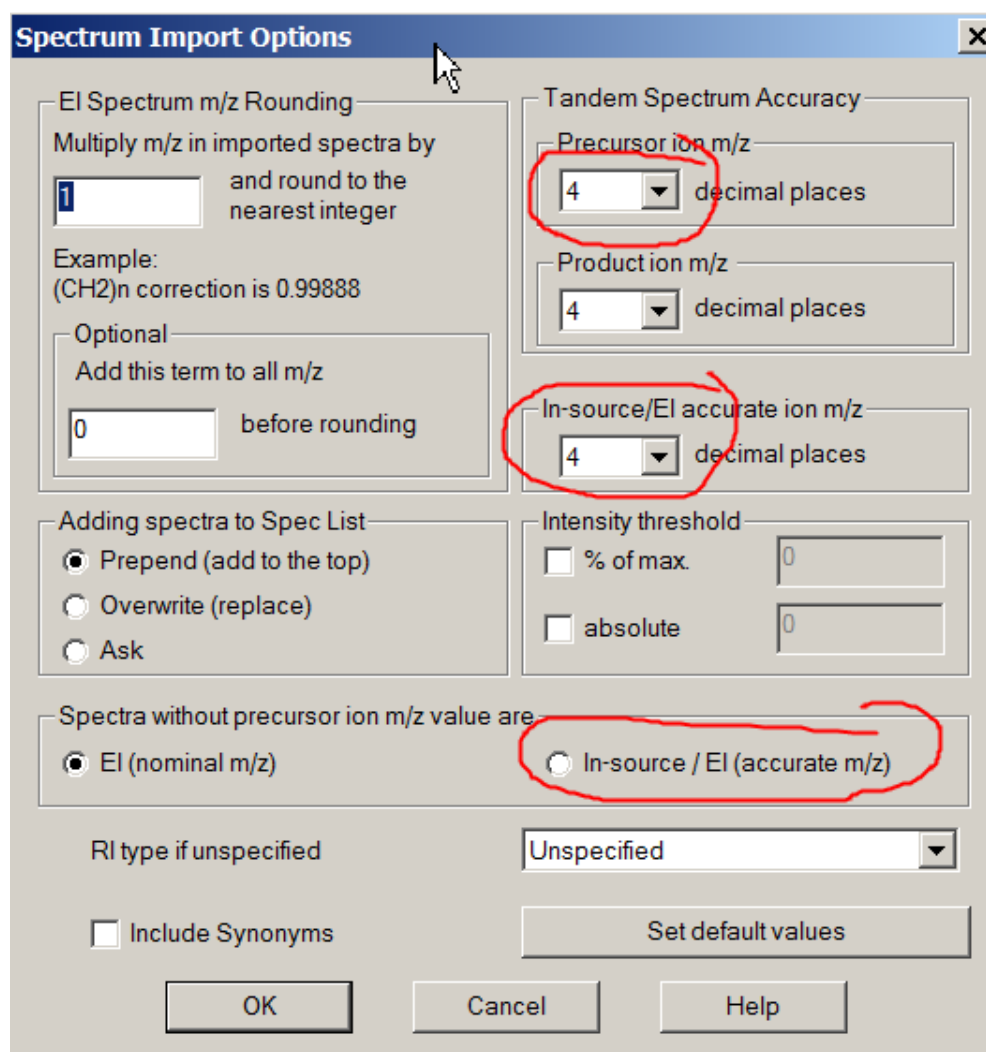
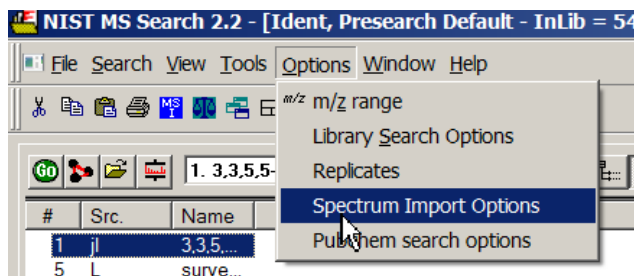


Accurate Mass Capabilities in NIST14 Search Software

- Ability to add accurate mass EI and MS/MS data to library
- No longer lose valuable accurate mass information in spectra
- Ability to limit the number of significant figures for m/z values for spectra added to library
- Other import options such as minimum intensity, append/overwrite/ask

New Spectrum Import Option Window Highlighting Accurate Mass Import Options



Example of Search of Accurate Mass Spectrum with Accurate Mass Library Result

NIST MS Search 2.2 - [Ident, Presearch Default - InLib = 818, 98 spectra]

File Search View Tools Options Window Help

1. 3,3,5,5-tetramethyl-4-((trimethylsilyloxy)tetrahydro-2H-pyran-2-one)

#	Src.	Name
1	jl	3,3,5...
2	jl	3,3,5...
6	L	surve...
7	L	surve...
8	L	surve...
9	L	surve...

Names Structures Spec List

mainlib, ecc: jl_user, new, palisade, wr10, wr10r, dd2014; 1182813 total spectra

Plot/Text of Search Spectrum Plot of Search Spectrum Spec List

(jl_user) 3,3,5,5-tetramethyl-4-((trimethylsilyloxy)tetrahydro-2H-pyran-2-one [in-source]

Name: 3,3,5,5-tetramethyl-4-((trimethylsilyloxy)tetrahydro-2H-pyran-2-one
 Formula: C₁₂H₂₄O₃Si
 MW: 244 Exact Mass: 244.149471 ID#: 3656 DB: jl_user
 Comment: Proposed Structure, A. Howard, J Little, June 2014
 Spectrum type: in-source
 Synonyms: no synonyms.

Head to Tail MF=999 RMF=999

3,3,5,5-tetramethyl-4-((trimethylsilyloxy)tetrahydro-2H-pyran-2-one

Difference Head to Tail Side by Side Subtraction

999 999R

#	Library	Match	R.Match	Name
1	jl_user	999	999	3,3,5...
2	new	852	858	HPH...
3	jl_user	852	858	3,3,5...
4	new	603	677	Prop...
5	jl_user	600	661	ADA...
6	jl_user	600	661	A2,2,4...
7	new	600	661	ADA...
8	new	600	661	A2,2,4...
9	jl_user	587	670	2,2,4...
10	new	587	670	2,2,4...
11	new	584	659	Prop...
12	jl_user	584	639	?2,2,4...
13	new	584	639	?2,2,4...
14	ecc	577	604	struct...
15	new	575	676	TMC...
16	jl_user	571	660	?mon...
17	jl_user	570	634	?Unk...
18	ecc	568	678	HTM...
19	new	568	609	2-met...
20	new	564	696	TMC...
21	new	564	654	ethyl (...)
22	ecc	563	759	1,1,3...
23	ecc	557	846	Partia...
24	ecc	557	561	??...

Names Structures InLib = 818, Hit List

Plot/Text of Hit Plot of Hit

(jl_user) 3,3,5,5-tetramethyl-4-((trimethylsilyloxy)tetrahydro-2H-pyran-2-one [in-source]

Name: 3,3,5,5-tetramethyl-4-((trimethylsilyloxy)tetrahydro-2H-pyran-2-one
 Formula: C₁₂H₂₄O₃Si
 MW: 244 Exact Mass: 244.149471 ID#: 3656 DB: jl_user
 Comment: Proposed Structure, A. Howard, J Little, June 2014
 Spectrum type: in-source
 Synonyms: no synonyms.

Example of Search of Accurate Mass Spectrum with Nominal Mass Library Result

NIST MS Search 2.2 - [Ident, Presearch Default - InLib = 818, 98 spectra]

File Search View Tools Options Window Help

1. 3,3,5,5-tetramethyl-4-((trimethylsilyloxy)tetrahydro-2H-pyran-2-one)

#	Src.	Name
1	jl	3,3,5...
2	jl	3,3,5...
6	L	surve...
7	L	surve...
8	L	surve...
9	L	surve...

Names / Structures / Spec List

mainlib; ecc; jl_user; new; palisade; wr10; wr10r; dd2014; 1182813 total spectra

#	Library	Match	R.Match	N...
1	jl_user	999	999	3...
2	new	852	858	H...
3	jl_user	852	858	3...
4	new	603	677	P...
5	jl_user	600	661	A...
6	jl_user	600	661	A...
7	new	600	661	A...
8	new	600	661	A...
9	jl_user	587	670	2...
10	new	587	670	2...
11	new	584	659	P...
12	jl_user	584	639	?...
13	new	584	639	?...
14	ecc	577	604	st...
15	new	575	676	T...
16	jl_user	571	660	?...
17	jl_user	570	634	?...
18	ecc	568	678	H...
19	new	568	609	2...
20	new	564	696	T...
21	new	564	654	et...
22	ecc	563	759	1...
23	ecc	557	846	P...
24	new	557	561	?...

InLib = 818, Hit List

Lib. Search | Other Search | Names | Compare | Librarian | MSMS

(jl_user) 3,3,5,5-tetramethyl-4-((trimethylsilyloxy)tetrahydro-2H-pyran-2-one) [in-source]

Plot/Text of Search Spectrum / Plot of Search Spectrum / Spec List

Name: 3,3,5,5-tetramethyl-4-((trimethylsilyloxy)tetrahydro-2H-pyran-2-one)
 Formula: C₁₂H₂₄O₃Si
 MW: 244 Exact Mass: 244.149471 ID#: 3656 DB: jl_user
 Comment: Proposed Structure. A. Howard, J Little, June 2014
 Spectrum type: in-source
 Synonyms: no synonyms.

(jl_user) 3,3,5,5-tetramethyl-4-((trimethylsilyloxy)tetrahydro-2H-pyran-2-one)

Plot/Text of Hit / Plot of Hit

Name: 3,3,5,5-tetramethyl-4-((trimethylsilyloxy)tetrahydro-2H-pyran-2-one)
 Formula: C₁₂H₂₄O₃Si
 MW: 244 Exact Mass: 244.149471 ID#: 3655 DB: jl_user
 Comment: MW confirmed by ammonia and methylamine CI. Molecular formula confirmed by accurate mass MS. A. Howard, J.Zewe, J.Little, June 2014
 Synonyms: no synonyms.

Example of Search of Accurate Mass MS/MS Spectrum with Standard Search

NIST MS Search 2.2 - [Quick, Presearch Definit - InLib = 617, 100 spectra]

File Search View Tools Options Window Help

1. Badge-BPA

#	Source	Name
1	nist_m...	1'-Hy...
2	nist_m...	1'-Hy...
3	msms...	Badg...
4	jl_user	3.3.5...
5	jl_user	3.3.5...
9	Spec...	surve...
10	Spec...	surve...
11	Spec...	surve...
12	Spec...	surve...

Names Structures Spec List

nist_msms: msms_neg.msms_pos.msms_pos_jl.wmsn1.msms_neg_jl.mwto2014; 219894 total spectra

#	Library	Match	R.Match	Prob. (...)	RI	N...
1	msms_p...	999	999	49.1	-	B...
2	msms_p...	999	999	49.1	-	B...
3	msms_p...	817	903	0.82	-	B...
4	msms_p...	817	903	0.82	-	B...
5	msms_p...	692	926	0.03	-	R...
6	msms_p...	692	926	0.03	-	R...
7	msms_p...	654	662	0.00	-	B...
8	msms_p...	654	662	0.00	-	B...
9	msms_p...	590	708	0.00	-	R...
10	msms_p...	590	708	0.00	-	R...
11	msms_p...	554	597	0.00	-	c...
12	msms_p...	554	597	0.00	-	c...
13	msms_p...	535	582	0.00	-	c...
14	msms_p...	535	582	0.00	-	c...
15	msms_p...	514	667	0.00	-	E...
16	msms_p...	514	667	0.00	-	E...
17	msms_p...	503	666	0.00	-	C...
18	msms_p...	503	666	0.00	-	C...
19	nist_msms	499	839	0.00	-	1...
20	msms_p...	463	960	0.00	-	R...
21	msms_p...	463	960	0.00	-	R...
22	nist_msms	447	841	0.00	-	F...

Names Structures InLib = 617, Hit List

Lib. Search Other Search Names Compare Librarian MSMS

(msms_pos_jl) Badge-BPA

Name: Badge-BPA
 Formula: C₃₆H₄₀O₆
 MW: 568 Exact Mass: 568.28249 ID#: 556 DB: msms_pos_jl
 Comment: see J Little Electronic notebook EX-233-118 for details; Component in Epon 82
 Instrument type: Q-TOF MS
 Spectrum type: ms2
 Precursor m/z: 586.3100
 Collision energy: 20 V
 Ionization: ESI
 10 largest peaks:
 135.0801 999.00 | 191.1064 508.27 | 419.2216 333.11 | 420.2248 137.07 | 136.0838 11
 475.2474 93.88 | 192.1098 74.99 | 586.3158 49.10 | 325.1795 48.52 | 476.2506 4
 Synonyms:
 no synonyms.

(msms_pos_jl) Badge-BPA

Name: Badge-BPA
 Formula: C₃₆H₄₀O₆
 MW: 568 Exact Mass: 568.28249 ID#: 556 DB: msms_pos_jl
 Comment: see J Little Electronic notebook EX-233-118 for details; Component in Epon 82
 Instrument type: Q-TOF MS
 Spectrum type: ms2
 Precursor m/z: 586.3100
 Collision energy: 20 V
 Ionization: ESI
 10 largest peaks:
 135.0801 999.00 | 191.1064 508.27 | 419.2216 333.11 | 420.2248 137.07 | 136.0838 11
 475.2474 93.88 | 192.1098 74.99 | 586.3158 49.10 | 325.1795 48.52 | 476.2506 4
 Synonyms:
 no synonyms.

Difference Head to Tail Side by Side Subtraction

Head to Tail MF=999 RMF=999

999 999R 49.1P

(msms_pos_jl) Badge-BPA

Name: Badge-BPA
 Formula: C₃₆H₄₀O₆
 MW: 568 Exact Mass: 568.28249 ID#: 556 DB: msms_pos_jl
 Comment: see J Little Electronic notebook EX-233-118 for details; Component in Epon 82
 Instrument type: Q-TOF MS
 Spectrum type: ms2
 Precursor m/z: 586.3100
 Collision energy: 20 V
 Ionization: ESI
 10 largest peaks:
 135.0801 999.00 | 191.1064 508.27 | 419.2216 333.11 | 420.2248 137.07 | 136.0838 11
 475.2474 93.88 | 192.1098 74.99 | 586.3158 49.10 | 325.1795 48.52 | 476.2506 4
 Synonyms:
 no synonyms.

Names Structures InLib = 617, Hit List

Lib. Search Other Search Names Compare Librarian MSMS

Library Search Option for MS/MS with Narrow Precursor Window for m/z 586.3100

Library Search Options

Search | MS/MS | Libraries | Automation | Limits | Constraints | RI (GC)

Spectrum Search Type
 Identity Similarity
MS/MS

Precursor Ion m/z
 in spectrum 586.3100

Spectrum Search Options
 Reverse Search
 Penalize rare compounds

Presearch
 Default Fast Off
 MW 315

Other Options
 Automation
 Auto Report
 Apply Limits
 Use Constraints

Structure Similarity Search Options
 Match Number of Rings Show Homologues

OK Cancel Help

Library Search Options

Search | MS/MS | Libraries | Automation | Limits | Constraints | RI (GC)

MS/MS and In-source HiRes search options

Search m/z Tolerance
Precursor \pm 20 ppm
Productions \pm 0.8 m/z

Ignore Precursor More Options
 Use alt. peak matching

Scoring
 Peptide

OK Cancel Help

Library Search Option for MS/MS with Narrow Precursor Window for m/z 586.3100 Yielding Fewer Results

NIST MS Search 2.2 - [MS/MS, Presearch Default - 8 spectra]

File Search View Tools Options Window Help

1. Badge-BPA

#	Source	Name
1	nist_m...	1-Hy...
2	nist_m...	1-Hy...
3	msms...	Badg...
4	j_user	3,3,5...
5	j_user	3,3,5...
9	Spec...	surve...
10	Spec...	surve...
11	Spec...	surve...
12	Spec...	surve...

Names / Structures / Spec List

nist_msms: msms_neg; msms_pos; msms_pos_jl; wmsn1; msms_neg_jl; mwtx2014; 219894 total spectra

#	Library	Score	DotPro...	Prob. (...)	N...
1	msms_p...	999	999	99.0	B...
2	msms_p...	999	999	99.0	B...
3	msms_p...	803	942	99.0	B...
4	msms_p...	802	942	99.0	B...
5	msms_p...	657	884	99.0	B...
6	msms_p...	656	884	99.0	B...
7	msms_p...	448	764	0.99	c...
8	msms_p...	446	763	0.99	c...

Names / Structures / Hit List

Lib. Search Other Search Names Compare Librarian MSMS

(msms_pos_jl) Badge-BPA

Plot/Text of Search Spectrum / Plot of Search Spectrum / Spec List

Name: Badge-BPA
Formula: C₃₆H₄₀O₆
MW: 568 Exact Mass: 568.28249 ID#: 556 DB: msms_pos_jl
Comment: see J Little Electronic notebook EX-233-118 for details; Component in Epon 82
Instrument type: Q-TOF MS
Spectrum type: ms2
Precursor m/z: 586.3100
Collision energy: 20 V
Ionization: ESI
10 largest peaks:
135.0801 999.00 | 191.1064 508.27 | 419.2216 333.11 | 420.2248 137.07 | 136.0838 11
475.2474 93.88 | 192.1098 74.99 | 586.3158 49.10 | 325.1795 48.52 | 476.2506 4
Synonyms:
no synonyms.

(msms_pos_jl) Badge-BPA

Plot/Text of Hit / Plot of Hit /

Name: Badge-BPA
Formula: C₃₆H₄₀O₆
MW: 568 Exact Mass: 568.28249 ID#: 556 DB: msms_pos_jl
Comment: see J Little Electronic notebook EX-233-118 for details; Component in Epon 82
Instrument type: Q-TOF MS
Spectrum type: ms2
Precursor m/z: 586.3100
Collision energy: 20 V
Ionization: ESI
10 largest peaks:
135.0801 999.00 | 191.1064 508.27 | 419.2216 333.11 | 420.2248 137.07 | 136.0838 11
475.2474 93.88 | 192.1098 74.99 | 586.3158 49.10 | 325.1795 48.52 | 476.2506 4
Synonyms:
no synonyms.

Difference Head to Tail (Side by Side) Subtraction / 999 999R 99.0P