

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU052120\
 Data File : VU038262.D
 Acq On : 21 May 2020 14:21
 Operator : JC/MD
 Sample : L2724-19
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BE4W5

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	1.600	73	81	93	rVB2	218198	368752	15.70%	1.910%
2	1.703	106	113	134	rVB	56102	72228	3.08%	0.374%
3	1.932	176	184	195	rVB	161102	206291	8.78%	1.069%
4	2.594	375	390	401	rBV	249359	415709	17.70%	2.154%
5	2.665	401	412	438	rVB	153930	349851	14.90%	1.812%
6	3.253	567	595	648	rBV2	199653	956258	40.72%	4.954%
7	3.620	693	709	724	rBV2	13389	30271	1.29%	0.157%
8	4.481	955	977	1014	rBV	896312	2348271	100.00%	12.165%
9	4.671	1020	1036	1054	rBV	302045	781478	33.28%	4.049%
10	5.102	1153	1170	1193	rBV	265786	580834	24.73%	3.009%
11	5.423	1253	1270	1284	rBV3	38975	88896	3.79%	0.461%
12	5.761	1351	1375	1406	rBV2	521952	1381580	58.83%	7.157%
13	6.282	1516	1537	1562	rVB	451602	899838	38.32%	4.662%
14	6.420	1567	1580	1598	rBV2	42207	85315	3.63%	0.442%
15	6.719	1658	1673	1691	rBV	338549	659316	28.08%	3.416%
16	7.157	1790	1809	1817	rBV	872213	1806750	76.94%	9.360%
17	7.591	1931	1944	1970	rBV	164248	291546	12.42%	1.510%
18	7.922	2034	2047	2061	rBV	605077	1089875	46.41%	5.646%
19	7.992	2062	2069	2081	rVV2	45752	85400	3.64%	0.442%
20	8.201	2120	2134	2146	rBV	106931	190061	8.09%	0.985%
21	8.497	2217	2226	2239	rVB5	18496	43161	1.84%	0.224%
22	8.655	2262	2275	2287	rBV	1070458	1866572	79.49%	9.670%
23	8.806	2312	2322	2332	rBV3	31584	54250	2.31%	0.281%
24	9.436	2504	2518	2550	rVB	636399	1111778	47.34%	5.760%
25	10.359	2795	2805	2818	rVB3	26851	43231	1.84%	0.224%
26	10.462	2825	2837	2849	rBV	17121	28096	1.20%	0.146%
27	10.771	2919	2933	2945	rBV	275971	447733	19.07%	2.320%
28	10.902	2960	2974	2987	rVB6	18685	34942	1.49%	0.181%
29	11.041	3007	3017	3030	rVB3	15831	30918	1.32%	0.160%
30	11.825	3248	3261	3280	rVB	681018	1147862	48.88%	5.947%
31	12.079	3329	3340	3363	rBV4	14996	39829	1.70%	0.206%
32	12.205	3363	3379	3395	rVV	626575	1023647	43.59%	5.303%
33	12.459	3447	3458	3466	rBV4	14971	25805	1.10%	0.134%
34	12.520	3468	3477	3486	rBV	29671	47524	2.02%	0.246%

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ClientSampleId :
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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

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

35	12.796	3553	3563	3572	rBV4	12780	23857	1.02%	0.124%
36	12.909	3584	3598	3607	rVB5	23597	41574	1.77%	0.215%
37	14.114	3960	3973	3985	rBV	89598	145474	6.19%	0.754%
38	14.356	4036	4048	4061	rBV2	135372	215070	9.16%	1.114%
39	15.092	4267	4277	4300	rBV4	54564	117899	5.02%	0.611%
40	15.748	4470	4481	4497	rBV4	67057	125071	5.33%	0.648%

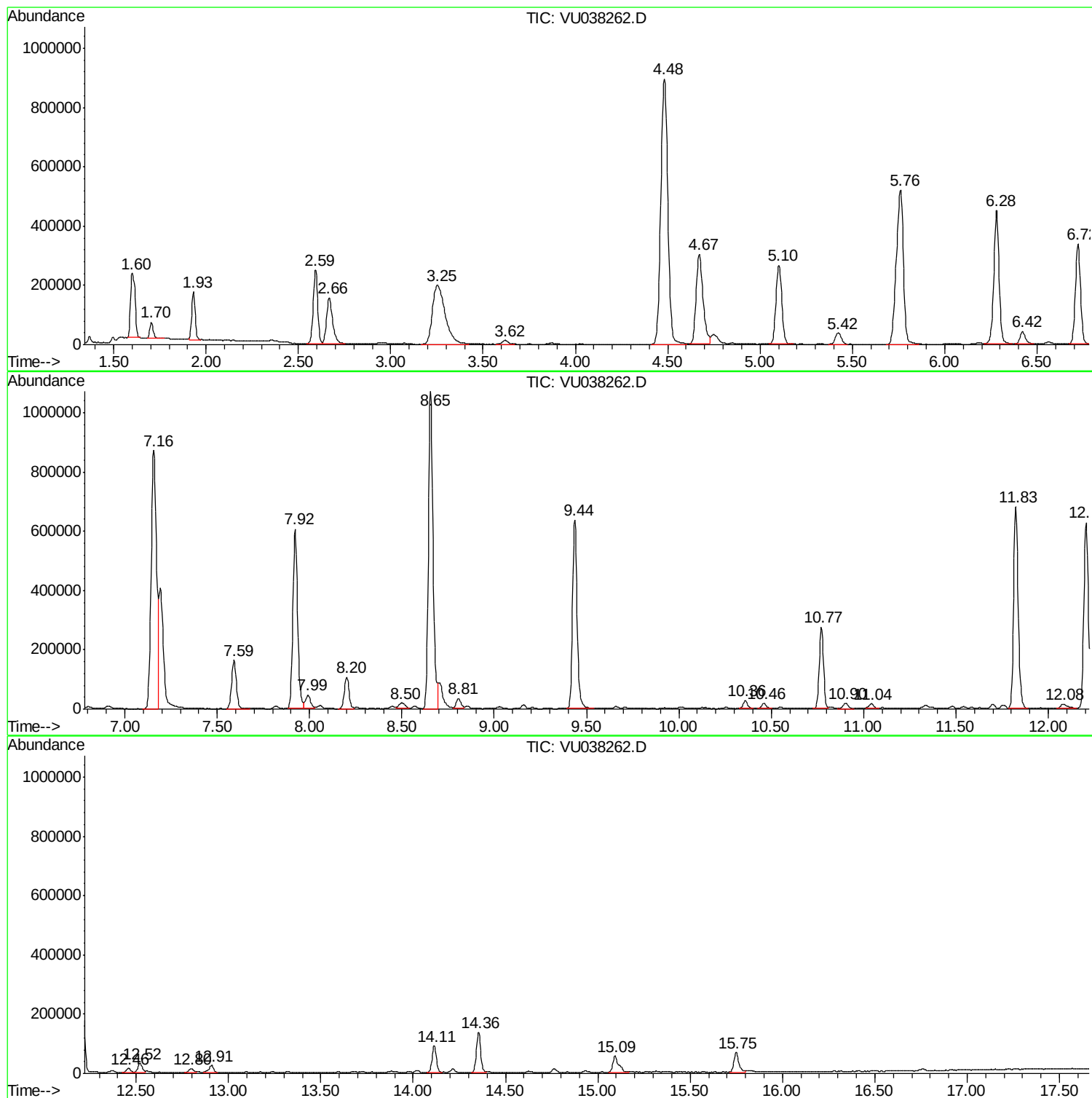
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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



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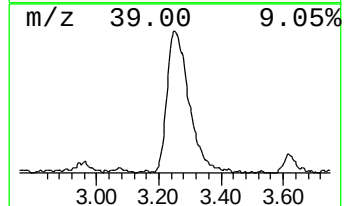
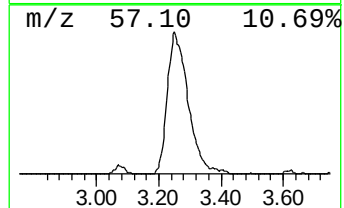
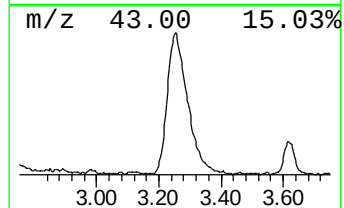
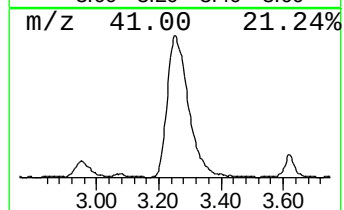
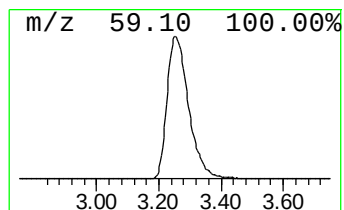
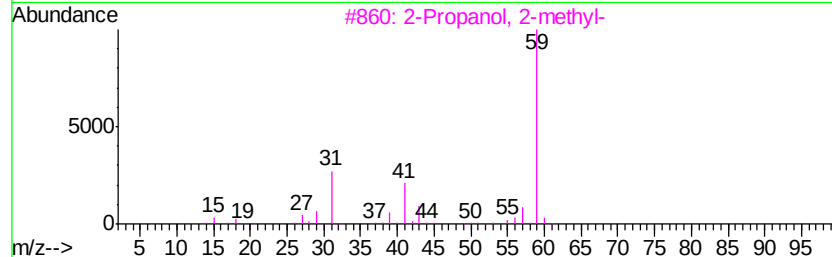
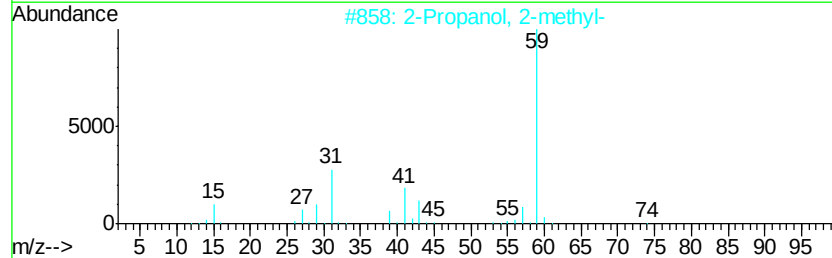
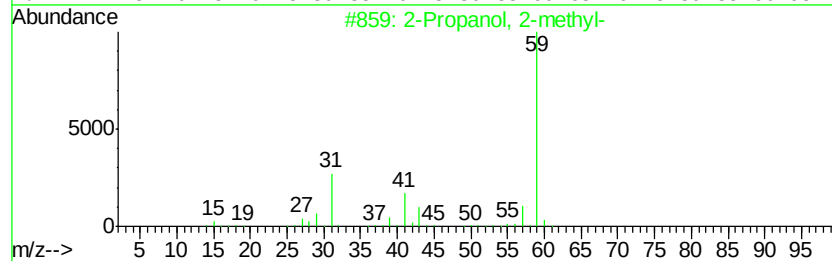
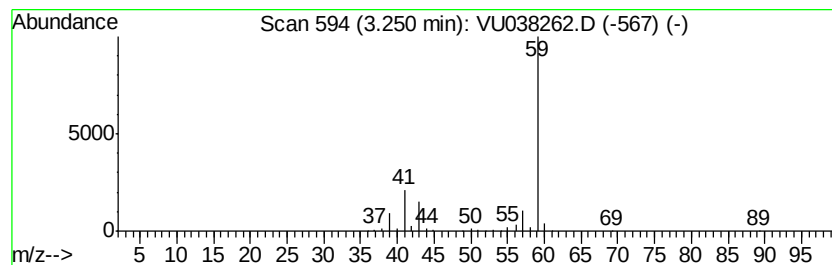
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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	5.31 ug/L	956258	1,4-Difluorobenzene	6.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	78
2			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	64
3			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	64
4			3-Pentanol	88	C5H12O	000584-02-1	64
5			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	37



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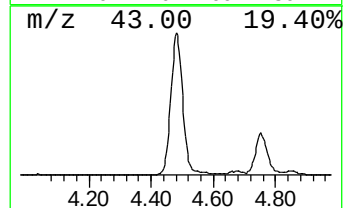
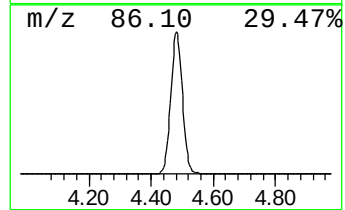
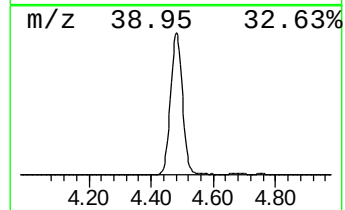
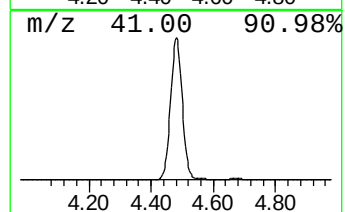
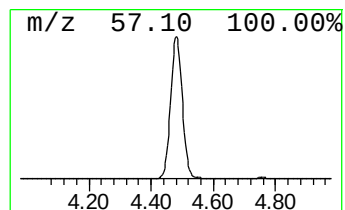
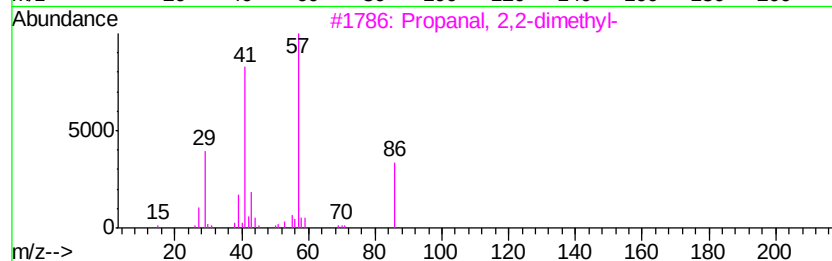
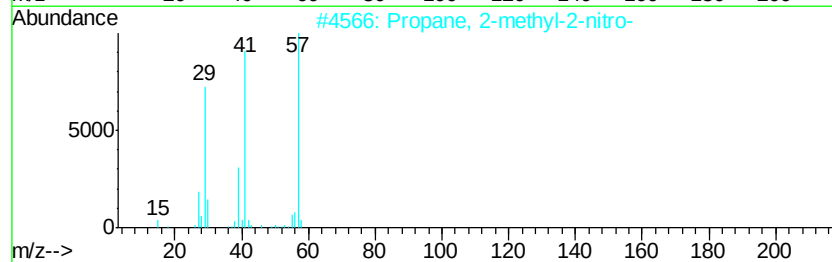
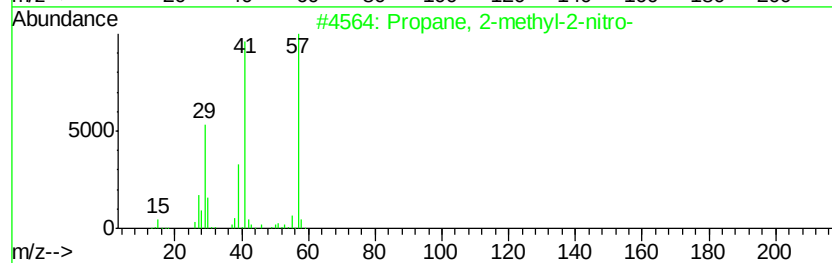
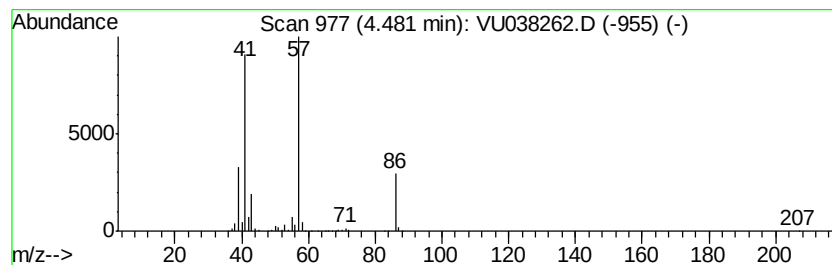
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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	13.05 ug/L	2348270	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	59
2		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	50
3		Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	50
4		3-Pentanone	86	C5H10O	000096-22-0	40
5		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	40



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Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampled :
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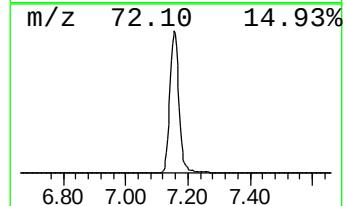
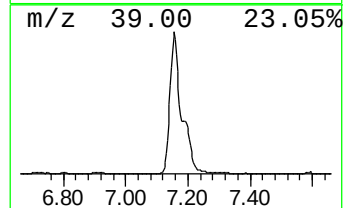
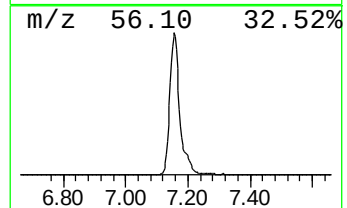
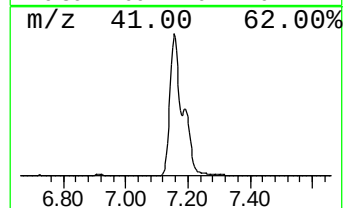
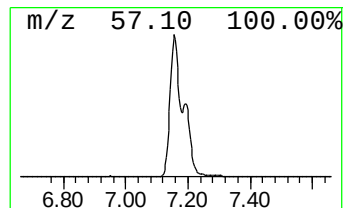
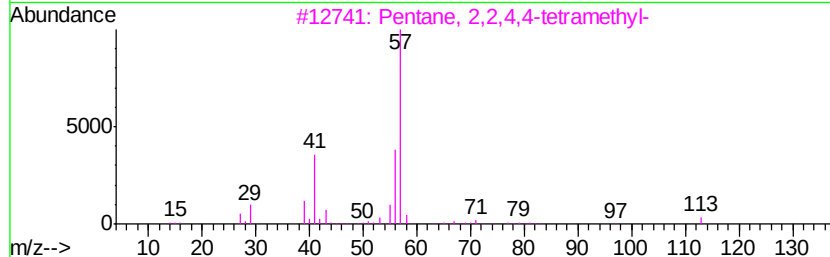
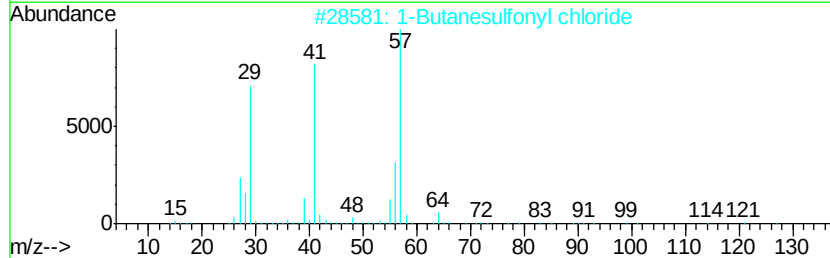
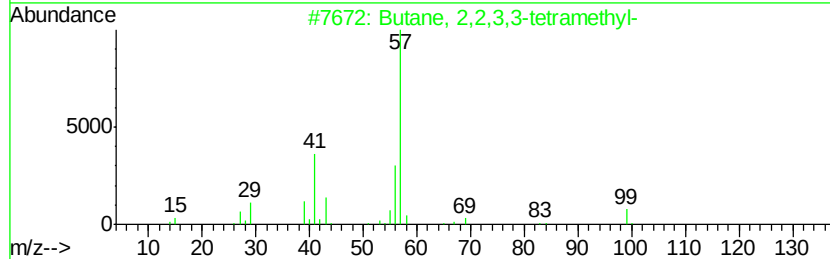
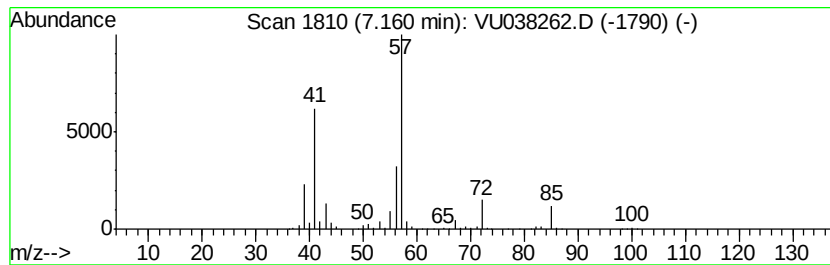
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.16	10.04 ug/L	1806750	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	40
2		1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	40
3		Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	40
4		1-Cyclopentyl-2,2-dimethyl-1-pro...	156	C10H20O	337966-85-5	40
5		Oxirane, 2-methyl-3-propyl-, trans-	100	C6H12O	006124-91-0	38



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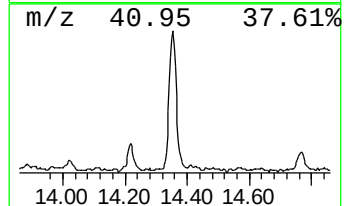
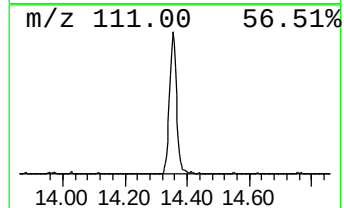
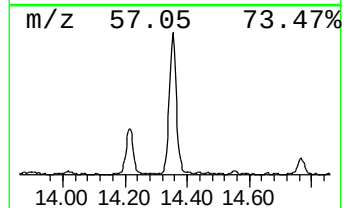
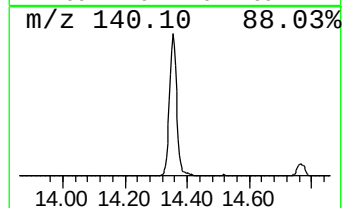
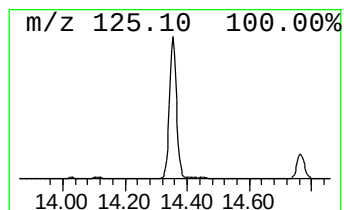
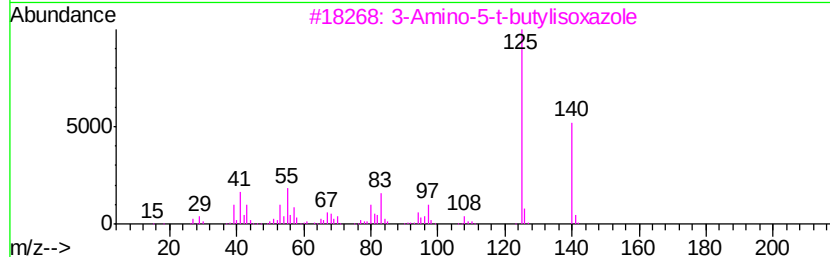
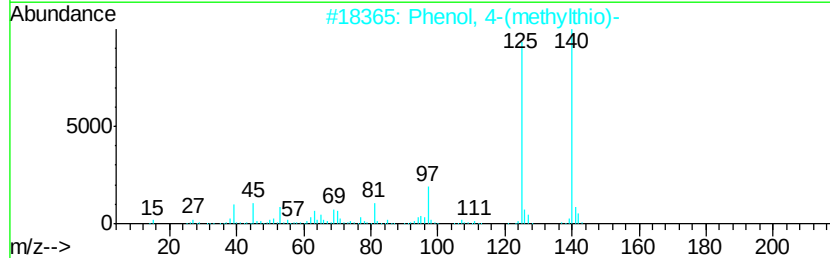
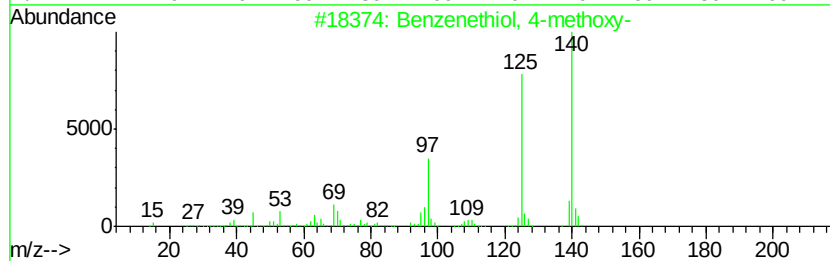
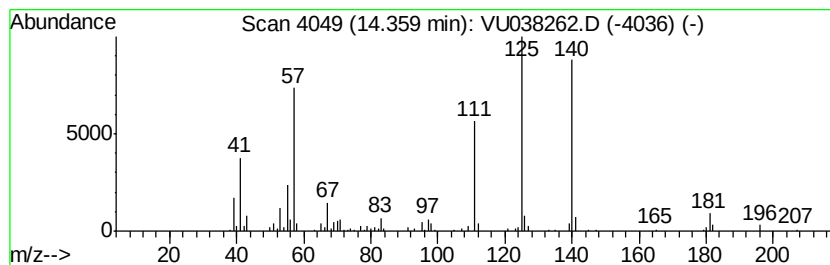
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzenethiol, 4-methoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	0.94 ug/L	215070	1,4-Dichlorobenzene-d4	11.83
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzenethiol, 4-methoxy-	140 C7H8OS	000696-63-9 53
2		Phenol, 4-(methylthio)-	140 C7H8OS	001073-72-9 53
3		3-Amino-5-t-butylisoxazole	140 C7H12N2O	055809-36-4 50
4		1-(2-Thienyl)-1-propanone	140 C7H8OS	013679-75-9 43
5		Benzenethiol, 2-methoxy-	140 C7H8OS	007217-59-6 43



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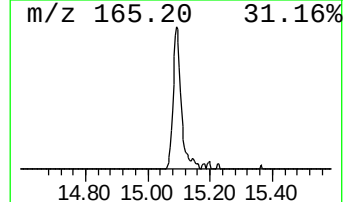
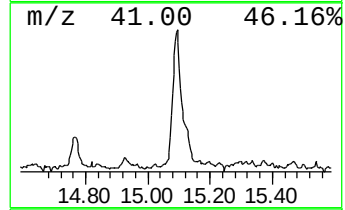
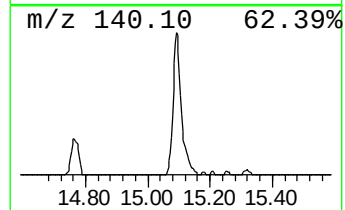
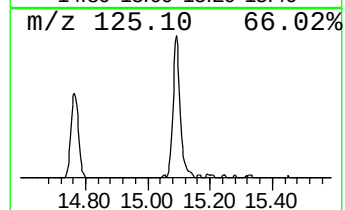
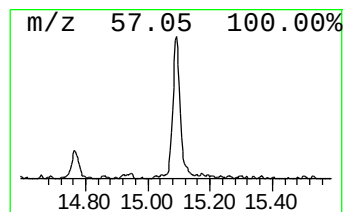
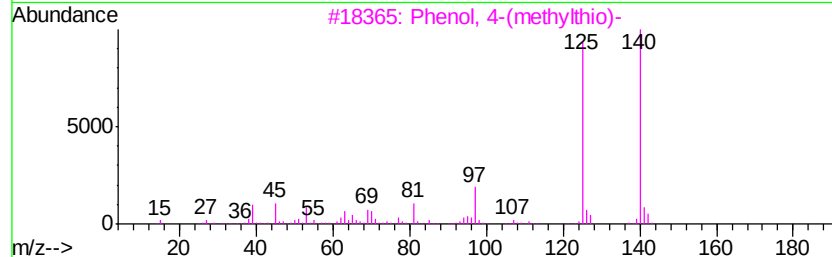
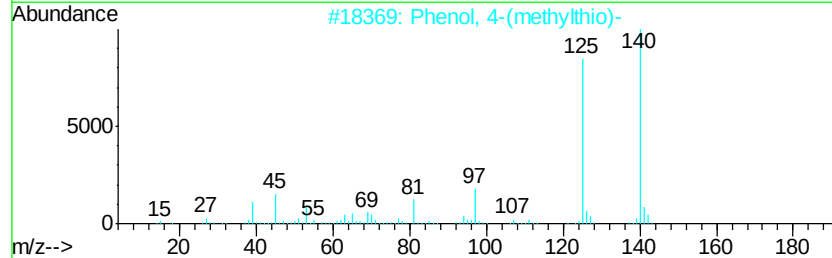
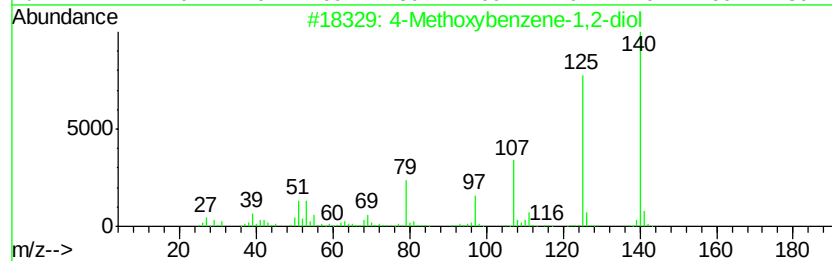
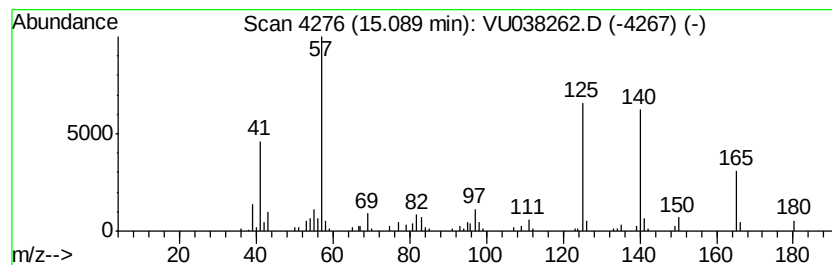
Instrument :
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 4-Methoxybenzene-1,2-diol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.09	0.51 ug/L	117899	1,4-Dichlorobenzene-d4	11.83		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Methoxybenzene-1,2-diol	140	C7H8O3	003934-97-2	58
2		Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	52
3		Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	52
4		Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	52
5		3-tert-Butyl-2-pyrazolin-5-one	140	C7H12N2O	029211-68-5	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU052120\
Data File : VU038262.D
Acq On : 21 May 2020 14:21
Operator : JC/MD
Sample : L2724-19
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 6 Sample Multiplier: 1

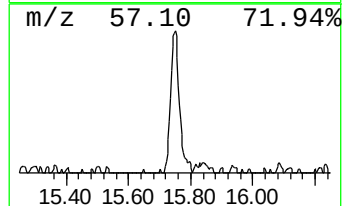
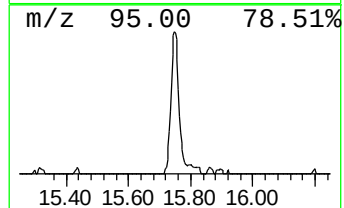
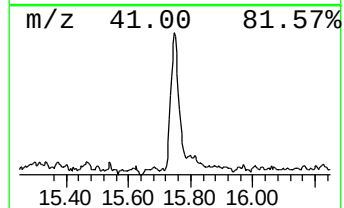
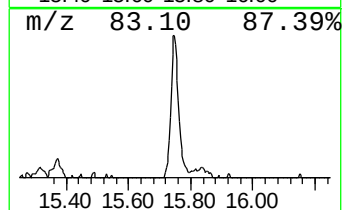
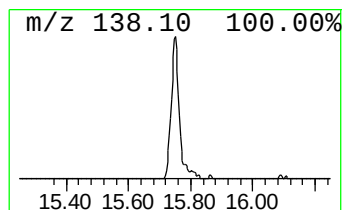
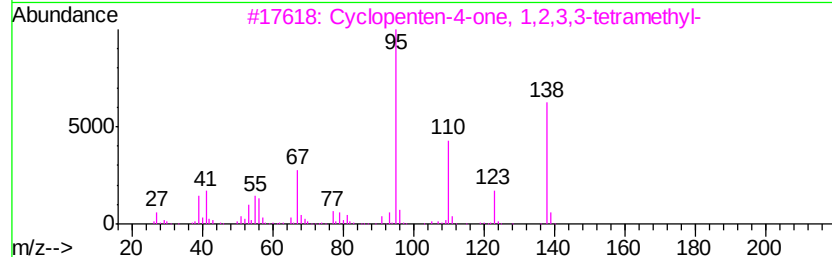
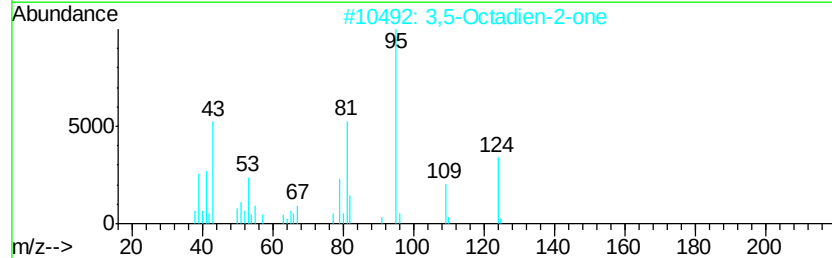
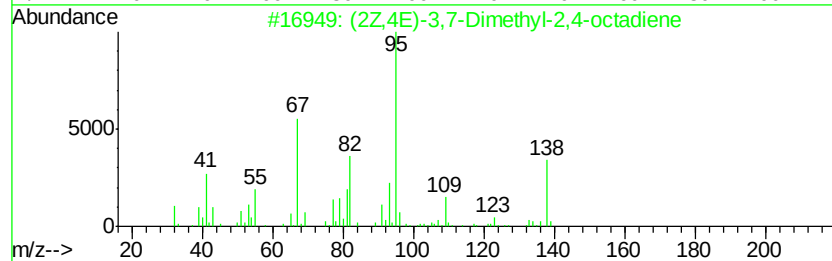
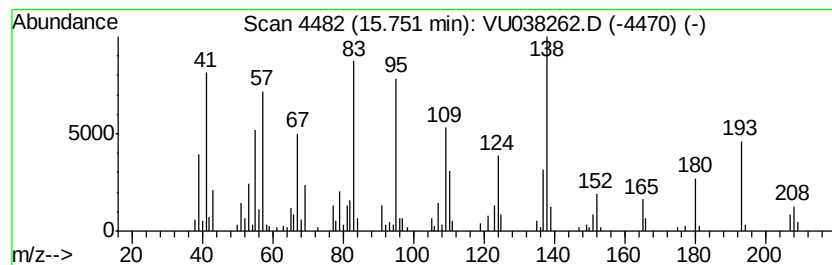
Instrument :
MSVOA_U
ClientSampleId :
BE4W5

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 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.75	0.54 ug/L	125071	1,4-Dichlorobenzene-d4	11.83	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(2Z,4E)-3,7-Dimethyl-2,4-octadiene	138	C10H18	1000374-08-4	38
2	3,5-Octadien-2-one	124	C8H12O	038284-27-4	35
3	Cyclopenten-4-one, 1,2,3,3-tetra...	138	C9H14O	1000163-38-6	30
4	10.alpha.-Eremophilane	208	C15H28	003242-05-5	27
5	Spiro[2.3]hexane-5-carboxylic ac...	278	C18H30O2	1000152-25-7	22



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU052120\
Data File : VU038262.D
Acq On : 21 May 2020 14:21
Operator : JC/MD
Sample : L2724-19
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BE4W5

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	5.3	ug/L	956258	1	6.28	899838	5.0
Propane, 2-methyl...	4.48	13.1	ug/L	2348270	1	6.28	899838	5.0
(DEL) Alkane: Str...	7.16	10.0	ug/L	1806750	1	6.28	899838	5.0
Benzenethiol, 4-m...	14.36	0.9	ug/L	215070	3	11.83	1147860	5.0
4-Methoxybenzene-...	15.09	0.5	ug/L	117899	3	11.83	1147860	5.0
unknown-01	15.75	0.5	ug/L	125071	3	11.83	1147860	5.0