LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112618\
Data File : VX006176.D
Acq On : 26 Nov 2018 15:38
Operator : JC/MD
Sample : J6044-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 30003

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112018W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.483	51	54	68	rBV	7464605	9071221	25.07%	8.573%
2	2.154	151	164	168	rBV	7591889	16615473	45.92%	15.703%
3	2.355	192	197	206	rVV	1167595	1890619	5.22%	1.787%
4	2.446	206	212	228	rVB	1170886	1910206	5.28%	1.805%
5	2.855	273	279	293	rVB	270060	525247	1.45%	0.496%
6	3.068	301	314	325	rBV	670092	1535364	4.24%	1.451%
7	3.416	363	371	383	rBV	263037	608890	1.68%	0.575%
8	4.019	459	470	479	rBV	619129	1602503	4.43%	1.514%
9	4.354	513	525	538	rBV	1562269	4344580	12.01%	4.106%
10	4.702	571	582	599	rBV	554144	1556825	4.30%	1.471%
11	5.501	703	713	727	rVB	188087	532747	1.47%	0.503%
12	5.665	727	740	755	rBV	324305	907996	2.51%	0.858%
13	6.068	796	806	819	rBV2	204836	548097	1.51%	0.518%
14	6.263	826	838	852	rBV	169163	448298	1.24%	0.424%
15	6.860	925	936	951	rBV	480334	1168634	3.23%	1.104%
16	7.336	1004	1014	1026	rBV	2049985	4147225	11.46%	3.919%
17	7.665	1060	1068	1075	rBV	864367	1593318	4.40%	1.506%
18	8.713	1234	1240	1247	rBV	984549	1555322	4.30%	1.470%
19	9.305	1331	1337	1345	rBV	326347	510379	1.41%	0.482%
20	10.061	1454	1461	1465	rBV	164499	387998	1.07%	0.367%
21	10.116	1465	1470	1481	rVV	1059863	1742331	4.82%	1.647%
22	10.213	1481	1486	1497	rVV	700913	993567	2.75%	0.939%
23	10.689	1559	1564	1568	rVV	389962	595266	1.65%	0.563%
24	10.737	1568	1572	1578	rVV	2344219	2923608	8.08%	2.763%
25	10.823	1578	1586	1592	rVB2	629987	1271533	3.51%	1.202%
26	11.140	1632	1638	1643	rBV	877402	1179681	3.26%	1.115%
27	11.475	1688	1693	1698	rBV	516295	651195	1.80%	0.615%
28	11.664	1721	1724	1730	rVB3	352846	552362	1.53%	0.522%
29	12.079	1788	1792	1800	rVB	1173078	1424643	3.94%	1.346%
30	12.286	1819	1826	1836	rBV	27172989	36185409	100.00%	34.198%
31	12.621	1875	1881	1891	rBV4	231409	502630	1.39%	0.475%
32	13.231	1972	1981	1991	rBV	3410122	5886893	16.27%	5.564%
33	13.310	1991	1994	2007	rVB	304869	441767	1.22%	0.418%

LSC Area Percent Report

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ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 30003

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112018W.M
Title : SW846 8260

Sum of corrected areas: 105811827

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112618\
Data File : VX006176.D
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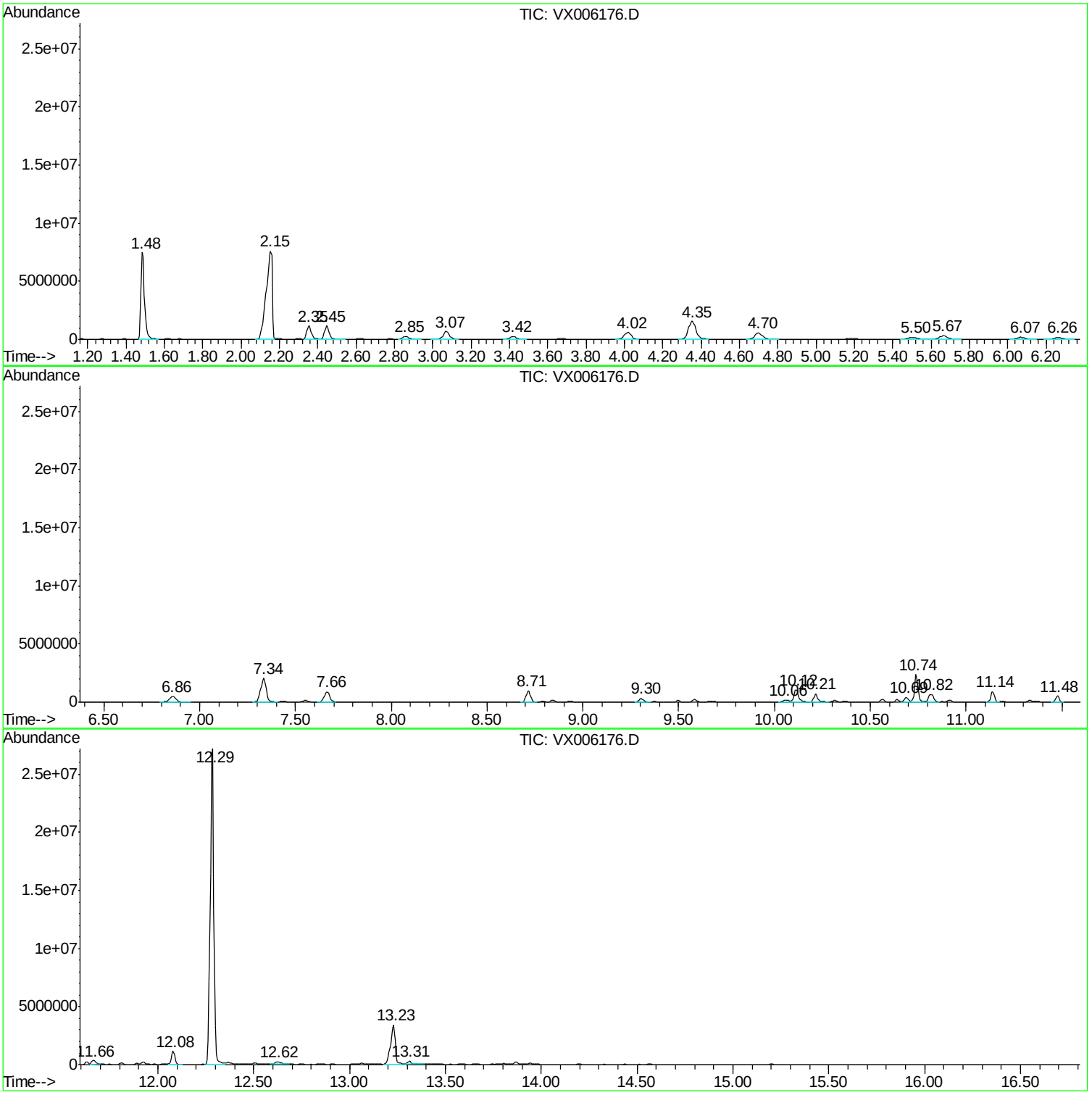
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
30003

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112018W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

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Data File : VX006176.D
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112018W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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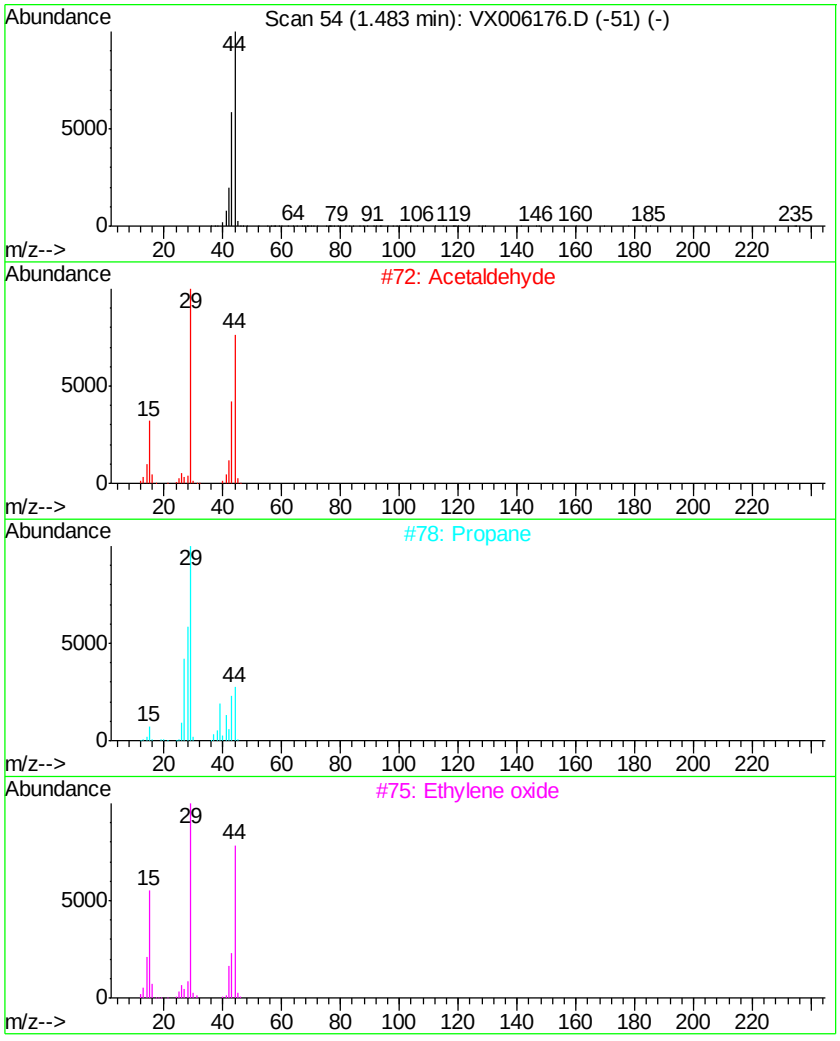
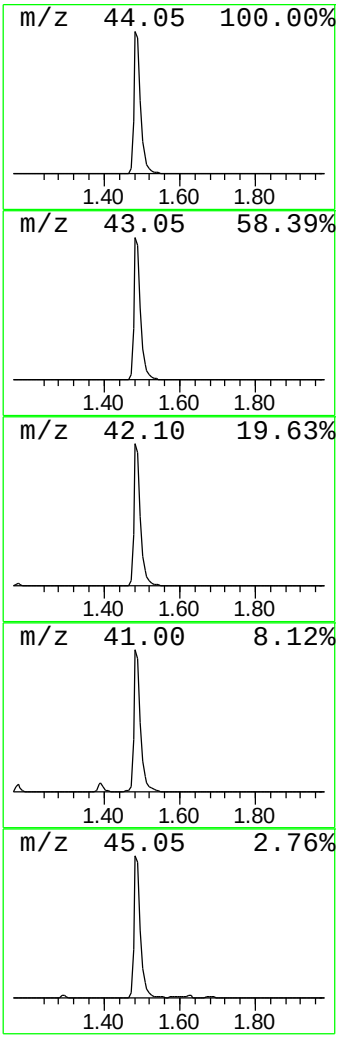
Peak Number 1 Acetaldehyde Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.48	499.52 ug/l	9071220	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	74
2	Propane	44	C3H8	000074-98-6	5
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Alanine	89	C3H7NO2	000056-41-7	4
5	Ethyne, fluoro-	44	C2HF	002713-09-9	3





Library Search Compound Report

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Data File : VX006176.D
Acq On : 26 Nov 2018 15:38
Operator : JC/MD
Sample : J6044-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 30003

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112018W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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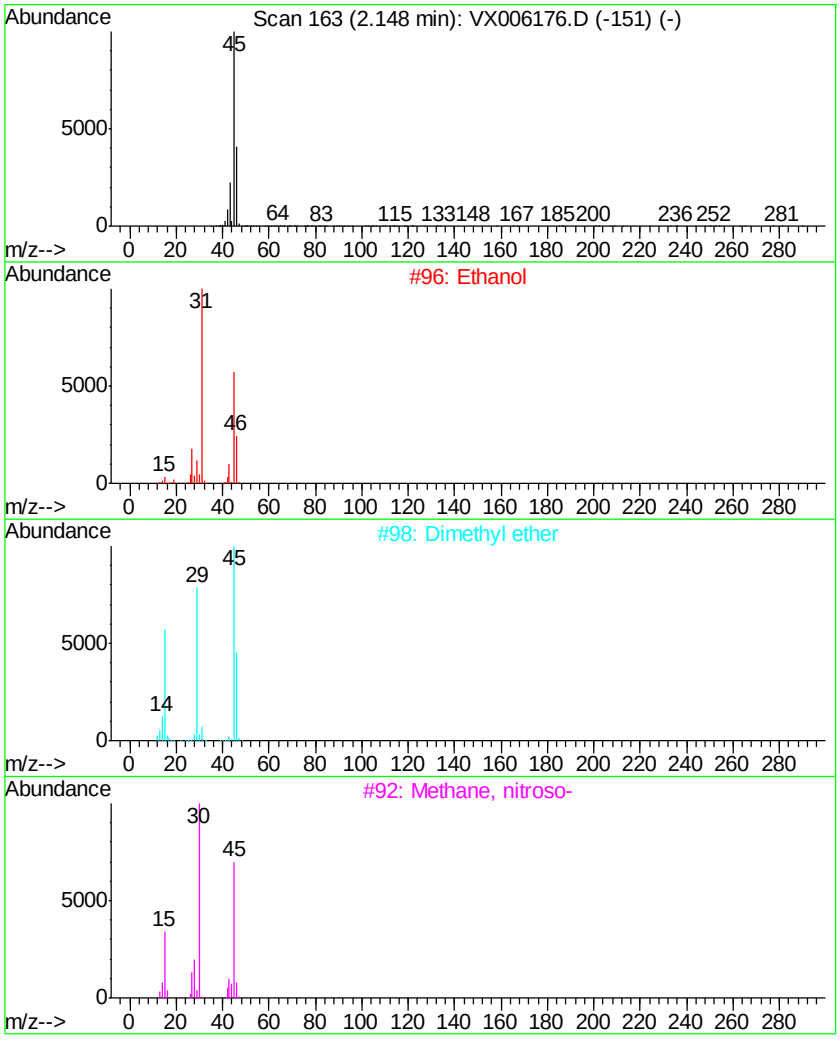
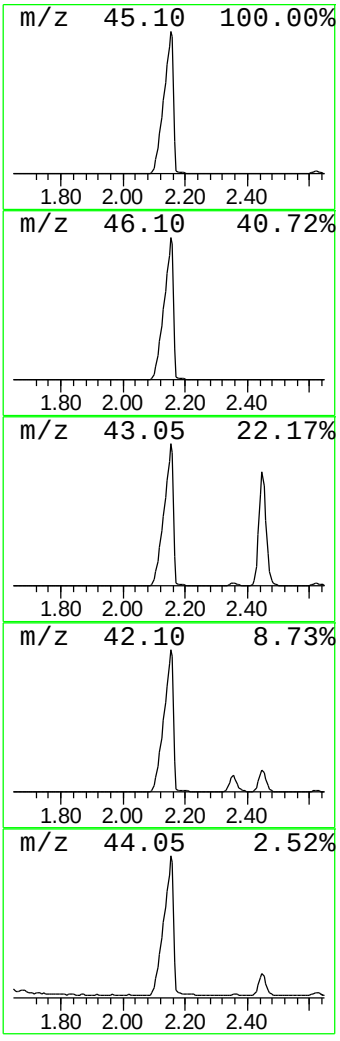
Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	914.95 ug/l	16615500	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	83
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Formic acid	46	CH2O2	000064-18-6	4
5	Oxalic acid	90	C2H2O4	000144-62-7	4





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112618\
Data File : VX006176.D
Acq On : 26 Nov 2018 15:38
Operator : JC/MD
Sample : J6044-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 30003

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112018W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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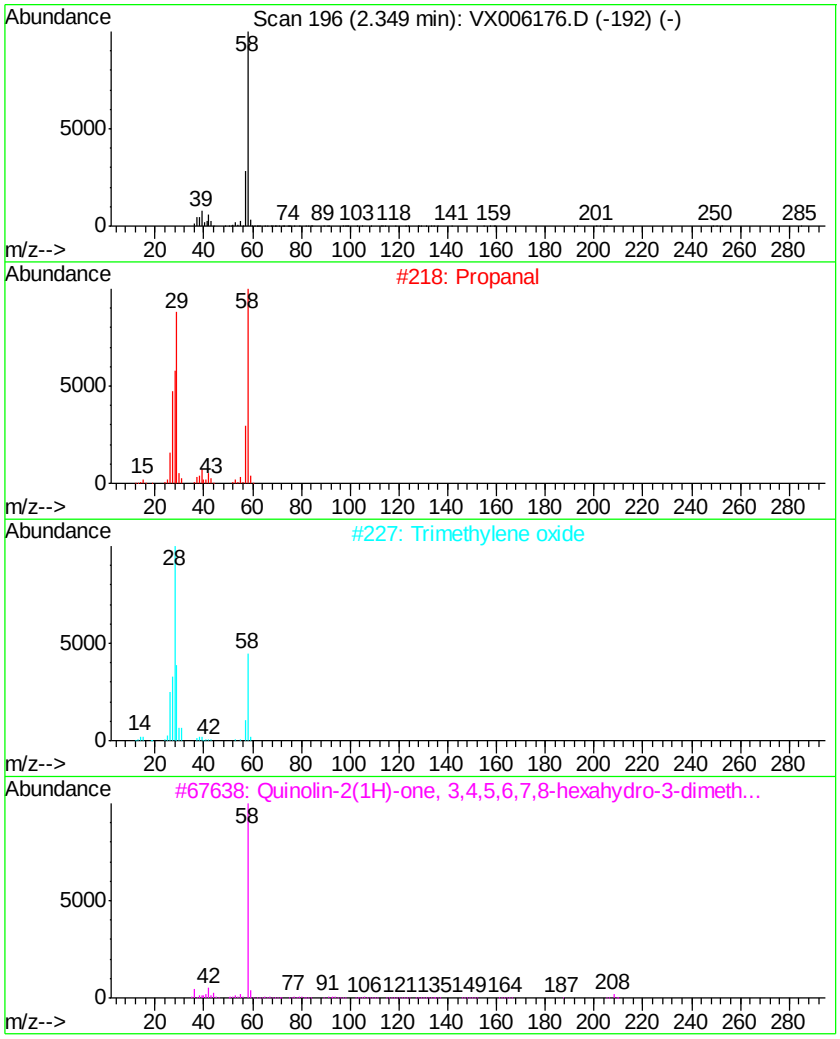
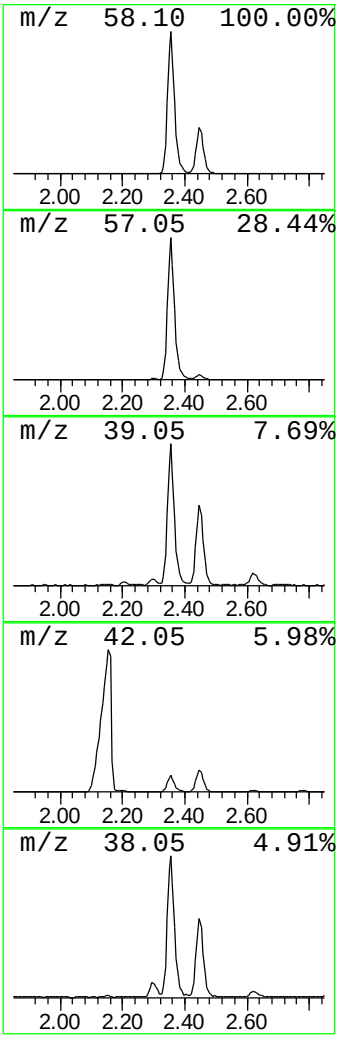
Peak Number 3 Propanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.35	104.11 ug/l	1890620	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal	58	C3H6O	000123-38-6	78
2	Trimethylene oxide	58	C3H6O	000503-30-0	56
3	Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
4	Propylene oxide	58	C3H6O	000075-56-9	7
5	Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7





Library Search Compound Report

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Acq On : 26 Nov 2018 15:38
Operator : JC/MD
Sample : J6044-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 30003

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112018W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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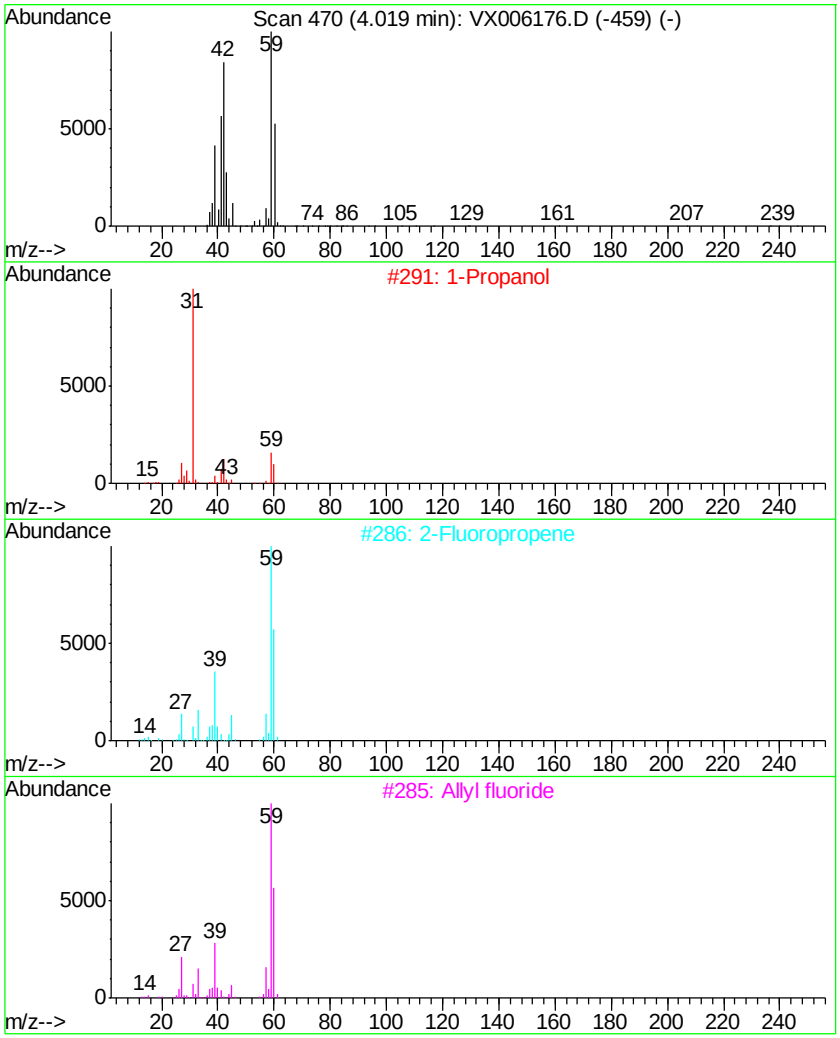
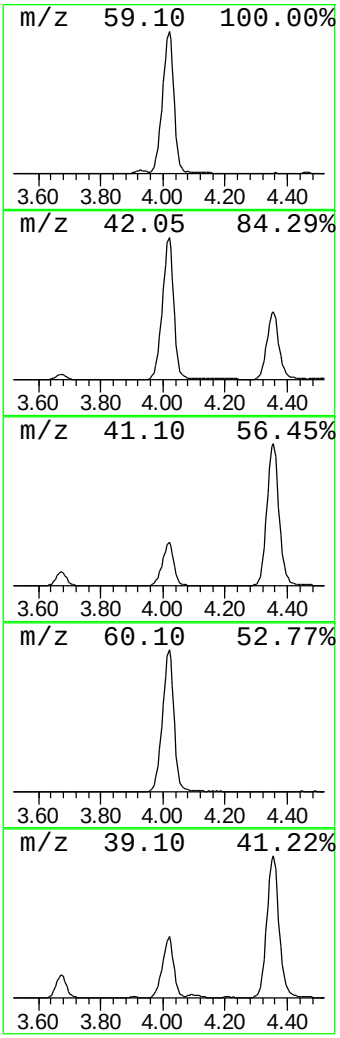
Peak Number 4 1-Propanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.02	88.24 ug/l	1602500	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	59
2	2-Fluoropropene	60	C3H5F	001184-60-7	52
3	Allyl fluoride	60	C3H5F	000818-92-8	38
4	Cyclopropane	42	C3H6	000075-19-4	25
5	2-Butanol, 3-methoxy-	104	C5H12O2	053778-72-6	10





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Operator : JC/MD
Sample : J6044-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 30003

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112018W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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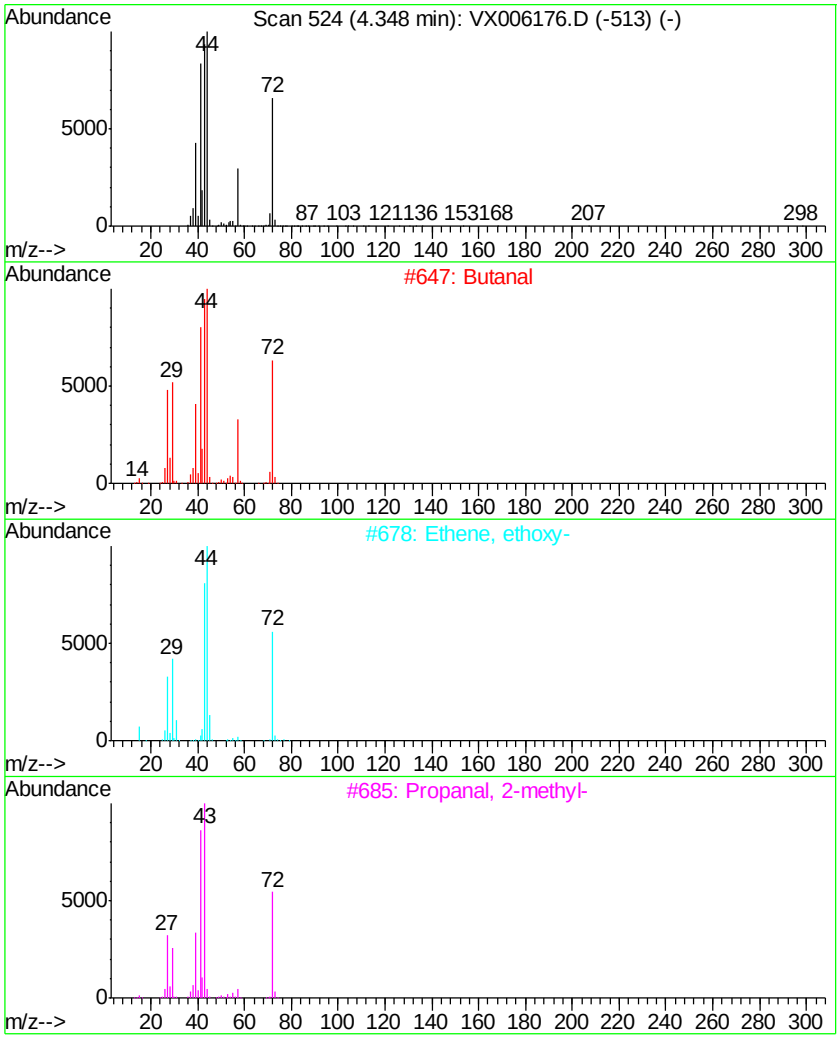
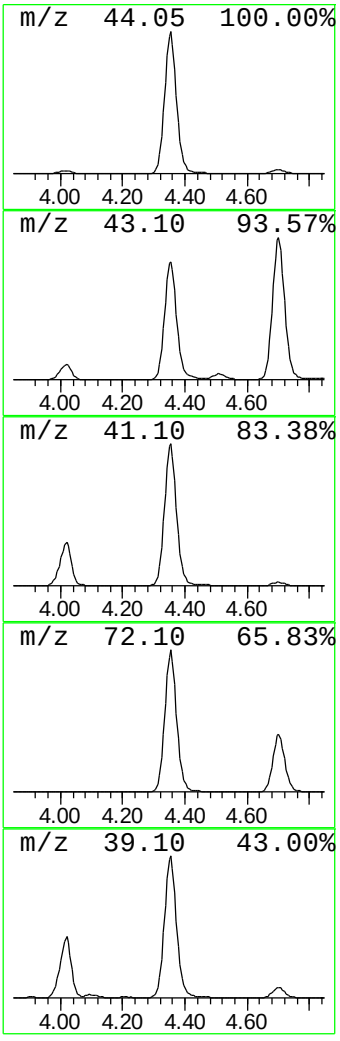
Peak Number 5 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.35	239.24 ug/l	4344580	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	52
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	52
4	Isobutylene epoxide	72	C4H8O	000558-30-5	22
5	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	12





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ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 30003

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112018W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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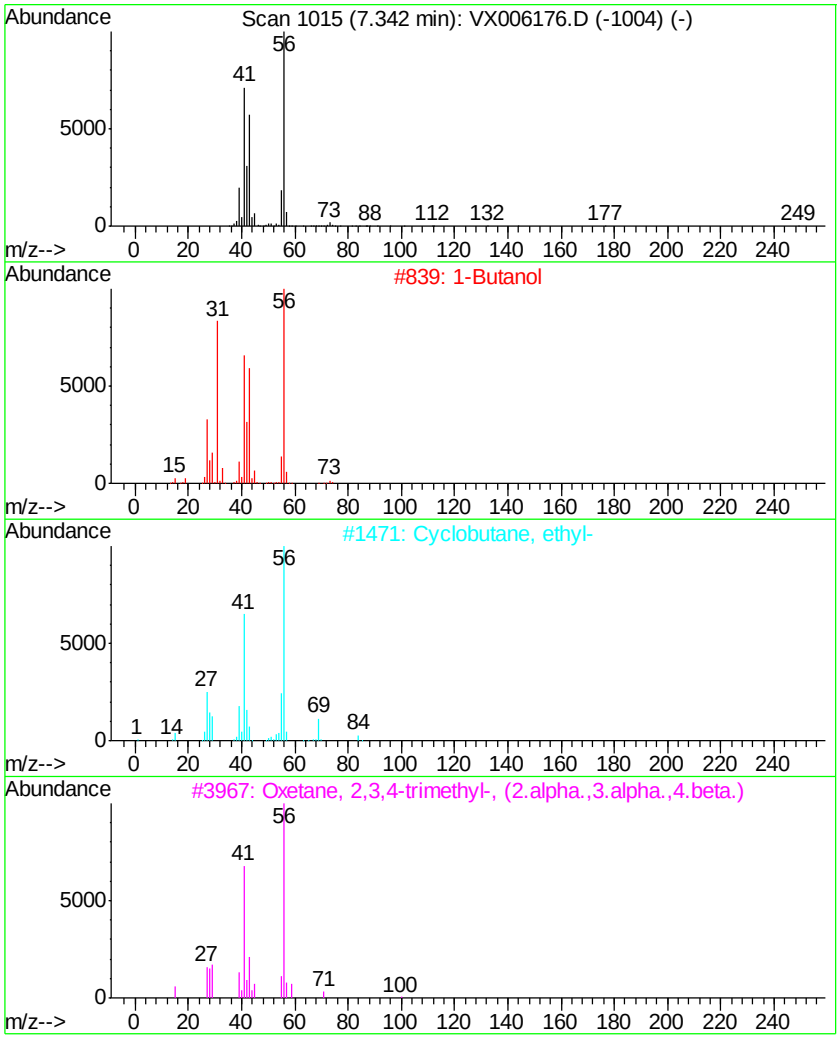
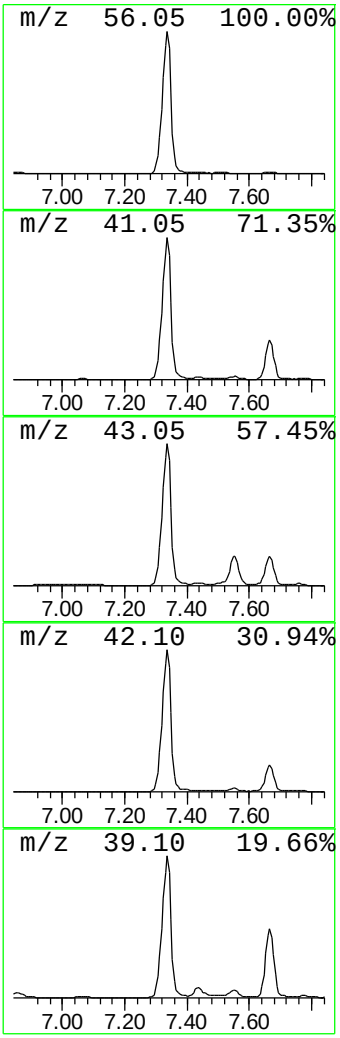
Peak Number 6 1-Butanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.34	177.44 ug/l	4147230	1,4-Difluorobenzene	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	91
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	9
3	Oxetane, 2,3,4-trimethyl-, (2.al...	100	C6H12O	032347-12-9	9
4	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	9
5	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9





Library Search Compound Report

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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 30003

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112018W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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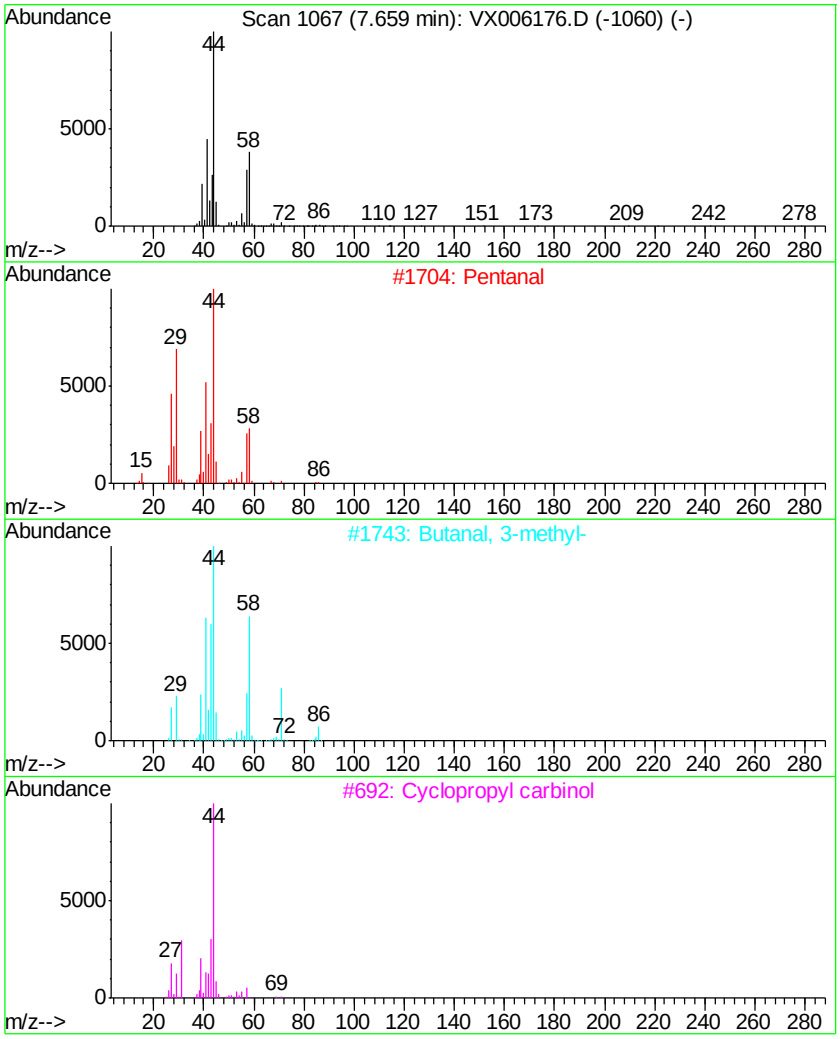
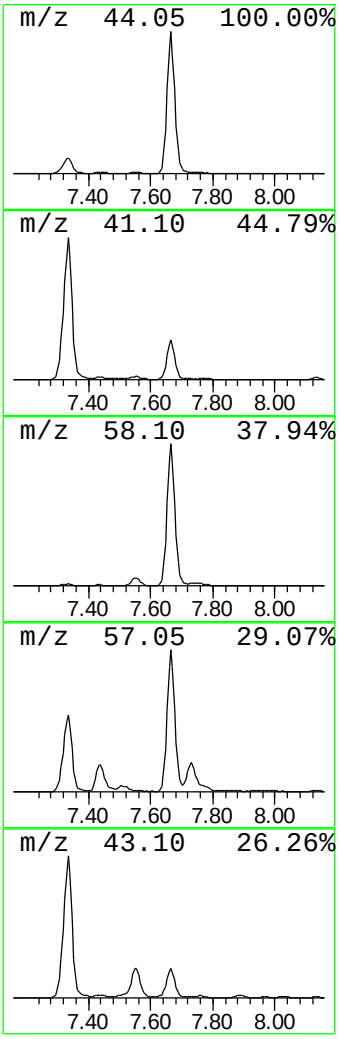
Peak Number 7 Pentanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	68.17 ug/l	1593320	1,4-Difluorobenzene	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal	86	C5H10O	000110-62-3	83
2	Butanal, 3-methyl-	86	C5H10O	000590-86-3	74
3	Cyclopropyl carbinol	72	C4H8O	002516-33-8	38
4	Glycidol	74	C3H6O2	000556-52-5	36
5	2-Propanamine	59	C3H9N	000075-31-0	9





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ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 30003

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112018W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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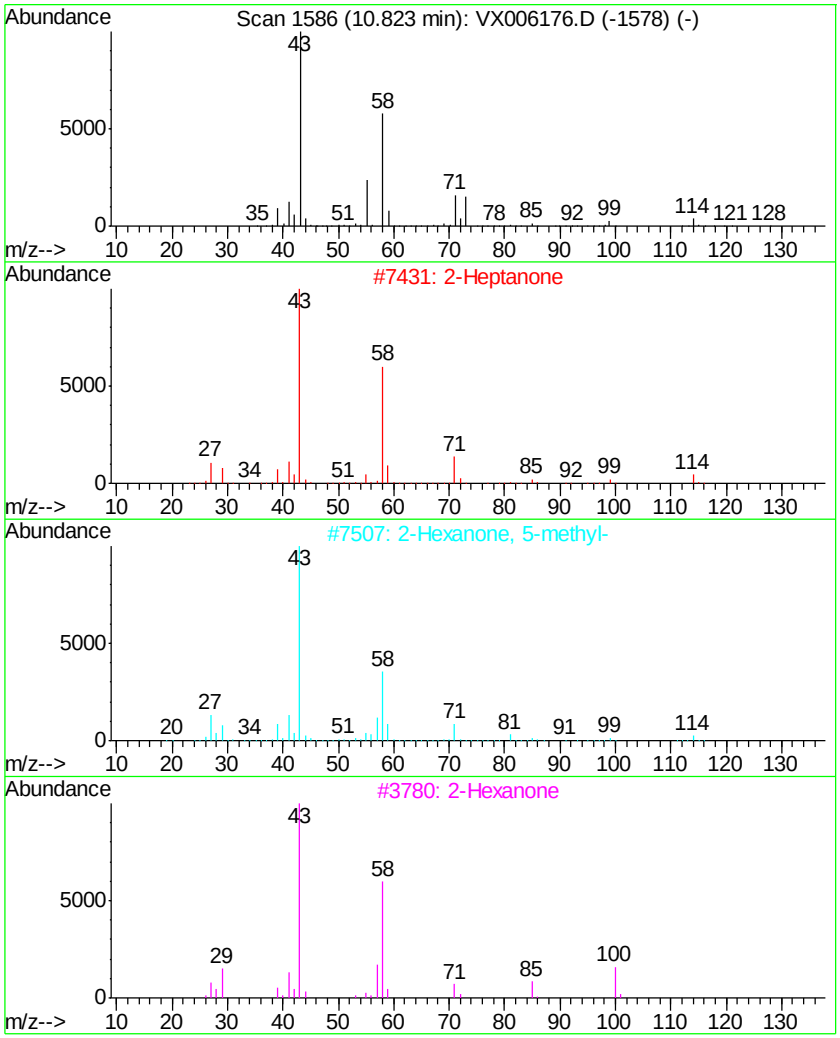
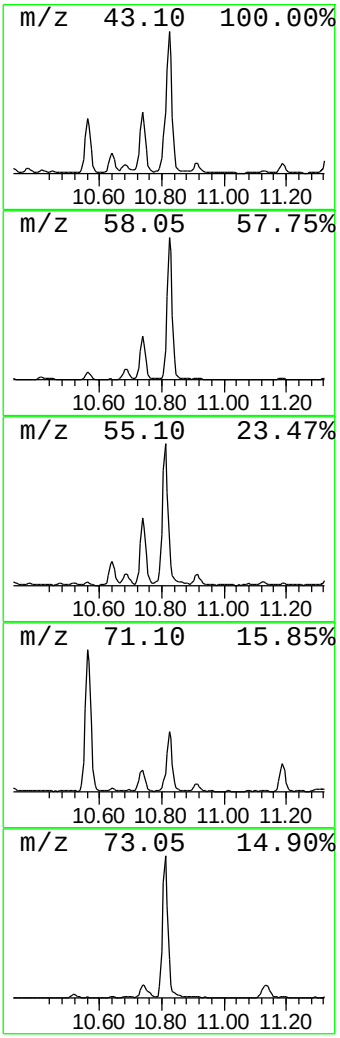
Peak Number 8 2-Heptanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.82	36.49 ug/l	1271530	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone	114	C7H14O	000110-43-0	80
2	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	50
3	2-Hexanone	100	C6H12O	000591-78-6	42
4	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	39
5	Propanamide, N,2-dimethyl-	101	C5H11NO	002675-88-9	36





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Sample : J6044-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 30003

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112018W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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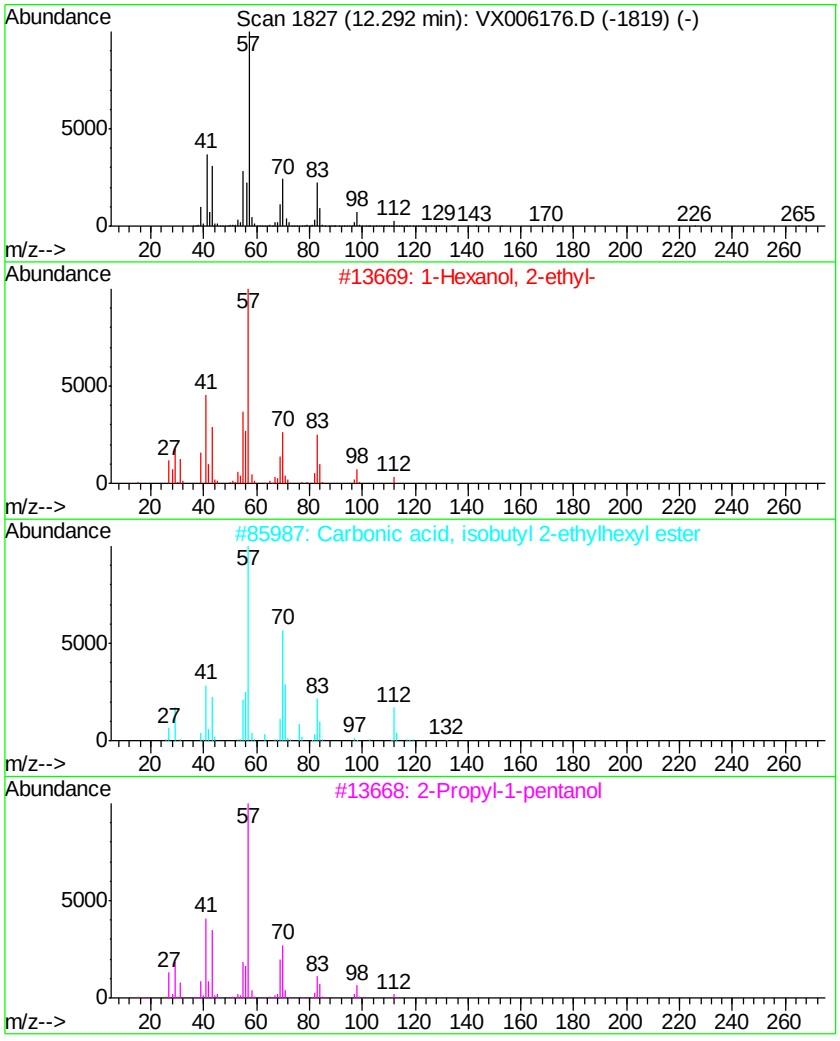
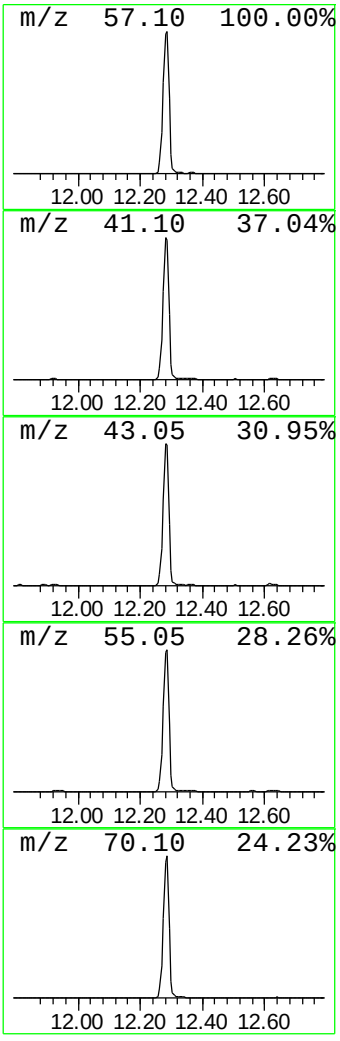
Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	1269.98 ug/l	36185400	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000357-82-9	59
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
4	1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	50
5	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112618\
Data File : VX006176.D
Acq On : 26 Nov 2018 15:38
Operator : JC/MD
Sample : J6044-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 30003

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112018W.M
Quant Title : SW846 8260

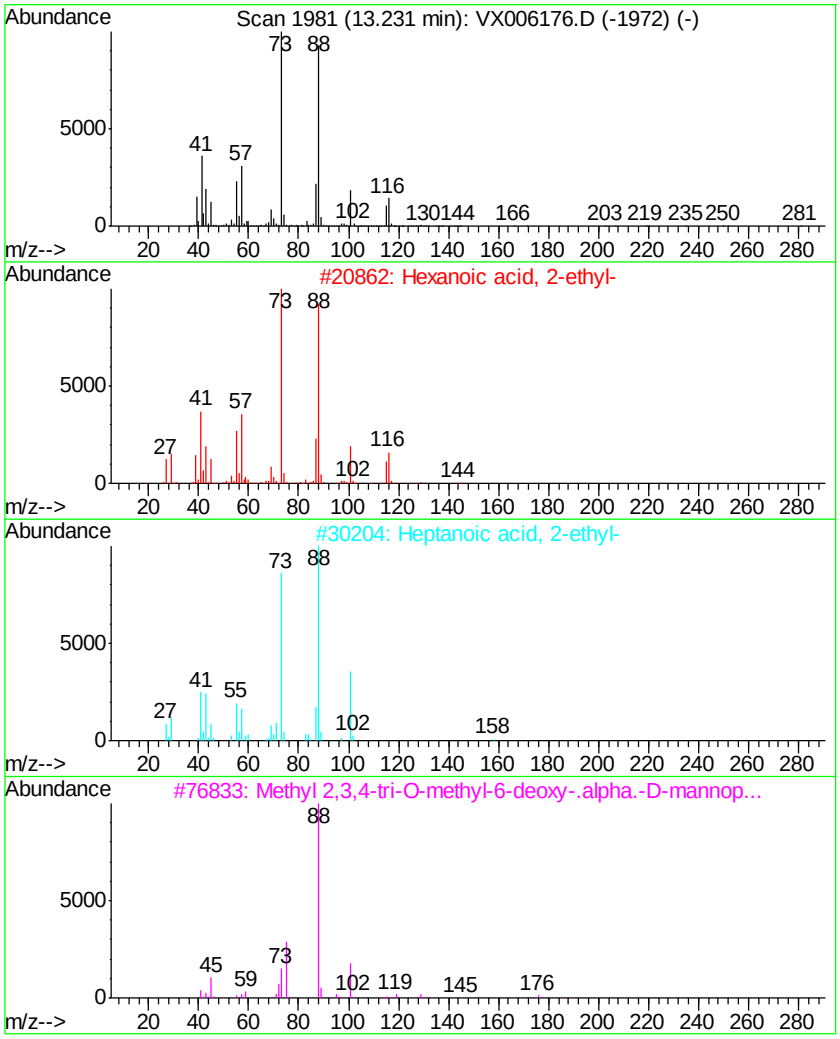
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

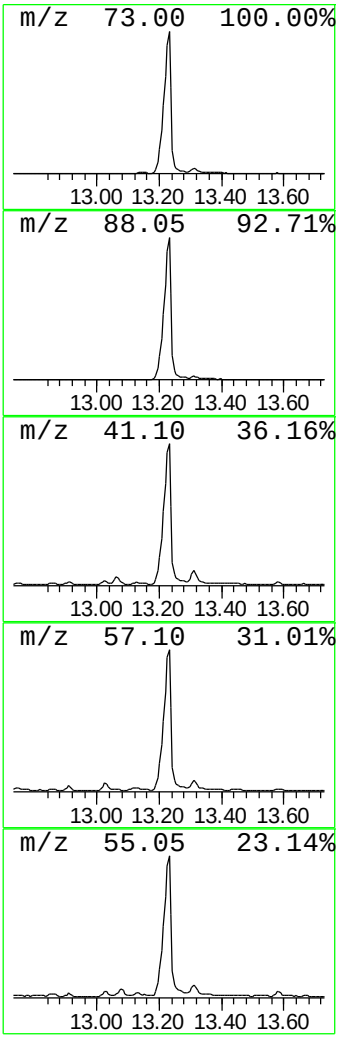
****

Peak Number 10 Hexanoic acid, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.23	206.61 ug/l	5886890	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	91
2	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	42
3	Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	40
4	Methyl-4-deoxy-2,3-di-O-methyl.b...	218	C9H14O6	1000312-09-9	40
5	Octanoic acid, 2-methyl-, methyl...	172	C10H20O2	002177-86-8	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112618\
Data File : VX006176.D
Acq On : 26 Nov 2018 15:38
Operator : JC/MD
Sample : J6044-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 30003

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112018W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Acetaldehyde	1.48	499.5	ug/l	9071220	1	5.67	907996	50.0
Ethanol	2.15	915.0	ug/l	16615500	1	5.67	907996	50.0
Propanal	2.35	104.1	ug/l	1890620	1	5.67	907996	50.0
1-Propanol	4.02	88.2	ug/l	1602500	1	5.67	907996	50.0
Butanal	4.35	239.2	ug/l	4344580	1	5.67	907996	50.0
1-Butanol	7.34	177.4	ug/l	4147230	2	6.86	1168630	50.0
Pentanal	7.66	68.2	ug/l	1593320	2	6.86	1168630	50.0
2-Heptanone	10.82	36.5	ug/l	1271530	3	10.12	1742330	50.0
1-Hexanol, 2-ethyl-	12.29	1270.0	ug/l	36185400	4	12.08	1424640	50.0
Hexanoic acid, 2-...	13.23	206.6	ug/l	5886890	4	12.08	1424640	50.0