KnowItAll Mass Spectrometry Training

Vendor Neutral Data Processing Solution for Spectral Analyses

WILEY

KnowItAll™

"Structure Tips and Structure Searches in ChemWindow"

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Handouts for Videos:
Website: Little Mass Spec and Sailing
https://littlemsandsailing.wordpress.com

NOTE: Series of other training videos/handouts for KnowItAll mass spectrometry software on my personal web site.

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Tips in ChemWindow (1 of 3)

-Make Chemistry/Add Implicit Hydrogens and Show Implicit Hydrogens is selected
-Functions well defined in video
-Use pointer to hover over end of double bond
-use various hot keys to get element
-if you keep clicking on an atom with H's, it will keep "stripping" them off

Hot Atom Keys	**Element**
C	CH_3
Shift C	Cl
H	H
Shift H	Cbz
P	PH_3
Shift P	Ph
S	SH
Shift S	SiH_3
O	OH
Shift O	COOH
N	NH_2
Shift N	NO_2
B	Br
Shift B	BH_2
I	I
F	F
Shift F	CF_3

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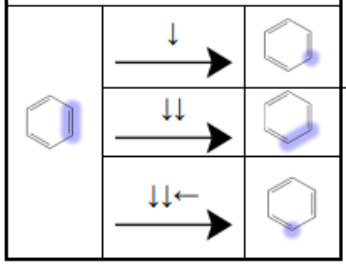
ChemWindow® Hotkeys

Tips in ChemWindow (2 of 3)

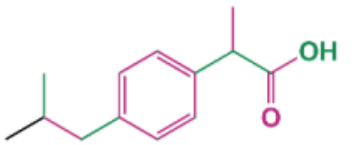
What's Possible:

Selection Arrows



Molecule Example

0, ↓, ↓, 1, 1, a, 1, 0, ↓, ↓, 1, 2, o

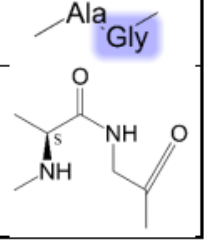


Predefined Substituents

Enter, Ala, Esc, →, →, Enter, Gly, Esc

Choose **Chemistry**, **Make Stick Structure**

For a full list of abbreviated substituents, select **Chemistry**, **Show Predefined Substituents**.



Hotkeys / Shortcuts:

Atom	0	1	2	3 or a	4	5	6	7	8	9	Enter	Space	'
			O								Edit Label	Remove Label	Tags with Number
	A	Ctrl+A	B	b	C	c	Ctrl+C	d	E	e	Ctrl+E	F	f
	Ac	A	BH_2	Br	Cl	CH_3	Ca	D	$COOCH_3$	Et	E	CF_3	F
	H	h	i	k	L	l	M	m	Ctrl+M	N	n or w	Ctrl+N	O
	Cbz	H	I	K	Li	Cl	MgBr	Me	M	NO_2	NH_2	Na	COOH
	o	P	p	Q	q	r	S	s	x	y	Z	z	+ or -
	OH	Ph	PH_2	Fmoc	Q	R	SiH_3	SH	X	Boc	N_3		Changes Charge

Bond	0	1	2	3	4	5	6	7	8	9	a	v	z
		Multiple to single bond											

Bond	B	b	c	d	H	h or W	w	y

Keep cursor away from structure when using Hotkeys. Many hotkeys can be typed multiple times to toggle through options.

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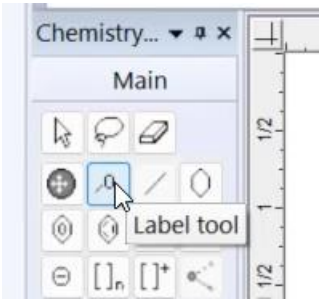
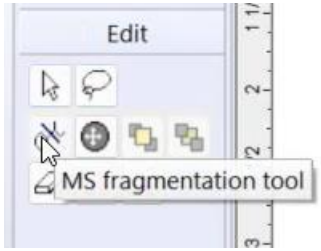
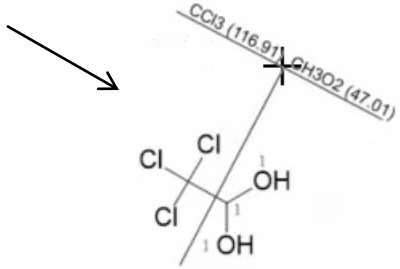
Tips in ChemWindow (3 of 3)

-To add elements which are not defined by hot keys
-Click on Label tool and hover end of bond, can add elements such as Aluminum, Al
-Can use Edit Mass Spec fragmentation tool

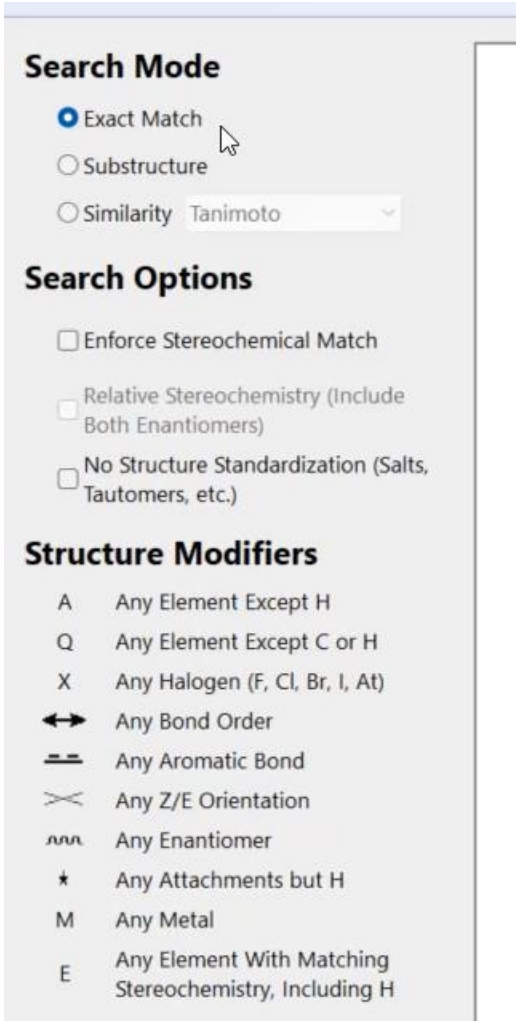






Tips in ChemWindow (1 of 2)

-To date, I have only done “Exact Match”
-And “Similarity Tanimoto”



Conclusions

- Atom keys are defined for common elements or species in ChemWindow
- When using them, the primary one is selected from the keypad
- A secondary one is selected with the same key when the shift key is depressed
- Special undefined elements can be added with the “label tool”
- Structures can be searched by a variety of approaches by exporting to SearchIt
- Two common searches demonstrated, exact and similar (Tanimoto)

NOTE: **Be sure to see my other videos for Mass Spec KnowItAll training on my personal website**