

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
 Data File : VU047927.D
 Acq On : 11 Apr 2022 23:46
 Operator : SY/MD
 Sample : N2293-15ME
 Misc : 6.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNP3ME

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: VU047927.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	72	80	111	rVB	71187	145267	10.26%	1.314%
2	1.825	120	151	152	rBV6	35281	122987	8.69%	1.112%
3	2.539	361	373	385	rBV	193141	332403	23.48%	3.006%
4	2.739	432	435	438	rBV3	482	356	0.03%	0.003%
5	2.755	438	440	449	rVB6	720	1042	0.07%	0.009%
6	3.099	542	547	549	rBV2	447	295	0.02%	0.003%
7	3.118	549	553	556	rBV3	405	334	0.02%	0.003%
8	3.173	566	570	572	rBV2	516	431	0.03%	0.004%
9	3.208	578	581	582	rBV4	897	508	0.04%	0.005%
10	3.260	593	597	600	rVB2	478	365	0.03%	0.003%
11	3.292	603	607	611	rVB3	321	275	0.02%	0.002%
12	3.452	651	657	660	rBV2	361	410	0.03%	0.004%
13	3.469	660	662	668	rVB2	404	312	0.02%	0.003%
14	3.510	668	675	679	rBV2	322	411	0.03%	0.004%
15	3.674	723	726	733	rVB4	647	769	0.05%	0.007%
16	3.845	776	779	786	rVB3	359	286	0.02%	0.003%
17	3.893	790	794	799	rBV2	324	272	0.02%	0.002%
18	4.636	1010	1025	1071	rBV	95505	316571	22.36%	2.863%
19	5.060	1141	1157	1185	rBV	198634	454071	32.07%	4.106%
20	5.157	1185	1187	1193	rVB4	491	373	0.03%	0.003%
21	5.295	1222	1230	1232	rBV	529	627	0.04%	0.006%
22	5.343	1237	1245	1251	rBV4	1261	2234	0.16%	0.020%
23	5.530	1300	1303	1310	rVB2	332	331	0.02%	0.003%
24	5.575	1310	1317	1319	rBV3	780	579	0.04%	0.005%
25	5.719	1339	1362	1374	rBV2	438433	1156171	81.66%	10.455%
26	5.983	1439	1444	1450	rBV3	783	972	0.07%	0.009%
27	6.021	1450	1456	1458	rBV2	310	282	0.02%	0.003%
28	6.124	1481	1488	1497	rVB7	1617	2803	0.20%	0.025%
29	6.247	1508	1526	1554	rBV	475200	932432	65.86%	8.432%
30	6.523	1605	1612	1621	rVV5	1460	2514	0.18%	0.023%
31	6.690	1647	1664	1689	rBV	259394	524375	37.04%	4.742%
32	6.803	1694	1699	1704	rVV3	803	945	0.07%	0.009%
33	6.825	1704	1706	1710	rVB4	457	264	0.02%	0.002%
34	7.063	1766	1780	1781	rBV5	843	1350	0.10%	0.012%
35	7.189	1804	1819	1832	rBV2	7589	17017	1.20%	0.154%
36	7.443	1895	1898	1900	rBV2	392	294	0.02%	0.003%

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Instrument :
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 ClientSampleId :
 ETNP3ME

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	7.497	1908	1915	1924	rBV5	1525	2160	0.15%	0.020%
38	7.568	1924	1937	1956	rVV	123773	239576	16.92%	2.167%
39	7.690	1969	1975	1976	rBV3	1257	1052	0.07%	0.010%
40	7.774	1997	2001	2006	rVB2	367	252	0.02%	0.002%
41	7.819	2012	2015	2021	rBV3	318	312	0.02%	0.003%
42	7.899	2024	2040	2055	rBV	488856	878620	62.06%	7.946%
43	7.970	2056	2062	2079	rVB	15758	29537	2.09%	0.267%
44	8.127	2105	2111	2116	rBV5	1301	1518	0.11%	0.014%
45	8.182	2116	2128	2152	rVV2	82851	164050	11.59%	1.484%
46	8.391	2189	2193	2199	rVB5	479	574	0.04%	0.005%
47	8.652	2258	2274	2314	rBV	381380	779878	55.08%	7.053%
48	8.857	2336	2338	2345	rVB4	337	342	0.02%	0.003%
49	8.989	2377	2379	2385	rVB3	301	299	0.02%	0.003%
50	9.182	2435	2439	2441	rBV	412	330	0.02%	0.003%
51	9.253	2458	2461	2467	rVB	290	245	0.02%	0.002%
52	9.365	2487	2496	2500	rBV5	7510	11088	0.78%	0.100%
53	9.423	2501	2514	2519	rBV	713373	1341604	94.76%	12.132%
54	9.578	2556	2562	2572	rVB5	3535	6139	0.43%	0.056%
55	9.693	2587	2598	2600	rBV5	3031	3722	0.26%	0.034%
56	9.825	2635	2639	2645	rBV3	221	296	0.02%	0.003%
57	10.108	2717	2727	2733	rBV4	2261	3212	0.23%	0.029%
58	10.433	2825	2828	2838	rVB3	524	822	0.06%	0.007%
59	10.481	2838	2843	2845	rBV2	512	457	0.03%	0.004%
60	10.661	2888	2899	2911	rVB10	3002	6054	0.43%	0.055%
61	10.764	2917	2931	2950	rBV	456879	763293	53.91%	6.903%
62	10.889	2963	2970	2973	rBV5	741	845	0.06%	0.008%
63	10.976	2990	2997	2998	rBV2	1287	1360	0.10%	0.012%
64	11.092	3027	3033	3039	rBV3	761	1084	0.08%	0.010%
65	11.150	3047	3051	3056	rVB2	374	298	0.02%	0.003%
66	11.288	3089	3094	3095	rBV2	719	469	0.03%	0.004%
67	11.414	3126	3133	3134	rBV3	449	492	0.03%	0.004%
68	11.462	3142	3148	3149	rBV3	1730	1536	0.11%	0.014%
69	11.561	3174	3179	3180	rBV	449	293	0.02%	0.003%
70	11.693	3217	3220	3227	rVB6	755	951	0.07%	0.009%
71	11.751	3232	3238	3245	rBV5	1790	2160	0.15%	0.020%
72	11.815	3245	3258	3273	rBV	896111	1415774	100.00%	12.803%
73	11.957	3296	3302	3305	rBV6	1665	2056	0.15%	0.019%
74	12.102	3344	3347	3355	rVB4	704	777	0.05%	0.007%
75	12.198	3359	3377	3396	rBV	603006	979453	69.18%	8.857%
76	12.475	3456	3463	3478	rBV7	2981	5448	0.38%	0.049%

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 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNP3ME

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	12.577	3491	3495	3501	rVB4	730	784	0.06%	0.007%
78	12.635	3507	3513	3516	rBV4	421	372	0.03%	0.003%
79	12.651	3516	3518	3522	rBV2	290	269	0.02%	0.002%
80	12.709	3533	3536	3543	rVB4	1538	1540	0.11%	0.014%
81	12.767	3551	3554	3562	rVB4	899	1256	0.09%	0.011%
82	12.822	3568	3571	3574	rBV2	419	299	0.02%	0.003%
83	12.880	3583	3589	3594	rBV4	1363	1793	0.13%	0.016%
84	12.973	3608	3618	3629	rBV3	17980	28167	1.99%	0.255%
85	13.034	3629	3637	3645	rVB3	958	1454	0.10%	0.013%
86	13.163	3670	3677	3686	rVB6	3393	5040	0.36%	0.046%
87	13.339	3725	3732	3735	rBV3	1211	1553	0.11%	0.014%
88	13.378	3735	3744	3756	rVB2	45175	67066	4.74%	0.606%
89	13.774	3864	3867	3869	rBV3	386	261	0.02%	0.002%
90	13.844	3884	3889	3898	rVB5	2383	3422	0.24%	0.031%
91	14.092	3960	3966	3967	rBV3	1668	1282	0.09%	0.012%
92	14.311	4030	4034	4035	rBV2	719	453	0.03%	0.004%
93	14.429	4062	4071	4081	rBV7	17815	29064	2.05%	0.263%
94	14.497	4081	4092	4104	rBV3	52311	83847	5.92%	0.758%
95	14.568	4111	4114	4115	rBV3	793	445	0.03%	0.004%
96	14.671	4143	4146	4150	rBV3	590	537	0.04%	0.005%
97	15.204	4306	4312	4314	rBV5	1268	1325	0.09%	0.012%
98	15.500	4401	4404	4407	rBV2	780	657	0.05%	0.006%
99	15.545	4408	4418	4430	rVV2	77162	120252	8.49%	1.087%
100	15.886	4512	4524	4525	rBV3	25657	37557	2.65%	0.340%

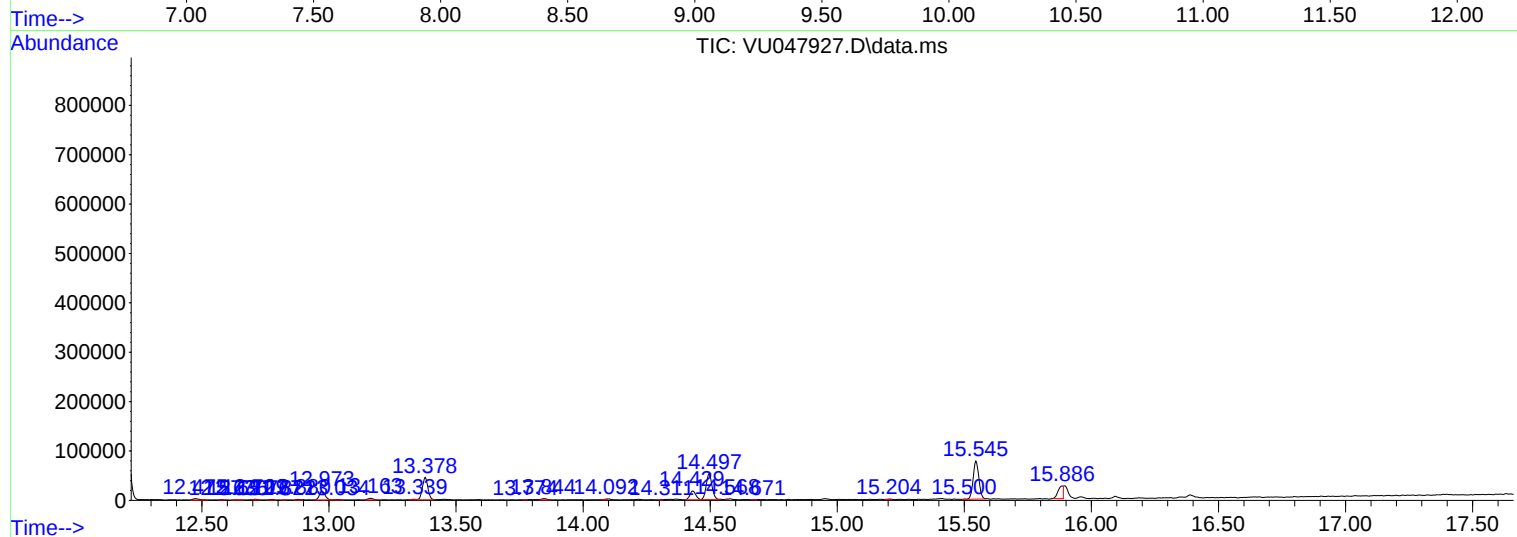
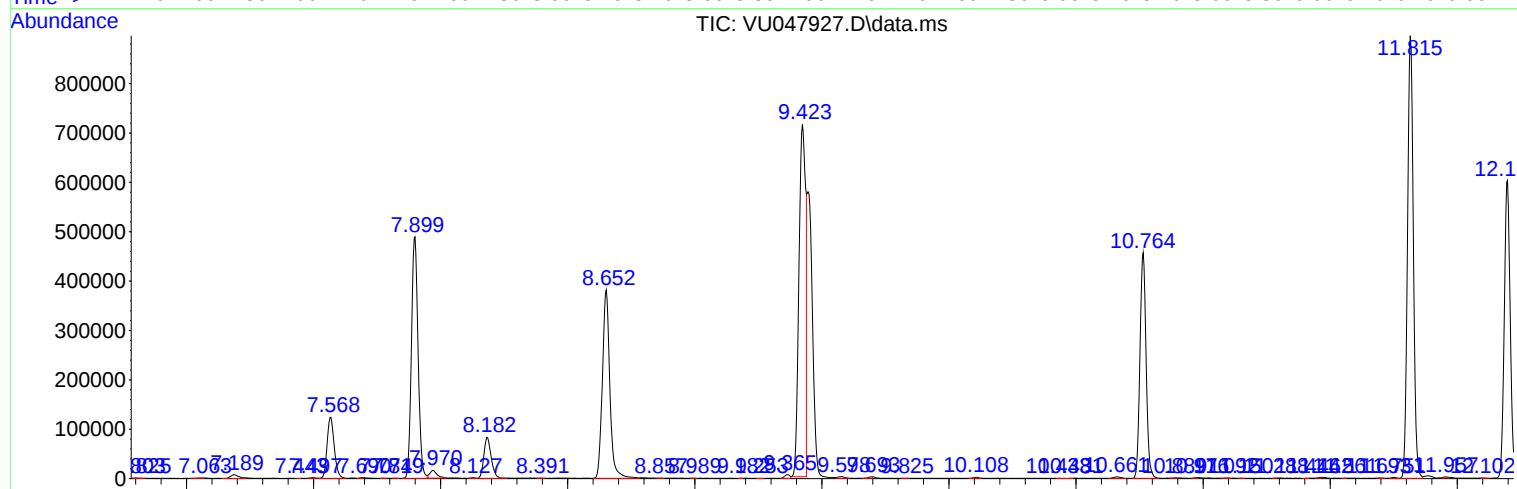
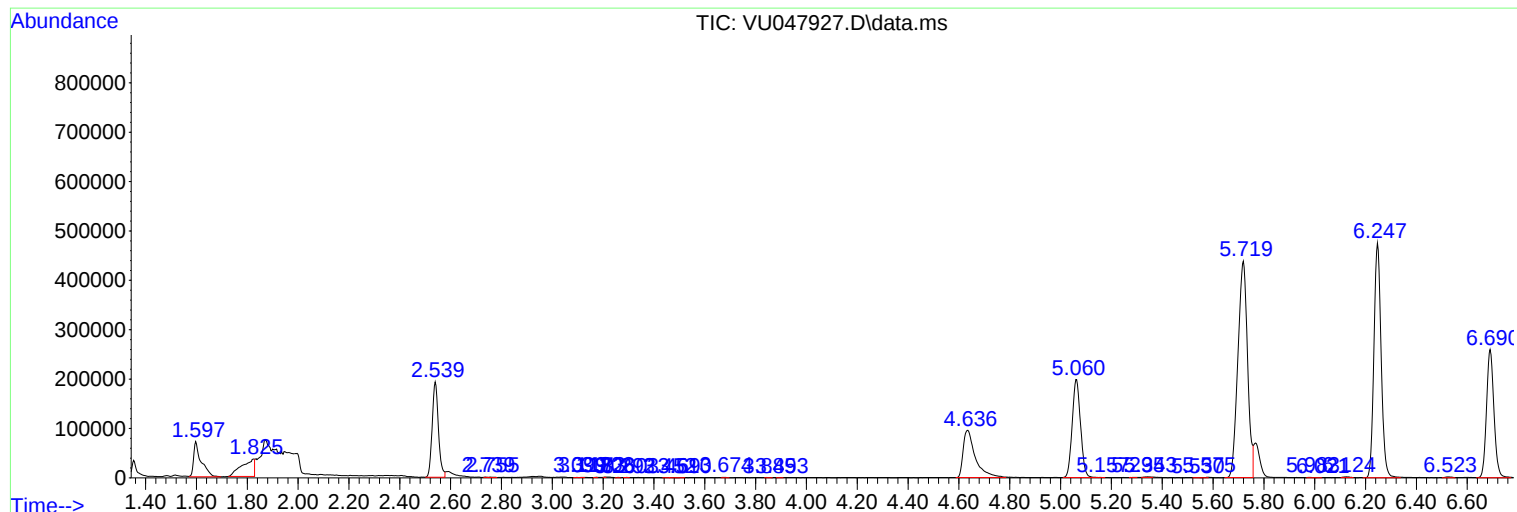
Sum of corrected areas: 11058051

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
Data File : VU047927.D
Acq On : 11 Apr 2022 23:46
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Sample : N2293-15ME
Misc : 6.71g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP3ME

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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ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP3ME

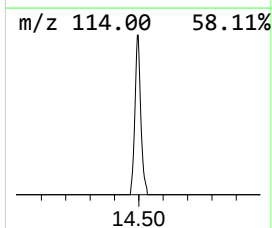
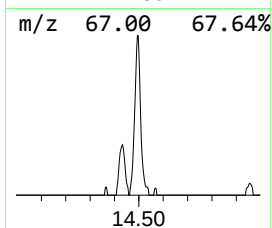
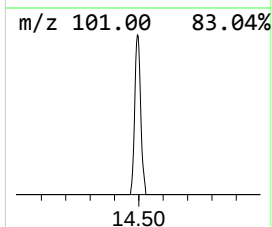
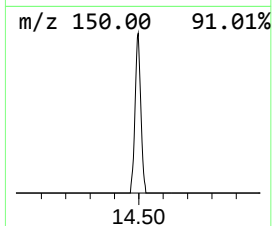
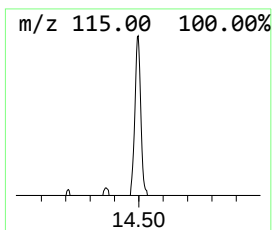
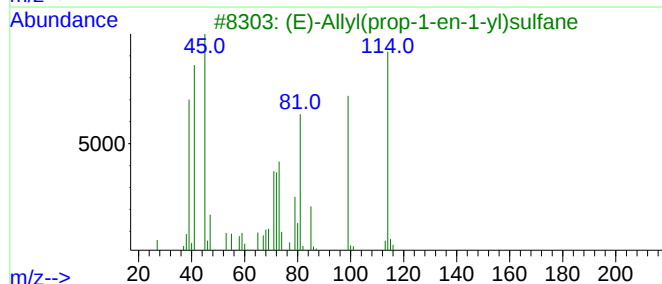
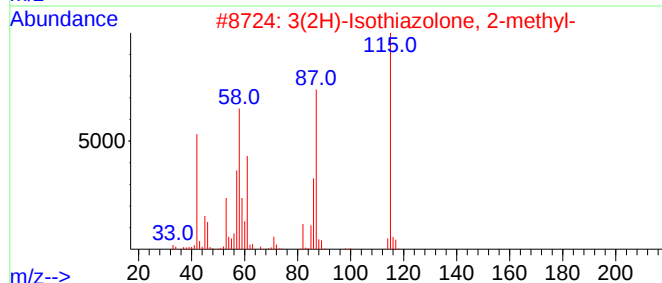
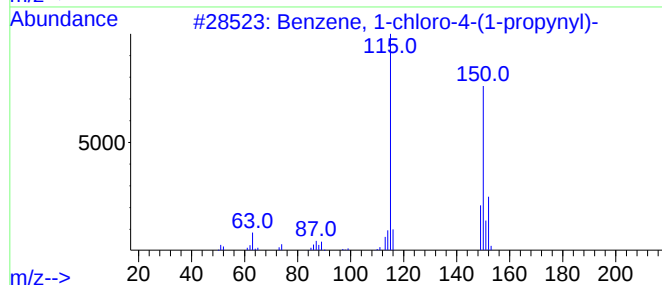
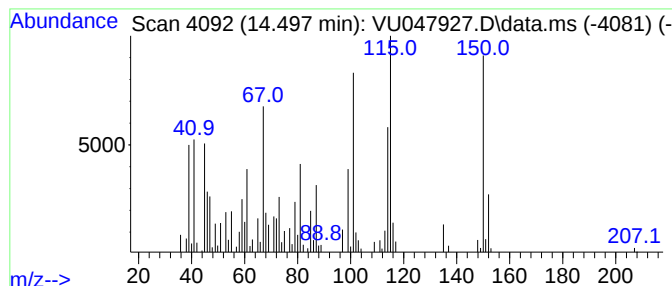
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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.
14.497	2.96 ug/L	83847	1,4-Dichlorobenzene-d4	11.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-chloro-4-(1-propynyl)-	150	C9H7Cl	002809-65-6	43
2			3(2H)-Isothiazolone, 2-methyl-	115	C4H5NOS	002682-20-4	18
3			(E)-Allyl(prop-1-en-1-yl)sulfane	114	C6H10S	104324-36-9	15
4			Benzo[b]thiophene-2-ol	150	C8H6OS	000496-31-1	11
5			2-Piperidinethione	115	C5H9NS	013070-01-4	11



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Instrument :
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ClientSampleId :
ETNP3ME

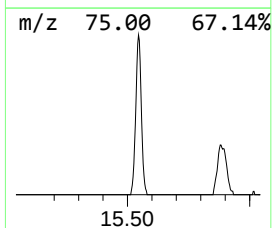
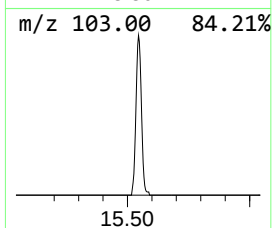
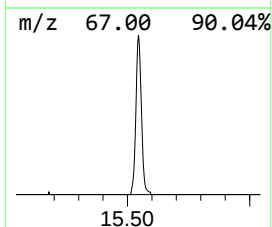
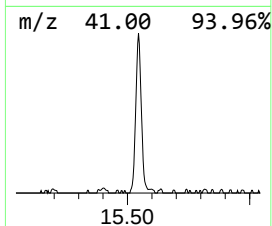
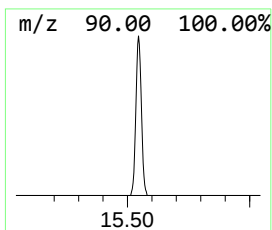
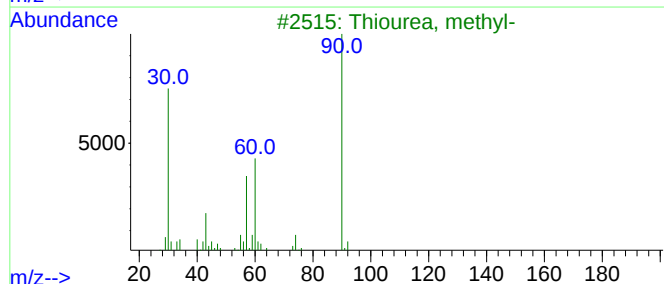
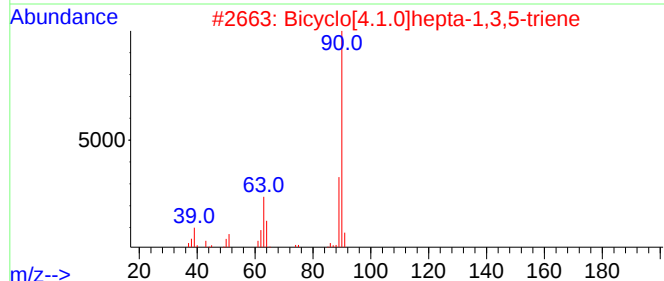
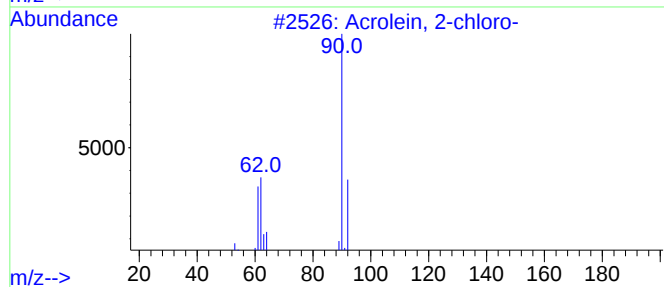
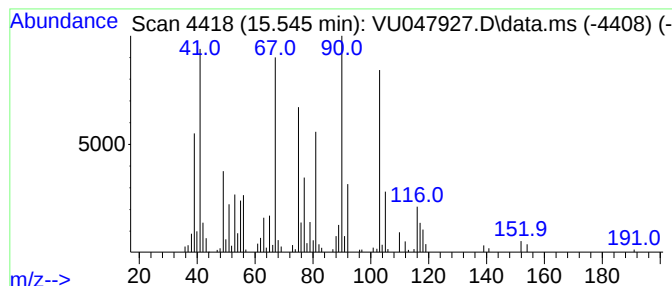
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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.
15.545	4.25 ug/L	120252	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	38
3			Thiourea, methyl-	90	C2H6N2S	000598-52-7	35
4			Propane, 2-(methylthio)-	90	C4H10S	001551-21-9	28
5			1,3,5-Trichloro-4-methyl-2-penta...	202	C6H9Cl3O	1000140-03-8	25



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ClientSampleId :
ETNP3ME

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	14.497	3.0	ug/L	83847	3	11.815	1415770	50.0
unknown-02	15.545	4.3	ug/L	120252	3	11.815	1415770	50.0