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*Article*

# Supplementary Material:

# UV-Vis Spectroscopy and Chemometrics for Monitoring of Organosolv Pretreatments

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**Table S1.** Reference concentrations in data block 1

| Sample No. | Lignin | HMF | Furfural | AcOH |
|---|---|---|---|---|
| | mg/L | | | |
| 1 | 0.189 | 0.00200 | 0.00200 | 6.00 |
| 2 | 0.472 | 0.00600 | 0.00600 | 4.00 |
| 3 | 0.944 | 0.00800 | 0.00800 | 8.00 |
| 4 | 1.89 | 0.0100 | 0.0100 | 10.0 |
| 5 | 2.83 | 0.0200 | 0.0200 | 15.0 |
| 6 | 3.78 | 0.0400 | 0.0400 | 25.0 |
| 7 | 5.67 | 0.0600 | 0.0600 | 64.0 |
| 8 | 7.55 | 0.0800 | 0.0800 | 80.0 |
| 9 | 9.44 | 0.100 | 0.100 | 200 |
| 10 | 11.3 | 0.200 | 0.200 | 1000 |
| 11 | 14.2 | 0.500 | 1.00 | |
| 12 | 18.9 | 1.00 | 5.00 | |
| 13 | 23.6 | 5.00 | 10.0 | |
| 14 | 30.2 | 10.0 | | |
| Mean | 9.35 | 1.22 | 1.27 | 141 |
| STD | 9.35 | 2.85 | 2.96 | 308 |

**Table S2.** Reference concentrations in data block 2

| Sample No. | Lignin | HMF | Furfural | AcOH |
|---|---|---|---|---|
| | mg/L | | | |
| 1 | 0.189 | 0.00200 | 0.00200 | 6.00 |
| 1 | 2.83 | 0.0500 | 0.0500 | 1.00 |
| 2 | 2.83 | 0.750 | 0.0500 | 15.0 |
| 3 | 2.83 | 0.750 | 0.0500 | 1.00 |
| 4 | 2.83 | 0.0500 | 0.0500 | 15.0 |
| 5 | 2.83 | 0.750 | 0.750 | 1.00 |
| 6 | 2.83 | 0.0500 | 0.750 | 1.00 |
| 7 | 2.83 | 0.750 | 0.750 | 15.0 |
| 8 | 2.83 | 0.0500 | 0.750 | 15.0 |
| 9 | 2.83 | 0.400 | 0.400 | 8.00 |
| 10 | 13.2 | 0.750 | 0.400 | 8.00 |
| 11 | 13.2 | 0.400 | 0.400 | 1.00 |
| 12 | 13.2 | 0.400 | 0.0500 | 8.00 |
| 13 | 13.2 | 0.400 | 0.400 | 8.00 |
| 14 | 13.2 | 0.400 | 0.400 | 8.00 |
| 15 | 13.2 | 0.400 | 0.750 | 8.00 |
| 16 | 13.2 | 0.0500 | 0.400 | 8.00 |
| 17 | 13.2 | 0.400 | 0.400 | 8.00 |
| 18 | 13.2 | 0.400 | 0.400 | 15.0 |
| 19 | 23.6 | 0.750 | 0.750 | 1.00 |
| 20 | 23.6 | 0.0500 | 0.750 | 15.0 |
| 21 | 23.6 | 0.750 | 0.750 | 15.0 |
| 22 | 23.6 | 0.750 | 0.0500 | 1.00 |
| 23 | 23.6 | 0.0500 | 0.750 | 1.00 |
| 24 | 23.6 | 0.750 | 0.0500 | 15.0 |
| Mean | 11.9 | 0.429 | 0.429 | 8.00 |
| STD | 8.28 | 0.290 | 0.290 | 5.84 |

**Table S3.** Reference concentrations in data block 3

| Sample No. | Lignin | HMF | Furfural | AcOH |
|---|---|---|---|---|
| | mg/L | | | |
| 1 | 0.189 | 0.00200 | 0.00200 | 6.00 |
| 1 | 6.25 | 0.00706 | 0.00766 | 1.43 |
| 2 | 8.61 | 0.00706 | 0.00766 | 1.43 |
| 3 | 9.37 | 0.0106 | 0.0115 | 2.15 |
| 4 | 11.0 | 0.00706 | 0.00766 | 1.43 |
| 5 | 11.7 | 0.0106 | 0.0115 | 2.15 |
| 6 | 12.5 | 0.0141 | 0.0153 | 2.87 |
| 7 | 13.3 | 0.00706 | 0.00766 | 1.43 |
| 8 | 14.1 | 0.0106 | 0.0115 | 2.15 |
| 9 | 14.4 | 0.0141 | 0.0153 | 2.87 |
| 10 | 15.7 | 0.00706 | 0.00766 | 1.43 |
| 11 | 16.5 | 0.0106 | 0.0115 | 2.15 |
| 12 | 17.2 | 0.0141 | 0.0153 | 2.87 |
| 13 | 18.1 | 0.00706 | 0.00766 | 1.43 |
| 14 | 18.8 | 0.0106 | 0.0115 | 2.15 |
| 15 | 20.4 | 0.00706 | 0.00766 | 1.43 |
| 16 | 21.2 | 0.0106 | 0.0115 | 2.15 |
| 17 | 21.9 | 0.0141 | 0.0153 | 2.87 |
| 18 | 23.5 | 0.0106 | 0.0115 | 2.15 |
| 19 | 26.7 | 0.0141 | 0.0153 | 2.87 |
| 20 | 28.3 | 0.0106 | 0.0115 | 2.15 |
| 21 | 31.4 | 0.0141 | 0.0153 | 2.87 |
| 22 | 36.1 | 0.0141 | 0.0153 | 2.87 |
| 23 | 40.8 | 0.0141 | 0.0153 | 2.87 |
| Mean | 19.0 | 0.0107 | 0.0117 | 2.18 |
| STD | 8.85 | 0.00291 | 0.00316 | 0.591 |

**Table S4.** Reference concentrations in data block 4

| Sample No. | Lignin | HMF | Furfural | AcOH |
|---|---|---|---|---|
| | mg/L | | | |
| 1 | 3.01 | 0.00093 | 0.00315 | 0.696 |
| 2 | 3.20 | 0.00087 | 0.00301 | 0.726 |
| 3 | 3.20 | 0.00093 | 0.00313 | 0.701 |
| 4 | 6.30 | 0.00168 | 0.00564 | 1.41 |
| 5 | 6.46 | 0.00182 | 0.00603 | 1.44 |
| 6 | 6.69 | 0.00239 | 0.0117 | 1.48 |
| 7 | 6.69 | 0.00239 | 0.0117 | 1.48 |
| 8 | 6.88 | 0.00216 | 0.00753 | 1.47 |
| 9 | 6.88 | 0.00173 | 0.00550 | 1.42 |
| 10 | 7.51 | 0.00249 | 0.00825 | 1.59 |
| 11 | 9.02 | 0.00280 | 0.00944 | 2.09 |
| 12 | 9.60 | 0.00261 | 0.00902 | 2.18 |
| 13 | 11.3 | 0.00374 | 0.0124 | 2.39 |
| 14 | 12.6 | 0.00336 | 0.0113 | 2.82 |
| 15 | 12.9 | 0.00339 | 0.0111 | 2.84 |
| 16 | 13.4 | 0.00478 | 0.0235 | 2.96 |
| 17 | 13.8 | 0.00432 | 0.0151 | 2.94 |
| 18 | 15.0 | 0.00499 | 0.0165 | 3.18 |
| 19 | 15.0 | 0.00466 | 0.0157 | 3.48 |
| 20 | 16.0 | 0.00435 | 0.0150 | 3.63 |
| 21 | 18.9 | 0.00505 | 0.0169 | 4.23 |
| 22 | 19.4 | 0.00508 | 0.0166 | 4.26 |
| 23 | 20.6 | 0.00518 | 0.0165 | 4.26 |
| 24 | 22.4 | 0.00651 | 0.0219 | 4.91 |
| 25 | 22.6 | 0.00638 | 0.0211 | 5.05 |
| 26 | 25.6 | 0.00744 | 0.0250 | 5.61 |
| 27 | 25.9 | 0.00678 | 0.0222 | 5.67 |
| 28 | 27.5 | 0.00864 | 0.0301 | 5.87 |
| 29 | 27.5 | 0.00690 | 0.0220 | 5.68 |
| 30 | 29.0 | 0.00820 | 0.0271 | 6.50 |
| Mean | 14.2 | 0.00408 | 0.0141 | 3.10 |
| STD | 8.08 | 0.00223 | 0.00750 | 1.75 |

**Table S5.** Reference concentrations in data block 5

| Sample No. | Lignin | HMF | Furfural | AcOH |
|---|---|---|---|---|
| | mg/L | | | |
| 1 | 4.96 | 0.00296 | 0.0213 | 1.02 |
| 2 | 6.16 | 0.00164 | 0.00425 | 1.29 |
| 3 | 12.3 | 0.00328 | 0.00850 | 2.58 |
| 4 | 14.9 | 0.00889 | 0.0638 | 3.06 |
| 5 | 18.5 | 0.00493 | 0.0128 | 3.87 |
| 6 | 24.8 | 0.0148 | 0.106 | 5.11 |
| Mean | 13.6 | 0.00609 | 0.0362 | 2.82 |
| STD | 7.51 | 0.00496 | 0.0406 | 1.55 |

**Table S6.** Overview of datasets used for PLS modeling after different pre-processing methods of Block 1. Matrix sizes ($n \times m$) are given in no. of samples (rows) times no. of variables (columns).

| Preprocessing | Lignin | AcOH | HMF | Furfural |
|---|---|---|---|---|
| | Size of matrix $\boldsymbol{X}$ ($n \times m$) | | | |
| Raw | 14 × 251 | 10 × 251 | 14 × 251 | 13 × 251 |
| 1st Derivative | 14 × 247 | 10 × 247 | 14 × 247 | 13 × 247 |
| 2nd Derivative | 14 × 247 | 10 × 247 | 14 × 247 | 13 × 247 |
| $\Delta_{284/320\ nm}$ | 14 × 251 | 10 × 251 | 14 × 251 | 13 × 251 |

**Table S7.** Overview of datasets used for chemometric modeling after different pre-processing methods of Block 2 to 5. Matrix sizes ($n \times m$) are given in no. of samples (rows) times no. of variables (columns).

| Preprocessing | Block 2 | Block 3 | Block 4 | Block 5 |
|---|---|---|---|---|
| | Size of matrix $\boldsymbol{X}$ ($n \times m$) | | | |
| Raw | 24 × 251 | 23 × 251 | 30 × 251 | 6 × 251 |
| 1st Derivative | 24 × 247 | 23 × 247 | 30 × 247 | 6 × 247 |
| 2nd Derivative | 24 × 247 | 23 × 247 | 30 × 247 | 6 × 247 |
| $\Delta_{284/320\ nm}$ | 24 × 251 | 23 × 251 | 30 × 251 | 6 × 251 |