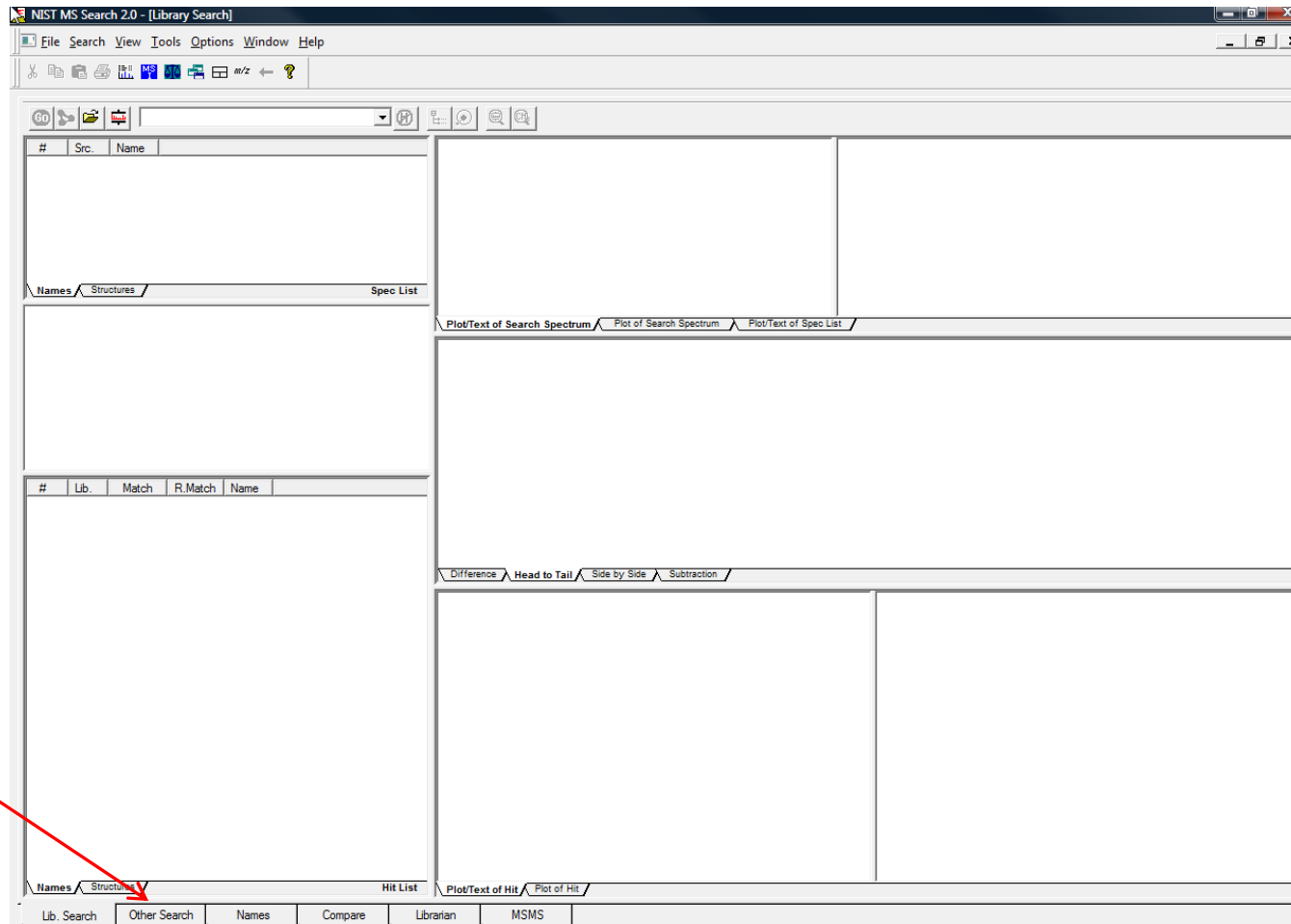


Using NIST Exact Mass Capabilities to Identify Known Unknowns

1. Used Version 2.0 g. build May 19, 2011
2. Select "Other Search" tab at bottom of page

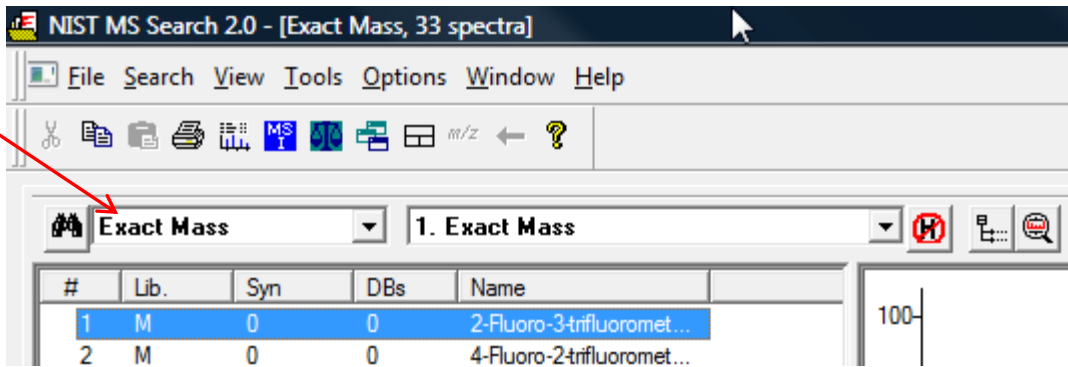
2



Using NIST Exact Mass Capabilities to Identify Known Unknowns

1. Select "Exact Mass" menu option from top left corner of menu

1



The screenshot shows the NIST MS Search 2.0 software interface. The title bar reads "NIST MS Search 2.0 - [Exact Mass, 33 spectra]". The menu bar includes "File", "Search", "View", "Tools", "Options", "Window", and "Help". The toolbar contains icons for various functions, including a search icon. The "Exact Mass" menu option is selected, and the search results table is displayed below. The table has columns for "#", "Lib.", "Syn", "DBs", and "Name". The first row is highlighted in blue and shows "# 1", "Lib. M", "Syn 0", "DBs 0", and "Name 2-Fluoro-3-trifluoromet...". The second row shows "# 2", "Lib. M", "Syn 0", "DBs 0", and "Name 4-Fluoro-2-trifluoromet...". A red arrow points from the number "1" to the "Exact Mass" menu option. A search input field on the right contains the number "100".

#	Lib.	Syn	DBs	Name
1	M	0	0	2-Fluoro-3-trifluoromet...
2	M	0	0	4-Fluoro-2-trifluoromet...

Using NIST Exact Mass Capabilities to Identify Known Unknowns

1. Enter accurate mass
2. Select appropriate uncertainty, mass error in ppm
3. Select Libraries tab
4. Select mainlib *only* as library to search
5. Select "OK" button
6. Select "OK" button

The image displays two screenshots of the NIST Exact Mass Search dialog box, illustrating the steps to identify known unknowns.

Left Screenshot (Step 1-3): The "Accurate Precursor Mass Search" tab is active. The search value is 308.104859, and the uncertainty is 5 ppm. The "Libraries" tab is selected, as indicated by arrow 3. The "OK" button is highlighted by arrow 6.

Right Screenshot (Step 4-5): The "Libraries" tab is active. The "Included Libs" list contains "mainlib", as indicated by arrow 4. The "OK" button is highlighted by arrow 5.

Using NIST Exact Mass Capabilities to Identify Known Unknowns

1. Add DB (Database) and Synonym Columns to Display by right clicking on window and selecting properties box
2. Select No. Synonyms and No. Other Databases boxes
3. Then OK

The left screenshot shows the NIST MS Search 2.0 interface with a list of search results. A context menu is open over the 'Properties' option, indicated by a red arrow labeled '1'. The right screenshot shows the same interface with a mass spectrum plot on the right and a 'Search (Others) Properties' dialog box open. The dialog box has 'No. Synonyms' and 'No. Other DBs' checked, and 'OK' is highlighted, indicated by red arrows labeled '2' and '3'.

#	Lib.	Name
1	M	2-Fluoro-3-trifluoromethylbenz...
2	M	4-Fluoro-2-trifluoromethylbenz...
3	M	3-Fluoro-4-trifluoromethylbenz...
4	M	2-Fluoro-6-trifluoromethylbenz...
5	M	Silane, diphenyldi(2-fluoroetho...
6	M	Phthalic acid, but-3-yn-2-yl 3-...
7	M	Acetic acid 4-(2-ethyl-benzofu...
8	M	Spiro[cyclopropane-1,9'-[9H]fl...
9	M	1,3,4,6-Hexanetetrone, 1-(4-m...
10	M	1,5-Diformyl-2,6-dimethoxy-9-...
11	M	3,6-Dihydroxy-7,8-dimethyl-2(...
12	M	1-Cyclopentene-3-carboxylic ...
13	M	Methyl 5-(4-biphenyloxy)meth...
14	M	2-(2-Butoxyethoxy)ethyl 2,2,3...
15	M	Warfarin

Search (Others) Properties

Structure View Options

Structure Size in %: 50

Structures Only

Items to Display

Order Number

Brief Origin Name

Full Origin Name

No Origin Name

No. Synonyms

No. Other DBs

Clear History on Exit

Color Settings

Bonds and Rings

Atomic Symbols

Compound Name

Font Settings

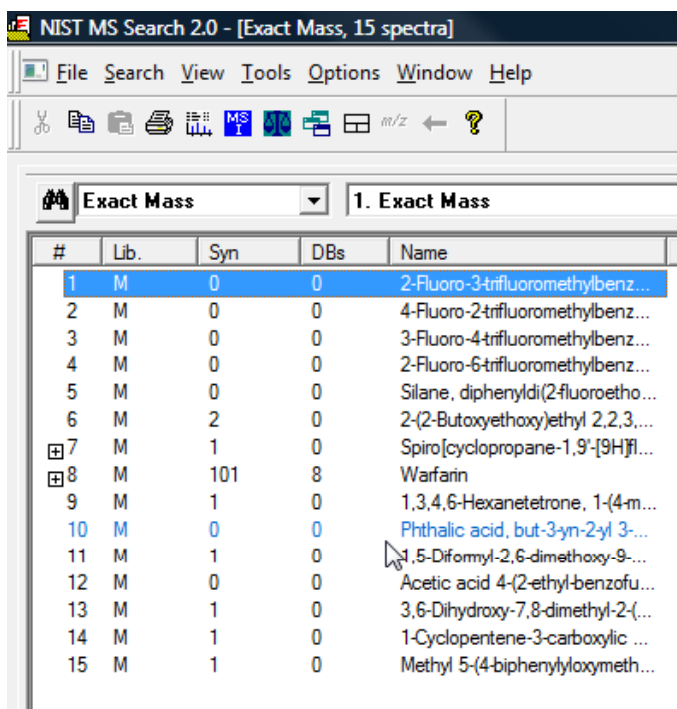
Select Font Set for all views

OK Cancel Apply Help

Using NIST Exact Mass Capabilities to Identify Known Unknowns

1. Then click to sort descending by either Syn or DBs column to get most useful results to top of list for consideration, sort by either Syn or DBs, I like Syn best

1

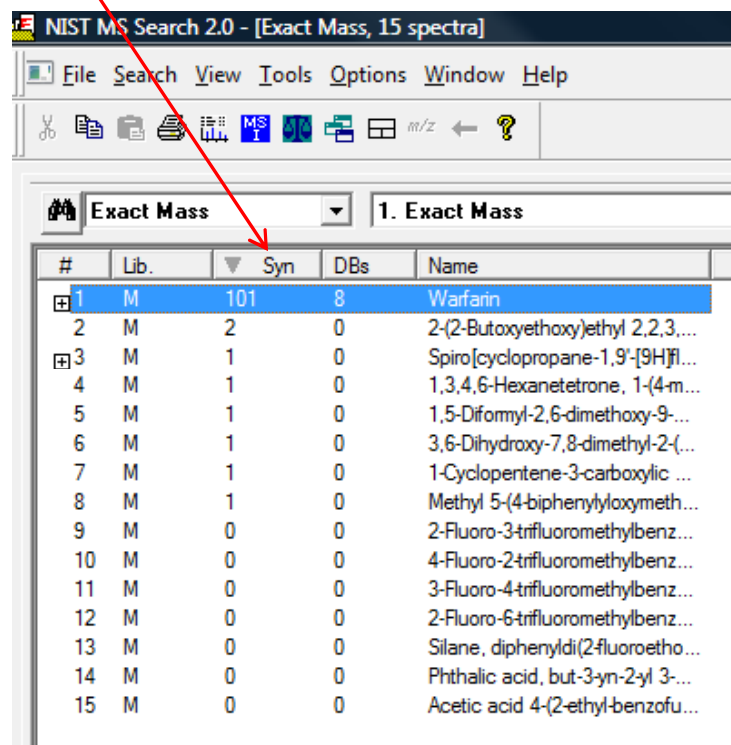


NIST MS Search 2.0 - [Exact Mass, 15 spectra]

File Search View Tools Options Window Help

Exact Mass 1. Exact Mass

#	Lib.	Syn	DBs	Name
1	M	0	0	2-Fluoro-3-trifluoromethylbenz...
2	M	0	0	4-Fluoro-2-trifluoromethylbenz...
3	M	0	0	3-Fluoro-4-trifluoromethylbenz...
4	M	0	0	2-Fluoro-6-trifluoromethylbenz...
5	M	0	0	Silane, diphenyldi(2-fluoroetho...
6	M	2	0	2-(2-Butoxyethoxy)ethyl 2,2,3...
7	M	1	0	Spiro[cyclopropane-1,9'-(9H)]f...
8	M	101	8	Warfarin
9	M	1	0	1,3,4,6-Hexanetetrone, 1-(4-m...
10	M	0	0	Phthalic acid, but-3-yn-2-yl 3-...
11	M	1	0	1,5-Difomyl-2,6-dimethoxy-9-...
12	M	0	0	Acetic acid 4-(2-ethyl-benzofu...
13	M	1	0	3,6-Dihydroxy-7,8-dimethyl-2-(...
14	M	1	0	1-Cyclopentene-3-carboxylic ...
15	M	1	0	Methyl 5-(4-biphenyloxy)meth...



NIST MS Search 2.0 - [Exact Mass, 15 spectra]

File Search View Tools Options Window Help

Exact Mass 1. Exact Mass

#	Lib.	Syn	DBs	Name
1	M	101	8	Warfarin
2	M	2	0	2-(2-Butoxyethoxy)ethyl 2,2,3...
3	M	1	0	Spiro[cyclopropane-1,9'-(9H)]f...
4	M	1	0	1,3,4,6-Hexanetetrone, 1-(4-m...
5	M	1	0	1,5-Difomyl-2,6-dimethoxy-9-...
6	M	1	0	3,6-Dihydroxy-7,8-dimethyl-2-(...
7	M	1	0	1-Cyclopentene-3-carboxylic ...
8	M	1	0	Methyl 5-(4-biphenyloxy)meth...
9	M	0	0	2-Fluoro-3-trifluoromethylbenz...
10	M	0	0	4-Fluoro-2-trifluoromethylbenz...
11	M	0	0	3-Fluoro-4-trifluoromethylbenz...
12	M	0	0	2-Fluoro-6-trifluoromethylbenz...
13	M	0	0	Silane, diphenyldi(2-fluoroetho...
14	M	0	0	Phthalic acid, but-3-yn-2-yl 3-...
15	M	0	0	Acetic acid 4-(2-ethyl-benzofu...