

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120923\
 Data File : VX039112.D
 Acq On : 08 Dec 2023 18:04
 Operator : JC/MD
 Sample : 05646-02ME
 Misc : 5.14g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COAT6ME

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: VX039112.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	10	11	15	rVV2	1590	1908	0.02%	0.010%
2	1.240	22	25	32	rBV3	4912	11185	0.12%	0.060%
3	1.368	43	46	57	rBV	116544	157450	1.74%	0.849%
4	1.471	61	63	72	rVB	7489	18807	0.21%	0.101%
5	1.642	86	91	99	rBV2	36732	64507	0.71%	0.348%
6	1.703	99	101	106	rVB4	3984	6418	0.07%	0.035%
7	1.782	109	114	116	rBV6	1257	2188	0.02%	0.012%
8	1.807	116	118	121	rBV2	10109	15439	0.17%	0.083%
9	2.093	164	165	168	rBV2	1153	1476	0.02%	0.008%
10	2.233	184	188	191	rVV	3219	5860	0.06%	0.032%
11	2.288	191	197	207	rVB	246166	396979	4.38%	2.141%
12	2.392	212	214	215	rVV	2986	2389	0.03%	0.013%
13	2.410	215	217	220	rVB2	2592	2748	0.03%	0.015%
14	2.617	250	251	255	rBV	1377	1411	0.02%	0.008%
15	2.715	263	267	273	rVB2	5495	9367	0.10%	0.051%
16	2.782	276	278	283	rVV2	2221	3094	0.03%	0.017%
17	2.849	283	289	296	rVB2	15904	31228	0.34%	0.168%
18	2.941	299	304	313	rBV2	7473	19992	0.22%	0.108%
19	3.233	350	352	356	rBV	1499	1570	0.02%	0.008%
20	3.965	470	472	474	rBV	1504	1463	0.02%	0.008%
21	4.166	501	505	506	rBV2	998	1478	0.02%	0.008%
22	4.203	508	511	513	rBV	1577	1827	0.02%	0.010%
23	4.306	526	528	533	rVB	1499	1516	0.02%	0.008%
24	4.379	536	540	543	rBV	2181	3094	0.03%	0.017%
25	4.477	547	556	578	rBV	69310	273765	3.02%	1.476%
26	4.684	589	590	592	rBV	1939	1562	0.02%	0.008%
27	5.056	641	651	670	rVV	133458	433027	4.78%	2.335%
28	5.751	763	765	766	rBV	1776	1523	0.02%	0.008%
29	5.788	769	771	774	rBV	1144	1453	0.02%	0.008%
30	5.843	778	780	783	rBV	1686	1860	0.02%	0.010%
31	5.873	783	785	788	rVB	1468	1571	0.02%	0.008%
32	5.964	789	800	808	rBV2	386291	1133381	12.51%	6.111%
33	6.166	830	833	836	rBV2	1461	2507	0.03%	0.014%
34	6.196	836	838	839	rBV2	1553	1415	0.02%	0.008%
35	6.349	860	863	865	rVV	1210	1392	0.02%	0.008%
36	6.416	873	874	877	rVB	2010	1475	0.02%	0.008%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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

37	6.531	890	893	895	rBV	1027	1635	0.02%	0.009%
38	6.605	902	905	907	rVB	1669	1976	0.02%	0.011%
39	6.757	921	930	946	rBV	362125	887825	9.80%	4.787%
40	7.068	978	981	983	rBV	1128	1783	0.02%	0.010%

41	7.104	984	987	989	rBV2	2034	2269	0.03%	0.012%
42	7.165	995	997	999	rBV	1615	1717	0.02%	0.009%
43	7.306	1012	1020	1034	rBV	224440	507053	5.60%	2.734%
44	7.519	1051	1055	1057	rVB	1540	1941	0.02%	0.010%
45	7.610	1069	1070	1073	rBV	1731	1818	0.02%	0.010%

46	7.927	1120	1122	1125	rBV2	1096	1411	0.02%	0.008%
47	8.123	1152	1154	1159	rBV	1322	2663	0.03%	0.014%
48	8.190	1163	1165	1167	rBV	1526	1737	0.02%	0.009%
49	8.324	1181	1187	1201	rBV	161906	275790	3.05%	1.487%
50	8.647	1234	1240	1252	rBV	559363	917340	10.13%	4.946%

51	8.952	1284	1290	1298	rBV	118469	185900	2.05%	1.002%
52	9.226	1333	1335	1338	rVB	2050	1490	0.02%	0.008%
53	9.397	1356	1363	1377	rBV	377370	648170	7.16%	3.495%
54	10.080	1465	1475	1491	rBV2	5465582	9056885	100.00%	48.835%
55	10.232	1499	1500	1503	rVB	2480	1558	0.02%	0.008%

56	10.762	1585	1587	1589	rBV	1883	2033	0.02%	0.011%
57	10.836	1596	1599	1600	rVV2	1228	1605	0.02%	0.009%
58	11.025	1627	1630	1632	rBV	1499	1742	0.02%	0.009%
59	11.195	1651	1658	1667	rBV	424695	545156	6.02%	2.940%
60	11.366	1681	1686	1692	rBV	355428	456024	5.04%	2.459%

61	11.415	1692	1694	1697	rVV	7078	9855	0.11%	0.053%
62	11.457	1697	1701	1709	rVV	89045	115748	1.28%	0.624%
63	11.531	1711	1713	1716	rBV	1411	1541	0.02%	0.008%
64	11.634	1728	1730	1733	rVV	1637	1643	0.02%	0.009%
65	11.689	1736	1739	1742	rBV	1627	2635	0.03%	0.014%

66	11.756	1747	1750	1752	rBV	1825	2112	0.02%	0.011%
67	11.829	1759	1762	1764	rBV	1446	1732	0.02%	0.009%
68	11.854	1764	1766	1768	rBV	1282	1413	0.02%	0.008%
69	11.969	1783	1785	1788	rBV2	2623	3633	0.04%	0.020%
70	12.024	1788	1794	1803	rBV2	880388	1363183	15.05%	7.350%

71	12.323	1837	1843	1849	rBV	607927	802663	8.86%	4.328%
72	12.695	1902	1904	1908	rBV	1408	1928	0.02%	0.010%
73	12.823	1919	1925	1927	rBV2	1699	2859	0.03%	0.015%
74	13.030	1956	1959	1960	rVV	1618	1693	0.02%	0.009%
75	13.073	1960	1966	1972	rVV2	31843	50151	0.55%	0.270%

76	13.116	1972	1973	1975	rVV	2017	1687	0.02%	0.009%
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 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AT6ME

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

77	13.359	2011	2013	2015	rBV2	1312	1476	0.02%	0.008%
78	13.591	2046	2051	2055	rBV2	1876	3800	0.04%	0.020%
79	13.780	2079	2082	2085	rVB	5034	5005	0.06%	0.027%
80	13.914	2103	2104	2108	rVB	1892	2094	0.02%	0.011%
81	13.975	2110	2114	2115	rBV2	1399	1983	0.02%	0.011%
82	13.993	2115	2117	2121	rVB3	2816	3901	0.04%	0.021%
83	14.036	2122	2124	2127	rBV	1635	1783	0.02%	0.010%
84	14.317	2169	2170	2173	rBV	2448	1646	0.02%	0.009%
85	14.432	2185	2189	2191	rBV	2596	2920	0.03%	0.016%
86	14.615	2215	2219	2224	rBV	1315	2963	0.03%	0.016%
87	14.810	2249	2251	2254	rVB	2192	1861	0.02%	0.010%
88	14.847	2254	2257	2259	rVB	1598	1606	0.02%	0.009%
89	14.926	2268	2270	2272	rBV	1785	2032	0.02%	0.011%
90	14.945	2272	2273	2275	rVV	2424	1580	0.02%	0.009%
91	14.975	2275	2278	2280	rVB	1793	1835	0.02%	0.010%
92	15.188	2310	2313	2314	rBV	2189	2366	0.03%	0.013%
93	15.310	2331	2333	2335	rBV	1872	1878	0.02%	0.010%
94	15.408	2347	2349	2351	rVB	2208	1700	0.02%	0.009%
95	15.444	2351	2355	2358	rBV	1853	3457	0.04%	0.019%
96	15.536	2366	2370	2371	rBV2	1557	2310	0.03%	0.012%
97	15.670	2390	2392	2394	rBV2	1926	2001	0.02%	0.011%
98	15.761	2405	2407	2409	rBV	1428	1394	0.02%	0.008%
99	15.896	2427	2429	2430	rBV	2021	1561	0.02%	0.008%
100	16.450	2518	2520	2522	rBV	2474	2352	0.03%	0.013%

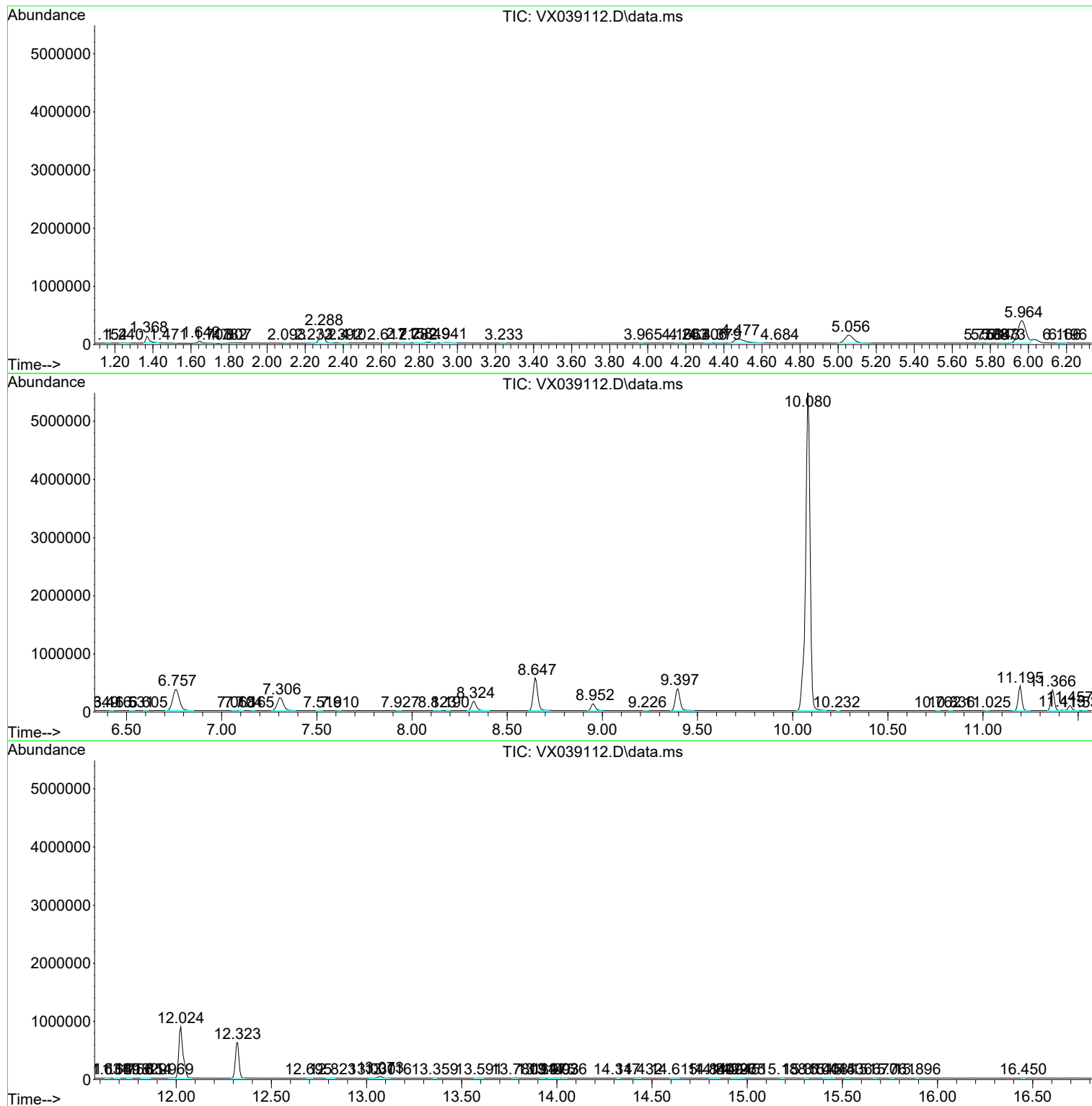
Sum of corrected areas: 18545826

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ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
C0AT6ME

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

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



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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AT6ME

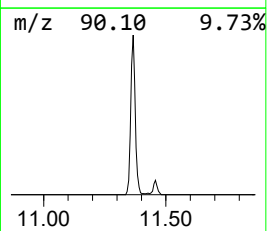
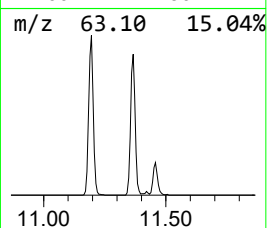
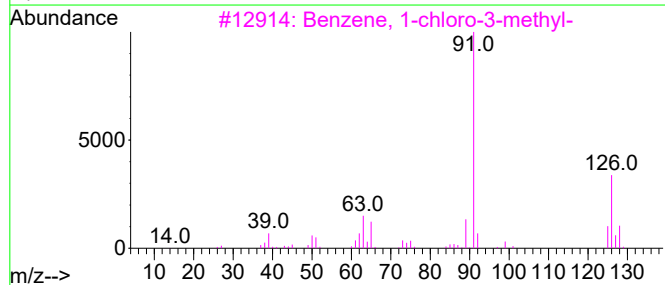
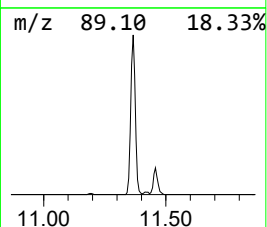
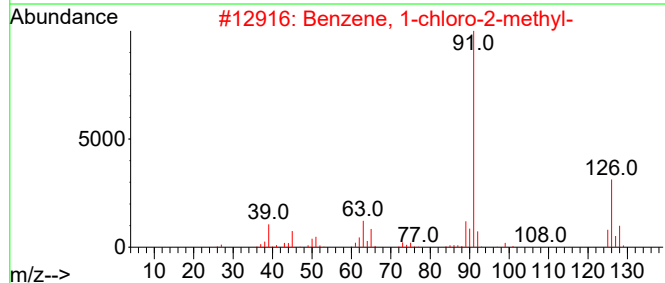
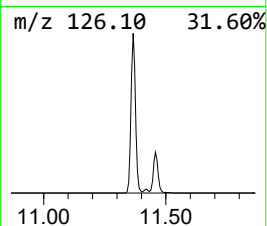
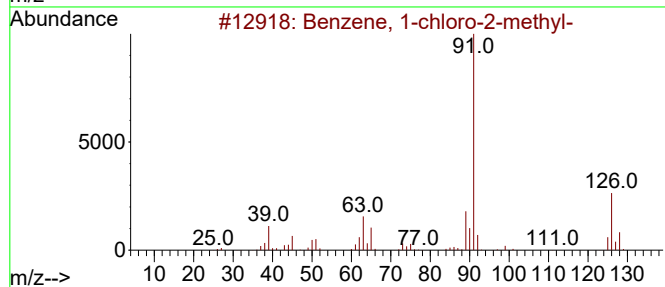
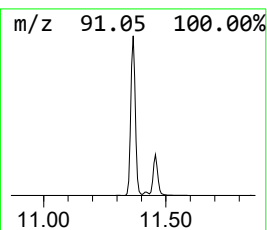
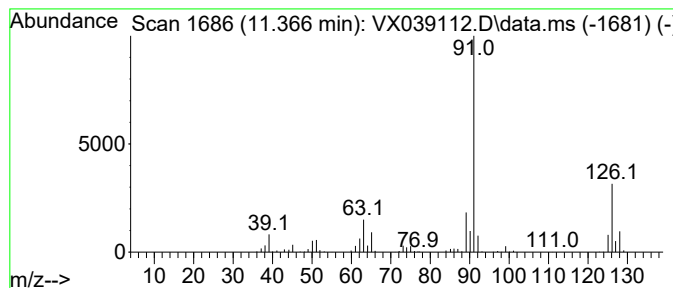
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.366	16.73 ug/L	456024	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	95
4			Benzene, 1-chloro-2-methyl-	126	C7H7Cl	000095-49-8	95
5			Benzene, 1-chloro-2-methyl-	126	C7H7Cl	000095-49-8	94



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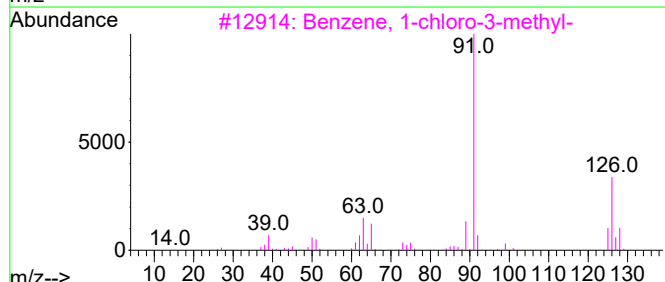
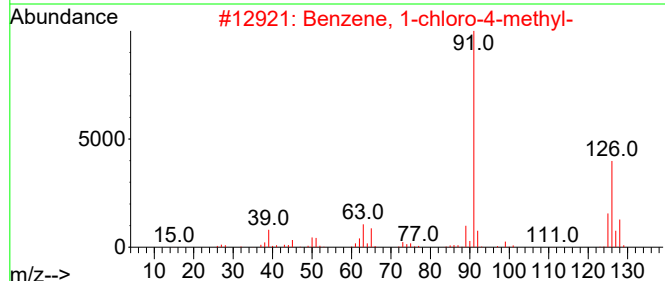
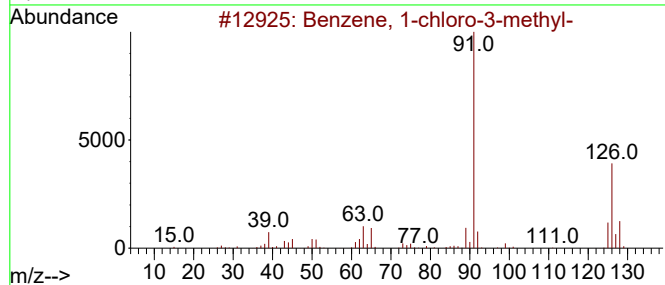
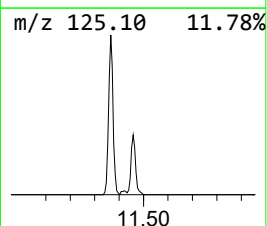
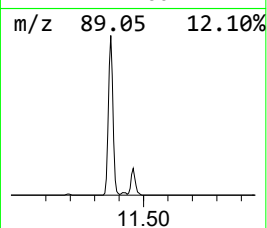
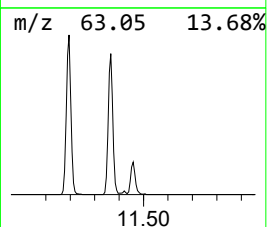
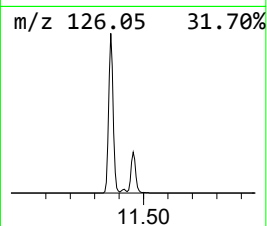
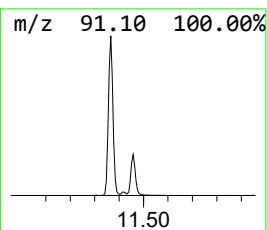
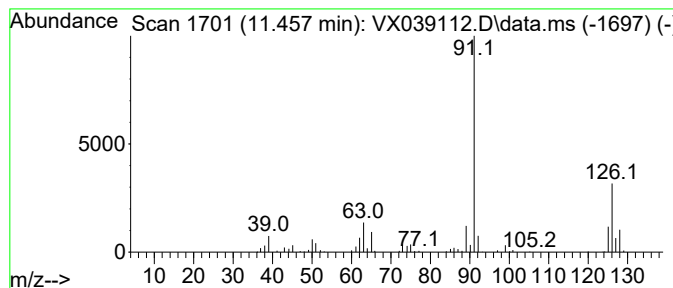
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Benzene, 1-chloro-3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.457	4.25 ug/L	115748	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-chloro-3-methyl-	126	C7H7Cl	000108-41-8	97
2			Benzene, 1-chloro-4-methyl-	126	C7H7Cl	000106-43-4	97
3			Benzene, 1-chloro-3-methyl-	126	C7H7Cl	000108-41-8	96
4			Benzene, 1-chloro-4-methyl-	126	C7H7Cl	000106-43-4	94
5			Benzene, 1-chloro-2-methyl-	126	C7H7Cl	000095-49-8	94



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120523WMA.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-chlo...	11.366	16.7	ug/L	456024	3	12.024	1363180	50.0
Benzene, 1-chlo...	11.457	4.3	ug/L	115748	3	12.024	1363180	50.0