LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX101918\
Data File : VX005463.D
Acq On : 19 Oct 2018 17:27
Operator : JC/MD
Sample : J5604-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MS-VB-25868-BOX-1

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\82X101218W.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	1.489	51	55	66	rVB	232699	266995	3.72%	1.077%
2	2.117	153	158	166	rVB	50680	75677	1.05%	0.305%
3	2.446	205	212	226	rBV	615459	1018330	14.18%	4.109%
4	2.617	233	240	252	rVB	241491	444107	6.18%	1.792%
5	4.354	511	525	534	rBV3	71478	210867	2.94%	0.851%
6	4.708	572	583	604	rVB	54139	156245	2.18%	0.630%
7	5.171	652	659	674	rVB6	20831	79408	1.11%	0.320%
8	5.507	701	714	729	rBV2	144049	417043	5.81%	1.683%
9	5.665	729	740	754	rBV2	242745	700778	9.76%	2.828%
10	6.067	795	806	813	rBV2	162480	422467	5.88%	1.705%
11	6.135	813	817	832	rVB	63899	169473	2.36%	0.684%
12	6.756	909	919	927	rBV	70025	171982	2.39%	0.694%
13	6.860	927	936	958	rVV	342066	848296	11.81%	3.423%
14	7.061	961	969	987	rVV	246439	546190	7.60%	2.204%
15	7.348	1004	1016	1032	rBV	3778926	7182611	100.00%	28.981%
16	7.555	1044	1050	1065	rVB	46036	99451	1.38%	0.401%
17	8.134	1136	1145	1162	rBV	252024	436614	6.08%	1.762%
18	8.719	1234	1241	1248	rVV	680520	1132737	15.77%	4.570%
19	8.787	1248	1252	1259	rVB	61053	104840	1.46%	0.423%
20	9.555	1373	1378	1382	rVB	67851	97472	1.36%	0.393%
21	9.896	1425	1434	1442	rBV	90765	134914	1.88%	0.544%
22	10.116	1461	1470	1476	rBV	710091	1016659	14.15%	4.102%
23	10.329	1499	1505	1517	rVB2	219487	366839	5.11%	1.480%
24	10.829	1577	1587	1597	rBV	43397	80774	1.12%	0.326%
25	10.939	1597	1605	1612	rBV6	42733	112683	1.57%	0.455%
26	11.054	1618	1624	1633	rBV	3609928	4498462	62.63%	18.151%
27	11.140	1633	1638	1645	rVB	633879	861843	12.00%	3.477%
28	12.030	1780	1784	1787	rBV	70897	81324	1.13%	0.328%
29	12.079	1787	1792	1800	rVV	833662	1035444	14.42%	4.178%
30	12.274	1816	1824	1835	rBV	154446	274691	3.82%	1.108%
31	13.804	2071	2075	2087	rBV2	813190	1154263	16.07%	4.657%
32	15.133	2289	2293	2301	rVB2	61236	116969	1.63%	0.472%
33	15.316	2319	2323	2340	rVB	255994	467225	6.50%	1.885%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX101918\
Data File : VX005463.D
Acq On : 19 Oct 2018 17:27
Operator : JC/MD
Sample : J5604-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MS-VB-25868-BOX-1

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\82X101218W.M
Title : SW846 8260

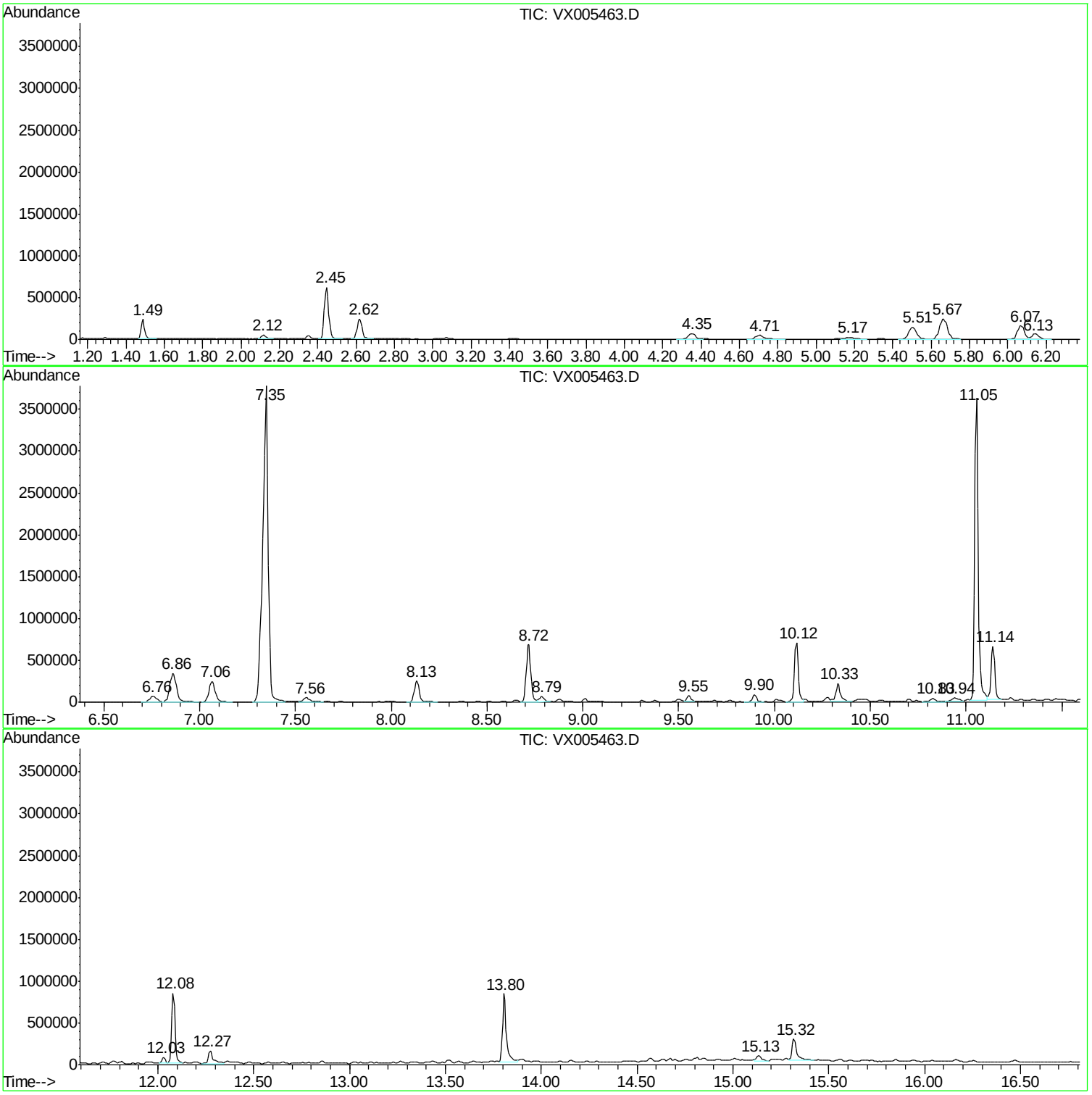
Sum of corrected areas: 24783673

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX101918\
Data File : VX005463.D
Acq On : 19 Oct 2018 17:27
Operator : JC/MD
Sample : J5604-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MS-VB-25868-BOX-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X101218W.M
Quant Title : SW846 8260

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX101918\
Data File : VX005463.D
Acq On : 19 Oct 2018 17:27
Operator : JC/MD
Sample : J5604-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MS-VB-25868-BOX-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X101218W.M
Quant Title : SW846 8260

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

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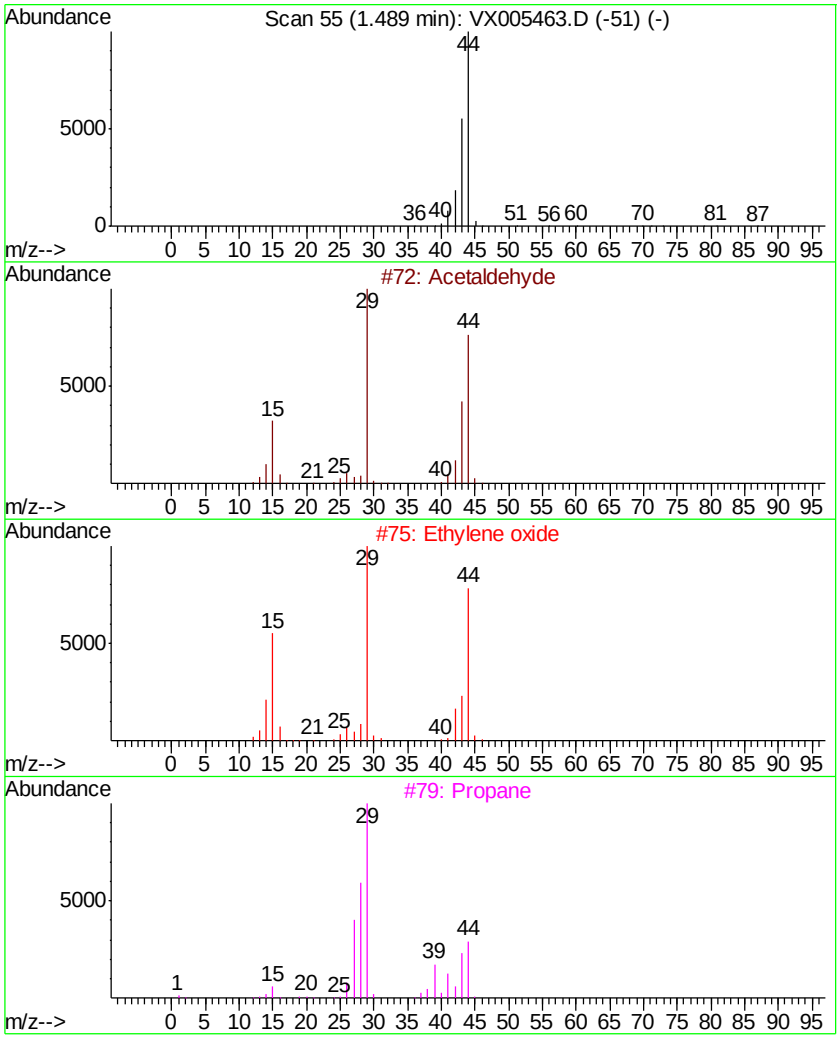
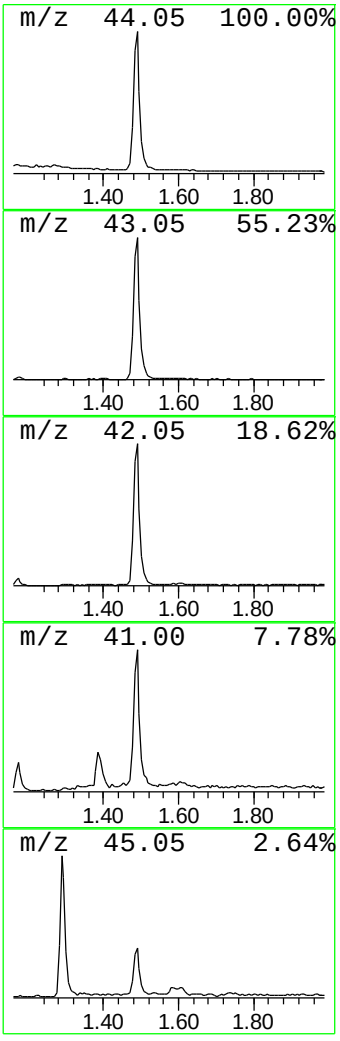
Peak Number 1 Acetaldehyde Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.49	19.05 ug/l	266995	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	56
2	Ethylene oxide	44	C2H4O	000075-21-8	5
3	Propane	44	C3H8	000074-98-6	4
4	Alanine	89	C3H7NO2	000056-41-7	4
5	Ethyne, fluoro-	44	C2HF	002713-09-9	3





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX101918\
Data File : VX005463.D
Acq On : 19 Oct 2018 17:27
Operator : JC/MD
Sample : J5604-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MS-VB-25868-BOX-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X101218W.M
Quant Title : SW846 8260

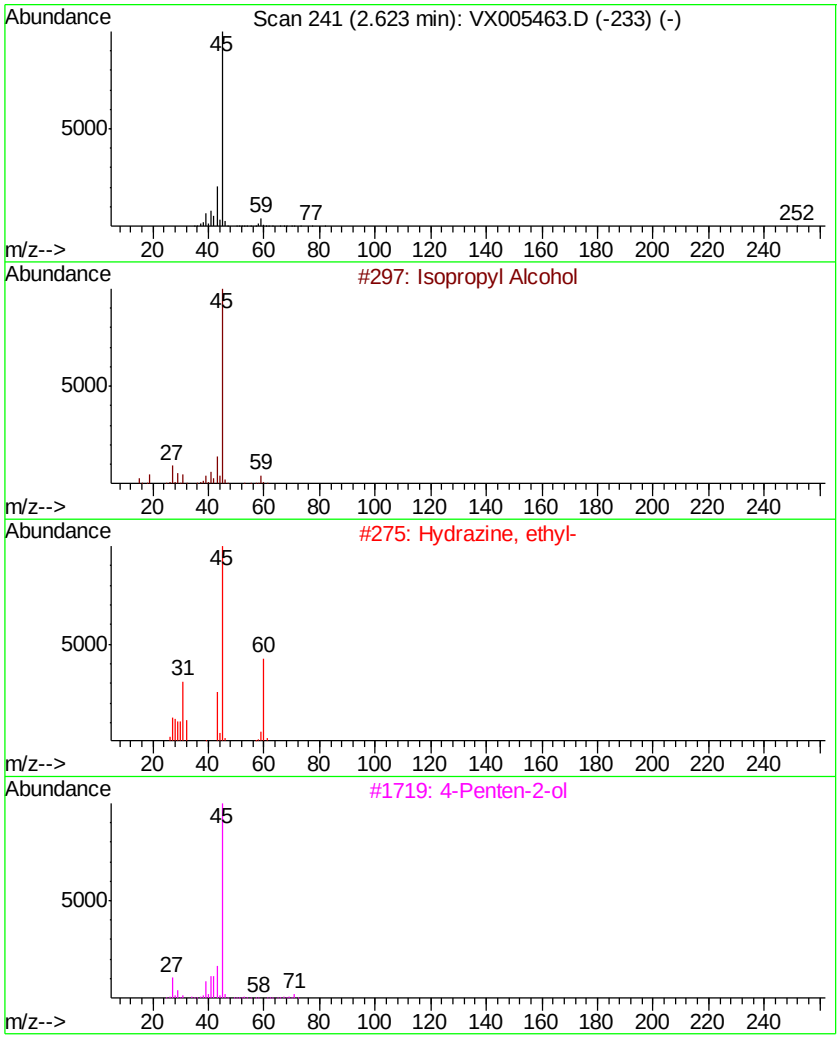
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

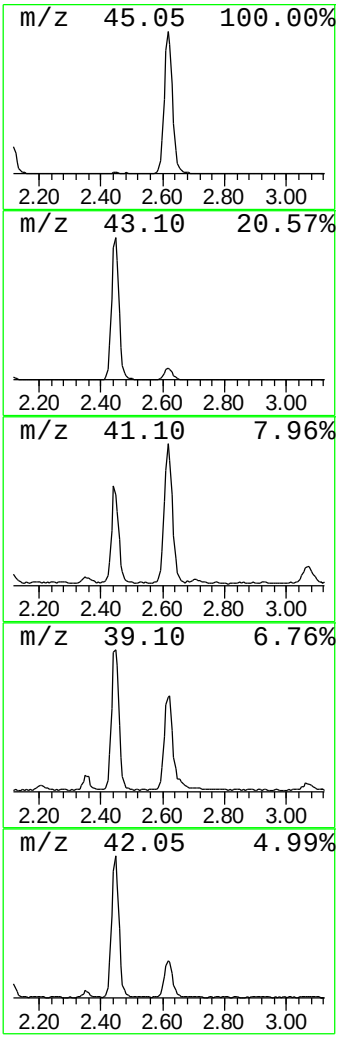
****

Peak Number 2 Isopropyl Alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.62	31.69 ug/l	444107	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	86
2	Hydrazine, ethyl-	60	C2H8N2	000624-80-6	40
3	4-Penten-2-ol	86	C5H10O	000625-31-0	9
4	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
5	Formamide	45	CH3NO	000075-12-7	4





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX101918\
Data File : VX005463.D
Acq On : 19 Oct 2018 17:27
Operator : JC/MD
Sample : J5604-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MS-VB-25868-BOX-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X101218W.M
Quant Title : SW846 8260

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

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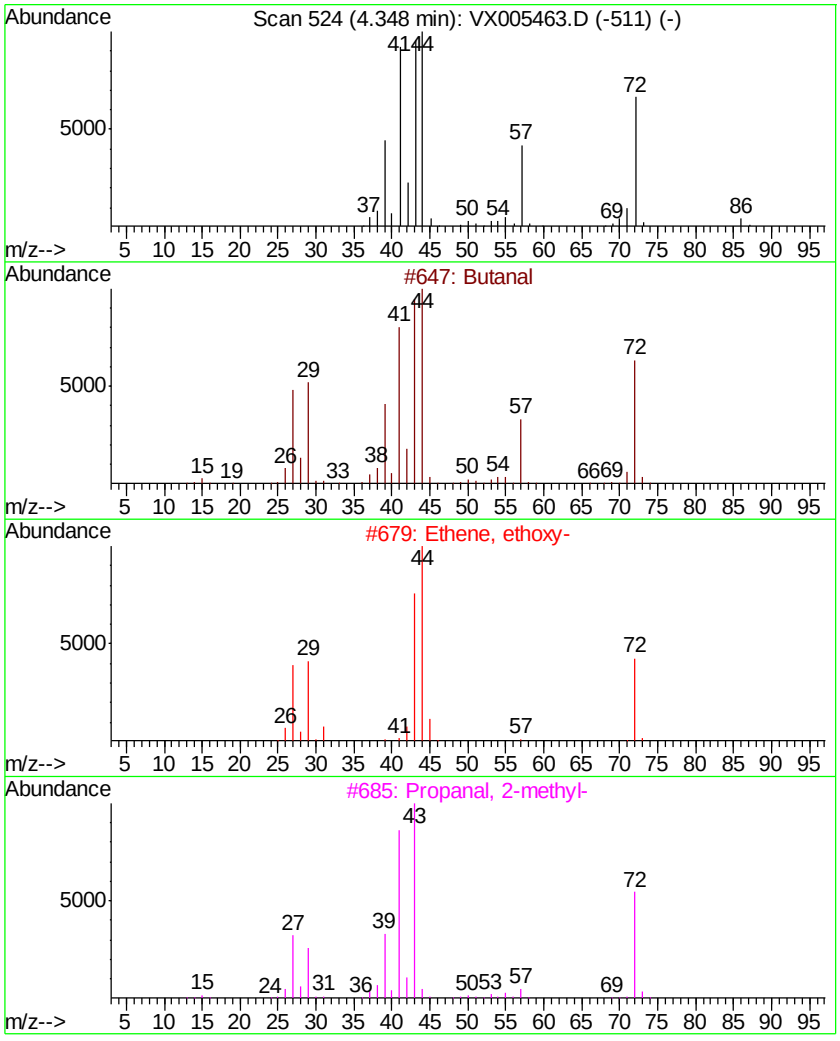
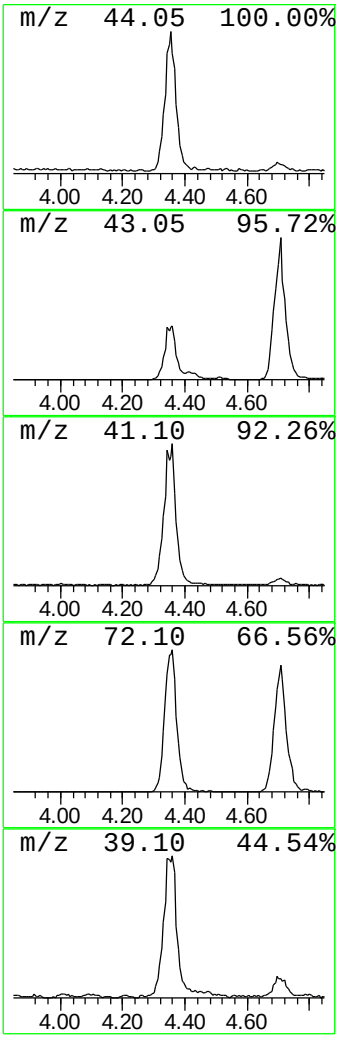
Peak Number 3 Butanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.35	15.05 ug/l	210867	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	50
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	49
4	O-Methylisourea	74	C2H6N2O	002440-60-0	36
5	Cyclopropyl carbinol	72	C4H8O	002516-33-8	25





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX101918\
Data File : VX005463.D
Acq On : 19 Oct 2018 17:27
Operator : JC/MD
Sample : J5604-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MS-VB-25868-BOX-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X101218W.M
Quant Title : SW846 8260

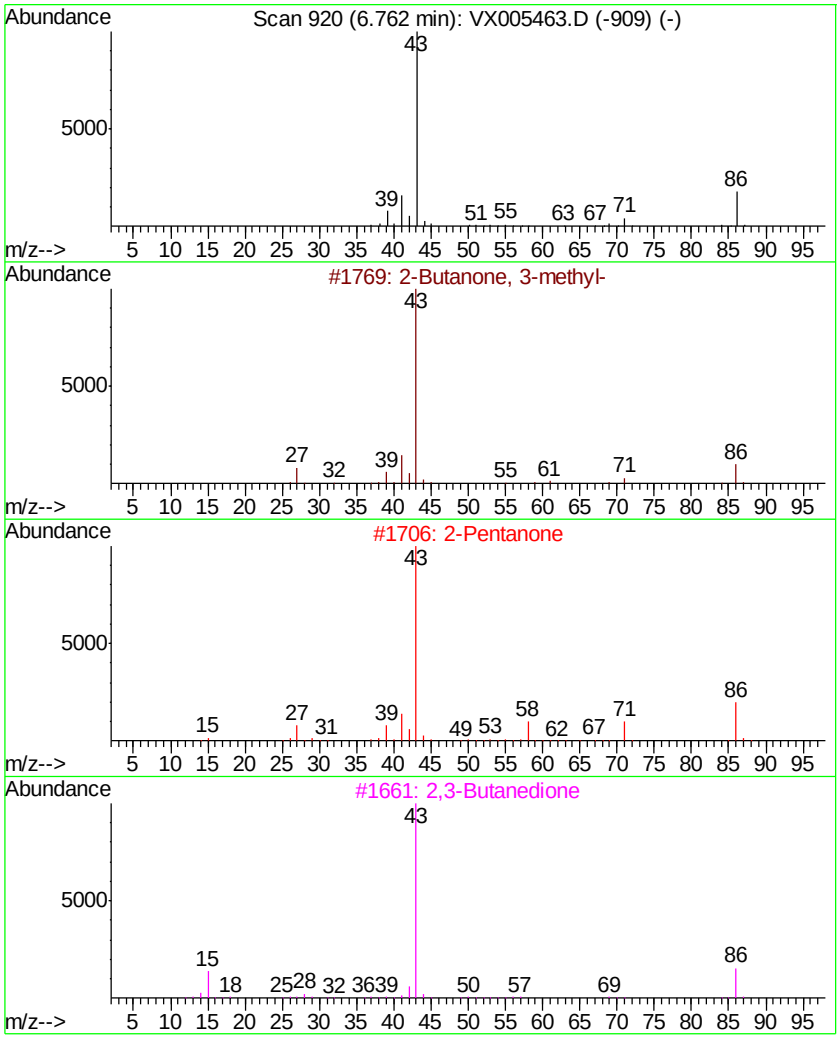
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

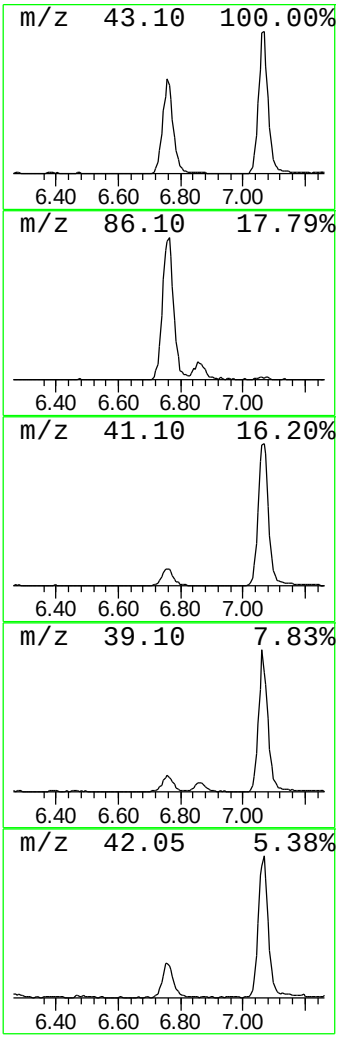
****

Peak Number 4 2-Butanone, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.76	10.14 ug/l	171982	1,4-Difluorobenzene	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	72
2	2-Pentanone	86	C5H10O	000107-87-9	53
3	2,3-Butanedione	86	C4H6O2	000431-03-8	50
4	2,3-Hexanedione	114	C6H10O2	003848-24-6	9
5	2-Pentanone, 3-ethyl-	114	C7H14O	006137-03-7	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX101918\
Data File : VX005463.D
Acq On : 19 Oct 2018 17:27
Operator : JC/MD
Sample : J5604-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MS-VB-25868-BOX-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X101218W.M
Quant Title : SW846 8260

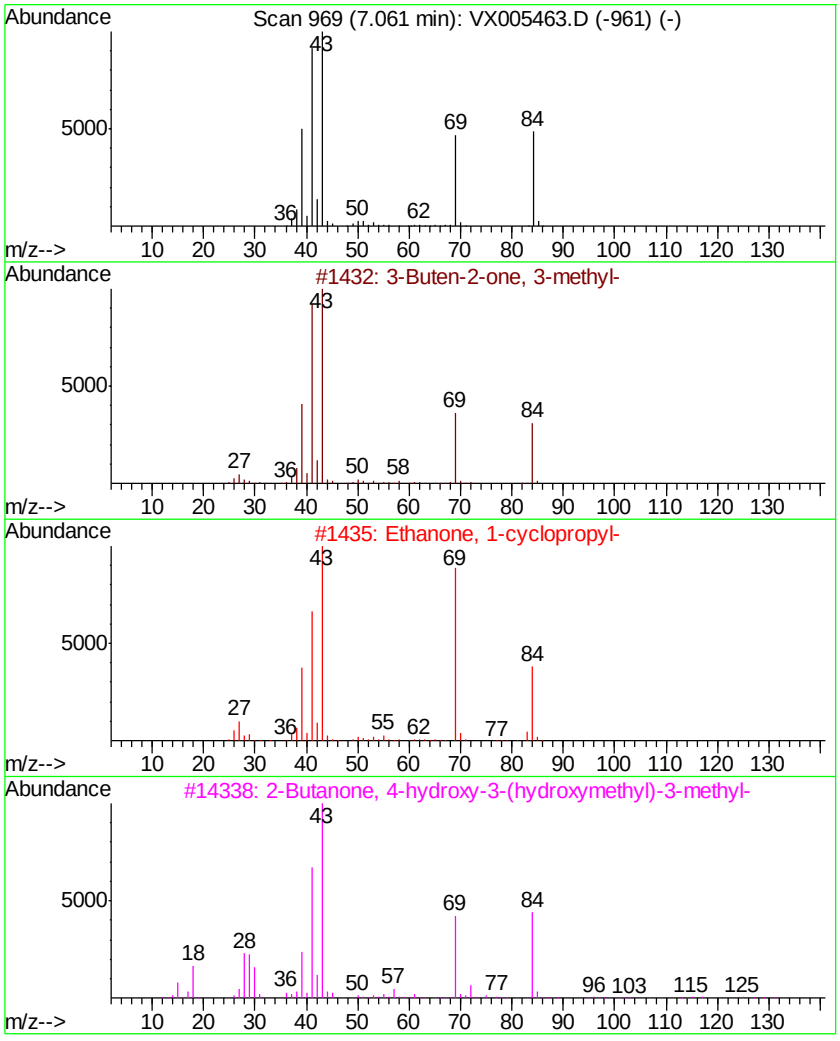
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

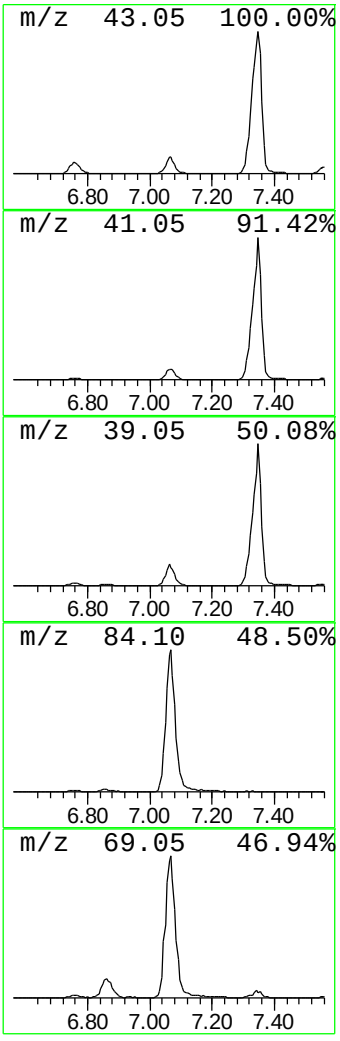
****

Peak Number 5 3-Buten-2-one, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.06	32.19 ug/l	546190	1,4-Difluorobenzene	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-2-one, 3-methyl-	84	C5H8O	000814-78-8	91
2	Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	62
3	2-Butanone, 4-hydroxy-3-(hydroxy...	132	C6H12O3	006868-97-9	38
4	(Z)-1,3-Butadien-1-ol	70	C4H6O	070415-58-6	25
5	2,2,6-Trimethyl-4H-1,3-dioxin-4-one	142	C7H10O3	005394-63-8	25





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX101918\
Data File : VX005463.D
Acq On : 19 Oct 2018 17:27
Operator : JC/MD
Sample : J5604-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MS-VB-25868-BOX-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X101218W.M
Quant Title : SW846 8260

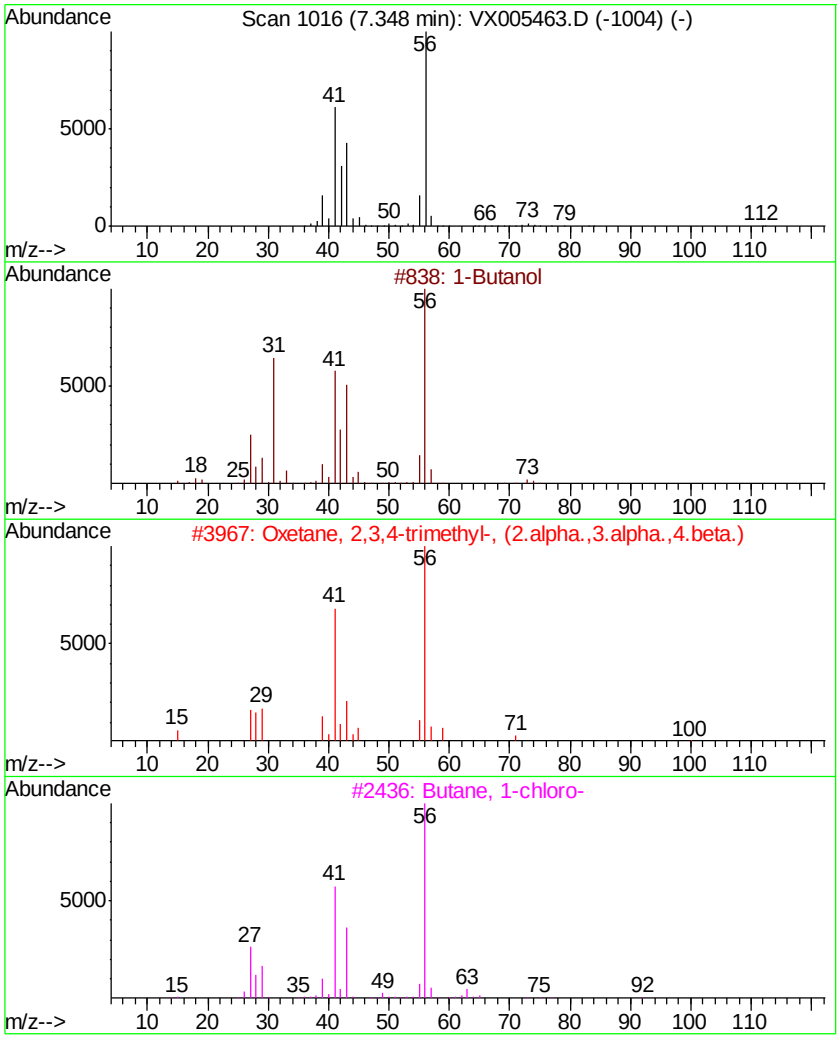
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

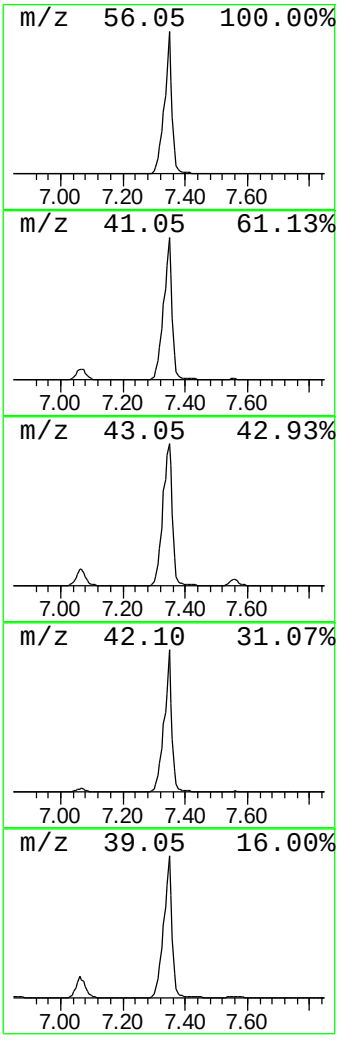
****

Peak Number 6 1-Butanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.35	423.36 ug/l	7182610	1,4-Difluorobenzene	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	83
2	Oxetane, 2,3,4-trimethyl-, (2.al...	100	C6H12O	032347-12-9	45
3	Butane, 1-chloro-	92	C4H9Cl	000109-69-3	38
4	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	36
5	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX101918\
Data File : VX005463.D
Acq On : 19 Oct 2018 17:27
Operator : JC/MD
Sample : J5604-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MS-VB-25868-BOX-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X101218W.M
Quant Title : SW846 8260

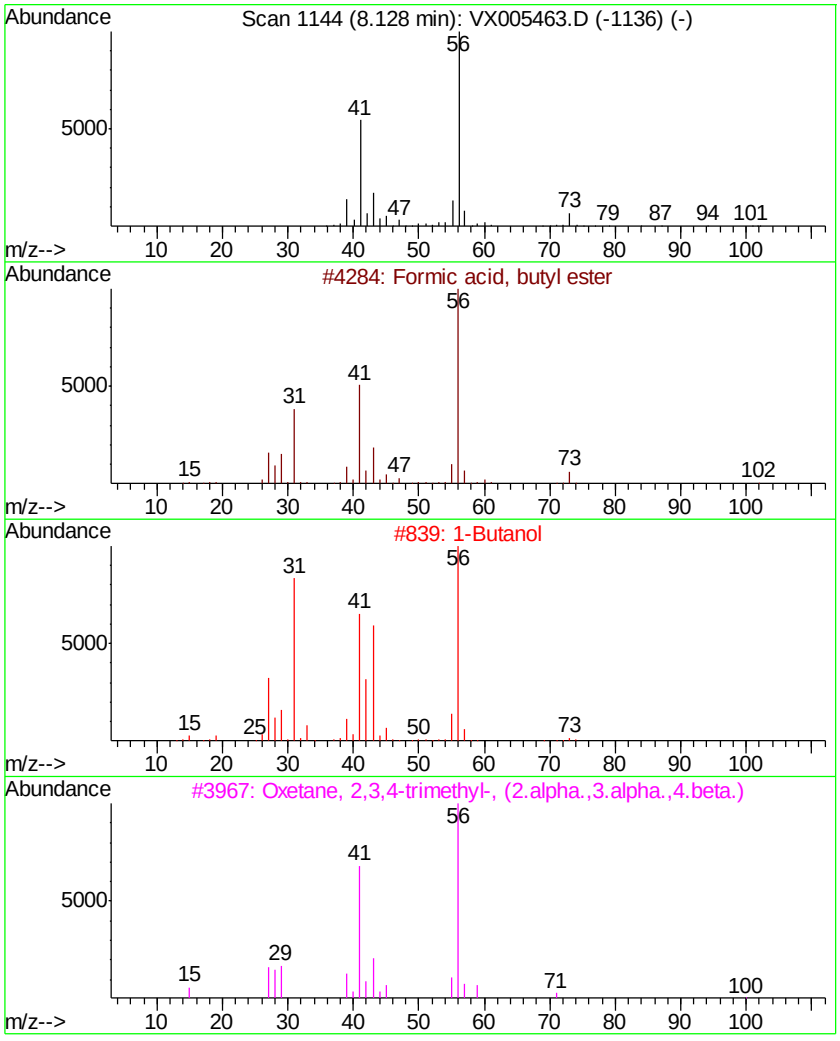
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

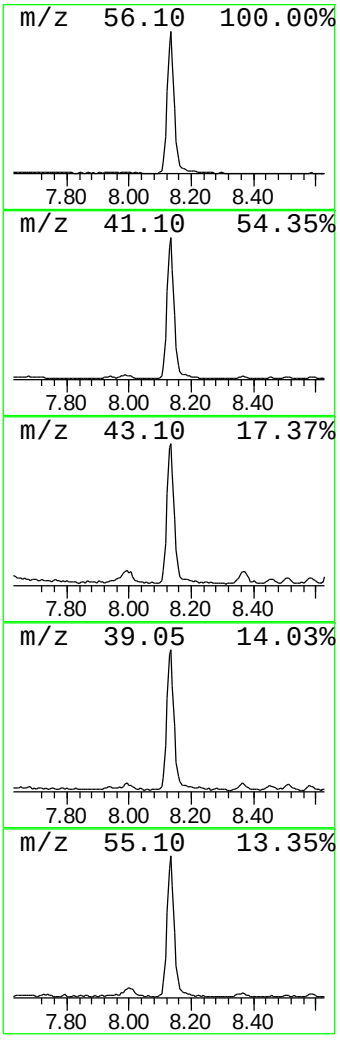
****

Peak Number 7 Formic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.13	25.73 ug/l	436614	1,4-Difluorobenzene	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Formic acid, butyl ester	102	C5H10O2	000592-84-7	83
2	1-Butanol	74	C4H10O	000071-36-3	72
3	Oxetane, 2,3,4-trimethyl-, (2.al...	100	C6H12O	032347-12-9	72
4	Butane, 1-chloro-	92	C4H9Cl	000109-69-3	64
5	Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	50





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX101918\
Data File : VX005463.D
Acq On : 19 Oct 2018 17:27
Operator : JC/MD
Sample : J5604-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MS-VB-25868-BOX-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X101218W.M
Quant Title : SW846 8260

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

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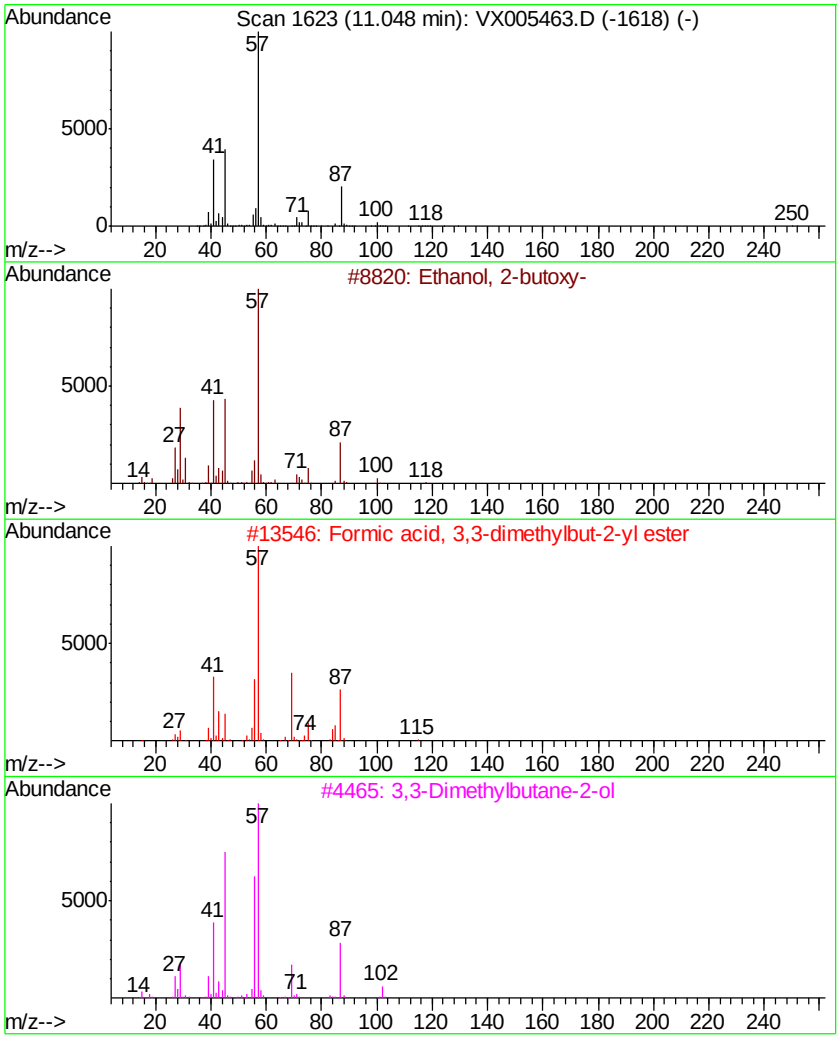
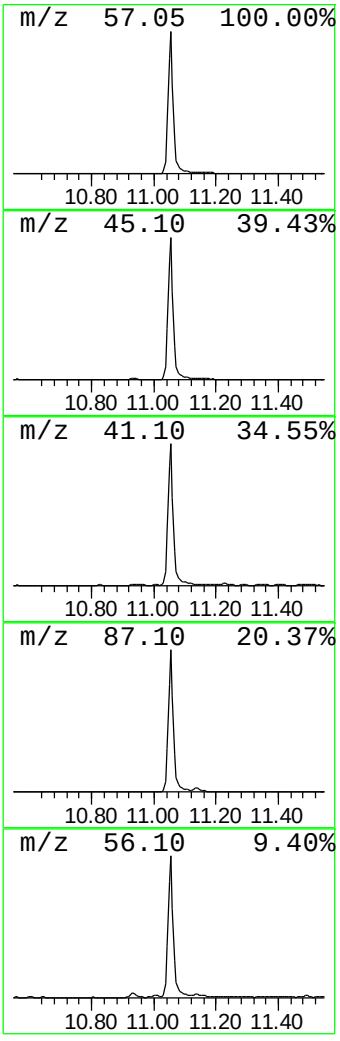
Peak Number 8 Ethanol, 2-butoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.05	221.24 ug/l	4498460	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	91
2	Formic acid, 3,3-dimethylbut-2-y...	130	C7H14O2	1000368-20-5	50
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	42
4	n-Butyl ether	130	C8H18O	000142-96-1	17
5	Propane, 1-(chloromethoxy)-2-met...	122	C5H11ClO	034180-11-5	16





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX101918\
Data File : VX005463.D
Acq On : 19 Oct 2018 17:27
Operator : JC/MD
Sample : J5604-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MS-VB-25868-BOX-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X101218W.M
Quant Title : SW846 8260

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

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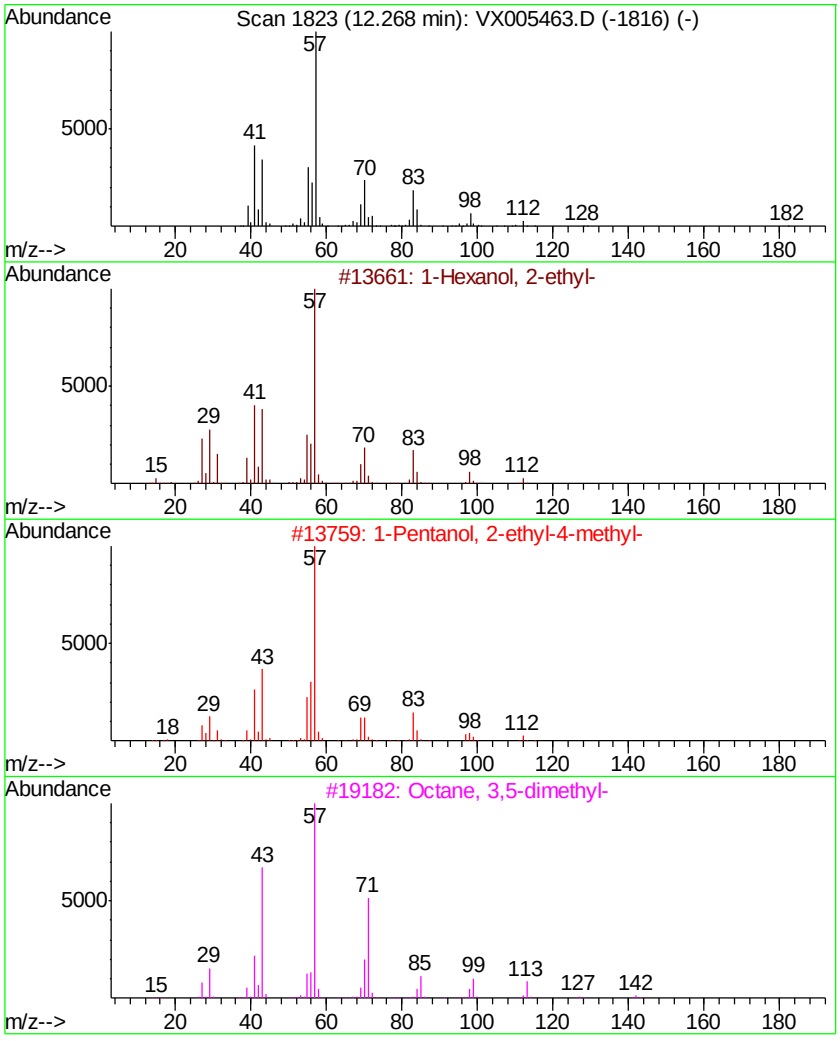
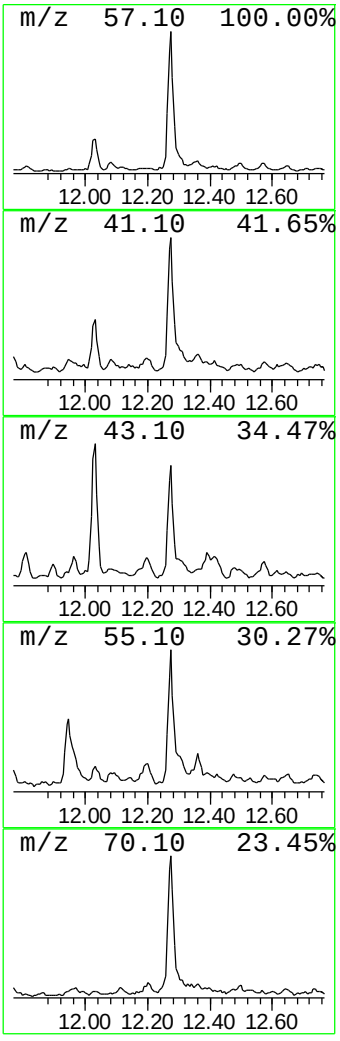
Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.27	13.26 ug/l	274691	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	90
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	53
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	47





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX101918\
Data File : VX005463.D
Acq On : 19 Oct 2018 17:27
Operator : JC/MD
Sample : J5604-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MS-VB-25868-BOX-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X101218W.M
Quant Title : SW846 8260

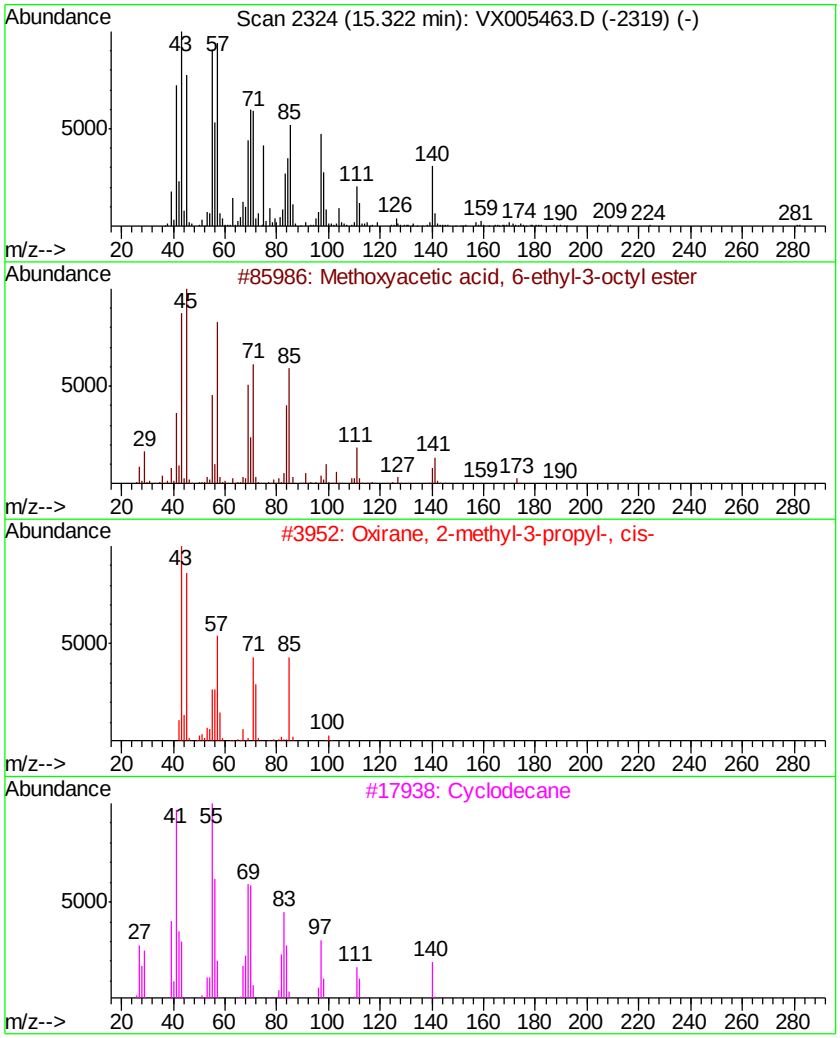
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

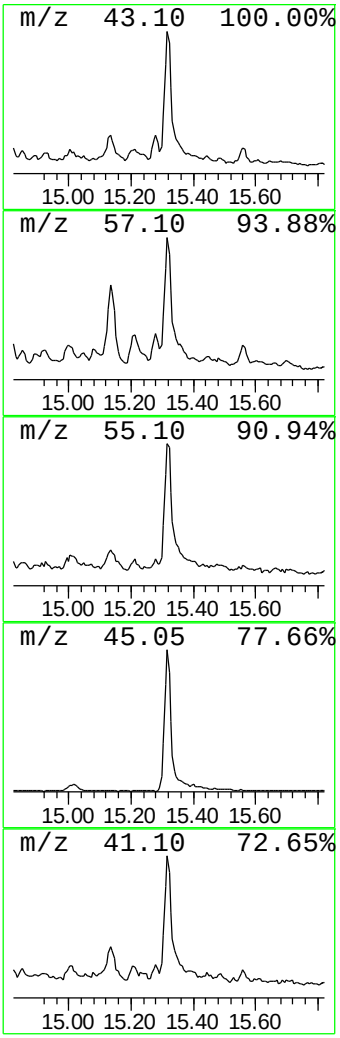
****

Peak Number 10 unknown Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.32	22.56 ug/l	467225	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methoxyacetic acid, 6-ethyl-3-oc...	230	C13H26O3	1000282-69-8	46
2	Oxirane, 2-methyl-3-propyl-, cis-	100	C6H12O	006124-90-9	43
3	Cyclodecane	140	C10H20	000293-96-9	41
4	3-Hexadecene, (Z)-	224	C16H32	034303-81-6	38
5	Cyclopropane, 1-(2-methylbutyl)-...	168	C12H24	064723-36-0	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX101918\
Data File : VX005463.D
Acq On : 19 Oct 2018 17:27
Operator : JC/MD
Sample : J5604-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MS-VB-25868-BOX-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X101218W.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	1.49	19.1	ug/l	266995	1	5.67	700778	50.0
Isopropyl Alcohol	2.62	31.7	ug/l	444107	1	5.67	700778	50.0
Butanal	4.35	15.1	ug/l	210867	1	5.67	700778	50.0
2-Butanone, 3-met...	6.76	10.1	ug/l	171982	2	6.87	848296	50.0
3-Buten-2-one, 3-...	7.06	32.2	ug/l	546190	2	6.87	848296	50.0
1-Butanol	7.35	423.4	ug/l	7182610	2	6.87	848296	50.0
Formic acid, buty...	8.13	25.7	ug/l	436614	2	6.87	848296	50.0
Ethanol, 2-butoxy-	11.05	221.2	ug/l	4498460	3	10.12	1016660	50.0
1-Hexanol, 2-ethyl-	12.27	13.3	ug/l	274691	4	12.08	1035440	50.0
unknown	15.32	22.6	ug/l	467225	4	12.08	1035440	50.0