

Using MetFrag with SciFinder and ChemSpider

1. The accurate mass data for Trazodone was obtained on Agilent QTOF
2. The data automatically exported into NIST Search program from MassHunter
3. The accurate mass data was exported from NIST Search to msp file
4. Spectrum (m/z , intensity) from NIST file pasted into MetFrag
5. <http://msbi.ipb-halle.de/MetFrag/>
6. Candidate structures obtained from SciFinder (SDF file manually from SciFinder) or ChemSpider (automatically with MetFrag Interface)
7. Best results obtained by sorting MetFrag by # of Explained Peaks
8. Note if isomers present, need to expand MetFrag display with :



Data Acquired on Agilent QTOF and Exported to NIST Search Software

Agilent MassHunter Qualitative Analysis 8.06.00 - lc-ms_default.m

File Edit View Find Identify Spectra Chromatograms Method Wizards Actions Configuration Tools Help

Data Navigator Compound List

Sort by Data File

Automatically Show Columns

Label	Show/Hide	Cpd	File	Name	Saturated
Cpd 8: Hydrocodone	<input checked="" type="checkbox"/>	8	For_Tox_mix_1AMSMS2.cdf	Hydrocodone	
Cpd 9: Methylenedioxyamphetam...	<input checked="" type="checkbox"/>	9	For_Tox_mix_1AMSMS2.cdf	Methylenedioxyametha...	
Cpd 10: Methamphetamine	<input checked="" type="checkbox"/>	10	For_Tox_mix_1AMSMS2.cdf	Methamphetamine	
Cpd 11: Strychnine	<input checked="" type="checkbox"/>	11	For_Tox_mix_1AMSMS2.cdf	Strychnine	
Cpd 12: Cocaine	<input checked="" type="checkbox"/>	12	For_Tox_mix_1AMSMS2.cdf	Cocaine	
Cpd 13: Meperidine (Pethidin...	<input checked="" type="checkbox"/>	13	For_Tox_mix_1AMSMS2.cdf	Meperidine (Pethidin...	
Cpd 14: Trazodone	<input checked="" type="checkbox"/>	14	For_Tox_mix_1AMSMS2.cdf	Trazodone	
Cpd 15: 3.506	<input checked="" type="checkbox"/>	15	For_Tox_mix_1AMSMS2.cdf		
Cpd 16: Phenacetin (APC)	<input checked="" type="checkbox"/>	16	For_Tox_mix_1AMSMS2.cdf	Phenacetin (APC)	

Chromatogram Results

x10⁸ +ESI TIC MS(all) Frag=110.0V For_Tox_mix_1AMSMS2.d

Chromatogram Results | Spectrum Identification Results

MS Spectrum Results

x10⁴ Cpd 14: +ESI Product Ion (3.346 min, 1 Scans) Frag=110.0V CID@20.0 (372.16[z=1] -> *)

Method Explorer: lc-ms_default.m

Chromatogram

Spectrum

General

Reports

Find Compounds

Find Compounds by Formula

Identify Compounds

Compound Automation Steps

Worklist Automation

Export

ASR Options

CEF Options

Compound Summary CSV Options

MGF Options

mzData Options

MS/MS Inclusion List Options

Extract EIC

Extract Chromatograms...

Subtract Background Spectrum

Subtract Any Spectrum

Add Any Spectrum

Convert Profile to Centroid

Convert Profile to Centroid and Replace

Find Spectrum Peaks

Create Compound from Spectra

MS Spectrum Peak List 1

MS Spectrum Peak List 2

MS Actuals

Adjust Peak Threshold

Search Database for Compounds

Search Database for Spectrum Peaks

Generate Formulas from Compound

Generate Formulas from Spectrum Peaks

Search Library for Compounds

Search Library for Spectra

Search Using NIST MS Program

Add/Edit Manual Identification

Deconvolute (Resolved Isotope)

Recalibrate

Restore Original Calibration in Data File

Set Anchor

Clear Anchor

Assign Ranges to

Move to Background Spectrum

Copy to User Spectra

Clear Spectrum Results

Delete

Unzoom

Assign Random Colors

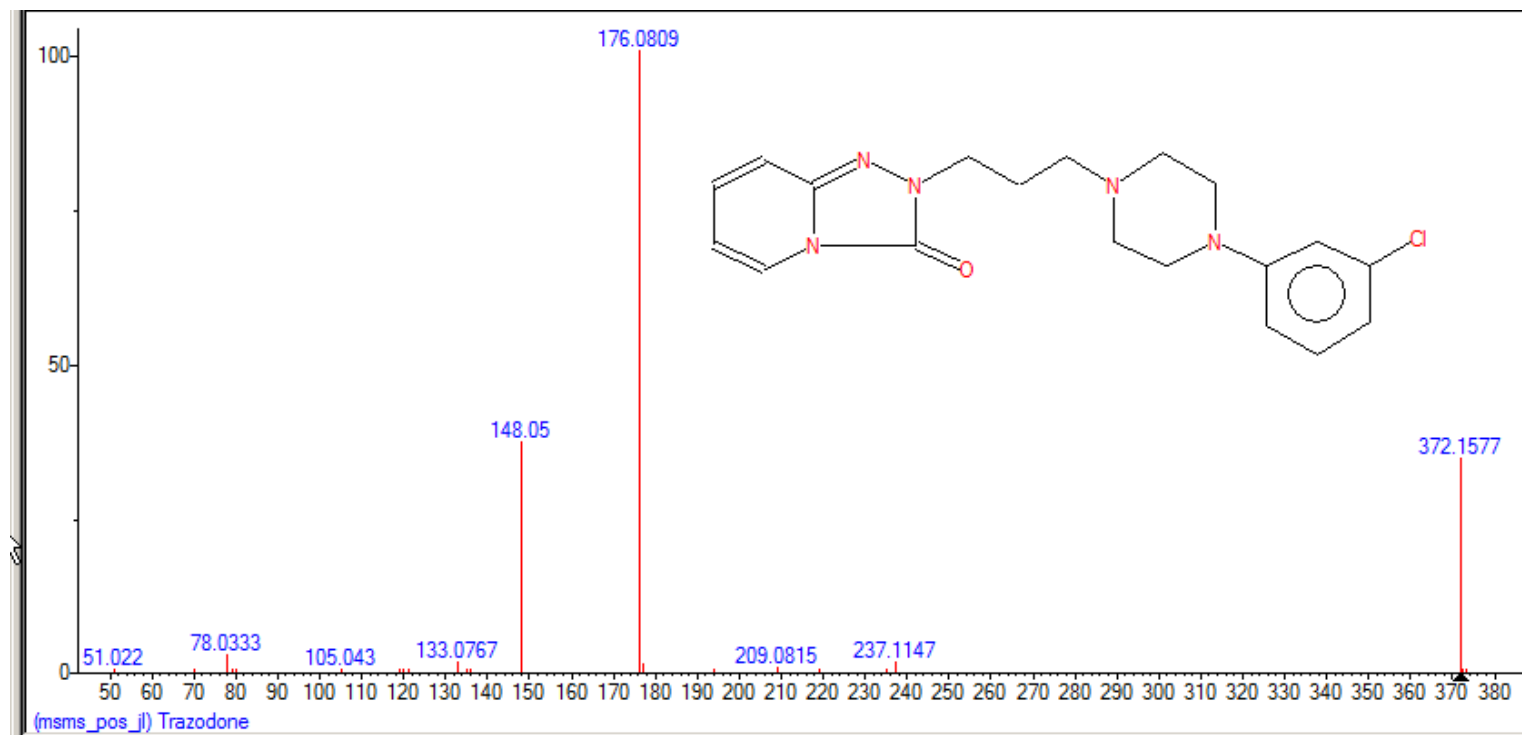
Choose Defined Color

Copy to Clipboard Ctrl+C

Print...

Export...

Spectrum in NIST Search Software Exported from MassHunter



Name: Trazodone
Formula: C₁₉H₂₂ClN₅O
MW: 371 **Exact Mass:** 371.151287 **CAS#:** 19794-93-5 **ID#:** 304 **DB:** msms_pos_jl
Other DBs: None
Comment: J Little, Mar 2012
Instrument type: Q-TOF MS
Spectrum type: ms2
Precursor m/z: 372.1588
Collision energy: 20 V
Ionization: ESI
10 largest peaks:
176.0809 999.00 | 148.05 368.47 | 372.1577 344.13 | 148.0857 69.57 | 78.0333 28.45 |
237.1147 17.03 | 133.0767 16.35 | 177.0823 11.95 | 209.0815 5.90 | 235.0928 5.15 |
Synonyms:
1. Agilent QTOF

MSP File Exported from NIST Search to Paste Into MetFrag

```
trazodone.MSP - Notepad
File Edit Format View Help
Name: Trazodone
Instrument_type: Q-TOF MS
Spectrum_type: ms2
Collision_energy: 20 V
Ionization: ESI
Synon: Agilent QTOF
Formula: C19H22ClN5O
MW: 371
ExactMass: 371.151287
PrecursorMZ: 372.1588
CAS#: 19794-93-5
DB#: 304
Comments: J Little, Mar 2012
Num Peaks: 29
51.022 2.19
70.0668 3.10
78.0333 28.45
79.0399 2.14
80.0479 2.85
105.043 4.56
119.075 2.45
120.0342 2.97
120.0563 2.58
121.0373 4.66
121.0777 4.23
133.0767 16.35
135.0434 4.29
136.0495 2.12
148.05 368.47
148.0857 69.57
148.1651 4.07
176.0809 999.00
177.0823 11.95
194.0627 3.68
209.0815 5.90
219.1203 2.07
235.0928 5.15
237.1147 17.03
372.1577 344.13
372.2581 4.72
372.3382 3.60
373.1529 2.58
373.1733 2.14
```

Search Results for C₁₉H₂₂ClN₅O from SciFinder Sorted by No. of References

SciFinder - Substance Answer Set - Windows Internet Explorer provided by Eastman Chemical Company

https://scifinder.cas.org/scifinder/view/scifinder/scifinderExplore.jsf

SciFinder - Substance Answer Set | Google | MetFrag | MetFusion | MetFusion

File Edit View Favorites Tools Help

Convert Select

Suggested Sites | Get more Add-ons | myeastman

Page Safety Tools

SciFinder®

Explore References | Explore Substances | Explore Reactions

Welcome Jim Little | Sign Out

Add KMP Alert | Molecular Formula "C19 H22 Cl N5 O" > substances (604)

Substances | Get References | Get Reactions | Tools | Send to SciPlanner

Save answers locally. To save answers on the SciFinder server, use Save.

Save Print Export

Sort by: Number of References

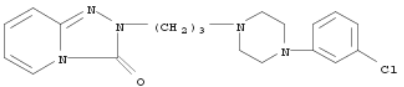
Answers per Page [15] View: [Icons]

0 of 604 Substances Selected

Page: 1 of 41

1. Substance Detail
19794-93-5

~1500

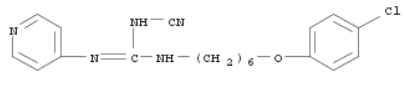


C₁₉H₂₂ClN₅O
1,2,4-Triazolo[4,3-*a*]pyridin-3(2*H*)-one, 2-[3-[4-(3-chlorophenyl)-1-piperazinyl]propyl]-

Spectra
Experimental Properties

2. Substance Detail
200484-11-3

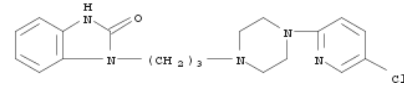
~67



C₁₉H₂₂ClN₅O
Guanidine, *N*'-[6-(4-chlorophenoxy)hexyl]-*N*'-cyano-*N*'-4-pyridinyl-

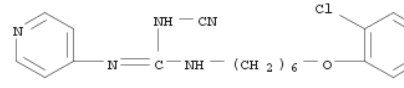
3. Substance Detail
174800-83-0

~4



4. Substance Detail
200484-22-6

~4



Analysis Refine

Analyze by: Substance Role

Click bar to view only those substances within the current answer set

Preparation	273
Biological Study	258
Uses	255
Prophetic in Patents	139
Properties	13
Reactant or Reagent	13
Analytical Study	6
Process	5
Miscellaneous	2
Occurrence	1

Show More

Exported All Components with >2 References (44) as SDF File from SciFinder

Export * Required

Export:

All
 Selected
 Range

Example: 2-20

For:

Offline review

Portable Document Format (*.pdf)
 Rich Text Format (*.rtf)
 Properties Only - Microsoft Excel Worksheet (*.xls)
 Answer Keys (*.txt)
 Quoted Format (*.txt)
 Tagged Format (*.txt)

Saving locally

Answer Key eXchange (*.akx)

Chemical structure processing

SDFFile (*.sdf)

Details:

File Name: *

Search MetFrag with Accurate Mass Spectrum and SciFinder SDF File



MetFrag

In silico fragmentation for computer assisted identification of metabolite mass spectra

MetFrag MzAnnotate Viewer About / News

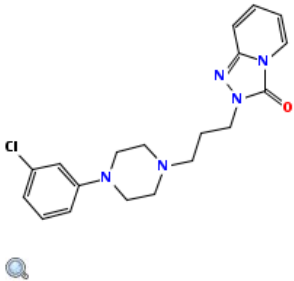
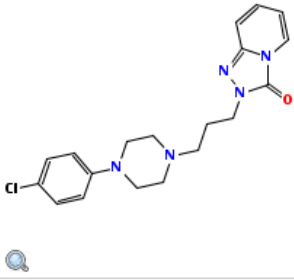
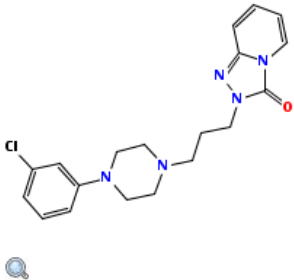
Database Settings
Database: KEGG PubChem ChemSpider Local SDF
Upload SDF: Browse... Upload
trazodone_test.sdf
Limit # of structures:
Search upstream DB 44 hits!

MetFrag Settings
Mode: [M+H] [M-H] [M]
Charge: pos. neg.
Mzabs (e.g. 0.01):
Mzppm (e.g. 10):
8 of 44 compounds processed
Process all 44 compounds! START Stop

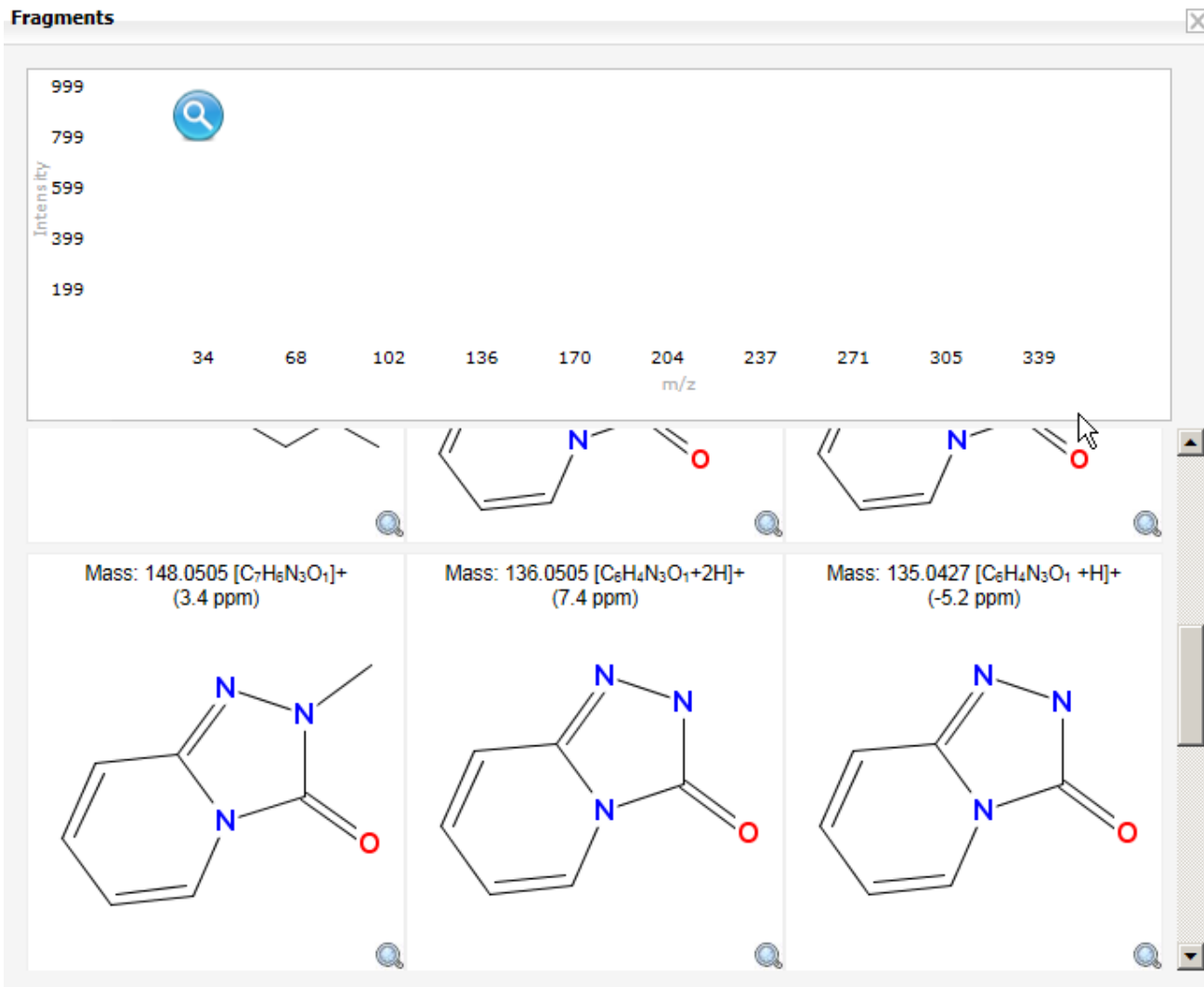
Parent ion: Neutral
Peaks:
51.022 2.19
70.0668 3.10
78.0333 28.45
79.0399 2.14
80.0479 2.85
105.043 4.56
119.075 2.45
120.0342 2.97
120.0563 2.58
121.0373 4.66
121.0777 4.23
133.0767 16.35
135.0434 4.29
136.0495 2.12
148.05 368.47
148.0857 69.57
148.1651 4.07
176.0809 999.00
177.0823 11.95
194.0627 3.68
209.0815 5.90
219.1203 2.07
235.0928 5.15
237.1147 17.03
372.1577 344.13
373.1581 4.72

[View spectrum](#)

Sort MetFrag Results by # Explained Peaks

Score	# Explained Peaks	Trivial Name	Exact Mass	Structure	Database ID	Actions
0.879	13	1,2,4-Triazolo[4,3-a]pyridin-3(2H)-one, 2-[3-[4-(3-chlorophenyl)-1-piperaziny...	C ₁₉ H ₂₂ Cl ₁ N ₅ O ₁ 371.1513		8	Fragments Download
0.879	13	1,2,4-Triazolo[4,3-a]pyridin-3(2H)-one, 2-[3-[4-(4-chlorophenyl)-1-piperaziny...	C ₁₉ H ₂₂ Cl ₁ N ₅ O ₁ 371.1513		32	Fragments Download
0.879	13	1,2,4-Triazolo[4,3-a]pyridin-3(2H)-one, 2-[3-[4-(3-chlorophenyl)-1-piperaziny...	C ₁₉ H ₂₂ Cl ₁ N ₅ O ₁ 371.1513		43	Fragments Download

Fragment Display Window in MetFrag



Using MetFrag with ChemSpider



MetFrag

In silico fragmentation for computer assisted identification of metabolite mass spectra

MetFrag MzAnnotate Viewer About / News

Database Settings

Database: KEGG PubChem ChemSpider Local SDF

Neutral exact mass: Search PPM:

Molecular formula:

Only biological compounds:

Limit # of structures:

Database ID's:

243 hits!

MetFrag Settings

Mode: [M+H] [M-H] [M]

Charge: pos. neg.

Mzabs (e.g. 0.01):

Mzppm (e.g. 10):

Parent ion: Neutral

Peaks:

51.022	2.19
70.0668	3.10
78.0333	28.45
79.0399	2.14
80.0479	2.85
105.043	4.56
119.075	2.45
120.0342	2.97
120.0563	2.58
121.0373	4.66
121.0777	4.23
133.0767	16.35
135.0434	4.29
136.0495	2.12
148.05	368.47
148.0857	69.57
148.1651	4.07
176.0809	999.00
177.0823	11.95
194.0627	3.68
209.0815	5.90
219.1203	2.07
235.0928	5.15
237.1147	17.03
372.1577	344.13
373.1581	4.72

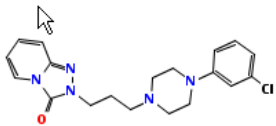
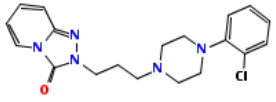
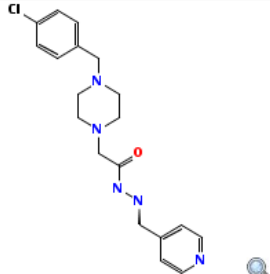
[View spectrum](#)

Results of MetFrag with ChemSpider

Log

[1](#)
[2](#)
[3](#)
[4](#)
[5](#)
[6](#)
[7](#)
[8](#)
[9](#)

Download complete table: [Generate output files](#)

	Score	# Explained Peaks	Trivial Name	Exact Mass	Structure	Database ID	Actions
	0.872	13	5332	C ₁₉ H ₂₂ Cl ₁ N ₅ O ₁ 371.1513		5332	Fragments Download
	0.872	13	7977308	C ₁₉ H ₂₂ Cl ₁ N ₅ O ₁ 371.1513		7977308	Fragments Download
	0.957	10	1263762	C ₁₉ H ₂₂ Cl ₁ N ₅ O ₁ 371.1513		1263762	Fragments Download
					