SUPPLEMENTAL FILES

TITLE:
Integrated Cell Manipulation Platform Coupled with the Single-probe for Mass Spectrometry Analysis of Drugs and Metabolites in Single Suspension Cells

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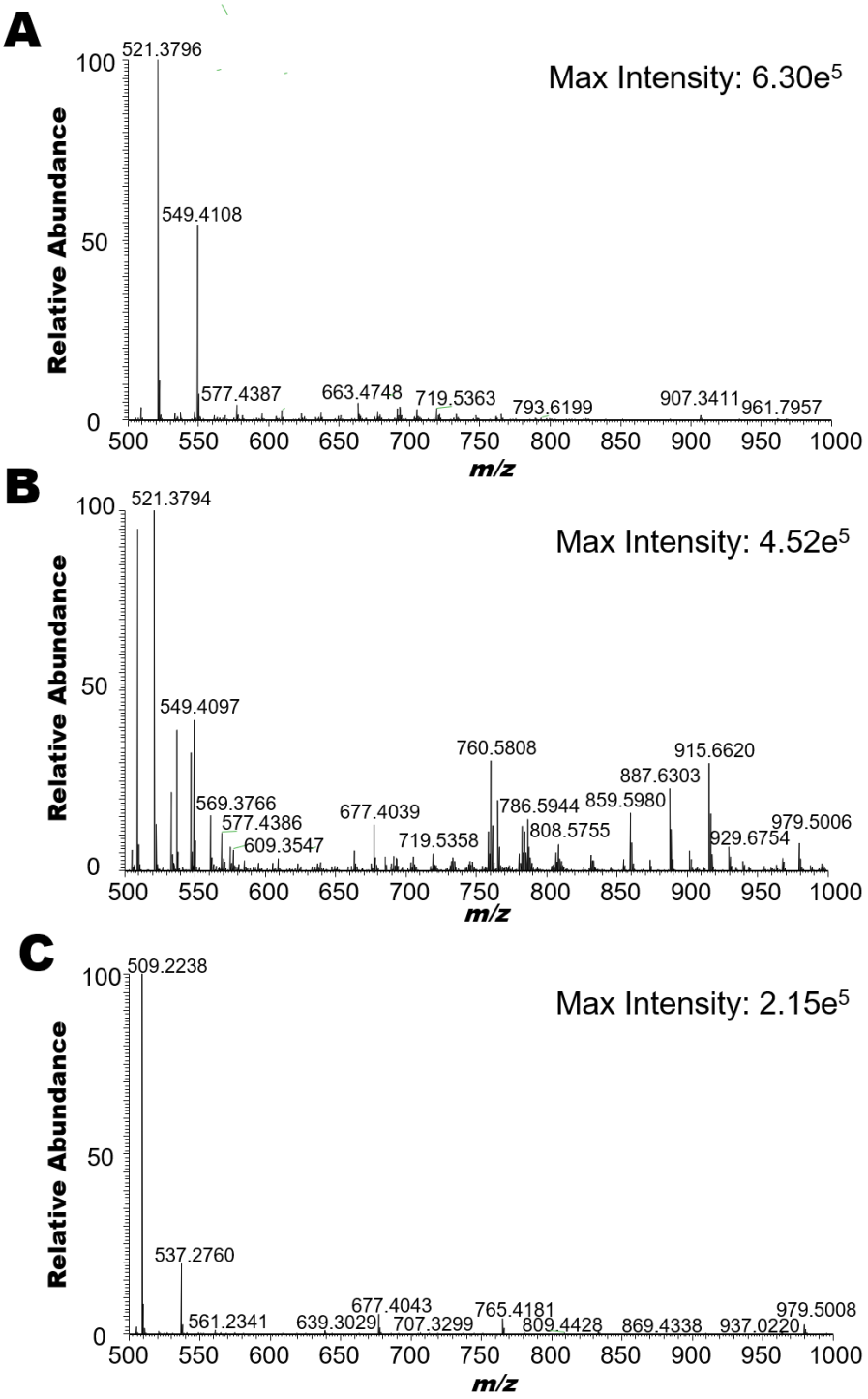
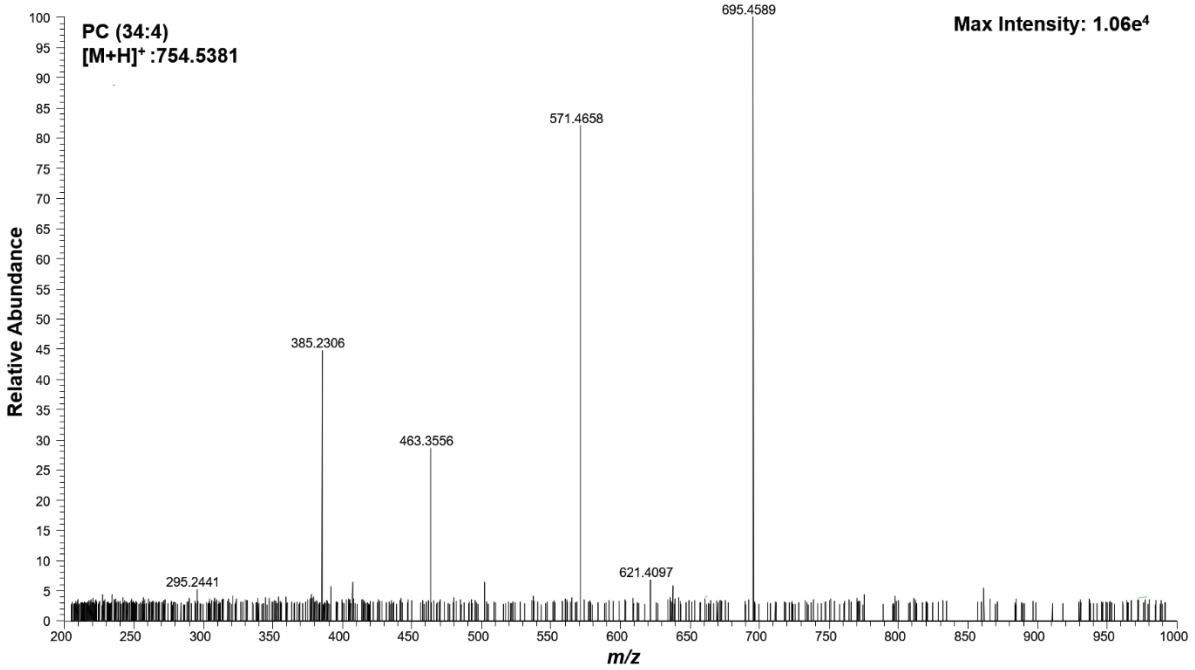
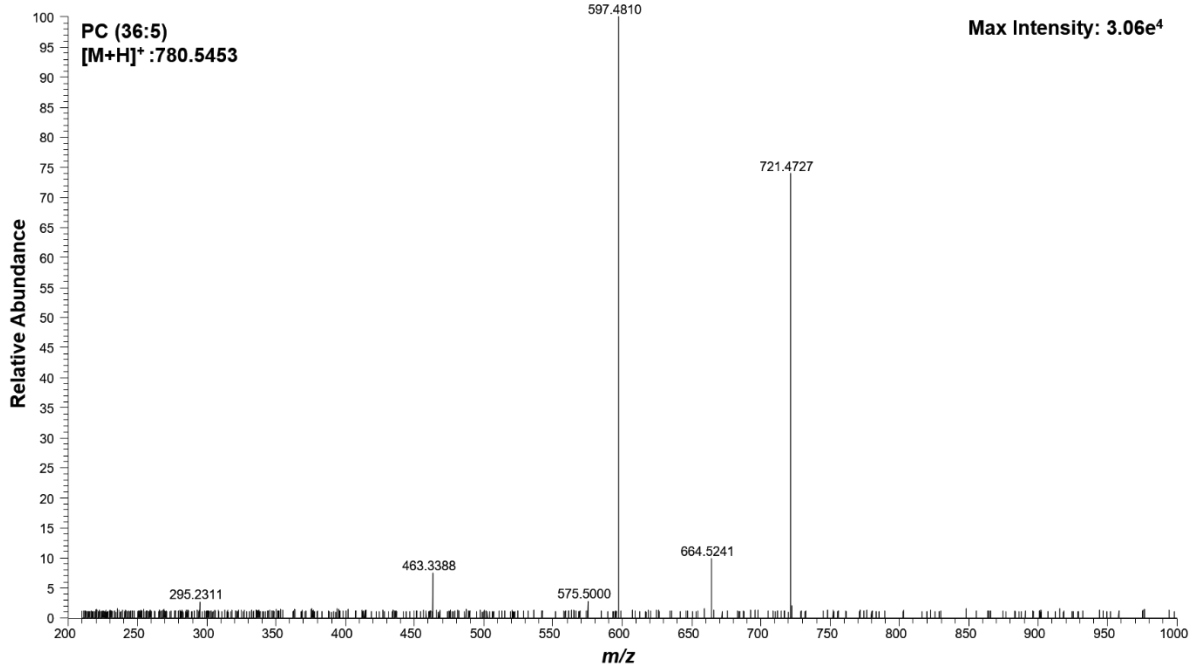


Figure S1. The zoomed-in mass spectra (*m/*z 500-1000) showing changes of ion signals (A) before analysis of a cell, (B) during acquisition of the cell, and (C) after cell analysis using the suspended cell platform.

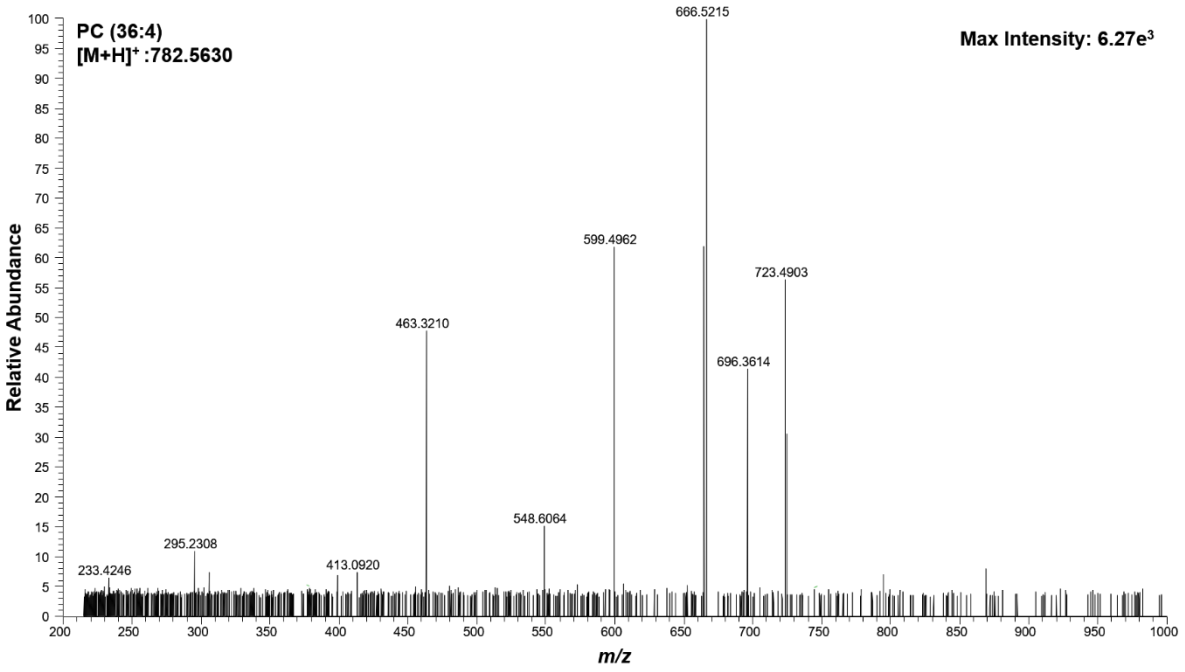
(a)


PC (34:4)
[M+H]+ :754.5381
Max Intensity: 1.06e4
695.4589
571.4658
385.2306
463.3556
621.4097
295.2441
Relative Abundance
m/z

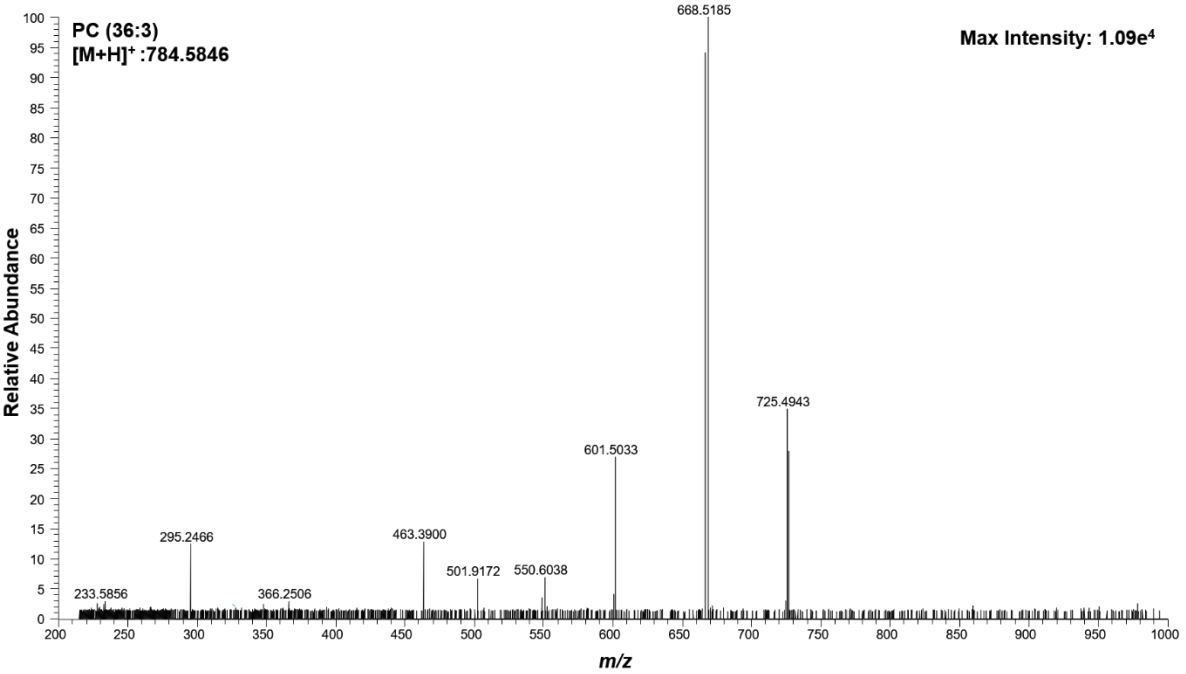
(b)


PC (36:5)
[M+H]+ :780.5453
Max Intensity: 3.06e4
597.4810
721.4727
664.5241
463.3388
295.2311
575.5000
Relative Abundance
m/z

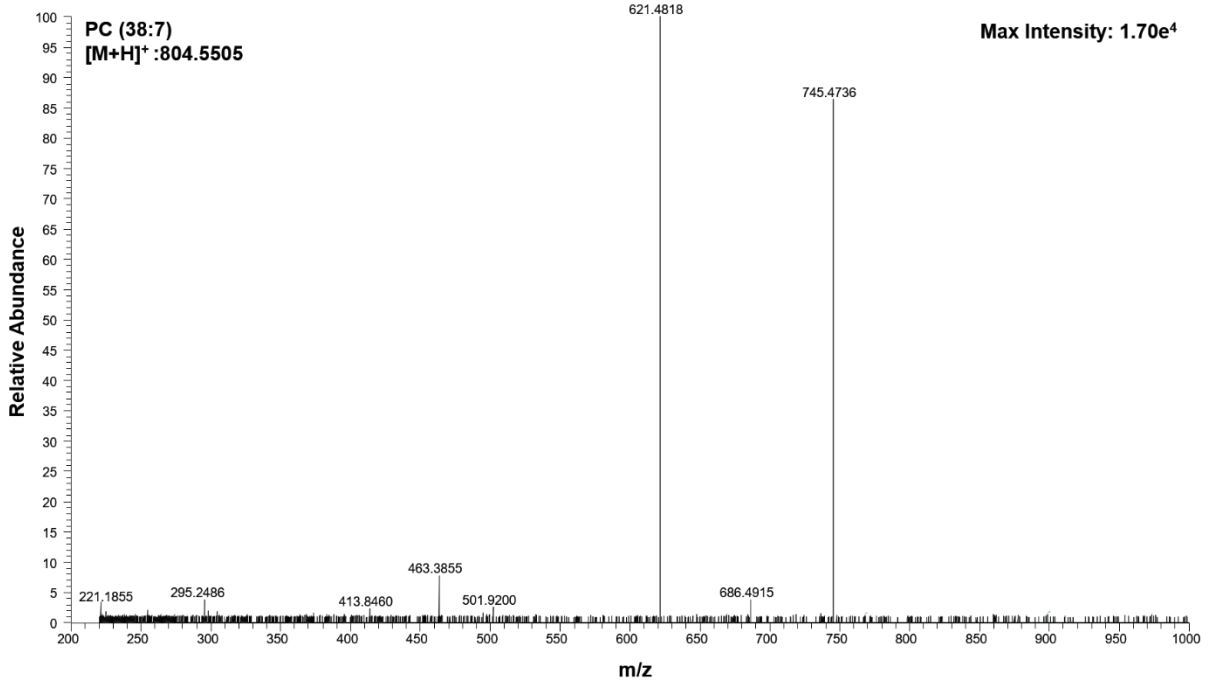
(c)


PC (36:4)
[M+H]+ :782.5630
Max Intensity: 6.27e3
Relative Abundance
m/z
666.5215
599.4962
723.4903
463.3210
696.3614
548.6064
295.2308
413.0920
233.4246

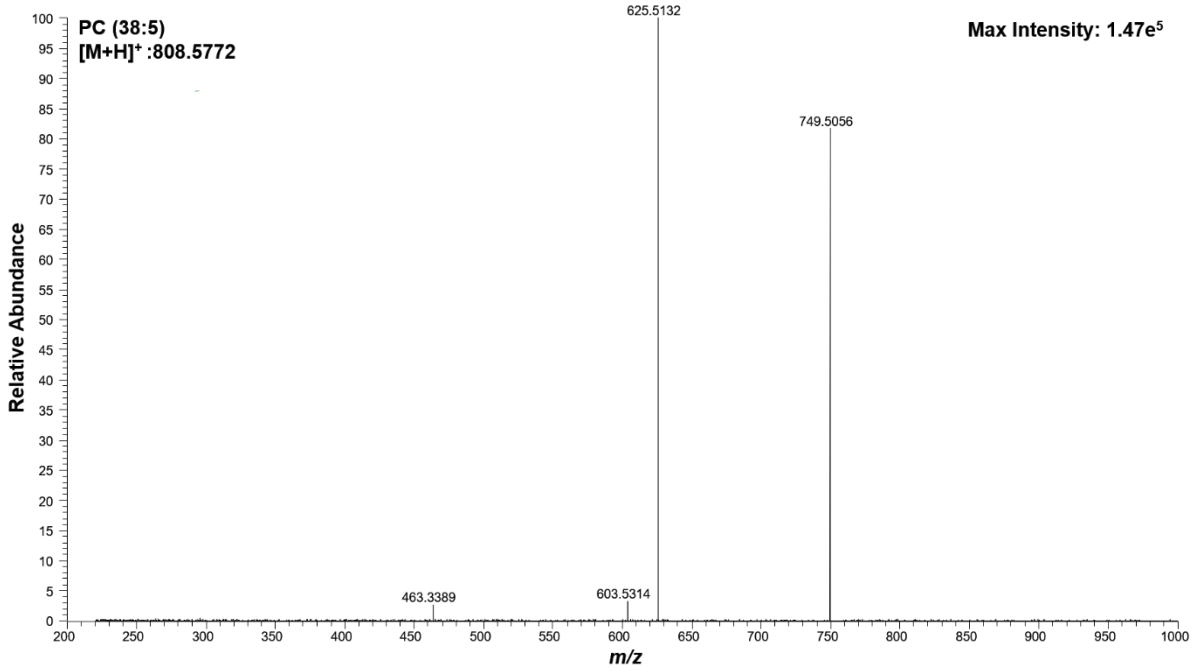
(d)


PC (36:3)
[M+H]+ :784.5846
Max Intensity: 1.09e4
Relative Abundance
m/z
668.5185
725.4943
601.5033
295.2466
463.3900
501.9172
550.6038
233.5856
366.2506

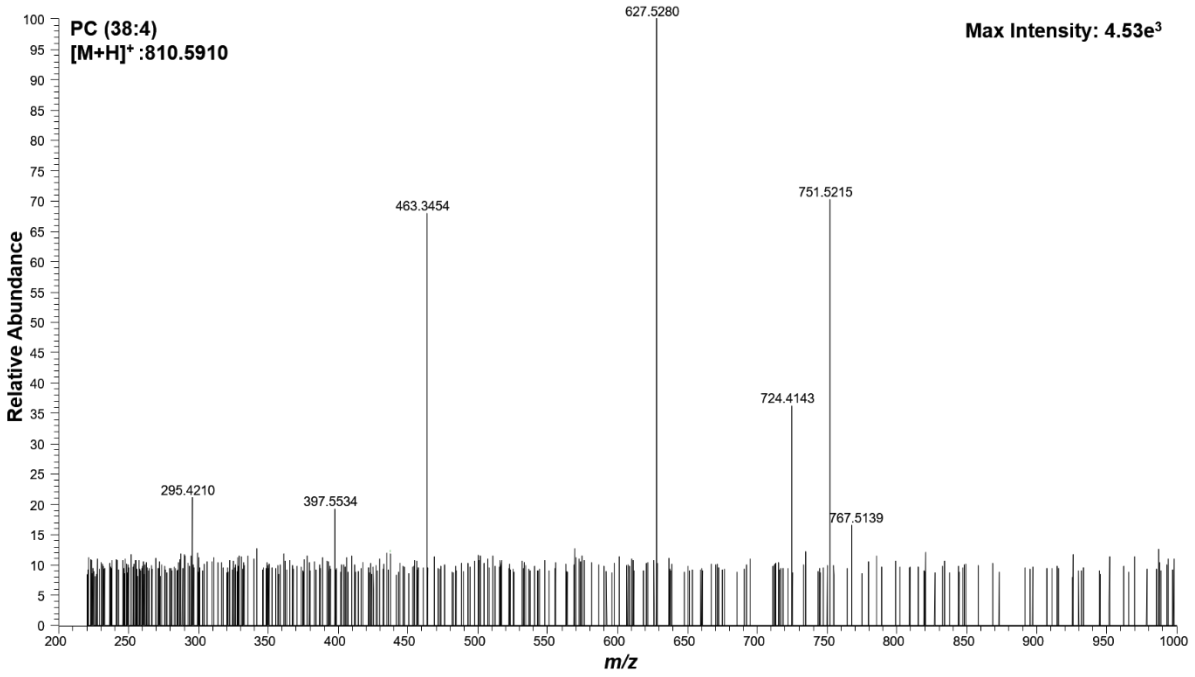
(e)


PC (38:7)
[M+H]+ :804.5505
Max Intensity: 1.70e4
621.4818
745.4736
463.3855
221.1855
295.2486
413.8460
501.9200
686.4915
Relative Abundance
m/z

(f)


PC (38:5)
[M+H]+ :808.5772
Max Intensity: 1.47e5
625.5132
749.5056
463.3389
603.5314
Relative Abundance
m/z

(g)



(h)

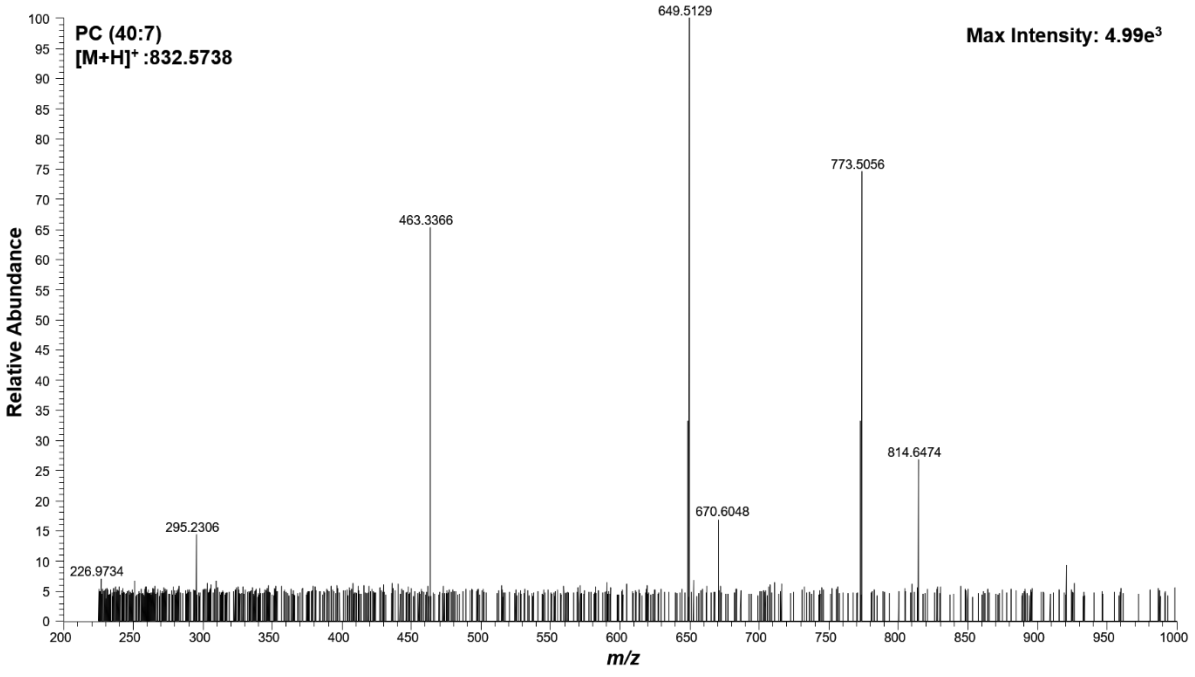


Figure S2. MS/MS verification of lipids with 10-40 manufacturer's unit energy at: (a) *m/z* 754.5 (b) *m/z* 780.5 (c) *m/z* 782.5 (d) *m/z* 784.5 (e) *m/z* 804.5 (f) *m/z* 808.5 (g) *m/z* 810.5 (h) *m/z* 832.5. Reprinted with permission from Standke et al[1]. Copyright 2019 American Chemical Society.

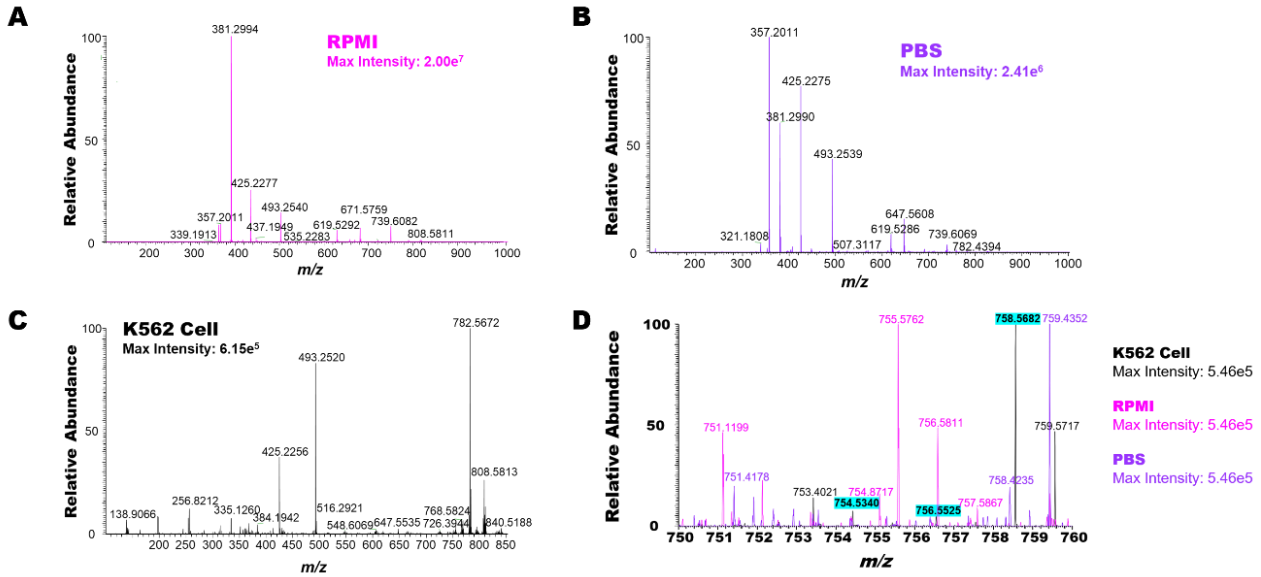


Figure S3. Mass spectra of (A) RPMI cell culture medium, (B) PBS, and (C) an individual K562 cell. (D) A zoomed-in region (m/z 750-760) of the combined three spectra (manually combined) from an individual K562 cell, RPMI media, and PBS showing the differences among them, indicating the identified PC species (highlighted) from the cell can be clearly distinguished.

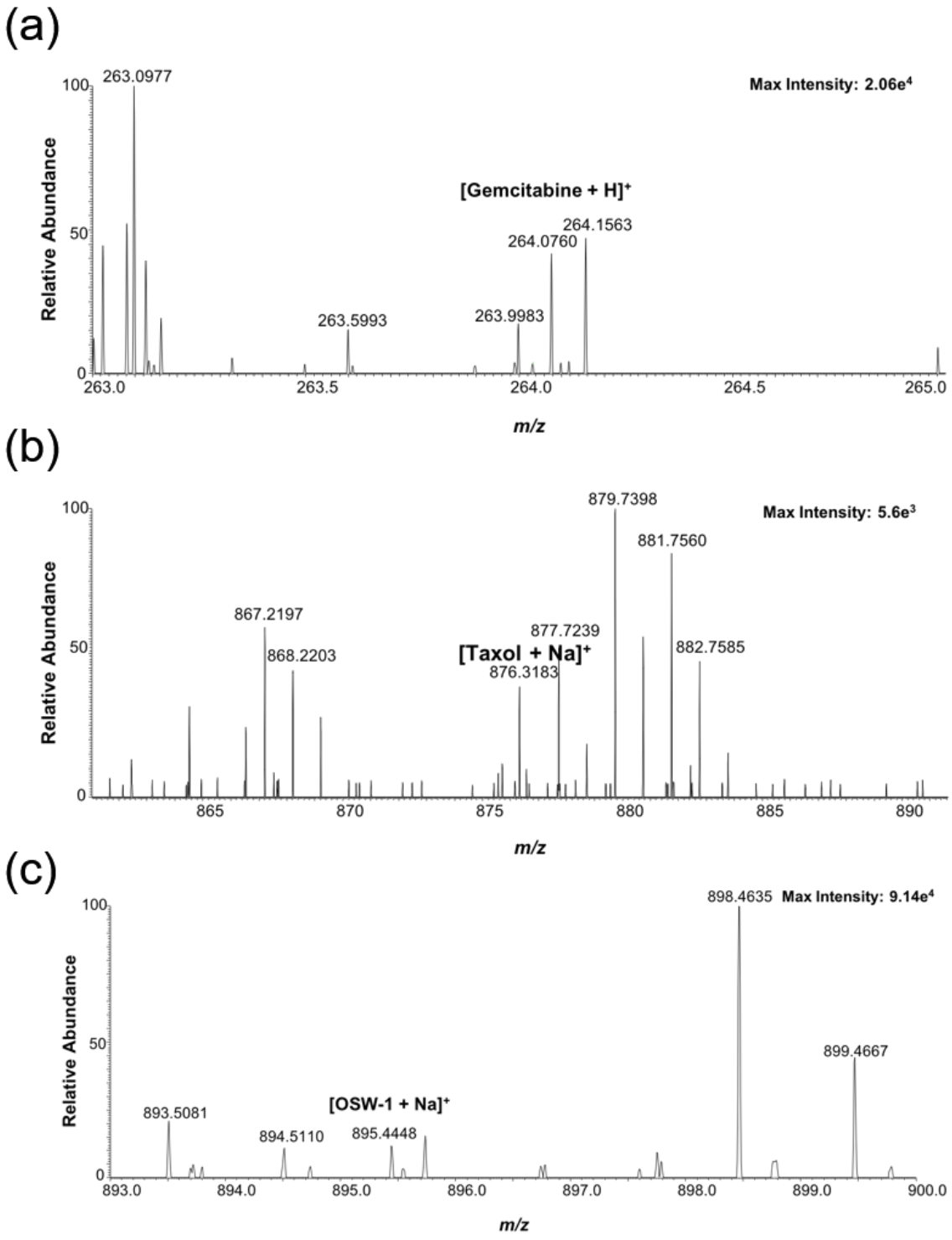


Figure S4. Mass spectra obtained from treating individual K562 cells with: (A) gemcitabine (1 µM, 1 hr) (B) taxol (1 µM, 1 hr) and (C) OSW-1 (100 nM, 4 hr). Reprinted with permission from Standke et al[1]. Copyright 2019 American Chemical Society.

REFERENCES

1. Standke, S.J., Colby, D.H., Bensen, R.C., Burgett, A.W.G., Yang, Z. Mass Spectrometry Measurement of Single Suspended Cells Using a Combined Cell Manipulation System and a Single-Probe Device. *Analytical Chemistry*. **91** (3), 1738–1742, doi: 10.1021/acs.analchem.8b05774 (2019).