LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU071618\
Data File : VU025432.D
Acq On : 16 Jul 2018 18:29
Operator : MD/SY
Sample : J3937-08
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BEMG6

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\SOMULM071618WMA.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	0.629	6	12	14	rVV4	570	502	0.01%	0.004%
2	0.667	23	24	27	rVB	901	347	0.01%	0.002%
3	0.802	64	66	71	rVB4	815	635	0.02%	0.004%
4	0.844	71	79	81	rBV5	990	950	0.03%	0.007%
5	0.918	98	102	108	rVB6	435	437	0.01%	0.003%
6	0.947	108	111	114	rBV3	637	341	0.01%	0.002%
7	0.973	116	119	123	rBV4	448	367	0.01%	0.003%
8	1.037	134	139	140	rBV3	799	746	0.02%	0.005%
9	1.082	140	153	171	rBV	3217067	3776740	100.00%	26.460%
10	1.391	243	249	266	rVB	124334	140710	3.73%	0.986%
11	1.674	330	337	353	rVB	97862	129367	3.43%	0.906%
12	2.272	511	523	539	rBV	211590	345839	9.16%	2.423%
13	4.169	1111	1113	1115	rBV3	992	604	0.02%	0.004%
14	4.227	1115	1131	1171	rVV2	61783	254767	6.75%	1.785%
15	4.400	1181	1185	1191	rVB8	1538	1909	0.05%	0.013%
16	4.645	1247	1261	1285	rBV2	184899	454233	12.03%	3.182%
17	4.889	1326	1337	1341	rBV9	2491	4285	0.11%	0.030%
18	4.934	1348	1351	1353	rBV4	785	452	0.01%	0.003%
19	5.133	1411	1413	1418	rVB4	1379	990	0.03%	0.007%
20	5.162	1420	1422	1426	rVB4	721	389	0.01%	0.003%
21	5.246	1444	1448	1450	rBV3	954	570	0.02%	0.004%
22	5.336	1453	1476	1497	rBV2	391188	1076781	28.51%	7.544%
23	5.426	1499	1504	1505	rBV4	2988	2459	0.07%	0.017%
24	5.796	1606	1619	1637	rBV	377765	842219	22.30%	5.901%
25	5.899	1639	1651	1668	rVV	376427	779075	20.63%	5.458%
26	6.349	1780	1791	1807	rBV	248398	504715	13.36%	3.536%
27	6.439	1809	1819	1878	rVB	430686	931018	24.65%	6.523%
28	7.239	2056	2068	2089	rVB2	134525	244374	6.47%	1.712%
29	7.577	2159	2173	2185	rBV	494943	858126	22.72%	6.012%
30	7.860	2250	2261	2277	rBV	92822	156865	4.15%	1.099%
31	8.011	2305	2308	2312	rBV4	1139	1077	0.03%	0.008%
32	8.149	2347	2351	2356	rBV6	1057	971	0.03%	0.007%
33	8.236	2376	2378	2382	rVB3	1322	942	0.02%	0.007%
34	8.326	2387	2406	2416	rBV	312644	554609	14.68%	3.886%

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Instrument : MSVOA_U
ClientSampleId : BEMG6

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\SOMULM071618WMA.M
Title : VOC Analysis

35	8.545	2471	2474	2477	rVB2	1261	783	0.02%	0.005%
36	8.725	2526	2530	2535	rVB4	967	799	0.02%	0.006%
37	8.747	2535	2537	2540	rBV2	580	370	0.01%	0.003%
38	8.825	2557	2561	2562	rBV2	1099	861	0.02%	0.006%
39	9.098	2633	2646	2686	rVB	490438	923033	24.44%	6.467%
40	9.976	2917	2919	2924	rBV4	796	737	0.02%	0.005%
41	10.027	2932	2935	2939	rBV5	862	949	0.03%	0.007%
42	10.107	2957	2960	2965	rVB4	1244	858	0.02%	0.006%
43	10.162	2974	2977	2978	rBV2	1006	582	0.02%	0.004%
44	10.313	3021	3024	3029	rBV4	596	484	0.01%	0.003%
45	10.439	3051	3063	3084	rVB	325188	599262	15.87%	4.198%
46	10.609	3108	3116	3117	rBV5	1491	1635	0.04%	0.011%
47	10.693	3139	3142	3146	rBV4	525	428	0.01%	0.003%
48	10.750	3157	3160	3165	rBV4	888	814	0.02%	0.006%
49	10.773	3165	3167	3174	rVB4	898	843	0.02%	0.006%
50	10.873	3195	3198	3202	rVB4	786	555	0.01%	0.004%
51	10.976	3228	3230	3235	rVB4	654	432	0.01%	0.003%
52	11.046	3249	3252	3258	rBV5	736	634	0.02%	0.004%
53	11.072	3258	3260	3263	rBV3	970	535	0.01%	0.004%
54	11.140	3277	3281	3283	rBV5	1175	1047	0.03%	0.007%
55	11.310	3329	3334	3338	rBV7	781	793	0.02%	0.006%
56	11.371	3345	3353	3360	rBV8	1434	2065	0.05%	0.014%
57	11.426	3368	3370	3372	rVB3	798	330	0.01%	0.002%
58	11.490	3373	3390	3406	rBV	479938	799478	21.17%	5.601%
59	11.599	3421	3424	3426	rBV4	789	568	0.02%	0.004%
60	11.709	3454	3458	3460	rBV4	587	397	0.01%	0.003%
61	11.754	3466	3472	3473	rBV5	2554	2368	0.06%	0.017%
62	11.866	3494	3507	3525	rBV	470771	799485	21.17%	5.601%
63	11.959	3534	3536	3539	rBV3	521	361	0.01%	0.003%
64	12.021	3552	3555	3561	rBV5	1309	1260	0.03%	0.009%
65	12.146	3591	3594	3598	rBV4	660	556	0.01%	0.004%
66	12.226	3617	3619	3620	rBV	687	323	0.01%	0.002%
67	12.258	3626	3629	3630	rBV3	730	447	0.01%	0.003%
68	12.291	3635	3639	3642	rBV5	765	721	0.02%	0.005%
69	12.348	3652	3657	3659	rBV3	675	608	0.02%	0.004%
70	12.361	3659	3661	3665	rVV4	542	357	0.01%	0.003%
71	12.410	3673	3676	3678	rBV2	790	581	0.02%	0.004%

LSC Area Percent Report

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ClientSampleId : BEMG6

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\SOMULM071618WMA.M
Title : VOC Analysis

72	12.477	3692	3697	3698	rBV5	877	700	0.02%	0.005%
73	12.574	3717	3727	3742	rVV4	19548	31852	0.84%	0.223%
74	12.660	3752	3754	3758	rBV5	732	493	0.01%	0.003%
75	12.718	3770	3772	3776	rVB2	595	355	0.01%	0.002%
76	12.805	3797	3799	3802	rVB3	758	399	0.01%	0.003%
77	12.824	3802	3805	3808	rBV4	1242	908	0.02%	0.006%
78	12.892	3819	3826	3827	rBV5	1344	1321	0.03%	0.009%
79	12.937	3837	3840	3841	rBV2	747	403	0.01%	0.003%
80	13.056	3874	3877	3881	rVB5	967	890	0.02%	0.006%
81	13.114	3893	3895	3900	rVB4	1167	852	0.02%	0.006%
82	13.143	3900	3904	3906	rBV4	905	733	0.02%	0.005%
83	13.255	3936	3939	3944	rBV5	478	464	0.01%	0.003%
84	13.287	3946	3949	3954	rBV4	621	435	0.01%	0.003%
85	13.329	3954	3962	3964	rBV6	4642	5592	0.15%	0.039%
86	13.622	4048	4053	4054	rBV5	930	765	0.02%	0.005%
87	13.750	4089	4093	4106	rVB6	2820	3528	0.09%	0.025%
88	13.802	4106	4109	4112	rVB2	900	563	0.01%	0.004%
89	13.821	4112	4115	4116	rBV2	853	460	0.01%	0.003%
90	13.947	4152	4154	4157	rBV2	625	374	0.01%	0.003%
91	13.985	4164	4166	4169	rBV3	1018	736	0.02%	0.005%
92	14.001	4169	4171	4176	rVB4	1139	637	0.02%	0.004%
93	14.104	4200	4203	4206	rBV2	867	473	0.01%	0.003%
94	14.143	4213	4215	4222	rVB6	1012	727	0.02%	0.005%
95	14.384	4286	4290	4292	rBV4	1084	805	0.02%	0.006%
96	14.631	4365	4367	4371	rVB5	1069	478	0.01%	0.003%
97	14.664	4374	4377	4379	rBV4	1106	912	0.02%	0.006%
98	14.734	4397	4399	4405	rVB6	934	610	0.02%	0.004%
99	15.236	4552	4555	4560	rBV6	1165	1442	0.04%	0.010%
100	15.387	4599	4602	4604	rBV3	1180	755	0.02%	0.005%

Sum of corrected areas: 14273412

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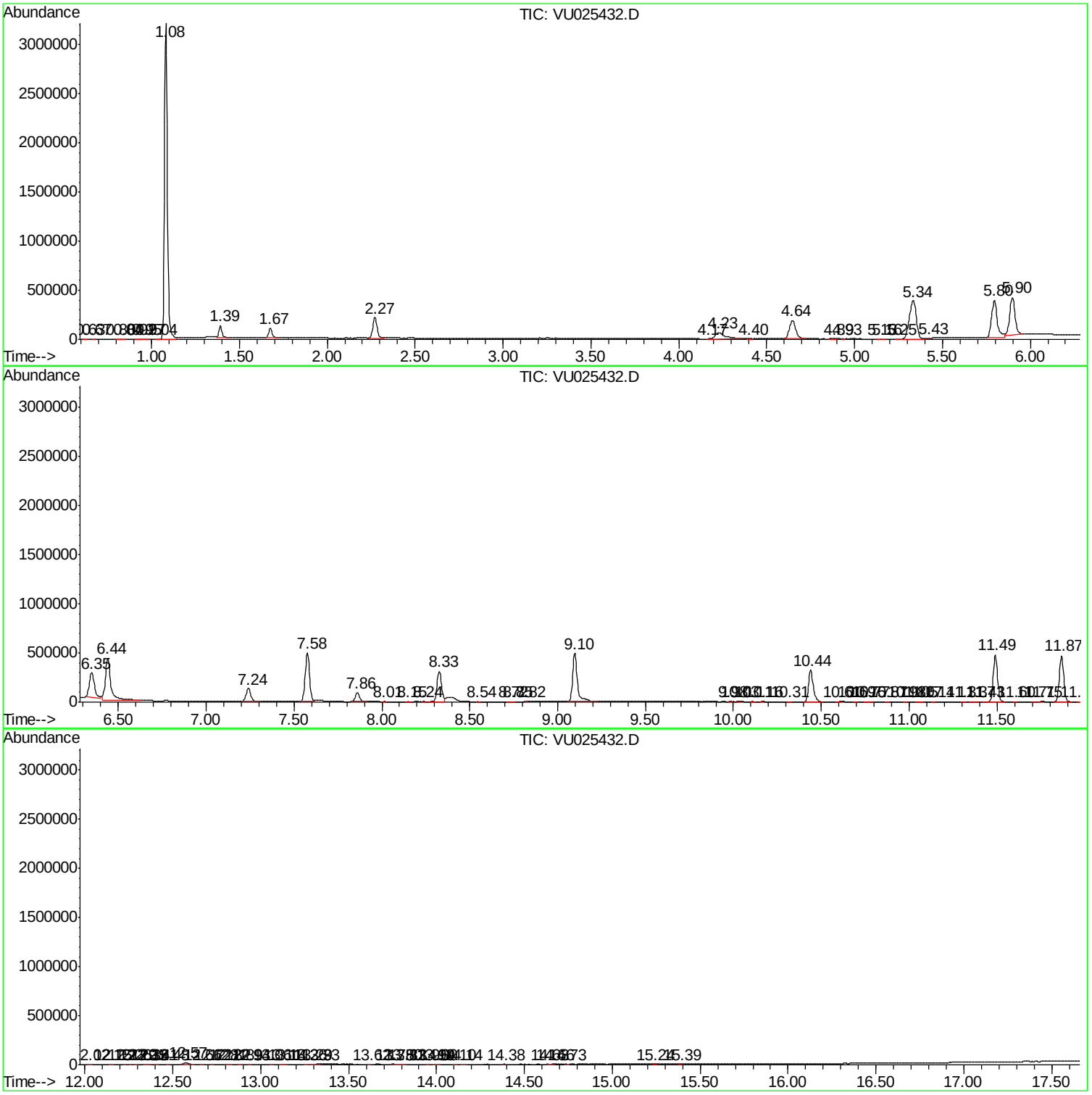
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM071618WMA.M
Quant Title : VOC Analysis

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU071618\
Data File : VU025432.D
Acq On : 16 Jul 2018 18:29
Operator : MD/SY
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Instrument : MSVOA_U
ClientSampleId : BEMG6

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM071618WMA.M
Quant Title : VOC Analysis

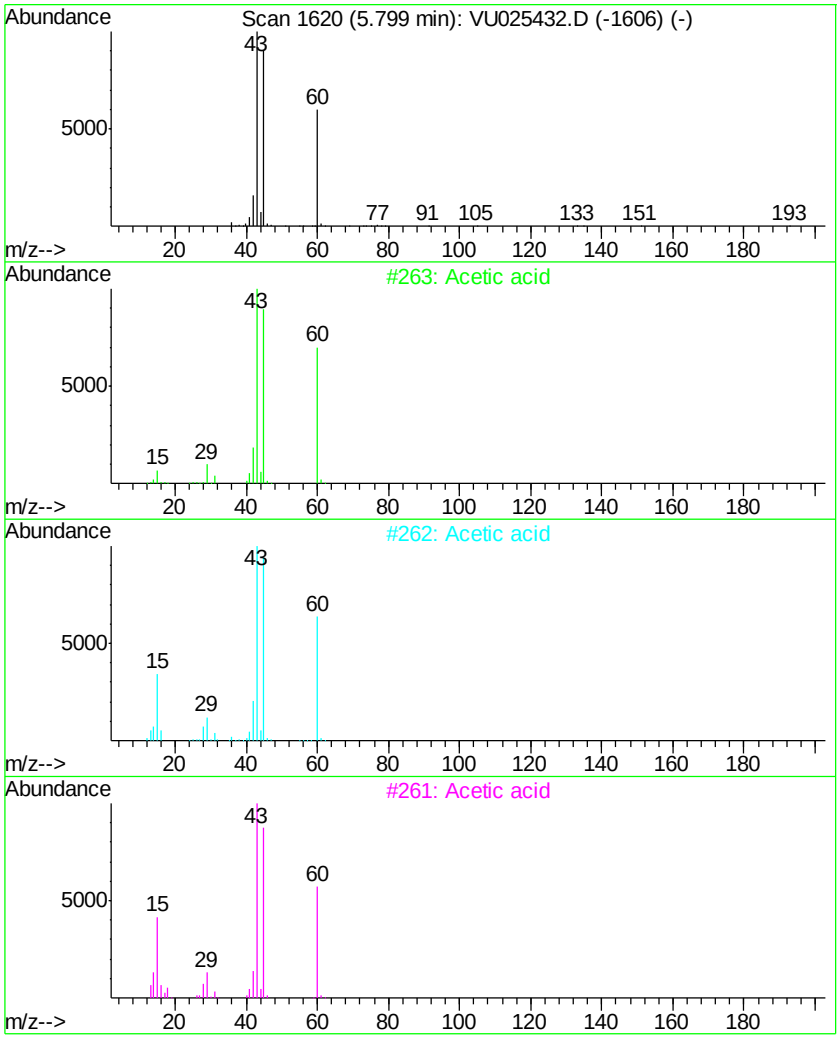
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

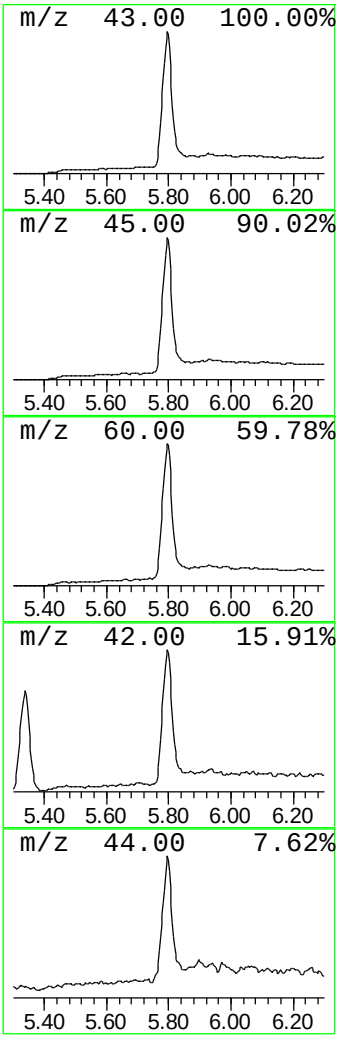
****

Peak Number 2 Acetic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.80	54.05 ug/L	842219	1,4-Difluorobenzene	5.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	91
2	Acetic acid	60	C2H4O2	000064-19-7	90
3	Acetic acid	60	C2H4O2	000064-19-7	90
4	Acetic acid	60	C2H4O2	000064-19-7	83
5	Ammonium acetate	77	C2H7NO2	000631-61-8	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU071618\
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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
Acetic acid	5.80	54.0	ug/L	842219	1	5.90	779075	50.0