

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
 Data File : VX025623.D
 Acq On : 08 Dec 2021 15:59
 Operator : JC/MD
 Sample : M4884-22ME
 Misc : 2.47g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EW9K6ME

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\SFAMXLM112221WMA.M
 Title : VOC Analysis

Signal : TIC: VX025623.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	37	rVB4	4062	8498	1.68%	0.191%
2	1.367	43	46	54	rVB	47668	56264	11.12%	1.263%
3	1.544	68	75	77	rBV3	3449	7607	1.50%	0.171%
4	1.648	88	92	100	rBV	29713	37340	7.38%	0.838%
5	2.282	190	196	207	rBV	85468	138706	27.41%	3.114%
6	2.843	286	288	289	rVB	770	441	0.09%	0.010%
7	2.953	300	306	317	rVB2	6353	16657	3.29%	0.374%
8	3.526	399	400	403	rVB	512	431	0.09%	0.010%
9	3.721	431	432	436	rBV	529	407	0.08%	0.009%
10	4.495	548	559	583	rBV	18071	83897	16.58%	1.883%
11	4.946	631	633	636	rBV	464	698	0.14%	0.016%
12	5.068	642	653	669	rVV	48534	159811	31.58%	3.588%
13	5.275	683	687	692	rVB	475	796	0.16%	0.018%
14	5.452	712	716	717	rBV2	580	488	0.10%	0.011%
15	5.592	737	739	740	rBV	554	552	0.11%	0.012%
16	5.885	785	787	788	rBV	508	438	0.09%	0.010%
17	5.970	791	801	819	rVB2	141914	409495	80.92%	9.193%
18	6.360	860	865	877	rVB4	2210	7064	1.40%	0.159%
19	6.440	877	878	881	rVB	615	466	0.09%	0.010%
20	6.464	881	882	885	rBV	472	417	0.08%	0.009%
21	6.525	888	892	894	rBV	420	545	0.11%	0.012%
22	6.763	922	931	946	rVB	97721	251722	49.74%	5.651%
23	7.123	982	990	1002	rBV	217985	493292	97.48%	11.074%
24	7.312	1013	1021	1039	rVB	76829	184661	36.49%	4.145%
25	7.433	1039	1041	1044	rBV2	366	454	0.09%	0.010%
26	7.647	1074	1076	1079	rBV	439	455	0.09%	0.010%
27	7.702	1082	1085	1087	rBV	494	658	0.13%	0.015%
28	8.330	1181	1188	1197	rBV	43631	77362	15.29%	1.737%
29	8.476	1210	1212	1215	rVB	370	409	0.08%	0.009%
30	8.653	1231	1241	1249	rBV	204363	337329	66.66%	7.573%
31	8.720	1249	1252	1258	rVB2	3495	5579	1.10%	0.125%
32	8.830	1268	1270	1274	rBV	388	516	0.10%	0.012%
33	8.958	1285	1291	1302	rVB2	26865	47798	9.45%	1.073%
34	9.165	1323	1325	1329	rVB	1111	1276	0.25%	0.029%
35	9.201	1329	1331	1335	rBV2	434	697	0.14%	0.016%
36	9.275	1337	1343	1350	rBV	82021	119464	23.61%	2.682%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
 Data File : VX025623.D
 Acq On : 08 Dec 2021 15:59
 Operator : JC/MD
 Sample : M4884-22ME
 Misc : 2.47g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EW9K6ME

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\SFAMXLM112221WMA.M
 Title : VOC Analysis

37	9.397	1357	1363	1372	rBV	108021	179794	35.53%	4.036%
38	9.573	1389	1392	1398	rVB3	684	1198	0.24%	0.027%
39	9.616	1398	1399	1401	rBV	574	478	0.09%	0.011%
40	9.714	1409	1415	1422	rBV3	1109	2207	0.44%	0.050%
41	10.012	1461	1464	1465	rBV	431	483	0.10%	0.011%
42	10.061	1466	1472	1480	rBV	193920	290082	57.32%	6.512%
43	10.226	1497	1499	1502	rVB	500	517	0.10%	0.012%
44	10.305	1508	1512	1517	rBV3	3225	4772	0.94%	0.107%
45	10.646	1565	1568	1575	rVB2	1699	2390	0.47%	0.054%
46	10.976	1619	1622	1624	rBV2	359	480	0.09%	0.011%
47	11.122	1639	1646	1649	rVV2	1704	2439	0.48%	0.055%
48	11.195	1653	1658	1665	rBV	142751	188330	37.22%	4.228%
49	11.390	1686	1690	1693	rBV3	562	738	0.15%	0.017%
50	11.457	1697	1701	1708	rBV3	2209	3614	0.71%	0.081%
51	11.542	1711	1715	1717	rBV	377	484	0.10%	0.011%
52	11.567	1717	1719	1723	rVB	449	671	0.13%	0.015%
53	11.610	1724	1726	1731	rVB2	452	516	0.10%	0.012%
54	11.756	1745	1750	1755	rVB3	5455	7285	1.44%	0.164%
55	11.811	1757	1759	1762	rBV3	417	432	0.09%	0.010%
56	11.933	1774	1779	1781	rBV2	874	1449	0.29%	0.033%
57	12.024	1789	1794	1800	rBV	243732	290823	57.47%	6.529%
58	12.085	1802	1804	1809	rVB2	1026	1233	0.24%	0.028%
59	12.146	1812	1814	1818	rVB3	1014	1290	0.25%	0.029%
60	12.219	1824	1826	1828	rBV	709	782	0.15%	0.018%
61	12.323	1838	1843	1851	rVB	243707	298467	58.98%	6.700%
62	12.414	1854	1858	1863	rVB2	7010	9522	1.88%	0.214%
63	12.536	1876	1878	1881	rBV2	508	673	0.13%	0.015%
64	12.664	1895	1899	1900	rBV2	586	508	0.10%	0.011%
65	12.890	1933	1936	1939	rBV2	1440	1815	0.36%	0.041%
66	12.969	1946	1949	1957	rVB3	3598	5479	1.08%	0.123%
67	13.048	1961	1962	1965	rVB3	531	418	0.08%	0.009%
68	13.134	1973	1976	1979	rBV2	340	475	0.09%	0.011%
69	13.176	1981	1983	1985	rVB2	548	445	0.09%	0.010%
70	13.262	1996	1997	1999	rBV2	810	748	0.15%	0.017%
71	13.286	1999	2001	2006	rVB4	1452	2313	0.46%	0.052%
72	13.347	2006	2011	2014	rBV2	2006	3183	0.63%	0.071%
73	13.426	2020	2024	2030	rVB3	2304	3407	0.67%	0.076%
74	13.646	2057	2060	2061	rBV2	343	447	0.09%	0.010%
75	13.780	2076	2082	2090	rBV	405121	506032	100.00%	11.360%
76	13.871	2094	2097	2103	rVB	7978	9905	1.96%	0.222%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
 Data File : VX025623.D
 Acq On : 08 Dec 2021 15:59
 Operator : JC/MD
 Sample : M4884-22ME
 Misc : 2.47g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EW9K6ME

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

77	13.963	2110	2112	2114	rBV	632	483	0.10%	0.011%
78	14.018	2118	2121	2122	rBV	525	499	0.10%	0.011%
79	14.133	2136	2140	2144	rVB2	1858	2565	0.51%	0.058%
80	14.225	2153	2155	2158	rBV2	442	607	0.12%	0.014%
81	14.420	2186	2187	2191	rVB2	484	402	0.08%	0.009%
82	14.481	2191	2197	2198	rBV	404	494	0.10%	0.011%
83	14.572	2209	2212	2214	rVB3	359	399	0.08%	0.009%
84	14.603	2214	2217	2218	rVV2	589	765	0.15%	0.017%
85	14.639	2218	2223	2231	rVB	70312	85236	16.84%	1.913%
86	14.725	2234	2237	2241	rVV4	744	1136	0.22%	0.026%
87	14.780	2241	2246	2257	rVV	38067	48270	9.54%	1.084%
88	15.213	2313	2317	2324	rBV2	4340	5768	1.14%	0.129%
89	15.377	2341	2344	2345	rBV	1157	1051	0.21%	0.024%
90	15.481	2355	2361	2367	rBV3	3723	6551	1.29%	0.147%
91	15.615	2379	2383	2387	rBV2	4160	7161	1.42%	0.161%
92	15.834	2416	2419	2425	rVB4	1202	2534	0.50%	0.057%
93	15.883	2425	2427	2429	rBV	679	477	0.09%	0.011%
94	16.097	2456	2462	2466	rBV3	2232	3701	0.73%	0.083%
95	16.170	2472	2474	2476	rBV	507	444	0.09%	0.010%
96	16.267	2488	2490	2493	rVB	578	573	0.11%	0.013%
97	16.328	2496	2500	2511	rVB2	2226	4434	0.88%	0.100%
98	16.432	2515	2517	2519	rBV2	324	400	0.08%	0.009%
99	16.578	2538	2541	2544	rBV2	589	928	0.18%	0.021%
100	16.657	2551	2554	2555	rBV	625	675	0.13%	0.015%

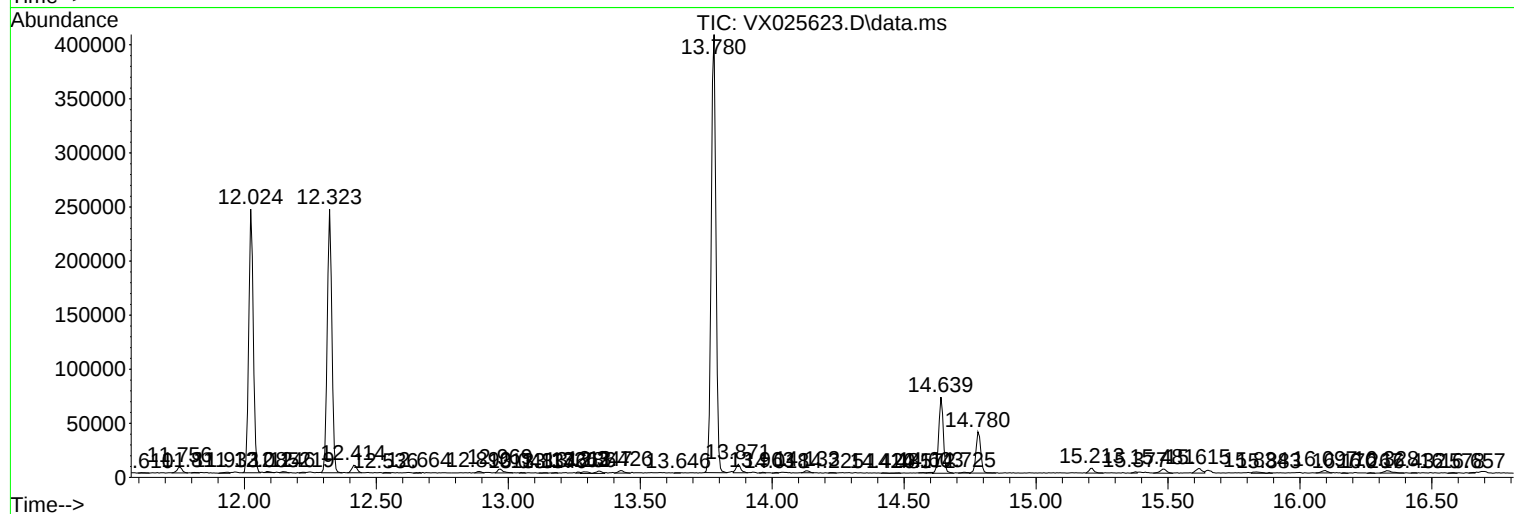
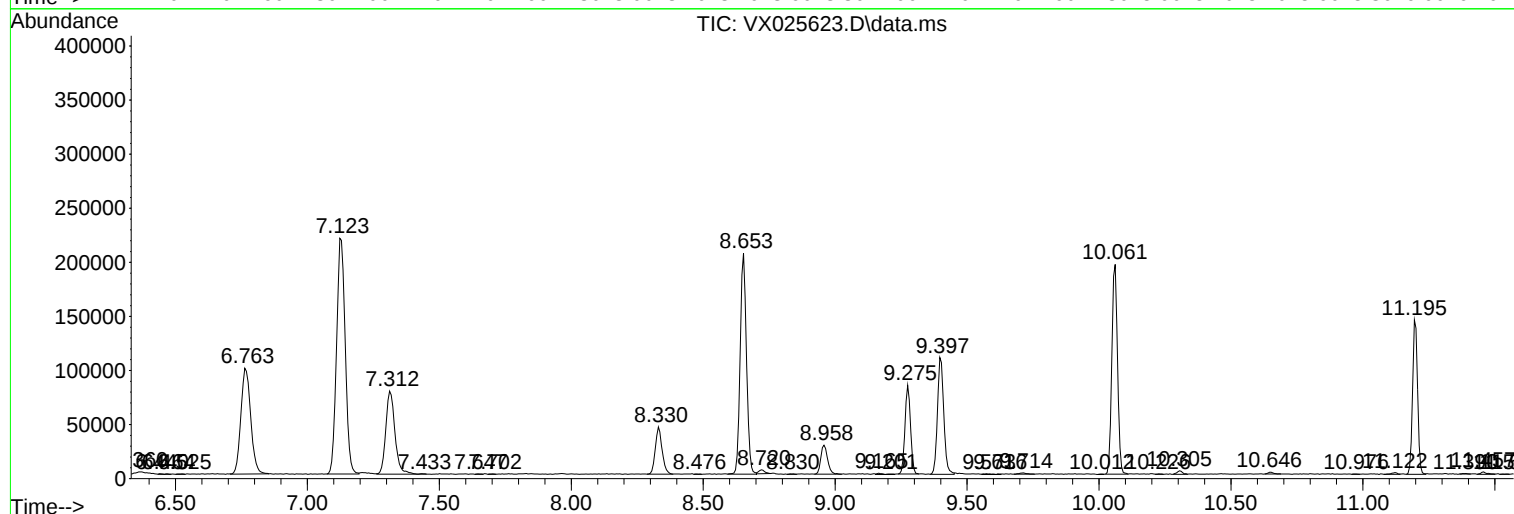
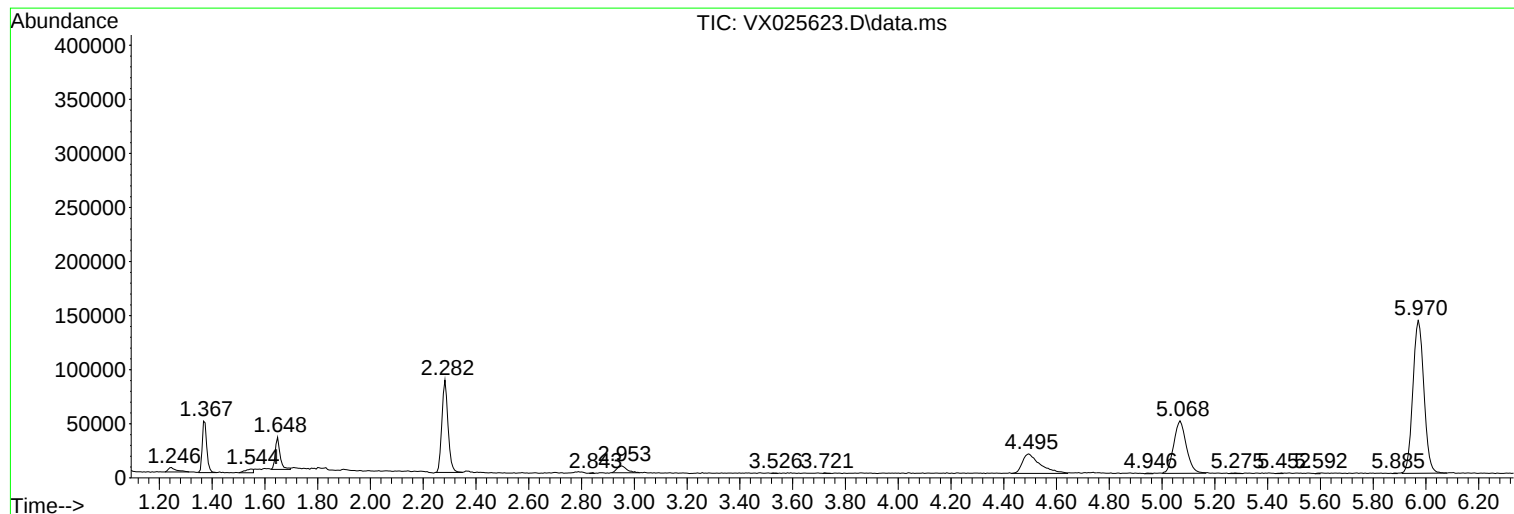
Sum of corrected areas: 4454567

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
Data File : VX025623.D
Acq On : 08 Dec 2021 15:59
Operator : JC/MD
Sample : M4884-22ME
Misc : 2.47g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9K6ME

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
Data File : VX025623.D
Acq On : 08 Dec 2021 15:59
Operator : JC/MD
Sample : M4884-22ME
Misc : 2.47g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9K6ME

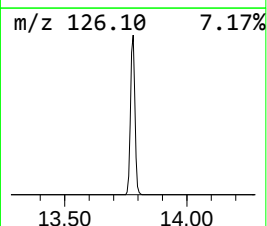
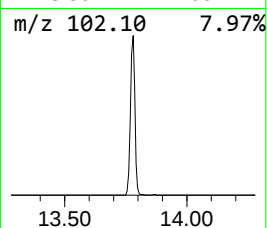
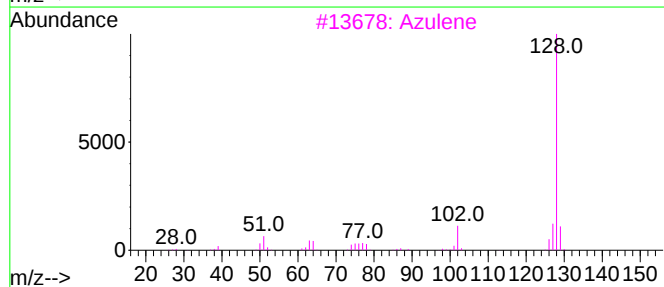
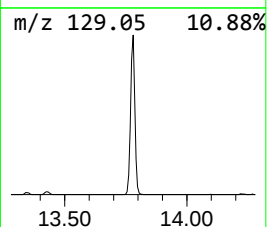
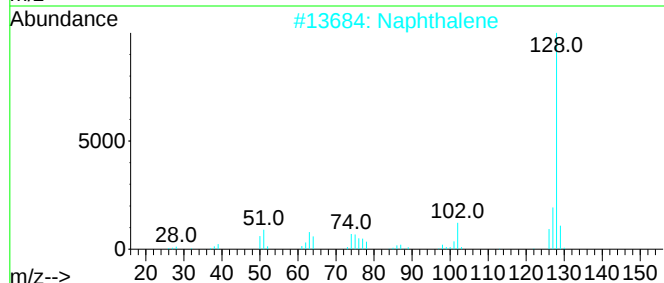
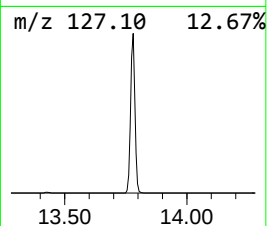
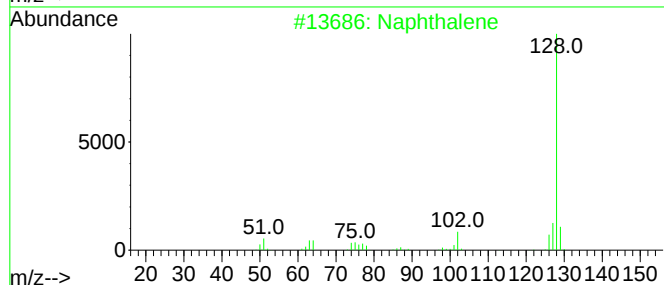
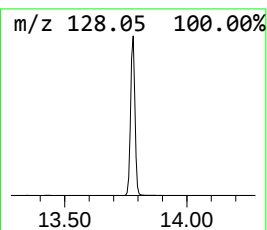
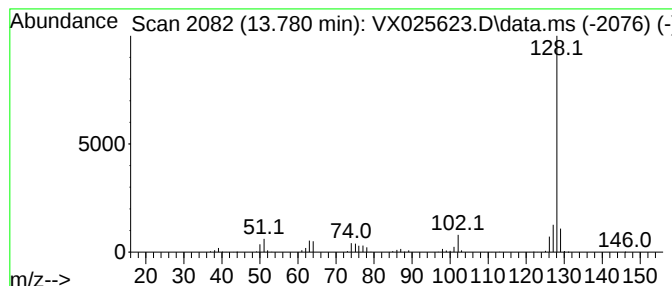
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.780	87.00 ug/L	506032	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			Azulene	128	C10H8	000275-51-4	91
5			Azulene	128	C10H8	000275-51-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
Data File : VX025623.D
Acq On : 08 Dec 2021 15:59
Operator : JC/MD
Sample : M4884-22ME
Misc : 2.47g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9K6ME

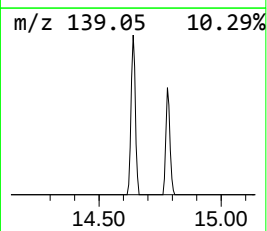
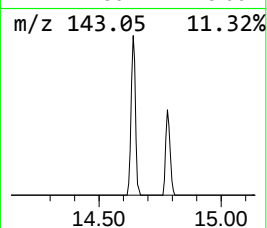
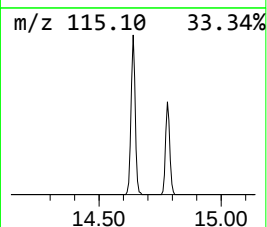
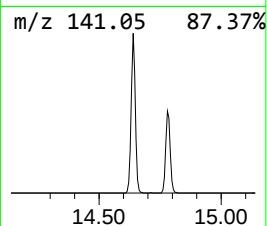
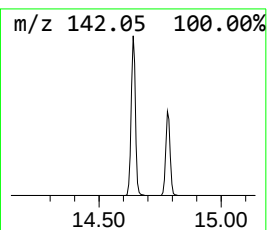
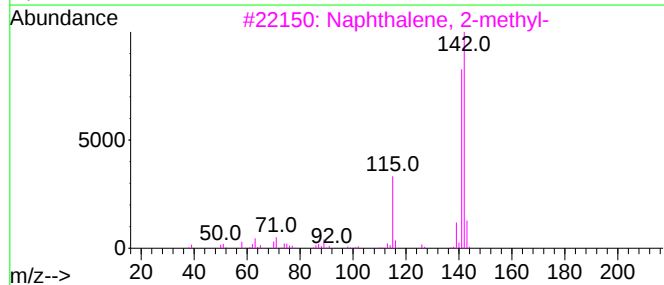
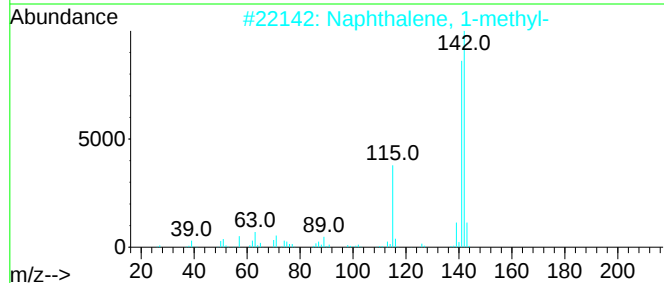
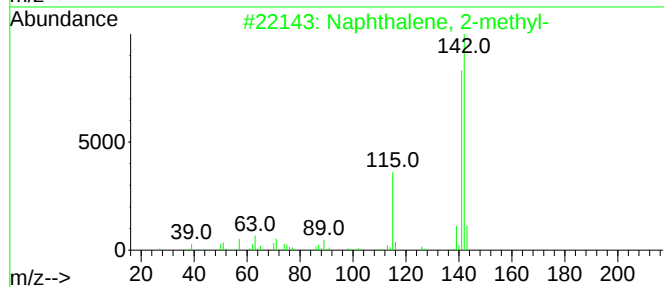
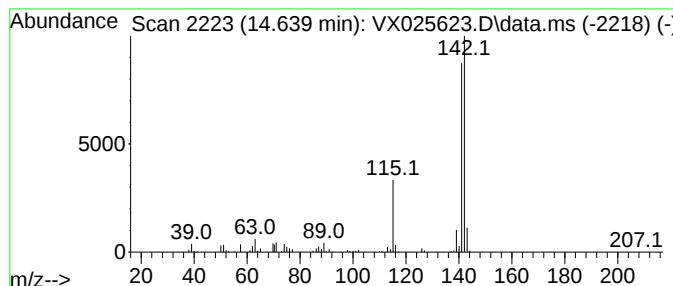
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	14.65 ug/L	85236	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, 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	95
5			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
Data File : VX025623.D
Acq On : 08 Dec 2021 15:59
Operator : JC/MD
Sample : M4884-22ME
Misc : 2.47g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9K6ME

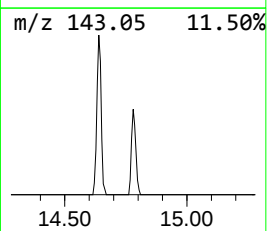
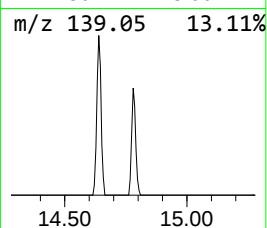
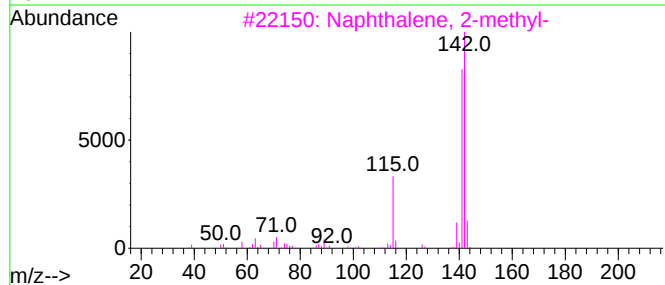
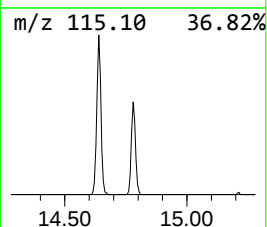
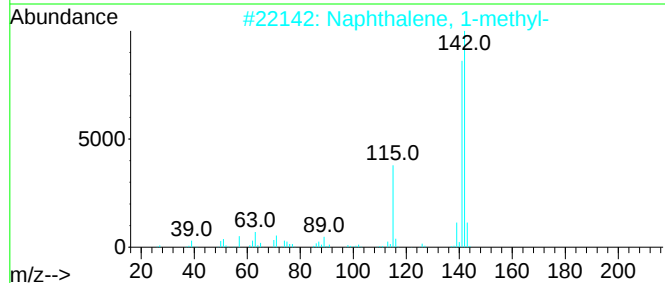
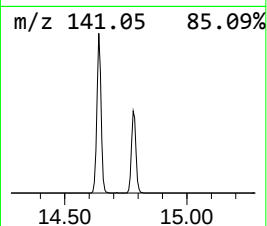
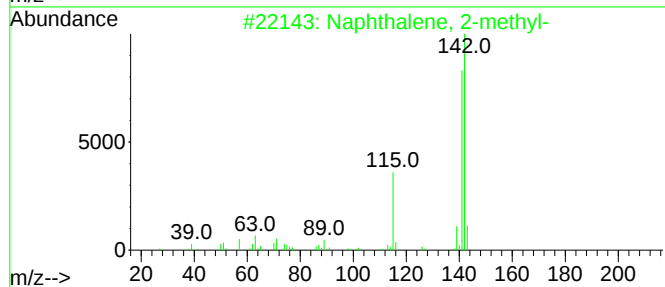
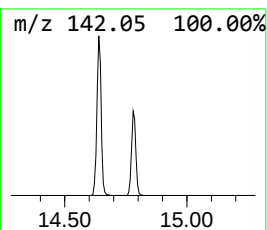
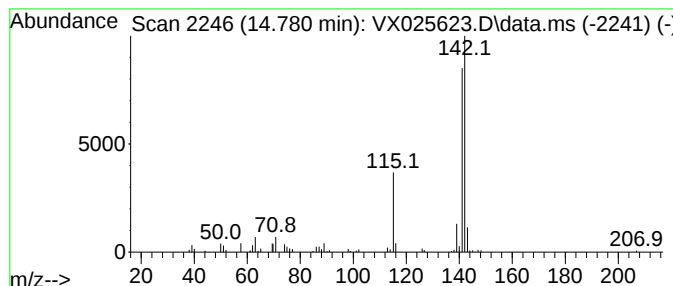
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	8.30 ug/L	48270	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, 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, 1-methyl-	142	C11H10	000090-12-0	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
Data File : VX025623.D
Acq On : 08 Dec 2021 15:59
Operator : JC/MD
Sample : M4884-22ME
Misc : 2.47g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9K6ME

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Azulene	13.780	87.0	ug/L	506032	3	12.024	290823	50.0
Naphthalene, 2-...	14.640	14.7	ug/L	85236	3	12.024	290823	50.0
Naphthalene, 1-...	14.780	8.3	ug/L	48270	3	12.024	290823	50.0