LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU072019\
Data File : VU033352.D
Acq On : 20 Jul 2019 01:07
Operator : JC/SP
Sample : K3890-04
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : A52W4

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\SOMUTR071619WMA.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	1.174	20	26	35	rVB3	12148	13938	2.80%	0.314%
2	1.389	80	93	105	rBV	69560	87032	17.49%	1.962%
3	1.534	133	138	150	rBV2	9746	13401	2.69%	0.302%
4	1.672	174	181	196	rVB	61639	80508	16.18%	1.815%
5	2.261	353	364	371	rBV	126987	189920	38.16%	4.281%
6	2.309	371	379	394	rVB	134993	214388	43.08%	4.833%
7	2.428	411	416	428	rVB3	6085	9941	2.00%	0.224%
8	4.167	943	957	975	rBV	72901	190384	38.25%	4.292%
9	4.254	975	984	1010	rVB	23768	62967	12.65%	1.419%
10	4.624	1083	1099	1126	rBV2	110753	270672	54.39%	6.101%
11	5.315	1291	1314	1337	rBV2	147263	412301	82.85%	9.294%
12	5.865	1472	1485	1506	rBV2	135111	262482	52.74%	5.917%
13	6.309	1607	1623	1643	rBV	97608	199201	40.03%	4.490%
14	6.521	1681	1689	1703	rVB6	2907	5662	1.14%	0.128%
15	7.209	1888	1903	1925	rBV	45947	85064	17.09%	1.918%
16	7.450	1966	1978	1996	rBV3	15160	29266	5.88%	0.660%
17	7.547	1996	2008	2023	rVV	175769	306878	61.66%	6.918%
18	7.621	2024	2031	2040	rVB4	4830	7823	1.57%	0.176%
19	7.833	2087	2097	2117	rBV2	28808	50642	10.18%	1.142%
20	8.299	2229	2242	2275	rBV	263580	497672	100.00%	11.218%
21	8.450	2279	2289	2304	rVB3	24046	43764	8.79%	0.987%
22	9.074	2467	2483	2510	rBV	207094	353906	71.11%	7.978%
23	10.019	2766	2777	2788	rBV5	3322	5104	1.03%	0.115%
24	10.415	2888	2900	2915	rBV	87134	139460	28.02%	3.144%
25	11.129	3107	3122	3139	rBV5	6688	14564	2.93%	0.328%
26	11.360	3186	3194	3202	rBV4	4158	6482	1.30%	0.146%
27	11.469	3217	3228	3248	rBV	201768	327730	65.85%	7.388%
28	11.736	3299	3311	3331	rBV3	45723	102384	20.57%	2.308%
29	11.846	3334	3345	3368	rVB	195289	328016	65.91%	7.394%
30	12.556	3554	3566	3577	rBV7	10333	19168	3.85%	0.432%
31	12.630	3578	3589	3599	rVV6	7609	15923	3.20%	0.359%
32	12.688	3599	3607	3620	rVB2	9906	15207	3.06%	0.343%
33	12.952	3679	3689	3693	rBV8	3934	5637	1.13%	0.127%
34	13.109	3727	3738	3748	rBV4	15355	24641	4.95%	0.555%

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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

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Title : TRACE VOA SOM01.0

35	13.733	3922	3932	3946	rBV	21930	37630	7.56%	0.848%
36	17.341	5049	5054	5065	rVB4	4266	6429	1.29%	0.145%

Sum of corrected areas: 4436187

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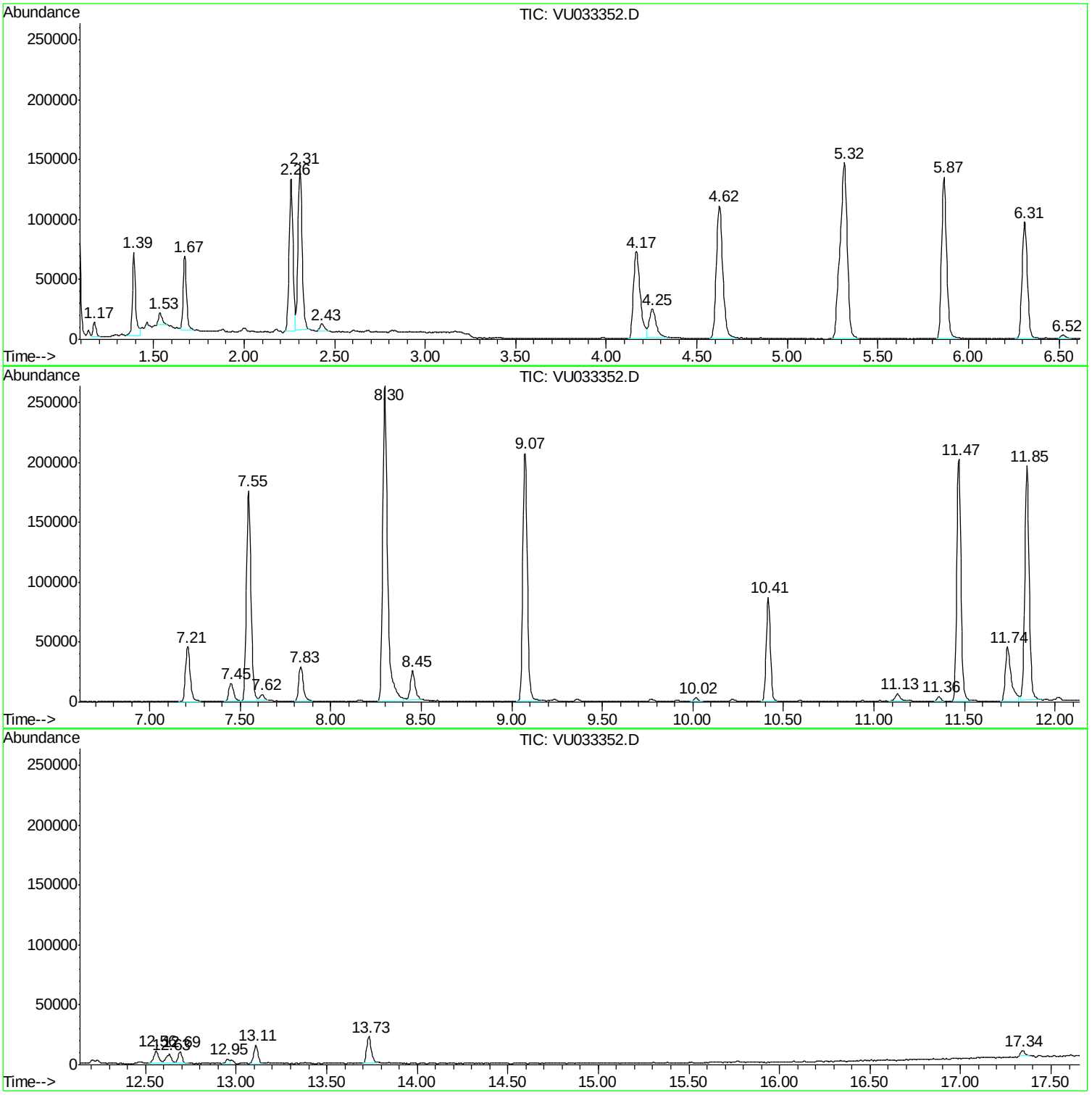
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR071619WMA.M
Quant Title : TRACE VOA SOM01.0

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU072019\
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Instrument : MSVOA_U
ClientSampleId : A52W4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR071619WMA.M
Quant Title : TRACE VOA SOM01.0

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

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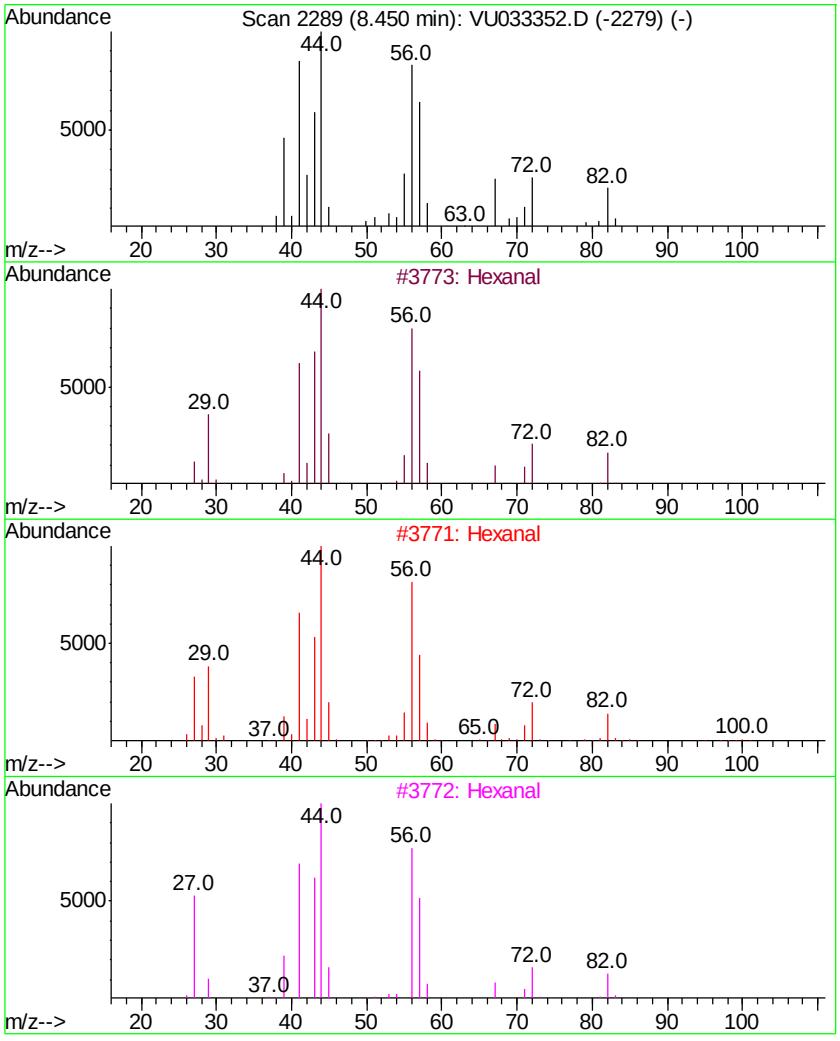
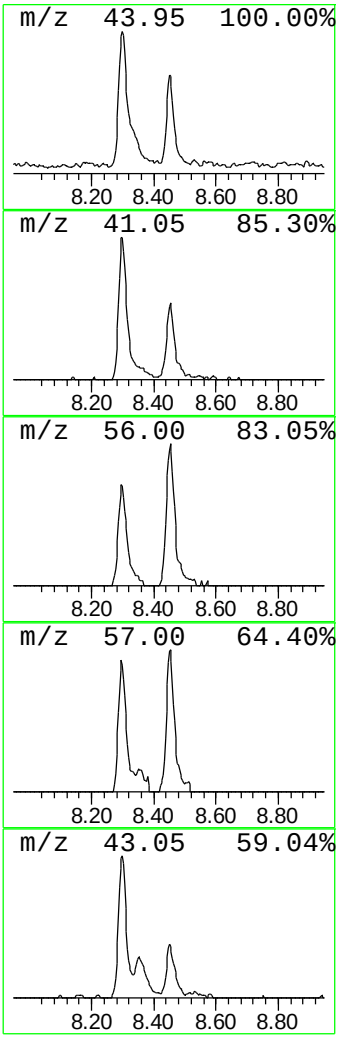
Peak Number 2 Hexanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.45	0.62 ug/L	43764	Chlorobenzene-d5	9.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	64
2	Hexanal	100	C6H12O	000066-25-1	50
3	Hexanal	100	C6H12O	000066-25-1	50
4	2-Hexen-1-ol, (E)-	100	C6H12O	000928-95-0	27
5	Hexanal	100	C6H12O	000066-25-1	25





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Instrument : MSVOA_U
ClientSampleId : A52W4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR071619WMA.M
Quant Title : TRACE VOA SOM01.0

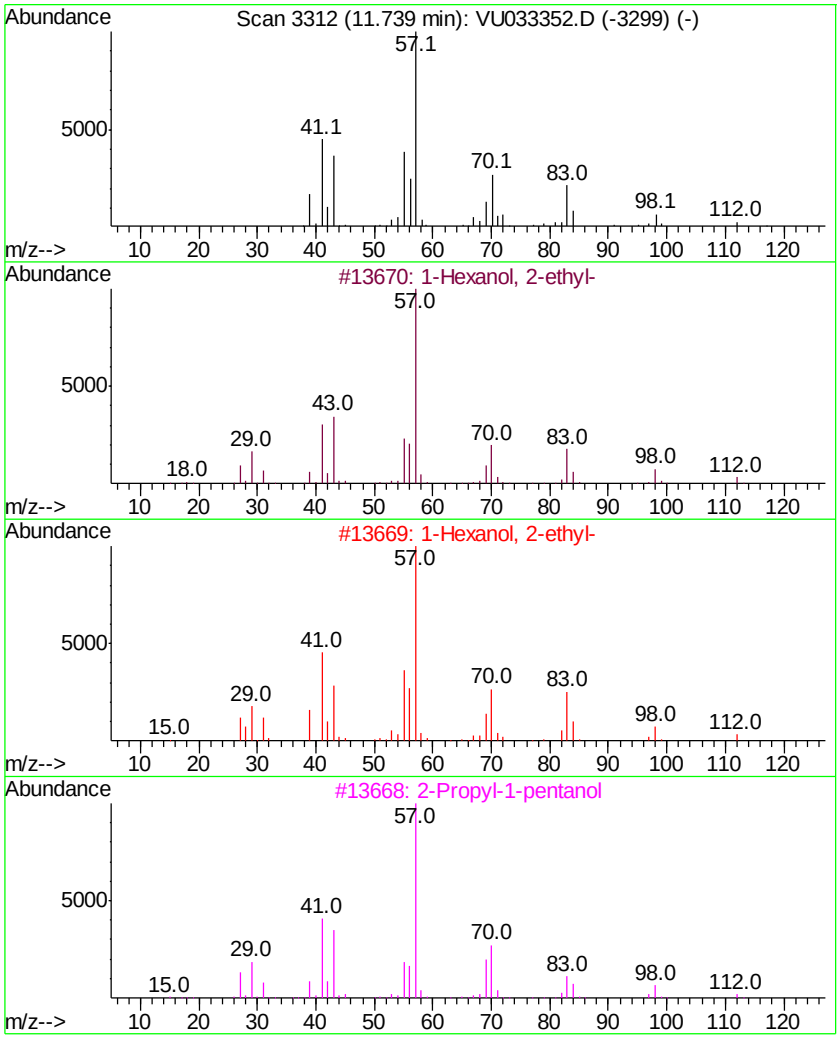
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

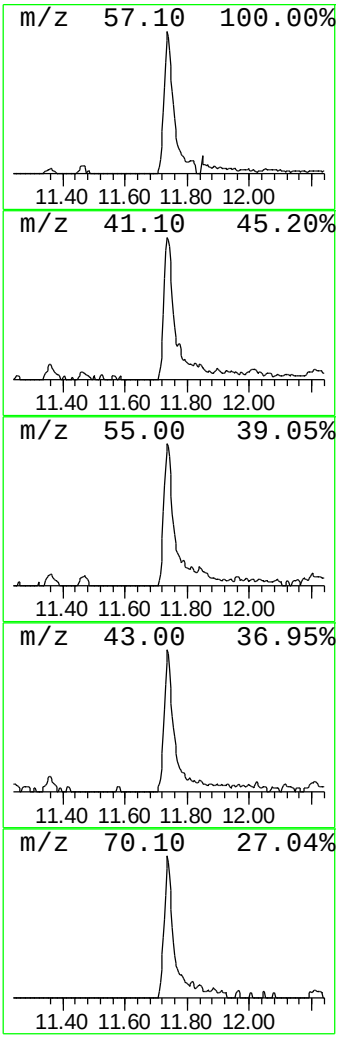
****

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.74	1.56 ug/L	102384	1,4-Dichlorobenzene-d4	11.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	56
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	50
5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	50





Tentatively Identified Compound (LSC) summary

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ClientSampleId : A52W4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR071619WMA.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
Hexanal	8.45	0.6	ug/L	43764	2	9.07	353906	5.0
1-Hexanol, 2-ethyl-	11.74	1.6	ug/L	102384	3	11.47	327730	5.0