

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121123\
 Data File : VX039137.D
 Acq On : 11 Dec 2023 12:42
 Operator : JC/MD
 Sample : 05646-02MEDL 5X
 Misc : 5.14g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AT6MEDL

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\SFAMXLM120523WMA.M
 Title : VOC Analysis

Signal : TIC: VX039137.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.367	43	46	57	rBV	132717	142464	7.92%	1.320%
2	1.648	89	92	102	rVB	84947	119865	6.66%	1.111%
3	2.300	193	199	211	rVB	237330	372437	20.70%	3.451%
4	2.507	231	233	236	rBV2	522	551	0.03%	0.005%
5	2.666	257	259	262	rBV2	435	577	0.03%	0.005%
6	2.702	263	265	273	rVV2	1417	2472	0.14%	0.023%
7	2.782	275	278	283	rVB3	1306	2427	0.13%	0.022%
8	2.855	283	290	297	rBV4	3041	7334	0.41%	0.068%
9	2.940	298	304	316	rVB	9895	23382	1.30%	0.217%
10	3.550	402	404	406	rVB2	368	326	0.02%	0.003%
11	3.574	406	408	410	rBV2	478	475	0.03%	0.004%
12	3.678	422	425	428	rBV2	249	331	0.02%	0.003%
13	3.891	458	460	462	rBV2	467	427	0.02%	0.004%
14	4.135	498	500	502	rBV	299	305	0.02%	0.003%
15	4.336	531	533	536	rBV2	313	294	0.02%	0.003%
16	4.452	544	552	567	rBV	96546	278108	15.45%	2.577%
17	4.921	628	629	631	rBV	337	297	0.02%	0.003%
18	5.056	640	651	668	rBV	135641	424663	23.60%	3.935%
19	5.306	691	692	695	rVB	382	295	0.02%	0.003%
20	5.366	699	702	703	rBV	438	430	0.02%	0.004%
21	5.549	724	732	736	rBV4	729	1906	0.11%	0.018%
22	5.964	789	800	825	rBV2	371781	1143502	63.55%	10.595%
23	6.385	867	869	871	rVB2	424	386	0.02%	0.004%
24	6.756	921	930	949	rBV	277693	681618	37.88%	6.315%
25	7.110	982	988	989	rBV4	1693	2823	0.16%	0.026%
26	7.305	1011	1020	1036	rBV	226218	501862	27.89%	4.650%
27	7.470	1045	1047	1048	rBV	604	411	0.02%	0.004%
28	7.586	1062	1066	1068	rBV	473	574	0.03%	0.005%
29	7.628	1070	1073	1075	rBV	403	406	0.02%	0.004%
30	7.762	1093	1095	1097	rBV2	359	324	0.02%	0.003%
31	7.903	1116	1118	1121	rBV2	218	294	0.02%	0.003%
32	7.970	1127	1129	1132	rVB3	599	511	0.03%	0.005%
33	8.061	1141	1144	1147	rVB2	299	296	0.02%	0.003%
34	8.323	1181	1187	1202	rBV	165992	279025	15.51%	2.585%
35	8.524	1219	1220	1224	rVB4	478	556	0.03%	0.005%
36	8.646	1234	1240	1256	rVV	573014	895763	49.78%	8.299%

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 Title : VOC Analysis

37	8.951	1284	1290	1300	rBV	122182	185736	10.32%	1.721%
38	9.287	1343	1345	1348	rBV2	325	429	0.02%	0.004%
39	9.384	1356	1361	1372	rBV	472870	661552	36.76%	6.129%
40	9.701	1410	1413	1417	rVB2	1537	2040	0.11%	0.019%
41	10.055	1465	1471	1472	rBV	657727	848833	47.17%	7.865%
42	10.079	1472	1475	1493	rVB	1297037	1799485	100.00%	16.673%
43	10.420	1529	1531	1533	rVV2	406	296	0.02%	0.003%
44	10.518	1544	1547	1549	rVV2	241	294	0.02%	0.003%
45	11.085	1635	1640	1644	rBV2	1048	1629	0.09%	0.015%
46	11.189	1652	1657	1670	rVV	417144	546241	30.36%	5.061%
47	11.365	1680	1686	1692	rBV	76163	99013	5.50%	0.917%
48	11.457	1697	1701	1709	rVB	17397	24784	1.38%	0.230%
49	11.676	1735	1737	1738	rBV2	461	305	0.02%	0.003%
50	11.707	1738	1742	1743	rVV2	360	370	0.02%	0.003%
51	11.780	1752	1754	1756	rBV	340	385	0.02%	0.004%
52	11.938	1777	1780	1783	rBV2	384	519	0.03%	0.005%
53	11.975	1783	1786	1788	rVV3	817	1259	0.07%	0.012%
54	12.024	1788	1794	1809	rVV	635936	907299	50.42%	8.406%
55	12.316	1837	1842	1855	rVB	602253	793441	44.09%	7.351%
56	12.554	1878	1881	1885	rBV2	340	530	0.03%	0.005%
57	12.640	1893	1895	1897	rVB2	305	296	0.02%	0.003%
58	12.658	1897	1898	1901	rBV2	360	282	0.02%	0.003%
59	12.682	1901	1902	1905	rVV	301	282	0.02%	0.003%
60	12.737	1909	1911	1913	rVV	332	320	0.02%	0.003%
61	12.761	1913	1915	1919	rVV3	448	576	0.03%	0.005%
62	13.072	1960	1966	1971	rVV3	6257	8873	0.49%	0.082%
63	13.115	1971	1973	1975	rVV	376	288	0.02%	0.003%
64	13.182	1982	1984	1990	rBV2	277	445	0.02%	0.004%
65	13.298	2001	2003	2004	rVB2	470	288	0.02%	0.003%
66	13.347	2009	2011	2015	rBV2	325	410	0.02%	0.004%
67	13.475	2030	2032	2035	rVB2	378	303	0.02%	0.003%
68	13.591	2048	2051	2054	rBV2	2163	2348	0.13%	0.022%
69	13.700	2068	2069	2071	rBV	453	297	0.02%	0.003%
70	13.786	2079	2083	2087	rBV2	889	1448	0.08%	0.013%
71	13.865	2094	2096	2101	rBV2	344	453	0.03%	0.004%
72	13.926	2101	2106	2108	rVV2	325	582	0.03%	0.005%
73	13.975	2109	2114	2116	rVB2	981	1434	0.08%	0.013%
74	13.993	2116	2117	2122	rBV2	480	479	0.03%	0.004%
75	14.048	2122	2126	2129	rBV2	317	552	0.03%	0.005%
76	14.091	2129	2133	2135	rVB3	396	512	0.03%	0.005%

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

77	14.127	2137	2139	2141	rVB	529	359	0.02%	0.003%
78	14.164	2141	2145	2149	rVB3	452	672	0.04%	0.006%
79	14.243	2156	2158	2160	rBV2	328	290	0.02%	0.003%
80	14.475	2194	2196	2198	rBV2	467	375	0.02%	0.003%
81	14.560	2207	2210	2213	rBV2	428	579	0.03%	0.005%
82	14.706	2232	2234	2237	rVB	405	327	0.02%	0.003%
83	14.737	2237	2239	2242	rBV	457	425	0.02%	0.004%
84	14.779	2244	2246	2248	rBV2	378	335	0.02%	0.003%
85	14.816	2250	2252	2254	rBV2	385	384	0.02%	0.004%
86	14.914	2267	2268	2270	rBV	498	299	0.02%	0.003%
87	14.987	2279	2280	2282	rVB	556	397	0.02%	0.004%
88	15.011	2282	2284	2285	rBV	482	350	0.02%	0.003%
89	15.029	2285	2287	2292	rVB2	327	372	0.02%	0.003%
90	15.182	2309	2312	2314	rBV2	414	421	0.02%	0.004%
91	15.310	2331	2333	2335	rVB	504	395	0.02%	0.004%
92	15.328	2335	2336	2337	rBV	563	394	0.02%	0.004%
93	15.670	2390	2392	2395	rVB2	541	467	0.03%	0.004%
94	15.791	2410	2412	2415	rVB2	291	369	0.02%	0.003%
95	15.834	2417	2419	2420	rBV	551	388	0.02%	0.004%
96	15.968	2438	2441	2442	rBV2	384	307	0.02%	0.003%
97	16.035	2448	2452	2454	rBV2	541	777	0.04%	0.007%
98	16.127	2466	2467	2469	rBV	352	378	0.02%	0.004%
99	16.316	2496	2498	2502	rBV3	339	486	0.03%	0.005%
100	16.694	2558	2560	2567	rBV3	672	952	0.05%	0.009%

Sum of corrected areas: 10793123

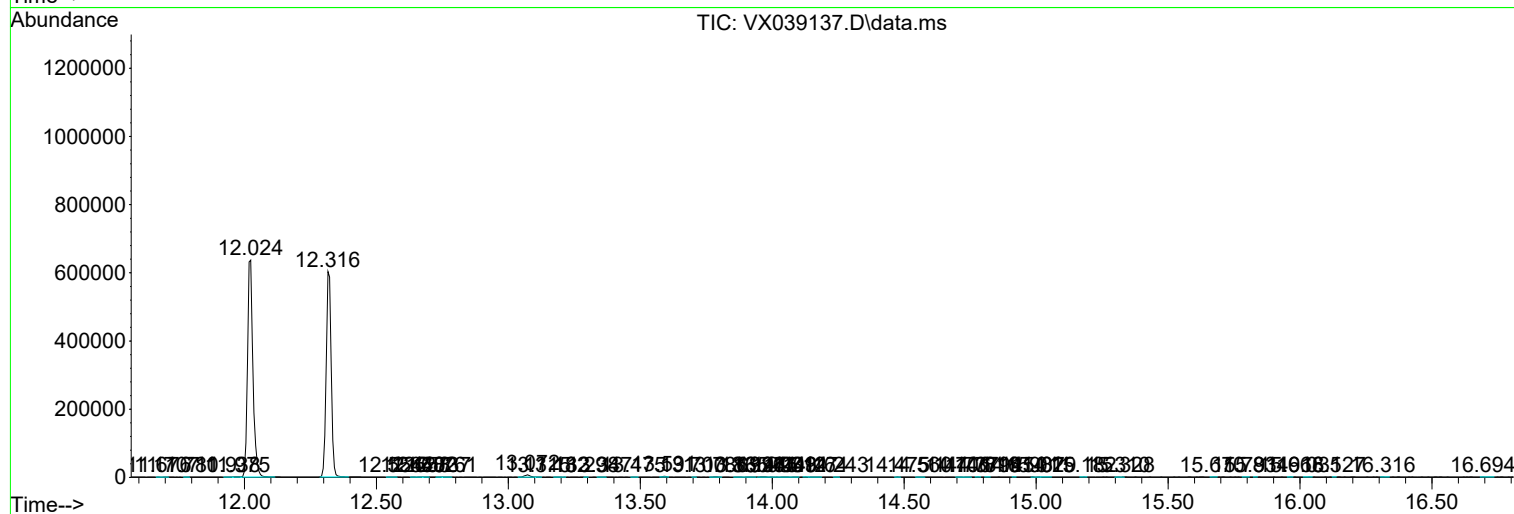
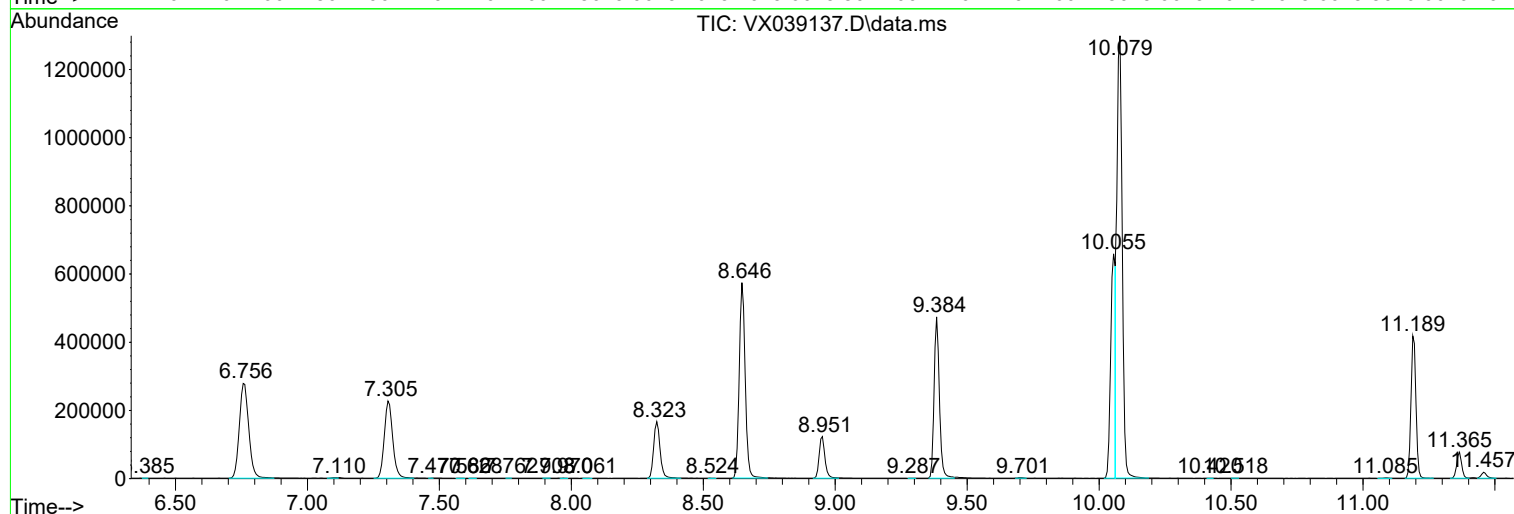
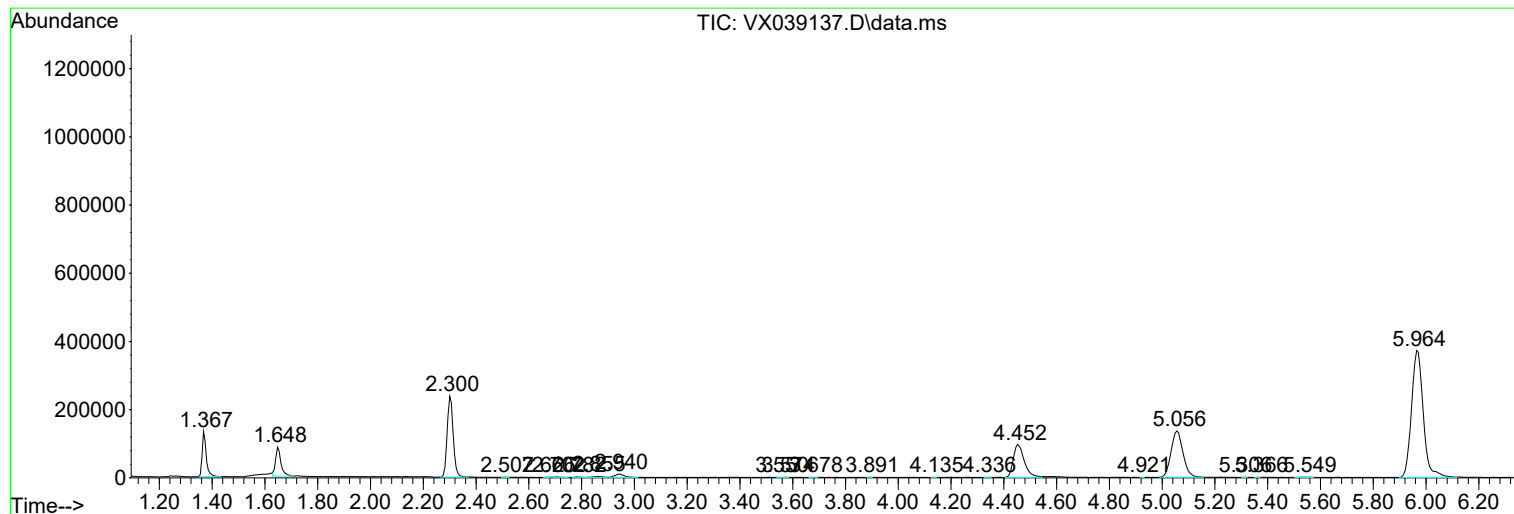
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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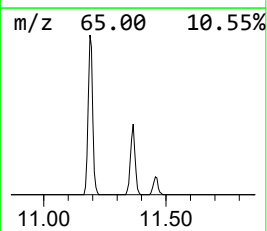
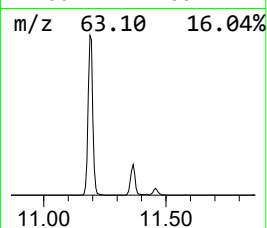
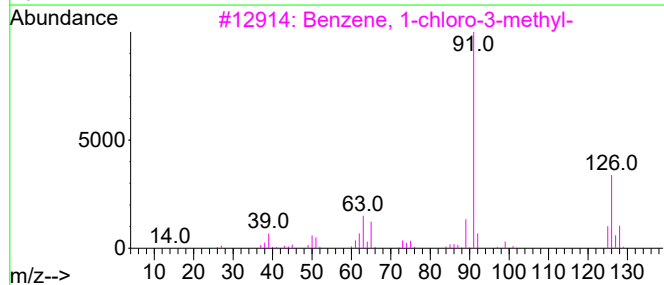
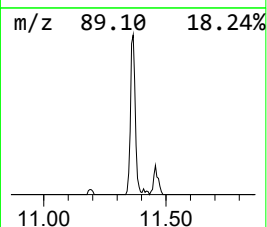
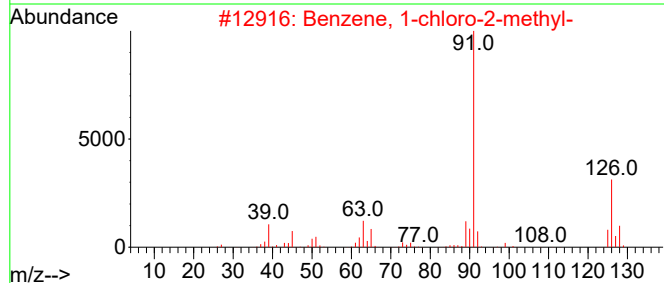
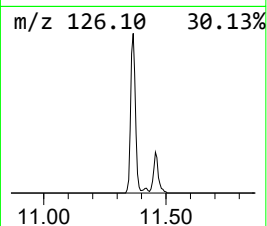
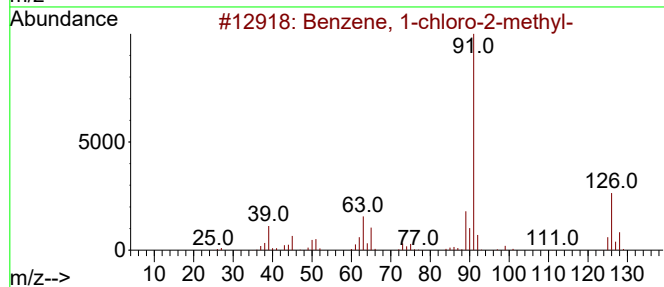
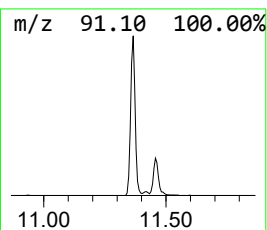
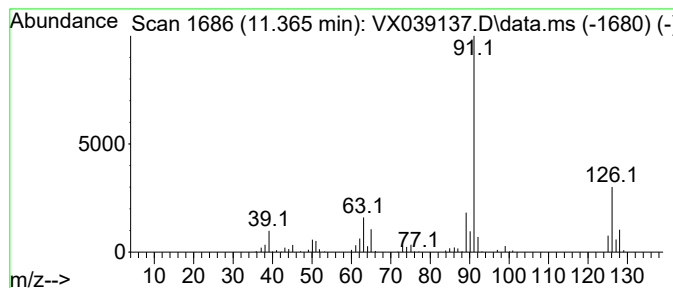
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Benzene, 1-chloro-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.365	5.46 ug/L	99013	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-chloro-2-methyl-	126	C7H7Cl	000095-49-8	96
2			Benzene, 1-chloro-2-methyl-	126	C7H7Cl	000095-49-8	95
3			Benzene, 1-chloro-3-methyl-	126	C7H7Cl	000108-41-8	94
4			Benzene, 1-chloro-2-methyl-	126	C7H7Cl	000095-49-8	94
5			Benzene, 1-chloro-2-methyl-	126	C7H7Cl	000095-49-8	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, 1-chlo...	11.365	5.5	ug/L	99013	3	12.024	907299	50.0