

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011322\
 Data File : VV024350.D
 Acq On : 13 Jan 2022 14:33
 Operator : SY/MD
 Sample : N1084-10DL 50X
 Misc : 12.29g/5.0mL/100ul/5.0mL/MSVOA_V/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BGLN3DL

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_V\Method\SFAMVLM123121WMA.M
 Title : VOC Analysis

Signal : TIC: VV024350.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.304	75	82	95	rVB	117409	119581	12.97%	1.471%
2	1.564	156	163	174	rBV	101619	109959	11.93%	1.353%
3	2.105	320	331	360	rVB	223078	331212	35.93%	4.075%
4	2.278	383	385	391	rBV3	420	368	0.04%	0.005%
5	2.404	422	424	428	rBV	190	118	0.01%	0.001%
6	2.503	451	455	456	rBV2	806	553	0.06%	0.007%
7	2.593	479	483	489	rVB	219	164	0.02%	0.002%
8	2.677	504	509	511	rBV2	350	292	0.03%	0.004%
9	2.709	515	519	523	rVV2	277	284	0.03%	0.003%
10	2.735	524	527	530	rVV3	387	323	0.04%	0.004%
11	2.754	530	533	540	rVB3	882	932	0.10%	0.011%
12	2.886	571	574	576	rBV	236	166	0.02%	0.002%
13	2.989	603	606	610	rBV2	198	126	0.01%	0.002%
14	3.040	616	622	628	rBV3	1020	1348	0.15%	0.017%
15	3.108	639	643	644	rBV	226	166	0.02%	0.002%
16	3.143	649	654	656	rBV	293	262	0.03%	0.003%
17	3.175	663	664	670	rVB2	170	121	0.01%	0.001%
18	3.204	670	673	676	rBV2	170	127	0.01%	0.002%
19	3.281	694	697	700	rBV	227	163	0.02%	0.002%
20	3.313	705	707	710	rVB2	233	123	0.01%	0.002%
21	3.358	718	721	726	rVB	297	257	0.03%	0.003%
22	3.384	727	729	732	rBB	225	107	0.01%	0.001%
23	3.407	733	736	737	rBV	147	101	0.01%	0.001%
24	3.416	737	739	741	rVB	264	127	0.01%	0.002%
25	3.452	747	750	753	rBV2	266	222	0.02%	0.003%
26	3.468	753	755	757	rVB	230	112	0.01%	0.001%
27	3.542	774	778	781	rBB2	266	194	0.02%	0.002%
28	3.577	786	789	791	rBV	170	144	0.02%	0.002%
29	3.667	812	817	820	rBV2	309	300	0.03%	0.004%
30	3.719	829	833	838	rBB	329	402	0.04%	0.005%
31	3.744	838	841	843	rBV	617	393	0.04%	0.005%
32	3.770	846	849	851	rBV3	364	200	0.02%	0.002%
33	3.876	872	882	916	rBV	53391	151920	16.48%	1.869%
34	4.204	979	984	987	rBV2	331	325	0.04%	0.004%
35	4.223	987	990	995	rBV3	411	346	0.04%	0.004%
36	4.342	1009	1027	1055	rBV	143261	353527	38.35%	4.349%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VW011322\
 Data File : VW024350.D
 Acq On : 13 Jan 2022 14:33
 Operator : SY/MD
 Sample : N1084-10DL 50X
 Misc : 12.29g/5.0mL/100ul/5.0mL/MSVOA_V/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BGLN3DL

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_V\Method\SFAMVLM123121WMA.M
 Title : VOC Analysis

37	4.477	1066	1069	1073	rBV	563	420	0.05%	0.005%
38	4.538	1086	1088	1091	rBV	231	174	0.02%	0.002%
39	4.555	1091	1093	1096	rVB2	253	142	0.02%	0.002%
40	4.574	1096	1099	1102	rBV	321	255	0.03%	0.003%
41	4.651	1120	1123	1124	rBV2	264	151	0.02%	0.002%
42	4.715	1141	1143	1146	rVB	260	142	0.02%	0.002%
43	4.735	1147	1149	1152	rBV2	255	170	0.02%	0.002%
44	4.786	1163	1165	1170	rBV	352	260	0.03%	0.003%
45	4.821	1174	1176	1179	rVB2	246	140	0.02%	0.002%
46	4.902	1194	1201	1205	rBV3	654	627	0.07%	0.008%
47	4.956	1215	1218	1222	rBV	253	248	0.03%	0.003%
48	5.040	1228	1244	1281	rBV2	321830	859445	93.24%	10.573%
49	5.249	1305	1309	1312	rBV2	439	264	0.03%	0.003%
50	5.365	1343	1345	1348	rVB2	232	108	0.01%	0.001%
51	5.487	1380	1383	1384	rBV	1346	733	0.08%	0.009%
52	5.612	1411	1422	1452	rBV	264349	523988	56.84%	6.446%
53	5.902	1500	1512	1531	rVB4	10799	23544	2.55%	0.290%
54	5.969	1531	1533	1535	rBB	357	137	0.01%	0.002%
55	6.005	1542	1544	1547	rBV	217	165	0.02%	0.002%
56	6.066	1550	1563	1587	rBV	180713	371985	40.35%	4.576%
57	6.210	1604	1608	1612	rBV6	833	728	0.08%	0.009%
58	6.297	1632	1635	1638	rVB	322	246	0.03%	0.003%
59	6.310	1638	1639	1641	rBV	431	187	0.02%	0.002%
60	6.368	1654	1657	1659	rBV	229	150	0.02%	0.002%
61	6.423	1668	1674	1676	rBV2	149	173	0.02%	0.002%
62	6.481	1689	1692	1697	rVB2	191	170	0.02%	0.002%
63	6.535	1706	1709	1714	rBB2	310	299	0.03%	0.004%
64	6.567	1715	1719	1720	rBV	341	132	0.01%	0.002%
65	6.587	1723	1725	1727	rVB	268	124	0.01%	0.002%
66	6.673	1750	1752	1757	rVB2	580	387	0.04%	0.005%
67	6.702	1757	1761	1763	rBB2	369	240	0.03%	0.003%
68	6.718	1763	1766	1769	rBB2	223	141	0.02%	0.002%
69	6.763	1776	1780	1784	rBV	359	396	0.04%	0.005%
70	6.873	1812	1814	1816	rBV	266	169	0.02%	0.002%
71	6.911	1822	1826	1827	rBV	328	217	0.02%	0.003%
72	6.921	1827	1829	1830	rVB	366	121	0.01%	0.001%
73	6.982	1837	1848	1872	rBV	103746	187573	20.35%	2.307%
74	7.181	1907	1910	1912	rBV	434	269	0.03%	0.003%
75	7.262	1926	1935	1939	rBV7	1588	2417	0.26%	0.030%
76	7.313	1940	1951	1967	rBV	398347	689894	74.84%	8.487%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011322\
 Data File : VV024350.D
 Acq On : 13 Jan 2022 14:33
 Operator : SY/MD
 Sample : N1084-10DL 50X
 Misc : 12.29g/5.0mL/100ul/5.0mL/MSVOA_V/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BGLN3DL

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_V\Method\SFAMVLM123121WMA.M
 Title : VOC Analysis

77	7.571	2021	2031	2036	rBV6	1861	2587	0.28%	0.032%
78	7.619	2037	2046	2072	rVB	74791	131843	14.30%	1.622%
79	7.751	2085	2087	2089	rBV	348	164	0.02%	0.002%
80	7.789	2092	2099	2101	rBV4	1261	1278	0.14%	0.016%
81	7.850	2116	2118	2120	rBV	151	108	0.01%	0.001%
82	7.979	2153	2158	2162	rVV4	606	595	0.06%	0.007%
83	8.021	2168	2171	2174	rBV2	291	276	0.03%	0.003%
84	8.085	2181	2191	2221	rBV	183960	353042	38.30%	4.343%
85	8.349	2263	2273	2280	rBV6	3716	5664	0.61%	0.070%
86	8.506	2319	2322	2326	rVB4	968	825	0.09%	0.010%
87	8.525	2326	2328	2331	rVB2	217	107	0.01%	0.001%
88	8.596	2334	2350	2356	rBV9	5623	14783	1.60%	0.182%
89	8.789	2400	2410	2418	rBV2	9476	16744	1.82%	0.206%
90	8.850	2418	2429	2448	rBV	395860	638702	69.29%	7.857%
91	9.011	2469	2479	2490	rBV	116420	183550	19.91%	2.258%
92	9.136	2508	2518	2531	rVB	383608	622818	67.57%	7.662%
93	9.410	2595	2603	2606	rBV5	2477	3266	0.35%	0.040%
94	9.545	2639	2645	2652	rBV	33059	46780	5.07%	0.575%
95	10.214	2845	2853	2871	rVB	291199	486852	52.82%	5.989%
96	10.445	2918	2925	2939	rBV	109922	225193	24.43%	2.770%
97	11.246	3166	3174	3184	rBV	474192	726682	78.83%	8.940%
98	11.622	3284	3291	3311	rVB2	531224	921804	100.00%	11.340%
99	14.763	4264	4268	4270	rBV5	2885	2169	0.24%	0.027%
100	15.120	4376	4379	4385	rBV6	849	815	0.09%	0.010%

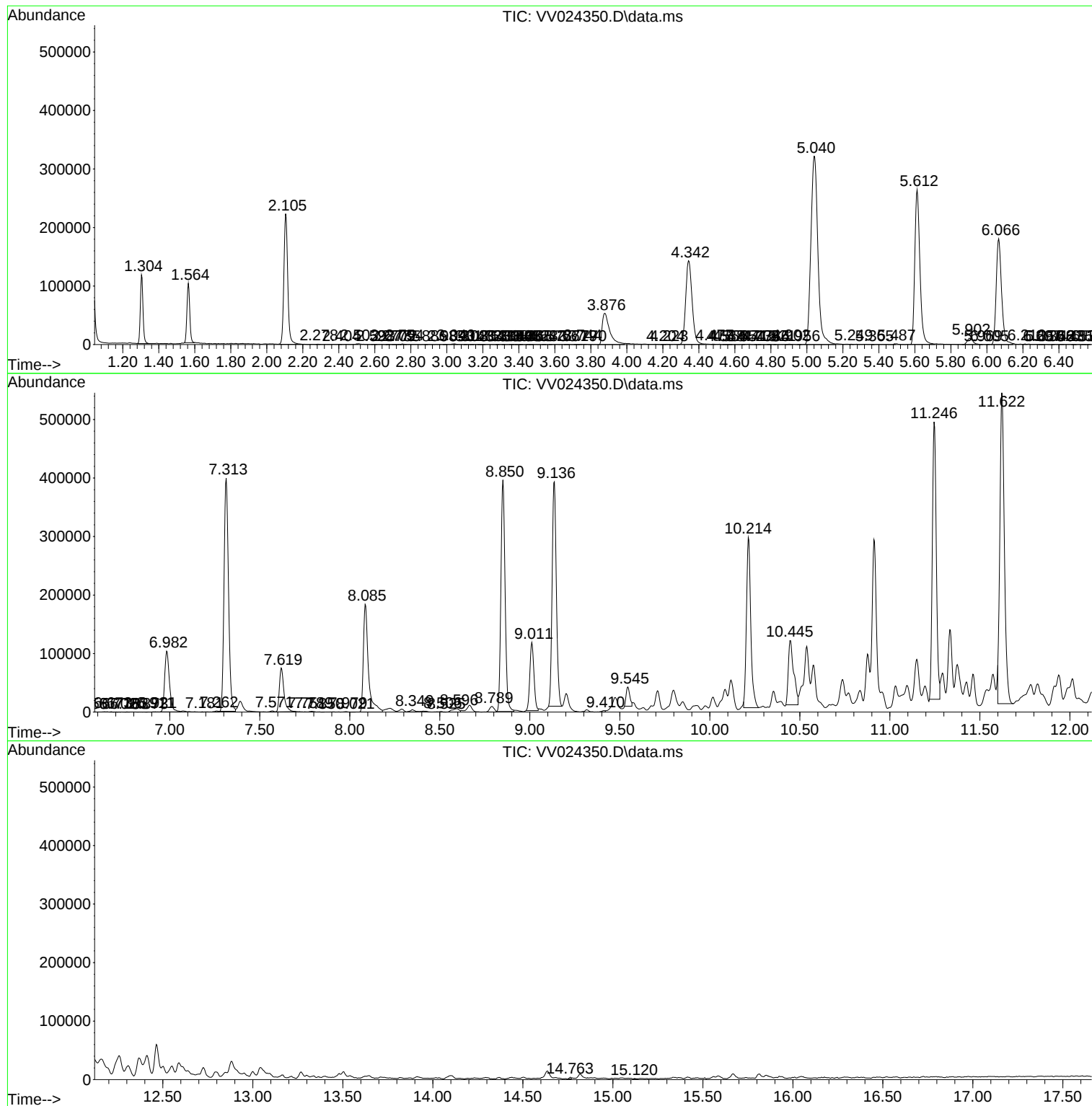
Sum of corrected areas: 8128843

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011322\
Data File : VV024350.D
Acq On : 13 Jan 2022 14:33
Operator : SY/MD
Sample : N1084-10DL 50X
Misc : 12.29g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGLN3DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011322\
Data File : VV024350.D
Acq On : 13 Jan 2022 14:33
Operator : SY/MD
Sample : N1084-10DL 50X
Misc : 12.29g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGLN3DL

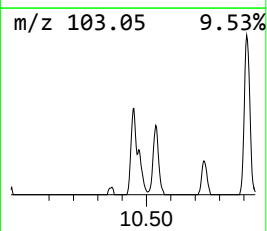
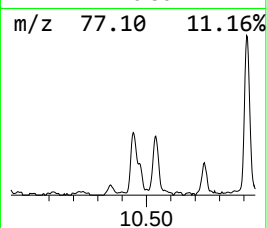
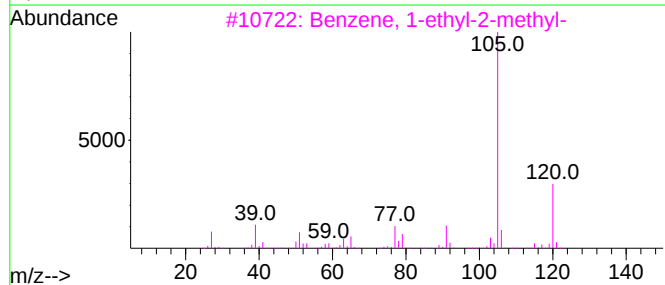
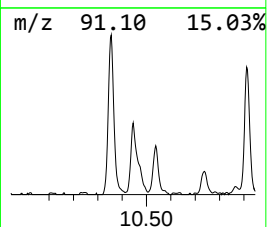
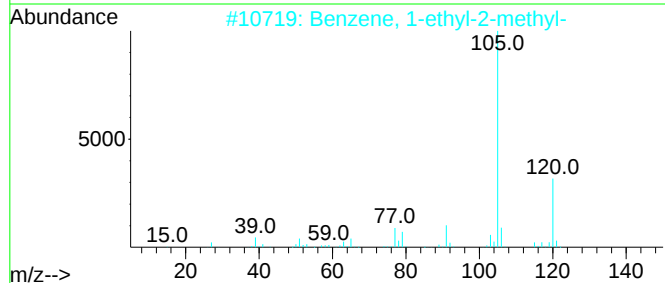
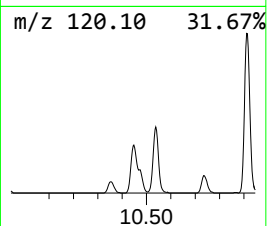
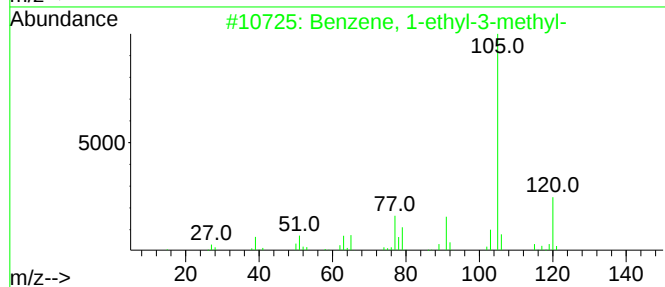
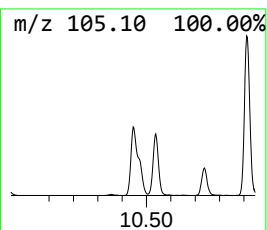
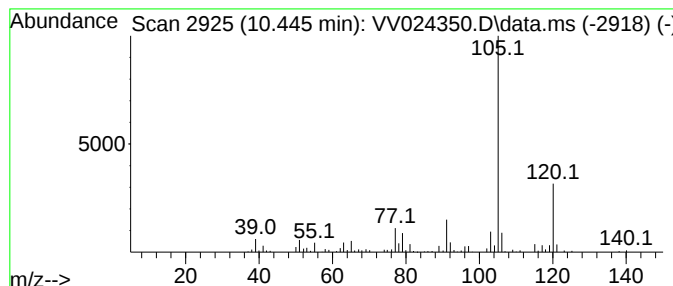
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Benzene, 1-ethyl-3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.445	15.49 ug/L	225193	1,4-Dichlorobenzene-d4	11.246

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
3			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
4			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011322\
Data File : VV024350.D
Acq On : 13 Jan 2022 14:33
Operator : SY/MD
Sample : N1084-10DL 50X
Misc : 12.29g/5.0mL/100ul/5.0mL/MSVOA_V/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BGLN3DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.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-ethy...	10.445	15.5	ug/L	225193	3	11.246	726682	50.0