

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
 Data File : VU042117.D
 Acq On : 20 Jan 2021 19:48
 Operator : SY/MD
 Sample : M1180-02
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F1E04

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\SOMUTR012021WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC: VU042117.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.363	3	7	17	rVB2	8835	10183	1.87%	0.180%
2	1.488	41	46	52	rBV2	5730	5639	1.04%	0.099%
3	1.601	70	81	90	rBV2	59559	88220	16.24%	1.556%
4	1.919	171	180	192	rVB	43178	56103	10.33%	0.989%
5	2.083	221	231	251	rBV2	11234	34536	6.36%	0.609%
6	2.366	304	319	327	rBV2	12373	28748	5.29%	0.507%
7	2.568	372	382	396	rVB	82721	131396	24.19%	2.317%
8	3.388	620	637	644	rBV5	5259	15641	2.88%	0.276%
9	4.472	956	974	991	rBV5	6347	20450	3.76%	0.361%
10	4.723	1022	1052	1097	rBV2	23101	166442	30.64%	2.935%
11	5.073	1148	1161	1180	rVB	82968	185367	34.13%	3.269%
12	5.732	1344	1366	1391	rBV2	173398	434467	79.99%	7.662%
13	6.256	1516	1529	1548	rVB	150205	283824	52.25%	5.005%
14	6.645	1642	1650	1655	rBV3	5256	8541	1.57%	0.151%
15	6.700	1655	1667	1694	rVB2	103795	208251	38.34%	3.672%
16	7.182	1796	1817	1835	rBV	87409	185288	34.11%	3.267%
17	7.575	1923	1939	1958	rBV	62927	111537	20.53%	1.967%
18	7.819	2000	2015	2018	rBV3	4143	8225	1.51%	0.145%
19	7.858	2018	2027	2030	rVV2	8777	15862	2.92%	0.280%
20	7.906	2030	2042	2058	rVV	209331	374960	69.03%	6.612%
21	7.970	2059	2062	2076	rVV5	3181	7356	1.35%	0.130%
22	8.047	2077	2086	2097	rVB	7727	14532	2.68%	0.256%
23	8.189	2118	2130	2150	rBV	40196	69481	12.79%	1.225%
24	8.501	2215	2227	2240	rBV	14226	25975	4.78%	0.458%
25	8.562	2240	2246	2255	rVB6	4341	6347	1.17%	0.112%
26	8.652	2260	2274	2287	rBV	240446	469978	86.53%	8.288%
27	8.796	2313	2319	2333	rVB3	4179	7613	1.40%	0.134%
28	9.423	2501	2514	2549	rVB	206208	362789	66.79%	6.398%
29	9.616	2554	2574	2576	rBV4	6864	11203	2.06%	0.198%
30	9.649	2576	2584	2594	rVB	29205	45940	8.46%	0.810%
31	9.774	2611	2623	2624	rBV2	6580	7320	1.35%	0.129%
32	9.928	2661	2671	2682	rBV2	12027	20092	3.70%	0.354%
33	10.118	2720	2730	2733	rBV7	3680	6804	1.25%	0.120%
34	10.247	2756	2770	2783	rBV4	5649	12129	2.23%	0.214%
35	10.356	2796	2804	2823	rVB7	3441	9408	1.73%	0.166%
36	10.655	2882	2897	2902	rVV3	5669	9435	1.74%	0.166%

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37	10.693	2902	2909	2920	rVV3	13072	21708	4.00%	0.383%
38	10.764	2920	2931	2945	rVV	81808	131625	24.23%	2.321%
39	10.896	2956	2972	2981	rBV9	5214	10987	2.02%	0.194%
40	10.973	2984	2996	3010	rBV	16472	29896	5.50%	0.527%
41	11.063	3015	3024	3037	rVB3	6556	11114	2.05%	0.196%
42	11.298	3084	3097	3106	rVB9	3813	9014	1.66%	0.159%
43	11.481	3145	3154	3163	rVB7	5436	8563	1.58%	0.151%
44	11.584	3178	3186	3196	rBV6	3503	6480	1.19%	0.114%
45	11.697	3214	3221	3231	rVB6	4213	7095	1.31%	0.125%
46	11.819	3247	3259	3276	rVV	223754	359537	66.19%	6.340%
47	11.902	3276	3285	3291	rBV5	3984	5796	1.07%	0.102%
48	11.986	3305	3311	3325	rVB4	6075	9728	1.79%	0.172%
49	12.073	3326	3338	3358	rBV	64423	134633	24.79%	2.374%
50	12.201	3366	3378	3393	rVB	206285	339476	62.50%	5.986%
51	12.333	3406	3419	3429	rBV	13777	23200	4.27%	0.409%
52	12.523	3468	3478	3480	rBV4	4899	7274	1.34%	0.128%
53	12.783	3550	3559	3569	rBV7	4764	8013	1.48%	0.141%
54	12.896	3586	3594	3604	rVB7	4711	7342	1.35%	0.129%
55	12.957	3604	3613	3623	rBV2	8130	12551	2.31%	0.221%
56	13.012	3623	3630	3637	rBV4	3780	5564	1.02%	0.098%
57	13.153	3660	3674	3683	rVB3	4402	10296	1.90%	0.182%
58	13.218	3684	3694	3709	rBV8	3900	7297	1.34%	0.129%
59	14.201	3985	4000	4014	rBV	116861	176892	32.57%	3.119%
60	14.327	4030	4039	4051	rVB2	11963	18744	3.45%	0.331%
61	15.008	4240	4251	4259	rBV6	10420	19701	3.63%	0.347%
62	15.111	4274	4283	4299	rBV2	6531	12364	2.28%	0.218%
63	15.301	4334	4342	4350	rBV4	5512	7333	1.35%	0.129%
64	15.462	4383	4392	4403	rBV2	8599	13235	2.44%	0.233%
65	15.558	4413	4422	4427	rBV6	7658	10472	1.93%	0.185%
66	15.594	4427	4433	4443	rVB3	8941	13534	2.49%	0.239%
67	15.648	4443	4450	4456	rBV6	4734	6158	1.13%	0.109%
68	15.703	4457	4467	4480	rVB4	17232	30192	5.56%	0.532%
69	16.143	4593	4604	4613	rBV2	39148	58441	10.76%	1.031%
70	16.282	4638	4647	4654	rBV5	4932	8075	1.49%	0.142%
71	16.359	4662	4671	4686	rVB7	4373	7689	1.42%	0.136%
72	16.780	4791	4802	4813	rBV2	75504	117453	21.62%	2.071%
73	16.896	4827	4838	4856	rBV	364745	543162	100.00%	9.578%

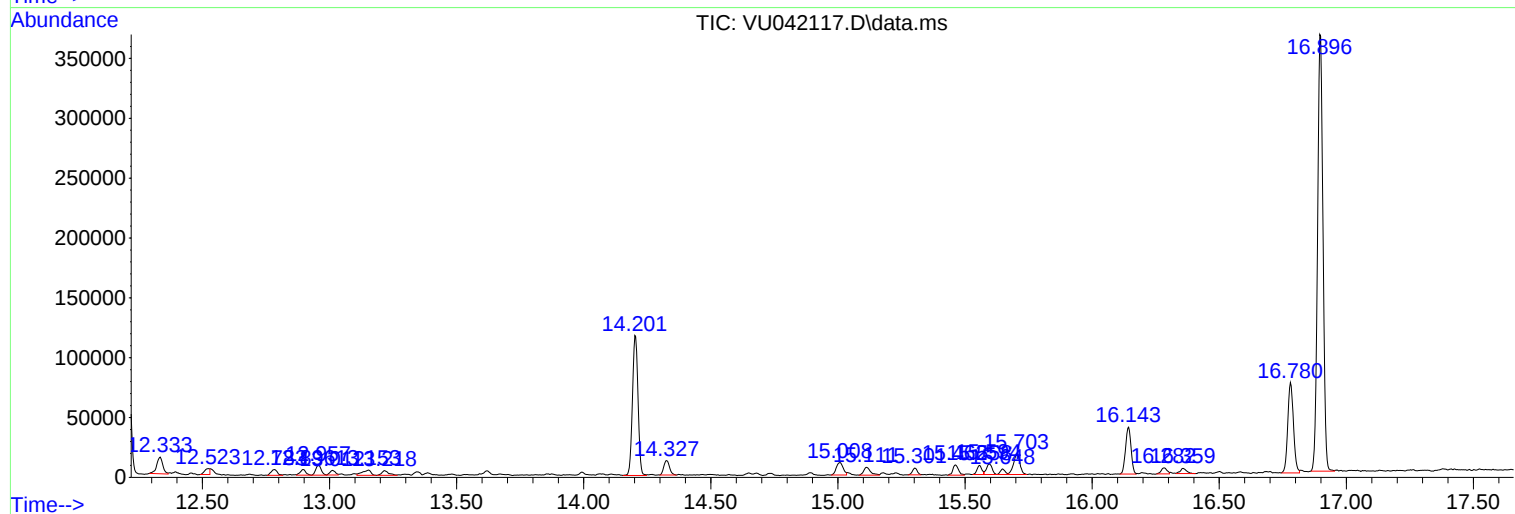
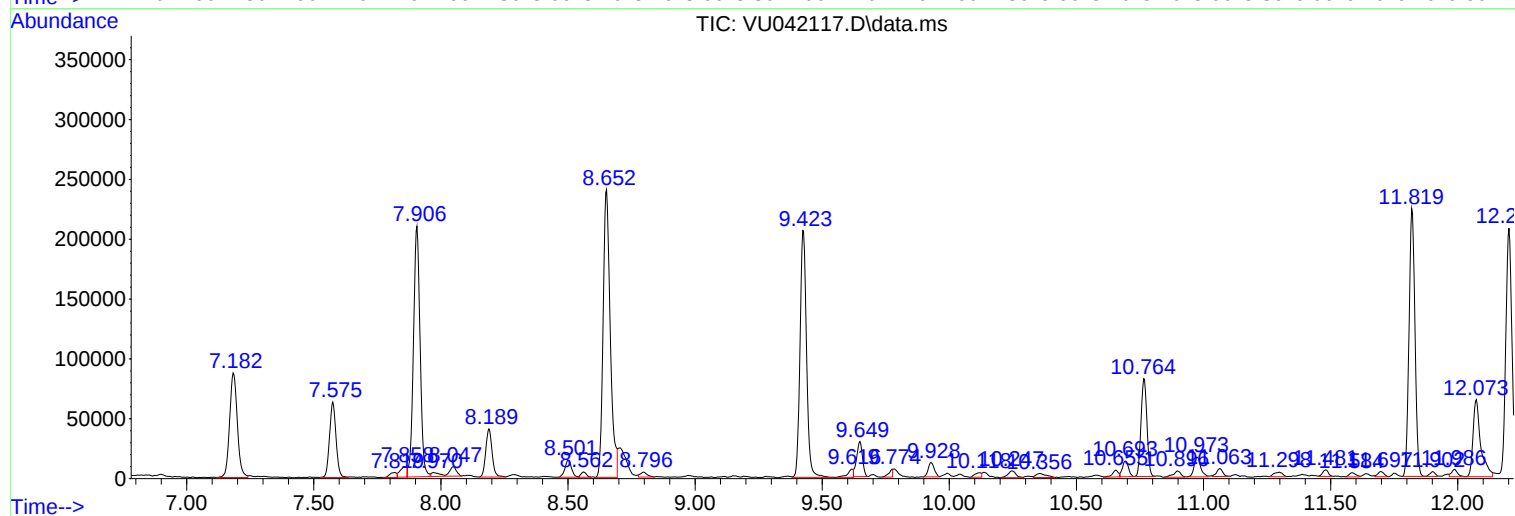
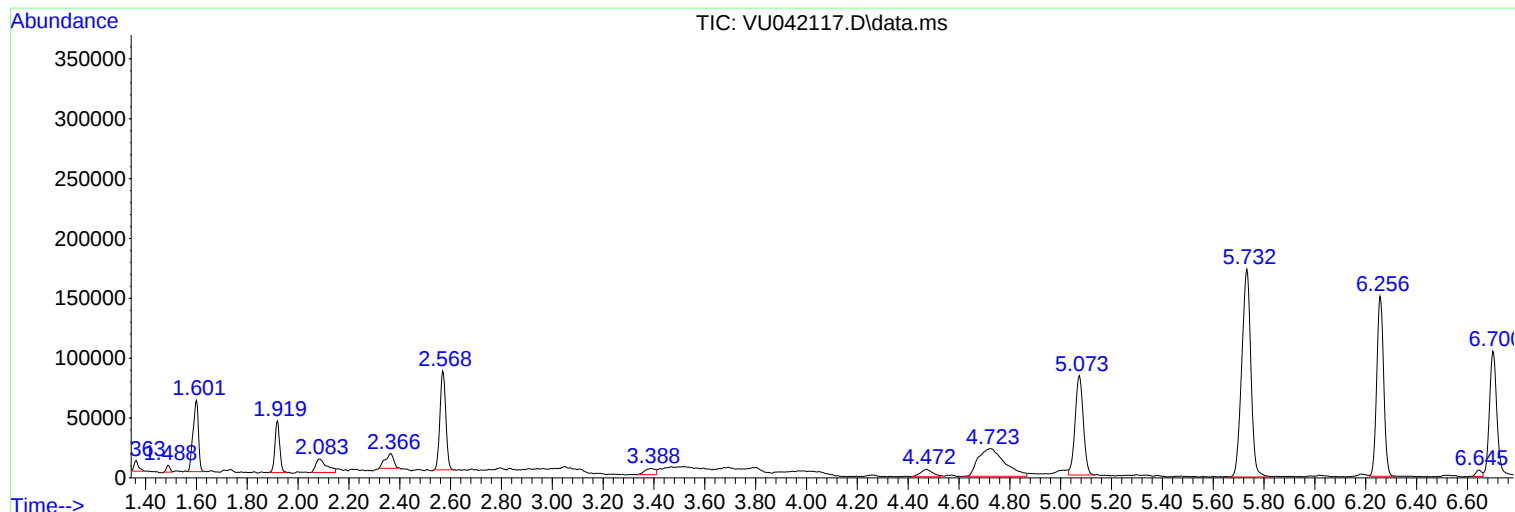
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ClientSampleId :
F1E04

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F1E04

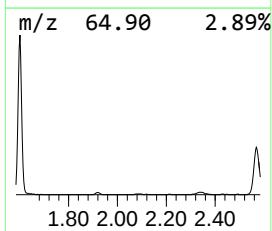
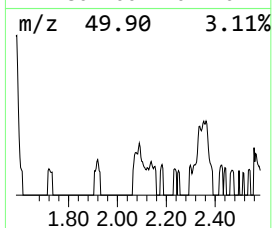
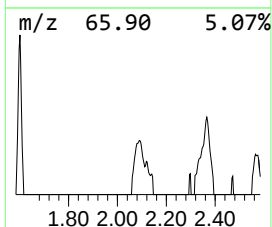
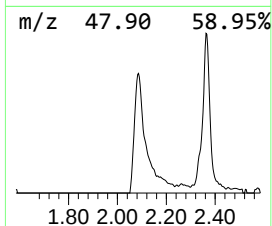
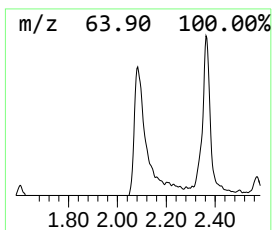
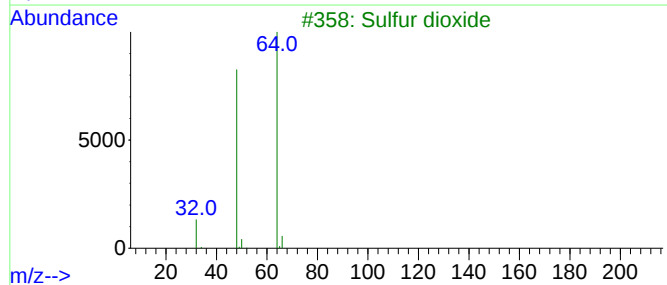
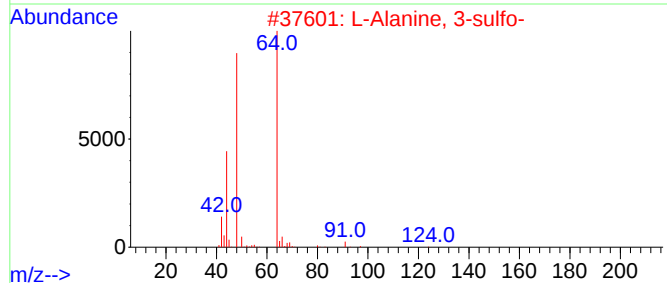
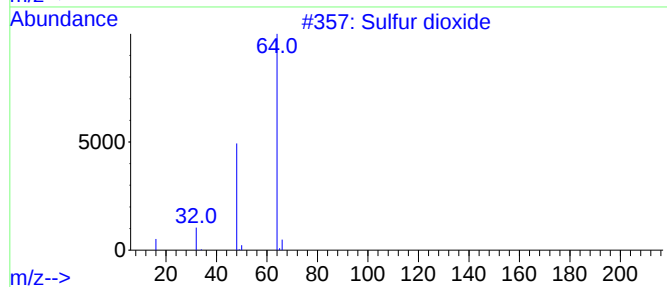
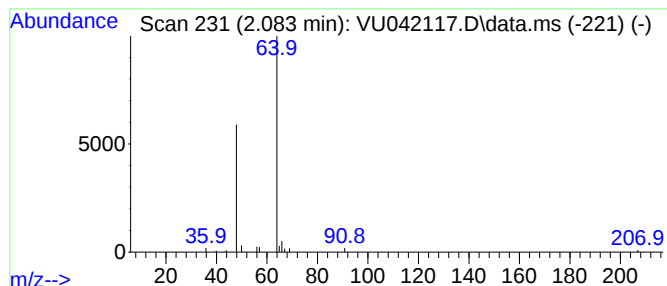
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.083	0.61 ug/L	34536	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
2			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	74
3			Sulfur dioxide	64	O2S	007446-09-5	74
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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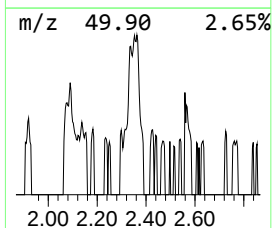
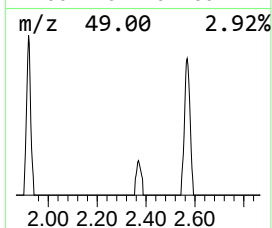
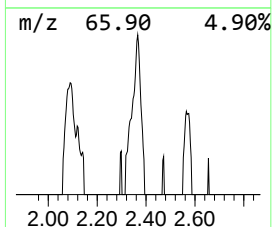
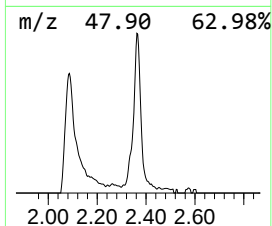
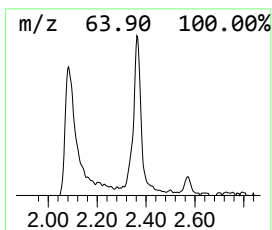
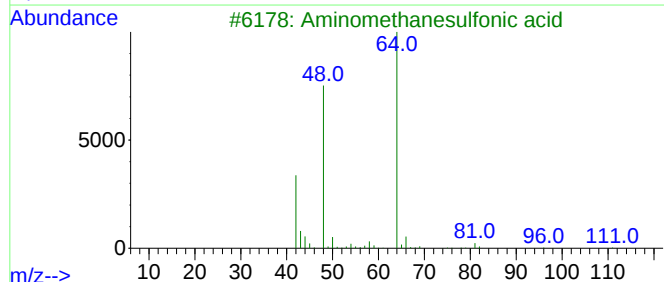
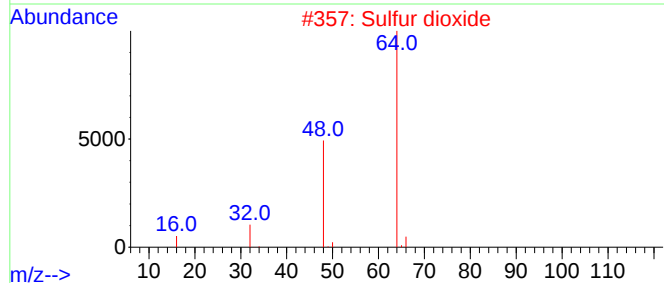
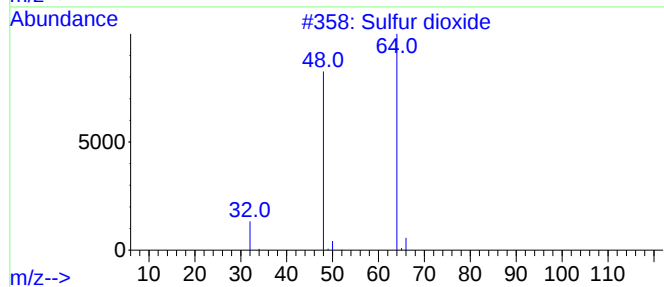
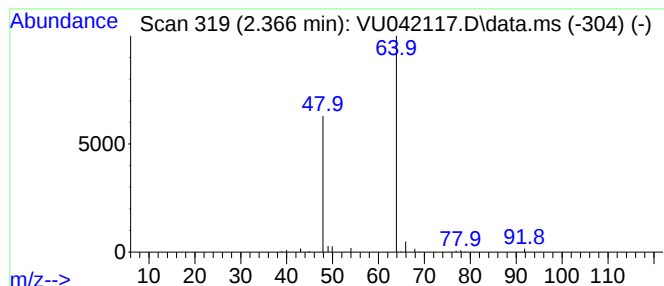
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 Aminomethanesulfonic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.366	0.51 ug/L	28748	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
2			Sulfur dioxide	64	O2S	007446-09-5	74
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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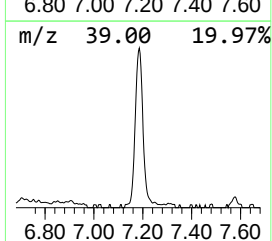
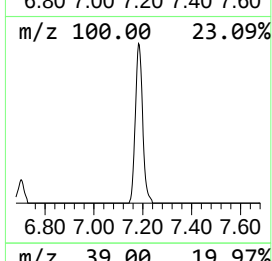
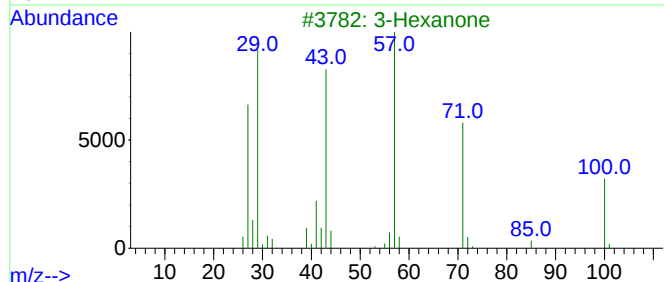
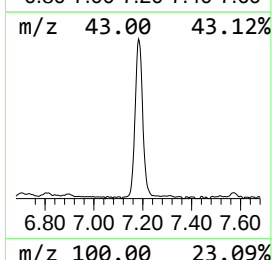
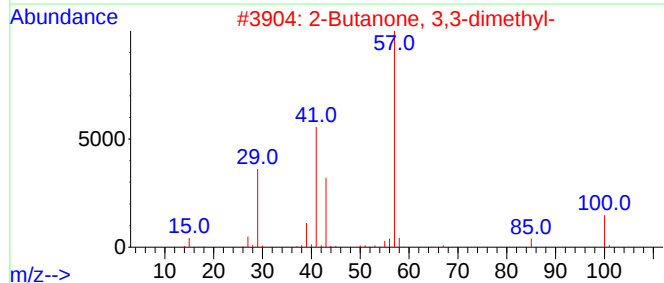
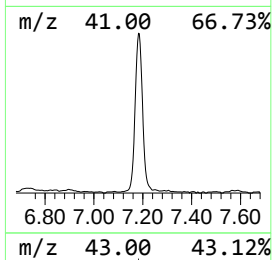
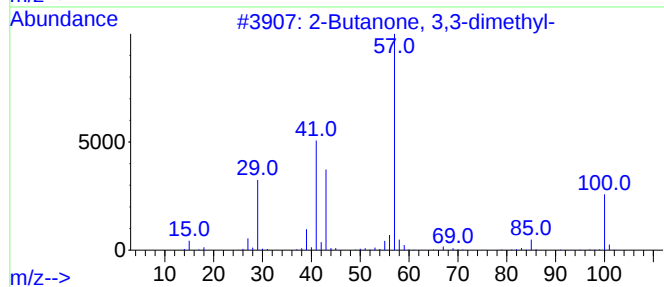
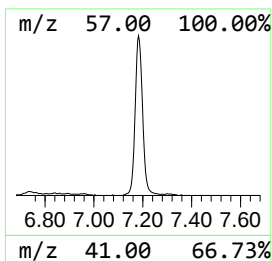
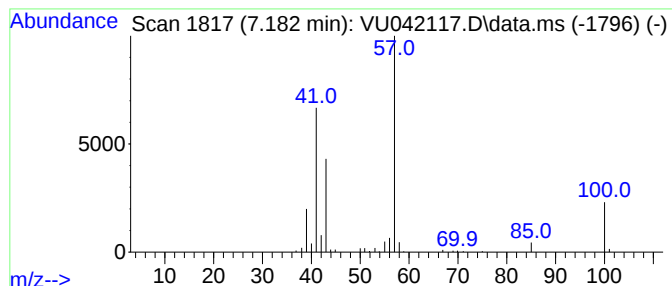
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Butanone, 3,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.182	3.26 ug/L	185288	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-			100	C6H12O	000075-97-8	90
2	2-Butanone, 3,3-dimethyl-			100	C6H12O	000075-97-8	64
3	3-Hexanone			100	C6H12O	000589-38-8	50
4	Diazene, bis(1,1-dimethylethyl)-			142	C8H18N2	000927-83-3	47
5	2-Butanone, 3,3-dimethyl-			100	C6H12O	000075-97-8	45



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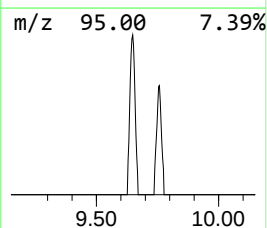
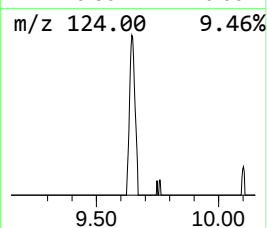
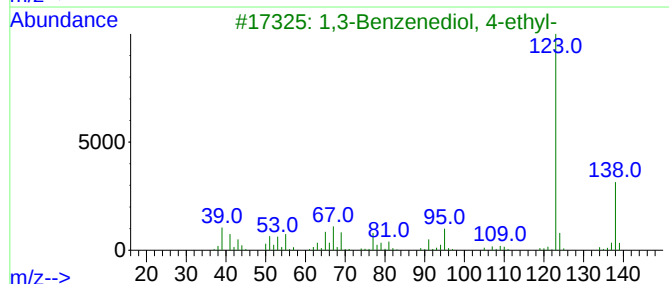
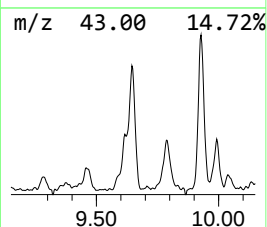
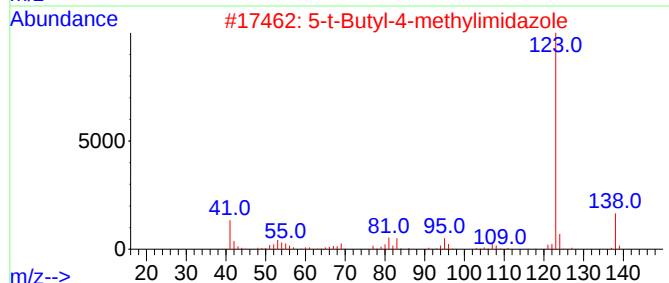
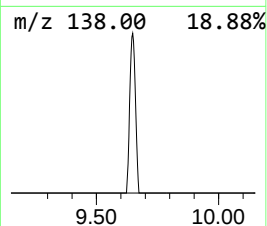
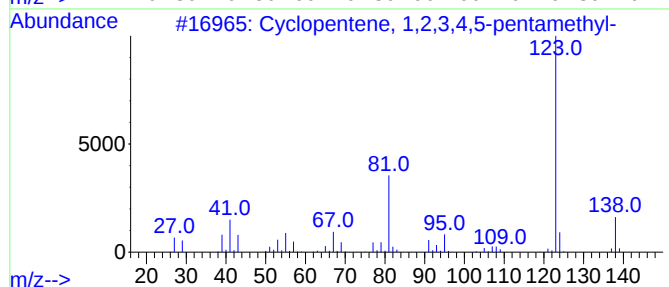
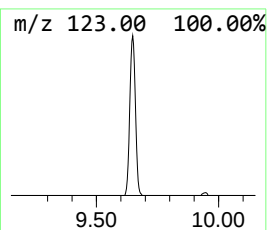
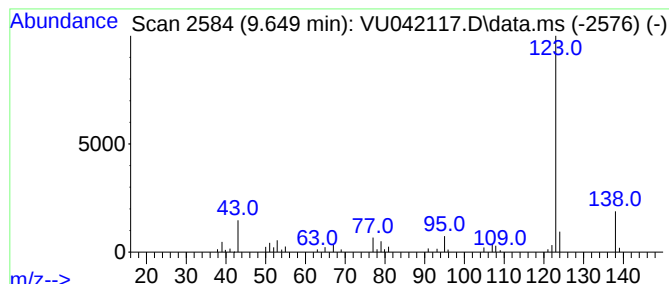
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 Cyclopentene, 1,2,3,4,5-pen... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.649	0.63 ug/L	45940	Chlorobenzene-d5	9.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentene, 1,2,3,4,5-pentamet...	138	C10H18	1000154-28-6	91
2			5-t-Butyl-4-methylimidazole	138	C8H14N2	146979-50-2	90
3			1,3-Benzenediol, 4-ethyl-	138	C8H10O2	002896-60-8	78
4			Cyclopentene, 1,2,3,3,4-pentamet...	138	C10H18	197390-29-7	78
5			Phenol, 4-amino-3-methyl-	123	C7H9NO	002835-99-6	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042117.D
Acq On : 20 Jan 2021 19:48
Operator : SY/MD
Sample : M1180-02
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F1E04

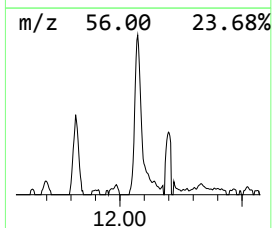
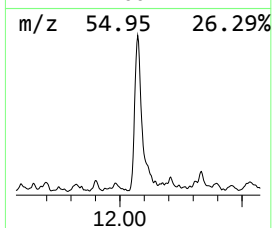
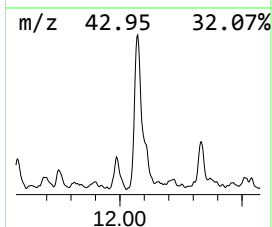
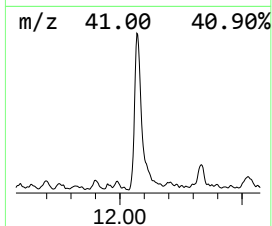
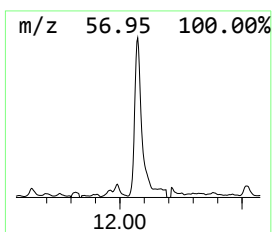
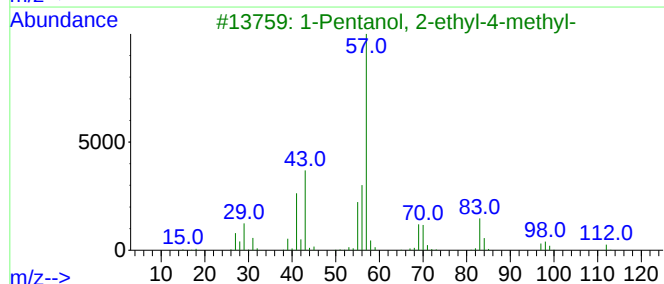
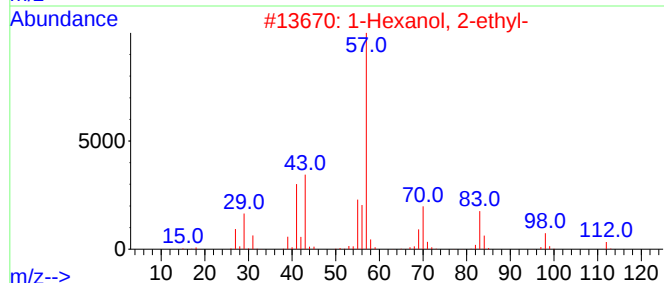
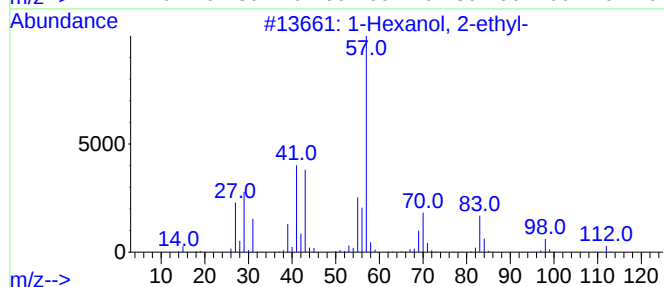
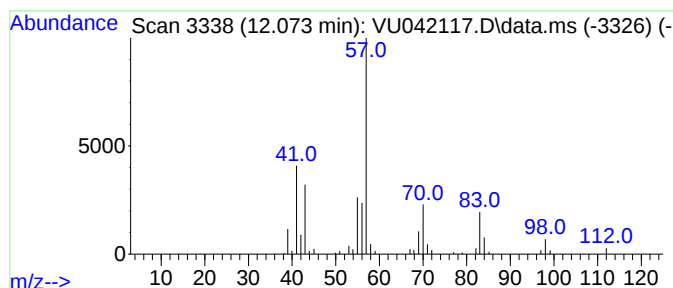
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.073	1.87 ug/L	134633	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
3			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	72
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
5			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042117.D
Acq On : 20 Jan 2021 19:48
Operator : SY/MD
Sample : M1180-02
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F1E04

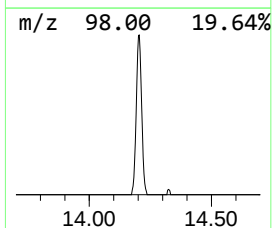
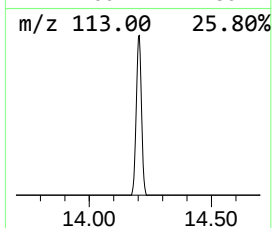
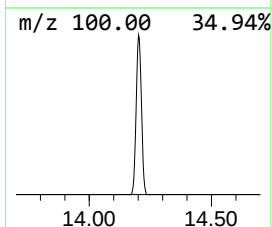
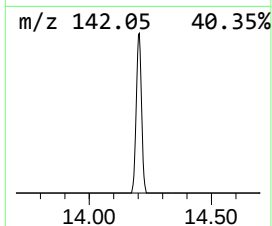
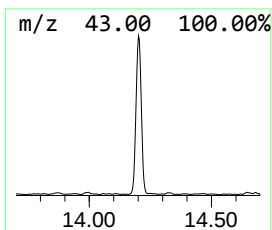
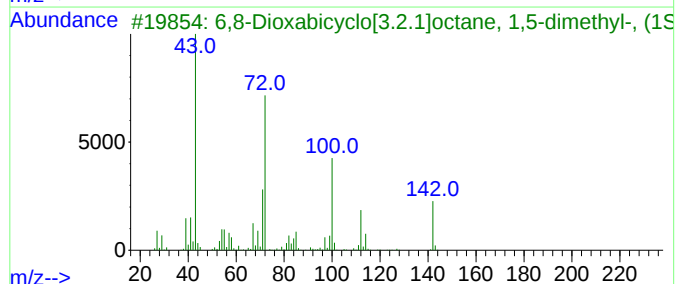
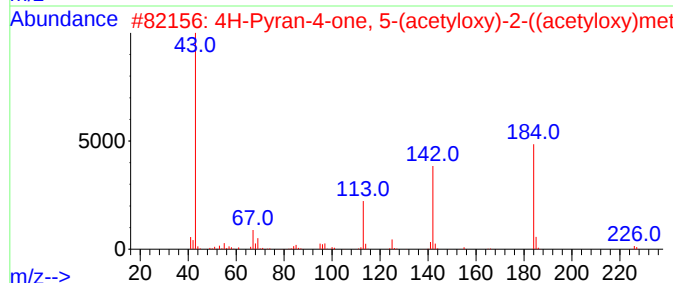
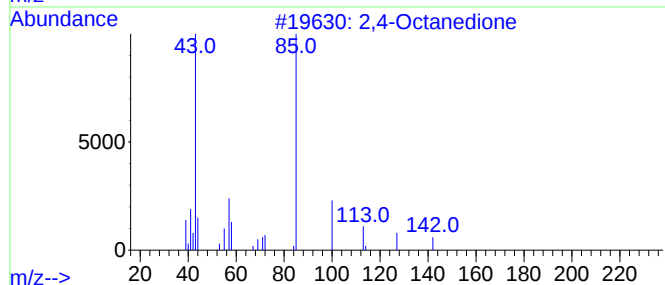
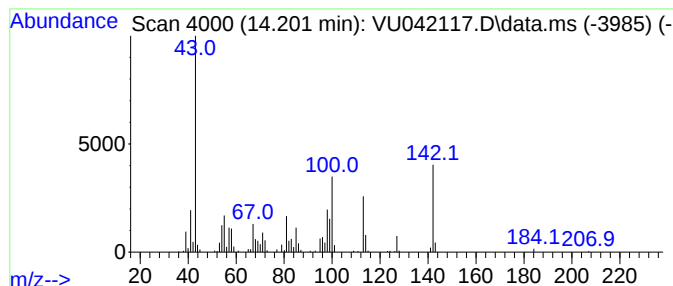
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.201	2.46 ug/L	176892	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Octanedione	142	C8H14O2	014090-87-0	47
2			4H-Pyran-4-one, 5-(acetyloxy)-2-...	226	C10H10O6	026209-93-8	38
3			6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	35
4			6-Dodecanone	184	C12H24O	006064-27-3	14
5			2,4,6-Heptanetrione	142	C7H10O3	000626-53-9	12



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042117.D
Acq On : 20 Jan 2021 19:48
Operator : SY/MD
Sample : M1180-02
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F1E04

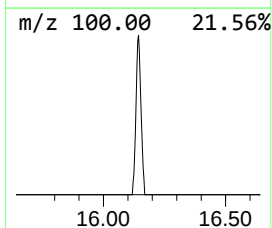
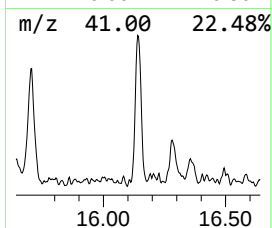
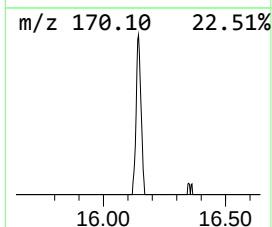
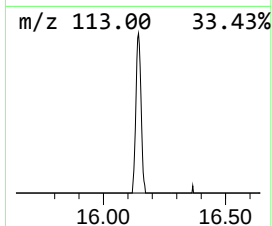
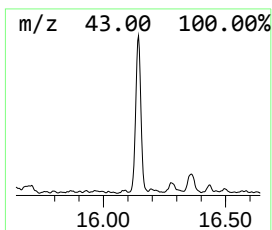
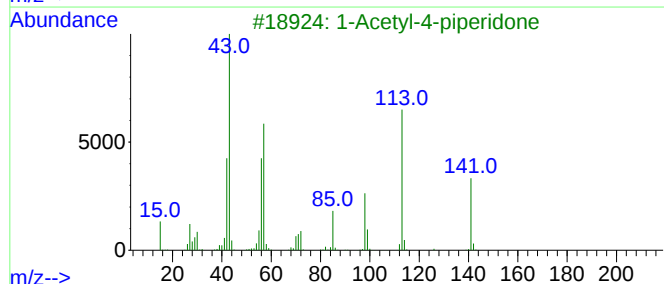
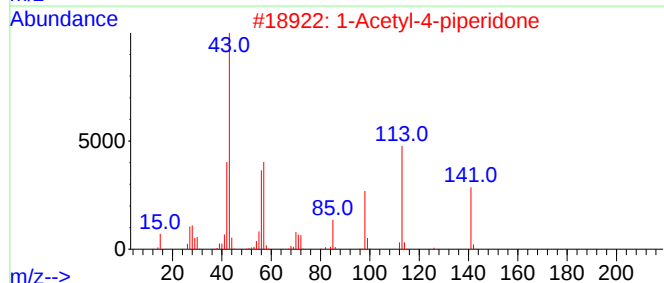
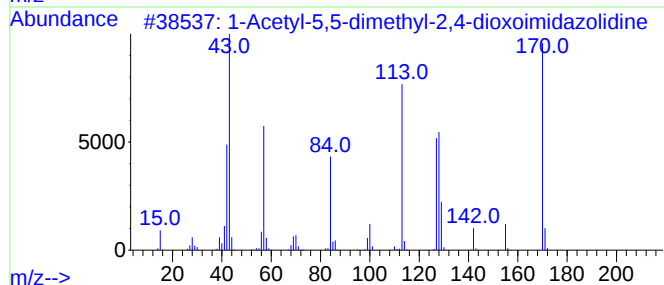
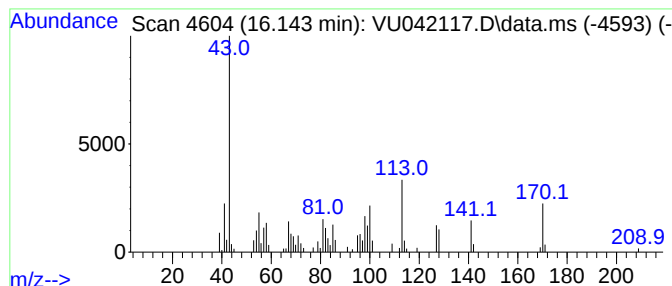
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 unknown-02 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.143	0.81 ug/L	58441	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Acetyl-5,5-dimethyl-2,4-dioxoi...	170	C7H10N2O3	006341-67-9	27
2			1-Acetyl-4-piperidone	141	C7H11NO2	032161-06-1	27
3			1-Acetyl-4-piperidone	141	C7H11NO2	032161-06-1	25
4			7-Pentadecanone	226	C15H30O	006064-38-6	22
5			3,4-Diethoxy-3-cyclobutene-1,2-d...	170	C8H10O4	005231-87-8	14



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042117.D
Acq On : 20 Jan 2021 19:48
Operator : SY/MD
Sample : M1180-02
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 25 Sample Multiplier: 1

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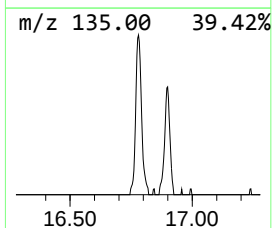
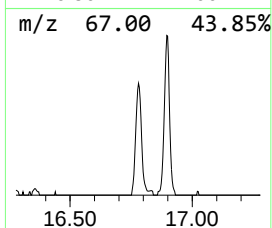
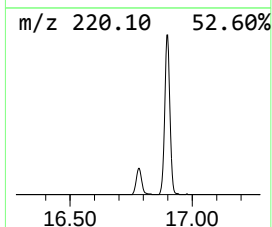
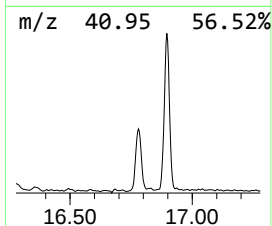
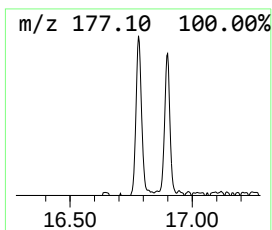
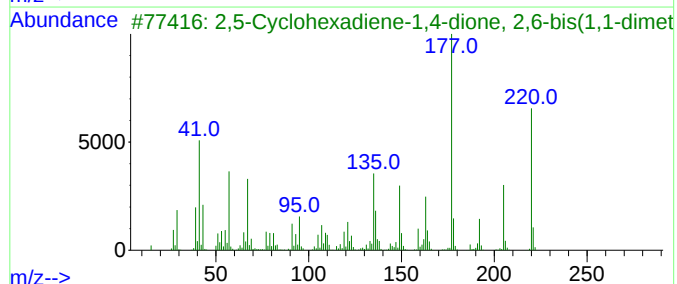
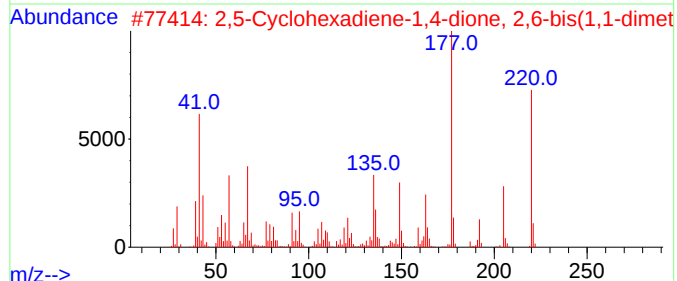
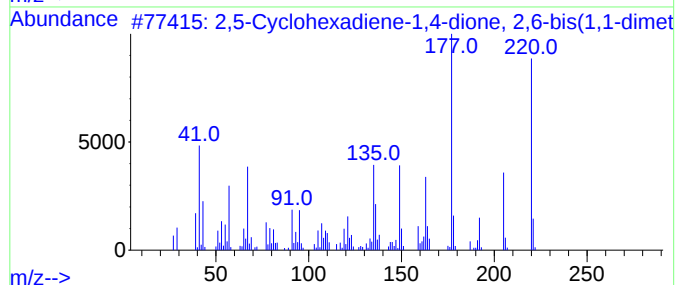
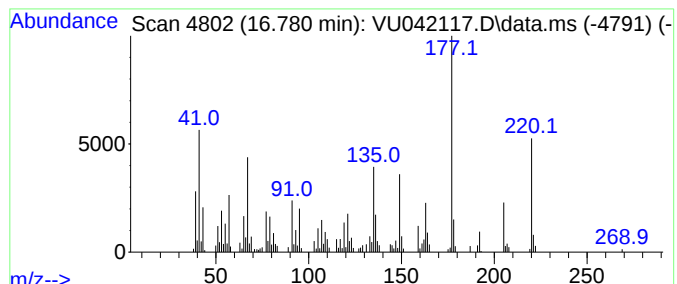
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 9 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.780	1.63 ug/L	117453	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	99
2			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	99
3			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	98
4			Thiocoumarine, 4,4,6,7-tetramethyl-	220	C13H16OS	1000128-90-2	49
5			trans-.beta.-Ionone	192	C13H20O	000079-77-6	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042117.D
Acq On : 20 Jan 2021 19:48
Operator : SY/MD
Sample : M1180-02
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F1E04

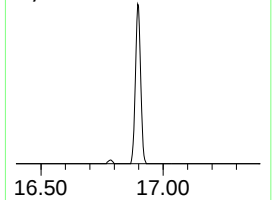
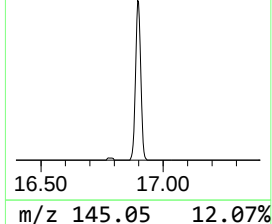
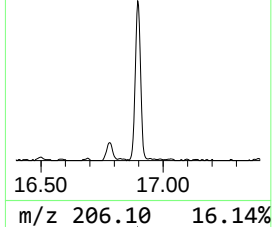
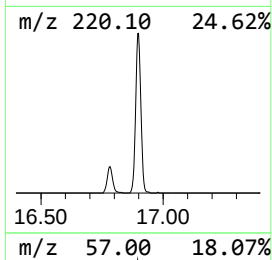
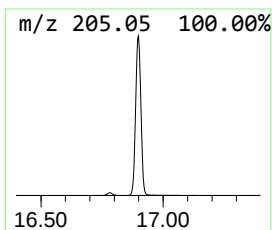
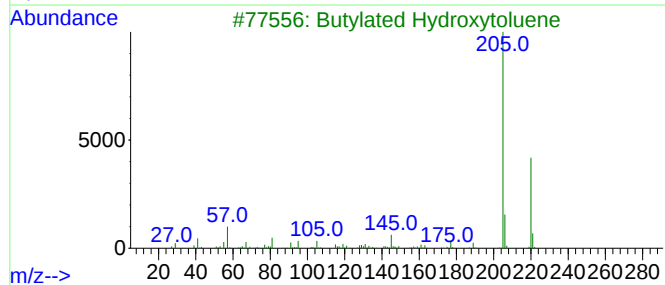
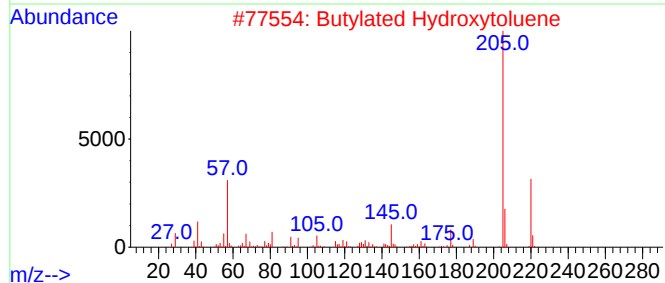
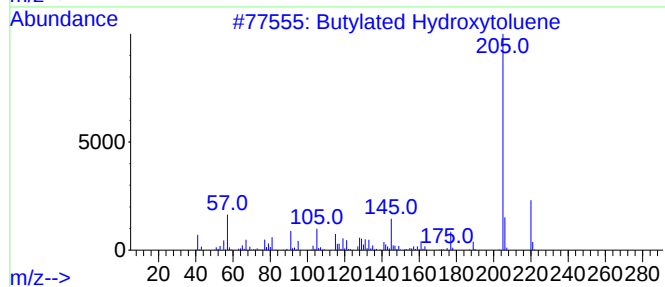
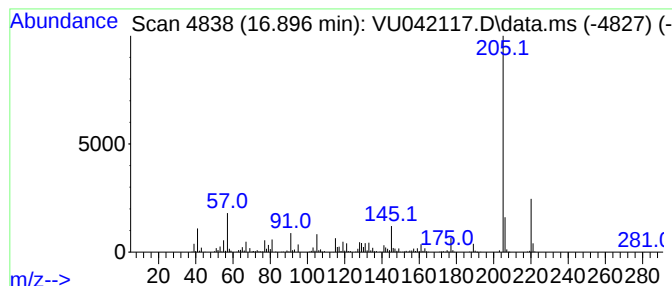
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 10 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.896	7.55 ug/L	543162	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	99
2			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	97
3			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	94
4			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	94
5			Phenol, 2,4,6-tris(1-methylethyl)-	220	C15H24O	002934-07-8	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042117.D
Acq On : 20 Jan 2021 19:48
Operator : SY/MD
Sample : M1180-02
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F1E04

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.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	2.083	0.6	ug/L	34536	1	6.256	283824	5.0
Aminomethanesul...	2.366	0.5	ug/L	28748	1	6.256	283824	5.0
2-Butanone, 3,3...	7.182	3.3	ug/L	185288	1	6.256	283824	5.0
Cyclopentene, 1...	9.649	0.6	ug/L	45940	2	9.427	362789	5.0
1-Hexanol, 2-et...	12.073	1.9	ug/L	134633	3	11.819	359537	5.0
unknown-01	14.201	2.5	ug/L	176892	3	11.819	359537	5.0
unknown-02	16.143	0.8	ug/L	58441	3	11.819	359537	5.0
2,5-Cyclohexadi...	16.780	1.6	ug/L	117453	3	11.819	359537	5.0
Butylated Hydro...	16.896	7.5	ug/L	543162	3	11.819	359537	5.0