

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU121319\
 Data File : VU036202.D
 Acq On : 13 Dec 2019 17:39
 Operator : JC/MD
 Sample : K6273-15
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFDR2

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\SOMUTR121319WMA.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	23	rVB	617073	599869	56.80%	5.842%
2	1.456	29	36	45	rBV	38011	41835	3.96%	0.407%
3	1.504	45	51	56	rVV	37302	36566	3.46%	0.356%
4	1.610	73	84	92	rBV3	360498	564865	53.48%	5.501%
5	1.707	107	114	121	rBV	74925	95940	9.08%	0.934%
6	1.745	121	126	137	rVB3	41681	59126	5.60%	0.576%
7	1.929	175	183	197	rVB	151665	197009	18.65%	1.919%
8	2.012	202	209	217	rVB2	41140	54029	5.12%	0.526%
9	2.173	250	259	267	rBV	62041	84251	7.98%	0.820%
10	2.224	267	275	284	rBV3	46194	77517	7.34%	0.755%
11	2.337	304	310	318	rVB5	8474	11446	1.08%	0.111%
12	2.433	335	340	351	rVB4	28290	43559	4.12%	0.424%
13	2.591	377	389	405	rBV	193243	317443	30.06%	3.091%
14	2.684	405	418	440	rBV	24630	65135	6.17%	0.634%
15	2.822	450	461	473	rVB	25234	41999	3.98%	0.409%
16	3.006	505	518	526	rBV7	4542	10881	1.03%	0.106%
17	3.392	629	638	654	rVB9	4636	11244	1.06%	0.109%
18	3.626	698	711	724	rBV4	14004	32899	3.11%	0.320%
19	3.742	733	747	759	rVB6	5620	13232	1.25%	0.129%
20	4.507	971	985	1003	rBV6	8347	21514	2.04%	0.210%
21	4.700	1029	1045	1065	rBV	134188	406705	38.51%	3.961%
22	5.112	1157	1173	1193	rBV2	176926	400927	37.96%	3.904%
23	5.768	1356	1377	1405	rBV2	345423	902819	85.48%	8.792%
24	6.289	1524	1539	1563	rBV	306244	594274	56.27%	5.787%
25	6.578	1617	1629	1648	rVB2	75377	144488	13.68%	1.407%
26	6.732	1662	1677	1694	rBV	217945	427683	40.49%	4.165%
27	6.922	1728	1736	1750	rBV6	9773	19980	1.89%	0.195%
28	7.115	1786	1796	1803	rBV	11502	21904	2.07%	0.213%
29	7.600	1931	1947	1968	rBV	105876	195616	18.52%	1.905%
30	7.932	2035	2050	2066	rBV	382846	672932	63.71%	6.553%
31	7.996	2066	2070	2081	rVB2	8111	14215	1.35%	0.138%
32	8.214	2126	2138	2152	rBV2	71427	128629	12.18%	1.253%
33	8.674	2269	2281	2312	rBV	514012	1056184	100.00%	10.286%
34	8.822	2319	2327	2344	rVB3	47997	81808	7.75%	0.797%

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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\SOMUTR121319WMA.M
Title : TRACE VOA SOM01.0

35	9.446	2508	2521	2556	rVB	461329	798581	75.61%	7.777%
36	10.375	2799	2810	2821	rBV7	17641	30343	2.87%	0.295%
37	10.784	2923	2937	2953	rBV	206846	333312	31.56%	3.246%
38	11.713	3215	3226	3238	rBV3	56281	91533	8.67%	0.891%
39	11.835	3252	3264	3281	rBV	426762	703726	66.63%	6.853%
40	12.086	3331	3342	3358	rBV4	15964	29455	2.79%	0.287%
41	12.218	3369	3383	3403	rVB	410313	676380	64.04%	6.587%
42	12.510	3463	3474	3483	rVB5	10476	15710	1.49%	0.153%
43	12.909	3584	3598	3612	rBV2	74380	113915	10.79%	1.109%
44	14.002	3930	3938	3948	rBV7	18061	27189	2.57%	0.265%

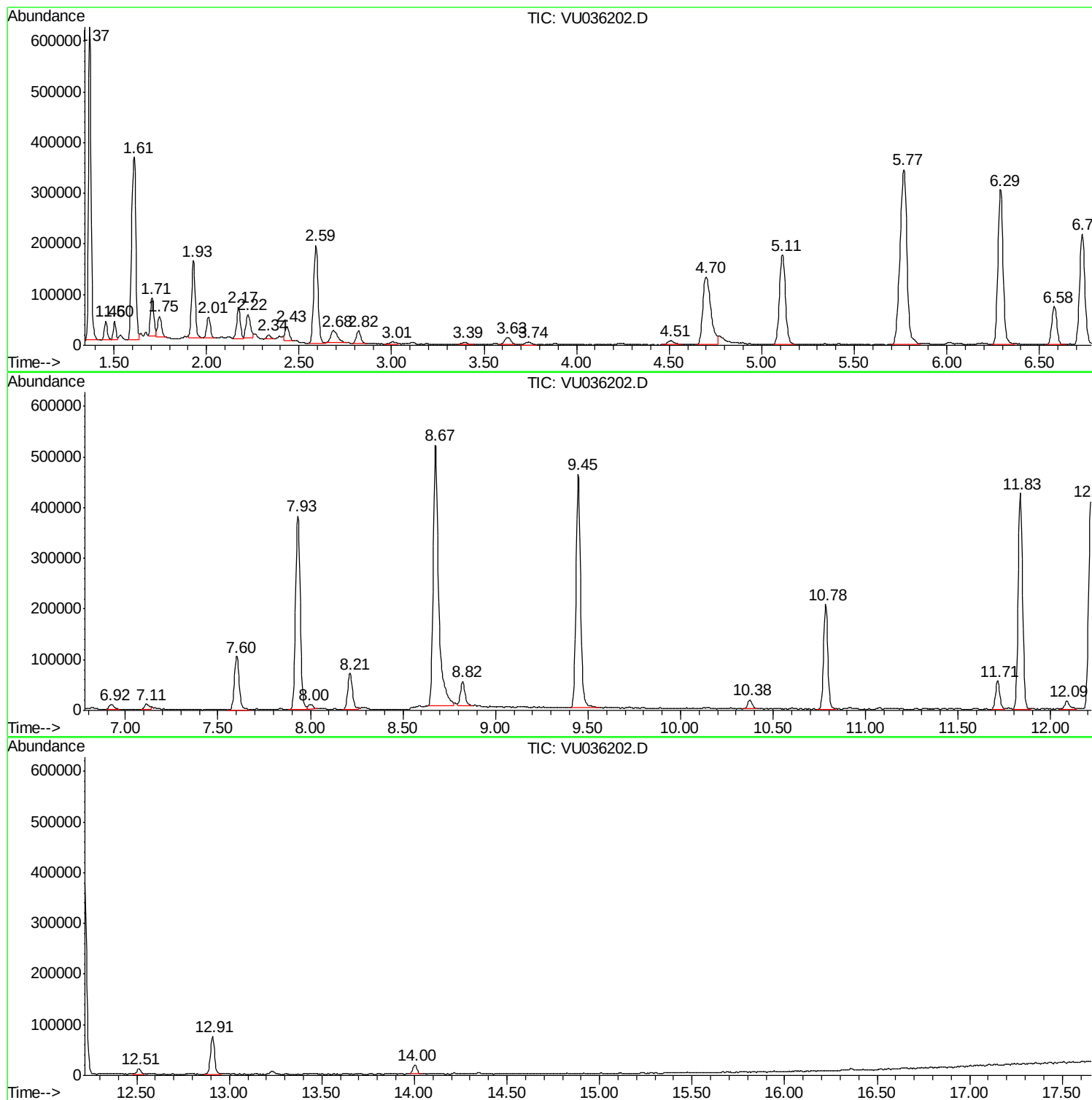
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121319WMA.M
Quant Title : TRACE VOA SOM01.0

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



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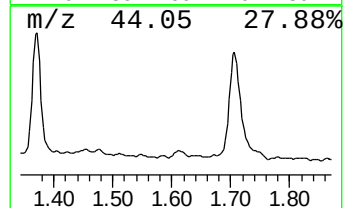
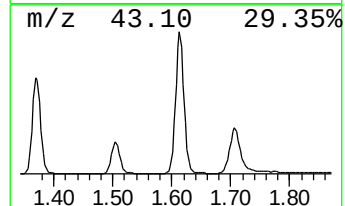
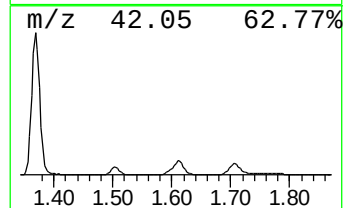
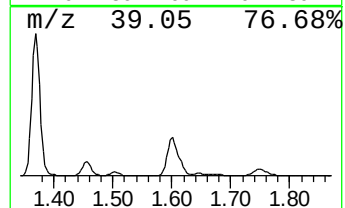
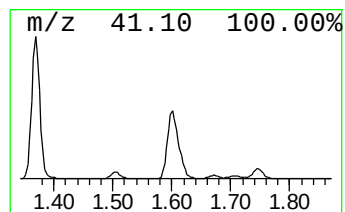
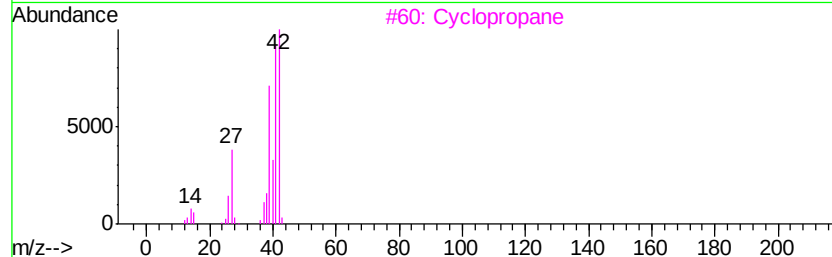
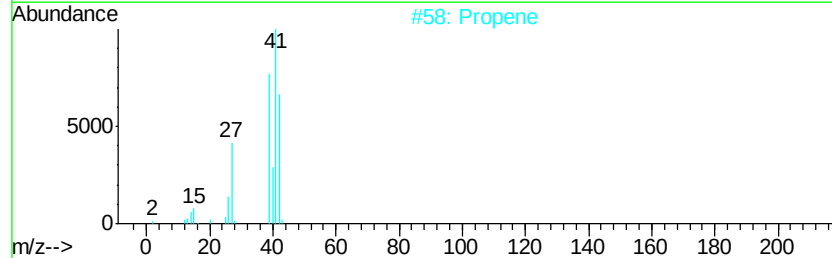
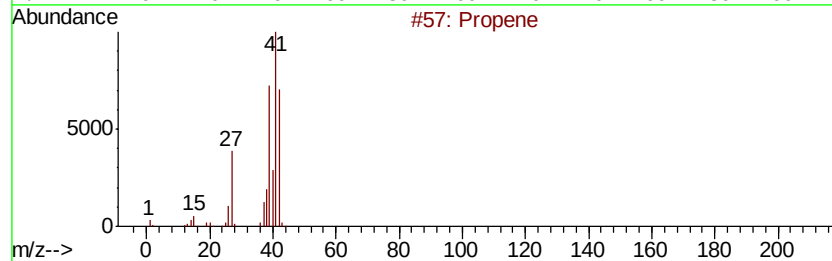
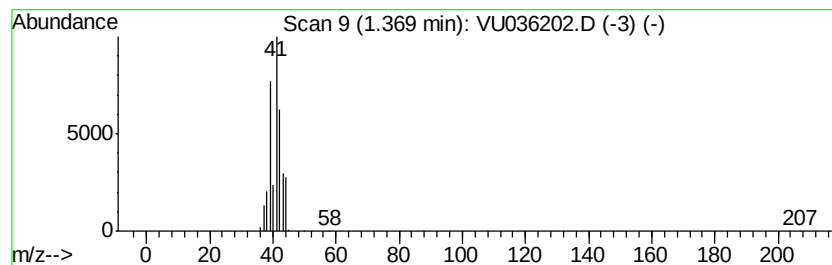
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Quant Title : TRACE VOA SOM01.0

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	5.05 ug/L	599869	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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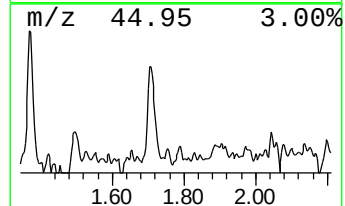
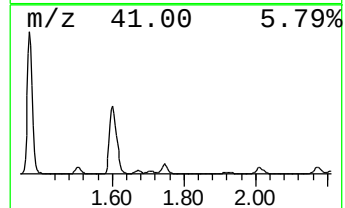
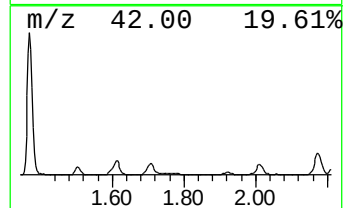
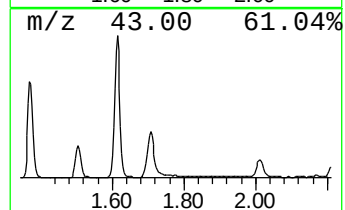
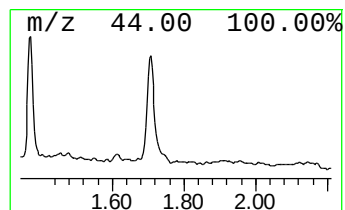
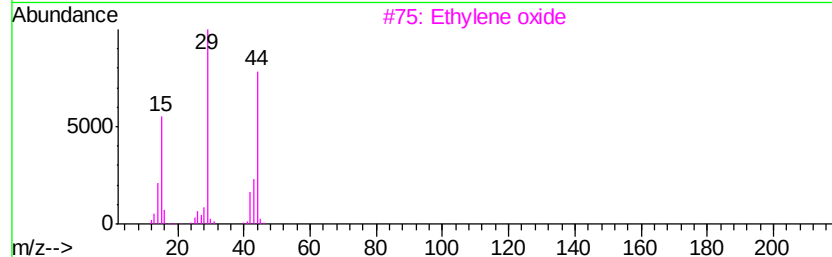
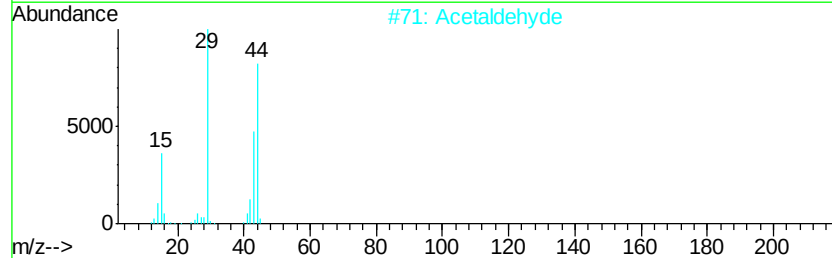
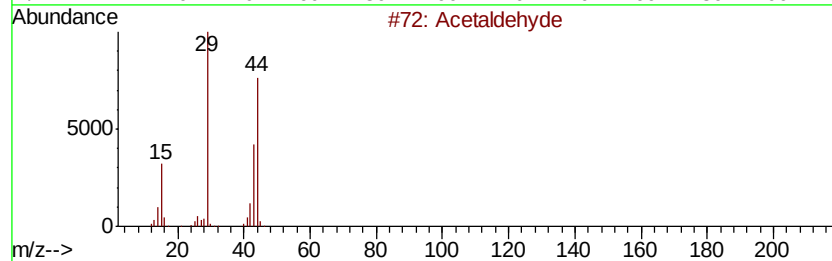
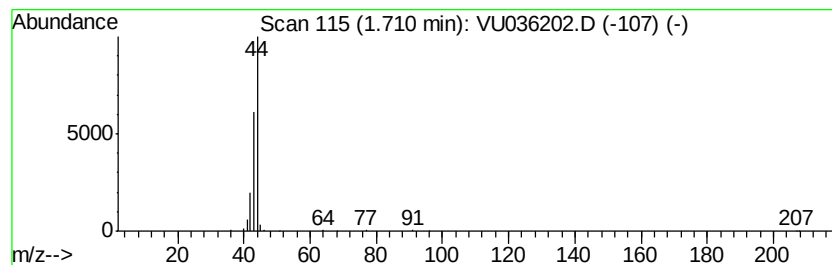
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121319WMA.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Acetaldehyde Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.71	0.81 ug/L	95940	1,4-Difluorobenzene	6.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde		44	C2H4O	000075-07-0	64
2	Acetaldehyde		44	C2H4O	000075-07-0	64
3	Ethylene oxide		44	C2H4O	000075-21-8	9
4	Propane		44	C3H8	000074-98-6	5
5	Ethylene oxide		44	C2H4O	000075-21-8	5



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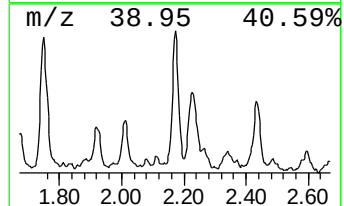
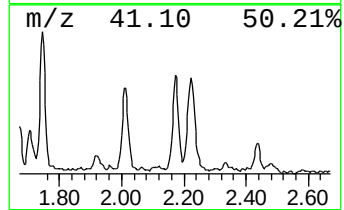
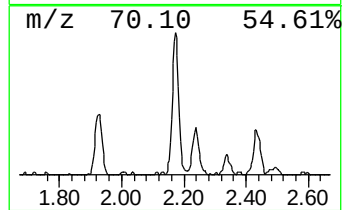
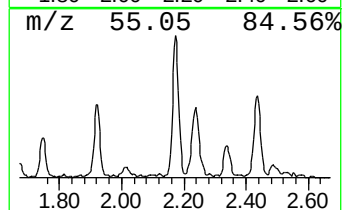
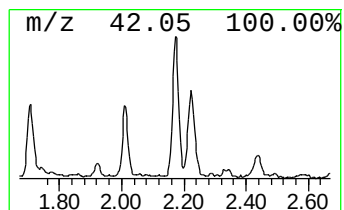
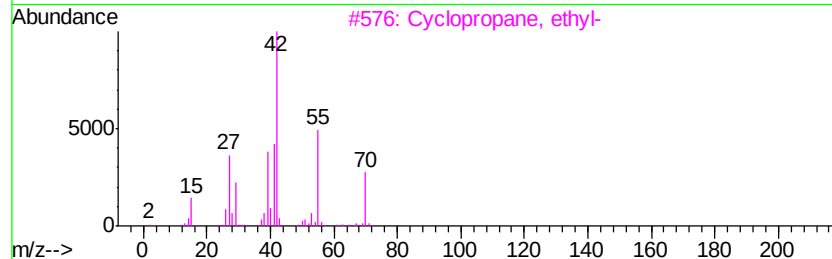
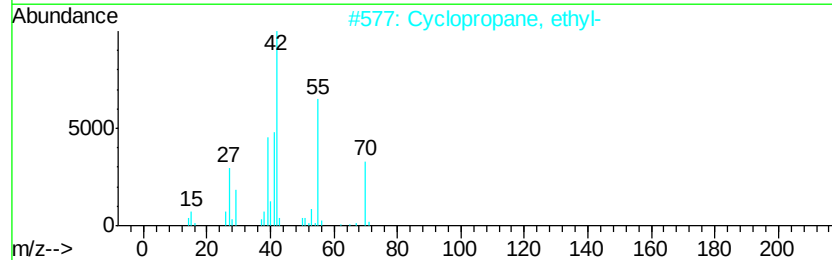
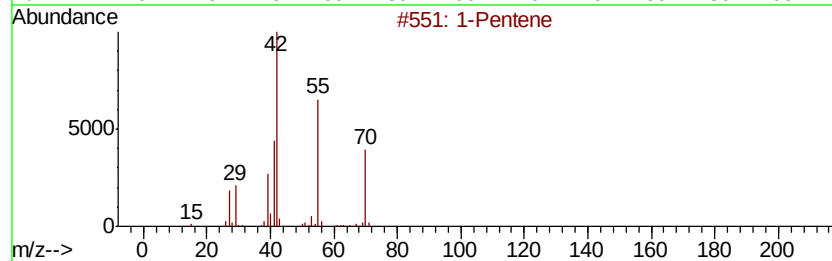
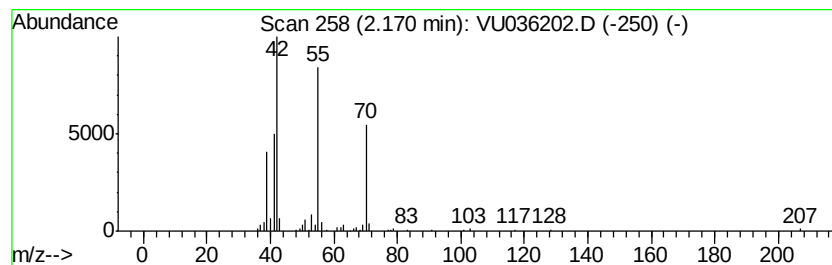
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121319WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 (DEL) Alkane: Cyclic2.17 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	0.71 ug/L	84251	1,4-Difluorobenzene	6.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Pentene	70	C5H10	000109-67-1	90
2		Cyclopropane, ethyl-	70	C5H10	001191-96-4	83
3		Cyclopropane, ethyl-	70	C5H10	001191-96-4	83
4		Cyclopropane, ethyl-	70	C5H10	001191-96-4	68
5		1-Pentene	70	C5H10	000109-67-1	62



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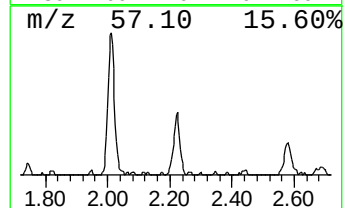
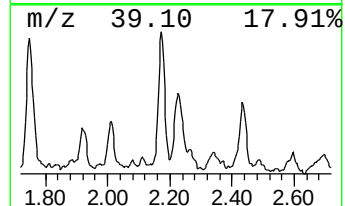
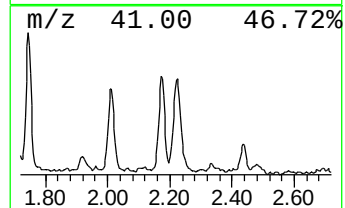
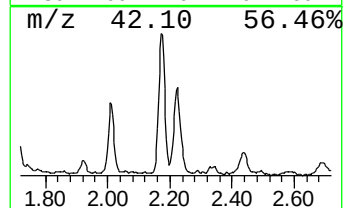
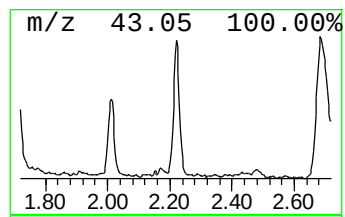
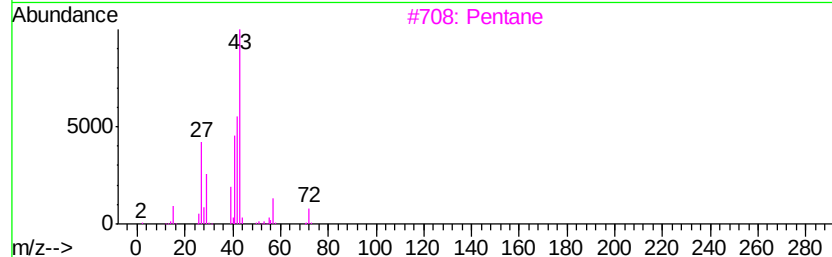
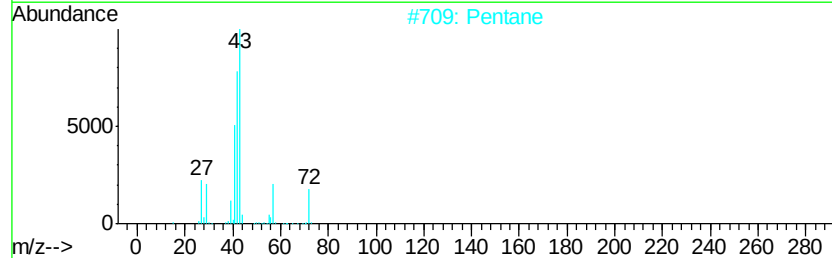
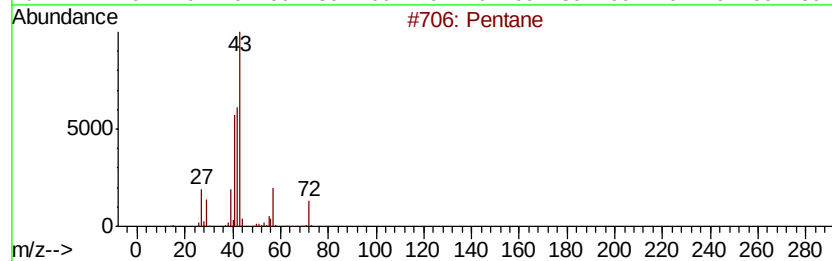
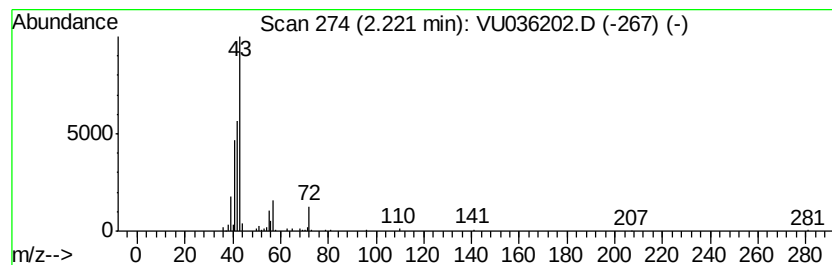
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	0.65 ug/L	77517	1,4-Difluorobenzene	6.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane	72	C5H12	000109-66-0	83
2		Pentane	72	C5H12	000109-66-0	80
3		Pentane	72	C5H12	000109-66-0	80
4		Pentane	72	C5H12	000109-66-0	80
5		Oxirane, ethyl-	72	C4H8O	000106-88-7	47



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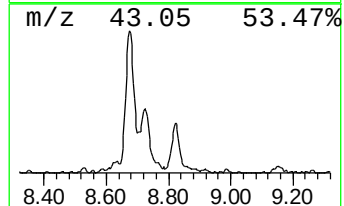
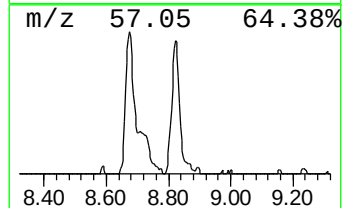
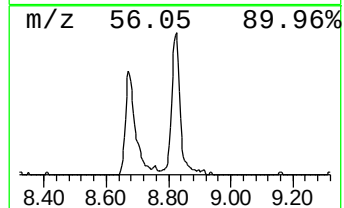
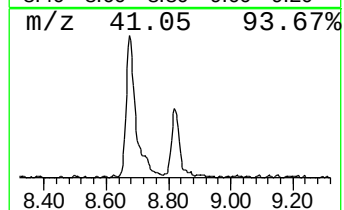
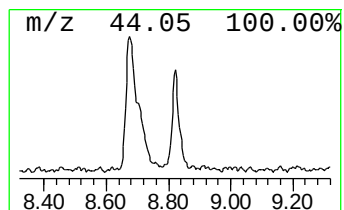
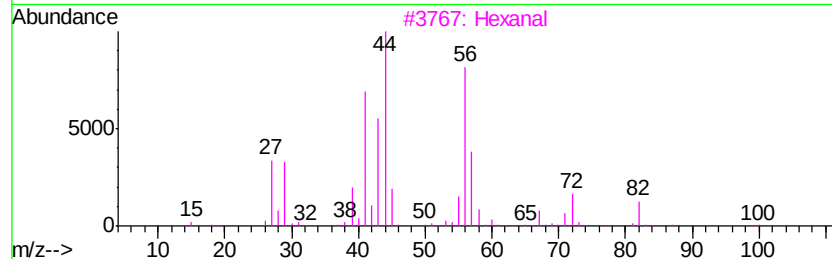
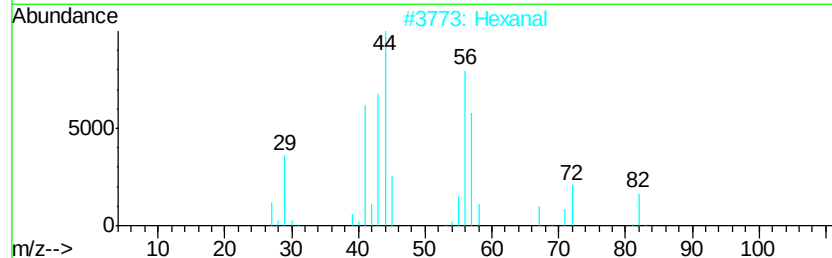
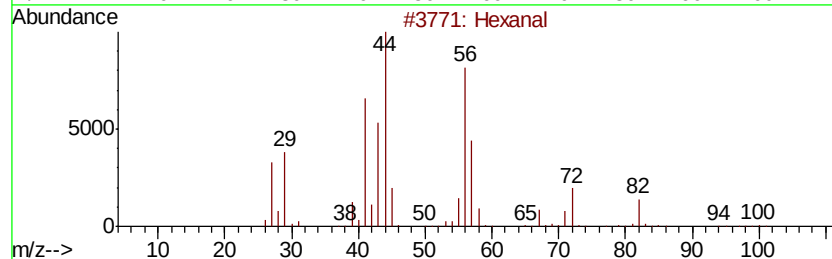
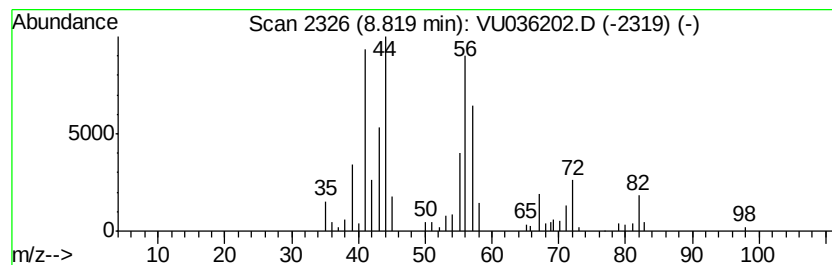
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121319WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 Hexanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.82	0.51 ug/L	81808	Chlorobenzene-d5	9.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanal	100	C6H12O	000066-25-1	83
2		Hexanal	100	C6H12O	000066-25-1	74
3		Hexanal	100	C6H12O	000066-25-1	72
4		Hexanal	100	C6H12O	000066-25-1	72
5		Butanal, 4-hydroxy-3-methyl-	102	C5H10O2	056805-34-6	25



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU121319\
Data File : VU036202.D
Acq On : 13 Dec 2019 17:39
Operator : JC/MD
Sample : K6273-15
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 15 Sample Multiplier: 1

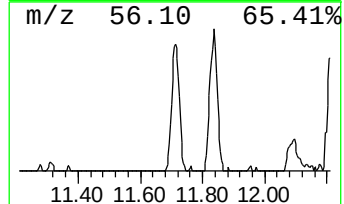
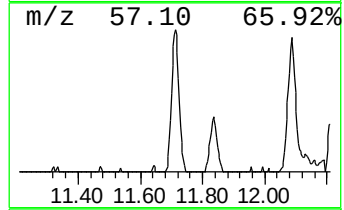
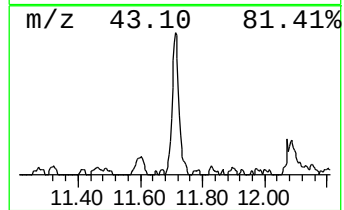
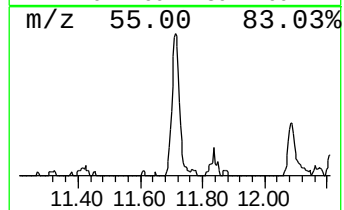
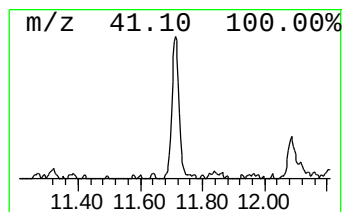
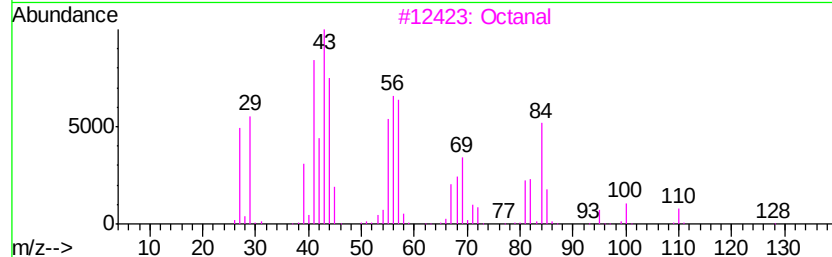
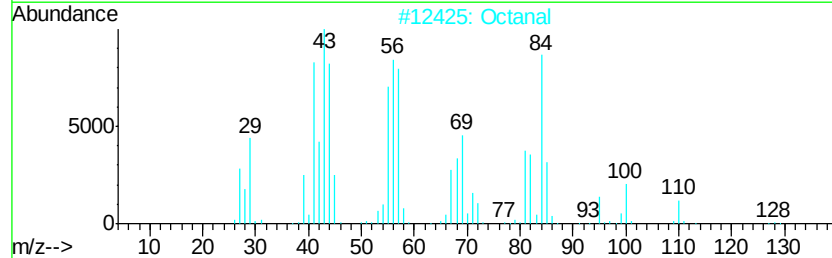
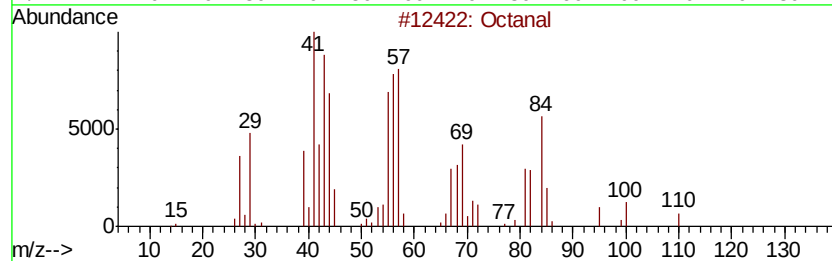
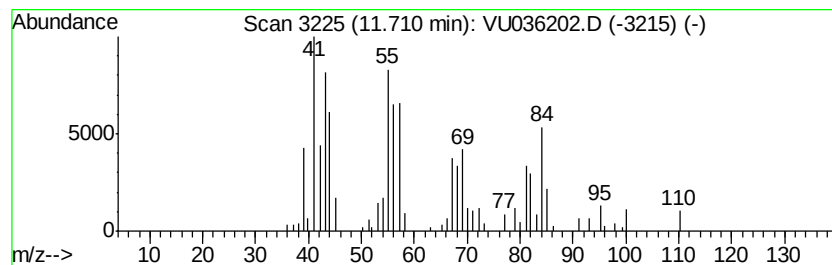
Instrument :
MSVOA_U
ClientSampleId :
BFDR2

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121319WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 Octanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.71	0.65 ug/L	91533	1,4-Dichlorobenzene-d4	11.83
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octanal		128 C8H16O	000124-13-0 91
2	Octanal		128 C8H16O	000124-13-0 86
3	Octanal		128 C8H16O	000124-13-0 86
4	Octanal		128 C8H16O	000124-13-0 78
5	3-Chlorohexane		120 C6H13Cl	002346-81-8 43



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU121319\
Data File : VU036202.D
Acq On : 13 Dec 2019 17:39
Operator : JC/MD
Sample : K6273-15
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFDR2

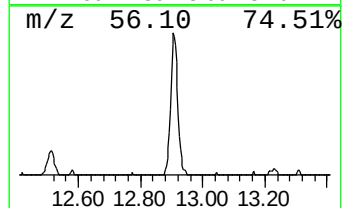
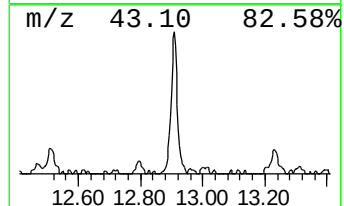
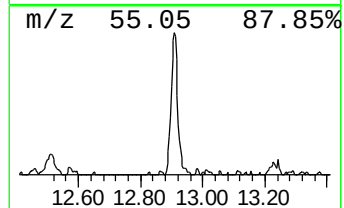
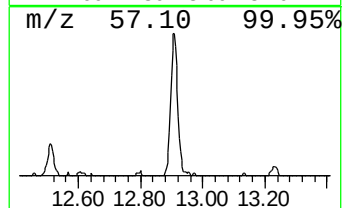
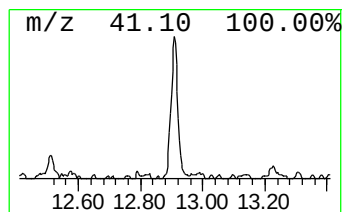
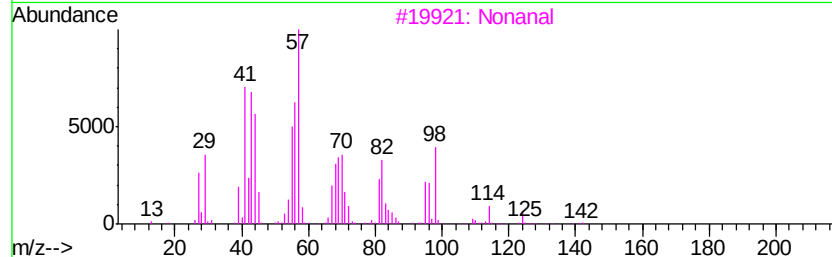
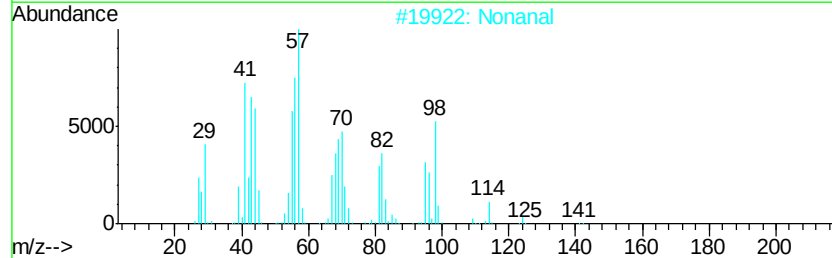
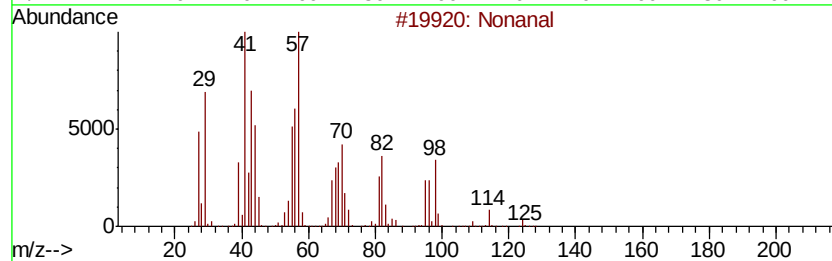
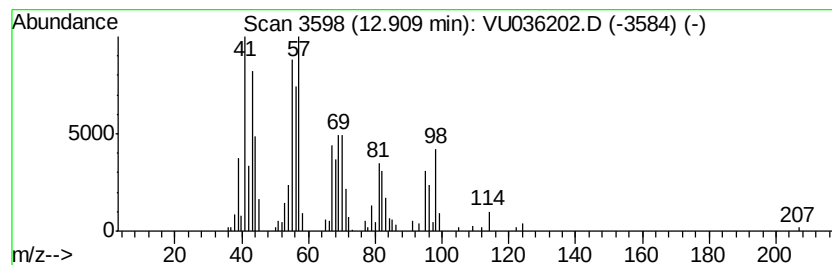
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121319WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 Nonanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.91	0.81 ug/L	113915	1,4-Dichlorobenzene-d4	11.83

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanal		142	C9H18O	000124-19-6	87
2	Nonanal		142	C9H18O	000124-19-6	87
3	Nonanal		142	C9H18O	000124-19-6	64
4	2-Heptene		98	C7H14	000592-77-8	30
5	Cyclohexanecarbonitrile, 1-hydroxy-		125	C7H11NO	000931-97-5	27



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121319\
Data File : VU036202.D
Acq On : 13 Dec 2019 17:39
Operator : JC/MD
Sample : K6273-15
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFDR2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121319WMA.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	5.0	ug/L	599869	1	6.29	594274	5.0
Acetaldehyde	1.71	0.8	ug/L	95940	1	6.29	594274	5.0
(DEL) Alkane: Cyc...	2.17	0.7	ug/L	84251	1	6.29	594274	5.0
(DEL) Alkane: Str...	2.22	0.7	ug/L	77517	1	6.29	594274	5.0
Hexanal	8.82	0.5	ug/L	81808	2	9.45	798581	5.0
Octanal	11.71	0.7	ug/L	91533	3	11.83	703726	5.0
Nonanal	12.91	0.8	ug/L	113915	3	11.83	703726	5.0