

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091224\
 Data File : VV037266.D
 Acq On : 12 Sep 2024 13:55
 Operator : SY/MD
 Sample : P3934-01
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BHMK7

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\SFAMVLM082624WMA.M
 Title : VOC Analysis

Signal : TIC: VV037266.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.179	37	43	48	rBV2	3457	5814	0.19%	0.022%
2	1.278	67	74	88	rBV	466055	496066	15.97%	1.916%
3	1.349	91	96	103	rVB	14176	14953	0.48%	0.058%
4	1.532	145	153	171	rVB	372311	435603	14.02%	1.683%
5	2.060	306	317	328	rBV	795199	1145879	36.89%	4.427%
6	2.111	328	333	356	rVB	69938	115843	3.73%	0.448%
7	2.445	431	437	447	rVB	34061	50835	1.64%	0.196%
8	3.191	666	669	670	rBV3	1461	895	0.03%	0.003%
9	3.256	685	689	693	rVB7	1944	1610	0.05%	0.006%
10	3.304	693	704	714	rBV6	13521	34469	1.11%	0.133%
11	3.503	764	766	769	rVB3	849	511	0.02%	0.002%
12	3.519	769	771	774	rBV4	715	475	0.02%	0.002%
13	3.535	774	776	780	rVB4	910	492	0.02%	0.002%
14	3.568	780	786	789	rBV5	1607	1586	0.05%	0.006%
15	3.625	801	804	805	rBV3	1510	879	0.03%	0.003%
16	3.642	807	809	810	rBV2	1318	565	0.02%	0.002%
17	3.735	834	838	839	rBV4	518	438	0.01%	0.002%
18	3.796	847	857	903	rBV	150549	438315	14.11%	1.693%
19	4.265	981	1003	1033	rBV4	365696	1227023	39.51%	4.740%
20	4.432	1053	1055	1060	rVB4	1465	943	0.03%	0.004%
21	4.455	1060	1062	1064	rBV3	878	469	0.02%	0.002%
22	4.484	1068	1071	1075	rBV5	927	952	0.03%	0.004%
23	4.558	1092	1094	1098	rVV4	687	390	0.01%	0.002%
24	4.596	1102	1106	1108	rBV4	424	372	0.01%	0.001%
25	4.625	1111	1115	1119	rVB5	842	598	0.02%	0.002%
26	4.651	1119	1123	1124	rBV4	898	457	0.01%	0.002%
27	4.690	1130	1135	1137	rBV4	1508	1374	0.04%	0.005%
28	4.706	1138	1140	1144	rVB5	937	708	0.02%	0.003%
29	4.728	1144	1147	1150	rBV5	1095	655	0.02%	0.003%
30	4.744	1150	1152	1157	rVB6	1310	998	0.03%	0.004%
31	4.809	1169	1172	1175	rVB4	945	604	0.02%	0.002%
32	4.841	1178	1182	1183	rBV3	513	375	0.01%	0.001%
33	4.850	1183	1185	1189	rVB4	680	381	0.01%	0.001%
34	4.873	1189	1192	1194	rBV2	679	365	0.01%	0.001%
35	4.950	1199	1216	1245	rBV2	1235093	3105935	100.00%	11.998%
36	5.211	1289	1297	1319	rBV4	16815	41064	1.32%	0.159%

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 Title : VOC Analysis

37	5.330	1331	1334	1338	rBV6	1457	1159	0.04%	0.004%
38	5.529	1384	1396	1431	rBV	823904	1672771	53.86%	6.462%
39	5.815	1473	1485	1504	rBV	494811	1026702	33.06%	3.966%
40	5.985	1525	1538	1569	rBV	685156	1414149	45.53%	5.463%
41	6.265	1617	1625	1651	rBV	67991	146092	4.70%	0.564%
42	6.834	1798	1802	1804	rBV5	1356	961	0.03%	0.004%
43	6.850	1805	1807	1809	rVB2	1330	470	0.02%	0.002%
44	6.863	1809	1811	1813	rBV2	670	410	0.01%	0.002%
45	6.908	1814	1825	1855	rBV	390797	732357	23.58%	2.829%
46	7.117	1881	1890	1901	rBV	96391	168134	5.41%	0.650%
47	7.236	1916	1927	1959	rBV	1414245	2499733	80.48%	9.657%
48	7.548	2015	2024	2054	rBV	257937	477929	15.39%	1.846%
49	7.812	2104	2106	2108	rVB3	1584	633	0.02%	0.002%
50	7.857	2108	2120	2141	rBV	590339	973799	31.35%	3.762%
51	7.947	2141	2148	2158	rVV2	34201	62813	2.02%	0.243%
52	8.021	2159	2171	2202	rVB3	699823	1449463	46.67%	5.599%
53	8.464	2306	2309	2313	rVB5	1530	1190	0.04%	0.005%
54	8.487	2313	2316	2320	rVB5	1529	1401	0.05%	0.005%
55	8.506	2320	2322	2324	rBV2	1066	574	0.02%	0.002%
56	8.519	2324	2326	2328	rBV3	1039	501	0.02%	0.002%
57	8.616	2345	2356	2387	rBV	942522	1487995	47.91%	5.748%
58	8.780	2395	2407	2445	rBV	1274155	2109932	67.93%	8.151%
59	9.255	2552	2555	2558	rBV3	812	748	0.02%	0.003%
60	9.294	2563	2567	2568	rBV4	1356	786	0.03%	0.003%
61	9.333	2571	2579	2599	rVV	15592	34357	1.11%	0.133%
62	9.426	2605	2608	2611	rBV5	2085	1309	0.04%	0.005%
63	9.497	2624	2630	2646	rBV5	5563	12192	0.39%	0.047%
64	9.641	2671	2675	2679	rBV5	1426	1565	0.05%	0.006%
65	9.709	2694	2696	2702	rVB6	1444	1117	0.04%	0.004%
66	9.789	2718	2721	2724	rVB4	1034	530	0.02%	0.002%
67	9.815	2727	2729	2732	rVV3	1335	790	0.03%	0.003%
68	9.831	2732	2734	2738	rVB5	1474	882	0.03%	0.003%
69	9.963	2771	2775	2779	rVB6	1131	972	0.03%	0.004%
70	10.001	2783	2787	2789	rVV4	1203	892	0.03%	0.003%
71	10.017	2789	2792	2796	rVV6	1202	1186	0.04%	0.005%
72	10.046	2798	2801	2804	rVB4	1217	890	0.03%	0.003%
73	10.149	2815	2833	2849	rVV	113912	190435	6.13%	0.736%
74	10.362	2897	2899	2902	rBV4	1161	822	0.03%	0.003%
75	10.432	2917	2921	2922	rBV3	1728	1071	0.03%	0.004%
76	10.516	2941	2947	2958	rVB9	5953	10228	0.33%	0.040%

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 Title : VOC Analysis

77	10.706	3003	3006	3008	rBV3	1233	831	0.03%	0.003%
78	10.770	3018	3026	3027	rBV6	1704	1850	0.06%	0.007%
79	10.808	3034	3038	3039	rBV3	1476	1023	0.03%	0.004%
80	10.860	3049	3054	3059	rBV8	2313	2636	0.08%	0.010%
81	10.908	3067	3069	3074	rVB5	1275	750	0.02%	0.003%
82	10.966	3082	3087	3092	rBV8	2902	3309	0.11%	0.013%
83	11.095	3119	3127	3128	rBV6	1989	2375	0.08%	0.009%
84	11.178	3143	3153	3179	rBV	1296230	2023526	65.15%	7.817%
85	11.500	3247	3253	3258	rBV9	4184	6835	0.22%	0.026%
86	11.554	3259	3270	3295	rVV	1369017	2170503	69.88%	8.385%
87	11.728	3318	3324	3330	rVB8	7748	9938	0.32%	0.038%
88	11.895	3374	3376	3377	rBV2	1164	502	0.02%	0.002%
89	12.169	3459	3461	3464	rBV4	1399	1037	0.03%	0.004%
90	12.297	3497	3501	3502	rBV4	2785	1849	0.06%	0.007%
91	12.439	3540	3545	3547	rBV6	2886	2277	0.07%	0.009%
92	12.484	3556	3559	3565	rBV9	1919	1625	0.05%	0.006%
93	12.821	3658	3664	3673	rBV8	8592	12692	0.41%	0.049%
94	13.030	3727	3729	3736	rVB6	1356	952	0.03%	0.004%
95	13.059	3736	3738	3739	rBV	1657	726	0.02%	0.003%
96	13.323	3815	3820	3825	rBV8	3393	4896	0.16%	0.019%
97	13.837	3974	3980	3986	rBV7	8982	12208	0.39%	0.047%
98	13.908	4000	4002	4005	rBV5	2228	1327	0.04%	0.005%
99	14.072	4051	4053	4055	rBV3	2081	794	0.03%	0.003%
100	14.696	4243	4247	4250	rBV5	3277	2949	0.09%	0.011%

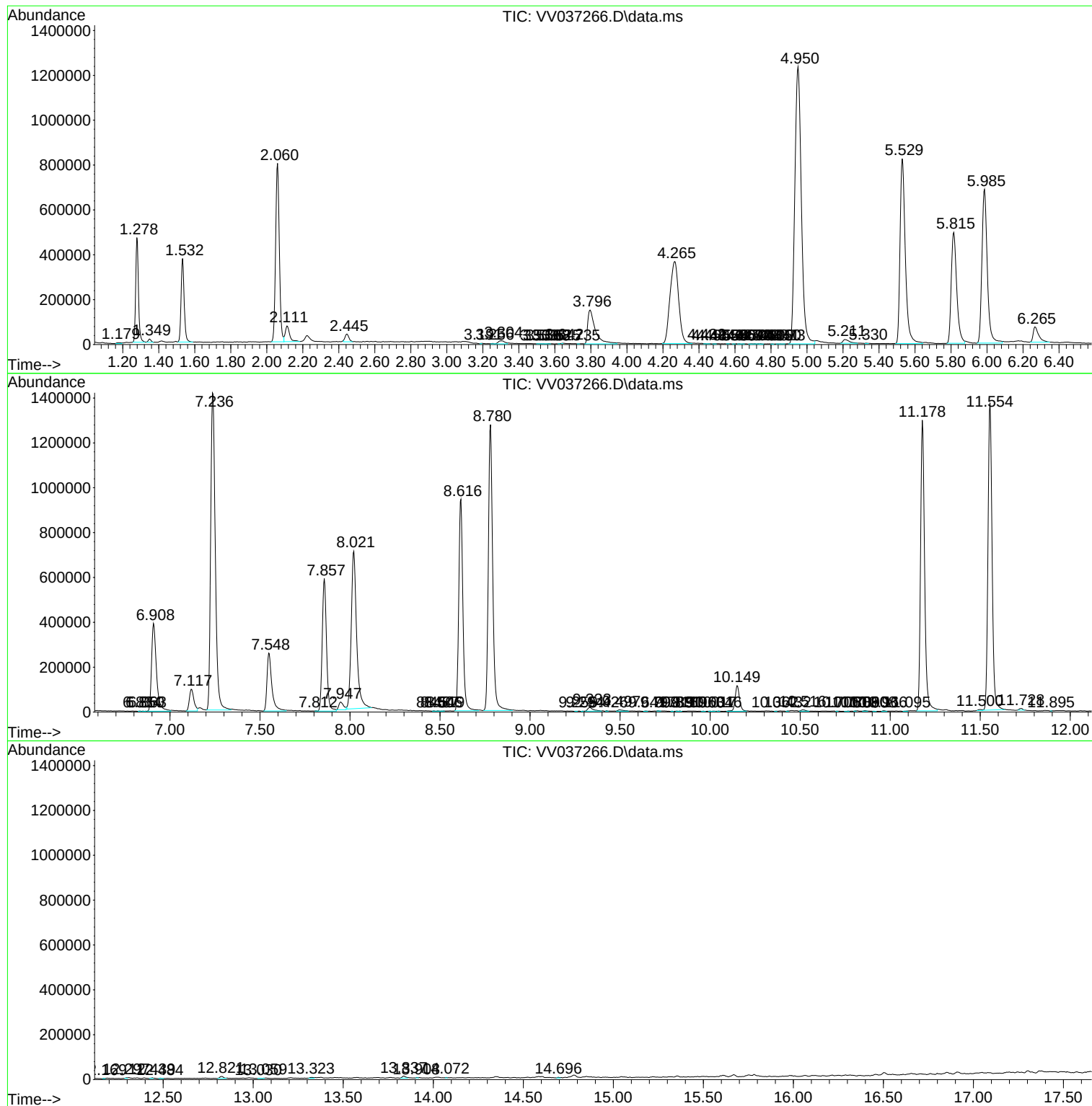
Sum of corrected areas: 25886241

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091224\
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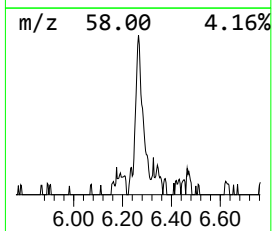
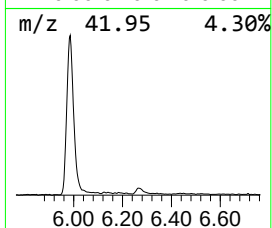
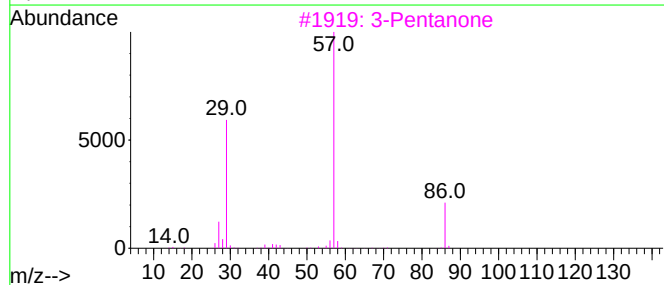
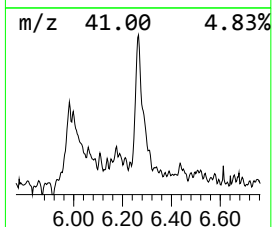
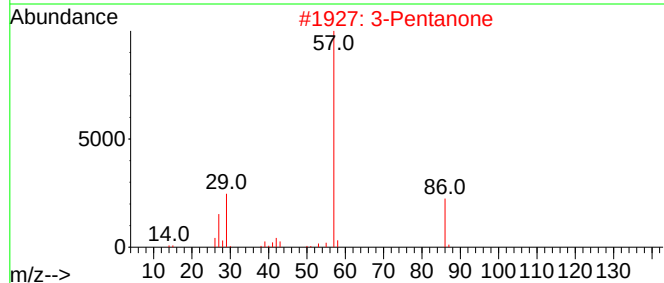
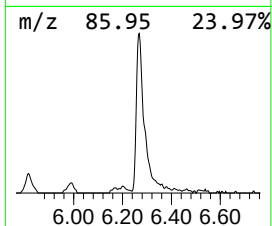
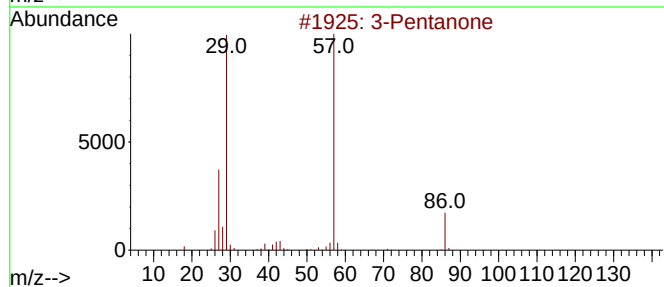
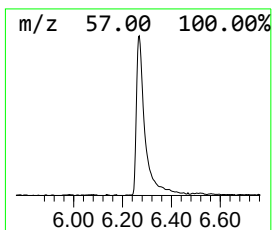
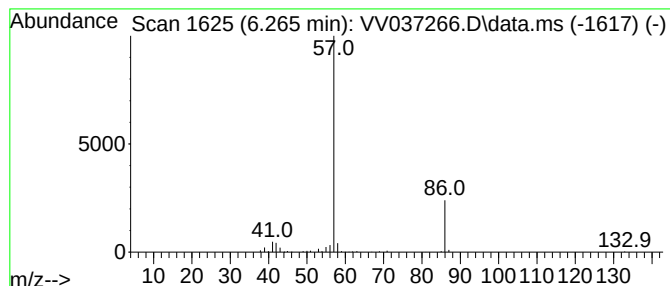
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 3-Pentanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.265	4.37 ug/L	146092	1,4-Difluorobenzene	5.529

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone		86	C5H10O	000096-22-0	80
2	3-Pentanone		86	C5H10O	000096-22-0	72
3	3-Pentanone		86	C5H10O	000096-22-0	64
4	3-Pentanone		86	C5H10O	000096-22-0	58
5	3-Pentanone		86	C5H10O	000096-22-0	9



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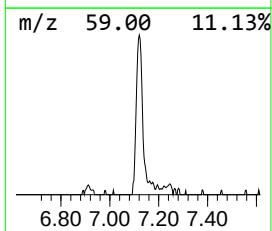
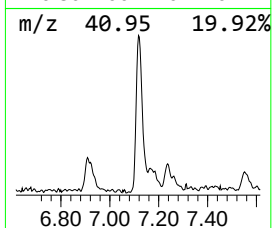
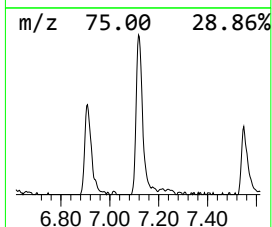
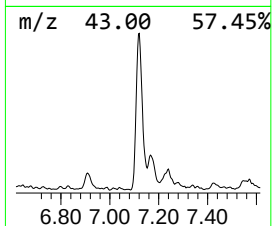
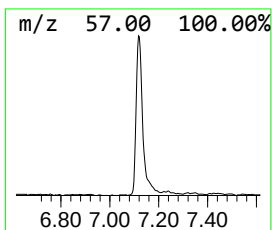
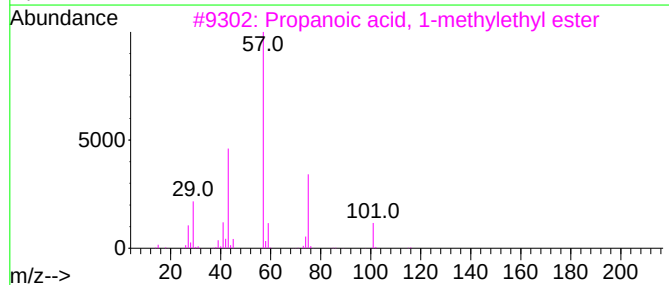
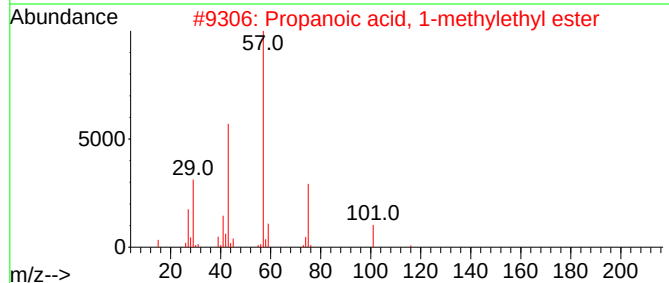
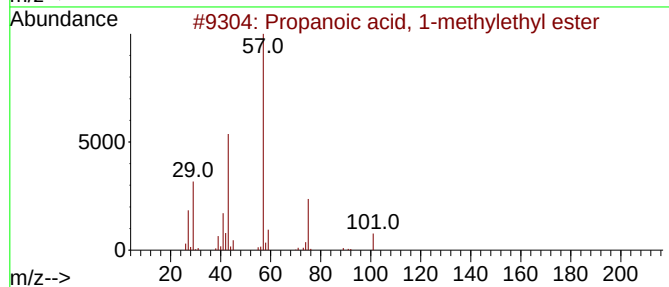
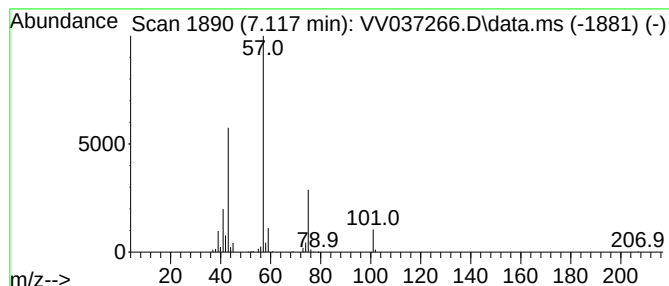
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.117	5.03 ug/L	168134	1,4-Difluorobenzene	5.529

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	86
2			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	78
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	59
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	50



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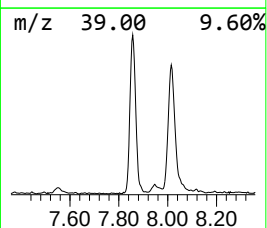
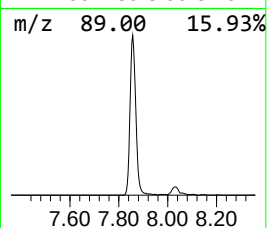
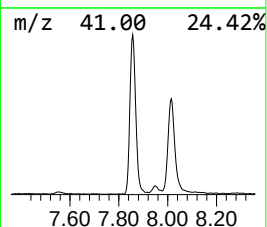
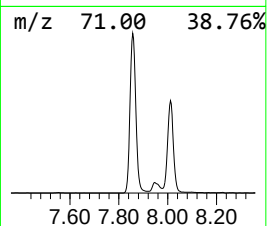
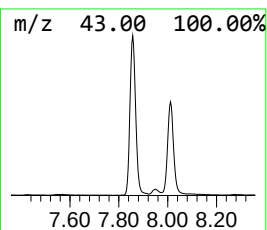
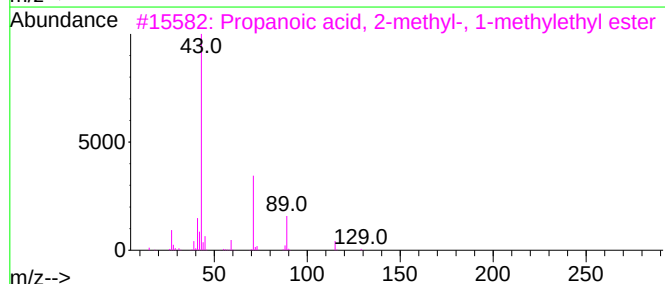
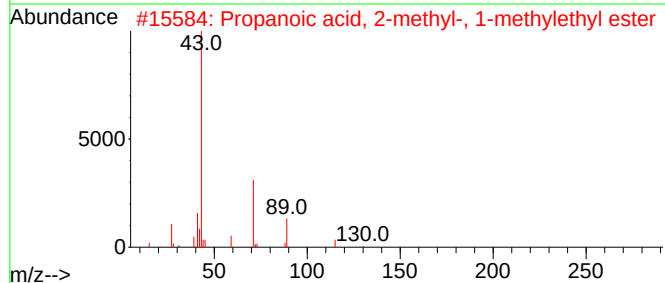
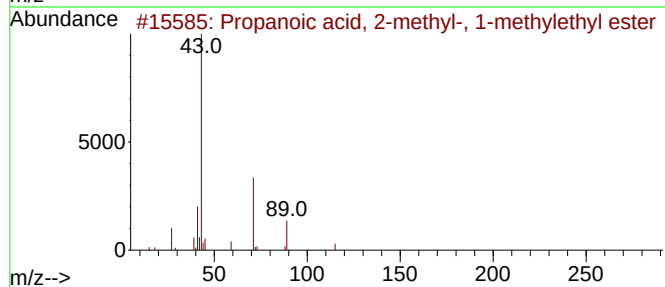
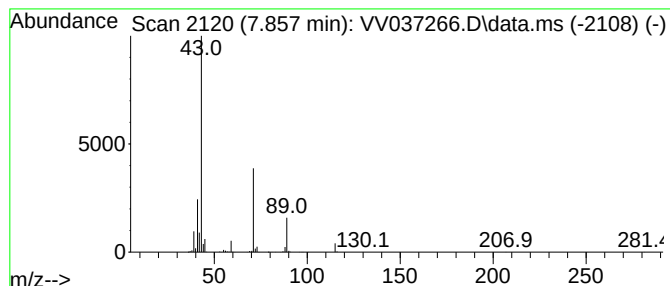
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Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.857	23.08 ug/L	973799	Chlorobenzene-d5	8.780

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
3			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
4			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
5			Isopropyl butyrate	130	C7H14O2	000638-11-9	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091224\
Data File : VV037266.D
Acq On : 12 Sep 2024 13:55
Operator : SY/MD
Sample : P3934-01
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BHMk7

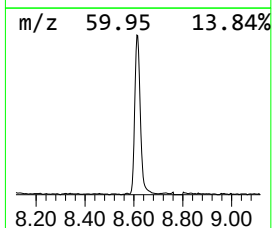
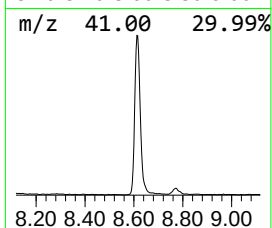
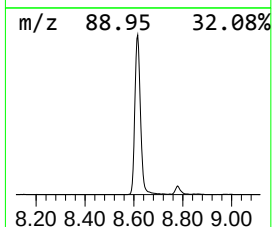
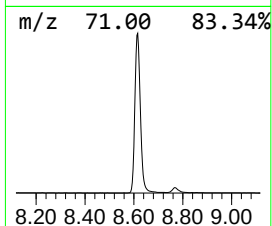
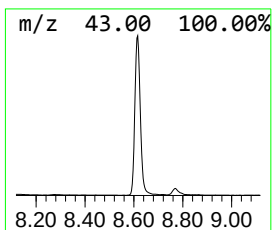
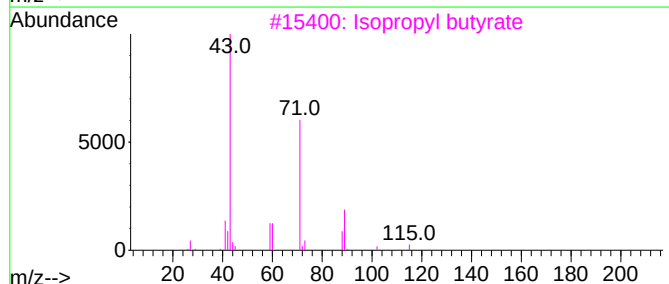
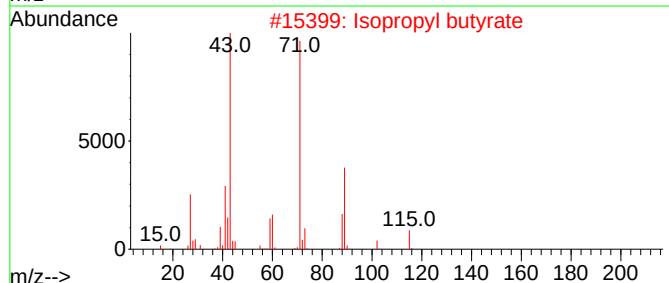
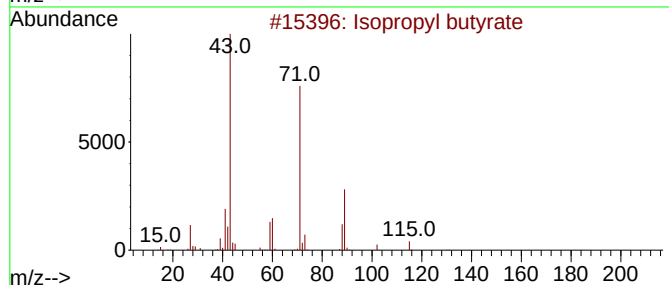
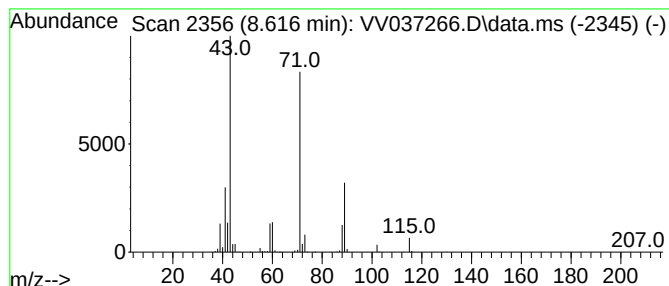
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Quant Title : VOC Analysis

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

Peak Number 6 Isopropyl butyrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.616	35.26 ug/L	1488000	Chlorobenzene-d5	8.780

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	95
2			Isopropyl butyrate	130	C7H14O2	000638-11-9	91
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	83
4			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091224\
Data File : VV037266.D
Acq On : 12 Sep 2024 13:55
Operator : SY/MD
Sample : P3934-01
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BHMK7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.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
3-Pentanone	6.265	4.4	ug/L	146092	1	5.529	1672770	50.0
Propanoic acid,...	7.117	5.0	ug/L	168134	1	5.529	1672770	50.0
Propanoic acid,...	7.857	23.1	ug/L	973799	2	8.780	2109930	50.0
Isopropyl butyrate	8.616	35.3	ug/L	1488000	2	8.780	2109930	50.0