LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU121919\
Data File : VU036300.D
Acq On : 19 Dec 2019 22:31
Operator : JC/MD
Sample : K6282-17
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDX3

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

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.427	19	27	43	rBV	411773	468233	71.18%	5.637%
2	1.571	67	72	77	rBV	40695	47820	7.27%	0.576%
3	1.690	99	109	127	rVB3	283792	493230	74.98%	5.938%
4	2.031	207	215	222	rBV	124220	166342	25.29%	2.003%
5	2.105	232	238	246	rBV3	52402	79157	12.03%	0.953%
6	2.321	298	305	328	rVB4	85544	192750	29.30%	2.320%
7	2.697	411	422	438	rVB	204505	334070	50.79%	4.022%
8	3.308	603	612	629	rVB3	23883	59060	8.98%	0.711%
9	3.723	736	741	742	rBV4	8518	6709	1.02%	0.081%
10	4.864	1081	1096	1120	rVB	44022	154071	23.42%	1.855%
11	5.192	1184	1198	1212	rBV	168831	362425	55.10%	4.363%
12	5.587	1302	1321	1346	rBV4	24582	78373	11.91%	0.944%
13	5.864	1388	1407	1439	rBV3	257343	657807	100.00%	7.919%
14	6.179	1489	1505	1532	rBV5	40352	141225	21.47%	1.700%
15	6.391	1554	1571	1587	rBV	245227	449745	68.37%	5.414%
16	6.626	1627	1644	1651	rBV3	37687	84835	12.90%	1.021%
17	6.668	1652	1657	1670	rVB2	38342	62627	9.52%	0.754%
18	6.819	1687	1704	1717	rBV	158922	300343	45.66%	3.616%
19	7.021	1753	1767	1799	rVB4	33925	102375	15.56%	1.232%
20	7.658	1955	1965	1984	rVB2	62079	107144	16.29%	1.290%
21	7.796	2003	2008	2017	rVB4	10345	14167	2.15%	0.171%
22	7.980	2054	2065	2076	rBV	266121	456702	69.43%	5.498%
23	8.102	2095	2103	2115	rVB2	33119	59215	9.00%	0.713%
24	8.253	2142	2150	2163	rVB2	38313	63554	9.66%	0.765%
25	8.356	2180	2182	2198	rVB5	11706	18752	2.85%	0.226%
26	8.713	2279	2293	2305	rBV	241609	457809	69.60%	5.511%
27	8.793	2311	2318	2330	rVB	63549	129097	19.63%	1.554%
28	8.854	2331	2337	2353	rVB5	28221	47202	7.18%	0.568%
29	9.471	2517	2529	2541	rBV	376297	655515	99.65%	7.892%
30	9.533	2542	2548	2567	rVB2	44257	83050	12.63%	1.000%
31	10.385	2804	2813	2838	rVB5	25370	53068	8.07%	0.639%
32	10.793	2928	2940	2960	rVB	120881	258296	39.27%	3.110%
33	10.928	2968	2982	2988	rBV7	3864	7984	1.21%	0.096%
34	11.719	3216	3228	3244	rVB3	45329	79200	12.04%	0.953%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU121919\
Data File : VU036300.D
Acq On : 19 Dec 2019 22:31
Operator : JC/MD
Sample : K6282-17
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDX3

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	11.841	3252	3266	3284	rVB	376615	642193	97.63%	7.731%
36	12.086	3332	3342	3357	rBV6	9676	21371	3.25%	0.257%
37	12.221	3371	3384	3398	rVB	316791	531394	80.78%	6.397%
38	12.793	3553	3562	3573	rBV9	4425	7494	1.14%	0.090%
39	12.909	3582	3598	3612	rBV4	92392	153865	23.39%	1.852%
40	13.407	3745	3753	3765	rVB4	6881	10715	1.63%	0.129%
41	13.661	3826	3832	3843	rVB9	7361	11173	1.70%	0.135%
42	14.002	3929	3938	3947	rBV5	24960	36687	5.58%	0.442%
43	14.105	3956	3970	3978	rBV3	8307	17949	2.73%	0.216%
44	14.204	3990	4001	4015	rVB3	6795	19680	2.99%	0.237%
45	14.655	4129	4141	4153	rBV9	8071	16084	2.45%	0.194%
46	14.860	4187	4205	4213	rBV10	20219	42220	6.42%	0.508%
47	15.889	4518	4525	4532	rVB6	12165	17325	2.63%	0.209%
48	16.535	4718	4726	4727	rBV7	6751	9324	1.42%	0.112%
49	17.056	4884	4888	4894	rVB7	9407	12080	1.84%	0.145%
50	17.143	4908	4915	4922	rBV2	17764	24960	3.79%	0.300%

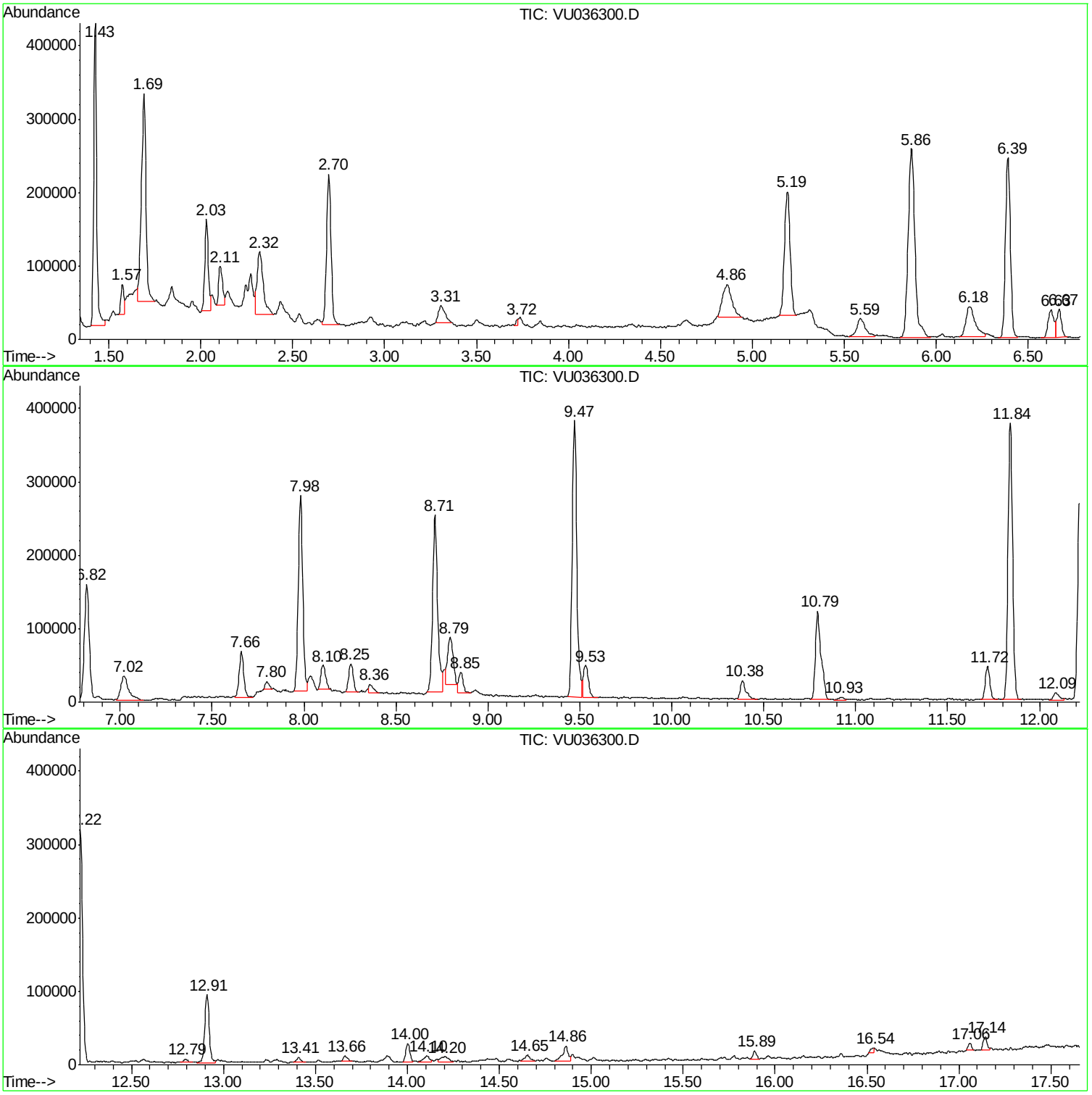
Sum of corrected areas: 8306466

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121919\
Data File : VU036300.D
Acq On : 19 Dec 2019 22:31
Operator : JC/MD
Sample : K6282-17
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDX3

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121919\
Data File : VU036300.D
Acq On : 19 Dec 2019 22:31
Operator : JC/MD
Sample : K6282-17
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDX3

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

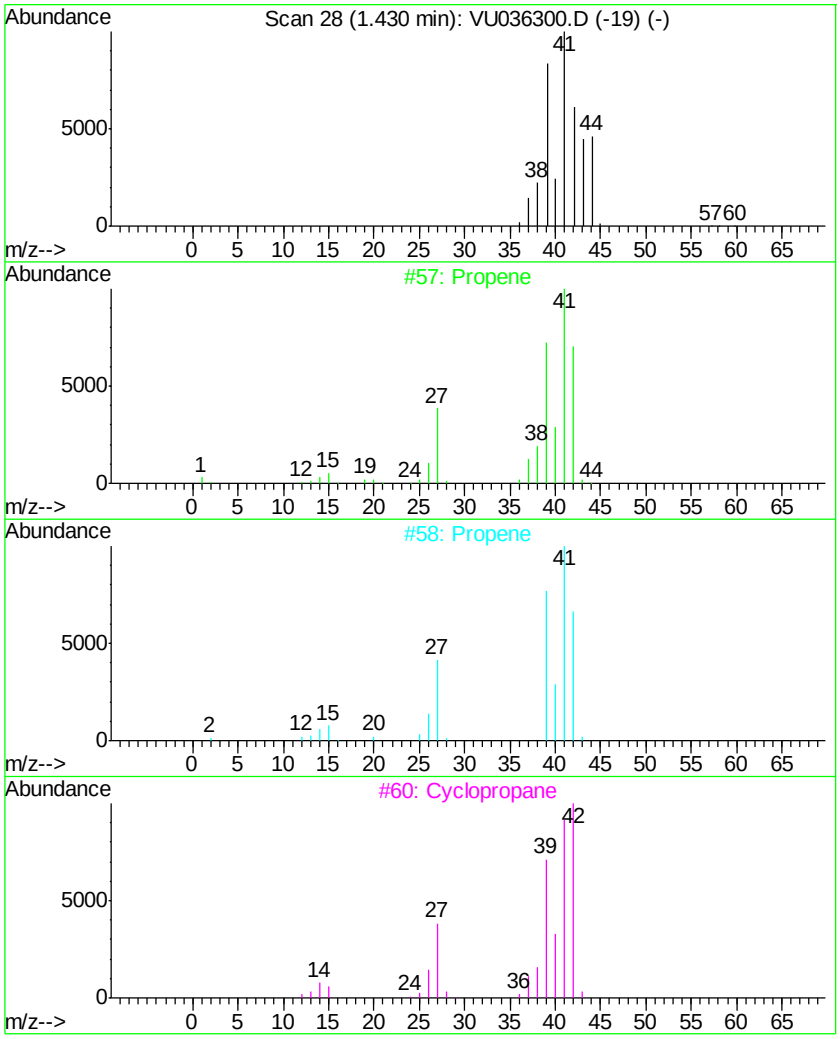
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

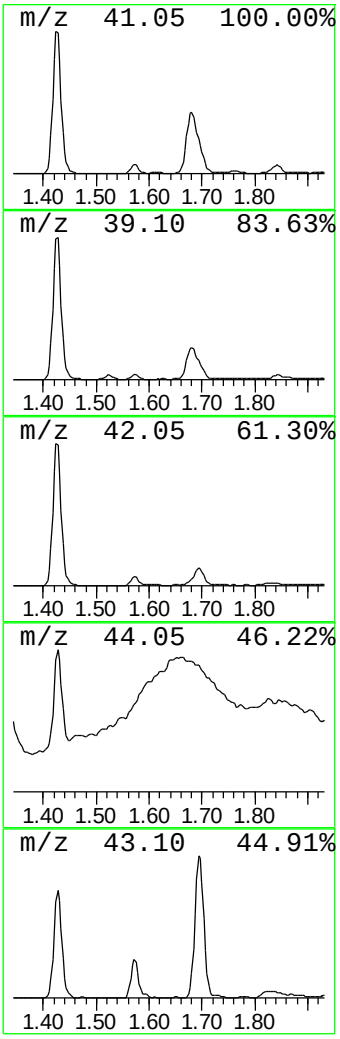
****

Peak Number 1 (DEL) Alkane: Cyclic1.43 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.43	5.21 ug/L	468233	1,4-Difluorobenzene	6.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	86
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





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU121919\
Data File : VU036300.D
Acq On : 19 Dec 2019 22:31
Operator : JC/MD
Sample : K6282-17
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDX3

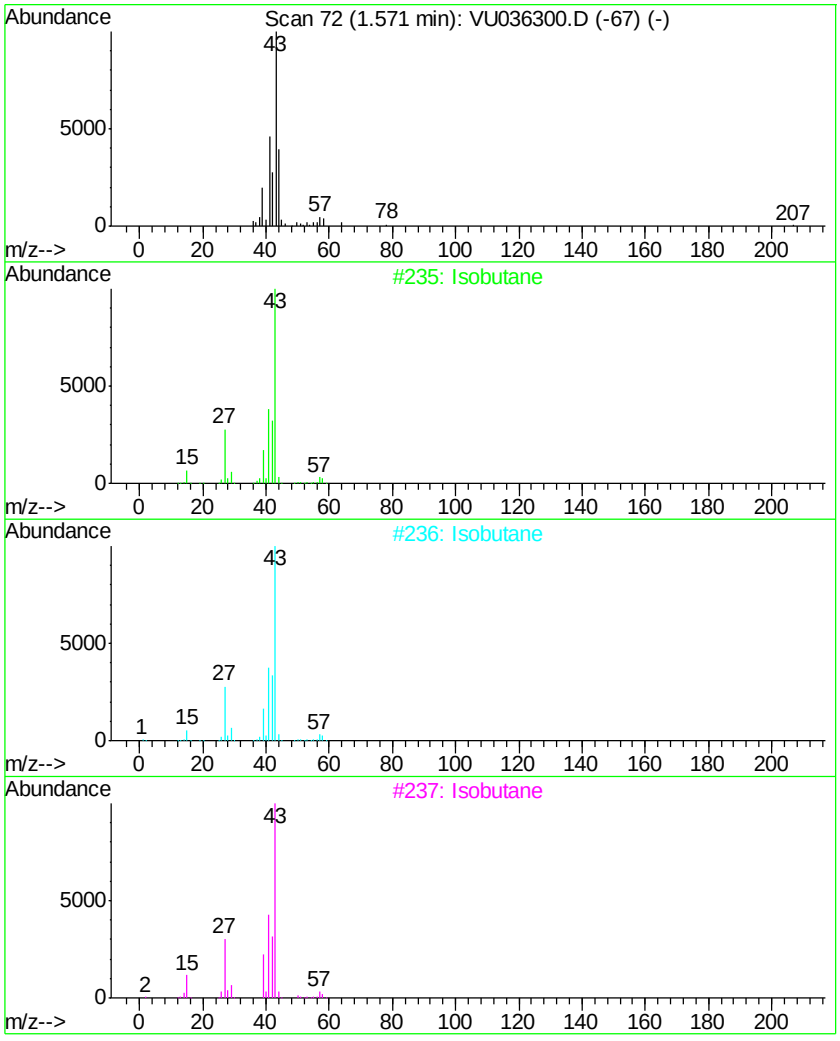
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR121319WMA.M
Quant Title : TRACE VOA SOM01.0

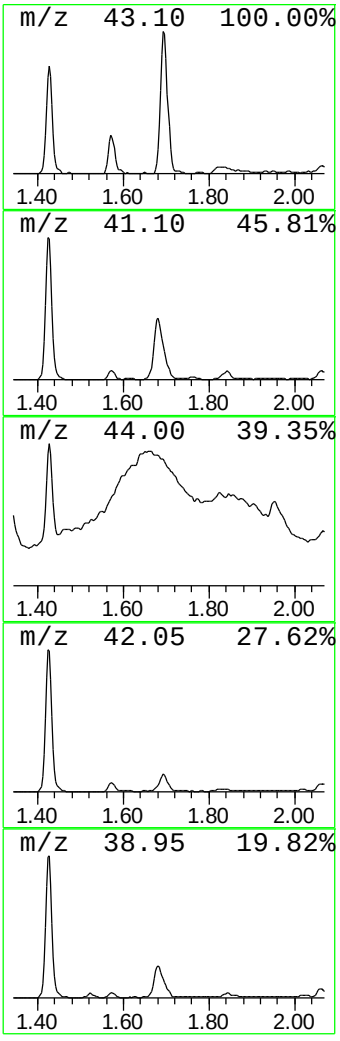
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.57	0.53 ug/L	47820	1,4-Difluorobenzene	6.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	43
2	Isobutane	58	C4H10	000075-28-5	37
3	Isobutane	58	C4H10	000075-28-5	32
4	Methyl Isobutyl Ketone	100	C6H12O	000108-10-1	9
5	2-Nitro-1-propanol	105	C3H7NO3	002902-96-7	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU121919\
Data File : VU036300.D
Acq On : 19 Dec 2019 22:31
Operator : JC/MD
Sample : K6282-17
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDX3

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

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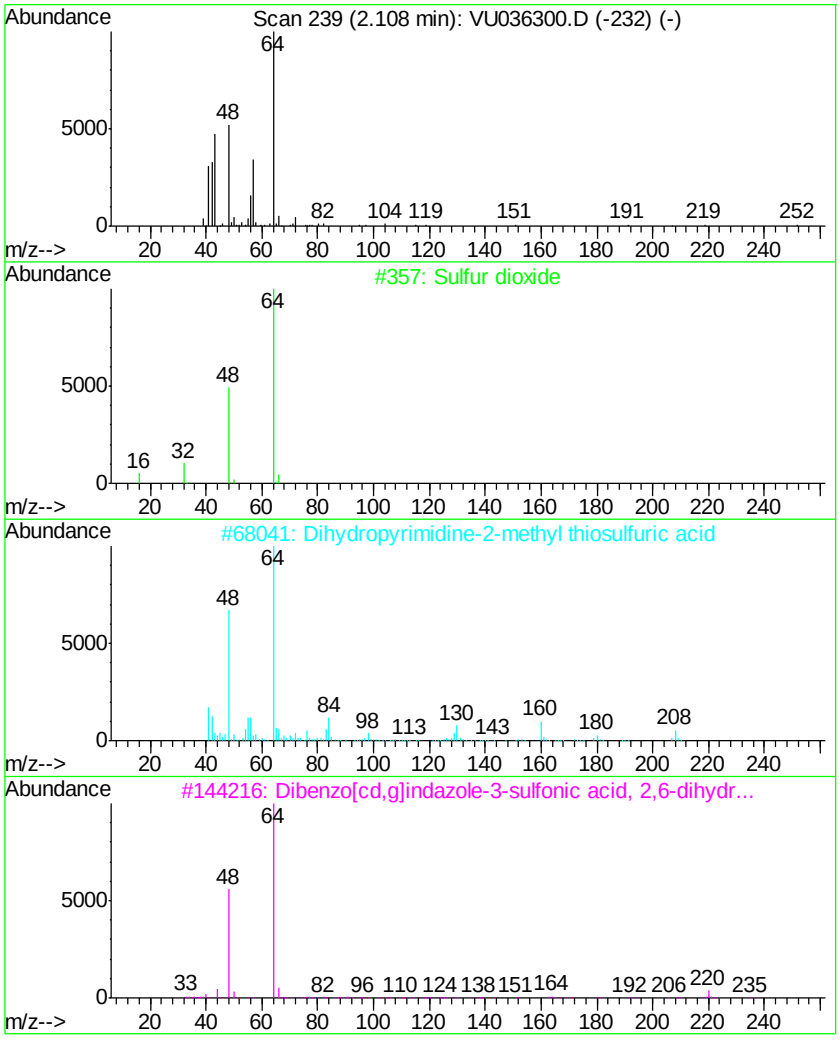
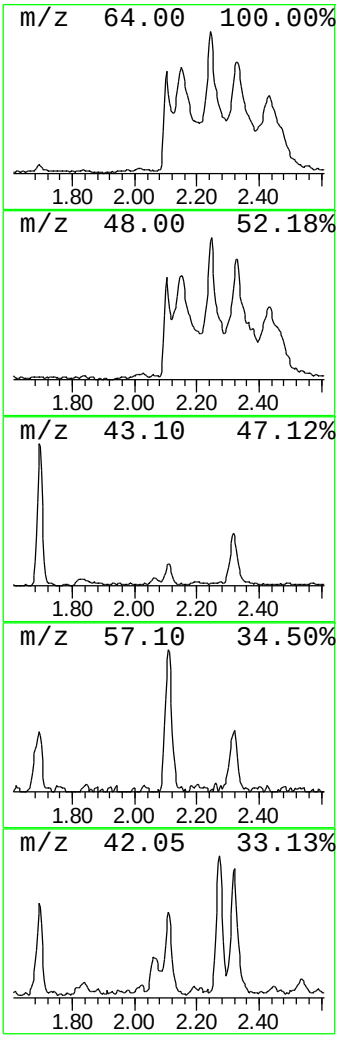
Peak Number 3 Sulfur dioxide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.11	0.88 ug/L	79157	1,4-Difluorobenzene	6.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	86
2	Dihydropyrimidine-2-methyl thios...	208	C5H8N2O3S2	1000256-28-8	74
3	Dibenzo[cd,g]indazole-3-sulfonic...	300	C14H8N2O4S	293765-87-4	64
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
5	N,N'-Nonamethylenebis[-S-3-amino...	466	C15H34N2O6S4	035871-58-0	64





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU121919\
Data File : VU036300.D
Acq On : 19 Dec 2019 22:31
Operator : JC/MD
Sample : K6282-17
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDX3

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

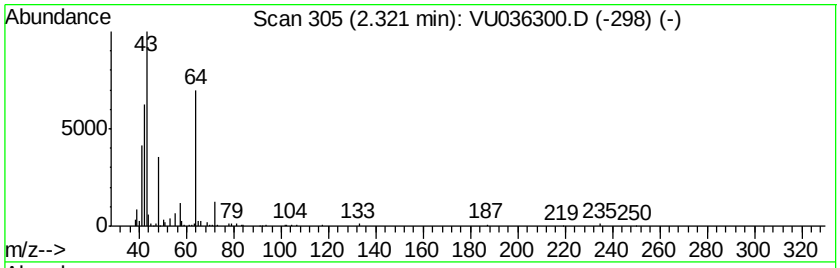
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

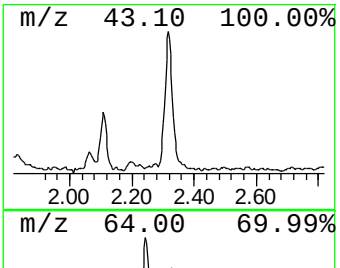
****

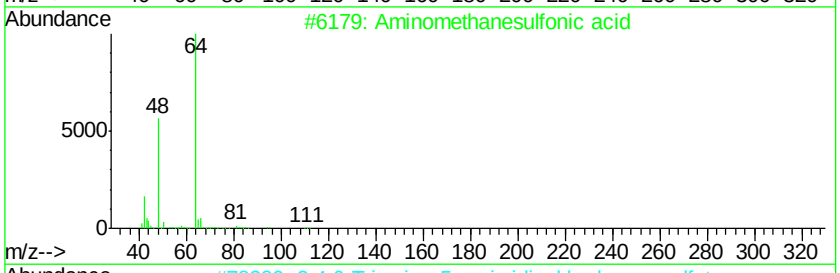
Peak Number 4 unknown-01 Concentration Rank 2

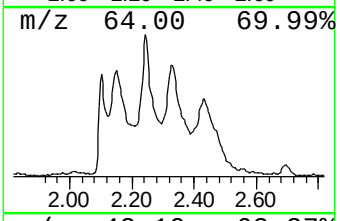
R.T.	EstConc	Area	Relative to ISTD	R.T.
2.32	2.14 ug/L	192750	1,4-Difluorobenzene	6.39

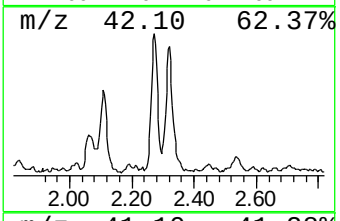
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	42
2	2,4,6-Triamino-5-pyrimidinyl hyd...	221	C4H7N5O4S	071552-23-3	40
3	Thiosulfuric acid (H2S2O3), S-(2...	320	C11H16N2O3S3	040284-00-2	33
4	Dibenzo[cd,g]indazole-3-sulfonic...	300	C14H8N2O4S	293765-87-4	33
5	Pentane	72	C5H12	000109-66-0	18

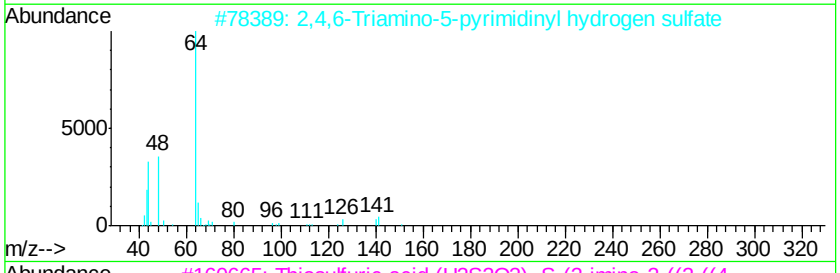


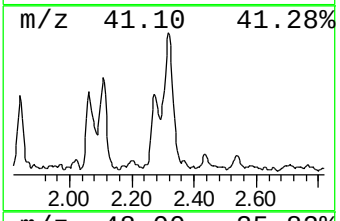


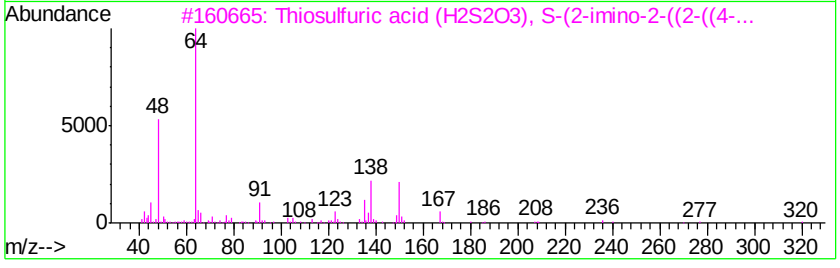


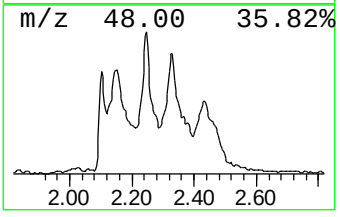












Library Search Compound Report

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ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDX3

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

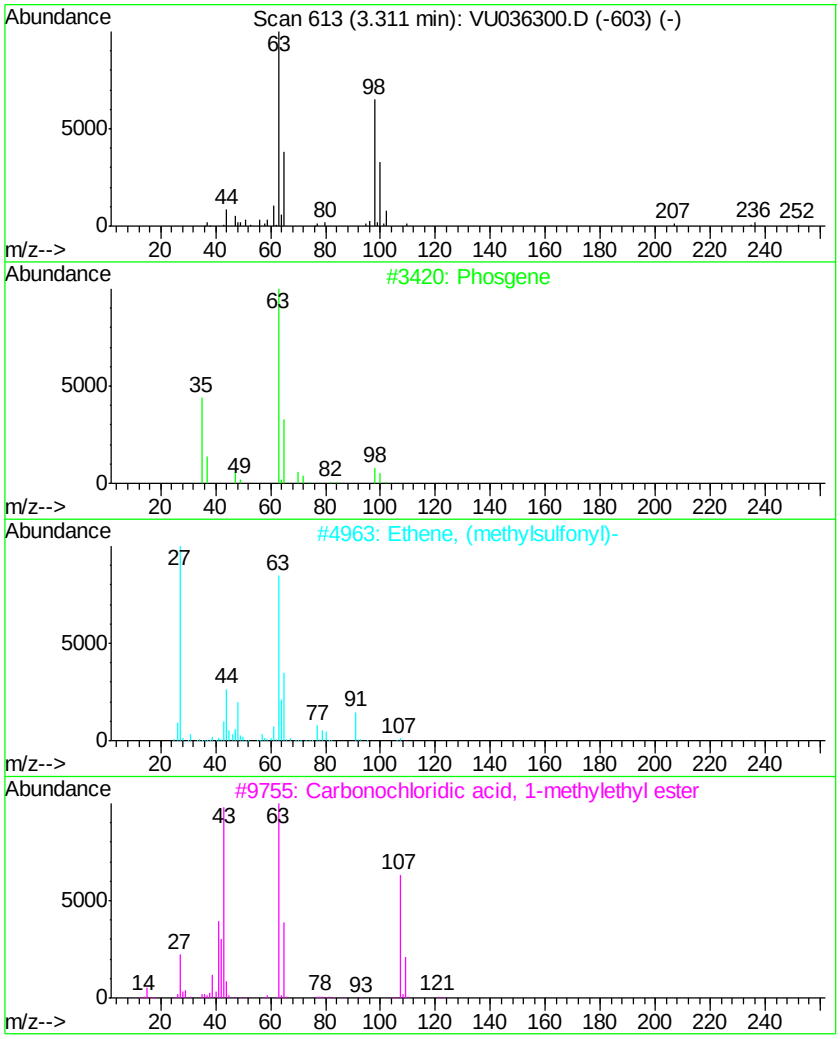
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

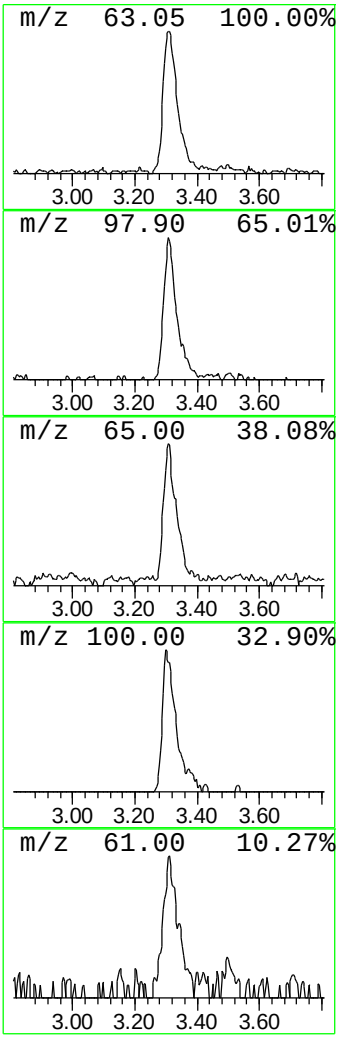
****

Peak Number 5 Phosgene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.31	0.66 ug/L	59060	1,4-Difluorobenzene	6.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phosgene	98	CCl2O	000075-44-5	83
2	Ethene, (methylsulfonyl)-	106	C3H6O2S	003680-02-2	56
3	Carbonochloridic acid, 1-methyle...	122	C4H7ClO2	000108-23-6	40
4	Ethane, 1,1-dichloro-	98	C2H4Cl2	000075-34-3	40
5	Ethane, 1,1-dichloro-	98	C2H4Cl2	000075-34-3	40





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU121919\
Data File : VU036300.D
Acq On : 19 Dec 2019 22:31
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Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDX3

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

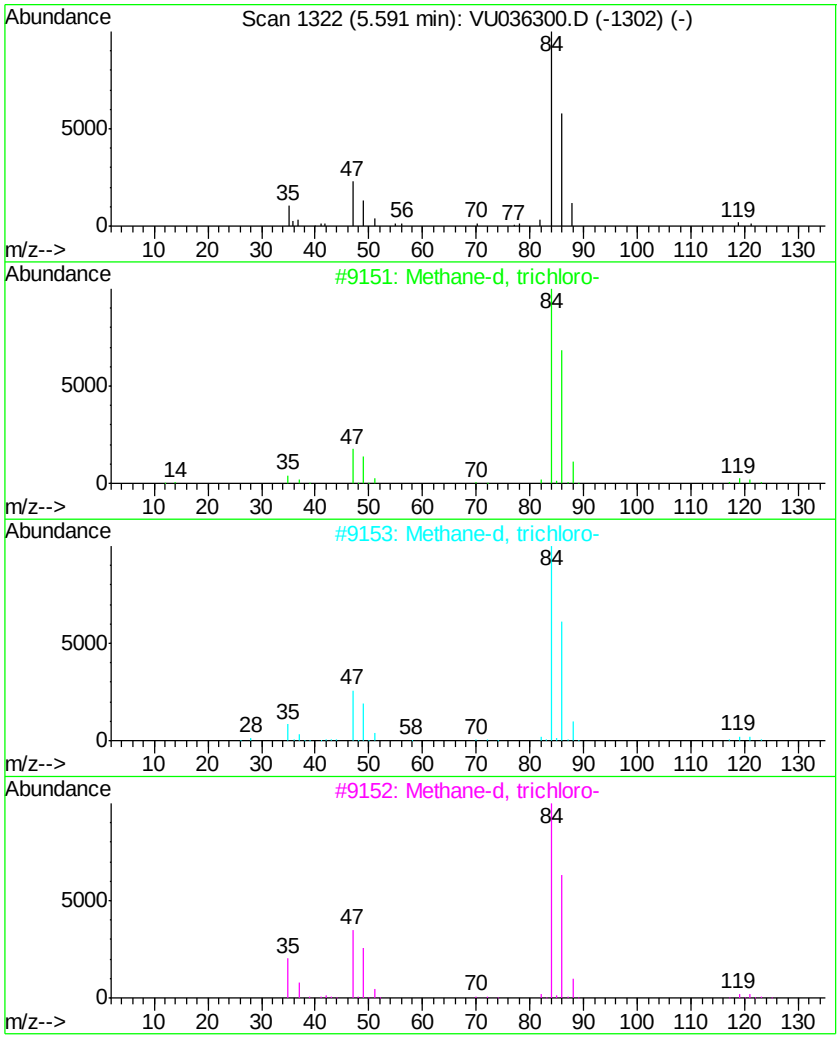
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

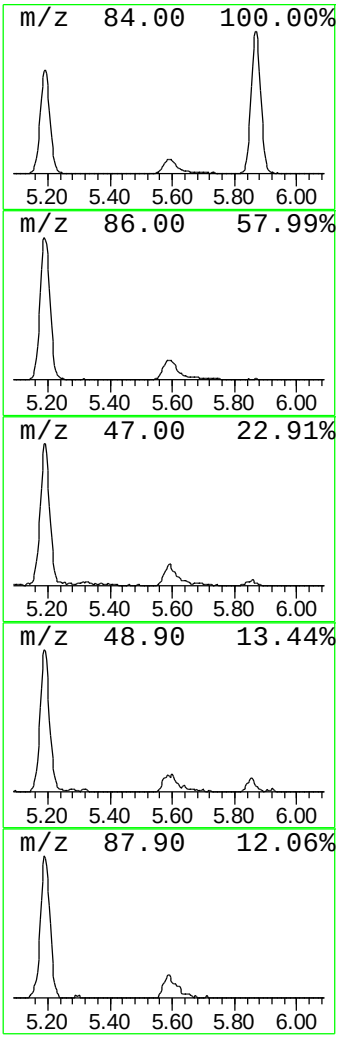
****

Peak Number 6 Methane-d, trichloro- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.59	0.87 ug/L	78373	1,4-Difluorobenzene	6.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methane-d, trichloro-	119	CDCl3	000865-49-6	90
2	Methane-d, trichloro-	119	CDCl3	000865-49-6	52
3	Methane-d, trichloro-	119	CDCl3	000865-49-6	47
4	Benzeneethanamine, .alpha.-methy...	177	C12H19N	033236-69-0	9
5	Benzeneethanamine, .alpha.-methy...	177	C12H19N	033236-69-0	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU121919\
Data File : VU036300.D
Acq On : 19 Dec 2019 22:31
Operator : JC/MD
Sample : K6282-17
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDX3

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

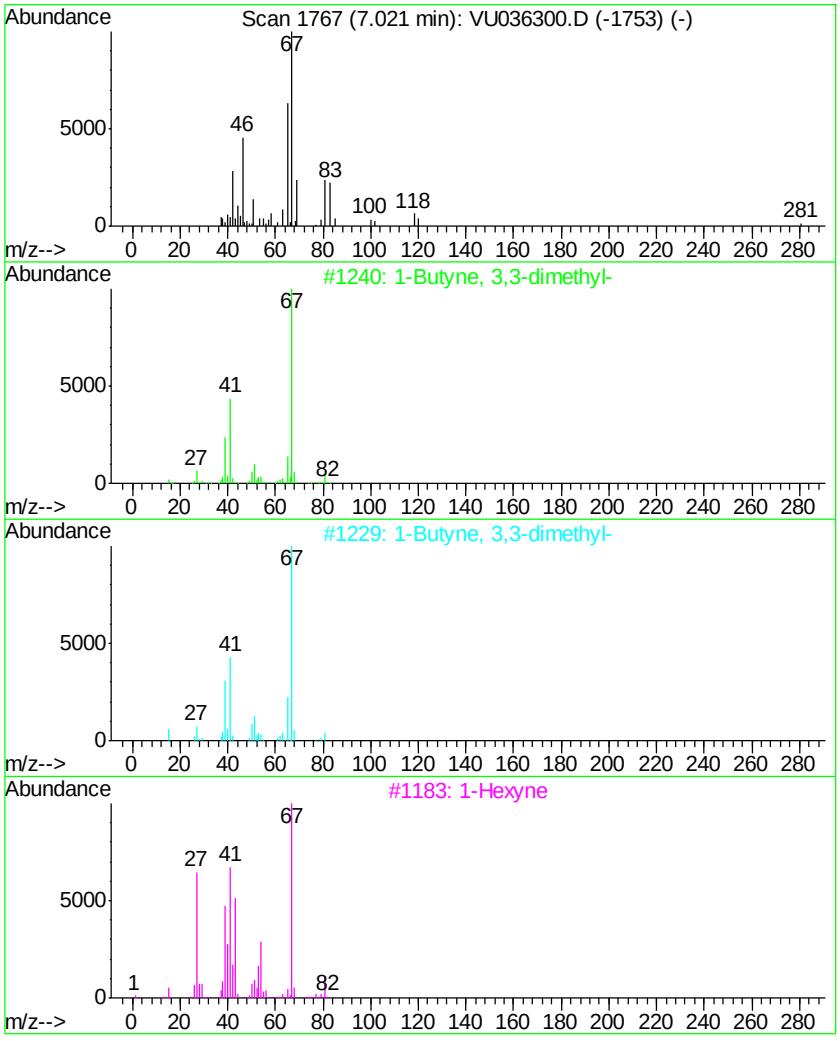
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

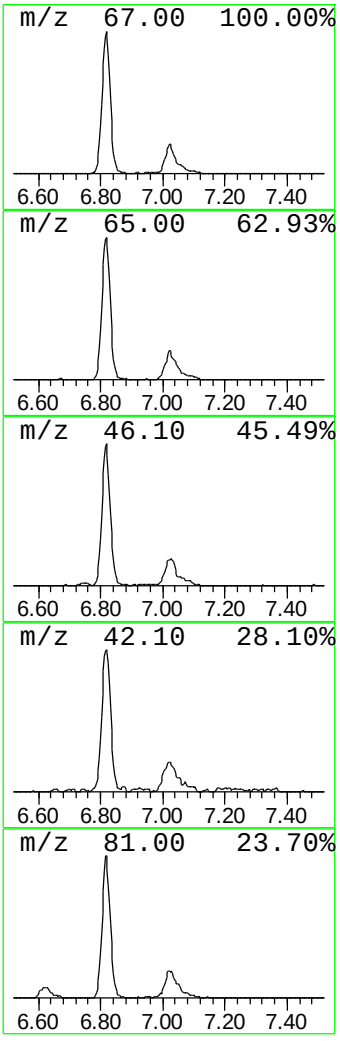
****

Peak Number 8 unknown-02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.02	1.14 ug/L	102375	1,4-Difluorobenzene	6.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butyne, 3,3-dimethyl-	82	C6H10	000917-92-0	9
2	1-Butyne, 3,3-dimethyl-	82	C6H10	000917-92-0	9
3	1-Hexyne	82	C6H10	000693-02-7	9
4	1-Hexyne	82	C6H10	000693-02-7	9
5	1-Hexyne	82	C6H10	000693-02-7	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU121919\
Data File : VU036300.D
Acq On : 19 Dec 2019 22:31
Operator : JC/MD
Sample : K6282-17
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDX3

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

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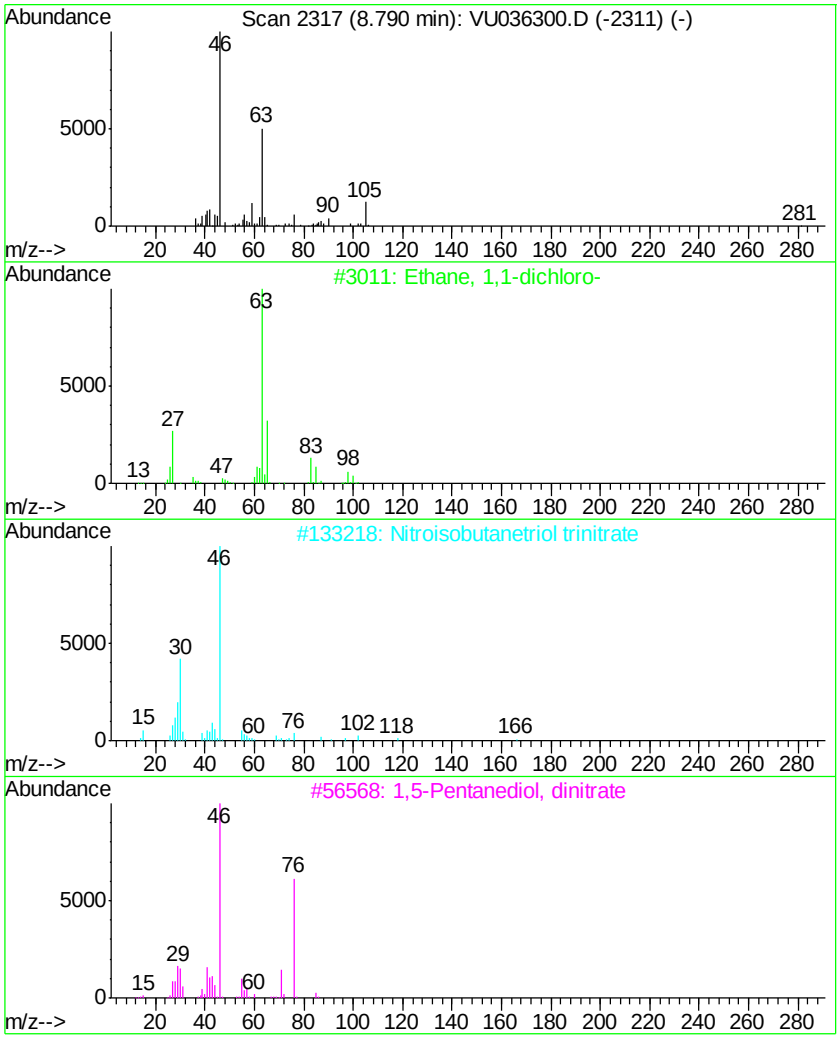
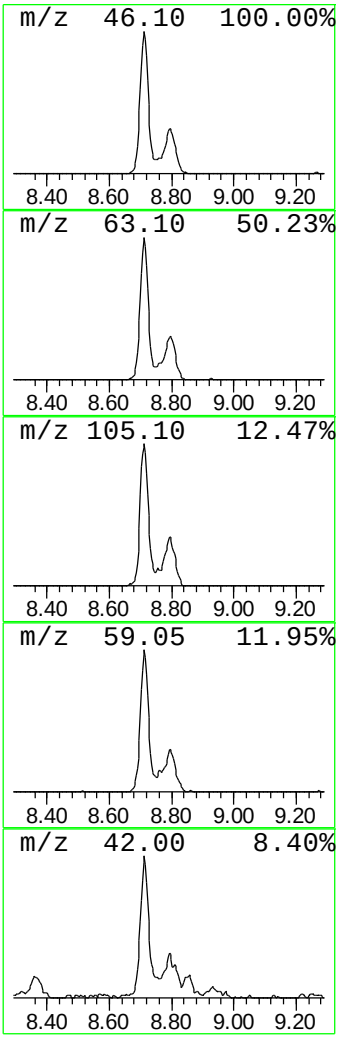
Peak Number 10 unknown-03 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.79	0.98 ug/L	129097	Chlorobenzene-d5	9.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethane, 1,1-dichloro-	98	C2H4Cl2	000075-34-3	28
2	Nitroisobutanetriol trinitrate	286	C4H6N4O11	020820-44-4	10
3	1,5-Pentanediol, dinitrate	194	C5H10N2O6	003457-92-9	10
4	1,2,3-Propanetriol, 1,3-dinitrate	182	C3H6N2O7	000623-87-0	10
5	Ethane, 1-chloro-2-nitro-	109	C2H4ClNO2	000625-47-8	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121919\
Data File : VU036300.D
Acq On : 19 Dec 2019 22:31
Operator : JC/MD
Sample : K6282-17
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDX3

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

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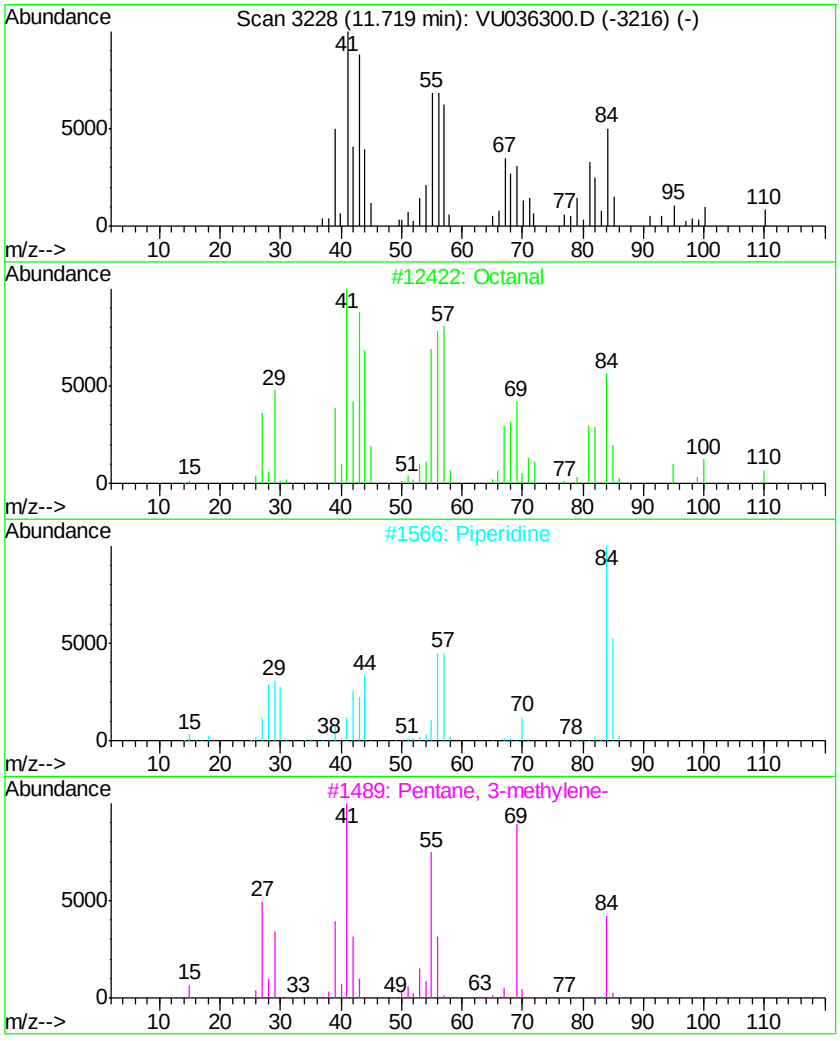
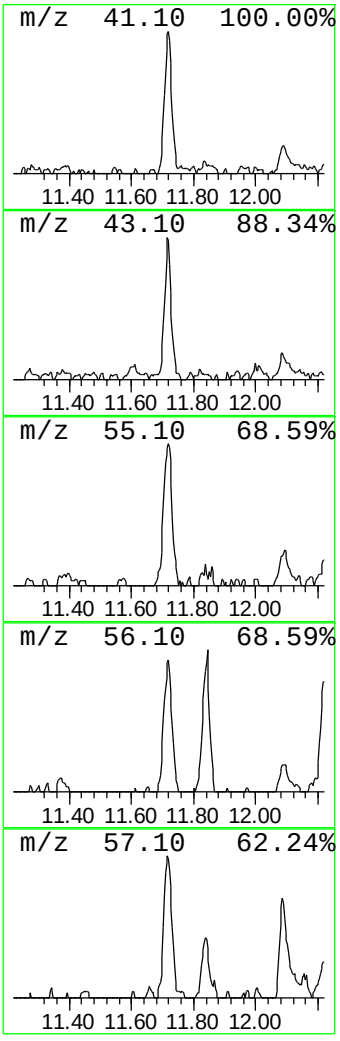
Peak Number 12 Octanal Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.72	0.62 ug/L	79200	1,4-Dichlorobenzene-d4	11.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanal	128	C8H16O	000124-13-0	64
2	Piperidine	85	C5H11N	000110-89-4	47
3	Pentane, 3-methylene-	84	C6H12	000760-21-4	30
4	Cyclopentanol, 2-methyl-, trans-	100	C6H12O	025144-04-1	30
5	Cyclopentanol, 2-methyl-, cis-	100	C6H12O	025144-05-2	30





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU121919\
Data File : VU036300.D
Acq On : 19 Dec 2019 22:31
Operator : JC/MD
Sample : K6282-17
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDX3

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

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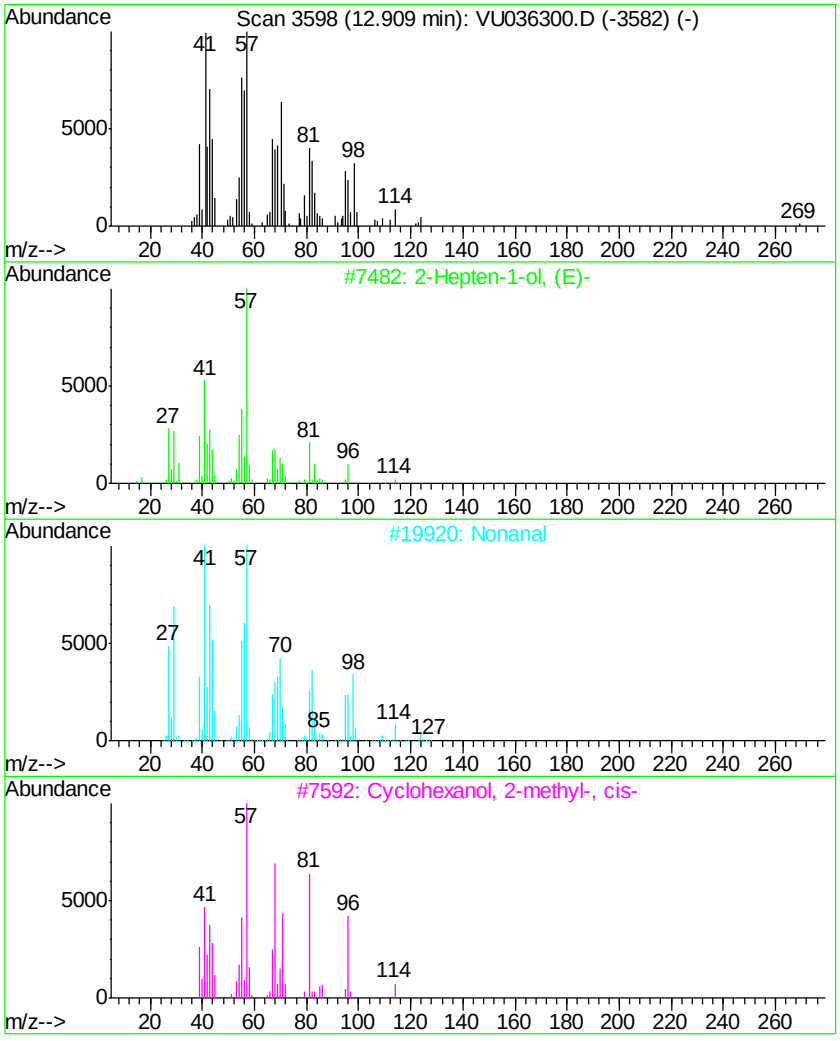
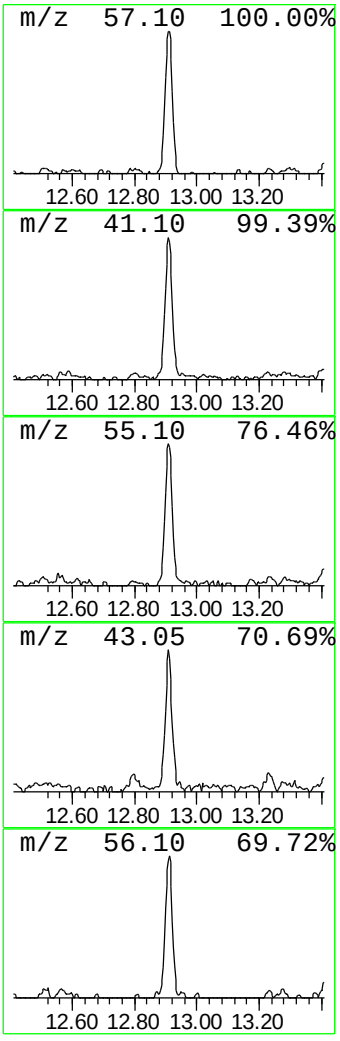
Peak Number 13 2-Hepten-1-ol, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.91	1.20 ug/L	153865	1,4-Dichlorobenzene-d4	11.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hepten-1-ol, (E)-	114	C7H14O	033467-76-4	58
2	Nonanal	142	C9H18O	000124-19-6	58
3	Cyclohexanol, 2-methyl-, cis-	114	C7H14O	007443-70-1	43
4	2-Nonen-1-ol, (Z)-	142	C9H18O	041453-56-9	38
5	Cycloheptane	98	C7H14	000291-64-5	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121919\
Data File : VU036300.D
Acq On : 19 Dec 2019 22:31
Operator : JC/MD
Sample : K6282-17
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BFDX3

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: Cyc...	1.43	5.2	ug/L	468233	1	6.39	449745	5.0
(DEL) Alkane: Str...	1.57	0.5	ug/L	47820	1	6.39	449745	5.0
Sulfur dioxide	2.11	0.9	ug/L	79157	1	6.39	449745	5.0
unknown-01	2.32	2.1	ug/L	192750	1	6.39	449745	5.0
Phosgene	3.31	0.7	ug/L	59060	1	6.39	449745	5.0
Methane-d, trichl...	5.59	0.9	ug/L	78373	1	6.39	449745	5.0
unknown-02	7.02	1.1	ug/L	102375	1	6.39	449745	5.0
unknown-03	8.79	1.0	ug/L	129097	2	9.47	655515	5.0
Octanal	11.72	0.6	ug/L	79200	3	11.84	642193	5.0
2-Hepten-1-ol, (E)-	12.91	1.2	ug/L	153865	3	11.84	642193	5.0