

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011121\
 Data File : VN065469.D
 Acq On : 11 Jan 2021 15:40
 Operator : JC/MD
 Sample : M1040-04 50X
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 41661

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: VN065469.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	198	rBV	347642	596257	15.33%	3.566%
2	3.261	456	473	498	rBV	48954	129409	3.33%	0.774%
3	7.553	1787	1808	1819	rBV2	140619	351864	9.05%	2.104%
4	7.627	1819	1831	1853	rVB	244812	599725	15.42%	3.587%
5	8.000	1926	1947	1977	rBV3	417933	1074976	27.65%	6.429%
6	8.553	2104	2119	2148	rBV	368906	774303	19.91%	4.631%
7	10.061	2572	2588	2597	rBV	608756	1114881	28.67%	6.668%
8	10.126	2597	2608	2641	rVB	2145886	3888266	100.00%	23.254%
9	10.820	2808	2824	2851	rBV2	24395	119838	3.08%	0.717%
10	11.380	2984	2998	3017	rBV	614196	1078961	27.75%	6.453%
11	11.482	3019	3030	3047	rVB	223800	380158	9.78%	2.274%
12	11.592	3049	3064	3087	rBV	695324	1314721	33.81%	7.863%
13	11.920	3147	3166	3183	rBV	399203	668301	17.19%	3.997%
14	12.376	3295	3308	3333	rVB	519357	908141	23.36%	5.431%
15	12.566	3353	3367	3376	rBV	33648	54261	1.40%	0.325%
16	12.627	3376	3386	3393	rBV	149431	246593	6.34%	1.475%
17	12.704	3403	3410	3421	rVB2	110038	173617	4.47%	1.038%
18	12.865	3445	3460	3471	rBV	76132	132950	3.42%	0.795%
19	13.013	3493	3506	3519	rBV	279702	446354	11.48%	2.669%
20	13.318	3588	3601	3620	rVB2	590558	1163867	29.93%	6.961%
21	13.518	3646	3663	3670	rBV2	106779	192446	4.95%	1.151%
22	13.556	3671	3675	3692	rVB4	38135	69957	1.80%	0.418%
23	13.646	3692	3703	3711	rBV	75687	118184	3.04%	0.707%
24	13.807	3748	3753	3762	rVV2	28771	41668	1.07%	0.249%
25	13.862	3762	3770	3779	rVB2	37716	54063	1.39%	0.323%
26	13.968	3794	3803	3814	rVB	47634	75251	1.94%	0.450%
27	14.222	3876	3882	3891	rVB	32755	50955	1.31%	0.305%
28	14.450	3945	3953	3960	rBV	30494	47964	1.23%	0.287%
29	14.498	3960	3968	3977	rVV	77341	106799	2.75%	0.639%
30	14.566	3977	3989	3998	rVV3	84026	166658	4.29%	0.997%
31	14.614	3998	4004	4017	rVB3	29071	51504	1.32%	0.308%
32	14.714	4025	4035	4051	rVB2	57673	102522	2.64%	0.613%
33	14.817	4054	4067	4075	rBV4	19615	42350	1.09%	0.253%
34	14.929	4091	4102	4112	rBV3	22070	46467	1.20%	0.278%
35	15.090	4141	4152	4165	rBV4	26959	75144	1.93%	0.449%
36	15.302	4210	4218	4231	rVB	56948	92145	2.37%	0.551%

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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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37	15.579	4298	4304	4317	rVB2	38229	67593	1.74%	0.404%
38	15.875	4384	4396	4406	rBV4	27271	57912	1.49%	0.346%
39	16.193	4485	4495	4505	rVB2	25596	43684	1.12%	0.261%

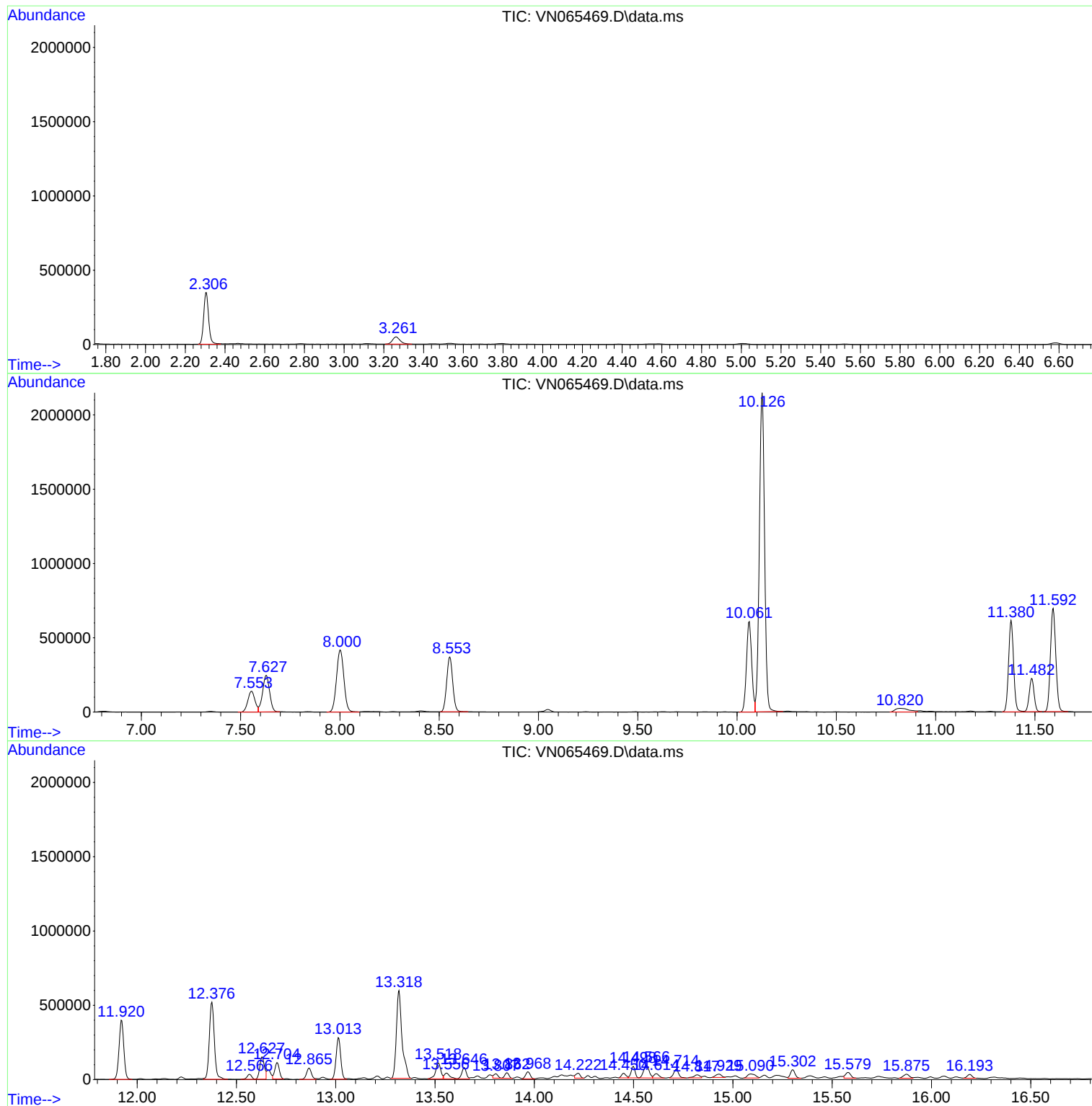
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Quant Title : SW846 8260

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



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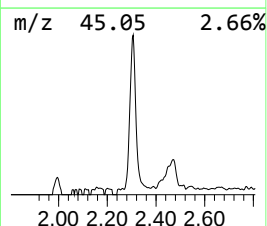
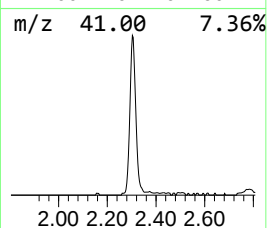
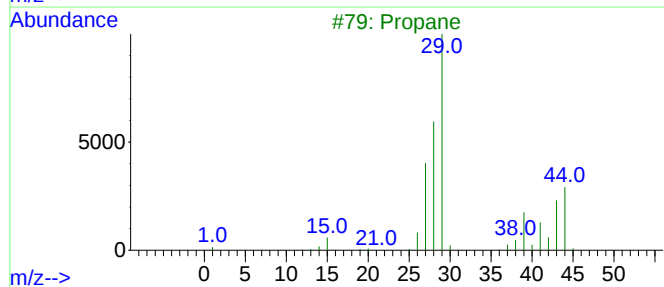
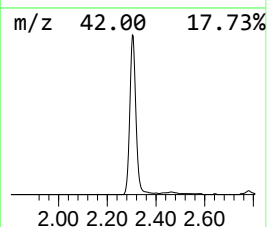
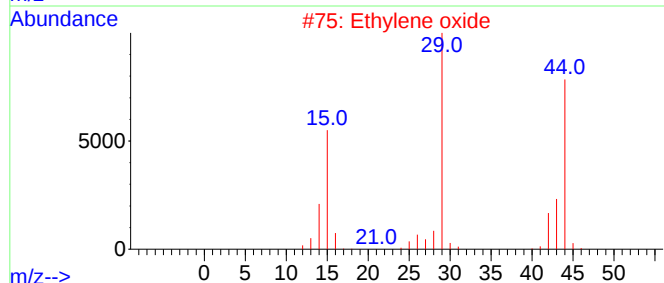
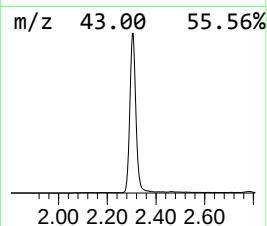
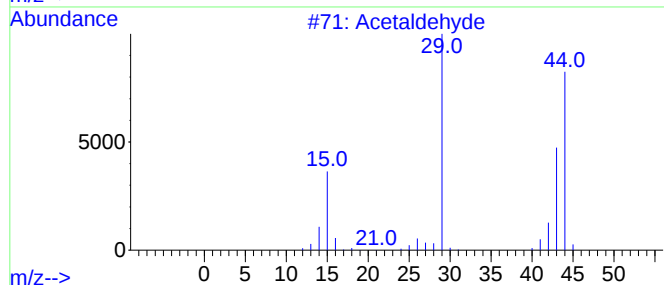
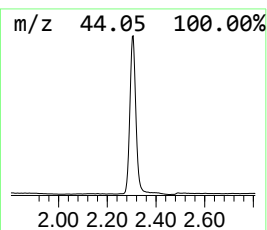
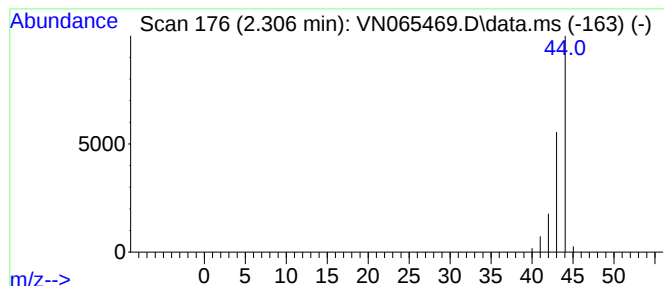
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

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	49.71 ug/l	596257	Pentafluorobenzene	7.631

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			1,2-Propanediamine	74	C3H10N2	000078-90-0	4



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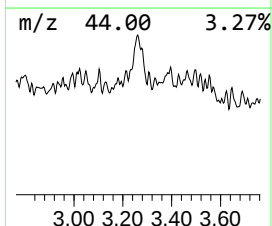
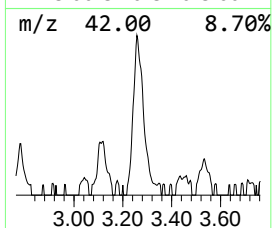
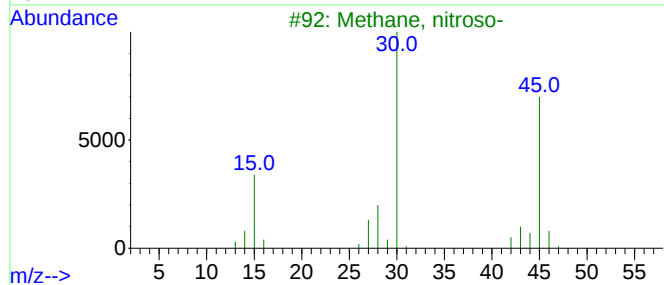
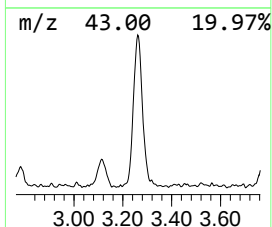
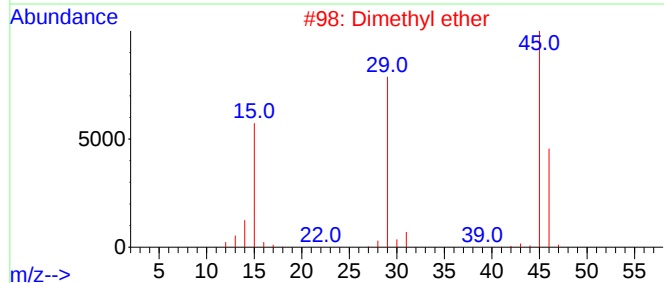
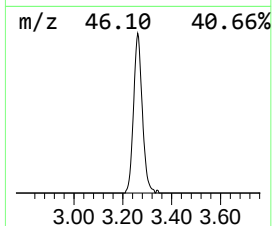
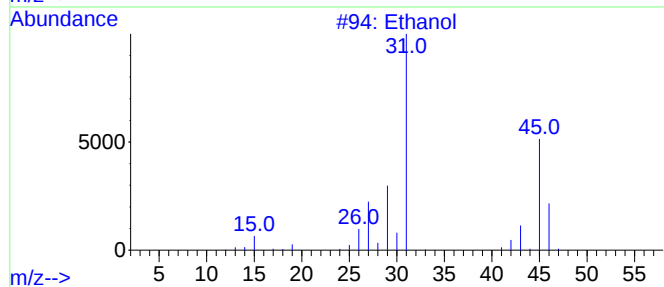
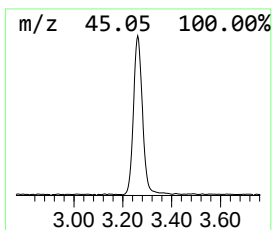
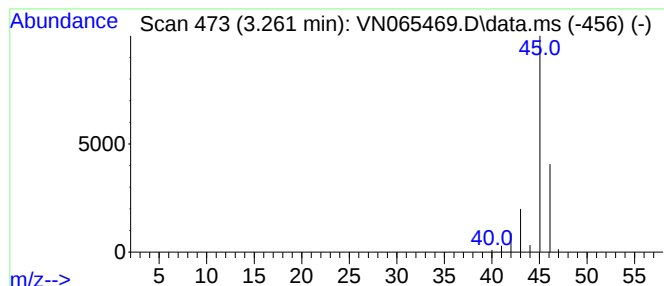
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.261	10.79 ug/l	129409	Pentafluorobenzene	7.631

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	90
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 : 13 Sample Multiplier: 1

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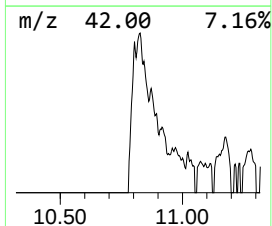
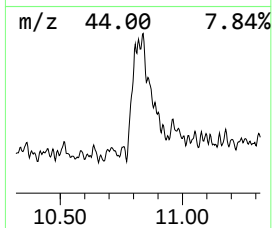
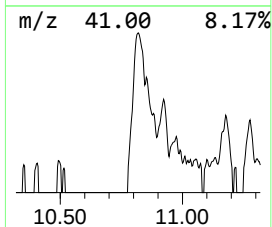
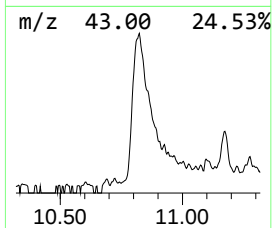
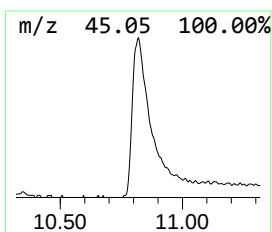
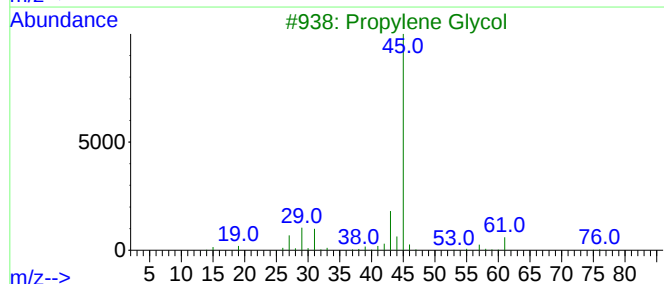
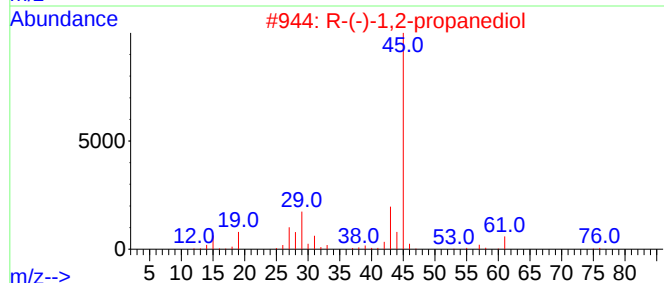
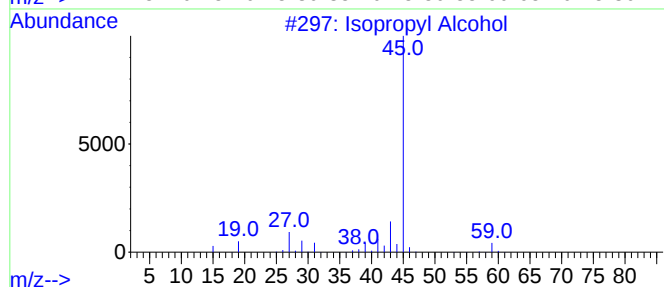
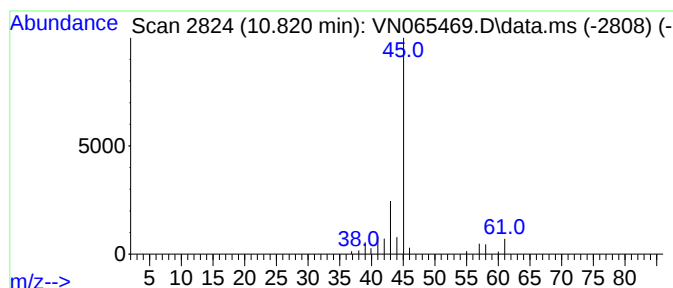
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Quant Title : SW846 8260

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

Peak Number 3 Isopropyl Alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.820	5.55 ug/l	119838	Chlorobenzene-d5	11.380

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isopropyl Alcohol	60	C3H8O	000067-63-0	50
2		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	40
3		Propylene Glycol	76	C3H8O2	000057-55-6	9
4		Methane, nitroso-	45	CH3NO	000865-40-7	4
5		Formamide	45	CH3NO	000075-12-7	4



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ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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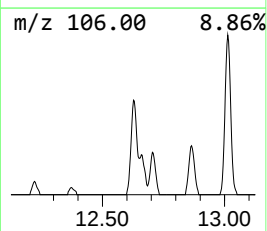
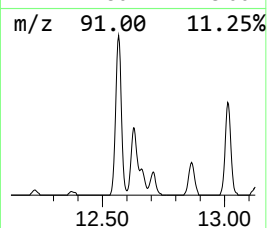
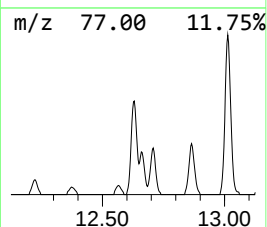
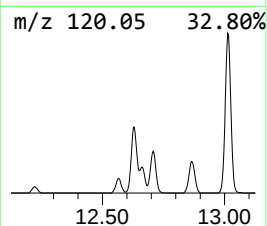
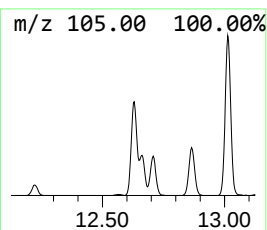
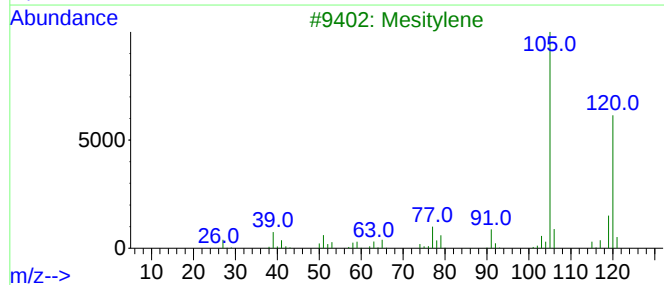
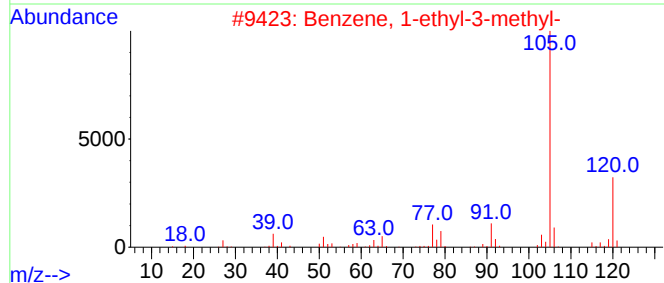
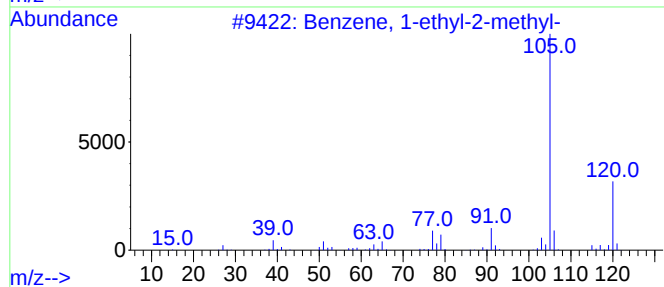
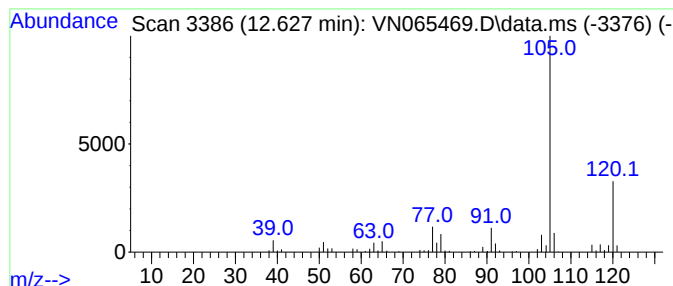
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Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.627	10.59 ug/l	246593	1,4-Dichlorobenzene-d4	13.318

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



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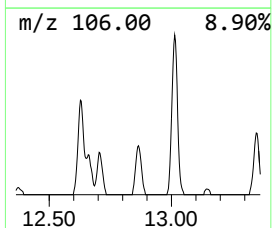
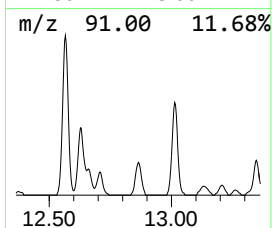
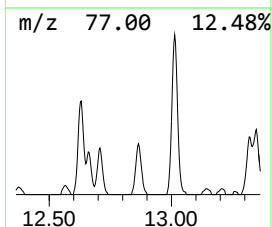
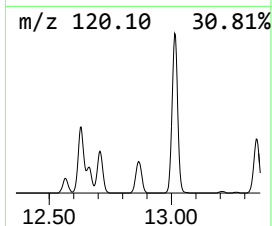
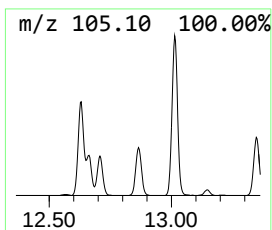
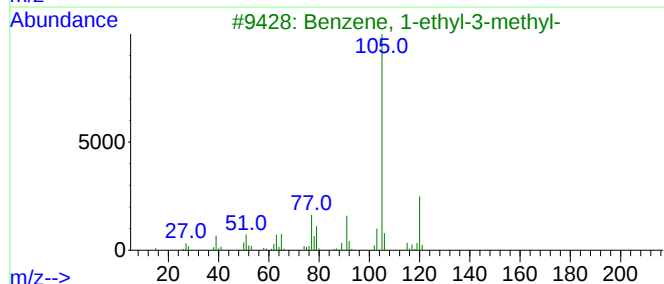
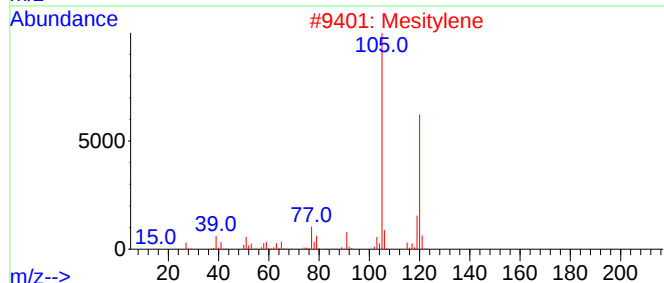
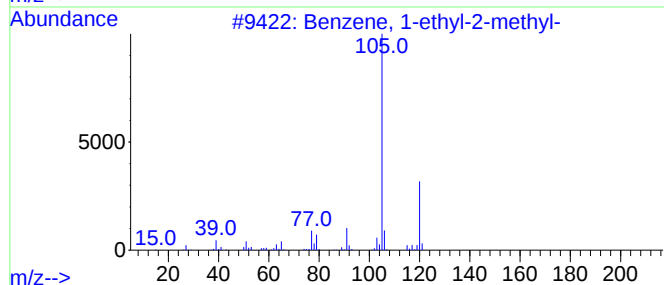
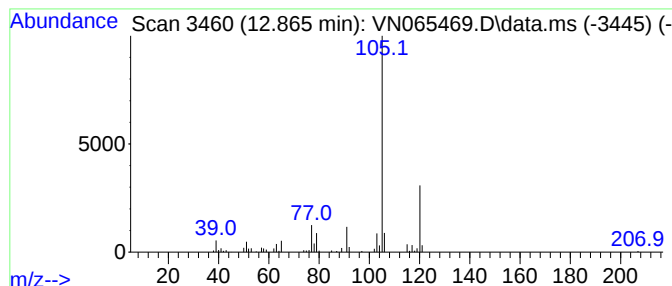
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Quant Title : SW846 8260

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

Peak Number 5 Mesitylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.865	5.71 ug/l	132950	1,4-Dichlorobenzene-d4	13.318

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Mesitylene	120	C9H12	000108-67-8	90
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011121\
Data File : VN065469.D
Acq On : 11 Jan 2021 15:40
Operator : JC/MD
Sample : M1040-04 50X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41661

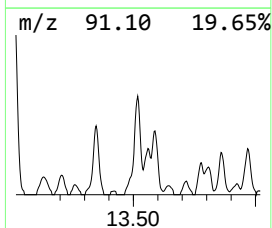
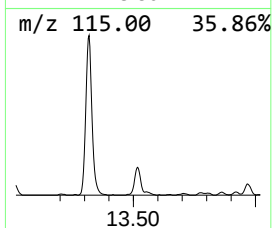
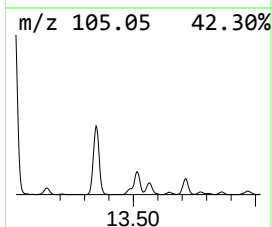
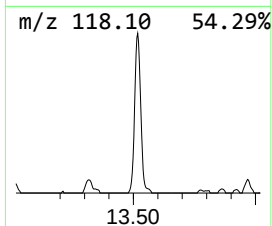
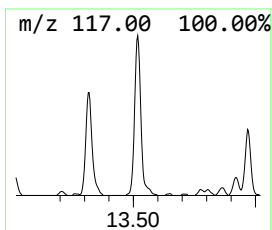
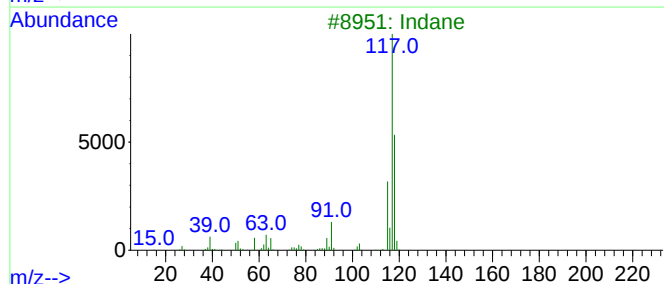
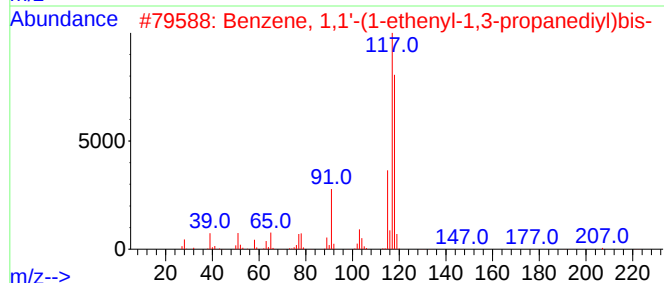
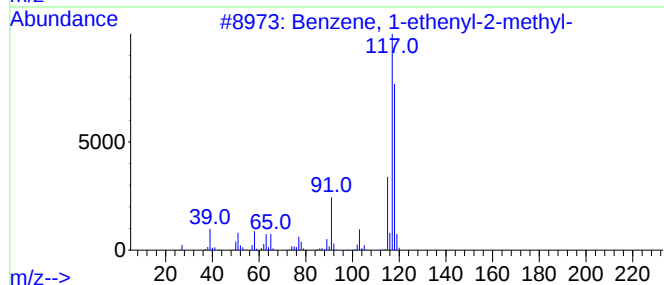
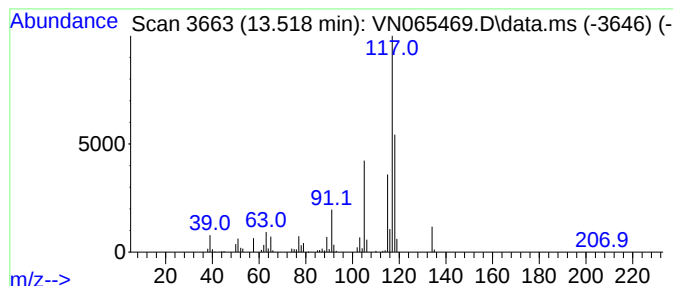
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-ethenyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.518	8.27 ug/l	192446	1,4-Dichlorobenzene-d4	13.318

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	94
2			Benzene, 1,1'-(1-ethenyl-1,3-pro...	222	C17H18	061141-97-7	80
3			Indane	118	C9H10	000496-11-7	76
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
5			Benzene, 2-propenyl-	118	C9H10	000300-57-2	76



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011121\
Data File : VN065469.D
Acq On : 11 Jan 2021 15:40
Operator : JC/MD
Sample : M1040-04 50X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41661

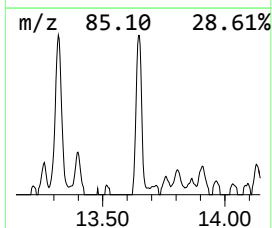
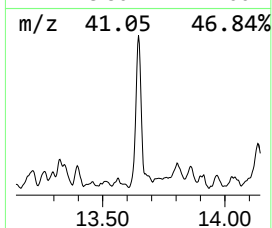
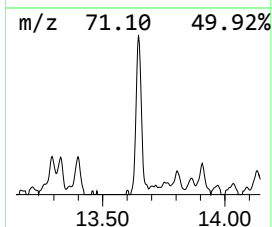
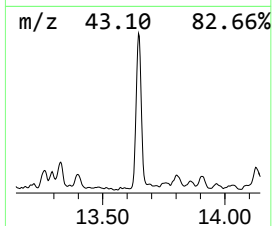
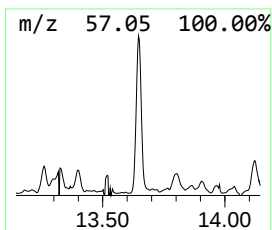
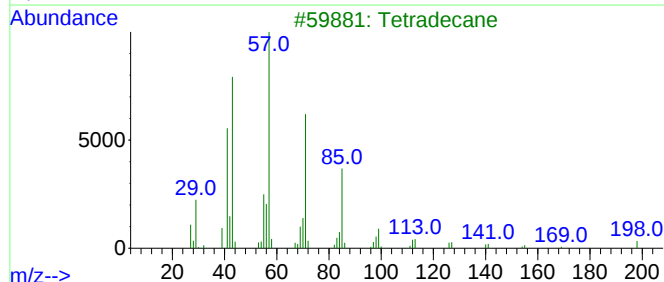
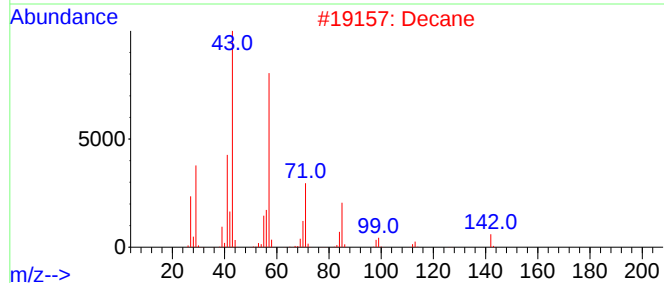
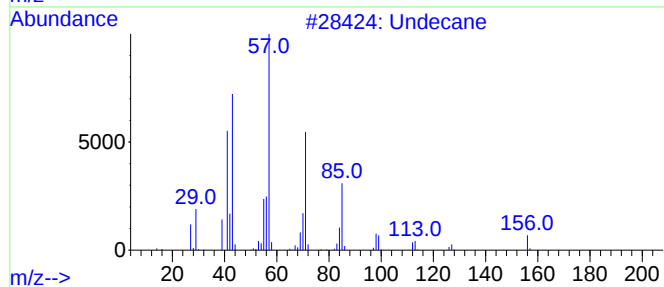
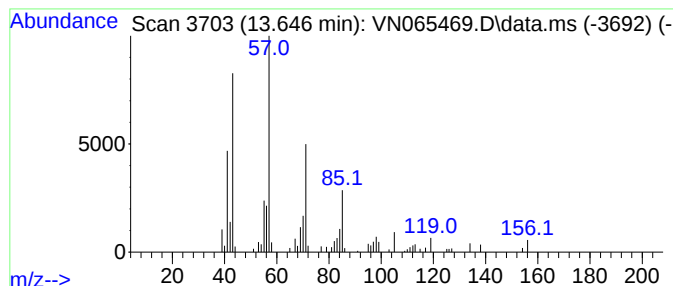
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

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

Peak Number 7 Undecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.646	5.08 ug/l	118184	1,4-Dichlorobenzene-d4	13.318

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	93
2	Decane			142	C10H22	000124-18-5	72
3	Tetradecane			198	C14H30	000629-59-4	64
4	Heptane, 2,6-dimethyl-			128	C9H20	001072-05-5	59
5	Hexadecane			226	C16H34	000544-76-3	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011121\
Data File : VN065469.D
Acq On : 11 Jan 2021 15:40
Operator : JC/MD
Sample : M1040-04 50X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41661

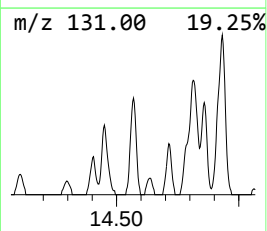
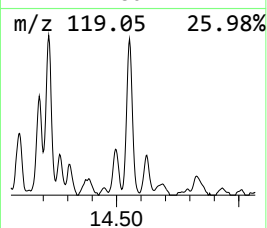
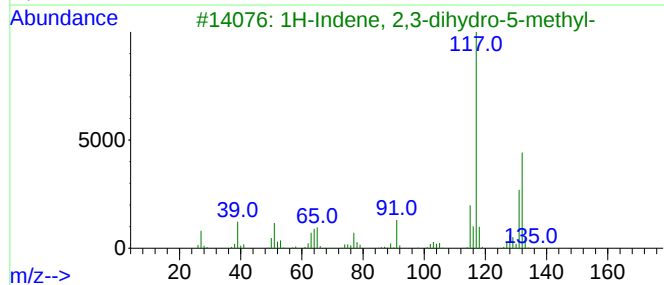
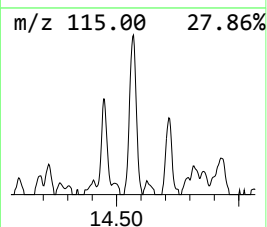
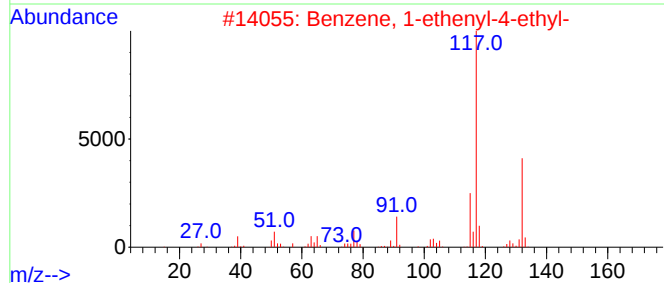
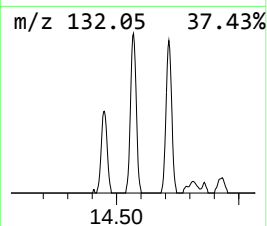
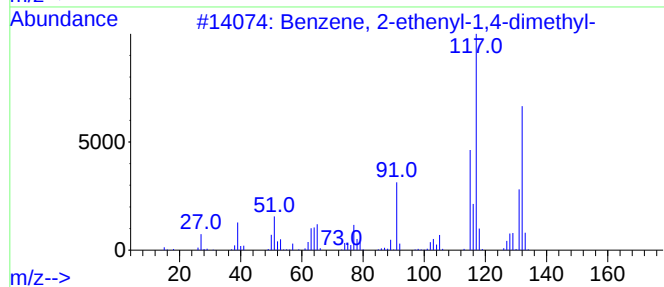
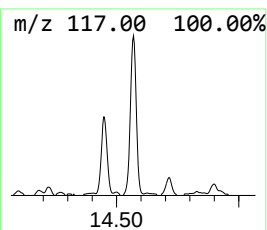
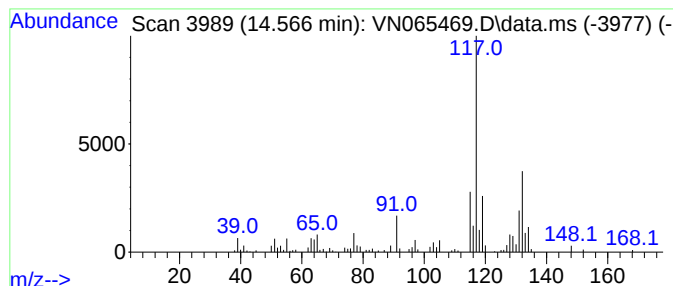
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

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

Peak Number 8 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.566	7.16 ug/l	166658	1,4-Dichlorobenzene-d4	13.318

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
2			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	86
3			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	76
4			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	76
5			3-Phenylbut-1-ene	132	C10H12	000934-10-1	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011121\
Data File : VN065469.D
Acq On : 11 Jan 2021 15:40
Operator : JC/MD
Sample : M1040-04 50X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41661

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	49.7	ug/l	596257	1	7.631	599725	50.0
Ethanol	3.261	10.8	ug/l	129409	1	7.631	599725	50.0
Isopropyl Alcohol	10.820	5.5	ug/l	119838	3	11.380	1078960	50.0
Benzene, 1-ethy...	12.627	10.6	ug/l	246593	4	13.318	1163870	50.0
Mesitylene	12.865	5.7	ug/l	132950	4	13.318	1163870	50.0
Benzene, 1-ethe...	13.518	8.3	ug/l	192446	4	13.318	1163870	50.0
Undecane	13.646	5.1	ug/l	118184	4	13.318	1163870	50.0
Benzene, 2-ethe...	14.566	7.2	ug/l	166658	4	13.318	1163870	50.0