

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120522\
 Data File : VX033241.D
 Acq On : 05 Dec 2022 21:13
 Operator : JC/MD
 Sample : N5875-07
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-41

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\82X112222W.M
 Title : SW846 8260

Signal : TIC: VX033241.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.136	300	336	364	rBV5	24966561	168820831	100.00%	70.133%
2	6.044	803	813	828	rVB	2708959	7100158	4.21%	2.950%
3	6.330	828	860	893	rVB	6923752	29198773	17.30%	12.130%
4	8.446	1193	1207	1213	rBV	1583250	3080264	1.82%	1.280%
5	8.525	1213	1220	1235	rVV	4681765	8416624	4.99%	3.497%
6	8.860	1264	1275	1289	rBV	4779735	8066591	4.78%	3.351%
7	10.031	1459	1467	1475	rBV2	1583702	2911406	1.72%	1.209%
8	10.153	1483	1487	1490	rVV	1900864	2432893	1.44%	1.011%
9	10.195	1490	1494	1498	rVV	1703880	2202622	1.30%	0.915%
10	10.305	1507	1512	1517	rVB	3239227	4436782	2.63%	1.843%
11	11.378	1683	1688	1695	rVV	1068675	1888774	1.12%	0.785%
12	11.750	1745	1749	1754	rBV	1799604	2158084	1.28%	0.897%

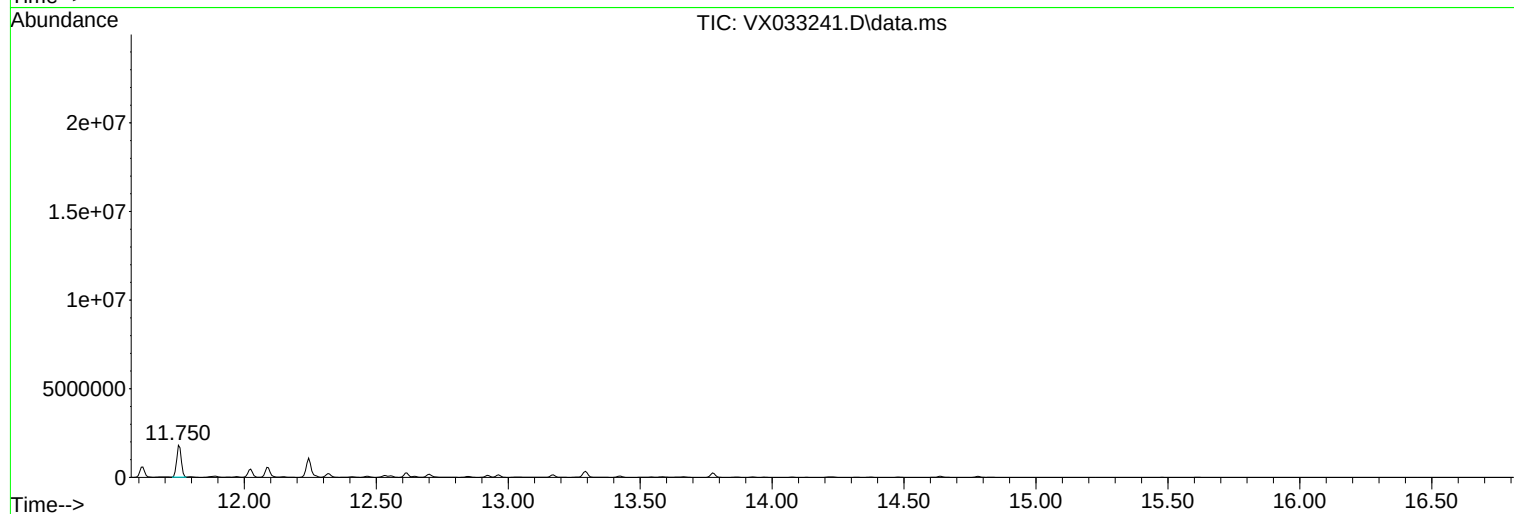
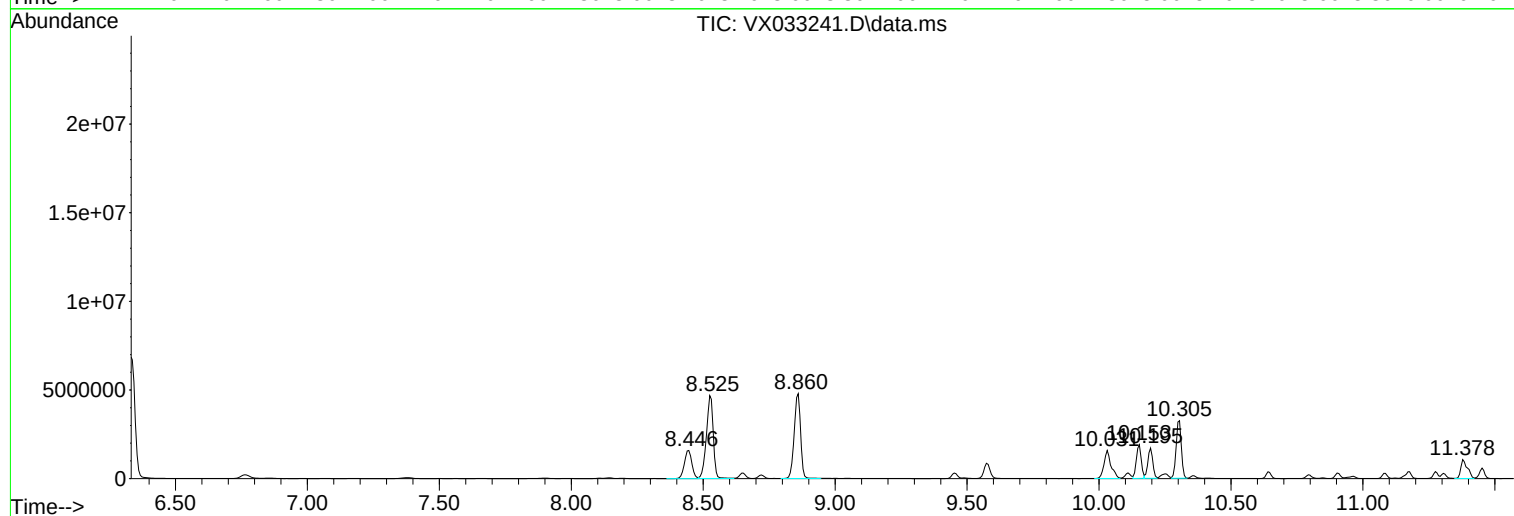
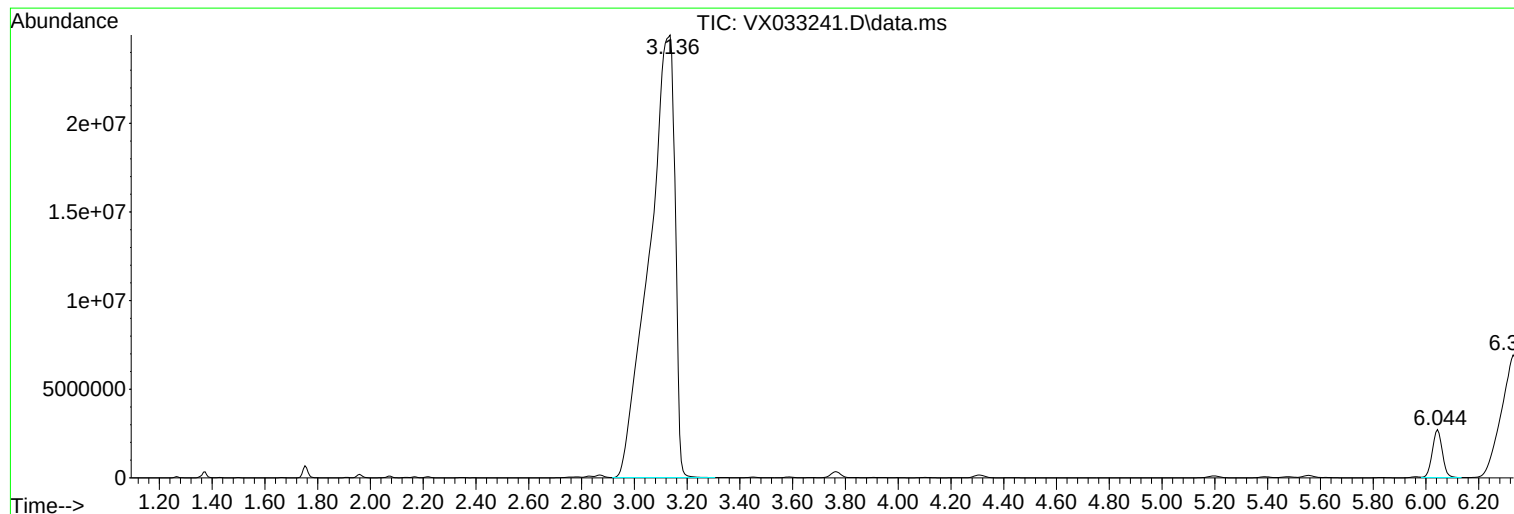
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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



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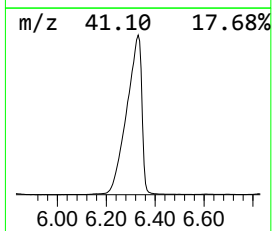
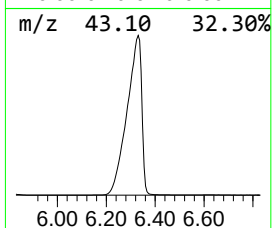
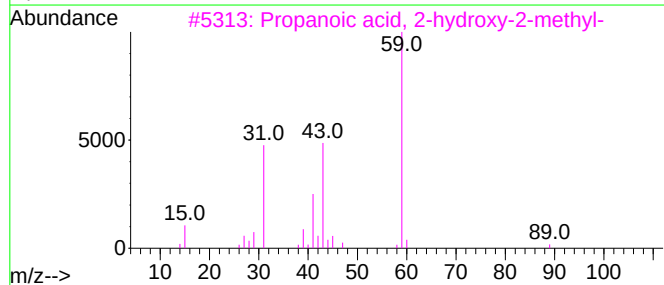
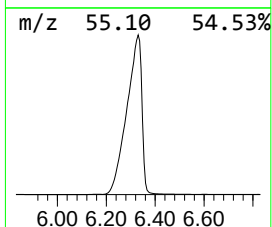
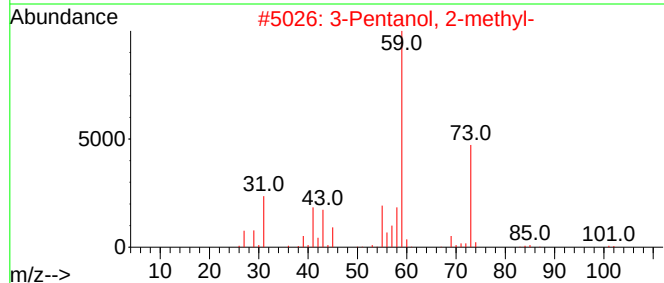
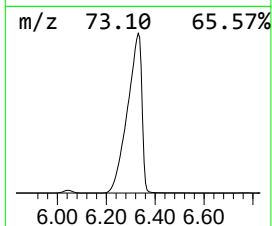
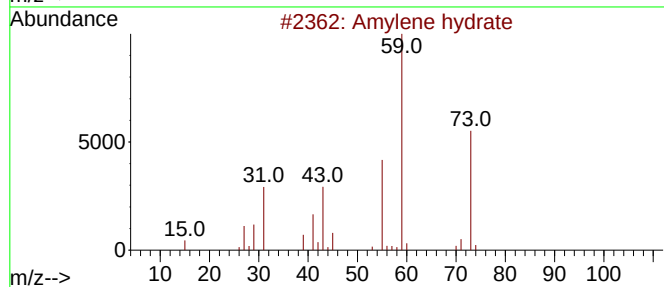
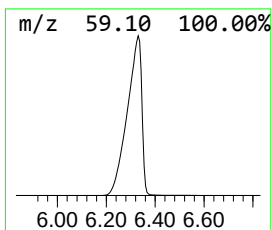
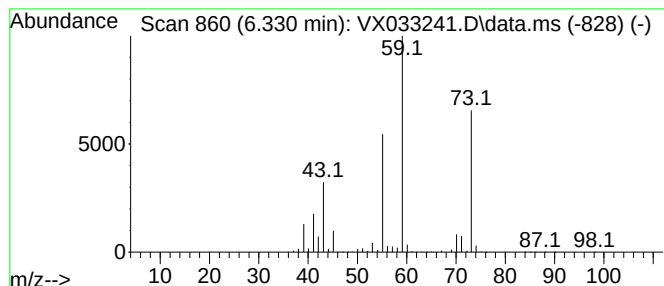
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

Peak Number 1 Amylene hydrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.330	50.00 ug/l	29198800	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Amylene hydrate	88	C5H12O	000075-85-4	83
2			3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	39
3			Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	36
4			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	22
5			Silane, trimethyl-	74	C3H10Si	000993-07-7	9



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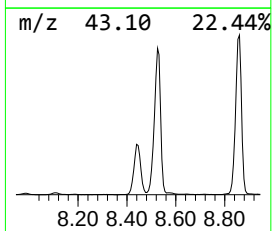
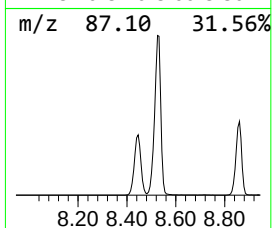
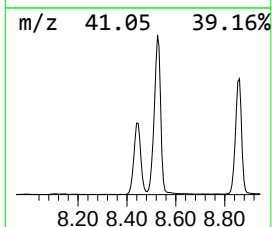
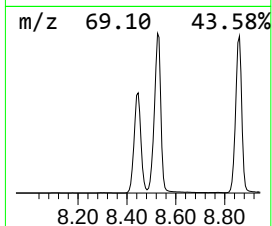
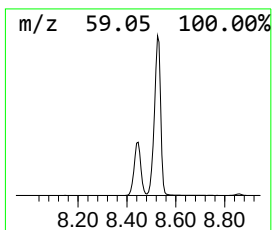
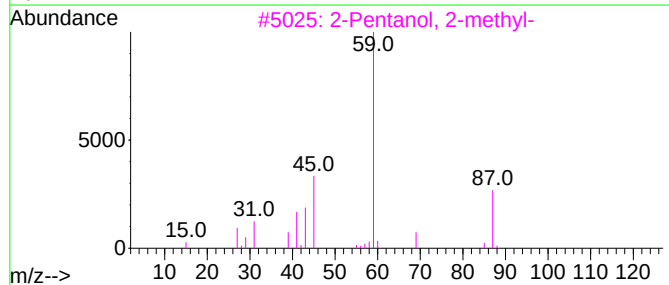
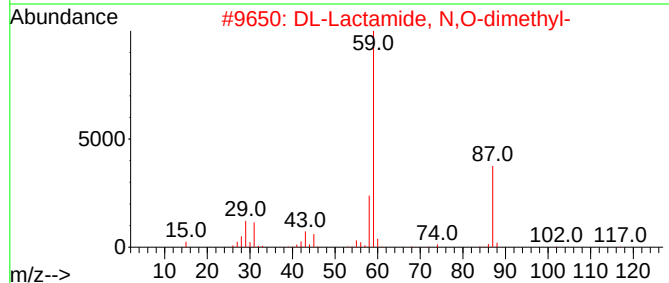
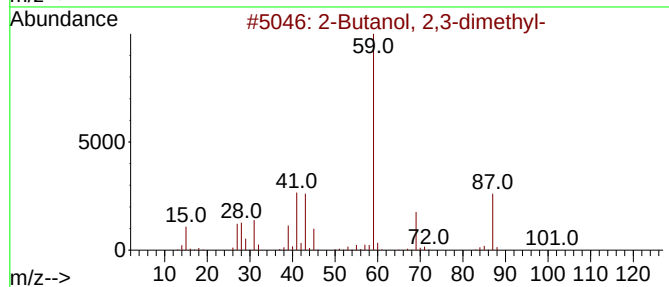
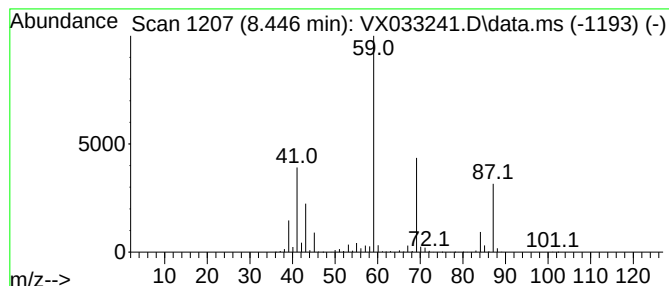
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Quant Title : SW846 8260

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

Peak Number 2 2-Butanol, 2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.446	52.90 ug/l	3080260	Chlorobenzene-d5	10.055

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	72
2		DL-Lactamide, N,O-dimethyl-	117	C5H11NO2	1000452-56-3	64
3		2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	59
4		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	45
5		3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	38



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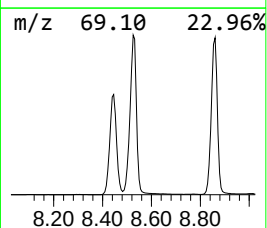
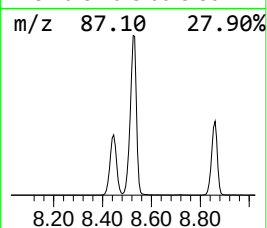
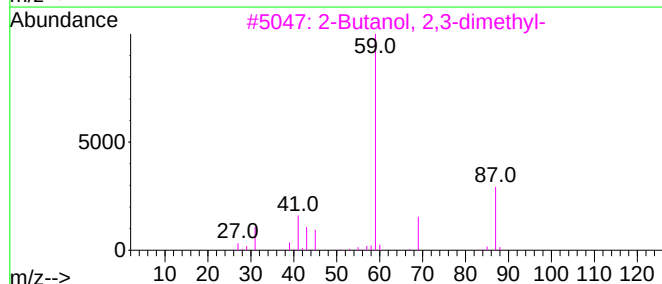
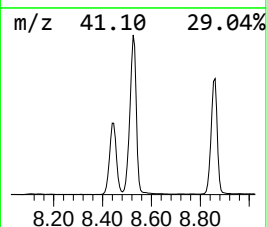
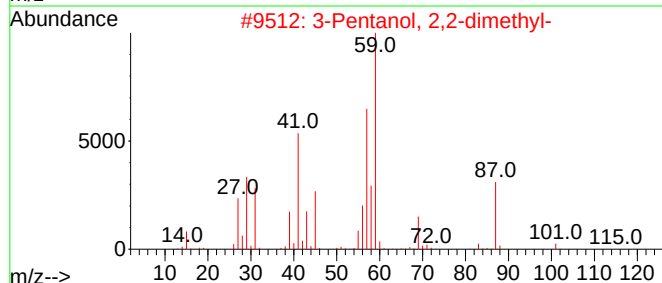
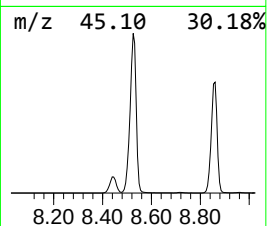
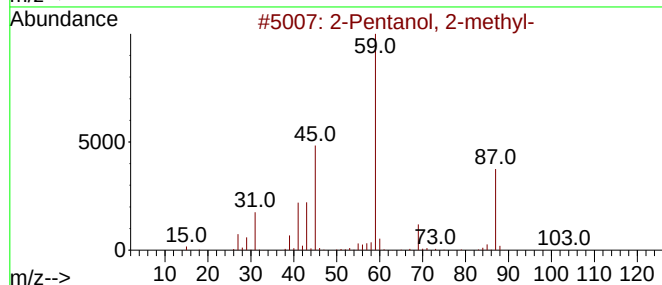
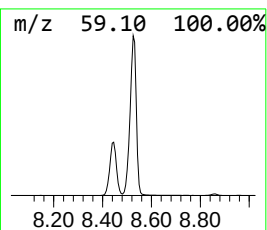
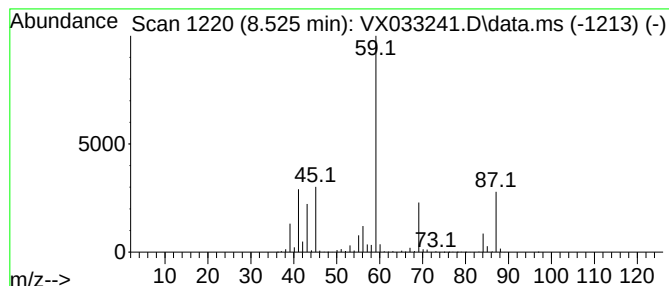
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Peak Number 3 2-Pentanol, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.525	144.55 ug/l	8416620	Chlorobenzene-d5	10.055

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	78
2		3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	56
3		2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	56
4		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	45
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	40



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ALS Vial : 26 Sample Multiplier: 1

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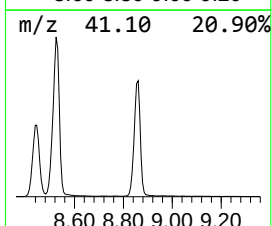
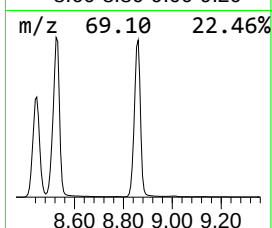
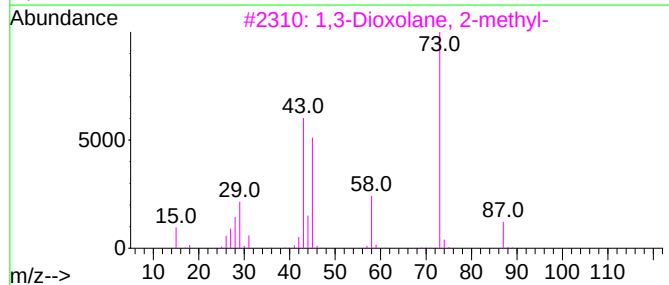
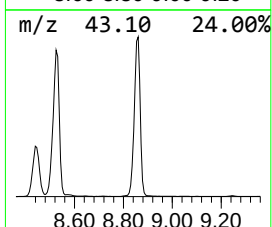
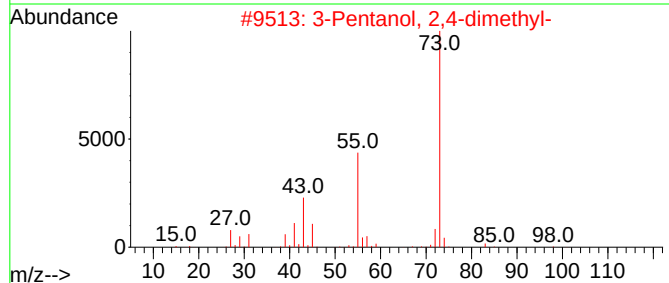
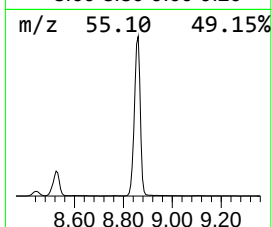
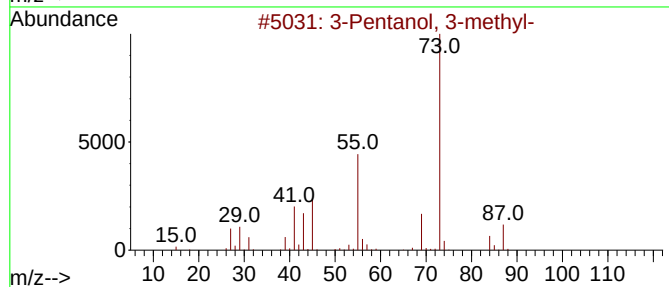
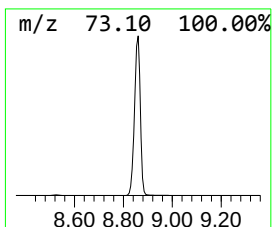
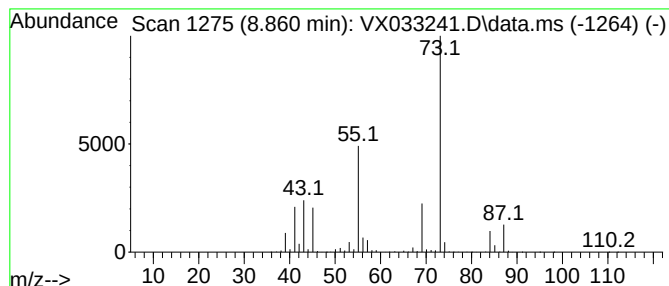
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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

Peak Number 4 3-Pentanol, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.860	138.53 ug/l	8066590	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	47
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	47
4			3-Methylpentan-3-yl propyl carbo...	188	C10H20O3	1000372-82-3	33
5			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	28



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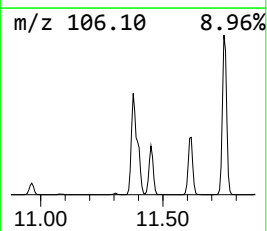
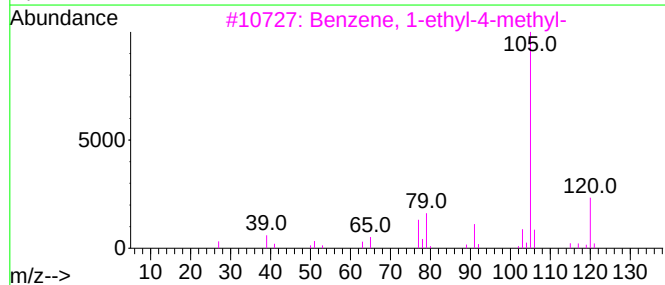
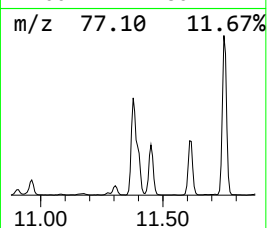
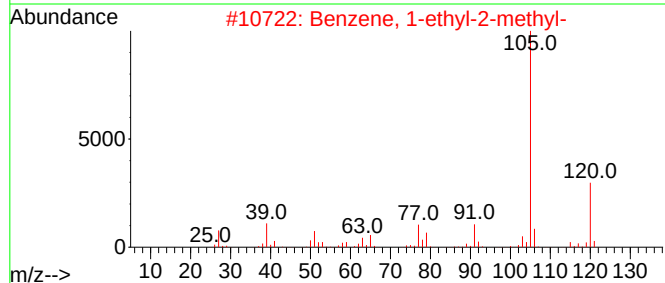
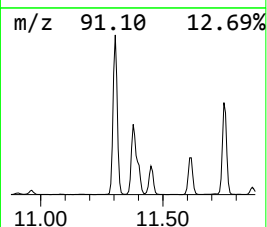
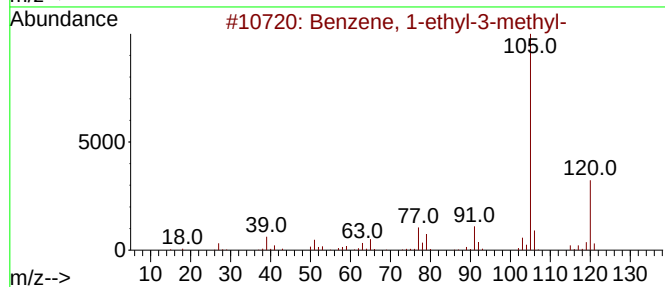
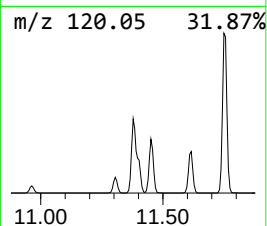
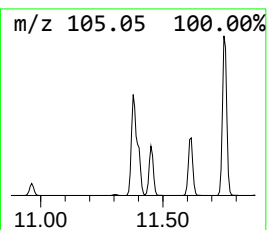
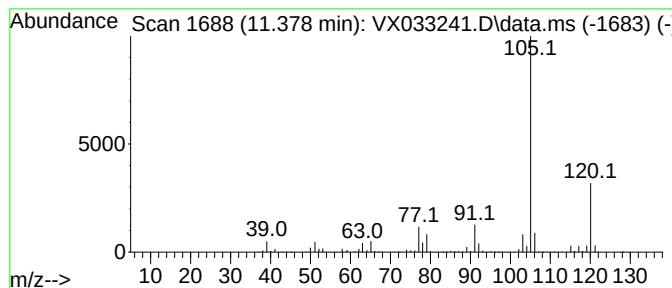
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzene, 1-ethyl-3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	43.76 ug/l	1888770	1,4-Dichlorobenzene-d4	12.024

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



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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
Amylene hydrate	6.330	50.0	ug/l	29198800	2	6.763	29198800	50.0
2-Butanol, 2,3-...	8.446	52.9	ug/l	3080260	3	10.055	2911410	50.0
2-Pentanol, 2-m...	8.525	144.6	ug/l	8416620	3	10.055	2911410	50.0
3-Pentanol, 3-m...	8.860	138.5	ug/l	8066590	3	10.055	2911410	50.0
Benzene, 1-ethy...	11.378	43.8	ug/l	1888770	4	12.024	2158080	50.0