

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011521\
 Data File : VV020027.D
 Acq On : 15 Jan 2021 16:22
 Operator : SY/MD
 Sample : M1147-12
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BG4Y6

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\SOMVLM011121WMA.M

Title : VOC Analysis

Signal : TIC: VV020027.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.110	3	6	19	rVB	85801	73249	4.78%	0.532%
2	1.309	59	68	80	rBV	241358	270932	17.69%	1.968%
3	1.570	141	149	159	rBV	203279	227607	14.86%	1.653%
4	1.766	205	210	217	rVB	11815	13345	0.87%	0.097%
5	2.110	305	317	338	rBV	405917	620948	40.55%	4.510%
6	2.296	366	375	384	rBV	3469	6309	0.41%	0.046%
7	2.441	417	420	423	rBV5	1291	1137	0.07%	0.008%
8	2.534	431	449	469	rVB2	47304	96988	6.33%	0.704%
9	2.766	504	521	544	rBV2	76731	160319	10.47%	1.164%
10	2.955	574	580	588	rVB10	2837	4546	0.30%	0.033%
11	3.045	594	608	629	rBV	261282	520261	33.97%	3.778%
12	3.235	663	667	671	rVB5	853	901	0.06%	0.007%
13	3.441	724	731	732	rBV3	884	891	0.06%	0.006%
14	3.467	736	739	744	rVV4	1497	1400	0.09%	0.010%
15	3.499	744	749	753	rVB4	869	944	0.06%	0.007%
16	3.769	813	833	855	rBV2	134711	344900	22.52%	2.505%
17	3.891	860	871	913	rBV	115235	341489	22.30%	2.480%
18	4.283	989	993	998	rBV5	596	840	0.05%	0.006%
19	4.354	998	1015	1046	rVV	256295	632567	41.31%	4.594%
20	4.634	1095	1102	1105	rBV7	1041	1416	0.09%	0.010%
21	4.659	1105	1110	1111	rBV3	1812	1209	0.08%	0.009%
22	4.907	1178	1187	1189	rBV8	2462	3238	0.21%	0.024%
23	5.052	1214	1232	1257	rBV2	592130	1531399	100.00%	11.122%
24	5.238	1281	1290	1305	rVB4	17833	42720	2.79%	0.310%
25	5.621	1395	1409	1436	rBV	455378	924697	60.38%	6.716%
26	5.913	1488	1500	1513	rBV2	23748	49516	3.23%	0.360%
27	6.074	1534	1550	1576	rBV	346879	711511	46.46%	5.167%
28	6.203	1585	1590	1600	rVV	3849	6752	0.44%	0.049%
29	6.267	1601	1610	1618	rVB8	7710	15081	0.98%	0.110%
30	6.447	1662	1666	1668	rBV4	1089	1008	0.07%	0.007%
31	6.466	1668	1672	1686	rVB8	3683	6439	0.42%	0.047%
32	6.659	1715	1732	1745	rBV2	24078	50642	3.31%	0.368%
33	6.782	1758	1770	1781	rBV4	22232	45260	2.96%	0.329%
34	6.849	1781	1791	1799	rVB6	6261	12209	0.80%	0.089%
35	6.923	1811	1814	1816	rBV4	1368	827	0.05%	0.006%
36	6.991	1821	1835	1857	rVV	183652	341853	22.32%	2.483%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011521\
 Data File : VV020027.D
 Acq On : 15 Jan 2021 16:22
 Operator : SY/MD
 Sample : M1147-12
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BG4Y6

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\SOMVLM011121WMA.M
 Title : VOC Analysis

37	7.267	1909	1921	1927	rBV3	15754	28831	1.88%	0.209%
38	7.322	1927	1938	1959	rVB	671808	1154847	75.41%	8.387%
39	7.489	1985	1990	1991	rBV5	1767	1636	0.11%	0.012%
40	7.627	2022	2033	2059	rBV	126700	234463	15.31%	1.703%
41	7.849	2097	2102	2106	rBV6	1325	1478	0.10%	0.011%
42	7.987	2135	2145	2152	rVB6	5690	9728	0.64%	0.071%
43	8.036	2157	2160	2163	rBV4	1191	932	0.06%	0.007%
44	8.093	2168	2178	2209	rBV2	382299	764321	49.91%	5.551%
45	8.360	2253	2261	2268	rBV9	5010	8319	0.54%	0.060%
46	8.486	2295	2300	2301	rBV3	1771	1386	0.09%	0.010%
47	8.579	2321	2329	2330	rBV5	3251	3821	0.25%	0.028%
48	8.672	2352	2358	2368	rVB8	6829	10987	0.72%	0.080%
49	8.714	2368	2371	2381	rVB7	1860	2644	0.17%	0.019%
50	8.798	2386	2397	2404	rBV6	7400	14009	0.91%	0.102%
51	8.859	2404	2416	2436	rBV	707680	1154614	75.40%	8.386%
52	9.199	2520	2522	2524	rBV3	1617	1046	0.07%	0.008%
53	9.373	2572	2576	2583	rVB5	924	841	0.05%	0.006%
54	9.418	2583	2590	2593	rBV9	1505	1702	0.11%	0.012%
55	9.482	2603	2610	2617	rVB8	6680	10448	0.68%	0.076%
56	9.679	2667	2671	2676	rBV7	2994	3721	0.24%	0.027%
57	10.023	2774	2778	2781	rBV5	1299	1289	0.08%	0.009%
58	10.135	2807	2813	2821	rVB8	5762	8373	0.55%	0.061%
59	10.222	2826	2840	2859	rBV	449124	712360	46.52%	5.174%
60	10.585	2947	2953	2957	rBV6	2221	2696	0.18%	0.020%
61	10.884	3042	3046	3048	rBV4	1055	939	0.06%	0.007%
62	11.158	3125	3131	3132	rVV5	2344	1904	0.12%	0.014%
63	11.199	3139	3144	3146	rBV5	1919	1569	0.10%	0.011%
64	11.257	3150	3162	3180	rBV	765488	1180816	77.11%	8.576%
65	11.473	3227	3229	3237	rVB6	1348	1298	0.08%	0.009%
66	11.556	3247	3255	3257	rBV5	6781	8067	0.53%	0.059%
67	11.630	3268	3278	3298	rVB	745482	1180259	77.07%	8.572%
68	11.826	3333	3339	3348	rVB5	6244	9640	0.63%	0.070%
69	11.923	3361	3369	3373	rBV5	5749	8444	0.55%	0.061%
70	12.026	3393	3401	3419	rVB	9512	18531	1.21%	0.135%
71	12.125	3427	3432	3433	rBV3	2516	1897	0.12%	0.014%
72	12.254	3462	3472	3474	rBV3	3897	5081	0.33%	0.037%
73	12.312	3487	3490	3496	rVB6	954	835	0.05%	0.006%
74	12.357	3499	3504	3509	rBV7	2690	3416	0.22%	0.025%
75	12.421	3517	3524	3531	rVB4	5218	7944	0.52%	0.058%
76	12.476	3534	3541	3553	rVB2	12101	17985	1.17%	0.131%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011521\
 Data File : VV020027.D
 Acq On : 15 Jan 2021 16:22
 Operator : SY/MD
 Sample : M1147-12
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BG4Y6

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\SOMVLM011121WMA.M

Title : VOC Analysis

77	12.559	3557	3567	3573	rBV3	9429	14531	0.95%	0.106%
78	12.624	3585	3587	3590	rVB3	1430	869	0.06%	0.006%
79	12.682	3596	3605	3613	rBV3	6673	12491	0.82%	0.091%
80	12.736	3615	3622	3631	rVB3	9840	14141	0.92%	0.103%
81	12.804	3637	3643	3649	rBV6	3347	4086	0.27%	0.030%
82	12.858	3653	3660	3665	rBV7	4242	6732	0.44%	0.049%
83	13.016	3701	3709	3713	rBV7	3079	3793	0.25%	0.028%
84	13.180	3750	3760	3767	rBV8	3681	6134	0.40%	0.045%
85	13.219	3767	3772	3773	rBV5	5743	4115	0.27%	0.030%
86	13.280	3783	3791	3798	rBV8	9567	14954	0.98%	0.109%
87	13.469	3846	3850	3857	rBV6	2834	3199	0.21%	0.023%
88	13.730	3921	3931	3936	rBV6	3663	6165	0.40%	0.045%
89	13.826	3953	3961	3963	rBV6	2182	2726	0.18%	0.020%
90	13.910	3983	3987	3988	rBV3	2369	1377	0.09%	0.010%
91	13.974	4005	4007	4011	rBV3	1390	1125	0.07%	0.008%
92	14.103	4037	4047	4050	rBV8	5284	8174	0.53%	0.059%
93	14.151	4058	4062	4066	rVB5	1037	916	0.06%	0.007%
94	14.244	4084	4091	4097	rBV5	2376	3747	0.24%	0.027%
95	14.315	4104	4113	4122	rVB9	3430	6783	0.44%	0.049%
96	14.428	4142	4148	4151	rBV6	811	845	0.06%	0.006%
97	14.887	4285	4291	4292	rVV2	1100	852	0.06%	0.006%
98	15.347	4431	4434	4436	rBV3	1503	939	0.06%	0.007%
99	15.575	4500	4505	4510	rBV5	1053	1049	0.07%	0.008%
100	16.215	4702	4704	4710	rBV5	1090	907	0.06%	0.007%

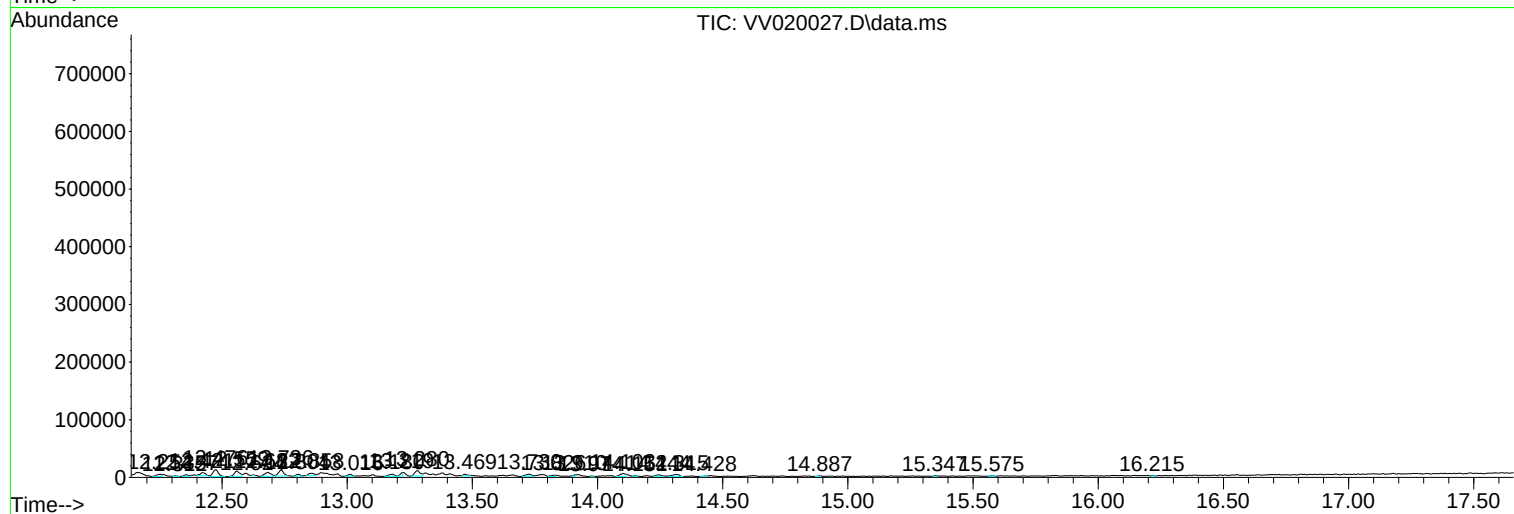
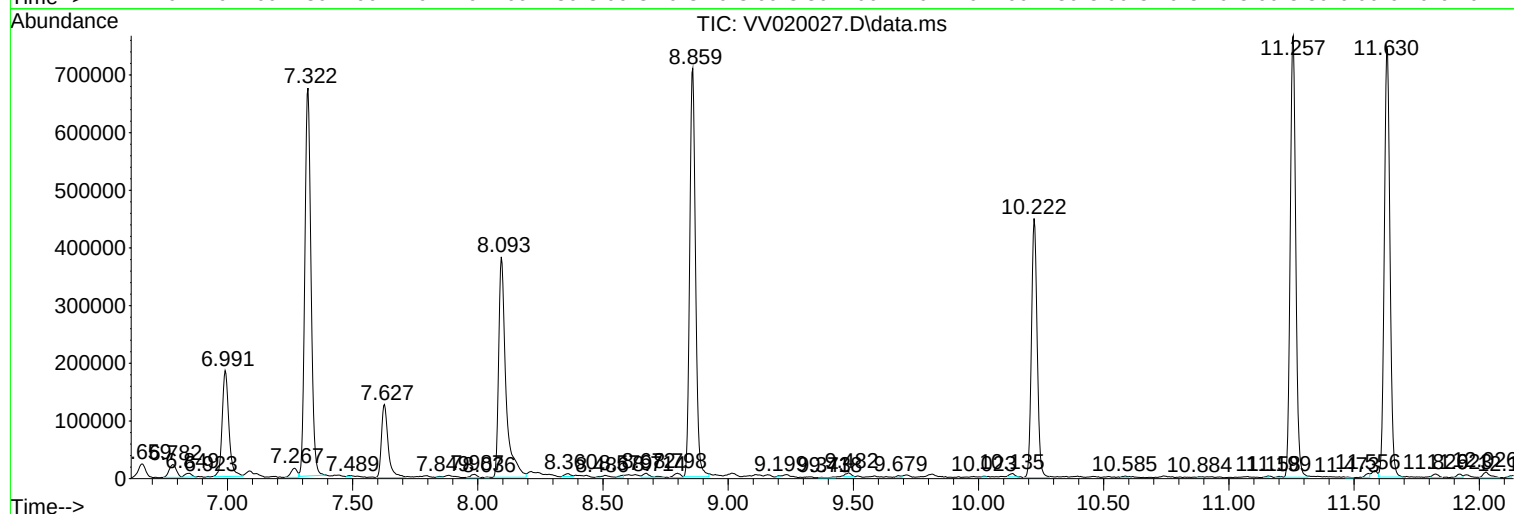
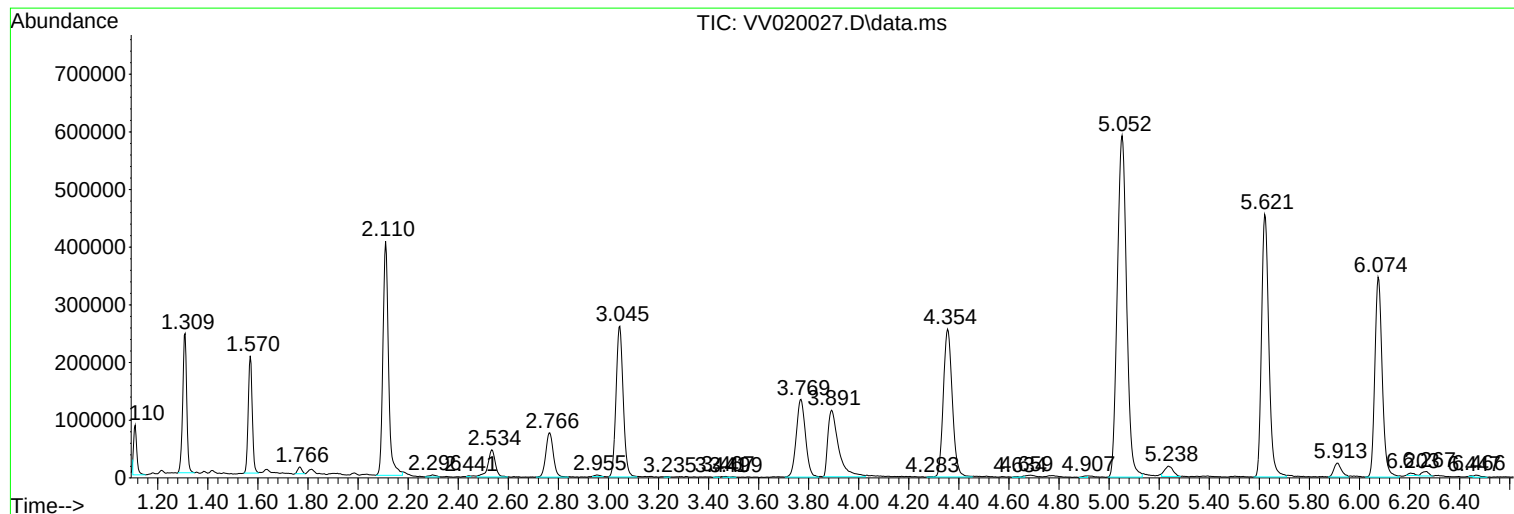
Sum of corrected areas: 13769117

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011521\
Data File : VV020027.D
Acq On : 15 Jan 2021 16:22
Operator : SY/MD
Sample : M1147-12
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BG4Y6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM011121WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011521\
Data File : VV020027.D
Acq On : 15 Jan 2021 16:22
Operator : SY/MD
Sample : M1147-12
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BG4Y6

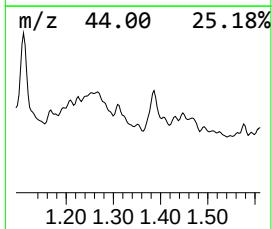
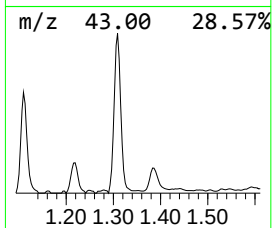
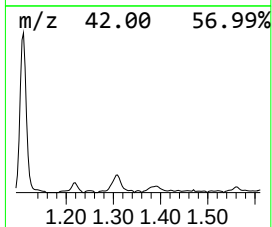
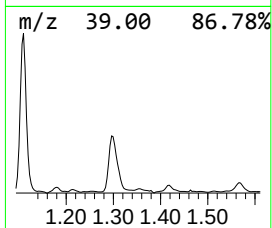
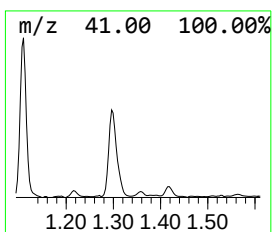
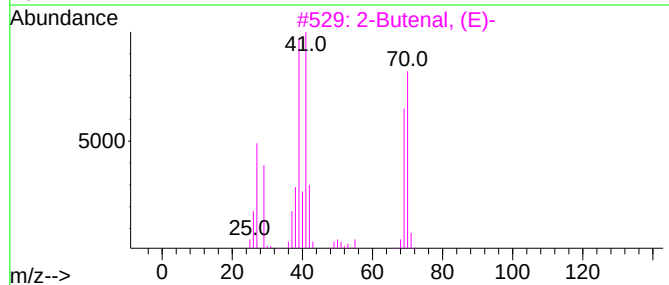
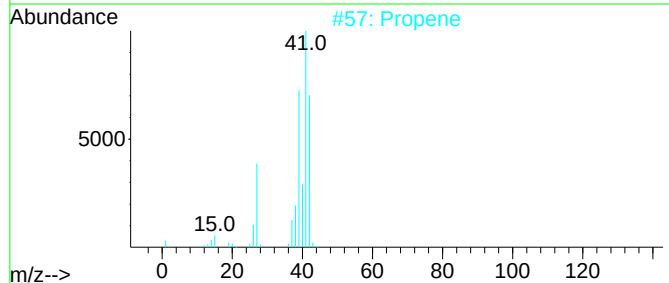
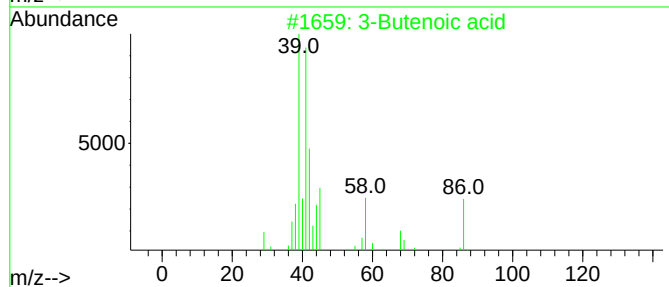
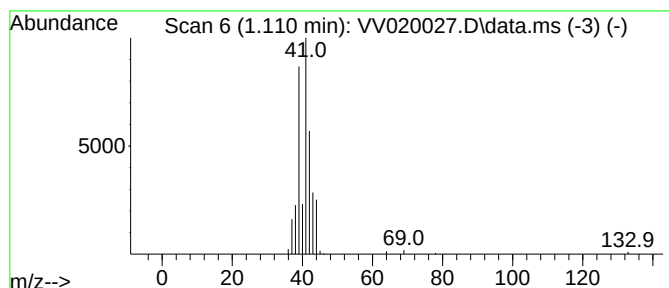
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM011121WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Butenoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.110	3.96 ug/L	73249	1,4-Difluorobenzene	5.621

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Butenoic acid	86	C4H6O2	000625-38-7	83
2			Propene	42	C3H6	000115-07-1	83
3			2-Butenal, (E)-	70	C4H6O	000123-73-9	78
4			Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	74
5			Cyclopropanecarboxylic acid	86	C4H6O2	001759-53-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011521\
Data File : VV020027.D
Acq On : 15 Jan 2021 16:22
Operator : SY/MD
Sample : M1147-12
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BG4Y6

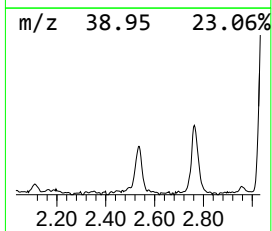
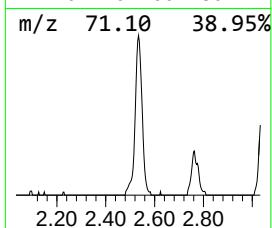
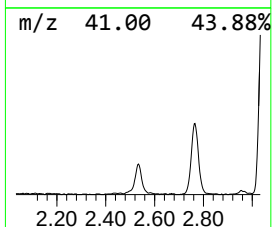
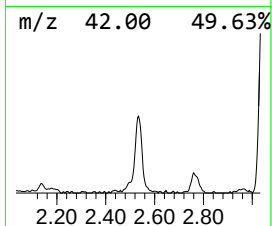
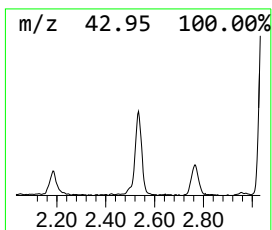
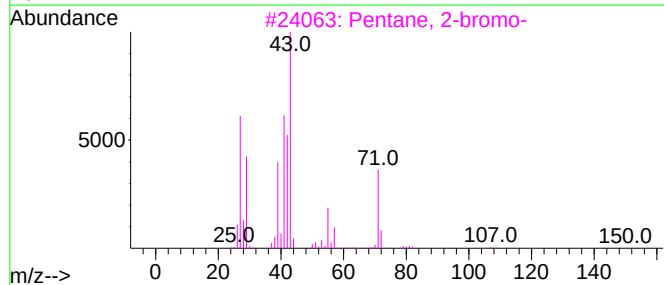
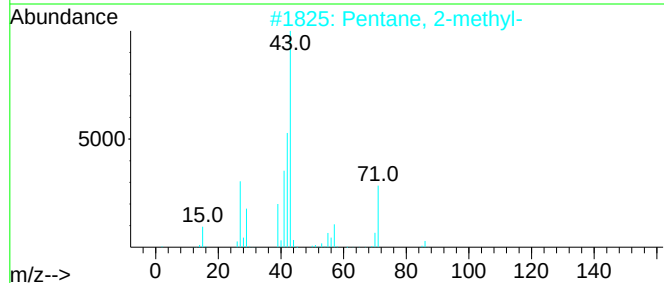
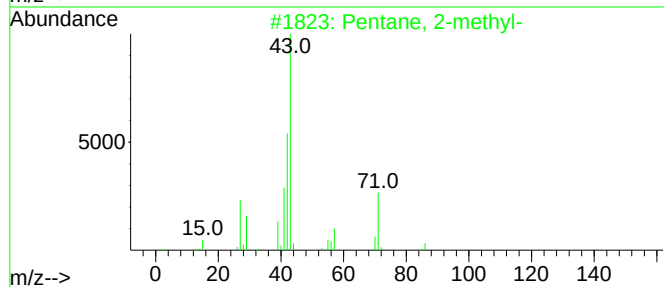
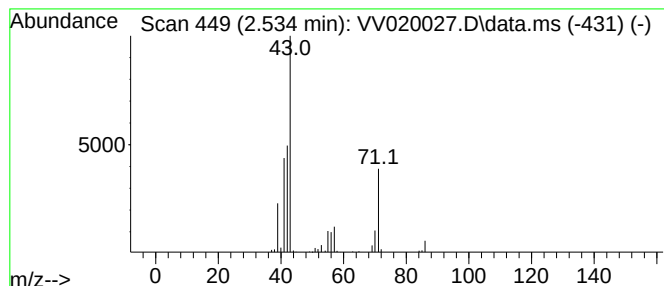
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM011121WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.534	5.24 ug/L	96988	1,4-Difluorobenzene	5.621

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	90
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	86
3	Pentane, 2-bromo-	150	C5H11Br	000107-81-3	59
4	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	58
5	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011521\
Data File : VV020027.D
Acq On : 15 Jan 2021 16:22
Operator : SY/MD
Sample : M1147-12
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BG4Y6

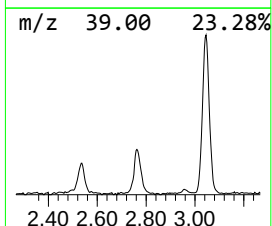
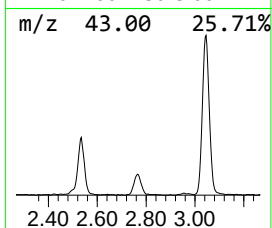
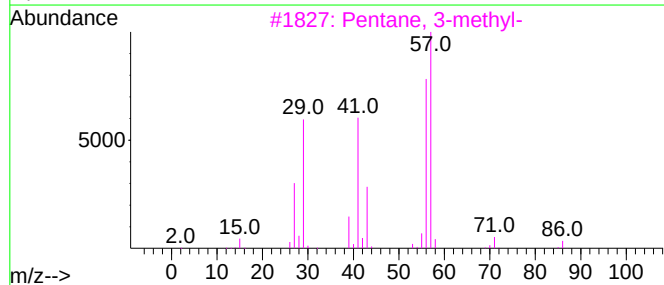
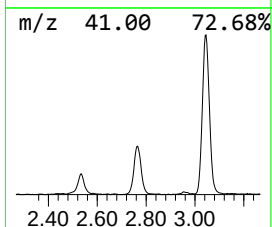
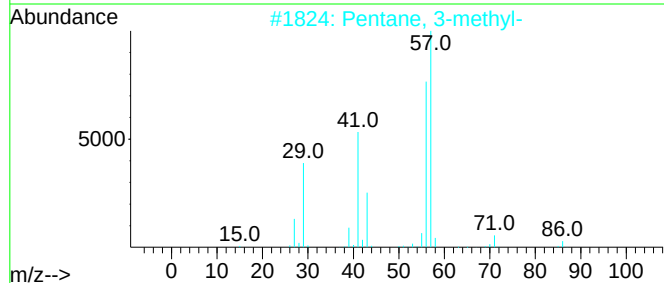
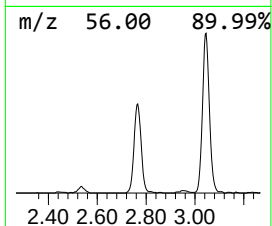
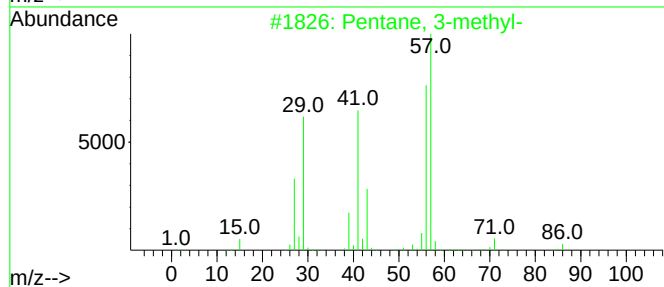
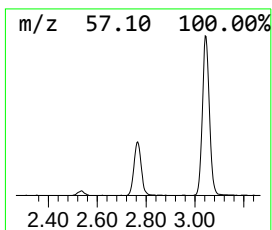
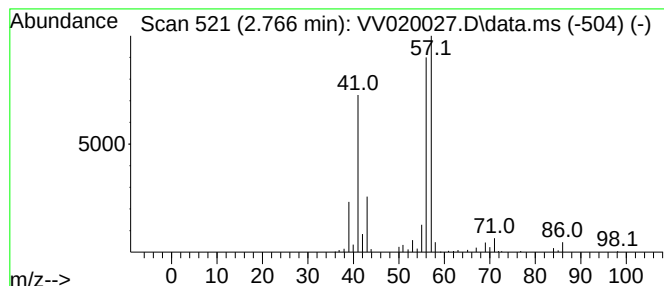
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM011121WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.766	8.67 ug/L	160319	1,4-Difluorobenzene	5.621

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentane, 3-methyl-	86	C6H14	000096-14-0	86
2		Pentane, 3-methyl-	86	C6H14	000096-14-0	80
3		Pentane, 3-methyl-	86	C6H14	000096-14-0	80
4		Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	72
5		Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011521\
Data File : VV020027.D
Acq On : 15 Jan 2021 16:22
Operator : SY/MD
Sample : M1147-12
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BG4Y6

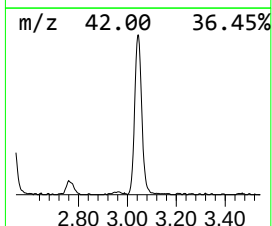
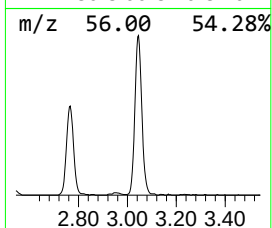
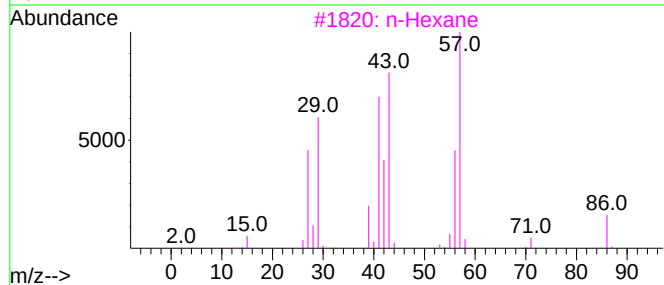
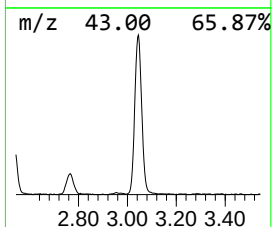
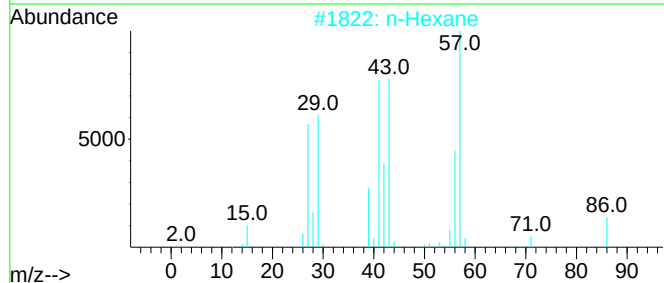
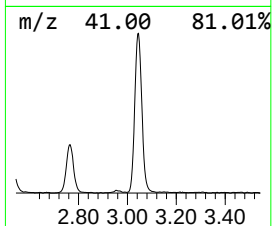
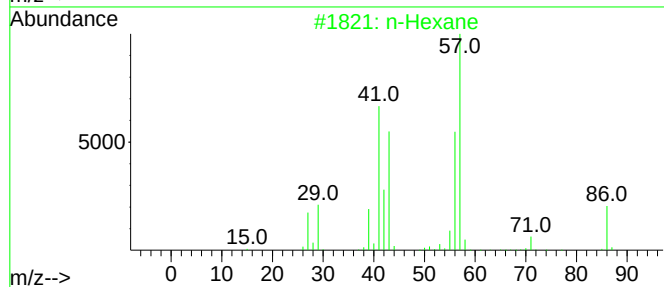
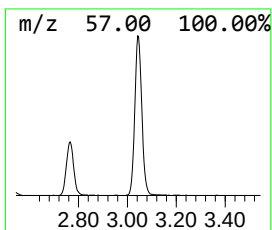
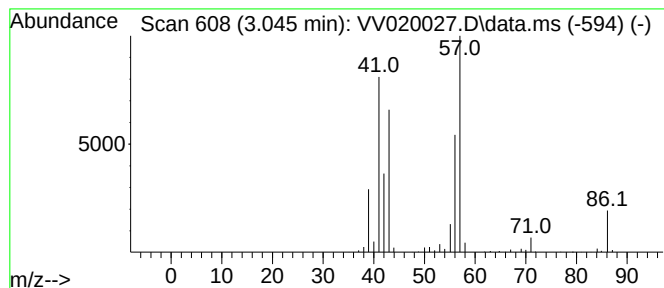
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM011121WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.045	28.13 ug/L	520261	1,4-Difluorobenzene	5.621

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexane	86	C6H14	000110-54-3	87
2		n-Hexane	86	C6H14	000110-54-3	72
3		n-Hexane	86	C6H14	000110-54-3	72
4		Furan, tetrahydro-3-methyl-	86	C5H10O	013423-15-9	53
5		Butanal, 2-methyl-	86	C5H10O	000096-17-3	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011521\
Data File : VV020027.D
Acq On : 15 Jan 2021 16:22
Operator : SY/MD
Sample : M1147-12
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BG4Y6

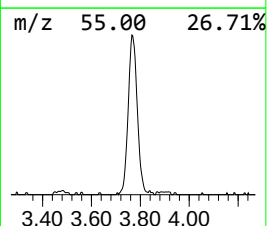
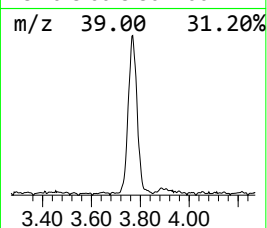
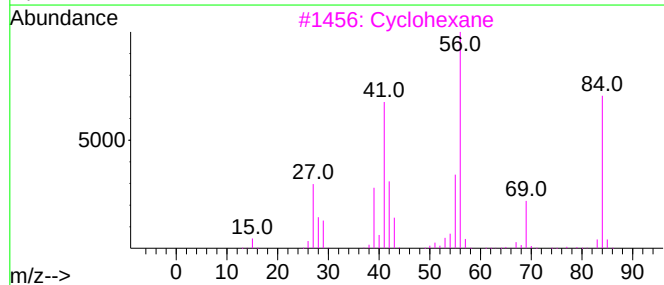
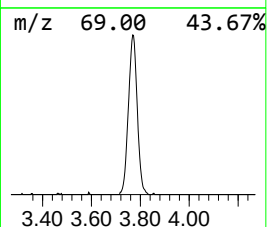
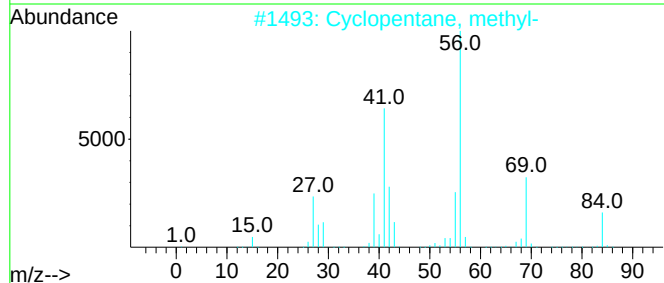
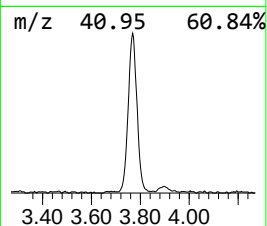
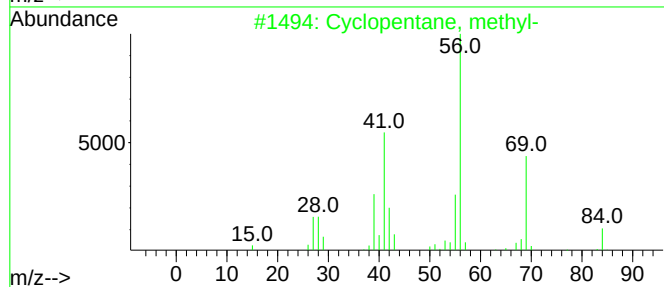
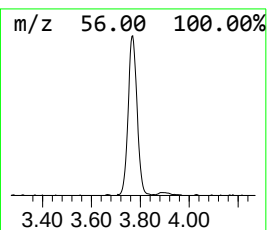
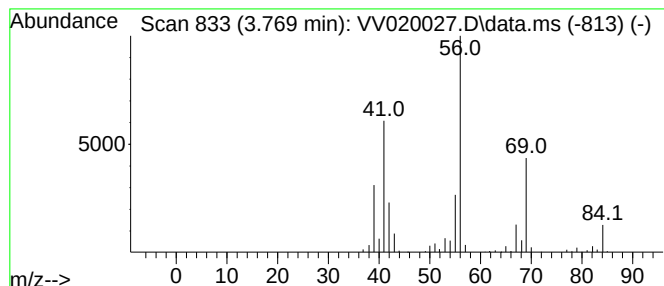
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM011121WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 (DEL) Alkane: Cyclic3.769 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.769	18.65 ug/L	344900	1,4-Difluorobenzene	5.621

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2			Cyclopentane, methyl-	84	C6H12	000096-37-7	87
3			Cyclohexane	84	C6H12	000110-82-7	86
4			Cyclohexane	84	C6H12	000110-82-7	86
5			Cyclohexane	84	C6H12	000110-82-7	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011521\
Data File : VV020027.D
Acq On : 15 Jan 2021 16:22
Operator : SY/MD
Sample : M1147-12
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BG4Y6

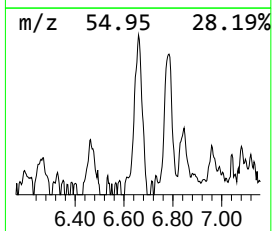
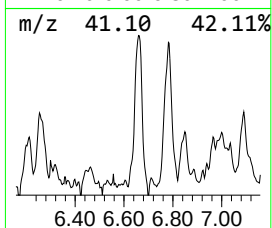
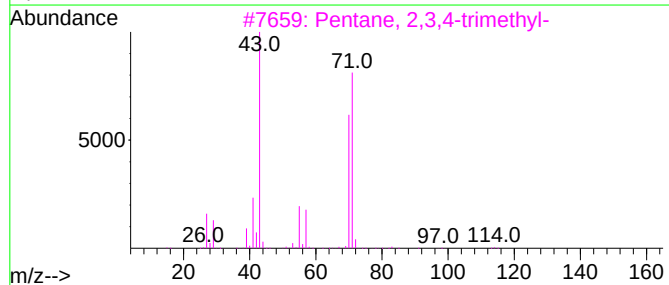
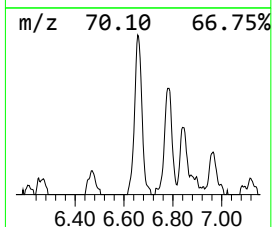
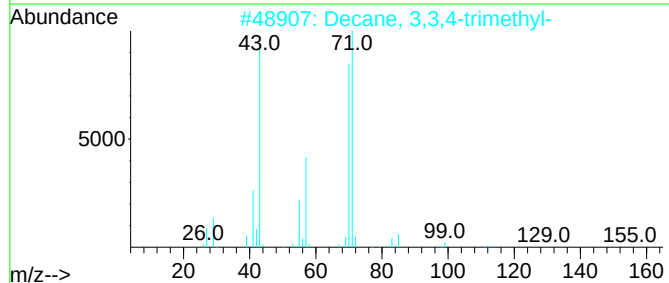
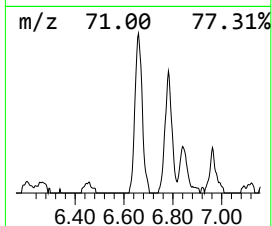
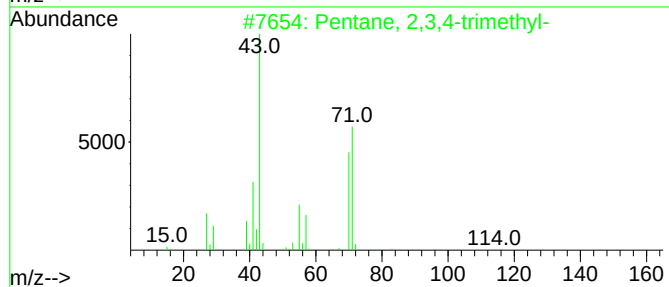
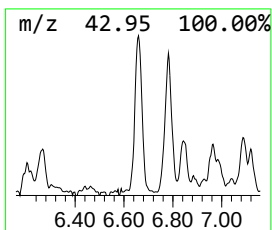
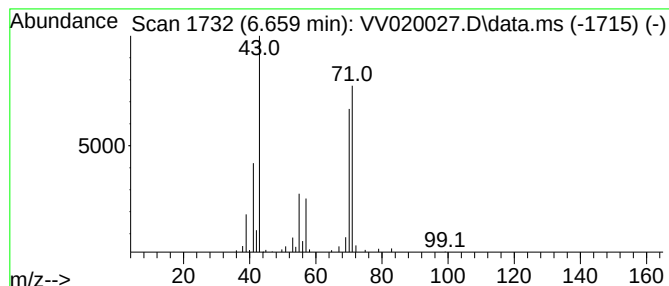
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM011121WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.659	2.74 ug/L	50642	1,4-Difluorobenzene	5.621

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	86
2		Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	72
3		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	64
4		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	64
5		Pentane, 3-ethyl-	100	C7H16	000617-78-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011521\
Data File : VV020027.D
Acq On : 15 Jan 2021 16:22
Operator : SY/MD
Sample : M1147-12
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BG4Y6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM011121WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Butenoic acid	1.110	4.0	ug/L	73249	1	5.621	924697	50.0
(DEL) Alkane: S...	2.534	5.2	ug/L	96988	1	5.621	924697	50.0
(DEL) Alkane: S...	2.766	8.7	ug/L	160319	1	5.621	924697	50.0
(DEL) Alkane: S...	3.045	28.1	ug/L	520261	1	5.621	924697	50.0
(DEL) Alkane: C...	3.769	18.6	ug/L	344900	1	5.621	924697	50.0
(DEL) Alkane: S...	6.659	2.7	ug/L	50642	1	5.621	924697	50.0