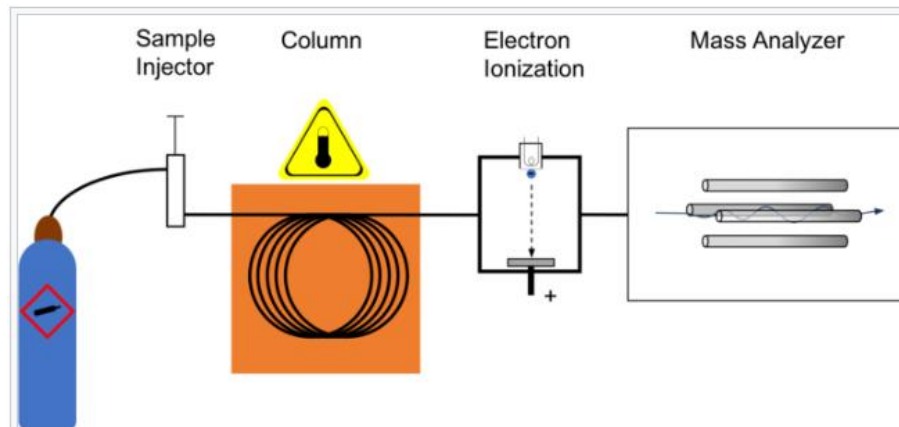


Free NIST GC-MS Software Lab for Universities:

Part 6: Structure Searches with Input from ChemSketch



James Little

August 29, 2023

38 years Eastman Chemical Company

7 years Mass Spec Interpretation Services

<https://littlemsandsailing.wpcomstaging.com/>

[Link to GCMS Schematic Above](#)

[Link to University Logos](#)

Free NIST GC-MS Software Lab for Universities

Part 1: Very Basic Theory of GCMS Analyses

Part 2: Installation of Software

Part 3: Library Searches

Part 4: Processing GCMS Data with AMDIS

Part 5: Understanding EI Fragmentation with MS Interpreter

Part 6: Structure Searches with Input from ChemSketch

Part 7: Creating a User Library

Part 8: Advanced Processing with NIST Software

A "Little" Mass Spec and Sailing
Organic Mass Spectrometry, NMR, Sailing, Tesla, Duplicate Bridge

Mass Spec Interpretation Services

Mass Spec Interpretation Services

Mass Spectrum Plot (m/z vs. Relative Abundance):

m/z	Relative Abundance (%)
15	~10
16	~5
27	~5
31	~5
39	~5
40	~5
43	100
44	~5
51	~5
53	~5

Chemical Structure: CC(=O)C (Acetone)

Mass Spectrometer Diagram: $C_{12}H_{10}O_2$ CAN COATING

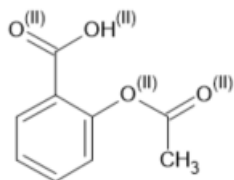
Computer Monitor: CAS NO. 20583.873

Navigation: About Me | My Topics | Others Links

[Link to Training Website](#)

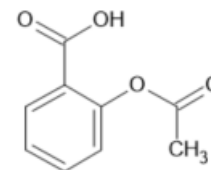
Bug in Pasting Structure from NIST to ChemSketch

-The oxidation state is transferred from NIST MS Search to ChemSketch



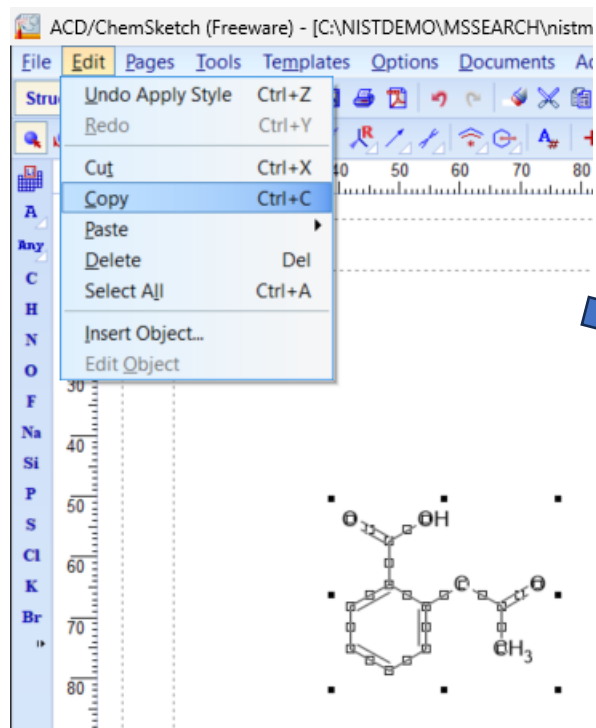
-Just circle the structure and change the style to normal

A screenshot of the ChemSketch software interface. The 'Set Structure Drawing Style' menu is open, showing various drawing styles. The 'Normal' style is selected. Below the menu, the chemical structure of 2-acetoxybenzoic acid is shown with a grid overlay, indicating it is selected for styling.

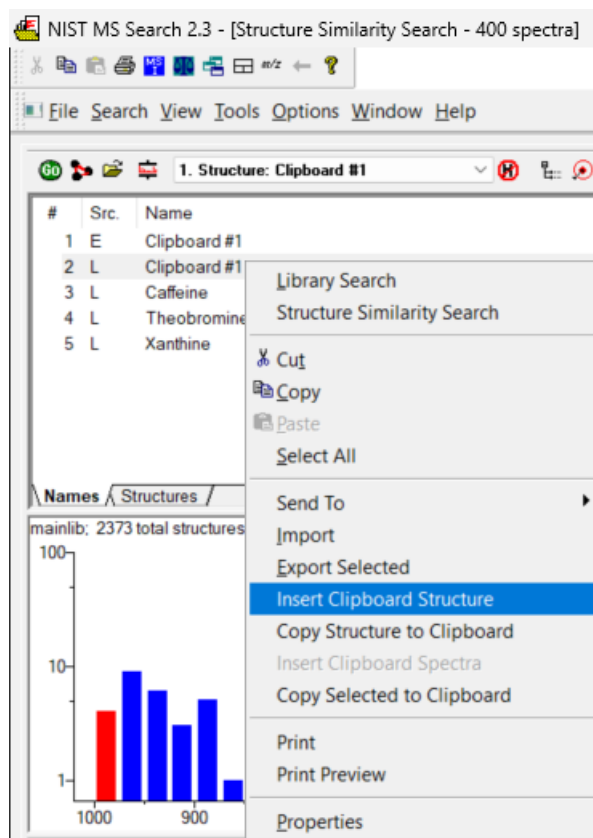


Sending Structure from ChemSketch to NIST Search Program

-Circle structure of interest and copy to clipboard



-Then insert clipboard structure with right click to get menu option



NIST MS Search 2.3 - [Structure Similarity Search - 400 spectra]

File Search View Tools Options Window Help

1. Structure: Clipboard #1

#	Src.	Name
1	E	Clipboard #1
2	L	Clipboard #1
3	L	Caffeine
4	L	Theobromine
5	L	Xanthine

Library Search
Structure Similarity Search

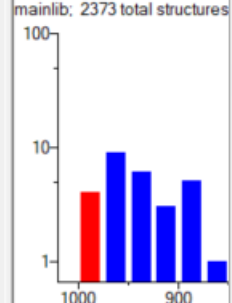
Cut
Copy
Paste
Select All

Send To
Import
Export Selected
Insert Clipboard Structure
Copy Structure to Clipboard
Insert Clipboard Spectra
Copy Selected to Clipboard

Print
Print Preview
Properties

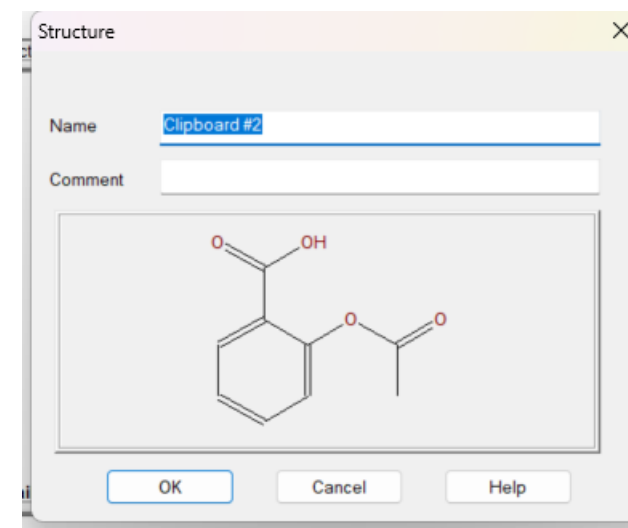
Names Structures /

mainlib: 2373 total structures



100
10
1

1000 900



Structure

Name Clipboard #2

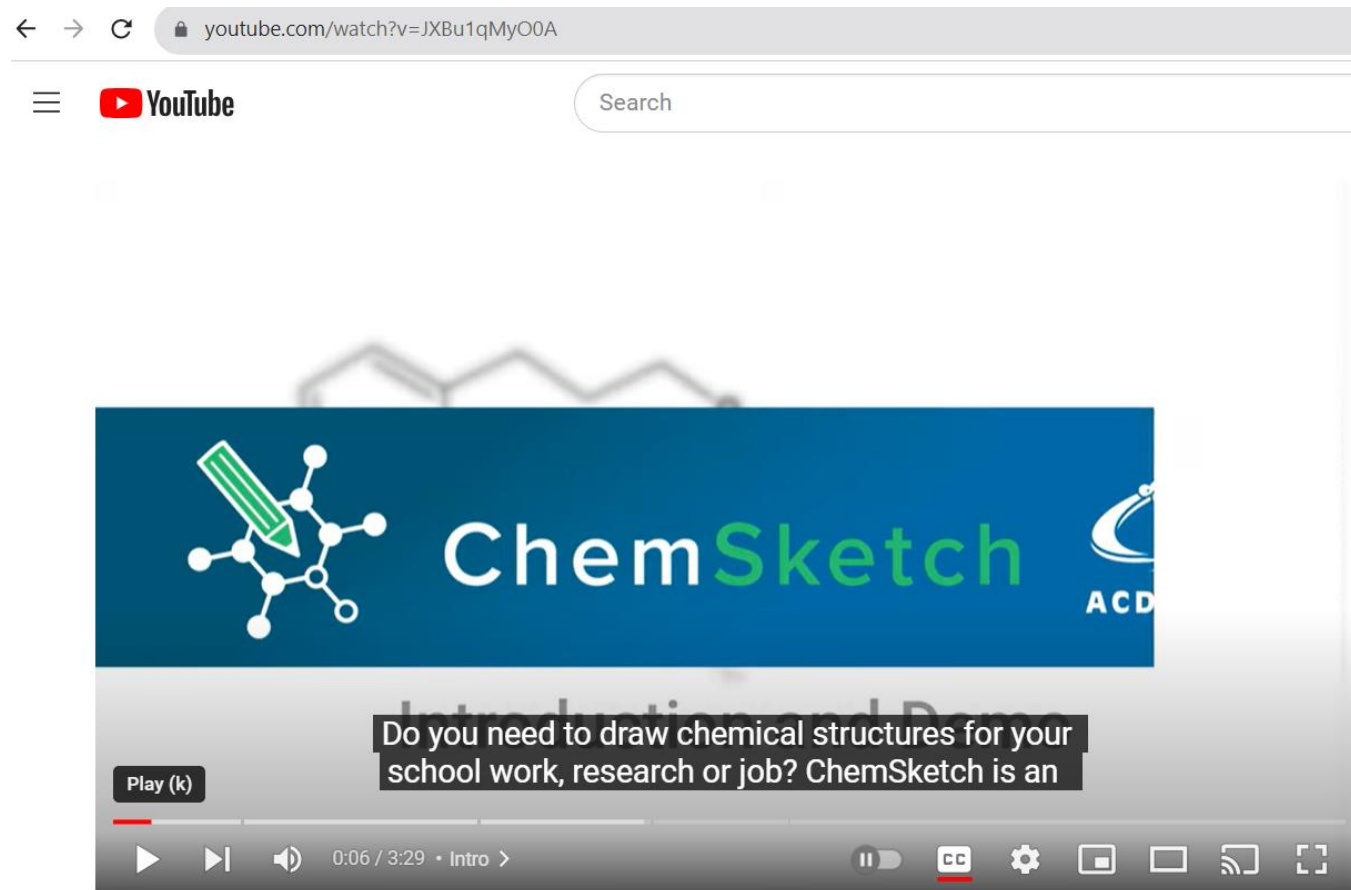
Comment

CC(=O)Oc1ccc(O)cc1

OK Cancel Help

Lots of Instructional Videos on YouTube for ChemSketch

-Included one in my video and also included link below:



The screenshot shows a YouTube video player interface. The address bar at the top displays the URL `youtube.com/watch?v=JXBu1qMyO0A`. The YouTube logo and a search bar are visible in the header. The video player itself features a blue banner with the ChemSketch logo, which includes a green pencil drawing a chemical structure. Below the banner, a subtitle reads: "Do you need to draw chemical structures for your school work, research or job? ChemSketch is an". The video progress bar at the bottom shows the video is at 0:06 / 3:29, with the word "Intro" and a right-pointing arrow next to it. Standard video control icons (play, pause, volume, full screen, etc.) are also present.

ChemSketch Introduction and Demo: How to Use ChemSketch (ACD/Labs)

[Link to YouTube Video](#)