

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
 Data File : VU048002.D
 Acq On : 13 Apr 2022 14:39
 Operator : SY/MD
 Sample : N2345-09
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0J87

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: VU048002.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	73	81	97	rBV	156422	188207	14.46%	1.690%
2	1.916	171	179	198	rVB	133836	184843	14.21%	1.660%
3	2.568	370	382	399	rBV	263335	443251	34.06%	3.981%
4	2.719	426	429	434	rVB3	468	397	0.03%	0.004%
5	2.864	471	474	480	rBV3	411	468	0.04%	0.004%
6	3.018	516	522	524	rBV3	292	358	0.03%	0.003%
7	3.044	524	530	531	rBV3	578	546	0.04%	0.005%
8	3.182	566	573	576	rBV3	960	1245	0.10%	0.011%
9	3.289	603	606	608	rBV3	354	276	0.02%	0.002%
10	3.356	623	627	628	rBV2	505	339	0.03%	0.003%
11	3.375	630	633	639	rVB3	766	660	0.05%	0.006%
12	3.459	653	659	663	rVB4	397	470	0.04%	0.004%
13	3.507	672	674	677	rVV3	421	251	0.02%	0.002%
14	3.533	679	682	687	rVB3	376	251	0.02%	0.002%
15	3.732	741	744	745	rBV	308	206	0.02%	0.002%
16	3.819	765	771	773	rBV2	489	394	0.03%	0.004%
17	3.871	785	787	791	rVB2	375	220	0.02%	0.002%
18	4.031	834	837	840	rVB	364	281	0.02%	0.003%
19	4.051	840	843	848	rBV2	369	374	0.03%	0.003%
20	4.166	871	879	885	rBV	367	321	0.02%	0.003%
21	4.350	931	936	940	rVB	332	368	0.03%	0.003%
22	4.436	957	963	964	rBV	237	220	0.02%	0.002%
23	4.498	978	982	987	rBV2	292	233	0.02%	0.002%
24	4.565	999	1003	1005	rBV2	274	207	0.02%	0.002%
25	4.633	1010	1024	1057	rBV	131828	351206	26.99%	3.154%
26	4.890	1099	1104	1106	rBV2	267	285	0.02%	0.003%
27	5.067	1141	1159	1185	rBV	231703	508897	39.11%	4.571%
28	5.292	1224	1229	1234	rBV4	900	1029	0.08%	0.009%
29	5.385	1254	1258	1263	rBV4	291	285	0.02%	0.003%
30	5.726	1343	1364	1398	rBV2	471770	1301242	100.00%	11.687%
31	6.041	1459	1462	1467	rVB3	319	229	0.02%	0.002%
32	6.250	1512	1527	1548	rBV	410841	783967	60.25%	7.041%
33	6.526	1607	1613	1616	rBV4	1207	1381	0.11%	0.012%
34	6.694	1648	1665	1686	rBV	293042	581236	44.67%	5.221%
35	6.800	1696	1698	1700	rBV3	409	243	0.02%	0.002%
36	7.038	1769	1772	1775	rBV	314	255	0.02%	0.002%

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 Title : VOC Analysis

37	7.182	1808	1817	1826	rBV4	3657	6487	0.50%	0.058%
38	7.237	1832	1834	1841	rVB3	510	413	0.03%	0.004%
39	7.449	1895	1900	1903	rBV3	366	290	0.02%	0.003%
40	7.568	1924	1937	1956	rBV	154001	273829	21.04%	2.459%
41	7.687	1966	1974	1986	rBV4	2285	4463	0.34%	0.040%
42	7.806	2008	2011	2015	rVB2	517	358	0.03%	0.003%
43	7.835	2015	2020	2026	rVB4	393	438	0.03%	0.004%
44	7.899	2026	2040	2057	rBV	594104	1030340	79.18%	9.254%
45	8.182	2114	2128	2143	rBV	107464	185297	14.24%	1.664%
46	8.356	2177	2182	2185	rBV3	1289	1324	0.10%	0.012%
47	8.385	2189	2191	2195	rBV4	337	254	0.02%	0.002%
48	8.475	2208	2219	2231	rVB3	2991	5076	0.39%	0.046%
49	8.636	2255	2269	2301	rBV	438736	791499	60.83%	7.109%
50	9.021	2386	2389	2395	rVB3	424	389	0.03%	0.003%
51	9.050	2396	2398	2404	rVB	423	243	0.02%	0.002%
52	9.166	2428	2434	2440	rVB3	542	618	0.05%	0.006%
53	9.247	2455	2459	2460	rBV	311	243	0.02%	0.002%
54	9.259	2460	2463	2465	rVV2	346	246	0.02%	0.002%
55	9.359	2490	2494	2498	rBV3	597	450	0.03%	0.004%
56	9.417	2498	2512	2547	rBV	614956	1058606	81.35%	9.508%
57	9.571	2555	2560	2565	rBV4	384	435	0.03%	0.004%
58	9.693	2590	2598	2606	rBV4	1138	1711	0.13%	0.015%
59	10.099	2719	2724	2731	rVV4	867	1054	0.08%	0.009%
60	10.214	2756	2760	2764	rBV3	346	345	0.03%	0.003%
61	10.234	2764	2766	2769	rVB	517	238	0.02%	0.002%
62	10.285	2778	2782	2786	rBV2	299	250	0.02%	0.002%
63	10.410	2817	2821	2826	rBV3	361	314	0.02%	0.003%
64	10.545	2858	2863	2864	rBV2	300	275	0.02%	0.002%
65	10.581	2868	2874	2875	rBV	329	283	0.02%	0.003%
66	10.671	2895	2902	2908	rVV5	2151	3031	0.23%	0.027%
67	10.758	2908	2929	2949	rVV	443491	720814	55.39%	6.474%
68	10.893	2958	2971	2983	rVB2	4686	8577	0.66%	0.077%
69	11.028	3009	3013	3018	rBV3	350	388	0.03%	0.003%
70	11.092	3028	3033	3036	rVB3	378	282	0.02%	0.003%
71	11.111	3036	3039	3042	rBV2	486	307	0.02%	0.003%
72	11.237	3076	3078	3083	rBV3	267	252	0.02%	0.002%
73	11.298	3095	3097	3103	rVB2	317	222	0.02%	0.002%
74	11.356	3111	3115	3117	rBV2	325	240	0.02%	0.002%
75	11.459	3140	3147	3159	rBV6	1811	3512	0.27%	0.032%
76	11.693	3216	3220	3221	rBV2	600	379	0.03%	0.003%

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Peak Location: TOP

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77	11.812	3242	3257	3285	rBV	695285	1106178	85.01%	9.935%
78	11.954	3293	3301	3315	rVB9	4935	9240	0.71%	0.083%
79	12.063	3325	3335	3349	rBV3	14814	29548	2.27%	0.265%
80	12.195	3358	3376	3393	rBV	620605	1021952	78.54%	9.179%
81	12.404	3438	3441	3443	rBV2	385	315	0.02%	0.003%
82	12.674	3520	3525	3530	rBV	344	417	0.03%	0.004%
83	12.777	3551	3557	3563	rVB2	1463	1971	0.15%	0.018%
84	12.828	3571	3573	3575	rBV2	414	214	0.02%	0.002%
85	12.970	3605	3617	3628	rVB5	8608	14975	1.15%	0.135%
86	13.070	3644	3648	3651	rBV2	342	288	0.02%	0.003%
87	13.115	3659	3662	3666	rBV3	542	353	0.03%	0.003%
88	13.330	3722	3729	3737	rBV2	6104	8809	0.68%	0.079%
89	13.378	3738	3744	3756	rVB4	7102	10742	0.83%	0.096%
90	13.465	3768	3771	3773	rBV3	499	409	0.03%	0.004%
91	14.063	3954	3957	3959	rBV3	793	572	0.04%	0.005%
92	14.307	4030	4033	4035	rBV	367	245	0.02%	0.002%
93	14.330	4036	4040	4043	rVV3	983	947	0.07%	0.009%
94	14.362	4045	4050	4061	rVB5	3198	4581	0.35%	0.041%
95	14.494	4085	4091	4100	rBV6	2033	2847	0.22%	0.026%
96	15.018	4252	4254	4260	rVB4	623	468	0.04%	0.004%
97	15.545	4407	4418	4433	rBV2	81106	125429	9.64%	1.127%
98	15.893	4515	4526	4540	rVB8	9478	24832	1.91%	0.223%
99	16.388	4670	4680	4692	rBV	163628	268314	20.62%	2.410%
100	17.346	4972	4978	4993	rVB5	24243	41624	3.20%	0.374%

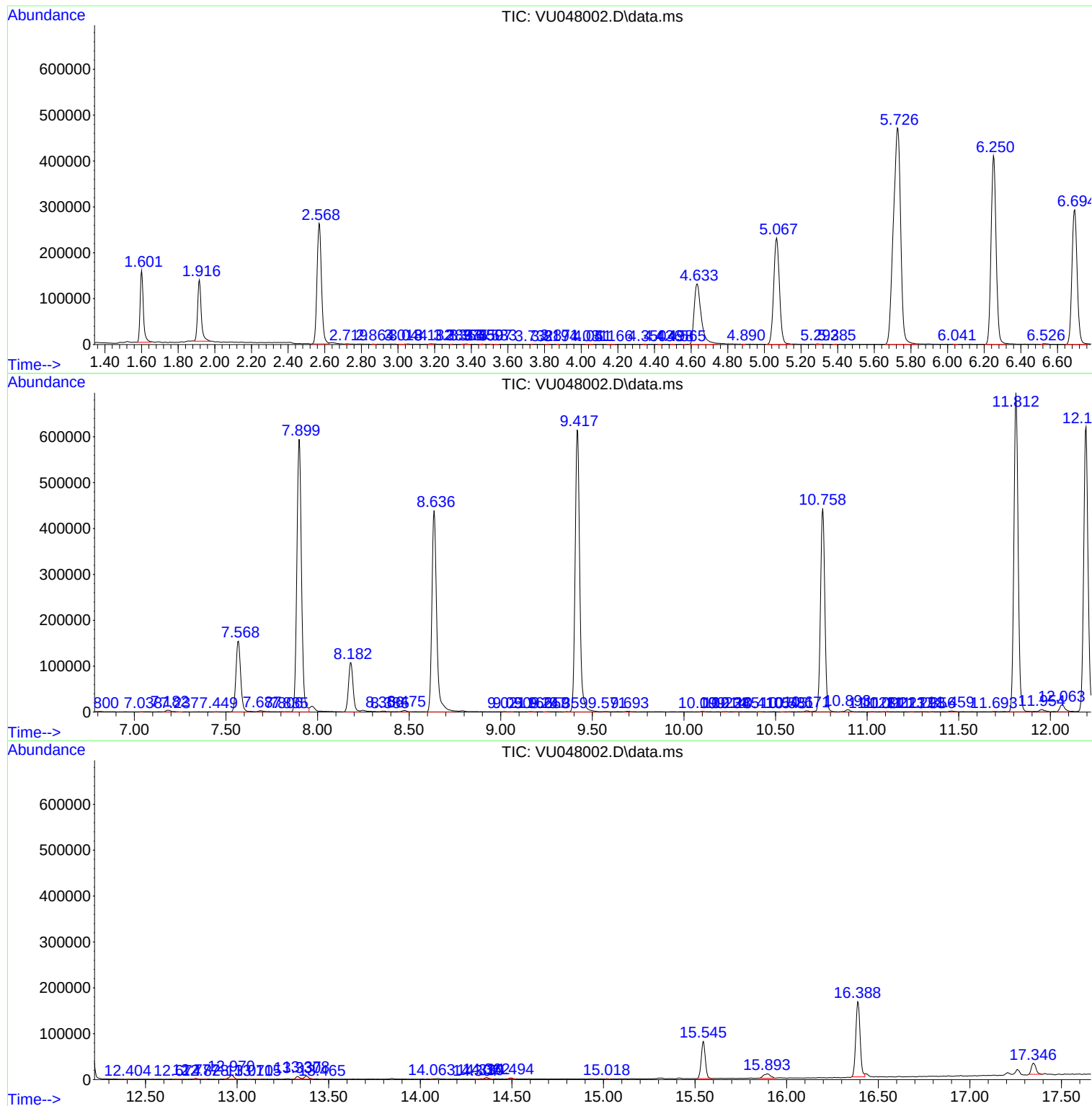
Sum of corrected areas: 11133683

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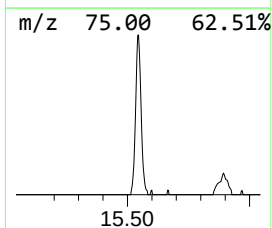
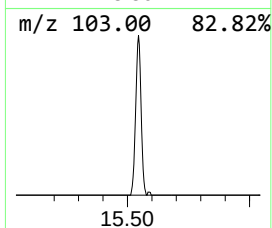
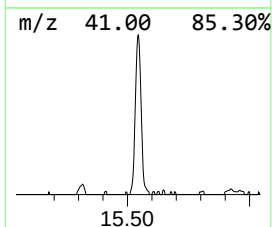
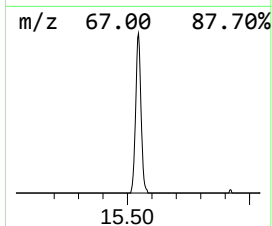
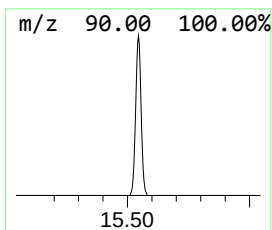
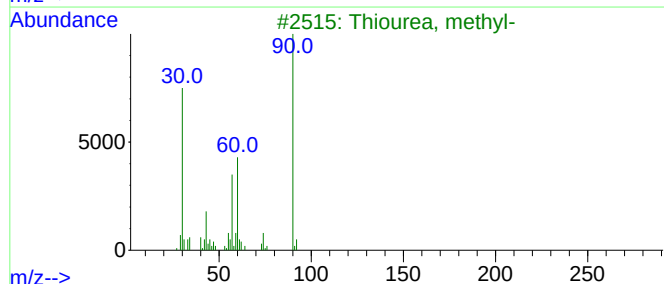
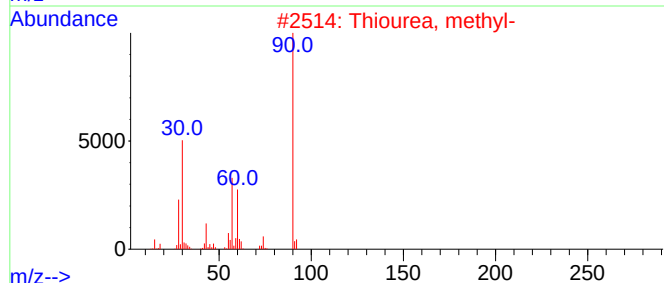
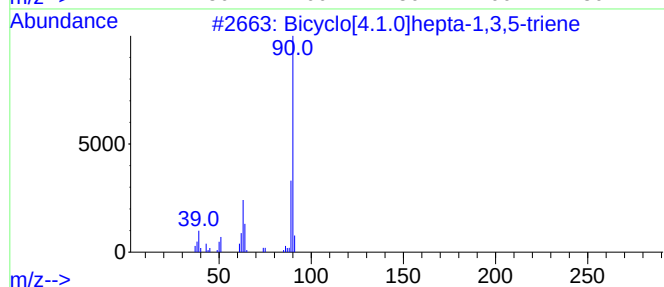
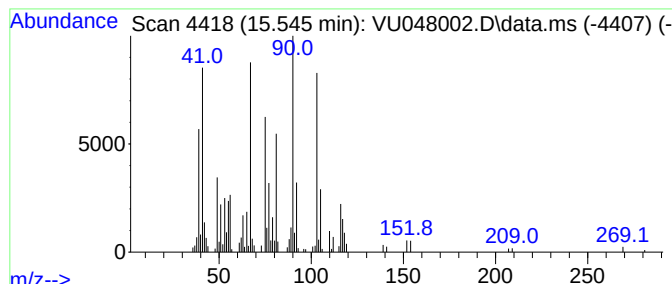
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.545	5.67 ug/L	125429	1,4-Dichlorobenzene-d4	11.812

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			Thiourea, methyl-	90	C2H6N2S	000598-52-7	35
3			Thiourea, methyl-	90	C2H6N2S	000598-52-7	35
4			1,3,5-Trichloro-4-methyl-2-penta...	202	C6H9Cl3O	1000140-03-8	28
5			Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	25



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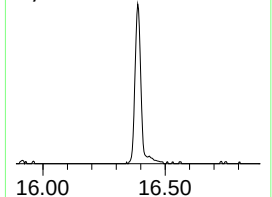
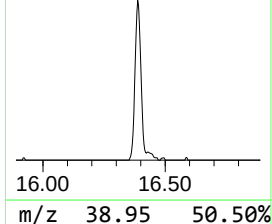
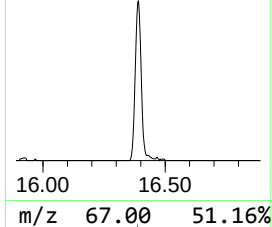
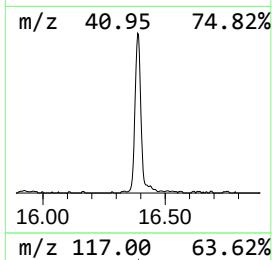
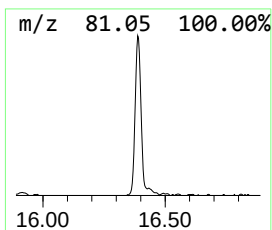
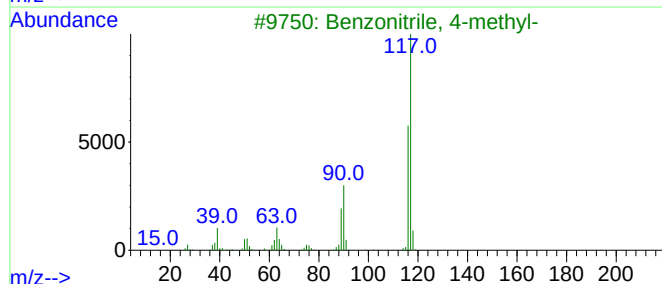
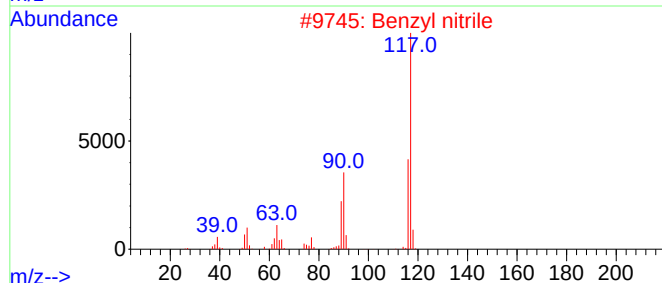
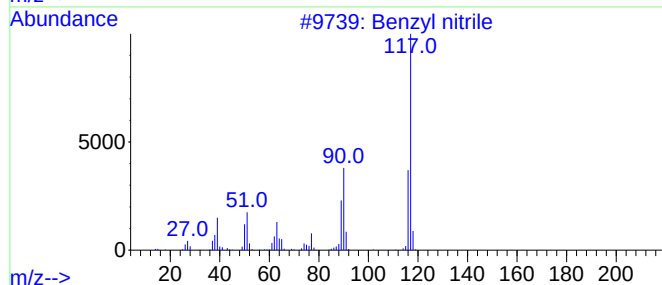
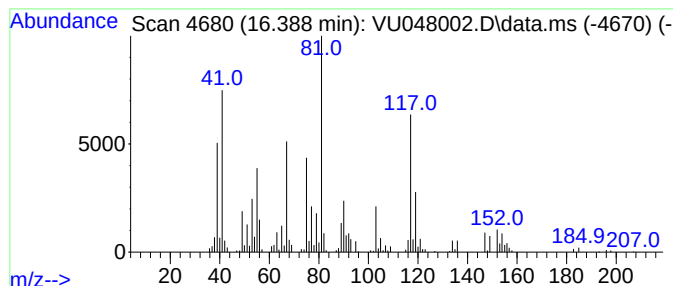
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.388	12.13 ug/L	268314	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzyl nitrile	117	C8H7N	000140-29-4	25
2			Benzyl nitrile	117	C8H7N	000140-29-4	25
3			Benzonitrile, 4-methyl-	117	C8H7N	000104-85-8	25
4			Benzonitrile, 4-methyl-	117	C8H7N	000104-85-8	15
5			Benzyl nitrile	117	C8H7N	000140-29-4	15



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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	15.545	5.7	ug/L	125429	3	11.812	1106180	50.0
unknown-02	16.388	12.1	ug/L	268314	3	11.812	1106180	50.0