

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX081020\
 Data File : VX017851.D
 Acq On : 10 Aug 2020 15:39
 Operator : JC/SP
 Sample : L3675-08
 Misc : 25.0mL/MSVOA X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 GAYA4

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR080720WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.160	9	12	20	rVB2	73834	81260	5.78%	0.766%
2	1.282	28	32	35	rBV3	30074	31622	2.25%	0.298%
3	1.386	44	49	55	rBV	176786	182972	13.00%	1.724%
4	1.471	61	63	67	rBV	19506	19968	1.42%	0.188%
5	1.581	77	81	86	rBV8	12276	21324	1.52%	0.201%
6	1.691	95	99	107	rVB	117132	147905	10.51%	1.393%
7	1.770	109	112	117	rBV5	14031	19401	1.38%	0.183%
8	1.983	144	147	152	rVB5	10858	14577	1.04%	0.137%
9	2.343	200	206	214	rBV	210443	353962	25.16%	3.335%
10	2.422	214	219	224	rVB	32317	65286	4.64%	0.615%
11	2.587	242	246	254	rVB	33765	56389	4.01%	0.531%
12	2.831	281	286	291	rBV3	15794	28397	2.02%	0.268%
13	4.538	557	566	577	rBV	203621	560236	39.82%	5.278%
14	4.666	577	587	599	rVV2	83723	296300	21.06%	2.792%
15	4.800	601	609	622	rVB2	52885	160502	11.41%	1.512%
16	5.141	653	665	677	rBV	154553	472904	33.61%	4.455%
17	5.471	711	719	724	rBV	5848	17119	1.22%	0.161%
18	5.629	739	745	748	rBV8	6831	15382	1.09%	0.145%
19	6.044	800	813	834	rBV3	375524	1148368	81.62%	10.819%
20	6.830	931	942	954	rBV	290694	678725	48.24%	6.394%
21	7.178	990	999	1003	rBV10	13452	35334	2.51%	0.333%
22	7.373	1022	1031	1039	rBV	253293	550045	39.09%	5.182%
23	8.373	1187	1195	1202	rBV	144084	242450	17.23%	2.284%
24	8.696	1242	1248	1255	rBV	504872	785328	55.81%	7.399%
25	8.763	1255	1259	1267	rVB	30996	54868	3.90%	0.517%
26	8.994	1291	1297	1302	rBV	97144	143721	10.21%	1.354%
27	9.427	1361	1368	1376	rBV	1021628	1407039	100.00%	13.256%
28	9.567	1387	1391	1396	rBV8	9743	15204	1.08%	0.143%
29	10.098	1471	1478	1488	rBV	604611	828772	58.90%	7.808%
30	11.232	1657	1664	1673	rVB	304759	397812	28.27%	3.748%
31	12.061	1794	1800	1807	rBV	619466	772993	54.94%	7.283%
32	12.256	1829	1832	1841	rBV	22143	39229	2.79%	0.370%
33	12.360	1844	1849	1859	rVB	711401	898284	63.84%	8.463%
34	14.676	2226	2229	2235	rBV5	12528	17701	1.26%	0.167%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 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\SOMXTR080720WMA.M
Title : TRACE VOA SOM01.0

35	15.176	2306	2311	2317	rBV6	13699	24142	1.72%	0.227%
36	15.268	2322	2326	2333	rVB4	17783	28740	2.04%	0.271%

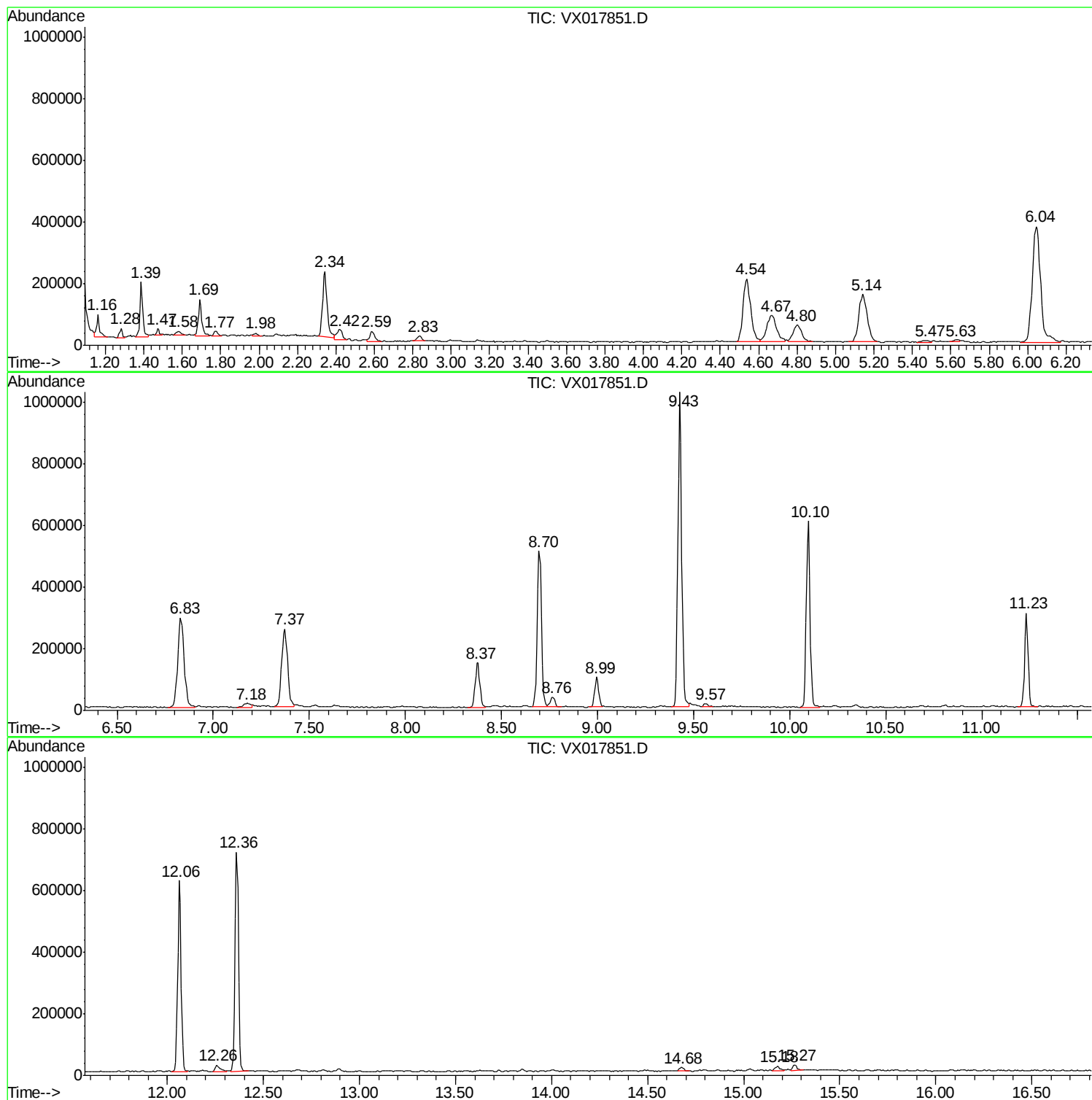
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR080720WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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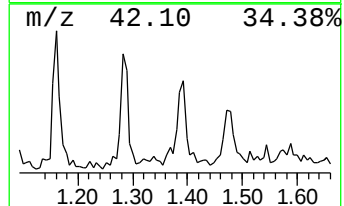
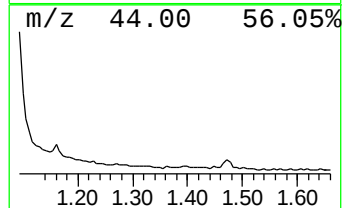
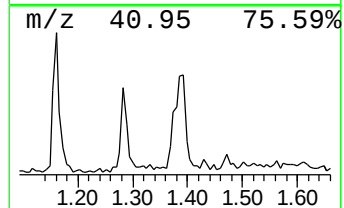
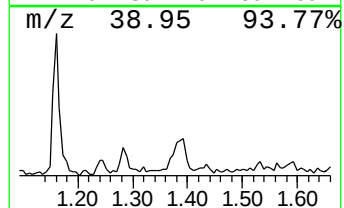
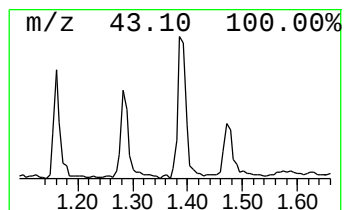
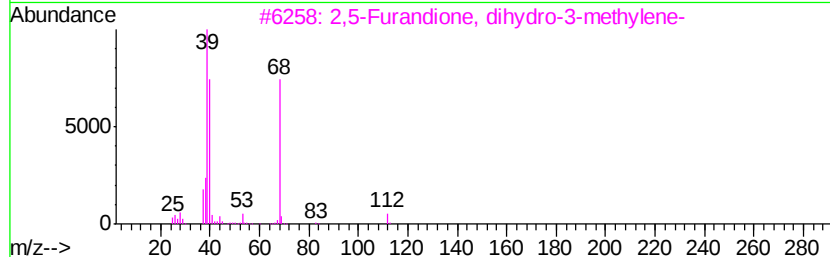
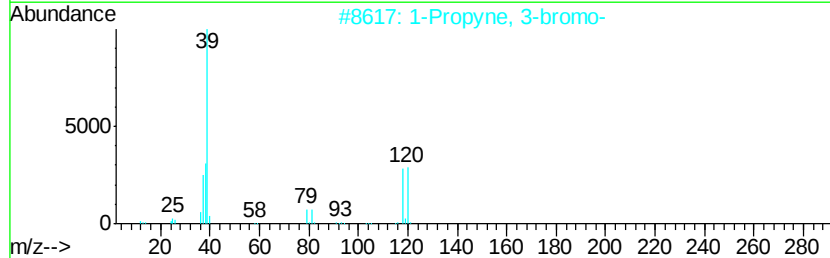
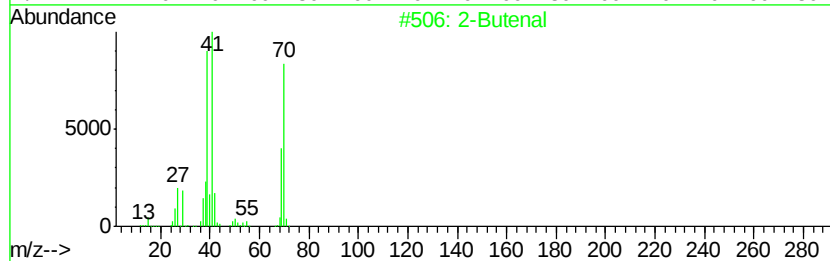
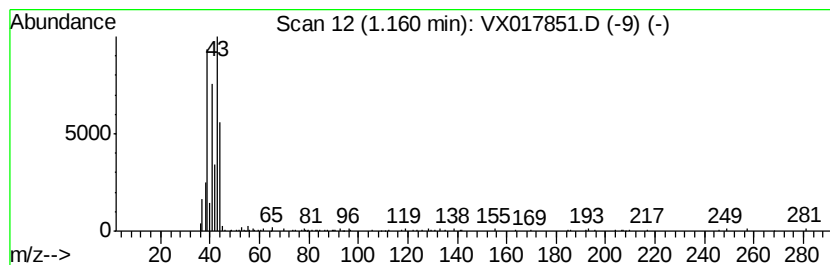
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TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Butenal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.16	0.60 ug/L	81260	1,4-Difluorobenzene	6.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butenal	70	C4H6O	004170-30-3	56
2			1-Propyne, 3-bromo-	118	C3H3Br	000106-96-7	50
3			2,5-Furandione, dihydro-3-methyl...	112	C5H4O3	002170-03-8	50
4			Acetoacetic acid, 1-thio-, S-all...	158	C7H10O2S	015780-65-1	40
5			2,5-Furandione, 3-methyl-	112	C5H4O3	000616-02-4	39



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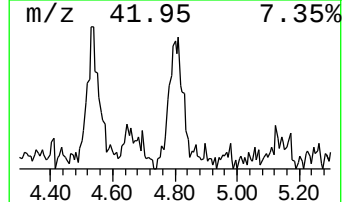
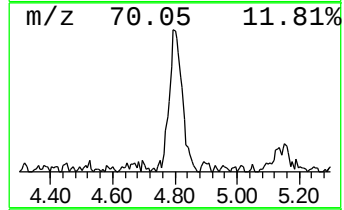
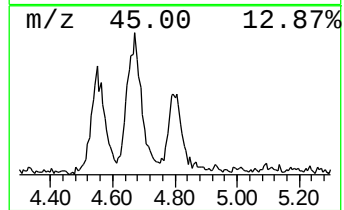
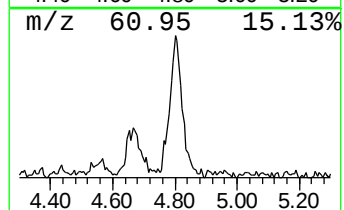
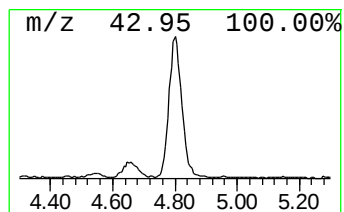
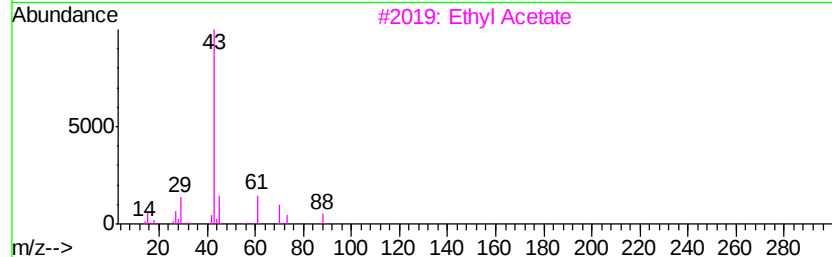
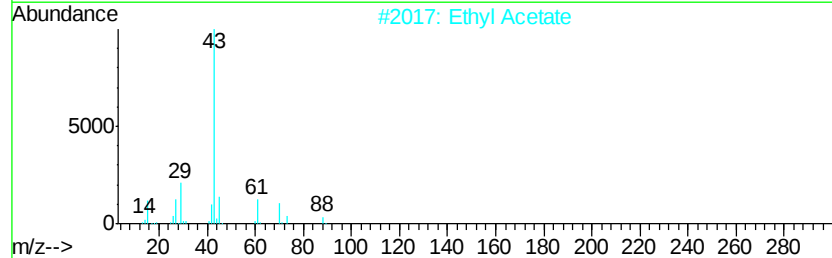
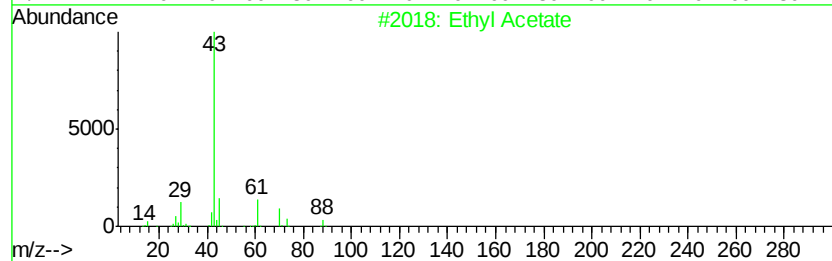
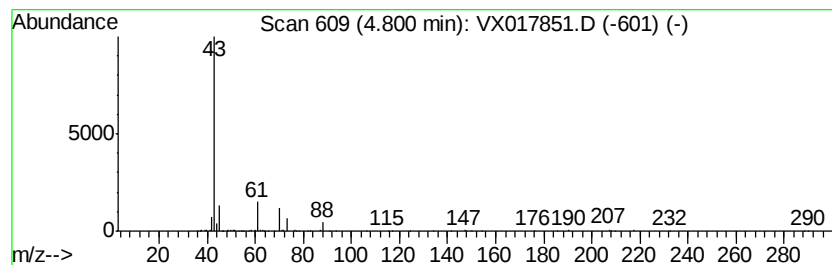
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethyl Acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	1.18 ug/L	160502	1,4-Difluorobenzene	6.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl Acetate	88	C4H8O2	000141-78-6	86
2			Ethyl Acetate	88	C4H8O2	000141-78-6	86
3			Ethyl Acetate	88	C4H8O2	000141-78-6	86
4			Ethyl Acetate	88	C4H8O2	000141-78-6	78
5			CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	33



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Butenal	1.16	0.6	ug/L	81260	1	6.83	678725	5.0
Ethyl Acetate	4.80	1.2	ug/L	160502	1	6.83	678725	5.0