

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
 Data File : VX039488.D
 Acq On : 27 Dec 2023 11:58
 Operator : JC/MD
 Sample : 05989-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 F7A60

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: VX039488.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	23	27	28	rBV	2740	3652	0.46%	0.051%
2	1.367	43	46	56	rVB2	175402	213972	26.68%	2.987%
3	1.666	91	95	109	rVB	58765	92537	11.54%	1.292%
4	2.306	193	200	207	rBV	153508	245950	30.67%	3.433%
5	2.373	208	211	217	rVB	6648	9756	1.22%	0.136%
6	2.526	230	236	243	rVB3	3804	8331	1.04%	0.116%
7	2.636	250	254	261	rVB2	771	1469	0.18%	0.021%
8	2.953	297	306	314	rVB3	2145	5353	0.67%	0.075%
9	3.099	324	330	336	rBV6	3611	7996	1.00%	0.112%
10	3.251	352	355	358	rBV2	191	296	0.04%	0.004%
11	3.477	389	392	394	rVB	268	275	0.03%	0.004%
12	3.739	432	435	437	rVB2	247	265	0.03%	0.004%
13	3.898	457	461	465	rVB2	188	322	0.04%	0.004%
14	4.026	478	482	485	rVB2	348	464	0.06%	0.006%
15	4.477	542	556	565	rBV2	136109	571886	71.31%	7.983%
16	4.836	613	615	619	rVB2	262	261	0.03%	0.004%
17	5.050	633	650	667	rBV	105130	323736	40.37%	4.519%
18	5.385	700	705	706	rBV3	755	847	0.11%	0.012%
19	5.537	728	730	731	rBV	362	316	0.04%	0.004%
20	5.708	756	758	761	rVB	328	231	0.03%	0.003%
21	5.964	787	800	826	rBV2	266231	801927	100.00%	11.194%
22	6.324	857	859	861	rVB2	250	206	0.03%	0.003%
23	6.623	906	908	911	rBV3	246	266	0.03%	0.004%
24	6.684	916	918	920	rVB2	319	243	0.03%	0.003%
25	6.757	920	930	945	rBV	224534	534677	66.67%	7.463%
26	6.982	965	967	970	rVB2	330	338	0.04%	0.005%
27	7.007	970	971	975	rBV2	284	337	0.04%	0.005%
28	7.135	988	992	993	rBV	301	414	0.05%	0.006%
29	7.305	1010	1020	1035	rBV	164520	368507	45.95%	5.144%
30	7.470	1042	1047	1054	rBV3	2206	5205	0.65%	0.073%
31	7.592	1063	1067	1071	rBV5	615	1065	0.13%	0.015%
32	7.811	1101	1103	1105	rVV	253	211	0.03%	0.003%
33	7.939	1120	1124	1127	rBV4	673	971	0.12%	0.014%
34	8.171	1159	1162	1164	rVB	239	219	0.03%	0.003%
35	8.324	1180	1187	1198	rBV	110222	185047	23.08%	2.583%
36	8.513	1212	1218	1219	rBV4	599	990	0.12%	0.014%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
Data File : VX039488.D
Acq On : 27 Dec 2023 11:58
Operator : JC/MD
Sample : 05989-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
F7A60

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

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

37	8.574	1225	1228	1233	rVB3	2324	3321	0.41%	0.046%
38	8.647	1233	1240	1247	rBV	385907	608233	75.85%	8.490%
39	8.714	1248	1251	1260	rVB	12247	20953	2.61%	0.292%
40	8.805	1265	1266	1270	rVV3	390	522	0.07%	0.007%
41	8.854	1270	1274	1278	rVB5	587	931	0.12%	0.013%
42	8.945	1284	1289	1299	rBV	77070	120291	15.00%	1.679%
43	9.244	1334	1338	1339	rBV2	599	630	0.08%	0.009%
44	9.275	1339	1343	1347	rVB3	1581	2366	0.30%	0.033%
45	9.378	1355	1360	1380	rBV	406269	601443	75.00%	8.395%
46	9.714	1413	1415	1419	rVB2	257	246	0.03%	0.003%
47	10.049	1465	1470	1488	rBV	453687	659484	82.24%	9.205%
48	10.201	1493	1495	1498	rVV2	557	421	0.05%	0.006%
49	10.305	1509	1512	1519	rVB3	1825	2877	0.36%	0.040%
50	10.378	1519	1524	1526	rBV3	736	1147	0.14%	0.016%
51	10.476	1536	1540	1542	rBV2	171	260	0.03%	0.004%
52	10.543	1550	1551	1557	rVB3	410	558	0.07%	0.008%
53	10.646	1564	1568	1572	rBV4	1835	2443	0.30%	0.034%
54	10.726	1580	1581	1584	rBV2	274	206	0.03%	0.003%
55	10.774	1586	1589	1593	rBV2	2165	3229	0.40%	0.045%
56	10.866	1600	1604	1606	rBV2	172	216	0.03%	0.003%
57	10.963	1616	1620	1624	rBB3	550	735	0.09%	0.010%
58	11.012	1626	1628	1630	rBV	324	201	0.03%	0.003%
59	11.085	1636	1640	1645	rBV4	2505	3588	0.45%	0.050%
60	11.189	1652	1657	1670	rVB	342837	435564	54.31%	6.080%
61	11.311	1673	1677	1681	rBV3	1660	2321	0.29%	0.032%
62	11.384	1685	1689	1690	rBV2	301	416	0.05%	0.006%
63	11.482	1703	1705	1710	rVB2	297	349	0.04%	0.005%
64	11.610	1725	1726	1732	rVB2	257	319	0.04%	0.004%
65	11.713	1740	1743	1745	rBV2	298	367	0.05%	0.005%
66	11.756	1745	1750	1761	rBV	75851	94710	11.81%	1.322%
67	11.853	1761	1766	1770	rBV	10231	14994	1.87%	0.209%
68	11.969	1782	1785	1788	rBV4	1151	1216	0.15%	0.017%
69	12.018	1788	1793	1802	rBV	462373	616372	76.86%	8.604%
70	12.146	1810	1814	1817	rVB4	1452	1880	0.23%	0.026%
71	12.225	1823	1827	1837	rBV4	1444	2873	0.36%	0.040%
72	12.317	1837	1842	1855	rVV	443358	557254	69.49%	7.778%
73	12.573	1879	1884	1886	rBV3	365	620	0.08%	0.009%
74	12.652	1895	1897	1900	rBV2	216	282	0.04%	0.004%
75	12.756	1910	1914	1918	rBV3	649	894	0.11%	0.012%
76	12.859	1926	1931	1934	rBV3	380	536	0.07%	0.007%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
 Data File : VX039488.D
 Acq On : 27 Dec 2023 11:58
 Operator : JC/MD
 Sample : 05989-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 F7A60

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	12.951	1943	1946	1951	rBV2	207	327	0.04%	0.005%
78	13.158	1978	1980	1986	rVB4	526	824	0.10%	0.012%
79	13.213	1986	1989	1991	rBV2	272	324	0.04%	0.005%
80	13.249	1991	1995	1997	rBV2	190	225	0.03%	0.003%
81	13.335	2008	2009	2012	rVB	322	234	0.03%	0.003%
82	13.487	2032	2034	2037	rVB2	262	274	0.03%	0.004%
83	13.591	2047	2051	2055	rVV3	973	1330	0.17%	0.019%
84	13.780	2079	2082	2088	rVV2	975	1449	0.18%	0.020%
85	13.847	2090	2093	2095	rBV2	172	243	0.03%	0.003%
86	13.865	2095	2096	2100	rVB2	239	239	0.03%	0.003%
87	13.963	2111	2112	2114	rVB	521	271	0.03%	0.004%
88	14.140	2135	2141	2143	rBV3	538	792	0.10%	0.011%
89	14.316	2166	2170	2172	rBV	218	294	0.04%	0.004%
90	14.554	2207	2209	2211	rVV	236	227	0.03%	0.003%
91	14.639	2221	2223	2227	rBV2	416	593	0.07%	0.008%
92	14.700	2231	2233	2235	rBV	346	282	0.04%	0.004%
93	14.725	2235	2237	2239	rVB	296	252	0.03%	0.004%
94	14.755	2239	2242	2244	rBV	224	268	0.03%	0.004%
95	15.152	2305	2307	2311	rBV2	345	510	0.06%	0.007%
96	15.261	2323	2325	2328	rBV2	280	271	0.03%	0.004%
97	15.700	2395	2397	2399	rBV2	270	242	0.03%	0.003%
98	16.078	2458	2459	2461	rVB	365	201	0.03%	0.003%
99	16.103	2461	2463	2466	rBV2	326	418	0.05%	0.006%
100	16.548	2535	2536	2538	rBV	265	225	0.03%	0.003%

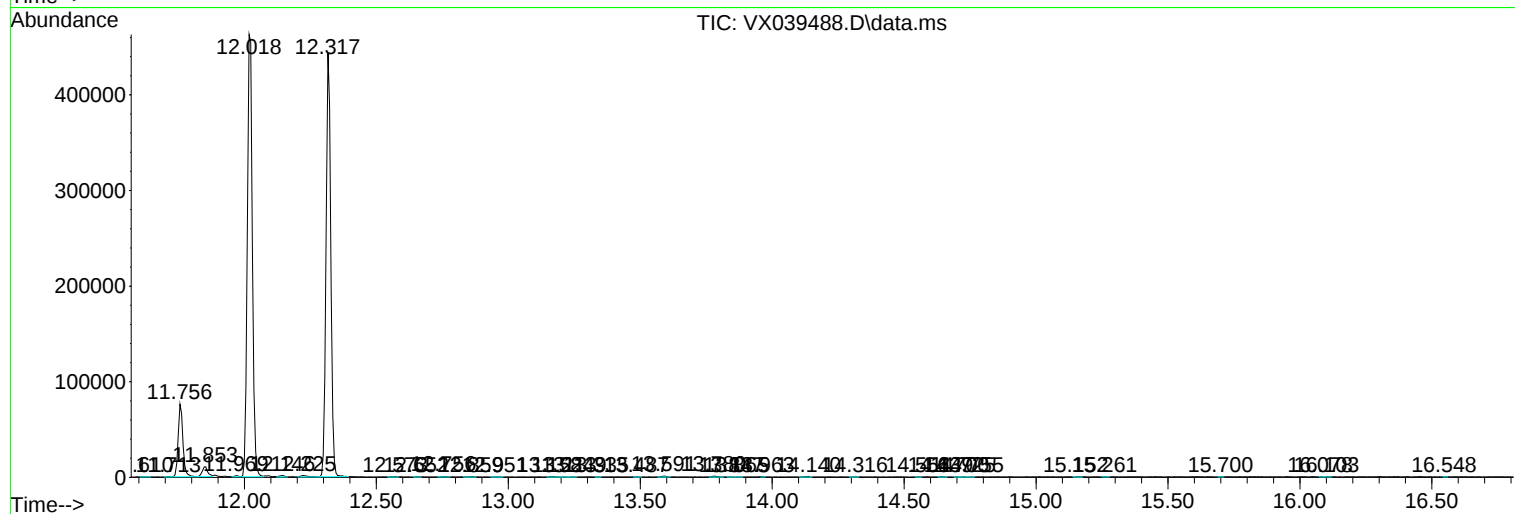
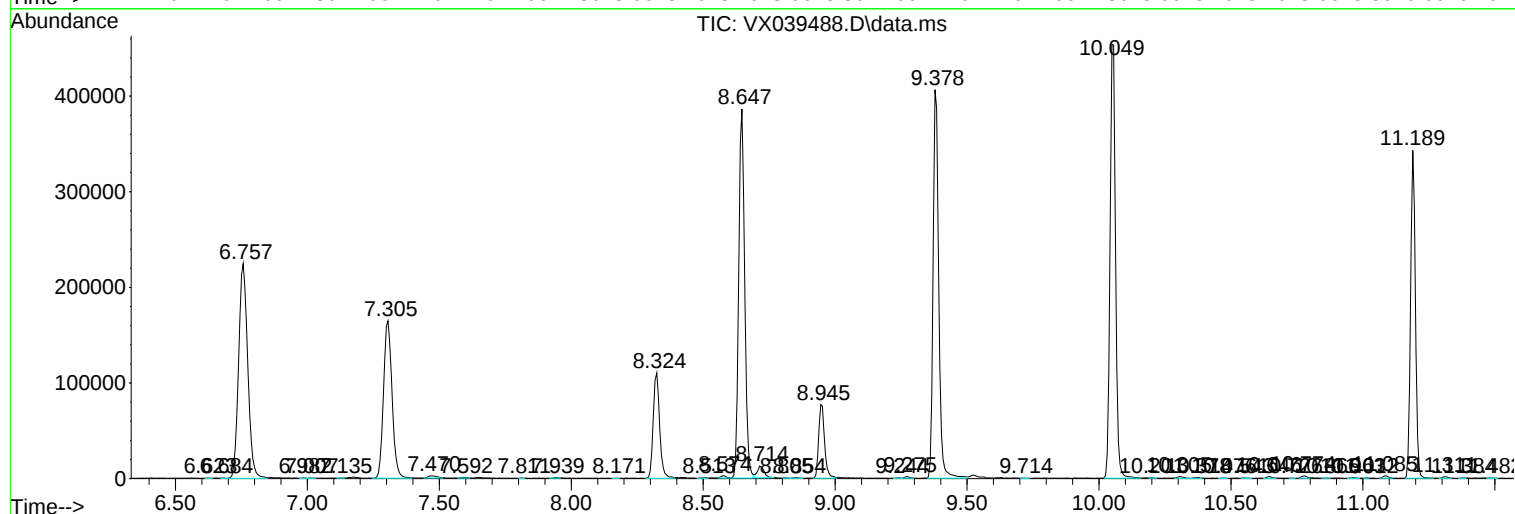
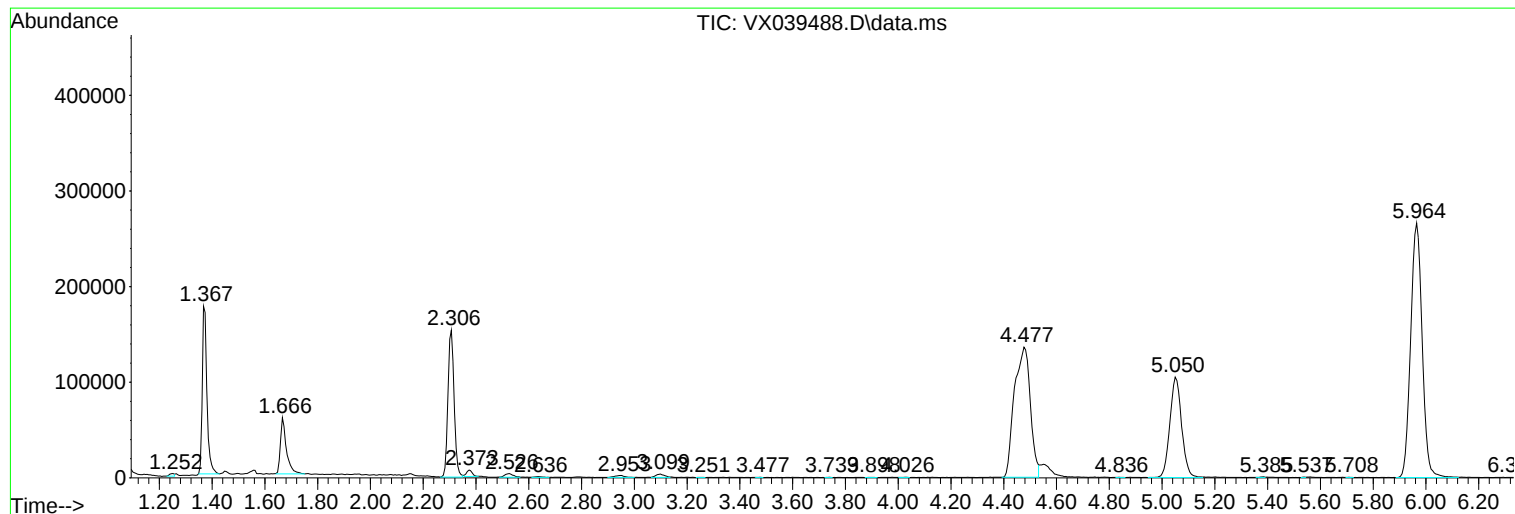
Sum of corrected areas: 7164121

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
Data File : VX039488.D
Acq On : 27 Dec 2023 11:58
Operator : JC/MD
Sample : 05989-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
F7A60

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
Data File : VX039488.D
Acq On : 27 Dec 2023 11:58
Operator : JC/MD
Sample : 05989-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
F7A60

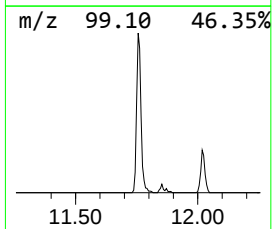
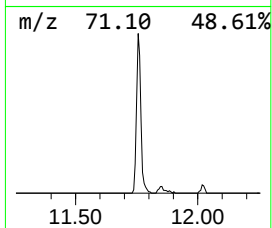
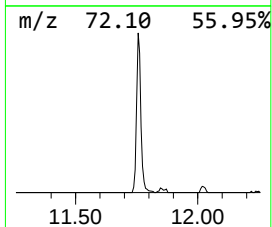
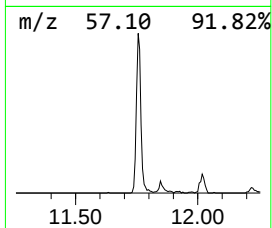
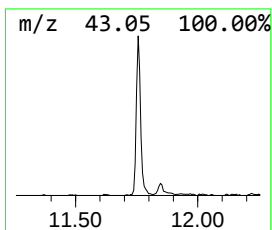
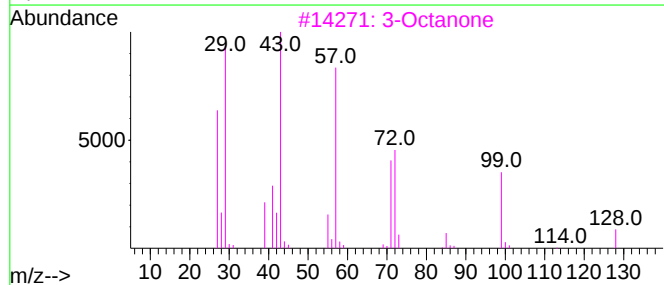
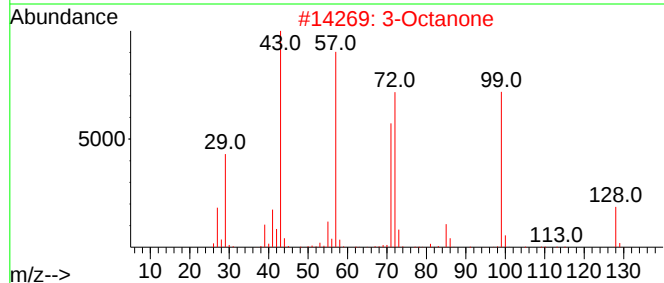
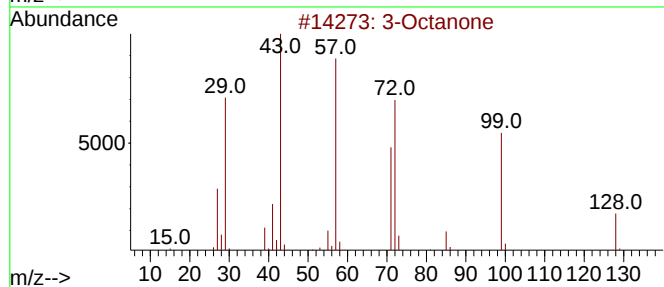
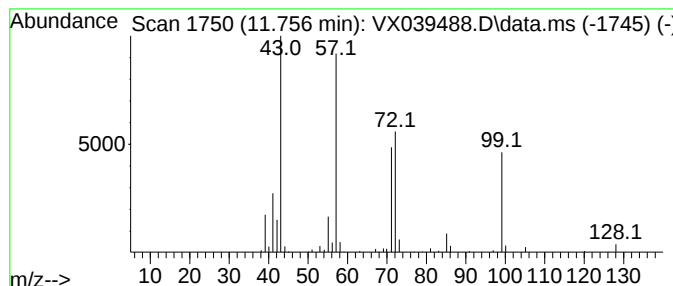
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 3-Octanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.756	7.68 ug/L	94710	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octanone			128	C8H16O	000106-68-3	91
2	3-Octanone			128	C8H16O	000106-68-3	78
3	3-Octanone			128	C8H16O	000106-68-3	74
4	3-Heptanone, 6-methyl-			128	C8H16O	000624-42-0	64
5	3-Heptanone, 5-methyl-			128	C8H16O	000541-85-5	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122723\
Data File : VX039488.D
Acq On : 27 Dec 2023 11:58
Operator : JC/MD
Sample : 05989-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
F7A60

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
3-Octanone	11.756	7.7	ug/L	94710	3	12.024	616372	50.0