

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010621\
 Data File : VN065403.D
 Acq On : 6 Jan 2021 16:28
 Operator : JC/MD
 Sample : M1022-05 50X
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 41098

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\82N122220W.M

Title : SW846 8260

Signal : TIC: VN065403.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.306	162	176	202	rBV	822142	1387525	100.00%	10.046%
2	3.258	454	472	499	rBV	478176	1177864	84.89%	8.528%
3	3.672	589	601	617	rVB	12815	30510	2.20%	0.221%
4	3.791	619	638	677	rBV	346852	909074	65.52%	6.582%
5	4.052	699	719	747	rVB2	128545	371512	26.78%	2.690%
6	6.023	1315	1332	1356	rBV3	9974	32018	2.31%	0.232%
7	6.508	1465	1483	1504	rBV2	44038	135338	9.75%	0.980%
8	6.811	1558	1577	1591	rBV2	7196	22198	1.60%	0.161%
9	6.901	1592	1605	1630	rVB3	10235	30359	2.19%	0.220%
10	7.553	1790	1808	1820	rBV2	172147	428440	30.88%	3.102%
11	7.630	1820	1832	1854	rVB	277671	666521	48.04%	4.826%
12	7.801	1873	1885	1905	rVB2	8552	22347	1.61%	0.162%
13	7.991	1927	1944	1965	rBV	173184	402482	29.01%	2.914%
14	8.553	2103	2119	2143	rBV	452184	937004	67.53%	6.784%
15	8.765	2171	2185	2213	rBV	58466	139481	10.05%	1.010%
16	9.135	2288	2300	2316	rBV4	9389	21660	1.56%	0.157%
17	10.061	2572	2588	2600	rBV	738828	1350111	97.30%	9.775%
18	10.126	2601	2608	2625	rVB	49151	90716	6.54%	0.657%
19	10.508	2715	2727	2737	rBV4	7533	16164	1.16%	0.117%
20	10.830	2816	2827	2839	rBV4	12914	24221	1.75%	0.175%
21	11.379	2984	2998	3025	rBV	727370	1295998	93.40%	9.384%
22	11.791	3103	3126	3145	rBV9	8077	29078	2.10%	0.211%
23	12.077	3175	3215	3220	rBV4	190690	779315	56.17%	5.643%
24	12.376	3295	3308	3330	rBV	605567	1078319	77.72%	7.808%
25	12.701	3402	3409	3419	rVB6	12612	20275	1.46%	0.147%
26	13.035	3496	3513	3526	rBV3	35107	63414	4.57%	0.459%
27	13.138	3534	3545	3554	rBV3	37863	69931	5.04%	0.506%
28	13.228	3559	3573	3579	rVV3	82541	211444	15.24%	1.531%
29	13.260	3579	3583	3590	rVV	76833	111886	8.06%	0.810%
30	13.318	3590	3601	3612	rVV	658908	1158916	83.52%	8.391%
31	13.379	3612	3620	3629	rVV	125747	219184	15.80%	1.587%
32	13.428	3629	3635	3646	rVV2	39828	73658	5.31%	0.533%
33	13.482	3647	3652	3669	rVB8	10875	20594	1.48%	0.149%
34	13.646	3693	3703	3712	rBV2	16817	25261	1.82%	0.183%
35	13.765	3730	3740	3745	rBV2	24015	36644	2.64%	0.265%
36	13.801	3745	3751	3768	rVB6	23277	46911	3.38%	0.340%

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37	13.926	3778	3790	3813	rVB6	18238	77986	5.62%	0.565%
38	14.498	3960	3968	3976	rVB2	26021	36591	2.64%	0.265%
39	14.559	3979	3987	3996	rBV7	10330	20498	1.48%	0.148%
40	14.617	3996	4005	4016	rBV2	38492	67426	4.86%	0.488%
41	14.820	4059	4068	4077	rBV6	19539	33845	2.44%	0.245%
42	15.084	4142	4150	4160	rBV4	11328	22831	1.65%	0.165%
43	15.302	4209	4218	4231	rVB3	26395	45069	3.25%	0.326%
44	15.579	4300	4304	4317	rVB10	10050	14699	1.06%	0.106%
45	16.125	4466	4474	4482	rVB3	12162	19509	1.41%	0.141%
46	16.193	4487	4495	4504	rVB2	12822	19488	1.40%	0.141%
47	16.309	4523	4531	4544	rBV5	7883	17000	1.23%	0.123%

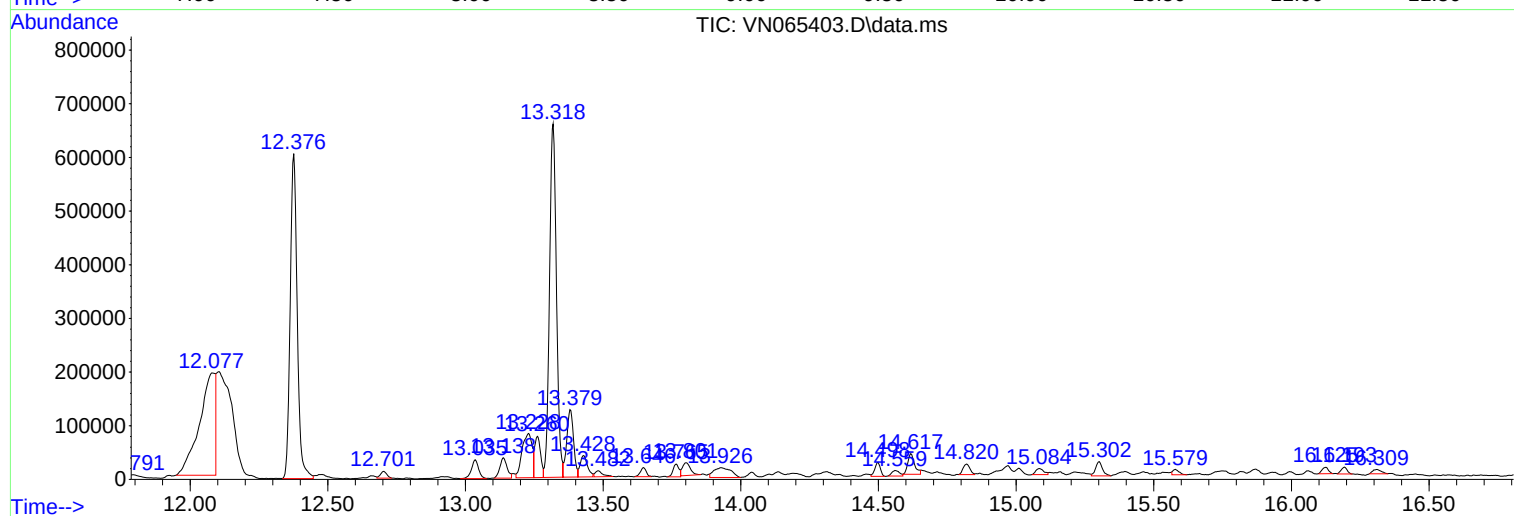
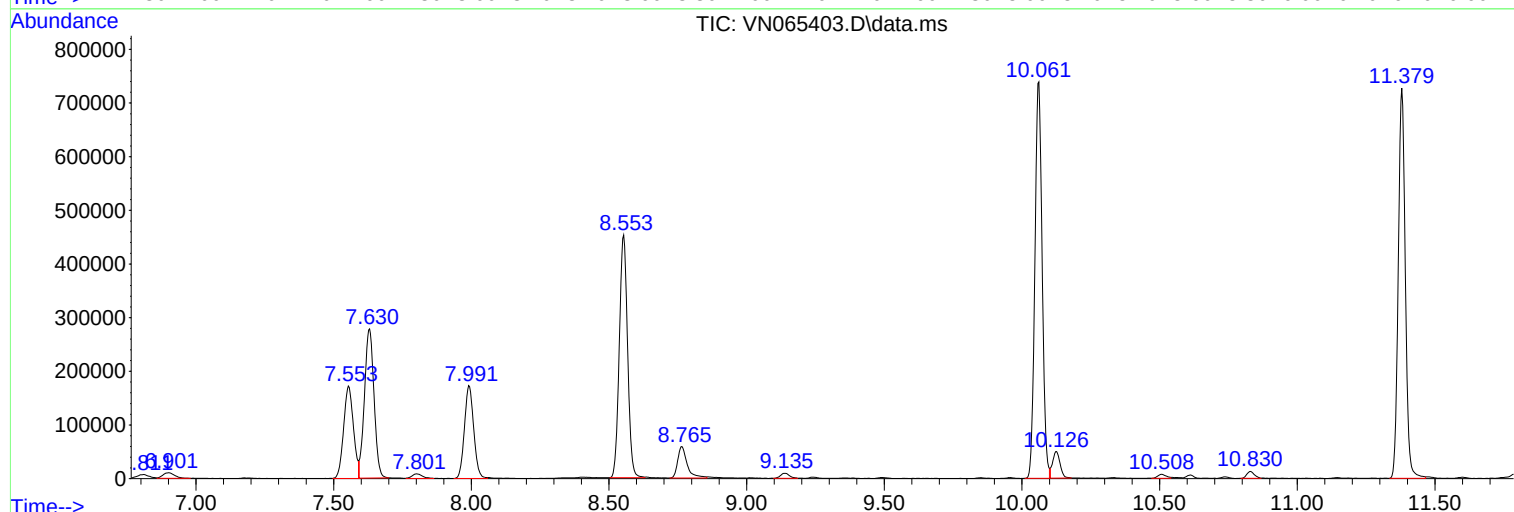
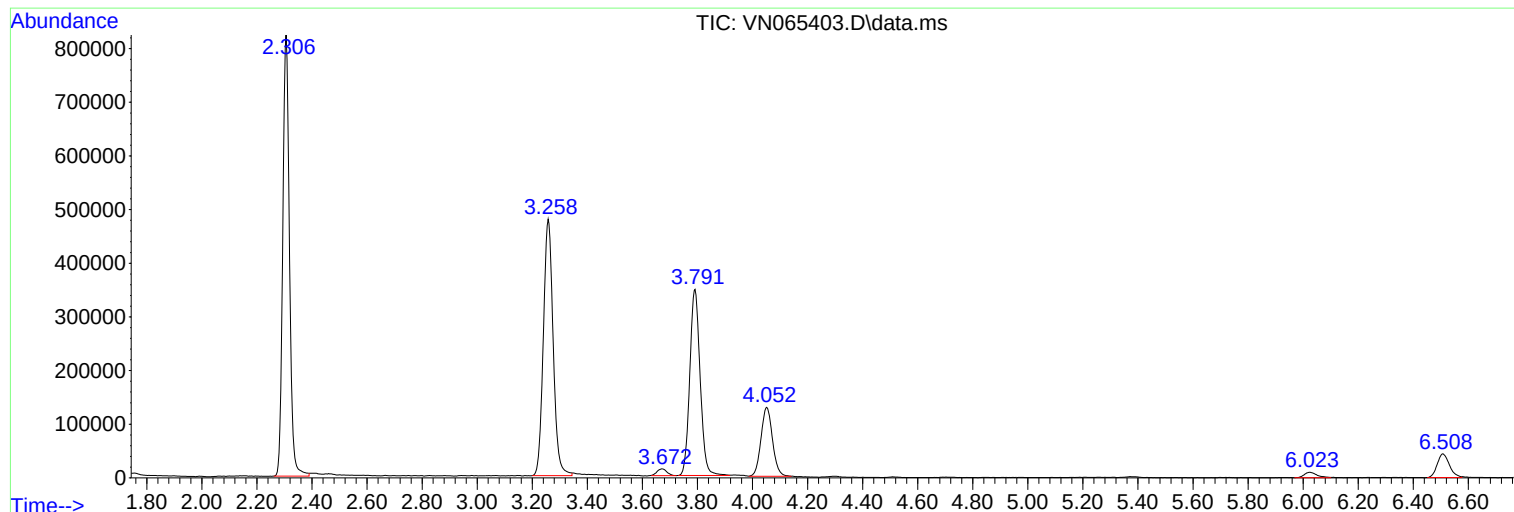
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

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



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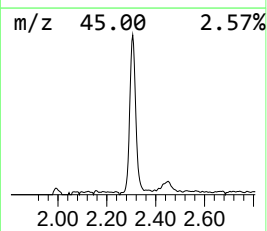
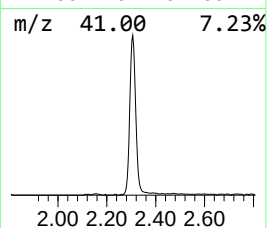
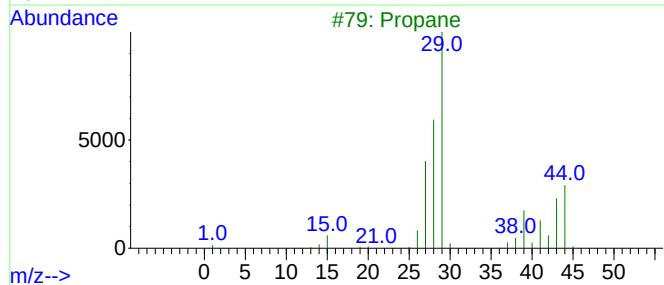
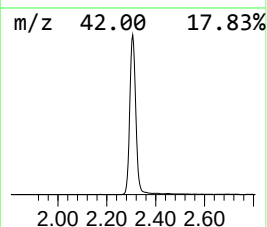
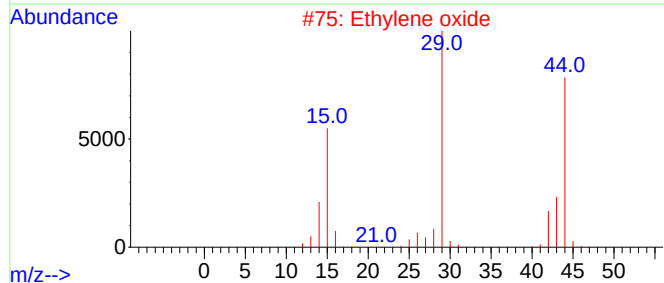
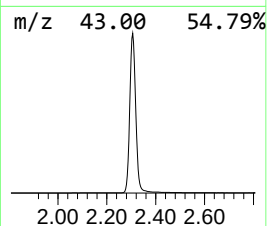
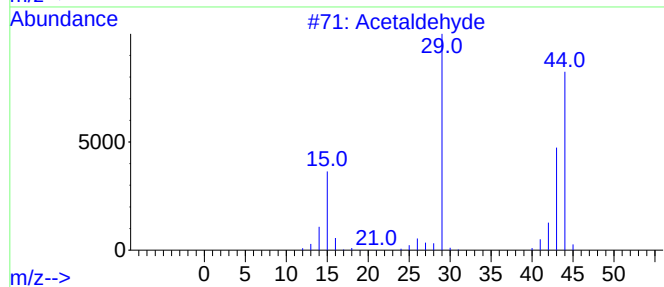
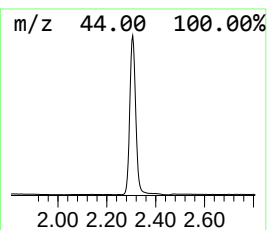
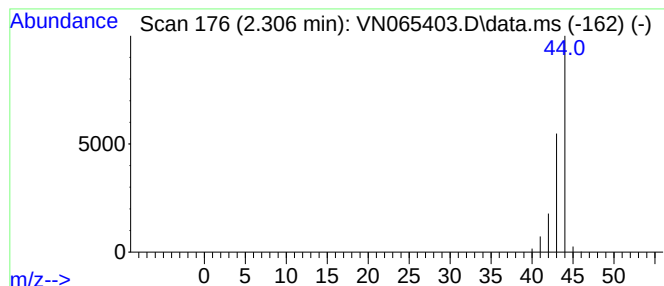
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.306	104.09 ug/l	1387530	Pentafluorobenzene	7.630

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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			Ethyne, fluoro-	44	C2HF	002713-09-9	3



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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41098

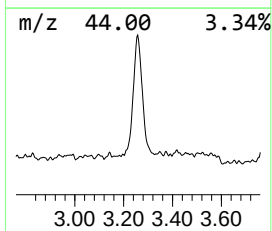
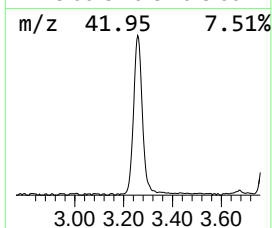
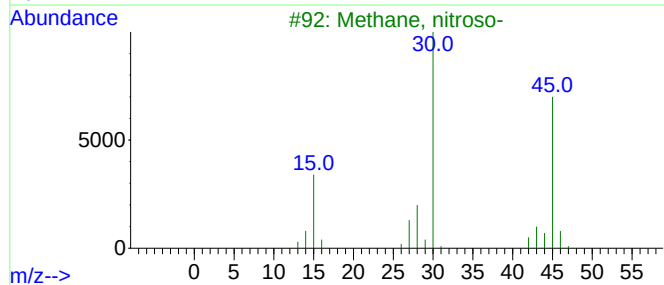
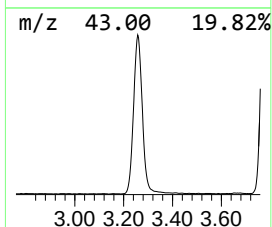
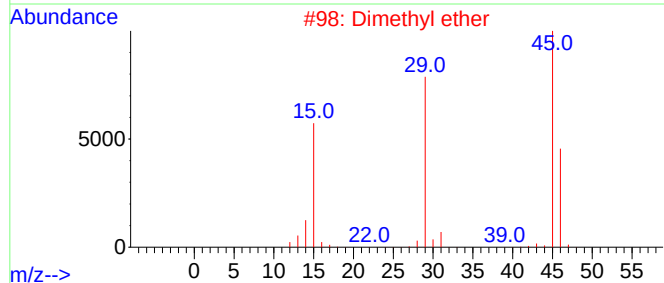
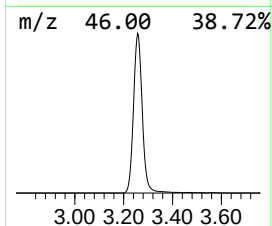
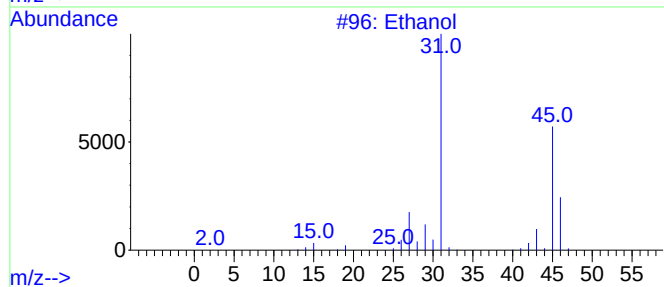
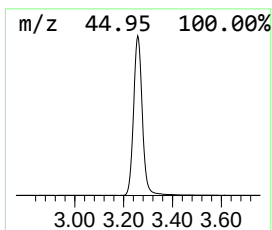
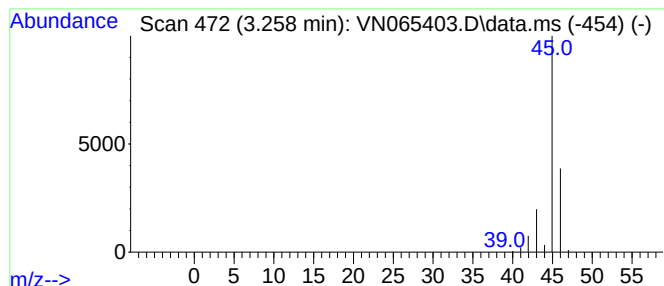
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N12220W.M
Quant Title : SW846 8260

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.
3.258	88.36 ug/l	1177860	Pentafluorobenzene	7.630

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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			L-Lactic acid	90	C3H6O3	000079-33-4	4
5			Formic acid	46	CH2O2	000064-18-6	4



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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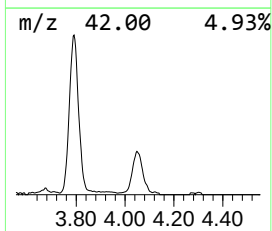
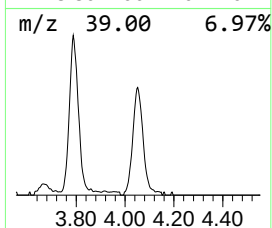
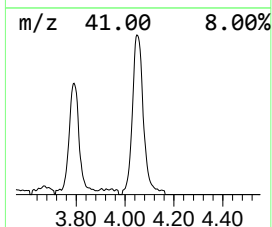
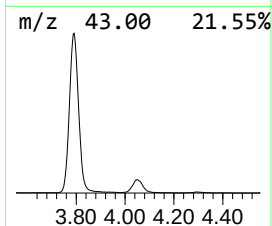
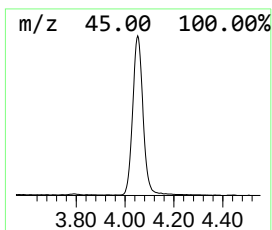
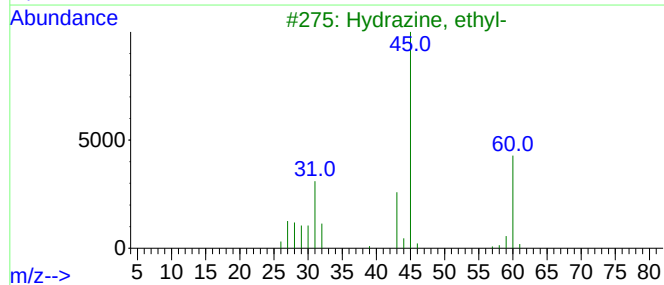
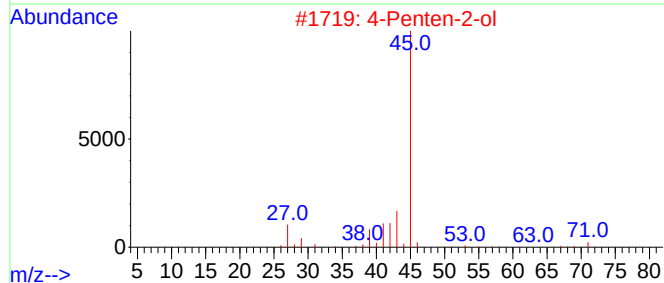
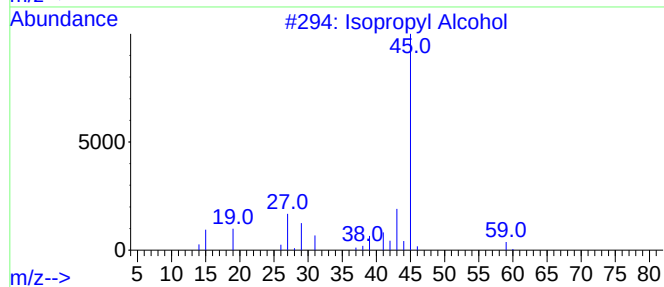
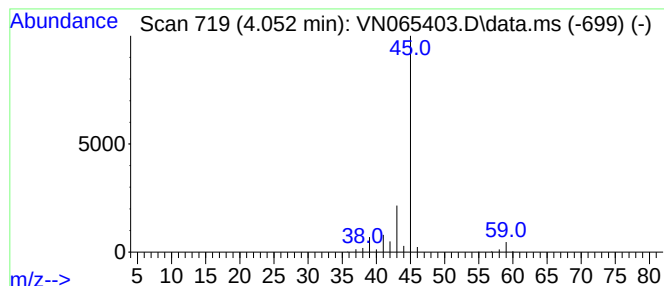
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

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

Peak Number 3 Isopropyl Alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.052	27.87 ug/l	371512	Pentafluorobenzene	7.630

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2			4-Penten-2-ol	86	C5H10O	000625-31-0	9
3			Hydrazine, ethyl-	60	C2H8N2	000624-80-6	9
4			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
5			Formamide	45	CH3NO	000075-12-7	5



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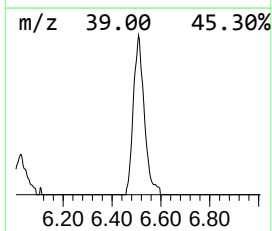
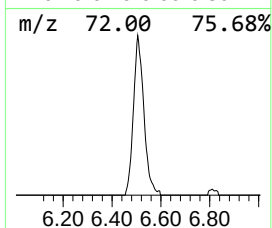
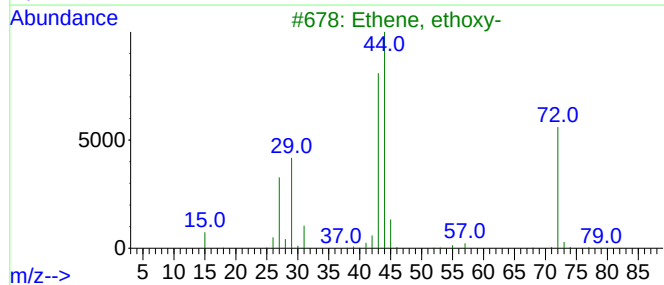
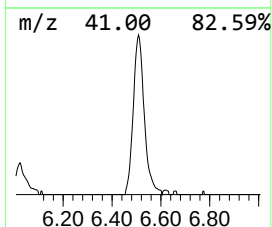
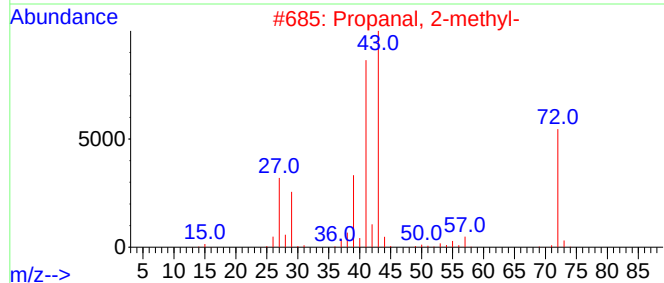
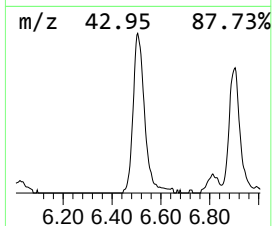
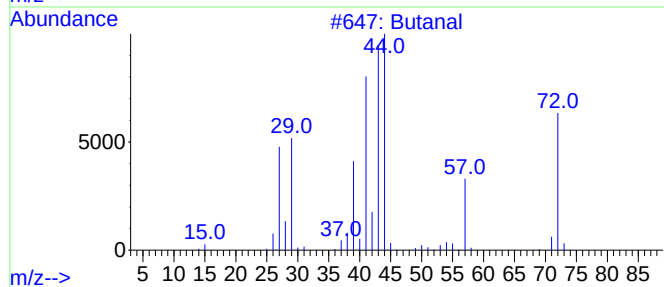
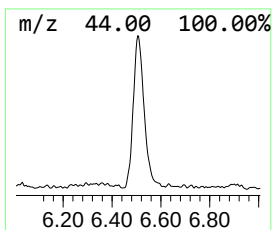
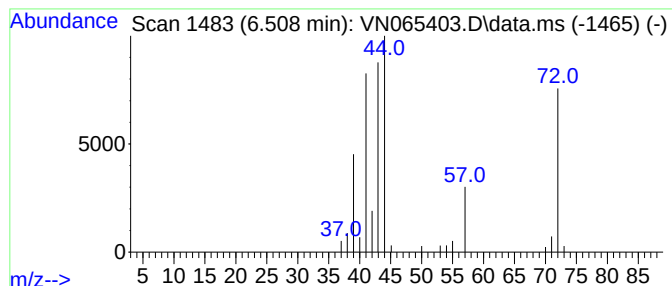
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Quant Title : SW846 8260

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

Peak Number 4 Butanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.508	10.15 ug/l	135338	Pentafluorobenzene	7.630

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanal	72	C4H8O	000123-72-8	94
2		Propanal, 2-methyl-	72	C4H8O	000078-84-2	37
3		Ethene, ethoxy-	72	C4H8O	000109-92-2	33
4		Isobutylene epoxide	72	C4H8O	000558-30-5	16
5		Methacrolein	70	C4H6O	000078-85-3	14



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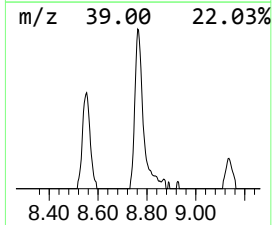
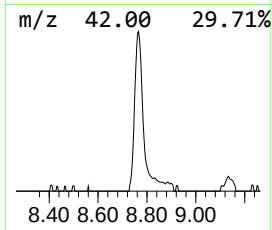
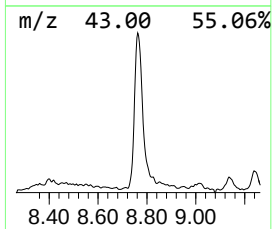
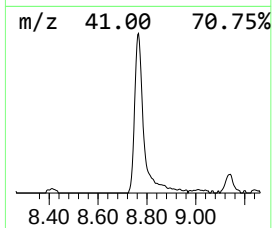
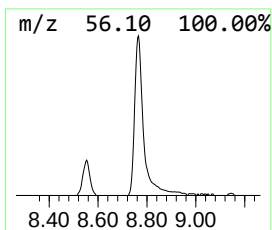
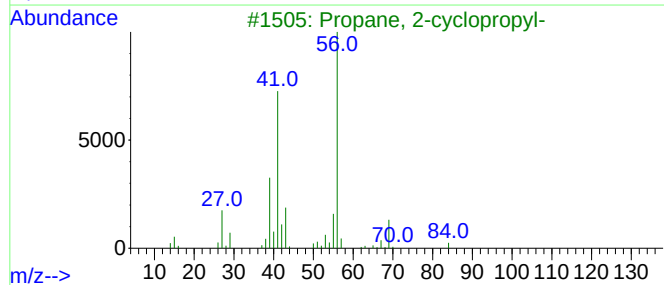
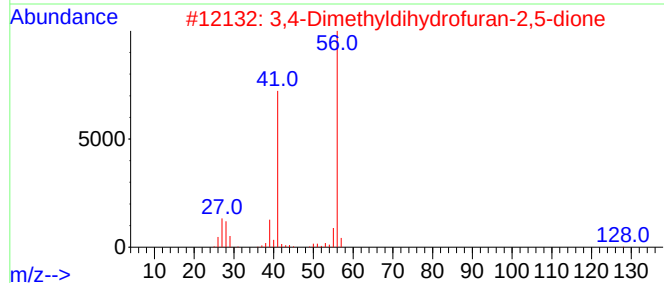
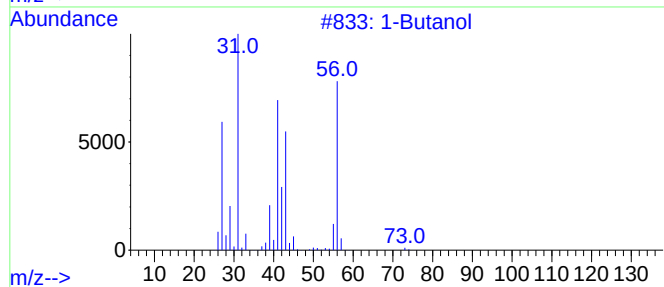
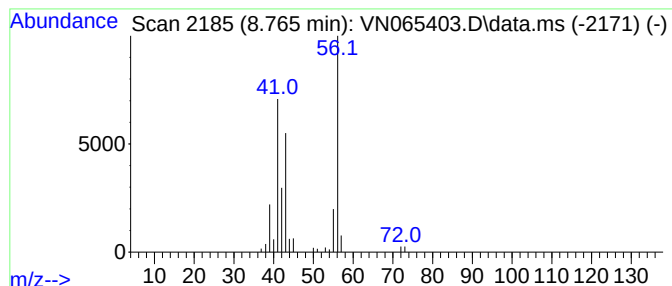
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Quant Title : SW846 8260

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

Peak Number 5 1-Butanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.765	7.44 ug/l	139481	1,4-Difluorobenzene	8.553

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	78
2			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	42
3			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	38
4			Formic acid, butyl ester	102	C5H10O2	000592-84-7	9
5			Oxetane, 2,3,4-trimethyl-, (2.al...	100	C6H12O	032347-12-9	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010621\
Data File : VN065403.D
Acq On : 6 Jan 2021 16:28
Operator : JC/MD
Sample : M1022-05 50X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41098

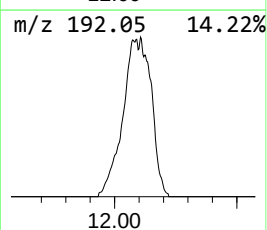
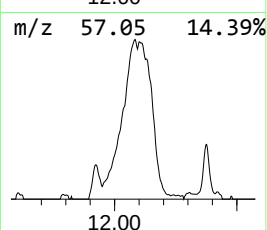
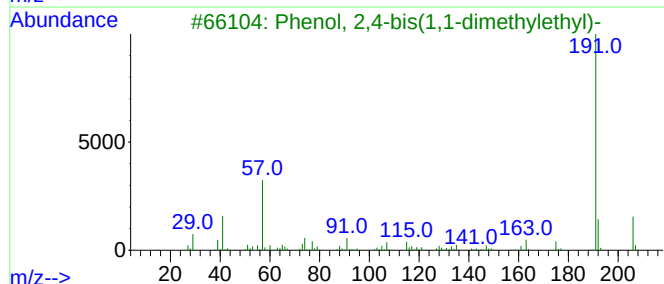
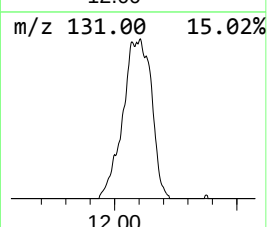
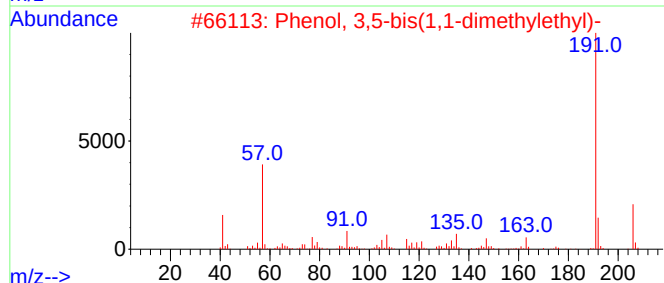
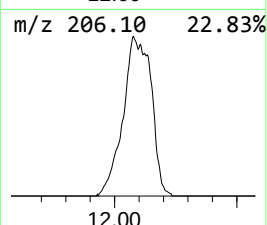
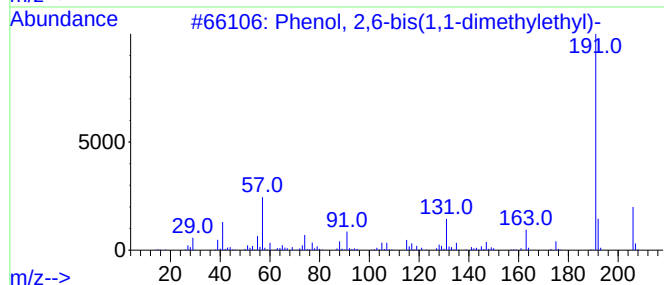
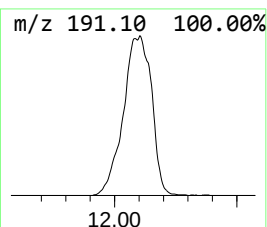
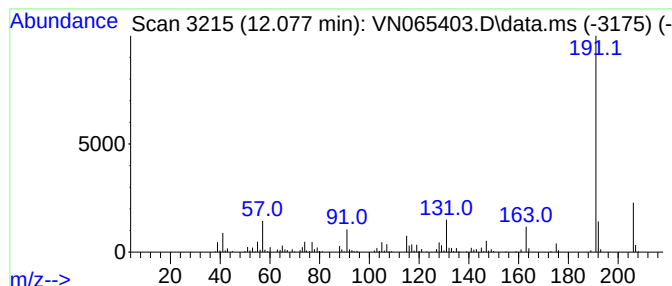
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Quant Title : SW846 8260

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

Peak Number 6 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.077	30.07 ug/l	779315	Chlorobenzene-d5	11.380

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	93
2			Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	81
3			Phenol, 2,4-bis(1,1-dimethylethyl)-	206	C14H22O	000096-76-4	80
4			Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	74
5			4'-Diethylaminoacetanilide	206	C12H18N2O	005326-57-8	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010621\
Data File : VN065403.D
Acq On : 6 Jan 2021 16:28
Operator : JC/MD
Sample : M1022-05 50X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41098

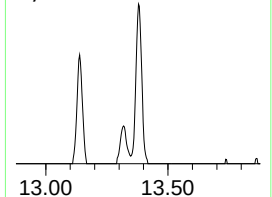
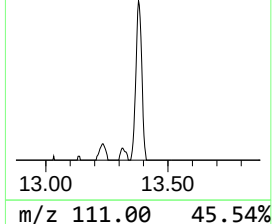
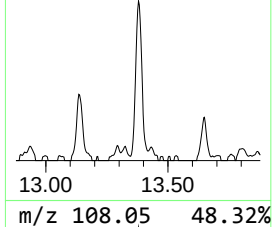
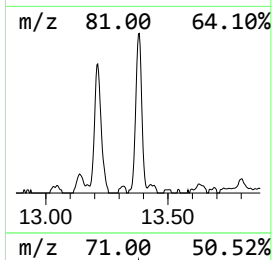
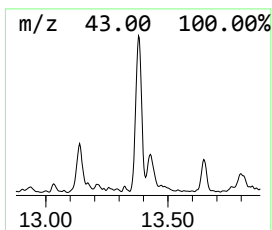
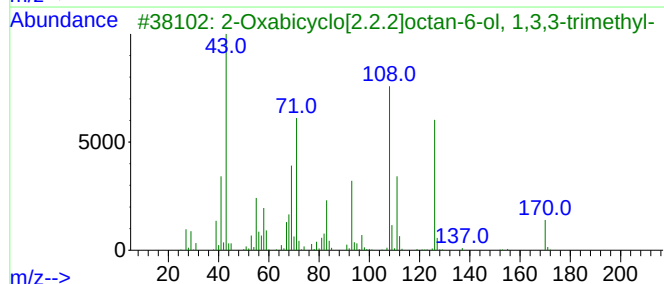
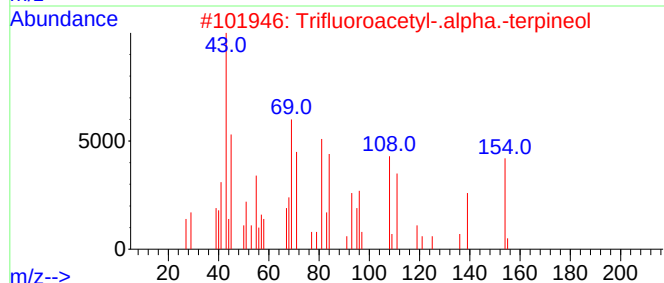
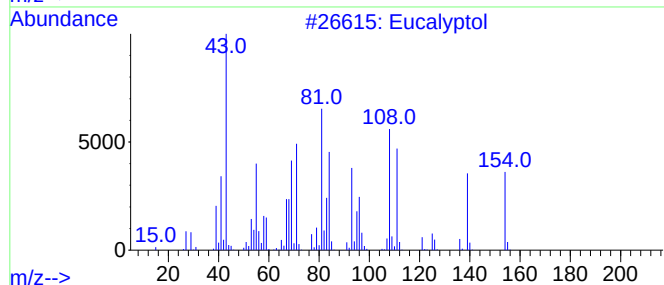
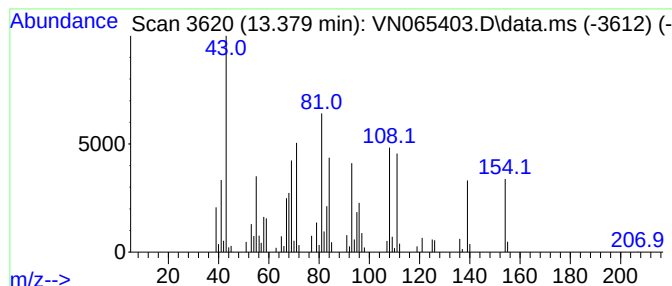
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Quant Title : SW846 8260

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

Peak Number 7 Eucalyptol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.379	9.46 ug/l	219184	1,4-Dichlorobenzene-d4	13.318

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	99
2			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	74
3			2-Oxabicyclo[2.2.2]octan-6-ol, 1...	170	C10H18O2	018679-48-6	35
4			2-Acetylcyclopentanone	126	C7H10O2	001670-46-8	27
5			2-Acetylcylohexanone	154	C9H14O2	006126-53-0	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010621\
Data File : VN065403.D
Acq On : 6 Jan 2021 16:28
Operator : JC/MD
Sample : M1022-05 50X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41098

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.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	2.306	104.1	ug/l	1387530	1	7.630	666521	50.0
Ethanol	3.258	88.4	ug/l	1177860	1	7.630	666521	50.0
Isopropyl Alcohol	4.052	27.9	ug/l	371512	1	7.630	666521	50.0
Butanal	6.508	10.2	ug/l	135338	1	7.630	666521	50.0
1-Butanol	8.765	7.4	ug/l	139481	2	8.553	937004	50.0
Phenol, 2,6-bis...	12.077	30.1	ug/l	779315	3	11.380	1296000	50.0
Eucalyptol	13.379	9.5	ug/l	219184	4	13.318	1158920	50.0