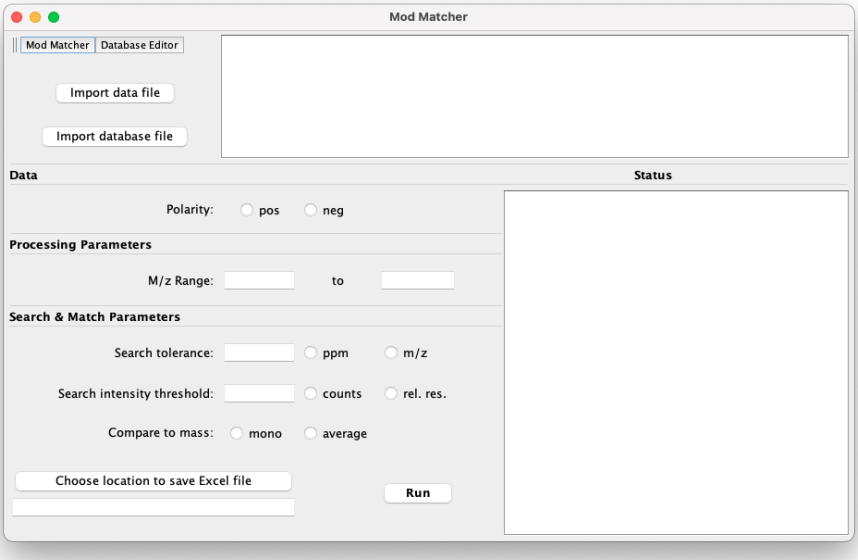
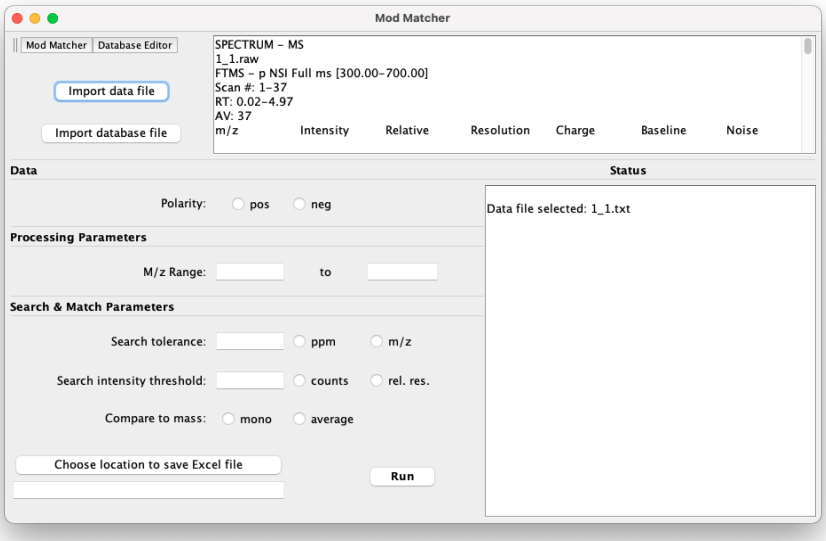
HOW TO USE MOD MATCHER

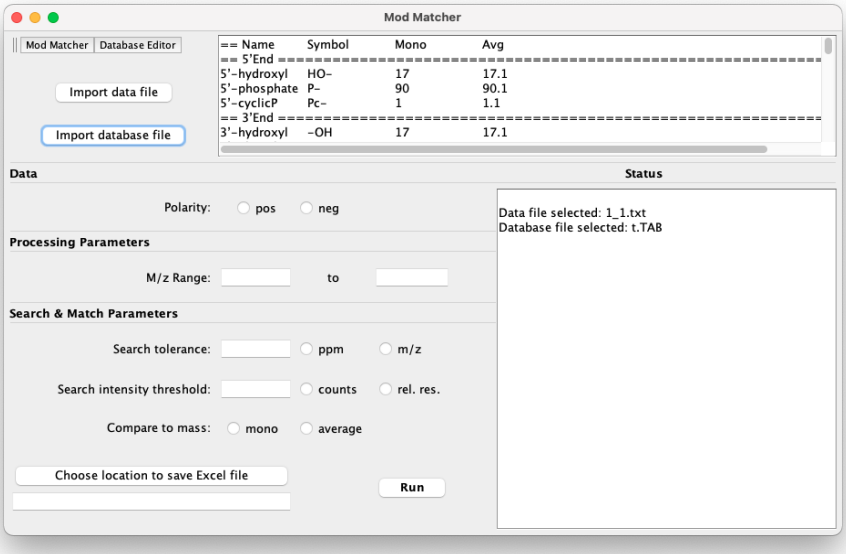
1. Always use command prompt to open ModMatcher.jar (otherwise the program will not be able to access your files). (Replace path with the actual path).
    a. *LINUX/MAC*: `java -jar` /path-to-jar/MassSpecAnalysis_java8.jar
    b. *WINDOWS*: `java -jar c:`\path-to-jar\MassSpecAnalysis_java8.jar
    c. **Note**: Program runs with JAVA SE1.8 and Java SE Runtime Environment 8



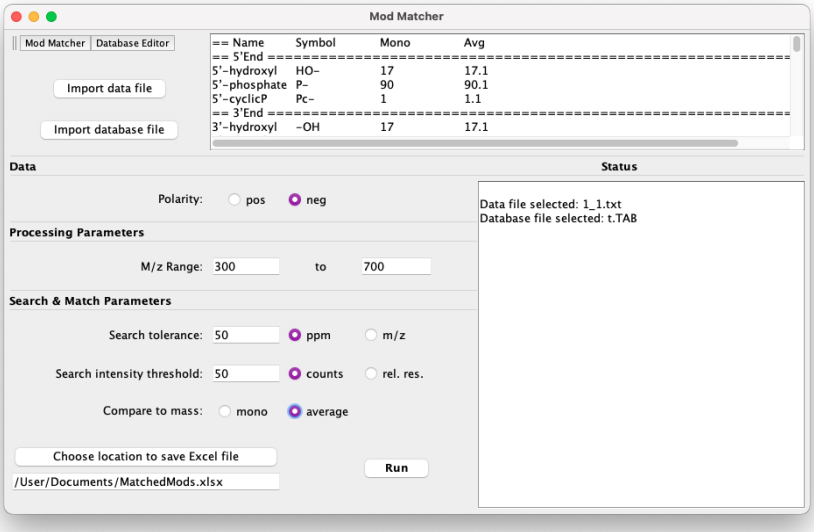
2. Click “Import data file”
3. Select data file (.txt)



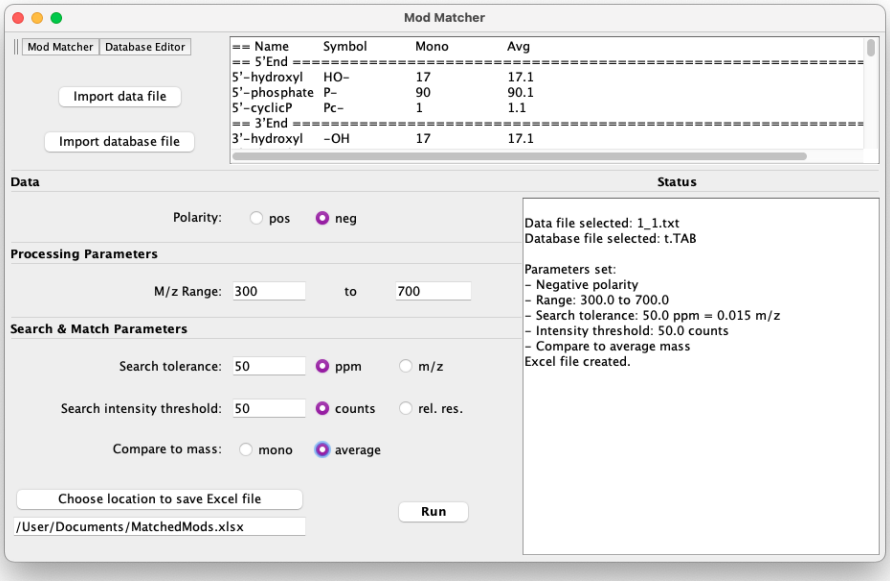
4. Click “Import database file”
5. Select database file called “t.TAB”



6. Set parameters.
    a. **Polarity**: select positive OR negative
    b. **M/z range**: enter *low range*, enter *high range*
    c. **Search tolerance**: enter *tolerance*, select ppm OR m/z
        i. This is the tolerance within which the experimental data will be compared to the database.
        ii. ***NOTE**: search tolerance does not apply to ACGU bases in order to calculate AvP, message will be shown in Excel file.
    d. **Search intensity threshold**: enter *intensity threshold*, select counts OR relative resolution
        i. This is the minimum intensity threshold (sets the noise level).
    e. **Compare to mass**: select mono OR average
        i. This is the database mass the experimental masses will be compared to.
    f. ***NOTE: Make sure ALL parameters are set or else the program will not work.**
7. Choose location to save the excel file, you can edit the name of the excel file here (default name is MatchedMods.xlsx).



8. Click “Run” button.



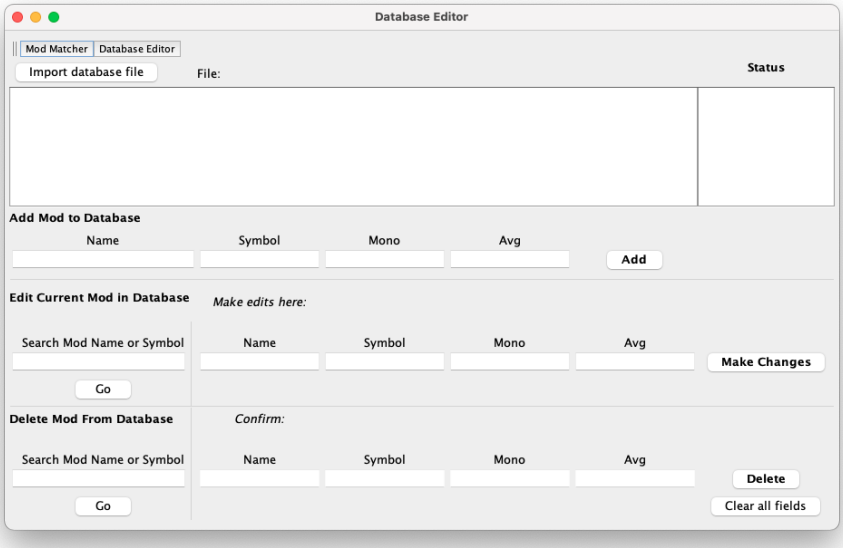
9. Excel file will be in the location you set.

	A	B	C	D	E	F	G	H	I	J
1	Name	Symbol	Experimental Mass	Experimental Intensity	Database Mono Mass	Database Avg Mass	AvP			
2	Cytidine	C	322.06524	28.3	322.03346	322.07712	0.133903013	*Intensity is below threshold		
3	Cytidine	C	322.06784	19.7	322.03346	322.07712	0.093211638	*Intensity is below threshold		
4	Cytidine	C	322.07489	38	322.03346	322.07712	0.179799098	*Intensity is below threshold		
5	Cytidine	C	322.0804	16.8	322.03346	322.07712	0.079490128	*Intensity is below threshold		
6	Cytidine	C	322.08906	291.9	322.03346	322.07712	1.381140967			
7	Uridine	U	323.04785	20821.7	323.01748	323.06184	98.51902322			
8	Uridine	U	323.05848	19	323.01748	323.06184	0.089899549	*Intensity is below threshold		
9	Adenosine	A	346.07874	11.9	346.0447	346.0912	0.056305507	*Intensity is below threshold		
10	Adenosine	A	346.09579	7.4	346.0447	346.0912	0.035013509	*Intensity is below threshold		
11	Adenosine	A	346.10297	5.8	346.0447	346.0912	0.02744302	*Intensity is below threshold		
12	Guanosine	G	362.07589	34.5	362.03961	362.0906	0.163238655	*Intensity is below threshold		
13	Guanosine	G	362.07789	33.3	362.03961	362.0906	0.157560789	*Intensity is below threshold		
14	Guanosine	G	362.08227	18.7	362.03961	362.0906	0.088480083	*Intensity is below threshold		
15	Guanosine	G	362.08664	25.7	362.03961	362.0906	0.121600969	*Intensity is below threshold		
16	Guanosine	G	362.09165	20	362.03961	362.0906	0.094631104	*Intensity is below threshold		
17	Guanosine	G	362.09285	19.4	362.03961	362.0906	0.091792171	*Intensity is below threshold		
18	Guanosine	G	362.09695	15.3	362.03961	362.0906	0.072392795	*Intensity is below threshold		
19	Guanosine	G	362.09888	11.4	362.03961	362.0906	0.053939729	*Intensity is below threshold		
20	Pseudouridine	Y	323.04785	20821.7	323.01748	323.06184	98.51902322			
21	3-methylcytidine	m3C	336.10427	110	336.04911	336.093	0.520471074			
22	5-methylcytidine	m5C	336.10427	110	336.04911	336.093	0.520471074			
23	2'-O-methylcytidine	Cm	336.10427	110	336.04911	336.093	0.520471074			
24	N4-methylcytidine	m4C	336.10427	110	336.04911	336.093	0.520471074			
25	2'-O-methyluridine	Um	337.07869	1439.9	337.03313	337.07772	6.812966354			
26	5-methyluridine	m5U	337.07869	1439.9	337.03313	337.07772	6.812966354			
27	1-methylpseudouridine	m1Y	337.07869	1439.9	337.03313	337.07772	6.812966354			
28	2'-O-methylpseudouridine	Ym	337.07869	1439.9	337.03313	337.07772	6.812966354			
29	3-methyluridine	m3U	337.07869	1439.9	337.03313	337.07772	6.812966354			
30	3-methylpseudouridine	m3Y	337.07869	1439.9	337.03313	337.07772	6.812966354			
31	5-hydroxyuridine	ho5U	339.05483	130	339.01239	339.06124	0.615102178			
32	5-hydroxyuridine	ho5U	339.05868	1375.7	339.01239	339.06124	6.509200509			
33	5-hydroxyuridine	ho5U	339.0674	545.8	339.01239	339.06124	2.582482836			
34	5-formyl-methyluridine	f5U	351.06309	635.5	351.01239	351.06124	3.006903339			
35	5-methoxyuridine	mo5U	353.06732	952.6	353.02804	353.07712	4.507279498			
36	Xanthosine	X	363.07354	88.8	363.02363	363.07532	0.420162103			
37	5-formyl-O-dimethyluridine	f5Um	365.06985	3752.2	365.02804	365.07712	17.75374148			
38	5-methylaminomethyluridine	mnm5U	366.11483	69.7	366.05968	366.10828	0.329789398			
39	5-carboxymethyluridine	cm5U	381.07405	299.1	381.02296	381.07652	1.415208165			
40	7-cyano-7-deazaguanosine	preQ0	386.09849	253	386.03961	386.0906	1.197083469			
41	5-carbamoylmethyl-2'-O-methyluridine	ncm5Um	394.09602	148	394.05459	394.10768	0.700270172			
42	5-methoxycarbonylmethyluridine	mcm5U	395.08978	2385.6	395.03861	395.0924	11.28759812			
43	Uridine 5-oxyacetic acid	cmo5U	397.08684	1143.5	397.01787	397.07592	5.410533388			
44	5-(carboxyhydroxymethyl)uridine	chm5U	397.08684	1143.5	397.01787	397.07592	5.410533388			
45	5-methoxycharbonylmethyl-2'-O-methyluridine	mcm5Um	409.10541	447.2	409.05426	409.10828	2.115951492			
46	Uridine 5-oxyacetic acid methyl ester	mcmo5U	411.10239	56.1	411.03352	411.0918	0.265440248			
47	5-(carboxyhydroxymethyl)uridine methyl ester	mchm5U	411.10239	56.1	411.03352	411.0918	0.265440248			
48	5-formyl-2-selenouridine	f5se2U	414.01339	142.3	414.934	414.02184	0.673300307			
49	5-aminomethyl-2-selenouridine	nm5se2U	415.05969	271.1	415.96563	415.053	1.282724619			
50	N6-glycinylcarbamoyladenosine	g6A	447.13421	847.1	447.05599	447.11996	4.008100423			
51	N6-methyl-N6-threonylcarbamoyladenosine	m6t6A	505.16034	668.9	505.09785	505.167	3.164937283			
52	N6-hydroxynorvalylcarbamoyladenosine	hn6A	505.16034	668.9	505.09785	505.167	3.164937283			
53										

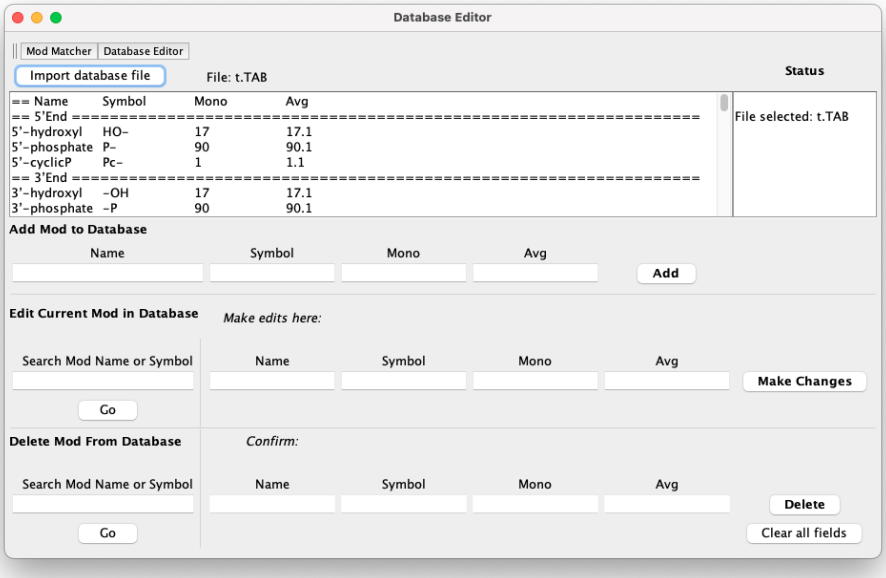
(Intensities for some or all ACGU canonical bases may be below the intensity threshold set by the user, but the ACGU bases that match their database masses within the mass search tolerance show in excel file in order for AvP to be calculated).

HOW TO USE DATABASE EDITOR

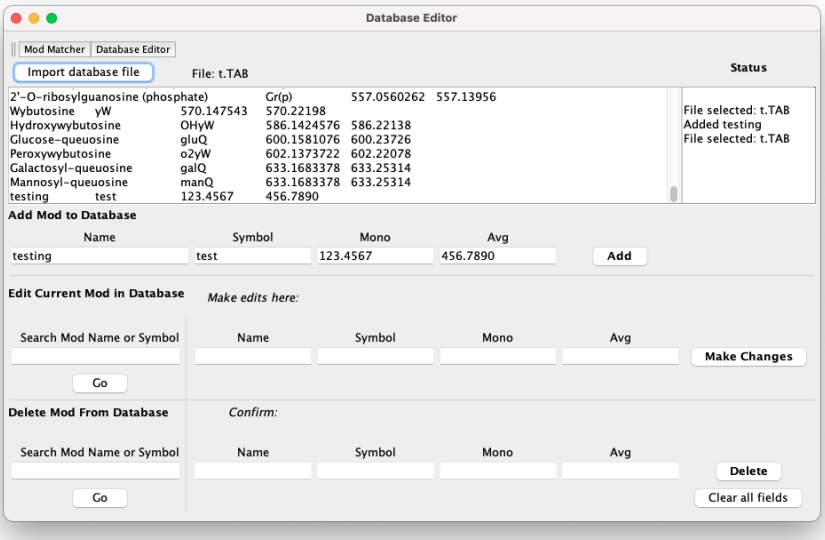
1. Click on “Database Editor” in top left corner of ModMatcher.java



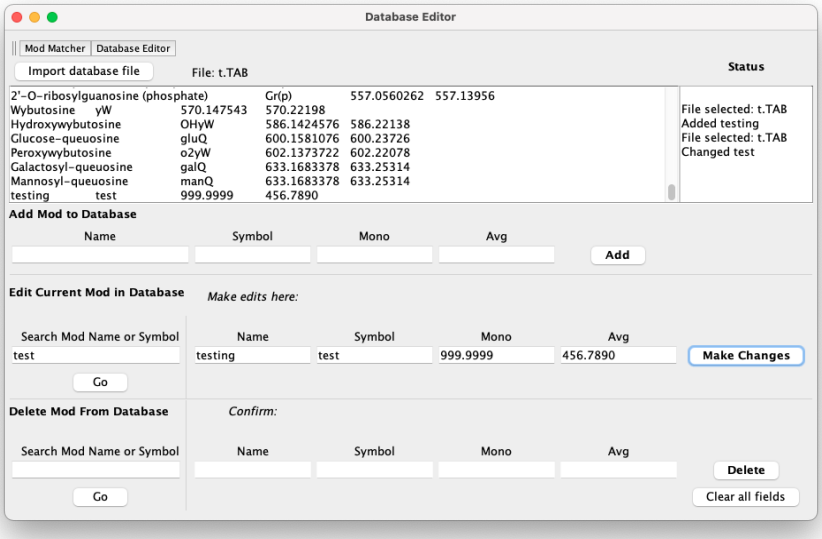
2. Click “Import database file” and select database file “t.TAB”



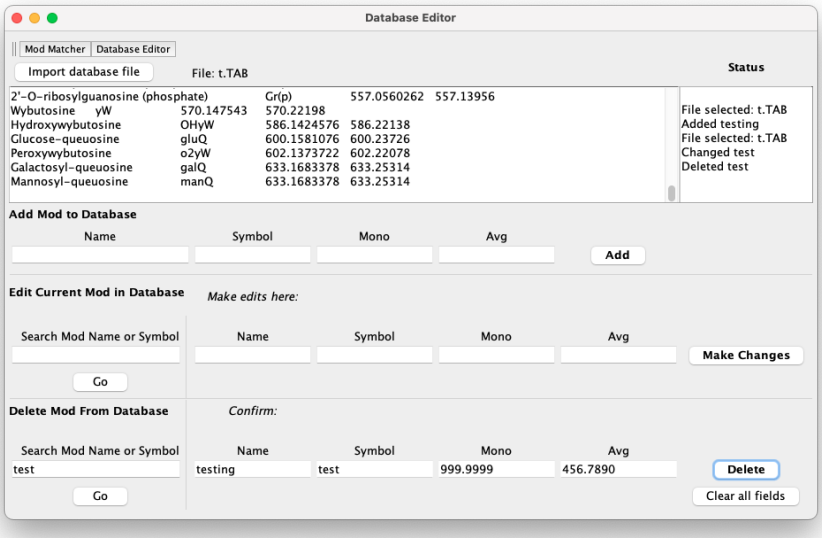
3. **ADD MOD**: Enter information in “Add Mod to Database” section and click “Add”
    a. ***NOTE**: the first time you add a mod, you may not be able to see it in the file viewer. However, if the status says that the mod has been added, you can be sure it has been added to the database. You can open the file itself to double-check, or simply import the database again and it will appear in the file viewer. You should be able to see the mod if you add more than one however.



4. **EDIT MOD**: Enter mod name or symbol exactly how it is written in the database in the “Edit Current Mod in Database” section and click “Go.” Make changes in the “Make edits here” section and click “Make Changes.” You will be able to see the changes immediately in the file viewer.



5. **DELETE MOD**: Enter mod name or symbol exactly how it is written in the database in the "Delete Mod From Database" section and click "Go." Confirm that it is the correct mod by reading the data in the "Confirm" section and click "Delete." You will be able to see the changes immediately in the file viewer.



6. Click "Clear all fields" if you want to reset all the text boxes.