

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV060421\
 Data File : VV021514.D
 Acq On : 04 Jun 2021 18:04
 Operator : SY/MD
 Sample : M2596-09ME
 Misc : 4.61g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BG5Q5ME

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\SFAMVLM052721WMA.M

Title : VOC Analysis

Signal : TIC: VV021514.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.214	49	54	56	rBV2	10386	10689	0.72%	0.088%
2	1.304	76	82	95	rBV	125069	151496	10.27%	1.250%
3	1.568	157	164	179	rBV	72629	109125	7.40%	0.901%
4	2.085	316	325	341	rVB	256166	369443	25.04%	3.049%
5	2.272	378	383	394	rVB2	5236	7570	0.51%	0.062%
6	2.420	427	429	433	rBV4	698	603	0.04%	0.005%
7	2.510	448	457	470	rVB4	15665	31515	2.14%	0.260%
8	2.616	479	490	505	rBV	7407	16402	1.11%	0.135%
9	2.748	518	531	557	rVB3	18391	41544	2.82%	0.343%
10	3.027	606	618	638	rVB3	10694	24079	1.63%	0.199%
11	3.130	647	650	654	rBV2	468	467	0.03%	0.004%
12	3.442	740	747	749	rBV5	672	736	0.05%	0.006%
13	3.577	784	789	791	rVB3	515	473	0.03%	0.004%
14	3.735	832	838	839	rBV4	500	451	0.03%	0.004%
15	3.815	859	863	865	rBV2	567	418	0.03%	0.003%
16	3.905	881	891	944	rBV	59450	308060	20.88%	2.542%
17	4.349	1014	1029	1061	rVB	213586	567814	38.48%	4.686%
18	4.664	1116	1127	1139	rBV4	6094	13714	0.93%	0.113%
19	4.751	1146	1154	1155	rBV4	5173	5398	0.37%	0.045%
20	4.902	1186	1201	1221	rBB2	25702	61152	4.14%	0.505%
21	5.043	1228	1245	1274	rBV2	558917	1435114	97.26%	11.844%
22	5.487	1375	1383	1399	rVB4	8616	18217	1.23%	0.150%
23	5.616	1410	1423	1453	rBV	496854	1085474	73.57%	8.959%
24	5.834	1489	1491	1495	rVB4	798	498	0.03%	0.004%
25	5.911	1504	1515	1535	rBV4	10040	29503	2.00%	0.243%
26	6.001	1536	1543	1550	rBV6	1294	2404	0.16%	0.020%
27	6.072	1550	1565	1594	rBV	292048	653945	44.32%	5.397%
28	6.365	1646	1656	1657	rBV6	2604	3053	0.21%	0.025%
29	6.464	1683	1687	1691	rVB4	981	928	0.06%	0.008%
30	6.567	1714	1719	1721	rBV3	1163	1265	0.09%	0.010%
31	6.747	1768	1775	1780	rBV10	1503	2525	0.17%	0.021%
32	6.783	1784	1786	1788	rBV3	838	530	0.04%	0.004%
33	6.915	1822	1827	1832	rBV8	2801	3793	0.26%	0.031%
34	6.989	1841	1850	1871	rVB	166913	329650	22.34%	2.721%
35	7.246	1926	1930	1932	rBV4	1416	1214	0.08%	0.010%
36	7.317	1940	1952	1972	rBV	644333	1183032	80.18%	9.764%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM052721WMA.M
 Title : VOC Analysis

37	7.571	2024	2031	2039	rVB3	10617	15652	1.06%	0.129%
38	7.625	2039	2048	2076	rBV	112574	234440	15.89%	1.935%
39	7.792	2096	2100	2102	rBV4	1703	1425	0.10%	0.012%
40	7.895	2128	2132	2135	rBV4	1362	1236	0.08%	0.010%
41	7.979	2150	2158	2169	rVB6	10299	17013	1.15%	0.140%
42	8.030	2170	2174	2182	rVB7	1128	1119	0.08%	0.009%
43	8.098	2183	2195	2198	rBV2	177397	261136	17.70%	2.155%
44	8.439	2293	2301	2307	rBV9	3550	6703	0.45%	0.055%
45	8.574	2337	2343	2349	rBV6	2646	3865	0.26%	0.032%
46	8.667	2367	2372	2383	rVB4	12982	20961	1.42%	0.173%
47	8.722	2383	2389	2399	rVB9	2264	3295	0.22%	0.027%
48	8.789	2401	2410	2419	rBV2	16376	26934	1.83%	0.222%
49	8.857	2419	2431	2454	rBV	718710	1323881	89.72%	10.926%
50	9.082	2493	2501	2505	rBV9	2733	4732	0.32%	0.039%
51	9.152	2515	2523	2531	rVB6	5869	10591	0.72%	0.087%
52	9.207	2533	2540	2548	rBV4	9641	13692	0.93%	0.113%
53	9.326	2568	2577	2584	rBV8	4187	6891	0.47%	0.057%
54	9.413	2599	2604	2605	rBV4	1255	1020	0.07%	0.008%
55	9.480	2619	2625	2631	rVB7	2718	3871	0.26%	0.032%
56	9.558	2643	2649	2651	rBV4	2556	2626	0.18%	0.022%
57	9.686	2681	2689	2691	rBV8	2943	3715	0.25%	0.031%
58	10.017	2784	2792	2802	rBV8	6804	12903	0.87%	0.106%
59	10.127	2821	2826	2836	rVB2	8112	11780	0.80%	0.097%
60	10.226	2836	2857	2875	rBV	455125	832483	56.42%	6.871%
61	10.461	2925	2930	2940	rVB9	3682	5595	0.38%	0.046%
62	10.583	2961	2968	2984	rVB5	11414	21820	1.48%	0.180%
63	10.660	2990	2992	2993	rBV	1066	487	0.03%	0.004%
64	10.924	3065	3074	3083	rBV4	8405	12813	0.87%	0.106%
65	11.201	3152	3160	3165	rBV7	3121	4234	0.29%	0.035%
66	11.252	3165	3176	3196	rBV	923366	1475522	100.00%	12.178%
67	11.464	3239	3242	3251	rVB5	2800	3236	0.22%	0.027%
68	11.574	3273	3276	3278	rBV3	1376	947	0.06%	0.008%
69	11.628	3282	3293	3317	rVB	766772	1245052	84.38%	10.276%
70	12.194	3466	3469	3473	rVB3	836	627	0.04%	0.005%
71	12.358	3514	3520	3527	rBV7	2297	3714	0.25%	0.031%
72	12.464	3551	3553	3561	rVB7	2042	2220	0.15%	0.018%
73	12.590	3587	3592	3600	rVB9	1570	1959	0.13%	0.016%
74	12.721	3630	3633	3634	rBV	852	397	0.03%	0.003%
75	12.795	3652	3656	3663	rBV6	1542	1766	0.12%	0.015%
76	12.860	3669	3676	3677	rBV6	1316	1262	0.09%	0.010%

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 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BG5Q5ME

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\SFAMVLM052721WMA.M
 Title : VOC Analysis

77	12.889	3680	3685	3688	rBV5	2865	2858	0.19%	0.024%
78	13.040	3728	3732	3734	rBV2	800	721	0.05%	0.006%
79	13.162	3768	3770	3774	rVB3	1108	576	0.04%	0.005%
80	13.217	3781	3787	3789	rBV4	1004	932	0.06%	0.008%
81	13.281	3798	3807	3816	rBV10	2401	5173	0.35%	0.043%
82	13.403	3842	3845	3847	rBV5	905	624	0.04%	0.005%
83	13.477	3865	3868	3869	rBV2	829	490	0.03%	0.004%
84	13.512	3871	3879	3891	rVB2	8252	14268	0.97%	0.118%
85	13.586	3899	3902	3909	rVB7	1679	1772	0.12%	0.015%
86	13.741	3946	3950	3951	rBV4	684	497	0.03%	0.004%
87	13.821	3973	3975	3978	rBV2	626	395	0.03%	0.003%
88	13.876	3986	3992	3997	rBV6	1333	1699	0.12%	0.014%
89	13.979	4021	4024	4027	rBV5	778	569	0.04%	0.005%
90	14.043	4042	4044	4048	rVB4	650	429	0.03%	0.004%
91	14.082	4052	4056	4057	rBV3	881	578	0.04%	0.005%
92	14.184	4086	4088	4093	rBV4	805	703	0.05%	0.006%
93	14.294	4120	4122	4125	rBV2	595	464	0.03%	0.004%
94	14.381	4147	4149	4153	rVV3	605	411	0.03%	0.003%
95	14.416	4158	4160	4164	rBV2	585	435	0.03%	0.004%
96	14.458	4170	4173	4176	rBV5	683	444	0.03%	0.004%
97	14.644	4224	4231	4235	rBV3	2983	3890	0.26%	0.032%
98	14.760	4264	4267	4268	rBV3	720	400	0.03%	0.003%
99	14.975	4331	4334	4336	rBV4	749	546	0.04%	0.005%
100	15.287	4428	4431	4435	rBV5	1562	1638	0.11%	0.014%

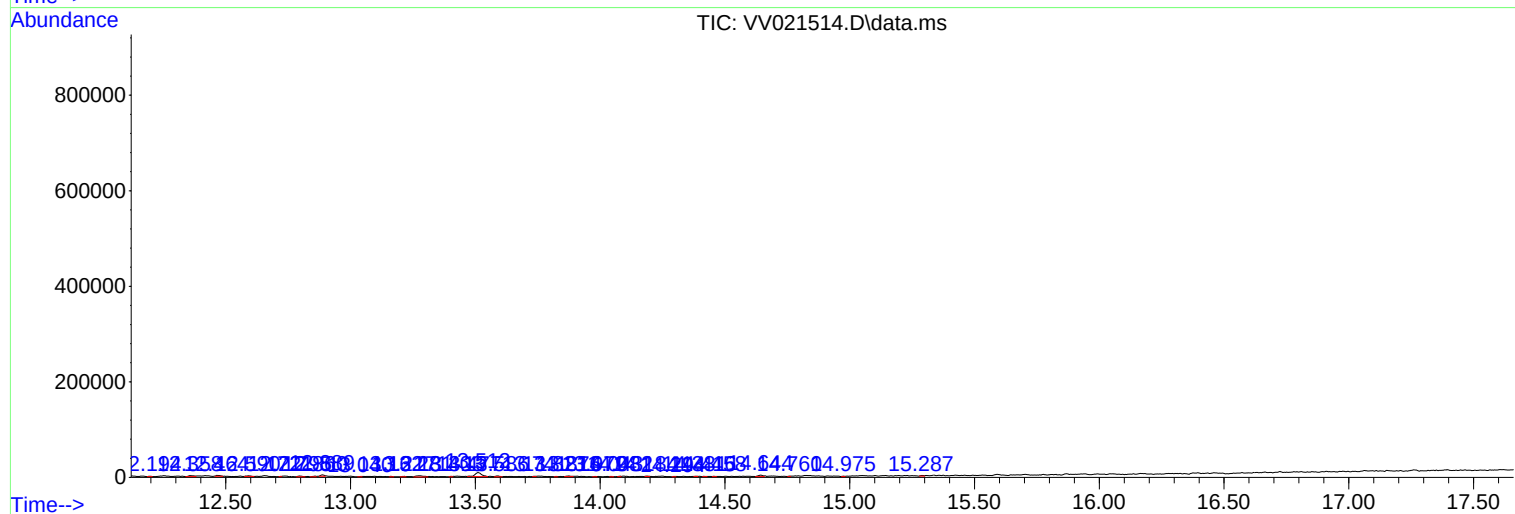
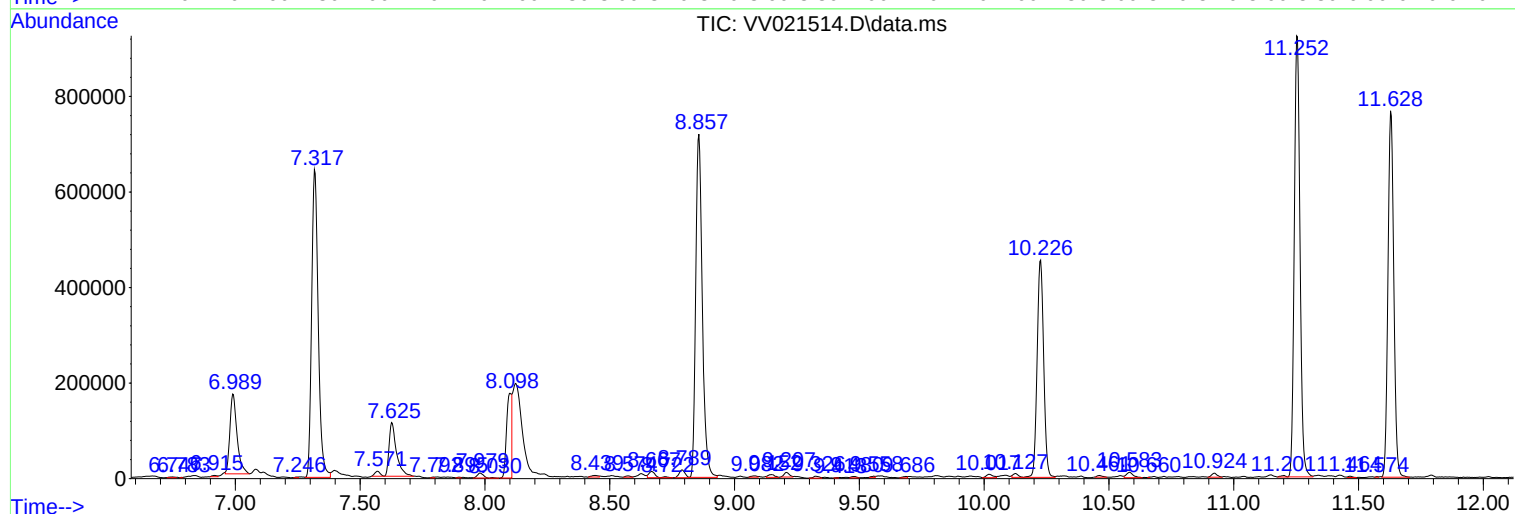
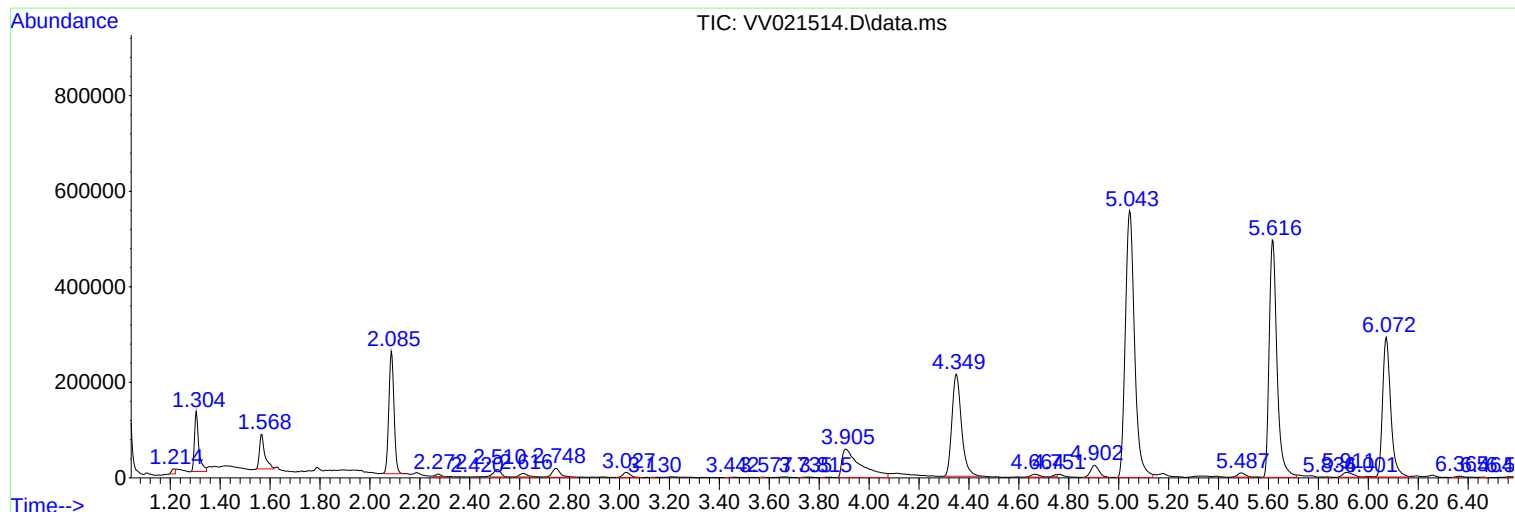
Sum of corrected areas: 12116421

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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BG5Q5ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM052721WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Instrument :
MSVOA_V
ClientSampleId :
BG5Q5ME

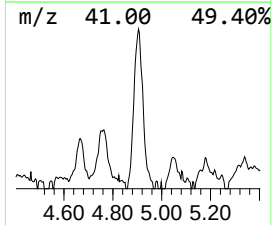
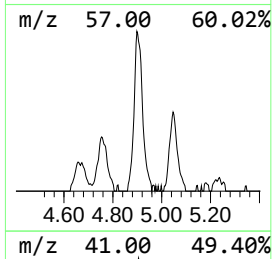
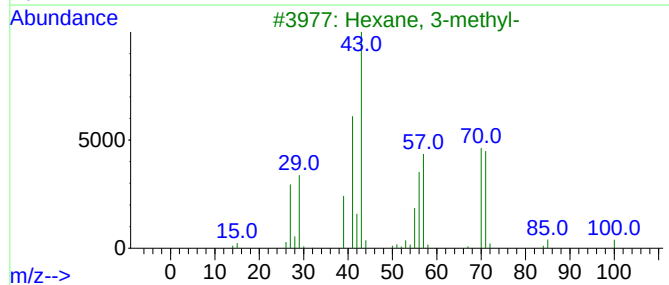
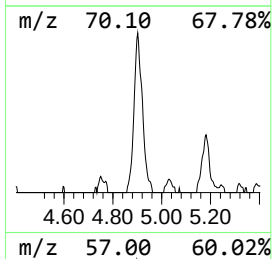
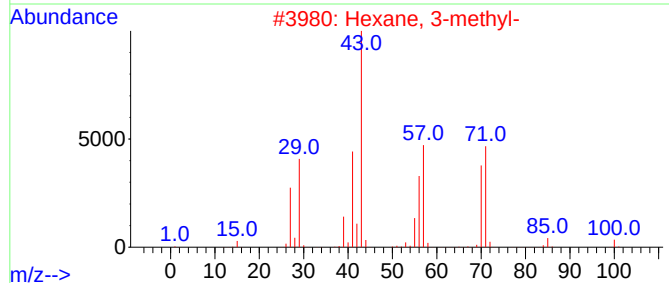
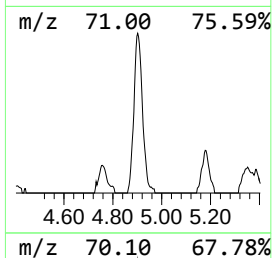
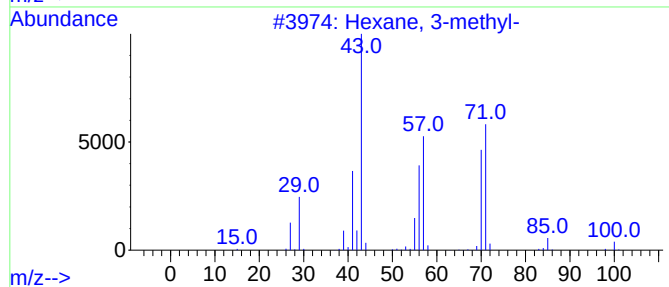
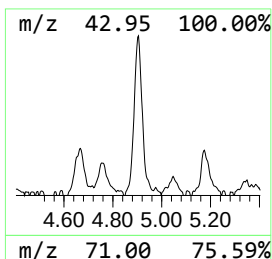
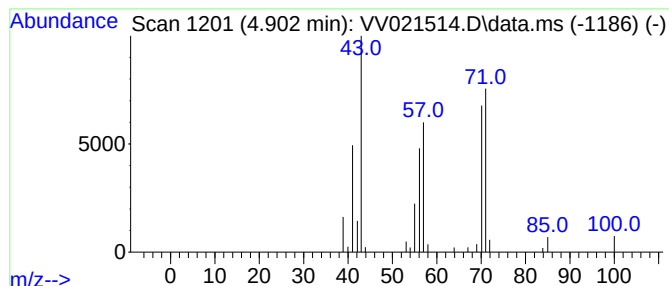
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM052721WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.902	2.82 ug/L	61152	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	91
2			Hexane, 3-methyl-	100	C7H16	000589-34-4	87
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	81
4			Heptane	100	C7H16	000142-82-5	64
5			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	4.902	2.8	ug/L	61152	1	5.619	1085470	50.0