

Supplementary Materials

Article

MALDI-MSI: A powerful approach to understand Primary Pancreatic Ductal Adenocarcinoma and Metastases

MALDI-MSI: A Powerful Approach to Understand Primary Pancreatic Ductal Adenocarcinoma and Metastases

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Table S1. Classification confusion matrices of the three algorithms trained with human PDAC primary and metastasis samples.

Confusion Matrices	RF	SVM	LDA
Accuracy	0.9319	0.9368	0.8972
95% CI	0.9177, 0.9444	0.923, 0.9488	0.8804, 0.9124
p-Value (Acc > NIR)	$< 2.2 \times 10^{-16}$	$< 2.2 \times 10^{-16}$	$< 2.2 \times 10^{-16}$
Kappa	0.8299	0.8476	0.7336
McNemar's Test p-Value	8.61×10^{-8}	0.8339	$< 2.2 \times 10^{-16}$
Sensitivity	0.9783	0.9567	0.9783
Specificity	0.8208	0.8892	0.7028
Pos Pred Value	0.929	0.9539	0.8875
Neg Pred Value	0.9405	0.8955	0.9313
Balanced accuracy	0.8996	0.9229	0.8406

Acc – accuracy; NIR – no information rate; Pos Pred Value – positive predictive value; Neg Pred Value – negative predictive value

Table S2. Top 10 features, calculated by forward feature selection

<i>m/z</i>	Accuracy	Possible ID
1198.71092	0.6237238	actin
2960.40253	0.6340433	Collagen alpha-2(1) chain precursor
3101.50179	0.6577561	
795.36804	0.6805357	Collagen alpha-1(III) chain
628.31276	0.7010649	
2705.33098	0.7119333	Collagen alpha-1(1) chain precursor
1832.87696	0.7215391	
1478.7627	0.7339993	Collagen alpha-2(1) chain precursor
898.460275	0.7460753	Collagen alpha-1(1) chain precursor
1139.57803	0.7512899	Collagen alpha-1(III) chain

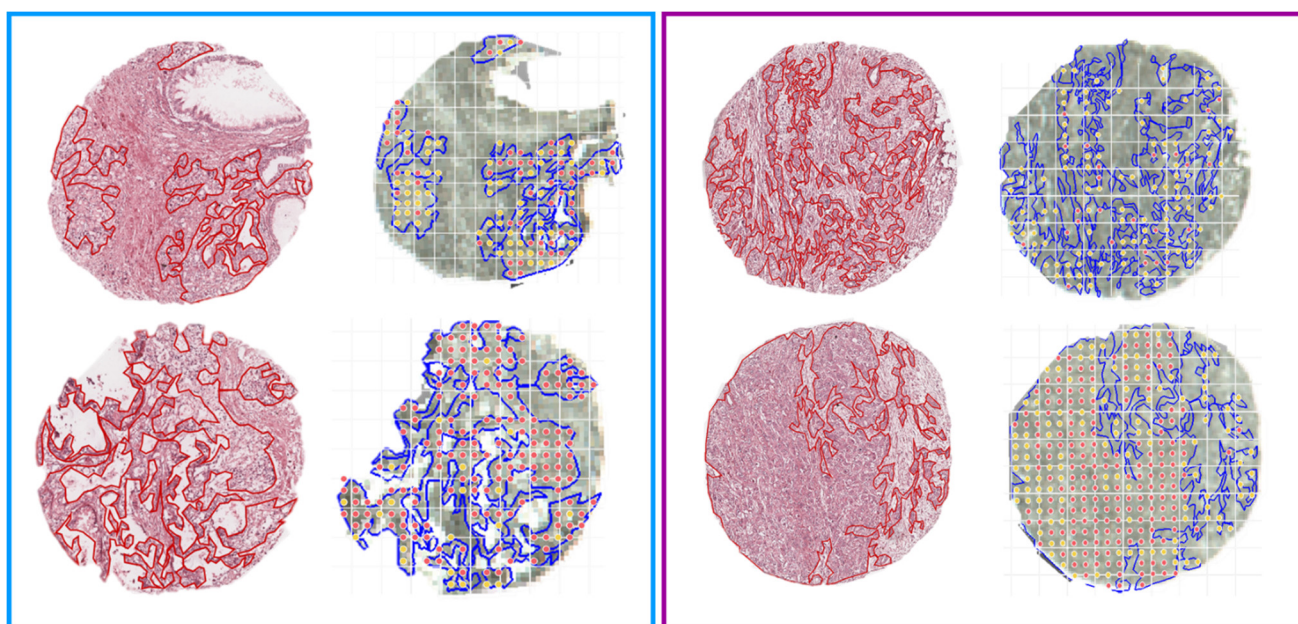


Figure S1. PDAC primary samples - the effect of the epithelial region size in the classification outcome. Two different regions from the primary PDAC tumor of the same patient are presented within the blue box and also in the purple box. On the top regions, which are more heterogeneous, it is possible to see that the classification outcome is not as accurate as in the bottom regions, where bigger areas of tumor (epithelial) regions are found. This effect might be due to an inefficient teaching, a deficient co-registration process and/or the measurement area per pixel not being adequate for the analysis of such detailed regions.

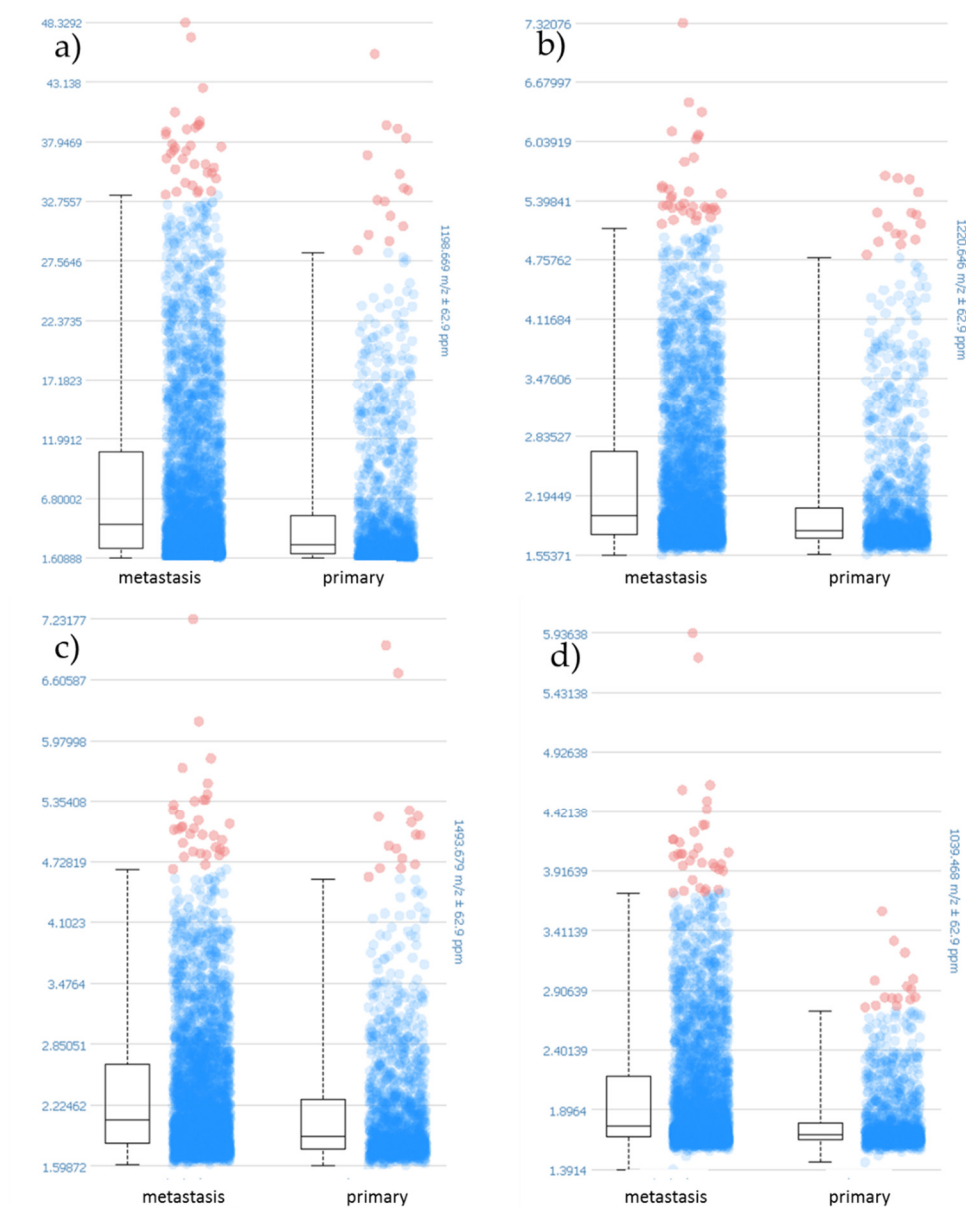


Figure S2. Feature expression comparison between primary tissue and metastasis in the mixed TMA. (a) $m/z = 1198.7$ (actin), (b) $m/z = 1220.6$ (COL4A3), (c) $m/z = 1493.7$ (COL1A2), and (d) $m/z = 1039.5$ (TBB2C).

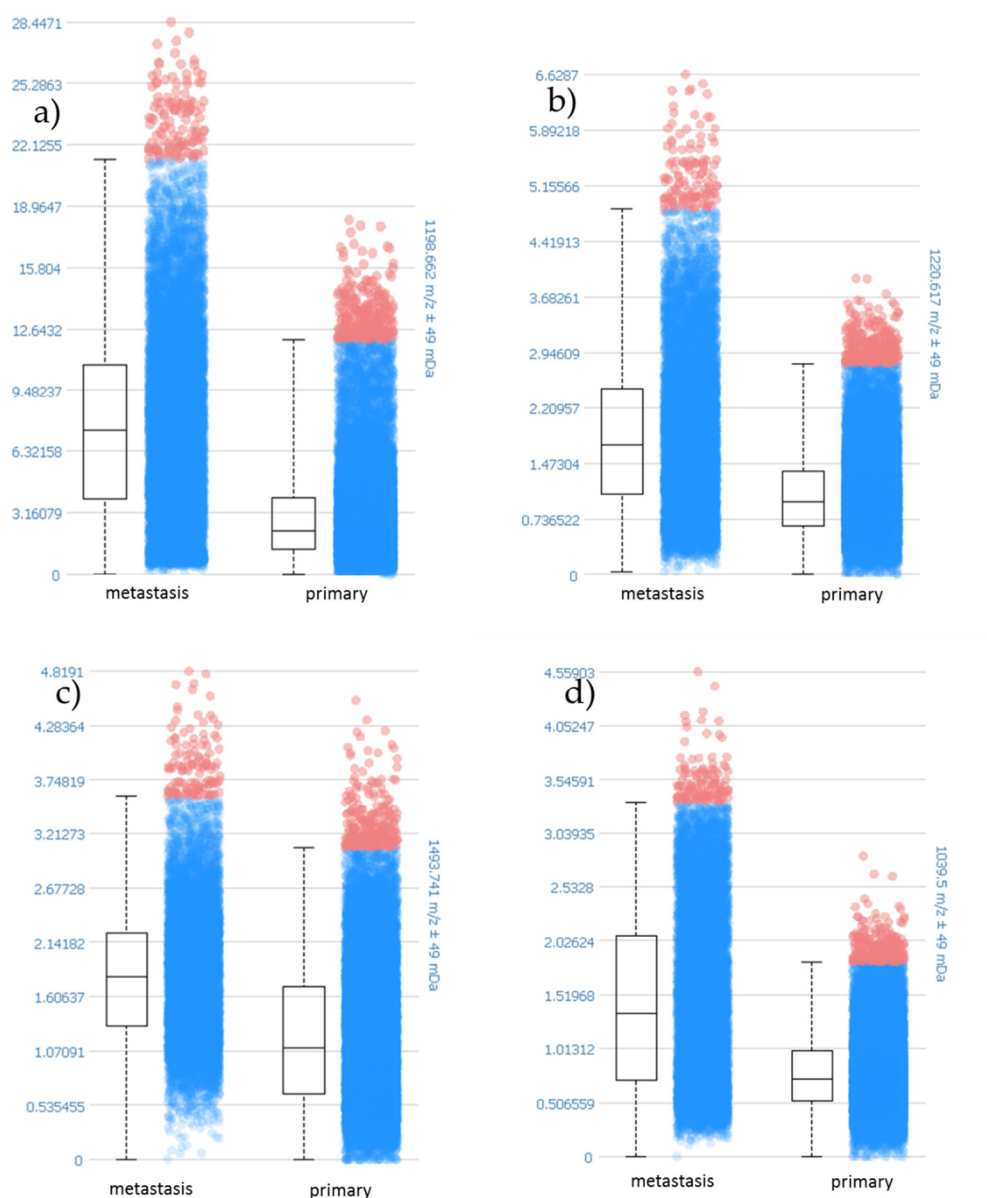


Figure S3. Feature expression comparison between primary tissue and metastasis in the validation dataset. (a) m/z = 1198.7 (actin), (b) m/z = 1220.6 (COL4A3), (c) m/z = 1493.7 (COL1A2), and (d) m/z = 1039.5 (TBB2C).

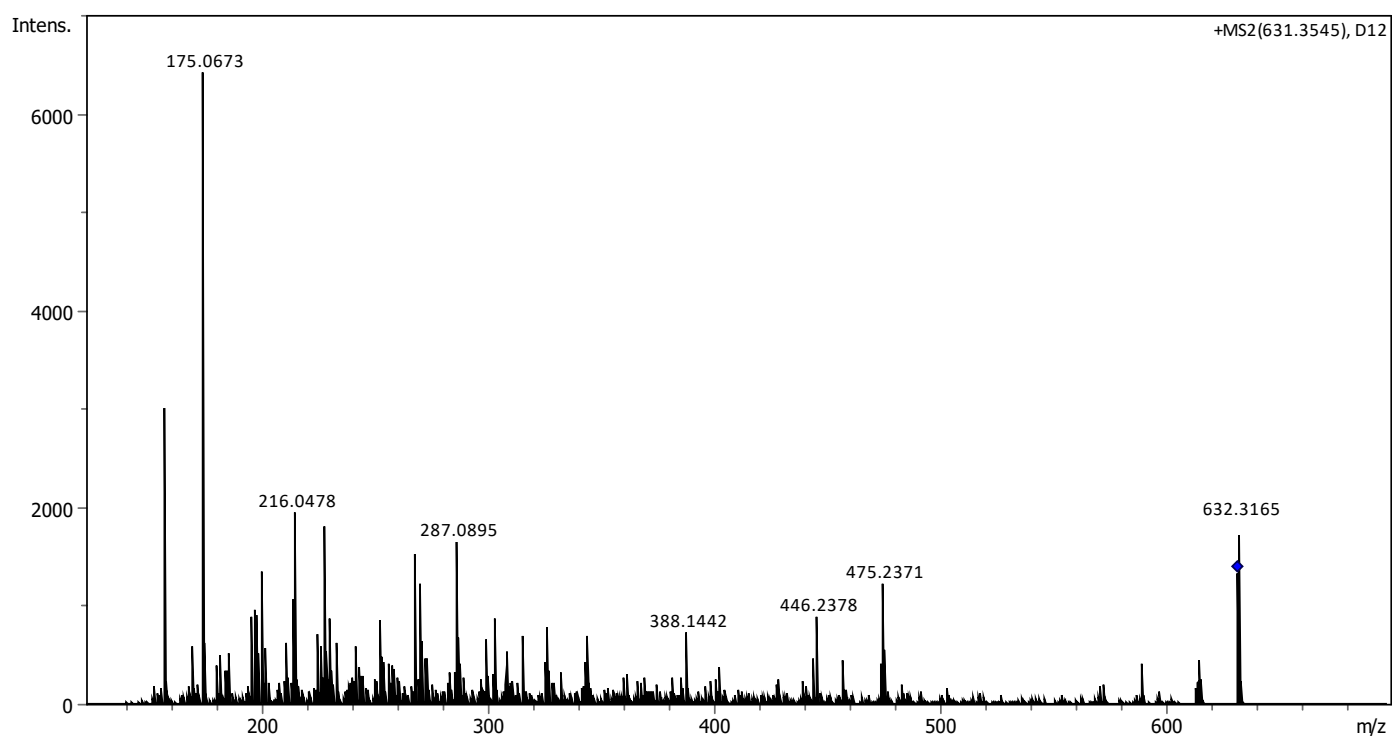


Figure S4. MS/MS fragmentation spectra utilized for the tentative identification of $m/z = 632.3$.

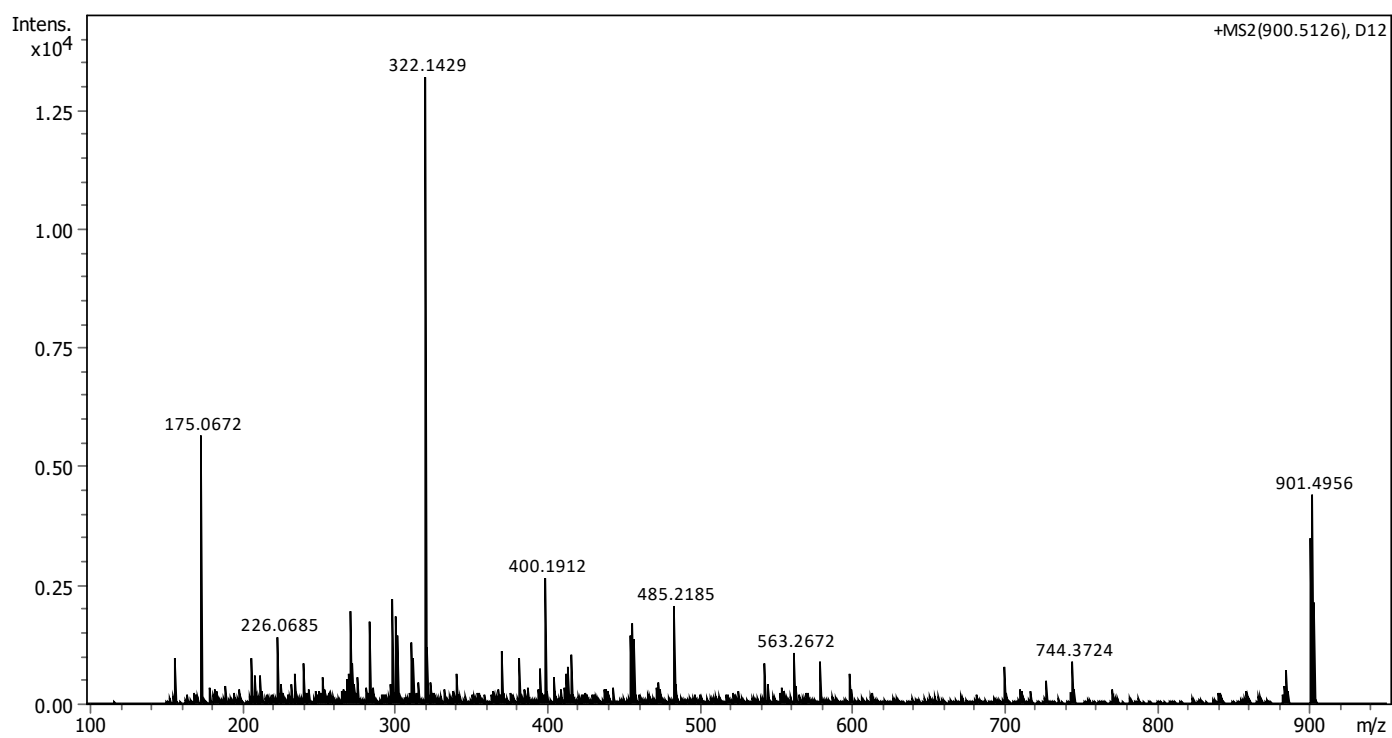


Figure S5. MS/MS fragmentation spectra utilized for the tentative identification of $m/z = 900.5$.

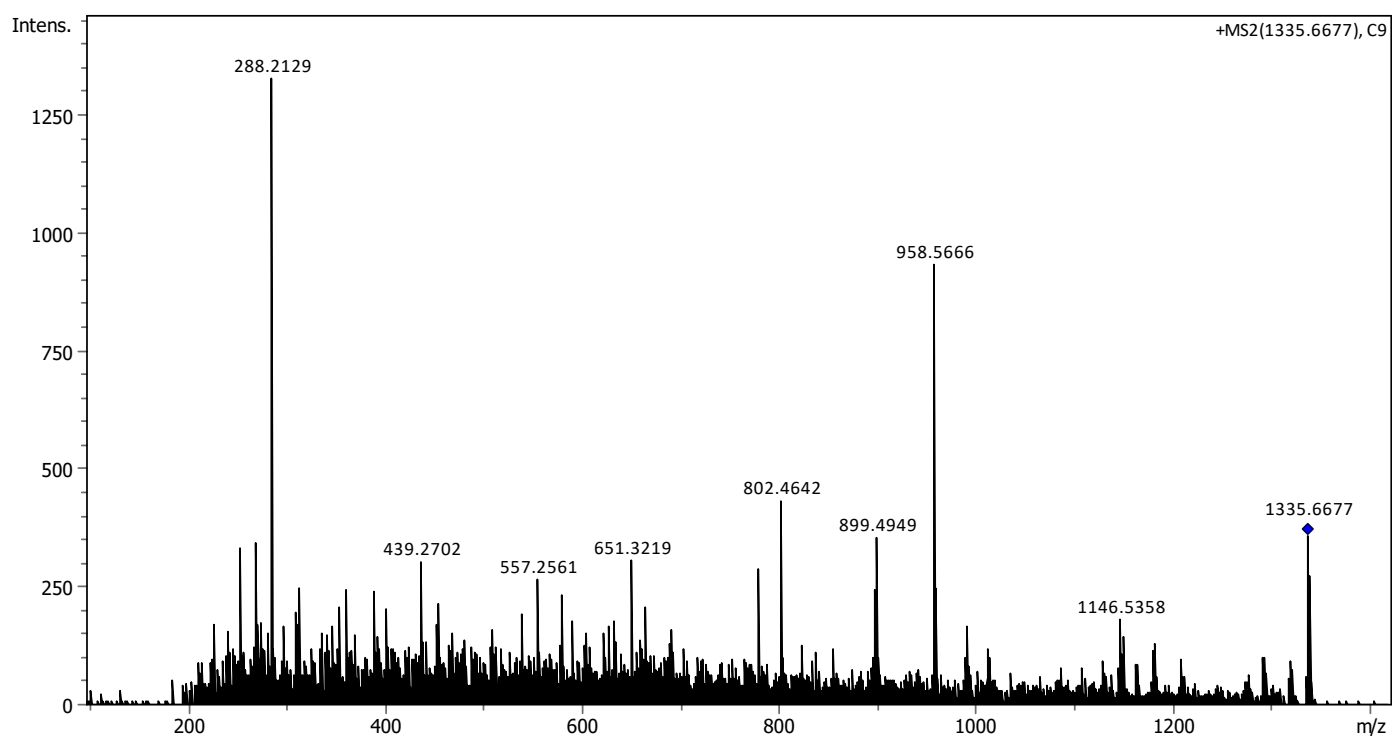


Figure S6. MS/MS fragmentation spectra utilized for the tentative identification of $m/z = 1335.7$.

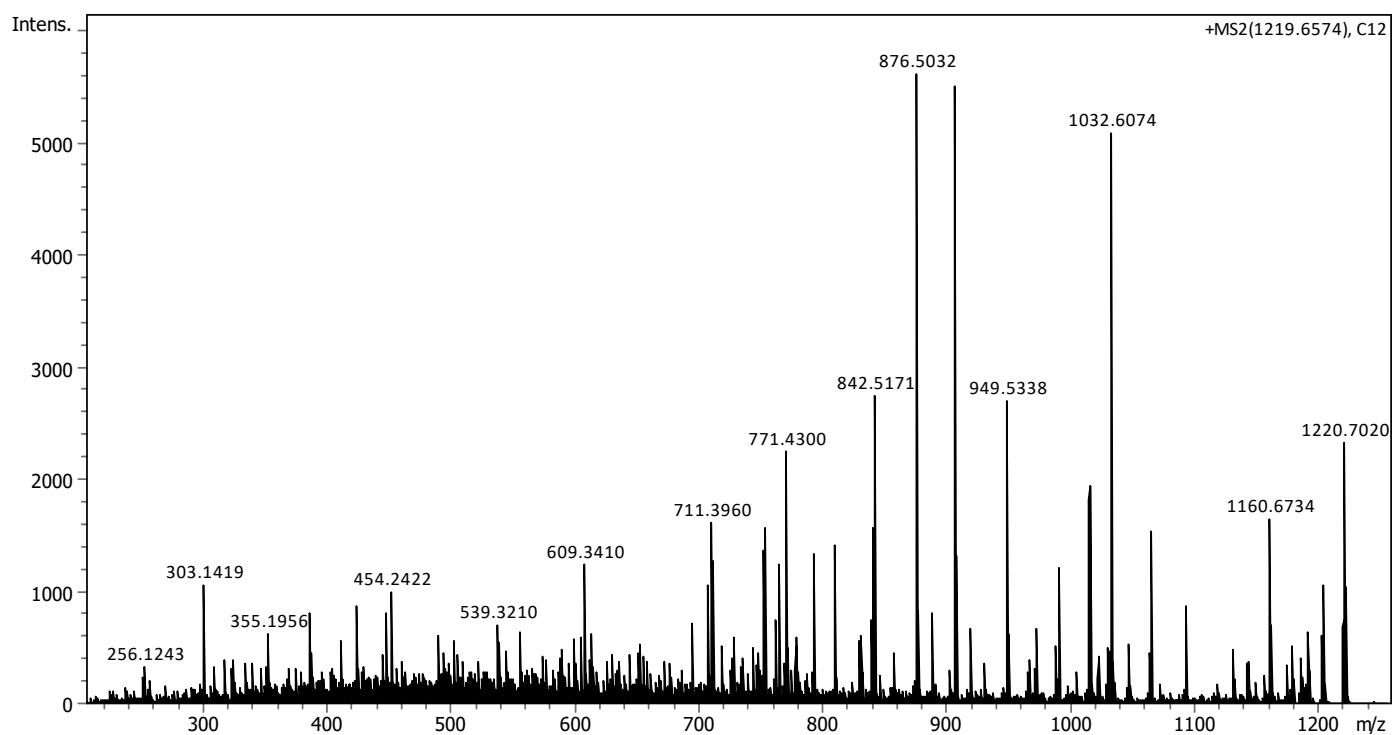


Figure S7. MS/MS fragmentation spectra utilized for the tentative identification of $m/z = 1220.7$.

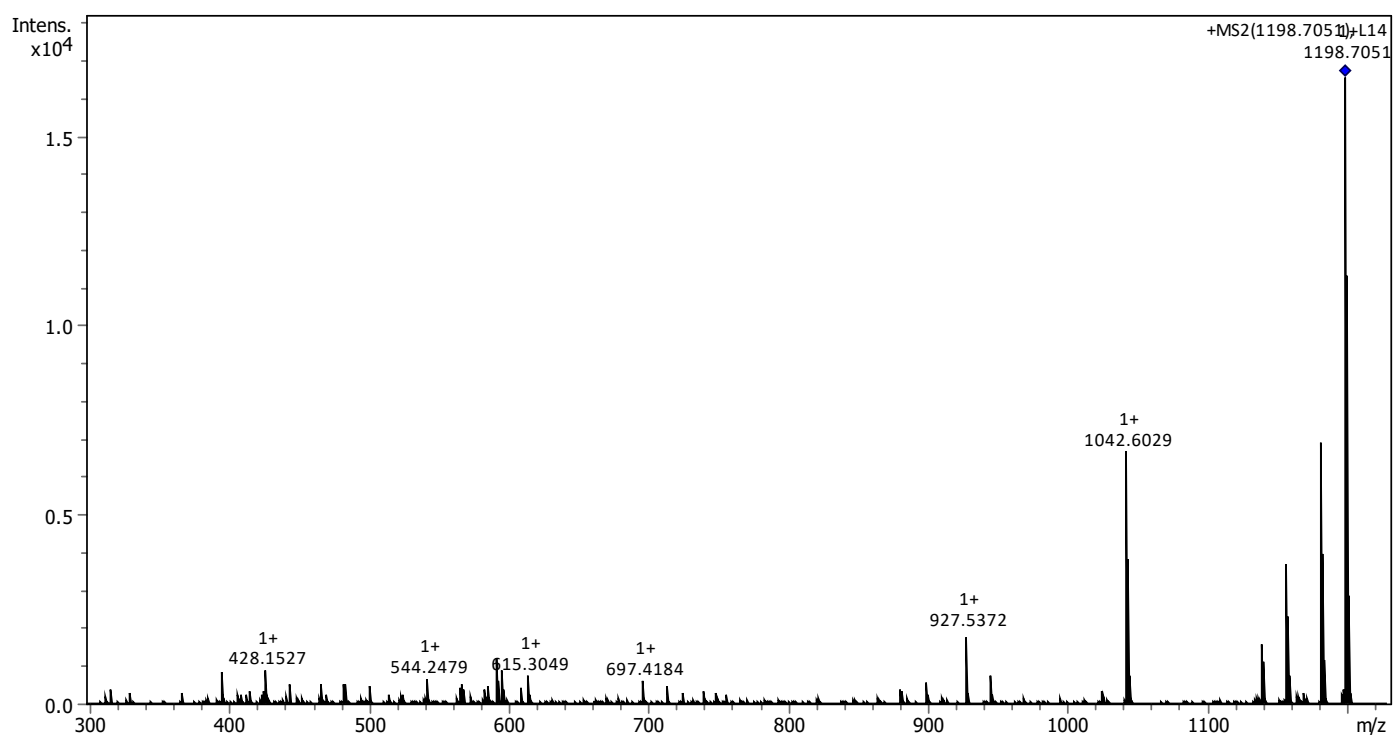


Figure S8. MS/MS fragmentation spectra utilized for the tentative identification of $m/z = 1198.7$.

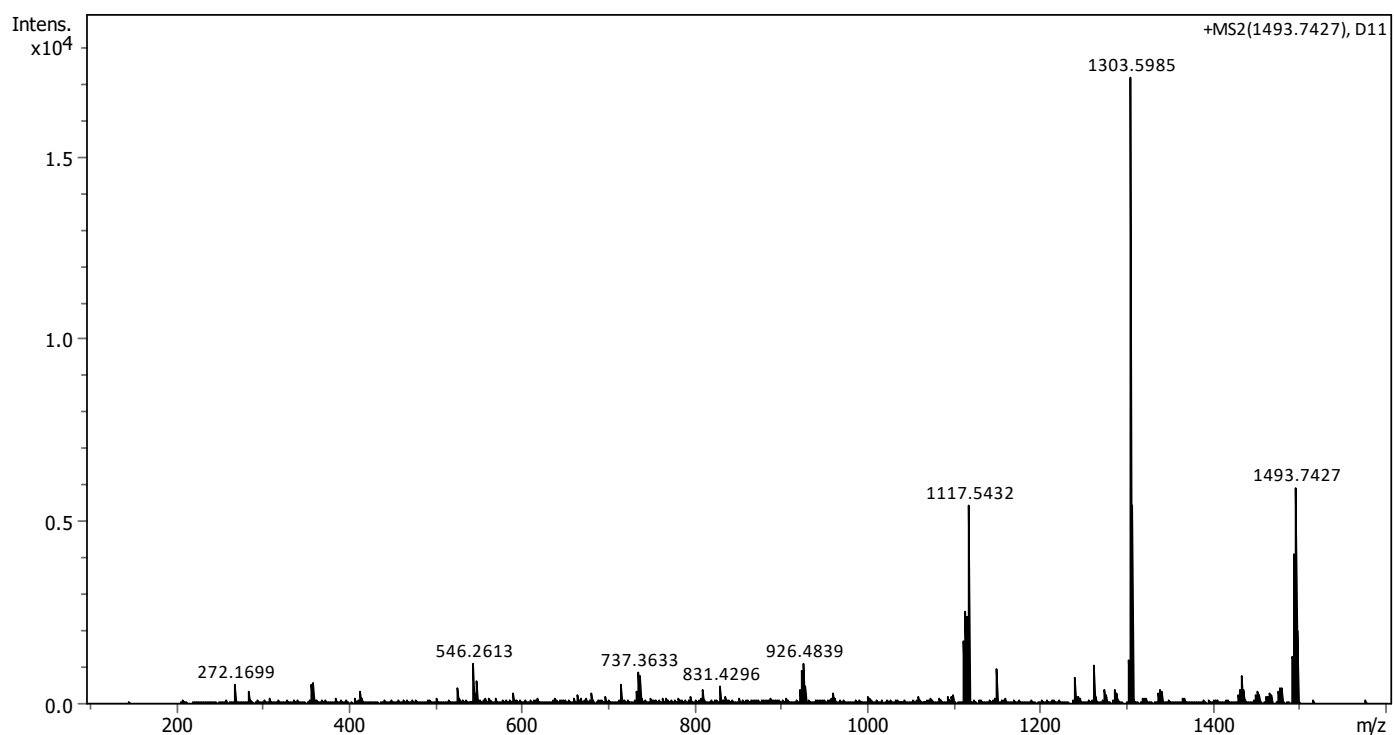


Figure S9. MS/MS fragmentation spectra utilized for the tentative identification of $m/z = 1493.7$.