LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU071318\
Data File : VU025394.D
Acq On : 13 Jul 2018 15:48
Operator : MD/SY
Sample : J3937-07 5X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BEMG5

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\SOMULM062918WMA.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	0.664	21	23	29	rVB5	1014	978	0.06%	0.009%
2	0.835	73	76	81	rBV6	610	626	0.04%	0.006%
3	0.960	110	115	118	rBV5	1013	880	0.05%	0.008%
4	1.082	144	153	174	rBV	1478413	1753869	100.00%	16.774%
5	1.326	225	229	238	rVB	16491	17271	0.98%	0.165%
6	1.397	245	251	268	rBV	102908	111981	6.38%	1.071%
7	1.658	326	332	346	rVB	80780	110373	6.29%	1.056%
8	2.265	512	521	532	rVB	181368	275660	15.72%	2.636%
9	2.693	648	654	665	rVB9	3163	5973	0.34%	0.057%
10	2.831	690	697	715	rVB5	5104	10203	0.58%	0.098%
11	3.204	810	813	817	rBV4	899	628	0.04%	0.006%
12	3.410	871	877	880	rBV5	882	848	0.05%	0.008%
13	3.577	924	929	932	rBV5	803	915	0.05%	0.009%
14	3.703	963	968	972	rBV6	1022	989	0.06%	0.009%
15	3.786	989	994	998	rVB5	1014	1048	0.06%	0.010%
16	3.989	1050	1057	1058	rBV6	789	901	0.05%	0.009%
17	4.031	1065	1070	1073	rBV5	736	725	0.04%	0.007%
18	4.079	1081	1085	1089	rBV4	653	564	0.03%	0.005%
19	4.117	1092	1097	1099	rBV6	773	697	0.04%	0.007%
20	4.172	1099	1114	1135	rBV	86153	232598	13.26%	2.225%
21	4.333	1160	1164	1169	rVB6	1182	1111	0.06%	0.011%
22	4.648	1243	1262	1281	rBV	150068	351197	20.02%	3.359%
23	4.786	1303	1305	1311	rVB5	821	707	0.04%	0.007%
24	4.815	1311	1314	1317	rBV3	776	618	0.04%	0.006%
25	4.982	1362	1366	1370	rVB4	673	565	0.03%	0.005%
26	5.037	1380	1383	1388	rVB5	1175	996	0.06%	0.010%
27	5.108	1400	1405	1409	rBV4	769	801	0.05%	0.008%
28	5.191	1425	1431	1437	rBV4	969	1498	0.09%	0.014%
29	5.239	1442	1446	1448	rBV3	691	589	0.03%	0.006%
30	5.339	1452	1477	1500	rBV2	291707	881826	50.28%	8.434%
31	5.551	1540	1543	1547	rBV5	970	975	0.06%	0.009%
32	5.680	1581	1583	1590	rVB5	801	647	0.04%	0.006%
33	5.715	1590	1594	1597	rBV4	976	809	0.05%	0.008%
34	5.741	1597	1602	1604	rBV3	814	675	0.04%	0.006%

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Instrument : MSVOA_U
ClientSampleId : BEMG5

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
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Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM062918WMA.M
Title : VOC Analysis

35	5.886	1631	1647	1676	rBV	494171	981128	55.94%	9.384%
36	6.333	1772	1786	1803	rBV	195894	395708	22.56%	3.785%
37	6.616	1863	1874	1889	rBV3	13488	30241	1.72%	0.289%
38	6.796	1927	1930	1934	rBV3	771	645	0.04%	0.006%
39	7.066	2011	2014	2018	rVB5	925	739	0.04%	0.007%
40	7.127	2029	2033	2037	rVB4	1037	878	0.05%	0.008%
41	7.156	2037	2042	2045	rBV6	1314	1246	0.07%	0.012%
42	7.230	2052	2065	2086	rBV	111840	201489	11.49%	1.927%
43	7.342	2092	2100	2103	rBV7	1532	2248	0.13%	0.021%
44	7.413	2119	2122	2125	rBV4	650	503	0.03%	0.005%
45	7.452	2129	2134	2135	rBV2	958	764	0.04%	0.007%
46	7.509	2149	2152	2154	rBV5	880	607	0.03%	0.006%
47	7.567	2156	2170	2188	rVV	408989	716020	40.83%	6.848%
48	7.850	2241	2258	2278	rBV	79867	138430	7.89%	1.324%
49	7.950	2287	2289	2293	rVB5	817	562	0.03%	0.005%
50	7.976	2293	2297	2299	rVB4	877	662	0.04%	0.006%
51	7.995	2299	2303	2306	rBV3	1054	1021	0.06%	0.010%
52	8.117	2334	2341	2343	rBV6	760	774	0.04%	0.007%
53	8.178	2352	2360	2371	rVB3	6586	11001	0.63%	0.105%
54	8.252	2378	2383	2386	rBV4	570	507	0.03%	0.005%
55	8.313	2389	2402	2419	rBV	318496	548392	31.27%	5.245%
56	8.529	2467	2469	2473	rVB5	950	691	0.04%	0.007%
57	8.558	2473	2478	2480	rBV3	680	647	0.04%	0.006%
58	8.577	2481	2484	2487	rBV4	883	542	0.03%	0.005%
59	8.693	2517	2520	2524	rVB4	715	676	0.04%	0.006%
60	9.091	2631	2644	2672	rBV	689080	1143305	65.19%	10.935%
61	9.271	2698	2700	2703	rVB4	891	540	0.03%	0.005%
62	9.378	2727	2733	2738	rBV7	2030	2990	0.17%	0.029%
63	10.091	2953	2955	2961	rVB5	899	823	0.05%	0.008%
64	10.124	2961	2965	2969	rBV5	975	835	0.05%	0.008%
65	10.310	3019	3023	3028	rBV4	778	854	0.05%	0.008%
66	10.368	3039	3041	3046	rVB4	949	638	0.04%	0.006%
67	10.435	3050	3062	3081	rVB	306776	494069	28.17%	4.725%
68	10.609	3108	3116	3127	rVB3	6708	11524	0.66%	0.110%
69	10.747	3157	3159	3164	rVB4	1053	750	0.04%	0.007%
70	10.773	3164	3167	3170	rBV5	696	577	0.03%	0.006%
71	11.140	3277	3281	3284	rBV3	957	787	0.04%	0.008%

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Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM062918WMA.M
Title : VOC Analysis

72	11.226	3305	3308	3314	rBV4	763	656	0.04%	0.006%
73	11.255	3314	3317	3319	rBV2	897	611	0.03%	0.006%
74	11.275	3319	3323	3331	rVB4	611	580	0.03%	0.006%
75	11.487	3374	3389	3412	rBV	728056	1147186	65.41%	10.972%
76	11.606	3422	3426	3430	rVV5	718	596	0.03%	0.006%
77	11.686	3446	3451	3453	rBV3	624	536	0.03%	0.005%
78	11.712	3456	3459	3464	rVB5	779	613	0.03%	0.006%
79	11.808	3484	3489	3492	rBV4	616	615	0.04%	0.006%
80	11.863	3494	3506	3524	rVB	443853	708536	40.40%	6.776%
81	12.072	3566	3571	3581	rVB8	2219	3093	0.18%	0.030%
82	12.204	3609	3612	3615	rVV3	603	545	0.03%	0.005%
83	12.230	3618	3620	3625	rVV3	1104	936	0.05%	0.009%
84	12.484	3690	3699	3708	rVV	8442	13170	0.75%	0.126%
85	12.567	3714	3725	3738	rBV2	34392	53293	3.04%	0.510%
86	12.648	3745	3750	3752	rVB3	835	679	0.04%	0.006%
87	12.744	3776	3780	3783	rBV5	603	520	0.03%	0.005%
88	12.921	3832	3835	3839	rVB3	1215	1108	0.06%	0.011%
89	12.947	3839	3843	3845	rBV4	1204	895	0.05%	0.009%
90	12.972	3845	3851	3853	rBV5	1120	1021	0.06%	0.010%
91	13.004	3857	3861	3863	rBV3	817	589	0.03%	0.006%
92	13.053	3867	3876	3886	rBV9	6528	11631	0.66%	0.111%
93	13.258	3935	3940	3943	rBV4	946	823	0.05%	0.008%
94	13.342	3949	3966	3970	rBV8	11484	26274	1.50%	0.251%
95	13.664	4064	4066	4071	rVB4	1416	1012	0.06%	0.010%
96	13.702	4076	4078	4081	rBV3	700	562	0.03%	0.005%
97	13.963	4155	4159	4163	rBV3	838	795	0.05%	0.008%
98	14.072	4187	4193	4200	rBV8	2235	3321	0.19%	0.032%
99	14.281	4251	4258	4268	rVB2	7175	10488	0.60%	0.100%
100	14.361	4281	4283	4285	rBV2	1014	609	0.03%	0.006%

Sum of corrected areas: 10455847

LSC Report - Integrated Chromatogram

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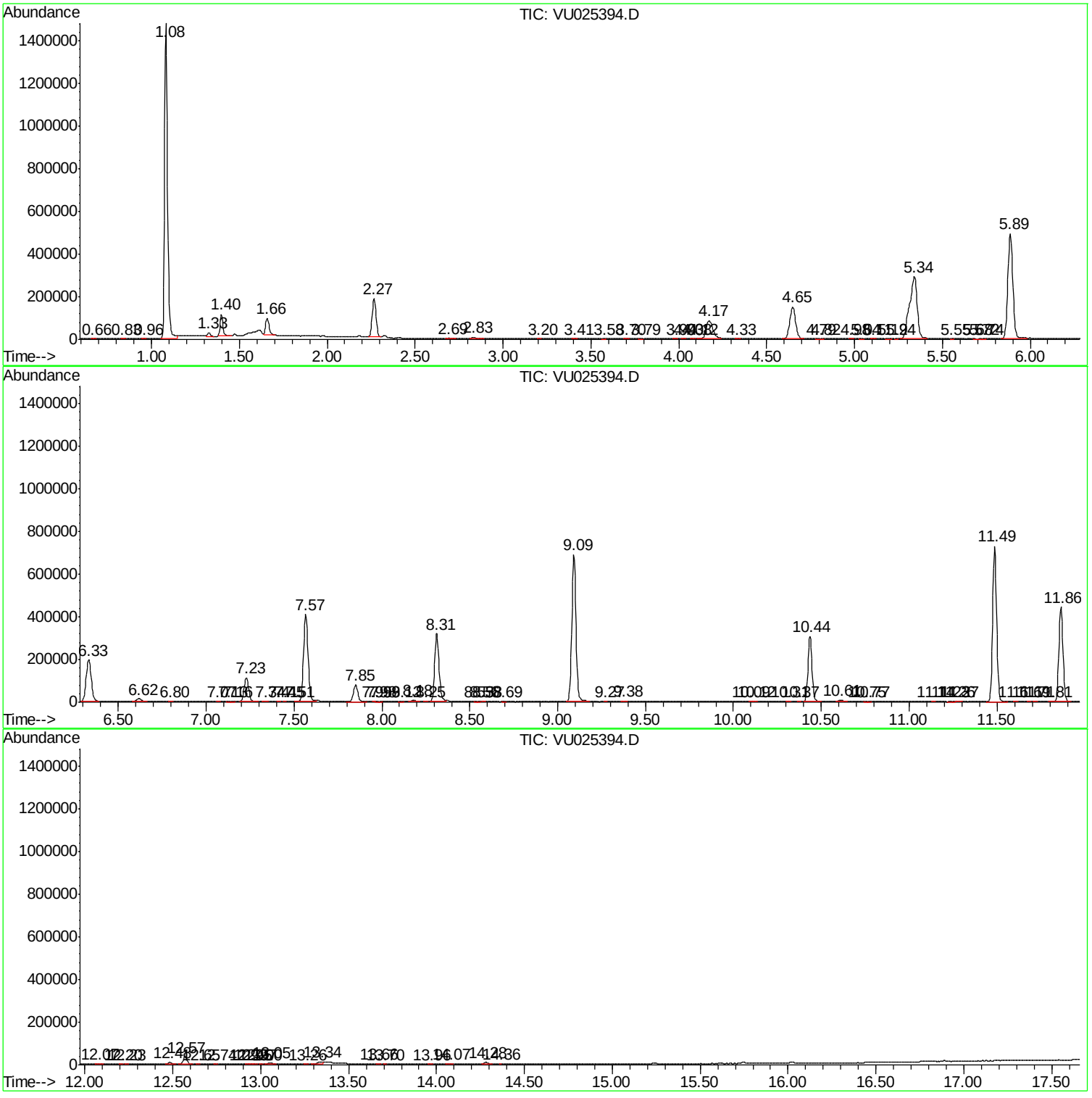
Instrument : MSVOA_U
ClientSampleId : BEMG5

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM062918WMA.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\VU071318\
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ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BEMG5

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM062918WMA.M
Quant Title : VOC Analysis

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

****

Peak Number 1 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.66	5.62 ug/L	110373	1,4-Difluorobenzene	5.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentyn-3-ol, 3-methyl-	98	C6H10O	000077-75-8	4
2	1H-1,2,3-Triazole	69	C2H3N3	000288-36-8	3
3	1H-1,2,4-Triazole	69	C2H3N3	000288-88-0	3
4	1H-1,2,4-Triazole	69	C2H3N3	000288-88-0	3
5	(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	3

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
unknown-01	1.66	5.6	ug/L	110373	1	5.89	981128	50.0