

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071522\
 Data File : VU049744.D
 Acq On : 15 Jul 2022 18:10
 Operator : SY/MD
 Sample : N3698-03ME
 Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5B68ME

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\SFAMULM071122WMA.M
 Title : VOC Analysis

Signal : TIC: VU049744.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.478	38	43	48	rBV2	2529	2974	0.16%	0.021%
2	1.594	70	79	113	rVB	118215	221515	11.74%	1.557%
3	1.877	125	167	195	rBV	112269	404059	21.41%	2.841%
4	2.289	292	295	299	rBV2	758	705	0.04%	0.005%
5	2.366	317	319	322	rBV2	735	421	0.02%	0.003%
6	2.385	322	325	328	rBV3	535	477	0.03%	0.003%
7	2.530	357	370	387	rBV	301641	484948	25.69%	3.410%
8	2.626	397	400	401	rBV	452	265	0.01%	0.002%
9	2.646	401	406	417	rVB2	1385	1915	0.10%	0.013%
10	2.935	490	496	498	rBV3	390	477	0.03%	0.003%
11	3.038	508	528	543	rVV6	8121	23156	1.23%	0.163%
12	3.105	546	549	554	rVB3	355	321	0.02%	0.002%
13	3.176	559	571	582	rBV	2583	4911	0.26%	0.035%
14	3.282	601	604	607	rBV	346	223	0.01%	0.002%
15	3.330	607	619	628	rBV3	4272	8583	0.45%	0.060%
16	3.668	716	724	736	rBV5	1607	2966	0.16%	0.021%
17	3.977	816	820	829	rVB	341	519	0.03%	0.004%
18	4.015	829	832	835	rBV2	272	247	0.01%	0.002%
19	4.244	897	903	907	rBV	257	371	0.02%	0.003%
20	4.263	907	909	914	rVB	445	351	0.02%	0.002%
21	4.337	927	932	936	rVB	248	249	0.01%	0.002%
22	4.411	942	955	970	rVB6	3622	8722	0.46%	0.061%
23	4.510	970	986	998	rVB5	3422	8122	0.43%	0.057%
24	4.636	1003	1025	1067	rBV	203644	660774	35.01%	4.646%
25	4.973	1127	1130	1132	rBV	316	239	0.01%	0.002%
26	5.057	1139	1156	1182	rBV	339812	769355	40.76%	5.409%
27	5.195	1192	1199	1204	rBV3	323	427	0.02%	0.003%
28	5.295	1222	1230	1238	rVB3	910	1610	0.09%	0.011%
29	5.369	1239	1253	1265	rBV8	4174	10444	0.55%	0.073%
30	5.446	1265	1277	1293	rVB3	20482	46431	2.46%	0.326%
31	5.581	1307	1319	1329	rBV4	4726	9763	0.52%	0.069%
32	5.716	1340	1361	1389	rBV2	726721	1887512	100.00%	13.271%
33	5.845	1390	1401	1403	rVV8	3690	5970	0.32%	0.042%
34	5.890	1404	1415	1430	rVB2	26476	61073	3.24%	0.429%
35	5.980	1431	1443	1456	rBV6	8570	18601	0.99%	0.131%
36	6.102	1472	1481	1483	rBV3	431	591	0.03%	0.004%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071522\
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 Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5B68ME

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\SFAMULM071122WMA.M
 Title : VOC Analysis

37	6.137	1489	1492	1498	rVB2	324	345	0.02%	0.002%
38	6.170	1498	1502	1504	rBV2	243	217	0.01%	0.002%
39	6.243	1511	1525	1547	rBV	373858	722707	38.29%	5.081%
40	6.404	1570	1575	1579	rBV3	315	373	0.02%	0.003%
41	6.526	1602	1613	1625	rBV7	8177	16764	0.89%	0.118%
42	6.600	1625	1636	1648	rBV3	3597	6993	0.37%	0.049%
43	6.687	1648	1663	1681	rBV	457236	919405	48.71%	6.464%
44	6.800	1694	1698	1707	rVB6	2442	3515	0.19%	0.025%
45	6.861	1707	1717	1727	rVB5	3578	6459	0.34%	0.045%
46	6.977	1744	1753	1762	rVB4	1507	2062	0.11%	0.014%
47	7.018	1762	1766	1773	rBV2	205	251	0.01%	0.002%
48	7.060	1775	1779	1783	rBV3	486	571	0.03%	0.004%
49	7.186	1809	1818	1825	rBV6	3639	7613	0.40%	0.054%
50	7.250	1831	1838	1851	rVB3	16156	31321	1.66%	0.220%
51	7.375	1864	1877	1886	rBV4	8706	17661	0.94%	0.124%
52	7.423	1887	1892	1902	rVV4	3707	5443	0.29%	0.038%
53	7.497	1909	1915	1918	rBV	332	313	0.02%	0.002%
54	7.565	1922	1936	1960	rBV	226822	420618	22.28%	2.957%
55	7.652	1960	1963	1967	rVV2	591	387	0.02%	0.003%
56	7.690	1967	1975	1986	rVV6	2284	3973	0.21%	0.028%
57	7.835	2011	2020	2024	rBV5	1725	2666	0.14%	0.019%
58	7.896	2025	2039	2059	rVB	780294	1360817	72.10%	9.568%
59	7.983	2061	2066	2067	rBV4	2395	1830	0.10%	0.013%
60	8.054	2086	2088	2089	rBV2	454	217	0.01%	0.002%
61	8.128	2108	2111	2114	rBV3	336	201	0.01%	0.001%
62	8.179	2114	2127	2154	rVV	147695	280784	14.88%	1.974%
63	8.343	2173	2178	2180	rBV4	929	733	0.04%	0.005%
64	8.423	2200	2203	2207	rBV2	253	262	0.01%	0.002%
65	8.497	2221	2226	2229	rBV2	281	312	0.02%	0.002%
66	8.649	2257	2273	2303	rBV2	626914	1439105	76.24%	10.118%
67	8.800	2316	2320	2329	rVB6	3435	4792	0.25%	0.034%
68	8.957	2366	2369	2372	rBV	362	221	0.01%	0.002%
69	9.211	2446	2448	2454	rVV	275	205	0.01%	0.001%
70	9.298	2472	2475	2477	rBV	299	240	0.01%	0.002%
71	9.420	2499	2513	2531	rBV	504925	889762	47.14%	6.256%
72	9.626	2573	2577	2581	rBV2	199	237	0.01%	0.002%
73	9.661	2586	2588	2591	rVV3	361	228	0.01%	0.002%
74	9.706	2598	2602	2608	rVV2	422	399	0.02%	0.003%
75	9.771	2619	2622	2626	rBV2	266	219	0.01%	0.002%
76	10.150	2737	2740	2745	rVB2	265	204	0.01%	0.001%

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 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5B68ME

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\SFAMULM071122WMA.M
 Title : VOC Analysis

77	10.237	2762	2767	2771	rBV2	198	212	0.01%	0.001%
78	10.594	2871	2878	2881	rBV2	332	283	0.01%	0.002%
79	10.616	2882	2885	2890	rVB2	256	243	0.01%	0.002%
80	10.703	2909	2912	2916	rBV	362	277	0.01%	0.002%
81	10.761	2916	2930	2955	rVV	726115	1197472	63.44%	8.419%
82	10.906	2967	2975	2978	rBV2	364	562	0.03%	0.004%
83	11.115	3035	3040	3048	rVB6	1259	1495	0.08%	0.011%
84	11.160	3050	3054	3055	rBV2	266	205	0.01%	0.001%
85	11.610	3191	3194	3198	rBV	300	279	0.01%	0.002%
86	11.648	3203	3206	3214	rVV2	750	831	0.04%	0.006%
87	11.687	3216	3218	3222	rVB2	312	211	0.01%	0.001%
88	11.816	3245	3258	3280	rBV	532432	846680	44.86%	5.953%
89	12.195	3363	3376	3398	rBV	859542	1369284	72.54%	9.627%
90	12.655	3514	3519	3521	rBV2	296	277	0.01%	0.002%
91	12.687	3521	3529	3533	rVV2	1320	1795	0.10%	0.013%
92	13.526	3787	3790	3792	rBV2	245	209	0.01%	0.001%
93	13.799	3872	3875	3878	rBV2	290	242	0.01%	0.002%
94	14.262	4016	4019	4021	rBV	316	224	0.01%	0.002%
95	14.275	4021	4023	4028	rVB2	537	403	0.02%	0.003%
96	14.420	4065	4068	4073	rVB	387	295	0.02%	0.002%
97	15.307	4341	4344	4349	rBV	466	481	0.03%	0.003%
98	15.629	4442	4444	4448	rBV2	446	259	0.01%	0.002%
99	15.960	4545	4547	4551	rBV3	590	382	0.02%	0.003%
100	16.378	4672	4677	4684	rBV3	717	976	0.05%	0.007%

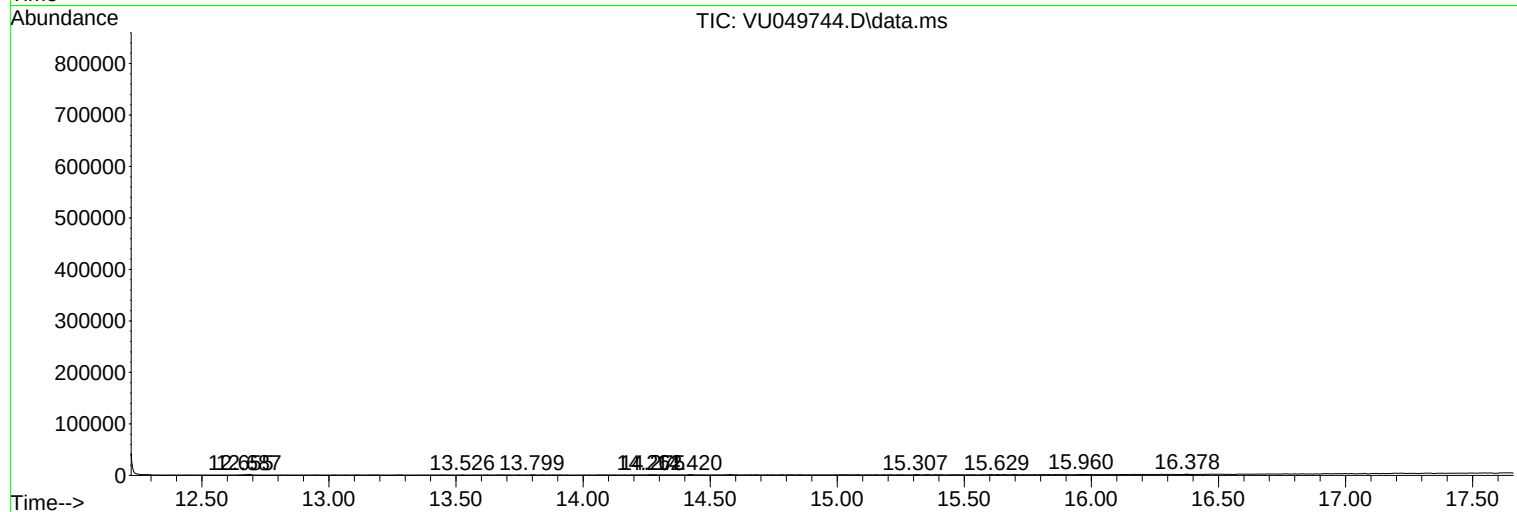
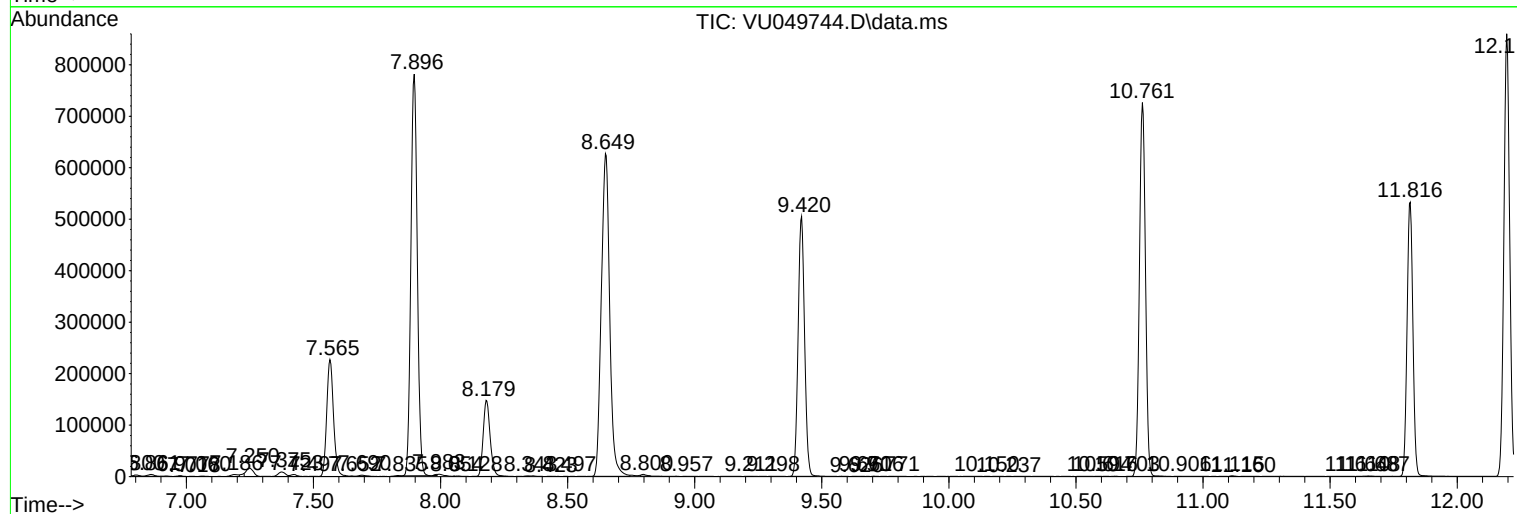
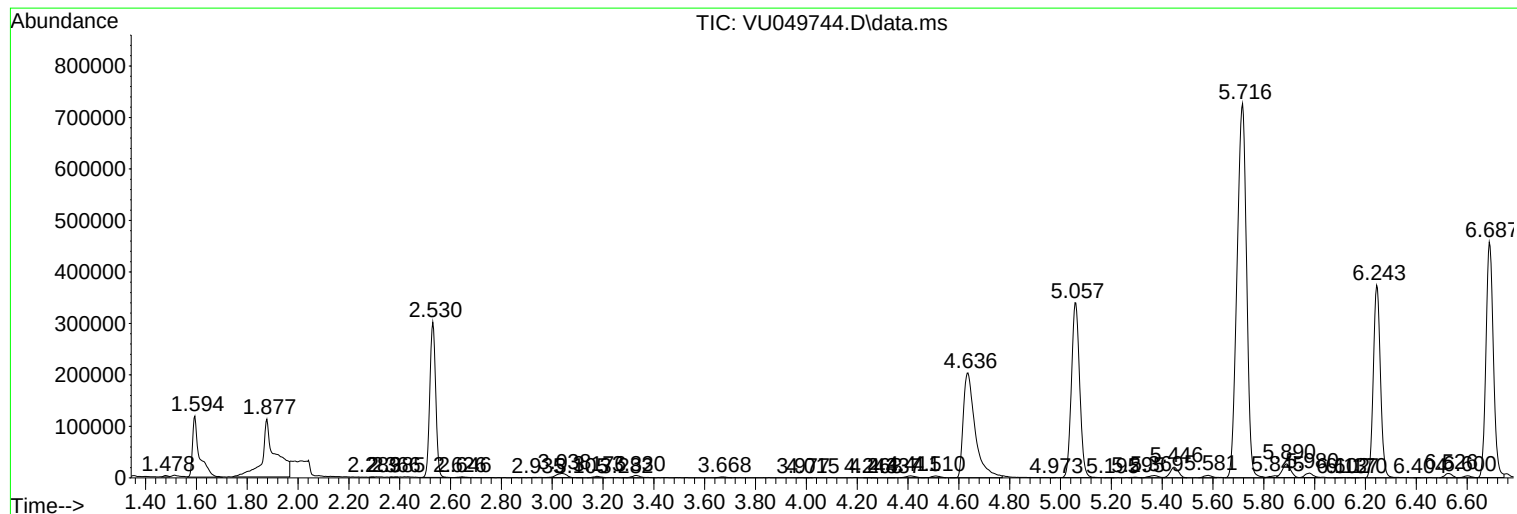
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Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071522\
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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5B68ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071522\
Data File : VU049744.D
Acq On : 15 Jul 2022 18:10
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Sample : N3698-03ME
Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5B68ME

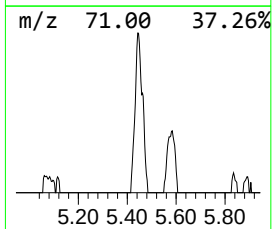
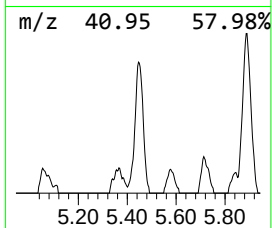
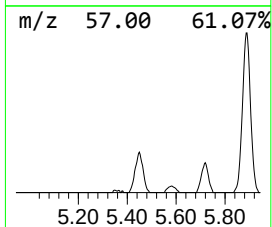
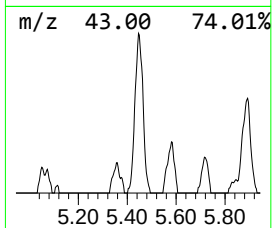
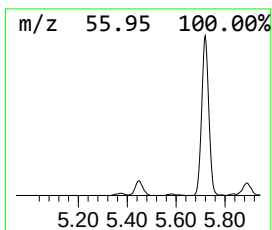
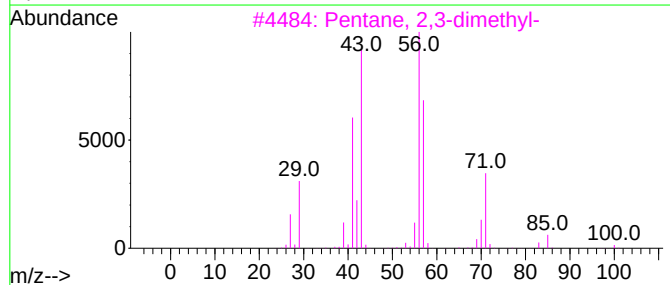
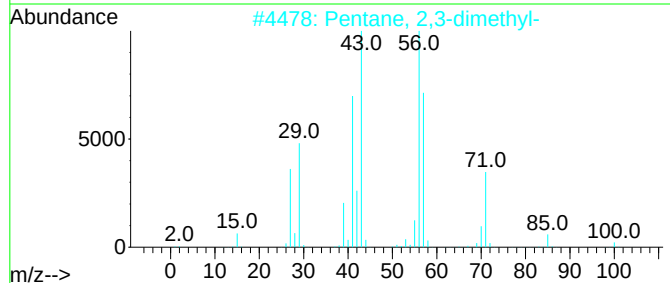
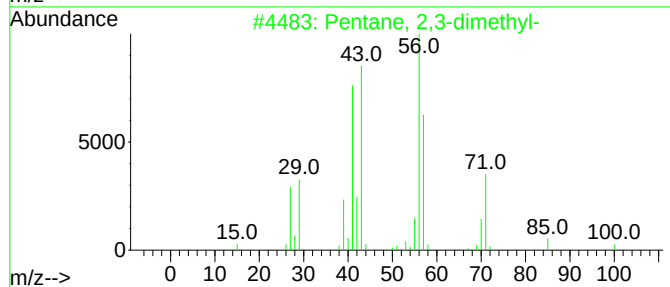
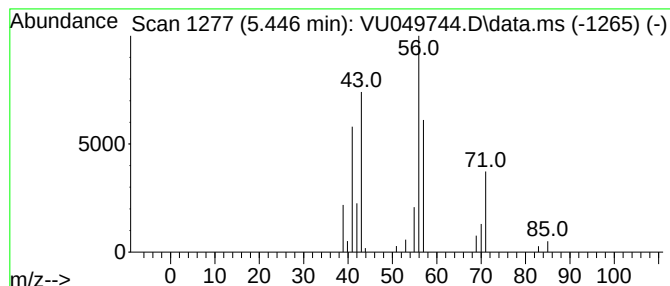
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.446	3.21 ug/L	46431	1,4-Difluorobenzene	6.243

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	90
2		Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	83
3		Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	83
4		Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	83
5		Pentane, 1-bromo-3,4-dimethyl-	178	C7H15Br	006570-92-9	38



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Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5B68ME

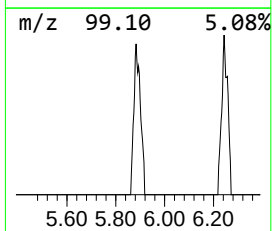
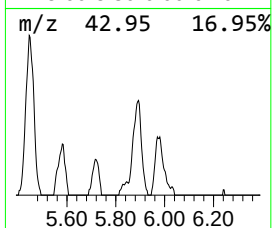
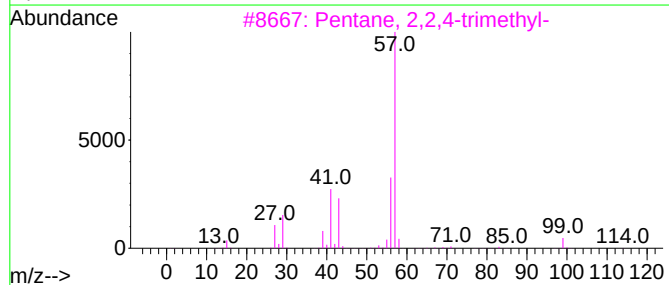
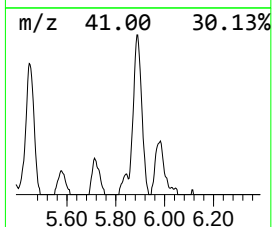
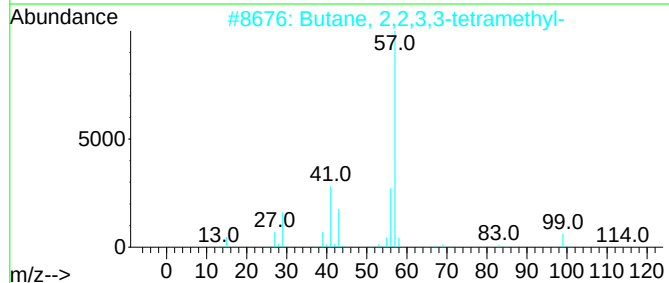
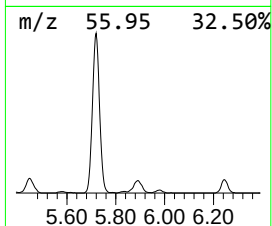
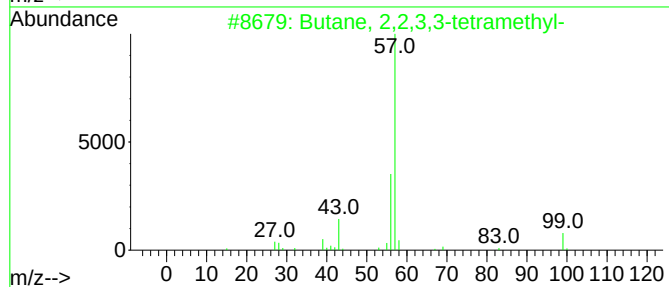
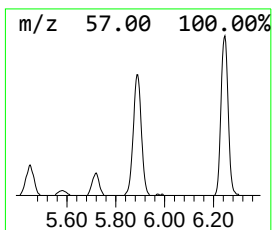
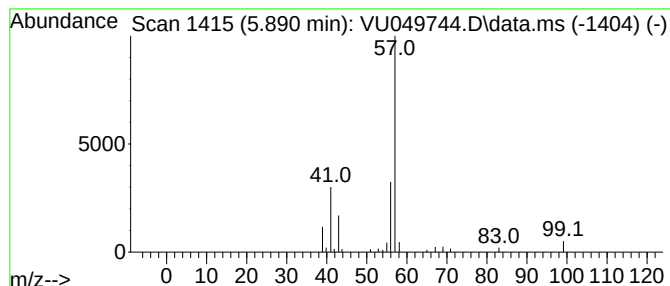
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

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.
5.890	4.23 ug/L	61073	1,4-Difluorobenzene	6.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
2			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
3			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	64
4			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	59
5			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	56



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Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
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
(DEL) Alkane: S...	5.446	3.2	ug/L	46431	1	6.243	722707	50.0
(DEL) Alkane: S...	5.890	4.2	ug/L	61073	1	6.243	722707	50.0