

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN112818\
 Data File : VN052530.D
 Acq On : 28 Nov 2018 19:55
 Operator : MD\SY
 Sample : J6044-04
 Misc : 5.00mL/MSVOA N/WATER
 ALS Vial : 26 Sample Multiplier: 28

Instrument :
 MSVOA_N
 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_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	1.815	4	13	28	rVB3	100651	146264	2.24%	0.243%
2	2.163	111	121	140	rVB	154094	230899	3.53%	0.384%
3	2.317	153	169	186	rBV	899856	1463579	22.37%	2.436%
4	3.265	446	464	508	rBV	838972	2081878	31.82%	3.465%
5	3.699	583	599	617	rBV	214016	537523	8.22%	0.895%
6	3.815	619	635	678	rVB	453031	1214770	18.57%	2.022%
7	4.056	694	710	732	rBV2	47130	139690	2.14%	0.232%
8	4.326	774	794	818	rBV	99635	290154	4.43%	0.483%
9	4.555	839	865	900	rBV	1126286	3469048	53.02%	5.773%
10	4.777	913	934	965	rVB	109275	386043	5.90%	0.642%
11	5.416	1107	1133	1157	rBV2	67237	231796	3.54%	0.386%
12	6.031	1305	1324	1351	rBV3	58523	193741	2.96%	0.322%
13	6.545	1460	1484	1503	rBV	806620	2461574	37.62%	4.097%
14	6.654	1504	1518	1545	rVB	256228	786752	12.02%	1.309%
15	6.838	1555	1575	1594	rBV	193510	566197	8.65%	0.942%
16	7.191	1669	1685	1717	rBV4	29628	97034	1.48%	0.161%
17	7.590	1788	1809	1820	rBV	819611	2045577	31.26%	3.404%
18	7.667	1821	1833	1855	rVB	1591573	3785223	57.85%	6.300%
19	8.027	1925	1945	1971	rBV	867085	2110291	32.25%	3.512%
20	8.587	2103	2119	2159	rVB	2282431	4766623	72.85%	7.933%
21	8.786	2166	2181	2195	rBV	185628	421142	6.44%	0.701%
22	9.043	2250	2261	2272	rBV2	48842	96355	1.47%	0.160%
23	9.165	2277	2299	2326	rVB3	305244	791449	12.10%	1.317%
24	10.091	2570	2587	2600	rBV	3556084	6542830	100.00%	10.889%
25	10.156	2600	2607	2630	rVB	153296	295841	4.52%	0.492%
26	10.854	2814	2824	2847	rVB2	118092	222601	3.40%	0.370%
27	11.407	2979	2996	3018	rBV	2983767	5331220	81.48%	8.872%
28	11.545	3018	3039	3051	rVV3	458230	904582	13.83%	1.505%
29	11.619	3051	3062	3087	rVB	327757	675728	10.33%	1.125%
30	11.776	3087	3111	3137	rBV	335599	605609	9.26%	1.008%
31	11.950	3152	3165	3177	rBV3	697484	1364696	20.86%	2.271%
32	12.027	3182	3189	3207	rVB	296498	507663	7.76%	0.845%
33	12.130	3212	3221	3232	rBV3	50016	82598	1.26%	0.137%
34	12.403	3273	3306	3328	rBV	2434035	4473180	68.37%	7.444%

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Integration Parameters: RTEINT.P

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35	12.657	3375	3385	3389	rBV	101495	158375	2.42%	0.264%
36	12.731	3401	3408	3426	rVB2	119240	199502	3.05%	0.332%
37	12.818	3426	3435	3439	rBV3	46262	67825	1.04%	0.113%
38	12.876	3441	3453	3457	rVV5	97689	235921	3.61%	0.393%
39	12.915	3458	3465	3481	rVB	223450	382893	5.85%	0.637%
40	13.040	3488	3504	3514	rBV	210921	436570	6.67%	0.727%
41	13.107	3516	3525	3545	rVB3	164313	321521	4.91%	0.535%
42	13.262	3562	3573	3585	rVB2	328086	565640	8.65%	0.941%
43	13.345	3585	3599	3618	rVB	2666452	4586548	70.10%	7.633%
44	13.451	3619	3632	3650	rBV	1798769	3003106	45.90%	4.998%
45	13.583	3669	3673	3689	rVB5	34596	65954	1.01%	0.110%
46	13.821	3738	3747	3762	rVB5	88084	159961	2.44%	0.266%
47	14.088	3823	3830	3838	rVB2	79093	109533	1.67%	0.182%
48	14.291	3886	3893	3906	rVB5	52401	91755	1.40%	0.153%
49	14.583	3977	3984	3997	rVB4	34662	67036	1.02%	0.112%
50	15.133	4143	4155	4166	rBV	75055	148810	2.27%	0.248%
51	16.162	4467	4475	4494	rVB2	40770	93416	1.43%	0.155%
52	16.355	4525	4535	4548	rBV2	34936	72572	1.11%	0.121%

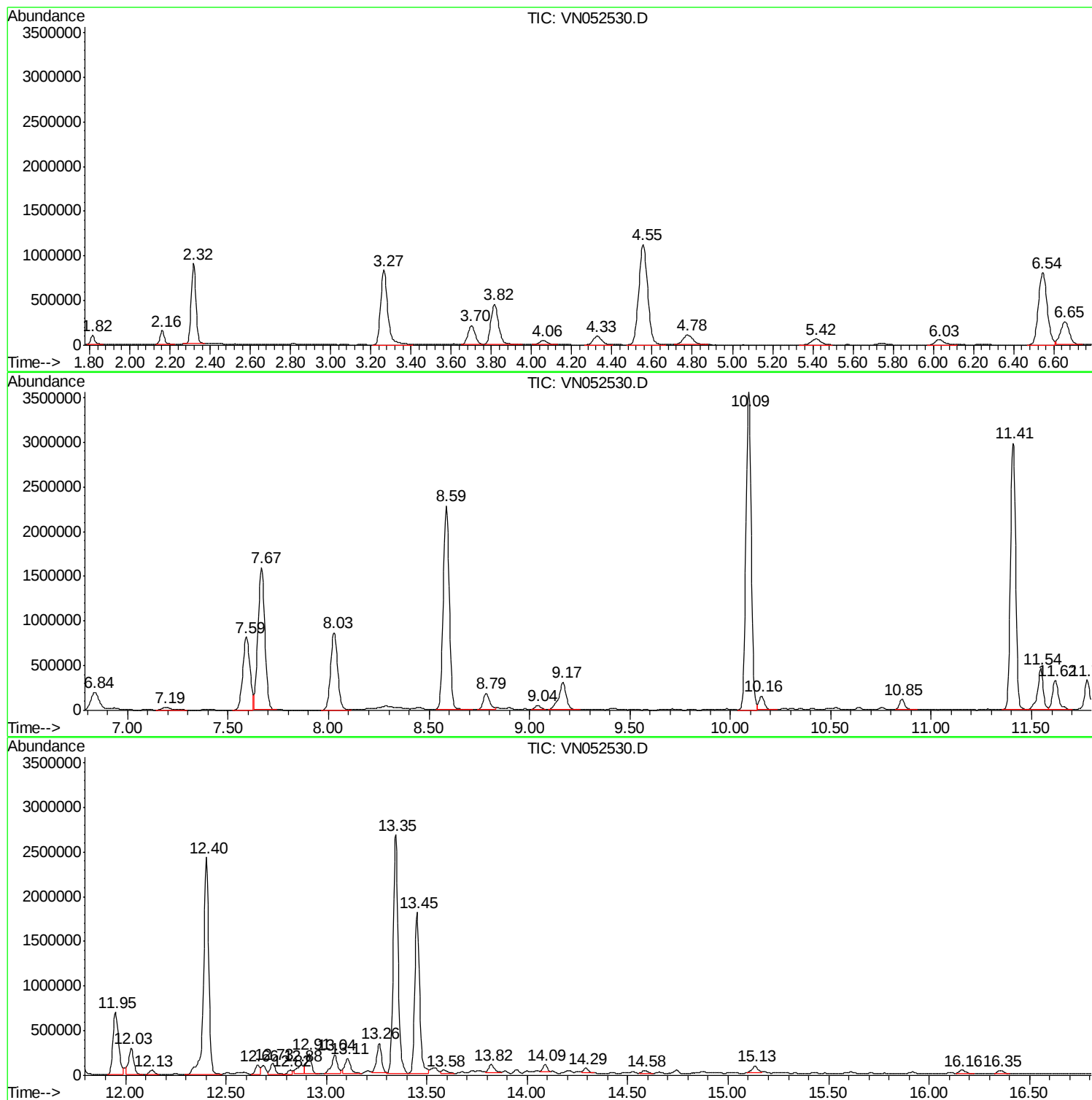
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N112718W.M
Quant Title : SW846 8260

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



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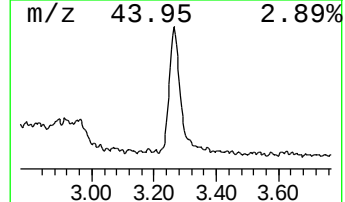
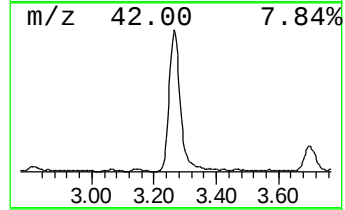
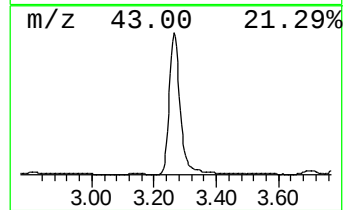
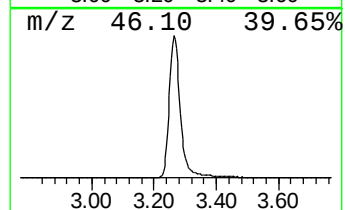
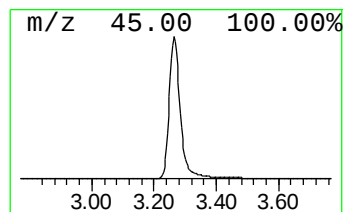
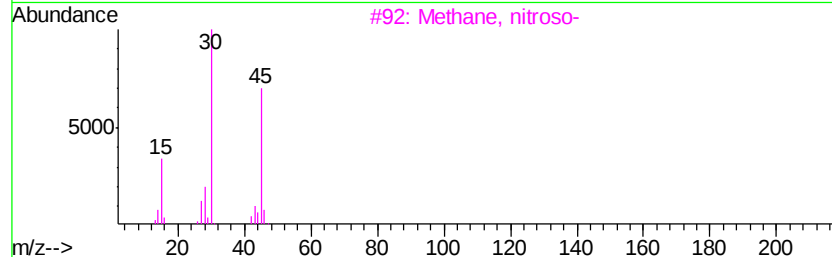
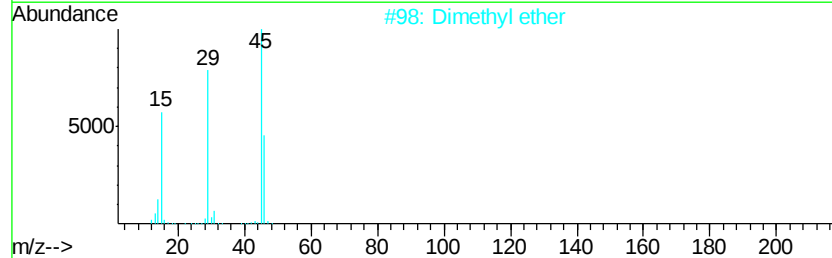
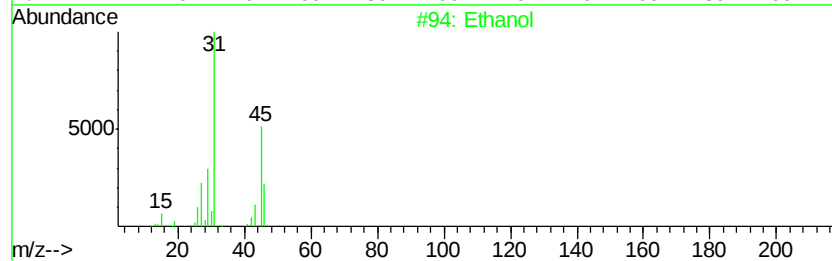
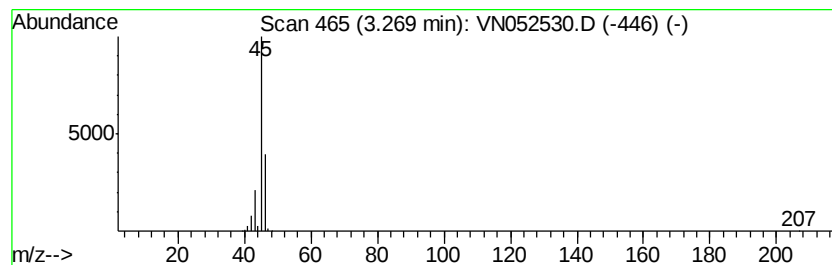
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N112718W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.27	27.50 ug/l	2081880	Pentafluorobenzene	7.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol	46	C2H6O	000064-17-5	74
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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ALS Vial : 26 Sample Multiplier: 28

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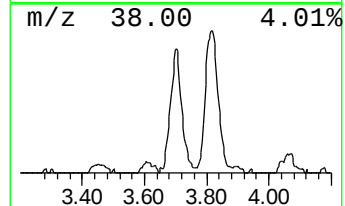
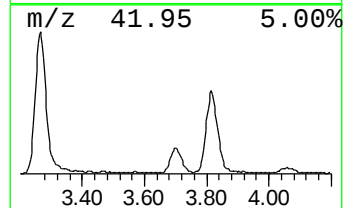
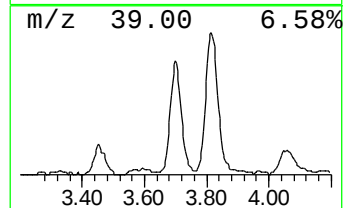
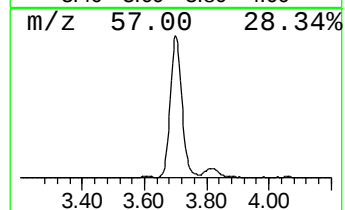
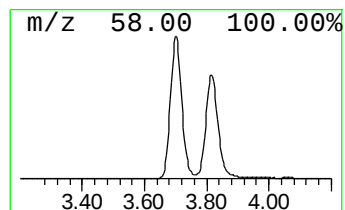
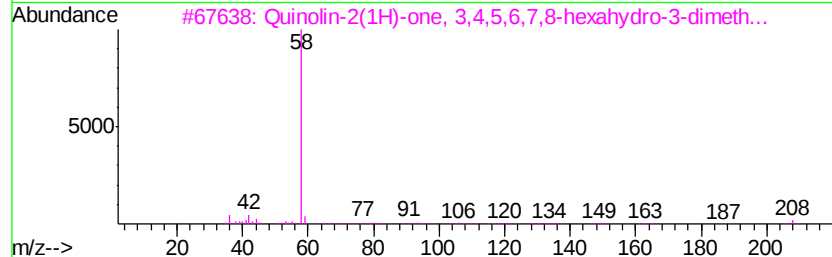
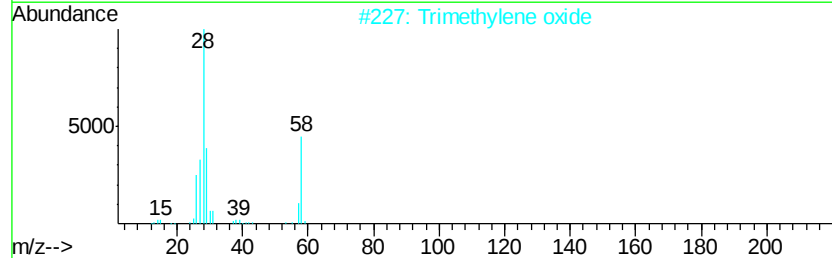
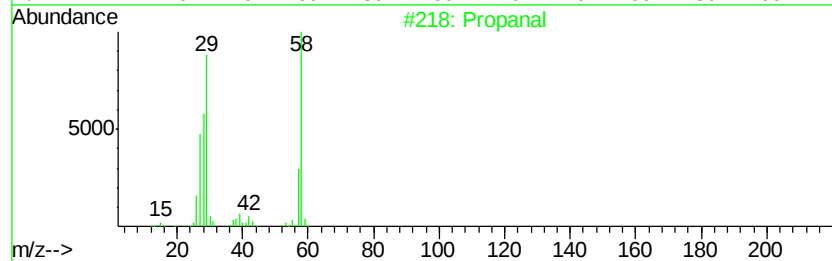
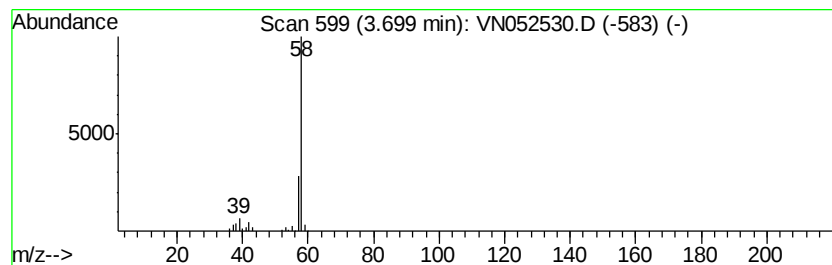
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N112718W.M
Quant Title : SW846 8260

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

Peak Number 3 Propanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.70	7.10 ug/l	537523	Pentafluorobenzene	7.67

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		Propylene oxide	58	C3H6O	000075-56-9	7
5		Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	4



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Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 26 Sample Multiplier: 28

Instrument :
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ClientSampleId :
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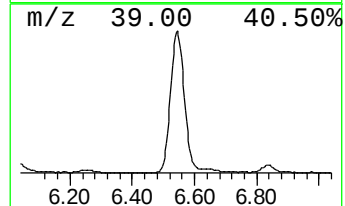
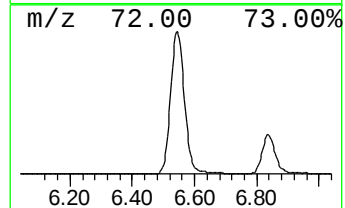
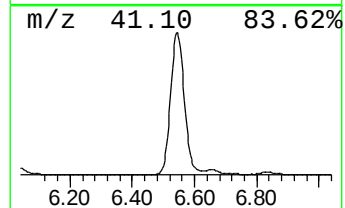
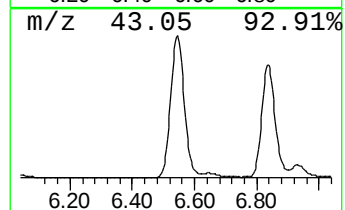
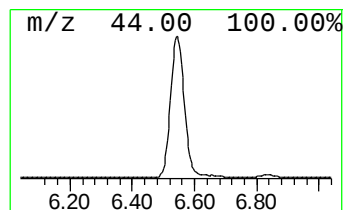
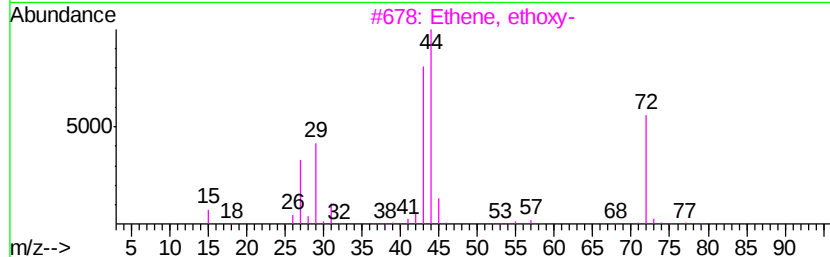
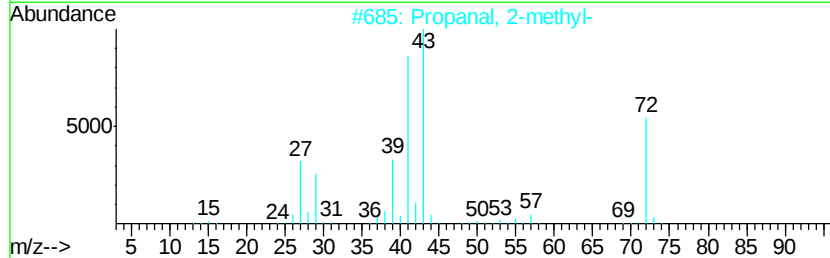
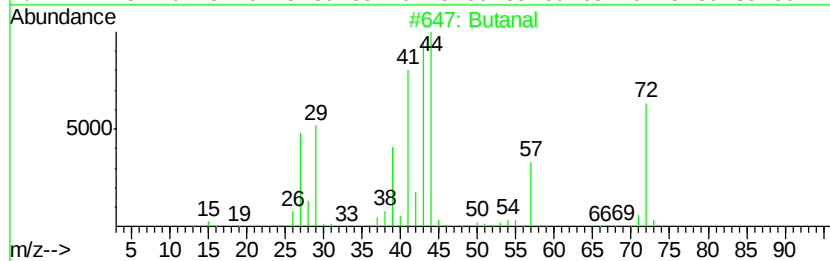
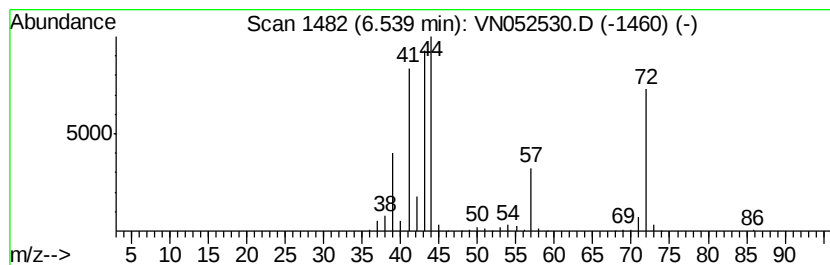
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Quant Title : SW846 8260

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

Peak Number 4 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	32.52 ug/l	2461570	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	58
3		Ethene, ethoxy-	72	C4H8O	000109-92-2	58
4		1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	38
5		Isobutylene epoxide	72	C4H8O	000558-30-5	35



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ALS Vial : 26 Sample Multiplier: 28

Instrument :
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ClientSampled :
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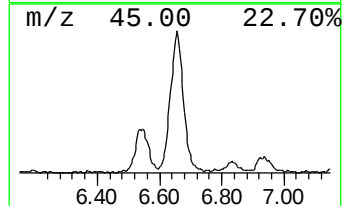
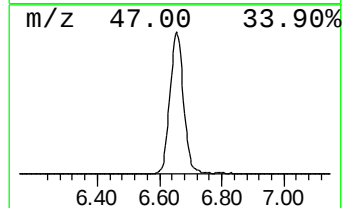
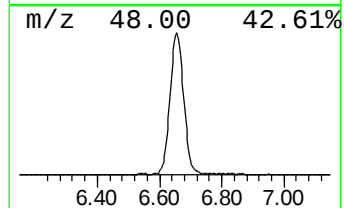
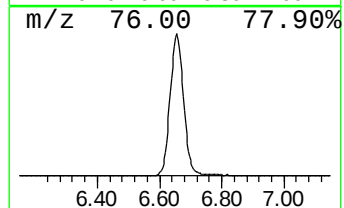
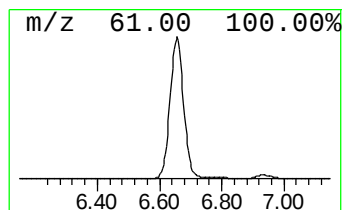
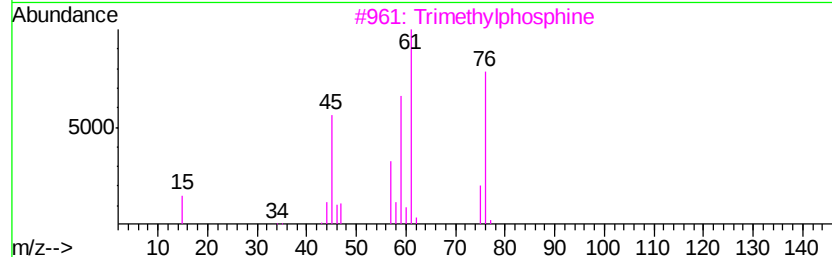
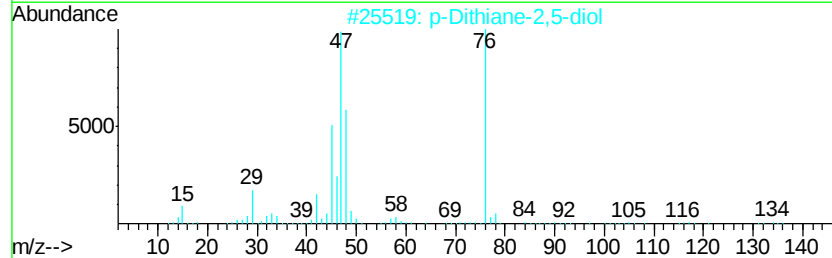
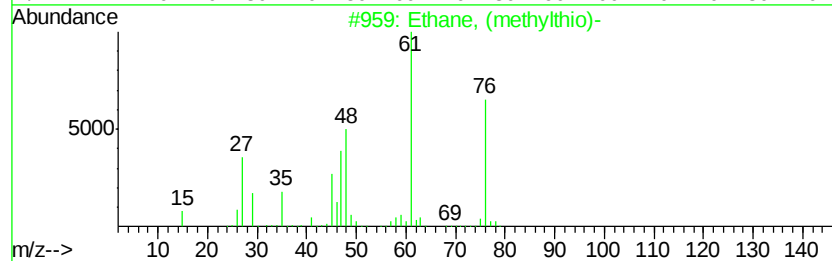
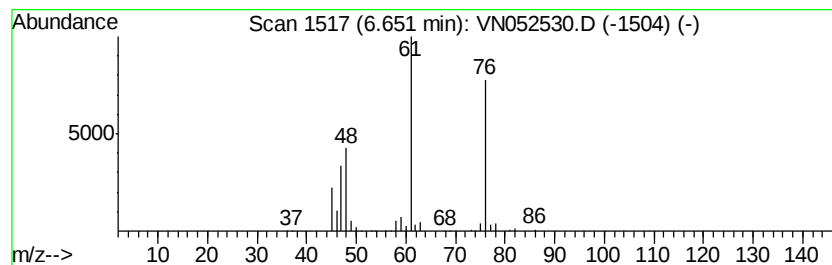
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Quant Title : SW846 8260

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

Peak Number 5 Ethane, (methylthio)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	10.39 ug/l	786752	Pentafluorobenzene	7.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethane, (methylthio)-	76	C3H8S	000624-89-5	95
2		p-Dithiane-2,5-diol	152	C4H8O2S2	040018-26-6	64
3		Trimethylphosphine	76	C3H9P	000594-09-2	50
4		Monomethyl carbonotrithioate	124	C2H4S3	001113-26-4	45
5		Propyl mercaptan	76	C3H8S	000107-03-9	42



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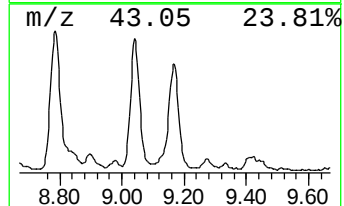
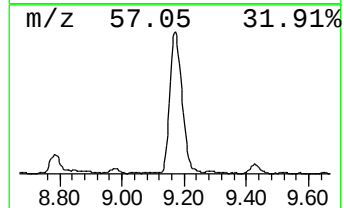
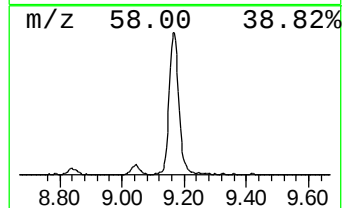
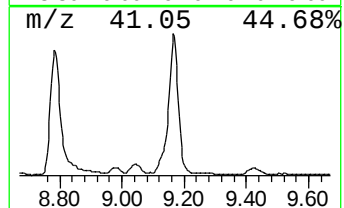
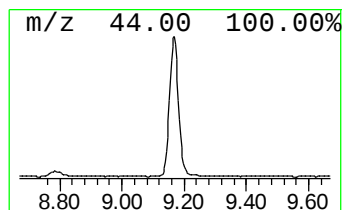
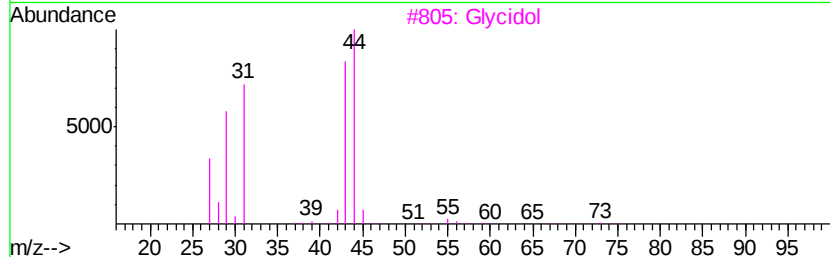
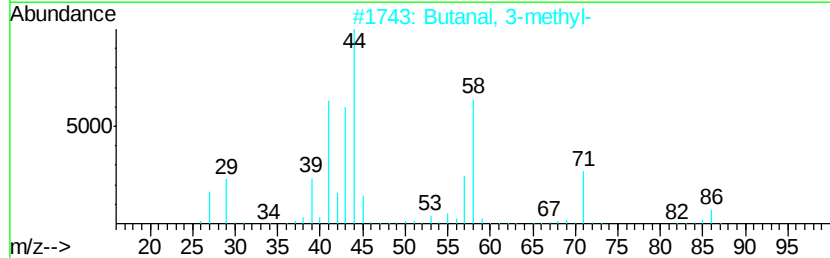
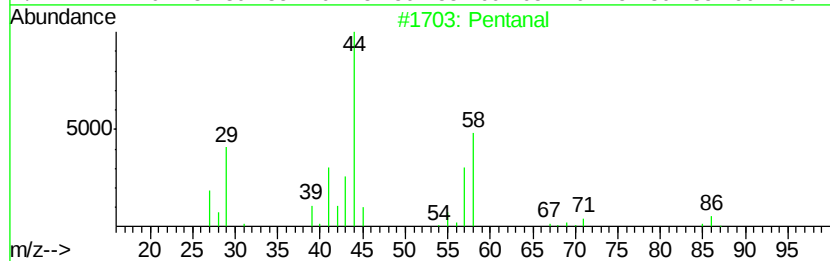
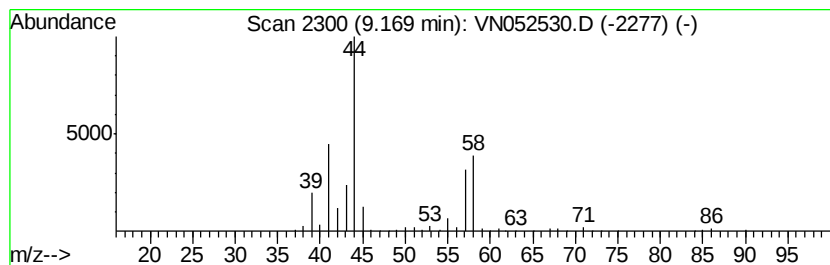
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Quant Title : SW846 8260

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

Peak Number 6 Pentanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.17	8.30 ug/l	791449	1,4-Difluorobenzene	8.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentanal	86	C5H10O	000110-62-3	64
2		Butanal, 3-methyl-	86	C5H10O	000590-86-3	42
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 : VN052530.D
Acq On : 28 Nov 2018 19:55
Operator : MD\SY
Sample : J6044-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 26 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
30002

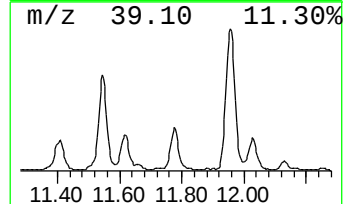
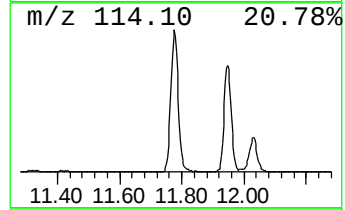
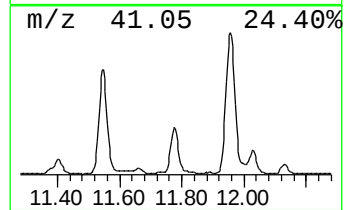
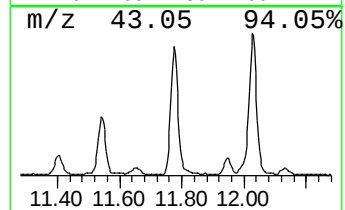
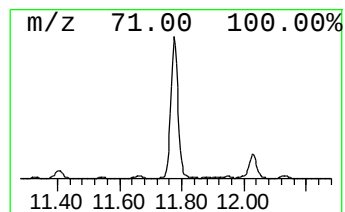
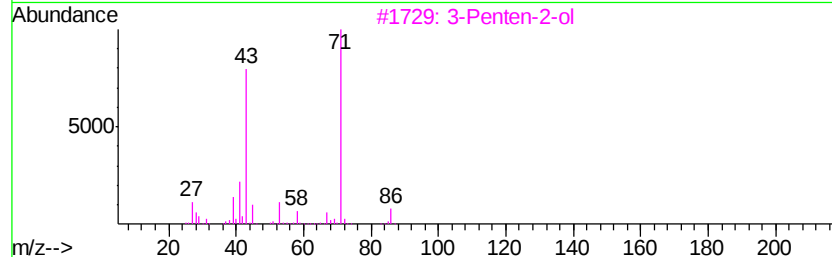
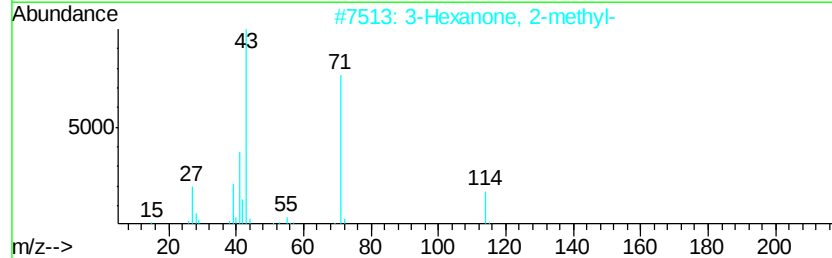
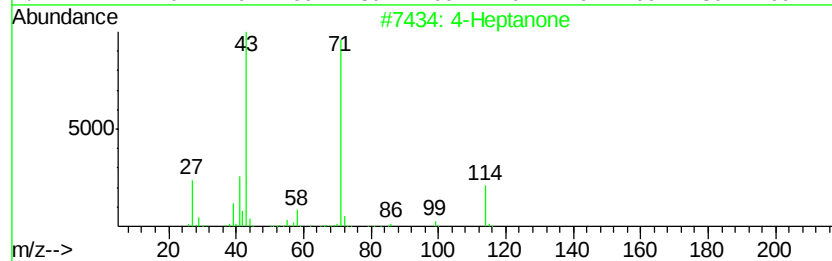
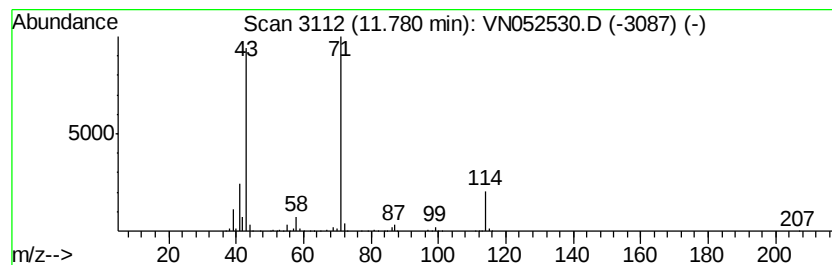
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Quant Title : SW846 8260

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

Peak Number 7 4-Heptanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	5.68 ug/l	605609	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Heptanone	114	C7H14O	000123-19-3	91
2		3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	78
3		3-Penten-2-ol	86	C5H10O	001569-50-2	59
4		Pentane, 3-bromo-	150	C5H11Br	001809-10-5	59
5		Propanoic acid, 2-methyl-, anhyd...	158	C8H14O3	000097-72-3	59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN112818\
Data File : VN052530.D
Acq On : 28 Nov 2018 19:55
Operator : MD\SY
Sample : J6044-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 26 Sample Multiplier: 28

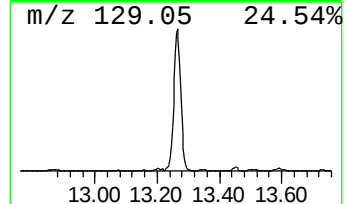
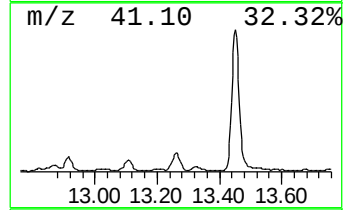
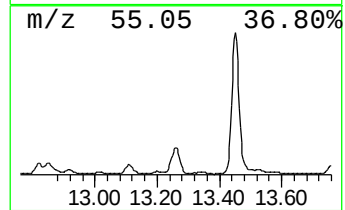
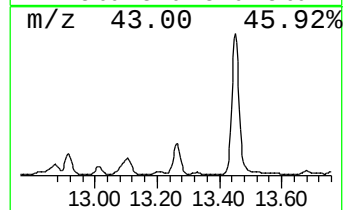
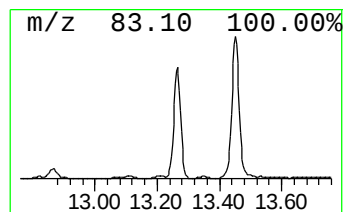
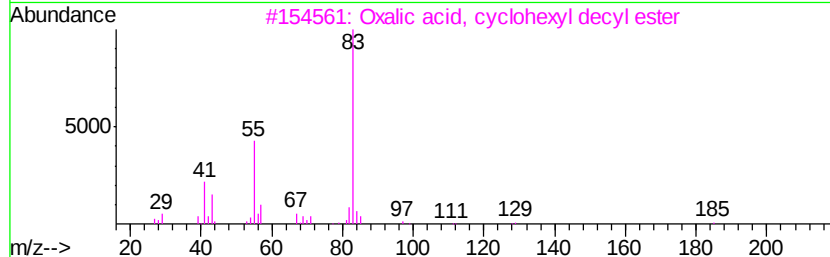
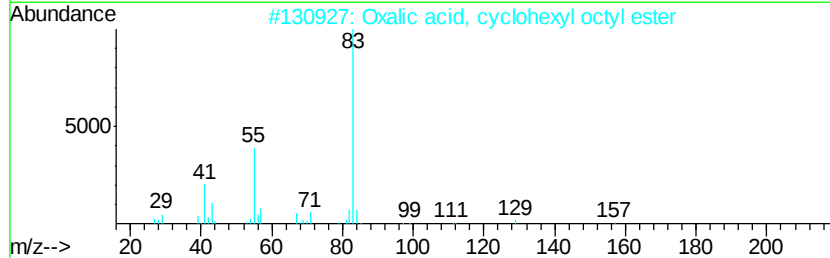
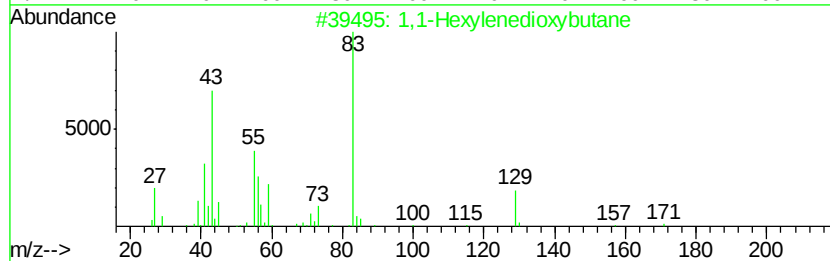
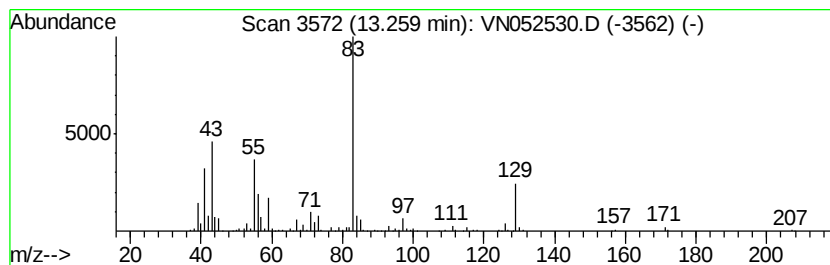
Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N112718W.M
Quant Title : SW846 8260

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

Peak Number 8 1,1-Hexylenedioxybutane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.26	6.17 ug/l	565640	1,4-Dichlorobenzene-d4	13.35		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,1-Hexylenedioxybutane	172	C10H20O2	1000249-77-4	83
2		Oxalic acid, cyclohexyl octyl ester	284	C16H28O4	1000309-31-0	50
3		Oxalic acid, cyclohexyl decyl ester	312	C18H32O4	1000309-31-2	50
4		Oxalic acid, cyclohexyl hexyl ester	256	C14H24O4	1000309-30-8	50
5		3-Methylbut-2-enoic acid, 4-nitr...	221	C11H11NO4	1000307-59-8	43



Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN112818\
Data File : VN052530.D
Acq On : 28 Nov 2018 19:55
Operator : MD\SY
Sample : J6044-04
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 26 Sample Multiplier: 28

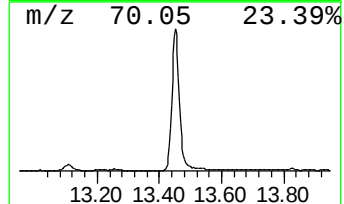
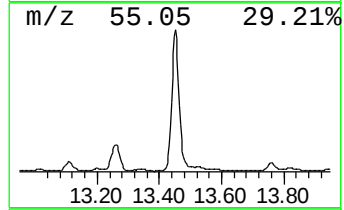
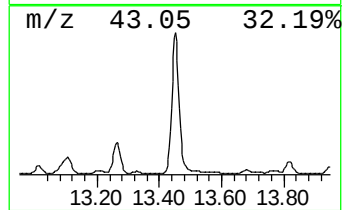
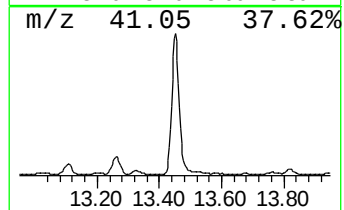
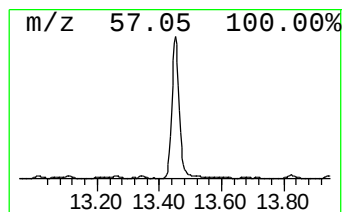
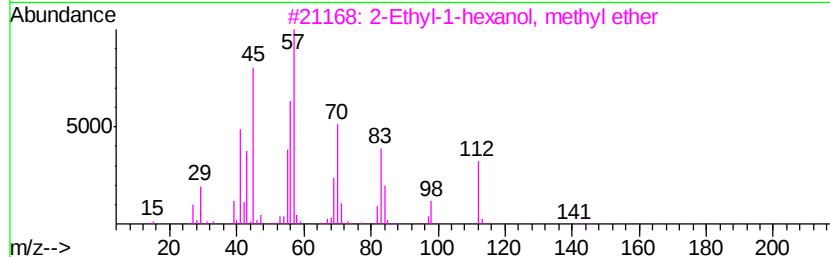
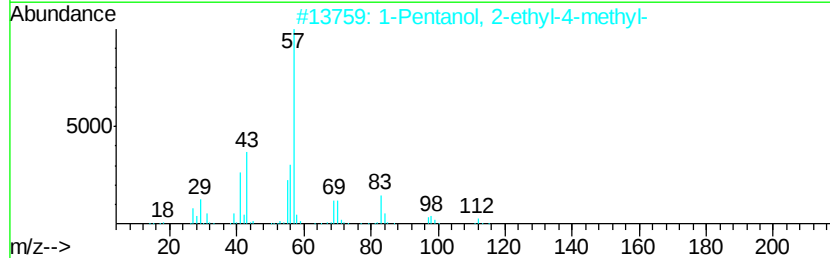
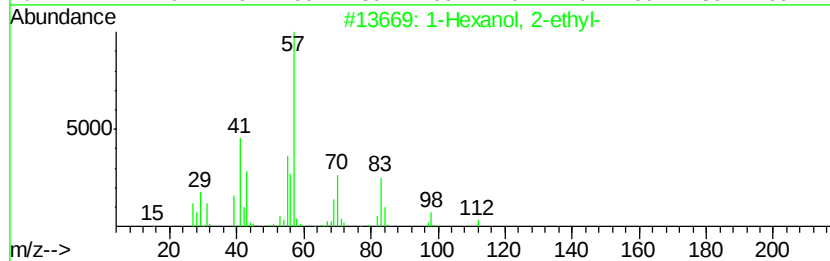
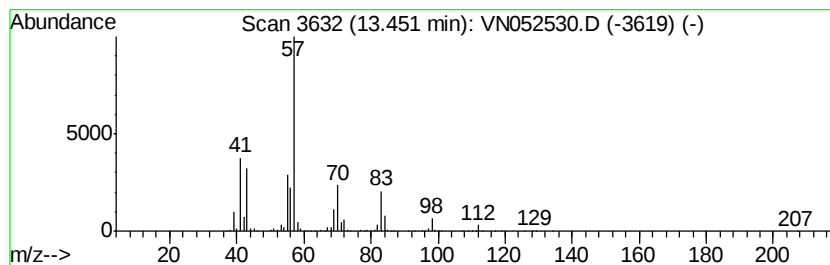
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MSVOA_N
ClientSampleId :
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N112718W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	32.74 ug/l	3003110	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Hexanol, 2-ethyl-	130 C8H18O	000104-76-7	78
2	1-Pentanol, 2-ethyl-4-methyl-	130 C8H18O	000106-67-2	56
3	2-Ethyl-1-hexanol, methyl ether	144 C9H20O	1000365-10-2	53
4	1-Decene, 2,4-dimethyl-	168 C12H24	055170-80-4	53
5	Oxalic acid, 2-ethylhexyl hexyl ...	286 C16H30O4	1000309-38-9	50



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Sample : J6044-04
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 28

Instrument :
MSVOA_N
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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
Ethanol	3.27	27.5	ug/l	2081880	1	7.67	3785220	50.0
Propanal	3.70	7.1	ug/l	537523	1	7.67	3785220	50.0
Butanal	6.54	32.5	ug/l	2461570	1	7.67	3785220	50.0
Ethane, (methylth...	6.65	10.4	ug/l	786752	1	7.67	3785220	50.0
Pentanal	9.17	8.3	ug/l	791449	2	8.59	4766620	50.0
4-Heptanone	11.78	5.7	ug/l	605609	3	11.41	5331220	50.0
1,1-Hexylenedioxy...	13.26	6.2	ug/l	565640	4	13.35	4586550	50.0
1-Hexanol, 2-ethyl-	13.45	32.7	ug/l	3003110	4	13.35	4586550	50.0