

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010621\
 Data File : VN065404.D
 Acq On : 6 Jan 2021 16:53
 Operator : JC/MD
 Sample : M1022-06 50X
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 41099

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: VN065404.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	163	176	203	rBV	838622	1418366	100.00%	11.405%
2	3.261	454	473	512	rBV	420577	1061705	74.85%	8.537%
3	3.672	587	601	615	rBV	13439	32566	2.30%	0.262%
4	3.791	620	638	667	rBV	318989	832850	58.72%	6.697%
5	4.052	700	719	745	rVB	124244	361340	25.48%	2.906%
6	6.029	1318	1334	1353	rBV7	8341	27617	1.95%	0.222%
7	6.508	1463	1483	1508	rBV2	40443	125343	8.84%	1.008%
8	6.804	1559	1575	1591	rBV2	7757	24208	1.71%	0.195%
9	6.897	1592	1604	1626	rVB2	10023	27350	1.93%	0.220%
10	7.553	1790	1808	1819	rBV	168901	417115	29.41%	3.354%
11	7.630	1820	1832	1857	rVB	277768	671501	47.34%	5.400%
12	7.804	1873	1886	1902	rVB2	8191	20111	1.42%	0.162%
13	7.991	1927	1944	1965	rBV	169793	399375	28.16%	3.211%
14	8.553	2102	2119	2148	rBV	451187	943694	66.53%	7.588%
15	8.765	2172	2185	2216	rBV	51770	124042	8.75%	0.997%
16	9.138	2289	2301	2315	rBV3	10048	21996	1.55%	0.177%
17	10.061	2571	2588	2601	rBV	733716	1361928	96.02%	10.952%
18	10.122	2601	2607	2622	rVB	32323	60145	4.24%	0.484%
19	10.830	2816	2827	2839	rBV7	12160	25322	1.79%	0.204%
20	11.379	2983	2998	3025	rBV	732122	1299365	91.61%	10.448%
21	11.794	3108	3127	3143	rBV7	6188	19870	1.40%	0.160%
22	11.923	3158	3167	3178	rBV	17711	28725	2.03%	0.231%
23	12.376	3291	3308	3331	rBV	603936	1050044	74.03%	8.444%
24	12.701	3401	3409	3421	rVB3	11523	18804	1.33%	0.151%
25	13.035	3501	3513	3527	rVB4	25813	48914	3.45%	0.393%
26	13.138	3531	3545	3554	rBV5	35309	65612	4.63%	0.528%
27	13.228	3559	3573	3579	rVV5	61959	154308	10.88%	1.241%
28	13.260	3579	3583	3590	rVV	55924	78678	5.55%	0.633%
29	13.318	3590	3601	3612	rVV	639093	1118808	78.88%	8.997%
30	13.379	3612	3620	3629	rVV	127014	214798	15.14%	1.727%
31	13.428	3629	3635	3645	rVB	28621	46365	3.27%	0.373%
32	13.646	3694	3703	3711	rVB3	17236	25380	1.79%	0.204%
33	13.765	3731	3740	3745	rBV5	17381	27801	1.96%	0.224%
34	13.801	3745	3751	3764	rVB7	21576	39713	2.80%	0.319%
35	14.039	3815	3825	3835	rBV7	8543	16065	1.13%	0.129%
36	14.498	3961	3968	3978	rVB	25664	35175	2.48%	0.283%

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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	14.563	3979	3988	3995	rBV8	10630	19019	1.34%	0.153%
38	14.617	3996	4005	4013	rBV2	34998	58300	4.11%	0.469%
39	14.820	4059	4068	4077	rBV6	17968	29417	2.07%	0.237%
40	15.084	4141	4150	4160	rBV7	12460	25990	1.83%	0.209%
41	15.299	4209	4217	4233	rVB3	22866	36695	2.59%	0.295%
42	16.190	4487	4494	4506	rVB3	13126	21567	1.52%	0.173%

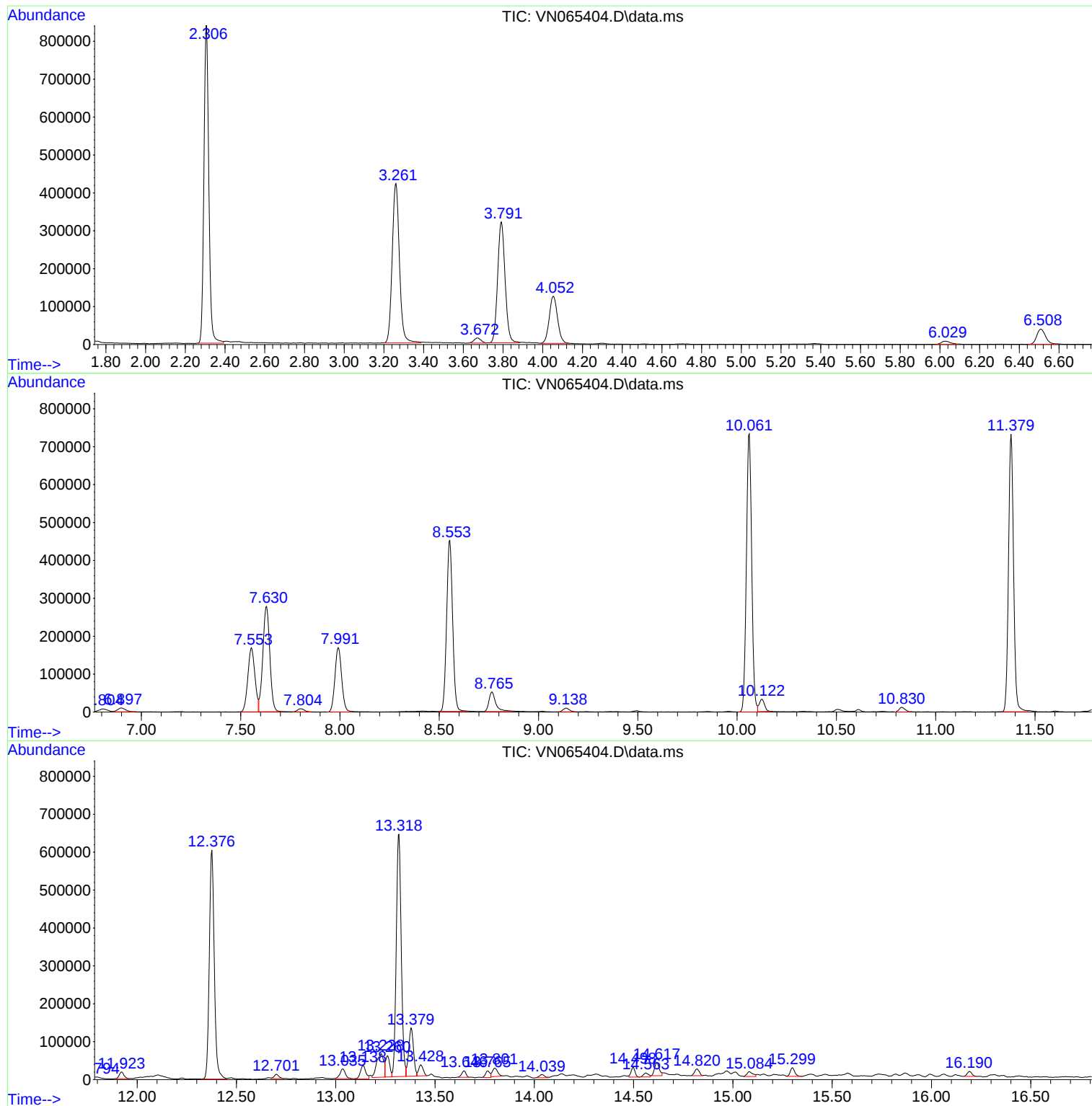
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

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



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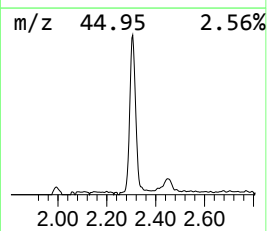
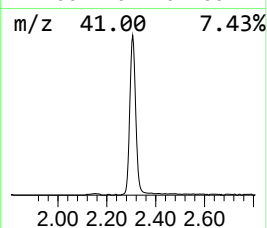
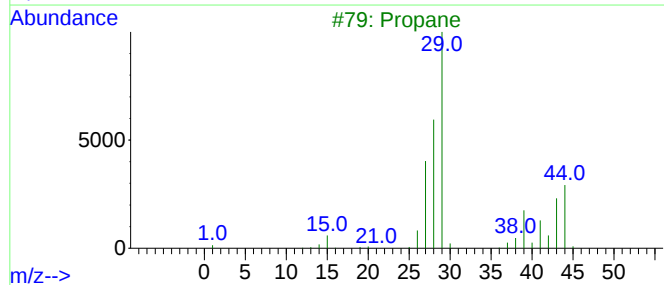
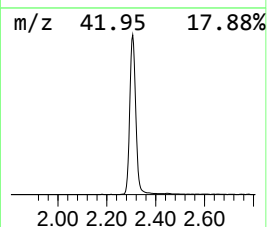
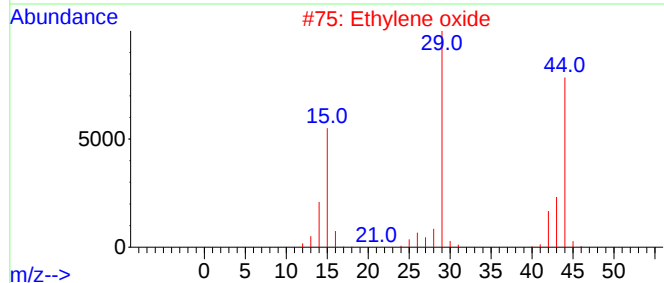
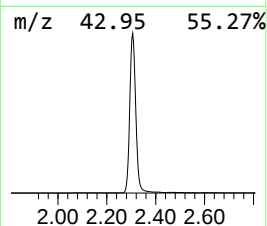
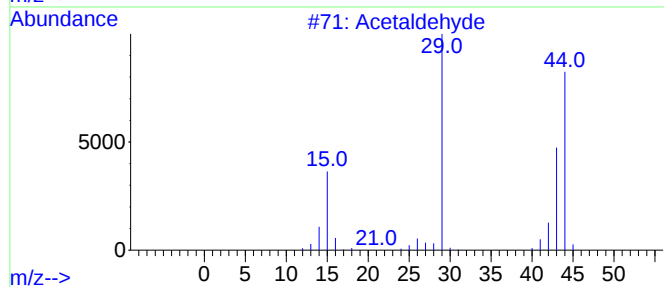
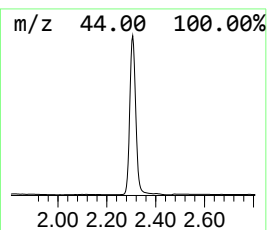
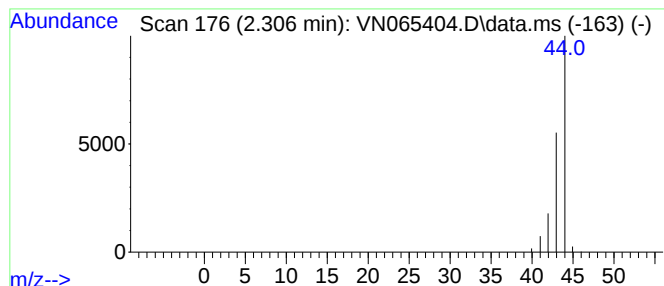
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

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	105.61 ug/l	1418370	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 : 18 Sample Multiplier: 1

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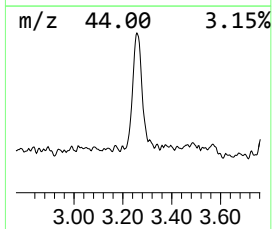
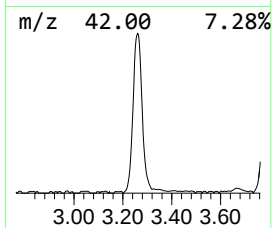
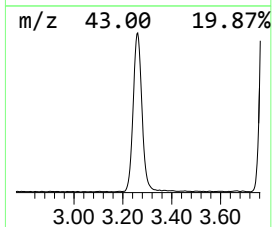
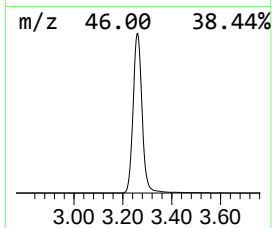
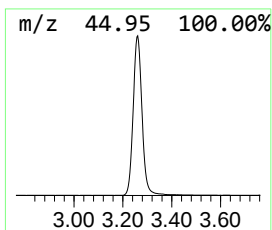
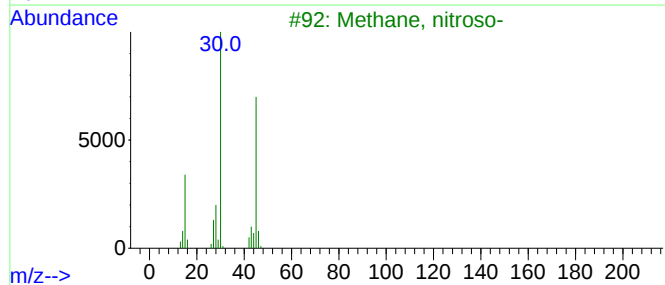
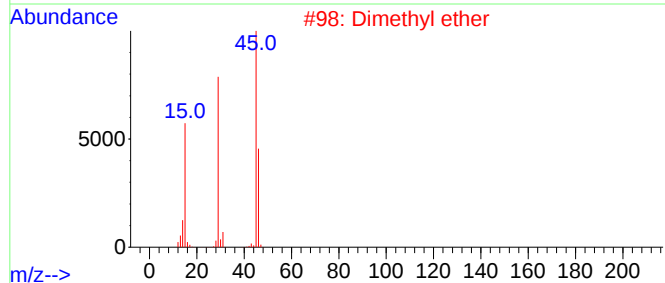
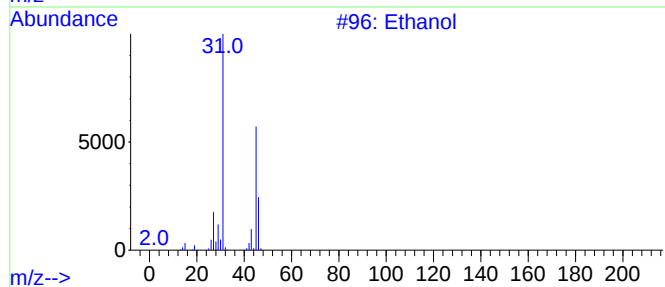
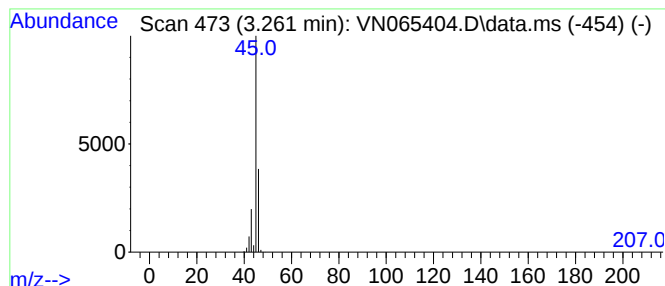
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N12220W.M
Quant Title : SW846 8260

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.
3.261	79.05 ug/l	1061710	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			Formic acid	46	CH2O2	000064-18-6	4
5			Methyltartronic acid	134	C4H6O5	000595-98-2	2



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

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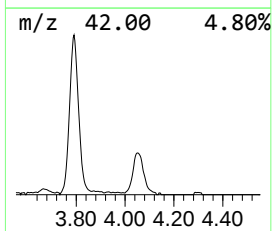
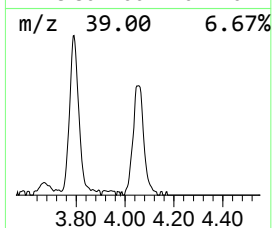
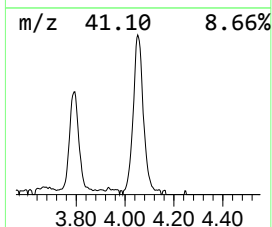
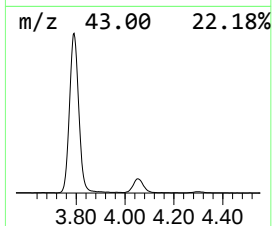
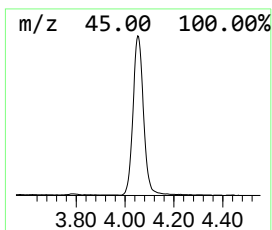
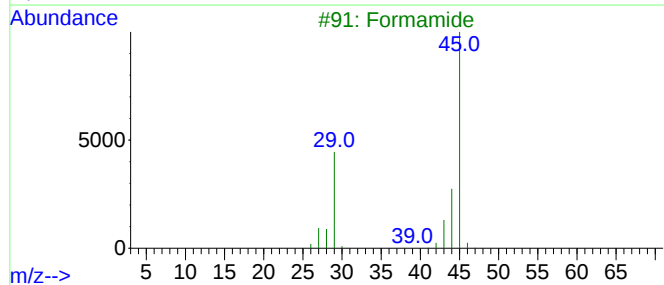
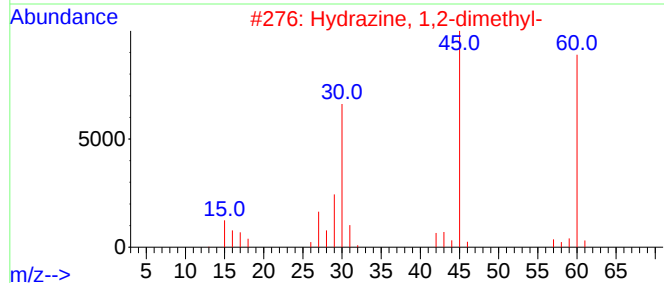
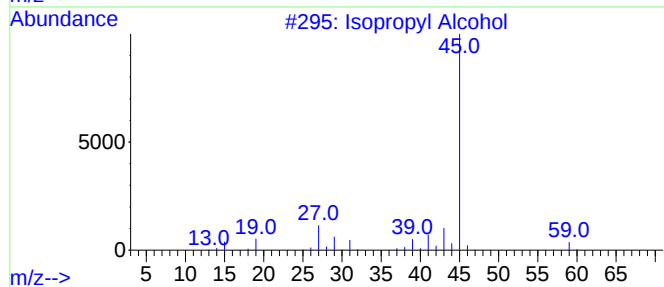
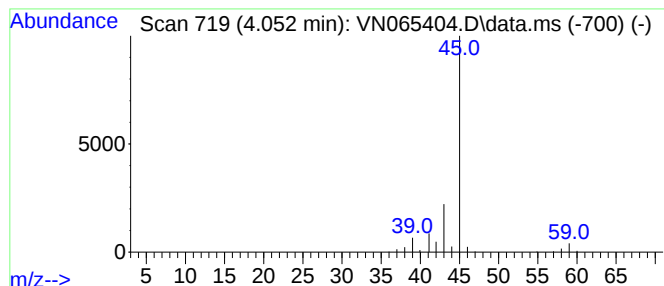
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

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

Peak Number 3 Isopropyl Alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.052	26.91 ug/l	361340	Pentafluorobenzene	7.630

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
3			Formamide	45	CH3NO	000075-12-7	5
4			Acetic acid, methoxy-	90	C3H6O3	000625-45-6	4
5			1-Butene, 4-methoxy	86	C5H10O	004696-30-4	4



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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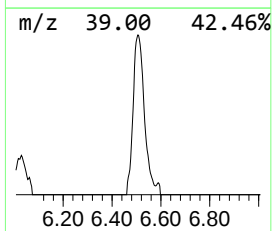
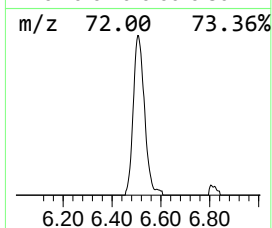
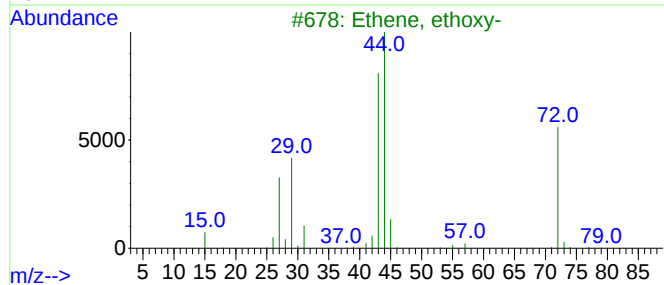
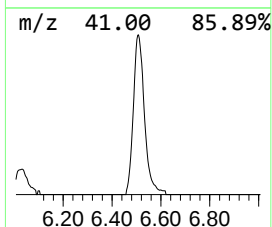
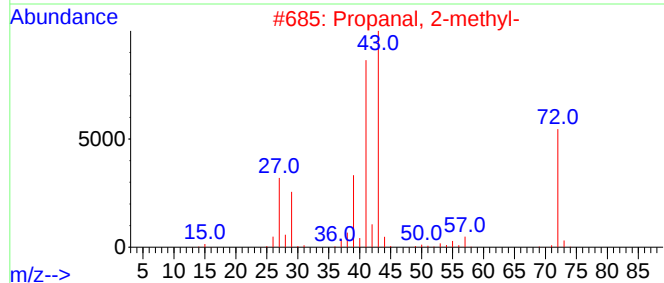
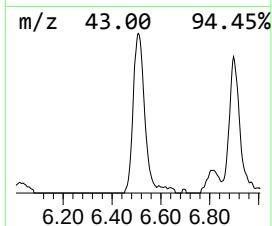
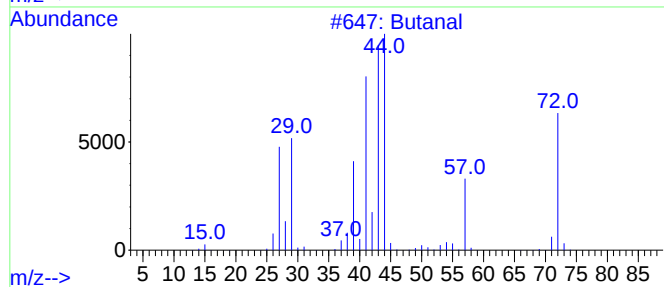
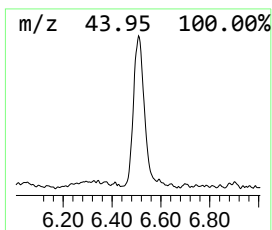
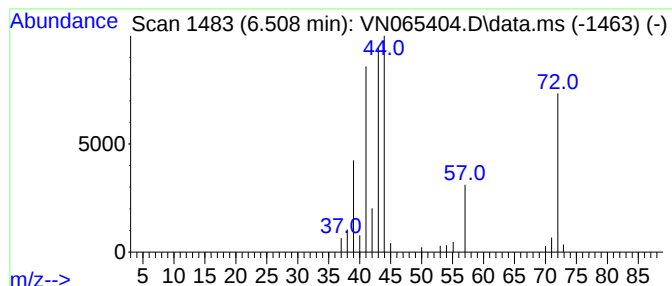
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Quant Title : SW846 8260

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

Peak Number 4 Butanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.508	9.33 ug/l	125343	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	52
3			Ethene, ethoxy-	72	C4H8O	000109-92-2	40
4			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37
5			Isobutylene epoxide	72	C4H8O	000558-30-5	27



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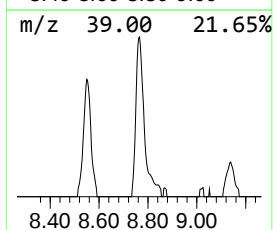
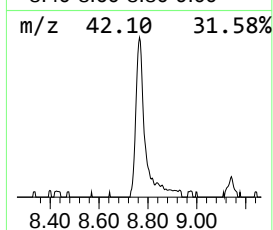
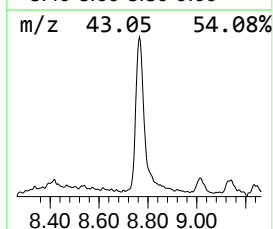
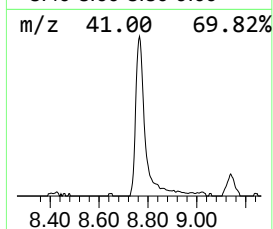
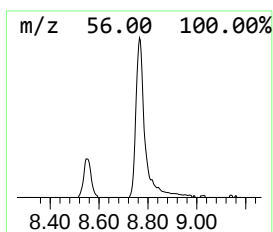
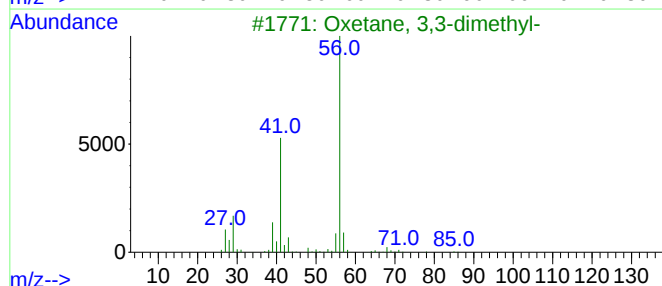
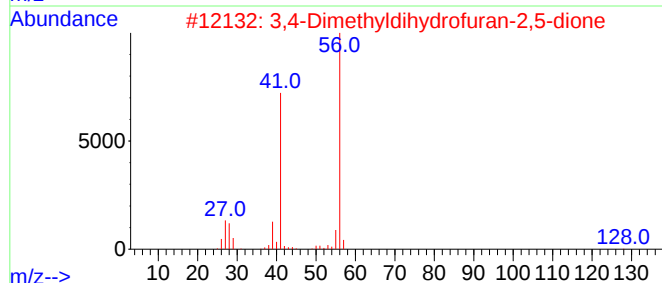
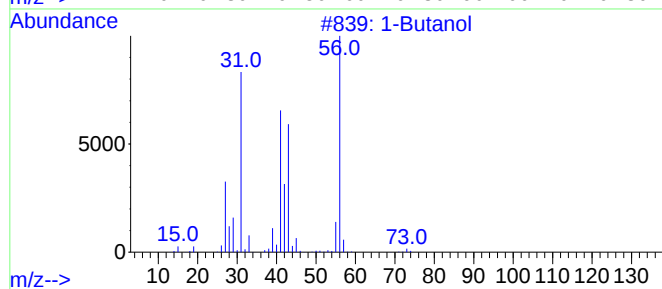
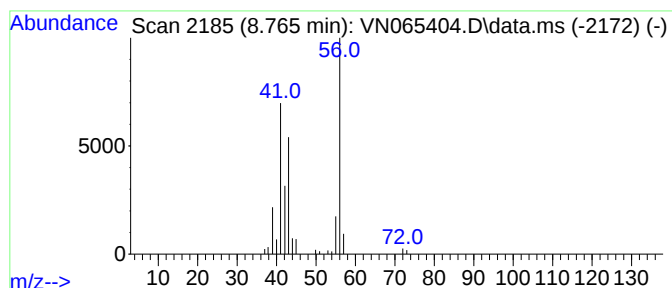
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

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

Peak Number 5 1-Butanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.765	6.57 ug/l	124042	1,4-Difluorobenzene	8.553

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	83
2			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	40
3			Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	36
4			1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	9
5			Butane, 1-chloro-	92	C4H9Cl	000109-69-3	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010621\
Data File : VN065404.D
Acq On : 6 Jan 2021 16:53
Operator : JC/MD
Sample : M1022-06 50X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41099

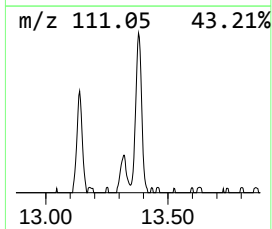
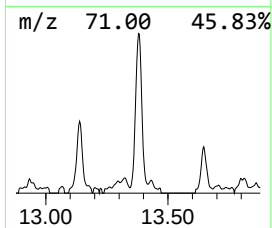
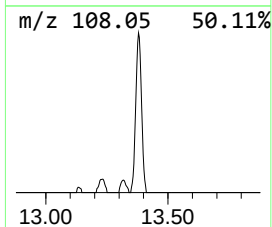
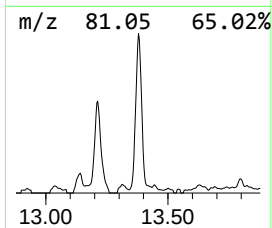
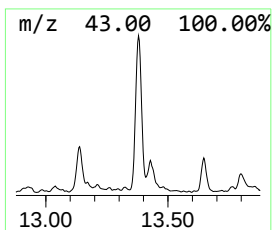
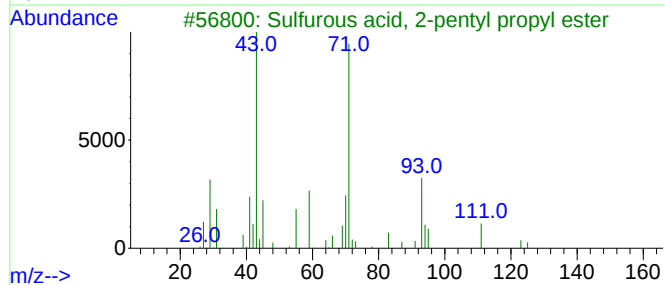
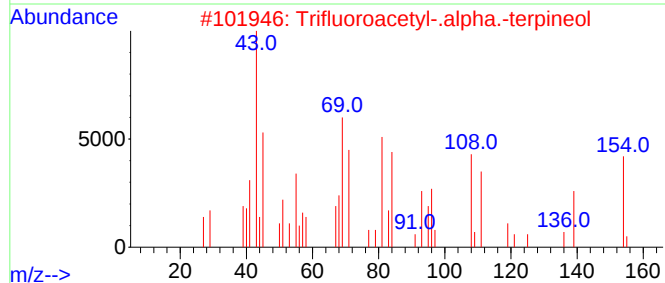
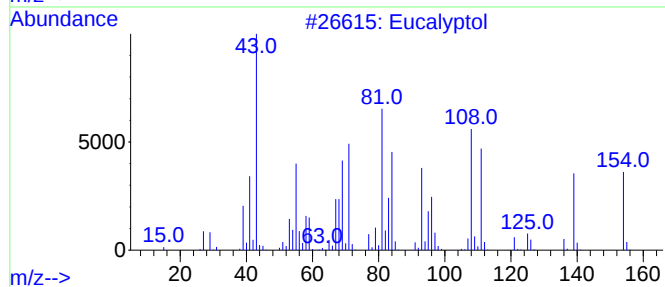
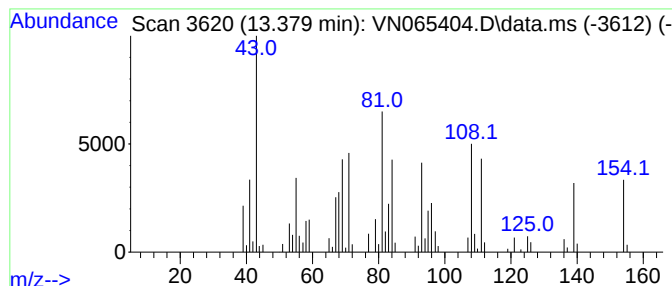
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Quant Title : SW846 8260

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

Peak Number 6 Eucalyptol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.379	9.60 ug/l	214798	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	80
3			Sulfurous acid, 2-pentyl propyl ...	194	C8H18O3S	1000309-15-1	22
4			trans-Cyclohexane-1,4-dimethanol...	228	C12H20O4	010412-78-9	22
5			3-Hepten-2-one, 3-propyl-	154	C10H18O	032064-69-0	15



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010621\
Data File : VN065404.D
Acq On : 6 Jan 2021 16:53
Operator : JC/MD
Sample : M1022-06 50X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41099

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	105.6	ug/l	1418370	1	7.630	671501	50.0
Ethanol	3.261	79.0	ug/l	1061710	1	7.630	671501	50.0
Isopropyl Alcohol	4.052	26.9	ug/l	361340	1	7.630	671501	50.0
Butanal	6.508	9.3	ug/l	125343	1	7.630	671501	50.0
1-Butanol	8.765	6.6	ug/l	124042	2	8.553	943694	50.0
Eucalyptol	13.379	9.6	ug/l	214798	4	13.318	1118810	50.0