

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102021\
 Data File : VN069074.D
 Acq On : 20 Oct 2021 20:23
 Operator : JC/MD
 Sample : M4253-07
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 133-134

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\82N101221W.M
 Title : SW846 8260

Signal : TIC: VN069074.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.260	85	101	113	rBV3	13428	24745	1.16%	0.130%
2	2.443	159	169	183	rVB	27393	43283	2.04%	0.227%
3	3.140	411	429	449	rBV	99358	223392	10.51%	1.171%
4	3.524	554	572	595	rVB4	16440	51610	2.43%	0.271%
5	5.090	1130	1156	1165	rBV4	8151	26578	1.25%	0.139%
6	5.618	1319	1353	1394	rBV2	590454	2126019	100.00%	11.144%
7	7.152	1899	1925	1947	rBV3	63863	184690	8.69%	0.968%
8	8.027	2228	2251	2261	rBV2	223988	532366	25.04%	2.791%
9	8.091	2262	2275	2298	rVB3	493787	1165524	54.82%	6.109%
10	8.442	2386	2406	2432	rBV	241643	563767	26.52%	2.955%
11	8.641	2439	2480	2492	rBV10	62253	309460	14.56%	1.622%
12	8.971	2584	2603	2629	rBV	647852	1329965	62.56%	6.971%
13	9.462	2758	2786	2802	rBV2	78259	198836	9.35%	1.042%
14	9.888	2931	2945	2957	rVB4	10910	22475	1.06%	0.118%
15	9.974	2964	2977	2985	rBV2	18746	35988	1.69%	0.189%
16	10.019	2986	2994	3011	rVB3	20406	39036	1.84%	0.205%
17	10.325	3097	3108	3120	rBV5	12232	22873	1.08%	0.120%
18	10.443	3134	3152	3184	rBV	989465	1874138	88.15%	9.824%
19	10.870	3296	3311	3328	rVB5	11571	28582	1.34%	0.150%
20	11.747	3619	3638	3665	rBV	916849	1654366	77.82%	8.672%
21	11.961	3700	3718	3743	rVB	185717	341471	16.06%	1.790%
22	12.283	3818	3838	3860	rVB	307733	523900	24.64%	2.746%
23	12.734	3988	4006	4030	rBV	699983	1226322	57.68%	6.428%
24	12.986	4086	4100	4105	rBV	94274	149708	7.04%	0.785%
25	13.018	4106	4112	4119	rVV2	138676	217206	10.22%	1.139%
26	13.061	4119	4128	4149	rVB	390852	642403	30.22%	3.367%
27	13.224	4168	4189	4208	rBV	533661	904967	42.57%	4.744%
28	13.560	4303	4314	4326	rVB2	24783	37955	1.79%	0.199%
29	13.678	4341	4358	4364	rBV	814684	1447594	68.09%	7.588%
30	13.841	4404	4419	4423	rBV2	57350	85254	4.01%	0.447%
31	13.879	4423	4433	4439	rBV	176253	279809	13.16%	1.467%
32	14.005	4467	4480	4492	rBV2	26846	42133	1.98%	0.221%
33	14.072	4492	4505	4516	rBV2	54078	83615	3.93%	0.438%
34	14.160	4518	4538	4548	rBV2	34763	71541	3.37%	0.375%
35	14.219	4548	4560	4573	rVB2	167031	259202	12.19%	1.359%
36	14.281	4573	4583	4589	rBV3	22418	33477	1.57%	0.175%

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37	14.329	4589	4601	4615	rVB3	173303	288398	13.57%	1.512%
38	14.461	4638	4650	4663	rVB2	84027	134375	6.32%	0.704%
39	14.541	4664	4680	4687	rVV	127264	207742	9.77%	1.089%
40	14.581	4687	4695	4705	rVV	142506	229570	10.80%	1.203%
41	14.624	4705	4711	4719	rVV2	30764	46327	2.18%	0.243%
42	14.662	4719	4725	4743	rVB7	19450	33226	1.56%	0.174%
43	14.766	4746	4764	4771	rBV6	15145	26924	1.27%	0.141%
44	14.812	4771	4781	4791	rVV4	49935	89430	4.21%	0.469%
45	14.933	4807	4826	4840	rBV5	286639	599262	28.19%	3.141%
46	14.997	4841	4850	4861	rVB6	17339	34647	1.63%	0.182%
47	15.086	4871	4883	4903	rBV3	47011	89318	4.20%	0.468%
48	15.201	4904	4926	4935	rBV4	58684	134289	6.32%	0.704%
49	15.314	4953	4968	4985	rVB5	69092	163937	7.71%	0.859%
50	15.810	5136	5153	5168	rBV3	17690	35275	1.66%	0.185%
51	15.987	5201	5219	5230	rBV3	22459	56836	2.67%	0.298%
52	16.113	5254	5266	5277	rBV2	12073	22295	1.05%	0.117%
53	16.193	5281	5296	5321	rVB6	15575	44863	2.11%	0.235%
54	16.346	5338	5353	5365	rBV4	17353	36460	1.71%	0.191%

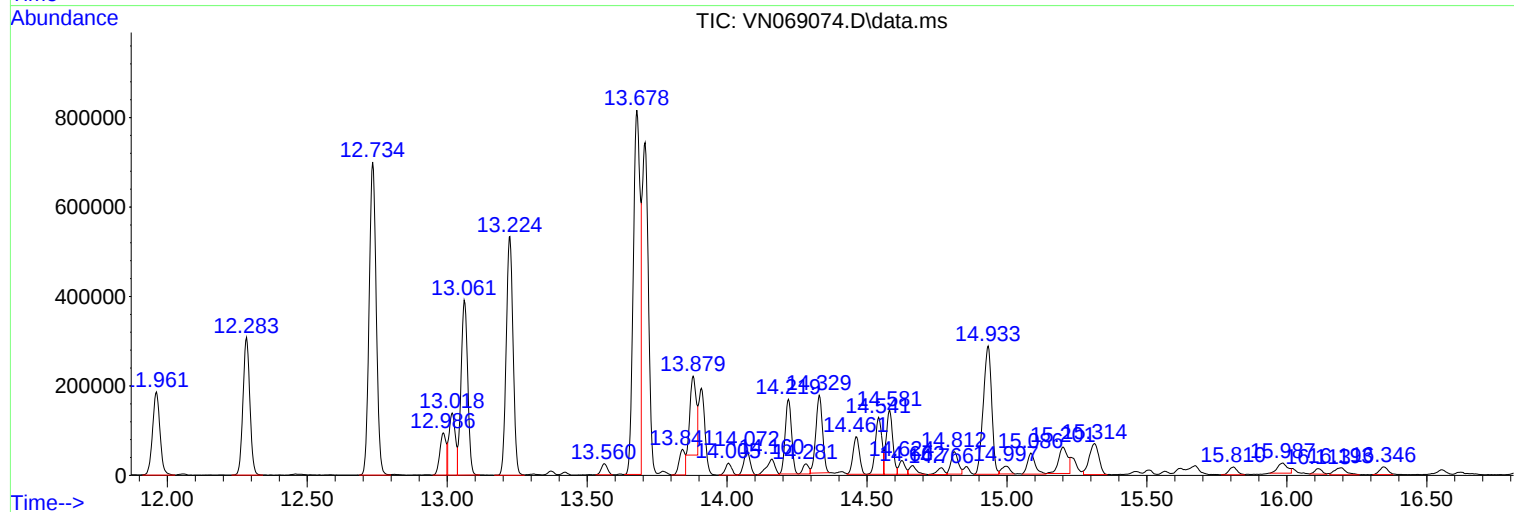
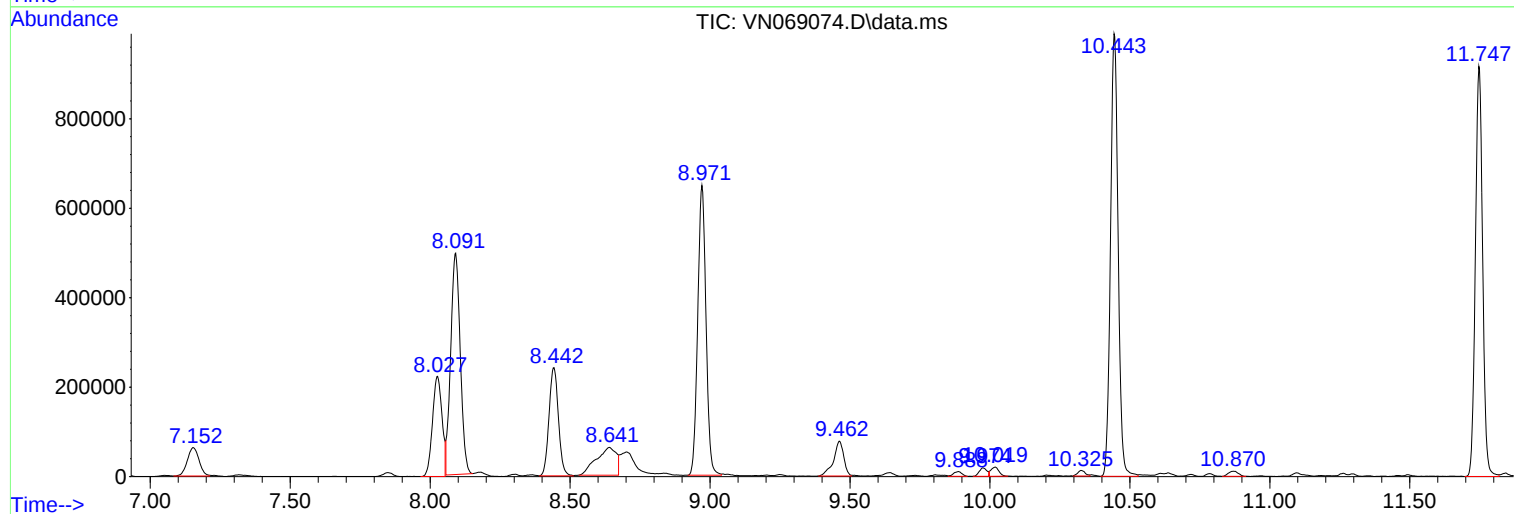
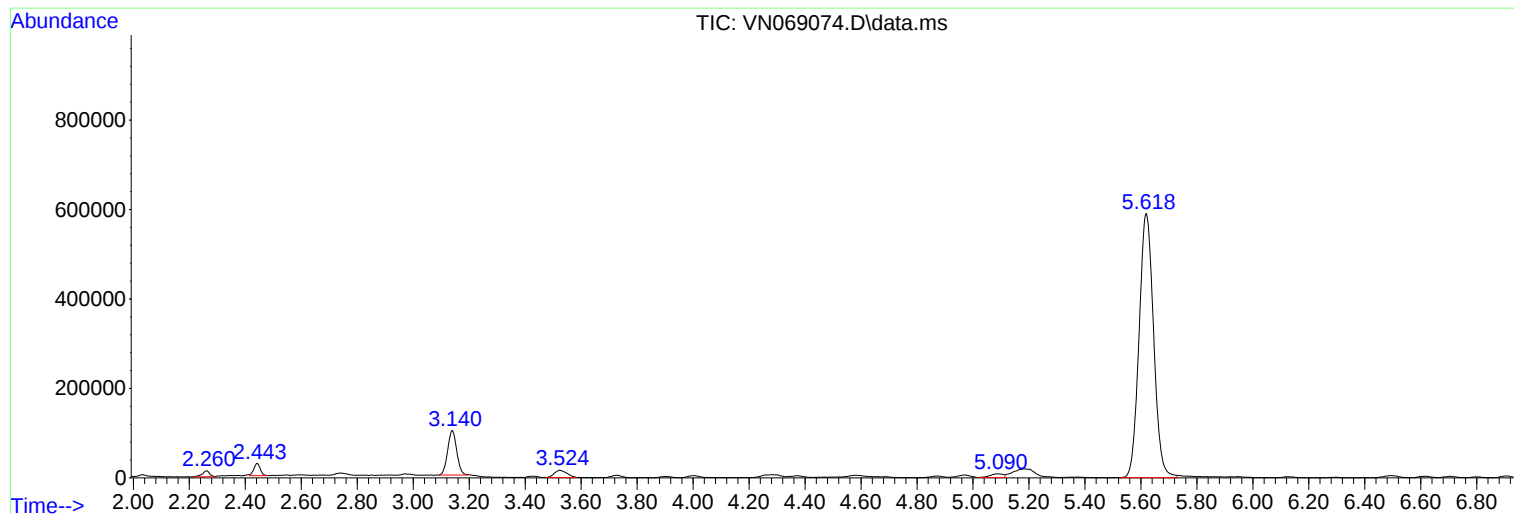
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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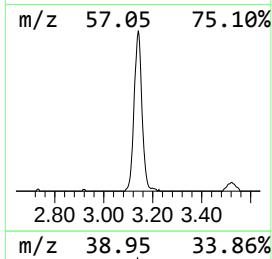
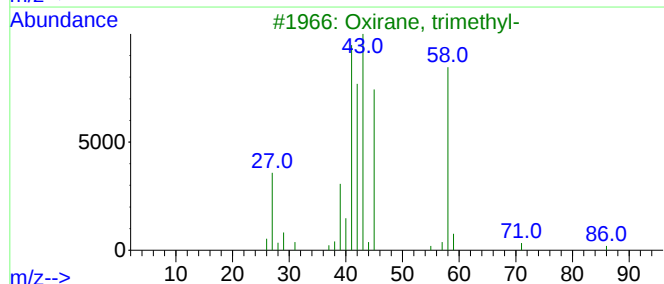
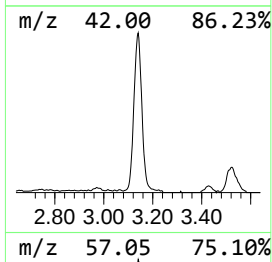
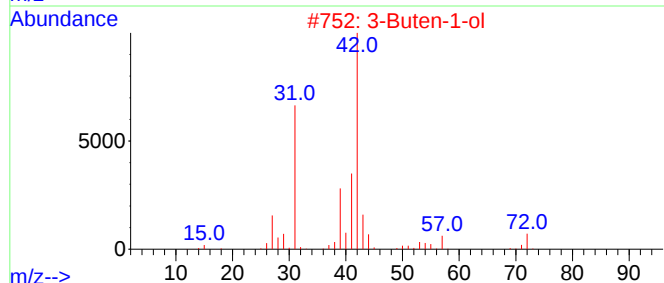
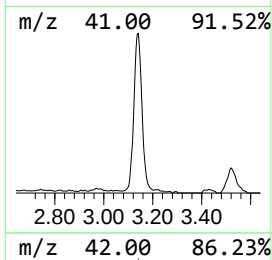
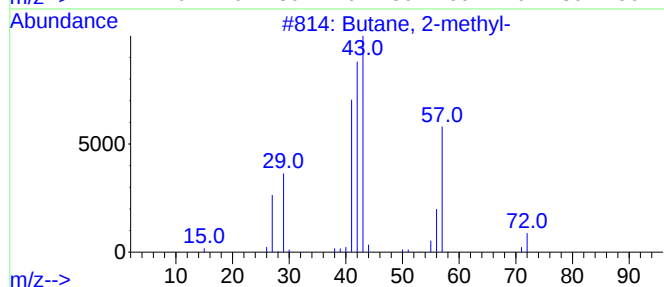
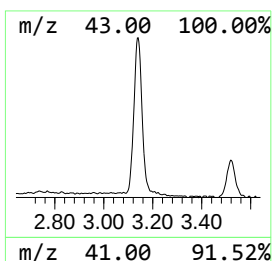
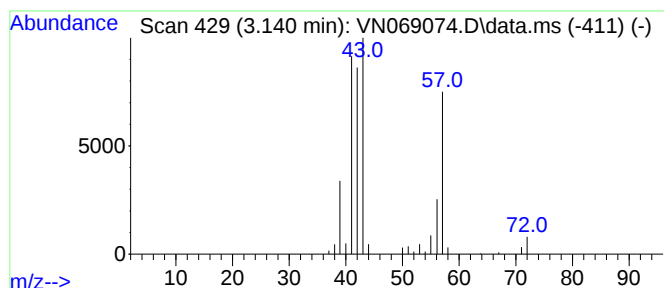
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.140	9.58 ug/l	223392	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	90
2			3-Buten-1-ol	72	C4H8O	000627-27-0	43
3			Oxirane, trimethyl-	86	C5H10O	005076-19-7	36
4			Pentane	72	C5H12	000109-66-0	33
5			2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	28



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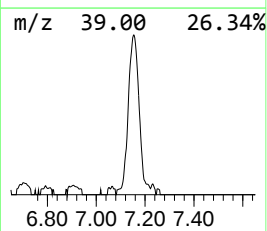
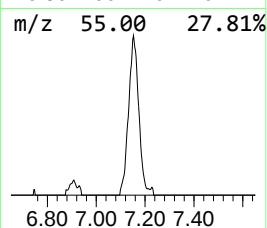
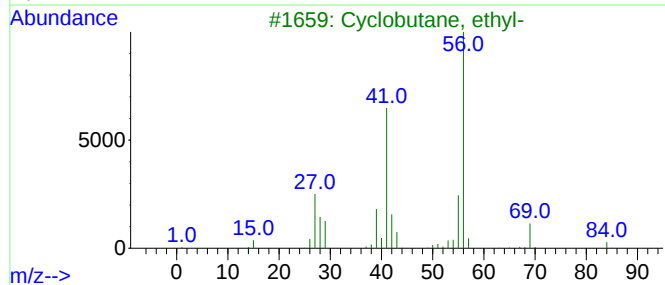
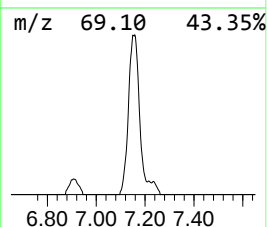
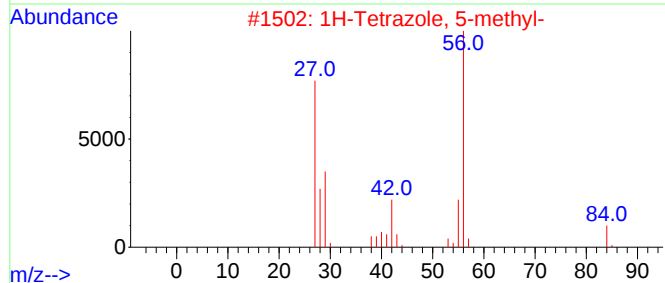
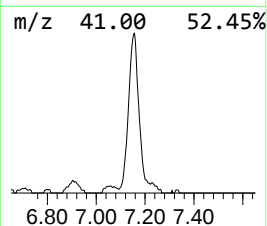
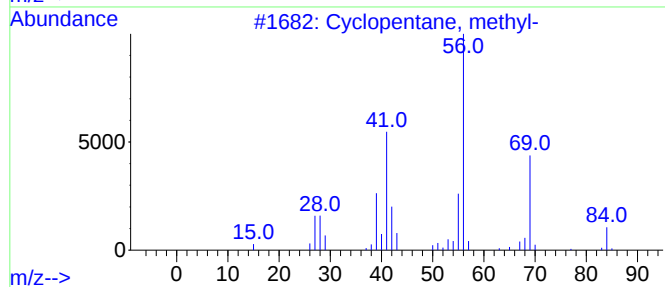
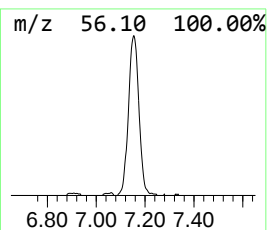
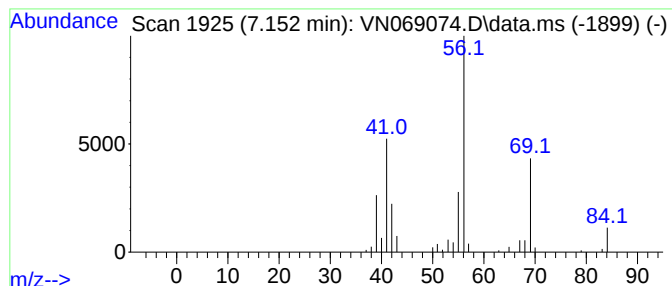
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclopentane, methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.152	7.92 ug/l	184690	Pentafluorobenzene	8.088

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
3			Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	56
5			Cyclobutane	56	C4H8	000287-23-0	50



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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
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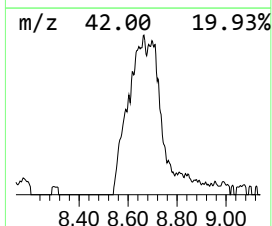
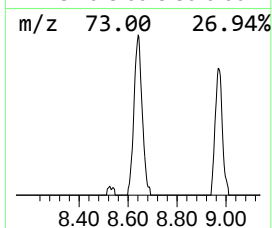
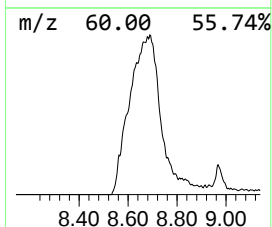
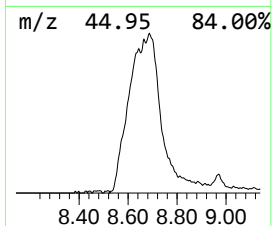
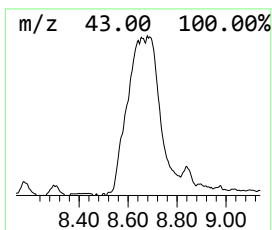
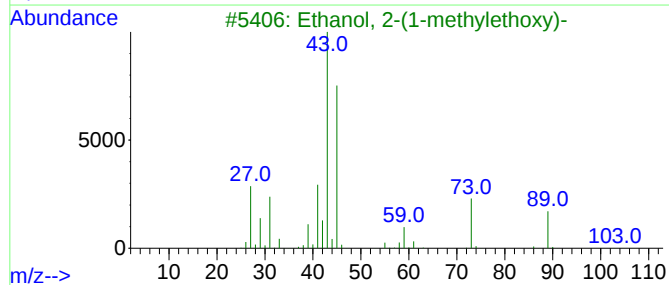
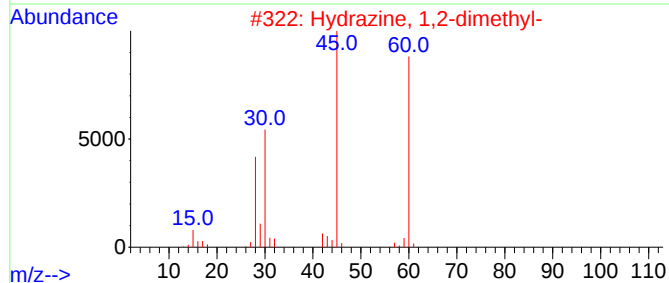
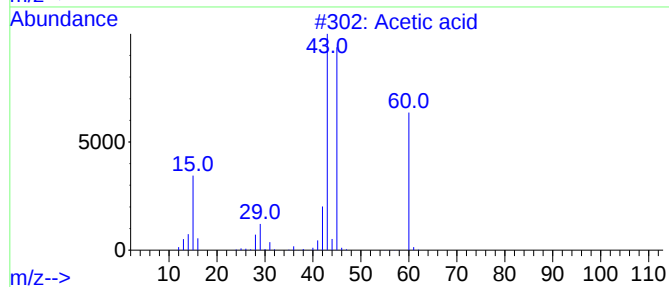
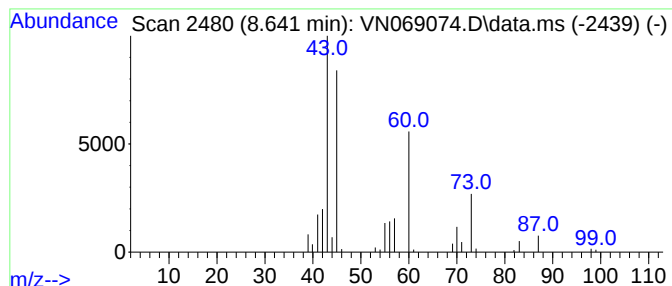
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Acetic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.641	11.63 ug/l	309460	1,4-Difluorobenzene	8.971

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid	60	C2H4O2	000064-19-7	64
2			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	38
3			Ethanol, 2-(1-methylethoxy)-	104	C5H12O2	000109-59-1	38
4			Ammonium acetate	77	C2H7NO2	000631-61-8	36
5			Hydroperoxide, 1-methylpentyl	118	C6H14O2	024254-55-5	33



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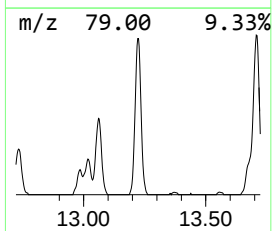
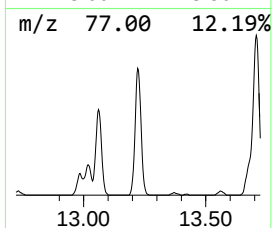
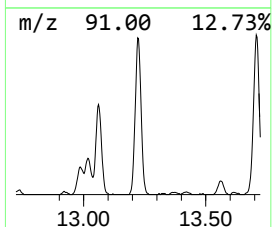
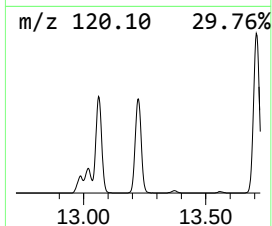
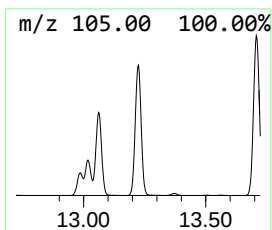
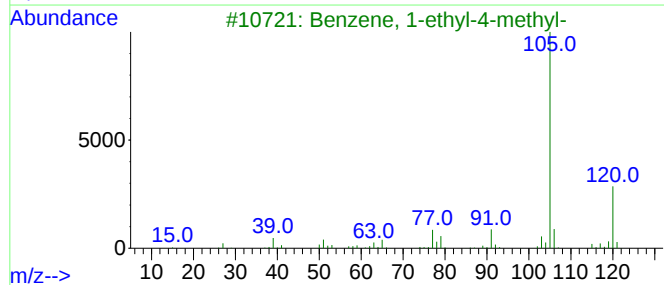
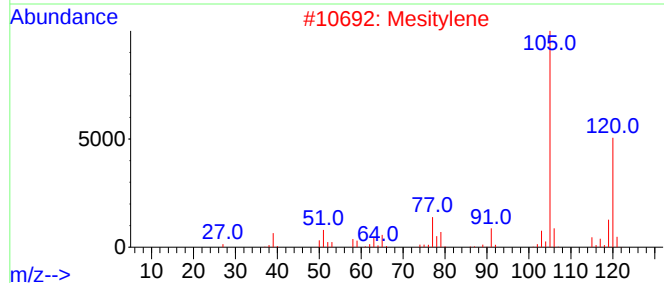
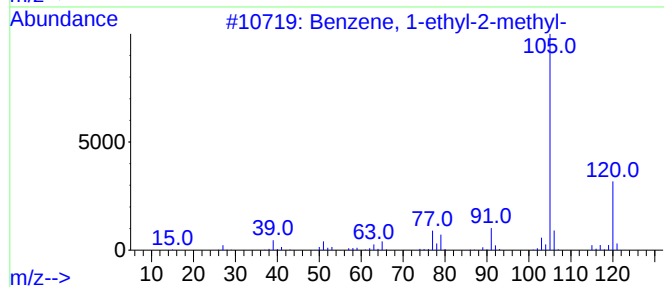
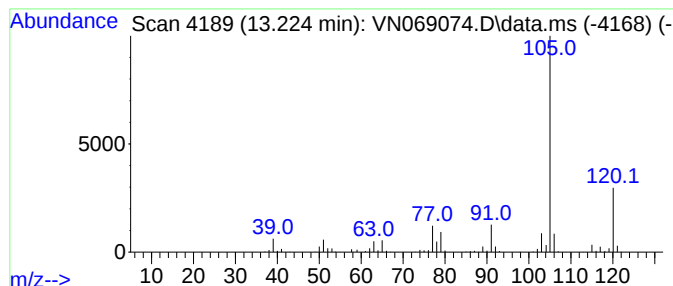
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.224	31.26 ug/l	904967	1,4-Dichlorobenzene-d4	13.678

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	91
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



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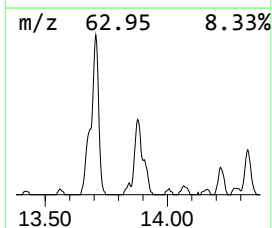
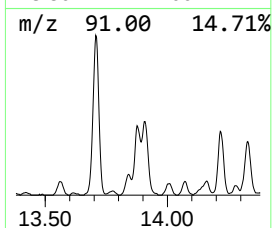
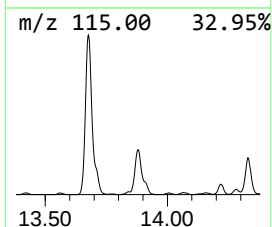
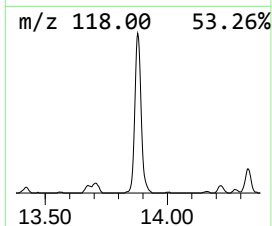
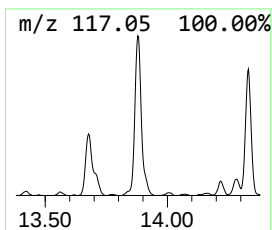
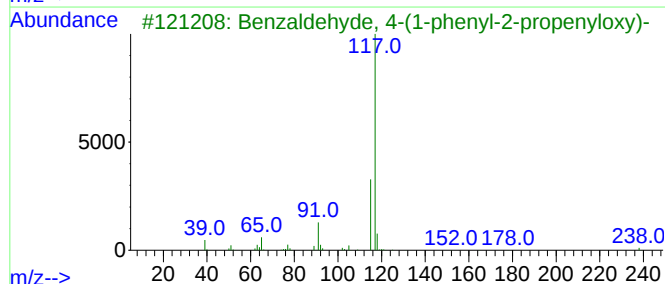
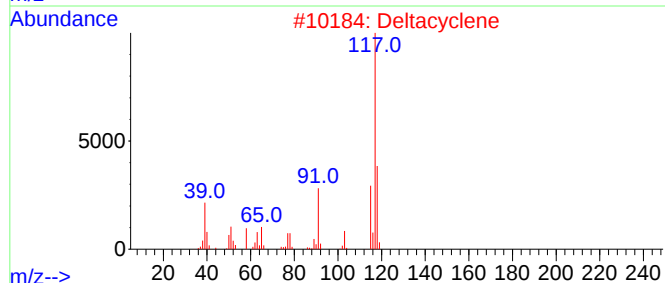
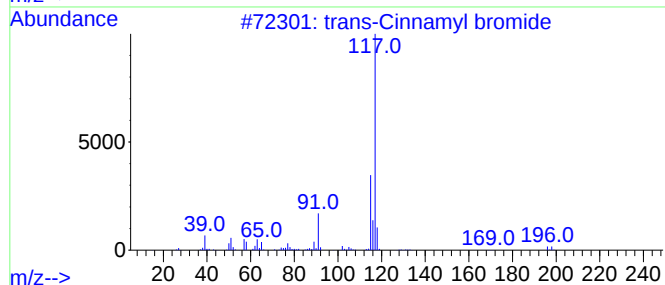
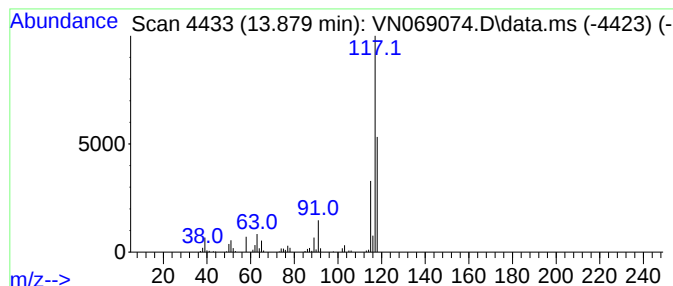
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 trans-Cinnamyl bromide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.879	9.66 ug/l	279809	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	59
2			Deltacyclene	118	C9H10	007785-10-6	59
3			Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	53
4			Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	43
5			Indole	117	C8H7N	000120-72-9	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102021\
Data File : VN069074.D
Acq On : 20 Oct 2021 20:23
Operator : JC/MD
Sample : M4253-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
133-134

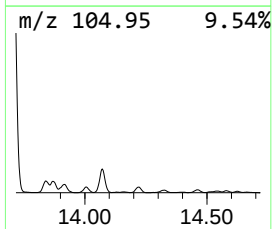
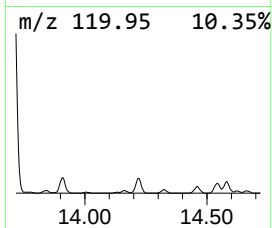
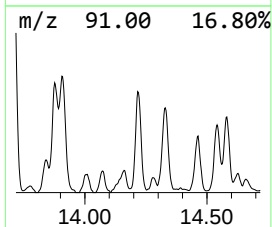
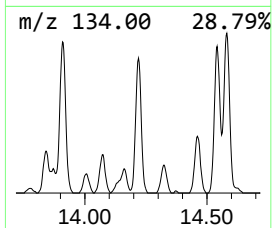
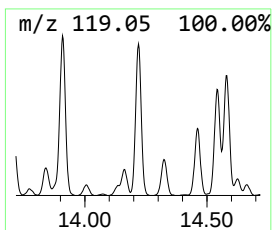
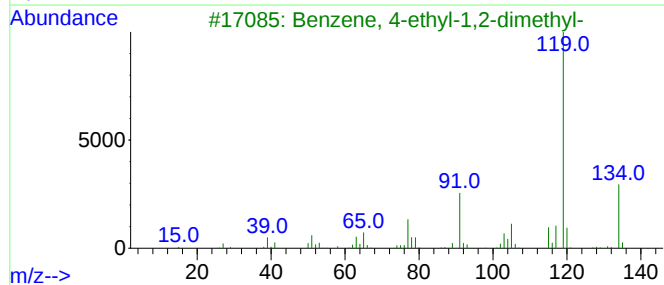
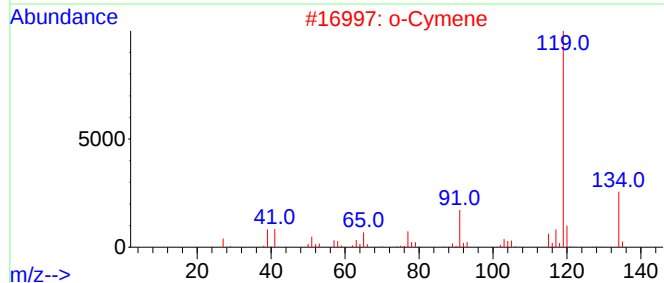
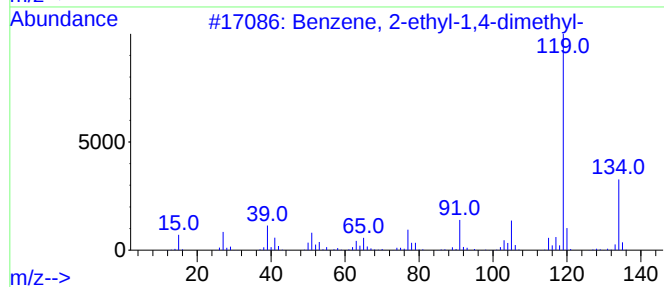
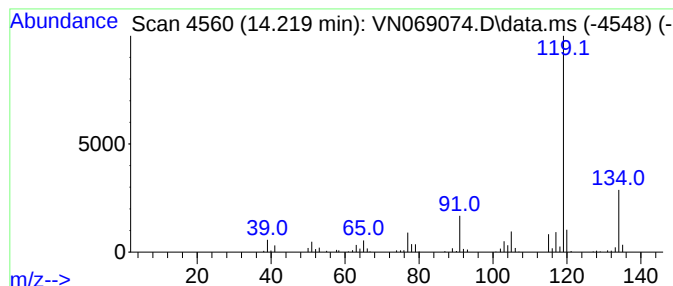
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.219	8.95 ug/l	259202	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
2			o-Cymene	134	C10H14	000527-84-4	95
3			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
4			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
5			p-Cymene	134	C10H14	000099-87-6	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102021\
Data File : VN069074.D
Acq On : 20 Oct 2021 20:23
Operator : JC/MD
Sample : M4253-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
133-134

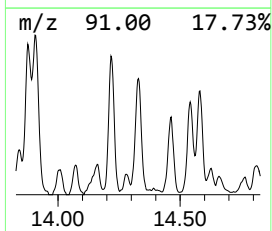
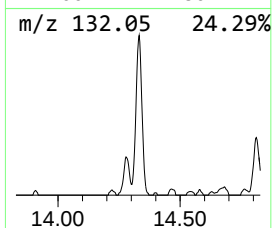
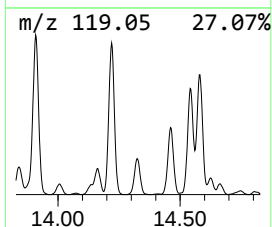
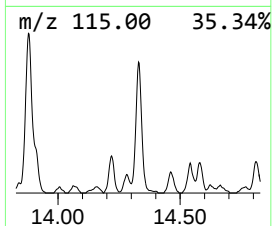
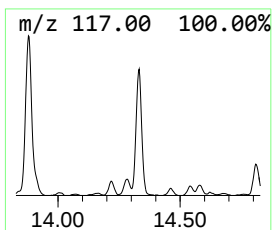
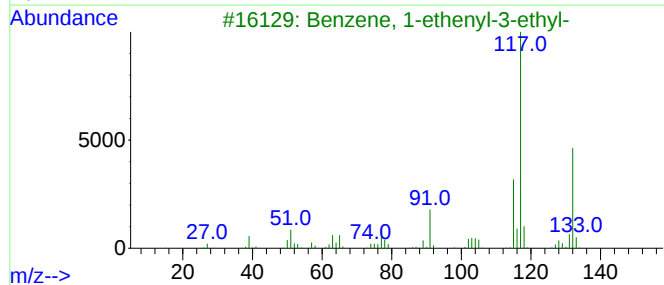
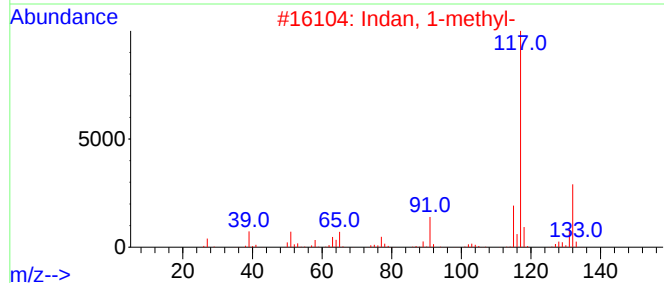
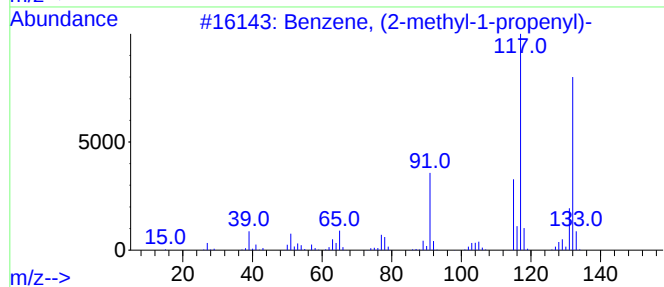
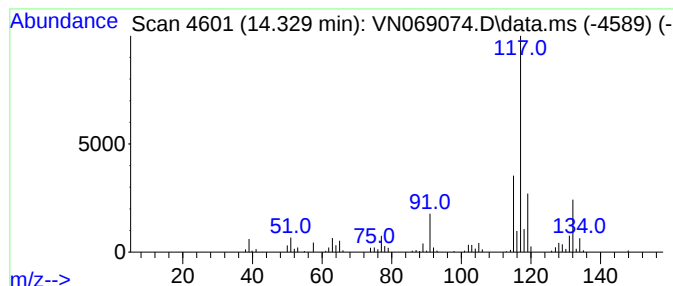
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Benzene, (2-methyl-1-propen... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	9.96 ug/l	288398	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	83
2			Indan, 1-methyl-	132	C10H12	000767-58-8	81
3			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	74
4			Benzene, 2-butenyl-	132	C10H12	001560-06-1	72
5			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102021\
Data File : VN069074.D
Acq On : 20 Oct 2021 20:23
Operator : JC/MD
Sample : M4253-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampled :
133-134

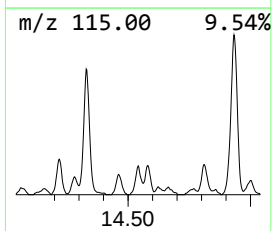
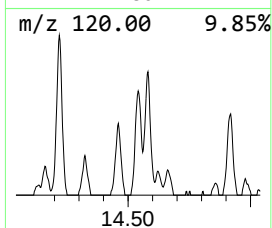
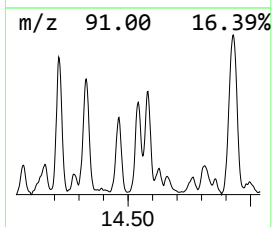
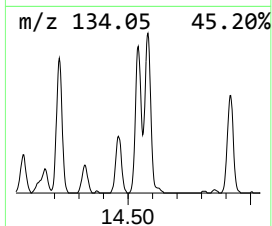
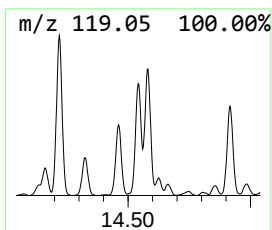
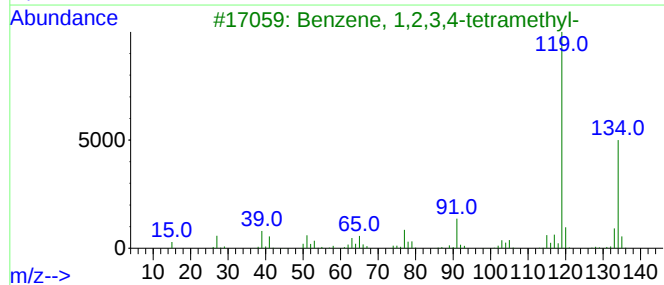
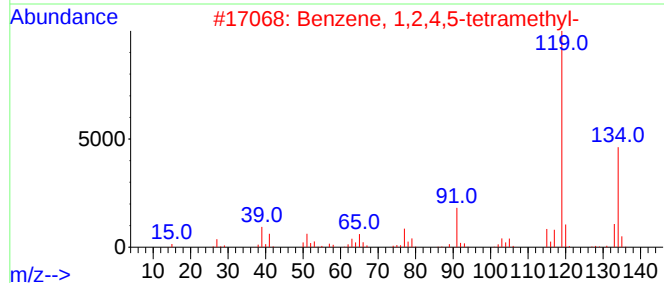
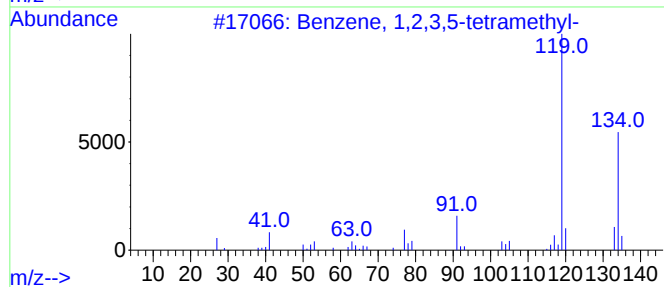
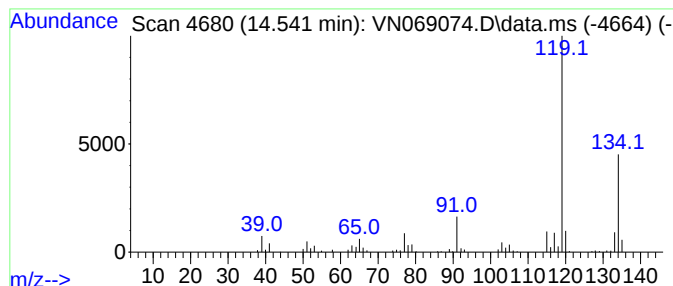
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.541	7.18 ug/l	207742	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	96
3			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
4			o-Cymene	134	C10H14	000527-84-4	95
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102021\
Data File : VN069074.D
Acq On : 20 Oct 2021 20:23
Operator : JC/MD
Sample : M4253-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
133-134

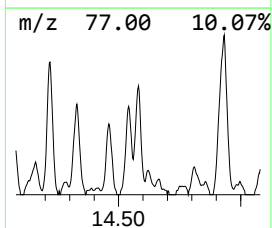
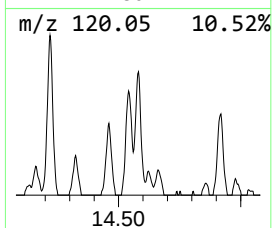
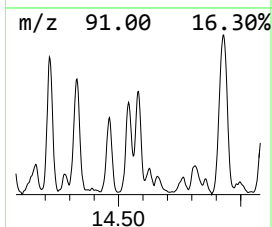
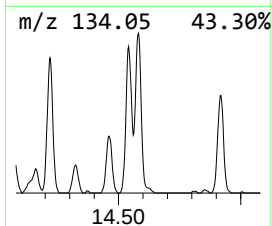
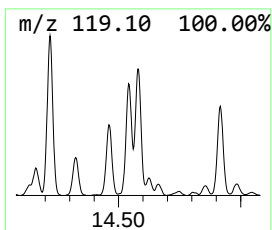
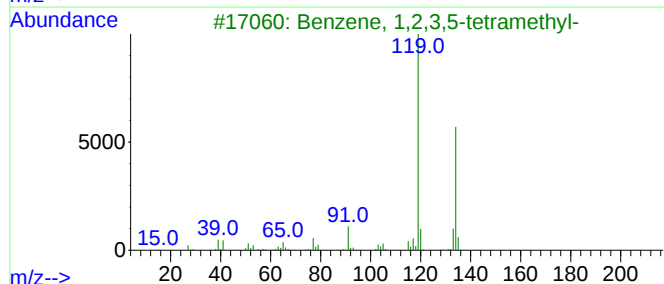
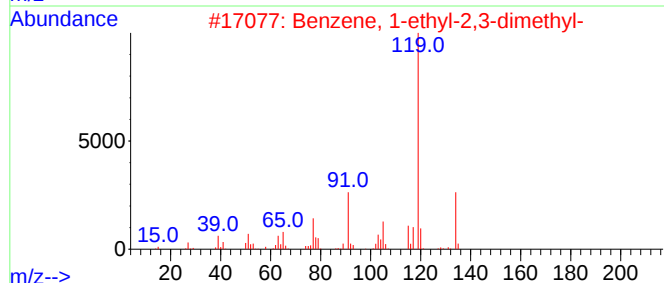
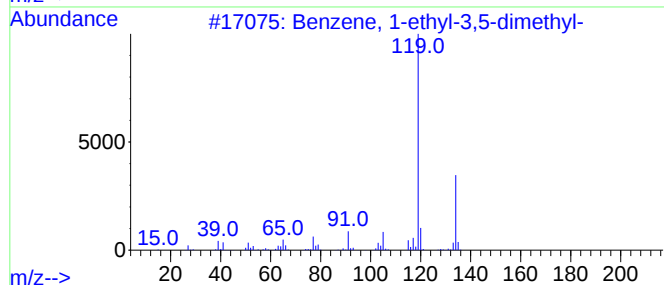
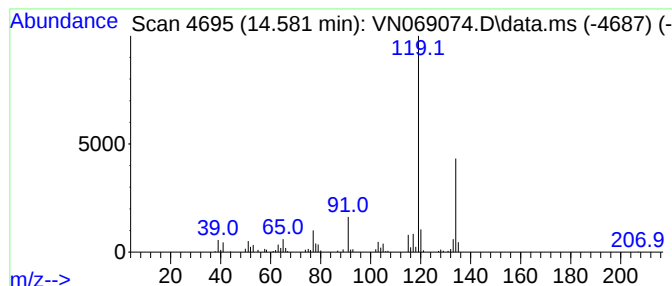
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Benzene, 1-ethyl-3,5-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.581	7.93 ug/l	229570	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	95
2			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
4			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	94
5			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102021\
Data File : VN069074.D
Acq On : 20 Oct 2021 20:23
Operator : JC/MD
Sample : M4253-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
133-134

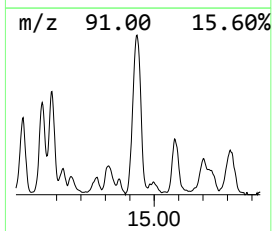
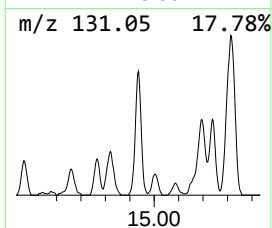
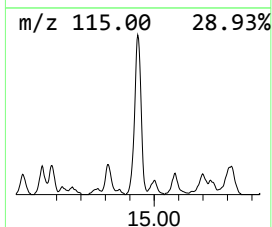
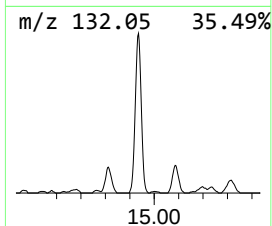
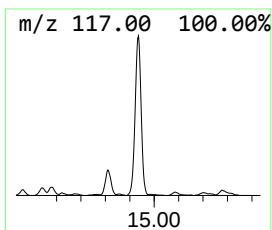
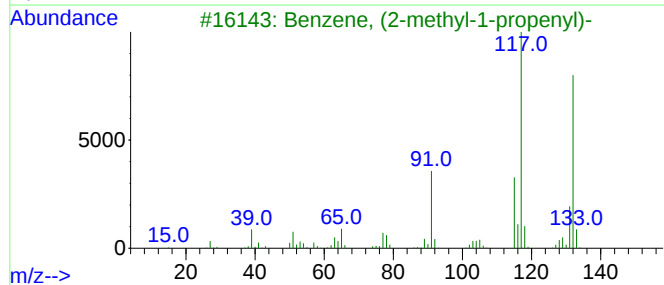
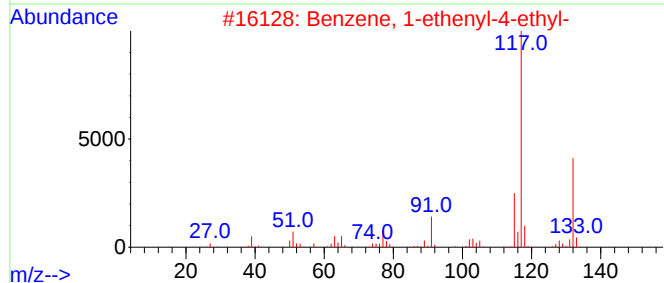
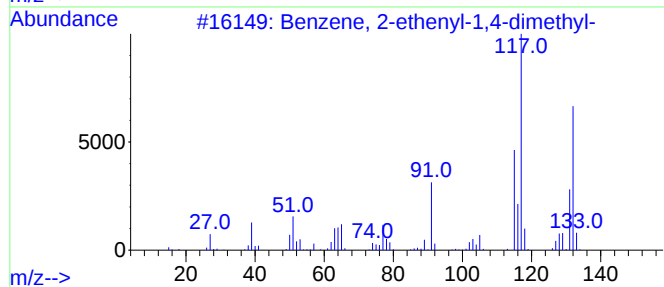
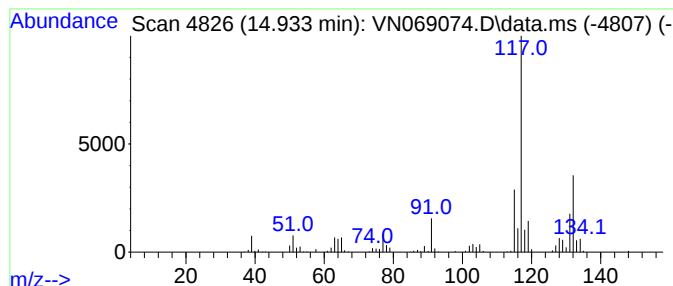
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.933	20.70 ug/l	599262	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
3			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	90
4			Indan, 1-methyl-	132	C10H12	000767-58-8	90
5			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102021\
Data File : VN069074.D
Acq On : 20 Oct 2021 20:23
Operator : JC/MD
Sample : M4253-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
133-134

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N101221W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methyl-	3.140	9.6	ug/l	223392	1	8.088	1165520	50.0
Cyclopentane, m...	7.152	7.9	ug/l	184690	1	8.088	1165520	50.0
Acetic acid	8.641	11.6	ug/l	309460	2	8.971	1329970	50.0
Benzene, 1-ethy...	13.224	31.3	ug/l	904967	4	13.678	1447590	50.0
trans-Cinnamyl ...	13.879	9.7	ug/l	279809	4	13.678	1447590	50.0
Benzene, 2-ethy...	14.219	8.9	ug/l	259202	4	13.678	1447590	50.0
Benzene, (2-met...	14.329	10.0	ug/l	288398	4	13.678	1447590	50.0
Benzene, 1,2,3,...	14.541	7.2	ug/l	207742	4	13.678	1447590	50.0
Benzene, 1-ethy...	14.581	7.9	ug/l	229570	4	13.678	1447590	50.0
Benzene, 2-ethe...	14.933	20.7	ug/l	599262	4	13.678	1447590	50.0