

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121623\
 Data File : VX039266.D
 Acq On : 16 Dec 2023 05:49
 Operator : JC/MD
 Sample : 05845-11
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 YCHE7

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: VX039266.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	7	9	13	rVB2	2860	2846	0.34%	0.035%
2	1.246	23	26	32	rVB2	3545	5854	0.71%	0.072%
3	1.368	41	46	57	rVB	96413	118798	14.39%	1.453%
4	1.672	91	96	107	rBV	58370	89513	10.85%	1.095%
5	2.319	194	202	208	rBV3	341374	645805	78.25%	7.897%
6	2.374	208	211	223	rVB	55397	88179	10.68%	1.078%
7	2.526	228	236	251	rBV	371678	672826	81.53%	8.227%
8	2.947	300	305	318	rVB2	6893	16354	1.98%	0.200%
9	3.105	327	331	339	rVB7	2066	4769	0.58%	0.058%
10	3.349	368	371	373	rBV	248	277	0.03%	0.003%
11	3.379	375	376	379	rVV2	263	198	0.02%	0.002%
12	3.611	405	414	424	rBV	33816	80574	9.76%	0.985%
13	3.745	433	436	437	rBV2	520	510	0.06%	0.006%
14	3.873	452	457	459	rVB2	195	277	0.03%	0.003%
15	3.892	459	460	463	rVB2	240	225	0.03%	0.003%
16	3.971	470	473	475	rBV2	166	188	0.02%	0.002%
17	4.184	506	508	509	rBV	254	209	0.03%	0.003%
18	4.446	543	551	563	rBV2	81324	328543	39.81%	4.017%
19	5.056	631	651	668	rBV	111815	362028	43.87%	4.427%
20	5.391	696	706	714	rBV4	6400	19324	2.34%	0.236%
21	5.806	771	774	776	rBV2	141	219	0.03%	0.003%
22	5.964	789	800	819	rBV2	269478	825281	100.00%	10.091%
23	6.373	866	867	871	rVB2	187	228	0.03%	0.003%
24	6.757	921	930	943	rBV	241729	583289	70.68%	7.132%
25	7.001	968	970	971	rVB	304	186	0.02%	0.002%
26	7.129	985	991	1000	rVB3	7643	17761	2.15%	0.217%
27	7.306	1011	1020	1036	rBV	171207	380925	46.16%	4.658%
28	7.671	1075	1080	1087	rVV2	1632	3153	0.38%	0.039%
29	7.787	1097	1099	1102	rBV2	284	283	0.03%	0.003%
30	7.866	1109	1112	1113	rVB	231	196	0.02%	0.002%
31	7.897	1113	1117	1124	rBV5	558	1522	0.18%	0.019%
32	7.958	1124	1127	1132	rVB2	309	563	0.07%	0.007%
33	8.110	1149	1152	1153	rBV	226	193	0.02%	0.002%
34	8.184	1161	1164	1167	rBV	185	192	0.02%	0.002%
35	8.226	1169	1171	1175	rVB2	250	202	0.02%	0.002%
36	8.324	1181	1187	1200	rBV	117663	189597	22.97%	2.318%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121623\
 Data File : VX039266.D
 Acq On : 16 Dec 2023 05:49
 Operator : JC/MD
 Sample : 05845-11
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 YCHE7

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

37	8.525	1216	1220	1222	rBV2	324	408	0.05%	0.005%
38	8.580	1226	1229	1233	rBV	220	287	0.03%	0.004%
39	8.647	1233	1240	1250	rBV	408120	644989	78.15%	7.887%
40	8.952	1284	1290	1307	rBV	79721	125384	15.19%	1.533%
41	9.275	1339	1343	1347	rVV2	929	1211	0.15%	0.015%
42	9.385	1355	1361	1383	rBV	348118	511368	61.96%	6.253%
43	9.689	1409	1411	1415	rVB2	246	298	0.04%	0.004%
44	9.756	1420	1422	1424	rVB2	234	217	0.03%	0.003%
45	9.793	1424	1428	1430	rBV2	322	398	0.05%	0.005%
46	9.958	1453	1455	1459	rBV2	188	203	0.02%	0.002%
47	10.049	1465	1470	1486	rBV	500927	717970	87.00%	8.779%
48	10.226	1497	1499	1505	rVB2	468	768	0.09%	0.009%
49	10.275	1505	1507	1508	rVB	355	196	0.02%	0.002%
50	10.305	1508	1512	1513	rBV3	694	773	0.09%	0.009%
51	10.360	1520	1521	1523	rVV	256	255	0.03%	0.003%
52	10.378	1523	1524	1531	rVV2	421	513	0.06%	0.006%
53	10.512	1544	1546	1553	rVB2	303	485	0.06%	0.006%
54	10.653	1563	1569	1571	rBV3	382	653	0.08%	0.008%
55	10.896	1606	1609	1611	rVB2	226	228	0.03%	0.003%
56	11.018	1624	1629	1633	rBV2	2489	3738	0.45%	0.046%
57	11.092	1636	1641	1648	rBV3	807	1344	0.16%	0.016%
58	11.189	1652	1657	1666	rBV	335463	418040	50.65%	5.112%
59	11.311	1674	1677	1684	rVB2	1054	1771	0.21%	0.022%
60	11.360	1684	1685	1688	rBV2	143	192	0.02%	0.002%
61	11.451	1697	1700	1701	rBV	225	241	0.03%	0.003%
62	11.762	1747	1751	1752	rBV2	415	473	0.06%	0.006%
63	11.866	1766	1768	1771	rBV2	176	250	0.03%	0.003%
64	11.957	1780	1783	1788	rVB2	343	605	0.07%	0.007%
65	12.018	1788	1793	1802	rBV	545627	700151	84.84%	8.561%
66	12.225	1822	1827	1837	rBV5	2837	5906	0.72%	0.072%
67	12.317	1837	1842	1858	rVB	467607	584988	70.88%	7.153%
68	12.536	1877	1878	1882	rBV	256	238	0.03%	0.003%
69	12.573	1882	1884	1885	rBV	374	219	0.03%	0.003%
70	12.591	1885	1887	1889	rVV2	403	286	0.03%	0.003%
71	12.701	1904	1905	1910	rBV	197	280	0.03%	0.003%
72	12.762	1910	1915	1919	rVV3	489	730	0.09%	0.009%
73	13.067	1961	1965	1968	rBV2	190	252	0.03%	0.003%
74	13.152	1978	1979	1981	rVV2	226	182	0.02%	0.002%
75	13.366	2010	2014	2015	rVB2	162	187	0.02%	0.002%
76	13.384	2015	2017	2021	rBV2	222	244	0.03%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121623\
 Data File : VX039266.D
 Acq On : 16 Dec 2023 05:49
 Operator : JC/MD
 Sample : 05845-11
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 YCHE7

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	13.433	2021	2025	2030	rBV2	733	1416	0.17%	0.017%
78	13.536	2038	2042	2043	rBV2	161	189	0.02%	0.002%
79	13.591	2048	2051	2056	rVV3	927	1068	0.13%	0.013%
80	13.731	2073	2074	2076	rBV2	230	200	0.02%	0.002%
81	13.780	2079	2082	2089	rVB2	628	1051	0.13%	0.013%
82	14.286	2162	2165	2166	rVB2	300	231	0.03%	0.003%
83	14.310	2166	2169	2170	rBV2	240	233	0.03%	0.003%
84	14.530	2203	2205	2207	rBV2	174	208	0.03%	0.003%
85	14.603	2214	2217	2221	rVB2	1111	1173	0.14%	0.014%
86	14.652	2223	2225	2226	rBV	223	185	0.02%	0.002%
87	14.841	2255	2256	2259	rBV	247	263	0.03%	0.003%
88	14.975	2276	2278	2279	rVB	345	211	0.03%	0.003%
89	15.255	2322	2324	2325	rBV2	238	188	0.02%	0.002%
90	15.292	2328	2330	2332	rBV3	246	241	0.03%	0.003%
91	15.481	2360	2361	2363	rBV2	476	278	0.03%	0.003%
92	15.548	2369	2372	2374	rBV2	342	355	0.04%	0.004%
93	15.737	2402	2403	2406	rVB	442	215	0.03%	0.003%
94	15.786	2410	2411	2414	rBV2	326	360	0.04%	0.004%
95	15.889	2427	2428	2431	rVB2	301	244	0.03%	0.003%
96	15.920	2431	2433	2436	rBV2	313	424	0.05%	0.005%
97	15.950	2436	2438	2440	rBV2	275	235	0.03%	0.003%
98	15.975	2440	2442	2446	rBV4	438	521	0.06%	0.006%
99	16.097	2460	2462	2464	rVB2	559	401	0.05%	0.005%
100	16.133	2464	2468	2469	rBV	274	309	0.04%	0.004%

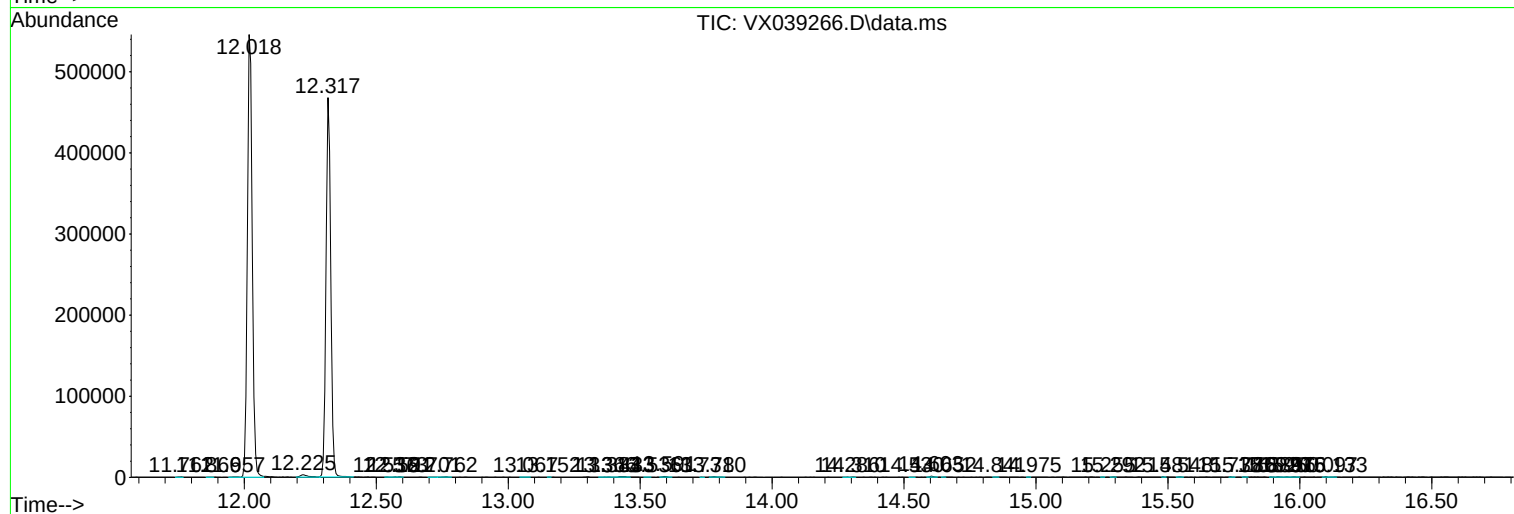
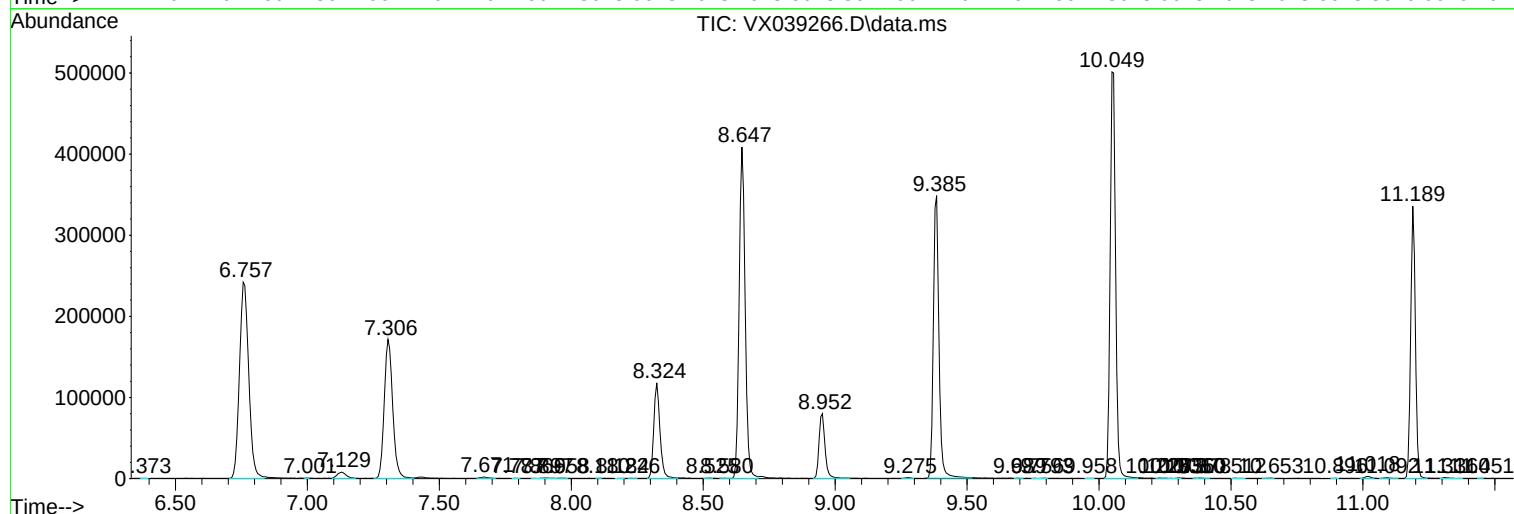
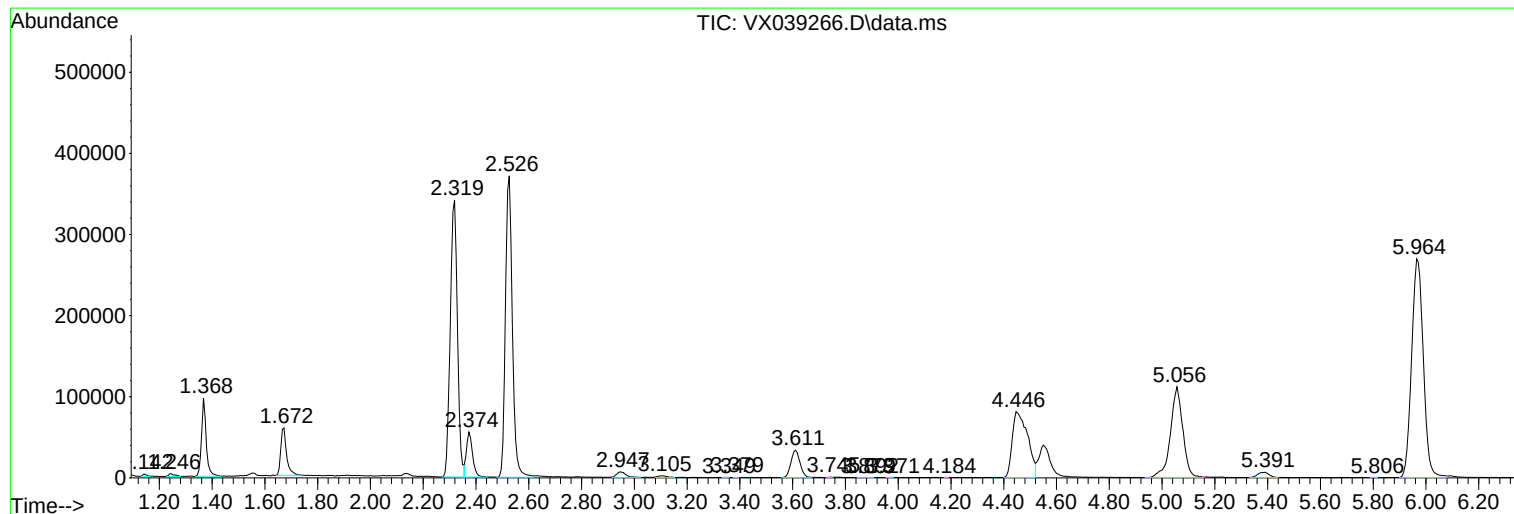
Sum of corrected areas: 8178207

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121623\
Data File : VX039266.D
Acq On : 16 Dec 2023 05:49
Operator : JC/MD
Sample : 05845-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YCHE7

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\VX121623\
Data File : VX039266.D
Acq On : 16 Dec 2023 05:49
Operator : JC/MD
Sample : 05845-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YCHE7

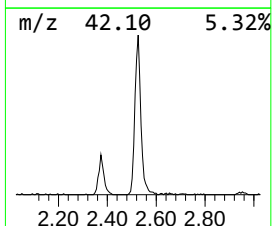
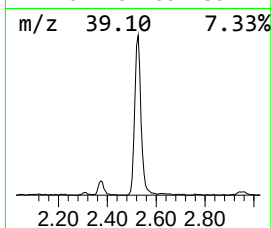
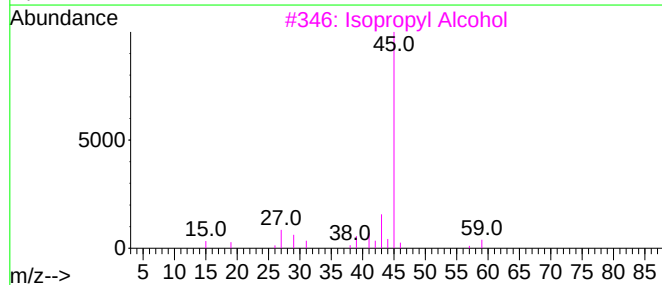
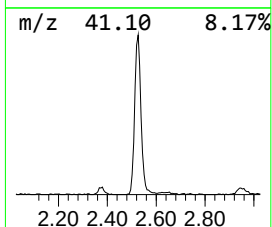
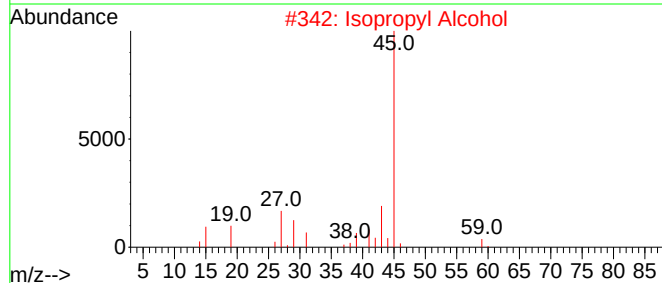
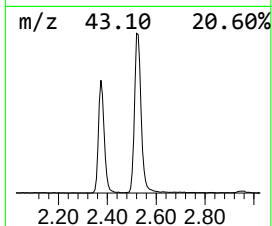
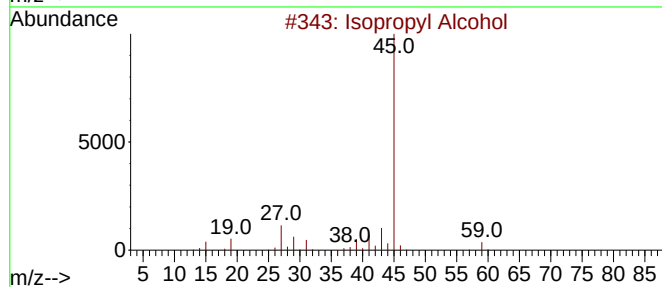
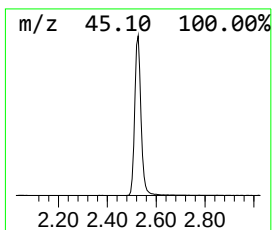
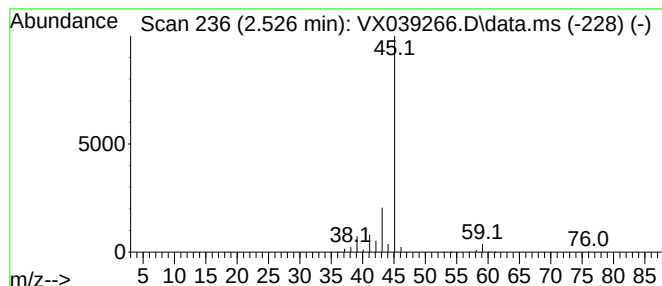
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.526	57.68 ug/L	672826	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	83
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
4			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
5			Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121623\
Data File : VX039266.D
Acq On : 16 Dec 2023 05:49
Operator : JC/MD
Sample : 05845-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
YCHE7

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
Isopropyl Alcohol	2.526	57.7	ug/L	672826	1	6.757	583289	50.0