

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
 Data File : VU047938.D
 Acq On : 12 Apr 2022 04:00
 Operator : SY/MD
 Sample : N2293-02ME
 Misc : 7.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNN2ME

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: VU047938.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	113	rVB	70252	160253	0.20%	0.171%
2	1.800	122	143	144	rBV8	24804	55550	0.07%	0.059%
3	1.855	154	160	166	rBV	149082	186560	0.23%	0.199%
4	2.485	349	356	361	rBV4	3968	5510	0.01%	0.006%
5	2.539	361	373	386	rBV	199726	341521	0.42%	0.365%
6	2.761	436	442	450	rBV2	1574	2396	0.00%	0.003%
7	2.929	491	494	495	rBV2	575	345	0.00%	0.000%
8	2.964	496	505	517	rVV4	3722	8566	0.01%	0.009%
9	3.038	518	528	547	rVB5	4308	9151	0.01%	0.010%
10	3.215	578	583	591	rVB4	1918	2888	0.00%	0.003%
11	3.305	605	611	615	rVB2	383	431	0.00%	0.000%
12	3.527	675	680	683	rBV2	387	415	0.00%	0.000%
13	3.851	776	781	782	rVV3	900	854	0.00%	0.001%
14	3.864	782	785	791	rVV5	1066	1194	0.00%	0.001%
15	4.392	941	949	955	rBV3	542	919	0.00%	0.001%
16	4.646	1011	1028	1077	rBV	102911	399521	0.49%	0.427%
17	5.064	1139	1158	1188	rVB	206816	481045	0.59%	0.514%
18	5.340	1237	1244	1246	rBV2	623	846	0.00%	0.001%
19	5.719	1341	1362	1371	rBV2	477316	1240688	1.51%	1.325%
20	5.977	1439	1442	1445	rBV4	929	720	0.00%	0.001%
21	6.031	1455	1459	1461	rBV3	396	322	0.00%	0.000%
22	6.086	1468	1476	1479	rBV3	529	650	0.00%	0.001%
23	6.247	1511	1526	1551	rVV	499188	992419	1.21%	1.060%
24	6.478	1586	1598	1606	rBV2	18527	38024	0.05%	0.041%
25	6.539	1608	1617	1632	rVB	51486	102341	0.12%	0.109%
26	6.690	1649	1664	1687	rBV	266393	557035	0.68%	0.595%
27	6.941	1737	1742	1746	rVB2	365	315	0.00%	0.000%
28	6.999	1754	1760	1765	rBV3	548	615	0.00%	0.001%
29	7.044	1771	1774	1775	rBV3	519	318	0.00%	0.000%
30	7.192	1808	1820	1837	rBV3	7175	18426	0.02%	0.020%
31	7.497	1905	1915	1926	rBV4	18416	41074	0.05%	0.044%
32	7.568	1926	1937	1959	rVB	130001	261122	0.32%	0.279%
33	7.694	1967	1976	1979	rBV4	1234	1817	0.00%	0.002%
34	7.899	2026	2040	2054	rBV	531004	984375	1.20%	1.052%
35	7.977	2054	2064	2095	rVB3	70848	202122	0.25%	0.216%
36	8.121	2105	2109	2110	rBV3	726	421	0.00%	0.000%

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Integration Parameters: LSCINT.P

Integrator: RTE

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

37	8.182	2116	2128	2151	rBV2	80113	177781	0.22%	0.190%
38	8.298	2154	2164	2174	rBV	12458	23233	0.03%	0.025%
39	8.472	2214	2218	2224	rVV3	496	540	0.00%	0.001%
40	8.581	2238	2252	2264	rBV	311460	659659	0.81%	0.705%
41	8.658	2265	2276	2312	rVB	420241	842342	1.03%	0.900%
42	8.922	2350	2358	2366	rBV4	4056	6360	0.01%	0.007%
43	9.118	2414	2419	2424	rVB3	652	671	0.00%	0.001%
44	9.160	2424	2432	2433	rBV4	911	706	0.00%	0.001%
45	9.292	2468	2473	2474	rBV	456	372	0.00%	0.000%
46	9.333	2482	2486	2489	rBV2	590	487	0.00%	0.001%
47	9.459	2499	2525	2569	rBV2	42320542	81902774	100.00%	87.498%
48	9.951	2667	2678	2688	rBV4	11767	21239	0.03%	0.023%
49	10.025	2693	2701	2705	rBV5	1023	1467	0.00%	0.002%
50	10.108	2718	2727	2736	rVB9	1831	3857	0.00%	0.004%
51	10.144	2736	2738	2743	rBV4	458	362	0.00%	0.000%
52	10.211	2756	2759	2761	rBV2	717	527	0.00%	0.001%
53	10.250	2764	2771	2775	rVV6	1675	2046	0.00%	0.002%
54	10.356	2800	2804	2807	rBV5	689	597	0.00%	0.001%
55	10.394	2810	2816	2822	rVB7	1645	2498	0.00%	0.003%
56	10.475	2836	2841	2842	rBV3	558	455	0.00%	0.000%
57	10.558	2863	2867	2871	rVB3	545	422	0.00%	0.000%
58	10.623	2884	2887	2892	rVB2	858	765	0.00%	0.001%
59	10.658	2892	2898	2899	rBV4	1840	1631	0.00%	0.002%
60	10.764	2918	2931	2958	rBV	497107	856947	1.05%	0.915%
61	10.996	3000	3003	3005	rBV3	916	621	0.00%	0.001%
62	11.095	3029	3034	3035	rBV4	1172	905	0.00%	0.001%
63	11.115	3035	3040	3041	rBV2	1043	876	0.00%	0.001%
64	11.189	3061	3063	3066	rBV4	490	353	0.00%	0.000%
65	11.295	3092	3096	3098	rBV	798	600	0.00%	0.001%
66	11.375	3118	3121	3123	rBV3	610	451	0.00%	0.000%
67	11.417	3129	3134	3141	rVB6	2062	2499	0.00%	0.003%
68	11.462	3141	3148	3149	rBV5	2587	2374	0.00%	0.003%
69	11.552	3170	3176	3179	rBV3	345	390	0.00%	0.000%
70	11.578	3179	3184	3191	rBV5	850	1148	0.00%	0.001%
71	11.693	3215	3220	3224	rBV3	1411	1611	0.00%	0.002%
72	11.819	3245	3259	3276	rBV	999485	1600402	1.95%	1.710%
73	11.935	3292	3295	3296	rBV2	752	529	0.00%	0.001%
74	12.079	3335	3340	3344	rBV5	617	697	0.00%	0.001%
75	12.198	3363	3377	3396	rBV	673569	1101535	1.34%	1.177%
76	12.330	3409	3418	3427	rBV9	4304	7070	0.01%	0.008%

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 ClientSampleId :
 ETNN2ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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Peak Location: TOP

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Peak separation: 5

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

77	12.664	3518	3522	3530	rVB4	1168	1400	0.00%	0.001%
78	12.742	3543	3546	3549	rVB3	436	345	0.00%	0.000%
79	12.767	3549	3554	3564	rBV9	1312	1646	0.00%	0.002%
80	12.825	3569	3572	3575	rBV3	701	455	0.00%	0.000%
81	12.973	3606	3618	3633	rVB	98991	161115	0.20%	0.172%
82	13.127	3664	3666	3668	rBV2	586	319	0.00%	0.000%
83	13.140	3668	3670	3674	rVB4	794	608	0.00%	0.001%
84	13.201	3685	3689	3692	rBV4	657	491	0.00%	0.001%
85	13.333	3721	3730	3738	rBV3	14638	23332	0.03%	0.025%
86	13.378	3739	3744	3753	rVB4	5716	7789	0.01%	0.008%
87	13.430	3755	3760	3767	rBV4	4165	5297	0.01%	0.006%
88	13.587	3801	3809	3817	rBV6	3914	6096	0.01%	0.007%
89	13.774	3864	3867	3874	rVB4	929	797	0.00%	0.001%
90	13.845	3883	3889	3898	rVB9	1533	2730	0.00%	0.003%
91	13.967	3921	3927	3929	rBV5	988	958	0.00%	0.001%
92	14.095	3962	3967	3971	rBV4	2995	2918	0.00%	0.003%
93	14.192	3992	3997	4006	rVB7	3330	4830	0.01%	0.005%
94	14.272	4019	4022	4026	rVB5	952	632	0.00%	0.001%
95	14.452	4070	4078	4086	rBV7	4731	7138	0.01%	0.008%
96	14.854	4201	4203	4206	rBV2	856	439	0.00%	0.000%
97	15.214	4307	4315	4316	rBV6	3614	4076	0.00%	0.004%
98	15.545	4411	4418	4428	rVB8	13698	21869	0.03%	0.023%
99	15.700	4464	4466	4468	rBV3	1300	645	0.00%	0.001%
100	16.391	4675	4681	4691	rVB10	12175	19182	0.02%	0.020%

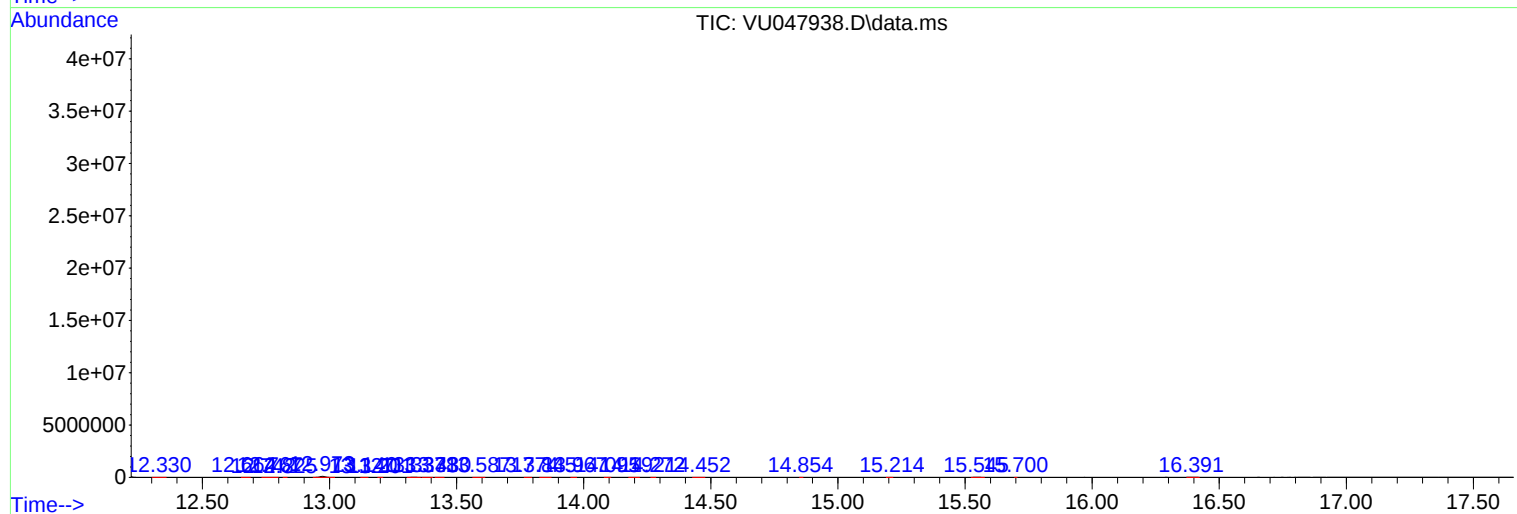
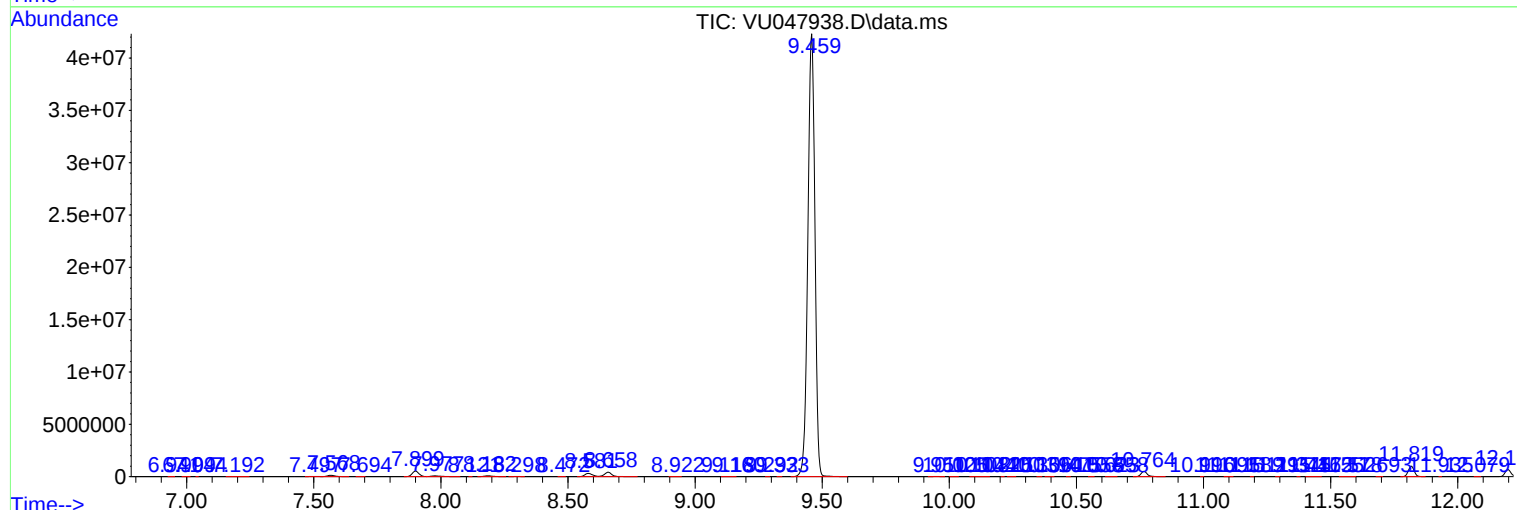
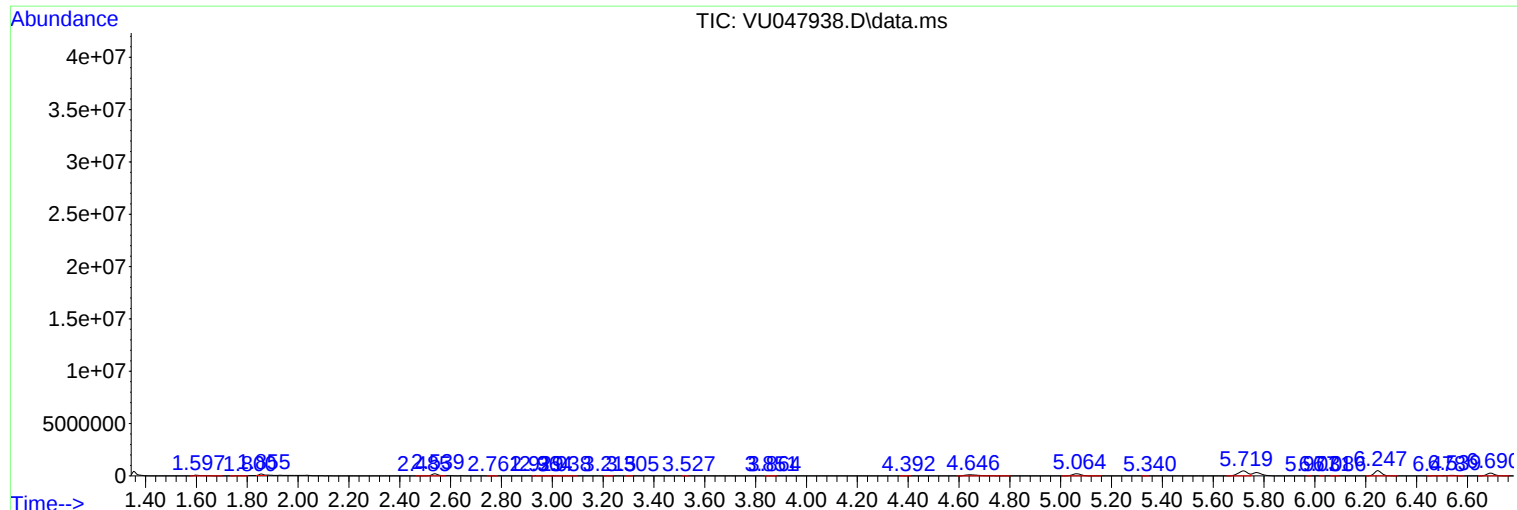
Sum of corrected areas: 93605675

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
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ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN2ME

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



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Instrument :
MSVOA_U
ClientSampleId :
ETNN2ME

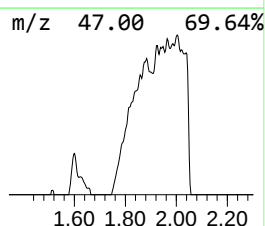
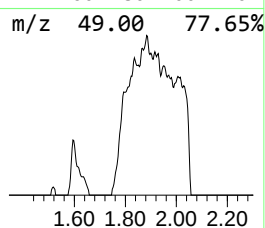
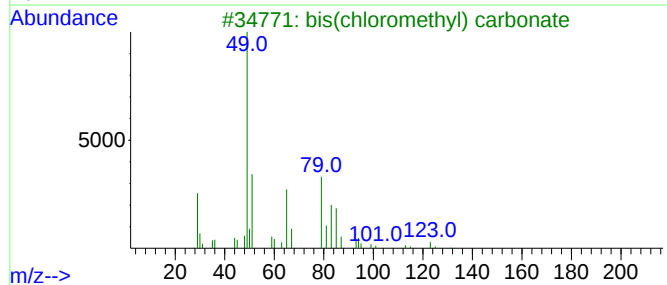
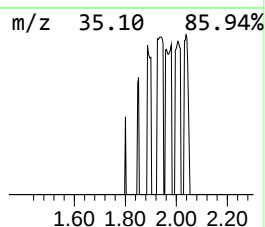
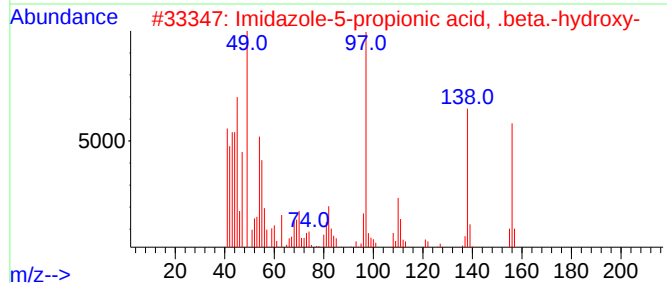
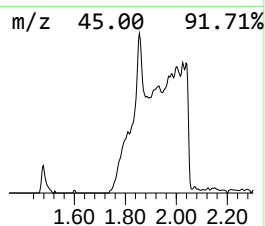
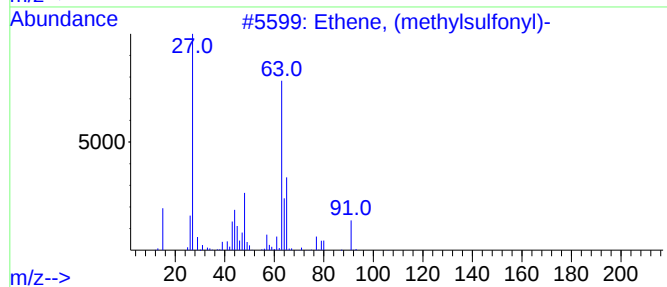
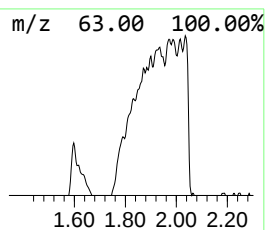
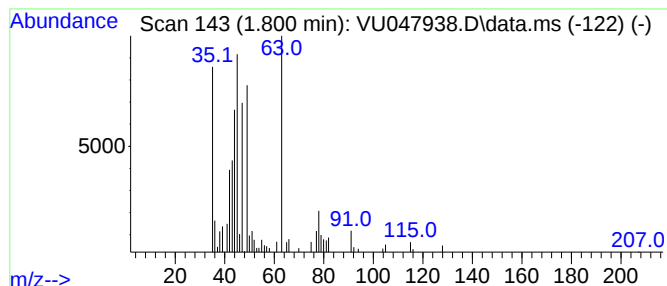
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.800	2.80 ug/L	55550	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethene, (methylsulfonyl)-	106	C3H6O2S	003680-02-2	9
2			Imidazole-5-propionic acid, .bet...	156	C6H8N2O3	1000129-47-8	9
3			bis(chloromethyl) carbonate	158	C3H4Cl2O3	1000404-37-0	9
4			Methane, chloromethoxy-	80	C2H5ClO	000107-30-2	7
5			Ethanol, 2-(2-chloroethoxy)-	124	C4H9ClO2	000628-89-7	4



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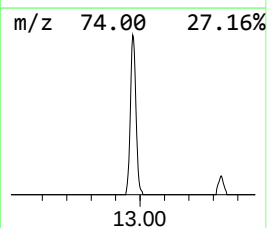
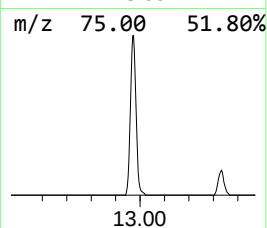
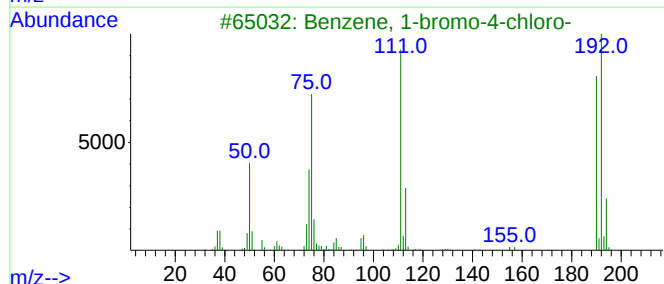
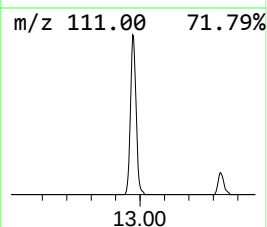
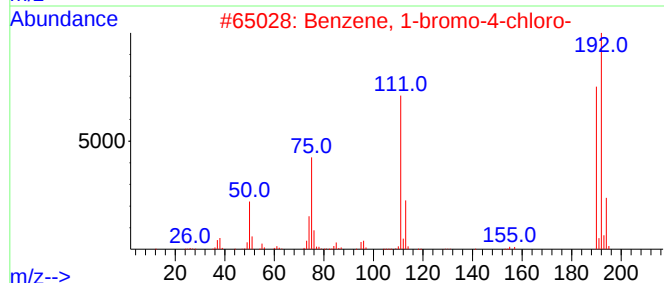
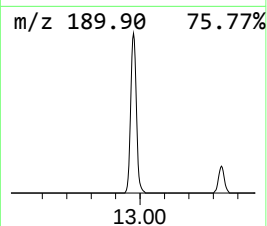
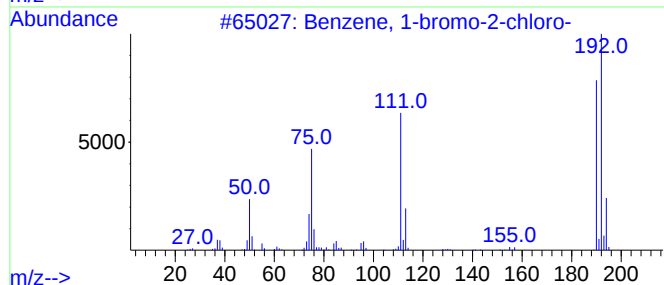
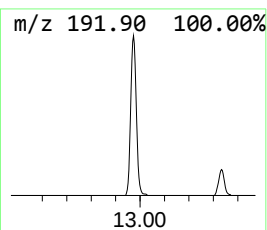
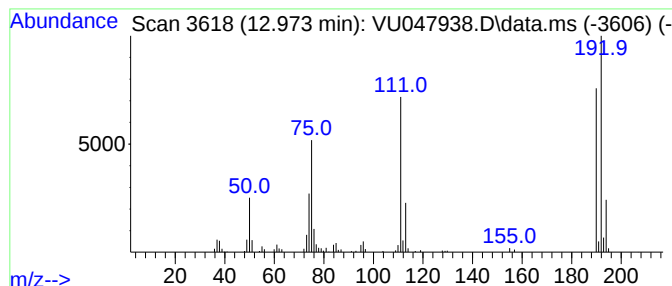
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.973	5.03 ug/L	161115	1,4-Dichlorobenzene-d4	11.819

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	98
3			Benzene, 1-bromo-4-chloro-	190	C6H4BrCl	000106-39-8	98
4			4-Chlorophenylselenol	192	C6H5ClSe	016645-10-6	97
5			Benzene, 1-bromo-2-chloro-	190	C6H4BrCl	000694-80-4	97



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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
unknown-01	1.800	2.8	ug/L	55550	1	6.247	992419	50.0
Benzene, 1-brom...	12.973	5.0	ug/L	161115	3	11.819	1600400	50.0