

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
 Data File : VU047995.D
 Acq On : 13 Apr 2022 12:01
 Operator : SY/MD
 Sample : N2345-07DL 100X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0J85DL

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: VU047995.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	74	81	98	rBV	163280	188844	6.69%	1.398%
2	1.916	171	179	201	rVB	128255	179136	6.35%	1.326%
3	2.572	370	383	398	rBV	274443	448452	15.90%	3.321%
4	2.790	448	451	453	rBV2	455	255	0.01%	0.002%
5	3.044	523	530	542	rVB4	2076	3849	0.14%	0.029%
6	3.105	546	549	556	rVB2	479	511	0.02%	0.004%
7	3.137	556	559	562	rBV2	420	318	0.01%	0.002%
8	3.163	563	567	569	rBV	298	238	0.01%	0.002%
9	3.179	569	572	575	rVV3	361	222	0.01%	0.002%
10	3.369	629	631	637	rVB3	370	319	0.01%	0.002%
11	3.404	637	642	645	rVB2	302	307	0.01%	0.002%
12	3.424	645	648	651	rBV2	506	357	0.01%	0.003%
13	3.491	666	669	673	rVB4	345	275	0.01%	0.002%
14	3.572	688	694	698	rBV2	437	510	0.02%	0.004%
15	3.851	777	781	789	rVB3	382	546	0.02%	0.004%
16	3.887	789	792	795	rVB2	405	253	0.01%	0.002%
17	3.916	795	801	803	rBV2	414	366	0.01%	0.003%
18	4.086	850	854	858	rBV2	264	277	0.01%	0.002%
19	4.105	858	860	865	rVB	367	248	0.01%	0.002%
20	4.150	868	874	878	rBV3	386	459	0.02%	0.003%
21	4.298	914	920	923	rBV3	333	369	0.01%	0.003%
22	4.620	1007	1020	1048	rBV	130168	313354	11.11%	2.320%
23	5.067	1140	1159	1186	rBV	230704	505016	17.90%	3.740%
24	5.282	1223	1226	1233	rVV3	669	739	0.03%	0.005%
25	5.420	1264	1269	1272	rVB3	248	223	0.01%	0.002%
26	5.481	1286	1288	1294	rVB2	301	239	0.01%	0.002%
27	5.729	1341	1365	1370	rBV2	480562	1212699	42.99%	8.980%
28	5.777	1372	1380	1404	rVB	1425443	2821104	100.00%	20.890%
29	6.034	1457	1460	1466	rVB4	621	732	0.03%	0.005%
30	6.063	1466	1469	1473	rBV5	686	507	0.02%	0.004%
31	6.121	1484	1487	1489	rBV2	455	232	0.01%	0.002%
32	6.163	1498	1500	1504	rBV2	330	224	0.01%	0.002%
33	6.250	1512	1527	1553	rBV	408978	780644	27.67%	5.781%
34	6.427	1578	1582	1587	rBV3	151	227	0.01%	0.002%
35	6.526	1607	1613	1616	rBV4	1261	1260	0.04%	0.009%
36	6.694	1649	1665	1693	rBV	294523	577259	20.46%	4.275%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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

37	6.813	1698	1702	1708	rVV5	1297	1578	0.06%	0.012%
38	6.838	1708	1710	1715	rVV2	422	384	0.01%	0.003%
39	6.880	1719	1723	1725	rBV2	322	232	0.01%	0.002%
40	6.896	1725	1728	1733	rVV3	413	373	0.01%	0.003%
41	6.973	1749	1752	1757	rVB2	282	309	0.01%	0.002%
42	7.015	1762	1765	1769	rBV3	239	250	0.01%	0.002%
43	7.189	1809	1819	1828	rBV3	3435	6443	0.23%	0.048%
44	7.304	1853	1855	1864	rVB2	489	583	0.02%	0.004%
45	7.568	1924	1937	1959	rBV	153406	270262	9.58%	2.001%
46	7.687	1966	1974	1981	rBV6	2324	3985	0.14%	0.030%
47	7.790	2003	2006	2018	rVB4	934	1245	0.04%	0.009%
48	7.899	2025	2040	2056	rBV	594791	1022099	36.23%	7.569%
49	8.179	2116	2127	2155	rBV	107057	185334	6.57%	1.372%
50	8.632	2255	2268	2301	rBV	377975	716911	25.41%	5.309%
51	8.886	2343	2347	2348	rBV2	335	256	0.01%	0.002%
52	9.047	2393	2397	2401	rBB2	391	374	0.01%	0.003%
53	9.166	2429	2434	2438	rVB4	495	559	0.02%	0.004%
54	9.192	2438	2442	2445	rVB2	327	288	0.01%	0.002%
55	9.221	2445	2451	2454	rBV2	323	409	0.01%	0.003%
56	9.420	2498	2513	2515	rBV	644761	884952	31.37%	6.553%
57	9.693	2589	2598	2609	rVB5	1354	2268	0.08%	0.017%
58	9.767	2618	2621	2623	rBV2	339	236	0.01%	0.002%
59	10.054	2705	2710	2715	rVB3	247	251	0.01%	0.002%
60	10.089	2715	2721	2722	rBV2	314	274	0.01%	0.002%
61	10.674	2895	2903	2910	rVB4	2421	3436	0.12%	0.025%
62	10.758	2916	2929	2953	rBV	434843	703663	24.94%	5.211%
63	10.864	2959	2962	2964	rBV2	452	283	0.01%	0.002%
64	10.886	2967	2969	2973	rVB3	337	276	0.01%	0.002%
65	11.092	3028	3033	3036	rBV3	594	486	0.02%	0.004%
66	11.124	3039	3043	3047	rVB3	445	369	0.01%	0.003%
67	11.465	3137	3149	3160	rVB8	2030	3814	0.14%	0.028%
68	11.574	3179	3183	3186	rBV2	374	253	0.01%	0.002%
69	11.700	3215	3222	3228	rVB3	943	1228	0.04%	0.009%
70	11.748	3230	3237	3245	rVB3	3679	4455	0.16%	0.033%
71	11.812	3245	3257	3280	rBV2	655512	1210094	42.89%	8.961%
72	11.951	3296	3300	3305	rBV6	1475	1753	0.06%	0.013%
73	11.976	3305	3308	3312	rVB4	1546	1292	0.05%	0.010%
74	12.018	3319	3321	3326	rVB3	375	328	0.01%	0.002%
75	12.044	3326	3329	3332	rBV2	315	257	0.01%	0.002%
76	12.099	3344	3346	3350	rBV3	394	286	0.01%	0.002%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M

Title : VOC Analysis

77	12.195	3360	3376	3398	rBV	605129	1028932	36.47%	7.619%
78	12.462	3456	3459	3461	rBV3	337	235	0.01%	0.002%
79	12.642	3511	3515	3522	rBV3	804	818	0.03%	0.006%
80	12.973	3606	3618	3630	rBV2	16468	26364	0.93%	0.195%
81	13.063	3643	3646	3650	rBV3	272	233	0.01%	0.002%
82	13.131	3665	3667	3671	rVB3	448	289	0.01%	0.002%
83	13.156	3671	3675	3677	rBV3	379	309	0.01%	0.002%
84	13.333	3719	3730	3738	rBV2	14019	22407	0.79%	0.166%
85	13.471	3769	3773	3774	rBV	404	293	0.01%	0.002%
86	13.716	3841	3849	3855	rBV3	2332	2710	0.10%	0.020%
87	13.848	3881	3890	3895	rBV5	3141	4337	0.15%	0.032%
88	14.092	3958	3966	3979	rBV2	2750	5199	0.18%	0.038%
89	14.333	4034	4041	4046	rVV4	1661	2345	0.08%	0.017%
90	14.404	4061	4063	4067	rBV	581	418	0.01%	0.003%
91	14.532	4101	4103	4112	rVB4	614	577	0.02%	0.004%
92	14.594	4113	4122	4135	rBV2	14259	21029	0.75%	0.156%
93	14.693	4151	4153	4156	rVB2	596	292	0.01%	0.002%
94	14.886	4211	4213	4216	rBV3	548	348	0.01%	0.003%
95	14.944	4229	4231	4238	rVB4	537	532	0.02%	0.004%
96	14.976	4238	4241	4245	rBV3	464	429	0.02%	0.003%
97	15.545	4409	4418	4430	rVB4	20268	29908	1.06%	0.221%
98	15.893	4510	4526	4542	rBV3	81387	204275	7.24%	1.513%
99	16.118	4592	4596	4604	rVB7	4944	6703	0.24%	0.050%
100	16.388	4674	4680	4692	rVB2	45893	72795	2.58%	0.539%

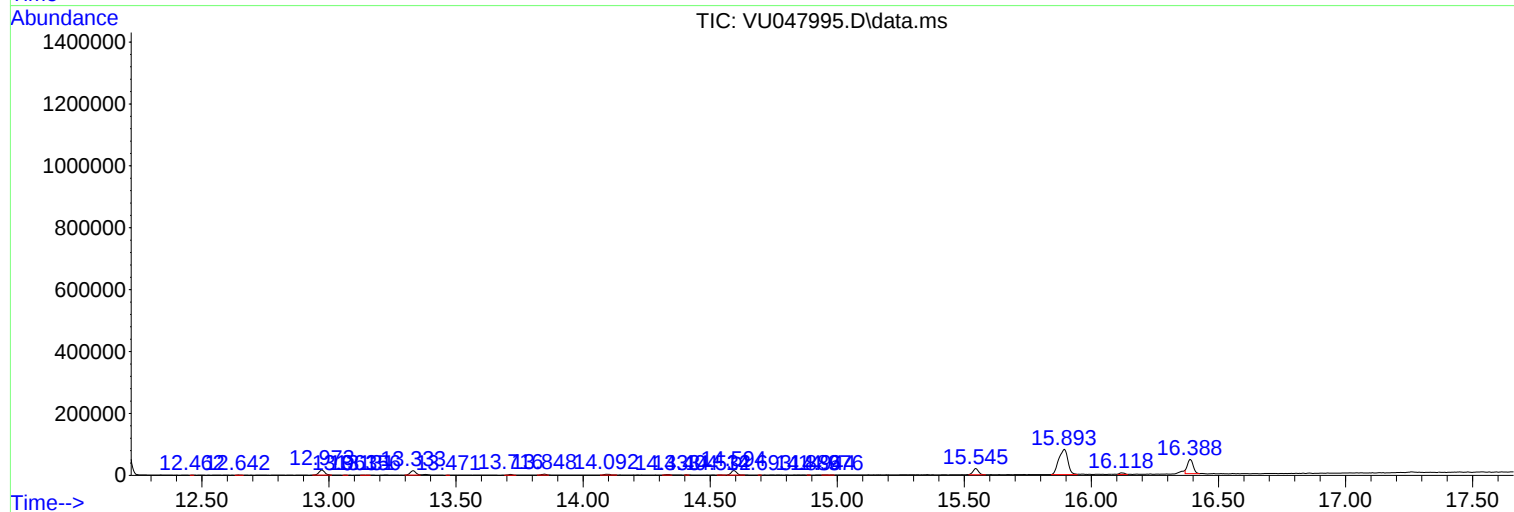
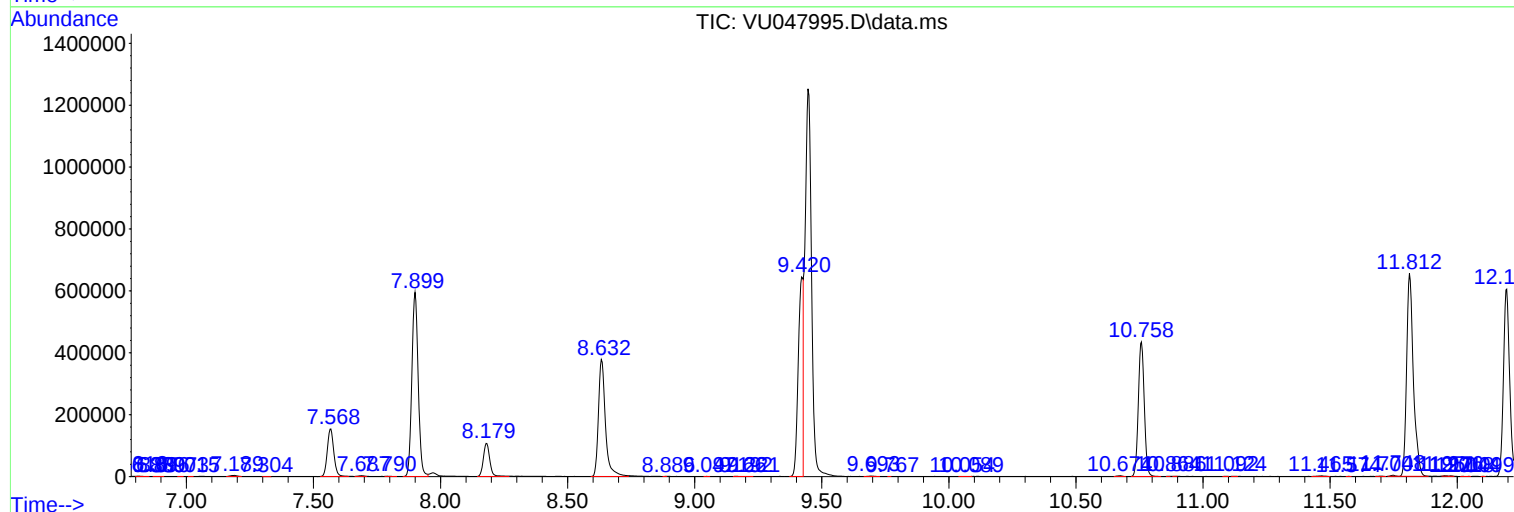
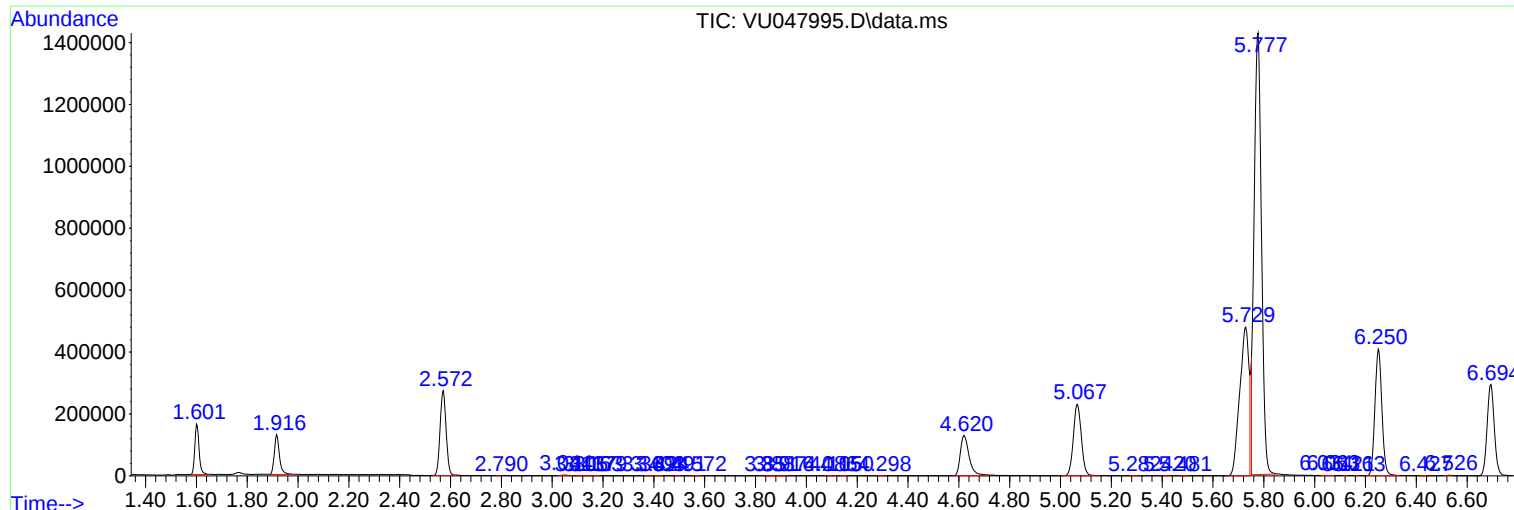
Sum of corrected areas: 13504475

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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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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



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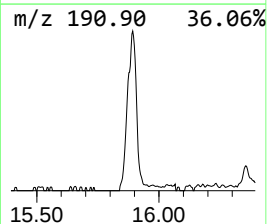
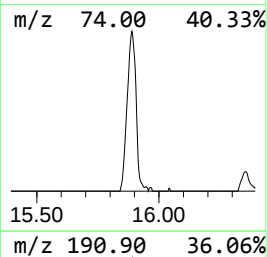
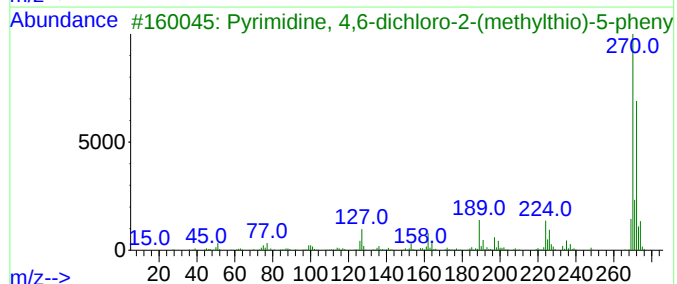
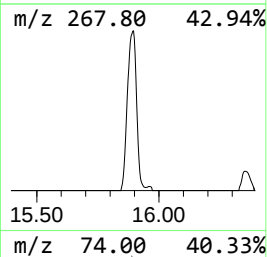
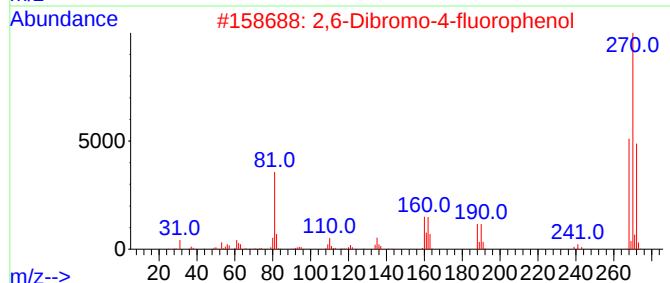
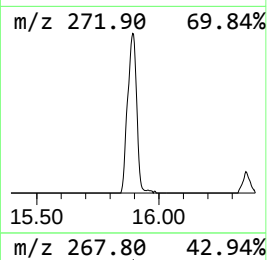
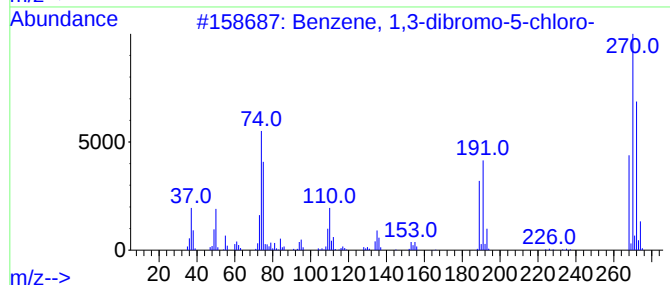
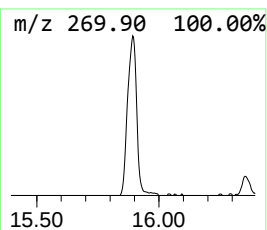
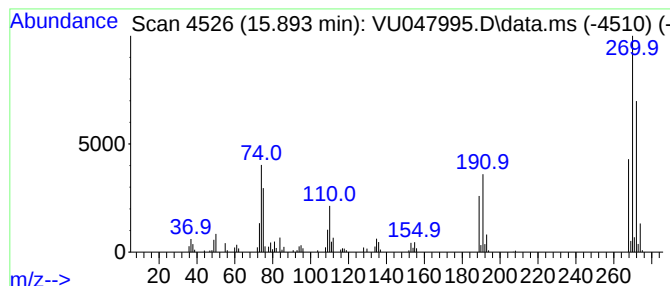
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Benzene, 1,3-dibromo-5-chloro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.893	8.44 ug/L	204275	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-dibromo-5-chloro-	268	C6H3Br2Cl	014862-52-3	94
2			2,6-Dibromo-4-fluorophenol	268	C6H3Br2FO	000344-20-7	49
3			Pyrimidine, 4,6-dichloro-2-(meth...	270	C11H8Cl2N2S	064415-11-8	32
4			3-Bromo-7-methylbenzo(b)thiophen...	270	C10H7BrO2S	001637-40-7	25
5			4,6-Dibromo-5-hydroxypyridazine ...	268	C4H2Br2N2O2	019971-61-0	25



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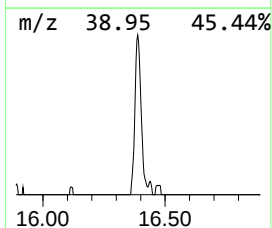
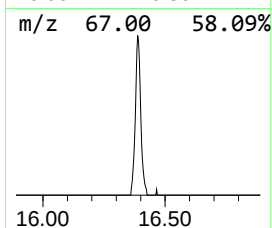
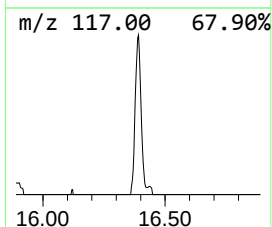
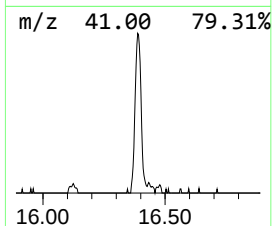
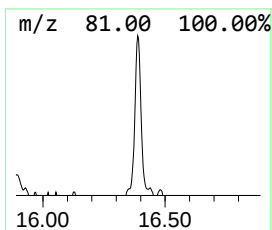
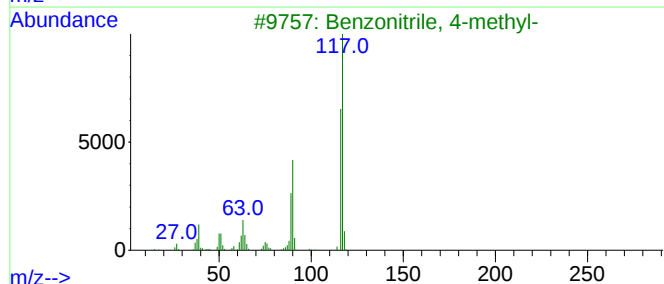
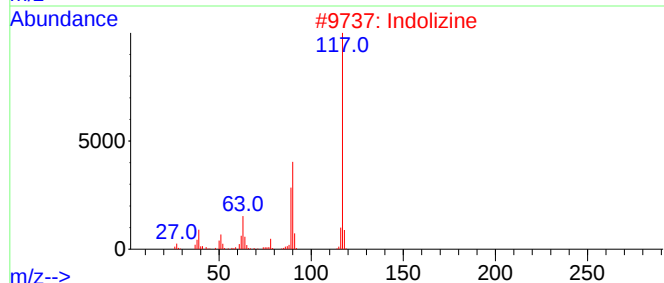
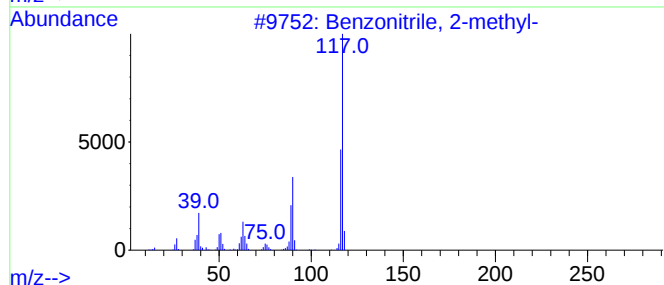
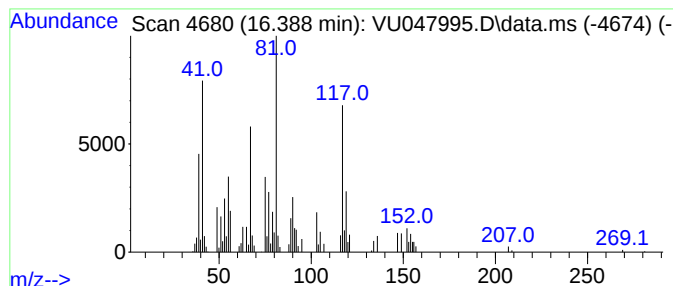
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.388	3.01 ug/L	72795	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzonitrile, 2-methyl-	117	C8H7N	000529-19-1	15
2			Indolizine	117	C8H7N	000274-40-8	15
3			Benzonitrile, 4-methyl-	117	C8H7N	000104-85-8	15
4			Benzonitrile, 4-methyl-	117	C8H7N	000104-85-8	15
5			Benzonitrile, 4-methyl-	117	C8H7N	000104-85-8	15



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, 1,3-di...	15.893	8.4	ug/L	204275	3	11.812	1210090	50.0
unknown-01	16.388	3.0	ug/L	72795	3	11.812	1210090	50.0