LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120721\
Data File : VX025567.D
Acq On : 07 Dec 2021 10:11
Operator : JC/MD
Sample : VX1207MBL01
Misc : 5.0g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK643

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\SFAMXLM112221WMA.M
Title : VOC Analysis

Signal : TIC: VX025567.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.368	42	46	54	rVB	95023	90651	16.19%	2.147%
2	1.666	91	95	105	rVB	64237	84234	15.05%	1.995%
3	2.306	194	200	214	rVB	132547	215710	38.54%	5.109%
4	2.782	276	278	282	rBV3	426	665	0.12%	0.016%
5	2.873	291	293	295	rBV2	145	121	0.02%	0.003%
6	3.160	338	340	341	rBV	73	73	0.01%	0.002%
7	3.197	345	346	347	rBV	153	72	0.01%	0.002%
8	3.654	419	421	423	rBV	106	93	0.02%	0.002%
9	3.928	464	466	467	rVB	148	101	0.02%	0.002%
10	4.044	483	485	487	rBB	122	71	0.01%	0.002%
11	4.306	524	528	529	rBV2	96	119	0.02%	0.003%
12	4.452	543	552	568	rVV	41956	117191	20.94%	2.776%
13	4.824	611	613	614	rBV	135	98	0.02%	0.002%
14	4.928	628	630	632	rBV2	125	95	0.02%	0.002%
15	5.056	639	651	668	rBV	71022	220494	39.39%	5.222%
16	5.221	676	678	680	rBV2	148	172	0.03%	0.004%
17	5.379	702	704	705	rBV	203	116	0.02%	0.003%
18	5.531	727	729	730	rBV	132	75	0.01%	0.002%
19	5.769	766	768	771	rVB2	117	94	0.02%	0.002%
20	5.970	788	801	819	rBV2	188922	559773	100.00%	13.258%
21	6.245	845	846	850	rVB	116	113	0.02%	0.003%
22	6.281	850	852	853	rBV	150	123	0.02%	0.003%
23	6.428	874	876	878	rBV	117	72	0.01%	0.002%
24	6.757	921	930	942	rBV	133927	318084	56.82%	7.534%
25	6.921	956	957	961	rBV2	160	171	0.03%	0.004%
26	6.952	961	962	965	rVB	138	99	0.02%	0.002%
27	7.104	982	987	994	rBV4	1650	3617	0.65%	0.086%
28	7.208	1002	1004	1006	rBV	74	73	0.01%	0.002%
29	7.306	1012	1020	1032	rBV	111548	246317	44.00%	5.834%
30	7.476	1043	1048	1053	rVB2	331	566	0.10%	0.013%
31	7.513	1053	1054	1057	rBV	121	103	0.02%	0.002%
32	7.677	1080	1081	1082	rBV	127	76	0.01%	0.002%
33	7.696	1082	1084	1085	rVV	121	93	0.02%	0.002%
34	7.775	1095	1097	1098	rBV	128	96	0.02%	0.002%
35	7.915	1118	1120	1126	rVB2	149	250	0.04%	0.006%
36	8.025	1136	1138	1139	rVB	133	76	0.01%	0.002%

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Instrument :
MSVOA_X
ClientSampleId :
VBLK643

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_X\Method\SFAMXLM112221WMA.M
Title : VOC Analysis

37	8.135	1155	1156	1159	rVB	134	87	0.02%	0.002%
38	8.220	1167	1170	1171	rBV	111	94	0.02%	0.002%
39	8.244	1172	1174	1176	rVB	163	86	0.02%	0.002%
40	8.275	1178	1179	1180	rBV	213	107	0.02%	0.003%
41	8.324	1180	1187	1200	rBV	80862	128146	22.89%	3.035%
42	8.464	1208	1210	1213	rBV2	184	220	0.04%	0.005%
43	8.647	1234	1240	1248	rBV	300704	471483	84.23%	11.167%
44	8.720	1248	1252	1258	rVB	4390	6313	1.13%	0.150%
45	8.866	1274	1276	1277	rBV	137	80	0.01%	0.002%
46	8.952	1284	1290	1298	rBV	54426	79138	14.14%	1.874%
47	9.238	1335	1337	1339	rBV2	89	75	0.01%	0.002%
48	9.293	1344	1346	1347	rVB	162	80	0.01%	0.002%
49	9.384	1355	1361	1376	rBV	187467	259962	46.44%	6.157%
50	9.866	1439	1440	1443	rBV	133	131	0.02%	0.003%
51	9.890	1443	1444	1447	rVV2	99	77	0.01%	0.002%
52	9.951	1452	1454	1456	rBV	150	140	0.03%	0.003%
53	10.055	1465	1471	1486	rBV	280802	378109	67.55%	8.955%
54	10.189	1491	1493	1496	rVB	351	388	0.07%	0.009%
55	10.220	1496	1498	1500	rVB	221	206	0.04%	0.005%
56	10.238	1500	1501	1504	rBV2	299	299	0.05%	0.007%
57	10.305	1508	1512	1516	rVB2	489	623	0.11%	0.015%
58	10.811	1593	1595	1597	rBV	100	93	0.02%	0.002%
59	10.957	1618	1619	1624	rVB2	162	169	0.03%	0.004%
60	11.122	1642	1646	1652	rVB2	2428	3097	0.55%	0.073%
61	11.195	1652	1658	1665	rBV	196829	260453	46.53%	6.169%
62	11.274	1669	1671	1679	rVV4	482	1288	0.23%	0.031%
63	11.451	1698	1700	1702	rBV	262	274	0.05%	0.006%
64	11.482	1702	1705	1711	rVB3	557	887	0.16%	0.021%
65	11.549	1713	1716	1719	rVB3	253	281	0.05%	0.007%
66	11.616	1725	1727	1729	rVB	175	138	0.02%	0.003%
67	11.750	1745	1749	1754	rBV3	1776	2378	0.42%	0.056%
68	11.841	1760	1764	1770	rVB3	322	401	0.07%	0.009%
69	11.890	1770	1772	1775	rBV2	97	119	0.02%	0.003%
70	11.933	1775	1779	1783	rVV2	960	1196	0.21%	0.028%
71	11.975	1784	1786	1789	rVV	316	339	0.06%	0.008%
72	12.024	1789	1794	1804	rVV	286815	356549	63.70%	8.445%
73	12.128	1808	1811	1812	rVV2	826	1058	0.19%	0.025%
74	12.152	1812	1815	1821	rVB3	1717	2411	0.43%	0.057%
75	12.201	1821	1823	1824	rBV	186	136	0.02%	0.003%
76	12.219	1824	1826	1829	rBV	89	135	0.02%	0.003%

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ALS Vial : 3 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : VBLK643

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_X\Method\SFAMXLM112221WMA.M
Title : VOC Analysis

77	12.323	1835	1843	1849	rBV	307302	400772	71.60%	9.492%
78	12.427	1858	1860	1864	rVB3	551	608	0.11%	0.014%
79	12.469	1864	1867	1868	rBV2	177	185	0.03%	0.004%
80	12.585	1884	1886	1890	rBV	94	122	0.02%	0.003%
81	12.664	1896	1899	1903	rBV2	218	287	0.05%	0.007%
82	12.768	1914	1916	1918	rBV	162	131	0.02%	0.003%
83	12.963	1947	1948	1950	rBV	137	78	0.01%	0.002%
84	13.030	1957	1959	1961	rBV2	127	108	0.02%	0.003%
85	13.055	1961	1963	1965	rVV	191	166	0.03%	0.004%
86	13.372	2013	2015	2020	rBV2	92	139	0.02%	0.003%
87	13.567	2046	2047	2049	rBV	122	125	0.02%	0.003%
88	13.591	2049	2051	2053	rVB	406	335	0.06%	0.008%
89	13.786	2079	2083	2085	rVB2	275	284	0.05%	0.007%
90	13.871	2095	2097	2101	rBV2	114	168	0.03%	0.004%
91	13.957	2109	2111	2114	rBV3	282	332	0.06%	0.008%
92	14.256	2158	2160	2164	rVB2	115	110	0.02%	0.003%
93	14.469	2193	2195	2196	rVB	157	98	0.02%	0.002%
94	14.493	2196	2199	2200	rBV2	158	181	0.03%	0.004%
95	14.920	2267	2269	2271	rBV2	162	147	0.03%	0.003%
96	15.018	2283	2285	2287	rBV	171	131	0.02%	0.003%
97	15.475	2358	2360	2362	rBV2	175	189	0.03%	0.004%
98	16.523	2530	2532	2534	rBV	181	145	0.03%	0.003%
99	16.566	2537	2539	2540	rBV	150	83	0.01%	0.002%
100	16.603	2543	2545	2548	rBV	174	136	0.02%	0.003%

Sum of corrected areas: 4222253

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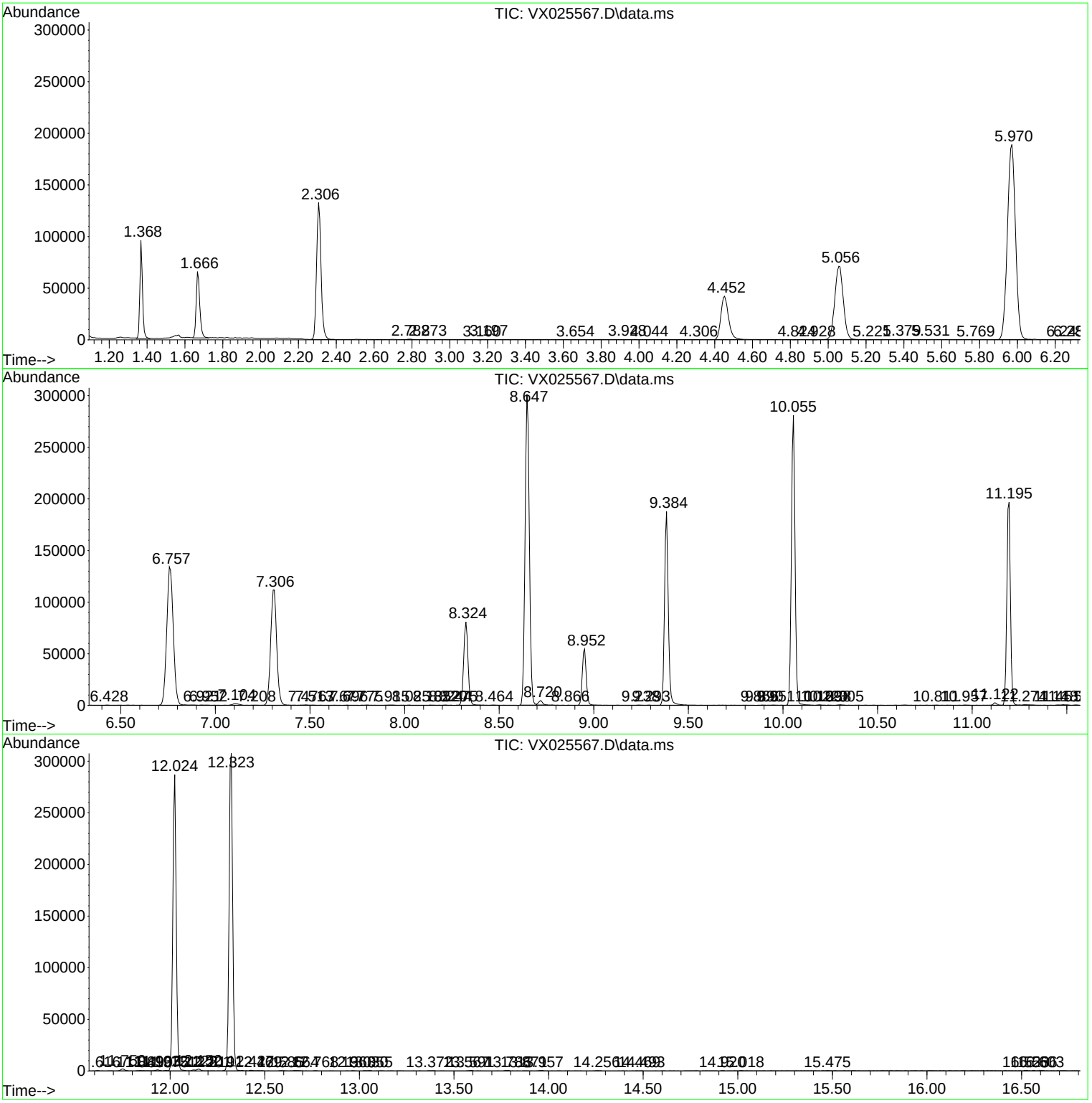
Instrument :
MSVOA_X
ClientSampleId :
VBLK643

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.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_X\Data\VX120721\
Data File : VX025567.D
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Misc : 5.0g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK643

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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

No Library Search Compounds Detected

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Tentatively Identified Compound (LSC) summary

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Instrument :
MSVOA_X
ClientSampleId :
VBLK643

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.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