LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052924\
Data File : VU059071.D
Acq On : 29 May 2024 23:00
Operator : MD/SY
Sample : P2586-01ME
Misc : 4.19g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A4D14ME

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: VU059071.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.480	55	59	65	rVB3	2451	2494	0.36%	0.045%
2	1.512	65	69	78	rVB3	1516	1998	0.29%	0.036%
3	1.592	86	94	116	rVB	57084	82523	12.05%	1.480%
4	1.808	135	161	162	rBV7	54441	147755	21.58%	2.651%
5	2.541	377	389	404	rBV	114641	185546	27.10%	3.329%
6	2.628	408	416	428	rBV3	3430	6253	0.91%	0.112%
7	2.772	453	461	465	rBV3	854	1291	0.19%	0.023%
8	2.869	488	491	494	rBV2	293	233	0.03%	0.004%
9	2.940	502	513	529	rBV	21308	42111	6.15%	0.755%
10	3.030	534	541	549	rVV3	3644	5755	0.84%	0.103%
11	3.094	559	561	567	rVB2	253	203	0.03%	0.004%
12	3.174	572	586	603	rBV2	8929	22050	3.22%	0.396%
13	3.583	709	713	719	rBV2	401	570	0.08%	0.010%
14	3.917	815	817	823	rVB	250	224	0.03%	0.004%
15	3.946	823	826	830	rBV2	247	254	0.04%	0.005%
16	4.071	862	865	868	rVB2	268	204	0.03%	0.004%
17	4.113	874	878	887	rVV2	246	328	0.05%	0.006%
18	4.618	1024	1035	1080	rBV2	57897	181409	26.50%	3.254%
19	4.930	1129	1132	1136	rVB2	329	250	0.04%	0.004%
20	4.978	1143	1147	1151	rVB	325	257	0.04%	0.005%
21	5.052	1155	1170	1192	rBV	110355	250779	36.63%	4.499%
22	5.374	1268	1270	1274	rVB2	261	218	0.03%	0.004%
23	5.711	1355	1375	1403	rBV2	232557	627257	91.62%	11.253%
24	5.914	1433	1438	1441	rBV3	254	212	0.03%	0.004%
25	5.975	1449	1457	1464	rBV7	1470	2503	0.37%	0.045%
26	6.071	1484	1487	1493	rVB2	211	207	0.03%	0.004%
27	6.120	1499	1502	1507	rVB3	294	239	0.03%	0.004%
28	6.171	1515	1518	1522	rBV2	368	290	0.04%	0.005%
29	6.238	1525	1539	1567	rBV	269619	522833	76.37%	9.380%
30	6.531	1619	1630	1641	rVB6	5051	9092	1.33%	0.163%
31	6.599	1641	1651	1663	rBV6	1693	3608	0.53%	0.065%
32	6.682	1664	1677	1694	rBV	144124	290056	42.37%	5.204%
33	6.862	1727	1733	1737	rBV2	243	278	0.04%	0.005%
34	7.148	1818	1822	1826	rBV2	257	284	0.04%	0.005%
35	7.206	1832	1840	1841	rBV2	745	709	0.10%	0.013%
36	7.255	1850	1855	1858	rBV2	289	344	0.05%	0.006%

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Misc : 4.19g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A4D14ME

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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Peak separation: 5

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

37	7.271	1858	1860	1868	rVB2	332	337	0.05%	0.006%
38	7.560	1938	1950	1969	rBV2	69742	127606	18.64%	2.289%
39	7.692	1987	1991	1993	rBV2	323	217	0.03%	0.004%
40	7.791	2019	2022	2025	rBV	421	272	0.04%	0.005%
41	7.891	2041	2053	2075	rBV	253824	446500	65.22%	8.010%
42	8.062	2104	2106	2112	rVB2	274	210	0.03%	0.004%
43	8.177	2131	2142	2159	rBV2	46550	85747	12.52%	1.538%
44	8.283	2169	2175	2180	rVB2	177	200	0.03%	0.004%
45	8.460	2225	2230	2232	rBV2	300	288	0.04%	0.005%
46	8.553	2252	2259	2267	rVB5	1229	1679	0.25%	0.030%
47	8.637	2273	2285	2325	rBV	155510	371187	54.22%	6.659%
48	8.865	2353	2356	2358	rBV2	419	289	0.04%	0.005%
49	9.145	2438	2443	2446	rVB2	210	202	0.03%	0.004%
50	9.248	2469	2475	2480	rVB2	259	301	0.04%	0.005%
51	9.348	2500	2506	2508	rBV	324	339	0.05%	0.006%
52	9.412	2513	2526	2551	rBV	392176	684619	100.00%	12.282%
53	9.566	2571	2574	2575	rBV	338	212	0.03%	0.004%
54	9.701	2608	2616	2628	rVB5	1375	2467	0.36%	0.044%
55	9.891	2671	2675	2678	rBV2	210	196	0.03%	0.004%
56	9.939	2684	2690	2693	rBV2	356	423	0.06%	0.008%
57	10.026	2708	2717	2720	rBV2	329	535	0.08%	0.010%
58	10.110	2734	2743	2746	rBV3	666	827	0.12%	0.015%
59	10.193	2763	2769	2773	rBV2	208	220	0.03%	0.004%
60	10.232	2778	2781	2785	rVB2	294	241	0.04%	0.004%
61	10.676	2915	2919	2924	rBV2	185	226	0.03%	0.004%
62	10.753	2928	2943	2962	rBV	227869	376903	55.05%	6.762%
63	10.865	2976	2978	2982	rVV	361	309	0.05%	0.006%
64	10.897	2985	2988	2993	rBV3	424	432	0.06%	0.008%
65	11.090	3041	3048	3050	rBV2	379	414	0.06%	0.007%
66	11.110	3050	3054	3056	rBV3	393	364	0.05%	0.007%
67	11.158	3065	3069	3073	rVB2	245	235	0.03%	0.004%
68	11.299	3110	3113	3120	rVB2	241	248	0.04%	0.004%
69	11.412	3145	3148	3151	rBV2	529	315	0.05%	0.006%
70	11.489	3166	3172	3173	rBV3	482	486	0.07%	0.009%
71	11.547	3186	3190	3192	rVB2	426	264	0.04%	0.005%
72	11.807	3260	3271	3292	rVV	387090	629521	91.95%	11.294%
73	11.933	3307	3310	3314	rVB4	497	345	0.05%	0.006%
74	12.094	3357	3360	3363	rBV	532	399	0.06%	0.007%
75	12.190	3377	3390	3415	rBV	244431	417074	60.92%	7.482%
76	12.656	3531	3535	3538	rVB2	229	197	0.03%	0.004%

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Instrument :
MSVOA_U
ClientSampleId :
A4D14ME

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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Peak separation: 5

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

77	12.714	3550	3553	3555	rBV2	318	203	0.03%	0.004%
78	12.762	3566	3568	3570	rBV	336	199	0.03%	0.004%
79	12.923	3613	3618	3619	rBV2	1003	763	0.11%	0.014%
80	13.418	3768	3772	3773	rBV	299	199	0.03%	0.004%
81	13.434	3773	3777	3783	rVB4	638	732	0.11%	0.013%
82	13.608	3828	3831	3834	rBV2	345	286	0.04%	0.005%
83	13.624	3834	3836	3842	rVB2	761	583	0.09%	0.010%
84	13.656	3843	3846	3850	rBV2	390	335	0.05%	0.006%
85	13.872	3910	3913	3916	rBV	300	198	0.03%	0.004%
86	14.029	3959	3962	3964	rBV	387	240	0.04%	0.004%
87	14.309	4046	4049	4052	rVB2	304	202	0.03%	0.004%
88	14.331	4052	4056	4060	rVB3	497	438	0.06%	0.008%
89	14.357	4060	4064	4065	rBV	301	212	0.03%	0.004%
90	14.450	4089	4093	4098	rVB3	701	669	0.10%	0.012%
91	14.479	4098	4102	4103	rBV	306	226	0.03%	0.004%
92	14.553	4121	4125	4126	rBV2	336	202	0.03%	0.004%
93	14.962	4240	4252	4270	rBV2	12597	22408	3.27%	0.402%
94	15.167	4313	4316	4319	rBV2	406	256	0.04%	0.005%
95	15.434	4394	4399	4403	rBV4	676	717	0.10%	0.013%
96	15.962	4561	4563	4566	rBV3	494	255	0.04%	0.005%
97	16.235	4646	4648	4650	rBV2	401	201	0.03%	0.004%
98	16.264	4655	4657	4662	rVV3	533	363	0.05%	0.007%
99	16.653	4776	4778	4781	rBV2	687	387	0.06%	0.007%
100	16.759	4809	4811	4812	rBV2	816	411	0.06%	0.007%

Sum of corrected areas: 5574148

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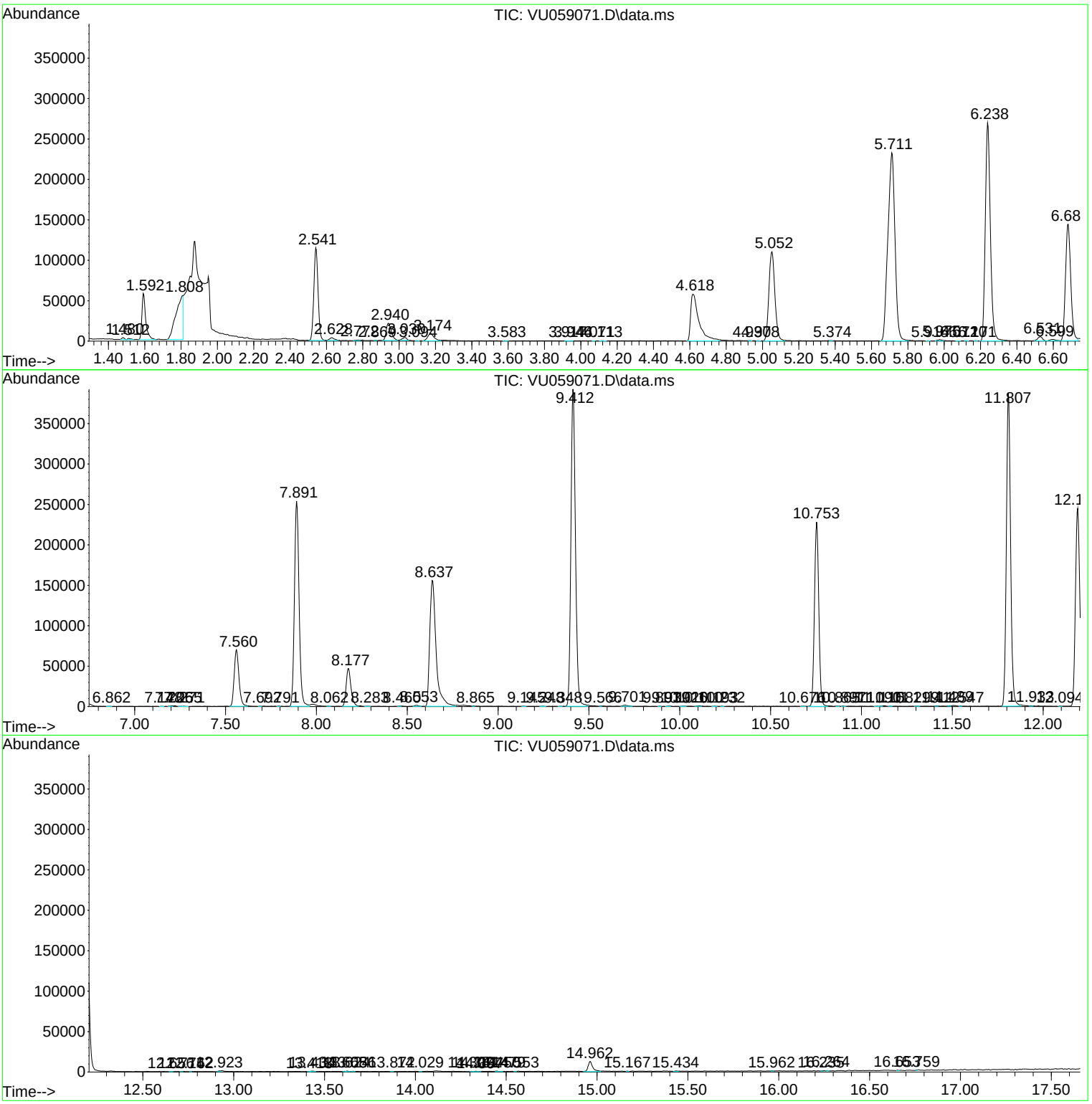
Instrument :
MSVOA_U
ClientSampleId :
A4D14ME

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\VU052924\
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ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A4D14ME

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

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052924\
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Instrument :
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ClientSampleId :
A4D14ME

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

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