

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
 Data File : VX025663.D
 Acq On : 09 Dec 2021 16:27
 Operator : JC/MD
 Sample : M4884-22MEDL 20X
 Misc : 2.47g/5mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EW9K6MEDL

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\SFAMXML112221WMA.M
 Title : VOC Analysis

Signal : TIC: VX025663.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.368	43	46	52	rVB	36048	35212	11.16%	1.090%
2	1.660	90	94	99	rBV	32849	40622	12.87%	1.258%
3	2.307	194	200	210	rVB	53836	89882	28.48%	2.782%
4	2.544	237	239	242	rVB2	449	380	0.12%	0.012%
5	2.788	275	279	284	rVB3	929	1538	0.49%	0.048%
6	2.861	288	291	292	rBV	367	381	0.12%	0.012%
7	2.953	299	306	311	rBV3	3841	8660	2.74%	0.268%
8	3.727	430	433	435	rBV	285	352	0.11%	0.011%
9	3.794	442	444	447	rBV2	267	364	0.12%	0.011%
10	3.861	453	455	458	rVB	251	278	0.09%	0.009%
11	3.892	458	460	462	rVB	380	280	0.09%	0.009%
12	3.922	462	465	468	rBB	298	357	0.11%	0.011%
13	3.953	468	470	472	rBV2	267	297	0.09%	0.009%
14	4.343	532	534	536	rBV2	280	241	0.08%	0.007%
15	4.459	542	553	567	rBV	35939	101466	32.15%	3.141%
16	4.562	567	570	573	rBV	469	518	0.16%	0.016%
17	4.818	610	612	615	rBV	267	222	0.07%	0.007%
18	4.965	633	636	638	rVB	346	402	0.13%	0.012%
19	5.062	640	652	668	rVV	45518	143173	45.36%	4.432%
20	5.739	759	763	766	rBV	290	480	0.15%	0.015%
21	5.824	775	777	780	rBV	247	287	0.09%	0.009%
22	5.885	786	787	789	rBV	324	220	0.07%	0.007%
23	5.971	789	801	820	rVV2	103650	314674	99.70%	9.741%
24	6.221	840	842	844	rBV	416	416	0.13%	0.013%
25	6.501	886	888	891	rBV2	191	228	0.07%	0.007%
26	6.544	893	895	900	rVB	290	286	0.09%	0.009%
27	6.623	906	908	909	rVB	374	270	0.09%	0.008%
28	6.763	922	931	945	rBV	108653	260312	82.48%	8.058%
29	6.989	965	968	972	rBV	245	337	0.11%	0.010%
30	7.129	983	991	1003	rBV	84777	187439	59.39%	5.803%
31	7.312	1013	1021	1032	rBV	70546	152255	48.24%	4.713%
32	7.525	1053	1056	1059	rBV	310	371	0.12%	0.011%
33	7.989	1129	1132	1135	rBV	310	417	0.13%	0.013%
34	8.019	1135	1137	1139	rBV	237	227	0.07%	0.007%
35	8.135	1153	1156	1159	rBV	358	423	0.13%	0.013%
36	8.263	1176	1177	1181	rBV	271	341	0.11%	0.011%

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 Title : VOC Analysis

37	8.324	1181	1187	1195	rBV	48768	78912	25.00%	2.443%
38	8.598	1229	1232	1234	rBV2	228	278	0.09%	0.009%
39	8.653	1234	1241	1248	rBV	143029	227285	72.01%	7.036%
40	8.903	1280	1282	1284	rBV	290	266	0.08%	0.008%
41	8.952	1284	1290	1297	rVV	34234	51123	16.20%	1.583%
42	9.031	1300	1303	1305	rBV	398	459	0.15%	0.014%
43	9.177	1324	1327	1331	rBV	305	394	0.12%	0.012%
44	9.275	1337	1343	1349	rVB	22169	33208	10.52%	1.028%
45	9.342	1352	1354	1356	rBV	234	296	0.09%	0.009%
46	9.385	1356	1361	1376	rBV	152829	218452	69.21%	6.763%
47	9.933	1449	1451	1454	rBV2	312	375	0.12%	0.012%
48	10.055	1465	1471	1480	rBV	233081	315622	100.00%	9.771%
49	10.177	1488	1491	1492	rBV2	374	449	0.14%	0.014%
50	10.299	1509	1511	1517	rVB3	746	1098	0.35%	0.034%
51	10.360	1517	1521	1524	rBV	404	511	0.16%	0.016%
52	10.610	1560	1562	1564	rBV	304	312	0.10%	0.010%
53	10.653	1564	1569	1570	rVV2	602	802	0.25%	0.025%
54	10.714	1575	1579	1582	rVB	383	555	0.18%	0.017%
55	10.738	1582	1583	1587	rBV	347	498	0.16%	0.015%
56	10.909	1610	1611	1616	rVB2	269	269	0.09%	0.008%
57	11.195	1652	1658	1668	rBV	161978	206510	65.43%	6.393%
58	11.311	1676	1677	1681	rVB2	287	329	0.10%	0.010%
59	11.378	1686	1688	1693	rVV2	369	572	0.18%	0.018%
60	11.433	1695	1697	1698	rBV	250	227	0.07%	0.007%
61	11.451	1698	1700	1701	rVV	526	415	0.13%	0.013%
62	11.622	1725	1728	1729	rBV2	344	345	0.11%	0.011%
63	11.756	1746	1750	1756	rVV2	1607	2157	0.68%	0.067%
64	11.841	1763	1764	1767	rBV2	245	227	0.07%	0.007%
65	11.976	1783	1786	1789	rBV2	260	480	0.15%	0.015%
66	12.024	1789	1794	1803	rVV	250135	300969	95.36%	9.317%
67	12.226	1826	1827	1829	rBV	329	280	0.09%	0.009%
68	12.323	1837	1843	1850	rVV	201420	260856	82.65%	8.075%
69	12.415	1855	1858	1863	rVV	1831	2339	0.74%	0.072%
70	12.616	1888	1891	1894	rVB2	313	416	0.13%	0.013%
71	12.646	1894	1896	1897	rBV	350	261	0.08%	0.008%
72	12.689	1902	1903	1907	rVB2	304	305	0.10%	0.009%
73	12.719	1907	1908	1911	rBB2	289	237	0.08%	0.007%
74	12.750	1911	1913	1914	rBV2	257	231	0.07%	0.007%
75	12.805	1919	1922	1924	rBV2	218	220	0.07%	0.007%
76	12.866	1929	1932	1933	rBV2	258	253	0.08%	0.008%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
 Title : VOC Analysis

77	12.921	1938	1941	1945	rVB2	377	497	0.16%	0.015%
78	12.963	1945	1948	1951	rBV3	774	1162	0.37%	0.036%
79	13.061	1961	1964	1965	rBV2	236	221	0.07%	0.007%
80	13.311	2002	2005	2008	rBV2	279	472	0.15%	0.015%
81	13.347	2008	2011	2013	rVB2	611	751	0.24%	0.023%
82	13.427	2020	2024	2028	rVB2	877	1042	0.33%	0.032%
83	13.725	2071	2073	2075	rBV2	397	332	0.11%	0.010%
84	13.774	2075	2081	2089	rBV	108447	141189	44.73%	4.371%
85	13.872	2094	2097	2100	rVV2	1813	1417	0.45%	0.044%
86	13.951	2108	2110	2113	rBV	236	299	0.09%	0.009%
87	14.134	2136	2140	2144	rBV2	713	902	0.29%	0.028%
88	14.207	2150	2152	2154	rVB	317	274	0.09%	0.008%
89	14.237	2154	2157	2159	rBV2	276	368	0.12%	0.011%
90	14.341	2172	2174	2177	rVV2	292	326	0.10%	0.010%
91	14.396	2181	2183	2186	rBV2	232	288	0.09%	0.009%
92	14.481	2196	2197	2199	rBV	257	242	0.08%	0.007%
93	14.640	2219	2223	2230	rVB	12899	15210	4.82%	0.471%
94	14.780	2242	2246	2251	rVB	7729	9456	3.00%	0.293%
95	15.207	2314	2316	2320	rVB2	804	916	0.29%	0.028%
96	15.420	2350	2351	2354	rBV	367	281	0.09%	0.009%
97	15.481	2358	2361	2364	rVB2	605	754	0.24%	0.023%
98	15.963	2438	2440	2442	rBV2	327	224	0.07%	0.007%
99	16.097	2458	2462	2464	rBV2	619	870	0.28%	0.027%
100	16.243	2485	2486	2489	rBV	487	413	0.13%	0.013%

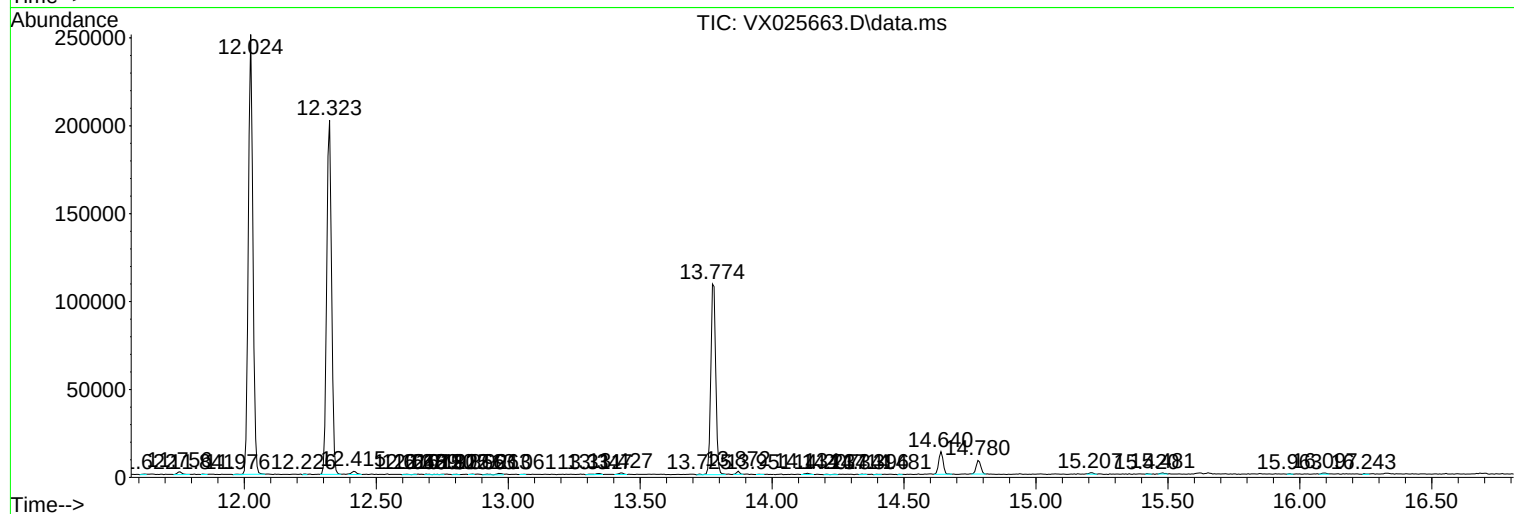
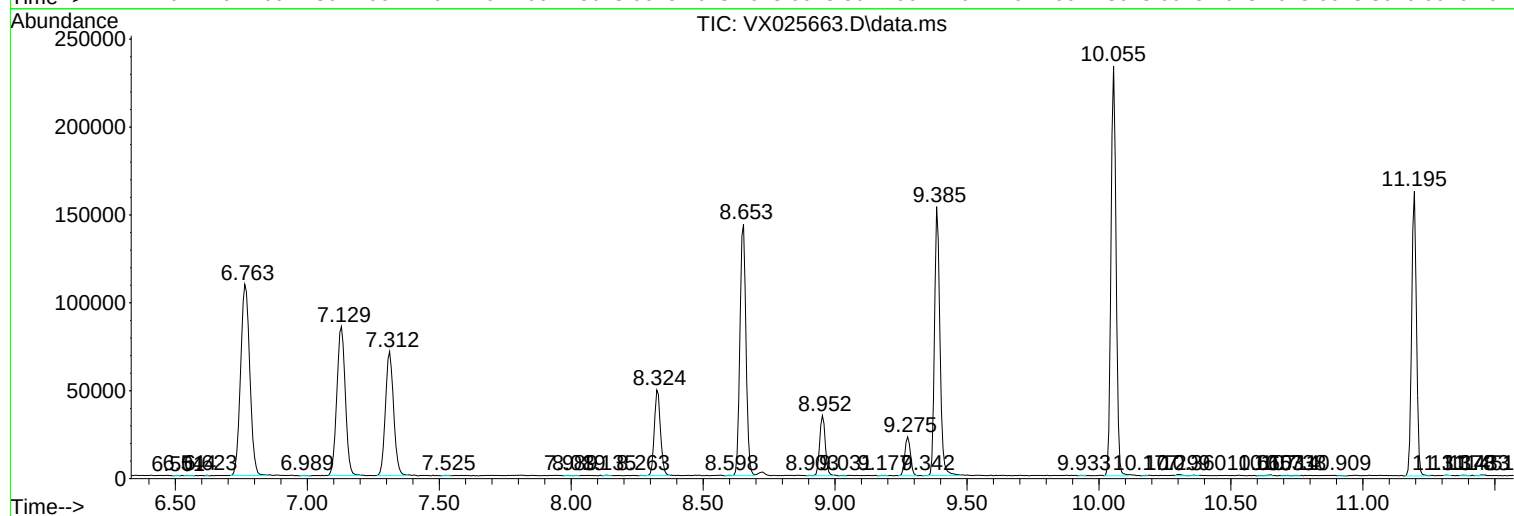
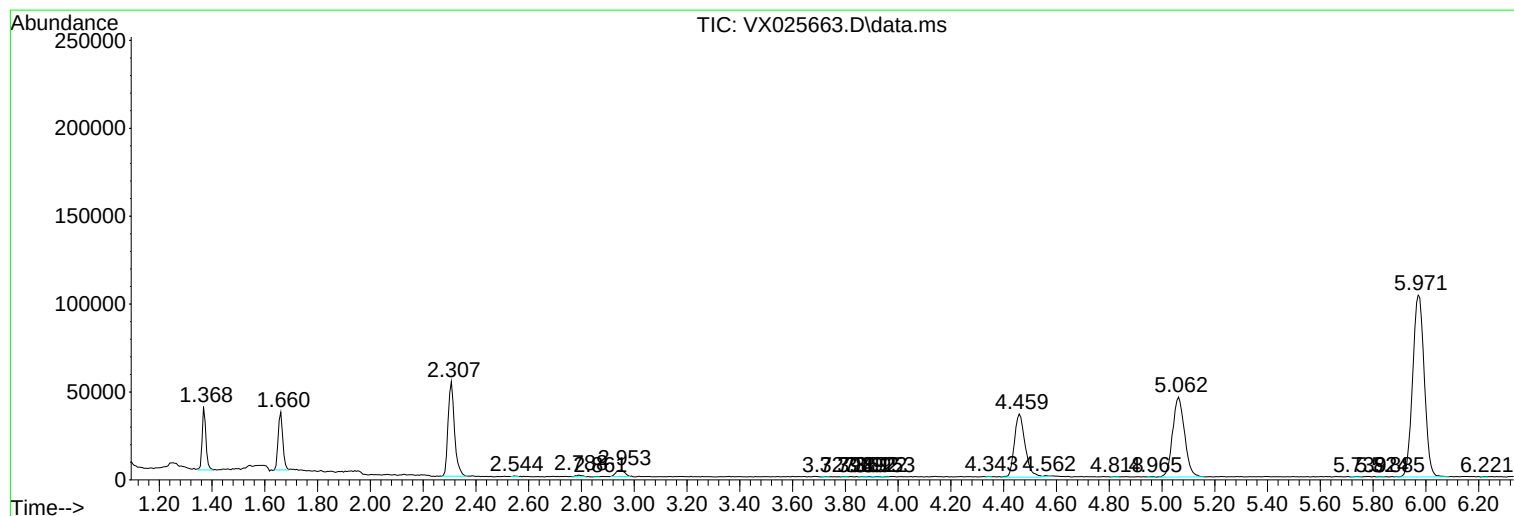
Sum of corrected areas: 3230307

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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



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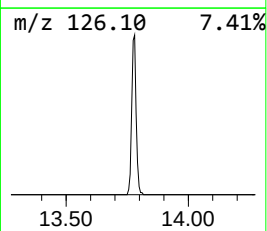
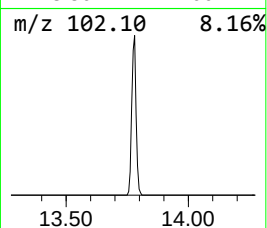
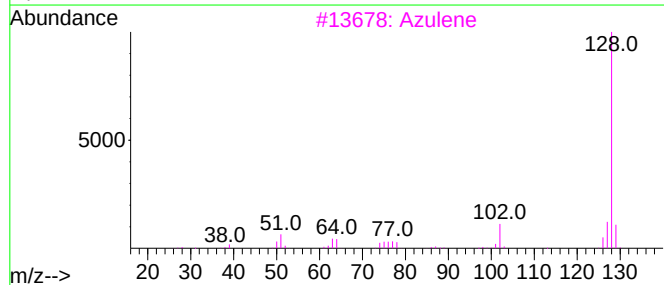
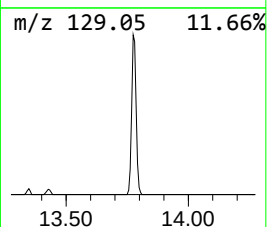
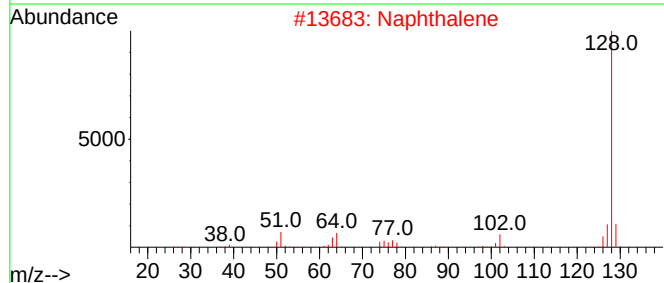
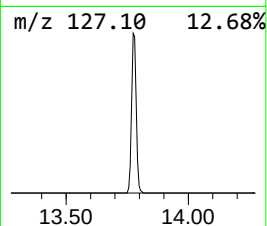
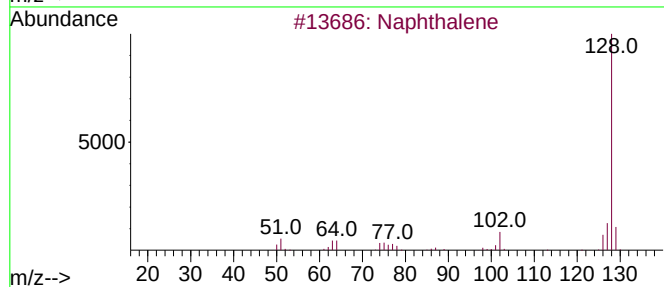
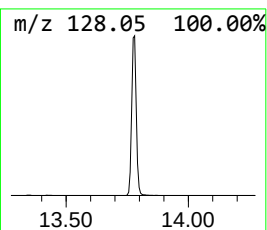
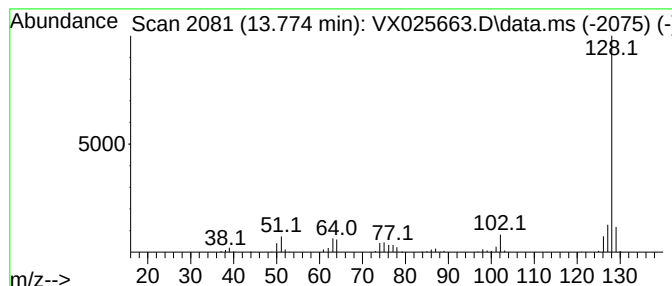
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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.
13.774	23.46 ug/L	141189	1,4-Dichlorobenzene-d4	12.024

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			Azulene	128	C10H8	000275-51-4	93
4			Naphthalene	128	C10H8	000091-20-3	91
5			Azulene	128	C10H8	000275-51-4	91



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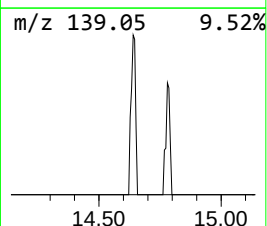
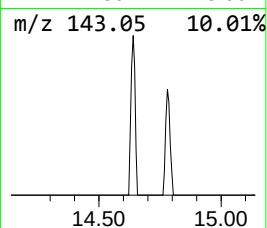
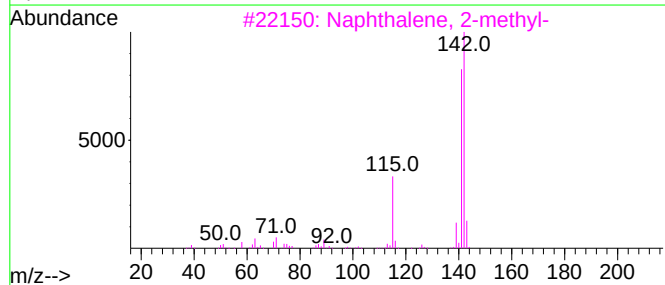
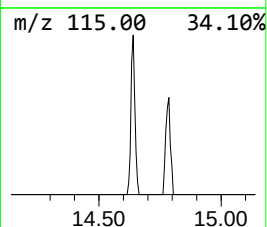
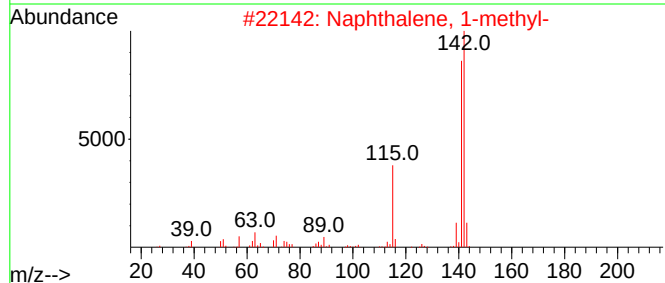
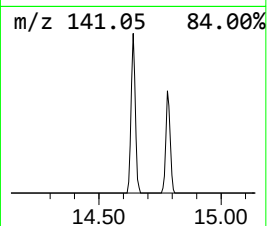
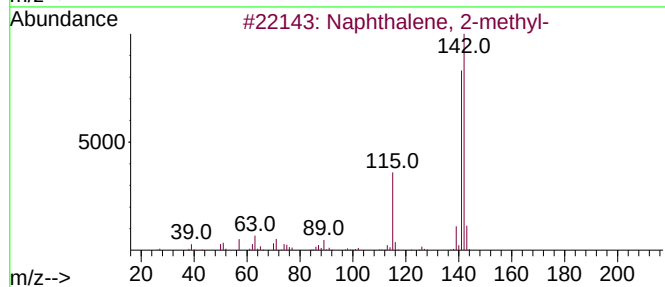
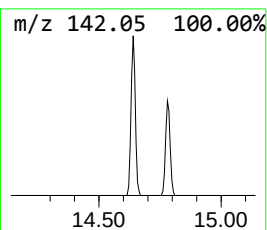
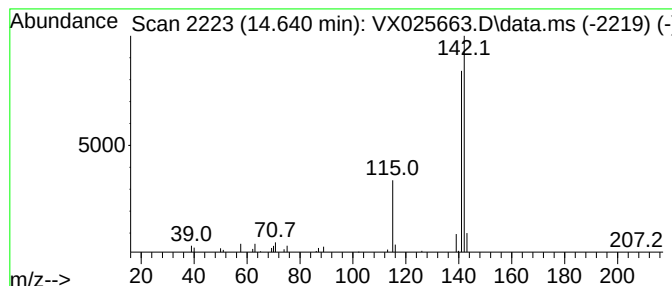
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML112221WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	2.53 ug/L	15210	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	95
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	95
3			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	94
4			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91
5			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Azulene	13.774	23.5	ug/L	141189	3	12.024	300969	50.0
Naphthalene, 2-...	14.640	2.5	ug/L	15210	3	12.024	300969	50.0