

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU111920\
 Data File : VU041348.D
 Acq On : 19 Nov 2020 17:13
 Operator : SY/MD
 Sample : L4790-06DL 100X
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 H4398DL

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\SOMUTR111620WMA.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	1.369	4	9	17	rVB	6778	6955	2.02%	0.209%
2	1.559	51	68	87	rBV3	10443	33554	9.75%	1.009%
3	1.687	99	108	117	rVB2	36141	45070	13.09%	1.355%
4	1.896	165	173	179	rBV3	6426	10149	2.95%	0.305%
5	2.025	206	213	223	rBV	25990	34864	10.13%	1.049%
6	2.115	229	241	253	rBV2	9629	30292	8.80%	0.911%
7	2.687	409	419	437	rVB	51420	88515	25.71%	2.662%
8	2.816	446	459	486	rVB	186897	344275	100.00%	10.354%
9	4.687	1026	1041	1055	rBV3	16188	37974	11.03%	1.142%
10	4.787	1055	1072	1084	rBV	93672	225338	65.45%	6.777%
11	5.182	1182	1195	1212	rVB	59162	128372	37.29%	3.861%
12	5.777	1372	1380	1387	rBV2	3768	5104	1.48%	0.153%
13	5.861	1387	1406	1421	rVV3	110063	285765	83.00%	8.594%
14	5.925	1421	1426	1446	rVB	16224	20964	6.09%	0.630%
15	6.372	1552	1565	1587	rVB	89174	160903	46.74%	4.839%
16	6.796	1681	1697	1714	rBV2	74297	142050	41.26%	4.272%
17	7.636	1947	1958	1972	rBV	33170	57428	16.68%	1.727%
18	7.960	2045	2059	2072	rBV	119732	203219	59.03%	6.112%
19	8.028	2072	2080	2091	rVB	13783	22110	6.42%	0.665%
20	8.231	2133	2143	2157	rVB2	21435	35263	10.24%	1.061%
21	8.684	2263	2284	2314	rBV	160343	316419	91.91%	9.516%
22	8.825	2320	2328	2338	rVB4	2320	3954	1.15%	0.119%
23	8.951	2356	2367	2373	rBV5	2964	5516	1.60%	0.166%
24	9.446	2509	2521	2538	rBV	121491	203210	59.03%	6.111%
25	9.597	2559	2568	2575	rBV3	6364	9631	2.80%	0.290%
26	9.716	2594	2605	2616	rBV2	8820	14863	4.32%	0.447%
27	10.118	2721	2730	2741	rBV3	6265	9847	2.86%	0.296%
28	10.767	2921	2932	2944	rBV	58127	90790	26.37%	2.730%
29	10.896	2963	2972	2984	rVB3	2751	4231	1.23%	0.127%
30	11.812	3246	3257	3270	rVB	110640	174761	50.76%	5.256%
31	12.192	3363	3375	3388	rBV	125298	196879	57.19%	5.921%
32	12.324	3408	3416	3425	rVB5	3910	5431	1.58%	0.163%
33	12.767	3546	3554	3564	rVB2	4173	6807	1.98%	0.205%
34	12.954	3598	3612	3619	rBV9	6191	12170	3.53%	0.366%

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 Title : TRACE VOA SOM01.0

35	12.999	3619	3626	3632	rVV2	4907	7004	2.03%	0.211%
36	13.041	3632	3639	3648	rVB5	7499	10848	3.15%	0.326%
37	13.124	3657	3665	3678	rVB4	8185	11841	3.44%	0.356%
38	13.423	3745	3758	3764	rBV2	10715	16892	4.91%	0.508%
39	13.578	3794	3806	3812	rVV4	7421	13231	3.84%	0.398%
40	13.616	3812	3818	3824	rVV7	6280	9670	2.81%	0.291%
41	13.668	3828	3834	3841	rVB6	4346	6879	2.00%	0.207%
42	13.716	3841	3849	3856	rBV5	2965	4164	1.21%	0.125%
43	13.799	3865	3875	3883	rBV4	3504	5077	1.47%	0.153%
44	13.970	3919	3928	3929	rBV4	12250	14298	4.15%	0.430%
45	14.037	3942	3949	3956	rVV2	11176	14804	4.30%	0.445%
46	14.082	3956	3963	3970	rVV3	13688	17612	5.12%	0.530%
47	14.166	3981	3989	4008	rVB4	18712	35426	10.29%	1.065%
48	14.439	4066	4074	4081	rBV2	10519	14480	4.21%	0.435%
49	14.565	4105	4113	4121	rBV7	6530	10394	3.02%	0.313%
50	14.661	4138	4143	4153	rVB7	4266	6264	1.82%	0.188%
51	14.790	4176	4183	4191	rBV10	4193	6016	1.75%	0.181%
52	14.928	4217	4226	4231	rBV6	8700	13271	3.85%	0.399%
53	14.960	4231	4236	4243	rVV5	6729	9083	2.64%	0.273%
54	15.008	4244	4251	4258	rVV7	10134	15019	4.36%	0.452%
55	15.053	4258	4265	4276	rVB10	6025	9172	2.66%	0.276%
56	15.131	4284	4289	4300	rVB6	7127	10298	2.99%	0.310%
57	15.192	4300	4308	4322	rVV6	7636	18197	5.29%	0.547%
58	15.259	4322	4329	4339	rVB7	5080	7595	2.21%	0.228%
59	15.394	4362	4371	4381	rBV4	7488	13026	3.78%	0.392%
60	15.494	4394	4402	4411	rVB8	5608	9706	2.82%	0.292%
61	15.590	4424	4432	4436	rBV8	2949	4426	1.29%	0.133%
62	15.745	4475	4480	4491	rVB8	2067	3535	1.03%	0.106%
63	15.918	4523	4534	4545	rBV9	7492	19309	5.61%	0.581%
64	16.249	4629	4637	4641	rBV7	6598	9072	2.64%	0.273%
65	16.394	4675	4682	4689	rBV6	4149	5806	1.69%	0.175%

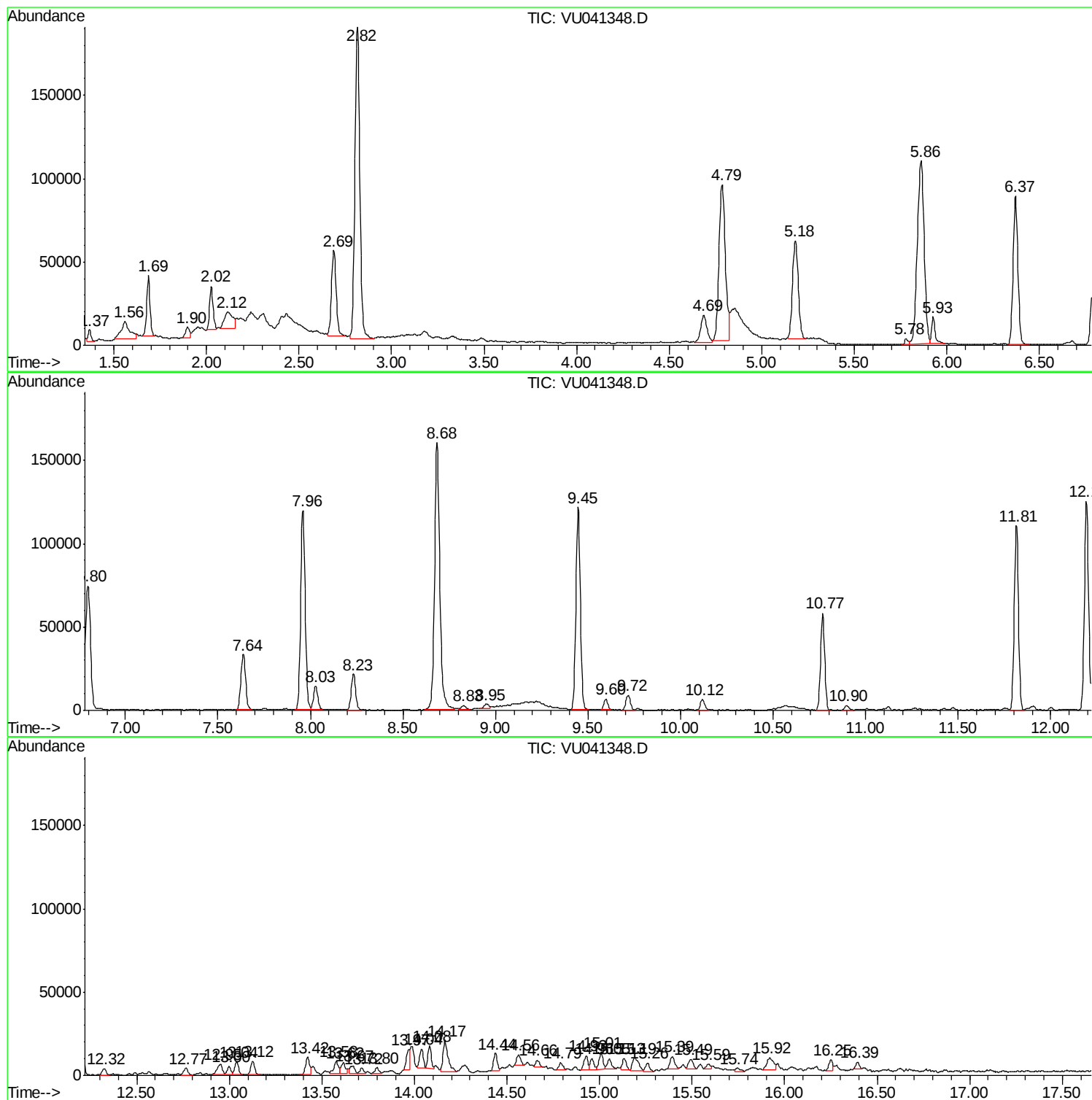
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ClientSampled :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR111620WMA.M
Quant Title : TRACE VOA SOM01.0

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



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ClientSampleId :
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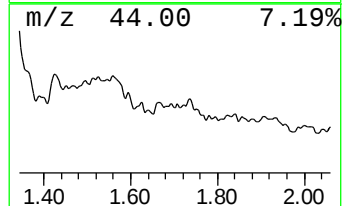
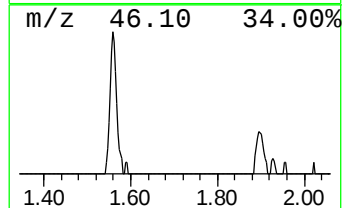
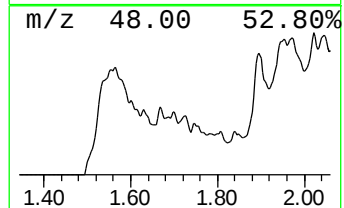
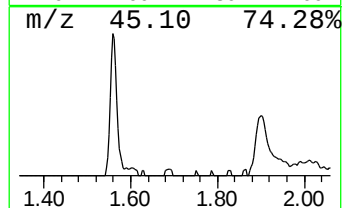
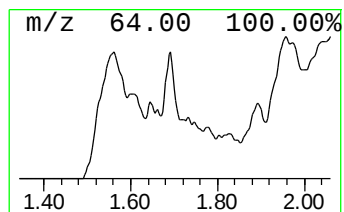
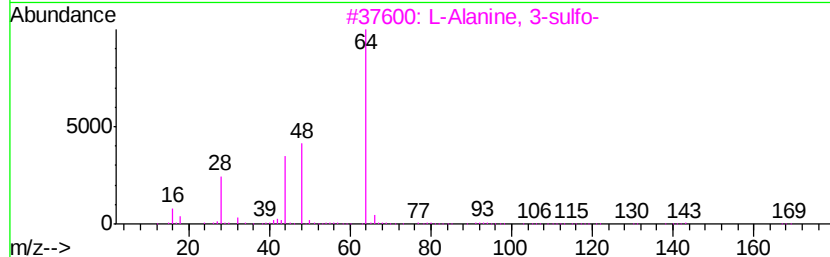
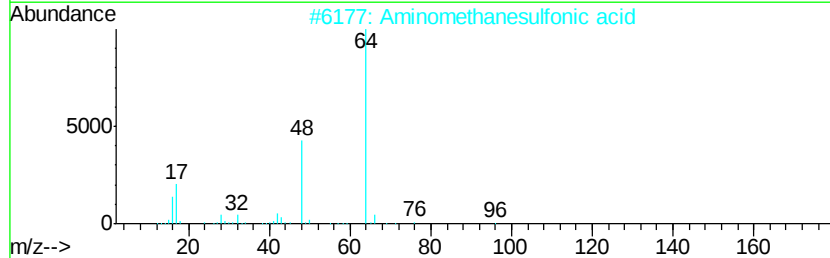
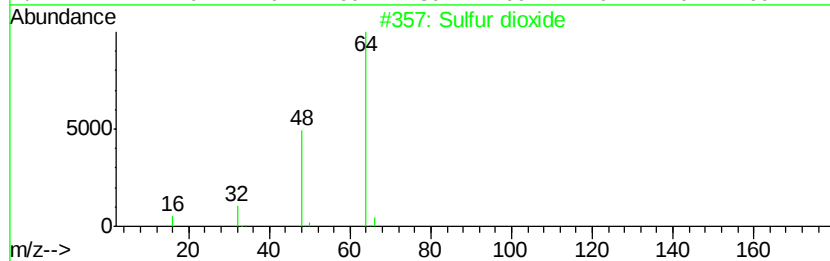
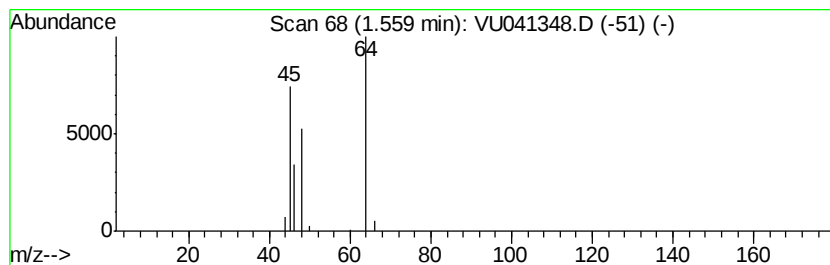
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR111620WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.56	1.04 ug/L	33554	1,4-Difluorobenzene	6.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfur dioxide	64	O2S	007446-09-5	45
2		Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
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	7



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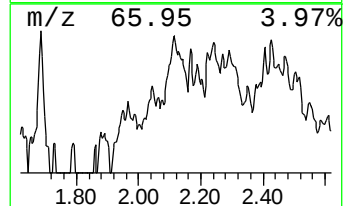
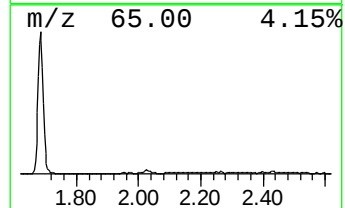
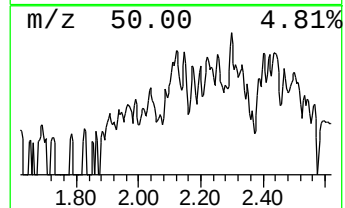
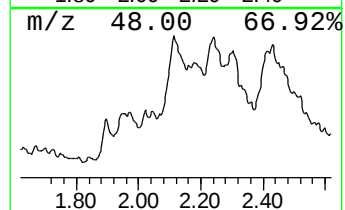
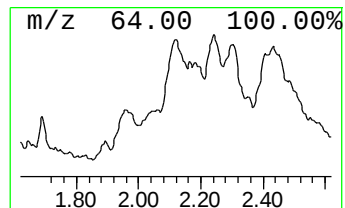
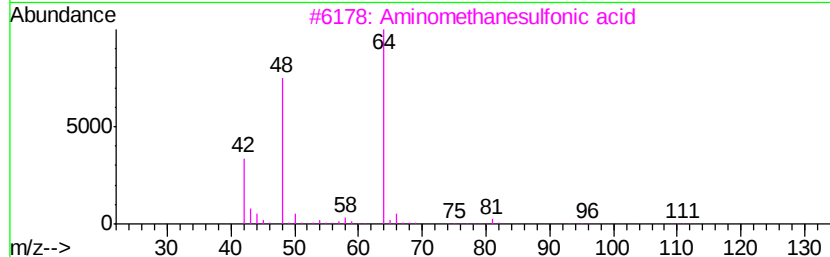
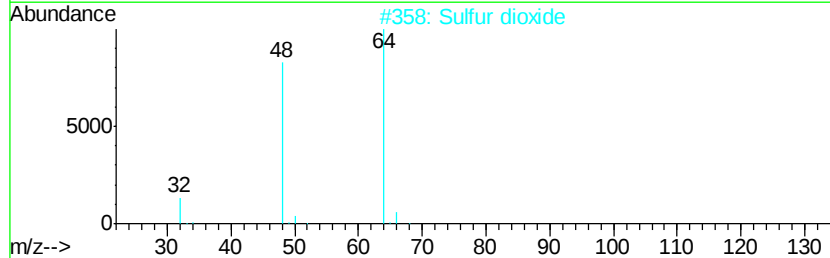
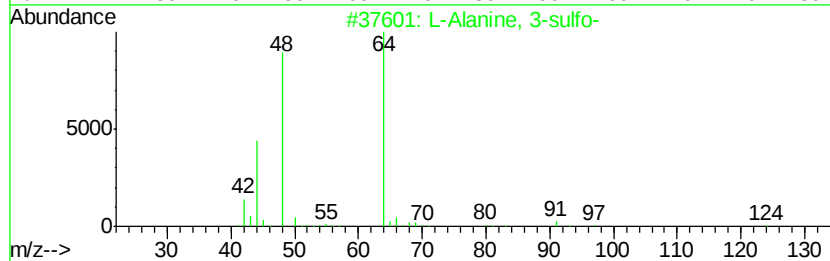
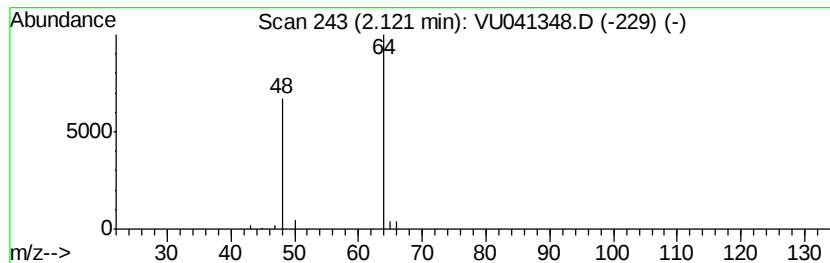
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR111620WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 L-Alanine, 3-sulfo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	0.94 ug/L	30292	1,4-Difluorobenzene	6.37

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		L-Alanine, 3-sulfo-	169	C3H7N05S	000498-40-8	74
2		Sulfur dioxide	64	O2S	007446-09-5	74
3		Aminomethanesulfonic acid	111	CH5N03S	013881-91-9	64
4		Aminomethanesulfonic acid	111	CH5N03S	013881-91-9	9
5		Sulfur dioxide	64	O2S	007446-09-5	7



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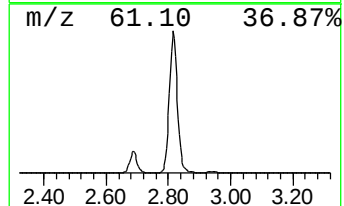
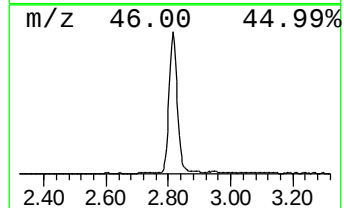
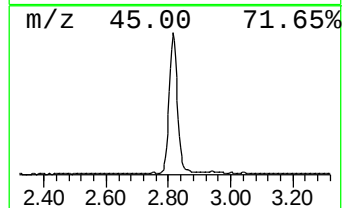
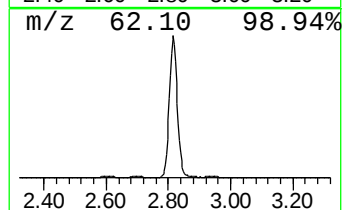
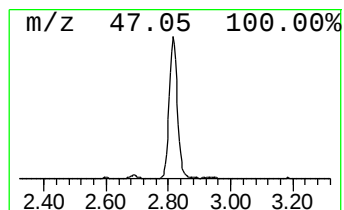
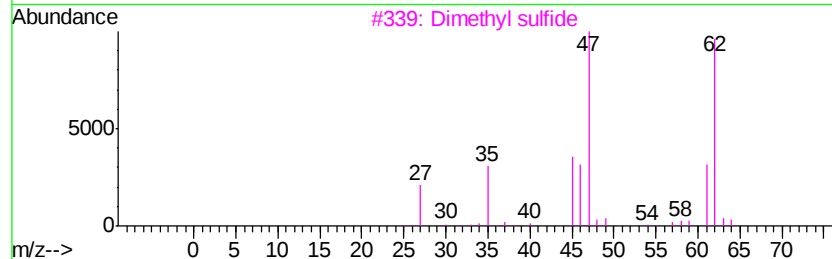
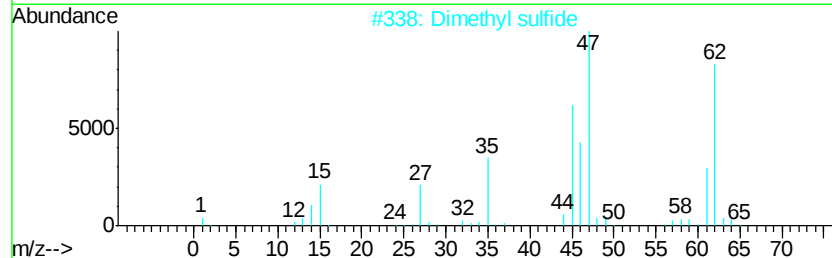
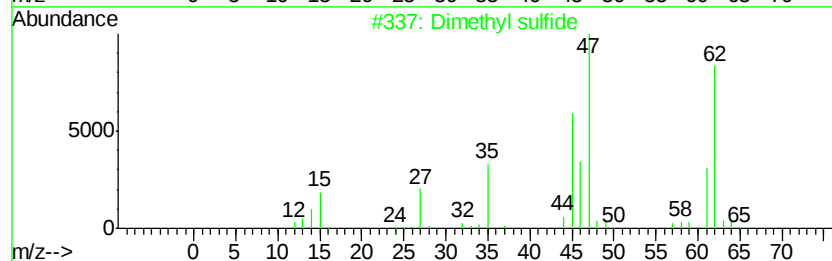
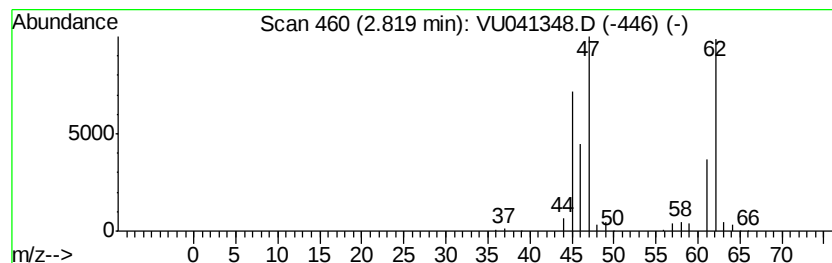
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 Dimethyl sulfide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.82	10.70 ug/L	344275	1,4-Difluorobenzene	6.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dimethyl sulfide	62	C2H6S	000075-18-3	94
2		Dimethyl sulfide	62	C2H6S	000075-18-3	94
3		Dimethyl sulfide	62	C2H6S	000075-18-3	91
4		Dimethyl sulfide	62	C2H6S	000075-18-3	91
5		Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	83



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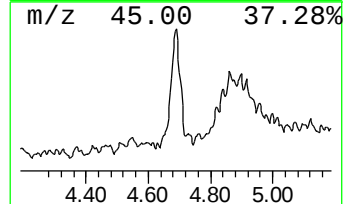
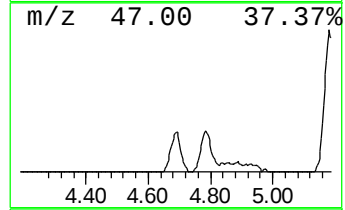
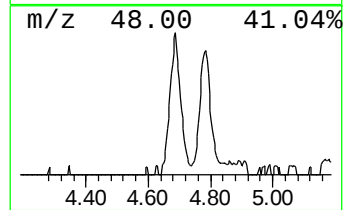
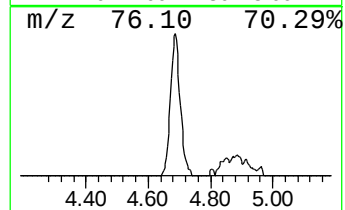
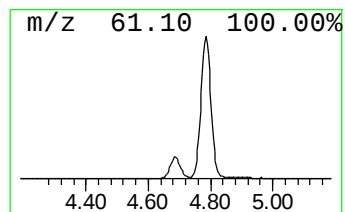
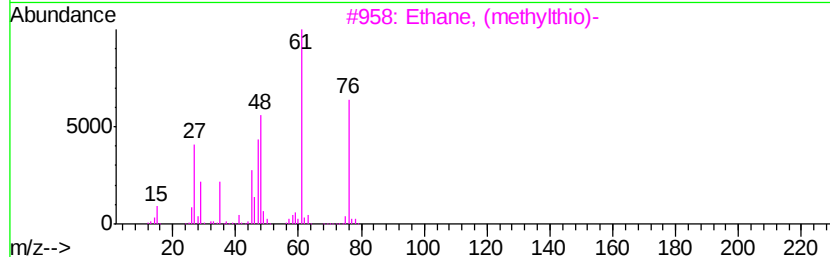
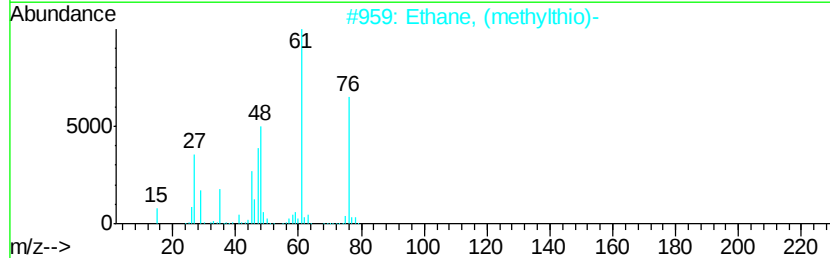
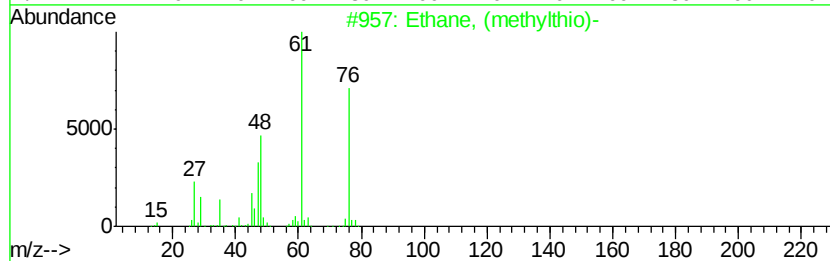
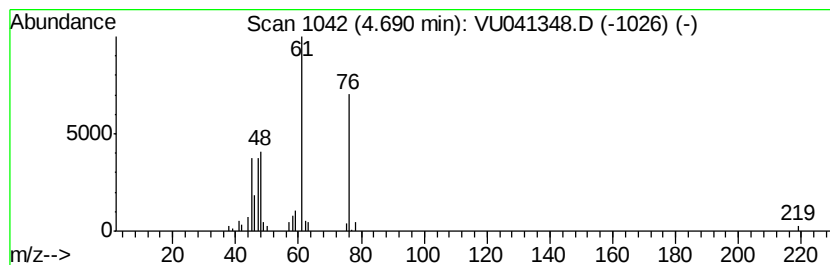
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR111620WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 Ethane, (methylthio)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.69	1.18 ug/L	37974	1,4-Difluorobenzene	6.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethane, (methylthio)-	76	C3H8S	000624-89-5	91
2		Ethane, (methylthio)-	76	C3H8S	000624-89-5	91
3		Ethane, (methylthio)-	76	C3H8S	000624-89-5	91
4		Trimethylphosphine	76	C3H9P	000594-09-2	59
5		3-(Methylthio)propyl 2,2,2-trifl...	202	C6H9F3O2S	1000367-07-4	53



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ClientSampleId :
H4398DL

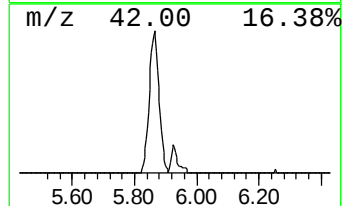
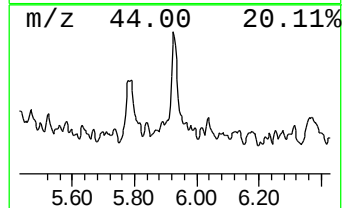
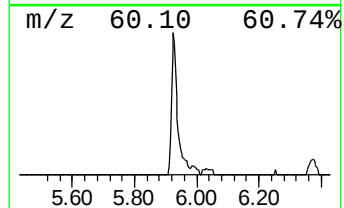
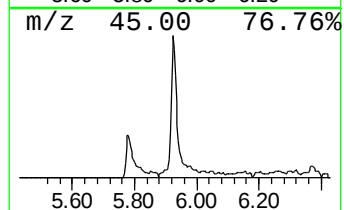
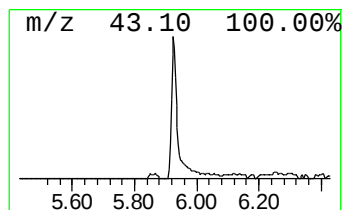
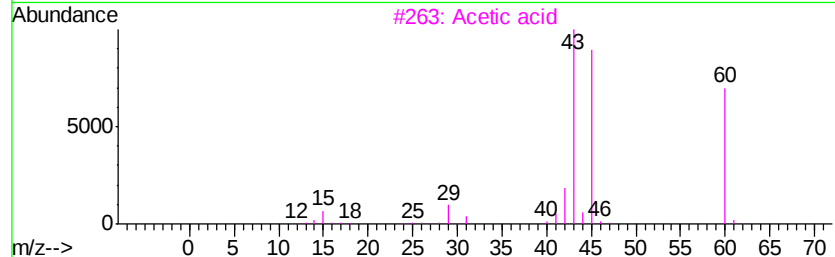
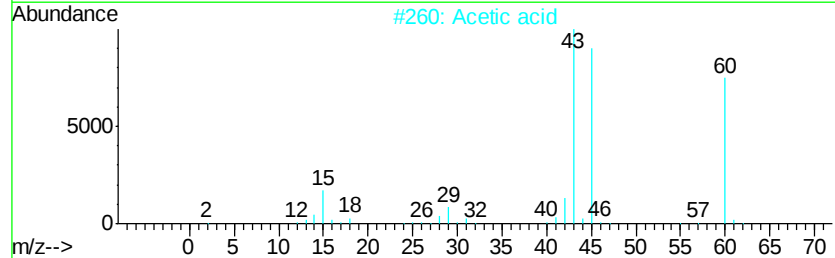
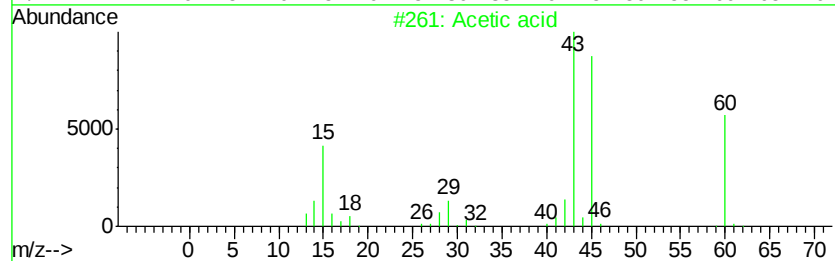
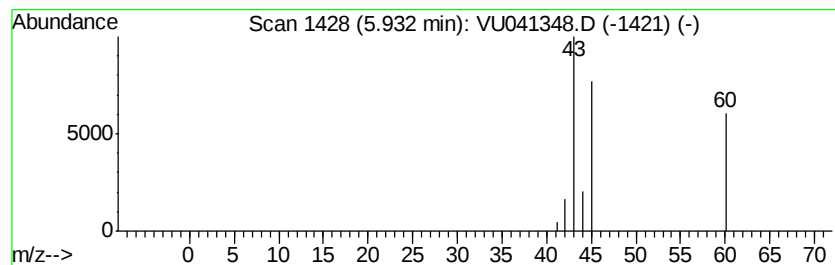
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 Acetic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.93	0.65 ug/L	20964	1,4-Difluorobenzene	6.37

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid			60	C2H4O2	000064-19-7	83
2	Acetic acid			60	C2H4O2	000064-19-7	83
3	Acetic acid			60	C2H4O2	000064-19-7	83
4	Acetic acid			60	C2H4O2	000064-19-7	83
5	Formic acid hydrazide			60	CH4N2O	000624-84-0	9



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU111920\
Data File : VU041348.D
Acq On : 19 Nov 2020 17:13
Operator : SY/MD
Sample : L4790-06DL 100X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
H4398DL

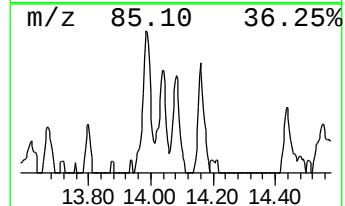
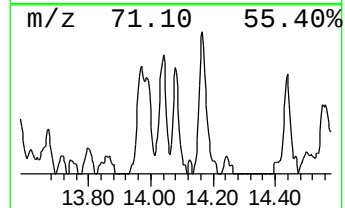
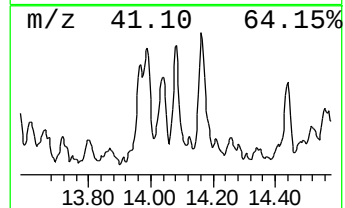
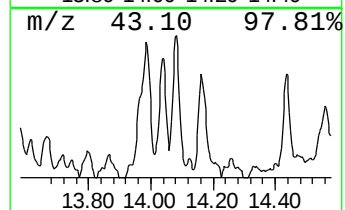
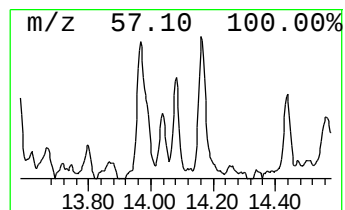
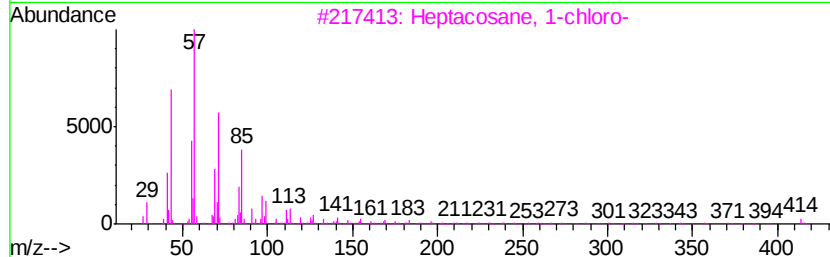
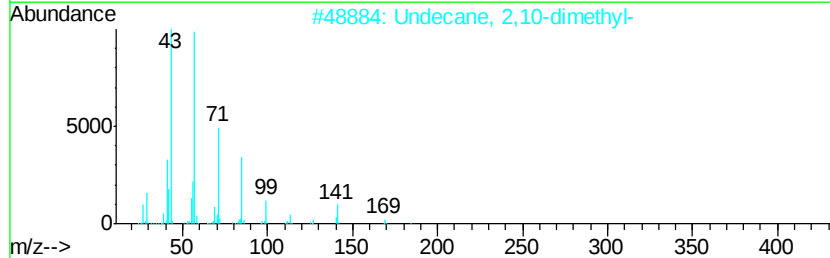
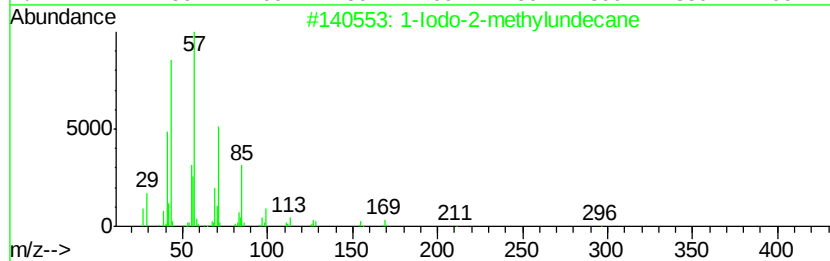
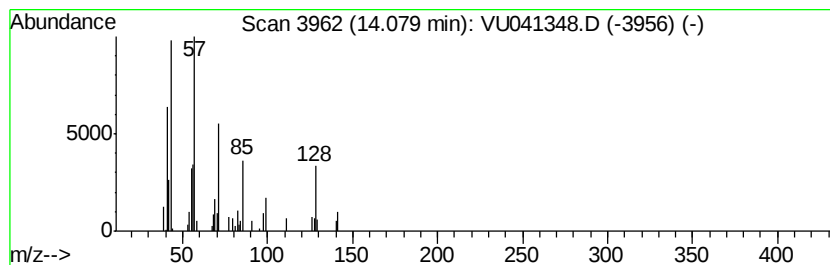
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 1-Iodo-2-methylundecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.08	0.50 ug/L	17612	1,4-Dichlorobenzene-d4	11.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	59
2			Undecane, 2,10-dimethyl-	184	C13H28	017301-27-8	59
3			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	50
4			Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	50
5			Dotriacontane	451	C32H66	000544-85-4	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU111920\
Data File : VU041348.D
Acq On : 19 Nov 2020 17:13
Operator : SY/MD
Sample : L4790-06DL 100X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
H4398DL

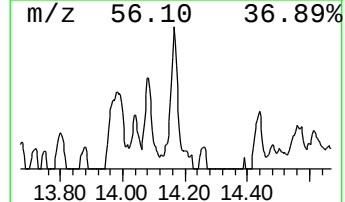
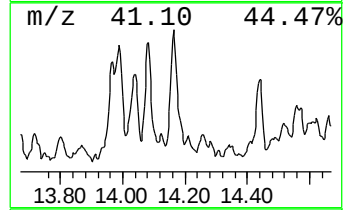
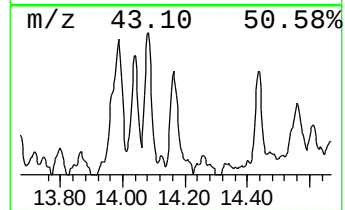
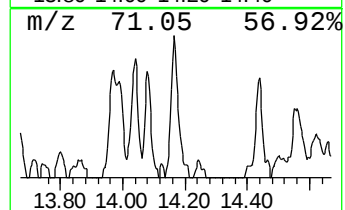
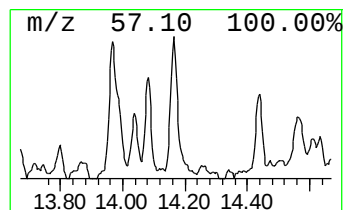
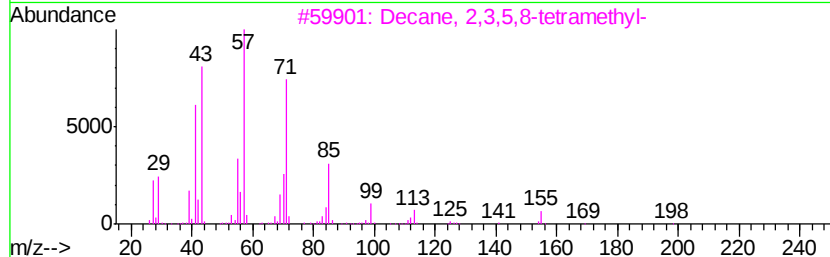
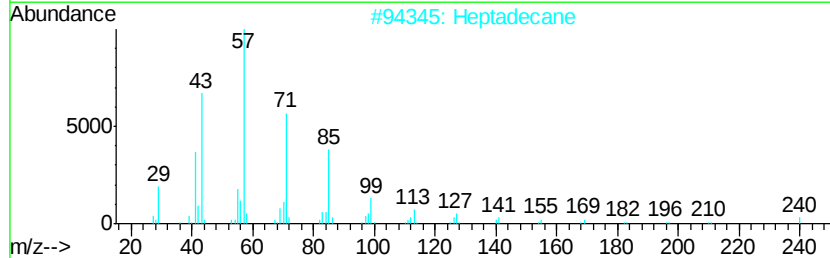
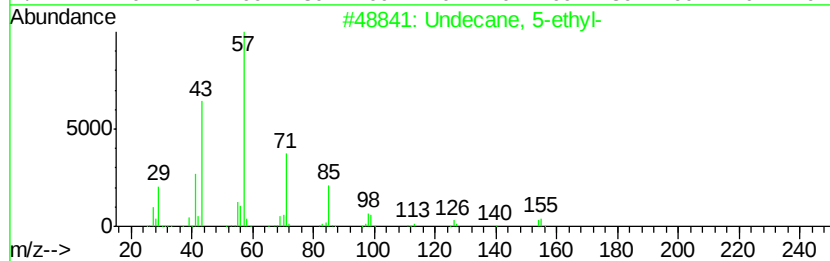
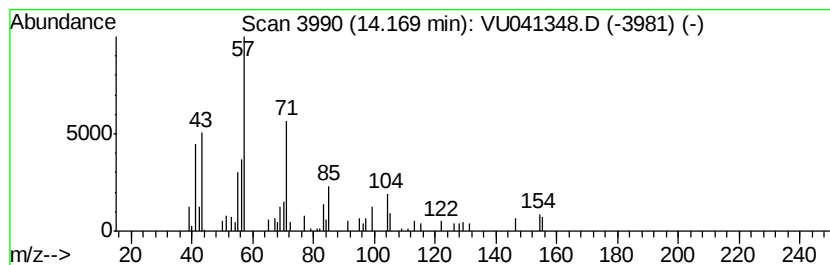
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.17	1.01 ug/L	35426	1,4-Dichlorobenzene-d4	11.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Undecane, 5-ethyl-	184	C13H28	017453-94-0	59
2		Heptadecane	240	C17H36	000629-78-7	53
3		Decane, 2,3,5,8-tetramethyl-	198	C14H30	192823-15-7	52
4		Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	50
5		Tridecane, 6-methyl-	198	C14H30	013287-21-3	50



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU111920\
Data File : VU041348.D
Acq On : 19 Nov 2020 17:13
Operator : SY/MD
Sample : L4790-06DL 100X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
H4398DL

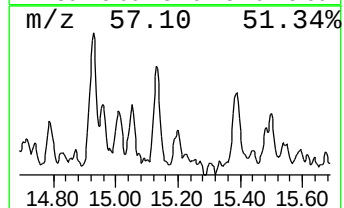
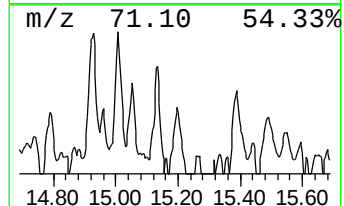
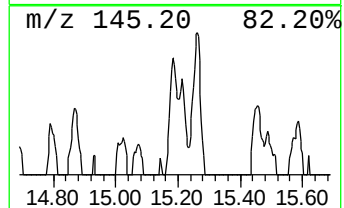
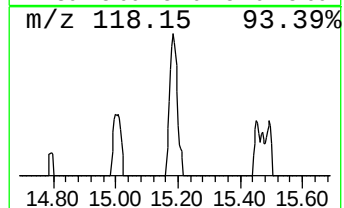
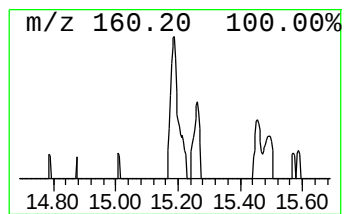
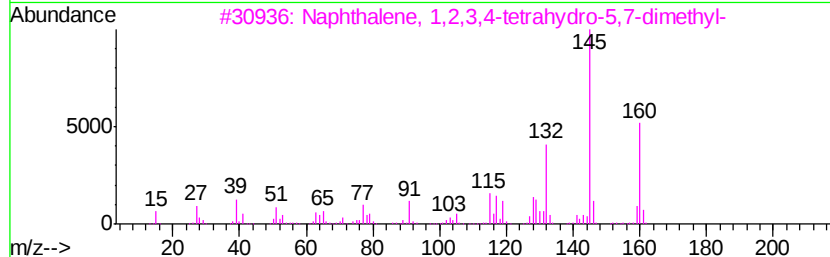
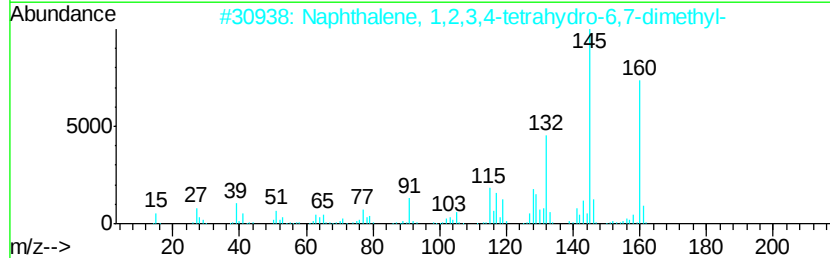
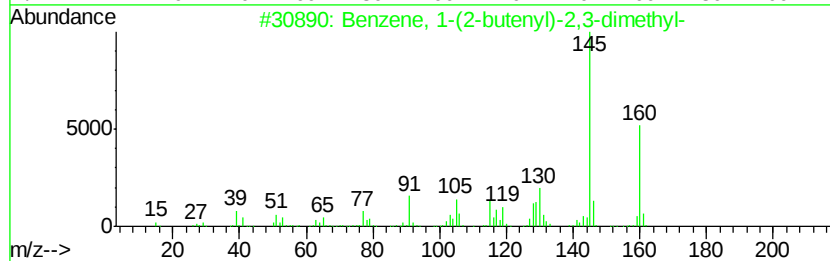
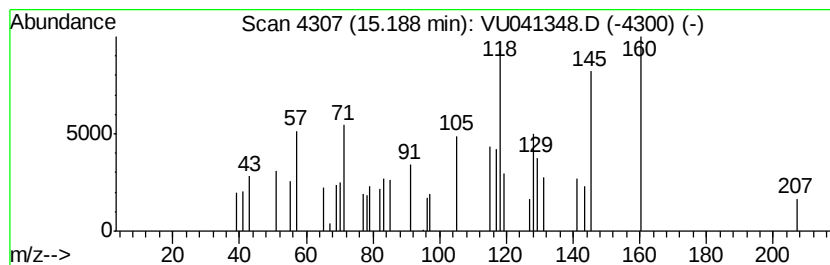
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 9 unknown-02 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.19	0.52 ug/L	18197	1,4-Dichlorobenzene-d4	11.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	35
2		Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	001076-61-5	35
3		Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021693-54-9	35
4		1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	27
5		Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	27



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU111920\
Data File : VU041348.D
Acq On : 19 Nov 2020 17:13
Operator : SY/MD
Sample : L4790-06DL 100X
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 36 Sample Multiplier: 1

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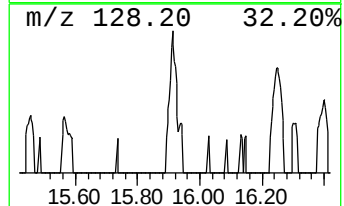
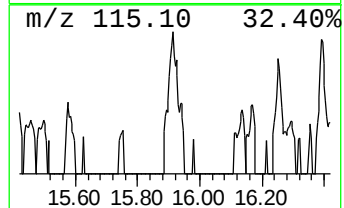
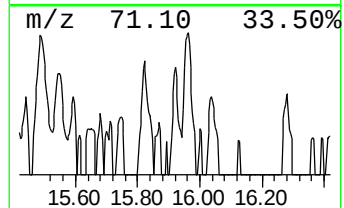
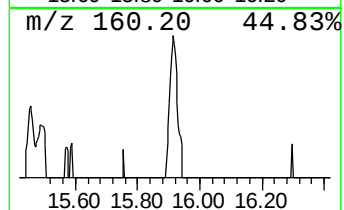
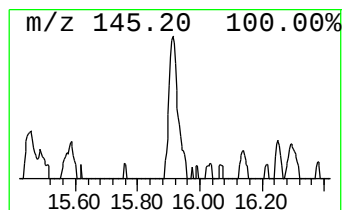
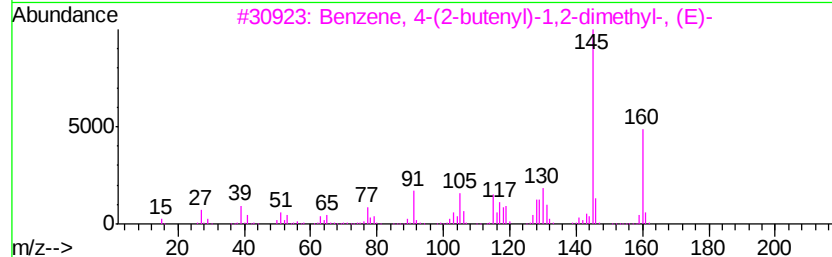
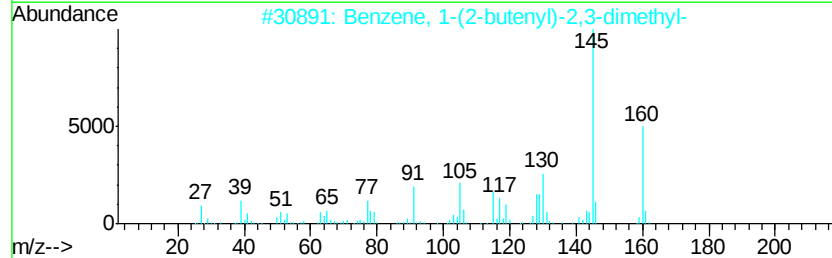
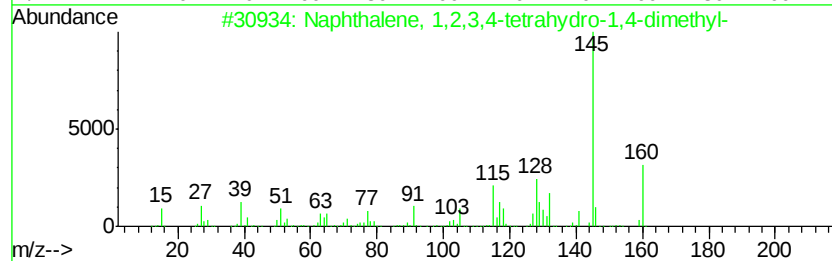
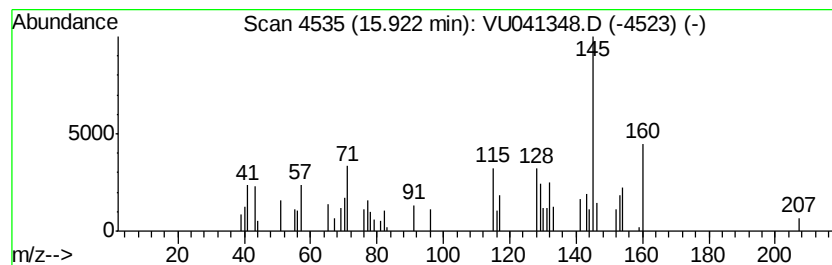
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 10 Naphthalene, 1,2,3,4-tetra... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.92	0.55 ug/L	19309	1,4-Dichlorobenzene-d4	11.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	93
2		Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	70
3		Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	58
4		Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	001076-61-5	58
5		Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	58



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU111920\
Data File : VU041348.D
Acq On : 19 Nov 2020 17:13
Operator : SY/MD
Sample : L4790-06DL 100X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
H4398DL

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR111620WMA.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	1.56	1.0	ug/L	33554	1	6.37	160903	5.0
L-Alanine, 3-sulfo-	2.12	0.9	ug/L	30292	1	6.37	160903	5.0
Dimethyl sulfide	2.82	10.7	ug/L	344275	1	6.37	160903	5.0
Ethane, (methylth...	4.69	1.2	ug/L	37974	1	6.37	160903	5.0
Acetic acid	5.93	0.7	ug/L	20964	1	6.37	160903	5.0
1-Iodo-2-methylun...	14.08	0.5	ug/L	17612	3	11.82	174761	5.0
(DEL) Alkane: Str...	14.17	1.0	ug/L	35426	3	11.82	174761	5.0
unknown-02	15.19	0.5	ug/L	18197	3	11.82	174761	5.0
Naphthalene, 1,2,...	15.92	0.6	ug/L	19309	3	11.82	174761	5.0