

Sensitivity, specificity, %undetermined, and quality (sensitivity + specificity - %undetermined) for each of the best distance-dependent 6-nearest neighbor classifiers using any of the 16 putative biomarkers.

| Metric | 1-ad | 2-ad | 3-ad | 1-rd | 2-rd | 3-rd | 2-cr | 3-cr | 2-sd | 3-sd |
|---------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| Sens | 63.4 | 81.0 | 75.7 | 57.5 | 74.2 | 84.4 | 75.6 | 82.9 | 75.6 | 79.4 |
| Spec | 59.5 | 59.0 | 73.5 | 61.9 | 67.6 | 76.7 | 62.2 | 71.4 | 62.2 | 79.4 |
| %Undet | 1.2 | 3.6 | 15.5 | 2.4 | 14.3 | 26.2 | 7.1 | 16.7 | 7.1 | 19.0 |
| Quality | 121.7 | 136.4 | 133.7 | 117.0 | 127.6 | 134.9 | 130.6 | 137.6 | 130.6 | 139.8 |

Sensitivity, specificity, %undetermined, and quality (sensitivity + specificity - %undetermined) for each of the best distance-dependent 6-nearest neighbor classifiers using any of the 16 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 | 63.4 | 81.0 | 68.3 | 57.5 | None | None | 70.0 | None | 70.0 | None |
| Spec | 59.5 | 59.0 | 66.7 | 61.9 | None | None | 62.5 | None | 62.5 | None |
| %Undet | 1.2 | 3.6 | 4.8 | 2.4 | None | None | 4.8 | None | 4.8 | None |
| Quality | 121.7 | 136.4 | 130.2 | 117.0 | None | None | 127.7 | None | 127.7 | 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% (1 sample) of a given State.

| Metric | 1% | | 1% | | 4% | | 4% | |
|-------------|-----------------|-------------------|-----------------|-------------------|-----------------|-------------------|-----------------|-------------------|
| | 1 st | 200 th |
| Sensitivity | 92.9 | 90.5 | 92.9 | 83.3 | 88.1 | 85.7 | 88.1 | 95.2 |
| Specificity | 95.2 | 95.2 | 92.9 | 95.2 | 95.2 | 95.2 | 95.2 | 85.7 |
| Quality | 188.1 | 185.7 | 185.7 | 178.6 | 183.3 | 181.0 | 183.3 | 181.0 |

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 28 Case-cells and 28 Control-cells.

| Metric | 5-Features | | 5-Features | | 6-Features | | 6-Features | | 7-Features | | 7-Features | |
|---------|-----------------|-------------------|-----------------|-------------------|-----------------|-------------------|-----------------|-------------------|-----------------|-------------------|-----------------|-------------------|
| | 1 st | 200 th |
| Sens | 100.0 | 100.0 | 92.9 | 88.1 | 100.0 | 100.0 | 97.6 | 92.9 | 100.0 | 100.0 | 97.6 | 95.2 |
| Spec | 97.6 | 88.1 | 100.0 | 100.0 | 97.6 | 92.9 | 100.0 | 100.0 | 96.7 | 92.9 | 100.0 | 100.0 |
| Quality | 197.6 | 188.1 | 192.9 | 188.1 | 197.6 | 192.9 | 197.6 | 192.9 | 197.6 | 192.9 | 197.6 | 195.2 |

(Last updated 4/21/07)