

Lipid annotation with MS2Analyzer

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Checklist before you start...

You need to have:

- 1.A computer with Java environment and Office(2003 or higher)
- 2.MS/MS spectra in MGF files
- 3.Latest version of MS2Analyzer jar file
- 4.Query text files

For additional validation with lipidblast, download the library and NIST search software in the following link(download the 87 MB full version):

<http://fiehnlab.ucdavis.edu/projects/LipidBlast>

Instruction outline

Step1: Using MS2Analyzer to search the spectra feature

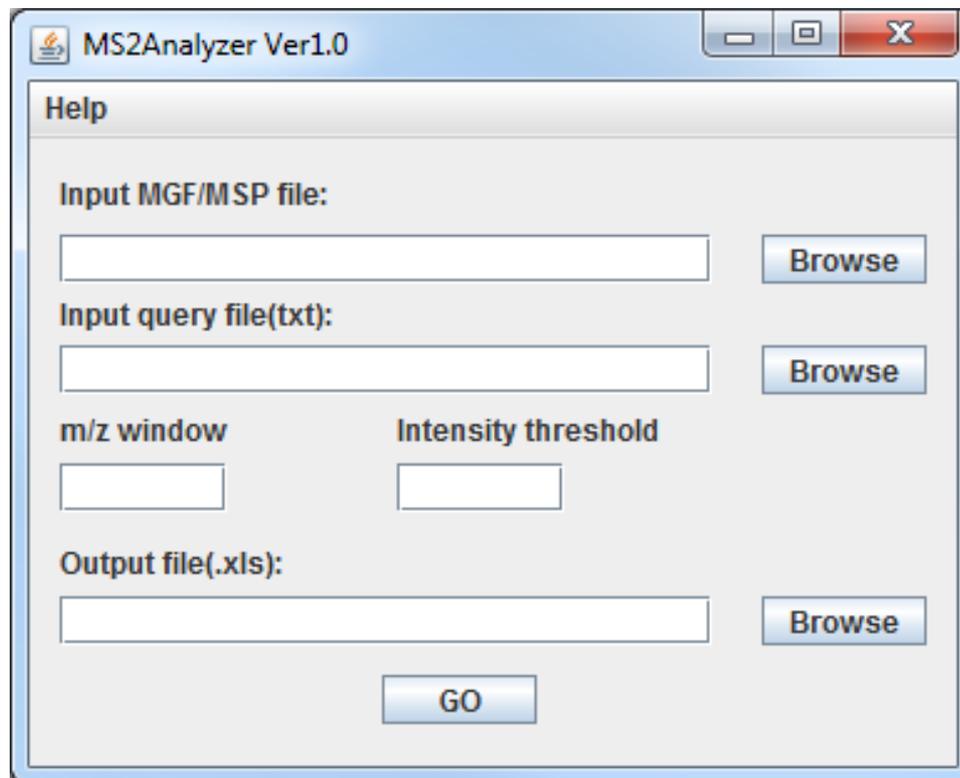
Step2: Using excel filters to annotate lipids

Step3: Confirmation by checking retention time
(optional)

Step 4:Using NIST search for library validation(optional)

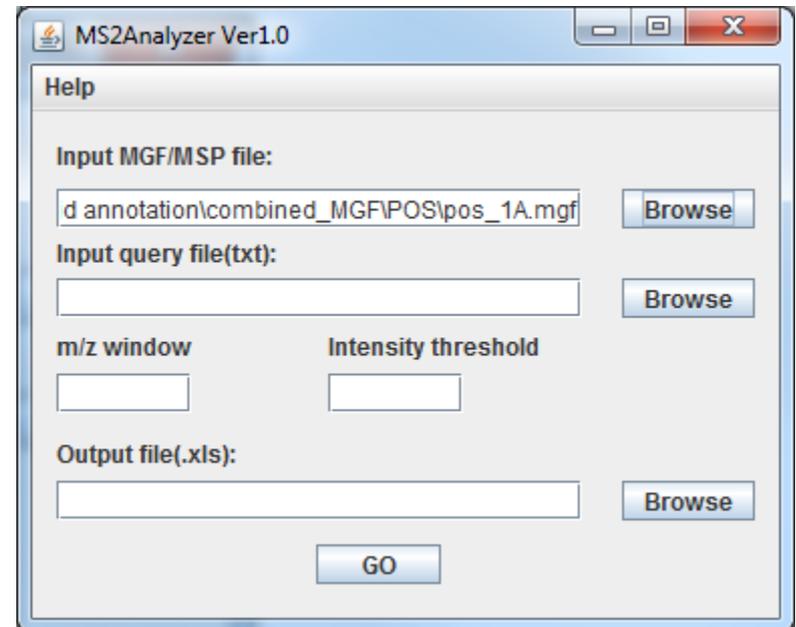
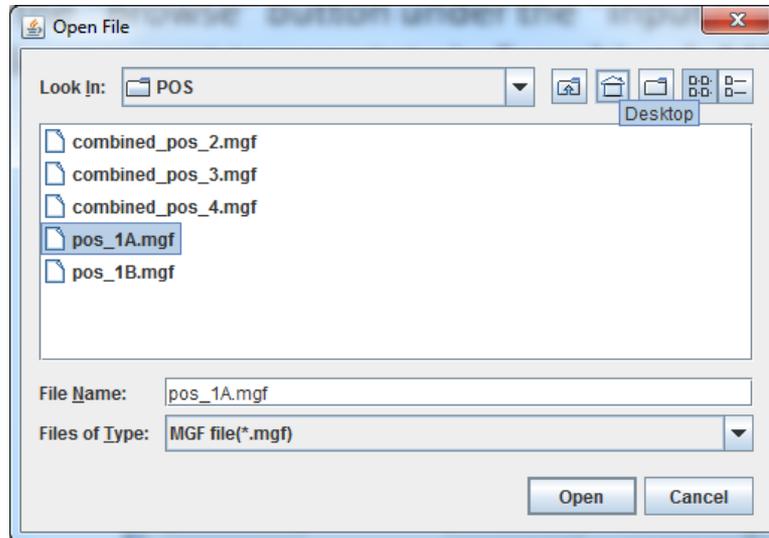
Step 1: Using MS2Analyzer to search the spectra feature

1. Double click on MS2Analyzer-ver1.jar to start the program



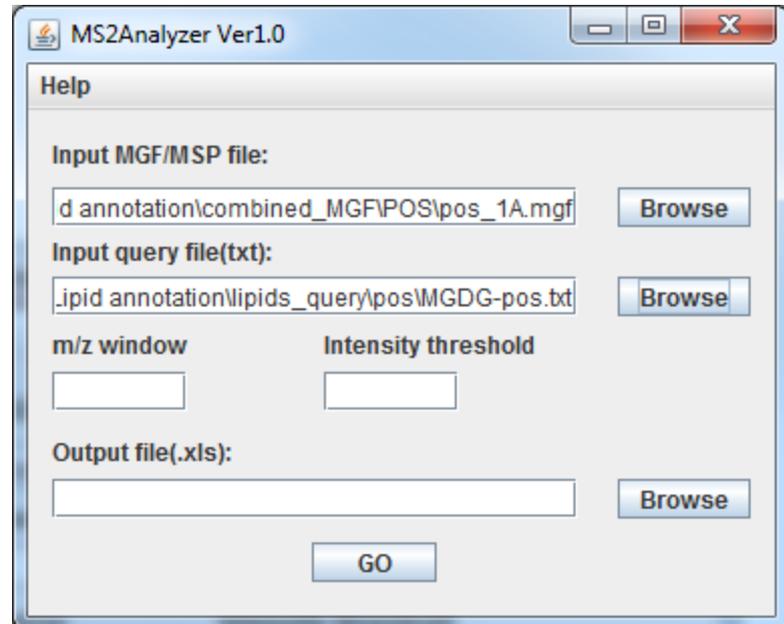
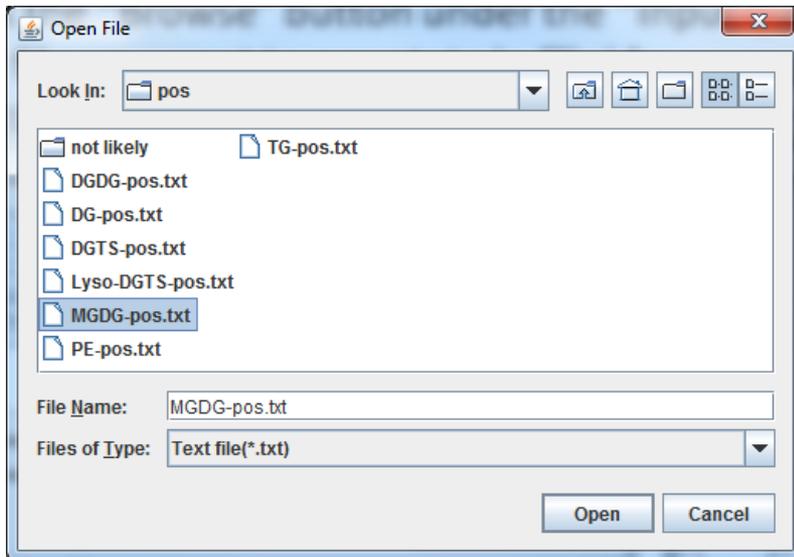
Step 1: Using MS2Analyzer to search the spectra feature

2. Click the “Browse” button under the “Input MGF/MSP file” and select the MGF file you want to annotate.



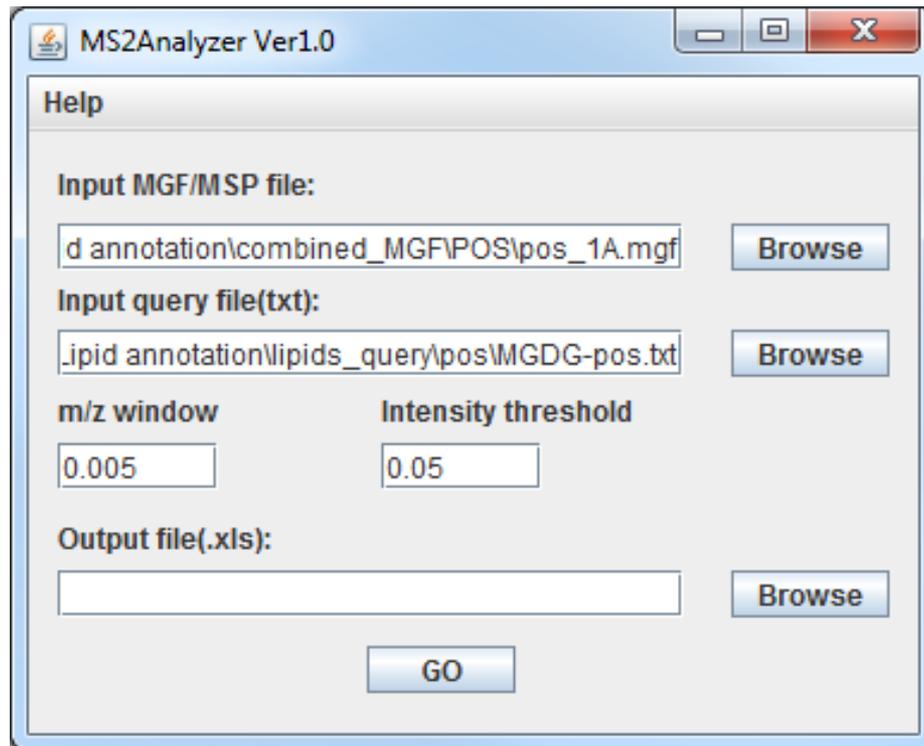
Step 1: Using MS2Analyzer to search the spectra feature

3. Click the “Browse” button under the “Input query file(txt)” and select the query file you want.



Step 1: Using MS2Analyzer to search the spectra feature

4.Type your desired parameters into “m/z window” and “intensity threshold”. The first one depends on the mass accuracy of the instrument and the second one depends how noisy the spectra are. Intensity threshold are relative intensity to the base peak, from 0 to 1.0.



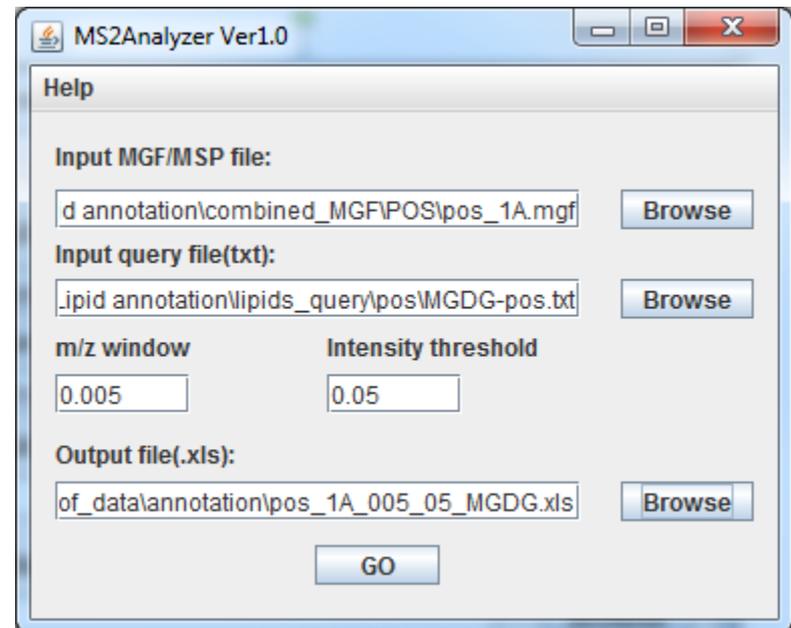
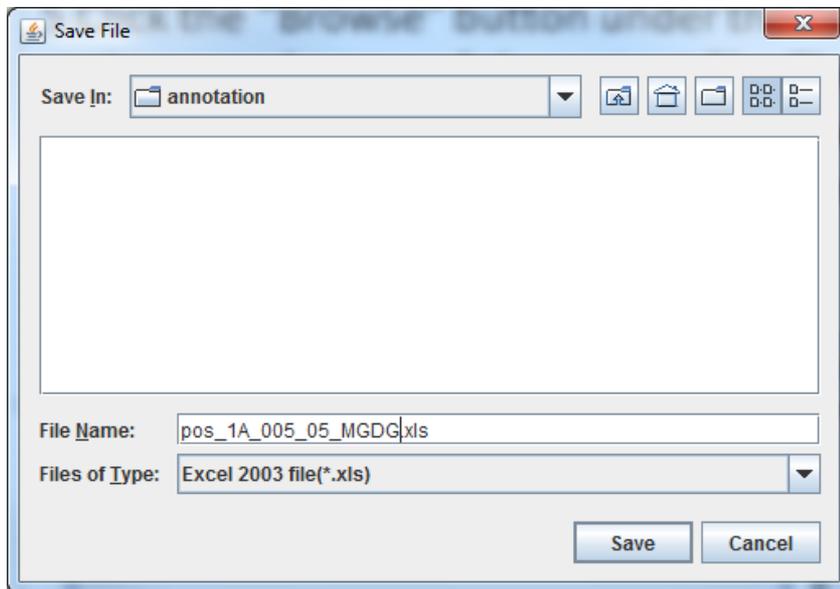
The screenshot shows the MS2Analyzer Ver1.0 application window. It features a title bar with the application name and standard window controls. The main interface includes a 'Help' section at the top. Below it, there are several input fields and buttons:

- Input MGF/MSP file:** A text box containing the path 'd annotation\combined_MGF\POS\pos_1A.mgf' and a 'Browse' button to the right.
- Input query file(txt):** A text box containing the path '.lipid annotation\lipids_query\pos\MGDG-pos.txt' and a 'Browse' button to the right.
- m/z window:** A text box containing the value '0.005'.
- Intensity threshold:** A text box containing the value '0.05'.
- Output file(.xls):** An empty text box and a 'Browse' button to the right.
- A large 'GO' button is centered at the bottom of the window.

Step 1: Using MS2Analyzer to search the spectra feature

5. Click the “Browse” button under the “Output files (.xls)” and choose the pathway and name of the output file.

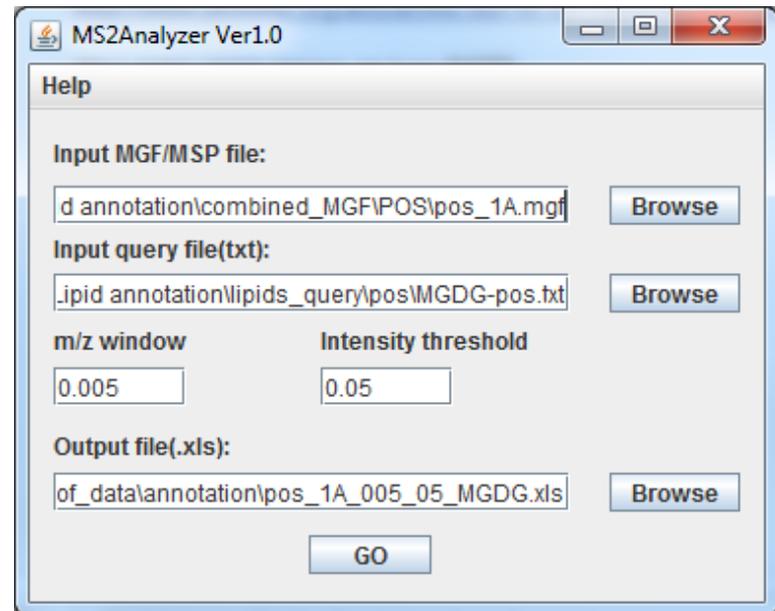
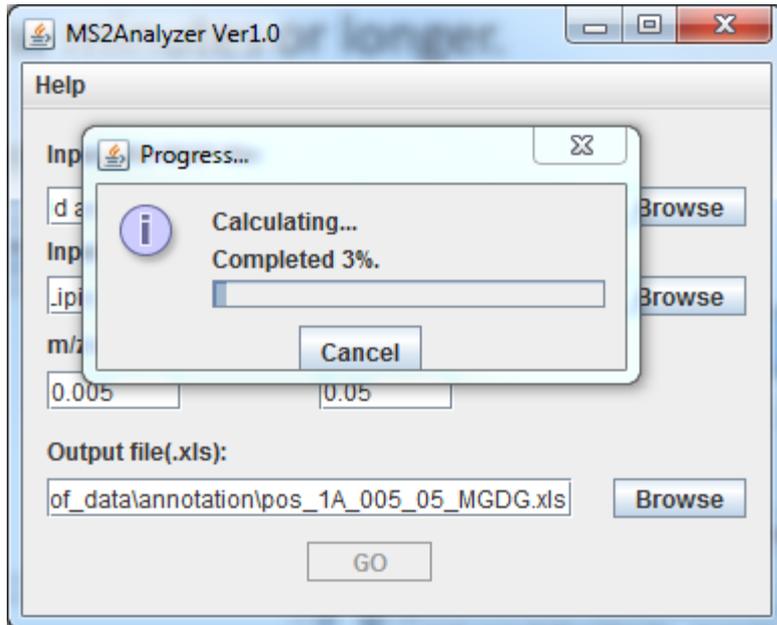
The default name of the output file is same as the name of the MGF files, but you may want to add more information about the lipid class and parameters. Here’s an example:



Step 1: Using MS2Analyzer to search the spectra feature

6. Click on “GO” button. The program will start searching mass spectra features in the MGF file and generate a Excel 2003 file.

Depending on the speed of the computer, it will take a few minutes or longer. A progress window will show up. When it's done, the progress window will disappear, and you are ready to move to the next Step!



Step 2: Using excel filters to annotate lipids

2.Set filters on the second row with Home-Sort&Filter-Filter (here's a example of excel 2010)

The screenshot shows an Excel spreadsheet with the following data in row 1 (headers):

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T
1		MGDG	16:0+179	16:1+179	16:2+179	16:3+179	16:4+179	18:0+179	18:1+179	18:2+179	18:3+179	18:4+179	4+	4+	4+	4+	4+	4+	4+	4+
2	Title	179.0793	435.3195	433.3039	431.2882	429.2726	427.2569	463.3508	461.3352	459.3195	457.3039	455.2882	748.5938	746.5781	744.5625	742.5468	740.5312	738.5155	736.4999	776.6251

Row 2 contains a list of lipid identifiers, such as '5h6kMSMSP.d, MS/MS of 237.0834021 0 at 0.04565 mins'. A filter is applied to this row, and a dropdown menu is visible over the 'MGDG34' cell, showing options for 'Filter', 'Clear', and 'Apply'.

Step 2: Using excel filters to annotate lipids

5. Check the 1 values in the acyl chain loss columns(16:0 to 18:4 in this case) and see if the sum of them matches the number in lipids name. If the sum matches, this is a correct hit!

Example 1: 16:4+18:3=34:7 which means this lipid is

MGDG 34:7(16:4/18:3) [M+NH4]⁺

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1		MGDG	16:0+179	16:1+179	16:2+179	16:3+179	16:4+179	18:0+179	18:1+179	18:2+179	18:3+179	18:4+179	MGDG34 :7[M+NH 4] ⁺	MGDG32 :0[M+NH 4] ⁺	MGDG32 :1[M+NH 4] ⁺
2	Title	179.0793	435.3195	433.3039	431.2882	429.2726	427.2569	463.3508	461.3352	459.3195	457.3039	455.2882	762.5155	748.5938	746.5781
1075	5h6kMSMSp.d, MS/MS of 762.5173035 1+ at 3.65928333333333 mins	69	862	37	878	386	894	846	354	862	37	878	952	412	92
4970			↑	0	0	0	0	↑	0	0	0	↑	0	1	0

Example 2: Sometimes there's only one acyl chain loss found, but maybe that's also a potential hit. In this case, the lipid name is written as

MGDG 34:7(16:4/18:3) [M+NH4]⁺

While 16:4 is found by program, and 18:3 is back calculated: 34:7-16:4=18:3

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1		MGDG	16:0+179	16:1+179	16:2+179	16:3+179	16:4+179	18:0+179	18:1+179	18:2+179	18:3+179	18:4+179	MGDG34 :7[M+NH 4] ⁺	MGDG32 :0[M+NH 4] ⁺
2	Title	179.0793	435.3195	433.3039	431.2882	429.2726	427.2569	463.3508	461.3352	459.3195	457.3039	455.2882	762.5155	748.5938
1075	5h6kMSMSp.d, MS/MS of 762.5173035 1+ at 3.65928333333333 mins	69	862	37	878	386	894	846	354	862	37	878	952	412
4970			↑	0	0	0	0	↑	0	0	0	0	0	1

Step 2: Using excel filters to annotate lipids

5. Example 3: Sometimes, there are multiple possibilities...

First spectra:

16:2+18:3=34:5 MGDG 34:5(16:2/18:3) [M+NH₄]⁺

Second spectra:

16:4+18:1=34:5 MGDG 34:5(16:4/18:1) [M+NH₄]⁺

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1		MGDG	16:0+179	16:1+179	16:2+179	16:3+179	16:4+179	18:0+179	18:1+179	18:2+179	18:3+179	18:4+179	MGDG34 :5[M+NH 4] ⁺	MGDG34 :7[M+NH 4] ⁺
2	Title	179.0793	435.3195	433.3039	431.2882	429.2726	427.2569	463.3508	461.3352	459.3195	457.3039	455.2882	766.5468	762.5155
1277	5h6kMSMSp.d, MS/MS of 766.5473429 0 at 4.128183333333333 mins	69	862	37	878	386	894	846	354	862	37	878	936	952
1387	5h6kMSMSp.d, MS/MS of 766.5473429 1+ at 4.38465 mins	69	862	37	878	386	894	846	354	862	37	878	936	952
4970														
4971														

Both are correct and should be reported separately.

Step 2: Using excel filters to annotate lipids

5. (Continue) After you are done with one lipid precursor m/z , clear the filter by checking the 0 value under its filter again, and move to the next precursor m/z.

The screenshot shows an Excel spreadsheet with the following data table:

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	
1		DGDG	16:0+NL	16:1+NL	16:2+NL	16:3+NL	16:4+NL	18:0+NL	18:1+NL	18:2+NL	18:3+NL	18:4+NL	DGDG34: 2[M+NH4]	DGDG34: 3[M+NH4]	DGDG34: 4[M+NH4]	DGDG32: 0[M+NH4]	1
2	Title	341.1321	597.3724	595.3567	593.3411	591.3254	589.3098	625.4037	623.3880	621.3724	619.3567	617.3411	934.6466	932.6310	930.6153	910.6466	9
1437	5h6kMSMSp.d, MS/MS of 932.6313477 1+ at 4.50706666666667 mins	9	072	58	088	596	104	056	564	072	58	088	622	13	638	622	0
1477	5h6kMSMSp.d, MS/MS of 932.6313477 1+ at 4.598 mins				0	0	0	0	0	0							0

The context menu for column M shows the following options:

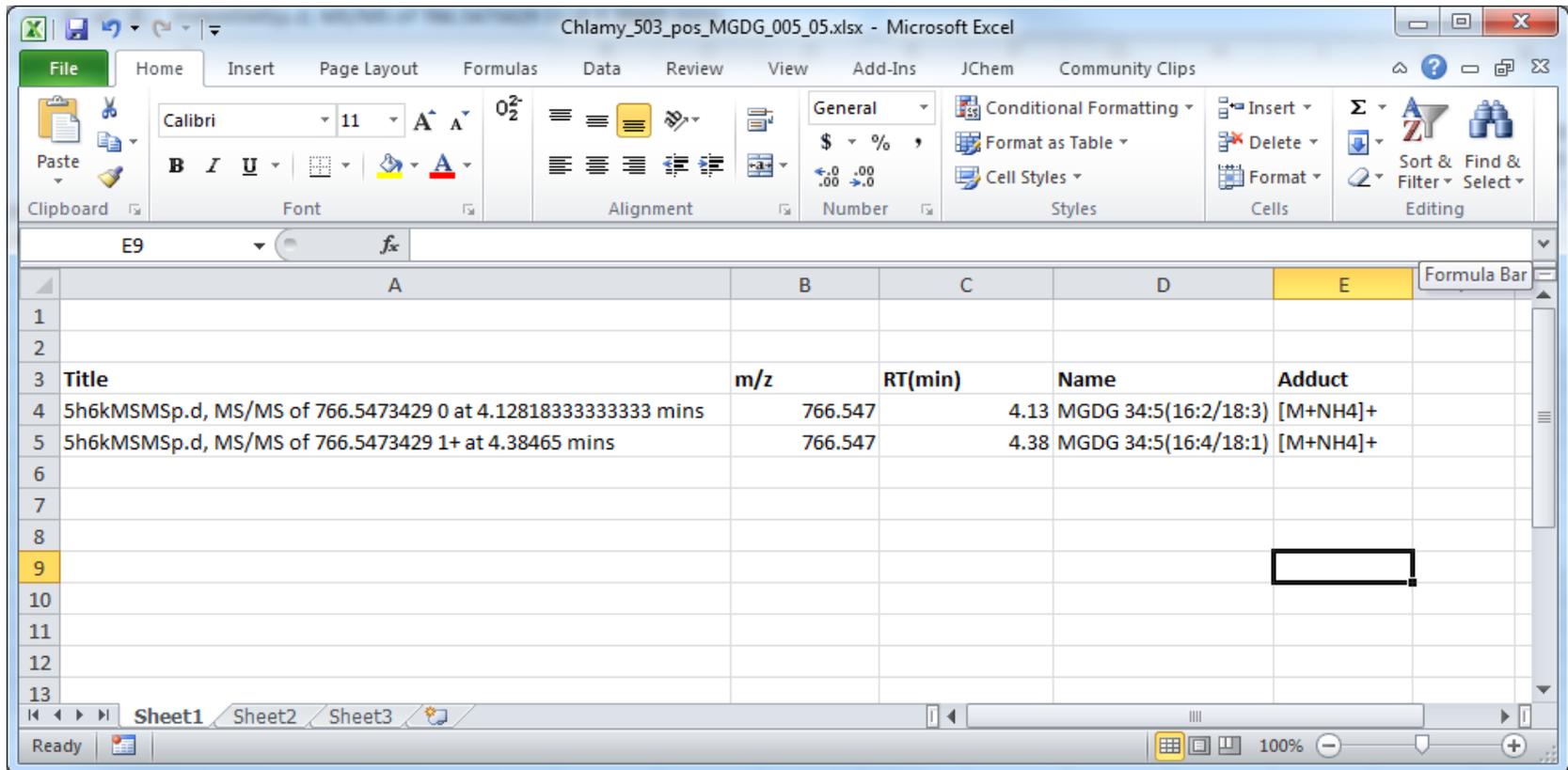
- Sort Smallest to Largest
- Sort Largest to Smallest
- Sort by Color
- Clear Filter From "932.631013"
- Filter by Color
- Number Filters
- Search
- (Select All)
- 0
- 1

Step 2: Using excel filters to annotate lipids

6. Write the result into a Excel file.

The following is an example of the report:

Report: Title, m/z(with 3 decimals, e.g. 766.547), RT(retention time, with 2 decimals, e.g. 4.13), Name of lipid, and Adduct



Chlamy_503_pos_MGDG_005_05.xlsx - Microsoft Excel

	A	B	C	D	E
1					
2					
3	Title	m/z	RT(min)	Name	Adduct
4	5h6kMSMSp.d, MS/MS of 766.5473429 0 at 4.12818333333333 mins	766.547	4.13	MGDG 34:5(16:2/18:3)	[M+NH4] ⁺
5	5h6kMSMSp.d, MS/MS of 766.5473429 1+ at 4.38465 mins	766.547	4.38	MGDG 34:5(16:4/18:1)	[M+NH4] ⁺
6					
7					
8					
9					
10					
11					
12					
13					

Step 2: Using excel filters to annotate lipids

TIPS:

MGDG, DGDG, DGTS, PE all have head groups and two acyl chains (same as the example).

Lyso-DGTS only has head group and one acyl chain, in this case, the acyl chain loss must be found in order to report.

DG and TG don't have head groups. Therefore,

DG: only look for the two acyl chain loss (both must be found)

TG: only look for the three acyl chain loss (at least two of them must be found)

Step3: Confirmation by checking retention time

If a RP column is used for the separation, among lipids in each lipid class, the retention times usually follow the following rule:

Retention times increase with the number of carbon, while decrease with the number of double bond.

This can be used as a further confirmation of the annotation.

Step3: Confirmation by checking retention time

For example

RT MGDG 34:0 < RT MGDG 36:0

RT DGDG 32:2 > RT DGDG 32:3

Quiz:

RT PE 34:1 ? RT PE 32:4

RT TG 50:4? RT DG 36:4

Step 4: Using NIST search for library validation

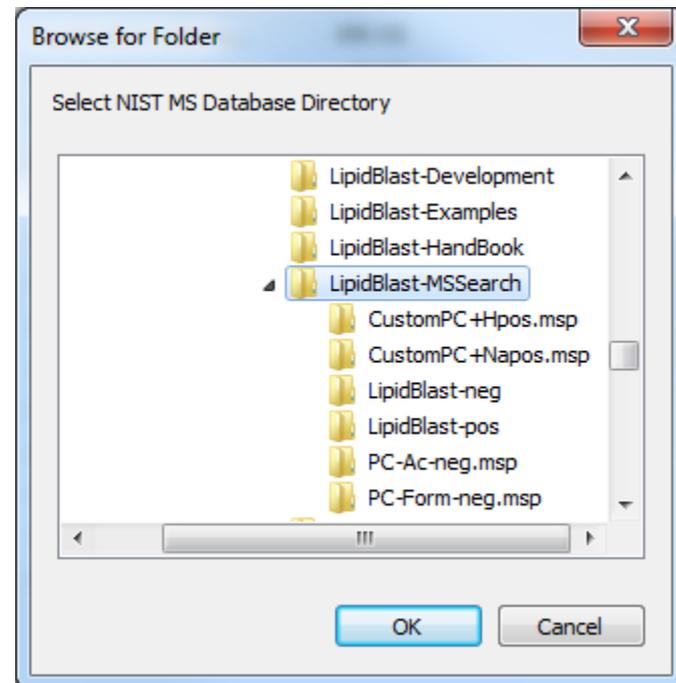
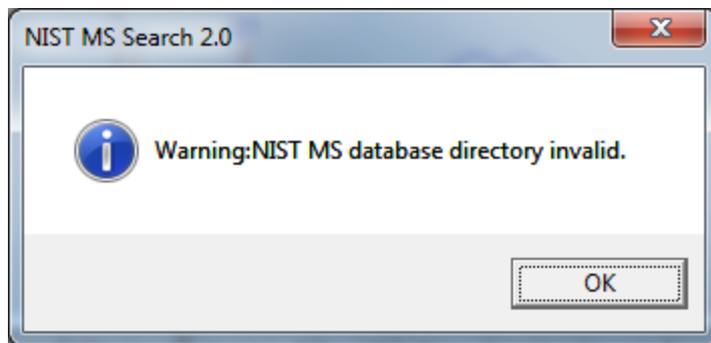
Now you have a list of potential lipid with its title and annotation, you can visualize the spectra in NIST search and search against available libraries to see if the annotation results match.

Here we use lipidblast library as an example.

Step 4: Using NIST search for library validation

1. Extract the LipidBlast-Full.zip file, and double click on the nistms.exe file in the LipidBlast-MSSearch folder.

When you open Nist search for the first time, it will give you a warning message. After clicking OK, a window pops up to ask you to select library directory. Here we just keep it highlighting LipidBlast-MSSearch and click OK, then the software will open.



Step 4: Using NIST search for library validation

2. Go to the import button, and select the MGF file where you have your lipids in.

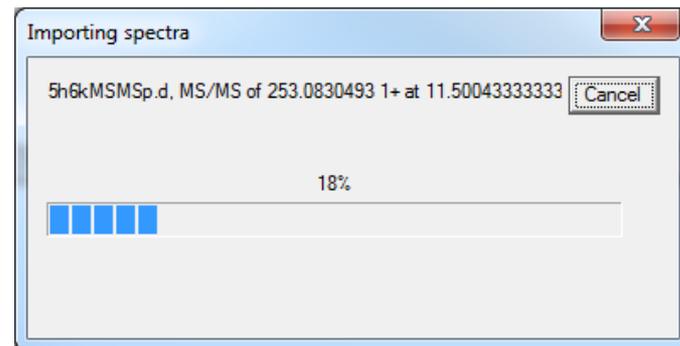
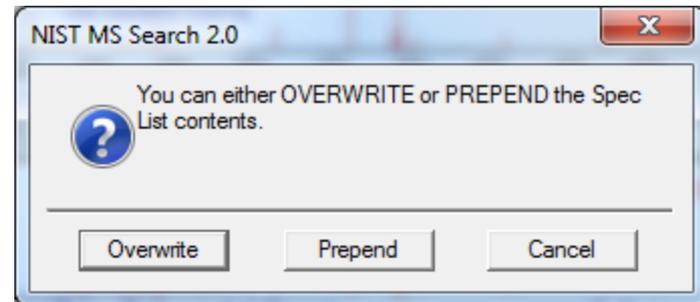
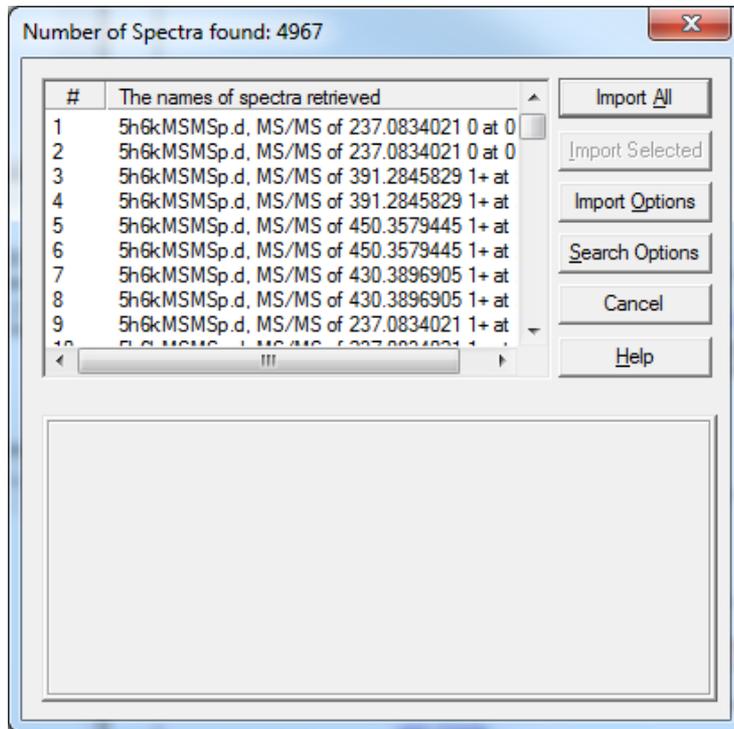
The screenshot shows the NIST MS Search 2.0 interface. The main window has a menu bar (File, Search, View, Tools, Options, Window, Help) and a toolbar with various icons. A red circle highlights the 'import' button (represented by a folder icon) in the toolbar. A blue box with the word 'import' is overlaid on the main window. Below the toolbar is a list of search results with columns for '#', 'Name', and 'Description'. The file selection dialog is open, showing the 'Look in' folder as 'POS'. The dialog contains a table of files:

Name	Date modified	Type	Size
combined_pos_2.mgf	10/22/2013 3:15 PM	MGF File	131,312 KB
combined_pos_3.mgf	10/22/2013 3:27 PM	MGF File	87,084 KB
combined_pos_4.mgf	10/22/2013 3:28 PM	MGF File	98,017 KB
pos_1A.mgf	10/7/2013 12:36 AM	MGF File	93,153 KB
pos_1B.mgf	10/7/2013 12:35 AM	MGF File	96,332 KB

The 'File name' field in the dialog contains 'pos_1A.mgf' and the 'Files of type' dropdown is set to 'All Files (*.*)'. The 'Open' button is highlighted.

Step 4: Using NIST search for library validation

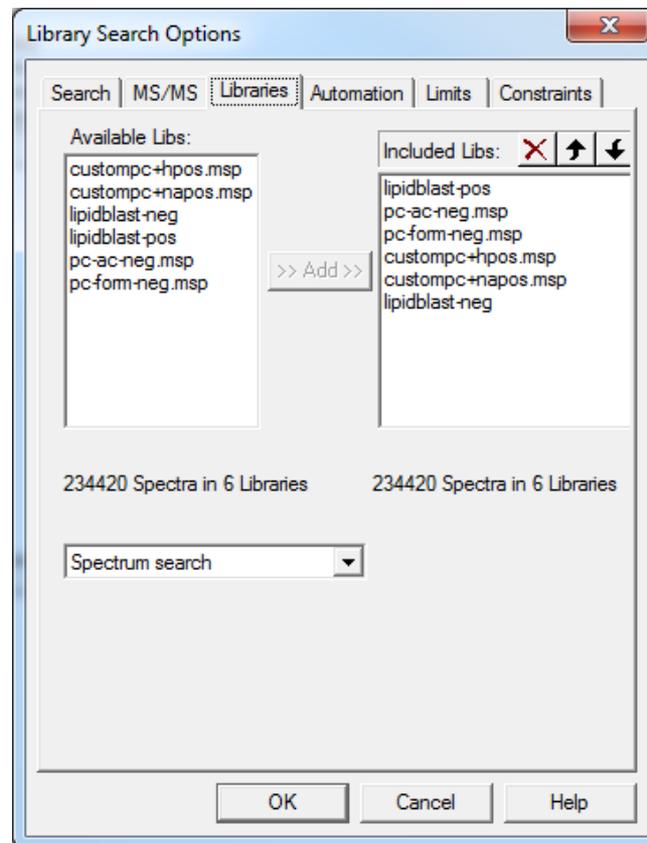
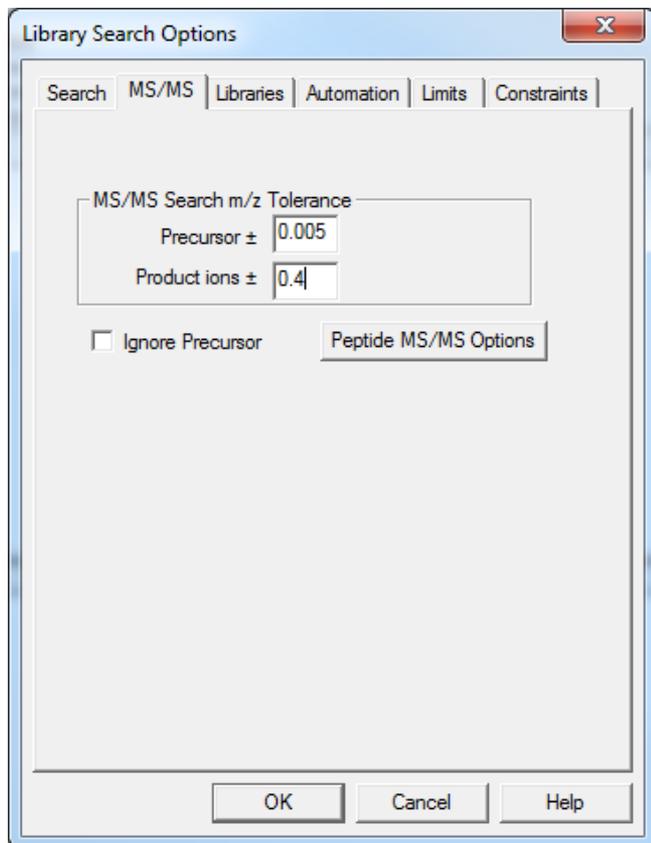
Click on "Import All" and in the next window, choose Overwrite or Prepend. It'll take some time to load all the spectra.



Step 4: Using NIST search for library validation

3. When the importing is done, go to the Library Search Options button, and set appropriate parameters.

For details, please refer to the user manual of lipidblast.

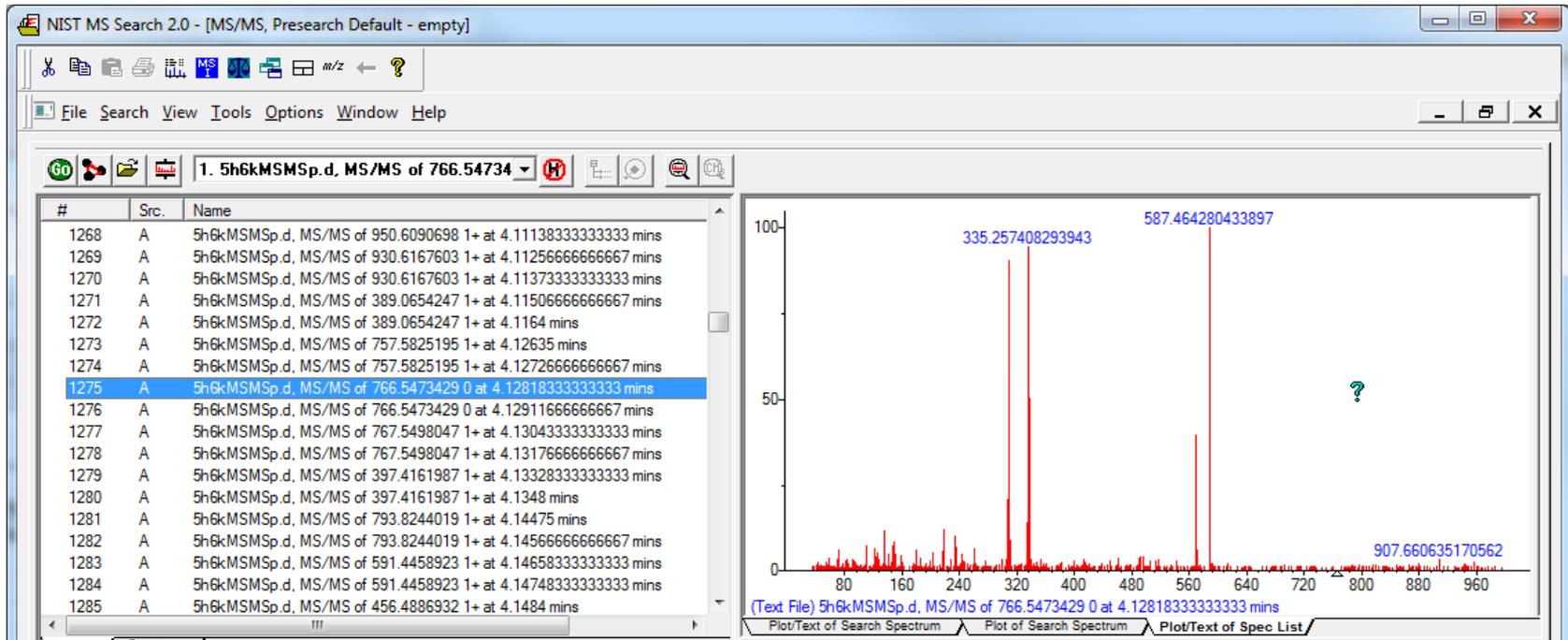


Step 4: Using NIST search for library validation

4. Scroll down in the upper-left window and find your potential lipids by its title (mainly RT, since RT is the increasing order).

Click on its title to show its spectra in the upper-right window.

Title	m/z	RT(min)	Name	Adduct
5h6kMSMSp.d, MS/MS of 766.5473429 0 at 4.128183333333333 mins	766.547	4.13	MGDG 34:5(16:2/18:3)	[M+NH4] ⁺



Step 4: Using NIST search for library validation

Double click on the title to search against libraries. Sometimes there's no good match in lipidblast because the specific lipid is not covered in lipidblast.

The screenshot displays the NIST MS Search 2.0 interface. The main window shows a search for a peptide with the title "1. 5h6kMMSp.d. MS/MS of 766.54734". The search results are displayed in a table with columns for #, Src, and Name. The top result is "1274 A 5h6kMMSp.d. MS/MS of 757.5825195 1+ at 4.12726666666667 mins".

Below the search results, there is a bar chart showing the distribution of spectra. The x-axis represents the number of spectra (0 to 1000), and the y-axis represents the number of spectra (1 to 1000). The chart shows a peak at approximately 1000 spectra.

The main search results table is as follows:

#	Src	Name
1274	A	5h6kMMSp.d. MS/MS of 757.5825195 1+ at 4.12726666666667 mins
1275	A	5h6kMMSp.d. MS/MS of 766.5473429 0 at 4.12818333333333 mins
1276	A	5h6kMMSp.d. MS/MS of 766.5473429 0 at 4.12911666666667 mins
1277	A	5h6kMMSp.d. MS/MS of 767.5498047 1+ at 4.13043333333333 mins
1278	A	5h6kMMSp.d. MS/MS of 767.5498047 1+ at 4.13176666666667 mins
1279	A	5h6kMMSp.d. MS/MS of 397.4161987 1+ at 4.13238333333333 mins
1280	A	5h6kMMSp.d. MS/MS of 397.4161987 1+ at 4.1348 mins
1281	A	5h6kMMSp.d. MS/MS of 793.8244019 1+ at 4.14475 mins
1282	A	5h6kMMSp.d. MS/MS of 793.8244019 1+ at 4.14566666666667 mins
1283	A	5h6kMMSp.d. MS/MS of 591.4458923 1+ at 4.14658333333333 mins
1284	A	5h6kMMSp.d. MS/MS of 591.4458923 1+ at 4.14748333333333 mins
1285	A	5h6kMMSp.d. MS/MS of 456.4886932 1+ at 4.1484 mins
1286	A	5h6kMMSp.d. MS/MS of 456.4886932 1+ at 4.14931666666667 mins

The interface also shows two mass spectra plots. The top plot is the "Plot of Search Spectrum" for the peptide, showing peaks at m/z 335.257408293943 and 587.464280433897. The bottom plot is the "Plot of Hit Spectrum" for the library entry "PE 38.4; [M-H]-; GPEn(18:3(6Z,9Z,12Z)/20:1(11E))", showing peaks at m/z 277.21662 and 474.26225. The library entry is highlighted in blue.

At the bottom of the interface, there is a table with columns for Lib, Score, Dot Pro..., Prob. (%), Rev-Dot, and Name. The table lists various library entries with their corresponding scores and names.

#	Lib	Score	Dot Pro...	Prob. (%)	Rev-Dot	Name
1	li	153	186	4.06	714	PE 38.4; [M-H]-; GPEn(18:3(6Z,9Z,12Z)/20:1(11E))
2	li	153	186	4.06	714	PE 38.4; [M-H]-; GPEn(18:3(6Z,9Z,12Z)/20:1(11Z))
3	li	153	186	4.06	714	PE 38.4; [M-H]-; GPEn(18:3(6Z,9Z,12Z)/20:1(13E))
4	li	153	186	4.06	714	PE 38.4; [M-H]-; GPEn(18:3(6Z,9Z,12Z)/20:1(13Z))
5	li	153	186	4.06	714	PE 38.4; [M-H]-; GPEn(18:3(9Z,12Z,15Z)/20:1(11E))
6	li	153	186	4.06	714	PE 38.4; [M-H]-; GPEn(18:3(9Z,12Z,15Z)/20:1(11Z))
7	li	153	186	4.06	714	PE 38.4; [M-H]-; GPEn(18:3(9Z,12Z,15Z)/20:1(13E))
8	li	153	186	4.06	714	PE 38.4; [M-H]-; GPEn(18:3(9Z,12Z,15Z)/20:1(13Z))
9	li	153	186	4.06	714	PE 38.4; [M-H]-; GPEn(20:1(11E)/18:3(6Z,9Z,12Z))
10	li	153	186	4.06	714	PE 38.4; [M-H]-; GPEn(20:1(11Z)/18:3(6Z,9Z,12Z))
11	li	153	186	4.06	714	PE 38.4; [M-H]-; GPEn(20:1(13E)/18:3(6Z,9Z,12Z))
12	li	153	186	4.06	714	PE 38.4; [M-H]-; GPEn(20:1(13Z)/18:3(6Z,9Z,12Z))
13	li	153	186	4.06	714	PE 38.4; [M-H]-; GPEn(20:1(13E)/18:3(9Z,12Z,15Z))
14	li	153	186	4.06	714	PE 38.4; [M-H]-; GPEn(20:1(13E)/18:3(9Z,12Z,15Z))
15	li	153	186	4.06	714	PE 38.4; [M-H]-; GPEn(20:1(13Z)/18:3(9Z,12Z,15Z))
16	li	153	186	4.06	714	PE 38.4; [M-H]-; GPEn(20:1(13Z)/18:3(9Z,12Z,15Z))
17	li	95	117	0.74	844	PE 38.4; [M-H]-; GPEn(18:2(6E,4E)/20:1(11Z,14Z))
18	li	95	117	0.74	844	PE 38.4; [M-H]-; GPEn(18:2(6E,4E)/20:2(5Z,8Z))
19	li	95	117	0.74	844	PE 38.4; [M-H]-; GPEn(18:2(6Z,9Z)/20:1(11Z,14Z))
20	li	95	117	0.74	844	PE 38.4; [M-H]-; GPEn(18:2(6Z,9Z)/20:2(5Z,8Z))
21	li	95	117	0.74	844	PE 38.4; [M-H]-; GPEn(18:2(9E,10E)/20:1(11Z,14Z))
22	li	95	117	0.74	844	PE 38.4; [M-H]-; GPEn(18:2(9E,10E)/20:2(5Z,8Z))
23	li	95	117	0.74	844	PE 38.4; [M-H]-; GPEn(18:2(9E,12E)/20:1(11Z,14Z))
24	li	95	117	0.74	844	PE 38.4; [M-H]-; GPEn(18:2(9E,12E)/20:2(5Z,8Z))
25	li	95	117	0.74	844	PE 38.4; [M-H]-; GPEn(18:2(9Z,11Z)/20:1(11Z,14Z))
26	li	95	117	0.74	844	PE 38.4; [M-H]-; GPEn(18:2(9Z,11Z)/20:2(5Z,8Z))

Step 4: Using NIST search for library validation

If the library search result match the MS2Analyzer result, then the annotation is further confirmed. Here's an example of good match.

Title	m/z	RT(min)	Name	Adduct
5h6kMSMSp.d, MS/MS of 586.5369873 1+ at 6.739 mins	586.537	6.74	DG 32:0(16:0/16:0)	[M+NH4] ⁺

NIST MS Search 2.0 - [Peptide, Research Default - 17 spectra]

File Search View Tools Options Window Help

1. 5h6kMSMSp.d, MS/MS of 586.5369873

Src. Name

2287	A	5h6kMSMSp.d, MS/MS of 552.434595 0 at 6.716583333333333 mins
2288	A	5h6kMSMSp.d, MS/MS of 552.434595 0 at 6.718133333333333 mins
2289	A	5h6kMSMSp.d, MS/MS of 553.4381104 1+ at 6.728666666666667 mins
2290	A	5h6kMSMSp.d, MS/MS of 553.4381104 1+ at 6.730166666666667 mins
2291	A	5h6kMSMSp.d, MS/MS of 628.5865479 1+ at 6.731916666666667 mins
2292	A	5h6kMSMSp.d, MS/MS of 628.5865479 1+ at 6.73365 mins
2293	A	5h6kMSMSp.d, MS/MS of 612.5553284 1+ at 6.73545 mins
2294	A	5h6kMSMSp.d, MS/MS of 612.5553284 1+ at 6.737233333333333 mins
2295	A	5h6kMSMSp.d, MS/MS of 586.5369873 1+ at 6.739 mins
2296	A	5h6kMSMSp.d, MS/MS of 586.5369873 1+ at 6.740766666666667 mins
2297	A	5h6kMSMSp.d, MS/MS of 654.6063232 1+ at 6.750716666666667 mins
2298	A	5h6kMSMSp.d, MS/MS of 654.6063232 1+ at 6.751633333333333 mins
2299	A	5h6kMSMSp.d, MS/MS of 371.0549708 1+ at 6.75235 mins

Names Structures Spec List

lipidblast-pos; pc-ac-neg.msp; pc-form-neg.msp; customcp-ppos.msp; customcp-nrpos.msp; lipidblast-neg; 234420 total spectra

#	Lib.	Score	Dot Pro...	Prob. (%)	Rev.Dot	Name
1	li	319	489	94.8	889	DG 32:0, [M+NH4] ⁺ , DG(16:0/16:0/0:0)
2	li	76	144	0.34	687	DG 32:0, [M+NH4] ⁺ , DG(14:0/18:0/0:0)
3	li	76	144	0.34	687	DG 32:0, [M+NH4] ⁺ , DG(18:0/14:0/0:0)
4	li	66	127	0.66	631	DG 32:0, [M+NH4] ⁺ , DG(15:0/17:0/0:0)
5	li	66	127	0.66	631	DG 32:0, [M+NH4] ⁺ , DG(17:0/15:0/0:0)
6	li	33	67	0.17	365	DG 32:0, [M+NH4] ⁺ , DG(12:0/20:0/0:0)
7	li	33	67	0.17	365	DG 32:0, [M+NH4] ⁺ , DG(20:0/12:0/0:0)
8	li	33	65	0.17	356	DG 32:0, [M+NH4] ⁺ , DG(8:0/24:0/0:0)
9	li	33	65	0.17	356	DG 32:0, [M+NH4] ⁺ , DG(13:0/19:0/0:0)
10	li	33	65	0.17	356	DG 32:0, [M+NH4] ⁺ , DG(19:0/13:0/0:0)
11	li	33	65	0.17	356	DG 32:0, [M+NH4] ⁺ , DG(24:0/8:0/0:0)
12	li	32	65	0.16	356	DG 32:0, [M+NH4] ⁺ , DG(9:0/23:0/0:0)
13	li	32	65	0.16	356	DG 32:0, [M+NH4] ⁺ , DG(23:0/9:0/0:0)
14	li	32	64	0.16	352	DG 32:0, [M+NH4] ⁺ , DG(10:0/22:0/0:0)
15	li	32	64	0.16	352	DG 32:0, [M+NH4] ⁺ , DG(22:0/10:0/0:0)
16	li	21	42	0.11	235	DG 32:0, [M+NH4] ⁺ , DG(11:0/21:0/0:0)
17	li	21	42	0.11	235	DG 32:0, [M+NH4] ⁺ , DG(21:0/11:0/0:0)

Names Structures Hit List

Lib. Search Other Search Names Compare Librarian

Peptide Peptide

Plot of Search Spectrum

Plot of Search Spectrum

Plot of Spec List

Difference Head to Tail Side by Side Subtraction

Head to Tail MF=319 RMF=489

DG 32:0, [M+NH4]⁺, DG(16:0/16:0/0:0)

319 489R 84.8P

Plot of Hit

Plot of Hit

DG 32:0, [M+NH4]⁺, DG(16:0/16:0/0:0)

Names Structures

MW: 586 [DB: 2363] DB: lipidblast-pos
Comment: Parent=586.54073 Mz_expect=586.54073; C35H68O5; [M+NH4]⁺; DG 32:0; DG(16:0/16:0/0:0)
3 largest peaks:
313.27410 999.00 | 551.52743 500.00 | 569.53799 200.00 |
3 m/z Values and Intensities:
313.27410 999.00 [M+NH4]⁺en1 | [M+NH4]⁺en2
551.52743 500.00 [M+NH4]⁺NH4+H2O (17-18)
569.53799 200.00 [M+NH4]⁺NH4 (17)
Synonyms:
no synonyms.

Names Structures

MW: N/A [DB: 2808] DB: Text File
Comment: Parent=586.5369873 CHARGE=1+ RTINSECONDS=404.34
10 largest peaks:
313.272450675758 999.00 | 551.498085796966 746.18 | 116.964630397103 100.31 | 195.03506296 35.0970631062332 59.86 | 239.24091277815 51.67 | 552.50775059238 50.33 | 95.081802816
Synonyms:
no synonyms.

That's it!

Thanks for using MS2Analyzer.

Feel free to email yanma@ucdavis.edu if you have any question and comment.