

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031723\
 Data File : VU053291.D
 Acq On : 18 Mar 2023 01:32
 Operator : JC/MD
 Sample : VIBLK114
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VIBLK114

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\SFAMULM031523WMA.M
 Title : VOC Analysis

Signal : TIC: VU053291.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.465	33	39	58	rBV	11182	20577	3.84%	0.507%
2	1.597	73	80	98	rVB	77850	87489	16.33%	2.156%
3	1.909	170	177	195	rVB	57073	78962	14.74%	1.946%
4	2.562	369	380	397	rVB	113156	183145	34.19%	4.513%
5	3.038	520	528	537	rVB3	1931	2918	0.54%	0.072%
6	3.221	583	585	586	rBV3	183	85	0.02%	0.002%
7	3.858	781	783	786	rBV	242	112	0.02%	0.003%
8	3.903	793	797	801	rVB2	202	204	0.04%	0.005%
9	4.076	848	851	855	rBV	206	185	0.03%	0.005%
10	4.266	908	910	915	rVB2	232	159	0.03%	0.004%
11	4.346	931	935	938	rBV	260	280	0.05%	0.007%
12	4.398	949	951	956	rVB	223	119	0.02%	0.003%
13	4.424	956	959	961	rBV	165	110	0.02%	0.003%
14	4.488	976	979	982	rBV	206	134	0.03%	0.003%
15	4.613	1006	1018	1042	rBV2	44488	106189	19.83%	2.617%
16	4.803	1070	1077	1080	rBV3	429	489	0.09%	0.012%
17	4.835	1084	1087	1089	rVV	320	194	0.04%	0.005%
18	4.851	1090	1092	1098	rVB2	339	197	0.04%	0.005%
19	4.896	1103	1106	1109	rBV2	195	107	0.02%	0.003%
20	5.057	1141	1156	1180	rBV	97352	211116	39.42%	5.202%
21	5.311	1231	1235	1237	rBV	159	81	0.02%	0.002%
22	5.366	1250	1252	1256	rBV	222	189	0.04%	0.005%
23	5.587	1319	1321	1324	rVB	226	143	0.03%	0.004%
24	5.610	1325	1328	1331	rBV	202	204	0.04%	0.005%
25	5.719	1341	1362	1390	rBV2	193704	535615	100.00%	13.198%
26	5.848	1399	1402	1404	rBV2	337	262	0.05%	0.006%
27	5.890	1410	1415	1418	rBV2	251	306	0.06%	0.008%
28	5.938	1424	1430	1432	rBV	233	287	0.05%	0.007%
29	6.015	1451	1454	1457	rBV	159	84	0.02%	0.002%
30	6.092	1475	1478	1481	rVB	223	143	0.03%	0.004%
31	6.243	1512	1525	1546	rBV	154849	292118	54.54%	7.198%
32	6.452	1586	1590	1591	rBV	362	216	0.04%	0.005%
33	6.517	1608	1610	1612	rBV	381	204	0.04%	0.005%
34	6.613	1635	1640	1645	rBV	227	336	0.06%	0.008%
35	6.684	1649	1662	1679	rBV	121732	236284	44.11%	5.822%
36	6.835	1706	1709	1711	rBV	190	129	0.02%	0.003%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
 Title : VOC Analysis

37	7.044	1772	1774	1778	rVB2	217	128	0.02%	0.003%
38	7.063	1778	1780	1785	rBV	227	132	0.02%	0.003%
39	7.112	1790	1795	1801	rVV2	233	292	0.05%	0.007%
40	7.185	1810	1818	1825	rBV4	897	1313	0.25%	0.032%
41	7.253	1836	1839	1845	rVB2	251	196	0.04%	0.005%
42	7.369	1872	1875	1880	rVB	157	110	0.02%	0.003%
43	7.436	1893	1896	1900	rBB	147	145	0.03%	0.004%
44	7.459	1900	1903	1904	rBV	281	183	0.03%	0.005%
45	7.562	1922	1935	1960	rBV	68678	118498	22.12%	2.920%
46	7.677	1967	1971	1973	rBV	407	314	0.06%	0.008%
47	7.735	1987	1989	1994	rVB2	186	120	0.02%	0.003%
48	7.816	2011	2014	2019	rBV	311	310	0.06%	0.008%
49	7.893	2025	2038	2059	rBV	246292	424939	79.34%	10.471%
50	8.025	2076	2079	2081	rBV2	213	144	0.03%	0.004%
51	8.073	2091	2094	2099	rBV	359	368	0.07%	0.009%
52	8.176	2114	2126	2145	rBV	48189	78662	14.69%	1.938%
53	8.269	2149	2155	2156	rBV	270	248	0.05%	0.006%
54	8.356	2177	2182	2185	rBV2	271	306	0.06%	0.008%
55	8.455	2209	2213	2216	rBV2	294	211	0.04%	0.005%
56	8.626	2254	2266	2300	rBV	132115	241489	45.09%	5.950%
57	8.806	2319	2322	2328	rBV	194	210	0.04%	0.005%
58	8.925	2357	2359	2362	rVB	227	104	0.02%	0.003%
59	9.086	2407	2409	2412	rVB2	203	115	0.02%	0.003%
60	9.189	2434	2441	2443	rBV	219	306	0.06%	0.008%
61	9.414	2497	2511	2532	rBV	210475	364167	67.99%	8.973%
62	9.697	2591	2599	2606	rVB	1119	1795	0.34%	0.044%
63	9.758	2616	2618	2621	rBV	172	92	0.02%	0.002%
64	9.825	2636	2639	2642	rBV2	170	101	0.02%	0.002%
65	9.938	2671	2674	2676	rBV2	172	119	0.02%	0.003%
66	9.973	2682	2685	2688	rBV2	233	168	0.03%	0.004%
67	10.076	2715	2717	2719	rBV2	196	95	0.02%	0.002%
68	10.105	2723	2726	2727	rBV	185	129	0.02%	0.003%
69	10.275	2776	2779	2781	rBV2	193	120	0.02%	0.003%
70	10.504	2847	2850	2852	rBV2	211	148	0.03%	0.004%
71	10.590	2874	2877	2880	rBV	154	83	0.02%	0.002%
72	10.706	2911	2913	2914	rBV	201	91	0.02%	0.002%
73	10.751	2915	2927	2944	rVB	165339	263194	49.14%	6.485%
74	11.468	3142	3150	3157	rBV2	925	1354	0.25%	0.033%
75	11.809	3244	3256	3276	rBV	213579	337284	62.97%	8.311%
76	12.124	3347	3354	3360	rBV	327	429	0.08%	0.011%

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77	12.188	3362	3374	3391	rBV	219238	355651	66.40%	8.763%
78	12.574	3486	3494	3497	rBV3	561	709	0.13%	0.017%
79	12.970	3615	3617	3618	rBV3	260	143	0.03%	0.004%
80	12.996	3623	3625	3629	rVB2	299	151	0.03%	0.004%
81	13.028	3629	3635	3636	rBV2	318	292	0.05%	0.007%
82	13.076	3648	3650	3652	rVB	336	119	0.02%	0.003%
83	13.105	3654	3659	3665	rVB2	294	316	0.06%	0.008%
84	13.346	3732	3734	3737	rBV	198	111	0.02%	0.003%
85	13.449	3759	3766	3772	rBV4	1066	1483	0.28%	0.037%
86	13.619	3812	3819	3828	rVB5	4047	5542	1.03%	0.137%
87	13.902	3904	3907	3910	rBV2	293	195	0.04%	0.005%
88	14.044	3948	3951	3955	rBV	480	369	0.07%	0.009%
89	14.089	3958	3965	3974	rVV	5541	8162	1.52%	0.201%
90	14.182	3992	3994	4002	rVB2	413	407	0.08%	0.010%
91	14.497	4088	4092	4093	rBV	231	148	0.03%	0.004%
92	14.658	4139	4142	4143	rBV2	326	181	0.03%	0.004%
93	14.687	4144	4151	4158	rVB4	2945	3603	0.67%	0.089%
94	15.015	4246	4253	4260	rVB3	3136	3788	0.71%	0.093%
95	15.156	4294	4297	4299	rBV	317	199	0.04%	0.005%
96	15.220	4307	4317	4331	rBV3	13547	22329	4.17%	0.550%
97	15.407	4366	4375	4389	rVB3	15508	23828	4.45%	0.587%
98	15.777	4487	4490	4494	rBV	390	346	0.06%	0.009%
99	16.259	4632	4640	4656	rVB4	7437	11573	2.16%	0.285%
100	16.407	4677	4686	4692	rBV3	13201	21202	3.96%	0.522%

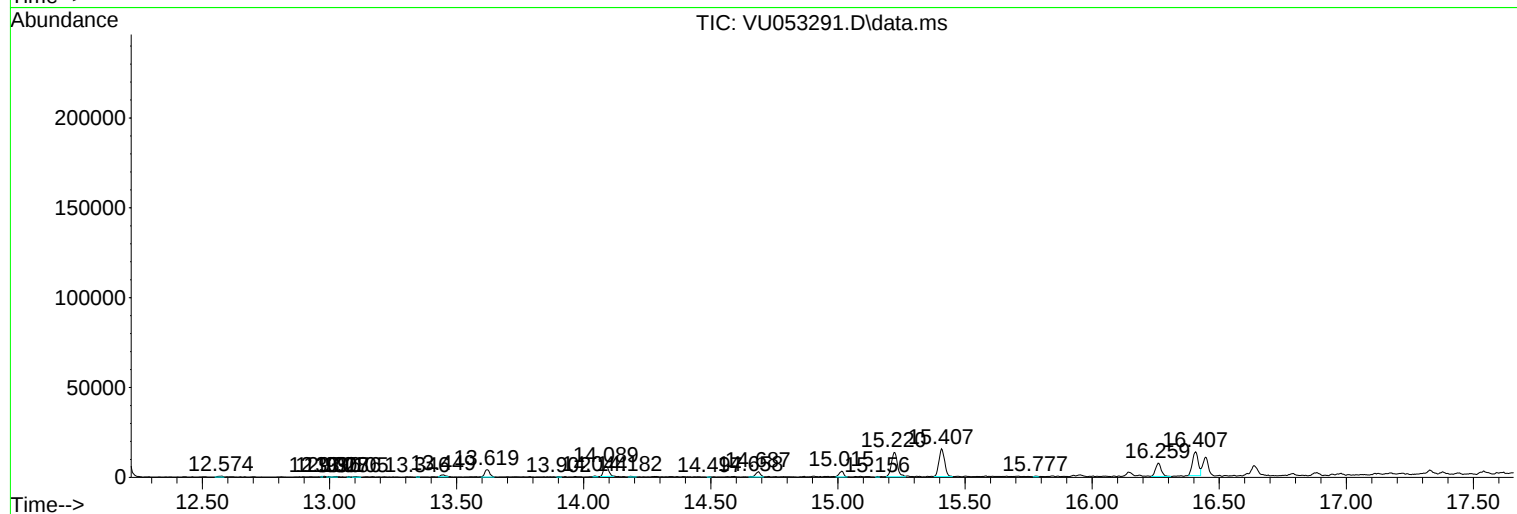
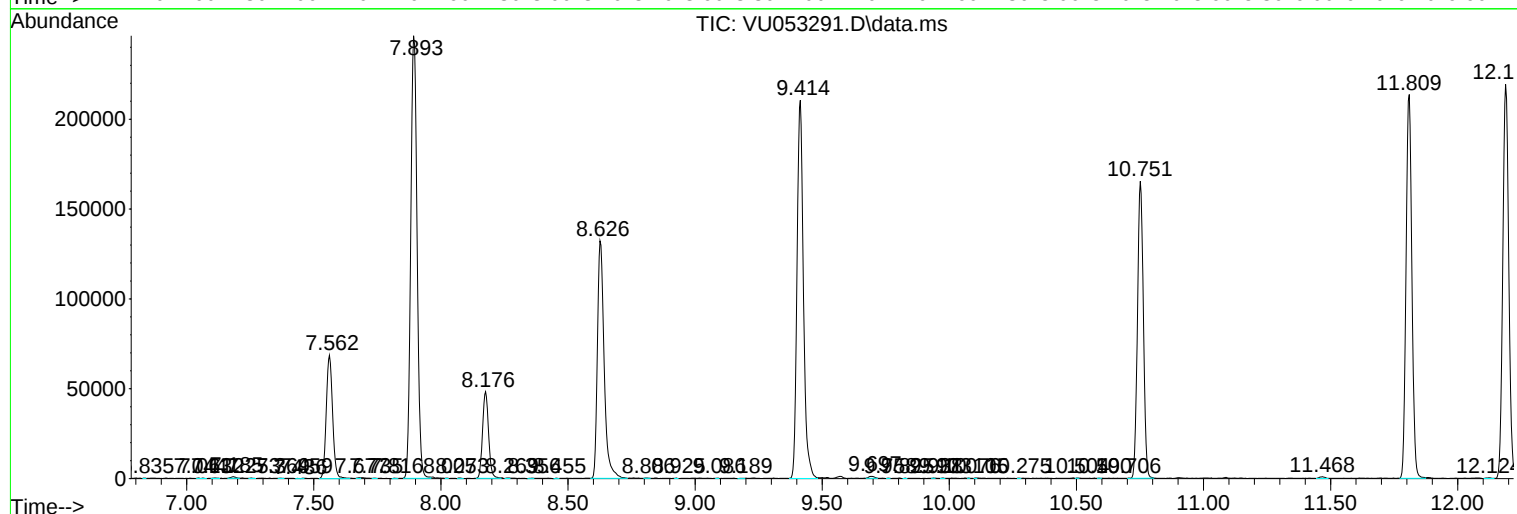
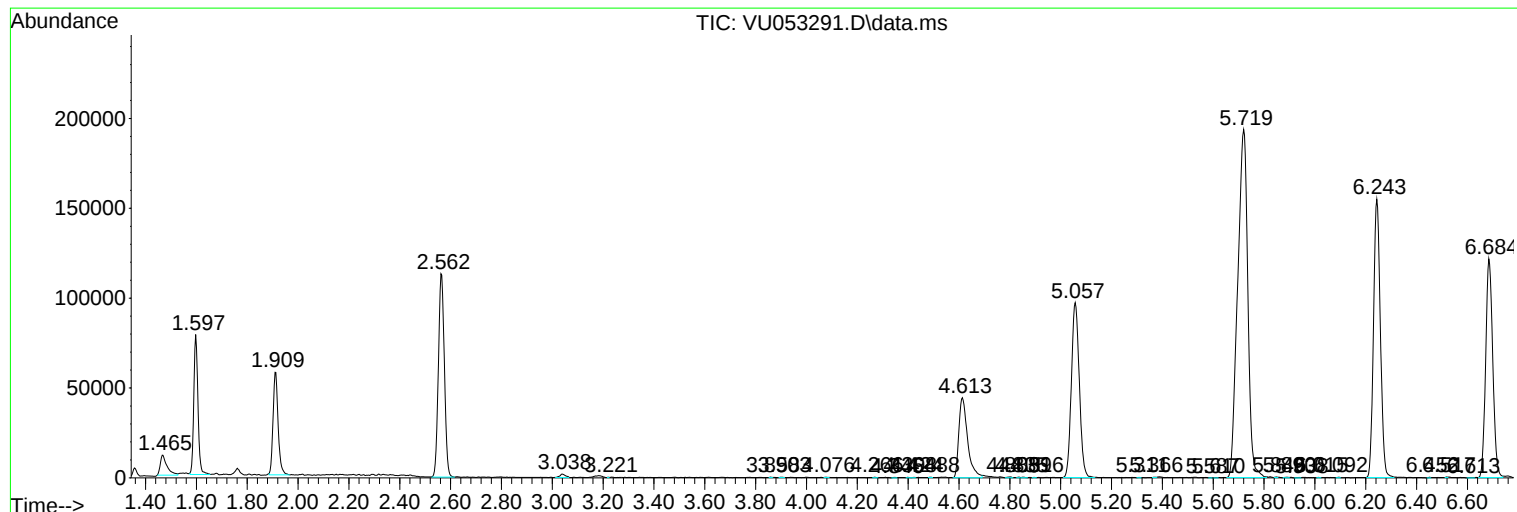
Sum of corrected areas: 4058431

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ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 41 Sample Multiplier: 1

Instrument :
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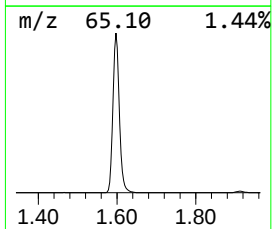
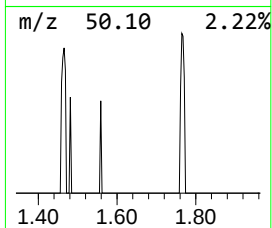
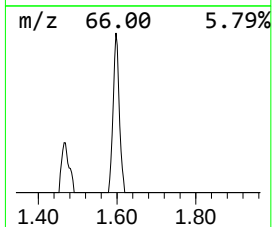
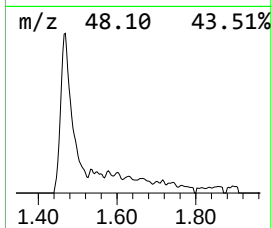
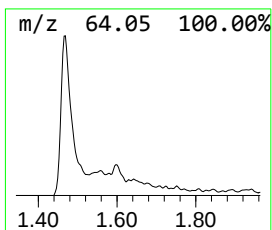
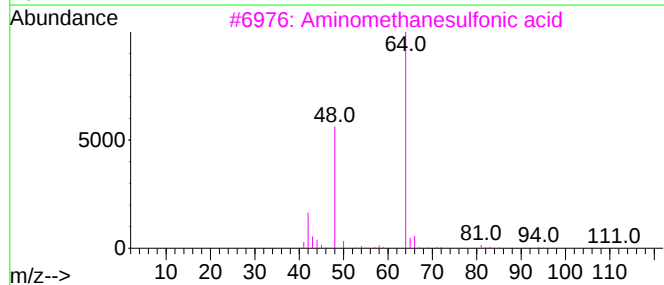
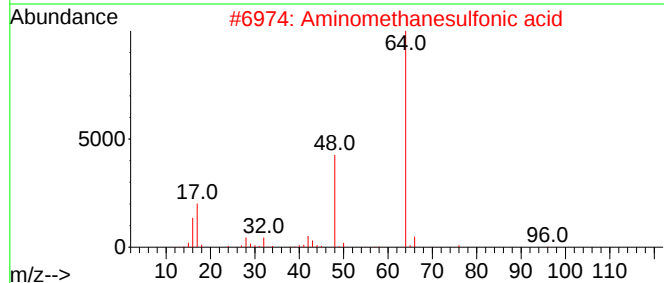
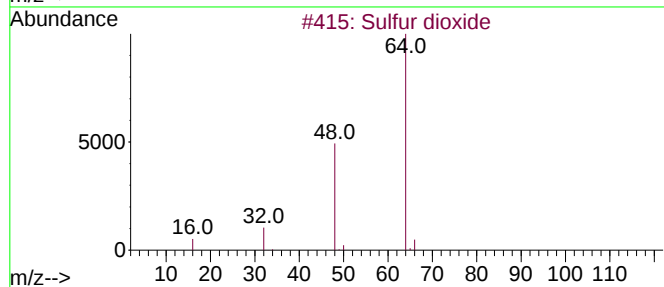
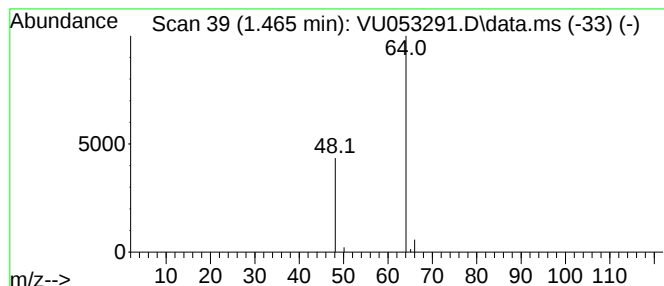
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.465	3.52 ug/L	20577	1,4-Difluorobenzene	6.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Sulfur dioxide	64	O2S	007446-09-5	5



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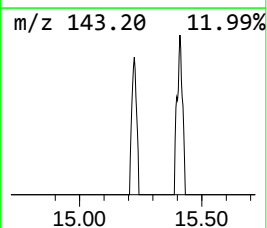
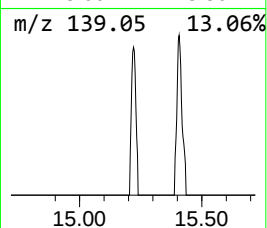
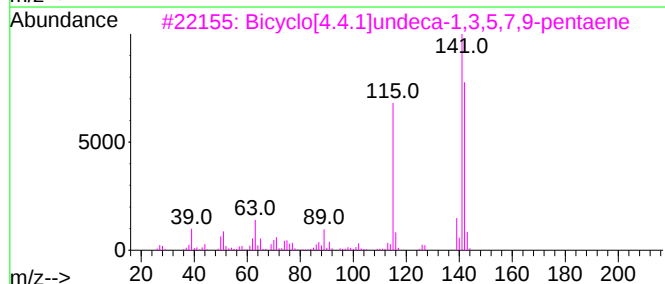
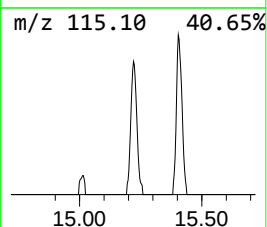
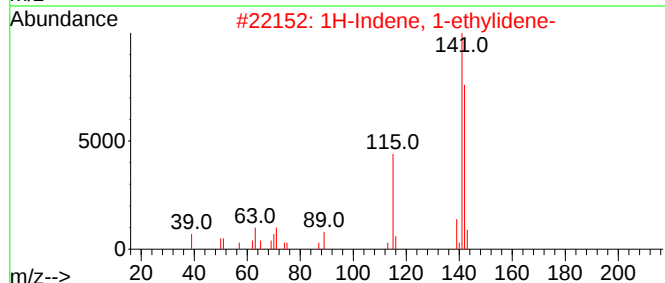
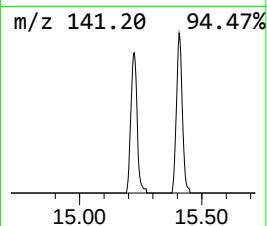
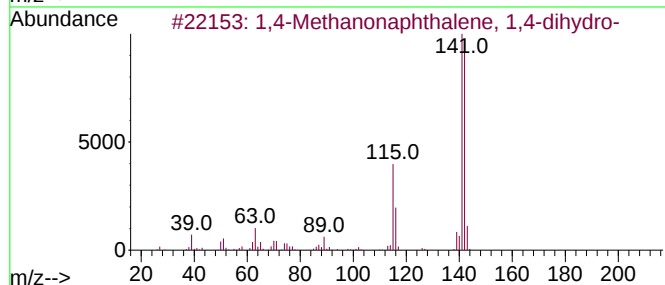
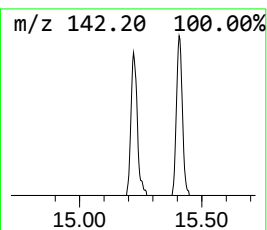
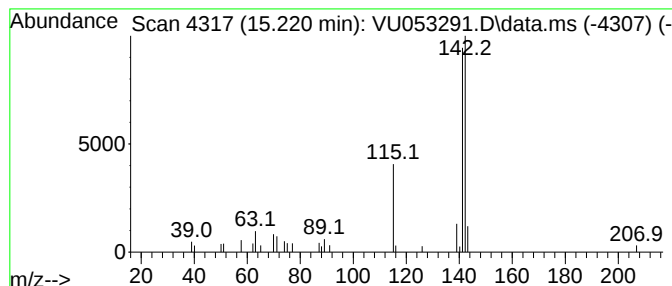
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 1,4-Methanonaphthalene, 1,4... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.220	3.31 ug/L	22329	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
2			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	91
3			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91
4			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	90
5			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	90



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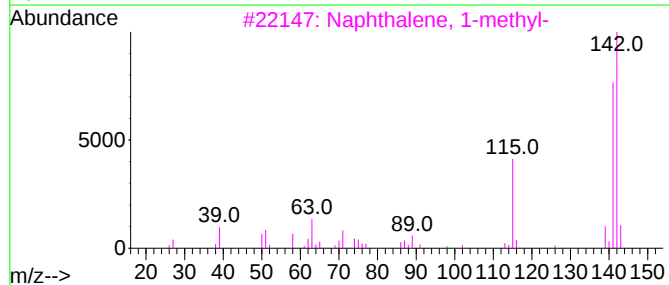
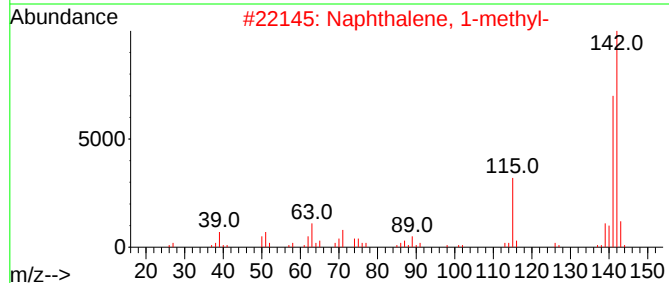
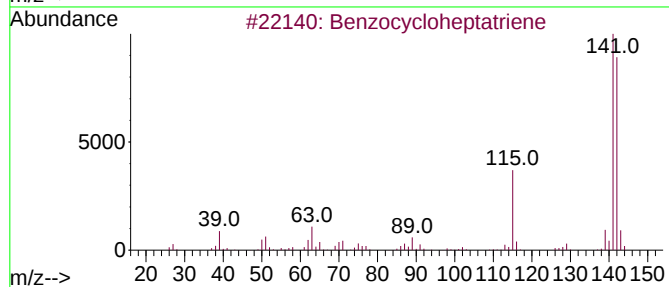
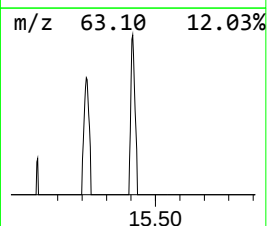
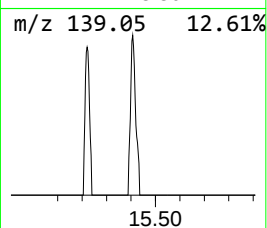
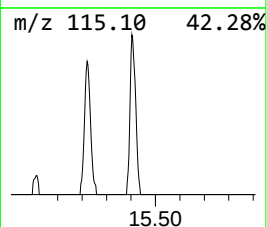
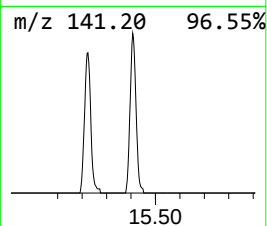
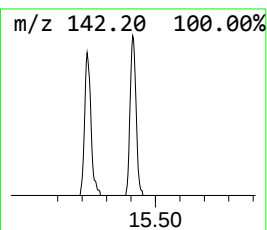
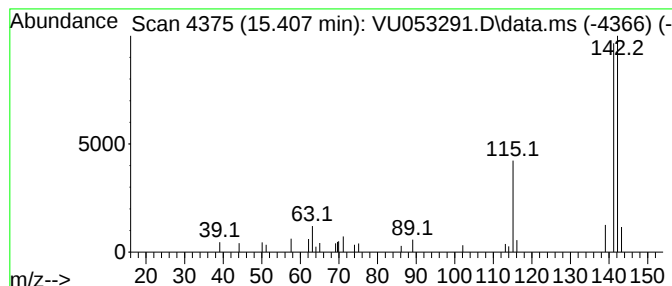
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Benzocycloheptatriene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.407	3.53 ug/L	23828	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzocycloheptatriene	142	C11H10	000264-09-5	94
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94
3			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94
4			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94
5			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031723\
Data File : VU053291.D
Acq On : 18 Mar 2023 01:32
Operator : JC/MD
Sample : VIBLK114
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VIBLK114

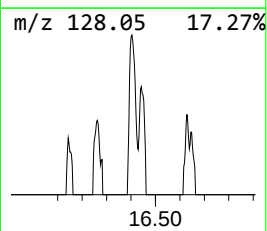
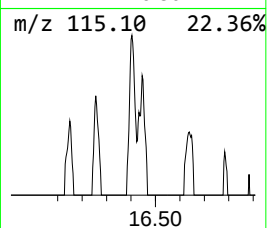
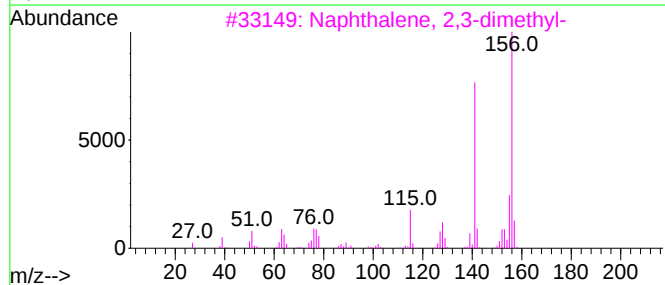
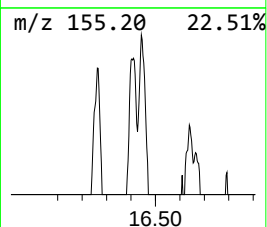
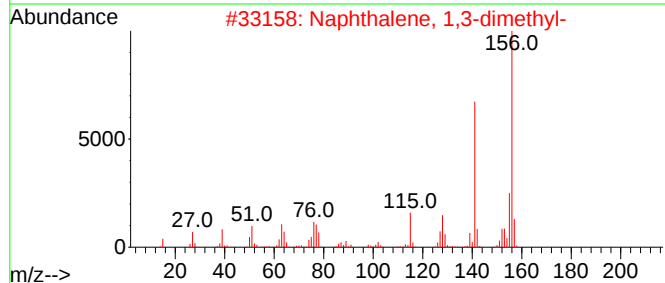
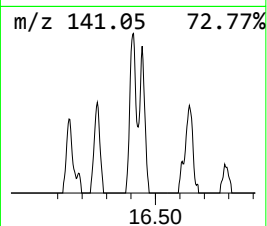
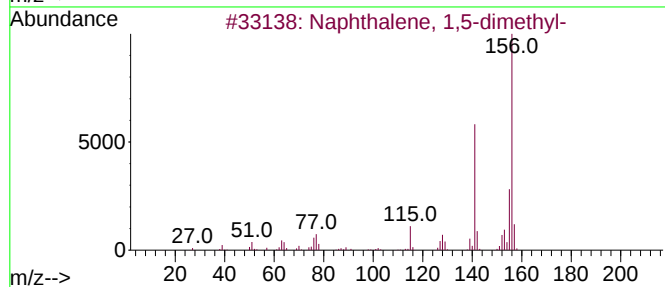
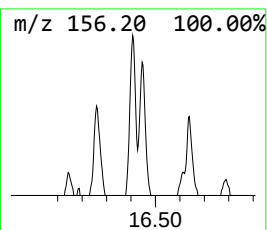
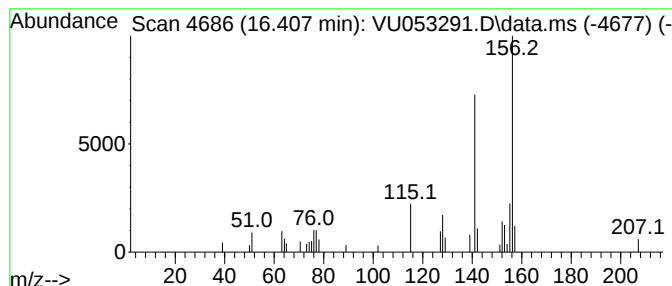
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Quant Title : VOC Analysis

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

Peak Number 5 Naphthalene, 1,5-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.407	3.14 ug/L	21202	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97
2			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96
3			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	96
4			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	96
5			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031723\
Data File : VU053291.D
Acq On : 18 Mar 2023 01:32
Operator : JC/MD
Sample : VIBLK114
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VIBLK114

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM031523WMA.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
Sulfur dioxide	1.465	3.5	ug/L	20577	1	6.243	292118	50.0
1,4-Methanonaph...	15.220	3.3	ug/L	22329	3	11.809	337284	50.0
Benzocyclohepta...	15.407	3.5	ug/L	23828	3	11.809	337284	50.0
Naphthalene, 1,...	16.407	3.1	ug/L	21202	3	11.809	337284	50.0