

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU010722\
 Data File : VU046696.D
 Acq On : 07 Jan 2022 15:52
 Operator : SY/MD
 Sample : N1025-04ME
 Misc : 6.80g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGLG8ME

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\SFAMULM010522WMA.M
 Title : VOC Analysis

Signal : TIC: VU046696.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.604	74	82	90	rBV	33974	58065	8.72%	0.851%
2	1.893	163	172	174	rBV	7536	9779	1.47%	0.143%
3	1.922	176	181	188	rVV	10822	16683	2.51%	0.244%
4	2.562	369	380	399	rBV	99600	172640	25.93%	2.530%
5	2.909	486	488	493	rVB	272	264	0.04%	0.004%
6	2.961	499	504	506	rBV2	304	279	0.04%	0.004%
7	3.051	524	532	533	rBV3	764	872	0.13%	0.013%
8	3.189	562	575	587	rBV	2496	5999	0.90%	0.088%
9	3.372	628	632	638	rBV	177	272	0.04%	0.004%
10	4.681	1019	1039	1085	rBV2	24950	171936	25.82%	2.520%
11	5.073	1145	1161	1198	rVB	96993	268030	40.25%	3.928%
12	5.726	1345	1364	1390	rBV2	267774	665864	100.00%	9.757%
13	5.989	1435	1446	1462	rBV4	3373	8699	1.31%	0.127%
14	6.134	1488	1491	1495	rBV2	441	364	0.05%	0.005%
15	6.253	1512	1528	1559	rBV	218193	456953	68.63%	6.696%
16	6.530	1608	1614	1617	rVV4	1156	1367	0.21%	0.020%
17	6.610	1629	1639	1652	rBV2	1611	3779	0.57%	0.055%
18	6.697	1652	1666	1693	rVB	138323	295539	44.38%	4.331%
19	7.224	1825	1830	1833	rVV3	641	589	0.09%	0.009%
20	7.240	1833	1835	1843	rVB2	678	711	0.11%	0.010%
21	7.571	1925	1938	1963	rVV	68943	146480	22.00%	2.146%
22	7.902	2027	2041	2058	rBV	274947	531400	79.81%	7.787%
23	8.189	2118	2130	2160	rVV2	38507	100988	15.17%	1.480%
24	8.697	2263	2288	2328	rBV	110638	386836	58.10%	5.669%
25	8.857	2336	2338	2352	rVB3	778	1124	0.17%	0.016%
26	8.922	2356	2358	2361	rBV2	466	276	0.04%	0.004%
27	8.954	2365	2368	2371	rBB3	369	277	0.04%	0.004%
28	9.127	2415	2422	2426	rVB3	597	825	0.12%	0.012%
29	9.163	2427	2433	2435	rBV	759	691	0.10%	0.010%
30	9.211	2440	2448	2458	rVB4	2821	4413	0.66%	0.065%
31	9.340	2480	2488	2496	rBB3	2954	3989	0.60%	0.058%
32	9.426	2499	2515	2547	rBV	228050	581241	87.29%	8.517%
33	9.578	2551	2562	2574	rBV	7902	14776	2.22%	0.217%
34	9.703	2588	2601	2617	rVV2	21987	49330	7.41%	0.723%
35	9.761	2617	2619	2624	rVV	614	499	0.07%	0.007%
36	10.021	2690	2700	2707	rBV6	3036	5107	0.77%	0.075%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM010522WMA.M
 Title : VOC Analysis

37	10.115	2718	2729	2740	rVV2	9280	18685	2.81%	0.274%
38	10.169	2741	2746	2753	rVB3	1116	1335	0.20%	0.020%
39	10.253	2763	2772	2782	rVB5	5757	8936	1.34%	0.131%
40	10.324	2784	2794	2795	rBV2	791	881	0.13%	0.013%
41	10.359	2797	2805	2811	rBV7	2781	4628	0.70%	0.068%
42	10.465	2832	2838	2840	rBV6	1309	1434	0.22%	0.021%
43	10.494	2840	2847	2856	rVB6	2596	4897	0.74%	0.072%
44	10.558	2856	2867	2875	rBV7	3942	7827	1.18%	0.115%
45	10.725	2914	2919	2920	rBV3	999	777	0.12%	0.011%
46	10.777	2922	2935	2957	rVB	218995	393536	59.10%	5.767%
47	10.918	2967	2979	2988	rBV	5336	10210	1.53%	0.150%
48	10.957	2988	2991	2998	rVB4	1197	1236	0.19%	0.018%
49	11.024	2998	3012	3020	rBV6	7248	19328	2.90%	0.283%
50	11.205	3057	3068	3075	rBV7	1740	3515	0.53%	0.052%
51	11.246	3075	3081	3082	rBV2	714	648	0.10%	0.009%
52	11.311	3090	3101	3114	rBV5	8157	16654	2.50%	0.244%
53	11.375	3115	3121	3127	rVV4	4823	6953	1.04%	0.102%
54	11.420	3128	3135	3142	rVV3	12545	19676	2.95%	0.288%
55	11.478	3143	3153	3172	rVB	53911	101682	15.27%	1.490%
56	11.578	3174	3184	3190	rBV3	5806	9478	1.42%	0.139%
57	11.709	3216	3225	3233	rBV8	8563	15572	2.34%	0.228%
58	11.822	3249	3260	3272	rBV	379544	614112	92.23%	8.999%
59	12.108	3339	3349	3360	rBV10	5812	12549	1.88%	0.184%
60	12.205	3366	3379	3392	rVB	336006	561354	84.30%	8.226%
61	12.275	3392	3401	3408	rBV6	1983	4617	0.69%	0.068%
62	12.388	3430	3436	3450	rVB6	6905	15102	2.27%	0.221%
63	12.475	3455	3463	3464	rBV	6050	6465	0.97%	0.095%
64	12.668	3517	3523	3531	rBV6	4535	6200	0.93%	0.091%
65	12.848	3566	3579	3585	rVB10	4379	9120	1.37%	0.134%
66	13.198	3685	3688	3692	rVB3	911	613	0.09%	0.009%
67	13.259	3703	3707	3711	rVB4	1037	720	0.11%	0.011%
68	13.291	3714	3717	3728	rVB7	2225	3243	0.49%	0.048%
69	13.352	3728	3736	3745	rBV7	2618	4285	0.64%	0.063%
70	13.462	3745	3770	3786	rBV7	9822	27998	4.20%	0.410%
71	13.532	3786	3792	3797	rBV7	1223	1879	0.28%	0.028%
72	13.590	3805	3810	3818	rVB2	5315	5810	0.87%	0.085%
73	13.735	3848	3855	3865	rBV6	1361	2280	0.34%	0.033%
74	13.844	3882	3889	3902	rVB10	4771	7197	1.08%	0.105%
75	13.947	3915	3921	3922	rBV	1119	858	0.13%	0.013%
76	13.960	3922	3925	3926	rBV2	1179	612	0.09%	0.009%

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 ClientSampleId :
 BGLG8ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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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\SFAMULM010522WMA.M

Title : VOC Analysis

77	14.092	3947	3966	3984	rVB	353418	561318	84.30%	8.225%
78	14.195	3986	3998	4014	rVB3	10049	20871	3.13%	0.306%
79	14.269	4019	4021	4022	rBV2	1145	379	0.06%	0.006%
80	14.452	4069	4078	4085	rBV2	6373	9422	1.42%	0.138%
81	14.491	4085	4090	4094	rVV4	2329	2337	0.35%	0.034%
82	14.648	4134	4139	4141	rBV4	1822	1695	0.25%	0.025%
83	14.854	4199	4203	4205	rBV5	736	592	0.09%	0.009%
84	14.876	4207	4210	4212	rBV3	922	534	0.08%	0.008%
85	14.921	4221	4224	4225	rBV3	646	407	0.06%	0.006%
86	14.944	4226	4231	4235	rVV6	1412	1471	0.22%	0.022%
87	15.024	4249	4256	4264	rBV8	3022	4646	0.70%	0.068%
88	15.073	4265	4271	4278	rVB6	2372	3373	0.51%	0.049%
89	15.224	4306	4318	4329	rBV	62377	101542	15.25%	1.488%
90	15.349	4349	4357	4359	rBV4	1132	1416	0.21%	0.021%
91	15.410	4365	4376	4400	rVB2	70866	123015	18.47%	1.803%
92	15.619	4439	4441	4445	rBV4	918	847	0.13%	0.012%
93	15.790	4490	4494	4497	rBV3	626	662	0.10%	0.010%
94	15.957	4531	4546	4548	rBV7	4818	9402	1.41%	0.138%
95	16.153	4599	4607	4612	rBV6	2503	3468	0.52%	0.051%
96	16.195	4613	4620	4629	rVB7	4210	7361	1.11%	0.108%
97	16.262	4633	4641	4645	rBV4	7612	11272	1.69%	0.165%
98	16.294	4646	4651	4660	rVB2	18499	24853	3.73%	0.364%
99	16.410	4681	4687	4695	rBV2	12883	17348	2.61%	0.254%
100	17.137	4908	4913	4922	rVB3	12237	16076	2.41%	0.236%

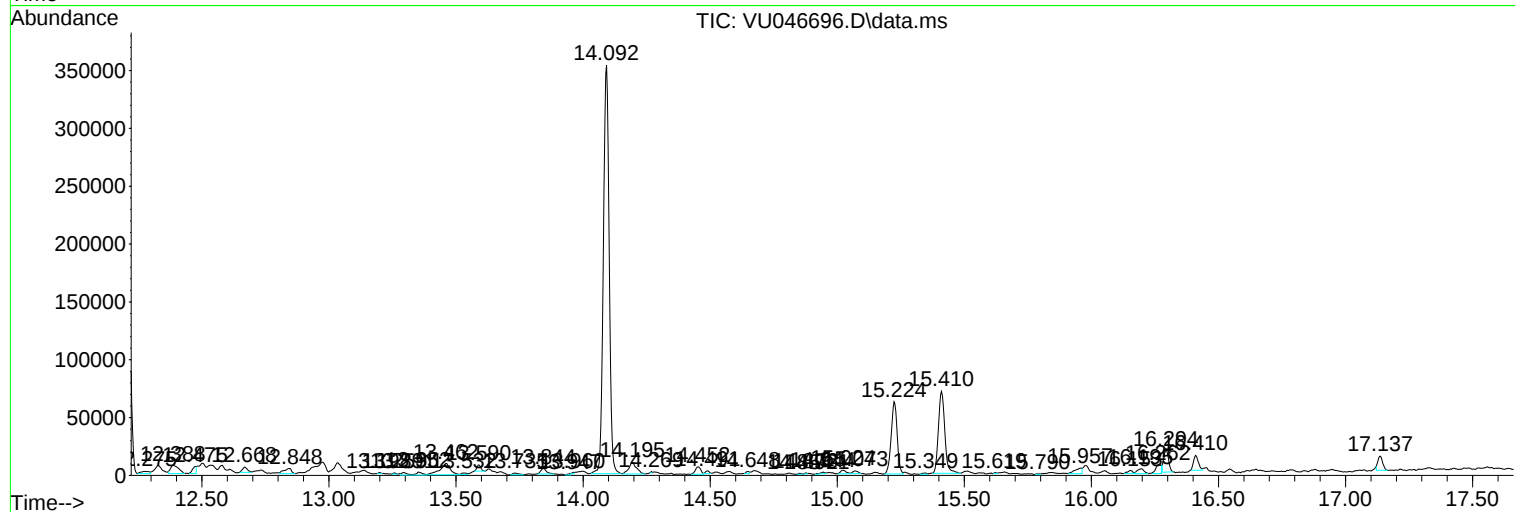
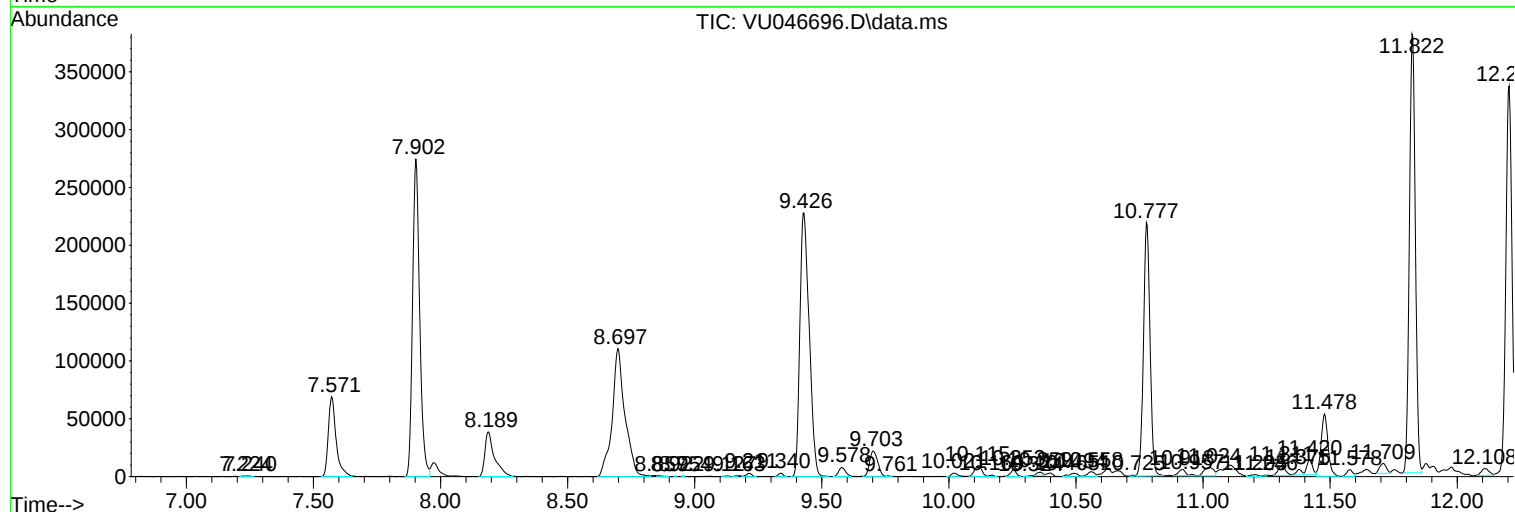
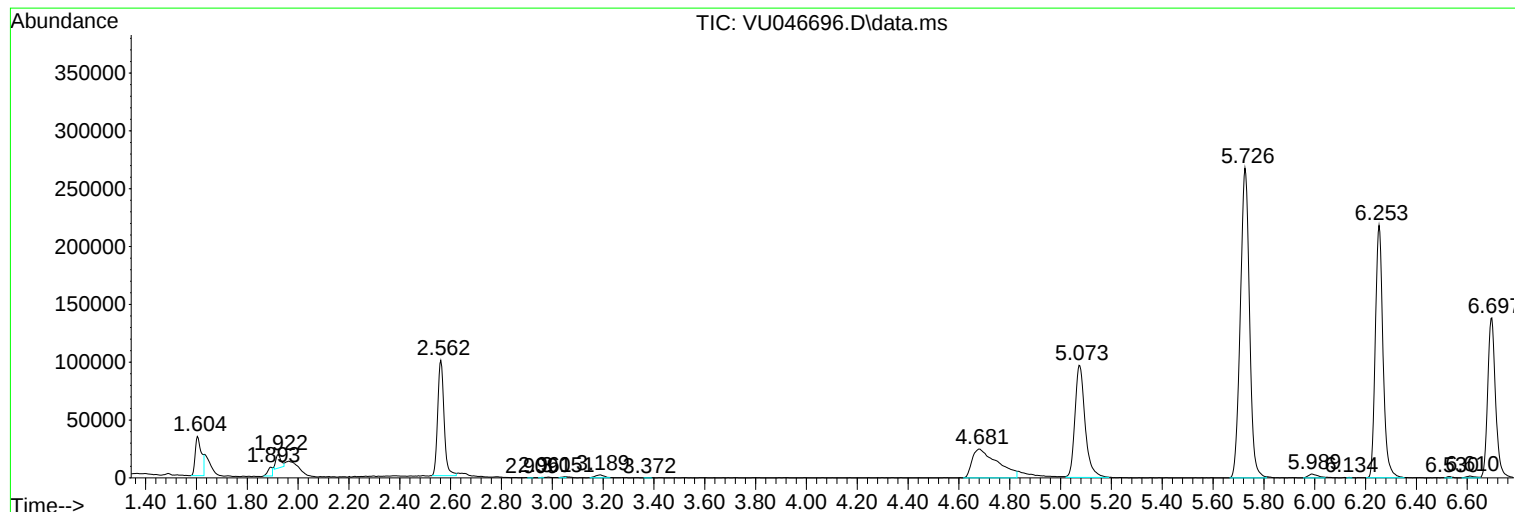
Sum of corrected areas: 6824145

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ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGLG8ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM010522WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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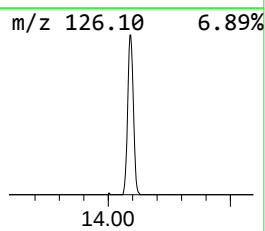
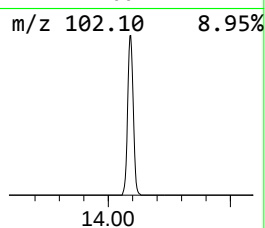
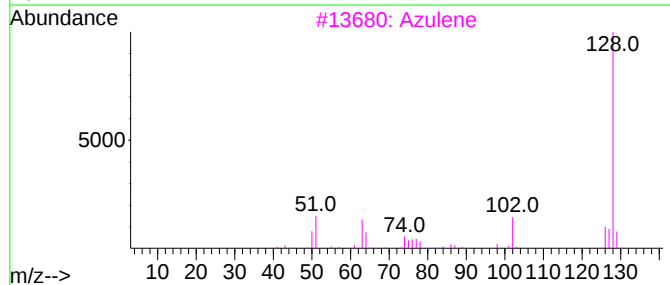
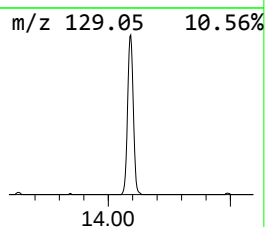
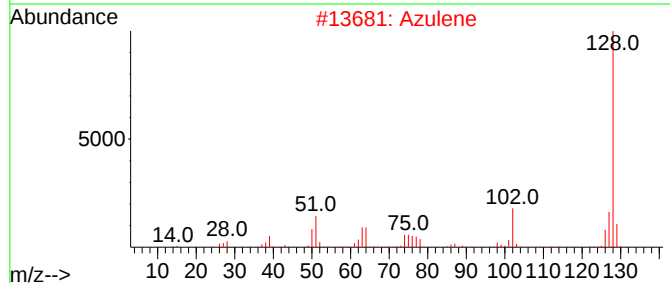
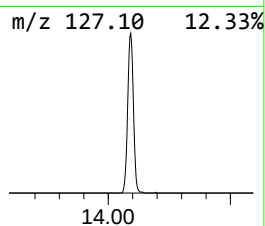
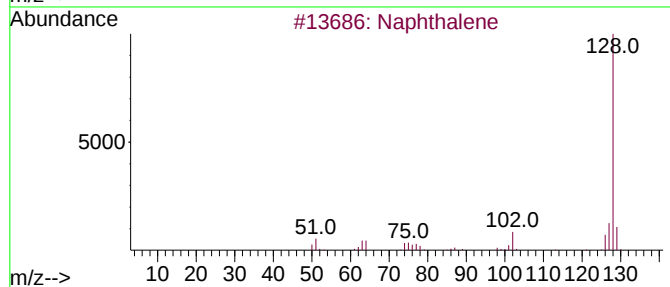
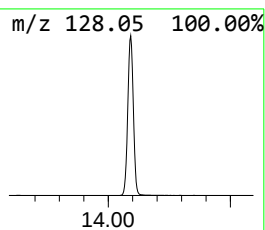
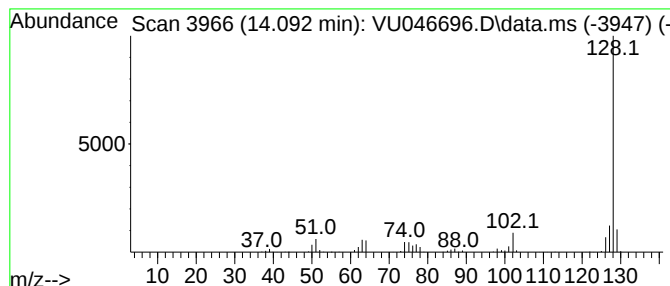
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM010522WMA.M
Quant Title : VOC Analysis

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.
14.092	45.70 ug/L	561318	1,4-Dichlorobenzene-d4	11.825

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Azulene	128	C10H8	000275-51-4	91
3			Azulene	128	C10H8	000275-51-4	91
4			Azulene	128	C10H8	000275-51-4	90
5			Azulene	128	C10H8	000275-51-4	90



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Instrument :
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ClientSampleId :
BGLG8ME

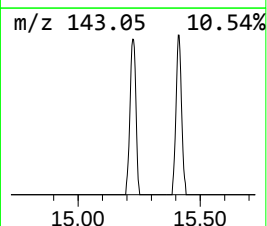
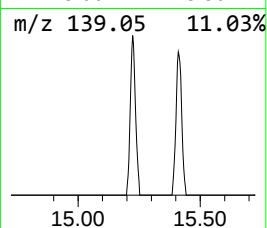
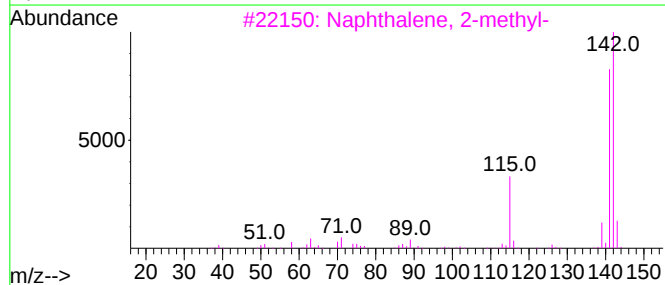
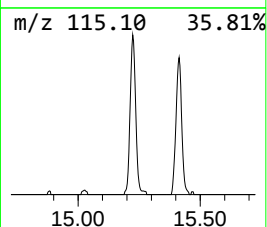
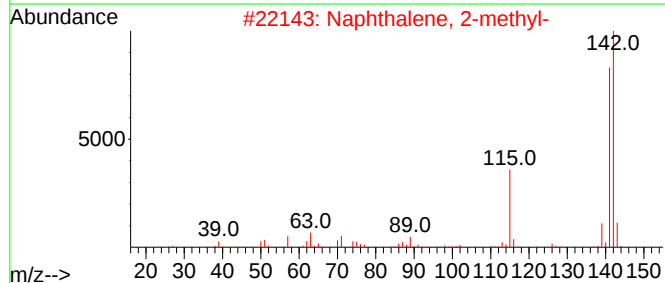
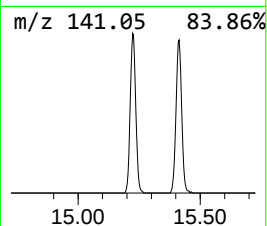
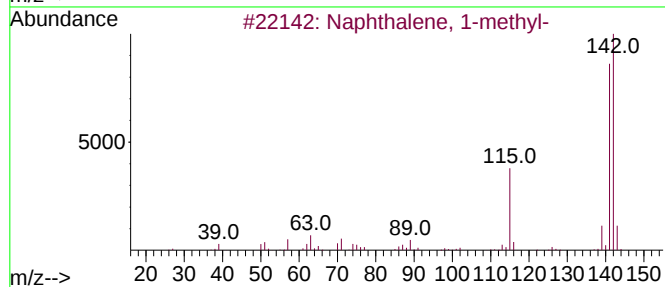
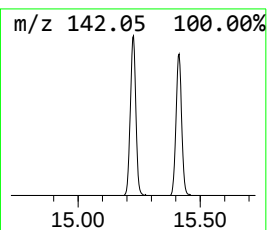
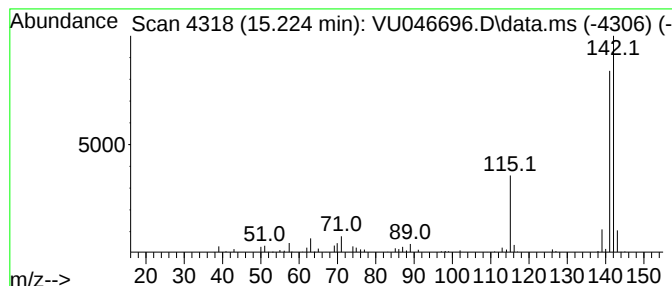
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM010522WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Naphthalene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.224	8.27 ug/L	101542	1,4-Dichlorobenzene-d4	11.825

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			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94
5			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94



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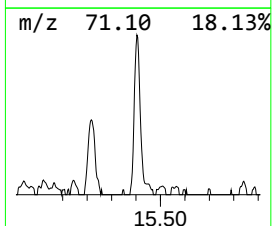
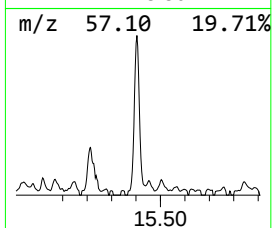
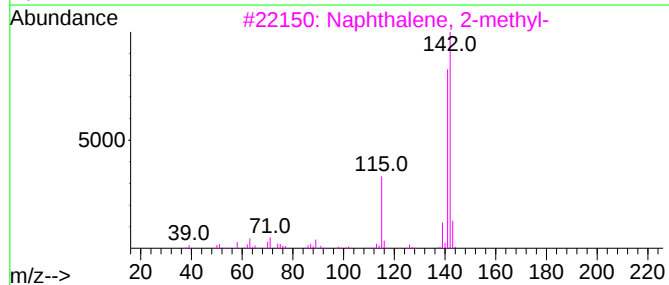
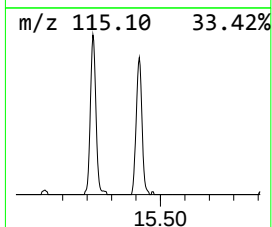
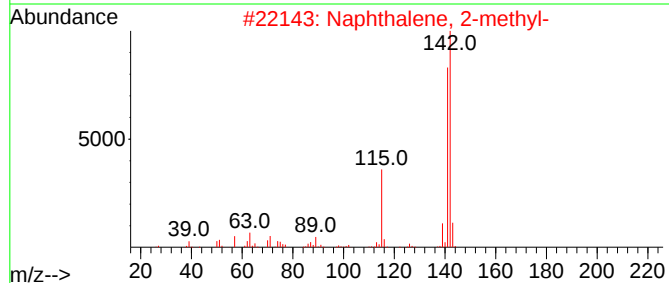
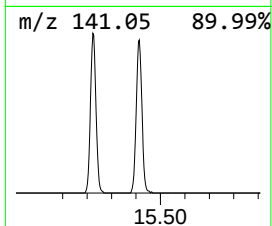
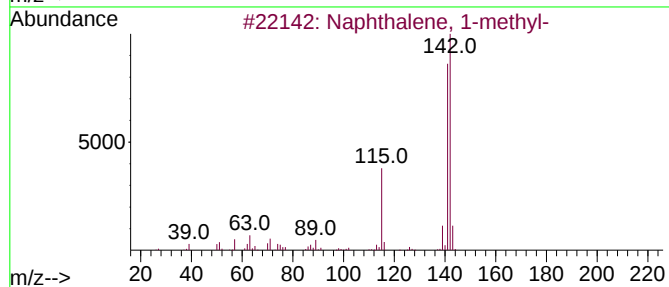
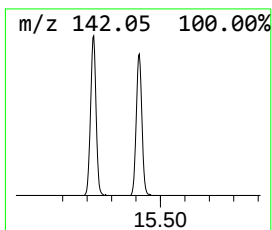
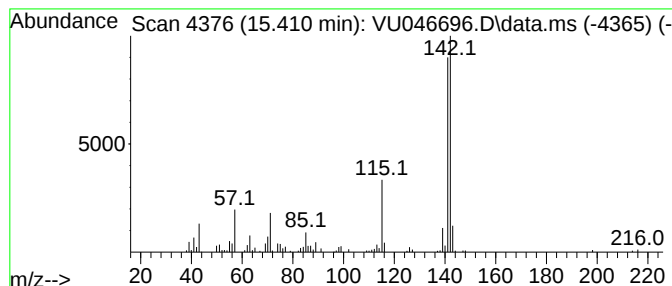
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM010522WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Naphthalene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.410	10.02 ug/L	123015	1,4-Dichlorobenzene-d4	11.825

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	95
4			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	95
5			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU010722\
Data File : VU046696.D
Acq On : 07 Jan 2022 15:52
Operator : SY/MD
Sample : N1025-04ME
Misc : 6.80g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGLG8ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM010522WMA.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	14.092	45.7	ug/L	561318	3	11.825	614112	50.0
Naphthalene, 1-...	15.224	8.3	ug/L	101542	3	11.825	614112	50.0
Naphthalene, 2-...	15.410	10.0	ug/L	123015	3	11.825	614112	50.0