

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU100320\
 Data File : VU040485.D
 Acq On : 03 Oct 2020 17:28
 Operator : SY/MD
 Sample : L4240-14
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BG3T4

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\SOMUTR092920WMA.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	1.366	3	8	19	rBV3	4961	6392	1.24%	0.146%
2	1.539	42	62	64	rBV2	23782	55662	10.83%	1.272%
3	1.607	77	83	98	rVB	50019	62064	12.07%	1.418%
4	1.922	174	181	193	rVB	38067	50624	9.85%	1.157%
5	2.581	374	386	401	rBV	80713	132088	25.69%	3.019%
6	3.099	538	547	561	rVB3	10636	21820	4.24%	0.499%
7	3.379	621	634	651	rBV2	20273	44737	8.70%	1.022%
8	3.719	725	740	758	rVB2	39247	86669	16.86%	1.981%
9	4.314	912	925	941	rVB6	3803	9749	1.90%	0.223%
10	4.456	955	969	981	rBV6	3464	8190	1.59%	0.187%
11	4.552	985	999	1016	rBV3	9450	22813	4.44%	0.521%
12	4.661	1016	1033	1075	rBV2	57547	219382	42.67%	5.014%
13	5.083	1139	1164	1181	rBV	74629	166502	32.38%	3.805%
14	5.742	1347	1369	1386	rBV4	142911	380366	73.98%	8.692%
15	6.263	1514	1531	1551	rBV	174251	327074	63.61%	7.475%
16	6.703	1652	1668	1686	rBV	94980	183592	35.71%	4.196%
17	7.575	1926	1939	1952	rBV	48183	83884	16.31%	1.917%
18	7.906	2028	2042	2055	rBV	163400	284119	55.26%	6.493%
19	7.973	2057	2063	2074	rVB3	3424	6000	1.17%	0.137%
20	8.185	2117	2129	2145	rBV2	34049	57893	11.26%	1.323%
21	8.642	2257	2271	2303	rBV	270307	514162	100.00%	11.750%
22	9.420	2498	2513	2547	rBV	251290	428009	83.24%	9.781%
23	9.690	2589	2597	2607	rBV2	5254	8194	1.59%	0.187%
24	10.754	2917	2928	2942	rBV	79478	128993	25.09%	2.948%
25	10.899	2960	2973	2986	rBV2	13215	23177	4.51%	0.530%
26	10.996	2992	3003	3021	rBV2	42346	87890	17.09%	2.009%
27	11.086	3021	3031	3042	rVB2	17936	26855	5.22%	0.614%
28	11.227	3067	3075	3085	rBV2	10626	15921	3.10%	0.364%
29	11.288	3085	3094	3104	rVB	20767	29582	5.75%	0.676%
30	11.465	3138	3149	3162	rVB2	35749	53314	10.37%	1.218%
31	11.809	3244	3256	3272	rBV	254147	410939	79.92%	9.391%
32	11.889	3272	3281	3291	rVB	20396	30715	5.97%	0.702%
33	12.089	3335	3343	3349	rBV3	8293	13575	2.64%	0.310%
34	12.118	3349	3352	3361	rVB2	6243	7808	1.52%	0.178%

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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	12.188	3361	3374	3387	rBV	191755	312276	60.73%	7.136%
36	12.565	3482	3491	3500	rVB3	6929	9648	1.88%	0.220%
37	12.873	3578	3587	3600	rVB5	5076	8749	1.70%	0.200%
38	13.446	3756	3765	3776	rVB6	4322	7154	1.39%	0.163%
39	13.828	3875	3884	3897	rVB2	21905	33480	6.51%	0.765%
40	14.076	3953	3961	3977	rVB	4616	7041	1.37%	0.161%
41	14.320	4029	4037	4045	rBV4	6420	8704	1.69%	0.199%

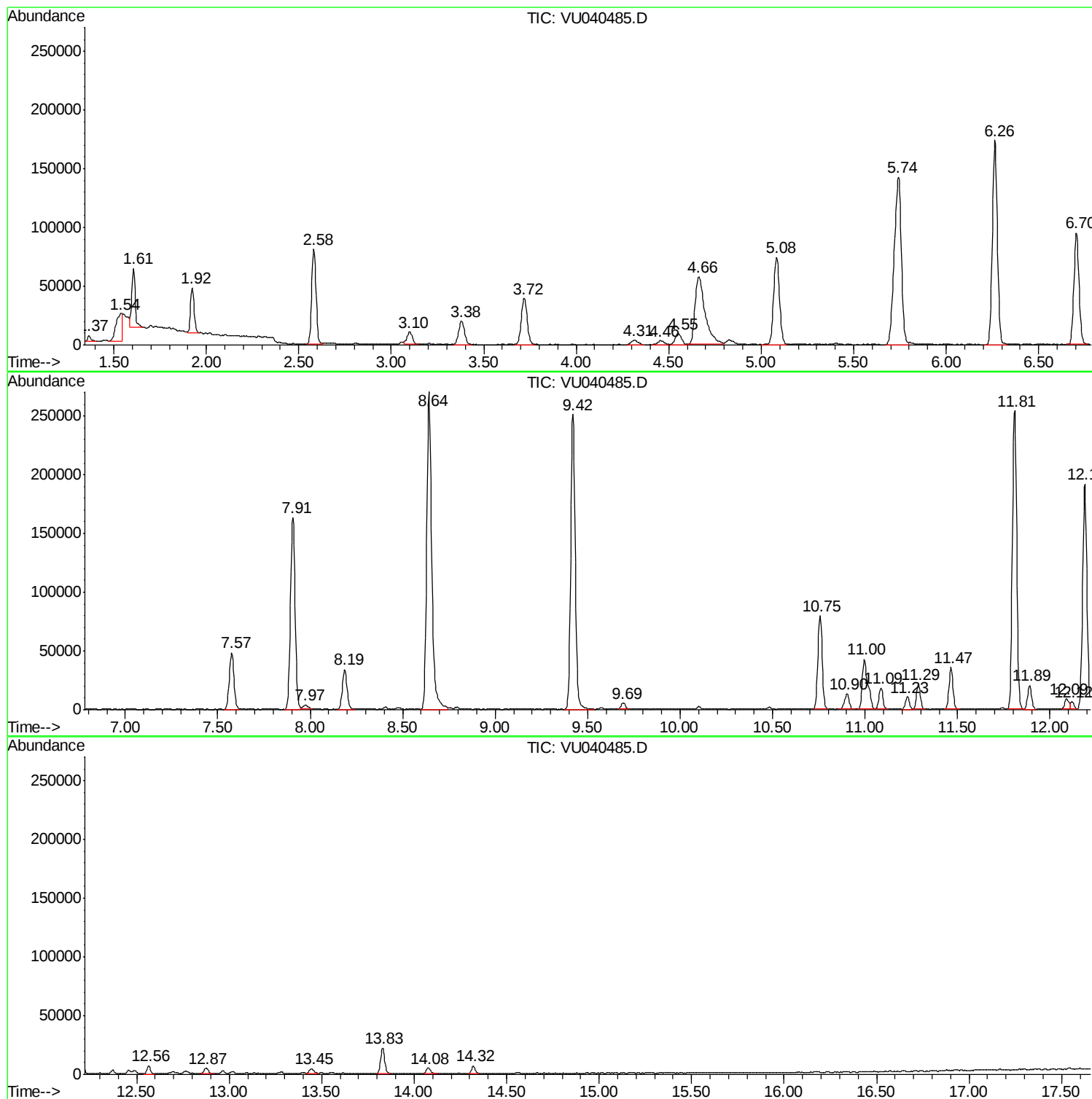
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR092920WMA.M
Quant Title : TRACE VOA SOM01.0

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



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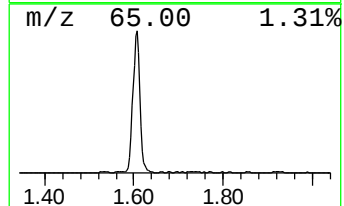
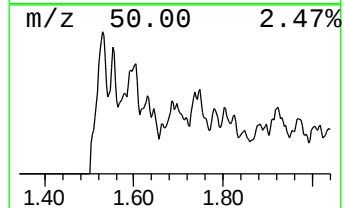
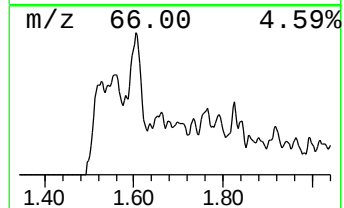
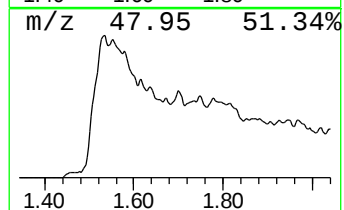
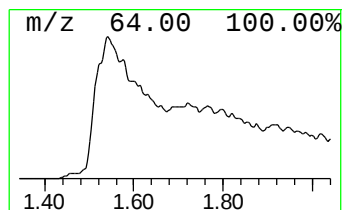
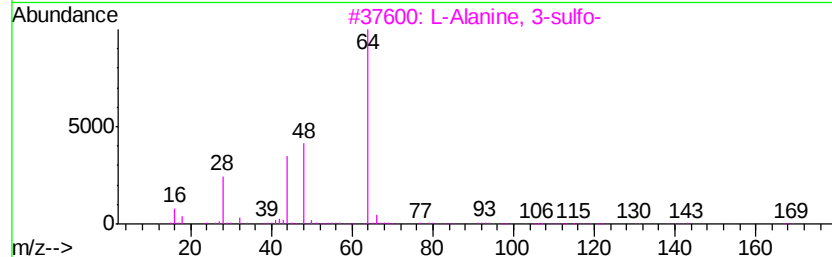
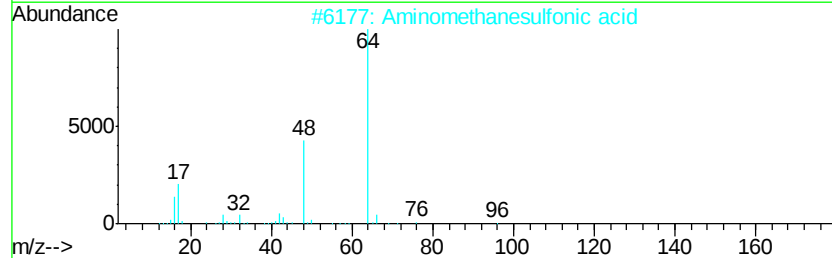
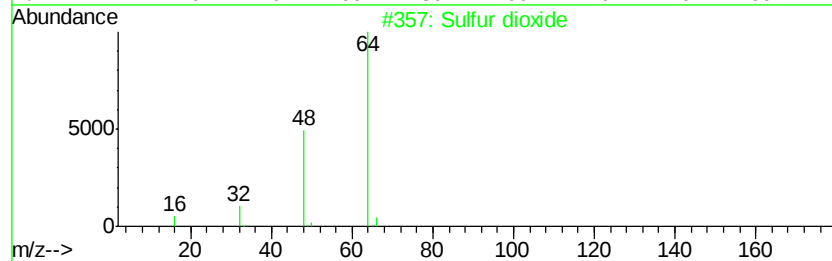
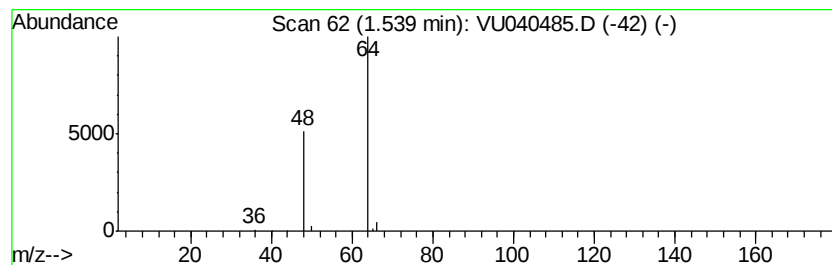
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR092920WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.54	0.85 ug/L	55662	1,4-Difluorobenzene	6.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfur dioxide	64	O2S	007446-09-5	90
2		Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3		L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4		Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5		Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	5



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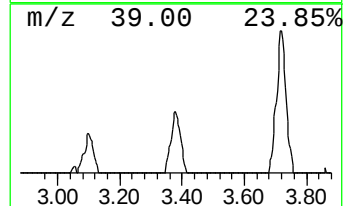
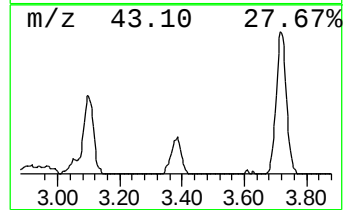
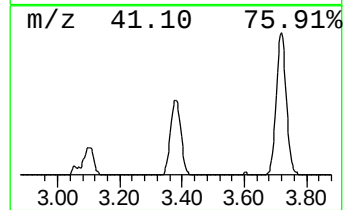
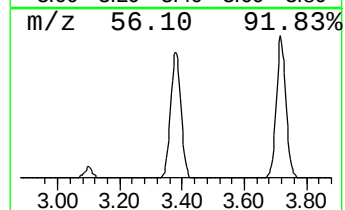
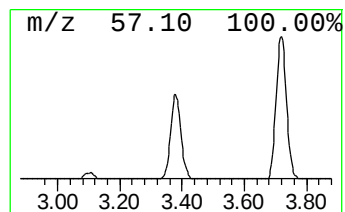
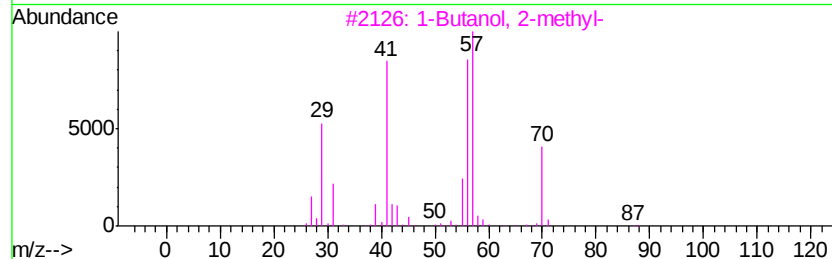
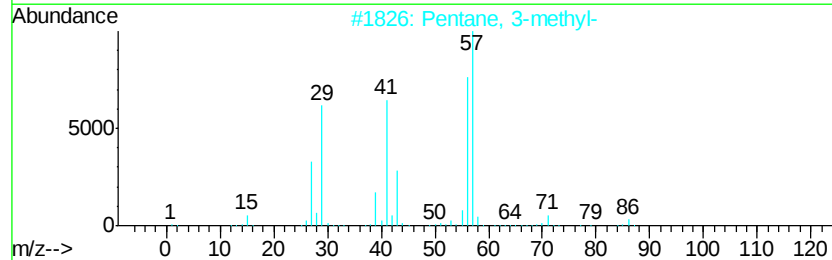
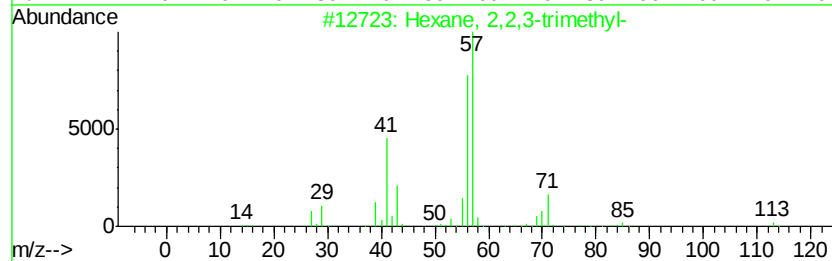
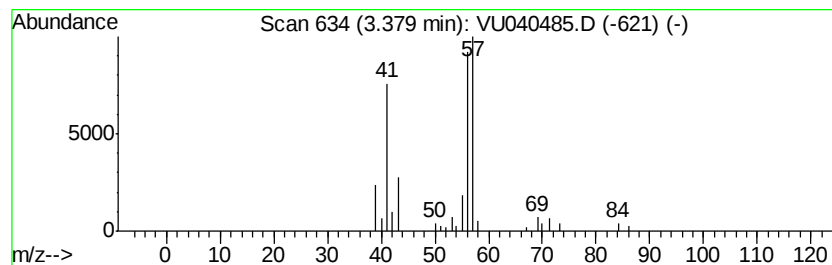
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.38	0.68 ug/L	44737	1,4-Difluorobenzene	6.26

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,2,3-trimethyl-		128	C9H20	016747-25-4	78
2	Pentane, 3-methyl-		86	C6H14	000096-14-0	72
3	1-Butanol, 2-methyl-		88	C5H12O	000137-32-6	72
4	Pentane, 3-methyl-		86	C6H14	000096-14-0	72
5	Pentane, 3-methyl-		86	C6H14	000096-14-0	64



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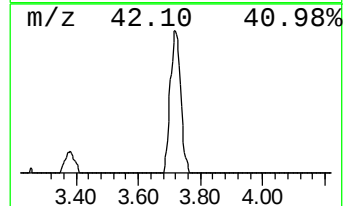
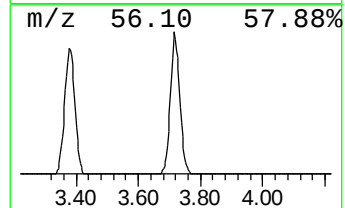
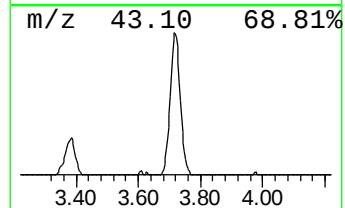
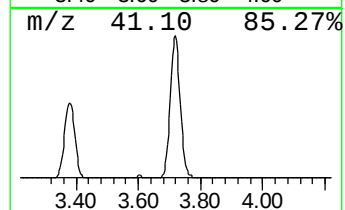
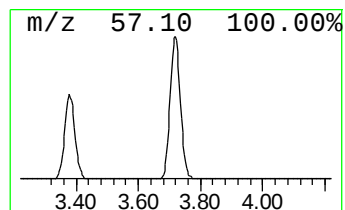
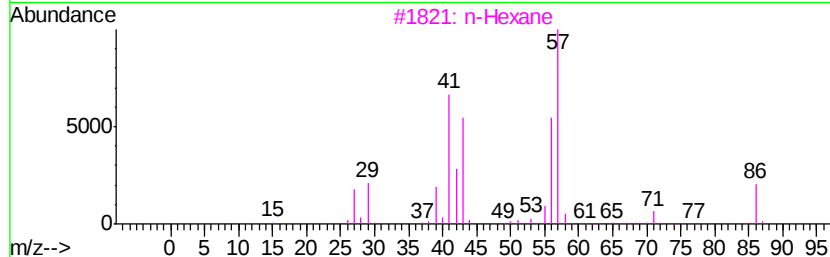
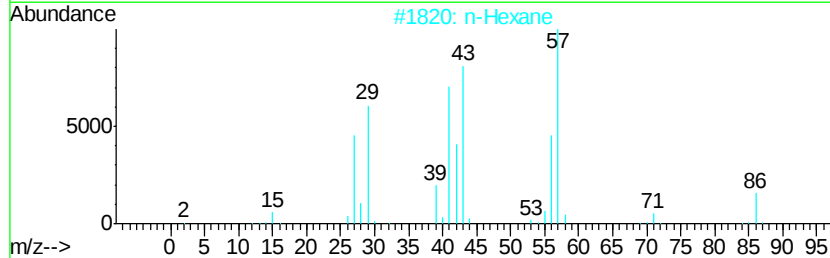
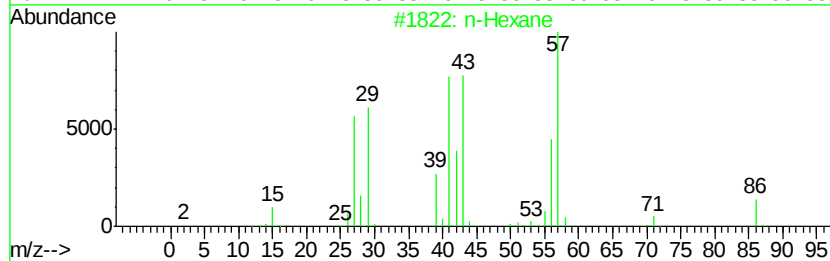
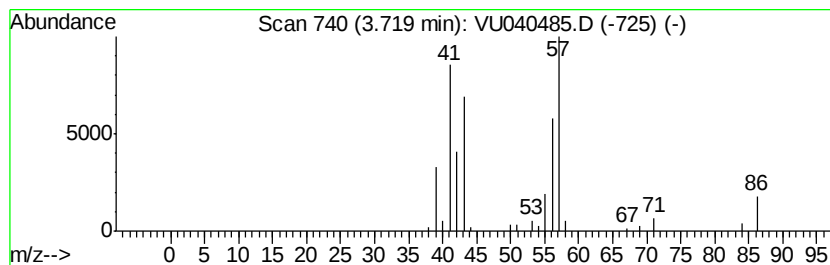
Instrument :
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
3.72	1.32 ug/L	86669	1,4-Difluorobenzene	6.26	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexane	86	C6H14	000110-54-3	90
2	n-Hexane	86	C6H14	000110-54-3	90
3	n-Hexane	86	C6H14	000110-54-3	72
4	Hydroperoxide, hexyl	118	C6H14O2	004312-76-9	50
5	1-Pentene, 4-methyl-	84	C6H12	000691-37-2	45



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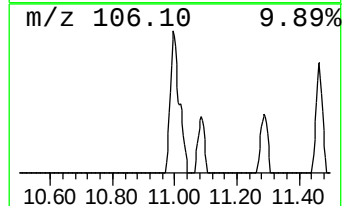
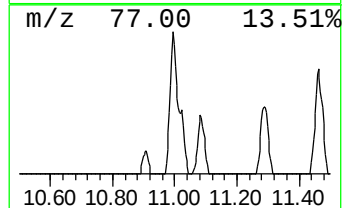
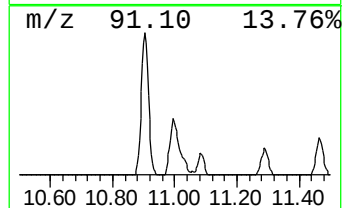
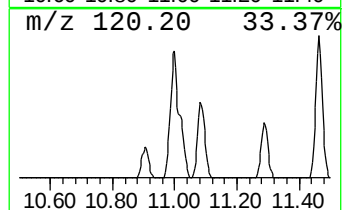
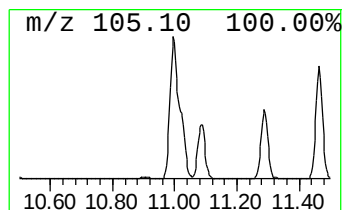
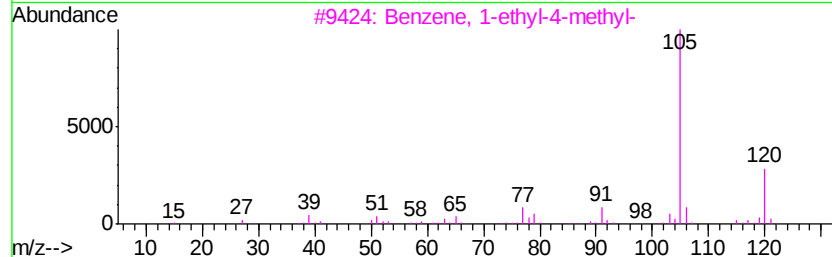
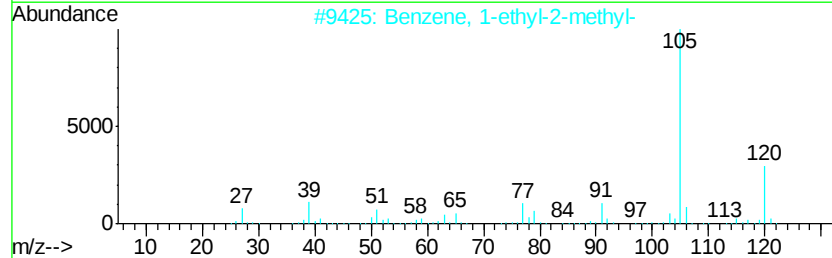
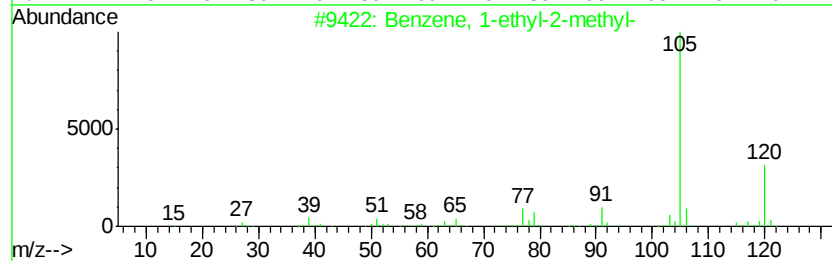
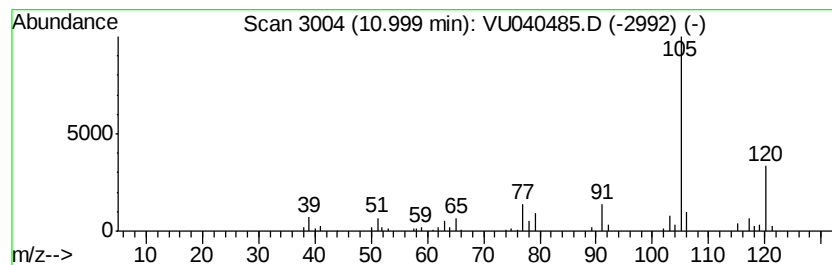
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.00	1.07 ug/L	87890	1,4-Dichlorobenzene-d4	11.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	91
2		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	91
3		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



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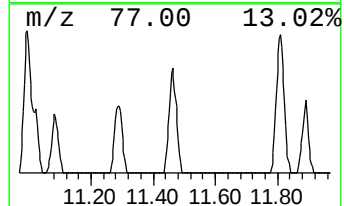
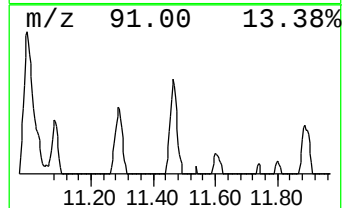
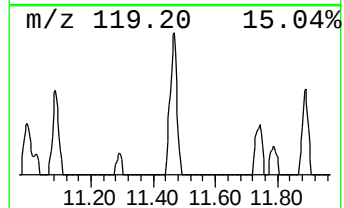
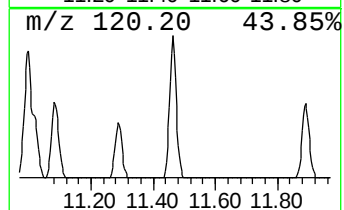
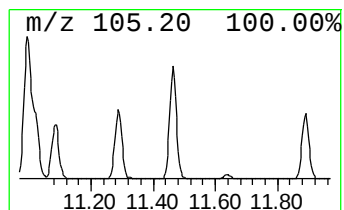
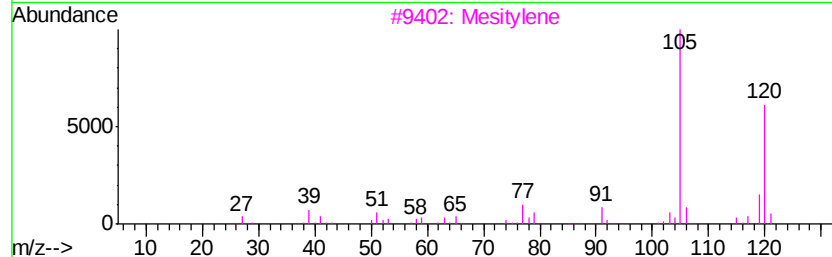
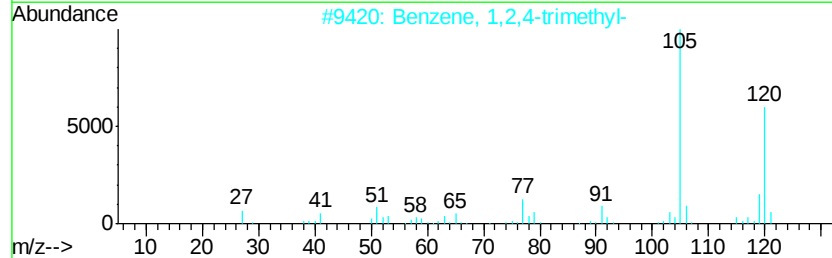
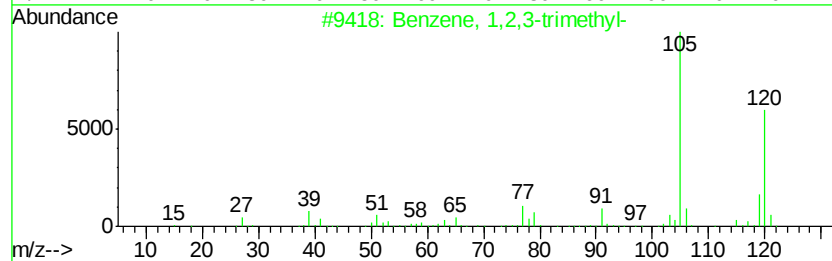
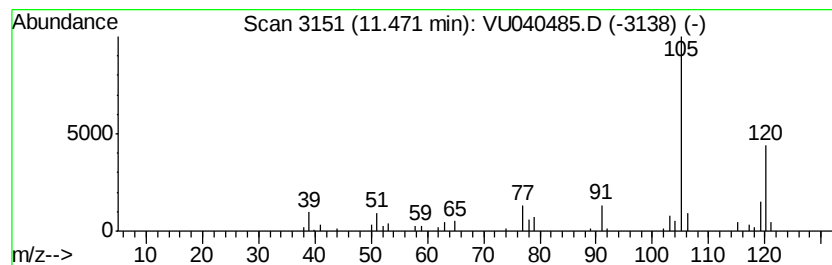
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR092920WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 Benzene, 1,2,3-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.47	0.65 ug/L	53314	1,4-Dichlorobenzene-d4	11.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
2		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
3		Mesitylene	120	C9H12	000108-67-8	91
4		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU100320\
Data File : VU040485.D
Acq On : 03 Oct 2020 17:28
Operator : SY/MD
Sample : L4240-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BG3T4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR092920WMA.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
Sulfur dioxide	1.54	0.8	ug/L	55662	1	6.26	327074	5.0
(DEL) Alkane: Str...	3.38	0.7	ug/L	44737	1	6.26	327074	5.0
(DEL) Alkane: Str...	3.72	1.3	ug/L	86669	1	6.26	327074	5.0
Benzene, 1-ethyl-...	11.00	1.1	ug/L	87890	3	11.81	410939	5.0
Benzene, 1,2,3-tr...	11.47	0.7	ug/L	53314	3	11.81	410939	5.0