

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032822\
 Data File : VX027756.D
 Acq On : 28 Mar 2022 17:42
 Operator : JC/MD
 Sample : N2154-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-4

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\82X032522W.M
 Title : SW846 8260

Signal : TIC: VX027756.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	21	26	34	rBV	18049	30473	7.70%	1.204%
2	1.453	56	60	64	rBV	4576	5670	1.43%	0.224%
3	2.056	153	159	167	rBV	16700	25977	6.56%	1.026%
4	2.379	206	212	216	rVV	25913	40422	10.21%	1.597%
5	2.422	216	219	225	rVB3	4705	8149	2.06%	0.322%
6	2.532	230	237	248	rBV	30431	56510	14.27%	2.233%
7	2.953	294	306	319	rBV2	43708	100488	25.38%	3.971%
8	3.849	445	453	469	rBV2	16585	45180	11.41%	1.785%
9	4.574	560	572	584	rBV	4882	15023	3.79%	0.594%
10	5.013	637	644	651	rBV5	1945	5591	1.41%	0.221%
11	5.099	654	658	666	rVB4	1860	4535	1.15%	0.179%
12	5.391	693	706	722	rBV	45159	132987	33.59%	5.255%
13	5.556	722	733	748	rVB	78837	219480	55.43%	8.672%
14	5.958	788	799	812	rBV	50063	135253	34.16%	5.344%
15	6.232	834	844	852	rBV5	1668	4076	1.03%	0.161%
16	6.763	922	931	947	rBV	126004	293722	74.18%	11.606%
17	7.226	997	1007	1011	rBV3	1697	4188	1.06%	0.165%
18	7.433	1034	1041	1053	rVB4	5684	13204	3.33%	0.522%
19	8.574	1222	1228	1234	rBV	6950	11890	3.00%	0.470%
20	8.653	1234	1241	1249	rBV	246728	395966	100.00%	15.646%
21	9.031	1299	1303	1308	rBV2	2673	4017	1.01%	0.159%
22	10.055	1465	1471	1480	rBV	271198	354700	89.58%	14.015%
23	10.299	1505	1511	1517	rBV2	3826	5120	1.29%	0.202%
24	11.085	1634	1640	1646	rBV	206326	270989	68.44%	10.708%
25	12.024	1788	1794	1801	rBV	265012	324125	81.86%	12.807%
26	12.219	1821	1826	1833	rBV2	16658	23053	5.82%	0.911%

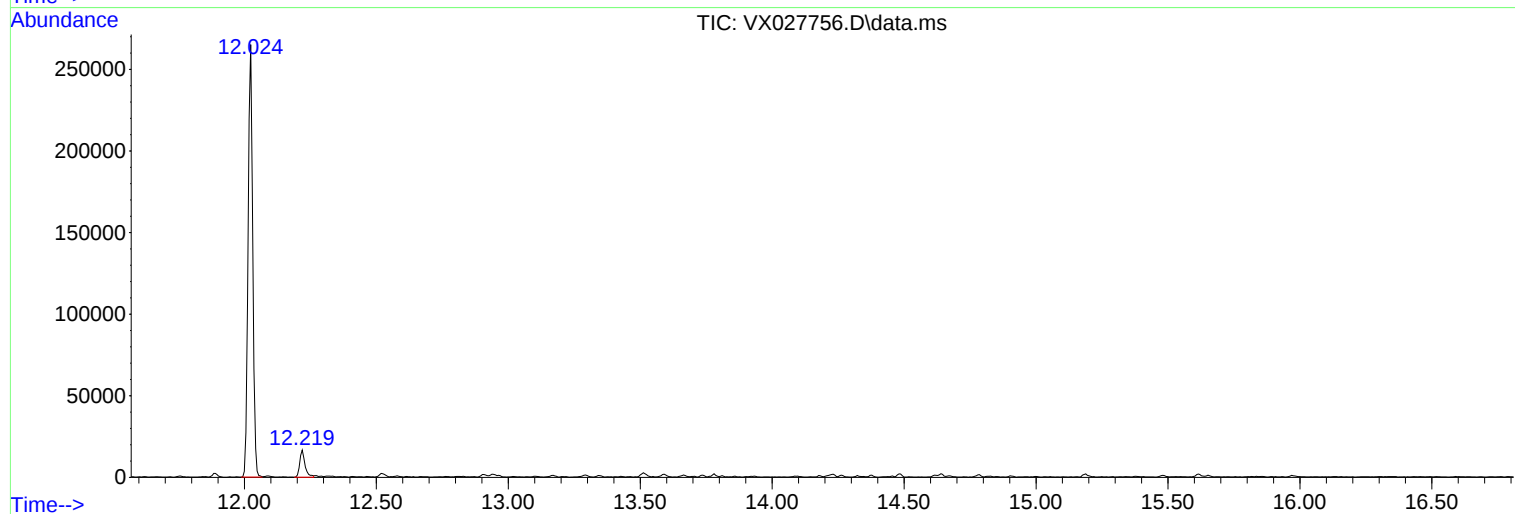
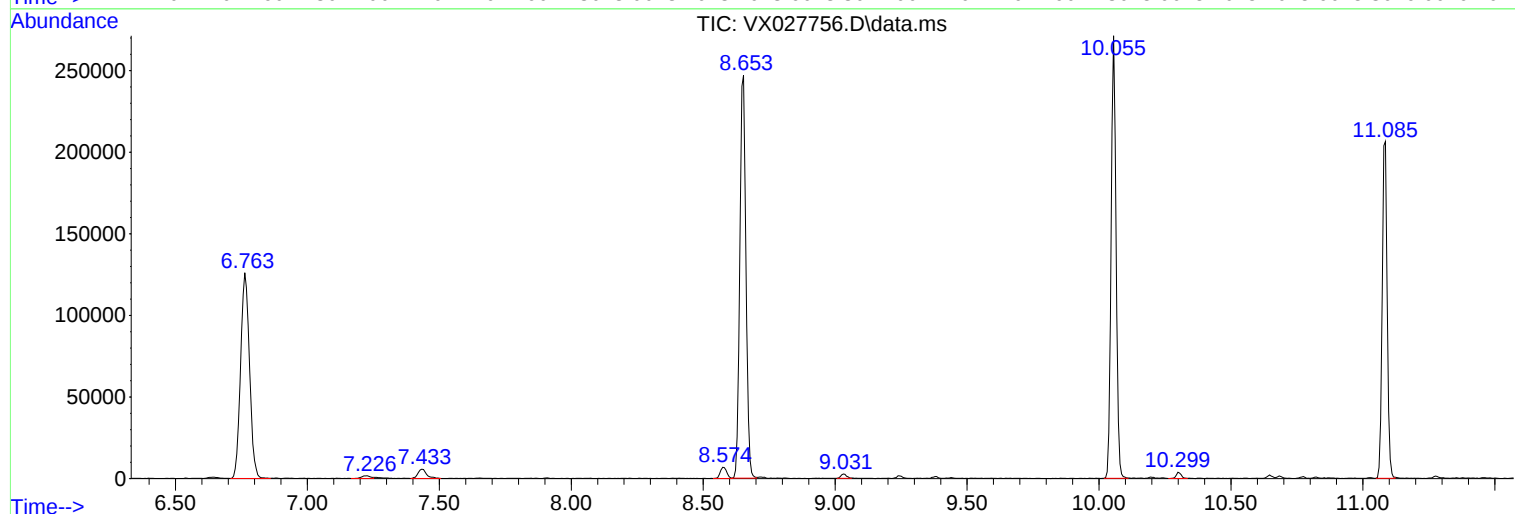
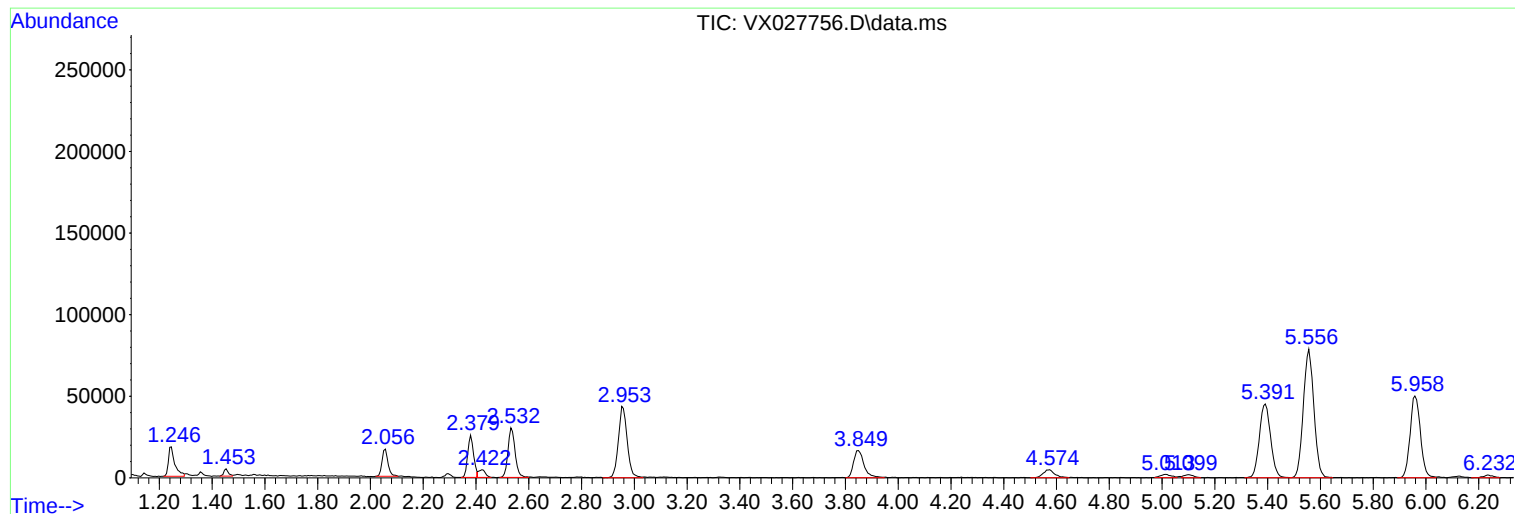
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032522W.M
Quant Title : SW846 8260

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



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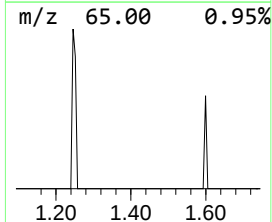
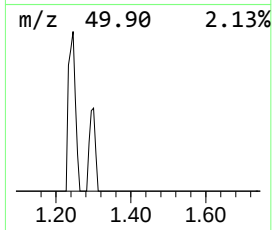
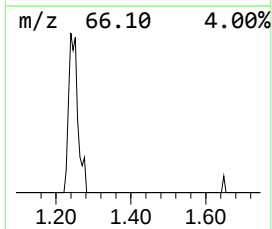
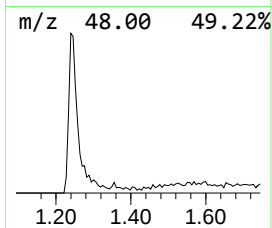
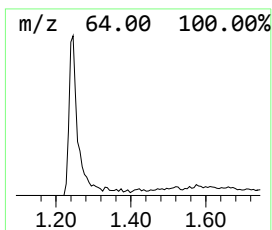
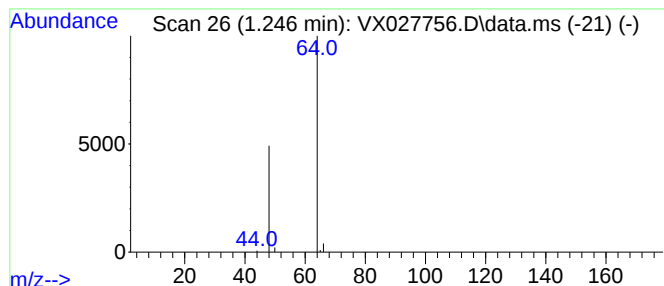
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032522W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	6.94 ug/l	30473	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
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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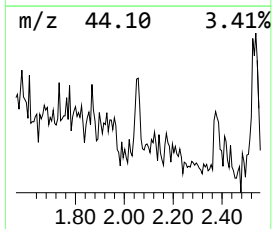
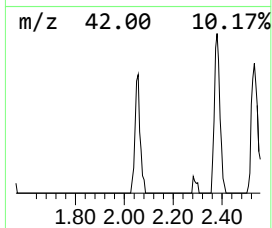
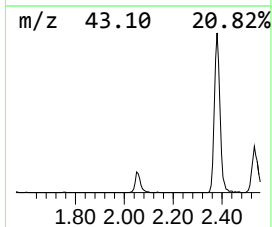
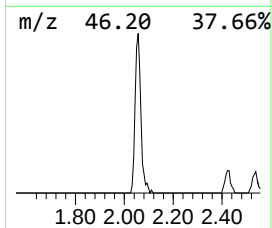
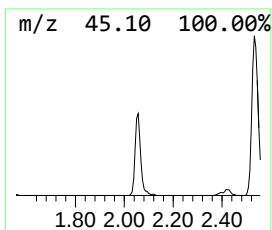
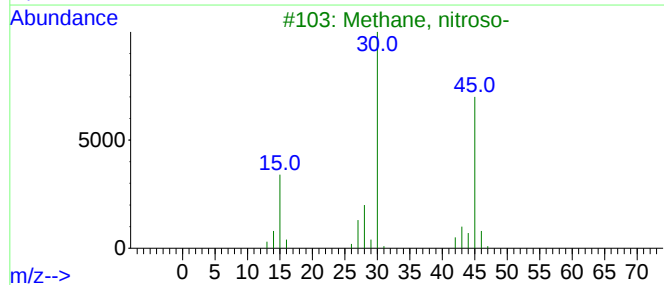
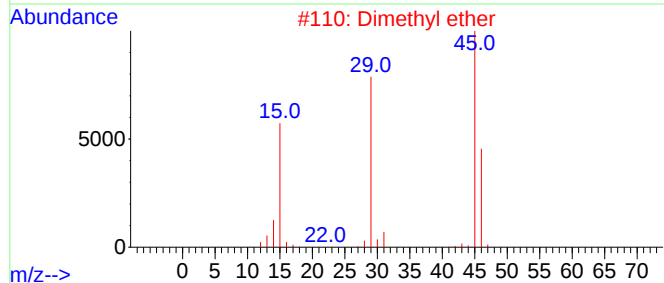
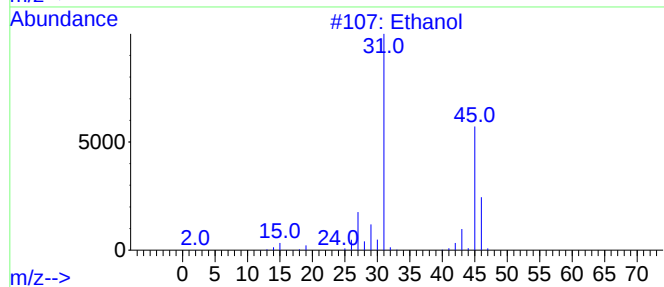
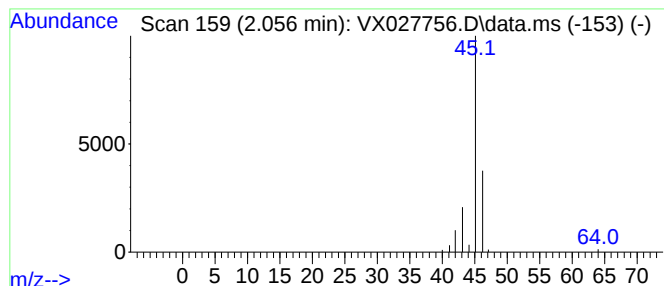
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Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.056	5.92 ug/l	25977	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			Dihydroxyacetic acid	92	C2H4O4	000563-96-2	2



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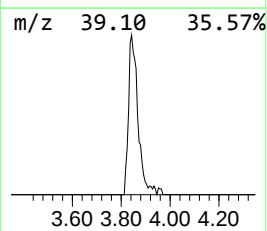
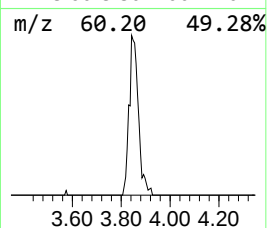
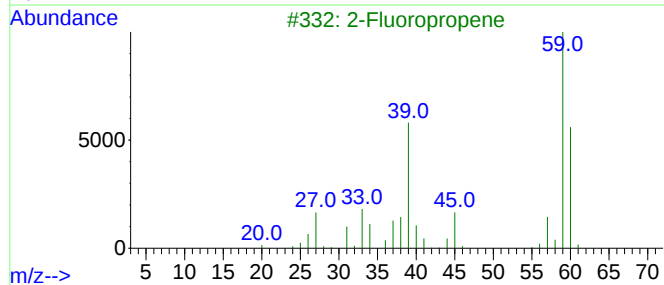
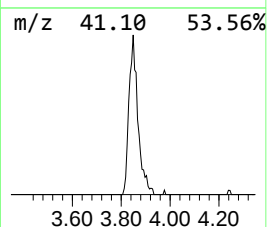
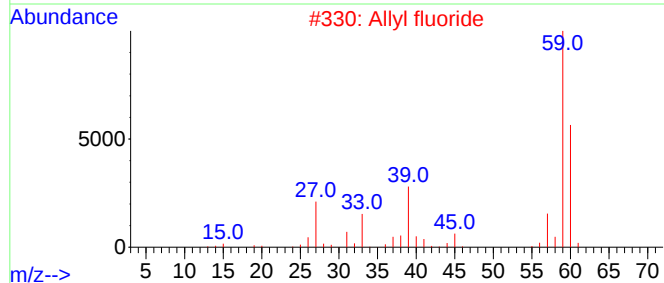
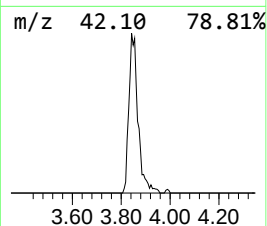
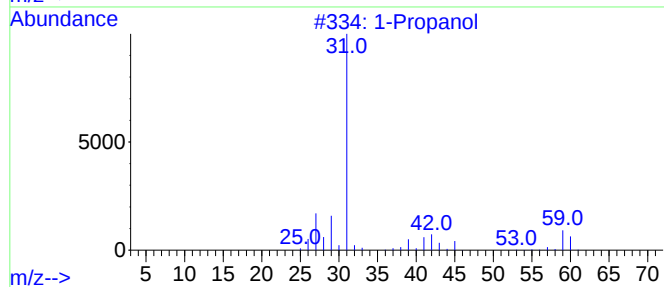
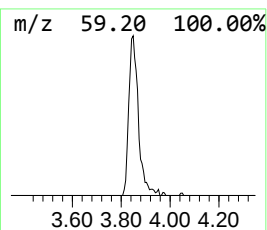
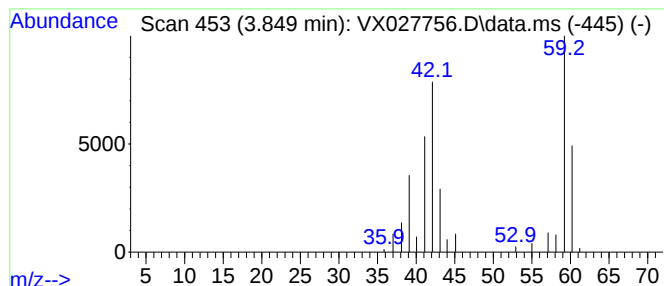
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.849	10.29 ug/l	45180	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propanol	60	C3H8O	000071-23-8	72
2			Allyl fluoride	60	C3H5F	000818-92-8	46
3			2-Fluoropropene	60	C3H5F	001184-60-7	37
4			Cyclopropane	42	C3H6	000075-19-4	16
5			3-Pentanol	88	C5H12O	000584-02-1	9



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.246	6.9	ug/l	30473	1	5.556	219480	50.0
Ethanol	2.056	5.9	ug/l	25977	1	5.556	219480	50.0
1-Propanol	3.849	10.3	ug/l	45180	1	5.556	219480	50.0