

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022024\
 Data File : VU057891.D
 Acq On : 20 Feb 2024 10:36
 Operator : MD/SY
 Sample : P1504-01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DCNF5

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\SFAMULM021924WMA.M
 Title : VOC Analysis

Signal : TIC: VU057891.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.515	63	70	84	rVB	113001	123517	3.43%	0.370%
2	1.596	87	95	114	rVB	132093	156733	4.35%	0.469%
3	1.895	180	188	206	rVB	97214	133456	3.70%	0.399%
4	2.287	308	310	313	rBV2	470	329	0.01%	0.001%
5	2.364	332	334	341	rVB4	653	496	0.01%	0.001%
6	2.563	381	396	407	rBV3	345506	687962	19.10%	2.059%
7	2.711	440	442	445	rVB2	415	187	0.01%	0.001%
8	2.776	458	462	463	rBV	767	462	0.01%	0.001%
9	3.033	527	542	568	rBV	303730	573709	15.92%	1.717%
10	3.348	621	640	669	rVV	692155	1602199	44.47%	4.796%
11	3.660	732	737	738	rBV3	276	266	0.01%	0.001%
12	3.946	822	826	831	rBV2	203	249	0.01%	0.001%
13	4.132	880	884	890	rBV2	189	287	0.01%	0.001%
14	4.222	909	912	918	rVB2	227	210	0.01%	0.001%
15	4.287	928	932	936	rVB2	292	301	0.01%	0.001%
16	4.325	936	944	945	rBV	204	257	0.01%	0.001%
17	4.357	951	954	963	rVB2	218	315	0.01%	0.001%
18	4.422	970	974	980	rBV2	221	291	0.01%	0.001%
19	4.612	1023	1033	1036	rBV	59122	96772	2.69%	0.290%
20	4.952	1135	1139	1144	rBV3	256	336	0.01%	0.001%
21	5.055	1154	1171	1199	rBV3	197153	588992	16.35%	1.763%
22	5.184	1208	1211	1215	rVB2	604	465	0.01%	0.001%
23	5.251	1230	1232	1236	rVB2	318	213	0.01%	0.001%
24	5.325	1242	1255	1265	rBV4	1436	3552	0.10%	0.011%
25	5.396	1272	1277	1284	rBV2	166	276	0.01%	0.001%
26	5.441	1287	1291	1294	rBV	262	234	0.01%	0.001%
27	5.505	1307	1311	1314	rVB2	244	226	0.01%	0.001%
28	5.541	1318	1322	1323	rBV2	249	194	0.01%	0.001%
29	5.579	1327	1334	1341	rBV2	258	354	0.01%	0.001%
30	5.615	1341	1345	1349	rVB	171	199	0.01%	0.001%
31	5.637	1349	1352	1356	rVB2	224	187	0.01%	0.001%
32	5.714	1356	1376	1388	rBV2	358231	965589	26.80%	2.890%
33	5.782	1388	1397	1421	rVB	235903	482827	13.40%	1.445%
34	6.042	1475	1478	1480	rVV4	321	273	0.01%	0.001%
35	6.068	1484	1486	1492	rVB3	430	371	0.01%	0.001%
36	6.238	1527	1539	1571	rBV	367327	710787	19.73%	2.128%

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Integrator: RTE

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021924WMA.M
 Title : VOC Analysis

37	6.383	1582	1584	1591	rVB2	565	520	0.01%	0.002%
38	6.534	1618	1631	1656	rBV	466353	876162	24.32%	2.623%
39	6.682	1663	1677	1694	rBV	221611	429475	11.92%	1.286%
40	6.782	1695	1708	1732	rVB	531067	1002993	27.84%	3.002%
41	6.910	1737	1748	1767	rVB2	70243	134423	3.73%	0.402%
42	7.097	1801	1806	1813	rVB3	431	639	0.02%	0.002%
43	7.164	1822	1827	1828	rBV2	344	263	0.01%	0.001%
44	7.213	1828	1842	1864	rBV2	28937	56258	1.56%	0.168%
45	7.438	1906	1912	1914	rBV2	606	554	0.02%	0.002%
46	7.560	1937	1950	1954	rBV2	130893	209999	5.83%	0.629%
47	7.599	1955	1962	1981	rVB	442892	761802	21.14%	2.280%
48	7.714	1992	1998	2007	rBV3	7260	10320	0.29%	0.031%
49	7.782	2007	2019	2041	rVV	550643	974781	27.06%	2.918%
50	7.891	2041	2053	2064	rVV	462887	795835	22.09%	2.382%
51	7.962	2064	2075	2108	rVB	1404206	2399174	66.59%	7.182%
52	8.174	2130	2141	2144	rBV	95135	139220	3.86%	0.417%
53	8.393	2196	2209	2230	rBV	446450	765972	21.26%	2.293%
54	8.547	2245	2257	2271	rBV	223729	379088	10.52%	1.135%
55	8.627	2272	2282	2290	rVV	205710	371445	10.31%	1.112%
56	8.676	2290	2297	2323	rVV	369699	679897	18.87%	2.035%
57	8.801	2325	2336	2359	rVV	381735	660149	18.32%	1.976%
58	8.917	2359	2372	2395	rVB	206540	352036	9.77%	1.054%
59	9.058	2415	2416	2419	rVB2	414	189	0.01%	0.001%
60	9.078	2419	2422	2425	rVB2	318	197	0.01%	0.001%
61	9.100	2425	2429	2432	rBV2	253	245	0.01%	0.001%
62	9.206	2453	2462	2465	rBV2	848	1332	0.04%	0.004%
63	9.412	2512	2526	2548	rBV	517983	871244	24.18%	2.608%
64	9.524	2549	2561	2588	rVB	977376	1643859	45.63%	4.921%
65	9.688	2597	2612	2639	rBV	746542	1235571	34.29%	3.699%
66	9.852	2659	2663	2666	rVB2	219	211	0.01%	0.001%
67	9.939	2684	2690	2694	rBV3	241	269	0.01%	0.001%
68	10.100	2725	2740	2773	rBV4	1777976	3602775	100.00%	10.785%
69	10.283	2785	2797	2818	rVB	134611	232036	6.44%	0.695%
70	10.483	2849	2859	2872	rBV4	4257	7005	0.19%	0.021%
71	10.750	2930	2942	2953	rVV	263032	432075	11.99%	1.293%
72	10.817	2953	2963	2985	rVB	377651	618886	17.18%	1.853%
73	10.910	2990	2992	2998	rVB4	375	290	0.01%	0.001%
74	10.994	3013	3018	3026	rVB5	1148	1499	0.04%	0.004%
75	11.081	3032	3045	3066	rBV	649947	992496	27.55%	2.971%
76	11.293	3100	3111	3121	rBV3	2513	4067	0.11%	0.012%

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Integration Parameters: LSCINT.P

Integrator: RTE

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 Title : VOC Analysis

77	11.377	3130	3137	3143	rVB4	748	1109	0.03%	0.003%
78	11.460	3150	3163	3190	rVB	595780	919738	25.53%	2.753%
79	11.743	3242	3251	3258	rBV6	1393	1734	0.05%	0.005%
80	11.807	3258	3271	3296	rBV3	572413	1229850	34.14%	3.681%
81	12.203	3376	3394	3416	rBV2	1268214	2615522	72.60%	7.829%
82	12.344	3437	3438	3444	rVB2	407	320	0.01%	0.001%
83	12.412	3455	3459	3461	rBV2	325	238	0.01%	0.001%
84	12.428	3461	3464	3468	rVV2	360	367	0.01%	0.001%
85	12.470	3470	3477	3486	rVB5	3419	4589	0.13%	0.014%
86	12.766	3567	3569	3577	rVB3	391	330	0.01%	0.001%
87	12.856	3591	3597	3600	rBV2	193	221	0.01%	0.001%
88	12.991	3628	3639	3657	rVV	116121	188459	5.23%	0.564%
89	13.219	3705	3710	3712	rBV4	1123	879	0.02%	0.003%
90	13.630	3835	3838	3844	rVB2	202	262	0.01%	0.001%
91	13.833	3889	3901	3926	rBV	391658	640342	17.77%	1.917%
92	14.013	3946	3957	3968	rBV2	424108	654565	18.17%	1.959%
93	14.081	3968	3978	4008	rVB	210748	360563	10.01%	1.079%
94	14.257	4031	4033	4036	rBV3	280	189	0.01%	0.001%
95	14.328	4046	4055	4064	rBV5	4563	7471	0.21%	0.022%
96	14.389	4071	4074	4077	rVB2	431	228	0.01%	0.001%
97	14.601	4137	4140	4142	rBV	333	253	0.01%	0.001%
98	14.794	4196	4200	4202	rBV2	312	283	0.01%	0.001%
99	15.547	4431	4434	4436	rBV2	345	251	0.01%	0.001%
100	16.248	4649	4652	4654	rBV	786	489	0.01%	0.001%

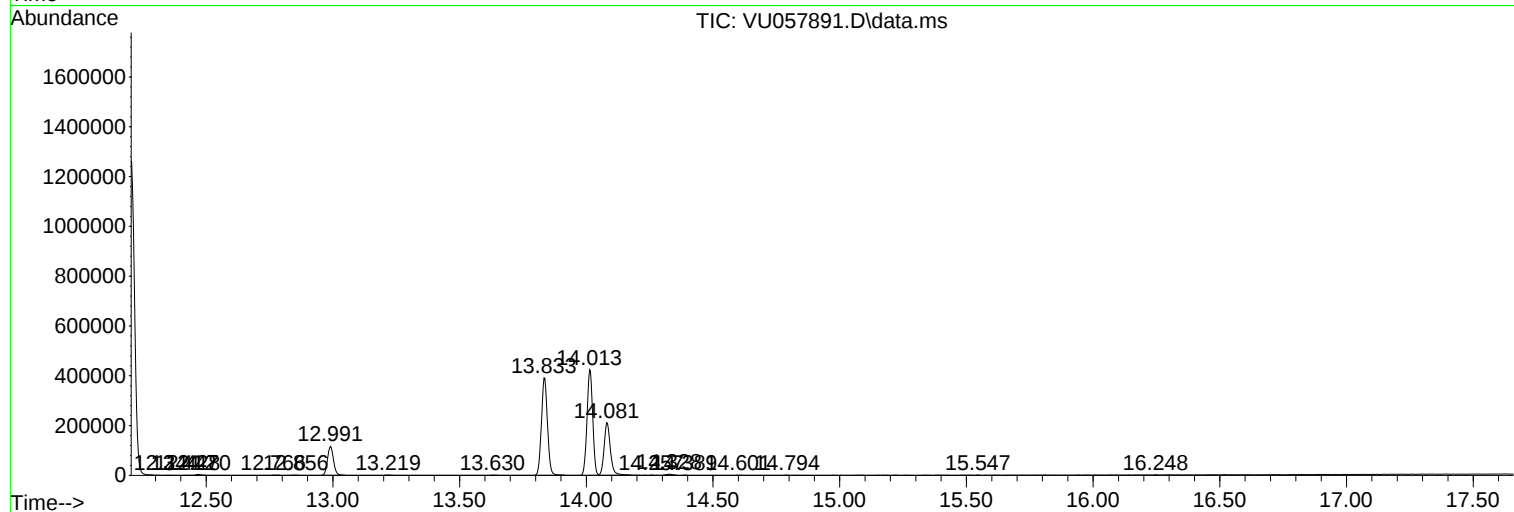
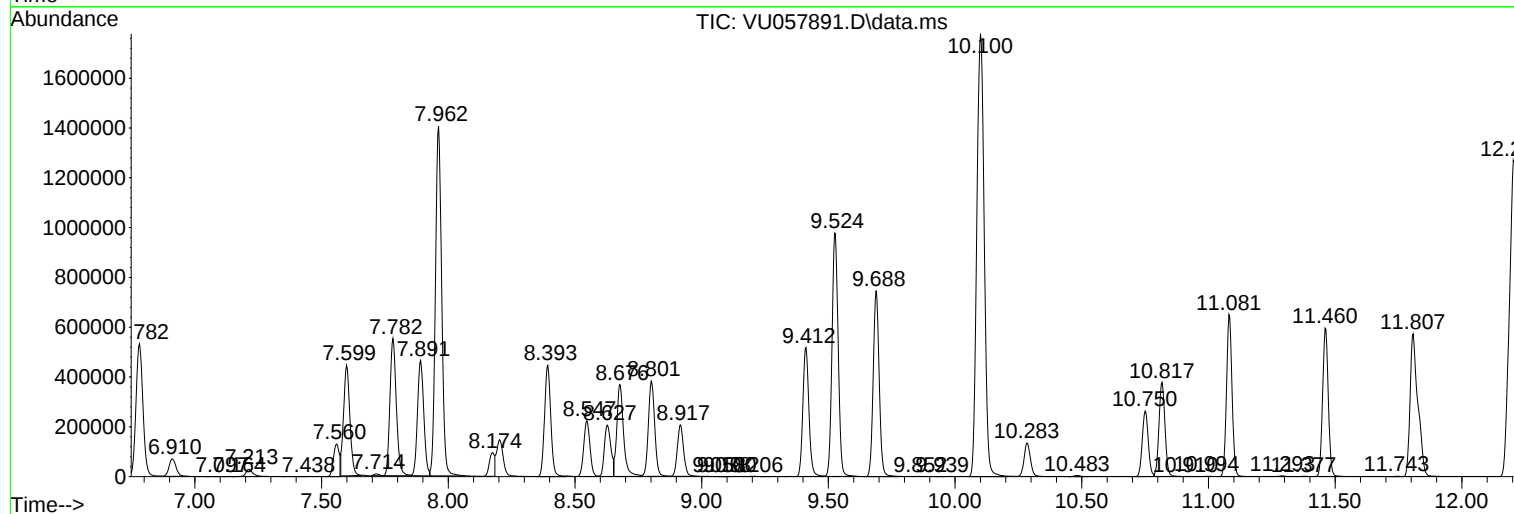
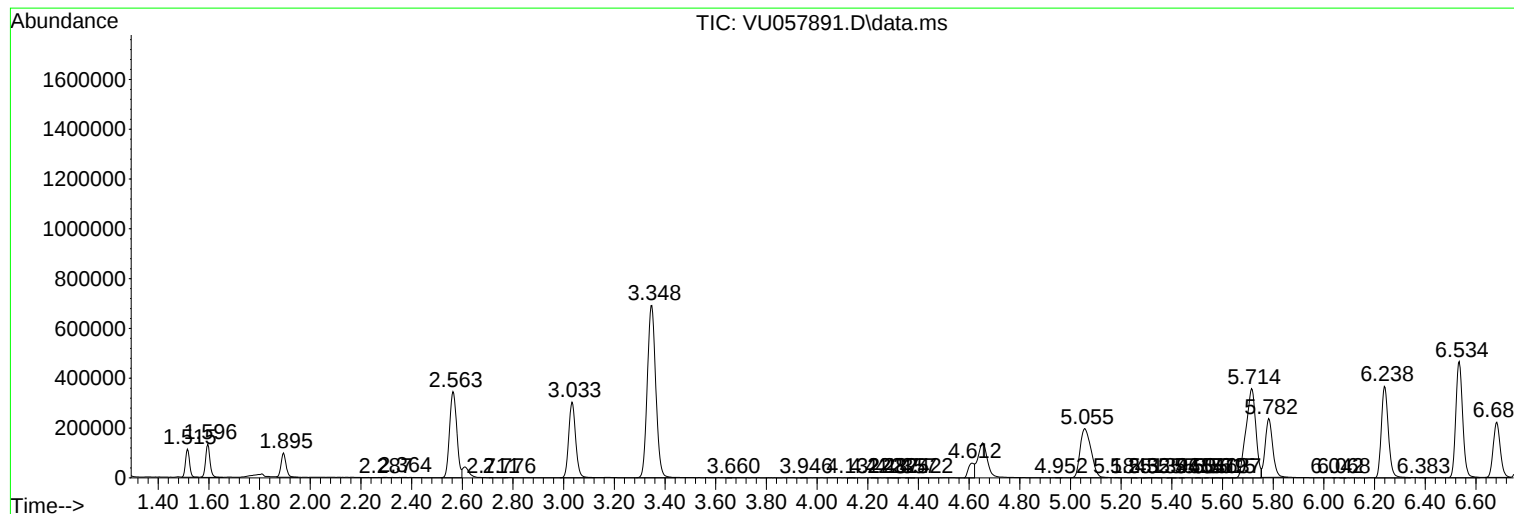
Sum of corrected areas: 33406576

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021924WMA.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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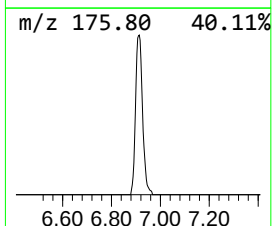
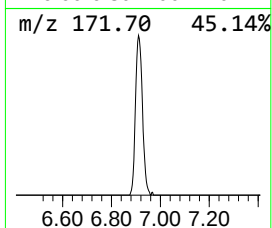
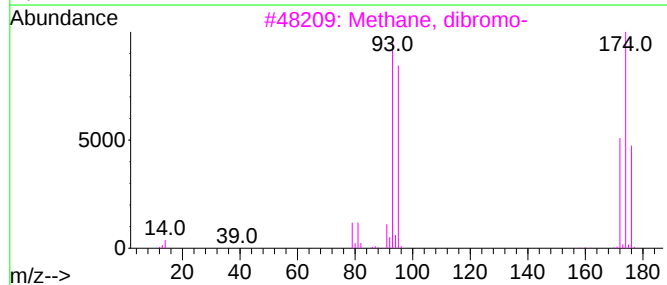
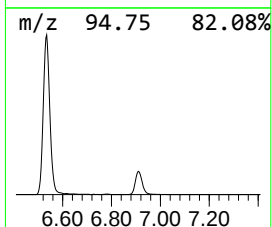
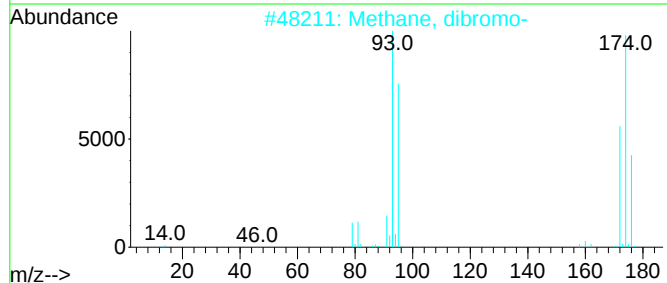
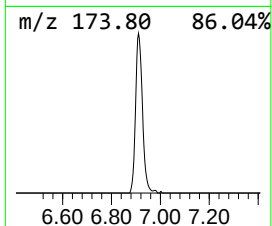
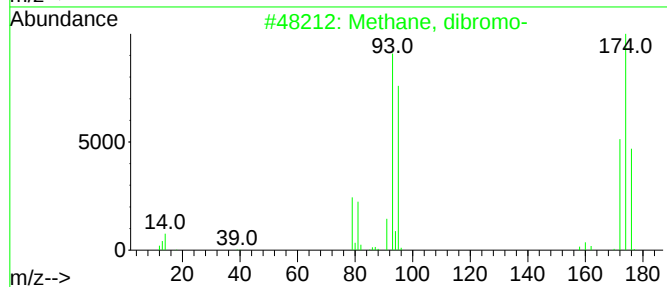
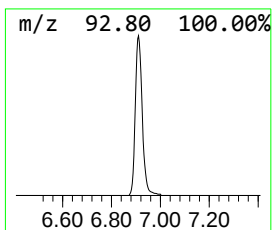
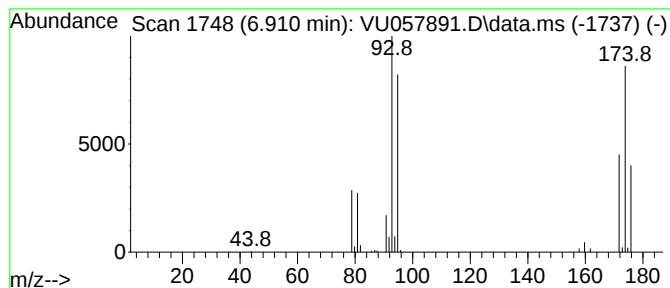
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021924WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Methane, dibromo- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.910	9.46 ug/L	134423	1,4-Difluorobenzene	6.238

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	96
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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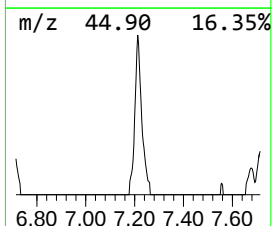
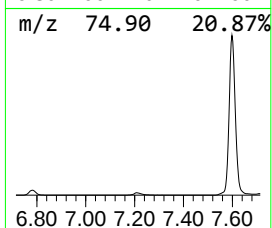
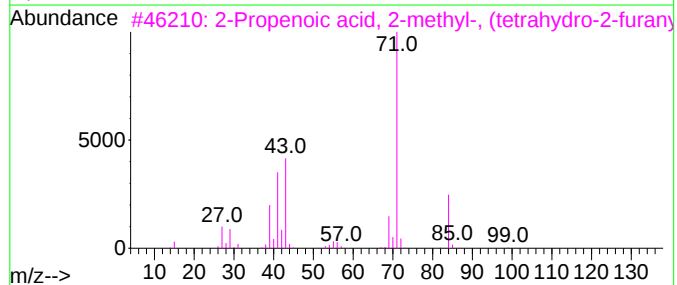
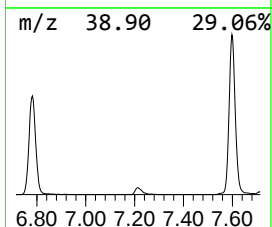
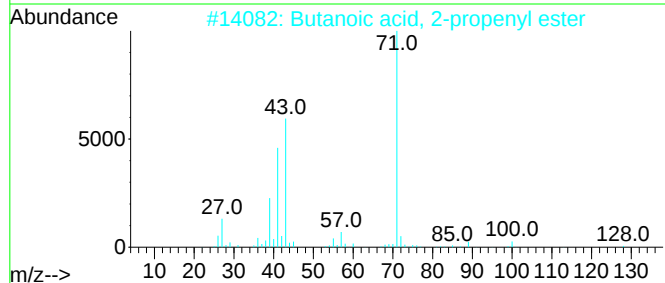
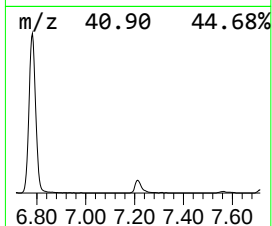
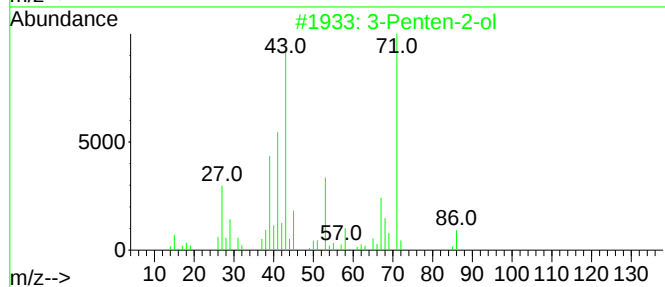
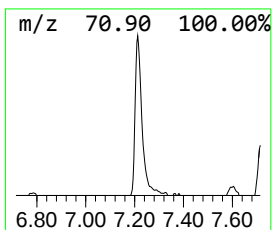
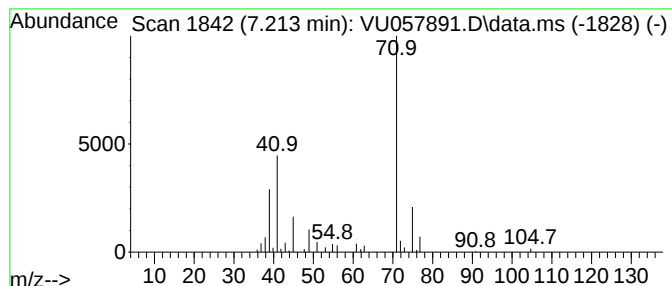
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021924WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.213	3.96 ug/L	56258	1,4-Difluorobenzene	6.238

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-ol	86	C5H10O	001569-50-2	33
2		Butanoic acid, 2-propenyl ester	128	C7H12O2	002051-78-7	9
3		2-Propenoic acid, 2-methyl-, (te...	170	C9H14O3	002455-24-5	9
4		3-Methoxy-1-pentene	100	C6H12O	014092-18-3	9
5		2-Hexene, 1-methoxy-, (E)-	114	C7H14O	056052-83-6	9



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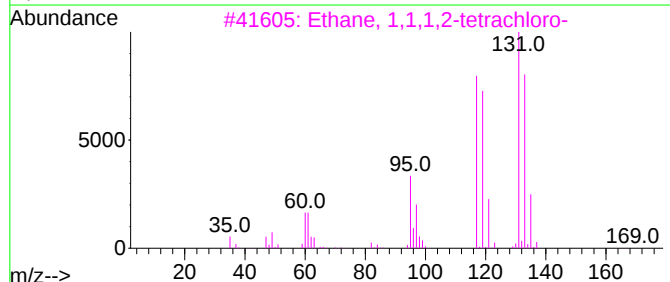
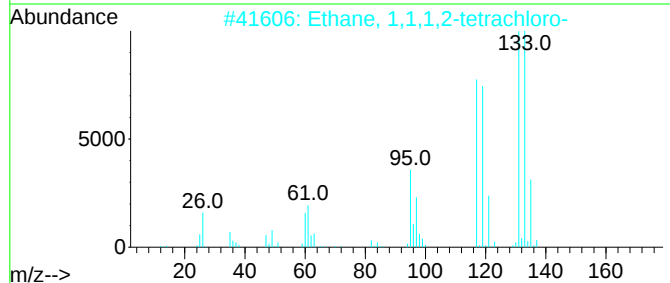
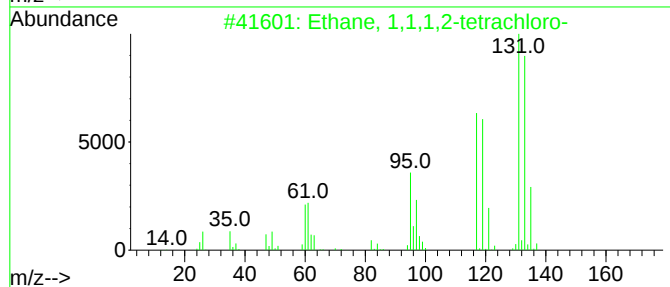
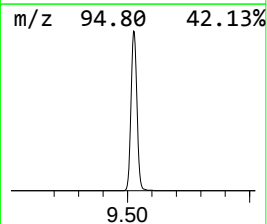
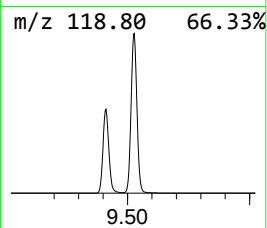
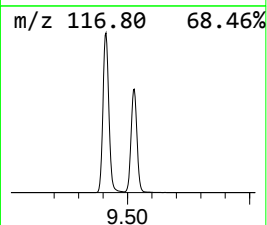
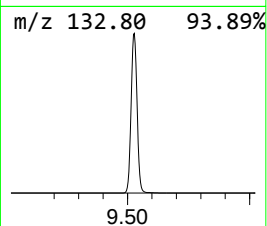
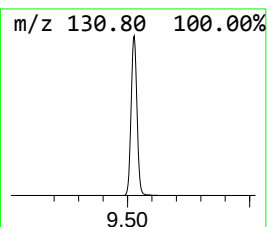
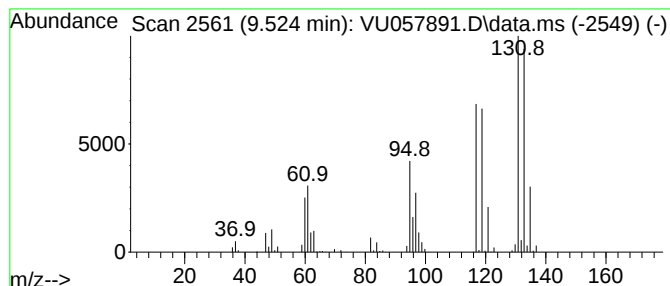
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021924WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Ethane, 1,1,1,2-tetrachloro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.524	94.34 ug/L	1643860	Chlorobenzene-d5	9.412

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	90
2			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	83
3			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	72
4			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	59
5			Carbon Tetrachloride	152	CCl4	000056-23-5	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022024\
Data File : VU057891.D
Acq On : 20 Feb 2024 10:36
Operator : MD/SY
Sample : P1504-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DCNF5

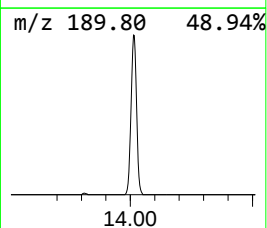
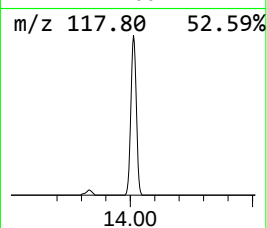
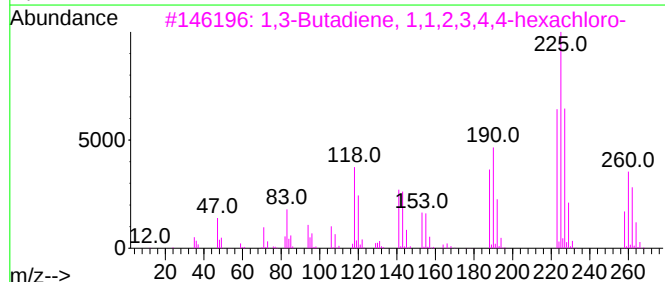
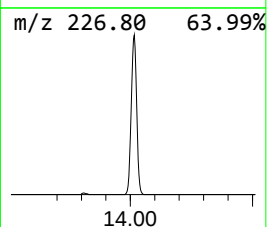
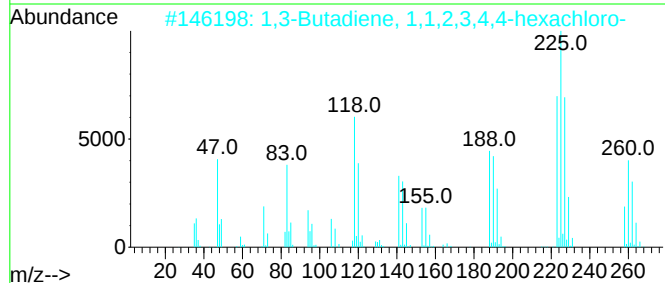
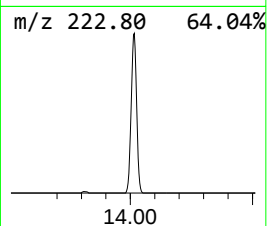
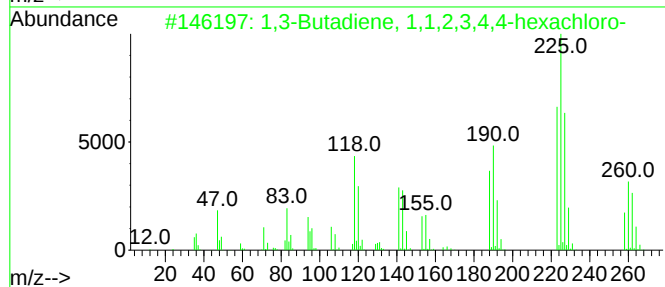
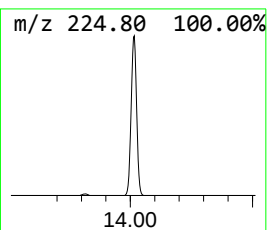
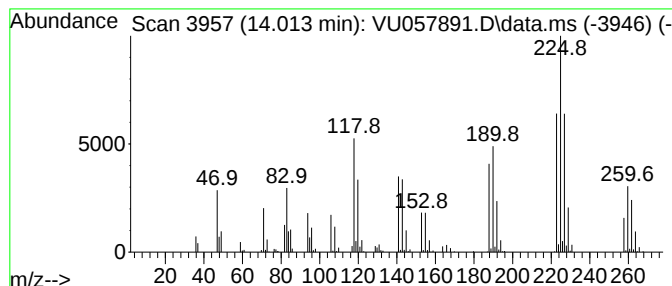
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021924WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 1,3-Butadiene, 1,1,2,3,4,4-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.013	26.61 ug/L	654565	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	99
2			1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	99
3			1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	99
4			1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	99
5			Tin(IV) chloride	260	Cl4Sn	007646-78-8	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022024\
Data File : VU057891.D
Acq On : 20 Feb 2024 10:36
Operator : MD/SY
Sample : P1504-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DCNF5

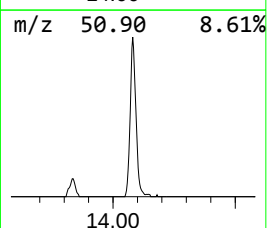
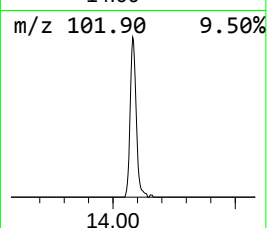
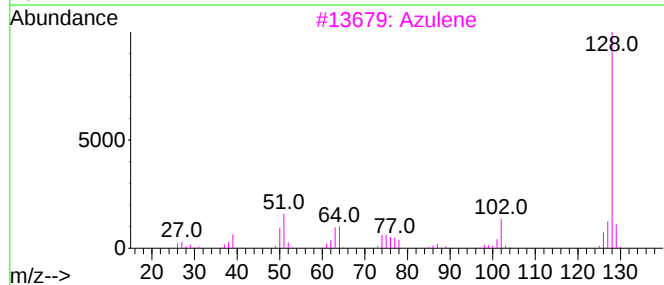
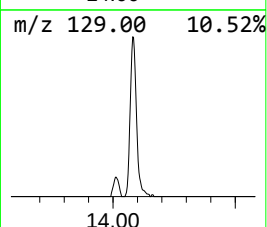
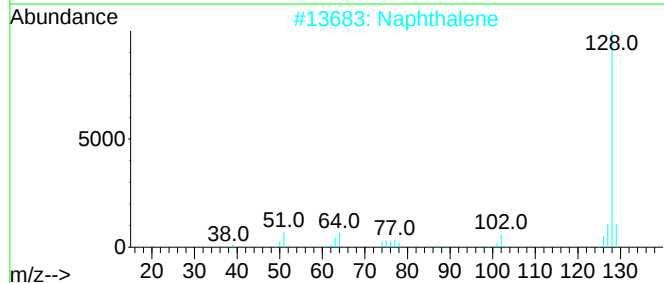
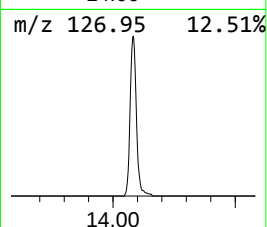
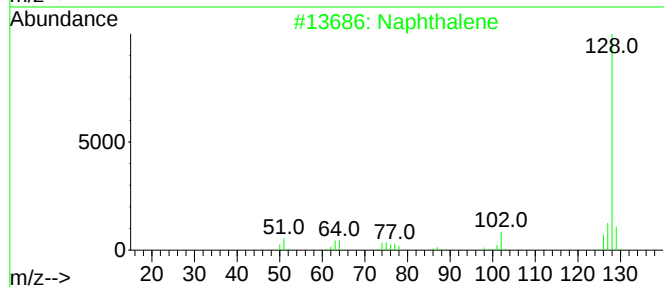
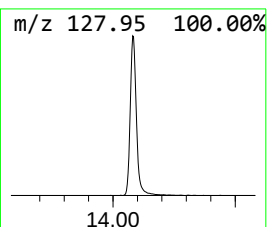
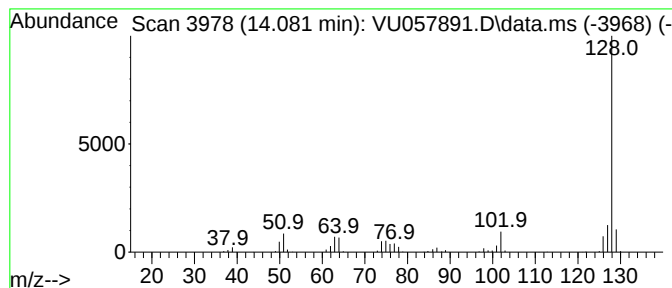
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021924WMA.M
Quant Title : VOC Analysis

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.
14.081	14.66 ug/L	360563	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Naphthalene	128	C10H8	000091-20-3	94
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\VU022024\
Data File : VU057891.D
Acq On : 20 Feb 2024 10:36
Operator : MD/SY
Sample : P1504-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DCNF5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021924WMA.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	9.5	ug/L	134423	1	6.238	710787	50.0
unknown-01	7.213	4.0	ug/L	56258	1	6.238	710787	50.0
Ethane, 1,1,1,2...	9.524	94.3	ug/L	1643860	2	9.412	871244	50.0
1,3-Butadiene, ...	14.013	26.6	ug/L	654565	3	11.807	1229850	50.0
Azulene	14.081	14.7	ug/L	360563	3	11.807	1229850	50.0