LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU091020\
Data File : VU040091.D
Acq On : 10 Sep 2020 19:11
Operator : SY/MD
Sample : L3961-10
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y34

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\SOMUTR083120WMA.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	1.604	72	82	92	rVB2	51992	71885	12.05%	1.687%
2	1.707	96	114	115	rBV	49256	105503	17.69%	2.476%
3	1.922	177	181	199	rVB	43055	58904	9.88%	1.383%
4	2.581	373	386	397	rBV	79443	129481	21.71%	3.039%
5	2.655	397	409	432	rBV2	35450	96048	16.10%	2.254%
6	2.826	439	462	522	rBV2	107722	596452	100.00%	14.000%
7	3.382	623	635	648	rVB4	5342	11598	1.94%	0.272%
8	3.890	776	793	812	rBV	32451	78981	13.24%	1.854%
9	4.526	977	991	1003	rVB5	4385	10522	1.76%	0.247%
10	4.652	1010	1030	1051	rBV	59593	159256	26.70%	3.738%
11	4.825	1072	1084	1103	rVB2	22449	52526	8.81%	1.233%
12	5.083	1148	1164	1181	rBV2	68426	150164	25.18%	3.525%
13	5.742	1347	1369	1380	rBV3	129618	350352	58.74%	8.223%
14	6.263	1516	1531	1552	rBV	140685	264101	44.28%	6.199%
15	6.504	1595	1606	1619	rBV3	13668	28125	4.72%	0.660%
16	6.703	1652	1668	1683	rBV2	84001	162778	27.29%	3.821%
17	7.468	1897	1906	1921	rVB5	8916	16338	2.74%	0.383%
18	7.575	1925	1939	1954	rBV	41504	72660	12.18%	1.705%
19	7.719	1971	1984	1995	rBV7	4090	8197	1.37%	0.192%
20	7.906	2020	2042	2055	rBV	150976	264615	44.36%	6.211%
21	8.185	2114	2129	2140	rBV2	27328	45924	7.70%	1.078%
22	8.639	2256	2270	2298	rBV	225645	410312	68.79%	9.631%
23	8.928	2347	2360	2373	rBV	5274	13554	2.27%	0.318%
24	9.420	2500	2513	2530	rBV	210326	345797	57.98%	8.116%
25	10.754	2915	2928	2942	rVB2	68031	111662	18.72%	2.621%
26	11.472	3143	3151	3159	rBV6	4364	6872	1.15%	0.161%
27	11.809	3243	3256	3270	rBV	202495	322788	54.12%	7.576%
28	12.057	3321	3333	3352	rBV3	30518	54507	9.14%	1.279%
29	12.189	3362	3374	3387	rVB	159496	254086	42.60%	5.964%
30	13.201	3681	3689	3697	rBV3	5061	6473	1.09%	0.152%

Sum of corrected areas: 4260461

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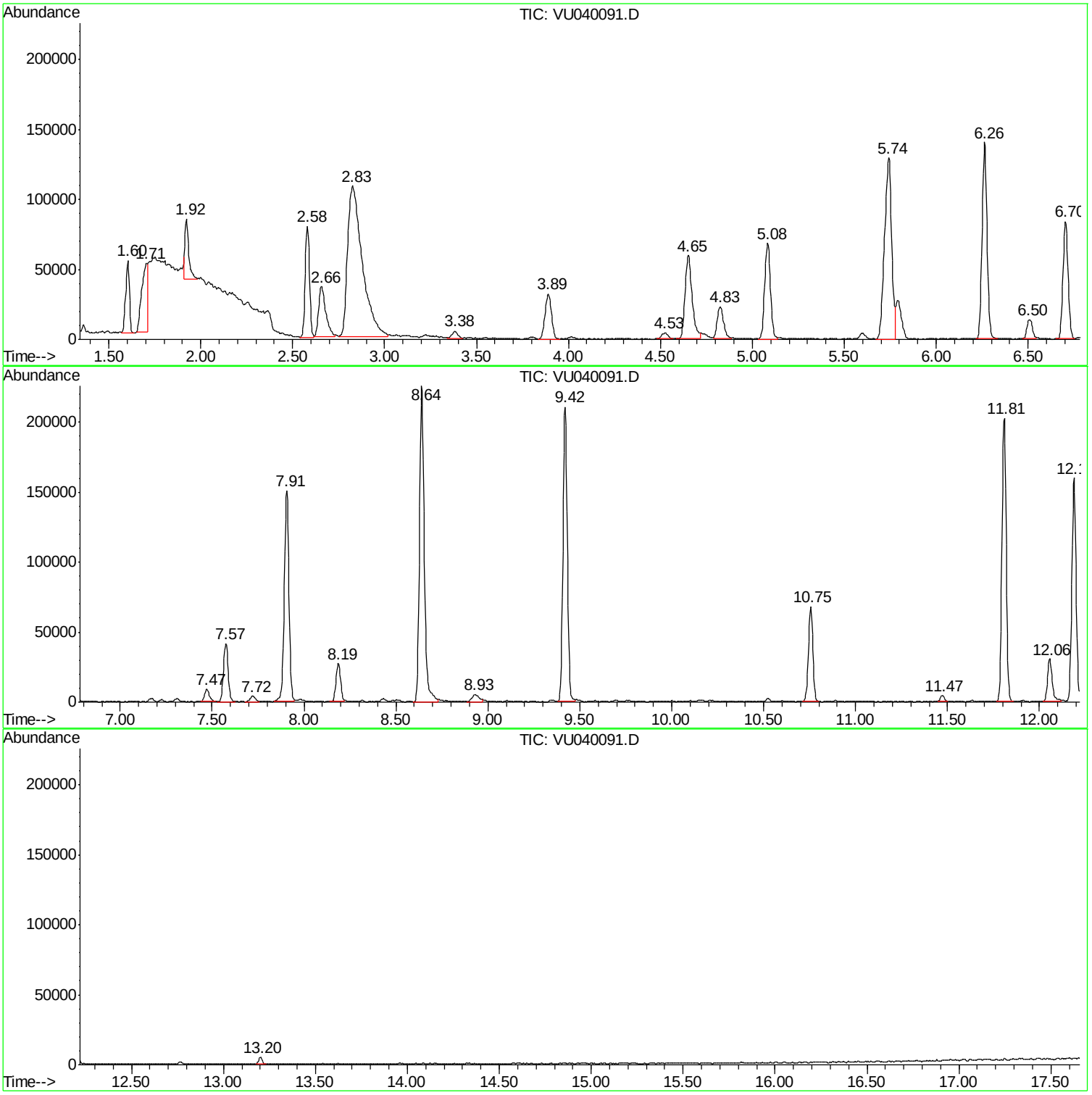
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y34

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR083120WMA.M
Quant Title : TRACE VOA SOM01.0

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



Library Search Compound Report

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

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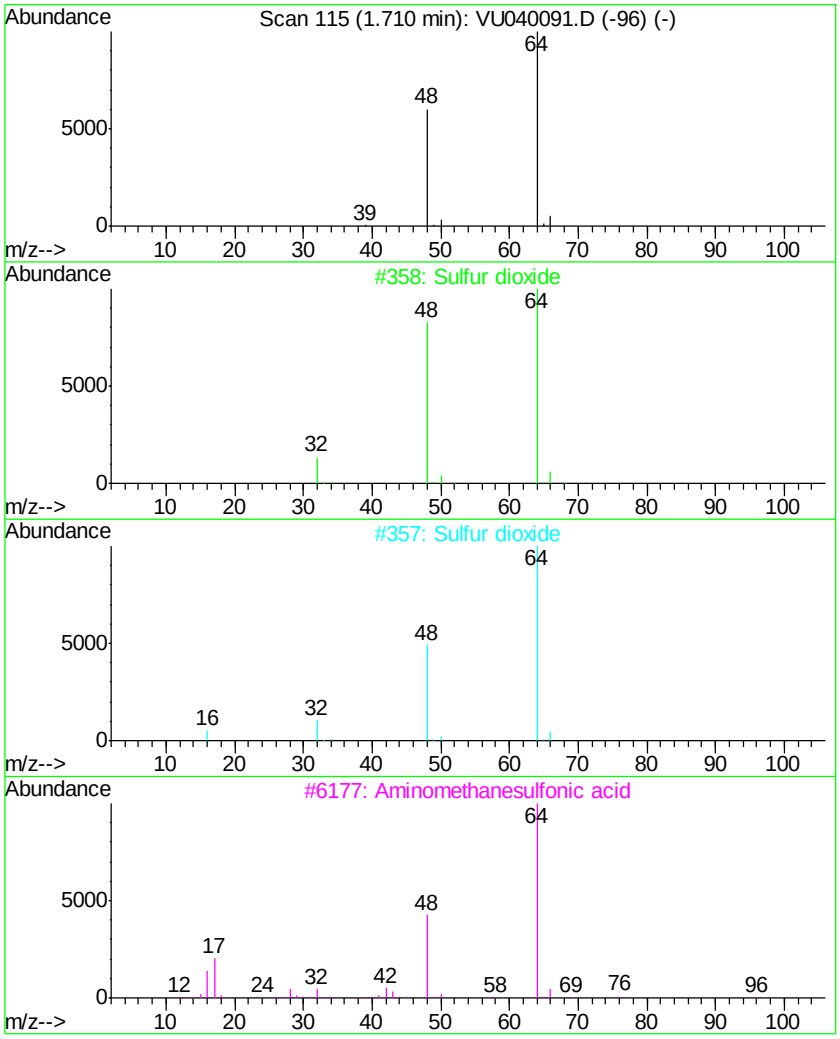
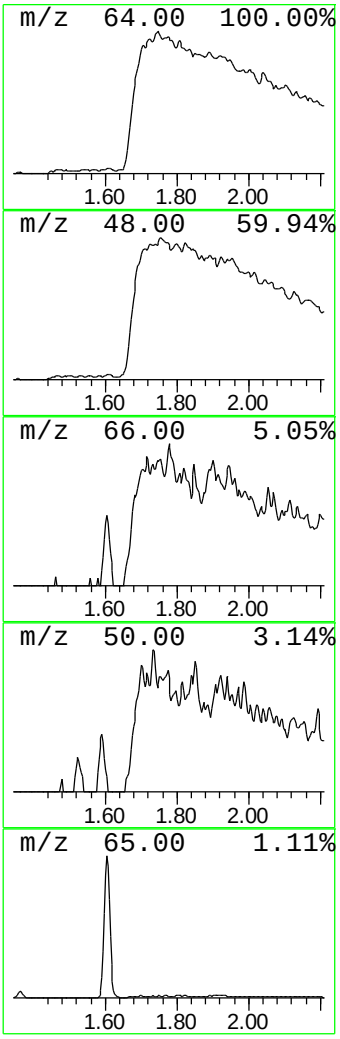
Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.71	2.00 ug/L	105503	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Sulfur dioxide	64	O2S	007446-09-5	83
3	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
4	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9





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Acq On : 10 Sep 2020 19:11
Operator : SY/MD
Sample : L3961-10
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y34

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR083120WMA.M
Quant Title : TRACE VOA SOM01.0

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

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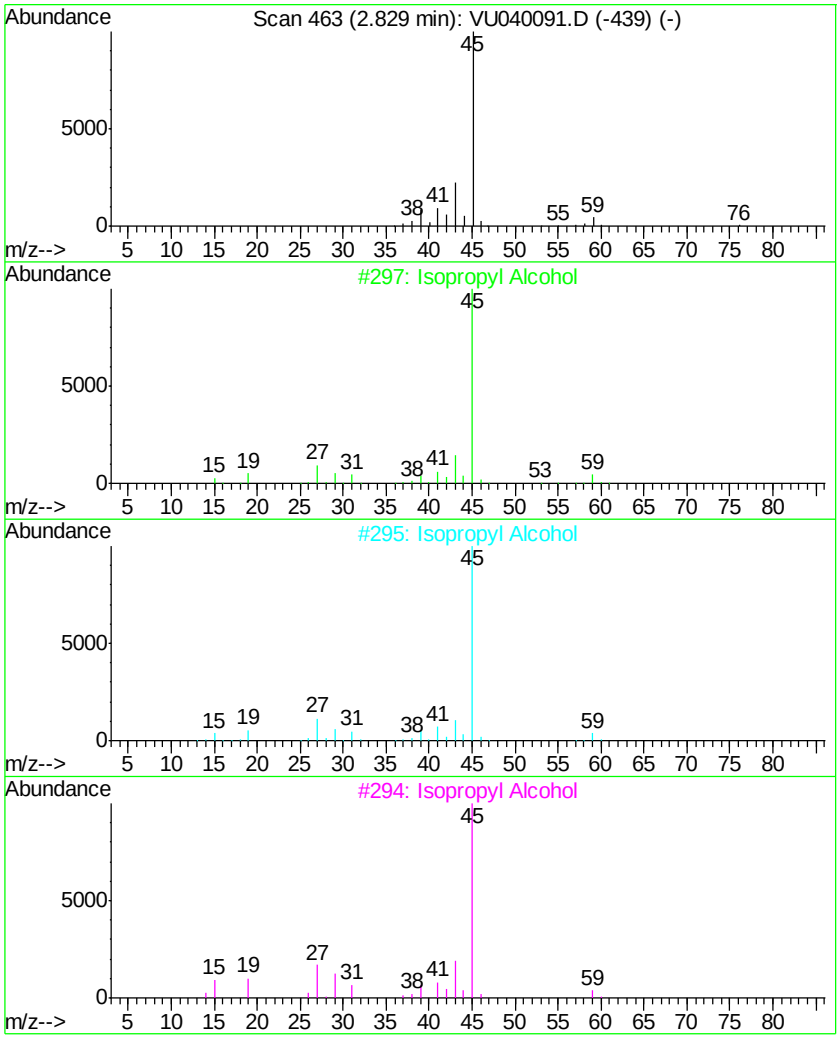
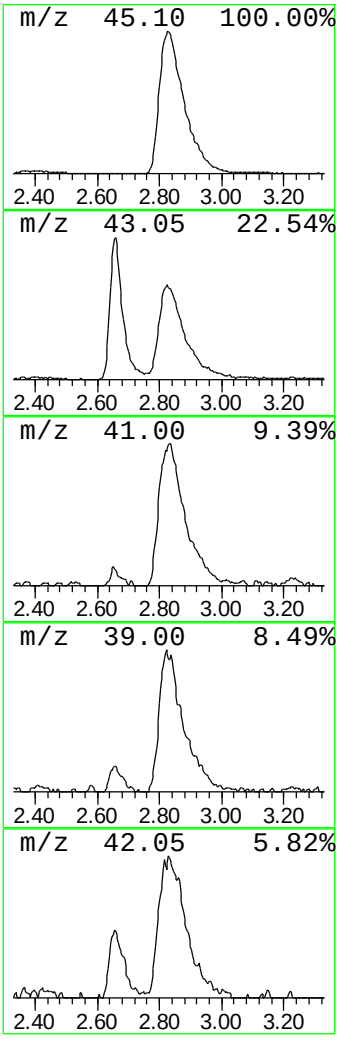
Peak Number 2 Isopropyl Alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.83	11.29 ug/L	596452	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	86
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	78
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	78
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	72
5	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	40





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU091020\
Data File : VU040091.D
Acq On : 10 Sep 2020 19:11
Operator : SY/MD
Sample : L3961-10
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y34

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR083120WMA.M
Quant Title : TRACE VOA SOM01.0

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

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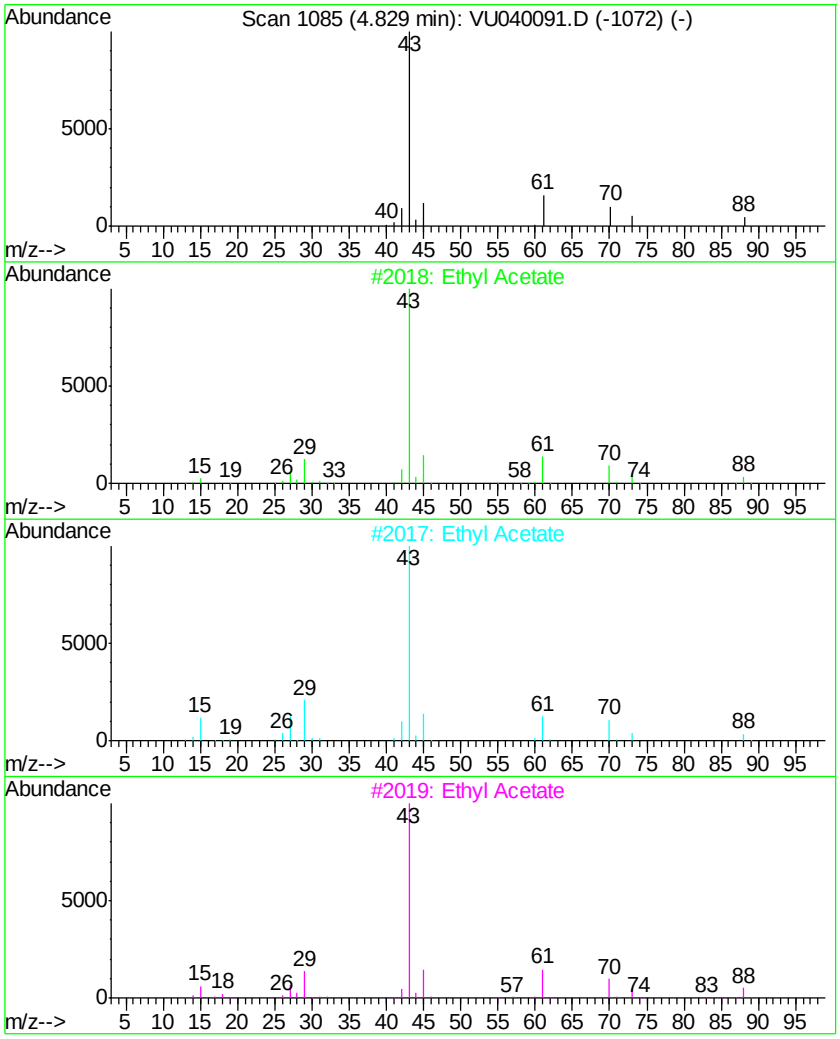
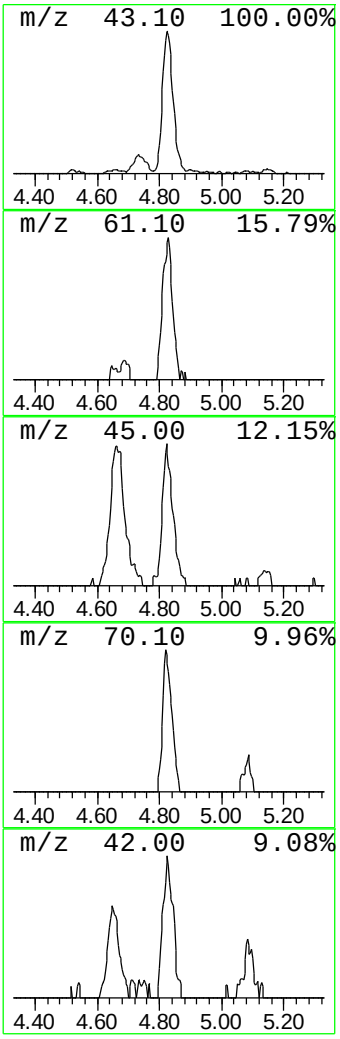
Peak Number 3 Ethyl Acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	0.99 ug/L	52526	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl Acetate	88	C4H8O2	000141-78-6	90
2	Ethyl Acetate	88	C4H8O2	000141-78-6	90
3	Ethyl Acetate	88	C4H8O2	000141-78-6	78
4	Ethyl Acetate	88	C4H8O2	000141-78-6	59
5	CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	36





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ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y34

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR083120WMA.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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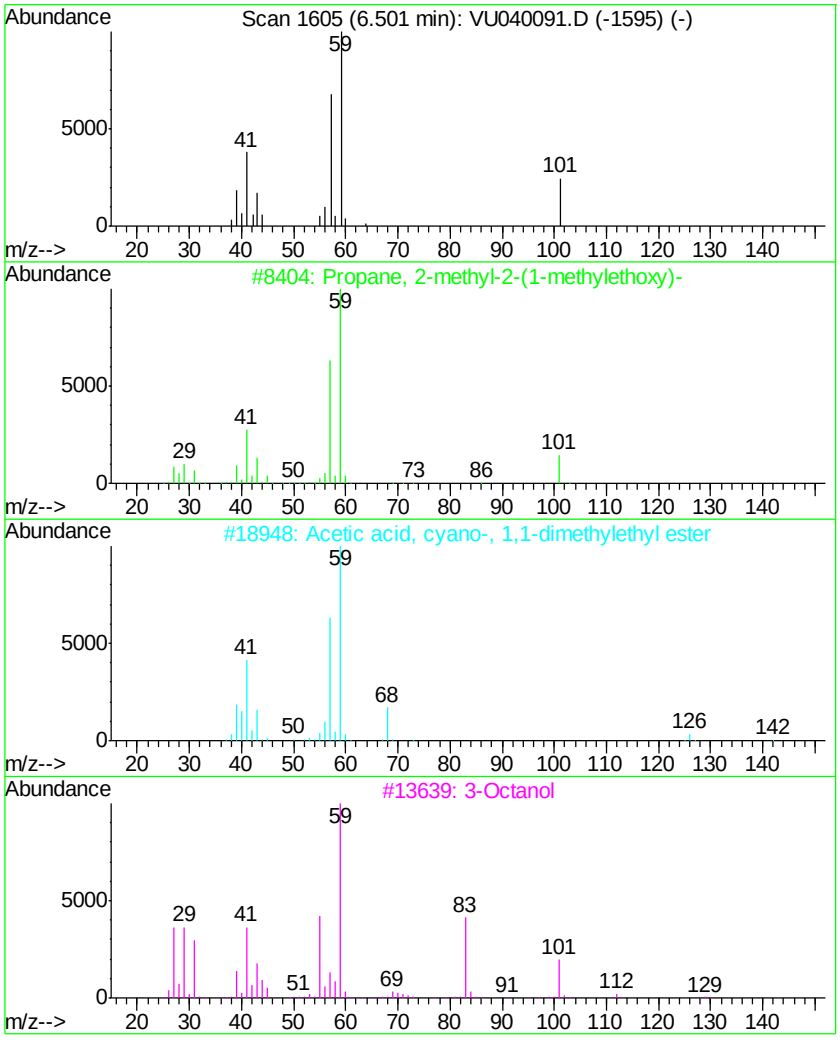
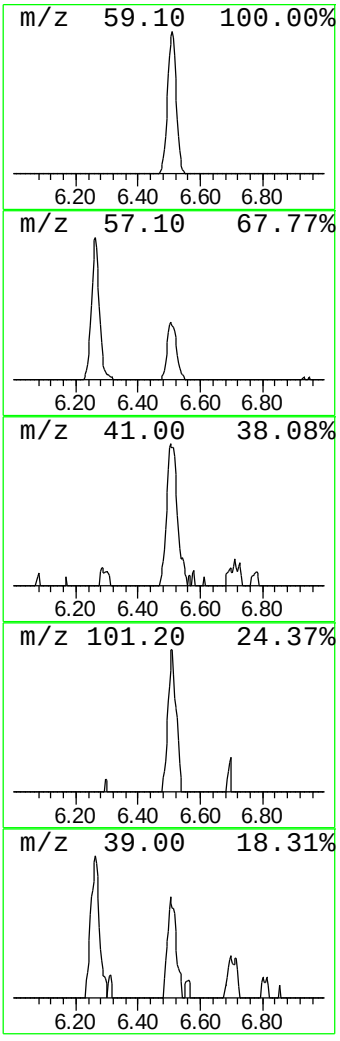
Peak Number 4 Propane, 2-methyl-2-(1-meth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	0.53 ug/L	28125	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	74
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	64
3	3-Octanol	130	C8H18O	000589-98-0	40
4	3-Hexanol	102	C6H14O	000623-37-0	39
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	38





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Instrument : MSVOA_U
ClientSampleId : F4Y34

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TIC Library : C:\DATABASE\NIST11.L
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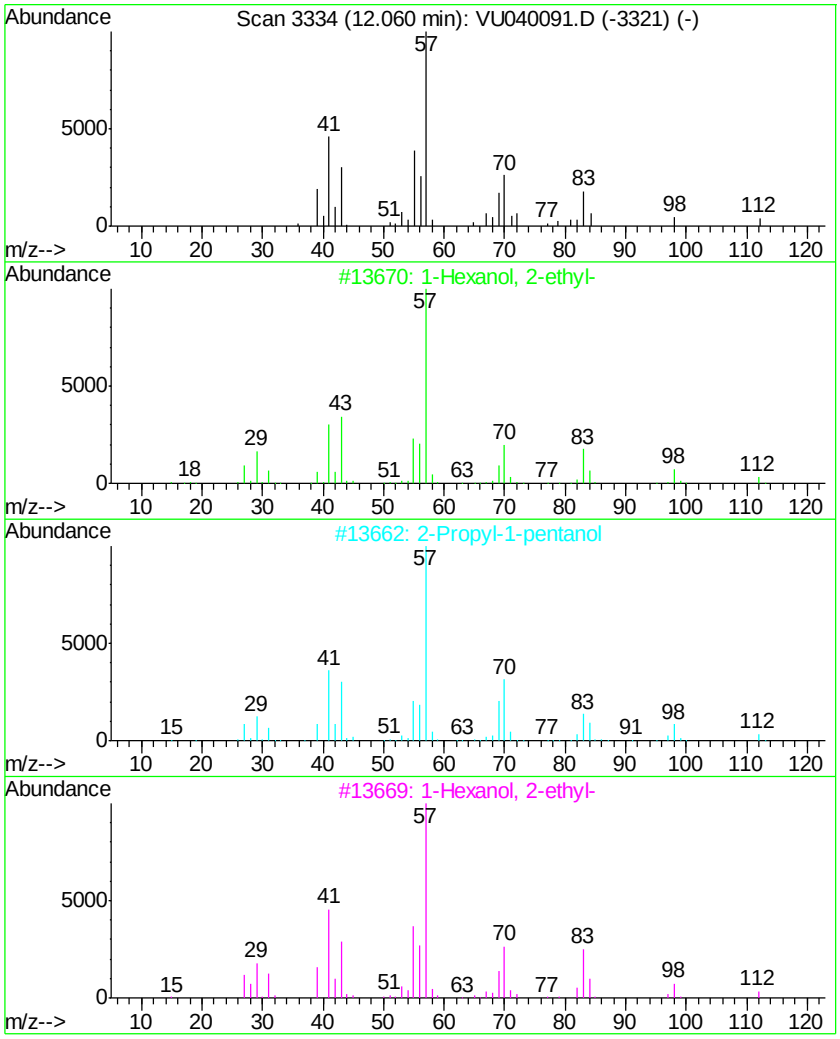
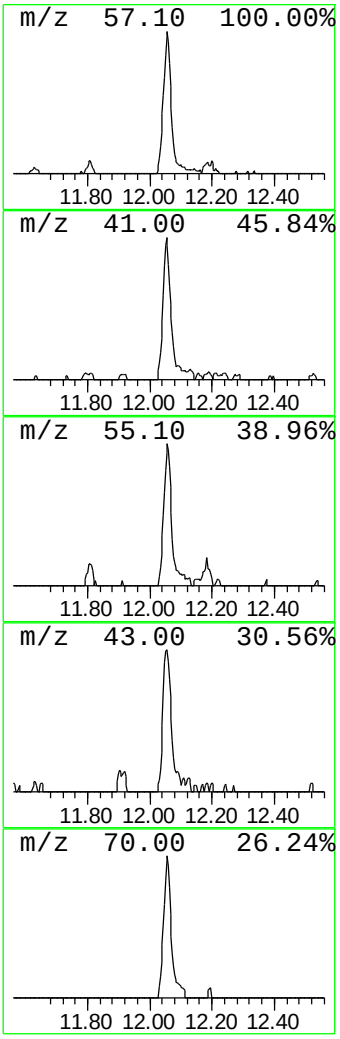
Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.06	0.84 ug/L	54507	1,4-Dichlorobenzene-d4	11.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	64
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	53
5	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	53





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Sulfur dioxide	1.71	2.0	ug/L	105503	1	6.26	264101	5.0
Isopropyl Alcohol	2.83	11.3	ug/L	596452	1	6.26	264101	5.0
Ethyl Acetate	4.83	1.0	ug/L	52526	1	6.26	264101	5.0
Propane, 2-methyl...	6.50	0.5	ug/L	28125	1	6.26	264101	5.0
1-Hexanol, 2-ethyl-	12.06	0.8	ug/L	54507	3	11.81	322788	5.0