Employing the CAS Registry (SciFinder^{n}) to Identify Seized Drugs Using Data from the NIST Hybrid EI Mass Spec Searches

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SciFinder®
A CAS SOLUTION

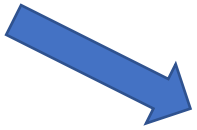
“Spectraless” Database Approach for Known Unknown Identications

Used as Supporting Information for the Presentation on My Website

Suggest New Users Watch Training Videos on SciFinder^{n} on My Website

Click Here for Website link

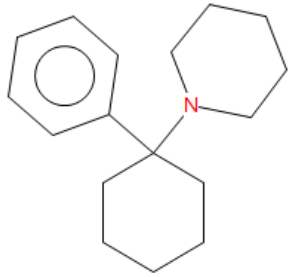
Excellent CAS training videos are available on a variety of topics. I have links to a few essential videos that I captured below that will be very useful for the new user of this powerful software package. They have many more on their website.



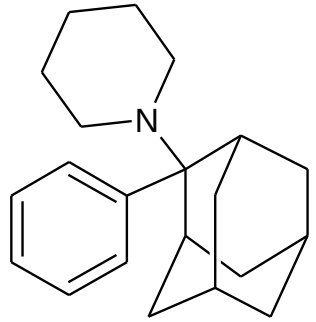
Basic Searching a Topic and Filtering (download or view Google Drive)
Basic Structure Searches (download or view Google Drive)
Searching for Specra and Properties of a Chemical (download or view Google Drive)

Conclusions Leading to Identification of Unknown

- Hybrid search was critical in suggesting PCP-related substructure
- Molecular formula from Accurate mass DART critical step (E. Sisco, NIST)
- Testing SciFinder and CAS Registry as a ***much simpler approach*** than shown in presentation
- Also demonstrated in separate video on website using ChemSpider



"Angel Dust"
Phenylcyclohexyl piperidine
PCP
Phencyclidine



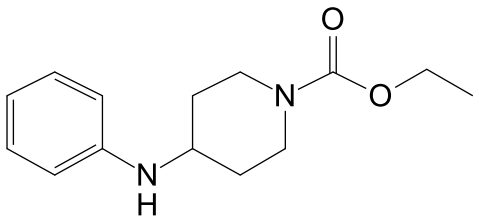
Identity of PCP-Related Unknown
CAS No. 72241-00-7

$C_{21}H_{29}N$
MW 295

Another Compound Identified in Presentation

- Hybrid search showed substructure and presence of carbamate group by MS and IR
- A molecular formula of $C_{14}H_{20}N_2O_2$ from hybrid data
- No accurate mass data really needed, such a simple deltaMass of oxygen, 16!
- IR and mass spectral data matched that obtained from another laboratory
- ***If it had not matched, could we have found other candidate structures with SciFinder^n***

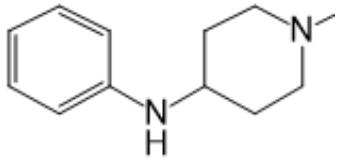
Identified Structure:



$C_{14}H_{20}N_2O_2$

MW 248

Other Possibilities for This Side of Ring?



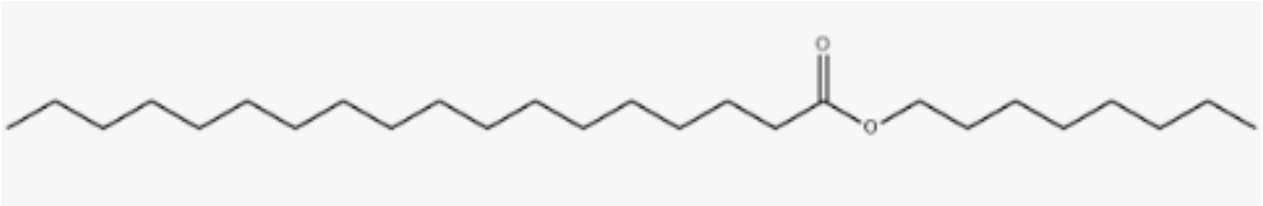
Searching or Limiting Searches in SciFinder by Molecular Weight

Molecular weight uses ***exclusively*** in SciFinder, ***but*** ChemSpider uses monoisotopic, nominal, and molecular weight.

Molecular weight calculated using the average molecular weight of the nuclides, thus those present in the periodic table. Typically used by chemists to calculate molar ratios for reactions.

Nominal Mass is calculated using the mass number of the most abundant isotope of each atom, without regard for the mass defect. All molecular ions and fragment ions are corrected to nominal mass when imported into in the NIST search program.

Monoisotopic Mass is calculated by taking the sum of the accurate masses (including mass defect) of the most abundant naturally occurring stable isotope of each atom in the molecule.



$C_{28}H_{56}O_2$

Molecular Weight	396.690
Nominal Molecular Weight	396
Monoisotopic Mass	396.39673

Calculating Molecular Weight from Mass Spec Data

- Not easy to easily determine by mass spec using most data systems
- Would have to normalize the isotopic data and m/z values to 1 or more places to right side of decimal
- Also know the standard deviation for the measurement
- See the following *link* to our JASMS article
- Not very practical

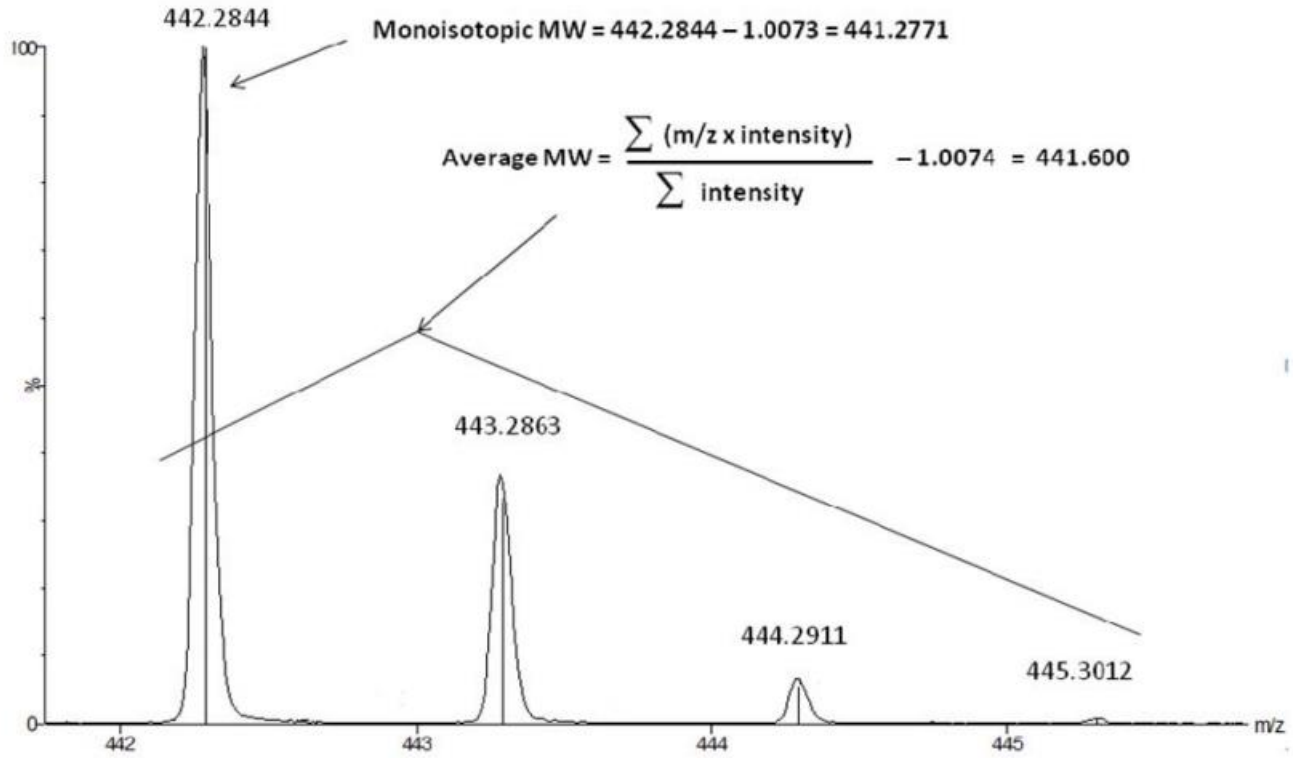


Figure 1: Determining the average MW of "known unknown" from centroided data for M+H species.

Relationship of Species Present to Molecular Weight (MW) Noted

- Carbon and hydrogen increase MW the most
- S, O, N, F, Si, I, etc. don't change significantly due to their value or the number typically present in a compound
- Cl and Br can have a significant effect, especially as the number present increase