

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010322\
 Data File : VN070443.D
 Acq On : 3 Jan 2022 17:42
 Operator : JC/MD
 Sample : M5251-07
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-6S

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\82N122721W.M
 Title : SW846 8260

Signal : TIC: VN070443.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.231	79	90	102	rBV2	311191	690301	13.08%	1.852%
2	2.443	161	169	185	rVB2	149108	241505	4.58%	0.648%
3	3.140	416	429	457	rVB2	151796	357942	6.78%	0.960%
4	3.518	557	570	592	rVB6	59050	166146	3.15%	0.446%
5	3.714	631	643	662	rVB4	69706	173159	3.28%	0.465%
6	3.990	730	746	778	rVB3	61634	172293	3.27%	0.462%
7	4.283	819	855	879	rBV4	58814	282603	5.36%	0.758%
8	5.079	1126	1152	1173	rBV4	69971	278874	5.29%	0.748%
9	7.150	1904	1924	1937	rVV5	23882	73108	1.39%	0.196%
10	7.321	1969	1988	2015	rVB7	16727	60978	1.16%	0.164%
11	8.021	2226	2249	2260	rBV2	662213	1604256	30.40%	4.304%
12	8.083	2260	2272	2294	rVV	1325557	3022006	57.27%	8.107%
13	8.174	2297	2306	2326	rVB7	31172	77268	1.46%	0.207%
14	8.437	2384	2404	2427	rBV	846781	1950744	36.97%	5.233%
15	8.614	2453	2470	2493	rVB2	172663	427880	8.11%	1.148%
16	8.965	2582	2601	2635	rBV	1984841	4157091	78.78%	11.152%
17	9.880	2925	2942	2961	rVB3	66277	135437	2.57%	0.363%
18	10.011	2968	2991	3007	rBV4	82997	178554	3.38%	0.479%
19	10.440	3131	3151	3167	rBV	2839265	5276658	100.00%	14.156%
20	10.502	3168	3174	3195	rVB	112679	208686	3.95%	0.560%
21	11.057	3366	3381	3402	rBV2	38131	88397	1.68%	0.237%
22	11.744	3619	3637	3661	rBV	2533967	4628994	87.73%	12.418%
23	11.843	3662	3674	3692	rVB	262736	465043	8.81%	1.248%
24	11.950	3697	3714	3746	rVB	739685	1543715	29.26%	4.141%
25	12.278	3820	3836	3858	rBV	239183	427874	8.11%	1.148%
26	12.731	3986	4005	4028	rBV	1974236	3530797	66.91%	9.472%
27	12.916	4065	4074	4086	rBV	35244	59761	1.13%	0.160%
28	12.983	4086	4099	4106	rBV2	130602	226335	4.29%	0.607%
29	13.058	4119	4127	4139	rVB2	71728	119332	2.26%	0.320%
30	13.222	4174	4188	4200	rBV2	56160	96557	1.83%	0.259%
31	13.366	4230	4242	4262	rVB	306782	517754	9.81%	1.389%
32	13.672	4339	4356	4386	rBV	1883374	3447827	65.34%	9.249%
33	13.876	4420	4432	4467	rVB	233568	483762	9.17%	1.298%
34	14.329	4590	4601	4619	rVB3	51896	94796	1.80%	0.254%
35	14.809	4768	4780	4792	rBV5	31131	52921	1.00%	0.142%
36	14.927	4805	4824	4839	rBV5	45616	109032	2.07%	0.292%

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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	15.504	5014	5039	5061	rBV	758864	1532468	29.04%	4.111%
38	15.603	5065	5076	5092	rVB2	30470	60425	1.15%	0.162%
39	16.614	5437	5453	5473	rVB2	109946	254714	4.83%	0.683%

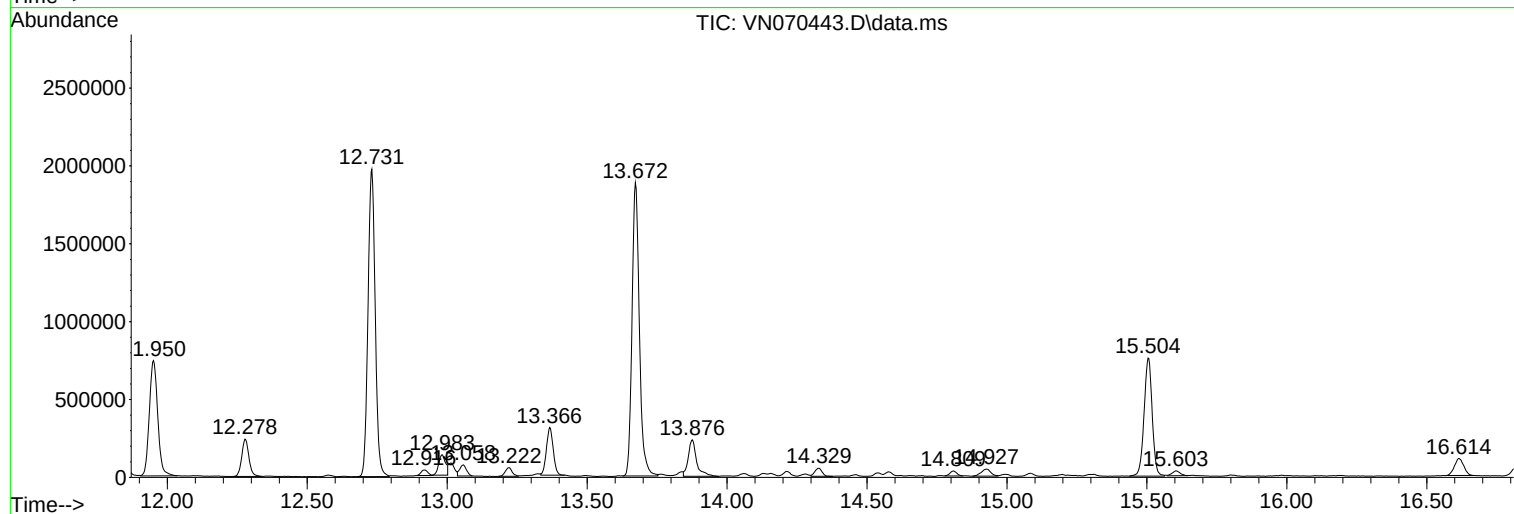
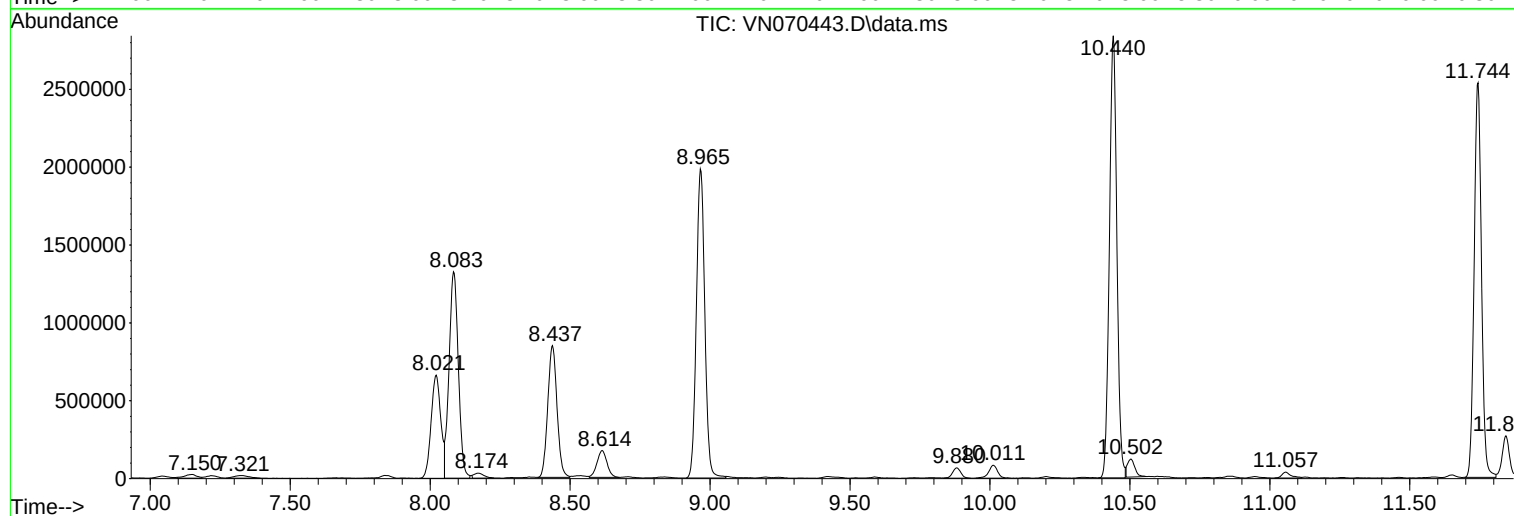
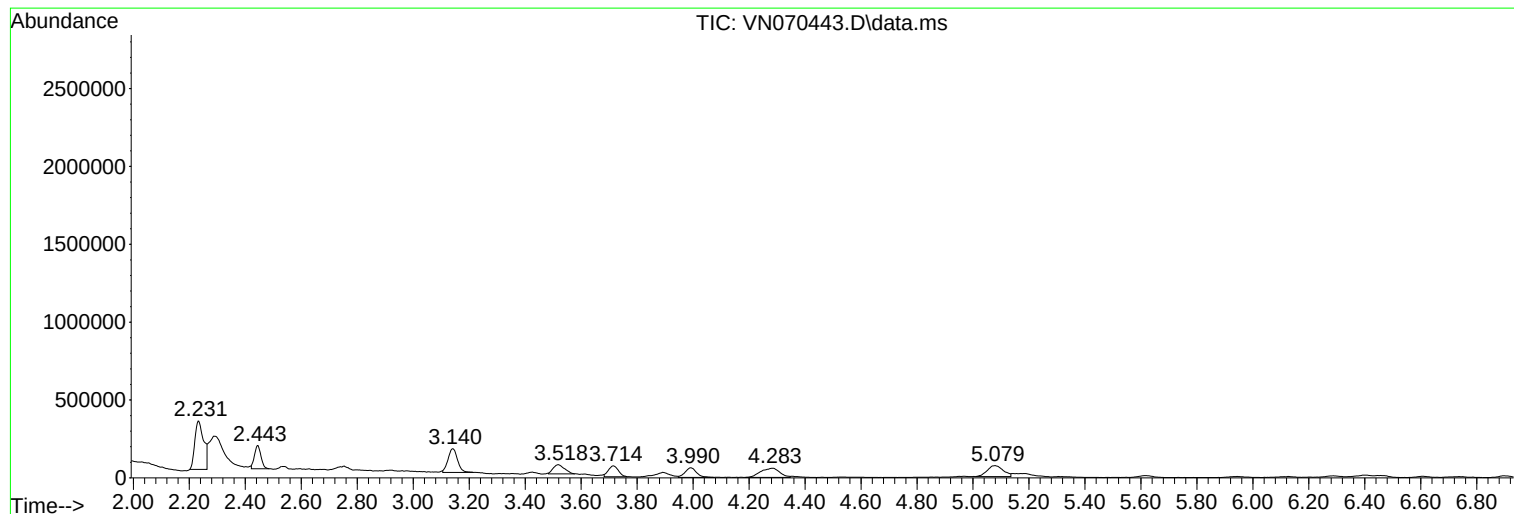
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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



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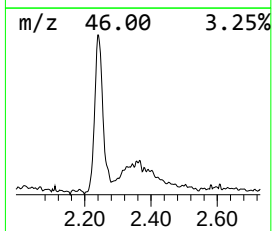
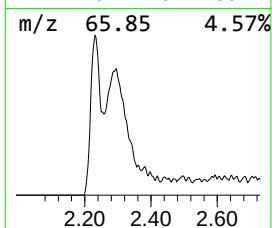
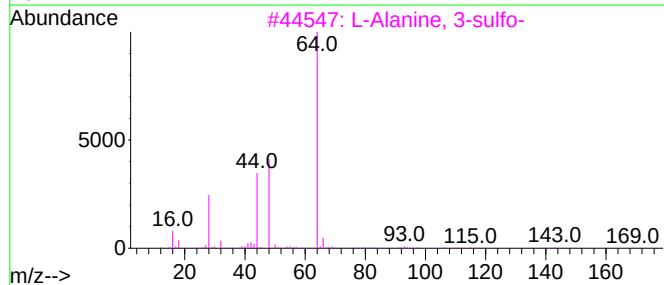
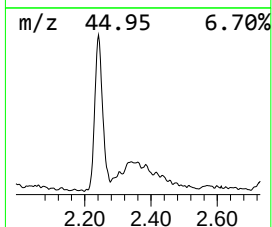
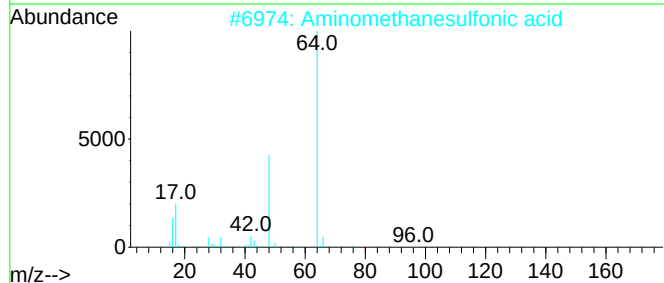
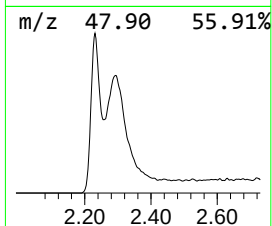
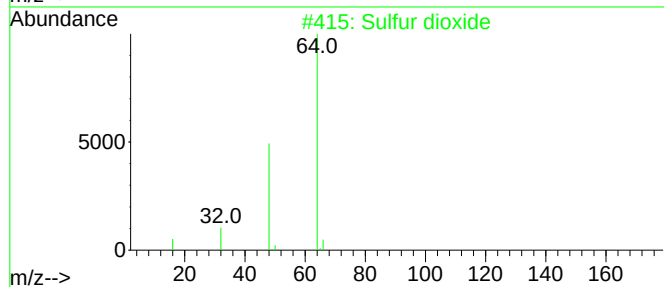
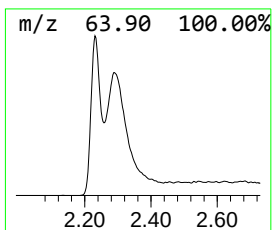
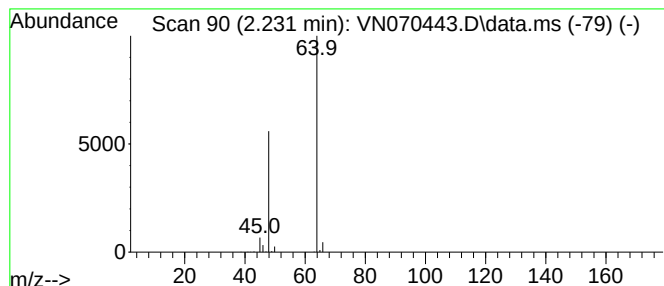
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.231	11.42 ug/l	690301	Pentafluorobenzene	8.083

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	5
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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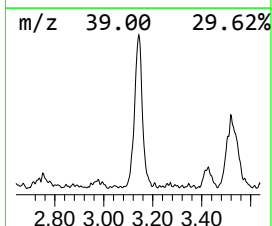
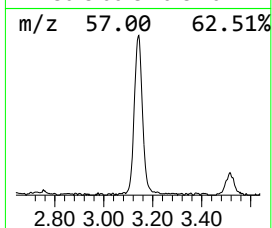
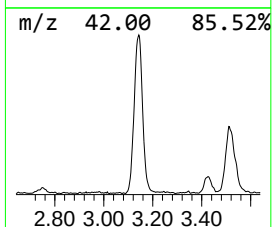
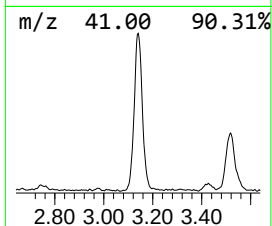
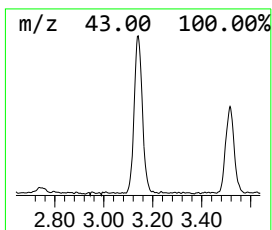
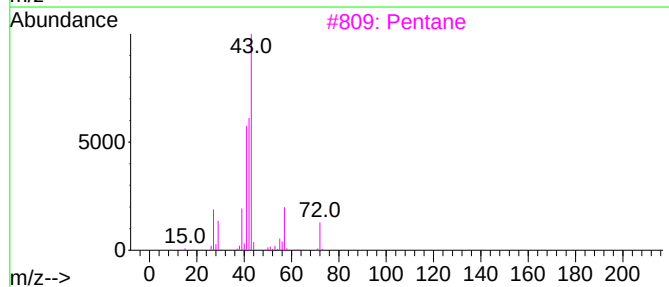
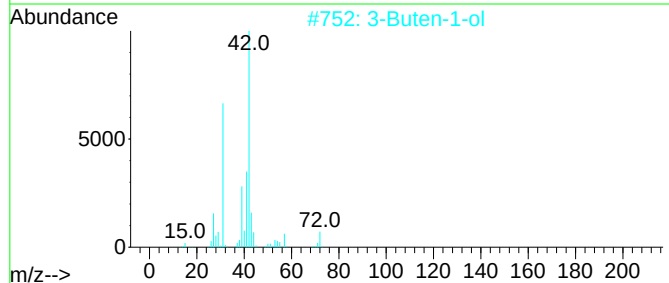
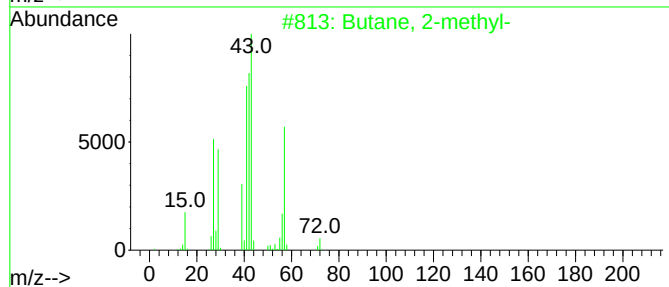
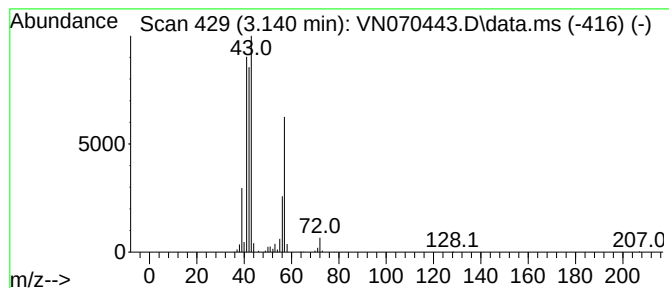
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Butane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.140	5.92 ug/l	357942	Pentafluorobenzene	8.083

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	86
2			3-Buten-1-ol	72	C4H8O	000627-27-0	47
3			Pentane	72	C5H12	000109-66-0	40
4			2,5-Furandione, dihydro-3-methyl-	114	C5H6O3	004100-80-5	23
5			Butane, 1-isocyano-	83	C5H9N	002769-64-4	12



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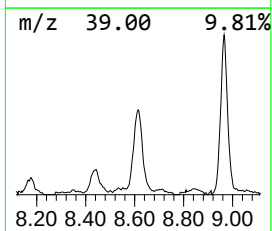
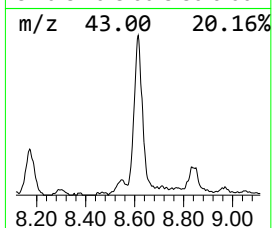
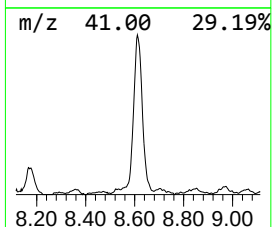
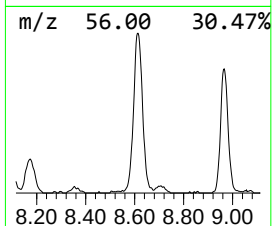
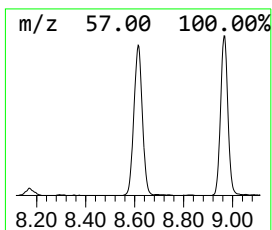
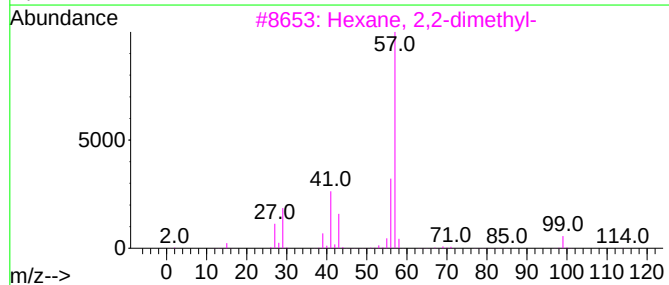
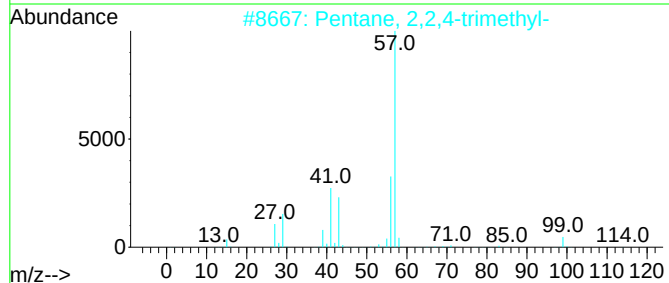
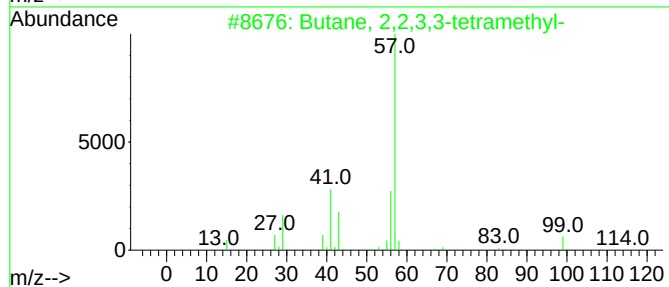
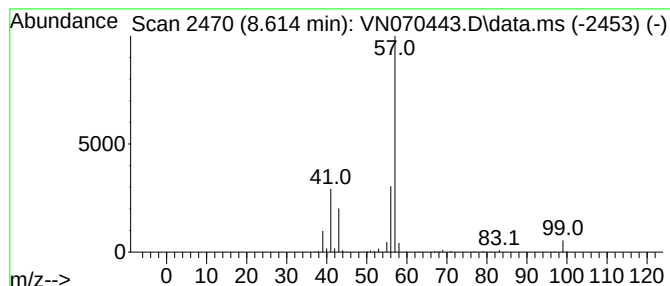
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Quant Title : SW846 8260

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

Peak Number 3 Butane, 2,2,3,3-tetramethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.614	5.15 ug/l	427880	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	83
2			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	78
3			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
4			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	64
5			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59



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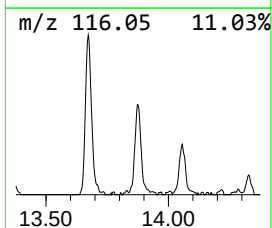
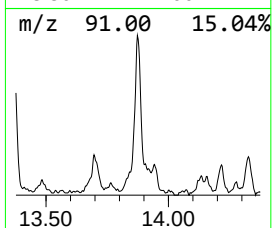
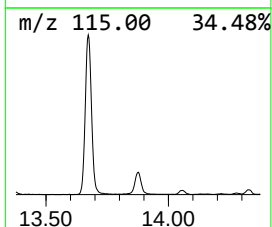
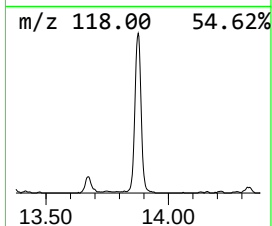
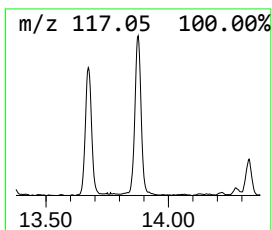
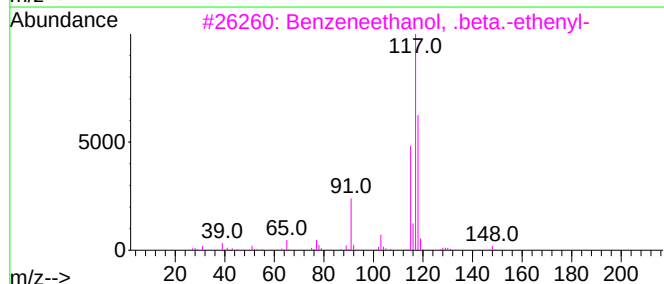
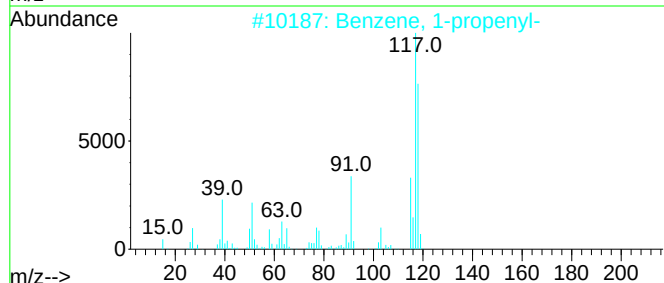
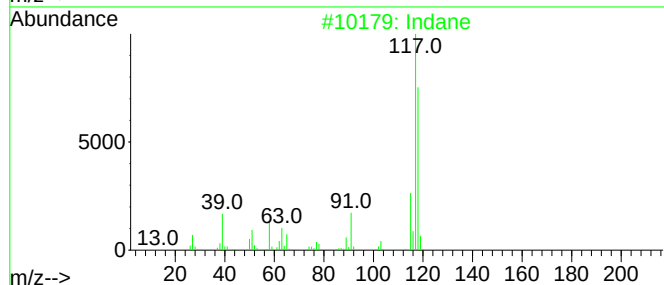
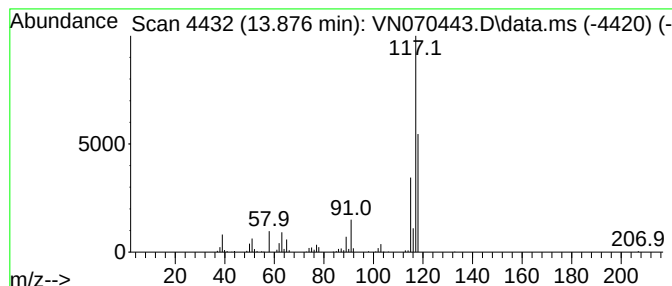
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Peak Number 4 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	7.02 ug/l	483762	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	95
2			Benzene, 1-propenyl-	118	C9H10	000637-50-3	72
3			Benzeneethanol, .beta.-ethenyl-	148	C10H12O	006052-63-7	72
4			Benzene, 2-propenyl-	118	C9H10	000300-57-2	64
5			Benzene, cyclopropyl-	118	C9H10	000873-49-4	64



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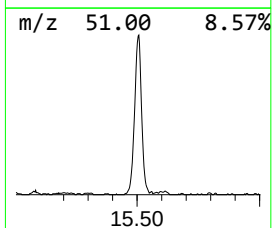
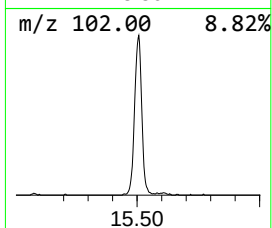
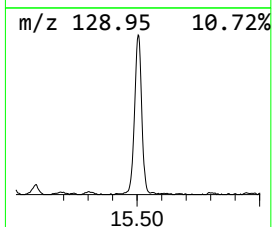
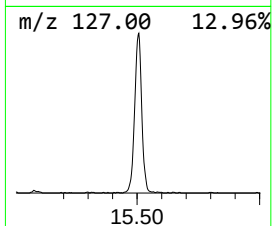
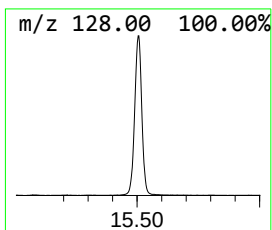
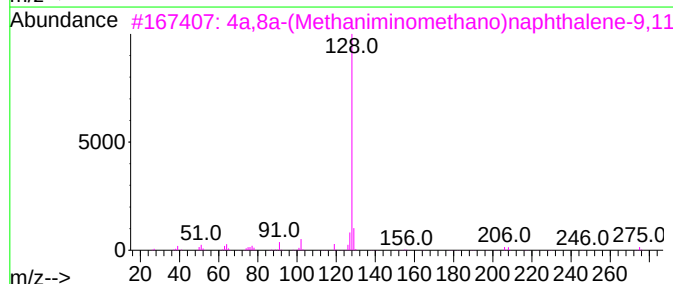
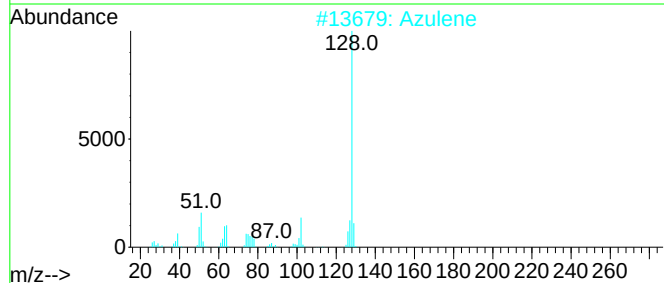
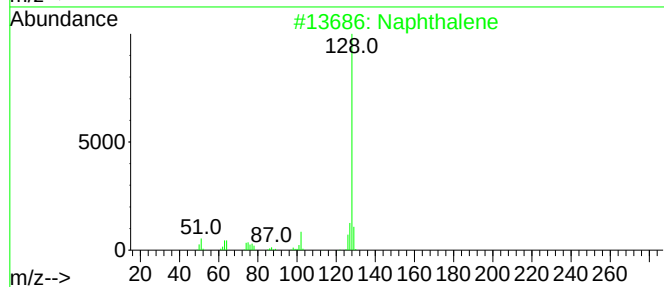
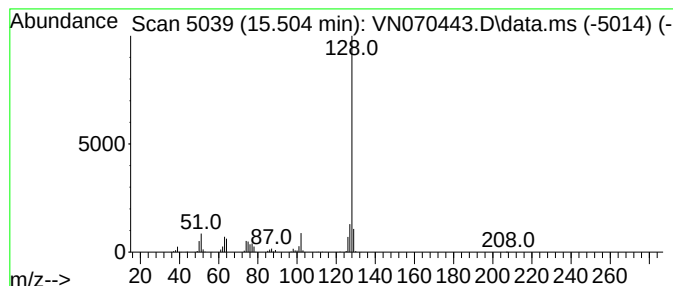
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 5 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.504	22.22 ug/l	1532470	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Azulene	128	C10H8	000275-51-4	91
3			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	74
4			[4.2.2]Propella-2,4,7,9-tetraene	128	C10H8	088090-34-0	64
5			1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010322\
Data File : VN070443.D
Acq On : 3 Jan 2022 17:42
Operator : JC/MD
Sample : M5251-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-6S

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.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
Sulfur dioxide	2.231	11.4	ug/l	690301	1	8.083	3022010	50.0
Butane, 2-methyl-	3.140	5.9	ug/l	357942	1	8.083	3022010	50.0
Butane, 2,2,3,3...	8.614	5.2	ug/l	427880	2	8.965	4157090	50.0
Indane	13.876	7.0	ug/l	483762	4	13.672	3447830	50.0
Azulene	15.504	22.2	ug/l	1532470	4	13.672	3447830	50.0