

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
 Data File : VU043727.D
 Acq On : 14 May 2021 02:43
 Operator : SY/MD
 Sample : M2320-04DL 20X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F3A08DL

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\SFAMULM051421WMA.M
 Title : VOC Analysis

Signal : TIC: VU043727.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.491	43	47	53	rVB2	9601	8790	0.48%	0.055%
2	1.604	73	82	95	rBV	287426	324557	17.79%	2.040%
3	1.913	170	178	190	rVB	177544	229497	12.58%	1.443%
4	1.996	195	204	216	rVB	120624	168055	9.21%	1.056%
5	2.472	348	352	354	rBV3	624	466	0.03%	0.003%
6	2.572	370	383	415	rVB	387212	684641	37.52%	4.303%
7	2.961	499	504	511	rVB5	613	774	0.04%	0.005%
8	3.051	518	532	553	rBV2	59801	140924	7.72%	0.886%
9	3.144	553	561	568	rVV2	10121	19897	1.09%	0.125%
10	3.192	570	576	594	rVB2	11788	26573	1.46%	0.167%
11	3.372	610	632	660	rBV	699228	1606349	88.03%	10.097%
12	3.572	686	694	699	rBV5	602	965	0.05%	0.006%
13	3.720	737	740	745	rVB2	287	316	0.02%	0.002%
14	3.790	754	762	767	rBV	309	352	0.02%	0.002%
15	3.835	767	776	781	rBV2	912	1267	0.07%	0.008%
16	3.977	815	820	823	rBV2	708	788	0.04%	0.005%
17	4.305	909	922	923	rBV3	3208	4847	0.27%	0.030%
18	4.443	946	965	981	rBV3	14990	36561	2.00%	0.230%
19	4.543	983	996	1007	rBV6	2829	6658	0.36%	0.042%
20	4.629	1007	1023	1059	rBV	204600	505838	27.72%	3.180%
21	4.890	1100	1104	1110	rVB2	244	300	0.02%	0.002%
22	5.073	1143	1161	1177	rBV	321448	701781	38.46%	4.411%
23	5.205	1199	1202	1205	rBV2	450	350	0.02%	0.002%
24	5.298	1221	1231	1234	rBV5	1664	2400	0.13%	0.015%
25	5.392	1248	1260	1270	rBV7	3238	7783	0.43%	0.049%
26	5.472	1270	1285	1300	rVB3	48227	110517	6.06%	0.695%
27	5.597	1316	1324	1326	rBV3	1960	2182	0.12%	0.014%
28	5.732	1345	1366	1392	rBV2	688731	1824688	100.00%	11.469%
29	5.855	1396	1404	1411	rVV5	15433	29006	1.59%	0.182%
30	5.909	1412	1421	1445	rVB4	40180	124825	6.84%	0.785%
31	6.115	1480	1485	1486	rBV2	521	487	0.03%	0.003%
32	6.256	1514	1529	1565	rBV	491865	929705	50.95%	5.844%
33	6.404	1568	1575	1577	rBV5	1361	1339	0.07%	0.008%
34	6.472	1590	1596	1599	rVB3	484	492	0.03%	0.003%
35	6.549	1606	1620	1631	rBV7	11389	24288	1.33%	0.153%
36	6.600	1631	1636	1638	rBV3	380	371	0.02%	0.002%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
 Title : VOC Analysis

37	6.697	1651	1666	1690	rBV	421980	836349	45.84%	5.257%
38	6.816	1696	1703	1711	rVB7	5597	8816	0.48%	0.055%
39	6.874	1713	1721	1731	rVV3	7445	13520	0.74%	0.085%
40	6.932	1735	1739	1750	rVB5	2046	2964	0.16%	0.019%
41	6.993	1755	1758	1760	rBV2	592	362	0.02%	0.002%
42	7.076	1768	1784	1794	rBV10	3642	9265	0.51%	0.058%
43	7.173	1808	1814	1815	rBV2	732	571	0.03%	0.004%
44	7.263	1828	1842	1854	rVB2	22340	45074	2.47%	0.283%
45	7.346	1858	1868	1869	rBV6	669	898	0.05%	0.006%
46	7.388	1869	1881	1891	rBV2	21428	39057	2.14%	0.246%
47	7.478	1903	1909	1920	rBV7	1076	1780	0.10%	0.011%
48	7.571	1924	1938	1953	rBV	216706	385608	21.13%	2.424%
49	7.700	1968	1978	1988	rVB9	3052	4731	0.26%	0.030%
50	7.774	1994	2001	2008	rBV5	1513	2345	0.13%	0.015%
51	7.906	2012	2042	2056	rBV	828200	1433531	78.56%	9.011%
52	8.028	2077	2080	2085	rBV7	1612	1752	0.10%	0.011%
53	8.186	2117	2129	2142	rBV	150585	254579	13.95%	1.600%
54	8.375	2175	2188	2195	rBV6	4339	7869	0.43%	0.049%
55	8.417	2195	2201	2211	rVB2	5098	7283	0.40%	0.046%
56	8.555	2242	2244	2255	rVB5	514	462	0.03%	0.003%
57	8.639	2256	2270	2302	rBV	584794	1050140	57.55%	6.601%
58	8.870	2337	2342	2351	rVB6	1555	2155	0.12%	0.014%
59	8.915	2353	2356	2357	rBV	667	369	0.02%	0.002%
60	8.964	2366	2371	2376	rBV5	641	581	0.03%	0.004%
61	9.054	2395	2399	2400	rBV	655	408	0.02%	0.003%
62	9.169	2431	2435	2436	rBV2	1013	631	0.03%	0.004%
63	9.253	2457	2461	2463	rBV3	308	272	0.01%	0.002%
64	9.340	2480	2488	2496	rBV6	1873	2864	0.16%	0.018%
65	9.423	2499	2514	2533	rBV	664497	1102414	60.42%	6.929%
66	9.578	2555	2562	2566	rBV5	897	1010	0.06%	0.006%
67	9.697	2592	2599	2603	rBV6	1815	1999	0.11%	0.013%
68	9.768	2614	2621	2623	rBV4	1066	1026	0.06%	0.006%
69	10.031	2698	2703	2710	rVB4	1189	1575	0.09%	0.010%
70	10.301	2784	2787	2792	rVB4	328	305	0.02%	0.002%
71	10.359	2800	2805	2806	rBV	369	309	0.02%	0.002%
72	10.472	2836	2840	2841	rVV	496	281	0.02%	0.002%
73	10.488	2841	2845	2850	rVB4	551	610	0.03%	0.004%
74	10.677	2895	2904	2912	rBV2	4043	5836	0.32%	0.037%
75	10.761	2917	2930	2949	rBV	574752	922378	50.55%	5.798%
76	10.874	2958	2965	2967	rBV4	1003	1321	0.07%	0.008%

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77	10.986	2996	3000	3002	rBV	309	254	0.01%	0.002%
78	11.092	3028	3033	3035	rBV2	415	397	0.02%	0.002%
79	11.211	3066	3070	3074	rVB3	348	284	0.02%	0.002%
80	11.465	3140	3149	3159	rBV5	2485	4442	0.24%	0.028%
81	11.620	3189	3197	3204	rVB3	2718	3298	0.18%	0.021%
82	11.700	3212	3222	3229	rBV5	2032	3115	0.17%	0.020%
83	11.751	3235	3238	3245	rVB3	644	574	0.03%	0.004%
84	11.819	3246	3259	3282	rBV	628840	980884	53.76%	6.166%
85	11.948	3291	3299	3303	rBV7	1193	1860	0.10%	0.012%
86	11.980	3303	3309	3315	rVB4	2268	3112	0.17%	0.020%
87	12.079	3337	3340	3342	rBV3	394	257	0.01%	0.002%
88	12.198	3360	3377	3397	rBV	769372	1220541	66.89%	7.672%
89	12.404	3436	3441	3444	rVB2	662	546	0.03%	0.003%
90	12.597	3498	3501	3505	rBV2	448	372	0.02%	0.002%
91	12.767	3551	3554	3557	rBV2	352	294	0.02%	0.002%
92	12.899	3590	3595	3600	rVB6	1068	1173	0.06%	0.007%
93	13.124	3660	3665	3671	rVB3	562	595	0.03%	0.004%
94	13.156	3671	3675	3682	rBV2	503	537	0.03%	0.003%
95	13.893	3899	3904	3913	rVB3	1352	1667	0.09%	0.010%
96	14.018	3939	3943	3945	rBV2	358	270	0.01%	0.002%
97	14.095	3963	3967	3974	rVB5	1197	1391	0.08%	0.009%
98	14.327	4037	4039	4043	rBV2	418	324	0.02%	0.002%
99	14.896	4209	4216	4219	rBV4	497	668	0.04%	0.004%
100	15.102	4277	4280	4284	rVB3	469	307	0.02%	0.002%

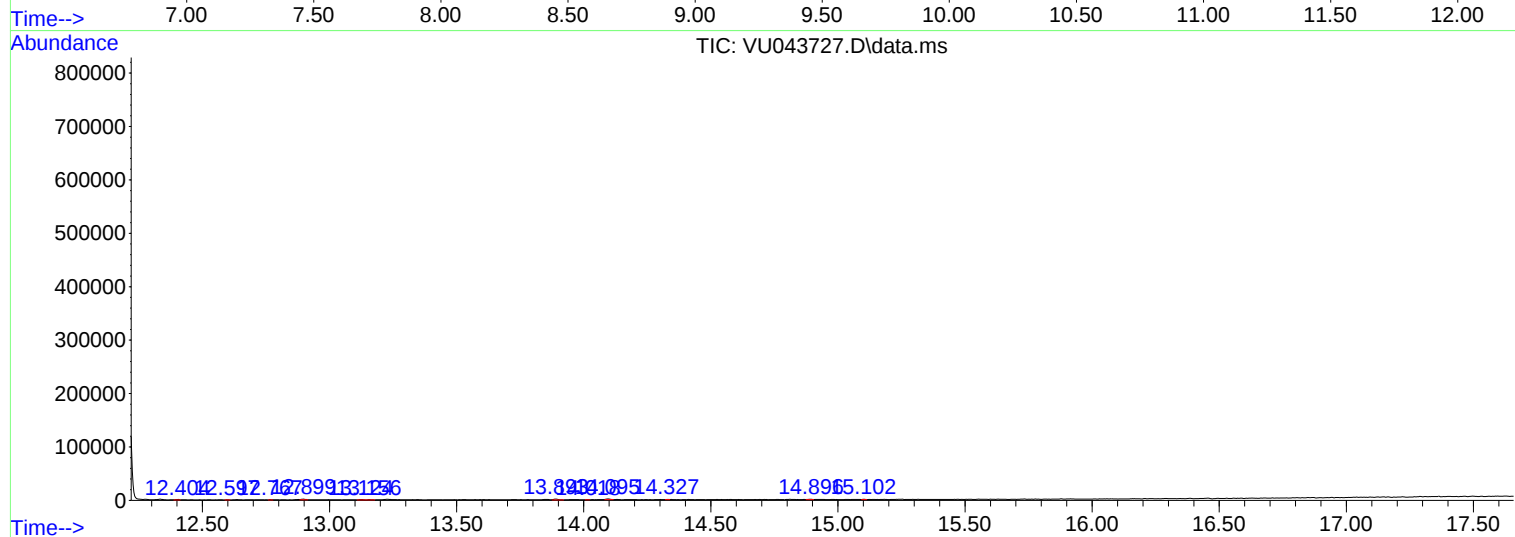
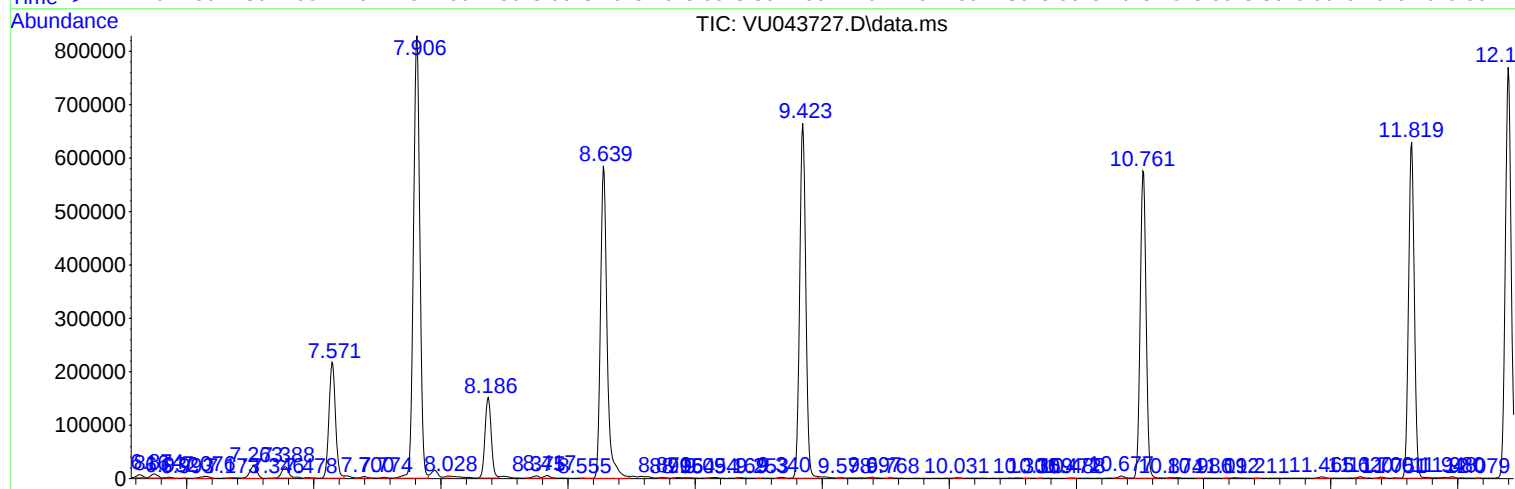
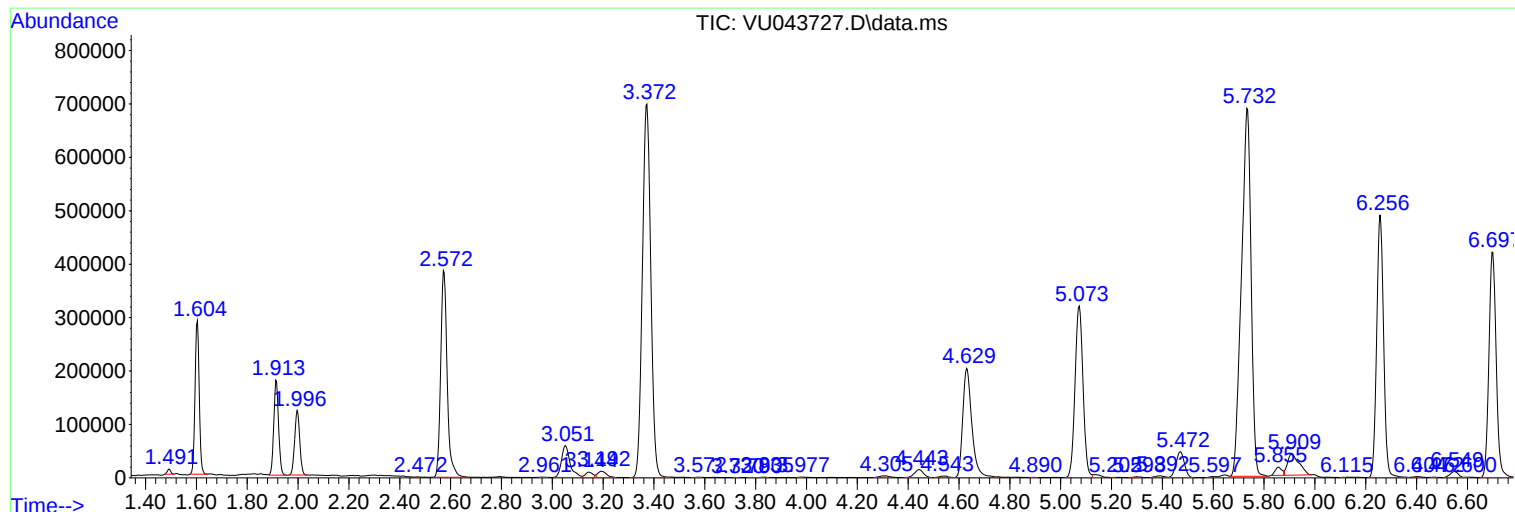
Sum of corrected areas: 15909091

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

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



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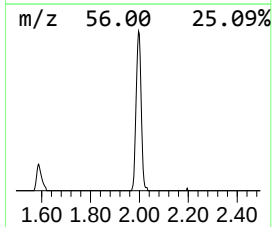
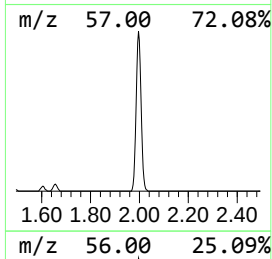
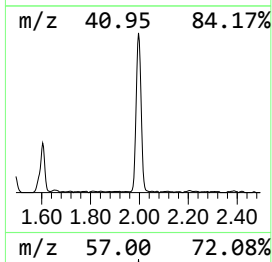
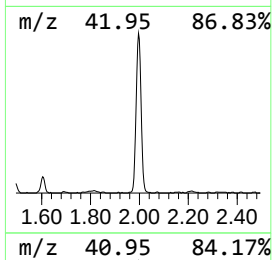
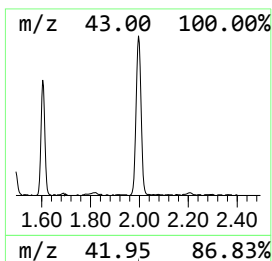
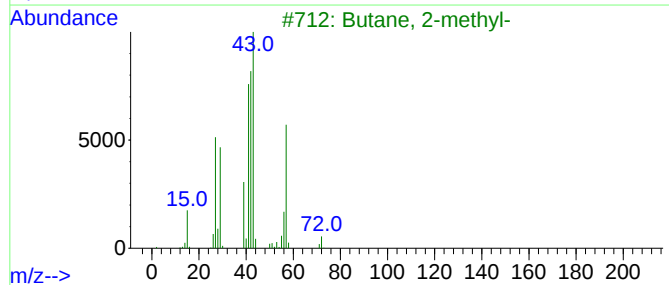
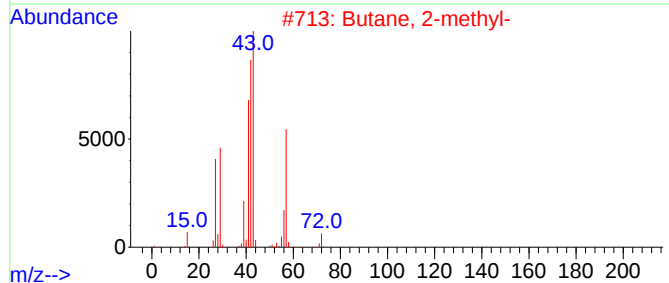
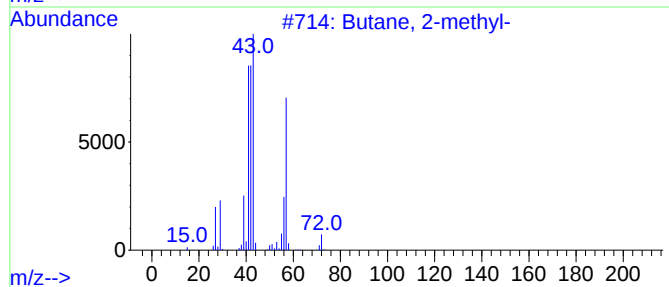
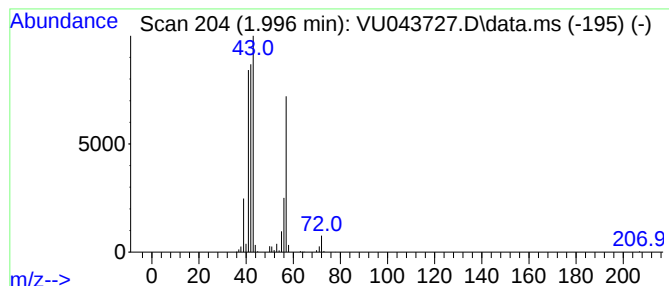
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

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.
1.996	9.04 ug/L	168055	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-			72	C5H12	000078-78-4	91
2	Butane, 2-methyl-			72	C5H12	000078-78-4	91
3	Butane, 2-methyl-			72	C5H12	000078-78-4	86
4	Pentane			72	C5H12	000109-66-0	42
5	Butane, 2,3-dimethyl-			86	C6H14	000079-29-8	33



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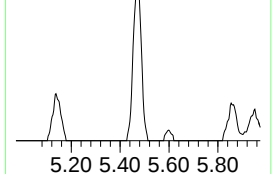
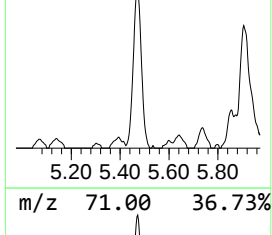
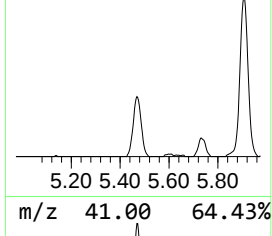
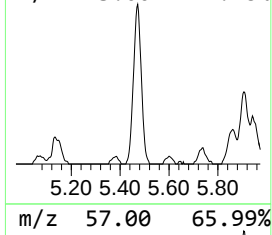
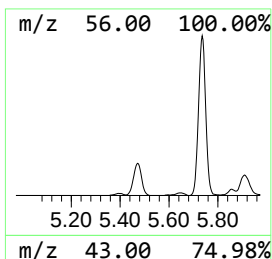
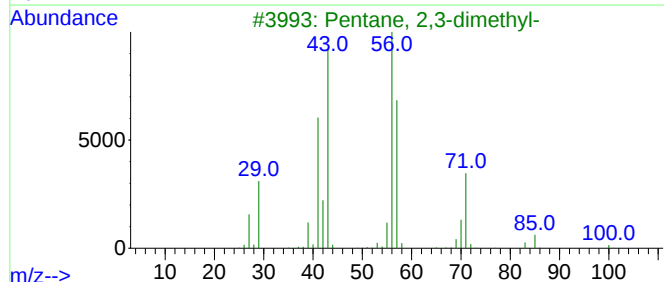
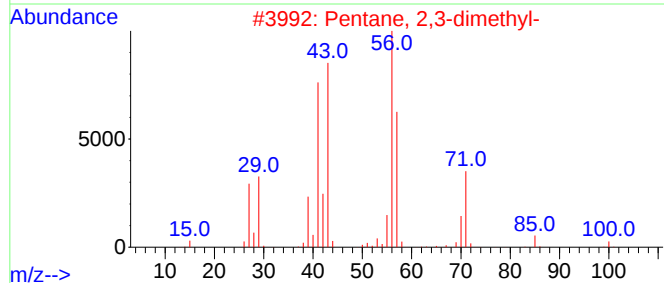
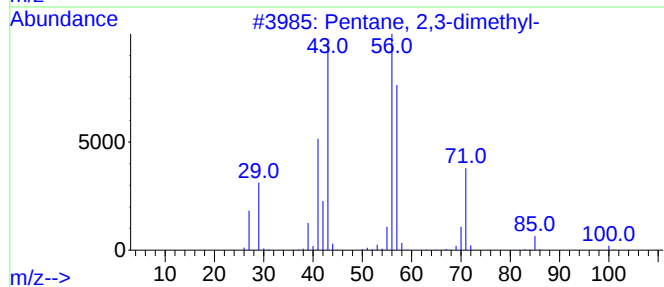
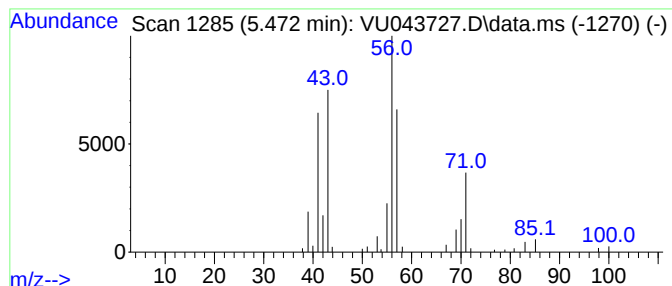
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Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.472	5.94 ug/L	110517	1,4-Difluorobenzene	6.256

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2		Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	87
3		Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	68
4		Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	64
5		Nonane, 5-methylene-	140	C10H20	006795-79-5	53



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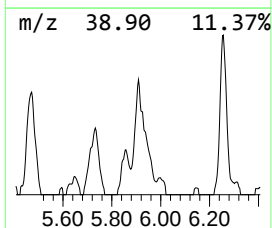
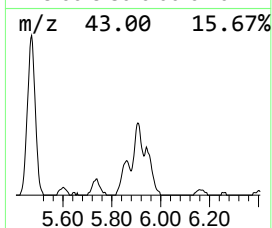
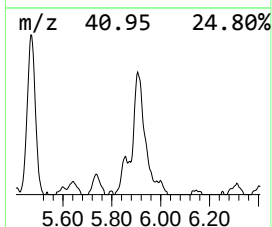
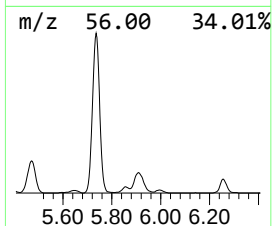
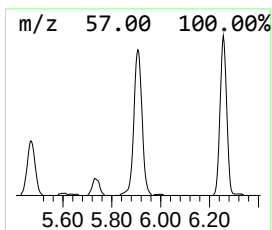
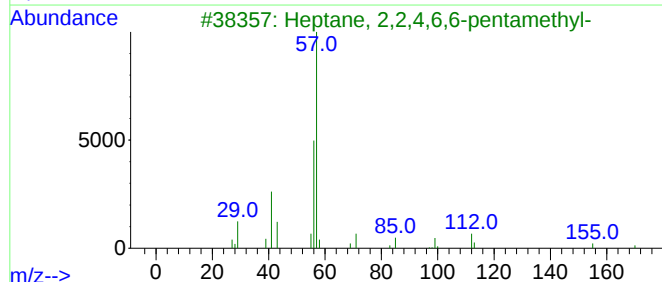
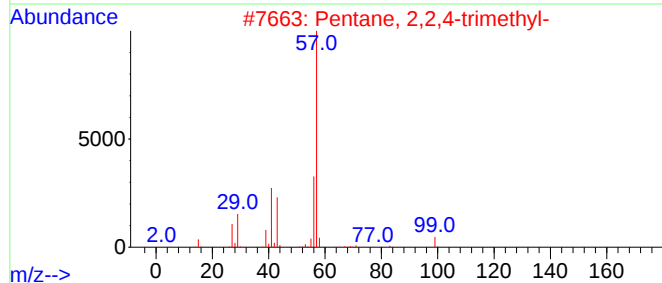
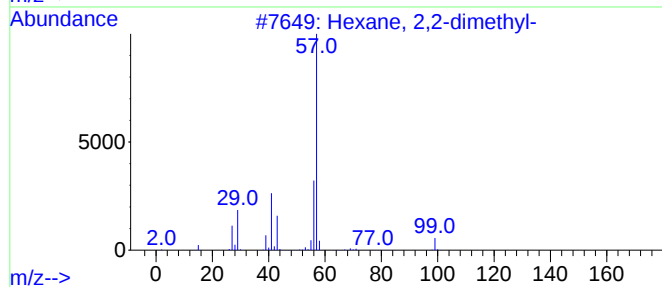
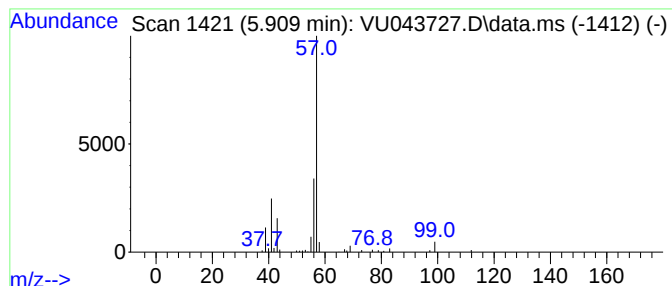
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.909	6.71 ug/L	124825	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	64
2			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	64
3			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	56
4			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	50
5			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043727.D
Acq On : 14 May 2021 02:43
Operator : SY/MD
Sample : M2320-04DL 20X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F3A08DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	1.996	9.0	ug/L	168055	1	6.256	929705	50.0
(DEL) Alkane: S...	5.472	5.9	ug/L	110517	1	6.256	929705	50.0
(DEL) Alkane: S...	5.909	6.7	ug/L	124825	1	6.256	929705	50.0