

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031221\
 Data File : VN066190.D
 Acq On : 12 Mar 2021 18:35
 Operator : JC/MD
 Sample : M1647-18
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 COMP1-41730:31

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_N\methods\82N031221W.M
 Title : SW846 8260

Signal : TIC: VN066190.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.783	26	35	53	rVB3	104045	137736	6.17%	0.706%
2	1.966	91	103	116	rBV3	17984	31393	1.41%	0.161%
3	2.121	152	161	167	rBV	27099	39927	1.79%	0.205%
4	2.274	207	218	236	rVB	115917	181476	8.13%	0.930%
5	3.208	552	566	583	rBV2	54368	129145	5.79%	0.662%
6	3.739	750	764	780	rBV2	76794	186824	8.37%	0.958%
7	4.243	933	952	977	rVB	48227	136010	6.09%	0.697%
8	4.726	1109	1132	1136	rBV4	27788	68774	3.08%	0.352%
9	5.855	1526	1553	1581	rBV3	108127	388170	17.39%	1.989%
10	6.453	1750	1776	1802	rBV3	163377	503519	22.56%	2.581%
11	6.748	1868	1886	1908	rBV2	17030	53324	2.39%	0.273%
12	7.510	2148	2170	2184	rBV2	275118	696290	31.20%	3.569%
13	7.587	2184	2199	2225	rVB2	517509	1241257	55.62%	6.362%
14	7.955	2315	2336	2358	rBV4	542230	1423246	63.77%	7.295%
15	8.515	2527	2545	2568	rBV	789212	1637818	73.39%	8.394%
16	8.730	2610	2625	2643	rBV4	59124	135519	6.07%	0.695%
17	9.103	2751	2764	2787	rVB6	18424	49094	2.20%	0.252%
18	10.028	3090	3109	3122	rBV	1217570	2231784	100.00%	11.439%
19	10.092	3122	3133	3152	rVB	650780	1164560	52.18%	5.969%
20	10.481	3264	3278	3296	rBV4	36514	80809	3.62%	0.414%
21	10.747	3367	3377	3387	rVB5	15284	23478	1.05%	0.120%
22	10.819	3387	3404	3423	rBV	438603	805591	36.10%	4.129%
23	11.350	3584	3602	3613	rBV	1140926	2089571	93.63%	10.710%
24	11.452	3634	3640	3659	rVB2	30430	51192	2.29%	0.262%
25	11.559	3668	3680	3703	rVB3	99026	192594	8.63%	0.987%
26	11.691	3714	3729	3746	rBV5	115139	226371	10.14%	1.160%
27	11.844	3773	3786	3792	rBV6	24494	41018	1.84%	0.210%
28	11.895	3794	3805	3818	rVV7	65765	141255	6.33%	0.724%
29	11.945	3819	3824	3837	rVB3	23230	39059	1.75%	0.200%
30	12.063	3860	3868	3879	rVB8	20097	34821	1.56%	0.178%
31	12.128	3879	3892	3901	rVV6	41796	74323	3.33%	0.381%
32	12.179	3903	3911	3927	rVB3	41761	75975	3.40%	0.389%
33	12.345	3956	3973	4001	rBV	759682	1345264	60.28%	6.895%
34	12.616	4062	4074	4090	rVB5	64155	130353	5.84%	0.668%
35	12.766	4118	4130	4133	rBV5	34835	49456	2.22%	0.253%
36	12.860	4154	4165	4190	rBV2	146280	257095	11.52%	1.318%

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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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Title : SW846 8260

37	12.962	4194	4203	4221	rVB9	54600	125855	5.64%	0.645%
38	13.053	4225	4237	4251	rBV2	103521	191047	8.56%	0.979%
39	13.142	4263	4270	4280	rBV4	38776	68060	3.05%	0.349%
40	13.286	4311	4324	4350	rVB	795100	1362849	61.07%	6.985%
41	13.396	4353	4365	4388	rBV	716808	1342066	60.13%	6.879%
42	13.667	4458	4466	4484	rVB3	62990	109206	4.89%	0.560%
43	15.043	4970	4979	4984	rBV3	135618	217767	9.76%	1.116%

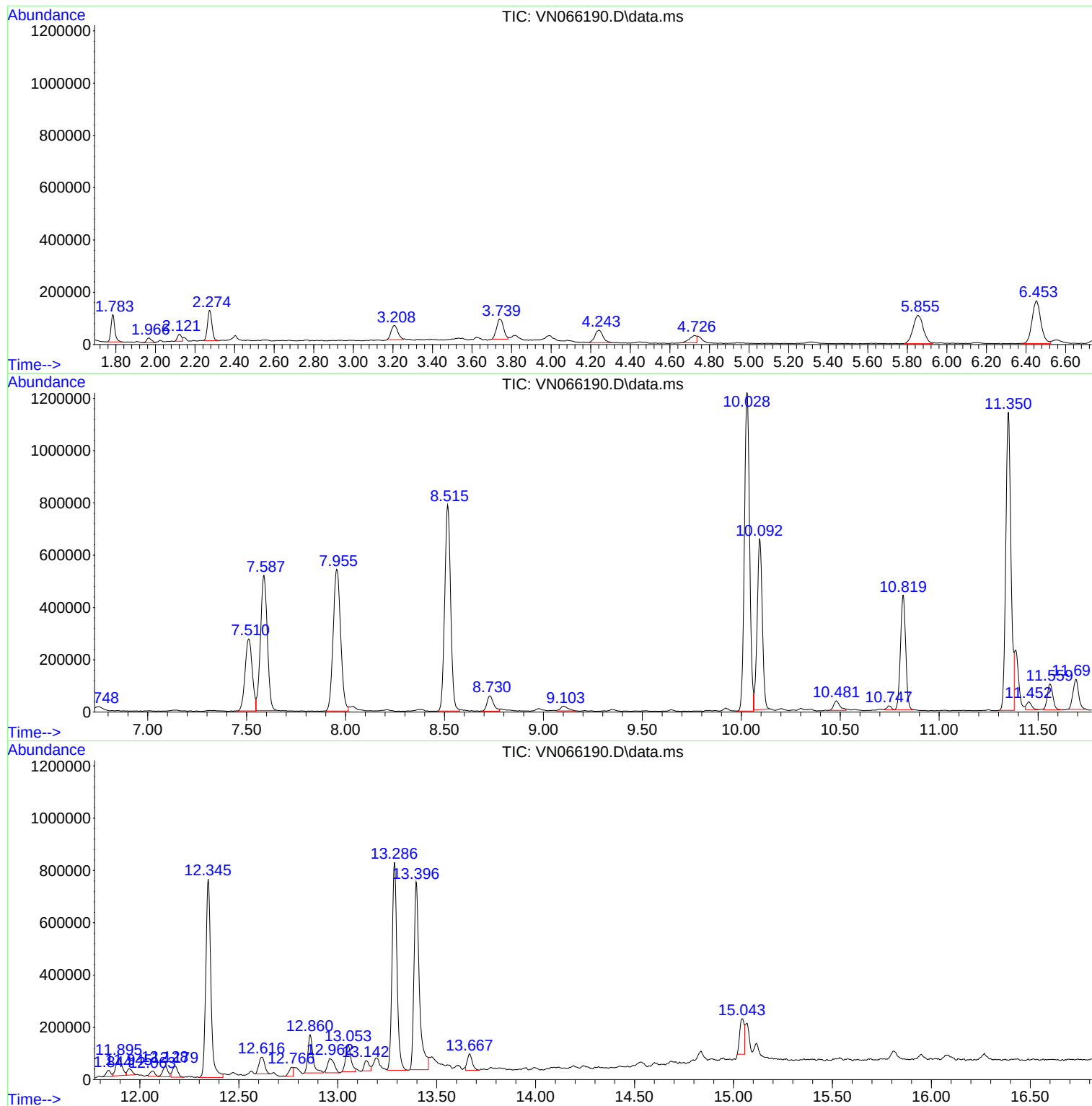
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031221W.M
Quant Title : SW846 8260

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



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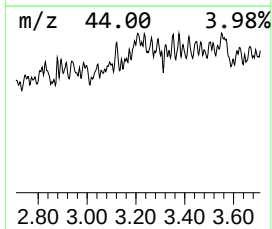
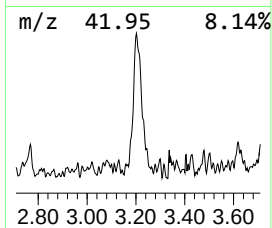
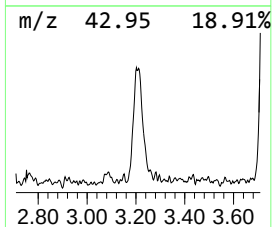
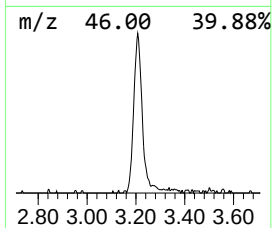
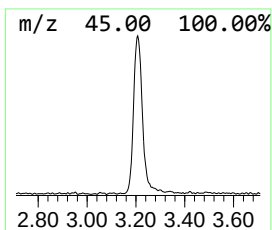
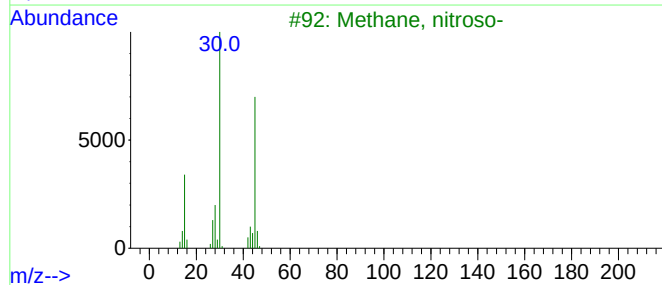
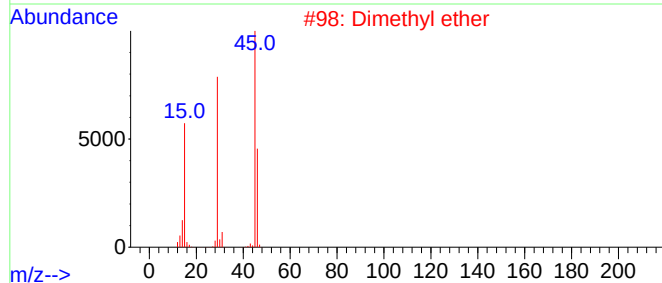
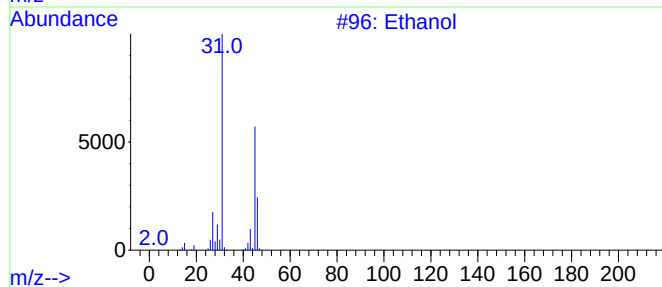
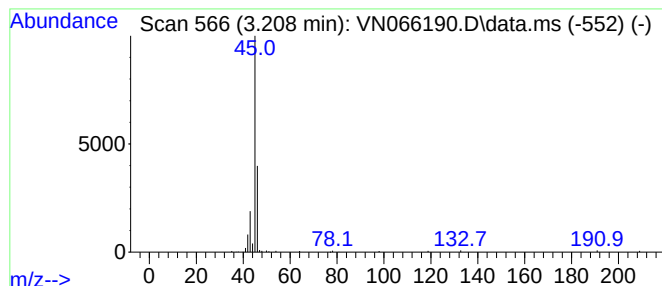
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031221W.M
Quant Title : SW846 8260

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

Peak Number 3 Ethanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.208	5.20 ug/l	129145	Pentafluorobenzene	7.590

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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			2,2-Dichloroethyl methyl ether	128	C3H6Cl2O	034862-07-2	4
5			Oxalic acid	90	C2H2O4	000144-62-7	4



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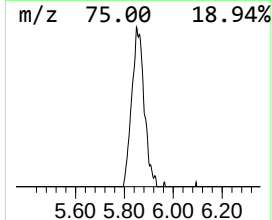
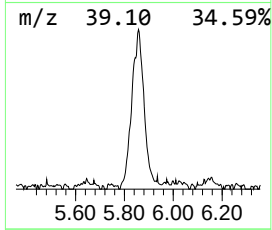
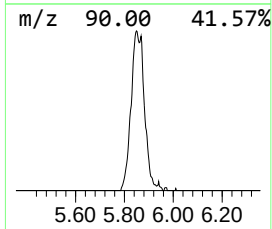
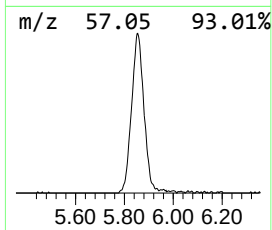
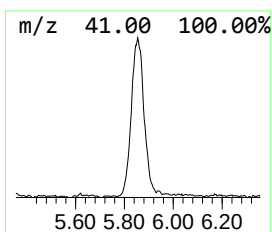
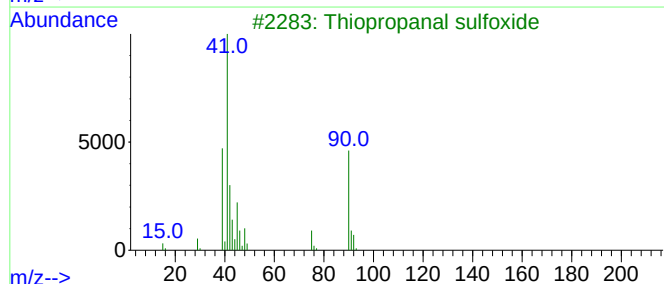
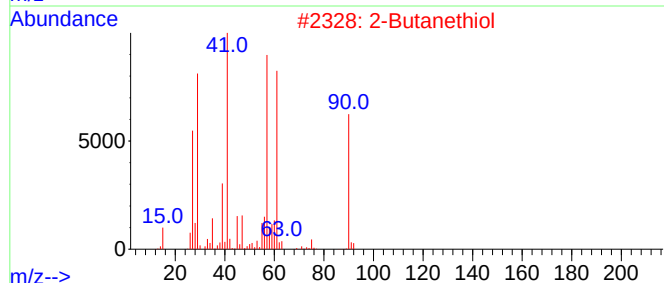
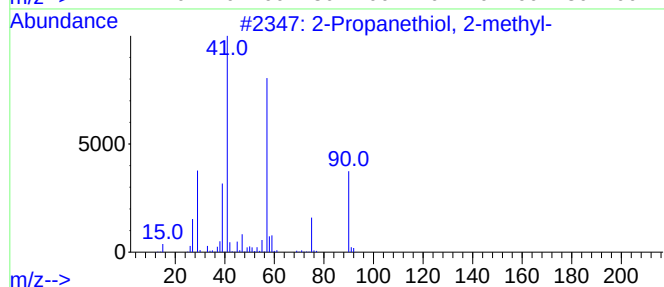
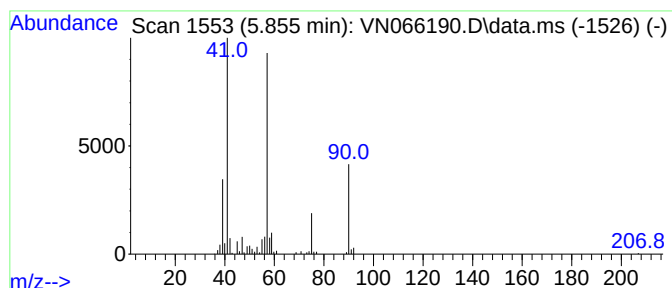
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031221W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Propanethiol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.855	15.64 ug/l	388170	Pentafluorobenzene	7.590

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	91
2			2-Butanethiol	90	C4H10S	000513-53-1	47
3			Thiopropenal sulfoxide	90	C3H6OS	1000322-28-4	38
4			Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	27
5			Acetoacetic acid, 1,3-dithio-, S...	190	C8H14OS2	020383-06-6	25



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ALS Vial : 17 Sample Multiplier: 1

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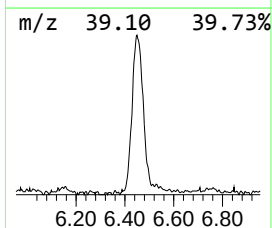
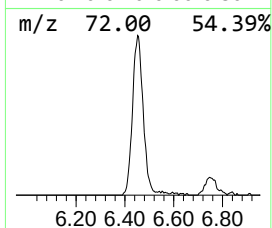
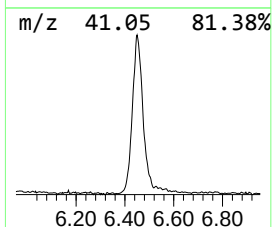
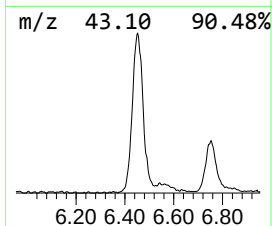
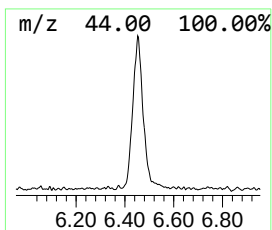
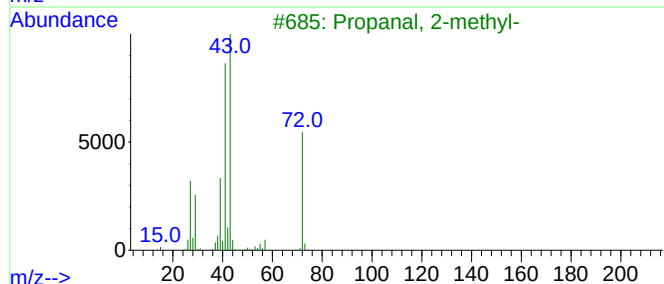
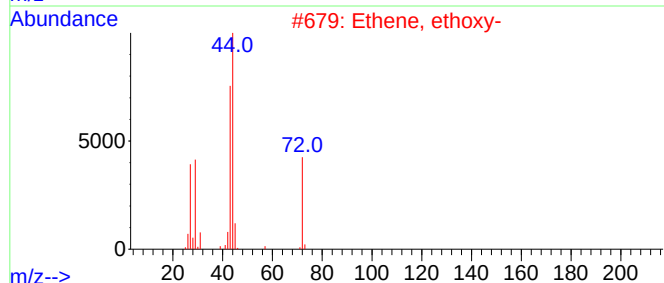
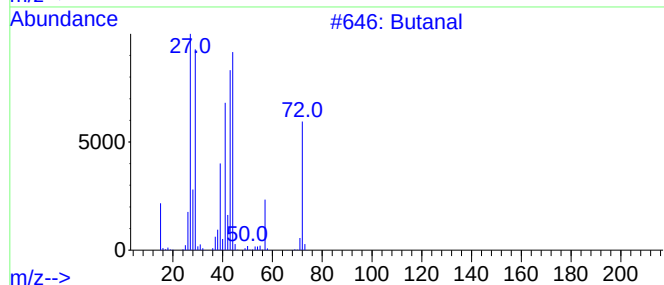
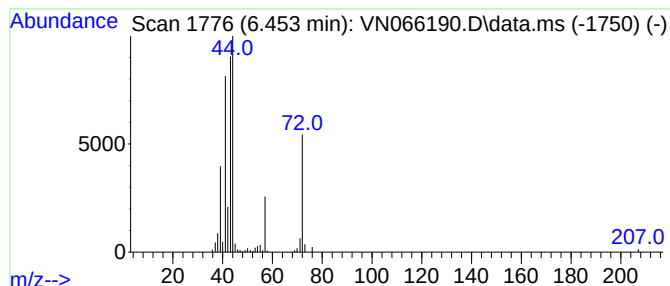
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031221W.M
Quant Title : SW846 8260

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

Peak Number 5 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.453	20.28 ug/l	503519	Pentafluorobenzene	7.590

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	91
2			Ethene, ethoxy-	72	C4H8O	000109-92-2	50
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	49
4			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	38
5			O-Methylisourea	74	C2H6N2O	002440-60-0	36



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ALS Vial : 17 Sample Multiplier: 1

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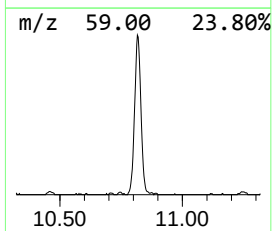
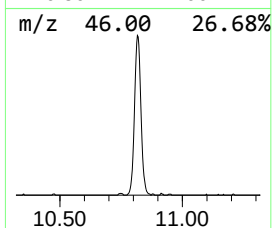
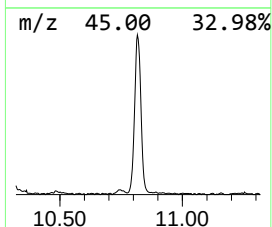
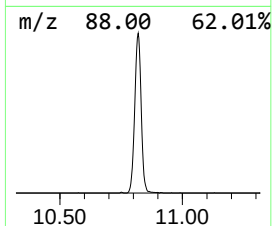
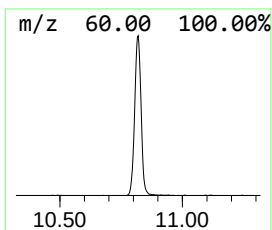
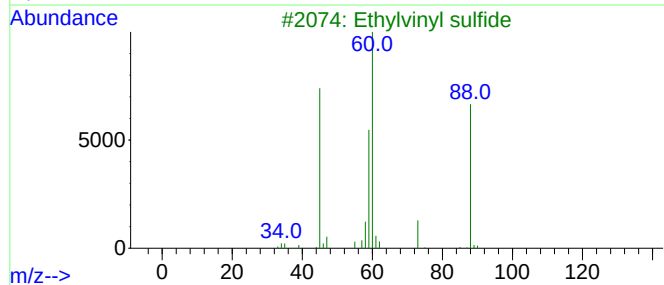
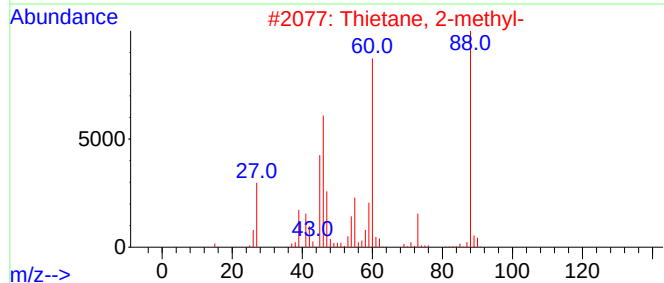
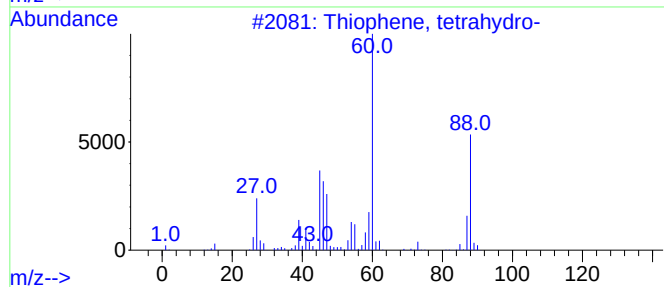
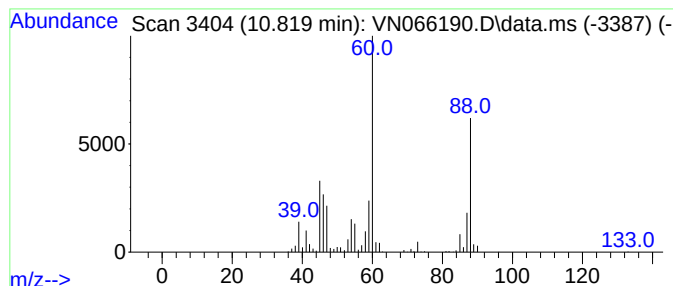
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Quant Title : SW846 8260

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

Peak Number 6 Thiophene, tetrahydro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.819	19.28 ug/l	805591	Chlorobenzene-d5	11.350

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, tetrahydro-	88	C4H8S	000110-01-0	97
2			Thietane, 2-methyl-	88	C4H8S	017837-41-1	72
3			Ethylvinyl sulfide	88	C4H8S	000627-50-9	40
4			Sulfide, allyl methyl	88	C4H8S	010152-76-8	27
5			Ethanol, 2-mercapto-	78	C2H6OS	000060-24-2	23



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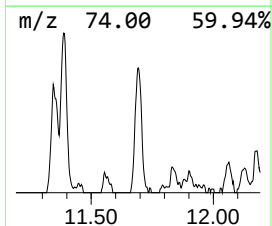
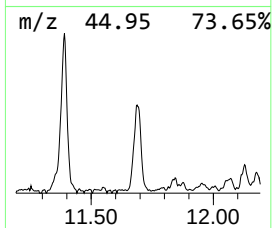
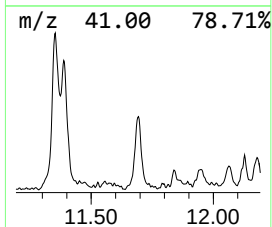
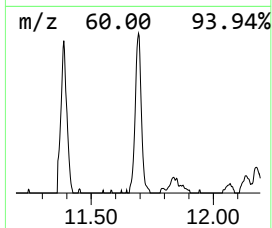
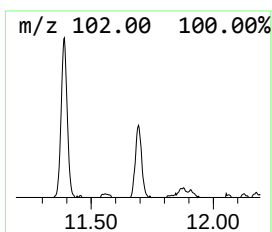
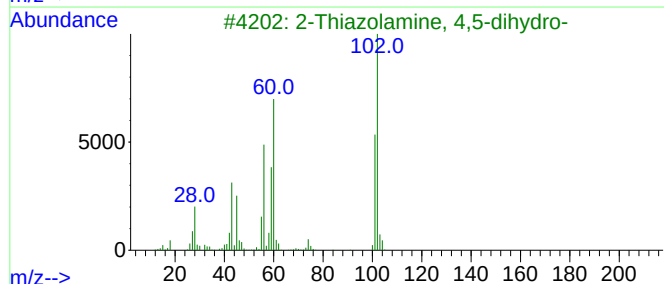
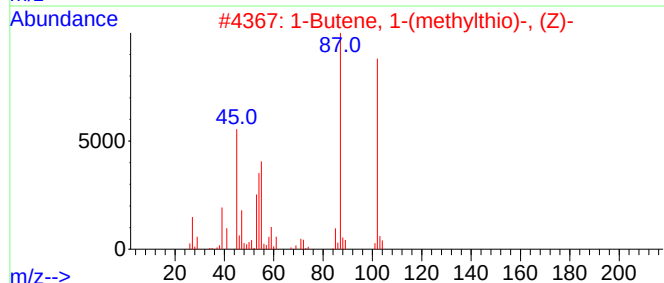
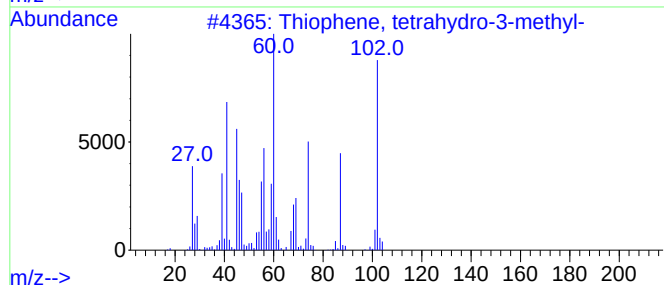
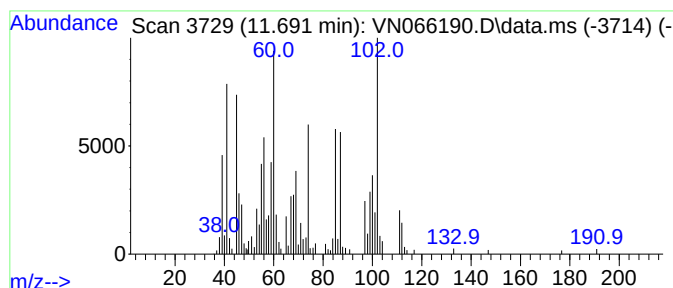
Instrument :
MSVOA_N
ClientSampleId :
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Quant Title : SW846 8260

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

Peak Number 7 Thiophene, tetrahydro-3-met... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.691	5.42 ug/l	226371	Chlorobenzene-d5	11.350	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, tetrahydro-3-methyl-	102	C5H10S	004740-00-5	89
2	1-Butene, 1-(methylthio)-, (Z)-	102	C5H10S	017414-15-2	45
3	2-Thiazolamine, 4,5-dihydro-	102	C3H6N2S	001779-81-3	43
4	3-Ethylthio-1-propene	102	C5H10S	005296-62-8	43
5	Thiazole, 4,5-dihydro-2-methyl-	101	C4H7NS	002346-00-1	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031221\
Data File : VN066190.D
Acq On : 12 Mar 2021 18:35
Operator : JC/MD
Sample : M1647-18
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP1-41730:31

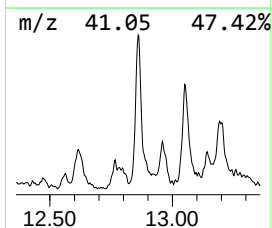
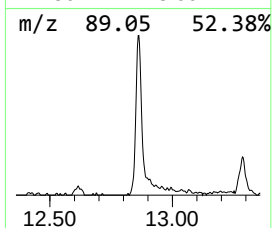
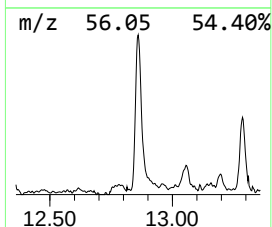
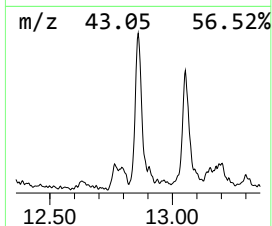
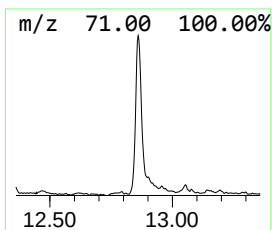
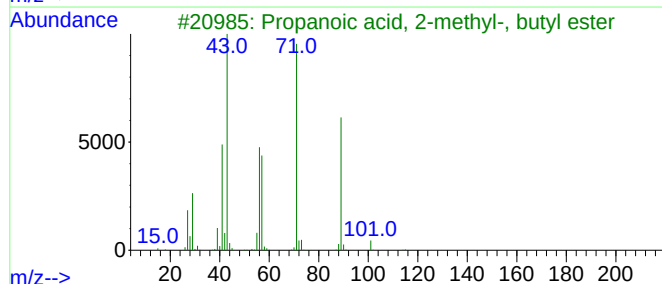
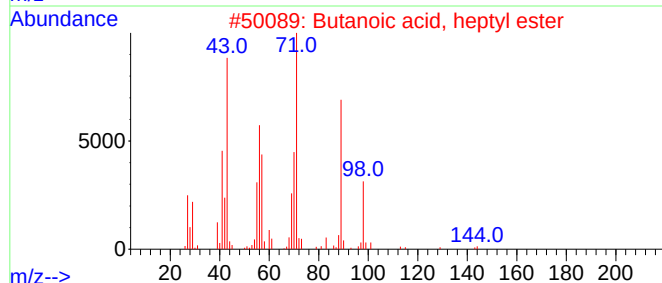
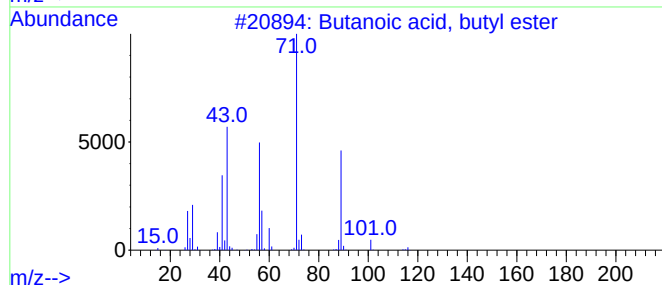
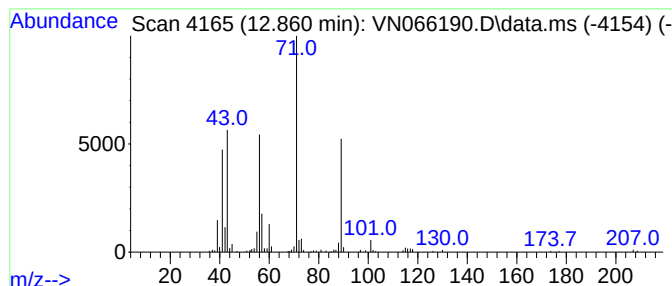
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Quant Title : SW846 8260

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

Peak Number 8 Butanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.860	9.43 ug/l	257095	1,4-Dichlorobenzene-d4	13.287

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2			Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	72
3			Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	64
4			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	64
5			Propanoic acid, 2-methyl-, 3-hyd...	216	C12H24O3	074367-34-3	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031221\
Data File : VN066190.D
Acq On : 12 Mar 2021 18:35
Operator : JC/MD
Sample : M1647-18
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP1-41730:31

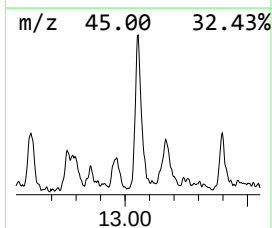
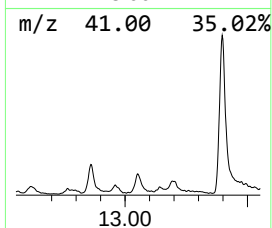
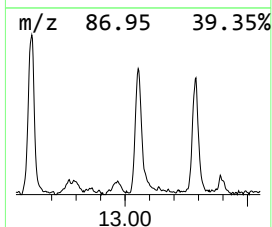
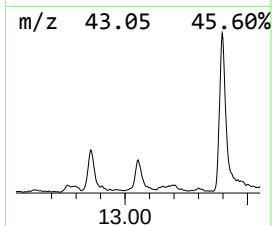
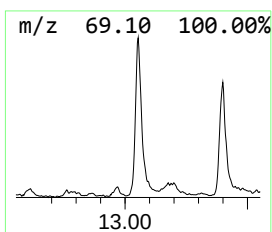
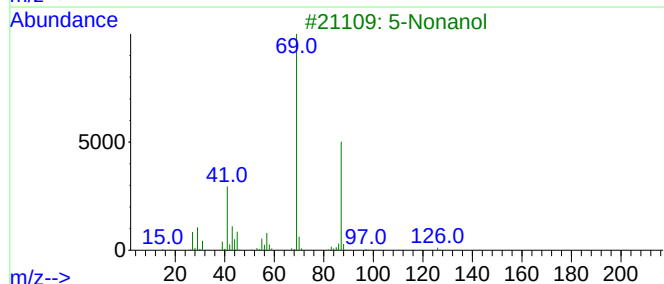
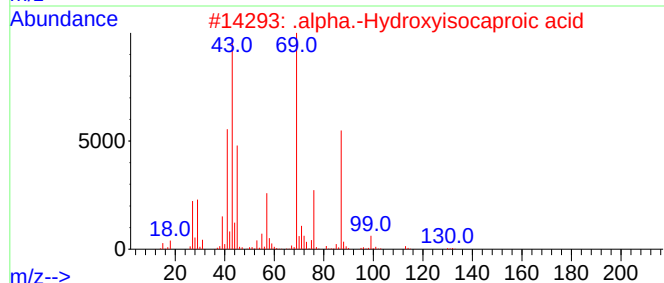
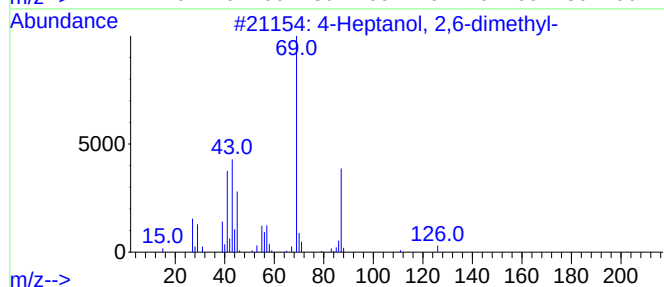
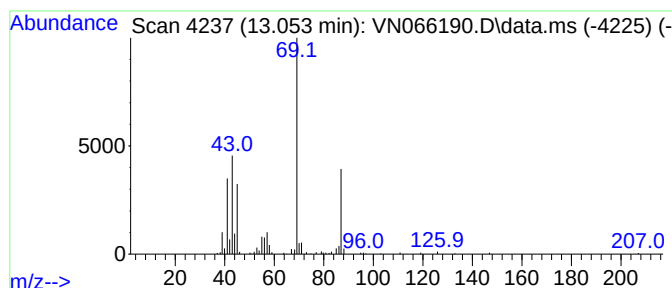
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Quant Title : SW846 8260

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

Peak Number 9 4-Heptanol, 2,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.053	7.01 ug/l	191047	1,4-Dichlorobenzene-d4	13.287

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	83
2			.alpha.-Hydroxyisocaproic acid	132	C6H12O3	000498-36-2	72
3			5-Nonanol	144	C9H20O	000623-93-8	72
4			1,2-Hexanediol	118	C6H14O2	006920-22-5	72
5			1-Octyn-4-ol	126	C8H14O	052517-92-7	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031221\
Data File : VN066190.D
Acq On : 12 Mar 2021 18:35
Operator : JC/MD
Sample : M1647-18
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP1-41730:31

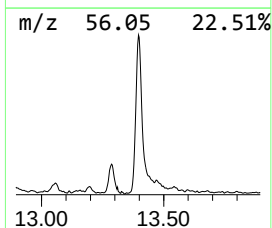
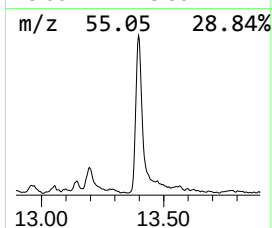
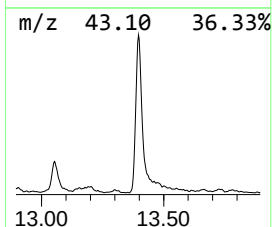
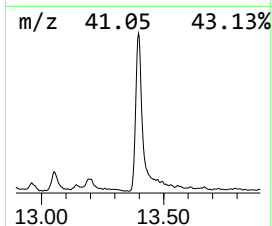
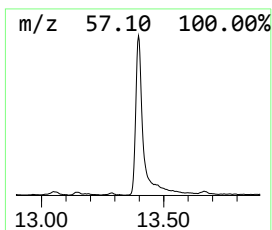
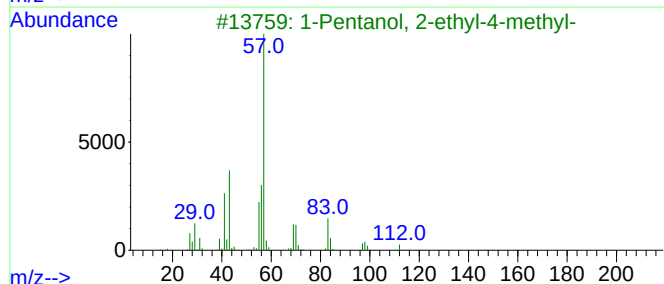
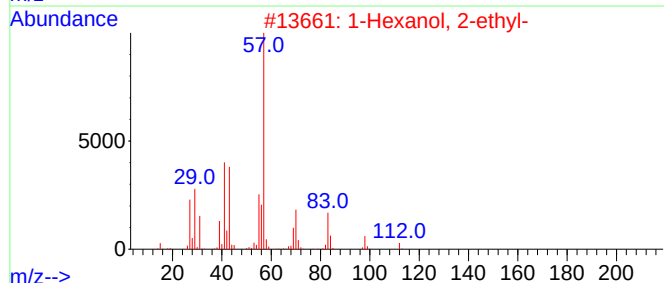
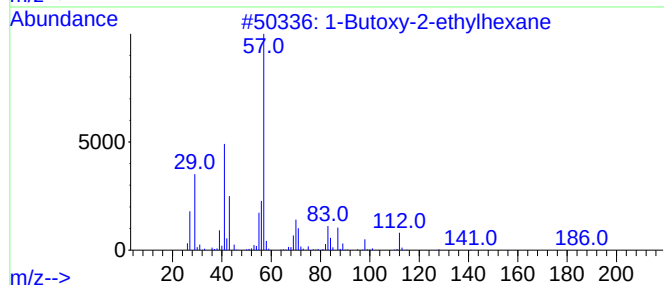
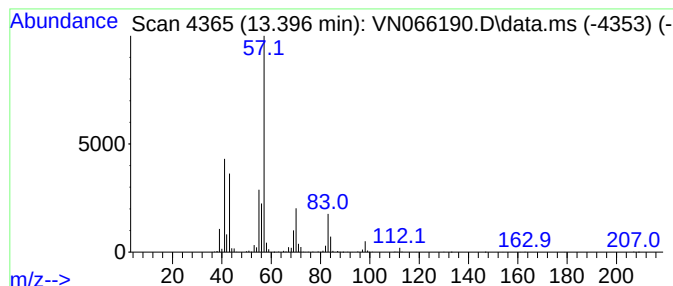
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031221W.M
Quant Title : SW846 8260

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

Peak Number 10 1-Butoxy-2-ethylhexane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.396	49.24 ug/l	1342070	1,4-Dichlorobenzene-d4	13.287

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butoxy-2-ethylhexane	186	C12H26O	062625-25-6	83
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	72
4			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	64
5			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031221\
Data File : VN066190.D
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Sample : M1647-18
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP1-41730:31

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031221W.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	3.208	5.2	ug/l	129145	1	7.590	1241260	50.0
2-Propanethiol,...	5.855	15.6	ug/l	388170	1	7.590	1241260	50.0
Butanal	6.453	20.3	ug/l	503519	1	7.590	1241260	50.0
Thiophene, tetr...	10.819	19.3	ug/l	805591	3	11.350	2089570	50.0
Thiophene, tetr...	11.691	5.4	ug/l	226371	3	11.350	2089570	50.0
Butanoic acid, ...	12.860	9.4	ug/l	257095	4	13.287	1362850	50.0
4-Heptanol, 2,6...	13.053	7.0	ug/l	191047	4	13.287	1362850	50.0
1-Butoxy-2-ethy...	13.396	49.2	ug/l	1342070	4	13.287	1362850	50.0