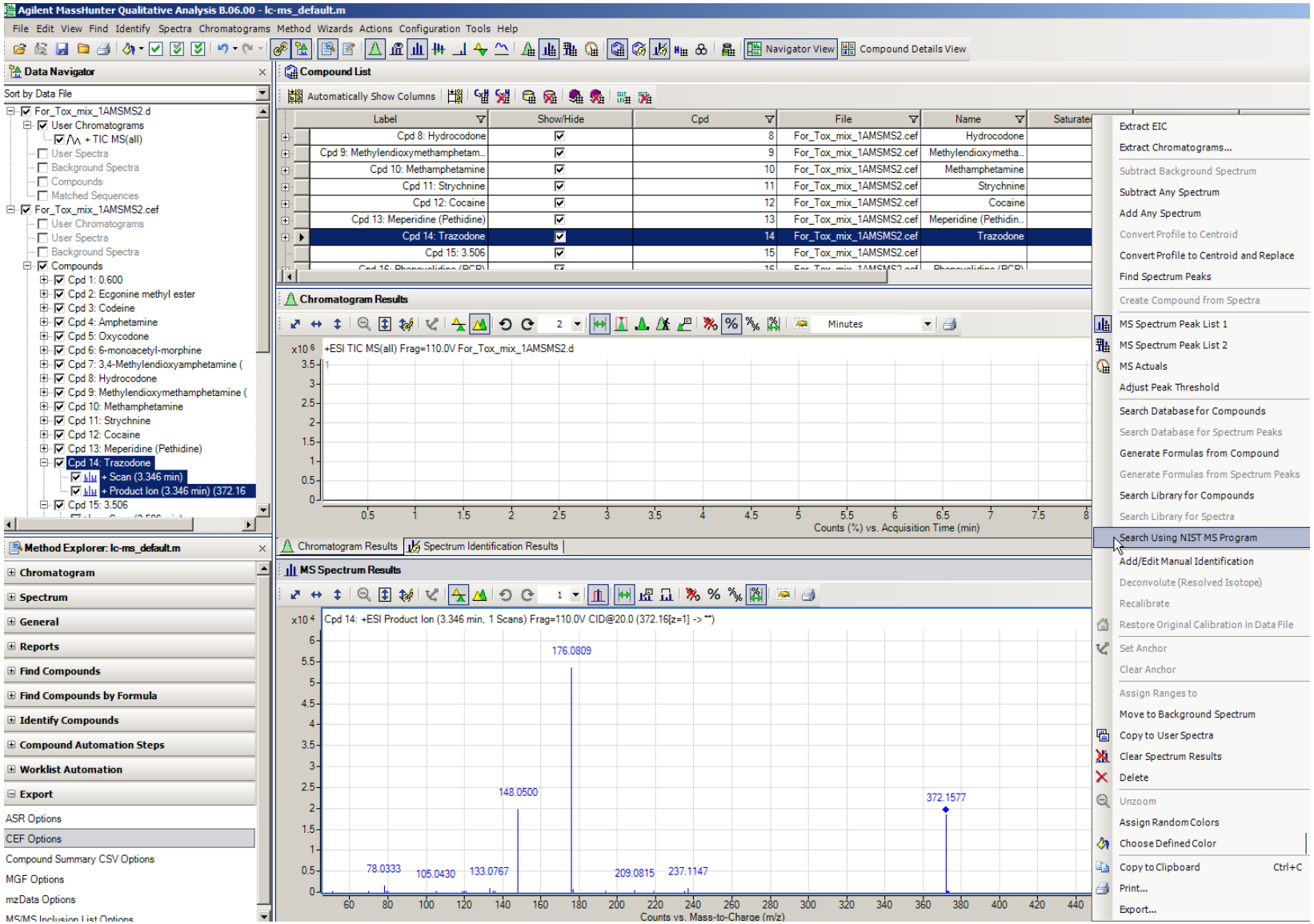
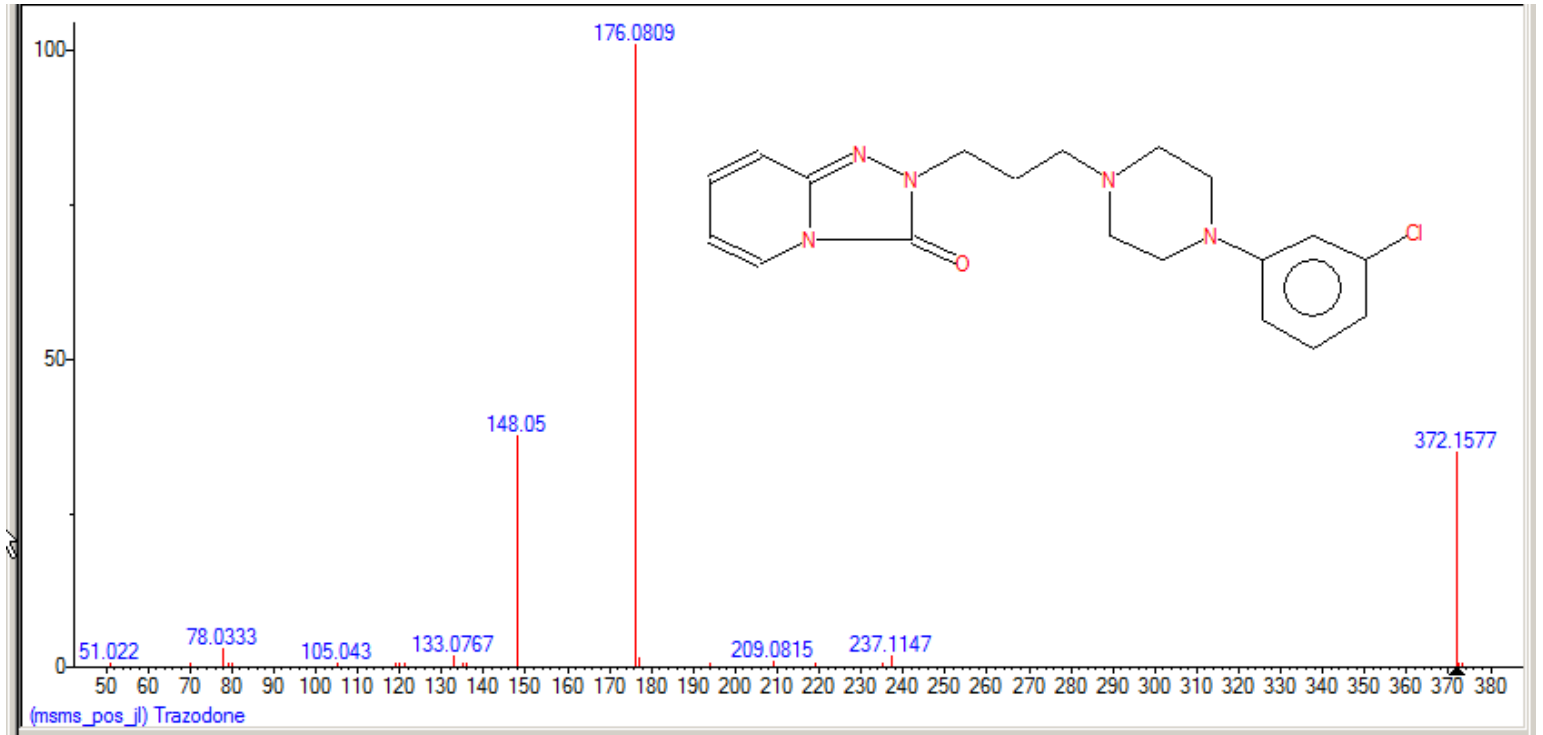
Using MetFrag with SciFinder and ChemSpider

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



Spectrum in NIST Search Software Exported from MassHunter

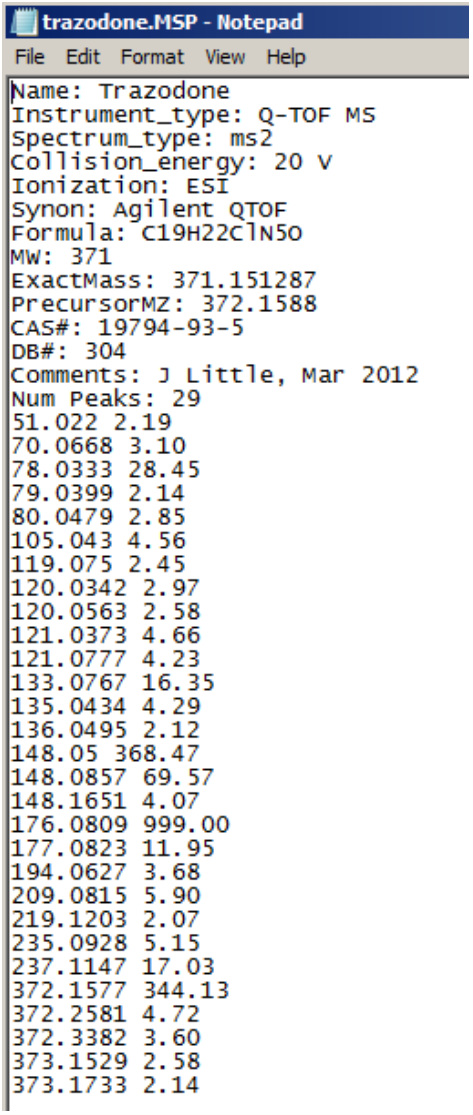


Name: Trazodone
Formula: $C_{19}H_{22}ClN_5O$
MW: 371 Exact Mass: 371.151287 CAS#: 19794-93-5 ID#: 304 DB: msms_pos_jl
Other DBs: None
Comment: J Little, Mar 2012
Instrument type: Q-TOF MS
Spectrum type: ms2
Precursor m/z: 372.1588
Collision energy: 20 V
Ionization: ESI
10 largest peaks:

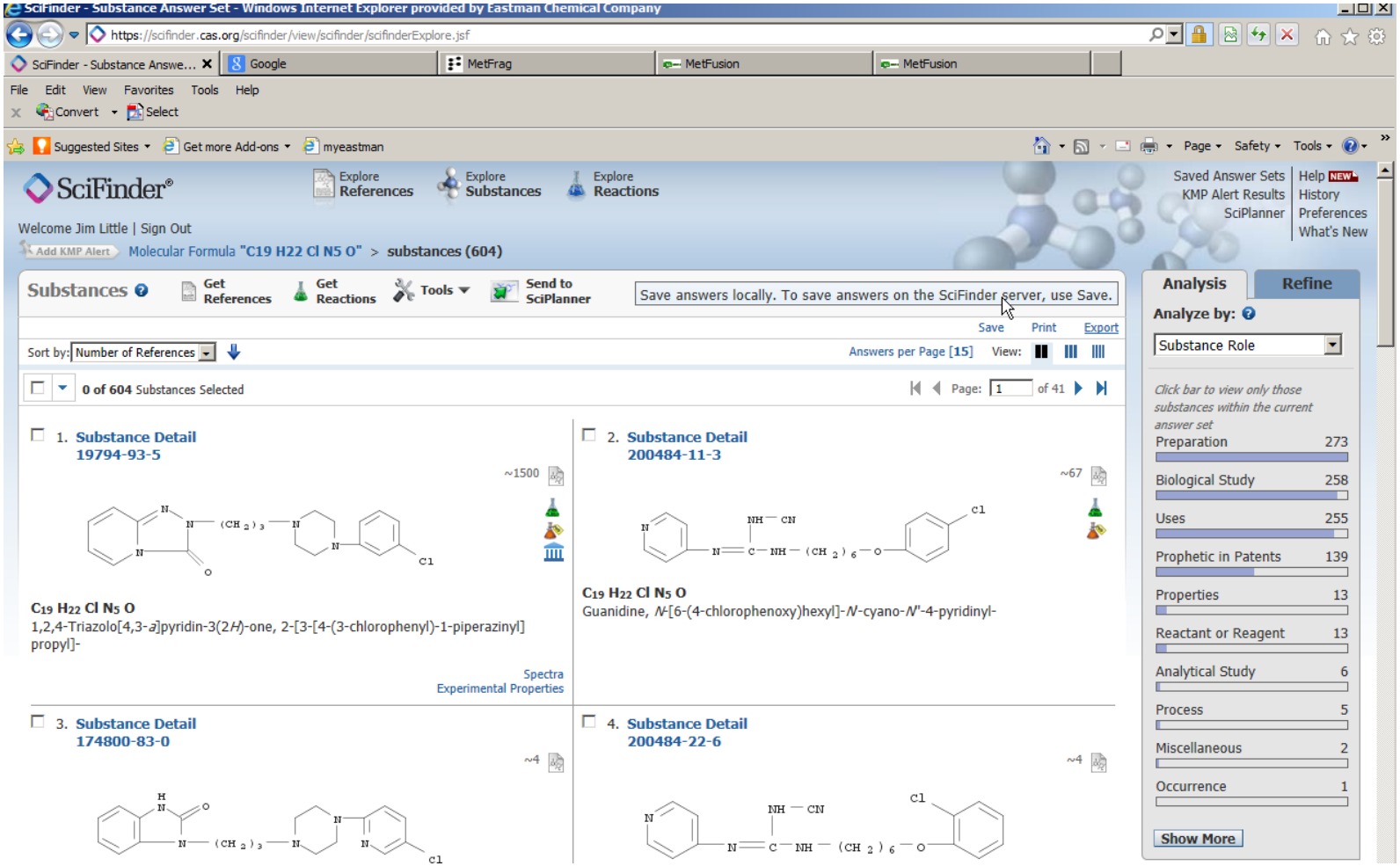
176.0809	999.00	148.05	368.47	372.1577	344.13	148.0857	69.57	78.0333	28.45
237.1147	17.03	133.0767	16.35	177.0823	11.95	209.0815	5.90	235.0928	5.15

Synonyms:
1.Agilent QTOF

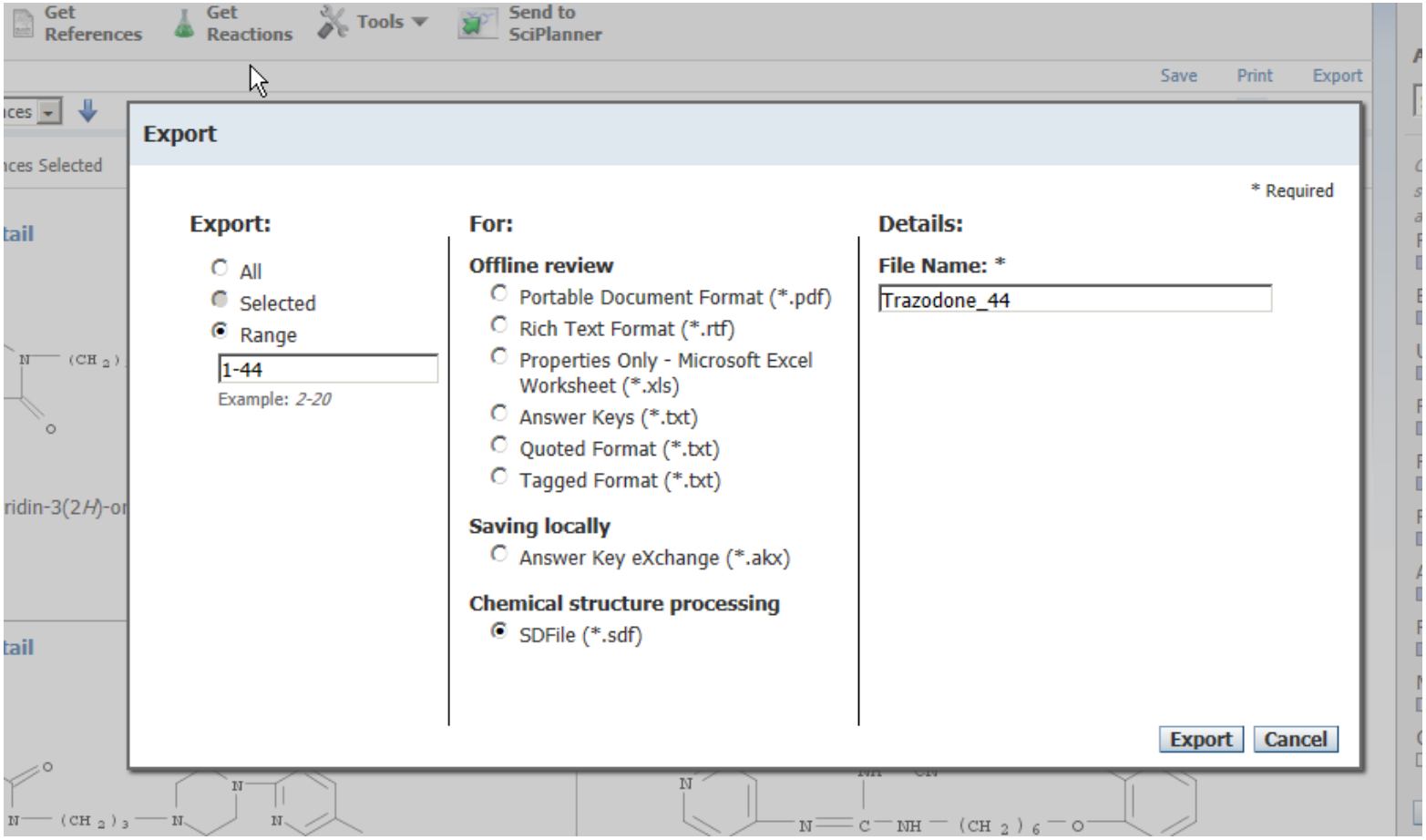
MSP File Exported from NIST Search to Paste Into MetFrag



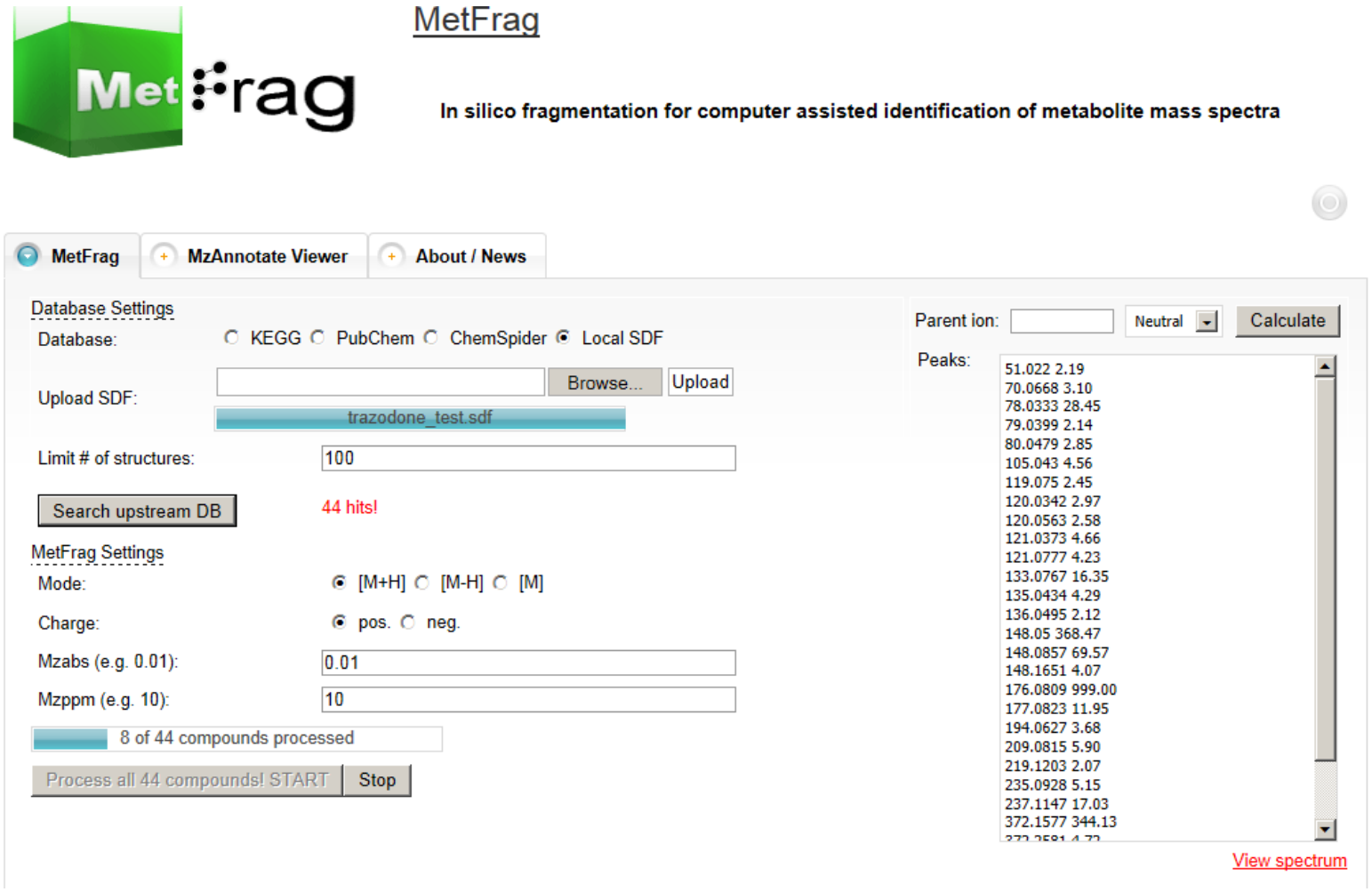
Search Results for $C_{19}H_{22}ClN_5O$ from SciFinder Sorted by No. of References



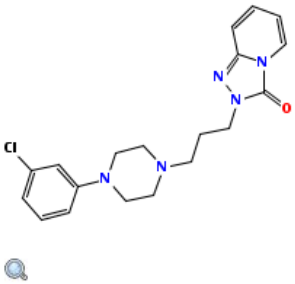
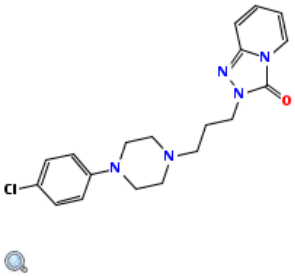
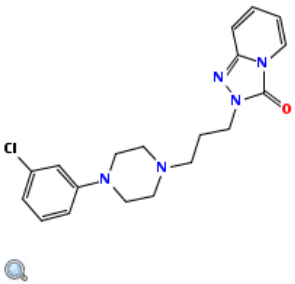
Exported All Components with >2 References (44) as SDF File from SciFinder



Search MetFrag with Accurate Mass Spectrum and SciFinder SDF File

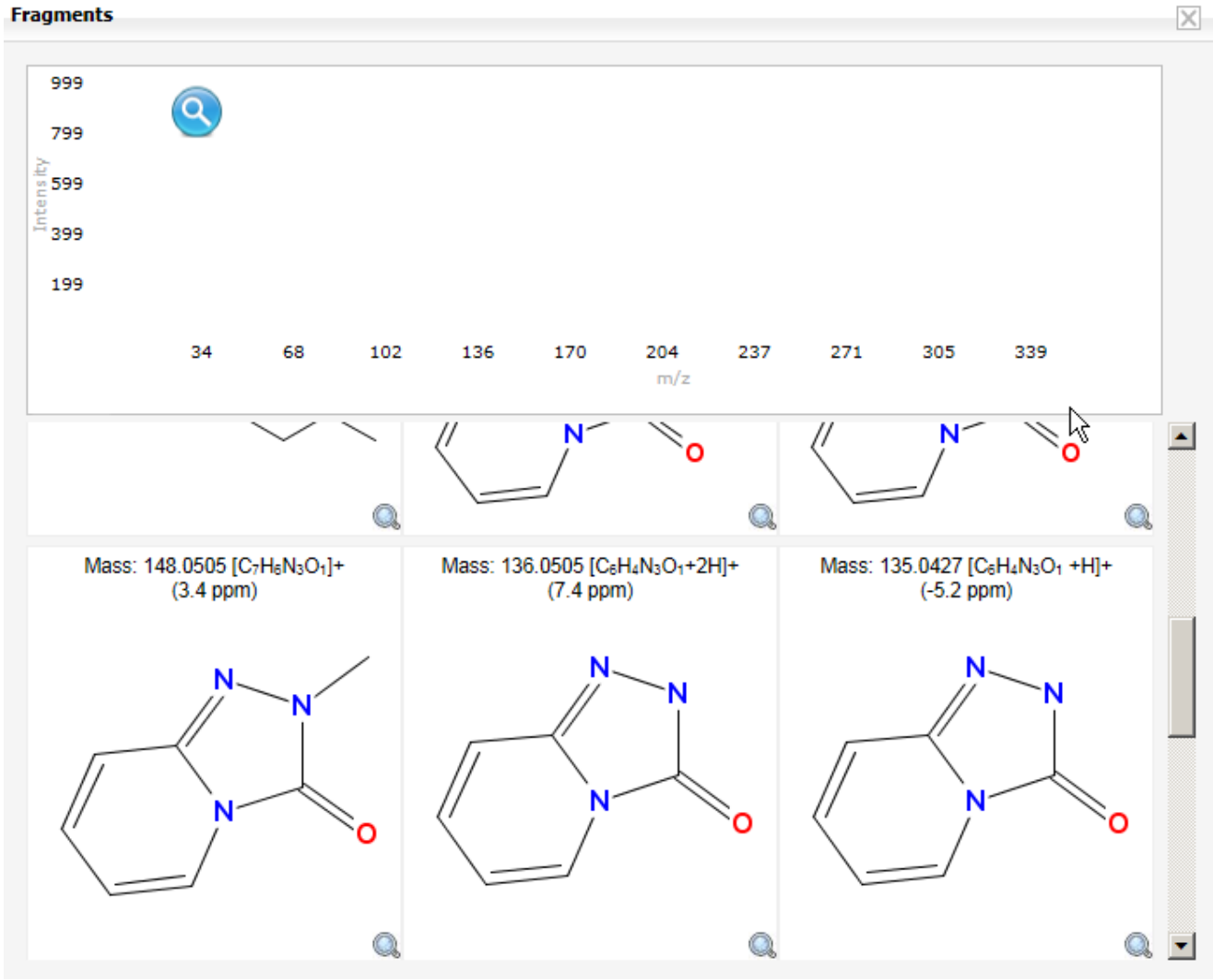


Sort MetFrag Results by # Explained Peaks

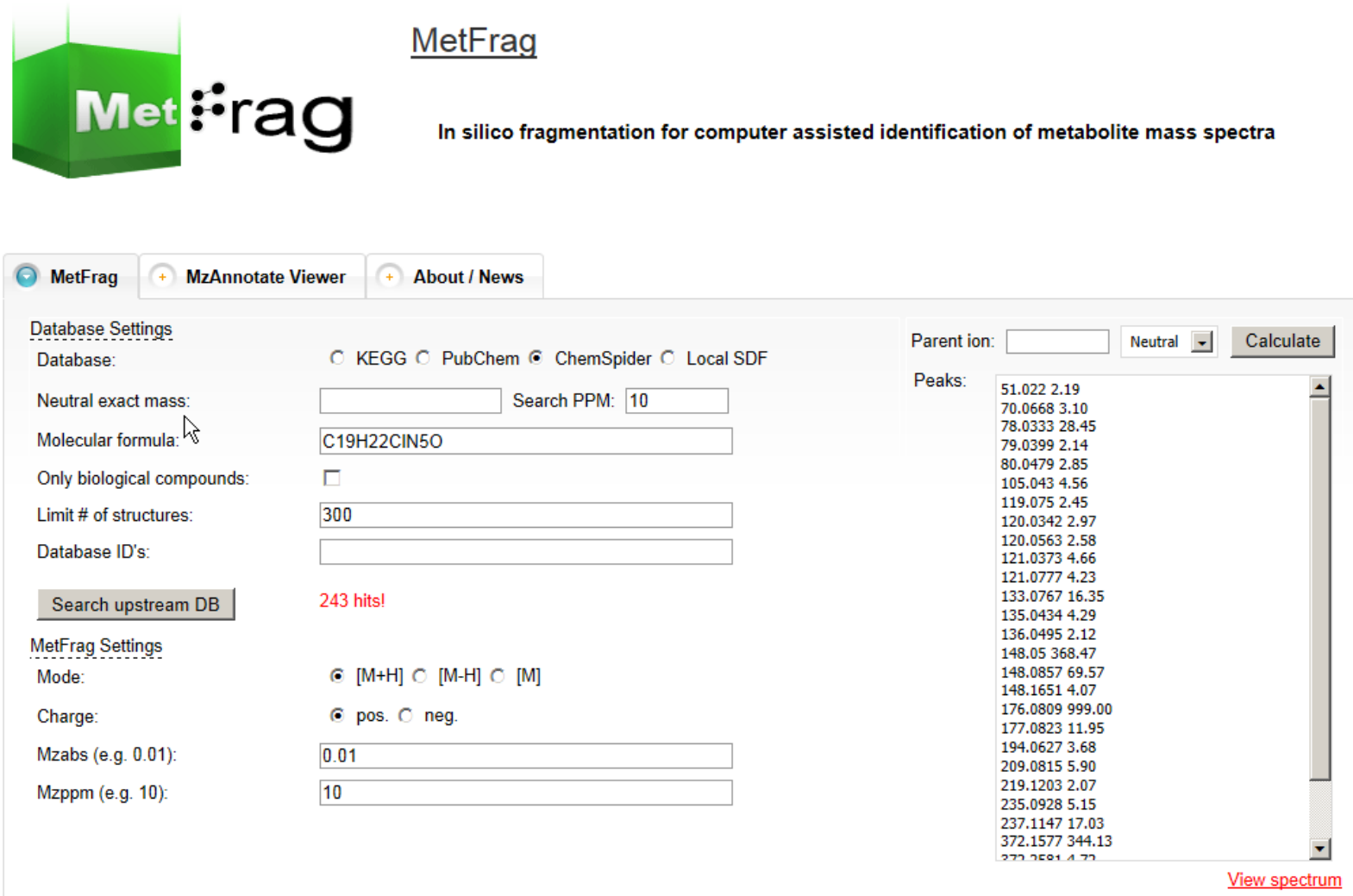
	Score	# Explained Peaks	Trivial Name	Exact Mass	Structure	Database ID	Actions
	0.879	13	1,2,4-Triazolo[4,3-a]pyridin-3(2H)-one, 2-[3-[4-(3-chlorophenyl)-1-piperaziny...	$C_{19}H_{22}Cl_1N_5O_1$ 371.1513		8	Fragments Download
	0.879	13	1,2,4-Triazolo[4,3-a]pyridin-3(2H)-one, 2-[3-[4-(4-chlorophenyl)-1-piperaziny...	$C_{19}H_{22}Cl_1N_5O_1$ 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...	$C_{19}H_{22}Cl_1N_5O_1$ 371.1513		43	Fragments Download

Feedback

Fragment Display Window in MetFrag



Using MetFrag with ChemSpider

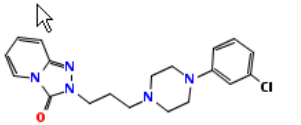
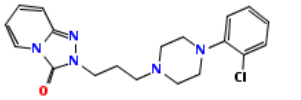
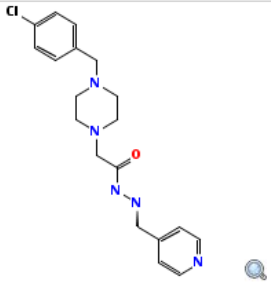


Results of MetFrag with ChemSpider

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	$C_{19}H_{22}Cl_1N_5O_1$ 371.1513		5332	Fragments Download
	0.872	13	7977308	$C_{19}H_{22}Cl_1N_5O_1$ 371.1513		7977308	Fragments Download
	0.957	10	1263762	$C_{19}H_{22}Cl_1N_5O_1$ 371.1513		1263762	Fragments Download