

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032123\
 Data File : VX034650.D
 Acq On : 21 Mar 2023 13:29
 Operator : JC/MD
 Sample : 02013-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 600

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\82X031023W.M
 Title : SW846 8260

Signal : TIC: VX034650.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	18	rVB	28973	27530	1.04%	0.231%
2	2.373	205	211	228	rBV	1667031	2642940	100.00%	22.203%
3	2.526	230	236	251	rBV	270022	494151	18.70%	4.151%
4	2.953	298	306	313	rBV2	12437	28029	1.06%	0.235%
5	4.227	504	515	535	rBV	244448	651366	24.65%	5.472%
6	4.550	560	568	586	rBV	99014	289830	10.97%	2.435%
7	5.385	694	705	720	rBV	151621	438377	16.59%	3.683%
8	5.550	720	732	747	rVB	264733	741562	28.06%	6.230%
9	5.952	788	798	808	rBV	175437	466830	17.66%	3.922%
10	6.763	920	931	947	rBV	403879	983409	37.21%	8.262%
11	7.458	1040	1045	1054	rBV	21171	43949	1.66%	0.369%
12	7.580	1058	1065	1071	rVV	22057	44860	1.70%	0.377%
13	7.641	1071	1075	1093	rVB	13044	32951	1.25%	0.277%
14	8.574	1221	1228	1234	rBV	141048	225635	8.54%	1.896%
15	8.647	1234	1240	1247	rVV	861175	1343385	50.83%	11.286%
16	8.714	1247	1251	1259	rVB2	22859	42067	1.59%	0.353%
17	10.055	1462	1471	1484	rBV	868797	1208553	45.73%	10.153%
18	10.506	1541	1545	1556	rBV	20624	29928	1.13%	0.251%
19	10.683	1570	1574	1582	rVB	56064	74087	2.80%	0.622%
20	10.768	1582	1588	1595	rBV3	16577	36006	1.36%	0.302%
21	11.079	1634	1639	1645	rBV	689005	867995	32.84%	7.292%
22	12.024	1788	1794	1802	rBV	811131	1025488	38.80%	8.615%
23	12.219	1821	1826	1842	rBV	70934	164565	6.23%	1.382%

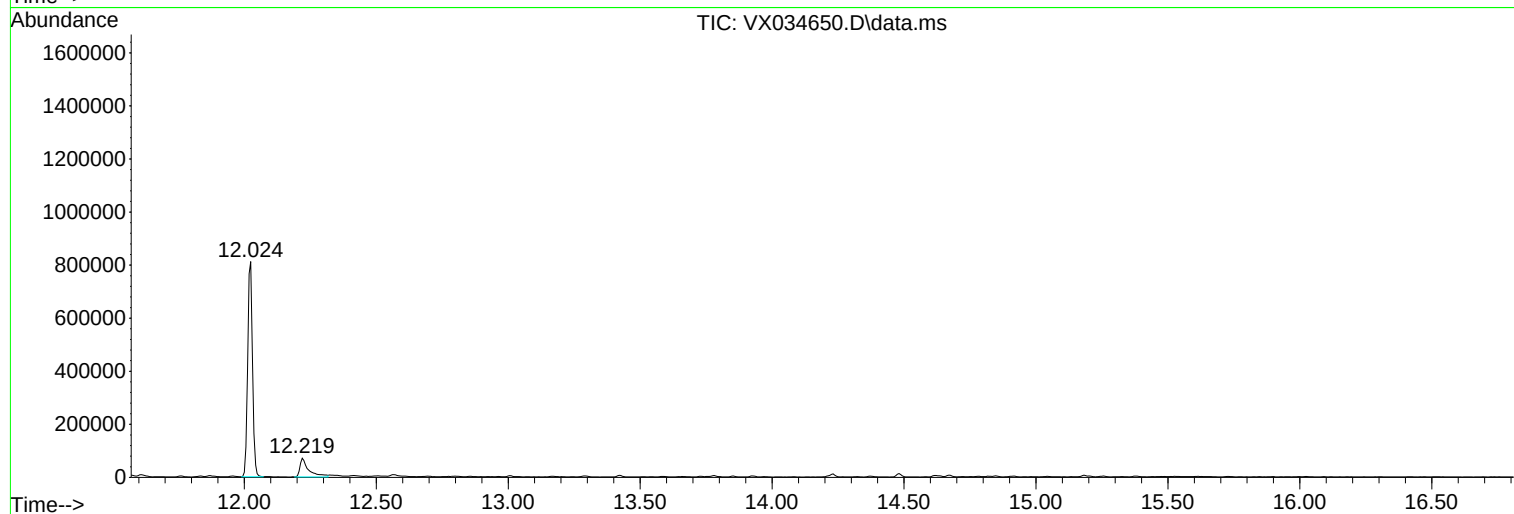
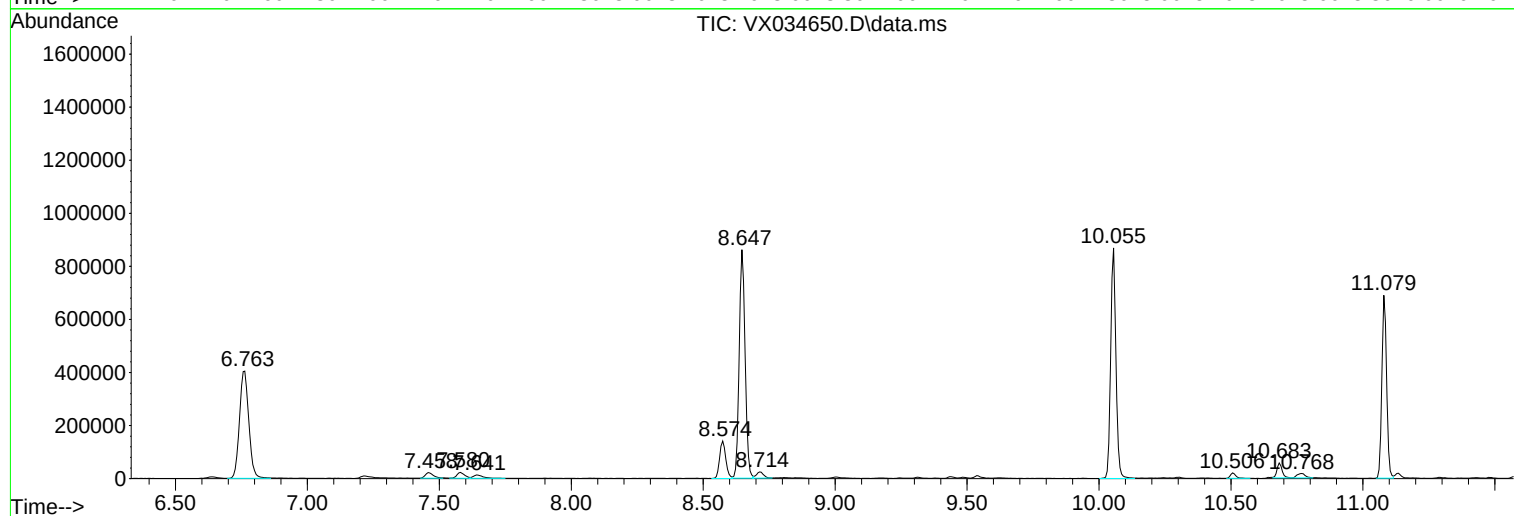
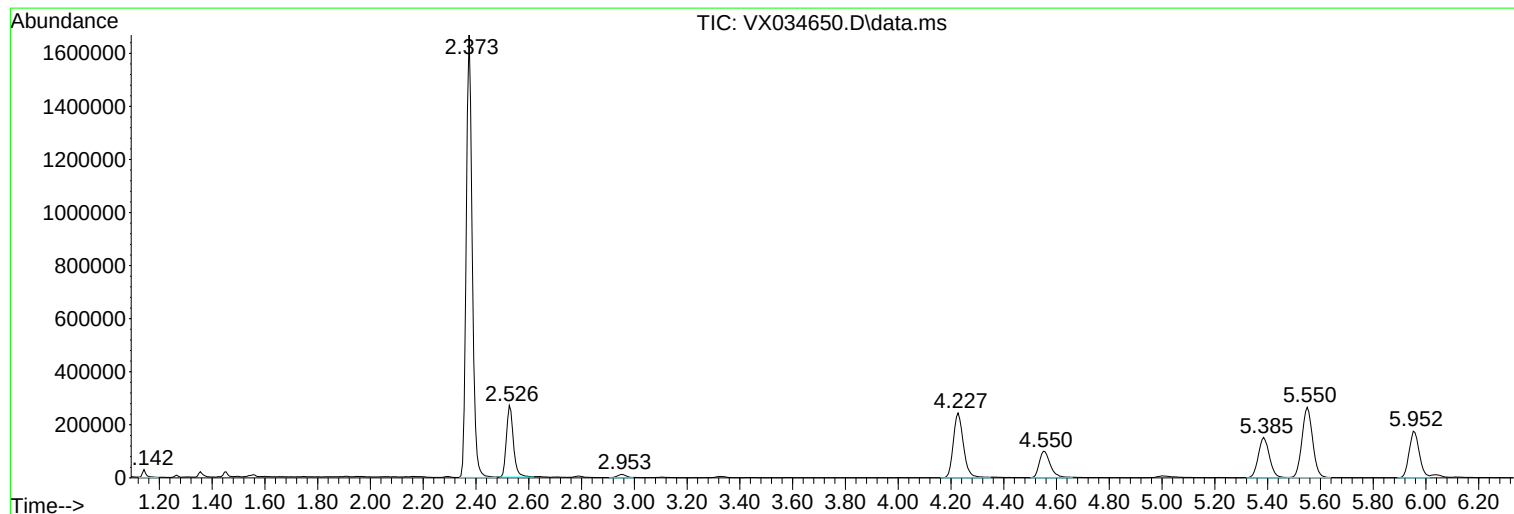
Sum of corrected areas: 11903493

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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



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Instrument :
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ClientSampleId :
600

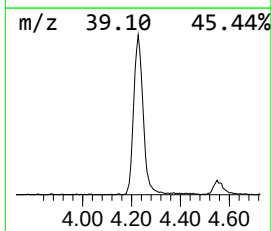
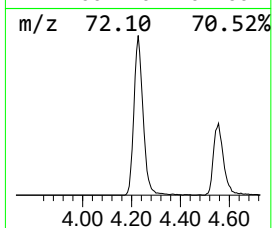
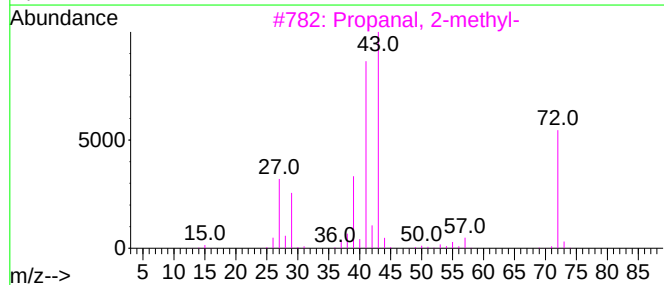
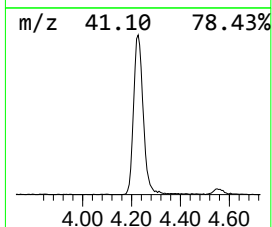
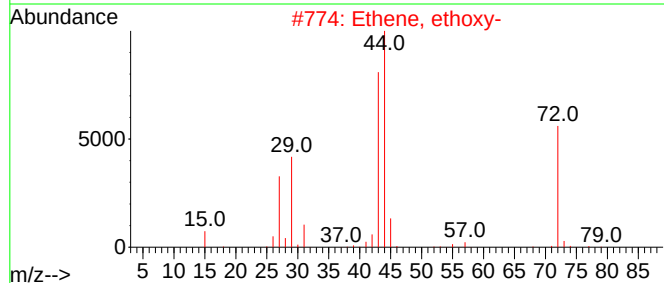
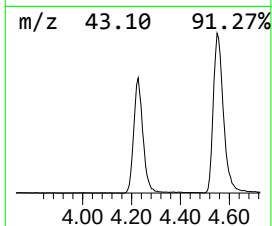
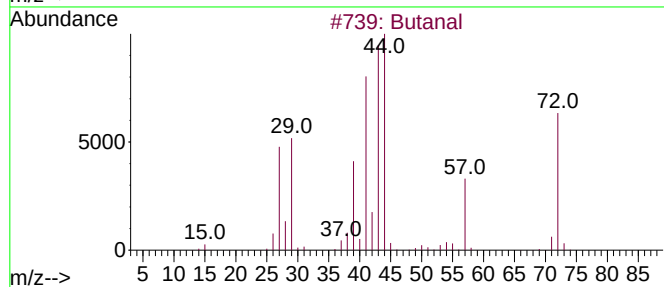
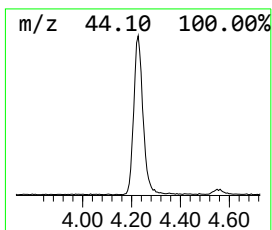
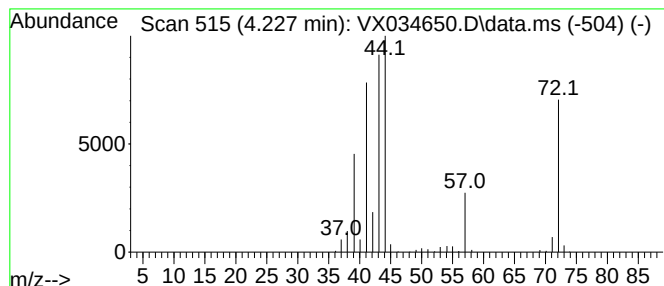
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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

Peak Number 1 Butanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	43.92 ug/l	651366	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	94
2			Ethene, ethoxy-	72	C4H8O	000109-92-2	52
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	35
5			Dimethylketene	70	C4H6O	000598-26-5	22



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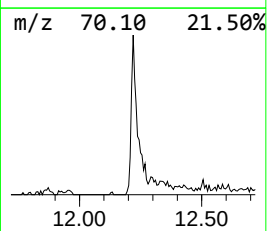
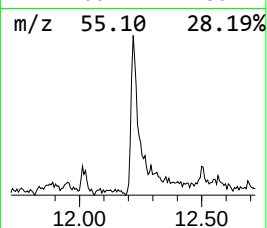
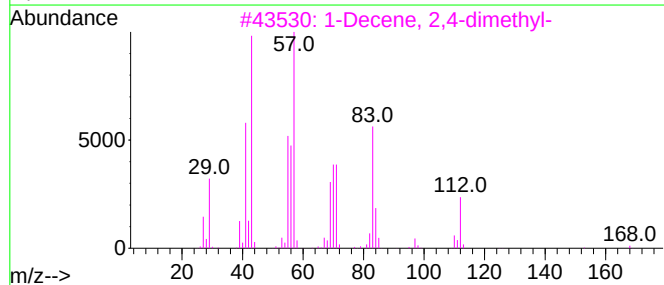
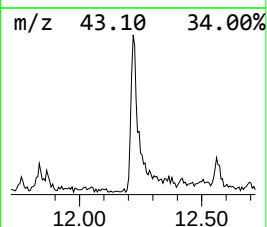
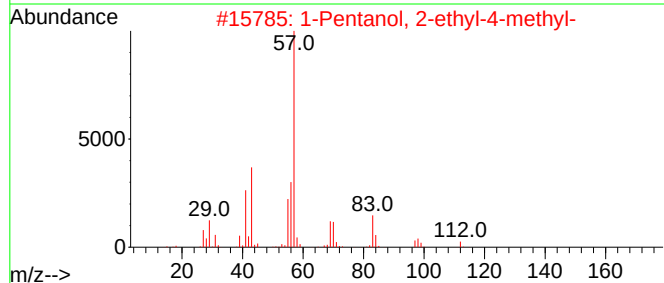
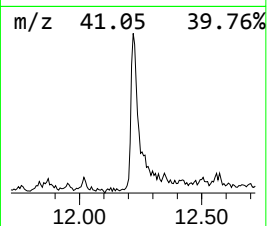
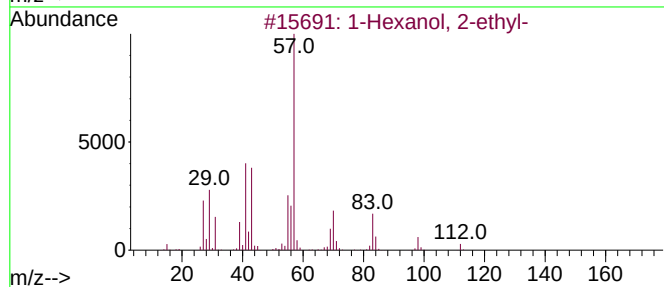
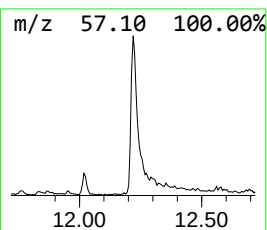
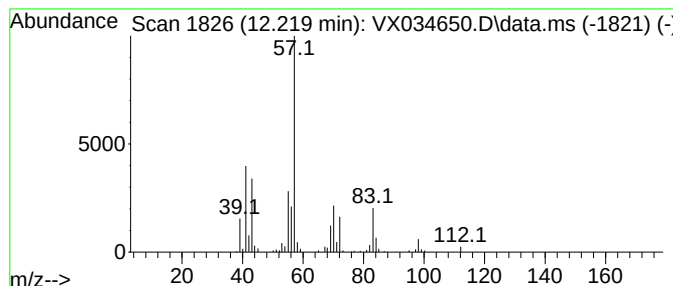
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Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	8.02 ug/l	164565	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	86
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50
3			1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	50
4			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	43
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanal	4.227	43.9	ug/l	651366	1	5.550	741562	50.0
1-Hexanol, 2-et...	12.219	8.0	ug/l	164565	4	12.024	1025490	50.0