

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU080620\
 Data File : VU039771.D
 Acq On : 06 Aug 2020 21:26
 Operator : SY/MD
 Sample : L3590-03
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 26 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: VU039772.D

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.485	27	45	49	rBV	12586	20508	5.40%	0.618%
2	1.597	70	80	92	rVB3	45756	71280	18.75%	2.147%
3	1.822	139	150	151	rBV5	3084	4957	1.30%	0.149%
4	1.916	172	179	190	rVB	35733	44373	11.67%	1.336%
5	2.392	320	327	341	rVB7	7260	14510	3.82%	0.437%
6	2.572	373	383	399	rVB	69950	112789	29.67%	3.397%
7	3.359	618	628	639	rBV5	10787	20930	5.51%	0.630%
8	4.687	1022	1041	1089	rBV3	76041	300325	79.01%	9.045%
9	5.083	1145	1164	1190	rBV	64394	151300	39.80%	4.557%
10	5.739	1347	1368	1381	rBV4	123741	305922	80.48%	9.213%
11	6.260	1519	1530	1547	rVB	105668	198158	52.13%	5.968%
12	6.549	1608	1620	1637	rBV	9388	19687	5.18%	0.593%
13	6.706	1655	1669	1684	rBV	79527	152258	40.06%	4.586%
14	6.806	1690	1700	1712	rBV3	4228	8831	2.32%	0.266%
15	6.899	1718	1729	1741	rBV2	13575	25080	6.60%	0.755%
16	7.575	1928	1939	1954	rBV2	35464	60293	15.86%	1.816%
17	7.813	2000	2013	2026	rBV2	15663	30443	8.01%	0.917%
18	7.903	2029	2041	2055	rVV	127381	221204	58.19%	6.662%
19	7.973	2057	2063	2074	rVB3	9543	15401	4.05%	0.464%
20	8.189	2118	2130	2142	rBV2	21477	35771	9.41%	1.077%
21	8.648	2260	2273	2299	rBV	204837	380115	100.00%	11.448%
22	8.793	2308	2318	2330	rBV3	18712	30952	8.14%	0.932%
23	9.420	2497	2513	2532	rBV	154603	252428	66.41%	7.602%
24	9.690	2582	2597	2609	rVB5	8889	15270	4.02%	0.460%
25	10.102	2712	2725	2731	rBV7	2760	4482	1.18%	0.135%
26	10.240	2757	2768	2777	rVB3	4897	8238	2.17%	0.248%
27	10.343	2790	2800	2813	rBV5	15060	25031	6.59%	0.754%
28	10.758	2914	2929	2941	rBV2	64988	104535	27.50%	3.148%
29	11.253	3072	3083	3091	rBV3	9323	13908	3.66%	0.419%
30	11.468	3140	3150	3159	rBV3	20046	31327	8.24%	0.943%
31	11.574	3172	3183	3196	rBV5	18637	36482	9.60%	1.099%
32	11.645	3197	3205	3214	rBV5	4978	6151	1.62%	0.185%
33	11.806	3242	3255	3267	rBV	158782	251506	66.17%	7.575%
34	12.057	3323	3333	3346	rBV5	4680	8337	2.19%	0.251%

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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	12.189	3362	3374	3388	rBV	149500	236303	62.17%	7.117%
36	12.529	3472	3480	3487	rVB7	3505	5491	1.44%	0.165%
37	12.674	3514	3525	3529	rBV6	2555	4744	1.25%	0.143%
38	12.767	3543	3554	3561	rBV	25649	40804	10.73%	1.229%
39	12.806	3561	3566	3582	rVV4	12862	21504	5.66%	0.648%
40	13.861	3880	3894	3910	rBV5	11577	22784	5.99%	0.686%
41	14.873	4199	4209	4218	rBV4	4172	5991	1.58%	0.180%

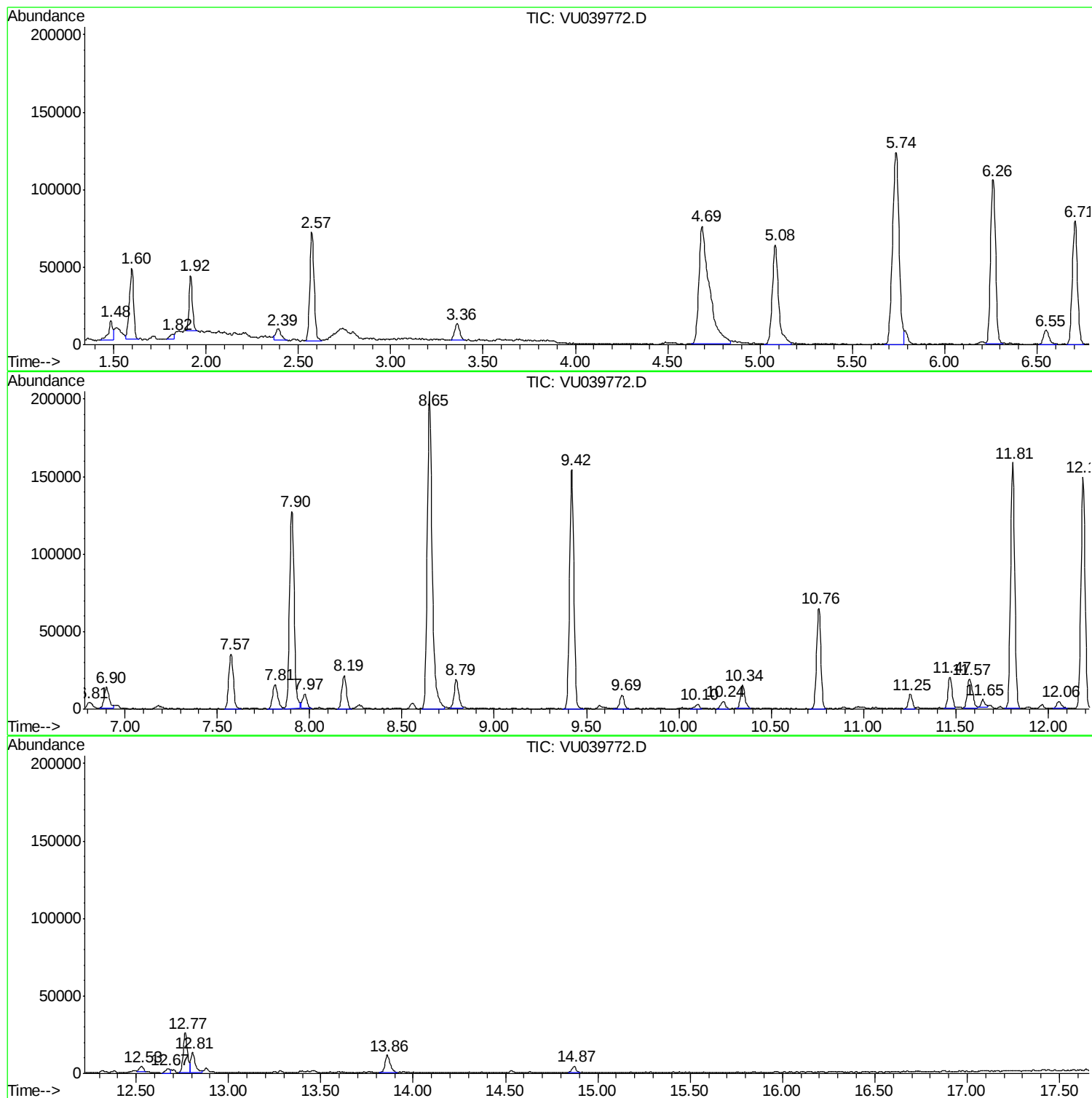
Sum of corrected areas: 3320403

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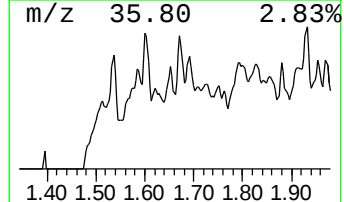
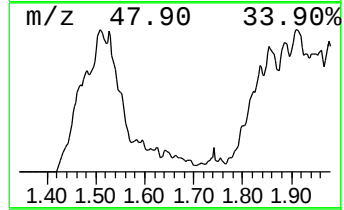
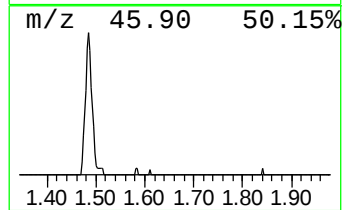
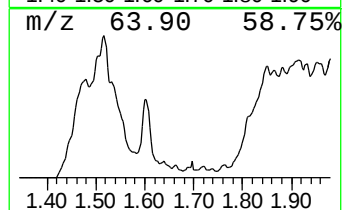
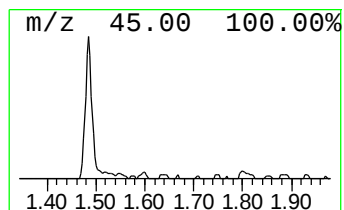
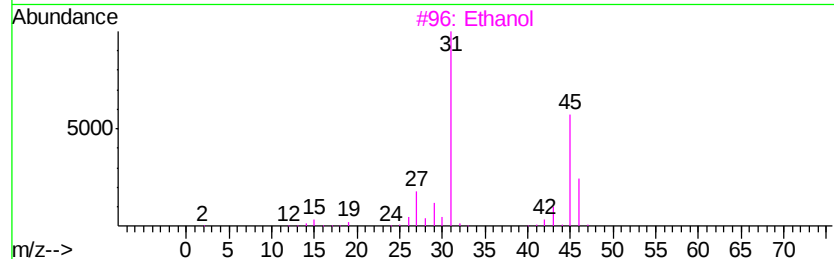
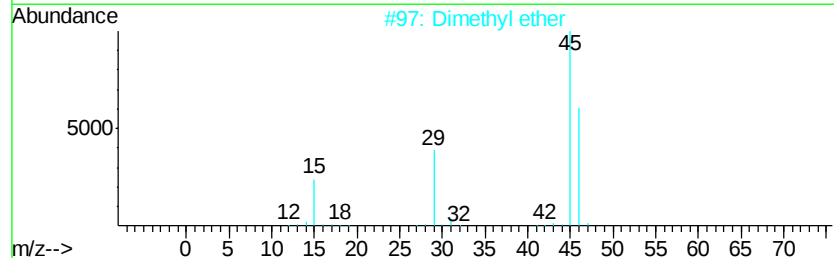
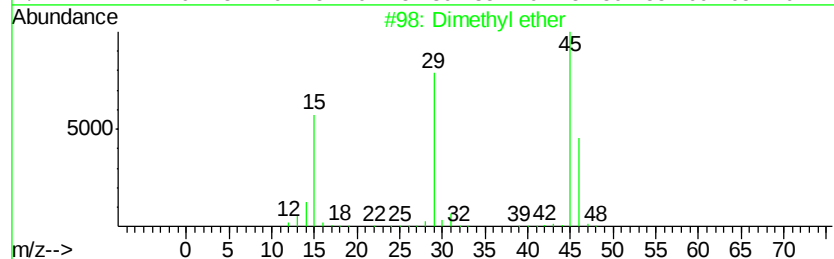
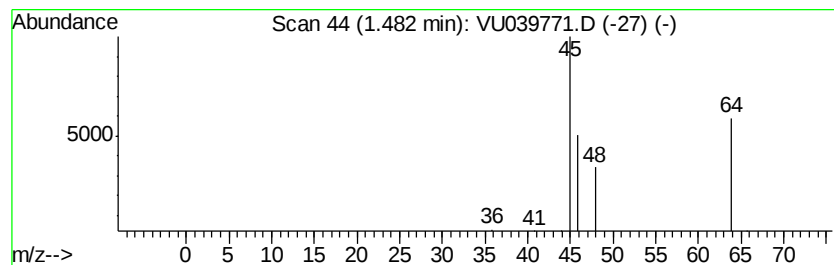
Instrument :
MSVOA_U
ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR080320WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.48	0.52 ug/L	20508	1,4-Difluorobenzene	6.26
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Dimethyl ether	46 C2H6O	000115-10-6 5
2		Dimethyl ether	46 C2H6O	000115-10-6 5
3		Ethanol	46 C2H6O	000064-17-5 4
4		Ethanol	46 C2H6O	000064-17-5 4
5		Ethanol	46 C2H6O	000064-17-5 4



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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampled :
F4L17

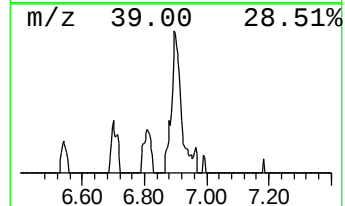
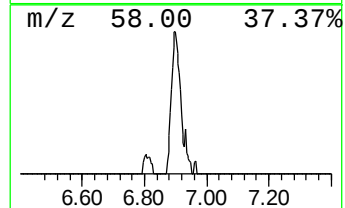
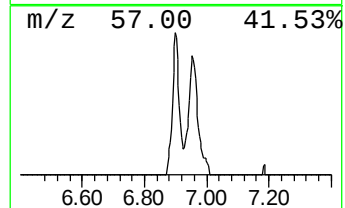
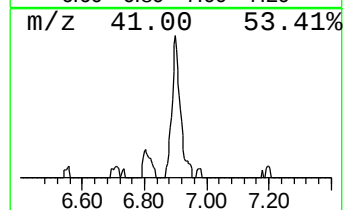
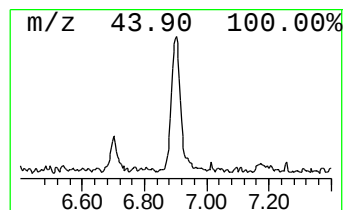
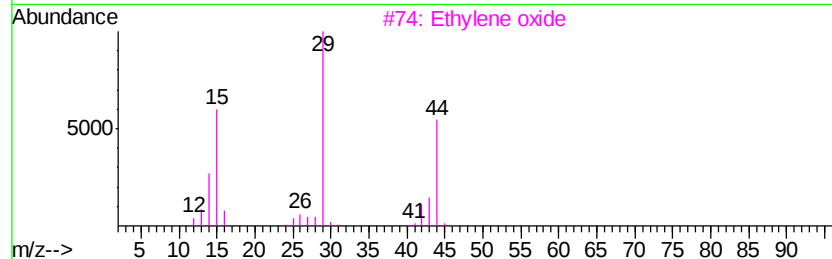
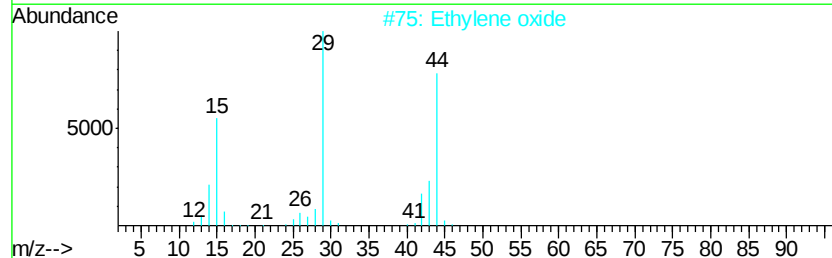
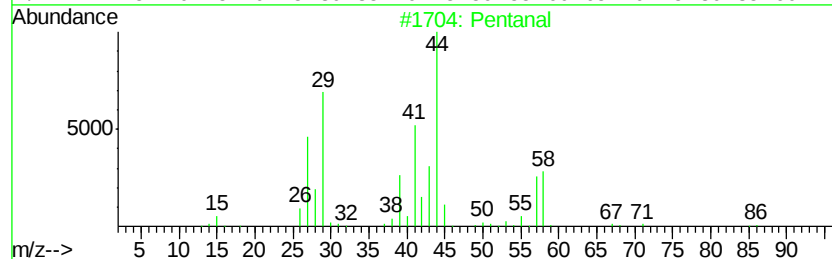
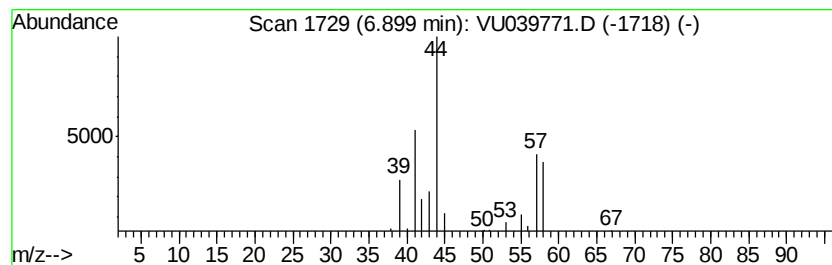
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR080320WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.90	0.63 ug/L	25080	1,4-Difluorobenzene	6.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentanal	86	C5H10O	000110-62-3	9
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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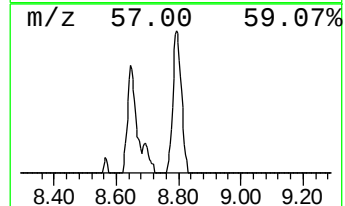
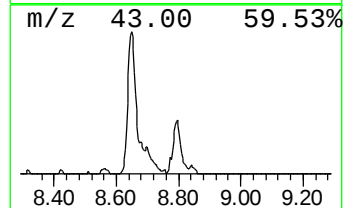
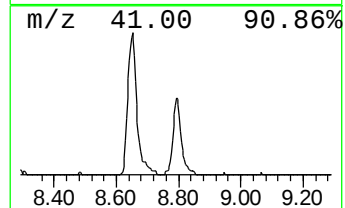
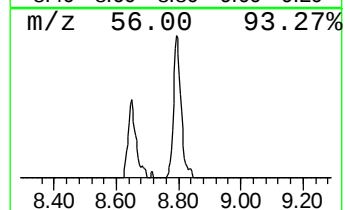
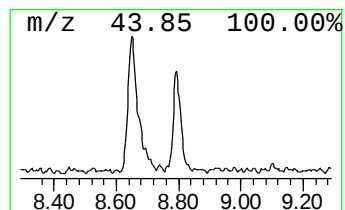
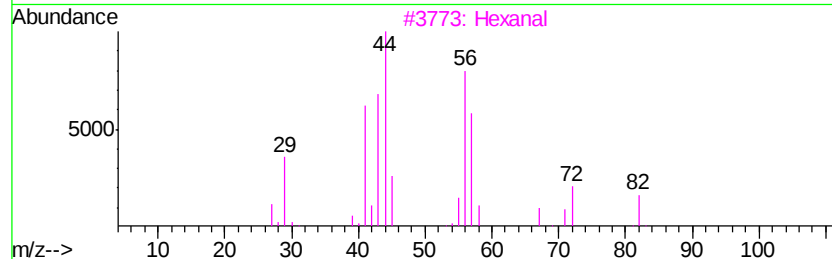
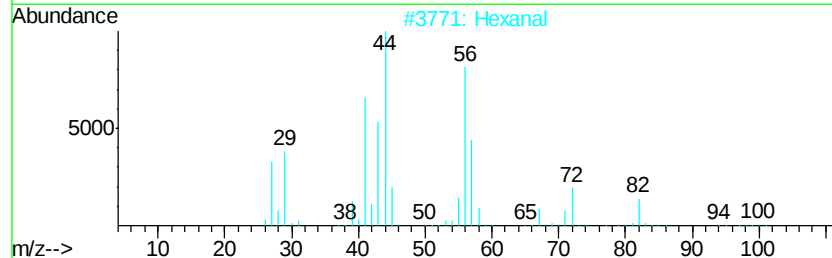
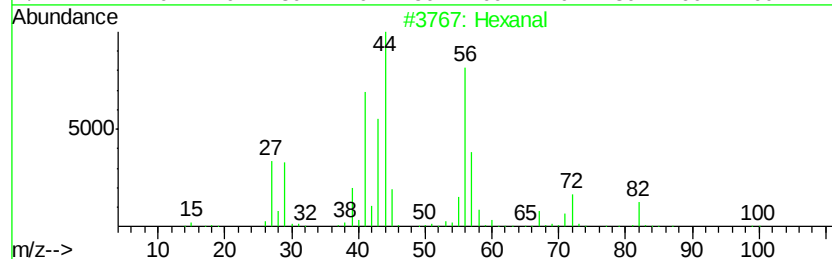
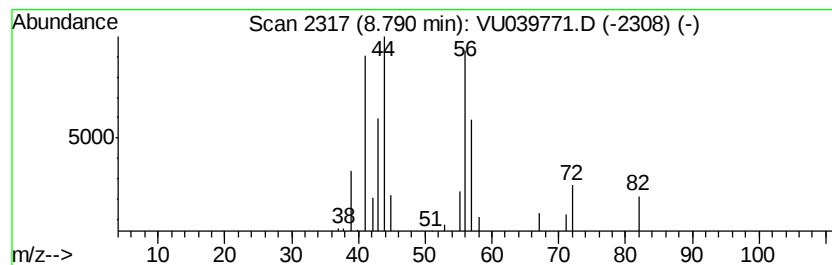
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 Hexanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.79	0.61 ug/L	30952	Chlorobenzene-d5	9.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanal	100	C6H12O	000066-25-1	72
2		Hexanal	100	C6H12O	000066-25-1	72
3		Hexanal	100	C6H12O	000066-25-1	64
4		Hexanal	100	C6H12O	000066-25-1	59
5		2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9	32



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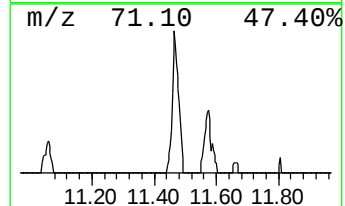
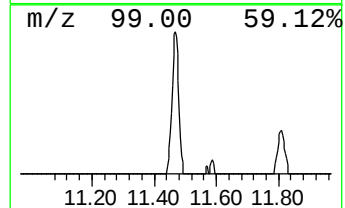
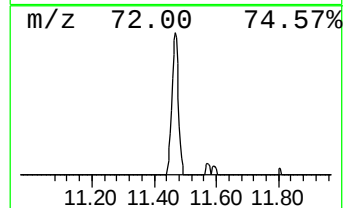
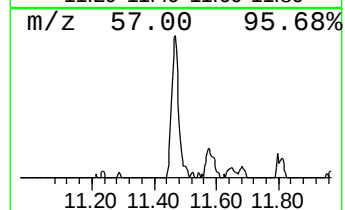
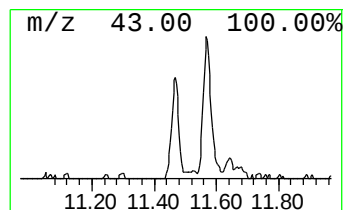
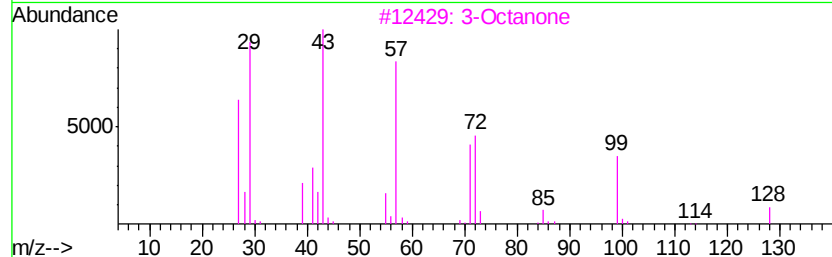
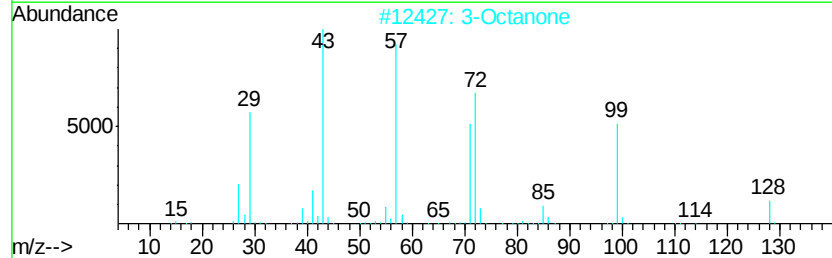
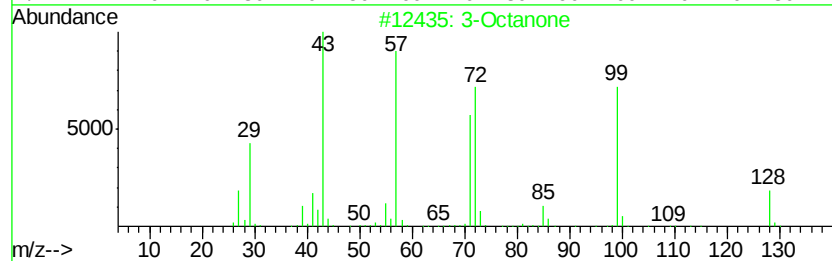
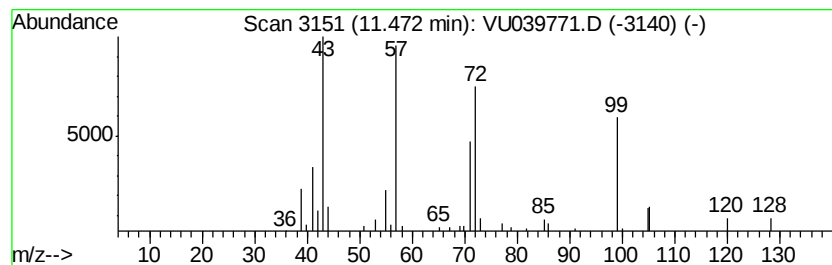
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 3-Octanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.47	0.62 ug/L	31327	1,4-Dichlorobenzene-d4	11.81

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octanone		128	C8H16O	000106-68-3	93
2	3-Octanone		128	C8H16O	000106-68-3	90
3	3-Octanone		128	C8H16O	000106-68-3	83
4	3-Octanone		128	C8H16O	000106-68-3	50
5	3-Heptanone, 6-methyl-		128	C8H16O	000624-42-0	50



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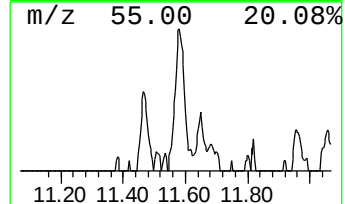
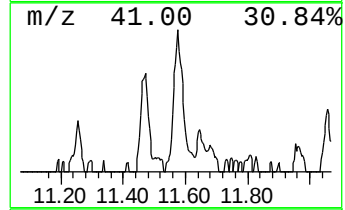
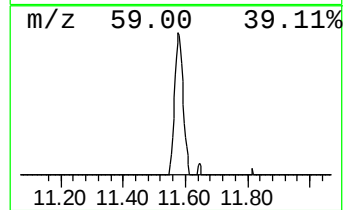
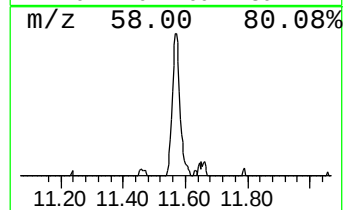
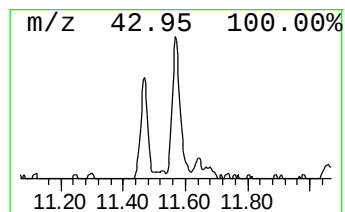
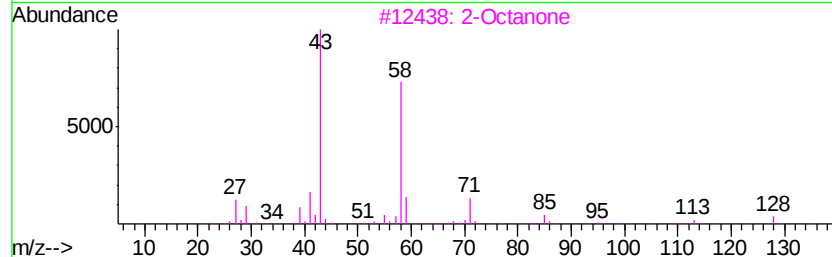
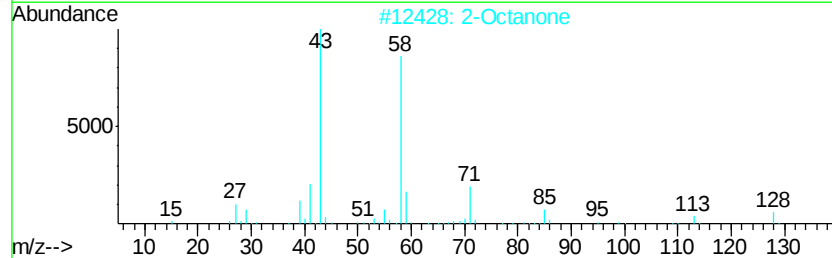
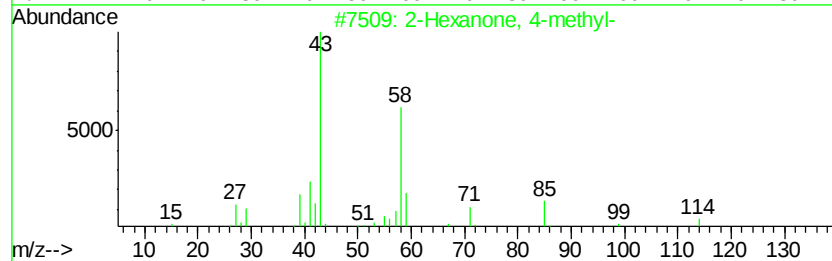
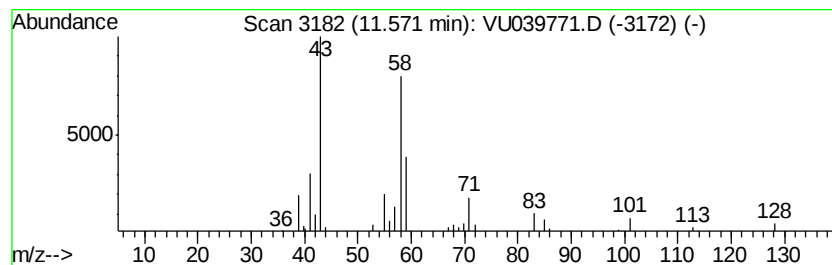
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 2-Hexanone, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.57	0.73 ug/L	36482	1,4-Dichlorobenzene-d4	11.81

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	53
2		2-Octanone	128	C8H16O	000111-13-7	50
3		2-Octanone	128	C8H16O	000111-13-7	50
4		2-Octanone	128	C8H16O	000111-13-7	50
5		Formamide, N-butyl-	101	C5H11NO	000871-71-6	47



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU080620\
Data File : VU039771.D
Acq On : 06 Aug 2020 21:26
Operator : SY/MD
Sample : L3590-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F4L17

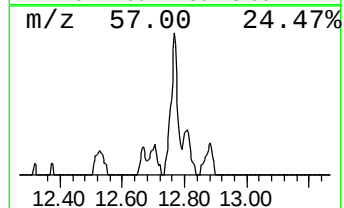
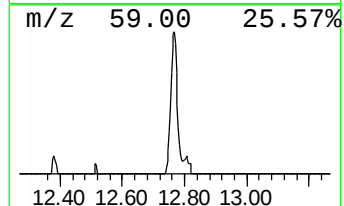
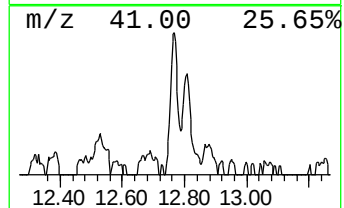
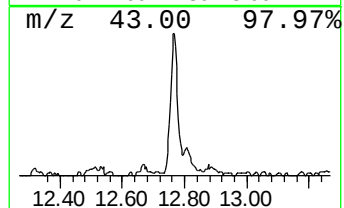
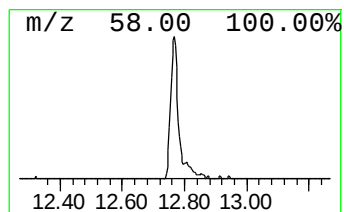
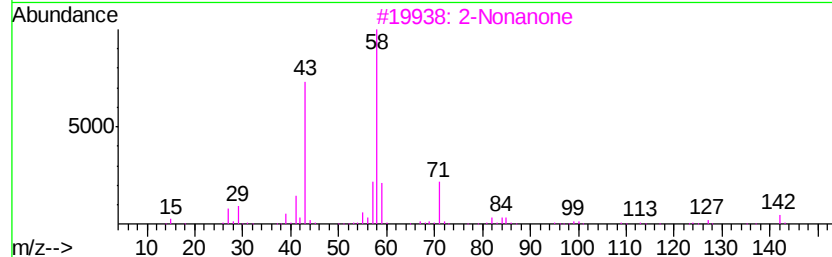
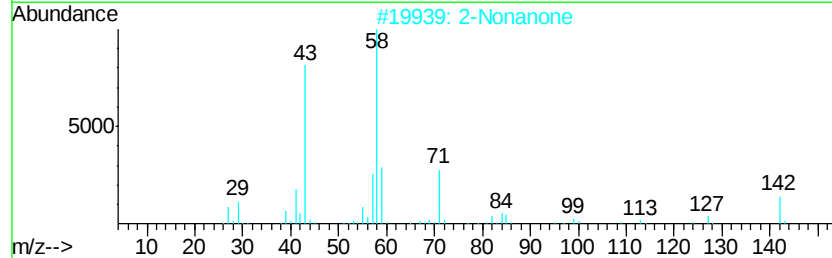
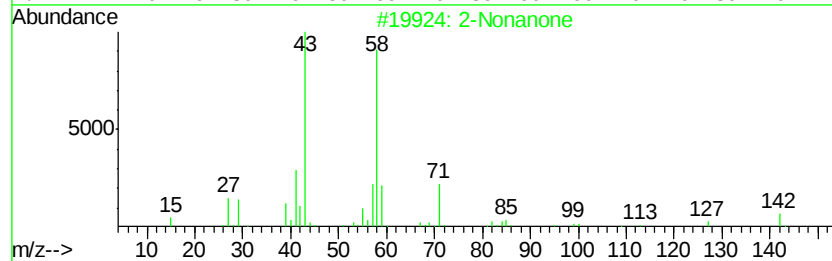
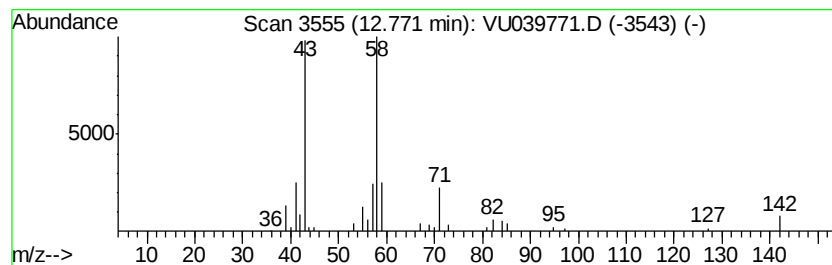
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Quant Title : TRACE VOA SOM01.0

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	40804	1,4-Dichlorobenzene-d4	11.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Nonanone	142	C9H18O	000821-55-6	91
2		2-Nonanone	142	C9H18O	000821-55-6	83
3		2-Nonanone	142	C9H18O	000821-55-6	83
4		2-Nonanone	142	C9H18O	000821-55-6	80
5		2-Dodecanone	184	C12H24O	006175-49-1	78



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU080620\
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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 26 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
unknown-01	1.48	0.5	ug/L	20508	1	6.26	198158	5.0
unknown-02	6.90	0.6	ug/L	25080	1	6.26	198158	5.0
Hexanal	8.79	0.6	ug/L	30952	2	9.42	252428	5.0
3-Octanone	11.47	0.6	ug/L	31327	3	11.81	251506	5.0
2-Hexanone, 4-met...	11.57	0.7	ug/L	36482	3	11.81	251506	5.0
2-Nonanone	12.77	0.8	ug/L	40804	3	11.81	251506	5.0