



Figure S2. Diatom endometabolome annotation methods. Representative peak(s) for compounds indicated on HSQC-TOCSY spectra (a and b). Additional structural validation (e.g., for polysaccharide β -1,3-glucan) by HSQC-TOCSY (c) and HMBC experiments (d). Peaks from HSQC experiments are overlaid and colored in red. A complete compound list is provided in Table 1, and chemical shift information used for annotation is provided in Table S1. 3-Hydroxybutyrate, 4-hydroxyphenylacetate, and uridine are not visible in a and b due to relatively low intensities. AA, amino acid alpha carbon.