

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU081720\
 Data File : VU039892.D
 Acq On : 17 Aug 2020 17:27
 Operator : SY/MD
 Sample : L3517-07 10X
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F4M01

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	1.604	74	82	89	rVB	28057	30695	9.43%	0.978%
2	1.919	171	180	191	rBV	28658	37179	11.42%	1.184%
3	2.578	372	385	397	rBV	47297	74181	22.79%	2.363%
4	2.694	398	421	461	rBV2	41097	236431	72.65%	7.533%
5	3.060	527	535	546	rVB4	4688	8351	2.57%	0.266%
6	4.678	1016	1038	1052	rBV3	35578	133238	40.94%	4.245%
7	5.083	1149	1164	1180	rBV2	53143	115795	35.58%	3.689%
8	5.742	1349	1369	1397	rBV4	94407	253290	77.83%	8.070%
9	6.263	1516	1531	1544	rVV	104805	195630	60.11%	6.233%
10	6.546	1610	1619	1621	rBV6	2903	3912	1.20%	0.125%
11	6.703	1655	1668	1684	rBV2	64926	125808	38.66%	4.008%
12	6.790	1684	1695	1714	rVB3	10732	24539	7.54%	0.782%
13	6.938	1732	1741	1754	rBV2	3885	7520	2.31%	0.240%
14	7.575	1928	1939	1953	rVB2	32512	56042	17.22%	1.785%
15	7.803	1998	2010	2029	rBV2	37422	73634	22.63%	2.346%
16	7.906	2029	2042	2056	rVV	105141	182918	56.21%	5.828%
17	7.976	2057	2064	2074	rVB3	7190	10950	3.36%	0.349%
18	8.185	2120	2129	2140	rBV	22654	37078	11.39%	1.181%
19	8.555	2238	2244	2252	rVB6	3707	5054	1.55%	0.161%
20	8.642	2257	2271	2298	rBV	169269	325432	100.00%	10.368%
21	8.919	2347	2357	2369	rBV4	6210	10154	3.12%	0.323%
22	9.420	2501	2513	2526	rBV	157007	257214	79.04%	8.195%
23	9.571	2550	2560	2572	rVB3	13052	19698	6.05%	0.628%
24	9.693	2585	2598	2609	rBV2	41860	65521	20.13%	2.087%
25	10.099	2714	2724	2746	rBV3	12742	20761	6.38%	0.661%
26	10.237	2755	2767	2780	rBV	35539	56372	17.32%	1.796%
27	10.359	2798	2805	2817	rVB4	5845	9828	3.02%	0.313%
28	10.754	2916	2928	2941	rVB	56974	90363	27.77%	2.879%
29	11.465	3137	3149	3162	rBV2	31170	46346	14.24%	1.477%
30	11.571	3172	3182	3196	rBV3	23282	43385	13.33%	1.382%
31	11.645	3196	3205	3213	rVB2	8957	13427	4.13%	0.428%
32	11.806	3242	3255	3277	rVB	173032	267651	82.24%	8.527%
33	12.053	3324	3332	3340	rBV4	5147	8285	2.55%	0.264%
34	12.188	3362	3374	3386	rBV2	124822	204385	62.80%	6.512%

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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_U\METHOD\SOMUTR080320WMA.M
Title : TRACE VOA SOM01.0

35	12.764	3543	3553	3560	rBV	41468	60735	18.66%	1.935%
36	12.806	3560	3566	3575	rVB3	15250	23170	7.12%	0.738%
37	14.076	3951	3961	3973	rVB4	2680	3823	1.17%	0.122%

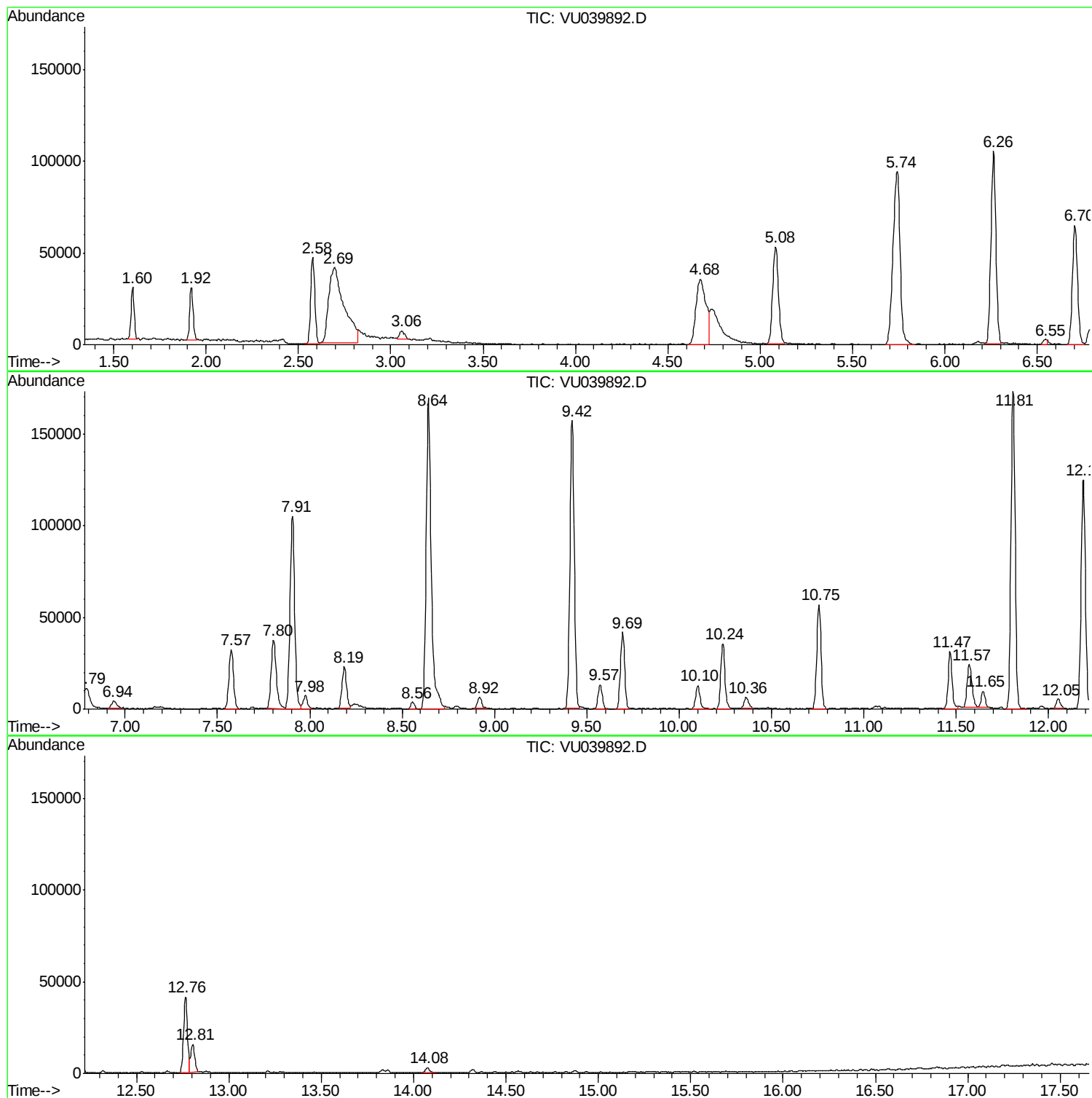
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR080320WMA.M
Quant Title : TRACE VOA SOM01.0

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



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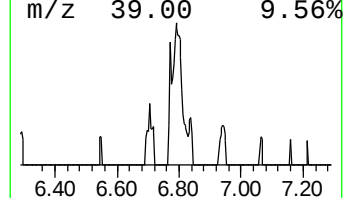
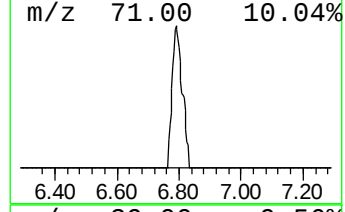
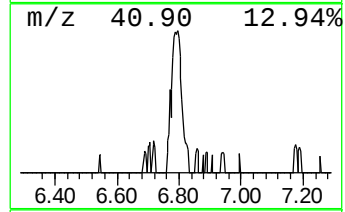
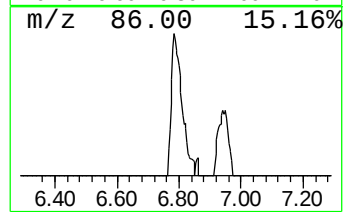
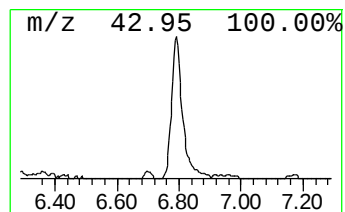
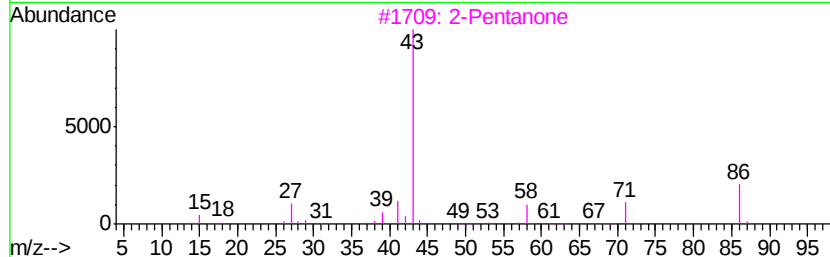
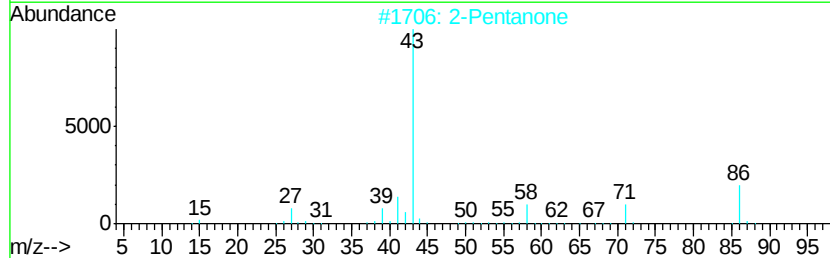
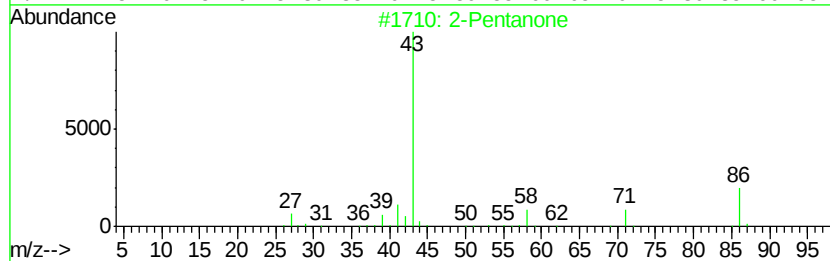
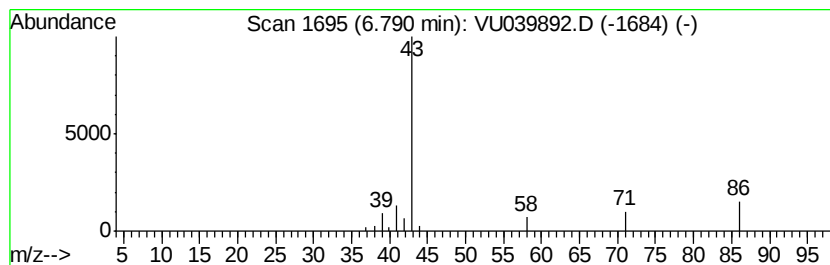
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 2-Pentanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.79	0.63 ug/L	24539	1,4-Difluorobenzene	6.26

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone	86	C5H10O	000107-87-9	90
2			2-Pentanone	86	C5H10O	000107-87-9	83
3			2-Pentanone	86	C5H10O	000107-87-9	78
4			2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	72
5			2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	72



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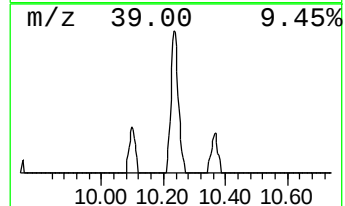
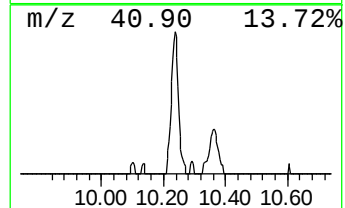
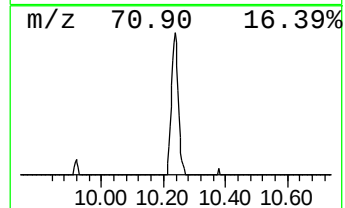
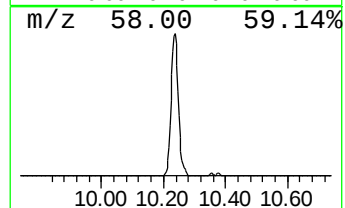
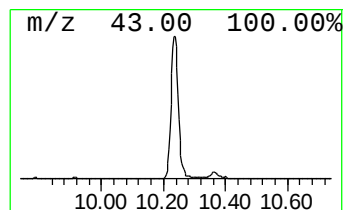
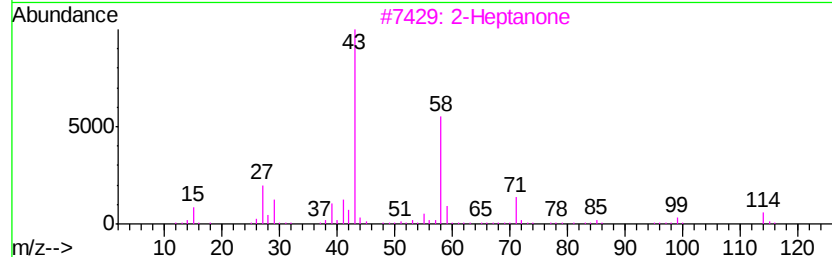
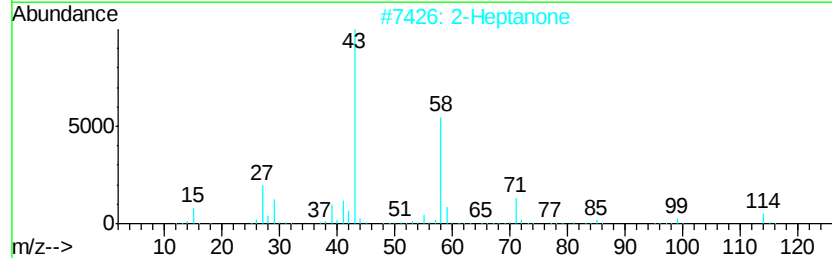
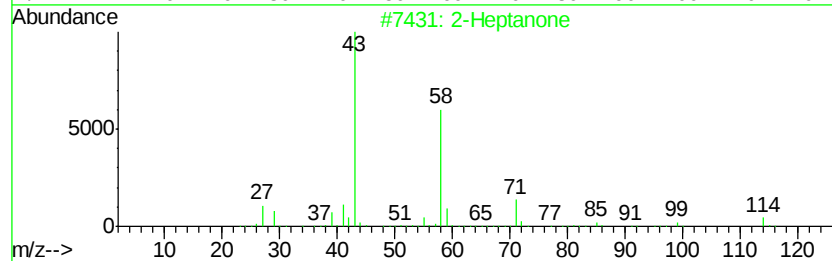
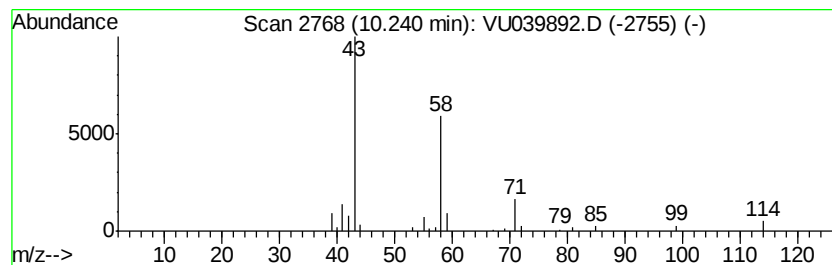
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR080320WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 2-Heptanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.24	1.10 ug/L	56372	Chlorobenzene-d5	9.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Heptanone	114	C7H14O	000110-43-0	91
2		2-Heptanone	114	C7H14O	000110-43-0	91
3		2-Heptanone	114	C7H14O	000110-43-0	90
4		2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	83
5		2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	72



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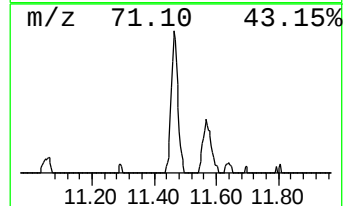
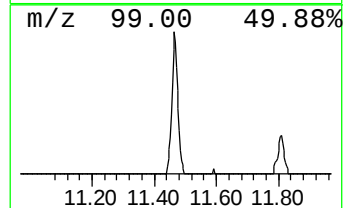
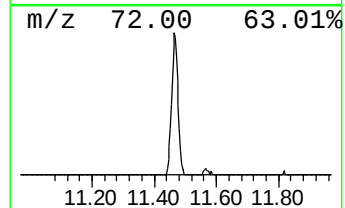
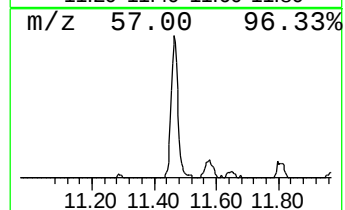
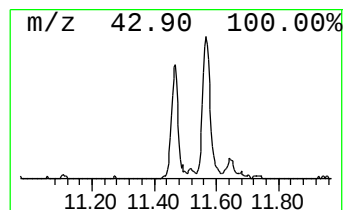
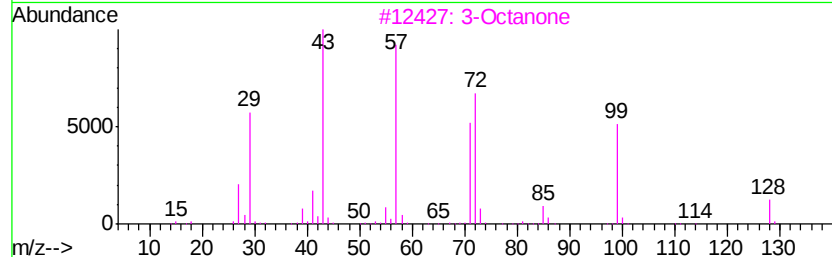
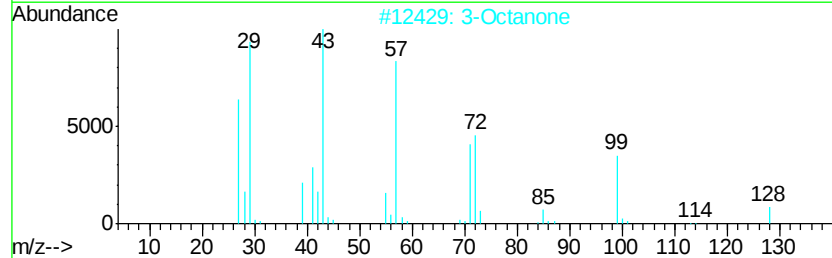
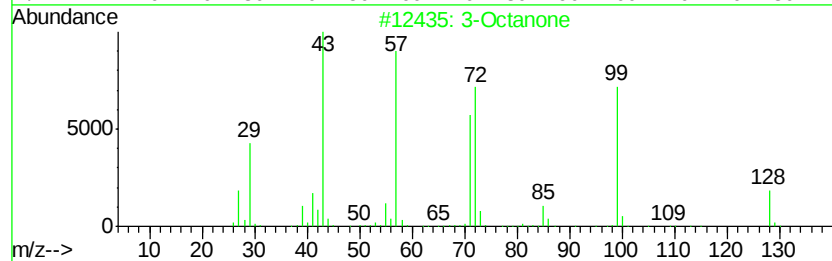
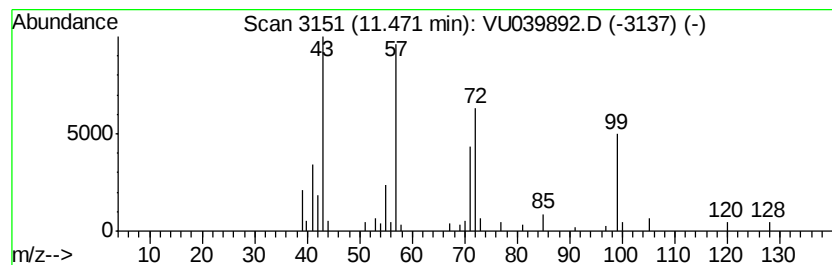
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 3-Octanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.47	0.87 ug/L	46346	1,4-Dichlorobenzene-d4	11.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Octanone	128	C8H16O	000106-68-3	91
2		3-Octanone	128	C8H16O	000106-68-3	64
3		3-Octanone	128	C8H16O	000106-68-3	59
4		3-Heptanone, 6-methyl-	128	C8H16O	000624-42-0	58
5		3-Octanone	128	C8H16O	000106-68-3	53



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Sample : L3517-07 10X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 19 Sample Multiplier: 1

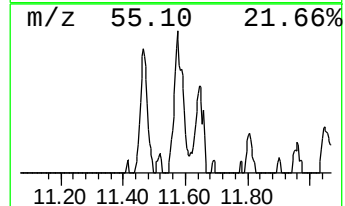
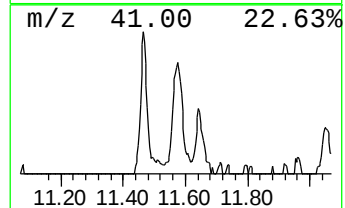
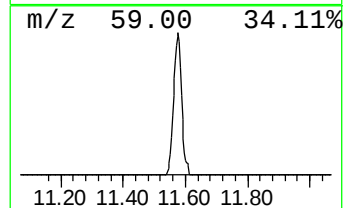
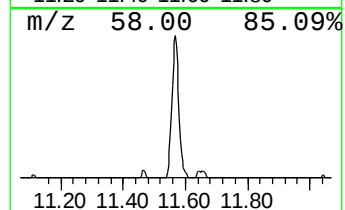
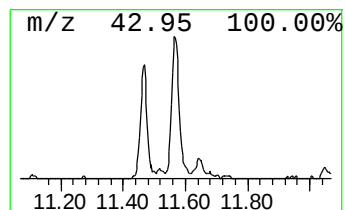
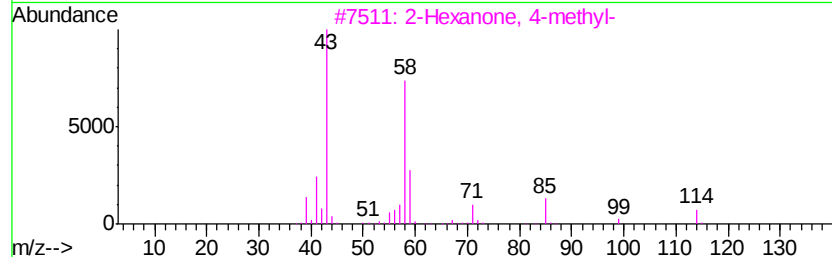
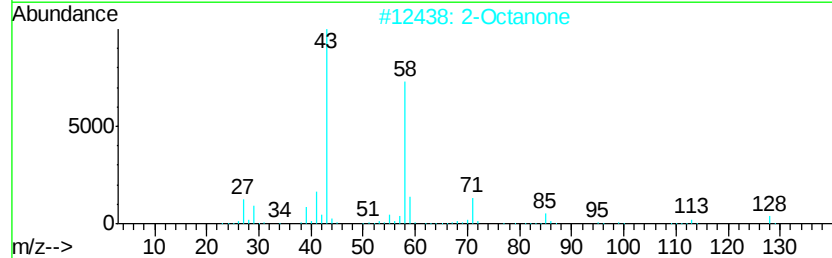
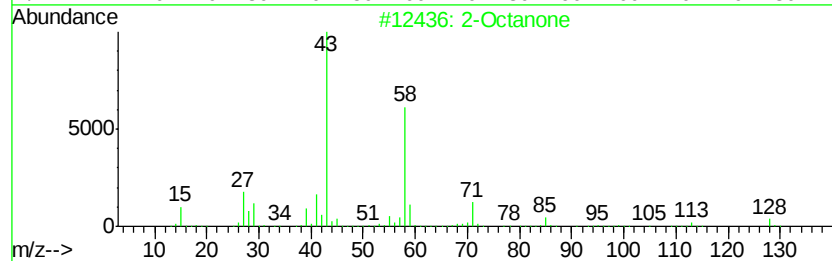
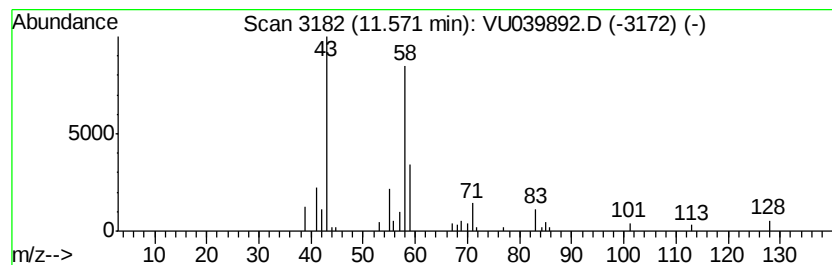
Instrument :
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 2-Hexanone, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.57	0.81 ug/L	43385	1,4-Dichlorobenzene-d4	11.81	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanone	128	C8H16O	000111-13-7	80
2	2-Octanone	128	C8H16O	000111-13-7	72
3	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	72
4	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	72
5	2-Octanone	128	C8H16O	000111-13-7	72



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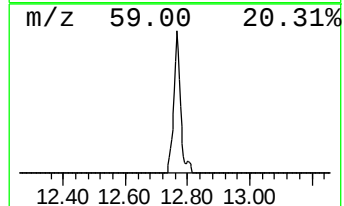
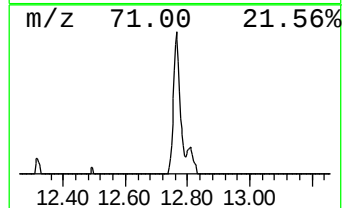
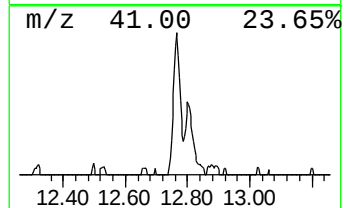
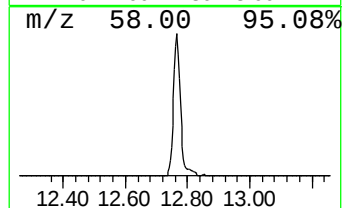
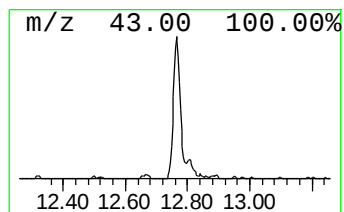
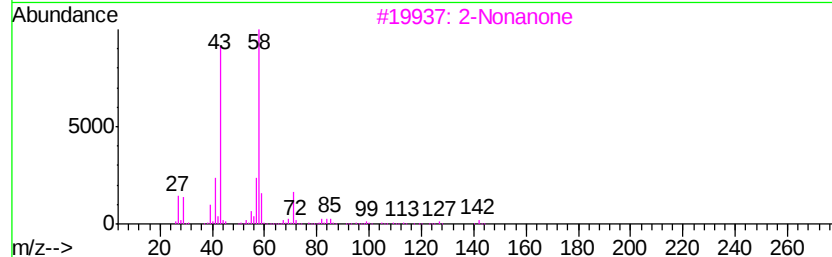
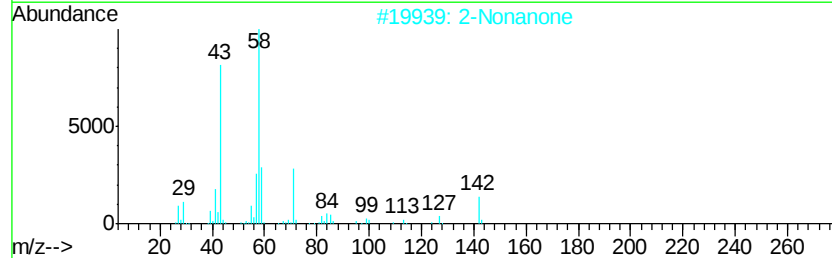
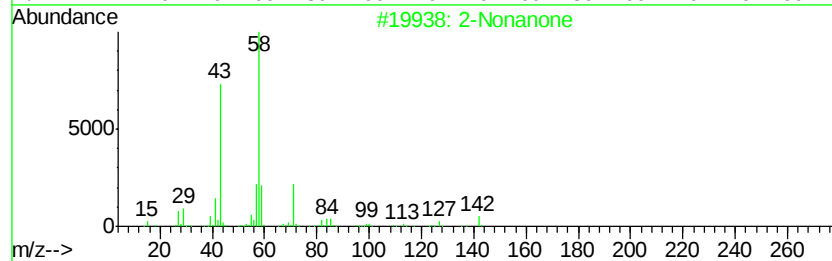
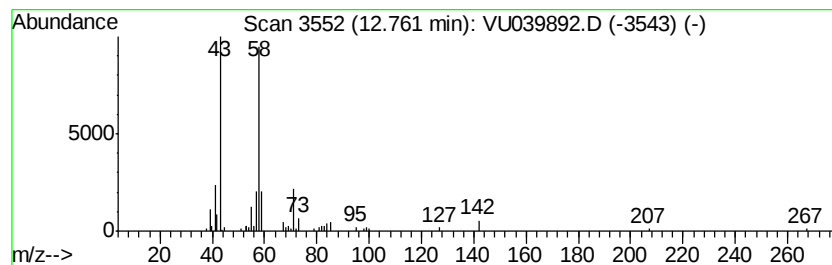
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR080320WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 2-Nonanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.76	1.13 ug/L	60735	1,4-Dichlorobenzene-d4	11.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Nonanone	142	C9H18O	000821-55-6	87
2		2-Nonanone	142	C9H18O	000821-55-6	87
3		2-Nonanone	142	C9H18O	000821-55-6	78
4		Pentanal, 2-methyl-	100	C6H12O	000123-15-9	59
5		2-Octanone	128	C8H16O	000111-13-7	56



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU081720\
Data File : VU039892.D
Acq On : 17 Aug 2020 17:27
Operator : SY/MD
Sample : L3517-07 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F4M01

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
2-Pentanone	6.79	0.6	ug/L	24539	1	6.26	195630	5.0
2-Heptanone	10.24	1.1	ug/L	56372	2	9.42	257214	5.0
3-Octanone	11.47	0.9	ug/L	46346	3	11.81	267651	5.0
2-Hexanone, 4-met...	11.57	0.8	ug/L	43385	3	11.81	267651	5.0
2-Nonanone	12.76	1.1	ug/L	60735	3	11.81	267651	5.0