

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
 Data File : VU046157.D
 Acq On : 07 Dec 2021 22:10
 Operator : SY/MD
 Sample : M4887-15ME
 Misc : 4.56g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EX8C9ME

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_U\Method\SFAMULM112921WMA.M
 Title : VOC Analysis

Signal : TIC: VU046157.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	73	81	97	rVB	174191	218905	14.25%	2.010%
2	1.916	170	179	198	rBV	104214	166299	10.83%	1.527%
3	2.549	365	376	392	rBV	299629	481662	31.36%	4.422%
4	2.967	504	506	511	rVB3	429	278	0.02%	0.003%
5	3.035	520	527	528	rBV2	1411	1312	0.09%	0.012%
6	3.183	552	573	597	rBV	11101	29990	1.95%	0.275%
7	3.382	631	635	639	rVB3	229	183	0.01%	0.002%
8	3.453	653	657	660	rBB	194	173	0.01%	0.002%
9	3.485	664	667	672	rBV	170	213	0.01%	0.002%
10	3.732	738	744	749	rBB	169	274	0.02%	0.003%
11	3.764	749	754	756	rBV	163	185	0.01%	0.002%
12	3.806	764	767	772	rBV	175	223	0.01%	0.002%
13	3.871	784	787	792	rBB	137	168	0.01%	0.002%
14	3.896	792	795	798	rBV	141	141	0.01%	0.001%
15	3.996	822	826	831	rBB	163	184	0.01%	0.002%
16	4.057	843	845	850	rBV	124	155	0.01%	0.001%
17	4.121	862	865	869	rBB	176	163	0.01%	0.001%
18	4.314	922	925	928	rBV	203	186	0.01%	0.002%
19	4.533	990	993	995	rBV	145	133	0.01%	0.001%
20	4.655	1012	1031	1073	rBV	78649	355561	23.15%	3.264%
21	5.063	1142	1158	1182	rVB	239594	586139	38.16%	5.381%
22	5.292	1228	1229	1238	rVB2	314	315	0.02%	0.003%
23	5.340	1241	1244	1248	rBB	139	141	0.01%	0.001%
24	5.366	1249	1252	1255	rBV	136	140	0.01%	0.001%
25	5.391	1257	1260	1263	rBV	139	136	0.01%	0.001%
26	5.475	1283	1286	1289	rBV	123	132	0.01%	0.001%
27	5.517	1296	1299	1301	rBV	138	123	0.01%	0.001%
28	5.636	1331	1336	1340	rBB	180	228	0.01%	0.002%
29	5.723	1341	1363	1385	rBV2	599982	1535857	100.00%	14.101%
30	5.893	1412	1416	1421	rVB2	281	319	0.02%	0.003%
31	5.977	1433	1442	1457	rBV3	5049	13340	0.87%	0.122%
32	6.073	1471	1472	1476	rVB	327	150	0.01%	0.001%
33	6.115	1482	1485	1489	rBB2	263	218	0.01%	0.002%
34	6.250	1510	1527	1555	rBV	223008	452832	29.48%	4.157%
35	6.539	1604	1617	1633	rBV	159057	306595	19.96%	2.815%
36	6.690	1650	1664	1694	rVB	336075	681517	44.37%	6.257%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
 Data File : VU046157.D
 Acq On : 07 Dec 2021 22:10
 Operator : SY/MD
 Sample : M4887-15ME
 Misc : 4.56g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EX8C9ME

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_U\Method\SFAMULM112921WMA.M
 Title : VOC Analysis

37	6.809	1694	1701	1709	rBV4	696	995	0.06%	0.009%
38	7.060	1775	1779	1782	rBV2	225	211	0.01%	0.002%
39	7.186	1811	1818	1820	rBV3	567	540	0.04%	0.005%
40	7.215	1825	1827	1829	rVV2	327	188	0.01%	0.002%
41	7.388	1878	1881	1886	rBB	136	142	0.01%	0.001%
42	7.417	1887	1890	1892	rBV	158	126	0.01%	0.001%
43	7.568	1923	1937	1966	rBV	185849	368538	24.00%	3.384%
44	7.790	1997	2006	2025	rBV2	3682	7830	0.51%	0.072%
45	7.899	2025	2040	2057	rBV	701379	1321789	86.06%	12.135%
46	8.060	2088	2090	2094	rVB3	334	244	0.02%	0.002%
47	8.182	2116	2128	2157	rVB2	108248	249498	16.24%	2.291%
48	8.298	2159	2164	2173	rVB2	225	257	0.02%	0.002%
49	8.472	2213	2218	2226	rVB	220	358	0.02%	0.003%
50	8.555	2235	2244	2255	rBV5	5667	9312	0.61%	0.085%
51	8.677	2258	2282	2315	rBV	256222	802539	52.25%	7.368%
52	8.838	2328	2332	2334	rBV	171	131	0.01%	0.001%
53	8.951	2359	2367	2375	rVV2	638	1309	0.09%	0.012%
54	9.423	2500	2514	2538	rBV	262094	578917	37.69%	5.315%
55	9.575	2554	2561	2566	rBV3	475	724	0.05%	0.007%
56	9.703	2591	2601	2612	rVB2	1274	2163	0.14%	0.020%
57	10.111	2724	2728	2732	rVV3	428	360	0.02%	0.003%
58	10.163	2741	2744	2751	rBV	203	332	0.02%	0.003%
59	10.227	2761	2764	2766	rBV2	219	147	0.01%	0.001%
60	10.468	2836	2839	2841	rBV	209	143	0.01%	0.001%
61	10.671	2893	2902	2912	rBV2	6423	9165	0.60%	0.084%
62	10.771	2918	2933	2949	rBV	477860	802202	52.23%	7.365%
63	10.867	2956	2963	2964	rBV3	1073	1052	0.07%	0.010%
64	10.925	2979	2981	2988	rVB2	795	558	0.04%	0.005%
65	11.005	3000	3006	3007	rBV2	315	225	0.01%	0.002%
66	11.121	3030	3042	3050	rBV7	1622	3400	0.22%	0.031%
67	11.205	3066	3068	3074	rVB2	513	401	0.03%	0.004%
68	11.362	3114	3117	3120	rBV3	417	325	0.02%	0.003%
69	11.414	3128	3133	3138	rBV4	606	678	0.04%	0.006%
70	11.459	3138	3147	3159	rVB4	4356	7837	0.51%	0.072%
71	11.578	3179	3184	3192	rVB4	899	1152	0.08%	0.011%
72	11.697	3214	3221	3229	rVB5	2631	3873	0.25%	0.036%
73	11.819	3246	3259	3283	rVB	382211	610619	39.76%	5.606%
74	11.902	3283	3285	3286	rBV	300	155	0.01%	0.001%
75	11.941	3291	3297	3301	rVV4	2272	3304	0.22%	0.030%
76	11.973	3302	3307	3314	rVB3	4345	5791	0.38%	0.053%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
 Data File : VU046157.D
 Acq On : 07 Dec 2021 22:10
 Operator : SY/MD
 Sample : M4887-15ME
 Misc : 4.56g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EX8C9ME

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_U\Method\SFAMULM112921WMA.M
 Title : VOC Analysis

77	12.198	3359	3377	3391	rBV	751327	1221933	79.56%	11.219%
78	12.272	3396	3400	3405	rVB3	904	958	0.06%	0.009%
79	12.327	3410	3417	3429	rVB3	3201	4569	0.30%	0.042%
80	12.394	3433	3438	3439	rBV2	1050	842	0.05%	0.008%
81	12.594	3495	3500	3502	rBV2	267	276	0.02%	0.003%
82	12.639	3510	3514	3518	rVB3	589	515	0.03%	0.005%
83	12.774	3549	3556	3562	rBV3	510	755	0.05%	0.007%
84	12.816	3563	3569	3574	rVV4	663	871	0.06%	0.008%
85	12.992	3621	3624	3629	rVB	194	124	0.01%	0.001%
86	13.137	3665	3669	3670	rBV2	366	230	0.01%	0.002%
87	13.430	3757	3760	3764	rVB3	543	329	0.02%	0.003%
88	13.513	3777	3786	3795	rVB2	15783	21734	1.42%	0.200%
89	13.706	3843	3846	3849	rBV	200	130	0.01%	0.001%
90	14.089	3959	3965	3974	rVV	792	1236	0.08%	0.011%
91	14.449	4073	4077	4083	rBV4	544	556	0.04%	0.005%
92	14.504	4090	4094	4095	rBV	204	143	0.01%	0.001%
93	14.581	4110	4118	4129	rVB2	1101	1767	0.12%	0.016%
94	14.648	4135	4139	4142	rBV2	176	182	0.01%	0.002%
95	14.719	4158	4161	4164	rVB2	224	153	0.01%	0.001%
96	14.777	4174	4179	4181	rBV2	210	202	0.01%	0.002%
97	14.947	4229	4232	4238	rVB	403	429	0.03%	0.004%
98	15.227	4312	4319	4327	rVB2	784	1328	0.09%	0.012%
99	15.365	4360	4362	4365	rBV2	206	146	0.01%	0.001%
100	15.404	4369	4374	4375	rBV3	767	566	0.04%	0.005%

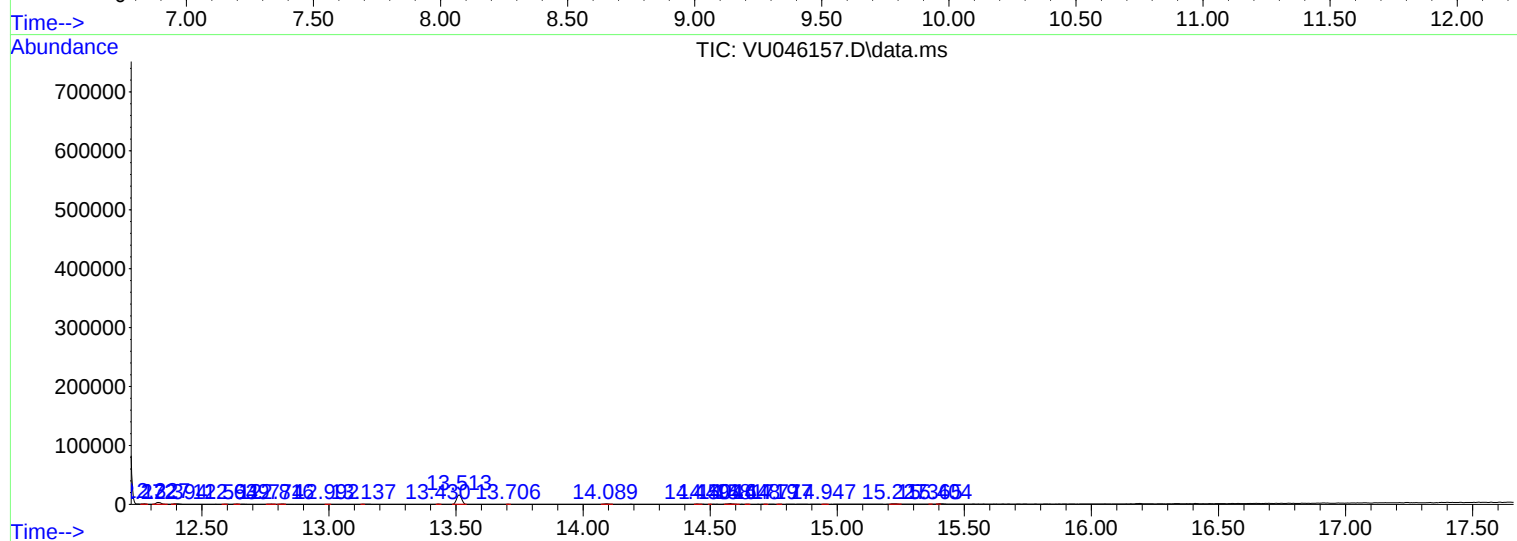
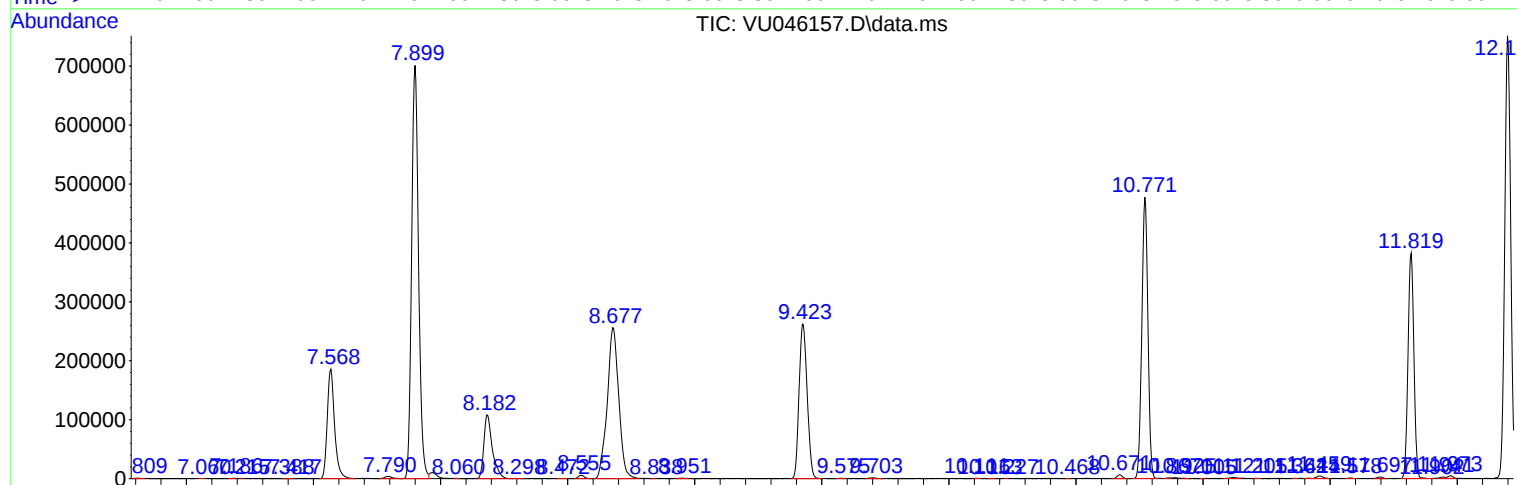
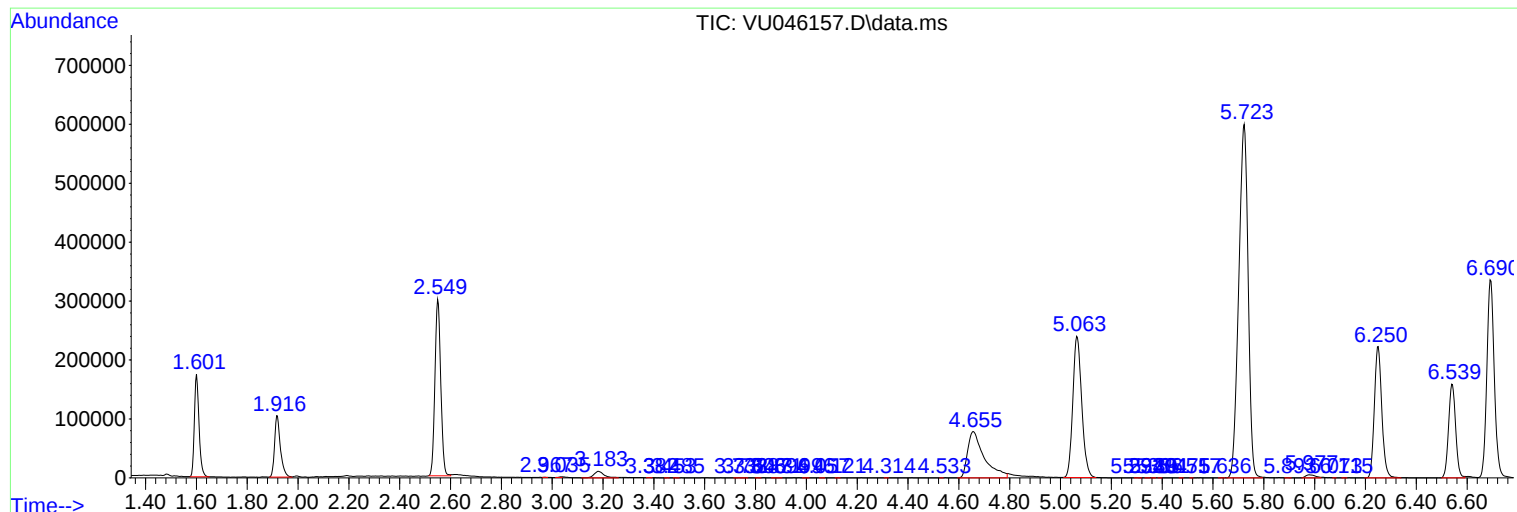
Sum of corrected areas: 10892074

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
Data File : VU046157.D
Acq On : 07 Dec 2021 22:10
Operator : SY/MD
Sample : M4887-15ME
Misc : 4.56g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EX8C9ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
Data File : VU046157.D
Acq On : 07 Dec 2021 22:10
Operator : SY/MD
Sample : M4887-15ME
Misc : 4.56g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EX8C9ME

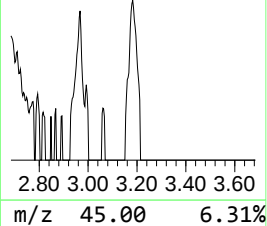
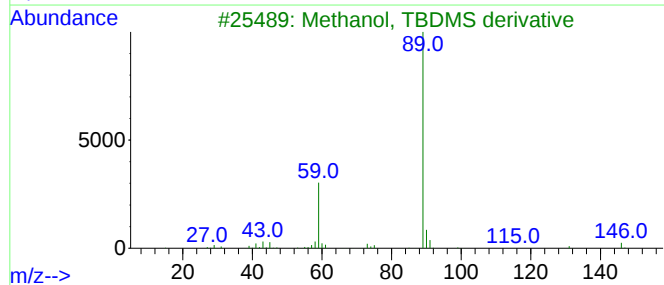
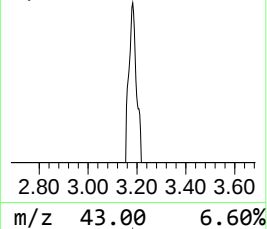
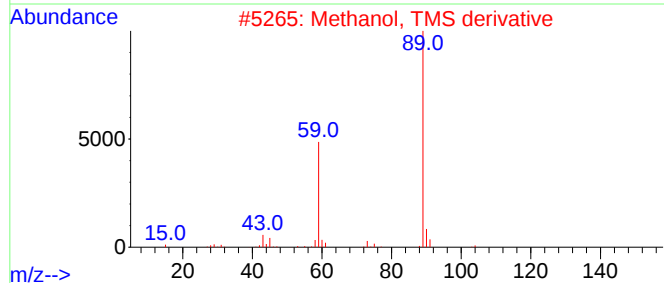
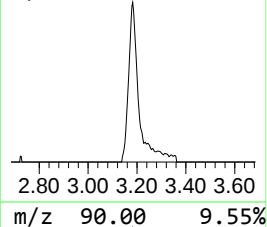
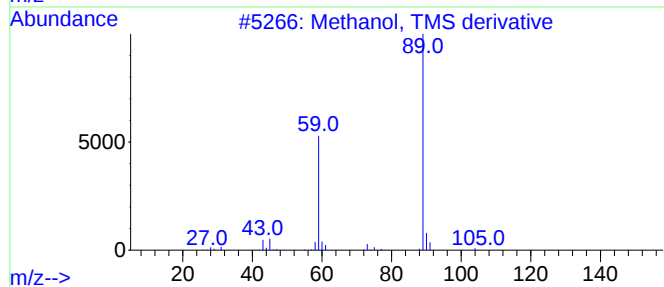
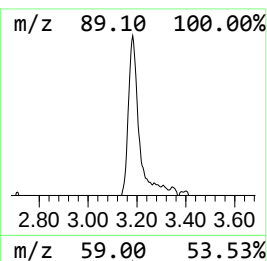
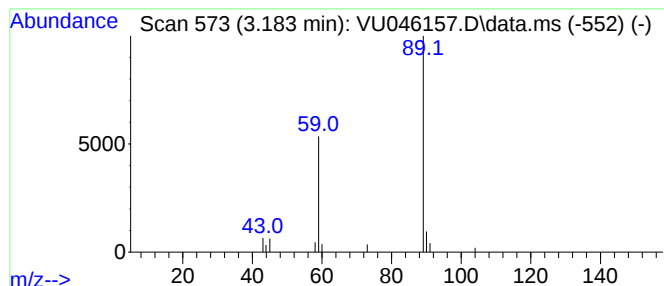
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Methanol, TMS derivative Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.183	3.31 ug/L	29990	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanol, TMS derivative	104	C4H12OSi	001825-61-2	90
2			Methanol, TMS derivative	104	C4H12OSi	001825-61-2	83
3			Methanol, TBDMS derivative	146	C7H18OSi	1000364-10-7	74
4			Ethyl(dimethyl)methoxysilane	118	C5H14OSi	052686-75-6	74
5			Silane, (2-methoxyethyl)trimethyl-	132	C6H16OSi	018173-63-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
Data File : VU046157.D
Acq On : 07 Dec 2021 22:10
Operator : SY/MD
Sample : M4887-15ME
Misc : 4.56g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EX8C9ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.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
Methanol, TMS d...	3.183	3.3	ug/L	29990	1	6.250	452832	50.0