

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062624\
 Data File : VU059529.D
 Acq On : 26 Jun 2024 17:15
 Operator : MD/SY
 Sample : P2909-11ME
 Misc : 4.37g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A4CP0ME

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\SFAMULM052924WMA.M
 Title : VOC Analysis

Signal : TIC: VU059529.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.593	85	94	116	rBV	84232	146164	13.79%	1.536%
2	1.869	136	180	202	rBV5	94272	538944	50.84%	5.664%
3	2.538	376	388	410	rVB	205662	336311	31.72%	3.534%
4	2.625	412	415	416	rBV2	1739	909	0.09%	0.010%
5	2.760	453	457	460	rBV	671	698	0.07%	0.007%
6	2.946	502	515	529	rBV	17813	36187	3.41%	0.380%
7	3.030	530	541	551	rVB3	4947	9701	0.92%	0.102%
8	3.175	568	586	600	rBV2	7495	19491	1.84%	0.205%
9	3.695	743	748	752	rBV2	294	336	0.03%	0.004%
10	4.184	890	900	903	rBV2	348	461	0.04%	0.005%
11	4.557	1011	1016	1021	rBV	318	314	0.03%	0.003%
12	4.618	1025	1035	1073	rBV	96808	286396	27.02%	3.010%
13	4.888	1117	1119	1126	rVB3	330	312	0.03%	0.003%
14	5.052	1153	1170	1197	rVV	187513	420217	39.64%	4.416%
15	5.184	1206	1211	1218	rVB4	355	397	0.04%	0.004%
16	5.345	1253	1261	1266	rBV2	243	339	0.03%	0.004%
17	5.711	1355	1375	1398	rBV2	399826	1060103	100.00%	11.140%
18	6.043	1472	1478	1482	rBV3	343	395	0.04%	0.004%
19	6.239	1526	1539	1574	rBV	335468	650927	61.40%	6.840%
20	6.528	1619	1629	1640	rVB5	3099	5833	0.55%	0.061%
21	6.599	1645	1651	1653	rBV	240	255	0.02%	0.003%
22	6.682	1663	1677	1702	rBV	238401	472726	44.59%	4.968%
23	6.805	1710	1715	1718	rBV3	571	609	0.06%	0.006%
24	6.875	1732	1737	1742	rBV2	249	302	0.03%	0.003%
25	7.036	1782	1787	1795	rBV2	187	294	0.03%	0.003%
26	7.203	1829	1839	1842	rBV4	1548	2184	0.21%	0.023%
27	7.560	1938	1950	1978	rBV	123555	227280	21.44%	2.388%
28	7.653	1978	1979	1986	rVB3	430	305	0.03%	0.003%
29	7.708	1989	1996	2002	rBV4	830	1119	0.11%	0.012%
30	7.891	2039	2053	2073	rBV	471358	831951	78.48%	8.743%
31	8.174	2131	2141	2162	rVV2	84149	153308	14.46%	1.611%
32	8.467	2224	2232	2243	rBV3	941	1753	0.17%	0.018%
33	8.634	2272	2284	2316	rBV	306814	639090	60.29%	6.716%
34	8.850	2346	2351	2358	rBV4	488	766	0.07%	0.008%
35	8.924	2370	2374	2378	rVB4	381	373	0.04%	0.004%
36	9.116	2432	2434	2440	rVB3	528	407	0.04%	0.004%

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 Title : VOC Analysis

37	9.206	2455	2462	2465	rBV3	1112	958	0.09%	0.010%
38	9.332	2492	2501	2513	rVB3	2258	3289	0.31%	0.035%
39	9.412	2513	2526	2562	rBV	489875	838001	79.05%	8.806%
40	9.599	2576	2584	2594	rVB5	2161	3871	0.37%	0.041%
41	9.644	2594	2598	2600	rBV2	335	271	0.03%	0.003%
42	9.657	2600	2602	2608	rVB2	827	664	0.06%	0.007%
43	9.689	2608	2612	2613	rBV2	1080	694	0.07%	0.007%
44	9.747	2626	2630	2631	rBV	475	388	0.04%	0.004%
45	9.760	2631	2634	2642	rVB3	846	852	0.08%	0.009%
46	9.943	2688	2691	2692	rBV2	623	358	0.03%	0.004%
47	10.017	2706	2714	2721	rBV6	4757	8028	0.76%	0.084%
48	10.113	2733	2744	2752	rBV5	4868	8448	0.80%	0.089%
49	10.245	2774	2785	2798	rVB2	17096	29428	2.78%	0.309%
50	10.313	2798	2806	2808	rBV4	2349	2784	0.26%	0.029%
51	10.351	2810	2818	2824	rVV7	7244	12636	1.19%	0.133%
52	10.390	2825	2830	2842	rVB4	9930	15010	1.42%	0.158%
53	10.460	2844	2852	2855	rBV5	2668	3269	0.31%	0.034%
54	10.554	2867	2881	2890	rBV9	9915	21869	2.06%	0.230%
55	10.618	2895	2901	2914	rVB4	16576	26940	2.54%	0.283%
56	10.753	2929	2943	2977	rVB	426998	706946	66.69%	7.429%
57	10.895	2977	2987	2989	rBV8	1945	2911	0.27%	0.031%
58	10.943	2997	3002	3005	rBV7	2096	2049	0.19%	0.022%
59	11.058	3031	3038	3048	rBV6	8527	14334	1.35%	0.151%
60	11.197	3072	3081	3088	rBV8	1730	3187	0.30%	0.033%
61	11.239	3090	3094	3099	rBV5	1438	1745	0.16%	0.018%
62	11.312	3110	3117	3126	rVB7	7579	11518	1.09%	0.121%
63	11.370	3128	3135	3140	rBV5	6809	10241	0.97%	0.108%
64	11.412	3140	3148	3156	rVB2	45407	63366	5.98%	0.666%
65	11.567	3189	3196	3204	rBV6	6437	10677	1.01%	0.112%
66	11.705	3233	3239	3247	rBV6	10156	14136	1.33%	0.149%
67	11.811	3260	3272	3285	rBV	551566	898439	84.75%	9.442%
68	12.094	3351	3360	3361	rBV8	3520	4136	0.39%	0.043%
69	12.190	3375	3390	3405	rBV	532405	879600	82.97%	9.244%
70	12.431	3462	3465	3468	rBV4	815	665	0.06%	0.007%
71	12.489	3471	3483	3486	rBV10	3833	7647	0.72%	0.080%
72	12.663	3529	3537	3546	rBV7	4309	6971	0.66%	0.073%
73	12.698	3546	3548	3551	rBV4	715	510	0.05%	0.005%
74	12.753	3563	3565	3567	rBV2	594	347	0.03%	0.004%
75	12.792	3574	3577	3582	rBV3	1013	948	0.09%	0.010%
76	12.817	3582	3585	3586	rBV2	759	364	0.03%	0.004%

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Instrument :
 MSVOA_U
 ClientSampleId :
 A4CP0ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
 Title : VOC Analysis

77	12.878	3599	3604	3605	rBV3	583	577	0.05%	0.006%
78	12.927	3609	3619	3626	rBV3	6206	12261	1.16%	0.129%
79	13.046	3649	3656	3665	rVB6	4224	5973	0.56%	0.063%
80	13.103	3670	3674	3675	rBV2	474	327	0.03%	0.003%
81	13.123	3677	3680	3691	rVB6	1972	2903	0.27%	0.031%
82	13.193	3691	3702	3703	rBV4	858	900	0.08%	0.009%
83	13.338	3742	3747	3748	rBV2	324	279	0.03%	0.003%
84	13.354	3748	3752	3757	rVB3	718	602	0.06%	0.006%
85	13.399	3761	3766	3770	rBV3	562	537	0.05%	0.006%
86	13.457	3774	3784	3795	rVB6	2337	4147	0.39%	0.044%
87	13.521	3801	3804	3810	rVB3	548	510	0.05%	0.005%
88	13.579	3810	3822	3829	rBV7	1633	3073	0.29%	0.032%
89	13.695	3853	3858	3862	rVB2	405	397	0.04%	0.004%
90	13.785	3882	3886	3896	rBV3	283	423	0.04%	0.004%
91	13.849	3902	3906	3909	rVB3	550	479	0.05%	0.005%
92	13.946	3932	3936	3940	rBV2	417	435	0.04%	0.005%
93	14.097	3973	3983	3998	rBV	6048	12120	1.14%	0.127%
94	14.345	4057	4060	4065	rBV2	534	421	0.04%	0.004%
95	14.570	4123	4130	4138	rBV4	754	1255	0.12%	0.013%
96	14.721	4174	4177	4182	rBV2	403	285	0.03%	0.003%
97	15.203	4324	4327	4333	rBV2	410	400	0.04%	0.004%
98	15.264	4338	4346	4350	rBV5	923	1137	0.11%	0.012%
99	15.914	4546	4548	4552	rBV2	453	328	0.03%	0.003%
100	16.248	4650	4652	4654	rBV2	614	361	0.03%	0.004%

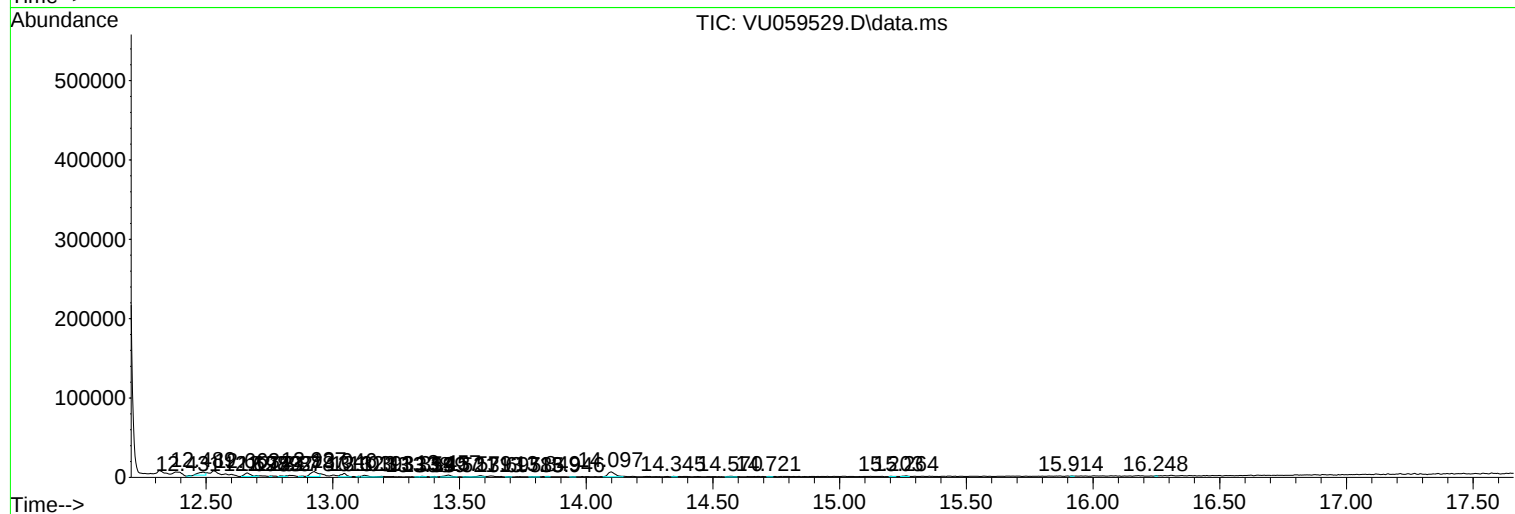
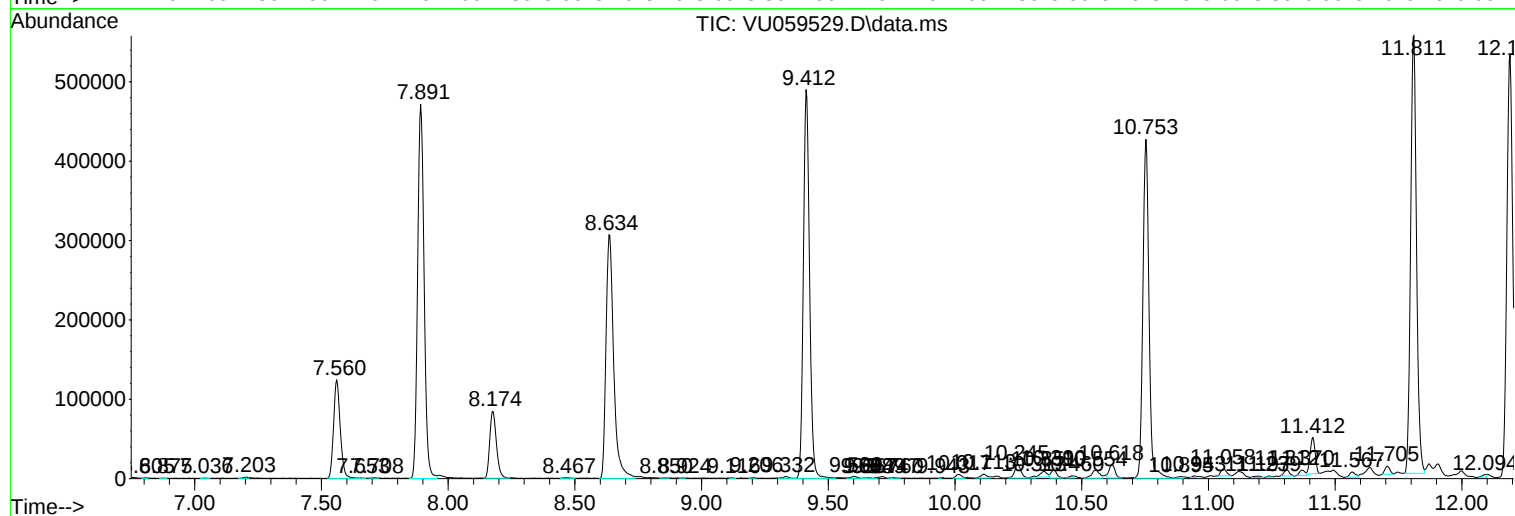
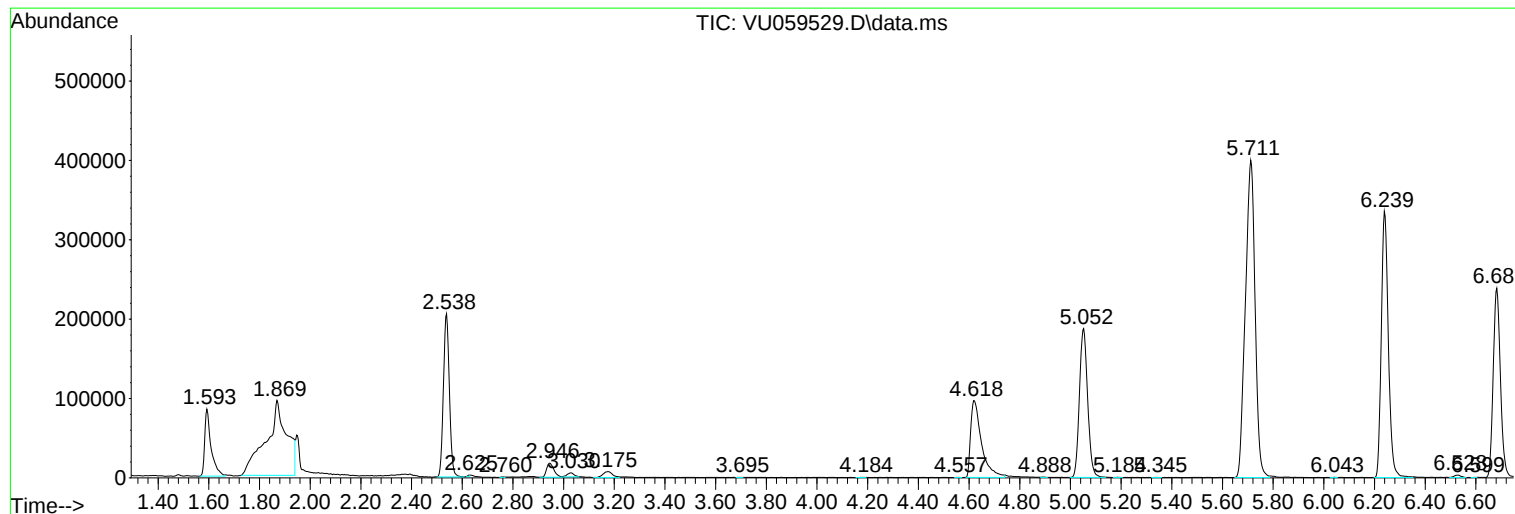
Sum of corrected areas: 9515782

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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A4CP0ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A4CP0ME

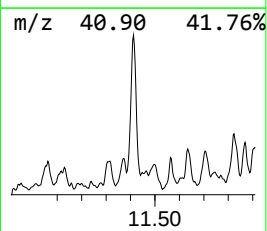
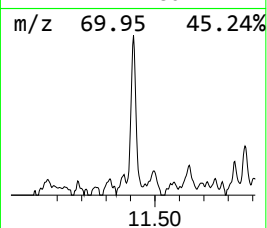
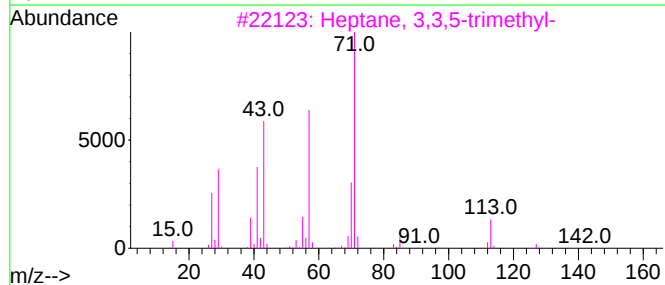
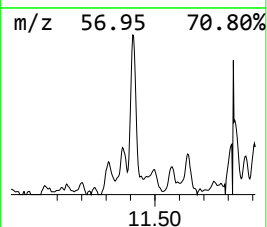
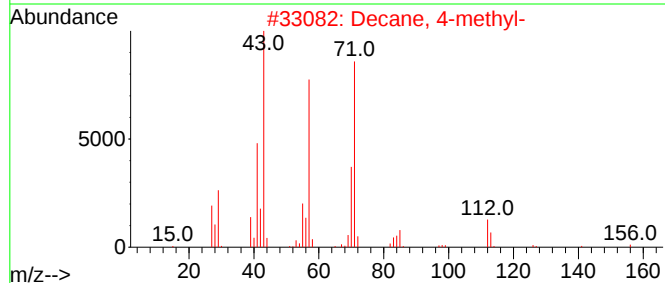
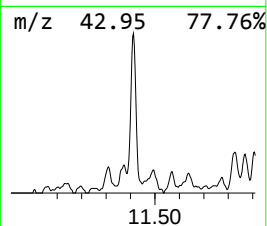
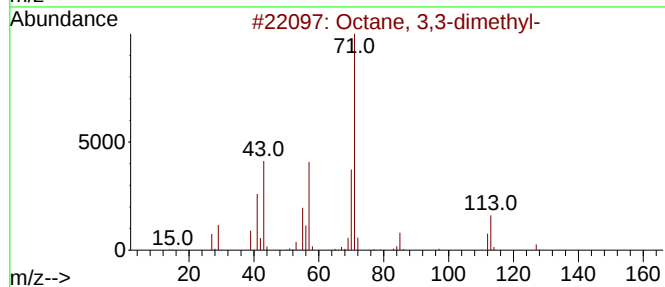
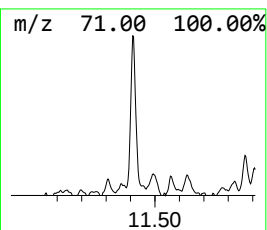
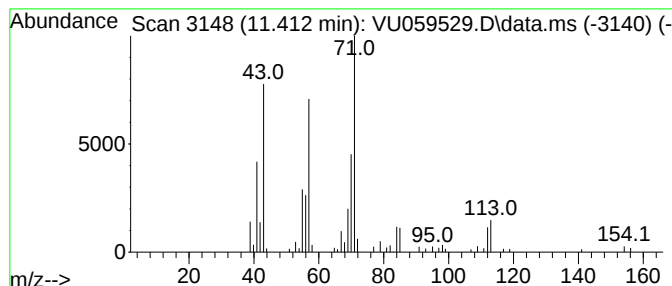
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.412	3.53 ug/L	63366	1,4-Dichlorobenzene-d4	11.811

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	64
2			Decane, 4-methyl-	156	C11H24	002847-72-5	64
3			Heptane, 3,3,5-trimethyl-	142	C10H22	007154-80-5	59
4			Carbonic acid, neopentyl 2-ethyl...	244	C14H28O3	1000357-85-7	59
5			Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	11.412	3.5	ug/L	63366	3	11.811	898439	50.0