LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038956.D
Acq On : 17 Jun 2020 19:58
Operator : SY/MD
Sample : L3040-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L25

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\SOMUTR061720WMA.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	1.626	79	89	103	rVB	122668	156086	10.00%	1.146%
2	1.954	184	191	200	rBV	103867	133813	8.57%	0.982%
3	2.218	266	273	277	rBV2	18437	24086	1.54%	0.177%
4	2.420	331	336	355	rVB2	32212	69235	4.43%	0.508%
5	2.607	384	394	407	rVB	293649	461937	29.58%	3.391%
6	3.289	593	606	607	rBV2	13651	27601	1.77%	0.203%
7	3.600	700	703	713	rVB3	10647	16543	1.06%	0.121%
8	4.549	975	998	1019	rBV6	19271	73221	4.69%	0.538%
9	4.800	1047	1076	1107	rBV2	92132	462165	29.60%	3.393%
10	5.153	1169	1186	1209	rVB	201524	434261	27.81%	3.188%
11	5.796	1365	1386	1409	rBV2	415339	1008329	64.57%	7.403%
12	6.311	1533	1546	1564	rVB	324057	596827	38.22%	4.382%
13	6.687	1652	1663	1671	rBV5	16327	32506	2.08%	0.239%
14	6.748	1671	1682	1703	rVV	250085	493860	31.63%	3.626%
15	7.227	1807	1831	1844	rBV	96674	203806	13.05%	1.496%
16	7.610	1935	1950	1965	rBV2	124527	212683	13.62%	1.561%
17	7.883	2011	2035	2040	rBV7	16557	42708	2.73%	0.314%
18	7.935	2040	2051	2067	rVB	439734	756150	48.42%	5.551%
19	8.079	2087	2096	2105	rVB2	10238	16240	1.04%	0.119%
20	8.214	2127	2138	2154	rBV	81917	136707	8.75%	1.004%
21	8.526	2221	2235	2246	rBV3	8705	16762	1.07%	0.123%
22	8.674	2263	2281	2318	rVV2	676759	1561599	100.00%	11.465%
23	8.816	2318	2325	2352	rVV4	19652	43511	2.79%	0.319%
24	8.947	2352	2366	2391	rVB3	8977	28608	1.83%	0.210%
25	9.443	2505	2520	2542	rBV	470680	790232	50.60%	5.802%
26	9.661	2567	2588	2599	rBV	58504	100958	6.47%	0.741%
27	9.787	2611	2627	2642	rBV5	14629	32796	2.10%	0.241%
28	9.941	2665	2675	2686	rVB3	12464	19282	1.23%	0.142%
29	10.150	2720	2740	2752	rVB6	6719	15673	1.00%	0.115%
30	10.256	2758	2773	2788	rBV	111411	185978	11.91%	1.365%
31	10.381	2798	2812	2829	rVB7	18301	51808	3.32%	0.380%
32	10.703	2904	2912	2922	rVB2	18469	29042	1.86%	0.213%
33	10.774	2922	2934	2948	rBV	216404	352820	22.59%	2.590%
34	10.983	2990	2999	3013	rVB	33174	52735	3.38%	0.387%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038956.D
Acq On : 17 Jun 2020 19:58
Operator : SY/MD
Sample : L3040-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L25

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\SOMUTR061720WMA.M
Title : TRACE VOA SOM01.0

35	11.063	3015	3024	3033	rVB3	20624	33347	2.14%	0.245%
36	11.584	3173	3186	3199	rBV2	130633	201433	12.90%	1.479%
37	11.661	3203	3210	3216	rVV2	25491	44658	2.86%	0.328%
38	11.700	3216	3222	3230	rVV3	35356	57049	3.65%	0.419%
39	11.751	3233	3238	3249	rVV9	10639	18751	1.20%	0.138%
40	11.825	3249	3261	3277	rVB	529771	831856	53.27%	6.107%
41	11.902	3277	3285	3296	rBV3	9832	17022	1.09%	0.125%
42	11.989	3305	3312	3322	rVB6	9742	15779	1.01%	0.116%
43	12.076	3325	3339	3368	rBV	675643	1357460	86.93%	9.966%
44	12.205	3368	3379	3402	rVB	546201	906952	58.08%	6.658%
45	12.336	3411	3420	3437	rVB2	40459	66156	4.24%	0.486%
46	12.793	3551	3562	3571	rBV	126260	199781	12.79%	1.467%
47	12.835	3571	3575	3588	rVV2	27736	52233	3.34%	0.383%
48	12.906	3589	3597	3607	rVV3	41524	68336	4.38%	0.502%
49	14.015	3933	3942	3951	rBV5	16779	25970	1.66%	0.191%
50	14.227	3994	4008	4020	rVB2	46230	74802	4.79%	0.549%
51	14.703	4143	4156	4164	rBV10	7686	16682	1.07%	0.122%
52	14.873	4200	4209	4215	rBV4	15154	29138	1.87%	0.214%
53	14.922	4219	4224	4233	rVV8	18551	32572	2.09%	0.239%
54	15.147	4288	4294	4306	rVB4	11209	16602	1.06%	0.122%
55	15.745	4462	4480	4493	rBV6	43242	79651	5.10%	0.585%
56	16.835	4809	4819	4832	rBV2	95973	160440	10.27%	1.178%
57	16.963	4847	4859	4879	rBV	397640	673827	43.15%	4.947%

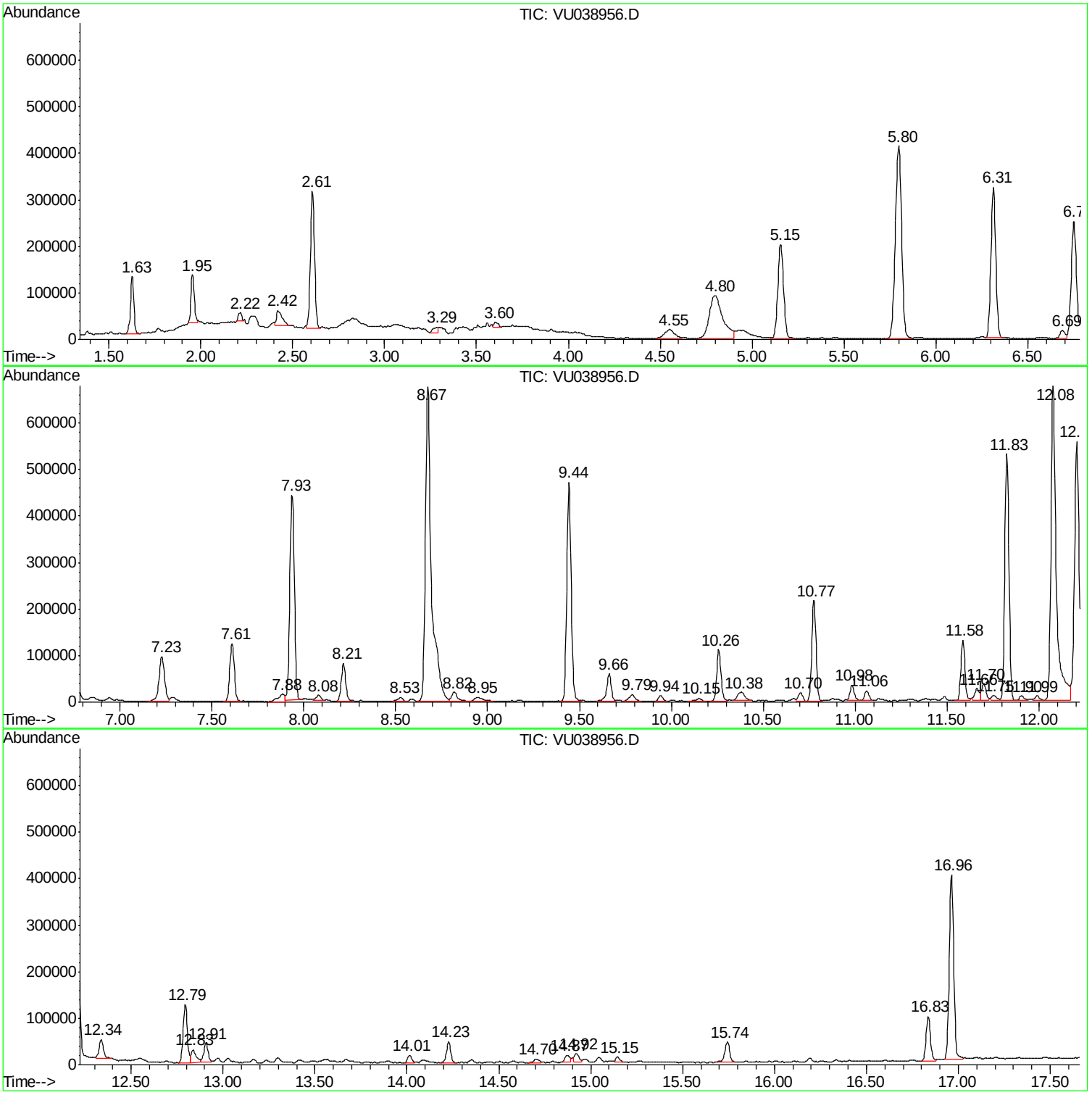
Sum of corrected areas: 13621065

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061720\
Data File : VU038956.D
Acq On : 17 Jun 2020 19:58
Operator : SY/MD
Sample : L3040-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L25

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038956.D
Acq On : 17 Jun 2020 19:58
Operator : SY/MD
Sample : L3040-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L25

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

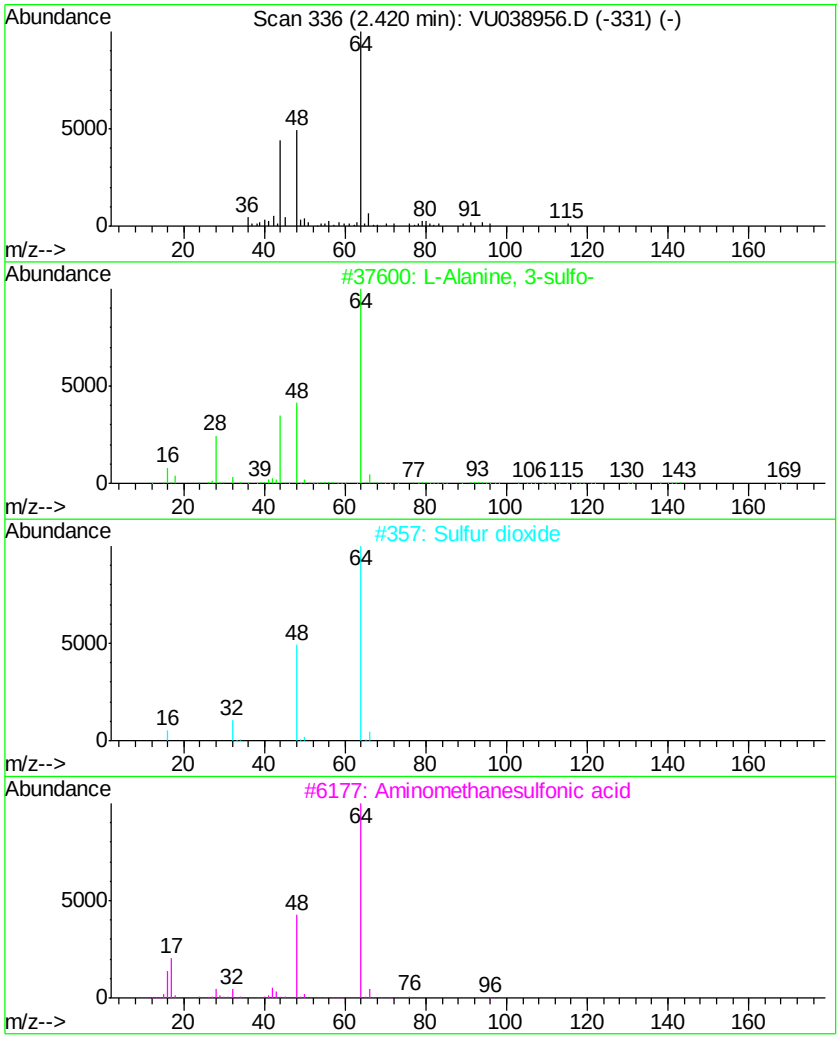
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

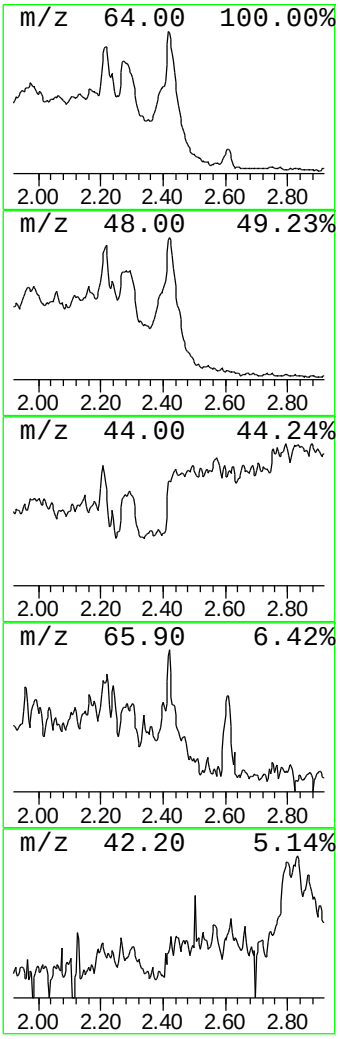
****

Peak Number 1 Sulfur dioxide Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.42	0.58 ug/L	69235	1,4-Difluorobenzene	6.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	83
2	Sulfur dioxide	64	O2S	007446-09-5	80
3	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	72
4	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	56
5	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	40





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061720\
Data File : VU038956.D
Acq On : 17 Jun 2020 19:58
Operator : SY/MD
Sample : L3040-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L25

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

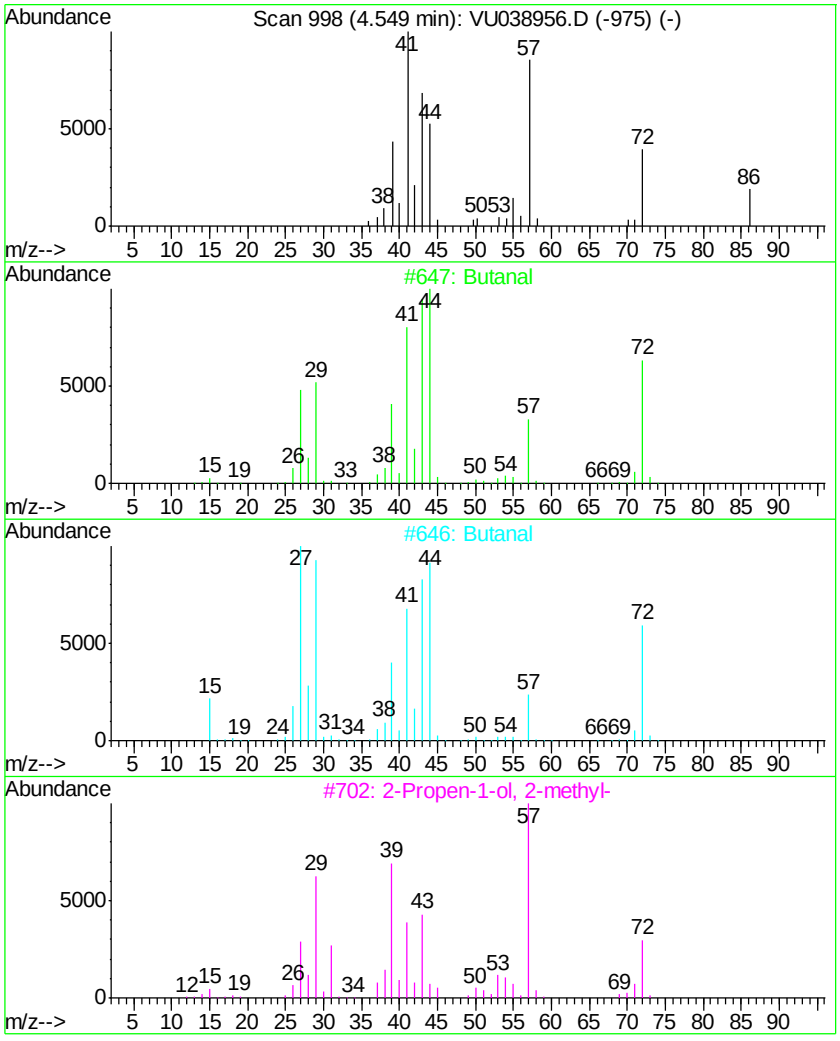
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

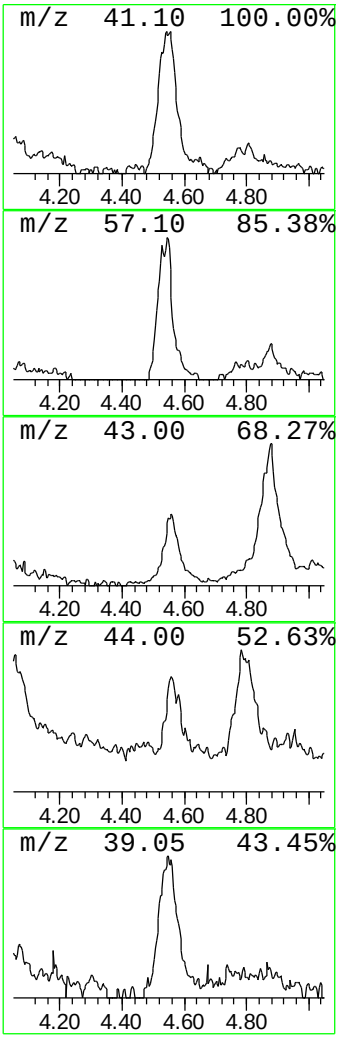
****

Peak Number 2 unknown-01 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	0.61 ug/L	73221	1,4-Difluorobenzene	6.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	49
2	Butanal	72	C4H8O	000123-72-8	43
3	2-Propen-1-ol, 2-methyl-	72	C4H8O	000513-42-8	38
4	Cyclobutanol, 2-ethyl-	100	C6H12O	035301-43-0	37
5	Cyclopropanecarboxamide	85	C4H7NO	006228-73-5	37





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038956.D
Acq On : 17 Jun 2020 19:58
Operator : SY/MD
Sample : L3040-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L25

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

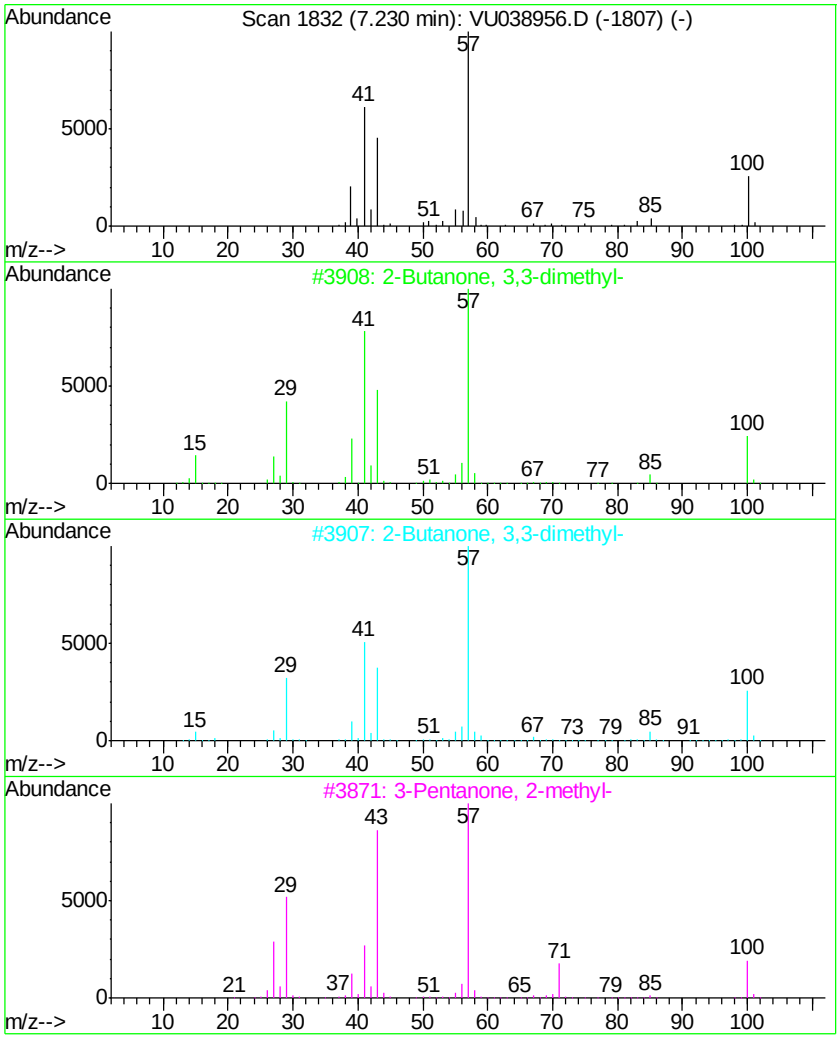
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

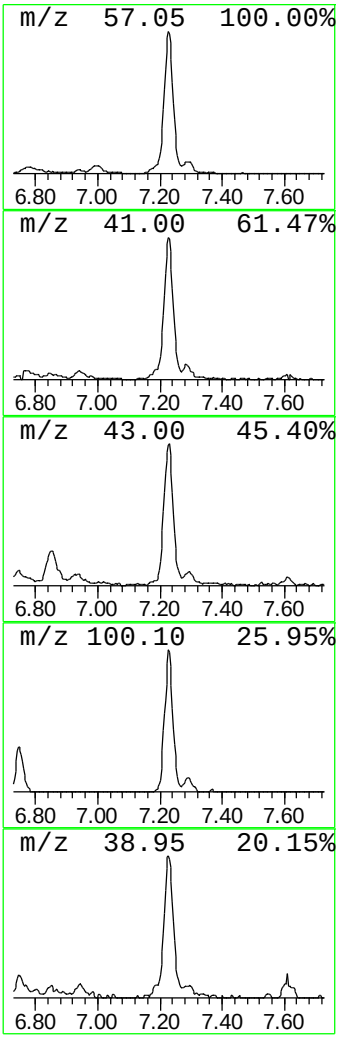
****

Peak Number 3 2-Butanone, 3,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.23	1.71 ug/L	203806	1,4-Difluorobenzene	6.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	91
2	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	90
3	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	64
4	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	50
5	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	49





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038956.D
Acq On : 17 Jun 2020 19:58
Operator : SY/MD
Sample : L3040-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L25

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

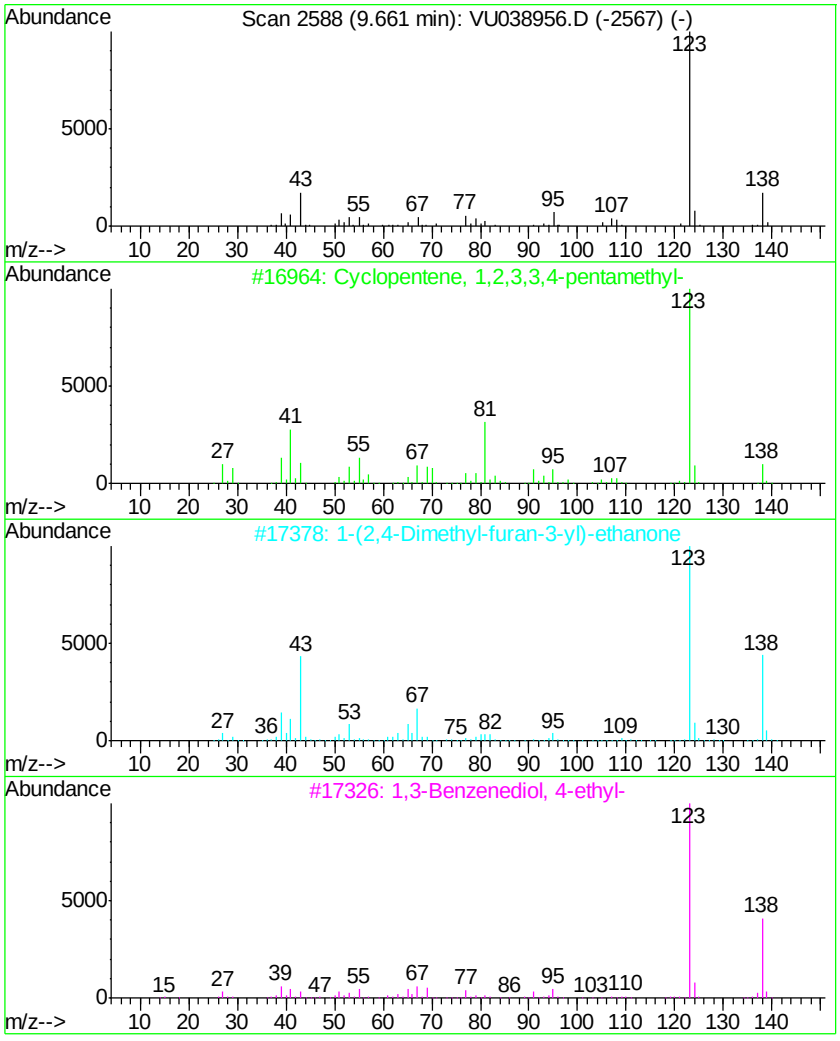
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

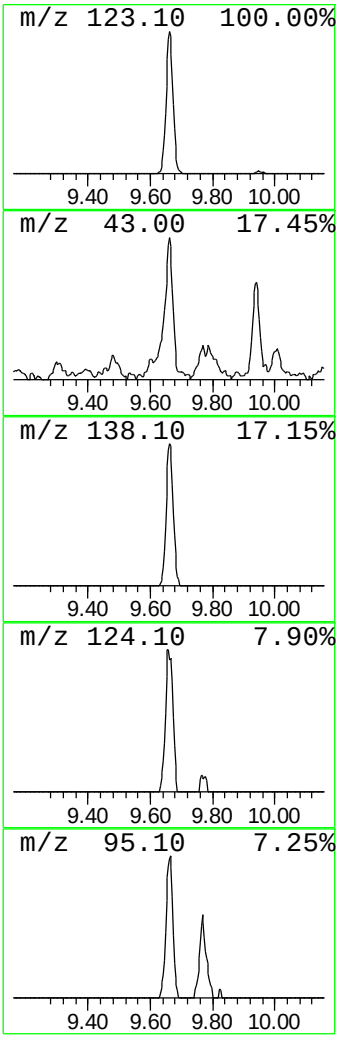
****

Peak Number 5 Cyclopentene, 1,2,3,3,4-pen... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.66	0.64 ug/L	100958	Chlorobenzene-d5	9.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene, 1,2,3,3,4-pentamet...	138	C10H18	197390-29-7	90
2	1-(2,4-Dimethyl-furan-3-yl)-etha...	138	C8H10O2	032933-07-6	72
3	1,3-Benzenediol, 4-ethyl-	138	C8H10O2	002896-60-8	72
4	Phenol, 4-amino-3-methyl-	123	C7H9NO	002835-99-6	72
5	Benzene, 1,4-dimethoxy-	138	C8H10O2	000150-78-7	64





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038956.D
Acq On : 17 Jun 2020 19:58
Operator : SY/MD
Sample : L3040-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L25

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

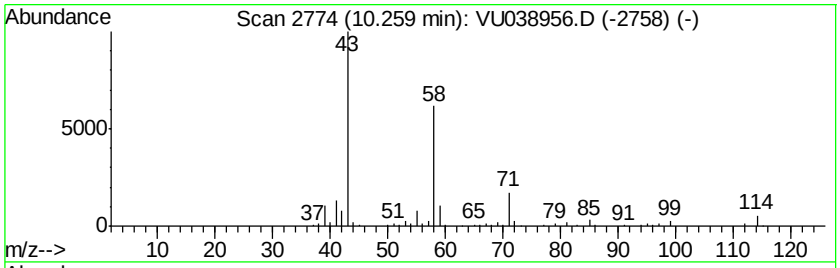
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

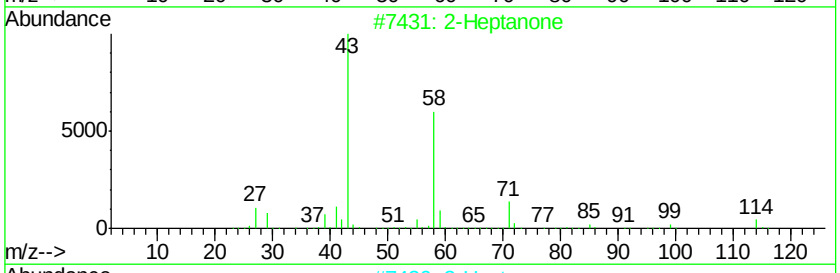
****

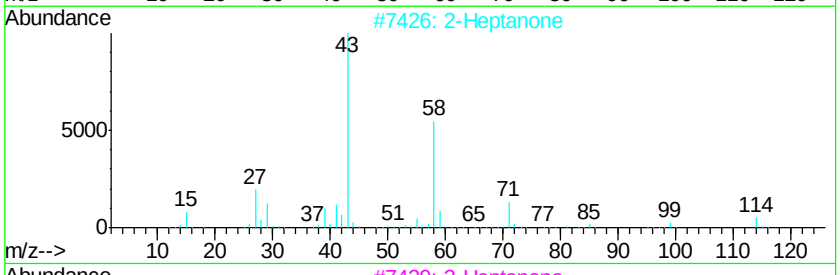
Peak Number 6 2-Heptanone Concentration Rank 7

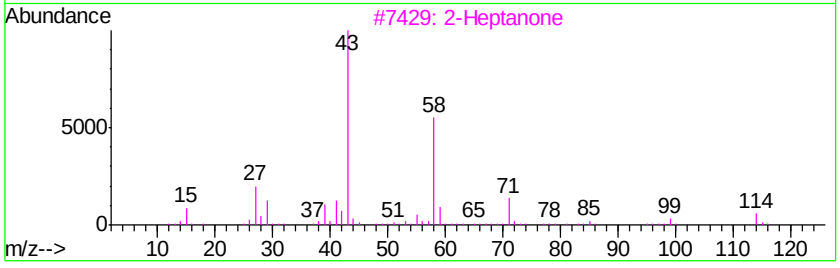
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.26	1.18 ug/L	185978	Chlorobenzene-d5	9.44

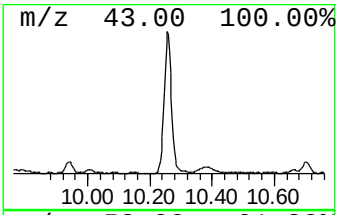
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone	114	C7H14O	000110-43-0	90
2	2-Heptanone	114	C7H14O	000110-43-0	90
3	2-Heptanone	114	C7H14O	000110-43-0	87
4	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	78
5	2-Heptanone	114	C7H14O	000110-43-0	78

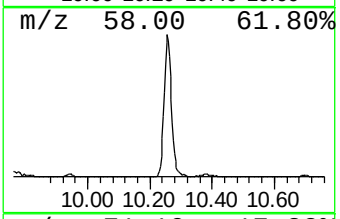


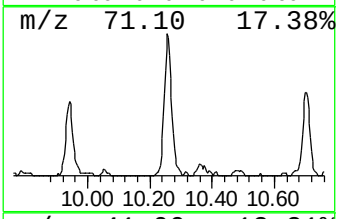


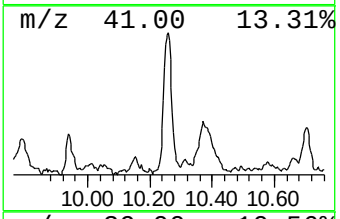


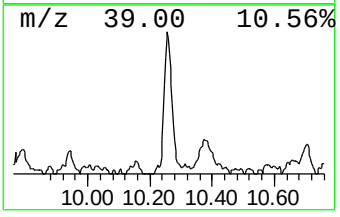












Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038956.D
Acq On : 17 Jun 2020 19:58
Operator : SY/MD
Sample : L3040-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L25

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

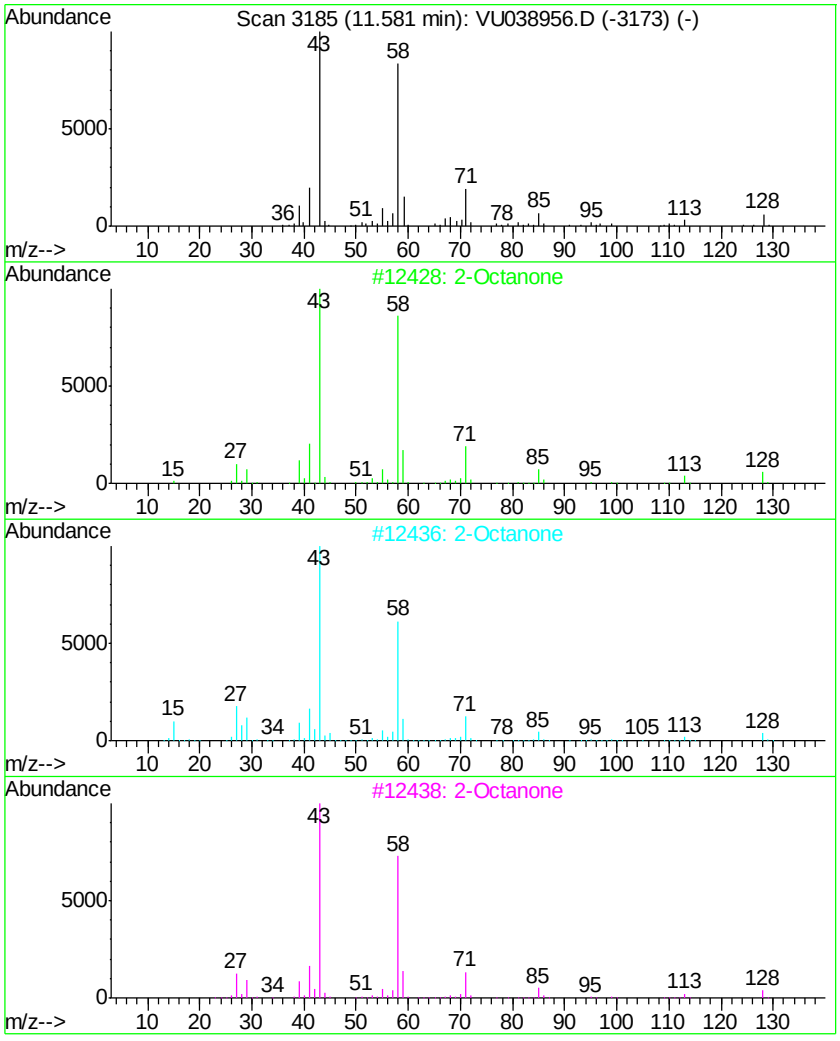
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

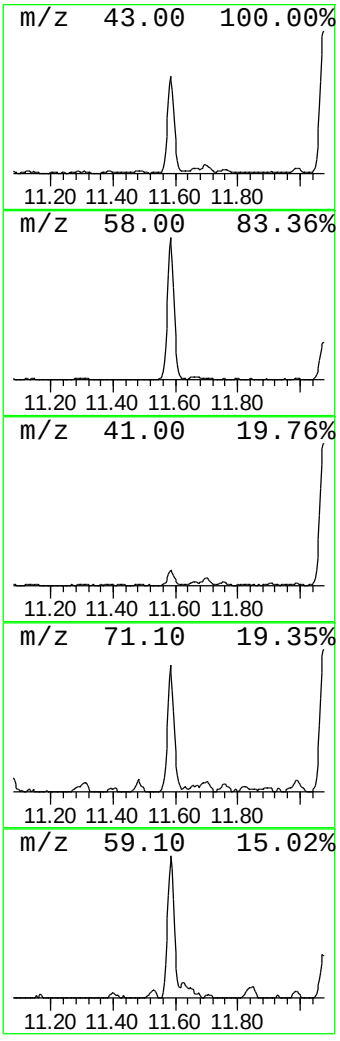
****

Peak Number 7 2-Octanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.58	1.21 ug/L	201433	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanone	128	C8H16O	000111-13-7	91
2	2-Octanone	128	C8H16O	000111-13-7	91
3	2-Octanone	128	C8H16O	000111-13-7	91
4	2-Octanone	128	C8H16O	000111-13-7	91
5	2-Octanone	128	C8H16O	000111-13-7	83





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038956.D
Acq On : 17 Jun 2020 19:58
Operator : SY/MD
Sample : L3040-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L25

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

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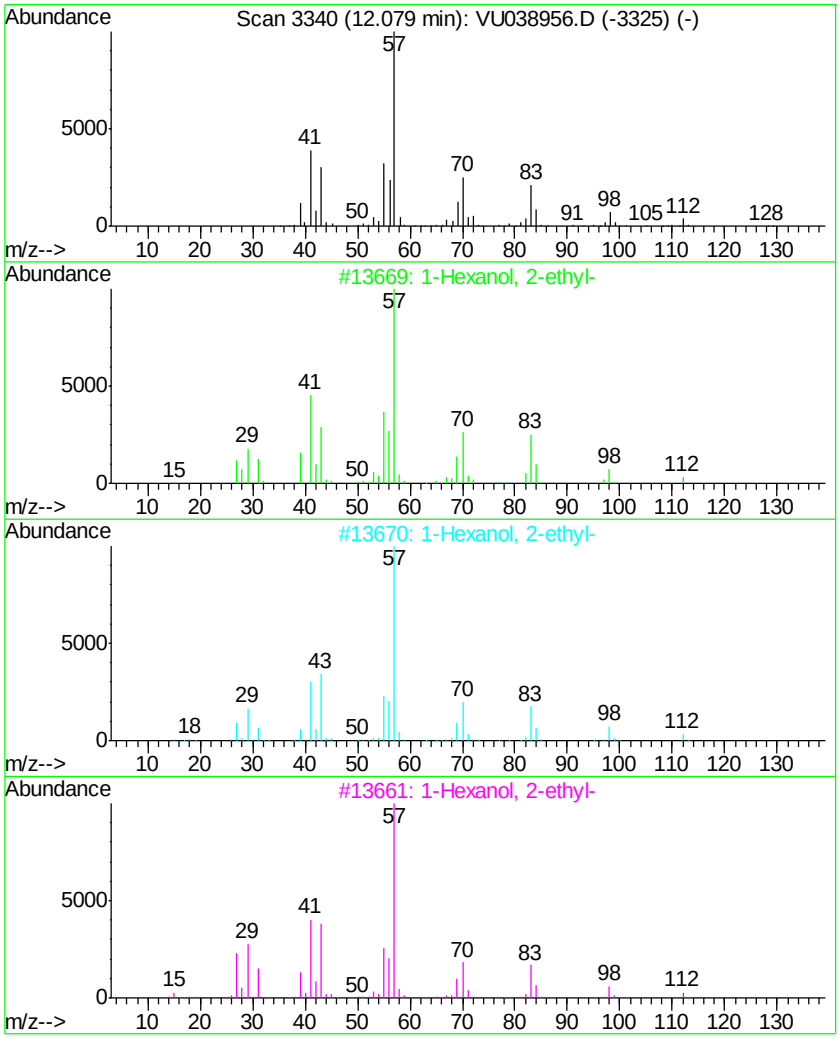
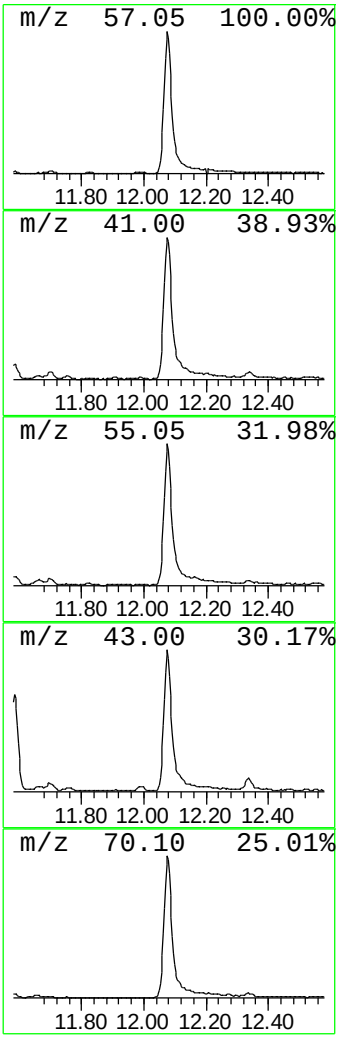
Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.08	8.16 ug/L	1357460	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
5	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59





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Data File : VU038956.D
Acq On : 17 Jun 2020 19:58
Operator : SY/MD
Sample : L3040-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L25

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

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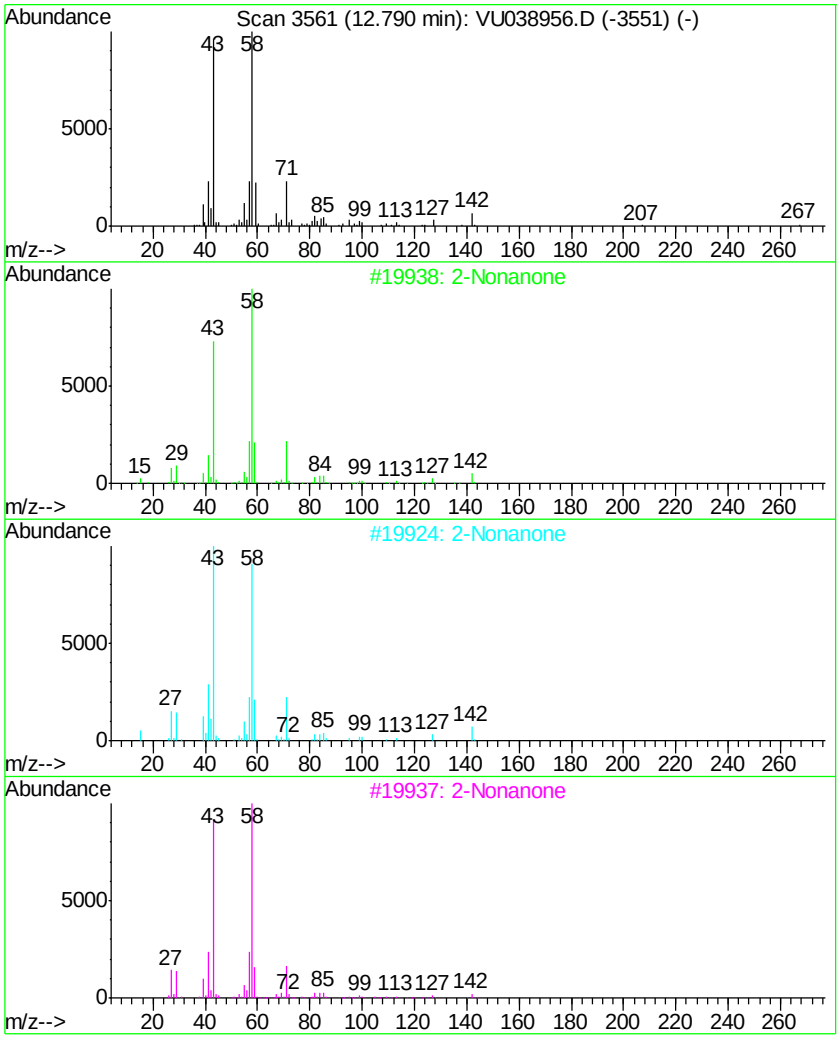
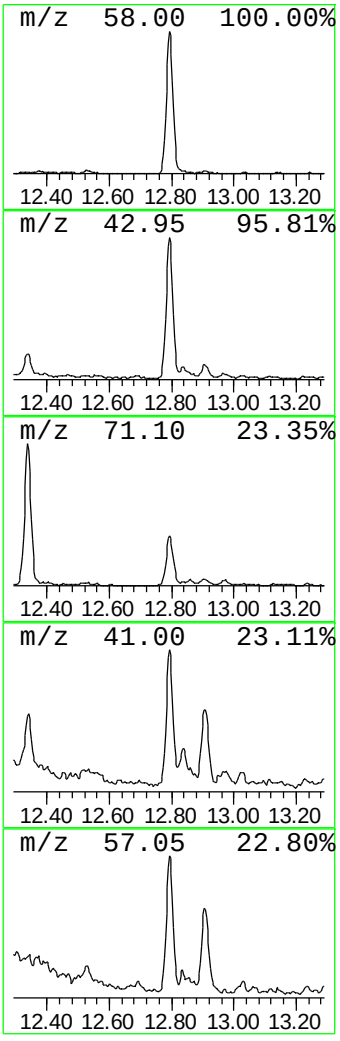
Peak Number 9 2-Nonanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	1.20 ug/L	199781	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonanone	142	C9H18O	000821-55-6	95
2	2-Nonanone	142	C9H18O	000821-55-6	94
3	2-Nonanone	142	C9H18O	000821-55-6	87
4	2-Nonanone	142	C9H18O	000821-55-6	87
5	2-Decanone	156	C10H20O	000693-54-9	64





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Data File : VU038956.D
Acq On : 17 Jun 2020 19:58
Operator : SY/MD
Sample : L3040-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L25

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

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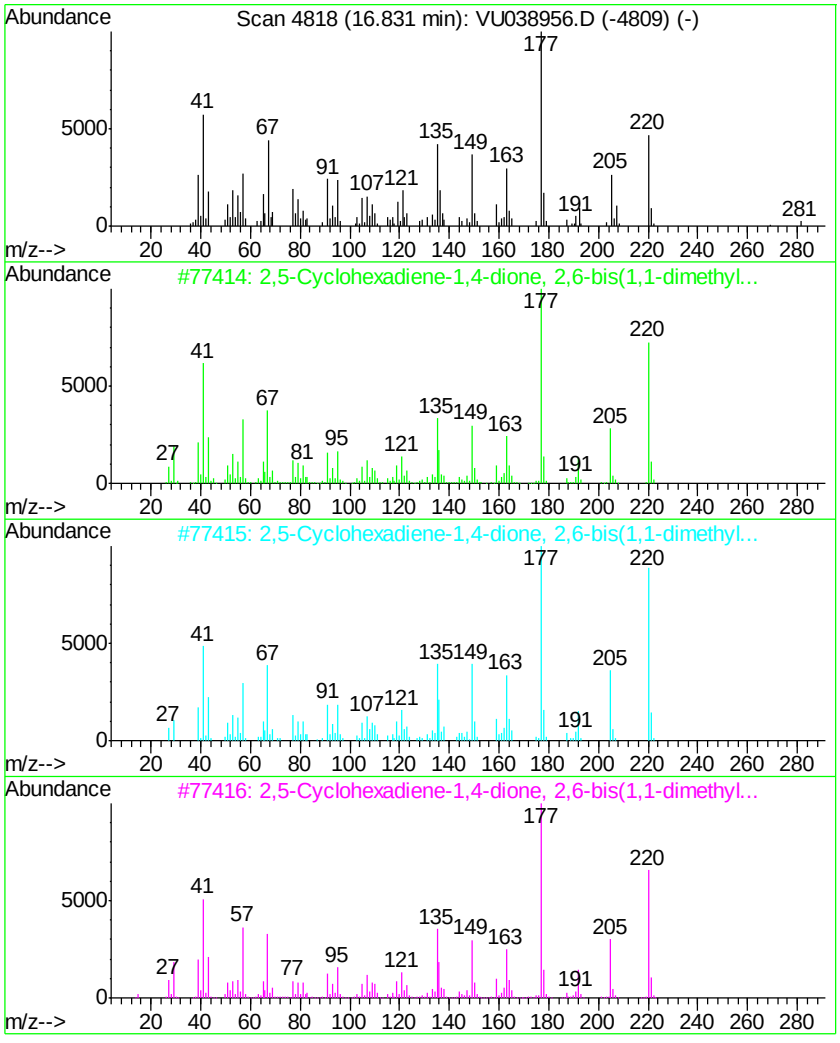
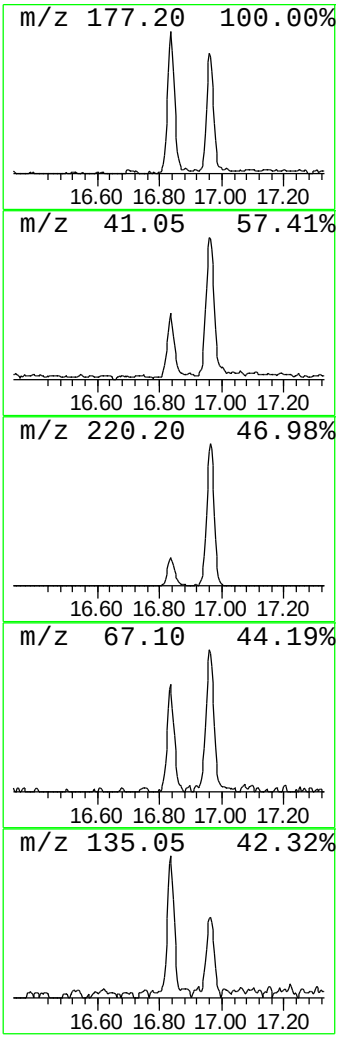
Peak Number 10 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.83	0.96 ug/L	160440	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	98
2	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	60
3	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	55
4	Thiocoumarin, 4,4,6,8-tetramethyl-	220	C13H16OS	1000128-90-3	43
5	trans-.beta.-Ionone	192	C13H20O	000079-77-6	38





Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038956.D
Acq On : 17 Jun 2020 19:58
Operator : SY/MD
Sample : L3040-12
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L25

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

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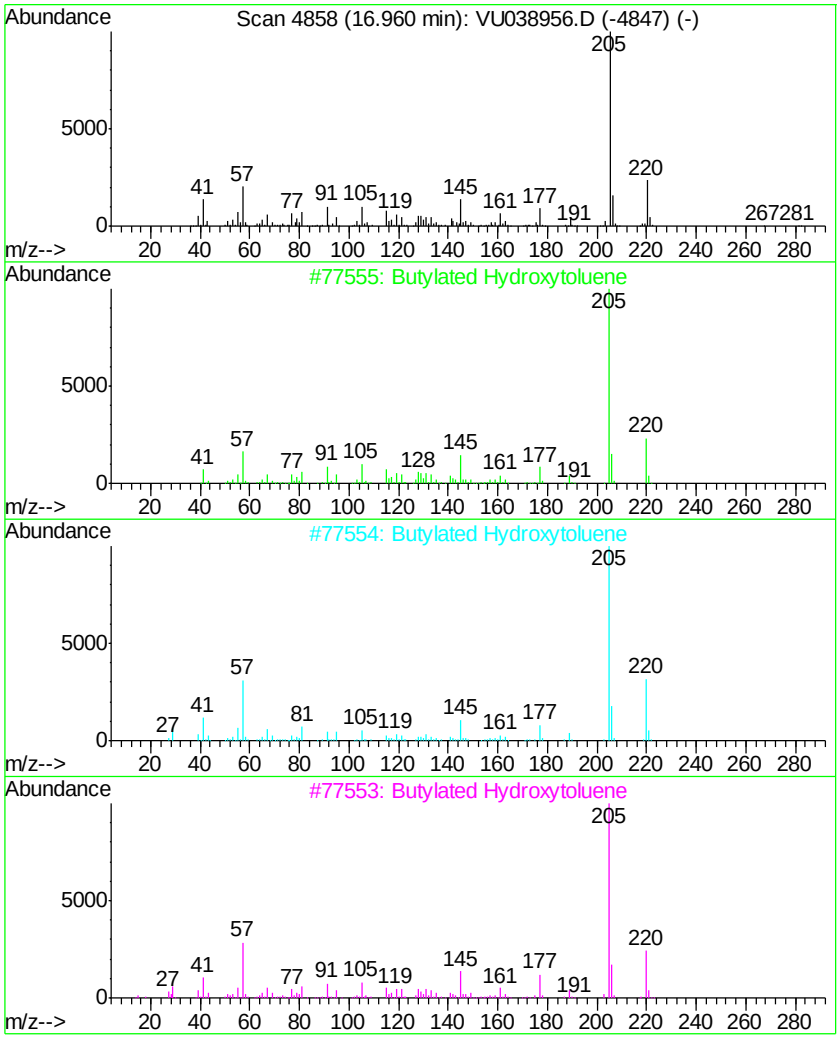
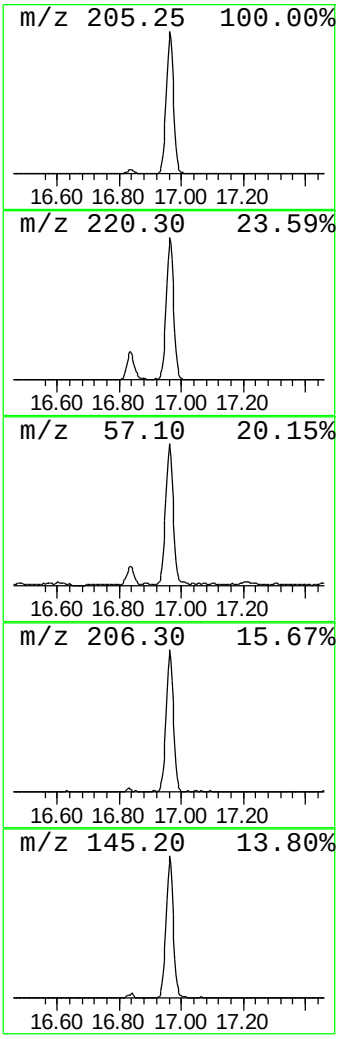
Peak Number 11 Butylated Hydroxytoluene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.96	4.05 ug/L	673827	1,4-Dichlorobenzene-d4	11.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	99
2	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	97
3	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	94
4	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	94
5	Phenol, 4,6-di(1,1-dimethylethyl...	220	C15H24O	000616-55-7	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061720\
Data File : VU038956.D
Acq On : 17 Jun 2020 19:58
Operator : SY/MD
Sample : L3040-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F9L25

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.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
Sulfur dioxide	2.42	0.6	ug/L	69235	1	6.31	596827	5.0
unknown-01	4.55	0.6	ug/L	73221	1	6.31	596827	5.0
2-Butanone, 3,3-d...	7.23	1.7	ug/L	203806	1	6.31	596827	5.0
Cyclopentene, 1,2...	9.66	0.6	ug/L	100958	2	9.44	790232	5.0
2-Heptanone	10.26	1.2	ug/L	185978	2	9.44	790232	5.0
2-Octanone	11.58	1.2	ug/L	201433	3	11.83	831856	5.0
1-Hexanol, 2-ethyl-	12.08	8.2	ug/L	1357460	3	11.83	831856	5.0
2-Nonanone	12.79	1.2	ug/L	199781	3	11.83	831856	5.0
2,5-Cyclohexadien...	16.83	1.0	ug/L	160440	3	11.83	831856	5.0
Butylated Hydroxy...	16.96	4.0	ug/L	673827	3	11.83	831856	5.0