**Sample preparation protocol:**

Filter samples were transferred into 15-mL of ultrapure MilliQ water in 50-mL tubes, and diatom cells were removed from the filters by sonication in an ice-water bath for 7 min (cycle: 50 s on and 10 s off). The liquid fraction was subsequently collected in new tubes and the procedure repeated three times, after which fractions were combined and stored at -80°C until further processing*1*. Samples were lyophilized (Labconco, Kansas City, MO, USA) and pellets mixed with 600 μL of phosphate buffer (30 mmol L-1 phosphate in deuterated water, pH 7.4) and 1 mmol L-1 internal standard 2,2-dimethyl-2-silapentane-5-sulfonate (DSS). Samples were vortexed for 5 min, centrifuged at 20,800 relative centrifugal force (RCF) for 10 min, and supernatants were transferred to 5-mm NMR tubes (Bruker, Billerica, MA, USA). Extraction and buffer blank controls were also prepared. Additionally, one pooled control sample was prepared by combining aliquots of all the samples and used for annotation.

*1*Uchimiya M, Tsuboi Y, Ito K, Date Y, Kikuchi J. Bacterial substrate transformation tracked by stable-isotope-guided NMR metabolomics: application in a natural aquatic microbial community. Metabolites. 2017;7:52.