

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071825\
 Data File : VX047051.D
 Acq On : 18 Jul 2025 15:42
 Operator : JC/MD
 Sample : Q2646-01 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FRAC TANK

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\82X070225W.M
 Title : SW846 8260

Signal : TIC: VX047051.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.179	13	15	24	rVB2	21462	35424	1.38%	0.167%
2	1.270	26	30	59	rBV	602839	2058715	80.30%	9.693%
3	1.465	60	62	74	rVV2	56130	157176	6.13%	0.740%
4	1.557	74	77	90	rVB2	27768	66757	2.60%	0.314%
5	1.971	140	145	153	rVV2	55120	92095	3.59%	0.434%
6	2.057	154	159	169	rVV	68412	137299	5.36%	0.646%
7	2.166	173	177	186	rVB5	14466	33068	1.29%	0.156%
8	2.392	208	214	218	rBV	19223	33977	1.33%	0.160%
9	2.532	231	237	248	rBV2	21452	66427	2.59%	0.313%
10	3.849	446	453	476	rVB	58674	172915	6.74%	0.814%
11	4.568	562	571	591	rBV	118068	378742	14.77%	1.783%
12	4.995	631	641	670	rBV	125934	476574	18.59%	2.244%
13	5.397	696	707	724	rBV3	272695	854090	33.31%	4.021%
14	5.562	724	734	757	rVB	433611	1351449	52.71%	6.363%
15	5.964	789	800	822	rBV2	299409	869260	33.90%	4.093%
16	6.769	922	932	957	rVB	723382	1881696	73.39%	8.860%
17	7.226	1001	1007	1020	rBV2	12014	30752	1.20%	0.145%
18	7.586	1061	1066	1074	rBV3	24000	58009	2.26%	0.273%
19	8.647	1234	1240	1250	rBV	1559791	2563879	100.00%	12.072%
20	9.238	1331	1337	1347	rBV2	23736	48198	1.88%	0.227%
21	9.519	1378	1383	1395	rVB	539818	765649	29.86%	3.605%
22	10.055	1465	1471	1487	rBV	1673211	2325548	90.70%	10.950%
23	10.299	1504	1511	1517	rBV3	18659	39806	1.55%	0.187%
24	10.579	1550	1557	1564	rBV	77792	127704	4.98%	0.601%
25	10.640	1564	1567	1579	rVB4	23232	46819	1.83%	0.220%
26	10.774	1584	1589	1598	rBV2	23177	42581	1.66%	0.200%
27	10.854	1598	1602	1606	rBV5	16574	26299	1.03%	0.124%
28	11.079	1634	1639	1650	rBV	1424729	1807236	70.49%	8.509%
29	11.378	1684	1688	1696	rBV	26101	51891	2.02%	0.244%
30	11.476	1702	1704	1710	rVB2	28435	33357	1.30%	0.157%
31	11.616	1723	1727	1732	rBV	213646	272494	10.63%	1.283%
32	11.658	1732	1734	1738	rVV4	25155	37365	1.46%	0.176%
33	11.726	1741	1745	1747	rVV	54356	84254	3.29%	0.397%
34	11.750	1747	1749	1756	rVB	77362	96112	3.75%	0.453%
35	12.018	1788	1793	1800	rBV	1853490	2257016	88.03%	10.627%
36	12.085	1800	1804	1811	rVB2	29624	51233	2.00%	0.241%

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Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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

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37	12.244	1824	1830	1832	rBV3	32896	46384	1.81%	0.218%
38	12.317	1837	1842	1848	rVB6	25100	46749	1.82%	0.220%
39	12.421	1848	1859	1863	rBV	61387	91241	3.56%	0.430%
40	12.549	1873	1880	1883	rBV4	27889	58563	2.28%	0.276%
41	12.591	1883	1887	1894	rVB2	64917	110970	4.33%	0.522%
42	12.695	1899	1904	1916	rVB7	15145	45538	1.78%	0.214%
43	12.963	1945	1948	1954	rVB3	24794	45491	1.77%	0.214%
44	13.036	1954	1960	1964	rBV6	15778	26747	1.04%	0.126%
45	13.164	1974	1981	1986	rBV4	21419	36732	1.43%	0.173%
46	13.268	1992	1998	2000	rBV	84050	120826	4.71%	0.569%
47	13.292	2000	2002	2007	rVB	55532	67414	2.63%	0.317%
48	13.420	2019	2023	2032	rVB	51015	86128	3.36%	0.406%
49	13.768	2077	2080	2087	rVB2	17344	31774	1.24%	0.150%
50	13.841	2087	2092	2098	rVB4	37054	70821	2.76%	0.333%
51	13.926	2098	2106	2110	rBV9	20278	41482	1.62%	0.195%
52	14.036	2120	2124	2127	rVB	103531	107834	4.21%	0.508%
53	14.225	2150	2155	2158	rBV2	47341	71546	2.79%	0.337%
54	14.475	2192	2196	2206	rVB7	37246	87271	3.40%	0.411%
55	14.560	2206	2210	2215	rVB7	18836	27806	1.08%	0.131%
56	14.609	2215	2218	2221	rBV2	54238	71134	2.77%	0.335%
57	14.755	2234	2242	2245	rBV2	133967	215107	8.39%	1.013%
58	14.841	2250	2256	2259	rVB8	15491	28867	1.13%	0.136%
59	15.176	2307	2311	2313	rBV4	22477	30343	1.18%	0.143%
60	15.207	2313	2316	2320	rVV	45292	62252	2.43%	0.293%
61	15.487	2357	2362	2367	rBV	98854	135323	5.28%	0.637%
62	16.371	2502	2507	2513	rVB2	25007	42608	1.66%	0.201%

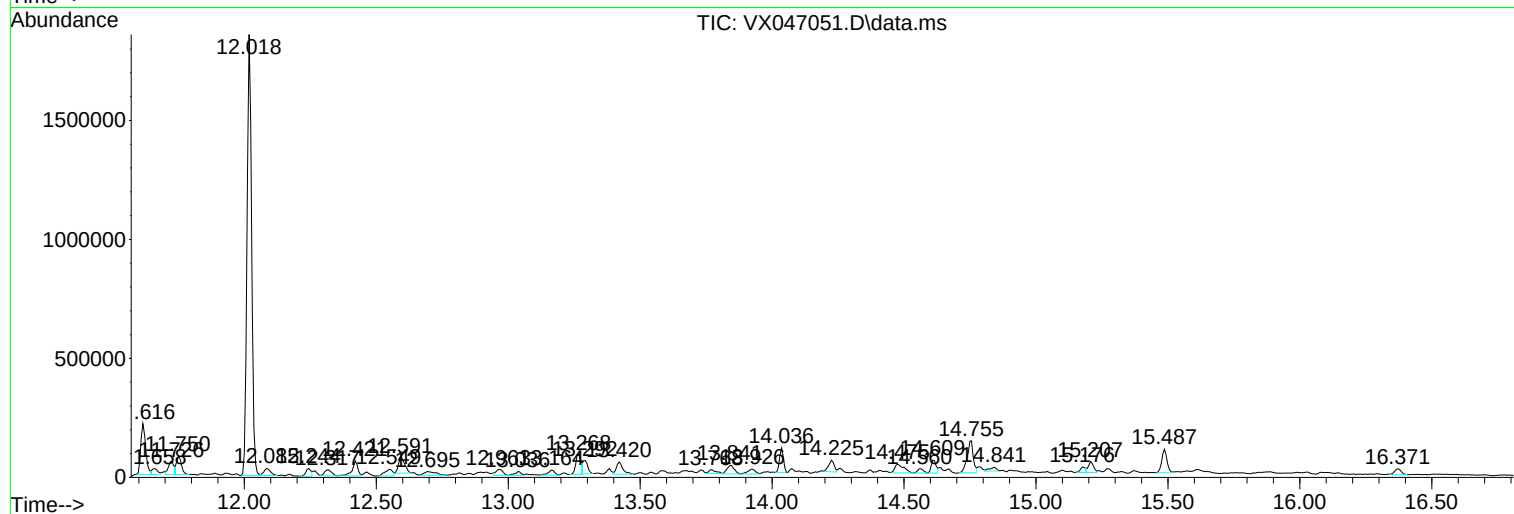
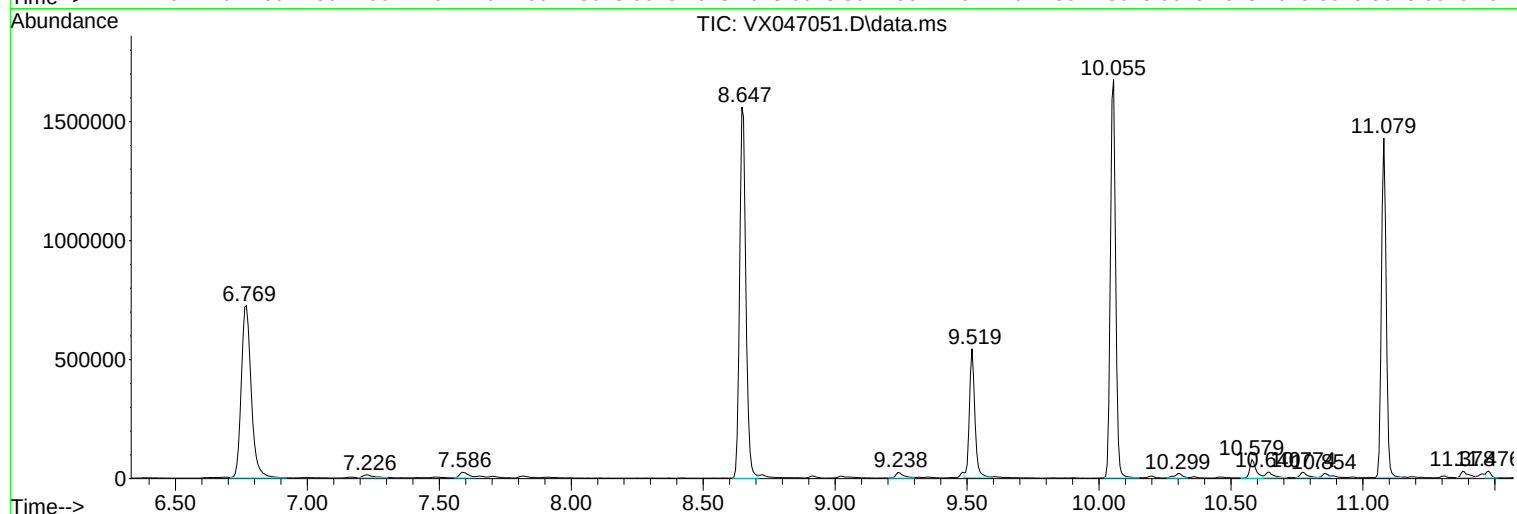
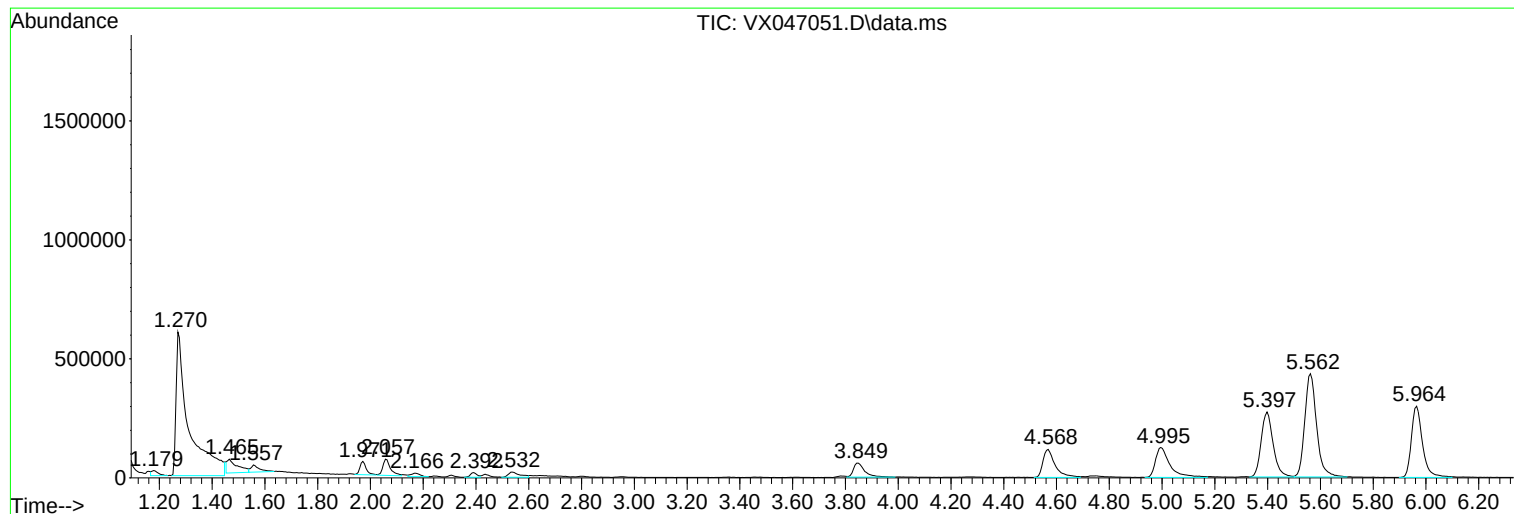
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Quant Title : SW846 8260

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



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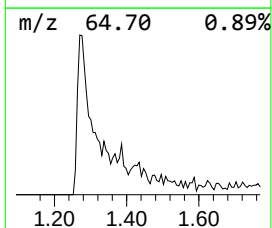
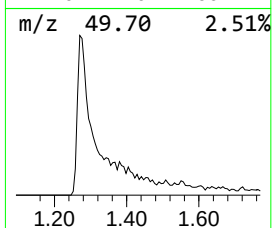
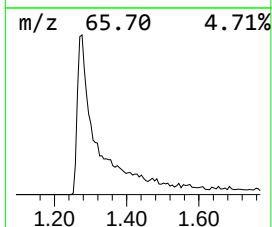
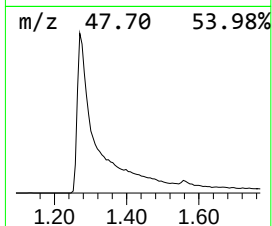
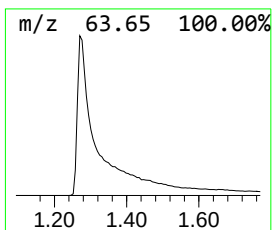
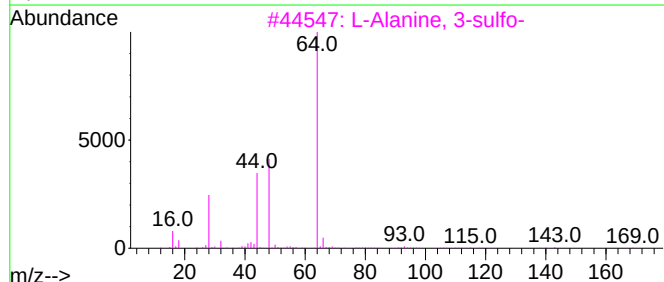
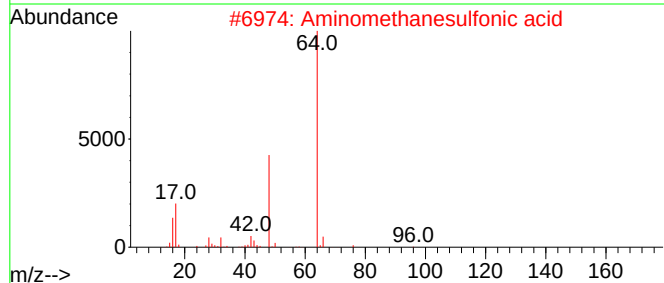
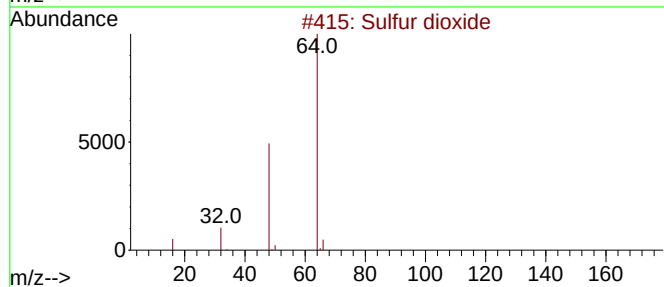
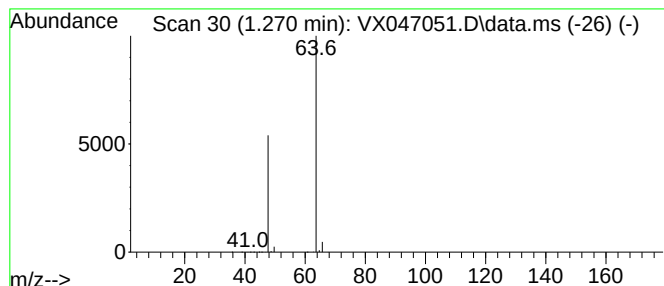
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Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.270	76.17 ug/l	2058720	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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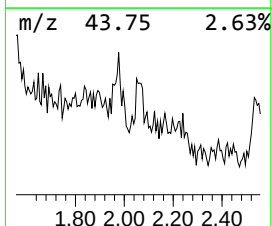
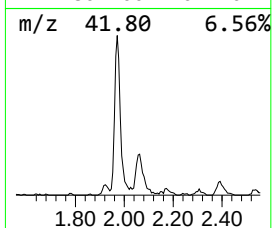
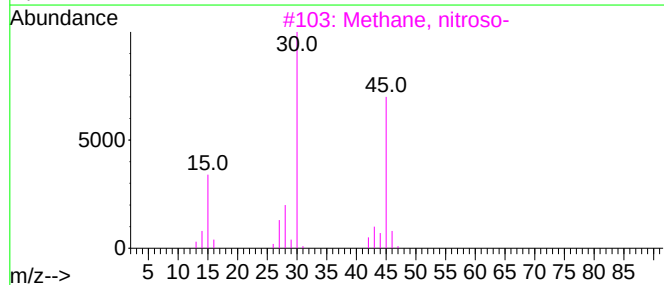
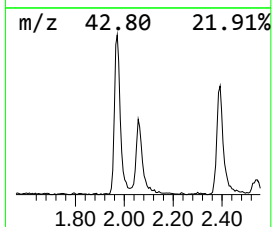
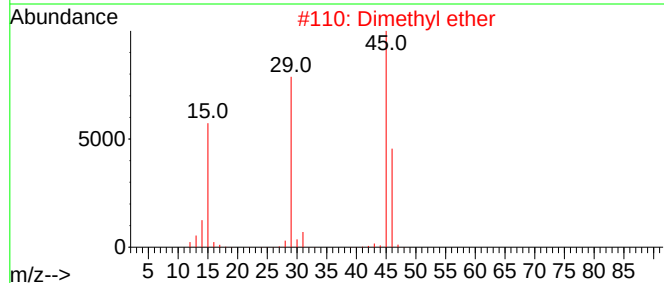
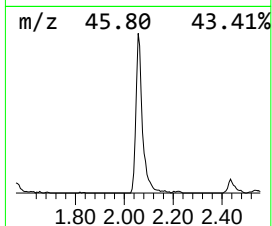
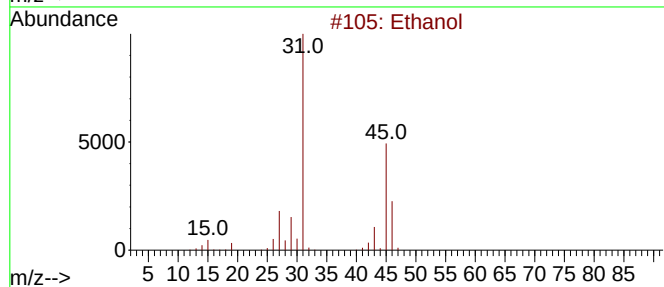
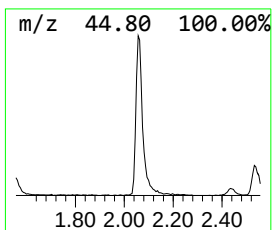
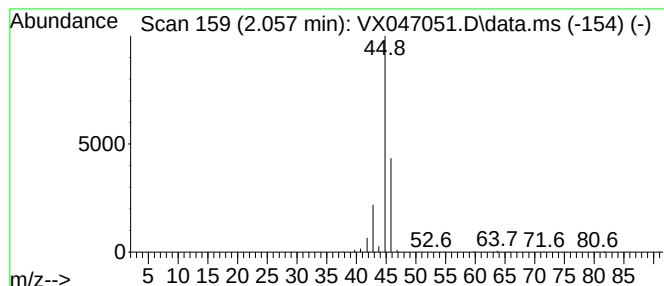
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070225W.M
Quant Title : SW846 8260

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

Peak Number 3 Ethanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.057	5.08 ug/l	137299	Pentafluorobenzene	5.562

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol		46	C2H6O	000064-17-5	78
2	Dimethyl ether		46	C2H6O	000115-10-6	9
3	Methane, nitroso-		45	CH3NO	000865-40-7	4
4	Isopropyl Alcohol		60	C3H8O	000067-63-0	4
5	Formic acid		46	CH2O2	000064-18-6	4



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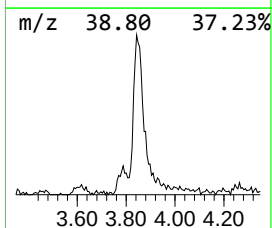
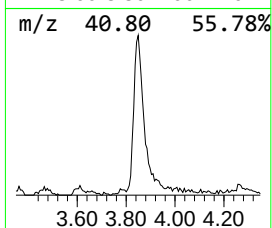
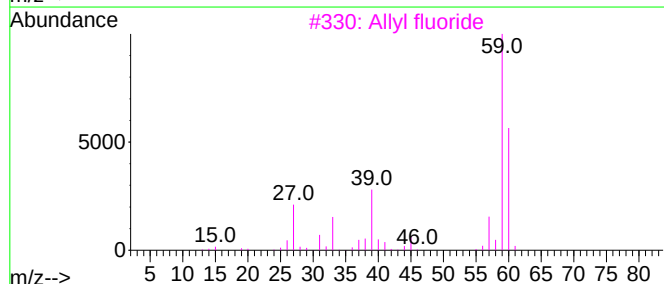
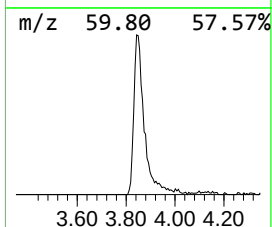
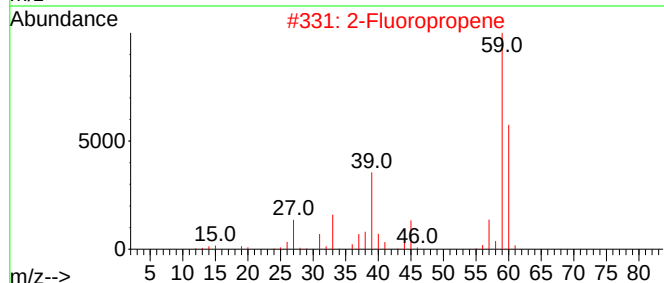
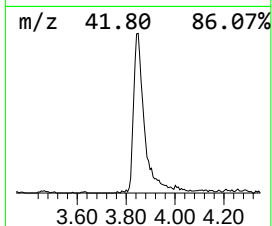
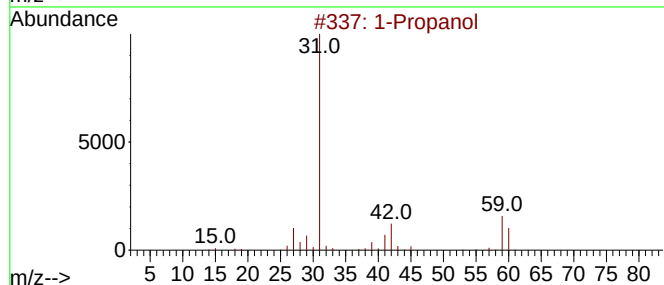
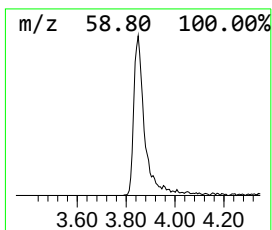
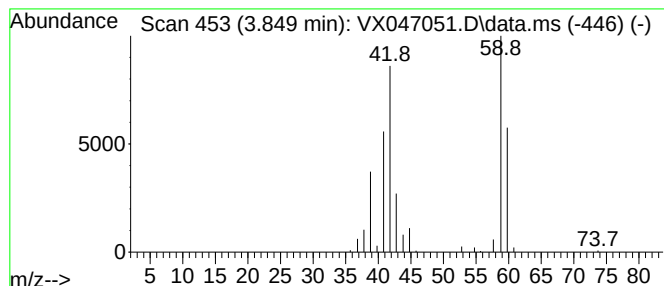
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070225W.M
Quant Title : SW846 8260

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

Peak Number 4 1-Propanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.849	6.40 ug/l	172915	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propanol	60	C3H8O	000071-23-8	80
2			2-Fluoropropene	60	C3H5F	001184-60-7	49
3			Allyl fluoride	60	C3H5F	000818-92-8	49
4			3-Buten-1-ol	72	C4H8O	000627-27-0	12
5			Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9



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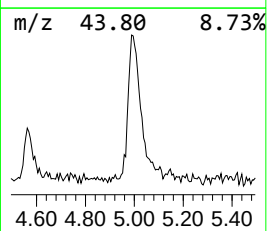
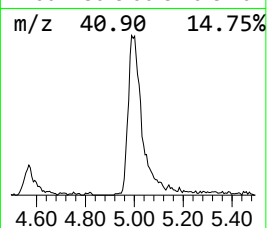
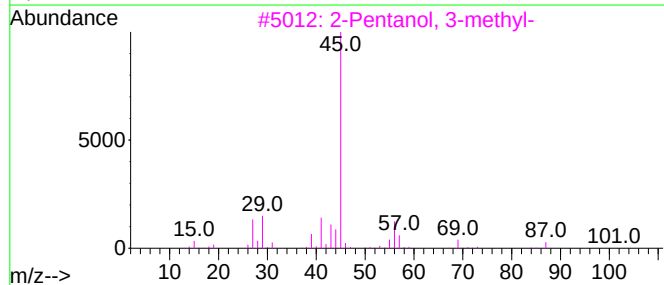
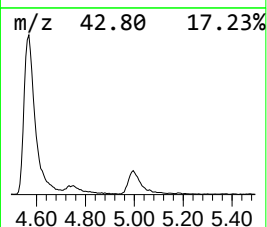
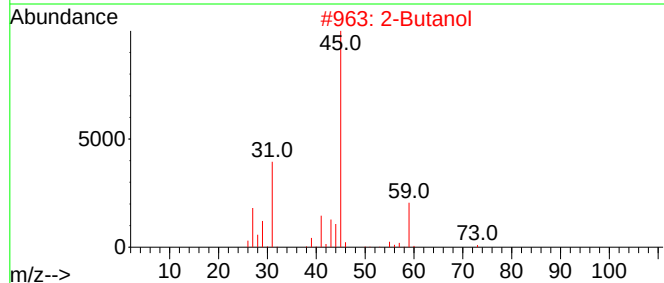
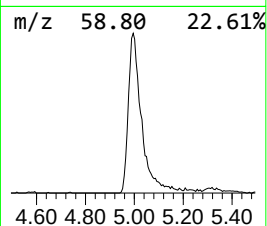
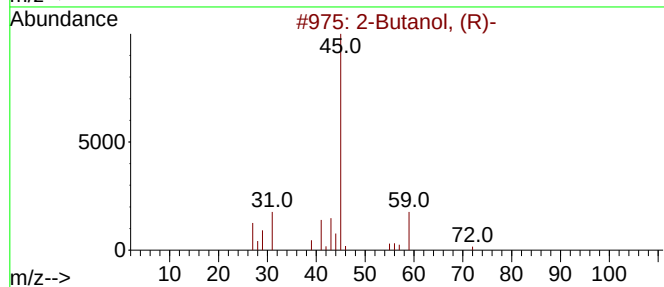
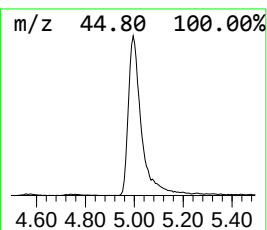
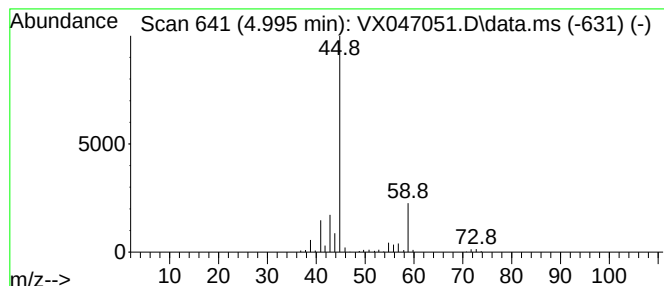
Instrument :
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ClientSampleId :
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Quant Title : SW846 8260

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

Peak Number 5 2-Butanol, (R)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.995	17.63 ug/l	476574	Pentafluorobenzene	5.562	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, (R)-	74	C4H10O	014898-79-4	83
2	2-Butanol	74	C4H10O	000078-92-2	78
3	2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	42
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	40
5	Isoamyl lactate	160	C8H16O3	019329-89-6	38



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FRAC TANK

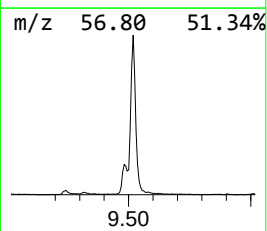
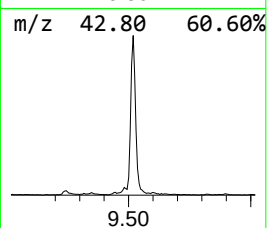
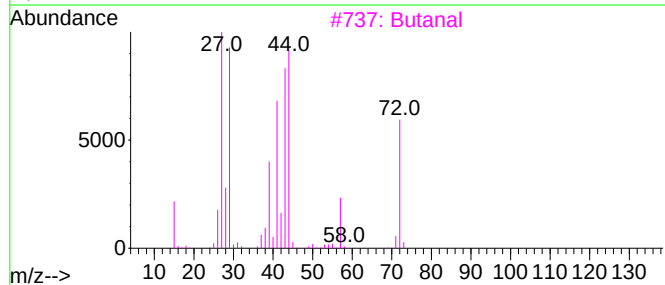
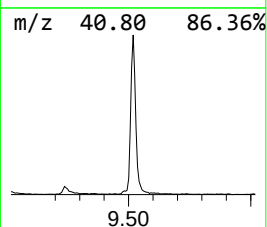
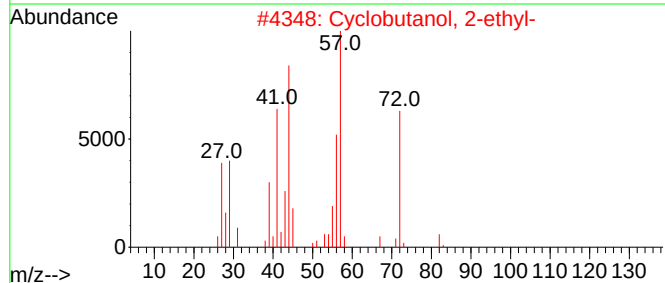
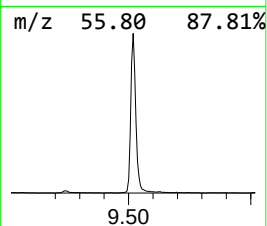
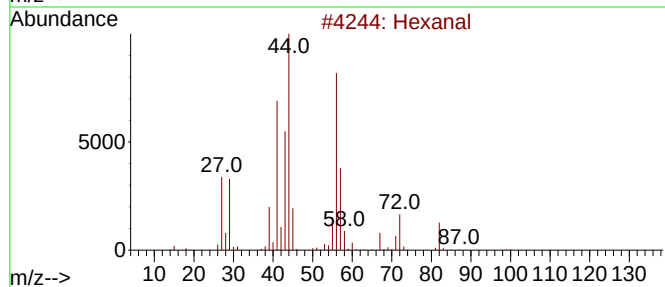
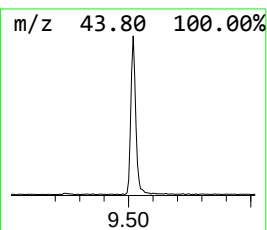
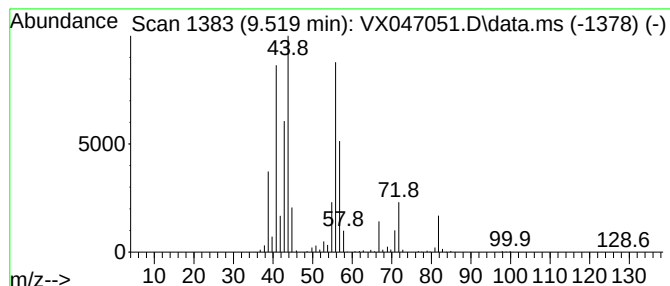
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Quant Title : SW846 8260

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

Peak Number 6 Hexanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.519	16.46 ug/l	765649	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal	100	C6H12O	000066-25-1	91
2			Cyclobutanol, 2-ethyl-	100	C6H12O	035301-43-0	50
3			Butanal	72	C4H8O	000123-72-8	30
4			Glutaraldehyde	100	C5H8O2	000111-30-8	25
5			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071825\
Data File : VX047051.D
Acq On : 18 Jul 2025 15:42
Operator : JC/MD
Sample : Q2646-01 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FRAC TANK

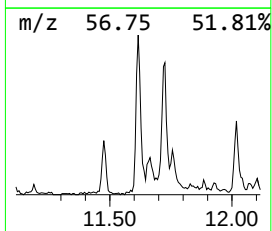
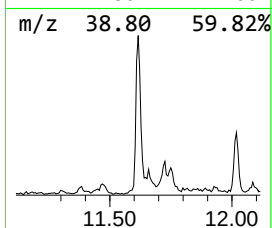
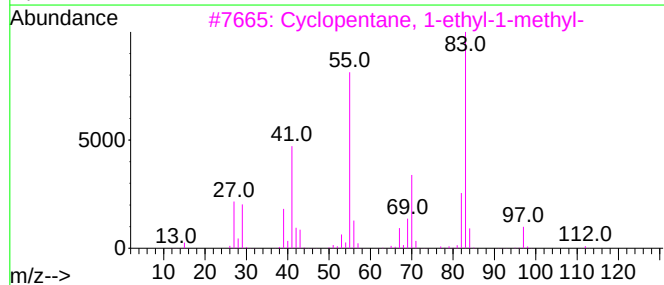
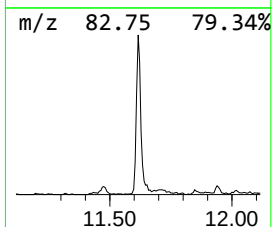
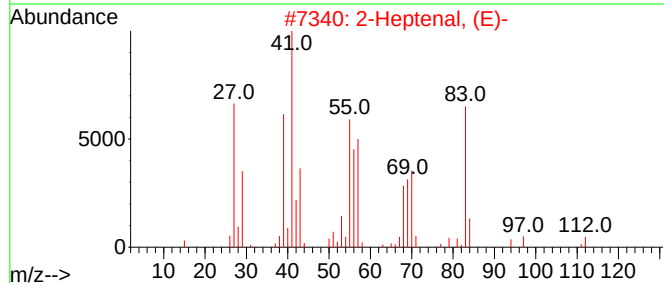
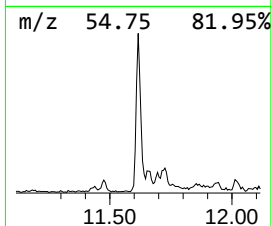
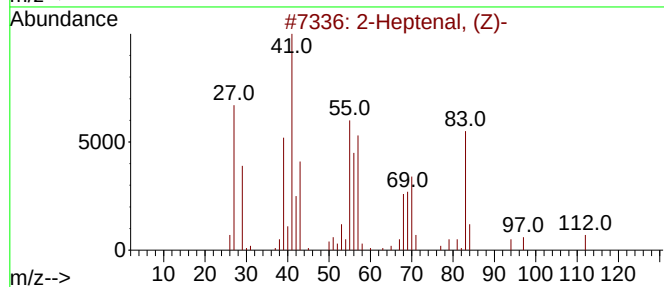
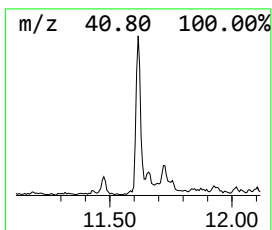
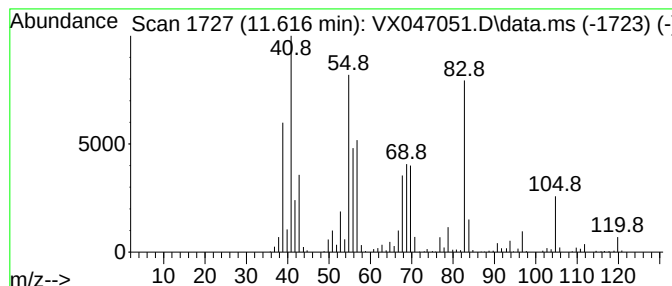
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Quant Title : SW846 8260

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

Peak Number 7 2-Heptenal, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	6.04 ug/l	272494	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptenal, (Z)-	112	C7H12O	057266-86-1	86
2			2-Heptenal, (E)-	112	C7H12O	018829-55-5	76
3			Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	43
4			2-Undecanethiol, 2-methyl-	202	C12H26S	010059-13-9	43
5			Cyclododecane	168	C12H24	000294-62-2	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071825\
Data File : VX047051.D
Acq On : 18 Jul 2025 15:42
Operator : JC/MD
Sample : Q2646-01 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FRAC TANK

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070225W.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
Sulfur dioxide	1.270	76.2	ug/l	2058720	1	5.562	1351450	50.0
Ethanol	2.057	5.1	ug/l	137299	1	5.562	1351450	50.0
1-Propanol	3.849	6.4	ug/l	172915	1	5.562	1351450	50.0
2-Butanol, (R)-	4.995	17.6	ug/l	476574	1	5.562	1351450	50.0
Hexanal	9.519	16.5	ug/l	765649	3	10.055	2325550	50.0
2-Heptenal, (Z)-	11.616	6.0	ug/l	272494	4	12.018	2257020	50.0