

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122023\
 Data File : VX039396.D
 Acq On : 20 Dec 2023 13:11
 Operator : JC/MD
 Sample : 05869-07
 Misc : 4.22g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AT3

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: VX039396.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	23	28	34	rBV4	1761	3634	0.35%	0.041%
2	1.373	43	47	59	rBV	83529	131368	12.83%	1.483%
3	1.495	65	67	68	rBV2	461	404	0.04%	0.005%
4	1.648	68	92	110	rBV2	44415	185133	18.08%	2.089%
5	2.288	191	197	209	rVB	210833	334620	32.67%	3.777%
6	2.404	211	216	220	rBV2	1066	1849	0.18%	0.021%
7	2.495	228	231	232	rBV4	615	562	0.05%	0.006%
8	2.648	252	256	257	rVV	344	401	0.04%	0.005%
9	2.715	260	267	275	rVV2	3755	7981	0.78%	0.090%
10	2.788	275	279	283	rVV3	1665	3057	0.30%	0.035%
11	2.849	284	289	298	rVV2	4698	9345	0.91%	0.105%
12	2.946	298	305	312	rVV2	3767	8823	0.86%	0.100%
13	3.324	365	367	372	rVB3	418	660	0.06%	0.007%
14	3.434	380	385	388	rVB2	276	398	0.04%	0.004%
15	3.605	412	413	417	rVB2	276	328	0.03%	0.004%
16	3.647	417	420	425	rBV2	235	371	0.04%	0.004%
17	4.470	546	555	581	rBV	62047	261423	25.53%	2.951%
18	4.726	595	597	602	rVB3	823	1223	0.12%	0.014%
19	5.062	639	652	672	rVV	118079	397666	38.83%	4.488%
20	5.214	674	677	683	rVB3	467	752	0.07%	0.008%
21	5.458	713	717	720	rBV2	477	802	0.08%	0.009%
22	5.556	729	733	740	rBV4	451	808	0.08%	0.009%
23	5.702	754	757	760	rVB2	286	329	0.03%	0.004%
24	5.964	788	800	821	rBV2	347087	1024091	100.00%	11.558%
25	6.244	845	846	850	rVB3	341	372	0.04%	0.004%
26	6.555	890	897	900	rVB2	289	483	0.05%	0.005%
27	6.757	919	930	945	rBV	251433	623893	60.92%	7.041%
28	7.067	977	981	983	rBV	225	322	0.03%	0.004%
29	7.116	983	989	995	rVB4	1877	3567	0.35%	0.040%
30	7.220	1000	1006	1011	rBV3	271	647	0.06%	0.007%
31	7.305	1011	1020	1039	rBV	207194	471708	46.06%	5.324%
32	7.470	1044	1047	1049	rVV3	599	583	0.06%	0.007%
33	7.488	1049	1050	1052	rVV	526	420	0.04%	0.005%
34	7.506	1052	1053	1057	rVB	496	428	0.04%	0.005%
35	7.958	1123	1127	1130	rVV3	430	624	0.06%	0.007%
36	7.994	1132	1133	1136	rVV	472	365	0.04%	0.004%

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

37	8.262	1170	1177	1180	rBV2	1019	1578	0.15%	0.018%
38	8.323	1181	1187	1208	rVV	127140	233801	22.83%	2.639%
39	8.464	1208	1210	1213	rVV2	371	361	0.04%	0.004%
40	8.500	1213	1216	1218	rVV2	371	439	0.04%	0.005%
41	8.525	1218	1220	1221	rVV2	501	362	0.04%	0.004%
42	8.646	1234	1240	1261	rBV	493077	800371	78.15%	9.033%
43	8.842	1270	1272	1276	rVB3	364	525	0.05%	0.006%
44	8.951	1285	1290	1309	rVB	92480	154102	15.05%	1.739%
45	9.274	1341	1343	1347	rVB	344	429	0.04%	0.005%
46	9.396	1357	1363	1378	rBV	346522	610524	59.62%	6.891%
47	9.713	1410	1415	1420	rVB3	1042	1541	0.15%	0.017%
48	10.055	1465	1471	1473	rBV	528970	788289	76.97%	8.897%
49	10.311	1508	1513	1517	rBV4	780	1195	0.12%	0.013%
50	10.585	1556	1558	1561	rVB2	655	592	0.06%	0.007%
51	10.646	1565	1568	1569	rBV2	701	718	0.07%	0.008%
52	10.780	1586	1590	1595	rVB4	1187	1810	0.18%	0.020%
53	10.853	1599	1602	1603	rBV3	516	567	0.06%	0.006%
54	10.896	1605	1609	1614	rVB4	1212	1861	0.18%	0.021%
55	10.939	1614	1616	1619	rBV3	495	735	0.07%	0.008%
56	11.024	1627	1630	1637	rBV3	1362	1901	0.19%	0.021%
57	11.091	1637	1641	1648	rVB4	1266	2148	0.21%	0.024%
58	11.195	1651	1658	1670	rBV	387063	502360	49.05%	5.670%
59	11.317	1673	1678	1681	rBV2	1746	2523	0.25%	0.028%
60	11.365	1681	1686	1694	rBV	114895	147317	14.39%	1.663%
61	11.426	1694	1696	1698	rBV3	1553	2022	0.20%	0.023%
62	11.457	1698	1701	1711	rVB2	14684	23314	2.28%	0.263%
63	11.548	1714	1716	1718	rBV2	573	413	0.04%	0.005%
64	11.573	1718	1720	1722	rVB2	481	297	0.03%	0.003%
65	11.597	1722	1724	1727	rBV3	769	867	0.08%	0.010%
66	11.628	1727	1729	1734	rBV4	1800	2331	0.23%	0.026%
67	11.683	1734	1738	1740	rBV3	2077	2391	0.23%	0.027%
68	11.713	1740	1743	1746	rBV2	4073	4376	0.43%	0.049%
69	11.750	1746	1749	1752	rBV5	826	1278	0.12%	0.014%
70	11.841	1759	1764	1766	rBV4	2810	4106	0.40%	0.046%
71	11.890	1766	1772	1776	rVV5	4026	7483	0.73%	0.084%
72	11.945	1776	1781	1782	rVV4	2458	3910	0.38%	0.044%
73	11.975	1782	1786	1789	rVV3	6808	9261	0.90%	0.105%
74	12.024	1789	1794	1805	rVB	652825	849180	82.92%	9.584%
75	12.103	1805	1807	1810	rBV4	2480	2396	0.23%	0.027%
76	12.231	1826	1828	1830	rBV3	1765	2191	0.21%	0.025%

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 Title : VOC Analysis

77	12.323	1837	1843	1849	rBV	559677	740665	72.32%	8.359%
78	12.554	1874	1881	1883	rBV6	5292	11893	1.16%	0.134%
79	12.640	1891	1895	1898	rBV5	2913	4360	0.43%	0.049%
80	12.682	1898	1902	1906	rBV4	9237	12403	1.21%	0.140%
81	12.762	1913	1915	1920	rVB3	7307	8280	0.81%	0.093%
82	12.816	1920	1924	1930	rVB7	14885	21732	2.12%	0.245%
83	12.884	1930	1935	1937	rBV4	12007	20286	1.98%	0.229%
84	12.944	1942	1945	1948	rBV4	5519	6275	0.61%	0.071%
85	12.981	1948	1951	1958	rVB5	9901	12856	1.26%	0.145%
86	13.042	1958	1961	1964	rBV2	10971	13089	1.28%	0.148%
87	13.207	1985	1988	1991	rBV3	10510	12529	1.22%	0.141%
88	13.298	1999	2003	2008	rVB5	20820	31724	3.10%	0.358%
89	13.347	2008	2011	2013	rBV4	6773	8766	0.86%	0.099%
90	13.383	2014	2017	2020	rBV	23258	30849	3.01%	0.348%
91	13.414	2020	2022	2024	rBV3	12646	12429	1.21%	0.140%
92	13.700	2066	2069	2072	rBV	23622	22393	2.19%	0.253%
93	13.798	2082	2085	2088	rBV4	24698	26845	2.62%	0.303%
94	13.841	2088	2092	2095	rBV2	36650	48072	4.69%	0.543%
95	13.993	2114	2117	2119	rBV4	14845	20232	1.98%	0.228%
96	14.133	2138	2140	2143	rVB3	17499	17645	1.72%	0.199%
97	14.615	2216	2219	2222	rBV3	27199	32826	3.21%	0.370%
98	14.847	2254	2257	2260	rBV3	20007	26108	2.55%	0.295%
99	15.420	2348	2351	2356	rVB4	26108	37184	3.63%	0.420%
100	15.743	2401	2404	2408	rVB5	20362	29525	2.88%	0.333%

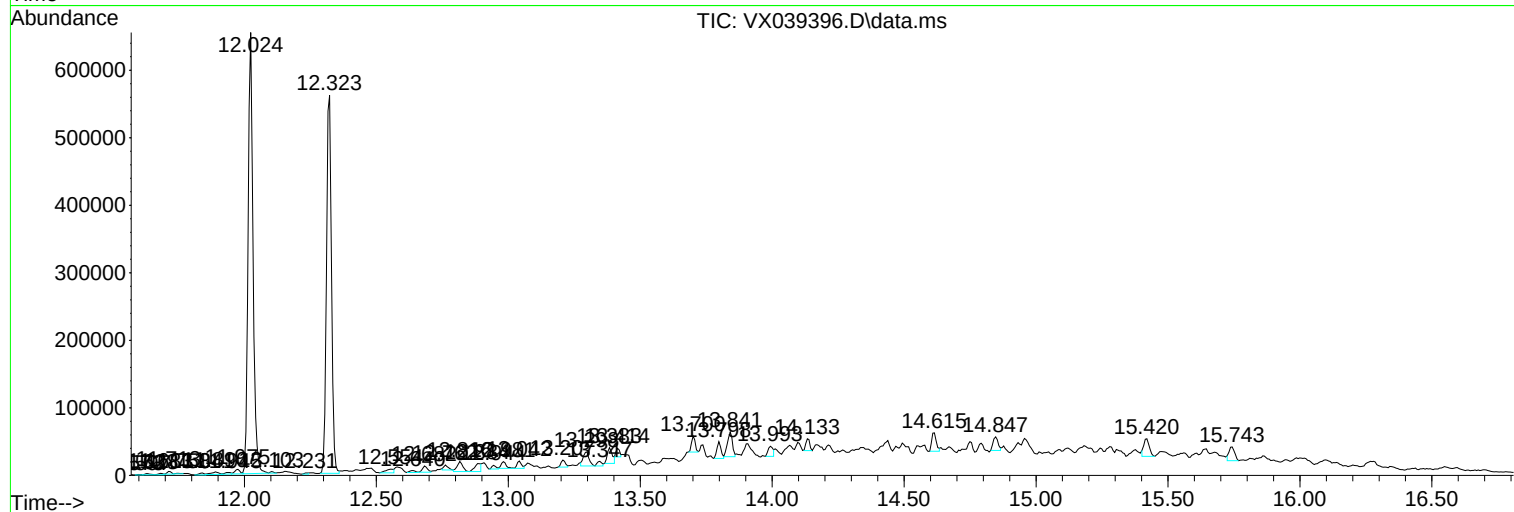
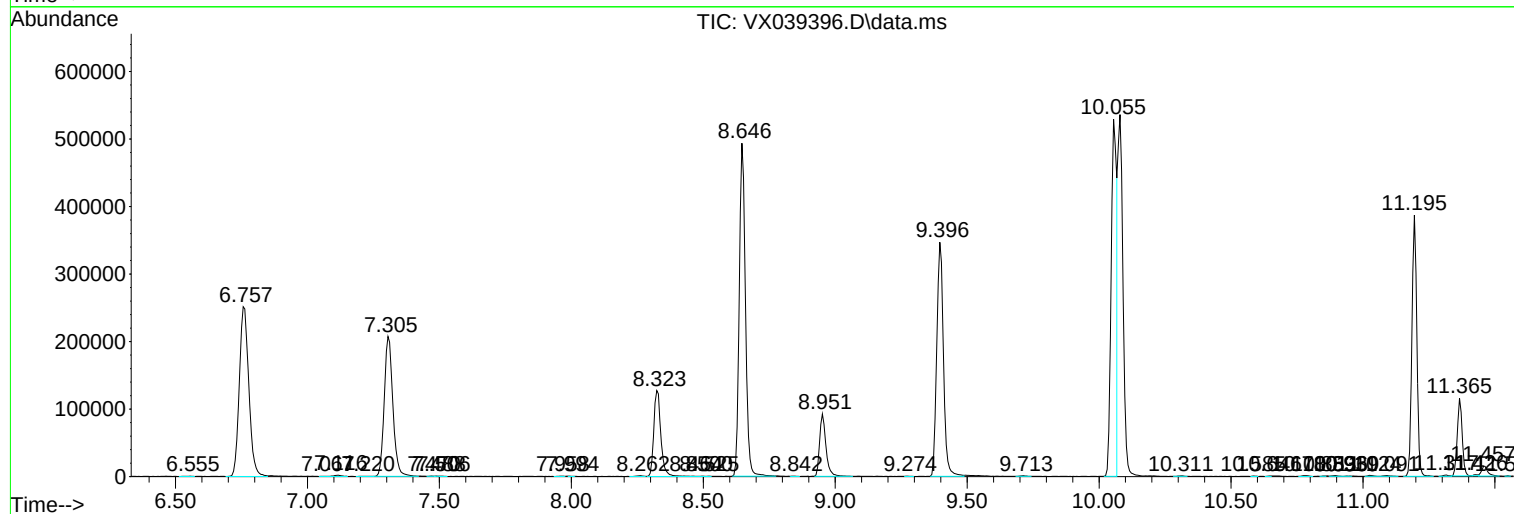
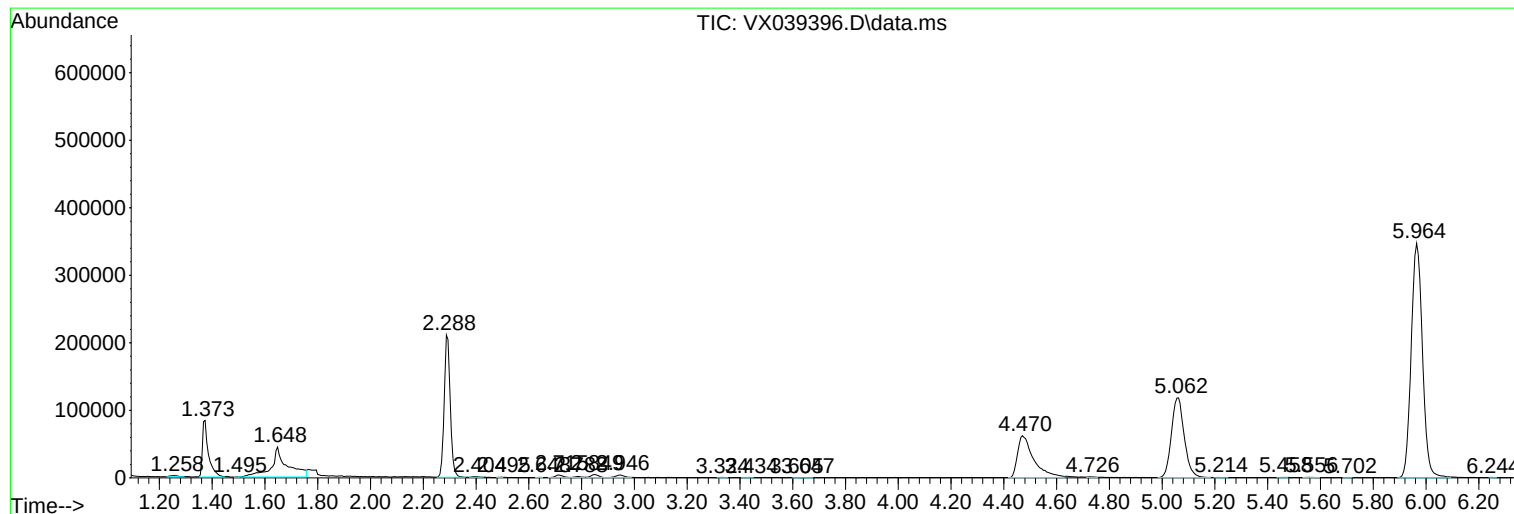
Sum of corrected areas: 8860271

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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



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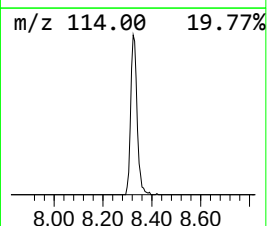
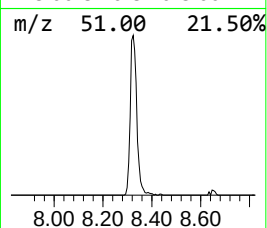
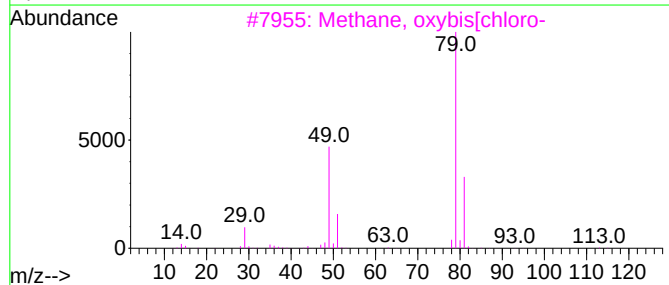
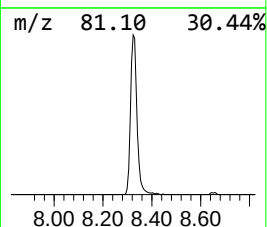
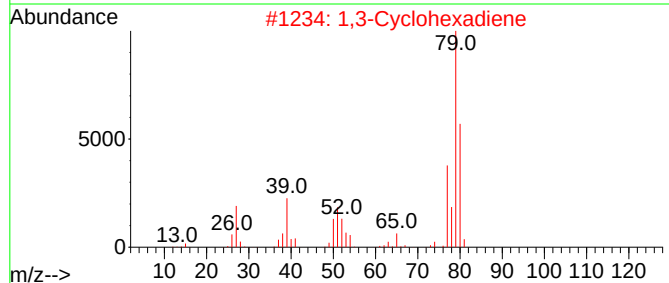
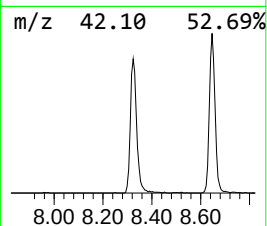
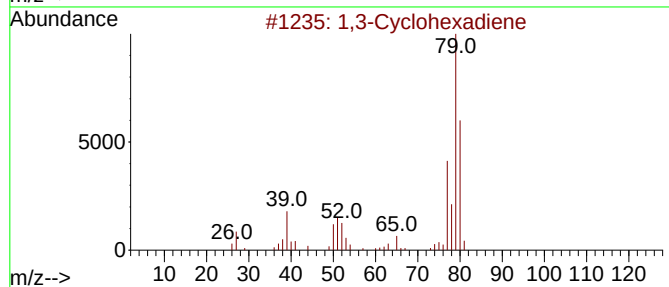
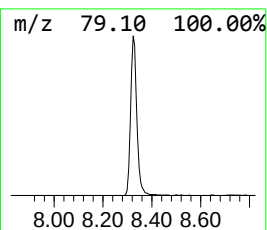
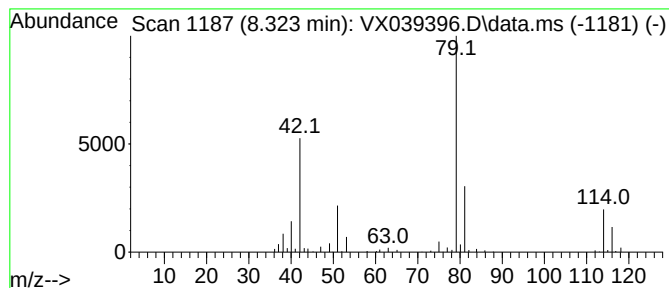
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.323	18.74 ug/L	233801	1,4-Difluorobenzene	6.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Cyclohexadiene	80	C6H8	000592-57-4	37
2		1,3-Cyclohexadiene	80	C6H8	000592-57-4	25
3		Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	25
4		1,3-Cyclohexadiene	80	C6H8	000592-57-4	25
5		n-Propyl chloride	78	C3H7Cl	000540-54-5	9



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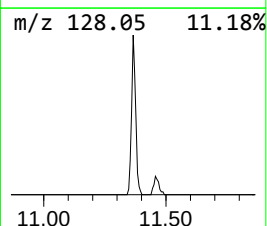
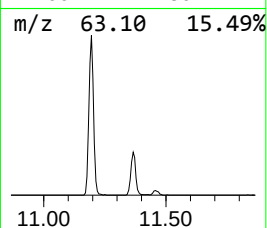
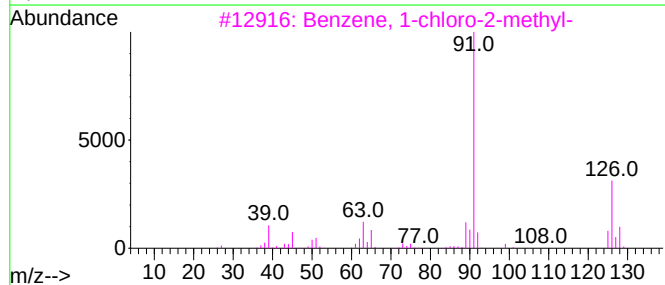
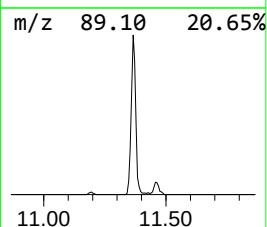
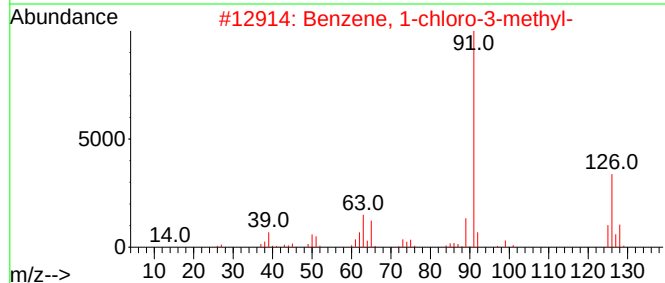
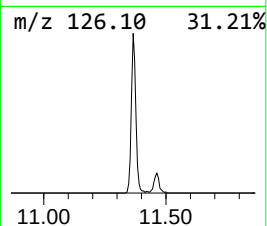
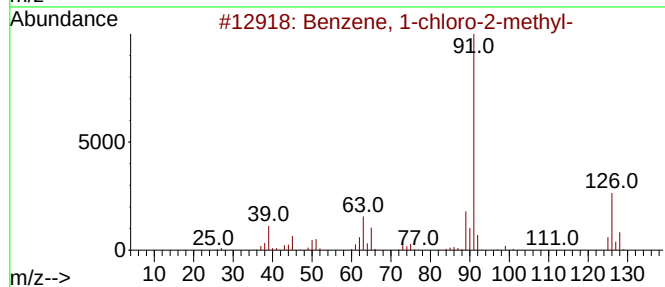
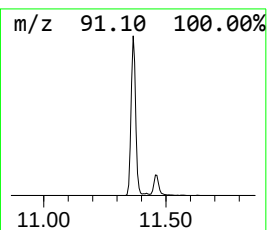
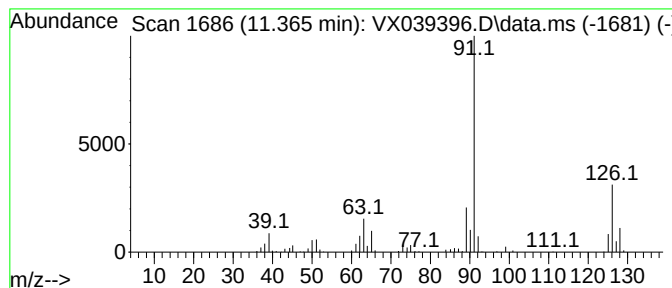
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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.
11.366	8.67 ug/L	147317	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-3-methyl-	126	C7H7Cl	000108-41-8	95
3			Benzene, 1-chloro-2-methyl-	126	C7H7Cl	000095-49-8	94
4			Benzene, 1-chloro-2-methyl-	126	C7H7Cl	000095-49-8	93
5			Benzene, 1-chloro-2-methyl-	126	C7H7Cl	000095-49-8	90



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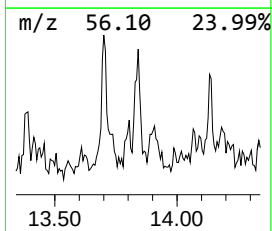
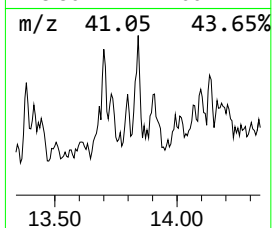
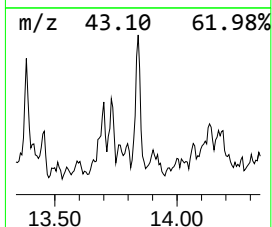
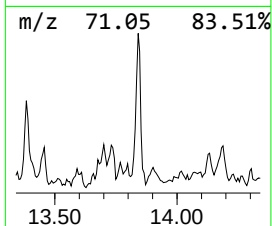
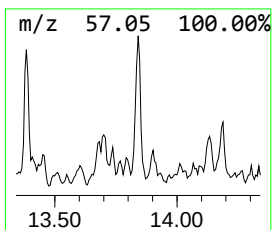
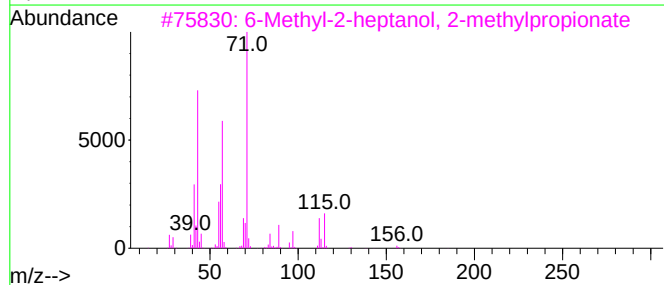
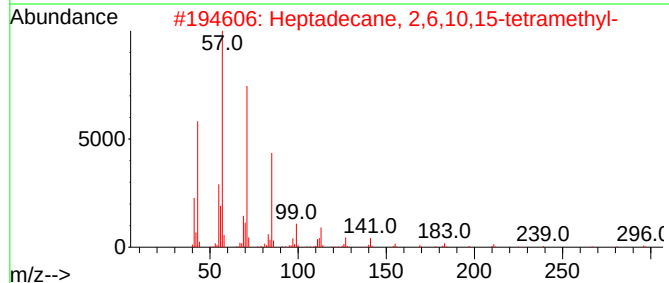
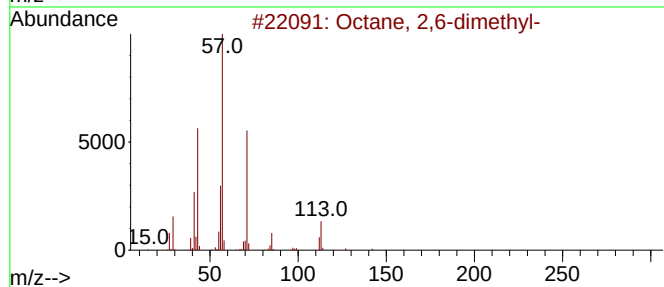
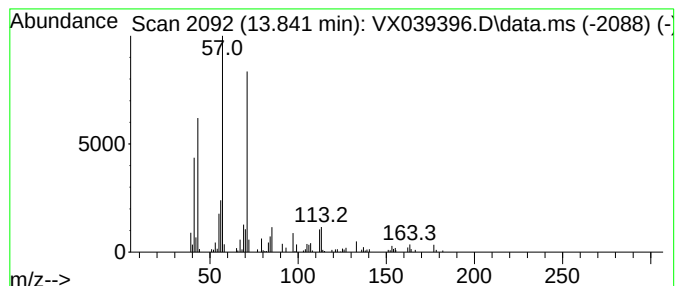
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Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.841	2.83 ug/L	48072	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,6-dimethyl-		142	C10H22		002051-30-1	78
2	Heptadecane, 2,6,10,15-tetramethyl-		296	C21H44		054833-48-6	64
3	6-Methyl-2-heptanol, 2-methylpro...		200	C12H24O2		1000447-36-7	53
4	Sulfurous acid, 2-ethylhexyl pen...		264	C13H28O3S		1000309-18-9	53
5	Threitol, 2-O-octyl-		234	C12H26O4		163776-14-5	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122023\
Data File : VX039396.D
Acq On : 20 Dec 2023 13:11
Operator : JC/MD
Sample : 05869-07
Misc : 4.22g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AT3

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
unknown-01	8.323	18.7	ug/L	233801	1	6.763	623893	50.0
Benzene, 1-chlo...	11.366	8.7	ug/L	147317	3	12.024	849180	50.0
(DEL) Alkane: S...	13.841	2.8	ug/L	48072	3	12.024	849180	50.0