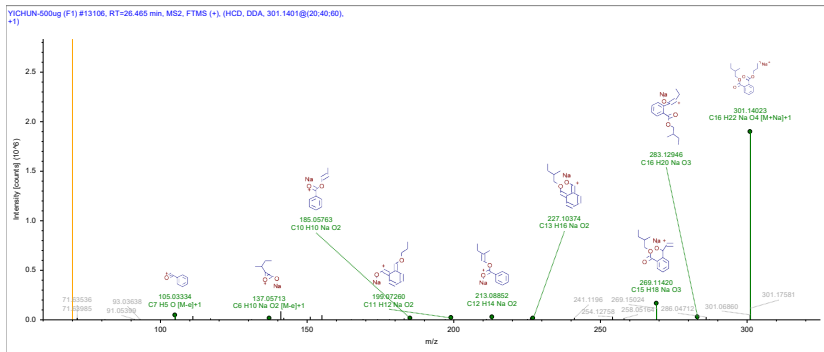


26.419 min 2-methyl butyl propyl phthalate

MS

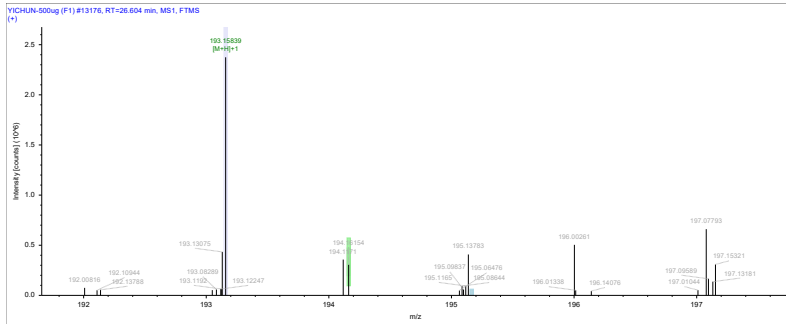


MS/MS

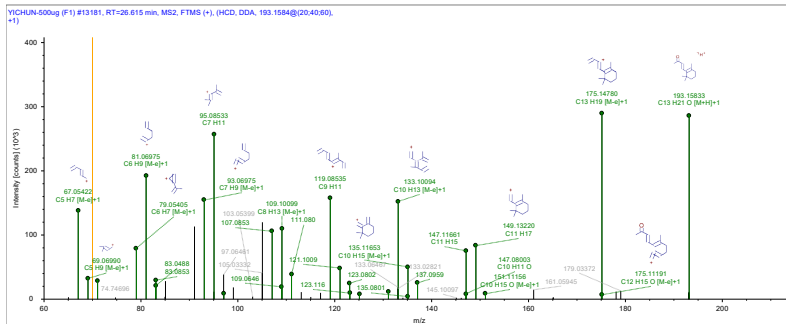


26.622 min β-Ionone

MS

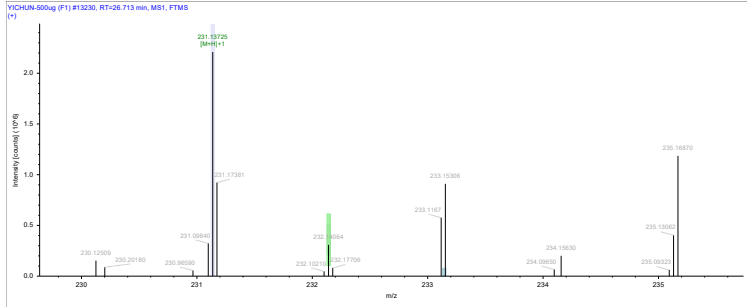


MS/MS

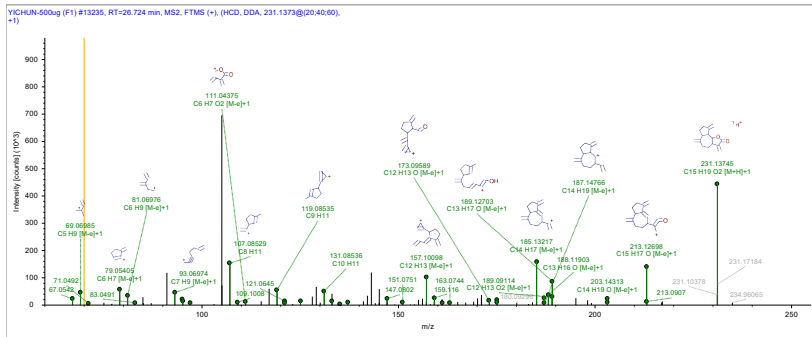


26.727 min Dehydrocostus lactone

MS

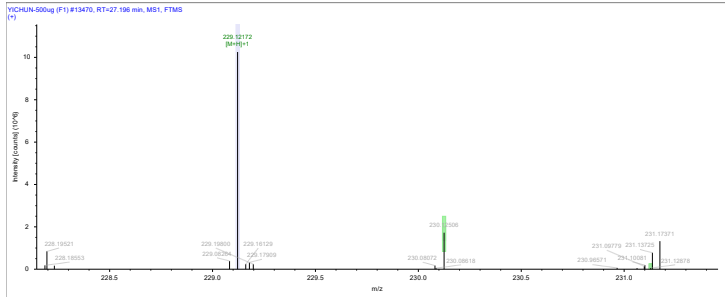


MS/MS

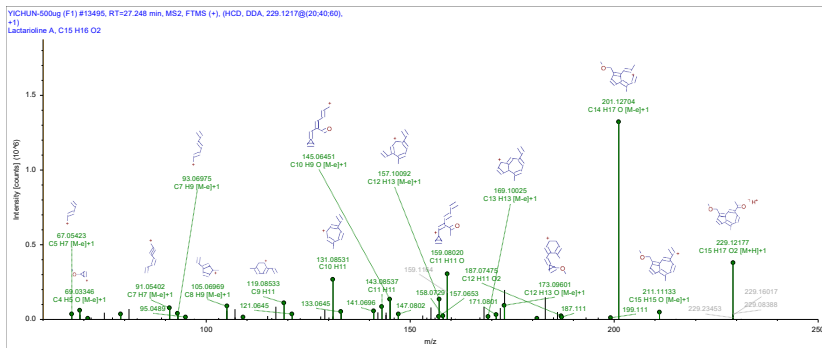


27.194 min Lactarioline A

MS

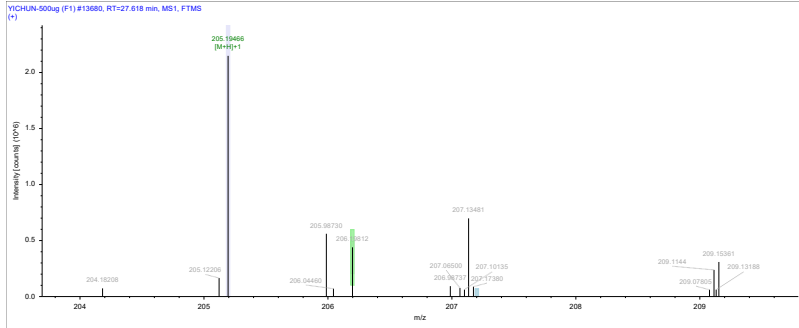


MS/MS

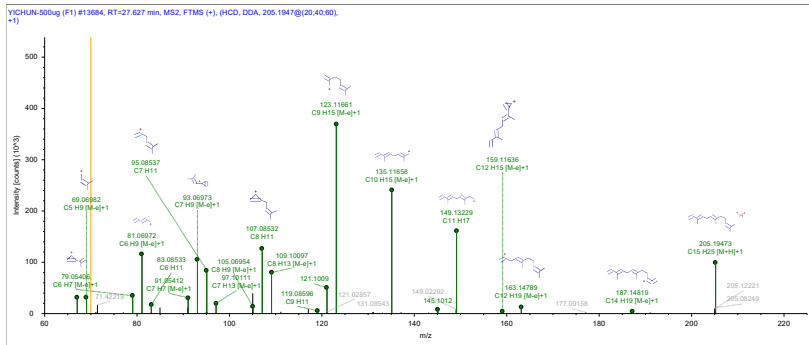


27.639 min α -Farnesene

MS

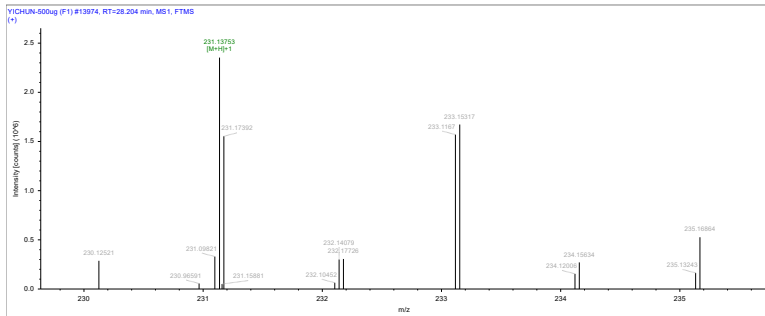


MS/MS

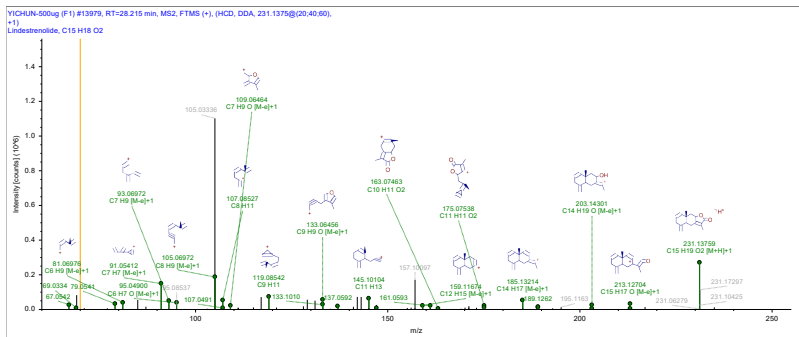


27.999 min Lindrestrenolide

MS

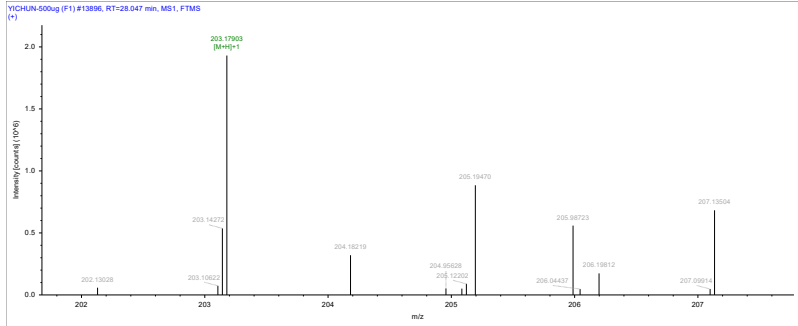


MS/MS

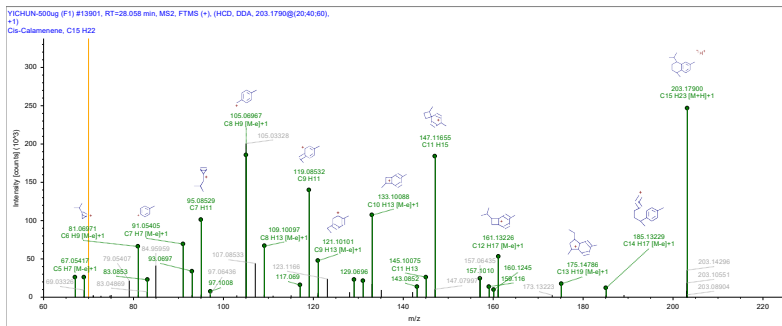


28.054 min Calamenene

MS

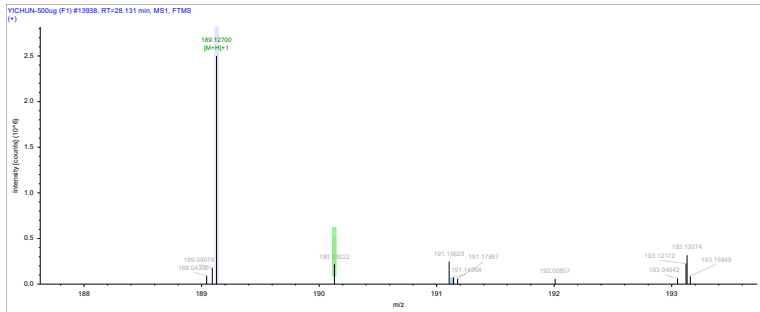


MS/MS

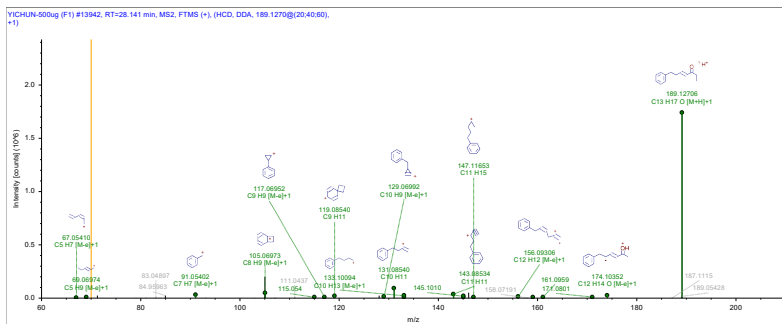


28.159 min 1-Phenylhept-3-en-4-one

MS

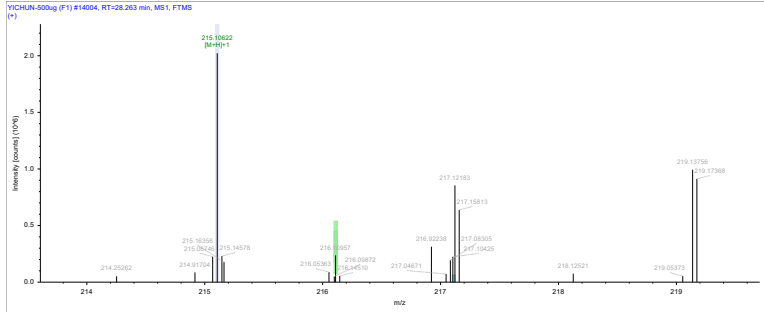


MS/MS

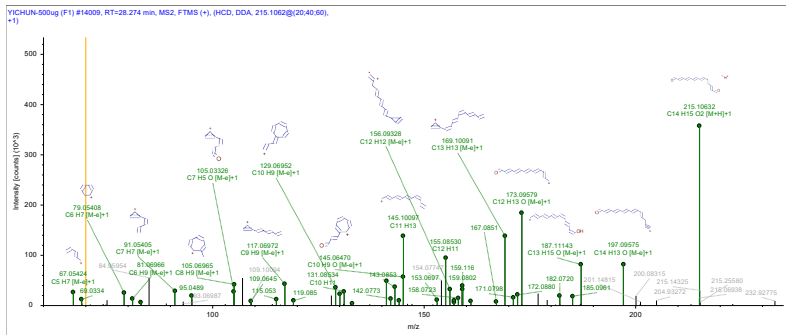


28.288 min 2,4,6,8,10,12-tetradeca-1,14-hexenedial

MS

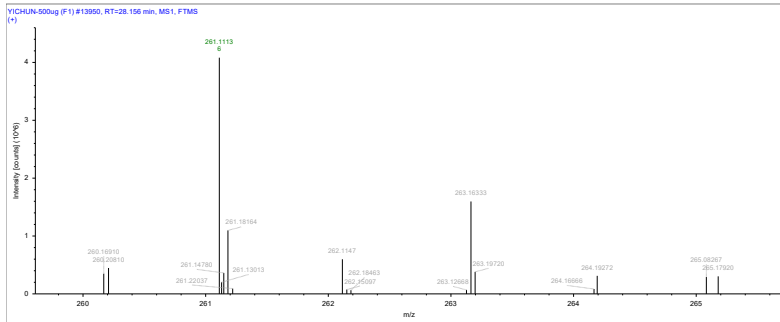


MS/MS

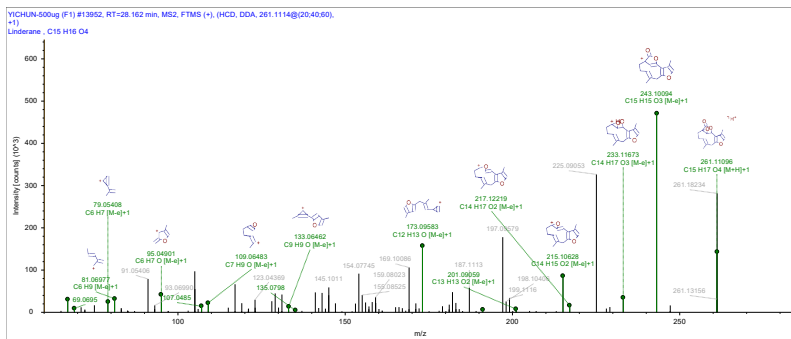


28.299 min Linderane

MS

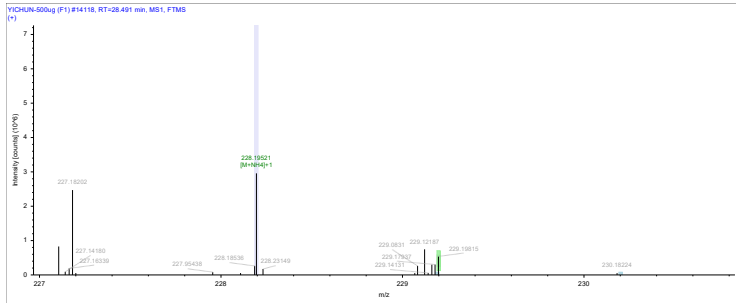


MS/MS

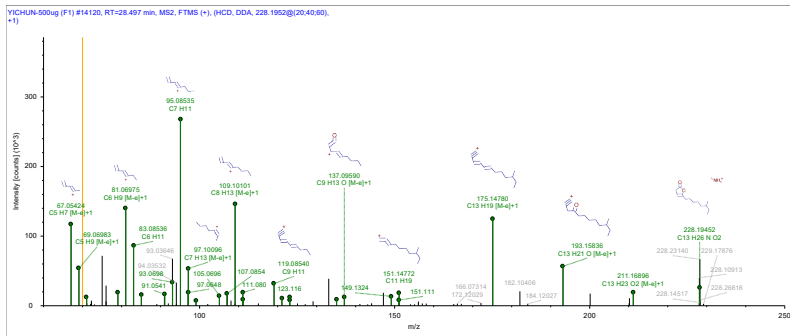


28.448 min 10-Methyldodec-3-en-4-olide

MS

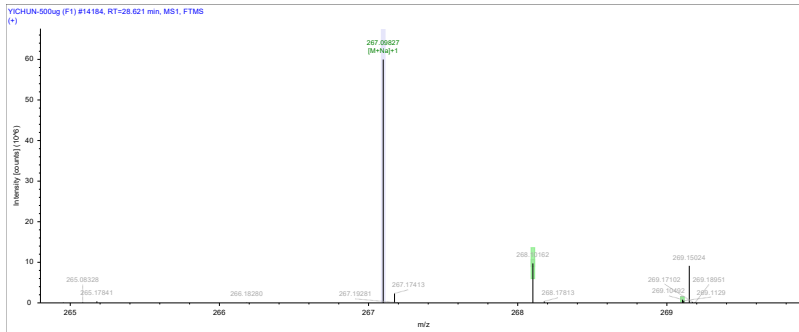


MS/MS

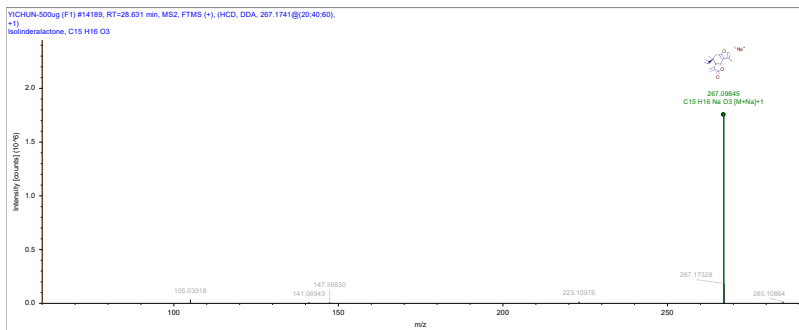


28.695 min Isolinderalactone

MS

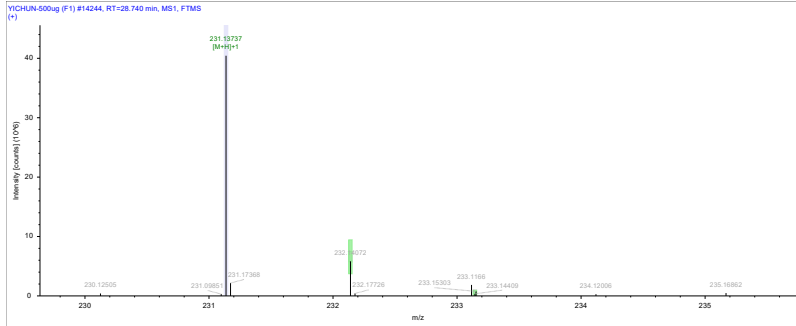


MS/MS

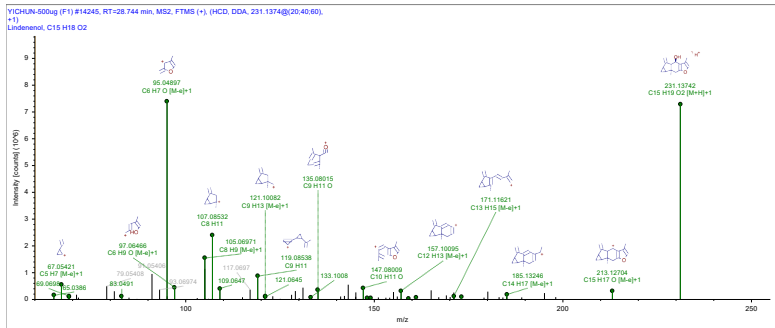


28.742 min Lindenol

MS

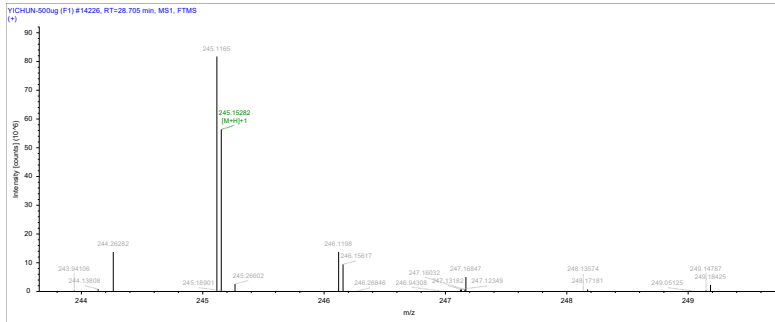


MS/MS

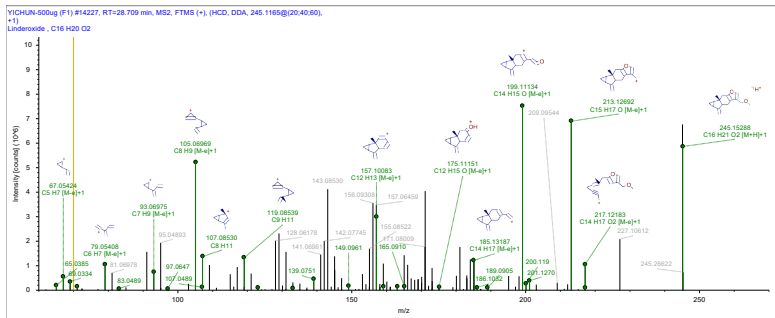


28.74 min Linderoxide

MS

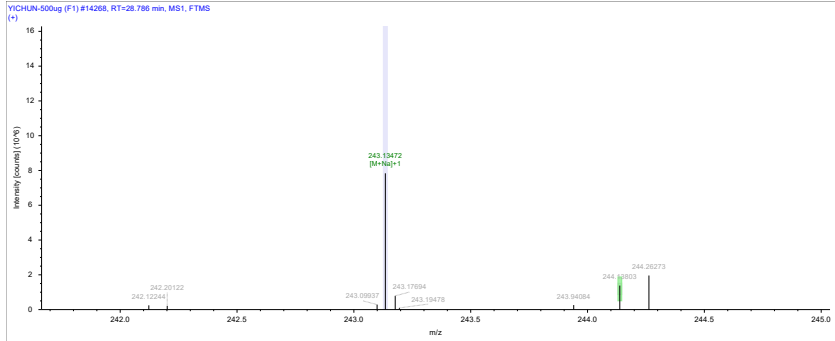


MS/MS

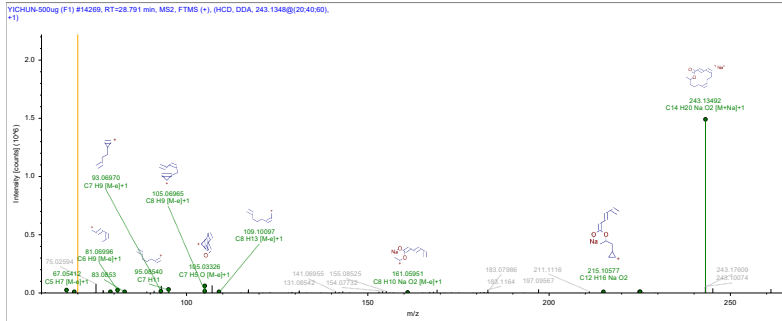


28.764 min Benquone

MS

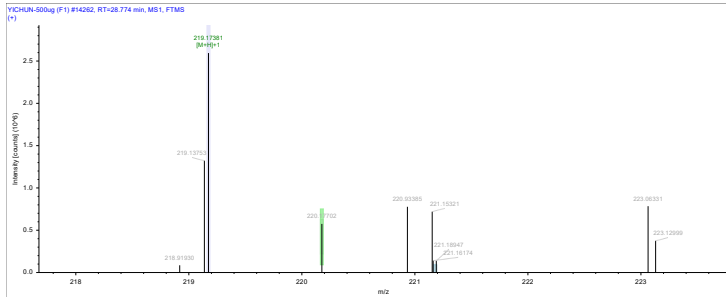


MS/MS

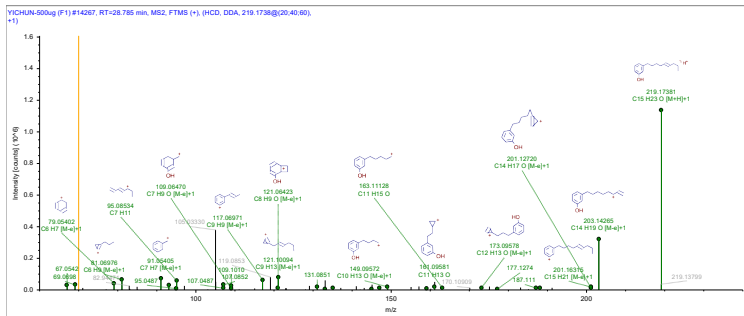


28.807min Anaephene A

MS

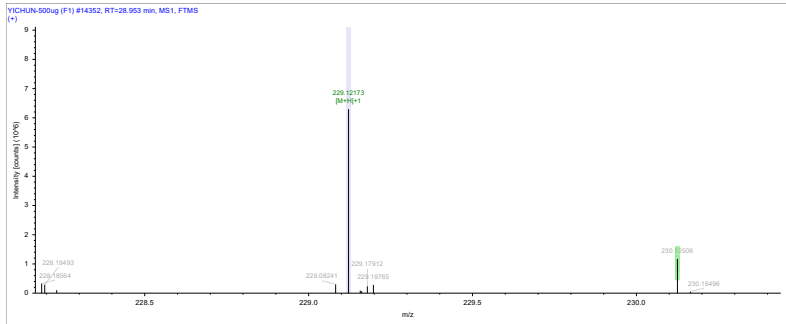


MS/MS

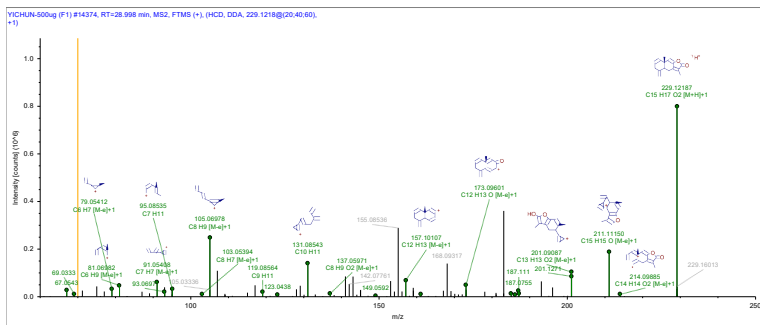


28.957 min Dehydrolindestrenolide

MS

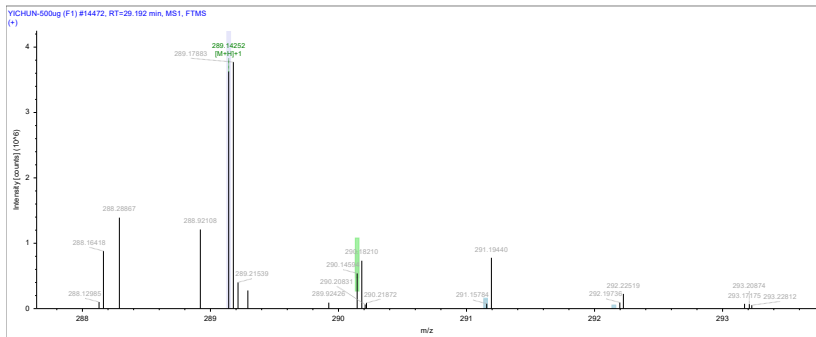


MS/MS

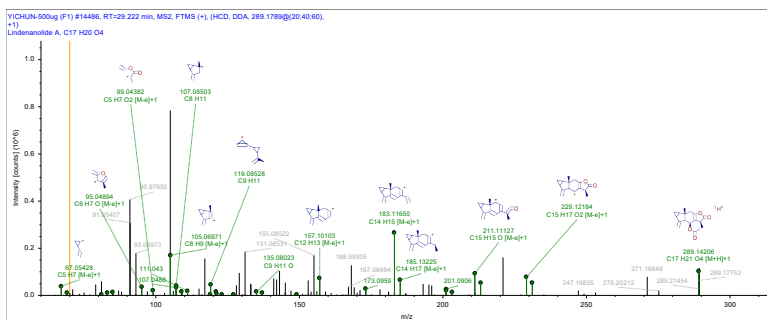


29.195 min Lindenanolide A

MS

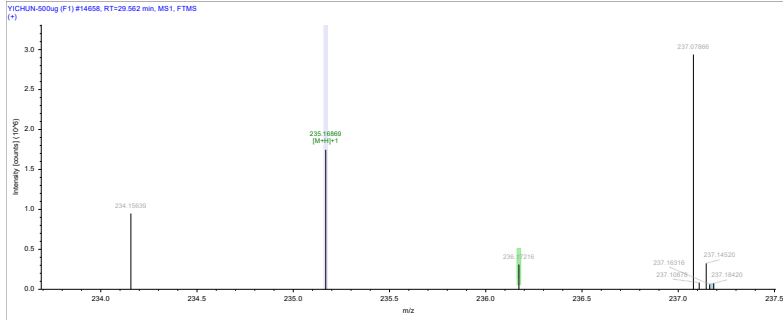


MS/MS

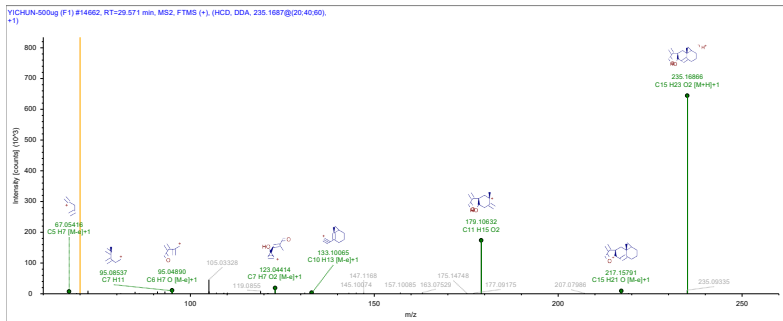


29.58 min Nigriterpene E

MS

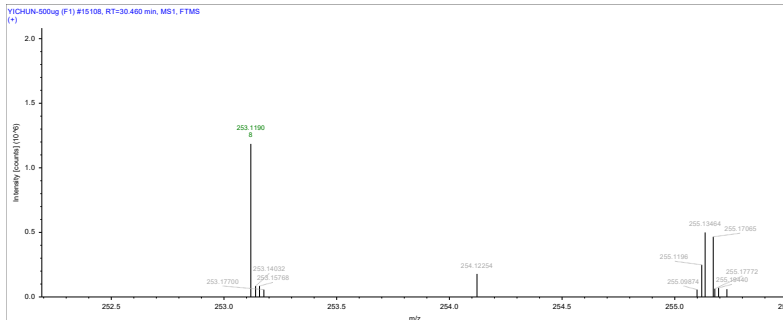


MS/MS

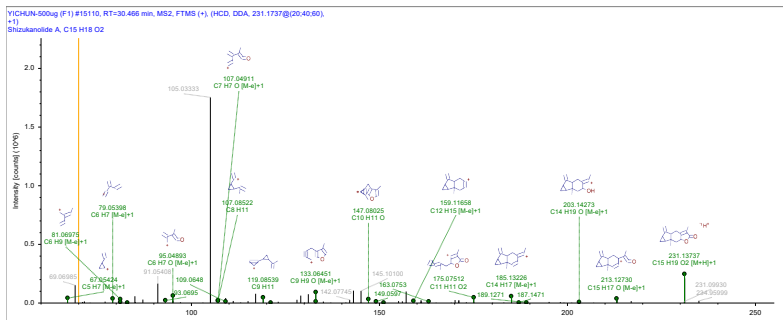


30.521 min Shizukanolide A

MS

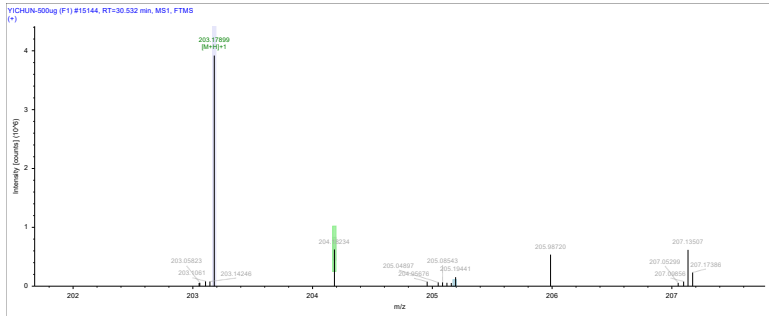


MS/MS

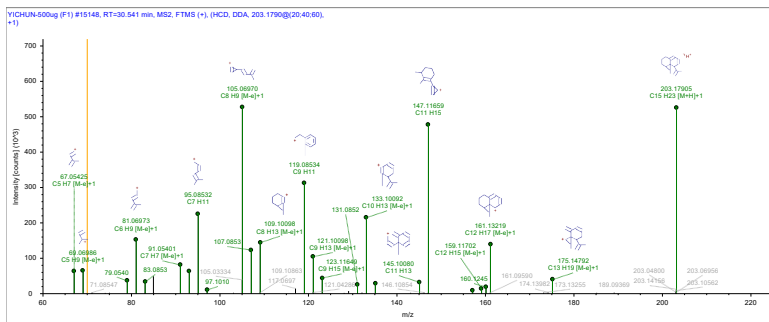


30.57 min Rulepidadiene B

MS



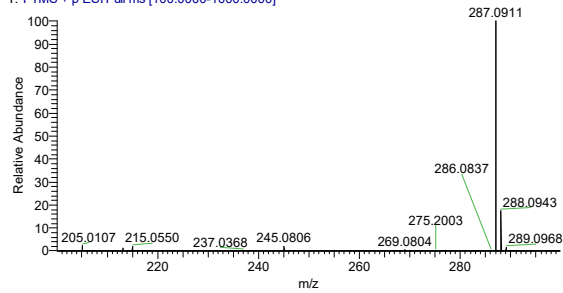
MS/MS



33.03 min Linderone

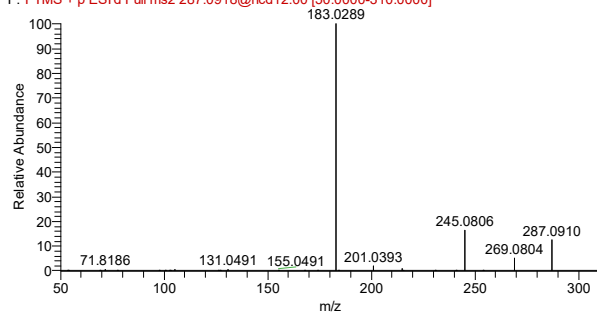
MS

Mix-Tie-6kinds-5ul #7950 RT: 33.04 AV: 1 NL: 1.72E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]



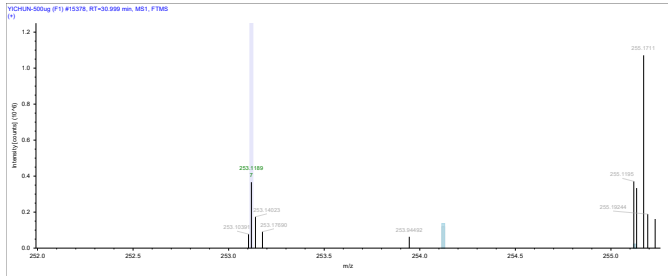
MS/MS

Mix-Tie-6kinds-5ul #7935 RT: 32.98 AV: 1 NL: 4.80E8
F: FTMS + p ESI d Full ms2 287.0918@hcd12.00 [50.0000-310.0000]

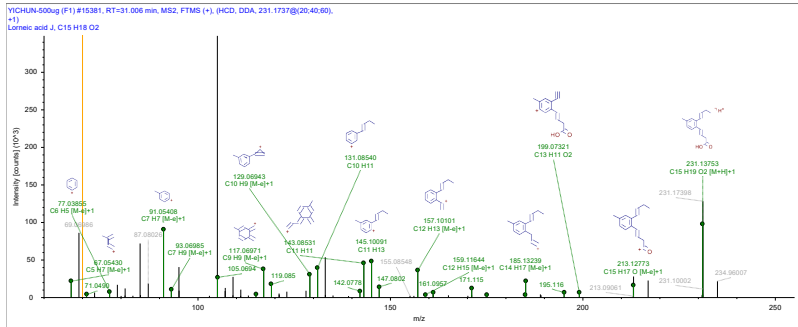


31.272 min Lorneic acid J

MS

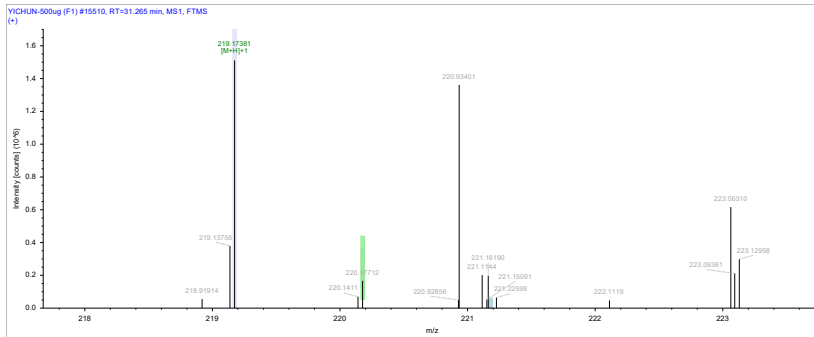


MS/MS

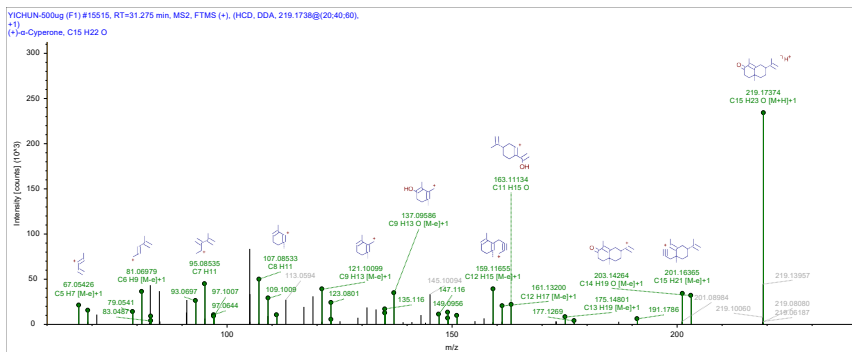


31.299 min (+)- α -Cyperone

MS

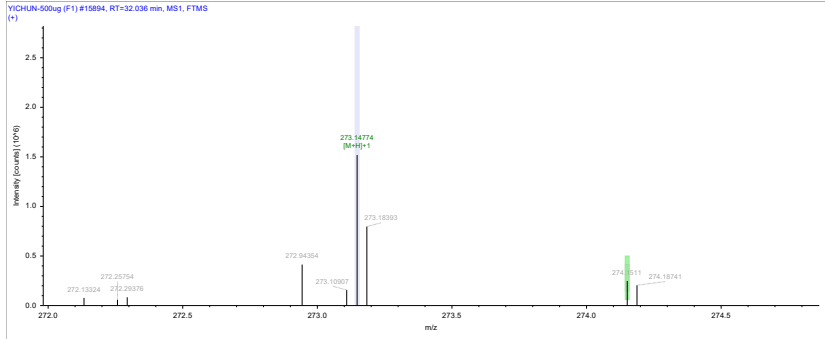


MS/MS

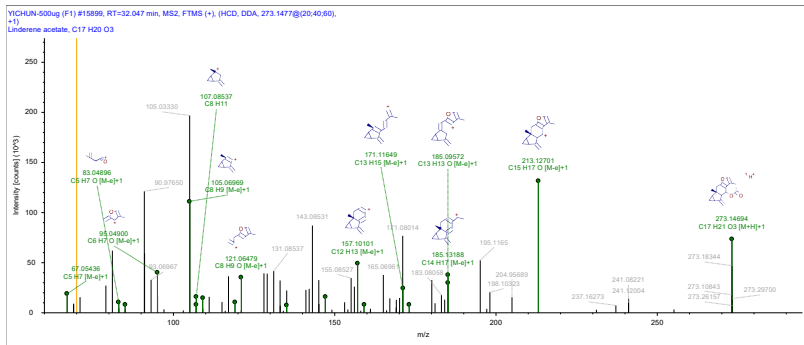


32.087 min Linderenyl acetate

MS

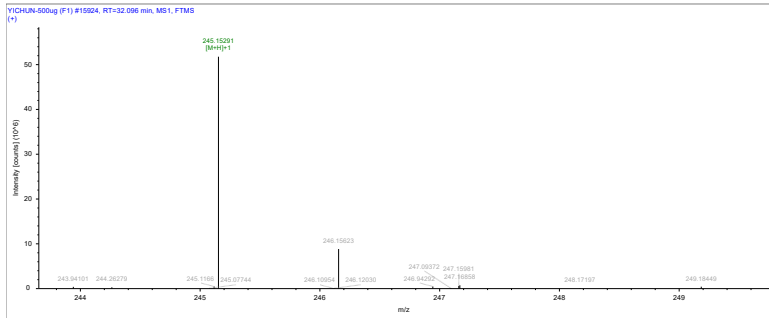


MS/MS

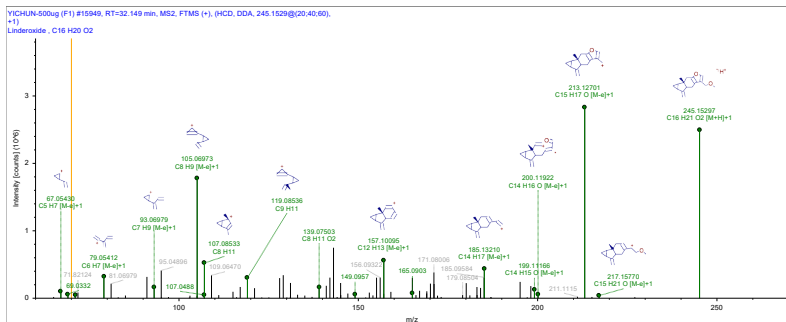


32.093 min Isolinderoxide

MS



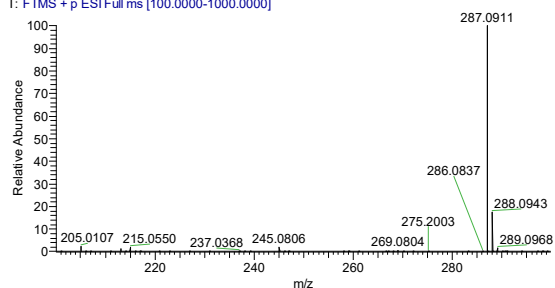
MS/MS



32.92 min (2E,3R,4S)-2-dodecylinene-3-hydroxy-4-ethoxy-4-methylbutanolide

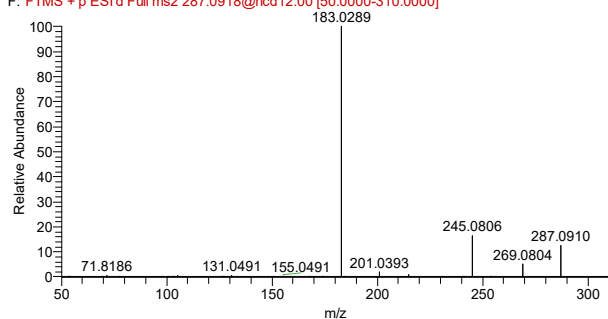
MS

Mix-Tie-6kinds-5ul #7950 RT: 33.04 AV: 1 NL: 1.72E9
T: FTMS + p ESI Full ms [100.0000-1000.0000]



MS/MS

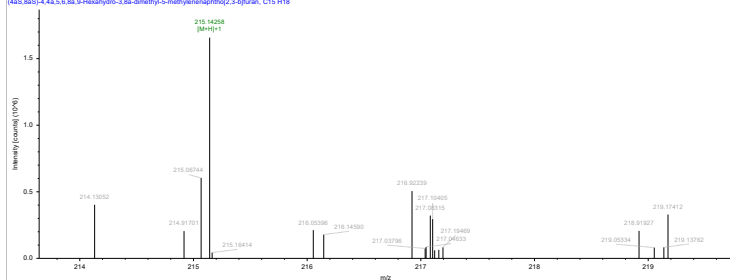
Mix-Tie-6kinds-5ul #7935 RT: 32.98 AV: 1 NL: 4.80E8
F: FTMS + p ESI d Full ms2 287.0918@hcd12.00 [50.0000-310.0000]



32.966 min (4aS,8aS)-4,4a,5,6,8a,9-Hexahydro-3,8a-dimethyl-5-methylenenaphtho[2,3-b]furan

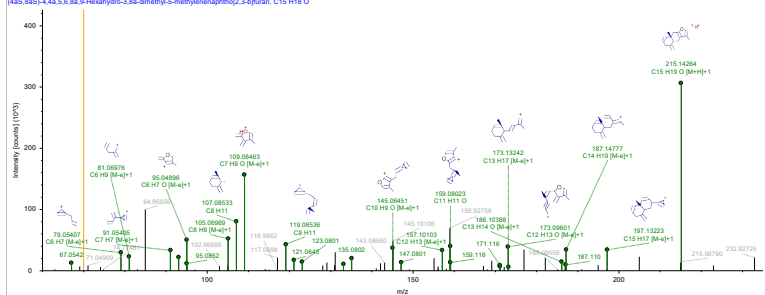
MS

VICHUN-500ug (F1) #18320, RT:32.89 min, MS1, FTMS (+)
(4aS,8aS)-4,4a,5,6,8a,9-Hexahydro-3,8a-dimethyl-5-methylenenaphtho[2,3-b]furan, C15 H18



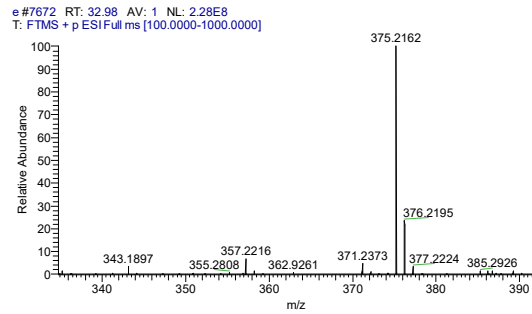
MS/MS

VICHUN-500ug (F1) #18320, RT:32.901 min, MS2, FTMS (+), (HCD, DDA, 215.14258@20:40:60)
(4aS,8aS)-4,4a,5,6,8a,9-Hexahydro-3,8a-dimethyl-5-methylenenaphtho[2,3-b]furan, C15 H18 O

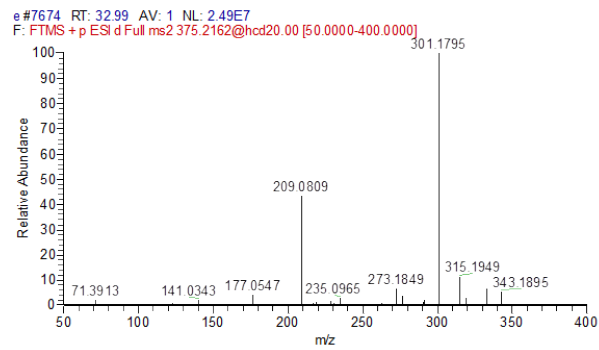


32.99 min 1-acetyl-4-methoxyl-denudaquinol

MS

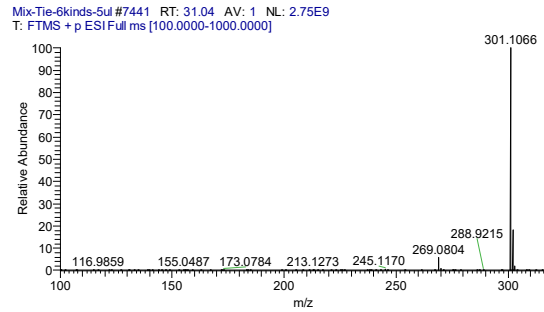


MS/MS

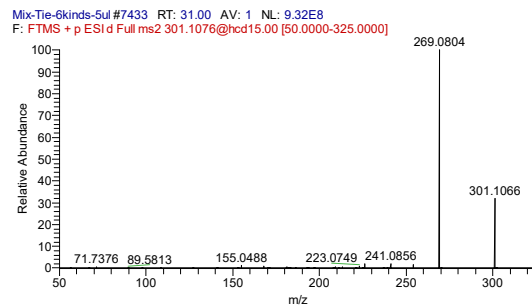


33.03 min methylinderone

MS



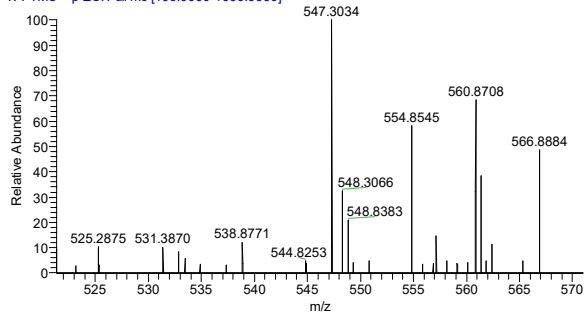
MS/MS



33.29 min linderin B

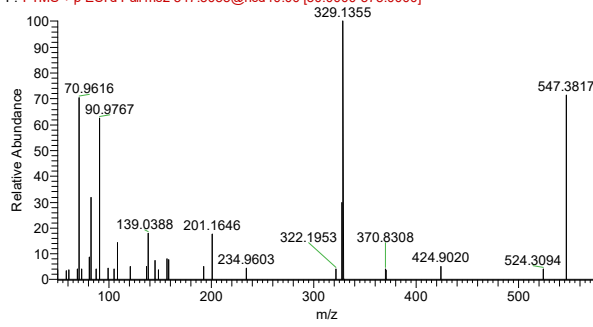
MS

a #8071 RT: 33.29 AV: 1 NL: 1.57E6
T: FTMS + p ESI Full ms [100.0000-1000.0000]



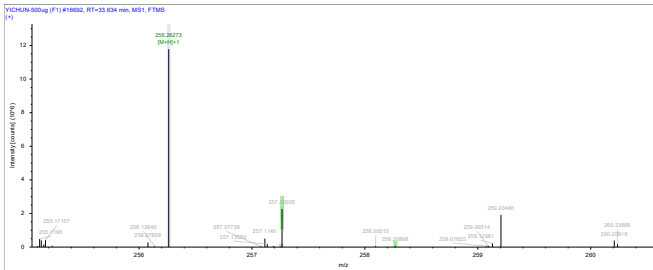
MS/MS

a #8064 RT: 33.27 AV: 1 NL: 3.47E4
F: FTMS + p ESI d Full ms2 547.3035@hcd40.00 [50.0000-575.0000]

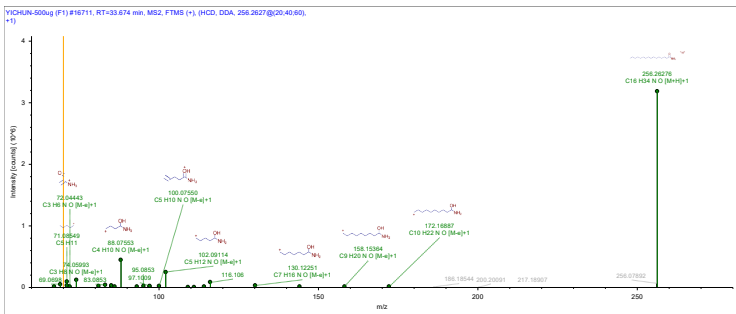


33.634 min Hexadecanamide

MS



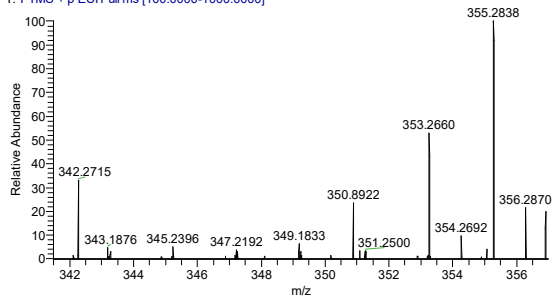
MS/MS



34.49 min (2E,3R,4S)-2-tetradecylinene-3-hydroxy-4-ethoxy-4-methylbutanolid

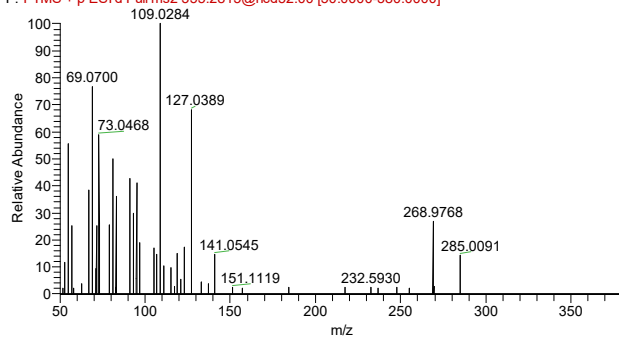
MS

1#7941 RT: 34.20 AV: 1 NL: 1.13E7
T: FTMS + p ESI Full ms [100.0000-1000.0000]



MS/MS

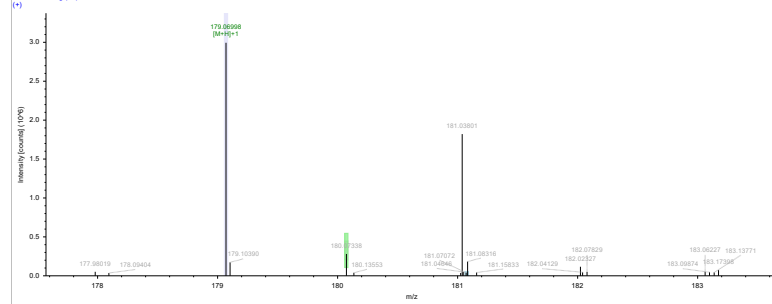
1#8010 RT: 34.49 AV: 1 NL: 3.96E5
F: FTMS + p ESI d Full ms 2 355.2815@hcd52.00 [50.0000-380.0000]



34.558 min Coniferyl aldehyde

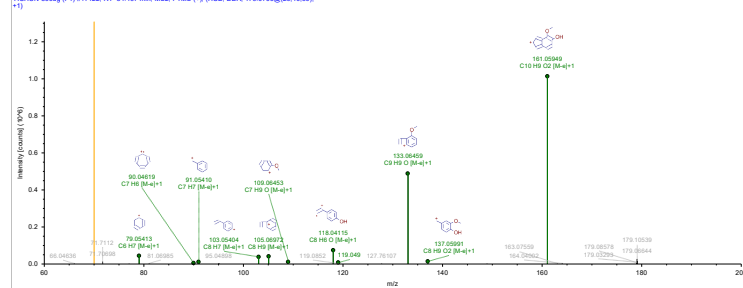
MS

VICHUN-500ug (F1) #17154 RT=34.561 min, MS1, FTMS



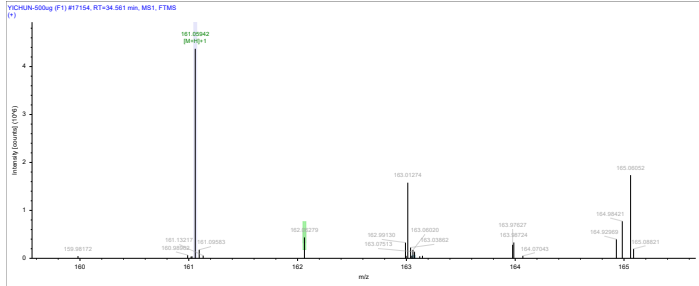
MS/MS

VICHUN-500ug (F1) #17122 RT=34.497 min, MS2, FTMS (+) (HCD, DDA, 179.0700@20.45.60)

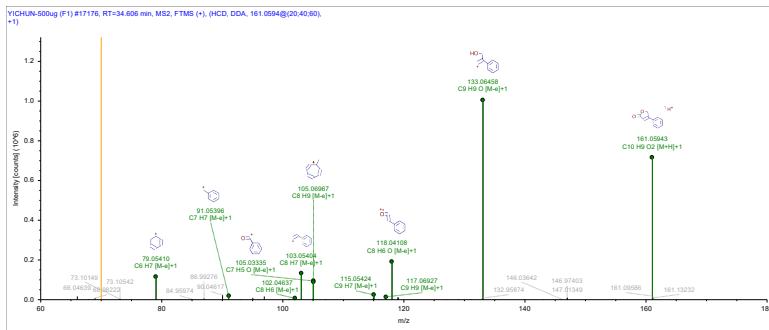


34.559 min Ralfuranone A

MS



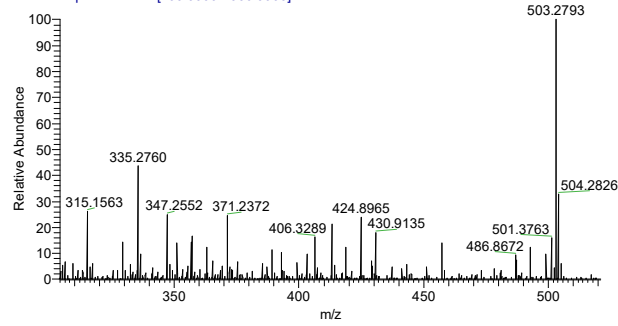
MS/MS



34.83 min lindechunisin A

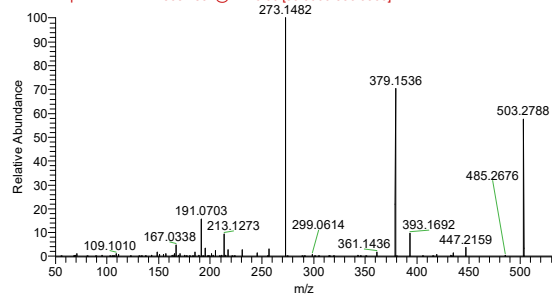
MS

b #8114 RT: 34.82 AV: 1 NL: 1.82E7
T: FTMS + p ESI Full ms [100.0000-1000.0000]



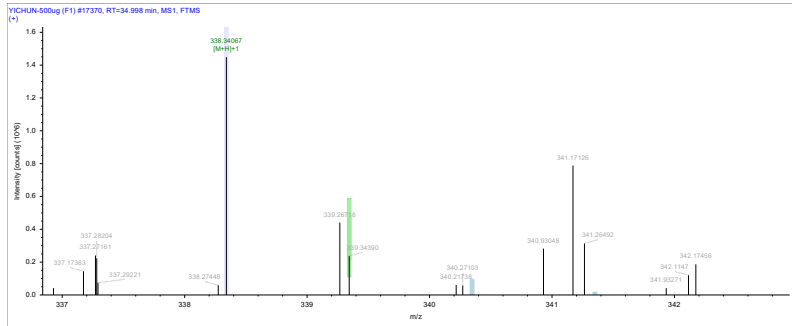
MS/MS

b #8107 RT: 34.80 AV: 1 NL: 3.66E6
F: FTMS + p ESI Full ms2 503.2832@hcd20.00 [50.0000-530.0000]

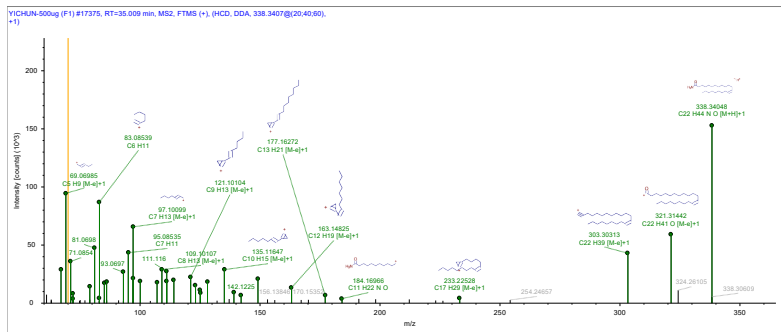


35.129 min Erucamide

MS

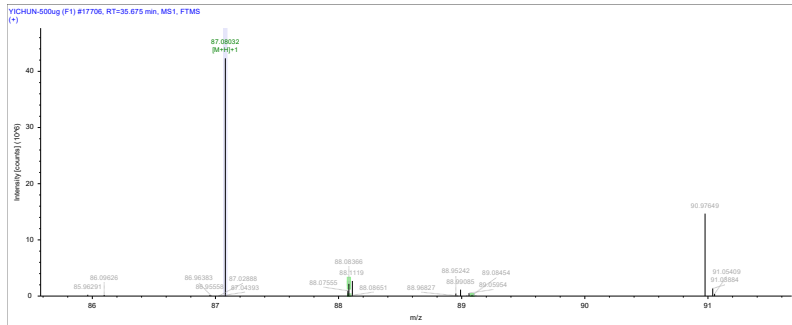


MS/MS

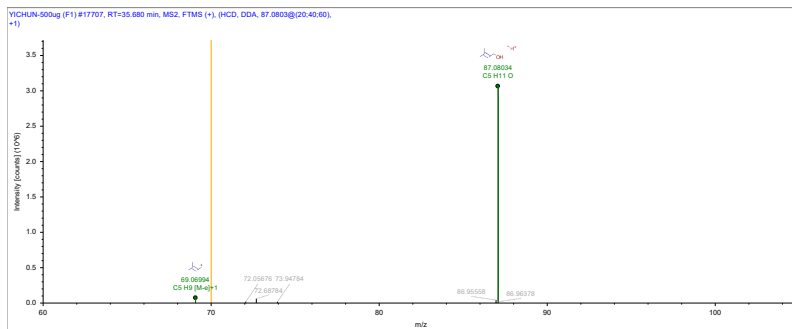


36.031 min Prenol

MS

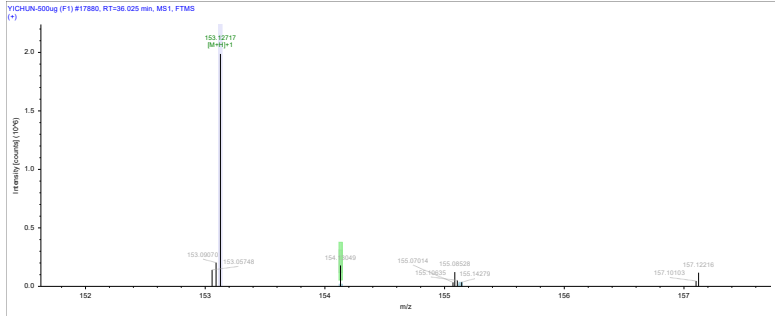


MS/MS

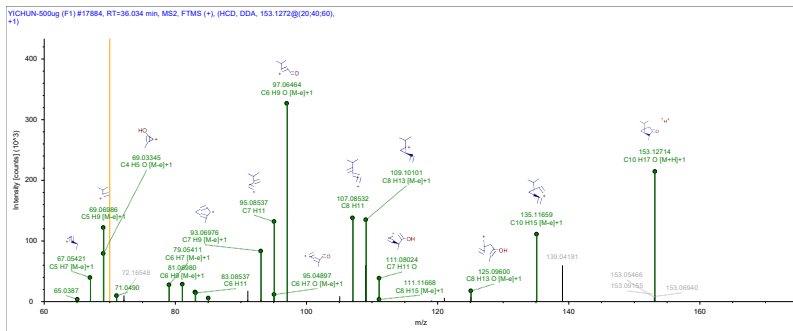


36.26 min Isothujone

MS

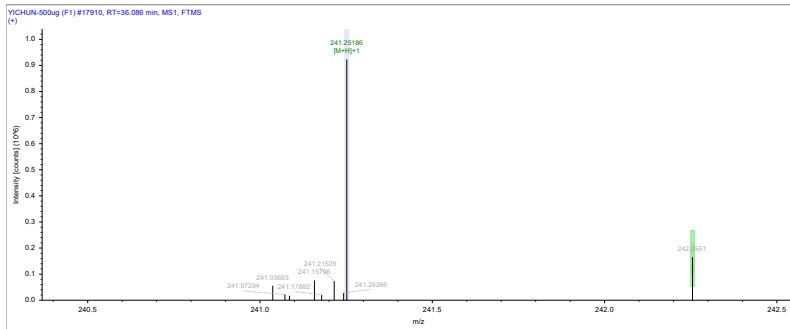


MS/MS

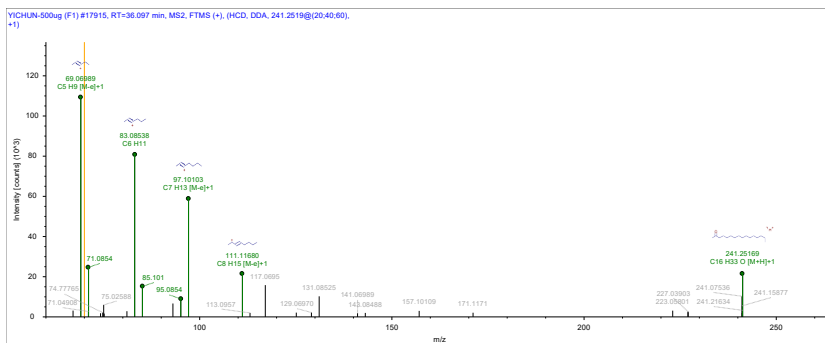


36.486 min Hexadecan-2-one

MS

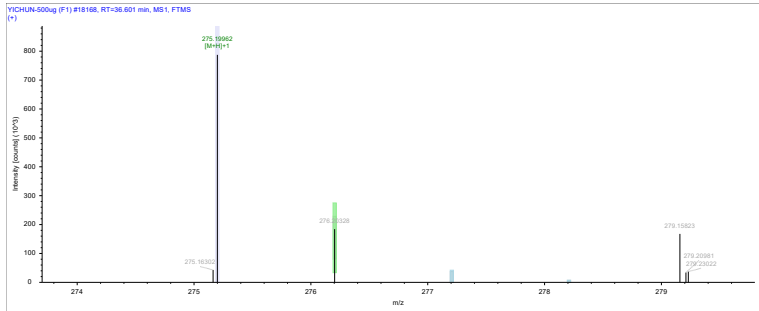


MS/MS

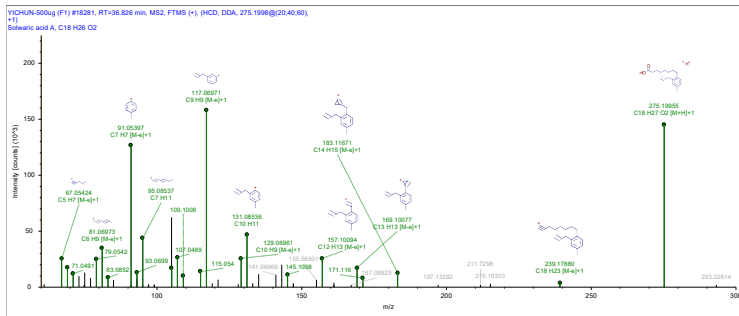


36.858 min Solwaric acid A

MS

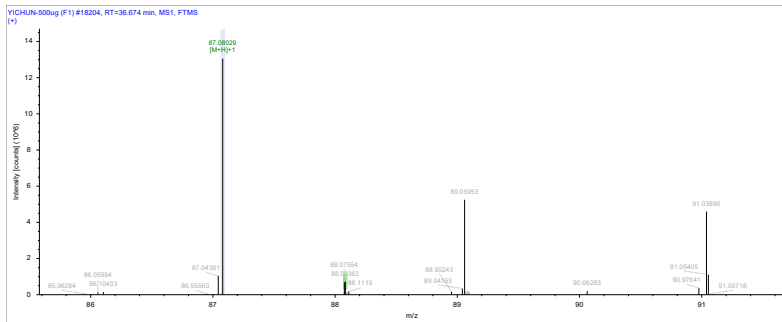


MS/MS



36.873 min Isoprenol

MS



MS/MS

