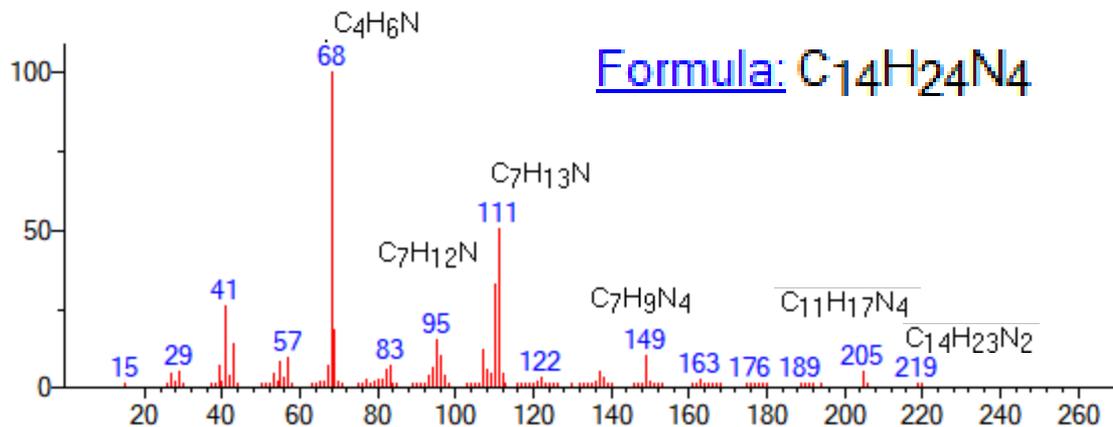


Comparison of Google Image Search to CAS and ChemSpider for Unknown Identifications Using Molecular Formula from Accurate Mass EI or MSMS

- For many years, we have used accurate mass data and either ChemSpider or SciFinder (CAS) to identify unknowns in commercial samples, extractables, etc.
- We refer^{1,2,3} to these as “*known unknowns*”
- They are **generally known** in a variety such of databases such as ChemSpider or the CAS Registry
- However**, their EI or MSMS spectra are not found in commercially available libraries
- This presentation compares using Google Image as another approach instead of ChemSpider or SciFinder for these type of identifications
- Possibly a viable approach which could compliment ChemSpider and SciFinder

Example:

Accurate Mass EI and CI Data Obtainable from Orbitrap
Identity **Not Found** In NIST or Wiley EI Libraries Searches



Google Search Results for C₁₄H₂₄N₄

- View results of Google search using *image* option
- Nitrile-azo compound shows up 7 times out of the 23 structures displayed
- the proposed structure fits the EI fragmentation pattern

Correct Structure

Use Image Display Option

structures synthesis anion

CC(C)C(C)(C)C#N[N+]=[N-]C(C)(C)C#N

CC1CN(C)CCN(C1)C2=CC=CN=C2

CC1=CN(C)CCN1

SciFinder (CAS Registry) Search Results for C₁₄H₂₄N₄

- Search with SciFinder and sort by descending associating references
- See top two references, would be hard to tell which isomer by EI
- However, more references could indicate that the isobutyl more likely

Substances search for "C₁₄H₂₄N₄" Molecular Formula

References

Reactions

Suppliers



Filter Behavior

Filter by

Exclude

Reaction Role

- Product (166)
- Reactant (67)
- Reagent (4)
- Catalyst (9)
- Solvent (1)

Reference Role

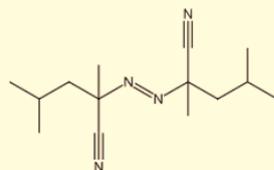
- Preparation (191)
- Synthetic Preparation (177)

15,448 Results

Sort: Number of References: Descending

1

4419-11-8



C₁₄H₂₄N₄

2,2'-Azobis[2,4-dimethylvaleronitrile]

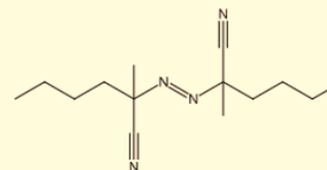
4,994
References

19K
Reactions

28
Suppliers

2

15545-95-6



C₁₄H₂₄N₄

2,2'-Azobis[2-methylhexanenitrile]

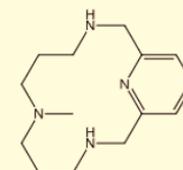
1,177
References

256
Reactions

3
Suppliers

3

106202-21-5



C₁₄H₂₄N₄

7-Methyl-3,7,11,17-tetraazaabicyclo[11.3.1]heptadeca-1(17),13,11,7-tetraene

25
References

10
Reactions

ChemSpider Search Results for C₁₄H₂₄N₄

- Search with ChemSpider and sort by descending associated references
- Top one consistent with EI fragmentation

Matches any text strings used to describe a molecule.

Systematic Name, Synonym, Trade Name, Registry Number, SMILES, InChI or CSID ?

▾

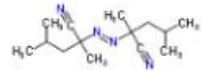
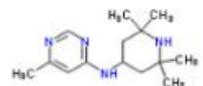
Search Hits Limit: ▾

Found 14345 results

Search term: **C14H24N4** (Found by molecular formula)



1 2 3 4 5

ID	Structure	Molecular Formula	Molecular Weight	# of Data Sources	# of References	# of PubMed	# of RSC
82654  - 0/2 defined		C ₁₄ H ₂₄ N ₄	248.3672	52	120	85	16
20518212		C ₁₄ H ₂₄ N ₄	248.3672	20	25	0	0

Conclusions

- Using Google search of a molecular formula from accurate mass data with subsequent display by images useful in getting possible candidate structures
- Then use EI or MSMS fragmentation to determine if reasonable
- SciFinder CAS registry search still likely the best, but not a free service
- ChemSpider is free and allows one to sort by relevant database, data sources, references to bring most likely structures to top of list
- Also, ChemSpider can be searched by accurate m/z values +/- error, SciFinder cannot
- Searching by accurate mass useful for higher molecular weight compounds (>500) when unsure of the molecular formula

References

1. [Unknown Identification Using SciFinder \(CAS Registry\)](#)
2. [Unknown Identification Using ChemSpider](#)
3. [LCGC Article Giving Overview with Examples](#)