

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
 Data File : VX025645.D
 Acq On : 09 Dec 2021 01:19
 Operator : JC/MD
 Sample : M4975-10
 Misc : 6.62g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BGKT4

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\SFAMXLM112221WMA.M
 Title : VOC Analysis

Signal : TIC: VX025645.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.239	23	25	34	rVB2	3113	4707	0.50%	0.095%
2	1.373	43	47	54	rVB	55394	63302	6.78%	1.274%
3	1.648	89	92	99	rVB	35891	42109	4.51%	0.847%
4	2.282	190	196	206	rBV	99838	165732	17.74%	3.335%
5	2.946	300	305	316	rVB	4233	10103	1.08%	0.203%
6	3.489	393	394	395	rBV	475	303	0.03%	0.006%
7	3.605	411	413	418	rVB3	404	506	0.05%	0.010%
8	3.800	443	445	447	rBV	310	219	0.02%	0.004%
9	4.355	535	536	540	rBV2	233	247	0.03%	0.005%
10	4.501	549	560	586	rBV2	20796	101431	10.86%	2.041%
11	4.903	625	626	628	rBV	248	188	0.02%	0.004%
12	5.068	641	653	672	rVB	58228	195508	20.93%	3.934%
13	5.263	681	685	686	rBV2	331	455	0.05%	0.009%
14	5.379	696	704	712	rVB4	4943	13285	1.42%	0.267%
15	5.763	765	767	770	rBV2	347	395	0.04%	0.008%
16	5.879	784	786	790	rBV2	320	418	0.04%	0.008%
17	5.970	790	801	819	rVV2	171027	497834	53.29%	10.018%
18	6.561	896	898	903	rBV2	351	588	0.06%	0.012%
19	6.604	903	905	909	rVV	294	320	0.03%	0.006%
20	6.641	909	911	912	rVB	441	256	0.03%	0.005%
21	6.659	912	914	919	rVB	466	636	0.07%	0.013%
22	6.702	919	921	922	rBV	323	333	0.04%	0.007%
23	6.763	922	931	947	rVV	131656	342255	36.64%	6.887%
24	7.128	982	991	1000	rBV4	12171	28665	3.07%	0.577%
25	7.214	1001	1005	1007	rBV3	688	1067	0.11%	0.021%
26	7.311	1013	1021	1034	rVB	92652	219836	23.53%	4.424%
27	7.574	1062	1064	1068	rBV2	379	481	0.05%	0.010%
28	7.695	1082	1084	1085	rBV	366	255	0.03%	0.005%
29	7.781	1097	1098	1100	rBV	415	245	0.03%	0.005%
30	7.927	1120	1122	1123	rBV2	307	267	0.03%	0.005%
31	8.055	1140	1143	1144	rBV2	288	317	0.03%	0.006%
32	8.329	1182	1188	1198	rBV	56611	103470	11.08%	2.082%
33	8.476	1210	1212	1213	rVB	455	253	0.03%	0.005%
34	8.518	1217	1219	1222	rVB	282	257	0.03%	0.005%
35	8.543	1222	1223	1227	rBV2	487	501	0.05%	0.010%
36	8.653	1234	1241	1249	rBV	244399	410478	43.94%	8.260%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
 Data File : VX025645.D
 Acq On : 09 Dec 2021 01:19
 Operator : JC/MD
 Sample : M4975-10
 Misc : 6.62g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BGKT4

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\SFAMXLM112221WMA.M
 Title : VOC Analysis

37	8.720	1249	1252	1259	rVB	4182	6914	0.74%	0.139%
38	8.957	1285	1291	1299	rVV	36932	64598	6.91%	1.300%
39	9.079	1310	1311	1314	rBV	330	254	0.03%	0.005%
40	9.128	1317	1319	1322	rBV	500	319	0.03%	0.006%
41	9.171	1325	1326	1328	rVB	470	221	0.02%	0.004%
42	9.195	1328	1330	1333	rBV	347	334	0.04%	0.007%
43	9.274	1336	1343	1354	rVV	633657	934200	100.00%	18.798%
44	9.402	1357	1364	1378	rVV	130531	223036	23.87%	4.488%
45	9.628	1399	1401	1403	rBV2	365	325	0.03%	0.007%
46	9.969	1453	1457	1458	rBV	454	491	0.05%	0.010%
47	10.061	1466	1472	1481	rBV	272979	401294	42.96%	8.075%
48	10.195	1492	1494	1499	rVB2	480	614	0.07%	0.012%
49	10.305	1508	1512	1517	rVV	2892	3634	0.39%	0.073%
50	10.457	1536	1537	1539	rBV	549	441	0.05%	0.009%
51	10.536	1549	1550	1552	rBV	299	210	0.02%	0.004%
52	10.652	1566	1569	1572	rBV2	854	1296	0.14%	0.026%
53	10.738	1580	1583	1584	rBV	270	208	0.02%	0.004%
54	10.817	1593	1596	1598	rBV	525	501	0.05%	0.010%
55	10.878	1603	1606	1607	rBV2	334	292	0.03%	0.006%
56	10.951	1615	1618	1620	rVB2	687	794	0.08%	0.016%
57	11.012	1626	1628	1629	rBV	356	206	0.02%	0.004%
58	11.122	1642	1646	1649	rBV2	2264	2784	0.30%	0.056%
59	11.195	1653	1658	1667	rVV	175956	234193	25.07%	4.713%
60	11.305	1674	1676	1677	rBV	411	236	0.03%	0.005%
61	11.750	1746	1749	1754	rVB3	1813	2539	0.27%	0.051%
62	11.841	1762	1764	1767	rBV2	393	515	0.06%	0.010%
63	11.939	1776	1780	1784	rVB2	1143	1488	0.16%	0.030%
64	11.969	1784	1785	1789	rVB2	496	488	0.05%	0.010%
65	12.024	1789	1794	1800	rBV	324230	399742	42.79%	8.044%
66	12.128	1806	1811	1812	rBV3	989	1320	0.14%	0.027%
67	12.225	1825	1827	1828	rBV	289	203	0.02%	0.004%
68	12.243	1828	1830	1831	rVB	442	233	0.02%	0.005%
69	12.323	1836	1843	1850	rBV	297468	372220	39.84%	7.490%
70	12.426	1856	1860	1863	rVB2	2400	2857	0.31%	0.057%
71	12.481	1866	1869	1872	rBV4	432	645	0.07%	0.013%
72	12.512	1872	1874	1877	rVB	236	190	0.02%	0.004%
73	12.621	1890	1892	1894	rBV	261	229	0.02%	0.005%
74	12.658	1896	1898	1901	rBV2	494	705	0.08%	0.014%
75	12.792	1918	1920	1922	rBV	325	241	0.03%	0.005%
76	13.005	1953	1955	1958	rVB	322	354	0.04%	0.007%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
 Data File : VX025645.D
 Acq On : 09 Dec 2021 01:19
 Operator : JC/MD
 Sample : M4975-10
 Misc : 6.62g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BGKT4

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\SFAMXLM112221WMA.M
 Title : VOC Analysis

77	13.060	1963	1964	1966	rVB	389	271	0.03%	0.005%
78	13.085	1966	1968	1970	rBV2	232	259	0.03%	0.005%
79	13.152	1977	1979	1982	rBV	324	319	0.03%	0.006%
80	13.182	1982	1984	1986	rVB2	399	295	0.03%	0.006%
81	13.201	1986	1987	1990	rBV	444	382	0.04%	0.008%
82	13.316	2005	2006	2007	rBV	405	202	0.02%	0.004%
83	13.432	2022	2025	2029	rBV	346	527	0.06%	0.011%
84	13.505	2034	2037	2039	rBV2	304	247	0.03%	0.005%
85	13.688	2066	2067	2069	rBV	484	431	0.05%	0.009%
86	13.780	2080	2082	2087	rVB2	326	401	0.04%	0.008%
87	13.828	2087	2090	2092	rBV2	320	323	0.03%	0.006%
88	13.938	2107	2108	2110	rBV	337	342	0.04%	0.007%
89	14.030	2121	2123	2125	rBV	325	292	0.03%	0.006%
90	14.194	2149	2150	2152	rVB2	475	200	0.02%	0.004%
91	14.353	2174	2176	2178	rBV	337	399	0.04%	0.008%
92	14.993	2279	2281	2282	rBV2	314	210	0.02%	0.004%
93	15.060	2287	2292	2295	rVV5	3272	4763	0.51%	0.096%
94	15.133	2301	2304	2308	rVB3	2846	3231	0.35%	0.065%
95	15.346	2333	2339	2344	rBV	46041	68421	7.32%	1.377%
96	15.511	2363	2366	2371	rVB5	2413	3298	0.35%	0.066%
97	15.718	2396	2400	2407	rVB5	3070	5939	0.64%	0.120%
98	15.804	2407	2414	2419	rBV3	5710	8907	0.95%	0.179%
99	16.005	2446	2447	2448	rBV	384	191	0.02%	0.004%
100	16.188	2475	2477	2482	rVB4	917	1120	0.12%	0.023%

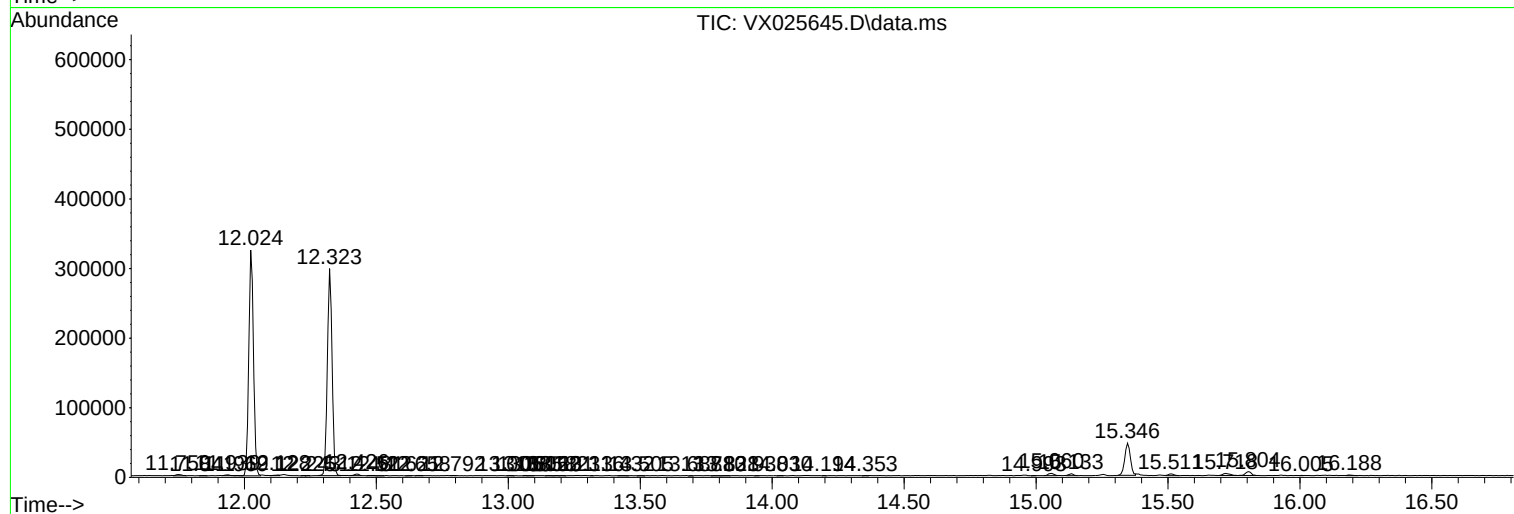
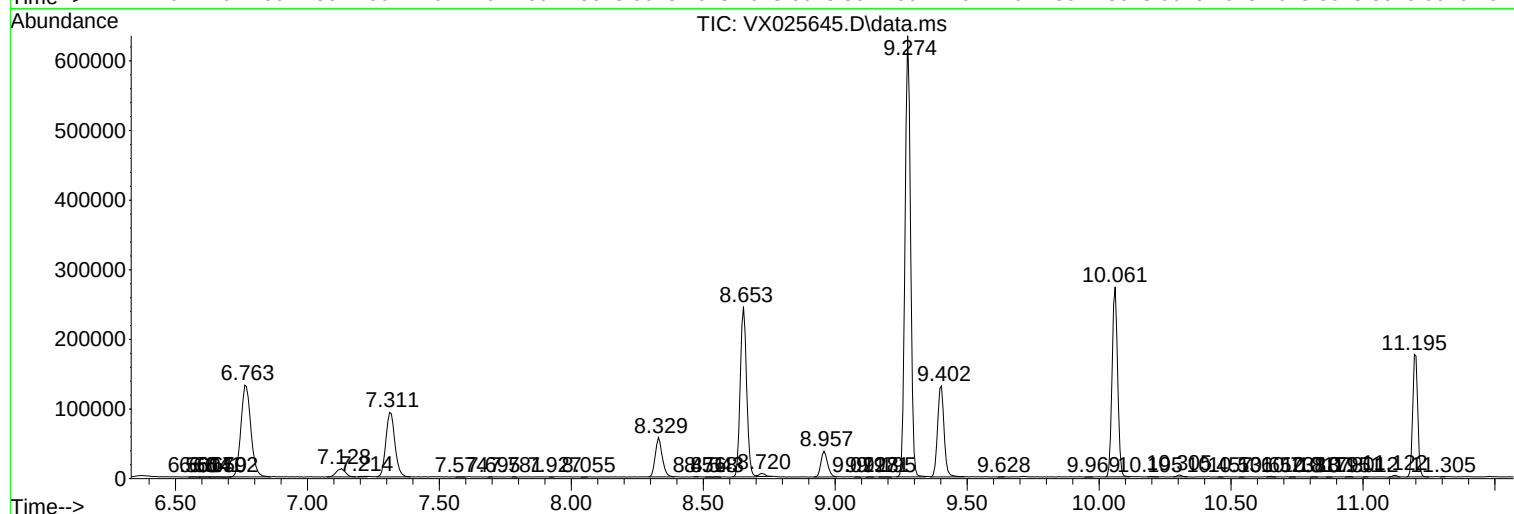
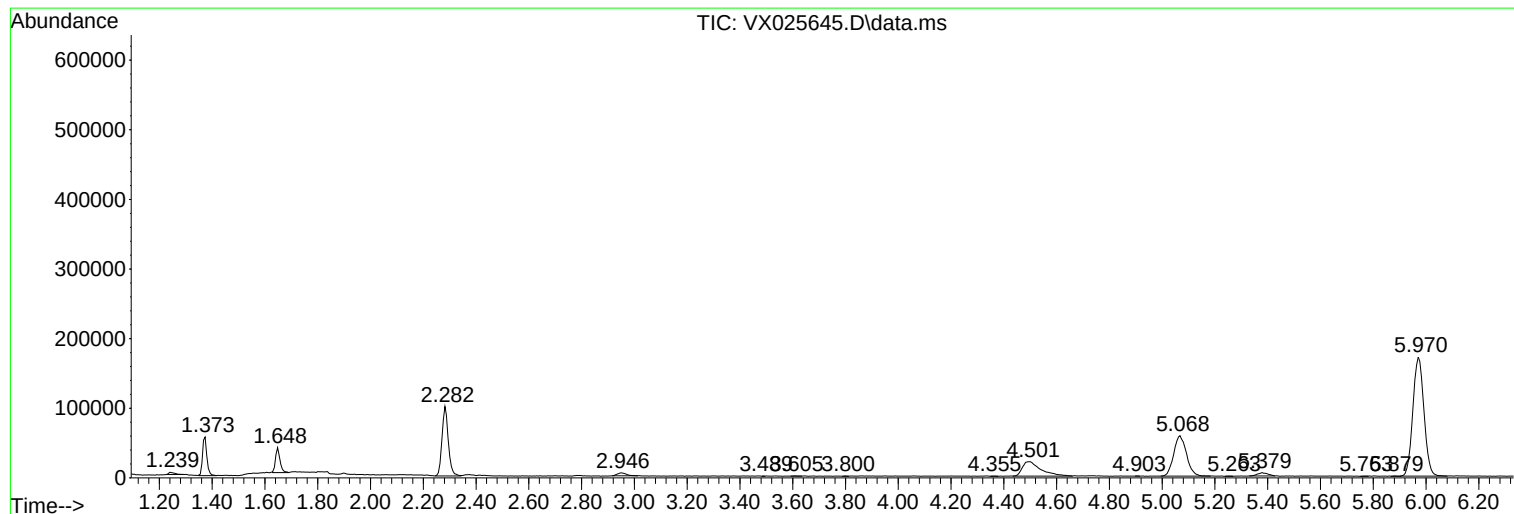
Sum of corrected areas: 4969556

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
Data File : VX025645.D
Acq On : 09 Dec 2021 01:19
Operator : JC/MD
Sample : M4975-10
Misc : 6.62g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGKT4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
Data File : VX025645.D
Acq On : 09 Dec 2021 01:19
Operator : JC/MD
Sample : M4975-10
Misc : 6.62g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGKT4

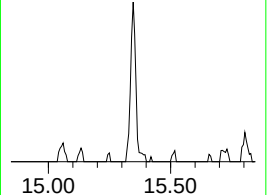
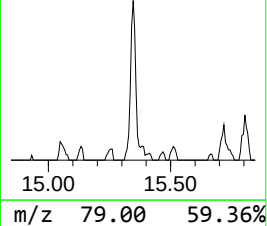
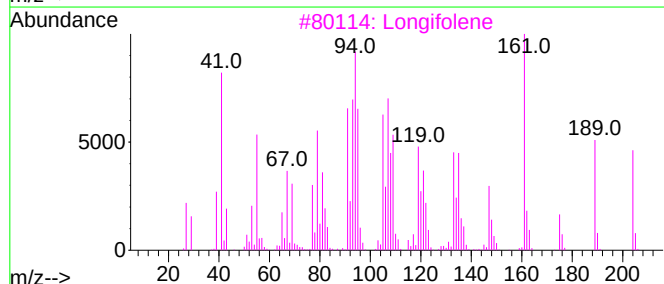
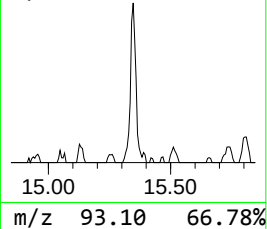
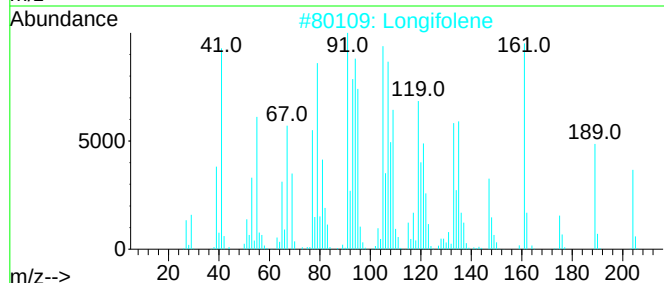
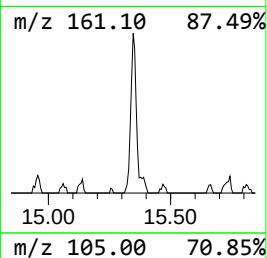
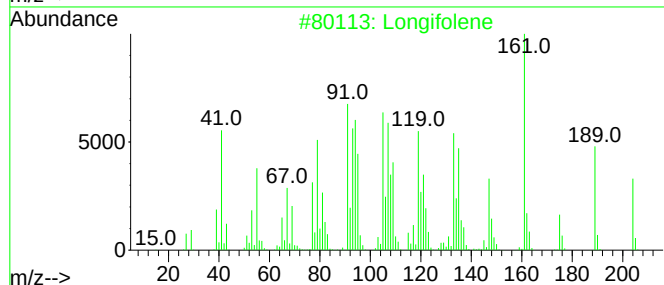
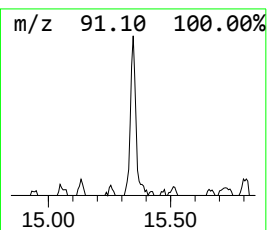
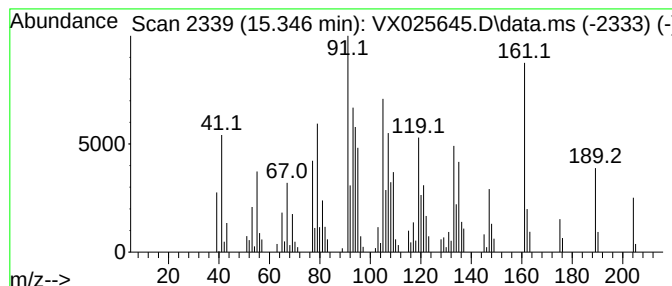
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Longifolene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.347	8.56 ug/L	68421	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Longifolene	204	C15H24	000475-20-7	99
2			Longifolene	204	C15H24	000475-20-7	99
3			Longifolene	204	C15H24	000475-20-7	99
4			Longifolene	204	C15H24	000475-20-7	99
5			(3R,4aS,5R)-4a,5-Dimethyl-3-(pro...	204	C15H24	024741-64-8	99



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
Data File : VX025645.D
Acq On : 09 Dec 2021 01:19
Operator : JC/MD
Sample : M4975-10
Misc : 6.62g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGKT4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML112221WMA.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
Longifolene	15.347	8.6	ug/L	68421	3	12.024	399742	50.0