

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU052120\
 Data File : VU038263.D
 Acq On : 21 May 2020 14:44
 Operator : JC/MD
 Sample : L2724-18
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BE4W4

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\SOMUTR050720WMA.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	1.498	41	49	56	rBV2	19488	25398	1.08%	0.129%
2	1.601	73	81	95	rBV2	227886	387386	16.47%	1.970%
3	1.703	106	113	125	rBV	57710	81967	3.49%	0.417%
4	1.932	176	184	197	rVB	161964	205500	8.74%	1.045%
5	2.594	372	390	401	rBV	250314	415641	17.68%	2.114%
6	2.668	401	413	438	rVB	147505	355235	15.11%	1.807%
7	3.253	571	595	659	rBV2	201026	1044015	44.40%	5.310%
8	3.620	694	709	725	rVB2	12624	30752	1.31%	0.156%
9	4.481	956	977	1007	rBV	905054	2351546	100.00%	11.959%
10	4.671	1020	1036	1055	rBV	297971	792804	33.71%	4.032%
11	5.102	1151	1170	1191	rBV	261490	575148	24.46%	2.925%
12	5.423	1253	1270	1287	rBV5	38652	89479	3.81%	0.455%
13	5.761	1352	1375	1405	rBV2	518032	1371730	58.33%	6.976%
14	6.279	1517	1536	1565	rVV	431397	890984	37.89%	4.531%
15	6.420	1568	1580	1602	rBV2	42814	91101	3.87%	0.463%
16	6.722	1657	1674	1691	rBV	339250	660072	28.07%	3.357%
17	7.157	1792	1809	1817	rBV	888438	1803728	76.70%	9.173%
18	7.591	1931	1944	1963	rBV	167445	296714	12.62%	1.509%
19	7.922	2032	2047	2062	rBV	606677	1106648	47.06%	5.628%
20	7.989	2062	2068	2081	rVV	45188	87421	3.72%	0.445%
21	8.202	2121	2134	2146	rBV	110313	193162	8.21%	0.982%
22	8.504	2218	2228	2239	rVB6	13807	30579	1.30%	0.156%
23	8.655	2261	2275	2287	rBV	1109362	1909020	81.18%	9.709%
24	8.806	2313	2322	2331	rBV3	30342	49584	2.11%	0.252%
25	9.436	2504	2518	2541	rBV	637842	1089643	46.34%	5.542%
26	10.359	2793	2805	2816	rBV3	27445	43645	1.86%	0.222%
27	10.462	2827	2837	2847	rBV	16876	25843	1.10%	0.131%
28	10.771	2920	2933	2945	rBV	277533	449228	19.10%	2.285%
29	10.902	2961	2974	2985	rVB7	15044	26566	1.13%	0.135%
30	11.041	3007	3017	3029	rVB3	15188	30165	1.28%	0.153%
31	11.825	3248	3261	3281	rVB	677658	1139122	48.44%	5.793%
32	12.082	3330	3341	3358	rBV2	15179	34832	1.48%	0.177%
33	12.205	3366	3379	3392	rBV	637426	1028309	43.73%	5.230%
34	12.520	3467	3477	3486	rBV	31948	52823	2.25%	0.269%

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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	12.909	3588	3598	3615	rVB4	23784	40029	1.70%	0.204%
36	14.114	3961	3973	3986	rBV	92535	154119	6.55%	0.784%
37	14.211	3995	4003	4018	rVB2	14934	24668	1.05%	0.125%
38	14.352	4037	4047	4059	rBV	140221	225658	9.60%	1.148%
39	14.764	4164	4175	4184	rBV2	13532	23792	1.01%	0.121%
40	14.928	4218	4226	4236	rBV4	15336	23529	1.00%	0.120%
41	15.089	4265	4276	4296	rBV2	77553	140349	5.97%	0.714%
42	15.748	4469	4481	4497	rBV3	124175	228564	9.72%	1.162%
43	16.754	4783	4794	4805	rBV6	18878	36219	1.54%	0.184%

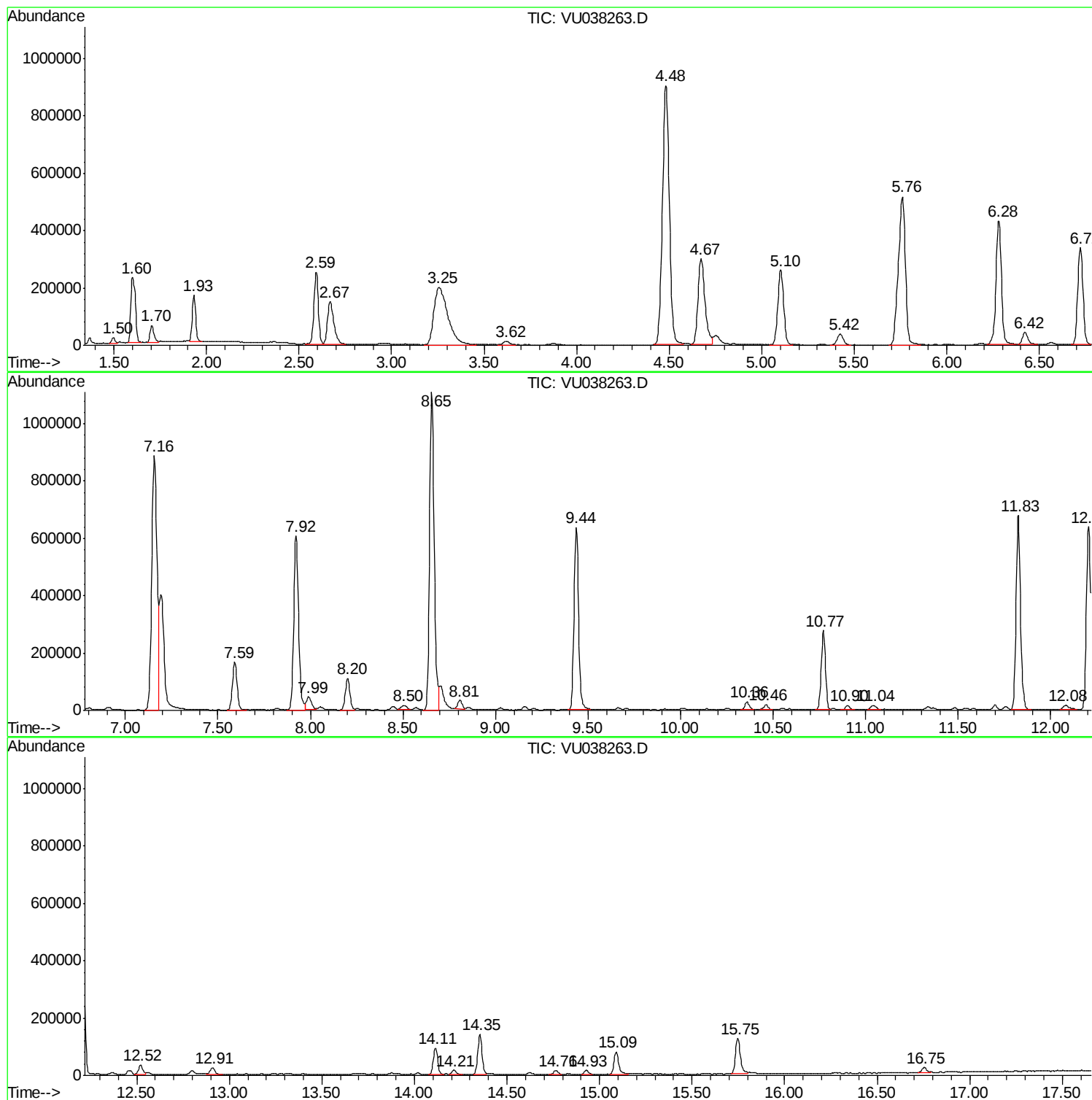
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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



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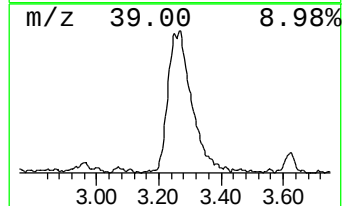
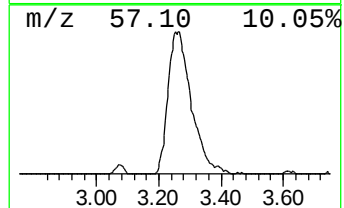
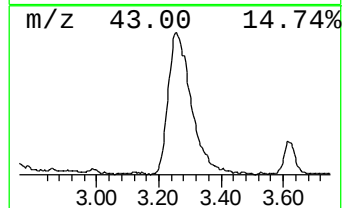
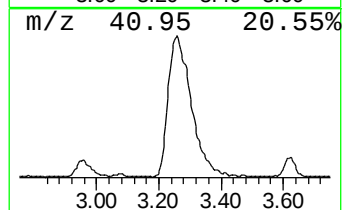
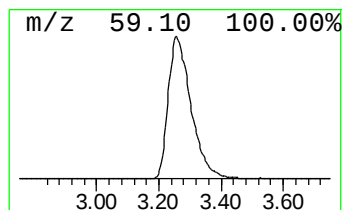
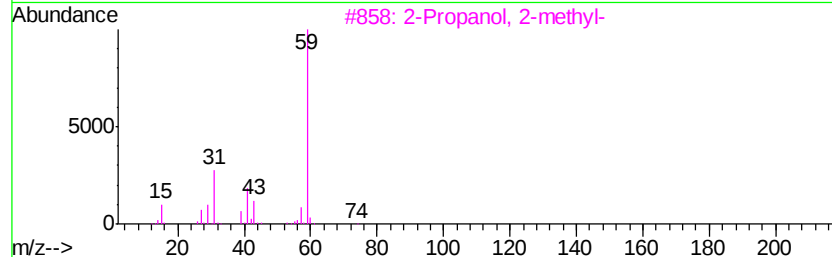
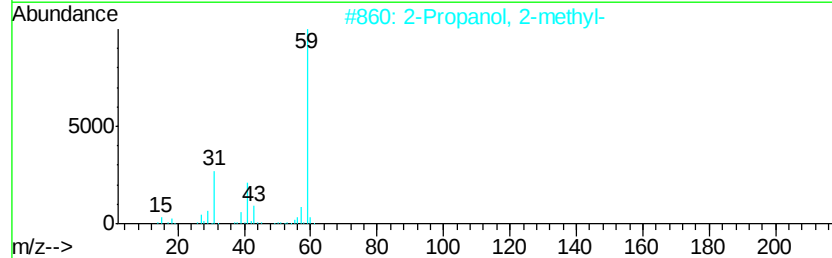
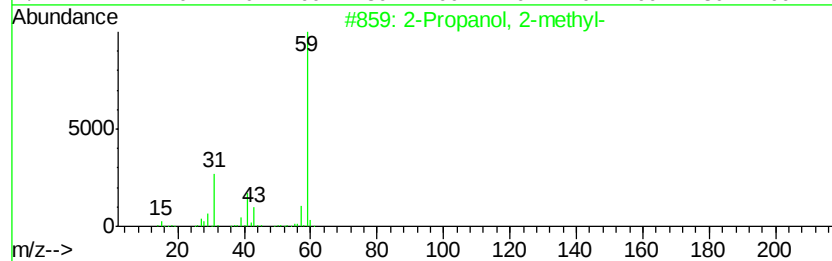
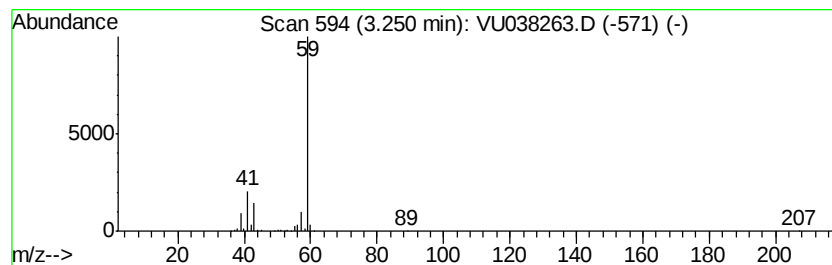
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 2-Propanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.25	5.86 ug/L	1044020	1,4-Difluorobenzene	6.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	74
2			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	64
3			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	64
4			Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	9
5			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	9



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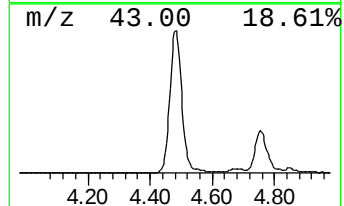
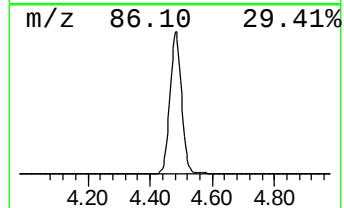
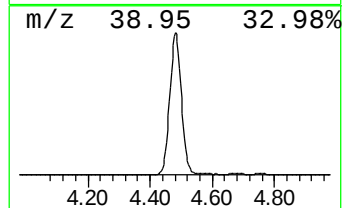
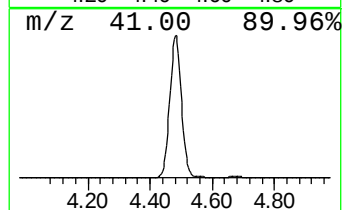
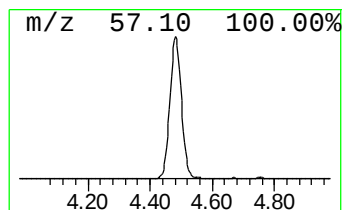
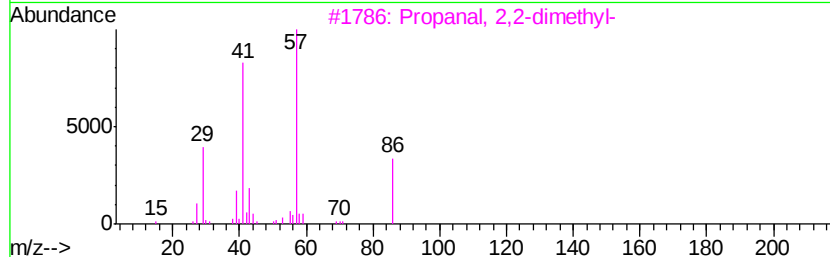
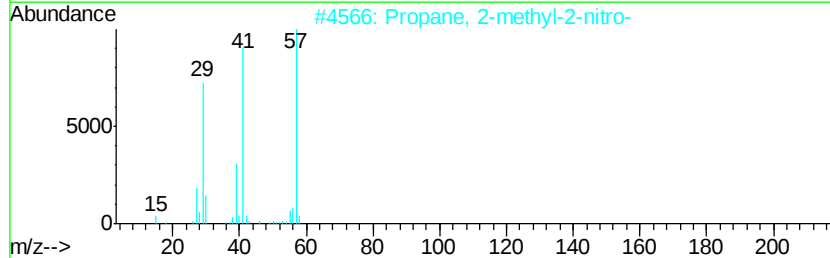
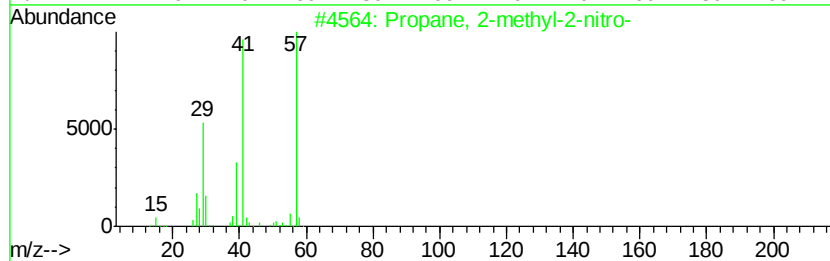
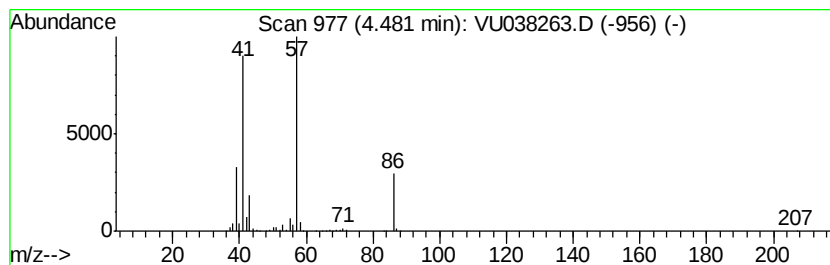
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 Propane, 2-methyl-2-nitro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.48	13.20 ug/L	2351550	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	53
2		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	53
3		Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	47
4		Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	45
5		Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	42



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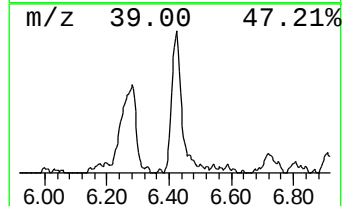
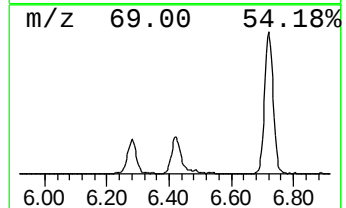
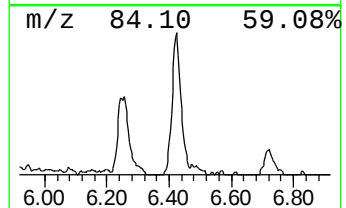
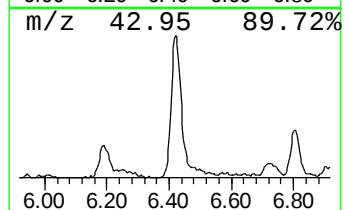
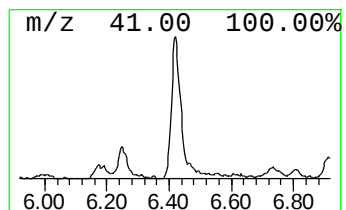
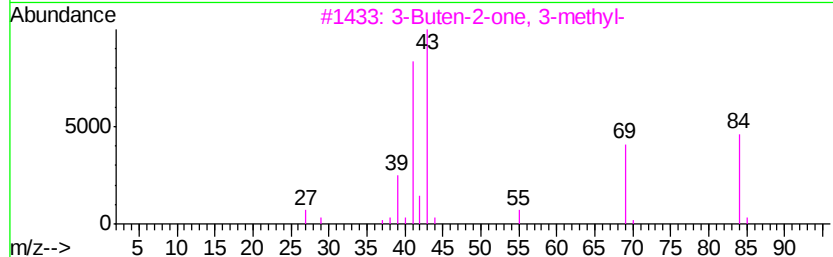
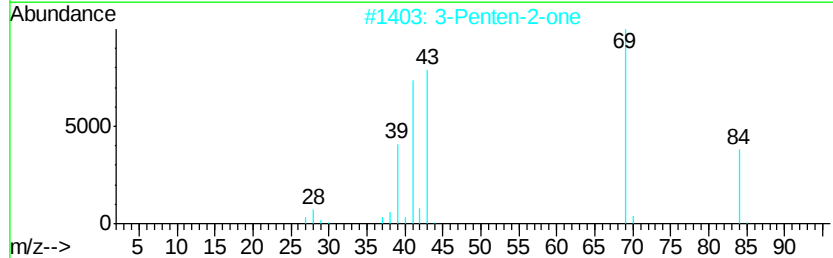
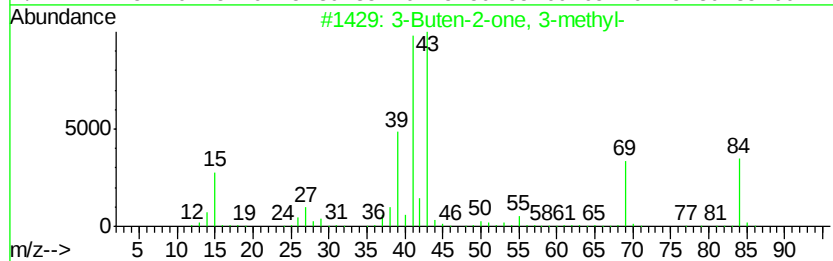
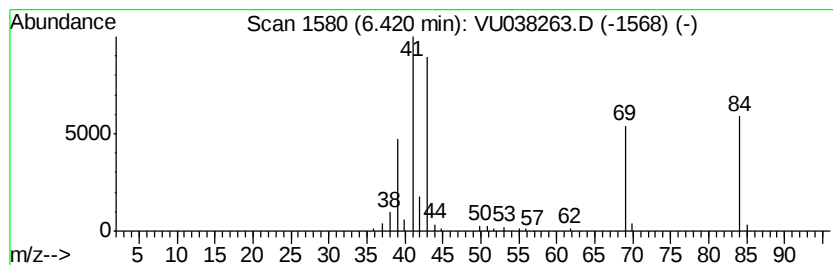
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 3-Buten-2-one, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	0.51 ug/L	91101	1,4-Difluorobenzene	6.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Buten-2-one, 3-methyl-	84	C5H8O	000814-78-8	90
2			3-Penten-2-one	84	C5H8O	000625-33-2	78
3			3-Buten-2-one, 3-methyl-	84	C5H8O	000814-78-8	58
4			Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	58
5			Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	47



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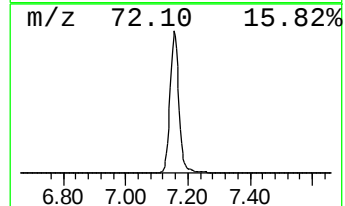
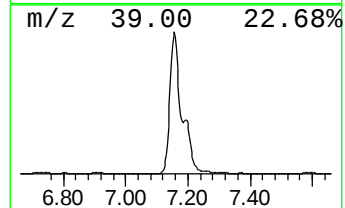
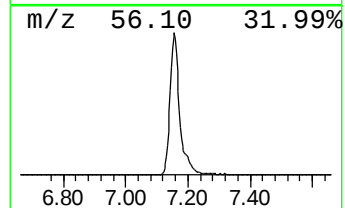
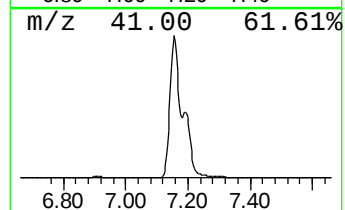
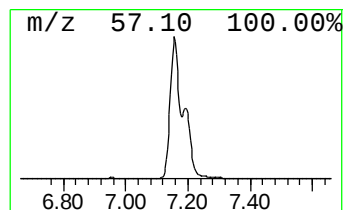
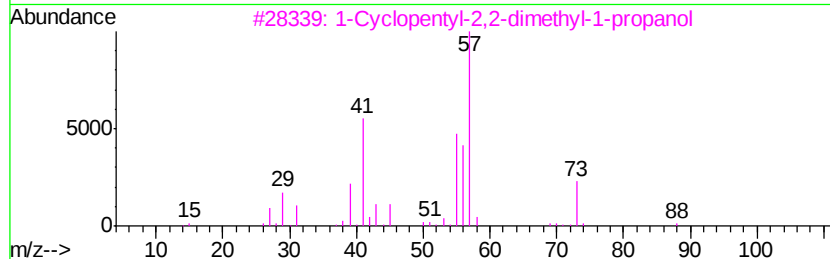
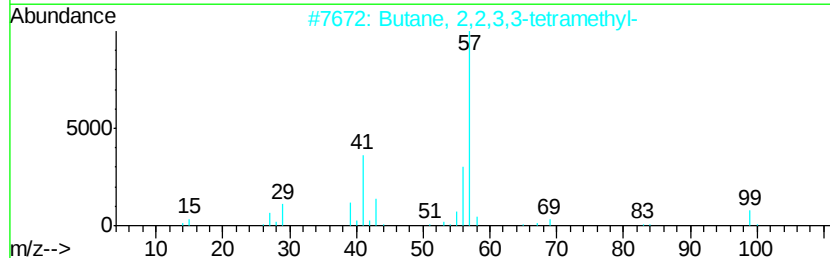
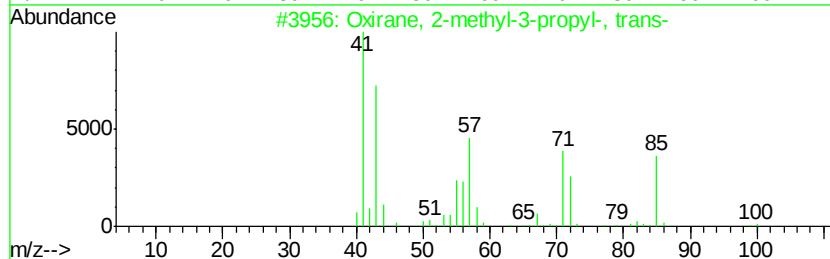
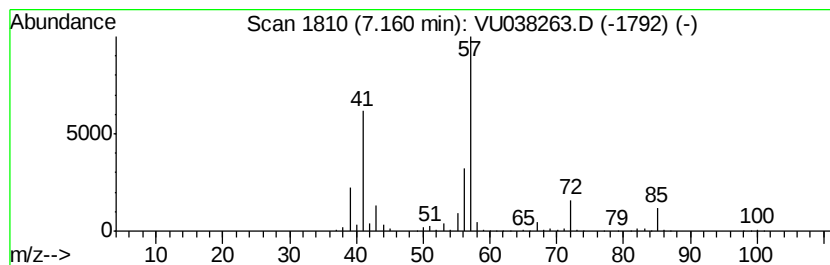
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Peak Number 4 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.16	10.12 ug/L	1803730	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, 2-methyl-3-propyl-, trans-	100	C6H12O	006124-91-0	46
2		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	40
3		1-Cyclopentyl-2,2-dimethyl-1-propanol	156	C10H20O	337966-85-5	40
4		1-Butanol, 3,3-dimethyl-	102	C6H14O	000624-95-3	36
5		Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	36



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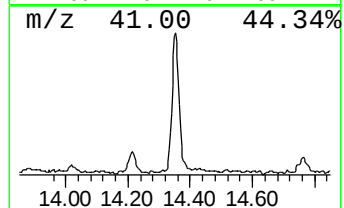
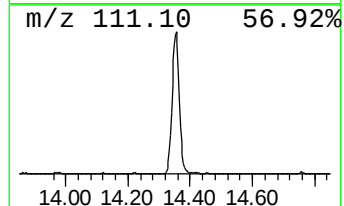
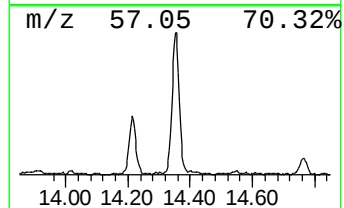
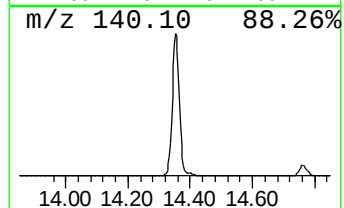
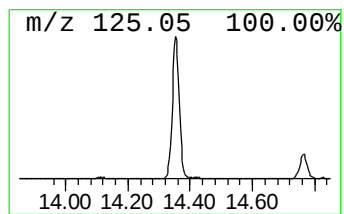
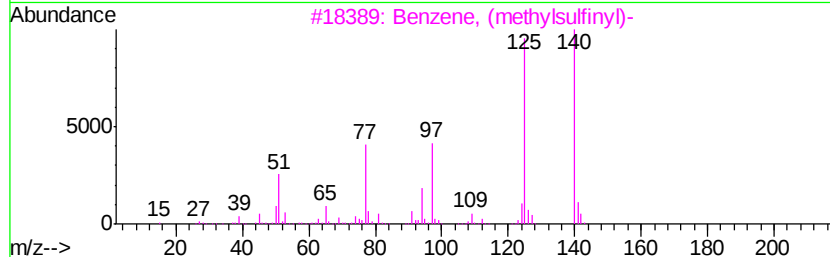
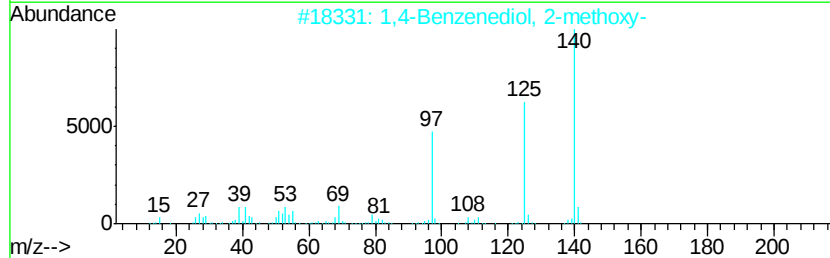
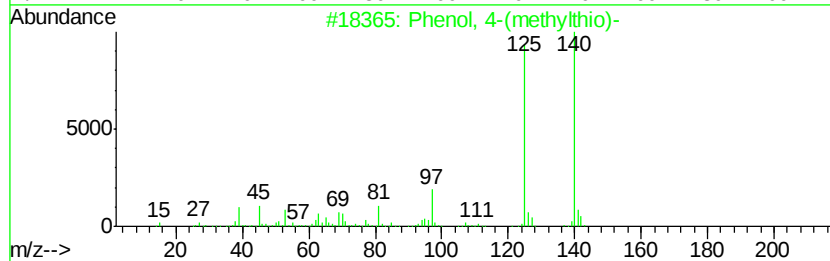
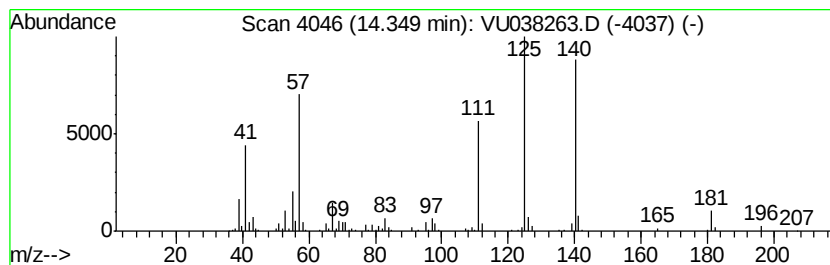
Instrument :
MSVOA_U
ClientSampleId :
BE4W4

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 Phenol, 4-(methylthio)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	0.99 ug/L	225658	1,4-Dichlorobenzene-d4	11.82
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Phenol, 4-(methylthio)-	140 C7H8OS	001073-72-9 59
2		1,4-Benzenediol, 2-methoxy-	140 C7H8O3	000824-46-4 42
3		Benzene, (methylsulfinyl)-	140 C7H8OS	001193-82-4 42
4		Flamenol	140 C7H8O3	002174-64-3 37
5		4-(Methylmercapto)phenol, acetate	182 C9H10O2S	1000353-05-2 37



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU052120\
Data File : VU038263.D
Acq On : 21 May 2020 14:44
Operator : JC/MD
Sample : L2724-18
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BE4W4

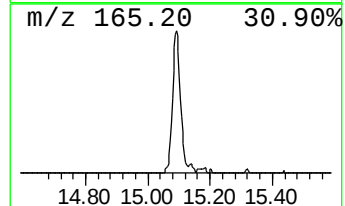
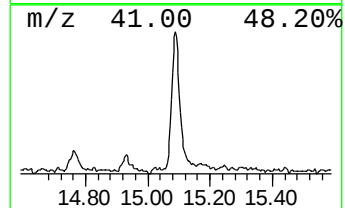
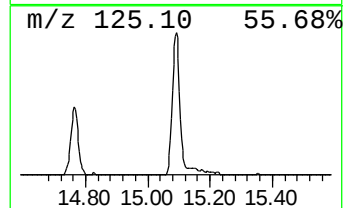
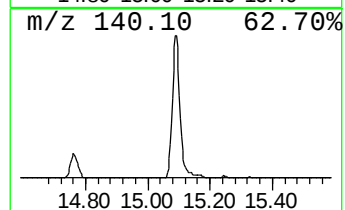
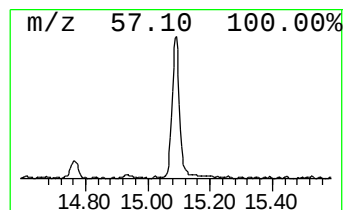
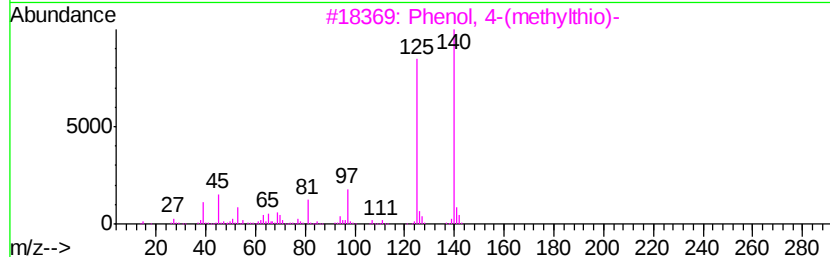
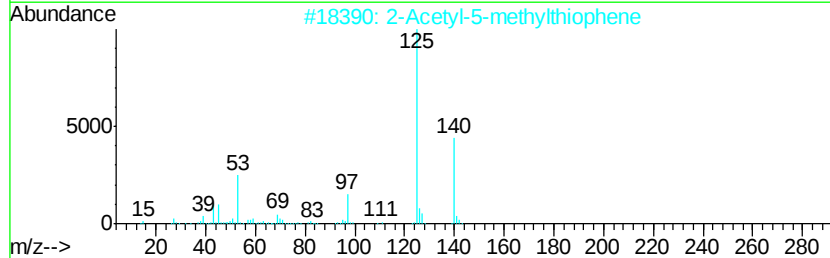
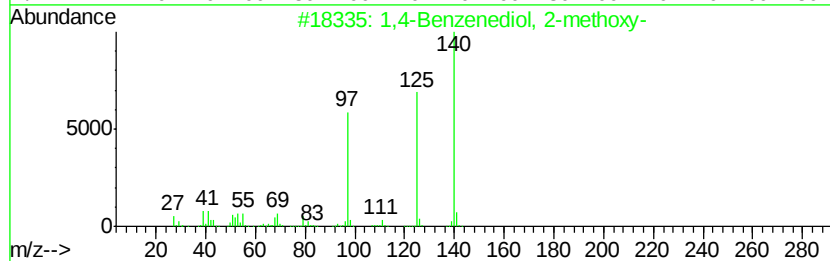
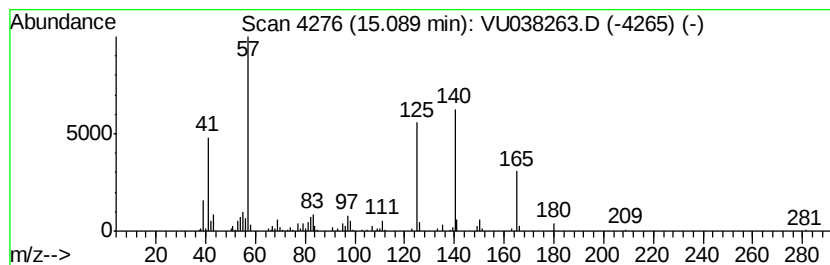
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 unknown-02 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	0.62 ug/L	140349	1,4-Dichlorobenzene-d4	11.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Benzenediol, 2-methoxy-	140	C7H8O3	000824-46-4	49
2		2-Acetyl-5-methylthiophene	140	C7H8OS	013679-74-8	49
3		Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	47
4		Cyclohexanone, 2-acetyl-	140	C8H12O2	000874-23-7	47
5		1-Allylimidazole-2-thione	140	C6H8N2S	121690-22-0	47



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU052120\
Data File : VU038263.D
Acq On : 21 May 2020 14:44
Operator : JC/MD
Sample : L2724-18
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampled :
BE4W4

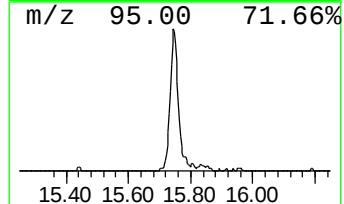
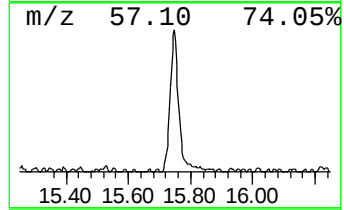
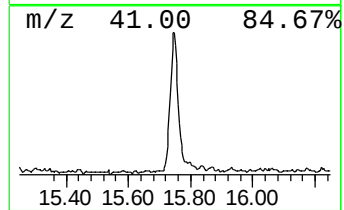
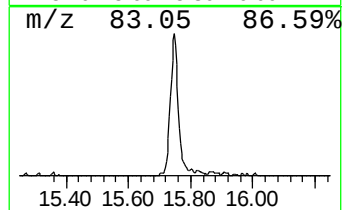
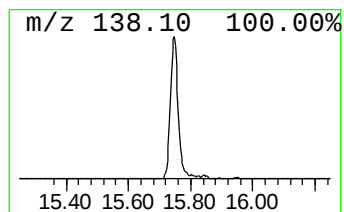
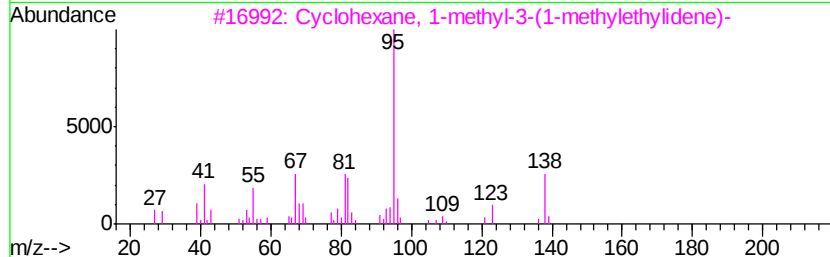
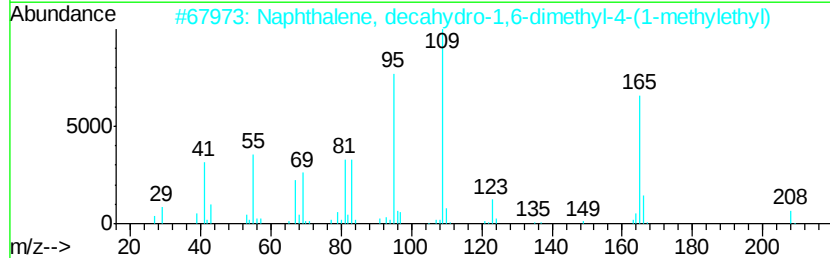
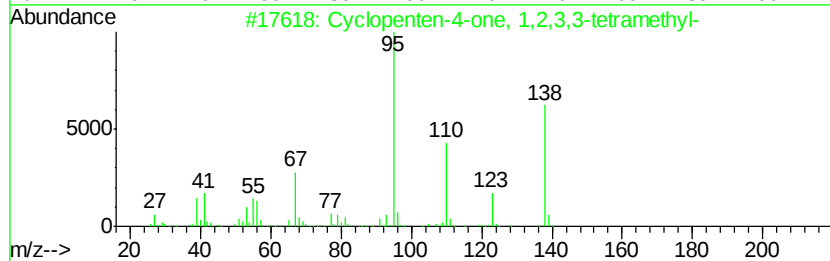
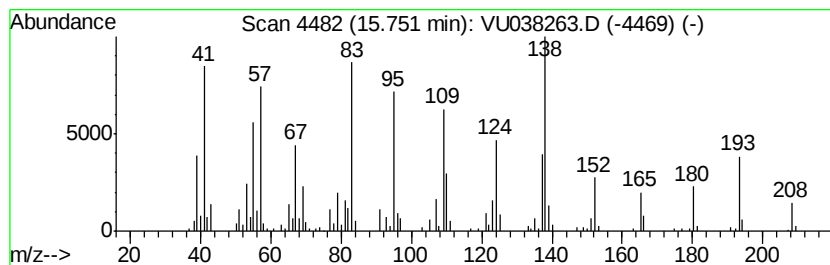
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 9 unknown-03 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.75	1.00 ug/L	228564	1,4-Dichlorobenzene-d4	11.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopenten-4-one, 1,2,3,3-tetra...	138	C9H14O	1000163-38-6	42
2		Naphthalene, decahydro-1,6-dimet...	208	C15H28	029788-41-8	38
3		Cyclohexane, 1-methyl-3-(1-methyl...	138	C10H18	013828-34-7	38
4		1,3-Hexadiene, 3-ethyl-2-methyl-...	124	C9H16	074752-97-9	30
5		1,2-Dimethyl-4-oxocyclohex-2-ene...	152	C9H12O2	1000187-01-2	25



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU052120\
Data File : VU038263.D
Acq On : 21 May 2020 14:44
Operator : JC/MD
Sample : L2724-18
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BE4W4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.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-Propanol, 2-met...	3.25	5.9	ug/L	1044020	1	6.28	890984	5.0
Propane, 2-methyl...	4.48	13.2	ug/L	2351550	1	6.28	890984	5.0
3-Buten-2-one, 3-...	6.42	0.5	ug/L	91101	1	6.28	890984	5.0
unknown-01	7.16	10.1	ug/L	1803730	1	6.28	890984	5.0
Phenol, 4-(methyl...	14.35	1.0	ug/L	225658	3	11.82	1139120	5.0
unknown-02	15.09	0.6	ug/L	140349	3	11.82	1139120	5.0
unknown-03	15.75	1.0	ug/L	228564	3	11.82	1139120	5.0