LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU091020\
Data File : VU040094.D
Acq On : 10 Sep 2020 20:22
Operator : SY/MD
Sample : L3961-13
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y37

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	49066	67445	10.59%	1.626%
2	1.752	102	128	129	rBV	49834	161520	25.37%	3.893%
3	1.922	177	181	193	rVB	44924	49970	7.85%	1.204%
4	2.581	372	386	399	rBV	76994	126293	19.83%	3.044%
5	2.665	399	412	435	rBV2	24486	76524	12.02%	1.844%
6	2.858	444	472	527	rBV	75521	636749	100.00%	15.347%
7	3.887	783	792	806	rVB5	4114	9215	1.45%	0.222%
8	4.652	1014	1030	1071	rBV2	52325	170504	26.78%	4.110%
9	4.829	1071	1085	1103	rVV2	24559	57318	9.00%	1.382%
10	5.083	1147	1164	1181	rBV	70262	152909	24.01%	3.685%
11	5.742	1348	1369	1395	rBV3	128460	339277	53.28%	8.177%
12	6.263	1515	1531	1550	rBV2	139854	263110	41.32%	6.342%
13	6.703	1651	1668	1684	rBV2	82846	164383	25.82%	3.962%
14	7.575	1927	1939	1954	rBV2	40774	69770	10.96%	1.682%
15	7.906	2029	2042	2058	rBV	148161	250716	39.37%	6.043%
16	8.186	2116	2129	2143	rBV2	27066	44517	6.99%	1.073%
17	8.639	2258	2270	2290	rBV	219616	399399	62.72%	9.626%
18	8.935	2350	2362	2378	rBV3	4818	12173	1.91%	0.293%
19	9.420	2501	2513	2532	rBV	211093	346971	54.49%	8.363%
20	10.755	2916	2928	2942	rVB	68296	108739	17.08%	2.621%
21	11.806	3240	3255	3275	rVB	203483	323176	50.75%	7.789%
22	12.054	3320	3332	3353	rBV2	33659	60801	9.55%	1.465%
23	12.186	3362	3373	3393	rVB	159657	257477	40.44%	6.206%

Sum of corrected areas: 4148956

LSC Report - Integrated Chromatogram

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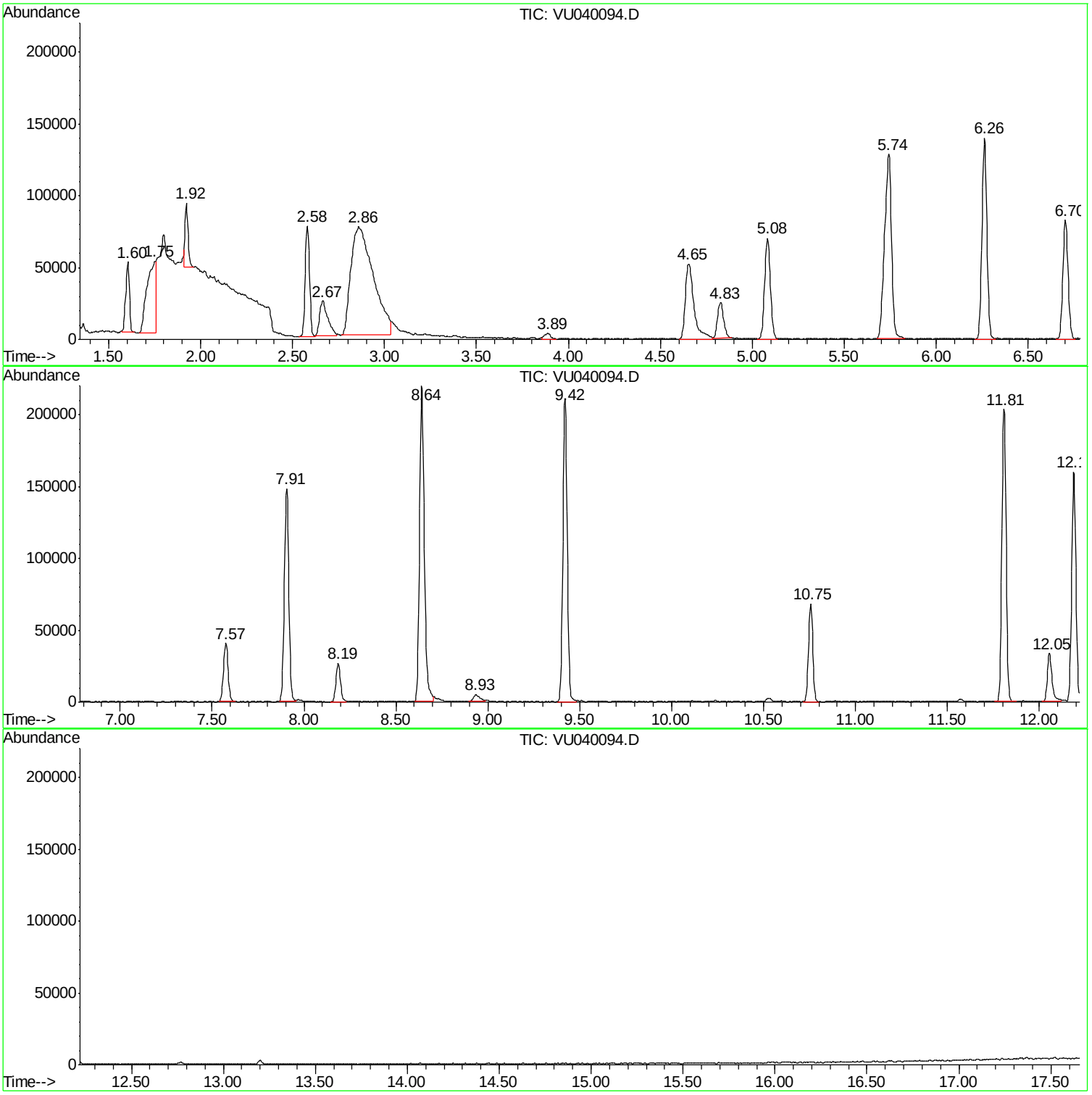
ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y37

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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Quant Title : TRACE VOA SOM01.0

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

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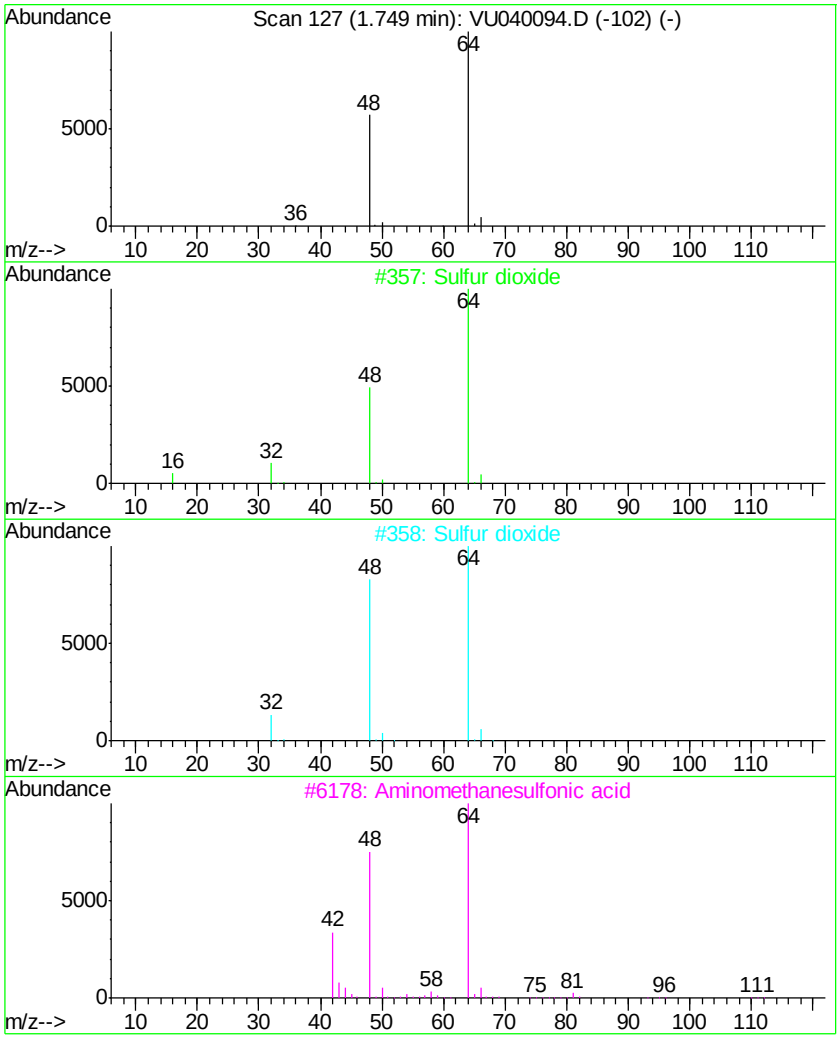
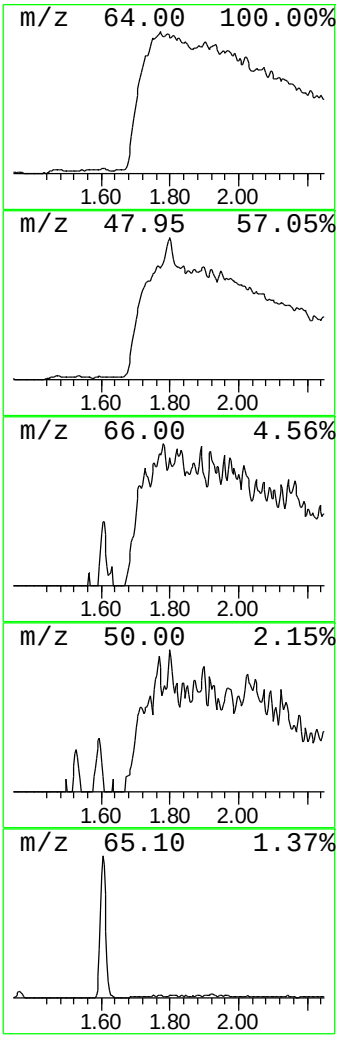
Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.75	3.07 ug/L	161520	1,4-Difluorobenzene	6.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	90
2	Sulfur dioxide	64	O2S	007446-09-5	83
3	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
5	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU091020\
Data File : VU040094.D
Acq On : 10 Sep 2020 20:22
Operator : SY/MD
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ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y37

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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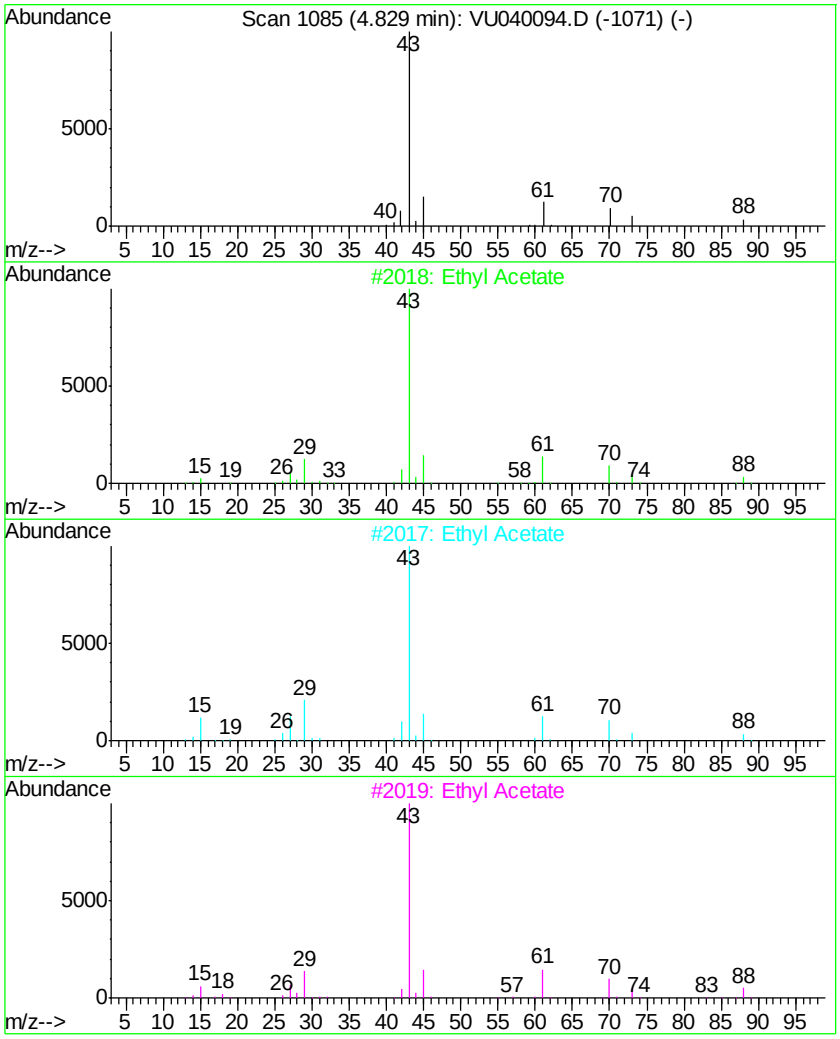
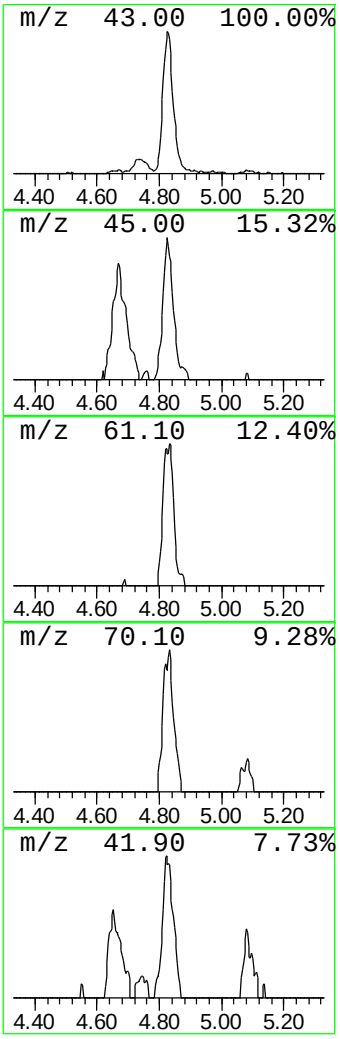
Peak Number 2 Ethyl Acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	1.09 ug/L	57318	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	64
5	CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	38





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ALS Vial : 28 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : F4Y37

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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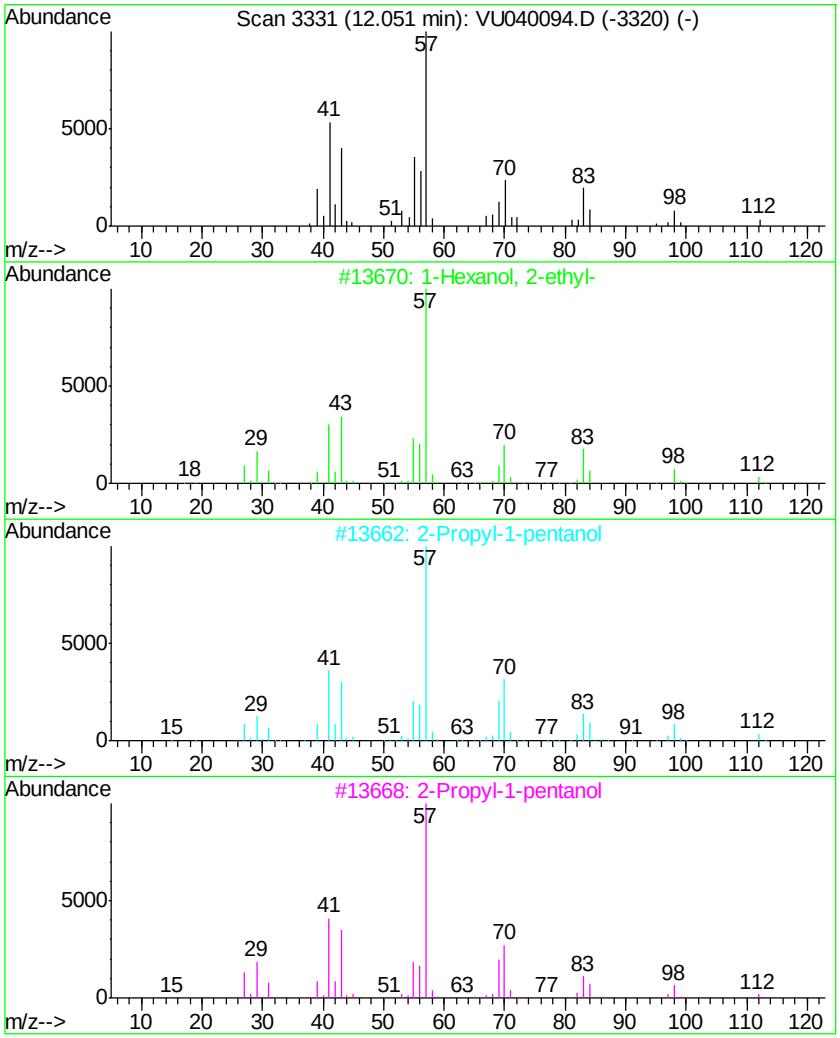
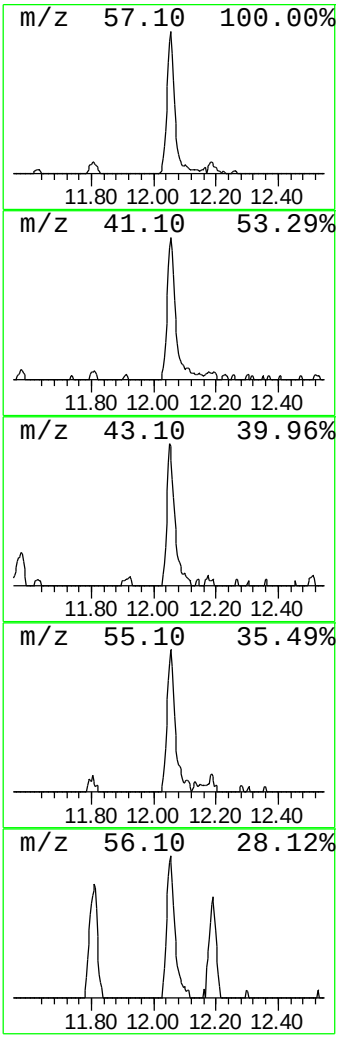
Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	0.94 ug/L	60801	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	64
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
4	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59
5	Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	53





Tentatively Identified Compound (LSC) summary

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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	3.1	ug/L	161520	1	6.26	263110	5.0
Ethyl Acetate	4.83	1.1	ug/L	57318	1	6.26	263110	5.0
1-Hexanol, 2-ethyl-	12.05	0.9	ug/L	60801	3	11.81	323176	5.0