

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030623\
 Data File : VX034349.D
 Acq On : 06 Mar 2023 15:00
 Operator : JC/MD
 Sample : 01816-04
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMP-VOC

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\82X021723W.M
 Title : SW846 8260

Signal : TIC: VX034349.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.374	205	211	230	rBV	1269439	2118766	10.01%	5.905%
2	4.556	560	569	586	rBV	126036	359423	1.70%	1.002%
3	5.385	694	705	718	rBV	153213	449342	2.12%	1.252%
4	5.550	722	732	751	rVB	257434	735645	3.47%	2.050%
5	5.958	788	799	806	rBV	170514	461022	2.18%	1.285%
6	6.038	806	812	823	rVB	200208	520559	2.46%	1.451%
7	6.763	921	931	947	rBV	414121	988618	4.67%	2.755%
8	8.647	1234	1240	1246	rBV	860508	1366524	6.45%	3.809%
9	8.720	1246	1252	1271	rVB	13265686	21172189	100.00%	59.008%
10	9.580	1386	1393	1398	rBV	378403	519555	2.45%	1.448%
11	10.055	1465	1471	1479	rBV	845645	1161299	5.49%	3.237%
12	10.195	1489	1494	1499	rVB	509040	654192	3.09%	1.823%
13	10.299	1504	1511	1523	rVB	1694306	2250627	10.63%	6.273%
14	10.640	1562	1567	1580	rVB	673079	922720	4.36%	2.572%
15	11.079	1634	1639	1645	rBV	697008	880115	4.16%	2.453%
16	12.024	1788	1794	1801	rVB	785062	1029488	4.86%	2.869%
17	12.219	1821	1826	1837	rBV	172010	290213	1.37%	0.809%

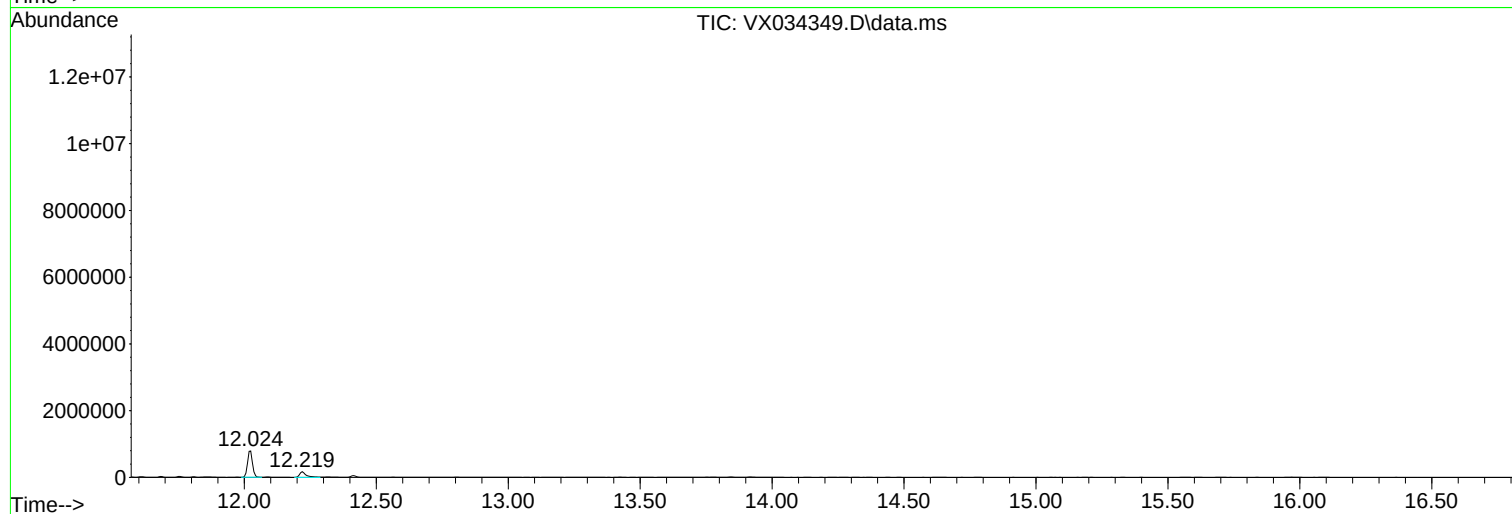
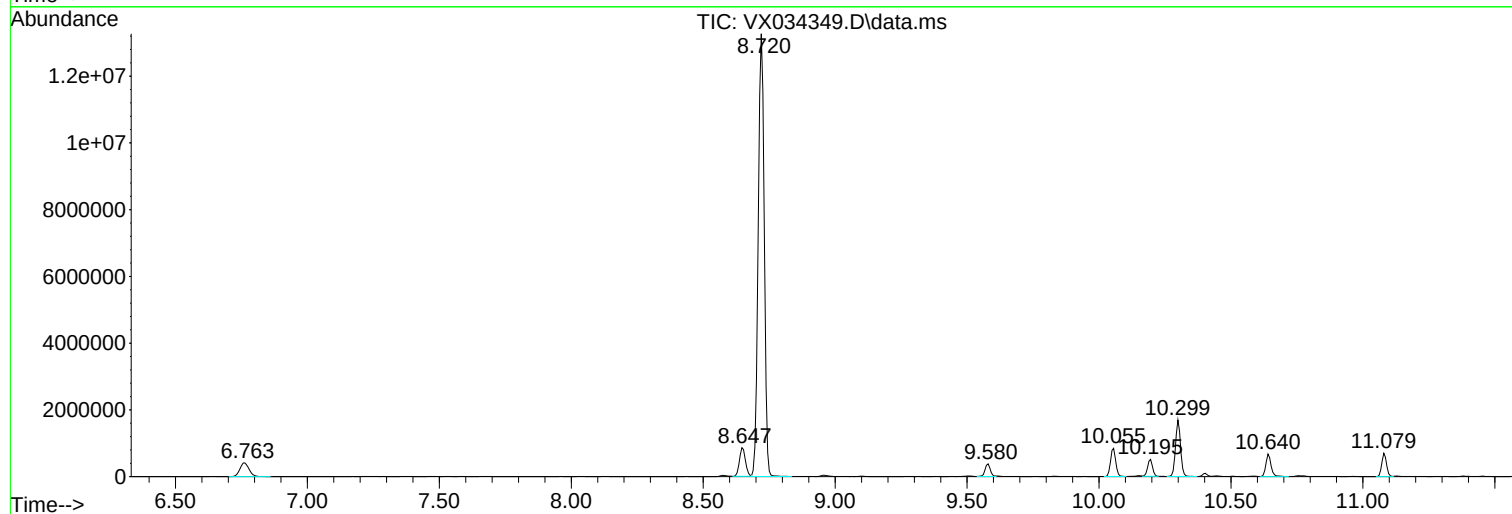
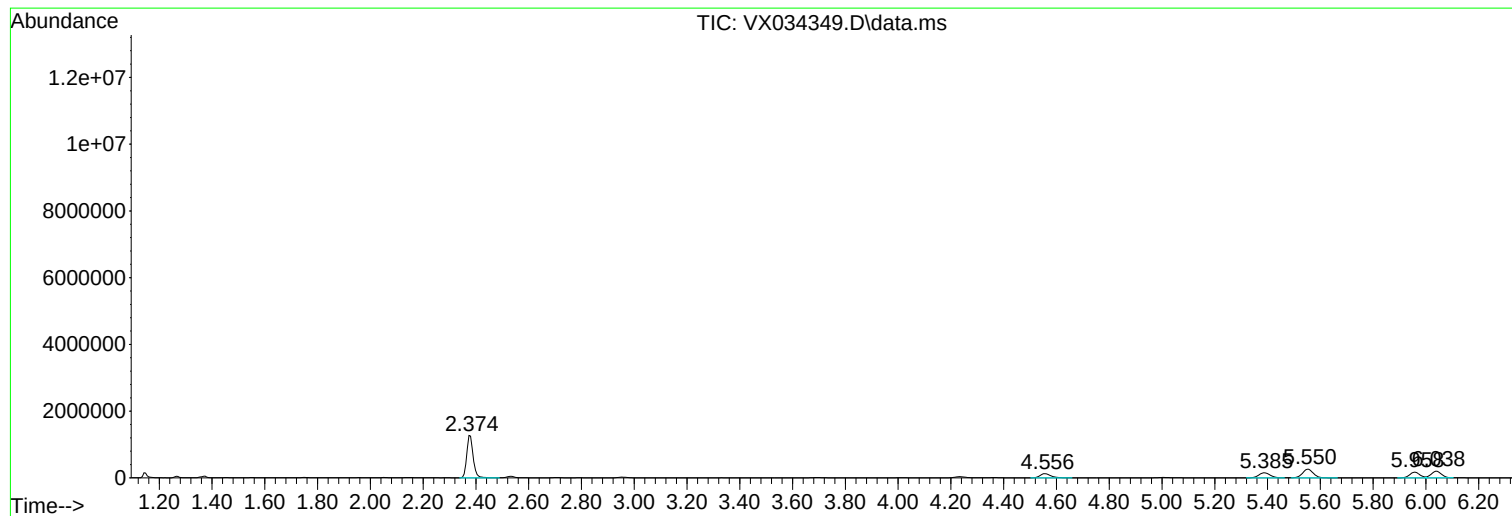
Sum of corrected areas: 35880297

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

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



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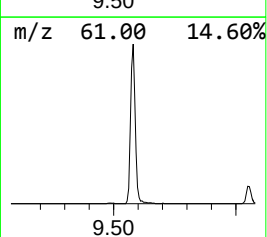
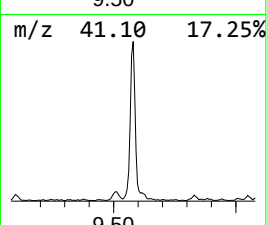
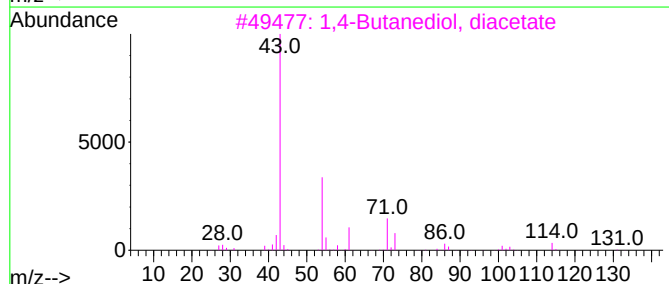
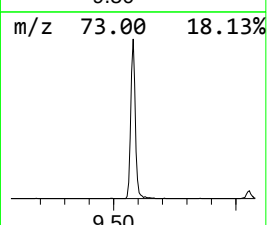
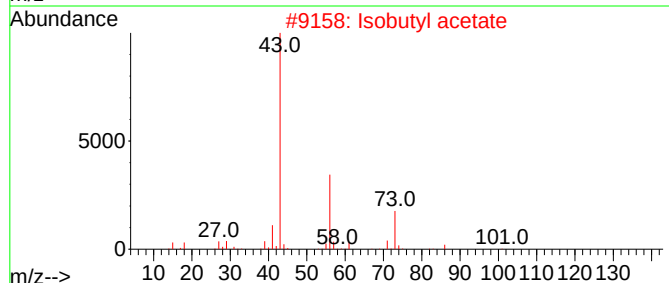
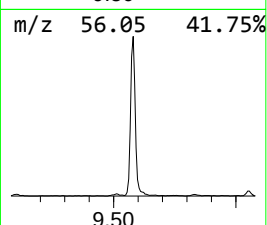
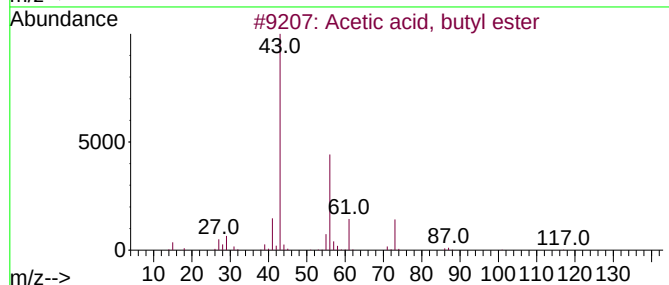
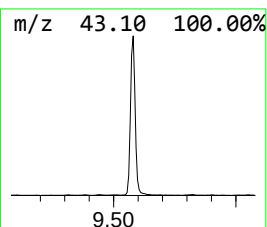
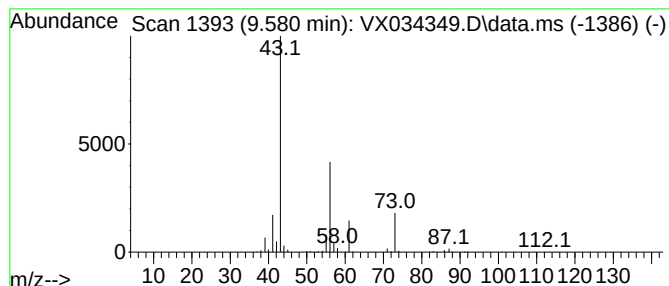
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetic acid, butyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.580	22.37 ug/l	519555	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2			Isobutyl acetate	116	C6H12O2	000110-19-0	40
3			1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	17
4			Isobutylamine	73	C4H11N	000078-81-9	9
5			3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	9



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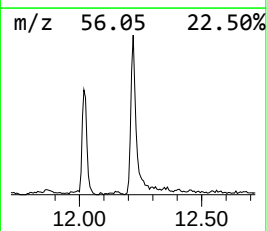
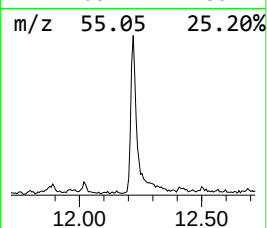
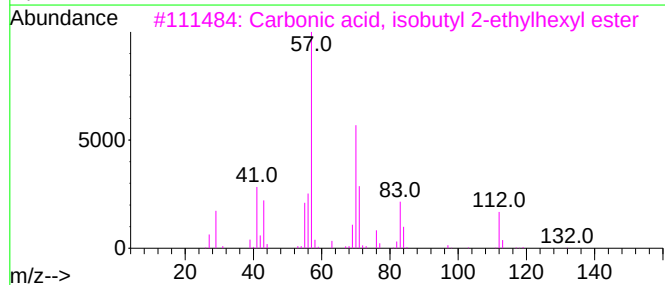
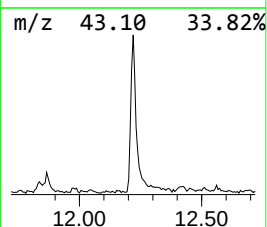
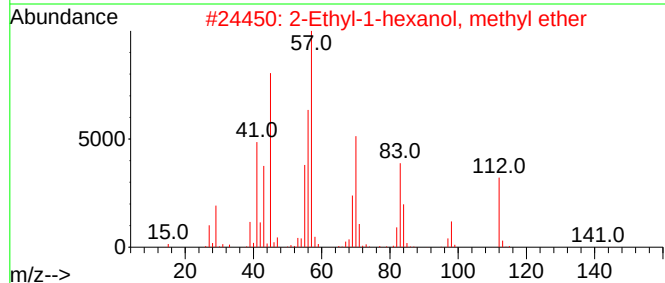
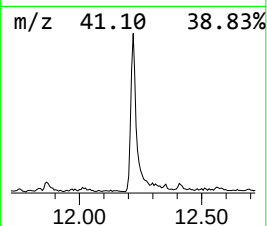
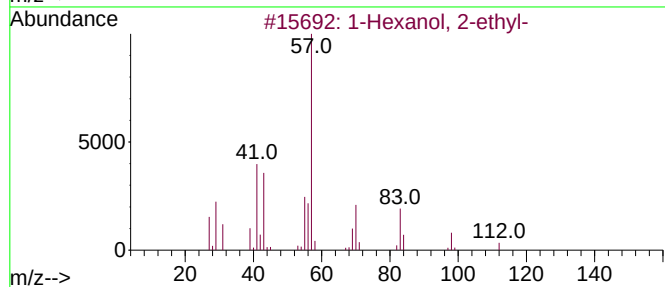
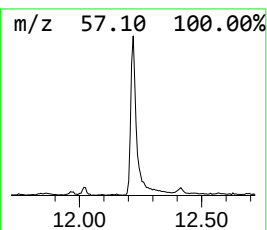
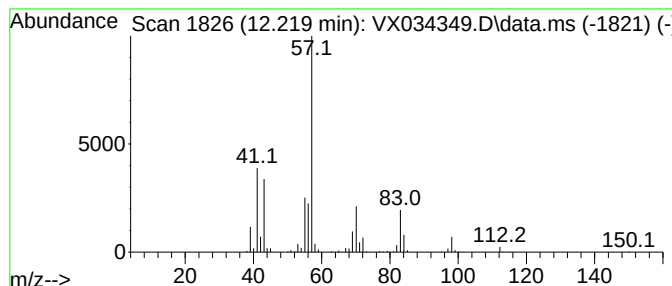
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	14.10 ug/l	290213	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			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	53
3			Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	53
4			Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	47
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetic acid, bu...	9.580	22.4	ug/l	519555	3	10.055	1161300	50.0
1-Hexanol, 2-et...	12.219	14.1	ug/l	290213	4	12.024	1029490	50.0