

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022824\
 Data File : VX040514.D
 Acq On : 28 Feb 2024 16:26
 Operator : JC/MD
 Sample : P1613-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 1847

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\82X022624W.M
 Title : SW846 8260

Signal : TIC: VX040514.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	11446	12746	2.86%	0.430%
2	2.380	204	212	225	rBV	20305	35937	8.07%	1.213%
3	4.227	506	515	530	rBV4	19096	53321	11.98%	1.799%
4	5.385	694	705	717	rBV2	52529	154074	34.62%	5.199%
5	5.556	721	733	745	rBV	85024	242242	54.43%	8.174%
6	5.952	788	798	811	rBV	61838	164296	36.91%	5.544%
7	6.763	921	931	946	rBV	136396	332885	74.79%	11.232%
8	7.958	1121	1127	1134	rBV3	2400	4802	1.08%	0.162%
9	8.647	1232	1240	1249	rBV	283470	445068	100.00%	15.017%
10	8.720	1249	1252	1257	rVB3	3563	5154	1.16%	0.174%
11	10.055	1465	1471	1484	rBV	303904	426877	95.91%	14.404%
12	10.305	1505	1512	1519	rBV3	4153	7141	1.60%	0.241%
13	10.506	1540	1545	1553	rVB	7944	11190	2.51%	0.378%
14	10.762	1582	1587	1602	rBV2	12888	34321	7.71%	1.158%
15	11.079	1634	1639	1644	rBV	255071	336402	75.58%	11.351%
16	11.128	1644	1647	1652	rVB	18028	24079	5.41%	0.812%
17	11.280	1668	1672	1681	rVB4	4679	7782	1.75%	0.263%
18	11.579	1715	1721	1724	rBV3	10075	18455	4.15%	0.623%
19	11.610	1724	1726	1734	rVV3	8138	15920	3.58%	0.537%
20	11.683	1734	1738	1748	rVB	80021	97669	21.94%	3.296%
21	12.024	1788	1794	1802	rVB	338916	439263	98.70%	14.822%
22	12.237	1822	1829	1836	rBV5	6263	19155	4.30%	0.646%
23	13.676	2058	2065	2070	rBV	36349	43153	9.70%	1.456%
24	14.030	2119	2123	2129	rVB2	7273	9163	2.06%	0.309%
25	14.140	2136	2141	2151	rVB2	9036	12254	2.75%	0.413%
26	14.274	2158	2163	2168	rVB	8053	10318	2.32%	0.348%

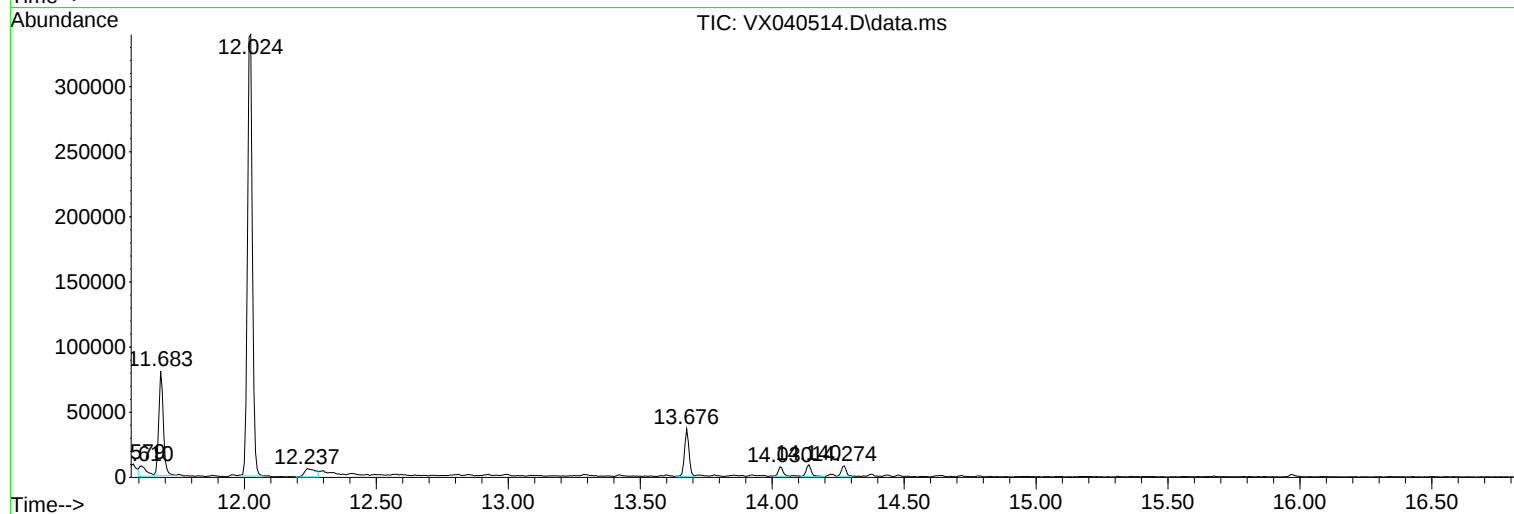
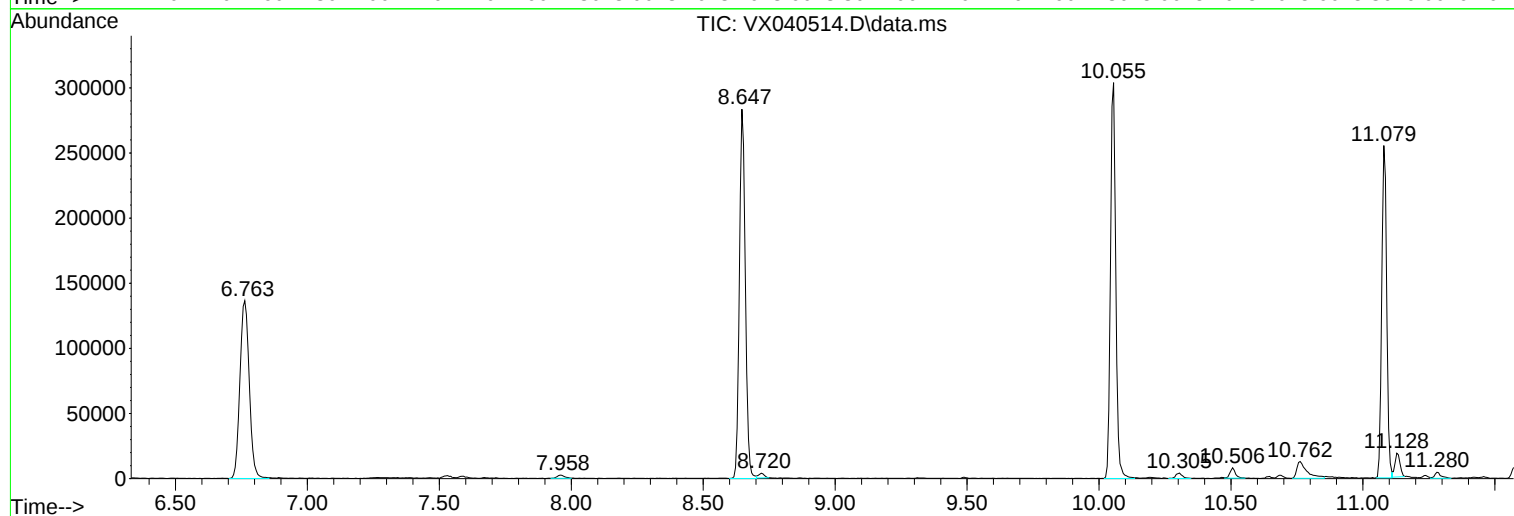
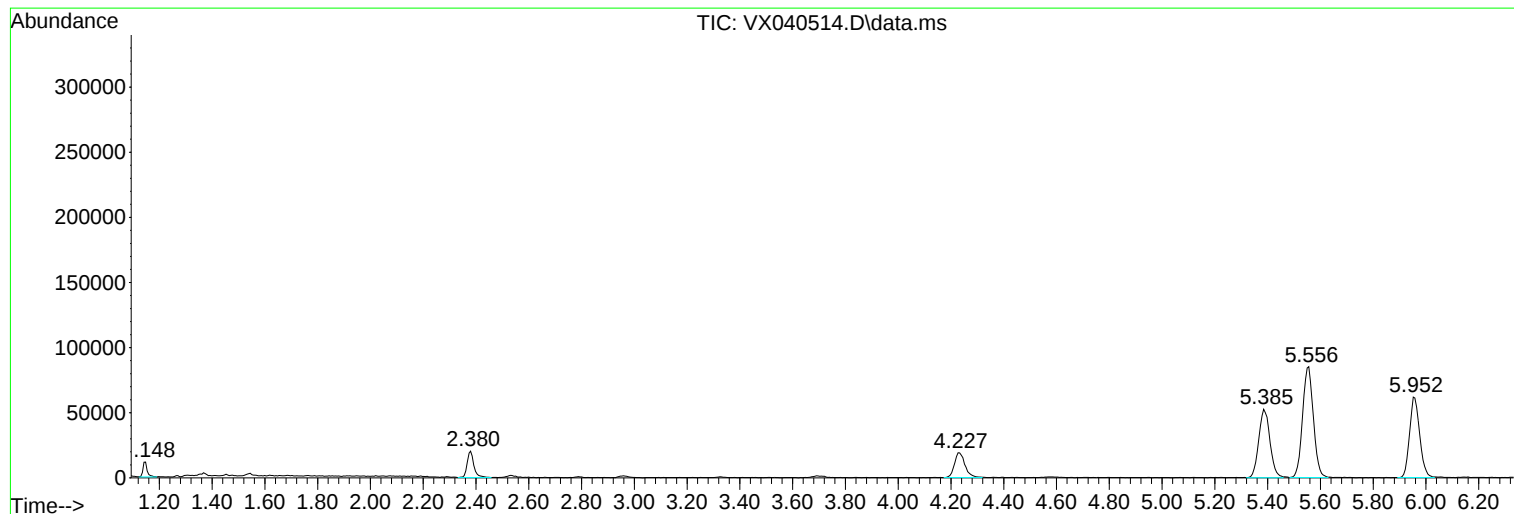
Sum of corrected areas: 2963667

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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022624W.M
Quant Title : SW846 8260

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



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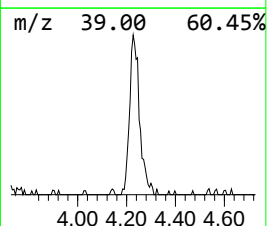
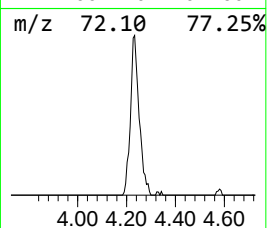
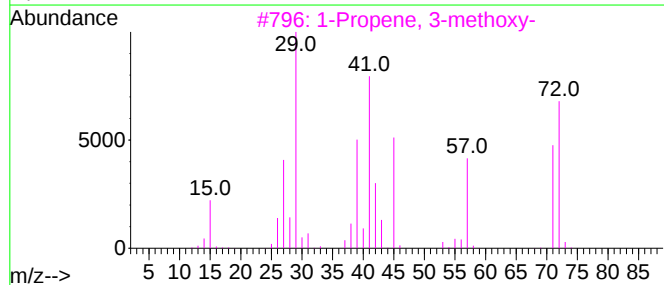
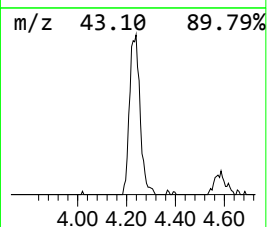
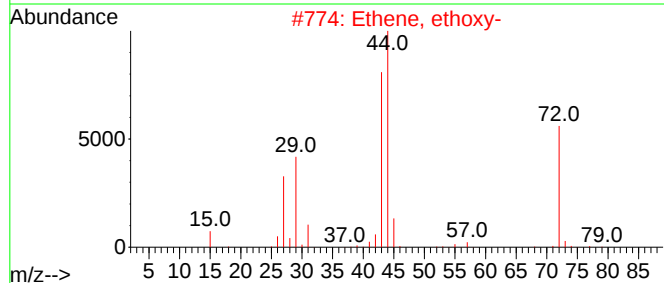
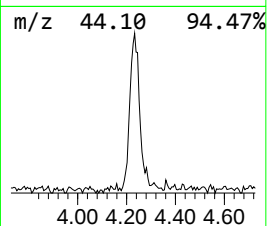
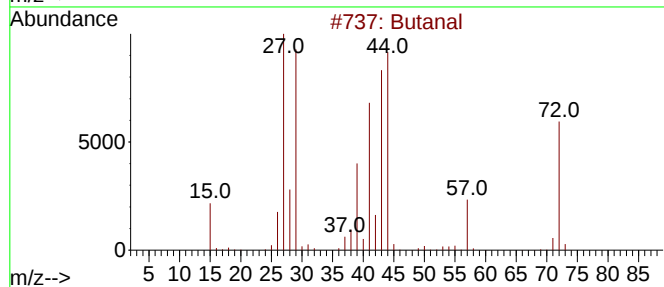
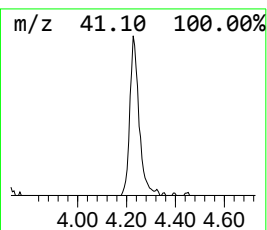
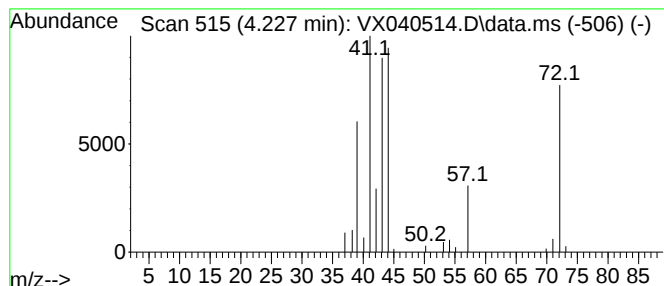
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022624W.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 1 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	11.01 ug/l	53321	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	86
2			Ethene, ethoxy-	72	C4H8O	000109-92-2	47
3			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	43
4			Methacrolein	70	C4H6O	000078-85-3	22
5			Propanal, 2-methyl-	72	C4H8O	000078-84-2	16



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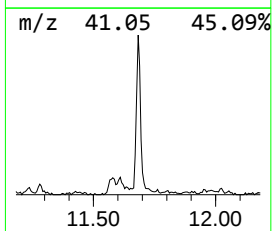
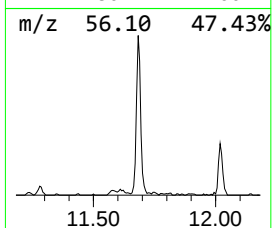
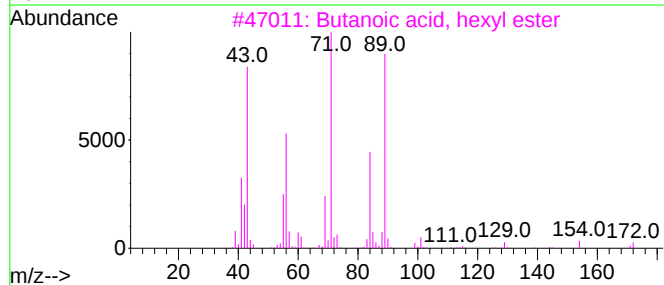
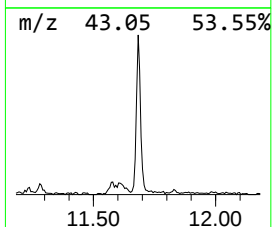
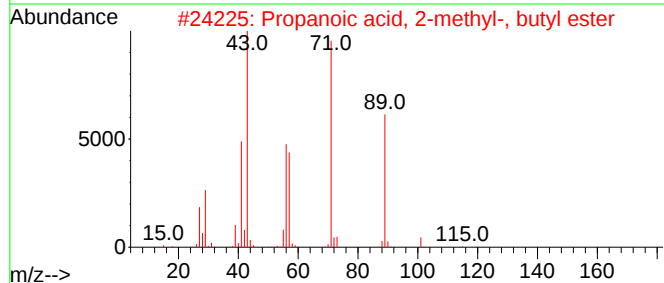
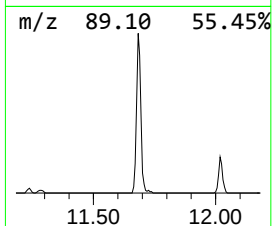
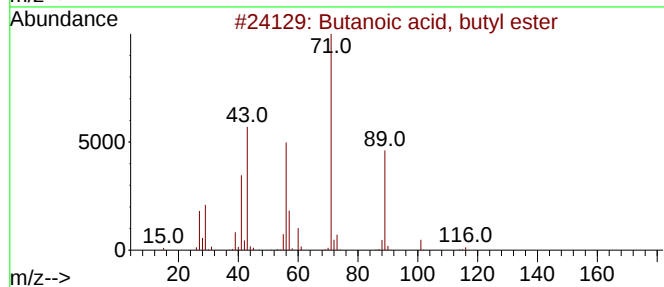
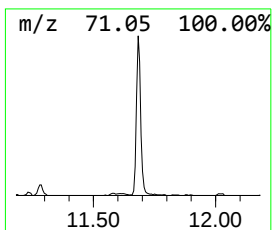
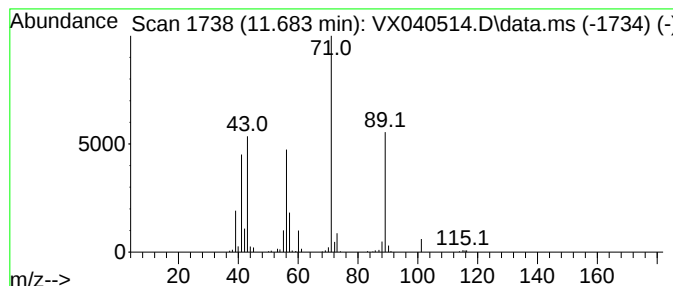
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Butanoic acid, butyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.683	11.12 ug/l	97669	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2			Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	78
3			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	74
4			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	64
5			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanal	4.227	11.0	ug/l	53321	1	5.556	242242	50.0
Butanoic acid, ...	11.683	11.1	ug/l	97669	4	12.024	439263	50.0