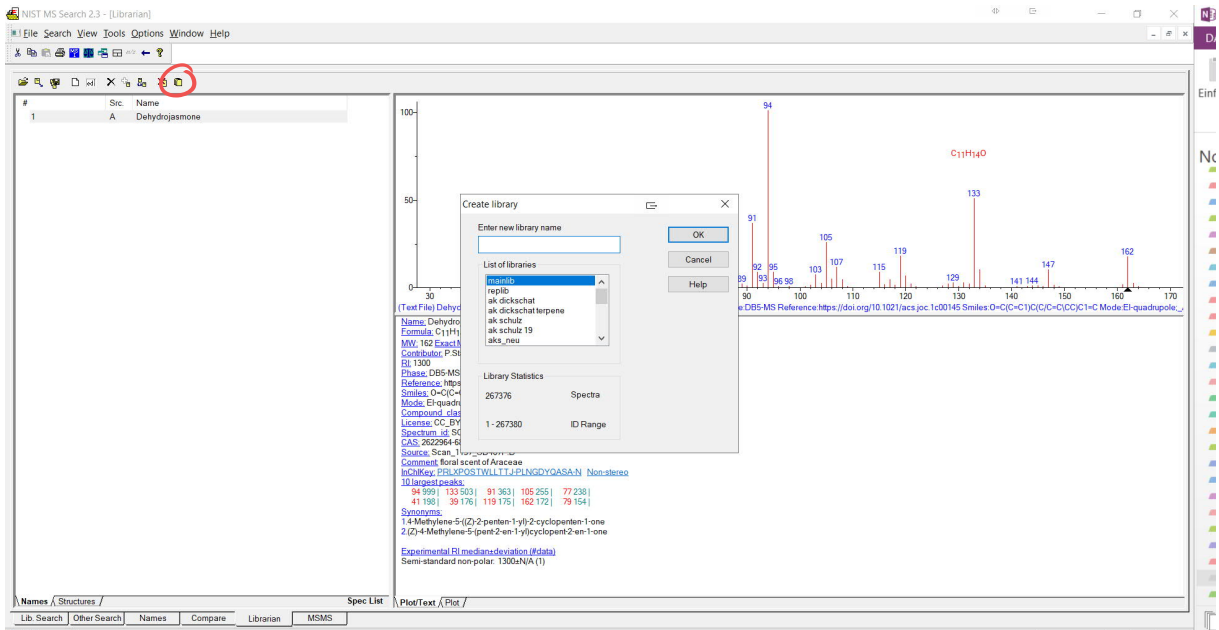


Quick guide to implement MACE in MSSearch

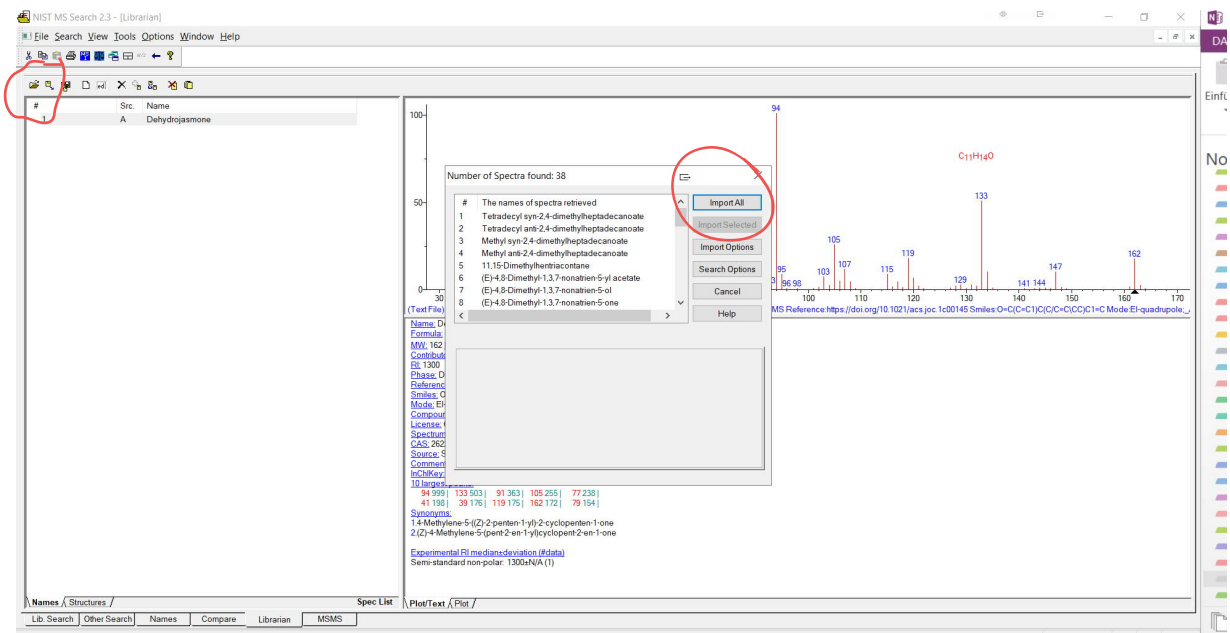
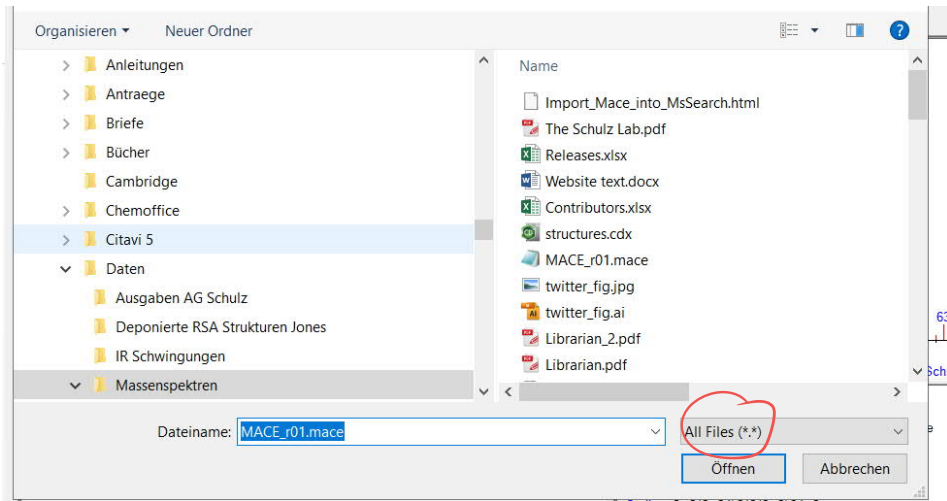
1. Go to Librarian in MsSearch 2.3



2. Create MACE database by clicking icon far right and follow instructions.



3. Clicking import, far left, and select MACE_rX.mace file for import. Make sure to first select All Files. May take some time.



4. Select all entries.

NIST MS Search 2.3 - [Librarian]

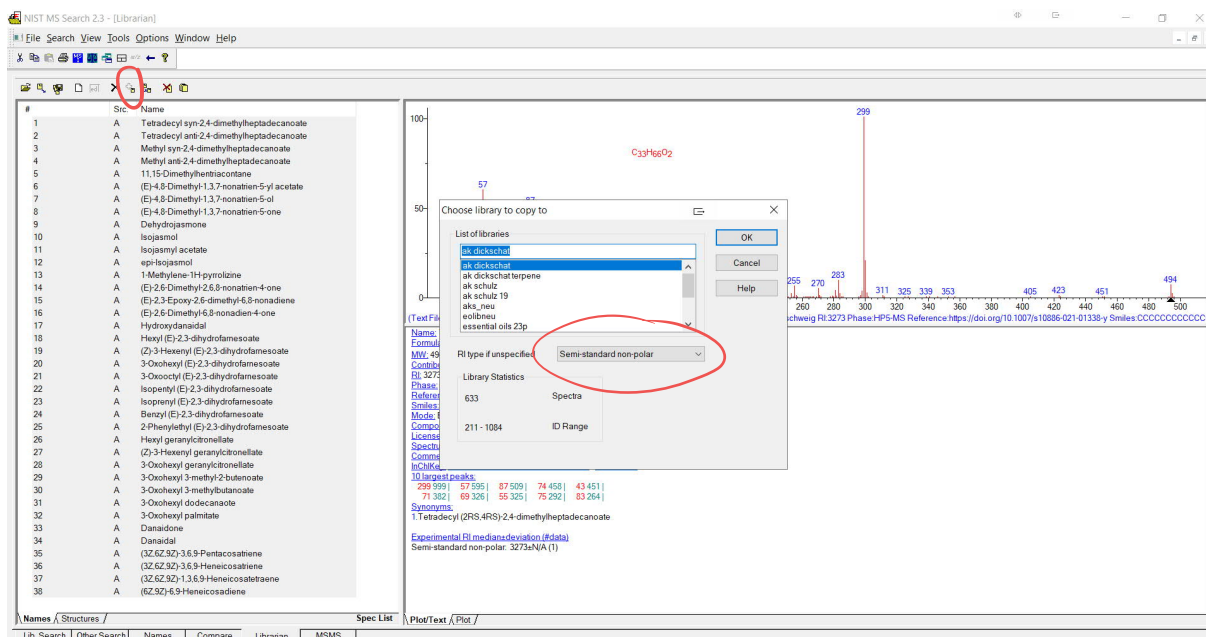
File Search View Tools Options Window Help

MS

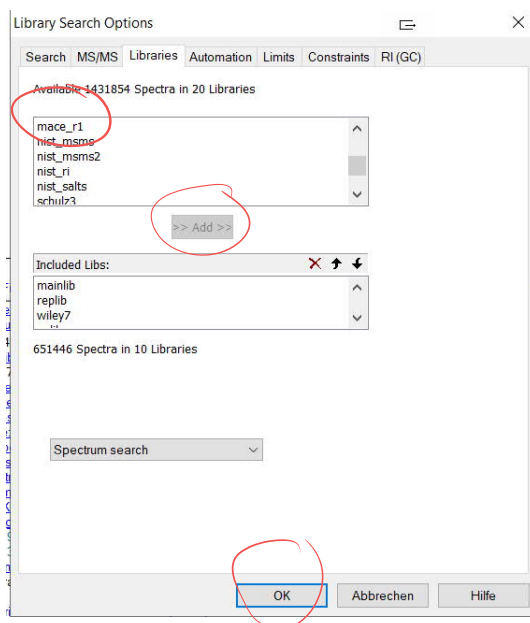
#	Src.	Name
1	A	Tetradecyl syn-2,4-dimethylheptadecanoate
2	A	Tetradecyl anti-2,4-dimethylheptadecanoate
3	A	Methyl syn-2,4-dimethylheptadecanoate
4	A	Methyl anti-2,4-dimethylheptadecanoate
5	A	11,15-Dimethylhentriacontane
6	A	(E)-4,8-Dimethyl-1,3,7-nonatrien-5-yl acetate
7	A	(E)-4,8-Dimethyl-1,3,7-nonatrien-5-ol
8	A	(E)-4,8-Dimethyl-1,3,7-nonatrien-5-one
9	A	Dehydrojasnone
10	A	Isojasmonol
11	A	Isojasmyl acetate
12	A	epi-Isojasmonol
13	A	1-Methylene-1H-pyrrolizine
14	A	(E)-2,6-Dimethyl-2,6,8-nonatrien-4-one
15	A	(E)-2,3-Epoxy-2,6-dimethyl-6,8-nonadiene
16	A	(E)-2,6-Dimethyl-6,8-nonadien-4-one
17	A	Hydroxydanaidal
18	A	Hexyl (E)-2,3-dihydrofarnesoate
19	A	(Z)-3-Hexenyl (E)-2,3-dihydrofarnesoate
20	A	3-Oxoethyl (E)-2,3-dihydrofarnesoate
21	A	3-Oxoethyl (E)-2,3-dihydrofarnesoate
22	A	Isopentyl (E)-2,3-dihydrofarnesoate
23	A	Isoprenyl (E)-2,3-dihydrofarnesoate
24	A	Benzyl (E)-2,3-dihydrofarnesoate
25	A	2-Phenylethyl (E)-2,3-dihydrofarnesoate
26	A	Hexyl geranylcitronellate
27	A	(Z)-3-Hexenyl geranylcitronellate
28	A	3-Oxoethyl geranylcitronellate
29	A	3-Oxoethyl 3-methyl-2-butenolate
30	A	3-Oxoethyl 3-methylbutanoate
31	A	3-Oxoethyl dodecanoate
32	A	3-Oxoethyl palmitate
33	A	Danaidone
34	A	Danaidal
35	A	(3Z,6Z,9Z)-3,6,9-Pentacosatriene
36	A	(3Z,6Z,9Z)-3,6,9-Heneicosatriene
37	A	(3Z,6Z,9Z)-1,3,6,9-Heneicosatetraene
38	A	(6Z,9Z)-6,9-Heneicosadiene

Names Structures Spec List

5. Add to MACE library by clicking 7th icon, add to library. Select semi-standard non-polar retention index. Click ok.



6. Go to options, select library search option. Select libraries tab. Select mace, click add and then ok. The library is now added to your search libraries.



7. Go to view, select Comment field options. Fill in tags, one line after the others.
Contributor
Phase
Reference
Smiles
Mode

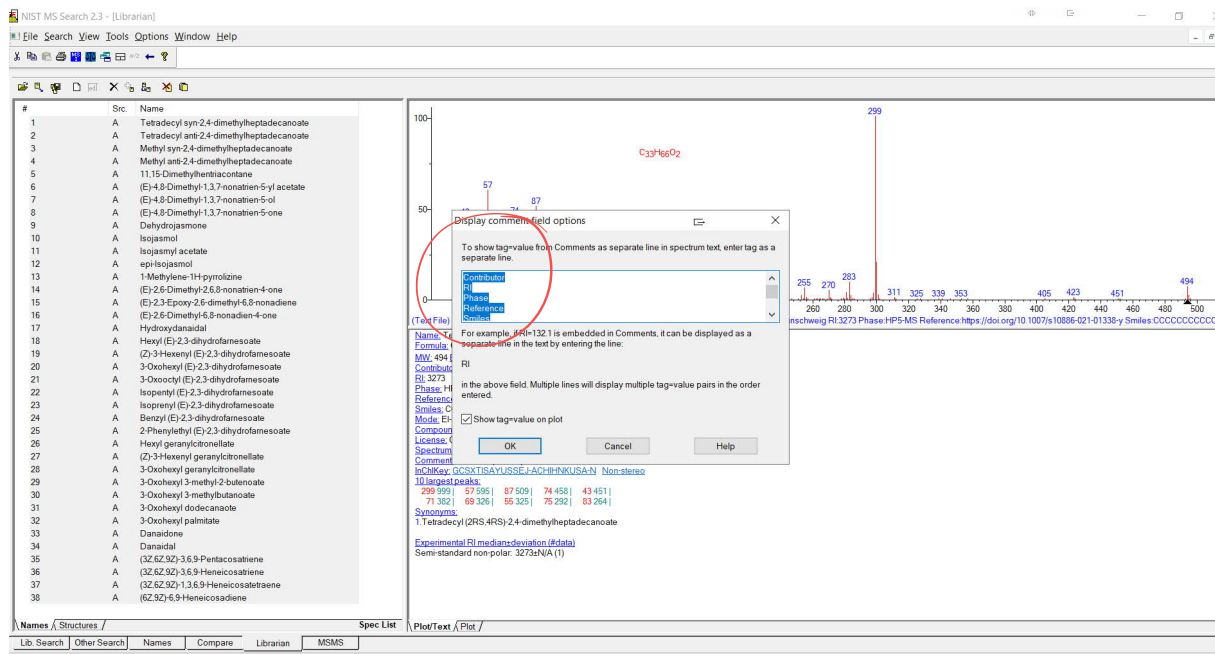
Compound_class

License

Spectrum_id

Source

Please note: If you click on the InChiKey of a spectrum, the pubchem page of this compound will be opened with information on compound occurrence and references.



S. Schulz, A. Möllerke, 17. May 2022