

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050622\
 Data File : VU048462.D
 Acq On : 06 May 2022 18:05
 Operator : SY/MD
 Sample : N2638-09ME
 Misc : 4.94g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXL04ME

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\SFAMULM050622WMA.M
 Title : VOC Analysis

Signal : TIC: VU048462.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.478	35	43	71	rBV	203946	383737	15.44%	2.170%
2	1.597	73	80	86	rBV	114506	182426	7.34%	1.032%
3	2.527	356	369	384	rBV	420075	771241	31.02%	4.362%
4	2.813	455	458	461	rBV4	520	361	0.01%	0.002%
5	2.861	470	473	477	rVB2	673	575	0.02%	0.003%
6	2.954	491	502	516	rBV2	10444	24882	1.00%	0.141%
7	3.173	556	570	590	rBV	29269	76075	3.06%	0.430%
8	3.433	648	651	654	rVB2	587	404	0.02%	0.002%
9	3.517	671	677	679	rBV	407	348	0.01%	0.002%
10	3.552	679	688	690	rBV4	2050	2256	0.09%	0.013%
11	4.060	838	846	848	rBV2	1362	1451	0.06%	0.008%
12	4.639	1010	1026	1040	rBV	180027	568368	22.86%	3.215%
13	5.063	1141	1158	1186	rBV	419528	1067519	42.94%	6.038%
14	5.202	1190	1201	1233	rVB	55012	141390	5.69%	0.800%
15	5.452	1274	1279	1284	rVB4	532	543	0.02%	0.003%
16	5.485	1286	1289	1294	rVB2	393	358	0.01%	0.002%
17	5.716	1340	1361	1390	rBV2	989716	2486144	100.00%	14.062%
18	5.848	1400	1402	1406	rVB	1211	648	0.03%	0.004%
19	5.870	1406	1409	1411	rBV2	516	379	0.02%	0.002%
20	5.977	1431	1442	1463	rVV2	17867	46208	1.86%	0.261%
21	6.124	1485	1488	1489	rBV2	1041	603	0.02%	0.003%
22	6.166	1490	1501	1513	rVV3	20605	56996	2.29%	0.322%
23	6.247	1513	1526	1553	rVB	424315	903673	36.35%	5.111%
24	6.398	1561	1573	1602	rVB3	51343	123765	4.98%	0.700%
25	6.523	1603	1612	1620	rBV8	4319	8073	0.32%	0.046%
26	6.597	1627	1635	1637	rBV7	8405	10488	0.42%	0.059%
27	6.690	1649	1664	1683	rBV	525209	1130269	45.46%	6.393%
28	6.784	1684	1693	1725	rVB	35285	129239	5.20%	0.731%
29	6.932	1729	1739	1769	rVB2	36949	118316	4.76%	0.669%
30	7.189	1807	1819	1845	rBV3	91249	232581	9.36%	1.315%
31	7.337	1862	1865	1869	rVB3	1224	707	0.03%	0.004%
32	7.359	1870	1872	1875	rBV3	580	333	0.01%	0.002%
33	7.568	1923	1937	1962	rBV	269239	565553	22.75%	3.199%
34	7.674	1967	1970	1971	rVV2	794	464	0.02%	0.003%
35	7.694	1971	1976	1989	rVB6	2540	4564	0.18%	0.026%
36	7.790	1996	2006	2015	rBV7	3578	6669	0.27%	0.038%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Stop Thrs : 0

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
 Title : VOC Analysis

37	7.899	2024	2040	2056	rBV	1041112	1992997	80.16%	11.272%
38	8.185	2116	2129	2157	rBV3	209849	490430	19.73%	2.774%
39	8.311	2164	2168	2171	rVB2	756	519	0.02%	0.003%
40	8.353	2175	2181	2182	rBV4	1206	1085	0.04%	0.006%
41	8.546	2232	2241	2242	rBV5	3217	2715	0.11%	0.015%
42	8.658	2258	2276	2312	rBV	650831	1592772	64.07%	9.009%
43	8.922	2355	2358	2360	rBV	539	342	0.01%	0.002%
44	9.073	2402	2405	2410	rVV2	413	339	0.01%	0.002%
45	9.144	2424	2427	2432	rVV6	677	698	0.03%	0.004%
46	9.166	2432	2434	2439	rVB2	521	416	0.02%	0.002%
47	9.218	2447	2450	2456	rVB3	748	506	0.02%	0.003%
48	9.285	2466	2471	2475	rBV2	574	603	0.02%	0.003%
49	9.423	2499	2514	2545	rBV	543990	1099288	44.22%	6.218%
50	9.549	2549	2553	2554	rBV3	634	433	0.02%	0.002%
51	9.574	2555	2561	2565	rBV6	1877	2172	0.09%	0.012%
52	9.697	2590	2599	2609	rVB4	5421	9528	0.38%	0.054%
53	9.960	2677	2681	2688	rVV3	395	463	0.02%	0.003%
54	10.108	2716	2727	2729	rBV5	3772	4582	0.18%	0.026%
55	10.230	2760	2765	2766	rBV2	523	449	0.02%	0.003%
56	10.488	2839	2845	2850	rBV2	693	848	0.03%	0.005%
57	10.674	2893	2903	2912	rBV5	4064	6618	0.27%	0.037%
58	10.767	2917	2932	2952	rBV	680771	1120706	45.08%	6.339%
59	10.873	2960	2965	2968	rBV4	559	553	0.02%	0.003%
60	11.012	3004	3008	3012	rVB2	447	479	0.02%	0.003%
61	11.092	3029	3033	3035	rVV2	438	367	0.01%	0.002%
62	11.124	3035	3043	3059	rVB7	1773	3688	0.15%	0.021%
63	11.205	3064	3068	3074	rVB4	746	675	0.03%	0.004%
64	11.243	3074	3080	3082	rBV2	421	427	0.02%	0.002%
65	11.317	3092	3103	3108	rBV4	1071	2051	0.08%	0.012%
66	11.372	3113	3120	3123	rBV4	1122	1195	0.05%	0.007%
67	11.414	3127	3133	3135	rBV3	1529	1385	0.06%	0.008%
68	11.462	3140	3148	3150	rBV6	2696	3443	0.14%	0.019%
69	11.574	3177	3183	3191	rBV5	2016	3090	0.12%	0.017%
70	11.639	3196	3203	3209	rBV5	1279	1667	0.07%	0.009%
71	11.697	3215	3221	3227	rVB4	2494	3191	0.13%	0.018%
72	11.754	3228	3239	3243	rBV5	1467	2167	0.09%	0.012%
73	11.816	3245	3258	3272	rBV	534012	856635	34.46%	4.845%
74	11.925	3289	3292	3293	rBV3	629	374	0.02%	0.002%
75	11.947	3293	3299	3302	rBV5	1606	1991	0.08%	0.011%
76	12.034	3322	3326	3330	rBV4	411	349	0.01%	0.002%

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Instrument :
 MSVOA_U
 ClientSampleId :
 EXL04ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
 Title : VOC Analysis

77	12.076	3335	3339	3341	rBV2	714	426	0.02%	0.002%
78	12.198	3359	3377	3397	rBV	848285	1385230	55.72%	7.835%
79	12.327	3409	3417	3425	rBV8	2117	3188	0.13%	0.018%
80	12.410	3437	3443	3446	rVB5	729	831	0.03%	0.005%
81	12.549	3482	3486	3490	rVB2	576	419	0.02%	0.002%
82	12.629	3507	3511	3513	rBV4	962	862	0.03%	0.005%
83	12.844	3574	3578	3581	rBV3	547	362	0.01%	0.002%
84	13.018	3629	3632	3635	rVV	663	390	0.02%	0.002%
85	13.147	3667	3672	3676	rBV5	890	780	0.03%	0.004%
86	13.227	3690	3697	3705	rVB6	1063	1754	0.07%	0.010%
87	13.291	3712	3717	3720	rBV4	549	503	0.02%	0.003%
88	13.433	3754	3761	3770	rBV5	1839	2525	0.10%	0.014%
89	13.574	3801	3805	3806	rBV2	896	642	0.03%	0.004%
90	13.848	3883	3890	3900	rBV7	2339	3187	0.13%	0.018%
91	14.044	3948	3951	3954	rBV2	634	379	0.02%	0.002%
92	14.089	3958	3965	3978	rVV2	6138	10401	0.42%	0.059%
93	14.230	4004	4009	4014	rBV2	459	537	0.02%	0.003%
94	14.262	4014	4019	4020	rBV3	614	487	0.02%	0.003%
95	14.333	4035	4041	4049	rBV8	3199	4951	0.20%	0.028%
96	14.806	4182	4188	4191	rBV	421	517	0.02%	0.003%
97	14.822	4191	4193	4197	rVB2	726	456	0.02%	0.003%
98	15.401	4370	4373	4377	rBV4	874	534	0.02%	0.003%
99	15.536	4412	4415	4416	rBV2	626	377	0.02%	0.002%
100	15.806	4496	4499	4503	rVB4	930	621	0.02%	0.004%

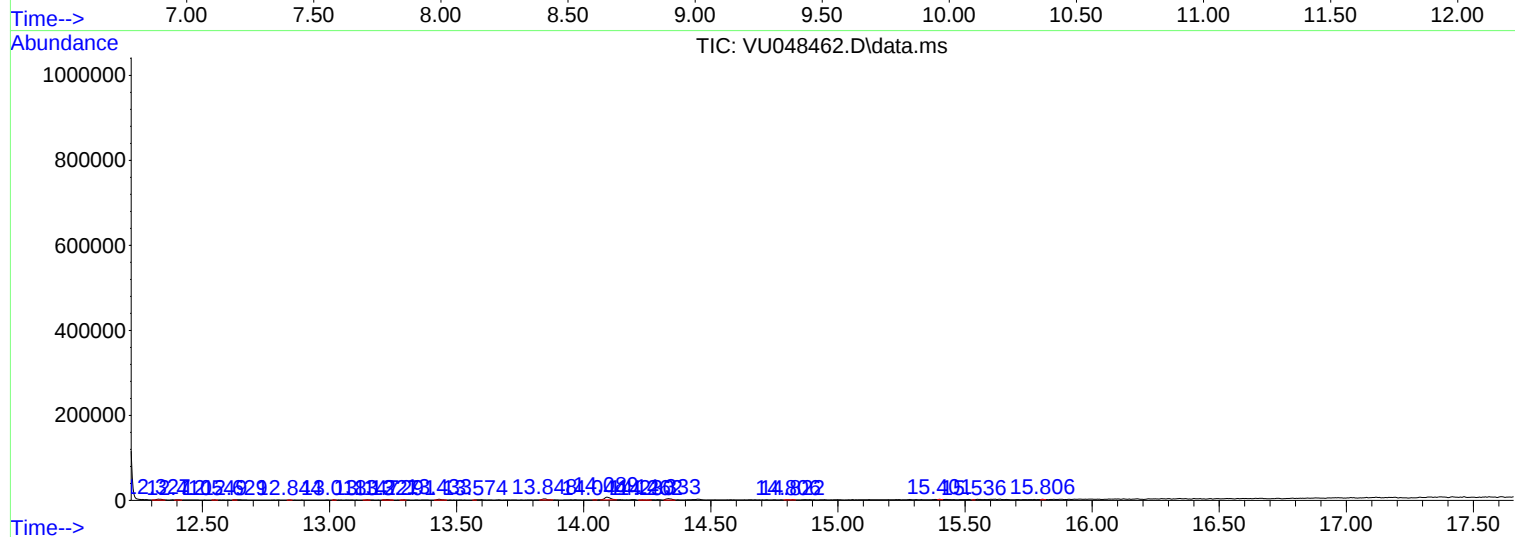
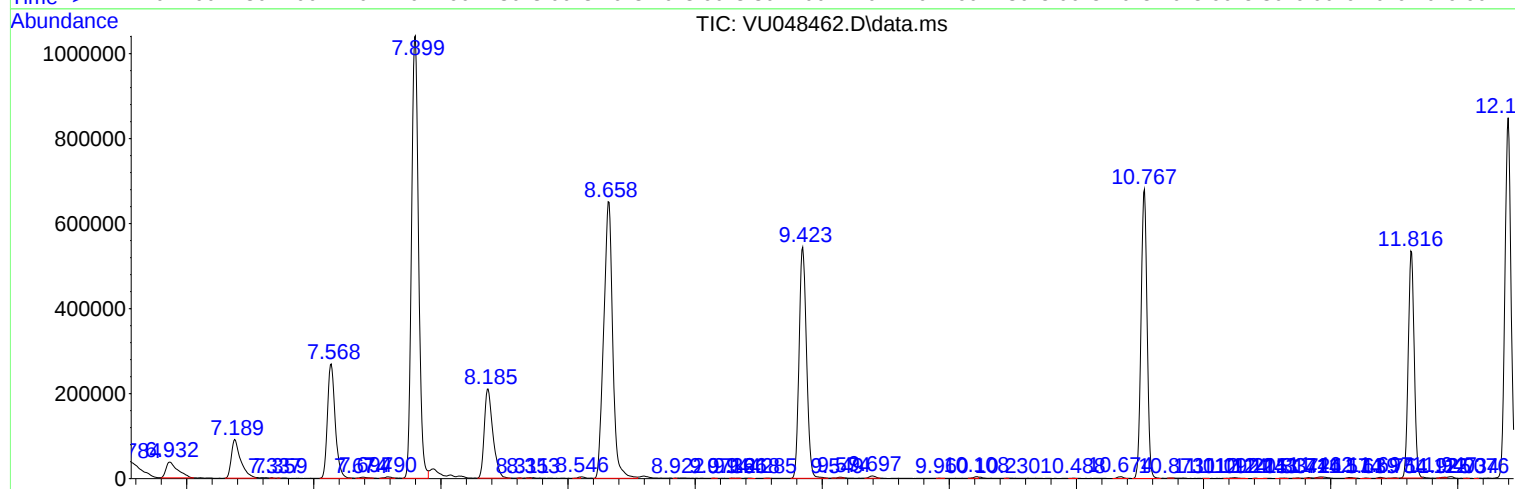
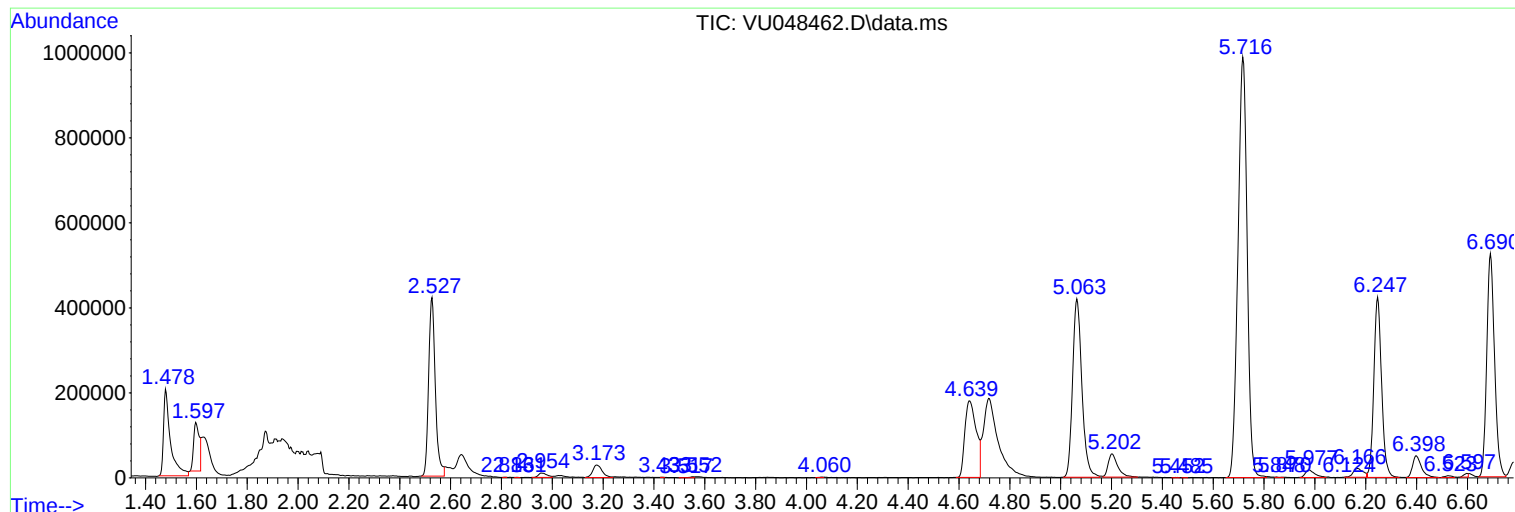
Sum of corrected areas: 17680201

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Instrument :
MSVOA_U
ClientSampleId :
EXL04ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050622\
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ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL04ME

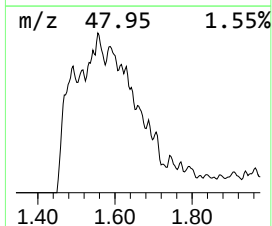
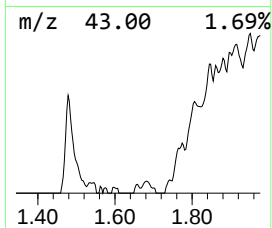
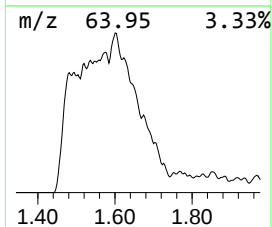
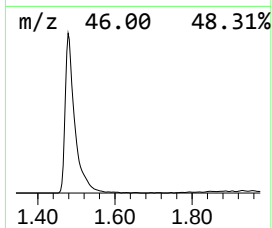
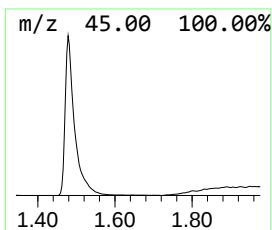
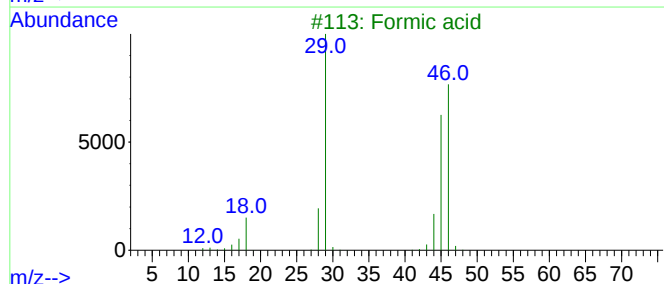
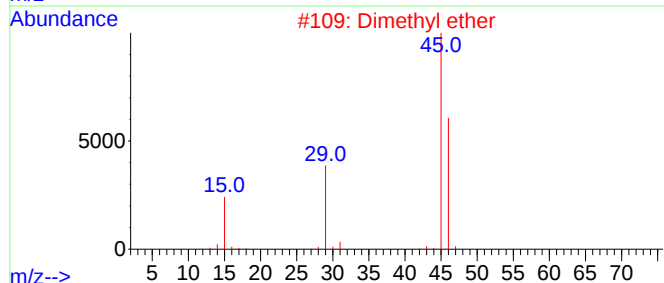
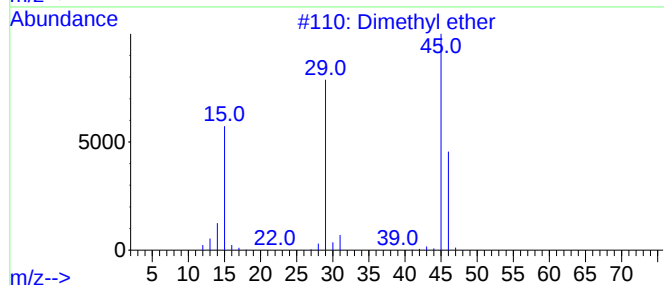
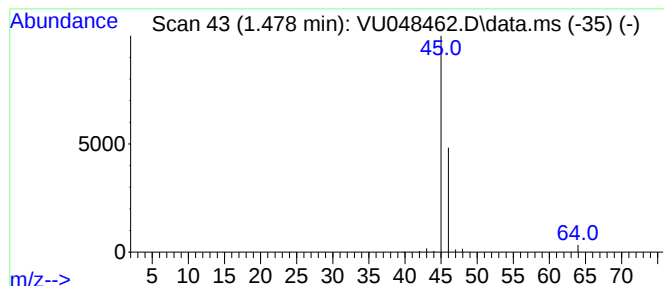
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Dimethyl ether Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.478	21.23 ug/L	383737	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl ether	46	C2H6O	000115-10-6	90
2			Dimethyl ether	46	C2H6O	000115-10-6	74
3			Formic acid	46	CH2O2	000064-18-6	7
4			Ethanol	46	C2H6O	000064-17-5	7
5			Ethanol	46	C2H6O	000064-17-5	7



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Instrument :
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ClientSampleId :
EXL04ME

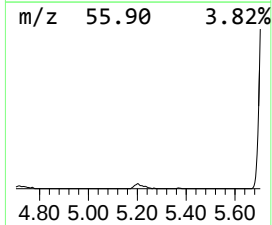
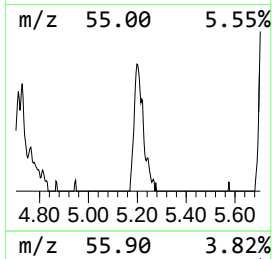
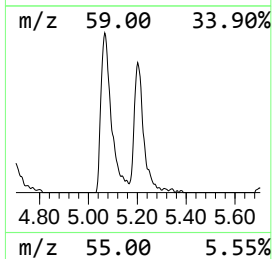
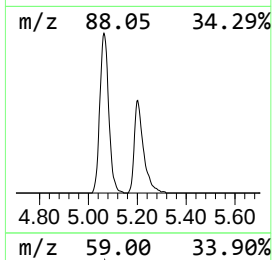
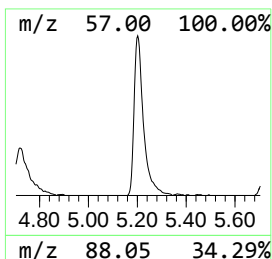
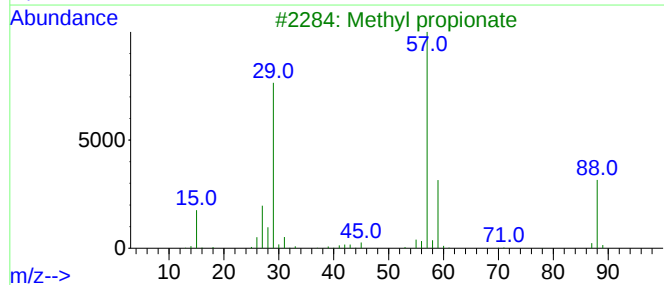
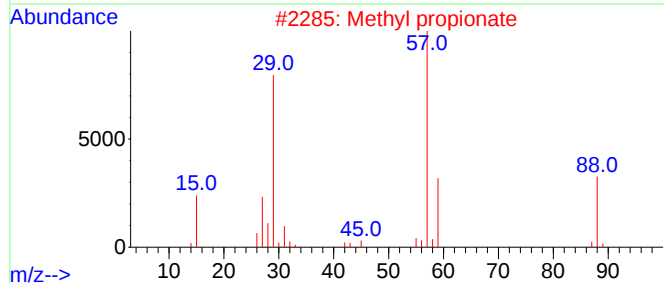
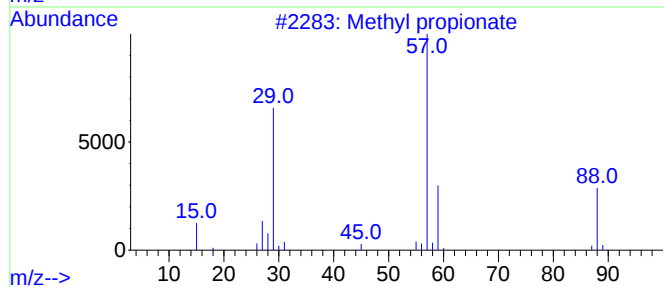
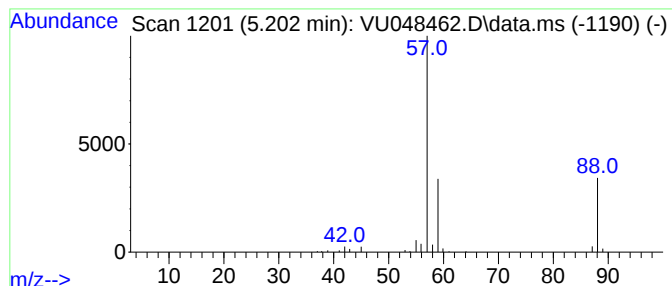
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Methyl propionate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.202	7.82 ug/L	141390	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl propionate	88	C4H8O2	000554-12-1	90
2			Methyl propionate	88	C4H8O2	000554-12-1	90
3			Methyl propionate	88	C4H8O2	000554-12-1	86
4			Methyl propionate	88	C4H8O2	000554-12-1	72
5			Glycerol, 1-tert-butyl ether	148	C7H16O3	1010381-75-8	33



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ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL04ME

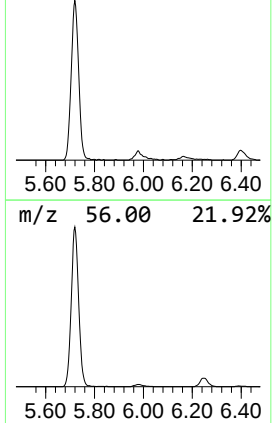
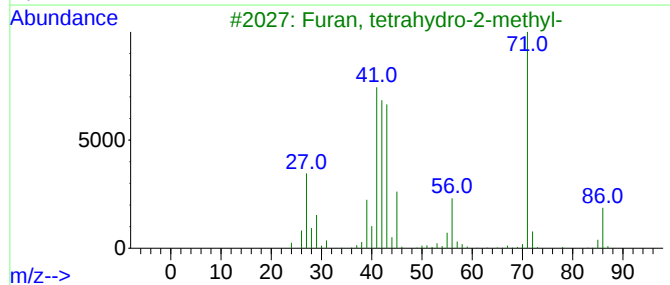
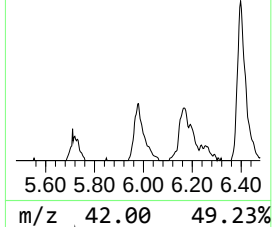
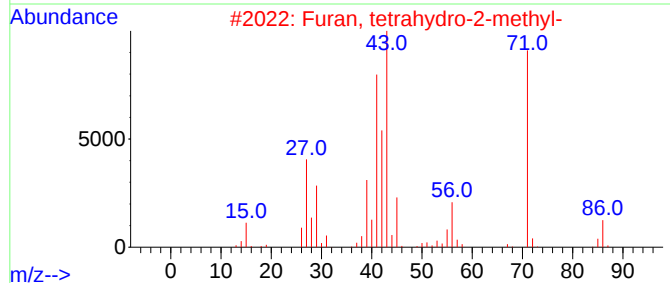
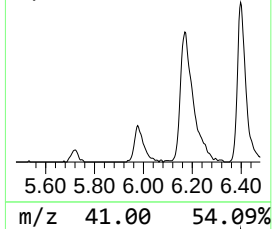
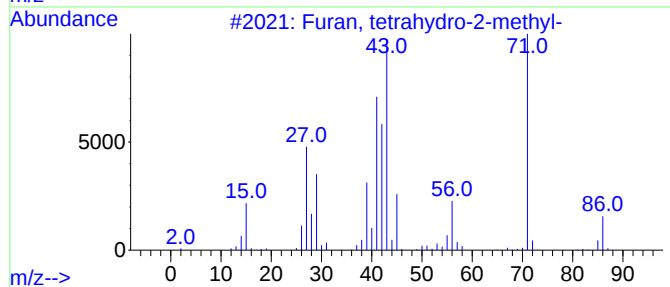
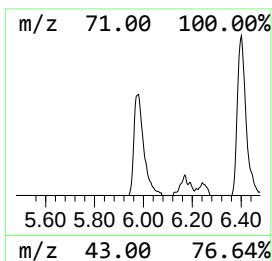
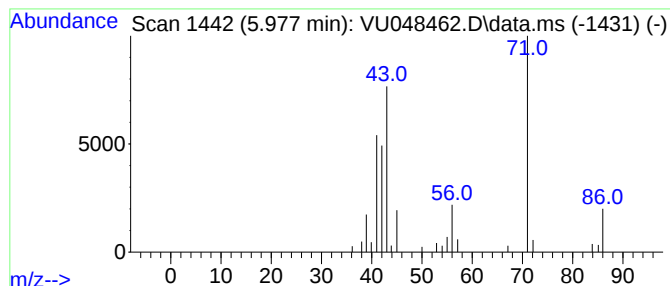
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Furan, tetrahydro-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.977	2.56 ug/L	46208	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	91
2			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	78
3			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	47
4			Prenol	86	C5H10O	000556-82-1	38
5			Prenol	86	C5H10O	000556-82-1	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050622\
Data File : VU048462.D
Acq On : 06 May 2022 18:05
Operator : SY/MD
Sample : N2638-09ME
Misc : 4.94g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL04ME

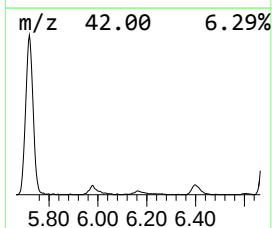
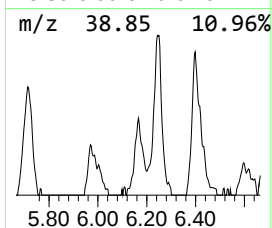
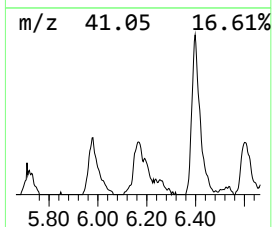
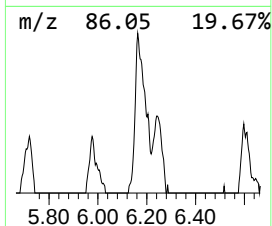
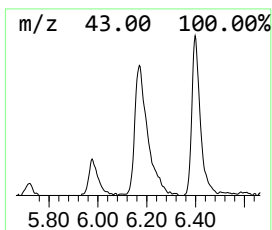
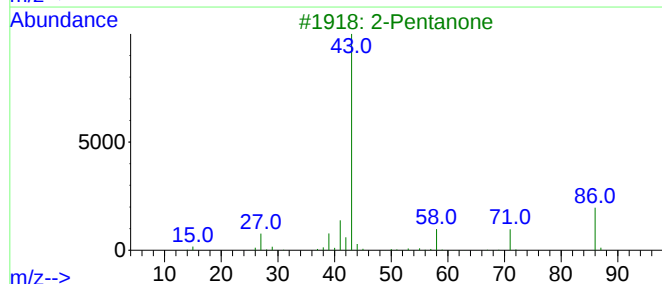
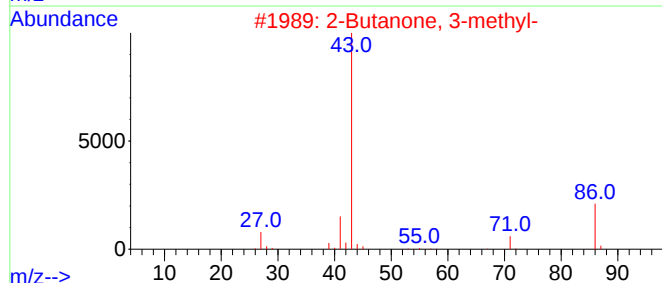
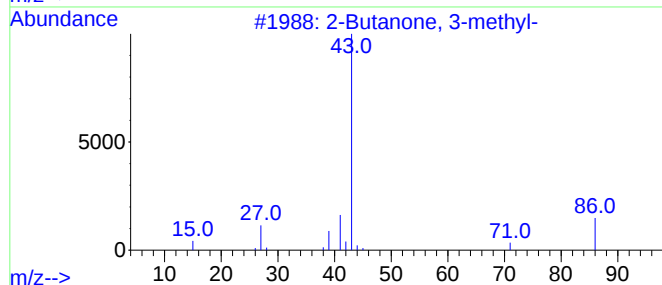
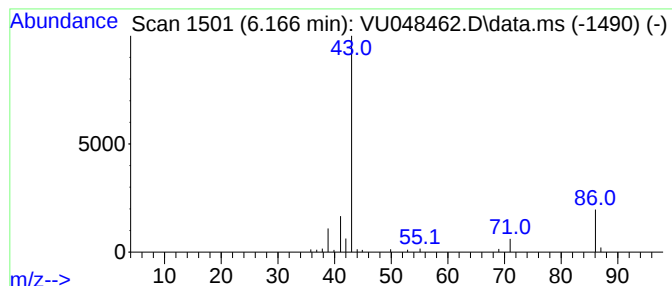
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Quant Title : VOC Analysis

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

Peak Number 5 2-Butanone, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.166	3.15 ug/L	56996	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3-methyl-			86	C5H10O	000563-80-4	59
2	2-Butanone, 3-methyl-			86	C5H10O	000563-80-4	53
3	2-Pentanone			86	C5H10O	000107-87-9	45
4	2-Pentanone			86	C5H10O	000107-87-9	36
5	2-Butanone, 3-methyl-			86	C5H10O	000563-80-4	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050622\
Data File : VU048462.D
Acq On : 06 May 2022 18:05
Operator : SY/MD
Sample : N2638-09ME
Misc : 4.94g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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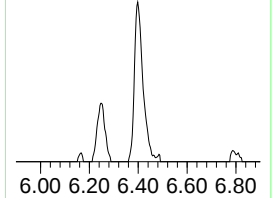
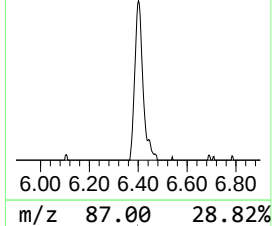
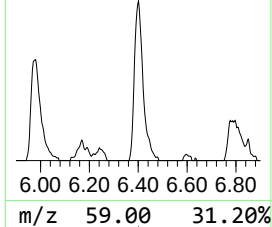
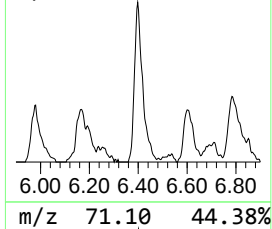
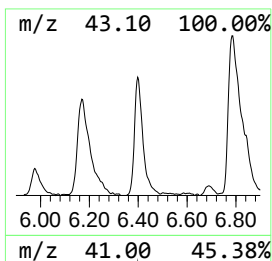
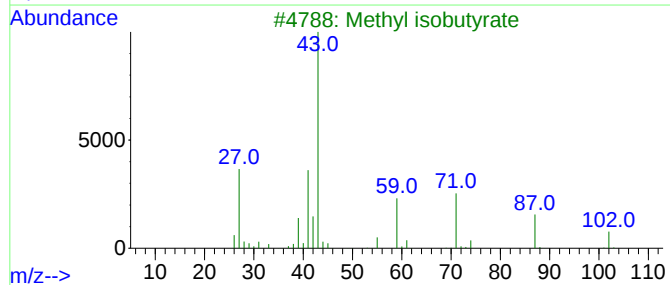
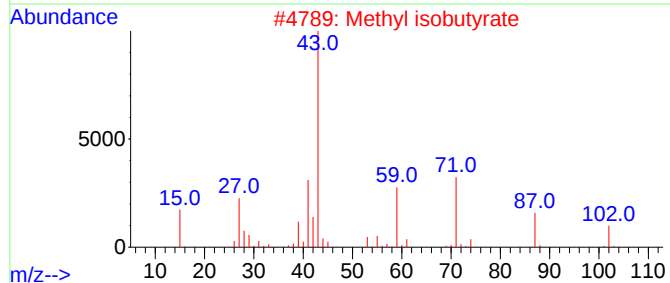
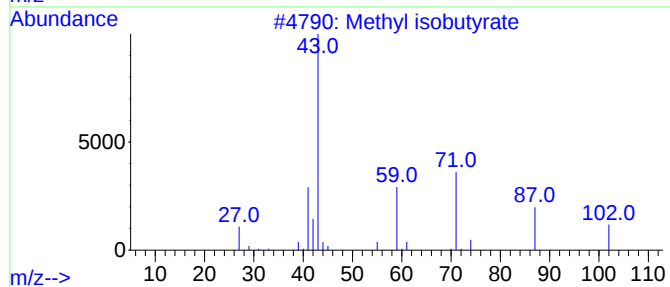
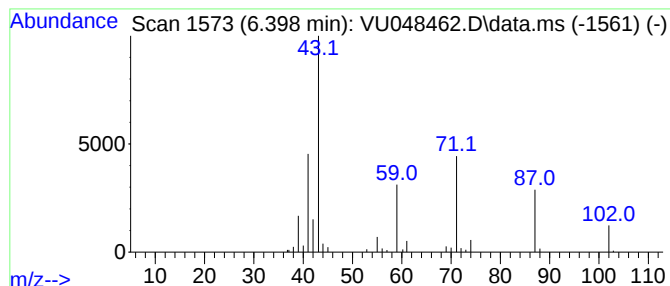
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Quant Title : VOC Analysis

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

Peak Number 6 Methyl isobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.398	6.85 ug/L	123765	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl isobutyrate	102	C5H10O2	000547-63-7	91
2			Methyl isobutyrate	102	C5H10O2	000547-63-7	91
3			Methyl isobutyrate	102	C5H10O2	000547-63-7	91
4			Methyl isobutyrate	102	C5H10O2	000547-63-7	72
5			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050622\
Data File : VU048462.D
Acq On : 06 May 2022 18:05
Operator : SY/MD
Sample : N2638-09ME
Misc : 4.94g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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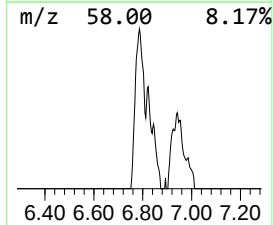
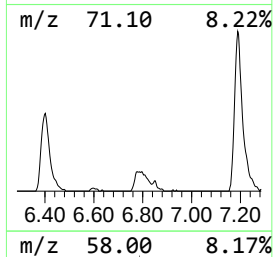
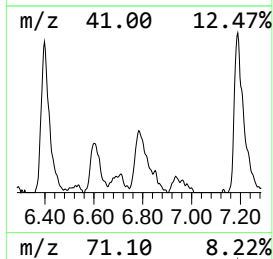
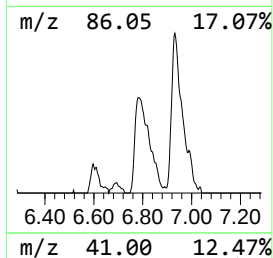
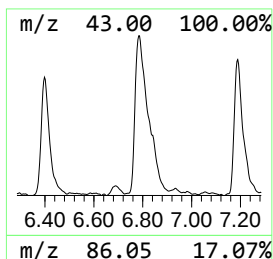
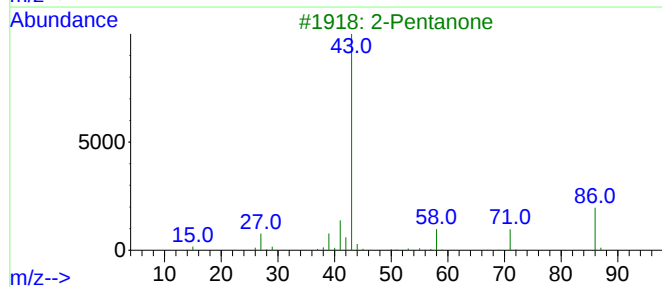
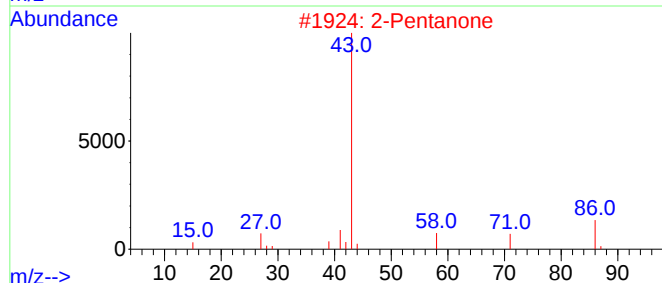
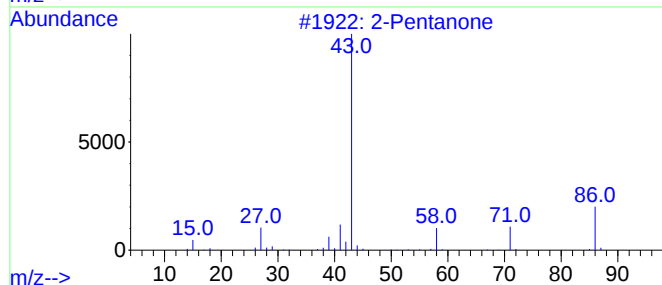
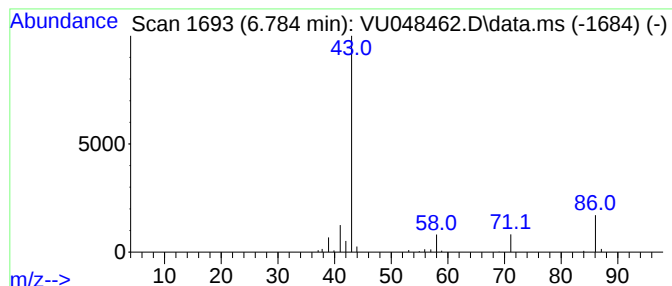
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Quant Title : VOC Analysis

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

Peak Number 7 2-Pentanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.784	7.15 ug/L	129239	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone			86	C5H10O	000107-87-9	72
2	2-Pentanone			86	C5H10O	000107-87-9	72
3	2-Pentanone			86	C5H10O	000107-87-9	72
4	2-Butanone, 3-methyl-			86	C5H10O	000563-80-4	72
5	2-Pentanone			86	C5H10O	000107-87-9	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050622\
Data File : VU048462.D
Acq On : 06 May 2022 18:05
Operator : SY/MD
Sample : N2638-09ME
Misc : 4.94g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL04ME

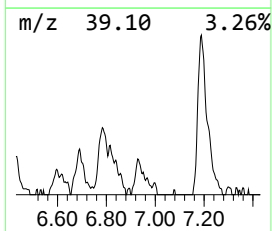
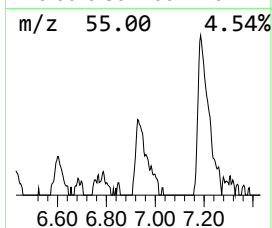
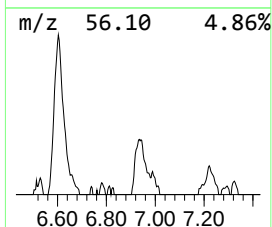
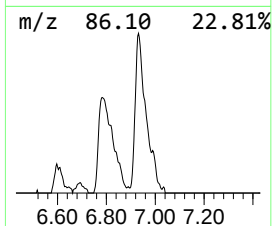
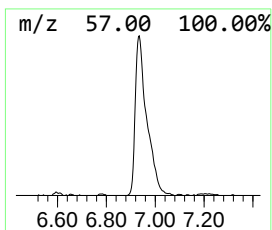
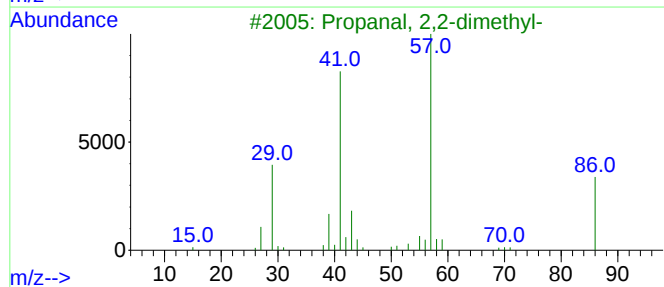
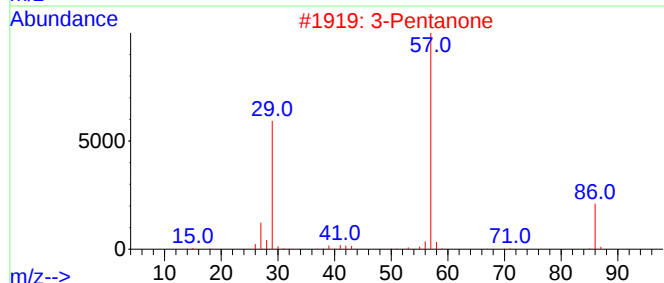
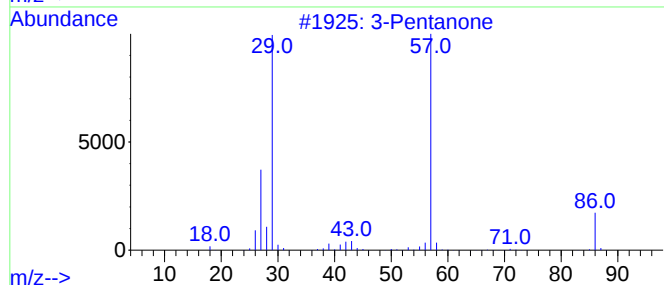
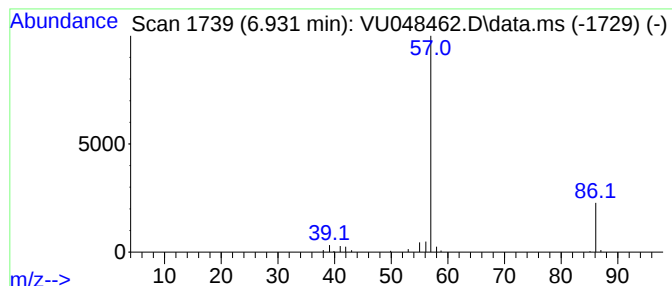
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Quant Title : VOC Analysis

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

Peak Number 8 3-Pentanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.931	6.55 ug/L	118316	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanone	86	C5H10O	000096-22-0	78
2			3-Pentanone	86	C5H10O	000096-22-0	72
3			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	9
4			3-Pentanone	86	C5H10O	000096-22-0	9
5			3-Pentanone	86	C5H10O	000096-22-0	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050622\
Data File : VU048462.D
Acq On : 06 May 2022 18:05
Operator : SY/MD
Sample : N2638-09ME
Misc : 4.94g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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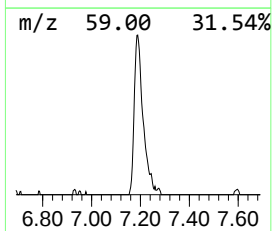
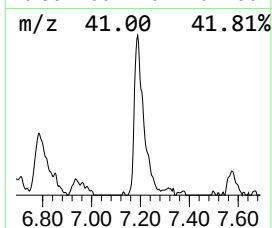
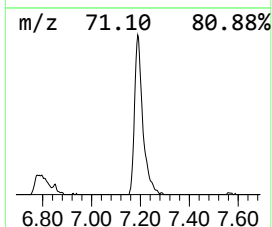
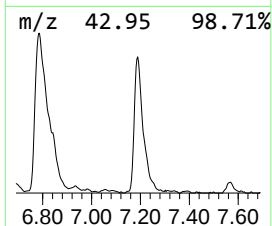
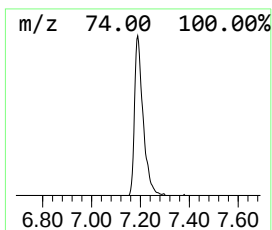
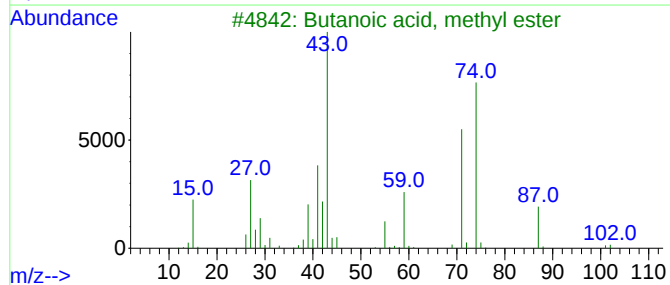
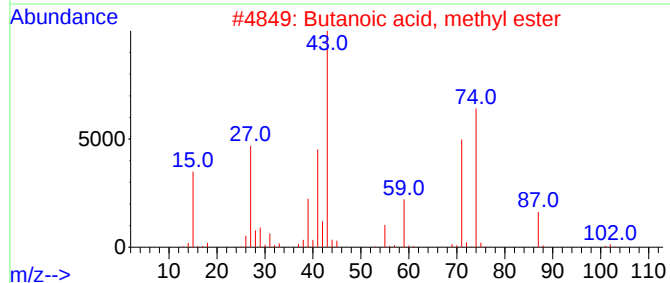
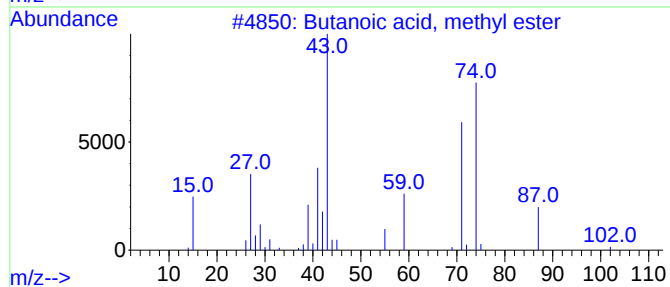
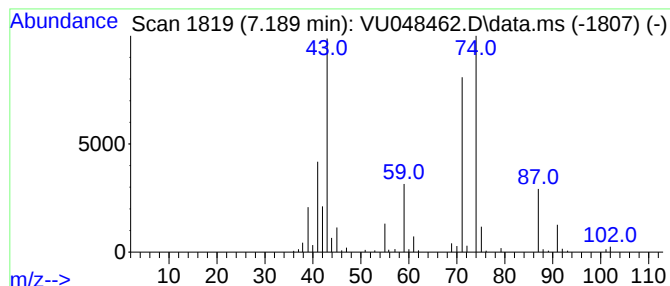
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Quant Title : VOC Analysis

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

Peak Number 9 Butanoic acid, methyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.189	12.87 ug/L	232581	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	87
2			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	72
3			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	52
4			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	47
5			Methyl isobutyrate	102	C5H10O2	000547-63-7	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050622\
Data File : VU048462.D
Acq On : 06 May 2022 18:05
Operator : SY/MD
Sample : N2638-09ME
Misc : 4.94g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXL04ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.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
Dimethyl ether	1.478	21.2	ug/L	383737	1	6.247	903673	50.0
Methyl propionate	5.202	7.8	ug/L	141390	1	6.247	903673	50.0
Furan, tetrahyd...	5.977	2.6	ug/L	46208	1	6.247	903673	50.0
2-Butanone, 3-m...	6.166	3.1	ug/L	56996	1	6.247	903673	50.0
Methyl isobutyrate	6.398	6.8	ug/L	123765	1	6.247	903673	50.0
2-Pentanone	6.784	7.2	ug/L	129239	1	6.247	903673	50.0
3-Pentanone	6.931	6.5	ug/L	118316	1	6.247	903673	50.0
Butanoic acid, ...	7.189	12.9	ug/L	232581	1	6.247	903673	50.0