Table S4. Results of hierarchical partitioning analysis of DOC compound-specific characteristics as predictors for mass transfer to the streambed. Given are percentage independent contributions applicable to each single variable as predictor of compound-specific mass transfer coefficients (n=276). The sum of independent contributions corresponds to  $R^2$  of the full model (given in the last line). Predictor variables are: Intransformed relative peak intensity in the inflow (*rI*<sub>inflow</sub>), aromaticity index (*AI*), indication of aromatic structures (*AI*>0.5), ratio of oxygen to carbon atoms (*O:C*), ratio of hydrogen to carbon atoms (*H:C*), presence of nitrogen (*N*), molecule size (*m/z*). Significance was tested using 500 random permutations of values of each variable and calculating critical percentiles of distributions of randomized independent contributions (\*\*\*...P<0.001, \*\*...P<0.01, \*...P<0.05, <sup>ns</sup>...non-significant). Subsets of predictor variables identified by the Akaike and Schwarz Bayesian Information Criteria to define the most parsimonious model are marked by <sup>AIC</sup> and <sup>BIC</sup>.

| 1                           | Height of bedforms in the mesocosms – flow heterogeneity treatment |                            |                            |                            |                            |                            |
|-----------------------------|--|----------------------------|----------------------------|----------------------------|----------------------------|----------------------------|
|                             | no bedforms  | 2 cm                       | 4 cm                       | 6 cm                       | 8 cm                       | 10 cm                      |
| <i>rl</i> <sub>inflow</sub> | 43.2*** <sup>BIC,AIC</sup>   | 60.2*** <sup>BIC,AIC</sup> |                            |                            | 63.7*** <sup>BIC,AIC</sup> | 45.5*** <sup>BIC,AIC</sup> |
| 0:C                         | 30.7*** <sup>BIC,AIC</sup>   | 17.1*** <sup>BIC,AIC</sup> | 12.7*** <sup>BIC,AIC</sup> | 30.9*** <sup>BIC,AIC</sup> | 10.6** <sup>BIC,AIC</sup>  | 22.3*** <sup>BIC,AIC</sup> |
| H:C                         | 9.1*** <sup>AIC</sup>  | 8.4**                      | 6.3**                      | 24.9*** <sup>BIC,AIC</sup> |                            | 18.3*** <sup>BIC,AIC</sup> |
| AI>0.5                      | 8.4*** <sup>BIC,AIC</sup>  | 9.1** <sup>BIC,AIC</sup>   | 8.1** <sup>BIC,AIC</sup>   | 6.8** <sup>AIC</sup>       | 11.2** <sup>BIC,AIC</sup>  | 10.1** <sup>AIC</sup>      |
| m/z                         | 5.5** <sup>AIC</sup>   | 0.7 <sup>ns</sup>          | 2.7 <sup>ns</sup>          | 0.6 <sup>ns</sup>          | 0.8 <sup>ns</sup>          | 1.2 <sup>ns</sup>          |
| AI                          | 2.1 <sup>ns</sup>  | 2.4 <sup>ns</sup>          | 2.4 <sup>ns</sup>          | 2.7 <sup>ns</sup>          | 1.5 <sup>ns</sup>          | 1.9 <sup>ns</sup>          |
| Ν                           | 1.1 <sup>ns</sup>  | 2.2 <sup>ns</sup>          | 2.7 <sup>ns</sup>          | 0.7 <sup>ns</sup>          | 1.1 <sup>ns</sup>          | 0.7 <sup>ns</sup>          |
| $R^2$                       | 0.48   | 0.31                       | 0.38                       | 0.44                       | 0.27                       | 0.26                       |