

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072922\
 Data File : VV027091.D
 Acq On : 29 Jul 2022 17:44
 Operator : SY/MD
 Sample : N3899-01 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DBUR0

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_V\Method\SFAMVLM072822WMA.M

Title : VOC Analysis

Signal : TIC: VV027091.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.301	74	81	102	rVB	318924	343845	4.63%	1.407%
2	1.565	155	163	177	rVB	269504	312702	4.21%	1.279%
3	2.101	319	330	347	rBV	574409	812068	10.93%	3.323%
4	2.500	446	454	470	rVB2	11571	20070	0.27%	0.082%
5	2.616	481	490	499	rVV4	3468	6433	0.09%	0.026%
6	2.822	547	554	556	rBV2	320	430	0.01%	0.002%
7	2.912	577	582	587	rVB2	667	542	0.01%	0.002%
8	3.204	669	673	679	rVB2	348	350	0.00%	0.001%
9	3.352	716	719	722	rBV3	416	331	0.00%	0.001%
10	3.455	749	751	756	rBV	393	326	0.00%	0.001%
11	3.587	787	792	795	rBV2	368	355	0.00%	0.001%
12	3.892	873	887	913	rBV2	106568	403396	5.43%	1.650%
13	4.343	1012	1027	1051	rBV	362200	891828	12.00%	3.649%
14	4.870	1188	1191	1196	rVB3	553	433	0.01%	0.002%
15	4.944	1211	1214	1222	rVB3	428	392	0.01%	0.002%
16	5.040	1227	1244	1296	rBV2	872771	2294145	30.86%	9.386%
17	5.375	1344	1348	1354	rVB6	876	1018	0.01%	0.004%
18	5.400	1354	1356	1358	rBV2	509	339	0.00%	0.001%
19	5.413	1358	1360	1368	rVB6	911	819	0.01%	0.003%
20	5.506	1384	1389	1395	rVB4	508	645	0.01%	0.003%
21	5.613	1410	1422	1460	rBV	559195	1171881	15.77%	4.795%
22	5.905	1502	1513	1529	rBV4	14650	31313	0.42%	0.128%
23	6.066	1547	1563	1598	rBV	496763	1044955	14.06%	4.275%
24	6.275	1625	1628	1635	rVB4	807	728	0.01%	0.003%
25	6.320	1639	1642	1646	rVB3	436	317	0.00%	0.001%
26	6.365	1652	1656	1660	rBV3	577	460	0.01%	0.002%
27	6.529	1703	1707	1709	rBV2	404	326	0.00%	0.001%
28	6.584	1720	1724	1728	rVB4	911	712	0.01%	0.003%
29	6.664	1743	1749	1751	rBV2	871	915	0.01%	0.004%
30	6.751	1774	1776	1780	rVB3	526	405	0.01%	0.002%
31	6.773	1780	1783	1787	rVB4	366	358	0.00%	0.001%
32	6.879	1811	1816	1819	rBV2	453	405	0.01%	0.002%
33	6.982	1838	1848	1873	rBV	221650	428009	5.76%	1.751%
34	7.204	1914	1917	1921	rVB5	861	735	0.01%	0.003%
35	7.313	1939	1951	1985	rBV	952209	1706509	22.96%	6.982%
36	7.619	2036	2046	2081	rVV	161081	301936	4.06%	1.235%

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.M
 Title : VOC Analysis

37	7.844	2113	2116	2119	rBV3	688	452	0.01%	0.002%
38	7.973	2151	2156	2158	rBV3	2021	1686	0.02%	0.007%
39	8.092	2181	2193	2229	rBV	434082	1023156	13.77%	4.186%
40	8.593	2347	2349	2352	rBV2	432	332	0.00%	0.001%
41	8.667	2368	2372	2376	rBV3	415	321	0.00%	0.001%
42	8.776	2400	2406	2407	rBV3	465	333	0.00%	0.001%
43	8.850	2417	2429	2451	rBV	884282	1457107	19.60%	5.962%
44	9.043	2487	2489	2494	rVB4	556	424	0.01%	0.002%
45	9.143	2511	2520	2537	rBV	21355	37999	0.51%	0.155%
46	9.304	2567	2570	2577	rVB3	632	630	0.01%	0.003%
47	9.365	2583	2589	2593	rBV3	405	352	0.00%	0.001%
48	9.458	2615	2618	2621	rBV3	392	326	0.00%	0.001%
49	9.545	2636	2645	2662	rBV	27231	44616	0.60%	0.183%
50	9.802	2721	2725	2733	rVB3	515	633	0.01%	0.003%
51	9.937	2758	2767	2776	rBV4	2800	4116	0.06%	0.017%
52	10.001	2783	2787	2790	rBV2	400	320	0.00%	0.001%
53	10.050	2799	2802	2807	rVB2	384	391	0.01%	0.002%
54	10.079	2807	2811	2813	rBV2	533	398	0.01%	0.002%
55	10.153	2830	2834	2840	rBV2	240	324	0.00%	0.001%
56	10.214	2840	2853	2882	rBV	725137	1170000	15.74%	4.787%
57	10.391	2906	2908	2913	rBV3	524	451	0.01%	0.002%
58	10.477	2932	2935	2939	rVV3	698	643	0.01%	0.003%
59	10.545	2950	2956	2963	rVV4	1079	1310	0.02%	0.005%
60	10.664	2990	2993	2998	rBV	442	332	0.00%	0.001%
61	10.709	3000	3007	3009	rBV2	459	523	0.01%	0.002%
62	10.738	3010	3016	3029	rVB4	2906	4818	0.06%	0.020%
63	10.847	3045	3050	3052	rBV3	547	503	0.01%	0.002%
64	10.915	3061	3071	3085	rVV	17837	28611	0.38%	0.117%
65	11.172	3139	3151	3163	rBV	31592	49721	0.67%	0.203%
66	11.249	3163	3175	3196	rVV	839396	1307299	17.59%	5.349%
67	11.336	3196	3202	3215	rVB2	13605	22067	0.30%	0.090%
68	11.484	3242	3248	3252	rBV3	381	497	0.01%	0.002%
69	11.529	3253	3262	3263	rBV4	4150	4460	0.06%	0.018%
70	11.622	3278	3291	3318	rBV	947175	1474019	19.83%	6.031%
71	11.747	3324	3330	3340	rVB2	10455	15990	0.22%	0.065%
72	12.027	3411	3417	3420	rVV3	1143	1104	0.01%	0.005%
73	12.117	3434	3445	3454	rBV4	8737	12839	0.17%	0.053%
74	12.198	3467	3470	3478	rVB2	431	567	0.01%	0.002%
75	12.307	3500	3504	3507	rBV4	625	525	0.01%	0.002%
76	12.365	3513	3522	3531	rBV3	10029	16043	0.22%	0.066%

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 Title : VOC Analysis

77	12.413	3531	3537	3544	rVB4	1586	1973	0.03%	0.008%
78	12.468	3545	3554	3564	rBV4	24180	44121	0.59%	0.181%
79	12.725	3628	3634	3647	rBV5	1786	3006	0.04%	0.012%
80	12.850	3669	3673	3676	rVV3	415	359	0.00%	0.001%
81	12.886	3676	3684	3691	rVV5	3471	5160	0.07%	0.021%
82	13.043	3726	3733	3734	rBV3	613	615	0.01%	0.003%
83	13.130	3757	3760	3763	rVB2	689	421	0.01%	0.002%
84	13.300	3809	3813	3816	rBV4	511	412	0.01%	0.002%
85	13.329	3818	3822	3825	rBV5	529	445	0.01%	0.002%
86	13.368	3830	3834	3840	rBV4	824	847	0.01%	0.003%
87	13.500	3862	3875	3901	rBV	5204563	7432906	100.00%	30.411%
88	13.622	3903	3913	3936	rVB	166746	275943	3.71%	1.129%
89	13.812	3967	3972	3976	rBV3	1014	908	0.01%	0.004%
90	13.915	4002	4004	4009	rVB4	905	577	0.01%	0.002%
91	14.085	4051	4057	4058	rBV4	1258	1173	0.02%	0.005%
92	14.127	4066	4070	4073	rBV4	830	601	0.01%	0.002%
93	14.175	4083	4085	4090	rVB2	627	453	0.01%	0.002%
94	14.310	4123	4127	4129	rBV3	511	442	0.01%	0.002%
95	14.580	4204	4211	4218	rVV5	3550	5215	0.07%	0.021%
96	14.632	4218	4227	4248	rVV	50182	79958	1.08%	0.327%
97	14.815	4273	4284	4304	rBV	72451	115749	1.56%	0.474%
98	15.368	4452	4456	4462	rBV5	1848	2164	0.03%	0.009%
99	15.484	4490	4492	4494	rBV2	767	415	0.01%	0.002%
100	15.541	4507	4510	4512	rBV4	916	692	0.01%	0.003%

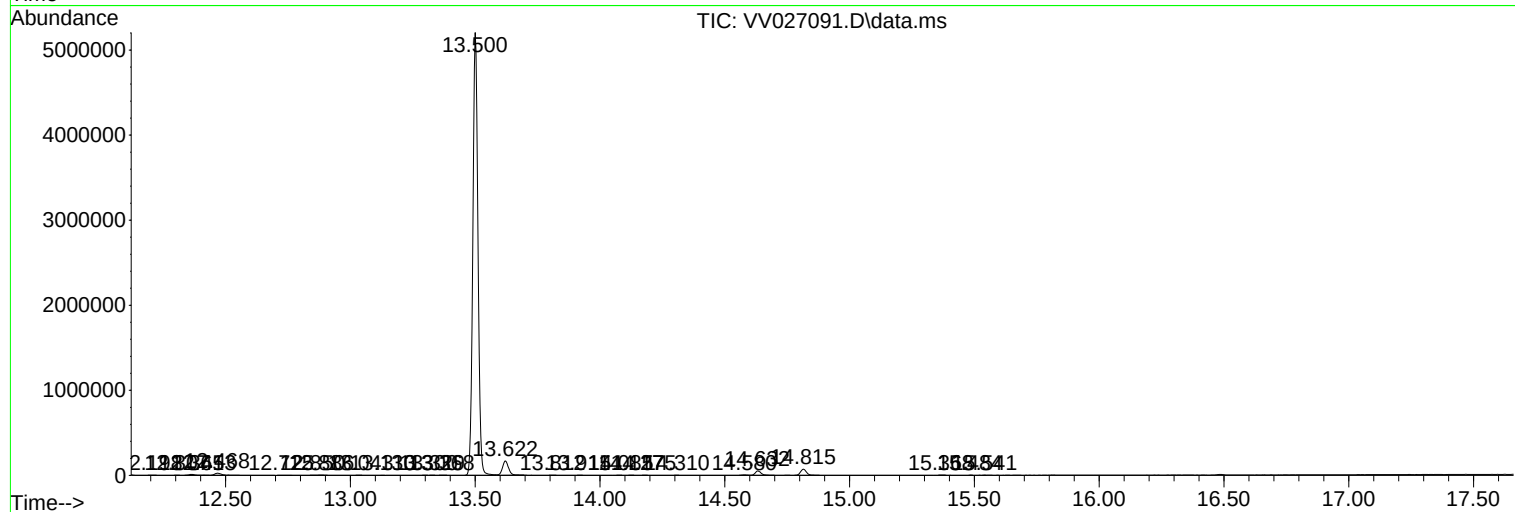
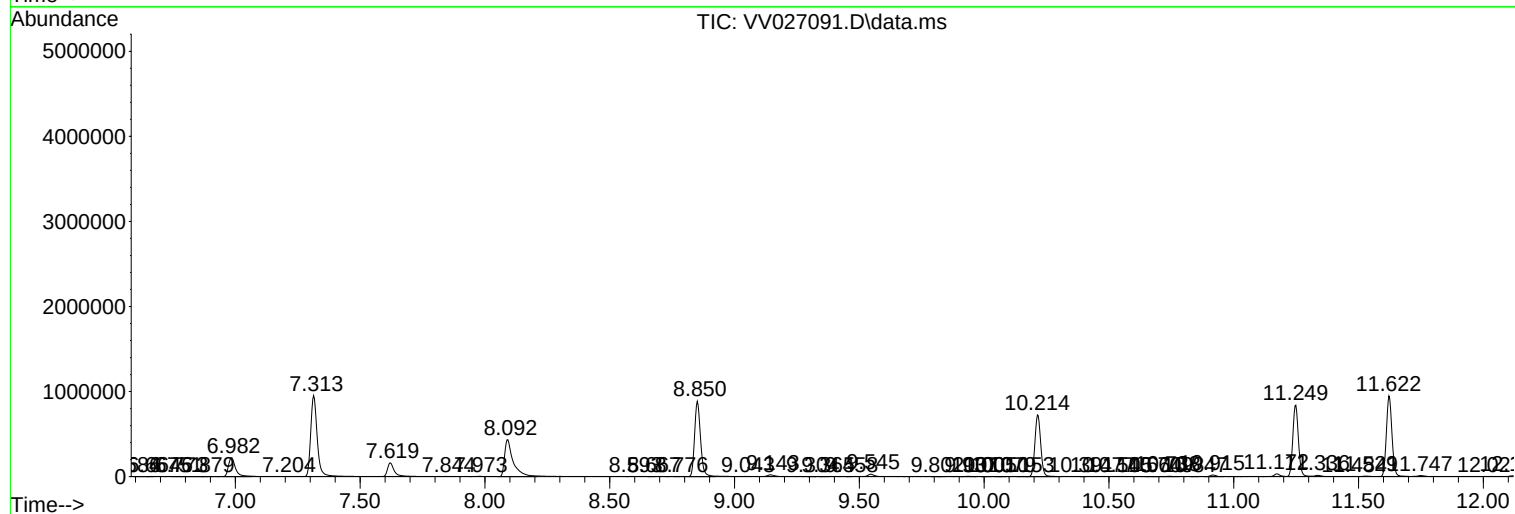
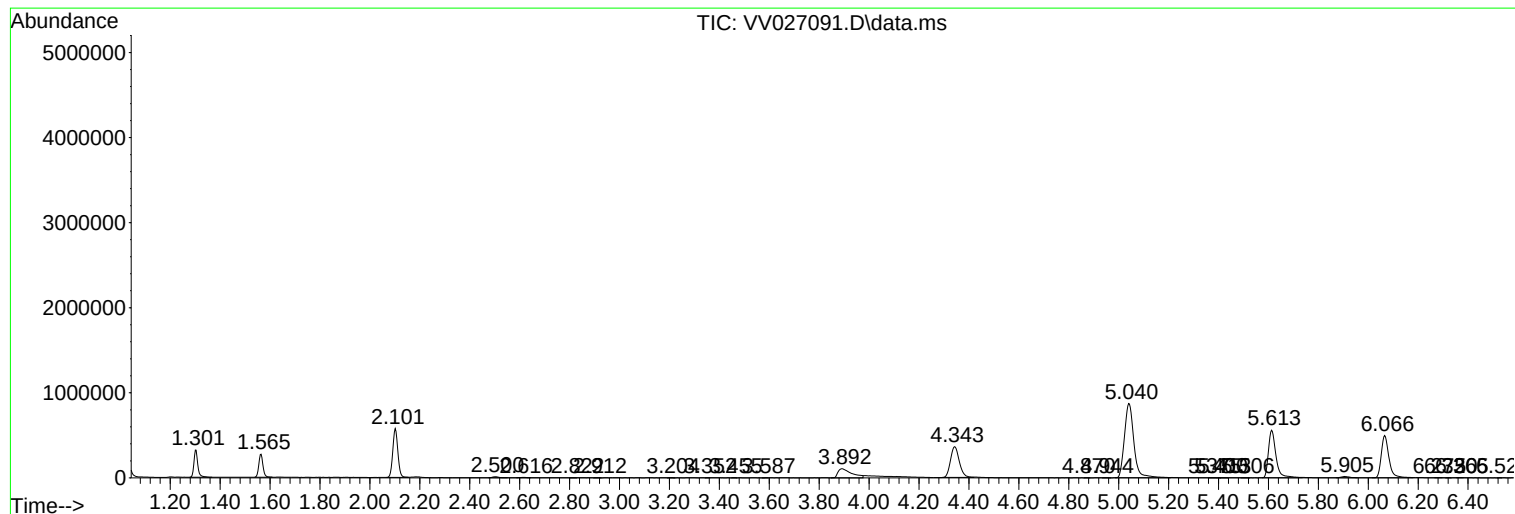
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.M
Quant Title : VOC Analysis

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



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DBUR0

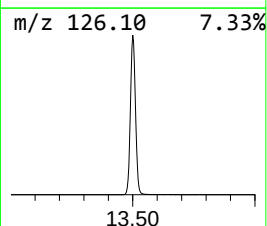
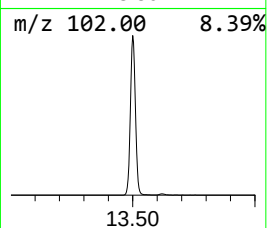
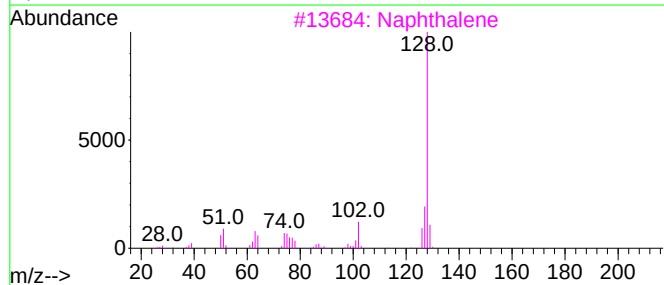
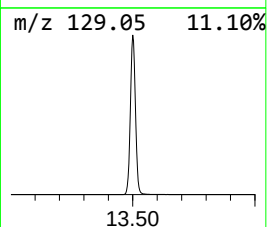
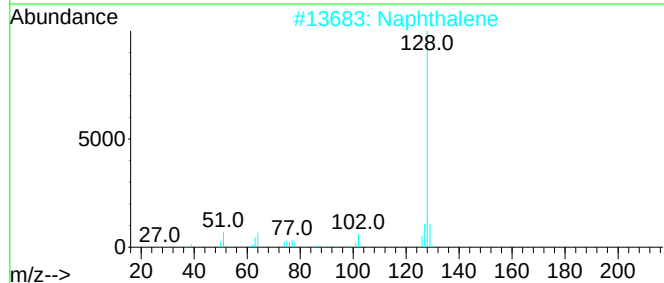
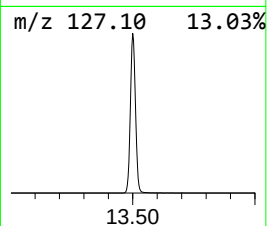
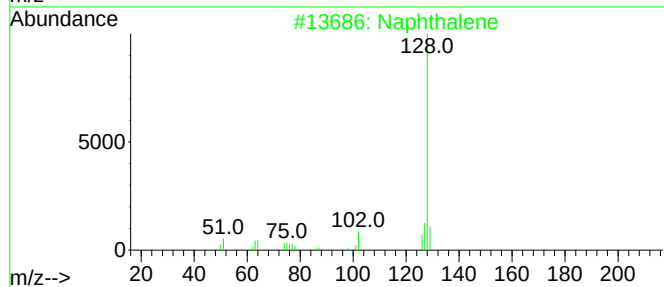
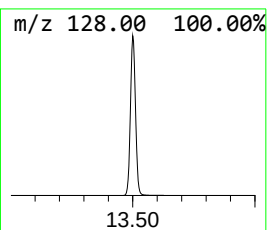
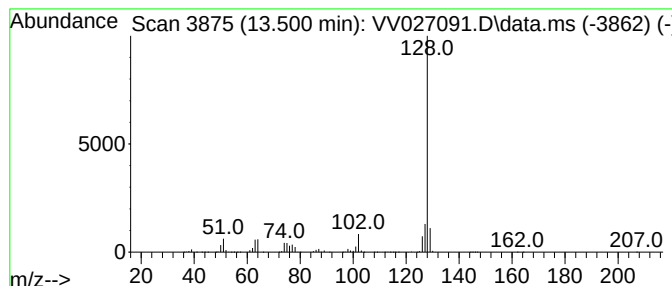
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.500	284.29 ug/L	7432910	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Naphthalene	128	C10H8	000091-20-3	94
3			Naphthalene	128	C10H8	000091-20-3	94
4			Azulene	128	C10H8	000275-51-4	93
5			Azulene	128	C10H8	000275-51-4	91



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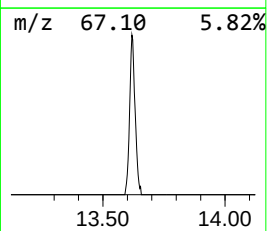
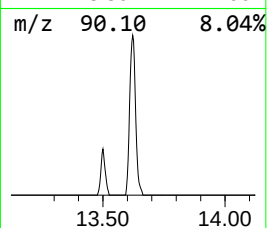
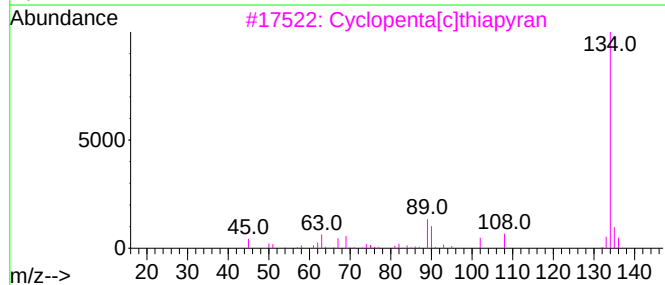
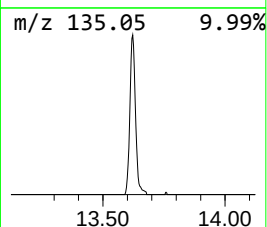
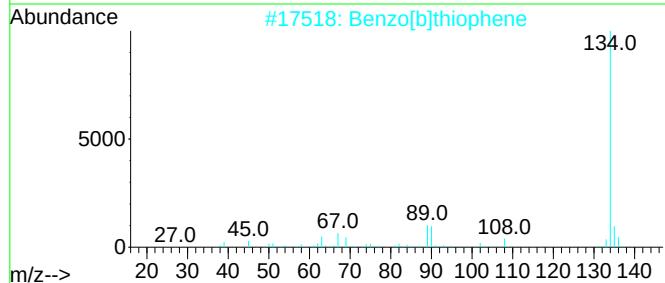
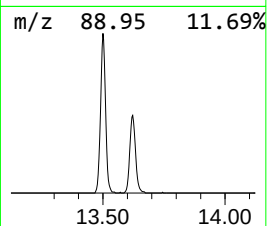
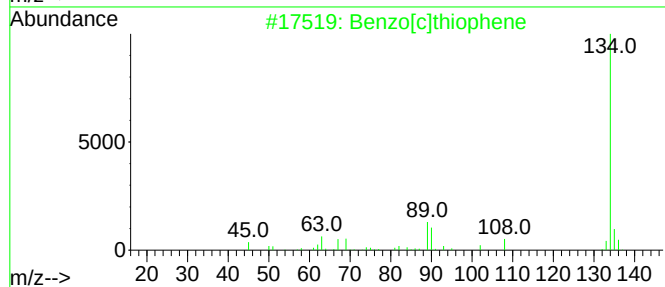
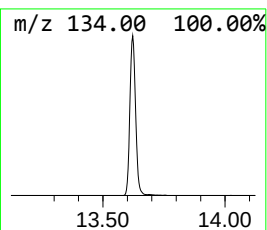
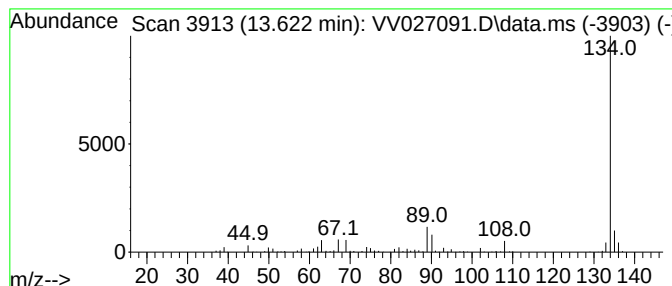
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Benzo[c]thiophene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.622	10.55 ug/L	275943	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[c]thiophene	134	C8H6S	000270-82-6	97
2			Benzo[b]thiophene	134	C8H6S	000095-15-8	95
3			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	94
4			Benzo[b]thiophene	134	C8H6S	000095-15-8	93
5			Benzo[b]thiophene	134	C8H6S	000095-15-8	91



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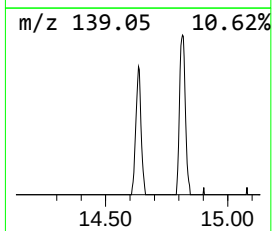
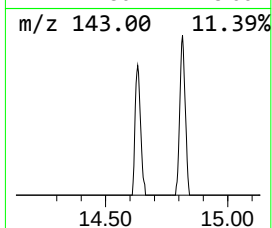
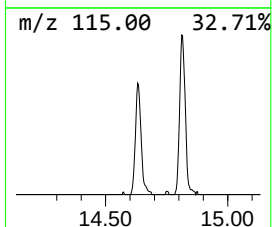
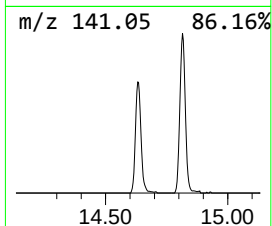
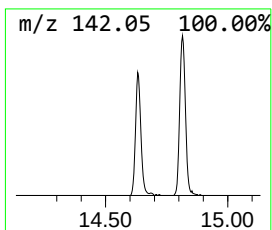
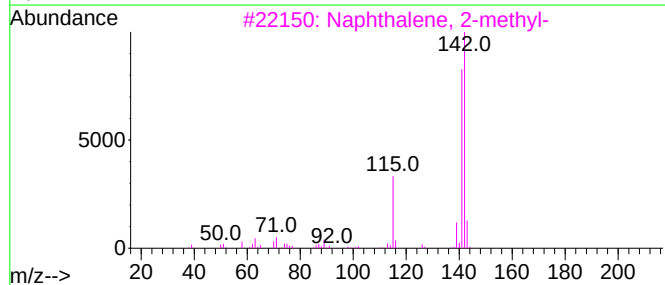
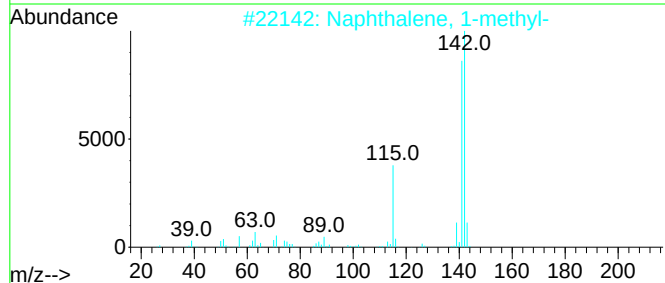
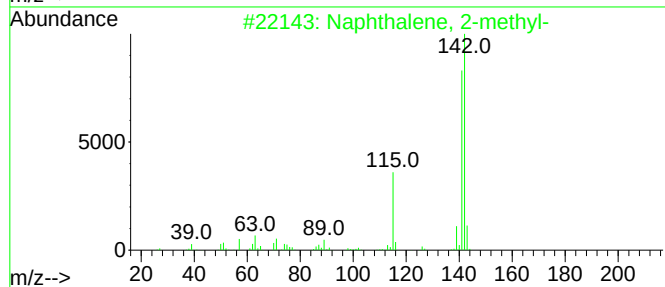
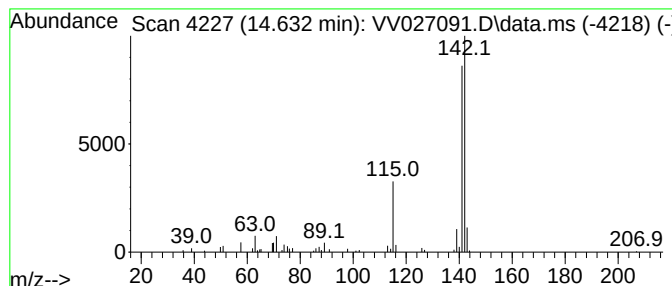
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Naphthalene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.632	3.06 ug/L	79958	1,4-Dichlorobenzene-d4	11.249

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
4		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94
5		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072922\
Data File : VV027091.D
Acq On : 29 Jul 2022 17:44
Operator : SY/MD
Sample : N3899-01 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DBUR0

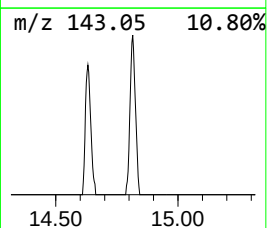
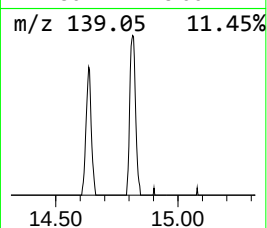
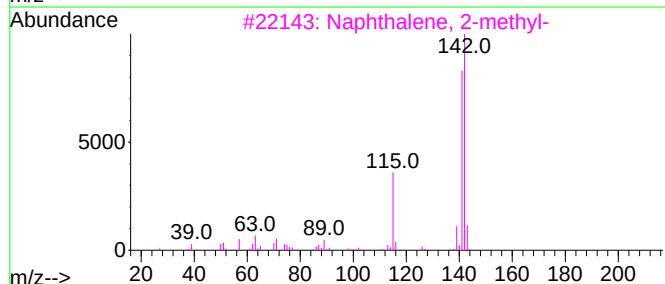
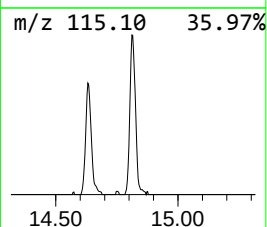
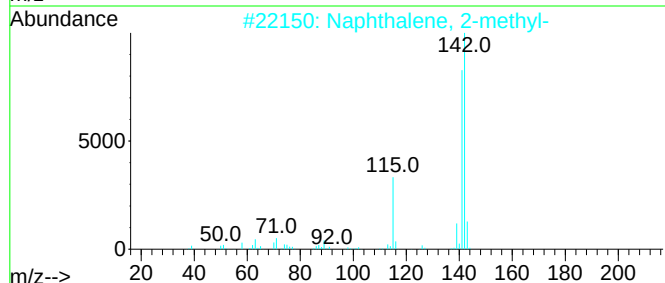
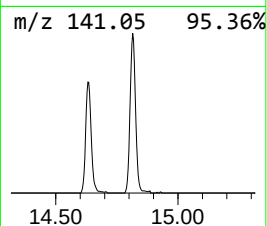
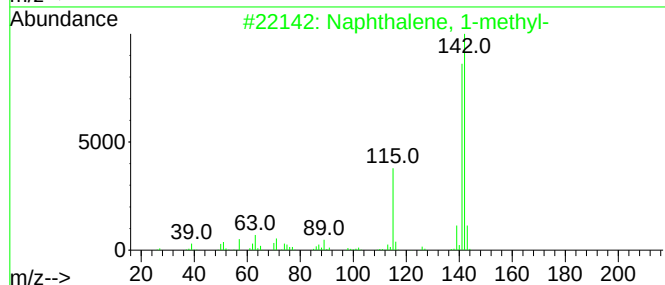
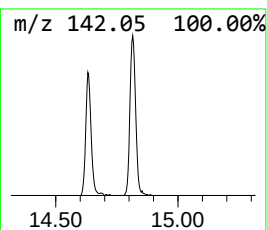
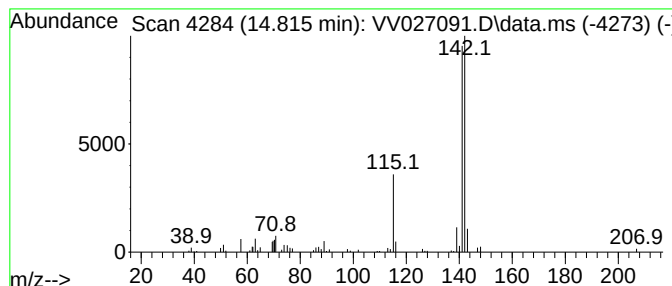
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Quant Title : VOC Analysis

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

Peak Number 5 Naphthalene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.815	4.43 ug/L	115749	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072922\
Data File : VV027091.D
Acq On : 29 Jul 2022 17:44
Operator : SY/MD
Sample : N3899-01 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DBUR0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072822WMA.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
Azulene	13.500	284.3	ug/L	7432910	3	11.249	1307300	50.0
Benzo[c]thiophene	13.622	10.6	ug/L	275943	3	11.249	1307300	50.0
Naphthalene, 2-...	14.632	3.1	ug/L	79958	3	11.249	1307300	50.0
Naphthalene, 1-...	14.815	4.4	ug/L	115749	3	11.249	1307300	50.0