LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU041119\
Data File : VU031113.D
Acq On : 12 Apr 2019 08:38
Operator : JC/SP
Sample : K2341-14
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 105 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DB736

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % 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\SOMULM040519WMA.M
Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.180	23	28	38	rVB	31070	29998	0.07%	0.040%
2	1.396	87	95	106	rBV	243968	262898	0.66%	0.346%
3	1.469	115	118	126	rVB	12878	11015	0.03%	0.015%
4	1.678	174	183	196	rBV	188491	245944	0.61%	0.324%
5	2.267	355	366	377	rBV2	384341	589652	1.47%	0.777%
6	2.437	408	419	442	rBV	71696	134965	0.34%	0.178%
7	2.637	477	481	484	rBV4	871	573	0.00%	0.001%
8	2.659	484	488	490	rBV4	1317	1028	0.00%	0.001%
9	2.694	495	499	508	rVB8	2477	3684	0.01%	0.005%
10	2.768	519	522	523	rBV3	760	438	0.00%	0.001%
11	2.833	530	542	555	rBV6	6300	14482	0.04%	0.019%
12	2.981	576	588	609	rVV	73849	138927	0.35%	0.183%
13	3.087	619	621	628	rVB2	697	598	0.00%	0.001%
14	3.183	649	651	653	rBV2	822	471	0.00%	0.001%
15	3.415	720	723	728	rVB2	975	787	0.00%	0.001%
16	3.476	738	742	749	rBV2	583	546	0.00%	0.001%
17	3.556	762	767	772	rBV3	704	680	0.00%	0.001%
18	3.637	787	792	796	rBV3	785	659	0.00%	0.001%
19	3.682	802	806	807	rBV2	630	448	0.00%	0.001%
20	3.736	820	823	828	rVB3	573	553	0.00%	0.001%
21	3.842	853	856	862	rBV3	884	719	0.00%	0.001%
22	4.019	906	911	915	rBV4	999	1174	0.00%	0.002%
23	4.109	935	939	941	rBV2	777	633	0.00%	0.001%
24	4.219	941	973	1015	rBV	3537714	9170845	22.87%	12.087%
25	4.643	1089	1105	1129	rBV	311096	801995	2.00%	1.057%
26	4.797	1150	1153	1155	rBV	1806	913	0.00%	0.001%
27	4.952	1197	1201	1206	rBV4	870	909	0.00%	0.001%
28	5.045	1227	1230	1235	rVB4	795	817	0.00%	0.001%
29	5.067	1235	1237	1243	rBV4	802	715	0.00%	0.001%
30	5.334	1289	1320	1352	rBV2	622906	1876344	4.68%	2.473%
31	5.617	1401	1408	1412	rBV8	2049	2412	0.01%	0.003%
32	5.714	1433	1438	1441	rBV3	584	595	0.00%	0.001%
33	5.743	1441	1447	1449	rBV4	568	579	0.00%	0.001%
34	5.794	1459	1463	1464	rVV2	947	700	0.00%	0.001%

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Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 105 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DB736

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % 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\SOMULM040519WMA.M
Title : VOC Analysis

35	5.881	1476	1490	1515	rBV	624195	1265092	3.15%	1.667%
36	6.180	1567	1583	1612	rBV	5702634	10962253	27.34%	14.448%
37	6.325	1617	1628	1657	rVB	431404	896319	2.24%	1.181%
38	6.759	1752	1763	1774	rBV3	10699	22148	0.06%	0.029%
39	7.061	1855	1857	1862	rVB2	517	441	0.00%	0.001%
40	7.128	1875	1878	1882	rBV2	642	522	0.00%	0.001%
41	7.225	1897	1908	1931	rBV	214486	404340	1.01%	0.533%
42	7.562	1999	2013	2026	rBV	769414	1355469	3.38%	1.786%
43	7.633	2027	2035	2058	rVB	153316	296064	0.74%	0.390%
44	7.845	2090	2101	2122	rBV2	144409	269402	0.67%	0.355%
45	8.138	2189	2192	2196	rBV4	714	532	0.00%	0.001%
46	8.167	2199	2201	2202	rBV2	1178	506	0.00%	0.001%
47	8.225	2202	2219	2236	rBV	23685137	40100484	100.00%	52.851%
48	8.305	2238	2244	2280	rVB	684062	1557744	3.88%	2.053%
49	8.466	2286	2294	2317	rVB5	52992	104487	0.26%	0.138%
50	8.733	2373	2377	2379	rBV2	702	565	0.00%	0.001%
51	8.752	2381	2383	2389	rVB5	1143	922	0.00%	0.001%
52	8.794	2394	2396	2398	rBV	1148	673	0.00%	0.001%
53	8.832	2405	2408	2413	rVB5	924	692	0.00%	0.001%
54	8.887	2422	2425	2430	rVB4	1046	877	0.00%	0.001%
55	9.003	2457	2461	2462	rBV2	596	482	0.00%	0.001%
56	9.087	2474	2487	2513	rBV	922586	1586163	3.96%	2.091%
57	9.296	2549	2552	2555	rBV3	837	524	0.00%	0.001%
58	9.427	2591	2593	2598	rVB3	828	551	0.00%	0.001%
59	9.514	2612	2620	2623	rBV3	725	903	0.00%	0.001%
60	9.723	2680	2685	2686	rBV2	654	502	0.00%	0.001%
61	9.781	2700	2703	2704	rBV2	1289	726	0.00%	0.001%
62	9.807	2705	2711	2717	rVV8	2436	3518	0.01%	0.005%
63	9.955	2753	2757	2765	rBV7	1079	1507	0.00%	0.002%
64	9.993	2766	2769	2774	rVB3	977	944	0.00%	0.001%
65	10.045	2774	2785	2796	rBV7	7595	17210	0.04%	0.023%
66	10.090	2796	2799	2801	rBV2	717	474	0.00%	0.001%
67	10.154	2817	2819	2825	rVB3	558	477	0.00%	0.001%
68	10.276	2854	2857	2861	rVB3	1150	861	0.00%	0.001%
69	10.337	2873	2876	2879	rBV3	815	495	0.00%	0.001%
70	10.363	2879	2884	2888	rVB5	786	790	0.00%	0.001%
71	10.427	2892	2904	2926	rBV	606599	989192	2.47%	1.304%

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ALS Vial : 105 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DB736

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % 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\SOMULM040519WMA.M
Title : VOC Analysis

72	10.572	2946	2949	2951	rBV2	907	600	0.00%	0.001%
73	10.607	2957	2960	2964	rBV5	1683	1546	0.00%	0.002%
74	10.730	2995	2998	3005	rVB3	944	798	0.00%	0.001%
75	10.916	3051	3056	3059	rBV3	726	633	0.00%	0.001%
76	10.939	3059	3063	3064	rBV2	860	515	0.00%	0.001%
77	11.257	3158	3162	3164	rBV2	576	450	0.00%	0.001%
78	11.376	3190	3199	3213	rBV7	13645	27128	0.07%	0.036%
79	11.479	3220	3231	3257	rBV	850223	1388573	3.46%	1.830%
80	11.797	3328	3330	3333	rVB3	1774	764	0.00%	0.001%
81	11.855	3333	3348	3372	rBV	772211	1286429	3.21%	1.695%
82	12.546	3560	3563	3566	rVB3	839	541	0.00%	0.001%
83	12.594	3568	3578	3580	rBV6	4711	6343	0.02%	0.008%
84	12.742	3621	3624	3626	rBV3	1405	894	0.00%	0.001%
85	12.800	3639	3642	3645	rBV3	1541	1292	0.00%	0.002%
86	12.910	3672	3676	3679	rVB4	1310	1039	0.00%	0.001%
87	12.996	3699	3703	3705	rBV3	873	784	0.00%	0.001%
88	13.373	3816	3820	3826	rBV	3498	3999	0.01%	0.005%
89	13.401	3826	3829	3831	rBV2	1694	1167	0.00%	0.002%
90	13.472	3849	3851	3854	rBV2	1479	1011	0.00%	0.001%
91	13.594	3886	3889	3892	rBV2	1079	798	0.00%	0.001%
92	13.652	3905	3907	3911	rVB3	1062	544	0.00%	0.001%
93	13.717	3925	3927	3933	rBV3	846	857	0.00%	0.001%
94	13.868	3971	3974	3978	rVB4	1136	831	0.00%	0.001%
95	13.948	3996	3999	4000	rBV2	956	591	0.00%	0.001%
96	13.983	4008	4010	4013	rVB2	1101	579	0.00%	0.001%
97	14.003	4013	4016	4018	rBV2	1136	754	0.00%	0.001%
98	14.064	4032	4035	4036	rBV	1115	602	0.00%	0.001%
99	14.106	4046	4048	4053	rVB4	804	524	0.00%	0.001%
100	14.996	4323	4325	4328	rBV2	1348	760	0.00%	0.001%

Sum of corrected areas: 75873893

LSC Report - Integrated Chromatogram

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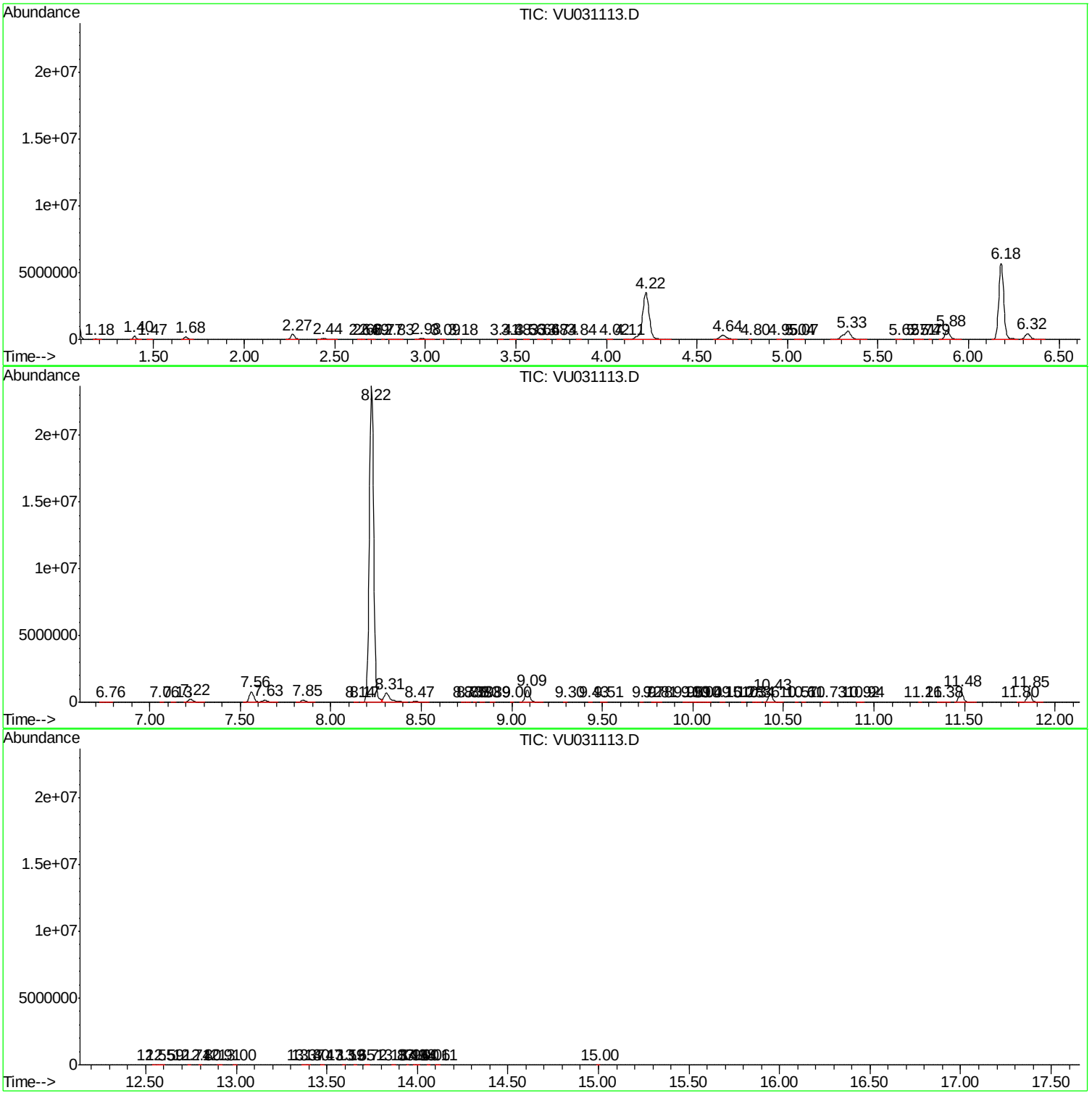
Sample : K2341-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 105 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DB736

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM040519WMA.M
Quant Title : VOC Analysis

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU041119\
Data File : VU031113.D
Acq On : 12 Apr 2019 08:38
Operator : JC/SP
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Misc : 5.0mL/MSVOA_U/WATER
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Instrument : MSVOA_U
ClientSampleId : DB736

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM040519WMA.M
Quant Title : VOC Analysis

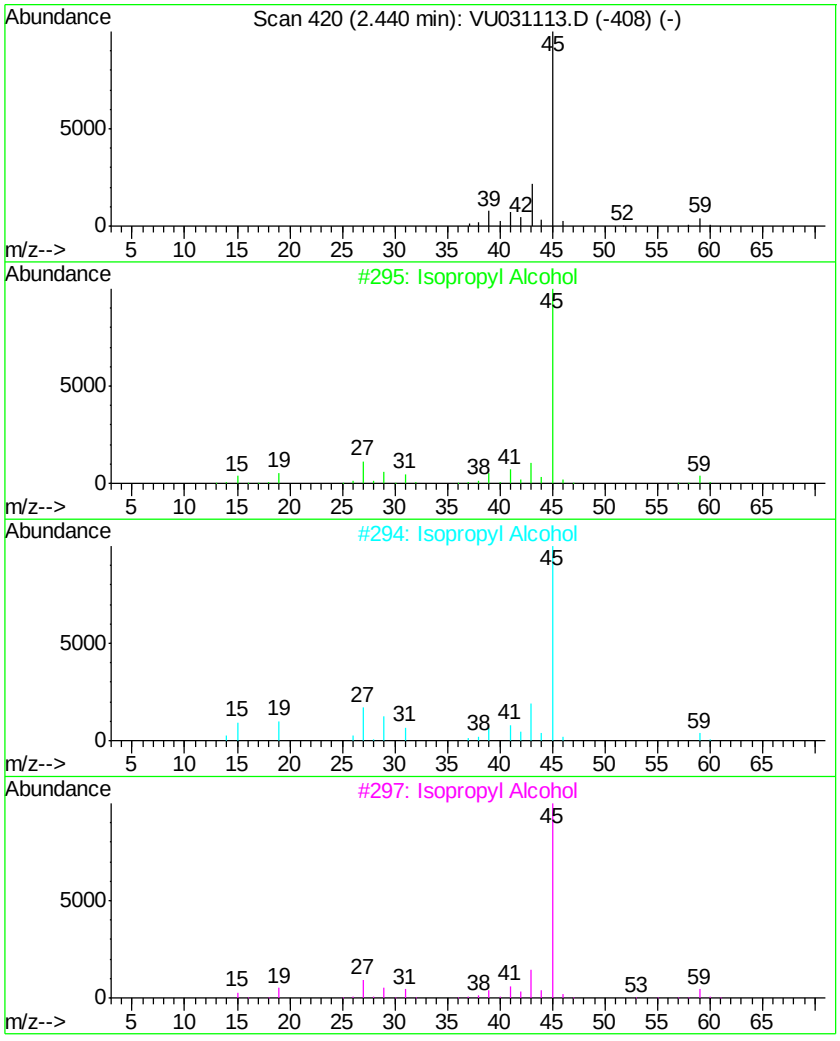
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

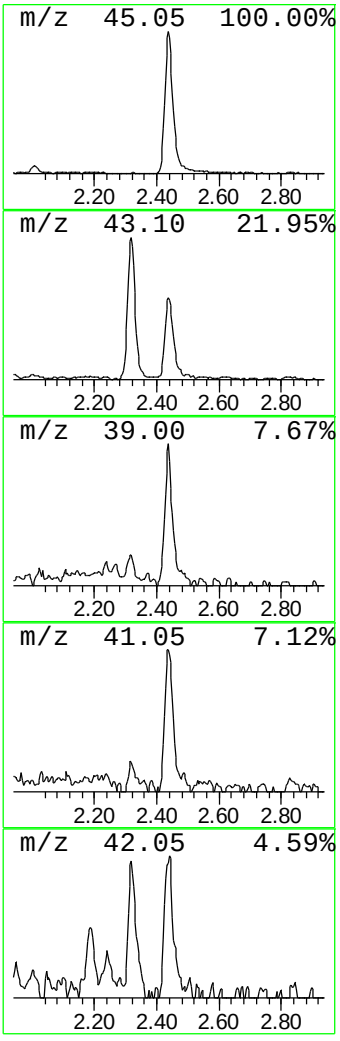
****

Peak Number 1 Isopropyl Alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.44	5.33 ug/L	134965	1,4-Difluorobenzene	5.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	90
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	83
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	83
4	4-Penten-2-ol	86	C5H10O	000625-31-0	50
5	Formamide	45	CH3NO	000075-12-7	5





Library Search Compound Report

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Acq On : 12 Apr 2019 08:38
Operator : JC/SP
Sample : K2341-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 105 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DB736

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM040519WMA.M
Quant Title : VOC Analysis

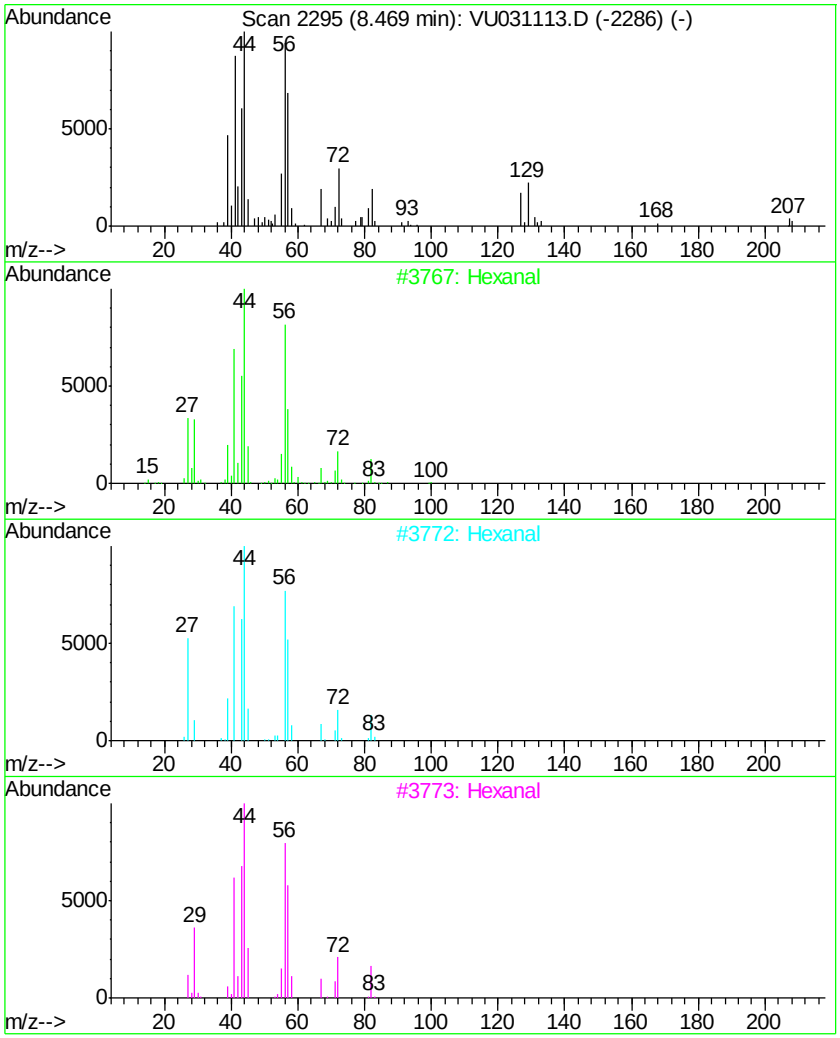
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

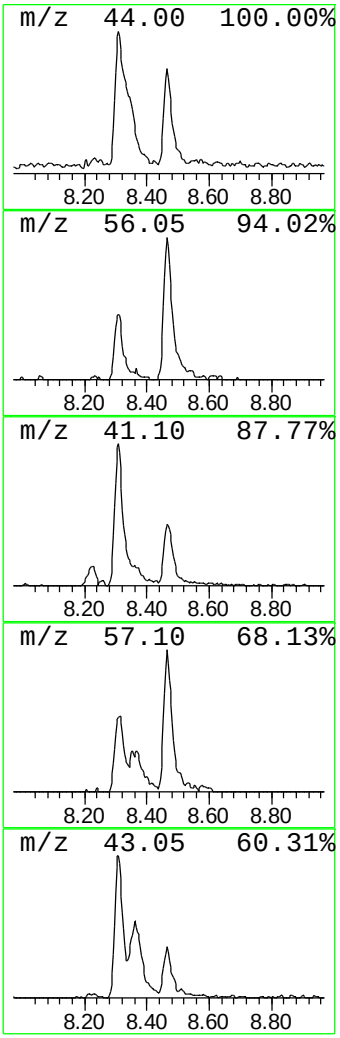
****

Peak Number 3 Hexanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.47	3.29 ug/L	104487	Chlorobenzene-d5	9.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	53
2	Hexanal	100	C6H12O	000066-25-1	47
3	Hexanal	100	C6H12O	000066-25-1	42
4	Hexanal	100	C6H12O	000066-25-1	40
5	2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9	32





Tentatively Identified Compound (LSC) summary

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Quant Title : VOC Analysis

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Isopropyl Alcohol	2.44	5.3	ug/L	134965	1	5.88	1265090	50.0
Hexanal	8.47	3.3	ug/L	104487	2	9.09	1586160	50.0