

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112618\
 Data File : VX006204.D
 Acq On : 27 Nov 2018 04:57
 Operator : JC/MD
 Sample : J6044-04
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 30002

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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	1.392	35	39	45	rVB	49414	55617	1.61%	0.203%
2	1.489	51	55	65	rBV	832327	943931	27.40%	3.445%
3	2.117	151	158	171	rBV	2005479	3030798	87.97%	11.061%
4	2.355	191	197	205	rVB	238206	382919	11.11%	1.397%
5	2.446	205	212	228	rVV	607156	1027974	29.84%	3.752%
6	2.611	230	239	250	rVB	97546	181479	5.27%	0.662%
7	2.776	261	266	272	rBV	75970	132381	3.84%	0.483%
8	2.855	273	279	292	rVB	524162	985825	28.61%	3.598%
9	3.062	304	313	324	rBV	299063	656171	19.05%	2.395%
10	3.416	362	371	381	rBV	55795	125712	3.65%	0.459%
11	3.666	407	412	421	rVB2	14286	39051	1.13%	0.143%
12	4.001	457	467	478	rBV	103198	262639	7.62%	0.958%
13	4.348	510	524	535	rBV	497139	1335233	38.76%	4.873%
14	4.458	535	542	560	rVB2	62102	191254	5.55%	0.698%
15	4.702	571	582	594	rBV	136276	386055	11.21%	1.409%
16	5.178	651	660	672	rBV	38092	111733	3.24%	0.408%
17	5.501	703	713	727	rVB	168729	471212	13.68%	1.720%
18	5.665	729	740	756	rBV	283802	787058	22.84%	2.872%
19	6.068	796	806	817	rBV	181622	478083	13.88%	1.745%
20	6.257	828	837	848	rBV	33853	90414	2.62%	0.330%
21	6.860	926	936	946	rBV	421281	976406	28.34%	3.563%
22	6.982	951	956	965	rVB4	13529	37501	1.09%	0.137%
23	7.317	1002	1011	1026	rBV	301898	623548	18.10%	2.276%
24	7.549	1041	1049	1054	rBV	30828	59421	1.72%	0.217%
25	7.665	1062	1068	1075	rVB	160620	287832	8.35%	1.050%
26	8.713	1233	1240	1247	rBV	869385	1346791	39.09%	4.915%
27	8.787	1247	1252	1256	rVB	33047	52686	1.53%	0.192%
28	9.299	1331	1336	1344	rBV	48194	75922	2.20%	0.277%
29	9.494	1362	1368	1375	rBV	20853	35893	1.04%	0.131%
30	9.585	1378	1383	1389	rVV3	45595	81044	2.35%	0.296%
31	10.116	1461	1470	1481	rBV	854669	1208722	35.08%	4.411%
32	10.213	1481	1486	1490	rBV	90201	121778	3.53%	0.444%
33	10.311	1497	1502	1506	rBV2	54299	81902	2.38%	0.299%
34	10.372	1506	1512	1518	rVB2	383209	574869	16.69%	2.098%

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35	10.561	1538	1543	1551	rBV	199261	259312	7.53%	0.946%
36	10.689	1559	1564	1569	rVV2	160425	280422	8.14%	1.023%
37	10.737	1569	1572	1577	rVV	271017	334866	9.72%	1.222%
38	10.823	1577	1586	1596	rVV2	251918	418619	12.15%	1.528%
39	10.908	1596	1600	1608	rVB2	26045	38348	1.11%	0.140%
40	11.085	1625	1629	1633	rBV	25489	36435	1.06%	0.133%
41	11.140	1633	1638	1643	rVV	747764	987233	28.65%	3.603%
42	11.207	1643	1649	1657	rVB2	122344	184672	5.36%	0.674%
43	11.365	1672	1675	1680	rVB2	35118	45512	1.32%	0.166%
44	11.432	1682	1686	1691	rBV	24996	40752	1.18%	0.149%
45	11.628	1713	1718	1720	rBV2	48387	61134	1.77%	0.223%
46	11.670	1720	1725	1732	rVV4	77994	163631	4.75%	0.597%
47	11.737	1732	1736	1741	rVV	81294	99698	2.89%	0.364%
48	11.810	1743	1748	1752	rVB2	99366	126964	3.69%	0.463%
49	11.920	1763	1766	1774	rVB2	64917	95144	2.76%	0.347%
50	12.042	1778	1786	1788	rBV4	38153	69415	2.01%	0.253%
51	12.079	1788	1792	1800	rVV2	1038175	1426302	41.40%	5.205%
52	12.274	1819	1824	1835	rBV	2815482	3445301	100.00%	12.573%
53	12.359	1835	1838	1852	rVB4	59298	111813	3.25%	0.408%
54	12.560	1867	1871	1875	rBV	24507	34678	1.01%	0.127%
55	12.621	1877	1881	1887	rVV4	58435	103240	3.00%	0.377%
56	12.853	1911	1919	1925	rVB4	38004	82191	2.39%	0.300%
57	12.926	1925	1931	1937	rVB	28274	43455	1.26%	0.159%
58	13.018	1937	1946	1950	rBV4	28399	61642	1.79%	0.225%
59	13.060	1950	1953	1958	rBV2	25392	45041	1.31%	0.164%
60	13.207	1971	1977	1989	rBV	472933	668515	19.40%	2.440%
61	13.298	1989	1992	1997	rBV	41449	49211	1.43%	0.180%
62	13.804	2072	2075	2077	rBV	46830	48997	1.42%	0.179%
63	13.835	2077	2080	2082	rVV	45277	51503	1.49%	0.188%
64	13.865	2082	2085	2089	rVB3	34354	46533	1.35%	0.170%
65	13.975	2100	2103	2113	rVB4	20259	34555	1.00%	0.126%
66	14.694	2215	2221	2225	rBV	35499	53543	1.55%	0.195%
67	14.840	2241	2245	2249	rBV	30196	38151	1.11%	0.139%
68	15.200	2299	2304	2309	rBV2	38344	56925	1.65%	0.208%
69	15.273	2312	2316	2322	rVB	29645	45652	1.33%	0.167%
70	15.377	2328	2333	2341	rBV	31278	50748	1.47%	0.185%
71	15.560	2358	2363	2368	rBV3	49054	85123	2.47%	0.311%

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Integration Parameters: RTEINT.P

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72	15.688	2378	2384	2387	rBV2	21896	38753	1.12%	0.141%
73	15.749	2387	2394	2400	rVB2	35908	75775	2.20%	0.277%
74	16.054	2437	2444	2451	rBV2	96444	182114	5.29%	0.665%
75	16.176	2459	2464	2471	rVB	21564	39693	1.15%	0.145%

Sum of corrected areas: 27401465

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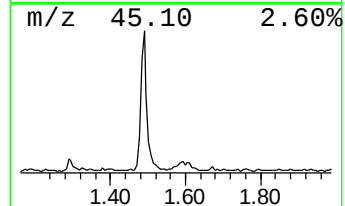
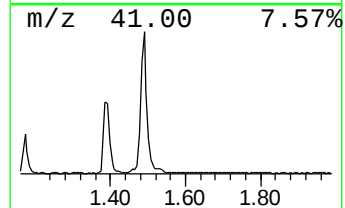
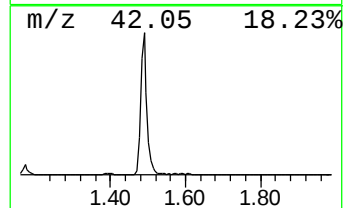
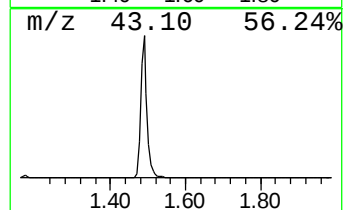
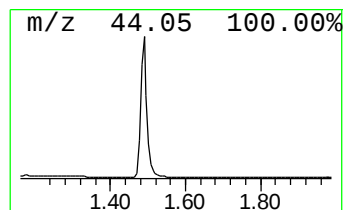
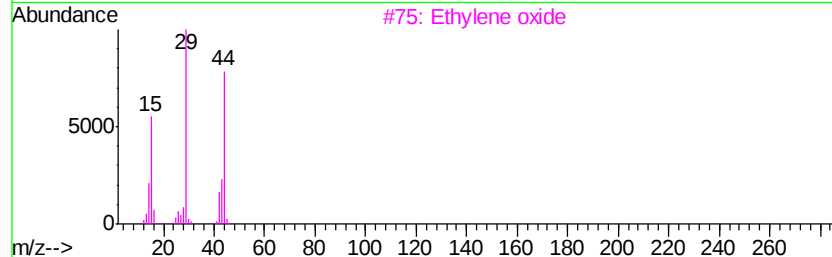
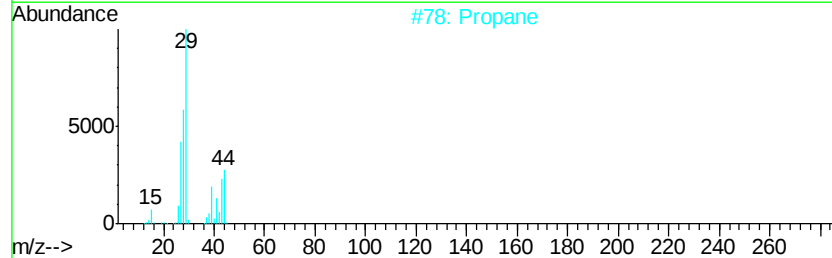
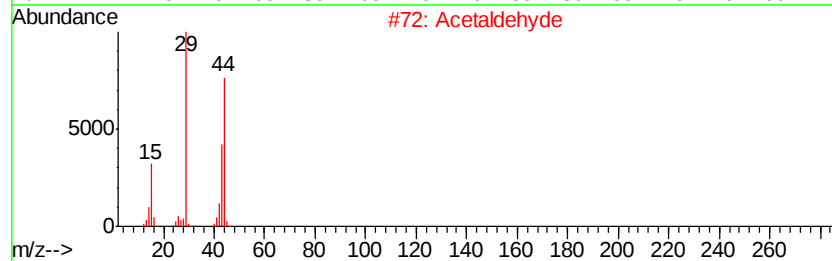
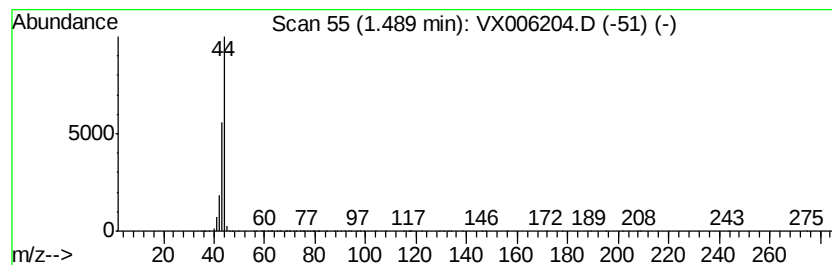
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X112018W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Acetaldehyde Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.49	59.97 ug/l	943931	Pentafluorobenzene	5.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde		44	C2H4O	000075-07-0	56
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



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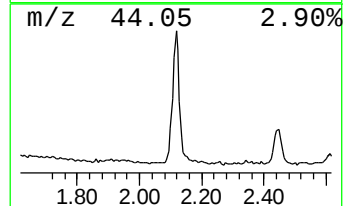
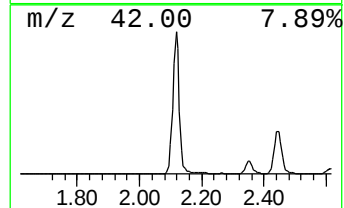
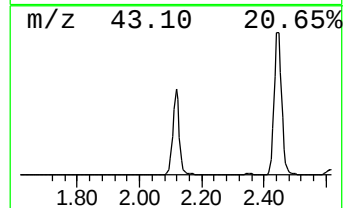
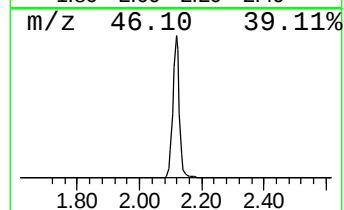
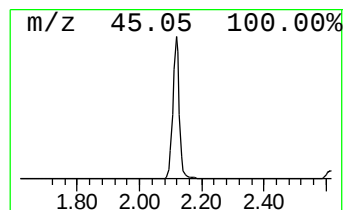
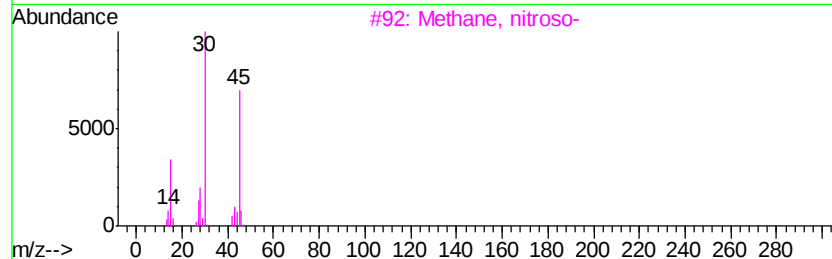
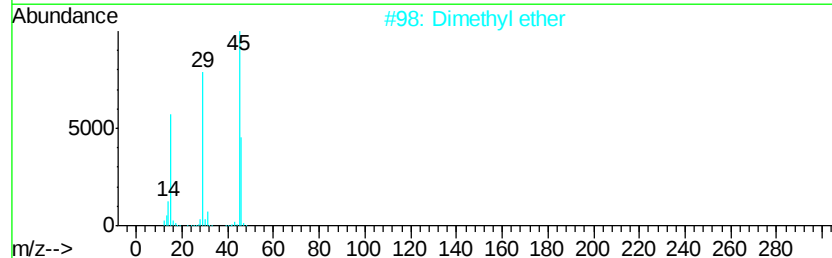
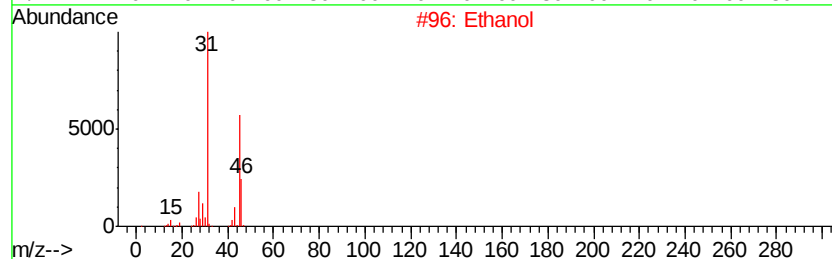
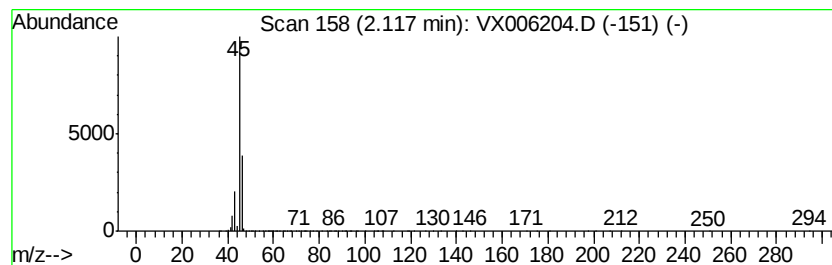
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X112018W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	192.54 ug/l	3030800	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol	46	C2H6O	000064-17-5	64
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



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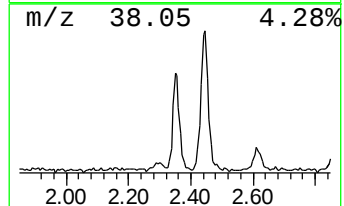
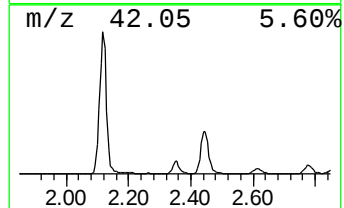
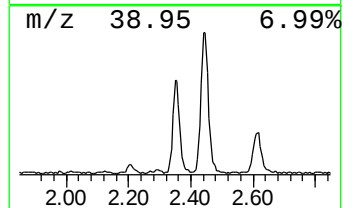
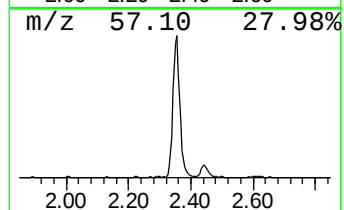
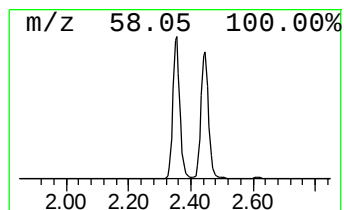
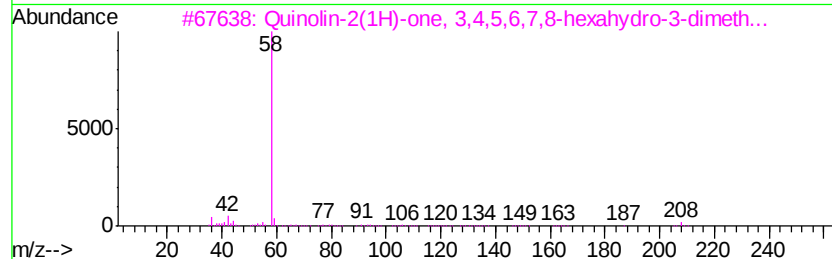
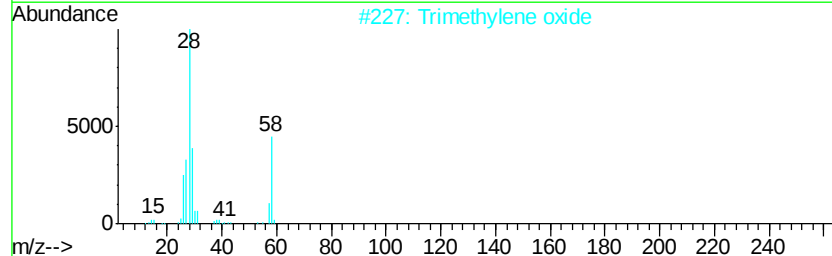
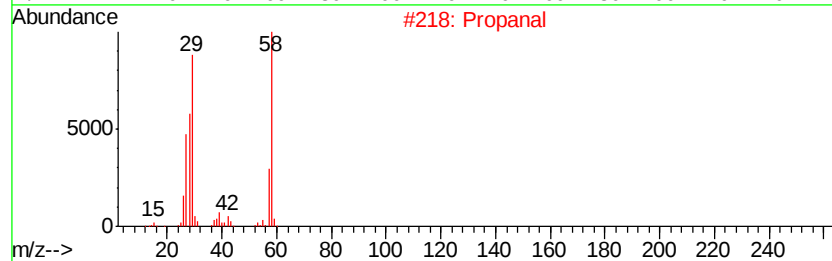
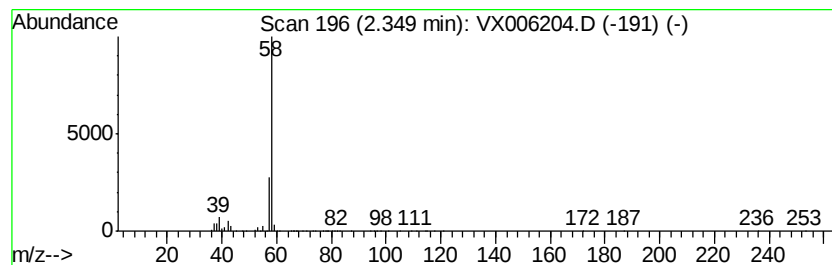
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Propanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.35	24.33 ug/l	382919	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7
5		Propylene oxide	58	C3H6O	000075-56-9	7



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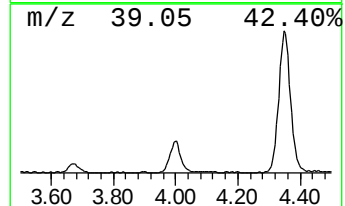
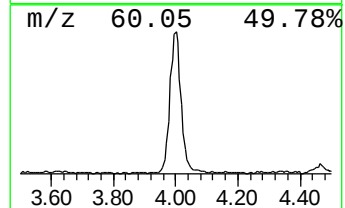
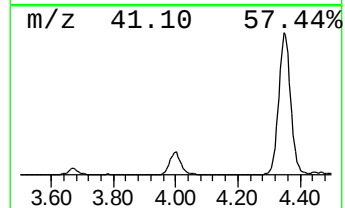
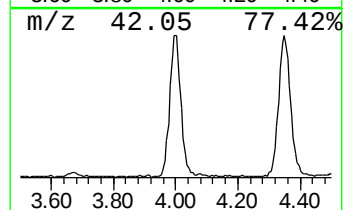
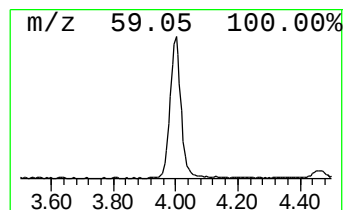
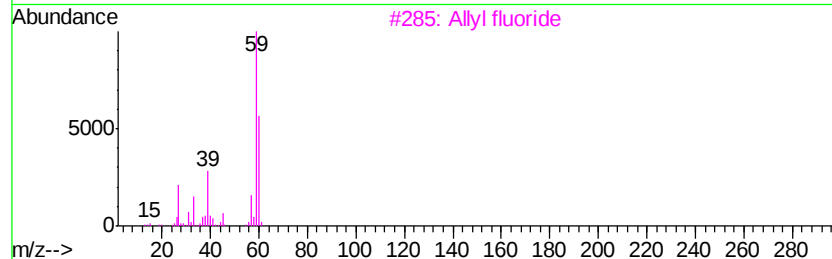
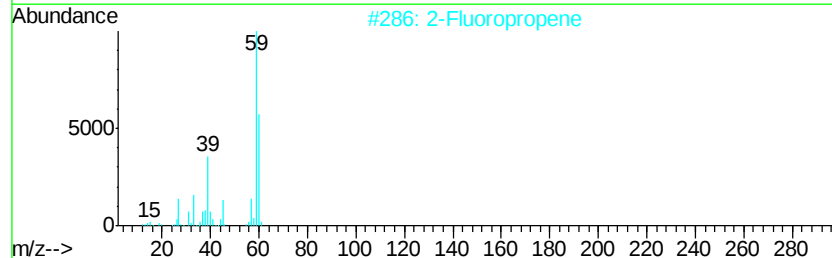
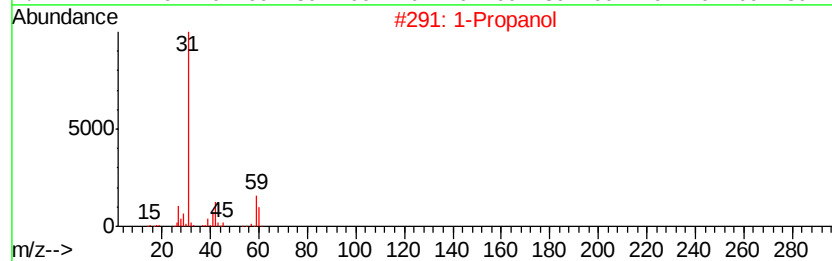
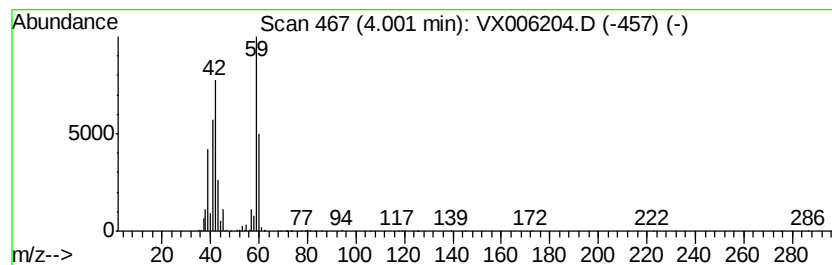
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Propanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.00	16.68 ug/l	262639	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Propanol	60	C3H8O	000071-23-8	64
2		2-Fluoropropene	60	C3H5F	001184-60-7	52
3		Allyl fluoride	60	C3H5F	000818-92-8	38
4		3-Buten-1-ol	72	C4H8O	000627-27-0	38
5		Isoxazolidine, 4-ethyl-2,5-dimet...	129	C7H15NO	056728-13-3	33



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Data File : VX006204.D
Acq On : 27 Nov 2018 04:57
Operator : JC/MD
Sample : J6044-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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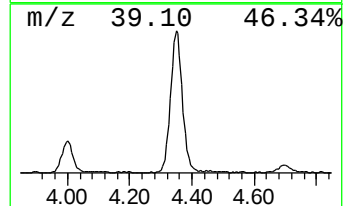
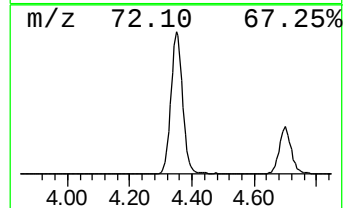
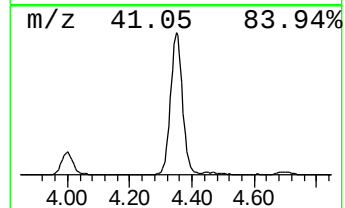
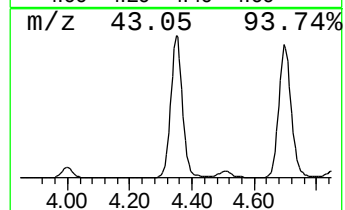
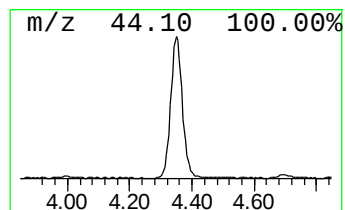
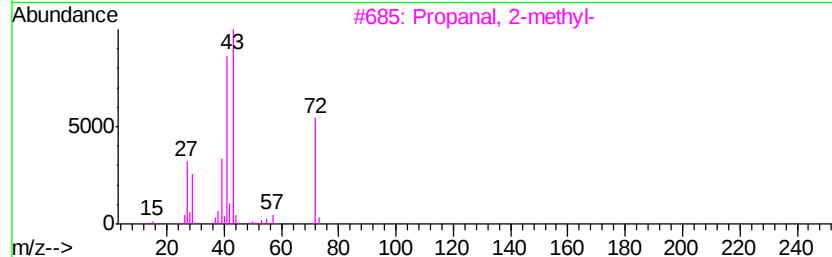
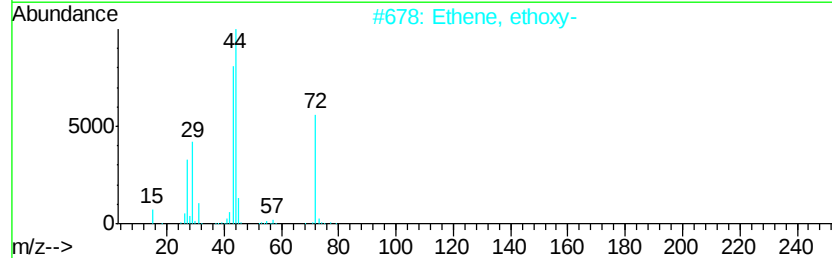
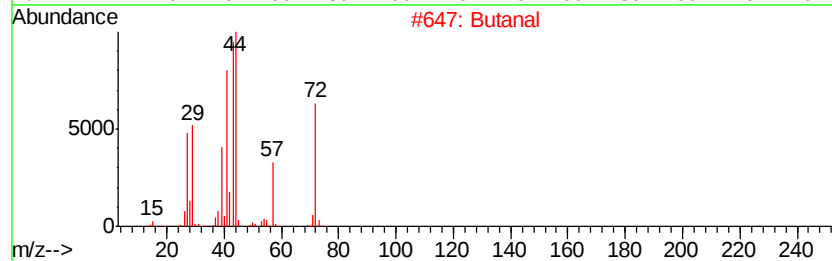
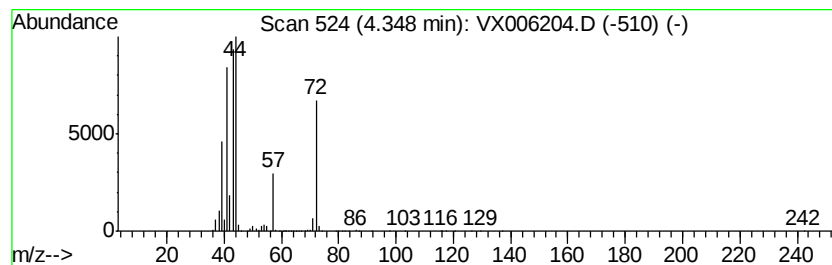
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Quant Title : SW846 8260

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

Peak Number 5 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.35	84.82 ug/l	1335230	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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	43
4		Methacrolein	70	C4H6O	000078-85-3	22
5		Cyclopropanecarboxamide	85	C4H7NO	006228-73-5	17



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX112618\
Data File : VX006204.D
Acq On : 27 Nov 2018 04:57
Operator : JC/MD
Sample : J6044-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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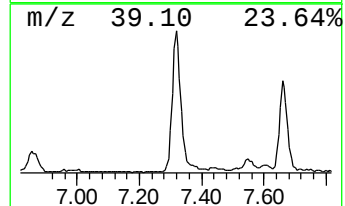
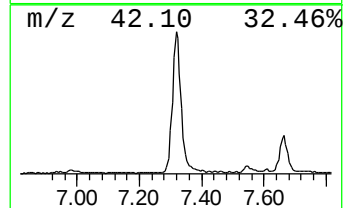
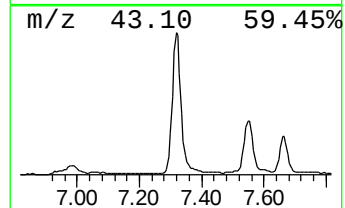
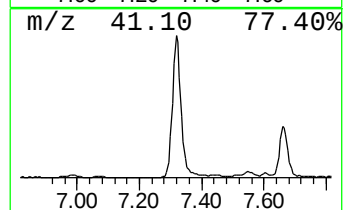
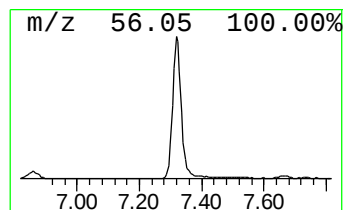
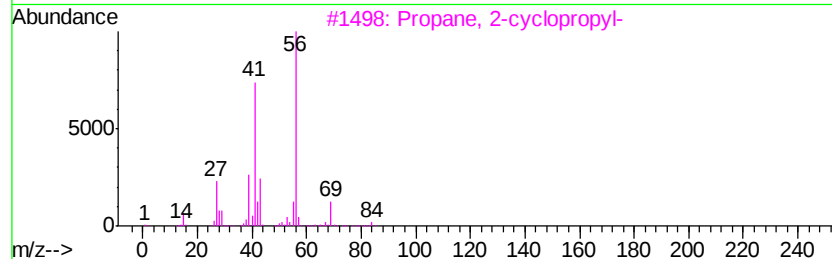
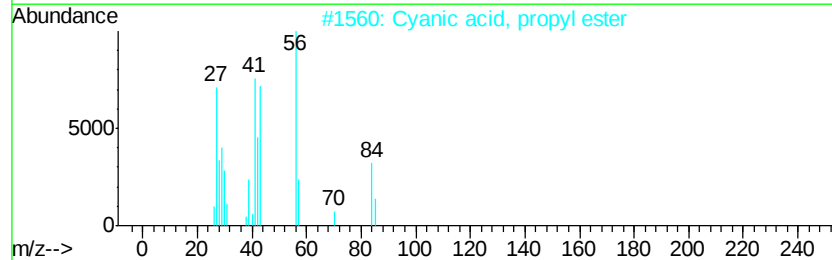
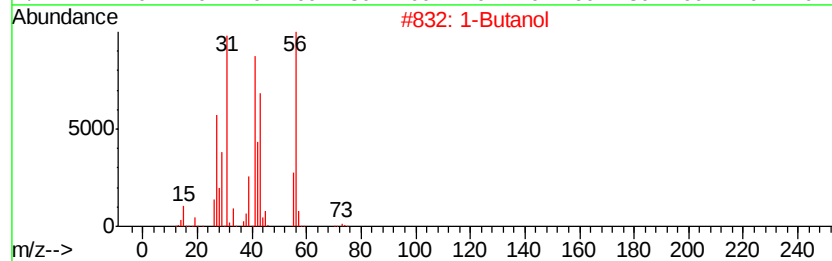
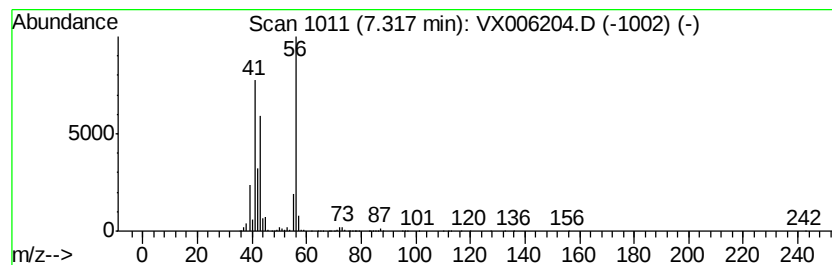
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Quant Title : SW846 8260

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

Peak Number 6 1-Butanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.32	31.93 ug/l	623548	1,4-Difluorobenzene	6.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol		74	C4H10O	000071-36-3	87
2	Cyanoic acid, propyl ester		85	C4H7NO	001768-36-1	56
3	Propane, 2-cyclopropyl-		84	C6H12	003638-35-5	40
4	2H-Pyran-2-one, tetrahydro-5,6-d...		128	C7H12O2	024405-16-1	36
5	Cyclopropane, propyl-		84	C6H12	002415-72-7	9



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX112618\
Data File : VX006204.D
Acq On : 27 Nov 2018 04:57
Operator : JC/MD
Sample : J6044-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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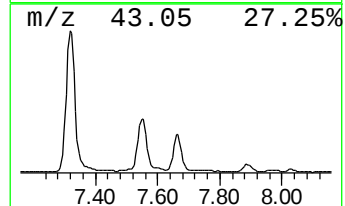
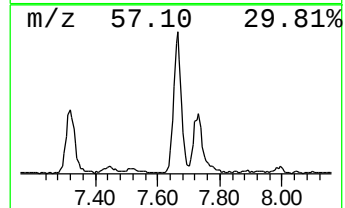
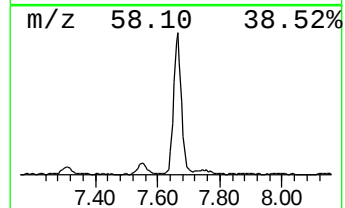
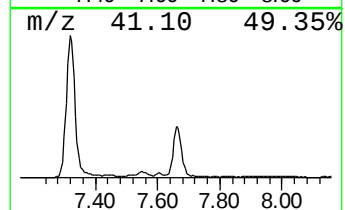
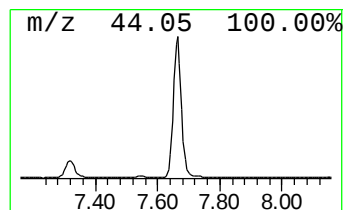
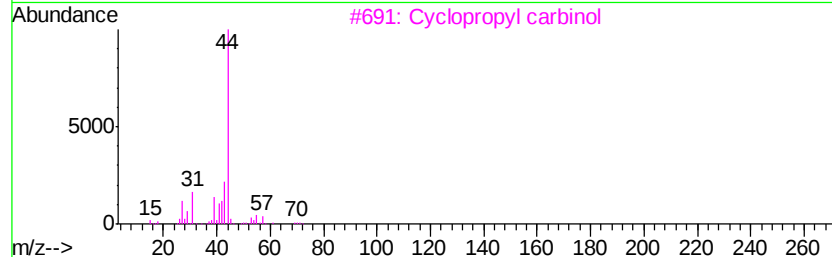
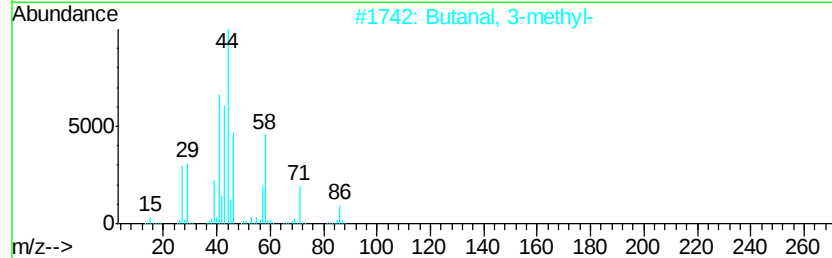
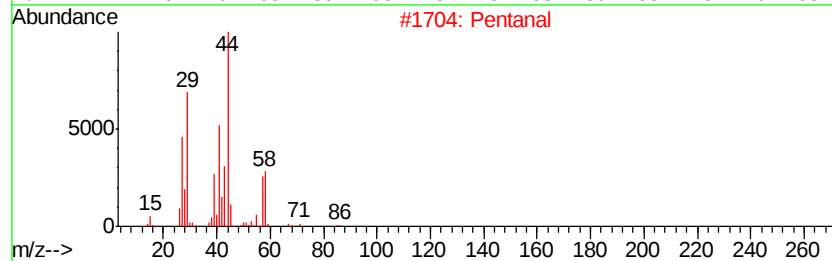
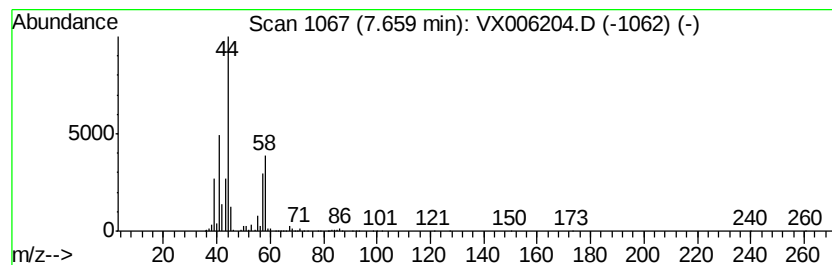
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Quant Title : SW846 8260

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

Peak Number 7 Pentanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	14.74 ug/l	287832	1,4-Difluorobenzene	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentanal	86	C5H10O	000110-62-3	90
2		Butanal, 3-methyl-	86	C5H10O	000590-86-3	64
3		Cyclopropyl carbinol	72	C4H8O	002516-33-8	33
4		Succindialdehyde	86	C4H6O2	000638-37-9	9
5		Cyclobutanol	72	C4H8O	002919-23-5	9



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX112618\
Data File : VX006204.D
Acq On : 27 Nov 2018 04:57
Operator : JC/MD
Sample : J6044-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 43 Sample Multiplier: 1

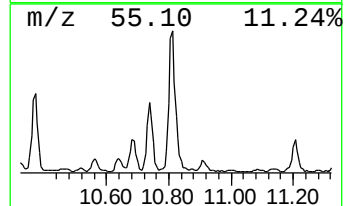
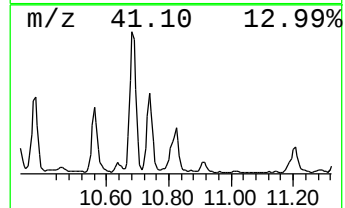
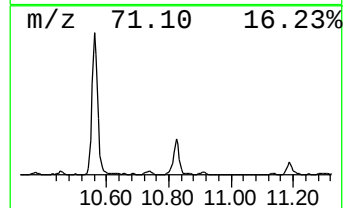
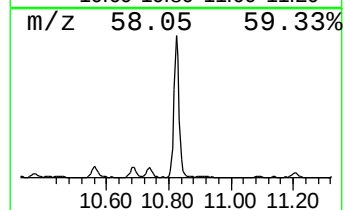
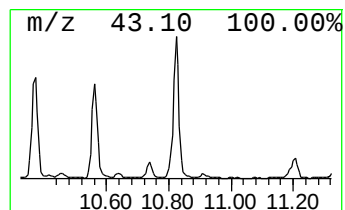
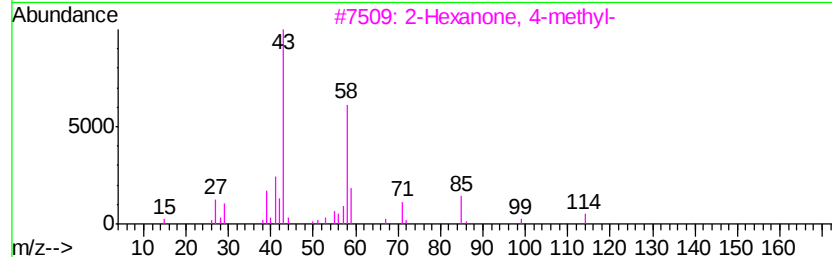
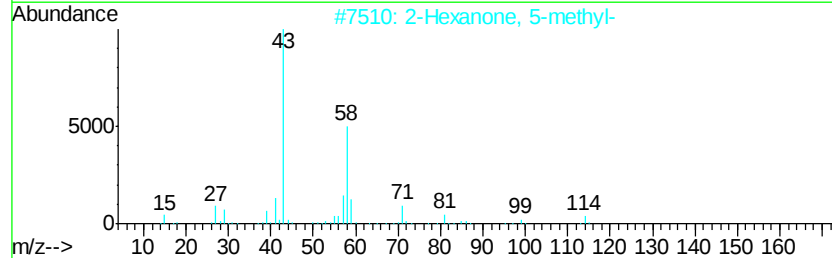
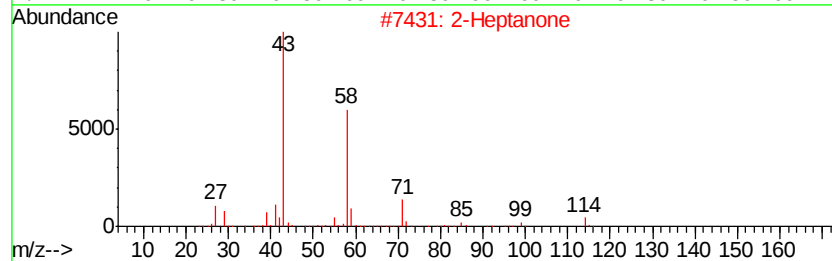
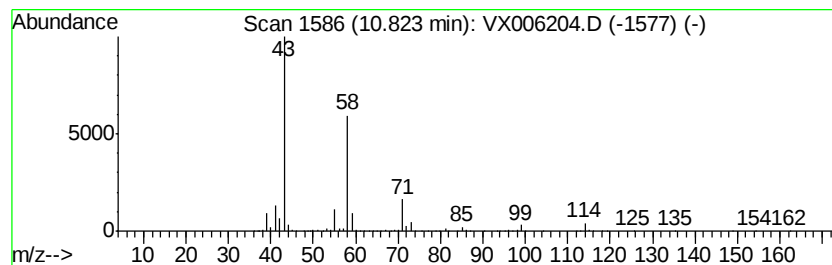
Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X112018W.M
Quant Title : SW846 8260

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

Peak Number 8 2-Heptanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.82	17.32 ug/l	418619	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	56
3	2-Hexanone, 4-methyl-	114 C7H14O	000105-42-0	56
4	Pentanal, 2-methyl-	100 C6H12O	000123-15-9	42
5	1-Butoxy-2-propanol acetate	174 C9H18O3	085409-76-3	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX112618\
Data File : VX006204.D
Acq On : 27 Nov 2018 04:57
Operator : JC/MD
Sample : J6044-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 43 Sample Multiplier: 1

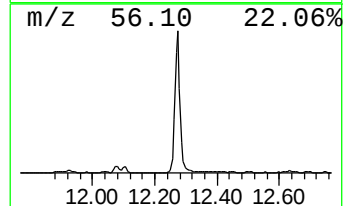
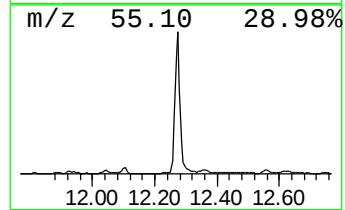
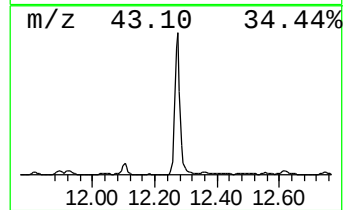
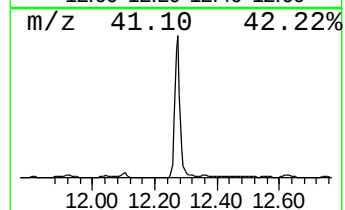
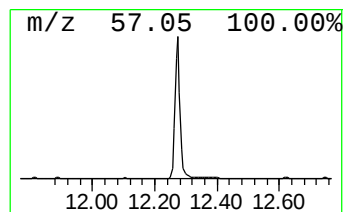
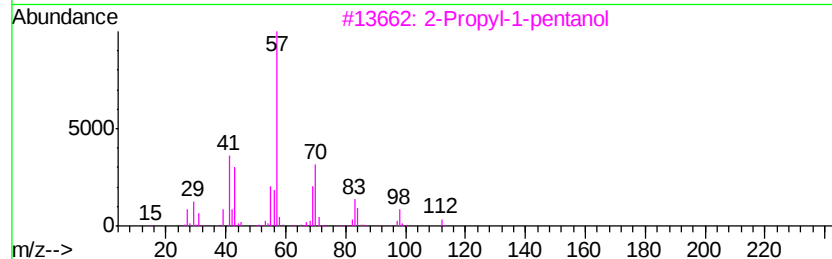
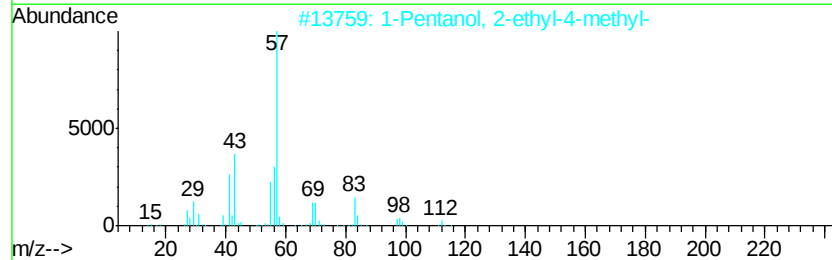
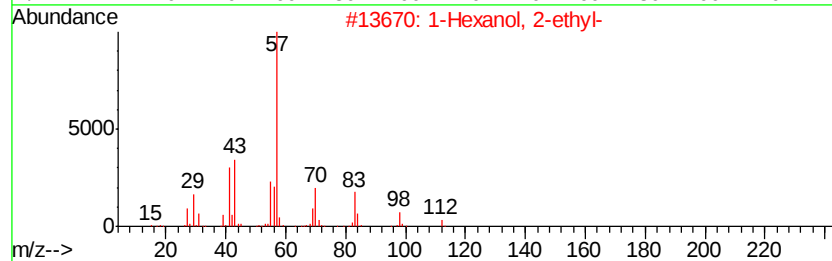
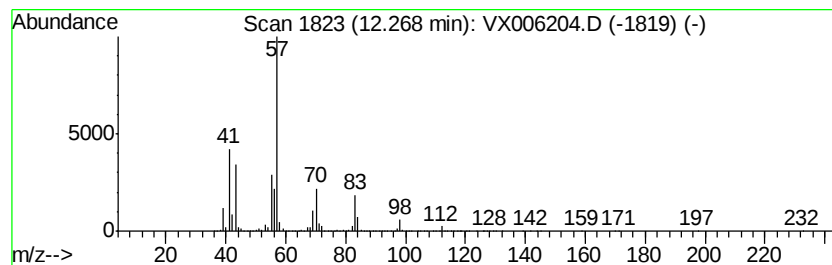
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X112018W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.27	120.78 ug/l	3445300	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	83
2	1-Pentanol, 2-ethyl-4-methyl-	130 C8H18O	000106-67-2	56
3	2-Propyl-1-pentanol	130 C8H18O	058175-57-8	50
4	2-Ethyl-1-hexanol, methyl ether	144 C9H20O	1000365-10-2	47
5	Carbonic acid, isobutyl 2-ethylh...	230 C13H26O3	1000357-82-9	45



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX112618\
Data File : VX006204.D
Acq On : 27 Nov 2018 04:57
Operator : JC/MD
Sample : J6044-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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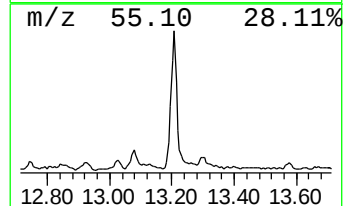
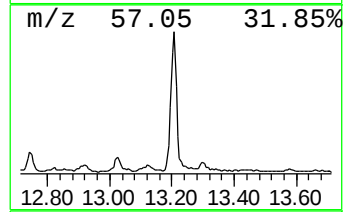
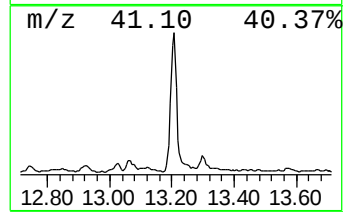
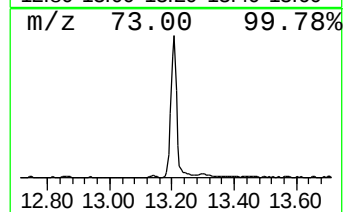
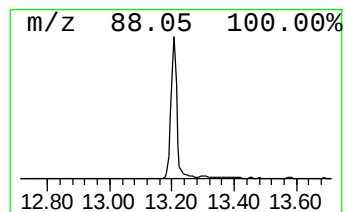
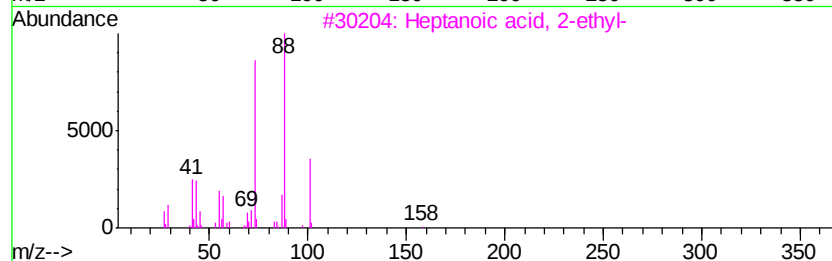
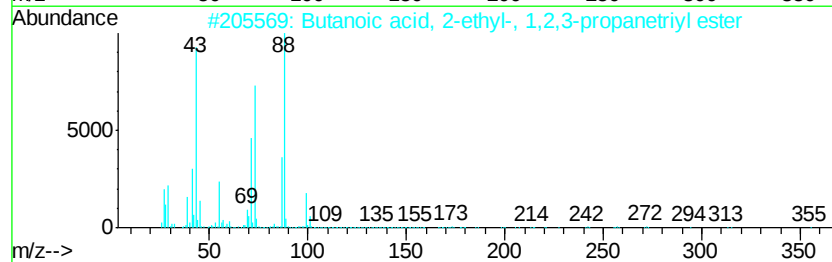
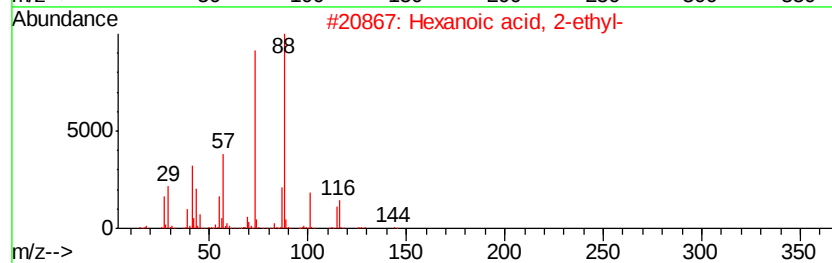
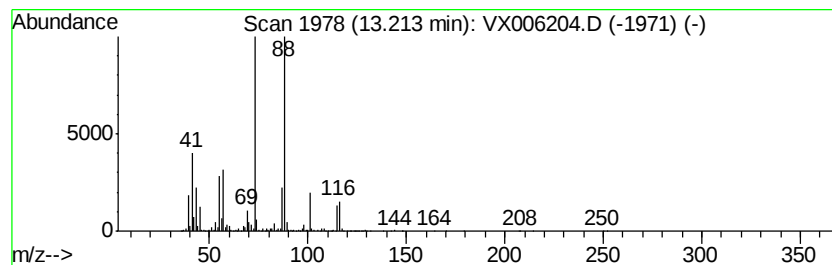
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Quant Title : SW846 8260

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

Peak Number 10 Hexanoic acid, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.21	23.44 ug/l	668515	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
2		Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	59
3		Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	42
4		Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	40
5		Methyl-4-deoxy-2,3-di-O-methyl.b...	218	C9H14O6	1000312-09-9	40



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112618\
Data File : VX006204.D
Acq On : 27 Nov 2018 04:57
Operator : JC/MD
Sample : J6044-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	1.49	60.0	ug/l	943931	1	5.67	787058	50.0
Ethanol	2.12	192.5	ug/l	3030800	1	5.67	787058	50.0
Propanal	2.35	24.3	ug/l	382919	1	5.67	787058	50.0
1-Propanol	4.00	16.7	ug/l	262639	1	5.67	787058	50.0
Butanal	4.35	84.8	ug/l	1335230	1	5.67	787058	50.0
1-Butanol	7.32	31.9	ug/l	623548	2	6.86	976406	50.0
Pentanal	7.66	14.7	ug/l	287832	2	6.86	976406	50.0
2-Heptanone	10.82	17.3	ug/l	418619	3	10.12	1208720	50.0
1-Hexanol, 2-ethyl-	12.27	120.8	ug/l	3445300	4	12.08	1426300	50.0
Hexanoic acid, 2-...	13.21	23.4	ug/l	668515	4	12.08	1426300	50.0