## Appendix B: PLSpredict assessment of the original model (PLS) vs. naive benchmark (LM)

|      | PLS       | Q²_predict | LM        | PLS-LM    |
|------|-----------|------------|-----------|----------|
|      | RMSE      | MAE        | RMSE      | MAE      | RMSE      | MAE      |
| BI1  | 1.085     | 0.878      | -0.003    | 1.084    | 0.88      | -0.001   | -0.002   |
| BI2  | 1.047     | 0.832      | 0.058     | 1.047    | 0.829     | 0         | 0.003     |
| BI3  | 1.117     | 0.921      | 0.043     | 1.115    | 0.917     | 0.002     | -0.004    |
| BI4  | 1.197     | 0.97       | 0.048     | 1.201    | 0.974     | -0.004    | -0.004    |
| BI5  | 1.083     | 0.869      | 0.052     | 1.084    | 0.865     | -0.001    | 0.004     |
| CTOP1| 1.323     | 1.159      | 0.034     | 1.323    | 1.158     | 0         | 0.001     |
| CTOP2| 1.235     | 1.014      | 0.033     | 1.235    | 1.011     | 0         | 0.003     |
| CTOP3| 1.125     | 0.866      | 0.002     | 1.126    | 0.851     | -0.001    | 0.015     |
| TSA1 | 1.158     | 0.938      | -0.011    | 1.152    | 0.939     | 0.006     | -0.001    |
| TSA2 | 1.208     | 0.901      | 0.043     | 1.208    | 0.889     | 0         | 0.012     |
| TSA3 | 1.073     | 0.867      | 0.069     | 1.063    | 0.861     | 0.01      | 0.006     |
| TSC1 | 1.202     | 0.992      | 0.024     | 1.204    | 0.982     | -0.002    | 0.01      |
| TSC2 | 1.178     | 0.966      | 0.009     | 1.18     | 0.967     | -0.002    | -0.001    |
| TSC3 | 1.146     | 0.856      | 0.018     | 1.148    | 0.855     | -0.002    | 0.001     |
| TSCC1| 1.152     | 0.905      | 0.018     | 1.149    | 0.902     | 0.003     | 0.003     |
| TSCC2| 1.089     | 0.886      | 0.099     | 1.082    | 0.864     | 0.007     | 0.022     |
| TSCC3| 1.307     | 1.065      | 0.038     | 1.307    | 1.068     | 0         | -0.003    |
| TSCPB1| 1.06      | 0.863      | 0.024     | 1.061    | 0.866     | -0.001    | -0.003    |
| TSCPB2| 1.077     | 0.892      | 0.017     | 1.074    | 0.887     | 0.003     | 0.005     |
| TSCPB3| 1.141     | 0.921      | 0.063     | 1.14     | 0.911     | 0.001     | 0.01      |
| TSCPC1| 1.178     | 1.015      | 0.023     | 1.181    | 1.018     | -0.003    | -0.003    |
| TSCPC2| 1.224     | 1.019      | 0.04      | 1.228    | 1.015     | -0.004    | 0.004     |
| TSCPC3| 1.115     | 0.876      | -0.01     | 1.113    | 0.88      | 0.002     | -0.004    |
| TSCP1| 1.045     | 0.828      | 0.099     | 1.037    | 0.804     | 0.008     | 0.024     |
| TSCP2| 1.187     | 0.972      | 0.035     | 1.19     | 0.977     | -0.003    | -0.005    |
| TSCP3| 1.057     | 0.85       | 0.06      | 1.057    | 0.847     | 0         | 0.003     |
| TSELLB1| 1.216     | 0.992      | 0.011     | 1.212    | 0.996     | 0.004     | -0.004    |
| TSELLB2| 1.158     | 0.964      | 0.023     | 1.162    | 0.967     | -0.004    | -0.003    |
| TSELLB3| 1.189     | 0.985      | 0.032     | 1.193    | 0.98      | -0.004    | 0.005     |
| TSELLC1| 1.304     | 1.148      | 0.021     | 1.303    | 1.15      | 0.001     | -0.002    |
| TSELLC2| 1.081     | 0.911      | 0.041     | 1.081    | 0.908     | 0         | 0.003     |
| TSELLC3| 1.177     | 0.962      | -0.045    | 1.155    | 0.956     | 0.022     | 0.026     |
| TSELLI1| 1.222     | 1.015      | 0.056     | 1.221    | 1.005     | -0.001    | 0.01      |
| TSELLI2| 1.138     | 0.912      | 0.055     | 1.135    | 0.9       | 0.003     | 0.012     |
| TSELLI3| 1.088     | 0.891      | 0.046     | 1.088    | 0.887     | 0         | 0.004     |