

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU111819\
 Data File : VU035741.D
 Acq On : 18 Nov 2019 13:55
 Operator : JC/SP
 Sample : K5911-01
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 GAQK6

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\SOMUTR110419WMA.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	1.372	3	10	22	rBV	749185	750423	82.68%	7.550%
2	1.459	31	37	42	rBV	24028	23971	2.64%	0.241%
3	1.507	45	52	59	rBV	66291	71406	7.87%	0.718%
4	1.613	75	85	94	rBV3	361370	609845	67.19%	6.136%
5	1.678	101	105	110	rVB	13366	11723	1.29%	0.118%
6	1.752	121	128	137	rBV3	45171	53145	5.86%	0.535%
7	1.877	162	167	175	rBV3	9290	13514	1.49%	0.136%
8	1.935	176	185	198	rVB	121179	170404	18.78%	1.714%
9	2.015	202	210	220	rVB	60799	83131	9.16%	0.836%
10	2.179	252	261	269	rBV	62567	87552	9.65%	0.881%
11	2.234	269	278	302	rVB4	66209	143611	15.82%	1.445%
12	2.443	334	343	352	rVB	24274	38606	4.25%	0.388%
13	2.597	379	391	406	rBV	189638	319884	35.25%	3.218%
14	2.665	407	412	423	rVB3	10183	18478	2.04%	0.186%
15	2.822	454	461	474	rVB	19285	31094	3.43%	0.313%
16	3.006	508	518	532	rVB7	5534	12422	1.37%	0.125%
17	3.115	542	552	562	rVB5	7230	14409	1.59%	0.145%
18	3.363	615	629	662	rBV	118083	267023	29.42%	2.687%
19	3.626	697	711	731	rVB6	16231	44161	4.87%	0.444%
20	3.739	731	746	762	rVB3	10669	23695	2.61%	0.238%
21	4.240	887	902	915	rBV10	4807	11370	1.25%	0.114%
22	4.700	1030	1045	1088	rBV2	134420	407331	44.88%	4.098%
23	5.115	1158	1174	1197	rBV	172471	398109	43.87%	4.005%
24	5.771	1357	1378	1410	rBV2	336759	907576	100.00%	9.131%
25	6.067	1461	1470	1488	rVB2	6869	17486	1.93%	0.176%
26	6.292	1525	1540	1563	rBV	214905	450518	49.64%	4.533%
27	6.591	1621	1633	1643	rVB	4037	9548	1.05%	0.096%
28	6.665	1643	1656	1664	rBV3	6350	12499	1.38%	0.126%
29	6.735	1664	1678	1695	rBV2	211155	428405	47.20%	4.310%
30	7.604	1933	1948	1970	rBV	90571	180302	19.87%	1.814%
31	7.935	2038	2051	2065	rBV	334958	626509	69.03%	6.303%
32	8.002	2065	2072	2085	rVV	42206	90066	9.92%	0.906%
33	8.070	2087	2093	2108	rVV10	17397	34324	3.78%	0.345%
34	8.160	2111	2121	2129	rVV3	29849	51472	5.67%	0.518%

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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\SOMUTR110419WMA.M
Title : TRACE VOA SOM01.0

35	8.218	2129	2139	2165	rVB2	52969	111631	12.30%	1.123%
36	8.700	2271	2289	2321	rBV2	257965	893149	98.41%	8.986%
37	8.838	2323	2332	2346	rVB6	46157	109878	12.11%	1.105%
38	9.452	2510	2523	2552	rBV	304076	638962	70.40%	6.429%
39	9.603	2562	2570	2587	rVB	14367	27141	2.99%	0.273%
40	9.729	2598	2609	2620	rBV	12008	22755	2.51%	0.229%
41	10.134	2725	2735	2747	rBV6	5366	9993	1.10%	0.101%
42	10.388	2805	2814	2835	rBV6	12030	28352	3.12%	0.285%
43	10.790	2925	2939	2962	rVB	164992	307490	33.88%	3.094%
44	11.726	3219	3230	3241	rBV5	25811	46322	5.10%	0.466%
45	11.845	3254	3267	3285	rBV	242705	470894	51.88%	4.738%
46	12.224	3372	3385	3401	rBV	258628	475183	52.36%	4.781%
47	12.915	3583	3600	3615	rBV	243627	383602	42.27%	3.859%

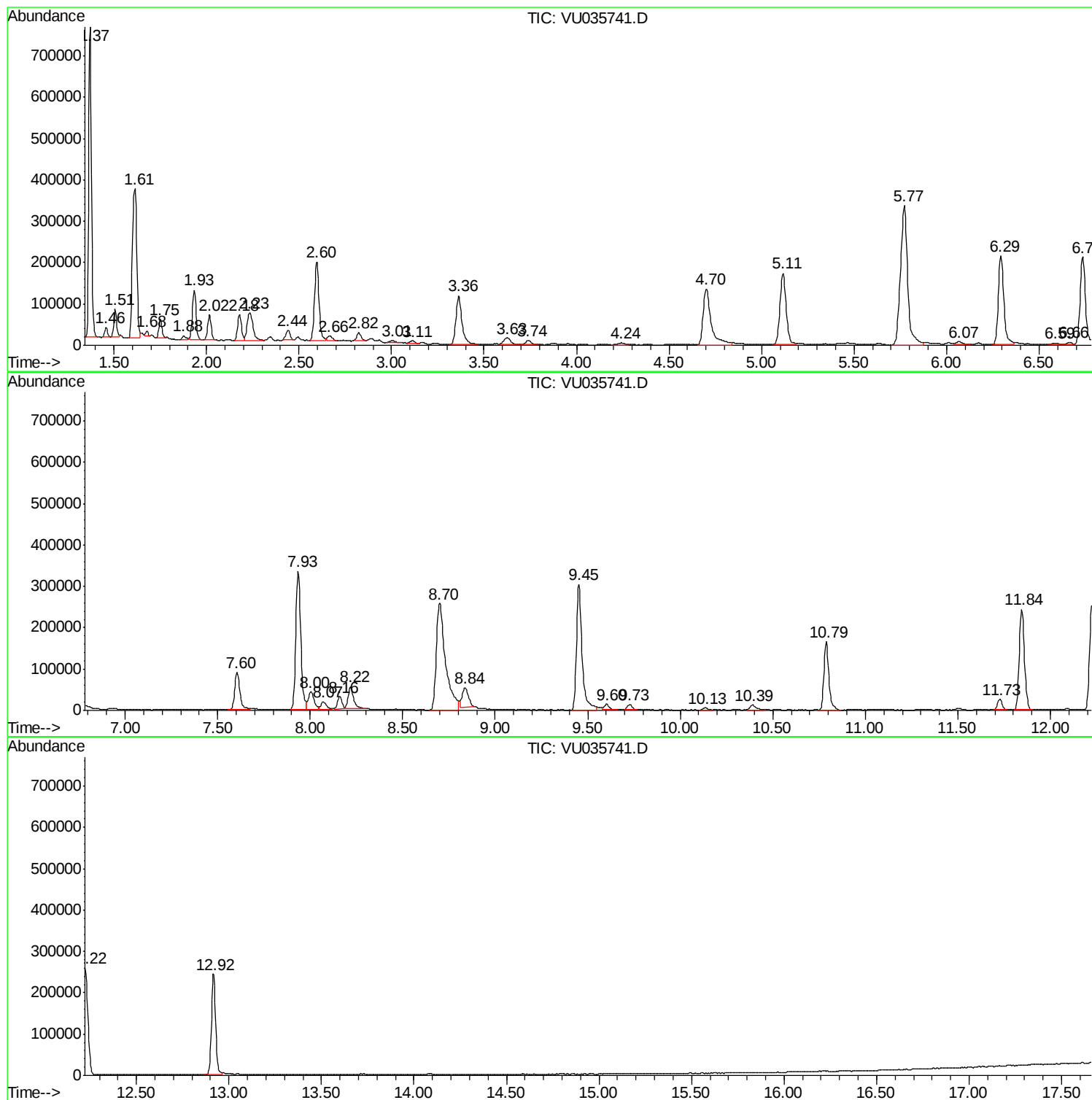
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR110419WMA.M
Quant Title : TRACE VOA SOM01.0

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



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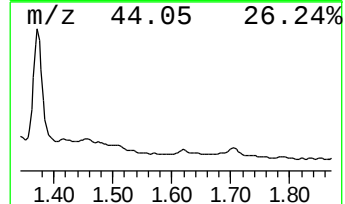
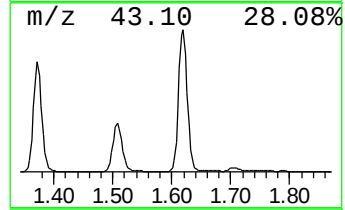
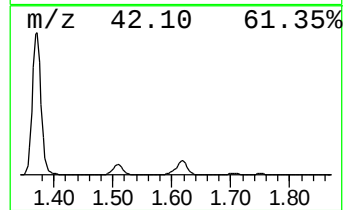
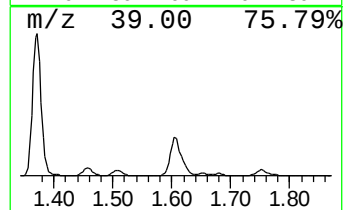
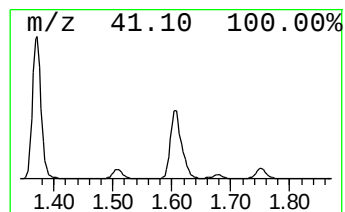
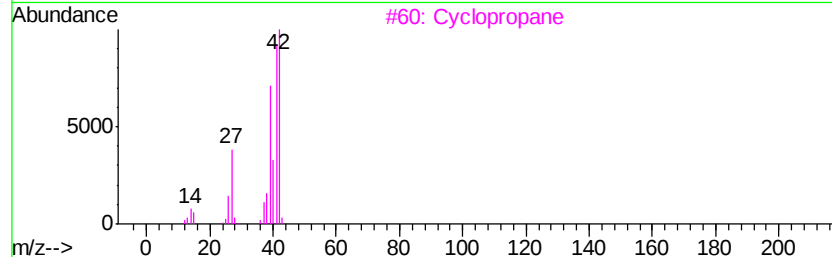
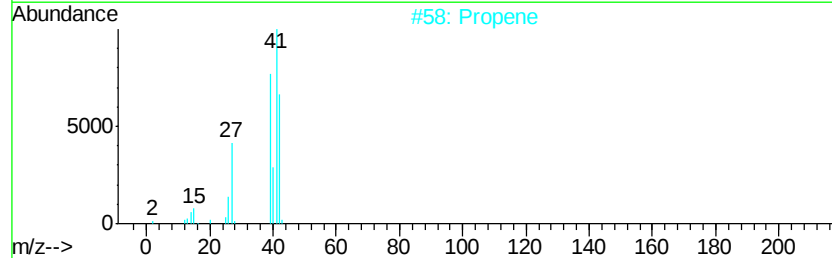
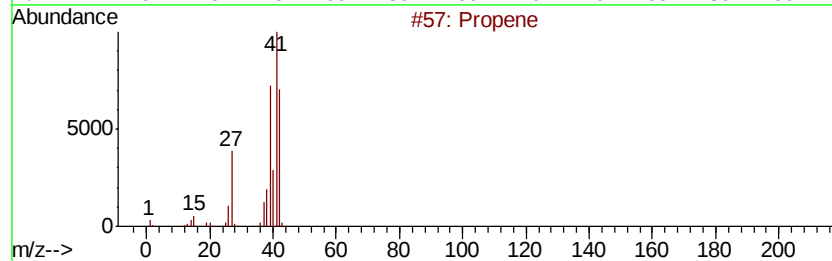
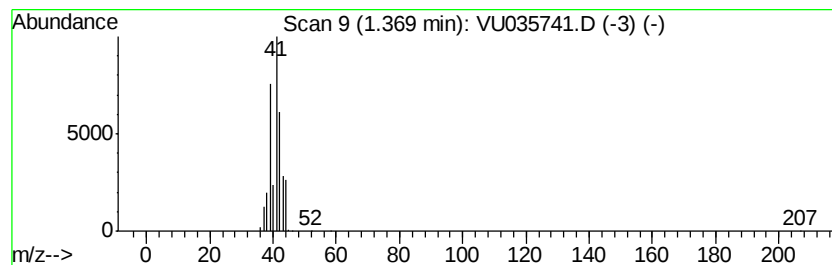
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Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.37	8.33 ug/L	750423	1,4-Difluorobenzene	6.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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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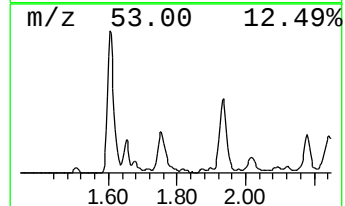
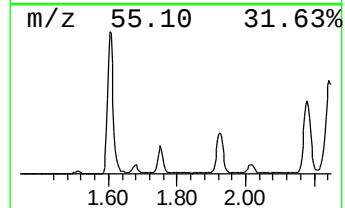
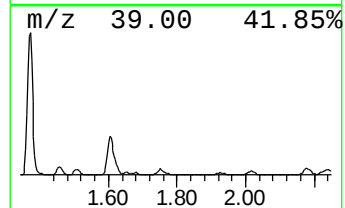
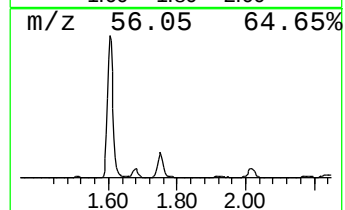
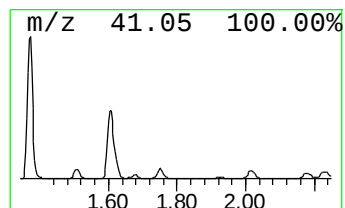
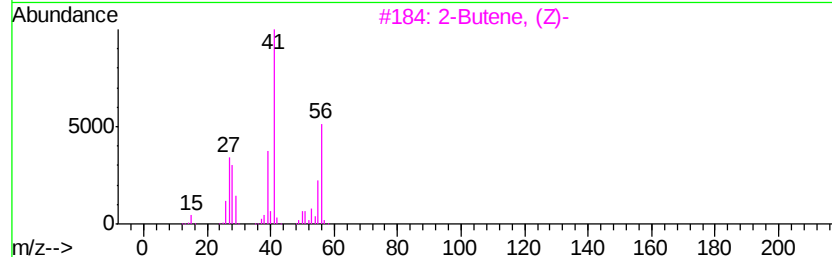
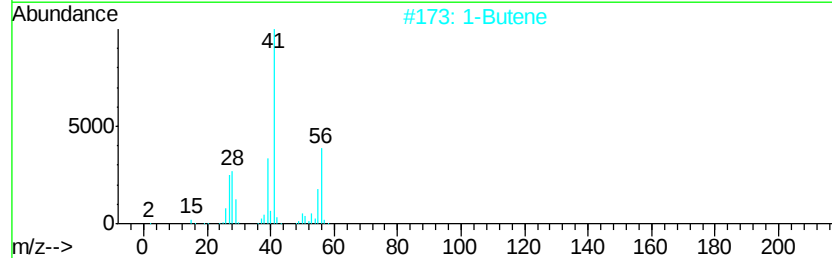
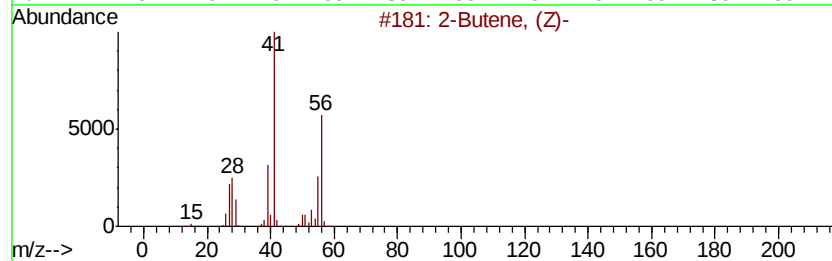
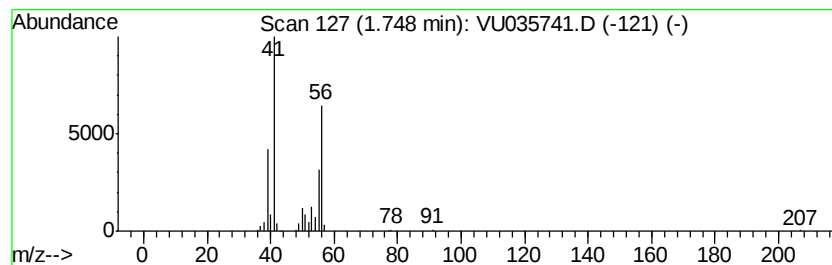
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR110419WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 (DEL) Alkane: Cyclic1.75 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.75	0.59 ug/L	53145	1,4-Difluorobenzene	6.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Butene, (Z)-	56	C4H8	000590-18-1	87
2		1-Butene	56	C4H8	000106-98-9	83
3		2-Butene, (Z)-	56	C4H8	000590-18-1	83
4		1-Butene	56	C4H8	000106-98-9	83
5		2-Butene, (E)-	56	C4H8	000624-64-6	83



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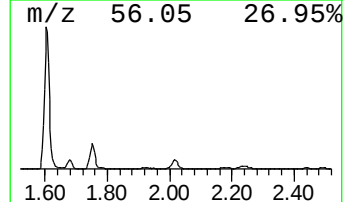
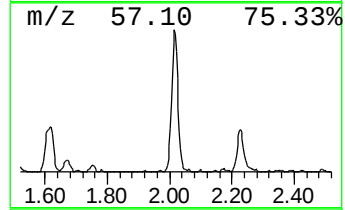
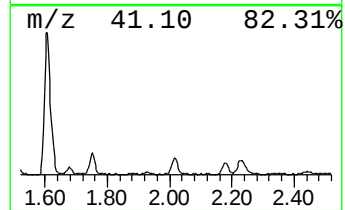
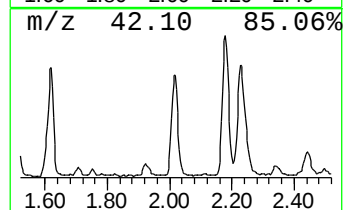
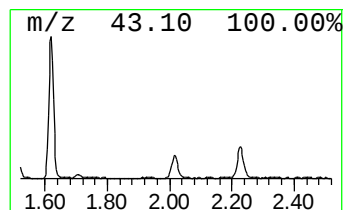
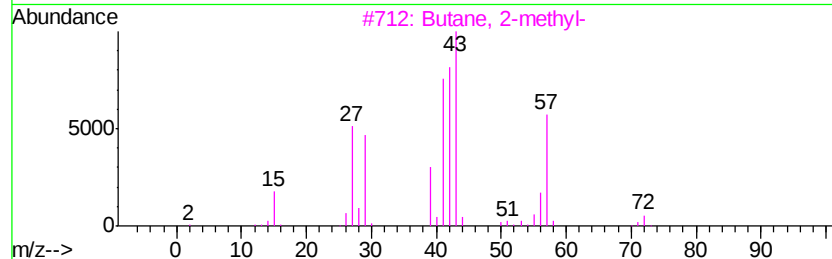
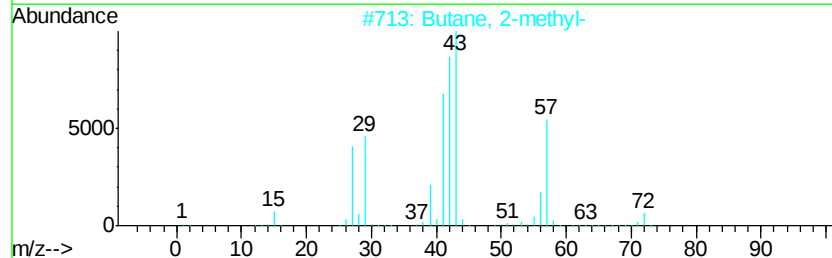
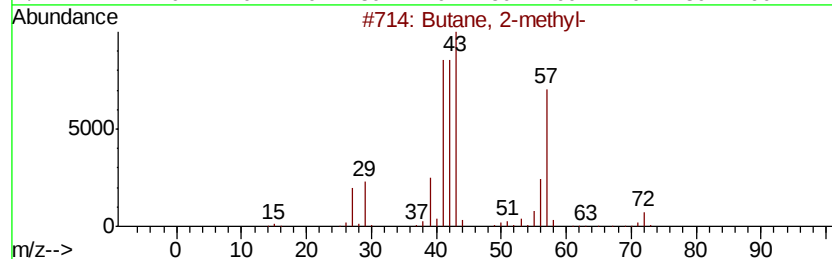
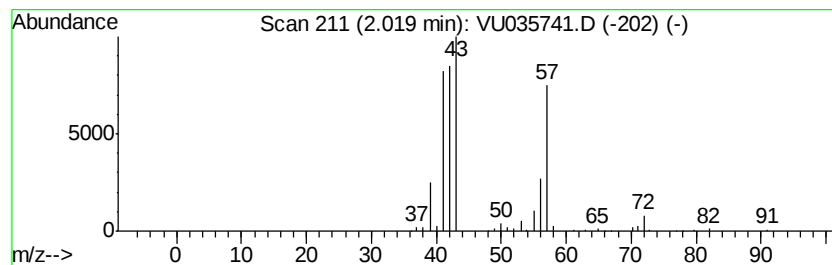
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR110419WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.02	0.92 ug/L	83131	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	80
3		Butane, 2-methyl-	72	C5H12	000078-78-4	80
4		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	33
5		Pentane	72	C5H12	000109-66-0	33



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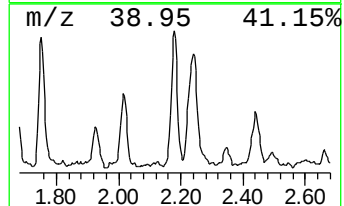
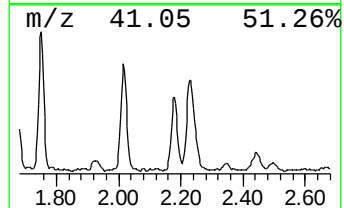
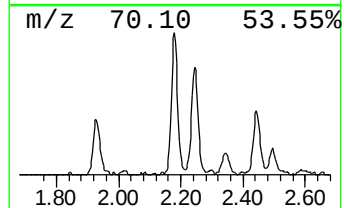
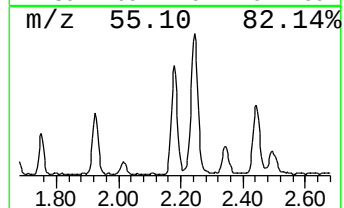
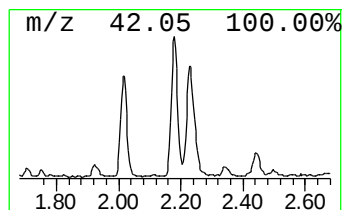
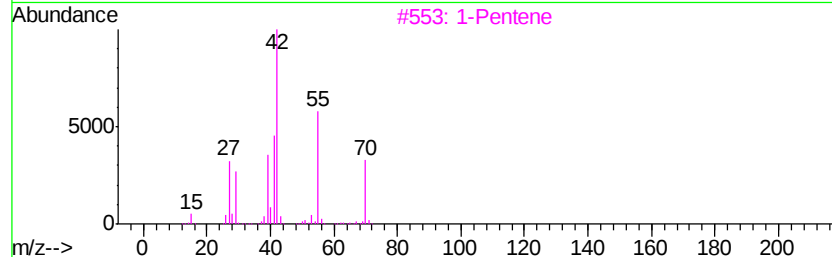
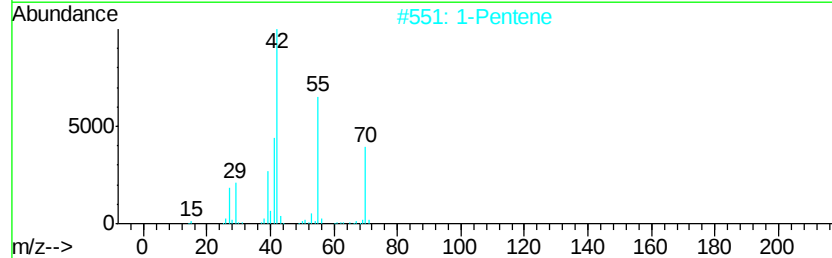
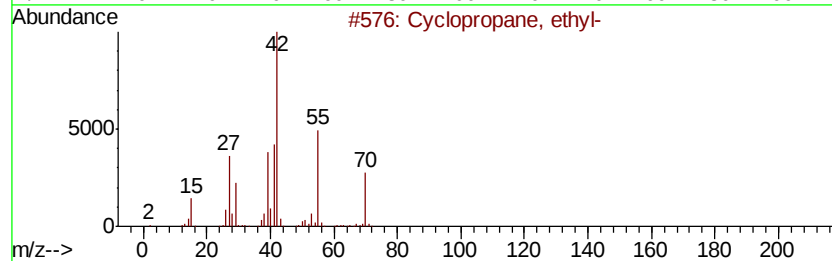
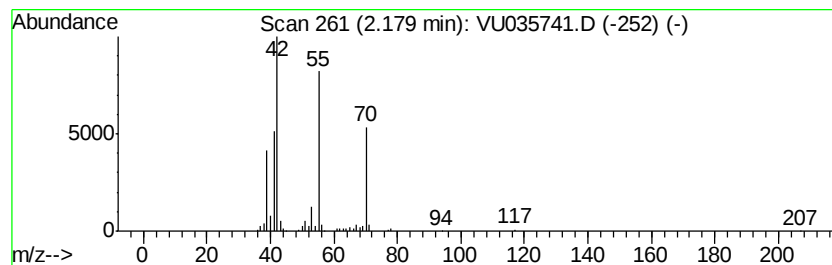
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 (DEL) Alkane: Cyclic2.18 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	0.97 ug/L	87552	1,4-Difluorobenzene	6.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopropane, ethyl-	70	C5H10	001191-96-4	78
2		1-Pentene	70	C5H10	000109-67-1	64
3		1-Pentene	70	C5H10	000109-67-1	64
4		Cyclopropane, ethyl-	70	C5H10	001191-96-4	58
5		2-Pentene	70	C5H10	000109-68-2	52



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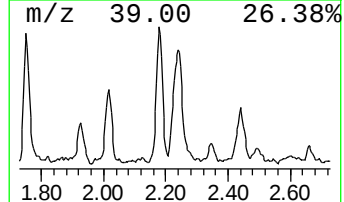
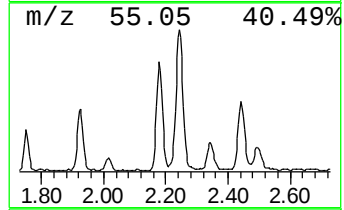
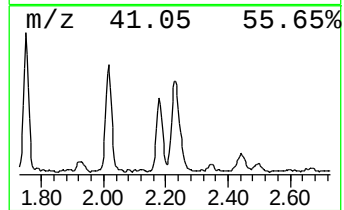
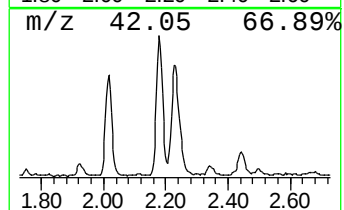
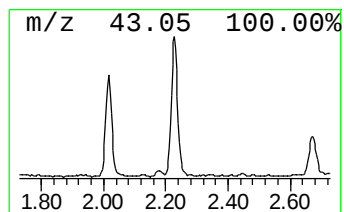
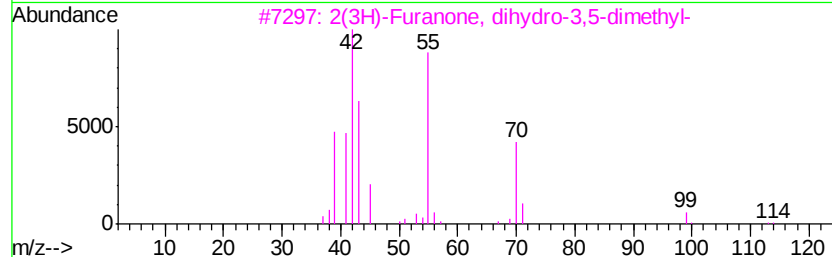
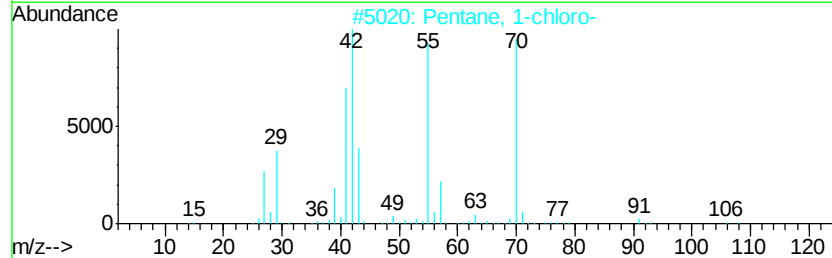
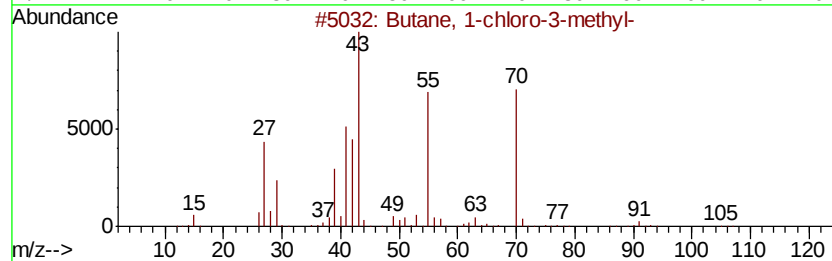
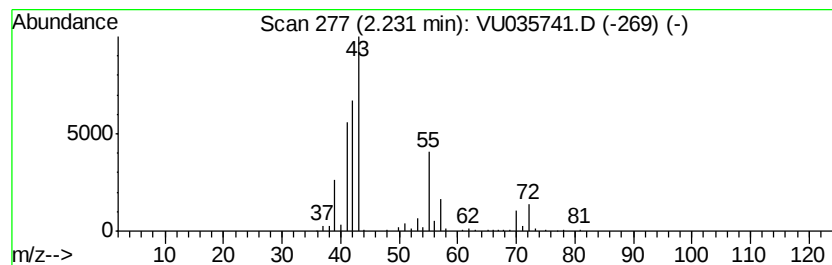
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 Butane, 1-chloro-3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.23	1.59 ug/L	143611	1,4-Difluorobenzene	6.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 1-chloro-3-methyl-	106	C5H11Cl	000107-84-6	64
2		Pentane, 1-chloro-	106	C5H11Cl	000543-59-9	53
3		2(3H)-Furanone, dihydro-3,5-dime...	114	C6H10O2	005145-01-7	50
4		1-Pentene	70	C5H10	000109-67-1	50
5		Pentane	72	C5H12	000109-66-0	47



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU111819\
Data File : VU035741.D
Acq On : 18 Nov 2019 13:55
Operator : JC/SP
Sample : K5911-01
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampled :
GAQK6

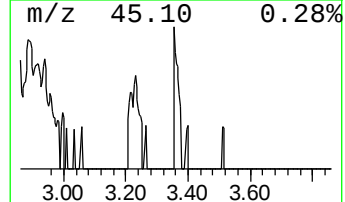
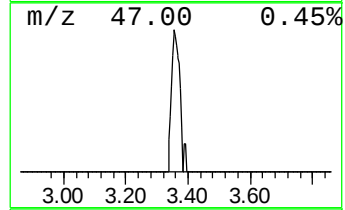
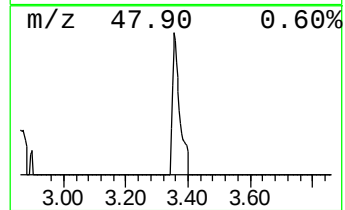
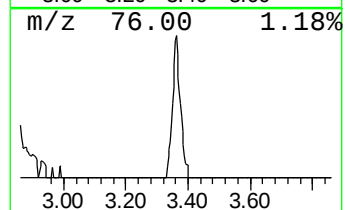
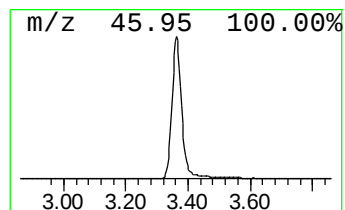
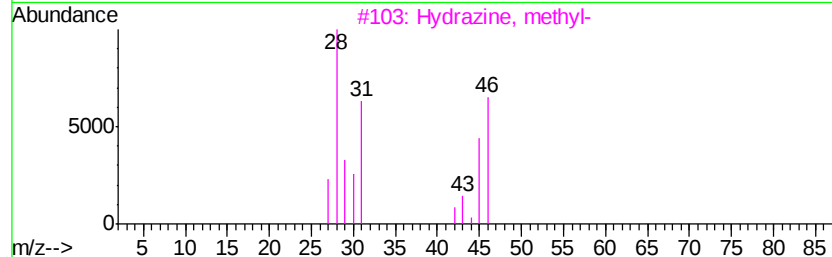
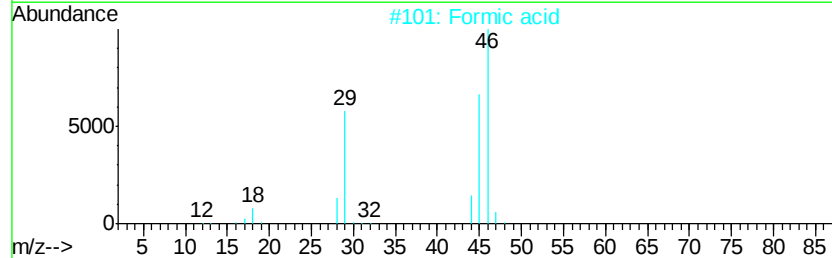
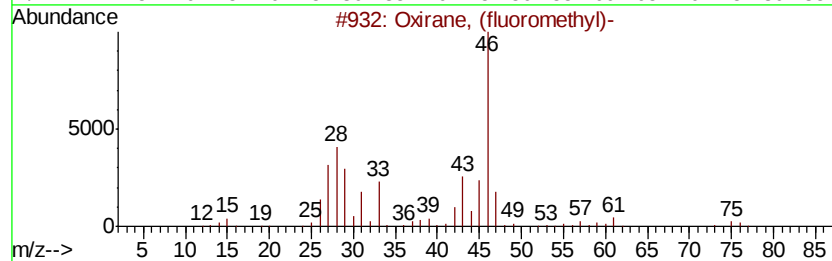
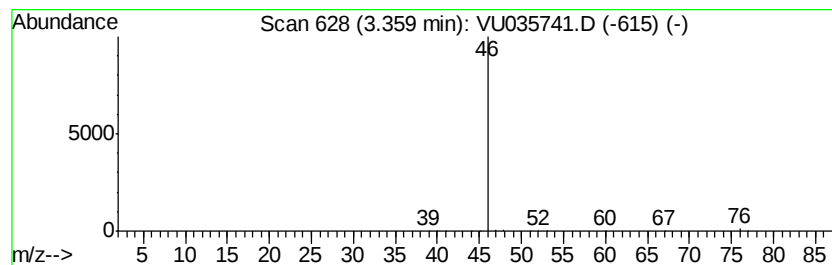
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.36	2.96 ug/L	267023	1,4-Difluorobenzene	6.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, (fluoromethyl)-	76	C3H5FO	000503-09-3	7
2		Formic acid	46	CH2O2	000064-18-6	4
3		Hvdrazine, methyl-	46	CH6N2	000060-34-4	3
4		Hvdrazine, methyl-	46	CH6N2	000060-34-4	3
5		Hydrazine, methyl-	46	CH6N2	000060-34-4	3



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU111819\
Data File : VU035741.D
Acq On : 18 Nov 2019 13:55
Operator : JC/SP
Sample : K5911-01
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 11 Sample Multiplier: 1

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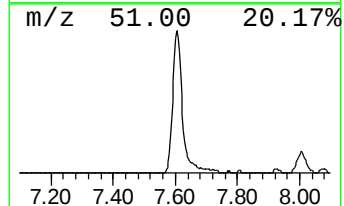
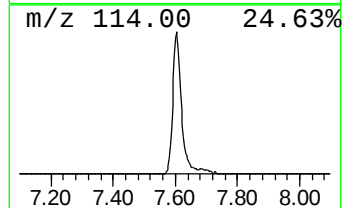
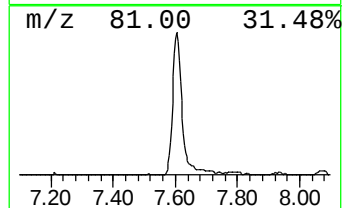
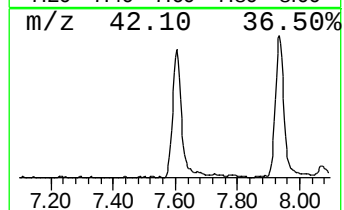
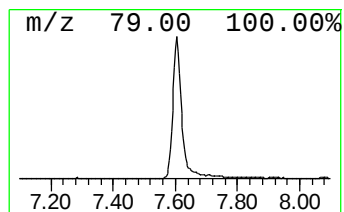
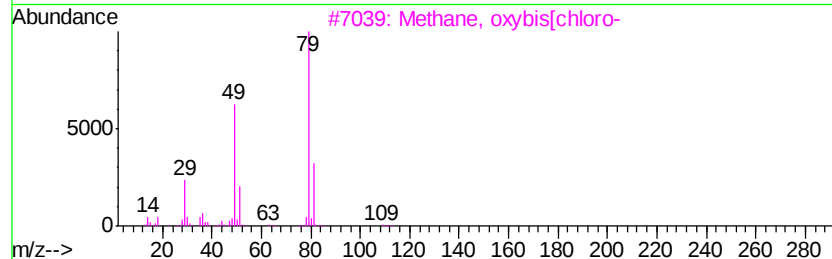
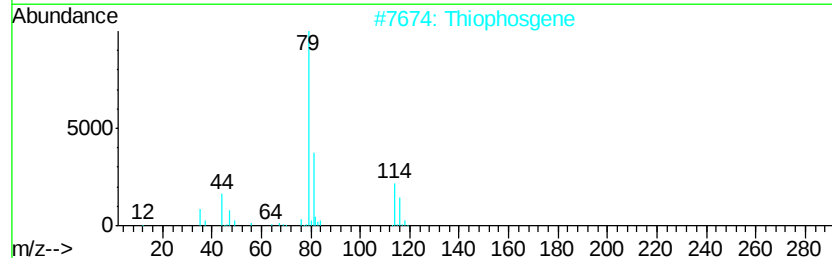
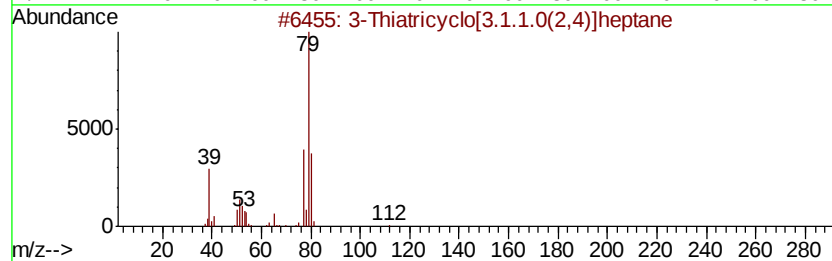
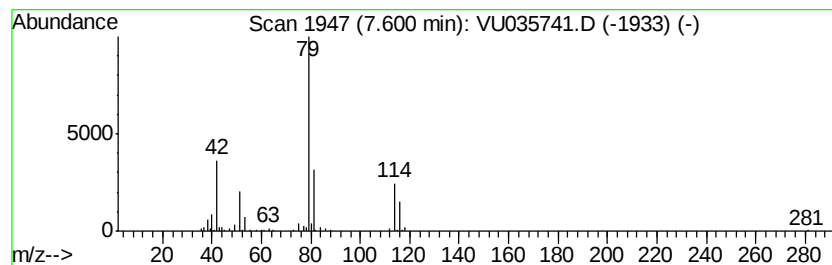
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.60	2.00 ug/L	180302	1,4-Difluorobenzene	6.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Thiatricyclo[3.1.1.0(2,4)]heptane	112	C6H8S	1000221-37-0	47
2		Thiophosgene	114	CCl2S	000463-71-8	42
3		Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	40
4		Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	33
5		1,3-Cyclohexadiene	80	C6H8	000592-57-4	28



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU111819\
Data File : VU035741.D
Acq On : 18 Nov 2019 13:55
Operator : JC/SP
Sample : K5911-01
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GAQK6

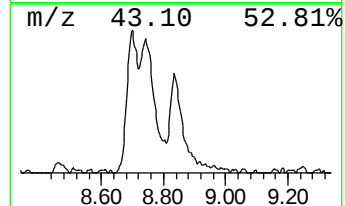
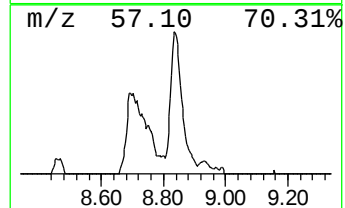
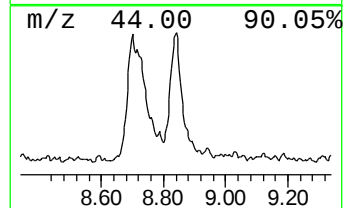
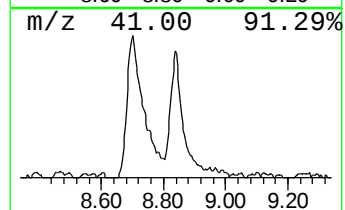
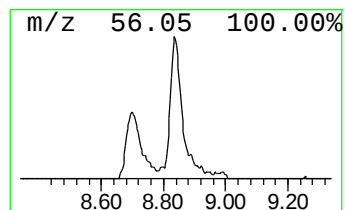
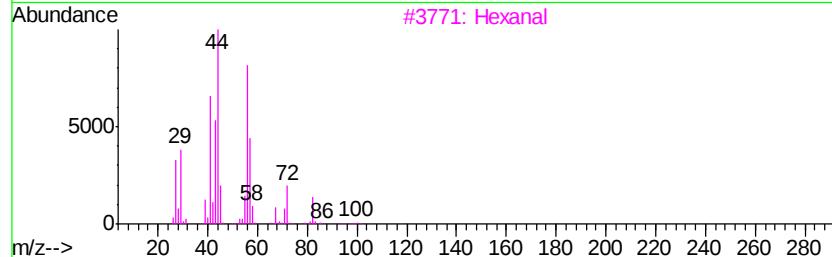
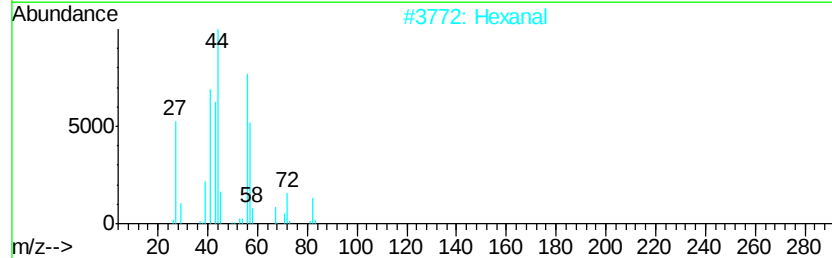
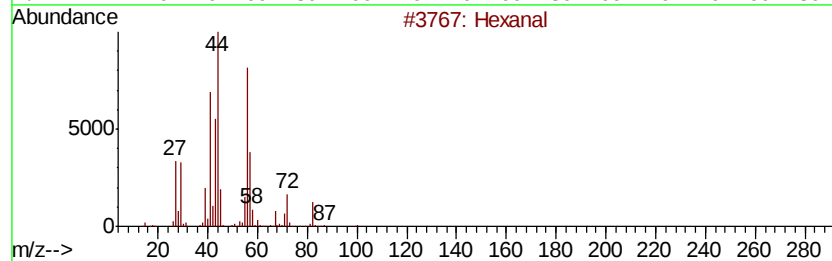
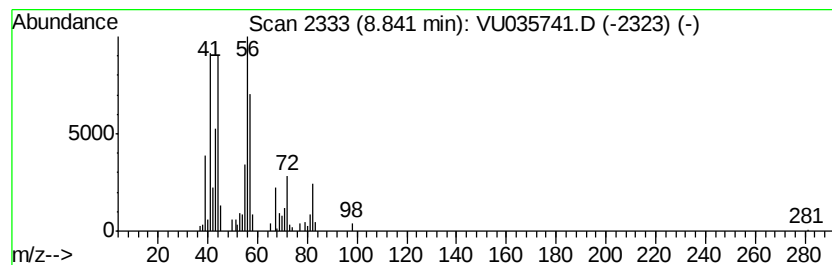
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 Hexanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.84	0.86 ug/L	109878	Chlorobenzene-d5	9.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanal	100	C6H12O	000066-25-1	59
2		Hexanal	100	C6H12O	000066-25-1	59
3		Hexanal	100	C6H12O	000066-25-1	42
4		4-Piperidinecarboxamide	128	C6H12N2O	039546-32-2	37
5		Butanal, 3-methyl-	86	C5H10O	000590-86-3	35



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU111819\
Data File : VU035741.D
Acq On : 18 Nov 2019 13:55
Operator : JC/SP
Sample : K5911-01
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GAQK6

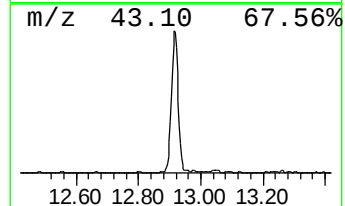
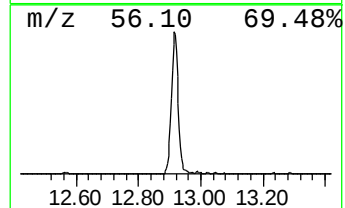
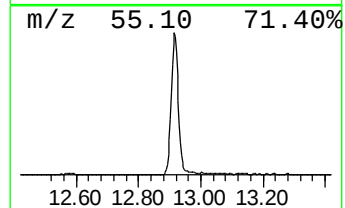
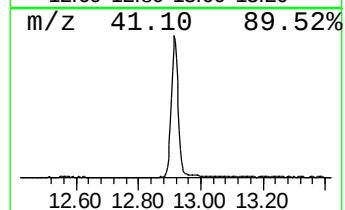
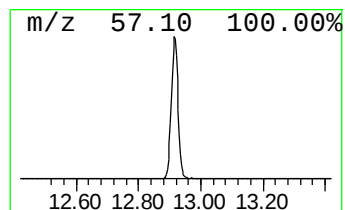
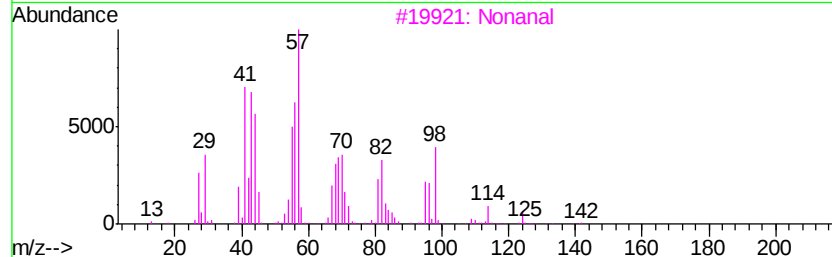
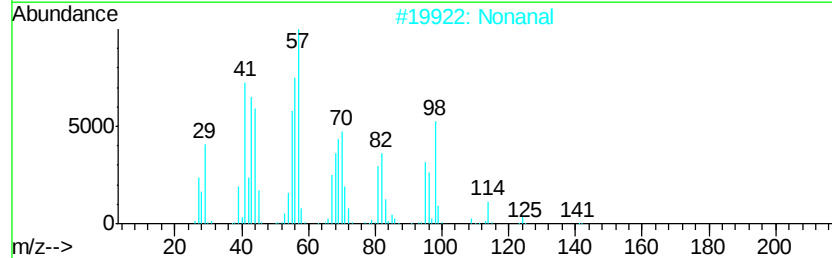
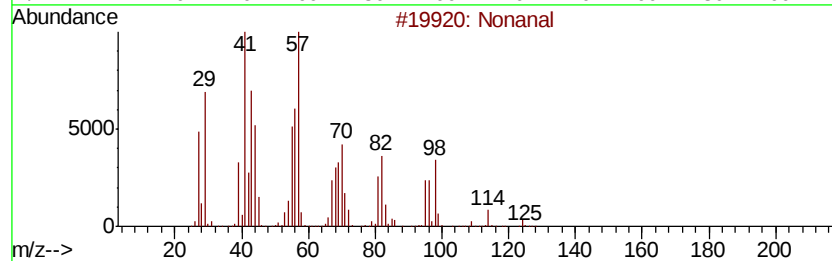
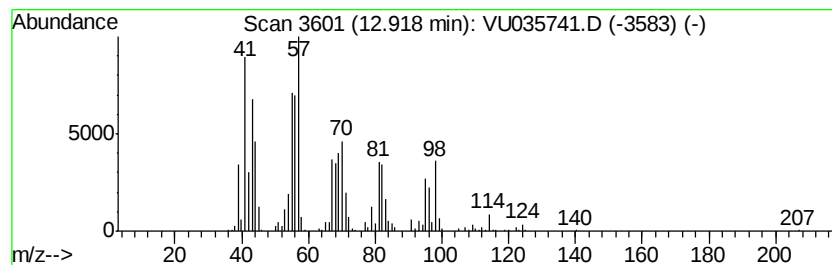
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 9 Nonanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.92	4.07 ug/L	383602	1,4-Dichlorobenzene-d4	11.84

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanal		142	C9H18O	000124-19-6	87
2	Nonanal		142	C9H18O	000124-19-6	86
3	Nonanal		142	C9H18O	000124-19-6	72
4	(R)-(-)-(Z)-14-Methyl-8-hexadec...		254	C17H34O	030689-78-2	38
5	Cyclohexanol, 2-methyl-, cis-		114	C7H14O	007443-70-1	38



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU111819\
Data File : VU035741.D
Acq On : 18 Nov 2019 13:55
Operator : JC/SP
Sample : K5911-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GAQK6

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR110419WMA.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: Cyc...	1.37	8.3	ug/L	750423	1	6.29	450518	5.0
(DEL) Alkane: Cyc...	1.75	0.6	ug/L	53145	1	6.29	450518	5.0
(DEL) Alkane: Str...	2.02	0.9	ug/L	83131	1	6.29	450518	5.0
(DEL) Alkane: Cyc...	2.18	1.0	ug/L	87552	1	6.29	450518	5.0
Butane, 1-chloro-...	2.23	1.6	ug/L	143611	1	6.29	450518	5.0
unknown-01	3.36	3.0	ug/L	267023	1	6.29	450518	5.0
unknown-02	7.60	2.0	ug/L	180302	1	6.29	450518	5.0
Hexanal	8.84	0.9	ug/L	109878	2	9.45	638962	5.0
Nonanal	12.92	4.1	ug/L	383602	3	11.84	470894	5.0