LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071524\
Data File : VU059957.D
Acq On : 15 Jul 2024 17:30
Operator : MD/SY
Sample : P3230-02MEDL 400X
Misc : 5.28g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHB33MEDL

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_U\Method\SFAMULM070224WMA.M
Title : VOC Analysis

Signal : TIC: VU059957.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.595	88	95	113	rBV	60824	76755	12.64%	1.429%
2	1.901	183	190	211	rVB	46902	72175	11.89%	1.344%
3	2.557	383	394	409	rBV	103321	167201	27.55%	3.112%
4	2.708	438	441	445	rBV2	294	204	0.03%	0.004%
5	2.763	454	458	460	rBV2	344	269	0.04%	0.005%
6	2.782	460	464	466	rVV3	436	324	0.05%	0.006%
7	3.039	533	544	556	rBV3	1951	3754	0.62%	0.070%
8	3.184	575	589	603	rVB2	5646	12707	2.09%	0.237%
9	3.467	673	677	680	rBV2	267	235	0.04%	0.004%
10	3.502	685	688	691	rVB	194	124	0.02%	0.002%
11	3.518	691	693	694	rBV	256	68	0.01%	0.001%
12	3.605	717	720	723	rBV	208	158	0.03%	0.003%
13	3.673	737	741	744	rBV2	310	266	0.04%	0.005%
14	3.782	769	775	781	rBV2	189	320	0.05%	0.006%
15	3.837	788	792	796	rBV2	243	256	0.04%	0.005%
16	3.930	819	821	828	rVB2	298	245	0.04%	0.005%
17	3.965	828	832	835	rBV2	237	197	0.03%	0.004%
18	4.052	850	859	863	rBV2	273	392	0.06%	0.007%
19	4.091	869	871	874	rVB2	137	75	0.01%	0.001%
20	4.129	880	883	886	rVB	335	218	0.04%	0.004%
21	4.148	886	889	891	rBV	252	150	0.02%	0.003%
22	4.193	900	903	904	rBV	219	125	0.02%	0.002%
23	4.251	919	921	923	rBV2	84	41	0.01%	0.001%
24	4.312	937	940	944	rVB	178	128	0.02%	0.002%
25	4.348	948	951	953	rBV	143	83	0.01%	0.002%
26	4.380	959	961	962	rBV	258	77	0.01%	0.001%
27	4.473	988	990	993	rVB	193	98	0.02%	0.002%
28	4.499	996	998	1001	rVB2	175	94	0.02%	0.002%
29	4.528	1001	1007	1010	rBV2	156	168	0.03%	0.003%
30	4.544	1010	1012	1016	rBV	98	72	0.01%	0.001%
31	4.618	1026	1035	1067	rBV2	70132	192549	31.72%	3.584%
32	5.055	1157	1171	1196	rBV2	107400	238775	39.34%	4.445%
33	5.274	1236	1239	1240	rBV2	181	97	0.02%	0.002%
34	5.512	1311	1313	1315	rBV2	146	83	0.01%	0.002%
35	5.717	1358	1377	1407	rBV2	206403	572553	94.32%	10.658%
36	5.965	1451	1454	1457	rBV2	193	128	0.02%	0.002%

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ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : BHB33MEDL

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_U\Method\SFAMULM070224WMA.M
Title : VOC Analysis

37	5.988	1457	1461	1464	rBV2	404	339	0.06%	0.006%
38	6.042	1475	1478	1481	rVB	156	102	0.02%	0.002%
39	6.062	1481	1484	1486	rBV	177	115	0.02%	0.002%
40	6.126	1500	1504	1506	rBV2	215	161	0.03%	0.003%
41	6.171	1515	1518	1520	rBV2	102	60	0.01%	0.001%
42	6.245	1527	1541	1565	rBV	246600	472499	77.84%	8.796%
43	6.483	1613	1615	1622	rVB3	400	351	0.06%	0.007%
44	6.541	1622	1633	1646	rVB8	5677	11505	1.90%	0.214%
45	6.595	1647	1650	1652	rBV	96	53	0.01%	0.001%
46	6.685	1665	1678	1700	rBV	136027	268994	44.31%	5.007%
47	6.997	1773	1775	1781	rBV2	136	81	0.01%	0.002%
48	7.074	1797	1799	1803	rVB	215	115	0.02%	0.002%
49	7.190	1832	1835	1836	rBV	211	112	0.02%	0.002%
50	7.264	1855	1858	1863	rBV2	116	121	0.02%	0.002%
51	7.325	1875	1877	1879	rVB	125	54	0.01%	0.001%
52	7.335	1879	1880	1881	rBV	184	36	0.01%	0.001%
53	7.351	1881	1885	1887	rBV	94	83	0.01%	0.002%
54	7.399	1895	1900	1903	rBV2	140	155	0.03%	0.003%
55	7.486	1921	1927	1931	rBV2	240	274	0.05%	0.005%
56	7.505	1931	1933	1935	rBV	172	96	0.02%	0.002%
57	7.563	1940	1951	1975	rVV	67598	119127	19.63%	2.218%
58	7.669	1981	1984	1986	rBV	288	189	0.03%	0.004%
59	7.772	2012	2016	2020	rBV2	172	172	0.03%	0.003%
60	7.894	2042	2054	2074	rBV	230815	402097	66.24%	7.485%
61	8.110	2119	2121	2124	rBV	175	117	0.02%	0.002%
62	8.177	2131	2142	2162	rBV	45755	80232	13.22%	1.494%
63	8.373	2196	2203	2206	rBV2	247	322	0.05%	0.006%
64	8.479	2229	2236	2245	rVB3	446	788	0.13%	0.015%
65	8.550	2245	2258	2273	rBV	270898	459858	75.76%	8.560%
66	8.631	2273	2283	2320	rVB	182912	340774	56.14%	6.344%
67	8.894	2363	2365	2367	rBV2	235	113	0.02%	0.002%
68	8.910	2367	2370	2374	rBV2	314	253	0.04%	0.005%
69	9.032	2405	2408	2409	rBV	114	64	0.01%	0.001%
70	9.190	2455	2457	2458	rBV	112	48	0.01%	0.001%
71	9.264	2477	2480	2484	rBV	209	157	0.03%	0.003%
72	9.415	2515	2527	2555	rBV	361715	607006	100.00%	11.300%
73	9.579	2577	2578	2585	rVB2	380	293	0.05%	0.005%
74	9.759	2628	2634	2636	rBV2	201	216	0.04%	0.004%
75	10.029	2715	2718	2720	rBV	182	103	0.02%	0.002%
76	10.225	2775	2779	2781	rBV	265	234	0.04%	0.004%

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Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
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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_U\Method\SFAMULM070224WMA.M
Title : VOC Analysis

77	10.328	2808	2811	2815	rBV	147	136	0.02%	0.003%
78	10.505	2861	2866	2868	rBV	312	264	0.04%	0.005%
79	10.537	2875	2876	2877	rBV	188	38	0.01%	0.001%
80	10.753	2930	2943	2963	rBV	227996	369168	60.82%	6.872%
81	10.862	2974	2977	2979	rBV	453	280	0.05%	0.005%
82	11.219	3084	3088	3094	rBV2	292	380	0.06%	0.007%
83	11.810	3259	3272	3304	rBV	310201	509921	84.01%	9.492%
84	11.965	3317	3320	3322	rBV	273	214	0.04%	0.004%
85	12.000	3330	3331	3333	rBV	266	123	0.02%	0.002%
86	12.190	3378	3390	3412	rBV	225729	381670	62.88%	7.105%
87	12.367	3442	3445	3447	rBB	320	152	0.03%	0.003%
88	12.682	3540	3543	3544	rBV	218	130	0.02%	0.002%
89	12.727	3555	3557	3560	rBV2	311	187	0.03%	0.003%
90	13.293	3730	3733	3738	rBV	324	295	0.05%	0.005%
91	14.055	3967	3970	3973	rBV	417	350	0.06%	0.007%

Sum of corrected areas: 5371941

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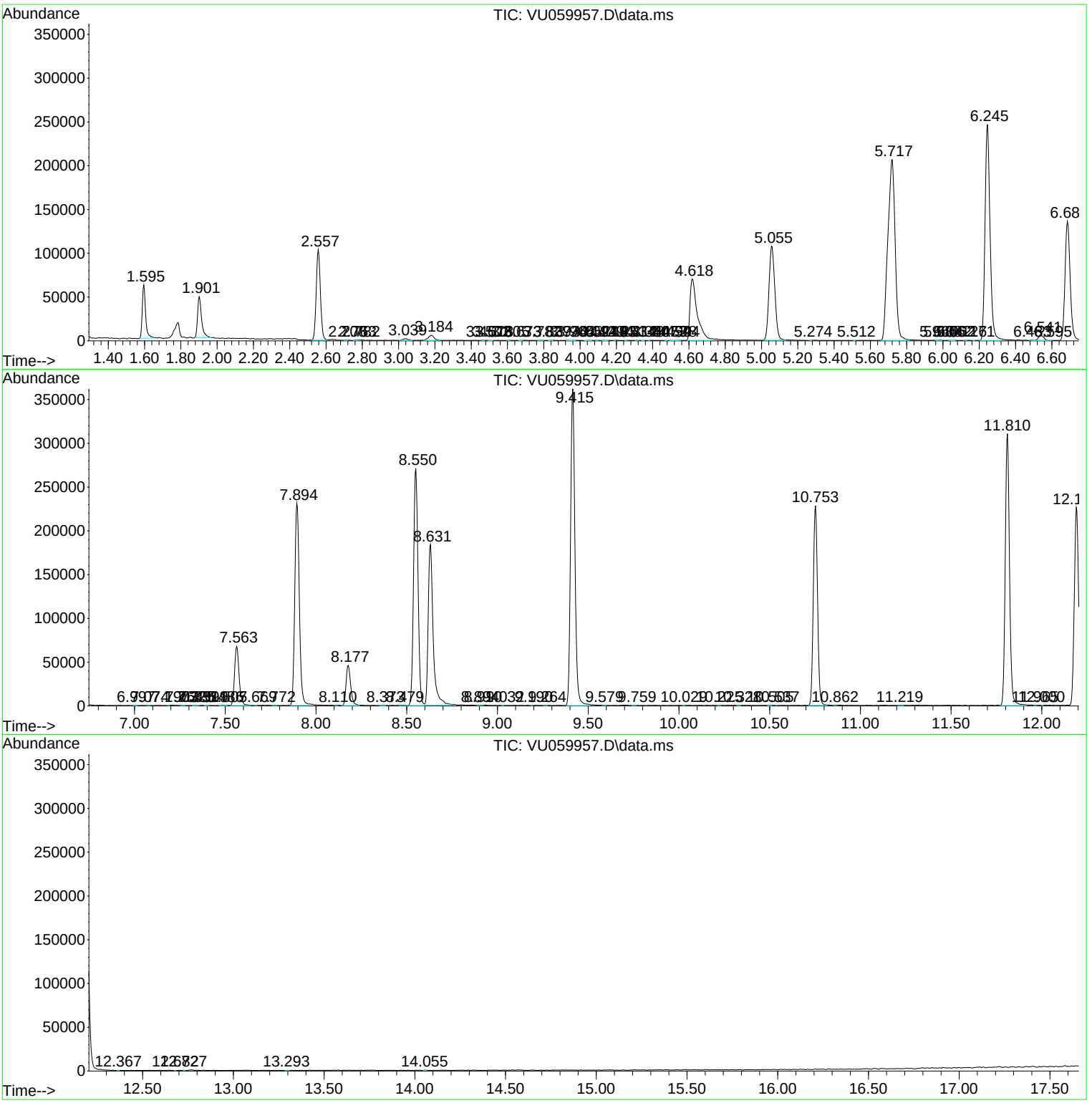
Instrument :
MSVOA_U
ClientSampleId :
BHB33MEDL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.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_U\Data\VU071524\
Data File : VU059957.D
Acq On : 15 Jul 2024 17:30
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Sample : P3230-02MEDL 400X
Misc : 5.28g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.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

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Instrument :
MSVOA_U
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.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