

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050923\
 Data File : VU054127.D
 Acq On : 09 May 2023 17:47
 Operator : JC/MD
 Sample : 02694-07
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 JREM7

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\SFAMULM042923WMA.M

Title : VOC Analysis

Signal : TIC: VU054127.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	73	80	101	rVB	67534	81990	11.22%	1.375%
2	1.906	169	176	194	rVB	59409	82742	11.32%	1.387%
3	2.562	365	380	393	rBV	133660	228005	31.19%	3.822%
4	2.623	394	399	411	rVB2	8549	13712	1.88%	0.230%
5	2.777	434	447	450	rBV5	2516	4728	0.65%	0.079%
6	3.022	521	523	524	rBV5	246	99	0.01%	0.002%
7	3.038	524	528	540	rVB4	1098	1636	0.22%	0.027%
8	3.080	540	541	543	rBV4	232	83	0.01%	0.001%
9	3.179	564	572	574	rBV3	1342	1911	0.26%	0.032%
10	3.372	630	632	633	rBV3	119	32	0.00%	0.001%
11	3.456	656	658	660	rBV	181	84	0.01%	0.001%
12	3.642	713	716	719	rBV	404	197	0.03%	0.003%
13	3.771	750	756	759	rBV2	398	443	0.06%	0.007%
14	3.816	768	770	771	rBV2	123	58	0.01%	0.001%
15	4.054	842	844	845	rBV	129	50	0.01%	0.001%
16	4.231	896	899	902	rBV	203	108	0.01%	0.002%
17	4.295	916	919	920	rBV	230	152	0.02%	0.003%
18	4.317	923	926	928	rVV	222	168	0.02%	0.003%
19	4.449	964	967	969	rBV2	361	263	0.04%	0.004%
20	4.559	997	1001	1004	rVB2	213	161	0.02%	0.003%
21	4.617	1008	1019	1044	rBV	60289	150318	20.56%	2.520%
22	4.967	1126	1128	1133	rBV2	177	147	0.02%	0.002%
23	5.057	1140	1156	1181	rBV	136074	302725	41.41%	5.075%
24	5.260	1216	1219	1224	rVB	452	264	0.04%	0.004%
25	5.424	1268	1270	1272	rBV	115	43	0.01%	0.001%
26	5.443	1272	1276	1279	rVB2	279	231	0.03%	0.004%
27	5.501	1291	1294	1295	rBV	188	105	0.01%	0.002%
28	5.530	1302	1303	1304	rBV	111	43	0.01%	0.001%
29	5.571	1314	1316	1319	rVB	215	101	0.01%	0.002%
30	5.620	1329	1331	1338	rBV	167	220	0.03%	0.004%
31	5.719	1341	1362	1385	rBV2	265689	731044	100.00%	12.256%
32	5.973	1439	1441	1442	rBV	180	57	0.01%	0.001%
33	6.002	1447	1450	1452	rBV2	196	143	0.02%	0.002%
34	6.038	1459	1461	1463	rVB	183	88	0.01%	0.001%
35	6.243	1511	1525	1551	rBV	266971	517613	70.80%	8.678%
36	6.494	1599	1603	1605	rBV3	204	146	0.02%	0.002%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042923WMA.M
 Title : VOC Analysis

37	6.523	1606	1612	1620	rVV3	1907	2990	0.41%	0.050%
38	6.584	1628	1631	1634	rBV2	338	212	0.03%	0.004%
39	6.600	1634	1636	1639	rBV2	245	142	0.02%	0.002%
40	6.684	1648	1662	1686	rBV	174825	340846	46.62%	5.714%
41	6.842	1708	1711	1714	rBV	355	198	0.03%	0.003%
42	6.883	1716	1724	1734	rBV4	1657	2629	0.36%	0.044%
43	7.060	1776	1779	1780	rBV	166	69	0.01%	0.001%
44	7.115	1792	1796	1800	rBV2	222	223	0.03%	0.004%
45	7.182	1807	1817	1823	rBV5	1043	1531	0.21%	0.026%
46	7.350	1865	1869	1871	rBV2	195	142	0.02%	0.002%
47	7.449	1898	1900	1904	rBV	309	215	0.03%	0.004%
48	7.472	1905	1907	1909	rBV	170	101	0.01%	0.002%
49	7.562	1923	1935	1950	rBV	94128	165301	22.61%	2.771%
50	7.790	1998	2006	2016	rBV5	2661	4360	0.60%	0.073%
51	7.893	2025	2038	2052	rBV	332626	569453	77.90%	9.547%
52	8.086	2096	2098	2101	rBV	321	148	0.02%	0.002%
53	8.173	2115	2125	2140	rBV	66714	113157	15.48%	1.897%
54	8.285	2156	2160	2164	rVB	276	186	0.03%	0.003%
55	8.340	2172	2177	2181	rBV	475	496	0.07%	0.008%
56	8.523	2231	2234	2236	rBV	189	143	0.02%	0.002%
57	8.629	2255	2267	2299	rBV2	180258	338102	46.25%	5.668%
58	8.784	2305	2315	2331	rVB2	25797	44831	6.13%	0.752%
59	8.960	2368	2370	2372	rBV	210	89	0.01%	0.001%
60	9.131	2421	2423	2425	rBV	168	68	0.01%	0.001%
61	9.179	2434	2438	2439	rBV	209	155	0.02%	0.003%
62	9.259	2460	2463	2471	rVB2	345	358	0.05%	0.006%
63	9.301	2474	2476	2478	rBV	164	84	0.01%	0.001%
64	9.411	2498	2510	2533	rBV	375679	628182	85.93%	10.531%
65	9.687	2584	2596	2604	rBV5	2027	3424	0.47%	0.057%
66	9.790	2626	2628	2629	rBV	149	39	0.01%	0.001%
67	9.819	2634	2637	2642	rBV2	307	233	0.03%	0.004%
68	9.874	2651	2654	2657	rBV	188	153	0.02%	0.003%
69	10.025	2698	2701	2706	rBV2	287	311	0.04%	0.005%
70	10.099	2718	2724	2726	rBV2	904	924	0.13%	0.015%
71	10.221	2759	2762	2763	rBV	234	119	0.02%	0.002%
72	10.346	2796	2801	2807	rVB3	1124	1341	0.18%	0.022%
73	10.484	2838	2844	2852	rBV2	422	650	0.09%	0.011%
74	10.591	2874	2877	2880	rVB2	246	159	0.02%	0.003%
75	10.751	2914	2927	2944	rBV	243315	395305	54.07%	6.627%
76	11.192	3062	3064	3065	rBV	209	87	0.01%	0.001%

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Peak Location: TOP

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Title : VOC Analysis

77	11.465	3144	3149	3160	rVB5	1008	1686	0.23%	0.028%
78	11.597	3187	3190	3194	rBV2	321	240	0.03%	0.004%
79	11.806	3243	3255	3276	rBV	400817	633434	86.65%	10.619%
80	11.999	3313	3315	3317	rVB	434	151	0.02%	0.003%
81	12.189	3361	3374	3396	rBV	351891	590987	80.84%	9.908%
82	13.025	3631	3634	3640	rVB2	409	367	0.05%	0.006%
83	13.221	3692	3695	3699	rVB2	655	512	0.07%	0.009%
84	13.690	3838	3841	3842	rBV	548	328	0.04%	0.005%
85	13.735	3852	3855	3857	rBV	336	196	0.03%	0.003%

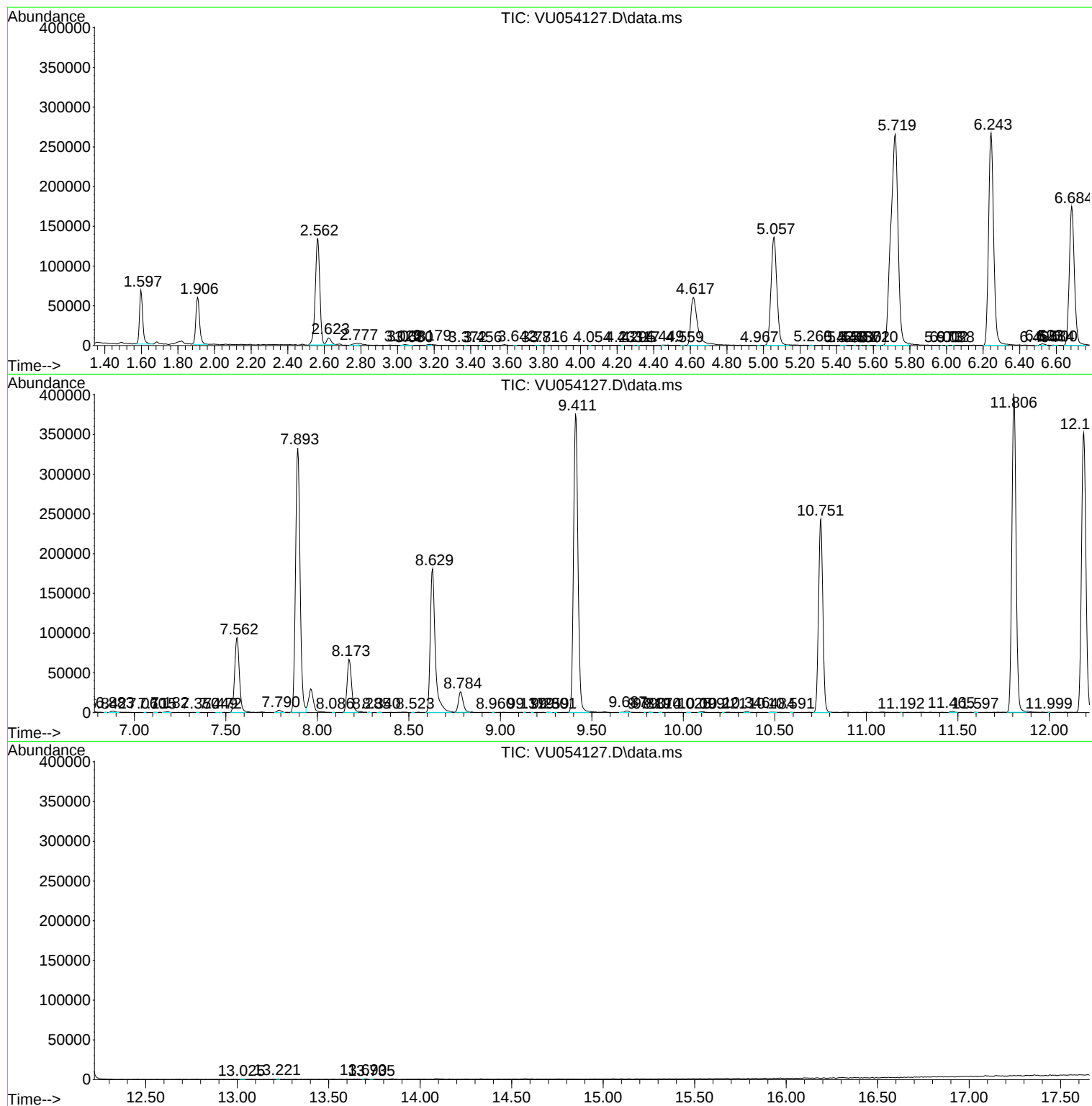
Sum of corrected areas: 5964967

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042923WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_U
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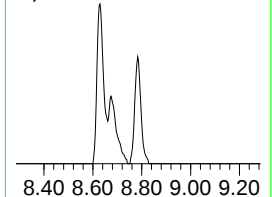
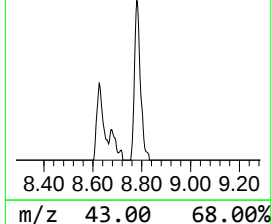
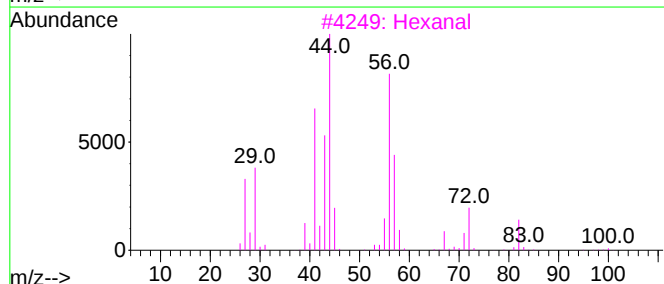
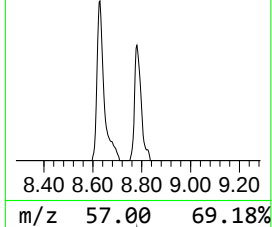
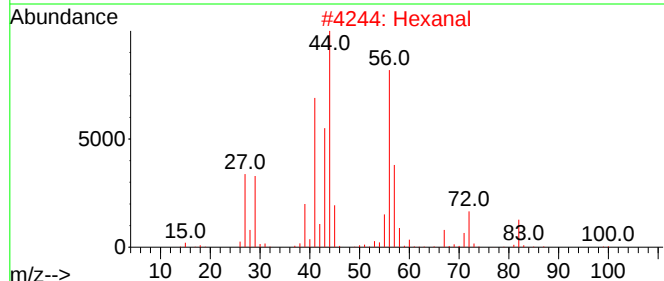
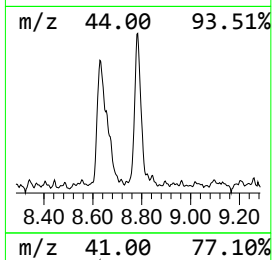
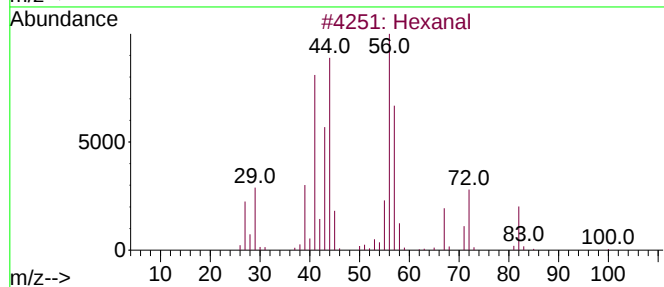
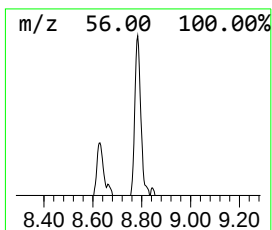
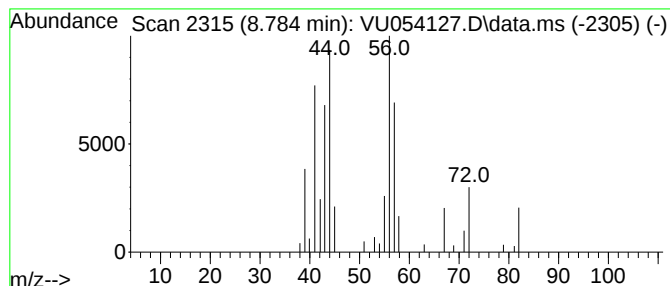
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042923WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Hexanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.784	3.57 ug/L	44831	Chlorobenzene-d5	9.411

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	72
2	Hexanal			100	C6H12O	000066-25-1	64
3	Hexanal			100	C6H12O	000066-25-1	64
4	Hexanal			100	C6H12O	000066-25-1	53
5	Hexanal			100	C6H12O	000066-25-1	53



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Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanal	8.784	3.6	ug/L	44831	2	9.411	628182	50.0