LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU091420\
Data File : VU040119.D
Acq On : 14 Sep 2020 14:27
Operator : SY/MD
Sample : L3961-20
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y45

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	71	82	93	rVB2	52279	81501	19.22%	2.077%
2	1.748	100	127	130	rBV2	52726	189119	44.61%	4.820%
3	1.922	176	181	192	rVB	41085	54177	12.78%	1.381%
4	2.581	373	386	399	rBV	81463	134982	31.84%	3.440%
5	2.678	399	416	446	rBV	17140	82174	19.38%	2.094%
6	2.928	450	494	497	rBV2	29098	150183	35.42%	3.827%
7	3.385	625	636	651	rVB5	6968	16022	3.78%	0.408%
8	3.887	774	792	806	rBV4	10529	28242	6.66%	0.720%
9	4.526	976	991	1005	rVB4	6844	17701	4.18%	0.451%
10	4.662	1017	1033	1058	rBV	45146	166022	39.16%	4.231%
11	4.829	1075	1085	1109	rVB	16082	41418	9.77%	1.056%
12	5.083	1149	1164	1180	rBV2	70814	155367	36.65%	3.959%
13	5.742	1348	1369	1395	rBV3	135335	353371	83.35%	9.006%
14	6.263	1514	1531	1546	rBV	148813	281517	66.40%	7.174%
15	6.510	1594	1608	1618	rBV4	8148	16635	3.92%	0.424%
16	6.703	1653	1668	1684	rBV2	88335	171305	40.41%	4.366%
17	7.308	1847	1856	1868	rVB6	4127	7734	1.82%	0.197%
18	7.575	1925	1939	1953	rBV	44378	75875	17.90%	1.934%
19	7.906	2020	2042	2056	rBV	159546	276972	65.33%	7.059%
20	8.185	2118	2129	2143	rBV2	27937	45904	10.83%	1.170%
21	8.642	2258	2271	2295	rBV	228904	423965	100.00%	10.805%
22	9.420	2500	2513	2533	rBV	220085	365172	86.13%	9.306%
23	10.755	2914	2928	2944	rBV	69302	114764	27.07%	2.925%
24	11.472	3138	3151	3159	rBV2	6263	9342	2.20%	0.238%
25	11.806	3243	3255	3269	rBV	216850	347139	81.88%	8.847%
26	12.054	3323	3332	3346	rBV3	27884	48803	11.51%	1.244%
27	12.189	3360	3374	3396	rVB	168510	268500	63.33%	6.843%

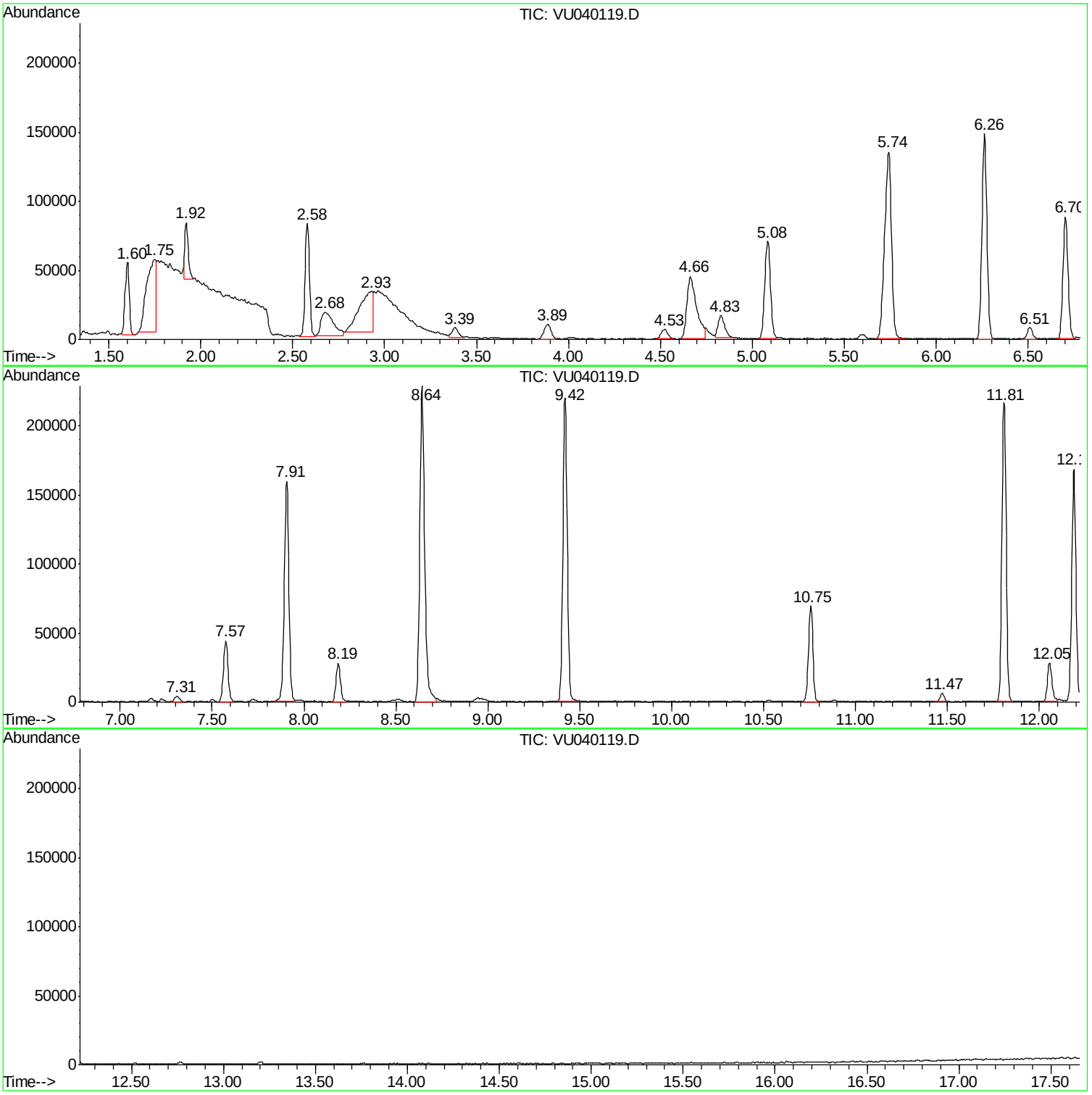
Sum of corrected areas: 3923906

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU091420\
Data File : VU040119.D
Acq On : 14 Sep 2020 14:27
Operator : SY/MD
Sample : L3961-20
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y45

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU091420\
Data File : VU040119.D
Acq On : 14 Sep 2020 14:27
Operator : SY/MD
Sample : L3961-20
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y45

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

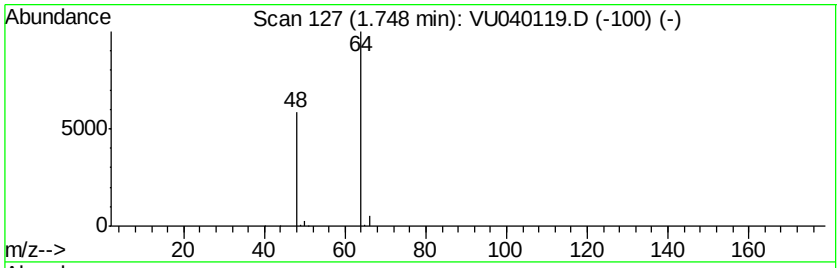
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

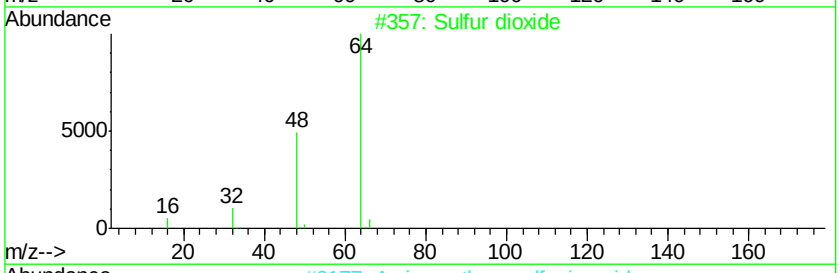
****

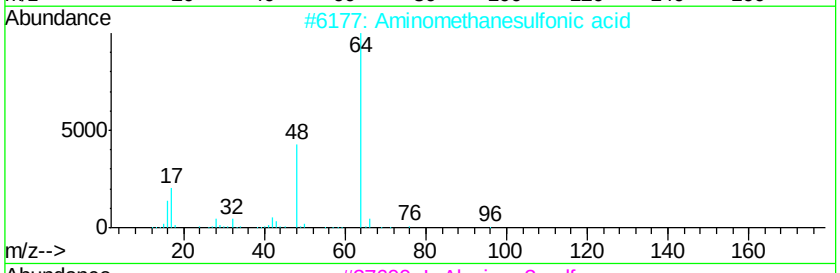
Peak Number 1 Sulfur dioxide Concentration Rank 1

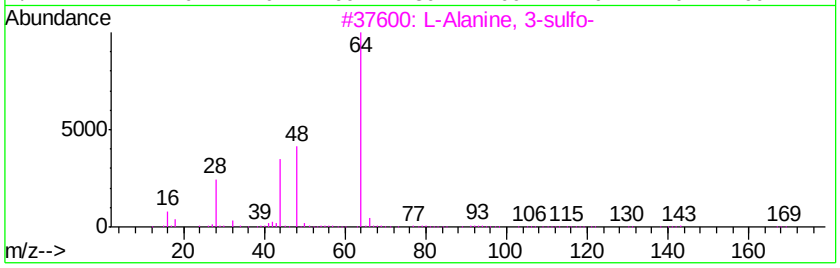
R.T.	EstConc	Area	Relative to ISTD	R.T.
1.75	3.36 ug/L	189119	1,4-Difluorobenzene	6.26

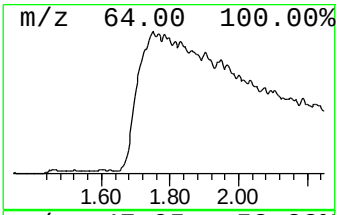
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9

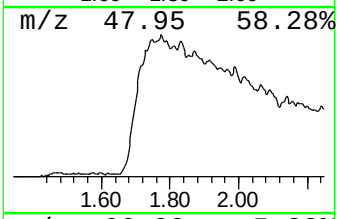


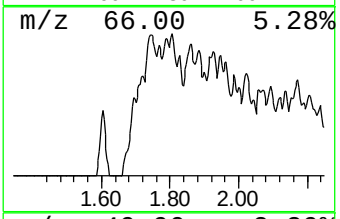


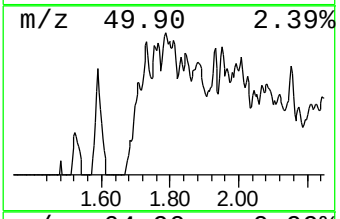


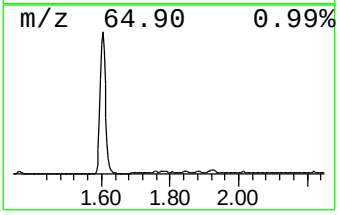












Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU091420\
Data File : VU040119.D
Acq On : 14 Sep 2020 14:27
Operator : SY/MD
Sample : L3961-20
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y45

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

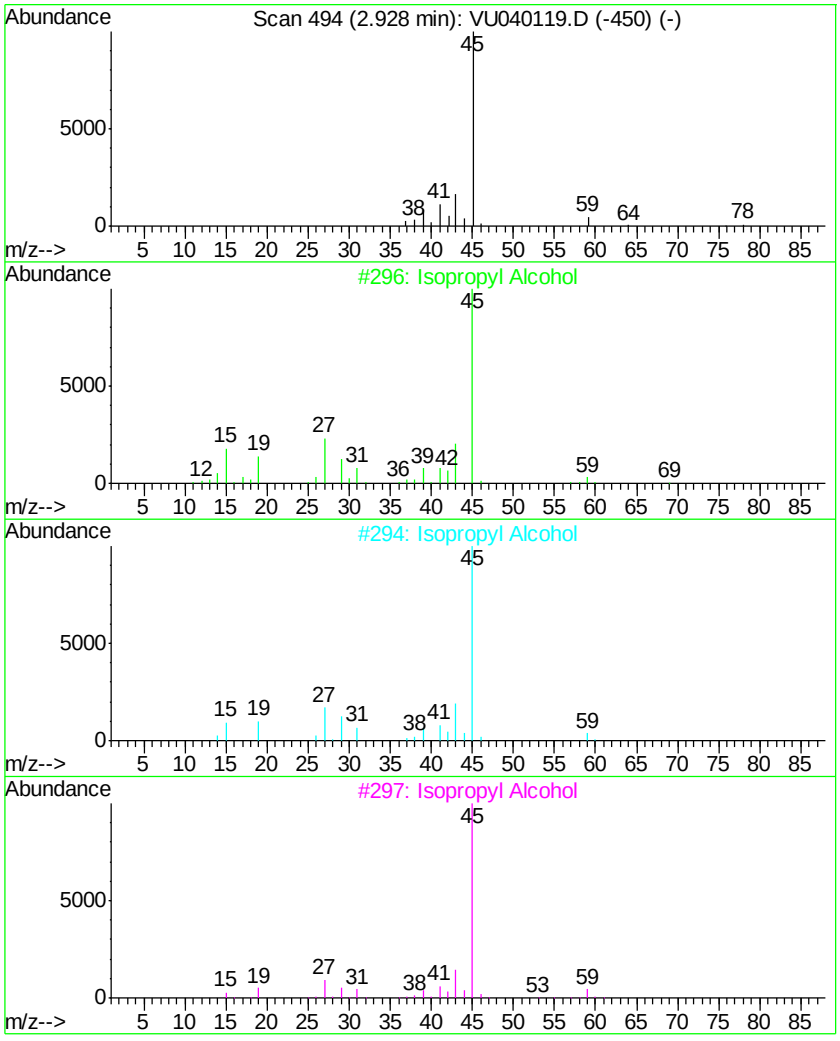
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

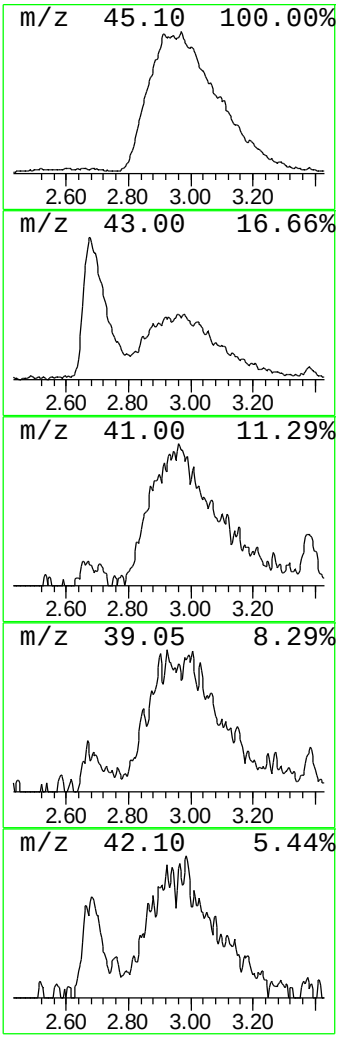
****

Peak Number 2 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.93	2.67 ug/L	150183	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4	Ethylamine	45	C2H7N	000075-04-7	5
5	Formamide	45	CH3NO	000075-12-7	4





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU091420\
Data File : VU040119.D
Acq On : 14 Sep 2020 14:27
Operator : SY/MD
Sample : L3961-20
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y45

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

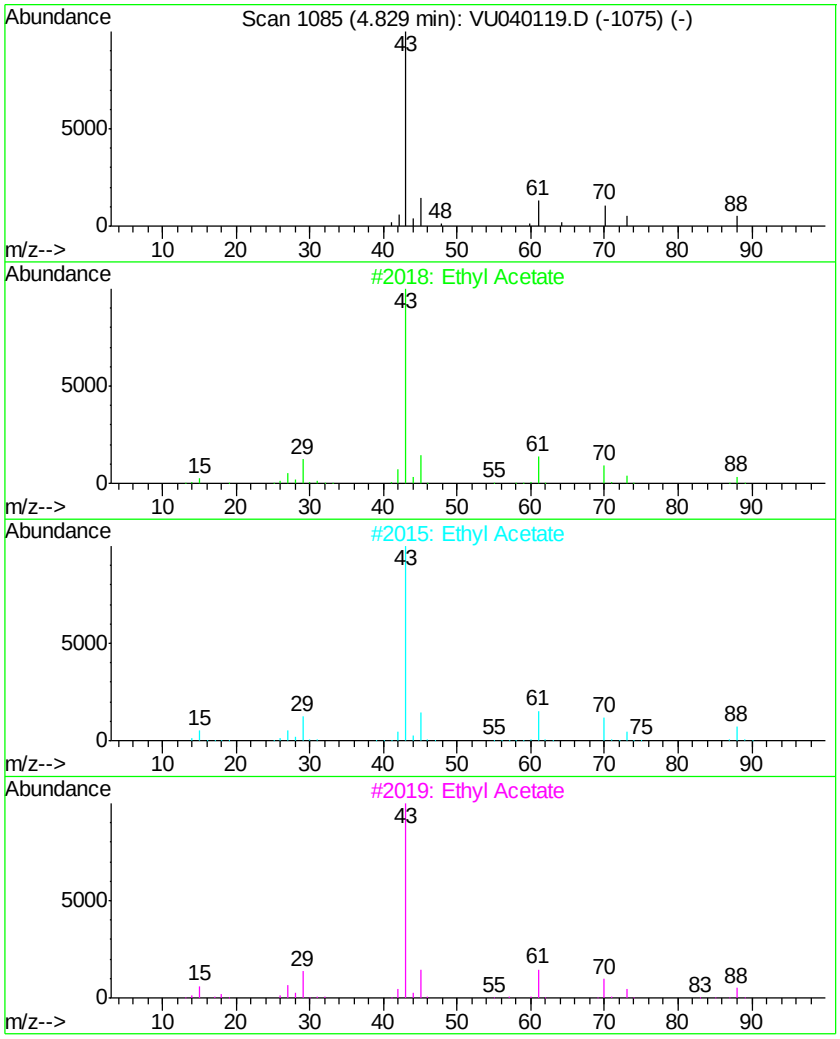
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

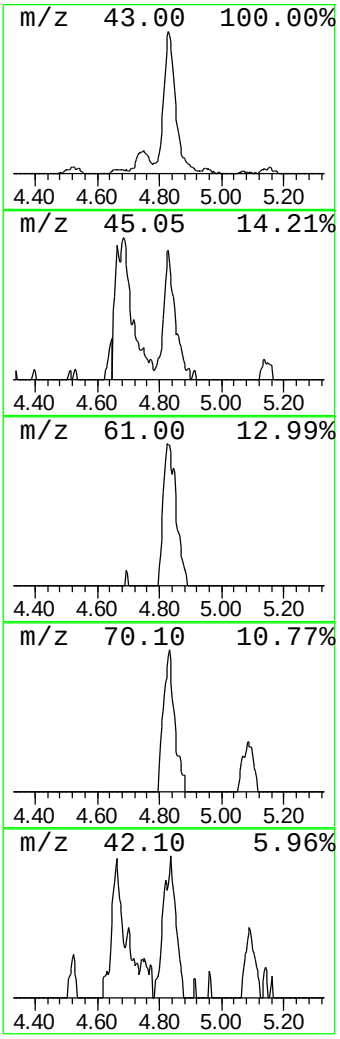
****

Peak Number 3 Ethyl Acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	0.74 ug/L	41418	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl Acetate	88	C4H8O2	000141-78-6	86
2	Ethyl Acetate	88	C4H8O2	000141-78-6	86
3	Ethyl Acetate	88	C4H8O2	000141-78-6	86
4	Ethyl Acetate	88	C4H8O2	000141-78-6	78
5	CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	42





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU091420\
Data File : VU040119.D
Acq On : 14 Sep 2020 14:27
Operator : SY/MD
Sample : L3961-20
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y45

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

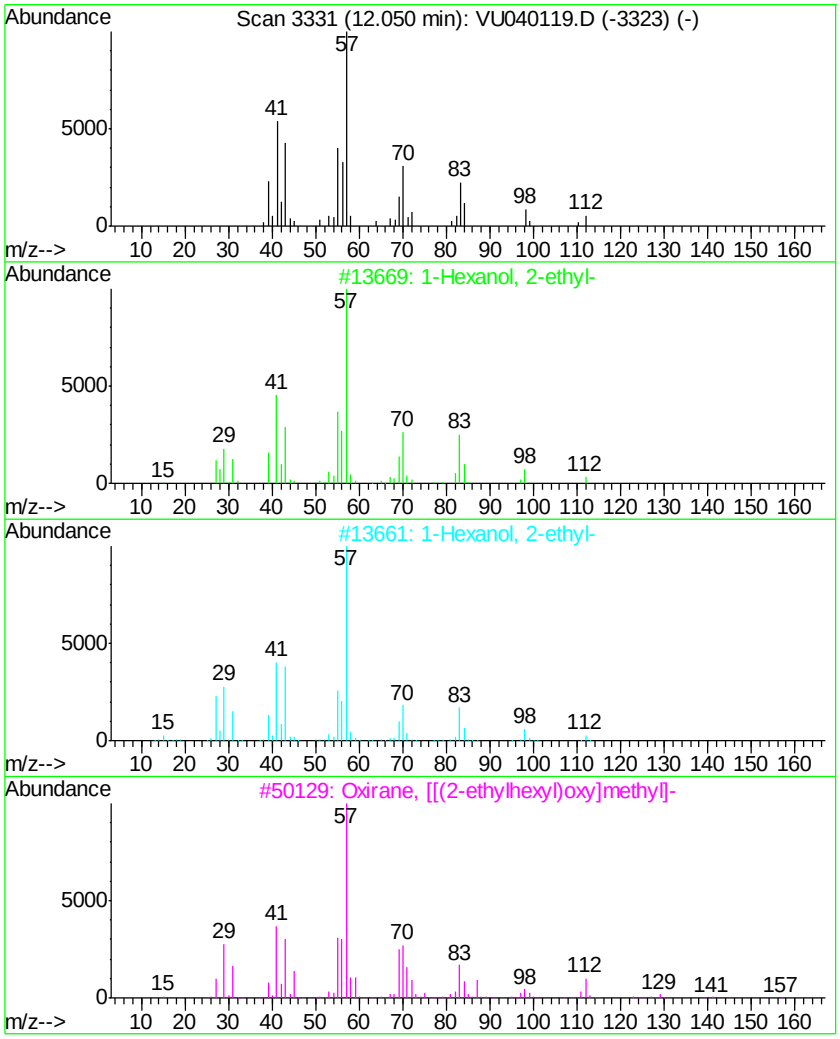
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

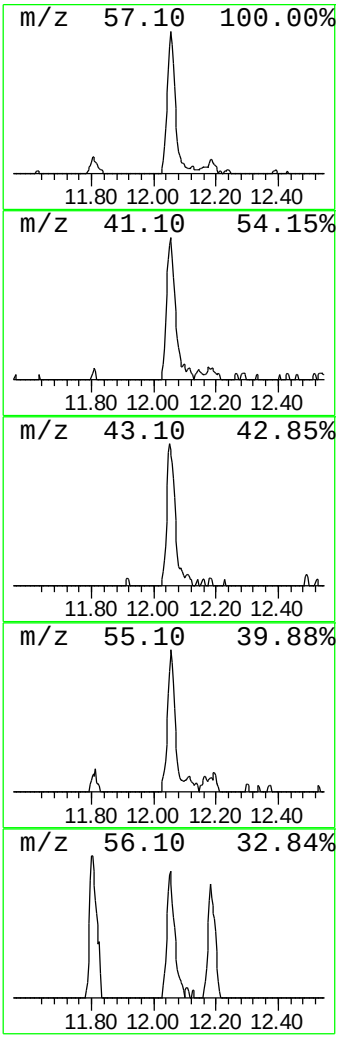
****

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	0.70 ug/L	48803	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	78
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
3	Oxirane, [[(2-ethylhexyl)oxy]met...	186	C11H22O2	002461-15-6	64
4	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59
5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU091420\
Data File : VU040119.D
Acq On : 14 Sep 2020 14:27
Operator : SY/MD
Sample : L3961-20
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y45

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Sulfur dioxide	1.75	3.4	ug/L	189119	1	6.26	281517	5.0
unknown-01	2.93	2.7	ug/L	150183	1	6.26	281517	5.0
Ethyl Acetate	4.83	0.7	ug/L	41418	1	6.26	281517	5.0
1-Hexanol, 2-ethyl-	12.05	0.7	ug/L	48803	3	11.81	347139	5.0