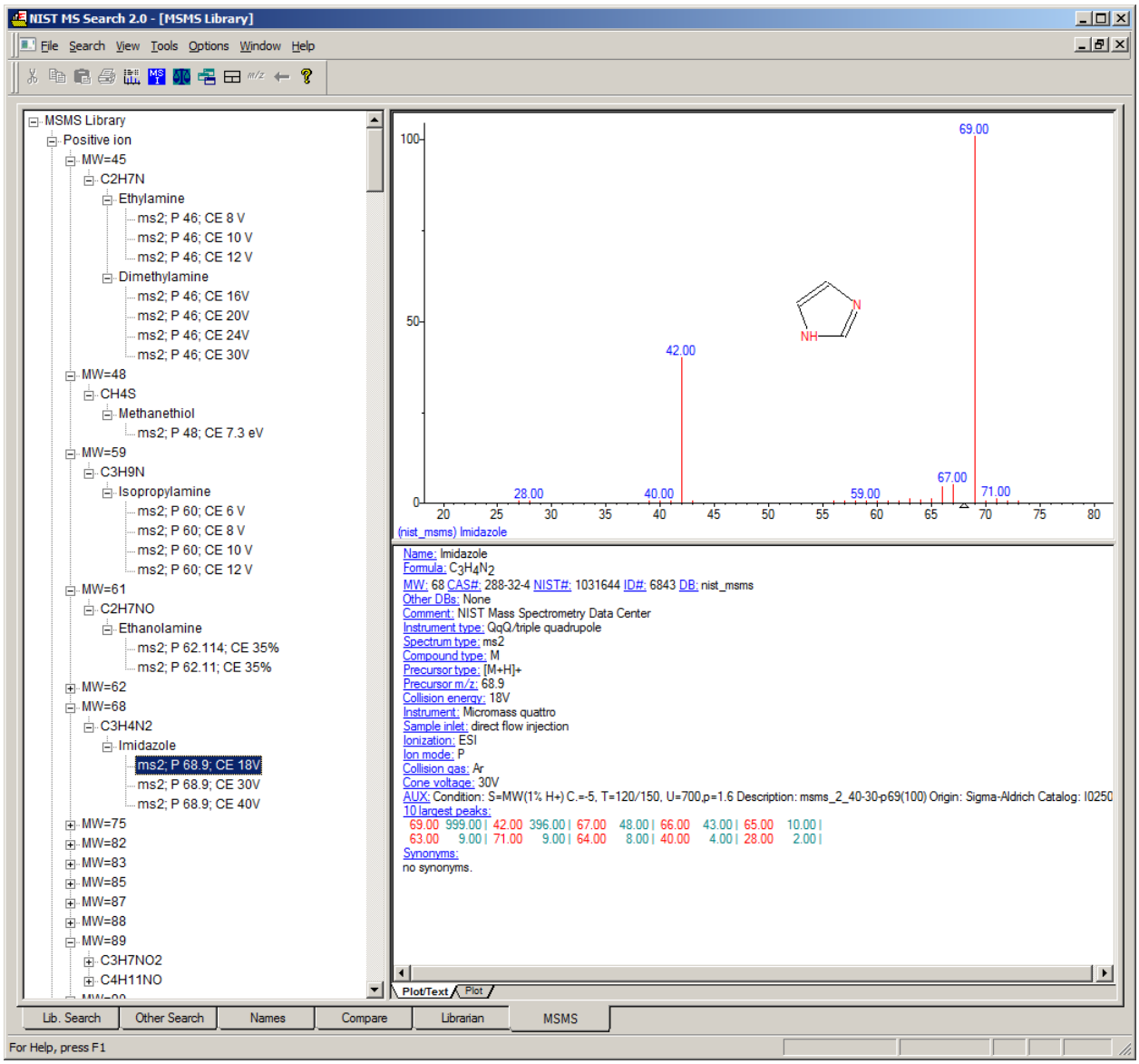
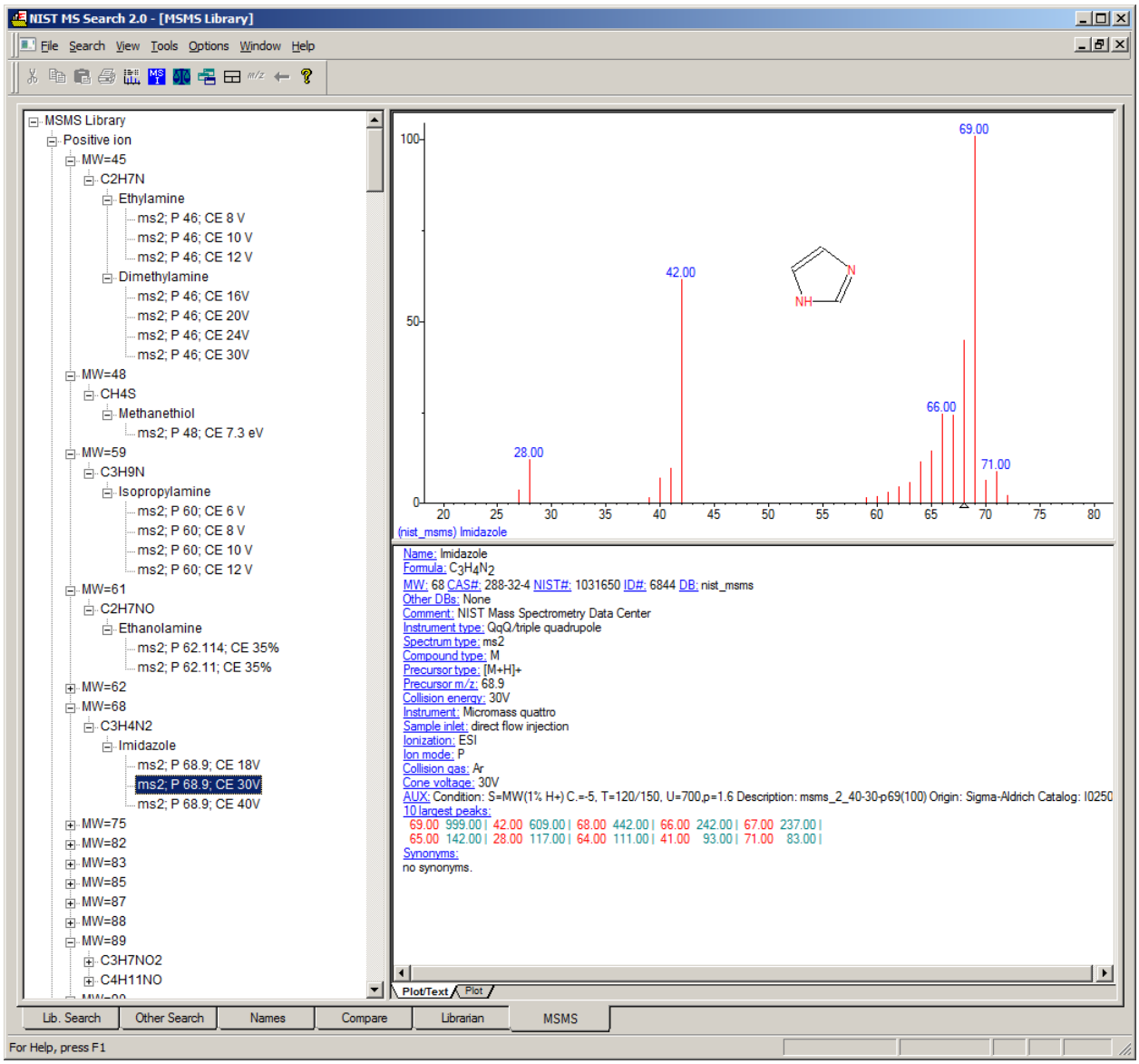
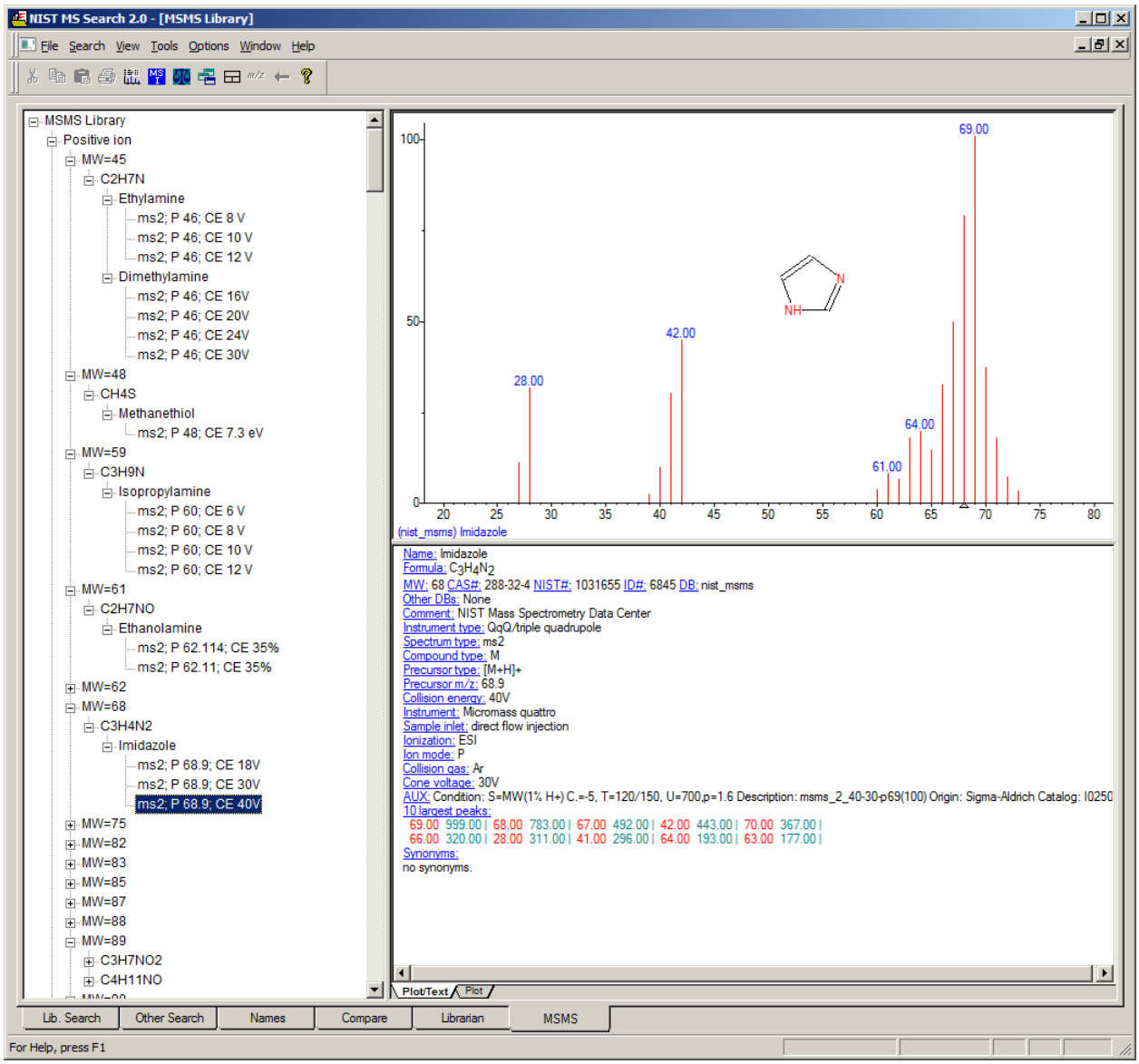
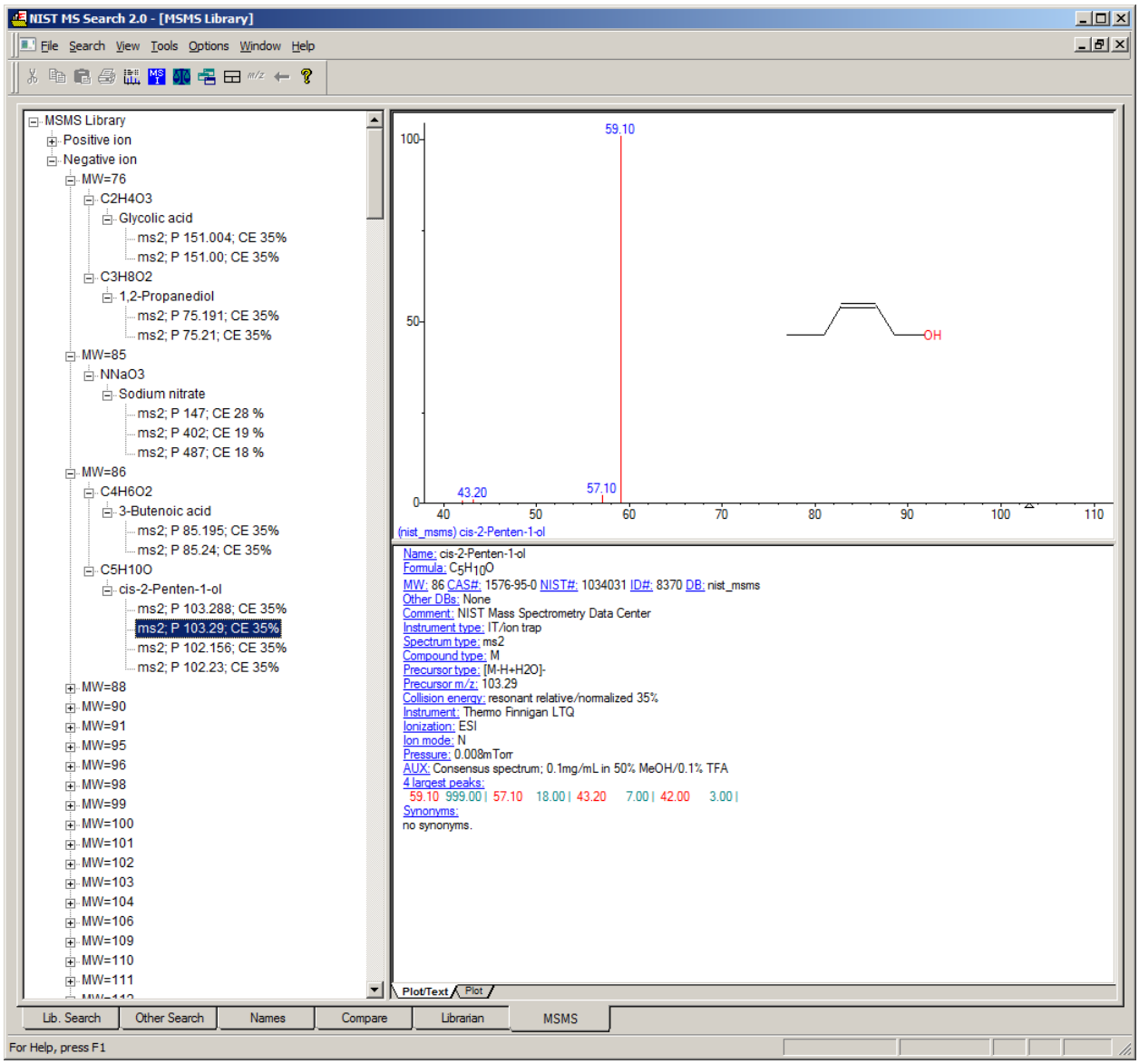
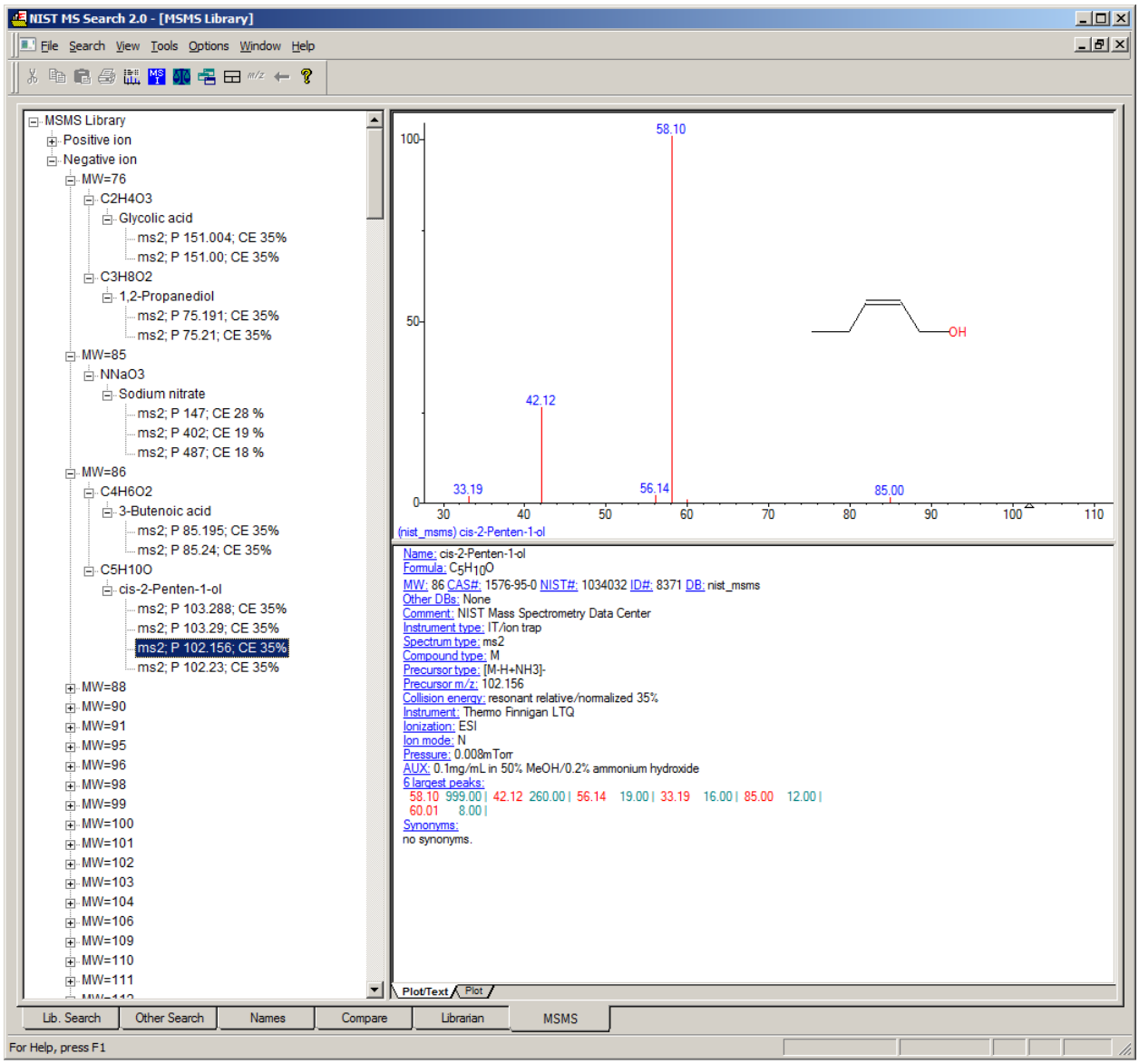
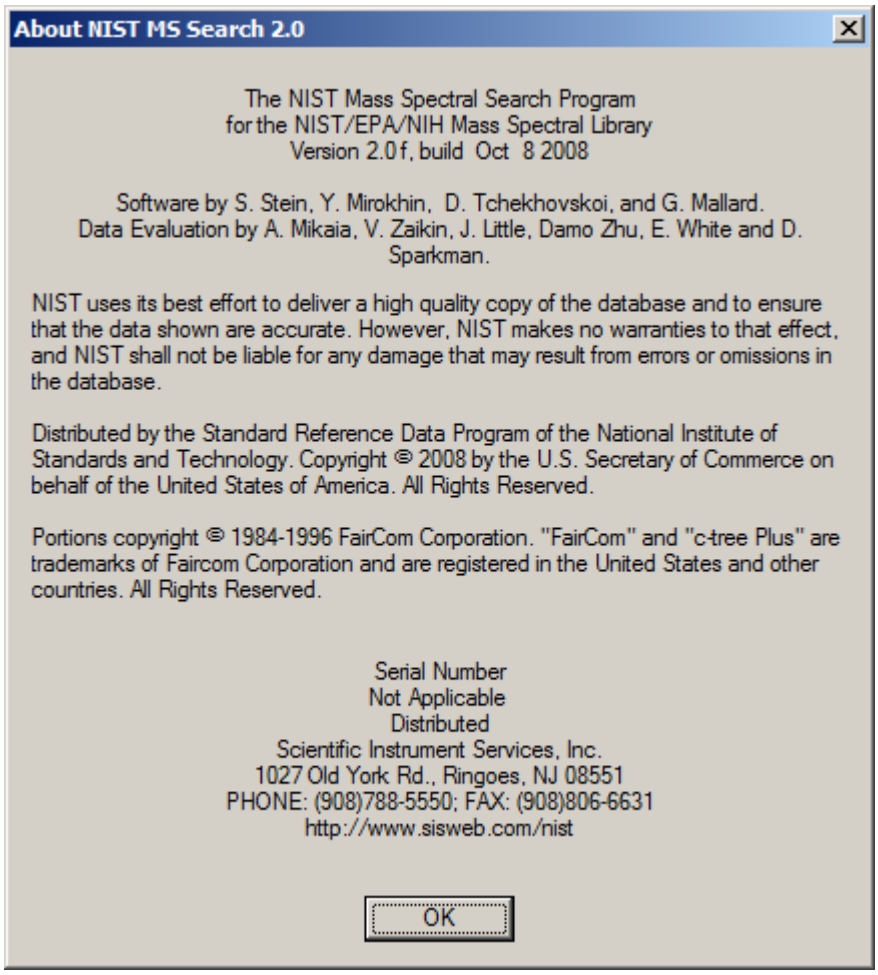

NIST MS Search 2.0 - [MSMS Library]
File Search View Tools Options Window Help
MSMS Library
Positive ion
MW=45
C2H7N
Ethylamine
ms2; P 46; CE 8 V
ms2; P 46; CE 10 V
ms2; P 46; CE 12 V
Dimethylamine
ms2; P 46; CE 16V
ms2; P 46; CE 20V
ms2; P 46; CE 24V
ms2; P 46; CE 30V
MW=48
CH4S
Methanethiol
ms2; P 48; CE 7.3 eV
MW=59
C3H9N
Isopropylamine
ms2; P 60; CE 6 V
ms2; P 60; CE 8 V
ms2; P 60; CE 10 V
ms2; P 60; CE 12 V
MW=61
C2H7NO
Ethanolamine
ms2; P 62.114; CE 35%
ms2; P 62.11; CE 35%
MW=62
MW=68
C3H4N2
Imidazole
ms2; P 68.9; CE 18V
ms2; P 68.9; CE 30V
ms2; P 68.9; CE 40V
MW=75
MW=82
MW=83
MW=85
MW=87
MW=88
MW=89
C3H7NO2
C4H11NO
69.00
42.00
28.00
40.00
59.00
67.00
71.00
(nist_msms) Imidazole
Name: Imidazole
Formula: C3H4N2
MW: 68 CAS#: 288-32-4 NIST#: 1031644 ID#: 6843 DB: nist_msms
Other DBs: None
Comment: NIST Mass Spectrometry Data Center
Instrument type: QqQ/triple quadrupole
Spectrum type: ms2
Compound type: M
Precursor type: [M+H]+
Precursor m/z: 68.9
Collision energy: 18V
Instrument: Micromass quattro
Sample inlet: direct flow injection
Ionization: ESI
Ion mode: P
Collision gas: Ar
Cone voltage: 30V
AUX: Condition: S=MW(1% H+) C.=-5, T=120/150, U=700,p=1.6 Description: msms_2_40-30-p69(100) Origin: Sigma-Aldrich Catalog: I0250
10 largest peaks:
69.00 999.00 | 42.00 396.00 | 67.00 48.00 | 66.00 43.00 | 65.00 10.00 |
63.00 9.00 | 71.00 9.00 | 64.00 8.00 | 40.00 4.00 | 28.00 2.00 |
Synonyms:
no synonyms.
Plot/Text
Plot
Lib. Search
Other Search
Names
Compare
Librarian
MSMS
For Help, press F1


NIST MS Search 2.0 - [MSMS Library]
File Search View Tools Options Window Help
MSMS Library
Positive ion
MW=45
C2H7N
Ethylamine
ms2; P 46; CE 8 V
ms2; P 46; CE 10 V
ms2; P 46; CE 12 V
Dimethylamine
ms2; P 46; CE 16V
ms2; P 46; CE 20V
ms2; P 46; CE 24V
ms2; P 46; CE 30V
MW=48
CH4S
Methanethiol
ms2; P 48; CE 7.3 eV
MW=59
C3H9N
Isopropylamine
ms2; P 60; CE 6 V
ms2; P 60; CE 8 V
ms2; P 60; CE 10 V
ms2; P 60; CE 12 V
MW=61
C2H7NO
Ethanolamine
ms2; P 62.114; CE 35%
ms2; P 62.11; CE 35%
MW=62
MW=68
C3H4N2
Imidazole
ms2; P 68.9; CE 18V
ms2; P 68.9; CE 30V
ms2; P 68.9; CE 40V
MW=75
MW=82
MW=83
MW=85
MW=87
MW=88
MW=89
C3H7NO2
C4H11NO
69.00
42.00
66.00
28.00
71.00
(nist_msms) Imidazole
Name: Imidazole
Formula: C3H4N2
MW: 68 CAS#: 288-32-4 NIST#: 1031650 ID#: 6844 DB: nist_msms
Other DBs: None
Comment: NIST Mass Spectrometry Data Center
Instrument type: QqQ/triple quadrupole
Spectrum type: ms2
Compound type: M
Precursor type: [M+H]+
Precursor m/z: 68.9
Collision energy: 30V
Instrument: Micromass quattro
Sample inlet: direct flow injection
Ionization: ESI
Ion mode: P
Collision gas: Ar
Cone voltage: 30V
AUX: Condition: S=MW(1% H+) C.=-5, T=120/150, U=700,p=1.6 Description: msms_2_40-30-p69(100) Origin: Sigma-Aldrich Catalog: I0250
10 largest peaks:
69.00 999.00 | 42.00 609.00 | 68.00 442.00 | 66.00 242.00 | 67.00 237.00 |
65.00 142.00 | 28.00 117.00 | 64.00 111.00 | 41.00 93.00 | 71.00 83.00 |
Synonyms:
no synonyms.
Plot/Text
Plot
Lib. Search
Other Search
Names
Compare
Librarian
MSMS
For Help, press F1


NIST MS Search 2.0 - [MSMS Library]
File Search View Tools Options Window Help
MSMS Library
Positive ion
MW=45
C2H7N
Ethylamine
ms2; P 46; CE 8 V
ms2; P 46; CE 10 V
ms2; P 46; CE 12 V
Dimethylamine
ms2; P 46; CE 16V
ms2; P 46; CE 20V
ms2; P 46; CE 24V
ms2; P 46; CE 30V
MW=48
CH4S
Methanethiol
ms2; P 48; CE 7.3 eV
MW=59
C3H9N
Isopropylamine
ms2; P 60; CE 6 V
ms2; P 60; CE 8 V
ms2; P 60; CE 10 V
ms2; P 60; CE 12 V
MW=61
C2H7NO
Ethanolamine
ms2; P 62.114; CE 35%
ms2; P 62.11; CE 35%
MW=62
MW=68
C3H4N2
Imidazole
ms2; P 68.9; CE 18V
ms2; P 68.9; CE 30V
ms2; P 68.9; CE 40V
MW=75
MW=82
MW=83
MW=85
MW=87
MW=88
MW=89
C3H7NO2
C4H11NO
69.00
42.00
28.00
64.00
61.00
(nist_msms) Imidazole
Name: Imidazole
Formula: C3H4N2
MW: 68 CAS#: 288-32-4 NIST#: 1031655 ID#: 6845 DB: nist_msms
Other DBs: None
Comment: NIST Mass Spectrometry Data Center
Instrument type: QqQ/triple quadrupole
Spectrum type: ms2
Compound type: M
Precursor type: [M+H]+
Precursor m/z: 68.9
Collision energy: 40V
Instrument: Micromass quattro
Sample inlet: direct flow injection
Ionization: ESI
Ion mode: P
Collision gas: Ar
Cone voltage: 30V
AUX: Condition: S=MW(1% H+) C.=-5, T=120/150, U=700,p=1.6 Description: msms_2_40-30-p69(100) Origin: Sigma-Aldrich Catalog: I0250
10 largest peaks:
69.00 999.00 | 68.00 783.00 | 67.00 492.00 | 42.00 443.00 | 70.00 367.00 |
66.00 320.00 | 28.00 311.00 | 41.00 296.00 | 64.00 193.00 | 63.00 177.00 |
Synonyms:
no synonyms.
Plot/Text
Plot
Lib. Search
Other Search
Names
Compare
Librarian
MSMS
For Help, press F1


NIST MS Search 2.0 - [MSMS Library]
File Search View Tools Options Window Help
MSMS Library
Positive ion
Negative ion
MW=76
C2H4O3
Glycolic acid
ms2; P 151.004; CE 35%
ms2; P 151.00; CE 35%
C3H8O2
1,2-Propanediol
ms2; P 75.191; CE 35%
ms2; P 75.21; CE 35%
MW=85
NNaO3
Sodium nitrate
ms2; P 147; CE 28 %
ms2; P 402; CE 19 %
ms2; P 487; CE 18 %
MW=86
C4H6O2
3-Butenoic acid
ms2; P 85.195; CE 35%
ms2; P 85.24; CE 35%
C5H10O
cis-2-Penten-1-ol
ms2; P 103.288; CE 35%
ms2; P 103.29; CE 35%
ms2; P 102.156; CE 35%
ms2; P 102.23; CE 35%
MW=88
MW=90
MW=91
MW=95
MW=96
MW=98
MW=99
MW=100
MW=101
MW=102
MW=103
MW=104
MW=106
MW=109
MW=110
MW=111
59.10
100
50
0
43.20
57.10
40
50
60
70
80
90
100
110
OH
(nist_msms) cis-2-Penten-1-ol
Name: cis-2-Penten-1-ol
Formula: C5H10O
MW: 86 CAS#: 1576-95-0 NIST#: 1034031 ID#: 8370 DB: nist_msms
Other DBs: None
Comment: NIST Mass Spectrometry Data Center
Instrument type: IT/ion trap
Spectrum type: ms2
Compound type: M
Precursor type: [M-H+H2O]-
Precursor m/z: 103.29
Collision energy: resonant relative/normalized 35%
Instrument: Thermo Finnigan LTQ
Ionization: ESI
Ion mode: N
Pressure: 0.008mTorr
AUX: Consensus spectrum; 0.1mg/mL in 50% MeOH/0.1% TFA
4 largest peaks:
59.10 999.00 | 57.10 18.00 | 43.20 7.00 | 42.00 3.00 |
Synonyms:
no synonyms.
Plot/Text
Plot
Lib. Search
Other Search
Names
Compare
Librarian
MSMS
For Help, press F1


NIST MS Search 2.0 - [MSMS Library]
File Search View Tools Options Window Help
MSMS Library
Positive ion
Negative ion
MW=76
C2H4O3
Glycolic acid
ms2; P 151.004; CE 35%
ms2; P 151.00; CE 35%
C3H8O2
1,2-Propanediol
ms2; P 75.191; CE 35%
ms2; P 75.21; CE 35%
MW=85
NNaO3
Sodium nitrate
ms2; P 147; CE 28 %
ms2; P 402; CE 19 %
ms2; P 487; CE 18 %
MW=86
C4H6O2
3-Butenoic acid
ms2; P 85.195; CE 35%
ms2; P 85.24; CE 35%
C5H10O
cis-2-Penten-1-ol
ms2; P 103.288; CE 35%
ms2; P 103.29; CE 35%
ms2; P 102.156; CE 35%
ms2; P 102.23; CE 35%
MW=88
MW=90
MW=91
MW=95
MW=96
MW=98
MW=99
MW=100
MW=101
MW=102
MW=103
MW=104
MW=106
MW=109
MW=110
MW=111
58.10
42.12
33.19
56.14
85.00
OH
(nist_msms) cis-2-Penten-1-ol
Name: cis-2-Penten-1-ol
Formula: C5H10O
MW: 86 CAS#: 1576-95-0 NIST#: 1034032 ID#: 8371 DB: nist_msms
Other DBs: None
Comment: NIST Mass Spectrometry Data Center
Instrument type: IT/ion trap
Spectrum type: ms2
Compound type: M
Precursor type: [M-H+NH3]-
Precursor m/z: 102.156
Collision energy: resonant relative/normalized 35%
Instrument: Thermo Finnigan LTQ
Ionization: ESI
Ion mode: N
Pressure: 0.008mTorr
AUX: 0.1mg/mL in 50% MeOH/0.2% ammonium hydroxide
6 largest peaks:
58.10 999.00 | 42.12 260.00 | 56.14 19.00 | 33.19 16.00 | 85.00 12.00 | 60.01 8.00 |
Synonyms:
no synonyms.
Plot/Text
Plot
Lib. Search
Other Search
Names
Compare
Librarian
MSMS
For Help, press F1


About NIST MS Search 2.0
The NIST Mass Spectral Search Program
for the NIST/EPA/NIH Mass Spectral Library
Version 2.0 f, build Oct 8 2008
Software by S. Stein, Y. Mirokhin, D. Tchekhovskoi, and G. Mallard.
Data Evaluation by A. Mikaia, V. Zaikin, J. Little, Damo Zhu, E. White and D. Sparkman.
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