

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV052323\
 Data File : VV031200.D
 Acq On : 23 May 2023 19:13
 Operator : SY/MD
 Sample : 02865-08
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 GBX63

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_V\Method\SFAMVLM051923WMA.M
 Title : VOC Analysis

Signal : TIC: VV031200.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.281	69	75	91	rVB	100259	114524	14.70%	1.813%
2	1.539	148	155	170	rVB	104876	131680	16.91%	2.085%
3	2.063	310	318	330	rBV	188076	275374	35.35%	4.359%
4	2.127	332	338	354	rVB	50094	85891	11.03%	1.360%
5	2.346	405	406	408	rVB2	1159	417	0.05%	0.007%
6	2.362	409	411	412	rBV2	1024	308	0.04%	0.005%
7	2.413	423	427	429	rBV5	1180	980	0.13%	0.016%
8	2.503	453	455	459	rBV5	1581	898	0.12%	0.014%
9	2.555	469	471	472	rBV2	822	269	0.03%	0.004%
10	2.773	537	539	541	rBV3	718	330	0.04%	0.005%
11	2.786	541	543	546	rVV4	1492	811	0.10%	0.013%
12	2.828	554	556	557	rBV2	1117	562	0.07%	0.009%
13	2.867	566	568	571	rVB4	1948	1011	0.13%	0.016%
14	2.889	571	575	576	rBV4	1060	877	0.11%	0.014%
15	2.934	587	589	590	rVB	748	229	0.03%	0.004%
16	2.947	590	593	594	rBV3	1395	758	0.10%	0.012%
17	2.966	597	599	604	rVB5	1962	1163	0.15%	0.018%
18	2.989	604	606	607	rBV2	1730	730	0.09%	0.012%
19	3.014	612	614	617	rVB3	1497	805	0.10%	0.013%
20	3.050	623	625	626	rBV2	1031	321	0.04%	0.005%
21	3.085	634	636	640	rVB4	1377	733	0.09%	0.012%
22	3.117	644	646	649	rBV4	882	702	0.09%	0.011%
23	3.185	664	667	668	rBV3	1458	680	0.09%	0.011%
24	3.217	676	677	680	rBV3	765	388	0.05%	0.006%
25	3.256	683	689	690	rBV6	1565	1417	0.18%	0.022%
26	3.291	696	700	703	rVB5	1417	1246	0.16%	0.020%
27	3.307	703	705	708	rBV4	1536	932	0.12%	0.015%
28	3.368	721	724	725	rBV3	1198	604	0.08%	0.010%
29	3.535	774	776	779	rBV4	1133	661	0.08%	0.010%
30	3.584	789	791	793	rBV3	1236	494	0.06%	0.008%
31	3.609	797	799	803	rVB4	1829	1173	0.15%	0.019%
32	3.629	803	805	806	rBV2	1032	541	0.07%	0.009%
33	3.658	812	814	815	rBV2	1427	589	0.08%	0.009%
34	3.802	848	859	881	rBV2	56265	168854	21.68%	2.673%
35	4.156	965	969	971	rBV5	2511	1809	0.23%	0.029%
36	4.259	989	1001	1025	rVB	128159	326214	41.88%	5.164%

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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_V\Method\SFAMVLM051923WMA.M
 Title : VOC Analysis

37	4.445	1056	1059	1063	rBV6	2119	2139	0.27%	0.034%
38	4.635	1116	1118	1123	rVB5	2576	1458	0.19%	0.023%
39	4.683	1129	1133	1136	rBV6	2546	2192	0.28%	0.035%
40	4.966	1205	1221	1245	rBV2	286743	778910	100.00%	12.331%
41	5.542	1389	1400	1419	rBV2	214097	436405	56.03%	6.909%
42	5.995	1530	1541	1563	rBV	175926	355414	45.63%	5.627%
43	6.349	1646	1651	1655	rBV8	2694	3264	0.42%	0.052%
44	6.448	1680	1682	1687	rBV6	2089	1499	0.19%	0.024%
45	6.738	1770	1772	1773	rBV2	1494	650	0.08%	0.010%
46	6.860	1808	1810	1815	rBV6	1266	1206	0.15%	0.019%
47	6.918	1819	1828	1847	rVV	84506	162815	20.90%	2.578%
48	7.169	1904	1906	1907	rBV2	1554	543	0.07%	0.009%
49	7.249	1921	1931	1945	rBV	325103	565109	72.55%	8.946%
50	7.558	2019	2027	2047	rVB2	65618	115952	14.89%	1.836%
51	8.034	2166	2175	2187	rBV	180781	332989	42.75%	5.272%
52	8.632	2356	2361	2363	rBV4	1928	1708	0.22%	0.027%
53	8.789	2399	2410	2434	rBV	344192	587129	75.38%	9.295%
54	9.085	2495	2502	2513	rBV4	10864	17586	2.26%	0.278%
55	9.259	2554	2556	2558	rBV3	1369	776	0.10%	0.012%
56	9.349	2580	2584	2586	rBV4	2905	2252	0.29%	0.036%
57	9.976	2770	2779	2783	rBV4	3324	5653	0.73%	0.089%
58	10.159	2825	2836	2850	rBV	244984	388342	49.86%	6.148%
59	10.574	2963	2965	2967	rBV3	2277	1476	0.19%	0.023%
60	10.673	2994	2996	2998	rBV3	1669	850	0.11%	0.013%
61	10.976	3087	3090	3092	rBV4	1775	1131	0.15%	0.018%
62	11.191	3147	3157	3174	rBV	352057	550703	70.70%	8.718%
63	11.426	3228	3230	3233	rBV4	2064	1039	0.13%	0.016%
64	11.487	3241	3249	3264	rBV	120303	224497	28.82%	3.554%
65	11.567	3266	3274	3294	rVB	388853	627305	80.54%	9.931%
66	12.168	3459	3461	3464	rBV4	1917	1486	0.19%	0.024%
67	12.262	3486	3490	3494	rBV6	1873	1862	0.24%	0.029%
68	12.754	3639	3643	3646	rBV5	1800	1682	0.22%	0.027%
69	13.635	3912	3917	3920	rBV6	2628	2783	0.36%	0.044%
70	13.908	4000	4002	4003	rBV2	1565	655	0.08%	0.010%
71	14.033	4039	4041	4046	rBV5	1790	1574	0.20%	0.025%
72	14.085	4054	4057	4059	rBV4	1770	1132	0.15%	0.018%
73	14.123	4066	4069	4073	rBV6	2882	1749	0.22%	0.028%
74	14.419	4158	4161	4165	rBV6	2307	1652	0.21%	0.026%
75	14.506	4181	4188	4189	rBV6	3607	3140	0.40%	0.050%
76	14.683	4240	4243	4245	rBV4	1587	1312	0.17%	0.021%

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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_V\Method\SFAMVLM051923WMA.M
Title : VOC Analysis

77	15.155	4388	4390	4394	rBV4	2478	1753	0.23%	0.028%
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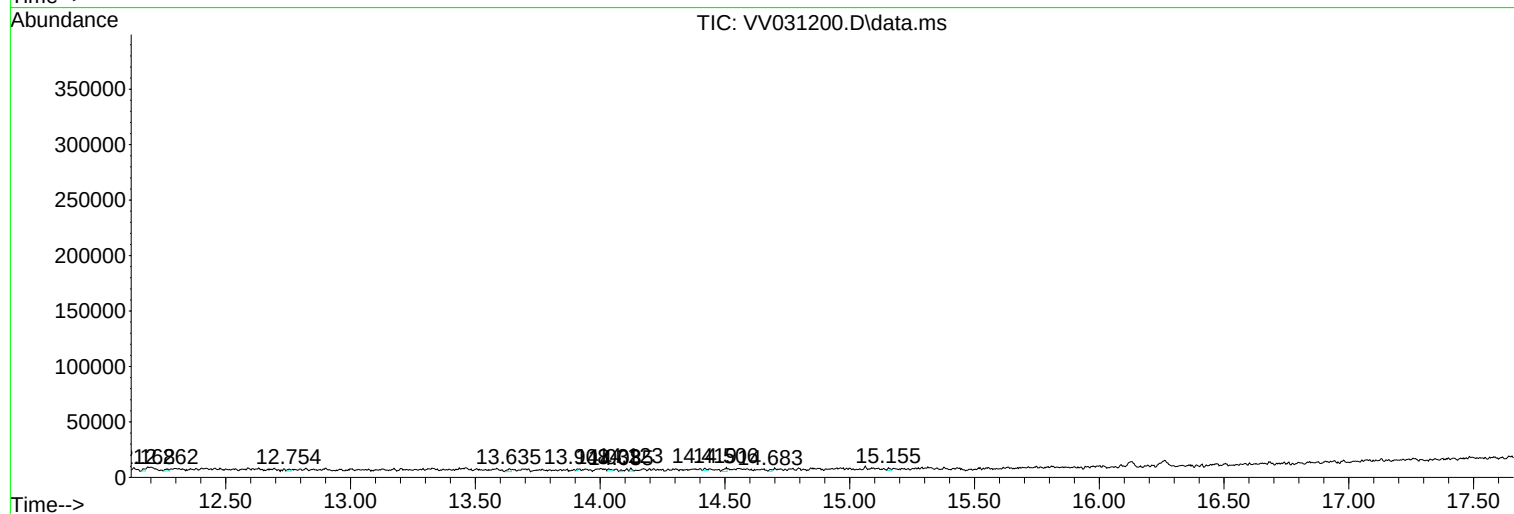
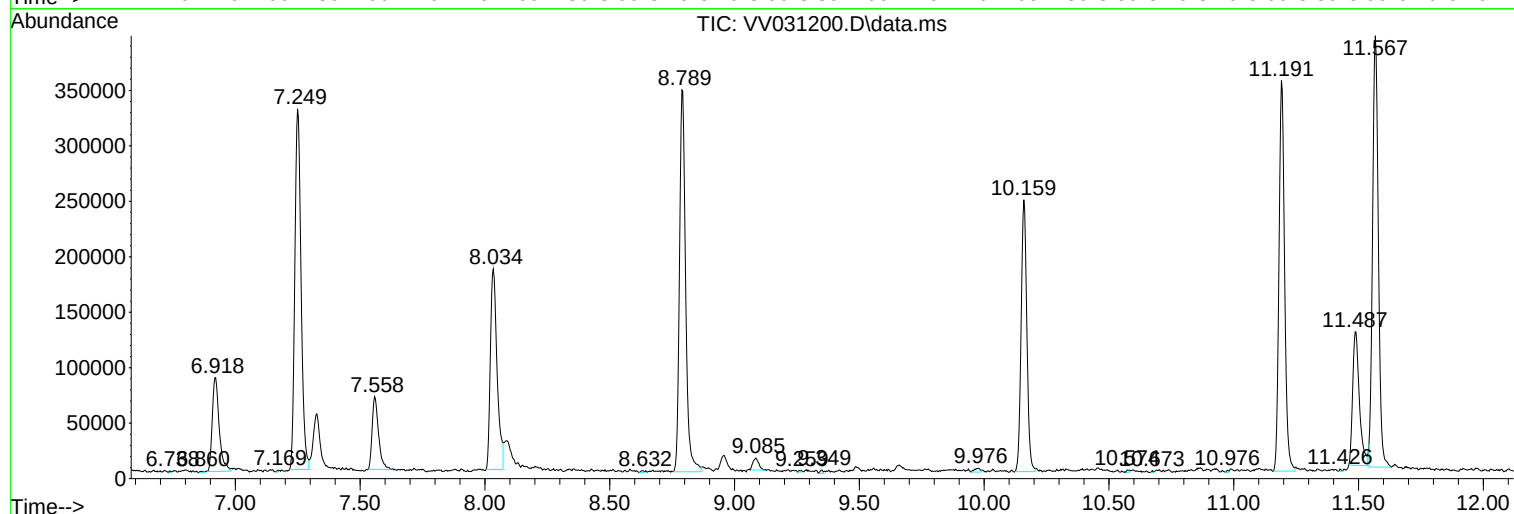
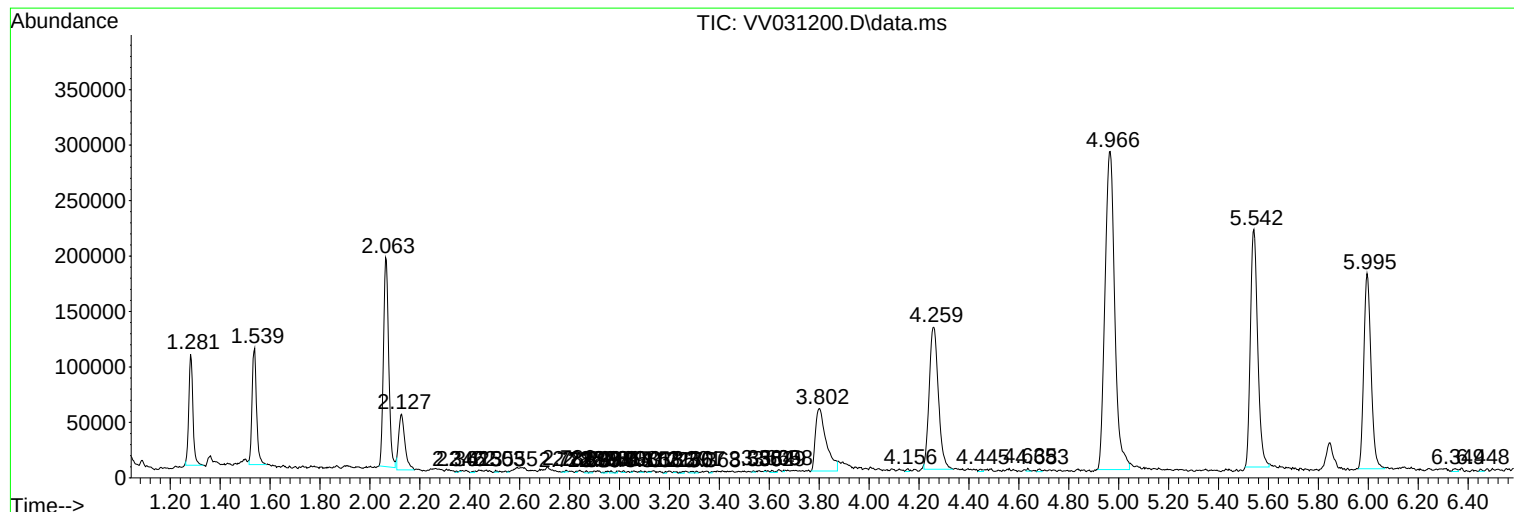
Sum of corrected areas: 6316747

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM051923WMA.M
Quant Title : VOC Analysis

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



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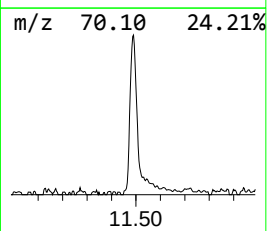
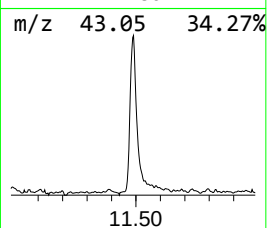
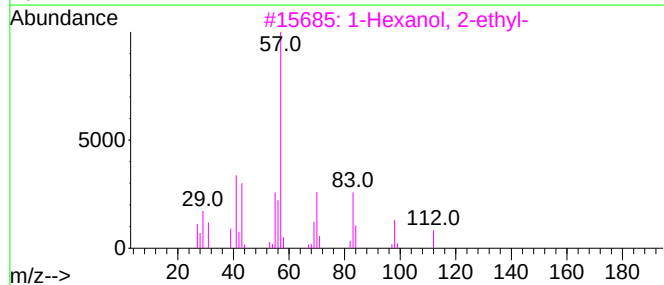
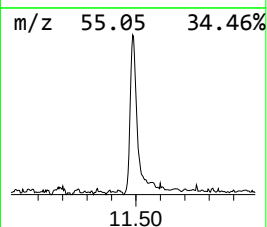
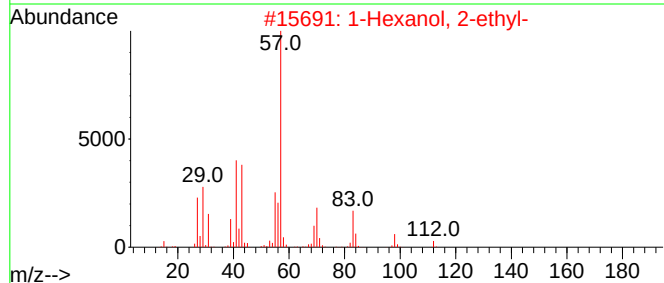
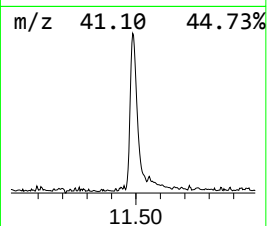
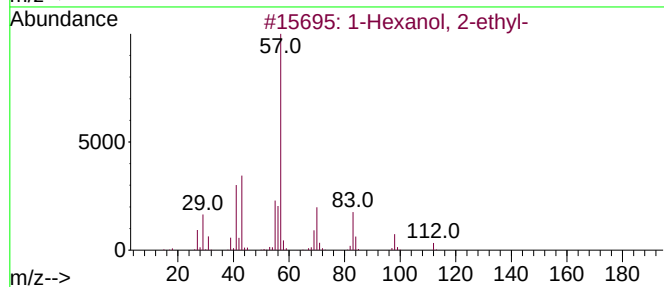
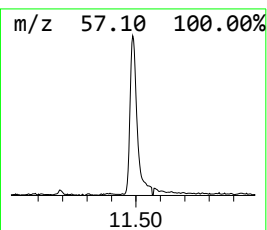
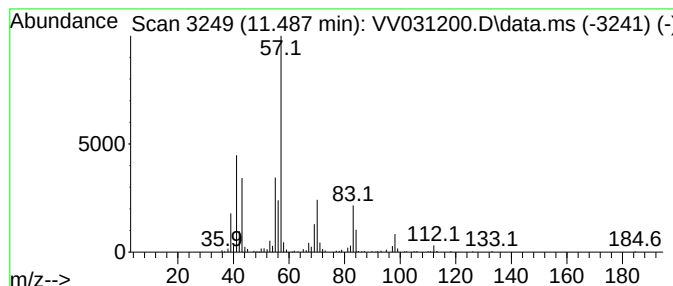
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM051923WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.487	20.38 ug/L	224497	1,4-Dichlorobenzene-d4	11.194

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	83
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	80
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
4	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
5	Carbonic acid, isobutyl 2-ethylh...			230	C13H26O3	1000383-13-3	59



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexanol, 2-et...	11.487	20.4	ug/L	224497	3	11.194	550703	50.0