

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120923\
 Data File : VX039111.D
 Acq On : 08 Dec 2023 17:41
 Operator : JC/MD
 Sample : 05646-01ME
 Misc : 3.79g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COAT5ME

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\SFAMXML120523WMA.M
 Title : VOC Analysis

Signal : TIC: VX039111.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.154	9	11	14	rBV2	1176	1301	0.03%	0.009%
2	1.246	20	26	28	rBV	5200	9006	0.18%	0.059%
3	1.368	43	46	59	rBV	140358	188999	3.78%	1.249%
4	1.544	72	75	81	rBV2	4355	8790	0.18%	0.058%
5	1.648	86	92	102	rBV2	47625	84298	1.69%	0.557%
6	1.746	107	108	109	rBV	1744	1178	0.02%	0.008%
7	1.800	115	117	120	rBV2	10390	16250	0.33%	0.107%
8	1.959	141	143	145	rBV2	1611	1425	0.03%	0.009%
9	2.209	182	184	187	rBV	4144	4880	0.10%	0.032%
10	2.288	191	197	206	rVV	289935	457560	9.16%	3.023%
11	2.599	246	248	251	rVB2	1445	1440	0.03%	0.010%
12	2.709	264	266	271	rVB3	4610	7041	0.14%	0.047%
13	2.849	284	289	296	rVB3	10093	20029	0.40%	0.132%
14	2.940	300	304	313	rVB3	7634	19008	0.38%	0.126%
15	3.087	326	328	333	rBV	1146	1489	0.03%	0.010%
16	3.434	383	385	389	rVB2	975	1182	0.02%	0.008%
17	3.593	409	411	412	rBV	2217	1488	0.03%	0.010%
18	4.154	501	503	504	rVV	1849	1162	0.02%	0.008%
19	4.269	518	522	525	rBV	1863	3107	0.06%	0.021%
20	4.477	547	556	574	rBV	87273	326990	6.54%	2.160%
21	4.800	608	609	611	rBV	1349	1292	0.03%	0.009%
22	5.056	640	651	666	rBV2	159475	504300	10.09%	3.332%
23	5.269	684	686	689	rBV	1719	2382	0.05%	0.016%
24	5.458	715	717	719	rBV	1213	1195	0.02%	0.008%
25	5.617	741	743	745	rBV	1853	2308	0.05%	0.015%
26	5.794	770	772	774	rVB	2372	1791	0.04%	0.012%
27	5.836	774	779	781	rBV	2494	4735	0.09%	0.031%
28	5.964	789	800	823	rBV2	468882	1353415	27.09%	8.941%
29	6.263	847	849	850	rBV	1682	1299	0.03%	0.009%
30	6.348	861	863	868	rVB	1737	1941	0.04%	0.013%
31	6.470	881	883	885	rVB	1777	1439	0.03%	0.010%
32	6.556	894	897	898	rBV	2207	1813	0.04%	0.012%
33	6.702	918	921	922	rBV	1509	1689	0.03%	0.011%
34	6.757	922	930	950	rVB	305395	755608	15.12%	4.992%
35	7.013	971	972	974	rBV	1637	1168	0.02%	0.008%
36	7.031	974	975	977	rBV	1682	1255	0.03%	0.008%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Filtering: 5

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120523WMA.M
 Title : VOC Analysis

37	7.104	982	987	988	rBV	2507	3677	0.07%	0.024%
38	7.306	1011	1020	1032	rBV	267519	602931	12.07%	3.983%
39	7.470	1045	1047	1050	rBV	1462	1568	0.03%	0.010%
40	7.787	1097	1099	1103	rBV	1131	1597	0.03%	0.011%
41	7.842	1106	1108	1110	rBV	1395	1302	0.03%	0.009%
42	7.940	1121	1124	1125	rBV	2175	2046	0.04%	0.014%
43	8.324	1181	1187	1197	rVV	194049	323094	6.47%	2.135%
44	8.470	1210	1211	1212	rBV	1897	1205	0.02%	0.008%
45	8.543	1220	1223	1224	rBV	1297	1161	0.02%	0.008%
46	8.647	1233	1240	1251	rBV	655419	1072791	21.47%	7.087%
47	8.952	1285	1290	1300	rBV	135028	214671	4.30%	1.418%
48	9.202	1329	1331	1334	rVB	1805	1319	0.03%	0.009%
49	9.262	1337	1341	1343	rBV	1635	1708	0.03%	0.011%
50	9.397	1357	1363	1374	rBV	447733	764259	15.30%	5.049%
51	9.708	1411	1414	1418	rBV4	2575	4257	0.09%	0.028%
52	9.811	1429	1431	1434	rBV2	1253	1778	0.04%	0.012%
53	9.860	1438	1439	1441	rBV	1659	1194	0.02%	0.008%
54	10.079	1465	1475	1490	rBV2	2866861	4996470	100.00%	33.009%
55	10.189	1491	1493	1496	rVV	1605	1180	0.02%	0.008%
56	10.384	1523	1525	1528	rVB	1348	1549	0.03%	0.010%
57	10.677	1570	1573	1574	rVB	1637	1494	0.03%	0.010%
58	10.805	1592	1594	1599	rVB	1358	1642	0.03%	0.011%
59	11.085	1637	1640	1641	rBV2	1930	1833	0.04%	0.012%
60	11.195	1652	1658	1667	rVV	499477	635228	12.71%	4.197%
61	11.311	1675	1677	1681	rVB	2430	2221	0.04%	0.015%
62	11.366	1682	1686	1692	rVV	22173	30710	0.61%	0.203%
63	11.421	1692	1695	1698	rVV2	3167	4331	0.09%	0.029%
64	11.463	1698	1702	1709	rVV	9818	14729	0.29%	0.097%
65	11.677	1733	1737	1740	rBV	1924	3309	0.07%	0.022%
66	11.969	1781	1785	1789	rBV	97260	123601	2.47%	0.817%
67	12.024	1789	1794	1803	rVB2	746387	1271363	25.45%	8.399%
68	12.164	1815	1817	1820	rVB	1606	1401	0.03%	0.009%
69	12.225	1825	1827	1832	rVV2	1381	1579	0.03%	0.010%
70	12.323	1837	1843	1853	rBV	707951	947571	18.96%	6.260%
71	12.463	1864	1866	1868	rVB	2603	2146	0.04%	0.014%
72	12.762	1911	1915	1918	rBV2	2557	4410	0.09%	0.029%
73	12.926	1940	1942	1943	rVB	1801	1258	0.03%	0.008%
74	12.945	1943	1945	1947	rBV2	1480	1826	0.04%	0.012%
75	13.067	1957	1965	1970	rBV2	33739	68145	1.36%	0.450%
76	13.115	1970	1973	1979	rVB2	6280	8848	0.18%	0.058%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120523WMA.M
 Title : VOC Analysis

77	13.243	1992	1994	1996	rBV	1158	1226	0.02%	0.008%
78	13.268	1996	1998	1999	rVB	2304	1167	0.02%	0.008%
79	13.439	2024	2026	2028	rVB	1825	1276	0.03%	0.008%
80	13.457	2028	2029	2031	rBV	2365	1505	0.03%	0.010%
81	13.585	2045	2050	2058	rBV2	45415	64314	1.29%	0.425%
82	13.670	2063	2064	2066	rBV	1493	1329	0.03%	0.009%
83	13.774	2079	2081	2087	rVB3	3635	5770	0.12%	0.038%
84	13.932	2105	2107	2108	rBV	2505	1825	0.04%	0.012%
85	13.963	2108	2112	2115	rVV3	16440	22838	0.46%	0.151%
86	13.987	2115	2116	2123	rVV3	5347	8555	0.17%	0.057%
87	14.054	2123	2127	2130	rVB3	3839	5170	0.10%	0.034%
88	14.213	2151	2153	2157	rVB2	3517	4552	0.09%	0.030%
89	14.255	2157	2160	2161	rBV	2409	3054	0.06%	0.020%
90	14.292	2165	2166	2168	rBV	2265	1865	0.04%	0.012%
91	14.444	2186	2191	2193	rBV	2056	2701	0.05%	0.018%
92	14.542	2203	2207	2209	rVB2	1792	2502	0.05%	0.017%
93	14.627	2218	2221	2225	rVB3	3555	5020	0.10%	0.033%
94	14.664	2225	2227	2229	rBV	1945	1730	0.03%	0.011%
95	14.780	2239	2246	2251	rBV4	12582	21341	0.43%	0.141%
96	15.054	2289	2291	2293	rBV	1294	1263	0.03%	0.008%
97	15.249	2317	2323	2328	rBV	28772	42081	0.84%	0.278%
98	15.786	2409	2411	2414	rBV	1384	1339	0.03%	0.009%
99	16.054	2453	2455	2458	rBV	1359	1947	0.04%	0.013%
100	16.505	2525	2529	2536	rVB2	6384	10614	0.21%	0.070%

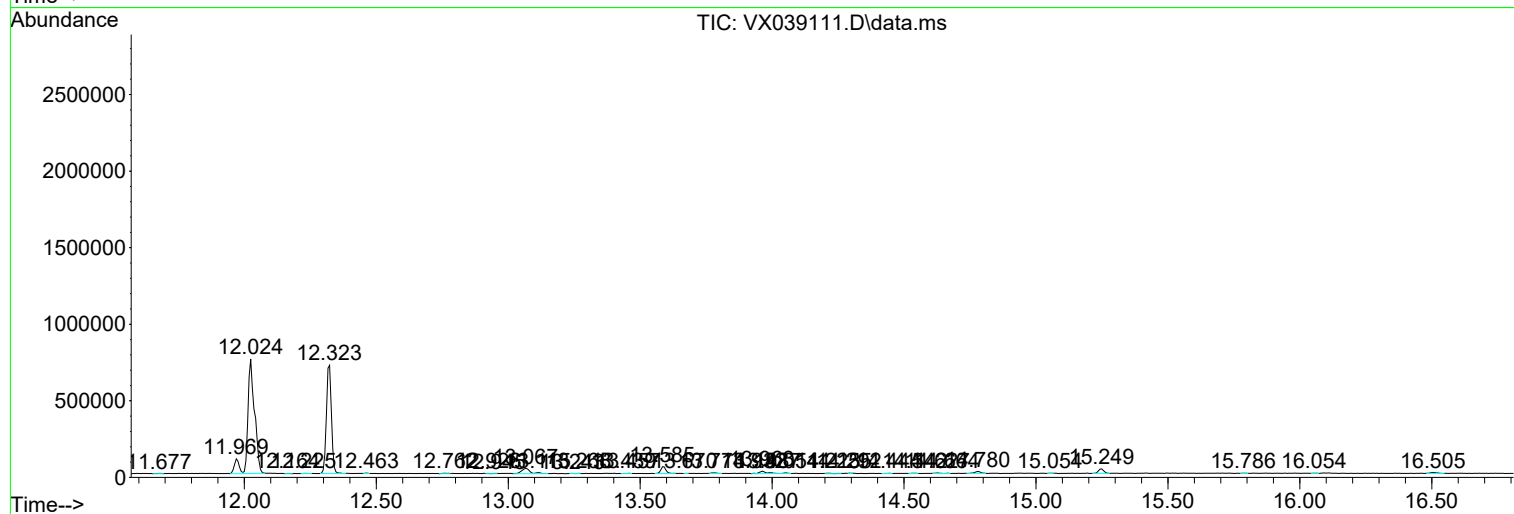
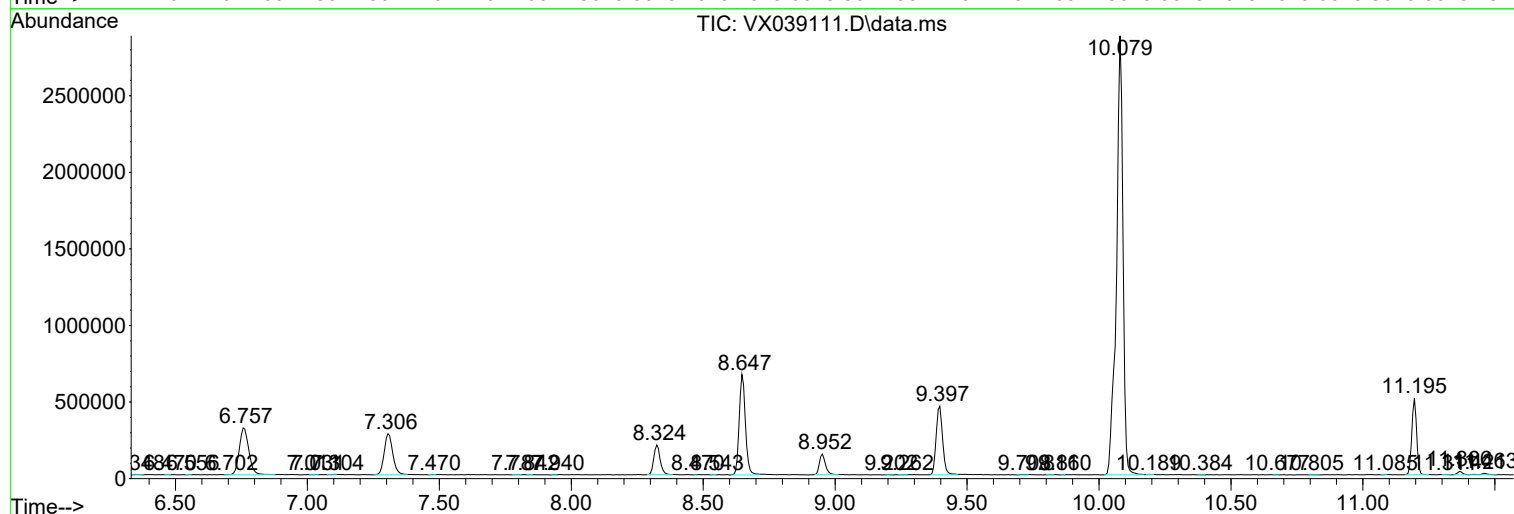
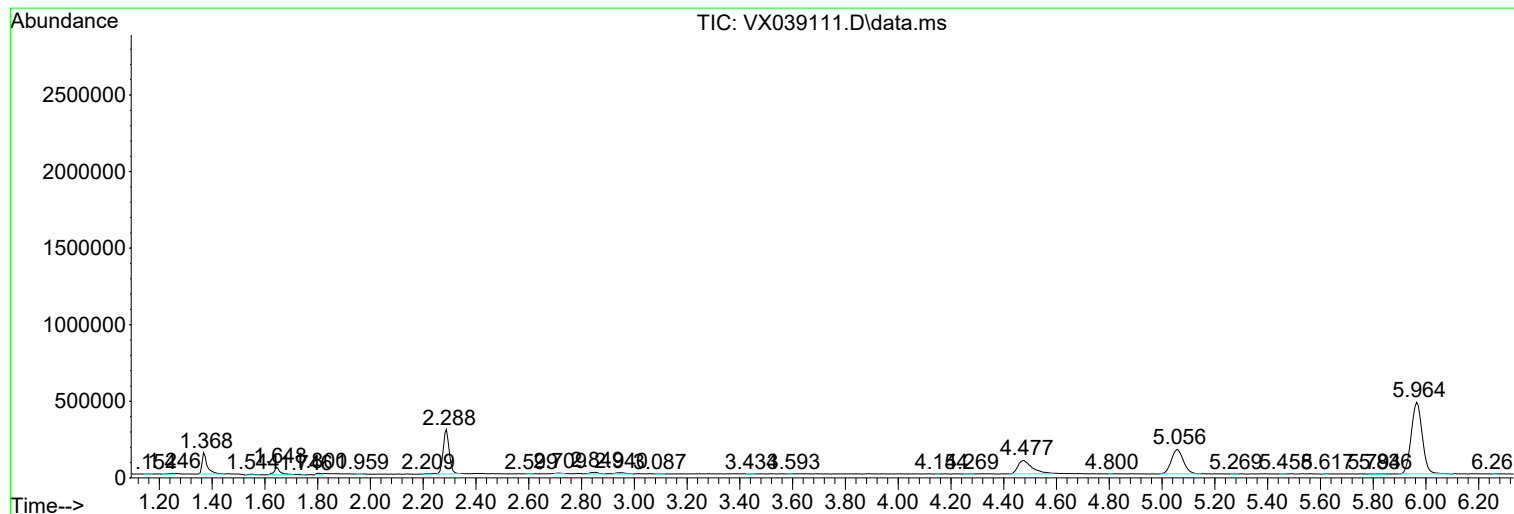
Sum of corrected areas: 15136639

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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COAT5ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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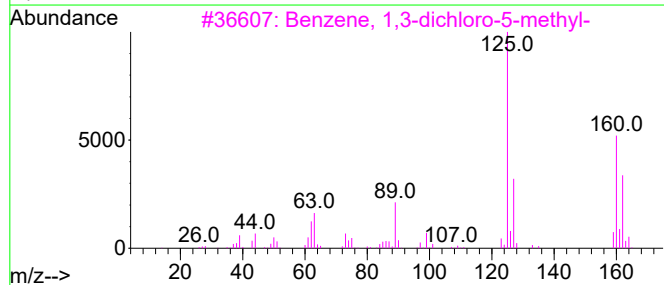
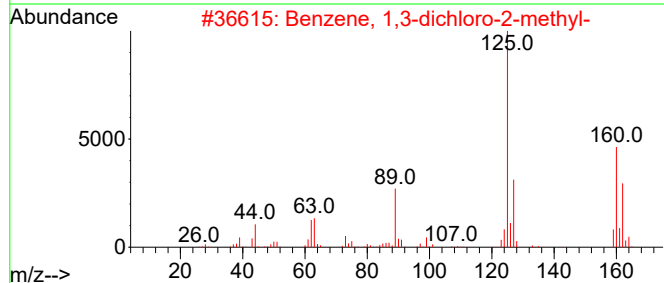
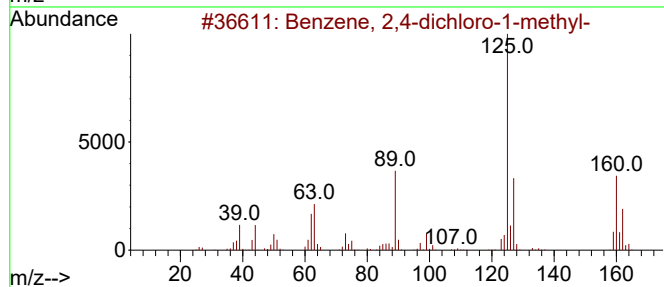
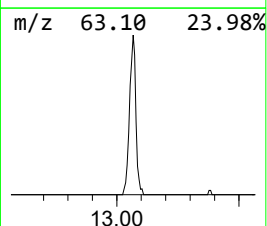
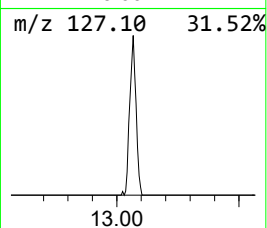
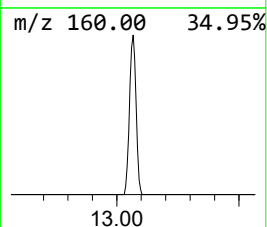
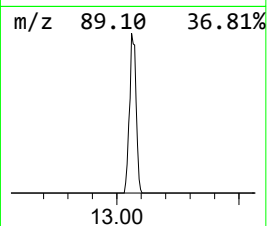
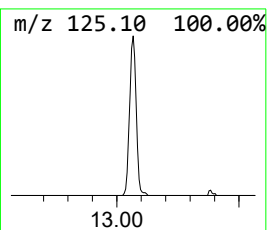
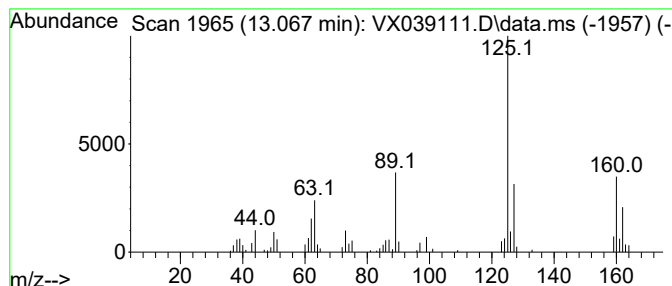
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Benzene, 2,4-dichloro-1-met... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.067	2.68 ug/L	68145	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2,4-dichloro-1-methyl-	160	C7H6Cl2	000095-73-8	98
2			Benzene, 1,3-dichloro-2-methyl-	160	C7H6Cl2	000118-69-4	97
3			Benzene, 1,3-dichloro-5-methyl-	160	C7H6Cl2	025186-47-4	97
4			Benzene, 1,3-dichloro-2-methyl-	160	C7H6Cl2	000118-69-4	97
5			Benzene, 1,2-dichloro-3-methyl-	160	C7H6Cl2	032768-54-0	97



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, 2,4-di...	13.067	2.7	ug/L	68145	3	12.024	1271360	50.0