

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120721\
 Data File : VX025586.D
 Acq On : 07 Dec 2021 18:13
 Operator : JC/MD
 Sample : M4881-10ME
 Misc : 3.96g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EW9E6ME

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: VX025586.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	22	25	33	rBV	4467	8768	2.44%	0.287%
2	1.368	43	46	54	rVB	38240	43511	12.09%	1.424%
3	1.648	88	92	97	rBV	21731	27478	7.64%	0.900%
4	2.282	189	196	205	rBV	65548	113195	31.46%	3.706%
5	2.721	260	268	269	rBV3	408	911	0.25%	0.030%
6	2.788	274	279	284	rVV4	1660	3260	0.91%	0.107%
7	2.947	298	305	319	rBV	6791	19569	5.44%	0.641%
8	4.282	520	524	531	rVB3	275	583	0.16%	0.019%
9	4.495	549	559	589	rBV	15842	73611	20.46%	2.410%
10	5.068	640	653	671	rVB	42146	138770	38.57%	4.543%
11	5.452	710	716	717	rBV4	648	910	0.25%	0.030%
12	5.550	729	732	738	rBV2	227	387	0.11%	0.013%
13	5.971	790	801	821	rBV2	121754	359782	100.00%	11.778%
14	6.361	858	865	882	rBV6	2322	7473	2.08%	0.245%
15	6.763	922	931	947	rVV	89067	229958	63.92%	7.528%
16	7.111	982	988	998	rVB6	1169	3208	0.89%	0.105%
17	7.220	998	1006	1013	rBV3	879	2551	0.71%	0.084%
18	7.312	1013	1021	1029	rBV	66660	155077	43.10%	5.077%
19	7.964	1123	1128	1132	rVB3	507	811	0.23%	0.027%
20	8.275	1174	1179	1182	rBV4	367	505	0.14%	0.017%
21	8.330	1182	1188	1198	rVV	35828	63576	17.67%	2.081%
22	8.598	1228	1232	1234	rBV2	758	958	0.27%	0.031%
23	8.653	1234	1241	1248	rVV	170314	283978	78.93%	9.296%
24	8.720	1248	1252	1265	rVB	10947	18964	5.27%	0.621%
25	8.915	1280	1284	1285	rBV3	382	465	0.13%	0.015%
26	8.958	1285	1291	1303	rVB2	23116	40161	11.16%	1.315%
27	9.275	1341	1343	1348	rVB3	383	432	0.12%	0.014%
28	9.403	1357	1364	1378	rBV	91816	157563	43.79%	5.158%
29	9.567	1385	1391	1394	rVB3	759	1197	0.33%	0.039%
30	9.616	1397	1399	1403	rVB2	559	614	0.17%	0.020%
31	9.708	1411	1414	1422	rVB3	874	1270	0.35%	0.042%
32	9.817	1427	1432	1435	rVB3	632	688	0.19%	0.023%
33	10.061	1466	1472	1483	rVB	175889	269843	75.00%	8.834%
34	10.201	1489	1495	1500	rVB3	742	1262	0.35%	0.041%
35	10.305	1508	1512	1517	rVV2	4266	6034	1.68%	0.198%
36	10.360	1517	1521	1525	rVB3	813	887	0.25%	0.029%

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Integrator: RTE

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

37	10.659	1564	1570	1577	rVV2	13633	20991	5.83%	0.687%
38	10.781	1588	1590	1592	rVB2	685	478	0.13%	0.016%
39	10.854	1600	1602	1605	rVB2	375	428	0.12%	0.014%
40	10.896	1605	1609	1613	rBV4	553	734	0.20%	0.024%
41	11.122	1642	1646	1651	rVB	2630	3055	0.85%	0.100%
42	11.195	1653	1658	1664	rBV	122344	166268	46.21%	5.443%
43	11.281	1668	1672	1673	rBV2	494	585	0.16%	0.019%
44	11.384	1685	1689	1696	rBV2	1239	1641	0.46%	0.054%
45	11.457	1698	1701	1702	rBV	956	1027	0.29%	0.034%
46	11.476	1702	1704	1708	rVB2	1467	1631	0.45%	0.053%
47	11.549	1713	1716	1718	rVB2	352	324	0.09%	0.011%
48	11.640	1724	1731	1735	rBV4	1712	2679	0.74%	0.088%
49	11.713	1740	1743	1745	rBV2	790	928	0.26%	0.030%
50	11.750	1745	1749	1754	rVB2	4259	5786	1.61%	0.189%
51	11.811	1754	1759	1763	rBV	35221	42887	11.92%	1.404%
52	11.848	1763	1765	1770	rVB	10430	11340	3.15%	0.371%
53	11.890	1770	1772	1775	rVB	592	602	0.17%	0.020%
54	11.933	1775	1779	1781	rBV3	1384	1848	0.51%	0.060%
55	11.963	1781	1784	1789	rVB3	2271	2969	0.83%	0.097%
56	12.024	1789	1794	1800	rBV	224181	281246	78.17%	9.207%
57	12.152	1813	1815	1824	rVB2	1734	2096	0.58%	0.069%
58	12.250	1827	1831	1833	rVV2	599	827	0.23%	0.027%
59	12.323	1837	1843	1850	rVB	221404	272285	75.68%	8.913%
60	12.421	1854	1859	1864	rVB	16553	22890	6.36%	0.749%
61	12.469	1864	1867	1868	rBV2	358	357	0.10%	0.012%
62	12.555	1875	1881	1884	rBV3	679	1115	0.31%	0.037%
63	12.591	1884	1887	1895	rVB4	1047	1570	0.44%	0.051%
64	12.664	1895	1899	1902	rBV2	1623	2302	0.64%	0.075%
65	12.750	1909	1913	1918	rVB	15951	18578	5.16%	0.608%
66	12.799	1918	1921	1928	rVB4	3176	3949	1.10%	0.129%
67	12.884	1932	1935	1938	rBV3	494	615	0.17%	0.020%
68	12.969	1945	1949	1953	rBV3	1209	1691	0.47%	0.055%
69	13.061	1959	1964	1969	rVB2	6149	7484	2.08%	0.245%
70	13.213	1986	1989	1993	rBV2	192	330	0.09%	0.011%
71	13.268	1995	1998	2001	rBV3	1316	1530	0.43%	0.050%
72	13.341	2007	2010	2014	rVB2	4355	4982	1.38%	0.163%
73	13.390	2014	2018	2019	rVV	432	491	0.14%	0.016%
74	13.427	2019	2024	2028	rVV	6932	9594	2.67%	0.314%
75	13.469	2029	2031	2035	rVB3	730	763	0.21%	0.025%
76	13.579	2046	2049	2052	rVB2	303	351	0.10%	0.011%

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Integrator: RTE

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 Title : VOC Analysis

77	13.676	2064	2065	2068	rBV2	372	389	0.11%	0.013%
78	13.780	2077	2082	2087	rVB	35426	46074	12.81%	1.508%
79	13.847	2089	2093	2095	rBV3	1493	1842	0.51%	0.060%
80	14.042	2121	2125	2127	rVB3	984	900	0.25%	0.029%
81	14.140	2134	2141	2146	rBV3	880	1885	0.52%	0.062%
82	14.189	2146	2149	2152	rVV3	367	564	0.16%	0.018%
83	14.219	2152	2154	2160	rVB4	776	1059	0.29%	0.035%
84	14.317	2168	2170	2177	rVB4	514	775	0.22%	0.025%
85	14.524	2201	2204	2206	rVB4	368	328	0.09%	0.011%
86	14.609	2214	2218	2219	rBV2	437	571	0.16%	0.019%
87	14.640	2219	2223	2227	rVB	10400	12357	3.43%	0.405%
88	14.780	2243	2246	2251	rVB	9552	11878	3.30%	0.389%
89	14.938	2269	2272	2275	rBV2	768	1130	0.31%	0.037%
90	15.115	2297	2301	2304	rBV3	490	722	0.20%	0.024%
91	15.213	2314	2317	2321	rVB6	1152	1433	0.40%	0.047%
92	15.475	2356	2360	2365	rBV3	3002	4439	1.23%	0.145%
93	15.615	2379	2383	2387	rBV2	6079	8992	2.50%	0.294%
94	15.737	2402	2403	2409	rVB3	546	542	0.15%	0.018%
95	15.810	2411	2415	2418	rBV3	1807	2744	0.76%	0.090%
96	16.097	2456	2462	2468	rBV3	1297	2151	0.60%	0.070%
97	16.292	2492	2494	2495	rBV2	498	390	0.11%	0.013%
98	16.335	2496	2501	2511	rVB3	3060	6627	1.84%	0.217%
99	16.597	2542	2544	2549	rVB4	1494	2157	0.60%	0.071%
100	16.658	2549	2554	2559	rBV4	2577	5358	1.49%	0.175%

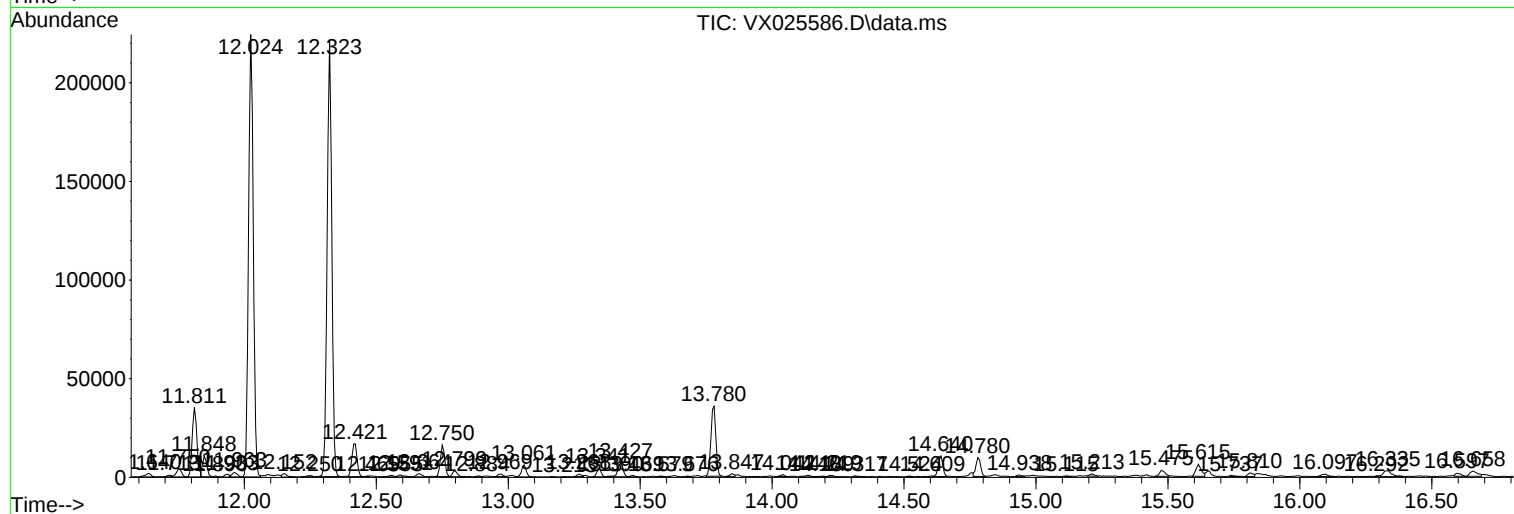
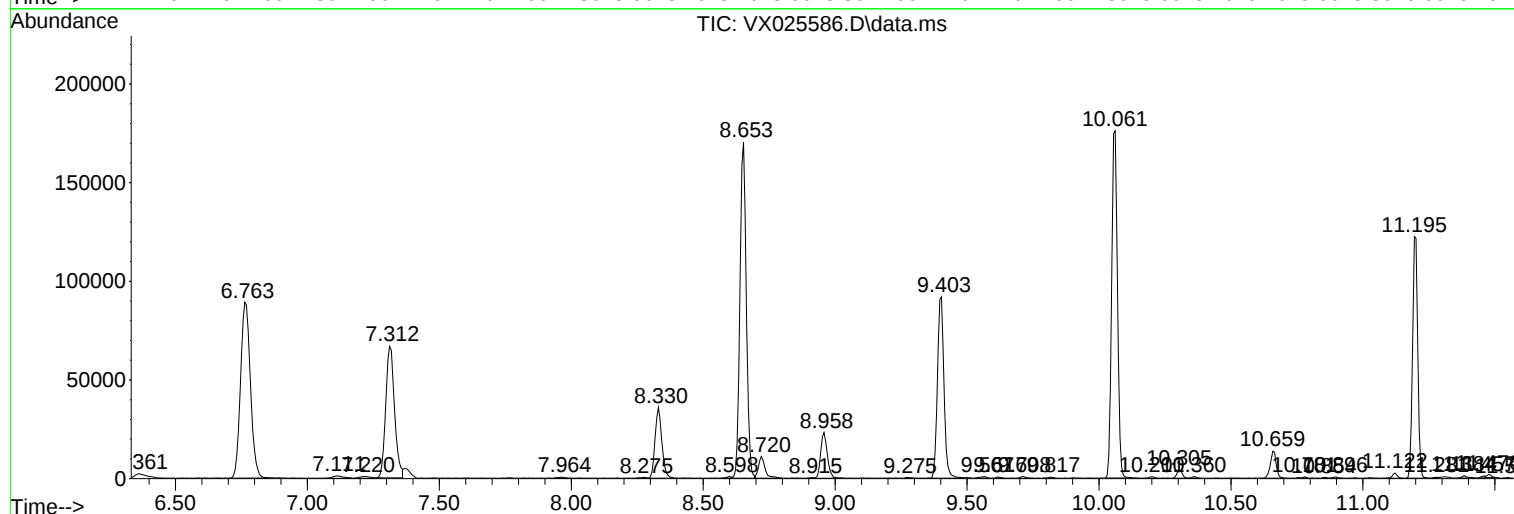
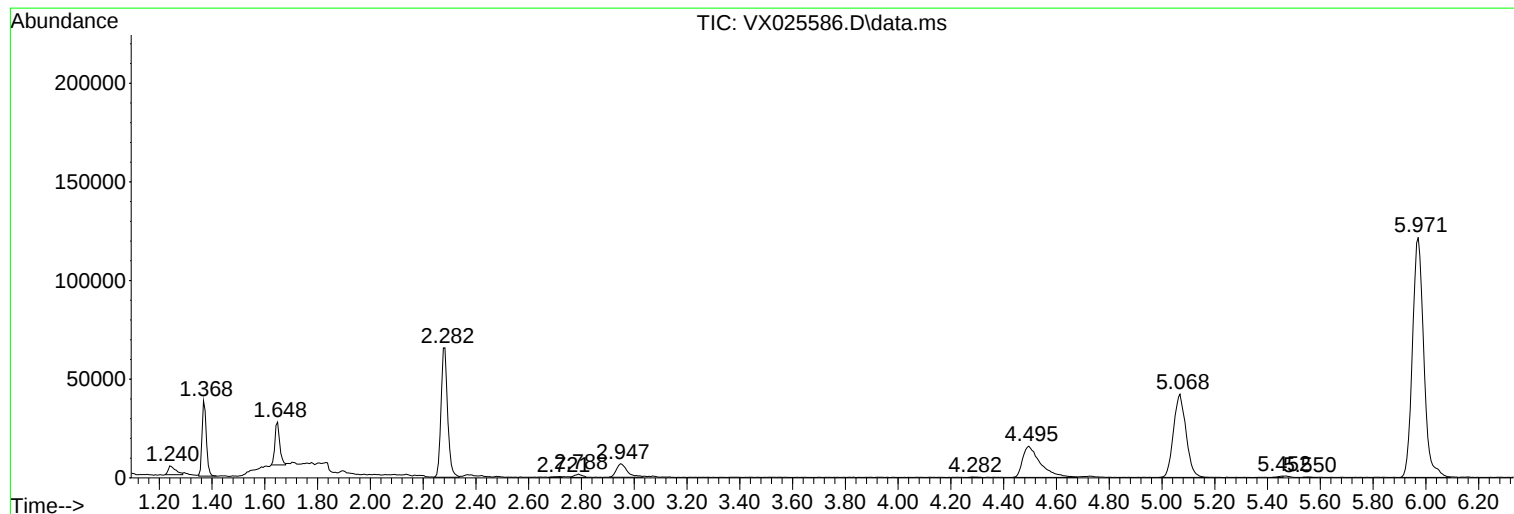
Sum of corrected areas: 3054764

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Instrument :
MSVOA_X
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EW9E6ME

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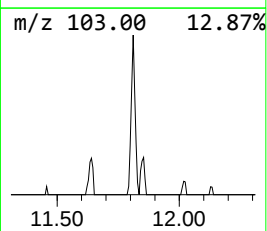
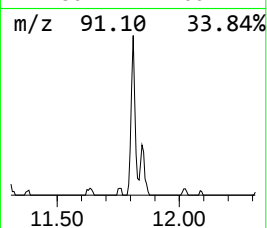
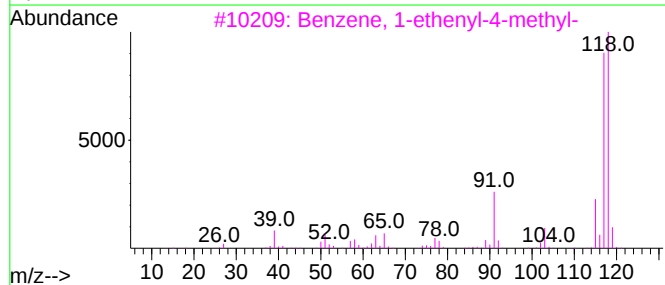
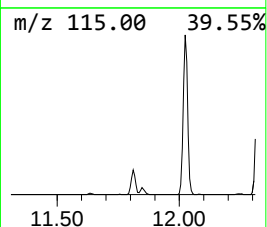
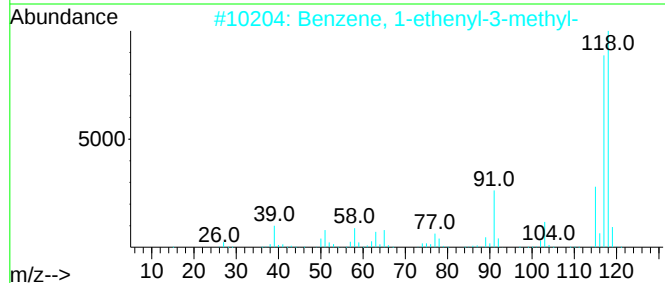
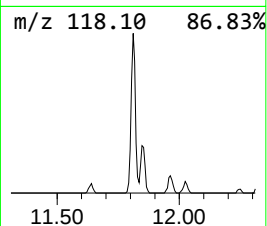
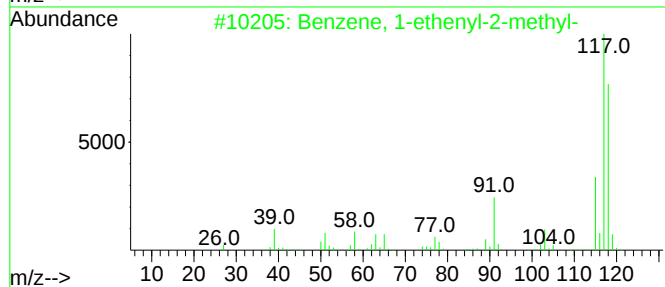
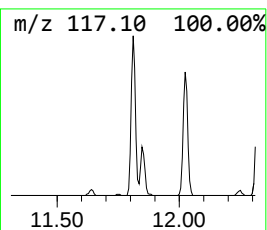
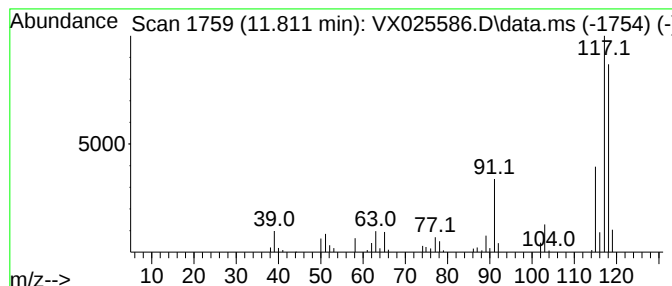
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Benzene, 1-ethenyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.811	7.62 ug/L	42887	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	94
2			Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	94
3			Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	94
4			Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	93
5			Benzene, 1,1'-(1-ethenyl-1,3-pro...	222	C17H18	061141-97-7	91



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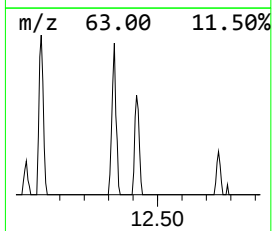
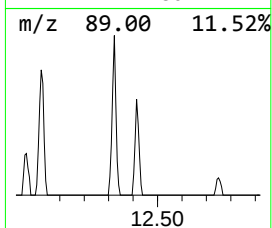
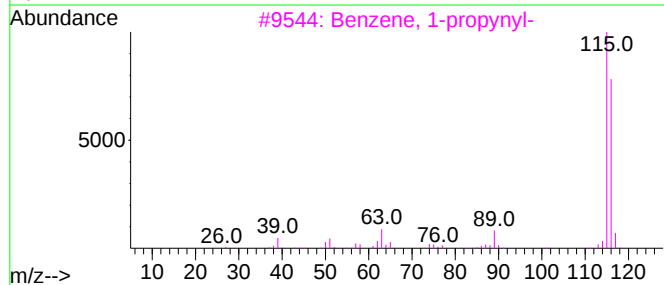
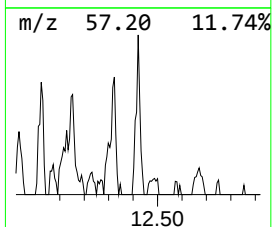
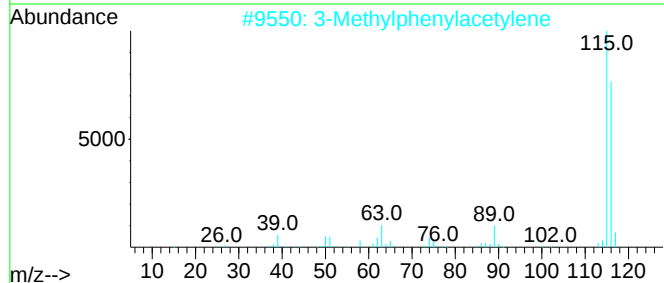
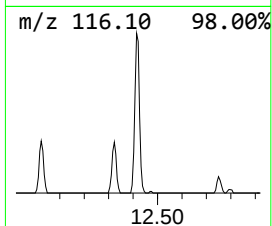
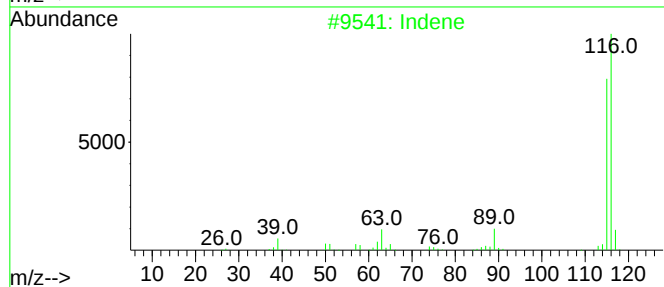
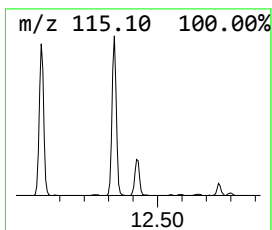
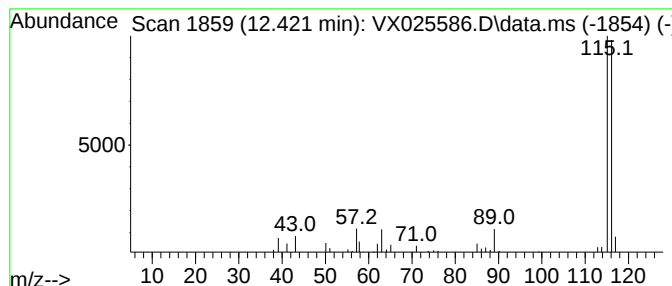
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Indene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.421	4.07 ug/L	22890	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	93
2	3-Methylphenylacetylene	116	C9H8	000766-82-5	93
3	Benzene, 1-propynyl-	116	C9H8	000673-32-5	90
4	Benzene, 1-propynyl-	116	C9H8	000673-32-5	90
5	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	87



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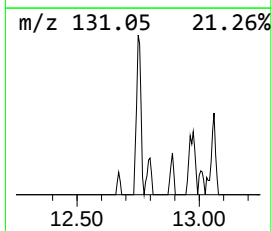
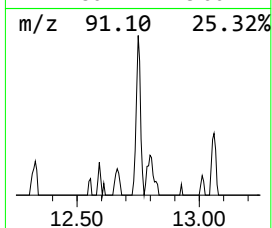
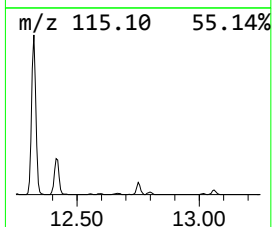
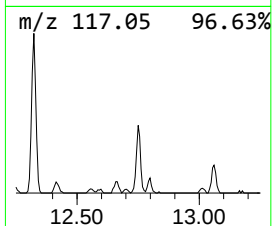
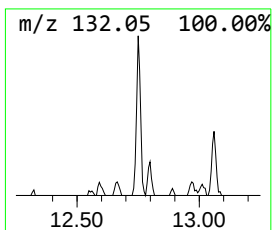
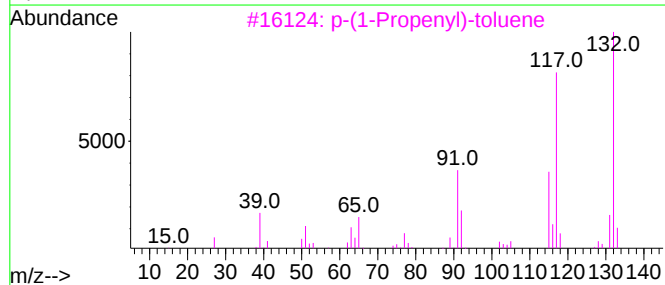
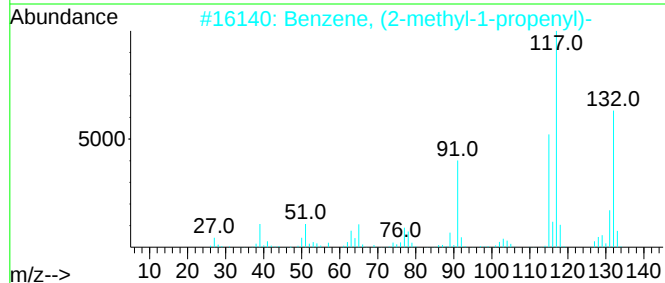
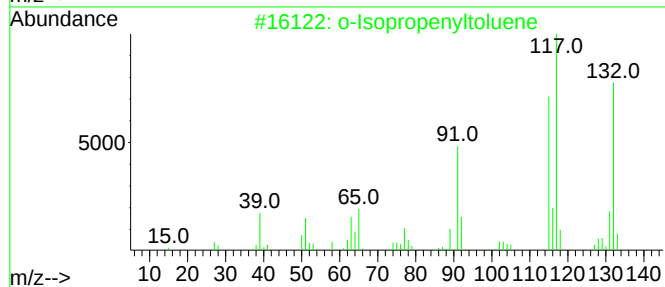
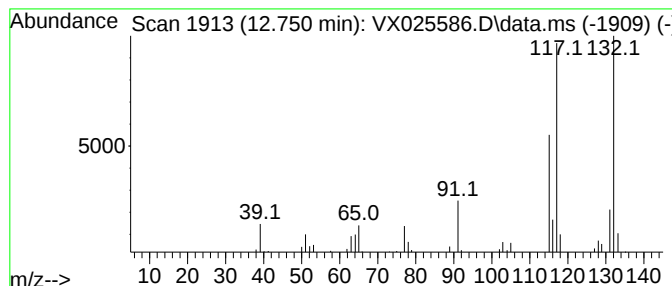
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Quant Title : VOC Analysis

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

Peak Number 5 o-Isopropenyltoluene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.750	3.30 ug/L	18578	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Isopropenyltoluene	132	C10H12	007399-49-7	94
2			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	94
3			p-(1-Propenyl)-toluene	132	C10H12	1000429-54-9	94
4			Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	93
5			Benzene, 2-butenyl-	132	C10H12	001560-06-1	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120721\
Data File : VX025586.D
Acq On : 07 Dec 2021 18:13
Operator : JC/MD
Sample : M4881-10ME
Misc : 3.96g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9E6ME

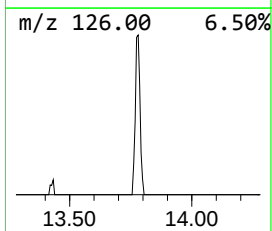
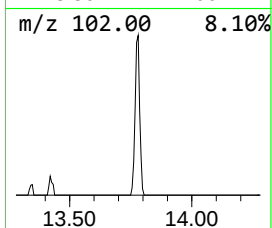
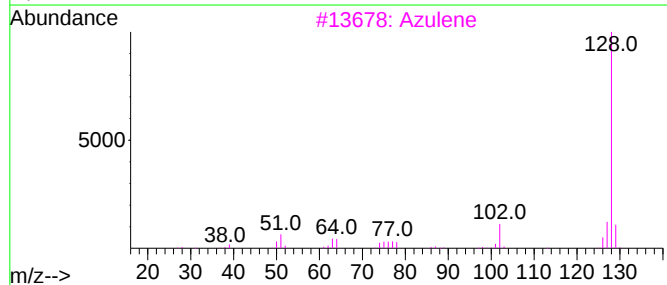
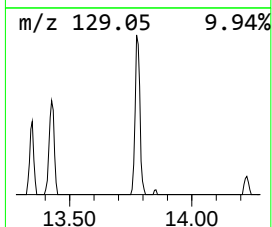
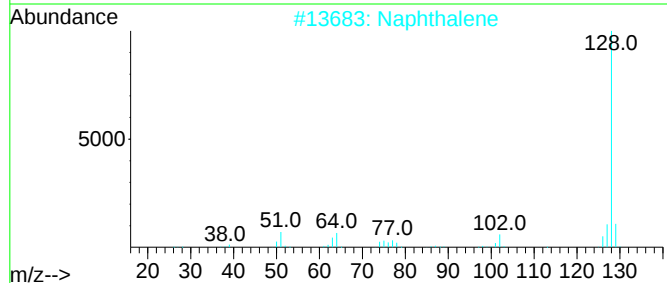
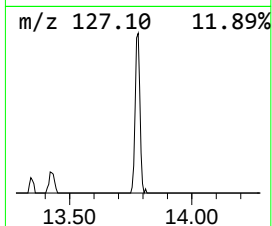
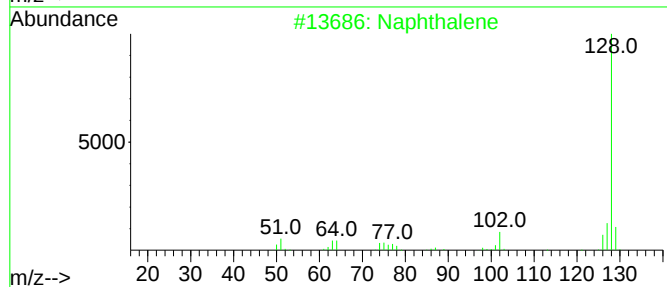
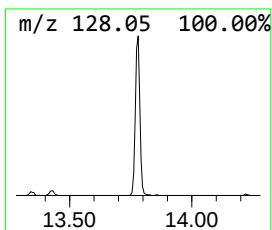
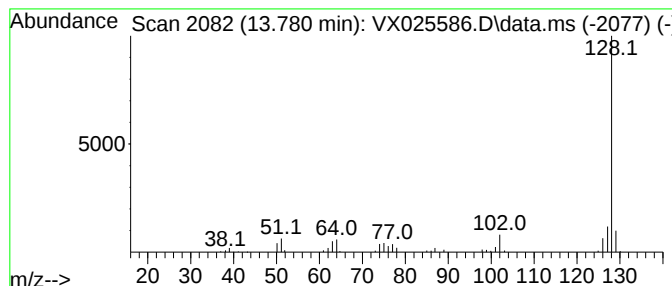
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Quant Title : VOC Analysis

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

Peak Number 6 Azulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.780	8.19 ug/L	46074	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\VX120721\
Data File : VX025586.D
Acq On : 07 Dec 2021 18:13
Operator : JC/MD
Sample : M4881-10ME
Misc : 3.96g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9E6ME

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
Benzene, 1-ethe...	11.811	7.6	ug/L	42887	3	12.024	281246	50.0
Indene	12.421	4.1	ug/L	22890	3	12.024	281246	50.0
o-Isopropenylto...	12.750	3.3	ug/L	18578	3	12.024	281246	50.0
Azulene	13.780	8.2	ug/L	46074	3	12.024	281246	50.0