ABCDom

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Data analysis report

R

The freely available software R version 4.2.1 (2022-06-23) in combination with RStudio (version 2022.7.1) 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, 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 54040 features in a total of 800 runs. Analysis was done on 44 runs of which 35 were samples and 9 blanks. Of those blanks, 9 were method blanks and 0 were instrument blanks (extraction solvents).

Data clean up

Flagging of contaminants present in blank

Contaminents were flagged and removed if $max(blanks) >= mean(peakarea) * 0.5$, thus over all samples. By comparing the datasets before and after gapfiling, the peak area background noise level was set on 5×10^4. Transient features are features that do not pass the background noise in at least 2 samples. These transient features were removed. Feature peak areas were normalized by $log10(peakarea)$ transformation. For all statistical analysis on normalized peak areas, a dataset was use where all peak areas that were replaced by 1000 + random number between 0 and 1 before the transformation.

GNPS

GNPS annotated 3620 features as a known compound based on their MS2 spectra. Another 0 features were matched to highly similar MS2 spectra, so called Analog hits. These analog hits might provide structual information on the unknown compounds.

Table 1: Metadata.

File Name	Sample Name	Injection_Type	Temp	Origin_PlanC	Field_Treatment	Bleaching_Status	Bleaching_Susceptability	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	Inoculum	Inoculum	Inoculum	Inoculum	Inoculum	PPL	T0	0	19	NA	NA	ABCDOM