

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
 Data File : VX025449.D
 Acq On : 03 Dec 2021 00:09
 Operator : JC/MD
 Sample : M4917-13
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-29

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_X\Method\82X111721W.M
 Title : SW846 8260

Signal : TIC: VX025449.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	41	rBV2	22571	79627	9.08%	1.409%
2	1.368	41	46	52	rVB	18930	24982	2.85%	0.442%
3	1.752	104	109	116	rVB	14814	21835	2.49%	0.386%
4	1.971	138	145	156	rVV3	12222	26710	3.05%	0.473%
5	2.069	156	161	171	rVV	14346	23902	2.73%	0.423%
6	2.166	171	177	180	rVV2	11093	18367	2.09%	0.325%
7	2.215	180	185	195	rVB	26663	40516	4.62%	0.717%
8	2.751	264	273	282	rBV	16136	31801	3.63%	0.563%
9	2.867	287	292	301	rVV2	10100	22101	2.52%	0.391%
10	2.965	301	308	321	rVV	28054	61199	6.98%	1.083%
11	3.117	324	333	346	rVB	41463	96966	11.06%	1.715%
12	3.763	427	439	446	rBV4	3206	12015	1.37%	0.213%
13	4.306	520	528	538	rVB4	4436	12644	1.44%	0.224%
14	5.391	693	706	717	rBV2	65663	189919	21.66%	3.360%
15	5.556	724	733	750	rVB	105779	302265	34.47%	5.347%
16	5.964	789	800	805	rBV	66912	176345	20.11%	3.120%
17	6.044	805	813	830	rVB	332564	876934	100.00%	15.514%
18	6.214	830	841	844	rBV4	3888	11301	1.29%	0.200%
19	6.763	922	931	949	rBV	167728	405694	46.26%	7.177%
20	8.653	1234	1241	1247	rVV	354947	548243	62.52%	9.699%
21	8.720	1247	1252	1262	rVB	67130	103302	11.78%	1.827%
22	9.458	1364	1373	1378	rBV2	7879	13373	1.52%	0.237%
23	10.055	1465	1471	1486	rVB	356729	473645	54.01%	8.379%
24	10.195	1488	1494	1501	rBV	266026	338092	38.55%	5.981%
25	10.305	1506	1512	1521	rVB	287092	383210	43.70%	6.779%
26	10.646	1562	1568	1575	rVB	142024	192757	21.98%	3.410%
27	11.085	1634	1640	1651	rVB	273651	355652	40.56%	6.292%
28	11.305	1671	1676	1682	rVB	11238	14368	1.64%	0.254%
29	11.384	1682	1689	1691	rBV	21834	34153	3.89%	0.604%
30	11.451	1696	1700	1705	rVB	11151	13596	1.55%	0.241%
31	11.616	1722	1727	1733	rBV	26851	33128	3.78%	0.586%
32	11.756	1745	1750	1757	rVB	87661	109593	12.50%	1.939%
33	12.024	1788	1794	1800	rBV	365253	442943	50.51%	7.836%
34	12.091	1800	1805	1811	rVB	33773	43187	4.92%	0.764%
35	12.244	1822	1830	1838	rBV	35889	48469	5.53%	0.857%
36	13.292	1998	2002	2008	rVB3	9471	11908	1.36%	0.211%

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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	13.780	2077	2082	2087	rVB	26884	32820	3.74%	0.581%
38	15.121	2297	2302	2310	rVB	18668	25145	2.87%	0.445%

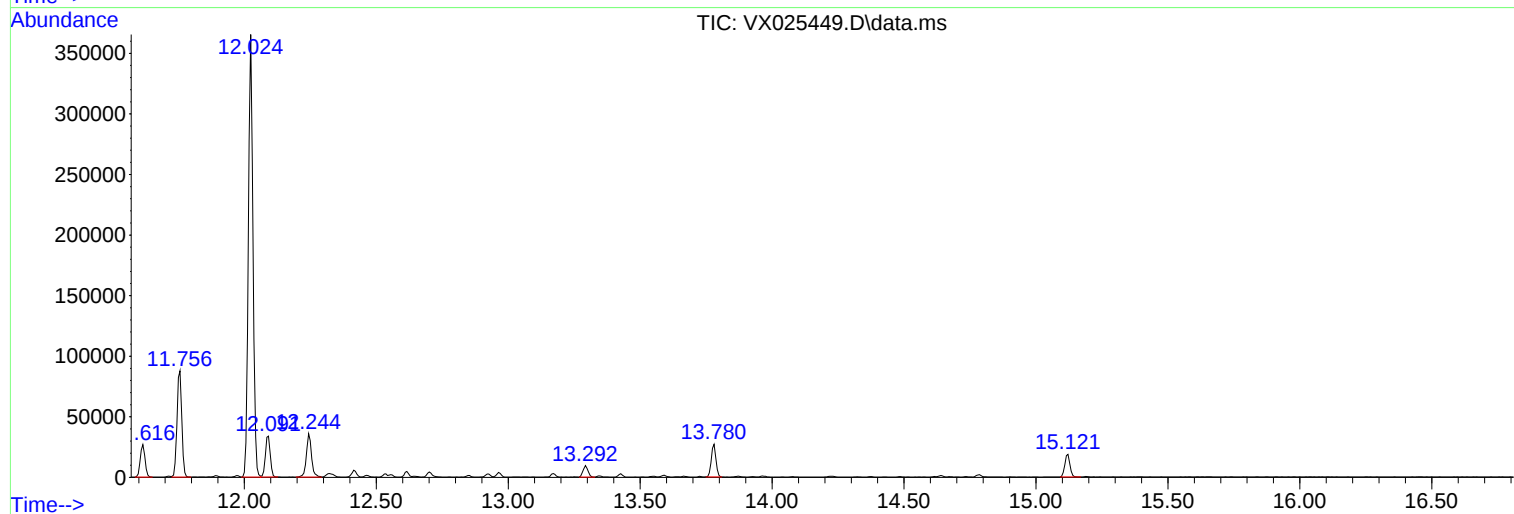
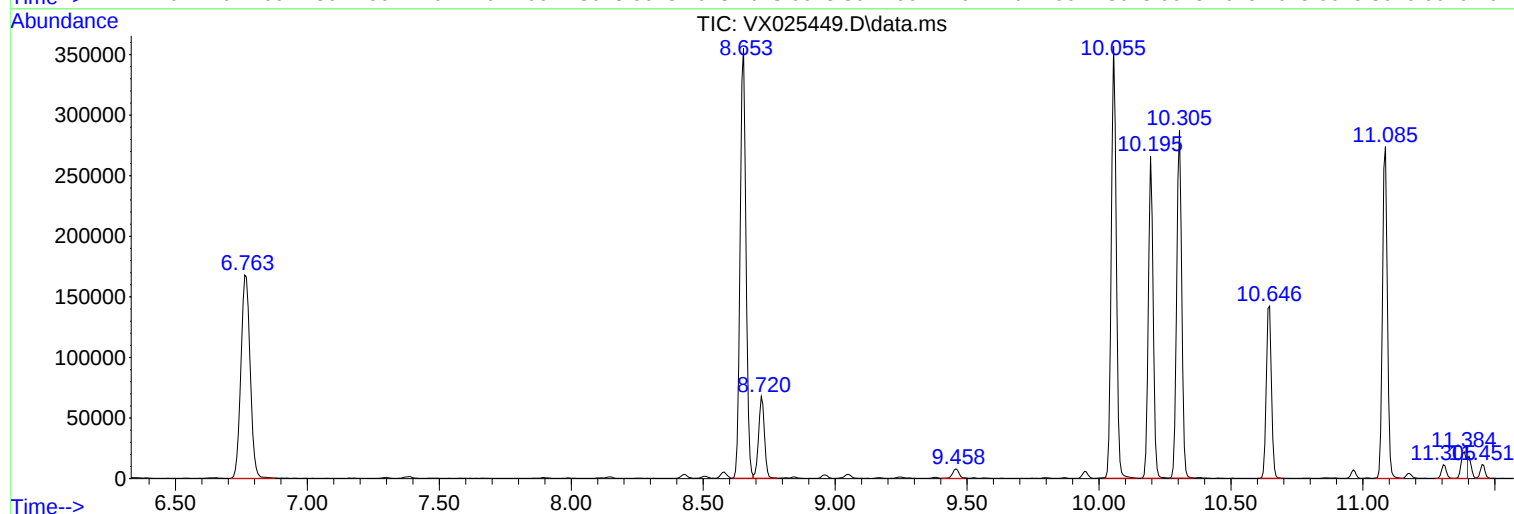
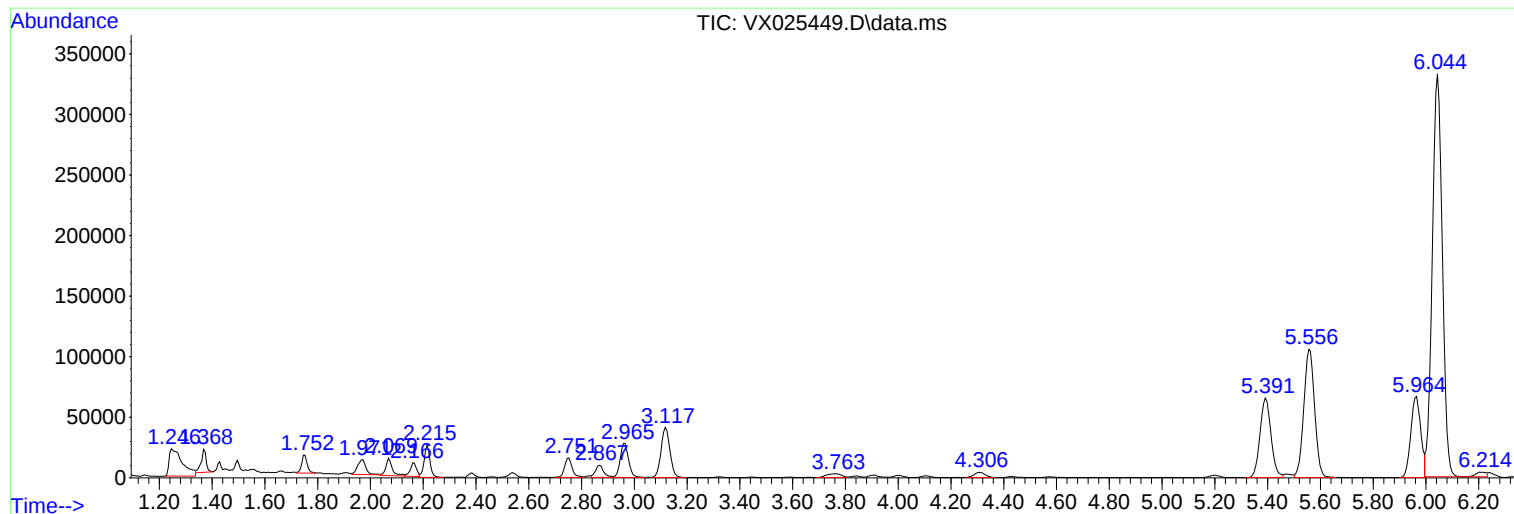
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Quant Title : SW846 8260

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



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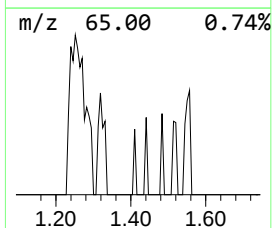
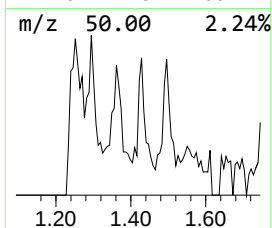
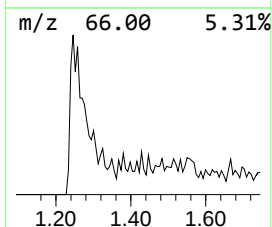
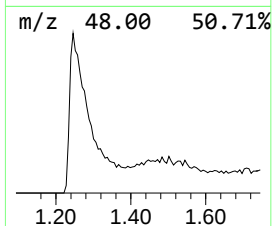
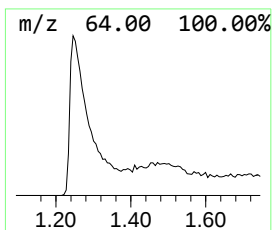
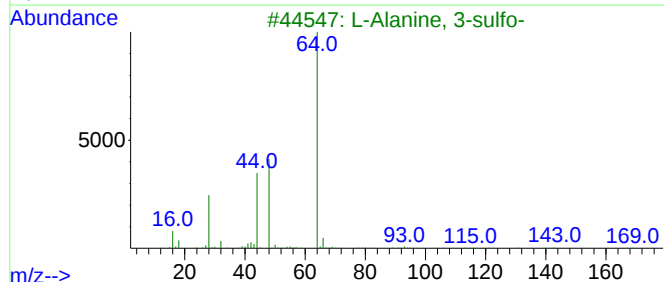
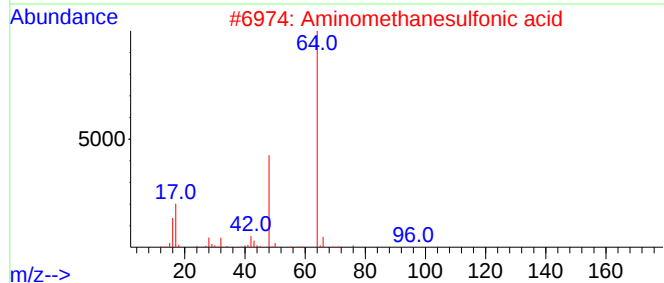
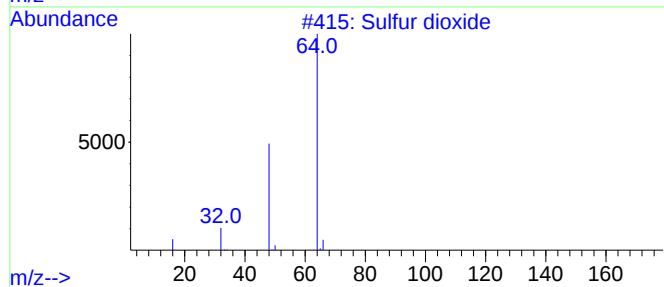
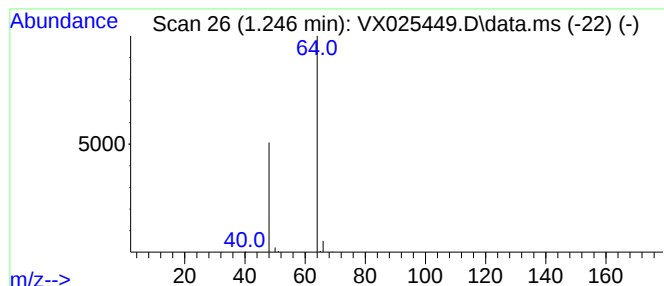
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	13.17 ug/l	79627	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	4



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Instrument :
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ClientSampleId :
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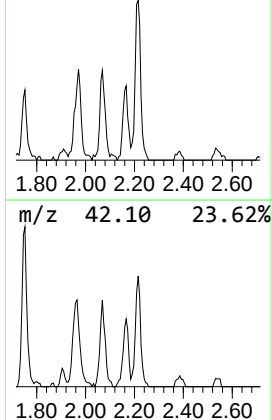
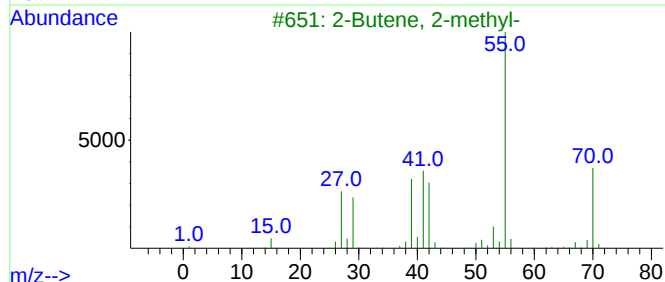
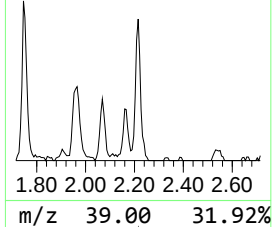
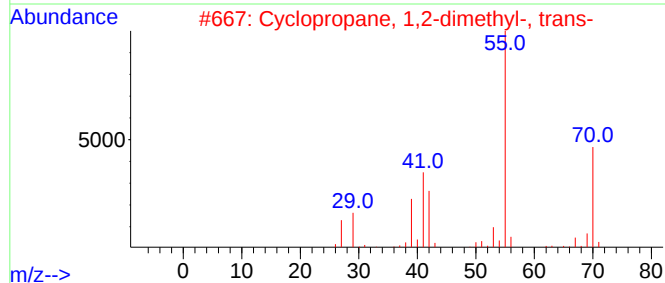
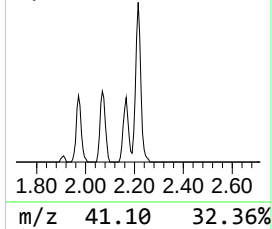
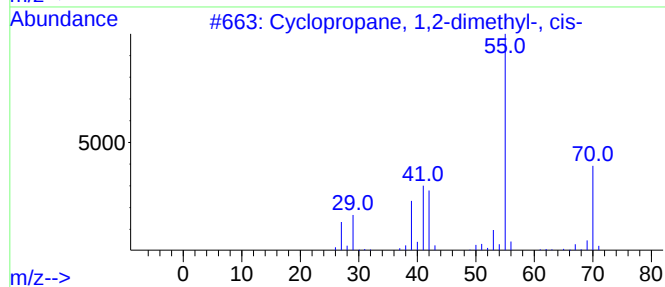
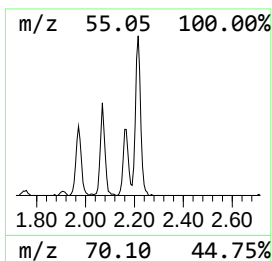
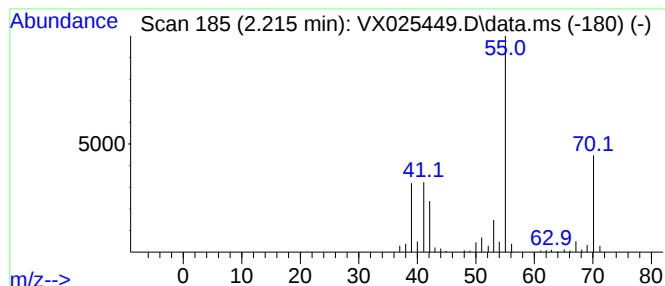
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 2 Cyclopropane, 1,2-dimethyl-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	6.70 ug/l	40516	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	86
2			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	80
3			2-Butene, 2-methyl-	70	C5H10	000513-35-9	78
4			1-Butene, 3-methyl-	70	C5H10	000563-45-1	72
5			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	72



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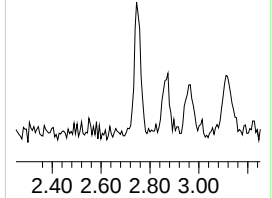
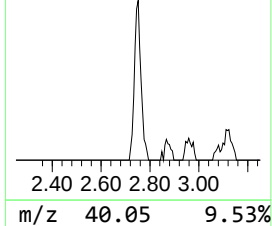
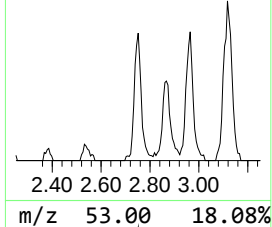
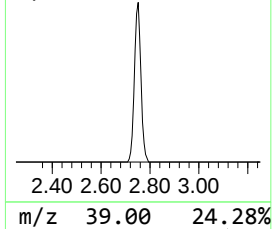
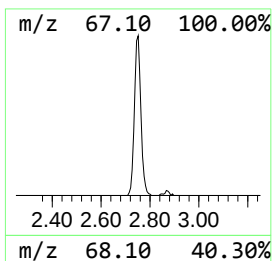
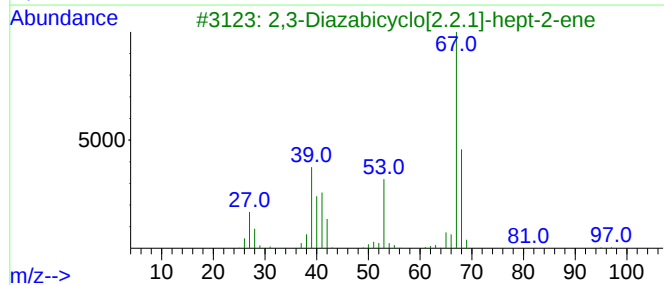
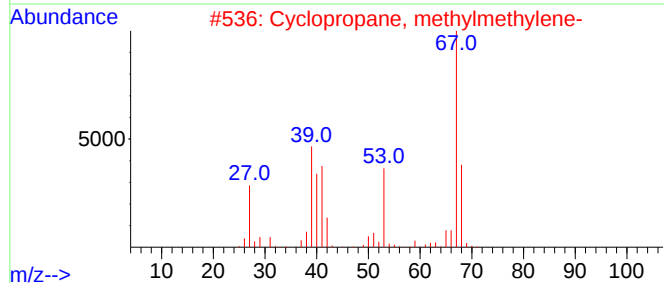
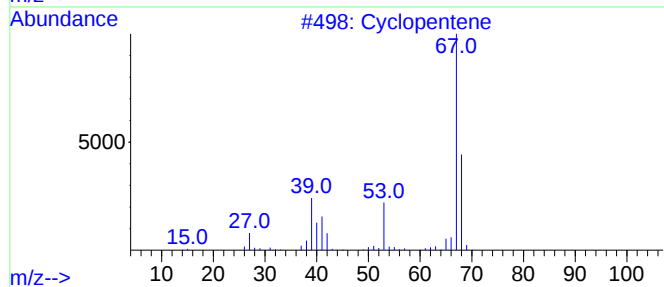
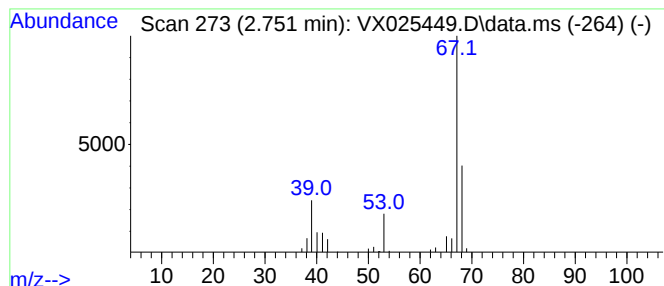
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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

Peak Number 3 Cyclopentene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.751	5.26 ug/l	31801	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentene	68	C5H8	000142-29-0	91
2			Cyclopropane, methylmethylene-	68	C5H8	018631-84-0	78
3			2,3-Diazabicyclo[2.2.1]-hept-2-ene	96	C5H8N2	002721-32-6	64
4			1,4-Pentadiene	68	C5H8	000591-93-5	58
5			1,3-Pentadiene	68	C5H8	000504-60-9	53



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Instrument :
MSVOA_X
ClientSampleId :
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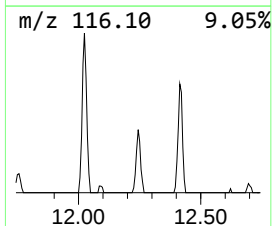
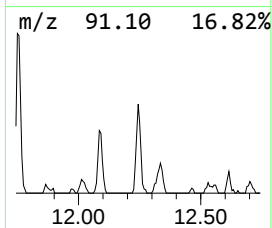
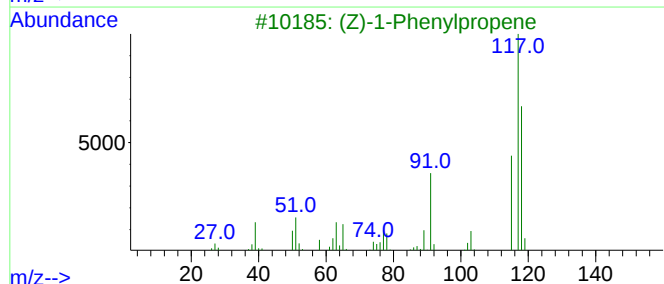
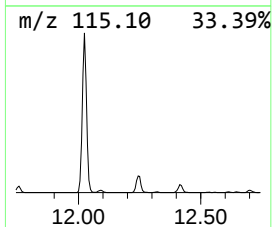
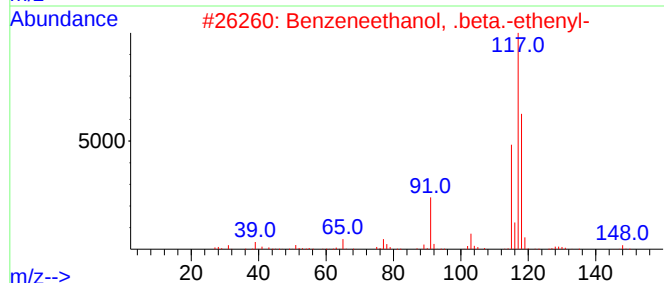
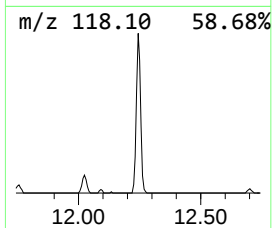
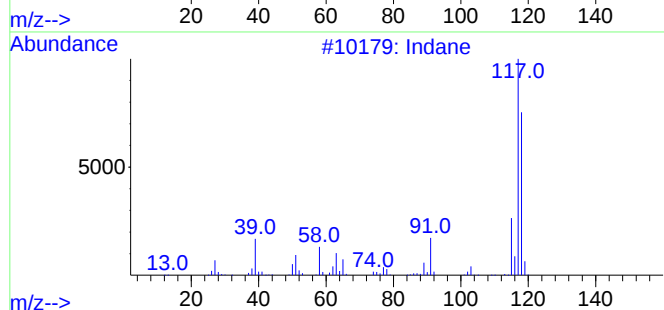
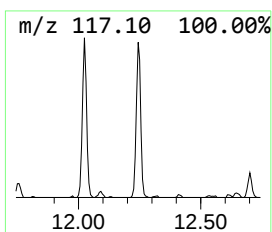
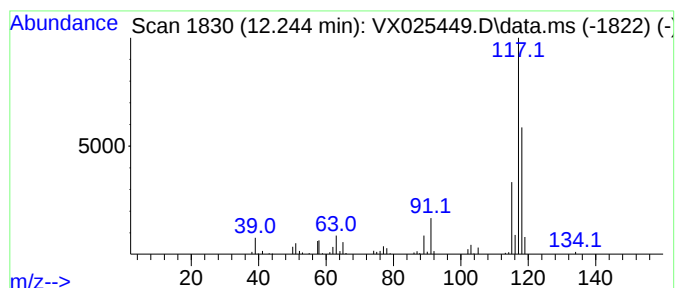
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Quant Title : SW846 8260

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

Peak Number 4 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	5.47 ug/l	48469	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	91
2			Benzeneethanol, .beta.-ethenyl-	148	C10H12O	006052-63-7	90
3			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	81
4			Benzene, 1-propenyl-	118	C9H10	000637-50-3	81
5			Benzene, cyclopropyl-	118	C9H10	000873-49-4	74



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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	1.246	13.2	ug/l	79627	1	5.556	302265	50.0
Cyclopropane, 1...	2.215	6.7	ug/l	40516	1	5.556	302265	50.0
Cyclopentene	2.751	5.3	ug/l	31801	1	5.556	302265	50.0
Indane	12.244	5.5	ug/l	48469	4	12.024	442943	50.0