LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU053024\
Data File : VU059087.D
Acq On : 30 May 2024 12:33
Operator : MD/SY
Sample : P2589-02ME
Misc : 5.89g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH5W3ME

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\SFAMULM052924WMA.M
Title : VOC Analysis

Signal : TIC: VU059087.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.592	86	94	120	rVB	52968	73356	12.07%	1.349%
2	1.875	137	182	197	rBV4	116337	607640	100.00%	11.173%
3	2.544	379	390	406	rVB	103356	169563	27.91%	3.118%
4	2.705	436	440	444	rBV2	276	244	0.04%	0.004%
5	2.763	456	458	461	rBV3	325	172	0.03%	0.003%
6	3.030	531	541	551	rBV4	4080	7852	1.29%	0.144%
7	3.171	573	585	602	rBV	8889	21928	3.61%	0.403%
8	3.518	688	693	695	rBV2	273	254	0.04%	0.005%
9	3.618	720	724	727	rBV2	203	177	0.03%	0.003%
10	3.679	740	743	747	rBV2	471	315	0.05%	0.006%
11	3.718	752	755	759	rBV	248	217	0.04%	0.004%
12	3.785	773	776	779	rBV2	210	191	0.03%	0.004%
13	3.817	783	786	790	rBV2	206	141	0.02%	0.003%
14	3.988	835	839	841	rBV	210	166	0.03%	0.003%
15	4.100	871	874	877	rBV2	324	220	0.04%	0.004%
16	4.264	921	925	929	rBV2	189	200	0.03%	0.004%
17	4.329	942	945	947	rBV	215	169	0.03%	0.003%
18	4.357	951	954	955	rBV	297	118	0.02%	0.002%
19	4.383	960	962	965	rBV	201	131	0.02%	0.002%
20	4.402	965	968	971	rBV2	271	206	0.03%	0.004%
21	4.576	1016	1022	1025	rBV	226	296	0.05%	0.005%
22	4.618	1025	1035	1074	rBV	49898	150857	24.83%	2.774%
23	5.052	1154	1170	1192	rVV	102990	232484	38.26%	4.275%
24	5.148	1198	1200	1202	rVB2	494	217	0.04%	0.004%
25	5.261	1232	1235	1236	rBV2	224	125	0.02%	0.002%
26	5.515	1309	1314	1316	rBV	287	275	0.05%	0.005%
27	5.711	1356	1375	1407	rBV3	209150	567292	93.36%	10.431%
28	5.843	1414	1416	1419	rVB2	404	153	0.03%	0.003%
29	5.965	1447	1454	1455	rBV2	1747	1460	0.24%	0.027%
30	6.001	1462	1465	1470	rVB3	719	568	0.09%	0.010%
31	6.084	1488	1491	1493	rBV	393	308	0.05%	0.006%
32	6.116	1498	1501	1506	rVV2	391	329	0.05%	0.006%
33	6.238	1526	1539	1560	rBV	238326	462646	76.14%	8.507%
34	6.483	1613	1615	1619	rBV2	185	162	0.03%	0.003%
35	6.521	1619	1627	1629	rBV4	4257	4899	0.81%	0.090%
36	6.595	1639	1650	1663	rBV7	2293	5321	0.88%	0.098%

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Misc : 5.89g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH5W3ME

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\SFAMULM052924WMA.M
Title : VOC Analysis

37	6.682	1663	1677	1698	rVV	136696	265353	43.67%	4.879%
38	6.898	1740	1744	1746	rBV	197	136	0.02%	0.003%
39	6.914	1746	1749	1752	rVB2	377	271	0.04%	0.005%
40	6.933	1752	1755	1760	rBV2	259	306	0.05%	0.006%
41	7.116	1807	1812	1814	rBV	157	148	0.02%	0.003%
42	7.132	1815	1817	1820	rBV2	184	111	0.02%	0.002%
43	7.174	1827	1830	1831	rBV	290	164	0.03%	0.003%
44	7.184	1831	1833	1834	rVV	409	201	0.03%	0.004%
45	7.203	1836	1839	1840	rVV	701	474	0.08%	0.009%
46	7.216	1840	1843	1848	rVB5	1090	1260	0.21%	0.023%
47	7.386	1894	1896	1900	rVB2	153	129	0.02%	0.002%
48	7.415	1902	1905	1910	rBV2	196	211	0.03%	0.004%
49	7.502	1929	1932	1934	rVB	192	110	0.02%	0.002%
50	7.560	1938	1950	1968	rBV2	67145	122995	20.24%	2.262%
51	7.711	1994	1997	2000	rVB2	529	310	0.05%	0.006%
52	7.737	2002	2005	2008	rBV	207	142	0.02%	0.003%
53	7.779	2016	2018	2020	rBV	196	132	0.02%	0.002%
54	7.891	2040	2053	2075	rBV	238540	412790	67.93%	7.590%
55	8.049	2099	2102	2104	rBV2	266	216	0.04%	0.004%
56	8.174	2130	2141	2161	rBV	46381	81668	13.44%	1.502%
57	8.415	2214	2216	2218	rBV	172	117	0.02%	0.002%
58	8.460	2225	2230	2239	rBB3	573	809	0.13%	0.015%
59	8.508	2243	2245	2249	rBV2	141	152	0.03%	0.003%
60	8.637	2273	2285	2319	rBV	136563	323336	53.21%	5.946%
61	8.878	2357	2360	2363	rBV2	263	180	0.03%	0.003%
62	8.936	2374	2378	2379	rBV	160	146	0.02%	0.003%
63	8.955	2379	2384	2387	rVV2	400	369	0.06%	0.007%
64	8.994	2390	2396	2397	rBV	331	302	0.05%	0.006%
65	9.126	2434	2437	2439	rBV	213	174	0.03%	0.003%
66	9.184	2452	2455	2458	rVB2	232	133	0.02%	0.002%
67	9.344	2499	2505	2510	rBV2	284	415	0.07%	0.008%
68	9.412	2514	2526	2549	rBV	355303	605684	99.68%	11.137%
69	9.705	2606	2617	2626	rVB4	1193	2444	0.40%	0.045%
70	9.746	2626	2630	2631	rBV	195	162	0.03%	0.003%
71	9.785	2640	2642	2646	rBV	162	131	0.02%	0.002%
72	9.833	2651	2657	2661	rBV2	258	334	0.05%	0.006%
73	9.914	2678	2682	2685	rBV2	142	119	0.02%	0.002%
74	10.036	2717	2720	2725	rVB2	224	178	0.03%	0.003%
75	10.103	2739	2741	2742	rBV2	333	129	0.02%	0.002%
76	10.258	2785	2789	2791	rBV	347	292	0.05%	0.005%

LSC Area Percent Report

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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH5W3ME

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

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Title : VOC Analysis

77	10.441	2843	2846	2850	rBV2	249	196	0.03%	0.004%
78	10.531	2867	2874	2876	rBV2	336	344	0.06%	0.006%
79	10.753	2931	2943	2966	rBV	206702	345589	56.87%	6.355%
80	10.949	3000	3004	3009	rVB2	286	311	0.05%	0.006%
81	11.016	3020	3025	3027	rBV2	265	268	0.04%	0.005%
82	11.097	3047	3050	3054	rBV2	208	190	0.03%	0.003%
83	11.367	3131	3134	3137	rBV2	252	231	0.04%	0.004%
84	11.415	3142	3149	3151	rBV2	356	378	0.06%	0.007%
85	11.563	3192	3195	3197	rBV2	210	159	0.03%	0.003%
86	11.807	3260	3271	3295	rBV	339520	562136	92.51%	10.337%
87	12.190	3377	3390	3416	rBV	231218	391926	64.50%	7.207%
88	12.489	3479	3483	3487	rBV2	307	345	0.06%	0.006%
89	12.585	3511	3513	3514	rBV	249	130	0.02%	0.002%
90	12.865	3597	3600	3602	rBV	392	240	0.04%	0.004%
91	13.251	3717	3720	3721	rBV	191	122	0.02%	0.002%
92	13.698	3857	3859	3863	rBV2	234	135	0.02%	0.002%
93	13.849	3903	3906	3908	rVB	471	277	0.05%	0.005%
94	14.138	3991	3996	3999	rBV2	463	537	0.09%	0.010%
95	14.656	4155	4157	4161	rBV2	257	235	0.04%	0.004%
96	14.688	4165	4167	4170	rBV2	286	132	0.02%	0.002%
97	14.711	4171	4174	4179	rBV2	346	406	0.07%	0.007%
98	15.196	4323	4325	4327	rBV	369	163	0.03%	0.003%
99	15.486	4413	4415	4417	rBV	368	240	0.04%	0.004%
100	16.341	4679	4681	4682	rBV	470	187	0.03%	0.003%

Sum of corrected areas: 5438262

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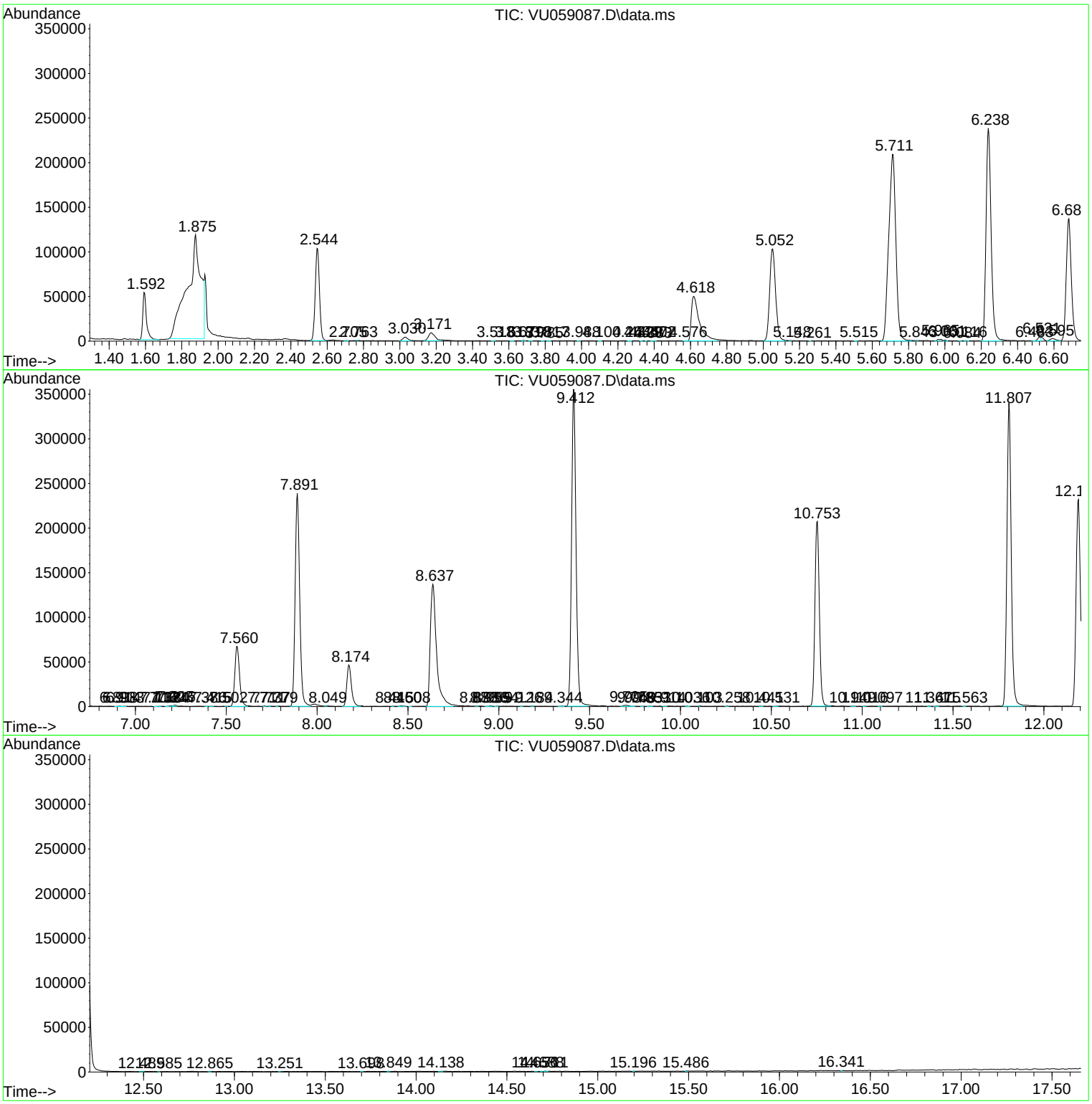
Instrument :
MSVOA_U
ClientSampleId :
BH5W3ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU053024\
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Sample : P2589-02ME
Misc : 5.89g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH5W3ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

No Library Search Compounds Detected
****

Tentatively Identified Compound (LSC) summary

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Misc : 5.89g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH5W3ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc