

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122623\
 Data File : VX039467.D
 Acq On : 26 Dec 2023 15:04
 Operator : JC/MD
 Sample : 06014-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 AUD-1307

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\82X121323W.M
 Title : SW846 8260

Signal : TIC: VX039467.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	21	rVB	186332	184689	23.59%	2.607%
2	1.239	21	25	27	rBV	19907	25118	3.21%	0.355%
3	1.264	27	29	33	rVB2	18803	19025	2.43%	0.269%
4	1.374	42	47	53	rVB	20315	20710	2.65%	0.292%
5	1.453	56	60	66	rBV	456385	574637	73.40%	8.111%
6	1.514	66	70	84	rVB	56620	129069	16.49%	1.822%
7	1.721	101	104	110	rVB2	6353	9189	1.17%	0.130%
8	2.099	158	166	177	rVB	28052	60462	7.72%	0.853%
9	2.386	206	213	223	rVB	14046	26750	3.42%	0.378%
10	2.995	298	313	324	rBV3	19453	69130	8.83%	0.976%
11	4.245	509	518	522	rBV5	3194	8572	1.09%	0.121%
12	5.385	694	705	717	rBV2	82556	245540	31.36%	3.466%
13	5.550	723	732	756	rVB	121529	353681	45.18%	4.992%
14	5.958	785	799	805	rBV	95556	262715	33.56%	3.708%
15	6.037	805	812	826	rVB	254053	672865	85.95%	9.498%
16	6.763	922	931	947	rBV	227681	552678	70.59%	7.801%
17	7.244	1005	1010	1020	rBV4	4409	11604	1.48%	0.164%
18	7.385	1026	1033	1039	rVB4	5492	12798	1.63%	0.181%
19	7.903	1112	1118	1127	rBV3	4330	9916	1.27%	0.140%
20	8.647	1233	1240	1248	rBV	501564	782894	100.00%	11.051%
21	8.720	1248	1252	1264	rVB	31550	54775	7.00%	0.773%
22	9.488	1367	1378	1387	rBV3	13348	24344	3.11%	0.344%
23	10.055	1465	1471	1484	rBV	539052	732745	93.59%	10.343%
24	10.195	1490	1494	1504	rVB	6398	9140	1.17%	0.129%
25	10.305	1504	1512	1524	rBV2	117440	188254	24.05%	2.657%
26	10.409	1524	1529	1533	rBV	30013	39023	4.98%	0.551%
27	10.640	1563	1567	1574	rBV	11857	16756	2.14%	0.237%
28	10.963	1615	1620	1625	rBV	11792	14796	1.89%	0.209%
29	11.079	1634	1639	1647	rBV	436439	568130	72.57%	8.019%
30	11.305	1669	1676	1683	rBV2	11987	19249	2.46%	0.272%
31	11.451	1697	1700	1711	rVB	25391	34091	4.35%	0.481%
32	11.610	1722	1726	1733	rVB	16964	23199	2.96%	0.327%
33	11.683	1733	1738	1745	rBV	40987	53333	6.81%	0.753%
34	11.750	1745	1749	1755	rVB	44800	60126	7.68%	0.849%
35	11.988	1782	1788	1789	rBV2	15262	19507	2.49%	0.275%
36	12.024	1789	1794	1800	rVV	540267	716938	91.58%	10.120%

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Integration Parameters: RTEINT.P

Integrator: RTE

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Filtering: 5

Sampling : 1

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Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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Title : SW846 8260

37	12.085	1800	1804	1810	rVB	44680	56424	7.21%	0.796%
38	12.219	1822	1826	1828	rBV	13640	17772	2.27%	0.251%
39	12.317	1838	1842	1851	rVB7	6245	12575	1.61%	0.178%
40	12.585	1881	1886	1901	rBV	66998	113890	14.55%	1.608%
41	13.676	2058	2065	2074	rBV	19452	32433	4.14%	0.458%
42	13.774	2077	2081	2088	rVB	38466	49247	6.29%	0.695%
43	14.194	2145	2150	2160	rBV2	36029	70273	8.98%	0.992%
44	14.566	2206	2211	2218	rBV2	24708	37207	4.75%	0.525%
45	14.780	2238	2246	2252	rBV2	9496	12641	1.61%	0.178%
46	16.090	2455	2461	2472	rBV2	46317	75558	9.65%	1.067%

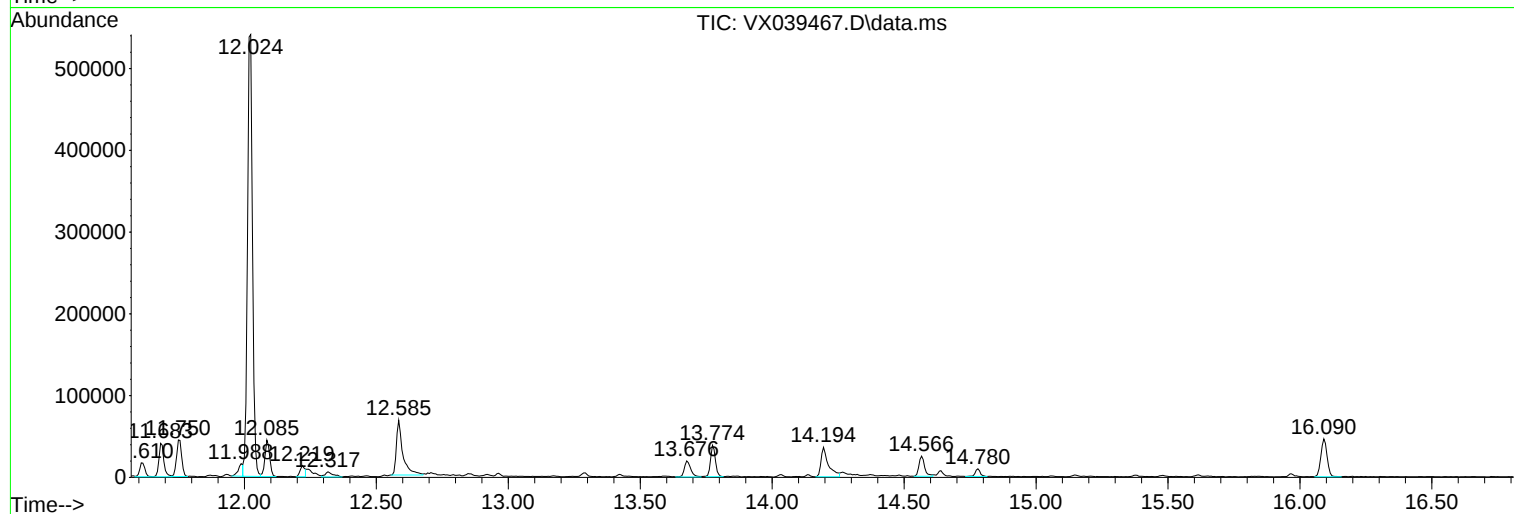
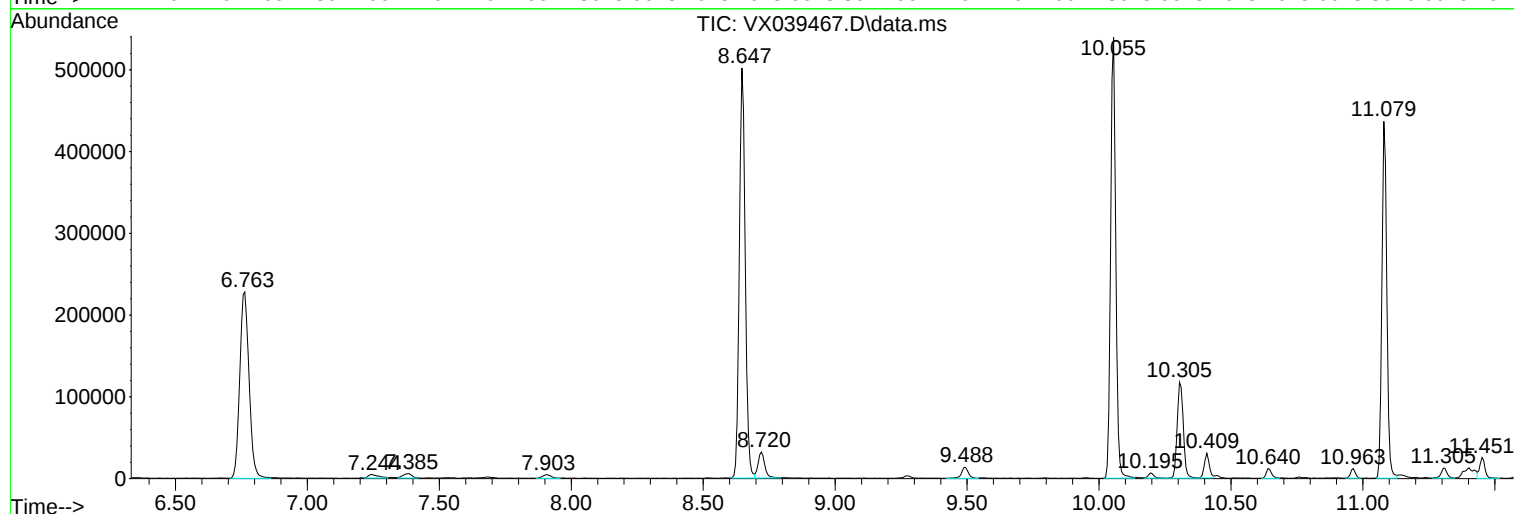
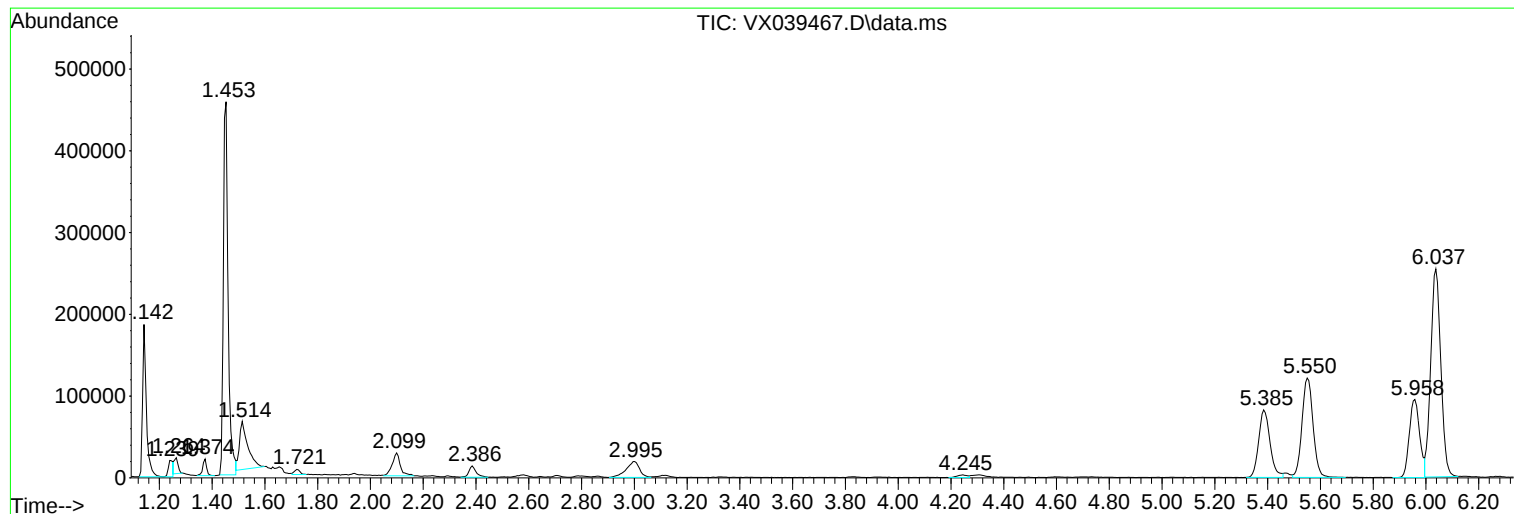
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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



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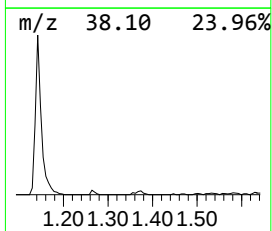
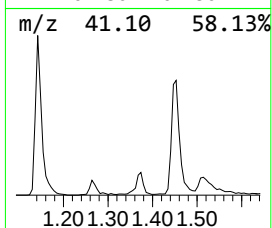
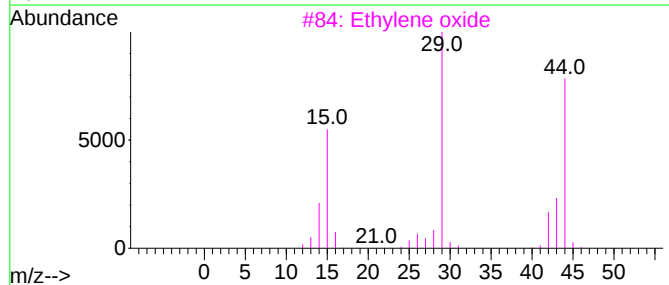
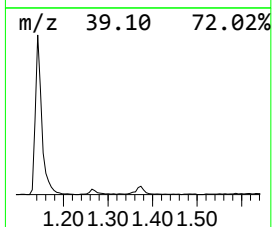
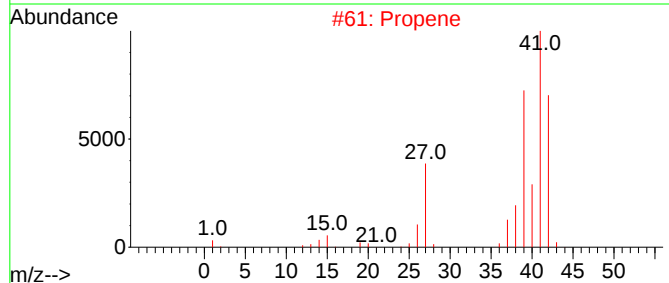
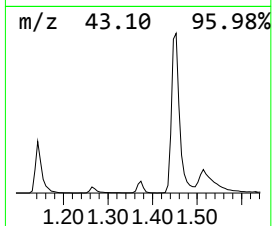
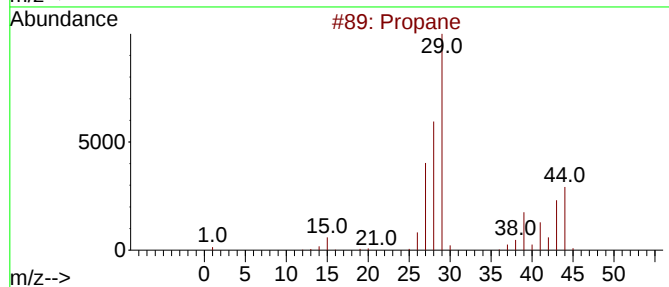
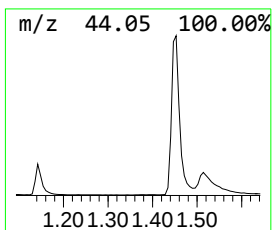
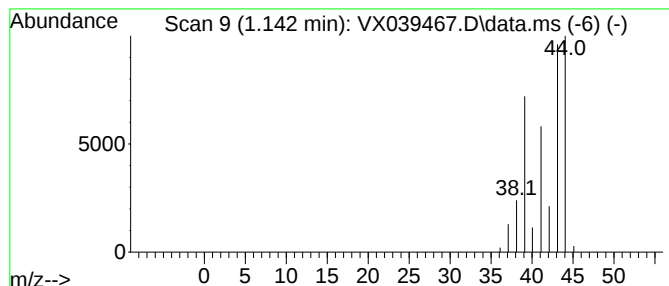
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 1 Propane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.142	26.11 ug/l	184689	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane			44	C3H8	000074-98-6	83
2	Propene			42	C3H6	000115-07-1	9
3	Ethylene oxide			44	C2H4O	000075-21-8	5
4	Acetonitrile-d3			44	C2D3N	002206-26-0	4
5	Acetaldehyde			44	C2H4O	000075-07-0	4



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Instrument :
MSVOA_X
ClientSampleId :
AUD-1307

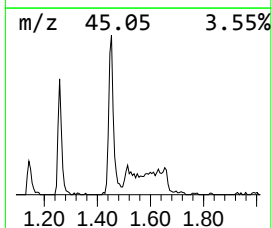
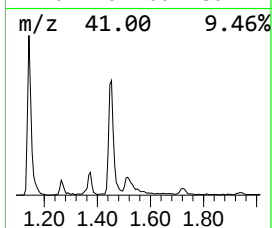
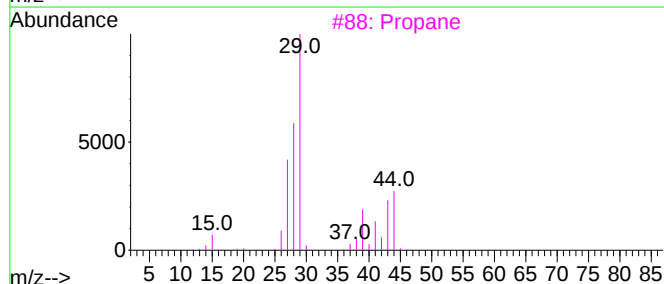
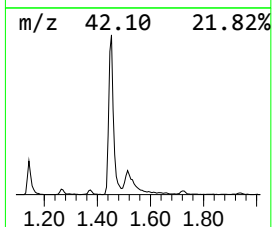
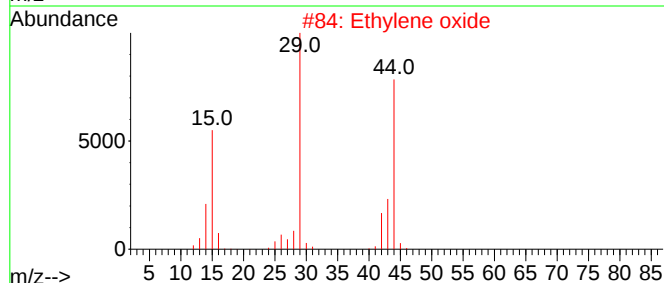
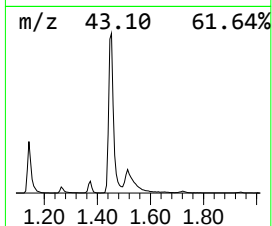
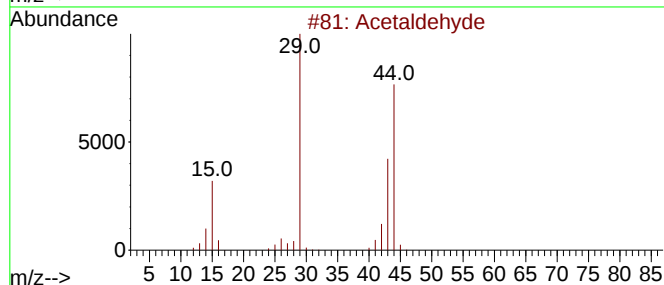
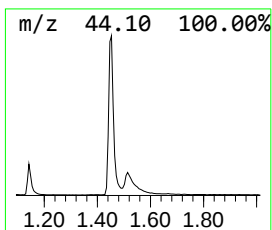
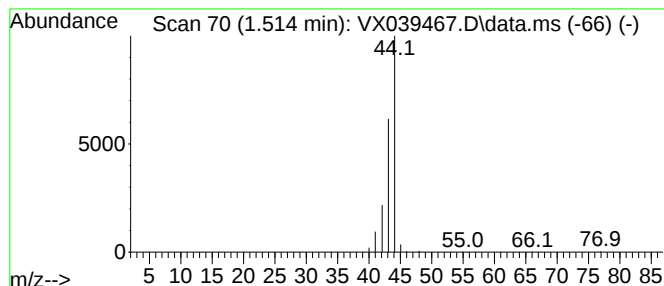
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 3 Acetaldehyde Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.514	18.25 ug/l	129069	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	64
2			Ethylene oxide	44	C2H4O	000075-21-8	9
3			Propane	44	C3H8	000074-98-6	5
4			Cyclopropyl carbinol	72	C4H8O	002516-33-8	4
5			2-(2-Aminoethanesulfonyl)propane	151	C5H13NO2S	320337-16-4	4



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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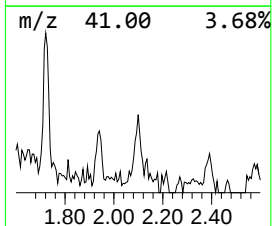
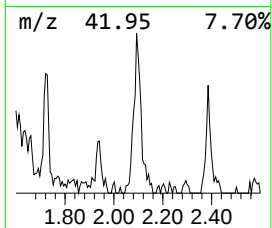
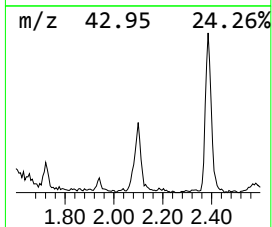
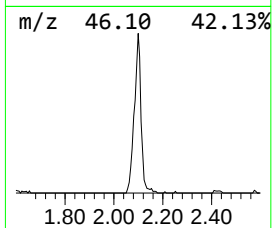
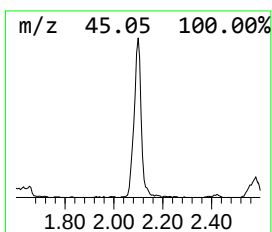
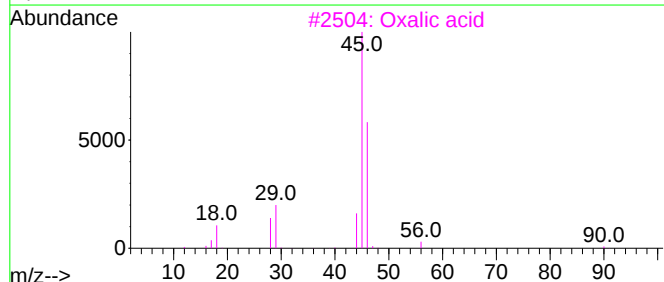
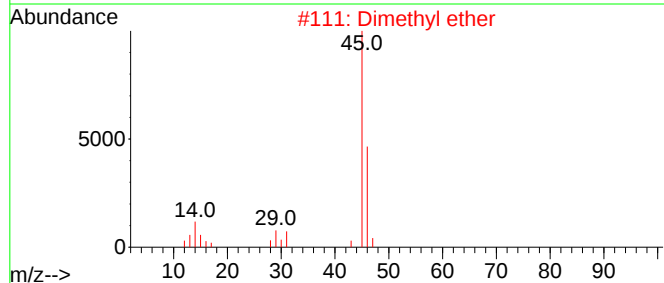
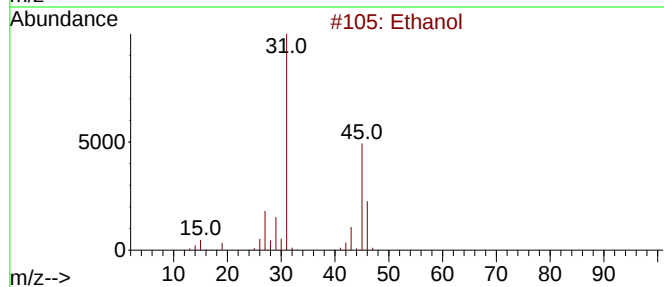
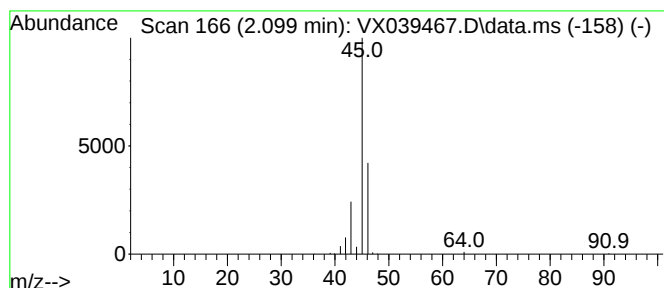
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 4 Ethanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.099	8.55 ug/l	60462	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	64
2			Dimethyl ether	46	C2H6O	000115-10-6	5
3			Oxalic acid	90	C2H2O4	000144-62-7	4
4			Propanedioic acid, dihydroxy-	136	C3H4O6	000560-27-0	4
5			Formic acid	46	CH2O2	000064-18-6	4



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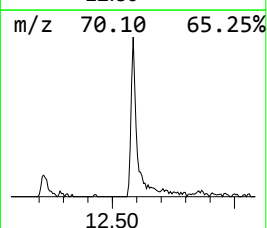
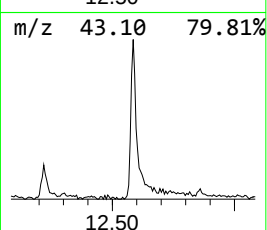
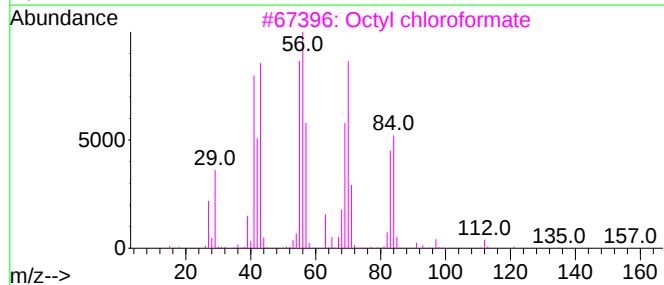
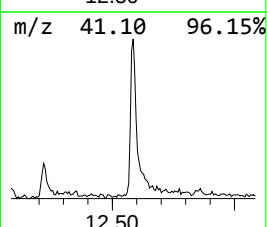
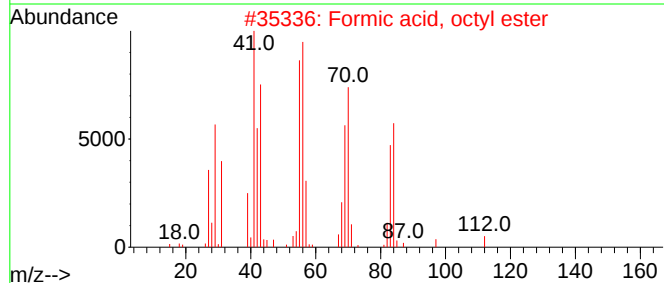
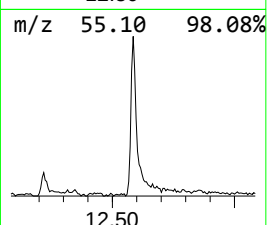
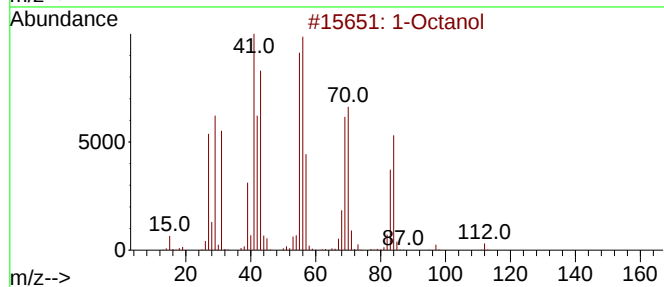
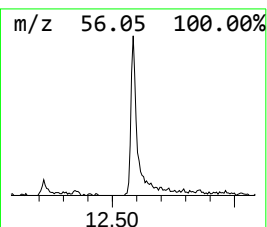
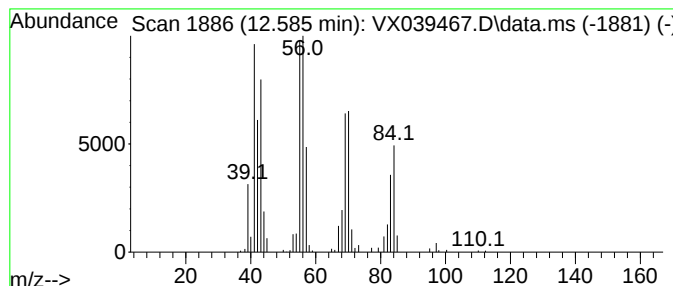
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Quant Title : SW846 8260

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

Peak Number 5 1-Octanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.585	7.94 ug/l	113890	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octanol	130	C8H18O	000111-87-5	91
2			Formic acid, octyl ester	158	C9H18O2	000112-32-3	90
3			Octyl chloroformate	192	C9H17ClO2	007452-59-7	78
4			1-Nonanol	144	C9H20O	000143-08-8	64
5			Cyclobutane, 1,2-diethyl-	112	C8H16	061141-83-1	64



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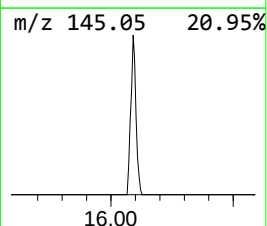
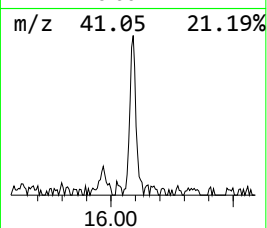
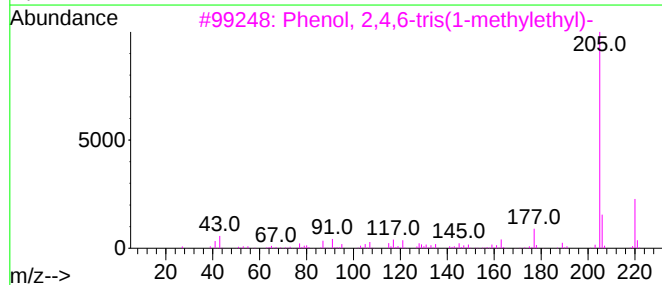
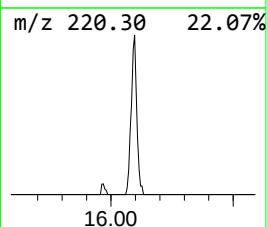
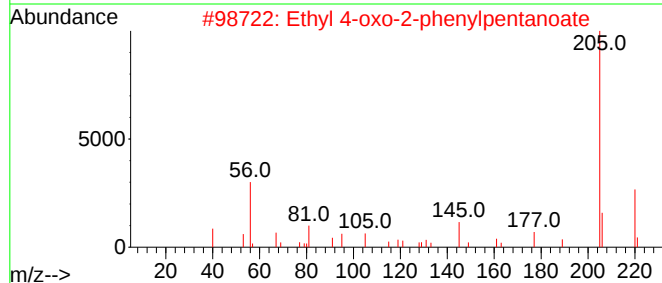
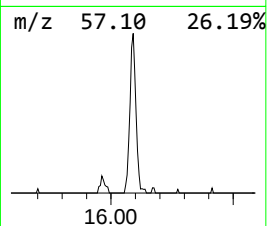
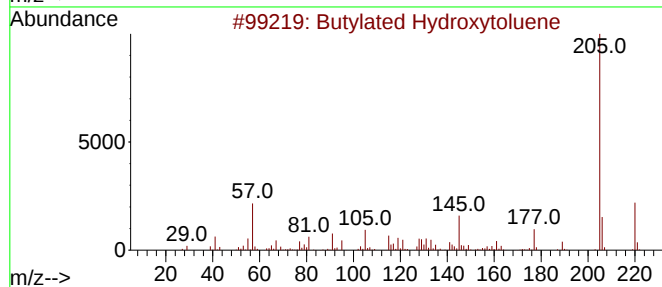
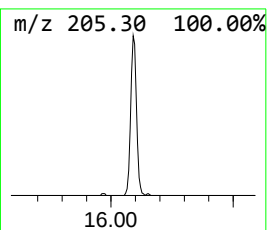
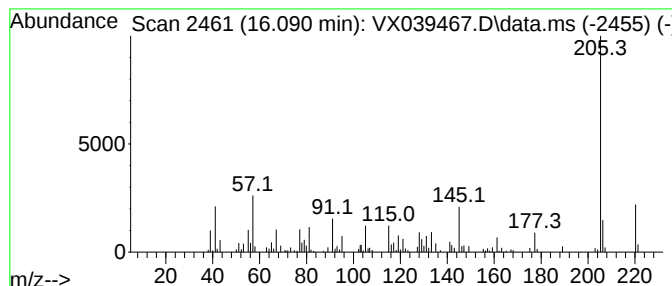
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

Peak Number 6 Butylated Hydroxytoluene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.090	5.27 ug/l	75558	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	95
2			Ethyl 4-oxo-2-phenylpentanoate	220	C13H16O3	1000427-11-2	76
3			Phenol, 2,4,6-tris(1-methylethyl)-	220	C15H24O	002934-07-8	76
4			2H-1-Benzopyran, 6,7-dimethoxy-2...	220	C13H16O3	000644-06-4	53
5			6-Methyl-1H,6H,7H-pyrrolo[2,3-c]...	220	C11H16N2OSi	1000504-47-6	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122623\
Data File : VX039467.D
Acq On : 26 Dec 2023 15:04
Operator : JC/MD
Sample : 06014-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-1307

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane	1.142	26.1	ug/l	184689	1	5.556	353681	50.0
Acetaldehyde	1.514	18.3	ug/l	129069	1	5.556	353681	50.0
Ethanol	2.099	8.6	ug/l	60462	1	5.556	353681	50.0
1-Octanol	12.585	7.9	ug/l	113890	4	12.024	716938	50.0
Butylated Hydro...	16.090	5.3	ug/l	75558	4	12.024	716938	50.0