

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU101920\
 Data File : VU040835.D
 Acq On : 20 Oct 2020 03:42
 Operator : SY/MD
 Sample : L4428-06
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 48 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETZ31

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\SOMUTR100820WMA.M
 Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.366	3	8	28	rVB	2048564	1924275	100.00%	23.617%
2	1.494	34	48	75	rBV2	625522	1267620	65.88%	15.558%
3	1.607	76	83	94	rVB2	591041	668477	34.74%	8.204%
4	1.922	175	181	191	rVB	43030	55503	2.88%	0.681%
5	2.006	199	207	217	rVB	93606	128073	6.66%	1.572%
6	2.215	263	272	287	rVB	68731	99461	5.17%	1.221%
7	2.581	373	386	400	rBV	72445	119478	6.21%	1.466%
8	3.153	555	564	578	rVB2	17598	34051	1.77%	0.418%
9	4.552	983	999	1015	rVB2	18218	41617	2.16%	0.511%
10	4.681	1015	1039	1084	rBV3	104440	412562	21.44%	5.063%
11	5.083	1147	1164	1190	rBV	88719	197112	10.24%	2.419%
12	5.407	1250	1265	1278	rVB3	19857	43064	2.24%	0.529%
13	5.742	1350	1369	1397	rVB2	158477	427805	22.23%	5.251%
14	6.263	1516	1531	1553	rBV	150024	277927	14.44%	3.411%
15	6.703	1654	1668	1682	rBV	110456	218533	11.36%	2.682%
16	6.774	1682	1690	1705	rVB4	14006	26875	1.40%	0.330%
17	7.575	1927	1939	1959	rBV	48602	84785	4.41%	1.041%
18	7.906	2029	2042	2058	rBV	157959	267875	13.92%	3.288%
19	8.185	2116	2129	2145	rBV	33707	55817	2.90%	0.685%
20	8.642	2257	2271	2305	rBV	355850	674540	35.05%	8.279%
21	9.420	2499	2513	2532	rBV	223059	364449	18.94%	4.473%
22	10.754	2917	2928	2942	rBV	101857	163957	8.52%	2.012%
23	11.806	3243	3255	3275	rBV	185470	297002	15.43%	3.645%
24	12.185	3361	3373	3389	rBV	184890	296964	15.43%	3.645%

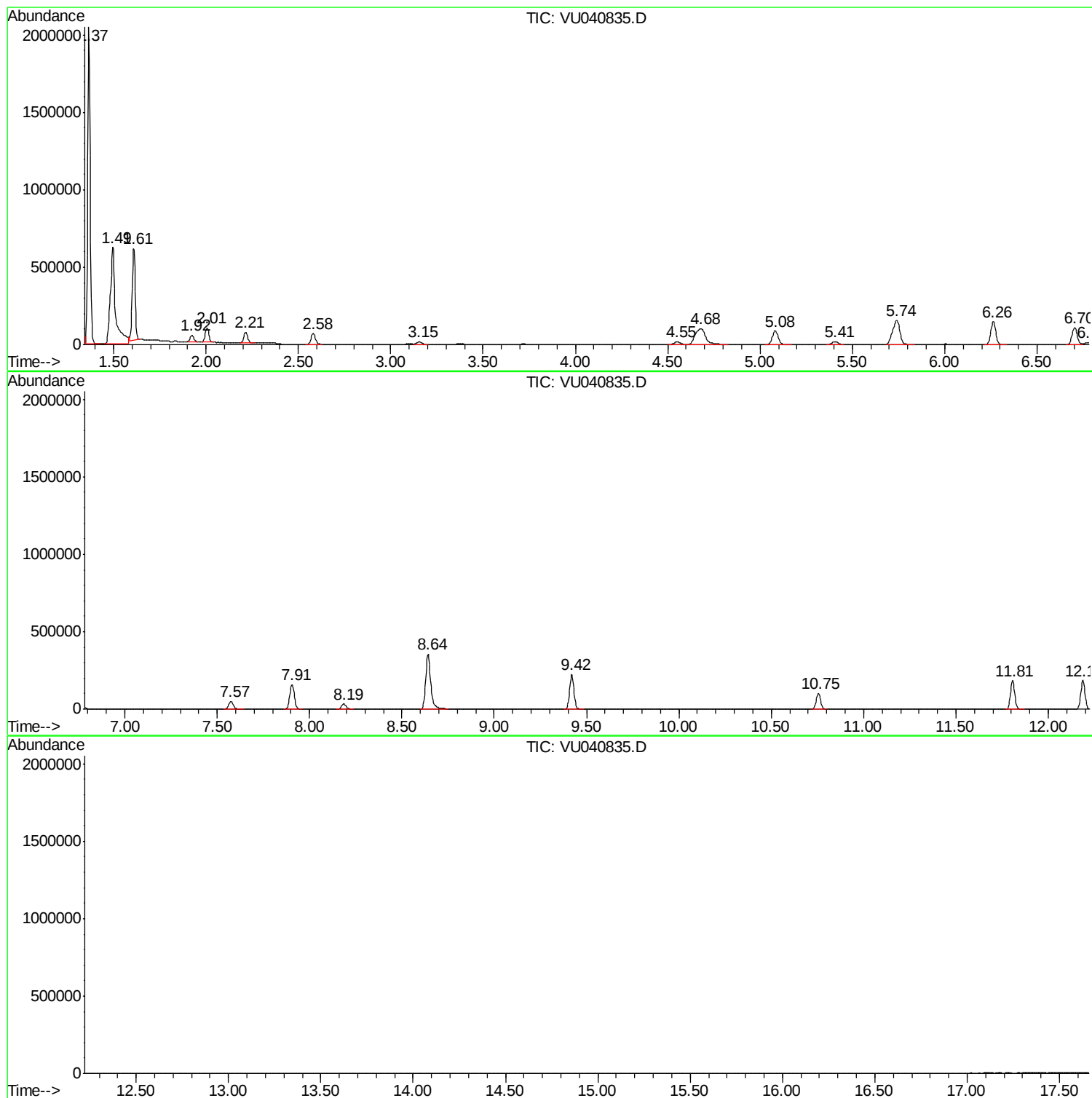
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR100820WMA.M
Quant Title : TRACE VOA SOM01.0

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



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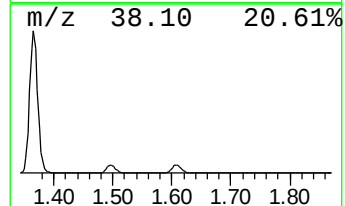
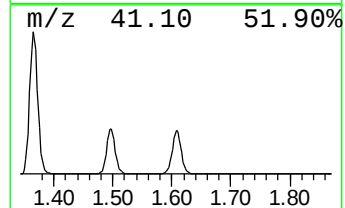
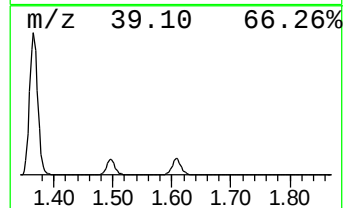
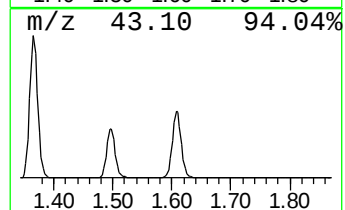
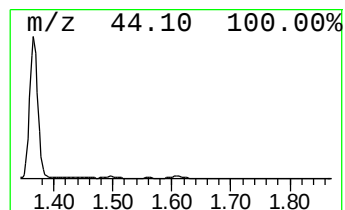
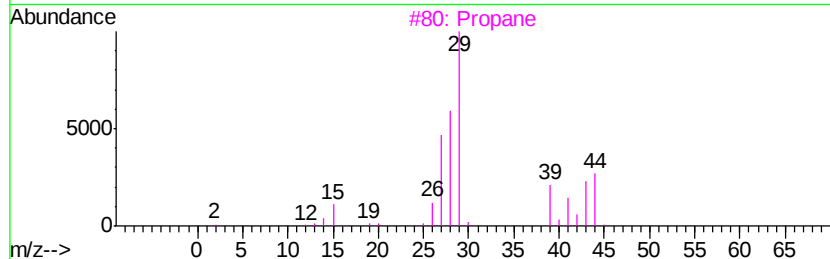
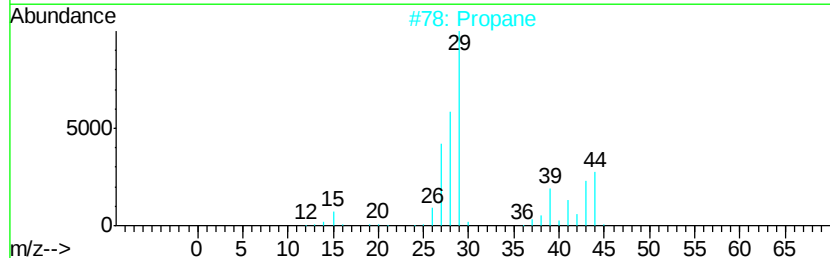
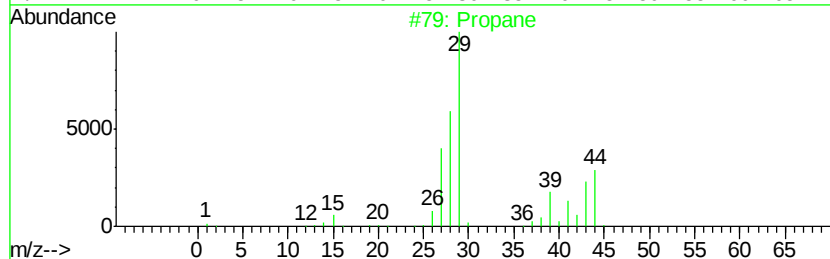
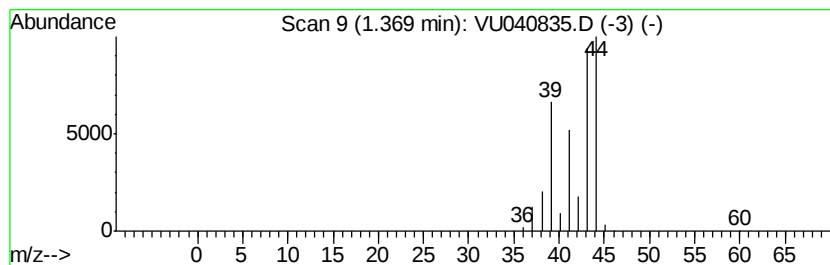
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Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.37	34.62 ug/L	1924280	1,4-Difluorobenzene	6.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane	44	C3H8	000074-98-6	83
2		Propane	44	C3H8	000074-98-6	83
3		Propane	44	C3H8	000074-98-6	9
4		Propene	42	C3H6	000115-07-1	9
5		Acetaldehyde	44	C2H4O	000075-07-0	5



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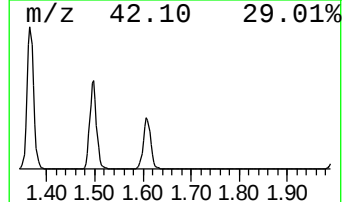
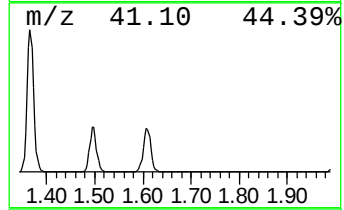
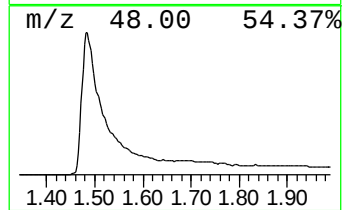
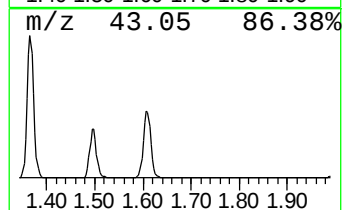
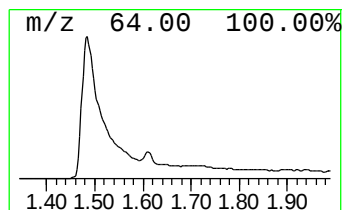
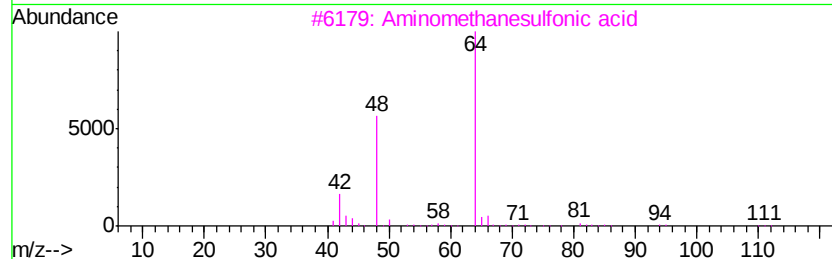
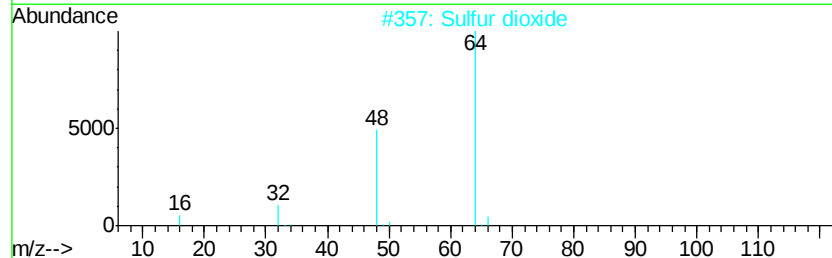
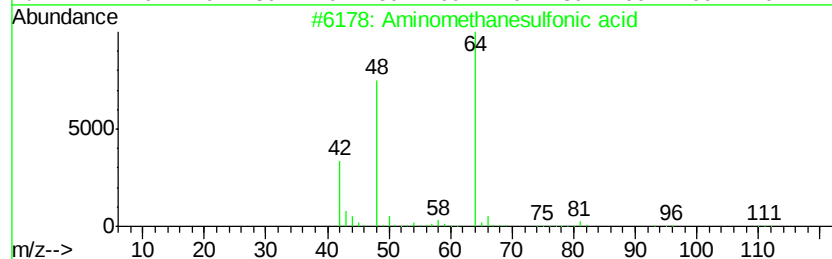
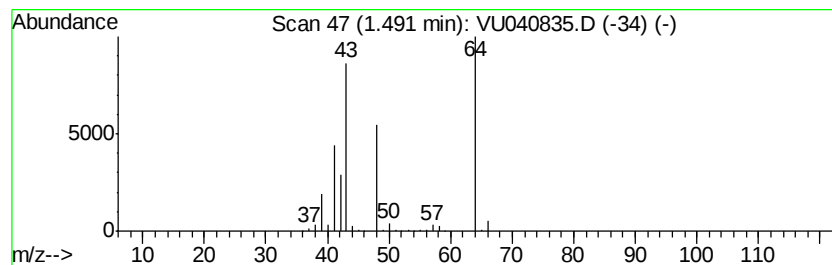
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 Aminomethanesulfonic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.49	22.80 ug/L	1267620	1,4-Difluorobenzene	6.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	83
2		Sulfur dioxide	64	O2S	007446-09-5	72
3		Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	43
4		L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5		Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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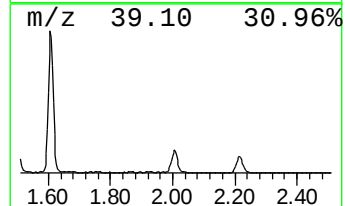
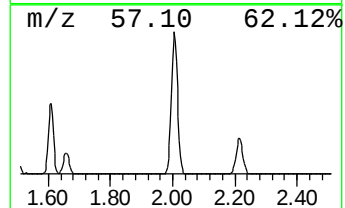
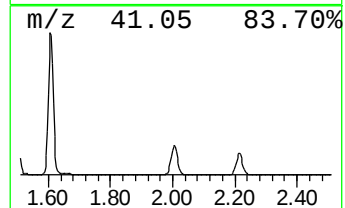
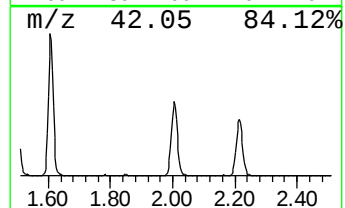
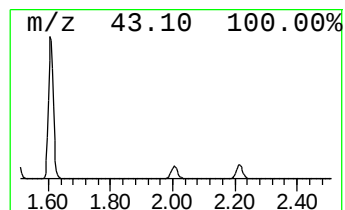
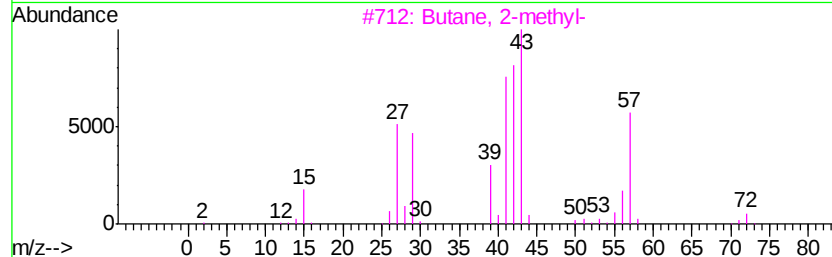
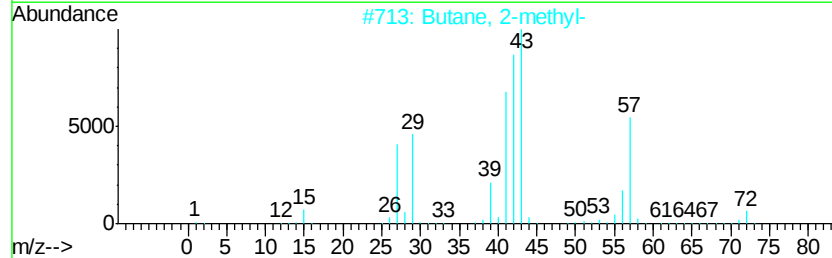
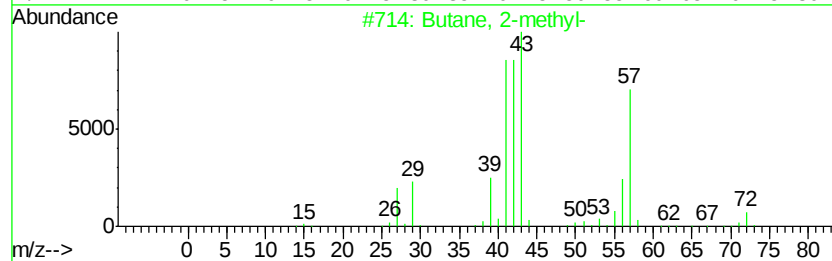
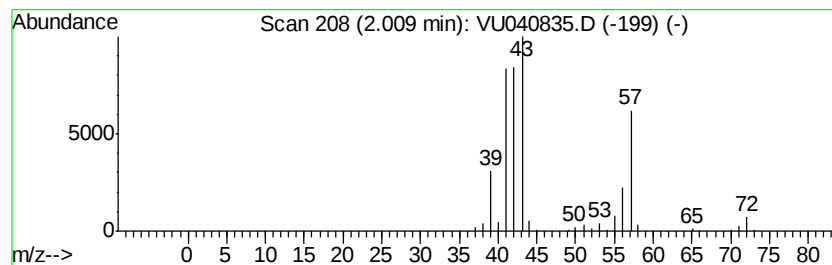
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Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.01	2.30 ug/L	128073	1,4-Difluorobenzene	6.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methyl-	72	C5H12	000078-78-4	94
2		Butane, 2-methyl-	72	C5H12	000078-78-4	91
3		Butane, 2-methyl-	72	C5H12	000078-78-4	91
4		Isobutylene epoxide	72	C4H8O	000558-30-5	53
5		3-Buten-1-ol	72	C4H8O	000627-27-0	47



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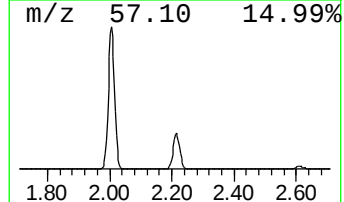
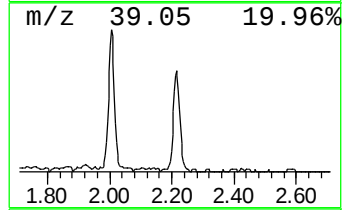
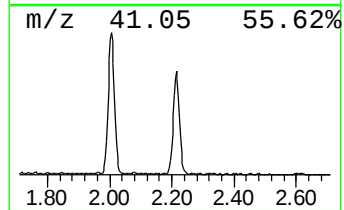
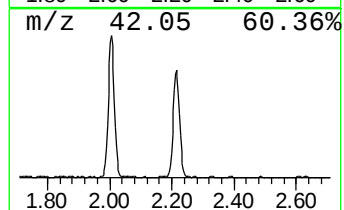
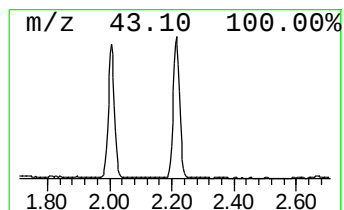
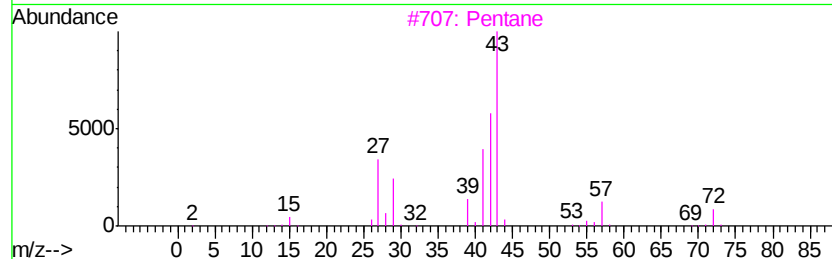
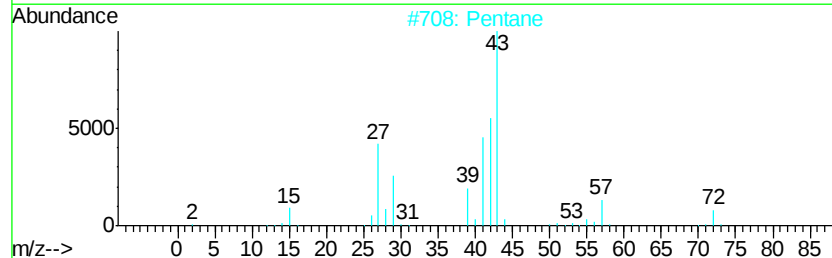
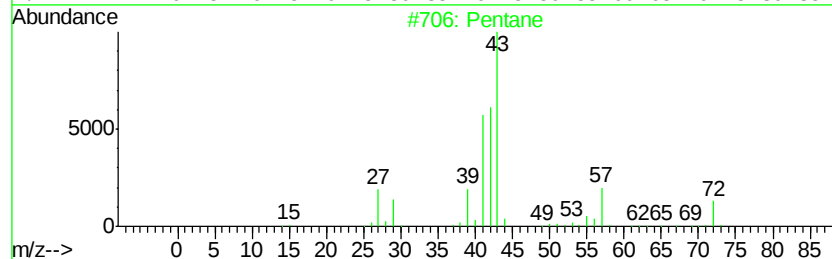
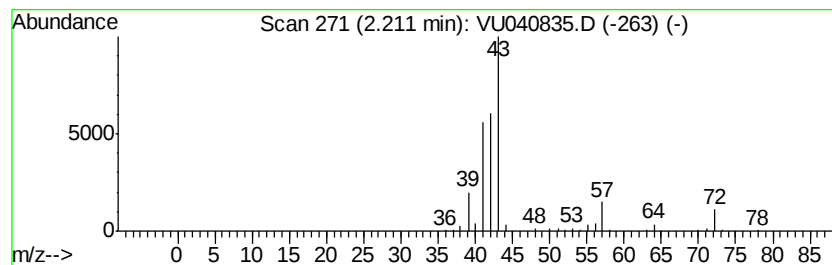
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.21	1.79 ug/L	99461	1,4-Difluorobenzene	6.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane	72	C5H12	000109-66-0	90
2		Pentane	72	C5H12	000109-66-0	86
3		Pentane	72	C5H12	000109-66-0	80
4		Pentane	72	C5H12	000109-66-0	64
5		Oxirane, ethyl-	72	C4H8O	000106-88-7	47



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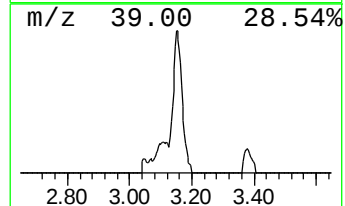
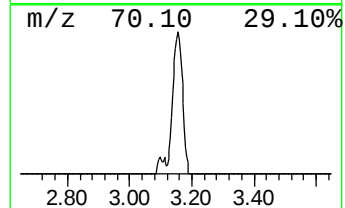
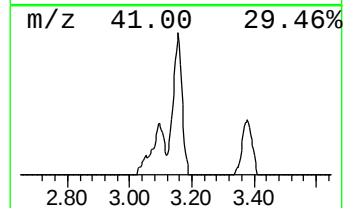
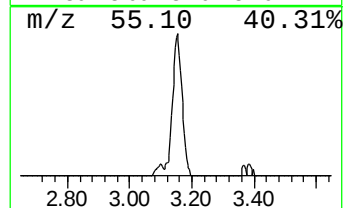
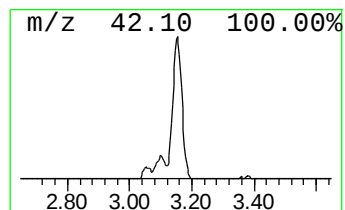
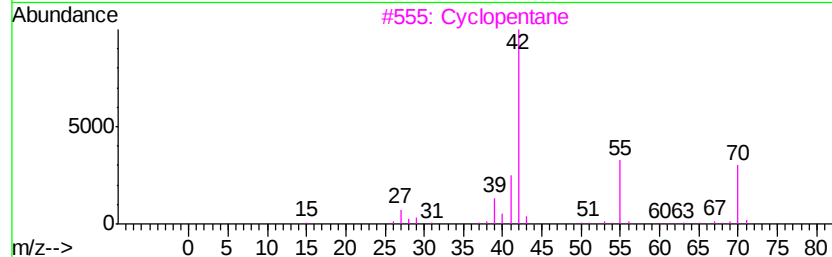
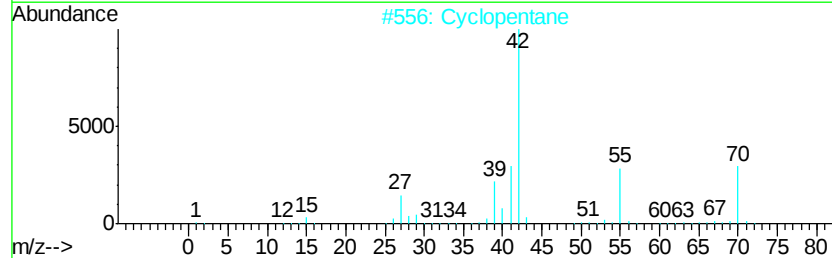
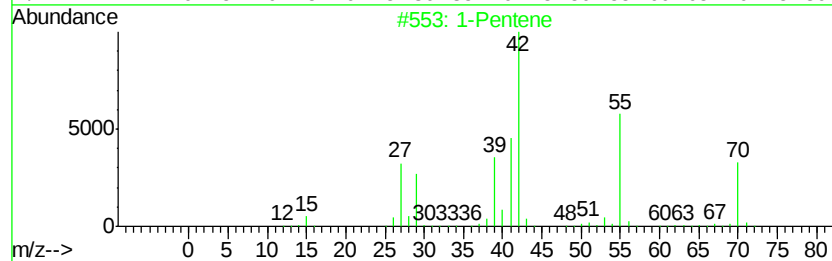
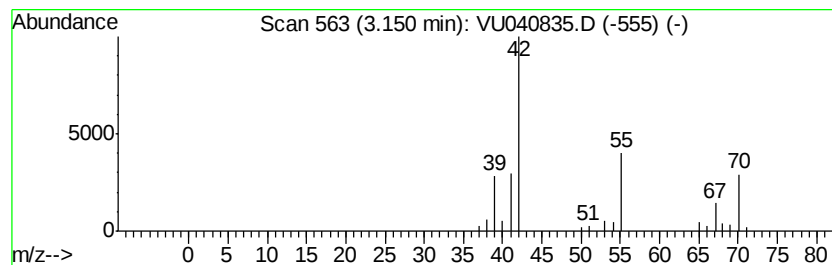
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.15	0.61 ug/L	34051	1,4-Difluorobenzene	6.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Pentene	70	C5H10	000109-67-1	72
2		Cyclopentane	70	C5H10	000287-92-3	64
3		Cyclopentane	70	C5H10	000287-92-3	64
4		1-Pentene	70	C5H10	000109-67-1	59
5		Cyclopropane, ethyl-	70	C5H10	001191-96-4	46



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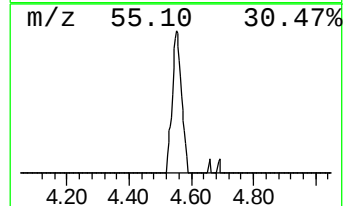
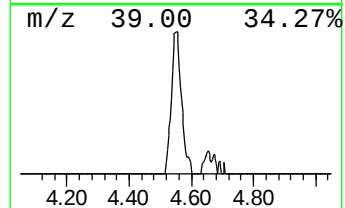
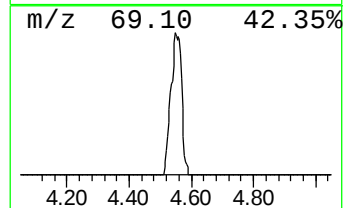
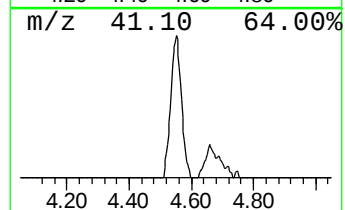
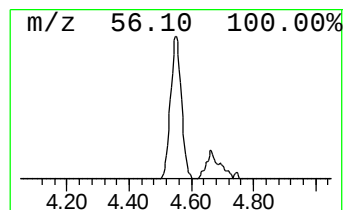
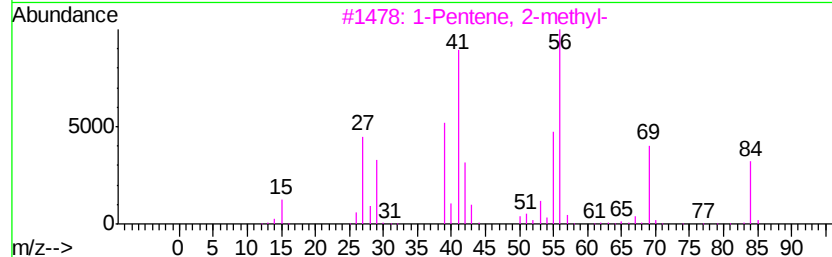
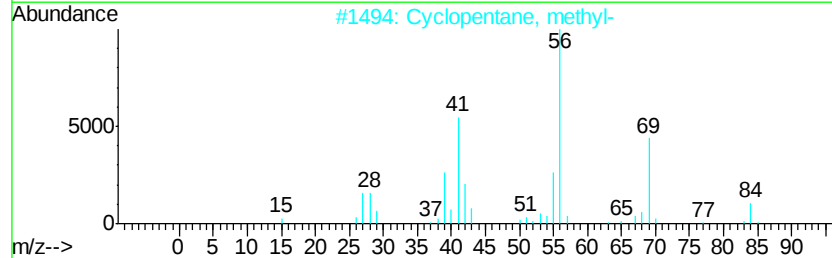
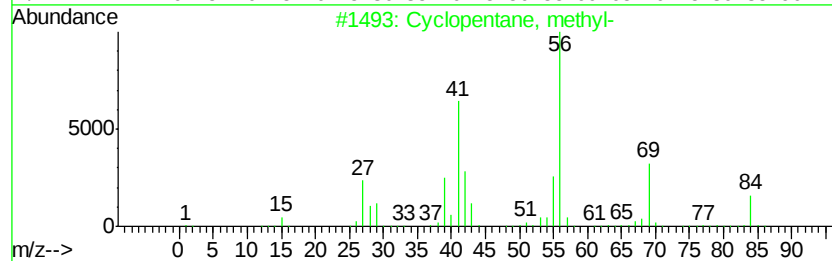
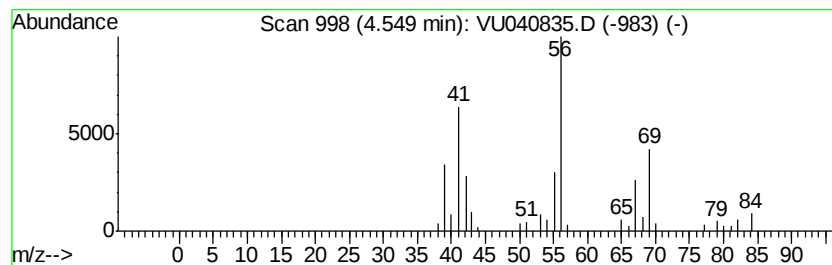
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR100820WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 (DEL) Alkane: Cyclic4.55 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	0.75 ug/L	41617	1,4-Difluorobenzene	6.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, methyl-	84	C6H12	000096-37-7	64
2		Cyclopentane, methyl-	84	C6H12	000096-37-7	58
3		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	53
4		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	50
5		Cyclobutane, ethyl-	84	C6H12	004806-61-5	47



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU101920\
Data File : VU040835.D
Acq On : 20 Oct 2020 03:42
Operator : SY/MD
Sample : L4428-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETZ31

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR100820WMA.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
(DEL) Alkane: Str...	1.37	34.6	ug/L	1924280	1	6.26	277927	5.0
Aminomethanesulfo...	1.49	22.8	ug/L	1267620	1	6.26	277927	5.0
(DEL) Alkane: Str...	2.01	2.3	ug/L	128073	1	6.26	277927	5.0
(DEL) Alkane: Str...	2.21	1.8	ug/L	99461	1	6.26	277927	5.0
(DEL) Alkane: Str...	3.15	0.6	ug/L	34051	1	6.26	277927	5.0
(DEL) Alkane: Cyc...	4.55	0.8	ug/L	41617	1	6.26	277927	5.0