

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071822\
 Data File : VU049765.D
 Acq On : 18 Jul 2022 17:13
 Operator : SY/MD
 Sample : N3698-03ME
 Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 18 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: VU049765.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.481	40	44	48	rBV3	1829	1573	0.24%	0.026%
2	1.594	71	79	87	rBV2	35849	53340	8.17%	0.866%
3	2.343	310	312	314	rBV	561	350	0.05%	0.006%
4	2.523	356	368	385	rVB	94484	154268	23.62%	2.506%
5	2.649	397	407	408	rBV4	1737	2059	0.32%	0.033%
6	2.748	429	438	447	rBV2	2059	3152	0.48%	0.051%
7	2.954	498	502	506	rBV2	466	360	0.06%	0.006%
8	3.173	555	570	592	rBV	28414	65301	10.00%	1.061%
9	3.324	605	617	629	rBV6	5875	13289	2.03%	0.216%
10	3.472	655	663	666	rBV	308	341	0.05%	0.006%
11	3.668	712	724	731	rBV4	1746	3321	0.51%	0.054%
12	3.851	776	781	782	rBV2	324	269	0.04%	0.004%
13	4.028	831	836	837	rBV	246	223	0.03%	0.004%
14	4.144	867	872	877	rBV2	208	250	0.04%	0.004%
15	4.266	906	910	914	rVV3	403	364	0.06%	0.006%
16	4.404	940	953	965	rBV4	4176	9517	1.46%	0.155%
17	4.504	973	984	998	rVB2	4186	8529	1.31%	0.139%
18	4.639	1012	1026	1065	rBV	84898	296557	45.41%	4.817%
19	4.825	1080	1084	1087	rVB3	628	454	0.07%	0.007%
20	4.964	1124	1127	1130	rVV3	611	454	0.07%	0.007%
21	4.980	1130	1132	1138	rVB5	608	542	0.08%	0.009%
22	5.060	1139	1157	1177	rBV	118802	272333	41.70%	4.424%
23	5.150	1182	1185	1188	rVV3	398	270	0.04%	0.004%
24	5.166	1188	1190	1199	rVV2	196	228	0.03%	0.004%
25	5.288	1222	1228	1231	rBV2	704	873	0.13%	0.014%
26	5.365	1241	1252	1263	rBV9	4789	10507	1.61%	0.171%
27	5.446	1263	1277	1292	rVB3	23120	51591	7.90%	0.838%
28	5.513	1293	1298	1306	rVB3	388	352	0.05%	0.006%
29	5.578	1306	1318	1330	rBV4	5071	10621	1.63%	0.173%
30	5.713	1340	1360	1389	rBV2	247339	653132	100.00%	10.610%
31	5.841	1389	1400	1402	rVV6	3491	5981	0.92%	0.097%
32	5.886	1404	1414	1431	rVB2	28159	65868	10.08%	1.070%
33	5.976	1431	1442	1456	rVB3	10890	23251	3.56%	0.378%
34	6.134	1485	1491	1497	rBV2	150	231	0.04%	0.004%
35	6.243	1510	1525	1552	rBV	252549	491071	75.19%	7.977%
36	6.391	1563	1571	1573	rBV2	183	231	0.04%	0.004%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071822\
 Data File : VU049765.D
 Acq On : 18 Jul 2022 17:13
 Operator : SY/MD
 Sample : N3698-03ME
 Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 18 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	6.526	1604	1613	1625	rVB7	6696	12891	1.97%	0.209%
38	6.597	1625	1635	1648	rBV5	3382	7502	1.15%	0.122%
39	6.687	1649	1663	1679	rBV	157494	323837	49.58%	5.260%
40	6.800	1695	1698	1706	rVB4	2244	2624	0.40%	0.043%
41	6.857	1706	1716	1727	rVB5	3573	6906	1.06%	0.112%
42	6.915	1728	1734	1736	rVV2	527	617	0.09%	0.010%
43	6.928	1736	1738	1742	rVB2	845	482	0.07%	0.008%
44	6.973	1745	1752	1762	rVB7	1564	2180	0.33%	0.035%
45	7.063	1776	1780	1788	rVB3	669	712	0.11%	0.012%
46	7.108	1788	1794	1799	rBV2	465	543	0.08%	0.009%
47	7.153	1803	1808	1811	rBV	371	338	0.05%	0.005%
48	7.189	1811	1819	1820	rBV3	2165	2215	0.34%	0.036%
49	7.250	1832	1838	1850	rVB2	19552	33206	5.08%	0.539%
50	7.298	1850	1853	1855	rBV2	524	325	0.05%	0.005%
51	7.333	1861	1864	1866	rBV2	435	281	0.04%	0.005%
52	7.375	1866	1877	1886	rBV2	9401	18422	2.82%	0.299%
53	7.478	1906	1909	1912	rVV2	460	313	0.05%	0.005%
54	7.565	1921	1936	1956	rBV2	76654	146903	22.49%	2.386%
55	7.693	1969	1976	1982	rBV4	1019	1439	0.22%	0.023%
56	7.803	2001	2010	2013	rBV4	3024	4561	0.70%	0.074%
57	7.896	2027	2039	2056	rVB	241923	425129	65.09%	6.906%
58	7.989	2061	2068	2081	rVV5	4531	10101	1.55%	0.164%
59	8.179	2116	2127	2154	rVV	51341	99146	15.18%	1.611%
60	8.346	2174	2179	2181	rBV3	1396	1185	0.18%	0.019%
61	8.407	2193	2198	2206	rVB4	657	768	0.12%	0.012%
62	8.471	2215	2218	2225	rBV2	188	246	0.04%	0.004%
63	8.552	2237	2243	2249	rBV3	1147	1271	0.19%	0.021%
64	8.648	2257	2273	2308	rBV3	223874	557154	85.30%	9.051%
65	8.796	2309	2319	2332	rVV8	3518	8279	1.27%	0.134%
66	8.857	2336	2338	2343	rVB2	667	534	0.08%	0.009%
67	8.925	2352	2359	2369	rBV6	625	1092	0.17%	0.018%
68	9.420	2499	2513	2534	rBV	336811	615718	94.27%	10.002%
69	9.574	2553	2561	2573	rVB2	2601	3840	0.59%	0.062%
70	9.700	2591	2600	2610	rVB2	2039	3456	0.53%	0.056%
71	10.108	2714	2727	2729	rBV3	3723	4847	0.74%	0.079%
72	10.227	2761	2764	2767	rBV	240	248	0.04%	0.004%
73	10.295	2780	2785	2788	rBV3	299	307	0.05%	0.005%
74	10.487	2837	2845	2855	rVB3	3074	5012	0.77%	0.081%
75	10.761	2918	2930	2945	rBV	273149	452508	69.28%	7.351%
76	10.825	2945	2950	2960	rVB5	1972	3100	0.47%	0.050%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071822\
 Data File : VU049765.D
 Acq On : 18 Jul 2022 17:13
 Operator : SY/MD
 Sample : N3698-03ME
 Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 18 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	11.092	3023	3033	3047	rVB7	3292	5996	0.92%	0.097%
78	11.471	3143	3151	3161	rBV3	4677	6371	0.98%	0.103%
79	11.542	3169	3173	3176	rBV	242	227	0.03%	0.004%
80	11.645	3202	3205	3211	rVB3	721	674	0.10%	0.011%
81	11.748	3230	3237	3245	rBV6	4439	6576	1.01%	0.107%
82	11.815	3245	3258	3275	rBV	357647	577242	88.38%	9.377%
83	12.195	3363	3376	3397	rBV	280365	474254	72.61%	7.704%
84	12.269	3397	3399	3403	rVV2	747	468	0.07%	0.008%
85	12.516	3473	3476	3481	rBV2	254	252	0.04%	0.004%
86	12.680	3518	3527	3539	rVB3	1613	2238	0.34%	0.036%
87	12.767	3550	3554	3557	rBV2	532	405	0.06%	0.007%
88	12.844	3575	3578	3583	rBV	243	263	0.04%	0.004%
89	12.999	3621	3626	3634	rVB5	1658	2401	0.37%	0.039%
90	13.108	3654	3660	3665	rBV2	330	414	0.06%	0.007%
91	13.220	3686	3695	3705	rBV5	7210	10538	1.61%	0.171%
92	13.622	3817	3820	3825	rVB	475	355	0.05%	0.006%
93	13.671	3832	3835	3841	rVB2	312	261	0.04%	0.004%
94	13.844	3880	3889	3905	rVB2	14803	21545	3.30%	0.350%
95	13.905	3905	3908	3911	rBV2	616	541	0.08%	0.009%
96	14.089	3954	3965	3984	rBV	31713	55134	8.44%	0.896%
97	14.330	4031	4040	4052	rBV3	18103	27300	4.18%	0.443%
98	14.436	4070	4073	4077	rVV2	279	234	0.04%	0.004%
99	15.143	4289	4293	4296	rBV2	480	465	0.07%	0.008%
100	16.728	4783	4786	4789	rBV3	884	595	0.09%	0.010%

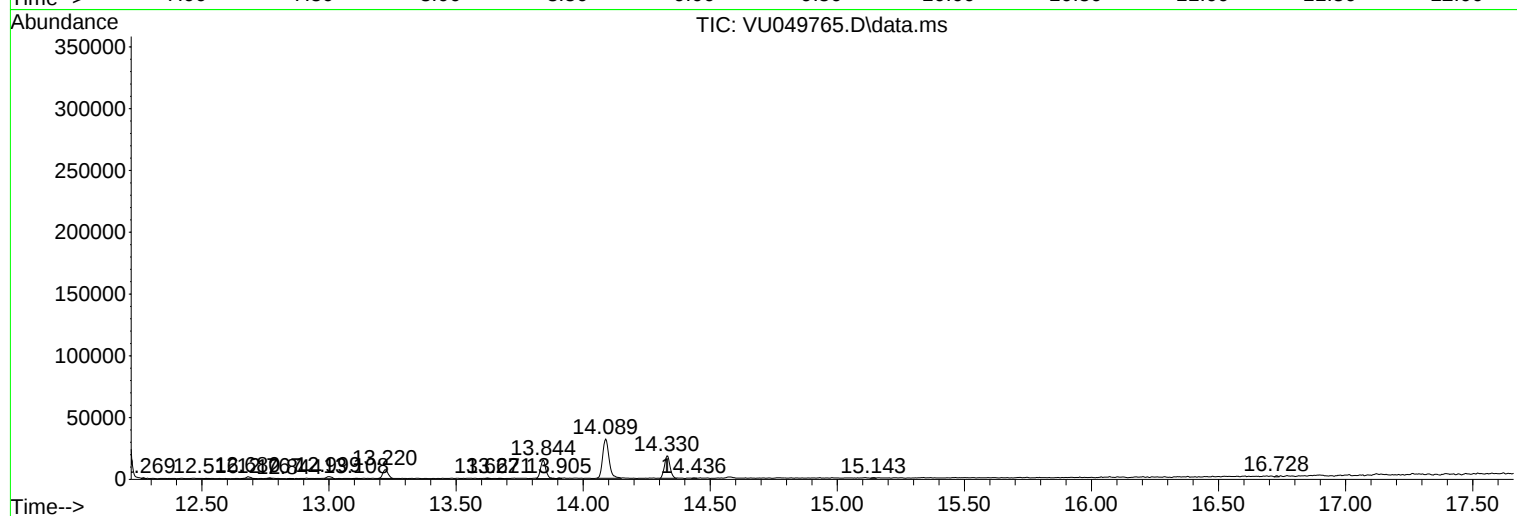
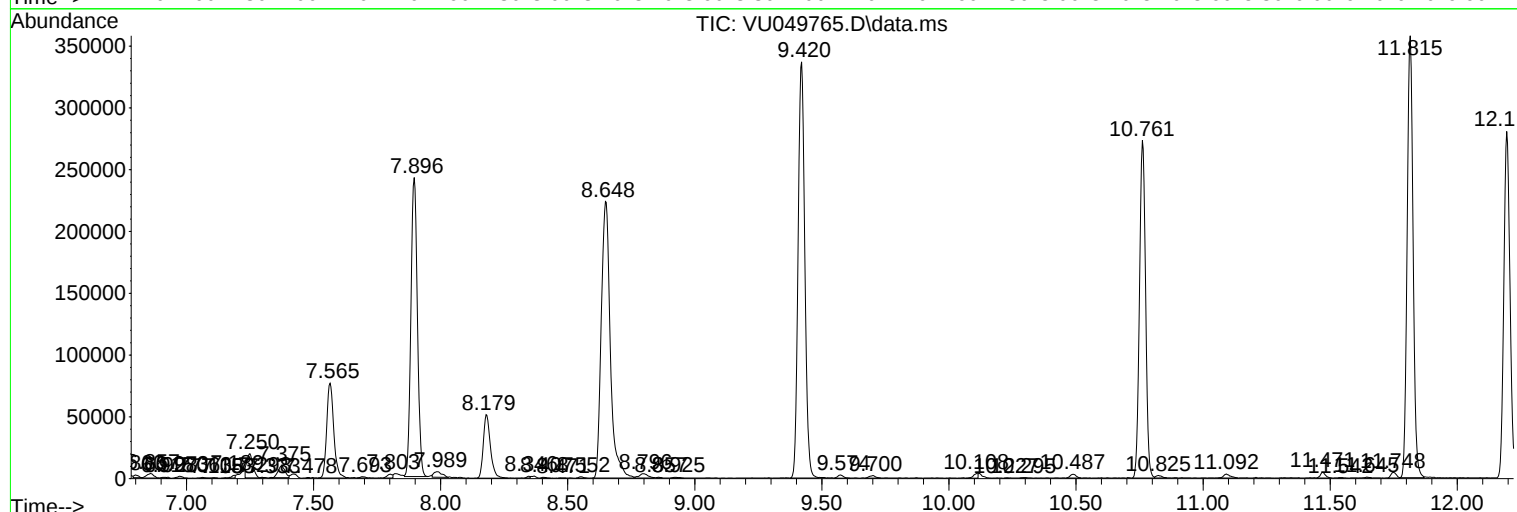
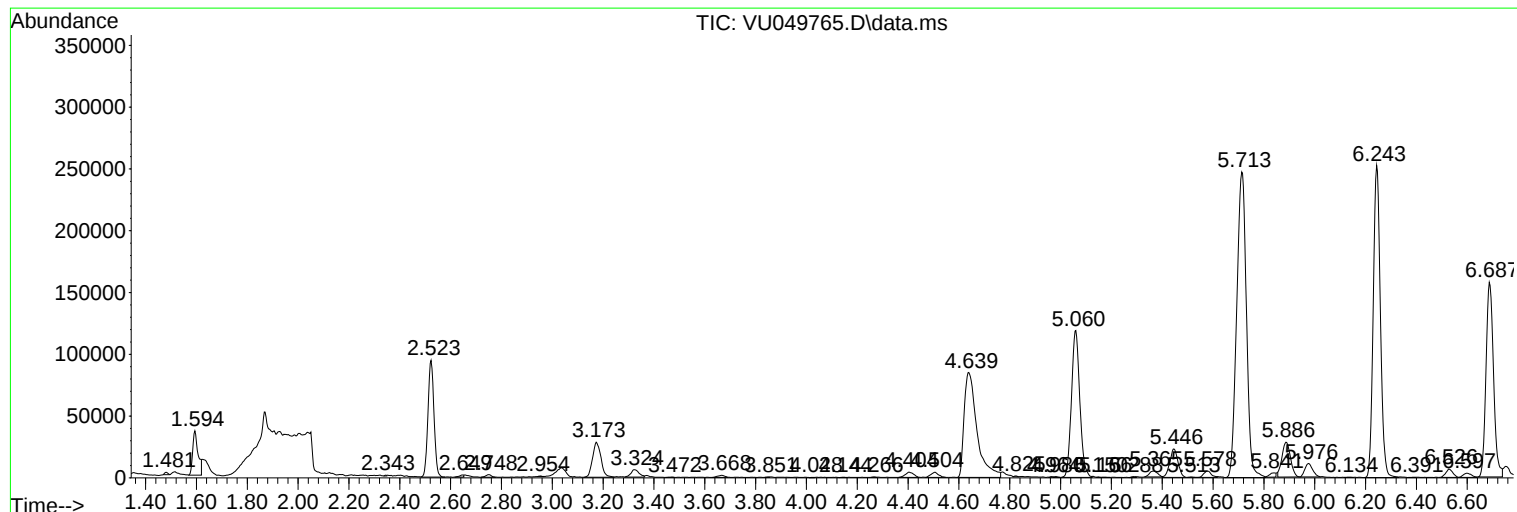
Sum of corrected areas: 6156040

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071822\
Data File : VU049765.D
Acq On : 18 Jul 2022 17:13
Operator : SY/MD
Sample : N3698-03ME
Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 18 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\VU071822\
Data File : VU049765.D
Acq On : 18 Jul 2022 17:13
Operator : SY/MD
Sample : N3698-03ME
Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5B68ME

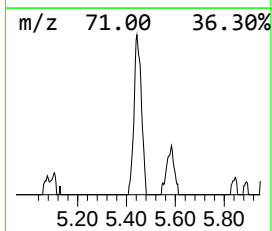
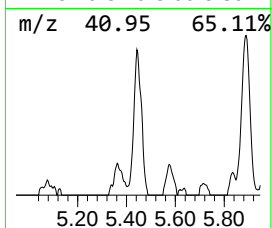
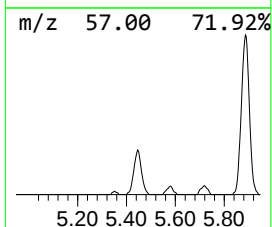
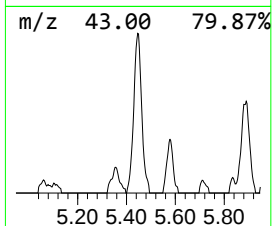
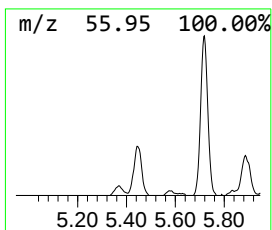
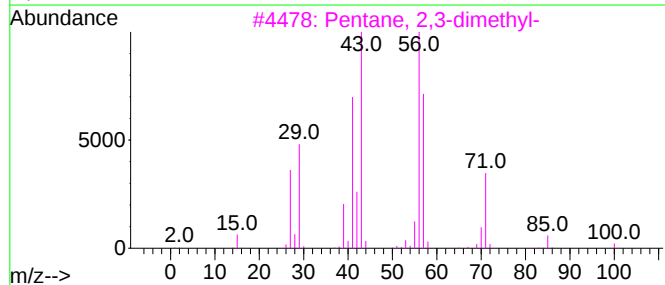
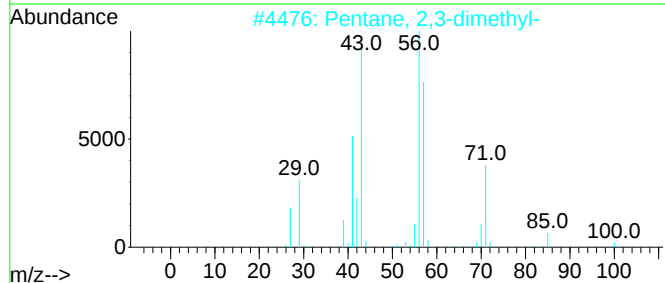
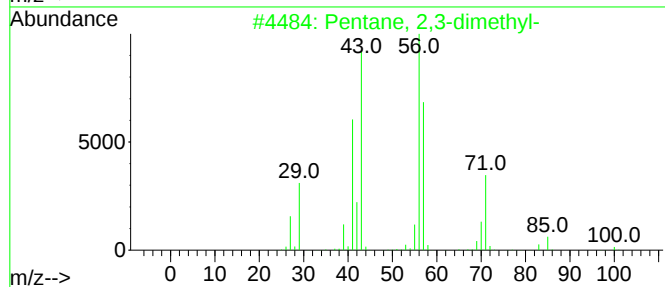
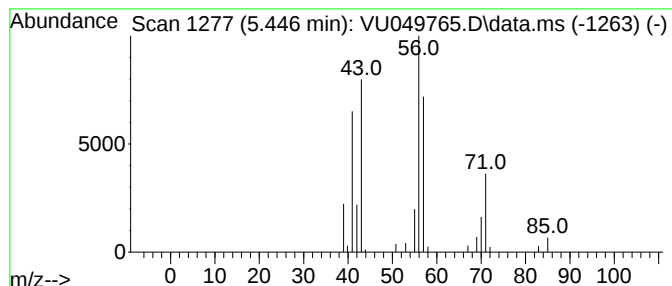
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.446	5.25 ug/L	51591	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			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071822\
Data File : VU049765.D
Acq On : 18 Jul 2022 17:13
Operator : SY/MD
Sample : N3698-03ME
Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5B68ME

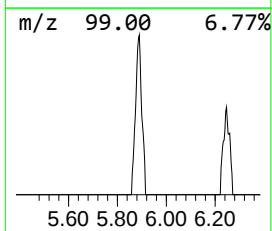
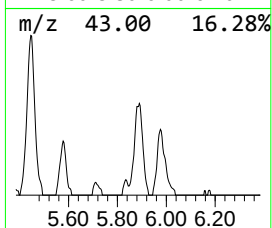
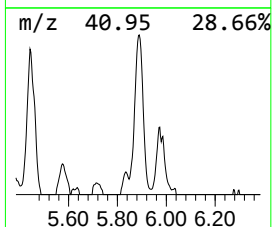
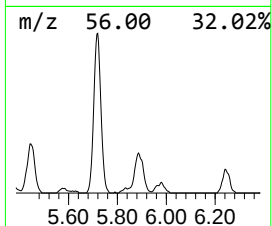
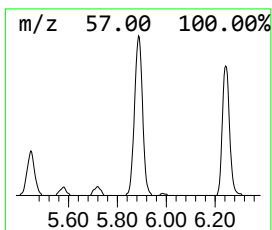
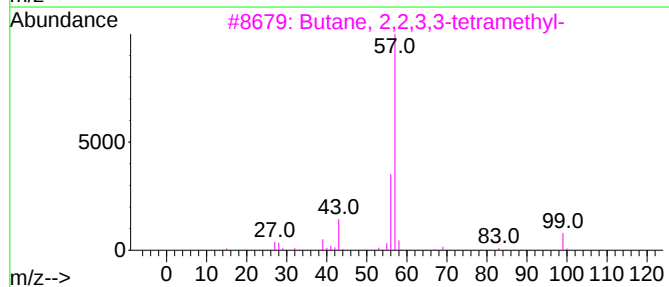
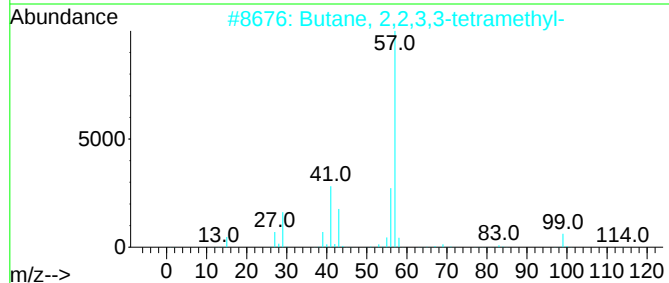
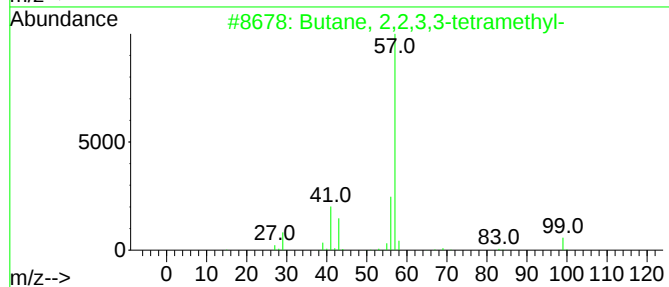
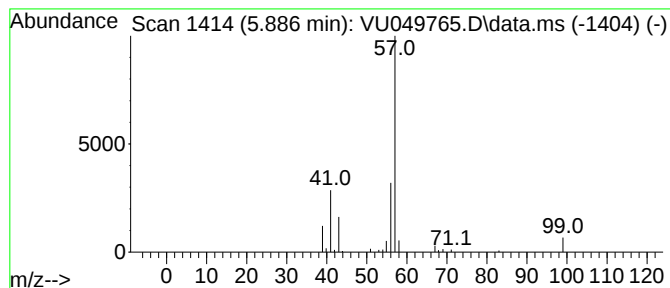
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.886	6.71 ug/L	65868	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		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
4		Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
5		Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071822\
Data File : VU049765.D
Acq On : 18 Jul 2022 17:13
Operator : SY/MD
Sample : N3698-03ME
Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5B68ME

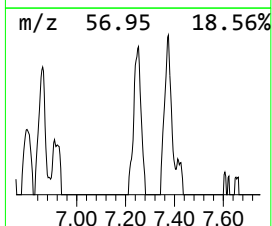
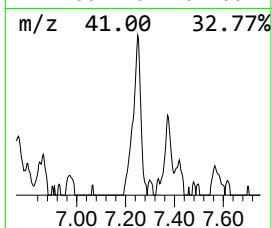
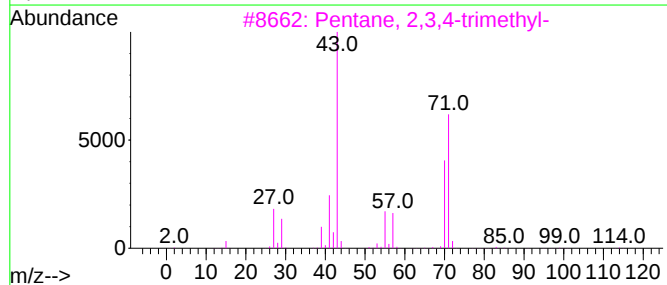
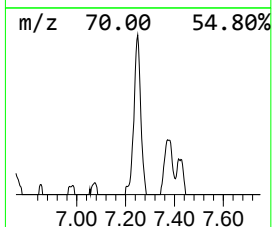
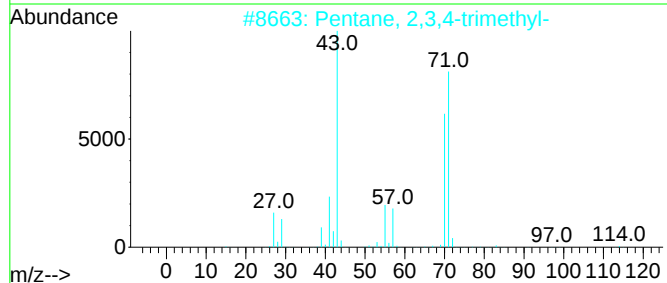
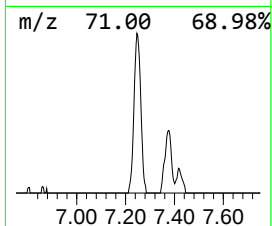
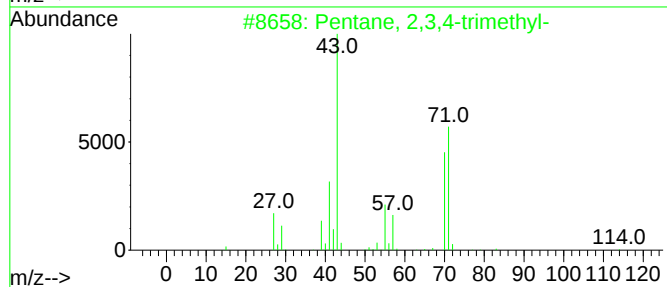
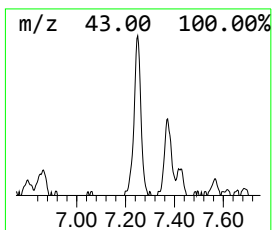
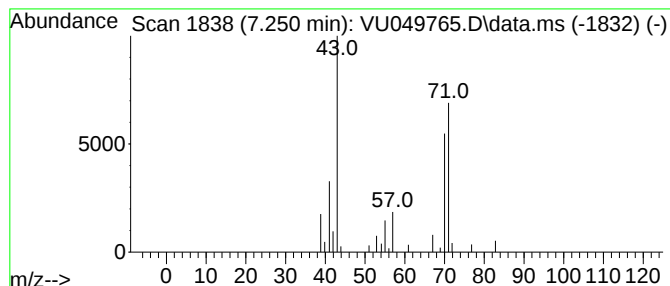
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.250	3.38 ug/L	33206	1,4-Difluorobenzene	6.243

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	72
2	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	72
3	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
4	Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	50
5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071822\
Data File : VU049765.D
Acq On : 18 Jul 2022 17:13
Operator : SY/MD
Sample : N3698-03ME
Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5B68ME

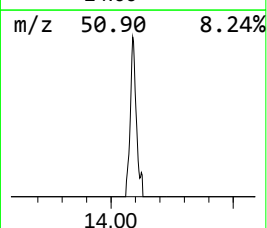
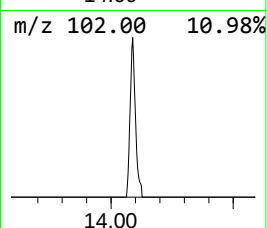
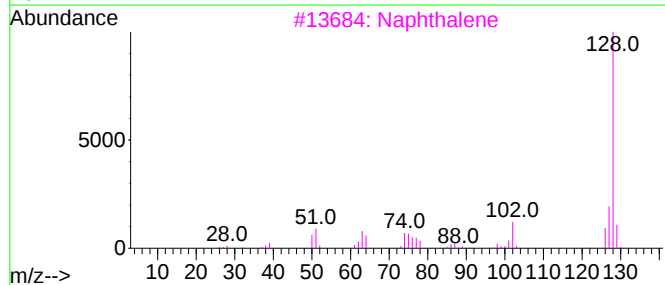
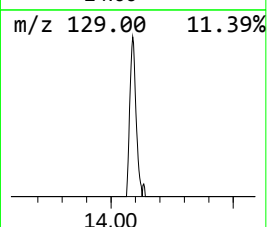
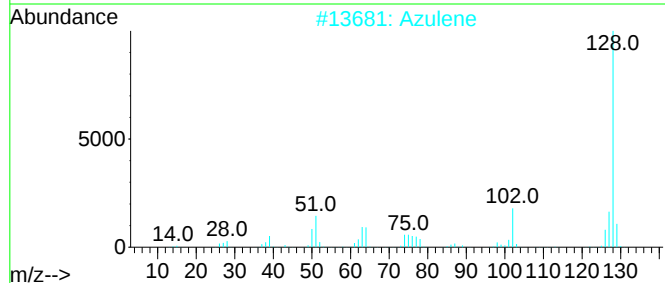
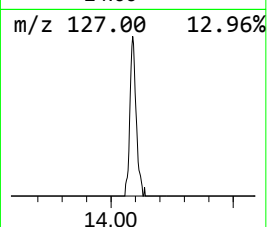
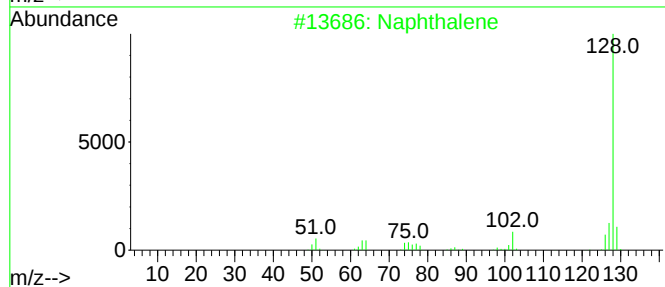
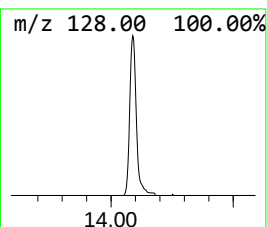
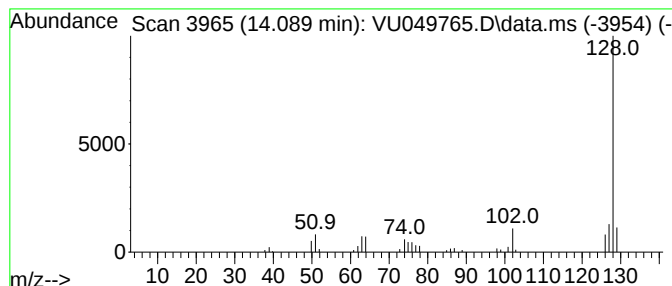
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 Azulene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.089	4.78 ug/L	55134	1,4-Dichlorobenzene-d4	11.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Azulene	128	C10H8	000275-51-4	94
3			Naphthalene	128	C10H8	000091-20-3	94
4			Azulene	128	C10H8	000275-51-4	91
5			Azulene	128	C10H8	000275-51-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071822\
Data File : VU049765.D
Acq On : 18 Jul 2022 17:13
Operator : SY/MD
Sample : N3698-03ME
Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 18 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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	5.446	5.3	ug/L	51591	1	6.243	491071	50.0
(DEL) Alkane: S...	5.886	6.7	ug/L	65868	1	6.243	491071	50.0
(DEL) Alkane: S...	7.250	3.4	ug/L	33206	1	6.243	491071	50.0
Azulene	14.089	4.8	ug/L	55134	3	11.815	577242	50.0