### Supplementary Table 2. Cross-validated results for different 1D input data types

| 1D Input data | Mean and standard deviation (k-folds=60) | Cross-correlation | $R^2$ | MCC(6) |
|---------------|------------------------------------------|-------------------|-------|--------|
| Imputed       |                                          | 0.340 ± 0.395     | 0.444 ± 0.187 | 0.407 ± 0.260 |
| Non-Imputed   |                                          | 0.305 ± 0.345     | 0.381 ± 0.172 | 0.360 ± 0.252 |

### Supplementary Table 3. Cross-validated results for different solvent system

| 1D input data | Mean and standard deviation (k-folds=60) | Cross-correlation | $R^2$ | MCC(6) |
|---------------|------------------------------------------|-------------------|-------|--------|
| E1            |                                          | 0.373 ± 0.421     | 0.502 ± 0.175 | 0.423 ± 0.251 |
| E2            |                                          | 0.306 ± 0.361     | 0.424 ± 0.188 | 0.411 ± 0.277 |
| E3            |                                          | 0.355 ± 0.412     | 0.306 ± 0.124 | 0.333 ± 0.195 |
| Non-Imputed   |                                          | 0.324 ± 0.376     | 0.396 ± 0.148 | 0.361 ± 0.237 |
|               |                                          | 0.287 ± 0.330     | 0.400 ± 0.189 | 0.376 ± 0.272 |
|               |                                          | 0.303 ± 0.367     | 0.251 ± 0.112 | 0.294 ± 0.203 |

### Suppl. Table 4. Significance test for solvent system analysis with imputed 1D input data

|          | Cross-correlation | $R^2$ | MCC(6) |
|----------|-------------------|-------|--------|
| E1       | 0                 | < 0.001 | < 0.0001 | < 0.0001 |
| E2       | 0.007             | < 0.0001 | < 0.0001 | < 0.0001 | < 0.0001 |
| E3       | < 0.001           | < 0.0001 | < 0.0001 | < 0.0001 | 0 |

### Suppl. Table 5. Significance for solvent system analysis with non-imputed 1D input data

|          | Cross-correlation | $R^2$ | MCC(6) |
|----------|-------------------|-------|--------|
| E1       | 0                 | < 0.001 | < 0.0001 | < 0.0001 |
| E2       | < 0.0001          | 0.0004 | 0.006 | < 0.0001 | < 0.0001 | 0 |
| E3       | < 0.001           | 0.0004 | < 0.0001 | < 0.0001 | 0 | < 0.0001 | < 0.0001 | 0 |