

## Supplementary Material

### Assessment of UV-VIS spectra analysis methods for quantifying the absorption properties of Chromophoric Dissolved Organic Matter (CDOM)

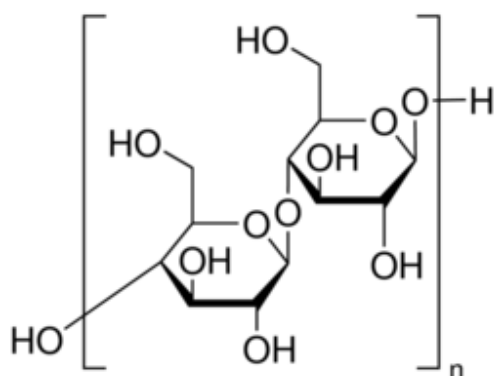
Ruosha Zeng\*, Chris M. Mannaerts, Caroline Lievens

\* Correspondence: r.zeng@utwente.nl

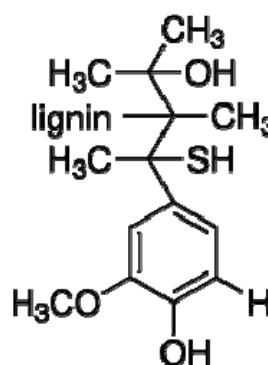
#### 1 Molecular structure of biomass constituent materials

Their molecular structures are shown in figure SI1. Because humic acid does not have a universal structural formula. It is composed of heterogenous compounds, including phenolic radicals and acids.

A)



B)



**Supplementary Figure 1.** Molecular structure of commercial cellulose(a) and lignin(b) used in our experiment.

## Supplementary Material

### 2 Component and DOC concentration information of samples

**Supplementary Table 2.** DOC concentrations measured by TOC analyzer and the component proportions of six three-component mixtures

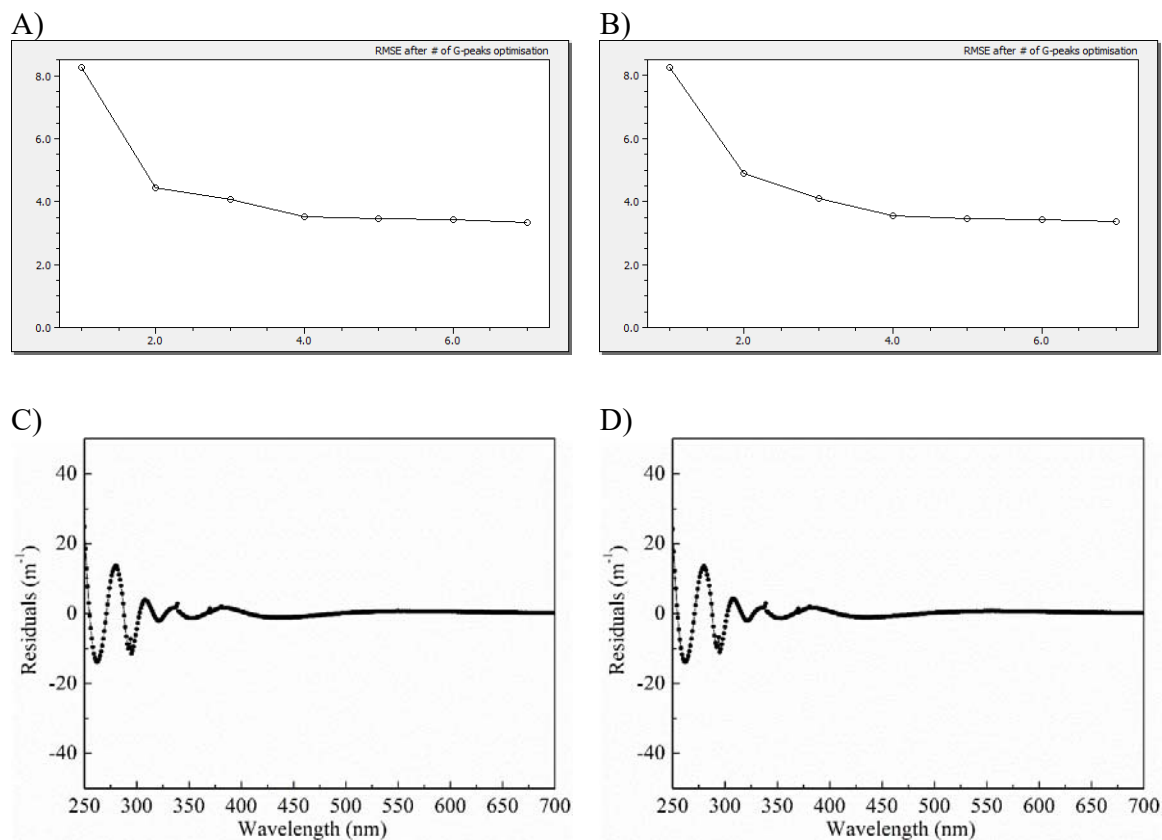
| Sample ID                                | wt%  | DOC(mg C/L) | C/HA | L/HA | C/L  |
|------------------------------------------|------|-------------|------|------|------|
| Cellulose dissolved solution 1 (CDS1)    | 0.1  | 10.06       | -    | -    | -    |
| Cellulose dissolved solution 2 (CDS2)    | 0.1  | 5.47        | -    | -    | -    |
| Lignin dissolved solution 1 (LDS1)       | 0.1  | 35.54       | -    | -    | -    |
| Lignin dissolved solution 2 (LDS2)       | 0.1  | 35.14       | -    | -    | -    |
| Humic acid dissolved solution 1 (HADS1)* | 0.1  | 11.54       | -    | -    | -    |
| Humic acid dissolved solution 2 (HADS2)* | 0.1  | 11.49       | -    | -    | -    |
| Mix solution1 (MIX1)*                    | 0.1  | 5.29        | 2.03 | 1    | 2.04 |
| Mix solution2 (MIX2)*                    | 0.1  | 4.60        | 1.97 | 0.98 | 2.02 |
| Mix solution3 (MIX3)*                    | 0.1  | 5.89        | 1.05 | 2    | 0.52 |
| Mix solution4 (MIX4)*                    | 0.11 | 6.16        | 0.91 | 1.96 | 0.46 |
| Mix solution 5 (MIX5)*                   | 0.1  | 8.18        | 0.51 | 0.51 | 0.99 |
| Mix solution 6 (MIX6)*                   | 0.1  | 7.90        | 0.5  | 0.49 | 1.01 |

\*ten times diluted from the sample after filtration.

C/HA denotes to the weight ratio of cellulose to humic acid in the solids; L/HA denotes to the weight ratio of lignin to humic acid in the solids; C/L denotes to the weight ratio of cellulose to lignin in the solids.

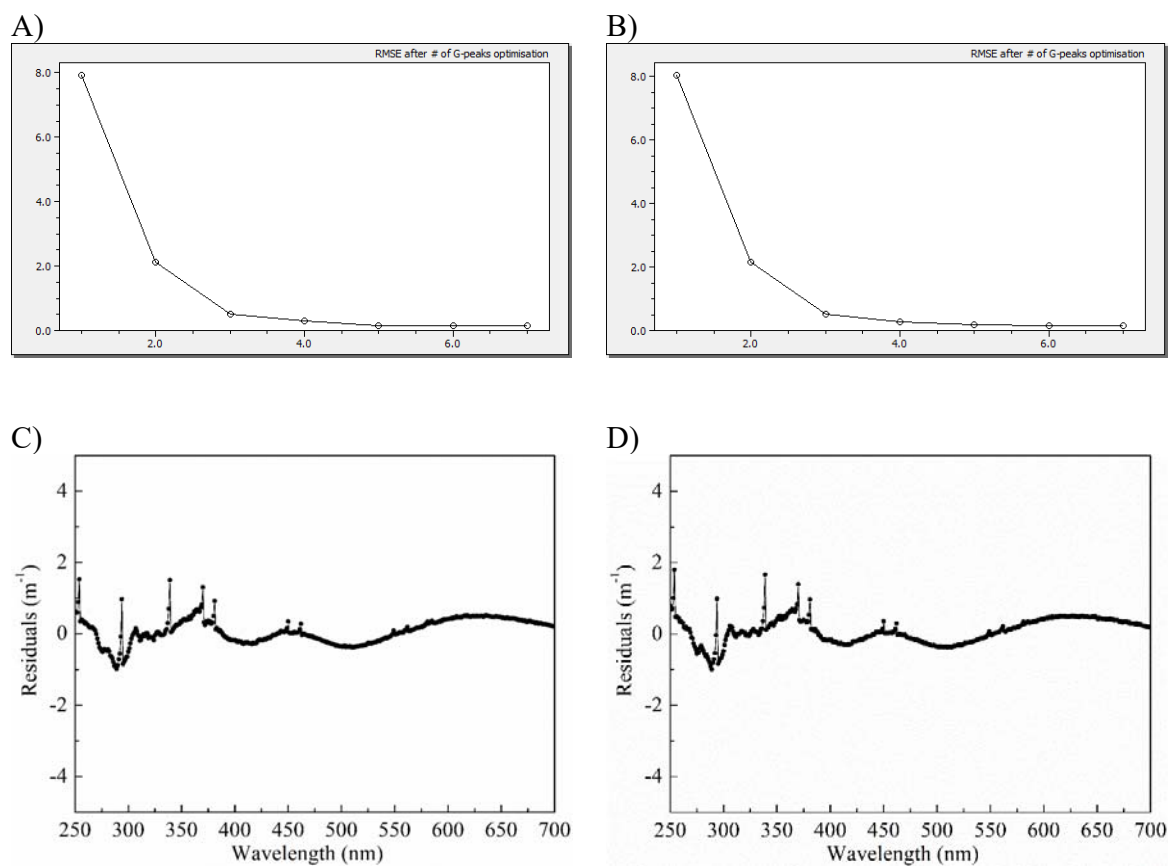
### 3 Details of Gaussian fit

#### 3.1 Gaussian fit only



**Supplementary Figure 2.** Residual's RMSE (ordinate) of optimization of peak numbers (abscissa) using only Gaussian fitting methods in ASFit for a) LDS1 and b) LDS2 absorption coefficient spectra; and residuals of c) LDS1 and d) LDS2 with the most optimized number ( $n=4$ ).

## Supplementary Material

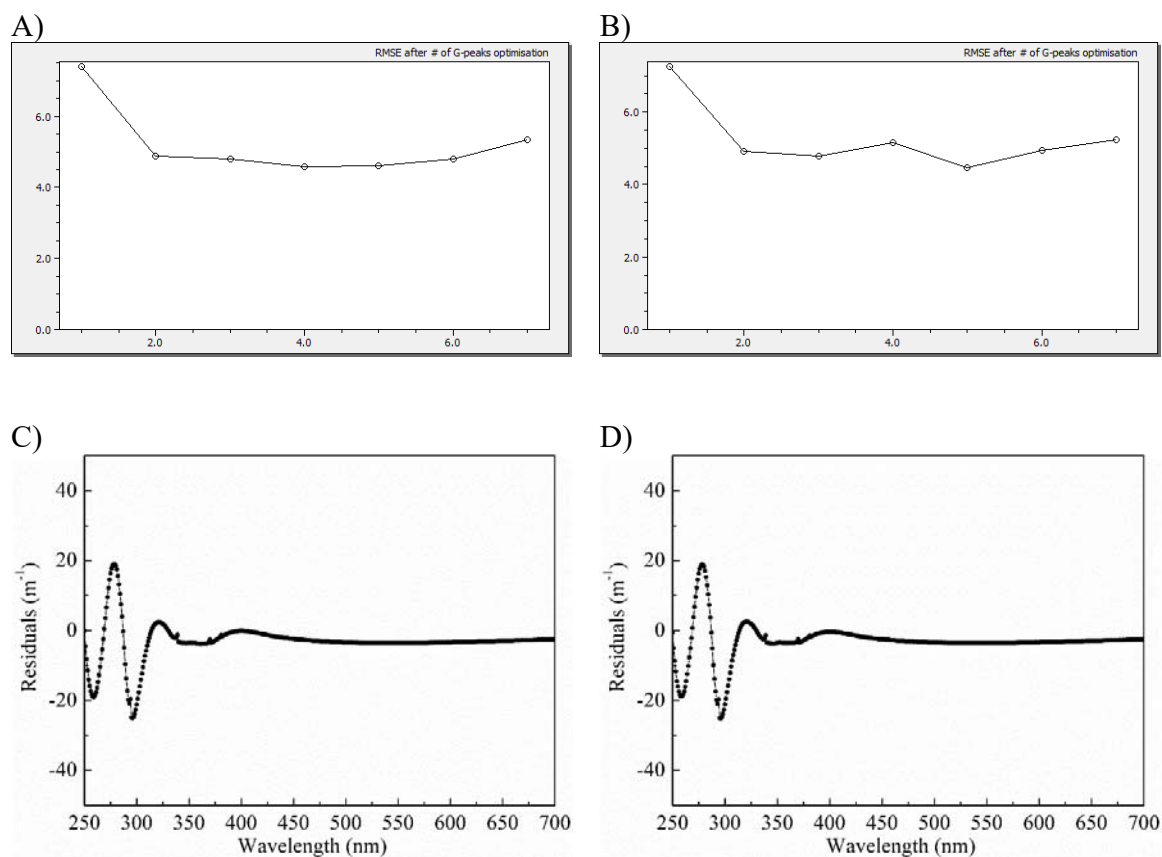


**Supplementary Figure 3.** Residual's RMSE (ordinate) of optimization of peak numbers (abscissa) using only Gaussian fitting methods in ASFit for a) HADS1 and b) HADS2 absorption coefficient spectra; and residuals of c) HADS1 and d) HADS2 with the most optimized number (n=2).

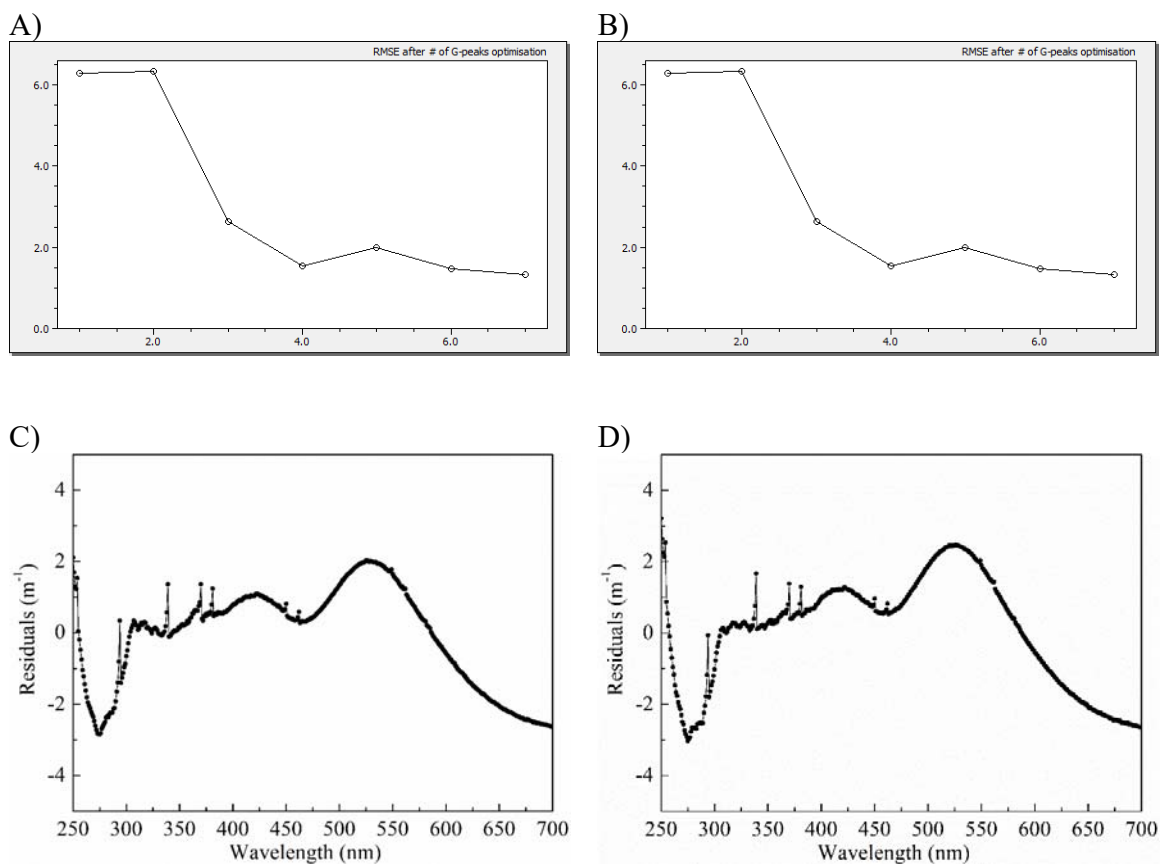
**Supplementary Table 2.** Details for Gaussian fit of LDS and HADS absorption coefficient spectra

| Gaussian peaks (GP) | GP1   | GP2   | GP3   | GP4   |
|---------------------|-------|-------|-------|-------|
| LDS1                |       |       |       |       |
| Position(nm)        | 272   | 318.4 | 342.1 | 368.3 |
| Height(m-1)         | 220.1 | 32.7  | 43.1  | 11.3  |
| Halfwidth(nm)       | 26.1  | 10    | 19.3  | 79.2  |
| LDS2                |       |       |       |       |
| Position(nm)        | 272   | 318.3 | 341.1 | 368.3 |
| Height(m-1)         | 221.4 | 33.6  | 41.2  | 10.9  |
| Halfwidth(nm)       | 26    | 10    | 19.4  | 79.3  |
| HADS1               |       |       |       |       |
| Position(nm)        | 215.2 | 327   |       |       |
| Height(m-1)         | 211   | 42.8  |       |       |
| Halfwidth(nm)       | 76.7  | 127   |       |       |
| HADS2               |       |       |       |       |
| Position(nm)        | 215.3 | 327   |       |       |
| Height(m-1)         | 214.8 | 43.4  |       |       |
| Halfwidth(nm)       | 76.8  | 126.8 |       |       |

### 3.2 Gaussian in combination with exponential



**Supplementary Figure 4.** Residual's RMSE (ordinate) of optimization of peak numbers (abscissa) using Gaussian in combination with exponential fitting methods in ASFit for a) LDS1 and b) LDS2 absorption coefficient spectra; and residuals of c) LDS1 and d) LDS2 with the most optimized number ( $n=2$ ).



**Supplementary Figure 5.** Residual's RMSE (ordinate) of optimization of peak numbers (abscissa) using Gaussian in combination with exponential fitting methods in ASFit for a) HADS1 and b) HADS2 absorption coefficient spectra; and residuals of c) HADS1 and d) HADS2 with the most optimized number ( $n=4$ ).

Supplementary Material

**Supplementary Table 3.** Details for Gaussian in combination with an exponential fit of LDS and HADS absorption coefficient spectra

| Gaussian peaks (GP) | GP1   | GP2   | GP3   | GP4   |
|---------------------|-------|-------|-------|-------|
| LDS1                |       |       |       |       |
| Position(nm)        | 271.2 | 342.9 |       |       |
| Height(m-1)         | 200.9 | 32.2  |       |       |
| Halfwidth(nm)       | 33.1  | 22.9  |       |       |
| LDS2                |       |       |       |       |
| Position(nm)        | 271.3 | 342.5 |       |       |
| Height(m-1)         | 201.7 | 30.1  |       |       |
| Halfwidth(nm)       | 33    | 23.3  |       |       |
| HADS1               |       |       |       |       |
| Position(nm)        | 241.4 | 331.9 | 376.8 | 440.5 |
| Height(m-1)         | 203.3 | 21.2  | 20.4  | 16.6  |
| Halfwidth(nm)       | 58.9  | 31.3  | 33.3  | 47.2  |
| HADS2               |       |       |       |       |
| Position(nm)        | 241.7 | 331.8 | 376.4 | 440.1 |
| Height(m-1)         | 205.5 | 22    | 20.4  | 16.8  |
| Halfwidth(nm)       | 58.6  | 32.7  | 33.3  | 45.7  |

#### 4 Derivative curve details

**Supplementary Table 4.** Details of peak positions of 3rd and 4th derivative curve

| Sample ID      | Peak position 1 (nm) | Peak position 2 (nm) | Peak position 3 (nm) | Peak position 4 (nm) |
|----------------|----------------------|----------------------|----------------------|----------------------|
| 3rd derivative |                      |                      |                      |                      |
| CDS1           | 264                  | 287                  | 309                  | 333                  |
| CDS2           | 258                  | 285                  | 312                  | 335                  |
| LDS1           | 287                  | 323                  | 362                  | -                    |
| LDS2           | 287                  | 323                  | 363                  | -                    |
| HADS1          | 276                  | 315                  | 344                  | 371                  |
| HADS2          | 276                  | 315                  | 344                  | 372                  |
| MIX1           | 287                  | 320                  | 344                  | 377                  |
| MIX2           | 287                  | 321                  | 345                  | 369                  |
| MIX3           | 287                  | 322                  | 342                  | 361                  |
| MIX4           | 287                  | 321                  | 341*                 | 359                  |
| MIX5           | 287                  | 319                  | 344                  | 377                  |
| MIX6           | 287                  | 318                  | 344                  | 376                  |
| 4th derivative |                      |                      |                      |                      |
| CDS1           | 283                  | 305                  | 326                  | 348                  |
| CDS2           | 280                  | 305                  | 329                  | 351                  |
| LDS1           | 279                  | 311                  | 354                  | -                    |
| LDS2           | 279                  | 311                  | 354                  | -                    |
| HADS1          | 267                  | 309                  | 339                  | 366                  |
| HADS2          | 268                  | 308                  | 339                  | 366                  |
| MIX1           | 278                  | 311                  | 340                  | 368                  |
| MIX2           | 278                  | 311                  | 340                  | 363                  |
| MIX3           | 278                  | 311                  | 340*                 | 356                  |
| MIX4           | 278                  | 311                  | 340*                 | 355                  |
| MIX5           | 278                  | 311                  | 339                  | 368                  |
| MIX6           | 278                  | 310                  | 339                  | 369                  |

\*Shoulder peak