

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
 Data File : VU047965.D
 Acq On : 12 Apr 2022 18:50
 Operator : SY/MD
 Sample : N2293-07ME
 Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 26 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: VU047965.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	103	rVB	76450	138478	3.81%	0.965%
2	2.543	362	374	387	rBV	202230	348410	9.59%	2.428%
3	3.038	519	528	536	rBV5	3590	7232	0.20%	0.050%
4	3.150	561	563	565	rBV2	187	97	0.00%	0.001%
5	3.166	565	568	570	rBV2	810	525	0.01%	0.004%
6	3.215	581	583	590	rVB3	375	306	0.01%	0.002%
7	3.272	599	601	605	rVB2	460	272	0.01%	0.002%
8	3.295	605	608	611	rBV2	357	273	0.01%	0.002%
9	3.433	648	651	654	rVB	220	149	0.00%	0.001%
10	3.456	654	658	660	rBV2	341	276	0.01%	0.002%
11	3.533	676	682	683	rBV	284	252	0.01%	0.002%
12	3.803	759	766	768	rBV2	221	253	0.01%	0.002%
13	3.919	800	802	806	rVB3	216	129	0.00%	0.001%
14	4.015	828	832	835	rVB2	195	152	0.00%	0.001%
15	4.038	835	839	842	rBV2	310	275	0.01%	0.002%
16	4.089	852	855	863	rVB2	300	223	0.01%	0.002%
17	4.137	867	870	871	rBV	163	106	0.00%	0.001%
18	4.276	907	913	919	rVB3	238	297	0.01%	0.002%
19	4.330	928	930	932	rBV2	222	111	0.00%	0.001%
20	4.388	946	948	952	rVB2	183	153	0.00%	0.001%
21	4.440	961	964	967	rVB2	183	119	0.00%	0.001%
22	4.568	1001	1004	1007	rBV	222	196	0.01%	0.001%
23	4.629	1007	1023	1069	rBV	122000	388548	10.69%	2.707%
24	5.063	1140	1158	1180	rBV	221934	502901	13.84%	3.504%
25	5.234	1205	1211	1214	rBV3	335	410	0.01%	0.003%
26	5.276	1222	1224	1225	rBV	309	171	0.00%	0.001%
27	5.423	1268	1270	1273	rVB2	332	157	0.00%	0.001%
28	5.491	1288	1291	1297	rBV3	262	241	0.01%	0.002%
29	5.549	1306	1309	1310	rBV2	241	148	0.00%	0.001%
30	5.719	1340	1362	1374	rBV2	469735	1261379	34.70%	8.789%
31	5.928	1425	1427	1429	rBV2	364	188	0.01%	0.001%
32	6.015	1451	1454	1456	rBV2	273	177	0.00%	0.001%
33	6.118	1483	1486	1489	rBV2	286	263	0.01%	0.002%
34	6.247	1512	1526	1554	rBV	466115	917298	25.24%	6.391%
35	6.478	1590	1598	1607	rBV4	2877	5002	0.14%	0.035%
36	6.587	1626	1632	1635	rBV2	356	413	0.01%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
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 Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 26 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	6.690	1649	1664	1689	rBV	285844	580661	15.97%	4.046%
38	6.989	1753	1757	1761	rBV2	201	158	0.00%	0.001%
39	7.025	1765	1768	1770	rBV2	246	149	0.00%	0.001%
40	7.047	1770	1775	1776	rBV3	1067	879	0.02%	0.006%
41	7.182	1806	1817	1835	rBV2	8461	19008	0.52%	0.132%
42	7.346	1865	1868	1871	rVB2	332	217	0.01%	0.002%
43	7.365	1871	1874	1880	rVB3	235	227	0.01%	0.002%
44	7.407	1880	1887	1890	rBV2	256	297	0.01%	0.002%
45	7.497	1904	1915	1925	rBV3	9382	18692	0.51%	0.130%
46	7.568	1925	1937	1959	rVB	143823	276656	7.61%	1.928%
47	7.655	1962	1964	1967	rBV3	352	236	0.01%	0.002%
48	7.697	1970	1977	1979	rBV2	1082	1282	0.04%	0.009%
49	7.780	2001	2003	2005	rBV3	276	183	0.01%	0.001%
50	7.899	2026	2040	2055	rBV	535503	961375	26.45%	6.699%
51	8.182	2116	2128	2146	rBV	98100	192788	5.30%	1.343%
52	8.362	2175	2184	2198	rBV9	6553	14119	0.39%	0.098%
53	8.472	2212	2218	2229	rVB3	1335	1973	0.05%	0.014%
54	8.533	2234	2237	2240	rBV2	245	190	0.01%	0.001%
55	8.648	2259	2273	2303	rBV	494376	958246	26.36%	6.677%
56	9.025	2382	2390	2406	rVB5	5013	9529	0.26%	0.066%
57	9.179	2434	2438	2444	rVV4	615	670	0.02%	0.005%
58	9.221	2447	2451	2454	rVB2	398	264	0.01%	0.002%
59	9.253	2459	2461	2465	rVB2	431	280	0.01%	0.002%
60	9.272	2465	2467	2469	rBV	278	141	0.00%	0.001%
61	9.311	2477	2479	2482	rVB2	248	105	0.00%	0.001%
62	9.340	2482	2488	2491	rBV3	440	509	0.01%	0.004%
63	9.449	2499	2522	2554	rBV2	1361521	3634922	100.00%	25.327%
64	9.764	2617	2620	2622	rBV	274	182	0.01%	0.001%
65	9.809	2632	2634	2636	rBV	181	102	0.00%	0.001%
66	9.848	2642	2646	2648	rBV	286	225	0.01%	0.002%
67	9.918	2666	2668	2671	rVB2	389	181	0.00%	0.001%
68	9.941	2673	2675	2680	rVB2	394	318	0.01%	0.002%
69	10.037	2701	2705	2707	rBV2	307	202	0.01%	0.001%
70	10.050	2707	2709	2712	rVB2	333	174	0.00%	0.001%
71	10.108	2717	2727	2733	rBV3	2156	3188	0.09%	0.022%
72	10.272	2776	2778	2781	rBV	206	157	0.00%	0.001%
73	10.333	2791	2797	2800	rBV	290	350	0.01%	0.002%
74	10.398	2814	2817	2820	rVV	241	133	0.00%	0.001%
75	10.465	2835	2838	2840	rBV2	343	292	0.01%	0.002%
76	10.571	2868	2871	2872	rBV	185	124	0.00%	0.001%

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 ALS Vial : 26 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	10.581	2872	2874	2876	rBV	276	158	0.00%	0.001%
78	10.655	2890	2897	2898	rBV3	3057	2965	0.08%	0.021%
79	10.764	2918	2931	2950	rBV	559204	900813	24.78%	6.277%
80	10.896	2967	2972	2982	rVB6	1894	3316	0.09%	0.023%
81	10.976	2989	2997	3002	rBV5	2953	4414	0.12%	0.031%
82	11.105	3027	3037	3046	rBV10	2804	6023	0.17%	0.042%
83	11.153	3050	3052	3055	rVB2	355	160	0.00%	0.001%
84	11.172	3055	3058	3060	rBV2	260	154	0.00%	0.001%
85	11.243	3077	3080	3087	rVB	269	237	0.01%	0.002%
86	11.285	3088	3093	3094	rBV2	679	494	0.01%	0.003%
87	11.420	3129	3135	3139	rBV4	654	779	0.02%	0.005%
88	11.584	3182	3186	3193	rVB6	1751	2223	0.06%	0.015%
89	11.751	3230	3238	3244	rBV3	2658	3383	0.09%	0.024%
90	11.815	3245	3258	3274	rBV	931623	1485919	40.88%	10.353%
91	12.024	3321	3323	3324	rBV	267	124	0.00%	0.001%
92	12.047	3328	3330	3332	rBV	407	284	0.01%	0.002%
93	12.195	3364	3376	3394	rBV	703184	1238295	34.07%	8.628%
94	12.327	3412	3417	3426	rVB5	4915	6659	0.18%	0.046%
95	12.738	3543	3545	3546	rBV5	428	193	0.01%	0.001%
96	12.912	3592	3599	3605	rBV7	2498	4152	0.11%	0.029%
97	12.970	3607	3617	3629	rVB	134926	211372	5.82%	1.473%
98	13.330	3718	3729	3740	rBV	106108	174795	4.81%	1.218%
99	13.844	3883	3889	3900	rVB5	6043	10218	0.28%	0.071%
100	15.796	4489	4496	4507	rVB2	27627	39850	1.10%	0.278%

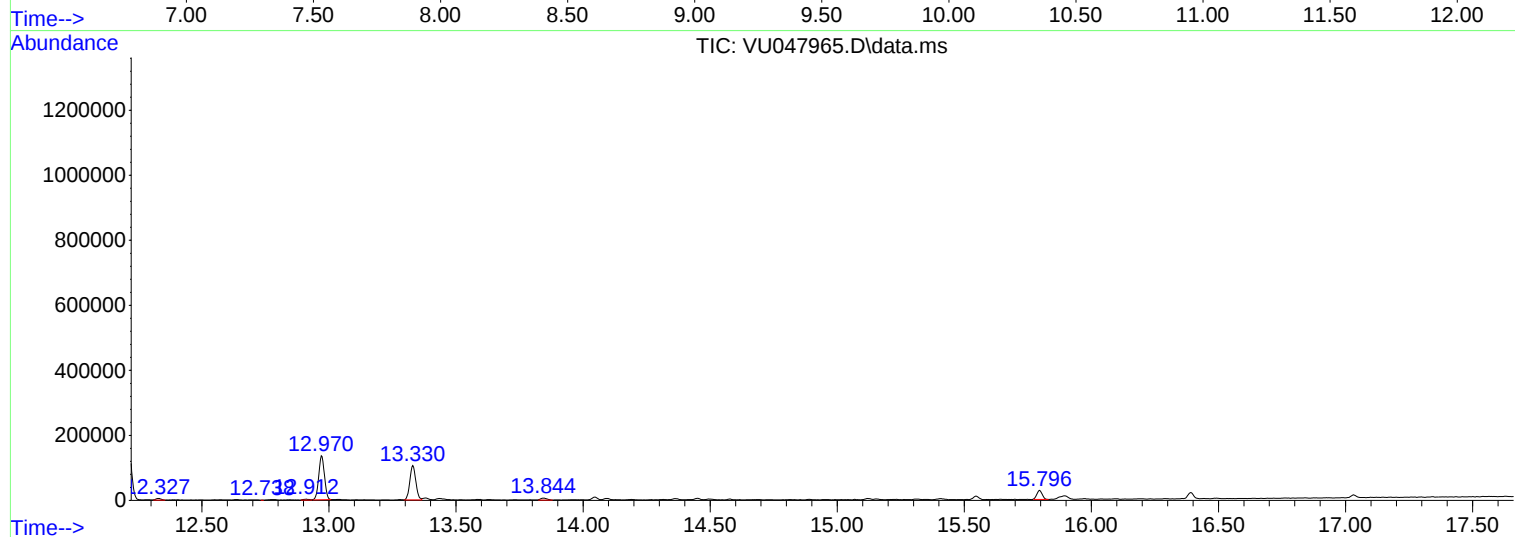
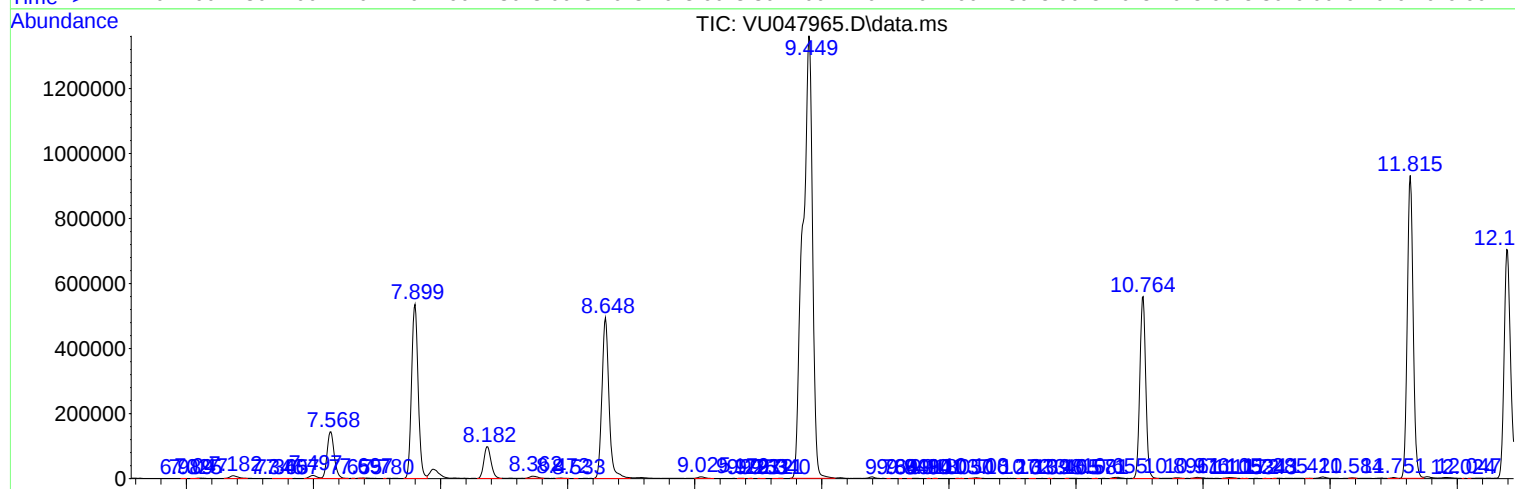
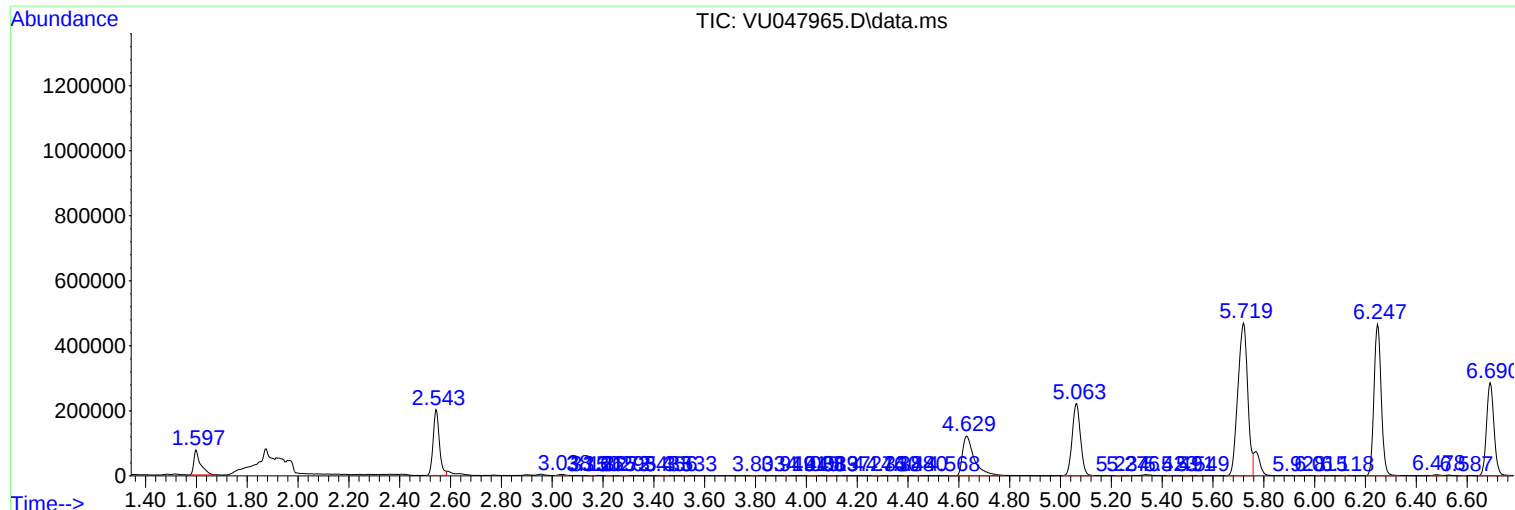
Sum of corrected areas: 14351944

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
Data File : VU047965.D
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Operator : SY/MD
Sample : N2293-07ME
Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 26 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\VU041222\
Data File : VU047965.D
Acq On : 12 Apr 2022 18:50
Operator : SY/MD
Sample : N2293-07ME
Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN7ME

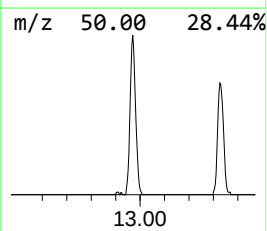
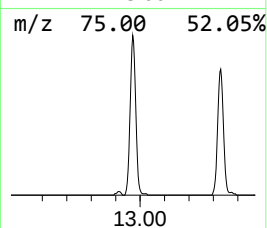
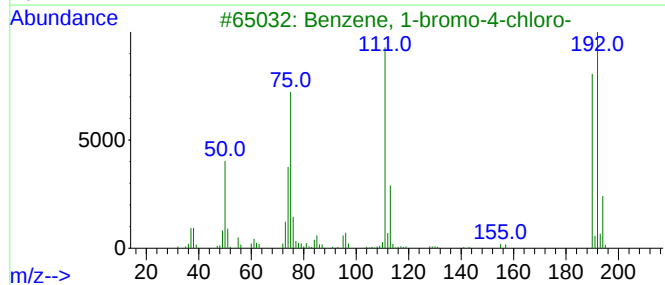
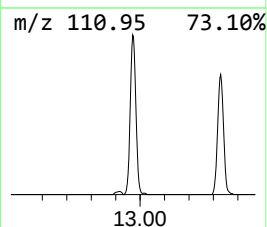
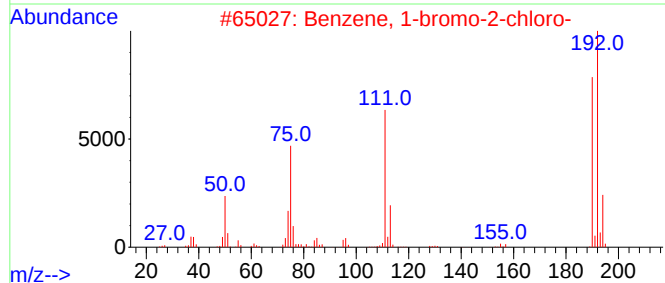
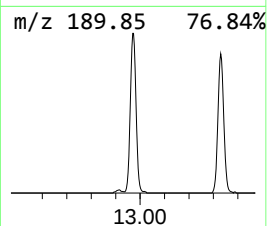
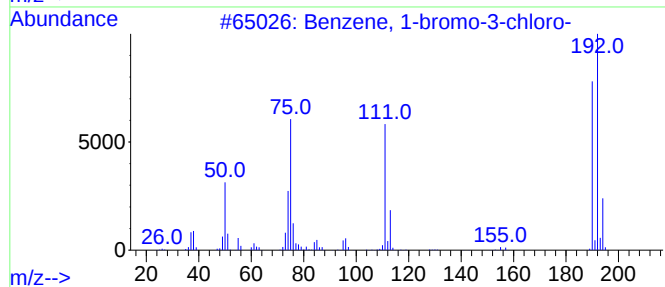
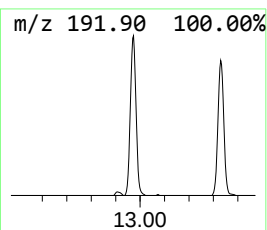
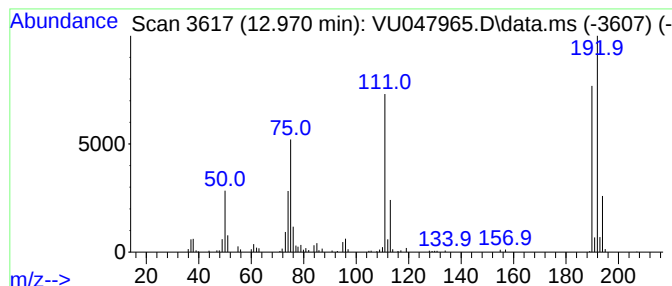
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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.
12.970	7.11 ug/L	211372	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	98
5			4-Chlorophenylselenol	192	C6H5ClSe	016645-10-6	97



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Operator : SY/MD
Sample : N2293-07ME
Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN7ME

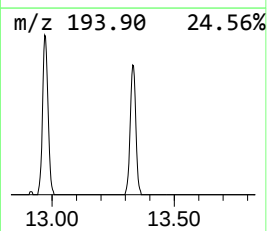
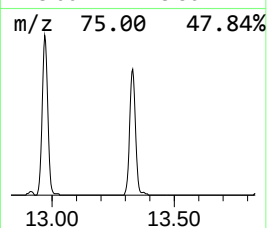
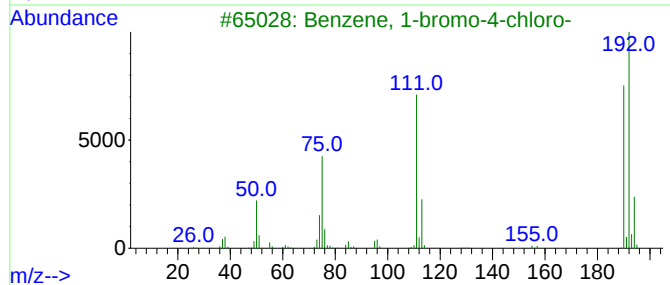
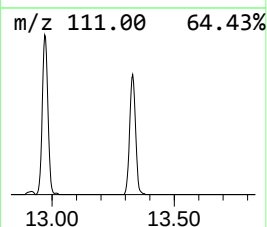
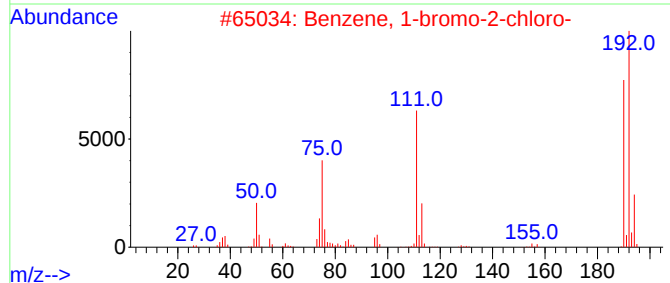
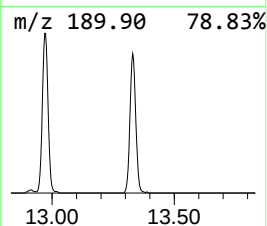
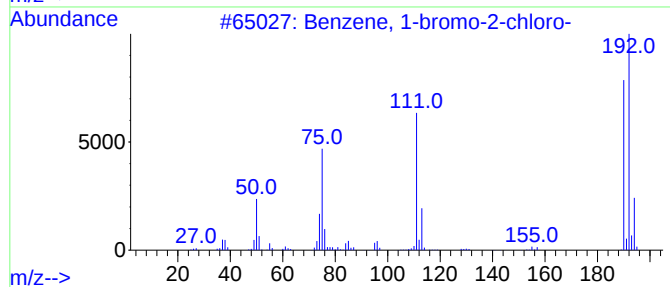
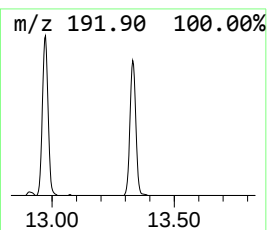
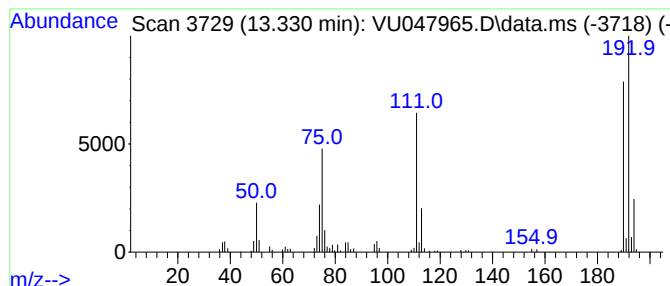
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.330	5.88 ug/L	174795	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-4-chloro-	190	C6H4BrCl	000106-39-8	98
4			Benzene, 1-bromo-4-chloro-	190	C6H4BrCl	000106-39-8	98
5			Benzene, 1-bromo-3-chloro-	190	C6H4BrCl	000108-37-2	97



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Misc : 6.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 26 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...	12.970	7.1	ug/L	211372	3	11.816	1485920	50.0
Benzene, 1-brom...	13.330	5.9	ug/L	174795	3	11.816	1485920	50.0