

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010322\
 Data File : VX026225.D
 Acq On : 03 Jan 2022 17:10
 Operator : JC/MD
 Sample : M5335-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 20966

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\82X123021W.M
 Title : SW846 8260

Signal : TIC: VX026225.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.148	6	10	15	rVB	37696	37811	3.41%	0.402%
2	2.051	150	158	172	rBV	155138	258221	23.28%	2.747%
3	2.380	203	212	217	rBV	52729	86791	7.83%	0.923%
4	2.532	230	237	249	rBV	27252	54074	4.88%	0.575%
5	2.953	298	306	315	rBV	11662	26848	2.42%	0.286%
6	4.233	505	516	531	rBV	61965	171033	15.42%	1.820%
7	4.568	558	571	585	rBV2	7968	24444	2.20%	0.260%
8	5.391	692	706	722	rBV	129401	381545	34.41%	4.060%
9	5.556	722	733	749	rVB	216799	617462	55.68%	6.570%
10	5.958	786	799	806	rBV	158194	404529	36.48%	4.304%
11	6.044	806	813	822	rVV2	98919	266528	24.03%	2.836%
12	6.111	822	824	837	rVB4	5675	11734	1.06%	0.125%
13	6.763	920	931	951	rBV	361963	866032	78.09%	9.215%
14	7.208	994	1004	1016	rBV	72013	159626	14.39%	1.698%
15	7.580	1056	1065	1073	rBV4	5998	13308	1.20%	0.142%
16	8.574	1221	1228	1234	rBV	18153	32953	2.97%	0.351%
17	8.653	1234	1241	1247	rVV	706659	1108961	100.00%	11.799%
18	8.720	1247	1252	1258	rVV	530781	797831	71.94%	8.489%
19	8.763	1258	1259	1270	rVB	15743	22648	2.04%	0.241%
20	8.958	1285	1291	1299	rBV3	8353	16733	1.51%	0.178%
21	9.232	1331	1336	1352	rBV	82689	125603	11.33%	1.336%
22	9.488	1373	1378	1383	rBV2	11871	21180	1.91%	0.225%
23	10.055	1465	1471	1480	rBV	727496	965432	87.06%	10.272%
24	10.153	1480	1487	1490	rVV	28131	40075	3.61%	0.426%
25	10.195	1490	1494	1500	rVV	42906	59913	5.40%	0.637%
26	10.299	1504	1511	1518	rVB	160464	224452	20.24%	2.388%
27	10.579	1552	1557	1563	rBV	13382	21027	1.90%	0.224%
28	10.640	1563	1567	1573	rBV	57452	81091	7.31%	0.863%
29	10.750	1581	1585	1595	rBV	23861	35866	3.23%	0.382%
30	11.079	1634	1639	1645	rBV	552213	719824	64.91%	7.659%
31	11.573	1715	1720	1723	rBV2	12069	16218	1.46%	0.173%
32	11.604	1723	1725	1731	rVV3	10479	15010	1.35%	0.160%
33	11.683	1736	1738	1747	rVB	13416	17981	1.62%	0.191%
34	11.872	1765	1769	1779	rVB	19053	33305	3.00%	0.354%
35	12.024	1789	1794	1802	rVB	706462	880005	79.35%	9.363%
36	12.219	1821	1826	1837	rBV	546749	693317	62.52%	7.377%

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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	12.305	1837	1840	1849	rVB4	21067	36810	3.32%	0.392%
38	12.585	1879	1886	1893	rBV8	6435	16259	1.47%	0.173%
39	13.311	1997	2005	2012	rVB5	7935	11426	1.03%	0.122%
40	15.975	2436	2442	2457	rBV5	10106	24585	2.22%	0.262%

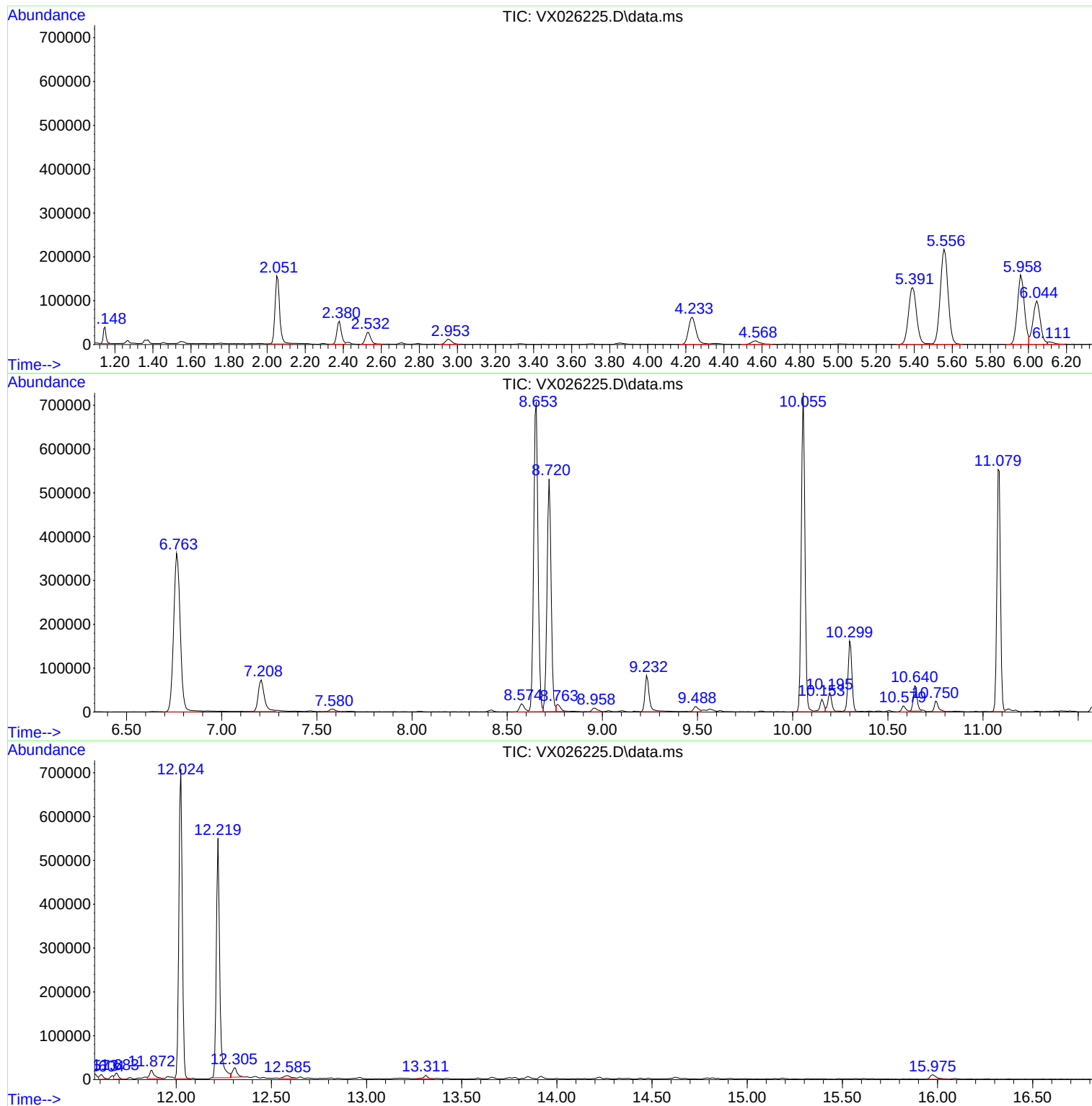
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.M
Quant Title : SW846 8260

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



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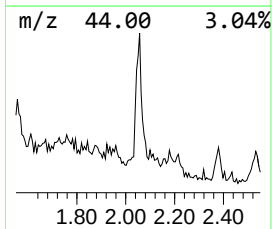
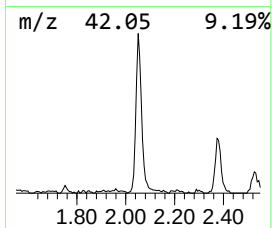
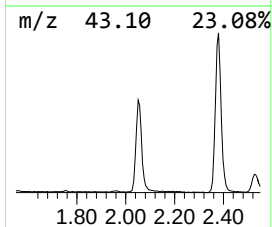
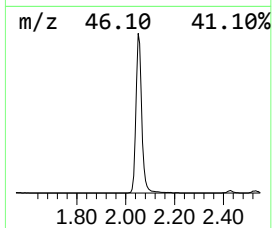
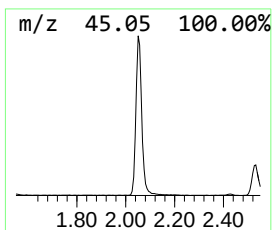
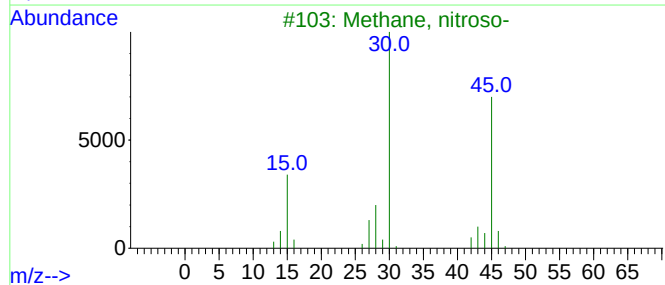
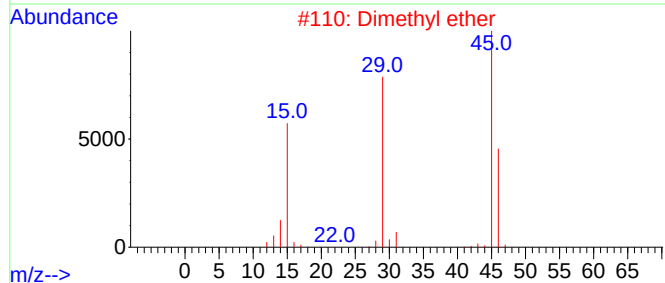
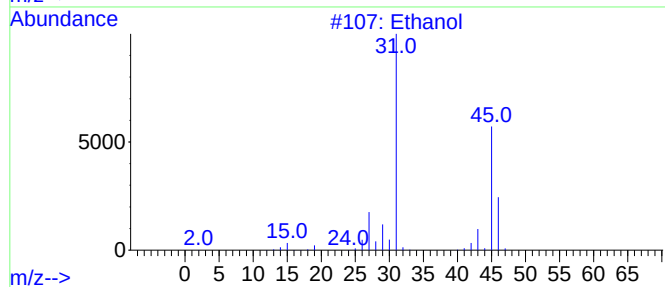
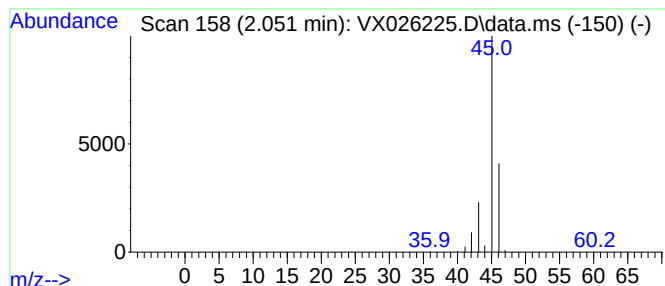
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.051	20.91 ug/l	258221	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	74
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Methane, nitroso-	45	CH3NO	000865-40-7	4
4			Formic acid	46	CH2O2	000064-18-6	4
5			Oxalic acid	90	C2H2O4	000144-62-7	4



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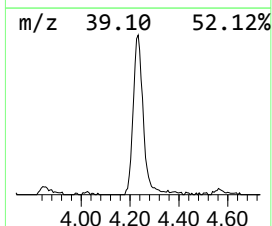
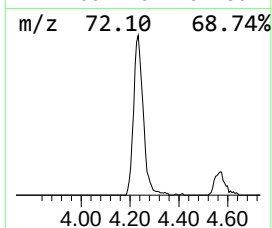
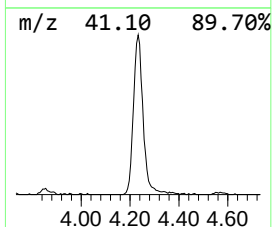
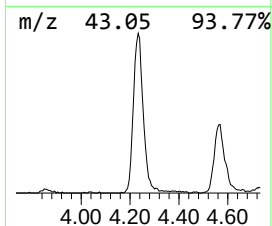
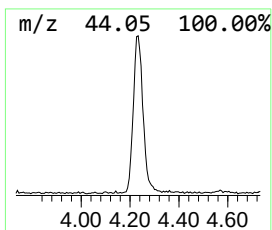
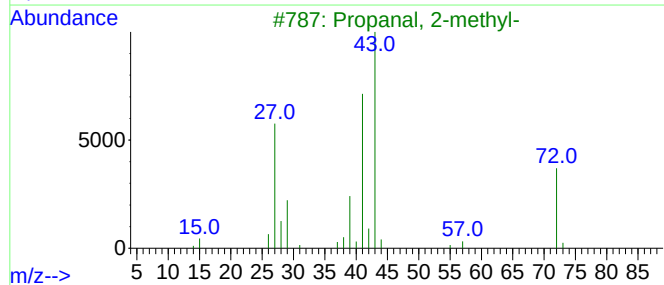
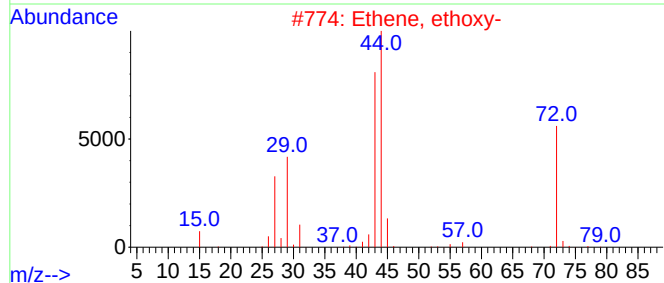
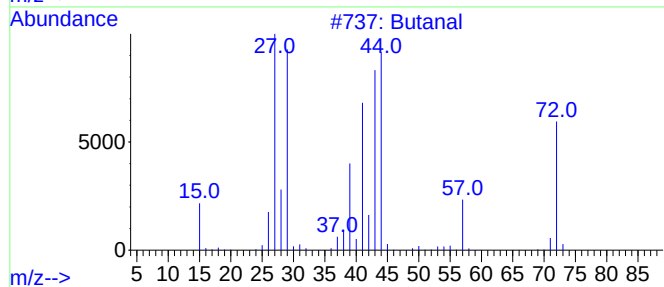
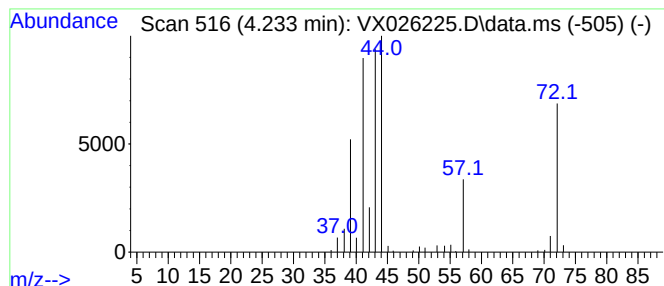
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.M
Quant Title : SW846 8260

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

Peak Number 2 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.233	13.85 ug/l	171033	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	91
2			Ethene, ethoxy-	72	C4H8O	000109-92-2	47
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
4			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	25
5			2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	17



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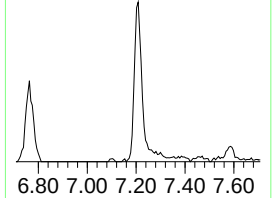
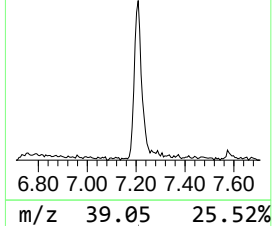
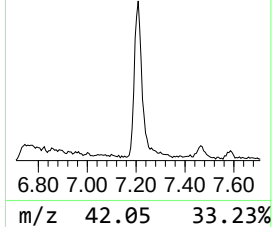
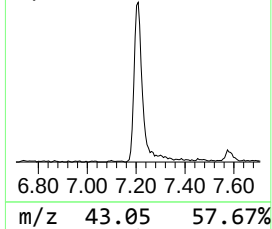
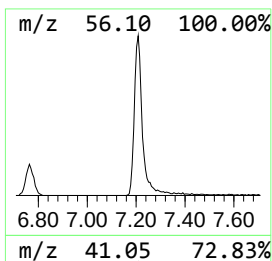
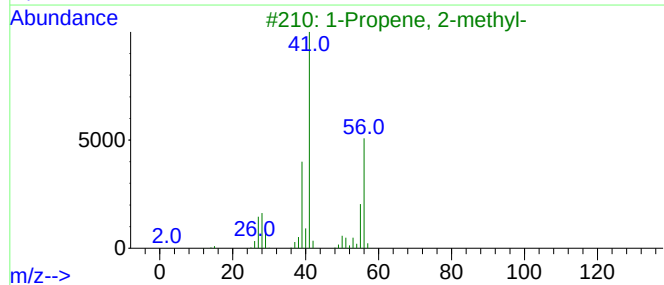
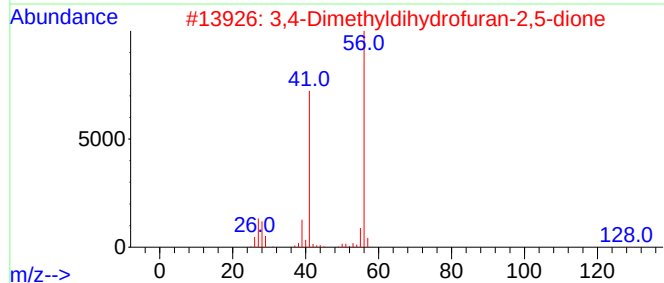
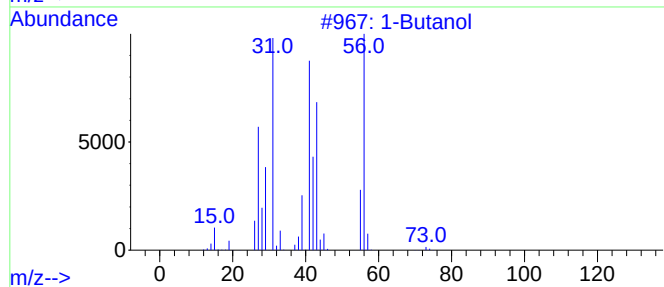
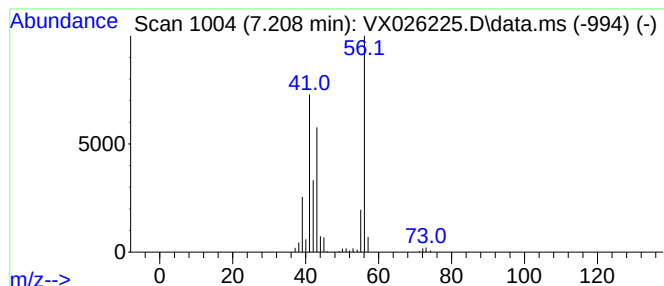
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.M
Quant Title : SW846 8260

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

Peak Number 3 1-Butanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	9.22 ug/l	159626	1,4-Difluorobenzene	6.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol		74	C4H10O	000071-36-3	91
2	3,4-Dimethyldihydrofuran-2,5-dione		128	C6H8O3	007475-92-5	42
3	1-Propene, 2-methyl-		56	C4H8	000115-11-7	40
4	Propane, 2-cyclopropyl-		84	C6H12	003638-35-5	38
5	Propanenitrile, 2-hydroxy-		71	C3H5NO	000078-97-7	9



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ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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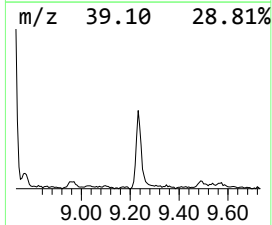
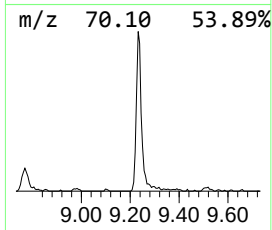
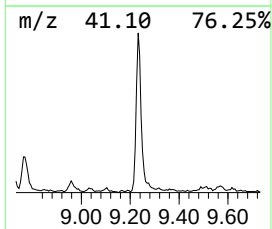
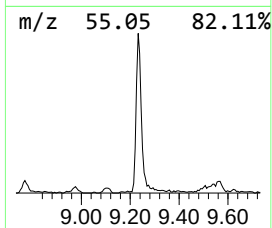
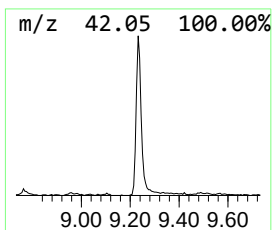
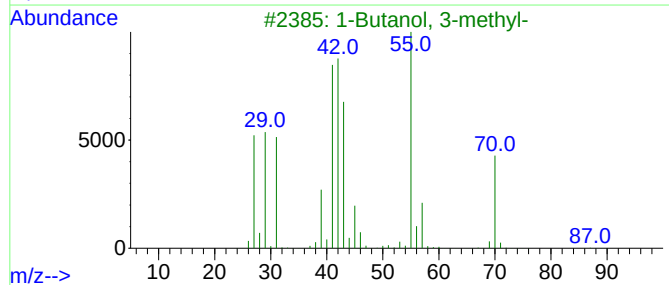
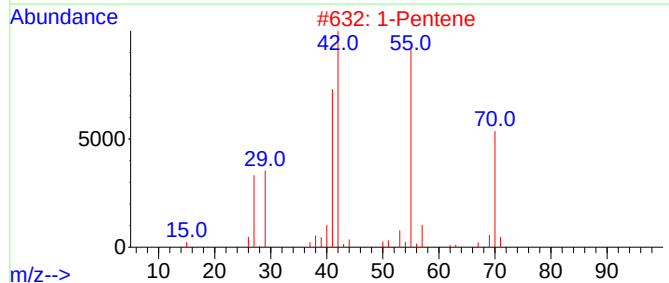
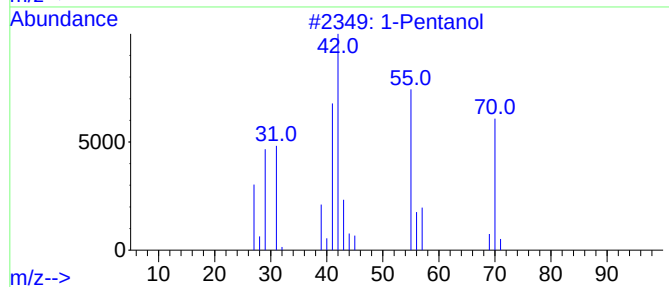
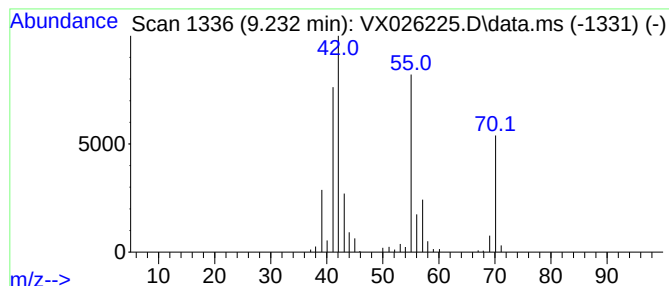
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.M
Quant Title : SW846 8260

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

Peak Number 4 1-Pentanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.232	6.51 ug/l	125603	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol			88	C5H12O	000071-41-0	78
2	1-Pentene			70	C5H10	000109-67-1	72
3	1-Butanol, 3-methyl-			88	C5H12O	000123-51-3	64
4	Cyclopentane			70	C5H10	000287-92-3	59
5	Carbonochloridic acid, pentyl ester			150	C6H11ClO2	000638-41-5	39



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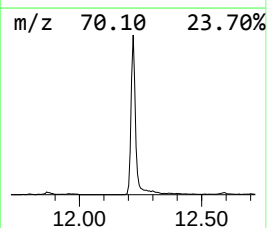
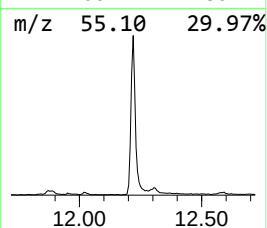
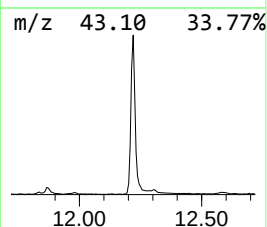
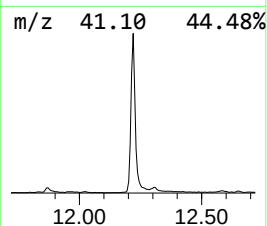
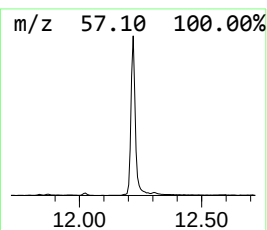
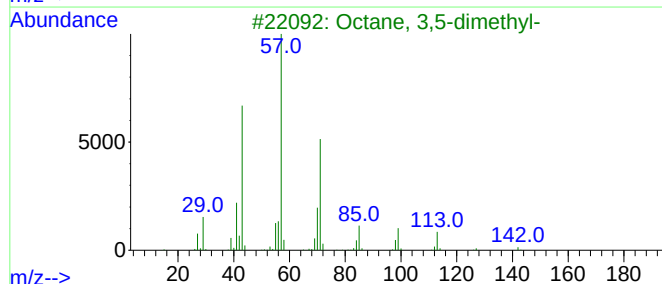
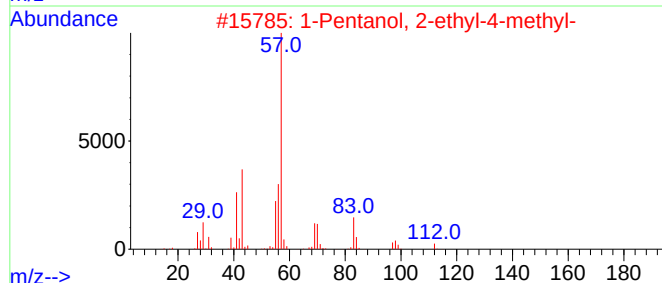
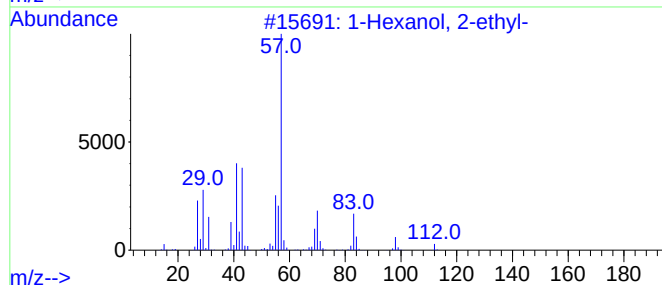
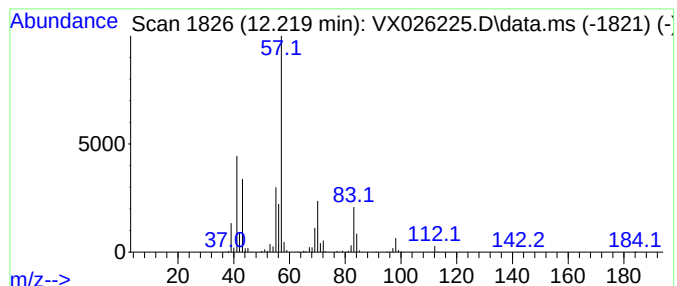
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.M
Quant Title : SW846 8260

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

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	39.39 ug/l	693317	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59
3			Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	53
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5			Carbonic acid, octyl vinyl ester	200	C11H20O3	1000383-25-5	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010322\
Data File : VX026225.D
Acq On : 03 Jan 2022 17:10
Operator : JC/MD
Sample : M5335-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20966

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.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
Ethanol	2.051	20.9	ug/l	258221	1	5.556	617462	50.0
Butanal	4.233	13.9	ug/l	171033	1	5.556	617462	50.0
1-Butanol	7.208	9.2	ug/l	159626	2	6.763	866032	50.0
1-Pentanol	9.232	6.5	ug/l	125603	3	10.055	965432	50.0
1-Hexanol, 2-et...	12.219	39.4	ug/l	693317	4	12.024	880005	50.0