

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN112818\
 Data File : VN052526.D
 Acq On : 28 Nov 2018 18:08
 Operator : MD\SY
 Sample : J6044-03
 Misc : 5.00mL/MSVOA N/WATER
 ALS Vial : 22 Sample Multiplier: 28

Instrument :
 MSVOA_N
 ClientSampleId :
 30003

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_N\METHODS\82N112718W.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	2.163	110	121	136	rBV	201631	305776	1.17%	0.225%
2	2.317	151	169	198	rBV	8460810	13843941	52.97%	10.201%
3	3.269	445	465	512	rBV	6035668	14338252	54.86%	10.566%
4	3.609	556	571	583	rBV	121954	290157	1.11%	0.214%
5	3.700	583	599	619	rVV	1382870	3475142	13.30%	2.561%
6	3.815	619	635	673	rVB	1050261	2769331	10.60%	2.041%
7	4.555	840	865	898	rBV	815901	2502684	9.58%	1.844%
8	4.777	908	934	964	rBV2	310782	1112339	4.26%	0.820%
9	5.413	1106	1132	1167	rBV2	404951	1380367	5.28%	1.017%
10	5.741	1210	1234	1263	rBV4	176567	577569	2.21%	0.426%
11	6.027	1303	1323	1364	rBV	327355	1044289	4.00%	0.770%
12	6.249	1374	1392	1412	rVB2	93738	276673	1.06%	0.204%
13	6.545	1460	1484	1506	rBV	2258827	6756355	25.85%	4.979%
14	6.654	1510	1518	1541	rVB3	111594	323884	1.24%	0.239%
15	6.834	1554	1574	1596	rBV	673399	1950200	7.46%	1.437%
16	7.590	1787	1809	1820	rBV	824335	2065720	7.90%	1.522%
17	7.667	1821	1833	1860	rVB	1646094	3880704	14.85%	2.860%
18	8.027	1918	1945	1969	rBV2	945273	2431574	9.30%	1.792%
19	8.452	2063	2077	2088	rBV3	120366	281641	1.08%	0.208%
20	8.587	2105	2119	2136	rVB	2321719	4702626	17.99%	3.465%
21	8.783	2162	2180	2198	rBV	1092718	2353747	9.01%	1.734%
22	9.040	2250	2260	2278	rVB	151607	302237	1.16%	0.223%
23	9.166	2281	2299	2326	rVB	1355761	2782907	10.65%	2.051%
24	10.092	2569	2587	2599	rBV	3659767	6916256	26.46%	5.097%
25	10.156	2599	2607	2629	rVB	471794	873577	3.34%	0.644%
26	10.265	2629	2641	2652	rBV2	141070	266560	1.02%	0.196%
27	10.751	2778	2792	2805	rBV	146873	270394	1.03%	0.199%
28	10.854	2812	2824	2845	rBV	357327	623825	2.39%	0.460%
29	11.407	2965	2996	3017	rVB	3425823	6096501	23.33%	4.492%
30	11.548	3033	3040	3051	rVV	301291	535227	2.05%	0.394%
31	11.619	3051	3062	3084	rVB	451699	955319	3.66%	0.704%
32	11.776	3100	3111	3120	rBV	486745	792365	3.03%	0.584%
33	11.947	3151	3164	3175	rBV2	3065929	5242115	20.06%	3.863%
34	12.027	3183	3189	3209	rVB	716111	1195432	4.57%	0.881%

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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

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35	12.130	3211	3221	3246	rVB3	240820	455696	1.74%	0.336%
36	12.403	3293	3306	3327	rVB	2570829	4389562	16.80%	3.235%
37	12.686	3377	3394	3404	rBV	1438501	2470744	9.45%	1.821%
38	12.818	3426	3435	3439	rBV2	197788	299103	1.14%	0.220%
39	13.043	3499	3505	3516	rVV3	218085	536536	2.05%	0.395%
40	13.107	3517	3525	3544	rVB2	554597	976138	3.74%	0.719%
41	13.201	3545	3554	3565	rBV5	127747	268184	1.03%	0.198%
42	13.345	3585	3599	3618	rBV	2779733	4743048	18.15%	3.495%
43	13.452	3618	3632	3669	rBV	16065445	26134364	100.00%	19.258%
44	13.818	3737	3746	3762	rVB2	340340	584085	2.23%	0.430%
45	14.291	3886	3893	3917	rVB4	164916	362486	1.39%	0.267%
46	15.136	4145	4156	4177	rVB	312037	639619	2.45%	0.471%
47	16.162	4464	4475	4493	rVB	151898	330580	1.26%	0.244%

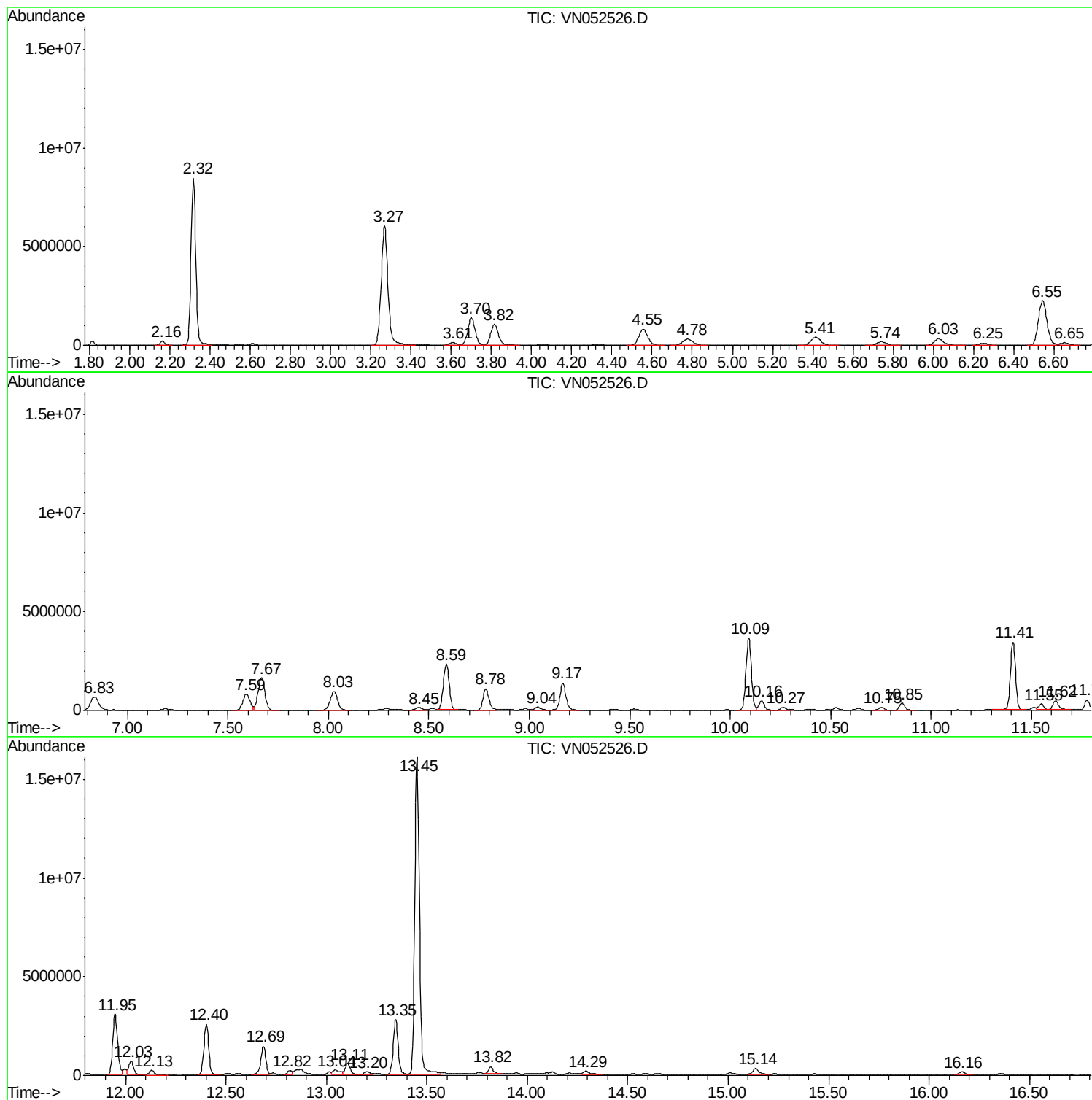
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N112718W.M
Quant Title : SW846 8260

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



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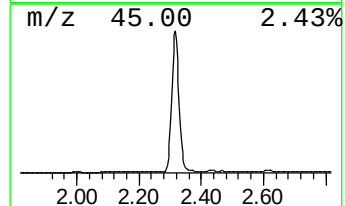
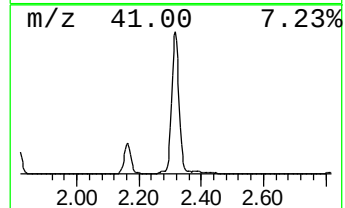
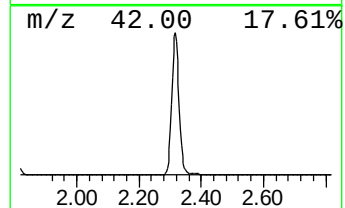
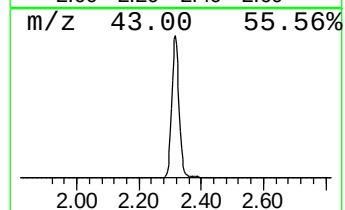
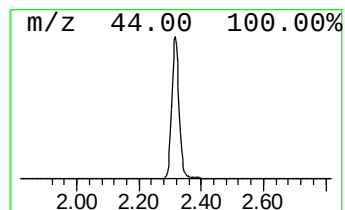
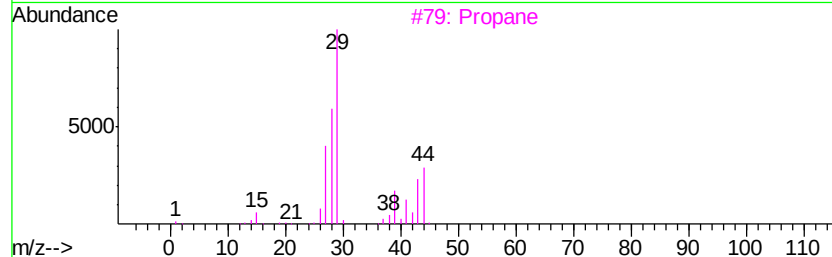
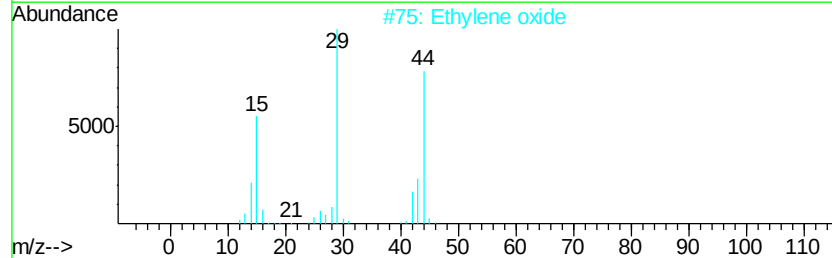
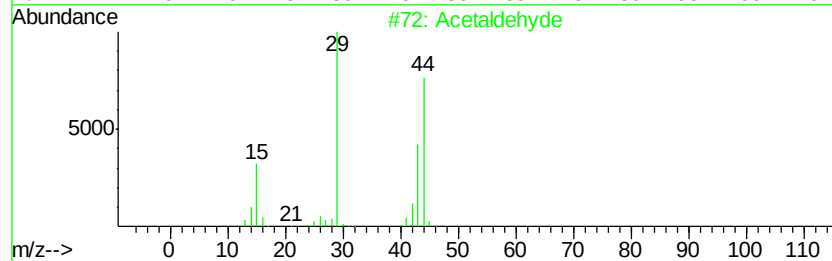
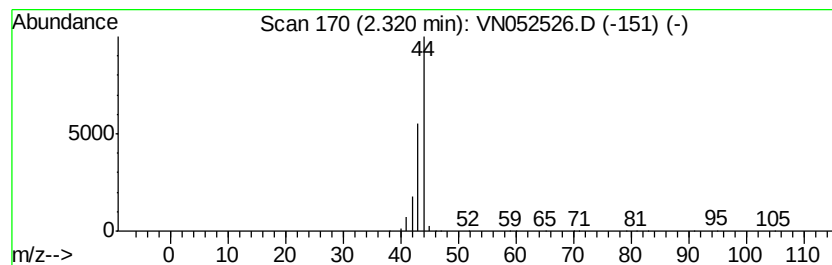
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N112718W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.32	178.37 ug/l	13843900	Pentafluorobenzene	7.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetaldehyde	44	C2H4O	000075-07-0	74
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		Carbon dioxide	44	CO2	000124-38-9	3



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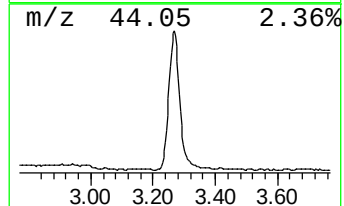
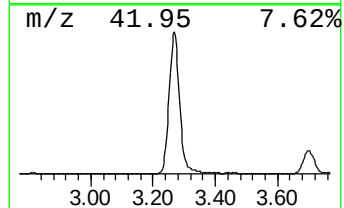
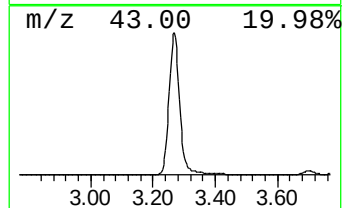
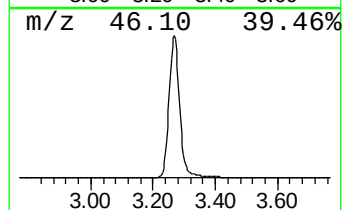
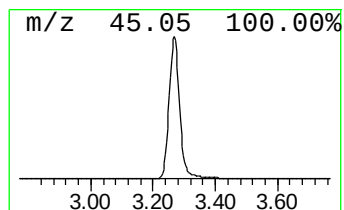
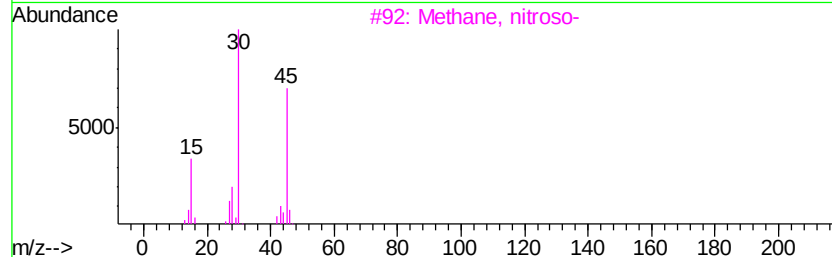
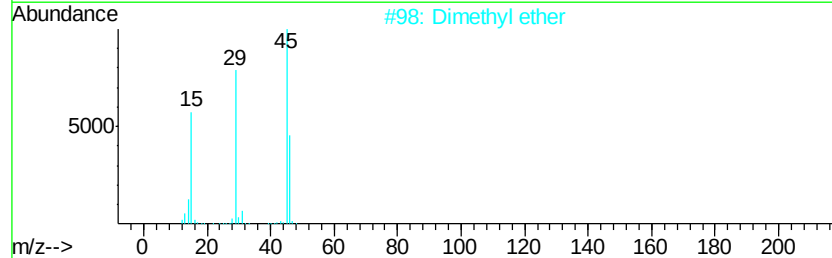
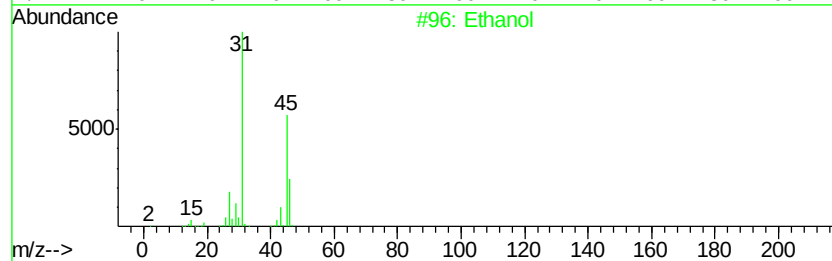
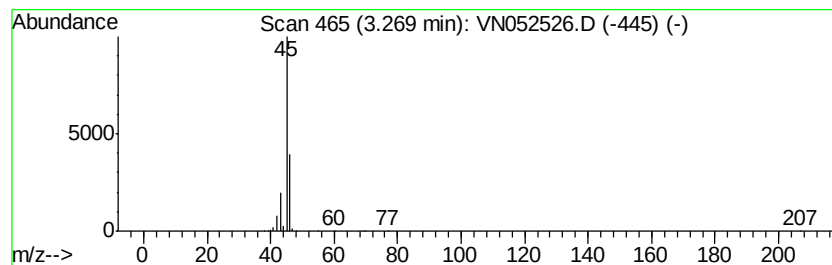
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N112718W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.27	184.74 ug/l	14338300	Pentafluorobenzene	7.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		L-Lactic acid	90	C3H6O3	000079-33-4	4



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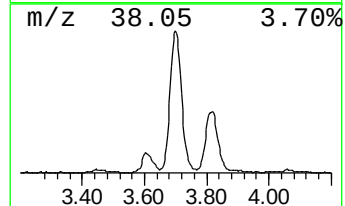
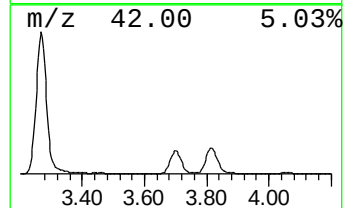
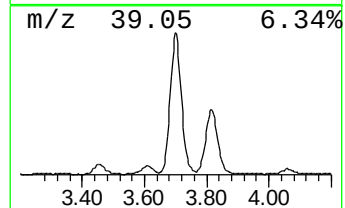
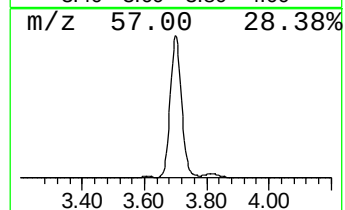
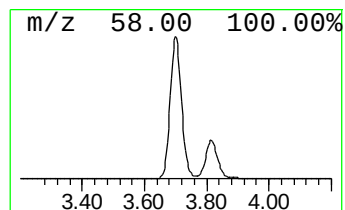
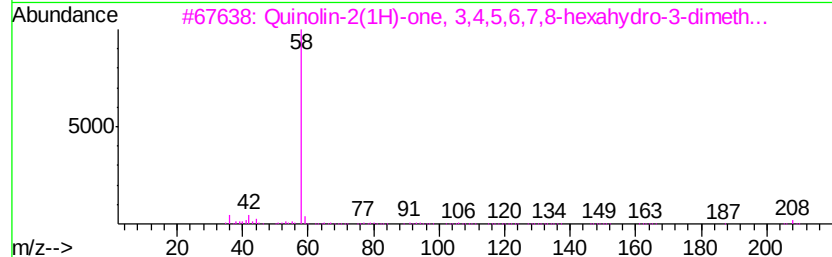
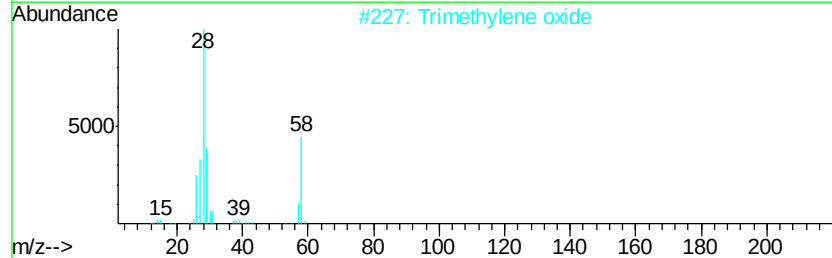
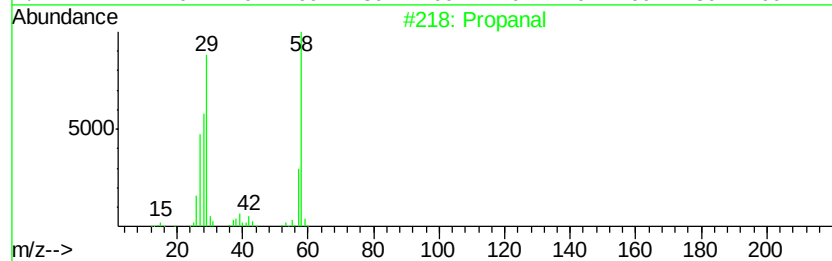
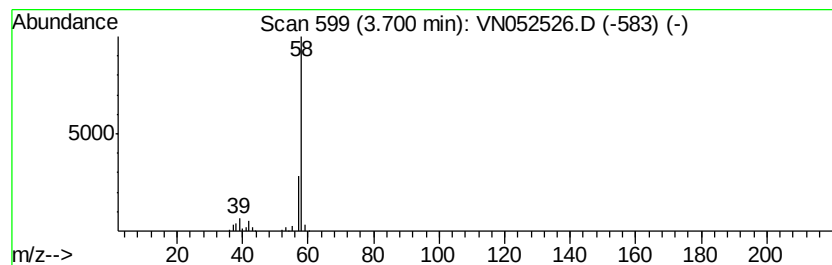
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N112718W.M
Quant Title : SW846 8260

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

Peak Number 3 Propanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.70	44.77 ug/l	3475140	Pentafluorobenzene	7.67

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	4



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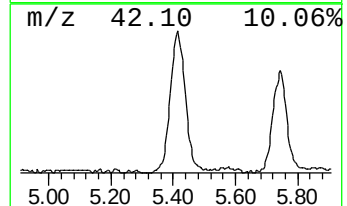
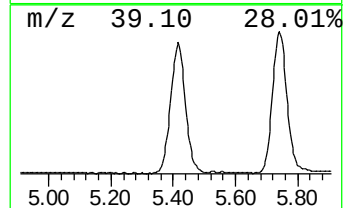
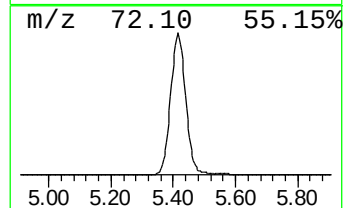
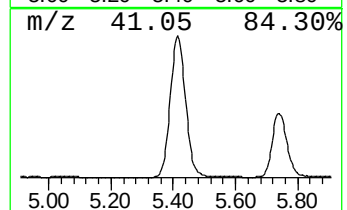
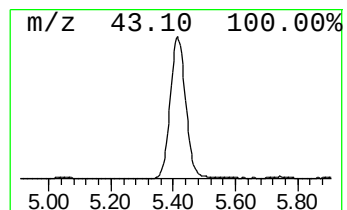
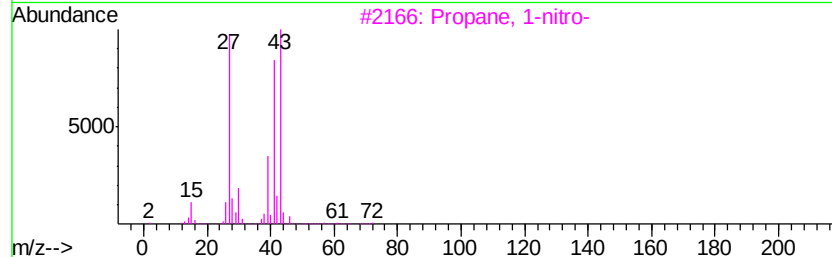
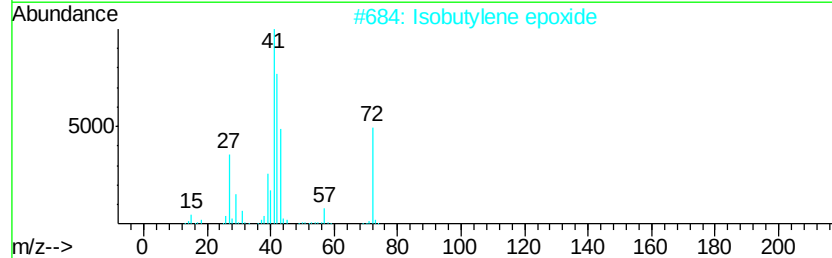
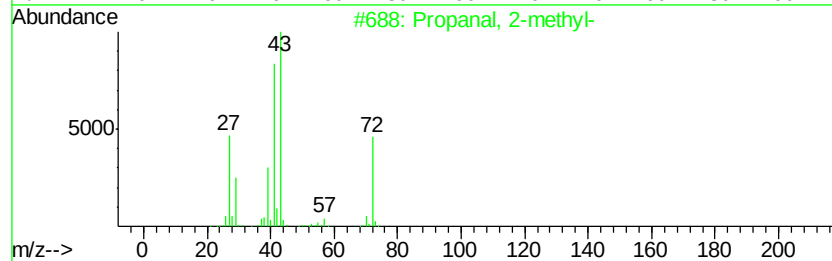
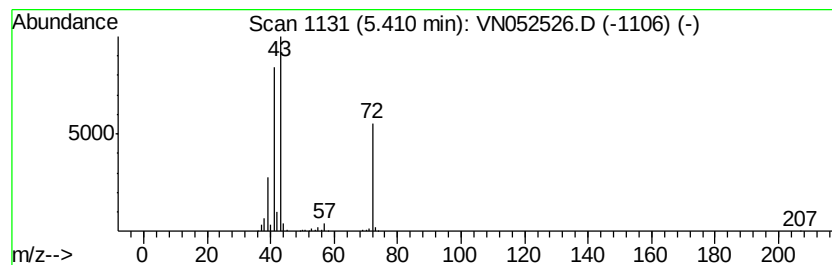
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Quant Title : SW846 8260

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

Peak Number 4 Propanal, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.41	17.79 ug/l	1380370	Pentafluorobenzene	7.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanal, 2-methyl-	72	C4H8O	000078-84-2	91
2		Isobutylene epoxide	72	C4H8O	000558-30-5	53
3		Propane, 1-nitro-	89	C3H7NO2	000108-03-2	37
4		Propane, 2-nitro-	89	C3H7NO2	000079-46-9	25
5		Isobutyl nitrite	103	C4H9NO2	000542-56-3	25



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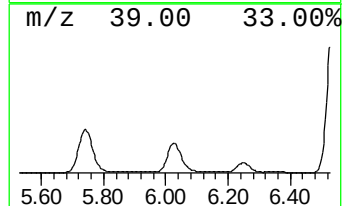
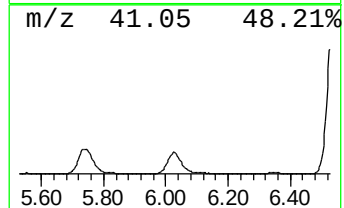
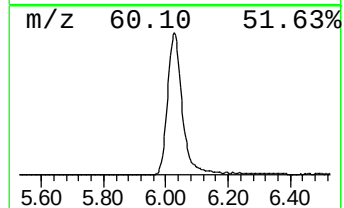
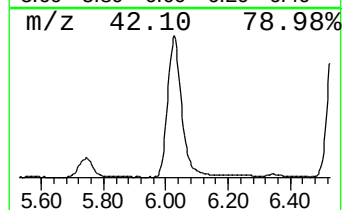
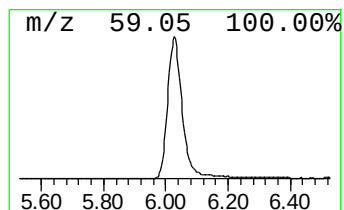
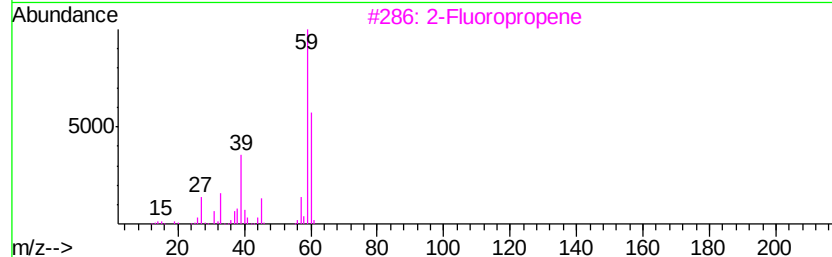
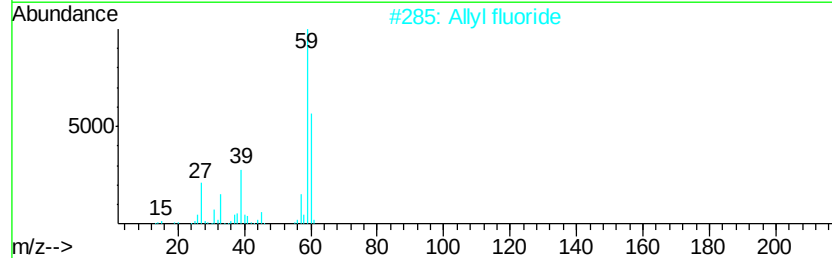
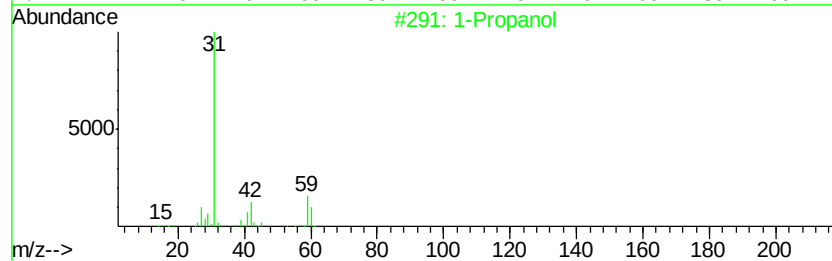
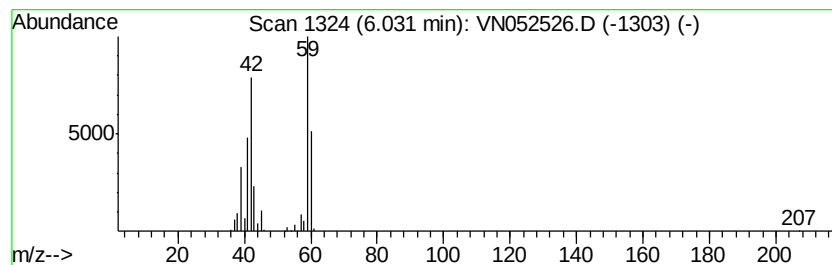
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N112718W.M
Quant Title : SW846 8260

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

Peak Number 5 1-Propanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.03	13.45 ug/l	1044290	Pentafluorobenzene	7.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Propanol	60	C3H8O	000071-23-8	78
2		Allyl fluoride	60	C3H5F	000818-92-8	47
3		2-Fluoropropene	60	C3H5F	001184-60-7	43
4		Methanamine, N-hydroxy-N-methyl-	61	C2H7NO	005725-96-2	23
5		Acetaldoxime	59	C2H5NO	000107-29-9	7



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN112818\
Data File : VN052526.D
Acq On : 28 Nov 2018 18:08
Operator : MD\SY
Sample : J6044-03
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 22 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampled :
30003

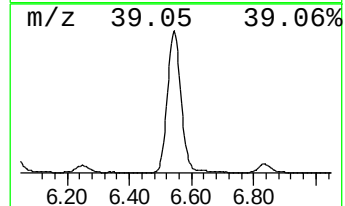
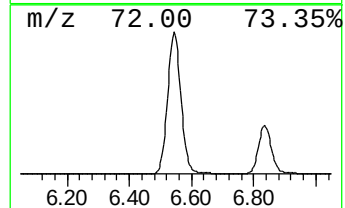
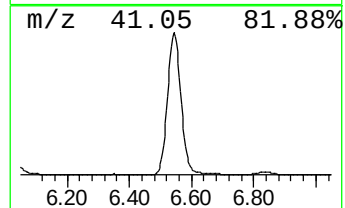
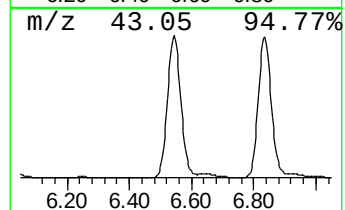
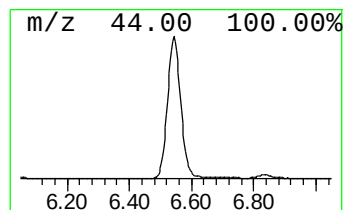
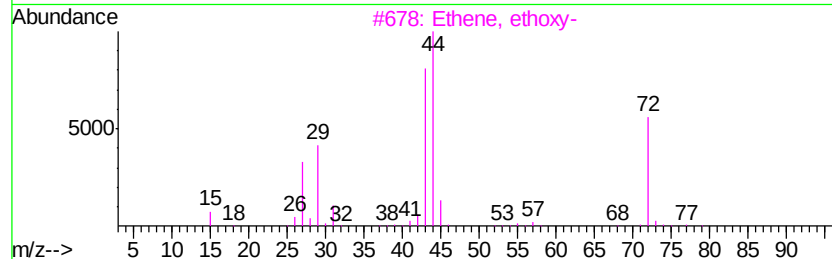
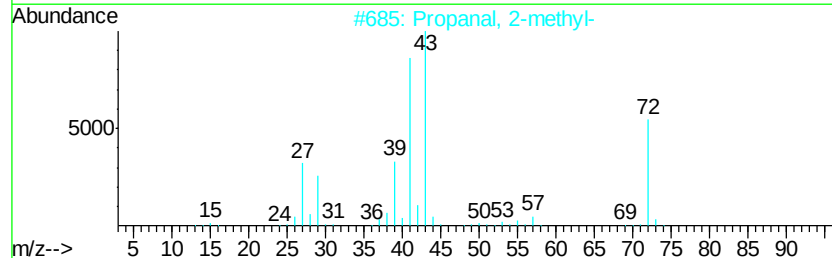
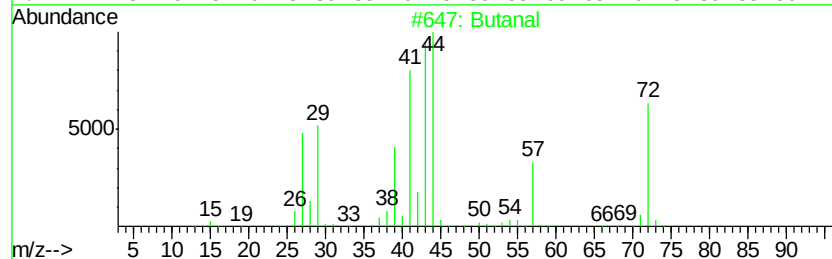
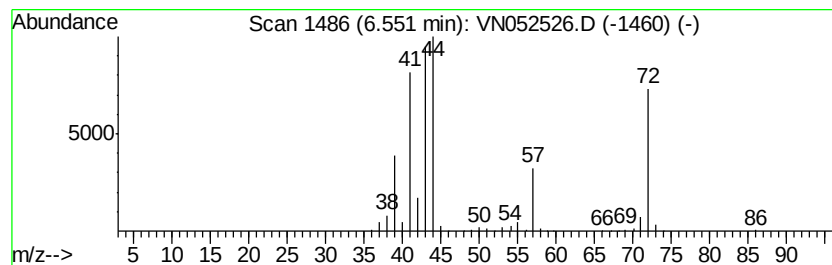
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Quant Title : SW846 8260

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

Peak Number 6 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	87.05 ug/l	6756360	Pentafluorobenzene	7.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanal	72	C4H8O	000123-72-8	94
2		Propanal, 2-methyl-	72	C4H8O	000078-84-2	52
3		Ethene, ethoxy-	72	C4H8O	000109-92-2	40
4		Butanal, 3-methyl-	86	C5H10O	000590-86-3	38
5		1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	32



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN112818\
Data File : VN052526.D
Acq On : 28 Nov 2018 18:08
Operator : MD\SY
Sample : J6044-03
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 22 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampled :
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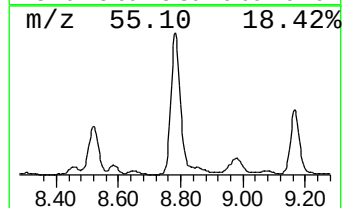
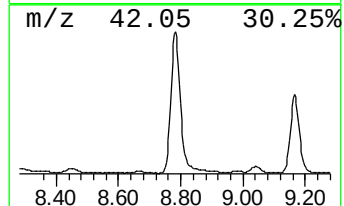
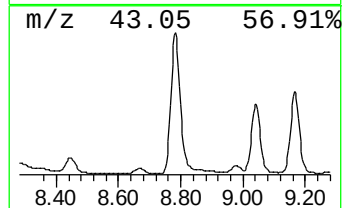
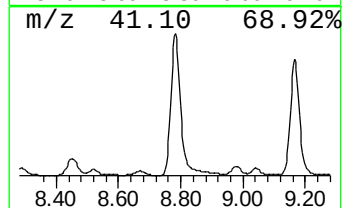
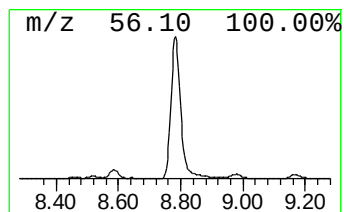
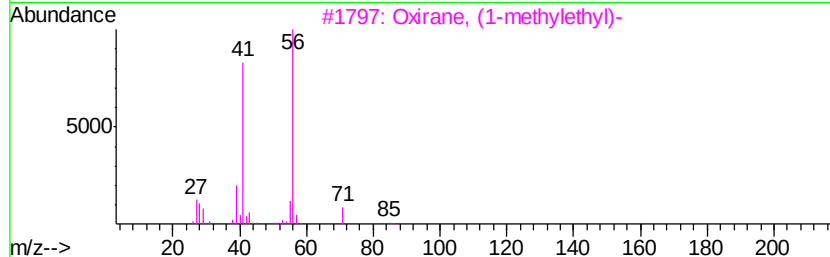
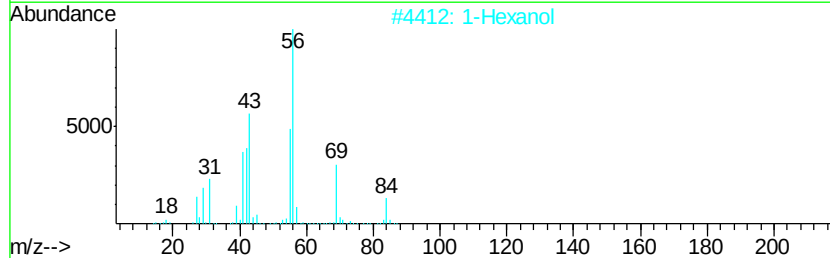
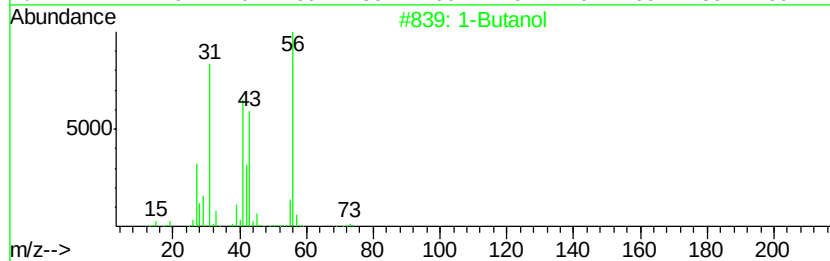
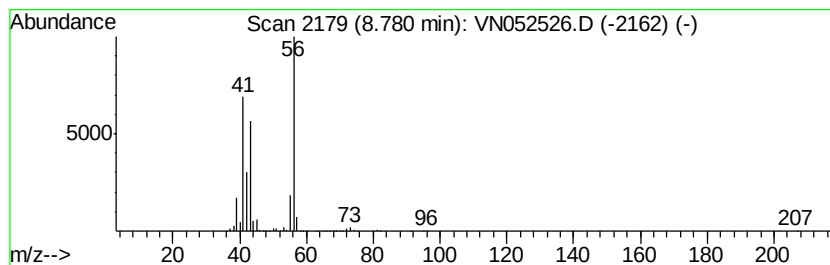
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Quant Title : SW846 8260

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

Peak Number 7 1-Butanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.78	25.03 ug/l	2353750	1,4-Difluorobenzene	8.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Butanol	74	C4H10O	000071-36-3	91
2		1-Hexanol	102	C6H14O	000111-27-3	43
3		Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	40
4		3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	33
5		.alpha.-Amino-.gamma.-butyrolactone	101	C4H7NO2	001192-20-7	9



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN112818\
Data File : VN052526.D
Acq On : 28 Nov 2018 18:08
Operator : MD\SY
Sample : J6044-03
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 22 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
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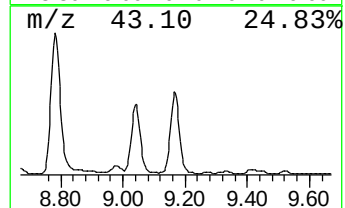
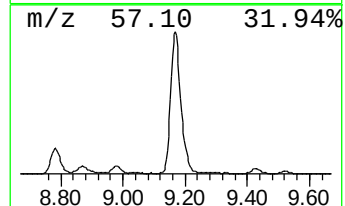
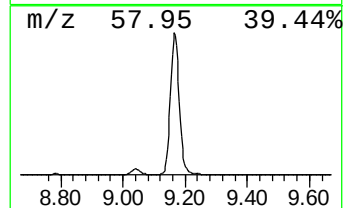
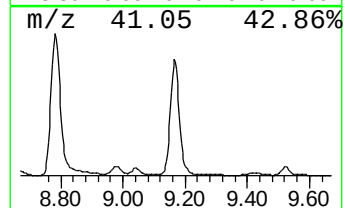
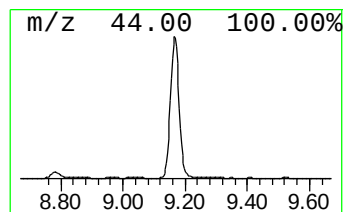
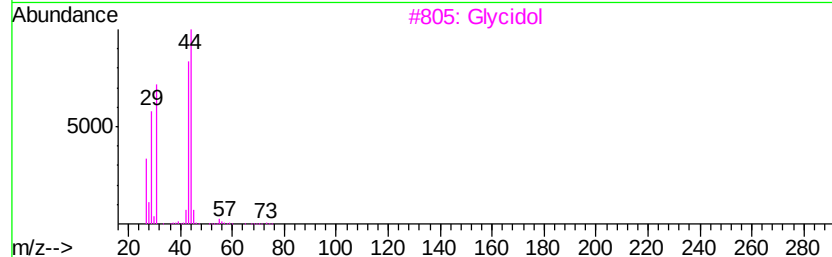
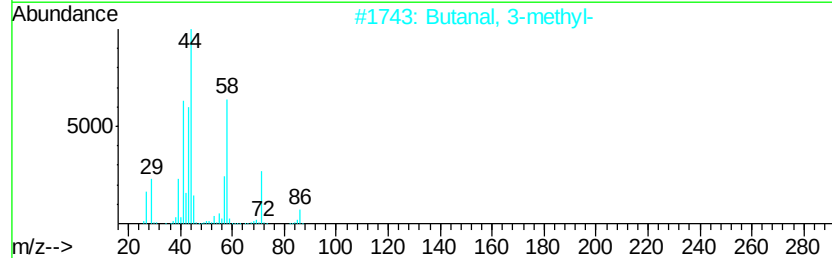
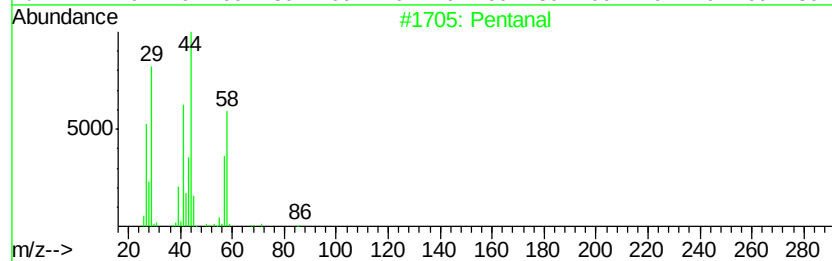
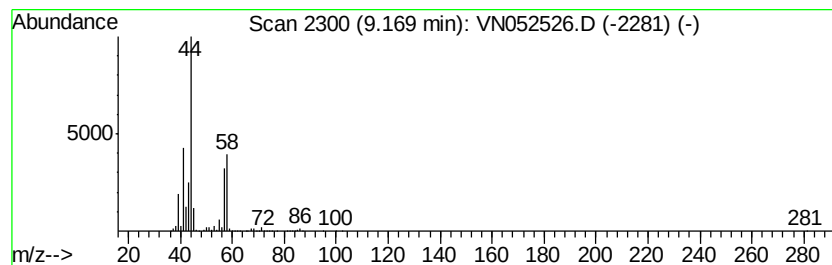
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Quant Title : SW846 8260

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

Peak Number 8 Pentanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.17	29.59 ug/l	2782910	1,4-Difluorobenzene	8.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentanal	86	C5H10O	000110-62-3	91
2		Butanal, 3-methyl-	86	C5H10O	000590-86-3	45
3		Glycidol	74	C3H6O2	000556-52-5	33
4		Cyclopropyl carbinol	72	C4H8O	002516-33-8	28
5		2-Propanamine	59	C3H9N	000075-31-0	9



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN112818\
Data File : VN052526.D
Acq On : 28 Nov 2018 18:08
Operator : MD\SY
Sample : J6044-03
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 22 Sample Multiplier: 28

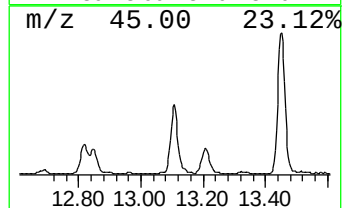
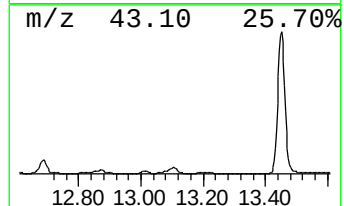
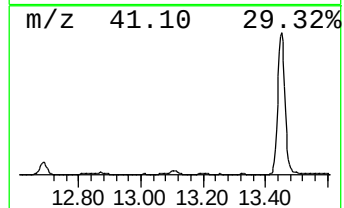
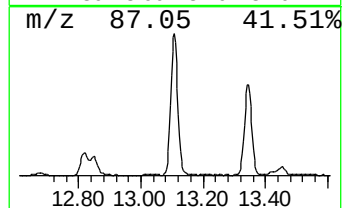
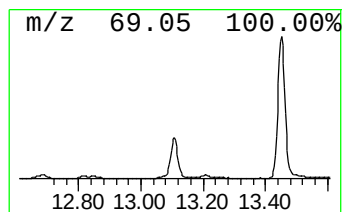
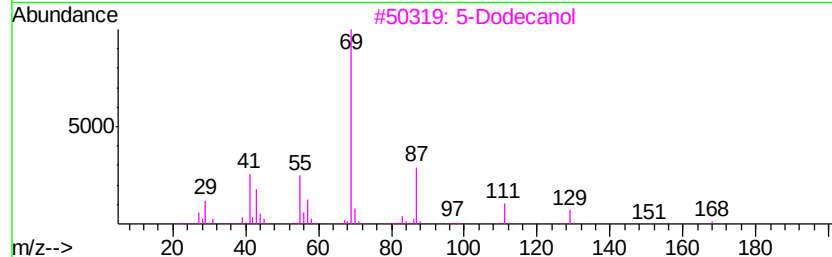
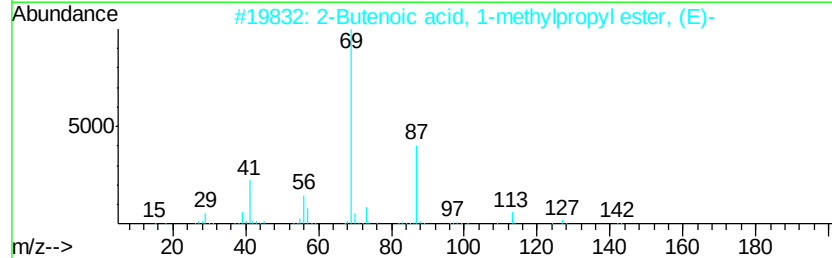
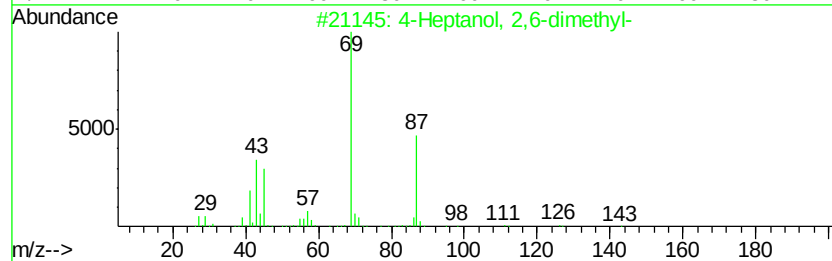
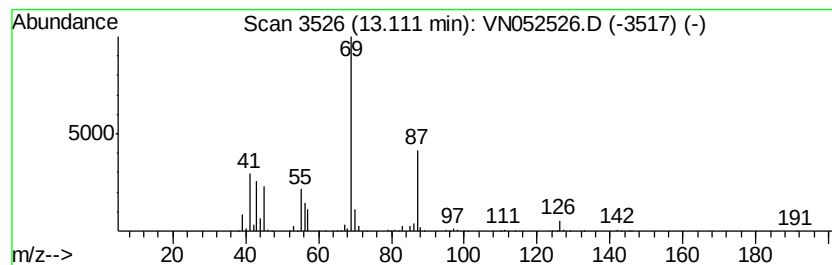
Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N112718W.M
Quant Title : SW846 8260

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

Peak Number 9 4-Heptanol, 2,6-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.11	10.29 ug/l	976138	1,4-Dichlorobenzene-d4	13.35	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	78
2	2-Butenoic acid, 1-methylpropyl ...	142	C8H14O2	010371-45-6	64
3	5-Dodecanol	186	C12H26O	010203-33-5	64
4	Pentanoic acid, 2-hydroxy-4-meth...	146	C7H14O3	040348-72-9	64
5	5-Nonanol	144	C9H20O	000623-93-8	64



Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN112818\
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Acq On : 28 Nov 2018 18:08
Operator : MD\SY
Sample : J6044-03
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ALS Vial : 22 Sample Multiplier: 28

Instrument :
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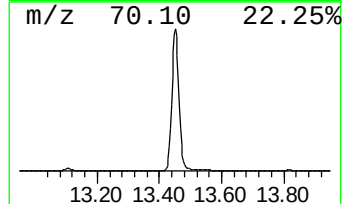
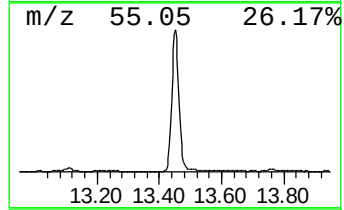
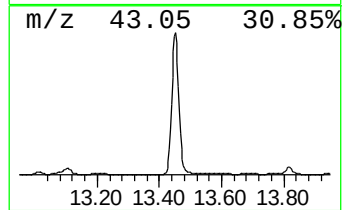
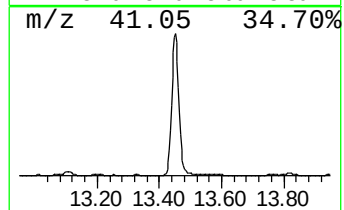
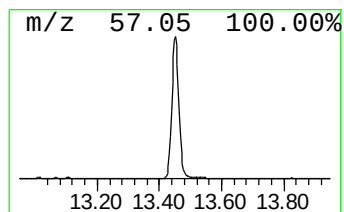
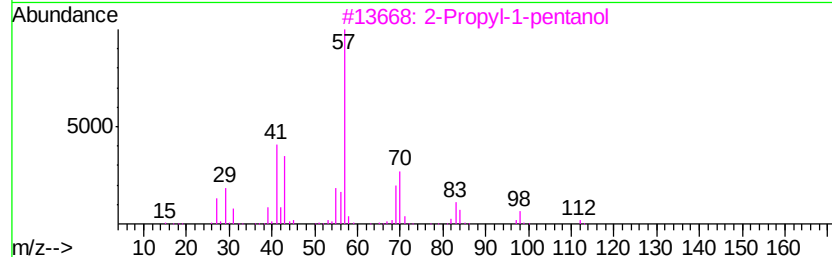
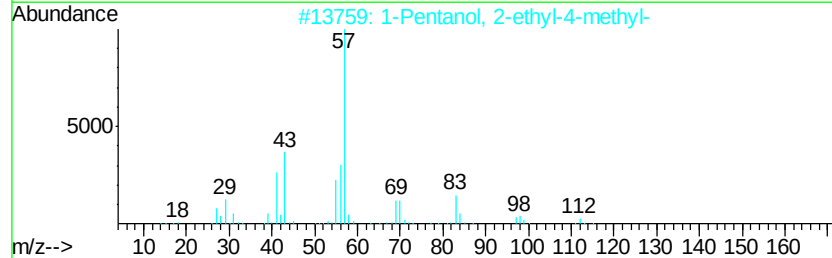
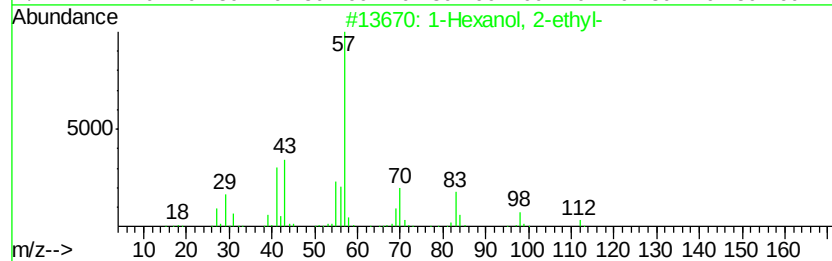
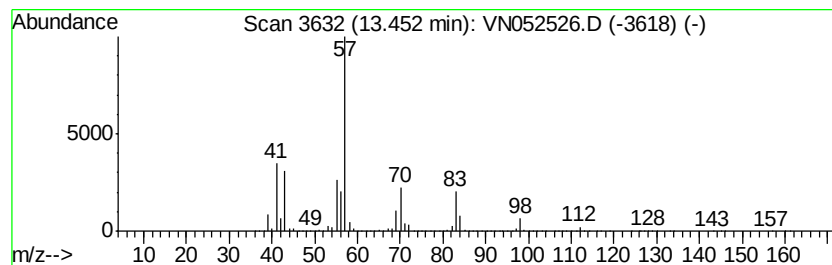
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Quant Title : SW846 8260

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

Peak Number 10 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	275.50 ug/l	26134400	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	42



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN112818\
Data File : VN052526.D
Acq On : 28 Nov 2018 18:08
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Sample : J6044-03
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112718W.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	2.32	178.4	ug/l	13843900	1	7.67	3880700	50.0
Ethanol	3.27	184.7	ug/l	14338300	1	7.67	3880700	50.0
Propanal	3.70	44.8	ug/l	3475140	1	7.67	3880700	50.0
Propanal, 2-methyl-	5.41	17.8	ug/l	1380370	1	7.67	3880700	50.0
1-Propanol	6.03	13.4	ug/l	1044290	1	7.67	3880700	50.0
Butanal	6.55	87.0	ug/l	6756360	1	7.67	3880700	50.0
1-Butanol	8.78	25.0	ug/l	2353750	2	8.59	4702630	50.0
Pentanal	9.17	29.6	ug/l	2782910	2	8.59	4702630	50.0
4-Heptanol, 2,6-d...	13.11	10.3	ug/l	976138	4	13.35	4743050	50.0
1-Hexanol, 2-ethyl-	13.45	275.5	ug/l	26134400	4	13.35	4743050	50.0