LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122921\
Data File : VX026129.D
Acq On : 29 Dec 2021 11:18
Operator : JC/MD
Sample : VX1229MBL01
Misc : 5.0g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK651

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\SFAMXLM122821WMA.M
Title : VOC Analysis

Signal : TIC: VX026129.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	43	46	53	rVB	105424	113753	15.46%	2.052%
2	1.672	92	96	104	rVB	90121	106548	14.48%	1.922%
3	2.313	194	201	219	rVB	174809	287588	39.08%	5.187%
4	2.514	232	234	236	rVB2	1027	667	0.09%	0.012%
5	2.587	243	246	248	rBV	703	941	0.13%	0.017%
6	2.654	256	257	260	rBV2	781	939	0.13%	0.017%
7	2.800	276	281	284	rVB4	2023	3811	0.52%	0.069%
8	2.849	287	289	291	rBV	475	475	0.06%	0.009%
9	2.947	298	305	313	rBV3	3214	7849	1.07%	0.142%
10	3.008	313	315	318	rVB2	681	805	0.11%	0.015%
11	3.038	318	320	321	rBV	511	407	0.06%	0.007%
12	3.319	364	366	368	rVB	633	472	0.06%	0.009%
13	3.440	383	386	387	rBV	801	632	0.09%	0.011%
14	4.111	495	496	497	rBV	934	503	0.07%	0.009%
15	4.459	544	553	566	rBV	52920	156127	21.22%	2.816%
16	4.885	620	623	624	rBV	379	459	0.06%	0.008%
17	4.916	626	628	631	rVB	655	583	0.08%	0.011%
18	5.056	639	651	666	rBV	95667	301474	40.97%	5.438%
19	5.385	700	705	707	rBV2	1097	1853	0.25%	0.033%
20	5.446	714	715	717	rBV	556	402	0.05%	0.007%
21	5.489	719	722	726	rBV	597	977	0.13%	0.018%
22	5.672	750	752	753	rBV	534	427	0.06%	0.008%
23	5.714	756	759	761	rBV2	372	513	0.07%	0.009%
24	5.775	768	769	770	rBV	717	406	0.06%	0.007%
25	5.970	787	801	815	rBV2	248617	735888	100.00%	13.273%
26	6.391	869	870	871	rBV	803	536	0.07%	0.010%
27	6.440	875	878	880	rVV2	437	447	0.06%	0.008%
28	6.544	893	895	897	rBV	679	612	0.08%	0.011%
29	6.568	897	899	901	rBV	428	404	0.05%	0.007%
30	6.635	907	910	912	rBV	596	557	0.08%	0.010%
31	6.763	922	931	943	rVV	187348	444194	60.36%	8.012%
32	6.964	963	964	968	rBV	778	742	0.10%	0.013%
33	7.111	982	988	997	rBV3	3361	7325	1.00%	0.132%
34	7.306	1012	1020	1033	rBV	150690	333875	45.37%	6.022%
35	7.452	1042	1044	1047	rBV2	607	831	0.11%	0.015%
36	7.586	1062	1066	1068	rBV	663	793	0.11%	0.014%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122921\
Data File : VX026129.D
Acq On : 29 Dec 2021 11:18
Operator : JC/MD
Sample : VX1229MBL01
Misc : 5.0g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK651

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\SFAMXLM122821WMA.M
Title : VOC Analysis

37	7.623	1071	1072	1077	rVB	781	1089	0.15%	0.020%
38	7.678	1080	1081	1083	rBV	578	397	0.05%	0.007%
39	7.995	1130	1133	1135	rVB	539	589	0.08%	0.011%
40	8.019	1135	1137	1138	rBV	555	524	0.07%	0.009%
41	8.110	1150	1152	1153	rBV	395	409	0.06%	0.007%
42	8.184	1162	1164	1166	rVB	542	405	0.06%	0.007%
43	8.214	1168	1169	1173	rBV2	390	515	0.07%	0.009%
44	8.324	1181	1187	1198	rVV	110342	178940	24.32%	3.227%
45	8.586	1228	1230	1232	rVB2	775	614	0.08%	0.011%
46	8.647	1234	1240	1248	rBV	357286	574847	78.12%	10.368%
47	8.726	1248	1253	1261	rVB3	5061	9262	1.26%	0.167%
48	8.836	1270	1271	1273	rBV	537	517	0.07%	0.009%
49	8.891	1278	1280	1283	rBV	580	631	0.09%	0.011%
50	8.952	1285	1290	1297	rVV	75256	113582	15.43%	2.049%
51	9.153	1321	1323	1326	rBV	907	707	0.10%	0.013%
52	9.177	1326	1327	1331	rVB2	589	798	0.11%	0.014%
53	9.214	1331	1333	1335	rBV	676	791	0.11%	0.014%
54	9.263	1338	1341	1343	rBV2	440	646	0.09%	0.012%
55	9.299	1346	1347	1349	rBV	517	414	0.06%	0.007%
56	9.385	1356	1361	1374	rVB	242408	337892	45.92%	6.094%
57	9.628	1397	1401	1403	rVB2	480	639	0.09%	0.012%
58	9.653	1403	1405	1408	rBV2	661	639	0.09%	0.012%
59	9.702	1411	1413	1415	rBV	561	595	0.08%	0.011%
60	9.756	1420	1422	1425	rVV	488	635	0.09%	0.011%
61	9.836	1432	1435	1437	rBV	677	793	0.11%	0.014%
62	9.970	1455	1457	1458	rVB	682	478	0.06%	0.009%
63	9.994	1458	1461	1464	rBV2	902	1275	0.17%	0.023%
64	10.055	1465	1471	1484	rVV	377194	512503	69.64%	9.244%
65	10.238	1500	1501	1504	rBV	573	602	0.08%	0.011%
66	10.299	1509	1511	1518	rVB2	1284	1963	0.27%	0.035%
67	10.409	1528	1529	1533	rVB	731	535	0.07%	0.010%
68	10.451	1533	1536	1537	rBV	593	754	0.10%	0.014%
69	10.646	1566	1568	1571	rBV3	716	788	0.11%	0.014%
70	10.762	1584	1587	1590	rBV	796	841	0.11%	0.015%
71	10.988	1621	1624	1625	rBV	920	889	0.12%	0.016%
72	11.122	1641	1646	1650	rBV4	2621	4241	0.58%	0.076%
73	11.195	1652	1658	1667	rVB	244470	324876	44.15%	5.860%
74	11.671	1735	1736	1739	rBV2	574	452	0.06%	0.008%
75	11.750	1745	1749	1754	rVB5	2533	3456	0.47%	0.062%
76	11.841	1762	1764	1769	rVB2	1380	1829	0.25%	0.033%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122921\
Data File : VX026129.D
Acq On : 29 Dec 2021 11:18
Operator : JC/MD
Sample : VX1229MBL01
Misc : 5.0g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK651

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\SFAMXLM122821WMA.M
Title : VOC Analysis

77	11.933	1775	1779	1783	rBV3	1486	1809	0.25%	0.033%
78	11.976	1783	1786	1787	rVB2	852	730	0.10%	0.013%
79	12.024	1789	1794	1801	rVV	353240	455822	61.94%	8.221%
80	12.122	1808	1810	1812	rBV2	1238	1371	0.19%	0.025%
81	12.323	1837	1843	1852	rVB	366152	473391	64.33%	8.538%
82	12.475	1866	1868	1873	rVB2	834	1531	0.21%	0.028%
83	12.677	1896	1901	1903	rBV3	476	886	0.12%	0.016%
84	13.195	1983	1986	1988	rBV2	720	1010	0.14%	0.018%
85	13.591	2047	2051	2055	rVB4	1170	1714	0.23%	0.031%
86	14.018	2120	2121	2123	rBV	643	523	0.07%	0.009%
87	14.652	2224	2225	2227	rBV	415	418	0.06%	0.008%
88	14.743	2237	2240	2242	rBV2	406	467	0.06%	0.008%
89	14.902	2264	2266	2268	rBV2	637	545	0.07%	0.010%
90	14.993	2278	2281	2283	rBV	805	766	0.10%	0.014%
91	15.609	2380	2382	2386	rBB2	715	738	0.10%	0.013%
92	15.682	2392	2394	2397	rBV	585	473	0.06%	0.009%
93	15.804	2412	2414	2416	rBV	618	515	0.07%	0.009%
94	15.865	2422	2424	2425	rBV	730	768	0.10%	0.014%
95	16.011	2447	2448	2450	rBV	580	401	0.05%	0.007%
96	16.152	2469	2471	2474	rBV2	683	790	0.11%	0.014%
97	16.444	2516	2519	2521	rBV2	594	665	0.09%	0.012%
98	16.542	2532	2535	2536	rVB2	851	598	0.08%	0.011%
99	16.651	2551	2553	2556	rVV2	503	410	0.06%	0.007%
100	16.767	2569	2572	2573	rBV	874	777	0.11%	0.014%

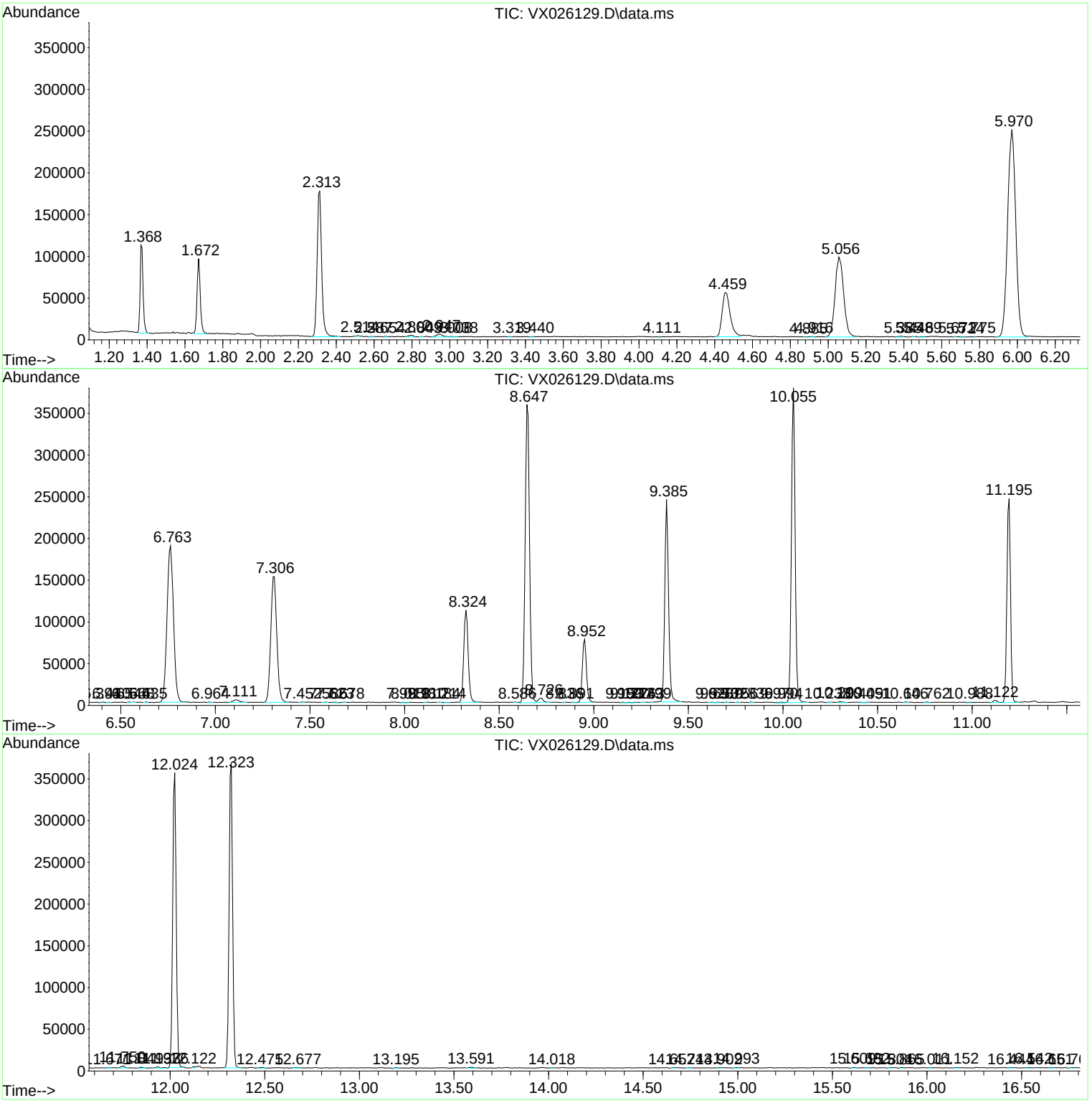
Sum of corrected areas: 5544285

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122921\
Data File : VX026129.D
Acq On : 29 Dec 2021 11:18
Operator : JC/MD
Sample : VX1229MBL01
Misc : 5.0g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK651

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122821WMA.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\VX122921\
Data File : VX026129.D
Acq On : 29 Dec 2021 11:18
Operator : JC/MD
Sample : VX1229MBL01
Misc : 5.0g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK651

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122821WMA.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\VX122921\
Data File : VX026129.D
Acq On : 29 Dec 2021 11:18
Operator : JC/MD
Sample : VX1229MBL01
Misc : 5.0g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK651

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122821WMA.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