LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072824\
Data File : VX042631.D
Acq On : 27 Jul 2024 04:08
Operator : JC/MD
Sample : P3344-09ME
Misc : 5.03g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 41 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BHB25ME

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_X\Method\SFAMXLM072624WMA.M
Title : VOC Analysis

Signal : TIC: VX042631.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	26	29	37	rVB2	8711	9807	2.25%	0.317%
2	1.374	43	47	63	rBV2	29836	78783	18.11%	2.545%
3	2.282	190	196	211	rBV	57027	105158	24.17%	3.397%
4	2.715	259	267	273	rBV2	2730	6114	1.41%	0.198%
5	2.941	299	304	312	rVB2	3480	8028	1.85%	0.259%
6	3.081	318	327	335	rBV2	9285	17786	4.09%	0.575%
7	3.313	363	365	368	rVB2	149	172	0.04%	0.006%
8	3.349	368	371	373	rBB	201	223	0.05%	0.007%
9	3.373	373	375	380	rBB	177	252	0.06%	0.008%
10	3.422	380	383	387	rBB2	192	306	0.07%	0.010%
11	3.483	391	393	395	rBV	217	233	0.05%	0.008%
12	3.630	415	417	418	rVB	298	168	0.04%	0.005%
13	3.867	454	456	459	rVB	336	264	0.06%	0.009%
14	3.995	474	477	479	rBV	233	307	0.07%	0.010%
15	4.056	486	487	491	rBV	215	238	0.05%	0.008%
16	4.105	491	495	497	rVV2	227	271	0.06%	0.009%
17	4.160	501	504	507	rBV	214	337	0.08%	0.011%
18	4.489	548	558	572	rBV	16640	59796	13.74%	1.932%
19	4.959	634	635	637	rBV	226	148	0.03%	0.005%
20	5.050	640	650	665	rVV	45269	139295	32.02%	4.500%
21	5.239	680	681	684	rVB	229	205	0.05%	0.007%
22	5.379	703	704	706	rBV	326	278	0.06%	0.009%
23	5.446	713	715	718	rBV	260	293	0.07%	0.009%
24	5.751	763	765	766	rBV	153	143	0.03%	0.005%
25	5.964	789	800	814	rBV2	120603	347364	79.84%	11.222%
26	6.263	847	849	850	rBV	247	206	0.05%	0.007%
27	6.330	858	860	863	rBV	266	253	0.06%	0.008%
28	6.452	878	880	883	rBV	169	215	0.05%	0.007%
29	6.757	921	930	946	rBV	156085	378802	87.07%	12.238%
30	7.220	1003	1006	1010	rVB2	517	700	0.16%	0.023%
31	7.306	1012	1020	1029	rBV	67749	151343	34.79%	4.889%
32	7.501	1050	1052	1054	rBB	320	252	0.06%	0.008%
33	7.525	1054	1056	1061	rBB2	160	293	0.07%	0.009%
34	7.592	1064	1067	1069	rBV	227	319	0.07%	0.010%
35	7.690	1081	1083	1084	rBB	258	145	0.03%	0.005%
36	7.714	1084	1087	1088	rBB	214	169	0.04%	0.005%

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Instrument :
MSVOA_X
ClientSampleId :
BHB25ME

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_X\Method\SFAMXLM072624WMA.M
Title : VOC Analysis

37	7.745	1090	1092	1093	rVV	255	184	0.04%	0.006%
38	7.824	1102	1105	1107	rVV	151	176	0.04%	0.006%
39	7.848	1107	1109	1114	rVB	190	205	0.05%	0.007%
40	7.964	1126	1128	1131	rBV	211	176	0.04%	0.006%
41	8.049	1141	1142	1146	rVB	180	193	0.04%	0.006%
42	8.092	1147	1149	1151	rBV	257	179	0.04%	0.006%
43	8.324	1182	1187	1198	rBV2	34561	61779	14.20%	1.996%
44	8.647	1234	1240	1248	rBV	177723	277603	63.81%	8.968%
45	8.872	1275	1277	1280	rBV2	343	330	0.08%	0.011%
46	8.952	1285	1290	1299	rBV2	23782	39506	9.08%	1.276%
47	9.092	1311	1313	1315	rBV2	189	150	0.03%	0.005%
48	9.129	1318	1319	1321	rVV	226	133	0.03%	0.004%
49	9.153	1321	1323	1328	rVB2	530	632	0.15%	0.020%
50	9.196	1328	1330	1331	rBV	198	168	0.04%	0.005%
51	9.244	1334	1338	1339	rBV	206	270	0.06%	0.009%
52	9.275	1339	1343	1346	rVB3	1667	1954	0.45%	0.063%
53	9.391	1357	1362	1377	rBV	64460	136887	31.46%	4.422%
54	9.763	1419	1423	1426	rVB	962	1543	0.35%	0.050%
55	9.824	1432	1433	1434	rBV	371	225	0.05%	0.007%
56	10.013	1460	1464	1465	rBV2	1051	1254	0.29%	0.041%
57	10.055	1465	1471	1487	rVB	306390	435066	100.00%	14.055%
58	10.305	1509	1512	1519	rVB2	904	1227	0.28%	0.040%
59	10.482	1539	1541	1543	rVB2	161	165	0.04%	0.005%
60	10.555	1551	1553	1555	rBV	206	245	0.06%	0.008%
61	10.653	1564	1569	1572	rBV2	371	674	0.15%	0.022%
62	10.744	1582	1584	1588	rBV	196	261	0.06%	0.008%
63	10.787	1588	1591	1592	rVB	206	184	0.04%	0.006%
64	10.927	1612	1614	1616	rBV	199	218	0.05%	0.007%
65	11.018	1626	1629	1634	rBV	348	541	0.12%	0.017%
66	11.153	1649	1651	1652	rBV	223	134	0.03%	0.004%
67	11.195	1652	1658	1666	rBV	117799	164354	37.78%	5.310%
68	11.311	1674	1677	1678	rBV2	247	211	0.05%	0.007%
69	11.457	1699	1701	1703	rBV	251	217	0.05%	0.007%
70	11.646	1730	1732	1734	rBV	225	259	0.06%	0.008%
71	11.732	1744	1746	1747	rBV	210	173	0.04%	0.006%
72	11.805	1755	1758	1761	rBV3	309	434	0.10%	0.014%
73	11.927	1777	1778	1781	rBV	225	230	0.05%	0.007%
74	11.976	1783	1786	1788	rBB	410	355	0.08%	0.011%
75	12.024	1788	1794	1802	rBV	285273	380753	87.52%	12.301%
76	12.189	1820	1821	1822	rBV	253	131	0.03%	0.004%

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Instrument : MSVOA_X
ClientSampleId : BHB25ME

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_X\Method\SFAMXLM072624WMA.M
Title : VOC Analysis

77	12.238	1828	1829	1830	rBV	314	181	0.04%	0.006%
78	12.317	1837	1842	1851	rBV	178750	229410	52.73%	7.411%
79	12.701	1903	1905	1908	rBV	263	260	0.06%	0.008%
80	12.744	1908	1912	1913	rBV	222	206	0.05%	0.007%
81	12.902	1936	1938	1940	rBV2	254	314	0.07%	0.010%
82	12.975	1948	1950	1952	rBV2	161	163	0.04%	0.005%
83	13.079	1966	1967	1970	rBV2	227	241	0.06%	0.008%
84	13.311	2002	2005	2008	rBB	187	226	0.05%	0.007%
85	13.353	2008	2012	2013	rBV2	216	341	0.08%	0.011%
86	13.512	2036	2038	2040	rBV2	267	266	0.06%	0.009%
87	13.561	2044	2046	2048	rBB2	187	155	0.04%	0.005%
88	13.585	2048	2050	2051	rBV2	173	152	0.03%	0.005%
89	13.737	2073	2075	2076	rBV	187	141	0.03%	0.005%
90	13.762	2077	2079	2082	rVV	191	196	0.05%	0.006%
91	13.878	2095	2098	2100	rBV	274	281	0.06%	0.009%
92	14.061	2125	2128	2131	rBV	170	318	0.07%	0.010%
93	14.128	2136	2139	2141	rBV2	406	475	0.11%	0.015%
94	14.378	2178	2180	2182	rBV	197	183	0.04%	0.006%
95	14.432	2185	2189	2193	rVV5	1321	1958	0.45%	0.063%
96	14.664	2224	2227	2228	rBV	315	363	0.08%	0.012%
97	15.060	2288	2292	2294	rBV3	400	636	0.15%	0.021%
98	15.195	2312	2314	2316	rBV2	260	229	0.05%	0.007%
99	15.231	2316	2320	2325	rVV5	6157	9199	2.11%	0.297%
100	16.091	2455	2461	2468	rVB	20011	31439	7.23%	1.016%

Sum of corrected areas: 3095378

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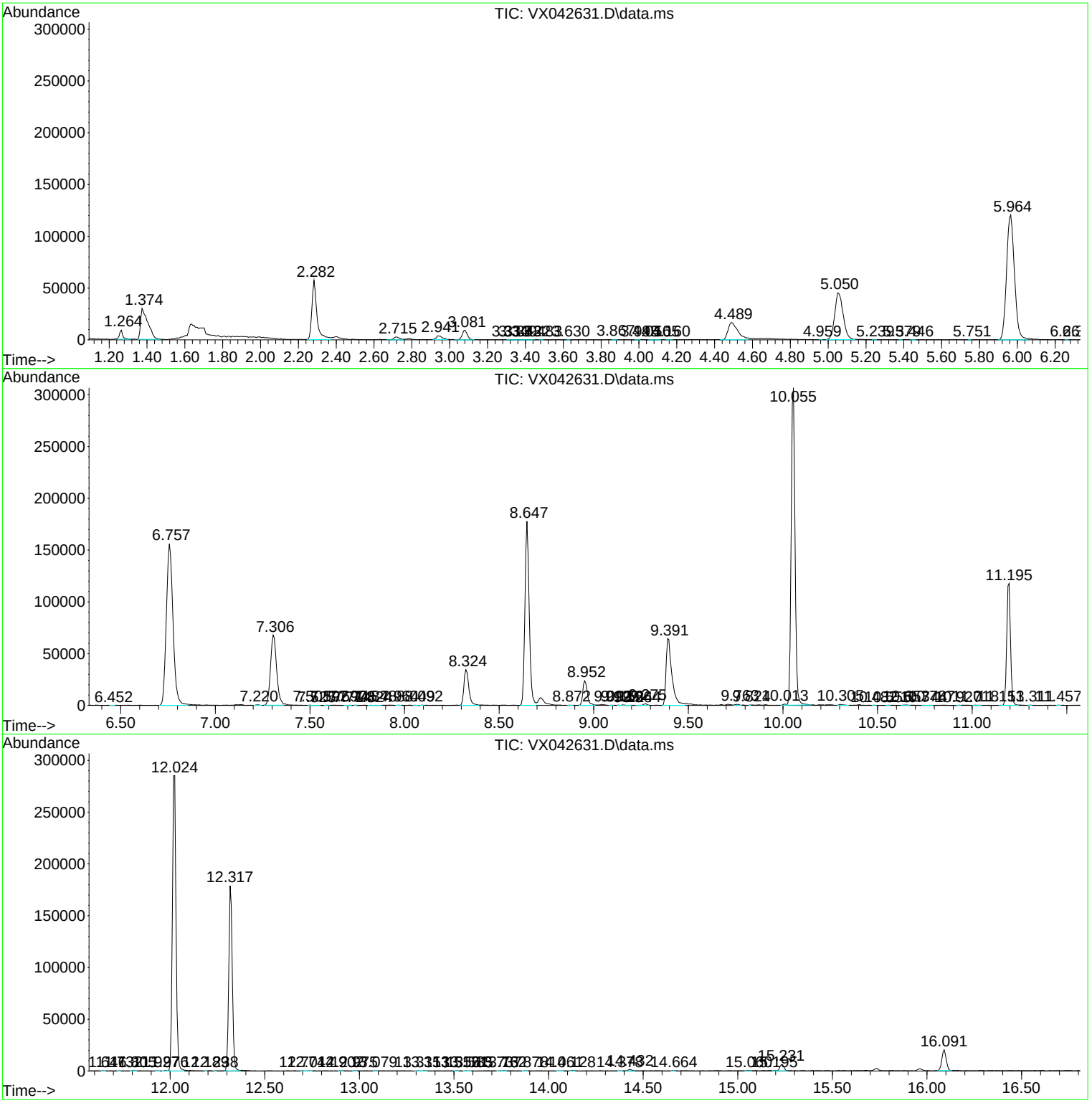
Instrument :
MSVOA_X
ClientSampleId :
BHB25ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM072624WMA.M
Quant Title : VOC Analysis

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



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MSVOA_X
ClientSampleId :
BHB25ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM072624WMA.M
Quant Title : VOC Analysis

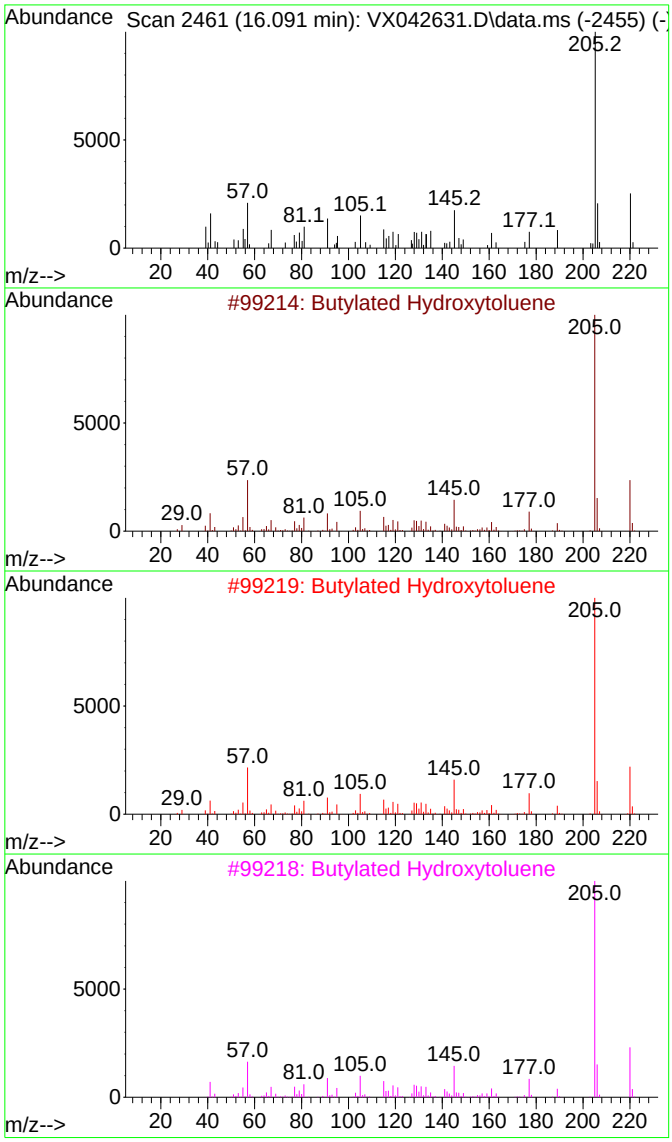
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

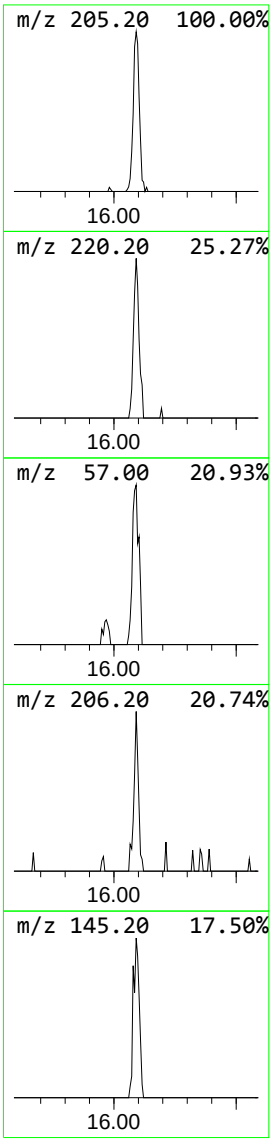
****

Peak Number 2 Butylated Hydroxytoluene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.091	4.13 ug/L	31439	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	94
2	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	91
3	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	91
4	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	90
5	Ethyl 4-oxo-2-phenylpentanoate	220	C13H16O3	1000427-11-2	87





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM072624WMA.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
Butylated Hydro...	16.091	4.1	ug/L	31439	3	12.024	380753	50.0