**Table A.2**

Optimised pre-processing and decision parameters for (1) DG-NIR, (2) HSI-NIR, (3) FTIR, (4) Raman

|   | Pre-processing | Origin | Instruments |
| --- | --- | --- | --- |
| 1 (DG-NIR) | 2 (HSI-NIR) | 3 (FTIR) | 4 (Raman) |
| Tvar% | RMSECV | RMSEC | RMSEP | MCC, Pred | Accuracy, Pred | F1, Pred | Tvar% | RMSECV | RMSEC | RMSEP | MCC, Pred | Accuracy, Pred | F1, Pred | Tvar% | RMSECV | RMSEC | RMSEP | MCC, Pred | Accuracy, Pred | F1, Pred | Tvar% | RMSECV | RMSEC | RMSEP | MCC, Pred | Accuracy, Pred | F1, Pred |
| 1 | MNCN | B | 98.54 | 0.300 | 0.290 | 0.408 | 0.832 | 0.909 | 0.917 | 99.69 | 0.317 | 0.310 | 0.380 | 0.655 | 0.800 | 0.833 | 99.69 | 0.436 | 0.418 | 0.486 | 0.156 | 0.476 | 0.000 | 99.91 | 0.384 | 0.373 | 0.342 | 0.894 | 0.944 | 0.947 |
| E |  | 0.383 | 0.379 | 0.434 | 0.109 | 0.458 | 0.209 |   | 0.426 | 0.414 | 0.499 | 0.000 | 0.500 | 0.000 |   | 0.355 | 0.343 | 0.647 | 0.429 | 0.286 | 0.286 |  | 0.381 | 0.371 | 0.422 | 0.447 | 0.667 | 0.500 |
| I |  | 0.289 | 0.274 | 0.632 | 0.000 | 0.500 | 0.000 |   | 0.331 | 0.318 | 0.309 | 1.000 | 1.000 | 1.000 |   | 0.410 | 0.400 | 0.529 | 0.224 | 0.452 | 0.000 |  | 0.164 | 0.160 | 0.238 | 0.845 | 0.917 | 0.909 |
| R |  | 0.379 | 0.375 | 0.419 | 0.589 | 0.792 | 0.805 |   | 0.415 | 0.407 | 0.496 | 0.816 | 0.900 | 0.889 |   | 0.414 | 0.403 | 0.416 | 0.202 | 0.595 | 0.514 |  | 0.347 | 0.343 | 0.316 | 0.837 | 0.912 | 0.919 |
| *Avg* |  | *0.338* | *0.329* | *0.473* | *0.383* | *0.665* | *0.483* |  | *0.372* | *0.362* | *0.421* | *0.618* | *0.800* | *0.681* |  | *0.404* | *0.391* | *0.520* | *0.253* | *0.452* | *0.200* |  | *0.319* | *0.312* | *0.329* | *0.756* | *0.860* | *0.819* |
| 2 | MSC, MNCN | B | 91.49 | 0.100 | 0.099 | 0.191 | 1.000 | 1.000 | 1.000 | 76.21 | 0.296 | 0.281 | 0.451 | 0.151 | 0.433 | 0.261 | 75.73 | 0.392 | 0.375 | 0.566 | 0.000 | 0.500 | 0.000 | 99.38 | 0.368 | 0.363 | 0.333 | 0.894 | 0.944 | 0.947 |
| E |  | 0.403 | 0.402 | 0.408 | 0.511 | 0.740 | 0.688 |   | 0.400 | 0.394 | 0.399 | 0.186 | 0.467 | 0.000 |   | 0.327 | 0.310 | 0.661 | 0.784 | 0.119 | 0.000 |  | 0.348 | 0.343 | 0.456 | 0.021 | 0.490 | 0.395 |
| I |  | 0.151 | 0.149 | 0.261 | 1.000 | 1.000 | 1.000 |   | 0.308 | 0.293 | 0.312 | 0.655 | 0.800 | 0.750 |   | 0.415 | 0.407 | 0.487 | 0.224 | 0.452 | 0.000 |  | 0.209 | 0.204 | 0.224 | 1.000 | 1.000 | 1.000 |
| R |  | 0.324 | 0.322 | 0.378 | 0.584 | 0.789 | 0.772 |   | 0.383 | 0.374 | 0.521 | 0.408 | 0.300 | 0.222 |   | 0.410 | 0.393 | 0.453 | 0.289 | 0.643 | 0.615 |  | 0.400 | 0.394 | 0.334 | 0.250 | 0.441 | 0.000 |
| *Avg* |  | *0.245* | *0.243* | *0.309* | *0.774* | *0.882* | *0.865* |  | *0.347* | *0.336* | *0.421* | *0.350* | *0.500* | *0.308* |  | *0.386* | *0.371* | *0.542* | *0.324* | *0.429* | *0.154* |  | *0.331* | *0.326* | *0.337* | *0.541* | *0.719* | *0.586* |
| 3 | SNV, MNCN | B | 91.49 | 0.100 | 0.099 | 0.191 | 1.000 | 1.000 | 1.000 | 76.20 | 0.296 | 0.281 | 0.451 | 0.151 | 0.433 | 0.261 | 75.68 | 0.392 | 0.375 | 0.566 | 0.000 | 0.500 | 0.000 | 99.36 | 0.368 | 0.363 | 0.333 | 0.894 | 0.944 | 0.947 |
| E |  | 0.403 | 0.402 | 0.408 | 0.511 | 0.740 | 0.688 |   | 0.400 | 0.394 | 0.399 | 0.186 | 0.467 | 0.000 |   | 0.327 | 0.310 | 0.661 | 0.784 | 0.119 | 0.000 |  | 0.348 | 0.343 | 0.456 | 0.021 | 0.490 | 0.395 |
| I |  | 0.151 | 0.149 | 0.261 | 1.000 | 1.000 | 1.000 |   | 0.308 | 0.293 | 0.312 | 0.655 | 0.800 | 0.750 |   | 0.415 | 0.407 | 0.486 | 0.224 | 0.452 | 0.000 |  | 0.209 | 0.203 | 0.224 | 1.000 | 1.000 | 1.000 |
| R |  | 0.324 | 0.322 | 0.378 | 0.584 | 0.789 | 0.772 |   | 0.383 | 0.374 | 0.521 | 0.408 | 0.300 | 0.222 |   | 0.409 | 0.393 | 0.453 | 0.289 | 0.643 | 0.615 |  | 0.399 | 0.394 | 0.334 | 0.250 | 0.441 | 0.000 |
| *Avg* |  | *0.245* | *0.243* | *0.309* | *0.774* | *0.882* | *0.865* |  | *0.347* | *0.336* | *0.421* | *0.350* | *0.500* | *0.308* |  | *0.386* | *0.371* | *0.542* | *0.324* | *0.429* | *0.154* |  | *0.331* | *0.326* | *0.337* | *0.541* | *0.719* | *0.586* |
| 4 | SNV, Detrend, MNCN | B | 91.32 | 0.101 | 0.099 | 0.191 | 1.000 | 1.000 | 1.000 | 75.65 | 0.297 | 0.282 | 0.450 | 0.392 | 0.367 | 0.000 | 70.33 | 0.392 | 0.376 | 0.517 | 0.000 | 0.500 | 0.000 | 99.37 | 0.368 | 0.363 | 0.333 | 0.894 | 0.944 | 0.947 |
| E |  | 0.403 | 0.402 | 0.408 | 0.511 | 0.740 | 0.688 |   | 0.400 | 0.394 | 0.400 | 0.267 | 0.433 | 0.000 |   | 0.326 | 0.305 | 0.629 | 0.670 | 0.190 | 0.000 |  | 0.348 | 0.343 | 0.456 | 0.021 | 0.490 | 0.395 |
| I |  | 0.151 | 0.148 | 0.260 | 1.000 | 1.000 | 1.000 |   | 0.309 | 0.294 | 0.314 | 0.655 | 0.800 | 0.750 |   | 0.417 | 0.409 | 0.472 | 0.324 | 0.405 | 0.000 |  | 0.209 | 0.203 | 0.224 | 1.000 | 1.000 | 1.000 |
| R |  | 0.324 | 0.322 | 0.378 | 0.584 | 0.789 | 0.772 |   | 0.382 | 0.374 | 0.520 | 0.471 | 0.267 | 0.214 |   | 0.409 | 0.393 | 0.448 | 0.239 | 0.619 | 0.600 |  | 0.399 | 0.394 | 0.334 | 0.250 | 0.441 | 0.000 |
| *Avg* |  | *0.245* | *0.243* | *0.309* | *0.774* | *0.882* | *0.865* |  | *0.347* | *0.336* | *0.421* | *0.446* | *0.467* | *0.241* |  | *0.386* | *0.371* | *0.516* | *0.308* | *0.429* | *0.150* |  | *0.331* | *0.326* | *0.337* | *0.541* | *0.719* | *0.586* |
| 5 | Normalisation, MNCN | B | 85.54 | 0.103 | 0.099 | 0.253 | 1.000 | 1.000 | 1.000 | 98.28 | 0.285 | 0.269 | 0.337 | 0.935 | 0.967 | 0.968 | 98.17 | 0.402 | 0.381 | 0.538 | 0.156 | 0.476 | 0.000 | 99.05 | 0.377 | 0.372 | 0.343 | 0.845 | 0.917 | 0.923 |
| E |   | 0.380 | 0.374 | 0.474 | 0.719 | 0.841 | 0.863 |   | 0.388 | 0.380 | 0.429 | 0.267 | 0.433 | 0.000 |   | 0.327 | 0.311 | 0.652 | 0.745 | 0.143 | 0.000 |  | 0.342 | 0.337 | 0.446 | 0.021 | 0.490 | 0.395 |
| I |   | 0.223 | 0.214 | 0.370 | 0.258 | 0.563 | 0.222 |   | 0.276 | 0.266 | 0.314 | 0.655 | 0.800 | 0.750 |   | 0.427 | 0.413 | 0.494 | 0.156 | 0.476 | 0.000 |  | 0.224 | 0.217 | 0.234 | 0.845 | 0.917 | 0.909 |
| R |   | 0.390 | 0.386 | 0.431 | 0.636 | 0.812 | 0.791 |   | 0.384 | 0.375 | 0.527 | 0.761 | 0.867 | 0.882 |   | 0.416 | 0.408 | 0.434 | 0.429 | 0.714 | 0.714 |  | 0.399 | 0.394 | 0.333 | 0.250 | 0.441 | 0.000 |
| *Avg* |  | *0.274* | *0.269* | *0.382* | *0.653* | *0.804* | *0.719* |  | *0.333* | *0.322* | *0.402* | *0.655* | *0.767* | *0.650* |  | *0.393* | *0.378* | *0.530* | *0.372* | *0.452* | *0.179* |  | 0.335 | 0.330 | 0.339 | *0.490* | *0.691* | *0.557* |
| 6 | SG (1der, 2poly, 7pts), MNCN | B | 88.01 | 0.251 | 0.243 | 0.346 | 1.000 | 1.000 | 1.000 | 53.10 | 0.314 | 0.296 | 0.320 | 0.935 | 0.967 | 0.968 | 98.89 | 0.400 | 0.383 | 0.493 | 0.074 | 0.524 | 0.231 | 99.72 | 0.418 | 0.414 | 0.381 | 0.259 | 0.617 | 0.511 |
| E |  | 0.396 | 0.394 | 0.323 | 0.218 | 0.455 | 0.000 |   | 0.388 | 0.383 | 0.480 | 0.186 | 0.467 | 0.000 |   | 0.329 | 0.313 | 0.667 | 0.526 | 0.238 | 0.273 |  | 0.334 | 0.323 | 0.392 | 0.632 | 0.804 | 0.773 |
| I |  | 0.097 | 0.094 | 0.160 | 1.000 | 1.000 | 1.000 |   | 0.277 | 0.249 | 0.229 | 0.816 | 0.900 | 0.889 |   | 0.424 | 0.412 | 0.561 | 0.224 | 0.452 | 0.000 |  | 0.322 | 0.316 | 0.424 | 0.086 | 0.466 | 0.238 |
| R |  | 0.359 | 0.355 | 0.422 | 0.396 | 0.698 | 0.703 |   | 0.374 | 0.363 | 0.417 | 0.761 | 0.867 | 0.882 |   | 0.429 | 0.417 | 0.414 | 0.000 | 0.500 | 0.222 |  | 0.343 | 0.335 | 0.308 | 0.889 | 0.941 | 0.944 |
| *Avg* |  | *0.276* | *0.272* | *0.313* | *0.654* | *0.788* | *0.676* |  | *0.338* | *0.323* | *0.362* | *0.675* | *0.800* | *0.685* |  | *0.395* | *0.382* | *0.534* | *0.206* | *0.429* | *0.181* |  | *0.354* | *0.347* | *0.376* | *0.466* | *0.707* | *0.616* |
| 7 | SG (1st der, 2nd poly, 9pts), MNCN | B | 89.34 | 0.251 | 0.243 | 0.345 | 1.000 | 1.000 | 1.000 | 57.43 | 0.314 | 0.296 | 0.312 | 0.935 | 0.967 | 0.968 | 99.26 | 0.401 | 0.387 | 0.492 | 0.074 | 0.524 | 0.231 | 99.72 | 0.418 | 0.414 | 0.381 | 0.259 | 0.617 | 0.511 |
| E |  | 0.397 | 0.395 | 0.323 | 0.218 | 0.455 | 0.000 |   | 0.388 | 0.382 | 0.470 | 0.186 | 0.467 | 0.000 |   | 0.328 | 0.314 | 0.663 | 0.526 | 0.238 | 0.273 |  | 0.335 | 0.324 | 0.394 | 0.632 | 0.804 | 0.773 |
| I |  | 0.093 | 0.090 | 0.154 | 1.000 | 1.000 | 1.000 |   | 0.280 | 0.253 | 0.234 | 1.000 | 1.000 | 1.000 |   | 0.421 | 0.412 | 0.558 | 0.224 | 0.452 | 0.000 |  | 0.323 | 0.317 | 0.425 | 0.086 | 0.466 | 0.238 |
| R |  | 0.358 | 0.355 | 0.422 | 0.396 | 0.698 | 0.703 |   | 0.374 | 0.364 | 0.430 | 0.535 | 0.767 | 0.774 |   | 0.429 | 0.418 | 0.414 | 0.000 | 0.500 | 0.222 |  | 0.343 | 0.335 | 0.308 | 0.889 | 0.941 | 0.944 |
| *Avg* |  | *0.275* | *0.271* | *0.311* | *0.654* | *0.788* | *0.676* |  | *0.339* | *0.323* | *0.362* | *0.664* | *0.800* | *0.685* |  | *0.395* | *0.383* | *0.532* | *0.206* | *0.429* | *0.181* |  | *0.355* | *0.348* | *0.377* | *0.466* | *0.707* | *0.616* |
| 8 | SG (1st der, 2nd poly, 15pts), MNCN | B | 91.3 | 0.250 | 0.243 | 0.344 | 1.000 | 1.000 | 1.000 | 68.87 | 0.322 | 0.301 | 0.279 | 0.874 | 0.933 | 0.938 | 99.61 | 0.404 | 0.392 | 0.491 | 0.162 | 0.548 | 0.240 | 99.71 | 0.419 | 0.415 | 0.380 | 0.259 | 0.617 | 0.511 |
| E |  | 0.398 | 0.396 | 0.324 | 0.218 | 0.455 | 0.000 |   | 0.383 | 0.375 | 0.416 | 0.336 | 0.667 | 0.643 |   | 0.332 | 0.319 | 0.658 | 0.526 | 0.238 | 0.273 |  | 0.337 | 0.326 | 0.399 | 0.632 | 0.804 | 0.773 |
| I |  | 0.089 | 0.087 | 0.150 | 1.000 | 1.000 | 1.000 |   | 0.277 | 0.253 | 0.279 | 1.000 | 1.000 | 1.000 |   | 0.420 | 0.411 | 0.554 | 0.277 | 0.429 | 0.000 |  | 0.323 | 0.317 | 0.426 | 0.086 | 0.466 | 0.238 |
| R |  | 0.357 | 0.354 | 0.421 | 0.396 | 0.698 | 0.703 |   | 0.382 | 0.373 | 0.482 | 0.333 | 0.600 | 0.333 |   | 0.428 | 0.416 | 0.414 | 0.000 | 0.500 | 0.222 |  | 0.342 | 0.335 | 0.309 | 0.889 | 0.941 | 0.944 |
| *Avg* |  | *0.274* | *0.270* | *0.310* | *0.654* | *0.788* | *0.676* |  | *0.341* | *0.325* | *0.364* | *0.636* | *0.800* | *0.728* |  | *0.396* | *0.384* | *0.529* | *0.241* | *0.429* | *0.184* |  | 0.355 | 0.348 | 0.379 | *0.466* | *0.707* | *0.616* |
| 9 | SG (2nd der, 2nd poly, 7pts), MNCN | B | 97.83 | 0.285 | 0.270 | 0.455 | 0.683 | 0.818 | 0.846 | 46.73 | 0.389 | 0.365 | 0.442 | 0.471 | 0.733 | 0.750 | 93.32 | 0.434 | 0.423 | 0.410 | 0.368 | 0.381 | 0.000 | 99.66 | 0.416 | 0.411 | 0.384 | 0.331 | 0.644 | 0.529 |
| E |  | 0.407 | 0.400 | 0.293 | 0.316 | 0.409 | 0.000 |   | 0.434 | 0.418 | 0.467 | 0.267 | 0.433 | 0.000 |   | 0.362 | 0.347 | 0.650 | 0.404 | 0.310 | 0.171 |  | 0.321 | 0.309 | 0.368 | 0.779 | 0.887 | 0.881 |
| I |  | 0.422 | 0.417 | 0.483 | 0.224 | 0.452 | 0.000 |   | 0.311 | 0.261 | 0.278 | 0.655 | 0.800 | 0.750 |   | 0.354 | 0.331 | 0.666 | 0.368 | 0.381 | 0.000 |  | 0.322 | 0.316 | 0.419 | 0.086 | 0.466 | 0.238 |
| R |  | 0.416 | 0.409 | 0.417 | 0.208 | 0.412 | 0.196 |   | 0.406 | 0.384 | 0.382 | 0.935 | 0.967 | 0.968 |   | 0.405 | 0.389 | 0.622 | 0.408 | 0.357 | 0.000 |  | 0.342 | 0.335 | 0.306 | 0.889 | 0.941 | 0.944 |
| *Avg* |  | *0.383* | *0.374* | *0.412* | *0.358* | *0.523* | *0.260* |  | *0.385* | *0.357* | *0.393* | *0.582* | *0.733* | *0.617* |  | *0.389* | *0.372* | *0.587* | *0.387* | *0.357* | *0.043* |  | *0.350* | *0.343* | *0.369* | *0.521* | *0.735* | *0.648* |
| 10 | SG (2nd der, 2nd poly, 9pts), MNCN | B | 95.52 | 0.283 | 0.268 | 0.452 | 0.683 | 0.818 | 0.846 | 53.91 | 0.379 | 0.356 | 0.433 | 0.535 | 0.767 | 0.774 | 96.29 | 0.414 | 0.387 | 0.376 | 0.191 | 0.595 | 0.585 | 99.71 | 0.416 | 0.412 | 0.385 | 0.259 | 0.617 | 0.511 |
| E |  | 0.408 | 0.400 | 0.295 | 0.053 | 0.481 | 0.216 |   | 0.431 | 0.417 | 0.481 | 0.000 | 0.500 | 0.000 |   | 0.360 | 0.344 | 0.658 | 0.596 | 0.238 | 0.000 |  | 0.325 | 0.314 | 0.372 | 0.632 | 0.804 | 0.773 |
| I |  | 0.421 | 0.415 | 0.488 | 0.224 | 0.452 | 0.000 |   | 0.300 | 0.254 | 0.231 | 1.000 | 1.000 | 1.000 |   | 0.419 | 0.364 | 0.614 | 0.368 | 0.381 | 0.000 |  | 0.322 | 0.316 | 0.420 | 0.086 | 0.466 | 0.238 |
| R |  | 0.416 | 0.409 | 0.417 | 0.160 | 0.435 | 0.202 |   | 0.397 | 0.380 | 0.388 | 0.874 | 0.933 | 0.938 |   | 0.432 | 0.421 | 0.499 | 0.000 | 0.500 | 0.000 |  | 0.343 | 0.336 | 0.305 | 0.889 | 0.941 | 0.944 |
| *Avg* |  | *0.382* | *0.373* | *0.413* | *0.280* | *0.547* | *0.316* |  | *0.377* | *0.352* | *0.383* | *0.602* | *0.800* | *0.678* |  | *0.406* | *0.379* | *0.537* | *0.288* | *0.429* | *0.146* |  | *0.351* | *0.344* | *0.370* | *0.466* | *0.707* | *0.616* |
| 11 | SG (2nd der, 2nd poly, 15pts), MNCN | B | 80.97 | 0.270 | 0.250 | 0.402 | 0.719 | 0.841 | 0.863 | 47.56 | 0.327 | 0.299 | 0.302 | 0.816 | 0.900 | 0.909 | 98.95 | 0.400 | 0.385 | 0.495 | 0.074 | 0.524 | 0.231 | 99.75 | 0.415 | 0.411 | 0.385 | 0.259 | 0.617 | 0.511 |
| E |  | 0.404 | 0.400 | 0.317 | 0.218 | 0.455 | 0.000 |   | 0.392 | 0.381 | 0.453 | 0.079 | 0.467 | 0.273 |   | 0.324 | 0.310 | 0.668 | 0.667 | 0.167 | 0.146 |  | 0.329 | 0.318 | 0.379 | 0.632 | 0.804 | 0.773 |
| I |  | 0.375 | 0.373 | 0.502 | 0.248 | 0.396 | 0.171 |   | 0.323 | 0.291 | 0.284 | 0.816 | 0.900 | 0.889 |   | 0.421 | 0.412 | 0.562 | 0.224 | 0.452 | 0.000 |  | 0.322 | 0.317 | 0.422 | 0.086 | 0.466 | 0.238 |
| R |  | 0.416 | 0.412 | 0.424 | 0.053 | 0.481 | 0.216 |   | 0.395 | 0.381 | 0.412 | 0.394 | 0.667 | 0.545 |   | 0.431 | 0.420 | 0.418 | 0.064 | 0.476 | 0.214 |  | 0.344 | 0.337 | 0.306 | 0.889 | 0.941 | 0.944 |
| *Avg* |  | *0.366* | *0.359* | *0.411* | *0.310* | *0.543* | *0.312* |  | *0.359* | *0.338* | *0.363* | *0.526* | *0.733* | *0.654* |  | *0.394* | *0.382* | *0.536* | *0.257* | *0.405* | *0.148* |  | *0.353* | *0.346* | *0.373* | *0.466* | *0.707* | *0.616* |
| 12 | MSC, SG (1st der, 2nd poly, 15pts), MNCN | B | 76.06 | 0.117 | 0.113 | 0.138 | 1.000 | 1.000 | 1.000 | 63.41 | 0.310 | 0.293 | 0.429 | 0.484 | 0.733 | 0.692 | 60.48 | 0.409 | 0.393 | 0.519 | 0.000 | 0.500 | 0.000 | 99.02 | 0.360 | 0.356 | 0.330 | 0.894 | 0.944 | 0.947 |
| E |  | 0.377 | 0.376 | 0.366 | 0.249 | 0.597 | 0.415 |   | 0.389 | 0.382 | 0.388 | 0.000 | 0.500 | 0.000 |   | 0.318 | 0.287 | 0.652 | 0.534 | 0.238 | 0.158 |  | 0.347 | 0.341 | 0.455 | 0.021 | 0.490 | 0.395 |
| I |  | 0.092 | 0.090 | 0.142 | 1.000 | 1.000 | 1.000 |   | 0.271 | 0.250 | 0.305 | 1.000 | 1.000 | 1.000 |   | 0.422 | 0.413 | 0.501 | 0.408 | 0.357 | 0.000 |  | 0.209 | 0.202 | 0.228 | 1.000 | 1.000 | 1.000 |
| R |  | 0.345 | 0.344 | 0.347 | 0.488 | 0.744 | 0.736 |   | 0.380 | 0.370 | 0.489 | 0.408 | 0.700 | 0.727 |   | 0.413 | 0.397 | 0.410 | 0.447 | 0.714 | 0.667 |  | 0.398 | 0.393 | 0.336 | 0.250 | 0.441 | 0.000 |
| *Avg* |  | *0.233* | *0.231* | *0.248* | *0.684* | *0.835* | *0.788* |  | *0.338* | *0.324* | *0.403* | *0.473* | *0.733* | *0.605* |  | *0.390* | *0.372* | *0.521* | *0.347* | *0.452* | *0.206* |  | 0.329 | 0.323 | 0.337 | *0.541* | *0.719* | *0.586* |
| 13 | MSC, SG (2nd der, 2nd poly, 7pts), MNCN | B | 98.2 | 0.425 | 0.418 | 0.436 | 0.402 | 0.695 | 0.652 | 47.78 | 0.388 | 0.365 | 0.472 | 0.134 | 0.433 | 0.414 | 69.05 | 0.446 | 0.417 | 0.477 | 0.447 | 0.333 | 0.000 | 87.97 | 0.344 | 0.337 | 0.324 | 0.845 | 0.917 | 0.923 |
| E |  | 0.389 | 0.384 | 0.389 | 0.385 | 0.669 | 0.564 |   | 0.441 | 0.426 | 0.460 | 0.186 | 0.467 | 0.000 |   | 0.425 | 0.359 | 0.683 | 0.447 | 0.333 | 0.000 |  | 0.346 | 0.341 | 0.453 | 0.021 | 0.490 | 0.395 |
| I |  | 0.106 | 0.103 | 0.135 | 1.000 | 1.000 | 1.000 |   | 0.289 | 0.259 | 0.254 | 0.816 | 0.900 | 0.889 |   | 0.388 | 0.362 | 0.797 | 0.121 | 0.452 | 0.207 |  | 0.212 | 0.203 | 0.239 | 0.845 | 0.917 | 0.909 |
| R |  | 0.426 | 0.420 | 0.404 | 0.014 | 0.506 | 0.367 |   | 0.403 | 0.383 | 0.409 | 0.218 | 0.600 | 0.500 |   | 0.385 | 0.372 | 0.698 | 0.485 | 0.310 | 0.000 |  | 0.393 | 0.387 | 0.337 | 0.250 | 0.441 | 0.000 |
| *Avg* |  | *0.336* | *0.331* | *0.341* | *0.450* | *0.718* | *0.646* |  | *0.380* | *0.358* | *0.399* | *0.339* | *0.600* | *0.451* |  | *0.411* | *0.378* | *0.664* | *0.375* | *0.357* | *0.052* |  | *0.324* | *0.317* | *0.338* | *0.490* | *0.691* | *0.557* |
| 14 | Normalisation, SG (1st der, 2nd poly, 15pts), MNCN | B | 77.31 | 0.170 | 0.166 | 0.251 | 1.000 | 1.000 | 1.000 | 85.79 | 0.284 | 0.272 | 0.287 | 0.874 | 0.933 | 0.938 | 97.12 | 0.392 | 0.354 | 0.404 | 0.243 | 0.595 | 0.414 | 98.94 | 0.340 | 0.335 | 0.310 | 0.894 | 0.944 | 0.947 |
| E |  | 0.354 | 0.351 | 0.416 | 0.719 | 0.841 | 0.863 |   | 0.370 | 0.359 | 0.428 | 0.089 | 0.533 | 0.300 |   | 0.401 | 0.368 | 0.491 | 0.052 | 0.476 | 0.353 |  | 0.355 | 0.348 | 0.466 | 0.149 | 0.574 | 0.540 |
| I |  | 0.079 | 0.075 | 0.140 | 1.000 | 1.000 | 1.000 |   | 0.261 | 0.245 | 0.293 | 1.000 | 1.000 | 1.000 |   | 0.396 | 0.362 | 0.547 | 0.074 | 0.524 | 0.231 |  | 0.190 | 0.184 | 0.221 | 1.000 | 1.000 | 1.000 |
| R |  | 0.387 | 0.384 | 0.361 | 0.000 | 0.500 | 0.000 |   | 0.382 | 0.375 | 0.491 | 0.484 | 0.733 | 0.692 |   | 0.418 | 0.392 | 0.517 | 0.196 | 0.405 | 0.324 |  | 0.399 | 0.393 | 0.339 | 0.174 | 0.471 | 0.000 |
| *Avg* |  | *0.247* | *0.244* | *0.292* | *0.680* | *0.835* | *0.716* |  | *0.324* | *0.313* | *0.375* | *0.612* | *0.800* | *0.732* |  | *0.402* | *0.369* | *0.490* | *0.141* | *0.500* | *0.330* |  | *0.321* | *0.315* | *0.334* | *0.554* | *0.747* | *0.622* |
| 15 | Normalisation, SG (2nd der, 2nd poly, 7pts), MNCN | B | 98.05 | 0.437 | 0.430 | 0.438 | 0.632 | 0.786 | 0.727 | 50.25 | 0.357 | 0.337 | 0.410 | 0.471 | 0.733 | 0.750 | 78.39 | 0.427 | 0.409 | 0.454 | 0.000 | 0.500 | 0.000 | 87.43 | 0.261 | 0.247 | 0.272 | 0.946 | 0.972 | 0.973 |
| E |  | 0.359 | 0.353 | 0.362 | 0.793 | 0.886 | 0.898 |   | 0.435 | 0.415 | 0.499 | 0.000 | 0.500 | 0.000 |   | 0.389 | 0.367 | 0.579 | 0.485 | 0.310 | 0.000 |  | 0.361 | 0.356 | 0.470 | 0.151 | 0.436 | 0.228 |
| I |  | 0.217 | 0.212 | 0.224 | 1.000 | 1.000 | 1.000 |   | 0.311 | 0.269 | 0.265 | 1.000 | 1.000 | 1.000 |   | 0.417 | 0.400 | 0.467 | 0.074 | 0.524 | 0.231 |  | 0.193 | 0.177 | 0.295 | 0.779 | 0.887 | 0.881 |
| R |  | 0.420 | 0.413 | 0.380 | 0.183 | 0.575 | 0.402 |   | 0.415 | 0.392 | 0.415 | 0.935 | 0.967 | 0.968 |   | 0.402 | 0.386 | 0.516 | 0.239 | 0.381 | 0.409 |  | 0.394 | 0.389 | 0.345 | 0.086 | 0.466 | 0.238 |
| *Avg* |  | *0.358* | *0.352* | *0.351* | *0.652* | *0.812* | *0.757* |  | *0.379* | *0.353* | *0.397* | *0.602* | *0.800* | *0.679* |  | *0.409* | *0.390* | *0.504* | *0.199* | *0.429* | *0.160* |  | *0.302* | *0.292* | *0.346* | *0.490* | *0.690* | *0.580* |
| 16 | SNV, Detrend, SG( 1st der, 2nd poly, 15pts), MNCN | B | 76.04 | 0.117 | 0.113 | 0.138 | 1.000 | 1.000 | 1.000 | 63.17 | 0.310 | 0.293 | 0.428 | 0.484 | 0.733 | 0.692 | 61.21 | 0.412 | 0.395 | 0.514 | 0.156 | 0.476 | 0.000 | 99.01 | 0.361 | 0.356 | 0.330 | 0.894 | 0.944 | 0.947 |
| E |  | 0.377 | 0.376 | 0.366 | 0.249 | 0.597 | 0.415 |   | 0.390 | 0.382 | 0.389 | 0.000 | 0.500 | 0.000 |   | 0.321 | 0.289 | 0.646 | 0.534 | 0.238 | 0.158 |  | 0.347 | 0.341 | 0.454 | 0.021 | 0.490 | 0.395 |
| I |  | 0.092 | 0.090 | 0.142 | 1.000 | 1.000 | 1.000 |   | 0.271 | 0.249 | 0.304 | 1.000 | 1.000 | 1.000 |   | 0.422 | 0.413 | 0.504 | 0.408 | 0.357 | 0.000 |  | 0.209 | 0.202 | 0.228 | 1.000 | 1.000 | 1.000 |
| R |  | 0.345 | 0.344 | 0.346 | 0.488 | 0.744 | 0.736 |   | 0.380 | 0.370 | 0.487 | 0.408 | 0.700 | 0.727 |   | 0.413 | 0.398 | 0.410 | 0.316 | 0.643 | 0.545 |  | 0.398 | 0.393 | 0.336 | 0.250 | 0.441 | 0.000 |
| *Avg* |  | *0.233* | *0.231* | *0.248* | *0.684* | *0.835* | *0.788* |  | *0.338* | *0.324* | *0.402* | *0.473* | *0.733* | *0.605* |  | *0.392* | *0.374* | *0.519* | *0.354* | *0.429* | *0.176* |  | *0.329* | *0.323* | *0.337* | *0.541* | *0.719* | *0.586* |
| 17 | SNV, Detrend, SG( 2nd der, 2nd poly, 7pts), MNCN | B | 98.2 | 0.425 | 0.418 | 0.436 | 0.402 | 0.695 | 0.652 | 47.78 | 0.388 | 0.365 | 0.472 | 0.134 | 0.433 | 0.414 | 68.93 | 0.449 | 0.419 | 0.461 | 0.485 | 0.310 | 0.000 | 87.39 | 0.344 | 0.337 | 0.324 | 0.845 | 0.917 | 0.923 |
| E |  | 0.388 | 0.384 | 0.389 | 0.385 | 0.669 | 0.564 |   | 0.440 | 0.426 | 0.460 | 0.186 | 0.467 | 0.000 |   | 0.429 | 0.364 | 0.664 | 0.408 | 0.357 | 0.000 |  | 0.346 | 0.341 | 0.452 | 0.021 | 0.490 | 0.395 |
| I |  | 0.106 | 0.103 | 0.135 | 1.000 | 1.000 | 1.000 |   | 0.289 | 0.259 | 0.254 | 0.816 | 0.900 | 0.889 |   | 0.389 | 0.362 | 0.792 | 0.121 | 0.452 | 0.207 |  | 0.211 | 0.202 | 0.238 | 0.845 | 0.917 | 0.909 |
| R |  | 0.426 | 0.420 | 0.404 | 0.014 | 0.506 | 0.367 |   | 0.403 | 0.383 | 0.408 | 0.218 | 0.600 | 0.500 |   | 0.384 | 0.371 | 0.699 | 0.485 | 0.310 | 0.000 |  | 0.393 | 0.387 | 0.337 | 0.250 | 0.441 | 0.000 |
| *Avg* |  | *0.336* | *0.331* | *0.341* | *0.450* | *0.718* | *0.646* |  | *0.380* | *0.358* | *0.399* | *0.339* | *0.600* | *0.451* |  | *0.413* | *0.379* | *0.654* | *0.375* | *0.357* | *0.052* |  | *0.324* | *0.317* | *0.338* | *0.490* | *0.691* | *0.557* |
| 18 | SNV, SG( 1st der, 2nd poly, 15pts), MNCN | B | 76.06 | 0.117 | 0.113 | 0.138 | 1.000 | 1.000 | 1.000 | 63.38 | 0.309 | 0.292 | 0.428 | 0.484 | 0.733 | 0.692 | 60.96 | 0.411 | 0.394 | 0.522 | 0.000 | 0.500 | 0.000 | 99.02 | 0.360 | 0.355 | 0.329 | 0.894 | 0.944 | 0.947 |
| E |  | 0.377 | 0.376 | 0.365 | 0.249 | 0.597 | 0.415 |   | 0.389 | 0.382 | 0.388 | 0.000 | 0.500 | 0.000 |   | 0.318 | 0.287 | 0.658 | 0.534 | 0.238 | 0.158 |  | 0.347 | 0.341 | 0.456 | 0.021 | 0.490 | 0.395 |
| I |  | 0.092 | 0.090 | 0.142 | 1.000 | 1.000 | 1.000 |   | 0.271 | 0.250 | 0.305 | 1.000 | 1.000 | 1.000 |   | 0.421 | 0.413 | 0.505 | 0.408 | 0.357 | 0.000 |  | 0.212 | 0.204 | 0.229 | 1.000 | 1.000 | 1.000 |
| R |  | 0.346 | 0.344 | 0.347 | 0.488 | 0.744 | 0.736 |   | 0.380 | 0.370 | 0.489 | 0.408 | 0.700 | 0.727 |   | 0.411 | 0.396 | 0.408 | 0.447 | 0.714 | 0.667 |  | 0.398 | 0.392 | 0.336 | 0.250 | 0.441 | 0.000 |
| *Avg* |  | *0.233* | *0.231* | *0.248* | *0.684* | *0.835* | *0.788* |  | *0.337* | *0.324* | *0.402* | *0.473* | *0.733* | *0.605* |  | *0.390* | *0.372* | *0.523* | *0.347* | *0.452* | *0.206* |  | *0.329* | *0.323* | *0.338* | *0.541* | *0.719* | *0.586* |
| 19 | SNV, SG( 2nd der, 2nd poly, 7pts), MNCN | B | 98.2 | 0.425 | 0.418 | 0.436 | 0.402 | 0.695 | 0.652 | 47.78 | 0.388 | 0.365 | 0.472 | 0.134 | 0.433 | 0.414 | 68.88 | 0.445 | 0.417 | 0.477 | 0.447 | 0.333 | 0.000 | 87.99 | 0.343 | 0.336 | 0.323 | 0.845 | 0.917 | 0.923 |
| E |  | 0.388 | 0.384 | 0.389 | 0.385 | 0.669 | 0.564 |   | 0.440 | 0.426 | 0.460 | 0.186 | 0.467 | 0.000 |   | 0.424 | 0.359 | 0.686 | 0.447 | 0.333 | 0.000 |  | 0.346 | 0.341 | 0.454 | 0.021 | 0.490 | 0.395 |
| I |  | 0.106 | 0.103 | 0.135 | 1.000 | 1.000 | 1.000 |   | 0.289 | 0.259 | 0.254 | 0.816 | 0.900 | 0.889 |   | 0.387 | 0.362 | 0.797 | 0.121 | 0.452 | 0.207 |  | 0.215 | 0.205 | 0.241 | 0.845 | 0.917 | 0.909 |
| R |  | 0.426 | 0.420 | 0.404 | 0.014 | 0.506 | 0.367 |   | 0.403 | 0.383 | 0.408 | 0.218 | 0.600 | 0.500 |   | 0.385 | 0.372 | 0.697 | 0.485 | 0.310 | 0.000 |  | 0.393 | 0.387 | 0.338 | 0.250 | 0.441 | 0.000 |
| *Avg* |  | *0.336* | *0.331* | *0.341* | *0.450* | *0.718* | *0.646* |  | *0.380* | *0.358* | *0.399* | *0.339* | *0.600* | *0.451* |  | *0.410* | *0.377* | *0.664* | *0.375* | *0.357* | *0.052* |  | *0.324* | *0.317* | *0.339* | *0.490* | *0.691* | *0.557* |
| 20 | EMSC, MNCN | B | 87.87 | 0.145 | 0.141 | 0.164 | 1.000 | 1.000 | 1.000 | 76.22 | 0.348 | 0.337 | 0.456 | 0.186 | 0.467 | 0.000 | 71.52 | 0.417 | 0.400 | 0.442 | 0.316 | 0.643 | 0.545 | 97.25 | 0.283 | 0.278 | 0.265 | 0.894 | 0.944 | 0.947 |
| E |  | 0.341 | 0.340 | 0.306 | 0.872 | 0.932 | 0.936 |   | 0.419 | 0.414 | 0.448 | 0.603 | 0.233 | 0.000 |   | 0.377 | 0.336 | 0.569 | 0.485 | 0.310 | 0.000 |  | 0.361 | 0.358 | 0.447 | 0.212 | 0.407 | 0.219 |
| I |  | 0.088 | 0.087 | 0.141 | 1.000 | 1.000 | 1.000 |   | 0.317 | 0.293 | 0.320 | 0.500 | 0.700 | 0.571 |   | 0.422 | 0.411 | 0.449 | 0.243 | 0.595 | 0.414 |  | 0.135 | 0.129 | 0.189 | 1.000 | 1.000 | 1.000 |
| R |  | 0.386 | 0.385 | 0.389 | 0.632 | 0.786 | 0.727 |   | 0.365 | 0.355 | 0.476 | 0.471 | 0.733 | 0.750 |   | 0.420 | 0.389 | 0.469 | 0.101 | 0.452 | 0.343 |  | 0.391 | 0.389 | 0.353 | 0.311 | 0.412 | 0.000 |
| *Avg* |  | *0.240* | *0.238* | *0.250* | *0.876* | *0.929* | *0.916* |  | *0.362* | *0.350* | *0.425* | *0.440* | *0.533* | *0.330* |  | *0.409* | *0.384* | *0.482* | *0.286* | *0.500* | *0.326* |  | *0.293* | *0.288* | *0.314* | *0.604* | *0.691* | *0.542* |
| 21 | WLS (2nd poly), MNCN | B | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 96.86 | 0.433 | 0.428 | 0.413 | 0.580 | 0.772 | 0.725 |
| E | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |  | 0.336 | 0.327 | 0.399 | 0.632 | 0.804 | 0.773 |
| I | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |  | 0.242 | 0.238 | 0.354 | 0.342 | 0.662 | 0.596 |
| R | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |  | 0.360 | 0.350 | 0.322 | 0.889 | 0.941 | 0.944 |
| *Avg* | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |   | *0.343* | *0.336* | *0.372* | *0.611* | *0.795* | *0.760* |
| 22 | WLS (2nd poly), normalisation, MNCN | B | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | 96.46 | 0.286 | 0.279 | 0.268 | 0.894 | 0.944 | 0.947 |
| E | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |  | 0.361 | 0.357 | 0.442 | 0.086 | 0.466 | 0.238 |
| I | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |  | 0.137 | 0.131 | 0.188 | 1.000 | 1.000 | 1.000 |
| R | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |  | 0.391 | 0.388 | 0.357 | 0.180 | 0.578 | 0.442 |
| *Avg* | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |   | *0.294* | *0.289* | *0.314* | *0.540* | *0.747* | *0.657* |
| *Notes: DG-NIR (Dispersive near-infrared), HSI (Hyperspectral Imaging), FTIR (Fourier Transform infrared/mid-infrared), RMSE(C/CV/P) (Root Mean Square Errors of Calibration/Cross-Validation/Prediction), TVar (Total variance explained), LVs (Number of Latent Variables), SG (#der, #poly, #pts) (Savitzky-Golay #derivative, #polynomial, #window points), WT (Wavelet Transform), MSC (Multiplicative Scatter Correction), SNV (Standard Normal Variate), MNCN (Mean centering), EMSC (Extended Multiplicative Scatter correction), MNCN (Mean centering), WLS (Weighted Least Squares), MCC (Matthew’s Correlation Coefficient)* |