

Supporting information for:

How to Apply Supervised Machine Learning Tools to MS Imaging Files: Case Study with Cancer Spheroids Undergoing Treatment with the Monoclonal Antibody, Cetuximab

David Hua¹, Xin Liu², Eden P. Go¹, Yijia Wang², Amanda B. Hummon², Heather Desaire^{1*}.

¹Department of Chemistry, University of Kansas, Lawrence, Kansas 66045, United States

2. Department of Chemistry and Biochemistry and the Comprehensive Cancer Center, The
Ohio State University, Columbus, Ohio 43210, United States

*Address correspondence to: Heather Desaire, phone: 785-864-3015, Email:hdesaire@ku.edu

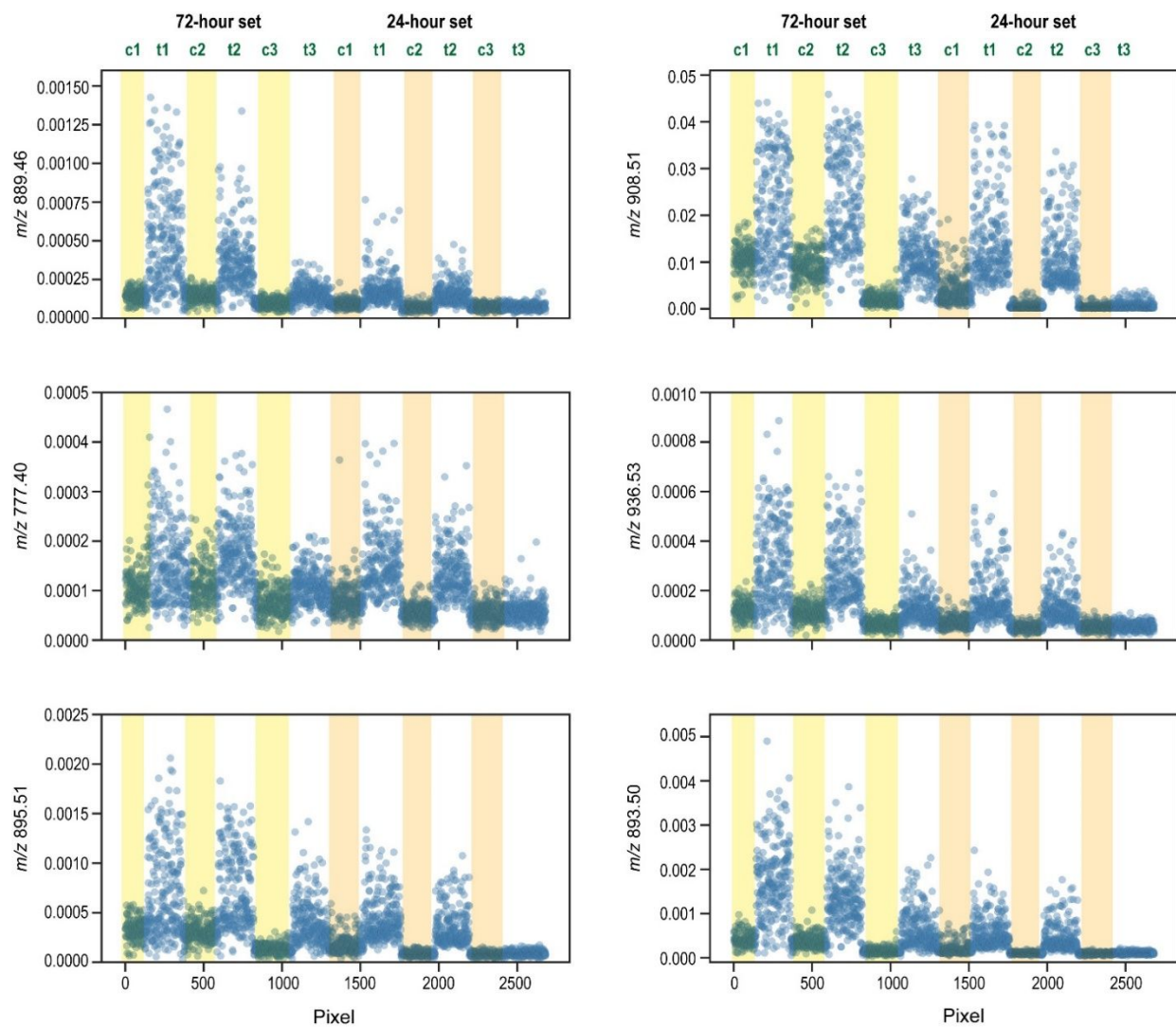


Figure S1: Pixel-vs-intensity plots for the 5th to the 10th most discriminating features at 24 hours.

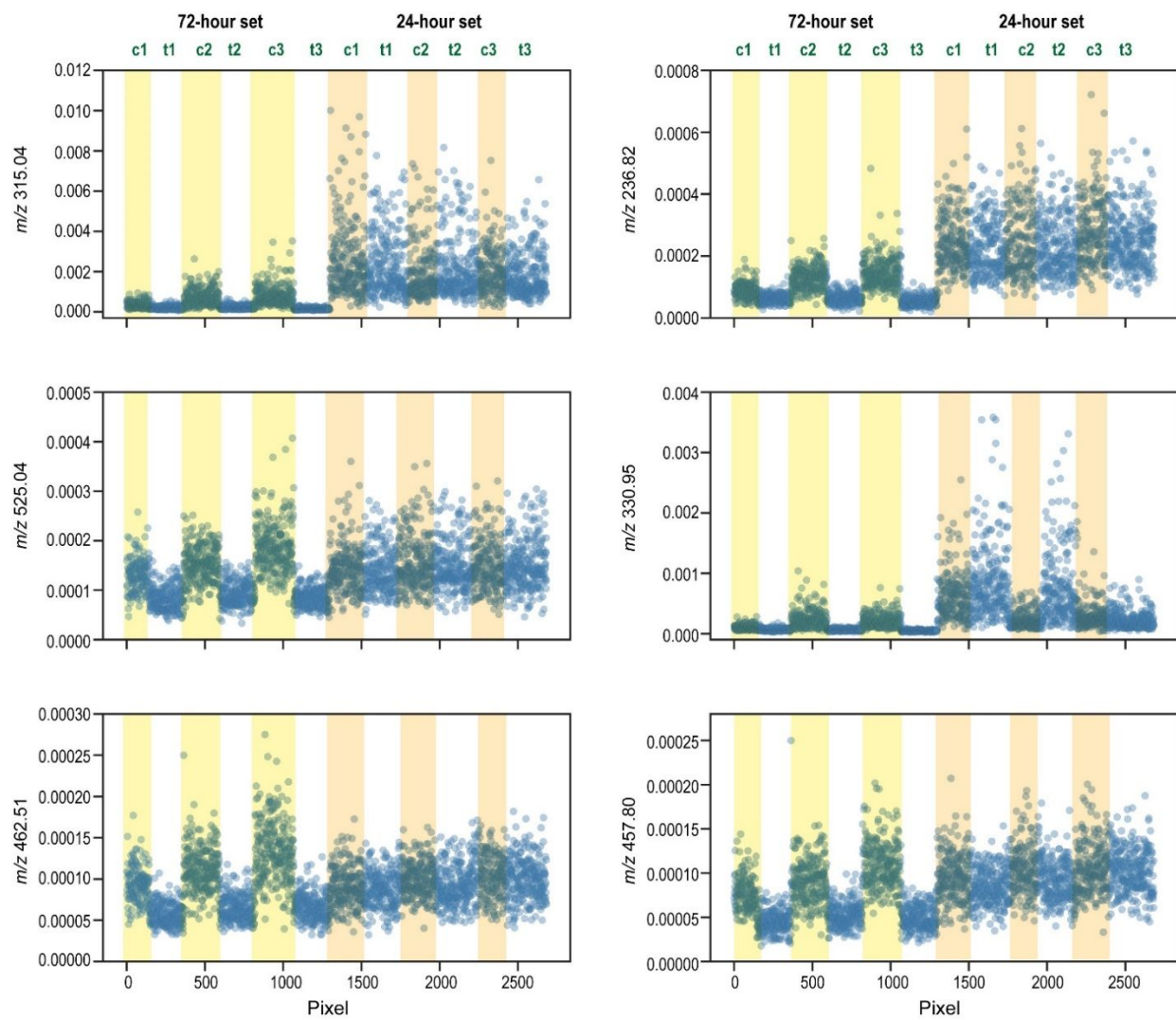


Figure S2: Pixel-vs-intensity plots for the 5th to the 10th most discriminating features at 72 hours.

Table S1: 50-most-discriminating m/z's at 24 hours.		
Rank	m/z	AUC (area under the receiver-operating curve)
1	891.48	0.78
2	781.44	0.78
3	540.06	0.77
4	779.42	0.77
5	893.5	0.76
6	936.53	0.76
7	908.51	0.76
8	895.51	0.76
9	777.4	0.76
10	889.46	0.76
11	650.33	0.76
12	835.67	0.76
13	861.45	0.75
14	505.99	0.75
15	885.43	0.75
16	833.43	0.75
17	751.4	0.74
18	906.5	0.74
19	859.43	0.74
20	910.53	0.74
21	259.23	0.74
22	887.45	0.74
23	880.5	0.74
24	904.48	0.74
25	408.05	0.74
26	934.51	0.74
27	876.46	0.74
28	850.47	0.74
29	652.34	0.73
30	466.32	0.73
31	852.48	0.73
32	921.51	0.73
33	735.27	0.73
34	822.45	0.73
35	941.46	0.73
36	624.33	0.73
37	863.47	0.73
38	211.27	0.73
39	281.42	0.73
40	883.41	0.73
41	865.48	0.73
42	857.41	0.73
43	878.48	0.73
44	792.42	0.73
45	783.45	0.73
46	538.26	0.72
47	824.47	0.72
48	882.52	0.72
49	835.45	0.72
50	863.69	0.72

Table S2: 50-most-discriminating m/z's at 72 hours.		
Rank	m/z	AUC (area under the receiver-operating curve)
1	331.17	0.971
2	539.16	0.968
3	271.56	0.963
4	523.92	0.958
5	457.80	0.954
6	330.95	0.952
7	236.82	0.948
8	462.51	0.946
9	525.04	0.942
10	315.04	0.942
11	457.58	0.940
12	523.02	0.939
13	514.51	0.938
14	271.78	0.938
15	349.10	0.935
16	365.24	0.933
17	347.09	0.930
18	260.35	0.925
19	741.99	0.924
20	353.36	0.922
21	891.48	0.921
22	338.12	0.919
23	338.35	0.917
24	289.49	0.914
25	508.01	0.909
26	271.33	0.909
27	893.50	0.908
28	379.14	0.907
29	332.07	0.906
30	508.90	0.906
31	428.44	0.906
32	499.49	0.906
33	538.94	0.904
34	249.15	0.903
35	287.70	0.902
36	462.29	0.901
37	319.52	0.901
38	288.59	0.901
39	562.47	0.901
40	272.68	0.899
41	272.01	0.898
42	428.00	0.896
43	443.46	0.896
44	270.66	0.894
45	555.07	0.893
46	439.87	0.892
47	439.65	0.891
48	405.58	0.890
49	523.25	0.890
50	459.60	0.889