

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010422\
 Data File : VX026270.D
 Acq On : 04 Jan 2022 14:41
 Operator : JC/MD
 Sample : M5335-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 8 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: VX026270.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	17	rVB	32225	30185	3.58%	0.422%
2	1.361	41	45	54	rVB2	7385	13226	1.57%	0.185%
3	1.550	70	76	81	rBV2	5724	9552	1.13%	0.133%
4	2.056	152	159	170	rBV	95451	162284	19.25%	2.268%
5	2.379	206	212	218	rBV	39910	66438	7.88%	0.928%
6	2.532	230	237	249	rBV	22368	43252	5.13%	0.604%
7	2.965	298	308	323	rBV4	15014	40480	4.80%	0.566%
8	3.702	413	429	441	rBV2	39326	111838	13.26%	1.563%
9	4.233	502	516	529	rBV	51944	151173	17.93%	2.113%
10	4.562	562	570	584	rBV2	5351	16417	1.95%	0.229%
11	5.391	693	706	719	rBV	100762	291558	34.58%	4.074%
12	5.556	723	733	746	rVB	168535	476367	56.50%	6.657%
13	5.958	789	799	806	rBV	120589	312173	37.03%	4.363%
14	6.043	806	813	835	rVB	74278	218513	25.92%	3.054%
15	6.763	921	931	945	rBV	270844	641537	76.09%	8.965%
16	7.208	996	1004	1014	rBV	47352	103451	12.27%	1.446%
17	7.580	1060	1065	1074	rVB	4865	9416	1.12%	0.132%
18	8.579	1221	1229	1234	rBV	13235	23761	2.82%	0.332%
19	8.653	1234	1241	1247	rVV	525331	843121	100.00%	11.783%
20	8.720	1247	1252	1258	rVV	397306	598261	70.96%	8.361%
21	8.768	1258	1260	1269	rVB	10392	14357	1.70%	0.201%
22	8.957	1284	1291	1299	rBV3	6009	11870	1.41%	0.166%
23	9.232	1331	1336	1351	rBV	50862	81973	9.72%	1.146%
24	9.488	1374	1378	1387	rBV6	4047	12621	1.50%	0.176%
25	10.055	1465	1471	1481	rBV	559887	729073	86.47%	10.189%
26	10.152	1481	1487	1490	rVV	16512	24291	2.88%	0.339%
27	10.195	1490	1494	1500	rVV	33255	44868	5.32%	0.627%
28	10.305	1503	1512	1519	rVV	121075	170031	20.17%	2.376%
29	10.585	1553	1558	1563	rBV2	7698	12271	1.46%	0.171%
30	10.646	1563	1568	1574	rBV	44666	63018	7.47%	0.881%
31	10.756	1580	1586	1600	rBV2	15164	26918	3.19%	0.376%
32	11.079	1634	1639	1646	rBV	424570	548586	65.07%	7.666%
33	11.573	1716	1720	1723	rBV	7659	10585	1.26%	0.148%
34	11.603	1723	1725	1732	rVV4	6368	10122	1.20%	0.141%
35	11.689	1732	1739	1747	rVV	11327	16534	1.96%	0.231%
36	11.872	1765	1769	1780	rVB2	11072	20255	2.40%	0.283%

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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	12.024	1789	1794	1802	rVB	545493	655424	77.74%	9.159%
38	12.219	1818	1826	1837	rBV	366914	497348	58.99%	6.950%
39	12.304	1837	1840	1851	rVB6	15501	33731	4.00%	0.471%
40	12.585	1879	1886	1894	rBV6	3638	8815	1.05%	0.123%

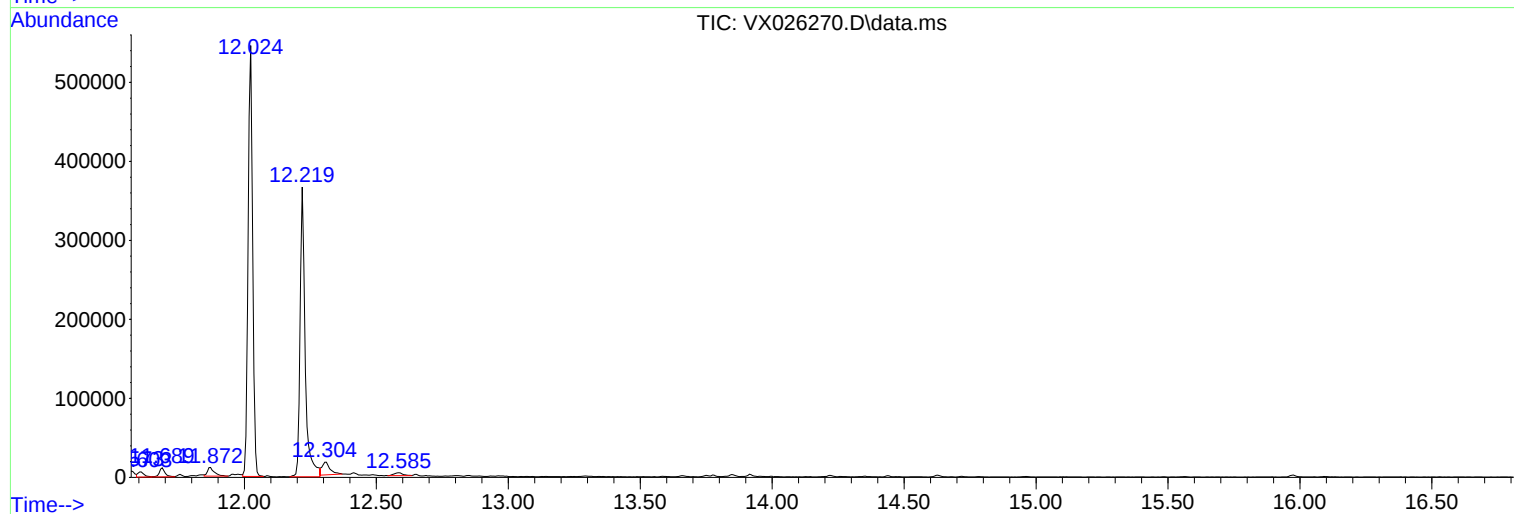
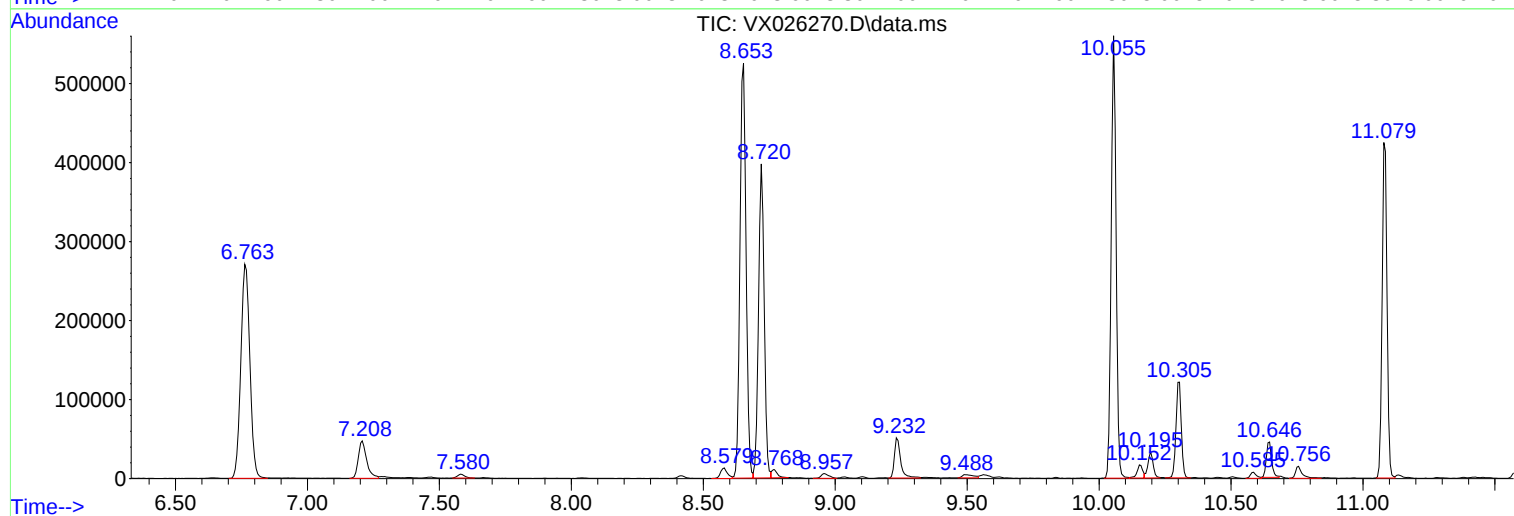
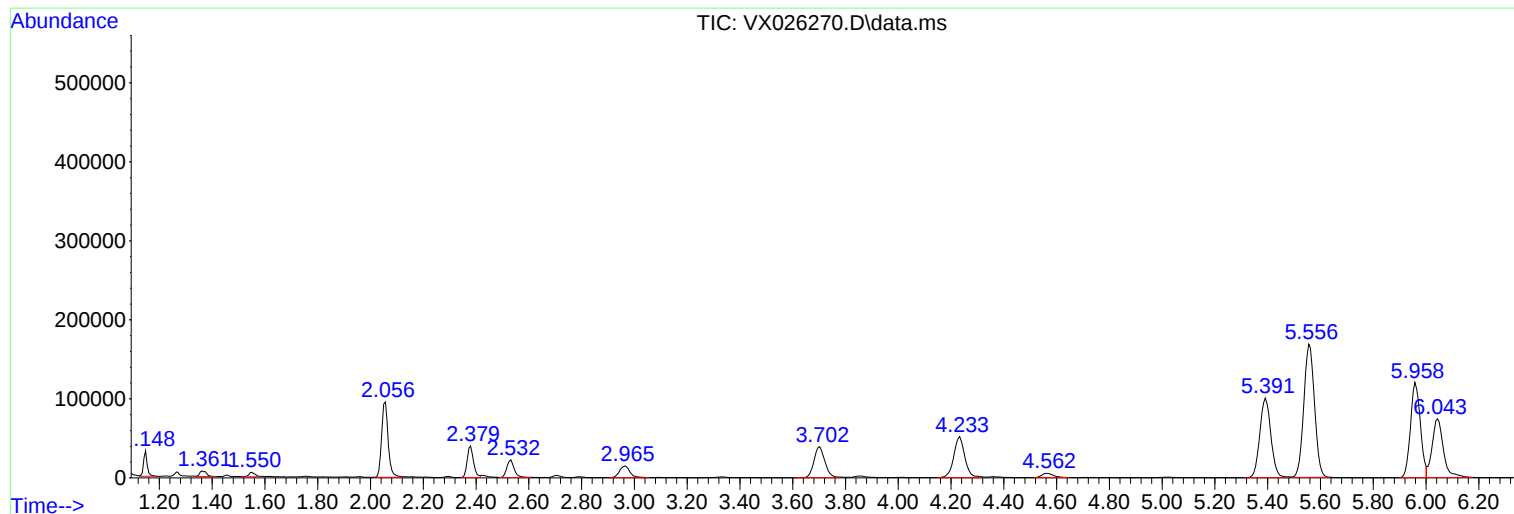
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\WX010422\
Data File : VX026270.D
Acq On : 04 Jan 2022 14:41
Operator : JC/MD
Sample : M5335-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

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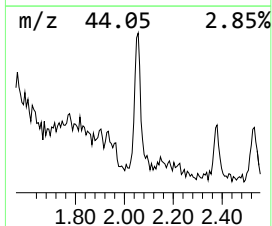
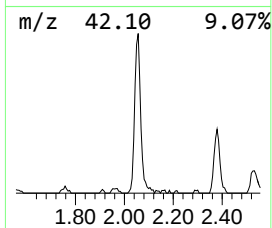
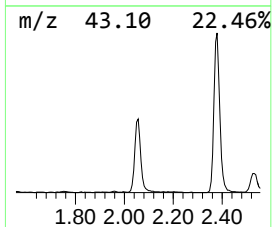
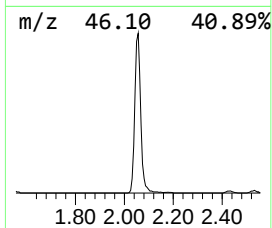
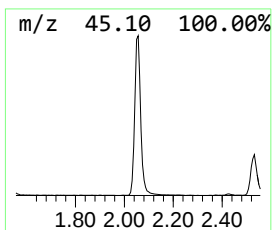
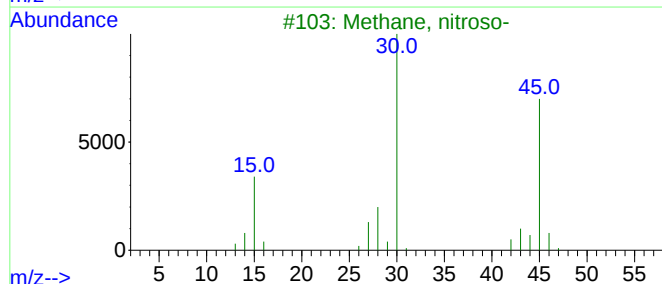
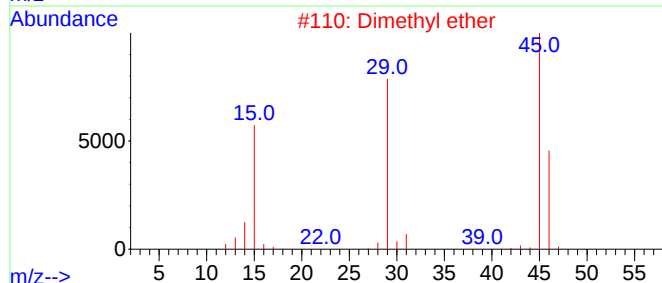
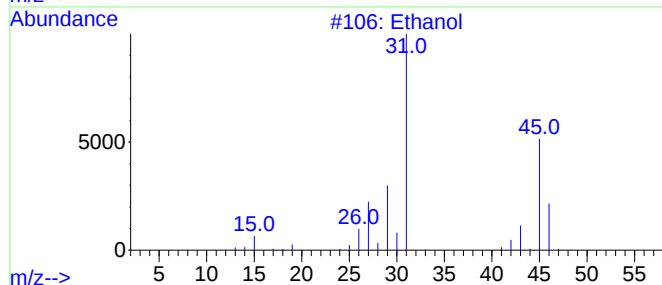
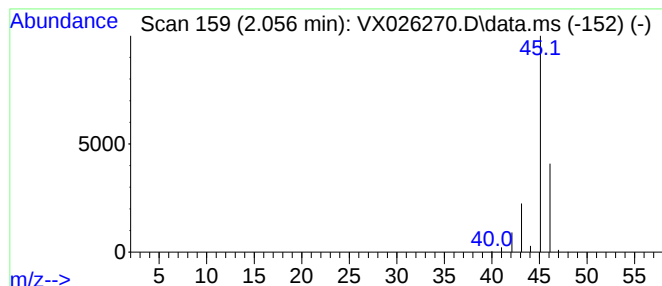
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.056	17.03 ug/l	162284	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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Instrument :
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ClientSampleId :
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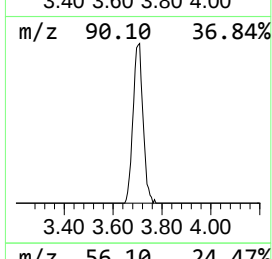
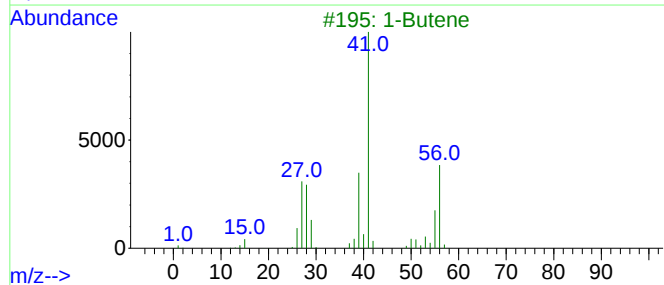
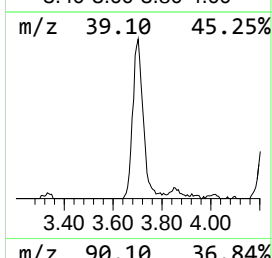
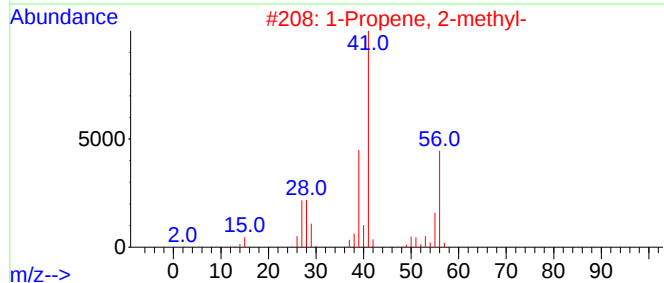
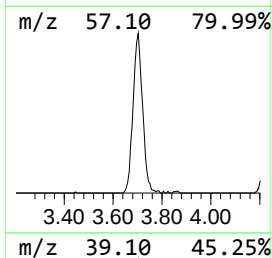
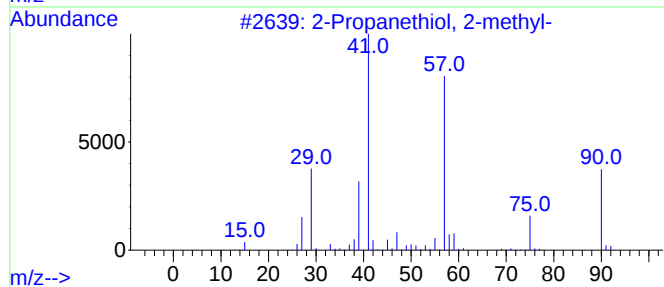
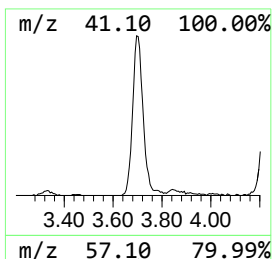
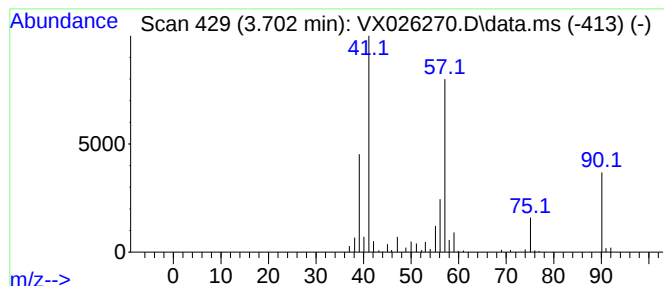
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.M
Quant Title : SW846 8260

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

Peak Number 2 2-Propanethiol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.702	11.74 ug/l	111838	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	53
2			1-Propene, 2-methyl-	56	C4H8	000115-11-7	49
3			1-Butene	56	C4H8	000106-98-9	46
4			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	38
5			Propane, 2-methyl-1-nitro-	103	C4H9NO2	000625-74-1	33



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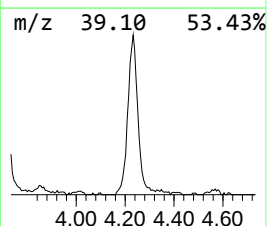
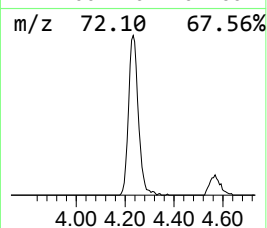
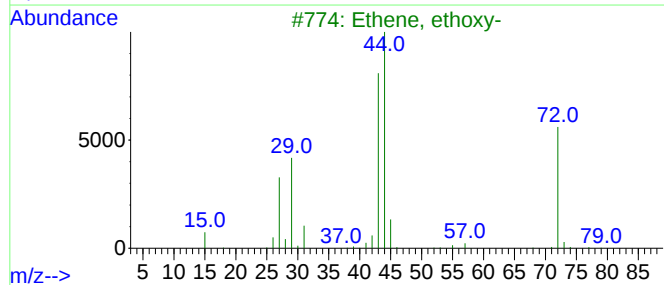
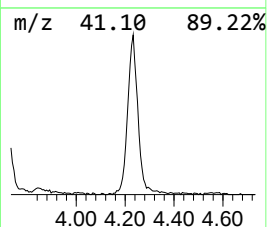
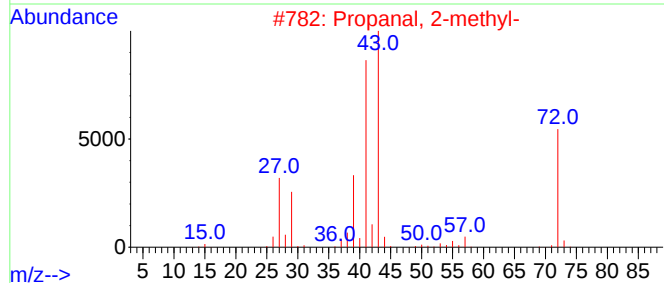
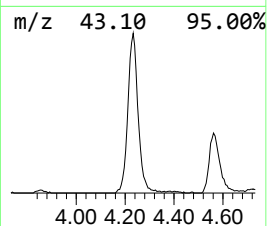
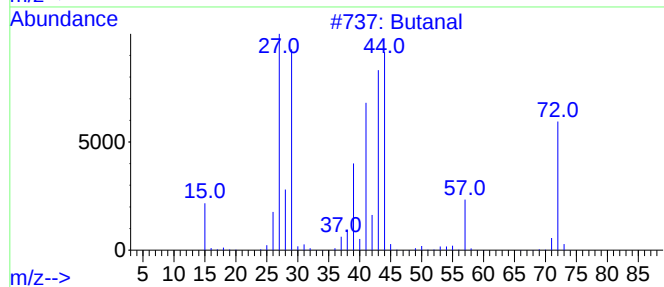
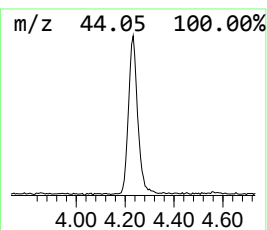
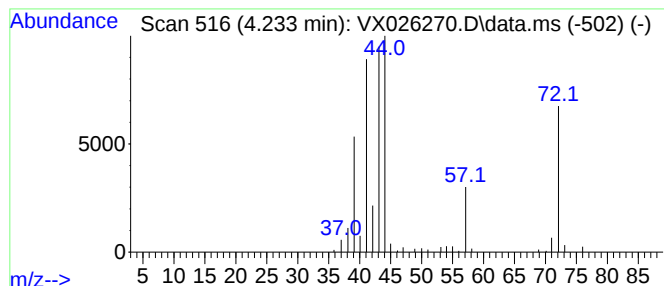
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.M
Quant Title : SW846 8260

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

Peak Number 3 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.233	15.87 ug/l	151173	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	91
2			Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
3			Ethene, ethoxy-	72	C4H8O	000109-92-2	38
4			O-Methylisourea	74	C2H6N2O	002440-60-0	36
5			Methacrolein	70	C4H6O	000078-85-3	27



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Instrument :
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ClientSampleId :
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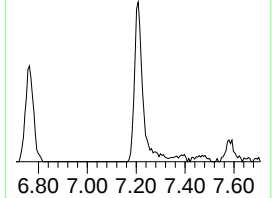
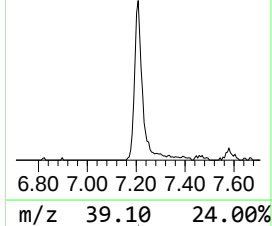
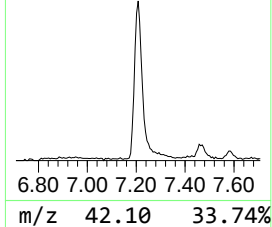
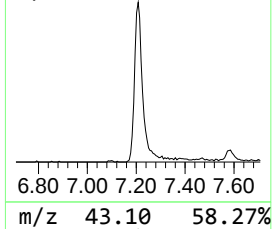
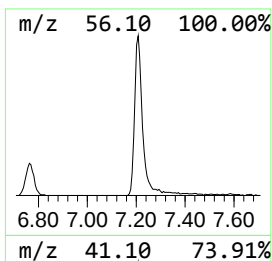
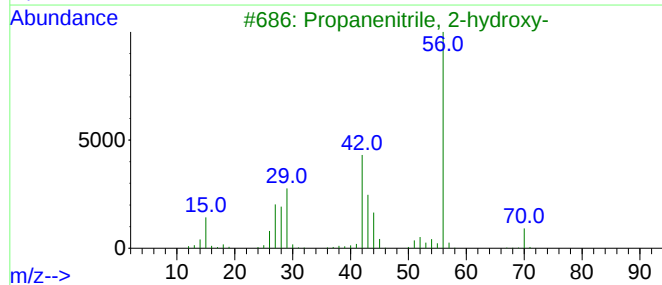
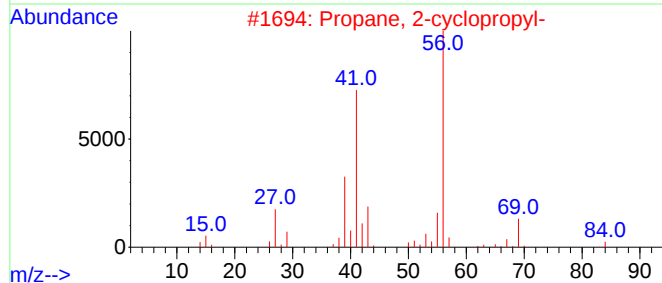
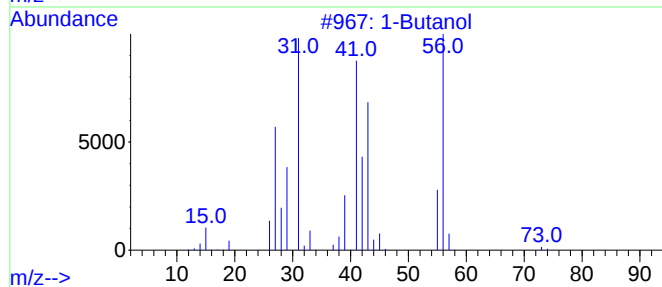
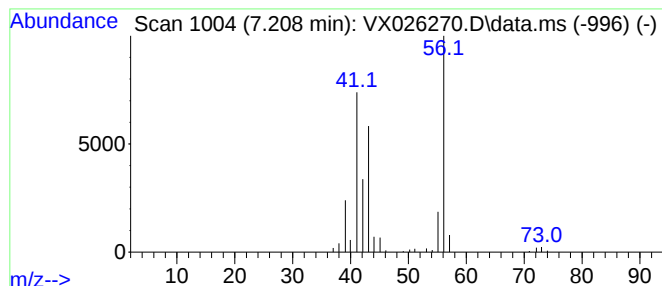
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Quant Title : SW846 8260

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

Peak Number 4 1-Butanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	8.06 ug/l	103451	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	90
2			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	39
3			Propanenitrile, 2-hydroxy-	71	C3H5NO	000078-97-7	9
4			Oxetane, 2,3,4-trimethyl-, (2.al...	100	C6H12O	032347-12-9	9
5			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	9



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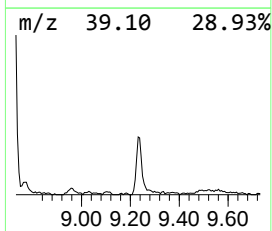
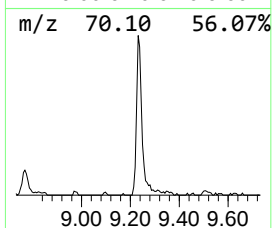
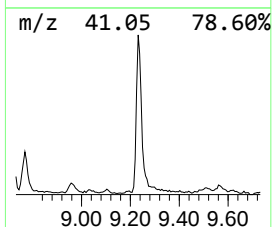
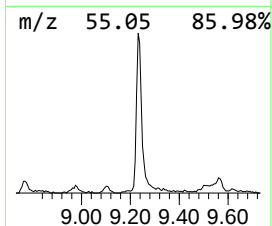
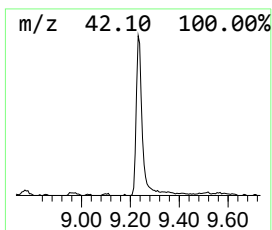
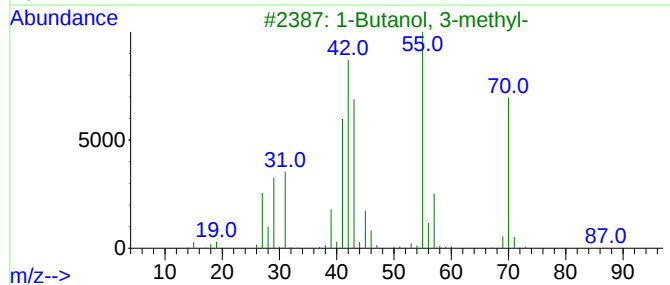
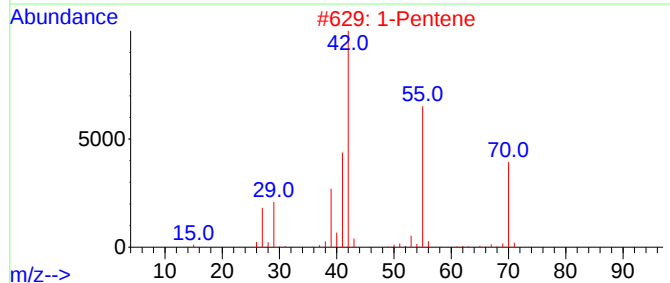
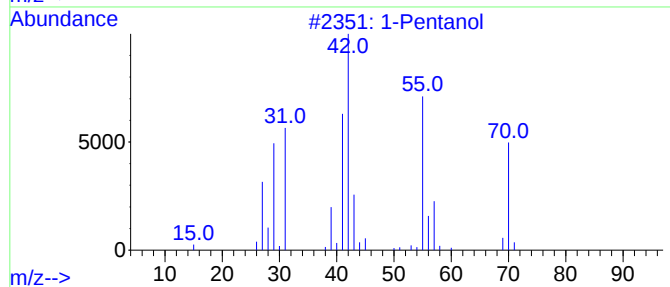
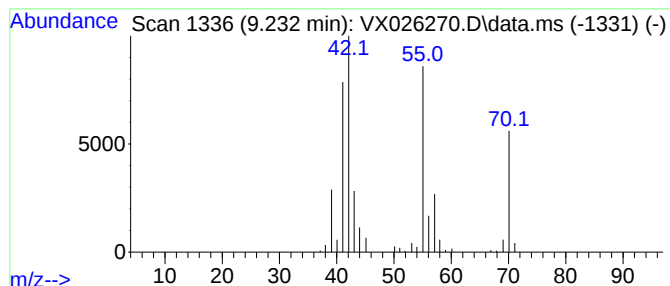
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.M
Quant Title : SW846 8260

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

Peak Number 5 1-Pentanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.232	5.62 ug/l	81973	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentanol	88	C5H12O	000071-41-0	83
2			1-Pentene	70	C5H10	000109-67-1	64
3			1-Butanol, 3-methyl-	88	C5H12O	000123-51-3	50
4			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	38
5			2H-Tetrazole, 2,5-dimethyl-	98	C3H6N4	004135-93-7	33



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010422\
Data File : VX026270.D
Acq On : 04 Jan 2022 14:41
Operator : JC/MD
Sample : M5335-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20966

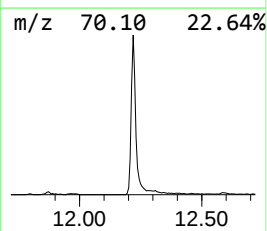
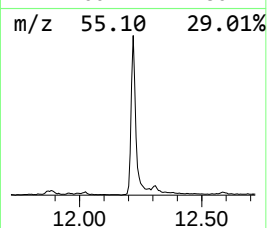
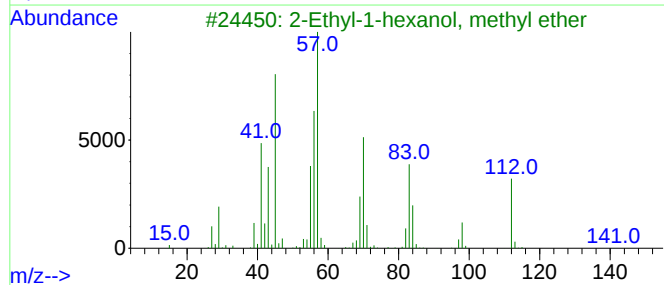
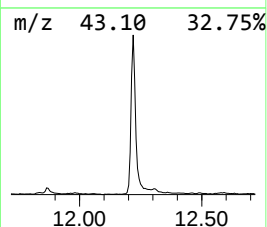
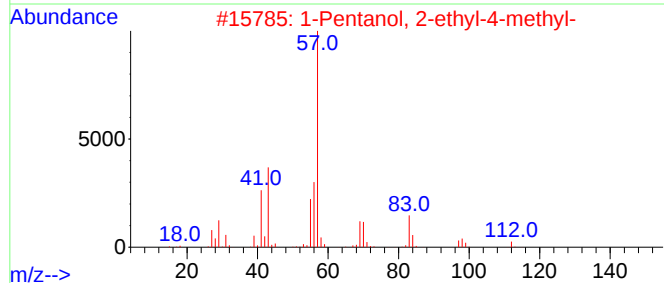
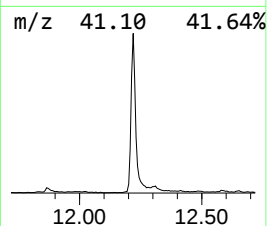
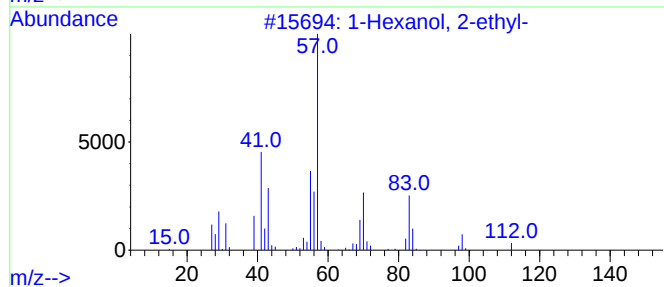
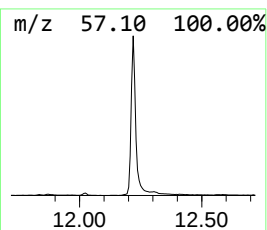
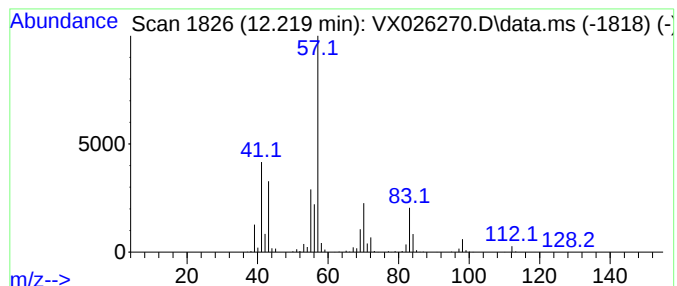
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Quant Title : SW846 8260

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

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	37.94 ug/l	497348	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	90
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
5			Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010422\
Data File : VX026270.D
Acq On : 04 Jan 2022 14:41
Operator : JC/MD
Sample : M5335-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 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	2.056	17.0	ug/l	162284	1	5.556	476367	50.0
2-Propanethiol,...	3.702	11.7	ug/l	111838	1	5.556	476367	50.0
Butanal	4.233	15.9	ug/l	151173	1	5.556	476367	50.0
1-Butanol	7.208	8.1	ug/l	103451	2	6.763	641537	50.0
1-Pentanol	9.232	5.6	ug/l	81973	3	10.055	729073	50.0
1-Hexanol, 2-et...	12.219	37.9	ug/l	497348	4	12.024	655424	50.0