

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU010522\
 Data File : VU046674.D
 Acq On : 05 Jan 2022 19:52
 Operator : SY/MD
 Sample : N1025-05
 Misc : 6.43g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGLG9

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\SFAMULM010522WMA.M
 Title : VOC Analysis

Signal : TIC: VU046674.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.604	73	82	111	rVB	69612	144305	15.49%	1.774%
2	1.919	172	180	218	rVB	35151	117075	12.57%	1.439%
3	2.555	366	378	399	rBV	160784	276311	29.66%	3.396%
4	2.870	472	476	479	rVB2	261	177	0.02%	0.002%
5	2.957	499	503	505	rBV2	261	181	0.02%	0.002%
6	2.983	509	511	514	rVB3	274	150	0.02%	0.002%
7	3.044	521	530	545	rBV2	1695	3869	0.42%	0.048%
8	3.186	562	574	592	rVB3	1800	4517	0.48%	0.056%
9	3.446	652	655	658	rBB	166	133	0.01%	0.002%
10	3.481	663	666	668	rBV	143	120	0.01%	0.001%
11	3.687	726	730	732	rBV2	679	442	0.05%	0.005%
12	3.761	749	753	756	rBV	142	165	0.02%	0.002%
13	4.089	850	855	857	rBV	159	172	0.02%	0.002%
14	4.665	1017	1034	1094	rBV2	34215	223311	23.97%	2.745%
15	5.067	1143	1159	1189	rVB	155417	366870	39.38%	4.509%
16	5.356	1246	1249	1253	rBV3	380	365	0.04%	0.004%
17	5.449	1275	1278	1281	rBV2	486	348	0.04%	0.004%
18	5.465	1281	1283	1286	rVB	316	188	0.02%	0.002%
19	5.587	1315	1321	1326	rVB3	850	863	0.09%	0.011%
20	5.722	1343	1363	1393	rVV2	365479	931700	100.00%	11.451%
21	5.854	1401	1404	1407	rBV2	247	171	0.02%	0.002%
22	5.899	1415	1418	1424	rVB3	673	509	0.05%	0.006%
23	5.983	1435	1444	1457	rBV5	3074	7028	0.75%	0.086%
24	6.128	1486	1489	1490	rBV	288	206	0.02%	0.003%
25	6.157	1496	1498	1502	rBV	240	238	0.03%	0.003%
26	6.176	1502	1504	1508	rVV	245	216	0.02%	0.003%
27	6.250	1512	1527	1551	rVV	233751	465657	49.98%	5.723%
28	6.349	1555	1558	1561	rBV	231	147	0.02%	0.002%
29	6.507	1597	1607	1609	rBV3	1923	2629	0.28%	0.032%
30	6.558	1620	1623	1627	rBB	156	129	0.01%	0.002%
31	6.607	1628	1638	1639	rBV2	919	1206	0.13%	0.015%
32	6.690	1650	1664	1691	rVV	193058	408211	43.81%	5.017%
33	6.800	1695	1698	1706	rVB3	847	1011	0.11%	0.012%
34	7.070	1775	1782	1783	rBV	272	343	0.04%	0.004%
35	7.189	1814	1819	1820	rBV	358	317	0.03%	0.004%
36	7.227	1828	1831	1833	rBV3	372	239	0.03%	0.003%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM010522WMA.M
 Title : VOC Analysis

37	7.243	1833	1836	1837	rVV	389	233	0.03%	0.003%
38	7.253	1837	1839	1842	rVV2	569	355	0.04%	0.004%
39	7.272	1842	1845	1849	rVB	335	237	0.03%	0.003%
40	7.497	1909	1915	1916	rBV2	541	554	0.06%	0.007%
41	7.568	1922	1937	1970	rBV	101084	219957	23.61%	2.703%
42	7.787	2001	2005	2006	rBV	648	483	0.05%	0.006%
43	7.841	2017	2022	2025	rBV	150	203	0.02%	0.002%
44	7.899	2025	2040	2058	rBV	417206	793362	85.15%	9.751%
45	8.185	2117	2129	2157	rBB2	52334	148211	15.91%	1.822%
46	8.365	2183	2185	2187	rBV	231	152	0.02%	0.002%
47	8.427	2201	2204	2208	rBB	167	152	0.02%	0.002%
48	8.472	2214	2218	2221	rBV2	363	384	0.04%	0.005%
49	8.681	2262	2283	2313	rBV2	179098	522515	56.08%	6.422%
50	8.864	2335	2340	2346	rVB4	928	1156	0.12%	0.014%
51	8.925	2350	2359	2366	rBV5	1315	2339	0.25%	0.029%
52	8.986	2376	2378	2380	rVB2	287	121	0.01%	0.001%
53	9.057	2390	2400	2406	rBV4	1008	1879	0.20%	0.023%
54	9.121	2413	2420	2428	rBV5	1384	2579	0.28%	0.032%
55	9.169	2428	2435	2440	rVV4	2231	3737	0.40%	0.046%
56	9.214	2442	2449	2459	rVB3	6122	10601	1.14%	0.130%
57	9.336	2479	2487	2497	rVB4	6111	9562	1.03%	0.118%
58	9.427	2501	2515	2536	rBV	257665	616241	66.14%	7.574%
59	9.500	2536	2538	2541	rBV2	232	163	0.02%	0.002%
60	9.571	2546	2560	2571	rVV6	1881	3902	0.42%	0.048%
61	9.623	2571	2576	2578	rVV2	384	419	0.04%	0.005%
62	9.645	2581	2583	2584	rVV	458	226	0.02%	0.003%
63	9.677	2584	2593	2594	rVV6	1273	1705	0.18%	0.021%
64	9.716	2598	2605	2612	rVV7	4328	7655	0.82%	0.094%
65	9.761	2615	2619	2635	rVB7	1694	3228	0.35%	0.040%
66	9.954	2674	2679	2683	rBV3	635	665	0.07%	0.008%
67	10.021	2690	2700	2714	rBV8	6570	14307	1.54%	0.176%
68	10.118	2723	2730	2738	rBV5	4655	7039	0.76%	0.087%
69	10.253	2755	2772	2785	rBV7	10765	20670	2.22%	0.254%
70	10.320	2785	2793	2795	rBV5	2301	3389	0.36%	0.042%
71	10.356	2797	2804	2811	rBV7	6760	11268	1.21%	0.138%
72	10.465	2830	2838	2842	rBV4	2791	4249	0.46%	0.052%
73	10.555	2854	2866	2875	rBV7	8086	17602	1.89%	0.216%
74	10.626	2876	2888	2893	rBV5	11362	20001	2.15%	0.246%
75	10.774	2914	2934	2958	rBV	320336	552563	59.31%	6.791%
76	11.018	3003	3010	3017	rBV7	3138	6005	0.64%	0.074%

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77	11.066	3019	3025	3033	rVB3	7701	11672	1.25%	0.143%
78	11.243	3076	3080	3087	rBV8	1513	1704	0.18%	0.021%
79	11.311	3088	3101	3114	rBV8	11916	27909	3.00%	0.343%
80	11.378	3115	3122	3128	rVV5	10038	15133	1.62%	0.186%
81	11.417	3128	3134	3141	rVV	24802	35377	3.80%	0.435%
82	11.475	3142	3152	3174	rVB3	31431	77201	8.29%	0.949%
83	11.578	3174	3184	3190	rBV2	12173	20774	2.23%	0.255%
84	11.706	3215	3224	3232	rBV7	16628	32076	3.44%	0.394%
85	11.819	3248	3259	3271	rBV	409300	662539	71.11%	8.143%
86	11.877	3272	3277	3284	rVB2	13003	15559	1.67%	0.191%
87	12.127	3335	3355	3363	rBV3	22485	55443	5.95%	0.681%
88	12.201	3365	3378	3391	rVB	496032	831539	89.25%	10.220%
89	12.385	3429	3435	3449	rVB5	16518	35822	3.84%	0.440%
90	12.471	3456	3462	3466	rBV3	10914	16000	1.72%	0.197%
91	13.587	3803	3809	3816	rBV	12702	16951	1.82%	0.208%
92	13.844	3882	3889	3903	rVB	8797	15163	1.63%	0.186%
93	14.089	3957	3965	3983	rVB	45706	77620	8.33%	0.954%
94	14.188	3989	3996	4010	rVB5	16875	32076	3.44%	0.394%
95	14.449	4070	4077	4084	rBV	22687	29437	3.16%	0.362%
96	15.018	4249	4254	4262	rBV7	5414	8285	0.89%	0.102%
97	15.211	4304	4314	4327	rBV8	14975	31567	3.39%	0.388%
98	15.404	4365	4374	4389	rBV3	44555	79161	8.50%	0.973%
99	16.291	4645	4650	4661	rVB3	17610	24933	2.68%	0.306%
100	16.407	4680	4686	4694	rBV4	9033	13040	1.40%	0.160%

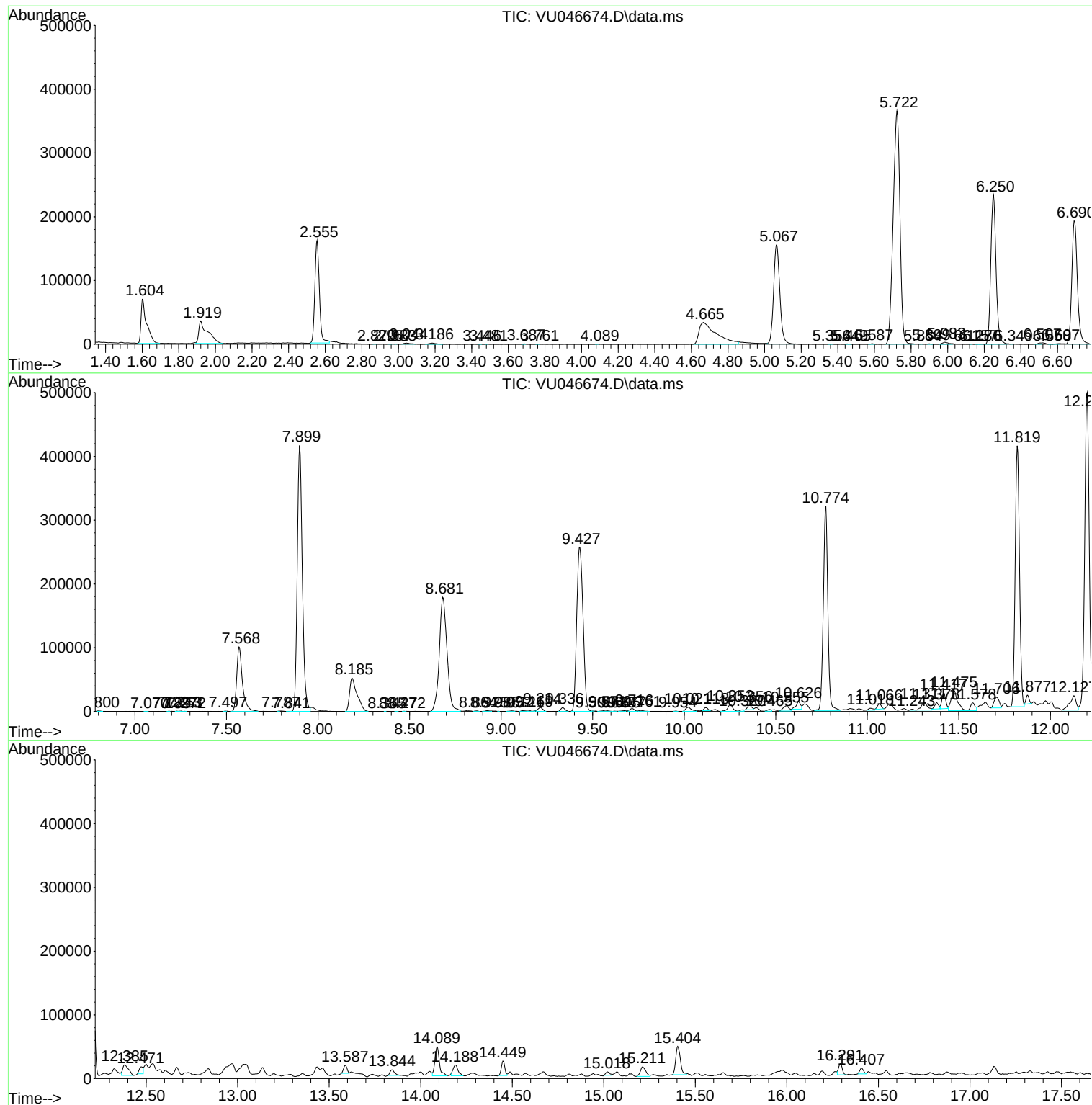
Sum of corrected areas: 8136569

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM010522WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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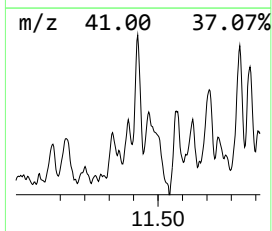
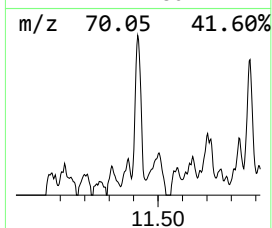
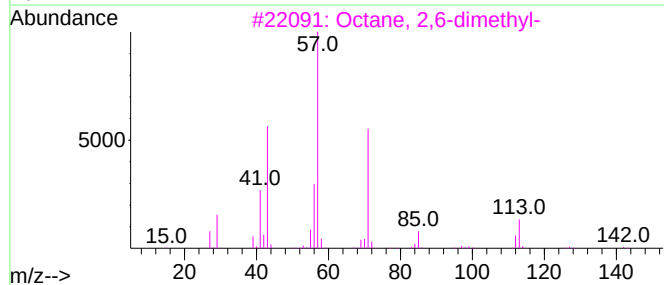
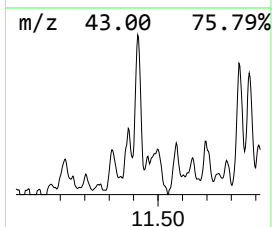
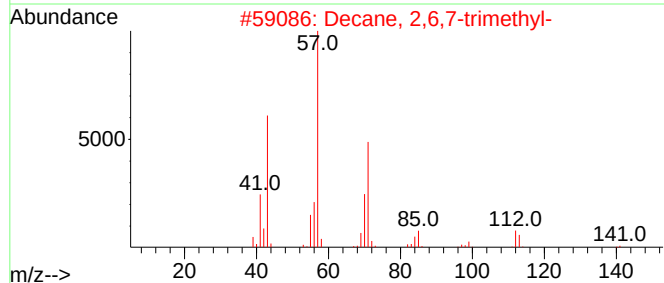
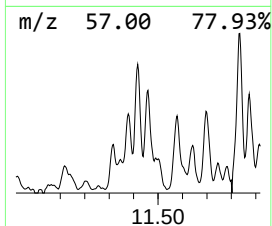
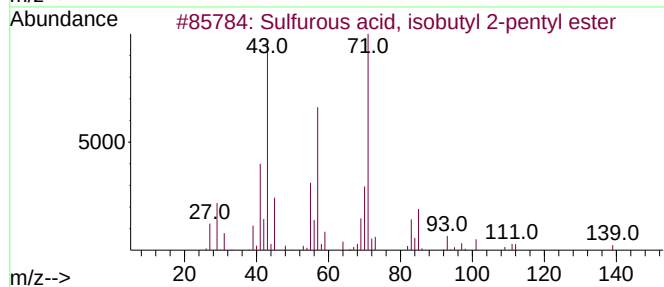
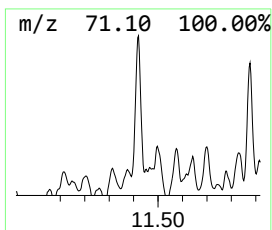
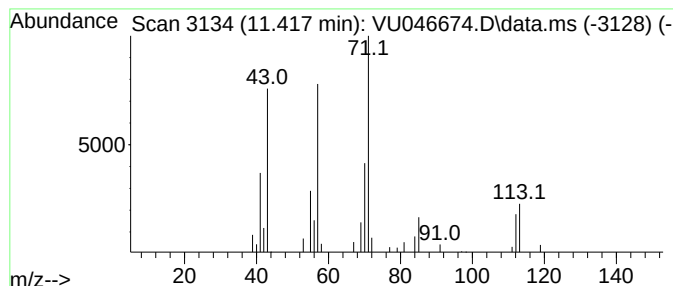
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM010522WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Sulfurous acid, isobutyl 2-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.417	2.67 ug/L	35377	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, isobutyl 2-penty...	208	C9H20O3S	1000309-15-2	64
2			Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	64
3			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	59
4			Heptane, 3-ethyl-5-methyl-	142	C10H22	052896-90-9	59
5			Octane, 3-ethyl-	142	C10H22	005881-17-4	59



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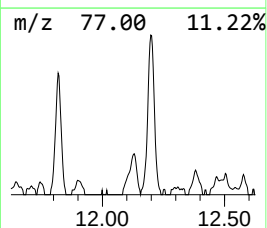
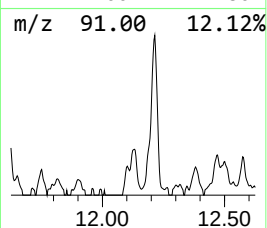
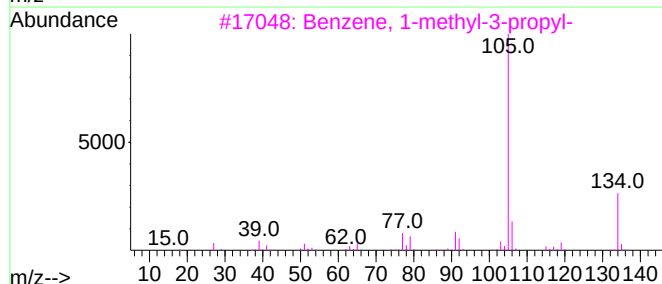
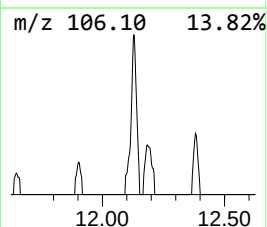
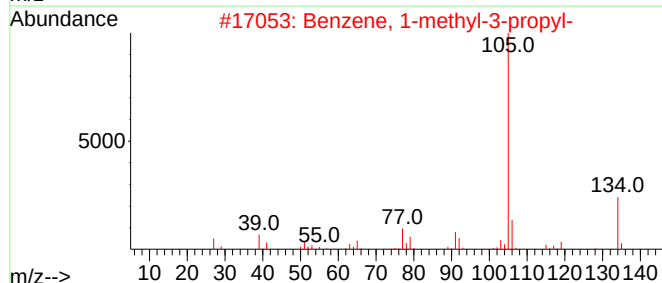
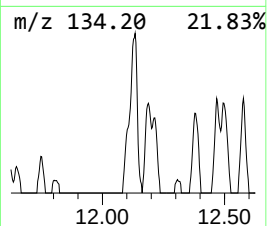
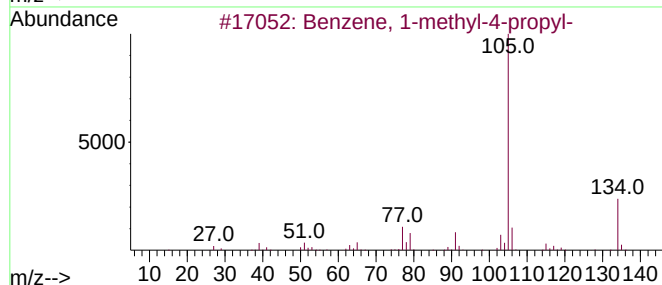
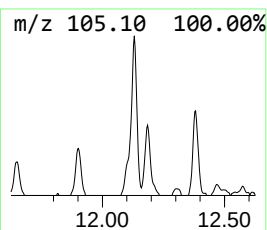
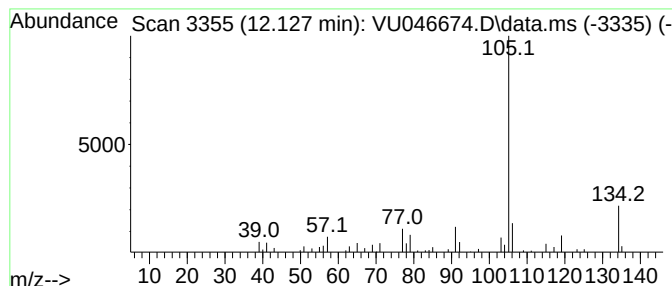
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM010522WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Benzene, 1-methyl-4-propyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.127	4.18 ug/L	55443	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-4-propyl-	134	C10H14	001074-55-1	91
2			Benzene, 1-methyl-3-propyl-	134	C10H14	001074-43-7	91
3			Benzene, 1-methyl-3-propyl-	134	C10H14	001074-43-7	91
4			2-Tolyloxirane	134	C9H10O	002783-26-8	91
5			Benzene, 1-methyl-2-propyl-	134	C10H14	001074-17-5	91



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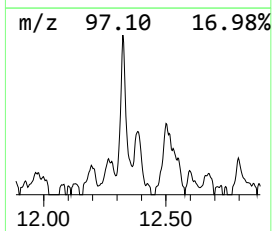
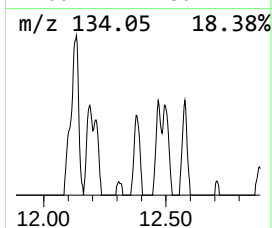
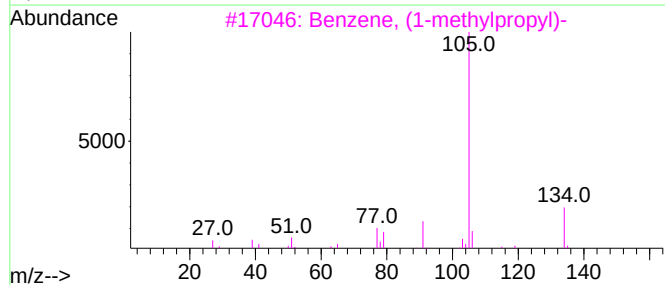
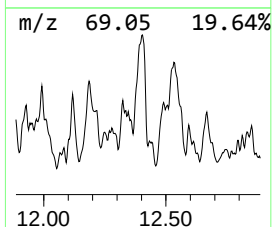
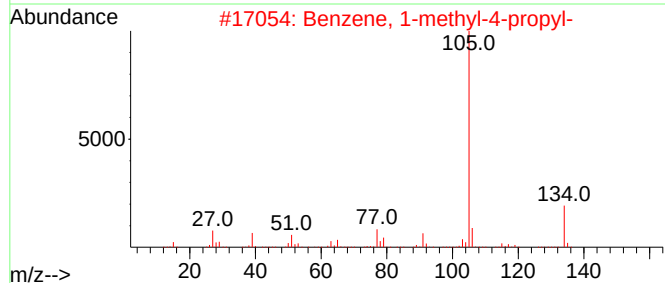
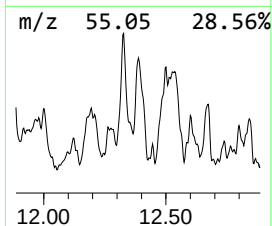
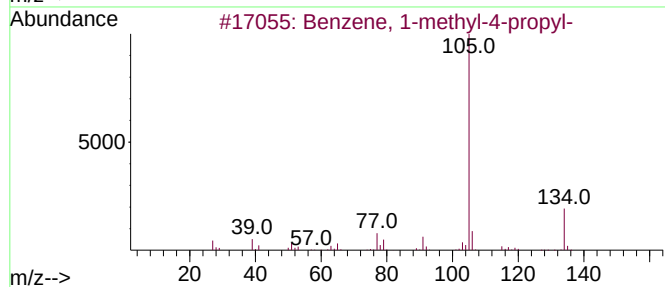
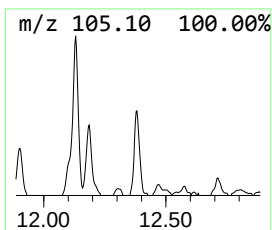
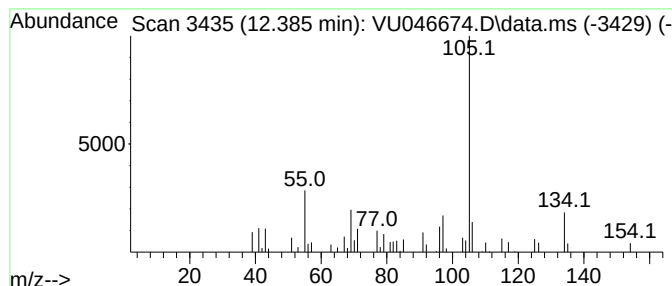
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM010522WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Benzene, (1-methylpropyl)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.385	2.70 ug/L	35822	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-4-propyl-	134	C10H14	001074-55-1	46
2			Benzene, 1-methyl-4-propyl-	134	C10H14	001074-55-1	46
3			Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	46
4			Benzene, 1-methyl-4-propyl-	134	C10H14	001074-55-1	43
5			Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU010522\
Data File : VU046674.D
Acq On : 05 Jan 2022 19:52
Operator : SY/MD
Sample : N1025-05
Misc : 6.43g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGLG9

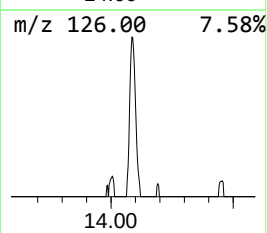
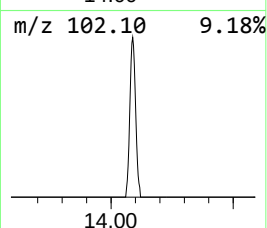
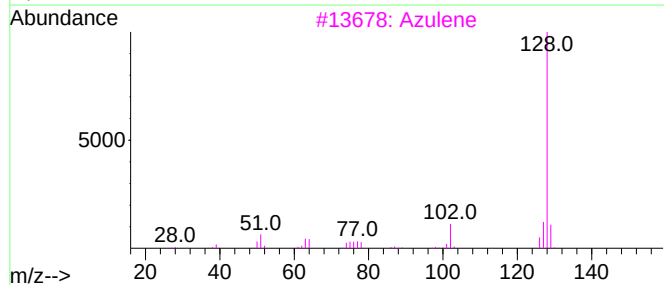
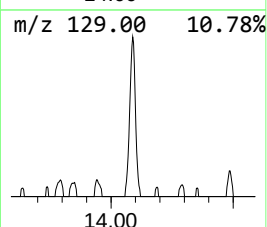
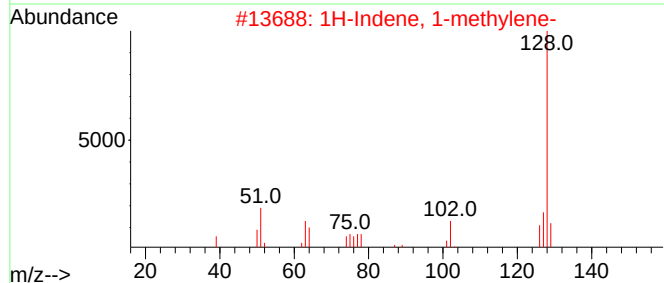
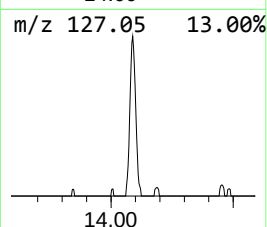
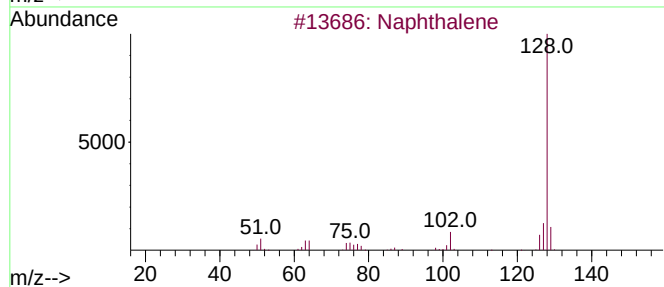
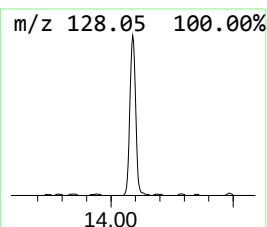
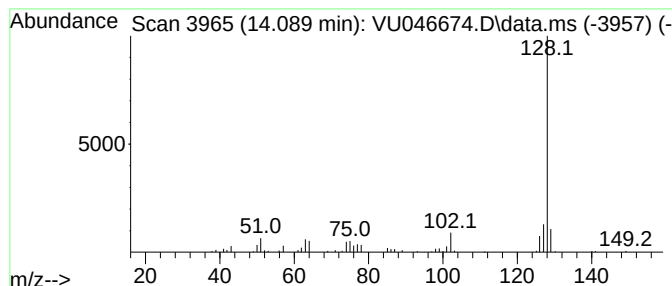
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Quant Title : VOC Analysis

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

Peak Number 5 Azulene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.089	5.86 ug/L	77620	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	95
3			Azulene	128	C10H8	000275-51-4	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\VU010522\
Data File : VU046674.D
Acq On : 05 Jan 2022 19:52
Operator : SY/MD
Sample : N1025-05
Misc : 6.43g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGLG9

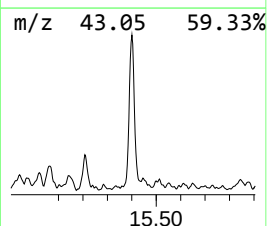
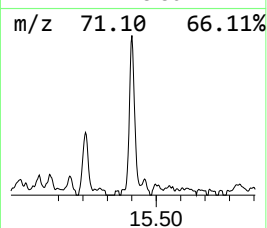
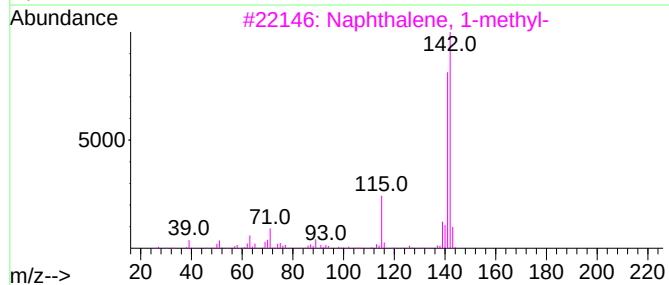
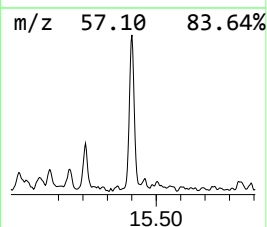
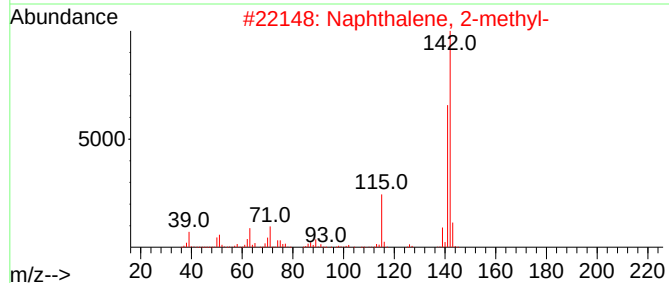
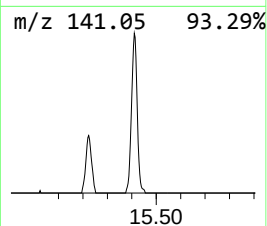
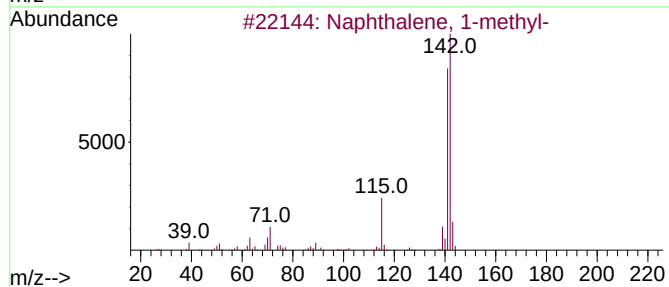
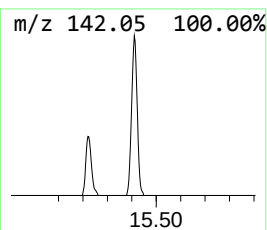
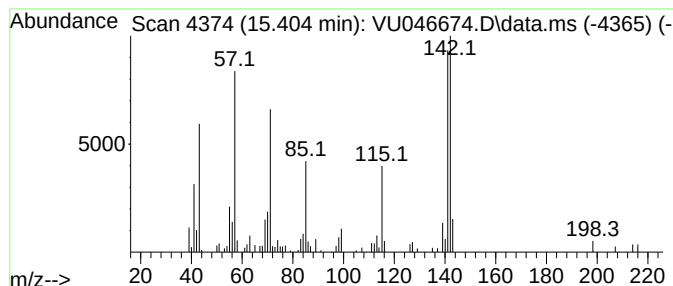
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM010522WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 Naphthalene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.404	5.97 ug/L	79161	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	81
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	81
3			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	72
4			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	70
5			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU010522\
Data File : VU046674.D
Acq On : 05 Jan 2022 19:52
Operator : SY/MD
Sample : N1025-05
Misc : 6.43g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGLG9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM010522WMA.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
Sulfurous acid,...	11.417	2.7	ug/L	35377	3	11.819	662539	50.0
Benzene, 1-meth...	12.127	4.2	ug/L	55443	3	11.819	662539	50.0
Benzene, (1-met...	12.385	2.7	ug/L	35822	3	11.819	662539	50.0
Azulene	14.089	5.9	ug/L	77620	3	11.819	662539	50.0
Naphthalene, 1-...	15.404	6.0	ug/L	79161	3	11.819	662539	50.0