

Sensitivity, specificity, %undetermined, and quality (sensitivity + specificity - %undetermined) for each of the best distance-dependent 6-nearest neighbor classifiers using any of the 27 putative biomarkers.

Metric	1-ad	2-ad	3-ad	1-rd	2-rd	3-rd	2-cr	3-cr	2-sd	3-sd
Sens	60.0	61.1	64.4	60.7	61.8	72.1	65.1	69.4	63.4	70.4
Spec	58.9	70.0	71.1	58.0	73.7	67.6	68.2	76.3	68.2	77.2
%Undet	0.0	0.0	0.0	1.7	15.5	25.0	6.7	17.8	7.2	16.7
Quality	118.9	131.1	135.6	117.0	120.0	114.7	126.6	128.0	124.4	131.0

Sensitivity, specificity, %undetermined, and quality (sensitivity + specificity - %undetermined) for each of the best distance-dependent 6-nearest neighbor classifiers using any of the 27 putative biomarkers with the caveat that %Undetermined cannot exceed 5.0%.

Metric	1-ad	2-ad	3-ad	1-rd	2-rd	3-rd	2-cr	3-cr	2-sd	3-sd
Sens	60.0	61.1	64.4	60.7	None	None	65.5	None	62.5	None
Spec	58.9	70.0	71.1	58.0	None	None	60.7	None	60.2	None
%Undet	0.0	0.0	0.0	1.7	None	None	5.0	None	5.0	None
Quality	118.9	131.1	135.6	117.0	None	None	121.2	None	117.7	None

Fingerprint Analysis

Sensitivity, specificity and quality (sensitivity + specificity) for the best and 200th best decision tree constructed from any of the 300 peak intensities. The evolutionary programming search used a population size of 200 and ran for 400 generations. A decision node became a terminal node when it contained 1% (no samples) or 4% (3 samples) of a given State.

Metric	1%		1%		4%		4%	
	1 st	200 th						
Sensitivity	83.3	81.1	85.6	83.3	80.0	81.1	76.7	74.4
Specificity	83.3	83.3	76.7	75.6	86.7	84.4	84.4	84.4
Quality	166.7	164.4	162.2	158.9	166.7	165.6	161.1	158.9

Sensitivity, specificity and quality (sensitivity + specificity) for the best and 200th best medoid classifier algorithm in each of the two runs using 5-, 6-, and 7-peak intensities from the set of 300. The evolutionary programming search used a population size of 400 and ran for 800 generations with the requirement that there are at most 60 Case-cells and 60 Control-cells.

Metric	5-Features		5-Features		6-Features		6-Features		7-Features		7-Features	
	1 st	200 th										
Sens	100.0	100.0	86.7	81.1	100.0	100.0	87.8	82.2	100.0	100.0	90.0	85.6
Spec	85.6	77.8	100.0	100.0	85.6	80.0	100.0	100.0	88.9	82.2	100.0	100.0
Quality	185.6	177.8	186.7	181.1	185.6	180.0	187.8	182.2	188.9	182.2	190.0	185.6

(Last updated 4/21/07)