

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU043023\
 Data File : VU054011.D
 Acq On : 30 Apr 2023 01:06
 Operator : JC/MD
 Sample : 02548-25ME
 Misc : 5.73g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DCCQ5ME

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\SFAMULM042923WMA.M
 Title : VOC Analysis

Signal : TIC: VU054011.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.488	40	46	52	rBV5	2626	3978	0.18%	0.027%
2	1.597	72	80	100	rBV	206959	289550	13.21%	1.938%
3	1.687	101	108	123	rVB	28787	40846	1.86%	0.273%
4	1.909	169	177	194	rBV	124059	209825	9.57%	1.405%
5	2.446	342	344	347	rBV	603	370	0.02%	0.002%
6	2.552	365	377	392	rBV	463637	748360	34.14%	5.010%
7	2.642	395	405	429	rVB	44362	106970	4.88%	0.716%
8	2.771	442	445	446	rBV2	439	245	0.01%	0.002%
9	2.951	493	501	505	rBV3	509	721	0.03%	0.005%
10	3.041	520	529	542	rBV4	3053	6164	0.28%	0.041%
11	3.179	569	572	577	rVV3	441	456	0.02%	0.003%
12	3.285	603	605	611	rVV2	282	254	0.01%	0.002%
13	3.581	693	697	699	rBV4	609	471	0.02%	0.003%
14	3.813	764	769	771	rVB2	416	311	0.01%	0.002%
15	4.067	837	848	851	rBV4	1682	2771	0.13%	0.019%
16	4.388	945	948	954	rBV2	325	265	0.01%	0.002%
17	4.632	1010	1024	1074	rBV	113123	420640	19.19%	2.816%
18	4.925	1113	1115	1121	rVB2	357	316	0.01%	0.002%
19	5.054	1138	1155	1185	rVV	375401	850119	38.78%	5.691%
20	5.298	1225	1231	1233	rBV	218	243	0.01%	0.002%
21	5.404	1258	1264	1266	rBV	242	256	0.01%	0.002%
22	5.436	1271	1274	1278	rBV	219	225	0.01%	0.002%
23	5.549	1299	1309	1312	rVB2	235	394	0.02%	0.003%
24	5.716	1339	1361	1395	rBV2	823193	2192170	100.00%	14.676%
25	5.970	1433	1440	1450	rVV6	2953	6185	0.28%	0.041%
26	6.025	1454	1457	1461	rVB4	517	349	0.02%	0.002%
27	6.044	1461	1463	1470	rVB3	344	273	0.01%	0.002%
28	6.134	1487	1491	1493	rBV	477	380	0.02%	0.003%
29	6.243	1511	1525	1555	rBV	255367	499387	22.78%	3.343%
30	6.401	1572	1574	1581	rVB2	653	532	0.02%	0.004%
31	6.526	1603	1613	1625	rBV8	8399	17558	0.80%	0.118%
32	6.600	1627	1636	1639	rBV6	1615	2428	0.11%	0.016%
33	6.684	1648	1662	1685	rBV	504051	991566	45.23%	6.638%
34	7.015	1758	1765	1767	rBV	273	286	0.01%	0.002%
35	7.160	1805	1810	1813	rBV2	184	241	0.01%	0.002%
36	7.192	1813	1820	1823	rBV4	2113	2661	0.12%	0.018%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU043023\
 Data File : VU054011.D
 Acq On : 30 Apr 2023 01:06
 Operator : JC/MD
 Sample : 02548-25ME
 Misc : 5.73g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DCCQ5ME

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\SFAMULM042923WMA.M
 Title : VOC Analysis

37	7.298	1847	1853	1856	rBV2	430	408	0.02%	0.003%
38	7.423	1888	1892	1896	rBV2	285	312	0.01%	0.002%
39	7.468	1902	1906	1911	rBV2	255	242	0.01%	0.002%
40	7.558	1922	1934	1962	rBV	261579	494888	22.58%	3.313%
41	7.693	1972	1976	1978	rBV3	557	490	0.02%	0.003%
42	7.893	2023	2038	2067	rBV	1014166	1834386	83.68%	12.281%
43	8.176	2113	2126	2151	rBV	163952	340814	15.55%	2.282%
44	8.314	2166	2169	2171	rBV2	310	260	0.01%	0.002%
45	8.472	2215	2218	2222	rVB2	486	359	0.02%	0.002%
46	8.549	2228	2242	2258	rBV	551025	954503	43.54%	6.390%
47	8.652	2259	2274	2304	rVB	440661	926681	42.27%	6.204%
48	8.877	2342	2344	2349	rVB3	310	284	0.01%	0.002%
49	9.163	2429	2433	2442	rVV3	427	629	0.03%	0.004%
50	9.340	2485	2488	2492	rVB2	315	248	0.01%	0.002%
51	9.417	2498	2512	2532	rBV	329906	606422	27.66%	4.060%
52	9.690	2591	2597	2609	rVB3	1406	2310	0.11%	0.015%
53	9.742	2609	2613	2617	rBV2	384	280	0.01%	0.002%
54	9.861	2648	2650	2655	rBV2	322	263	0.01%	0.002%
55	10.243	2765	2769	2773	rBV2	472	400	0.02%	0.003%
56	10.327	2790	2795	2799	rBV2	283	323	0.01%	0.002%
57	10.484	2841	2844	2850	rVB2	361	376	0.02%	0.003%
58	10.555	2863	2866	2875	rBV3	322	380	0.02%	0.003%
59	10.597	2875	2879	2882	rBV2	375	340	0.02%	0.002%
60	10.613	2882	2884	2887	rVV3	418	256	0.01%	0.002%
61	10.642	2891	2893	2901	rVB2	854	857	0.04%	0.006%
62	10.706	2906	2913	2915	rBV2	276	351	0.02%	0.002%
63	10.758	2916	2929	2946	rBV	663449	1053293	48.05%	7.051%
64	10.963	2990	2993	2999	rVB2	264	255	0.01%	0.002%
65	11.114	3034	3040	3043	rBV5	1070	1191	0.05%	0.008%
66	11.163	3053	3055	3060	rVB2	368	301	0.01%	0.002%
67	11.307	3093	3100	3103	rBV3	469	610	0.03%	0.004%
68	11.362	3114	3117	3119	rBV2	460	311	0.01%	0.002%
69	11.484	3148	3155	3163	rVV5	1762	3401	0.16%	0.023%
70	11.516	3163	3165	3169	rVV3	511	315	0.01%	0.002%
71	11.610	3190	3194	3197	rBV	302	248	0.01%	0.002%
72	11.696	3217	3221	3226	rBV	382	381	0.02%	0.003%
73	11.809	3240	3256	3274	rBV	386194	607581	27.72%	4.068%
74	11.957	3299	3302	3305	rVV2	346	245	0.01%	0.002%
75	12.192	3361	3375	3397	rVV	1052515	1695838	77.36%	11.353%
76	12.336	3418	3420	3424	rVB3	416	228	0.01%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU043023\
 Data File : VU054011.D
 Acq On : 30 Apr 2023 01:06
 Operator : JC/MD
 Sample : 02548-25ME
 Misc : 5.73g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DCCQ5ME

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\SFAMULM042923WMA.M
 Title : VOC Analysis

77	12.430	3447	3449	3453	rVB2	357	263	0.01%	0.002%
78	12.876	3581	3588	3593	rBV2	283	399	0.02%	0.003%
79	12.979	3614	3620	3622	rBV	349	394	0.02%	0.003%
80	13.060	3639	3645	3650	rBV2	347	511	0.02%	0.003%
81	13.259	3705	3707	3713	rVB	418	231	0.01%	0.002%
82	13.352	3730	3736	3739	rBV2	256	338	0.02%	0.002%
83	13.468	3767	3772	3773	rBV2	357	316	0.01%	0.002%
84	13.523	3784	3789	3790	rBV	340	250	0.01%	0.002%
85	13.532	3790	3792	3796	rVB2	501	314	0.01%	0.002%
86	13.555	3796	3799	3800	rBV	394	246	0.01%	0.002%
87	13.674	3833	3836	3841	rBV	348	305	0.01%	0.002%
88	13.706	3842	3846	3849	rBV	459	418	0.02%	0.003%
89	13.732	3849	3854	3856	rVB3	378	353	0.02%	0.002%
90	13.754	3856	3861	3862	rBV2	371	299	0.01%	0.002%
91	13.921	3910	3913	3915	rBV	493	269	0.01%	0.002%
92	13.979	3927	3931	3934	rBV3	325	290	0.01%	0.002%
93	13.999	3934	3937	3940	rBV	290	250	0.01%	0.002%
94	14.217	4001	4005	4006	rBV	329	240	0.01%	0.002%
95	14.278	4020	4024	4027	rBV	491	496	0.02%	0.003%
96	14.333	4037	4041	4046	rBV3	449	423	0.02%	0.003%
97	14.655	4138	4141	4142	rBV	366	234	0.01%	0.002%
98	15.449	4385	4388	4392	rBV2	542	316	0.01%	0.002%
99	15.860	4514	4516	4518	rBV2	521	230	0.01%	0.002%
100	16.175	4612	4614	4619	rBV4	798	765	0.03%	0.005%

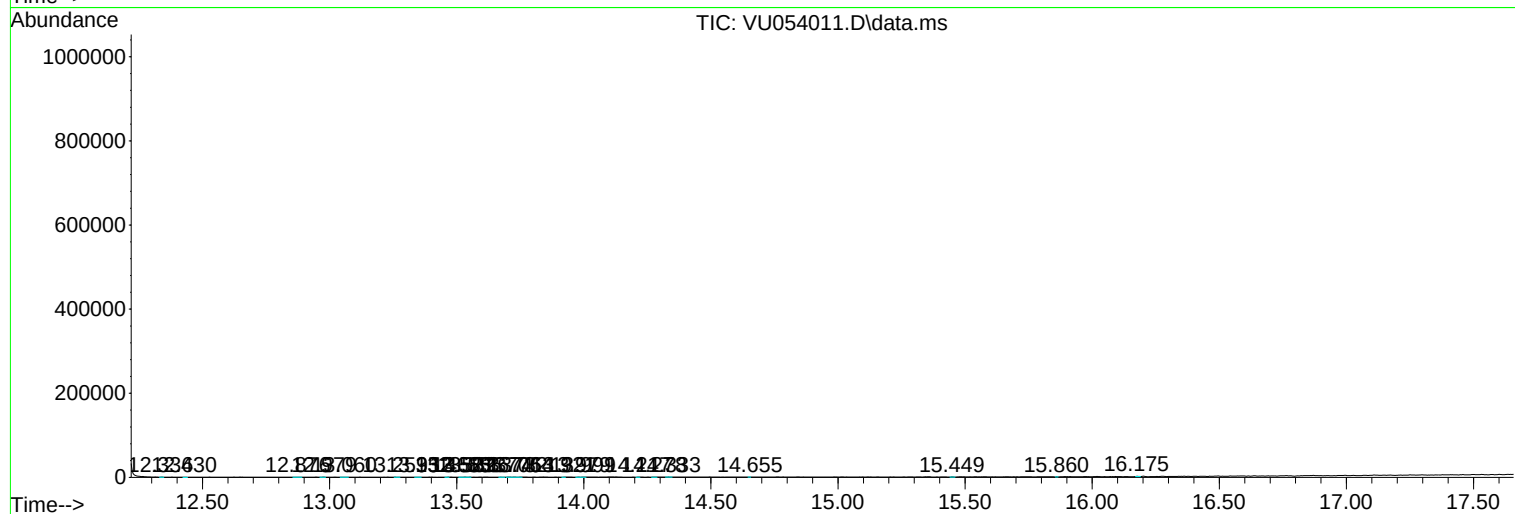
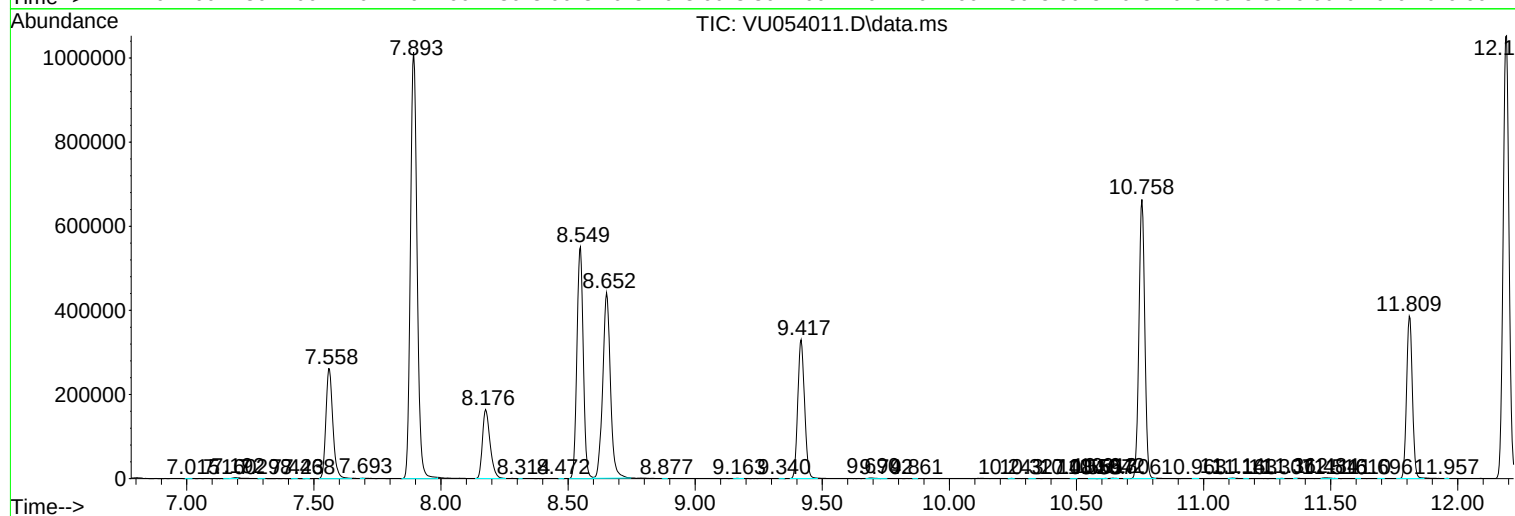
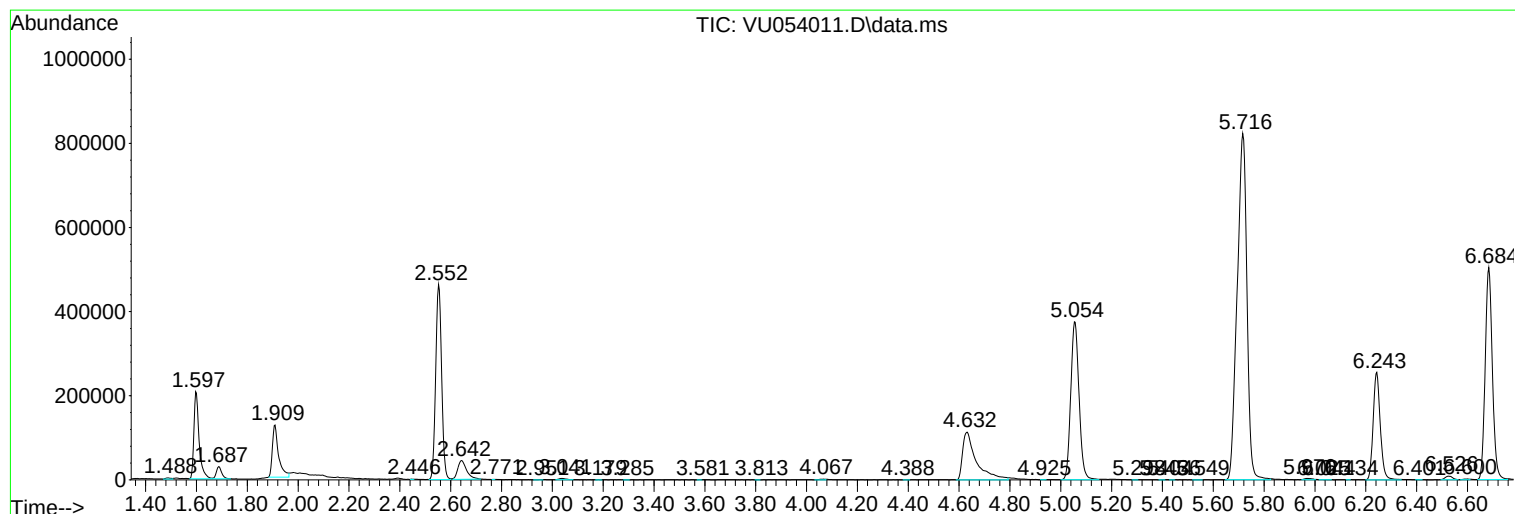
Sum of corrected areas: 14937176

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU043023\
Data File : VU054011.D
Acq On : 30 Apr 2023 01:06
Operator : JC/MD
Sample : 02548-25ME
Misc : 5.73g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 33 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DCCQ5ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042923WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU043023\
Data File : VU054011.D
Acq On : 30 Apr 2023 01:06
Operator : JC/MD
Sample : 02548-25ME
Misc : 5.73g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 33 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DCCQ5ME

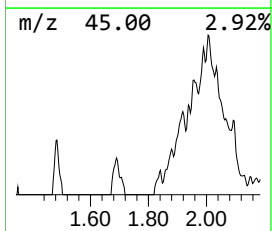
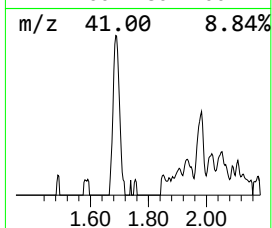
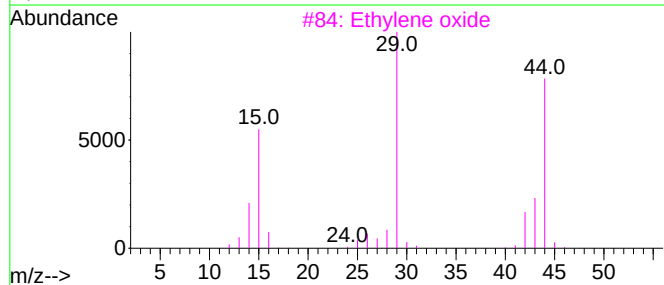
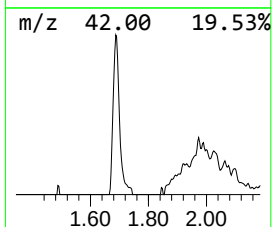
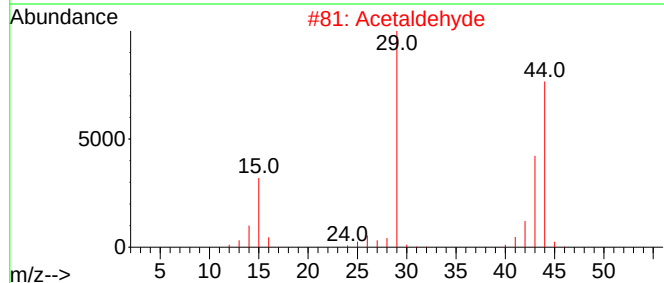
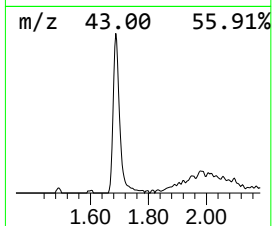
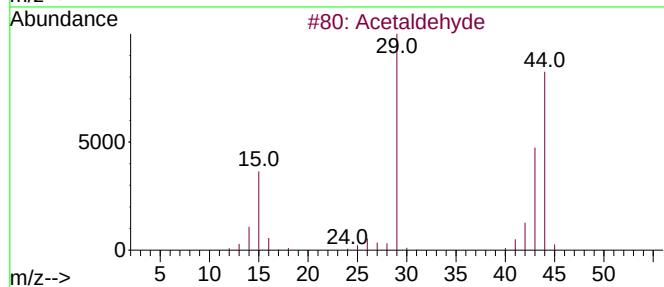
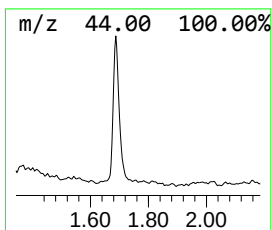
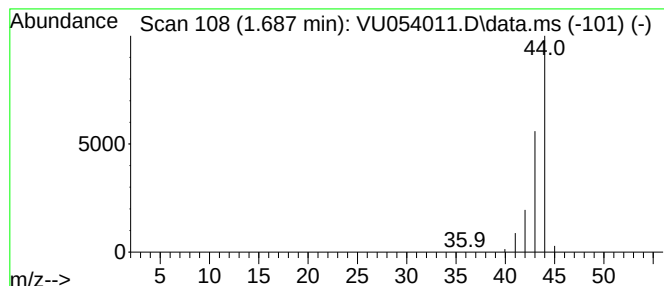
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042923WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.687	4.09 ug/L	40846	1,4-Difluorobenzene	6.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
2			Acetaldehyde	44	C2H4O	000075-07-0	74
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			Ethylene oxide	44	C2H4O	000075-21-8	5
5			Ethylene oxide	44	C2H4O	000075-21-8	5



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU043023\
Data File : VU054011.D
Acq On : 30 Apr 2023 01:06
Operator : JC/MD
Sample : 02548-25ME
Misc : 5.73g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 33 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DCCQ5ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042923WMA.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
Acetaldehyde	1.687	4.1	ug/L	40846	1	6.243	499387	50.0