SmetSearch tutorial

Objective

This project is to develop the formula 'identification' method by ultrahigh resolution MS instrument (we used FT-ICR). The point of this program is to utilize two type of data; 1) fully labeled (in our case, by 34S) biological samples; and 2) non-labeled samples as the control. The program generates formula candidates by means of non-labeled biological datum in combination with the strict mass tolerance (less than 2 mDa). The 34S labeled datum is used to check the 'metabolite peak shift' derived from its labeled element with respect to the formula candidates. The users can quickly perform the metabolite screenings from living organisms of interest.

Limitation:

1) The program needs two type 'direct infusion MS' data; 1) a 34S labeled biological dadum 2) a non-labeled sample datum.

2) The current SmetSearch program accepts the ASCII format file exported from Brucker DataAnalysis software.

Therefore, we produce the source code itself and please let us (hiroshi.tsugawa@riken.jp) know if you are using the different instrument (ex. Orbitrap or QTOF). We can help you as much as possible.

Main window

Graphical user interface of SmetSearch is simply developed for checking raw infusion MS spectra. The user can import two data, i.e. a labeled datum and a non-labeled datum. The result is generated in the same directory as the above files.
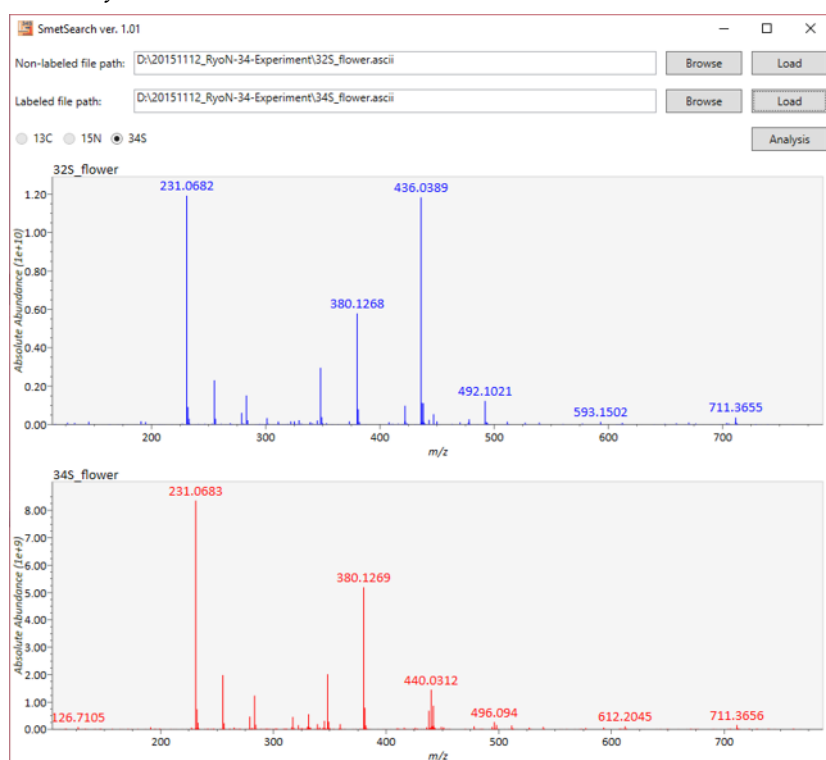
1. Select a file of non-labeled datum from 'Browse'. From 'Load', you can see raw MS spectra.
2. Select a file of labeled datum from 'Browse'. From 'Load', you can see raw MS spectra.
3. Click 'Analysis'.
4. The output will be generated in the same directory as the above files.

Result

Rank 1	Identification level	Formula	Mass error	Total score	Mass score	Isotopic score	Database score	Database	Non labeled	Non labeled	labeled ma	labeld inter	Rank 2	Identification	Formula	Mass error
1	1	C10H16SO4	0.0008935	2.468	0.905	0.986	0.576923	ChEBI,UNP	231.0688	1.7E+10	233.0648	3.03E+08				
1	1	C11H20SO6	1.29E-05	2.515	1	0.977	0.538462	UNPD	279.0908	7.1E+08	281.0867	13665036	2		C12H24S3	0.000882
1	4	C14H32N2SO2	0.0013228	0.811	0.804	0.507	0		291.2099	30013630	293.2069	8715278				
1	5	C10H20N2S2O4	-0.000257	2.516	0.992	0.986	0.538462	ChEBI	295.0794	46893688	0	0	2		C18H16SO	0.000394
1	3	C14H30SO5	-0.000441	1.975	0.976	0.961	0.538462	T3DB	309.1746	32416342	311.1691	23518958				
1	4	C16H36N2SO2	0.0009829	1.034	0.886	0.648	0		319.2415	22037060	321.2386	6960800				
1	1	C15H21N3SO3	-0.000524	2.628	0.966	0.97	0.692308	ChEBI,Dru	322.1236	1.45E+08	324.1195	5537181				
1	4	C16H34SO5	-0.000691	1.234	0.942	0.792	0		337.2061	9653801	339.2007	15351761	2		C17H30N4	0.000646
1	6	C12H40N2S4	-0.000533	1.763	0.965	0.798	0		339.2007	45804816	0	0	2		C19H32SO	-0.000751
1	4	C11H26N2S2O6	-0.000738	1.243	0.934	0.809	0		345.1167	6128790	349.1065	3.15E+08				
1	6	C20H42S2	8.69E-05	1.758	0.999	0.759	0		345.2654	34496364	0	0				
1	1	C16H19N3SO4	-0.000549	2.458	0.963	0.803	0.692308	ChEBI,Dru	348.1029	3.14E+09	350.0987	17559776	2		C9H27N5S	-0.000332
1	4	C13H22N2SO7	0.0010856	1.262	0.863	0.899	0		349.1064	4.05E+08	351.1023	9253539	2		C25H18S	-0.000765
1	4	C10H22N2SO11	0.0005441	1.109	0.964	0.645	0		377.0866	28881096	379.0837	12787804	2		C23H14N4	3.10E-05
1	4	C16H30N2S3O2	-0.000175	1.151	0.996	0.655	0		377.1398	9110776	383.1288	24089934	2		C24H26S2	0.000476
1	2	C17H23N3SO5	-0.000625	1.917	0.952	0.965	0		380.1292	4.68E+09	382.1243	5945733	2		C18H27N3	0.000244
1	4	C10H27N3SO10	0.0004386	1.343	0.976	0.867	0		380.134	7660319	382.1301	5604678	2		C22H23NS	-0.001412
1	4	C15H22N4SO6	-0.001071	1.152	0.866	0.786	0		385.1198	33159850	387.1156	5227140				
1	4	C10H29N5S3O6	-0.00028	1.225	0.99	0.735	0		410.121	17666718	416.1063	1.2E+08				
1	6	C7H17N3S3O11	-0.000235	1.857	0.993	0.864	0		413.9955	16465915	0	0	2		C15H13NS	0.000417
1	6	C15H31NS4O4	-6.40E-05	1.963	0.999	0.964	0		416.1064	1.01E+08	0	0	2		C15H23N5	0.000404
1	4	C7H19NSO17	-1.73E-05	0.946	1	0.446	0		420.0301	51090308	422.0273	6148451	2		C8H15N5S	0.00132
1	3	C13H17N5S2O8	-0.001262	1.801	0.82	0.75	0.730769	ChEBI,Dru	434.0458	11983925	438.0381	11261674	2		C8H21NSO	-9.72E-05
1	1	C12H23NS3O10	-0.001148	2.589	0.848	0.972	0.769231	ChEBI,Foo	436.0423	73094424	442.0297	13361795	2		C13H19NS	0.00019
1	3	C16H20N2S2O9	-0.001174	1.82	0.842	0.709	0.769231	ChEBI,Foo	447.0549	21144086	451.0466	13928907	2		C12H20N2	0.001328
1	4	C8H21NSO18	-5.26E-05	0.934	1	0.434	0		450.0407	8492443	452.0378	7080681	2		C9H17N5S	0.001285
1	3	C17H22N2S2O10	-0.00118	1.795	0.84	0.686	0.769231	ChEBI,Foo	477.0655	14714493	481.057	9882625	2		C13H22N2	0.001323
1	6	C18H29N3S4O4	-0.000296	1.729	0.989	0.74	0		478.0971	17053582	0	0	2		C26H25NS	0.000356
1	6	C17H36SO16	0.0003096	1.956	0.988	0.968	0		527.1648	95931768	0	0	2		C30H28N2	-0.000204
1	6	C19H43N5S3O11	-0.000616	1.584	0.954	0.63	0		612.2055	1.85E+08	0	0	2		C27H39N3	3.54E-05
1	4	C30H44SO13	0.000786	1.246	0.926	0.82	0		643.2422	19423026	645.2392	16998336	2		C43H36N2	0.000273
1	6	C34H58N4S3O2	-0.000126	1.472	0.998	0.474	0		649.365	80021320	0	0	2		C42H54N2	0.000525
1	4	C30H57N3SO10	0.0005196	0.885	0.967	0.418	0		650.3687	22892350	652.3658	9336955				

32S_leaf-34S_leaf

The program generates up to five candidates for a metabolite peak with the identification level as follows.

Level 1. Finding 34S isotopic ions (M+2) in non-labeled sample, AND finding the peak shift in labeld sample, AND reported in metabolome databases.

Level 2. Finding 34S isotopic ions (M+2) in non-labeled sample, AND finding the peak shift in labeld sample, AND unreported in metabolome databases.

Level 3. Cannot find 34S isotopic ions (M+2) in non-labeled sample, AND finding the peak shift in labeld sample, AND reported in metabolome databases.

Level 4. Cannot find 34S isotopic ions (M+2) in non-labeled sample, AND finding the peak shift in labeld sample, AND unreported in metabolome databases.

Level 5. Finding 34S isotopic ions (M+2) in non-labeled sample, AND cannot find the peak shift in labeld sample, AND reported in metabolome databases.

Level 6. Finding 34S isotopic ions (M+2) in non-labeled sample, AND cannot find the peak shift in labeld sample, AND unreported in metabolome databases.