LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013125\
Data File : VX044795.D
Acq On : 31 Jan 2025 14:40
Operator : JC/MD
Sample : Q1189-03ME
Misc : 15.32g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44Q6ME

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\SFAMXLM012825WMA.M
Title : VOC Analysis

Signal : TIC: VX044795.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	33	rBV2	13969	24965	2.13%	0.292%
2	1.368	43	46	49	rBV	90431	97758	8.33%	1.145%
3	1.648	89	92	95	rBV	20760	26309	2.24%	0.308%
4	2.282	190	196	212	rBV	243965	395471	33.71%	4.630%
5	2.861	287	291	292	rBV2	343	435	0.04%	0.005%
6	2.947	299	305	310	rBV2	3559	7749	0.66%	0.091%
7	3.410	375	381	382	rBV3	571	807	0.07%	0.009%
8	3.739	432	435	437	rVB2	420	486	0.04%	0.006%
9	4.245	516	518	521	rBV	407	471	0.04%	0.006%
10	4.477	548	556	578	rBV	56028	212705	18.13%	2.490%
11	4.818	610	612	614	rBV2	425	280	0.02%	0.003%
12	4.928	629	630	632	rBV	331	273	0.02%	0.003%
13	5.056	639	651	669	rBV	141130	447385	38.14%	5.238%
14	5.172	669	670	672	rVB	630	348	0.03%	0.004%
15	5.361	698	701	705	rBV2	415	626	0.05%	0.007%
16	5.397	705	707	710	rVB	533	382	0.03%	0.004%
17	5.550	728	732	733	rBV	563	497	0.04%	0.006%
18	5.708	754	758	761	rBV2	359	519	0.04%	0.006%
19	5.775	766	769	771	rVV	317	277	0.02%	0.003%
20	5.812	771	775	776	rVB2	357	349	0.03%	0.004%
21	5.964	788	800	822	rBV2	400893	1173160	100.00%	13.735%
22	6.373	865	867	869	rBV3	279	270	0.02%	0.003%
23	6.550	894	896	897	rBV	395	303	0.03%	0.004%
24	6.580	900	901	904	rVV	369	303	0.03%	0.004%
25	6.757	921	930	954	rVV	283448	708498	60.39%	8.295%
26	7.190	999	1001	1003	rBV2	381	333	0.03%	0.004%
27	7.220	1004	1006	1008	rVV2	431	365	0.03%	0.004%
28	7.306	1011	1020	1040	rBV	237975	529819	45.16%	6.203%
29	7.488	1049	1050	1053	rVB2	728	451	0.04%	0.005%
30	7.635	1070	1074	1076	rBV2	411	723	0.06%	0.008%
31	7.763	1093	1095	1098	rBV2	293	294	0.03%	0.003%
32	7.964	1126	1128	1129	rBV	415	342	0.03%	0.004%
33	7.982	1129	1131	1132	rVV	476	296	0.03%	0.003%
34	8.001	1132	1134	1135	rVB2	560	398	0.03%	0.005%
35	8.049	1140	1142	1145	rVB	502	451	0.04%	0.005%
36	8.116	1150	1153	1154	rVB2	467	420	0.04%	0.005%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013125\
Data File : VX044795.D
Acq On : 31 Jan 2025 14:40
Operator : JC/MD
Sample : Q1189-03ME
Misc : 15.32g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44Q6ME

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\SFAMXLM012825WMA.M
Title : VOC Analysis

37	8.135	1154	1156	1157	rBV2	330	281	0.02%	0.003%
38	8.165	1159	1161	1163	rBV	371	296	0.03%	0.003%
39	8.251	1171	1175	1176	rBV	303	301	0.03%	0.004%
40	8.324	1181	1187	1201	rVV	164738	280527	23.91%	3.284%
41	8.580	1227	1229	1230	rBV	343	296	0.03%	0.003%
42	8.592	1230	1231	1233	rBV	685	391	0.03%	0.005%
43	8.647	1233	1240	1258	rBV	566482	947516	80.77%	11.093%
44	8.903	1279	1282	1284	rBV3	941	1195	0.10%	0.014%
45	8.952	1284	1290	1306	rVB	111705	176951	15.08%	2.072%
46	9.092	1311	1313	1315	rVB	414	365	0.03%	0.004%
47	9.110	1315	1316	1320	rVB2	380	298	0.03%	0.003%
48	9.275	1338	1343	1350	rVB	5950	8985	0.77%	0.105%
49	9.330	1350	1352	1356	rBV2	373	347	0.03%	0.004%
50	9.391	1356	1362	1378	rBV	235195	417527	35.59%	4.888%
51	9.677	1408	1409	1411	rBV	473	460	0.04%	0.005%
52	9.708	1411	1414	1417	rVB5	911	1294	0.11%	0.015%
53	9.848	1435	1437	1440	rVB2	438	493	0.04%	0.006%
54	9.872	1440	1441	1444	rBV2	378	324	0.03%	0.004%
55	10.055	1465	1471	1491	rVV	575409	851857	72.61%	9.973%
56	10.305	1510	1512	1517	rVB3	610	804	0.07%	0.009%
57	10.445	1532	1535	1537	rBV2	430	556	0.05%	0.007%
58	10.555	1551	1553	1555	rBV2	463	617	0.05%	0.007%
59	10.646	1565	1568	1569	rBV2	418	532	0.05%	0.006%
60	10.732	1579	1582	1583	rBV	473	379	0.03%	0.004%
61	10.781	1588	1590	1594	rVB2	271	361	0.03%	0.004%
62	10.939	1614	1616	1617	rBV2	348	304	0.03%	0.004%
63	11.152	1649	1651	1652	rBV	404	313	0.03%	0.004%
64	11.189	1652	1657	1669	rVV	399083	533194	45.45%	6.243%
65	11.378	1687	1688	1691	rBV	338	312	0.03%	0.004%
66	11.433	1694	1697	1698	rBV2	389	412	0.04%	0.005%
67	11.482	1703	1705	1710	rVB4	1601	2020	0.17%	0.024%
68	11.604	1723	1725	1729	rVB2	305	279	0.02%	0.003%
69	11.713	1741	1743	1745	rBV2	390	448	0.04%	0.005%
70	11.750	1746	1749	1751	rBV4	945	1208	0.10%	0.014%
71	11.872	1764	1769	1774	rVB4	473	908	0.08%	0.011%
72	11.933	1774	1779	1783	rBV4	871	1523	0.13%	0.018%
73	12.018	1788	1793	1803	rBV	659230	836285	71.28%	9.791%
74	12.244	1827	1830	1835	rVB5	457	648	0.06%	0.008%
75	12.317	1837	1842	1858	rBV	623728	809915	69.04%	9.482%
76	12.640	1892	1895	1900	rVB3	537	945	0.08%	0.011%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013125\
Data File : VX044795.D
Acq On : 31 Jan 2025 14:40
Operator : JC/MD
Sample : Q1189-03ME
Misc : 15.32g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44Q6ME

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\SFAMXLM012825WMA.M
Title : VOC Analysis

77	12.701	1903	1905	1908	rVB2	405	392	0.03%	0.005%
78	12.762	1911	1915	1920	rVV	2754	3350	0.29%	0.039%
79	12.896	1935	1937	1938	rBV	458	312	0.03%	0.004%
80	12.987	1948	1952	1953	rBV2	483	598	0.05%	0.007%
81	13.036	1958	1960	1963	rBV2	431	477	0.04%	0.006%
82	13.079	1966	1967	1969	rVV2	516	315	0.03%	0.004%
83	13.195	1982	1986	1988	rBV2	580	611	0.05%	0.007%
84	13.268	1993	1998	2004	rBV4	1123	1812	0.15%	0.021%
85	13.341	2008	2010	2012	rBV2	365	308	0.03%	0.004%
86	13.737	2073	2075	2077	rBV2	405	468	0.04%	0.005%
87	13.835	2089	2091	2093	rVB3	815	614	0.05%	0.007%
88	13.969	2111	2113	2116	rBV3	585	492	0.04%	0.006%
89	14.036	2121	2124	2128	rBV2	1256	1633	0.14%	0.019%
90	14.091	2130	2133	2134	rBV	346	316	0.03%	0.004%
91	14.128	2135	2139	2143	rVB	4707	5999	0.51%	0.070%
92	14.280	2161	2164	2167	rBV3	471	688	0.06%	0.008%
93	14.335	2171	2173	2177	rVB4	593	829	0.07%	0.010%
94	14.371	2177	2179	2183	rBV3	697	870	0.07%	0.010%
95	14.512	2200	2202	2206	rVB3	504	627	0.05%	0.007%
96	14.548	2206	2208	2211	rBV2	634	678	0.06%	0.008%
97	14.694	2231	2232	2237	rVB2	615	624	0.05%	0.007%
98	14.755	2239	2242	2245	rVV2	1294	1508	0.13%	0.018%
99	15.578	2375	2377	2380	rBV2	778	799	0.07%	0.009%
100	16.286	2491	2493	2495	rVB2	718	742	0.06%	0.009%

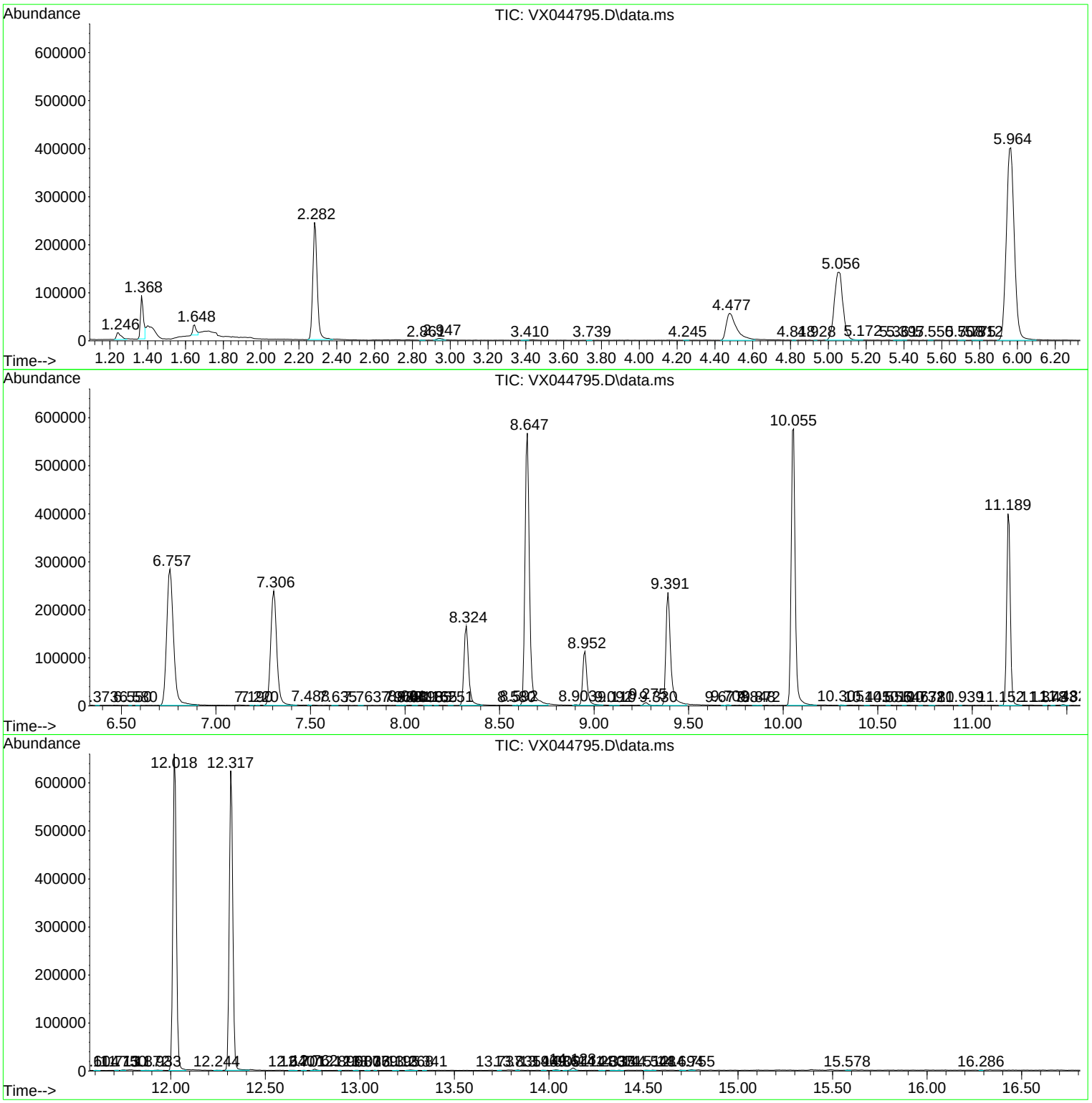
Sum of corrected areas: 8541247

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013125\
Data File : VX044795.D
Acq On : 31 Jan 2025 14:40
Operator : JC/MD
Sample : Q1189-03ME
Misc : 15.32g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44Q6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM012825WMA.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\VX013125\
Data File : VX044795.D
Acq On : 31 Jan 2025 14:40
Operator : JC/MD
Sample : Q1189-03ME
Misc : 15.32g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44Q6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM012825WMA.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\VX013125\
Data File : VX044795.D
Acq On : 31 Jan 2025 14:40
Operator : JC/MD
Sample : Q1189-03ME
Misc : 15.32g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44Q6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM012825WMA.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