

Data Path : C:\MSDCHEM\1\DATA\20-CRT-300\

Data File : 121_03.D

Acq On : 7 Jul 2020 20:03

Operator :

Sample : 121

Misc :

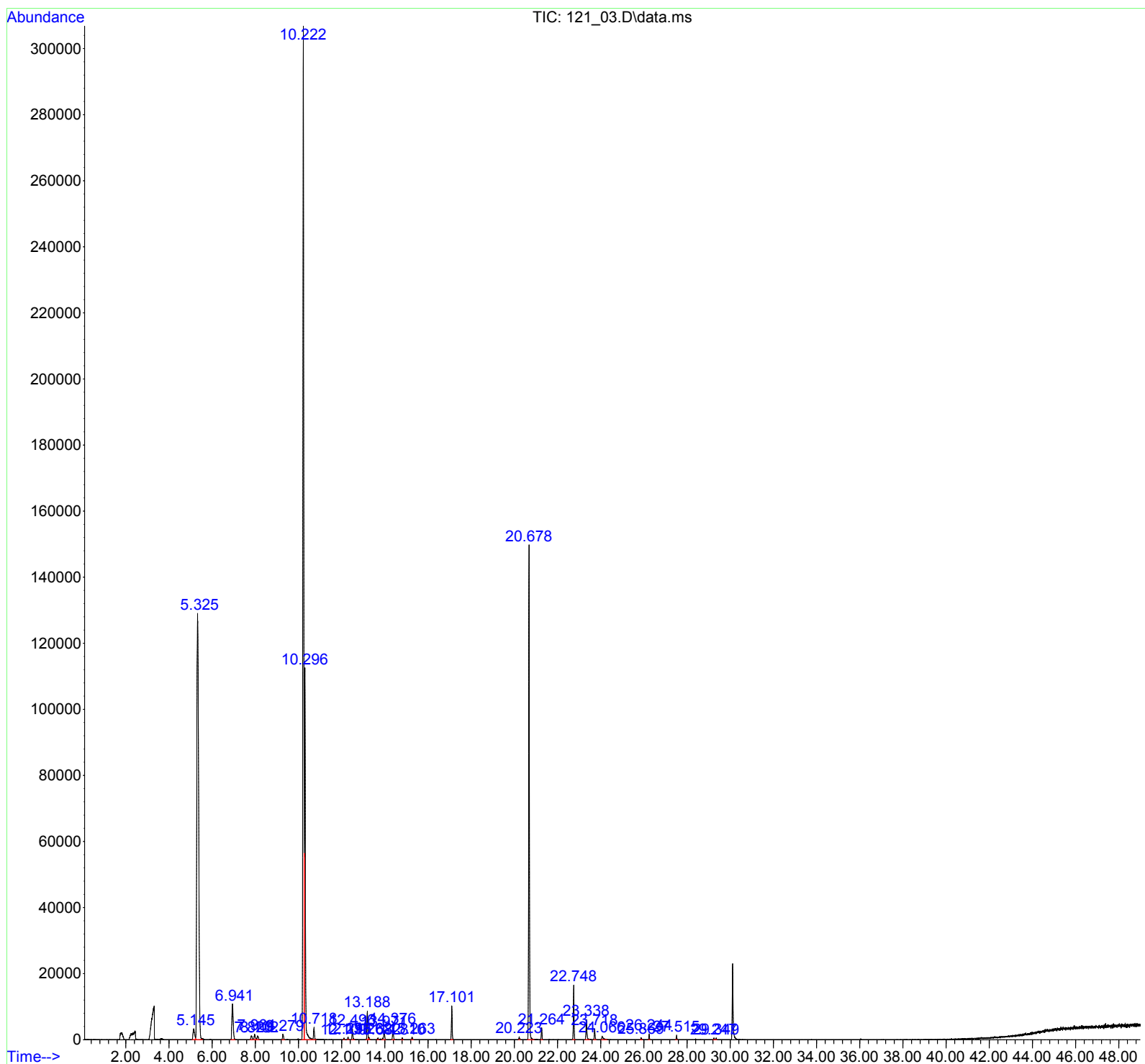
ALS Vial : 9 Sample Multiplier: 1

Search Libraries: C:\Database\NIST11.L

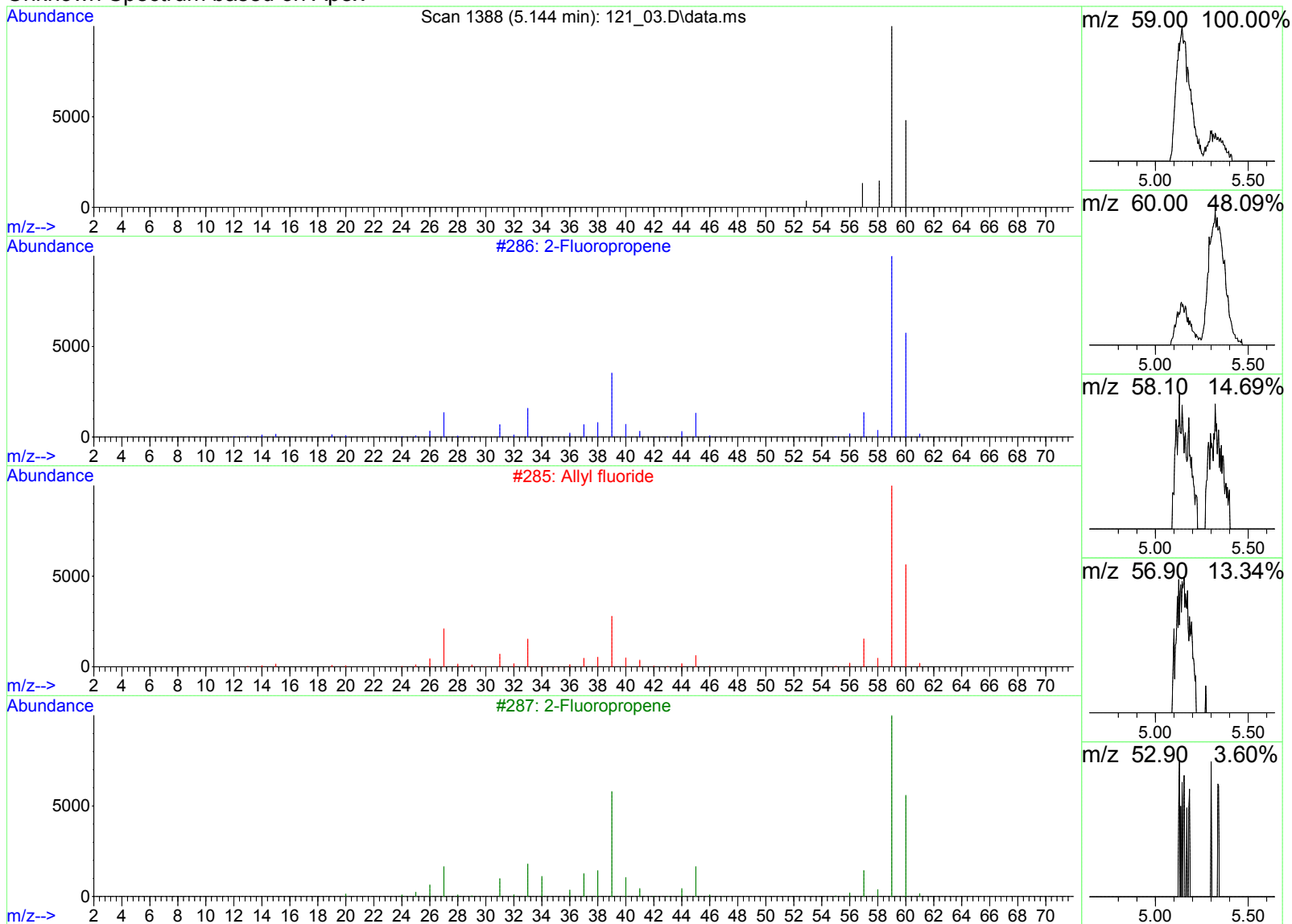
Minimum Quality: 0

Unknown Spectrum: Apex

Integration Events: ChemStation Integrator - autoint1.e



Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

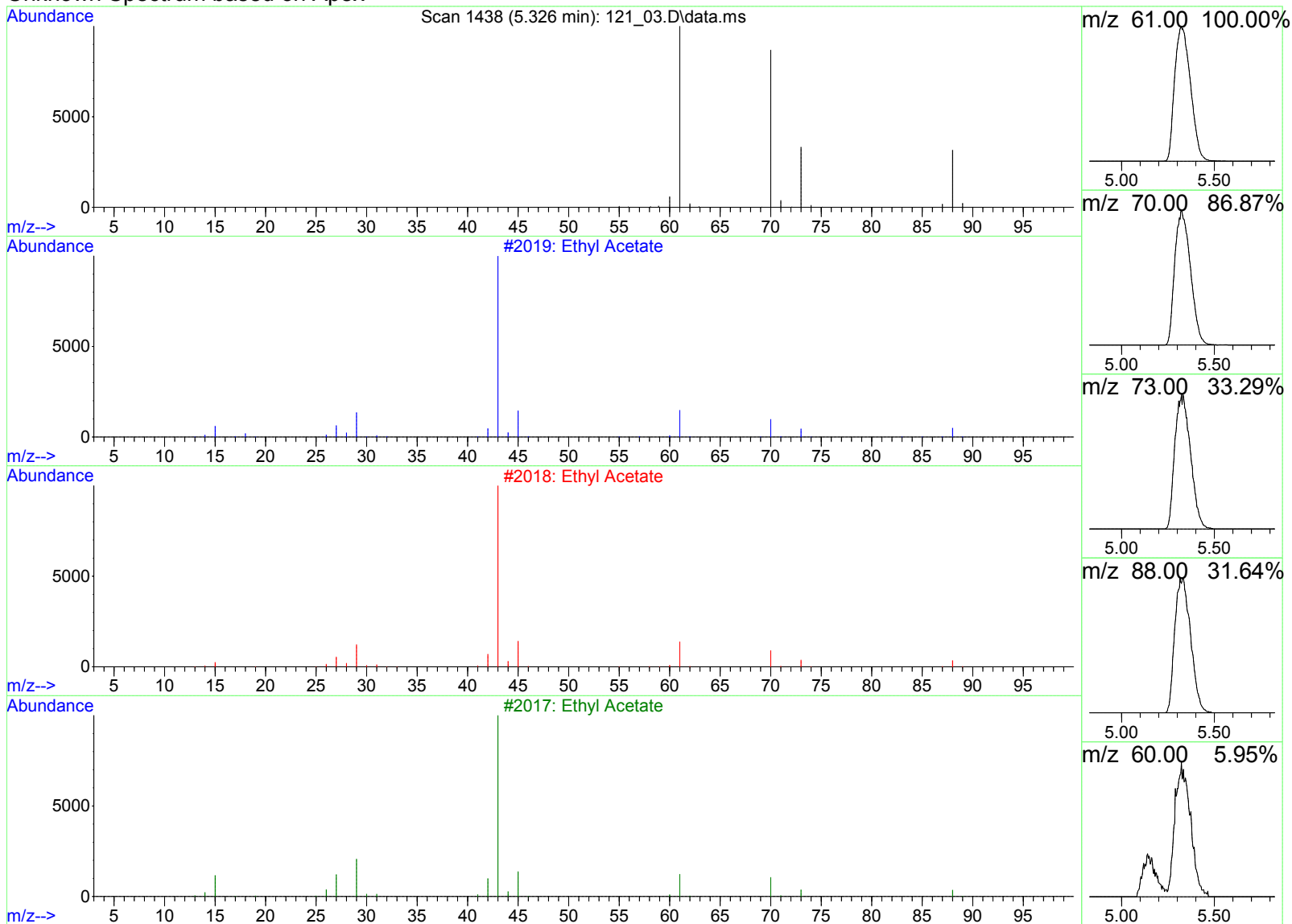
Sample : 121

Peak Number: 1 at 5.144 min Area: 164973 Area % 0.63

The 3 best hits from each library.

	Ref#	CAS#	Qual
C:\Database\NIST11.L			
1 2-Fluoropropene	286	001184-60-7	9
2 Allyl fluoride	285	000818-92-8	9
3 2-Fluoropropene	287	001184-60-7	9

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

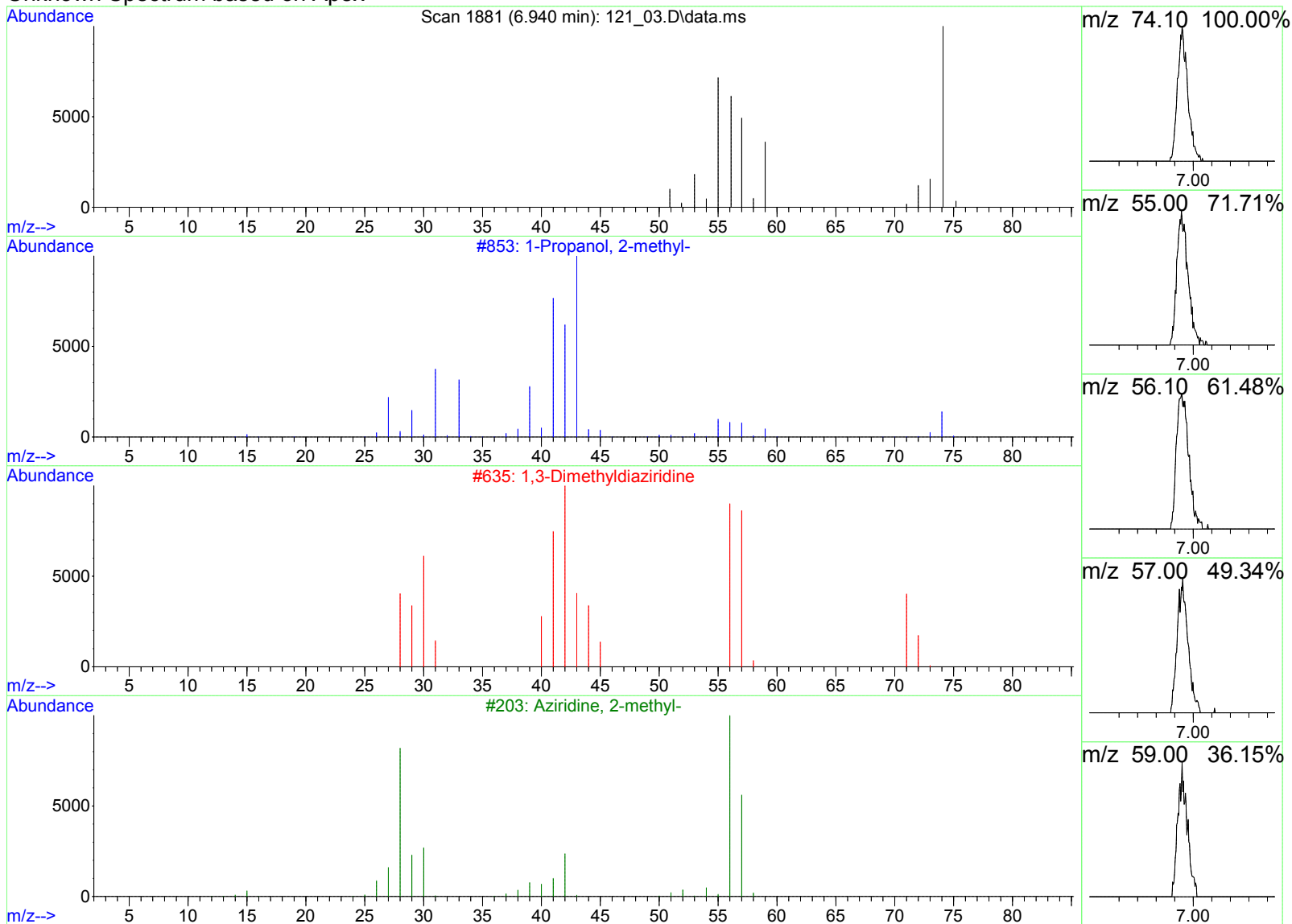
Peak Number: 2 at 5.326 min Area: 7625772 Area % 29.22

The 3 best hits from each library. Ref# CAS# Qual

C:\Database\NIST11.L

1 Ethyl Acetate	2019 000141-78-6	78
2 Ethyl Acetate	2018 000141-78-6	64
3 Ethyl Acetate	2017 000141-78-6	9

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

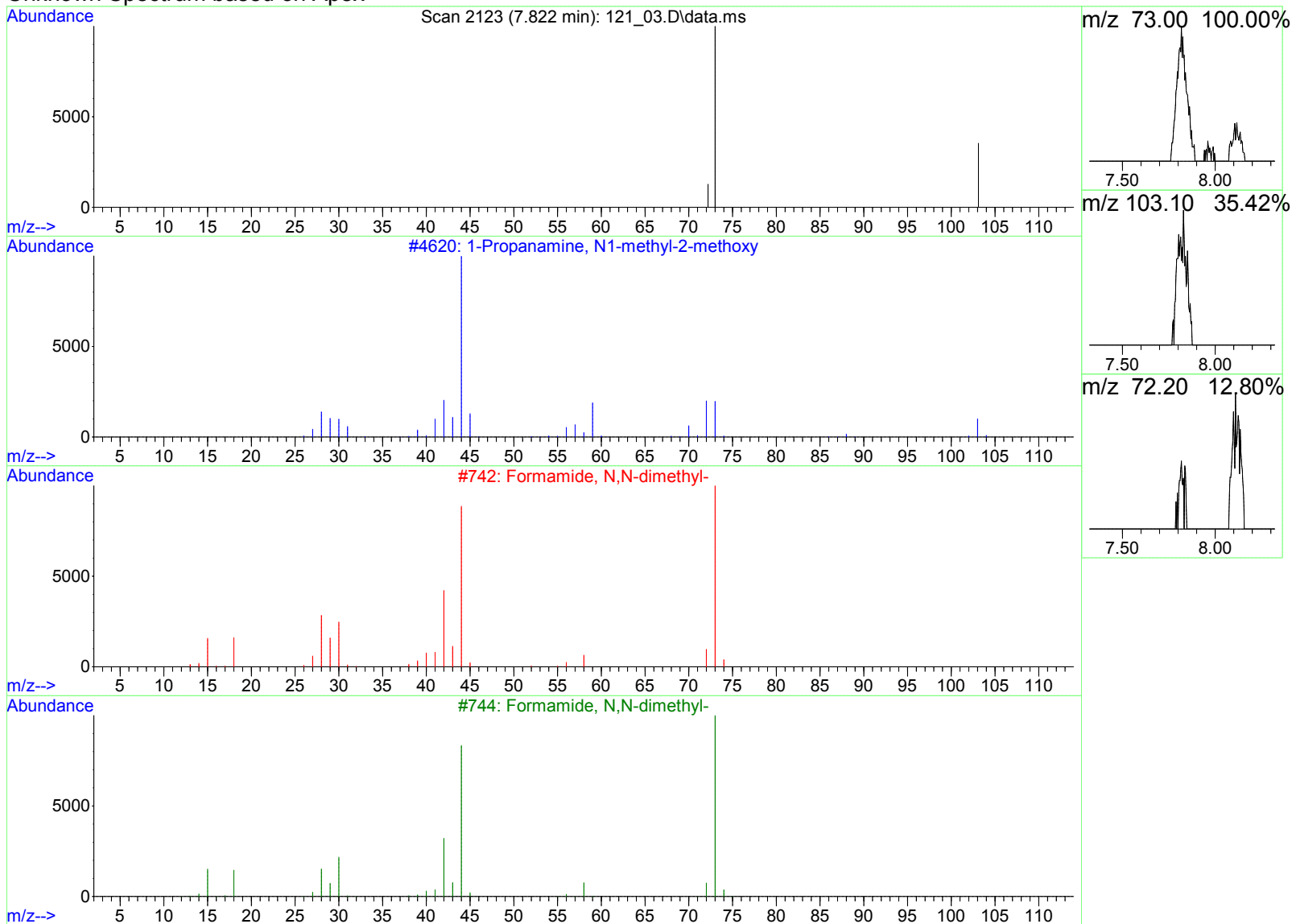
Peak Number: 3 at 6.940 min Area: 464843 Area % 1.78

The 3 best hits from each library. Ref# CAS# Qual

C:\Database\NIST11.L

1	1-Propanol, 2-methyl-	853	000078-83-1	50
2	1,3-Dimethyldiaziridine	635	026177-36-6	9
3	Aziridine, 2-methyl-	203	000075-55-8	9

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

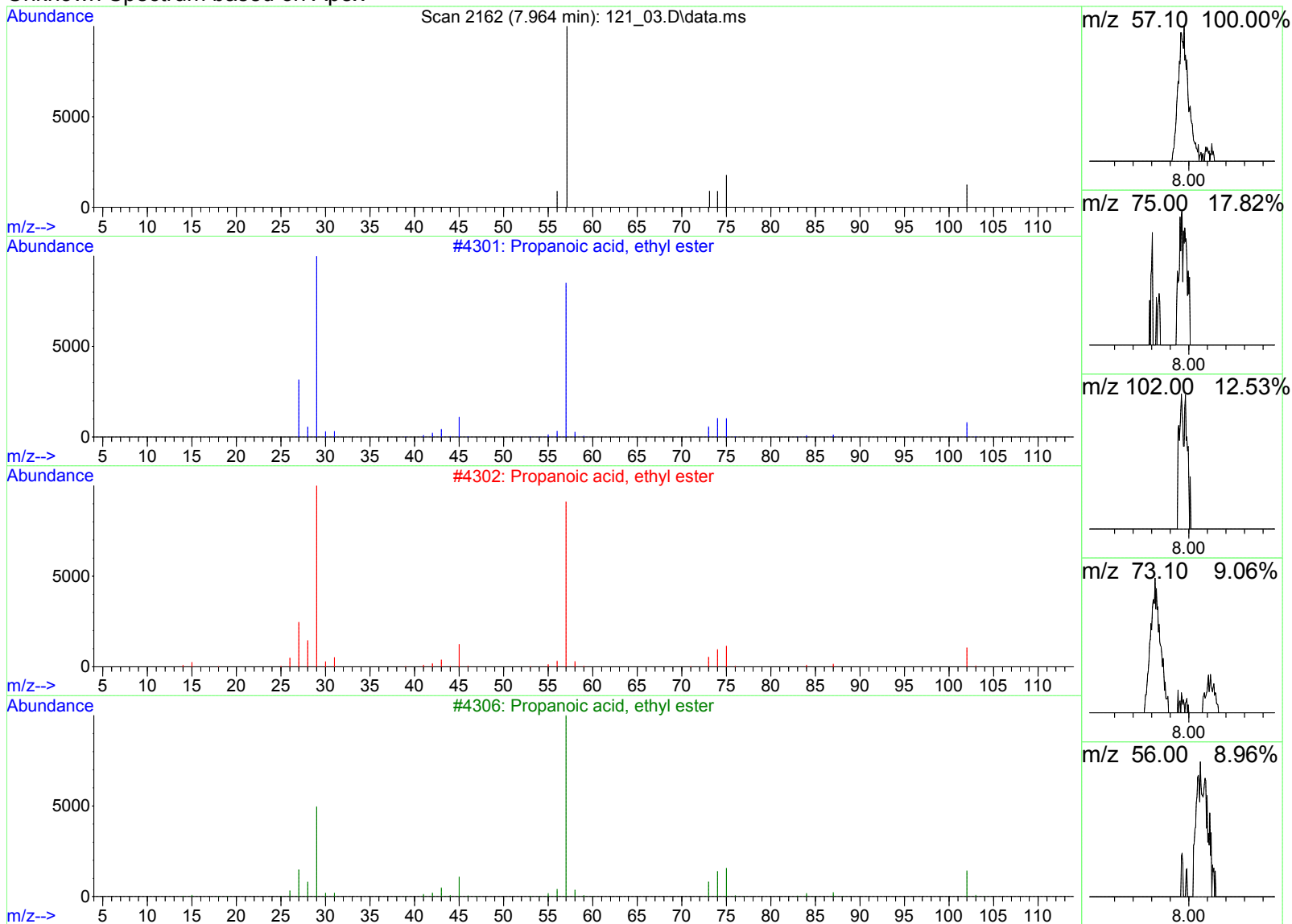
Peak Number: 4 at 7.822 min Area: 46138 Area % 0.18

The 3 best hits from each library. Ref# CAS# Qual

C:\Database\NIST11.L

1	1-Propanamine, N1-methyl-2-methoxy	4620	1000198-01-0	4
2	Formamide, N,N-dimethyl-	742	000068-12-2	4
3	Formamide, N,N-dimethyl-	744	000068-12-2	3

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

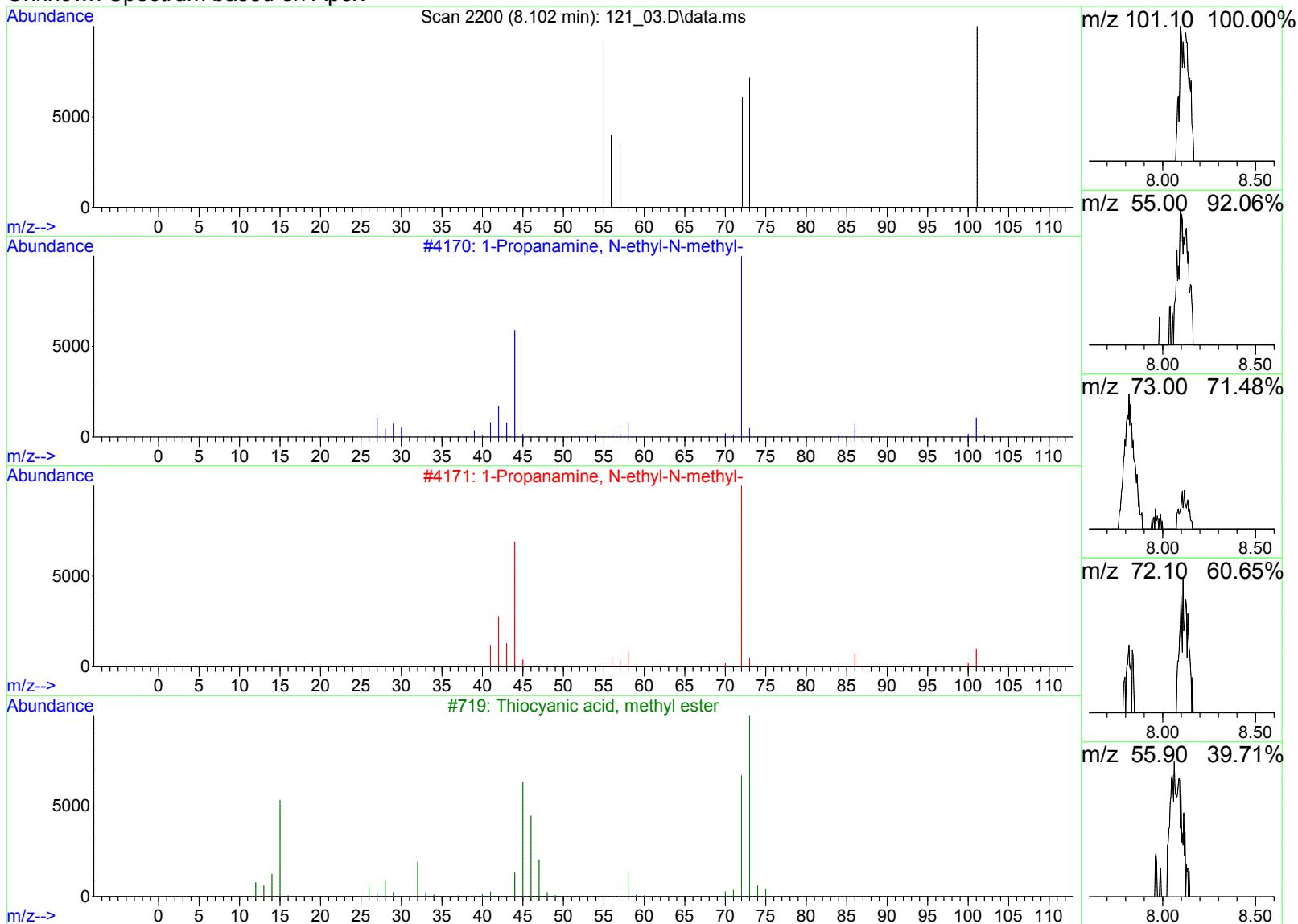
Peak Number: 5 at 7.964 min Area: 56204 Area % 0.22

The 3 best hits from each library. Ref# CAS# Qual

C:\Database\NIST11.L

1 Propanoic acid, ethyl ester	4301 000105-37-3	74
2 Propanoic acid, ethyl ester	4302 000105-37-3	9
3 Propanoic acid, ethyl ester	4306 000105-37-3	5

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

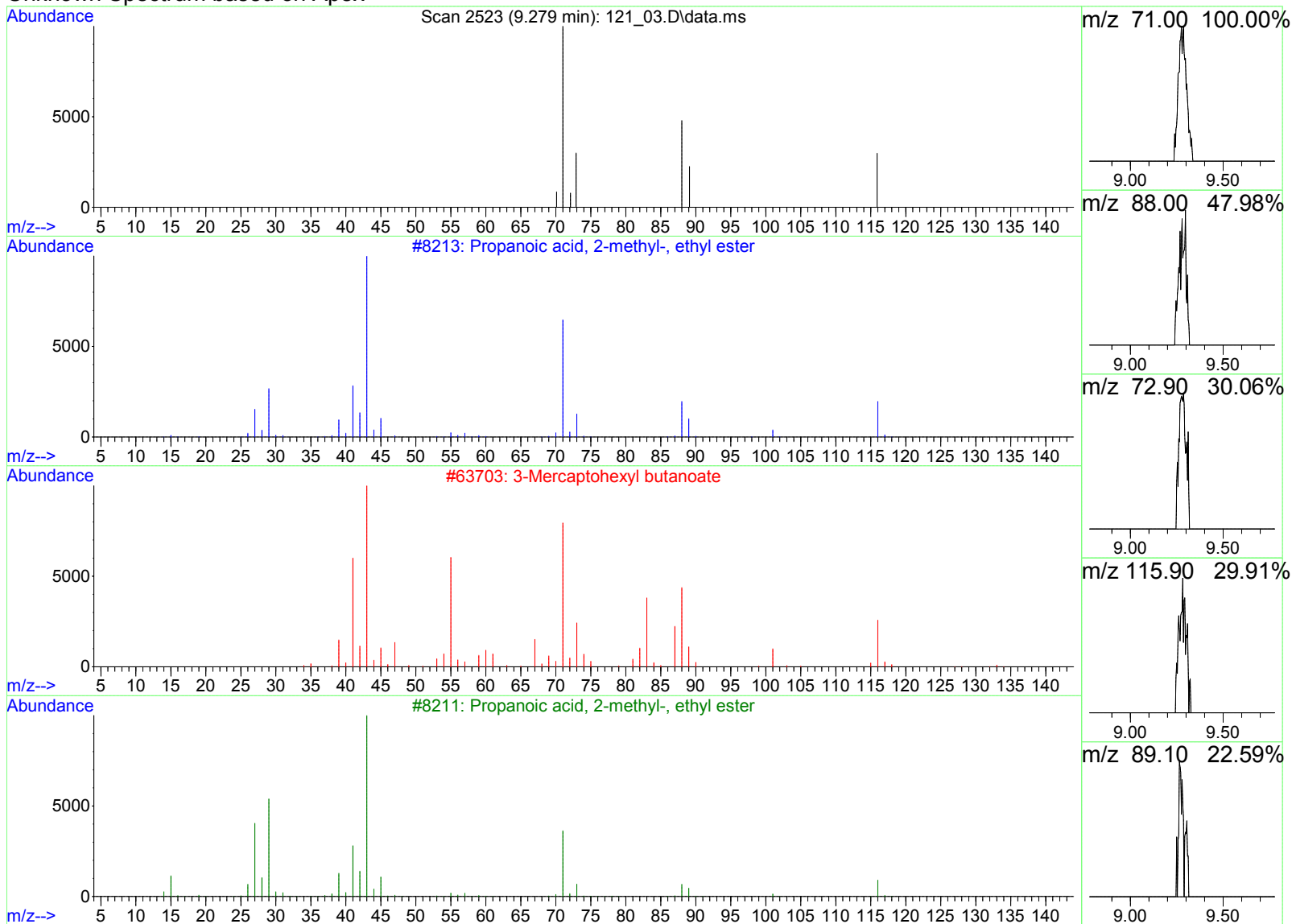
Peak Number: 6 at 8.102 min Area: 51663 Area % 0.20

The 3 best hits from each library. Ref# CAS# Qual

C:\Database\NIST11.L

1	1-Propanamine, N-ethyl-N-methyl-	4170	004458-32-6	5
2	1-Propanamine, N-ethyl-N-methyl-	4171	004458-32-6	5
3	Thiocyanic acid, methyl ester	719	000556-64-9	4

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

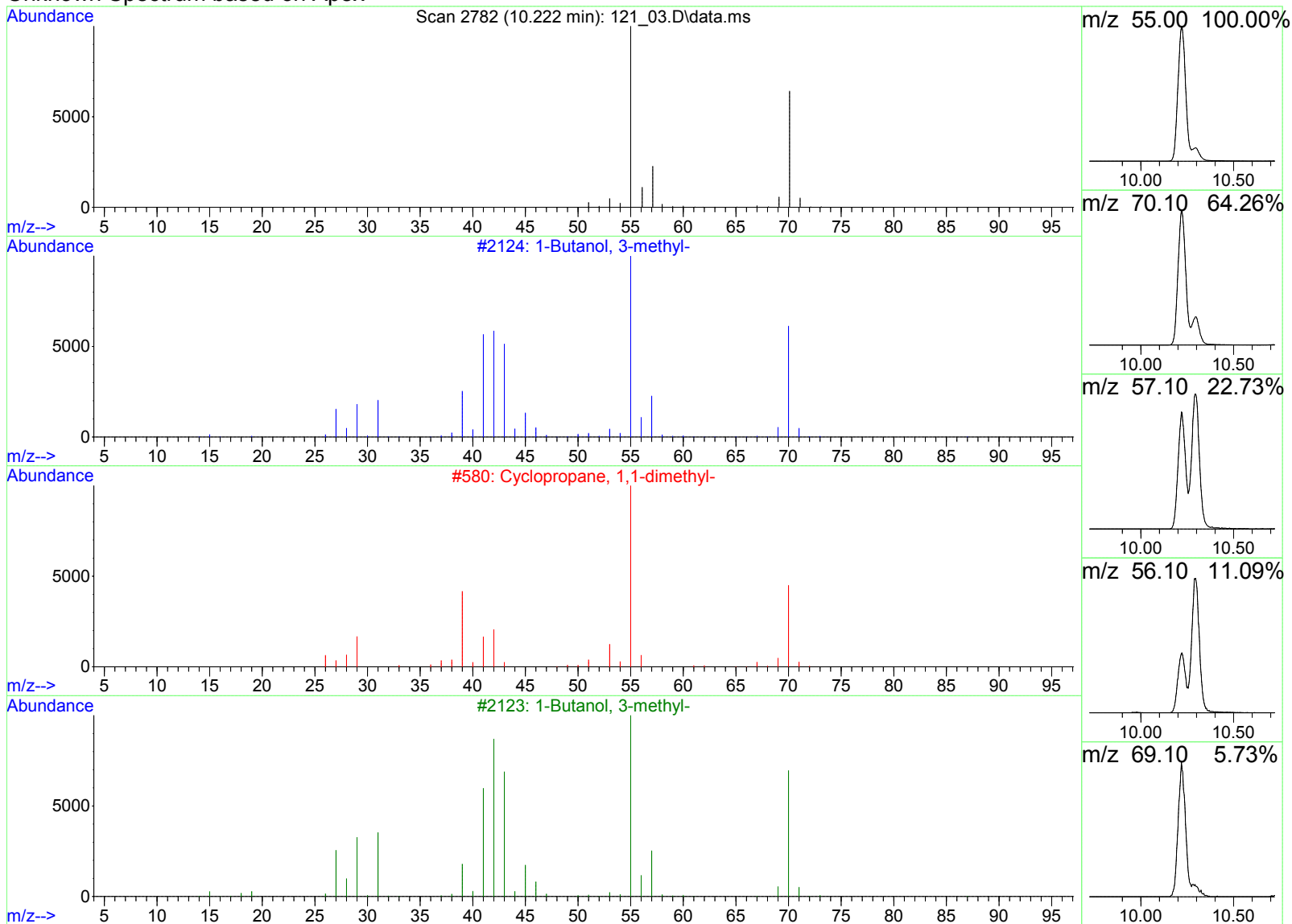
Peak Number: 7 at 9.279 min Area: 50481 Area % 0.19

The 3 best hits from each library. Ref# CAS# Qual

C:\Database\NIST11.L

1 Propanoic acid, 2-methyl-, ethyl...	8213 000097-62-1	83
2 3-Mercaptohexyl butanoate	63703 136954-21-7	64
3 Propanoic acid, 2-methyl-, ethyl...	8211 000097-62-1	9

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

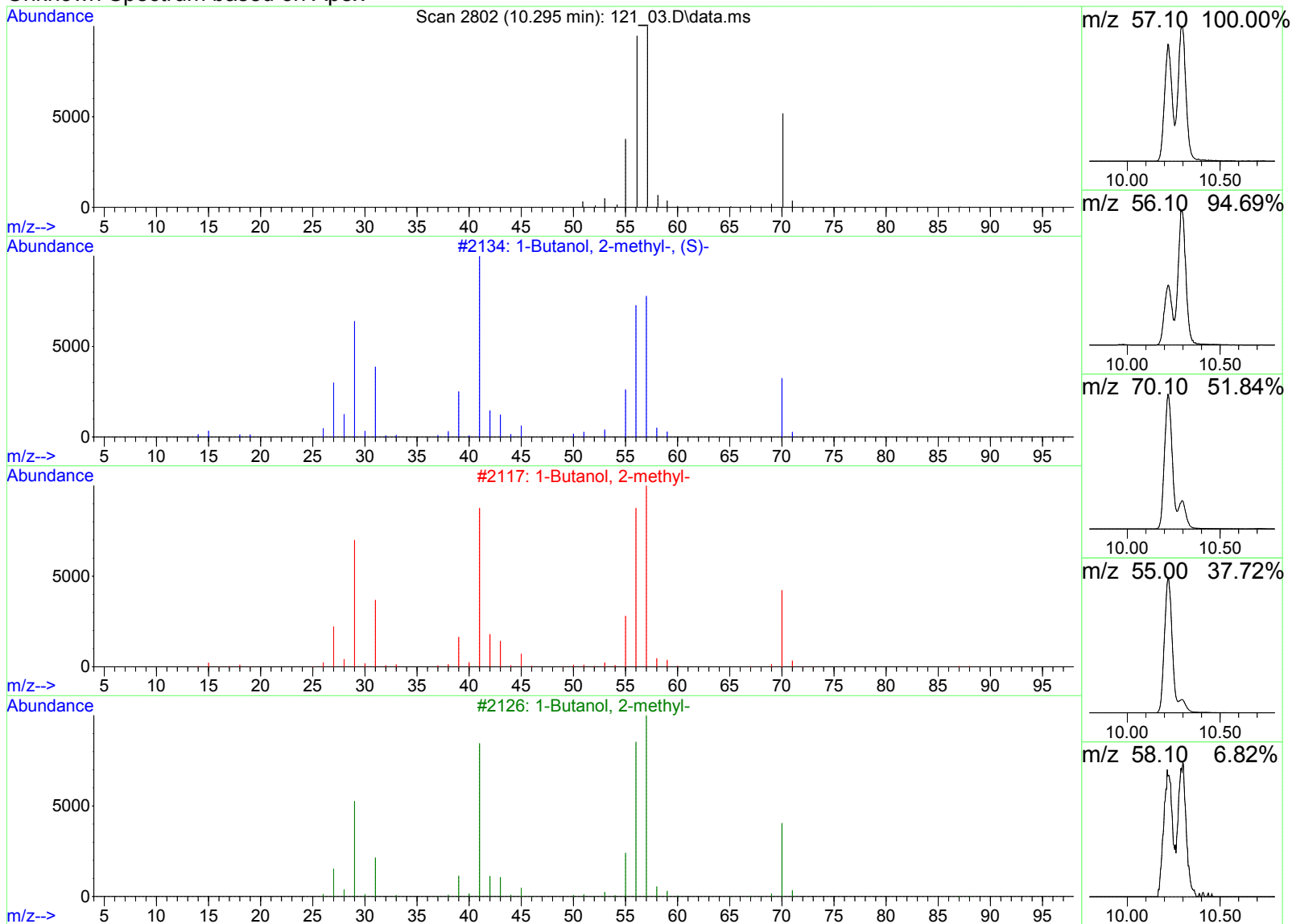
Peak Number: 8 at 10.222 min Area: 8829889 Area % 33.83

The 3 best hits from each library. Ref# CAS# Qual

C:\Database\NIST11.L

1 1-Butanol, 3-methyl-	2124	000123-51-3	64
2 Cyclopropane, 1,1-dimethyl-	580	001630-94-0	64
3 1-Butanol, 3-methyl-	2123	000123-51-3	56

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

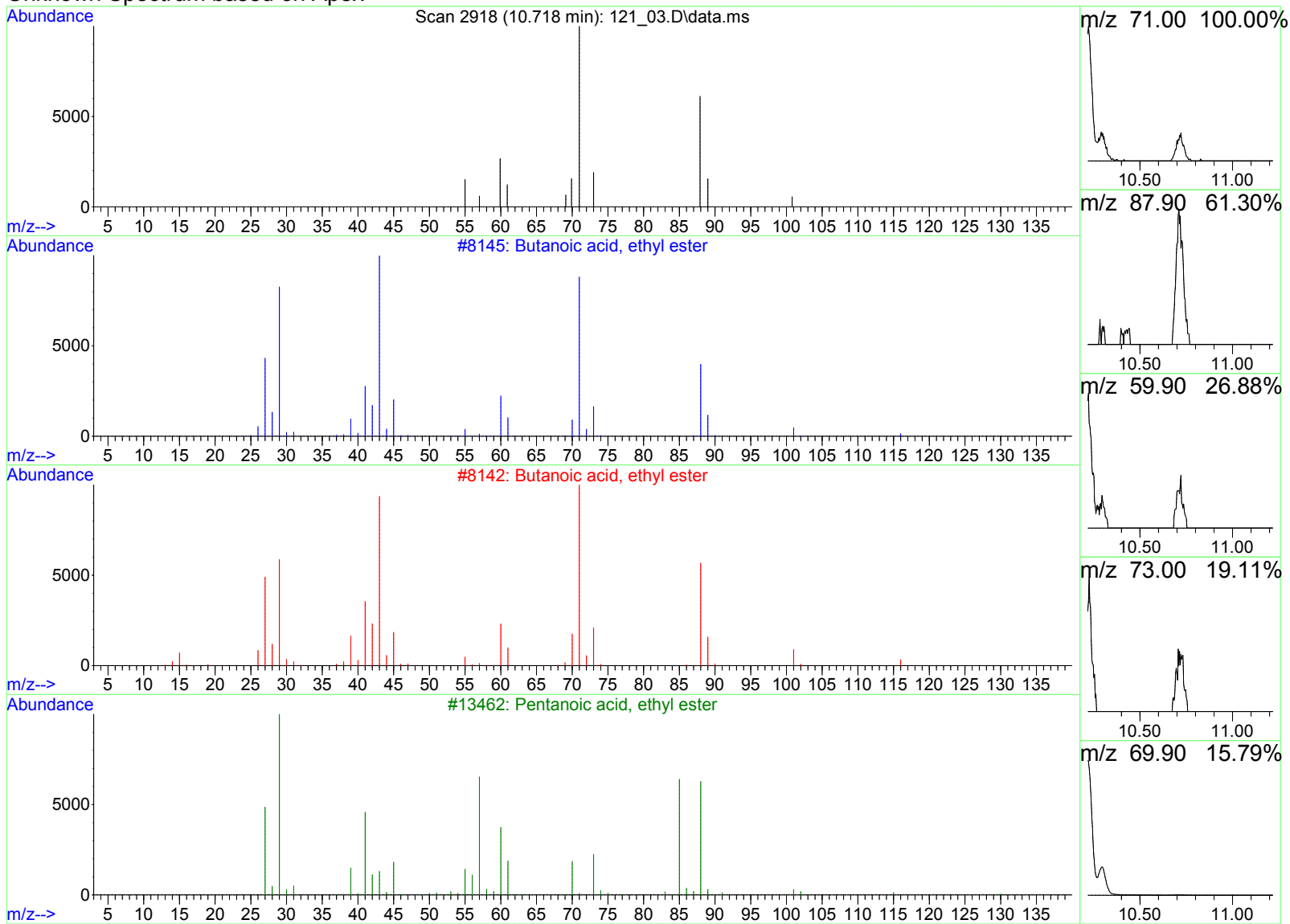
Peak Number: 9 at 10.295 min Area: 3382759 Area % 12.96

The 3 best hits from each library. Ref# CAS# Qual

C:\Database\NIST11.L

1	1-Butanol, 2-methyl-, (S)-	2134	001565-80-6	83
2	1-Butanol, 2-methyl-	2117	000137-32-6	78
3	1-Butanol, 2-methyl-	2126	000137-32-6	74

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

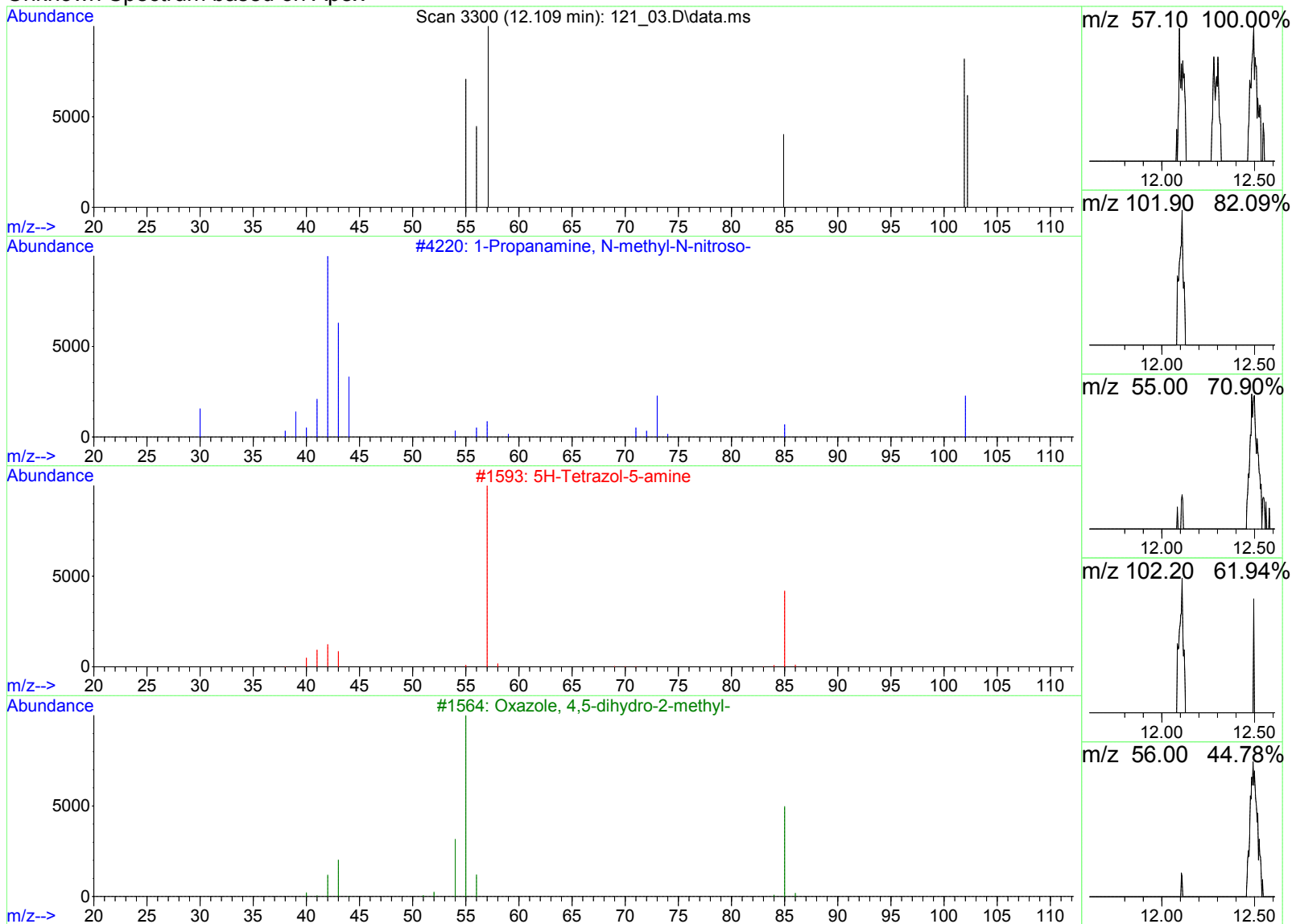
Peak Number: 10 at 10.718 min Area: 113086 Area % 0.43

The 3 best hits from each library. Ref# CAS# Qual

C:\Database\NIST11.L

1 Butanoic acid, ethyl ester	8145	000105-54-4	83
2 Butanoic acid, ethyl ester	8142	000105-54-4	43
3 Pentanoic acid, ethyl ester	13462	000539-82-2	25

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

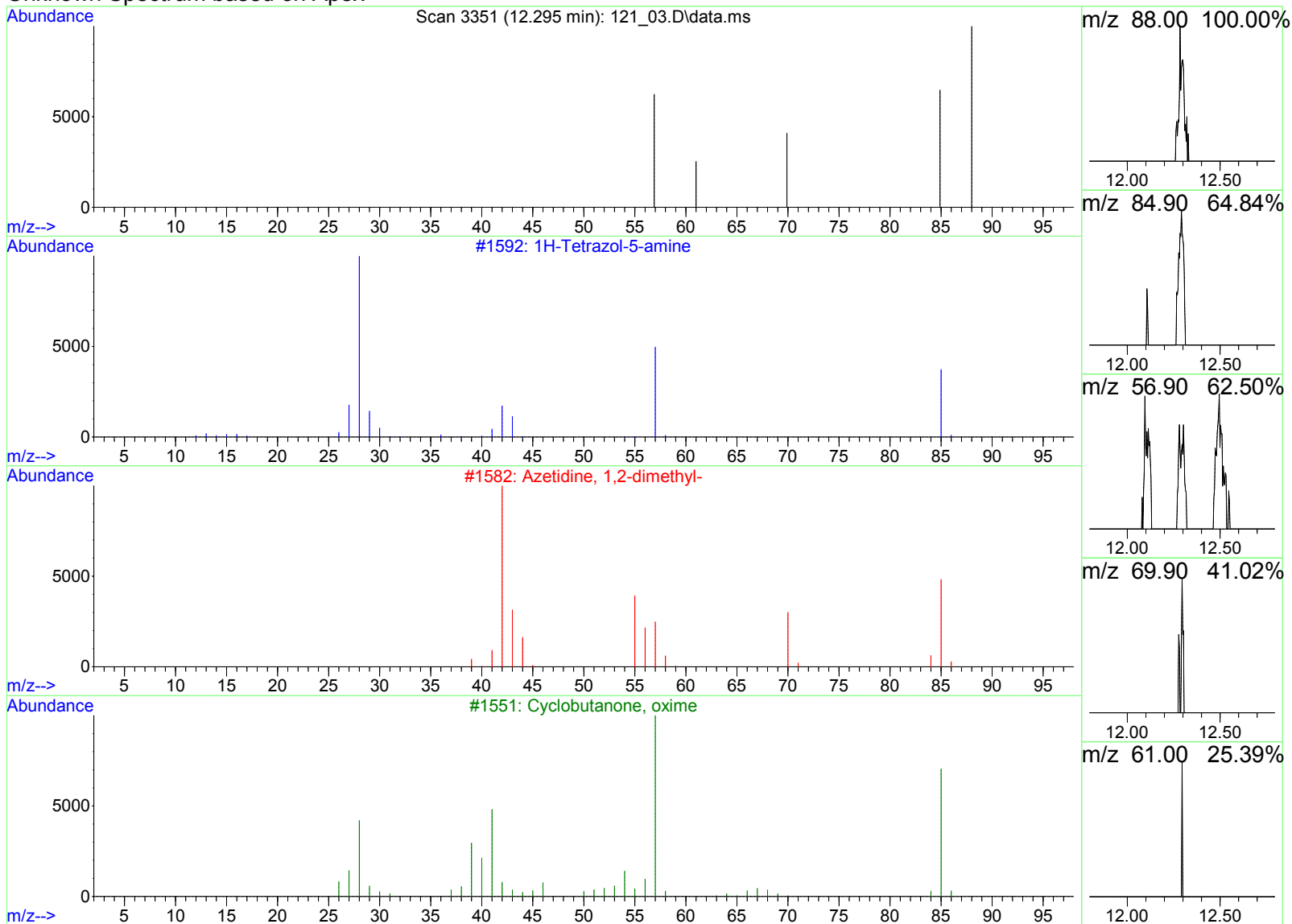
Peak Number: 11 at 12.109 min Area: 8271 Area % 0.03

The 3 best hits from each library. Ref# CAS# Qual

C:\Database\NIST11.L

1	1-Propanamine, N-methyl-N-nitroso-	4220	000924-46-9	5
2	5H-Tetrazol-5-amine	1593	1000273-02-0	4
3	Oxazole, 4,5-dihydro-2-methyl-	1564	001120-64-5	4

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

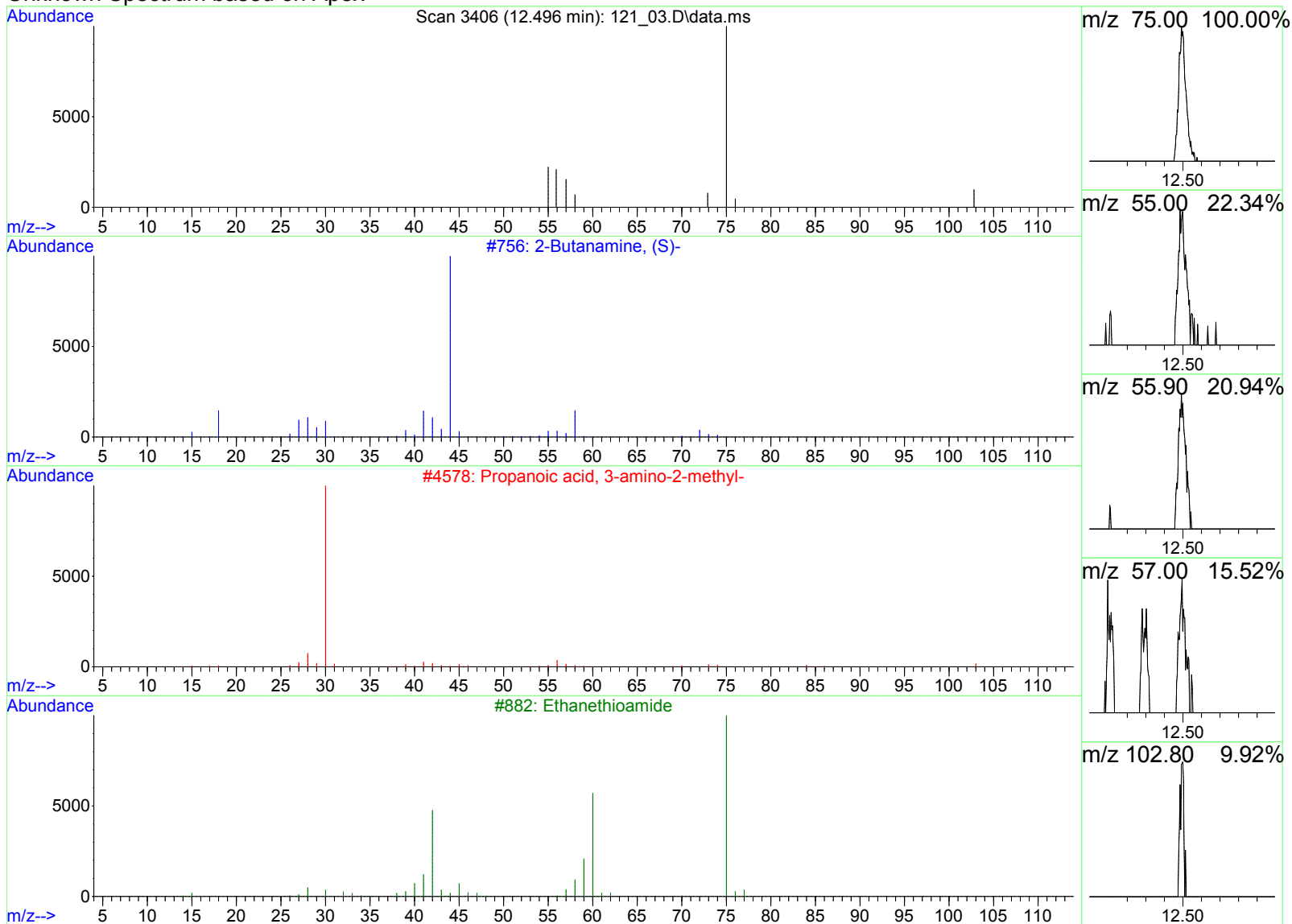
Peak Number: 12 at 12.295 min Area: 16308 Area % 0.06

The 3 best hits from each library. Ref# CAS# Qual

C:\Database\NIST11.L

1	1H-Tetrazol-5-amine	1592	004418-61-5	4
2	Azetidine, 1,2-dimethyl-	1582	051764-32-0	4
3	Cyclobutanone, oxime	1551	002972-05-6	4

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

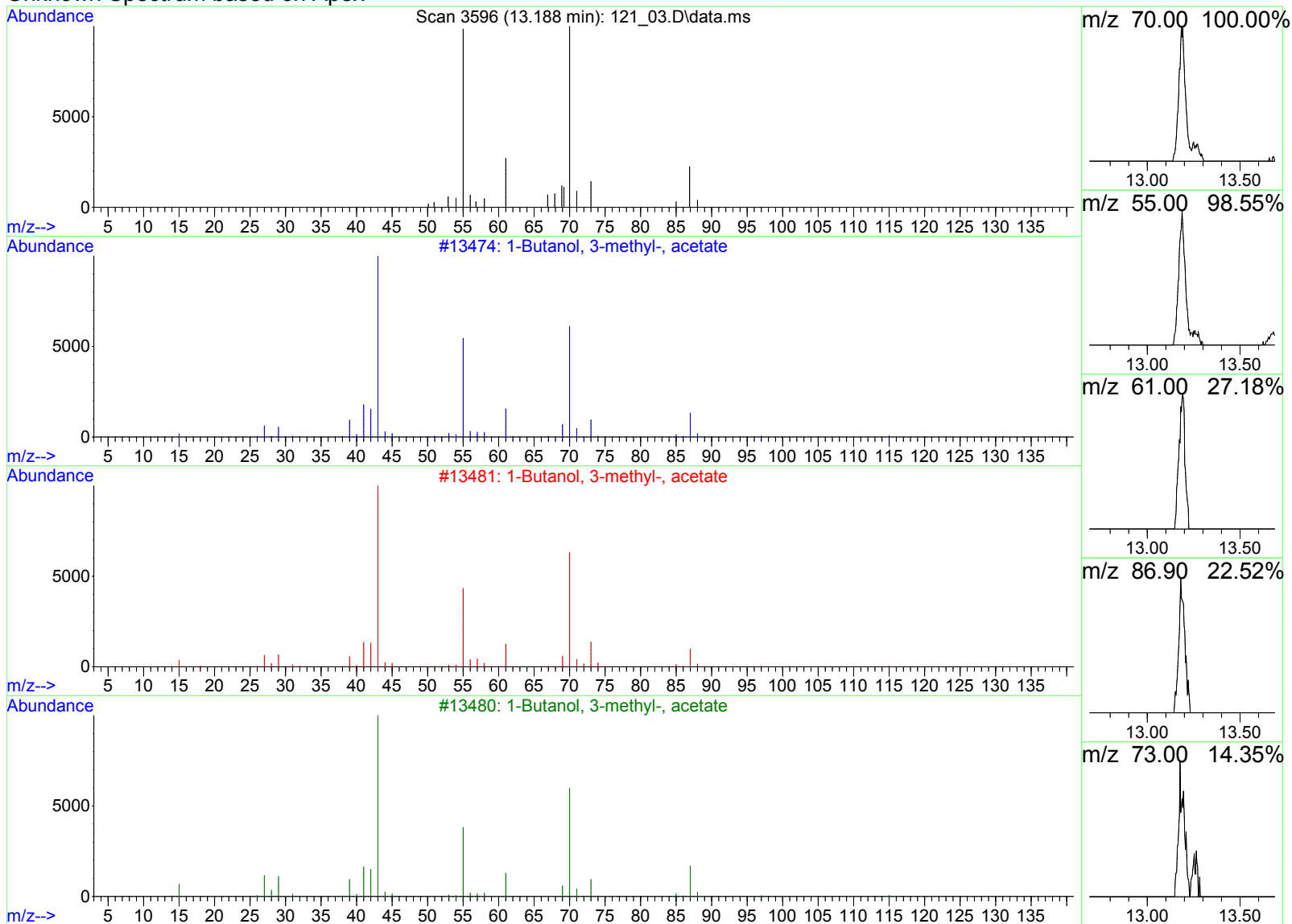
Peak Number: 13 at 12.496 min Area: 86982 Area % 0.33

The 3 best hits from each library. Ref# CAS# Qual

C:\Database\NIST11.L

1 2-Butanamine, (S)-	756 000513-49-5	5
2 Propanoic acid, 3-amino-2-methyl-	4578 000144-90-1	5
3 Ethanethioamide	882 000062-55-5	5

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

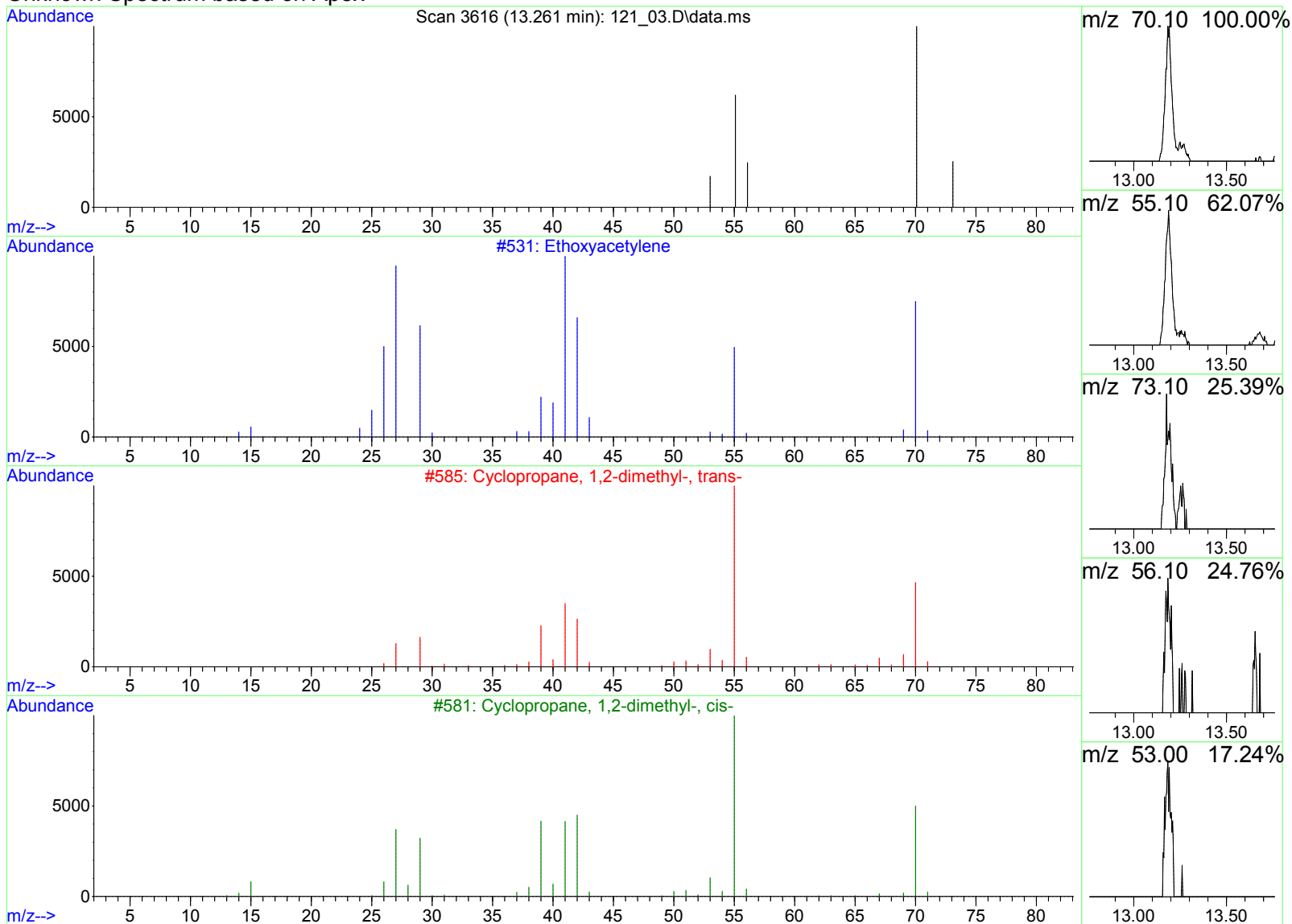
Peak Number: 14 at 13.188 min Area: 212711 Area % 0.81

The 3 best hits from each library. Ref# CAS# Qual

C:\Database\NIST11.L

1	1-Butanol, 3-methyl-, acetate	13474	000123-92-2	83
2	1-Butanol, 3-methyl-, acetate	13481	000123-92-2	74
3	1-Butanol, 3-methyl-, acetate	13480	000123-92-2	72

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

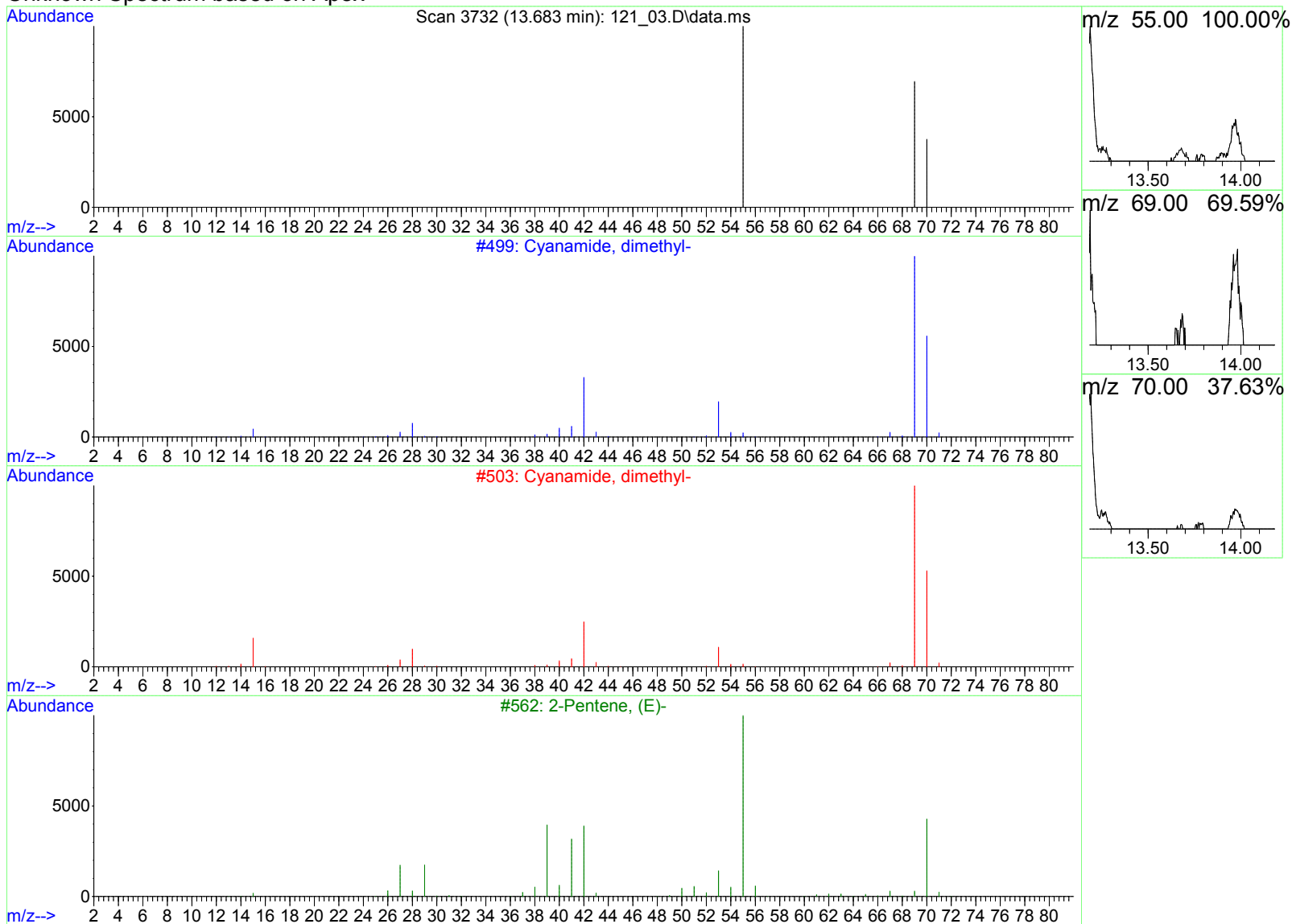
Peak Number: 15 at 13.261 min Area: 19105 Area % 0.07

The 3 best hits from each library. Ref# CAS# Qual

C:\Database\NIST11.L

- | | | | |
|---------------------------------------|-----|-------------|---|
| 1 Ethoxyacetylene | 531 | 000927-80-0 | 4 |
| 2 Cyclopropane, 1,2-dimethyl-, trans- | 585 | 002402-06-4 | 4 |
| 3 Cyclopropane, 1,2-dimethyl-, cis- | 581 | 000930-18-7 | 4 |

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

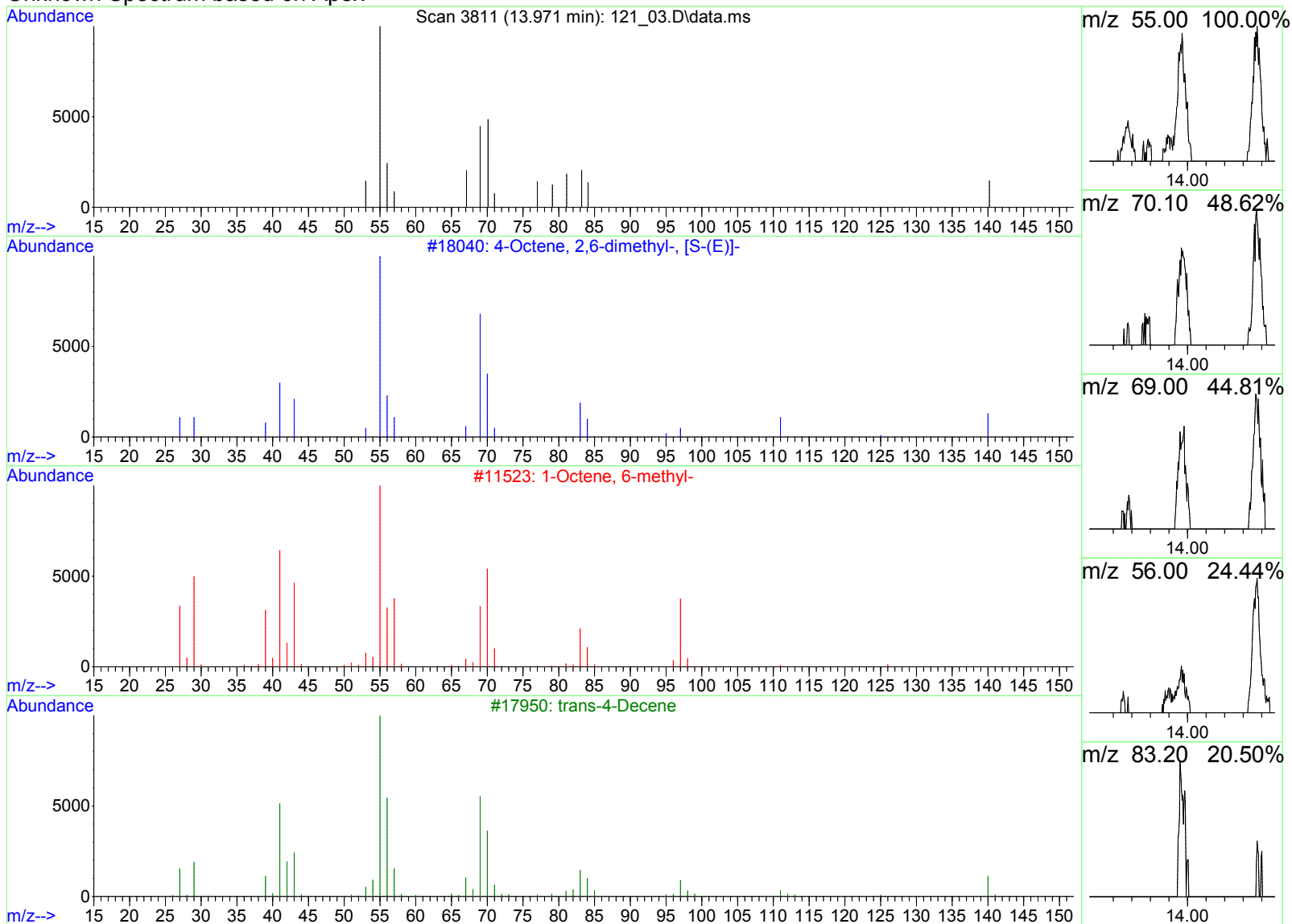
Peak Number: 16 at 13.683 min Area: 10672 Area % 0.04

The 3 best hits from each library. Ref# CAS# Qual

C:\Database\NIST11.L

1 Cyanamide, dimethyl-	499	001467-79-4	4
2 Cyanamide, dimethyl-	503	001467-79-4	4
3 2-Pentene, (E)-	562	000646-04-8	4

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

Peak Number: 17 at 13.971 min Area: 93636 Area % 0.36

The 3 best hits from each library. Ref# CAS# Qual

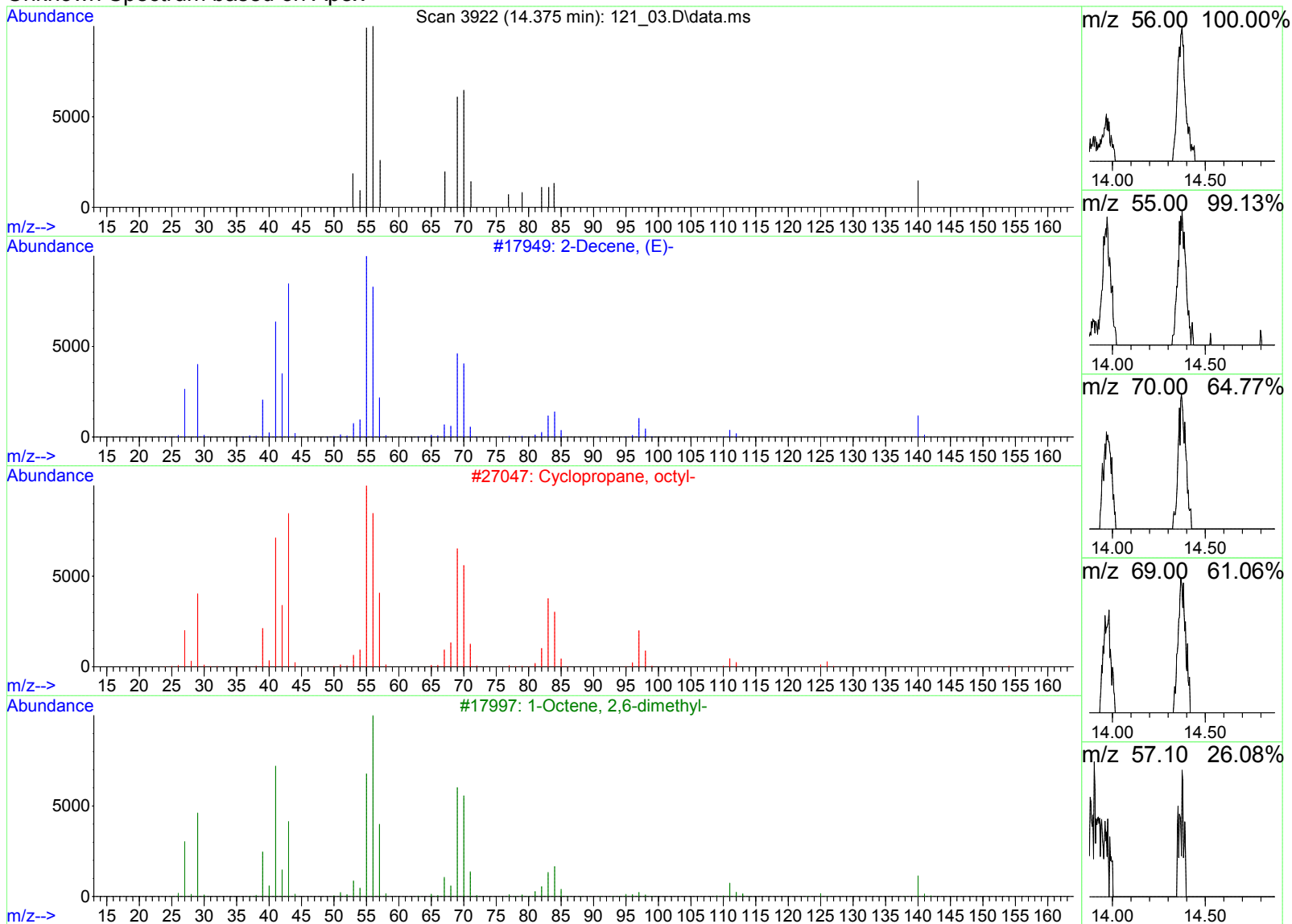
C:\Database\NIST11.L

1 4-Octene, 2,6-dimethyl-, [S-(E)]- 18040 062960-76-3 64

2 1-Octene, 6-methyl- 11523 013151-10-5 53

3 trans-4-Decene 17950 019398-89-1 50

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

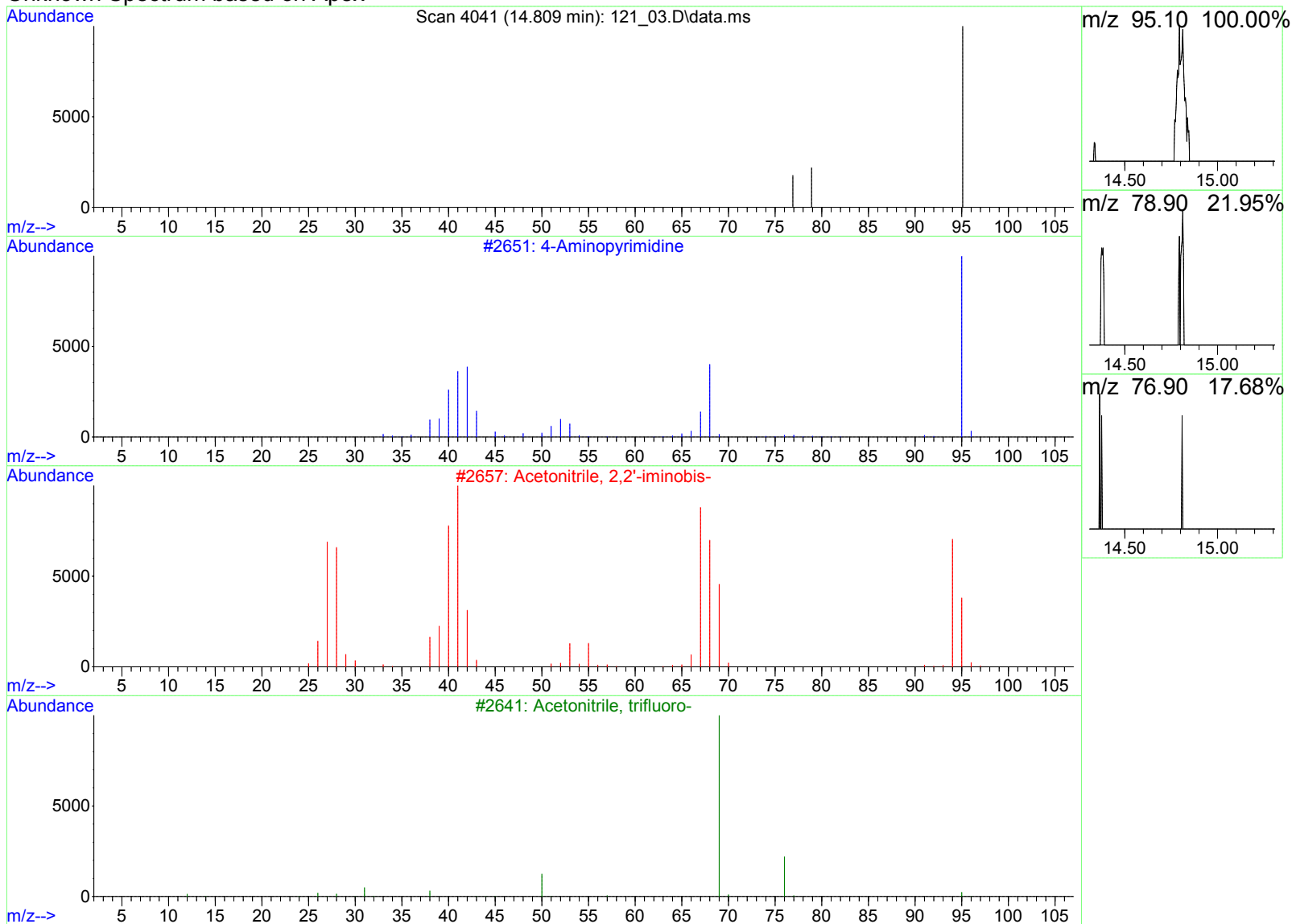
Peak Number: 18 at 14.375 min Area: 104344 Area % 0.40

The 3 best hits from each library. Ref# CAS# Qual

C:\Database\NIST11.L

1 2-Decene, (E)-	17949 020063-97-2	72
2 Cyclopropane, octyl-	27047 001472-09-9	64
3 1-Octene, 2,6-dimethyl-	17997 006874-29-9	64

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

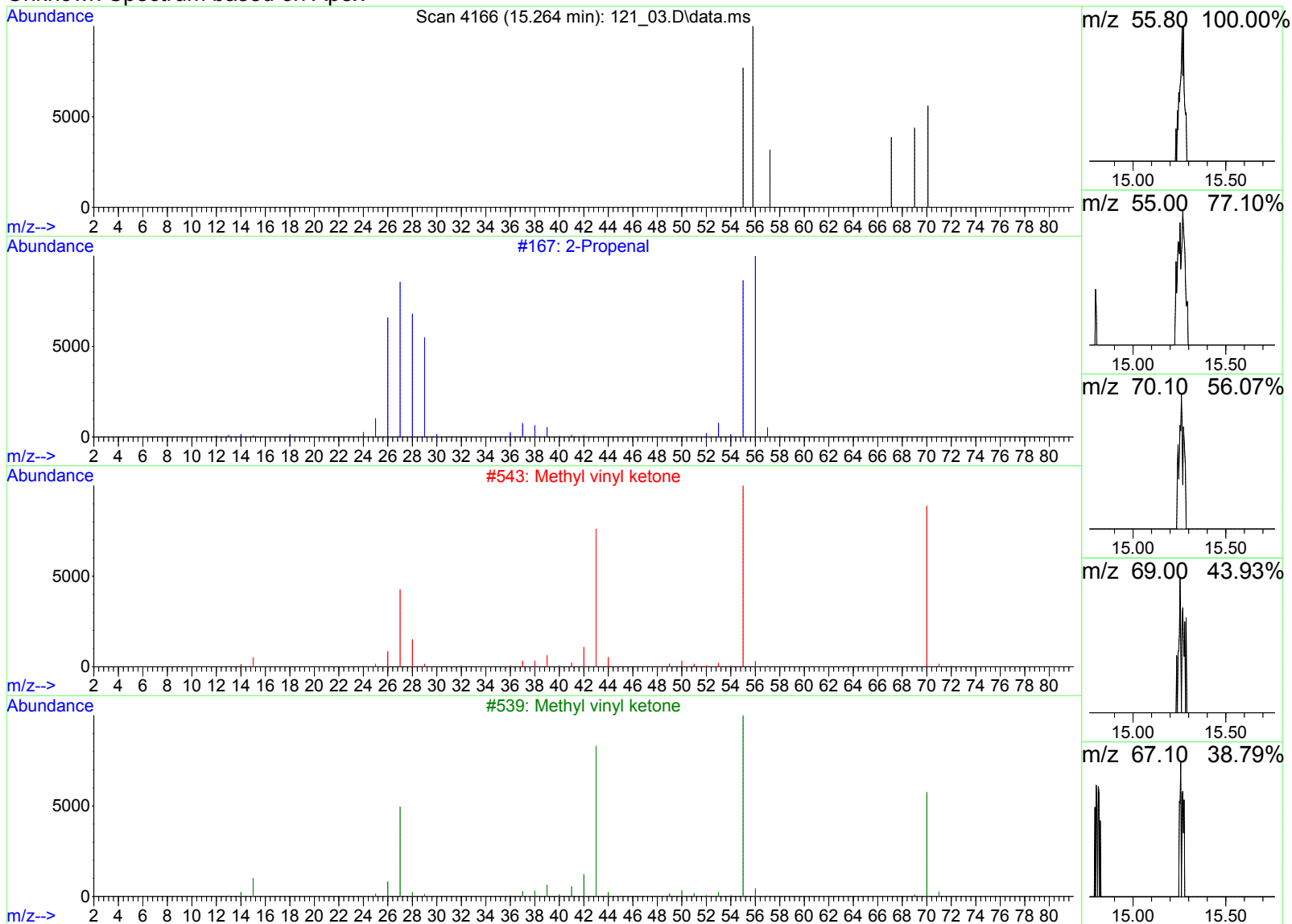
Peak Number: 19 at 14.809 min Area: 13230 Area % 0.05

The 3 best hits from each library. Ref# CAS# Qual

C:\Database\NIST11.L

1	4-Aminopyrimidine	2651	000591-54-8	2
2	Acetonitrile, 2,2'-iminobis-	2657	000628-87-5	2
3	Acetonitrile, trifluoro-	2641	000353-85-5	2

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

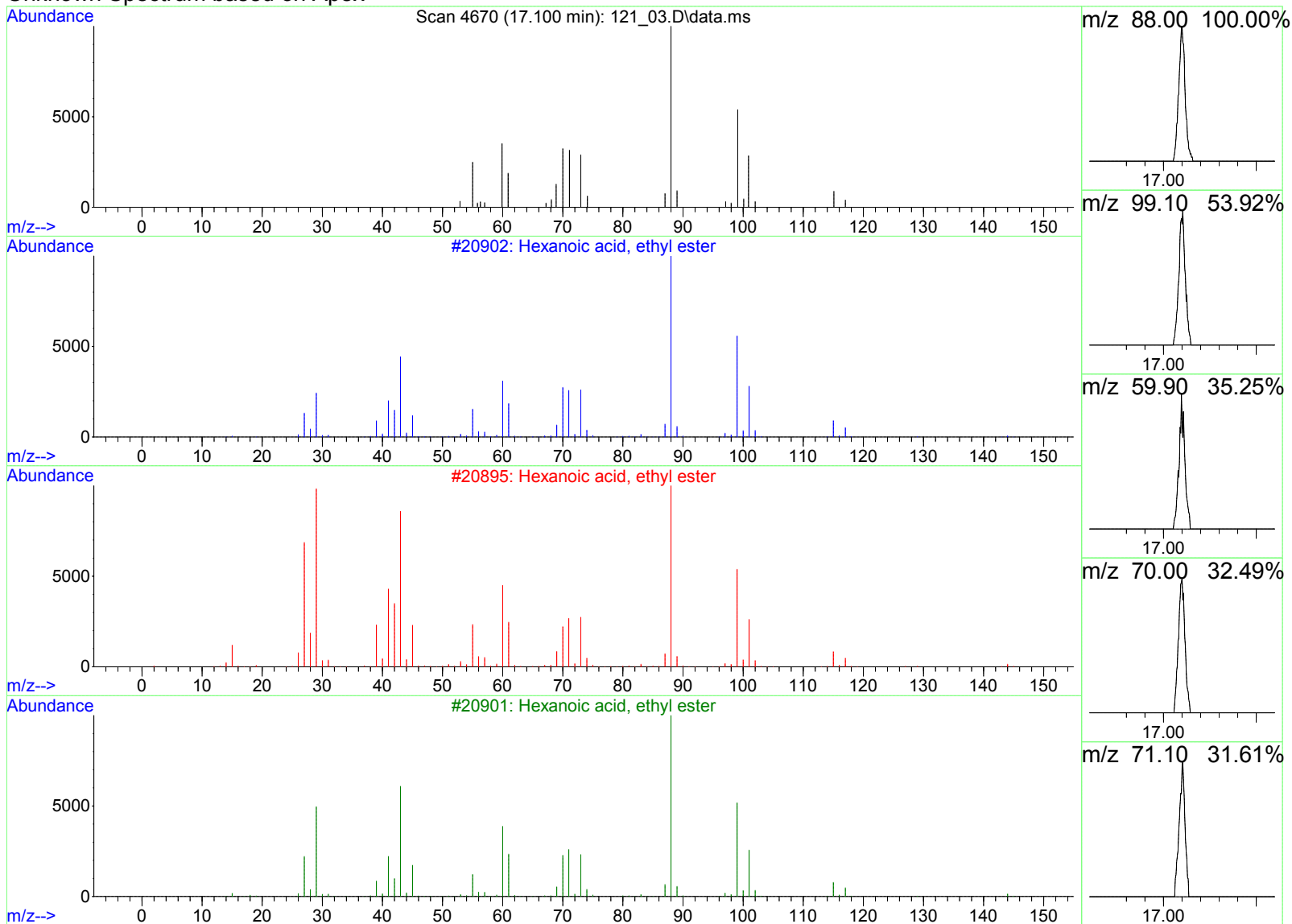
Peak Number: 20 at 15.264 min Area: 18462 Area % 0.07

The 3 best hits from each library. Ref# CAS# Qual

C:\Database\NIST11.L

1 2-Propenal	167 000107-02-8	4
2 Methyl vinyl ketone	543 000078-94-4	4
3 Methyl vinyl ketone	539 000078-94-4	4

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

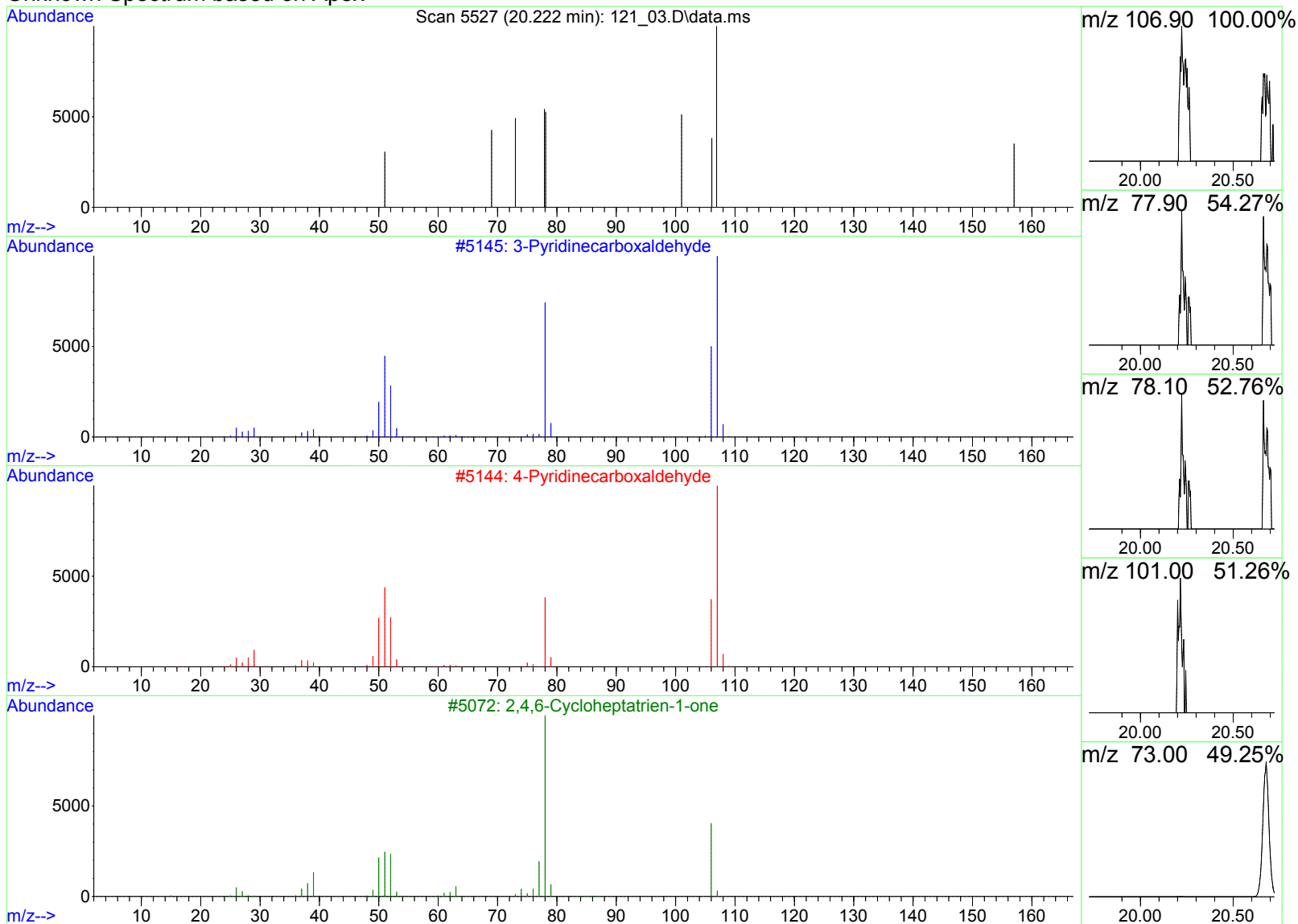
Peak Number: 21 at 17.100 min Area: 245749 Area % 0.94

The 3 best hits from each library. Ref# CAS# Qual

C:\Database\NIST11.L

1 Hexanoic acid, ethyl ester	20902	000123-66-0	90
2 Hexanoic acid, ethyl ester	20895	000123-66-0	78
3 Hexanoic acid, ethyl ester	20901	000123-66-0	78

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

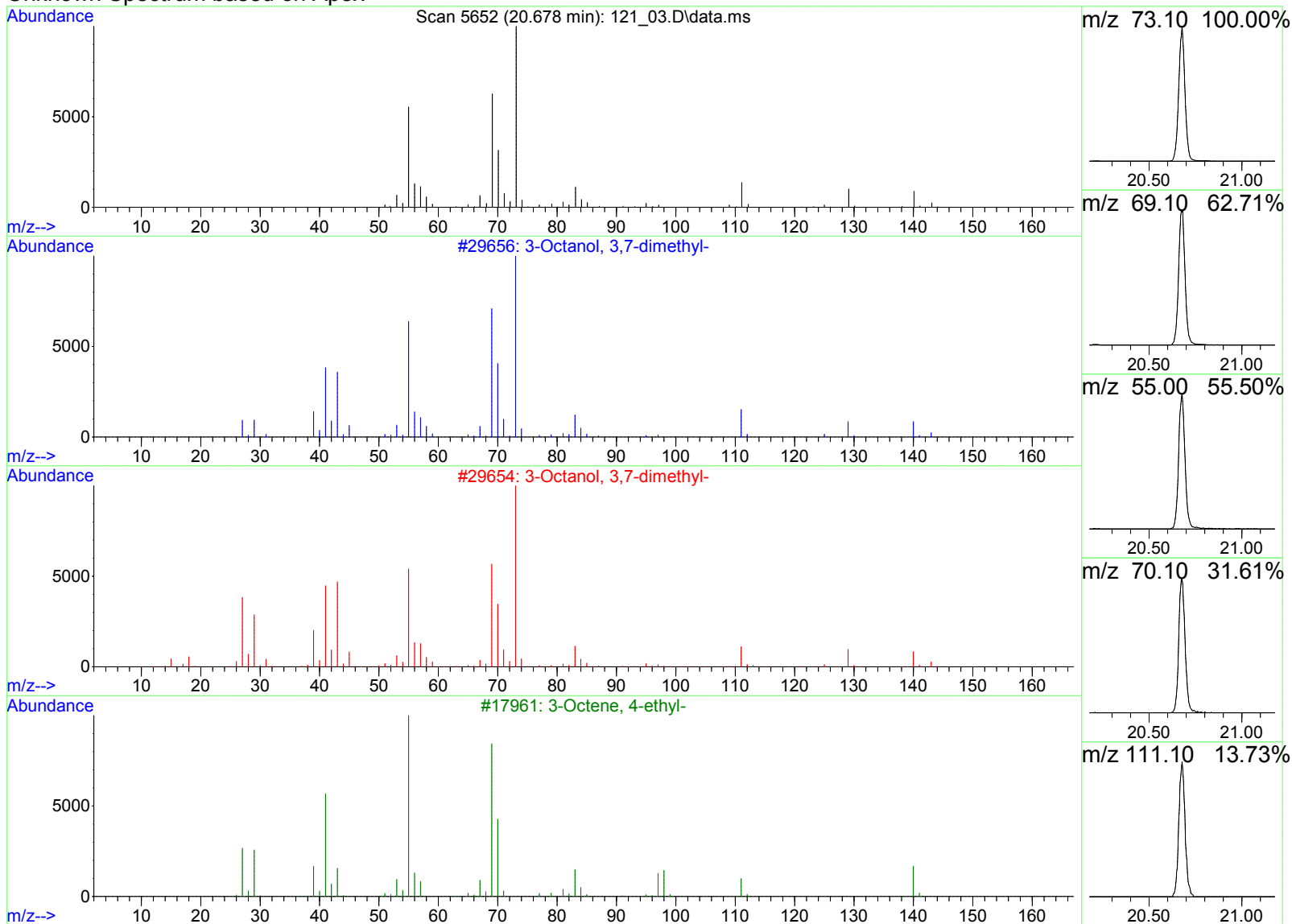
Peak Number: 22 at 20.222 min Area: 19109 Area % 0.07

The 3 best hits from each library. Ref# CAS# Qual

C:\Database\NIST11.L

1	3-Pyridinecarboxaldehyde	5145	000500-22-1	9
2	4-Pyridinecarboxaldehyde	5144	000872-85-5	9
3	2,4,6-Cycloheptatrien-1-one	5072	000539-80-0	9

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

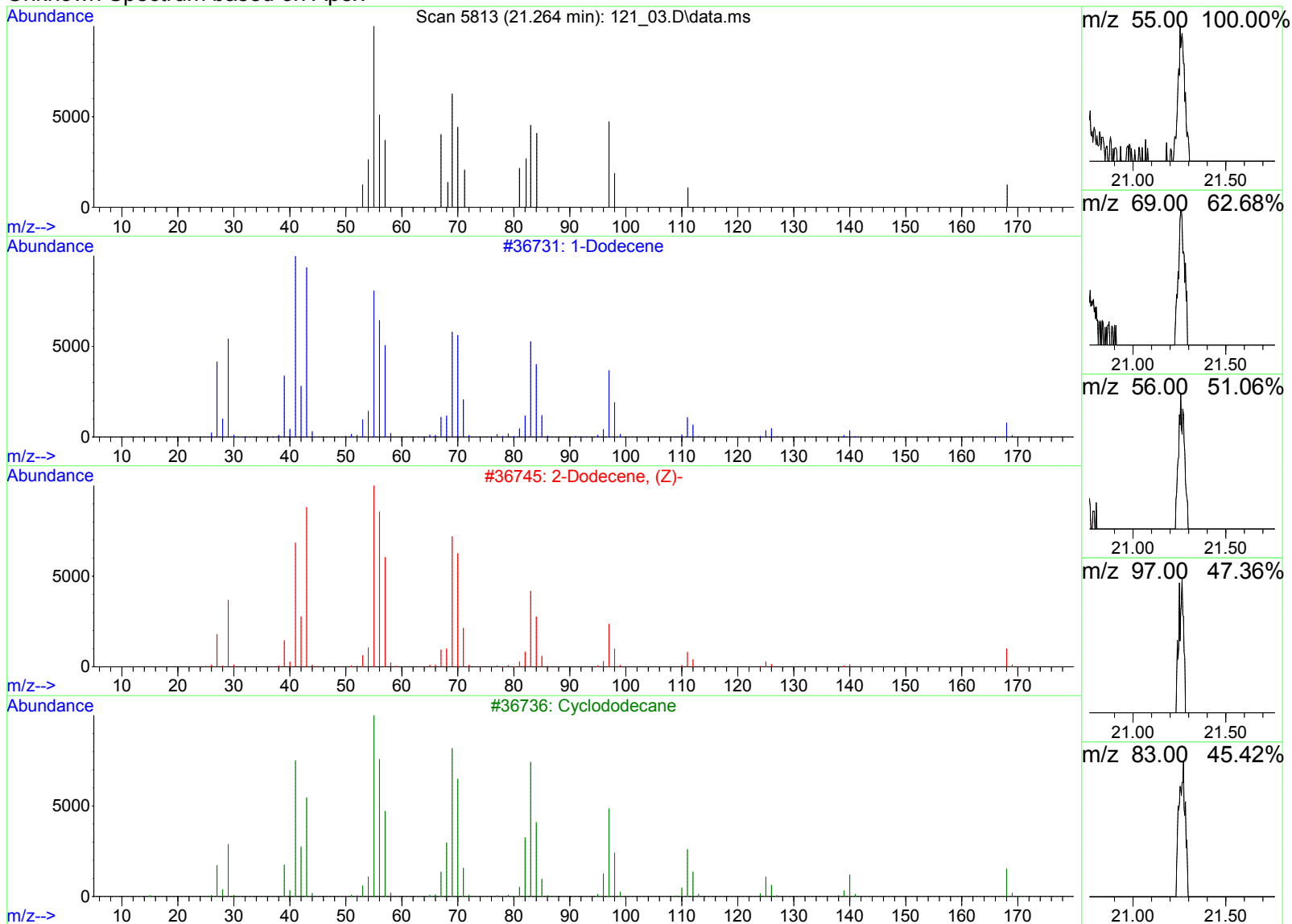
Peak Number: 23 at 20.678 min Area: 3627933 Area % 13.90

The 3 best hits from each library. Ref# CAS# Qual

C:\Database\NIST11.L

1	3-Octanol, 3,7-dimethyl-	29656	000078-69-3	90
2	3-Octanol, 3,7-dimethyl-	29654	000078-69-3	90
3	3-Octene, 4-ethyl-	17961	053966-51-1	60

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

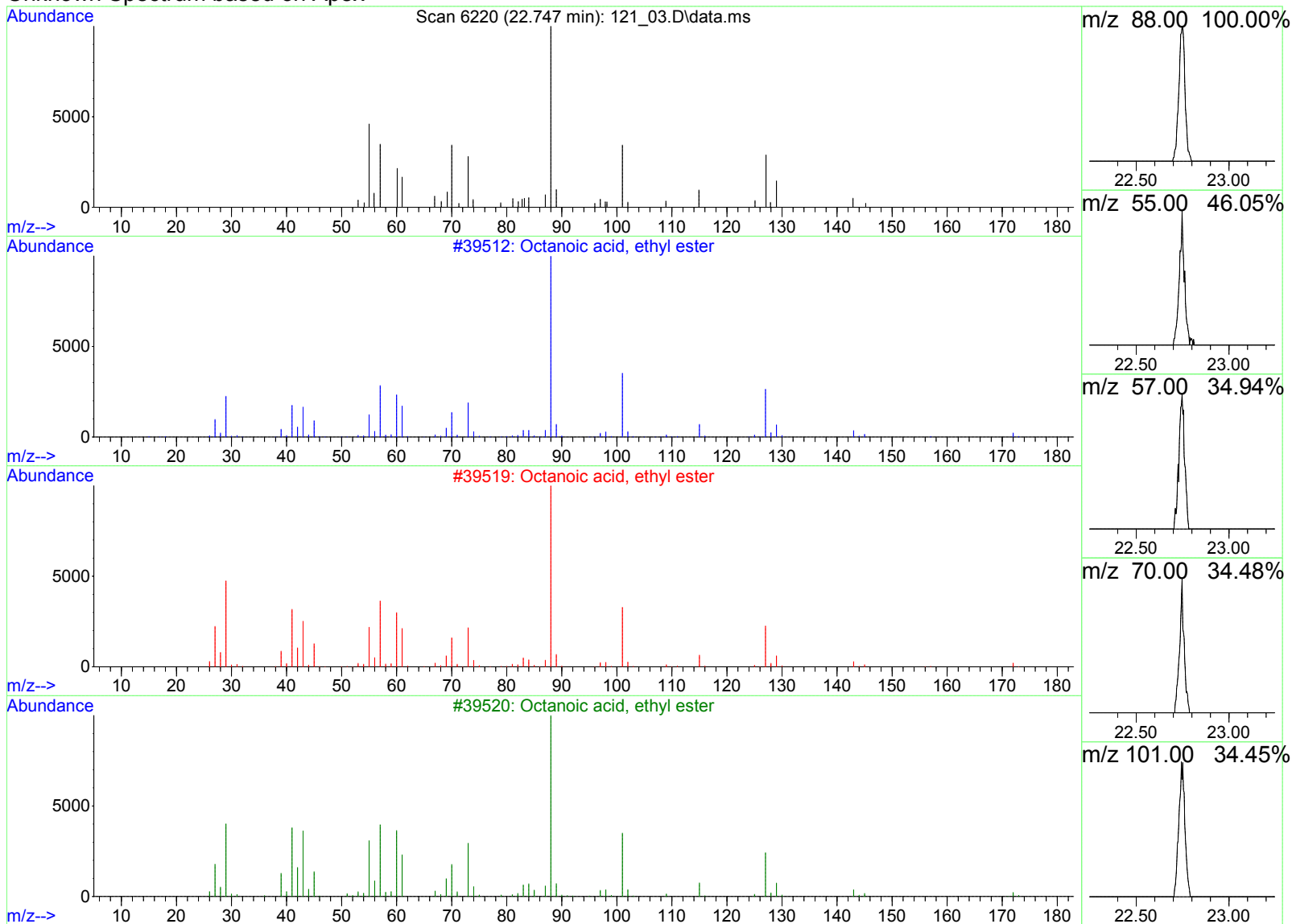
Peak Number: 24 at 21.264 min Area: 82859 Area % 0.32

The 3 best hits from each library. Ref# CAS# Qual

C:\Database\NIST11.L

1	1-Dodecene	36731	000112-41-4	70
2	2-Dodecene, (Z)-	36745	007206-26-0	58
3	Cyclododecane	36736	000294-62-2	53

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

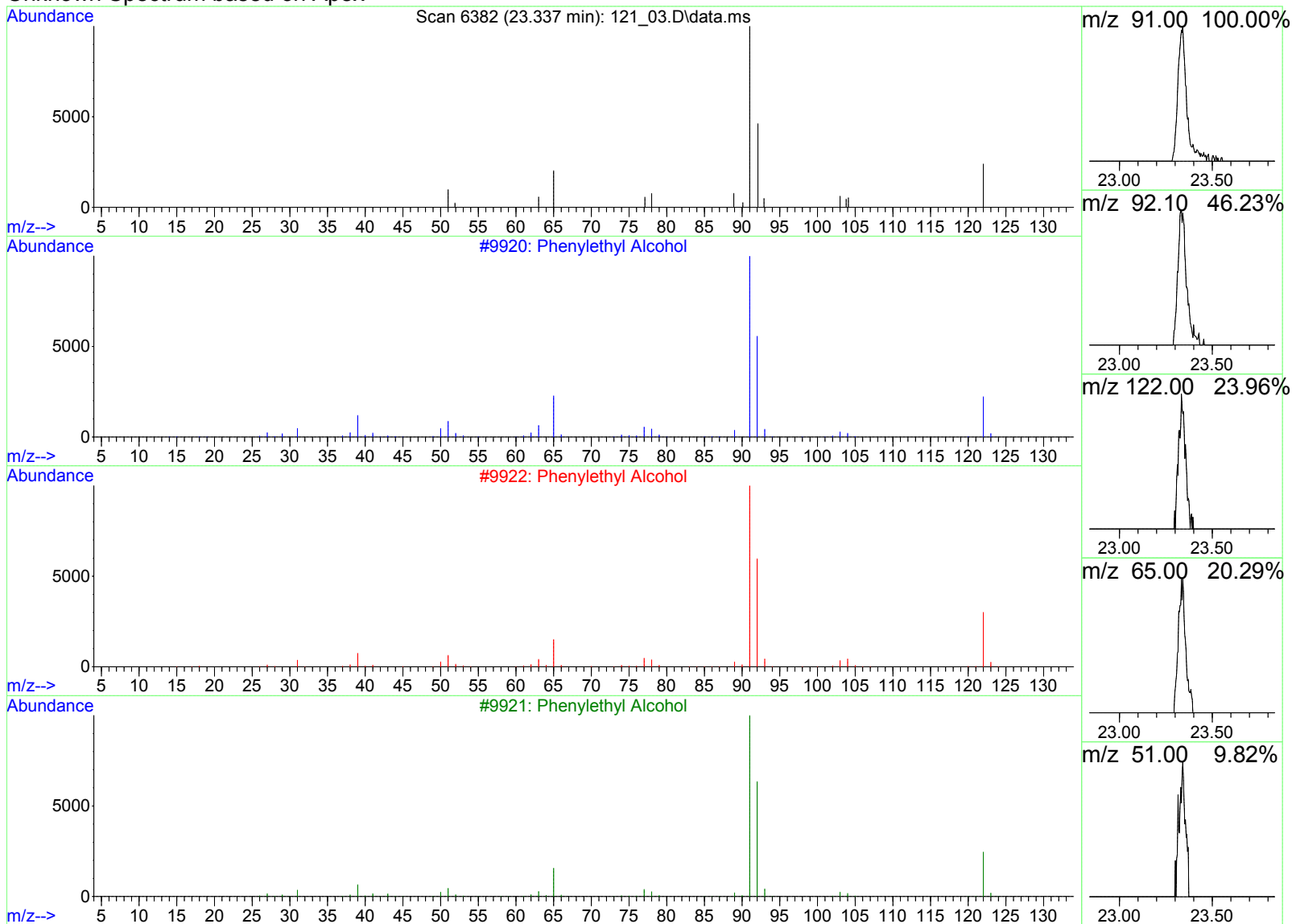
Peak Number: 25 at 22.747 min Area: 355837 Area % 1.36

The 3 best hits from each library. Ref# CAS# Qual

C:\Database\NIST11.L

1 Octanoic acid, ethyl ester	39512	000106-32-1	72
2 Octanoic acid, ethyl ester	39519	000106-32-1	64
3 Octanoic acid, ethyl ester	39520	000106-32-1	64

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

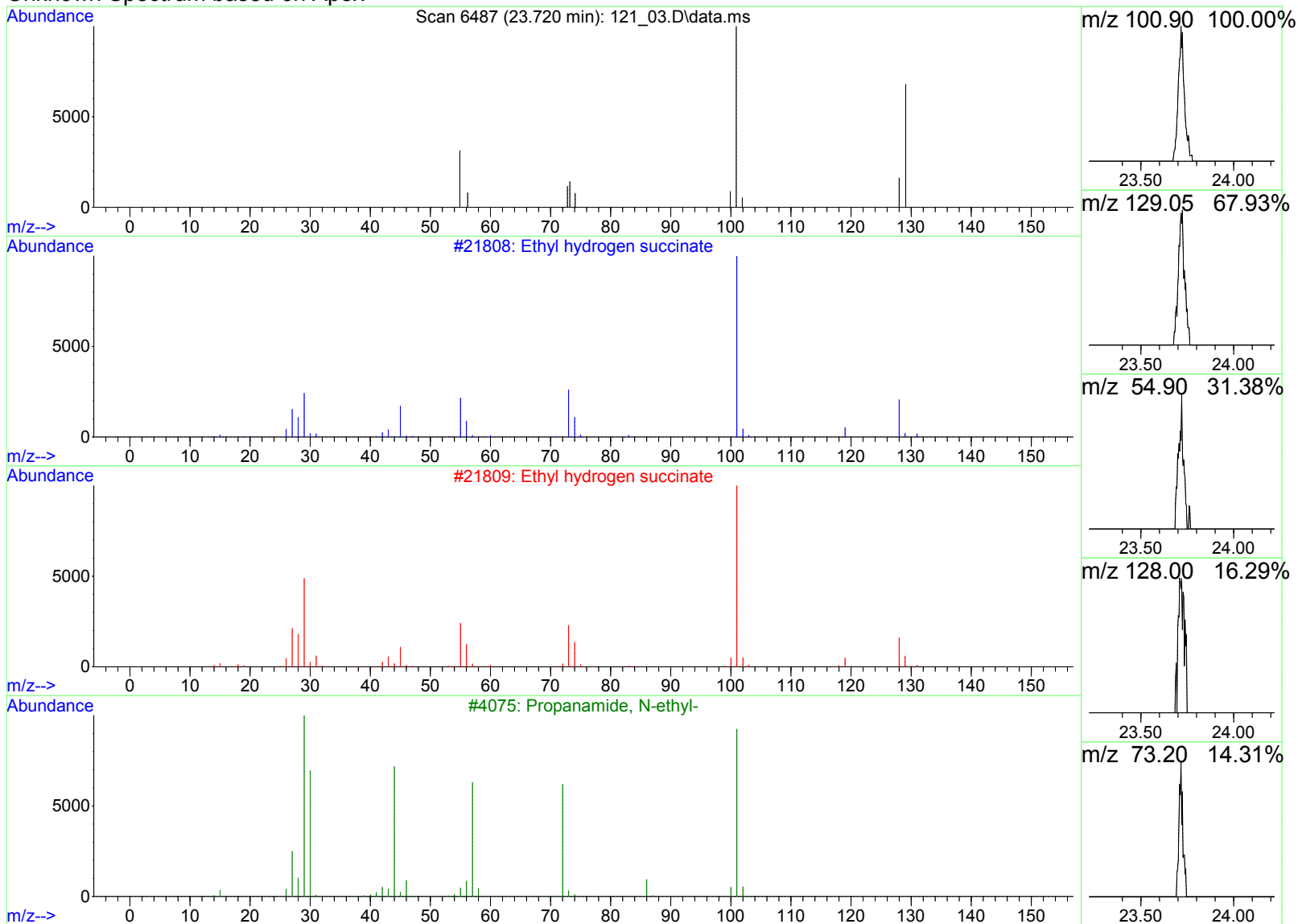
Peak Number: 26 at 23.337 min Area: 182830 Area % 0.70

The 3 best hits from each library. Ref# CAS# Qual

C:\Database\NIST11.L

1 Phenylethyl Alcohol	9920 000060-12-8	86
2 Phenylethyl Alcohol	9922 000060-12-8	72
3 Phenylethyl Alcohol	9921 000060-12-8	59

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

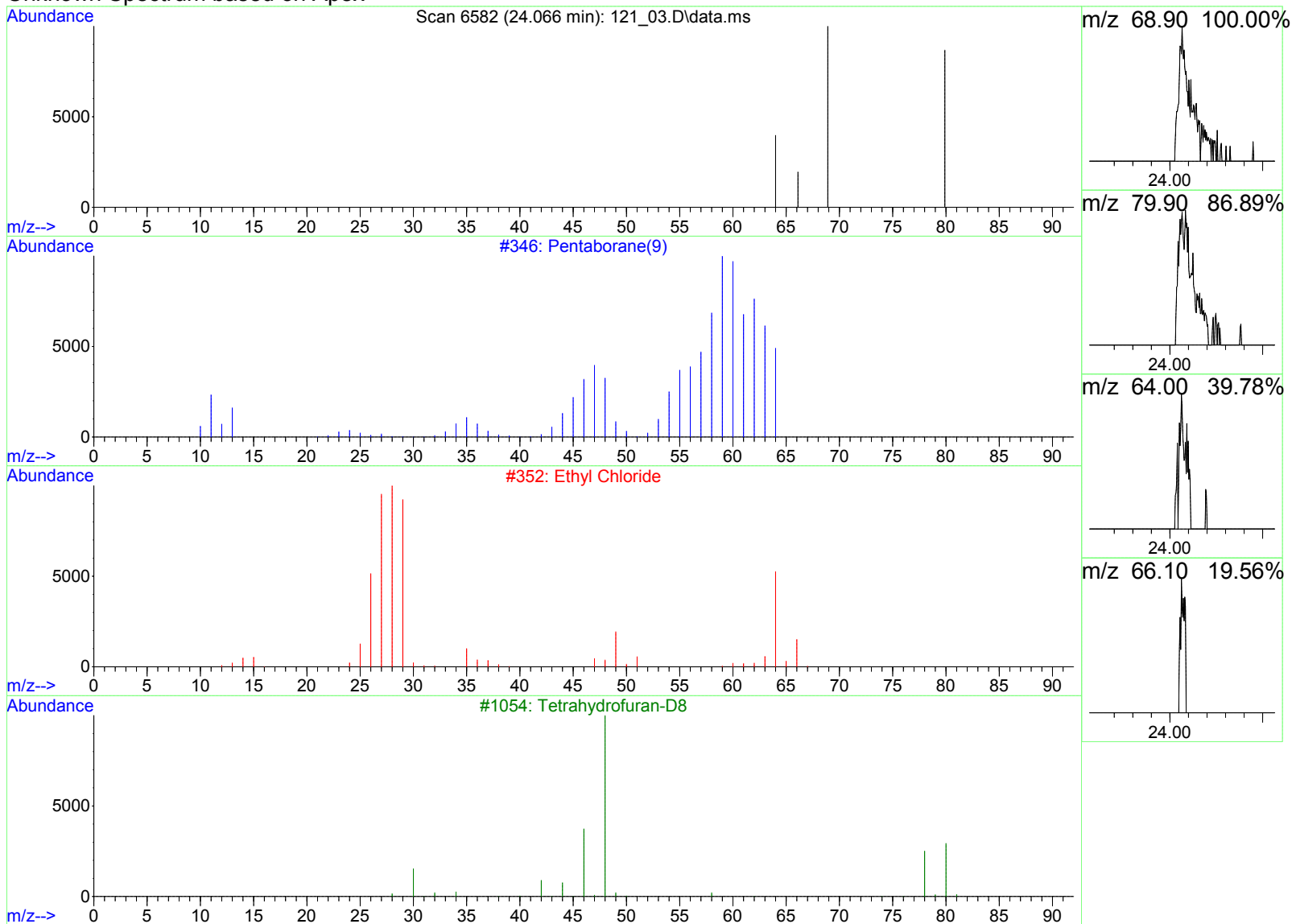
Peak Number: 27 at 23.720 min Area: 76285 Area % 0.29

The 3 best hits from each library. Ref# CAS# Qual

C:\Database\NIST11.L

1 Ethyl hydrogen succinate	21808	001070-34-4	53
2 Ethyl hydrogen succinate	21809	001070-34-4	45
3 Propanamide, N-ethyl-	4075	005129-72-6	9

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

Peak Number: 28 at 24.066 min Area: 51906 Area % 0.20

The 3 best hits from each library. Ref# CAS# Qual

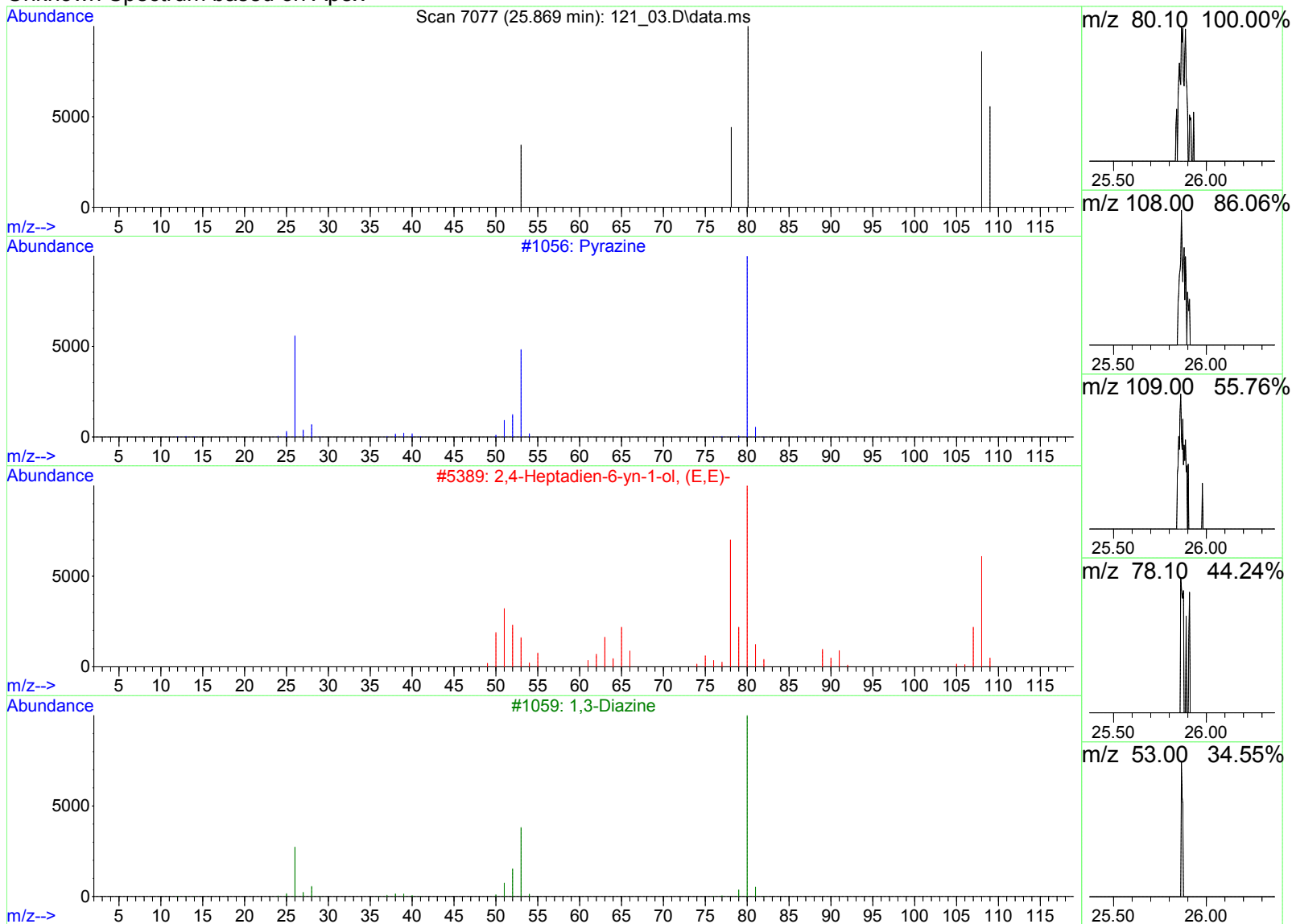
C:\Database\NIST11.L

1 Pentaborane(9) 346 019624-22-7 3

2 Ethyl Chloride 352 000075-00-3 3

3 Tetrahydrofuran-D8 1054 001693-74-9 2

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

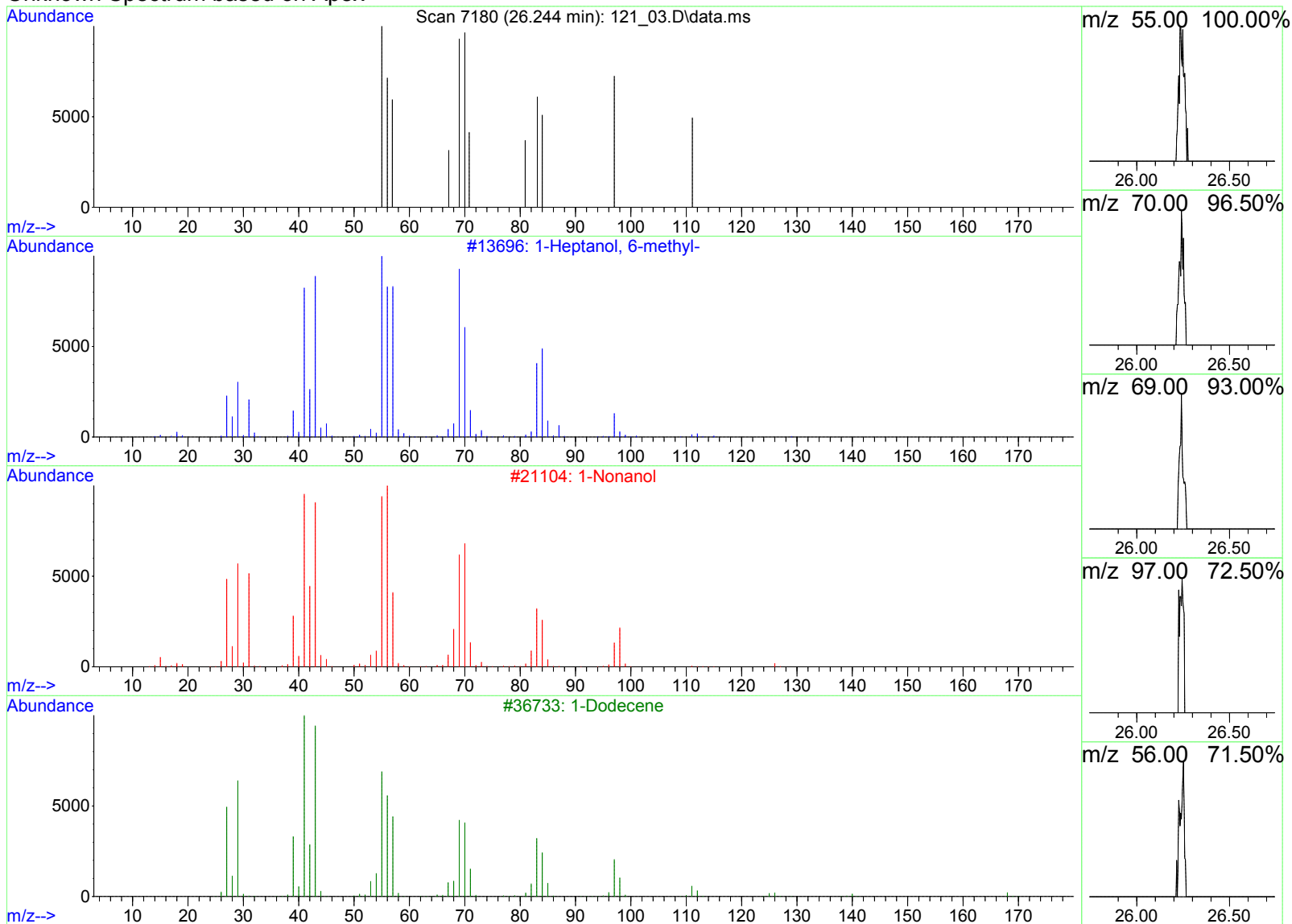
Peak Number: 29 at 25.869 min Area: 14472 Area % 0.06

The 3 best hits from each library. Ref# CAS# Qual

C:\Database\NIST11.L

1	Pyrazine	1056	000290-37-9	7
2	2,4-Heptadien-6-yn-1-ol, (E,E)-	5389	017098-71-4	7
3	1,3-Diazine	1059	000289-95-2	7

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

Peak Number: 30 at 26.244 min Area: 31177 Area % 0.12

The 3 best hits from each library. Ref# CAS# Qual

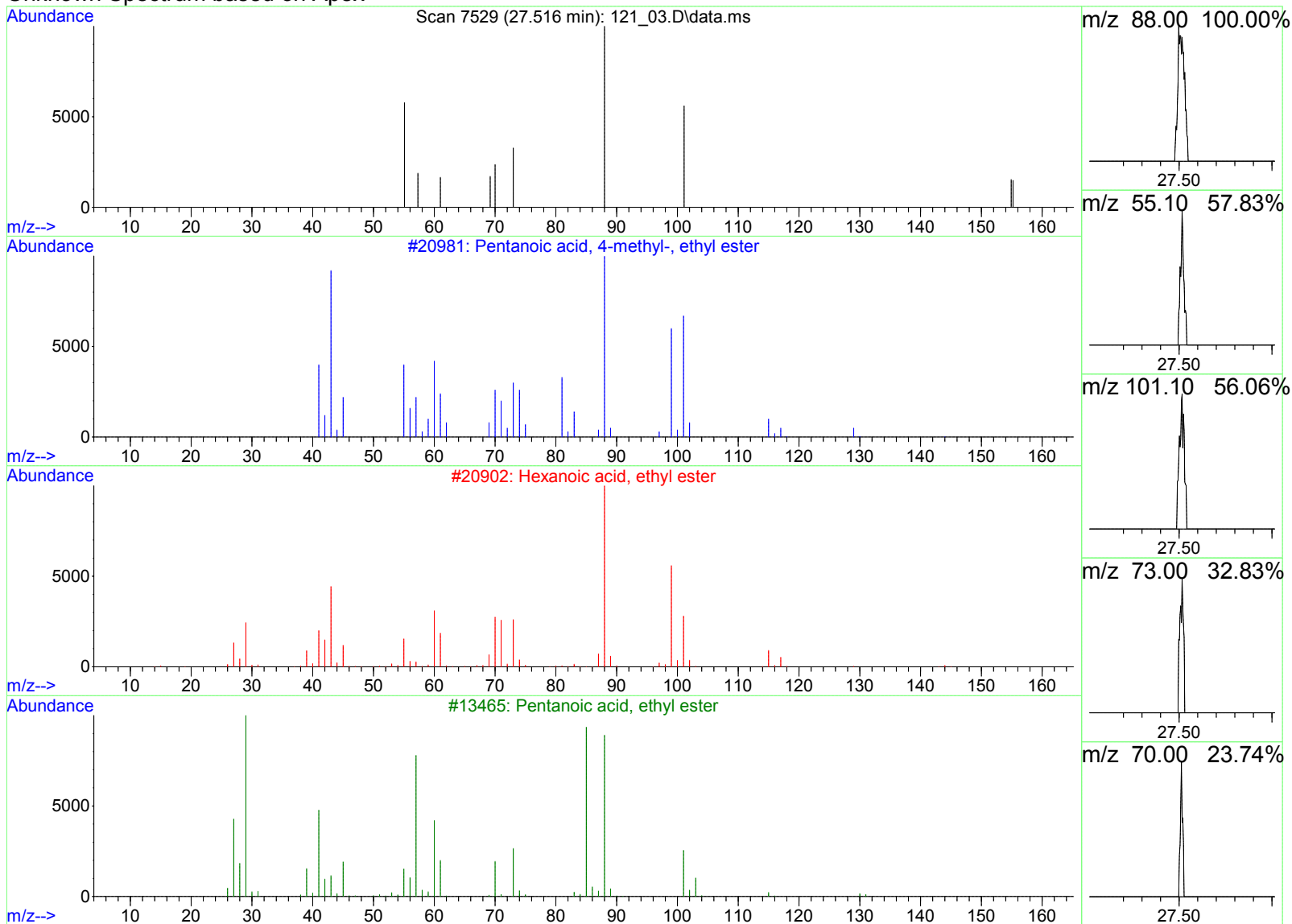
C:\Database\NIST11.L

1 1-Heptanol, 6-methyl- 13696 001653-40-3 47

2 1-Nonanol 21104 000143-08-8 42

3 1-Dodecene 36733 000112-41-4 39

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

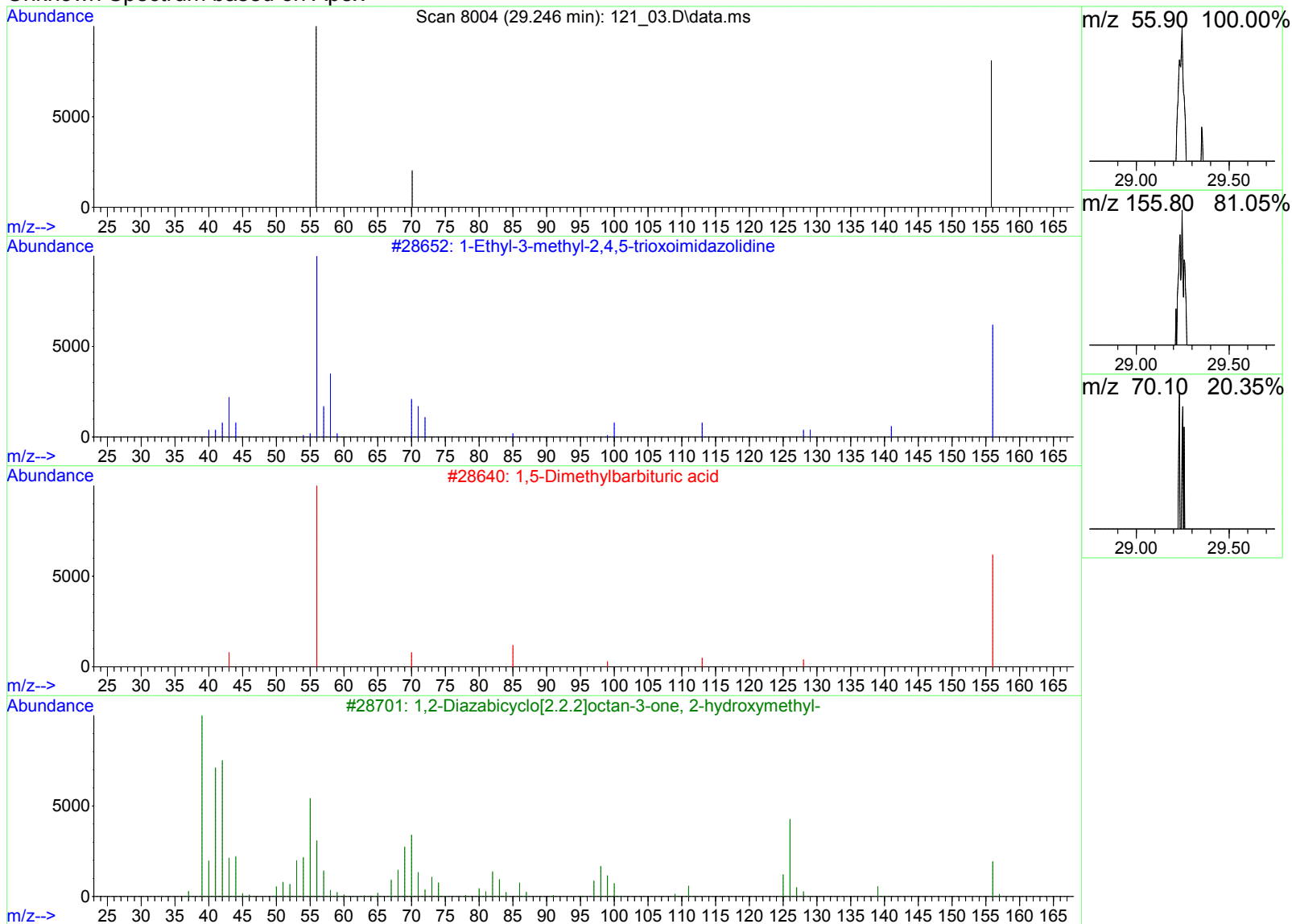
Peak Number: 31 at 27.516 min Area: 25071 Area % 0.10

The 3 best hits from each library. Ref# CAS# Qual

C:\Database\NIST11.L

1 Pentanoic acid, 4-methyl-, ethyl...	20981	025415-67-2	78
2 Hexanoic acid, ethyl ester	20902	000123-66-0	38
3 Pentanoic acid, ethyl ester	13465	000539-82-2	38

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

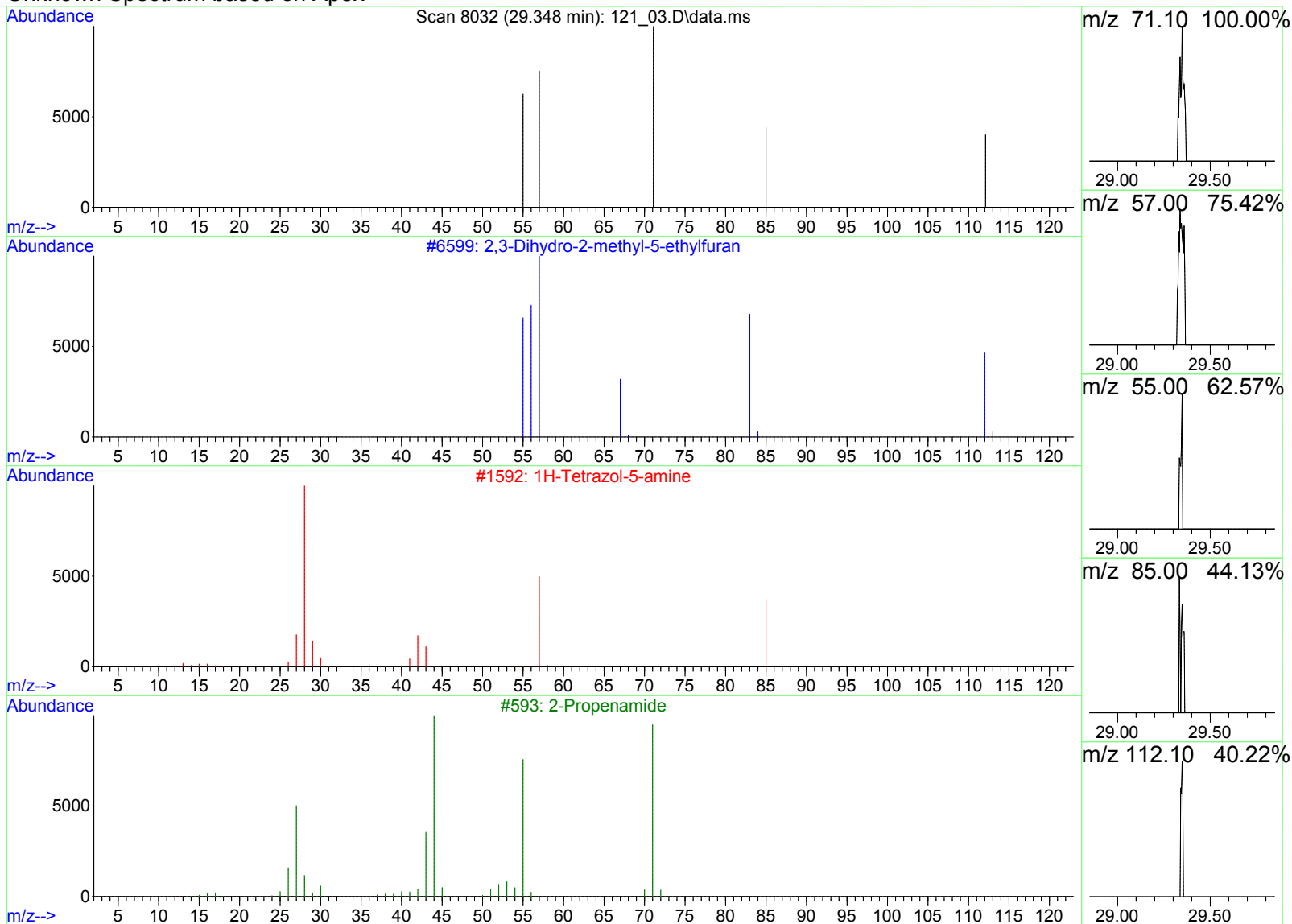
Peak Number: 32 at 29.246 min Area: 9975 Area % 0.04

The 3 best hits from each library. Ref# CAS# Qual

C:\Database\NIST11.L

1	1-Ethyl-3-methyl-2,4,5-trioximi...	28652	071194-99-5	9
2	1,5-Dimethylbarbituric acid	28640	007391-67-5	5
3	1,2-Diazabicyclo[2.2.2]octan-3-o...	28701	1000263-51-1	4

Unknown Spectrum based on Apex



Data File: C:\MSDCHEM\1\DATA\20-CRT-300\121_03.D

Sample : 121

Peak Number: 33 at 29.348 min Area: 8341 Area % 0.03

The 3 best hits from each library. Ref# CAS# Qual

C:\Database\NIST11.L

1 2,3-Dihydro-2-methyl-5-ethylfuran 6599 1000288-51-4 7

2 1H-Tetrazol-5-amine 1592 004418-61-5 4

3 2-Propenamide 593 000079-06-1 4