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Reactive organic carbon governing the ecosystem functions of permafrost soil and their response to climate change

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Permafrost soils contain a vast reservoir of organic carbon (OC), the potential release of which could trigger substantial positive feedback to climate change, resulting in accelerated temperature rises in tundra regions far exceeding the global average. Molecular-level understanding about the response of OC in permafrost soils to climate change is crucial for predicting the feedback response of tundra ecosystem to carbon cycles. This study has investigated the reactive OC in permafrost soils along a thaw gradient (palsa, bog, fen), by coupling high-performance liquid chromatography (HPLC)- high-resolution tandem mass spectrometry (HRMS/MS) analysis, and metabolomic tools. Organic carbon complexed with iron (Fe) as well as associated with poorly crystalline, crystalline, and reactive Fe oxides were extracted by selective reagents in addition to just deionized water. The HPLC-HRMS/MS features (2647 in total across all extractions) were detected and processed with MZmine before performing molecular networking analysis and library matching using GNPS platform. In addition, molecular formula and structures were predicted by SIRIUS. The major dominant features for different groups of permafrost soils and extractions were screened out. The reactive OC most important for the emissions of CO_2 and CH_4 was identified through multiple statistical analyses. Their roles were validated by key biogeochemical reactions as well as respiration rates, including redox properties for the possible inclusion in the methane oxidation or suppression. The molecular-level information of these compounds offered new insights into the chemistry of OC important for the Arctic soil ecosystem functions and impact of climate change. Identification of these key compounds can help make the next-generation modeling of carbon cycles in tundra soils under climate change more accurate.