

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011024\
 Data File : VV033563.D
 Acq On : 10 Jan 2024 16:18
 Operator : SY/MD
 Sample : PB158329TB 10X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VLEB329

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\SFAMVLM011024WMA.M

Title : VOC Analysis

Signal : TIC: VV033563.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.166	36	39	43	rVB	1419	1202	0.09%	0.011%
2	1.220	50	56	61	rBV6	2762	4650	0.33%	0.042%
3	1.278	68	74	91	rBV	201752	212255	15.27%	1.910%
4	1.529	145	152	174	rVB	152146	188665	13.57%	1.698%
5	2.060	308	317	331	rBV	312563	451959	32.51%	4.067%
6	2.449	430	438	453	rVB2	11291	20105	1.45%	0.181%
7	2.542	463	467	468	rBV3	539	383	0.03%	0.003%
8	2.638	495	497	502	rVB3	548	429	0.03%	0.004%
9	2.696	508	515	516	rBV4	2923	2610	0.19%	0.023%
10	2.802	546	548	552	rVB2	646	370	0.03%	0.003%
11	3.005	607	611	616	rBV4	557	550	0.04%	0.005%
12	3.066	625	630	632	rVB4	496	416	0.03%	0.004%
13	3.111	637	644	645	rBV4	780	698	0.05%	0.006%
14	3.275	690	695	697	rBV5	396	377	0.03%	0.003%
15	3.410	732	737	741	rBV6	452	457	0.03%	0.004%
16	3.465	748	754	757	rBV5	494	536	0.04%	0.005%
17	3.638	802	808	809	rBV4	677	400	0.03%	0.004%
18	3.783	844	853	892	rBV	88614	246206	17.71%	2.215%
19	4.159	967	970	974	rBV5	740	727	0.05%	0.007%
20	4.249	981	998	1024	rBV	207362	531360	38.22%	4.781%
21	4.452	1057	1061	1065	rVB6	891	774	0.06%	0.007%
22	4.474	1065	1068	1070	rBV4	597	356	0.03%	0.003%
23	4.635	1115	1118	1124	rVB7	642	677	0.05%	0.006%
24	4.670	1126	1129	1131	rVB3	684	415	0.03%	0.004%
25	4.793	1164	1167	1172	rBV5	464	427	0.03%	0.004%
26	4.957	1200	1218	1249	rBV2	521316	1390190	100.00%	12.508%
27	5.214	1287	1298	1311	rBV3	8182	20372	1.47%	0.183%
28	5.532	1386	1397	1433	rBV	364645	754910	54.30%	6.792%
29	5.834	1481	1491	1505	rBV6	6515	14157	1.02%	0.127%
30	5.989	1524	1539	1569	rBV	308529	640195	46.05%	5.760%
31	6.304	1629	1637	1644	rBV5	1956	4457	0.32%	0.040%
32	6.394	1657	1665	1700	rBV	107261	215702	15.52%	1.941%
33	6.757	1775	1778	1782	rVB2	486	364	0.03%	0.003%
34	6.815	1792	1796	1800	rVB4	508	376	0.03%	0.003%
35	6.911	1814	1826	1859	rBV	184976	349055	25.11%	3.141%
36	7.120	1882	1891	1902	rBV	25763	44260	3.18%	0.398%

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Integrator: RTE

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 Title : VOC Analysis

37	7.243	1918	1929	1953	rBV	628232	1110782	79.90%	9.994%
38	7.555	2015	2026	2053	rBV	153108	285853	20.56%	2.572%
39	7.780	2091	2096	2108	rVB	1953	4209	0.30%	0.038%
40	7.860	2108	2121	2134	rBV	33743	59700	4.29%	0.537%
41	7.976	2150	2157	2162	rVV7	7048	10423	0.75%	0.094%
42	8.024	2163	2172	2198	rVV	326721	626184	45.04%	5.634%
43	8.133	2199	2206	2227	rVB	48294	91120	6.55%	0.820%
44	8.249	2233	2242	2260	rBV	26395	48420	3.48%	0.436%
45	8.574	2340	2343	2348	rBV5	443	473	0.03%	0.004%
46	8.619	2348	2357	2375	rBV	96821	154916	11.14%	1.394%
47	8.783	2397	2408	2437	rBV	538244	916396	65.92%	8.245%
48	8.960	2457	2463	2471	rVB4	2866	4061	0.29%	0.037%
49	9.050	2487	2491	2493	rBV3	1043	811	0.06%	0.007%
50	9.088	2496	2503	2513	rVV7	2698	5552	0.40%	0.050%
51	9.127	2513	2515	2518	rVB4	713	352	0.03%	0.003%
52	9.169	2524	2528	2534	rVB7	592	539	0.04%	0.005%
53	9.252	2551	2554	2560	rBV4	548	547	0.04%	0.005%
54	9.432	2605	2610	2614	rVB6	406	510	0.04%	0.005%
55	9.490	2618	2628	2634	rBV2	9489	16923	1.22%	0.152%
56	9.670	2680	2684	2686	rBV3	985	609	0.04%	0.005%
57	9.834	2731	2735	2739	rBV5	518	428	0.03%	0.004%
58	9.873	2741	2747	2756	rBV4	1673	2343	0.17%	0.021%
59	10.008	2784	2789	2791	rBV3	570	427	0.03%	0.004%
60	10.024	2791	2794	2799	rVV4	567	396	0.03%	0.004%
61	10.091	2810	2815	2817	rBV4	634	522	0.04%	0.005%
62	10.107	2817	2820	2821	rVV4	628	422	0.03%	0.004%
63	10.152	2822	2834	2875	rVB	364668	593466	42.69%	5.340%
64	10.487	2930	2938	2943	rBV5	2108	2995	0.22%	0.027%
65	10.776	3023	3028	3031	rBV5	829	656	0.05%	0.006%
66	10.863	3047	3055	3065	rVB5	2968	4918	0.35%	0.044%
67	10.985	3089	3093	3097	rVV5	565	477	0.03%	0.004%
68	11.043	3107	3111	3115	rVB5	522	422	0.03%	0.004%
69	11.124	3132	3136	3138	rBV4	1397	1146	0.08%	0.010%
70	11.185	3144	3155	3182	rBV	573193	907117	65.25%	8.162%
71	11.294	3186	3189	3195	rVB7	809	809	0.06%	0.007%
72	11.365	3208	3211	3216	rVB4	570	503	0.04%	0.005%
73	11.561	3259	3272	3299	rBV	619842	997084	71.72%	8.971%
74	11.747	3328	3330	3332	rBV2	595	400	0.03%	0.004%
75	11.857	3358	3364	3369	rBV6	578	690	0.05%	0.006%
76	11.969	3396	3399	3401	rBV2	461	342	0.02%	0.003%

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Integrator: RTE

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Sampling : 1

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Peak separation: 5

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 Title : VOC Analysis

77	12.072	3427	3431	3435	rBV5	681	671	0.05%	0.006%
78	12.210	3470	3474	3477	rBV4	598	505	0.04%	0.005%
79	12.246	3480	3485	3488	rBV4	459	528	0.04%	0.005%
80	12.368	3513	3523	3532	rBV7	3994	6404	0.46%	0.058%
81	12.586	3587	3591	3603	rVV5	1959	2956	0.21%	0.027%
82	12.664	3612	3615	3619	rBV3	750	538	0.04%	0.005%
83	12.696	3623	3625	3630	rVB3	570	423	0.03%	0.004%
84	12.731	3630	3636	3639	rBV5	604	744	0.05%	0.007%
85	12.850	3667	3673	3675	rBV4	534	495	0.04%	0.004%
86	12.953	3701	3705	3706	rBV2	624	426	0.03%	0.004%
87	13.008	3718	3722	3725	rVV3	676	560	0.04%	0.005%
88	13.130	3758	3760	3765	rVV6	581	432	0.03%	0.004%
89	13.204	3773	3783	3796	rBV2	16636	27109	1.95%	0.244%
90	13.310	3810	3816	3818	rBV4	466	479	0.03%	0.004%
91	13.384	3832	3839	3846	rVV3	7779	9759	0.70%	0.088%
92	13.445	3849	3858	3875	rVV	56616	97521	7.01%	0.877%
93	13.689	3927	3934	3946	rVB6	3557	5863	0.42%	0.053%
94	13.786	3961	3964	3968	rVB4	798	681	0.05%	0.006%
95	13.853	3981	3985	3988	rBV3	577	412	0.03%	0.004%
96	14.303	4121	4125	4127	rBV4	460	392	0.03%	0.004%
97	14.390	4148	4152	4155	rBV2	651	513	0.04%	0.005%
98	14.574	4205	4209	4210	rBV2	662	422	0.03%	0.004%
99	14.689	4241	4245	4249	rBV4	637	583	0.04%	0.005%
100	15.123	4378	4380	4386	rBV5	720	660	0.05%	0.006%

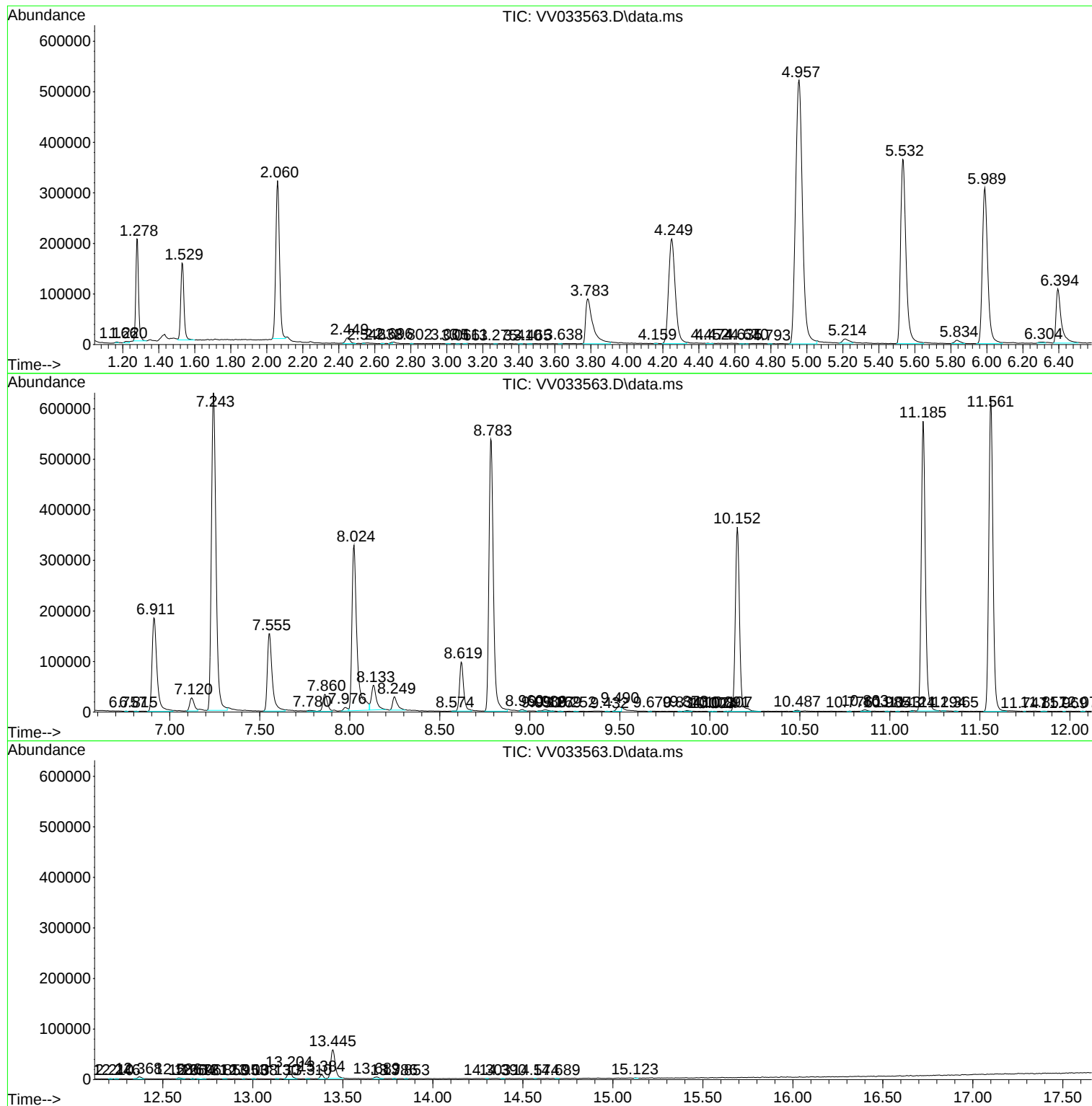
Sum of corrected areas: 11114061

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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



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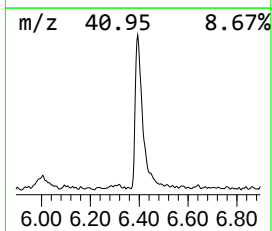
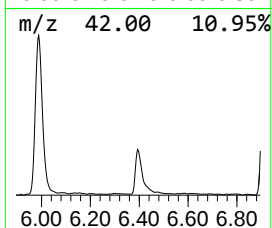
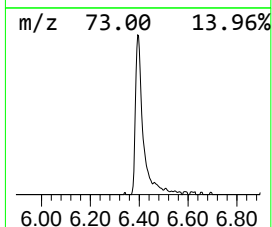
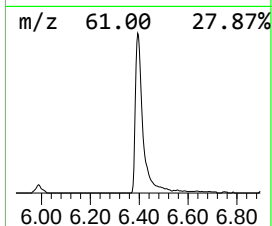
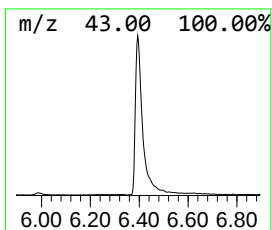
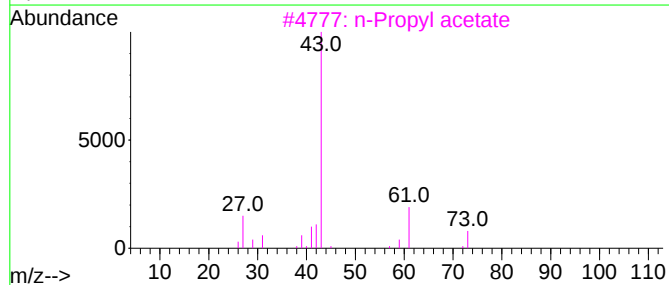
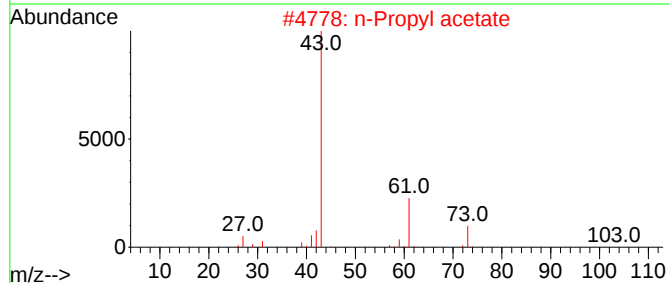
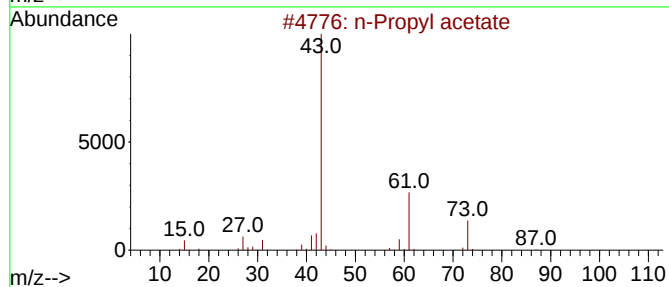
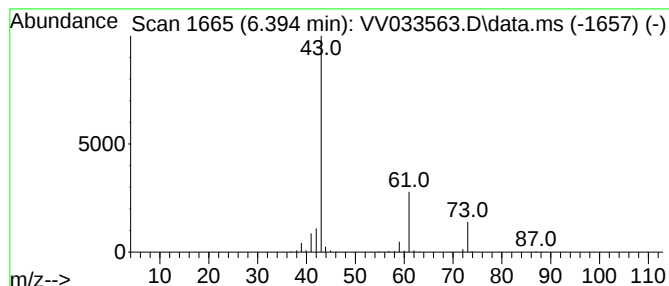
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.394	14.29 ug/L	215702	1,4-Difluorobenzene	5.535

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



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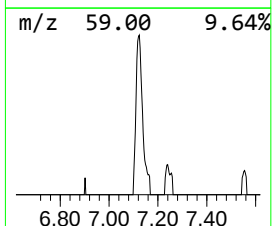
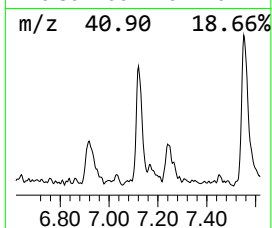
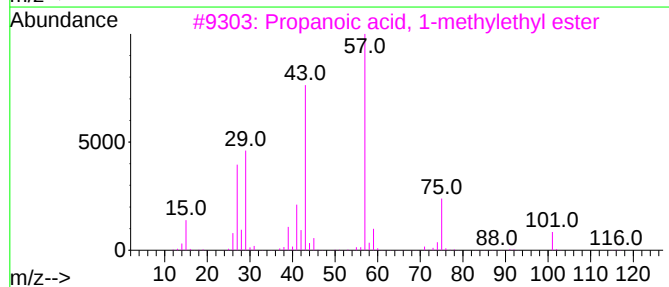
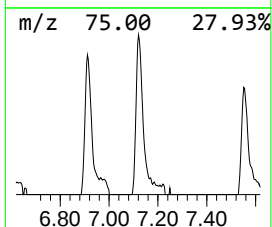
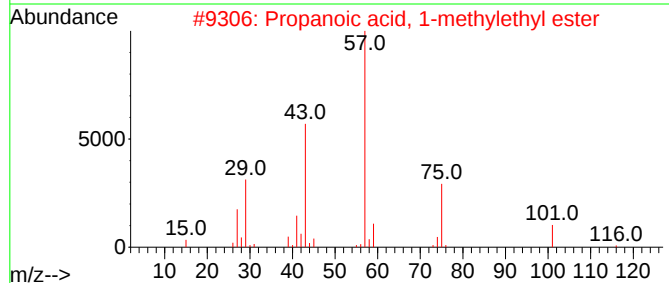
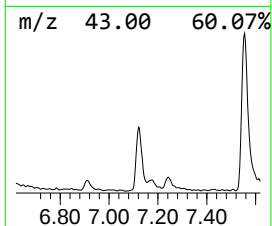
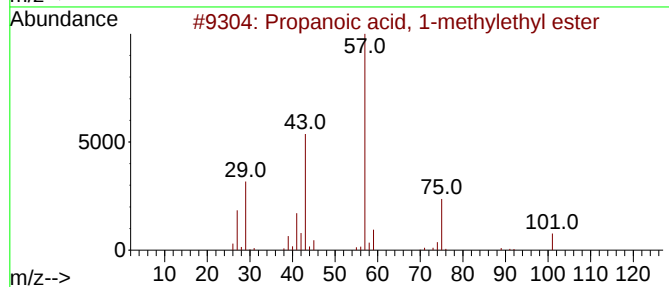
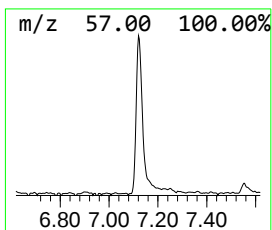
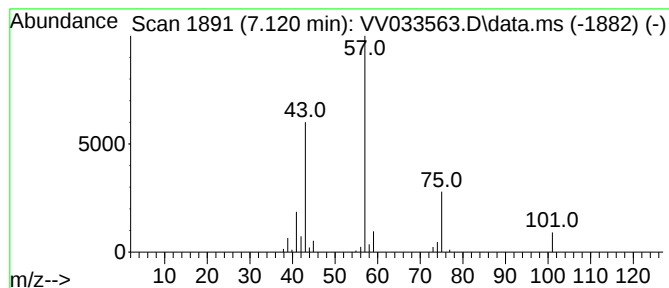
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.120	2.93 ug/L	44260	1,4-Difluorobenzene	5.535

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
2			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
4			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	64
5			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	36



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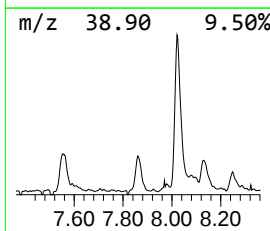
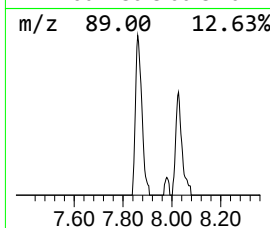
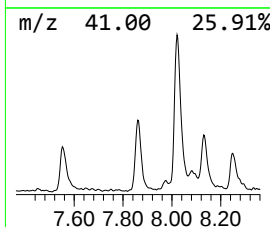
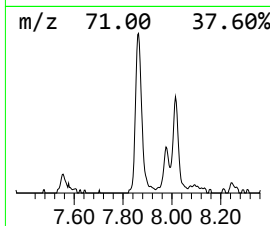
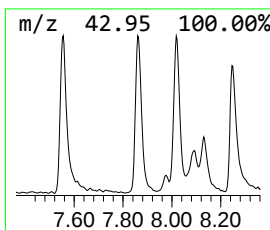
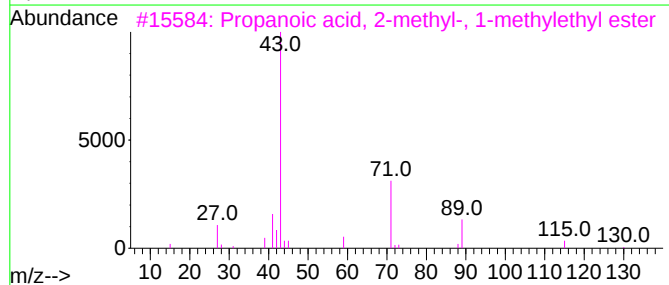
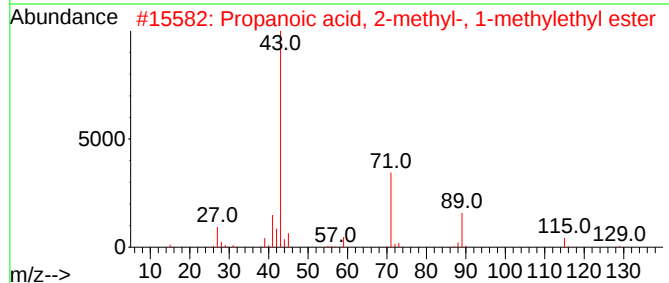
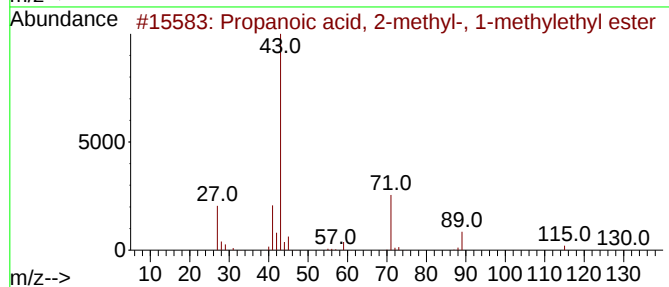
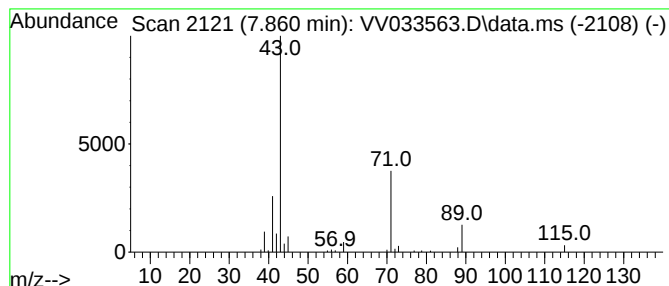
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.860	3.26 ug/L	59700	Chlorobenzene-d5	8.786

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-, 1-met...	130	C7H14O2	000617-50-5	83
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011024\
Data File : VV033563.D
Acq On : 10 Jan 2024 16:18
Operator : SY/MD
Sample : PB158329TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB329

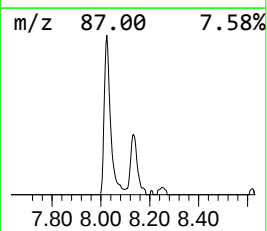
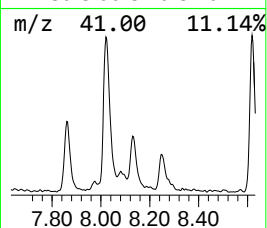
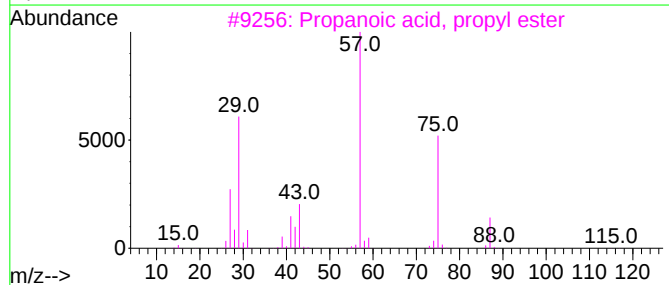
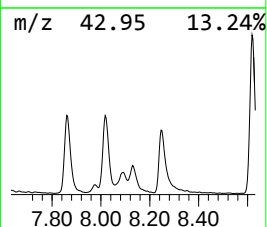
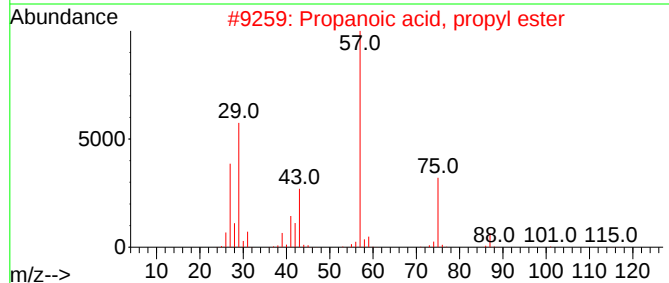
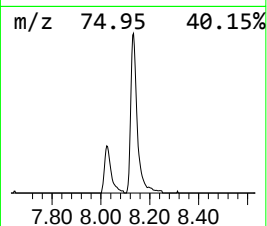
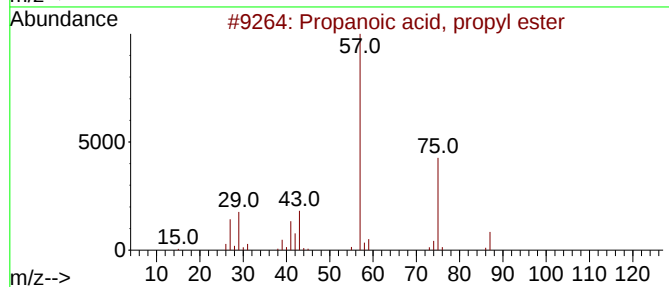
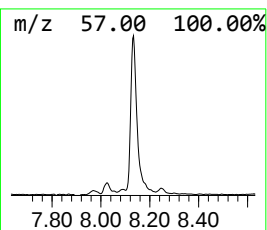
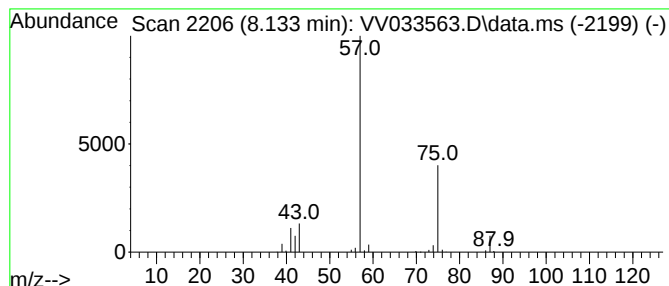
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Quant Title : VOC Analysis

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

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.133	4.97 ug/L	91120	Chlorobenzene-d5	8.786

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	74
3			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	72
4			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	72
5			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011024\
Data File : VV033563.D
Acq On : 10 Jan 2024 16:18
Operator : SY/MD
Sample : PB158329TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB329

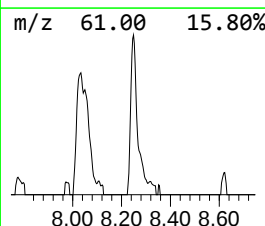
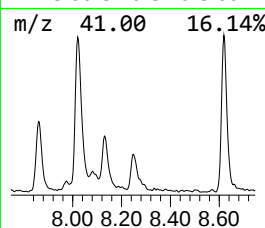
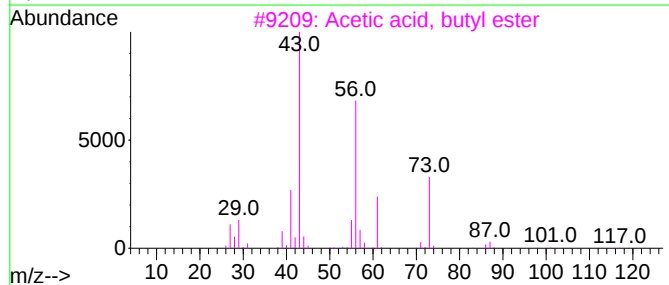
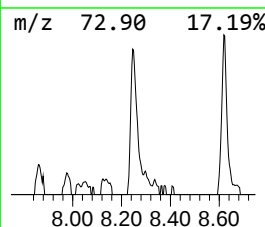
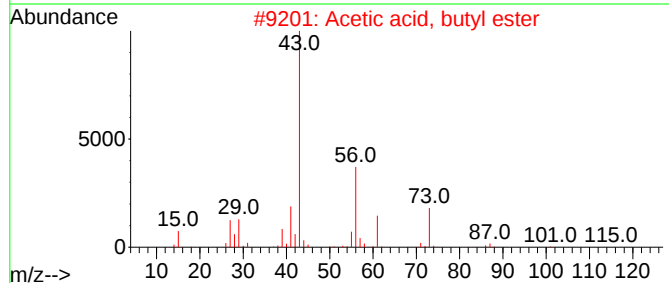
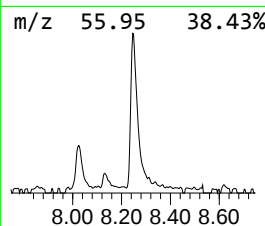
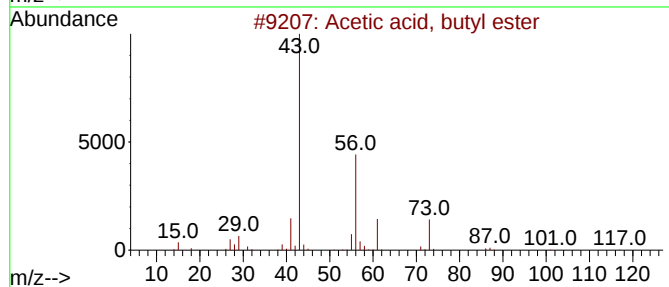
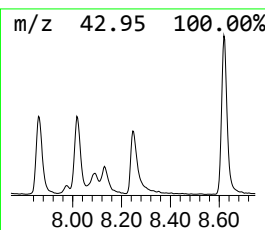
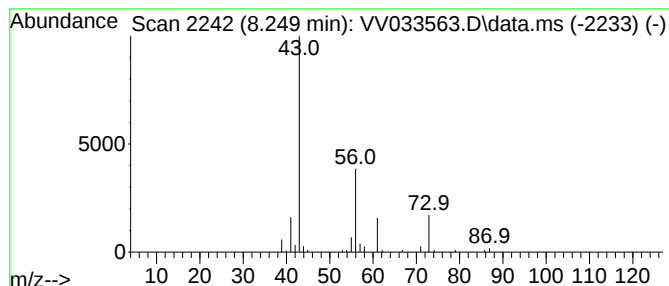
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Quant Title : VOC Analysis

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

Peak Number 6 Acetic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.249	2.64 ug/L	48420	Chlorobenzene-d5	8.786

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	90
2			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
3			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
5			Isobutyl acetate	116	C6H12O2	000110-19-0	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011024\
Data File : VV033563.D
Acq On : 10 Jan 2024 16:18
Operator : SY/MD
Sample : PB158329TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB329

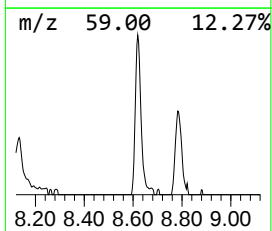
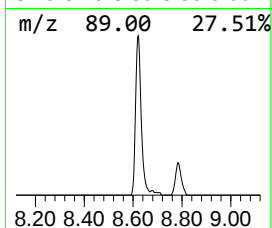
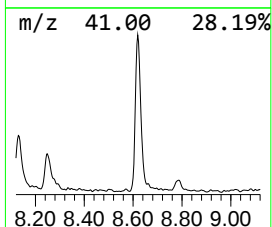
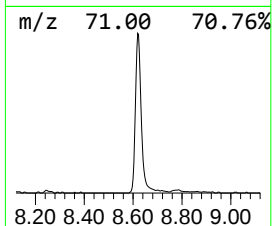
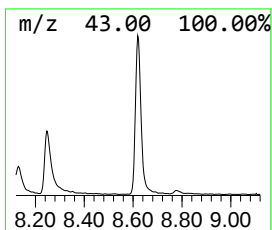
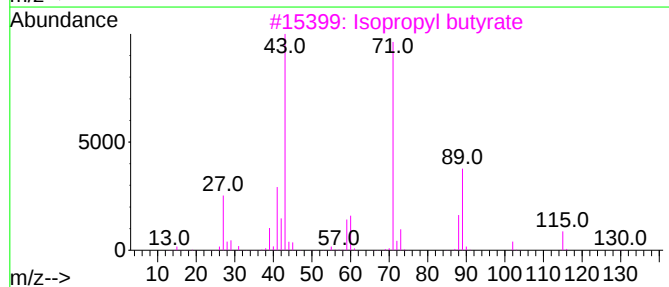
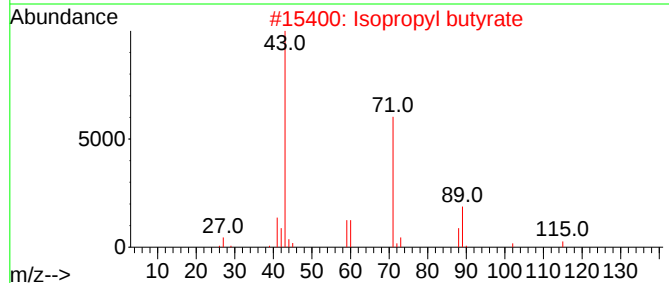
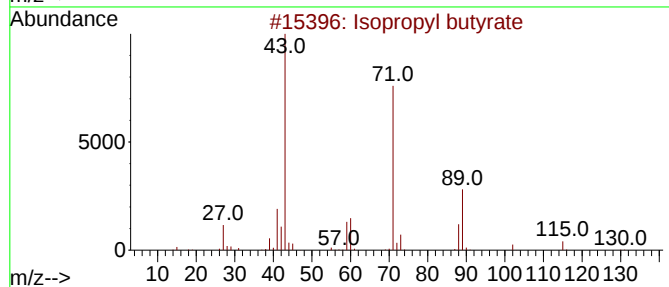
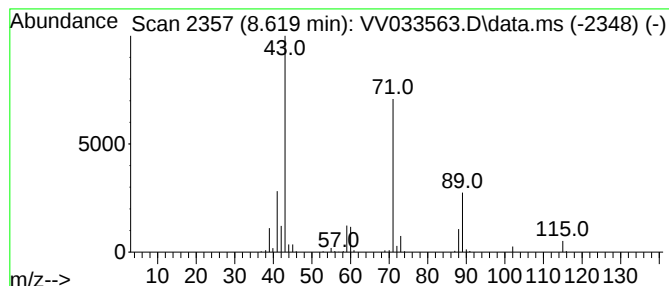
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Quant Title : VOC Analysis

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

Peak Number 7 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.619	8.45 ug/L	154916	Chlorobenzene-d5	8.786

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	86
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	86
4			Isopropyl butyrate	130	C7H14O2	000638-11-9	78
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011024\
Data File : VV033563.D
Acq On : 10 Jan 2024 16:18
Operator : SY/MD
Sample : PB158329TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB329

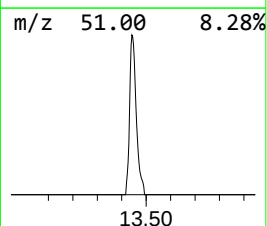
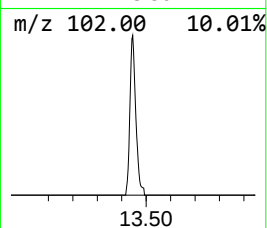
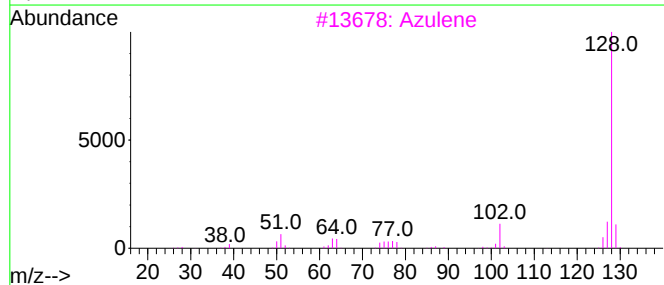
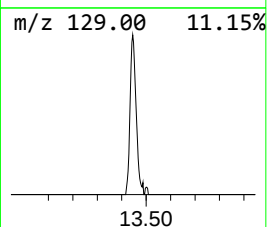
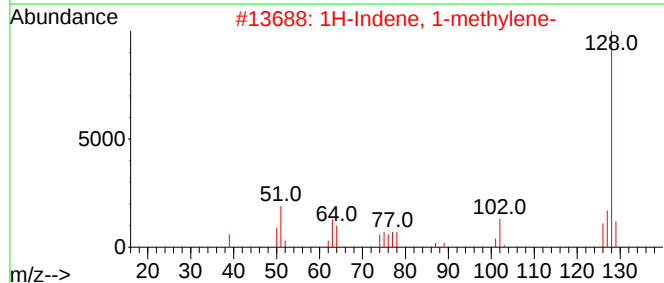
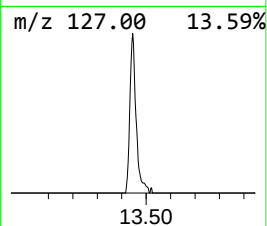
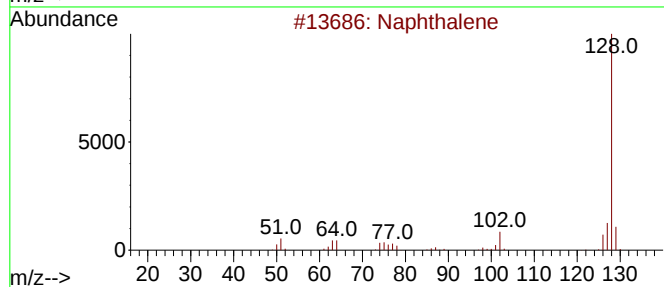
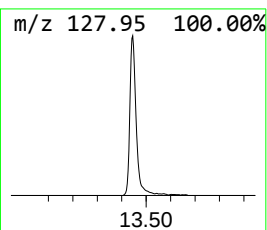
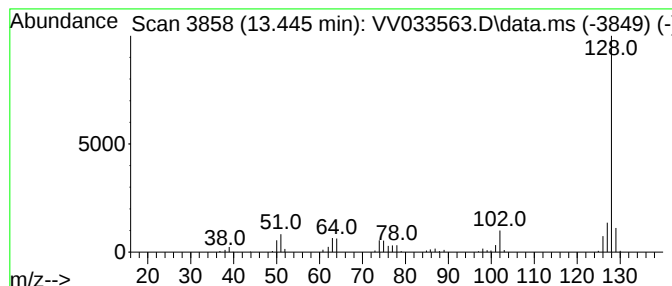
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Quant Title : VOC Analysis

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

Peak Number 8 Azulene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.445	5.38 ug/L	97521	1,4-Dichlorobenzene-d4	11.185

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	95
3			Azulene	128	C10H8	000275-51-4	94
4			Azulene	128	C10H8	000275-51-4	94
5			Naphthalene	128	C10H8	000091-20-3	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011024\
Data File : VV033563.D
Acq On : 10 Jan 2024 16:18
Operator : SY/MD
Sample : PB158329TB 10X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VLEB329

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.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	6.394	14.3	ug/L	215702	1	5.535	754910	50.0
Propanoic acid,...	7.120	2.9	ug/L	44260	1	5.535	754910	50.0
Propanoic acid,...	7.860	3.3	ug/L	59700	2	8.786	916396	50.0
Propanoic acid,...	8.133	5.0	ug/L	91120	2	8.786	916396	50.0
Acetic acid, bu...	8.249	2.6	ug/L	48420	2	8.786	916396	50.0
Isopropyl butyrate	8.619	8.4	ug/L	154916	2	8.786	916396	50.0
Azulene	13.445	5.4	ug/L	97521	3	11.185	907117	50.0