LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
Data File : VX025639.D
Acq On : 08 Dec 2021 22:59
Operator : JC/MD
Sample : M4975-04
Misc : 6.99g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGKS8

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: VX025639.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.239	23	25	32	rBV2	3452	4950	0.99%	0.127%
2	1.368	43	46	57	rVB	55365	65473	13.07%	1.677%
3	1.471	61	63	67	rBV2	470	421	0.08%	0.011%
4	1.648	88	92	97	rBV	35938	40234	8.03%	1.030%
5	2.282	190	196	207	rBV	101892	165827	33.10%	4.247%
6	2.562	240	242	246	rBV	391	661	0.13%	0.017%
7	2.642	252	255	257	rBV	378	419	0.08%	0.011%
8	2.782	274	278	284	rBV4	896	2018	0.40%	0.052%
9	2.886	292	295	297	rBV2	305	438	0.09%	0.011%
10	2.953	299	306	314	rVV	5999	15207	3.04%	0.389%
11	3.178	340	343	344	rBV	290	241	0.05%	0.006%
12	3.221	348	350	353	rVV	255	256	0.05%	0.007%
13	3.361	371	373	375	rVB	360	242	0.05%	0.006%
14	3.416	380	382	383	rBV	287	254	0.05%	0.007%
15	3.605	411	413	417	rVB	451	438	0.09%	0.011%
16	4.087	490	492	493	rBV	322	286	0.06%	0.007%
17	4.172	504	506	509	rBV	402	530	0.11%	0.014%
18	4.221	513	514	517	rBV	267	287	0.06%	0.007%
19	4.269	519	522	524	rBV	285	370	0.07%	0.009%
20	4.489	549	558	588	rBV	22260	105251	21.01%	2.695%
21	5.068	641	653	668	rBV	59311	197575	39.44%	5.060%
22	5.214	675	677	680	rBV	346	379	0.08%	0.010%
23	5.495	721	723	725	rBV	328	251	0.05%	0.006%
24	5.605	739	741	744	rVB	410	402	0.08%	0.010%
25	5.690	753	755	758	rVB	388	376	0.08%	0.010%
26	5.733	760	762	764	rBV	301	267	0.05%	0.007%
27	5.848	780	781	784	rBV2	350	341	0.07%	0.009%
28	5.970	789	801	818	rVV2	172521	500981	100.00%	12.830%
29	6.361	860	865	866	rBV	1883	2603	0.52%	0.067%
30	6.489	884	886	888	rVB	429	389	0.08%	0.010%
31	6.513	888	890	891	rBV	346	323	0.06%	0.008%
32	6.647	911	912	915	rBV	422	358	0.07%	0.009%
33	6.763	921	931	947	rBV	129087	334488	66.77%	8.566%
34	7.110	982	988	995	rBV4	2109	4925	0.98%	0.126%
35	7.220	1000	1006	1009	rBV5	1061	2216	0.44%	0.057%
36	7.312	1014	1021	1033	rVB	95702	220624	44.04%	5.650%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
Data File : VX025639.D
Acq On : 08 Dec 2021 22:59
Operator : JC/MD
Sample : M4975-04
Misc : 6.99g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGKS8

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

37	7.635	1071	1074	1075	rBV	378	356	0.07%	0.009%
38	7.665	1077	1079	1082	rVB	224	247	0.05%	0.006%
39	7.696	1082	1084	1086	rBV	315	257	0.05%	0.007%
40	7.818	1101	1104	1106	rBV2	319	313	0.06%	0.008%
41	7.921	1119	1121	1124	rBV2	448	392	0.08%	0.010%
42	8.007	1133	1135	1138	rVB	377	349	0.07%	0.009%
43	8.061	1141	1144	1146	rBV2	292	413	0.08%	0.011%
44	8.232	1170	1172	1175	rBV2	209	257	0.05%	0.007%
45	8.330	1181	1188	1198	rBV	57672	102291	20.42%	2.620%
46	8.653	1232	1241	1249	rBV	246931	415530	82.94%	10.642%
47	8.720	1249	1252	1256	rVB2	2752	4033	0.81%	0.103%
48	8.866	1274	1276	1279	rVB	333	387	0.08%	0.010%
49	8.897	1279	1281	1283	rBV2	306	316	0.06%	0.008%
50	8.958	1285	1291	1301	rVV	36649	63556	12.69%	1.628%
51	9.067	1305	1309	1310	rVV	297	347	0.07%	0.009%
52	9.104	1314	1315	1318	rBV	343	296	0.06%	0.008%
53	9.275	1339	1343	1349	rVB2	6281	9193	1.83%	0.235%
54	9.323	1349	1351	1353	rBV	226	248	0.05%	0.006%
55	9.397	1357	1363	1376	rBV	132925	223302	44.57%	5.719%
56	9.714	1412	1415	1420	rBV2	1103	1570	0.31%	0.040%
57	9.762	1420	1423	1428	rBV	324	542	0.11%	0.014%
58	9.890	1442	1444	1446	rVB	327	246	0.05%	0.006%
59	10.061	1466	1472	1479	rBV	260507	392161	78.28%	10.043%
60	10.159	1486	1488	1491	rBV2	316	309	0.06%	0.008%
61	10.305	1510	1512	1517	rVB	505	603	0.12%	0.015%
62	10.470	1537	1539	1541	rBV	347	382	0.08%	0.010%
63	10.665	1570	1571	1573	rBV	339	254	0.05%	0.007%
64	10.787	1588	1591	1594	rBV2	195	263	0.05%	0.007%
65	10.921	1611	1613	1615	rVB	312	264	0.05%	0.007%
66	10.969	1620	1621	1623	rBV	356	295	0.06%	0.008%
67	11.128	1639	1647	1651	rBV3	1492	2764	0.55%	0.071%
68	11.195	1653	1658	1665	rVV	179565	236766	47.26%	6.063%
69	11.280	1668	1672	1673	rBV2	271	351	0.07%	0.009%
70	11.482	1701	1705	1708	rVV3	449	582	0.12%	0.015%
71	11.555	1715	1717	1719	rVV	301	296	0.06%	0.008%
72	11.750	1746	1749	1753	rVB3	1127	1571	0.31%	0.040%
73	11.847	1760	1765	1767	rBV	363	447	0.09%	0.011%
74	11.933	1776	1779	1783	rVB4	509	752	0.15%	0.019%
75	12.024	1789	1794	1802	rBV	324959	389489	77.75%	9.975%
76	12.128	1809	1811	1812	rBV	438	328	0.07%	0.008%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
Data File : VX025639.D
Acq On : 08 Dec 2021 22:59
Operator : JC/MD
Sample : M4975-04
Misc : 6.99g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGKS8

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

77	12.244	1828	1830	1833	rVB	342	284	0.06%	0.007%
78	12.323	1834	1843	1849	rBV	301970	373838	74.62%	9.574%
79	12.414	1856	1858	1862	rBV2	270	313	0.06%	0.008%
80	12.561	1880	1882	1885	rBV	341	333	0.07%	0.009%
81	12.640	1891	1895	1897	rBV	274	273	0.05%	0.007%
82	12.713	1904	1907	1909	rBV	204	244	0.05%	0.006%
83	12.804	1919	1922	1923	rBV2	321	310	0.06%	0.008%
84	12.920	1936	1941	1942	rBV	344	404	0.08%	0.010%
85	13.061	1962	1964	1967	rBV	288	344	0.07%	0.009%
86	13.201	1985	1987	1990	rVV	306	306	0.06%	0.008%
87	13.390	2014	2018	2020	rBV2	226	277	0.06%	0.007%
88	13.463	2027	2030	2031	rBV	300	293	0.06%	0.008%
89	13.676	2062	2065	2068	rBV	384	457	0.09%	0.012%
90	13.884	2097	2099	2102	rBV	321	393	0.08%	0.010%
91	13.908	2102	2103	2107	rVV	211	262	0.05%	0.007%
92	14.066	2128	2129	2132	rVB	381	357	0.07%	0.009%
93	14.091	2132	2133	2135	rBV	277	291	0.06%	0.007%
94	14.127	2137	2139	2142	rVV	293	297	0.06%	0.008%
95	14.194	2148	2150	2151	rVB	428	290	0.06%	0.007%
96	14.213	2151	2153	2154	rBV	378	285	0.06%	0.007%
97	14.335	2172	2173	2176	rBV	301	359	0.07%	0.009%
98	14.457	2188	2193	2195	rBV2	380	631	0.13%	0.016%
99	14.585	2211	2214	2215	rVV	366	323	0.06%	0.008%
100	15.987	2440	2444	2447	rBV4	515	998	0.20%	0.026%

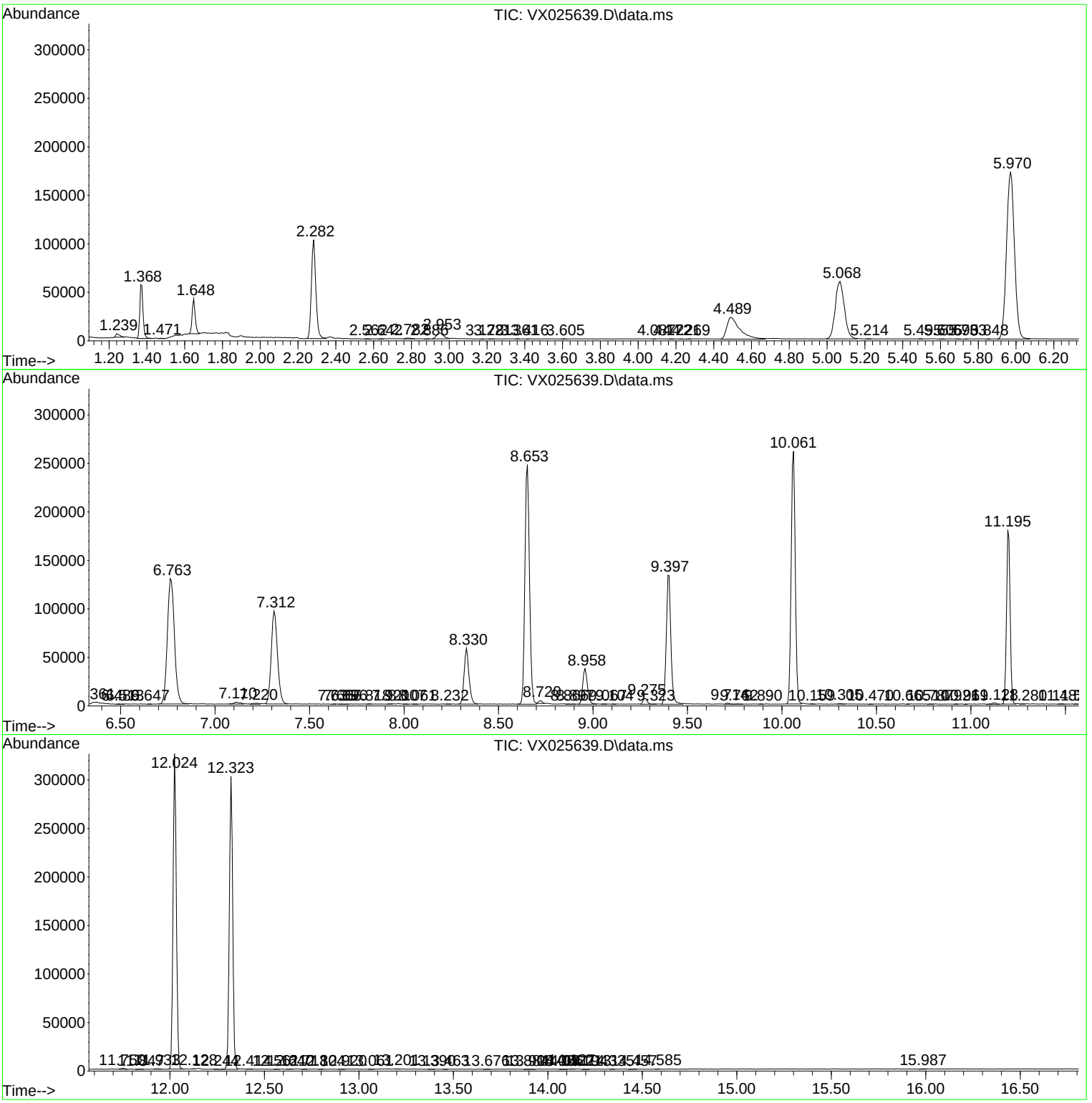
Sum of corrected areas: 3904781

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
Data File : VX025639.D
Acq On : 08 Dec 2021 22:59
Operator : JC/MD
Sample : M4975-04
Misc : 6.99g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGKS8

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\VX120821\
Data File : VX025639.D
Acq On : 08 Dec 2021 22:59
Operator : JC/MD
Sample : M4975-04
Misc : 6.99g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGKS8

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

****

Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
Data File : VX025639.D
Acq On : 08 Dec 2021 22:59
Operator : JC/MD
Sample : M4975-04
Misc : 6.99g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGKS8

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