Supplementary

Table 1: Average “peak” (± standard deviation) counts for the standard samples

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Method | Total peak count | Class A peaks | Class B peaks | Class C peaks | Class D peaks |
| Derivative based detection high threshold | | | | | |
| No background correction | 114±5 | 91±4 | 0±0 | 0±0 | 23±4 |
| Direct | 117±8 | 96±8 | 0±0 | 0±0 | 21±0 |
| SVD-BC | 60±15 | 31±5 | 0±0 | 8±10 | 21±0 |
| AWLS | 21±1 | 0±0 | 0±0 | 0±0 | 21±1 |
| Drain algorithm high threshold without baseline correction | | | | | |
| No background correction | 158±7 | 90±5 | 46±3 | 0±0 | 22±2 |
| Direct | 87±11 | 65±12 | 1±1 | 0±0 | 21±0 |
| SVD-BC | 59±11 | 27±9 | 3±7 | 7±7 | 21±0 |
| AWLS | 21±1 | 0±0 | 0±0 | 0±0 | 21±1 |
| Drain algorithm high threshold with baseline correction | | | | | |
| No background correction | 90±7 | 52±7 | 10±3 | 0±0 | 29±1 |
| Direct | 87±1 | 51±4 | 10±3 | 0±0 | 26±1 |
| SVD-BC | 41±5 | 15±4 | 5±2 | 0±0 | 21±0 |
| AWLS | 22±1 | 0±0 | 0±0 | 0±0 | 22±1 |
| Derivative based detection low threshold | | | | | |
| No background correction | 124±21 | 91±4 | 0±0 | 8±10 | 25±3 |
| Direct | 128±6 | 98±9 | 0±0 | 0±0 | 30±5 |
| SVD-BC | 181±54 | 61±12 | 0±0 | 79±83 | 41±13 |
| AWLS | 23±0 | 0±0 | 0±0 | 0±0 | 23±0 |
| Drain algorithm low threshold without baseline correction | | | | | |
| No background correction | 168±21 | 90±6 | 45±2 | 8±16 | 25±12 |
| Direct | 103±8 | 63±11 | 3±2 | 6±5 | 32±13 |
| SVD-BC | 160±35 | 58±14 | 1±0 | 61±15 | 40±8 |
| AWLS | 24±1 | 0±0 | 0±0 | 0±0 | 24±1 |
| Drain algorithm low threshold with baseline correction | | | | | |
| No background correction | 103±8 | 57±6 | 9±3 | 0±0 | 37±6 |
| Direct | 91±1 | 54±4 | 9±2 | 0±1 | 28±1 |
| SVD-BC | 63±5 | 29±1 | 5±1 | 2±2 | 28±2 |
| AWLS | 24±1 | 0±0 | 0±0 | 0±0 | 24±1 |

aTrue number of peaks is 21 for the high threshold and 23 peaks for the low threshold.

Table 2: Average “peak” (± standard deviation) counts for the maize samples

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Method | Total peak count | Class A peaks | Class B peaks | Class C peaks | Class D peaks |
| Derivative based detection high threshold | | | | | |
| No background correction | 256±10 | 91±5 | 0±0 | 0±0 | 165±9 |
| Direct | 247±15 | 95±6 | 0±0 | 0±1 | 151±14 |
| SVD-BC | 137±21 | 32±4 | 0±0 | 14±14 | 90±14 |
| AWLS | 83±4 | 0±0 | 0±0 | 0±0 | 83±4 |
| Drain algorithm high threshold without baseline correction | | | | | |
| No background correction | 269±15 | 88±8 | 41±10 | 0±0 | 140±12 |
| Direct | 173±13 | 64±8 | 2±1 | 0±0 | 105±9 |
| SVD-BC | 125±18 | 29±4 | 2±5 | 9±8 | 83±8 |
| AWLS | 81±3 | 0±0 | 0±0 | 0±0 | 81±3 |
| Drain algorithm high threshold with baseline correction | | | | | |
| No background correction | 129±5 | 47±4 | 9±2 | 0±0 | 73±2 |
| Direct | 132±9 | 53±8 | 5±2 | 0±0 | 74±5 |
| SVD-BC | 86±3 | 14±2 | 6±3 | 0±0 | 67±2 |
| AWLS | 73±4 | 0±0 | 0±0 | 0±0 | 73±4 |
| Derivative based detection low threshold | | | | | |
| No background correction | 316±24 | 90±5 | 0±0 | 21±12 | 204±11 |
| Direct | 298±21 | 96±7 | 0±0 | 19±13 | 183±13 |
| SVD-BC | 600±140 | 70±10 | 0±0 | 88±22 | 441±114 |
| AWLS | 118±4 | 0±0 | 0±0 | 0±0 | 117±4 |
| Drain algorithm low threshold without baseline correction | | | | | |
| No background correction | 321±25 | 88±8 | 44±3 | 0±0 | 190±21 |
| Direct | 262±25 | 67±8 | 27±8 | 19±12 | 150±10 |
| SVD-BC | 397±82 | 54±6 | 6±7 | 75±18 | 263±59 |
| AWLS | 97±3 | 0±0 | 0±0 | 0±0 | 98±3 |
| Drain algorithm low threshold with baseline correction | | | | | |
| No background correction | 162±8 | 57±8 | 8±3 | 0±0 | 97±3 |
| Direct | 148±4 | 51±3 | 6±2 | 1±1 | 90±4 |
| SVD-BC | 147±6 | 26±4 | 7±4 | 1±1 | 113±6 |
| AWLS | 93±3 | 0±0 | 0±0 | 0±0 | 93±3 |