

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040822\
 Data File : VX028021.D
 Acq On : 08 Apr 2022 12:51
 Operator : JC/MD
 Sample : N2333-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-1

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\82X040722W.M
 Title : SW846 8260

Signal : TIC: VX028021.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	21	29	39	rBV	19870	36062	4.29%	0.871%
2	1.374	43	47	51	rVV	22519	24011	2.85%	0.580%
3	1.752	104	109	118	rVB	27588	37968	4.51%	0.917%
4	2.215	180	185	191	rVB	8147	12473	1.48%	0.301%
5	2.337	200	205	210	rBV	5302	10981	1.30%	0.265%
6	2.776	267	277	285	rBV2	18590	44640	5.30%	1.079%
7	2.867	285	292	300	rVV	16132	31899	3.79%	0.771%
8	3.757	427	438	447	rBV6	4028	12438	1.48%	0.301%
9	4.221	503	514	521	rBV3	3750	11506	1.37%	0.278%
10	4.306	521	528	536	rVB3	3523	9335	1.11%	0.226%
11	5.391	694	706	718	rBV3	62337	187600	22.29%	4.533%
12	5.556	723	733	743	rBV	106459	300579	35.72%	7.263%
13	5.958	788	799	805	rBV	66929	178945	21.26%	4.324%
14	6.044	805	813	827	rVV	315511	841524	100.00%	20.334%
15	6.251	840	847	857	rVV	8456	26285	3.12%	0.635%
16	6.763	921	931	947	rBV	159550	383489	45.57%	9.267%
17	7.982	1125	1131	1139	rVB	8219	17209	2.04%	0.416%
18	8.110	1143	1152	1162	rBV	15893	32009	3.80%	0.773%
19	8.653	1226	1241	1248	rBV	328655	523252	62.18%	12.644%
20	8.964	1286	1292	1299	rVB4	8238	16732	1.99%	0.404%
21	9.049	1299	1306	1311	rBV	8684	13883	1.65%	0.335%
22	10.055	1465	1471	1481	rBV	356183	470469	55.91%	11.368%
23	10.963	1611	1620	1626	rBV	8063	10676	1.27%	0.258%
24	11.085	1634	1640	1645	rBV	282309	373909	44.43%	9.035%
25	11.305	1672	1676	1680	rBV	8782	10187	1.21%	0.246%
26	12.024	1789	1794	1804	rBV	376754	454248	53.98%	10.976%
27	12.244	1823	1830	1836	rBV	45974	57461	6.83%	1.388%
28	12.926	1938	1942	1946	rVB	6763	8655	1.03%	0.209%

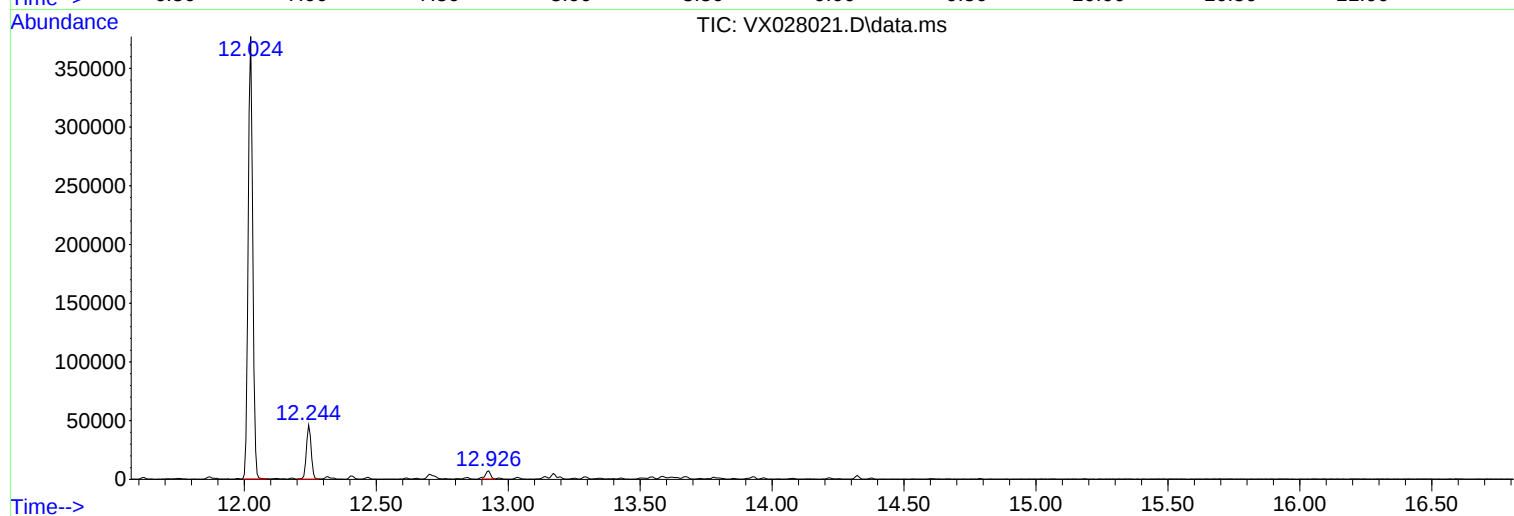
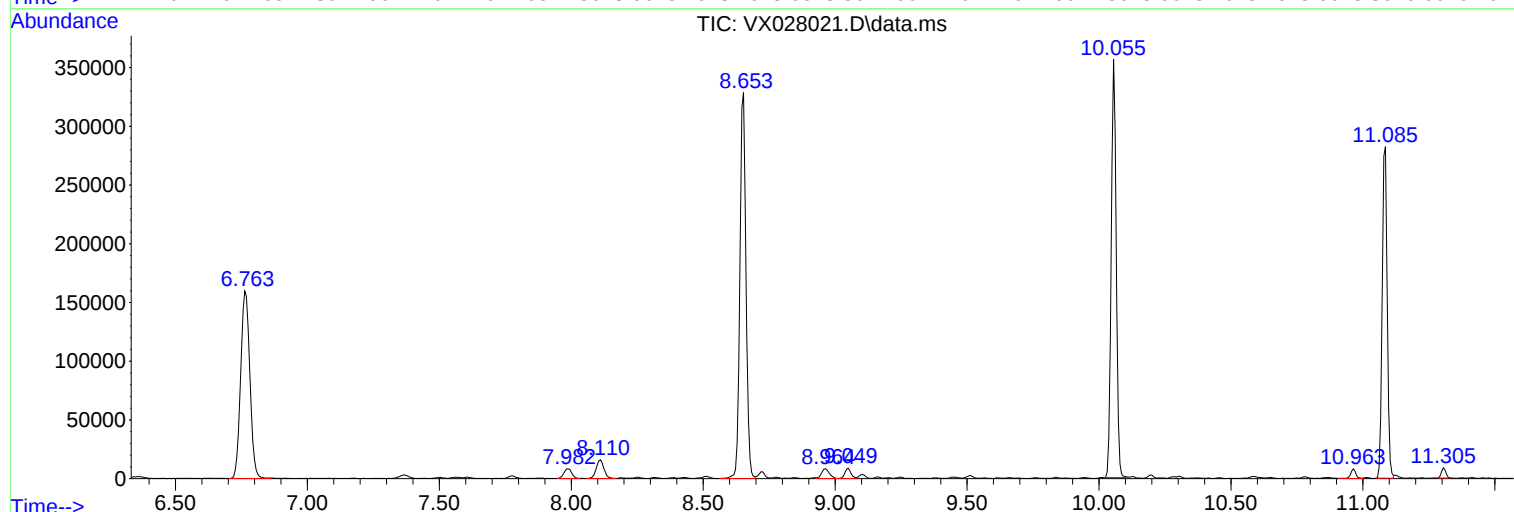
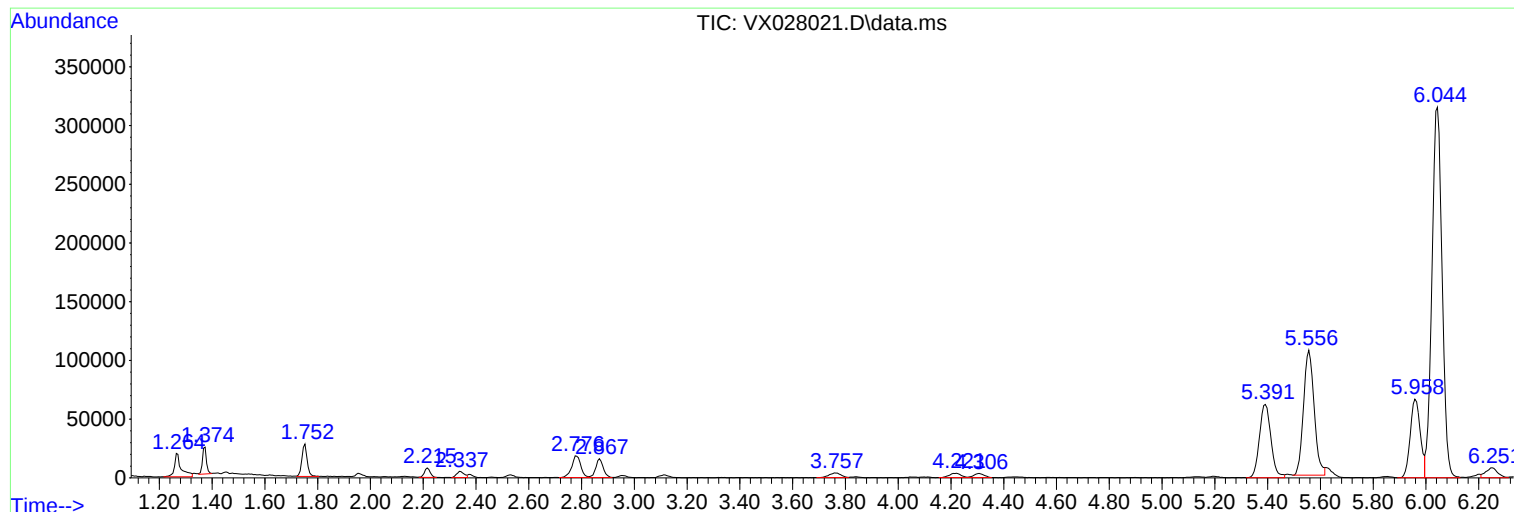
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Instrument :
MSVOA_X
ClientSampleId :
MW-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040722W.M
Quant Title : SW846 8260

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



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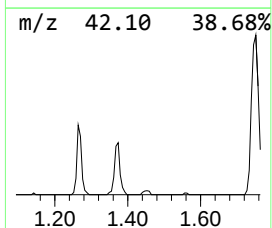
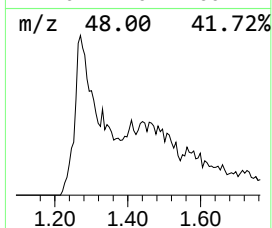
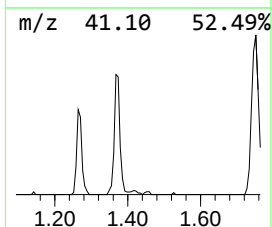
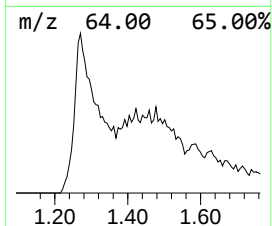
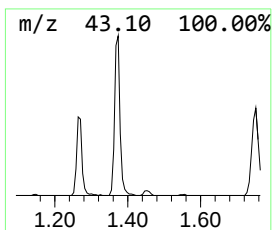
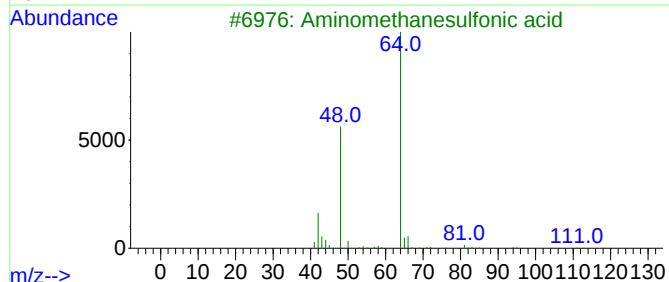
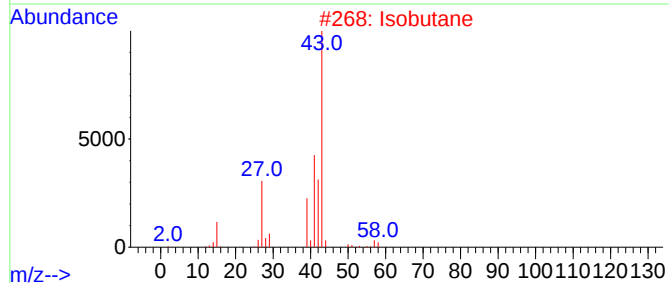
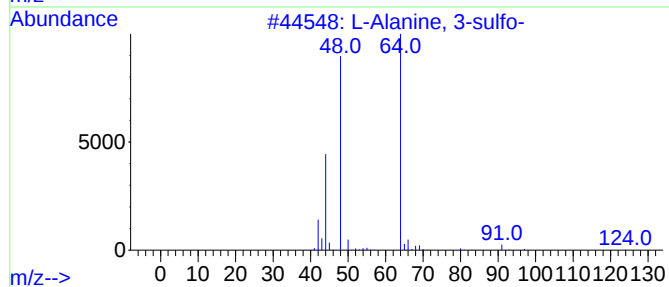
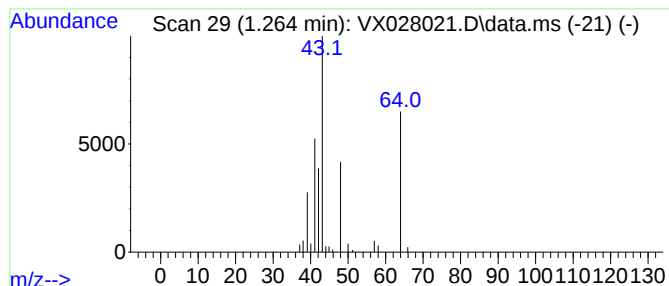
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040722W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown1.264 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	6.00 ug/l	36062	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	38
2			Isobutane	58	C4H10	000075-28-5	10
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			Propane, 1-chloro-2-methyl-	92	C4H9Cl	000513-36-0	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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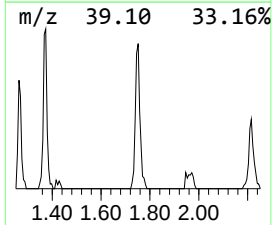
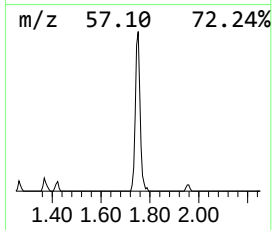
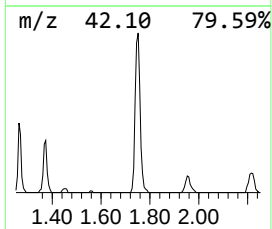
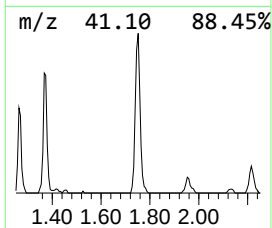
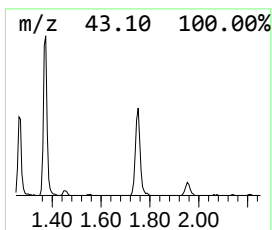
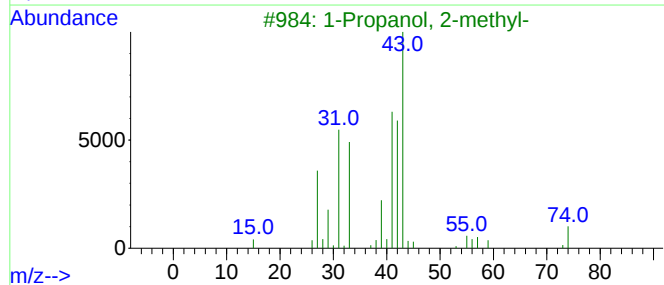
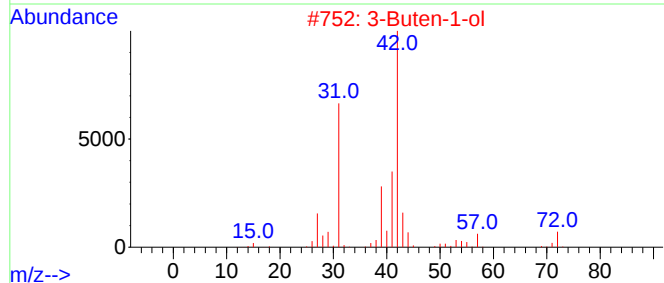
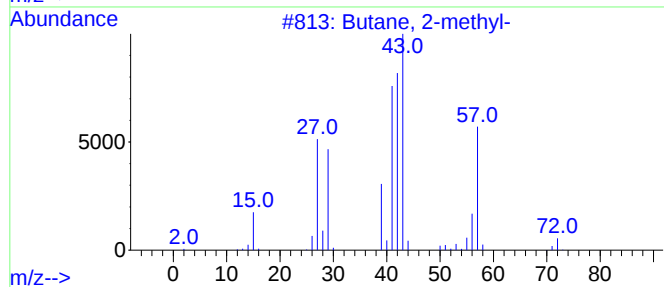
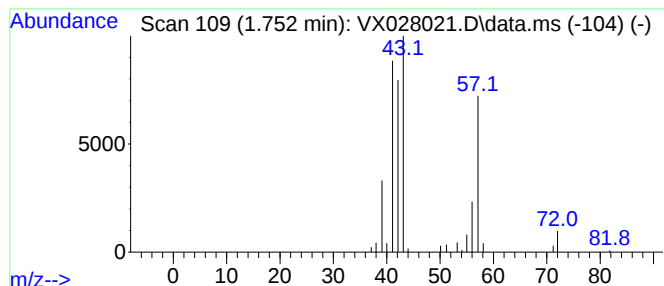
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040722W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	6.32 ug/l	37968	Pentafluorobenzene	5.556

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	47
3			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	38
4			Pentane	72	C5H12	000109-66-0	33
5			Oxirane, trimethyl-	86	C5H10O	005076-19-7	33



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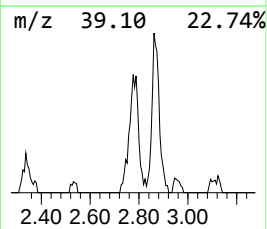
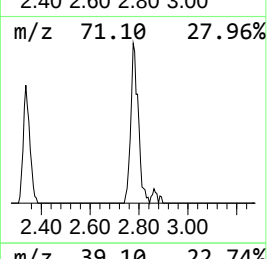
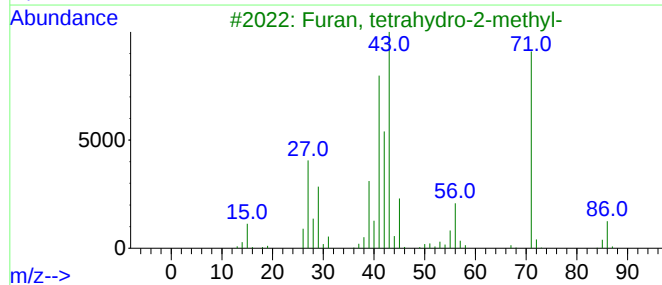
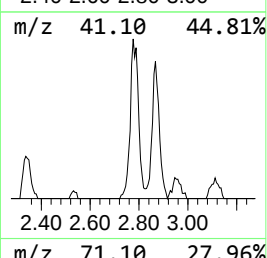
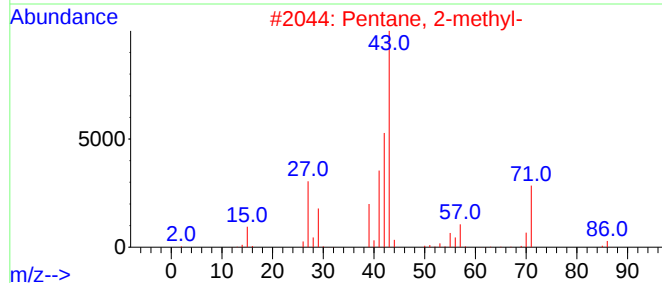
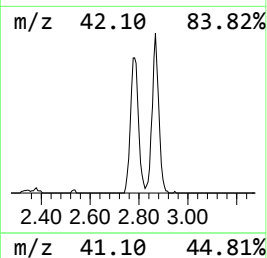
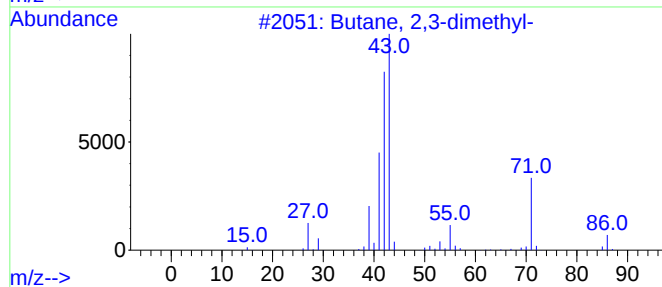
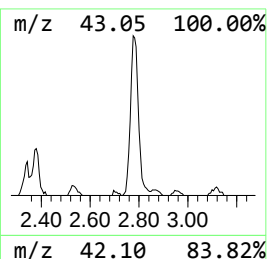
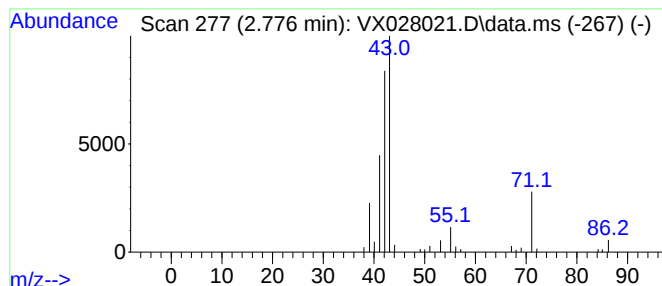
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040722W.M
Quant Title : SW846 8260

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

Peak Number 3 Butane, 2,3-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.776	7.43 ug/l	44640	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	14
4			3-Buten-2-ol, 3-methyl-	86	C5H10O	010473-14-0	9
5			Tetrahydrofuran	72	C4H8O	000109-99-9	9



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ClientSampleId :
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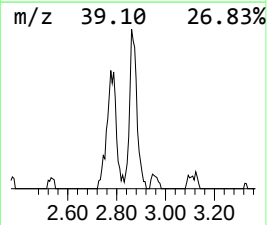
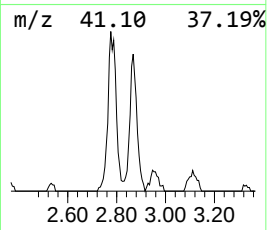
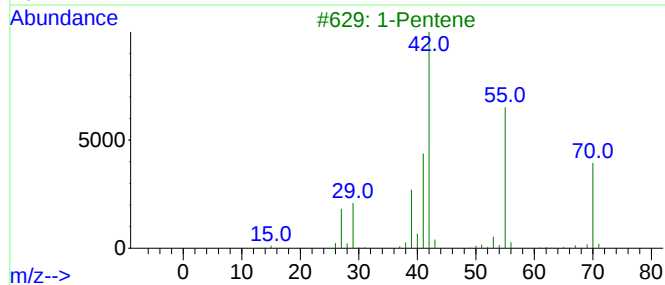
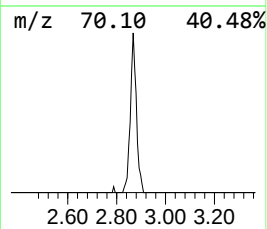
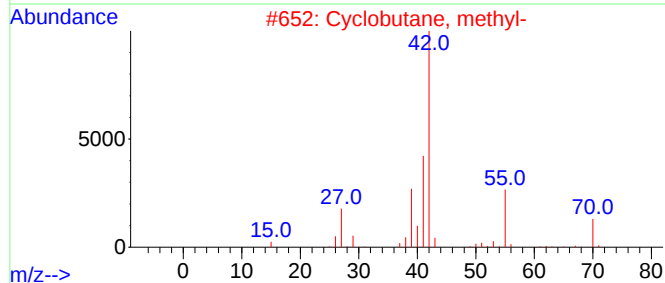
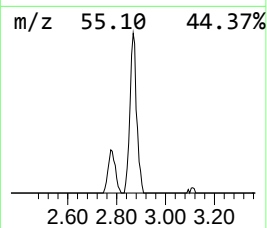
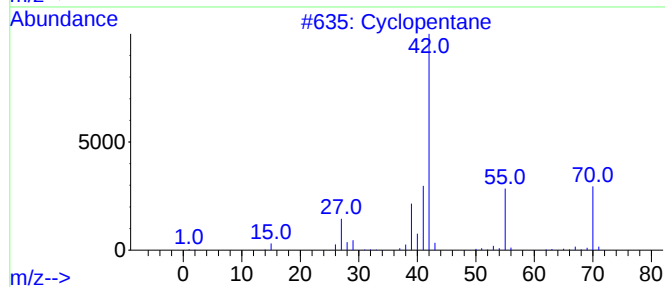
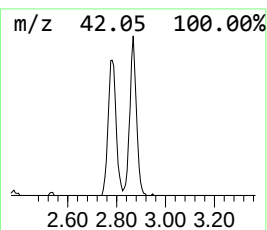
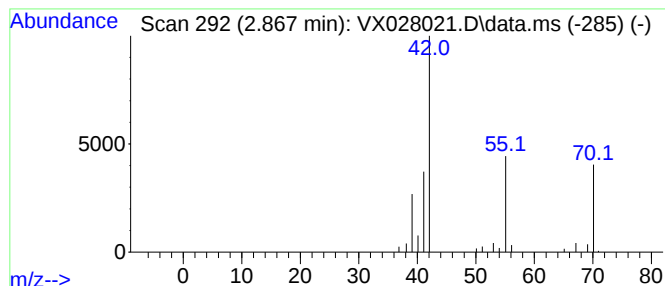
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Quant Title : SW846 8260

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

Peak Number 4 Cyclopentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	5.31 ug/l	31899	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane	70	C5H10	000287-92-3	90
2			Cyclobutane, methyl-	70	C5H10	000598-61-8	78
3			1-Pentene	70	C5H10	000109-67-1	72
4			Cyclopropane, ethyl-	70	C5H10	001191-96-4	39
5			Cyclobutanone	70	C4H6O	001191-95-3	9



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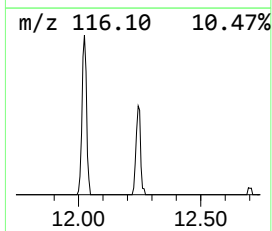
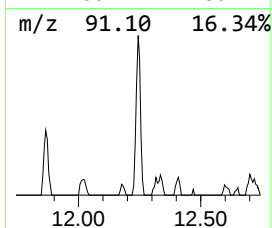
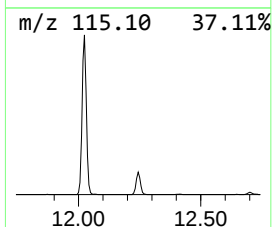
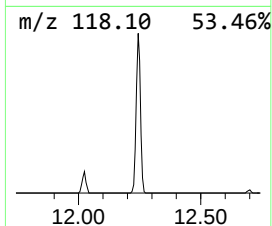
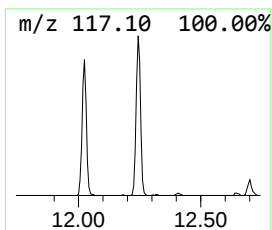
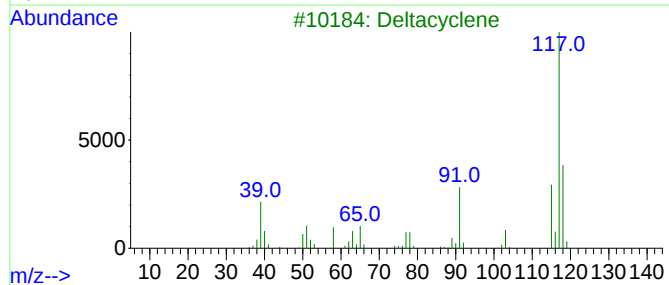
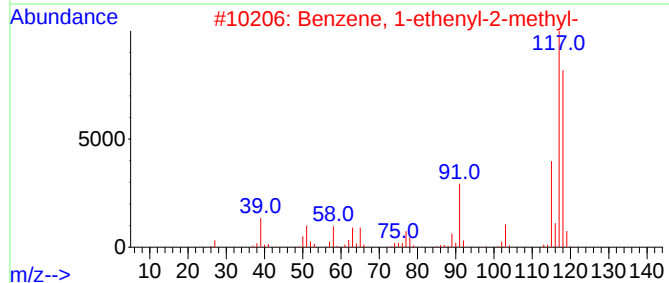
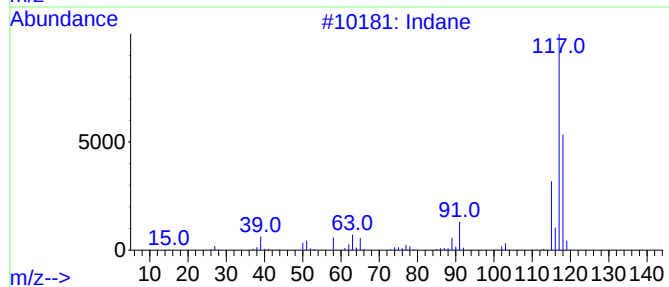
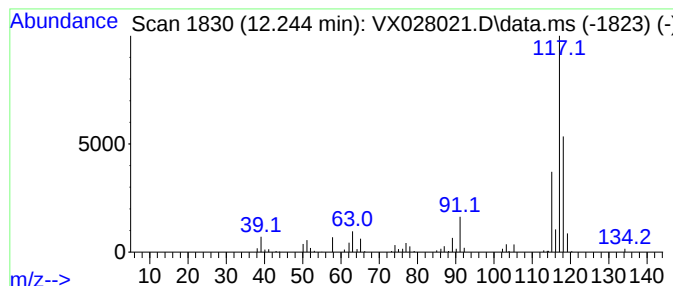
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040722W.M
Quant Title : SW846 8260

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

Peak Number 5 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	6.32 ug/l	57461	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	94
2			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	83
3			Deltacyclene	118	C9H10	007785-10-6	64
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
5			Benzene, 1-propenyl-	118	C9H10	000637-50-3	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.264	1.264	6.0	ug/l	36062	1	5.556	300579	50.0
Butane, 2-methyl-	1.752	6.3	ug/l	37968	1	5.556	300579	50.0
Butane, 2,3-dim...	2.776	7.4	ug/l	44640	1	5.556	300579	50.0
Cyclopentane	2.867	5.3	ug/l	31899	1	5.556	300579	50.0
Indane	12.244	6.3	ug/l	57461	4	12.024	454248	50.0