LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052424\
Data File : VU058985.D
Acq On : 24 May 2024 21:02
Operator : MD/SY
Sample : P2568-14ME
Misc : 6.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH634ME

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\SFAMULM052324WMA.M
Title : VOC Analysis

Signal : TIC: VU058985.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	87	94	112	rVB	102972	122270	14.54%	2.087%
2	1.885	179	185	201	rVB	81845	114452	13.61%	1.953%
3	2.554	381	393	410	rBV	152713	244087	29.02%	4.165%
4	2.862	486	489	492	rBV2	167	106	0.01%	0.002%
5	3.033	532	542	558	rBV4	4140	7329	0.87%	0.125%
6	3.171	572	585	606	rVB	13791	31791	3.78%	0.543%
7	3.248	606	609	615	rBV	310	257	0.03%	0.004%
8	3.293	619	623	627	rBV2	249	218	0.03%	0.004%
9	3.431	662	666	669	rBV2	216	232	0.03%	0.004%
10	3.499	681	687	690	rBV2	356	242	0.03%	0.004%
11	3.637	727	730	733	rBV	238	171	0.02%	0.003%
12	3.685	742	745	751	rBV2	281	261	0.03%	0.004%
13	3.747	762	764	767	rBV2	111	60	0.01%	0.001%
14	3.776	770	773	776	rVV	283	182	0.02%	0.003%
15	3.811	779	784	785	rBV	279	170	0.02%	0.003%
16	3.837	789	792	795	rBV	148	112	0.01%	0.002%
17	4.036	852	854	856	rBV	121	63	0.01%	0.001%
18	4.078	862	867	872	rBV	190	235	0.03%	0.004%
19	4.120	875	880	884	rVB2	269	255	0.03%	0.004%
20	4.145	884	888	895	rVB	240	202	0.02%	0.003%
21	4.184	895	900	906	rBB2	261	348	0.04%	0.006%
22	4.216	906	910	912	rBV2	243	207	0.02%	0.004%
23	4.274	926	928	931	rBV	163	115	0.01%	0.002%
24	4.309	937	939	941	rBV2	127	79	0.01%	0.001%
25	4.406	966	969	972	rVB2	289	181	0.02%	0.003%
26	4.425	972	975	979	rBV	249	179	0.02%	0.003%
27	4.470	987	989	991	rBV	105	54	0.01%	0.001%
28	4.560	1014	1017	1018	rBV2	127	67	0.01%	0.001%
29	4.608	1022	1032	1059	rBV	95512	237126	28.19%	4.047%
30	5.052	1155	1170	1189	rBV	148600	331114	39.37%	5.650%
31	5.210	1216	1219	1220	rBV	200	122	0.01%	0.002%
32	5.245	1228	1230	1233	rBV2	165	99	0.01%	0.002%
33	5.312	1248	1251	1256	rVB	412	282	0.03%	0.005%
34	5.335	1256	1258	1262	rBV2	300	190	0.02%	0.003%
35	5.357	1262	1265	1268	rVB2	269	162	0.02%	0.003%
36	5.377	1268	1271	1275	rBV2	192	176	0.02%	0.003%

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Acq On : 24 May 2024 21:02
Operator : MD/SY
Sample : P2568-14ME
Misc : 6.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH634ME

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\SFAMULM052324WMA.M
Title : VOC Analysis

37	5.467	1295	1299	1301	rBV2	214	150	0.02%	0.003%
38	5.480	1301	1303	1306	rBV	209	161	0.02%	0.003%
39	5.592	1335	1338	1341	rBV	168	110	0.01%	0.002%
40	5.714	1356	1376	1401	rBV2	304434	841093	100.00%	14.353%
41	5.994	1460	1463	1464	rBV	170	89	0.01%	0.002%
42	6.017	1468	1470	1474	rVV2	238	157	0.02%	0.003%
43	6.036	1474	1476	1479	rVV2	173	101	0.01%	0.002%
44	6.052	1479	1481	1487	rVV2	191	193	0.02%	0.003%
45	6.132	1504	1506	1507	rBV	48	17	0.00%	0.000%
46	6.155	1507	1513	1519	rVB2	333	336	0.04%	0.006%
47	6.184	1519	1522	1526	rBV	160	130	0.02%	0.002%
48	6.242	1527	1540	1560	rBV	201084	393661	46.80%	6.718%
49	6.444	1601	1603	1604	rBV	313	142	0.02%	0.002%
50	6.473	1609	1612	1614	rBV2	149	106	0.01%	0.002%
51	6.531	1620	1630	1642	rVB9	6211	12311	1.46%	0.210%
52	6.589	1642	1648	1650	rBV2	384	392	0.05%	0.007%
53	6.624	1656	1659	1661	rBV	235	146	0.02%	0.002%
54	6.682	1663	1677	1698	rVV	197281	387859	46.11%	6.619%
55	6.840	1724	1726	1730	rBV2	126	92	0.01%	0.002%
56	6.878	1735	1738	1743	rVB2	306	251	0.03%	0.004%
57	7.023	1777	1783	1784	rBV2	150	139	0.02%	0.002%
58	7.190	1831	1835	1837	rBV3	391	307	0.04%	0.005%
59	7.232	1842	1848	1849	rBV2	258	206	0.02%	0.004%
60	7.271	1858	1860	1863	rVB2	208	102	0.01%	0.002%
61	7.293	1863	1867	1871	rBV2	227	195	0.02%	0.003%
62	7.332	1876	1879	1881	rVV	216	167	0.02%	0.003%
63	7.361	1885	1888	1894	rBV2	141	141	0.02%	0.002%
64	7.390	1894	1897	1899	rBV	80	55	0.01%	0.001%
65	7.463	1915	1920	1925	rBV2	324	310	0.04%	0.005%
66	7.515	1932	1936	1938	rBV2	284	229	0.03%	0.004%
67	7.560	1939	1950	1970	rVV	93568	166491	19.79%	2.841%
68	7.711	1995	1997	1998	rBV	332	101	0.01%	0.002%
69	7.772	2012	2016	2018	rBV3	357	306	0.04%	0.005%
70	7.891	2040	2053	2078	rBV	324221	564019	67.06%	9.625%
71	8.116	2117	2123	2129	rVB3	482	530	0.06%	0.009%
72	8.174	2130	2141	2161	rBV	67413	113957	13.55%	1.945%
73	8.299	2177	2180	2182	rBV	129	67	0.01%	0.001%
74	8.338	2190	2192	2194	rBV	178	63	0.01%	0.001%
75	8.425	2217	2219	2221	rBV	172	99	0.01%	0.002%
76	8.473	2225	2234	2239	rVB3	557	1016	0.12%	0.017%

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Operator : MD/SY
Sample : P2568-14ME
Misc : 6.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BH634ME

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\SFAMULM052324WMA.M
Title : VOC Analysis

77	8.499	2239	2242	2244	rBV	124	78	0.01%	0.001%
78	8.518	2245	2248	2254	rVB	317	262	0.03%	0.004%
79	8.560	2254	2261	2263	rBV2	304	298	0.04%	0.005%
80	8.627	2271	2282	2326	rBV	251040	481246	57.22%	8.212%
81	8.917	2363	2372	2374	rBV2	615	587	0.07%	0.010%
82	9.116	2432	2434	2437	rBV2	226	108	0.01%	0.002%
83	9.412	2514	2526	2547	rBV	287979	481687	57.27%	8.220%
84	9.788	2640	2643	2645	rBV	350	216	0.03%	0.004%
85	10.016	2711	2714	2717	rBV2	176	107	0.01%	0.002%
86	10.550	2876	2880	2885	rBV	343	323	0.04%	0.006%
87	10.586	2889	2891	2894	rVV	154	85	0.01%	0.001%
88	10.618	2897	2901	2905	rBV	388	290	0.03%	0.005%
89	10.750	2929	2942	2961	rBV	281814	458968	54.57%	7.832%
90	10.865	2975	2978	2980	rBV2	343	190	0.02%	0.003%
91	10.933	2996	2999	3002	rBV	433	250	0.03%	0.004%
92	11.245	3093	3096	3099	rBV	195	164	0.02%	0.003%
93	11.476	3166	3168	3170	rBV2	206	81	0.01%	0.001%
94	11.756	3250	3255	3259	rBV	374	374	0.04%	0.006%
95	11.807	3259	3271	3288	rBV	241514	391788	46.58%	6.686%
96	12.007	3330	3333	3335	rBV	370	259	0.03%	0.004%
97	12.187	3377	3389	3409	rBV	273464	463111	55.06%	7.903%
98	12.373	3444	3447	3453	rBV2	439	332	0.04%	0.006%

Sum of corrected areas: 5859997

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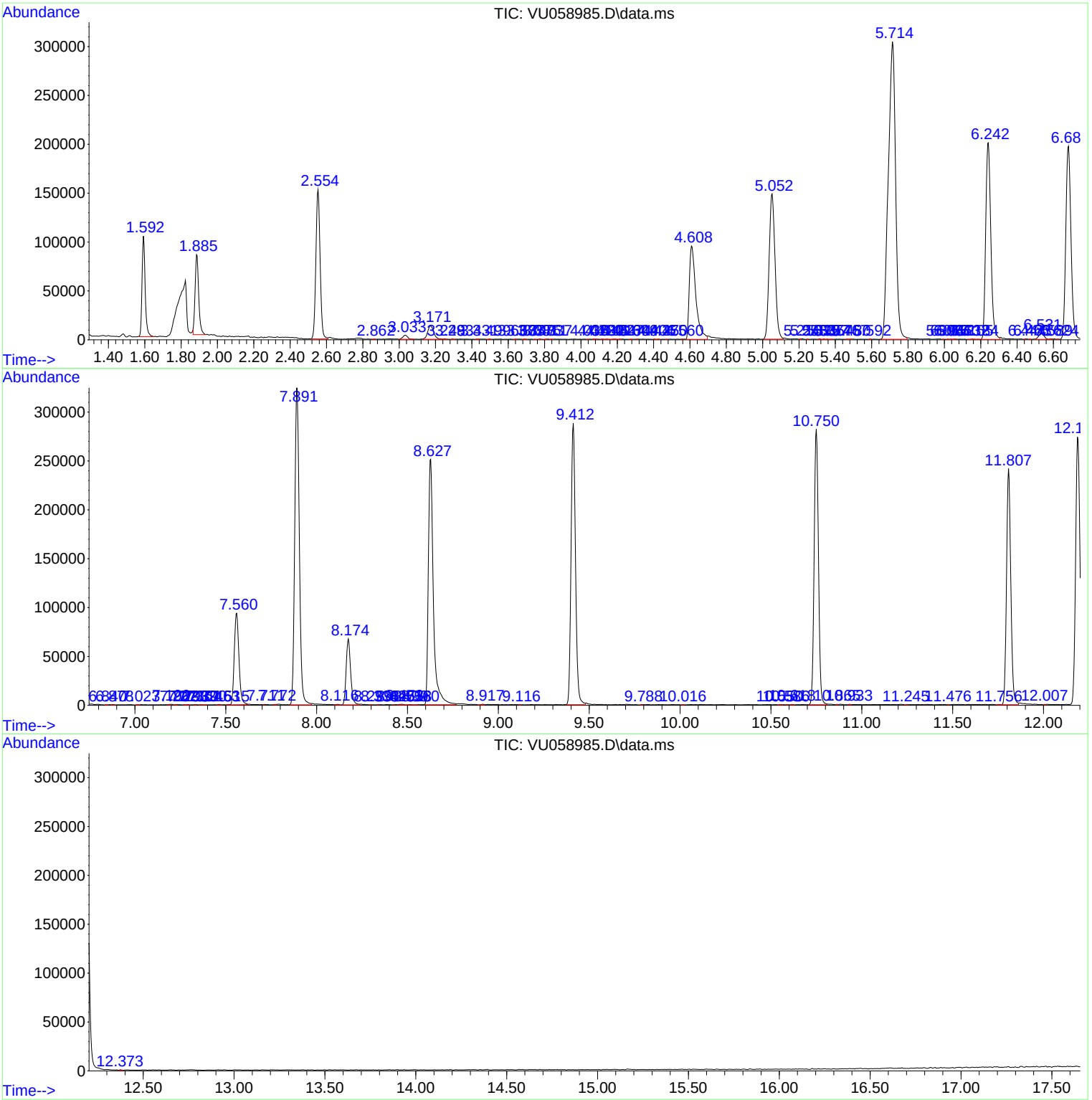
Sample : P2568-14ME
Misc : 6.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH634ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052324WMA.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\VU052424\
Data File : VU058985.D
Acq On : 24 May 2024 21:02
Operator : MD/SY
Sample : P2568-14ME
Misc : 6.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH634ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052324WMA.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\VU052424\
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Misc : 6.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
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Instrument :
MSVOA_U
ClientSampleId :
BH634ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052324WMA.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