

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041322\
 Data File : VU048011.D
 Acq On : 13 Apr 2022 18:07
 Operator : SY/MD
 Sample : N2316-10ME
 Misc : 6.49g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNQ9ME

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: VU048011.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	129851	277472	12.72%	1.582%
2	2.536	360	372	385	rBV	359395	625590	28.68%	3.566%
3	3.237	588	590	591	rBV2	264	95	0.00%	0.001%
4	3.478	663	665	667	rBV3	392	232	0.01%	0.001%
5	3.587	696	699	705	rBV3	409	310	0.01%	0.002%
6	3.713	733	738	739	rBV2	292	237	0.01%	0.001%
7	3.880	785	790	794	rBV2	383	348	0.02%	0.002%
8	3.899	794	796	800	rVB2	276	165	0.01%	0.001%
9	4.054	841	844	846	rBV	189	114	0.01%	0.001%
10	4.076	849	851	852	rBV	309	146	0.01%	0.001%
11	4.131	865	868	871	rBV	178	124	0.01%	0.001%
12	4.163	877	878	882	rVB	263	82	0.00%	0.000%
13	4.189	882	886	889	rBV2	263	210	0.01%	0.001%
14	4.240	900	902	904	rBV2	170	86	0.00%	0.000%
15	4.282	912	915	920	rBV2	139	120	0.01%	0.001%
16	4.321	924	927	929	rBV	269	181	0.01%	0.001%
17	4.497	977	982	983	rBV2	370	280	0.01%	0.002%
18	4.568	1003	1004	1005	rBV2	125	31	0.00%	0.000%
19	4.632	1010	1024	1069	rVV	171717	558783	25.61%	3.185%
20	4.960	1123	1126	1128	rBV	252	158	0.01%	0.001%
21	5.063	1141	1158	1186	rVB	352739	807898	37.03%	4.606%
22	5.227	1207	1209	1211	rBV	341	100	0.00%	0.001%
23	5.272	1221	1223	1224	rBV	387	197	0.01%	0.001%
24	5.430	1270	1272	1274	rBV	93	43	0.00%	0.000%
25	5.468	1282	1284	1287	rBV3	291	150	0.01%	0.001%
26	5.510	1295	1297	1298	rBV	167	51	0.00%	0.000%
27	5.616	1327	1330	1334	rBV2	279	218	0.01%	0.001%
28	5.645	1337	1339	1341	rVV2	325	141	0.01%	0.001%
29	5.719	1341	1362	1399	rVV2	808790	2181485	100.00%	12.436%
30	5.944	1430	1432	1438	rVB3	536	353	0.02%	0.002%
31	5.973	1438	1441	1447	rBV4	954	822	0.04%	0.005%
32	5.999	1447	1449	1451	rBV2	121	54	0.00%	0.000%
33	6.009	1451	1452	1453	rBV2	240	78	0.00%	0.000%
34	6.034	1458	1460	1462	rBV2	454	271	0.01%	0.002%
35	6.076	1471	1473	1474	rBV	123	33	0.00%	0.000%
36	6.092	1474	1478	1479	rBV	229	165	0.01%	0.001%

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 Title : VOC Analysis

37	6.121	1485	1487	1489	rBV2	539	262	0.01%	0.001%
38	6.247	1511	1526	1554	rBV	451129	904037	41.44%	5.154%
39	6.414	1576	1578	1580	rBV	305	137	0.01%	0.001%
40	6.430	1580	1583	1586	rVV	240	201	0.01%	0.001%
41	6.529	1606	1614	1624	rVB8	3217	5718	0.26%	0.033%
42	6.578	1627	1629	1631	rBV2	245	115	0.01%	0.001%
43	6.690	1648	1664	1696	rBV	469398	953816	43.72%	5.437%
44	6.919	1733	1735	1736	rVB	236	74	0.00%	0.000%
45	6.944	1740	1743	1744	rBV	136	58	0.00%	0.000%
46	6.954	1744	1746	1750	rVB	226	107	0.00%	0.001%
47	6.986	1751	1756	1757	rBV2	642	438	0.02%	0.002%
48	7.131	1799	1801	1804	rBV2	270	167	0.01%	0.001%
49	7.185	1806	1818	1835	rBV2	11288	25510	1.17%	0.145%
50	7.333	1862	1864	1867	rVB	262	139	0.01%	0.001%
51	7.356	1867	1871	1872	rBV2	181	101	0.00%	0.001%
52	7.369	1872	1875	1877	rBV2	275	165	0.01%	0.001%
53	7.433	1894	1895	1898	rBV2	274	122	0.01%	0.001%
54	7.494	1906	1914	1924	rBV6	4540	9119	0.42%	0.052%
55	7.568	1924	1937	1958	rVB	237142	461837	21.17%	2.633%
56	7.690	1970	1975	1986	rBV5	3451	5843	0.27%	0.033%
57	7.825	2015	2017	2018	rBV5	264	103	0.00%	0.001%
58	7.899	2026	2040	2055	rBV	954696	1723765	79.02%	9.827%
59	8.182	2116	2128	2149	rBV	161085	323212	14.82%	1.843%
60	8.507	2227	2229	2233	rBV	364	165	0.01%	0.001%
61	8.581	2243	2252	2258	rBV5	2733	4589	0.21%	0.026%
62	8.652	2259	2274	2305	rVV	714585	1398331	64.10%	7.971%
63	9.018	2386	2388	2394	rBV4	894	824	0.04%	0.005%
64	9.127	2419	2422	2425	rBV2	451	327	0.01%	0.002%
65	9.227	2450	2453	2456	rVB2	435	200	0.01%	0.001%
66	9.359	2489	2494	2495	rBV2	686	537	0.02%	0.003%
67	9.423	2500	2514	2544	rVV2	696248	1785416	81.84%	10.178%
68	9.700	2589	2600	2611	rVB3	3878	7196	0.33%	0.041%
69	9.742	2611	2613	2616	rBV2	322	165	0.01%	0.001%
70	10.108	2720	2727	2737	rVB7	3051	4822	0.22%	0.027%
71	10.192	2751	2753	2755	rBV	215	108	0.00%	0.001%
72	10.269	2775	2777	2780	rVB2	460	195	0.01%	0.001%
73	10.304	2786	2788	2792	rBV	201	105	0.00%	0.001%
74	10.526	2853	2857	2865	rBV5	1018	1183	0.05%	0.007%
75	10.668	2893	2901	2909	rBV5	5137	8506	0.39%	0.048%
76	10.764	2919	2931	2952	rVB	829267	1342637	61.55%	7.654%

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Integrator: RTE

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Stop Thrs : 0

Peak Location: TOP

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

Title : VOC Analysis

77	10.864	2958	2962	2965	rBV2	1156	1191	0.05%	0.007%
78	11.201	3065	3067	3075	rVB3	767	726	0.03%	0.004%
79	11.256	3082	3084	3087	rBV	363	199	0.01%	0.001%
80	11.295	3093	3096	3104	rVB4	1861	2153	0.10%	0.012%
81	11.468	3139	3150	3159	rBV5	5254	9373	0.43%	0.053%
82	11.581	3179	3185	3186	rBV3	1001	863	0.04%	0.005%
83	11.815	3245	3258	3276	rBV	916518	1449698	66.45%	8.264%
84	12.198	3360	3377	3401	rBV	1117068	1860766	85.30%	10.608%
85	12.973	3607	3618	3629	rBV3	38432	63009	2.89%	0.359%
86	14.497	4086	4092	4100	rVB6	10358	14799	0.68%	0.084%
87	15.545	4408	4418	4433	rBV	134636	207940	9.53%	1.185%
88	16.391	4671	4681	4692	rBV	329037	503968	23.10%	2.873%

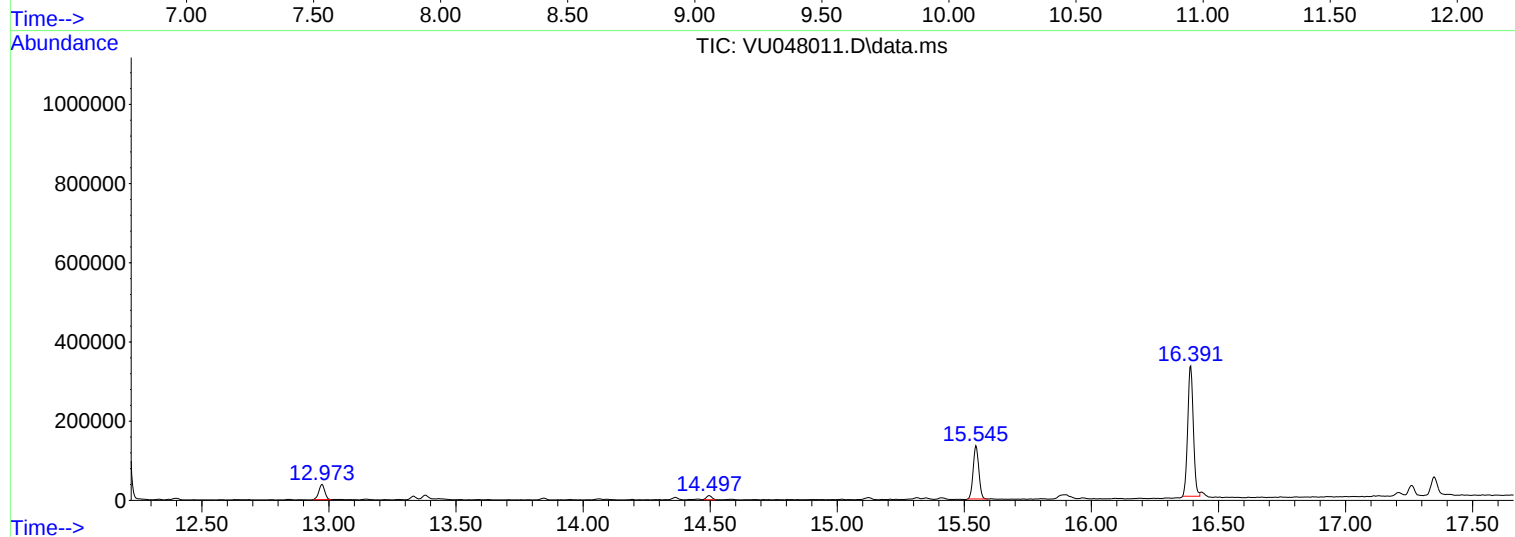
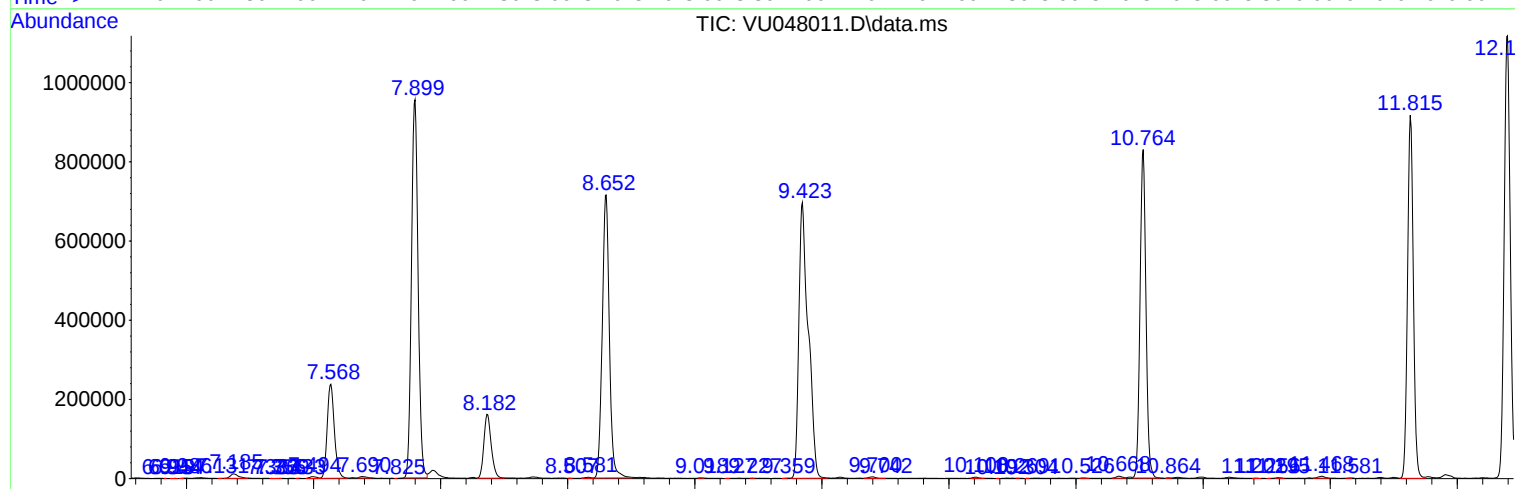
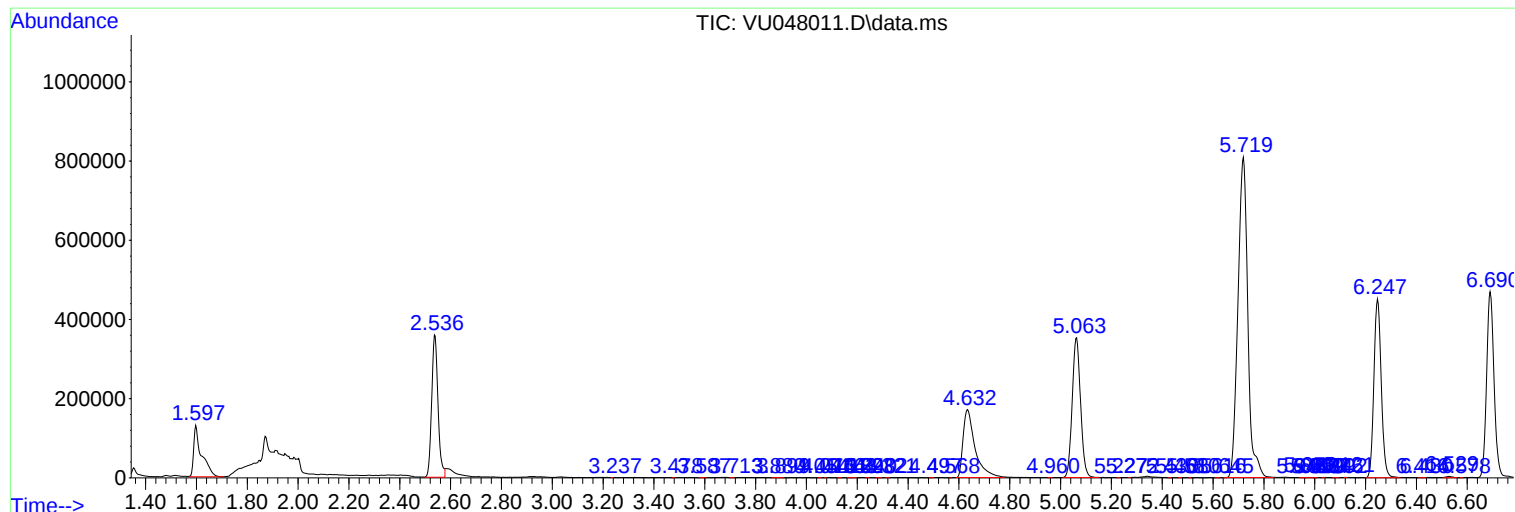
Sum of corrected areas: 17541860

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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNQ9ME

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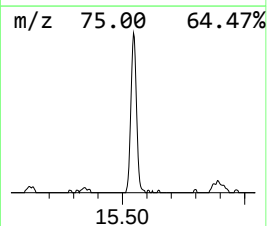
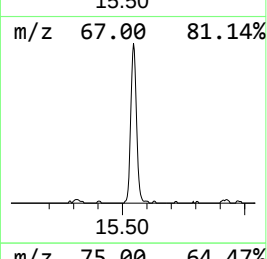
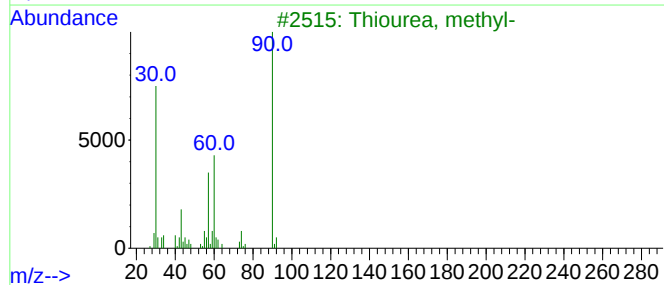
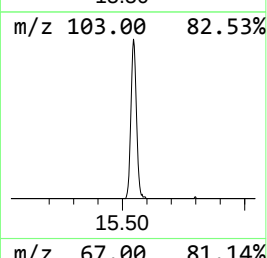
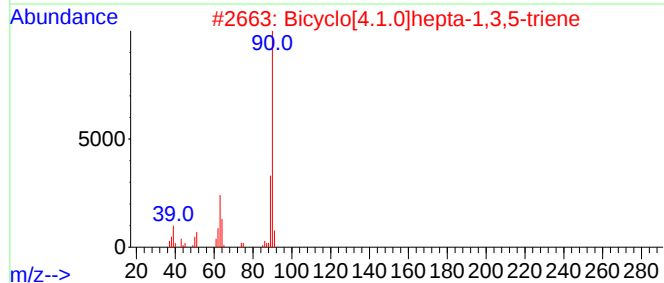
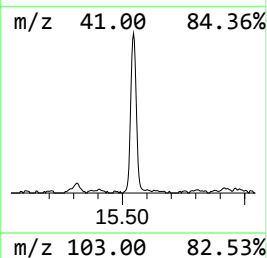
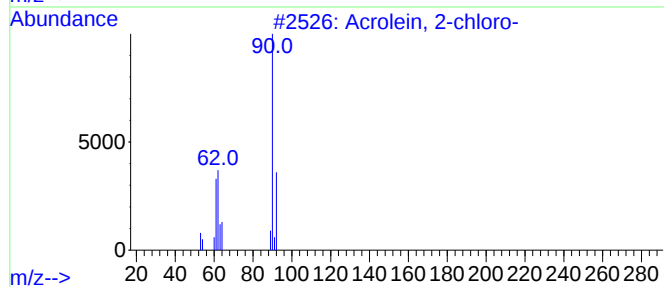
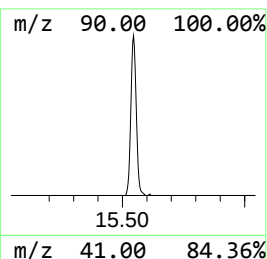
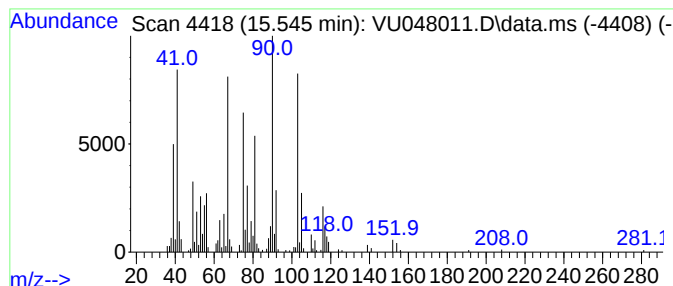
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.545	7.17 ug/L	207940	1,4-Dichlorobenzene-d4	11.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acrolein, 2-chloro-	90	C3H3ClO	000683-51-2	43
2			Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	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	28



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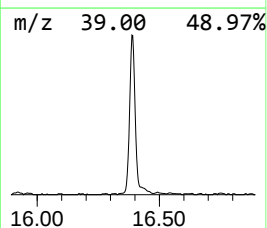
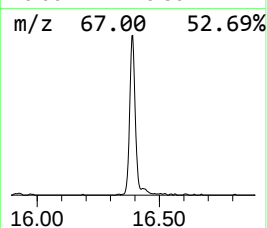
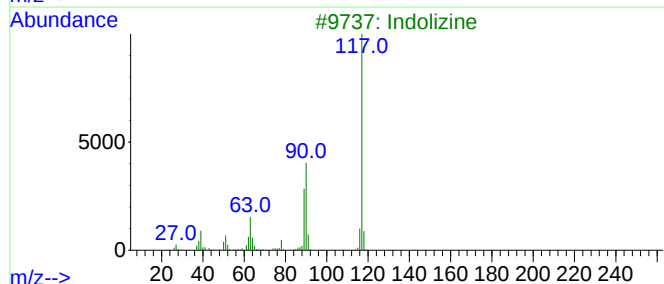
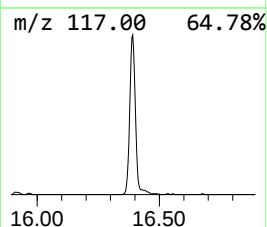
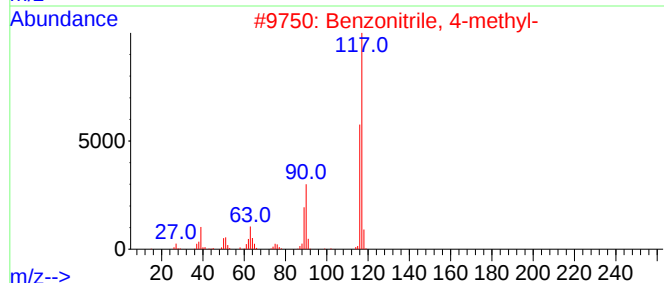
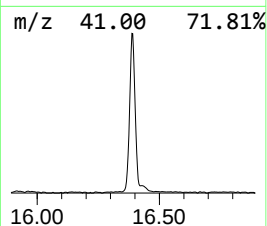
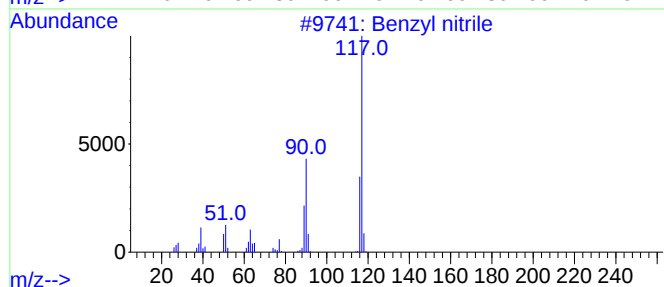
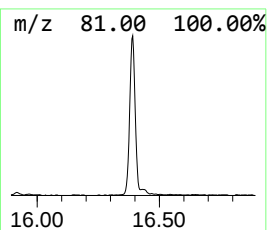
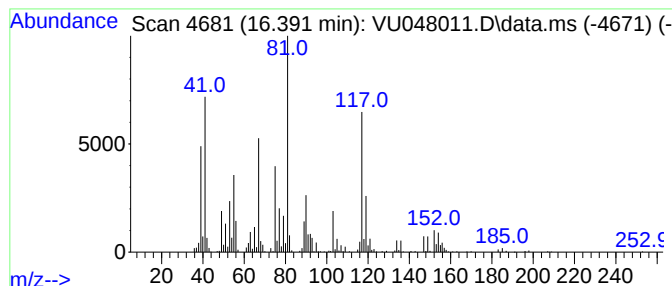
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.391	17.38 ug/L	503968	1,4-Dichlorobenzene-d4	11.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzyl nitrile	117	C8H7N	000140-29-4	25
2			Benzonitrile, 4-methyl-	117	C8H7N	000104-85-8	15
3			Indolizine	117	C8H7N	000274-40-8	15
4			Benzonitrile, 2-methyl-	117	C8H7N	000529-19-1	15
5			Benzyl nitrile	117	C8H7N	000140-29-4	15



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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	7.2	ug/L	207940	3	11.815	1449700	50.0
unknown-02	16.391	17.4	ug/L	503968	3	11.815	1449700	50.0