

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU081720\
 Data File : VU039890.D
 Acq On : 17 Aug 2020 16:15
 Operator : SY/MD
 Sample : L3517-07 10X
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 16 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	92	rVB	25993	31083	9.65%	0.981%
2	1.922	170	181	192	rBV	25792	33581	10.42%	1.060%
3	2.578	373	385	397	rBV	42337	68684	21.32%	2.168%
4	2.690	397	420	461	rBV	48346	262102	81.35%	8.275%
5	3.063	530	536	547	rVB6	5169	8457	2.62%	0.267%
6	4.671	1017	1036	1050	rBV3	34734	123379	38.29%	3.895%
7	5.083	1147	1164	1181	rBV	48526	105586	32.77%	3.333%
8	5.742	1348	1369	1394	rBV2	86741	230451	71.52%	7.275%
9	6.176	1494	1504	1510	rBV3	1941	3529	1.10%	0.111%
10	6.263	1517	1531	1546	rBV	126285	233438	72.45%	7.370%
11	6.549	1610	1620	1630	rVB7	2694	5327	1.65%	0.168%
12	6.703	1654	1668	1682	rBV3	59477	115286	35.78%	3.640%
13	6.787	1682	1694	1720	rVB2	12962	29327	9.10%	0.926%
14	6.941	1733	1742	1755	rBV	4049	7457	2.31%	0.235%
15	7.574	1926	1939	1950	rBV2	29335	49274	15.29%	1.556%
16	7.803	1998	2010	2028	rBV2	38717	73996	22.97%	2.336%
17	7.906	2028	2042	2055	rVV	97191	166967	51.82%	5.271%
18	7.976	2055	2064	2073	rVB2	6055	11143	3.46%	0.352%
19	8.185	2118	2129	2140	rBV2	20308	35964	11.16%	1.135%
20	8.555	2238	2244	2252	rVB5	4695	5797	1.80%	0.183%
21	8.642	2258	2271	2298	rBV	153247	287727	89.30%	9.084%
22	8.918	2348	2357	2373	rVB4	5435	10150	3.15%	0.320%
23	9.420	2499	2513	2526	rBV	191476	312073	96.85%	9.852%
24	9.571	2550	2560	2572	rBV	13744	20423	6.34%	0.645%
25	9.693	2585	2598	2609	rBV	41967	69197	21.48%	2.185%
26	10.098	2714	2724	2740	rVB3	12458	20148	6.25%	0.636%
27	10.233	2755	2766	2781	rBV	37040	57531	17.86%	1.816%
28	10.365	2795	2807	2820	rVB4	6446	11050	3.43%	0.349%
29	10.754	2915	2928	2941	rBV2	51927	82218	25.52%	2.596%
30	11.465	3140	3149	3159	rBV3	30382	44398	13.78%	1.402%
31	11.571	3171	3182	3196	rBV3	24188	43801	13.59%	1.383%
32	11.645	3196	3205	3216	rVB2	8319	13172	4.09%	0.416%
33	11.806	3242	3255	3269	rVB	211551	322208	100.00%	10.172%
34	12.053	3324	3332	3340	rBV3	5127	7642	2.37%	0.241%

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ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
F4M01

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	12.188	3362	3374	3387	rBV	113979	185111	57.45%	5.844%
36	12.764	3543	3553	3561	rBV	40110	60866	18.89%	1.922%
37	12.803	3561	3565	3576	rVB4	13589	18988	5.89%	0.599%

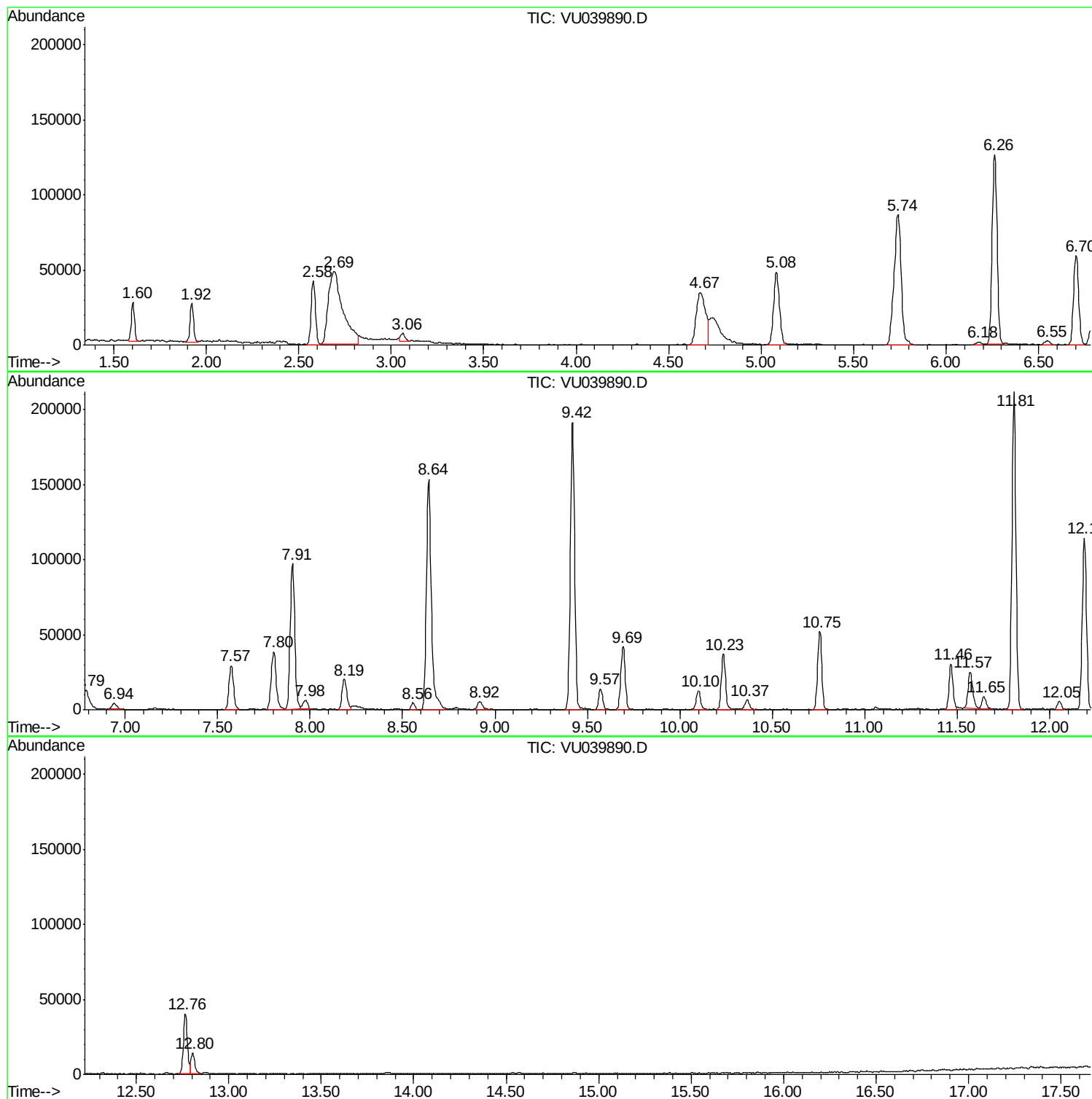
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR080320WMA.M
Quant Title : TRACE VOA SOM01.0

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



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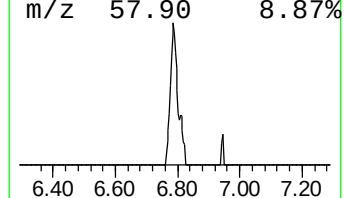
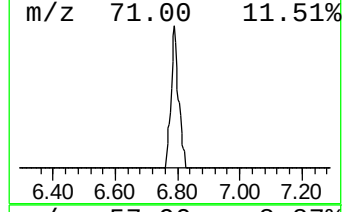
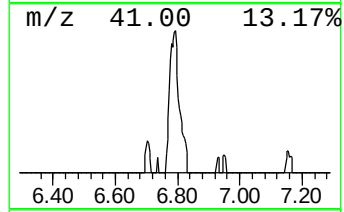
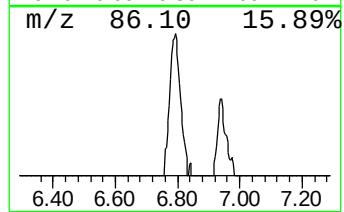
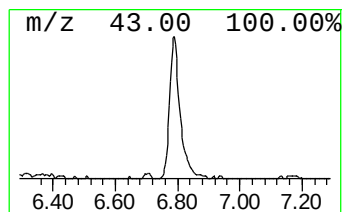
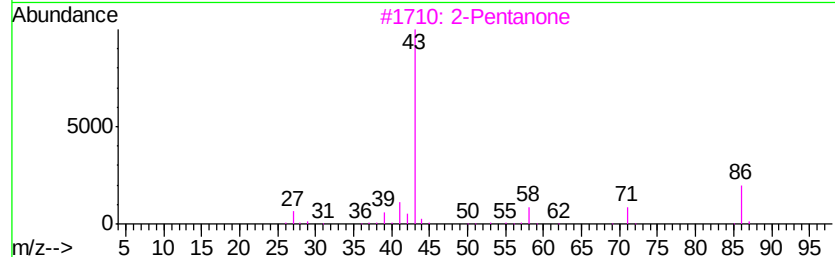
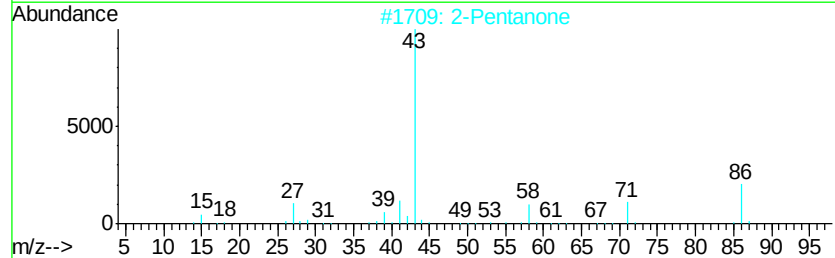
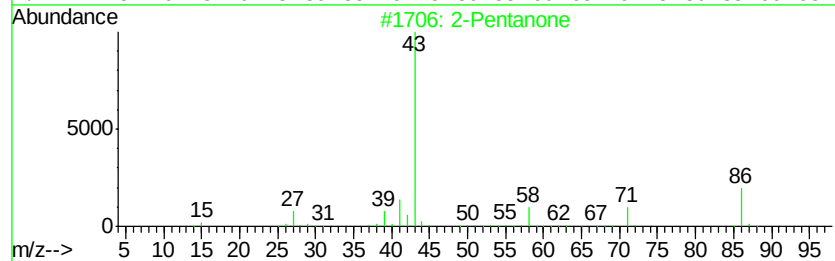
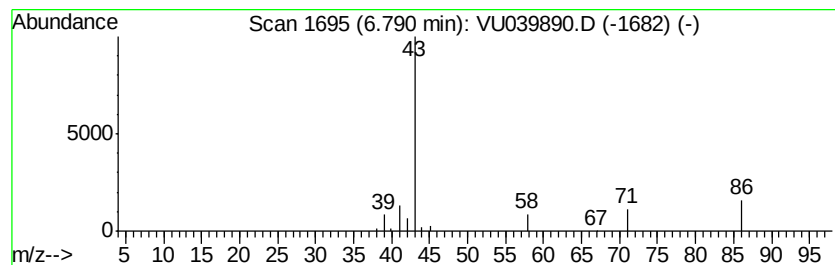
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR080320WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 2-Pentanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.79	0.63 ug/L	29327	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	78
3			2-Pentanone	86	C5H10O	000107-87-9	78
4			2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	64
5			2,3-Pentanedione, 4-methyl-	114	C6H10O2	007493-58-5	36



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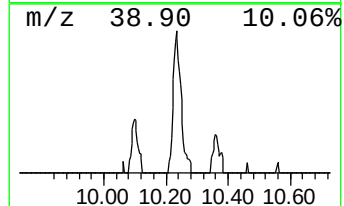
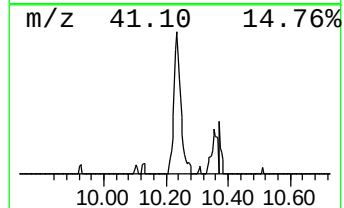
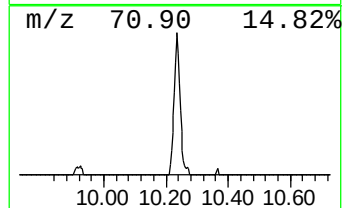
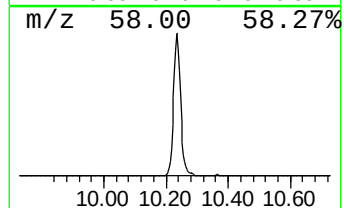
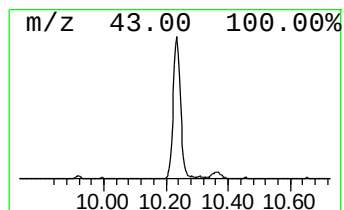
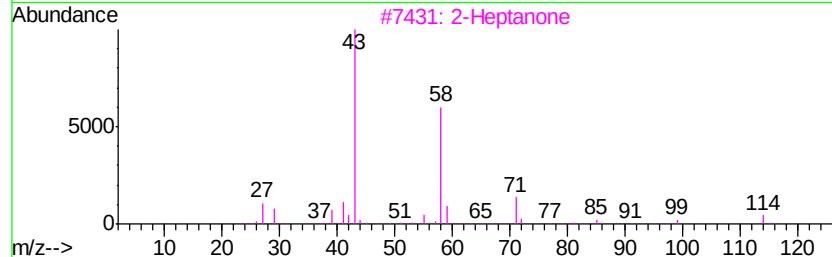
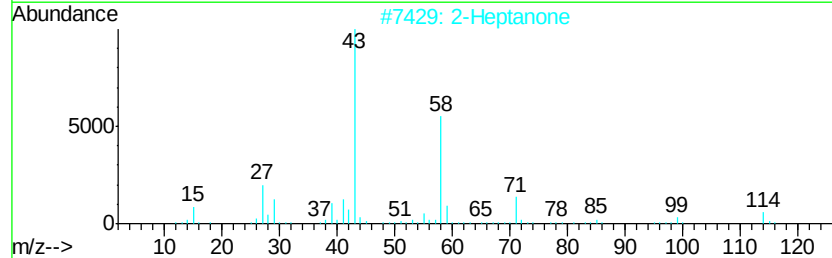
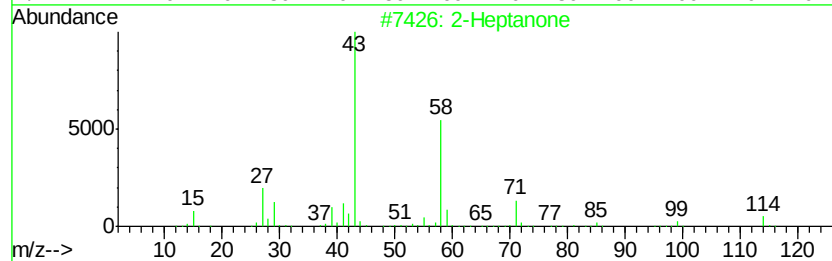
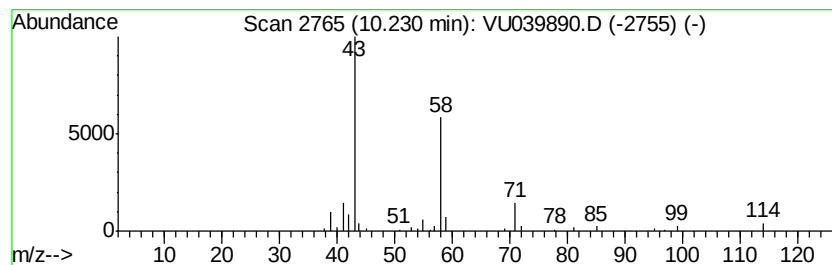
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 2-Heptanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.23	0.92 ug/L	57531	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	86
3		2-Heptanone	114	C7H14O	000110-43-0	80
4		2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	72
5		2-Hexanone	100	C6H12O	000591-78-6	64



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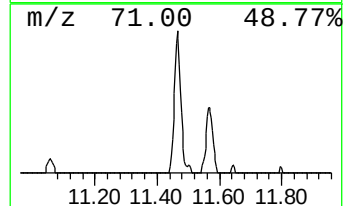
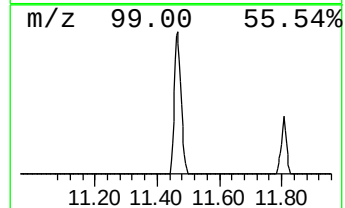
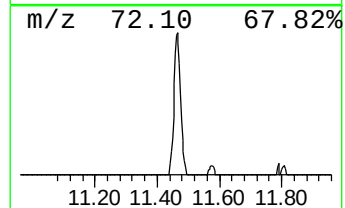
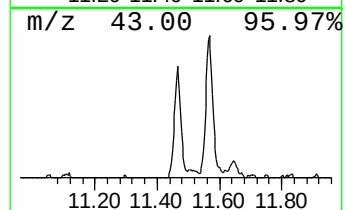
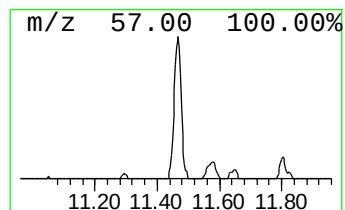
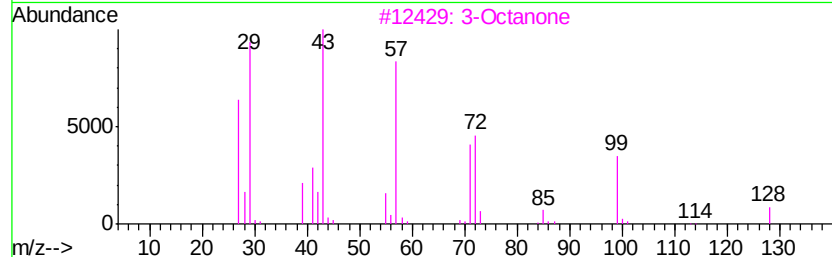
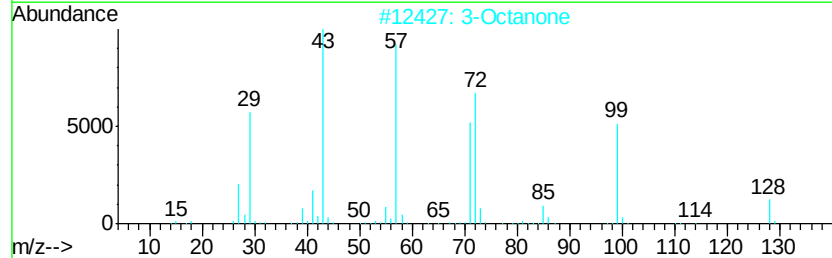
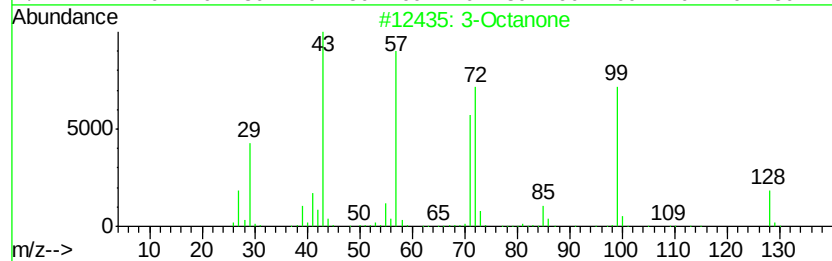
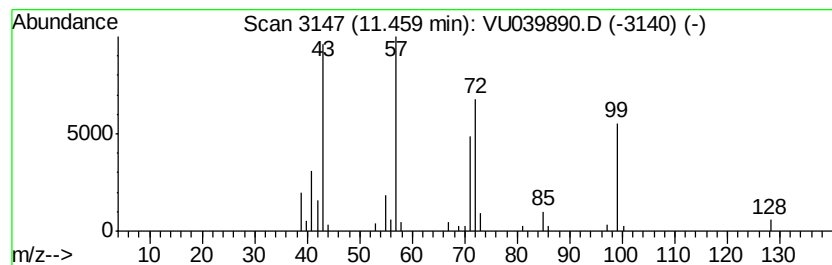
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Quant Title : TRACE VOA SOM01.0

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.
11.46	0.69 ug/L	44398	1,4-Dichlorobenzene-d4	11.81

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octanone		128	C8H16O	000106-68-3	87
2	3-Octanone		128	C8H16O	000106-68-3	80
3	3-Octanone		128	C8H16O	000106-68-3	64
4	3-Octanone		128	C8H16O	000106-68-3	58
5	3-Heptanone, 5-methyl-		128	C8H16O	000541-85-5	50



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ALS Vial : 16 Sample Multiplier: 1

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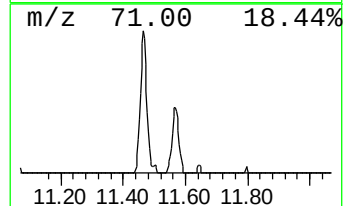
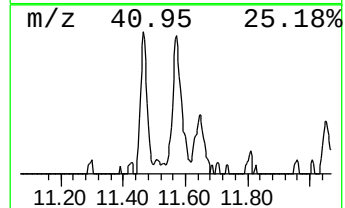
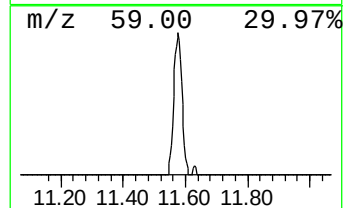
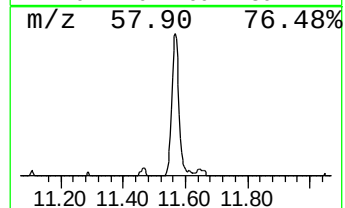
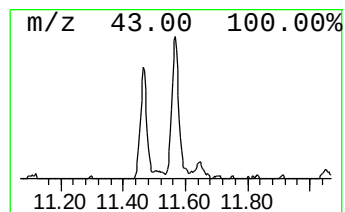
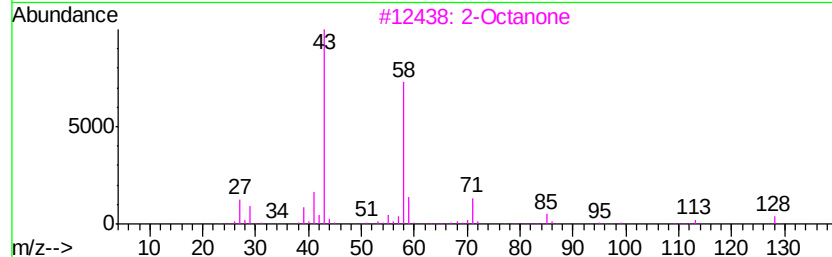
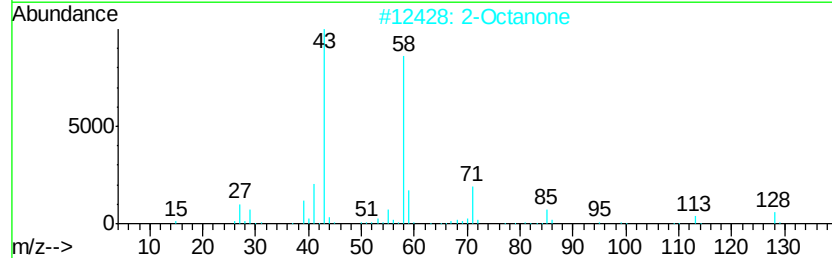
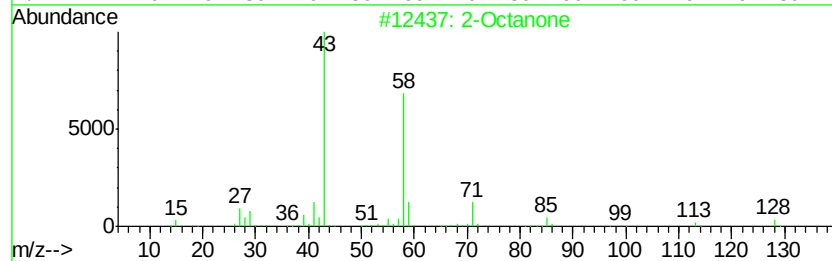
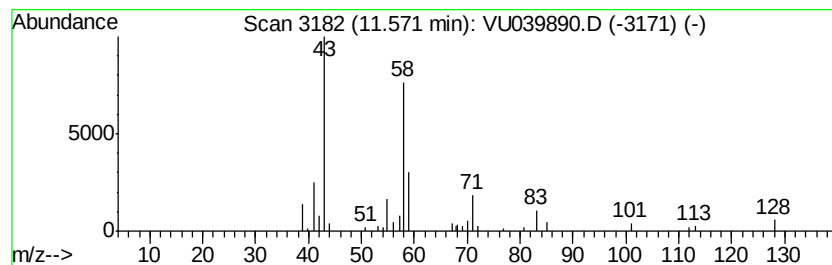
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Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.57	0.68 ug/L	43801	1,4-Dichlorobenzene-d4	11.81

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanone		128	C8H16O	000111-13-7	72
2	2-Octanone		128	C8H16O	000111-13-7	64
3	2-Octanone		128	C8H16O	000111-13-7	64
4	2-Octanone		128	C8H16O	000111-13-7	59
5	2-Heptanone, 4-methyl-		128	C8H16O	006137-06-0	50



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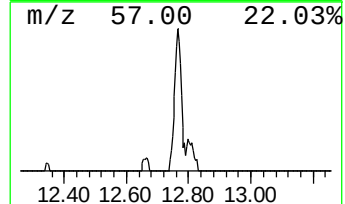
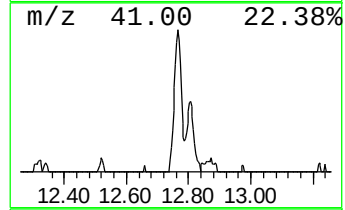
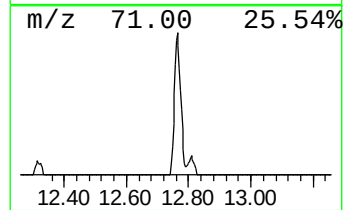
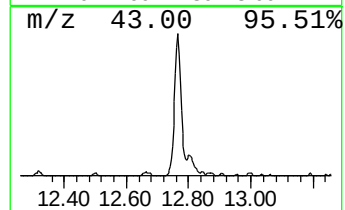
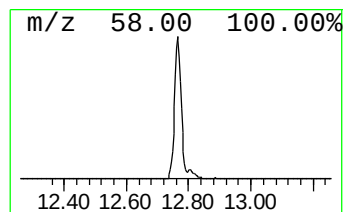
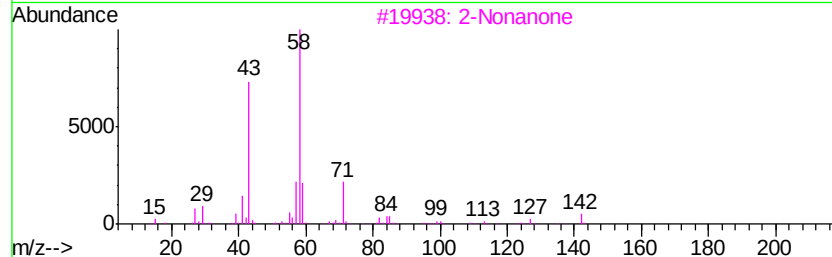
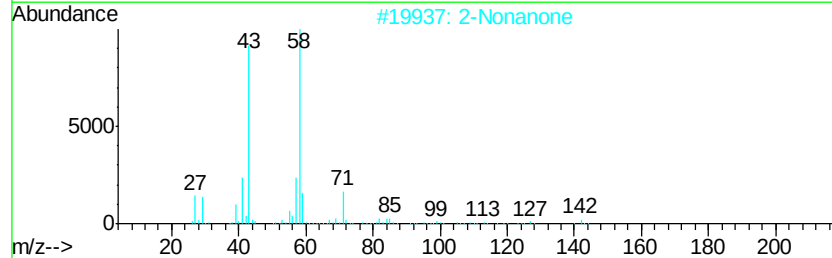
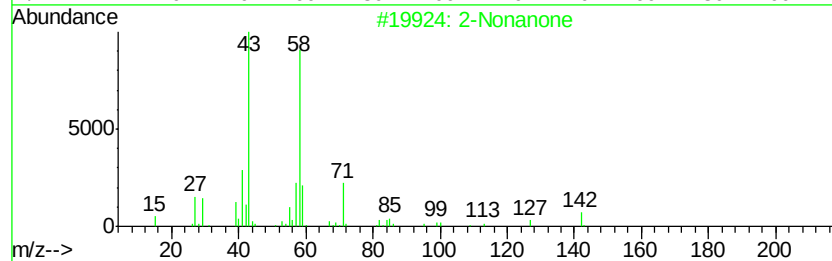
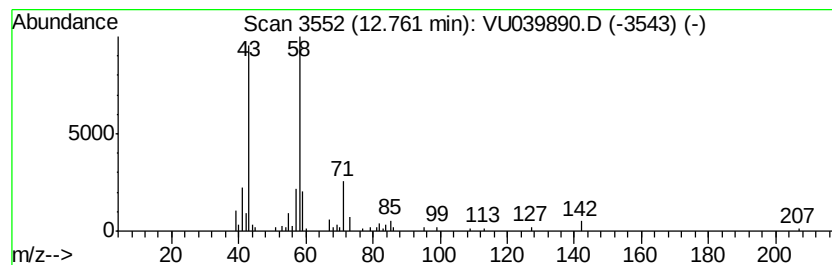
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 2-Nonanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.76	0.94 ug/L	60866	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	91
3	2-Nonanone		142	C9H18O	000821-55-6	90
4	2-Undecanone		170	C11H22O	000112-12-9	78
5	2-Nonanone		142	C9H18O	000821-55-6	72



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Sample : L3517-07 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F4M01

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone	6.79	0.6	ug/L	29327	1	6.26	233438	5.0
2-Heptanone	10.23	0.9	ug/L	57531	2	9.42	312073	5.0
3-Octanone	11.46	0.7	ug/L	44398	3	11.81	322208	5.0
2-Heptanone, 4-me...	11.57	0.7	ug/L	43801	3	11.81	322208	5.0
2-Nonanone	12.76	0.9	ug/L	60866	3	11.81	322208	5.0