

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091523\
 Data File : VV032124.D
 Acq On : 15 Sep 2023 16:12
 Operator : SY/MD
 Sample : PB155573TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VLEB573

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\SFAMVLM082323WMA.M

Title : VOC Analysis

Signal : TIC: VV032124.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.278	68	74	90	rBV	116952	124858	15.28%	1.762%
2	1.532	146	153	170	rVB	95676	114305	13.99%	1.613%
3	2.059	308	317	329	rBV	182853	266152	32.57%	3.756%
4	2.449	429	438	454	rVB	17265	29657	3.63%	0.419%
5	2.532	462	464	465	rBV	409	162	0.02%	0.002%
6	2.812	548	551	556	rBV3	300	271	0.03%	0.004%
7	2.966	596	599	600	rBV2	402	253	0.03%	0.004%
8	3.043	621	623	626	rVB2	249	119	0.01%	0.002%
9	3.076	627	633	636	rBV	271	220	0.03%	0.003%
10	3.092	636	638	640	rBV2	307	189	0.02%	0.003%
11	3.211	673	675	682	rVB2	298	226	0.03%	0.003%
12	3.240	682	684	686	rBV	160	113	0.01%	0.002%
13	3.272	690	694	698	rVB2	332	325	0.04%	0.005%
14	3.313	705	707	709	rVB	360	154	0.02%	0.002%
15	3.420	738	740	742	rBV2	227	148	0.02%	0.002%
16	3.465	750	754	755	rBV2	342	217	0.03%	0.003%
17	3.677	814	820	824	rBV2	295	304	0.04%	0.004%
18	3.699	824	827	831	rBV2	168	111	0.01%	0.002%
19	3.793	844	856	891	rBV2	70941	211693	25.91%	2.987%
20	4.256	985	1000	1024	rBV	120456	308096	37.71%	4.348%
21	4.529	1082	1085	1087	rBV3	409	293	0.04%	0.004%
22	4.629	1114	1116	1118	rVB	322	115	0.01%	0.002%
23	4.641	1118	1120	1123	rBV2	275	168	0.02%	0.002%
24	4.696	1133	1137	1142	rVB3	356	282	0.03%	0.004%
25	4.738	1146	1150	1151	rBV	238	163	0.02%	0.002%
26	4.776	1160	1162	1165	rBV	279	107	0.01%	0.002%
27	4.802	1168	1170	1173	rBV2	299	178	0.02%	0.003%
28	4.960	1198	1219	1245	rBV2	308084	817053	100.00%	11.530%
29	5.214	1290	1298	1314	rBV2	6667	16920	2.07%	0.239%
30	5.468	1373	1377	1378	rBV2	342	227	0.03%	0.003%
31	5.538	1384	1399	1423	rBV	235989	488406	59.78%	6.892%
32	5.831	1480	1490	1501	rBV4	8066	17433	2.13%	0.246%
33	5.908	1512	1514	1517	rBV3	292	154	0.02%	0.002%
34	5.992	1528	1540	1559	rBV	177156	369477	45.22%	5.214%
35	6.397	1657	1666	1691	rBV	100566	198445	24.29%	2.800%
36	6.918	1817	1828	1864	rBV	97468	190146	23.27%	2.683%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
 Title : VOC Analysis

37	7.127	1884	1893	1903	rBV	22951	38976	4.77%	0.550%
38	7.246	1919	1930	1964	rBV	369969	664178	81.29%	9.373%
39	7.558	2017	2027	2052	rBV	92422	172847	21.15%	2.439%
40	7.770	2090	2093	2095	rBV2	548	342	0.04%	0.005%
41	7.799	2099	2102	2105	rVB2	296	159	0.02%	0.002%
42	7.866	2114	2123	2146	rVB2	34846	66263	8.11%	0.935%
43	8.027	2165	2173	2198	rBV2	191320	352410	43.13%	4.973%
44	8.133	2201	2206	2232	rVB	49221	86157	10.54%	1.216%
45	8.249	2235	2242	2262	rVB2	26332	47561	5.82%	0.671%
46	8.500	2318	2320	2321	rBV	208	117	0.01%	0.002%
47	8.622	2348	2358	2378	rBV	91783	150569	18.43%	2.125%
48	8.789	2398	2410	2435	rBV	367957	620817	75.98%	8.761%
49	9.069	2489	2497	2498	rBV4	1175	1276	0.16%	0.018%
50	9.143	2516	2520	2528	rVB5	389	529	0.06%	0.007%
51	9.210	2538	2541	2543	rBV	224	178	0.02%	0.003%
52	9.349	2580	2584	2589	rBV3	596	643	0.08%	0.009%
53	9.497	2623	2630	2641	rBV3	6469	10907	1.33%	0.154%
54	9.632	2671	2672	2674	rBV	309	126	0.02%	0.002%
55	9.754	2707	2710	2712	rBV2	208	122	0.01%	0.002%
56	9.844	2735	2738	2740	rBV3	183	150	0.02%	0.002%
57	9.873	2740	2747	2752	rVV5	419	630	0.08%	0.009%
58	9.985	2780	2782	2784	rBV2	278	140	0.02%	0.002%
59	10.098	2814	2817	2819	rBV	244	140	0.02%	0.002%
60	10.156	2823	2835	2859	rBV	235198	371834	45.51%	5.247%
61	10.268	2868	2870	2874	rBV2	267	214	0.03%	0.003%
62	10.329	2879	2889	2899	rBV2	11027	17270	2.11%	0.244%
63	10.484	2935	2937	2943	rVB3	634	447	0.05%	0.006%
64	10.522	2947	2949	2951	rBV2	243	121	0.01%	0.002%
65	10.596	2970	2972	2974	rBV	225	111	0.01%	0.002%
66	10.635	2980	2984	2985	rBV2	252	189	0.02%	0.003%
67	10.699	3001	3004	3007	rBV3	223	140	0.02%	0.002%
68	10.725	3007	3012	3015	rBV	350	370	0.05%	0.005%
69	10.786	3029	3031	3033	rBV2	226	120	0.01%	0.002%
70	10.824	3041	3043	3044	rBV	271	114	0.01%	0.002%
71	10.940	3077	3079	3083	rVB2	280	163	0.02%	0.002%
72	10.966	3085	3087	3091	rVB2	198	133	0.02%	0.002%
73	11.043	3109	3111	3114	rBV2	379	186	0.02%	0.003%
74	11.120	3133	3135	3136	rBV	266	108	0.01%	0.002%
75	11.188	3145	3156	3175	rBV	416290	652200	79.82%	9.204%
76	11.361	3208	3210	3213	rVB2	330	108	0.01%	0.002%

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 Title : VOC Analysis

77	11.442	3231	3235	3238	rBV3	419	332	0.04%	0.005%
78	11.564	3260	3273	3297	rBV	368759	589441	72.14%	8.318%
79	11.728	3322	3324	3326	rBV2	583	280	0.03%	0.004%
80	11.850	3358	3362	3364	rVB3	304	155	0.02%	0.002%
81	11.869	3366	3368	3370	rBV2	231	115	0.01%	0.002%
82	11.988	3403	3405	3409	rBV2	182	151	0.02%	0.002%
83	12.033	3416	3419	3424	rVB3	264	249	0.03%	0.004%
84	12.062	3426	3428	3433	rVB2	302	183	0.02%	0.003%
85	12.139	3449	3452	3453	rBV2	201	100	0.01%	0.001%
86	12.197	3460	3470	3483	rVB	5828	9804	1.20%	0.138%
87	12.255	3485	3488	3489	rBV	287	143	0.02%	0.002%
88	12.439	3543	3545	3548	rVB2	232	106	0.01%	0.001%
89	12.599	3592	3595	3598	rBV2	278	166	0.02%	0.002%
90	12.876	3677	3681	3682	rBV	433	240	0.03%	0.003%
91	13.033	3727	3730	3733	rVB	384	249	0.03%	0.004%
92	13.252	3795	3798	3801	rBV	219	199	0.02%	0.003%
93	13.303	3812	3814	3820	rVB2	427	263	0.03%	0.004%
94	13.445	3846	3858	3874	rBV	34099	56475	6.91%	0.797%
95	13.574	3889	3898	3908	rBV4	1574	2525	0.31%	0.036%
96	13.644	3917	3920	3922	rBV	174	99	0.01%	0.001%
97	13.818	3972	3974	3978	rBV	263	172	0.02%	0.002%
98	13.898	3995	3999	4003	rBV2	448	454	0.06%	0.006%
99	14.281	4114	4118	4120	rBV	383	285	0.03%	0.004%
100	14.580	4203	4211	4224	rVB2	4865	7702	0.94%	0.109%

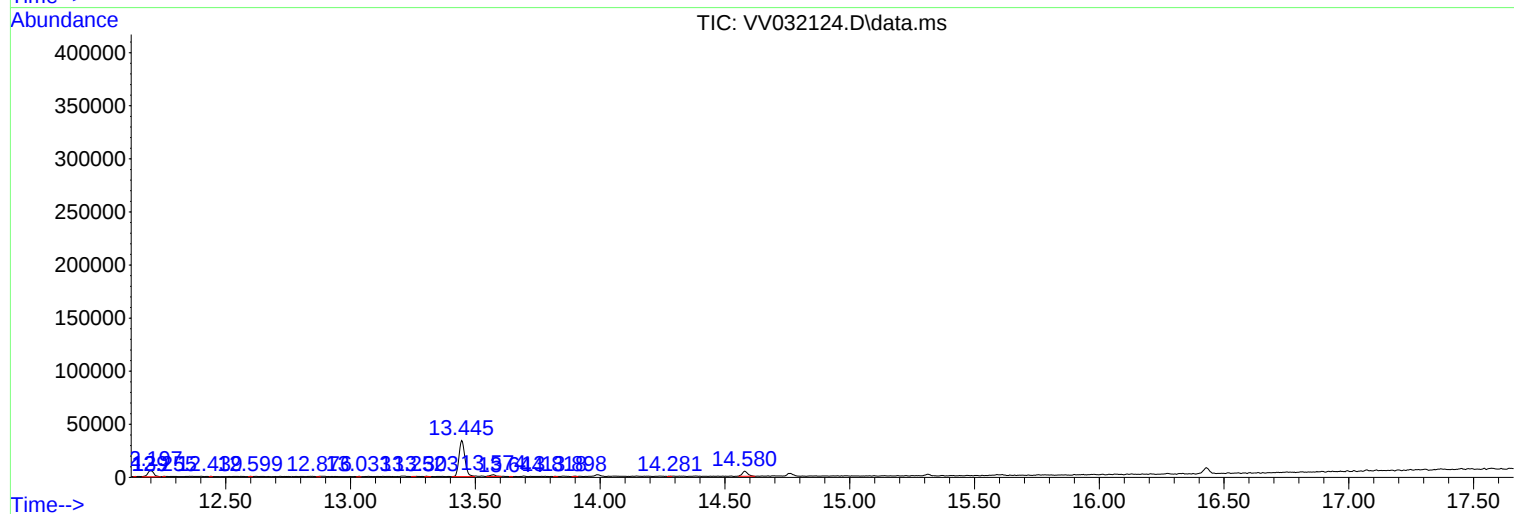
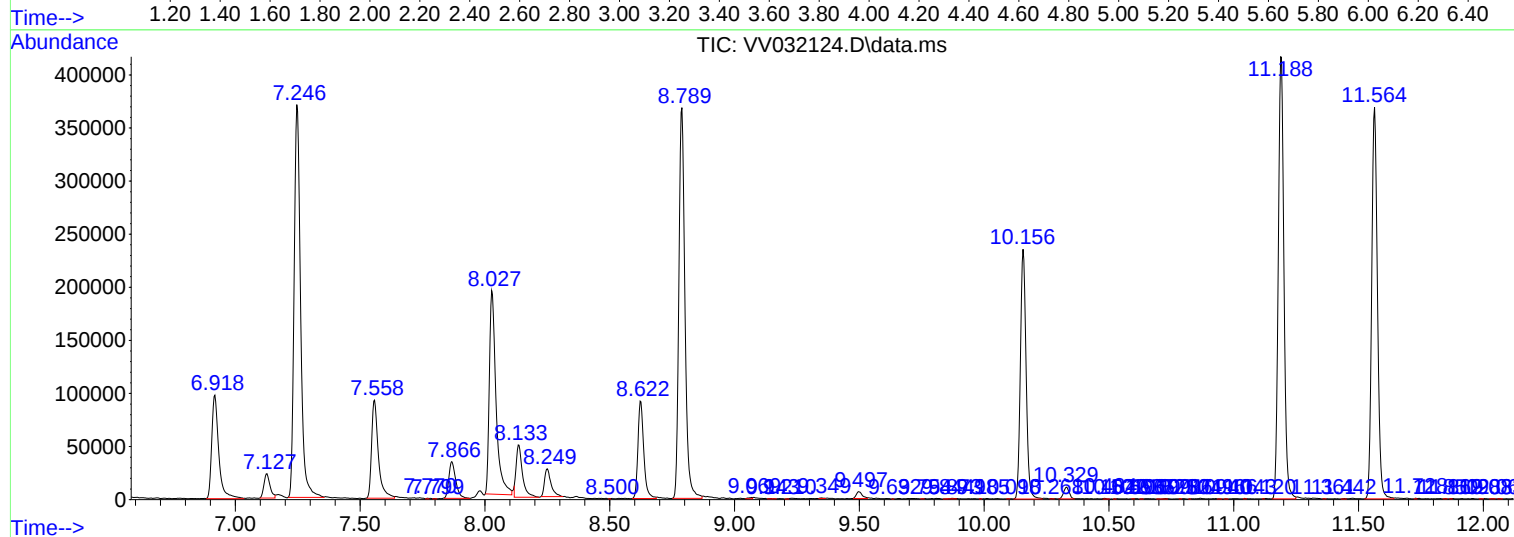
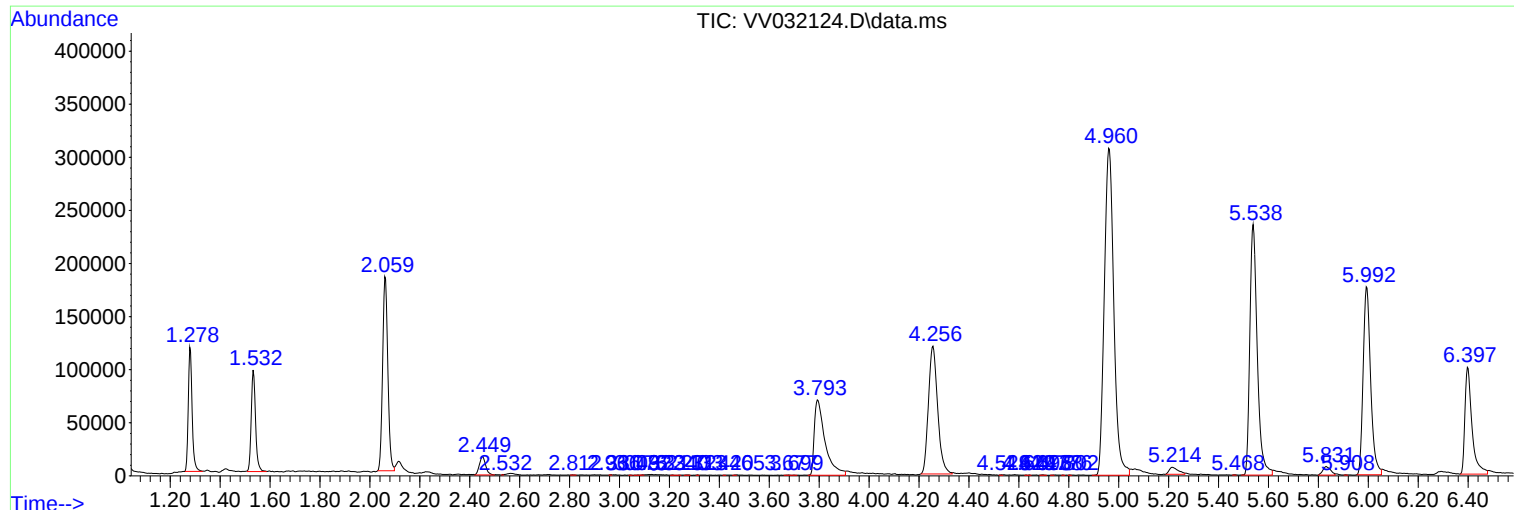
Sum of corrected areas: 7086093

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

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



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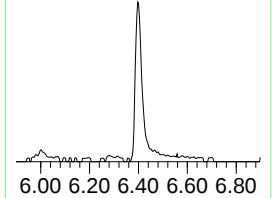
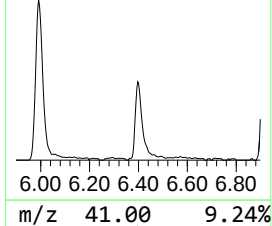
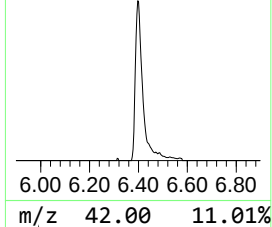
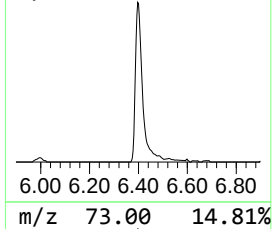
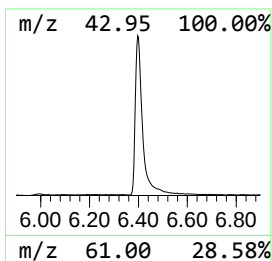
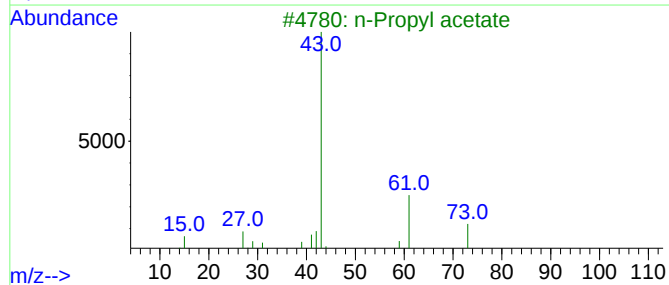
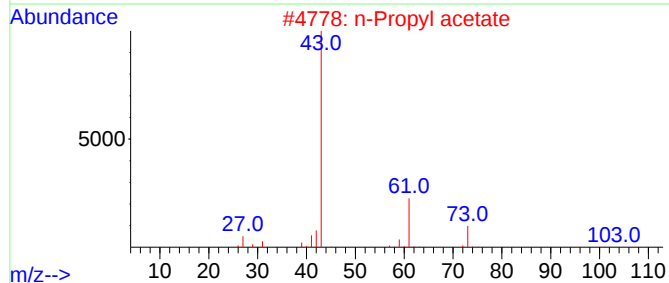
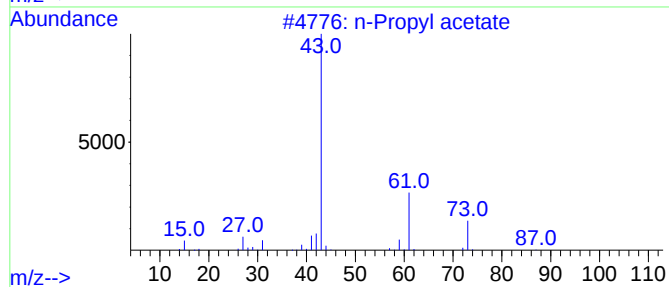
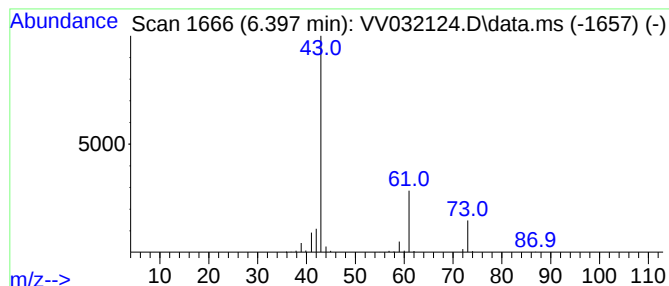
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.397	20.32 ug/L	198445	1,4-Difluorobenzene	5.538

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	78
3	n-Propyl acetate			102	C5H10O2	000109-60-4	72
4	n-Propyl acetate			102	C5H10O2	000109-60-4	64
5	n-Propyl acetate			102	C5H10O2	000109-60-4	56



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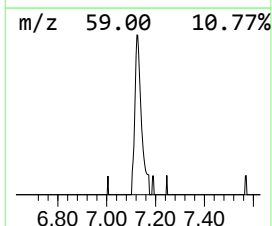
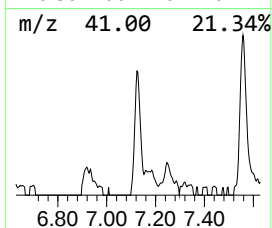
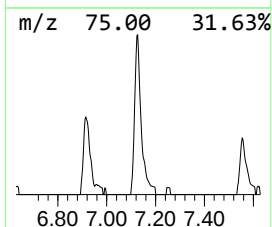
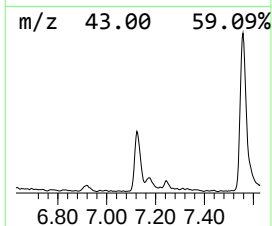
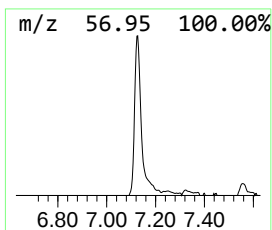
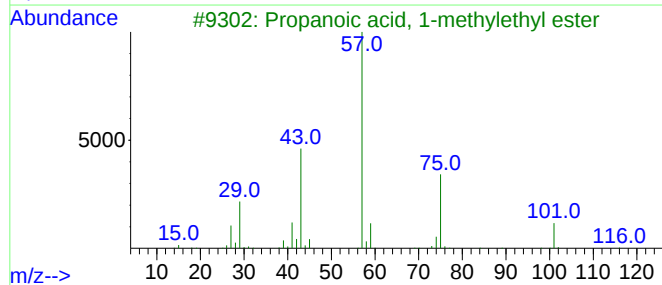
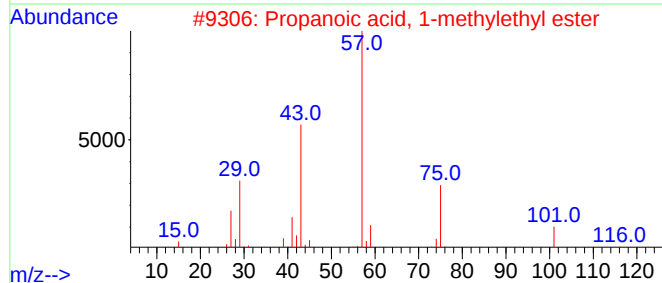
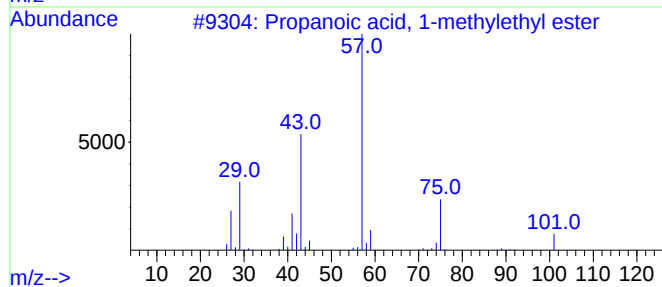
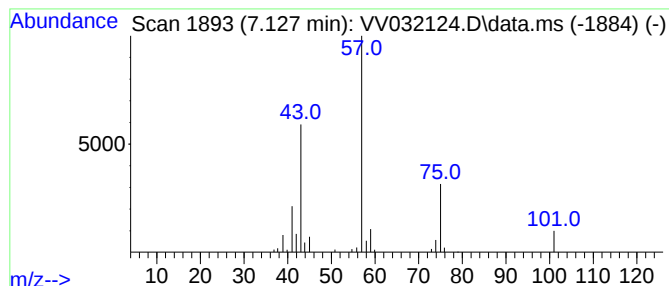
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.127	3.99 ug/L	38976	1,4-Difluorobenzene	5.538

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	78
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	72
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	59



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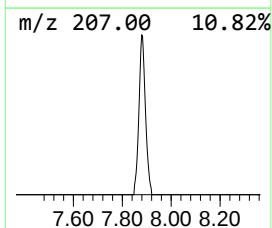
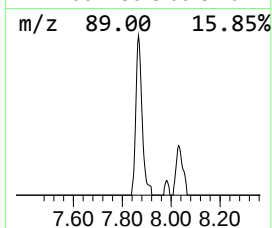
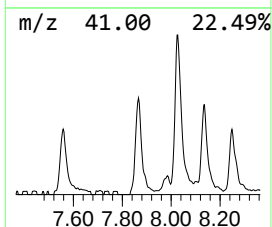
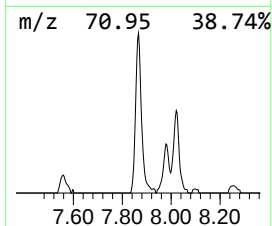
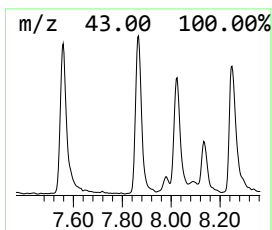
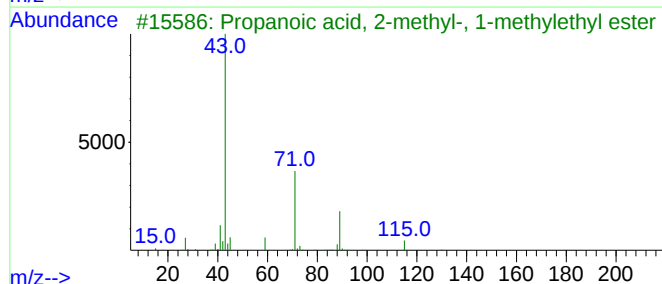
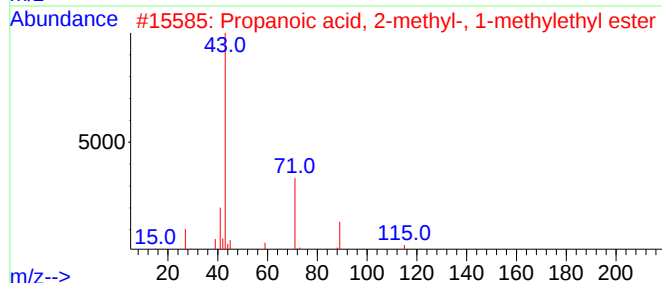
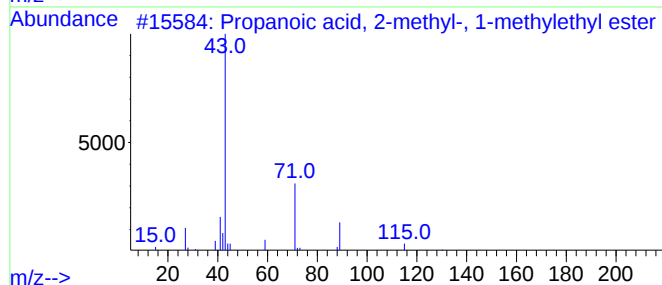
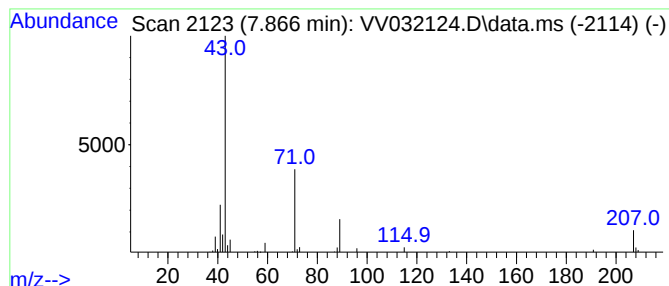
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.866	5.34 ug/L	66263	Chlorobenzene-d5	8.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59
2			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59
3			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091523\
Data File : VV032124.D
Acq On : 15 Sep 2023 16:12
Operator : SY/MD
Sample : PB155573TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB573

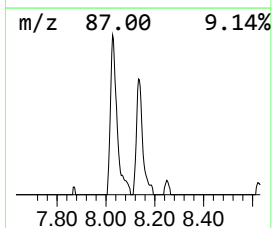
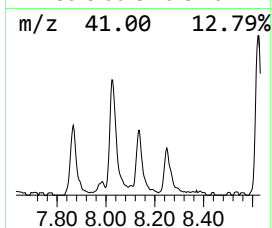
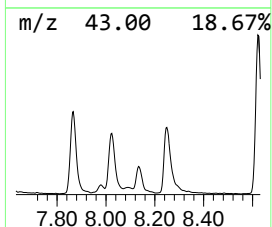
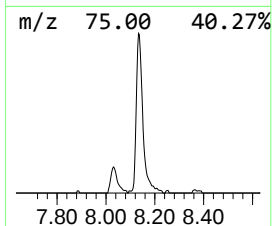
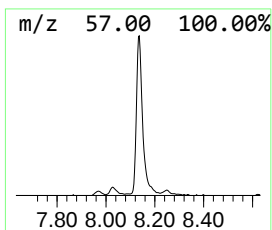
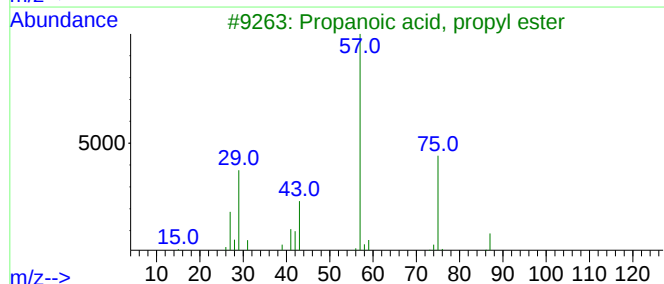
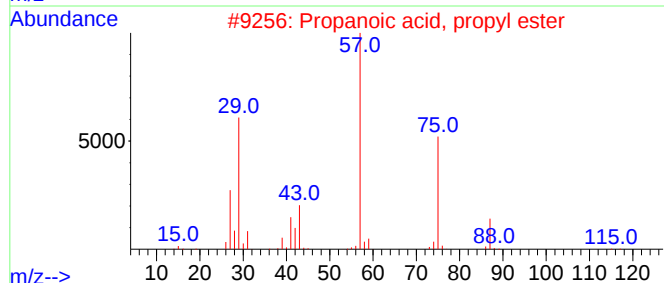
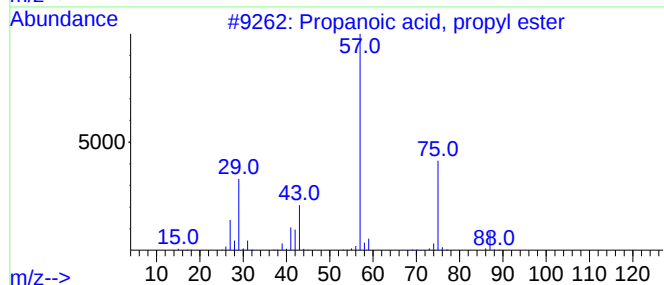
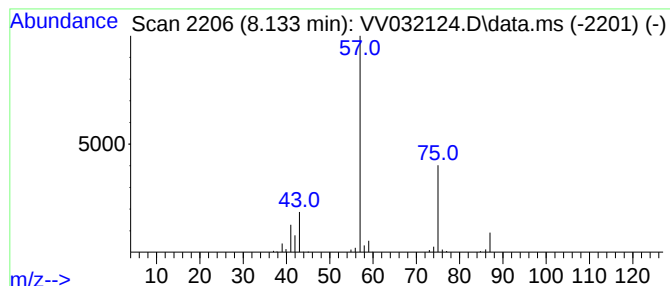
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Quant Title : VOC Analysis

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

Peak Number 6 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.133	6.94 ug/L	86157	Chlorobenzene-d5	8.789

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	74
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091523\
Data File : VV032124.D
Acq On : 15 Sep 2023 16:12
Operator : SY/MD
Sample : PB155573TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB573

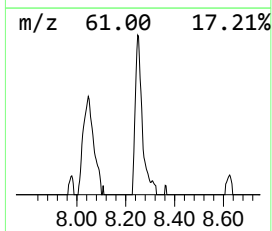
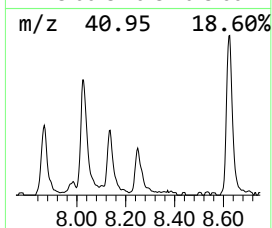
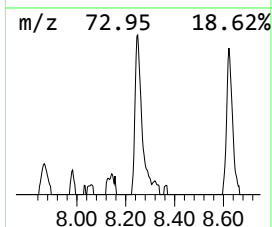
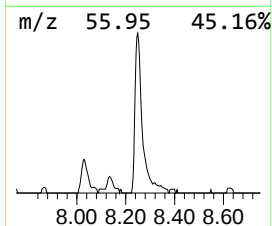
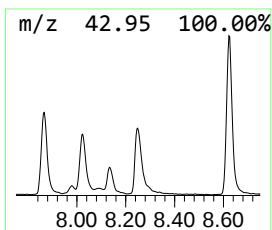
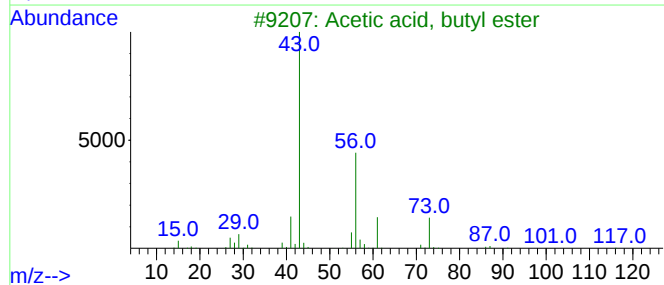
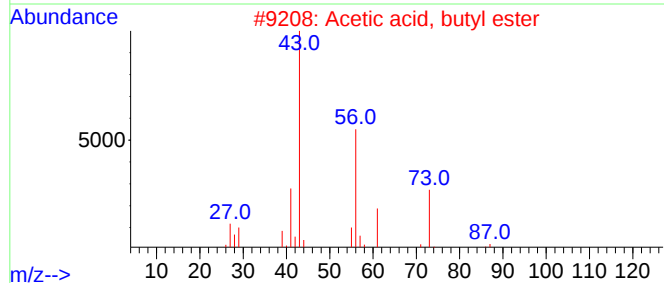
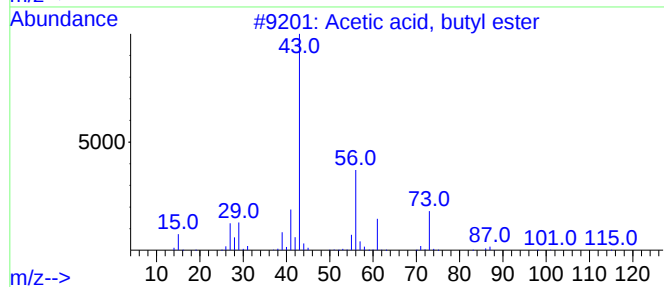
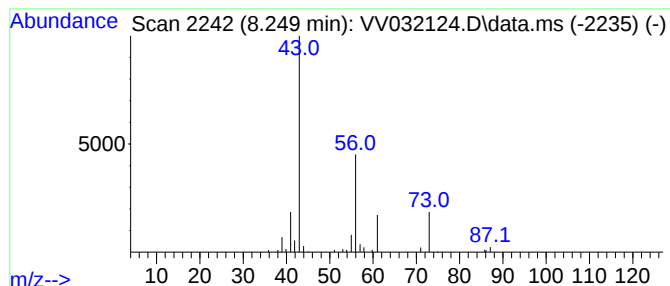
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Quant Title : VOC Analysis

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

Peak Number 7 Acetic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.249	3.83 ug/L	47561	Chlorobenzene-d5	8.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83		
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72		
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64		
4	Isobutyl acetate	116	C6H12O2	000110-19-0	50		
5	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	50		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091523\
Data File : VV032124.D
Acq On : 15 Sep 2023 16:12
Operator : SY/MD
Sample : PB155573TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB573

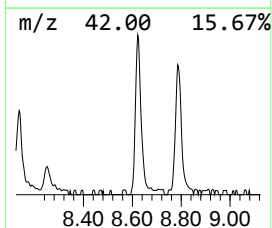
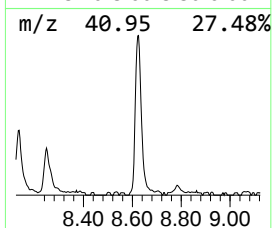
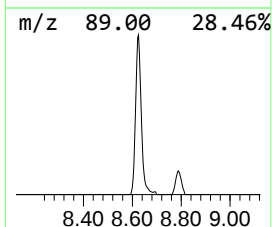
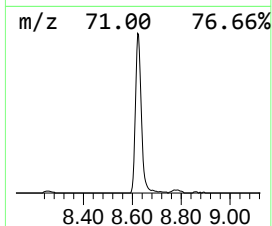
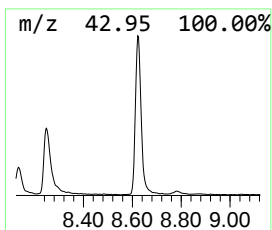
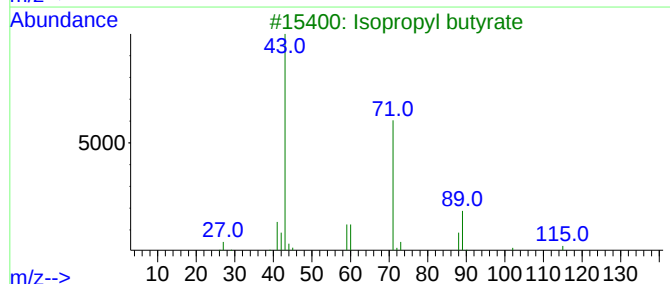
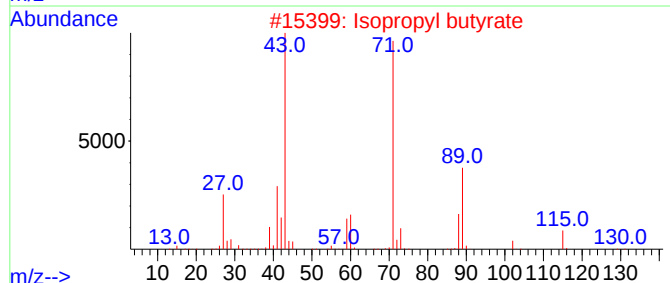
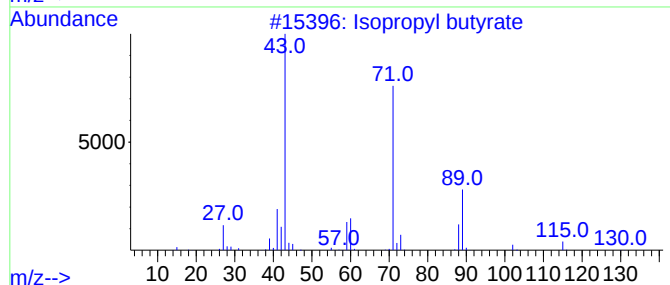
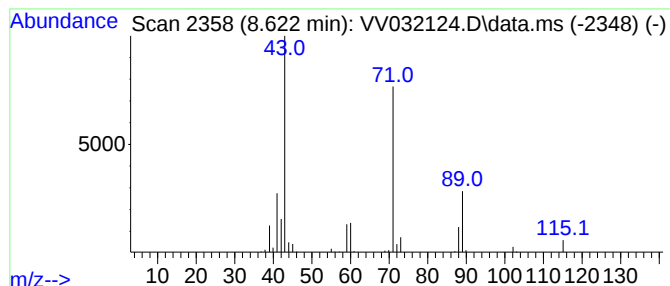
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Quant Title : VOC Analysis

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

Peak Number 8 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.622	12.13 ug/L	150569	Chlorobenzene-d5	8.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
2			Isopropyl butyrate	130	C7H14O2	000638-11-9	90
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	78
4			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091523\
Data File : VV032124.D
Acq On : 15 Sep 2023 16:12
Operator : SY/MD
Sample : PB155573TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB573

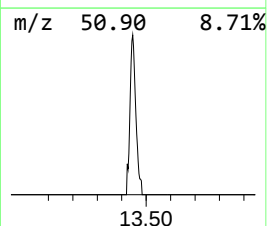
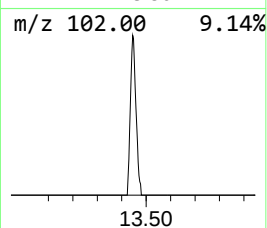
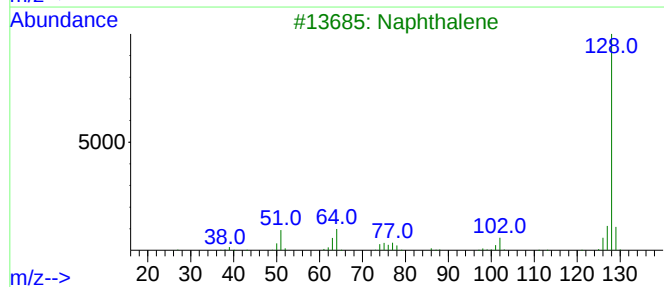
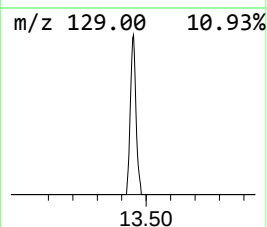
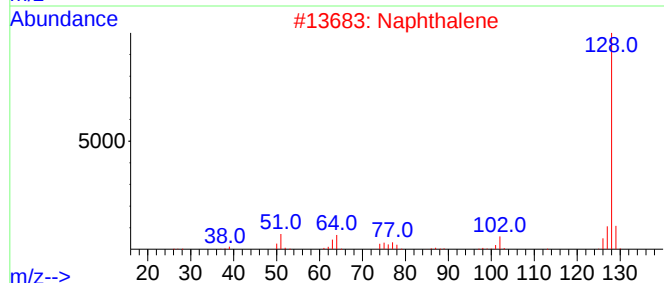
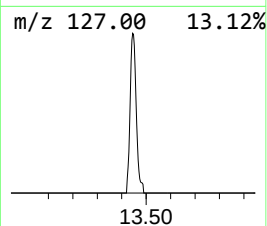
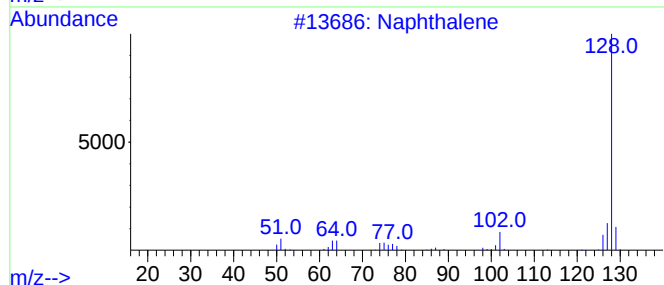
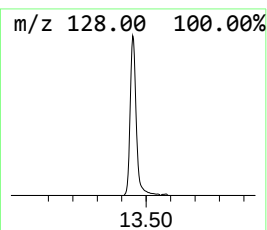
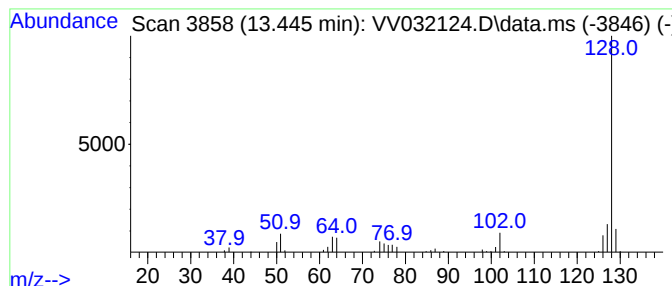
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Quant Title : VOC Analysis

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

Peak Number 9 Azulene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.445	4.33 ug/L	56475	1,4-Dichlorobenzene-d4	11.191

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			Naphthalene	128	C10H8	000091-20-3	93
4			Azulene	128	C10H8	000275-51-4	91
5			Azulene	128	C10H8	000275-51-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV091523\
Data File : VV032124.D
Acq On : 15 Sep 2023 16:12
Operator : SY/MD
Sample : PB155573TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB573

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	6.397	20.3	ug/L	198445	1	5.538	488406	50.0
Propanoic acid,...	7.127	4.0	ug/L	38976	1	5.538	488406	50.0
Propanoic acid,...	7.866	5.3	ug/L	66263	2	8.789	620817	50.0
Propanoic acid,...	8.133	6.9	ug/L	86157	2	8.789	620817	50.0
Acetic acid, bu...	8.249	3.8	ug/L	47561	2	8.789	620817	50.0
Isopropyl butyrate	8.622	12.1	ug/L	150569	2	8.789	620817	50.0
Azulene	13.445	4.3	ug/L	56475	3	11.191	652200	50.0