

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051022\
 Data File : VU048491.D
 Acq On : 10 May 2022 15:14
 Operator : SY/MD
 Sample : N2736-12
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXEW8

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\SFAMULM050622WMA.M
 Title : VOC Analysis

Signal : TIC: VU048491.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.600	75	81	93	rVB	137505	150649	13.74%	1.626%
2	1.912	171	178	192	rVB	95979	124765	11.38%	1.347%
3	2.205	263	269	286	rVB3	15822	22418	2.04%	0.242%
4	2.321	298	305	315	rVB3	5497	8773	0.80%	0.095%
5	2.475	344	353	362	rBV6	3569	6935	0.63%	0.075%
6	2.568	371	382	395	rBV	234211	380830	34.73%	4.111%
7	2.774	441	446	448	rBV	320	227	0.02%	0.002%
8	2.893	481	483	487	rBV	289	210	0.02%	0.002%
9	2.964	501	505	507	rBV2	770	579	0.05%	0.006%
10	3.366	614	630	644	rVB3	17334	39019	3.56%	0.421%
11	3.517	675	677	680	rBV	148	94	0.01%	0.001%
12	3.587	697	699	702	rBV	345	193	0.02%	0.002%
13	3.610	702	706	708	rBV2	267	173	0.02%	0.002%
14	3.626	708	711	713	rBV2	233	165	0.02%	0.002%
15	3.703	732	735	739	rVB	372	274	0.02%	0.003%
16	3.722	739	741	743	rBV	361	181	0.02%	0.002%
17	3.767	752	755	758	rVB2	537	353	0.03%	0.004%
18	3.784	758	760	762	rBV	175	114	0.01%	0.001%
19	3.832	771	775	780	rBV2	291	222	0.02%	0.002%
20	3.931	801	806	809	rBV3	417	311	0.03%	0.003%
21	3.980	809	821	822	rBV4	1599	2429	0.22%	0.026%
22	4.095	850	857	864	rVB3	1470	1947	0.18%	0.021%
23	4.256	899	907	910	rBV5	1562	1993	0.18%	0.022%
24	4.327	926	929	931	rBV2	626	445	0.04%	0.005%
25	4.433	952	962	965	rBV5	2525	3741	0.34%	0.040%
26	4.533	977	993	1007	rBV3	21099	51135	4.66%	0.552%
27	4.616	1007	1019	1042	rBV	135646	319609	29.15%	3.450%
28	5.063	1142	1158	1176	rBV2	208274	455683	41.56%	4.919%
29	5.195	1196	1199	1200	rBV	381	214	0.02%	0.002%
30	5.240	1210	1213	1215	rBV	278	174	0.02%	0.002%
31	5.253	1215	1217	1219	rBV	218	111	0.01%	0.001%
32	5.275	1222	1224	1227	rBV	366	261	0.02%	0.003%
33	5.292	1227	1229	1231	rBV	441	199	0.02%	0.002%
34	5.327	1237	1240	1244	rBV2	291	303	0.03%	0.003%
35	5.391	1244	1260	1272	rBV5	36767	84765	7.73%	0.915%
36	5.552	1307	1310	1313	rBV	241	173	0.02%	0.002%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
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37	5.632	1323	1335	1336	rBV3	9326	9913	0.90%	0.107%
38	5.726	1346	1364	1376	rBV2	404217	1096392	100.00%	11.836%
39	5.989	1435	1446	1460	rVB8	9536	20573	1.88%	0.222%
40	6.063	1467	1469	1471	rBV	276	137	0.01%	0.001%
41	6.124	1479	1488	1490	rBV3	599	880	0.08%	0.009%
42	6.153	1490	1497	1506	rVB4	1377	2128	0.19%	0.023%
43	6.189	1506	1508	1510	rBV2	336	172	0.02%	0.002%
44	6.250	1513	1527	1545	rBV	350317	657191	59.94%	7.095%
45	6.417	1576	1579	1580	rBV	311	130	0.01%	0.001%
46	6.446	1586	1588	1589	rBV	310	150	0.01%	0.002%
47	6.546	1608	1619	1620	rBV5	3650	4543	0.41%	0.049%
48	6.594	1632	1634	1638	rBV2	322	213	0.02%	0.002%
49	6.623	1639	1643	1646	rBV2	244	223	0.02%	0.002%
50	6.690	1650	1664	1693	rBV	254943	514447	46.92%	5.554%
51	6.925	1736	1737	1741	rVB2	421	168	0.02%	0.002%
52	7.005	1753	1762	1765	rBV4	1434	1934	0.18%	0.021%
53	7.060	1776	1779	1782	rBV2	331	207	0.02%	0.002%
54	7.108	1792	1794	1799	rBV	188	177	0.02%	0.002%
55	7.156	1801	1809	1810	rBV3	3986	3729	0.34%	0.040%
56	7.240	1833	1835	1839	rVB2	349	239	0.02%	0.003%
57	7.333	1861	1864	1868	rBV2	164	144	0.01%	0.002%
58	7.388	1870	1881	1882	rBV6	3449	3925	0.36%	0.042%
59	7.494	1911	1914	1917	rBV	427	351	0.03%	0.004%
60	7.568	1924	1937	1950	rBV2	104418	197339	18.00%	2.130%
61	7.690	1967	1975	1988	rVB6	5665	10510	0.96%	0.113%
62	7.761	1988	1997	2001	rBV7	1754	2222	0.20%	0.024%
63	7.899	2028	2040	2055	rVB	501261	860872	78.52%	9.293%
64	8.179	2115	2127	2140	rBV	76223	128013	11.68%	1.382%
65	8.369	2180	2186	2191	rBV4	1583	2300	0.21%	0.025%
66	8.484	2209	2222	2234	rVB3	9325	17409	1.59%	0.188%
67	8.578	2240	2251	2257	rBV2	18183	29812	2.72%	0.322%
68	8.632	2257	2268	2288	rBV	411241	720832	65.75%	7.782%
69	8.925	2356	2359	2361	rBV	369	185	0.02%	0.002%
70	8.938	2361	2363	2365	rBV	246	125	0.01%	0.001%
71	9.070	2402	2404	2407	rBV2	714	491	0.04%	0.005%
72	9.115	2416	2418	2420	rBV2	258	123	0.01%	0.001%
73	9.198	2437	2444	2453	rVB8	5421	8297	0.76%	0.090%
74	9.272	2453	2467	2476	rBV4	5503	9261	0.84%	0.100%
75	9.327	2476	2484	2499	rBV6	11700	21585	1.97%	0.233%
76	9.417	2499	2512	2536	rBV	494303	833437	76.02%	8.997%

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77	9.809	2631	2634	2635	rBV2	615	352	0.03%	0.004%
78	9.877	2648	2655	2663	rBV5	3590	5398	0.49%	0.058%
79	10.166	2741	2745	2750	rBV4	790	843	0.08%	0.009%
80	10.221	2759	2762	2765	rBV	363	271	0.02%	0.003%
81	10.301	2785	2787	2789	rBV2	409	183	0.02%	0.002%
82	10.362	2794	2806	2826	rBV3	56023	102207	9.32%	1.103%
83	10.758	2917	2929	2950	rVB	374349	613958	56.00%	6.628%
84	10.967	2989	2994	2996	rBV3	1100	1056	0.10%	0.011%
85	11.005	3002	3006	3009	rBV3	903	845	0.08%	0.009%
86	11.069	3017	3026	3038	rBV8	7417	12956	1.18%	0.140%
87	11.266	3084	3087	3092	rBV3	489	489	0.04%	0.005%
88	11.500	3158	3160	3161	rBV	266	103	0.01%	0.001%
89	11.523	3161	3167	3175	rVV6	2146	2605	0.24%	0.028%
90	11.812	3245	3257	3276	rBV	535269	850360	77.56%	9.180%
91	11.947	3293	3299	3304	rBV7	1473	2276	0.21%	0.025%
92	12.008	3311	3318	3324	rBV4	2299	2578	0.24%	0.028%
93	12.192	3364	3375	3396	rVB	524596	842557	76.85%	9.096%
94	12.912	3597	3599	3604	rVB3	740	450	0.04%	0.005%
95	12.944	3604	3609	3611	rBV3	616	597	0.05%	0.006%
96	13.192	3681	3686	3691	rBV3	664	798	0.07%	0.009%
97	13.243	3700	3702	3706	rBV2	332	255	0.02%	0.003%
98	13.266	3706	3709	3713	rBV	447	370	0.03%	0.004%
99	13.323	3724	3727	3729	rBV3	644	400	0.04%	0.004%
100	13.394	3744	3749	3752	rBV5	797	901	0.08%	0.010%

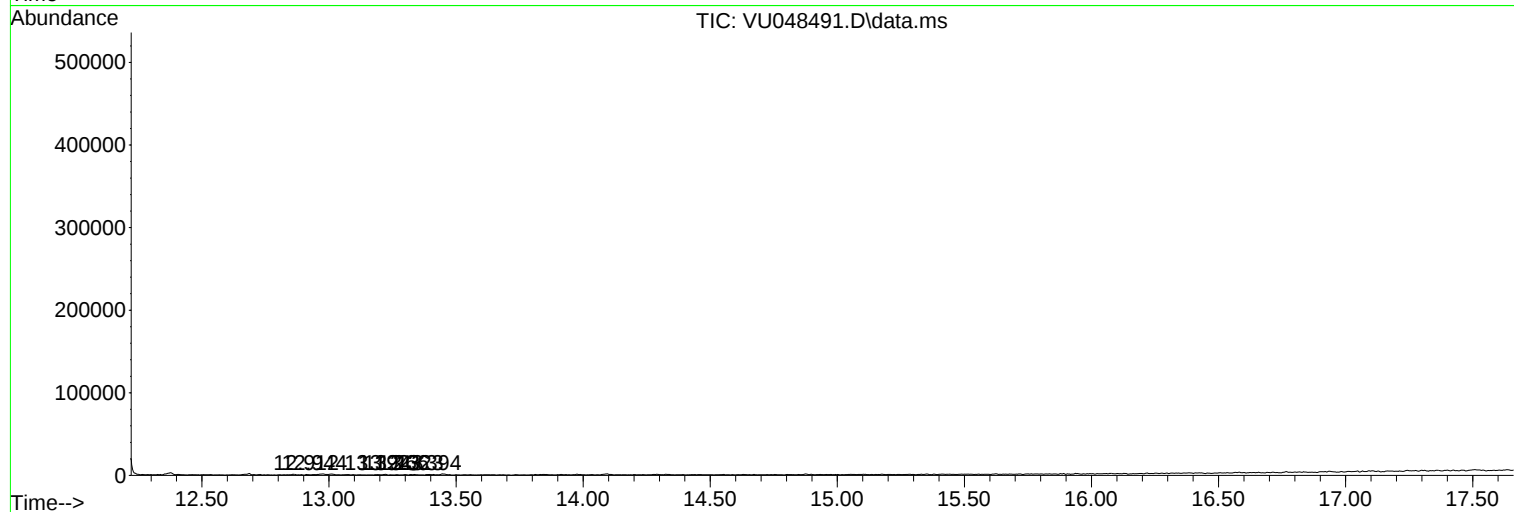
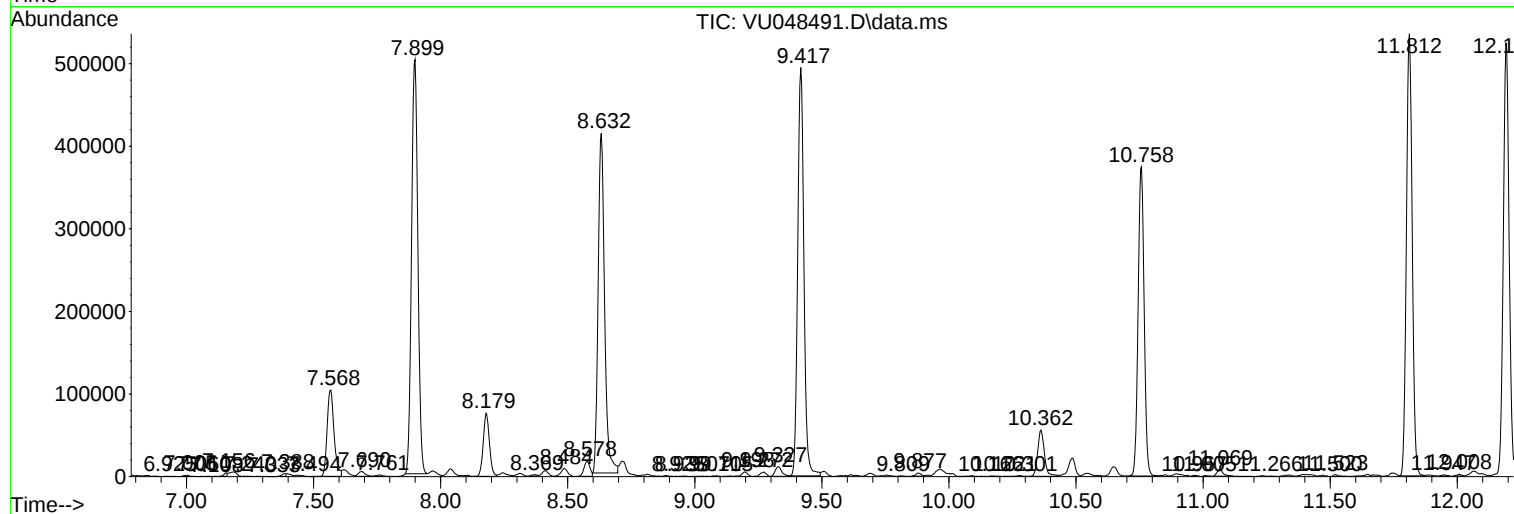
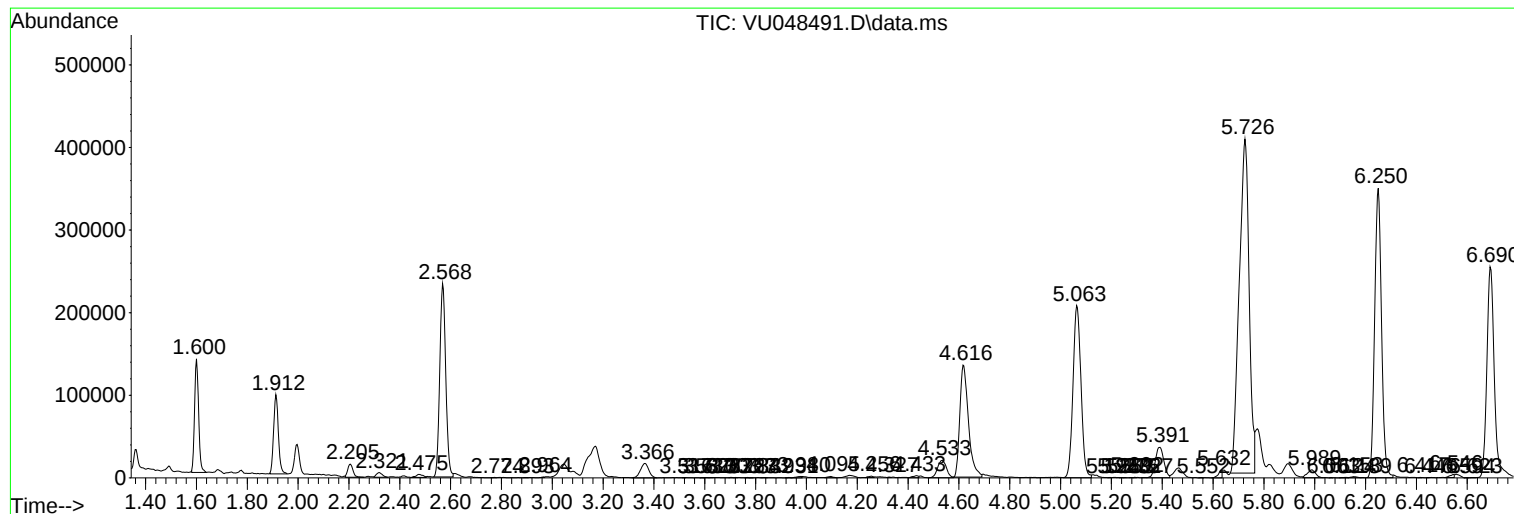
Sum of corrected areas: 9263254

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

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



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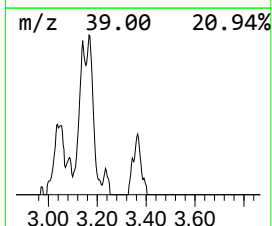
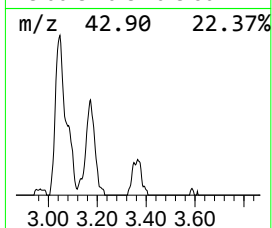
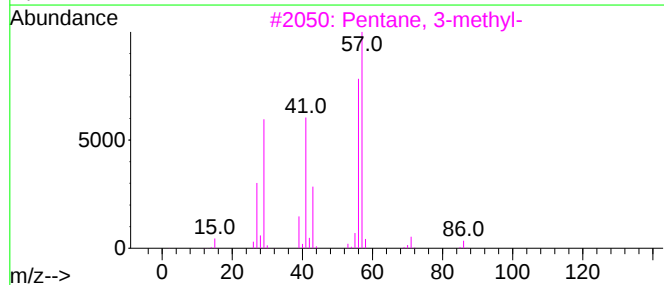
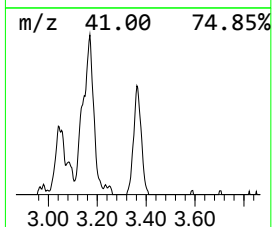
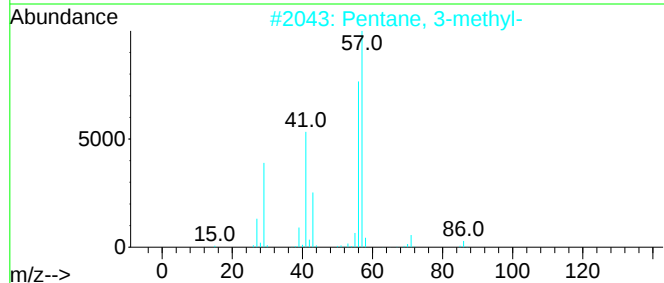
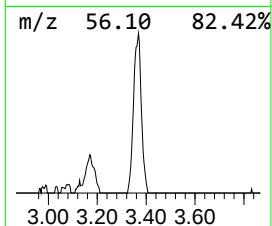
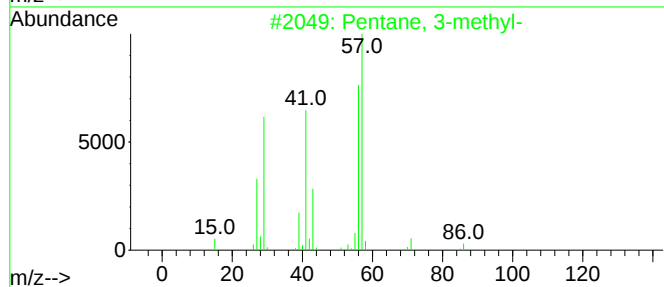
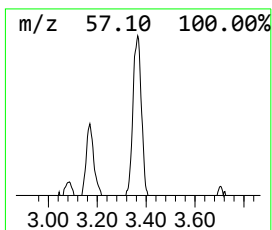
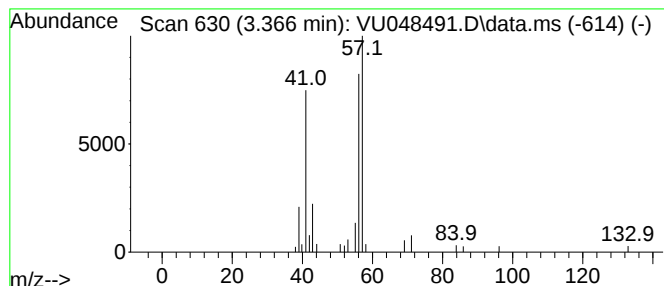
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.366	2.97 ug/L	39019	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	86
2			Pentane, 3-methyl-	86	C6H14	000096-14-0	72
3			Pentane, 3-methyl-	86	C6H14	000096-14-0	72
4			Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	64
5			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64



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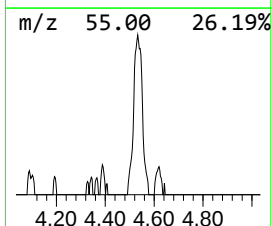
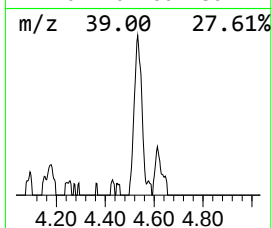
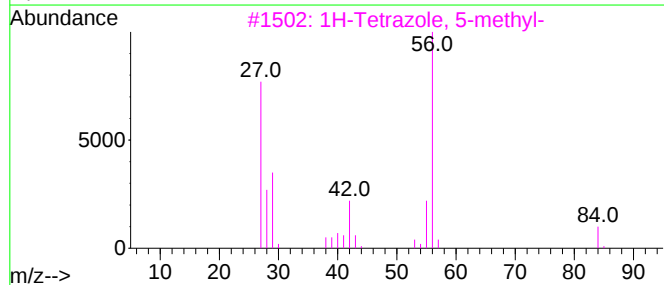
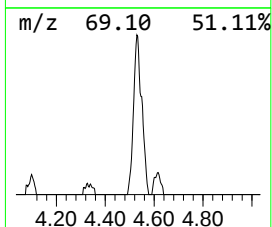
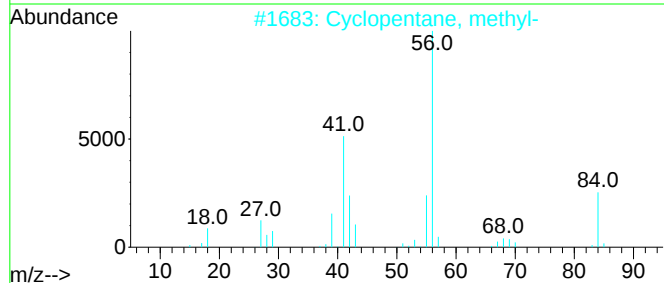
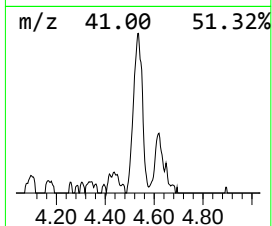
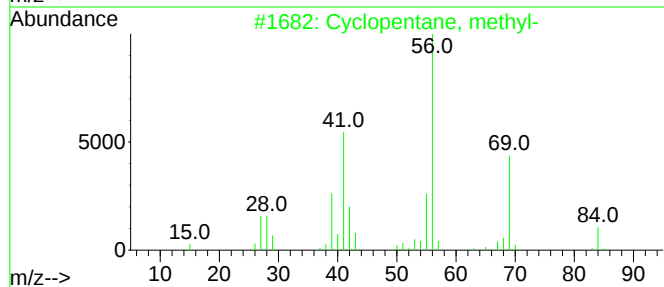
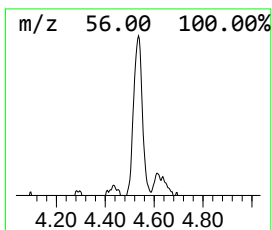
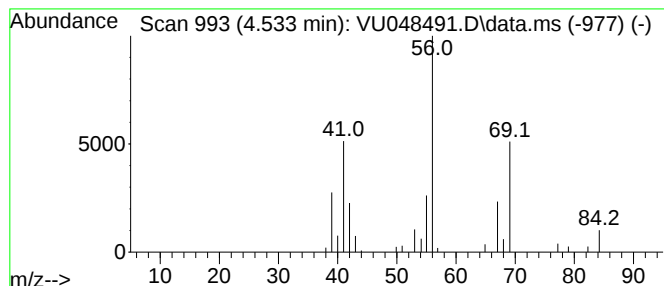
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Cyclic4.533 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.533	3.89 ug/L	51135	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	72
2			Cyclopentane, methyl-	84	C6H12	000096-37-7	59
3			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	53
4			Cyclobutane, ethyl-	84	C6H12	004806-61-5	53
5			Cyclobutane, ethyl-	84	C6H12	004806-61-5	50



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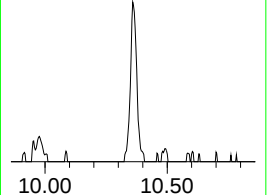
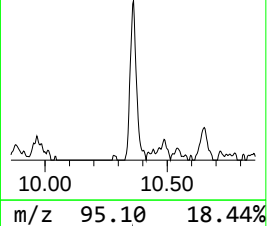
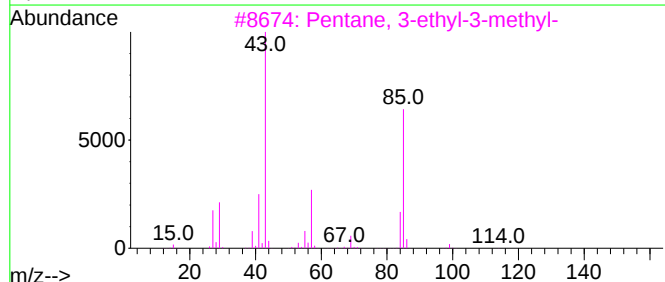
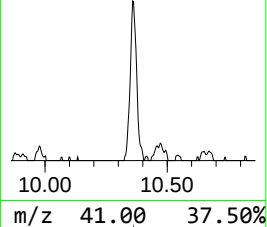
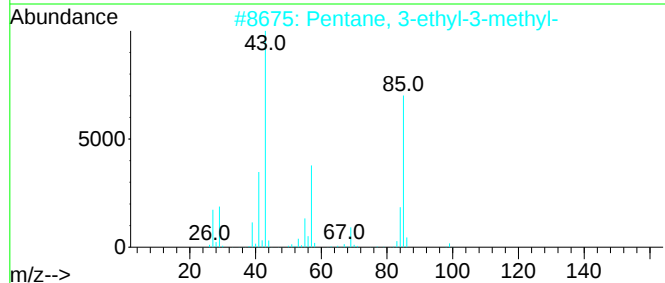
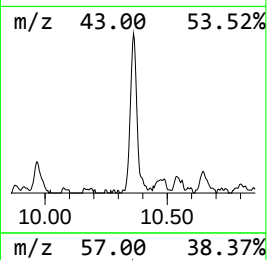
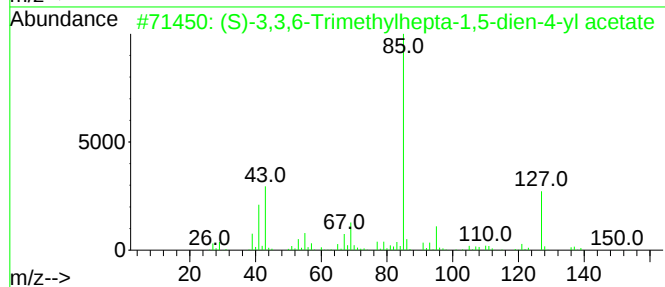
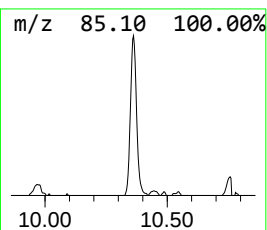
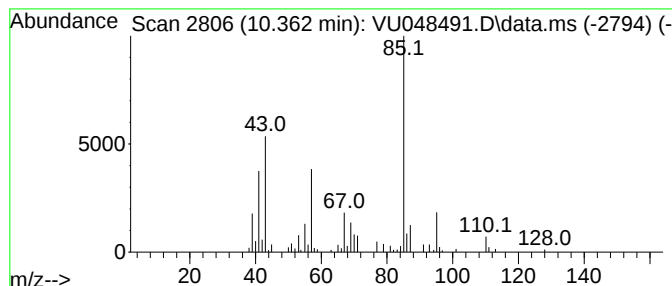
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 (S)-3,3,6-Trimethylhepta-1,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.362	6.13 ug/L	102207	Chlorobenzene-d5	9.417

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-3,3,6-Trimethylhepta-1,5-die...	196	C12H2002	003465-88-1	59		
2	Pentane, 3-ethyl-3-methyl-	114	C8H18	001067-08-9	59		
3	Pentane, 3-ethyl-3-methyl-	114	C8H18	001067-08-9	53		
4	Pentane, 3-ethyl-3-methyl-	114	C8H18	001067-08-9	53		
5	2H-Pyran-2-methanol, tetrahydro-	116	C6H1202	000100-72-1	53		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051022\
Data File : VU048491.D
Acq On : 10 May 2022 15:14
Operator : SY/MD
Sample : N2736-12
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEW8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.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...	3.366	3.0	ug/L	39019	1	6.250	657191	50.0
(DEL) Alkane: C...	4.533	3.9	ug/L	51135	1	6.250	657191	50.0
(S)-3,3,6-Trime...	10.362	6.1	ug/L	102207	2	9.417	833437	50.0