

Combining Desorption Electrospray Ionization Mass Spectrometry Imaging and Machine Learning for Molecular Recognition of Myocardial Infarction

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Table S1. Mass spectral peaks identified by GBDT algorithm as important for classification of each pixel as infarct or normally perfused myocardium arranged in descending order of relative importance.

	<i>m/z</i>	Importance	Mean difference	Prevalence
1	124	0.05547	-0.09989	Normal
2	79.95	0.04841	-0.04163	Normal
3	253.2	0.04740	0.05119	Infarct
4	327.25	0.04286	-0.31952	Normal
5	281.25	0.04186	0.20391	Infarct
6	282.25	0.03732	0.03581	Infarct
7	309.3	0.03580	-0.02105	Normal
8	113	0.03379	-0.01115	Normal
9	451.3	0.03328	-0.02117	Normal
10	303.25	0.03177	-0.08824	Normal
11	790.55	0.03127	-0.02869	Normal
12	311.15	0.02774	0.03276	Infarct
13	329.25	0.02774	-0.10815	Normal
14	284.25	0.02521	0.02315	Infarct
15	283.25	0.02370	0.11689	Infarct
16	299.2	0.02370	0.00579	Infarct
17	304.25	0.02269	-0.02325	Normal
18	89	0.02219	-0.09220	Normal
19	328.25	0.02219	-0.07940	Normal
20	255.25	0.02068	0.15295	Infarct
21	331.25	0.02017	-0.02731	Normal
22	307.25	0.01967	-0.01667	Normal
23	326.2	0.01916	0.00722	Infarct
24	427.3	0.01866	0.00025	Infarct
25	227.2	0.01866	0.02028	Infarct
26	183	0.01866	0.01805	Infarct
27	297.25	0.01715	-0.00763	Normal
28	277.2	0.01664	-0.01323	Normal
29	453.3	0.01563	-0.00872	Normal
30	280.25	0.01563	-0.08472	Normal
31	325.2	0.01563	0.04097	Infarct

	<i>m/z</i>	Importance	Mean difference	Prevalence
32	339.2	0.01513	0.02309	Infarct
33	256.25	0.01462	0.02220	Infarct
34	885.55	0.01362	-0.01307	Normal
35	115	0.01311	-0.08855	Normal
36	279.25	0.01261	-0.42116	Normal
37	305.25	0.01160	-0.04656	Normal
38	312.15	0.00908	0.00549	Infarct
39	197	0.00807	0.00008	Infarct
40	273.8	0.00656	0.03454	Infarct
41	297.15	0.00656	0.00804	Infarct
42	295.25	0.00454	-0.01265	Normal
43	747.5	0.00454	-0.01956	Normal
44	340.2	0.00353	0.00327	Infarct
45	114	0.00303	-0.01410	Normal
46	330.25	0.00303	-0.02568	Normal
47	452.3	0.00252	0.00002	Infarct
48	301.2	0.00252	-0.01129	Normal
49	117.05	0.00252	-0.00303	Normal
50	146.95	0.00252	0.07572	Infarct
51	459.35	0.00151	0.00020	Infarct
52	189.05	0.00151	-0.00235	Normal
53	205.15	0.00101	0.03261	Infarct
54	311.3	0.00101	0.00010	Infarct
55	332.25	0.00101	0.00098	Infarct
56	228.95	0.00050	0.00266	Infarct
57	455.3	0.00050	0.00019	Infarct
58	254.2	0.00050	0.00324	Infarct
59	102.95	0.00050	-0.00012	Normal
60	499.3	0.00050	-0.00461	Normal
61	130	0.00050	0.01312	Infarct
62	196.9	0.00050	0.00513	Infarct

Table S2. Performance of various classification algorithms on mass spectrometry imaging data collected during this study.

%	GBDT	PCA+LDA	SVM	Logistic Regression	RMMC	RF
Accuracy	97.43 ± 0.45	94.33±0.65	93.92±0.89	94.86±0.78	95.63±0.73	96.57±0.63
Recall	95.82 ± 1.46	91.32±1.84	88.07±2.27	89.45±1.20	90.92±1.98	94.03±0.72
Precision	94.84 ± 0.96	94.01±1.05	91.74±1.12	93.50±1.86	94.64±1.61	94.82±2.20