**Read me file for BARNES Goldstein Group GCxGC Speciated Organics- NonQuantified**

Emily Barnes, Goldstein Group, UC Berkeley

Contact [barnes\_emily@berkeley.edu](mailto:barnes_emily@berkeley.edu) with questions.

**Barnes\_SeaScape\_NascentSSA\_GCxGCspecorg**

Column 1 describes the date/time of beginning of sampling period. Samples are consecutive without breaks (sample 1 end time = sample 2 start time)

Columns 2:End: Headers correspond to compound library names (see Barnes\_SeaScape\_NascentSSA\_CompoundLibrary). Values correspond to normalized but not quantified units of instrument detected volume. Values have been normalized for instrument condition and sample duration but not recovery biases. Relative variability of individual compounds is accurate, but absolute quantities are not entirely representative of true mass distributions.

**Barnes\_SeaScape\_NascentSSA\_CompoundLibrary**

Column 1 corresponds to headers from Barnes\_SeaScape\_NascentSSA\_GCxGCspecorg

Column 2 corresponds to the measured d-alkane retention index (similar to kovats index but shifted forward by ~30), an indication of retention time relative to the volatility column.

Column 3 corresponds to the identity assigned by spectral comparison to the NIST main mass spectral database

Columns 4 and 5 correspond to the NIST match factor and reverse match factor. A match factor > 750 indicates high probability that the compound has been accurately identified within the NIST database. A match between 600 and 750 indicates no exact mass but chemical similarities between the novel organic and the assigned known compound. A match below 600 indicates that the NIST database contains no mass spectrally similar compounds.

Columns 6, 7, and 8 correspond to the n-alkane retention index, formula, and molecular weight recorded for the assigned NIST library known compound entry

* Important to note: Samples are derivatized with MSTFA- this technique replaces OH groups with O-Si(CH3)3 to improve recovery of polar species. This will be reflected in the mass spectra recorded, and matches to underivatized NIST entries containing OH groups should be viewed with skepticism