

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
 Data File : VU047935.D
 Acq On : 12 Apr 2022 02:51
 Operator : SY/MD
 Sample : N2293-07ME
 Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNN7ME

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: VU047935.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	114	rVB	137785	277597	7.75%	1.381%
2	2.546	362	375	388	rBV	384666	665613	18.59%	3.312%
3	3.182	568	573	576	rBV2	370	356	0.01%	0.002%
4	3.256	593	596	597	rBV	194	122	0.00%	0.001%
5	3.266	597	599	602	rVB2	477	270	0.01%	0.001%
6	3.289	602	606	607	rBV	337	195	0.01%	0.001%
7	3.440	651	653	655	rVB3	477	175	0.00%	0.001%
8	3.453	655	657	659	rBV	223	147	0.00%	0.001%
9	3.481	664	666	668	rVB2	207	77	0.00%	0.000%
10	3.645	715	717	720	rBV2	251	124	0.00%	0.001%
11	3.674	720	726	728	rBV4	597	619	0.02%	0.003%
12	3.742	744	747	751	rBV	336	264	0.01%	0.001%
13	3.761	751	753	754	rBV	212	86	0.00%	0.000%
14	3.777	754	758	764	rVB2	409	374	0.01%	0.002%
15	3.867	783	786	787	rBV	208	119	0.00%	0.001%
16	3.909	796	799	801	rVB2	303	158	0.00%	0.001%
17	3.941	807	809	812	rVB2	142	83	0.00%	0.000%
18	3.999	825	827	829	rBV2	271	119	0.00%	0.001%
19	4.054	842	844	847	rBV2	125	83	0.00%	0.000%
20	4.108	858	861	864	rBV2	253	200	0.01%	0.001%
21	4.144	870	872	875	rBV	135	92	0.00%	0.000%
22	4.170	878	880	884	rVB	248	159	0.00%	0.001%
23	4.272	905	912	915	rBV3	357	348	0.01%	0.002%
24	4.301	918	921	926	rBV4	229	184	0.01%	0.001%
25	4.330	926	930	934	rBV2	273	236	0.01%	0.001%
26	4.379	942	945	948	rBV	159	148	0.00%	0.001%
27	4.404	951	953	955	rVB2	213	96	0.00%	0.000%
28	4.449	964	967	968	rBV2	182	102	0.00%	0.001%
29	4.510	982	986	993	rBV3	590	617	0.02%	0.003%
30	4.565	1000	1003	1007	rVB3	509	361	0.01%	0.002%
31	4.642	1012	1027	1097	rBV2	169011	648413	18.11%	3.227%
32	5.063	1140	1158	1185	rBV	394478	896869	25.05%	4.463%
33	5.215	1202	1205	1210	rVB4	602	381	0.01%	0.002%
34	5.276	1221	1224	1226	rBV3	636	401	0.01%	0.002%
35	5.333	1239	1242	1243	rBV	385	221	0.01%	0.001%
36	5.343	1243	1245	1248	rVV2	395	242	0.01%	0.001%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
 Data File : VU047935.D
 Acq On : 12 Apr 2022 02:51
 Operator : SY/MD
 Sample : N2293-07ME
 Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNN7ME

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	5.395	1259	1261	1264	rVB3	486	192	0.01%	0.001%
38	5.465	1280	1283	1285	rVV2	396	220	0.01%	0.001%
39	5.481	1285	1288	1290	rVB	280	150	0.00%	0.001%
40	5.542	1304	1307	1314	rVB2	319	237	0.01%	0.001%
41	5.581	1315	1319	1320	rBV2	151	90	0.00%	0.000%
42	5.719	1341	1362	1376	rBV2	881953	2298777	64.20%	11.439%
43	6.076	1471	1473	1476	rVB2	279	102	0.00%	0.001%
44	6.092	1476	1478	1480	rBV2	223	124	0.00%	0.001%
45	6.108	1480	1483	1486	rBV3	391	330	0.01%	0.002%
46	6.131	1486	1490	1499	rVB6	1032	1032	0.03%	0.005%
47	6.169	1499	1502	1504	rBV	225	179	0.00%	0.001%
48	6.247	1507	1526	1556	rBV	466449	937417	26.18%	4.665%
49	6.481	1591	1599	1606	rBV6	2782	5127	0.14%	0.026%
50	6.690	1648	1664	1692	rBV	504725	1041844	29.10%	5.184%
51	6.877	1720	1722	1727	rVB3	368	238	0.01%	0.001%
52	6.903	1727	1730	1731	rBV3	263	146	0.00%	0.001%
53	6.944	1741	1743	1744	rBV	348	148	0.00%	0.001%
54	6.980	1751	1754	1755	rBV2	210	127	0.00%	0.001%
55	7.041	1771	1773	1774	rBV	256	129	0.00%	0.001%
56	7.195	1809	1821	1846	rBV5	7798	24567	0.69%	0.122%
57	7.311	1855	1857	1859	rBV	268	147	0.00%	0.001%
58	7.324	1859	1861	1864	rVB	290	158	0.00%	0.001%
59	7.366	1872	1874	1875	rBV	254	108	0.00%	0.001%
60	7.443	1892	1898	1899	rBV2	272	238	0.01%	0.001%
61	7.497	1905	1915	1925	rBV3	8458	18489	0.52%	0.092%
62	7.568	1925	1937	1962	rVB	246642	485092	13.55%	2.414%
63	7.899	2026	2040	2055	rBV	1013802	1832722	51.19%	9.120%
64	8.182	2115	2128	2150	rBV	154122	329445	9.20%	1.639%
65	8.375	2175	2188	2204	rVB9	6328	16785	0.47%	0.084%
66	8.504	2226	2228	2233	rVB3	541	264	0.01%	0.001%
67	8.562	2244	2246	2249	rBB	325	167	0.00%	0.001%
68	8.587	2249	2254	2255	rBV2	714	540	0.02%	0.003%
69	8.661	2259	2277	2310	rBV	735457	1510350	42.18%	7.516%
70	9.034	2382	2393	2406	rVB8	4251	10312	0.29%	0.051%
71	9.134	2421	2424	2427	rBV2	204	179	0.00%	0.001%
72	9.240	2455	2457	2461	rBV3	368	225	0.01%	0.001%
73	9.356	2489	2493	2495	rBV4	614	557	0.02%	0.003%
74	9.449	2500	2522	2550	rBV2	1276129	3580562	100.00%	17.817%
75	9.697	2589	2599	2610	rBV	5526	9086	0.25%	0.045%
76	9.742	2610	2613	2620	rVV5	609	482	0.01%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
 Data File : VU047935.D
 Acq On : 12 Apr 2022 02:51
 Operator : SY/MD
 Sample : N2293-07ME
 Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNN7ME

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	9.870	2650	2653	2654	rBV	301	125	0.00%	0.001%
78	9.912	2664	2666	2669	rVB2	328	115	0.00%	0.001%
79	10.009	2692	2696	2699	rBV2	300	224	0.01%	0.001%
80	10.108	2711	2727	2731	rBV5	3289	5232	0.15%	0.026%
81	10.340	2795	2799	2801	rBV2	527	371	0.01%	0.002%
82	10.462	2833	2837	2840	rBV4	450	315	0.01%	0.002%
83	10.484	2842	2844	2847	rVV3	527	305	0.01%	0.002%
84	10.668	2890	2901	2912	rVV5	7074	13442	0.38%	0.067%
85	10.764	2919	2931	2952	rVB	842550	1371995	38.32%	6.827%
86	10.841	2952	2955	2957	rBV3	665	355	0.01%	0.002%
87	10.980	2987	2998	3001	rBV5	2775	4110	0.11%	0.020%
88	11.115	3026	3040	3048	rBV9	3338	7313	0.20%	0.036%
89	11.465	3140	3149	3160	rBV5	5890	11663	0.33%	0.058%
90	11.584	3178	3186	3197	rVB6	2956	4724	0.13%	0.024%
91	11.635	3200	3202	3206	rBV3	545	396	0.01%	0.002%
92	11.751	3232	3238	3245	rVB4	3342	4283	0.12%	0.021%
93	11.816	3245	3258	3274	rBV	865167	1365160	38.13%	6.793%
94	12.198	3364	3377	3397	rVB	1149236	1957592	54.67%	9.741%
95	12.465	3456	3460	3461	rBV2	1005	627	0.02%	0.003%
96	12.973	3607	3618	3633	rVB	134121	210919	5.89%	1.050%
97	13.330	3719	3729	3738	rBV2	108862	173882	4.86%	0.865%
98	15.545	4409	4418	4432	rVB2	67344	103888	2.90%	0.517%
99	15.796	4488	4496	4505	rVB2	38036	56860	1.59%	0.283%
100	16.391	4673	4681	4692	rVB2	130053	199233	5.56%	0.991%

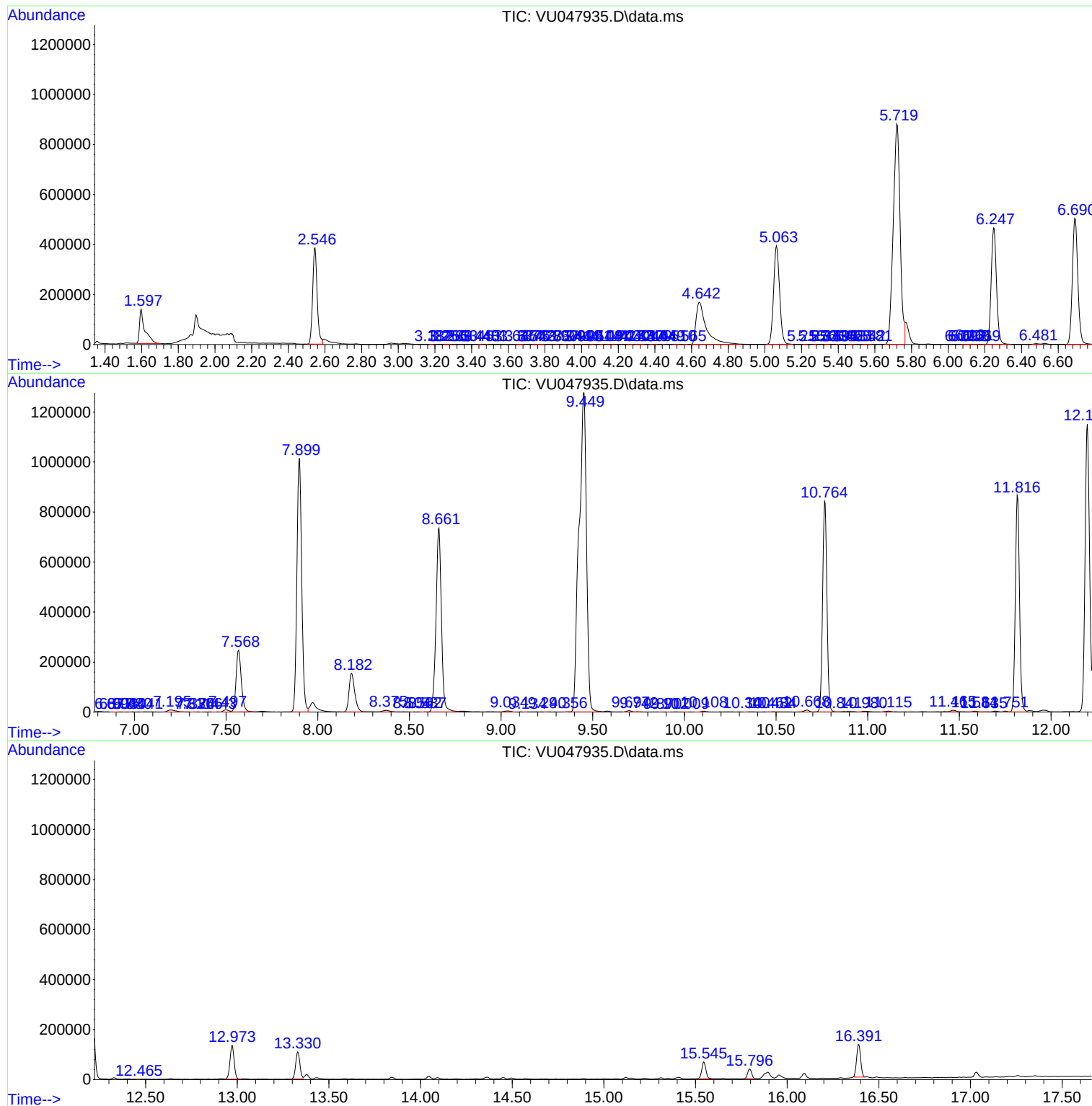
Sum of corrected areas: 20095864

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
Data File : VU047935.D
Acq On : 12 Apr 2022 02:51
Operator : SY/MD
Sample : N2293-07ME
Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN7ME

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\VU041122\
Data File : VU047935.D
Acq On : 12 Apr 2022 02:51
Operator : SY/MD
Sample : N2293-07ME
Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN7ME

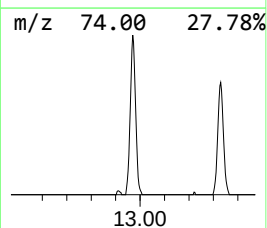
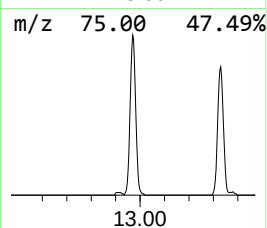
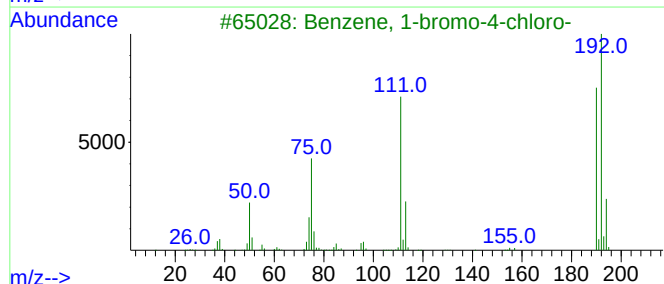
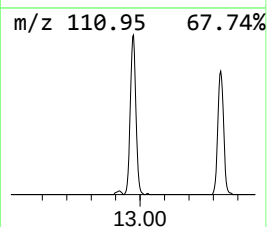
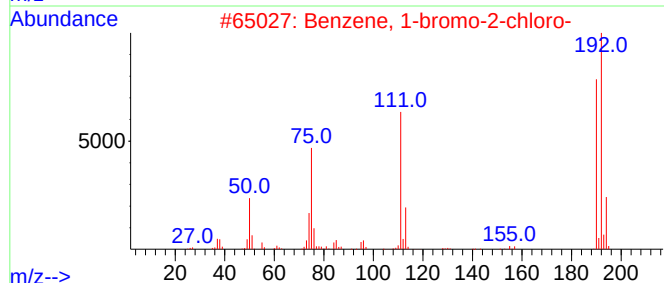
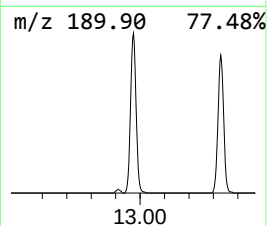
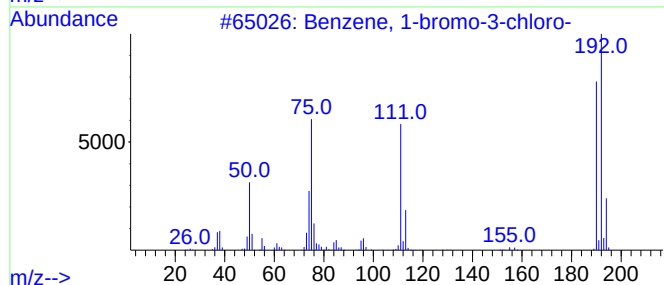
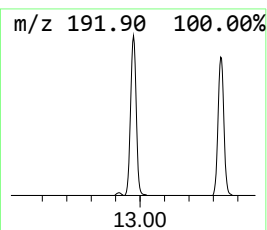
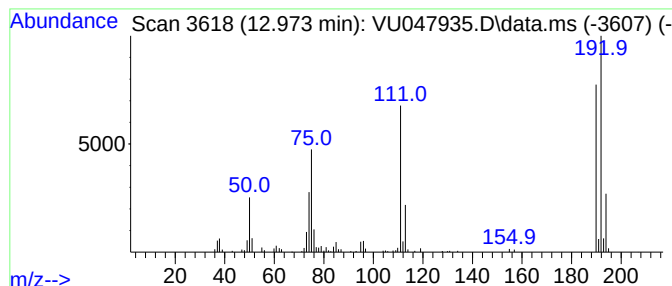
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.973	7.73 ug/L	210919	1,4-Dichlorobenzene-d4	11.816

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
Data File : VU047935.D
Acq On : 12 Apr 2022 02:51
Operator : SY/MD
Sample : N2293-07ME
Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN7ME

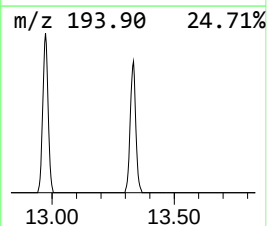
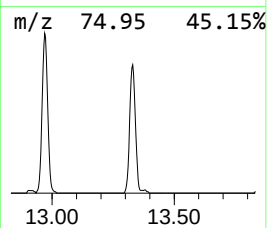
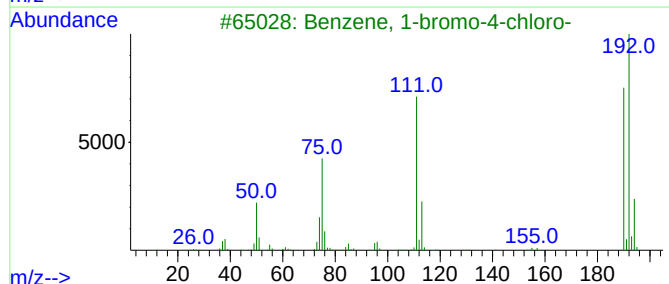
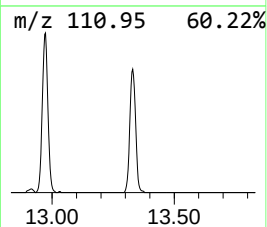
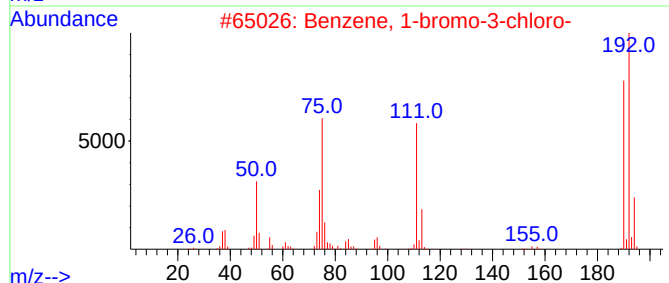
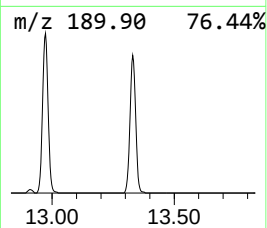
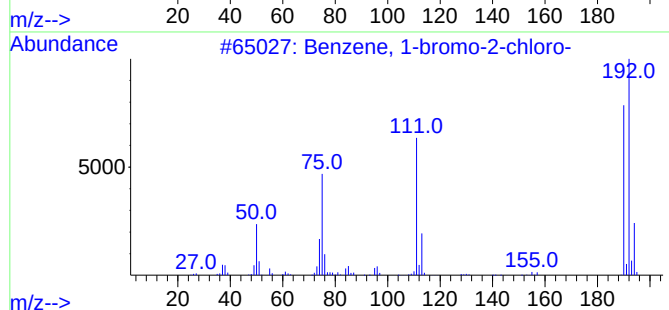
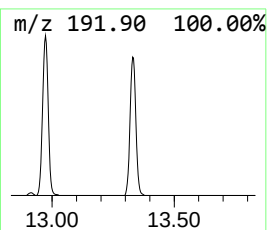
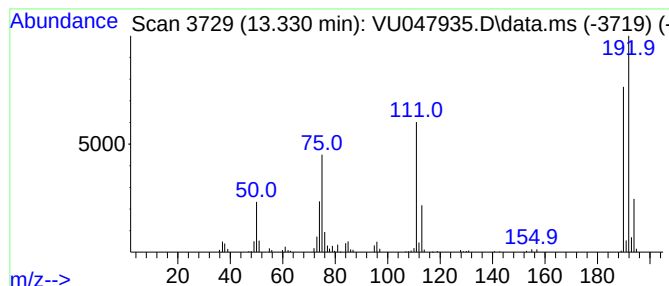
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Benzene, 1-bromo-2-chloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.330	6.37 ug/L	173882	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-3-chloro-	190	C6H4BrCl	000108-37-2	98
3			Benzene, 1-bromo-4-chloro-	190	C6H4BrCl	000106-39-8	98
4			Benzene, 1-bromo-3-chloro-	190	C6H4BrCl	000108-37-2	97
5			Benzene, 1-bromo-2-chloro-	190	C6H4BrCl	000694-80-4	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
Data File : VU047935.D
Acq On : 12 Apr 2022 02:51
Operator : SY/MD
Sample : N2293-07ME
Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN7ME

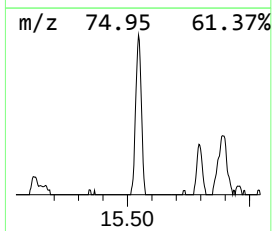
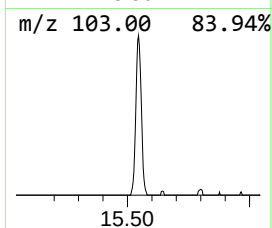
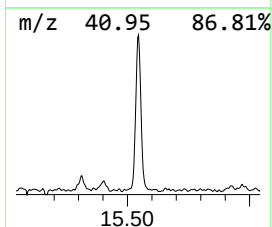
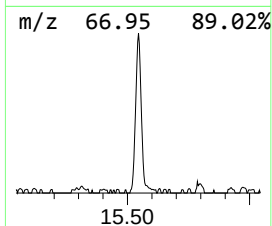
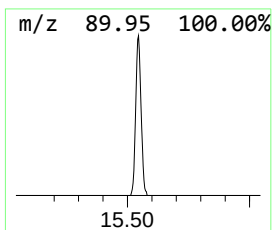
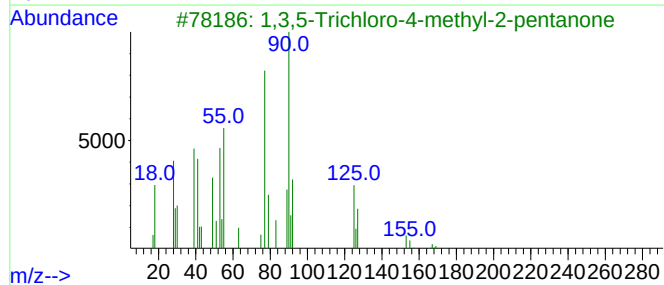
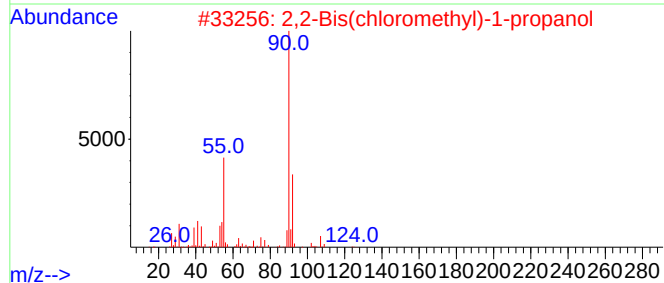
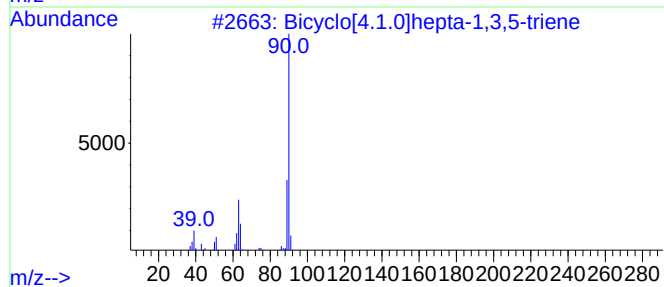
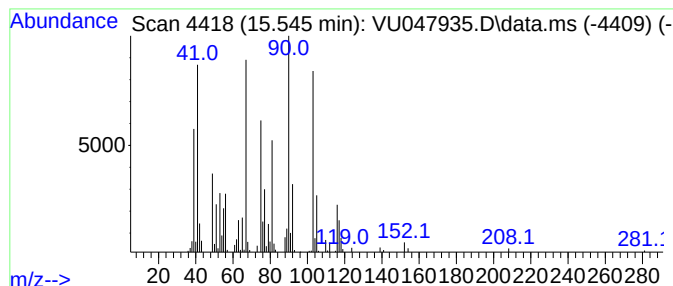
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.545	3.80 ug/L	103888	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	38
2			2,2-Bis(chloromethyl)-1-propanol	156	C5H10Cl2O	005355-54-4	38
3			1,3,5-Trichloro-4-methyl-2-penta...	202	C6H9Cl3O	1000140-03-8	28
4			Acrolein, 2-chloro-	90	C3H3ClO	000683-51-2	25
5			2,2-Bis(chloromethyl)-1-propanol	156	C5H10Cl2O	005355-54-4	23



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
Data File : VU047935.D
Acq On : 12 Apr 2022 02:51
Operator : SY/MD
Sample : N2293-07ME
Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN7ME

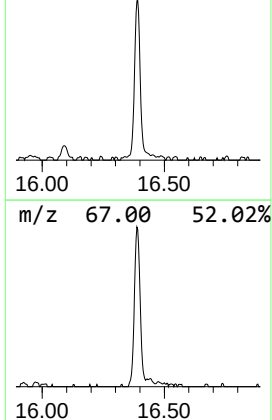
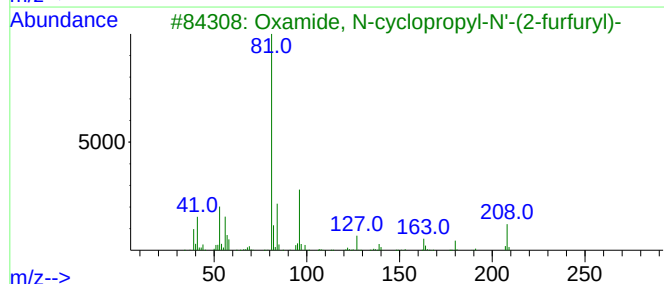
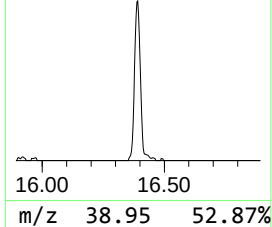
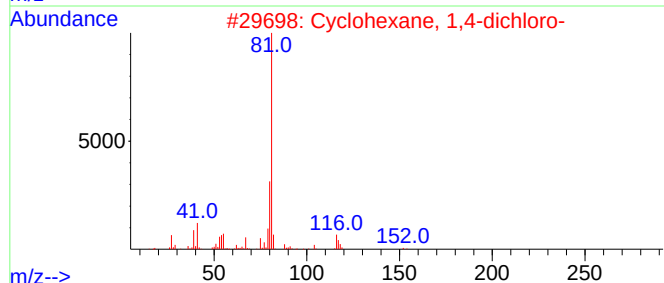
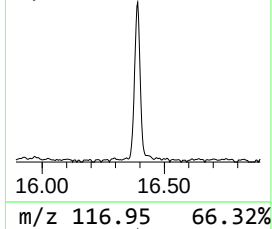
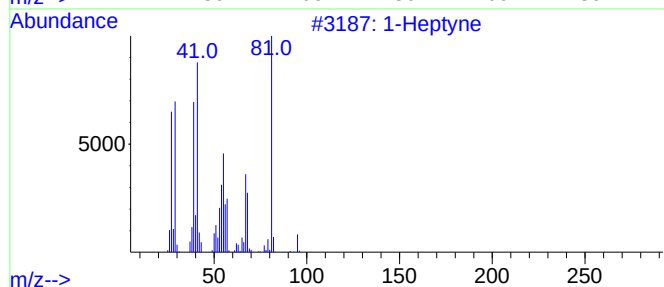
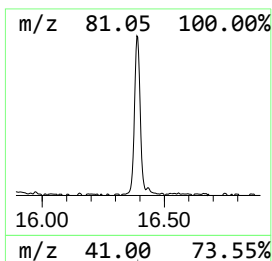
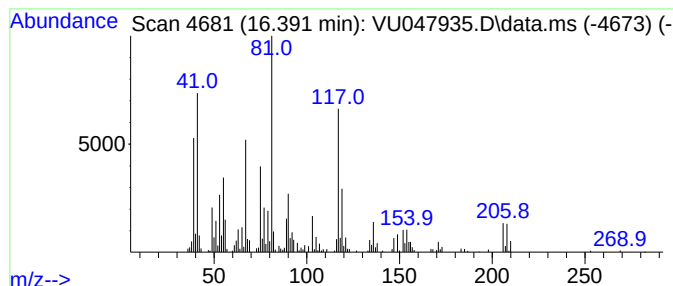
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 unknown-02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.391	7.30 ug/L	199233	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptyne	96	C7H12	000628-71-7	22
2			Cyclohexane, 1,4-dichloro-	152	C6H10Cl2	019398-57-3	14
3			Oxamide, N-cyclopropyl-N'-(2-fur...	208	C10H12N2O3	296773-01-8	11
4			3-Methyl-1-penten-4-yn-3-ol	96	C6H8O	003230-69-1	11
5			2,4-Dimethyl 1,4-pentadiene	96	C7H12	004161-65-3	11



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
Data File : VU047935.D
Acq On : 12 Apr 2022 02:51
Operator : SY/MD
Sample : N2293-07ME
Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN7ME

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...	12.973	7.7	ug/L	210919	3	11.816	1365160	50.0
Benzene, 1-brom...	13.330	6.4	ug/L	173882	3	11.816	1365160	50.0
unknown-01	15.545	3.8	ug/L	103888	3	11.816	1365160	50.0
unknown-02	16.391	7.3	ug/L	199233	3	11.816	1365160	50.0