

Tips for Converting Lab Data to Search Strategies

Type of Search	Lab Data	Sources	Values Searched	Error Range	Caveats
CAS Registry Number	Not available from lab data	SDBS, POC, DOC, SFS, Beilstein	68-85-0		Use CAS RN to find/confirm physical properties info, view spectral diagram, prep & rxn articles
MP	115	POC, DOC	110 - 120	+/- 5	Put Spaces between hyphens
BP	190	POC, DOC	185 - 195	+/- 5	Put Spaces between hyphens
MW	200	POC, DOC	(197 - 203) OR (397 - 403)	+/- 3	Convert equivalent weight into MW by multiplying values by 1 and 2
Number of Atoms	9-12 Hydrogens, No Nitrogen present	SDBS	Hydrogen 9 to 12, Nitrogen 0 to 0		
Number of Atoms	9-12 Hydrogens	POC, DOC	H9 OR H10 OR H11 OR H12		
Molecular Elements (All Present in MF)	Oxygen is only heteroatom	POC, DOC	- Only-C H O		Browse MF Index to see values available.
MF	C6H5Br	SDBS, POC, DOC	C6H5Br		Element symbols are case sensitive in many resources. Put MF in Hill System Order (Carbon 1st, Hydrogen 2nd, and then all other elements in alpha order)
Substructure Fragments	Benzene ring, Carboxylic Acid	POC, DOC	Draw using Structure Editor		Disconnected fragments okay, draw functional groups if shortcut symbols are ambiguous. Structures not present for all substances.

Type of Search	Lab Data	Sources	Values Searched	Error Range	Caveats
IR Peak	2800 AND 1400	SDBS	2800 1400	+/-10	Use either a space or a comma as the separator for multiple peaks. Use a hyphen to search a range of values (e.g. 550-750).
IR Peak	2800 AND 1400	POC	(2780 - 2820) AND (1380 - 1420)	+/- 20	Spectral data not present for all cmpds. Only use significant peaks.
H-NMR Peak	1.4 AND 7.2	SDBS	1.4,7.2	+/- 0.2 ppm	Comma is the separator for multiple shifts. Range is defined by two numbers separated by a space. Ranges for multiple peaks – put space between upper and lower range of each peak, use comma between each range with no space between comma and values. For no shift regions – only specify what you can see.
H-NMR Peak	1.4 AND 7.2	POC	(1.2 - 1.6) AND (7.0 - 7.4)	+/- 0.2 ppm	Spectral data not present for all cmpds. Only use significant peaks.
H-NMR Spectra, Predicted	Structure	ACD's ILab	Exact Structure		Use to refine DOC results. Note predictions weakest for ionic Hydrogen in an alcohol, amine, and acid.
C-13 Peak	128,129,130,134,173	SDBS	128,129,130,134,173 No Shift Regions 170 135	+/- 2.0	Comma is the separator for multiple shifts. Range is defined by two numbers separated by a space. Ranges for multiple peaks – put space between upper and lower range of each peak, use comma between each range with no space between comma and values. For no shift regions – only specify what you can see.
C-13 Peak	128,129,130,134,173	POC	(126 - 136) AND (171 - 175)	+/- 2.0	Spectral data not present for all cmpds.
C-13 Spectra, Predicted	Structure	ACD's ILab	Exact Structure		Use to refine DOC results. Note predictions weakest for alcohols and amines.

Don't use peaks from solvent!