

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
 Data File : VU059381.D
 Acq On : 20 Jun 2024 15:32
 Operator : MD/SY
 Sample : P2960-15
 Misc : 6.02g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHB52

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\SFAMULM052924WMA.M
 Title : VOC Analysis

Signal : TIC: VU059381.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.592	86	94	119	rVB	37139	66472	9.83%	1.253%
2	1.821	138	165	167	rBV3	40126	140303	20.74%	2.644%
3	2.534	376	387	403	rBV	99443	164767	24.36%	3.105%
4	2.624	411	415	416	rBV3	700	463	0.07%	0.009%
5	2.763	452	458	460	rBV3	481	555	0.08%	0.010%
6	3.023	528	539	550	rBV4	2637	5586	0.83%	0.105%
7	3.158	577	581	583	rBV2	805	675	0.10%	0.013%
8	3.293	618	623	627	rBV	213	245	0.04%	0.005%
9	3.319	627	631	636	rVV2	365	358	0.05%	0.007%
10	3.367	642	646	649	rVB2	315	255	0.04%	0.005%
11	3.386	649	652	662	rBV2	282	370	0.05%	0.007%
12	3.425	662	664	669	rBV	270	273	0.04%	0.005%
13	3.480	677	681	686	rVB2	255	255	0.04%	0.005%
14	3.512	686	691	693	rBV	314	305	0.05%	0.006%
15	3.705	744	751	757	rBV2	155	259	0.04%	0.005%
16	3.792	775	778	781	rVB2	335	259	0.04%	0.005%
17	3.827	784	789	796	rBV	661	838	0.12%	0.016%
18	4.303	934	937	942	rVB2	290	251	0.04%	0.005%
19	4.345	942	950	953	rBV2	259	386	0.06%	0.007%
20	4.624	1027	1037	1082	rBV	51297	158101	23.38%	2.979%
21	4.988	1145	1150	1155	rVB	319	251	0.04%	0.005%
22	5.052	1155	1170	1195	rBV	100194	229382	33.91%	4.322%
23	5.200	1213	1216	1221	rVB2	322	262	0.04%	0.005%
24	5.248	1229	1231	1237	rVB2	415	413	0.06%	0.008%
25	5.303	1245	1248	1254	rVB	355	344	0.05%	0.006%
26	5.399	1274	1278	1284	rBV2	248	253	0.04%	0.005%
27	5.579	1331	1334	1338	rVB2	352	322	0.05%	0.006%
28	5.605	1338	1342	1348	rBV2	277	410	0.06%	0.008%
29	5.637	1348	1352	1355	rVB	307	271	0.04%	0.005%
30	5.711	1355	1375	1400	rBV2	214761	570131	84.29%	10.743%
31	5.972	1452	1456	1458	rBV3	823	644	0.10%	0.012%
32	6.238	1527	1539	1563	rBV	262985	520930	77.02%	9.816%
33	6.393	1584	1587	1590	rBV3	329	280	0.04%	0.005%
34	6.521	1617	1627	1641	rVB8	3934	8116	1.20%	0.153%
35	6.605	1641	1653	1661	rBV6	1454	2882	0.43%	0.054%
36	6.682	1662	1677	1699	rVV2	128807	259521	38.37%	4.890%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
 Data File : VU059381.D
 Acq On : 20 Jun 2024 15:32
 Operator : MD/SY
 Sample : P2960-15
 Misc : 6.02g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHB52

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\SFAMULM052924WMA.M
 Title : VOC Analysis

37	6.840	1723	1726	1732	rBV2	276	334	0.05%	0.006%
38	6.949	1751	1760	1765	rVB2	295	536	0.08%	0.010%
39	6.988	1765	1772	1775	rBV2	341	490	0.07%	0.009%
40	7.058	1787	1794	1799	rBV2	207	301	0.04%	0.006%
41	7.123	1811	1814	1822	rVB2	324	345	0.05%	0.007%
42	7.197	1822	1837	1843	rBV5	1932	3701	0.55%	0.070%
43	7.560	1938	1950	1976	rVV	63852	115754	17.11%	2.181%
44	7.721	1986	2000	2008	rBV4	1068	2634	0.39%	0.050%
45	7.891	2041	2053	2073	rBV	239907	423373	62.60%	7.978%
46	8.052	2100	2103	2106	rBV	365	265	0.04%	0.005%
47	8.177	2131	2142	2165	rVB	42381	76875	11.37%	1.449%
48	8.261	2165	2168	2171	rVB2	370	249	0.04%	0.005%
49	8.287	2171	2176	2180	rBV2	212	249	0.04%	0.005%
50	8.547	2248	2257	2268	rVB4	5649	9134	1.35%	0.172%
51	8.640	2273	2286	2320	rBV3	145118	335076	49.54%	6.314%
52	9.151	2442	2445	2449	rBV	306	337	0.05%	0.006%
53	9.360	2506	2510	2513	rBV2	335	292	0.04%	0.006%
54	9.412	2514	2526	2561	rVV	381977	676361	100.00%	12.745%
55	9.614	2585	2589	2593	rBV3	280	278	0.04%	0.005%
56	9.698	2609	2615	2622	rBV4	916	1220	0.18%	0.023%
57	10.016	2708	2714	2718	rBV3	987	1117	0.17%	0.021%
58	10.116	2738	2745	2750	rBV4	1199	1368	0.20%	0.026%
59	10.164	2757	2760	2764	rVB3	494	330	0.05%	0.006%
60	10.248	2777	2786	2798	rVB5	4550	6996	1.03%	0.132%
61	10.309	2798	2805	2807	rBV2	522	594	0.09%	0.011%
62	10.348	2813	2817	2821	rBV3	1477	1146	0.17%	0.022%
63	10.389	2826	2830	2838	rVB4	2276	3165	0.47%	0.060%
64	10.454	2847	2850	2852	rBV	486	319	0.05%	0.006%
65	10.560	2876	2883	2890	rBV5	2305	3792	0.56%	0.071%
66	10.618	2897	2901	2908	rBV6	2379	2750	0.41%	0.052%
67	10.753	2930	2943	2962	rBV	224504	367896	54.39%	6.932%
68	10.952	3000	3005	3008	rBV2	459	391	0.06%	0.007%
69	11.007	3019	3022	3026	rBV2	457	328	0.05%	0.006%
70	11.065	3031	3040	3046	rBV5	3127	4624	0.68%	0.087%
71	11.113	3049	3055	3058	rBV3	1260	1346	0.20%	0.025%
72	11.306	3112	3115	3116	rBV2	452	262	0.04%	0.005%
73	11.373	3131	3136	3140	rBV4	778	906	0.13%	0.017%
74	11.412	3141	3148	3156	rVB7	5766	8719	1.29%	0.164%
75	11.447	3156	3159	3161	rBV3	794	504	0.07%	0.009%
76	11.466	3161	3165	3166	rBV3	1575	1113	0.16%	0.021%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
 Data File : VU059381.D
 Acq On : 20 Jun 2024 15:32
 Operator : MD/SY
 Sample : P2960-15
 Misc : 6.02g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHB52

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\SFAMULM052924WMA.M
 Title : VOC Analysis

77	11.566	3190	3196	3199	rBV3	485	604	0.09%	0.011%
78	11.595	3200	3205	3206	rBV2	444	358	0.05%	0.007%
79	11.630	3213	3216	3222	rBV5	1007	1164	0.17%	0.022%
80	11.708	3232	3240	3248	rBV7	2627	4015	0.59%	0.076%
81	11.753	3248	3254	3260	rVB4	1115	1409	0.21%	0.027%
82	11.811	3260	3272	3296	rBV	403489	660083	97.59%	12.438%
83	11.955	3315	3317	3321	rVB2	421	248	0.04%	0.005%
84	12.003	3327	3332	3337	rVB4	828	656	0.10%	0.012%
85	12.190	3378	3390	3413	rBV	261039	435961	64.46%	8.215%
86	12.360	3440	3443	3448	rVB3	798	657	0.10%	0.012%
87	12.537	3493	3498	3504	rBV	459	339	0.05%	0.006%
88	12.659	3532	3536	3542	rBV3	308	368	0.05%	0.007%
89	12.749	3561	3564	3570	rVB2	270	284	0.04%	0.005%
90	13.798	3887	3890	3895	rVB2	367	256	0.04%	0.005%
91	13.839	3901	3903	3906	rBV2	372	251	0.04%	0.005%
92	13.855	3906	3908	3912	rVB2	390	285	0.04%	0.005%
93	14.450	4091	4093	4098	rVB3	471	395	0.06%	0.007%
94	14.643	4142	4153	4156	rBV3	565	1130	0.17%	0.021%
95	14.772	4185	4193	4201	rBV3	469	891	0.13%	0.017%
96	14.810	4201	4205	4206	rBV2	362	279	0.04%	0.005%
97	15.402	4384	4389	4398	rVB5	975	1354	0.20%	0.026%
98	15.508	4419	4422	4424	rBV2	513	374	0.06%	0.007%
99	15.685	4474	4477	4480	rBV2	362	308	0.05%	0.006%
100	16.286	4659	4664	4678	rVB8	2260	4374	0.65%	0.082%

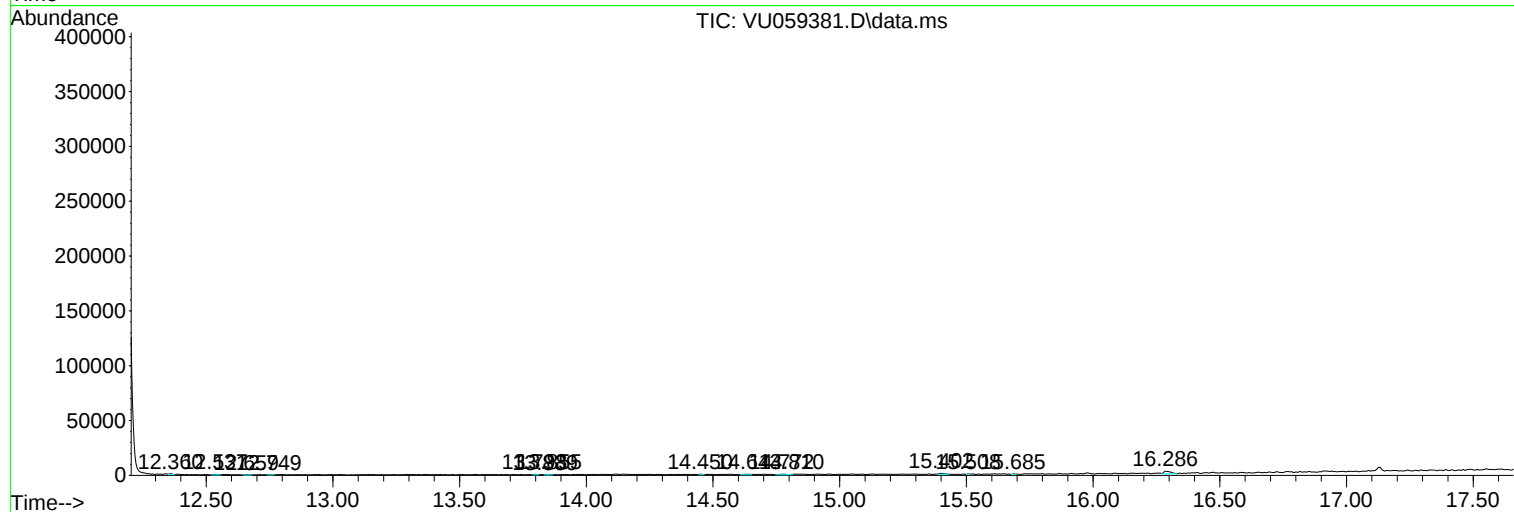
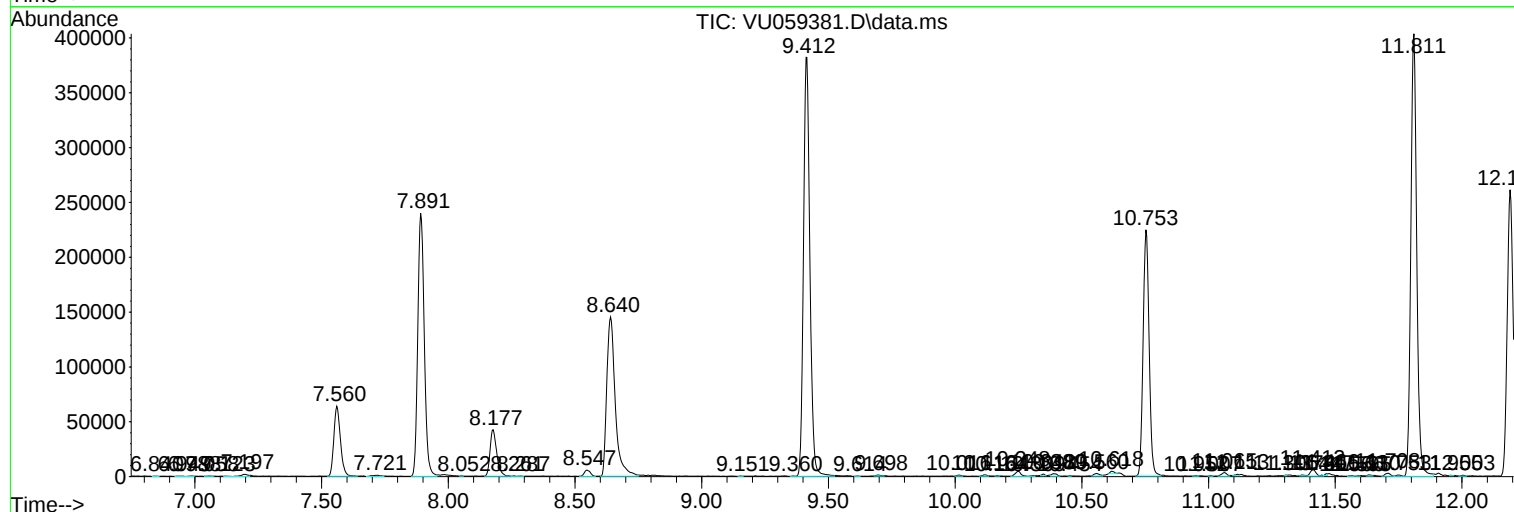
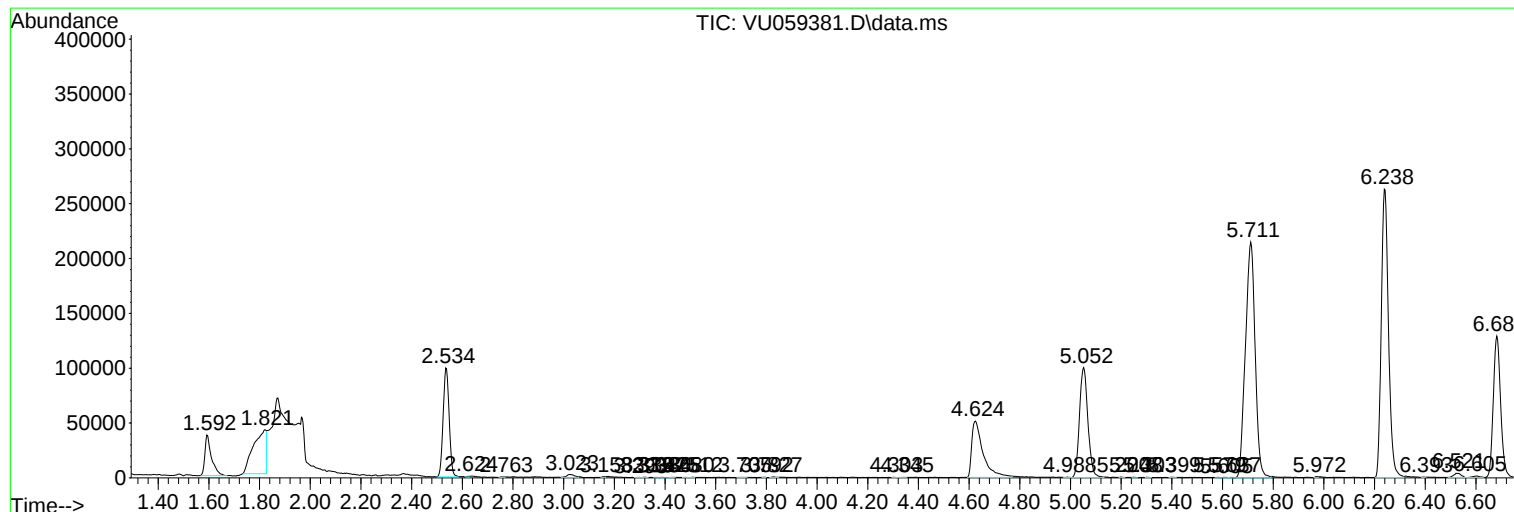
Sum of corrected areas: 5306901

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
Data File : VU059381.D
Acq On : 20 Jun 2024 15:32
Operator : MD/SY
Sample : P2960-15
Misc : 6.02g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHB52

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
Data File : VU059381.D
Acq On : 20 Jun 2024 15:32
Operator : MD/SY
Sample : P2960-15
Misc : 6.02g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHB52

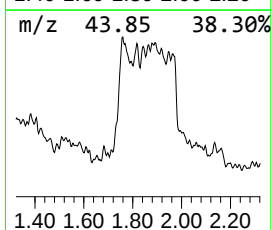
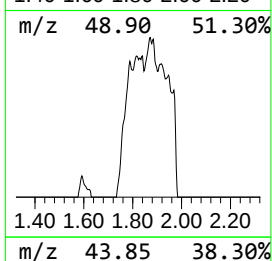
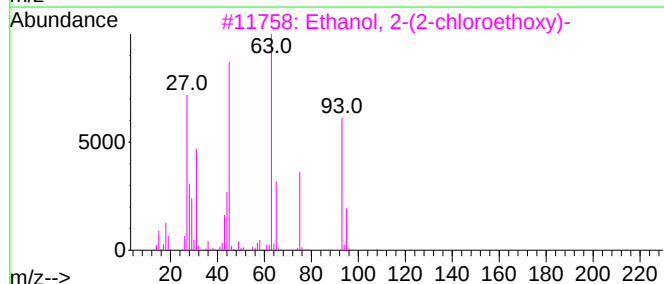
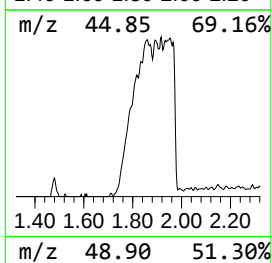
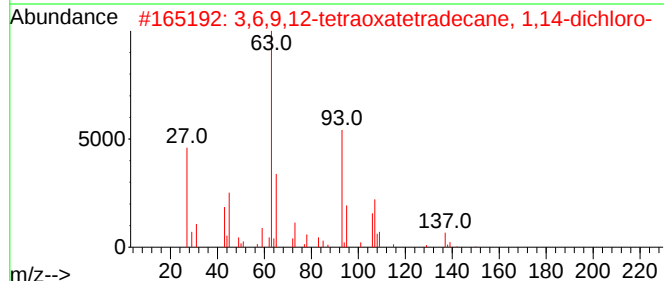
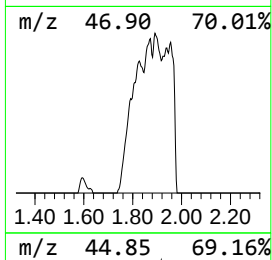
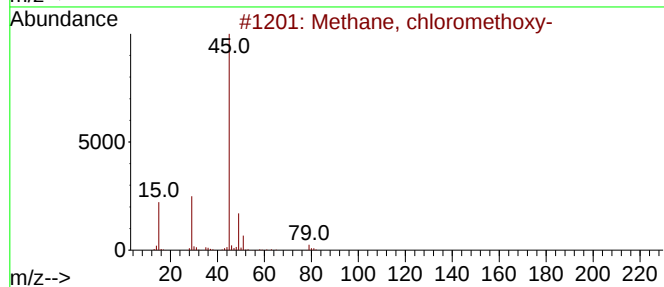
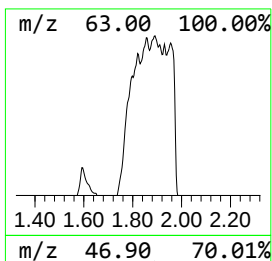
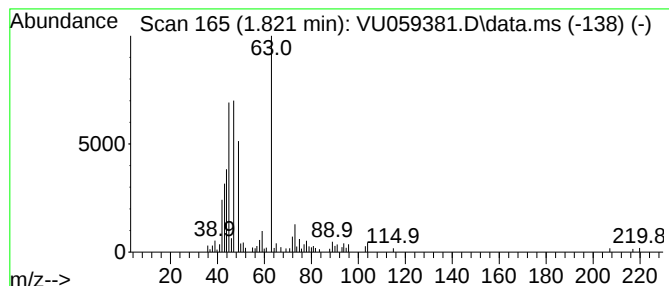
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.821	13.47 ug/L	140303	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methane, chloromethoxy-	80	C2H5ClO	000107-30-2	9
2			3,6,9,12-tetraoxatetradecane, 1,...	274	C10H20Cl2O4	1000401-80-9	9
3			Ethanol, 2-(2-chloroethoxy)-	124	C4H9ClO2	000628-89-7	9
4			2-Propanol, 1-chloro-3-fluoro-	112	C3H6ClFO	189937-18-6	9
5			Methane, chloromethoxy-	80	C2H5ClO	000107-30-2	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
Data File : VU059381.D
Acq On : 20 Jun 2024 15:32
Operator : MD/SY
Sample : P2960-15
Misc : 6.02g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHB52

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.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
unknown-01	1.821	13.5	ug/L	140303	1	6.242	520930	50.0