**Supplementary Information:**

**Utilization of UV-Vis spectroscopy and related data analyses for dissolved organic matter (DOM) studies: A review**

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Table S1. Common terms used in UV-Vis absorbance spectra

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Names | Abbreviation | Unit | Definitions | Algorithm |
| Light intensity | I | Number of photons or energy intensity of photons | Light intensity |  |
| Transmittance | T | % | The ratio of transmitted light to the incident light | $$T=\frac{I}{I\_{0}}$$ |
| Absorbance | A | Unitless | The negative algorithm of transmittance | $A=-log\_{10}($T) |
| Absorption coefficient | a | m-1 |  | $$a=2.303A/L$$ |
| Specific ultraviolet absorbance | SUVA | L mg-1 m-1 | UV absorbance divided by the DOC concentration  | $$SUVA=(\frac{A}{L})/DOC$$ |
| Molar absorptivity | ε | L mol-1 m-1 | Absorption per mole of organic carbon | $$ε=a/(\frac{DOC}{12.01})$$ |

Table S2. Applications of absorption ratio in DOM studies

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Absorbance ratios | Characteristics | Range | Relationships | DOM types | Note | References |
| A210/A254 | Aromaticity | 1.59-41.0 | Decrease with aromaticity | Commercial humic substances and polymers (SRHA, SRFA, BSA, Asparagine) | Interferences in wavelength range of 200-230 nm due to inorganic ions such as nitrates or sulfates. | (Her et al. 2008) |
| A210/A254 | Aromaticity, MW, THMFP a | 1.277-7.980 | Negatively correlate with aromaticity, MW and THMFP | Humic substances |  | (Rodríguez et al. 2016) |
| A210/A254 | Aromaticity | 0.02-0.76 (estimate from figure) | Correlate positively with aromaticity | Storm water |  | (Huang et al. 2016) |
| A220/A254 | Polarity | 1.39-1.85 | Correlate negatively with polarity | Lake  |  | (Erlandsson et al. 2012) |
| A240/A420 | Humification | 5.93-8.69 | Not correlated well | Biosolid |  | (Wang et al. 2013) |
| A250/A365 | MW | 6.2-10.3 | Negatively correlate with MW | Soil leachate |  | (Guo and Chorover 2003)  |
| A250/A365 | MW | 4.16-5.72 | Negatively correlate with aromaticity and MW | River, lake water humic substances |  | (Peuravuori and Pihlaja 1997) |
| A250/A365 | MW | 5.17-8.26 | Negatively correlate with MW | Estuary |  |  (Santos et al. 2016) |
| A250/A365 | Aromaticity, MW, THMFP | 2.623-5.858 | Negatively correlate with aromaticity, MW and THMFP | Humic substances |  | (Rodríguez et al. 2016) |
| Absorbance ratios | Characteristics | Range | Relationships | DOM types | Note | References |
| A250/A365 | Aromaticity and MW | 5.7-8.8 | Negatively correlate with aromaticity and MW | Aerosol |  | (Duarte et al. 2005) |
| A250/A364 | MW | 3.5-10.7 | Negatively correlate with MW | Lake  |  | (Erlandsson et al. 2012) |
| A254/A365 | Aromaticity and MW | - | Negatively correlate with aromaticity and MW | Plant and manure DOM |  | (Hunt and Ohno 2007) |
| A253/A203 | THMFP | 0.197-0.436 | Correlate positively with THMFP | Reservoir |  | (Korshin et al. 1997) |
| A254/A204 | Terrestrial/Autochonous | 0.462-0.755 | Source discrimination | Humic substances |  | (Hur et al. 2006) |
| A254/A204 | Hydrophobicity | 0.33-0.52 (estimate from figure | Positively correlated with hydrophobic/hydrophilic ratio | Lake and Pond |  | (Al-Juboori et al. 2016) |
| A254/A203 | Aromaticity, MW, THMFP | 0.140-0.730 | Positively correlate with aromaticity, MW and THMFP | Humic substances |  | (Rodríguez et al. 2016) |
| A254/A436 | Sources, aromaticity | 4.37-11.34 | Estimate the relative composition of autochthonous versus terrestrial DOM | River |  | (Battin 1998) |
| A254/A436 | Sources | 19.52-27.45 | Estimate the relative composition of autochthonous versus terrestrial DOM | Estuary (seawater) | Sensitive to photobleaching | (Jaffé et al. 2004) |
| A254/A436 | Sources | 5.32-7.81 | Estimate the relative composition of autochthonous versus terrestrial DOM | Humic substances |  | (Hur et al. 2006) |
| A254/A436 | Aromaticity, MW, THMFP | 4.867-17.324 | Negatively correlate with aromaticity, MW and THMFP | Humic substances |  | (Rodríguez et al. 2016) |
| Absorbance ratios | Characteristics | Range | Relationships | DOM types | Note | References |
| A265/A465 | Aromaticity, MW, THMFP | 5.677-22.304 | Negatively correlate with aromaticity, MW and THMFP | Humic substances |  | (Rodríguez et al. 2016) |
| A270/A400 | Aromaticity, MW, THMFP | 3.272-7.983 | Negatively correlate with aromaticity, MW and THMFP | Humic substances |  | (Rodríguez et al. 2016) |
| A270/A400 | DOM degradation | 3.2-5.4 | Source discrimination | Commercial humic substances |  | (Yakimenko et al. 2016) |
| A280/A350 | Aromaticity, MW, THMFP | 1.886-3.088 | Negatively correlate with aromaticity, MW and THMFP | Humic substances |  | (Rodríguez et al. 2016) |
| A280/A472 | Lignin proportion | 5.8-10.2 | Source discrimination | Commercial humic substances |  | (Yakimenko et al. 2016) |
| A280/A665 | Sources | 22.05-47.01 | Source discrimination (higher values were found in HA extracted from sediments in forest lakes than sediments in lakes drainingagricultural fields) | Lake sediment humic acids |  | (Cieslewicz and Gonet 2004) |
| A280/A665 | Humification degree | 29.7-47.4 | Source discrimination | Commercial humic substances | Not suitable for discrimination of peat from fossil humic substances | (Yakimenko et al. 2016) |
| A280/A664 | Humification | 10.75-27.17 | Not correlated well | Biosolid |  | (Wang et al. 2013) |
| A300/A400 | Humification | 2.67-3.10 | Correlate negatively with humification | Soil humic acids |  | (Claret et al. 2003) |
| A300/A400 | Humification | 5.14-7.03 | Correlate negatively with humification | Soil fulvic acids |  | (Claret et al. 2003) |
| Absorbance ratios | Characteristics | Range | Relationships | DOM types | Note | References |
| A300/A400 | Humification | 3.4-8.4 | Correlate negatively with humification | Lake  |  | (Erlandsson et al. 2012) |
| A340/A254 | Prediction of DOC | 0.20-0.38 | To predict DOC concentration | River |  | (Tipping et al. 2009) |
| Log(A400/A600) | Humification and aromaticity | 0.512-0.963 | Correlate negatively with humification and aromaticity | Soil humic acids |  | (Ikeya et al. 2015) |
| A465/A665 | MW | - | Correlate inversely with DOM MW | Soil DOM |  | (You et al. 1999) |
| A465/A665 | Sources | 3.35-6.71 | Source discrimination (higher values were found in HA extracted from sediments in forest lakes than sediments in lakes drainingagricultural fields) | Lake sediment humic acids |  | (Cieslewicz and Gonet 2004) |
| A465/A665 | Humification | 2.21-2.75 | Not correlated well  | Biosolid |  | (Wang et al. 2013) |
| A465/A665 | Humification | 3.85-7.65 | Correlate inversely with humification (the value of 3-5 is characteristic of humic acid and >5 for fulvic acid) | Soil DOM |  | (Kiss et al. 2014) |
| A465/A665 | Aromaticity, condensation, humification | 4.5-6.7 | No significant correlation between A465/A665 and aromaticity | Commercial humic substances |  | (Yakimenko et al. 2016) |
| A465/A465 | Aromaticity, MW, THMFP | 3.167-7.000 | Negatively related to both aromaticity and MW (Aldrich humic acid excluded) | Humic substances | Difficult to get reliable absorbance measurements at 665 nm | (Rodríguez et al. 2016) |

a: THMFP denotes trihalomethane formation potential

Table S3 Reponses of spectral slope and absorption ratio to environmental processes (composting, biodegradation, and photodegradation)

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Processes | S275-295 | S350-400 | Spectral slope a | Spectral slope ratio | E2:E3 | Sample Type | References |
| Biodegradation | - | - | S300-DL: Constant | - | - | Plant leachate | (Vahatalo and Wetzel 2008) |
| Biodegradation | Almost constant | - | - | - | Almost constant | Soil leachates | (Olefeldt et al. 2013) |
| Biodegradation | Decrease | - | - | Spectral slope, linear fitting | - | Plant (Rice, Cattail, Tule) DOM, Algae DOM | (Hansen et al. 2016) |
| Biodegradation | Almost constant | - | - | Spectral slope, linear fitting | - | Soil DOM | (Hansen et al. 2016) |
| Composting | - | - | - | Decrease | - | Compost DOM | (Zhao et al. 2016) |
| Composting | - | - | - | - | Decrease | Compost DOM | (Xi et al. 2012) |
| Composting | Decrease | Decrease | - | - | Decrease | Compost DOM | (He et al. 2011) |
| Photodegradation | Increase | Depends on source | S300-700: Decrease | Increase | Increase | River, Estuary and Ocean DOM | (Helms et al. 2008) |
| Photodegradation | Increase | - | - |  | Increase |  | (Olefeldt et al. 2013) |
| Photodegradation | Increase | Decrease | S300-700: No obvious trend | Increase | - | Ocean DOM | (Helms et al. 2013) |
| Photodegradation | - | - | S290-400: Increase | - | - | Estuarine freshwater DOM | (Moran et al. 2000) |
| Photodegradation | Increase | - | - | - | - | Riverine, coastal and ocean DOM | (Fichot and Benner 2012) |
| Photodegradation | - | - | S280-400: No significant impact | - | - | Lake DOM | (Bertilsson and Tranvik 2000) |
| Processes | S275-295 | S350-400 | Spectral slope a | Spectral slope ratio | E2:E3 | Sample Type | References |
| Photodegradation | Increase in first 10 days and decreased finally (57 days) (Exponential fitting) | Decrease (Exponential fitting) | - | Increase (Exponential fitting) | - | River DOM | (Spencer et al. 2009) |
| Photodegradation | - | - | S300-DL: Increase | - | - | Plant leachate | (Vahatalo and Wetzel 2008) |
| Photodegradation | - | - | S290-400: Increase (log-transformed linear fitting) | - | - | Swamp and lake DOM | (Obernosterer and Benner 2004) |
| Biodegradation (After photodegradation) | - | - | S290-400: Decrease | - | - | Estuarine freshwater DOM | (Moran et al. 2000) |
| Biodegradation+Photodegradation | Decrease | - | - | Spectral slope, linear fitting | - | Plant (Rice, Cattail, Tule) DOM, Algae DOM | (Hansen et al. 2016) |
| Biodegradation+Photodegradation | Almost constant | - | - | Spectral slope, linear fitting | - | Soil DOM | (Hansen et al. 2016) |

a: DL denotes detection limit of the instrument

Fig. S1. Boxplot for ratios of different spectral slope parameters obtained through two different methods. Method A: Log-transformed linear fitting, the calculation was based on Helms et al. (2008) and the algorithm was presented in Table 3. Method B: Non-linear fitting (exponential), the calculation was based on Stedmon et al. (2000) and the algorithm was presented in Table 3. The ratio is defined as the corresponding parameter obtained through Method A divided by that obtained through Method B. The original absorption spectra for calculation is shown in Fig. S1.



Fig. S2 Original absorption spectra used for the calculation in Fig. S1. The samples are pore water DOM from river sediments. All the samples were filtered through 0.7 μm pre-ashed GF/F filter (Whatman, UK). The absorbance spectra of all DOM samples were measured from 200 nm to 800 nm with 1 cm cell using a UV-1800 spectrophotometer (Shimadzu, Japan). Milli-Q water was used as a reference. Average absorbance between 680 nm and 700 nm was used for baseline correction for all samples. The raw spectra of these samples could be seen in Supporting Information II (Raw Spectra.xlsx).

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