

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120621\
 Data File : VU046119.D
 Acq On : 06 Dec 2021 18:19
 Operator : SY/MD
 Sample : M4938-09 10X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EX8E5

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\SFAMULM112921WMA.M
 Title : VOC Analysis

Signal : TIC: VU046119.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	73	81	93	rBV	92040	100558	12.77%	1.479%
2	1.916	170	179	193	rVB	68205	85068	10.80%	1.251%
3	2.202	265	268	273	rBV	276	201	0.03%	0.003%
4	2.289	292	295	297	rBV	225	157	0.02%	0.002%
5	2.375	320	322	326	rVB	293	187	0.02%	0.003%
6	2.453	344	346	353	rVB3	343	294	0.04%	0.004%
7	2.572	369	383	401	rBV	164027	274896	34.91%	4.044%
8	2.800	447	454	460	rBV2	504	746	0.09%	0.011%
9	3.054	524	533	542	rVB2	2333	4223	0.54%	0.062%
10	3.192	569	576	580	rBV2	466	645	0.08%	0.009%
11	4.208	888	892	894	rBV	301	245	0.03%	0.004%
12	4.629	1008	1023	1048	rBV	76158	192297	24.42%	2.829%
13	4.877	1096	1100	1102	rBV	241	157	0.02%	0.002%
14	4.932	1114	1117	1121	rBV3	282	243	0.03%	0.004%
15	5.067	1143	1159	1181	rBV	134277	306684	38.95%	4.512%
16	5.295	1225	1230	1231	rBV2	396	308	0.04%	0.005%
17	5.346	1242	1246	1249	rVB	226	183	0.02%	0.003%
18	5.469	1282	1284	1289	rVB	188	179	0.02%	0.003%
19	5.494	1289	1292	1294	rBV	209	177	0.02%	0.003%
20	5.729	1343	1365	1389	rBV2	293295	787355	100.00%	11.582%
21	5.912	1413	1422	1433	rVB4	917	1703	0.22%	0.025%
22	6.002	1446	1450	1452	rBV2	191	166	0.02%	0.002%
23	6.250	1513	1527	1548	rBV	245759	465745	59.15%	6.851%
24	6.542	1605	1618	1629	rVB4	14064	28155	3.58%	0.414%
25	6.694	1648	1665	1681	rBV	178345	345142	43.84%	5.077%
26	6.928	1721	1738	1750	rVB4	1063	2626	0.33%	0.039%
27	7.041	1761	1773	1790	rBV	48771	83977	10.67%	1.235%
28	7.185	1814	1818	1827	rVB4	597	688	0.09%	0.010%
29	7.568	1922	1937	1954	rBV	104267	178771	22.71%	2.630%
30	7.687	1972	1974	1977	rVV2	253	179	0.02%	0.003%
31	7.739	1981	1990	2003	rVV2	12905	21213	2.69%	0.312%
32	7.796	2003	2008	2015	rVB3	831	991	0.13%	0.015%
33	7.899	2025	2040	2056	rBV	377080	646710	82.14%	9.514%
34	8.182	2116	2128	2144	rBV	68190	115415	14.66%	1.698%
35	8.465	2208	2216	2226	rVB3	3052	4536	0.58%	0.067%
36	8.510	2226	2230	2235	rBV	271	245	0.03%	0.004%

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Integrator: RTE

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 Title : VOC Analysis

37	8.565	2235	2247	2257	rBV6	8772	20243	2.57%	0.298%
38	8.632	2257	2268	2288	rVV	238765	413158	52.47%	6.078%
39	8.729	2289	2298	2318	rVV	91369	142211	18.06%	2.092%
40	8.803	2318	2321	2324	rVV3	703	486	0.06%	0.007%
41	8.835	2324	2331	2340	rVB4	3964	5960	0.76%	0.088%
42	9.009	2380	2385	2388	rBV2	173	201	0.03%	0.003%
43	9.131	2419	2423	2427	rBV2	186	199	0.03%	0.003%
44	9.163	2430	2433	2437	rVB2	188	161	0.02%	0.002%
45	9.211	2437	2448	2460	rBV	55567	84978	10.79%	1.250%
46	9.365	2492	2496	2500	rBV2	303	308	0.04%	0.005%
47	9.420	2500	2513	2532	rBV	352959	583536	74.11%	8.584%
48	9.571	2554	2560	2567	rBV	610	855	0.11%	0.013%
49	9.693	2587	2598	2611	rVB2	6137	9418	1.20%	0.139%
50	10.028	2696	2702	2703	rBV	197	192	0.02%	0.003%
51	10.105	2712	2726	2735	rVB5	3211	5634	0.72%	0.083%
52	10.365	2804	2807	2810	rVV	213	158	0.02%	0.002%
53	10.481	2840	2843	2848	rBV2	195	201	0.03%	0.003%
54	10.674	2894	2903	2910	rVV3	1644	2290	0.29%	0.034%
55	10.758	2917	2929	2947	rBV	257607	409156	51.97%	6.019%
56	10.873	2959	2965	2969	rBV3	323	427	0.05%	0.006%
57	11.005	2999	3006	3010	rBV2	356	451	0.06%	0.007%
58	11.095	3024	3034	3038	rVB3	1030	1411	0.18%	0.021%
59	11.121	3038	3042	3046	rBV2	317	330	0.04%	0.005%
60	11.295	3092	3096	3099	rBV3	315	283	0.04%	0.004%
61	11.385	3122	3124	3129	rVB	290	158	0.02%	0.002%
62	11.465	3138	3149	3159	rBV3	3046	5155	0.65%	0.076%
63	11.700	3216	3222	3225	rVV3	671	677	0.09%	0.010%
64	11.732	3225	3232	3241	rVB2	4655	6741	0.86%	0.099%
65	11.812	3245	3257	3275	rBV	399851	620726	78.84%	9.131%
66	11.896	3278	3283	3288	rBV2	433	529	0.07%	0.008%
67	11.944	3295	3298	3301	rVV2	407	231	0.03%	0.003%
68	11.976	3301	3308	3317	rVB4	1563	2091	0.27%	0.031%
69	12.089	3339	3343	3344	rBV2	383	252	0.03%	0.004%
70	12.195	3358	3376	3392	rBV	388463	617239	78.39%	9.080%
71	12.272	3397	3400	3403	rVV2	261	206	0.03%	0.003%
72	12.314	3403	3413	3423	rVB2	4881	8068	1.02%	0.119%
73	12.642	3509	3515	3521	rVB3	347	406	0.05%	0.006%
74	12.925	3598	3603	3611	rBV2	1063	1288	0.16%	0.019%
75	13.034	3628	3637	3646	rBV3	1668	2683	0.34%	0.039%
76	13.118	3659	3663	3666	rBV2	293	276	0.04%	0.004%

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77	13.150	3670	3673	3677	rVB3	337	282	0.04%	0.004%
78	13.224	3692	3696	3699	rBV2	515	426	0.05%	0.006%
79	13.436	3757	3762	3763	rBV	209	182	0.02%	0.003%
80	13.549	3794	3797	3801	rVB2	318	259	0.03%	0.004%
81	13.578	3804	3806	3812	rVB2	216	174	0.02%	0.003%
82	13.626	3817	3821	3822	rBV	330	205	0.03%	0.003%
83	13.767	3862	3865	3868	rBV	265	202	0.03%	0.003%
84	13.835	3883	3886	3887	rBV	362	201	0.03%	0.003%
85	13.918	3908	3912	3915	rBV	287	260	0.03%	0.004%
86	13.934	3915	3917	3923	rBV	182	180	0.02%	0.003%
87	14.086	3953	3964	3978	rBV	108230	169498	21.53%	2.493%
88	14.208	3996	4002	4012	rVB	3752	5077	0.64%	0.075%
89	14.330	4034	4040	4046	rVB3	420	536	0.07%	0.008%
90	14.426	4066	4070	4071	rBV	214	165	0.02%	0.002%
91	14.584	4110	4119	4127	rBV2	922	1728	0.22%	0.025%
92	14.684	4147	4150	4152	rVB2	329	196	0.02%	0.003%
93	14.873	4204	4209	4215	rBV	441	593	0.08%	0.009%
94	14.915	4220	4222	4228	rBV2	271	237	0.03%	0.003%
95	14.954	4231	4234	4238	rBV2	294	236	0.03%	0.003%
96	15.028	4253	4257	4260	rBV2	310	266	0.03%	0.004%
97	15.227	4310	4319	4328	rVV	6379	9903	1.26%	0.146%
98	15.410	4369	4376	4384	rVB3	4326	6330	0.80%	0.093%
99	16.005	4559	4561	4566	rVB	367	271	0.03%	0.004%
100	16.092	4585	4588	4594	rBV2	403	357	0.05%	0.005%

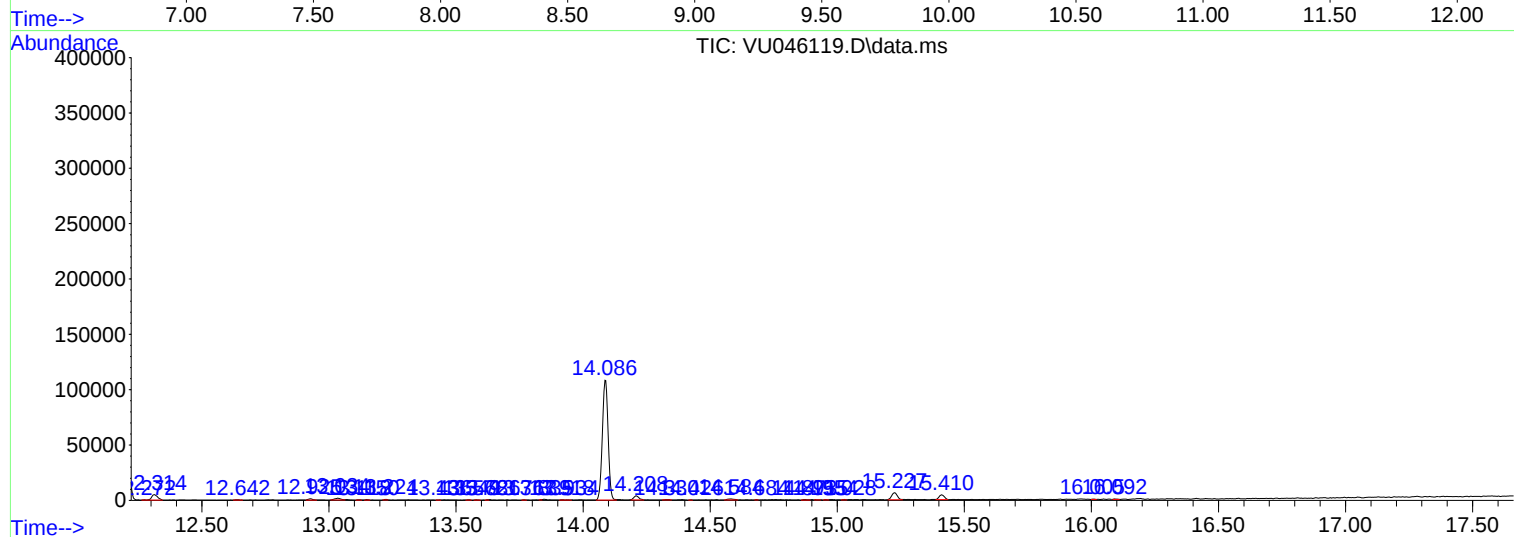
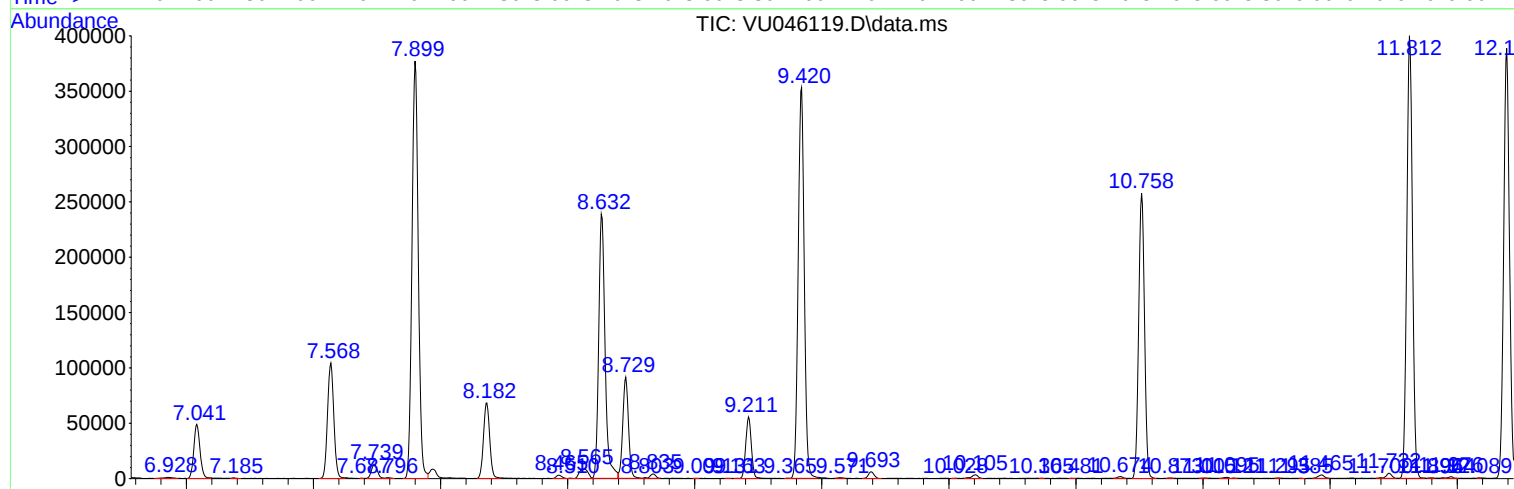
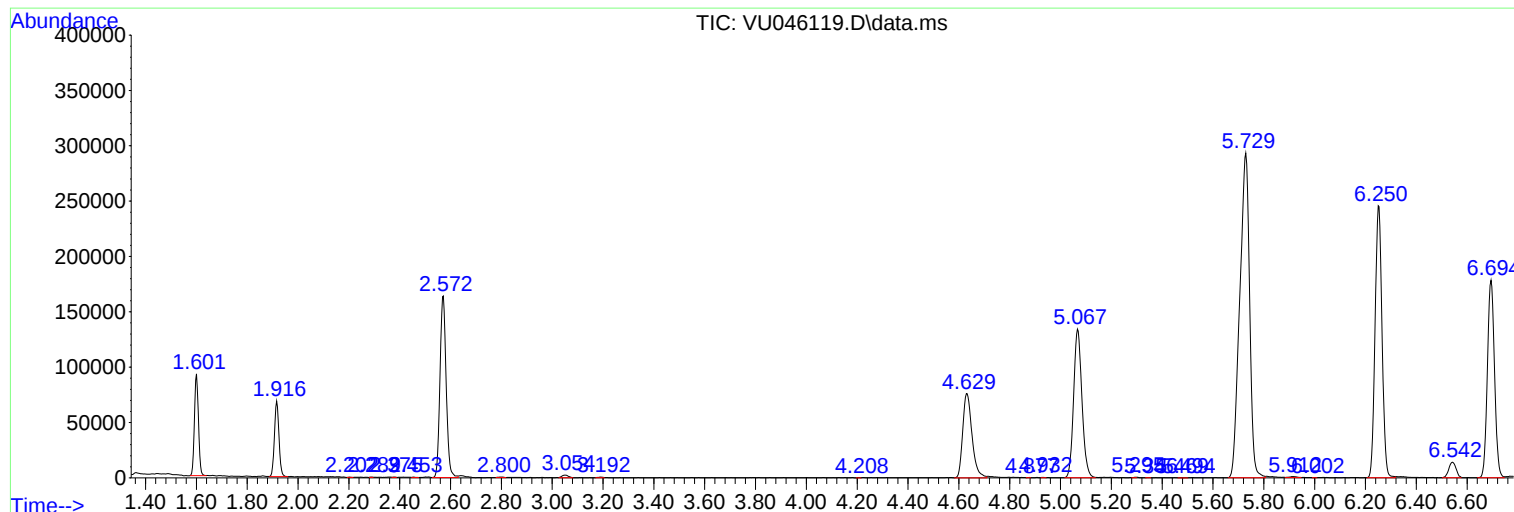
Sum of corrected areas: 6797802

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MSVOA_U
ClientSampleId :
EX8E5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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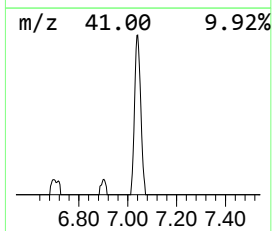
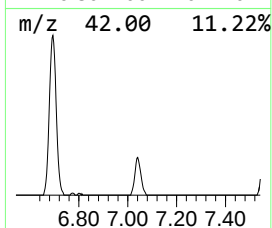
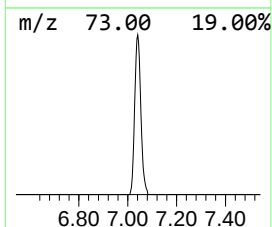
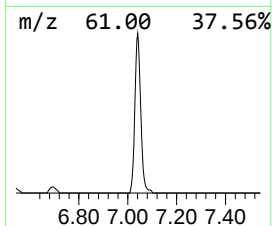
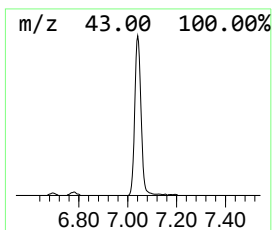
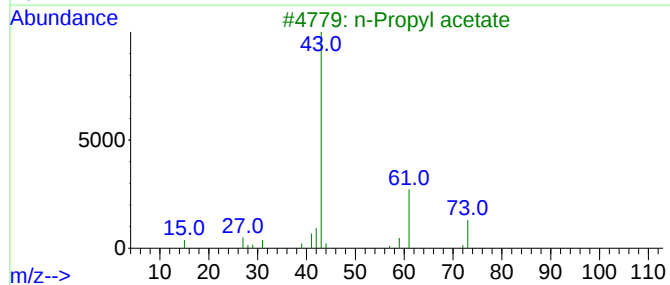
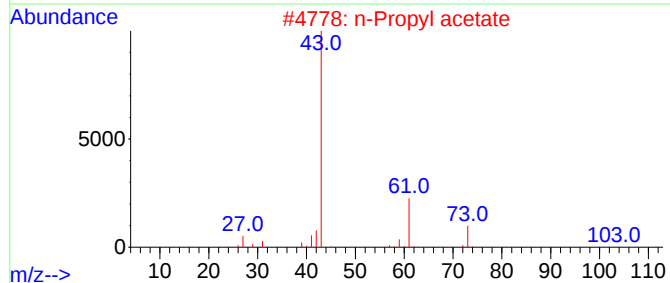
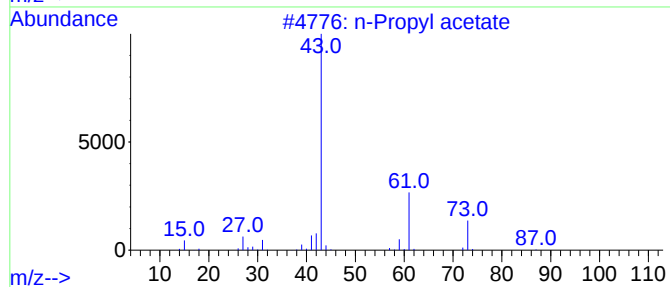
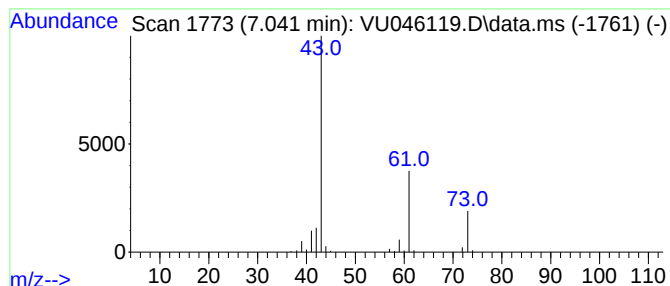
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 n-Propyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.041	9.02 ug/L	83977	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate			102	C5H10O2	000109-60-4	83
2	n-Propyl acetate			102	C5H10O2	000109-60-4	83
3	n-Propyl acetate			102	C5H10O2	000109-60-4	78
4	n-Propyl acetate			102	C5H10O2	000109-60-4	72
5	Propanal, 2,3-dihydroxy-, (S)-			90	C3H6O3	000497-09-6	36



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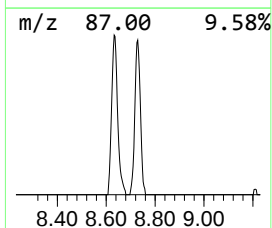
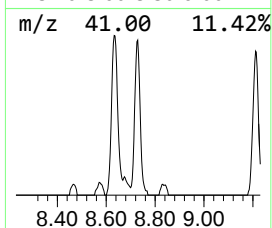
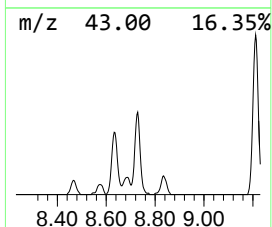
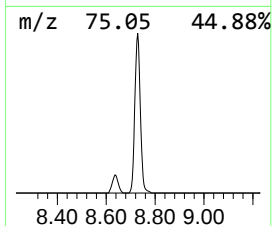
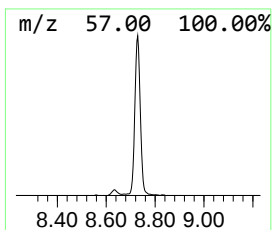
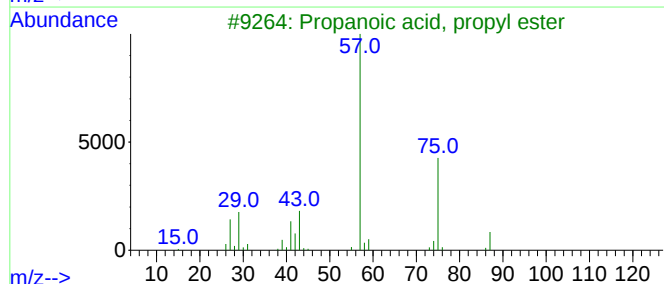
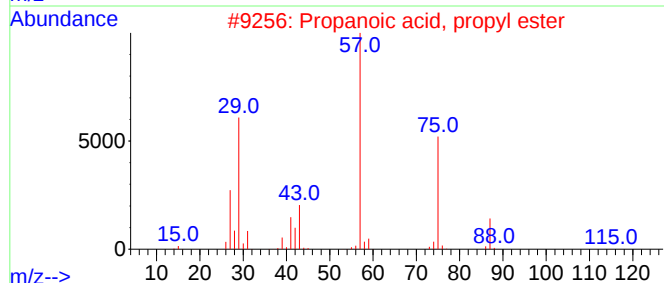
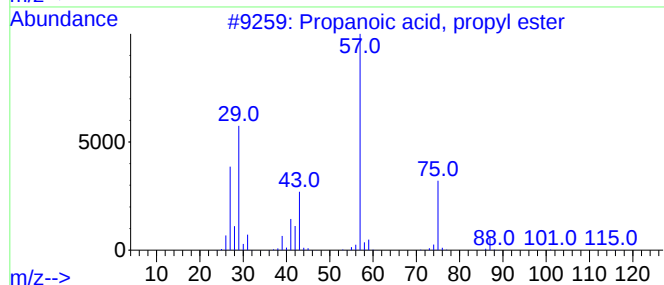
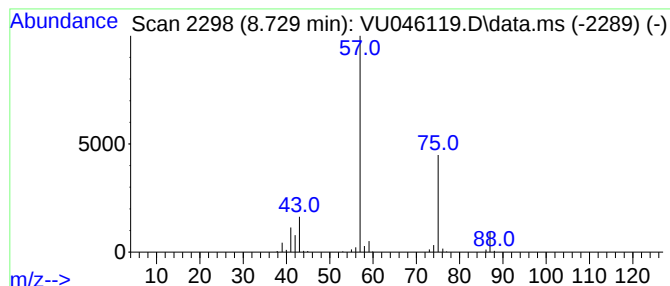
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Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.729	12.19 ug/L	142211	Chlorobenzene-d5	9.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
3			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83



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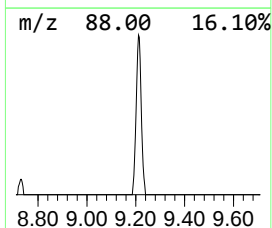
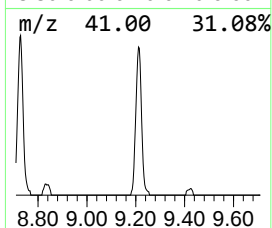
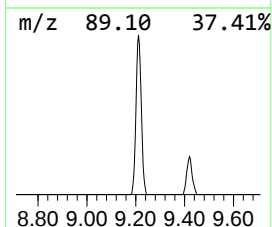
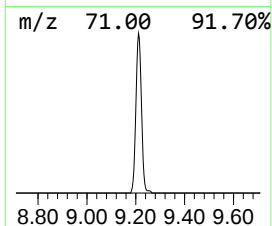
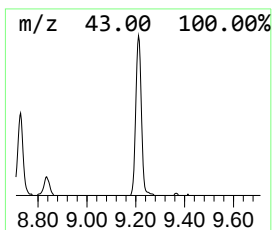
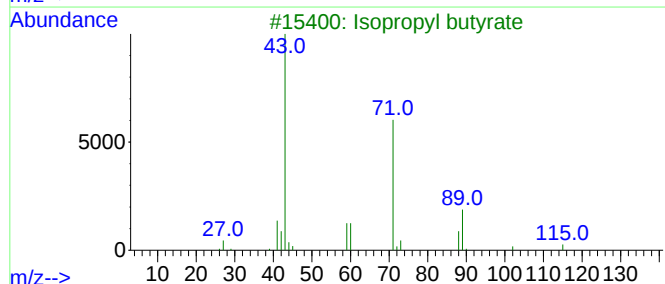
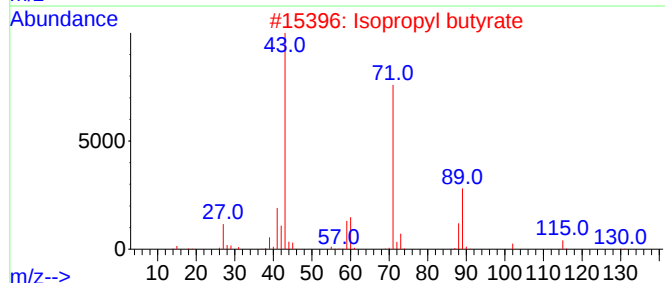
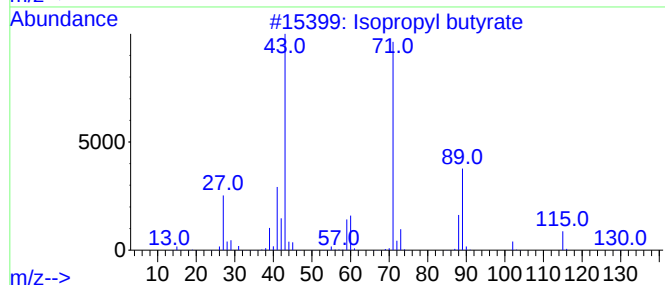
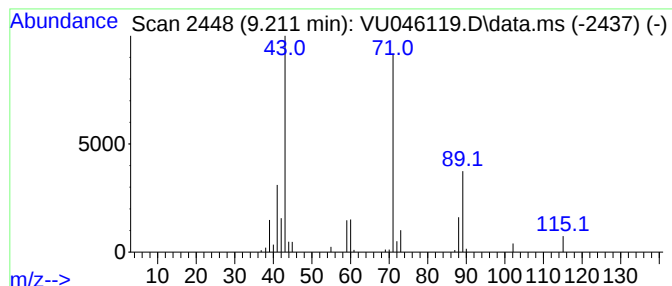
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 Isopropyl butyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.211	7.28 ug/L	84978	Chlorobenzene-d5	9.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	83
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120621\
Data File : VU046119.D
Acq On : 06 Dec 2021 18:19
Operator : SY/MD
Sample : M4938-09 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EX8E5

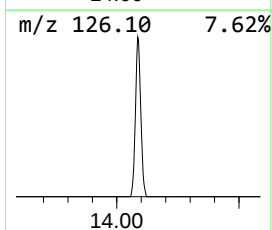
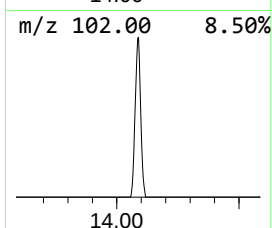
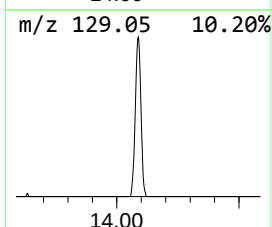
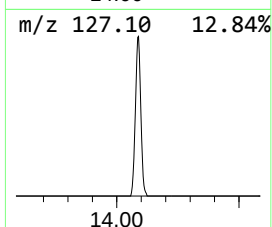
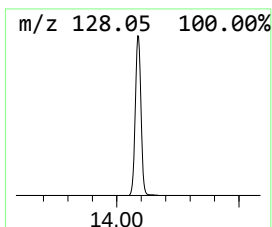
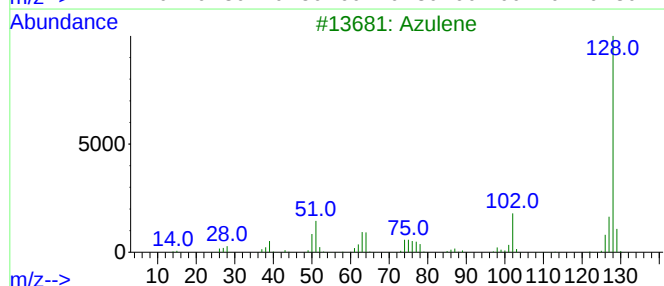
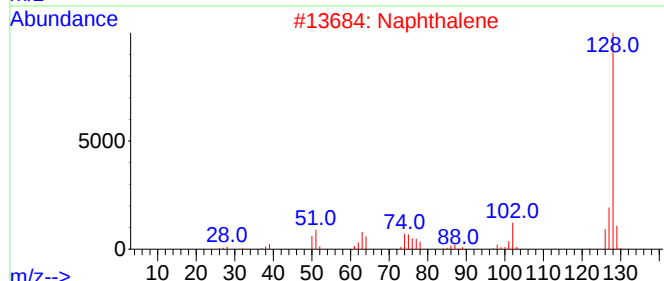
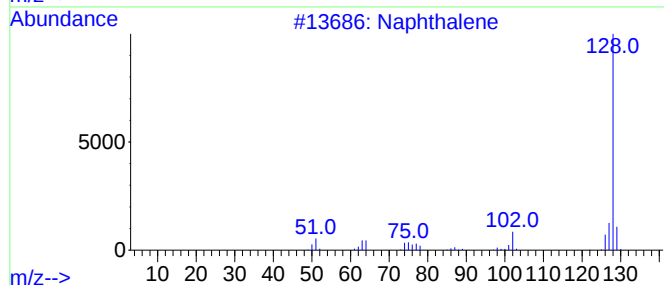
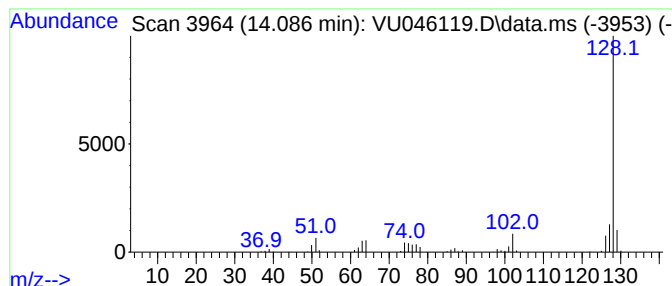
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Quant Title : VOC Analysis

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

Peak Number 6 Azulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.086	13.65 ug/L	169498	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene			128	C10H8	000091-20-3	95
2	Naphthalene			128	C10H8	000091-20-3	94
3	Azulene			128	C10H8	000275-51-4	91
4	Azulene			128	C10H8	000275-51-4	91
5	Azulene			128	C10H8	000275-51-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120621\
Data File : VU046119.D
Acq On : 06 Dec 2021 18:19
Operator : SY/MD
Sample : M4938-09 10X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EX8E5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.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
n-Propyl acetate	7.041	9.0	ug/L	83977	1	6.253	465745	50.0
Propanoic acid,...	8.729	12.2	ug/L	142211	2	9.420	583536	50.0
Isopropyl butyrate	9.211	7.3	ug/L	84978	2	9.420	583536	50.0
Azulene	14.086	13.7	ug/L	169498	3	11.812	620726	50.0