

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU080820\
 Data File : VU039803.D
 Acq On : 08 Aug 2020 11:44
 Operator : SY/MD
 Sample : L3590-03
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F4L17

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_U\METHOD\SOMUTR080320WMA.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	1.363	3	7	20	rVB2	2246	3587	1.12%	0.142%
2	1.485	39	45	50	rBV	5566	6161	1.92%	0.243%
3	1.601	70	81	94	rVB3	31193	52025	16.21%	2.053%
4	1.919	172	180	193	rVB	24214	31397	9.78%	1.239%
5	2.208	260	270	279	rBV7	2952	5144	1.60%	0.203%
6	2.388	318	326	343	rBV6	5673	13089	4.08%	0.517%
7	2.575	373	384	400	rBV	47714	78078	24.33%	3.081%
8	3.362	617	629	642	rVB6	7519	15826	4.93%	0.625%
9	4.719	1027	1051	1073	rBV2	37002	139320	43.41%	5.498%
10	5.083	1149	1164	1180	rBV2	48846	114160	35.57%	4.505%
11	5.735	1350	1367	1380	rBV5	93598	225316	70.21%	8.891%
12	6.263	1518	1531	1546	rVB2	88061	162147	50.53%	6.399%
13	6.546	1606	1619	1636	rBV10	8410	17213	5.36%	0.679%
14	6.706	1655	1669	1687	rBV2	61899	116496	36.30%	4.597%
15	6.813	1690	1702	1716	rBV3	3755	8127	2.53%	0.321%
16	6.899	1719	1729	1742	rVV3	12244	23686	7.38%	0.935%
17	7.575	1925	1939	1953	rBV2	27506	47455	14.79%	1.873%
18	7.812	2003	2013	2029	rBV3	15509	29527	9.20%	1.165%
19	7.902	2029	2041	2053	rVV	87019	150410	46.87%	5.935%
20	7.973	2057	2063	2075	rVB	8771	13988	4.36%	0.552%
21	8.185	2120	2129	2140	rBV2	17857	27875	8.69%	1.100%
22	8.269	2146	2155	2165	rBV6	2123	3440	1.07%	0.136%
23	8.555	2236	2244	2252	rVB4	2945	4549	1.42%	0.180%
24	8.648	2261	2273	2305	rBV	171734	320921	100.00%	12.664%
25	8.793	2309	2318	2336	rBV3	18339	30019	9.35%	1.185%
26	9.420	2500	2513	2530	rBV	127561	205546	64.05%	8.111%
27	9.568	2553	2559	2569	rBV3	2264	3309	1.03%	0.131%
28	9.690	2588	2597	2609	rVB2	7319	11511	3.59%	0.454%
29	10.102	2716	2725	2732	rBV6	2371	3333	1.04%	0.132%
30	10.240	2760	2768	2779	rVB4	4833	7200	2.24%	0.284%
31	10.343	2790	2800	2815	rVB5	13625	22938	7.15%	0.905%
32	10.754	2918	2928	2941	rBV	55292	87358	27.22%	3.447%
33	11.253	3071	3083	3091	rBV3	6953	10503	3.27%	0.414%
34	11.465	3140	3149	3159	rBV2	18074	26925	8.39%	1.063%

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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

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Title : TRACE VOA SOM01.0

35	11.574	3169	3183	3197	rBV4	16195	32420	10.10%	1.279%
36	11.648	3197	3206	3213	rBV5	4353	6738	2.10%	0.266%
37	11.806	3244	3255	3269	rVB	137483	214016	66.69%	8.445%
38	12.053	3324	3332	3343	rBV7	3728	7079	2.21%	0.279%
39	12.185	3362	3373	3388	rVB	113522	182051	56.73%	7.184%
40	12.668	3514	3523	3528	rBV6	1939	3421	1.07%	0.135%
41	12.767	3543	3554	3560	rBV2	22518	34824	10.85%	1.374%
42	12.806	3560	3566	3578	rVB4	9997	16075	5.01%	0.634%
43	13.857	3884	3893	3906	rVB4	8902	14745	4.59%	0.582%
44	14.867	4199	4207	4219	rBV5	2777	4152	1.29%	0.164%

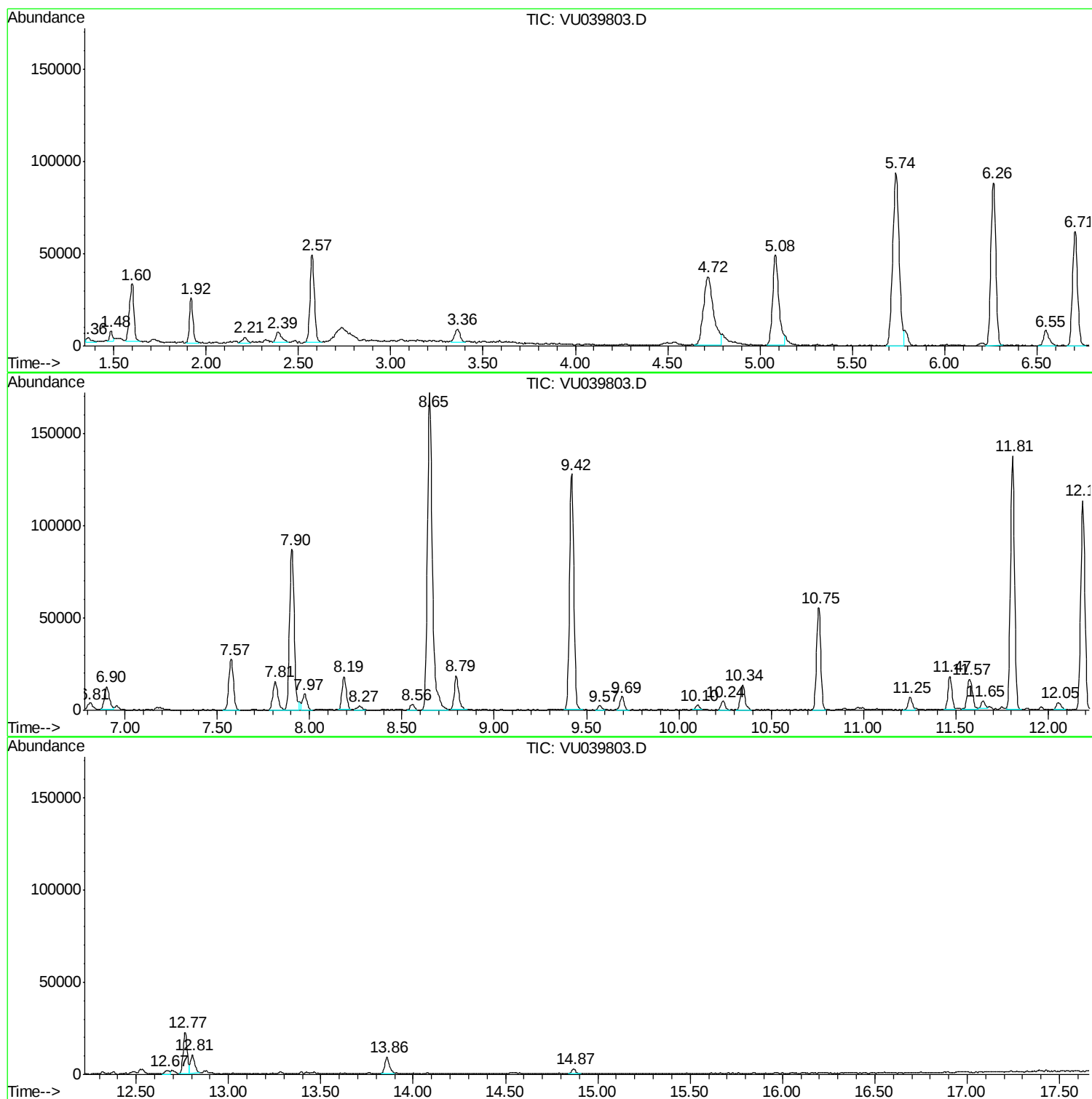
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ClientSampled :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR080320WMA.M
Quant Title : TRACE VOA SOM01.0

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



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Instrument :
MSVOA_U
ClientSampleId :
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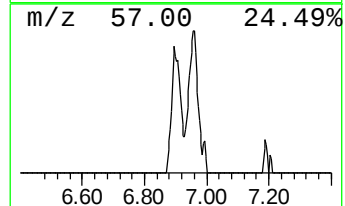
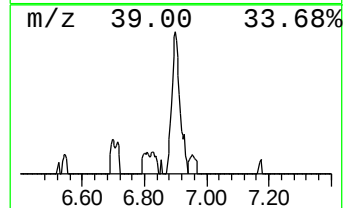
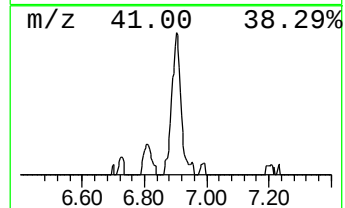
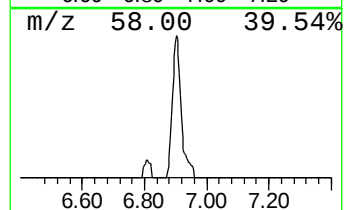
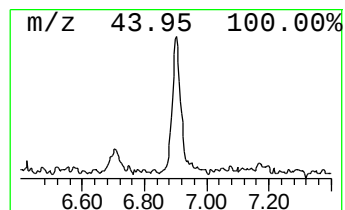
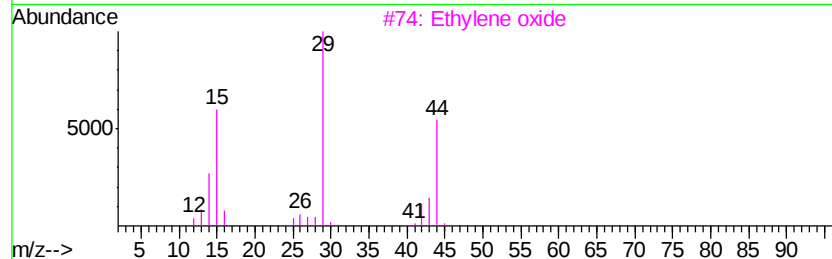
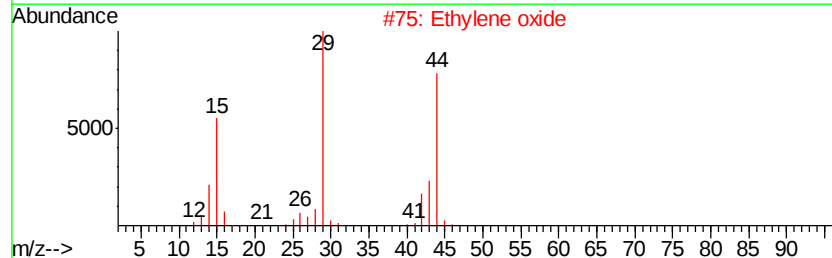
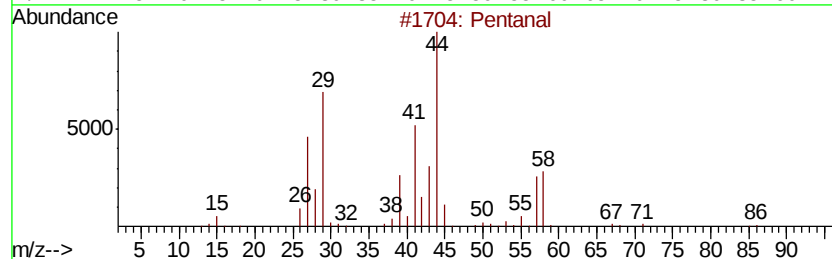
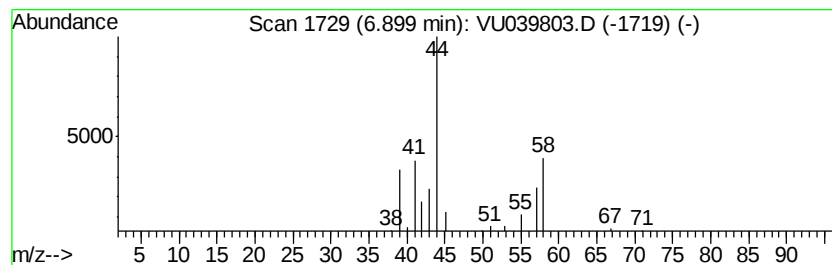
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Pentanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.90	0.73 ug/L	23686	1,4-Difluorobenzene	6.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentanal	86	C5H10O	000110-62-3	78
2		Ethylene oxide	44	C2H4O	000075-21-8	5
3		Ethylene oxide	44	C2H4O	000075-21-8	5
4		Propane	44	C3H8	000074-98-6	4
5		Propane	44	C3H8	000074-98-6	4



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Instrument :
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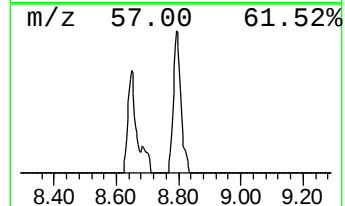
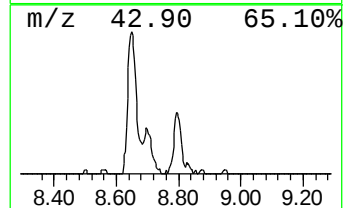
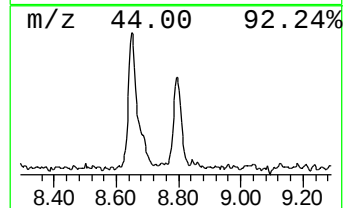
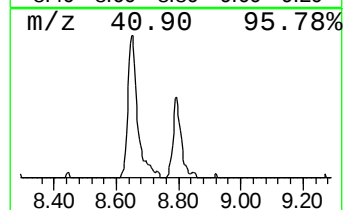
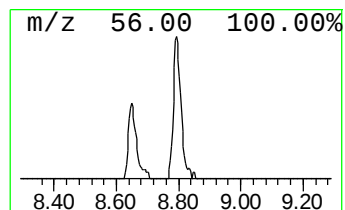
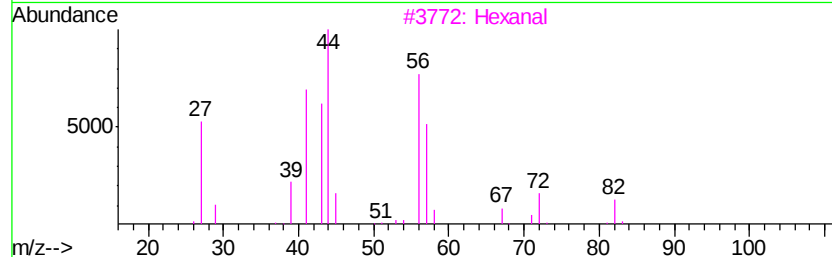
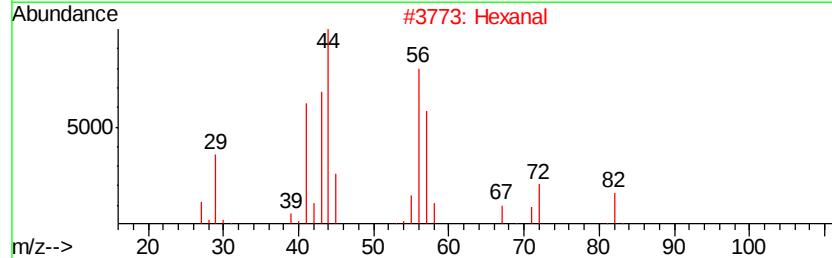
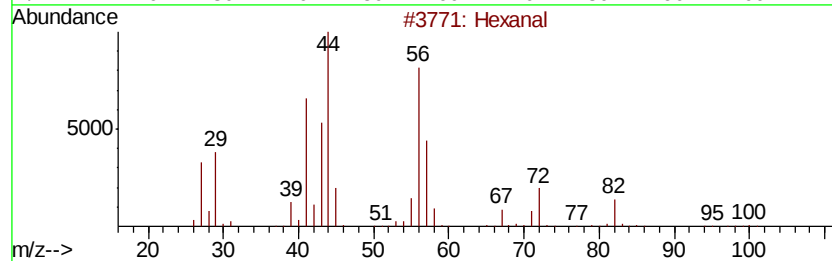
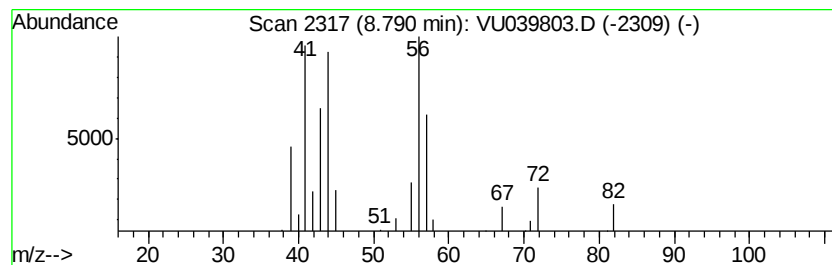
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR080320WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 Hexanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.79	0.73 ug/L	30019	Chlorobenzene-d5	9.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanal	100	C6H12O	000066-25-1	64
2		Hexanal	100	C6H12O	000066-25-1	59
3		Hexanal	100	C6H12O	000066-25-1	59
4		Hexanal	100	C6H12O	000066-25-1	45
5		2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9	37



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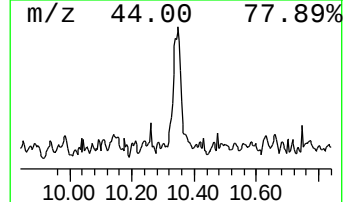
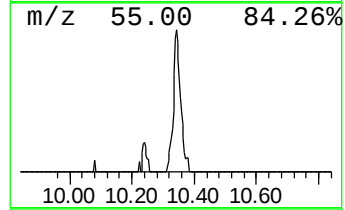
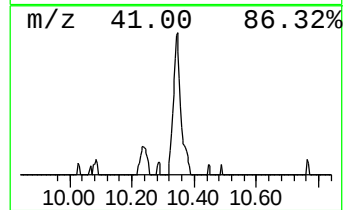
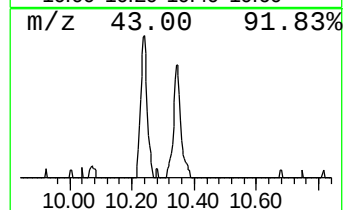
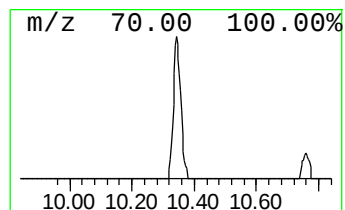
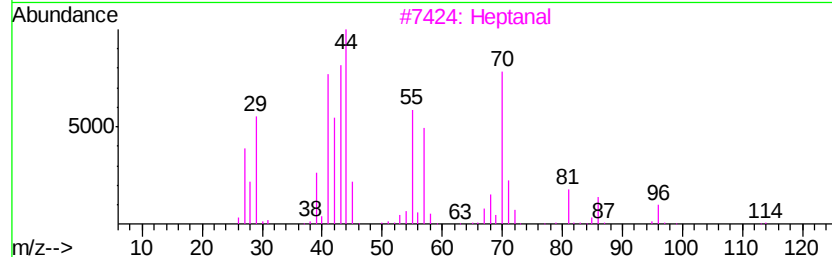
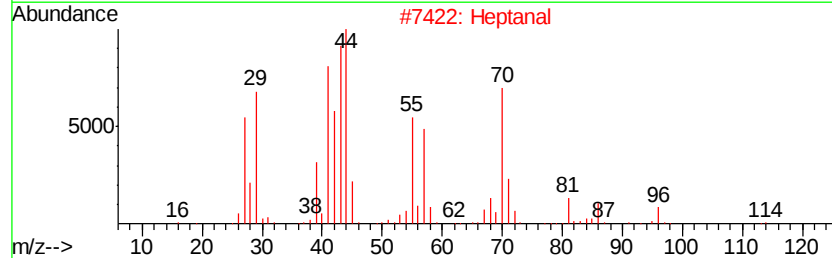
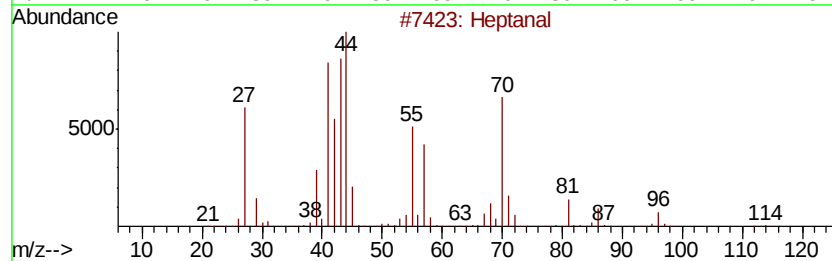
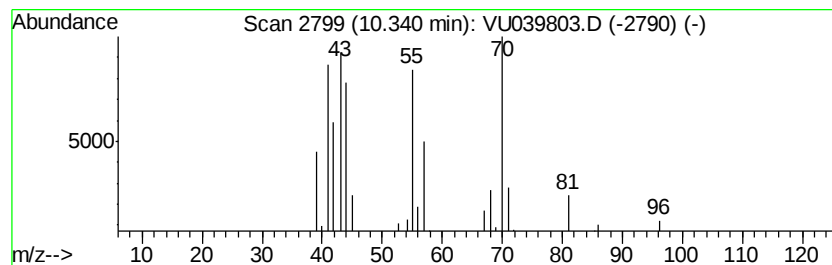
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR080320WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 Heptanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.34	0.56 ug/L	22938	Chlorobenzene-d5	9.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptanal	114	C7H14O	000111-71-7	53
2		Heptanal	114	C7H14O	000111-71-7	53
3		Heptanal	114	C7H14O	000111-71-7	50
4		Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	43
5		2-Pentene	70	C5H10	000109-68-2	43



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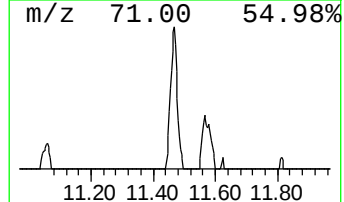
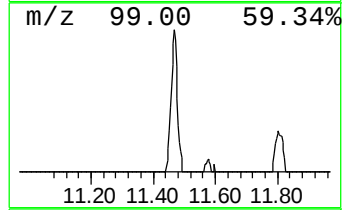
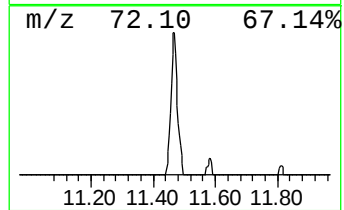
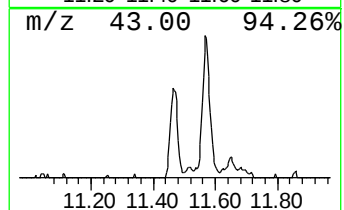
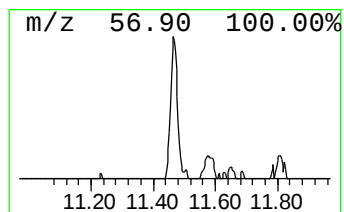
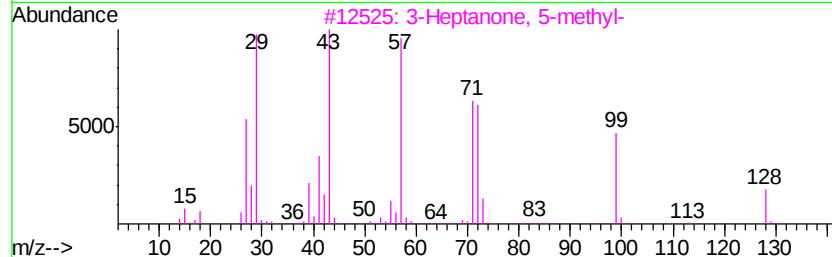
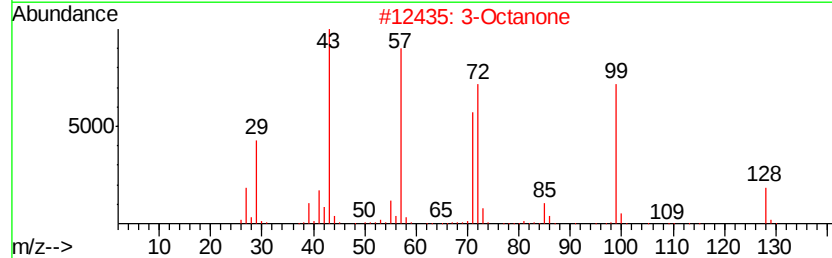
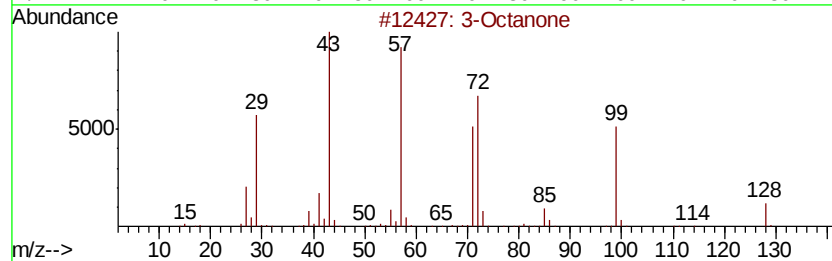
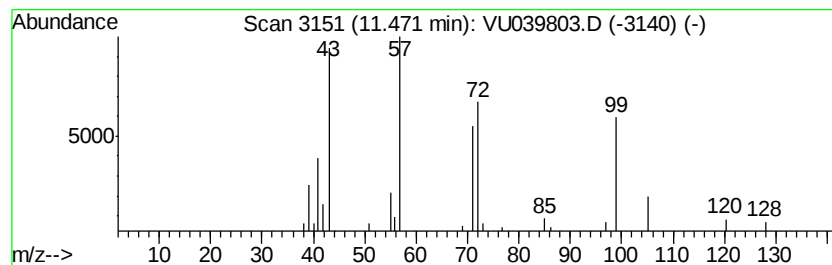
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 3-Octanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.47	0.63 ug/L	26925	1,4-Dichlorobenzene-d4	11.81

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octanone		128	C8H16O	000106-68-3	81
2	3-Octanone		128	C8H16O	000106-68-3	64
3	3-Heptanone, 5-methyl-		128	C8H16O	000541-85-5	59
4	3-Heptanone, 5-methyl-		128	C8H16O	000541-85-5	53
5	3-Octanone		128	C8H16O	000106-68-3	50



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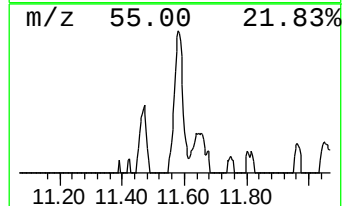
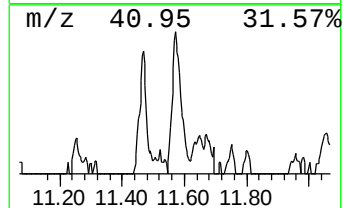
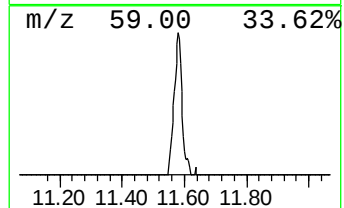
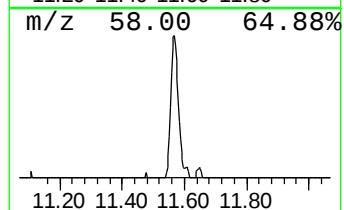
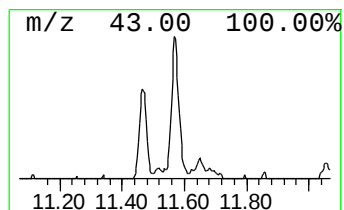
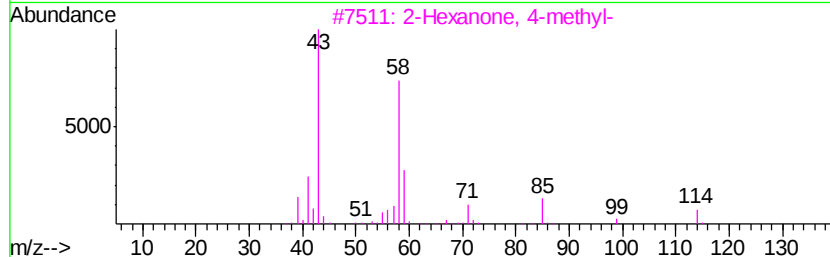
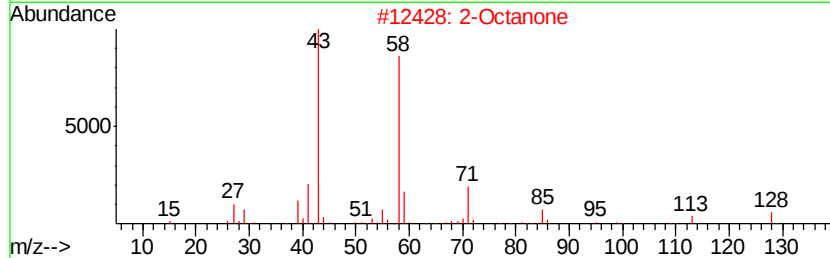
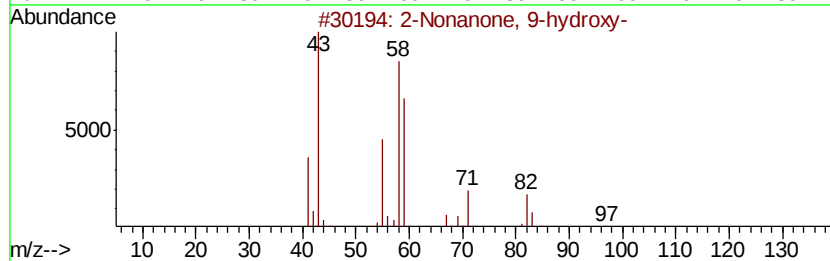
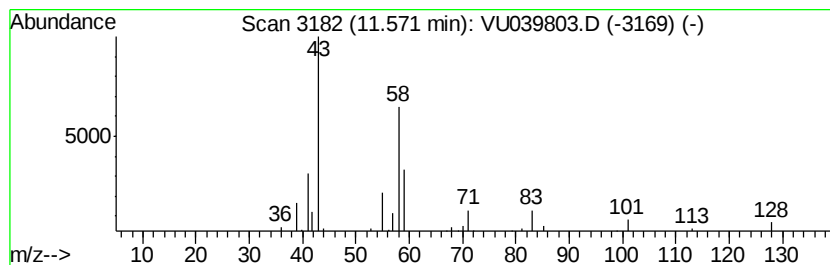
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 2-Nonanone, 9-hydroxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.57	0.76 ug/L	32420	1,4-Dichlorobenzene-d4	11.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	50
2			2-Octanone	128	C8H16O	000111-13-7	46
3			2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	43
4			Methylamine, N,N-dimethyl-	59	C3H9N	000075-50-3	37
5			2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	35



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU080820\
Data File : VU039803.D
Acq On : 08 Aug 2020 11:44
Operator : SY/MD
Sample : L3590-03
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F4L17

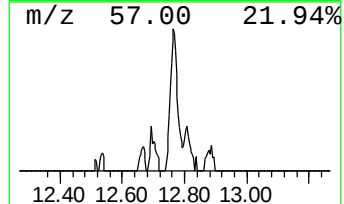
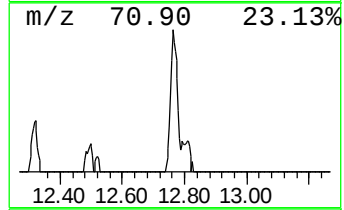
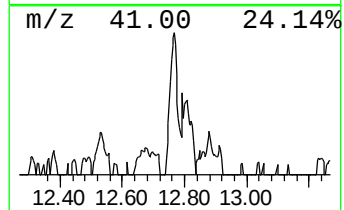
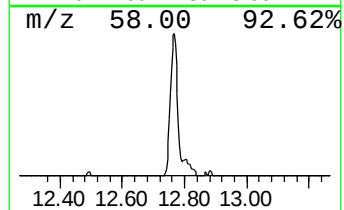
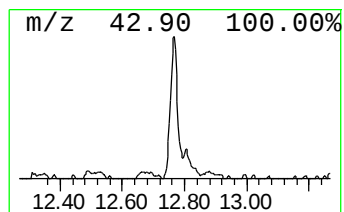
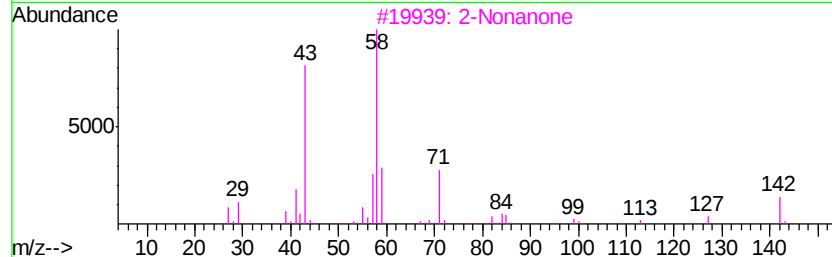
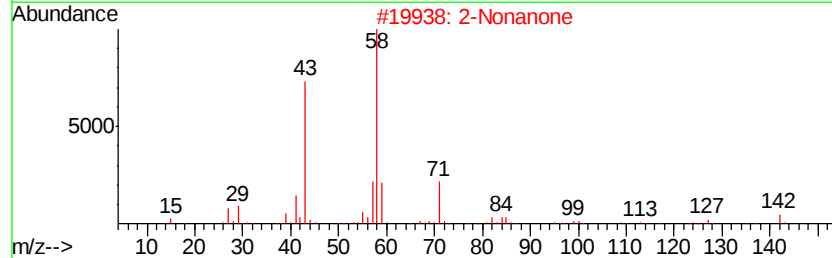
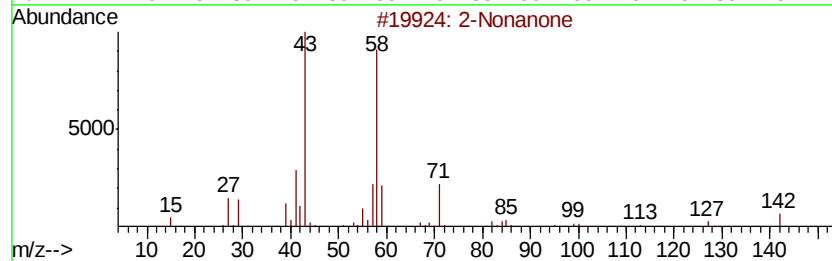
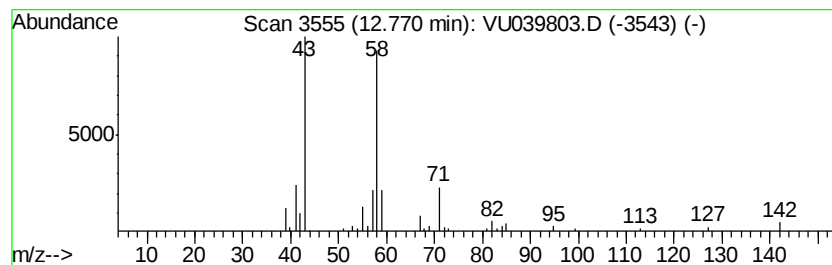
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 2-Nonanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	0.81 ug/L	34824	1,4-Dichlorobenzene-d4	11.81

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonanone		142	C9H18O	000821-55-6	91
2	2-Nonanone		142	C9H18O	000821-55-6	87
3	2-Nonanone		142	C9H18O	000821-55-6	78
4	2-Heptanone		114	C7H14O	000110-43-0	72
5	2-Dodecanone		184	C12H24O	006175-49-1	64



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU080820\
Data File : VU039803.D
Acq On : 08 Aug 2020 11:44
Operator : SY/MD
Sample : L3590-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F4L17

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR080320WMA.M
Quant Title : TRACE VOA SOM01.0

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

TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
Pentanal	6.90	0.7	ug/L	23686	1	6.27	162147	5.0
Hexanal	8.79	0.7	ug/L	30019	2	9.42	205546	5.0
Heptanal	10.34	0.6	ug/L	22938	2	9.42	205546	5.0
3-Octanone	11.47	0.6	ug/L	26925	3	11.81	214016	5.0
2-Nonanone, 9-hyd...	11.57	0.8	ug/L	32420	3	11.81	214016	5.0
2-Nonanone	12.77	0.8	ug/L	34824	3	11.81	214016	5.0