SpectraC Manual

Author
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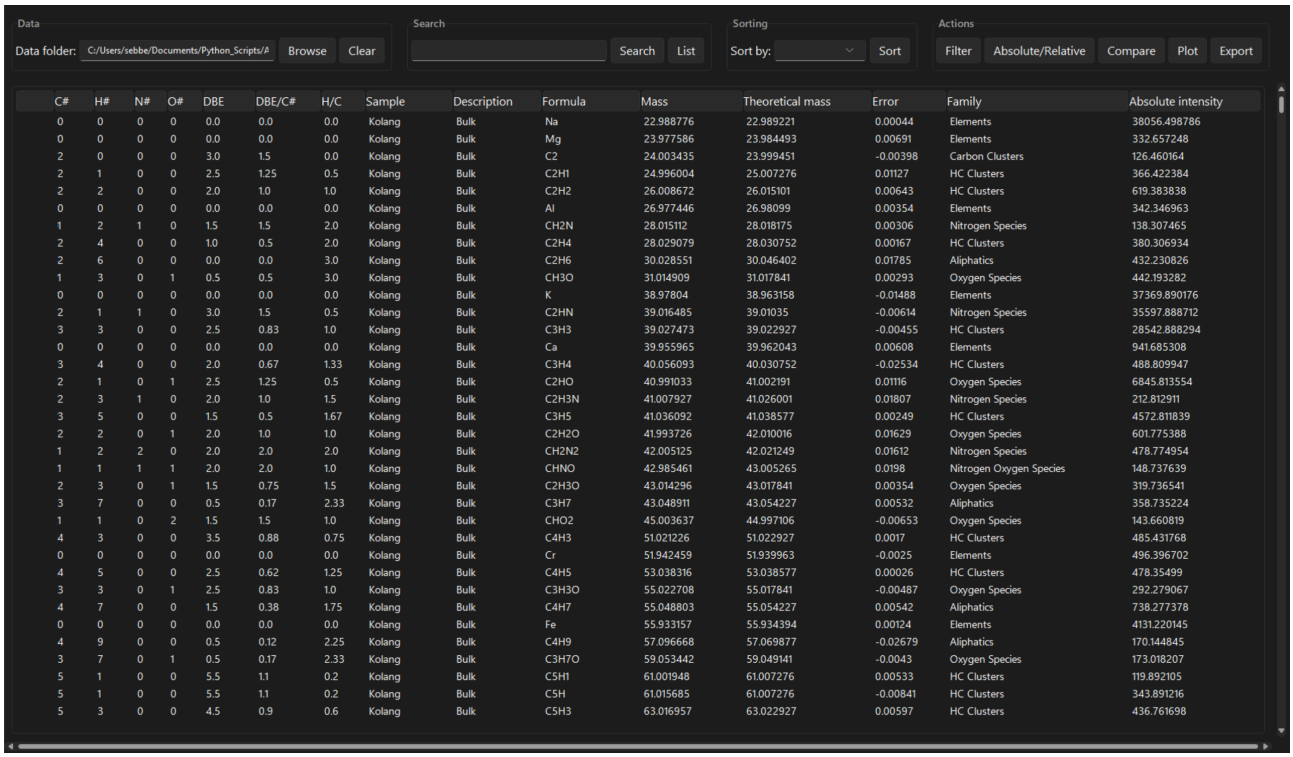


C#	H#	N#	O#	DBE	DBE/C#	H/C	Sample	Description	Formula	Mass	Theoretical mass	Error	Family	Absolute intensity
0	0	0	0	0.0	0.0	0.0	Kolang	Bulk	Na	22.988776	22.989221	0.00044	Elements	38056.498786
0	0	0	0	0.0	0.0	0.0	Kolang	Bulk	Mg	23.977586	23.984493	0.00691	Elements	332.657248
2	0	0	0	3.0	1.5	0.0	Kolang	Bulk	C2	24.003435	23.999451	-0.00398	Carbon Clusters	126.460164
2	1	0	0	2.5	1.25	0.5	Kolang	Bulk	C2H1	24.996004	25.007276	0.01127	HC Clusters	366.422384
2	2	0	0	2.0	1.0	1.0	Kolang	Bulk	C2H2	26.008672	26.015101	0.00643	HC Clusters	619.383838
0	0	0	0	0.0	0.0	0.0	Kolang	Bulk	Al	26.977446	26.98099	0.00354	Elements	342.346963
1	2	1	0	1.5	1.5	2.0	Kolang	Bulk	CH2N	28.015112	28.018175	0.00306	Nitrogen Species	138.307465
2	4	0	0	1.0	0.5	2.0	Kolang	Bulk	C2H4	28.029079	28.030752	0.00167	HC Clusters	380.306934
2	6	0	0	0.0	0.0	3.0	Kolang	Bulk	C2H6	30.028551	30.046402	0.01785	Aliphatics	432.230826
1	3	0	1	0.5	0.5	3.0	Kolang	Bulk	CH3O	31.014909	31.017841	0.00293	Oxygen Species	442.193282
0	0	0	0	0.0	0.0	0.0	Kolang	Bulk	K	38.97804	38.963158	-0.01488	Elements	37369.890176
2	1	1	0	3.0	1.5	0.5	Kolang	Bulk	C2HN	39.016485	39.01035	-0.00614	Nitrogen Species	35597.888712
3	3	0	0	2.5	0.83	1.0	Kolang	Bulk	C3H3	39.027473	39.022927	-0.00455	HC Clusters	28542.888294
0	0	0	0	0.0	0.0	0.0	Kolang	Bulk	Ca	39.955965	39.962043	0.00608	Elements	941.685308
3	4	0	0	2.0	0.67	1.33	Kolang	Bulk	C3H4	40.056093	40.030752	-0.02534	HC Clusters	488.809947
2	1	0	1	2.5	1.25	0.5	Kolang	Bulk	C2HO	40.991033	41.002191	0.01116	Oxygen Species	6845.813554
2	3	1	0	2.0	1.0	1.5	Kolang	Bulk	C2H3N	41.007927	41.026001	0.01807	Nitrogen Species	212.812911
3	5	0	0	1.5	0.5	1.67	Kolang	Bulk	C3H5	41.036092	41.038577	0.00249	HC Clusters	4572.811839
2	2	0	1	2.0	1.0	1.0	Kolang	Bulk	C2H2O	41.993726	42.010016	0.01629	Oxygen Species	601.775388
1	2	2	0	2.0	2.0	2.0	Kolang	Bulk	CH2N2	42.005125	42.021249	0.01612	Nitrogen Species	478.774954
1	1	1	1	2.0	2.0	1.0	Kolang	Bulk	CHNO	42.985461	43.005265	0.0198	Nitrogen Oxygen Species	148.737639
2	3	0	1	1.5	0.75	1.5	Kolang	Bulk	C2H3O	43.014296	43.017841	0.00354	Oxygen Species	319.736541
3	7	0	0	0.5	0.17	2.33	Kolang	Bulk	C3H7	43.048911	43.054227	0.00532	Aliphatics	358.735224
1	1	0	2	1.5	1.5	1.0	Kolang	Bulk	CHO2	45.003637	44.997106	-0.00653	Oxygen Species	143.660819
4	3	0	0	3.5	0.88	0.75	Kolang	Bulk	C4H3	51.021226	51.022927	0.0017	HC Clusters	485.431768
0	0	0	0	0.0	0.0	0.0	Kolang	Bulk	Cr	51.942459	51.939963	-0.0025	Elements	496.396702
4	5	0	0	2.5	0.62	1.25	Kolang	Bulk	C4H5	53.038316	53.038577	0.00026	HC Clusters	478.35499
3	3	0	1	2.5	0.83	1.0	Kolang	Bulk	C3H3O	55.022708	55.017841	-0.00487	Oxygen Species	292.279067
4	7	0	0	1.5	0.38	1.75	Kolang	Bulk	C4H7	55.048803	55.054227	0.00542	Aliphatics	738.277378
0	0	0	0	0.0	0.0	0.0	Kolang	Bulk	Fe	55.933157	55.934394	0.00124	Elements	4131.220145
4	9	0	0	0.5	0.12	2.25	Kolang	Bulk	C4H9	57.096668	57.069877	-0.02679	Aliphatics	170.144845
3	7	0	1	0.5	0.17	2.33	Kolang	Bulk	C3H7O	59.053442	59.049141	-0.0043	Oxygen Species	173.018207
5	1	0	0	5.5	1.1	0.2	Kolang	Bulk	C5H1	61.001948	61.007276	0.00533	HC Clusters	119.892105
5	1	0	0	5.5	1.1	0.2	Kolang	Bulk	C5H	61.015685	61.007276	-0.00841	HC Clusters	343.891216
5	3	0	0	4.5	0.9	0.6	Kolang	Bulk	C5H3	63.016957	63.022927	0.00597	HC Clusters	436.761698

September 28, 2023

Contents

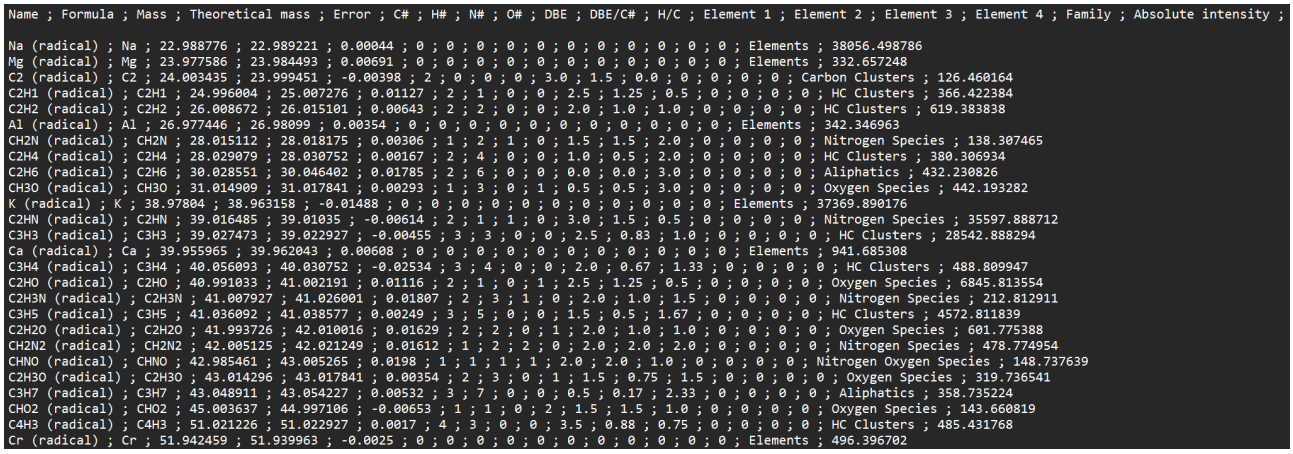
1 Description

SpectraC is an application developed in Python, leveraging the tkinter library for its intuitive graphical user interface (GUI). Tailored specifically for spectra attributed with the mMass software, files created by mMass with the "Generate DBE" tool can be directly loaded into SpectraC.

While simple, SpectraC can still be a powerful tool to help users rapidly understand the contents of mass spectra. The goal was to create a quick and user friendly solution for comparing and analysing multiple mass spectra at the same time and generating a visual database. While raw mass spectra and extensive lists of molecular formulas might be daunting and cryptic to most, a simplified visual representation can bridge the understanding gap. The core philosophy behind this application is the simplification and visual reduction of mass spectral data. This allows users to easily see the types of compounds, their aromaticity, and family groupings. By transforming complex mass spectral data into more digestible visualizations, SpectraC offers users a clearer perspective on the chemical composition within their samples.

2 Data Formatting

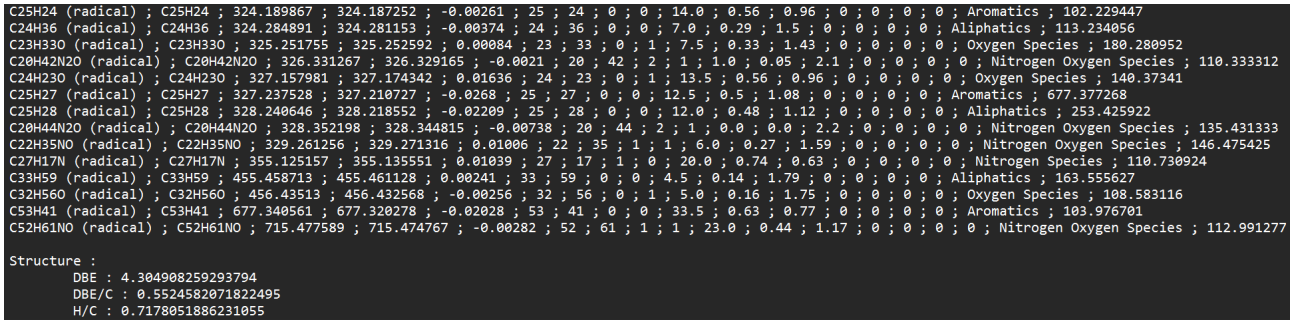
As mentioned, this software are specifically made to be able to upload the output files from the mMass software. Therefore the files that are to be uploaded shall follow the same format which can be seen in figure 1 & 2.



```
Name ; Formula ; Mass ; Theoretical mass ; Error ; C# ; H# ; N# ; O# ; DBE ; DBE/C# ; H/C ; Element 1 ; Element 2 ; Element 3 ; Element 4 ; Family ; Absolute intensity ;

Na (radical) ; Na ; 22.988776 ; 22.989221 ; 0.00044 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; Elements ; 38056.498786
Mg (radical) ; Mg ; 23.977586 ; 23.984493 ; 0.00691 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; Elements ; 332.657248
C2 (radical) ; C2 ; 24.003435 ; 23.999451 ; -0.00398 ; 2 ; 0 ; 0 ; 0 ; 3.0 ; 1.5 ; 0.0 ; 0 ; 0 ; 0 ; 0 ; Carbon Clusters ; 126.460164
C2H1 (radical) ; C2H1 ; 24.996004 ; 25.007276 ; 0.01127 ; 2 ; 1 ; 0 ; 0 ; 2.5 ; 1.25 ; 0.5 ; 0 ; 0 ; 0 ; 0 ; HC Clusters ; 366.422384
C2H2 (radical) ; C2H2 ; 26.008672 ; 26.015101 ; 0.00643 ; 2 ; 2 ; 0 ; 0 ; 2.0 ; 1.0 ; 1.0 ; 0 ; 0 ; 0 ; 0 ; HC Clusters ; 619.383838
Al (radical) ; Al ; 26.977446 ; 26.98099 ; 0.00354 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; Elements ; 342.346963
CH2N (radical) ; CH2N ; 28.015112 ; 28.018175 ; 0.00306 ; 1 ; 2 ; 1 ; 0 ; 1.5 ; 1.5 ; 2.0 ; 0 ; 0 ; 0 ; 0 ; Nitrogen Species ; 138.307465
C2H4 (radical) ; C2H4 ; 28.029079 ; 28.030752 ; 0.00167 ; 2 ; 4 ; 0 ; 0 ; 1.0 ; 0.5 ; 2.0 ; 0 ; 0 ; 0 ; 0 ; HC Clusters ; 380.306934
C2H6 (radical) ; C2H6 ; 30.028551 ; 30.046402 ; 0.01785 ; 2 ; 6 ; 0 ; 0 ; 0.0 ; 0.0 ; 3.0 ; 0 ; 0 ; 0 ; 0 ; Aliphatics ; 432.230826
CH3O (radical) ; CH3O ; 31.014909 ; 31.017841 ; 0.00293 ; 1 ; 3 ; 0 ; 1 ; 0.5 ; 0.5 ; 3.0 ; 0 ; 0 ; 0 ; 0 ; Oxygen Species ; 442.193282
K (radical) ; K ; 38.97804 ; 38.963158 ; -0.01488 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; Elements ; 37369.890176
C2HN (radical) ; C2HN ; 39.016485 ; 39.01035 ; -0.00614 ; 2 ; 1 ; 1 ; 0 ; 3.0 ; 1.5 ; 0.5 ; 0 ; 0 ; 0 ; 0 ; Nitrogen Species ; 35597.888712
C3H3 (radical) ; C3H3 ; 39.027473 ; 39.022927 ; -0.00455 ; 3 ; 3 ; 0 ; 0 ; 2.5 ; 0.83 ; 1.0 ; 0 ; 0 ; 0 ; 0 ; HC Clusters ; 28542.888294
Ca (radical) ; Ca ; 39.955965 ; 39.962043 ; 0.00608 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; Elements ; 941.685308
C3H4 (radical) ; C3H4 ; 40.056093 ; 40.030752 ; -0.02534 ; 3 ; 4 ; 0 ; 0 ; 2.0 ; 0.67 ; 1.33 ; 0 ; 0 ; 0 ; 0 ; HC Clusters ; 488.809947
C2HO (radical) ; C2HO ; 40.991033 ; 41.002191 ; 0.01116 ; 2 ; 1 ; 0 ; 1 ; 2.5 ; 1.25 ; 0.5 ; 0 ; 0 ; 0 ; 0 ; Oxygen Species ; 6845.813554
C2H3N (radical) ; C2H3N ; 41.007927 ; 41.026001 ; 0.01807 ; 2 ; 3 ; 1 ; 0 ; 2.0 ; 1.0 ; 1.5 ; 0 ; 0 ; 0 ; 0 ; Nitrogen Species ; 212.812911
C3H5 (radical) ; C3H5 ; 41.036092 ; 41.038577 ; 0.00249 ; 3 ; 5 ; 0 ; 0 ; 1.5 ; 0.5 ; 1.67 ; 0 ; 0 ; 0 ; 0 ; HC Clusters ; 4572.811839
C2H2O (radical) ; C2H2O ; 41.993726 ; 42.010016 ; 0.01629 ; 2 ; 2 ; 0 ; 1 ; 2.0 ; 1.0 ; 1.0 ; 0 ; 0 ; 0 ; 0 ; Oxygen Species ; 601.775388
CH2N2 (radical) ; CH2N2 ; 42.005125 ; 42.021249 ; 0.01612 ; 1 ; 2 ; 2 ; 0 ; 2.0 ; 2.0 ; 2.0 ; 0 ; 0 ; 0 ; 0 ; Nitrogen Species ; 478.774954
CHNO (radical) ; CHNO ; 42.985461 ; 43.005265 ; 0.0198 ; 1 ; 1 ; 1 ; 1 ; 2.0 ; 2.0 ; 1.0 ; 0 ; 0 ; 0 ; 0 ; Nitrogen Oxygen Species ; 148.737639
C2H3O (radical) ; C2H3O ; 43.014296 ; 43.017841 ; 0.00354 ; 2 ; 3 ; 0 ; 1 ; 1.5 ; 0.75 ; 1.5 ; 0 ; 0 ; 0 ; 0 ; Oxygen Species ; 319.736541
C3H7 (radical) ; C3H7 ; 43.048911 ; 43.054227 ; 0.00532 ; 3 ; 7 ; 0 ; 0 ; 0.5 ; 0.17 ; 2.33 ; 0 ; 0 ; 0 ; 0 ; Aliphatics ; 358.735224
CHO2 (radical) ; CHO2 ; 45.003637 ; 44.997106 ; -0.00653 ; 1 ; 1 ; 0 ; 2 ; 1.5 ; 1.5 ; 1.0 ; 0 ; 0 ; 0 ; 0 ; Oxygen Species ; 143.660819
C4H3 (radical) ; C4H3 ; 51.021226 ; 51.022927 ; 0.0017 ; 4 ; 3 ; 0 ; 0 ; 3.5 ; 0.88 ; 0.75 ; 0 ; 0 ; 0 ; 0 ; HC Clusters ; 485.431768
Cr (radical) ; Cr ; 51.942459 ; 51.939963 ; -0.0025 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; 0 ; Elements ; 496.396702
```

Figure 1: Screenshot showing the first few lines of a correctly formatted data file to be uploaded to SpectraC



```
C25H24 (radical) ; C25H24 ; 324.189867 ; 324.187252 ; -0.00261 ; 25 ; 24 ; 0 ; 0 ; 14.0 ; 0.56 ; 0.96 ; 0 ; 0 ; 0 ; 0 ; Aromatics ; 102.229447
C24H36 (radical) ; C24H36 ; 324.284891 ; 324.281153 ; -0.00374 ; 24 ; 36 ; 0 ; 0 ; 7.0 ; 0.29 ; 1.5 ; 0 ; 0 ; 0 ; 0 ; Aliphatics ; 113.234056
C23H33O (radical) ; C23H33O ; 325.251755 ; 325.252592 ; 0.00084 ; 23 ; 33 ; 0 ; 1 ; 7.5 ; 0.33 ; 1.43 ; 0 ; 0 ; 0 ; 0 ; Oxygen Species ; 180.280952
C20H42N2O (radical) ; C20H42N2O ; 326.331267 ; 326.329165 ; -0.0021 ; 20 ; 42 ; 2 ; 1 ; 1.0 ; 0.05 ; 2.1 ; 0 ; 0 ; 0 ; 0 ; Nitrogen Oxygen Species ; 110.333312
C24H23O (radical) ; C24H23O ; 327.157981 ; 327.174342 ; 0.01636 ; 24 ; 23 ; 0 ; 1 ; 13.5 ; 0.56 ; 0.96 ; 0 ; 0 ; 0 ; 0 ; Oxygen Species ; 140.37341
C25H27 (radical) ; C25H27 ; 327.237528 ; 327.210727 ; -0.0268 ; 25 ; 27 ; 0 ; 0 ; 12.5 ; 0.5 ; 1.08 ; 0 ; 0 ; 0 ; 0 ; Aromatics ; 677.377268
C25H28 (radical) ; C25H28 ; 328.240646 ; 328.218552 ; -0.02209 ; 25 ; 28 ; 0 ; 0 ; 12.0 ; 0.48 ; 1.12 ; 0 ; 0 ; 0 ; 0 ; Aliphatics ; 253.425922
C20H44N2O (radical) ; C20H44N2O ; 328.352198 ; 328.344815 ; -0.00738 ; 20 ; 44 ; 2 ; 1 ; 0.0 ; 0.0 ; 2.2 ; 0 ; 0 ; 0 ; 0 ; Nitrogen Oxygen Species ; 135.431333
C22H35NO (radical) ; C22H35NO ; 329.261256 ; 329.271316 ; 0.01006 ; 22 ; 35 ; 1 ; 1 ; 6.0 ; 0.27 ; 1.59 ; 0 ; 0 ; 0 ; 0 ; Nitrogen Oxygen Species ; 146.475425
C27H17N (radical) ; C27H17N ; 355.125157 ; 355.135551 ; 0.01039 ; 27 ; 17 ; 1 ; 0 ; 20.0 ; 0.74 ; 0.63 ; 0 ; 0 ; 0 ; 0 ; Nitrogen Species ; 110.730924
C33H59 (radical) ; C33H59 ; 455.458713 ; 455.461128 ; 0.00241 ; 33 ; 59 ; 0 ; 0 ; 4.5 ; 0.14 ; 1.79 ; 0 ; 0 ; 0 ; 0 ; Aliphatics ; 163.555627
C32H56O (radical) ; C32H56O ; 456.43513 ; 456.432568 ; -0.00256 ; 32 ; 56 ; 0 ; 1 ; 5.0 ; 0.16 ; 1.75 ; 0 ; 0 ; 0 ; 0 ; Oxygen Species ; 108.583116
C53H41 (radical) ; C53H41 ; 677.340561 ; 677.320278 ; -0.02028 ; 53 ; 41 ; 0 ; 0 ; 33.5 ; 0.63 ; 0.77 ; 0 ; 0 ; 0 ; 0 ; Aromatics ; 103.976701
C52H61NO (radical) ; C52H61NO ; 715.477589 ; 715.474767 ; -0.00282 ; 52 ; 61 ; 1 ; 1 ; 23.0 ; 0.44 ; 1.17 ; 0 ; 0 ; 0 ; 0 ; Nitrogen Oxygen Species ; 112.991277

Structure :
        DBE : 4.304908259293794
        DBE/C : 0.5524582071822495
        H/C : 0.7178051886231055
```

Figure 2: Screenshot showing the last few lines of a correctly formatted data file to be uploaded to SpectraC

Note that there are 4 extra lines at the end of the file, these are skipped by the software. So make sure to have 4 extra lines at the bottom of your file (they can be empty) otherwise the last 4 lines of data will be skipped.

The columns: **Name, Element 1, Element 2, Element 3 & Element 4** are automatically removed when uploaded since they are unnecessary. So these columns do not have to include anything of value, but they need to exist in order to upload the file.

The name of the file should be in the format of **"Sample_Description"** for example: **"Murchison_IOM"**. The reason for this naming is because two new columns will be created when files are uploaded with the name and the description in order to differentiate between the samples.

3 Getting started

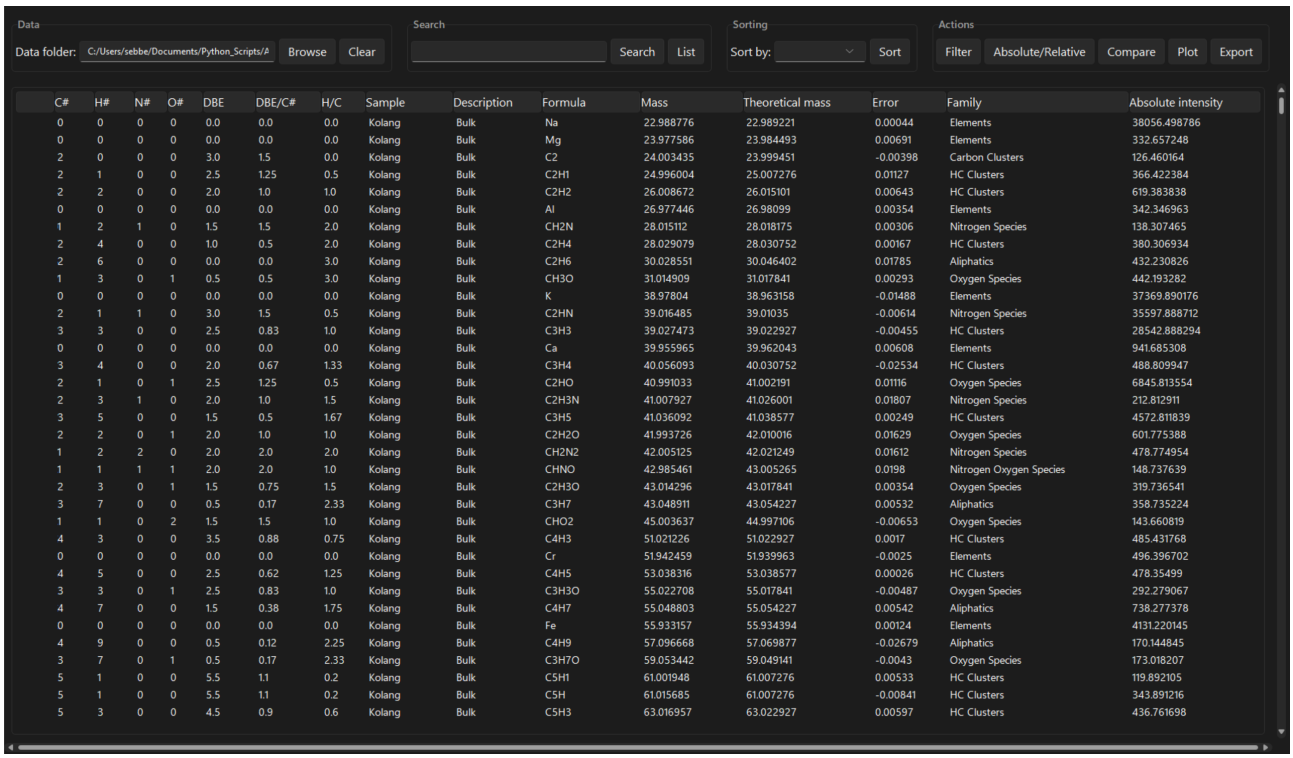
Here are a step by step explanation on how to start using SpectraC.

- **Step 1:** Download the code for the SpectraC software and the training data by clicking the links in the appendix which will take you to a GitHub repository where you can download the files.
- **Step 2:** Run the code using a IDE like Spyder for example or run it directly from the command prompt.
- **Step 3:** Unzip the file containing the training data. This file should contain three .txt files with the data for Murchison Bulk, IOM and SOM.
- **Step 4:** In the SpectraC software, click on the browse button and select the folder containing the training data. After a few seconds the data will be loaded and displayed on the screen.
- **Step 5:** You are now ready to use any of the different functionalities described in next section of this manual.
- **Step 6:** If you for any reason need to reupload the data or want to load a new set of data, simply press the "Clear" button and then you can load it again as done in step 4.

4 Functionalities

4.1 Load data

When the data are loaded into the application a new family is automatically added by splitting the aromatics family into aromatics (DBE<0.67) and condensed aromatics (DBE≥0.67). This is because the mMass software does not include condensed aromatics in its family analysis.



C#	H#	N#	O#	DBE	DBE/C#	H/C	Sample	Description	Formula	Mass	Theoretical mass	Error	Family	Absolute intensity
0	0	0	0	0.0	0.0	0.0	Kolang	Bulk	Na	22.988776	22.989221	0.00044	Elements	38056.498786
0	0	0	0	0.0	0.0	0.0	Kolang	Bulk	Mg	23.977586	23.984493	0.00691	Elements	332.657248
2	0	0	0	3.0	1.5	0.0	Kolang	Bulk	C2	24.003435	23.999451	-0.00398	Carbon Clusters	126.460164
2	1	0	0	2.5	1.25	0.5	Kolang	Bulk	C2H1	24.996004	25.007276	0.01127	HC Clusters	366.422384
2	2	0	0	2.0	1.0	1.0	Kolang	Bulk	C2H2	26.008672	26.015101	0.00643	HC Clusters	619.383838
0	0	0	0	0.0	0.0	0.0	Kolang	Bulk	Al	26.977446	26.98099	0.00354	Elements	342.346963
1	2	1	0	1.5	1.5	2.0	Kolang	Bulk	CH2N	28.015112	28.018175	0.00306	Nitrogen Species	138.307465
2	4	0	0	1.0	0.5	2.0	Kolang	Bulk	C2H4	28.029079	28.030752	0.00167	HC Clusters	380.306934
2	6	0	0	0.0	0.0	3.0	Kolang	Bulk	C2H6	30.028551	30.046402	0.01785	Aliphatics	432.230826
1	3	0	1	0.5	0.5	3.0	Kolang	Bulk	CH3O	31.014909	31.017841	0.00293	Oxygen Species	442.193282
0	0	0	0	0.0	0.0	0.0	Kolang	Bulk	K	38.97804	38.963158	-0.01488	Elements	37369.890176
2	1	1	0	3.0	1.5	0.5	Kolang	Bulk	C2HN	39.016485	39.01035	-0.00614	Nitrogen Species	35597.888712
3	3	0	0	2.5	0.83	1.0	Kolang	Bulk	C3H3	39.027473	39.022927	-0.00455	HC Clusters	28542.888294
0	0	0	0	0.0	0.0	0.0	Kolang	Bulk	Ca	39.955965	39.962043	0.00608	Elements	941.685308
3	4	0	0	2.0	0.67	1.33	Kolang	Bulk	C3H4	40.056093	40.030752	-0.02534	HC Clusters	488.809947
2	1	0	1	2.5	1.25	0.5	Kolang	Bulk	C2HO	40.991033	41.002191	0.01116	Oxygen Species	6845.813554
2	3	1	0	2.0	1.0	1.5	Kolang	Bulk	C2H3N	41.007927	41.026001	0.01807	Nitrogen Species	212.812911
3	5	0	0	1.5	0.5	1.67	Kolang	Bulk	C3H5	41.036092	41.038577	0.00249	HC Clusters	4572.811839
2	2	0	1	2.0	1.0	1.0	Kolang	Bulk	C2H2O	41.993726	42.010016	0.01629	Oxygen Species	601.775388
1	2	2	0	2.0	2.0	2.0	Kolang	Bulk	CH2N2	42.005125	42.021249	0.01612	Nitrogen Species	478.774954
1	1	1	1	2.0	2.0	1.0	Kolang	Bulk	CHNO	42.985461	43.005265	0.0198	Nitrogen Oxygen Species	148.737639
2	3	0	1	1.5	0.75	1.5	Kolang	Bulk	C2H3O	43.014296	43.017841	0.00354	Oxygen Species	319.736541
3	7	0	0	0.5	0.17	2.33	Kolang	Bulk	C3H7	43.048911	43.054227	0.00532	Aliphatics	358.735224
1	1	0	2	1.5	1.5	1.0	Kolang	Bulk	CHO2	45.003637	44.997106	-0.00653	Oxygen Species	143.660819
4	3	0	0	3.5	0.88	0.75	Kolang	Bulk	C4H3	51.021226	51.022927	0.0017	HC Clusters	485.431768
0	0	0	0	0.0	0.0	0.0	Kolang	Bulk	Cr	51.942459	51.939963	-0.0025	Elements	496.396702
4	5	0	0	2.5	0.62	1.25	Kolang	Bulk	C4H5	53.038316	53.038577	0.00026	HC Clusters	478.35499
3	3	0	1	2.5	0.83	1.0	Kolang	Bulk	C3H3O	55.022708	55.017841	-0.00487	Oxygen Species	292.279067
4	7	0	0	1.5	0.38	1.75	Kolang	Bulk	C4H7	55.048803	55.054227	0.00542	Aliphatics	738.277378
0	0	0	0	0.0	0.0	0.0	Kolang	Bulk	Fe	55.933157	55.934394	0.00124	Elements	4131.220145
4	9	0	0	0.5	0.12	2.25	Kolang	Bulk	C4H9	57.096668	57.069877	-0.02679	Aliphatics	170.144845
3	7	0	1	0.5	0.17	2.33	Kolang	Bulk	C3H7O	59.053442	59.049141	-0.0043	Oxygen Species	173.018207
5	1	0	0	5.5	1.1	0.2	Kolang	Bulk	C5H1	61.001948	61.007276	0.00533	HC Clusters	119.892105
5	1	0	0	5.5	1.1	0.2	Kolang	Bulk	C5H	61.015685	61.007276	-0.00841	HC Clusters	343.891216
5	3	0	0	4.5	0.9	0.6	Kolang	Bulk	C5H3	63.016957	63.022927	0.00597	HC Clusters	436.761698

Figure 3: Screenshot from the SpectraC software after data has been loaded

4.2 Search

Allows the user to search for peaks manually by typing in the search bar or through list matching by pressing the list button and uploading either a .txt or .csv file containing the list. The list should be a single column .txt or .csv file with one formula per row.

4.3 Sort

Makes it possible to sort the data based on the different columns.

4.4 Filter

By pressing the filter button the filter window is opened. Here the user can filter the data by family, C number, mass and intensity. For the C number and mass it is also possible to filter by multiple ranges, for example $C\#Ranges : 0 - 30, 60 - 90$.

In order to use the filter function, you should first press the "Select families" button and select the desired family/families, then press the "Update" button in the filter window. This will automatically be display the min and max values for each parameter for the selected family/families. These can then be edited as wished and if you want to redisplay the min and max values for a parameter, simply press the "All" button.

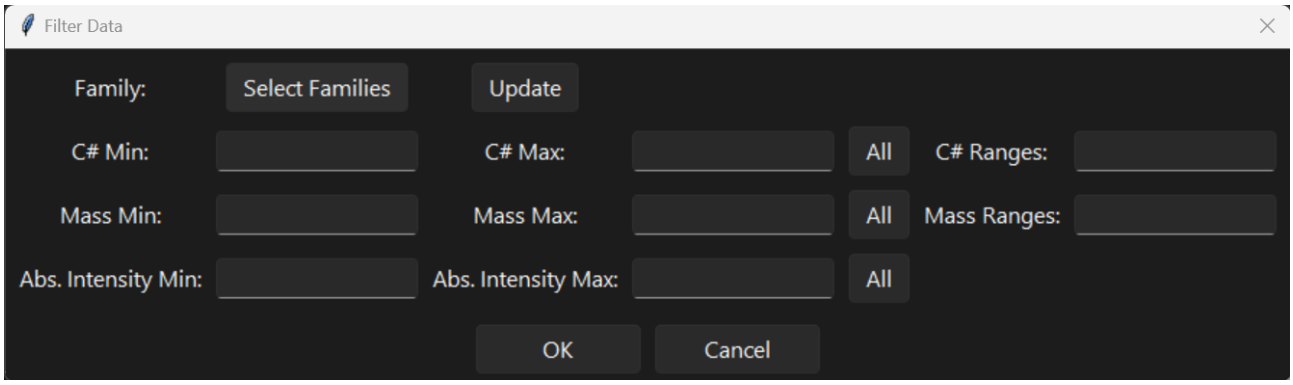


Figure 4: Screenshot from the SpectraC software showing the filter window

4.5 Absolute/Relative

This button enables the user to toggle the intensity column between absolute and relative intensity. The relative intensities are calculated relative the most intense peak for each respective sample individually.

4.6 Plot

When pressing this button the plotting window is opened in which the user can select the samples to be plotted and the type of plot, a separate plot is created for each selected sample.

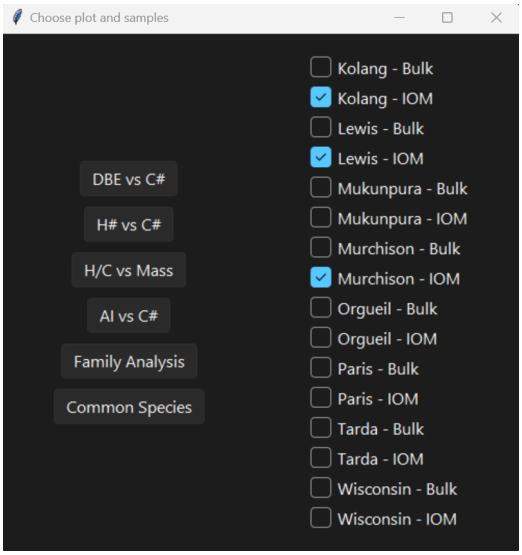


Figure 5: Screenshot from the SpectraC software showing the plot window

The "DBE vs C#", "H# vs C#", "H/C vs Mass" and "AI vs C#" plots can be largely customized. First, the user selects the group of species to be plotted (C and CH, CHN, CHO or CHNO species) if multiple are selected, a plot will be generated for each group. Then, when applicable, there is the option to add asymptotes/limits to the plot. Finally, the user can choose to customize the min and max values for the axes, as well as for the colorbar representing the intensity. Once the plot is generated, the user can effortlessly save it by clicking the "save" button at the bottom of the plot window. This allows the user to save both the plot and the data plotted in their preferred format.

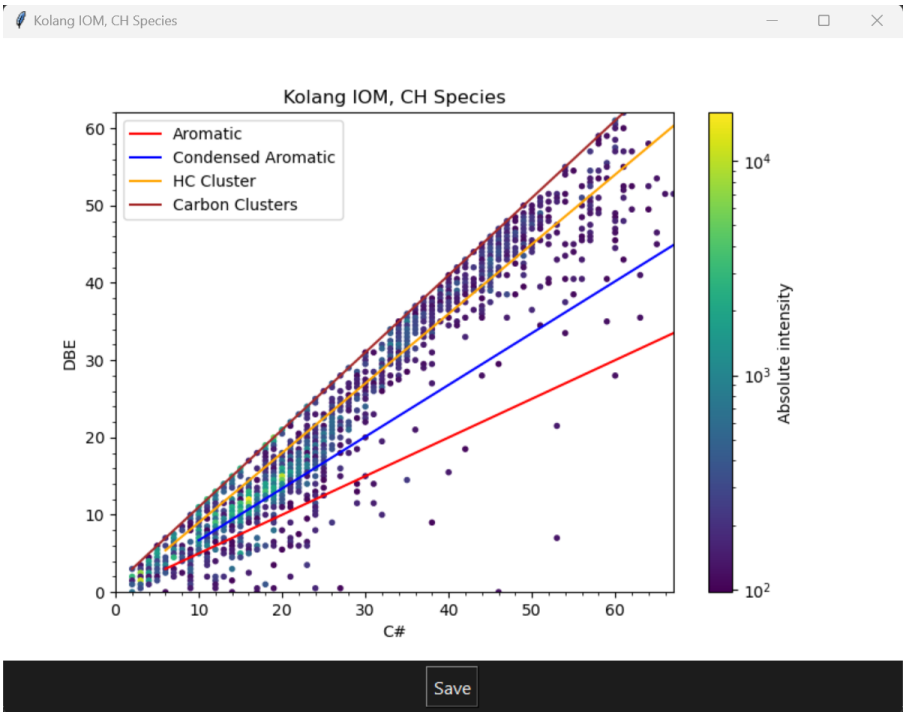


Figure 6: Screenshot from the SpectraC software showing an example of a generated DBE vs C# plot

The "Family Analysis" plot generates two bar plots for all selected samples. The x-axis are the same for both plots and contains the different samples with a group of bars for each sample. The groups of bars represents the different families inside the samples and the height of the bars are defined by the sum of the intensities for all species of the families in one of the plots and the number of species of the families in the other plot. Before the plot is generated the user is prompted to choose which families to include and if the height of the bars should be in linear or logarithmic scale.

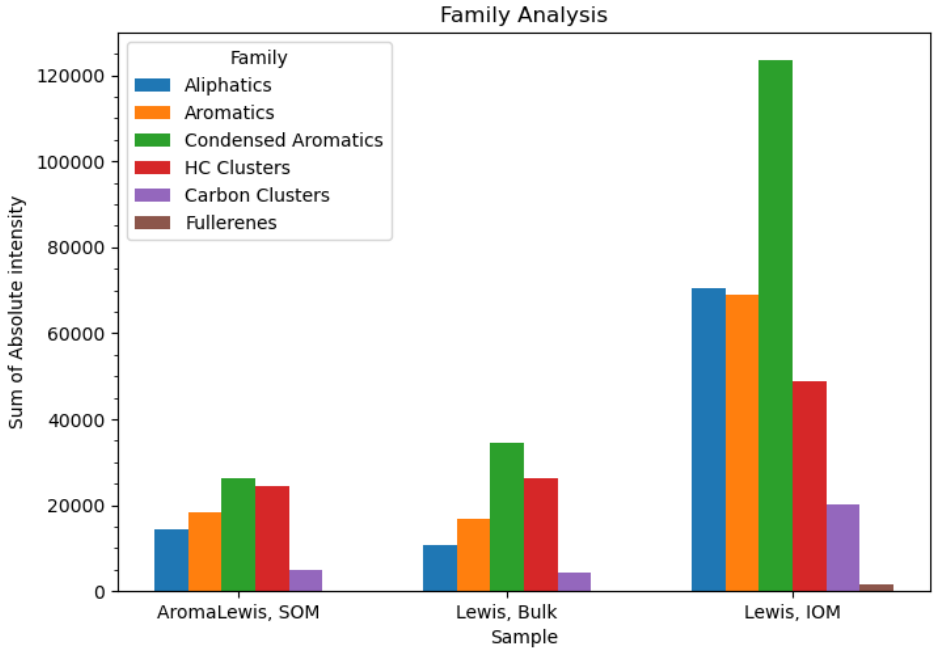


Figure 7: Example of a generated family analysis plot

For the "Common Species" option two samples are selected. It then generates a plot with three subplots with the DBE vs C# for the; larger sample, smaller sample and common species between the two. It also shows the percentage of species in the smaller sample which are also found in the larger sample.

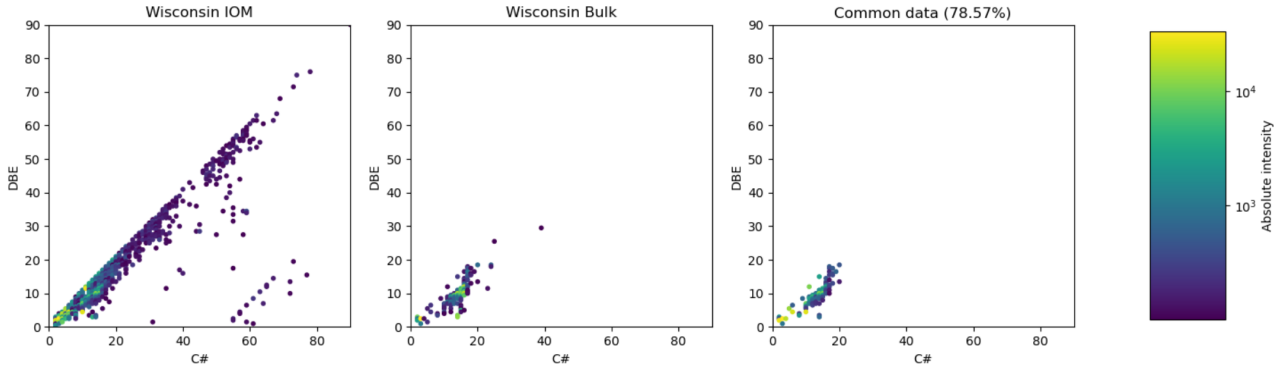


Figure 8: Example of a generated common species plot

4.7 Compare

In the compare window the user can choose to generate an average or common species list of the selected samples. In both cases this generates a new column with the average intensity which is then used for the plots. The key difference is that the "average" option will take the average of the full spectra, including non-common species, while the "common species" option will use only the species that are common to the selected samples.

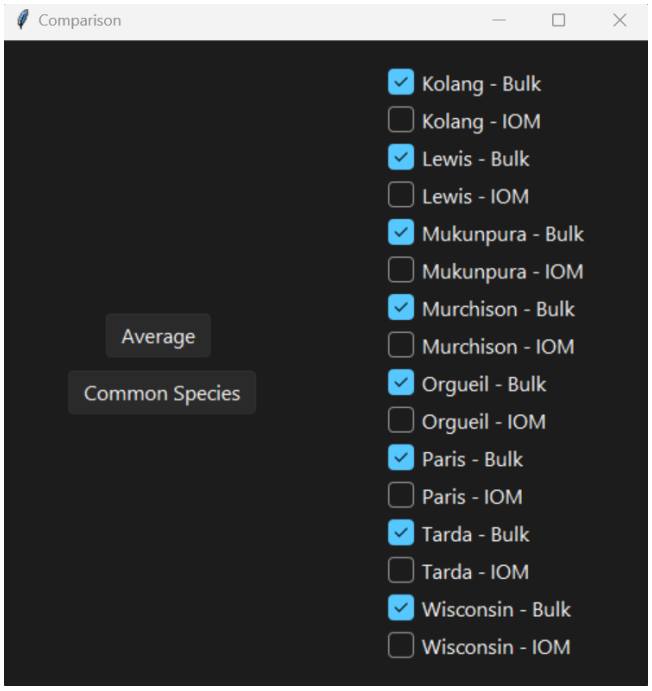


Figure 9: Screenshot from the SpectraC software showing the compare window

4.8 Export

Pressing this button at any time allows the user to export the currently displayed data as either a .txt or .csv file.

Appendices

A Appendix

A.1 Code for SpectraC

Click here to get to the download page

A.2 Training Data

Click here to get to the download page