

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102623\
 Data File : VU055904.D
 Acq On : 26 Oct 2023 14:48
 Operator : MD/SY
 Sample : 04961-06MERE
 Misc : 5.59g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 E0LJ2MERE

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\SFAMULM101023WMA.M
 Title : VOC Analysis

Signal : TIC: VU055904.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.473	49	57	66	rBV2	21881	48018	1.09%	0.252%
2	1.599	89	96	128	rVB	101864	182913	4.16%	0.959%
3	2.544	379	390	409	rBV	190346	318445	7.25%	1.670%
4	2.769	455	460	469	rBV	2785	3691	0.08%	0.019%
5	2.891	494	498	500	rBV3	442	351	0.01%	0.002%
6	3.036	532	543	563	rVV7	5804	15964	0.36%	0.084%
7	3.174	571	586	604	rBV2	28372	69122	1.57%	0.363%
8	3.473	672	679	682	rBV4	458	554	0.01%	0.003%
9	3.676	734	742	744	rBV4	1753	2176	0.05%	0.011%
10	3.743	756	763	767	rBV	482	532	0.01%	0.003%
11	3.894	804	810	812	rVB2	274	317	0.01%	0.002%
12	3.959	828	830	835	rBV2	518	433	0.01%	0.002%
13	4.164	891	894	900	rVB2	433	423	0.01%	0.002%
14	4.193	900	903	909	rVB	359	298	0.01%	0.002%
15	4.383	959	962	968	rVB2	324	325	0.01%	0.002%
16	4.428	973	976	980	rVB2	520	372	0.01%	0.002%
17	4.496	993	997	999	rBV2	385	307	0.01%	0.002%
18	4.627	1026	1038	1096	rBV2	133765	465874	10.60%	2.444%
19	5.058	1155	1172	1197	rBV	270735	648346	14.76%	3.401%
20	5.219	1220	1222	1224	rBV2	732	315	0.01%	0.002%
21	5.341	1245	1260	1269	rBV3	4332	11606	0.26%	0.061%
22	5.518	1312	1315	1321	rVB	396	325	0.01%	0.002%
23	5.573	1328	1332	1333	rBV2	592	381	0.01%	0.002%
24	5.714	1353	1376	1409	rBV2	531935	1469417	33.45%	7.708%
25	5.875	1425	1426	1430	rVB2	633	363	0.01%	0.002%
26	5.978	1447	1458	1465	rBV7	3754	8093	0.18%	0.042%
27	6.081	1486	1490	1493	rBV2	544	359	0.01%	0.002%
28	6.132	1500	1506	1516	rVB7	2114	3118	0.07%	0.016%
29	6.245	1526	1541	1573	rBV	616913	1246997	28.39%	6.541%
30	6.541	1618	1633	1645	rBV7	30608	64146	1.46%	0.336%
31	6.602	1645	1652	1663	rVB5	5252	9855	0.22%	0.052%
32	6.685	1665	1678	1699	rBV	351888	720690	16.41%	3.780%
33	7.010	1776	1779	1783	rBV2	460	301	0.01%	0.002%
34	7.045	1783	1790	1792	rVV4	391	441	0.01%	0.002%
35	7.193	1825	1836	1837	rBV4	4560	5085	0.12%	0.027%
36	7.293	1863	1867	1869	rBV2	772	602	0.01%	0.003%

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 Title : VOC Analysis

37	7.328	1876	1878	1886	rVB3	748	736	0.02%	0.004%
38	7.489	1923	1928	1937	rBV5	1821	2456	0.06%	0.013%
39	7.563	1937	1951	1973	rBV2	176597	354533	8.07%	1.860%
40	7.701	1987	1994	1996	rBV4	2417	2840	0.06%	0.015%
41	7.795	2013	2023	2033	rVB5	5463	10157	0.23%	0.053%
42	7.846	2036	2039	2041	rBV3	468	302	0.01%	0.002%
43	7.897	2041	2055	2074	rBV	545346	985488	22.43%	5.169%
44	8.071	2107	2109	2115	rVB4	801	654	0.01%	0.003%
45	8.129	2122	2127	2132	rVB5	1982	2216	0.05%	0.012%
46	8.184	2132	2144	2164	rBV	116773	249448	5.68%	1.308%
47	8.344	2186	2194	2197	rBV5	1561	2416	0.05%	0.013%
48	8.476	2224	2235	2241	rBV5	1676	2986	0.07%	0.016%
49	8.550	2243	2258	2276	rBV	2529376	4393059	100.00%	23.043%
50	8.650	2277	2289	2328	rVB	577727	1183066	26.93%	6.206%
51	8.872	2356	2358	2366	rVB6	1344	973	0.02%	0.005%
52	8.920	2366	2373	2375	rBV6	2676	3139	0.07%	0.016%
53	9.023	2402	2405	2407	rBV	968	494	0.01%	0.003%
54	9.116	2430	2434	2437	rBV3	1296	1078	0.02%	0.006%
55	9.158	2442	2447	2449	rBV3	1508	1453	0.03%	0.008%
56	9.209	2456	2463	2473	rVB9	4376	6990	0.16%	0.037%
57	9.335	2492	2502	2512	rBV8	3404	5073	0.12%	0.027%
58	9.422	2514	2529	2553	rBV	907431	1665385	37.91%	8.736%
59	9.573	2574	2576	2581	rVB6	1426	967	0.02%	0.005%
60	9.621	2587	2591	2595	rBV4	649	506	0.01%	0.003%
61	9.701	2606	2616	2622	rBV4	6091	9697	0.22%	0.051%
62	9.811	2646	2650	2655	rBV2	902	771	0.02%	0.004%
63	9.840	2655	2659	2662	rBV	484	399	0.01%	0.002%
64	9.875	2666	2670	2674	rVB2	729	514	0.01%	0.003%
65	9.952	2690	2694	2700	rVB3	622	493	0.01%	0.003%
66	10.026	2706	2717	2720	rBV6	1676	2759	0.06%	0.014%
67	10.042	2720	2722	2727	rVB3	1357	937	0.02%	0.005%
68	10.113	2732	2744	2746	rBV7	3149	4638	0.11%	0.024%
69	10.206	2768	2773	2774	rBV4	617	469	0.01%	0.002%
70	10.251	2779	2787	2800	rVB8	4497	7779	0.18%	0.041%
71	10.351	2810	2818	2824	rBV10	1780	3484	0.08%	0.018%
72	10.393	2825	2831	2842	rVB5	6026	9675	0.22%	0.051%
73	10.553	2868	2881	2884	rBV7	2958	4700	0.11%	0.025%
74	10.624	2894	2903	2908	rBV6	4251	6234	0.14%	0.033%
75	10.759	2931	2945	2980	rVV	738935	1207858	27.49%	6.336%
76	10.894	2984	2987	2991	rBV5	866	658	0.01%	0.003%

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 Title : VOC Analysis

77	10.946	3001	3003	3005	rBV2	597	359	0.01%	0.002%
78	10.987	3012	3016	3019	rBV3	827	726	0.02%	0.004%
79	11.010	3019	3023	3024	rBV3	758	499	0.01%	0.003%
80	11.055	3031	3037	3038	rBV6	1906	1640	0.04%	0.009%
81	11.113	3048	3055	3071	rVB2	17710	30107	0.69%	0.158%
82	11.203	3078	3083	3090	rVB5	1337	1787	0.04%	0.009%
83	11.257	3096	3100	3102	rBV4	789	664	0.02%	0.003%
84	11.309	3110	3116	3125	rBV6	3487	5668	0.13%	0.030%
85	11.376	3130	3137	3140	rVV6	2887	3894	0.09%	0.020%
86	11.415	3142	3149	3157	rVB4	13492	18935	0.43%	0.099%
87	11.566	3192	3196	3198	rBV4	1460	1234	0.03%	0.006%
88	11.637	3215	3218	3229	rVB8	5533	7808	0.18%	0.041%
89	11.708	3229	3240	3245	rBV10	2219	4418	0.10%	0.023%
90	11.814	3260	3273	3290	rBV	1068410	1748885	39.81%	9.174%
91	12.193	3375	3391	3409	rBV	858100	1425910	32.46%	7.479%
92	12.325	3424	3432	3444	rVB2	44375	68452	1.56%	0.359%
93	12.663	3530	3537	3547	rVB6	8047	12659	0.29%	0.066%
94	12.942	3608	3624	3636	rBV9	13265	42373	0.96%	0.222%
95	13.003	3639	3643	3650	rVV8	6898	9591	0.22%	0.050%
96	13.048	3652	3657	3664	rVB9	7995	10873	0.25%	0.057%
97	13.132	3679	3683	3693	rVB5	7067	9687	0.22%	0.051%
98	13.431	3767	3776	3800	rVB2	62476	107294	2.44%	0.563%
99	13.585	3815	3824	3836	rBV	31328	53623	1.22%	0.281%
100	14.447	4085	4092	4101	rVB2	42608	59278	1.35%	0.311%

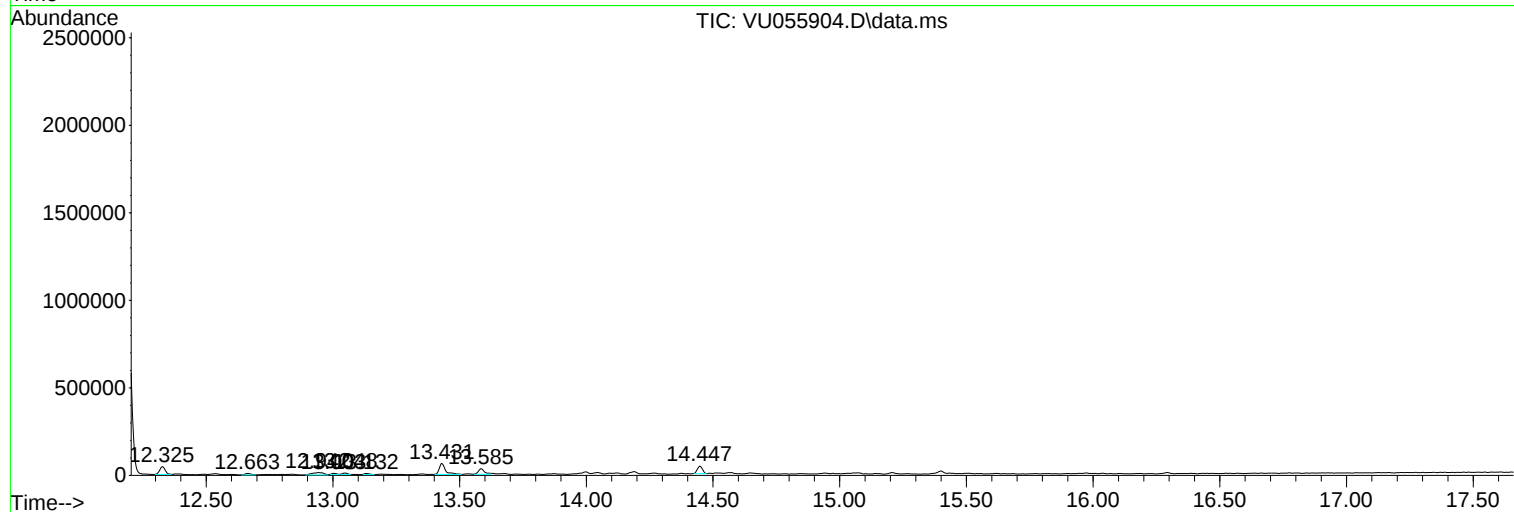
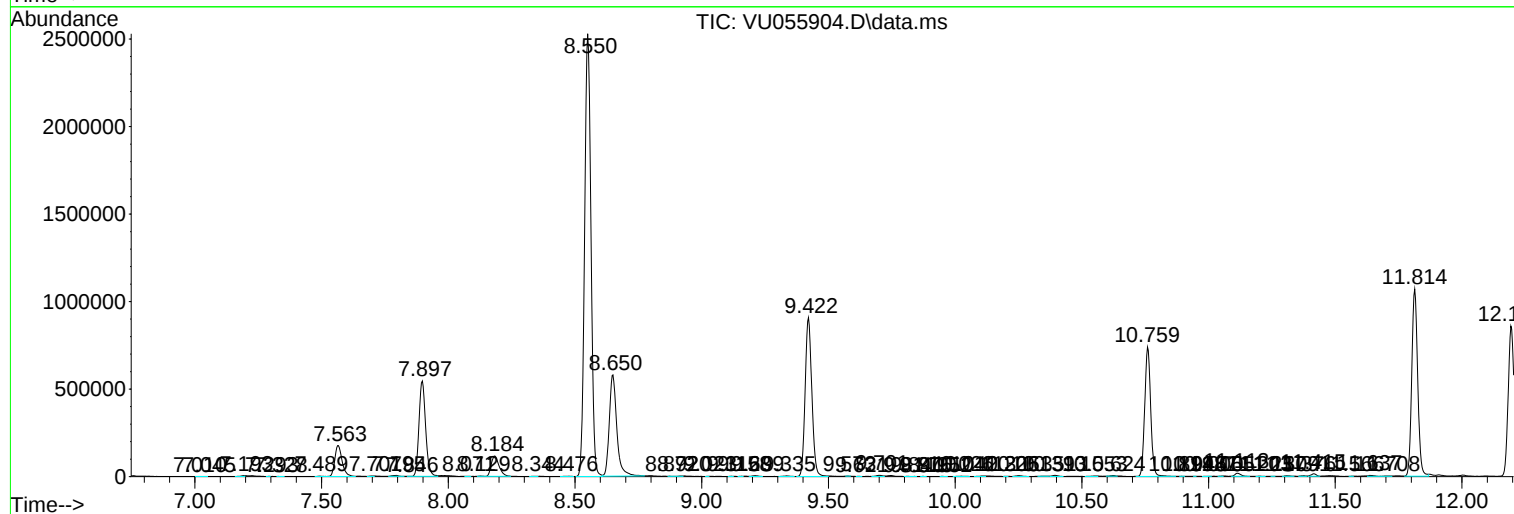
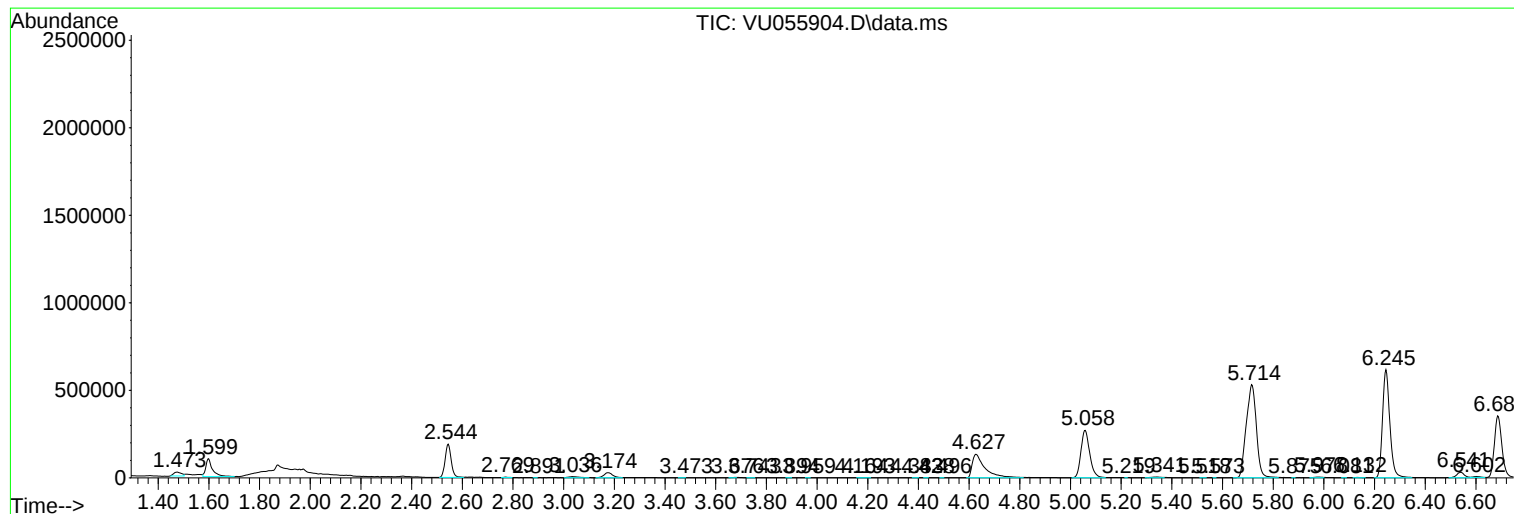
Sum of corrected areas: 19064399

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Instrument :
MSVOA_U
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.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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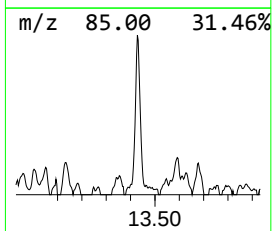
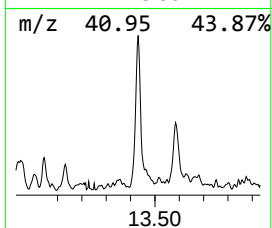
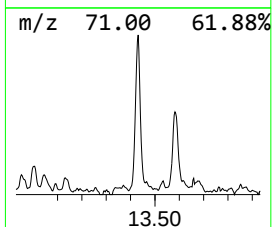
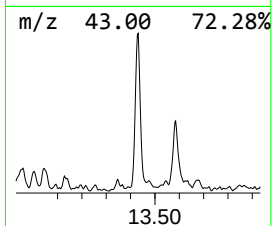
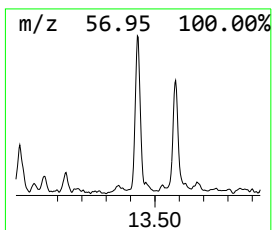
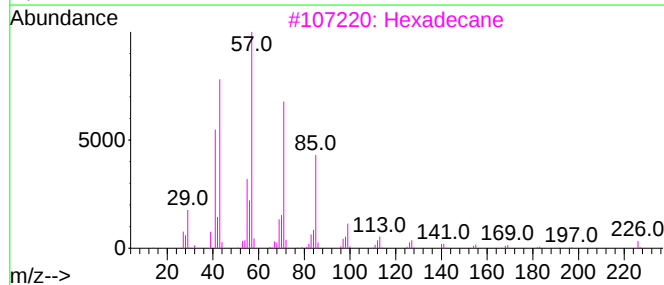
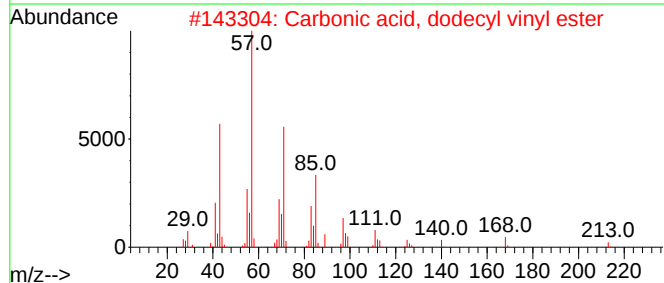
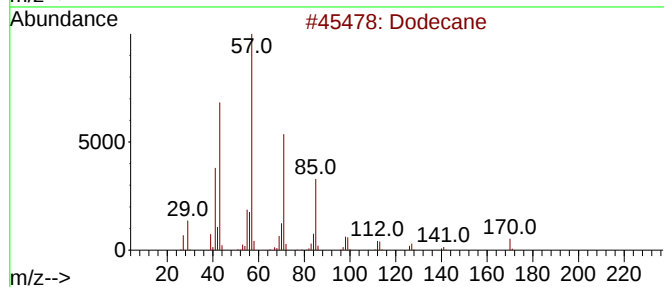
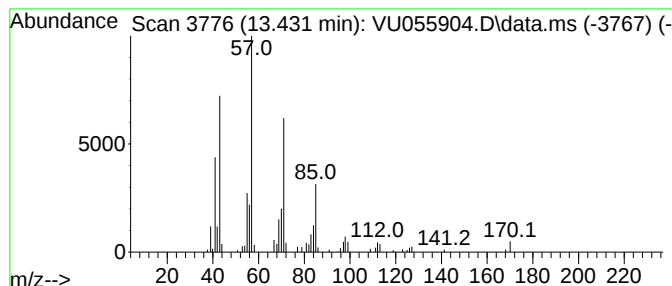
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.431	3.07 ug/L	107294	1,4-Dichlorobenzene-d4	11.814

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	93
2			Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	83
3			Hexadecane	226	C16H34	000544-76-3	80
4			Tetradecane	198	C14H30	000629-59-4	80
5			Undecane	156	C11H24	001120-21-4	78



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	13.431	3.1	ug/L	107294	3	11.814	1748890	50.0