

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV122123\
 Data File : VV033535.D
 Acq On : 21 Dec 2023 15:24
 Operator : SY/MD
 Sample : 05891-20
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCLT0

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\SFAMVLM121523WMA.M
 Title : VOC Analysis

Signal : TIC: VV033535.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	68	75	89	rVB	106665	112575	13.83%	1.716%
2	1.532	147	153	166	rVB	99785	119462	14.67%	1.821%
3	2.059	308	317	327	rBV	184986	274952	33.77%	4.191%
4	2.429	430	432	436	rBV5	1087	730	0.09%	0.011%
5	2.510	454	457	460	rBV4	1491	1235	0.15%	0.019%
6	2.545	466	468	471	rBV3	1421	1015	0.12%	0.015%
7	2.622	490	492	496	rBV6	1068	821	0.10%	0.013%
8	2.686	510	512	513	rBV	1168	420	0.05%	0.006%
9	2.767	536	537	538	rBV	920	275	0.03%	0.004%
10	2.812	546	551	552	rBV4	1495	1172	0.14%	0.018%
11	2.838	556	559	562	rBV5	1034	750	0.09%	0.011%
12	2.854	562	564	567	rBV3	1001	439	0.05%	0.007%
13	2.873	567	570	573	rBV4	2641	2432	0.30%	0.037%
14	3.021	615	616	617	rBV	732	168	0.02%	0.003%
15	3.030	617	619	623	rVB5	928	497	0.06%	0.008%
16	3.098	636	640	641	rBV4	1361	779	0.10%	0.012%
17	3.124	646	648	652	rBV4	902	684	0.08%	0.010%
18	3.191	667	669	671	rBV3	734	377	0.05%	0.006%
19	3.227	677	680	684	rBV6	980	800	0.10%	0.012%
20	3.291	698	700	702	rBV2	1315	582	0.07%	0.009%
21	3.310	703	706	708	rVV4	1287	706	0.09%	0.011%
22	3.333	710	713	714	rBV3	1149	566	0.07%	0.009%
23	3.342	714	716	718	rBV3	909	510	0.06%	0.008%
24	3.384	727	729	734	rBV6	1058	1072	0.13%	0.016%
25	3.413	736	738	742	rVB4	968	545	0.07%	0.008%
26	3.436	742	745	747	rBV3	1767	1349	0.17%	0.021%
27	3.493	761	763	764	rBV2	743	299	0.04%	0.005%
28	3.545	778	779	780	rBV	659	210	0.03%	0.003%
29	3.587	789	792	795	rVB4	1380	967	0.12%	0.015%
30	3.629	795	805	807	rBV8	3066	3722	0.46%	0.057%
31	3.786	845	854	880	rBV2	53478	153354	18.84%	2.338%
32	4.127	958	960	962	rBV3	936	562	0.07%	0.009%
33	4.159	968	970	971	rBV	1078	317	0.04%	0.005%
34	4.252	985	999	1030	rBV3	155834	492943	60.55%	7.514%
35	4.567	1095	1097	1100	rBV4	1096	590	0.07%	0.009%
36	4.583	1100	1102	1106	rVV5	1420	985	0.12%	0.015%

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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\SFAMVLM121523WMA.M
 Title : VOC Analysis

37	4.686	1128	1134	1137	rBV9	1615	2108	0.26%	0.032%
38	4.751	1152	1154	1160	rBV5	1448	953	0.12%	0.015%
39	4.809	1169	1172	1173	rBV3	986	454	0.06%	0.007%
40	4.879	1192	1194	1196	rBV2	769	401	0.05%	0.006%
41	4.956	1203	1218	1248	rBV2	301762	814123	100.00%	12.411%
42	5.535	1387	1398	1424	rBV	228567	481031	59.09%	7.333%
43	5.866	1494	1501	1525	rBV	79757	200200	24.59%	3.052%
44	6.915	1817	1827	1850	rBV	87124	170794	20.98%	2.604%
45	7.140	1893	1897	1898	rBV4	1467	955	0.12%	0.015%
46	7.243	1919	1929	1947	rBV	322959	575336	70.67%	8.770%
47	7.554	2018	2026	2041	rBV	62293	110820	13.61%	1.689%
48	7.873	2121	2125	2129	rBV6	2410	2365	0.29%	0.036%
49	8.024	2163	2172	2211	rBV	172806	386903	47.52%	5.898%
50	8.551	2333	2336	2337	rBV2	1591	816	0.10%	0.012%
51	8.580	2343	2345	2350	rBV6	1547	1045	0.13%	0.016%
52	8.786	2399	2409	2435	rBV	387175	637387	78.29%	9.716%
53	9.339	2578	2581	2584	rBV4	1574	1012	0.12%	0.015%
54	9.477	2621	2624	2627	rBV4	1373	1177	0.14%	0.018%
55	9.654	2676	2679	2681	rBV3	1749	1344	0.17%	0.020%
56	10.107	2817	2820	2821	rBV3	1638	855	0.11%	0.013%
57	10.152	2823	2834	2858	rVB	257532	410238	50.39%	6.254%
58	10.628	2981	2982	2984	rBV2	993	529	0.06%	0.008%
59	10.754	3019	3021	3023	rBV3	1012	519	0.06%	0.008%
60	11.069	3117	3119	3122	rVB	1123	423	0.05%	0.006%
61	11.184	3144	3155	3173	rBV	357503	566731	69.61%	8.639%
62	11.487	3239	3249	3262	rBV	157563	329752	40.50%	5.027%
63	11.561	3265	3272	3293	rVB	413762	671277	82.45%	10.233%
64	13.130	3757	3760	3762	rBV4	2136	1390	0.17%	0.021%
65	13.821	3973	3975	3977	rBV4	1363	722	0.09%	0.011%
66	13.898	3997	3999	4001	rBB3	1110	369	0.05%	0.006%
67	14.120	4066	4068	4070	rBV2	1213	666	0.08%	0.010%
68	14.162	4079	4081	4082	rBV3	847	279	0.03%	0.004%
69	14.172	4082	4084	4089	rVV4	827	764	0.09%	0.012%
70	14.278	4115	4117	4119	rBV2	952	408	0.05%	0.006%
71	14.319	4128	4130	4137	rBV8	1621	986	0.12%	0.015%
72	14.477	4177	4179	4183	rBV5	910	633	0.08%	0.010%
73	15.027	4347	4350	4353	rBV4	1705	1338	0.16%	0.020%
74	15.075	4361	4365	4370	rBV7	1312	1609	0.20%	0.025%
75	15.316	4438	4440	4443	rVB3	1628	989	0.12%	0.015%
76	15.512	4497	4501	4502	rBV3	1110	710	0.09%	0.011%

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DCLT0

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\SFAMVLM121523WMA.M
Title : VOC Analysis

77	15.702	4558	4560	4563	rVB3	1653	664	0.08%	0.010%
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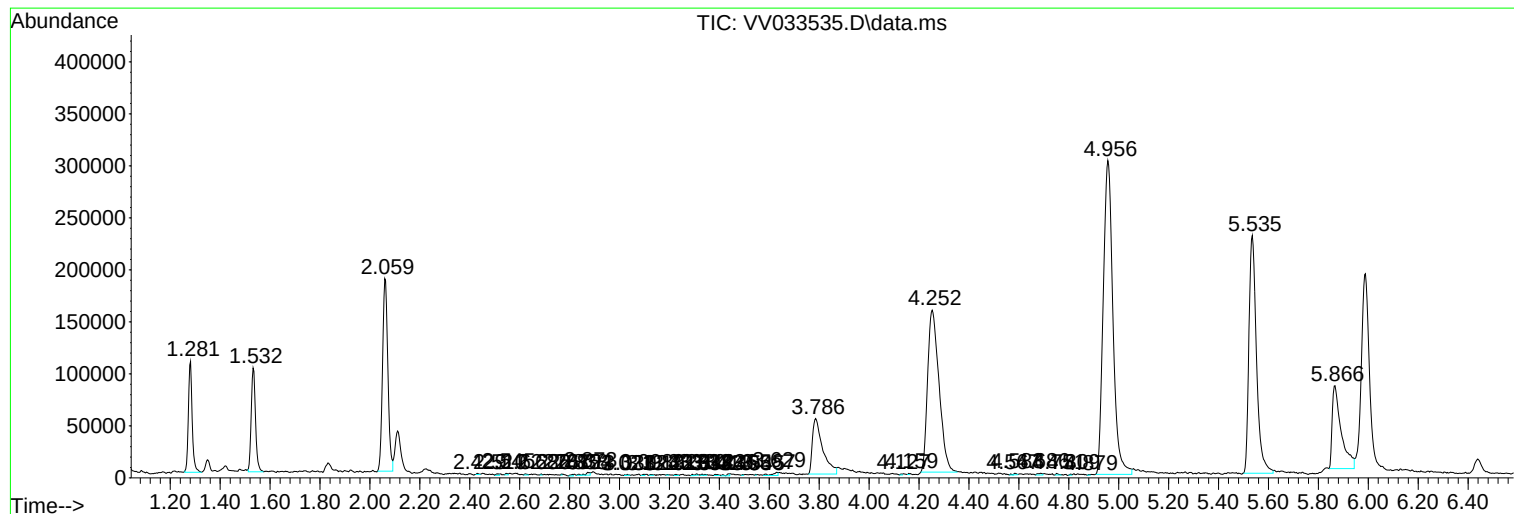
Sum of corrected areas: 6559937

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Instrument :
MSVOA_V
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM121523WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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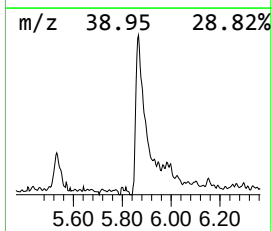
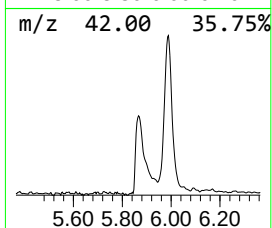
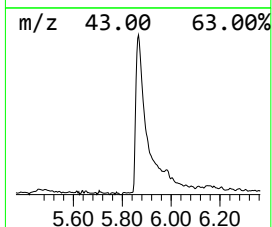
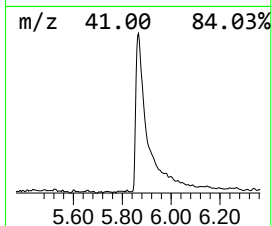
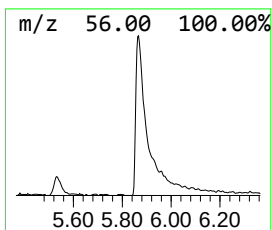
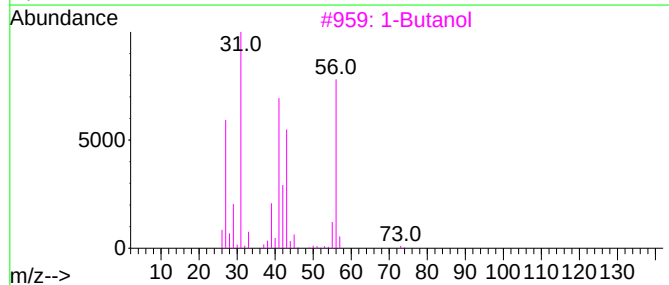
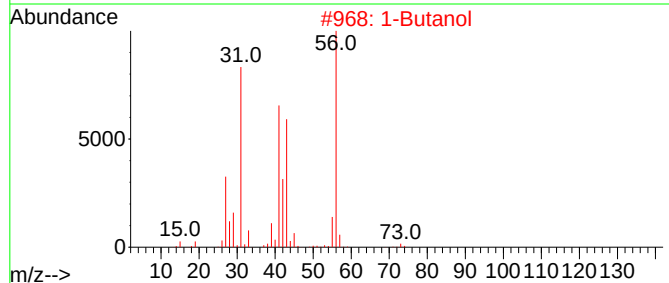
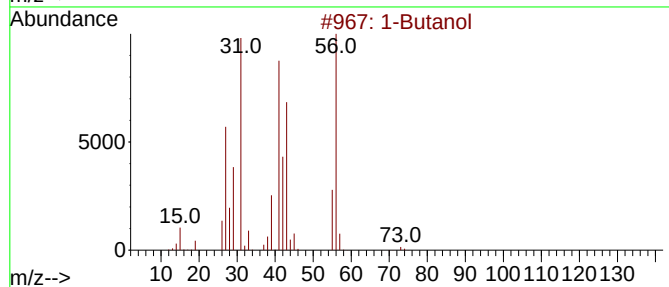
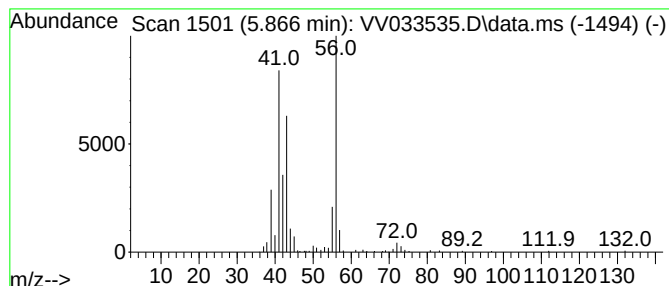
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM121523WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 1-Butanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.866	20.81 ug/L	200200	1,4-Difluorobenzene	5.535

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol			74	C4H10O	000071-36-3	80
2	1-Butanol			74	C4H10O	000071-36-3	80
3	1-Butanol			74	C4H10O	000071-36-3	72
4	1-Butanol			74	C4H10O	000071-36-3	64
5	1-Butanol			74	C4H10O	000071-36-3	43



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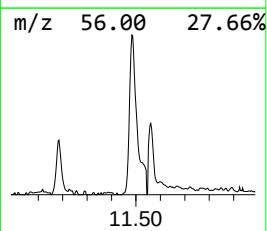
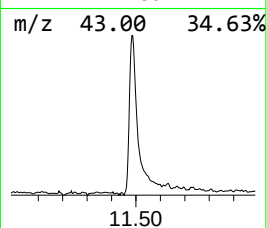
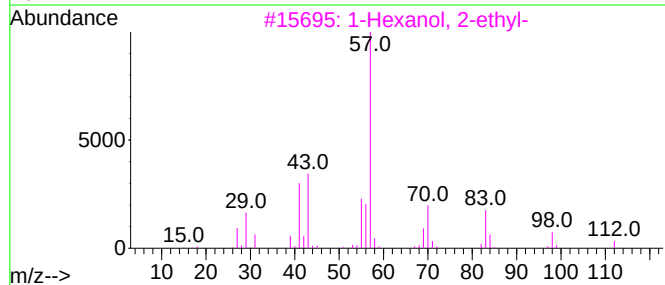
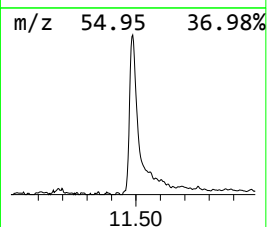
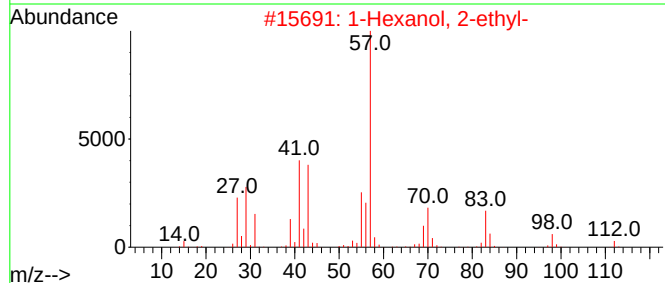
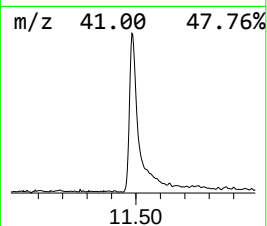
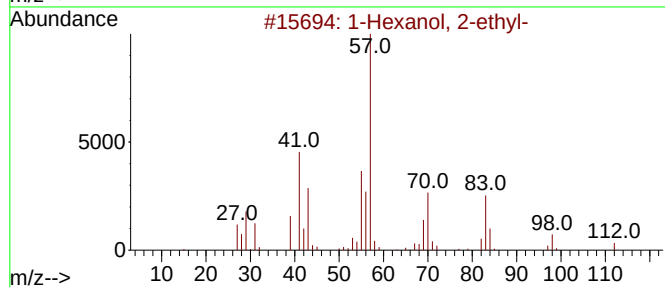
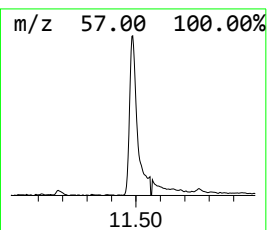
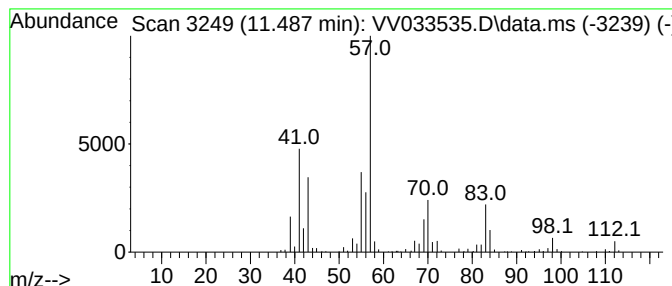
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM121523WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.487	29.09 ug/L	329752	1,4-Dichlorobenzene-d4	11.185

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	72
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	64
4	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	64
5	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	64



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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-Butanol	5.866	20.8	ug/L	200200	1	5.535	481031	50.0
1-Hexanol, 2-et...	11.487	29.1	ug/L	329752	3	11.185	566731	50.0