LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU121718\
Data File : VU028732.D
Acq On : 17 Dec 2018 19:56
Operator : MD/SY
Sample : J6440-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : COMP-4

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 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\82U120618W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.398	63	70	78	rVB	6144	7218	1.43%	0.225%
2	1.472	85	93	107	rBV	129262	143451	28.40%	4.472%
3	1.572	113	124	131	rVB10	5894	10833	2.14%	0.338%
4	2.321	348	357	370	rVB	12373	19481	3.86%	0.607%
5	2.447	384	396	411	rBV2	4742	8352	1.65%	0.260%
6	2.829	504	515	529	rBV3	2633	5993	1.19%	0.187%
7	3.990	864	876	892	rBV2	15416	39458	7.81%	1.230%
8	4.881	1136	1153	1170	rBV3	72821	162952	32.26%	5.079%
9	4.983	1170	1185	1212	rVB	110717	246637	48.82%	7.688%
10	5.308	1272	1286	1301	rBV	87503	183980	36.42%	5.735%
11	5.389	1301	1311	1328	rVB3	11672	25440	5.04%	0.793%
12	5.884	1448	1465	1486	rBV	187588	363040	71.87%	11.316%
13	6.508	1648	1659	1679	rBV4	6620	13771	2.73%	0.429%
14	7.565	1974	1988	2002	rBV	288378	505154	100.00%	15.746%
15	7.636	2003	2010	2031	rVB	17971	34121	6.75%	1.064%
16	8.456	2258	2265	2277	rBV5	4301	7000	1.39%	0.218%
17	9.089	2447	2462	2483	rBV	254656	421632	83.47%	13.143%
18	9.372	2541	2550	2563	rBV	12508	20272	4.01%	0.632%
19	9.777	2667	2676	2686	rBV2	5362	7626	1.51%	0.238%
20	9.896	2705	2713	2727	rBV2	6596	10711	2.12%	0.334%
21	10.308	2829	2841	2853	rBV	193362	302443	59.87%	9.427%
22	10.369	2855	2860	2869	rVB3	4963	7288	1.44%	0.227%
23	10.919	3019	3031	3037	rBV4	4766	6656	1.32%	0.207%
24	11.067	3069	3077	3089	rVB2	13872	20291	4.02%	0.632%
25	11.292	3138	3147	3159	rVB	23830	35788	7.08%	1.116%
26	11.482	3196	3206	3226	rVB	226716	354462	70.17%	11.049%
27	11.742	3275	3287	3303	rBV	124828	201803	39.95%	6.290%
28	13.745	3896	3910	3930	rBV	9026	18690	3.70%	0.583%
29	13.871	3940	3949	3962	rBV2	7940	12469	2.47%	0.389%
30	13.964	3970	3978	3987	rBV3	7345	11083	2.19%	0.345%

Sum of corrected areas: 3208095

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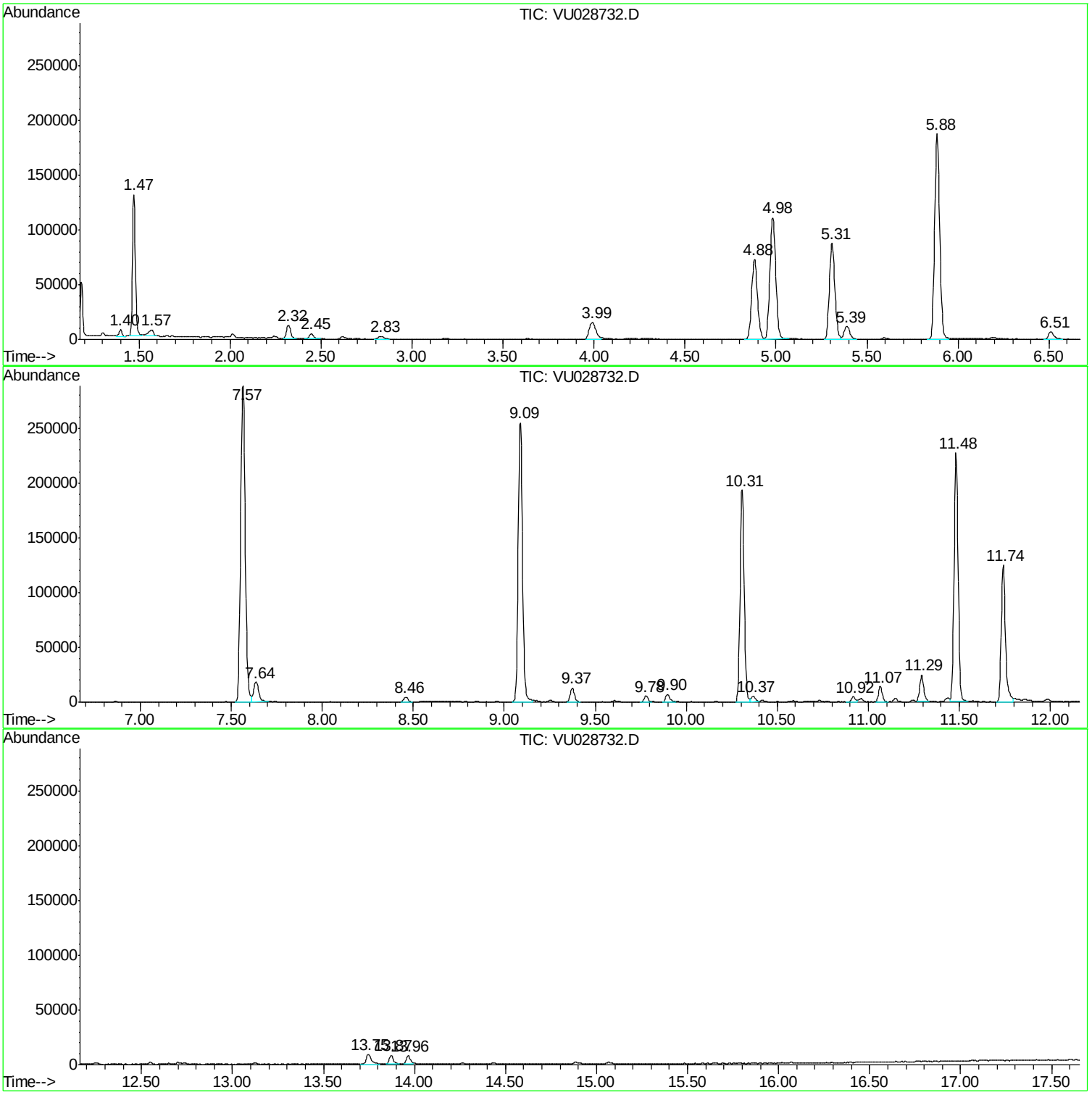
Instrument :
MSVOA_U
ClientSampleId :
COMP-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U120618W.M
Quant Title : SW846 8260

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



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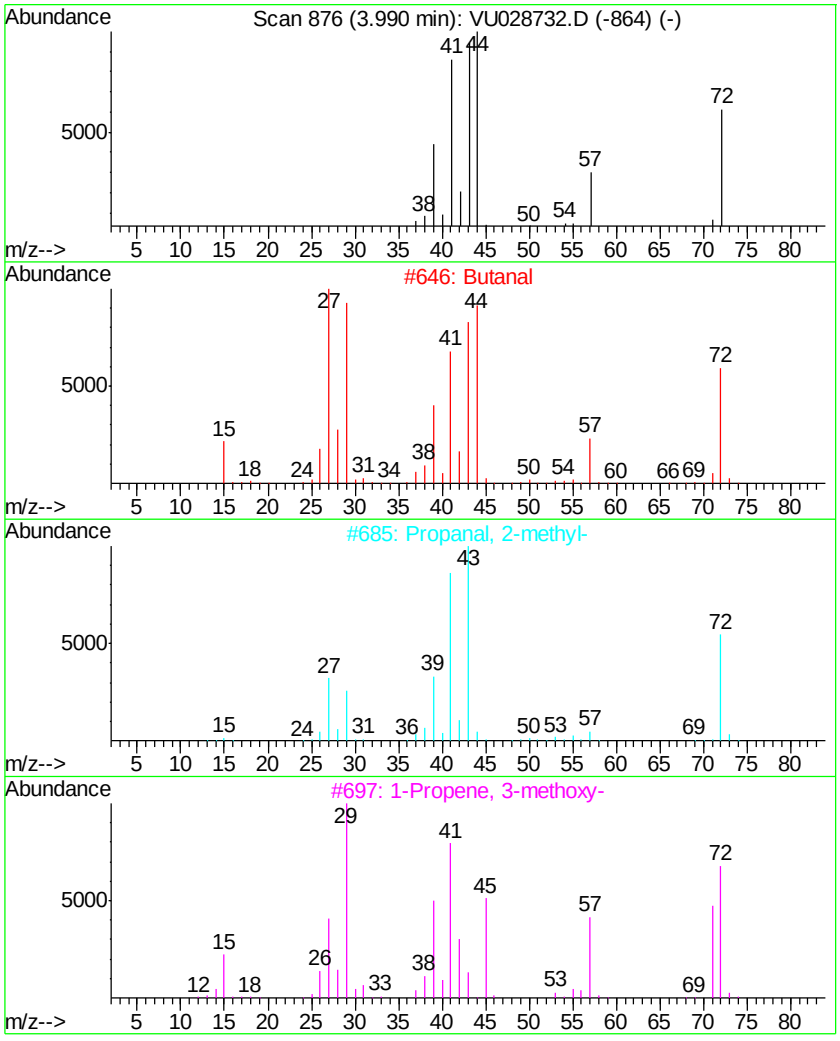
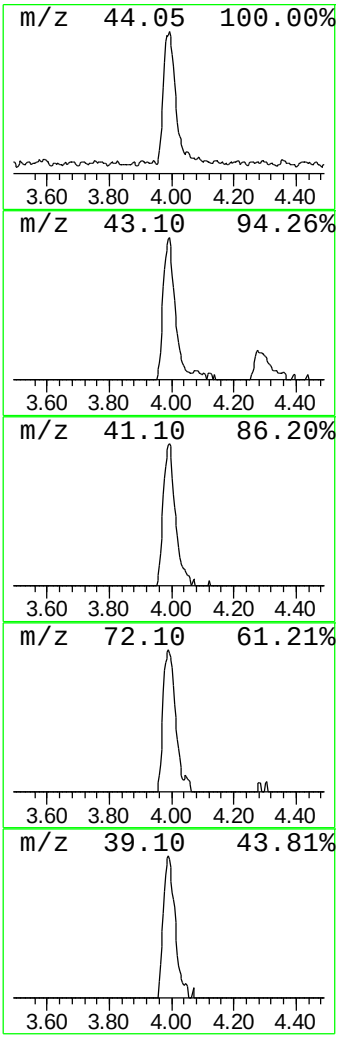
Peak Number 2 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.99	8.00 ug/l	39458	Pentafluorobenzene	4.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Propanal, 2-methyl-	72	C4H8O	000078-84-2	47
3	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	35
4	Cyclopropyl carbinol	72	C4H8O	002516-33-8	32
5	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	17





Library Search Compound Report

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Instrument : MSVOA_U
ClientSampleId : COMP-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U120618W.M
Quant Title : SW846 8260

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

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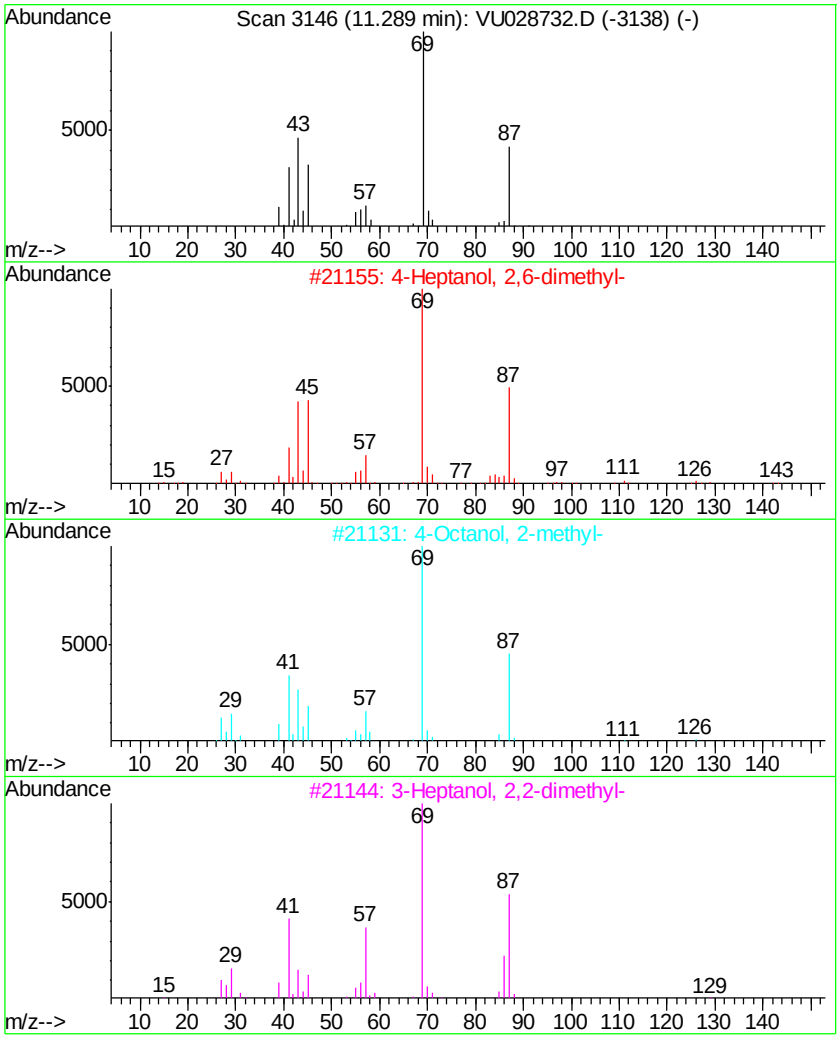
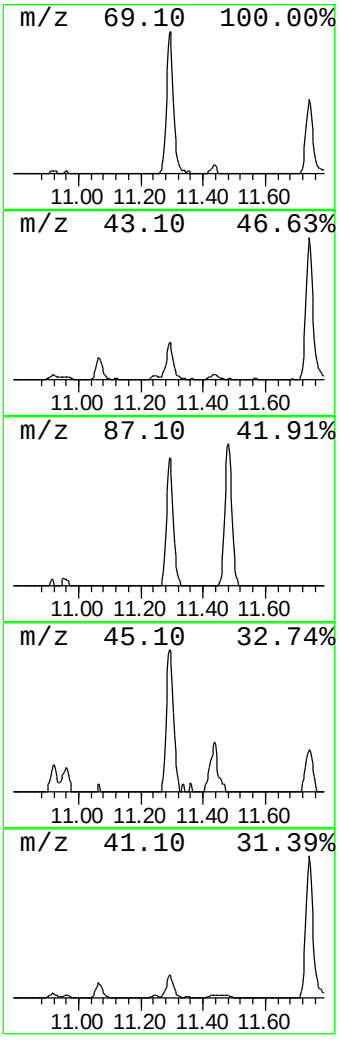
Peak Number 3 4-Heptanol, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.29	5.05 ug/l	35788	1,4-Dichlorobenzene-d4	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	83
2	4-Octanol, 2-methyl-	144	C9H20O	040575-41-5	72
3	3-Heptanol, 2,2-dimethyl-	144	C9H20O	019549-70-3	64
4	1-Octyn-4-ol	126	C8H14O	052517-92-7	64
5	1,2-Hexanediol	118	C6H14O2	006920-22-5	64





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ClientSampleId : COMP-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U120618W.M
Quant Title : SW846 8260

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

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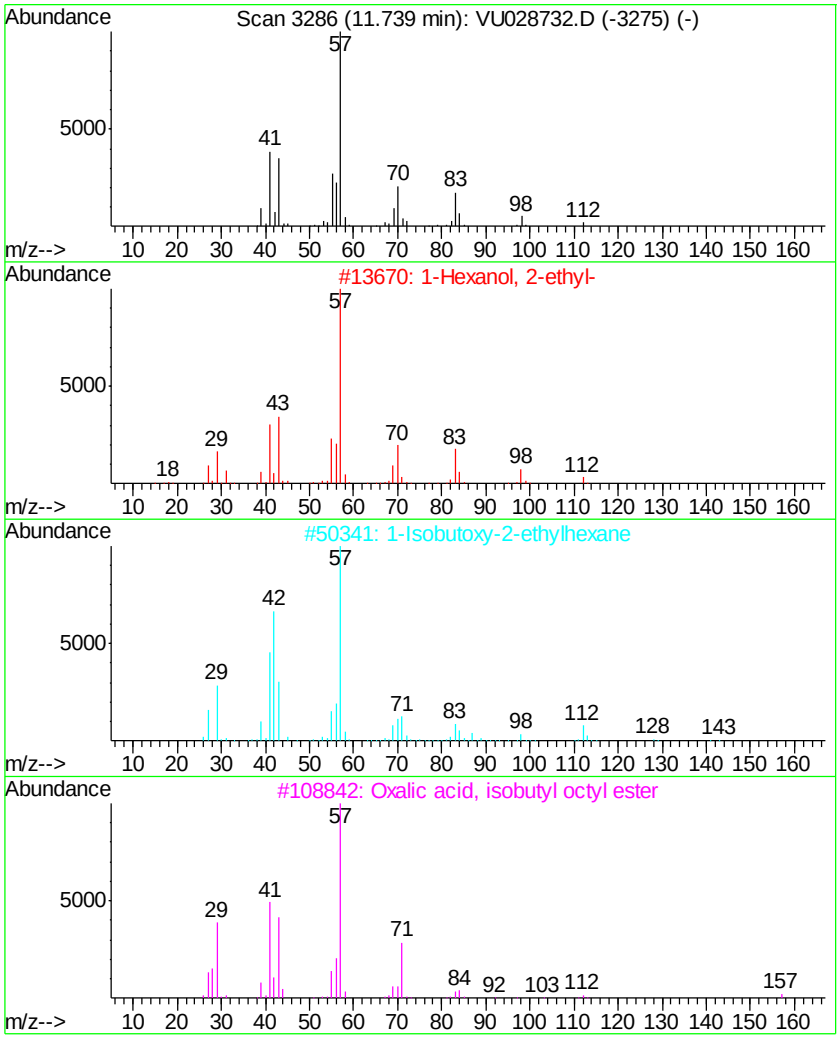
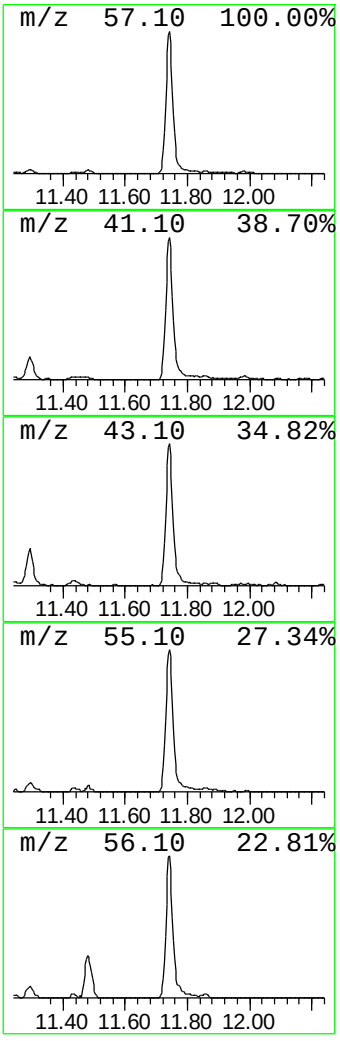
Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.74	28.47 ug/l	201803	1,4-Dichlorobenzene-d4	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
3	Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	53
4	1-Hexene, 5,5-dimethyl-	112	C8H16	007116-86-1	50
5	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U120618W.M
Quant Title : SW846 8260

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butanal	3.99	8.0	ug/l	39458	1	4.98	246637	50.0
4-Heptanol, 2,6-d...	11.29	5.0	ug/l	35788	4	11.48	354462	50.0
1-Hexanol, 2-ethyl-	11.74	28.5	ug/l	201803	4	11.48	354462	50.0