

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
 Data File : VU048012.D
 Acq On : 13 Apr 2022 18:30
 Operator : SY/MD
 Sample : N2316-11ME
 Misc : 6.23g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNR1ME

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\SFAMULM032422WMA.M
 Title : VOC Analysis

Signal : TIC: VU048012.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	73	80	112	rVB	74589	167563	10.49%	1.387%
2	1.771	119	134	135	rBV5	22018	36757	2.30%	0.304%
3	1.871	161	165	170	rBV2	32711	38193	2.39%	0.316%
4	2.533	360	371	386	rBV	209329	369618	23.15%	3.059%
5	2.752	436	439	441	rBV3	666	455	0.03%	0.004%
6	3.031	521	526	538	rVB6	1501	3050	0.19%	0.025%
7	3.170	564	569	571	rBV3	648	679	0.04%	0.006%
8	3.684	726	729	735	rVB4	476	422	0.03%	0.003%
9	4.636	1011	1025	1073	rVV2	97574	320051	20.05%	2.649%
10	5.060	1139	1157	1185	rBV	204091	474274	29.71%	3.926%
11	5.292	1224	1229	1233	rBV3	662	714	0.04%	0.006%
12	5.340	1233	1244	1253	rVV4	2908	6301	0.39%	0.052%
13	5.527	1295	1302	1308	rBV2	304	472	0.03%	0.004%
14	5.719	1338	1362	1393	rBV2	475977	1284298	80.44%	10.631%
15	5.880	1407	1412	1420	rBV3	545	826	0.05%	0.007%
16	5.986	1441	1445	1450	rVV6	464	470	0.03%	0.004%
17	6.247	1510	1526	1553	rBV	423274	838738	52.53%	6.943%
18	6.414	1575	1578	1582	rVB2	540	385	0.02%	0.003%
19	6.530	1604	1614	1624	rBV8	2615	4298	0.27%	0.036%
20	6.690	1648	1664	1691	rBV	268157	551719	34.56%	4.567%
21	7.047	1765	1775	1777	rBV3	1285	1580	0.10%	0.013%
22	7.186	1807	1818	1835	rBV4	9003	20869	1.31%	0.173%
23	7.407	1881	1887	1892	rBV4	459	536	0.03%	0.004%
24	7.501	1907	1916	1924	rBV5	2364	4385	0.27%	0.036%
25	7.565	1924	1936	1957	rVV	136274	263992	16.53%	2.185%
26	7.694	1970	1976	1979	rBV3	1336	1742	0.11%	0.014%
27	7.899	2025	2040	2055	rBV	544052	994816	62.31%	8.234%
28	8.182	2115	2128	2153	rBV	89024	182889	11.45%	1.514%
29	8.282	2153	2159	2160	rBV2	481	507	0.03%	0.004%
30	8.362	2175	2184	2185	rBV5	2222	2946	0.18%	0.024%
31	8.469	2215	2217	2227	rVB5	867	1069	0.07%	0.009%
32	8.578	2241	2251	2257	rBV7	2583	3935	0.25%	0.033%
33	8.652	2259	2274	2299	rBV	387699	789383	49.44%	6.534%
34	8.848	2332	2335	2340	rVB2	711	612	0.04%	0.005%
35	8.874	2340	2343	2346	rBV3	531	481	0.03%	0.004%
36	9.009	2381	2385	2386	rBV2	590	378	0.02%	0.003%

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 Misc : 6.23g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNR1ME

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\SFAMULM032422WMA.M
 Title : VOC Analysis

37	9.359	2491	2494	2499	rBV4	984	896	0.06%	0.007%
38	9.420	2499	2513	2552	rVB2	622163	1596604	100.00%	13.216%
39	9.568	2552	2559	2560	rBV4	1692	1539	0.10%	0.013%
40	9.697	2589	2599	2611	rVB4	2686	4176	0.26%	0.035%
41	9.948	2672	2677	2681	rVB5	651	604	0.04%	0.005%
42	10.105	2719	2726	2734	rBV6	2101	3239	0.20%	0.027%
43	10.423	2819	2825	2829	rVB3	333	447	0.03%	0.004%
44	10.491	2842	2846	2852	rVB3	856	847	0.05%	0.007%
45	10.575	2862	2872	2882	rBV3	3007	4968	0.31%	0.041%
46	10.668	2892	2901	2909	rBV6	3378	5911	0.37%	0.049%
47	10.713	2911	2915	2918	rVV2	1764	1851	0.12%	0.015%
48	10.764	2919	2931	2952	rVB	474882	781260	48.93%	6.467%
49	10.867	2960	2963	2964	rBV2	872	504	0.03%	0.004%
50	10.893	2964	2971	2976	rVV6	1188	1461	0.09%	0.012%
51	10.993	2993	3002	3010	rBV4	4954	8050	0.50%	0.067%
52	11.102	3027	3036	3047	rVV6	3903	6850	0.43%	0.057%
53	11.147	3048	3050	3055	rVB3	618	487	0.03%	0.004%
54	11.266	3083	3087	3090	rBV	1271	1145	0.07%	0.009%
55	11.417	3131	3134	3137	rBV2	615	490	0.03%	0.004%
56	11.472	3140	3151	3162	rVV6	4544	8598	0.54%	0.071%
57	11.581	3181	3185	3188	rBV2	462	391	0.02%	0.003%
58	11.648	3198	3206	3210	rBV3	452	671	0.04%	0.006%
59	11.697	3214	3221	3228	rBV6	1405	2251	0.14%	0.019%
60	11.751	3231	3238	3244	rBV4	1383	1792	0.11%	0.015%
61	11.816	3245	3258	3274	rBV	839546	1331452	83.39%	11.021%
62	11.954	3293	3301	3316	rVB	5697	12720	0.80%	0.105%
63	12.015	3316	3320	3322	rBV3	521	412	0.03%	0.003%
64	12.102	3341	3347	3352	rBV5	1405	1578	0.10%	0.013%
65	12.195	3362	3376	3394	rBV	670788	1099060	68.84%	9.097%
66	12.365	3423	3429	3431	rBV3	3862	4198	0.26%	0.035%
67	12.398	3434	3439	3450	rVB3	17420	26214	1.64%	0.217%
68	12.472	3456	3462	3467	rBV3	1187	1391	0.09%	0.012%
69	12.578	3487	3495	3500	rBV3	1621	1998	0.13%	0.017%
70	12.671	3520	3524	3525	rBV3	782	492	0.03%	0.004%
71	12.783	3551	3559	3568	rBV5	2831	4993	0.31%	0.041%
72	12.838	3571	3576	3577	rBV5	1010	890	0.06%	0.007%
73	12.877	3586	3588	3590	rBV3	724	459	0.03%	0.004%
74	12.915	3594	3600	3604	rBV7	1798	2068	0.13%	0.017%
75	12.970	3604	3617	3630	rBV2	94966	153155	9.59%	1.268%
76	13.144	3667	3671	3684	rVB6	4618	6902	0.43%	0.057%

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 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNR1ME

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\SFAMULM032422WMA.M
 Title : VOC Analysis

77	13.208	3688	3691	3692	rVV	612	364	0.02%	0.003%
78	13.224	3693	3696	3701	rVB5	1475	1343	0.08%	0.011%
79	13.269	3707	3710	3711	rBV2	990	539	0.03%	0.004%
80	13.330	3719	3729	3739	rBV	74369	118919	7.45%	0.984%
81	13.513	3782	3786	3794	rVB4	1326	1775	0.11%	0.015%
82	13.581	3798	3807	3815	rVV9	3526	5252	0.33%	0.043%
83	13.632	3815	3823	3831	rVB7	2980	4363	0.27%	0.036%
84	13.729	3850	3853	3858	rVB5	825	606	0.04%	0.005%
85	13.841	3879	3888	3900	rBV7	9481	16707	1.05%	0.138%
86	13.944	3914	3920	3923	rBV6	2935	3450	0.22%	0.029%
87	14.025	3941	3945	3947	rBV5	1432	1251	0.08%	0.010%
88	14.057	3947	3955	3962	rVV7	6634	10941	0.69%	0.091%
89	14.192	3991	3997	4009	rVB8	4436	6575	0.41%	0.054%
90	14.288	4020	4027	4036	rVV9	3270	5554	0.35%	0.046%
91	14.494	4084	4091	4108	rVB9	7616	13298	0.83%	0.110%
92	14.578	4111	4117	4125	rBV4	1943	2774	0.17%	0.023%
93	14.664	4140	4144	4157	rVB4	4593	9221	0.58%	0.076%
94	14.790	4181	4183	4185	rBV3	795	485	0.03%	0.004%
95	14.883	4207	4212	4218	rVB6	2428	2744	0.17%	0.023%
96	15.018	4248	4254	4264	rVB9	4685	7087	0.44%	0.059%
97	15.545	4408	4418	4430	rVB3	84059	131615	8.24%	1.089%
98	15.796	4492	4496	4505	rVB7	3745	4897	0.31%	0.041%
99	15.886	4515	4524	4527	rBV8	8148	13729	0.86%	0.114%
100	16.391	4670	4681	4691	rBV	161933	265220	16.61%	2.195%

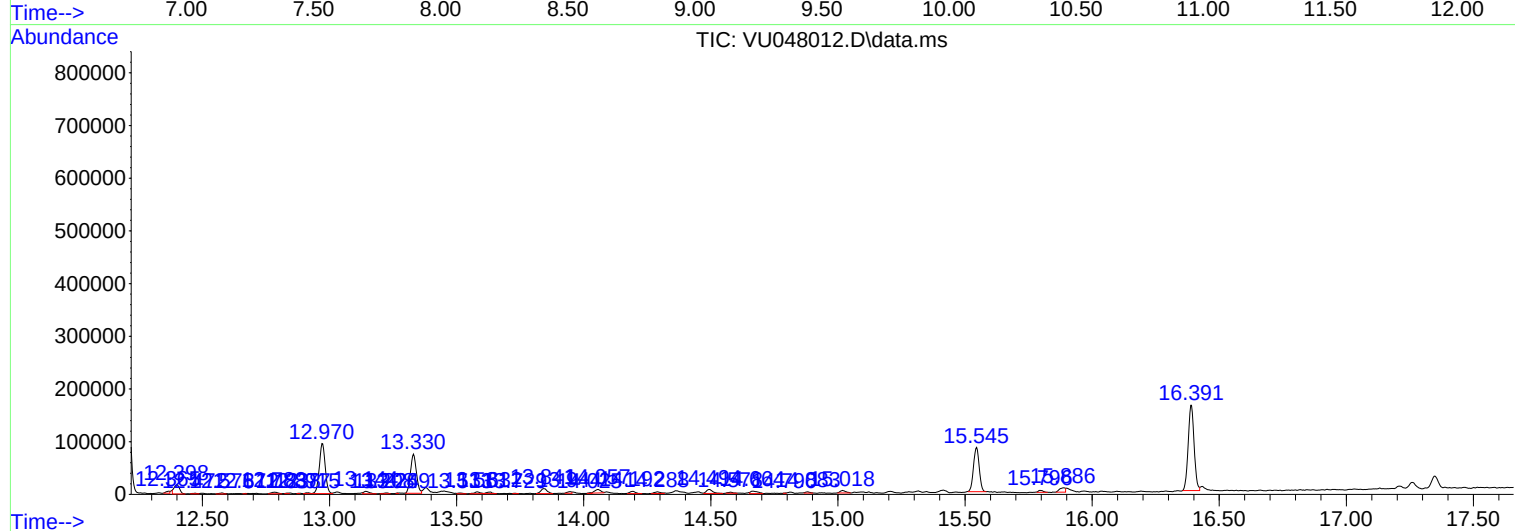
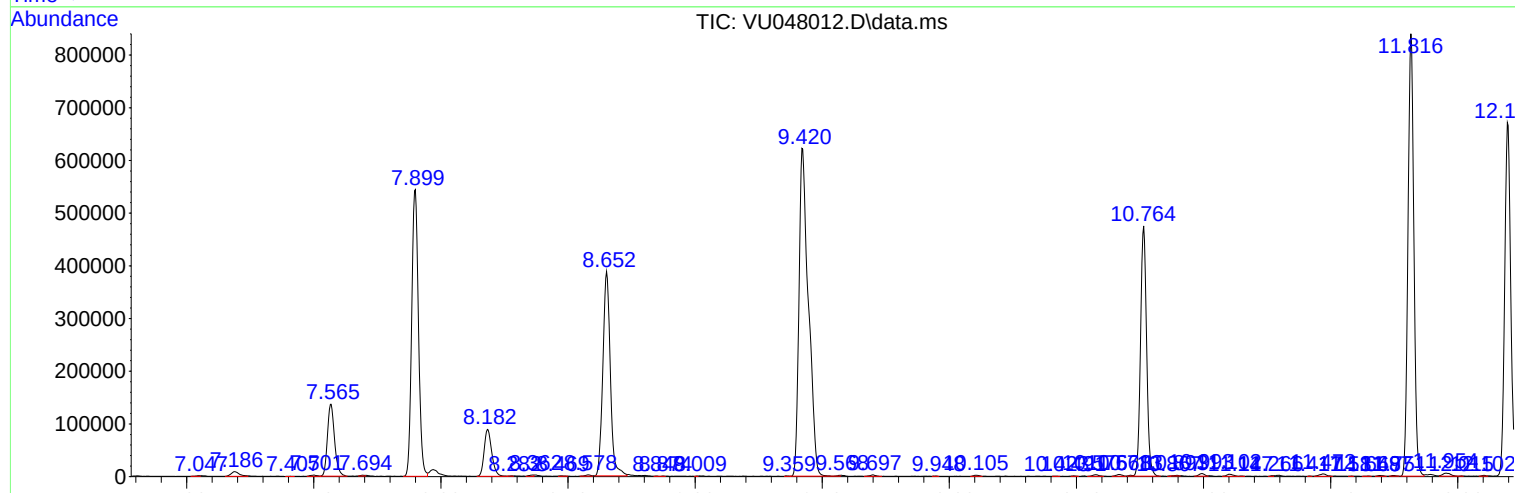
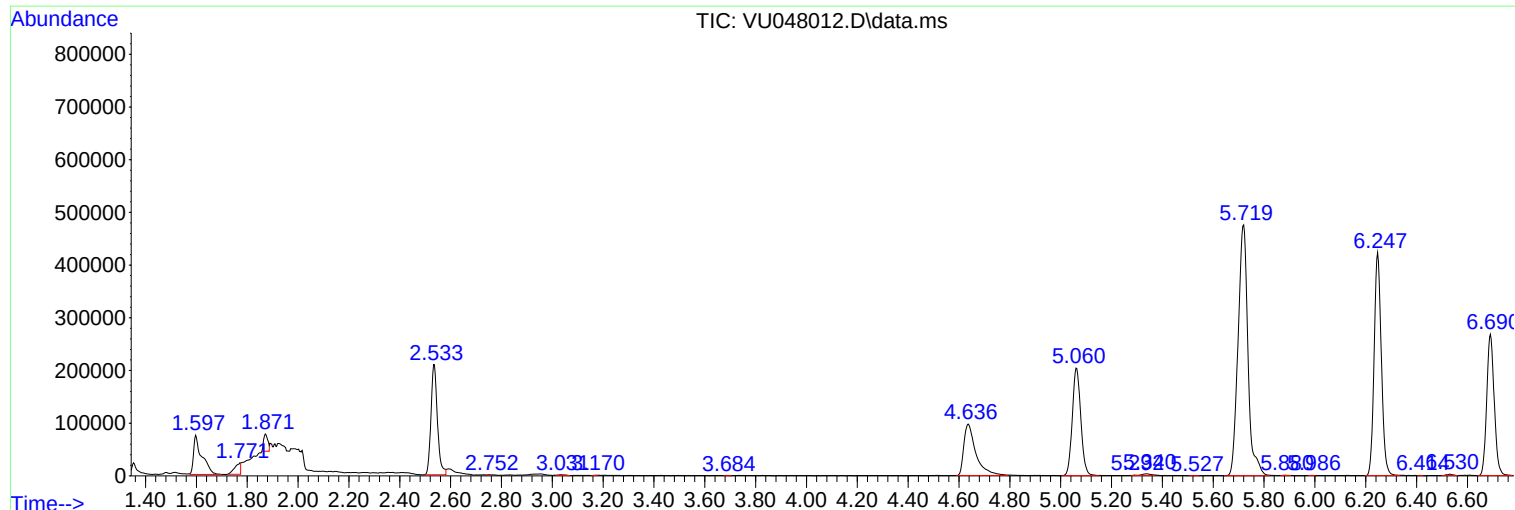
Sum of corrected areas: 12081126

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Misc : 6.23g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNR1ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
Data File : VU048012.D
Acq On : 13 Apr 2022 18:30
Operator : SY/MD
Sample : N2316-11ME
Misc : 6.23g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNR1ME

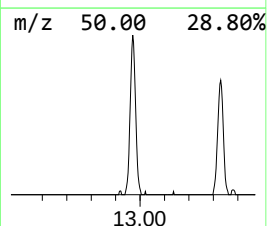
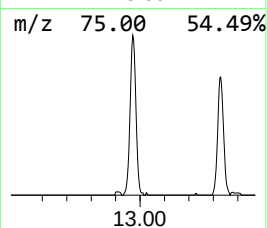
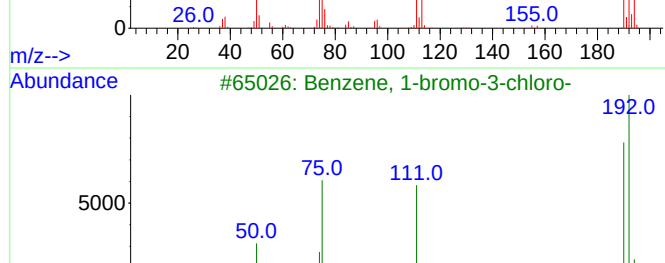
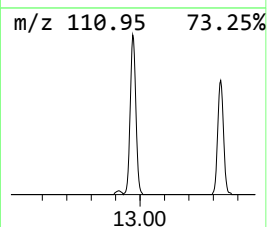
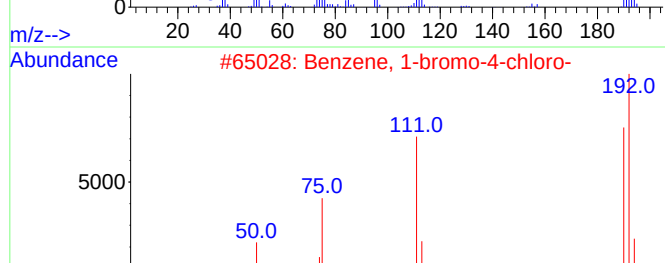
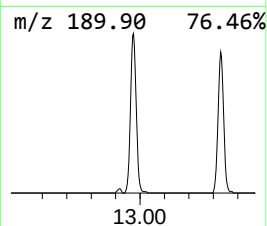
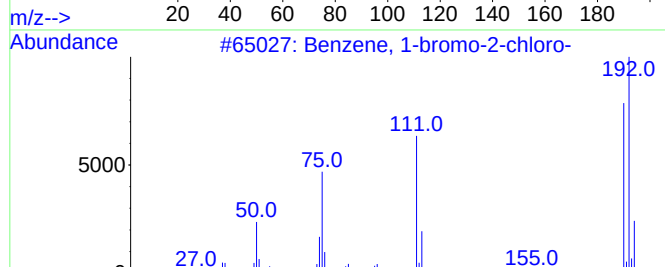
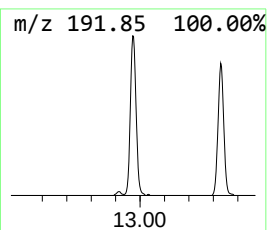
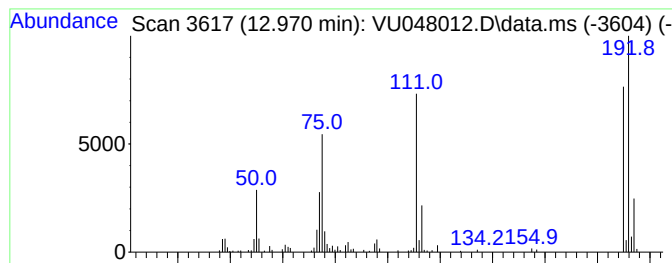
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Benzene, 1-bromo-2-chloro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.970	5.75 ug/L	153155	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-bromo-2-chloro-	190	C6H4BrCl	000694-80-4	98
2			Benzene, 1-bromo-4-chloro-	190	C6H4BrCl	000106-39-8	97
3			Benzene, 1-bromo-3-chloro-	190	C6H4BrCl	000108-37-2	97
4			4-Chlorophenylselenol	192	C6H5ClSe	016645-10-6	96
5			Benzene, 1-bromo-3-chloro-	190	C6H4BrCl	000108-37-2	96



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Misc : 6.23g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNR1ME

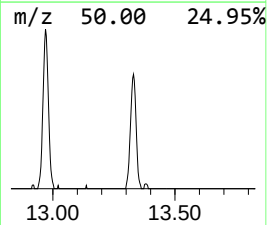
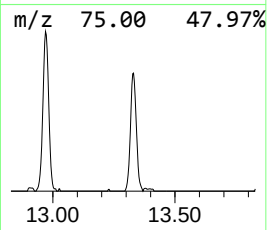
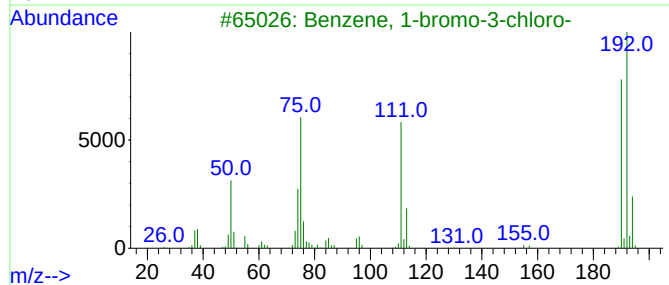
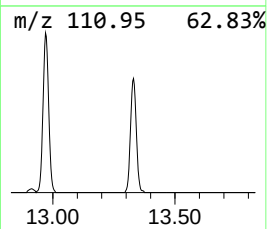
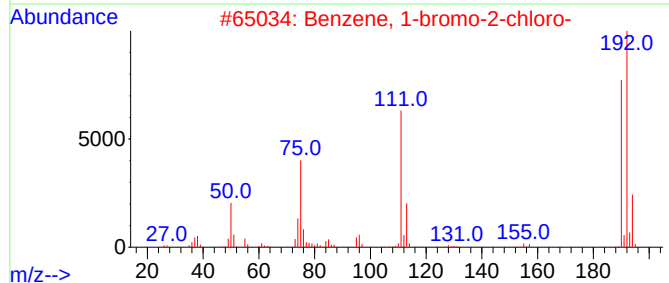
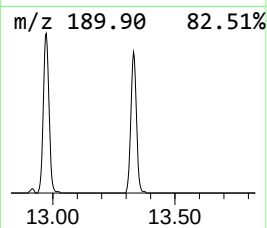
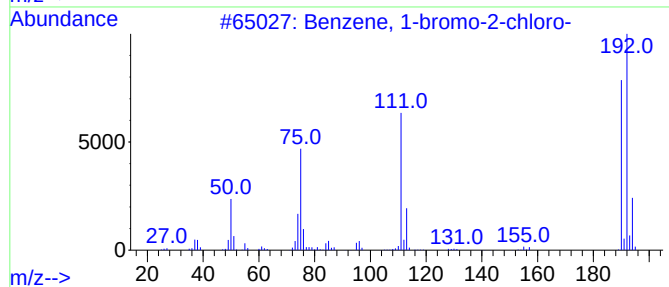
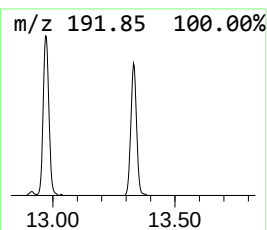
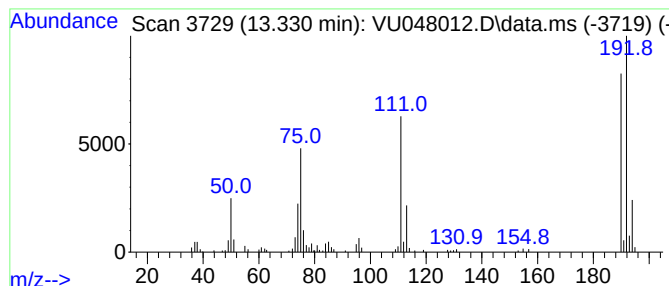
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Benzene, 1-bromo-3-chloro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.330	4.47 ug/L	118919	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-bromo-2-chloro-	190	C6H4BrCl	000694-80-4	99
2			Benzene, 1-bromo-2-chloro-	190	C6H4BrCl	000694-80-4	98
3			Benzene, 1-bromo-3-chloro-	190	C6H4BrCl	000108-37-2	98
4			Benzene, 1-bromo-4-chloro-	190	C6H4BrCl	000106-39-8	98
5			Benzene, 1-bromo-4-chloro-	190	C6H4BrCl	000106-39-8	98



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Misc : 6.23g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNR1ME

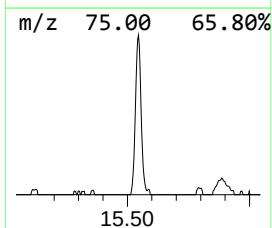
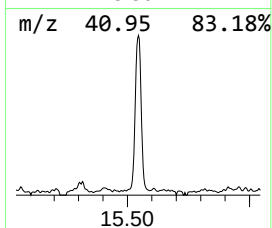
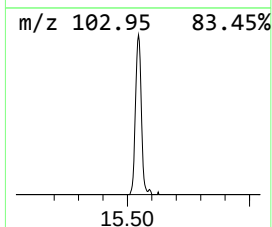
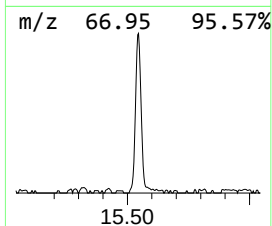
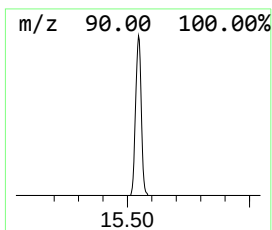
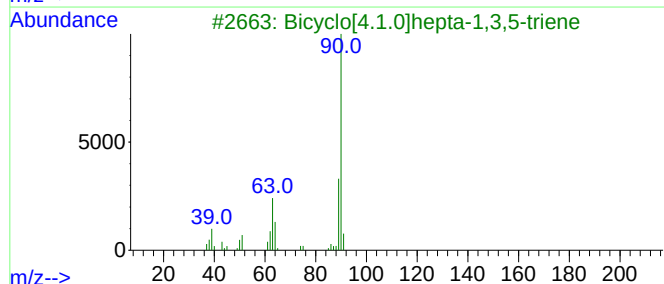
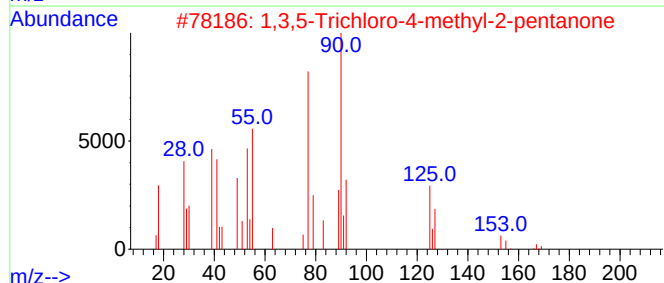
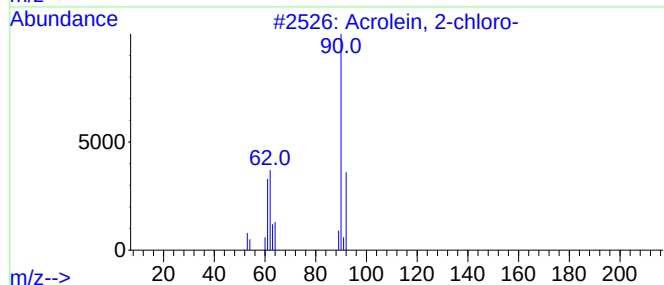
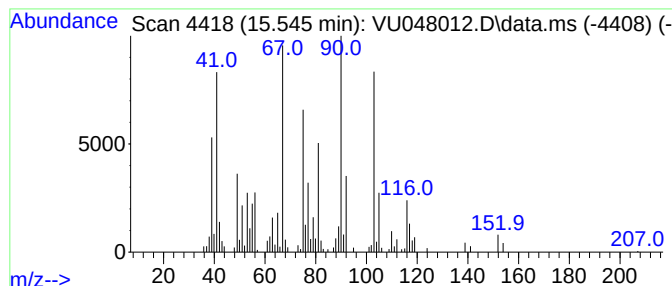
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Quant Title : VOC Analysis

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

Peak Number 4 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.545	4.94 ug/L	131615	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acrolein, 2-chloro-	90	C3H3ClO	000683-51-2	43
2			1,3,5-Trichloro-4-methyl-2-penta...	202	C6H9Cl3O	1000140-03-8	38
3			Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	35
4			Thiourea, methyl-	90	C2H6N2S	000598-52-7	35
5			2,2-Bis(chloromethyl)-1-propanol	156	C5H10Cl2O	005355-54-4	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
Data File : VU048012.D
Acq On : 13 Apr 2022 18:30
Operator : SY/MD
Sample : N2316-11ME
Misc : 6.23g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNR1ME

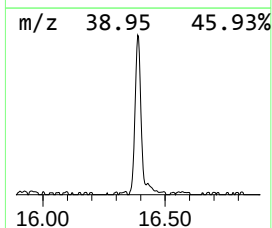
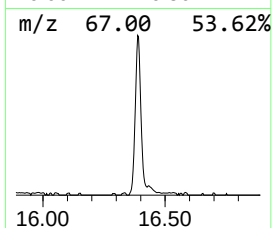
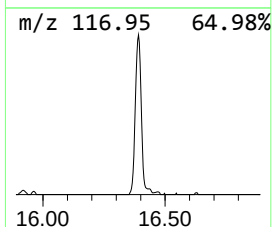
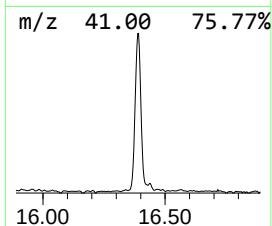
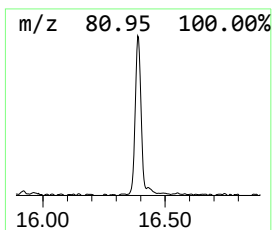
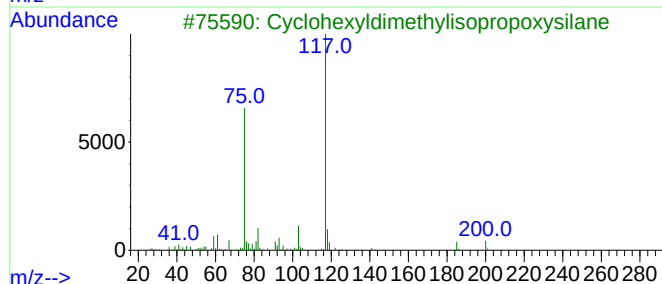
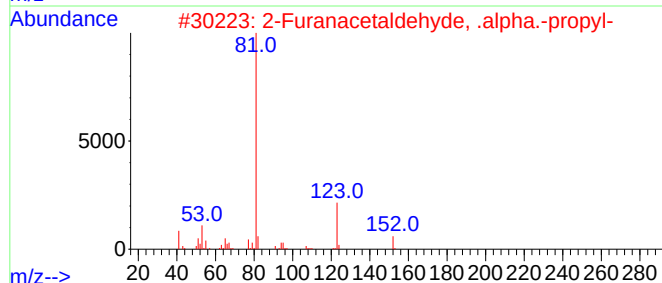
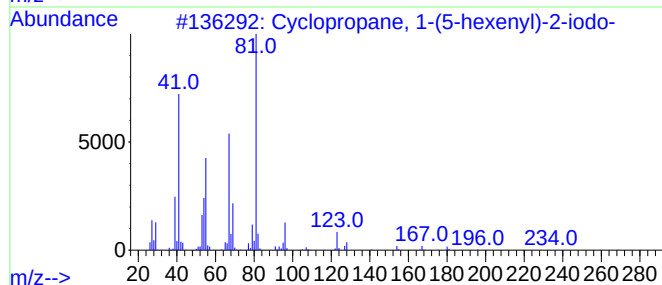
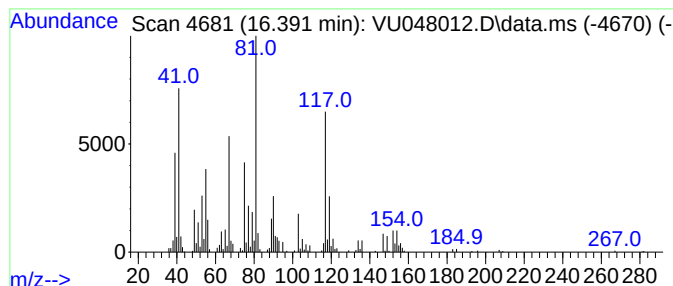
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Quant Title : VOC Analysis

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

Peak Number 5 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.391	9.96 ug/L	265220	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1-(5-hexenyl)-2-iodo-	250	C9H15I	074685-40-8	12
2			2-Furanacetaldehyde, .alpha.-pro...	152	C9H12O2	031681-26-2	10
3			Cyclohexyldimethylisopropoxysilane	200	C11H24OSi	1000282-21-5	10
4			Isomycorene	136	C10H16	006876-07-9	10
5			1,5-Hexadiene, 2-methyl-	96	C7H12	004049-81-4	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
Data File : VU048012.D
Acq On : 13 Apr 2022 18:30
Operator : SY/MD
Sample : N2316-11ME
Misc : 6.23g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNR1ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.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
Benzene, 1-brom...	12.970	5.8	ug/L	153155	3	11.816	1331450	50.0
Benzene, 1-brom...	13.330	4.5	ug/L	118919	3	11.816	1331450	50.0
unknown-01	15.545	4.9	ug/L	131615	3	11.816	1331450	50.0
unknown-02	16.391	10.0	ug/L	265220	3	11.816	1331450	50.0