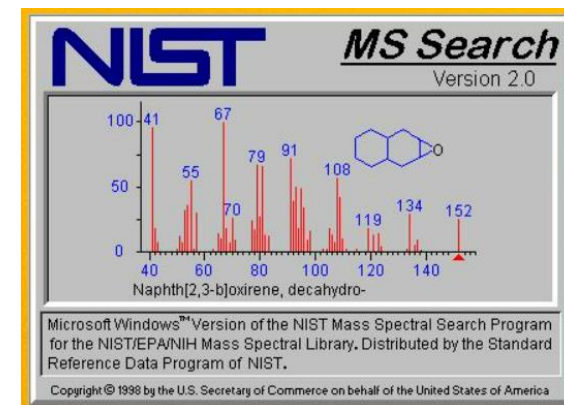


Creazione di una libreria con NIST MS Search

Davide Facciabene
Product Specialist GC & GC-MS



Per la creazione di una libreria personalizzata, bisogna tener presente che:

- 1) Non è possibile modificare e quindi aggiungere spettri di massa alle librerie precaricate, tipo la Mainlib
- 2) E' necessario utilizzare cromatogrammi con picchi intensi, ben definiti e senza coeluzioni, quindi bisogna iniettare qualche ppm di standard, ed acquisiti con range di scan larghi che coprono tutto lo spettro di massa del principio attivo in esame

NIST MS Search...

The screenshot displays the NIST MS Search 2.3 interface. At the top, the window title is "NIST MS Search 2.3 - [Ident, Presearch Default - InLib = -984, 100 spectra]". The main area is divided into several sections:

- File Search View Tools Options Window Help:** The top menu bar.
- File List:** Shows two files: "1. BLK01#1909 RT: 5.40 AV: 1 SB: 1" and "2. (Text File) BLK01#1908 RT: 5.40 AV: 1 S...".
- Mass Spectra:** A plot comparing the sample spectrum (top) with a library reference spectrum (bottom). The x-axis is m/z (0-220) and the y-axis is relative intensity (0-100). The sample spectrum has a base peak at m/z 91. The library reference spectrum for Toluene also has a base peak at m/z 91 and other characteristic peaks at 39, 51, 65, 77, 103, 131, 146, 164, and 182.
- Search Results:** A list of hits for "Toluene" with columns for retention time (RT), abundance (AV), and name. The top hit is "656 802 763 Toluene".
- Library Entry:** Detailed information for Toluene, including formula (C₇H₈), molecular weight (92), exact mass, CAS#, NIST#, ID#, and DB. It also lists synonyms: 1. Benzene, methyl; 2. Methacide; 3. Methylbenzene; 4. Methylbenzol; 5. Phenylmethane.
- Chemical Structure:** A skeletal structure of Toluene (a benzene ring with a methyl group) is shown.

At the bottom, there are tabs for "Lib. Search", "Other Search", "Names", "Compare", "Librarian", and "MSMS". The status bar at the very bottom indicates "For Help, press F1" and "Ident".

Schermata di partenza, in cui si arriva mediante esportazione dello spettro di massa per eseguire un' identificazione, utilizzando un software CDS, quale ad esempio Chromeleon, QualBrowser di Xcalibur/TraceFinder o il Qualitative di MassHunter.

NIST MS Search...

NIST MS Search 2.3 - [Ident, Presearch Default - InLib = -984, 100 spectra]

File Search View Tools Options Window Help

1. BLK01#1909 RT: 5.40 AV: 1 SB: 1

1 (Text File) BLK01#1909 RT: 5.40 AV: 1 S... 2 (Text File) BLK01#1908 RT: 5.40 AV: 1 S...

Names Structures Spec List

mainlib: replib. 346115 total spectra

Lib.	Match	R.Match	RI	Name
R	710	851	763	Toluene
R	695	849	763	Toluene
R	694	854	772	Spiro[2.4]hepta-4,6-diene
R	693	848	772	1,3,5-Cycloheptatriene
M	690	836	-	1,3,5-Cycloheptatriene
M	690	738	-	3-Benzylsulfanyl-3-fluoro-2-trifluoromethyl-acrylonitrile
R	687	825	772	1,3,5-Cycloheptatriene
M	674	836	-	Cyclobutene, 2-propenylidene-
M	673	813	-	Toluene
M	671	812	-	Spiro[2.4]hepta-4,6-diene
R	659	815	689	2,5-Norbornadiene
M	656	821	-	1,6-Heptadien-3-yne
R	656	802	763	Toluene
M	656	681	-	(1,3,3,3-Tetrafluoro-2-trifluoromethyl-propenylsulfanyl)met
M	656	667	-	3-Benzylsulfanyl-3-fluoro-2-trifluoromethyl-acrylic acid me
M	654	838	-	Propanal dibenzyl acetal
R	650	794	763	Toluene
R	650	790	763	Toluene
M	646	805	-	Spiro[3.3]hepta-1,5-diene
R	643	815	-	1,6-Heptadien-3-yne
R	643	794	1...	Benzeneacetamide
R	642	779	763	Toluene
R	629	790	1...	Benzeneacetaldehyde
M	626	757	-	Tetracyclo[3.2.0.0(2.7).0(4.6)]heptane

Names Structures Spec List

InLib = -984, Hit List

Lib. Search Other Search Names Compare Librarian MSMS

For Help, press F1

Ident Ident

Name: BLK01#1909 RT: 5.40 AV: 1 SB: 114 5.21-5.35 , 5.44-5.59
MW: N/A ID# 9 DB: Text File
Comment: T: {0,0} + c EI Full ms [45.00-230.00]
10 largest peaks:
91 999 | 51 489 | 92 422 | 65 197 | 63 146 |
46 82 | 45 74 | 131 62 | 62 54 | 50 52 |
Synonyms:
no synonyms.

(Text File) BLK01#1909 RT: 5.40 AV: 1 SB: 114 5.21-5.35 , 5.44-5.59

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

Name: Toluene
Formula: C₇H₈
MW: 92 Exact Mass: 92.0626 CAS# 108-88-3 NIST# 19587 ID# 15228 DB: replib
Other DBs: Fine, TSCA, RTECS, EPA, HODOG, NIH, EINECS, IRDB
InChIKey: YXFVVABEGXRONW-CHFFPAOYSA-N Non-stereo
10 largest peaks:
91 999 | 92 778 | 39 199 | 65 142 | 51 103 |
63 95 | 50 60 | 89 56 | 93 55 | 27 52 |
Synonyms:
1. Benzene, methyl
2. Methacide
3. Methylbenzene
4. Methylbenzol
5. Toluene

BLK01#1909 RT: 5.40 AV: 1 SB: 114 5.21-5.35 , 5.44-5.59 Head to Tail MF=710 RMF=851 Toluene

Difference Head to Tail Side by Side Subtraction / 710 851R 20.6P 763RI

(replib) Toluene

Plot/Text of Hit Plot of Hit /

COPIARE IL CAS NUMBER

NIST MS Search...

The screenshot displays the NIST MS Search 2.3 interface. On the left, a list of search results is shown:

#	Src.	Name
1	A	BLK01#1909 RT: 5.40 AV: 1 SB: 114 5.21-5.35
2	A	BLK01#1908 RT: 5.40 AV: 1 SB: 160 5.53-5.73
3	A	BLK01#1883 RT: 5.33 AV: 1 SB: 160 5.53-5.73
4	L	+EI Scan (rt 38.20 min) IPA NATIV.D
5	L	Caffeine
6	L	Theobromine
7	L	Xanthine

The main area shows a mass spectrum plot with the x-axis labeled 'm/z' ranging from 40 to 230 and the y-axis representing relative intensity from 0 to 100. The base peak is at m/z 91. Other significant peaks are labeled at m/z 46, 51, 65, 131, 157, 161, 166, 170, 175, 180, 184, 189, 195, 201, 205, 209, 219, and 223. A green question mark is visible on the plot.

Below the plot, the following text is displayed:

(Text File) BLK01#1909 RT: 5.40 AV: 1 SB: 114 5.21-5.35 5.44-5.59
[Name](#): BLK01#1909 RT: 5.40 AV: 1 SB: 114 5.21-5.35 5.44-5.59
[MW](#): N/A [ID#](#): 9 [DB](#): Text File
[Comment](#): T: (0,0) +c EI Full ms [45.00-230.00]
[10 largest peaks](#):
91 999 | 51 489 | 92 422 | 65 197 | 63 146 |
46 82 | 45 74 | 131 62 | 62 54 | 50 52 |
[Synonyms](#):
no synonyms.

A callout box with the text "SPOSTARSI SULLA SCHEDE LIBRARIAN" points to the "Librarian" button in the bottom navigation bar. The "Librarian" button is circled in red.

NIST MS Search...

The screenshot displays the NIST MS Search 2.3 interface. On the left, a table lists search results:

#	Src.	Name
1	A	BLK01#1909 RT: 5.40 AV: 1 SB: 114 5.21-5.35 ..
2	A	BLK01#1908 RT: 5.40 AV: 1 SB: 160 5.53-5.73 ..
3	A	BLK01#1883 RT: 5.33 AV: 1 SB: 160 5.53-5.73 ..
4	L	+EI Scan (rt. 38.20 min) IPA NATIV.D
5	L	Caffeine
6	L	Theobromine
7	L	Xanthine

The main area shows a mass spectrum plot for the selected entry (BLK01#1909). The x-axis represents m/z from 100 to 230, and the y-axis represents relative intensity from 50 to 100. The base peak is at m/z 91. Other labeled peaks include 51, 97, 102, 107, 111, 117, 122, 131, 139, 144, 157, 161, 166, 170, 175, 180, 184, 189, 195, 201, 205, 209, 219, and 223.

A text box with the text "PREMERE IL TASTO EDIT SPECTRUM" is overlaid on the plot area, with an arrow pointing to the 'Edit Spectrum' icon (a document with a pencil) in the toolbar.

Below the plot, the following information is displayed:

(Text File) BLK01#1909 RT: 5.40 AV: 1 SB: 114 5.21-5.35 , 5.44-5.59
[Name](#): BLK01#1909 RT: 5.40 AV: 1 SB: 114 5.21-5.35 , 5.44-5.59
[MW](#): N/A [ID#](#): 9 [DB](#): Text File
[Comment](#): T: (0,0) +c EI Full ms [45.00-230.00]
[10 largest peaks](#):
91 999 | 51 489 | 92 422 | 65 197 | 63 146 |
46 82 | 45 74 | 131 62 | 62 54 | 50 52 |
[Synonyms](#):
no synonyms.

At the bottom, there are navigation tabs: Names / Structures / Spec List / Plot/Text / Plot / Lib. Search / Other Search / Names / Compare / Librarian / MSMS.

NIST MS Search...

Spectrum Information

Name

Formula

Mol. Weight CAS Number

Library

ID Number

RI

Other Names (Synonyms)

Comments

T: {0,0} + c EI Full ms [45.00-230.00]

Peak information

m/z	Abund.	Annotation
45	74	
46	82	
50	52	
51	100	
55		
56		
57		
60		
61		

INSERIRE IL NOME ED IL
CAS NUMBER
PRECEDENTEMENTE
COPIATO

NIST MS Search...

Spectrum Information

Name

Formula

Mol. Weight CAS Number

Library Text File

ID Number 9

RI

Other Names (Synonyms)

Comments
T: {0,0} + c EI Full ms [45.00-230.00]

Peak information

m/z	Abund.	Annotation
45	74	
46	82	
50	52	
51	489	
55		
56		
57		
60		
61		

No structure

INSERIRE IL NOME ED IL
CAS NUMBER
PRECEDENTEMENTE
COPIATO

NIST MS Search...

Spectrum Information

Name: Toluene

Formula: From structure

Mol. Weight: 0 CAS Number: 108-88-3

Library: Text File ID Number: 9

RI: Edit RI

Other Names (Synonyms):

Comments: T: {0,0} + c EI Full ms [45.00-230.00]

Peak information

m/z	Abund.	Annotation
45	74	
46	82	
50	52	
51	489	
55	7	
56	11	
57	15	
60	15	
61	30	

Accept HiRes Spectrum Peaks 95

Attach Struct

Clipboard Struct

No structure

Exit Add to Library Replace Add to List Help

CLICCARE SUL PULSANTE
ATTACH STRUCT

NIST MS Search...

Spectrum Information

Name: Toluene

Formula: From structure

Mol. Weight: 0 CAS Number: 108-88-3

Library: Text File ID Number: 9

RI: Edit RI

Other Names (Synonyms):

Comments: T: {0,0} + c EI Full ms [45.00-230.00]

Peaks: 95

Attach Struct
Clipboard Struct

No structure

Exit Add to Library Replace Add to List Help

CLICCARE SUL PULSANTE FROM MAIN PER INSERIRE L'IMMAGINE DELLA FORMULA

NIST MS Search 2.3

Structure for CAS=108-88-3 is in the Main Library. Use this structure or attach another one ?

From Main Another Cancel

NIST MS Search...

Spectrum Information

Name

Formula

Mol. Weight CAS Number

Library

Peak information

m/z	Abund.	Annotation
45	74	
46	82	
50	52	
51	489	
55	7	
56	11	
57	15	
60	15	
61	30	

HiRes Spectrum Peaks 95

Cc1ccccc1

MAINLIB via CAS number

IL COMPOSTO ERA GIA
PRESENTE NELLA
LIBRERIA NIST,
IN QUESTO MODO HO
COLLEGATO L'IMMAGINE

IMMAGINE

NIST MS Search...

Spectrum Information

Name: Toluene

Formula: From structure

Mol. Weight: 0 CAS Number: 0

Library: Spec. List ID Number: 3 RI:

Other Names (Synonyms):

Comments: T: {0,0} + c EI Full ms [45.

Peak information

m/z	Abund.	Annotation
45	74	
46	82	

Choose library to save to

List of libraries

- custom
- test

RI type if unspecified: Unspecified

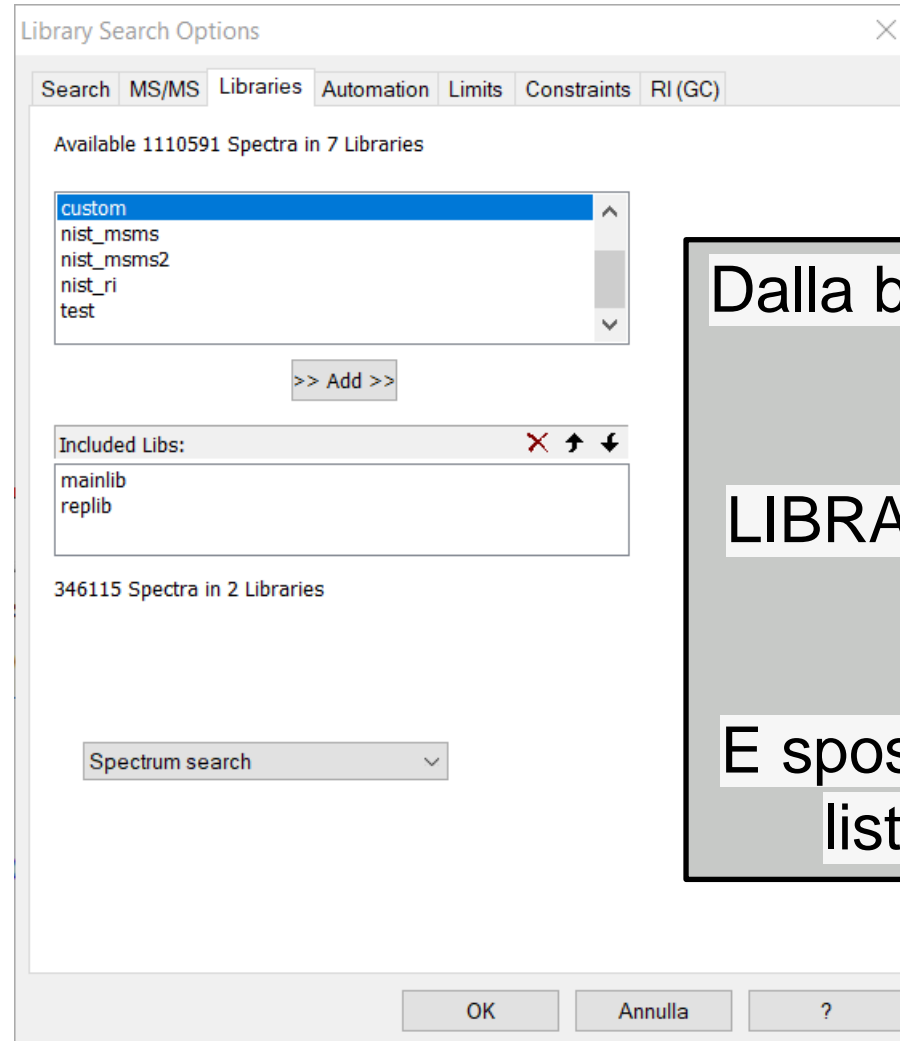
Library Statistics

- Spectra
- ID Range

Buttons: Exit, Add to Library, Replace, Add to List, Help

**CLICCARE SUL PULSANTE
Add to Library e digitare il
nome della libreria o
selezionarla dalla lista se già
presente**

NIST MS Search...

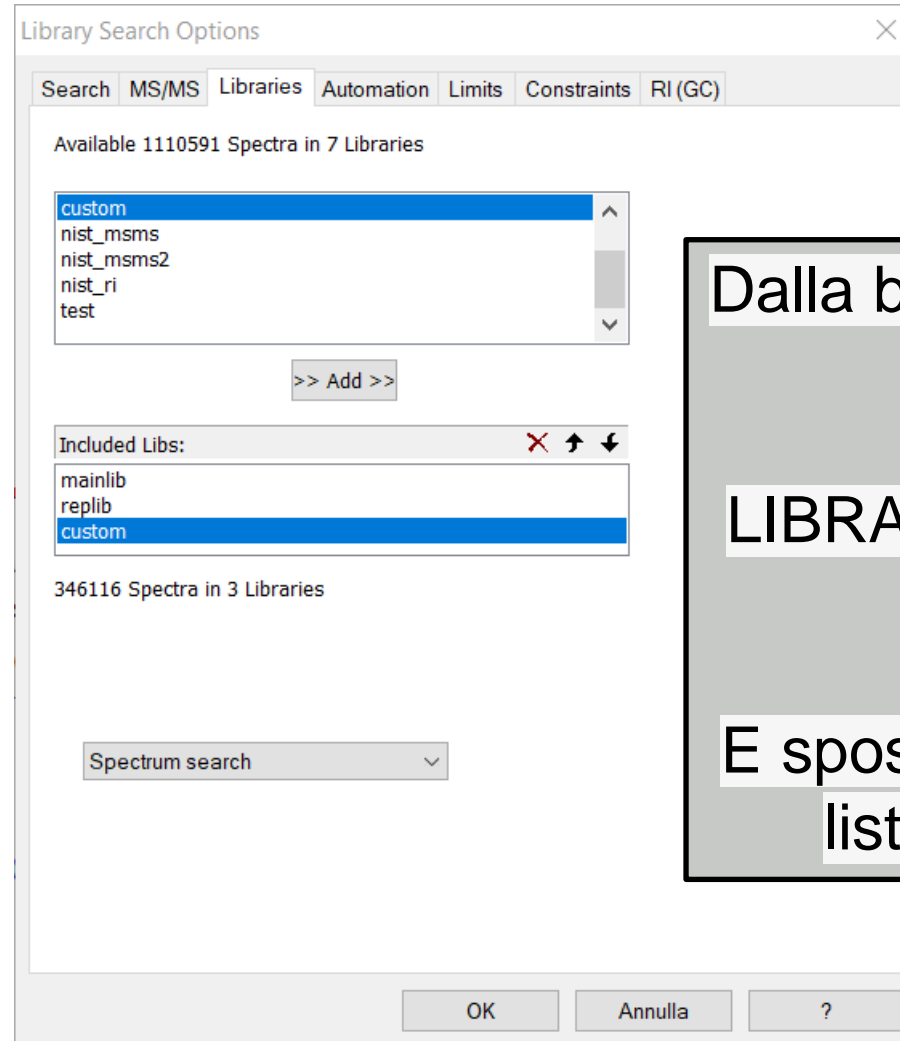


Dalla barra dei menu, cliccare su:

OPTIONS >
LIBRARY SEARCH OPTIONS >
LIBRARIES

E spostare la nuova libreria nella
lista attiva (Included Libs)

NIST MS Search...



Dalla barra dei menu, cliccare su:

OPTIONS >
LIBRARY SEARCH OPTIONS >
LIBRARIES

E spostare la nuova libreria nella
lista attiva (Included Libs)

Grazie per l'attenzione

