

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\U121219\
 Data File : VU036164.D
 Acq On : 12 Dec 2019 21:36
 Operator : JC/MD
 Sample : K6273-07
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFDQ4

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\SOMUTR121219WMA.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	3	9	29	rVB	1560356	1500243	100.00%	11.903%
2	1.456	31	36	44	rVB2	15935	17591	1.17%	0.140%
3	1.504	44	51	58	rBV	99989	103349	6.89%	0.820%
4	1.610	73	84	98	rBV3	710310	1173239	78.20%	9.308%
5	1.675	99	104	108	rVV	29854	33782	2.25%	0.268%
6	1.704	108	113	120	rVV2	26060	33662	2.24%	0.267%
7	1.749	120	127	139	rVB	95551	115462	7.70%	0.916%
8	1.929	174	183	197	rVB2	185739	261750	17.45%	2.077%
9	2.012	201	209	221	rVB	106268	143965	9.60%	1.142%
10	2.176	250	260	267	rBV	149818	206251	13.75%	1.636%
11	2.224	267	275	294	rVB3	132777	233520	15.57%	1.853%
12	2.340	304	311	319	rVB2	17688	24526	1.63%	0.195%
13	2.437	333	341	352	rVB	56956	91769	6.12%	0.728%
14	2.488	353	357	373	rVB2	11417	17373	1.16%	0.138%
15	2.594	377	390	405	rBV	229891	377593	25.17%	2.996%
16	2.675	405	415	427	rVB	12963	25672	1.71%	0.204%
17	2.822	449	461	475	rBV2	26941	48444	3.23%	0.384%
18	3.012	504	520	532	rBV10	12230	33640	2.24%	0.267%
19	3.118	544	553	562	rVB4	10148	18611	1.24%	0.148%
20	3.398	627	640	655	rVB6	13856	30119	2.01%	0.239%
21	3.626	697	711	728	rVB3	26193	59649	3.98%	0.473%
22	3.739	733	746	763	rVB5	16603	38660	2.58%	0.307%
23	4.691	1024	1042	1064	rBV	160055	444196	29.61%	3.524%
24	5.112	1156	1173	1194	rBV	213441	471066	31.40%	3.737%
25	5.771	1354	1378	1407	rBV2	400593	1051138	70.06%	8.339%
26	6.067	1461	1470	1482	rVB9	8461	16999	1.13%	0.135%
27	6.170	1488	1502	1514	rBV9	5743	15053	1.00%	0.119%
28	6.292	1525	1540	1559	rBV	317536	616319	41.08%	4.890%
29	6.584	1619	1631	1643	rBV5	18602	39676	2.64%	0.315%
30	6.732	1660	1677	1696	rBV	256280	499493	33.29%	3.963%
31	7.600	1934	1947	1961	rBV2	115073	205886	13.72%	1.633%
32	7.932	2035	2050	2064	rBV	429191	750821	50.05%	5.957%
33	7.999	2067	2071	2081	rVB5	11734	19189	1.28%	0.152%
34	8.215	2126	2138	2153	rBV3	85509	180548	12.03%	1.432%

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Instrument :
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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\SOMUTR121219WMA.M
Title : TRACE VOA SOM01.0

35	8.678	2269	2282	2310	rBV	550814	1129994	75.32%	8.965%
36	8.822	2321	2327	2338	rVB9	12010	20391	1.36%	0.162%
37	9.446	2509	2521	2554	rBV	483811	833724	55.57%	6.615%
38	10.784	2925	2937	2952	rBV	232653	375489	25.03%	2.979%
39	11.835	3251	3264	3280	rBV	379662	627946	41.86%	4.982%
40	12.214	3370	3382	3399	rVB	399561	667276	44.48%	5.294%
41	12.909	3588	3598	3608	rBV6	17162	25558	1.70%	0.203%
42	16.359	4664	4671	4681	rBV7	17601	24792	1.65%	0.197%

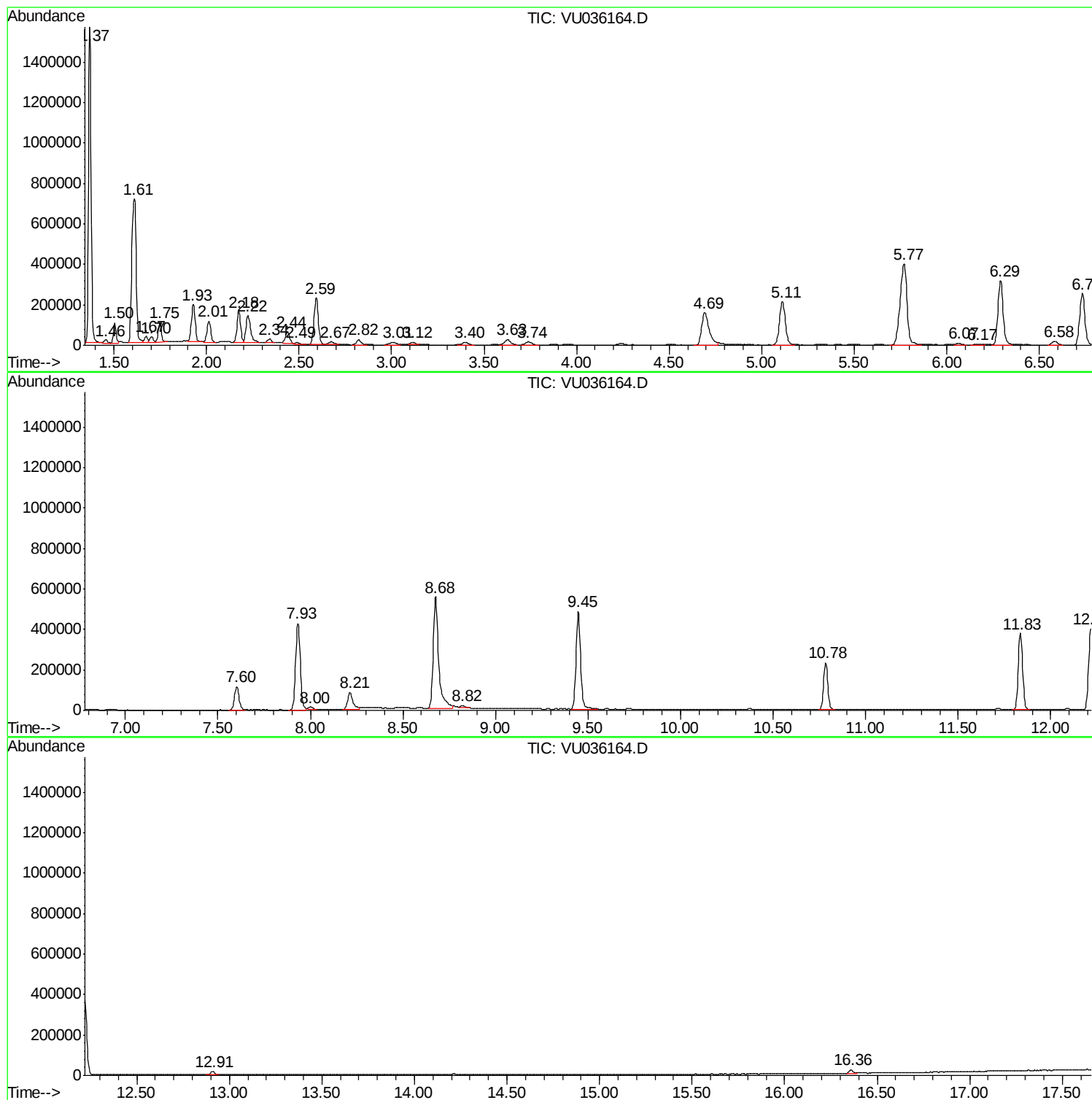
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BFDQ4

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121219WMA.M
Quant Title : TRACE VOA SOM01.0

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



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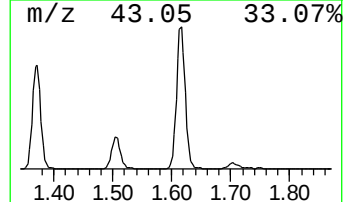
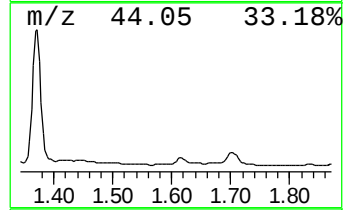
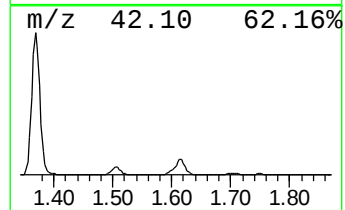
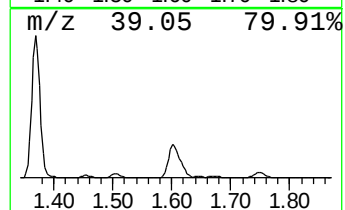
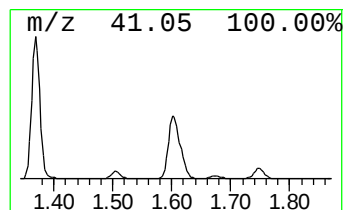
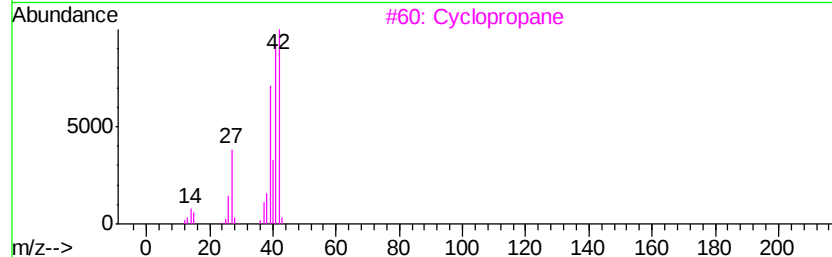
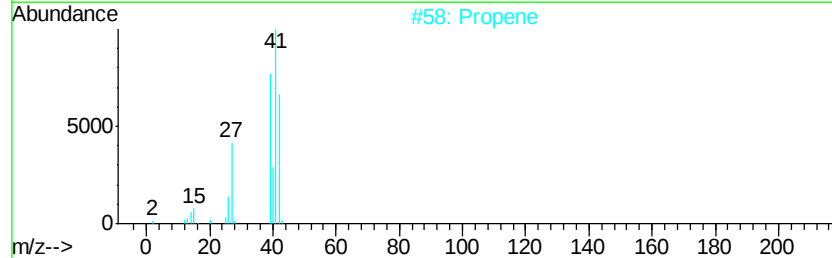
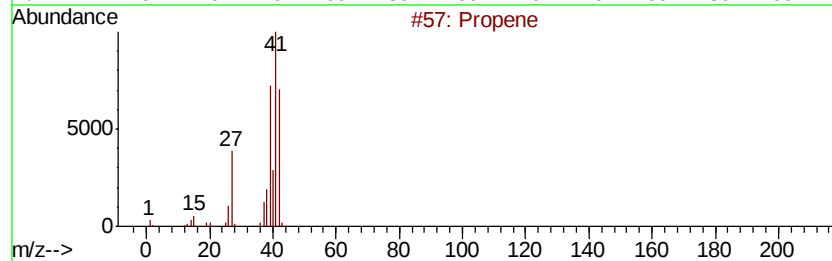
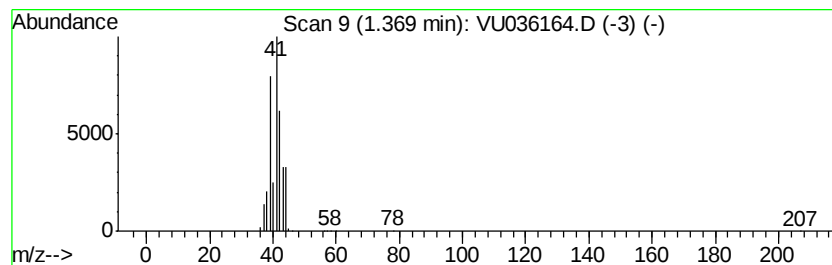
Instrument :
MSVOA_U
ClientSampleId :
BFDQ4

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121219WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 (DEL) Alkane: Cyclic1.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.37	12.17 ug/L	1500240	1,4-Difluorobenzene	6.29
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Propene		42 C3H6	000115-07-1 90
2	Propene		42 C3H6	000115-07-1 42
3	Cyclopropane		42 C3H6	000075-19-4 9
4	Cyclopropene		40 C3H4	002781-85-3 9
5	Cyclopropane		42 C3H6	000075-19-4 7



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Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFDQ4

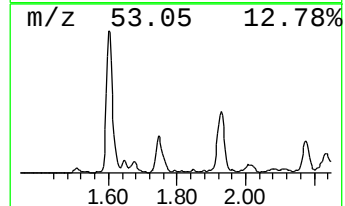
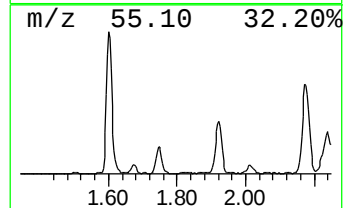
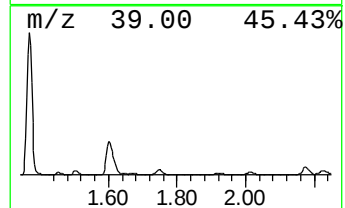
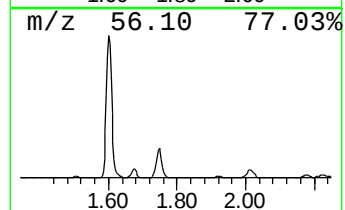
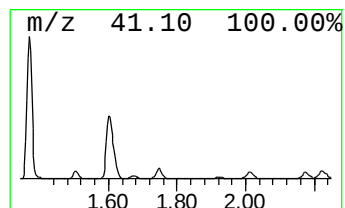
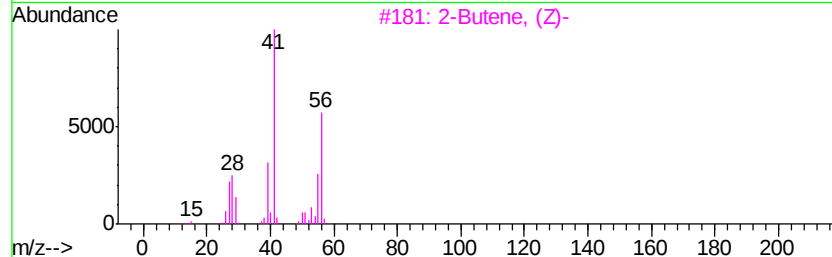
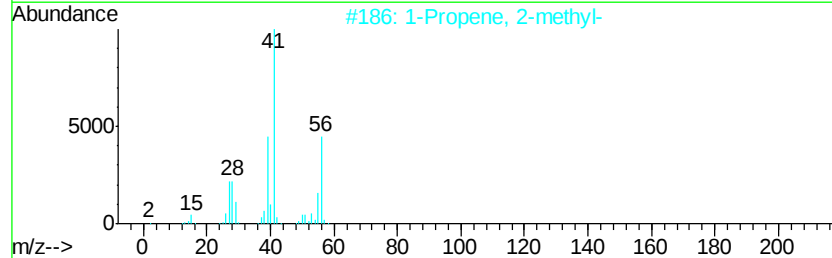
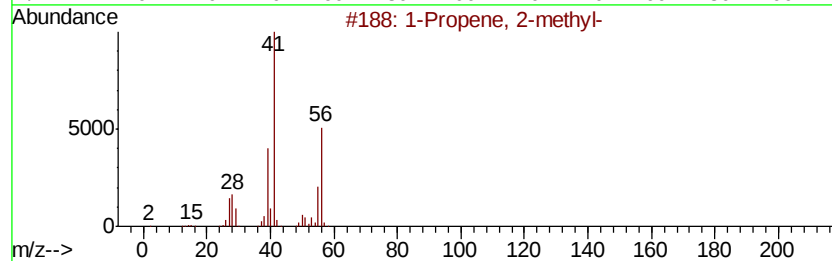
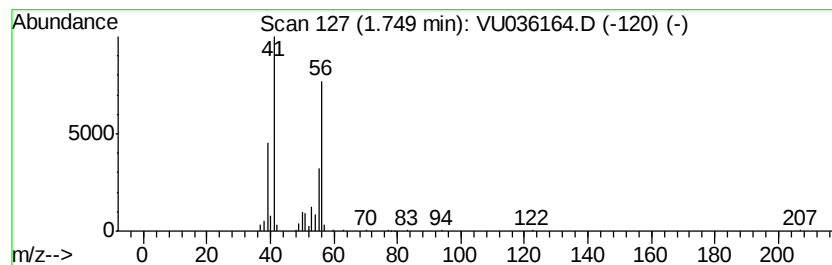
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121219WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 (DEL) Alkane: Cyclic1.75 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.75	0.94 ug/L	115462	1,4-Difluorobenzene	6.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-methyl-		56	C4H8	000115-11-7	80
2	1-Propene, 2-methyl-		56	C4H8	000115-11-7	80
3	2-Butene, (Z)-		56	C4H8	000590-18-1	80
4	2-Butene		56	C4H8	000107-01-7	74
5	2-Butene, (Z)-		56	C4H8	000590-18-1	74



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MSVOA_U
ClientSampleId :
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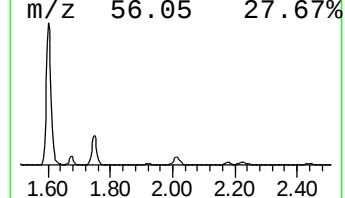
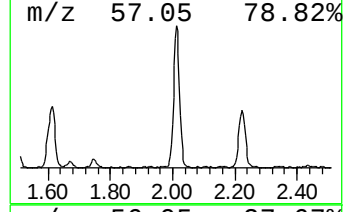
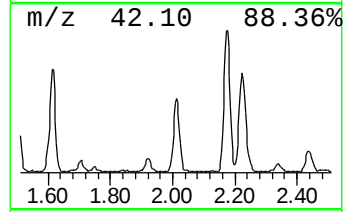
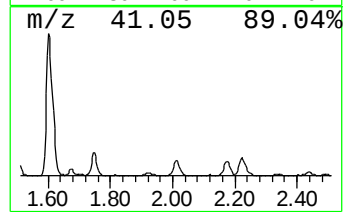
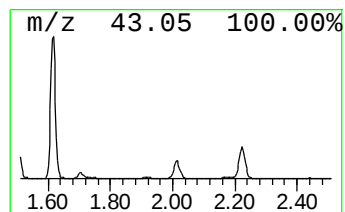
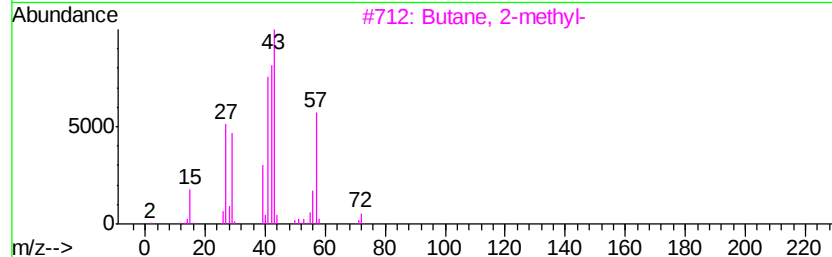
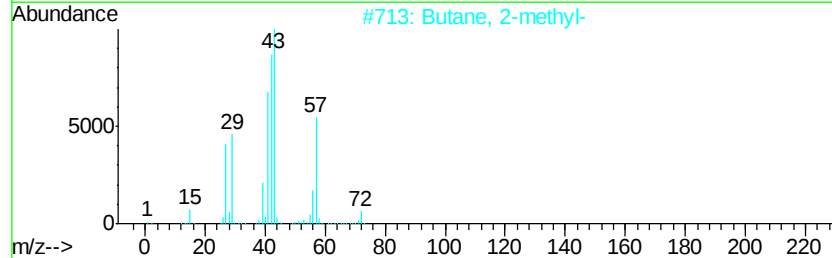
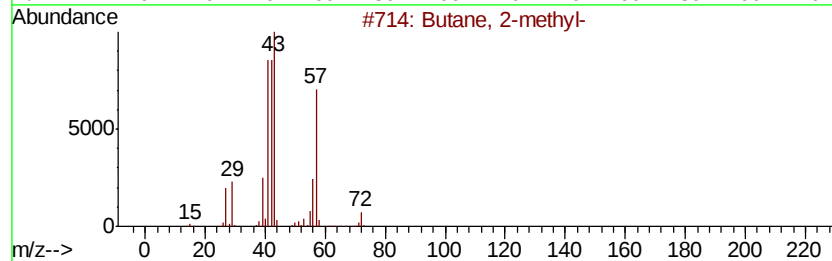
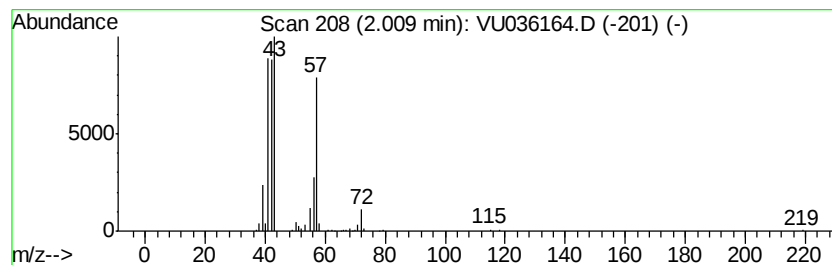
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121219WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.01	1.17 ug/L	143965	1,4-Difluorobenzene	6.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2		Butane, 2-methyl-	72	C5H12	000078-78-4	87
3		Butane, 2-methyl-	72	C5H12	000078-78-4	80
4		3-Buten-1-ol	72	C4H8O	000627-27-0	43
5		Pentane	72	C5H12	000109-66-0	42



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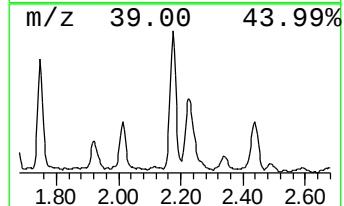
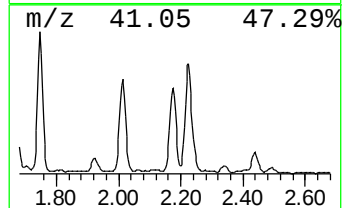
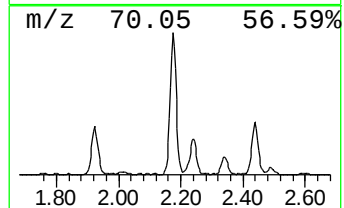
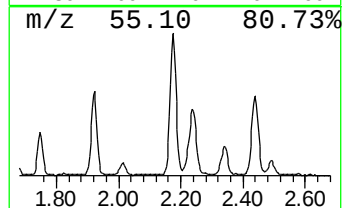
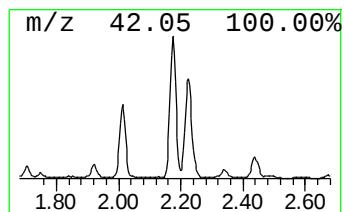
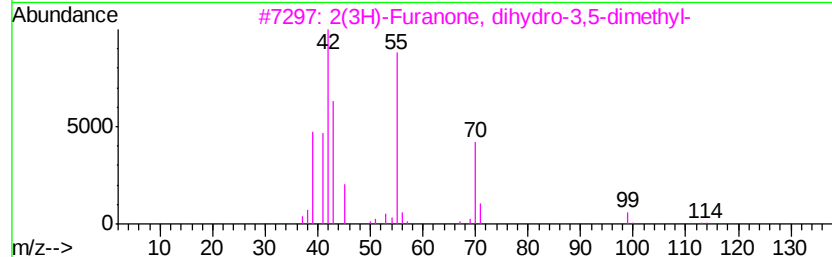
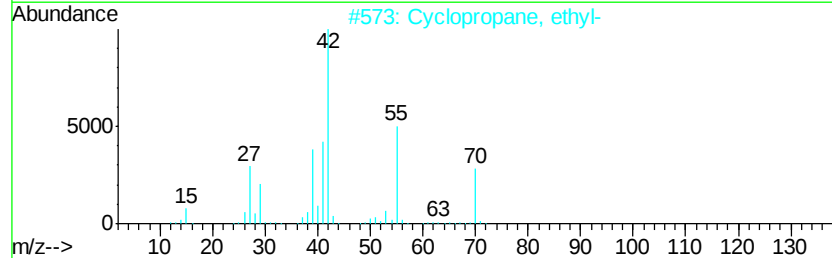
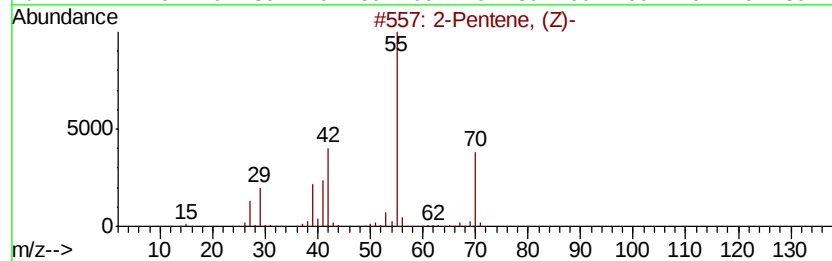
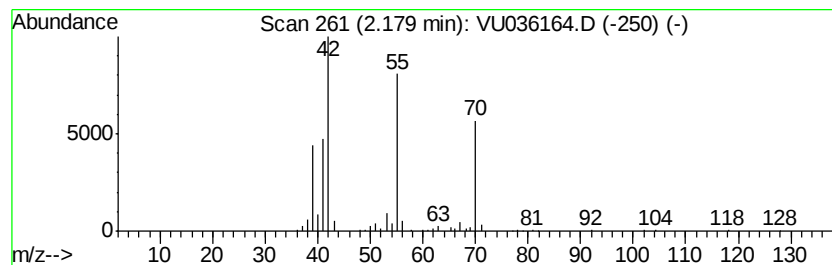
Instrument :
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ClientSampled :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 (DEL) Alkane: Cyclic2.18 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.18	1.67 ug/L	206251	1,4-Difluorobenzene	6.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, (Z)-	70	C5H10	000627-20-3	87
2	Cyclopropane, ethyl-	70	C5H10	001191-96-4	76
3	2(3H)-Furanone, dihydro-3,5-dime...	114	C6H10O2	005145-01-7	64
4	1-Pentene	70	C5H10	000109-67-1	64
5	1-Pentene	70	C5H10	000109-67-1	64



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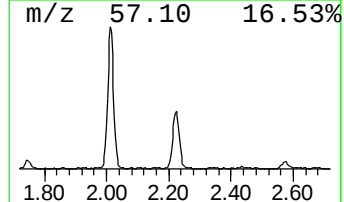
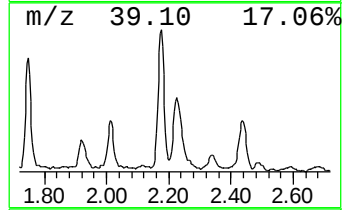
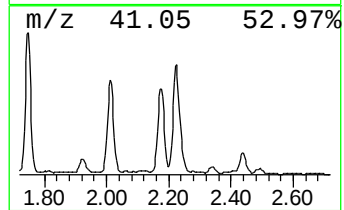
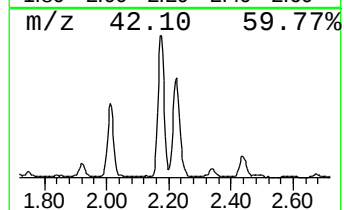
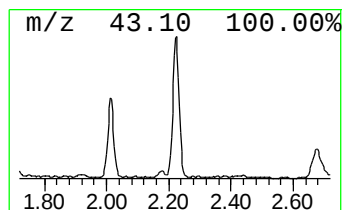
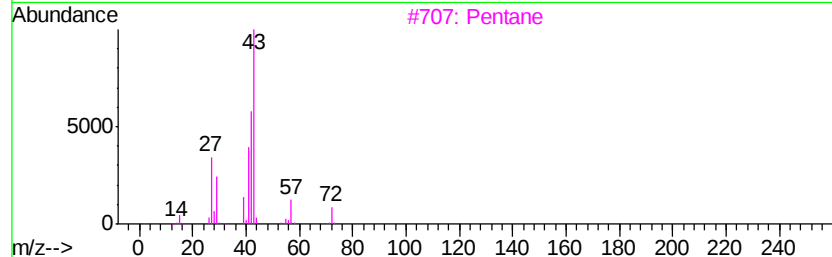
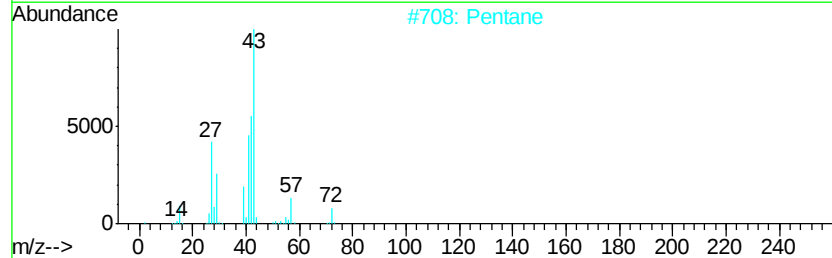
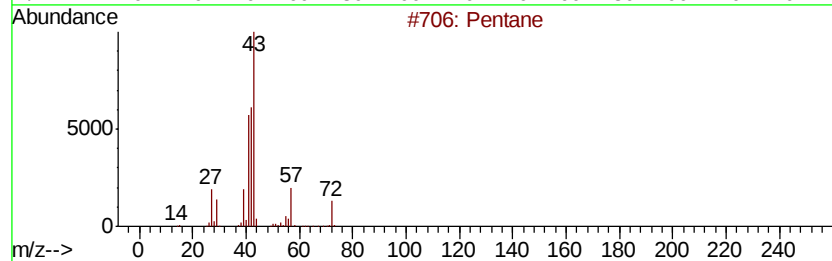
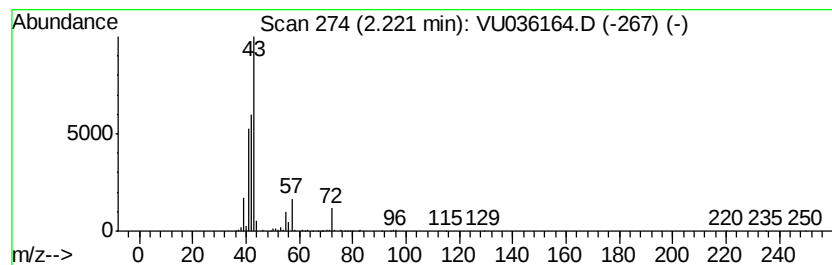
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121219WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	1.89 ug/L	233520	1,4-Difluorobenzene	6.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane	72	C5H12	000109-66-0	87
2		Pentane	72	C5H12	000109-66-0	80
3		Pentane	72	C5H12	000109-66-0	80
4		Pentane	72	C5H12	000109-66-0	64
5		Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	9



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU121219\
Data File : VU036164.D
Acq On : 12 Dec 2019 21:36
Operator : JC/MD
Sample : K6273-07
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFDQ4

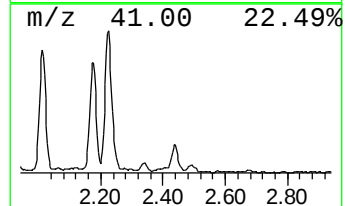
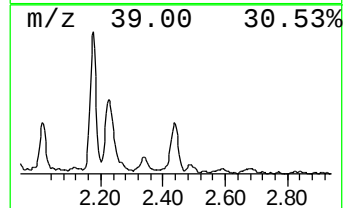
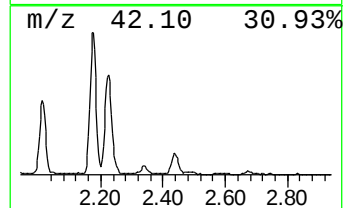
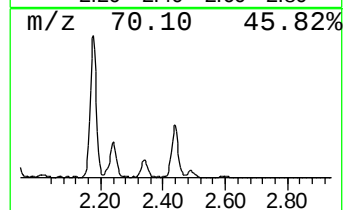
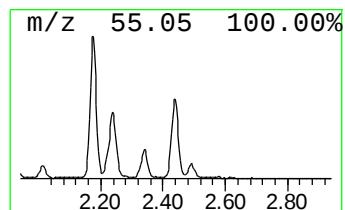
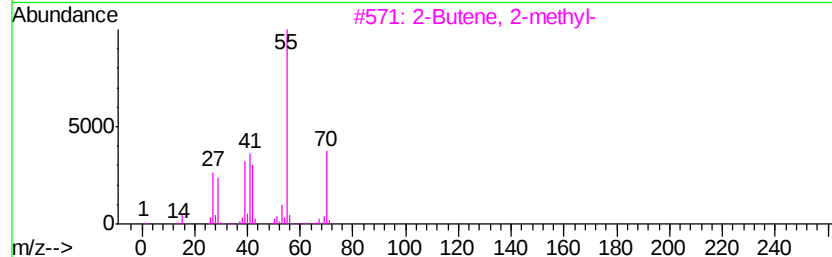
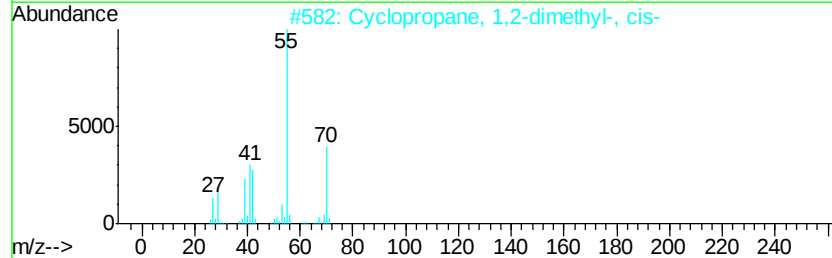
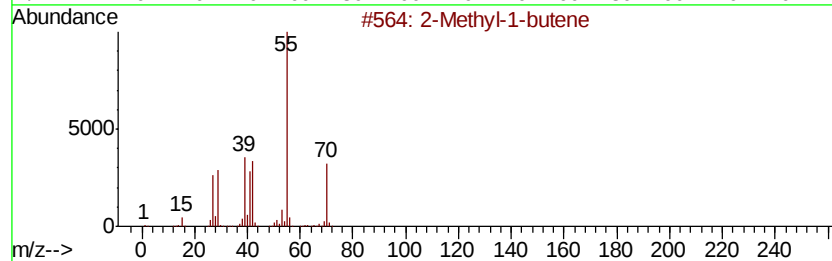
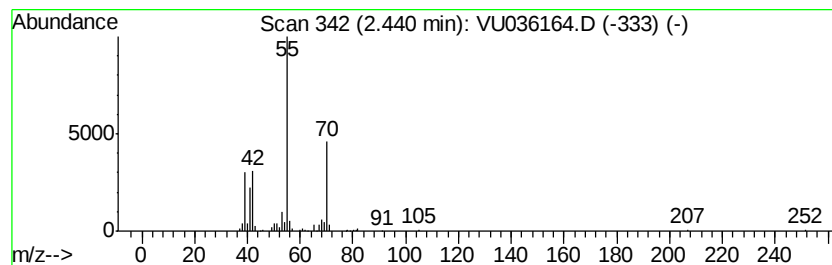
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 (DEL) Alkane: Cyclic2.44 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.44	0.74 ug/L	91769	1,4-Difluorobenzene	6.29

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methyl-1-butene	70	C5H10	000563-46-2	83
2			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	83
3			2-Butene, 2-methyl-	70	C5H10	000513-35-9	83
4			2-Methyl-1-butene	70	C5H10	000563-46-2	83
5			2-Butene, 2-methyl-	70	C5H10	000513-35-9	83



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121219\
Data File : VU036164.D
Acq On : 12 Dec 2019 21:36
Operator : JC/MD
Sample : K6273-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFDQ4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121219WMA.M
Quant Title : TRACE VOA SOM01.0

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

						--Internal Standard--			
TIC Top Hit name	RT	EstConc	Units	Response		#	RT	Resp	Conc
(DEL) Alkane: Cyc...	1.37	12.2	ug/L	1500240		1	6.29	616319	5.0
(DEL) Alkane: Cyc...	1.75	0.9	ug/L	115462		1	6.29	616319	5.0
(DEL) Alkane: Str...	2.01	1.2	ug/L	143965		1	6.29	616319	5.0
(DEL) Alkane: Cyc...	2.18	1.7	ug/L	206251		1	6.29	616319	5.0
(DEL) Alkane: Str...	2.22	1.9	ug/L	233520		1	6.29	616319	5.0
(DEL) Alkane: Cyc...	2.44	0.7	ug/L	91769		1	6.29	616319	5.0