

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090922\
 Data File : VX031258.D
 Acq On : 09 Sep 2022 15:44
 Operator : JC/MD
 Sample : N4495-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 ETGI-345

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\82X090722W.M
 Title : SW846 8260

Signal : TIC: VX031258.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.270	22	30	35	rBV3	2626	5465	1.27%	0.242%
2	2.386	207	213	226	rBB	26587	43245	10.06%	1.918%
3	2.550	234	240	253	rVB2	5757	12556	2.92%	0.557%
4	2.794	273	280	286	rBB2	4762	8166	1.90%	0.362%
5	5.391	695	706	720	rBB	52249	148008	34.42%	6.563%
6	5.556	723	733	746	rBV2	60314	171718	39.93%	7.614%
7	5.958	789	799	813	rBV	63524	168751	39.24%	7.483%
8	6.348	855	863	872	rBB2	4132	9453	2.20%	0.419%
9	6.763	922	931	944	rBV	103935	273588	63.62%	12.131%
10	7.641	1070	1075	1082	rBV	13471	25049	5.82%	1.111%
11	7.806	1095	1102	1113	rBB2	3843	7495	1.74%	0.332%
12	8.549	1218	1224	1234	rVB	17718	32863	7.64%	1.457%
13	8.653	1234	1241	1249	rBV	275992	430064	100.00%	19.070%
14	9.250	1333	1339	1345	rBV	26634	38044	8.85%	1.687%
15	9.311	1345	1349	1355	rVV	7516	11015	2.56%	0.488%
16	9.378	1355	1360	1367	rVB	37116	51792	12.04%	2.297%
17	9.915	1443	1448	1455	rBB2	13968	18314	4.26%	0.812%
18	10.055	1462	1471	1483	rBV	199472	269853	62.75%	11.966%
19	11.085	1634	1640	1645	rBV	221524	282328	65.65%	12.519%
20	11.762	1746	1751	1759	rVB	12337	15469	3.60%	0.686%
21	12.024	1789	1794	1800	rVB	190866	231953	53.93%	10.285%

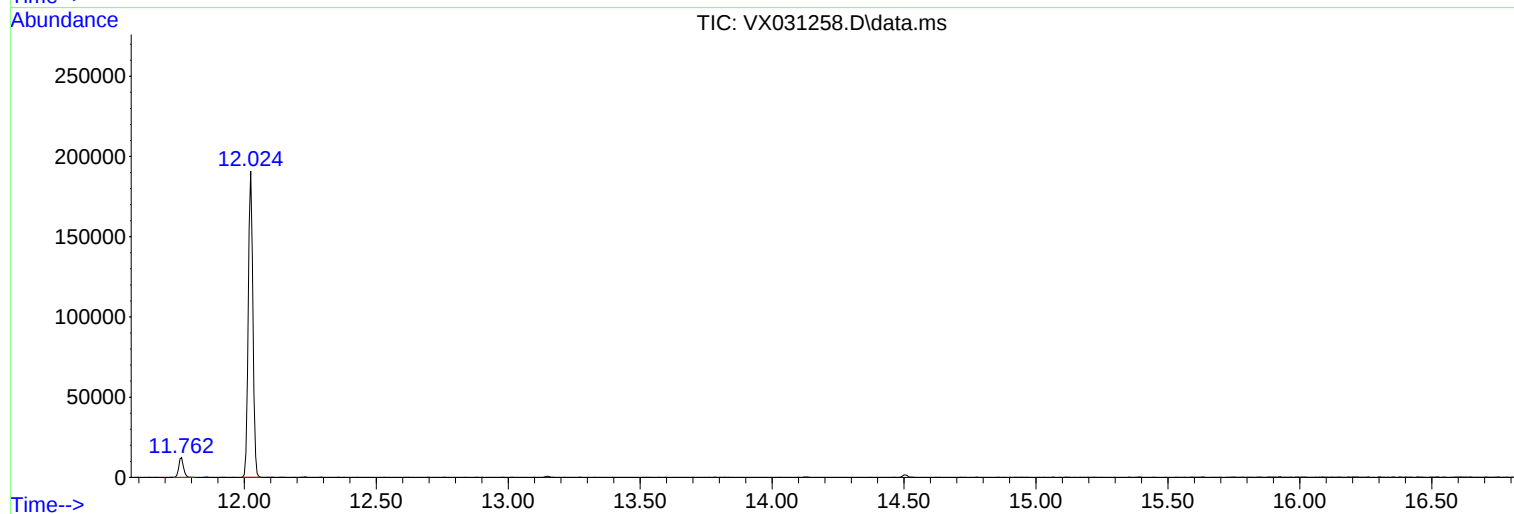
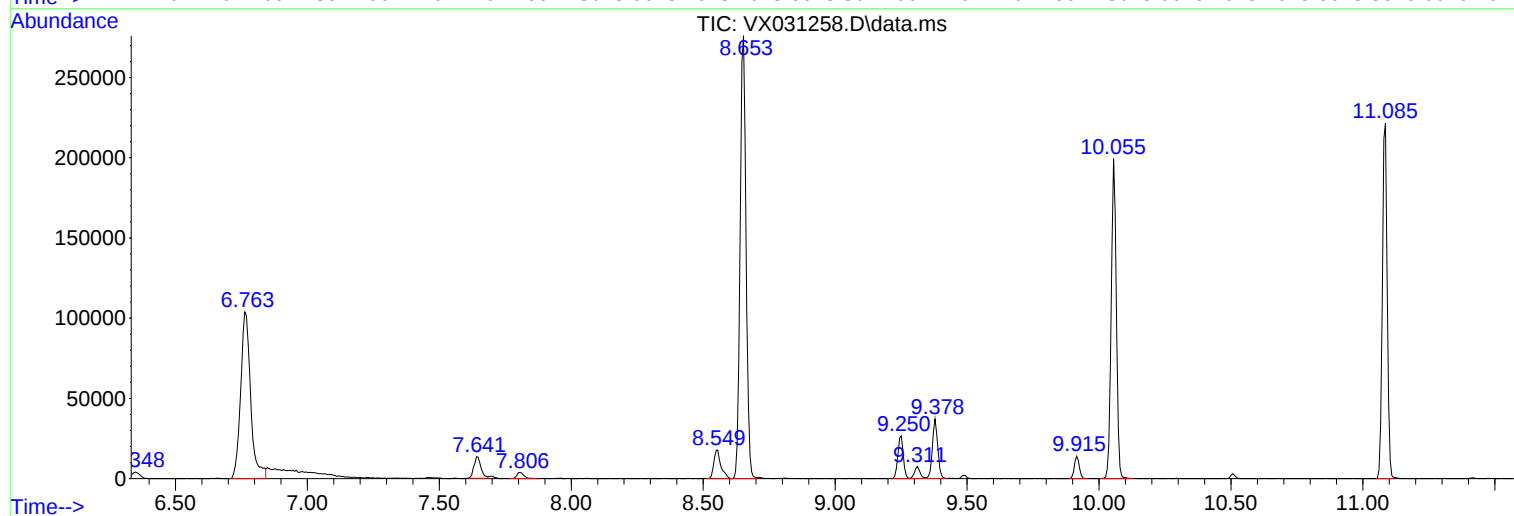
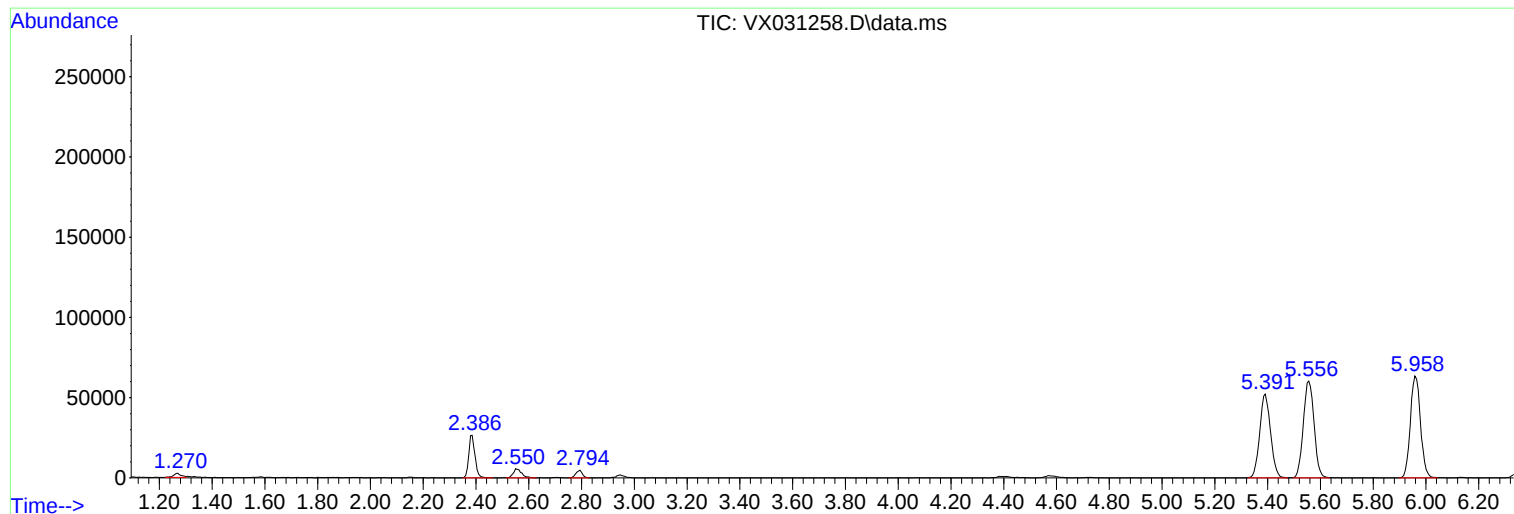
Sum of corrected areas: 2255189

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090722W.M
Quant Title : SW846 8260

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



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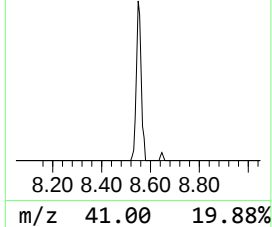
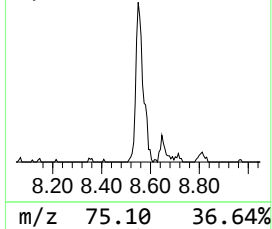
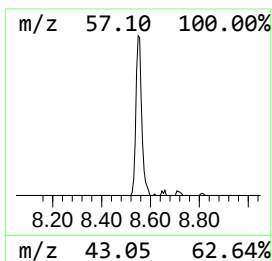
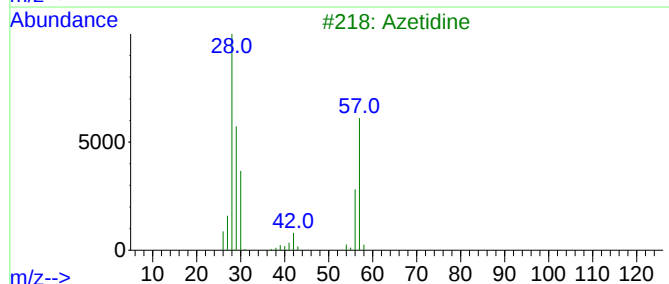
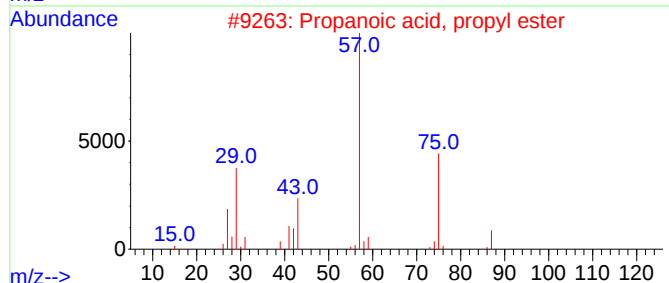
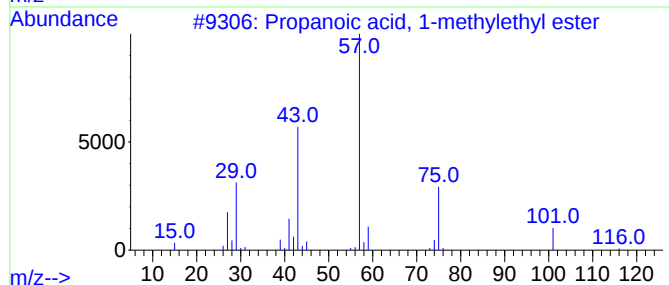
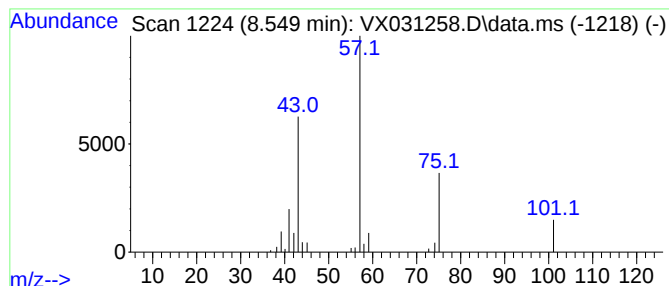
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Peak Number 1 Propanoic acid, 1-methyleth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.549	6.09 ug/l	32863	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
2			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50
3			Azetidine	57	C3H7N	000503-29-7	10
4			Diacetamide	101	C4H7NO2	000625-77-4	9
5			o-Isopropylhydroxylamine	75	C3H9NO	1000322-42-6	9



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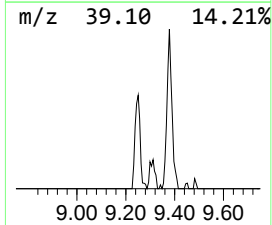
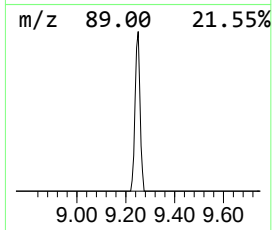
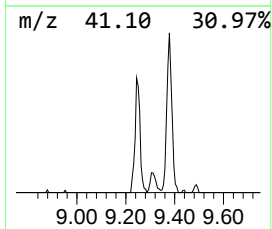
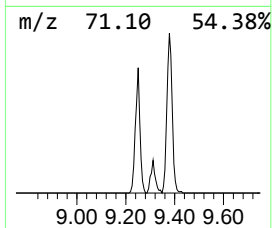
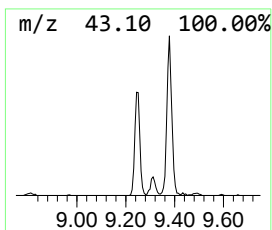
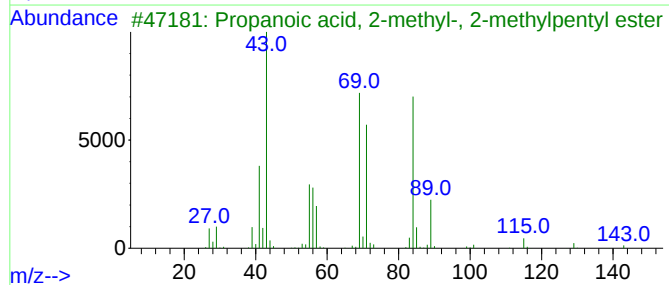
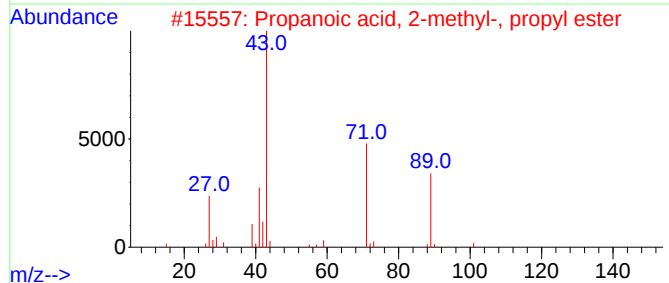
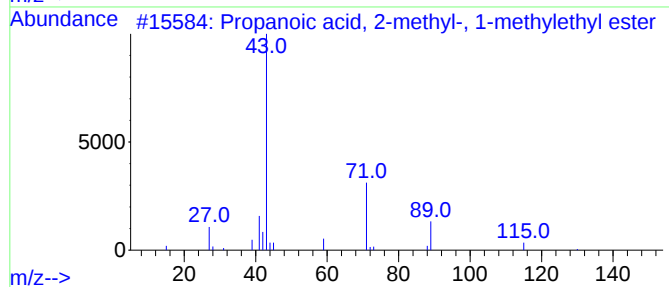
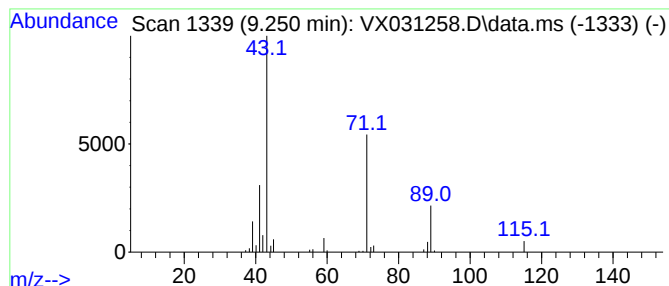
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Peak Number 2 Propanoic acid, 2-methyl-, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.250	7.05 ug/l	38044	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	74
2			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
3			Propanoic acid, 2-methyl-, 2-met...	172	C10H20O2	084254-82-0	39
4			Isopropyl butyrate	130	C7H14O2	000638-11-9	39
5			Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	33



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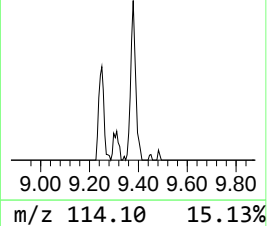
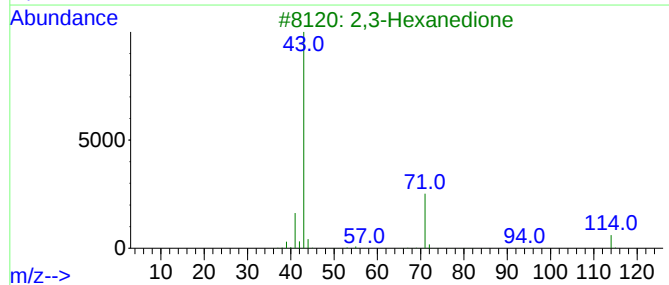
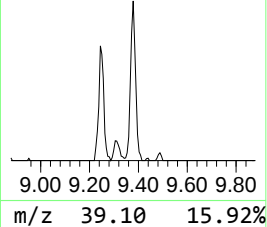
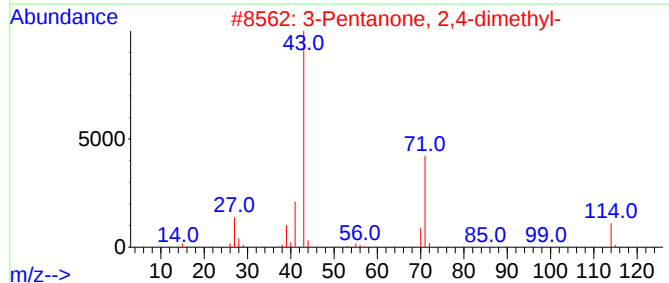
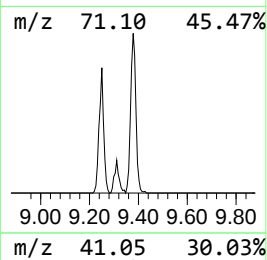
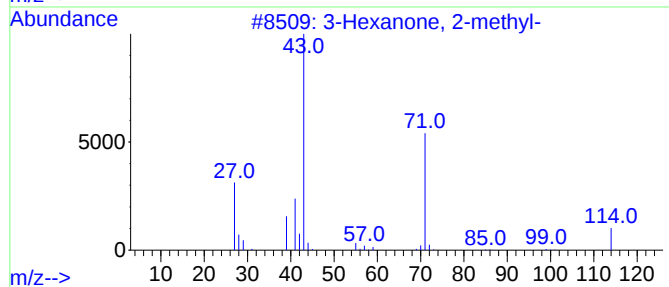
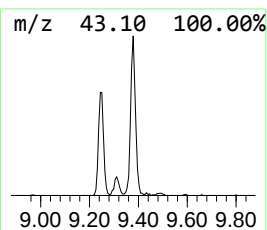
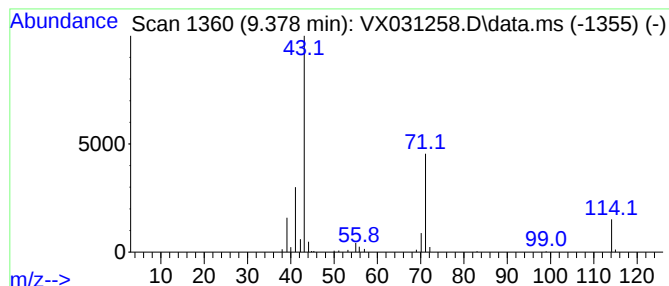
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Peak Number 3 3-Hexanone, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.378	9.60 ug/l	51792	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	90
2			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	86
3			2,3-Hexanedione	114	C6H10O2	003848-24-6	56
4			4-Heptanone	114	C7H14O	000123-19-3	45
5			2-Oxo-n-valeric acid	116	C5H8O3	001821-02-9	42



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	8.549	6.1	ug/l	32863	3	10.055	269853	50.0
Propanoic acid,...	9.250	7.0	ug/l	38044	3	10.055	269853	50.0
3-Hexanone, 2-m...	9.378	9.6	ug/l	51792	3	10.055	269853	50.0