

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020724\
 Data File : VU057837.D
 Acq On : 07 Feb 2024 13:58
 Operator : MD/SY
 Sample : P1081-01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AA1

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\SFAMULM020724WMA.M
 Title : VOC Analysis

Signal : TIC: VU057837.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.518	63	71	82	rVB	156030	170271	6.17%	0.503%
2	1.596	88	95	110	rVB	127706	153759	5.57%	0.454%
3	1.888	179	186	206	rVB	95762	134827	4.89%	0.398%
4	2.370	333	336	337	rBV2	671	344	0.01%	0.001%
5	2.560	382	395	405	rBV3	265296	498649	18.07%	1.473%
6	2.612	405	411	436	rVB	118958	213706	7.74%	0.631%
7	2.782	460	464	472	rVB2	1244	1685	0.06%	0.005%
8	2.956	511	518	523	rBV3	462	666	0.02%	0.002%
9	3.036	529	543	564	rVB	76366	142683	5.17%	0.421%
10	3.171	575	585	587	rBV3	2250	2984	0.11%	0.009%
11	3.351	619	641	674	rBV	554105	1271029	46.05%	3.754%
12	3.541	696	700	706	rBV4	519	454	0.02%	0.001%
13	4.653	1019	1046	1069	rBV2	380901	1032528	37.41%	3.050%
14	4.859	1107	1110	1115	rVB3	471	325	0.01%	0.001%
15	4.968	1142	1144	1150	rVB4	483	388	0.01%	0.001%
16	4.997	1150	1153	1155	rBV2	478	371	0.01%	0.001%
17	5.074	1155	1177	1207	rBV3	432390	1230403	44.58%	3.634%
18	5.319	1246	1253	1254	rBV4	469	449	0.02%	0.001%
19	5.393	1274	1276	1281	rVB2	338	234	0.01%	0.001%
20	5.515	1296	1314	1334	rBV	159981	350622	12.70%	1.036%
21	5.608	1340	1343	1347	rBV2	346	213	0.01%	0.001%
22	5.714	1356	1376	1386	rBV2	361045	973293	35.26%	2.875%
23	5.782	1389	1397	1418	rVB2	358632	786848	28.51%	2.324%
24	6.026	1469	1473	1478	rVB2	283	302	0.01%	0.001%
25	6.242	1526	1540	1562	rBV	307208	581971	21.09%	1.719%
26	6.480	1610	1614	1618	rBV2	288	242	0.01%	0.001%
27	6.534	1618	1631	1658	rBV	487143	916079	33.19%	2.706%
28	6.682	1664	1677	1695	rBV	223982	429269	15.55%	1.268%
29	6.782	1695	1708	1730	rVB	143734	276348	10.01%	0.816%
30	6.910	1736	1748	1771	rBV	127032	236825	8.58%	0.700%
31	7.097	1792	1806	1830	rBV	378917	694829	25.18%	2.052%
32	7.213	1830	1842	1860	rVB2	26799	51666	1.87%	0.153%
33	7.560	1938	1950	1955	rBV	134999	224493	8.13%	0.663%
34	7.599	1956	1962	1988	rVB	259414	448284	16.24%	1.324%
35	7.721	1991	2000	2008	rBV3	5159	9036	0.33%	0.027%
36	7.782	2008	2019	2040	rBV	293932	530967	19.24%	1.568%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

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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\SFAMULM020724WMA.M
 Title : VOC Analysis

37	7.891	2041	2053	2064	rBV	460551	782373	28.35%	2.311%
38	7.962	2064	2075	2093	rVB	856261	1455696	52.74%	4.300%
39	8.174	2129	2141	2146	rBV	92558	153132	5.55%	0.452%
40	8.393	2197	2209	2232	rBV	326103	559964	20.29%	1.654%
41	8.547	2245	2257	2272	rBV	237214	401743	14.56%	1.187%
42	8.627	2272	2282	2290	rVV	269990	459966	16.67%	1.359%
43	8.679	2291	2298	2324	rVV	268516	476981	17.28%	1.409%
44	8.801	2324	2336	2360	rVV	411056	708513	25.67%	2.093%
45	8.917	2360	2372	2388	rVB	86544	148013	5.36%	0.437%
46	9.016	2400	2403	2408	rVB3	374	294	0.01%	0.001%
47	9.100	2424	2429	2433	rVB2	260	231	0.01%	0.001%
48	9.197	2455	2459	2460	rBV2	457	269	0.01%	0.001%
49	9.206	2460	2462	2466	rVB	641	401	0.01%	0.001%
50	9.412	2514	2526	2529	rBV	471796	677550	24.55%	2.001%
51	9.528	2550	2562	2568	rBV	888092	1507455	54.62%	4.453%
52	9.563	2569	2573	2598	rVB	794650	1146022	41.52%	3.385%
53	9.685	2598	2611	2638	rVB	741416	1198203	43.41%	3.539%
54	9.917	2681	2683	2687	rVB	331	210	0.01%	0.001%
55	9.942	2687	2691	2695	rBV2	249	272	0.01%	0.001%
56	10.097	2723	2739	2773	rBV4	1408523	2759973	100.00%	8.153%
57	10.286	2787	2798	2819	rVB	77327	136192	4.93%	0.402%
58	10.479	2846	2858	2870	rBV2	3892	6572	0.24%	0.019%
59	10.544	2875	2878	2886	rBV2	292	387	0.01%	0.001%
60	10.753	2930	2943	2946	rBV	320754	490611	17.78%	1.449%
61	10.817	2955	2963	2983	rVB	957930	1574638	57.05%	4.651%
62	10.997	3011	3019	3022	rBV2	881	1123	0.04%	0.003%
63	11.013	3022	3024	3027	rVV4	505	302	0.01%	0.001%
64	11.084	3034	3046	3066	rVV	443334	684767	24.81%	2.023%
65	11.290	3095	3110	3117	rBV3	2821	4447	0.16%	0.013%
66	11.376	3128	3137	3145	rBV5	1430	2171	0.08%	0.006%
67	11.421	3145	3151	3152	rBV3	3729	3096	0.11%	0.009%
68	11.463	3152	3164	3179	rVB	721625	1096992	39.75%	3.240%
69	11.608	3200	3209	3215	rBV2	647	895	0.03%	0.003%
70	11.637	3216	3218	3225	rVB3	514	527	0.02%	0.002%
71	11.740	3237	3250	3261	rBV	709728	1111865	40.29%	3.284%
72	11.807	3261	3271	3296	rVB3	494471	1088909	39.45%	3.217%
73	11.933	3307	3310	3313	rBV2	377	222	0.01%	0.001%
74	12.203	3377	3394	3419	rBV2	728391	1727957	62.61%	5.104%
75	12.386	3449	3451	3455	rVB2	416	239	0.01%	0.001%
76	12.434	3461	3466	3470	rBV3	312	322	0.01%	0.001%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020724WMA.M
 Title : VOC Analysis

77	12.470	3475	3477	3484	rVB2	499	371	0.01%	0.001%
78	12.602	3515	3518	3523	rVB2	236	223	0.01%	0.001%
79	12.762	3562	3568	3576	rVB3	882	1493	0.05%	0.004%
80	12.862	3596	3599	3606	rVB2	290	296	0.01%	0.001%
81	12.991	3627	3639	3656	rBV	300410	486203	17.62%	1.436%
82	13.225	3706	3712	3723	rVB2	1115	1390	0.05%	0.004%
83	13.386	3760	3762	3766	rVV2	373	245	0.01%	0.001%
84	13.460	3783	3785	3791	rVB	334	224	0.01%	0.001%
85	13.637	3835	3840	3844	rBV2	399	346	0.01%	0.001%
86	13.782	3880	3885	3889	rBV2	250	291	0.01%	0.001%
87	13.839	3896	3903	3911	rBV5	2903	4107	0.15%	0.012%
88	13.942	3932	3935	3942	rVV3	345	333	0.01%	0.001%
89	14.081	3965	3978	4008	rVV	990093	1614798	58.51%	4.770%
90	14.331	4049	4056	4065	rVB8	2723	4004	0.15%	0.012%
91	14.386	4070	4073	4077	rVB3	425	326	0.01%	0.001%
92	14.444	4085	4091	4096	rBV2	393	340	0.01%	0.001%
93	14.502	4105	4109	4112	rVB3	303	271	0.01%	0.001%
94	14.518	4112	4114	4117	rBV3	317	225	0.01%	0.001%
95	14.785	4193	4197	4200	rBV2	330	288	0.01%	0.001%
96	15.100	4291	4295	4298	rBV4	431	359	0.01%	0.001%
97	15.605	4450	4452	4455	rBV2	323	242	0.01%	0.001%
98	15.634	4459	4461	4465	rVB3	509	283	0.01%	0.001%
99	15.736	4491	4493	4497	rBV2	432	241	0.01%	0.001%
100	15.862	4530	4532	4535	rBV2	556	311	0.01%	0.001%

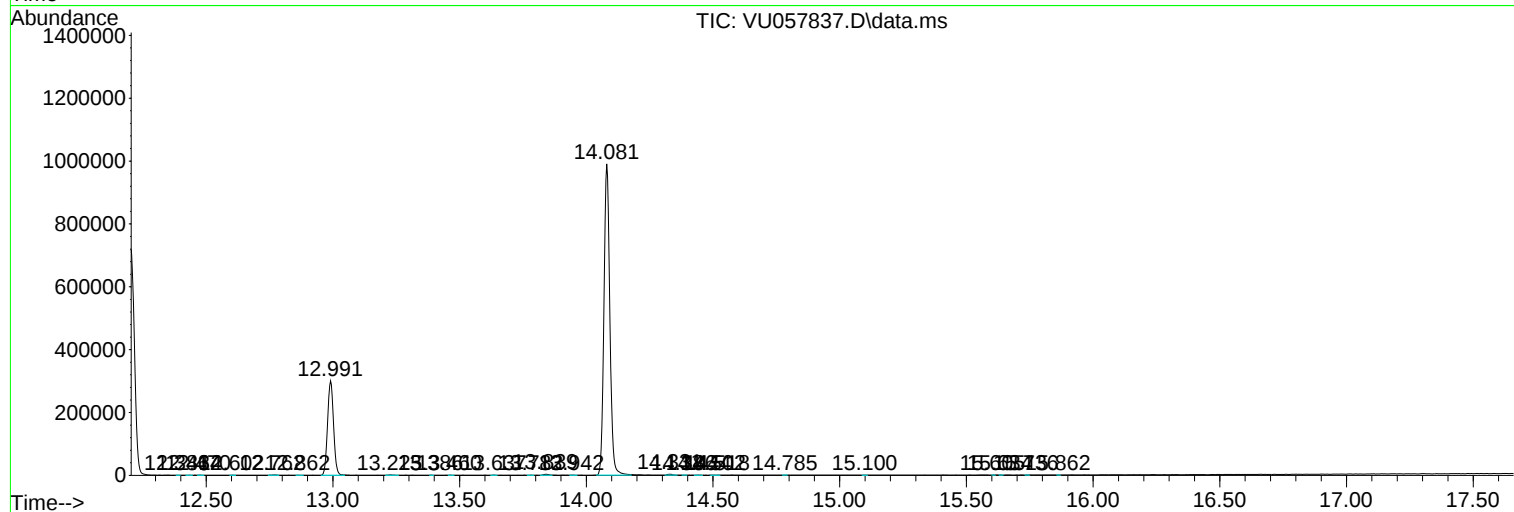
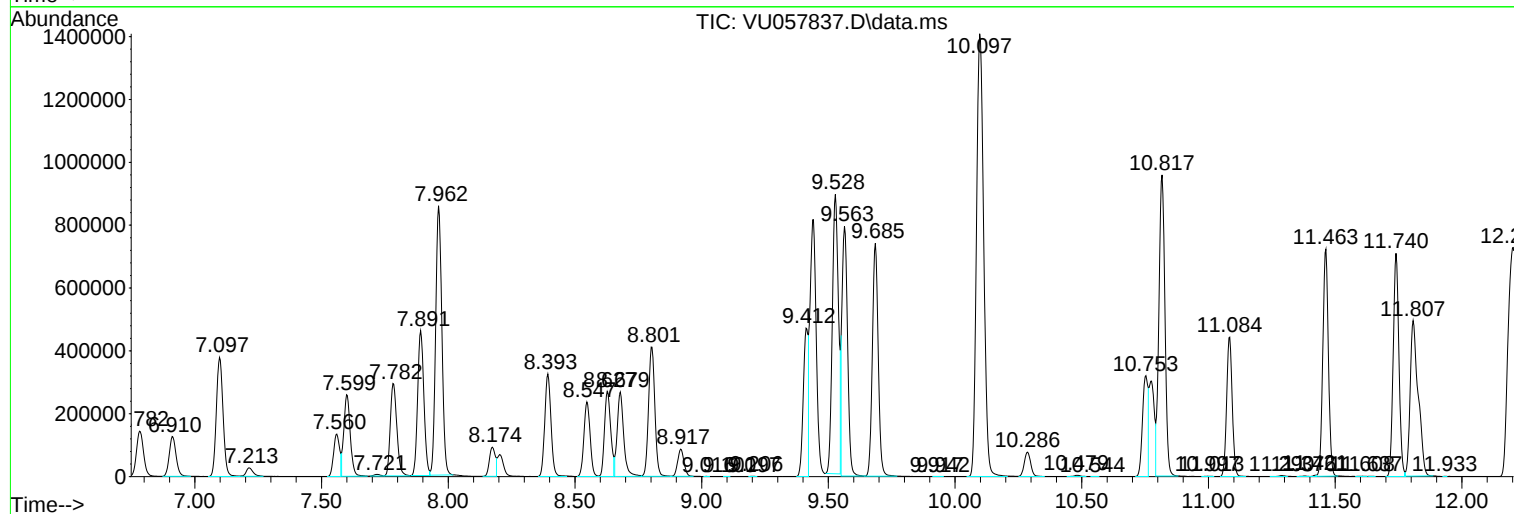
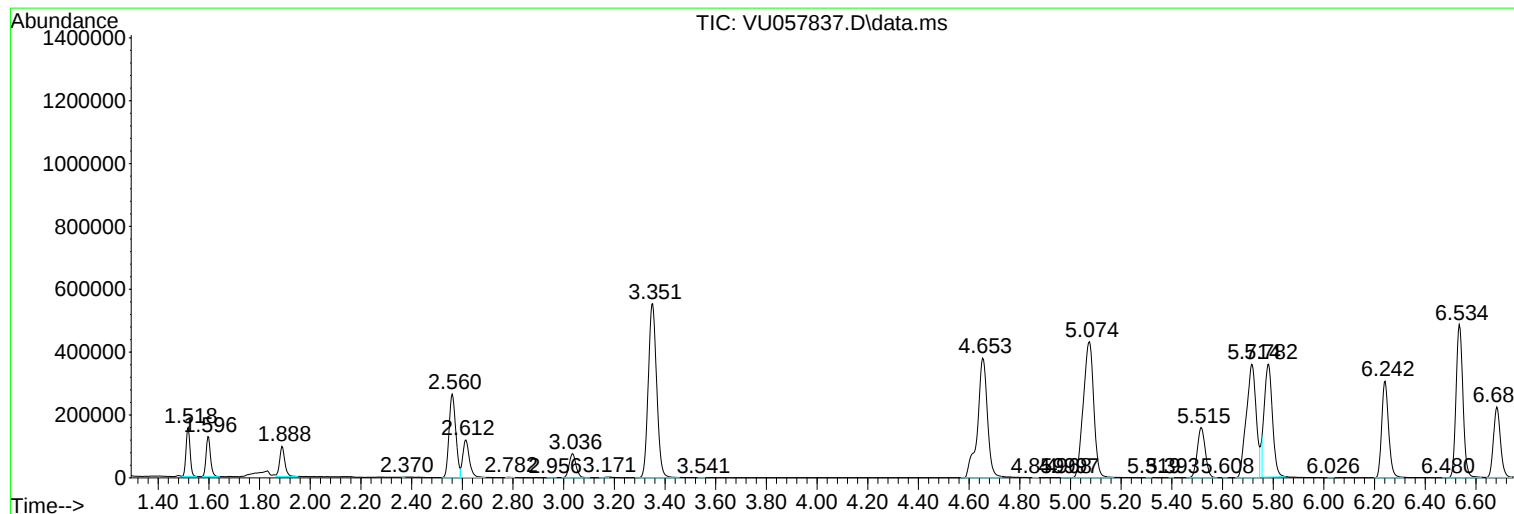
Sum of corrected areas: 33853747

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Instrument :
MSVOA_U
ClientSampleId :
C0AA1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020724WMA.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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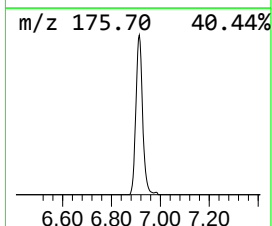
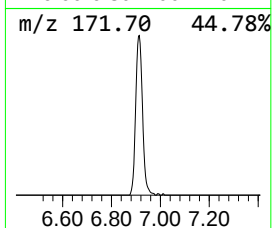
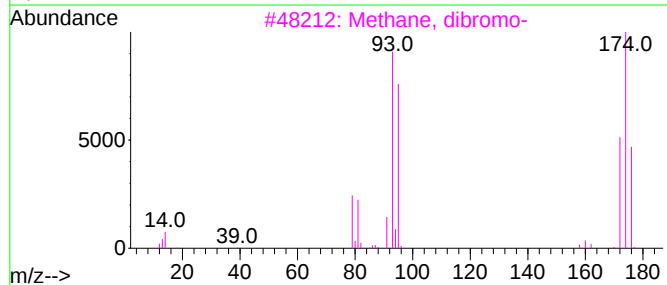
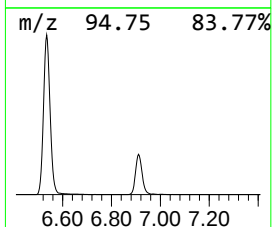
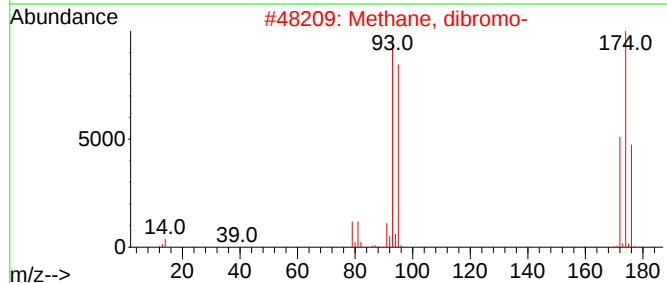
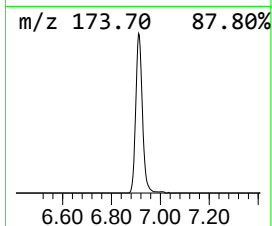
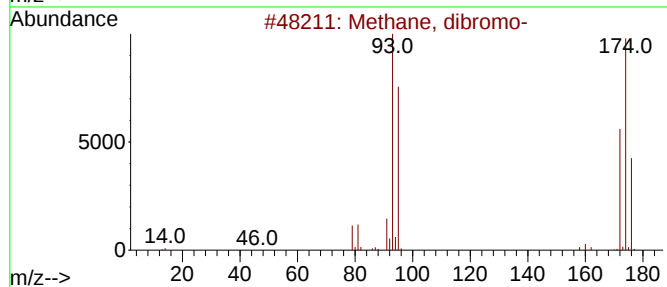
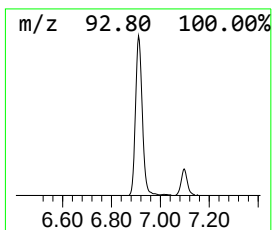
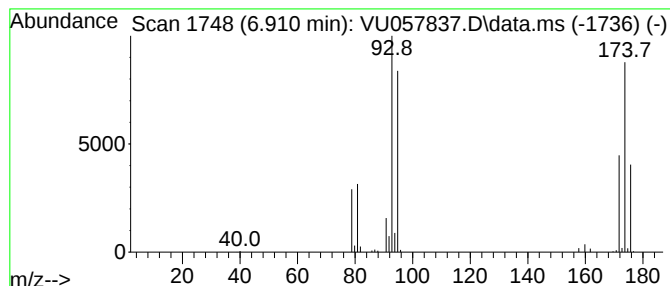
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020724WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Methane, dibromo- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.910	20.35 ug/L	236825	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methane, dibromo-	172	CH2Br2	000074-95-3	96
2			Methane, dibromo-	172	CH2Br2	000074-95-3	94
3			Methane, dibromo-	172	CH2Br2	000074-95-3	94
4			Methane, dibromo-	172	CH2Br2	000074-95-3	94
5			3-Chloro-6-methoxy-4-methylpyrid...	174	C6H7ClN2O2	050450-89-0	9



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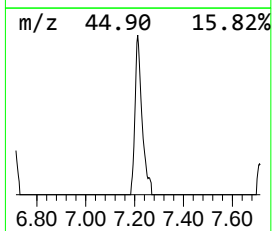
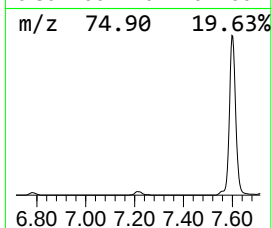
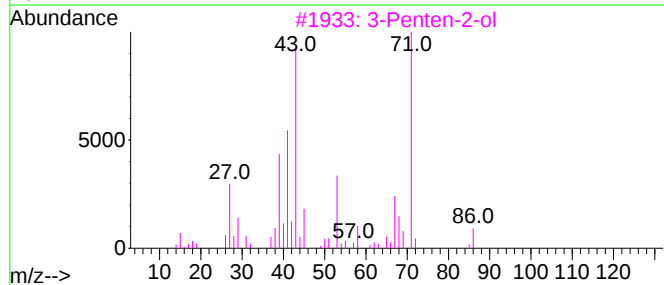
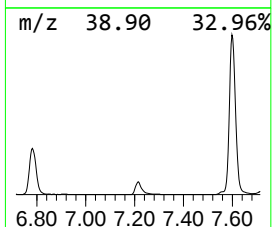
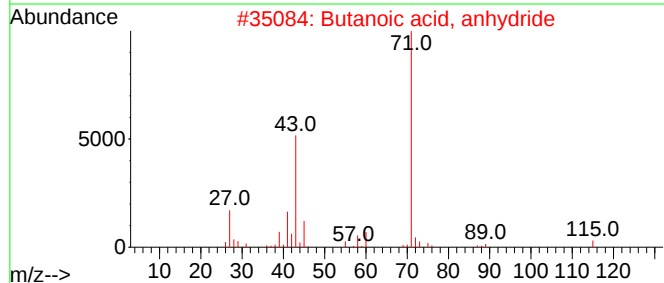
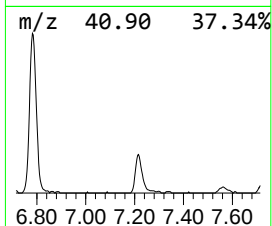
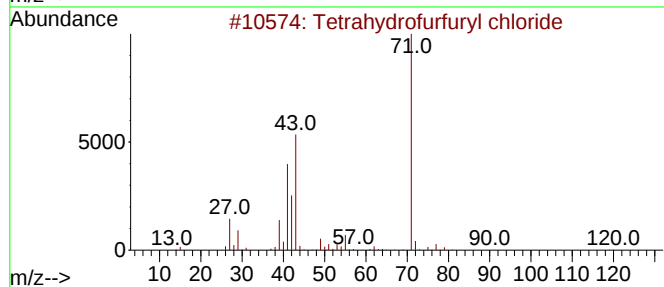
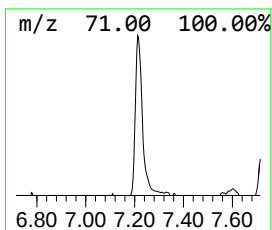
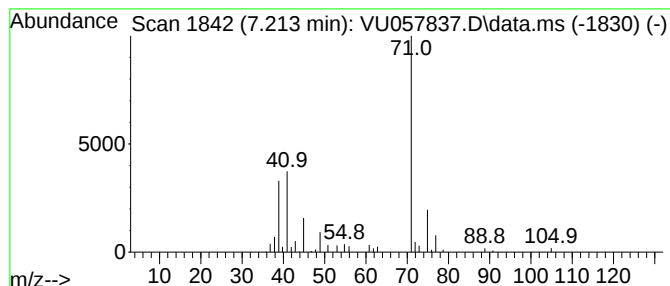
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020724WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.213	4.44 ug/L	51666	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetrahydrofurfuryl chloride	120	C5H9ClO	003003-84-7	42
2			Butanoic acid, anhydride	158	C8H14O3	000106-31-0	36
3			3-Penten-2-ol	86	C5H10O	001569-50-2	36
4			3-Methoxy-1-pentene	100	C6H12O	014092-18-3	10
5			2-Hydroperoxytetrahydrofuran, TM...	176	C7H16O3Si	1000368-50-8	9



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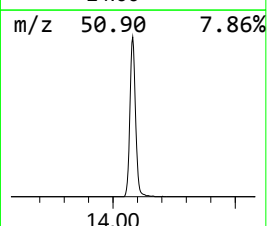
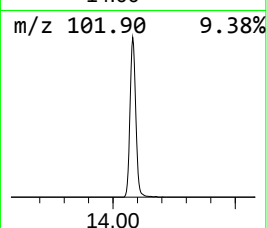
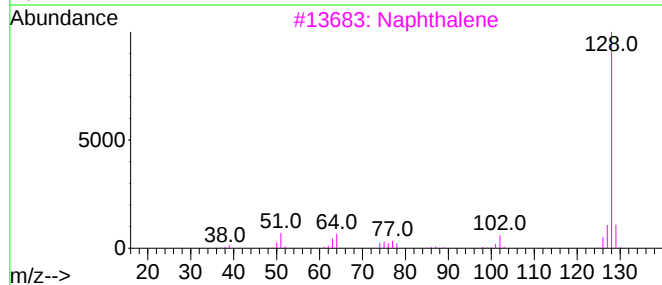
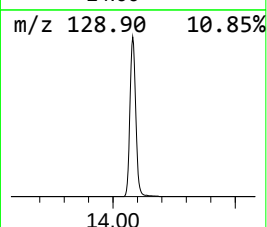
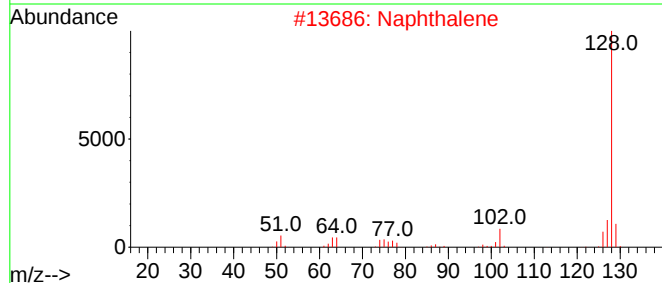
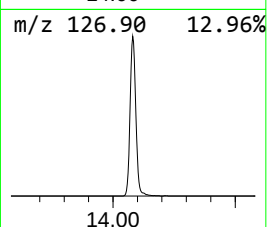
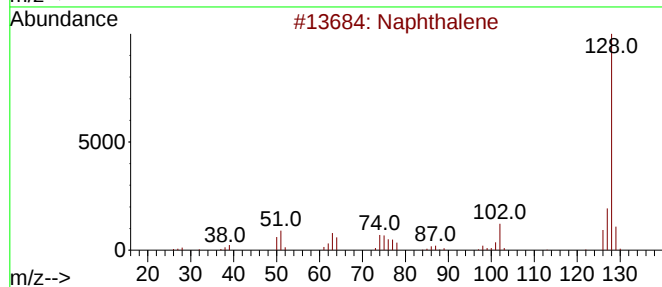
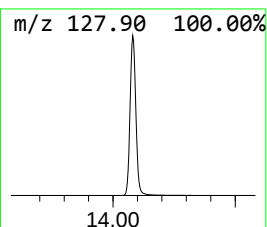
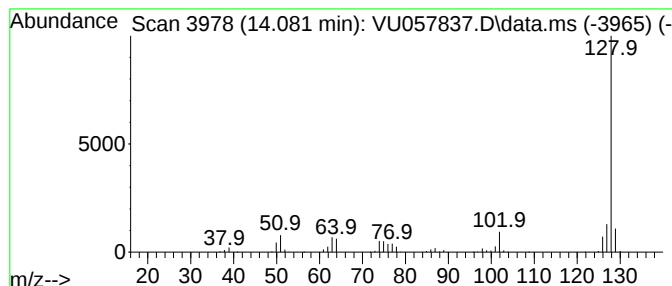
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020724WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.081	74.15 ug/L	1614800	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	97
2			Naphthalene	128	C10H8	000091-20-3	95
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\VU020724\
Data File : VU057837.D
Acq On : 07 Feb 2024 13:58
Operator : MD/SY
Sample : P1081-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AA1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020724WMA.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
Methane, dibromo-	6.910	20.4	ug/L	236825	1	6.242	581971	50.0
unknown-01	7.213	4.4	ug/L	51666	1	6.242	581971	50.0
Azulene	14.081	74.2	ug/L	1614800	3	11.807	1088910	50.0