

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122921\
 Data File : VX026138.D
 Acq On : 29 Dec 2021 14:57
 Operator : JC/MD
 Sample : M5194-17ME
 Misc : 6.63g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BGLC9ME

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_X\Method\SFAMXLM122821WMA.M
 Title : VOC Analysis

Signal : TIC: VX026138.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	43	47	56	rVB	150936	185950	13.60%	1.390%
2	1.660	90	94	102	rBV	103123	138994	10.17%	1.039%
3	2.288	191	197	206	rBV	330121	512818	37.51%	3.833%
4	2.782	274	278	286	rVB2	3466	7153	0.52%	0.053%
5	2.947	298	305	316	rBV	11993	27666	2.02%	0.207%
6	3.325	366	367	370	rBV2	894	797	0.06%	0.006%
7	3.349	370	371	374	rVB2	611	655	0.05%	0.005%
8	3.422	381	383	384	rBV2	768	615	0.04%	0.005%
9	3.514	396	398	403	rVB	830	816	0.06%	0.006%
10	3.684	423	426	427	rVB	736	650	0.05%	0.005%
11	3.709	427	430	432	rBV	1042	969	0.07%	0.007%
12	3.758	436	438	440	rVV2	681	589	0.04%	0.004%
13	4.117	494	497	500	rBV	783	964	0.07%	0.007%
14	4.294	522	526	528	rBV2	755	1084	0.08%	0.008%
15	4.489	549	558	594	rVV	61689	293337	21.46%	2.192%
16	5.062	640	652	672	rVV2	159218	547197	40.03%	4.090%
17	5.288	688	689	694	rVB	429	639	0.05%	0.005%
18	5.404	704	708	710	rBV2	647	659	0.05%	0.005%
19	5.489	720	722	725	rBV	773	769	0.06%	0.006%
20	5.532	727	729	732	rBV2	727	976	0.07%	0.007%
21	5.818	773	776	779	rBV	543	698	0.05%	0.005%
22	5.971	789	801	816	rVV2	486613	1367056	100.00%	10.217%
23	6.221	840	842	846	rBV	501	804	0.06%	0.006%
24	6.367	858	866	878	rBV5	3670	12126	0.89%	0.091%
25	6.544	888	895	896	rBV2	841	2007	0.15%	0.015%
26	6.763	920	931	943	rBV2	297775	729892	53.39%	5.455%
27	6.952	961	962	966	rBV2	586	636	0.05%	0.005%
28	7.037	973	976	978	rBV	740	941	0.07%	0.007%
29	7.117	982	989	999	rBV4	6863	18551	1.36%	0.139%
30	7.220	1001	1006	1007	rBV2	1304	2288	0.17%	0.017%
31	7.312	1012	1021	1036	rBV	292669	631851	46.22%	4.722%
32	7.464	1044	1046	1048	rBV3	760	946	0.07%	0.007%
33	7.604	1065	1069	1070	rBV	607	722	0.05%	0.005%
34	7.824	1102	1105	1107	rBV3	708	929	0.07%	0.007%
35	7.928	1121	1122	1124	rBV2	686	629	0.05%	0.005%
36	8.330	1182	1188	1198	rVV	195713	330170	24.15%	2.468%

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 BGLC9ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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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_X\Method\SFAMXLM122821WMA.M
 Title : VOC Analysis

37	8.482	1210	1213	1214	rBV2	902	617	0.05%	0.005%
38	8.653	1233	1241	1248	rBV	714780	1128163	82.53%	8.432%
39	8.720	1249	1252	1259	rVB	8499	14266	1.04%	0.107%
40	8.952	1285	1290	1302	rBV	139927	214552	15.69%	1.604%
41	9.116	1312	1317	1322	rVB3	1080	2193	0.16%	0.016%
42	9.244	1336	1338	1340	rVB	746	654	0.05%	0.005%
43	9.269	1340	1342	1344	rBV2	959	1051	0.08%	0.008%
44	9.342	1352	1354	1355	rBV2	791	779	0.06%	0.006%
45	9.409	1357	1365	1379	rVB	306213	653785	47.82%	4.886%
46	9.714	1413	1415	1422	rVB2	1359	1830	0.13%	0.014%
47	10.055	1466	1471	1489	rVB	562672	839064	61.38%	6.271%
48	10.195	1489	1494	1501	rBV	177124	238268	17.43%	1.781%
49	10.305	1506	1512	1525	rVB	432368	619699	45.33%	4.632%
50	10.464	1535	1538	1540	rBV2	658	625	0.05%	0.005%
51	10.586	1554	1558	1563	rBV4	1067	1890	0.14%	0.014%
52	10.647	1563	1568	1576	rVV	141993	188617	13.80%	1.410%
53	10.750	1583	1585	1587	rVV2	680	595	0.04%	0.004%
54	10.781	1588	1590	1594	rVB3	1590	1714	0.13%	0.013%
55	10.854	1600	1602	1606	rVB4	1328	1856	0.14%	0.014%
56	10.970	1614	1621	1625	rBV2	2562	4404	0.32%	0.033%
57	11.122	1642	1646	1652	rVB	7103	9965	0.73%	0.074%
58	11.201	1653	1659	1666	rBV	470223	639222	46.76%	4.777%
59	11.305	1674	1676	1684	rVB2	5822	9612	0.70%	0.072%
60	11.384	1684	1689	1696	rBV	19843	32954	2.41%	0.246%
61	11.451	1696	1700	1708	rVV	16345	25272	1.85%	0.189%
62	11.543	1713	1715	1719	rVB2	958	922	0.07%	0.007%
63	11.616	1723	1727	1734	rBV	12037	14855	1.09%	0.111%
64	11.720	1740	1744	1745	rBV2	1684	1759	0.13%	0.013%
65	11.756	1745	1750	1756	rVB	60703	76136	5.57%	0.569%
66	11.939	1776	1780	1782	rBV3	3837	5667	0.41%	0.042%
67	11.969	1782	1785	1789	rVB3	5208	7179	0.53%	0.054%
68	12.024	1789	1794	1801	rBV	667675	849206	62.12%	6.347%
69	12.091	1801	1805	1809	rVB	30394	35731	2.61%	0.267%
70	12.244	1826	1830	1834	rBV2	19199	30442	2.23%	0.228%
71	12.323	1838	1843	1851	rVB	834707	1028660	75.25%	7.688%
72	12.421	1855	1859	1863	rVB	17960	24567	1.80%	0.184%
73	12.469	1863	1867	1872	rVB	5747	7775	0.57%	0.058%
74	12.536	1874	1878	1879	rBV	6537	7262	0.53%	0.054%
75	12.616	1887	1891	1894	rBV	10811	12127	0.89%	0.091%
76	12.707	1902	1906	1914	rVB3	5129	11602	0.85%	0.087%

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 ClientSampleId :
 BGLC9ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Stop Thrs : 0

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML122821WMA.M
 Title : VOC Analysis

77	12.799	1918	1921	1924	rBV4	2200	2596	0.19%	0.019%
78	12.890	1933	1936	1939	rBV3	2898	4132	0.30%	0.031%
79	12.927	1939	1942	1945	rVV2	8545	10085	0.74%	0.075%
80	12.963	1945	1948	1956	rVV2	15982	21906	1.60%	0.164%
81	13.170	1979	1982	1986	rVB4	5219	6573	0.48%	0.049%
82	13.292	1998	2002	2007	rBV3	12778	19187	1.40%	0.143%
83	13.427	2021	2024	2032	rVB2	8091	10081	0.74%	0.075%
84	13.548	2041	2044	2046	rBV2	1163	1317	0.10%	0.010%
85	13.585	2046	2050	2057	rVB5	2418	4908	0.36%	0.037%
86	13.780	2076	2082	2093	rBV	236435	299149	21.88%	2.236%
87	13.872	2093	2097	2104	rVB2	5032	7031	0.51%	0.053%
88	14.079	2128	2131	2135	rVB2	2124	2722	0.20%	0.020%
89	14.219	2150	2154	2159	rBV3	3097	4349	0.32%	0.033%
90	14.378	2177	2180	2185	rVB3	3274	4015	0.29%	0.030%
91	14.573	2208	2212	2213	rBV3	1252	1378	0.10%	0.010%
92	14.597	2213	2216	2218	rVV2	7432	8868	0.65%	0.066%
93	14.640	2218	2223	2233	rVV	803599	957781	70.06%	7.158%
94	14.731	2233	2238	2241	rVV2	6807	9338	0.68%	0.070%
95	14.780	2241	2246	2255	rVB	275325	347077	25.39%	2.594%
96	15.207	2312	2316	2322	rBV	25642	34450	2.52%	0.257%
97	15.377	2340	2344	2348	rBV2	7477	10009	0.73%	0.075%
98	15.481	2356	2361	2367	rVB2	13220	18869	1.38%	0.141%
99	15.615	2379	2383	2387	rBV3	11011	16900	1.24%	0.126%
100	16.328	2495	2500	2505	rBV4	4342	8282	0.61%	0.062%

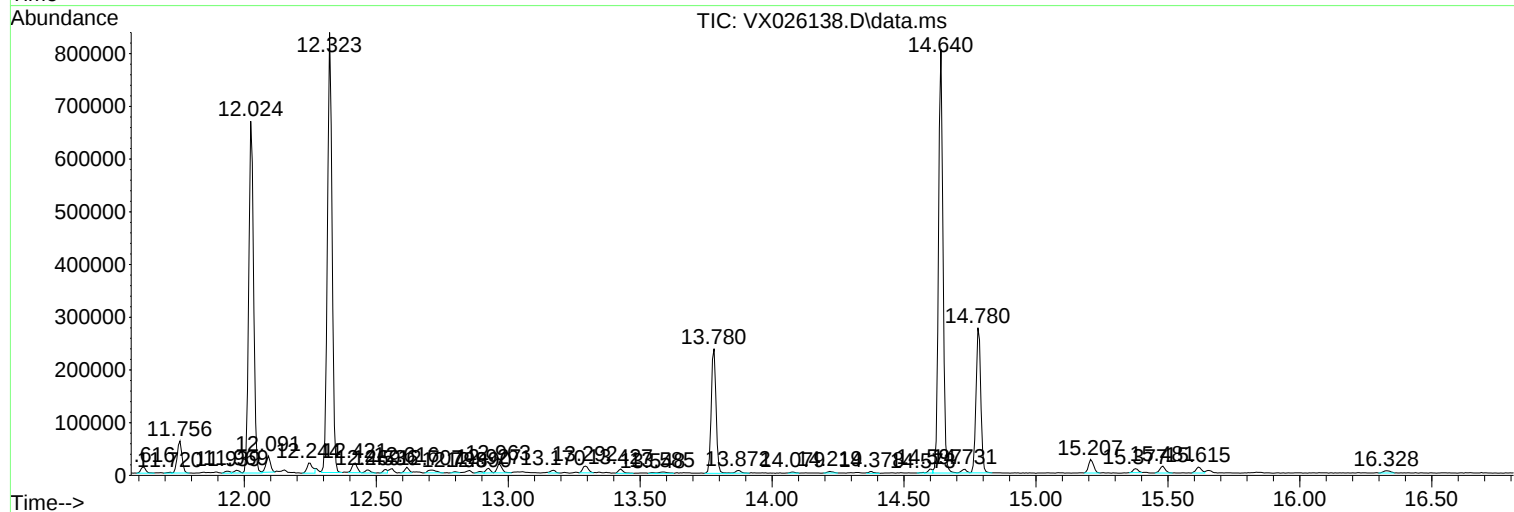
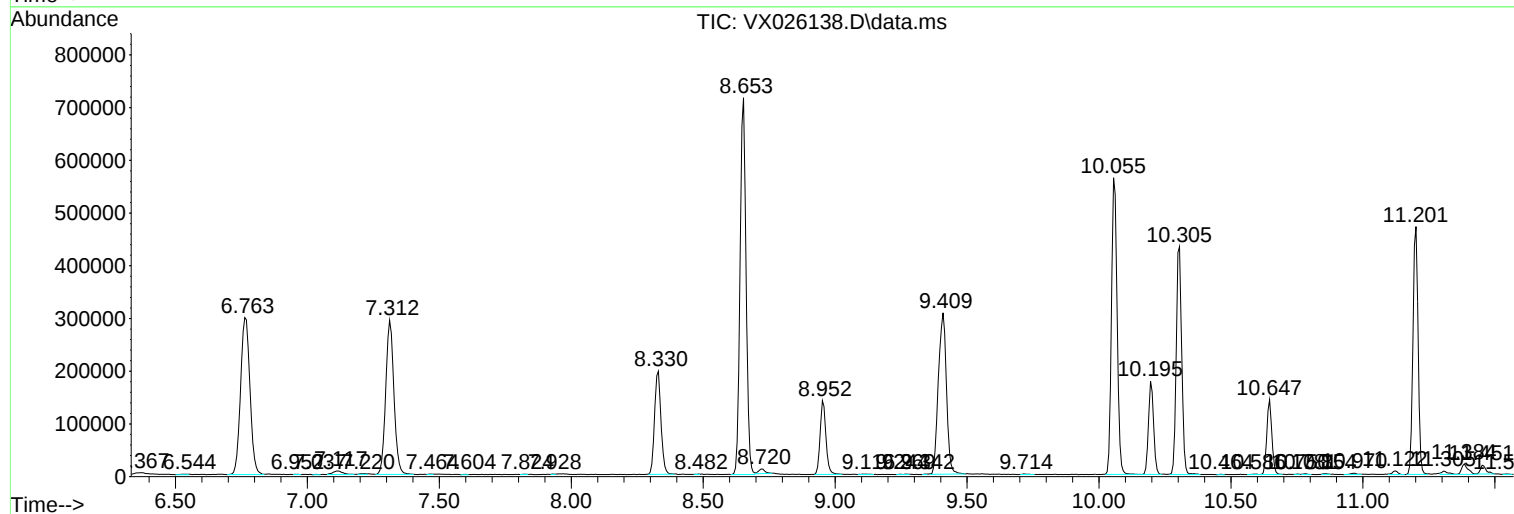
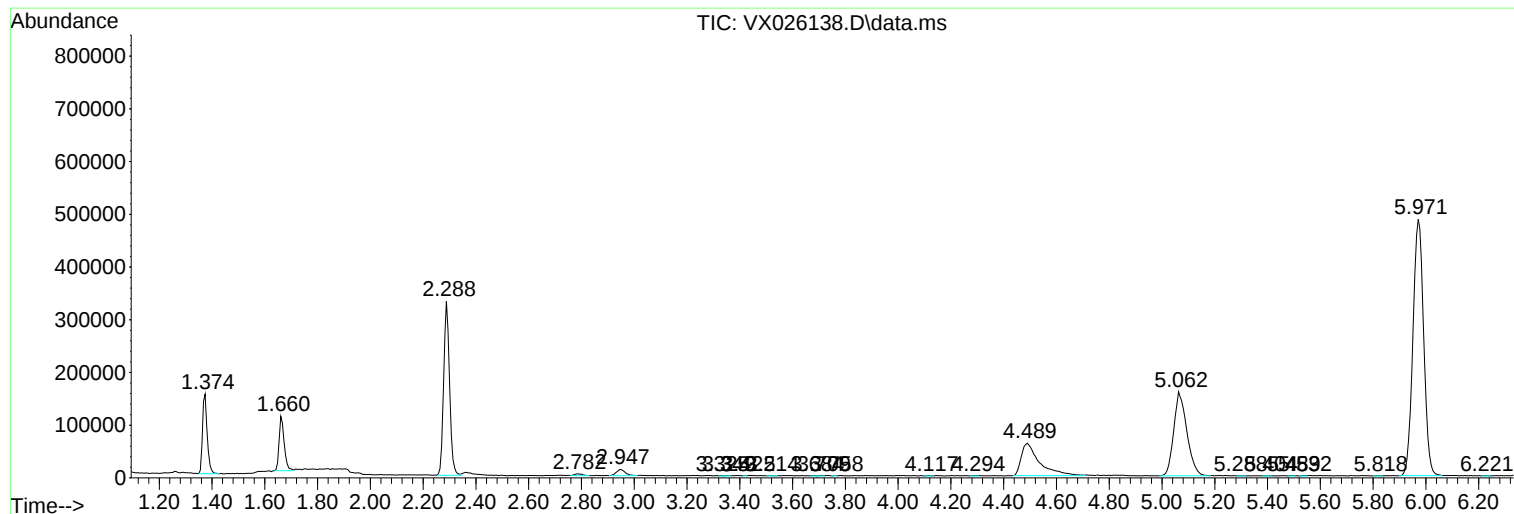
Sum of corrected areas: 13380083

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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGLC9ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122821WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGLC9ME

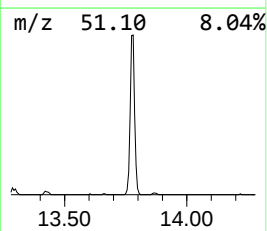
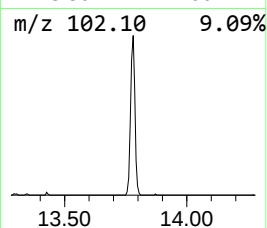
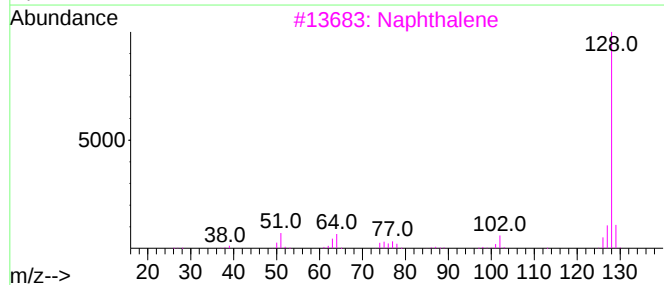
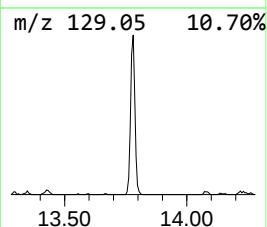
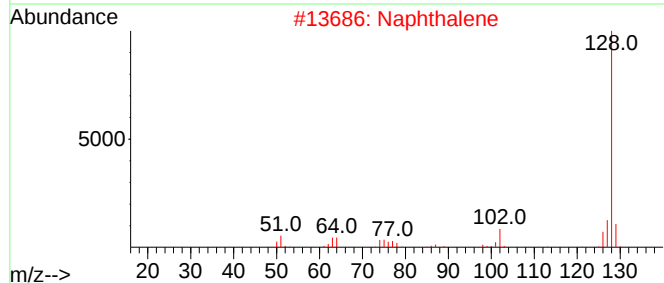
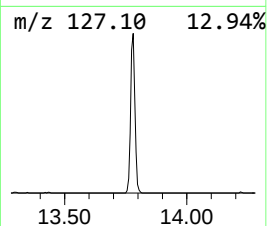
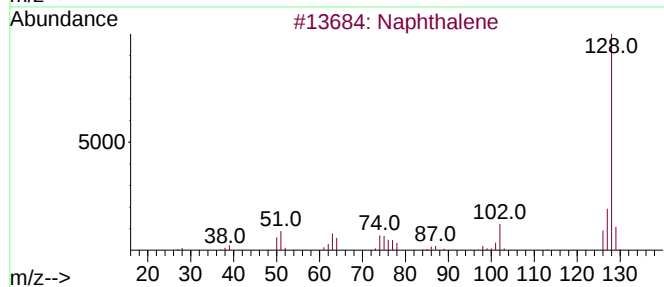
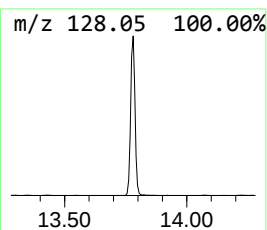
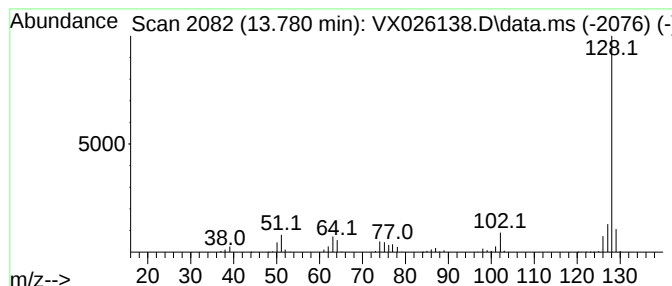
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122821WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Azulene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.780	17.61 ug/L	299149	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	97
2			Naphthalene	128	C10H8	000091-20-3	95
3			Naphthalene	128	C10H8	000091-20-3	91
4			Azulene	128	C10H8	000275-51-4	91
5			Azulene	128	C10H8	000275-51-4	91



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Instrument :
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ClientSampleId :
BGLC9ME

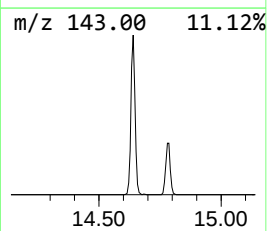
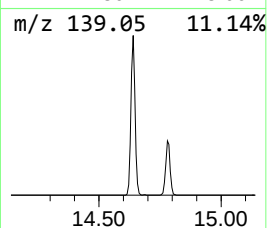
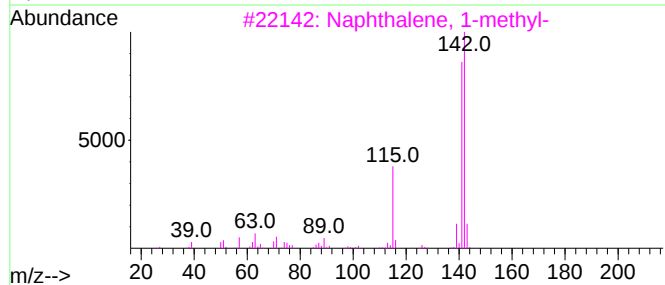
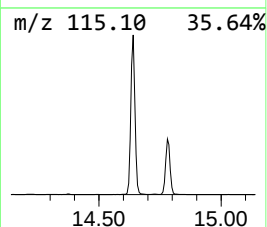
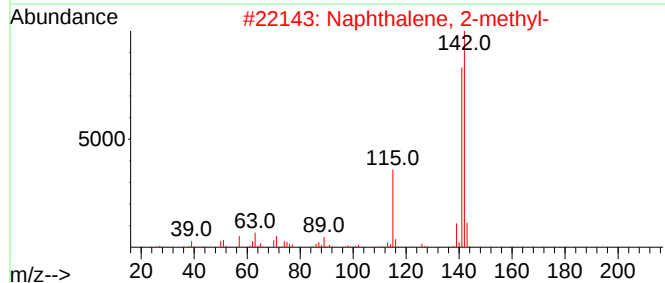
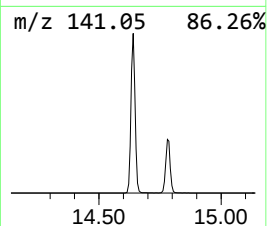
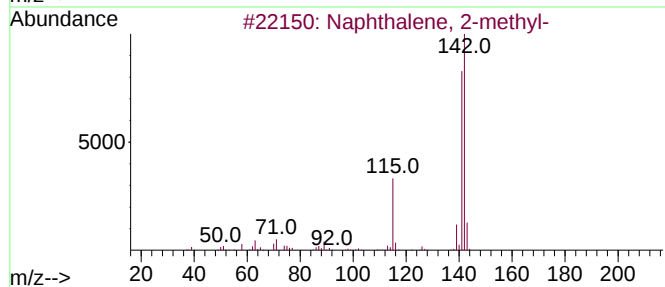
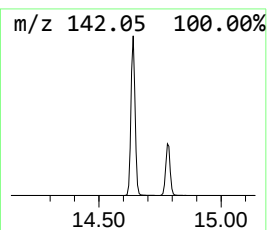
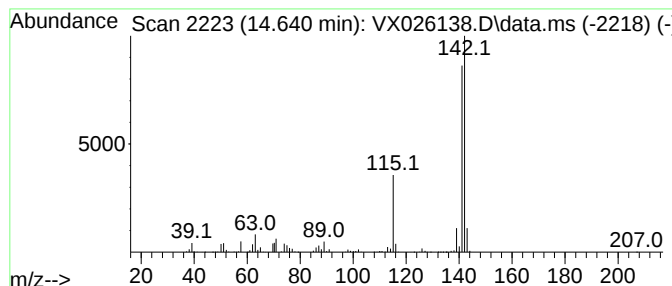
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122821WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Naphthalene, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	56.39 ug/L	957781	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
4			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	95
5			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94



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Instrument :
MSVOA_X
ClientSampleId :
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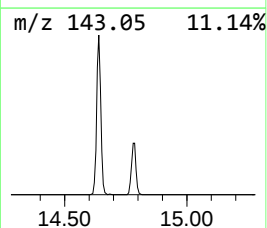
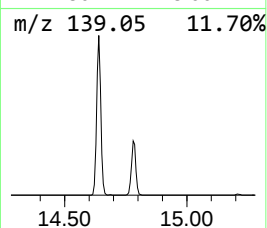
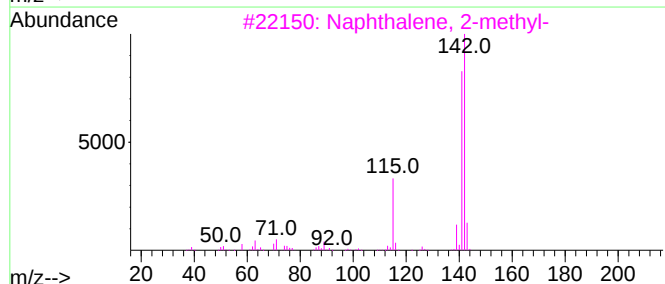
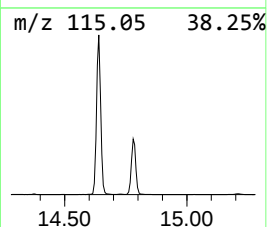
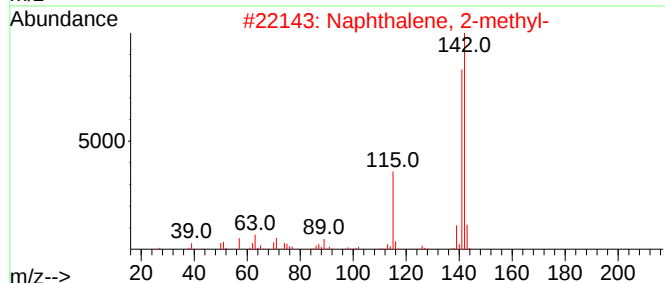
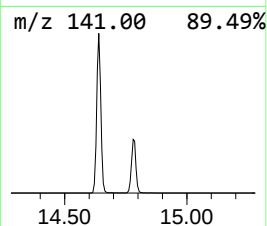
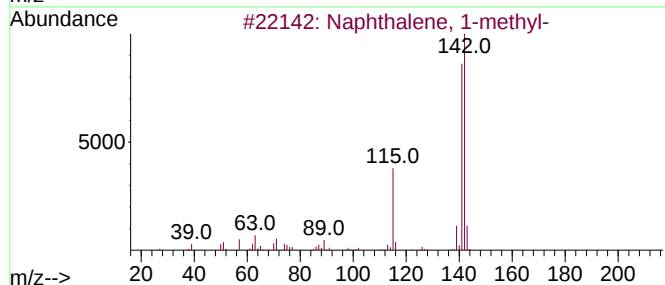
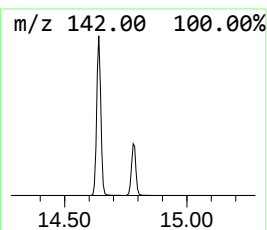
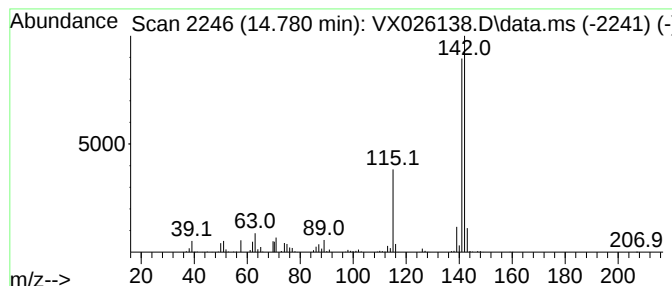
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122821WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	20.44 ug/L	347077	1,4-Dichlorobenzene-d4	12.024

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122921\
Data File : VX026138.D
Acq On : 29 Dec 2021 14:57
Operator : JC/MD
Sample : M5194-17ME
Misc : 6.63g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGLC9ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML122821WMA.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	13.780	17.6	ug/L	299149	3	12.024	849206	50.0
Naphthalene, 2-...	14.640	56.4	ug/L	957781	3	12.024	849206	50.0
Naphthalene, 1-...	14.780	20.4	ug/L	347077	3	12.024	849206	50.0