

ABCDom

Wesley Sparagon and Milou G.I. Arts

11 January 2022

Contents

| | |
|---|----------|
| Data analysis report | 1 |
| R | 1 |
| Raw data | 1 |
| Data clean up | 1 |
| Flagging of contaminants present in blank | 1 |
| GNPS | 1 |

Data analysis report

R

The freely available software R version 4.1.0 (2021-05-18) in combination with RStudio (version 1.4.1717) was used. Installed packages are textclean, rmarkdown, knitr, kableExtra, tictoc, expss, vegan, stringi, psych, nortest, binom, epitools, car, ape, wesanderson, RColorBrewer, data.table, DescTools, broom, readxl, multcomp, summarytools, scales, reshape, reshape2, cluster, ggfortify, rfPermute, plyr, tidyverse, tibble, dplyr, svglite, dunn.test, UpSetR, gridExtra, grid, ggpubr, rstatix, ComplexUpset, cowplot, scatterplot3d, pdftools, png, magick, devtools.

Raw data

Mzmine detected 10268 features in a total of 61 runs. Analysis was done on 61 runs of which 60 were samples and 1 blanks. Of those blanks, 1 was a method blank and 0 were instrument blanks (extraction solvents).

Data clean up

Flagging of contaminants present in blank

Contaminants were flagged and removed if $\max(blanks) \geq \text{mean}(peakarea) * 0.5$, thus over all samples. By comparing the datasets before and after gapfiling, the peak area background noise level was set on 1.4065×10^5 . Transient features are features that do not pass the background noise in at least 3 samples. These transient features were removed. Feature peak areas were relativized by the total ion current of each sample followed by $\text{asin}(\sqrt{x})$ normalization.. For all statistical analysis on normalized peak areas, a dataset was use where all peak areas that were replaced by + random number between 0 and 1 before the transformation.

GNPS

GNPS annotated 571 features as a known compound based on their MS2 spectra. Another 3884 features were matched to highly similar MS2 spectra, so called Analog hits. These analog hits might provide structural information on the unknown compounds.

Table 1: Metadata.

| File Name | Sample Name | Injection_Type | Temp | Origin_PlanC | Field_Treatment | Bleaching_Status | Bleaching_Susceptibility | Stress_status | Treatment_old | Treatment | Sample_Type | Timepoint_char | Timepoint | Bottle_NR | Notes | PLANC_aquaria | Experiment |
|---------------|-------------------|----------------|---------|--------------------|-------------------|------------------|--------------------------|----------------|-----------------------|------------------------|-------------|----------------|-----------|-----------|-----------|---------------|------------|
| Mo_2019_110 | PC_WA1_T7C | Sample | Ambient | control | Water Control | NA | NA | Ambient | Ambient Water Control | Ambient Water Control | PPL | T0 | 0 | 0 | NA | NA | PLANC |
| Mo_2019_111 | PC_WA2_T7C | Sample | Ambient | control | Water Control | NA | NA | Ambient | Ambient Water Control | Ambient Water Control | PPL | T0 | 0 | 0 | NA | NA | PLANC |
| Mo_2019_112 | PC_WA3_T7C | Sample | Ambient | control | Water Control | NA | NA | Ambient | Ambient Water Control | Ambient Water Control | PPL | T0 | 0 | 0 | NA | NA | PLANC |
| Mo_2019_113 | PC_HE1_T7C | Sample | Ambient | Healthy | Coral Control | Non Bleached | Resistant | Ambient | Control | Non-bleached + Ambient | PPL | T0 | 0 | 13 | NA | NA | PLANC |
| Mo_2019_114 | PC_HE2_T7C | Sample | Ambient | Healthy | Coral Control | Non Bleached | Resistant | Ambient | Control | Non-bleached + Ambient | PPL | T0 | 0 | 14 | NA | NA | PLANC |
| Mo_2019_115 | PC_HE3_T7C | Sample | Ambient | Healthy | Coral Control | Non Bleached | Resistant | Ambient | Control | Non-bleached + Ambient | PPL | T0 | 0 | 15 | NA | NA | PLANC |
| Mo_2019_116 | PC_PB1_T7C | Sample | Ambient | Partially Bleached | Bleaching | NA | Susceptible | Ambient | NA | NA | PPL | T0 | 0 | 0 | NA | NA | PLANC |
| Mo_2019_117 | PC_PB2_T7C | Sample | Ambient | Partially Bleached | Bleaching | NA | Susceptible | Ambient | NA | NA | PPL | T0 | 0 | 0 | NA | NA | PLANC |
| Mo_2019_118 | PC_PB3_T7C | Sample | Ambient | Partially Bleached | Bleaching | NA | Susceptible | Ambient | NA | NA | PPL | T0 | 0 | 0 | NA | NA | PLANC |
| Mo_2019_119 | PC_BL1_T7C | Sample | Ambient | Bleached | Recovering | Bleached | Susceptible | Ambient | Bleached | Bleached + Ambient | PPL | T0 | 0 | 10 | NA | BL1_T7C | PLANC |
| Mo_2019_120 | PC_BL2_T7C | Sample | Ambient | Bleached | Recovering | Bleached | Susceptible | Ambient | Bleached | Bleached + Ambient | PPL | T0 | 0 | 11 | NA | BL2_T7C | PLANC |
| Mo_2019_121 | PC_BL3_T7C | Sample | Ambient | Bleached | Recovering | Bleached | Susceptible | Ambient | Bleached | Bleached + Ambient | PPL | T0 | 0 | 12 | NA | BL3_T7C | PLANC |
| Mo_2019_122 | C PC_Blank | Blank method | Blank | Blank | Blank | Blank | Blank | Blank | Blank | Blank | PPL | T0 | 0 | 0 | NA | Blank | PLANC |
| Mo_2019_230 | PC_WA1_T7H | Sample | Hot | control | Hot Water Control | NA | NA | Thermal Stress | Heated Water Control | Heated Water Control | PPL | T0 | 0 | 0 | NA | NA | PLANC |
| Mo_2019_231 | PC_WA2_T7H | Sample | Hot | control | Hot Water Control | NA | NA | Thermal Stress | Heated Water Control | Heated Water Control | PPL | T0 | 0 | 0 | NA | NA | PLANC |
| Mo_2019_232 | PC_WA3_T7H | Sample | Hot | control | Hot Water Control | NA | NA | Thermal Stress | Heated Water Control | Heated Water Control | PPL | T0 | 0 | 0 | NA | NA | PLANC |
| Mo_2019_233 | PC_HE1_T7H | Sample | Hot | Healthy | Bleaching | Non Bleached | Resistant | Thermal Stress | Heated | Non-bleached + Heated | PPL | T0 | 0 | 0 | NA | NA | PLANC |
| Mo_2019_234 | PC_HE2_T7H | Sample | Hot | Healthy | Bleaching | Non Bleached | Resistant | Thermal Stress | Heated | Non-bleached + Heated | PPL | T0 | 0 | 5 | NA | HE2_T7H | PLANC |
| Mo_2019_235 | PC_HE3_T7H | Sample | Hot | Healthy | Bleaching | Non Bleached | Resistant | Thermal Stress | Heated | Non-bleached + Heated | PPL | T0 | 0 | 6 | NA | HE3_T7H | PLANC |
| Mo_2019_236 | PC_PB1_T7H | Sample | Hot | Partially Bleached | Dying | Bleached | SemiResistant | Thermal Stress | Bleached + Heated | Bleached + Heated | PPL | T0 | 0 | 1 | NA | PB1_T7H | PLANC |
| Mo_2019_237 | PC_PB2_T7H | Sample | Hot | Partially Bleached | Dying | Bleached | SemiResistant | Thermal Stress | Bleached + Heated | Bleached + Heated | PPL | T0 | 0 | 2 | NA | PB2_T7H | PLANC |
| Mo_2019_238 | PC_PB3_T7H | Sample | Hot | Partially Bleached | Dying | Bleached | SemiResistant | Thermal Stress | Bleached + Heated | Bleached + Heated | PPL | T0 | 0 | 3 | NA | PB3_T7H | PLANC |
| Mo_2019_239 | PC_BL1_T7H | Sample | Hot | Bleached | Dead | Bleached | Susceptible | Thermal Stress | Bleached + Heated | Bleached + Heated | PPL | T0 | 0 | 0 | NA | NA | PLANC |
| Mo_2019_240 | PC_BL2_T7H | Sample | Hot | Bleached | Dead | Bleached | Susceptible | Thermal Stress | Bleached + Heated | Bleached + Heated | PPL | T0 | 0 | 0 | NA | NA | PLANC |
| Mo_2019_241 | PC_BL3_T7H | Sample | Hot | Bleached | Dead | Bleached | Susceptible | Thermal Stress | Bleached + Heated | Bleached + Heated | PPL | T0 | 0 | 0 | NA | NA | PLANC |
| Mo_2019_320 | ABC_019 | Sample | Hot | Partially Bleached | Dying | Bleached | SemiResistant | Thermal Stress | Bleached + Heated | Bleached + Heated | PPL | T0 | 0 | 1 | NA | PB1_T7H | ABCDOM |
| Mo_2019_321 | ABC_020 | Sample | Hot | Partially Bleached | Dying | Bleached | SemiResistant | Thermal Stress | Bleached + Heated | Bleached + Heated | PPL | T0 | 0 | 2 | NA | PB2_T7H | ABCDOM |
| Mo_2019_322 | ABC_021 | Sample | Hot | Partially Bleached | Dying | Bleached | SemiResistant | Thermal Stress | Bleached + Heated | Bleached + Heated | PPL | T0 | 0 | 3 | NA | PB3_T7H | ABCDOM |
| Mo_2019_323 | ABC_023 | Sample | Hot | Healthy | Bleaching | Non Bleached | Resistant | Thermal Stress | Heated | Non-bleached + Heated | PPL | T0 | 0 | 5 | NA | HE2_T7H | ABCDOM |
| Mo_2019_324 | ABC_024 | Sample | Hot | Healthy | Bleaching | Non Bleached | Resistant | Thermal Stress | Heated | Non-bleached + Heated | PPL | T0 | 0 | 6 | NA | HE3_T7H | ABCDOM |
| Mo_2019_324_B | ABC_024 | Sample | Hot | Healthy | Bleaching | Non Bleached | Resistant | Thermal Stress | Heated | Non-bleached + Heated | PPL | T0 | 0 | 6 | NA | HE3_T7H | ABCDOM |
| Mo_2019_325 | ABC_025 | Sample | Hot | control | Hot Water Control | NA | NA | Thermal Stress | Heated Water Control | Heated Water Control | PPL | T0 | 0 | 7 | NA | NA | ABCDOM |
| Mo_2019_326 | ABC_026 | Sample | Hot | control | Hot Water Control | NA | NA | Thermal Stress | Heated Water Control | Heated Water Control | PPL | T0 | 0 | 8 | NA | NA | ABCDOM |
| Mo_2019_327 | ABC_027 | Sample | Hot | control | Hot Water Control | NA | NA | Thermal Stress | Heated Water Control | Heated Water Control | PPL | T0 | 0 | 9 | NA | NA | ABCDOM |
| Mo_2019_328 | ABC_028 | Sample | Ambient | Bleached | Recovering | Bleached | Susceptible | Ambient | Bleached | Bleached + Ambient | PPL | T0 | 0 | 10 | NA | BL1_T7C | ABCDOM |
| Mo_2019_329 | ABC_029 | Sample | Ambient | Bleached | Recovering | Bleached | Susceptible | Ambient | Bleached | Bleached + Ambient | PPL | T0 | 0 | 11 | NA | BL2_T7C | ABCDOM |
| Mo_2019_330 | ABC_030 | Sample | Ambient | Bleached | Recovering | Bleached | Susceptible | Ambient | Bleached | Bleached + Ambient | PPL | T0 | 0 | 12 | NA | BL3_T7C | ABCDOM |
| Mo_2019_331 | ABC_031 | Sample | Ambient | Healthy | Coral Control | Non Bleached | Resistant | Ambient | Control | Non-bleached + Ambient | PPL | T0 | 0 | 13 | NA | HE1_T7C | ABCDOM |
| Mo_2019_332 | ABC_032 | Sample | Ambient | Healthy | Coral Control | Non Bleached | Resistant | Ambient | Control | Non-bleached + Ambient | PPL | T0 | 0 | 14 | NA | HE2_T7C | ABCDOM |
| Mo_2019_333 | ABC_033 | Sample | Ambient | Healthy | Coral Control | Non Bleached | Resistant | Ambient | Control | Non-bleached + Ambient | PPL | T0 | 0 | 15 | NA | HE3_T7C | ABCDOM |
| Mo_2019_334 | ABC_034 | Sample | Ambient | control | Water Control | NA | NA | Ambient | Ambient Water Control | Ambient Water Control | PPL | T0 | 0 | 16 | NA | NA | ABCDOM |
| Mo_2019_335 | ABC_035 | Sample | Ambient | control | Water Control | NA | NA | Ambient | Ambient Water Control | Ambient Water Control | PPL | T0 | 0 | 17 | NA | NA | ABCDOM |
| Mo_2019_336 | ABC_036 | Sample | Ambient | control | Water Control | NA | NA | Ambient | Ambient Water Control | Ambient Water Control | PPL | T0 | 0 | 18 | NA | NA | ABCDOM |
| Mo_2019_337 | ABC_073 | Sample | Hot | Partially Bleached | Dying | Bleached | SemiResistant | Thermal Stress | Bleached + Heated | Bleached + Heated | PPL | Tend | 36 | 1 | NA | PB1_T7H | ABCDOM |
| Mo_2019_338 | ABC_074 | Sample | Hot | Partially Bleached | Dying | Bleached | SemiResistant | Thermal Stress | Bleached + Heated | Bleached + Heated | PPL | Tend | 36 | 2 | NA | PB2_T7H | ABCDOM |
| Mo_2019_339 | ABC_075 | Sample | Hot | Partially Bleached | Dying | Bleached | SemiResistant | Thermal Stress | Bleached + Heated | Bleached + Heated | PPL | Tend | 36 | 3 | NA | PB3_T7H | ABCDOM |
| Mo_2019_340 | ABC_077 | Sample | Hot | Healthy | Bleaching | Non Bleached | Resistant | Thermal Stress | Heated | Non-bleached + Heated | PPL | Tend | 36 | 5 | NA | HE2_T7H | ABCDOM |
| Mo_2019_341 | ABC_078 | Sample | Hot | Healthy | Bleaching | Non Bleached | Resistant | Thermal Stress | Heated | Non-bleached + Heated | PPL | Tend | 36 | 6 | NA | HE3_T7H | ABCDOM |
| Mo_2019_342 | ABC_079 | Sample | Hot | control | Hot Water Control | NA | NA | Thermal Stress | Heated Water Control | Heated Water Control | PPL | Tend | 36 | 7 | NA | NA | ABCDOM |
| Mo_2019_343 | ABC_080 | Sample | Hot | control | Hot Water Control | NA | NA | Thermal Stress | Heated Water Control | Heated Water Control | PPL | Tend | 36 | 8 | NA | NA | ABCDOM |
| Mo_2019_344 | ABC_081 | Sample | Hot | control | Hot Water Control | NA | NA | Thermal Stress | Heated Water Control | Heated Water Control | PPL | Tend | 36 | 9 | NA | NA | ABCDOM |
| Mo_2019_345 | ABC_082 | Sample | Ambient | Bleached | Recovering | Bleached | Susceptible | Ambient | Bleached | Bleached + Ambient | PPL | Tend | 36 | 10 | NA | BL1_T7C | ABCDOM |
| Mo_2019_346 | ABC_083 | Sample | Ambient | Bleached | Recovering | Bleached | Susceptible | Ambient | Bleached | Bleached + Ambient | PPL | Tend | 36 | 11 | NA | BL2_T7C | ABCDOM |
| Mo_2019_347 | ABC_084 | Sample | Ambient | Bleached | Recovering | Bleached | Susceptible | Ambient | Bleached | Bleached + Ambient | PPL | Tend | 36 | 12 | NA | BL3_T7C | ABCDOM |
| Mo_2019_348 | ABC_085 | Sample | Ambient | Healthy | Coral Control | Non Bleached | Resistant | Ambient | Control | Non-bleached + Ambient | PPL | Tend | 36 | 13 | NA | HE1_T7C | ABCDOM |
| Mo_2019_349 | ABC_086 | Sample | Ambient | Healthy | Coral Control | Non Bleached | Resistant | Ambient | Control | Non-bleached + Ambient | PPL | Tend | 36 | 14 | NA | HE2_T7C | ABCDOM |
| Mo_2019_350 | ABC_087 | Sample | Ambient | Healthy | Coral Control | Non Bleached | Resistant | Ambient | Control | Non-bleached + Ambient | PPL | Tend | 36 | 15 | NA | HE3_T7C | ABCDOM |
| Mo_2019_351 | ABC_088 | Sample | Ambient | control | Water Control | NA | NA | Ambient | Ambient Water Control | Ambient Water Control | PPL | Tend | 36 | 16 | NA | NA | ABCDOM |
| Mo_2019_352 | ABC_089 | Sample | Ambient | control | Water Control | NA | NA | Ambient | Ambient Water Control | Ambient Water Control | PPL | Tend | 36 | 17 | NA | NA | ABCDOM |
| Mo_2019_353 | ABC_090 | Sample | Ambient | control | Water Control | NA | NA | Ambient | Ambient Water Control | Ambient Water Control | PPL | Tend | 36 | 18 | NA | NA | ABCDOM |
| Mo_2019_542 | ABC_022 | Sample | Hot | Healthy | Bleaching | Non Bleached | Resistant | Thermal Stress | Heated | Non-bleached + Heated | PPL | T0 | 0 | 4 | Not taken | HE1_T7H | ABCDOM |
| Mo_2019_543 | ABC_inoculum_B_T0 | Sample | Ambient | Inoculum | Inoculum | NA | NA | NA | NA | NA | PPL | T0 | 0 | 19 | NA | NA | ABCDOM |