

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121123\
 Data File : VV033238.D
 Acq On : 12 Dec 2023 01:24
 Operator : SY/MD
 Sample : 05751-05
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 YCHA6

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\SFAMVLM120123WMA.M
 Title : VOC Analysis

Signal : TIC: VV033238.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	86	rVB	86928	89902	10.93%	1.292%
2	1.532	145	153	166	rVB	69906	83325	10.13%	1.197%
3	2.008	299	301	304	rBV	316	176	0.02%	0.003%
4	2.060	307	317	327	rBV	147697	213854	26.01%	3.072%
5	2.214	355	365	387	rBV	110848	196331	23.88%	2.820%
6	2.616	487	490	494	rVB2	378	241	0.03%	0.003%
7	2.703	513	517	519	rBV	372	280	0.03%	0.004%
8	2.744	528	530	532	rBV	406	235	0.03%	0.003%
9	2.857	563	565	568	rBV2	232	148	0.02%	0.002%
10	2.925	583	586	588	rBV2	262	171	0.02%	0.002%
11	2.960	596	597	600	rVB2	282	152	0.02%	0.002%
12	2.979	600	603	607	rBV	398	243	0.03%	0.003%
13	3.079	628	634	635	rBV	294	297	0.04%	0.004%
14	3.185	666	667	672	rBB2	374	297	0.04%	0.004%
15	3.243	681	685	687	rVB2	289	163	0.02%	0.002%
16	3.381	724	728	730	rBV	361	322	0.04%	0.005%
17	3.613	796	800	802	rBV	309	222	0.03%	0.003%
18	3.629	802	805	809	rVB2	237	207	0.03%	0.003%
19	3.780	844	852	870	rBV	51180	130971	15.93%	1.882%
20	4.166	969	972	973	rBV	516	284	0.03%	0.004%
21	4.249	981	998	1025	rBV	138289	369665	44.96%	5.311%
22	4.445	1055	1059	1062	rBV3	617	605	0.07%	0.009%
23	4.574	1097	1099	1100	rBV2	256	145	0.02%	0.002%
24	4.606	1104	1109	1113	rVB4	740	697	0.08%	0.010%
25	4.648	1119	1122	1125	rBV2	455	240	0.03%	0.003%
26	4.667	1125	1128	1131	rBV2	364	239	0.03%	0.003%
27	4.715	1140	1143	1147	rBV2	319	259	0.03%	0.004%
28	4.957	1201	1218	1251	rBV2	307866	822234	100.00%	11.812%
29	5.230	1301	1303	1306	rBV	395	285	0.03%	0.004%
30	5.371	1344	1347	1350	rVB	488	273	0.03%	0.004%
31	5.391	1350	1353	1355	rBV3	428	292	0.04%	0.004%
32	5.445	1368	1370	1372	rBV2	322	176	0.02%	0.003%
33	5.532	1386	1397	1426	rBV	290306	601467	73.15%	8.641%
34	5.777	1471	1473	1475	rBV	338	168	0.02%	0.002%
35	5.828	1479	1489	1504	rVV3	16561	34904	4.25%	0.501%
36	5.989	1526	1539	1566	rBV2	173363	362412	44.08%	5.206%

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 Title : VOC Analysis

37	6.185	1599	1600	1604	rVB3	662	330	0.04%	0.005%
38	6.310	1636	1639	1642	rBV	296	261	0.03%	0.004%
39	6.352	1648	1652	1657	rBV2	327	349	0.04%	0.005%
40	6.510	1700	1701	1705	rBV2	411	285	0.03%	0.004%
41	6.593	1723	1727	1728	rBV2	231	154	0.02%	0.002%
42	6.622	1734	1736	1739	rVV2	315	180	0.02%	0.003%
43	6.670	1747	1751	1757	rVB3	284	296	0.04%	0.004%
44	6.754	1774	1777	1778	rBV	320	147	0.02%	0.002%
45	6.828	1798	1800	1803	rVB	315	145	0.02%	0.002%
46	6.912	1816	1826	1848	rBV	98667	184844	22.48%	2.655%
47	7.149	1898	1900	1904	rBV2	296	258	0.03%	0.004%
48	7.243	1915	1929	1955	rBV	368153	650663	79.13%	9.347%
49	7.555	2016	2026	2041	rBV	73053	128396	15.62%	1.845%
50	7.703	2070	2072	2074	rBV	413	172	0.02%	0.002%
51	7.741	2080	2084	2087	rVB2	375	202	0.02%	0.003%
52	7.854	2116	2119	2120	rBV	523	304	0.04%	0.004%
53	7.915	2136	2138	2141	rVB2	472	274	0.03%	0.004%
54	7.963	2150	2153	2156	rBV2	372	245	0.03%	0.004%
55	8.021	2161	2171	2209	rBV	179205	361733	43.99%	5.197%
56	8.304	2252	2259	2272	rVB6	2708	5216	0.63%	0.075%
57	8.690	2376	2379	2383	rVB	346	199	0.02%	0.003%
58	8.715	2384	2387	2389	rBV2	387	274	0.03%	0.004%
59	8.783	2397	2408	2427	rBV	471526	771144	93.79%	11.078%
60	9.082	2498	2501	2505	rBV2	574	486	0.06%	0.007%
61	9.101	2505	2507	2509	rVB2	536	229	0.03%	0.003%
62	9.156	2521	2524	2526	rBV2	258	165	0.02%	0.002%
63	9.423	2604	2607	2610	rBV	293	218	0.03%	0.003%
64	9.551	2644	2647	2648	rBV	348	150	0.02%	0.002%
65	9.641	2673	2675	2679	rBV2	276	148	0.02%	0.002%
66	9.667	2679	2683	2689	rVB	310	300	0.04%	0.004%
67	9.731	2696	2703	2706	rBV2	413	562	0.07%	0.008%
68	9.876	2746	2748	2753	rBV3	330	271	0.03%	0.004%
69	9.918	2758	2761	2764	rBV	283	190	0.02%	0.003%
70	10.153	2823	2834	2859	rBV	257654	410134	49.88%	5.892%
71	10.481	2934	2936	2940	rBV	533	413	0.05%	0.006%
72	10.506	2942	2944	2948	rVV2	328	214	0.03%	0.003%
73	10.577	2964	2966	2971	rVB3	474	363	0.04%	0.005%
74	10.609	2971	2976	2977	rBV	362	271	0.03%	0.004%
75	10.690	2997	3001	3002	rBV	305	199	0.02%	0.003%
76	10.712	3007	3008	3012	rVB2	374	227	0.03%	0.003%

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 Title : VOC Analysis

77	10.937	3075	3078	3080	rBV2	300	204	0.02%	0.003%
78	11.185	3144	3155	3178	rBV	507718	787644	95.79%	11.315%
79	11.352	3204	3207	3210	rBV2	615	489	0.06%	0.007%
80	11.561	3257	3272	3292	rBV	468936	733229	89.18%	10.533%
81	11.747	3329	3330	3332	rBV	348	162	0.02%	0.002%
82	12.136	3449	3451	3455	rVB2	367	198	0.02%	0.003%
83	12.545	3576	3578	3581	rBV2	306	188	0.02%	0.003%
84	12.599	3592	3595	3598	rVB3	622	421	0.05%	0.006%
85	12.693	3621	3624	3627	rVB2	295	202	0.02%	0.003%
86	12.718	3627	3632	3634	rBV2	254	284	0.03%	0.004%
87	12.805	3654	3659	3660	rBV2	283	219	0.03%	0.003%
88	12.902	3685	3689	3690	rBV2	397	314	0.04%	0.005%
89	12.931	3694	3698	3702	rBV2	460	361	0.04%	0.005%
90	12.972	3708	3711	3714	rBV	564	366	0.04%	0.005%
91	13.030	3726	3729	3731	rBV	257	168	0.02%	0.002%
92	13.124	3753	3758	3762	rBV2	517	553	0.07%	0.008%
93	13.217	3782	3787	3790	rVB3	588	518	0.06%	0.007%
94	13.246	3795	3796	3799	rBV2	257	165	0.02%	0.002%
95	13.451	3855	3860	3865	rBV4	1035	1198	0.15%	0.017%
96	13.509	3875	3878	3884	rBV	363	430	0.05%	0.006%
97	13.654	3921	3923	3927	rVB	545	295	0.04%	0.004%
98	13.673	3927	3929	3930	rBV	301	154	0.02%	0.002%
99	14.107	4061	4064	4067	rBV3	611	543	0.07%	0.008%
100	14.625	4223	4225	4226	rBV	544	185	0.02%	0.003%

Sum of corrected areas: 6960983

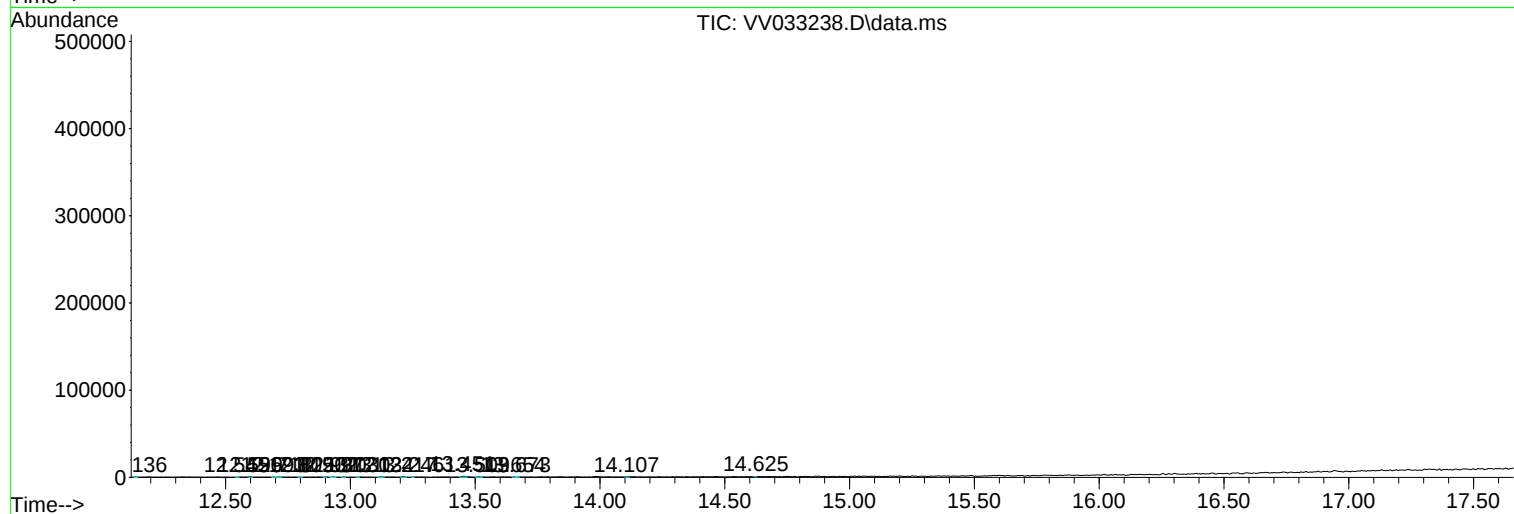
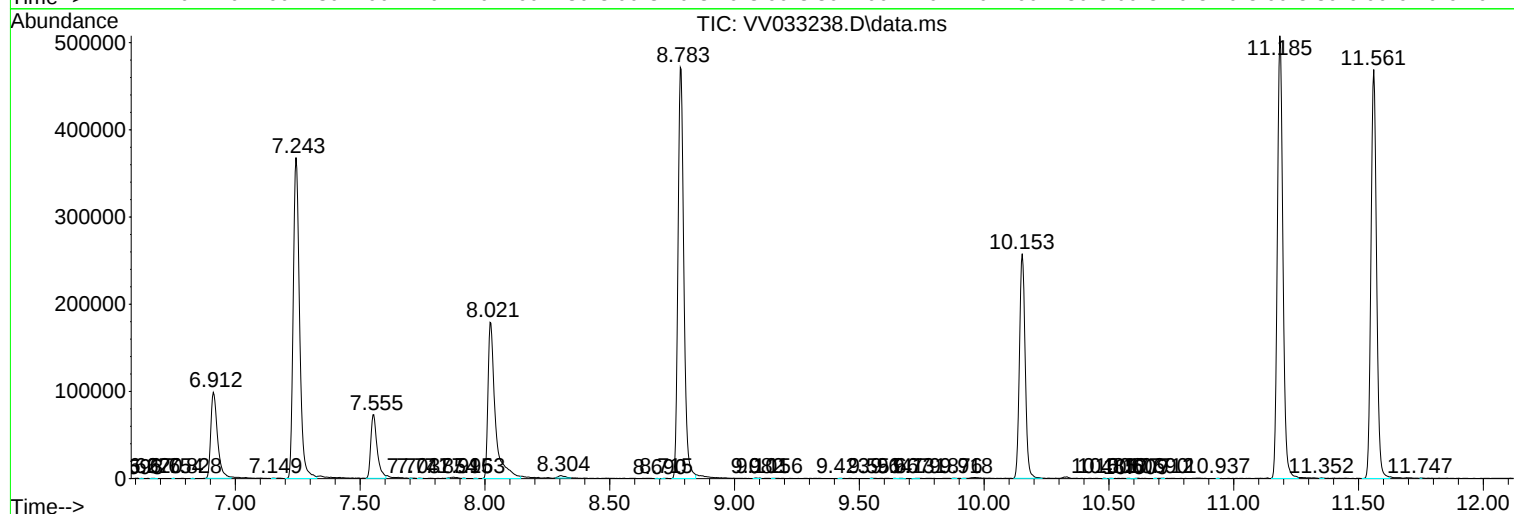
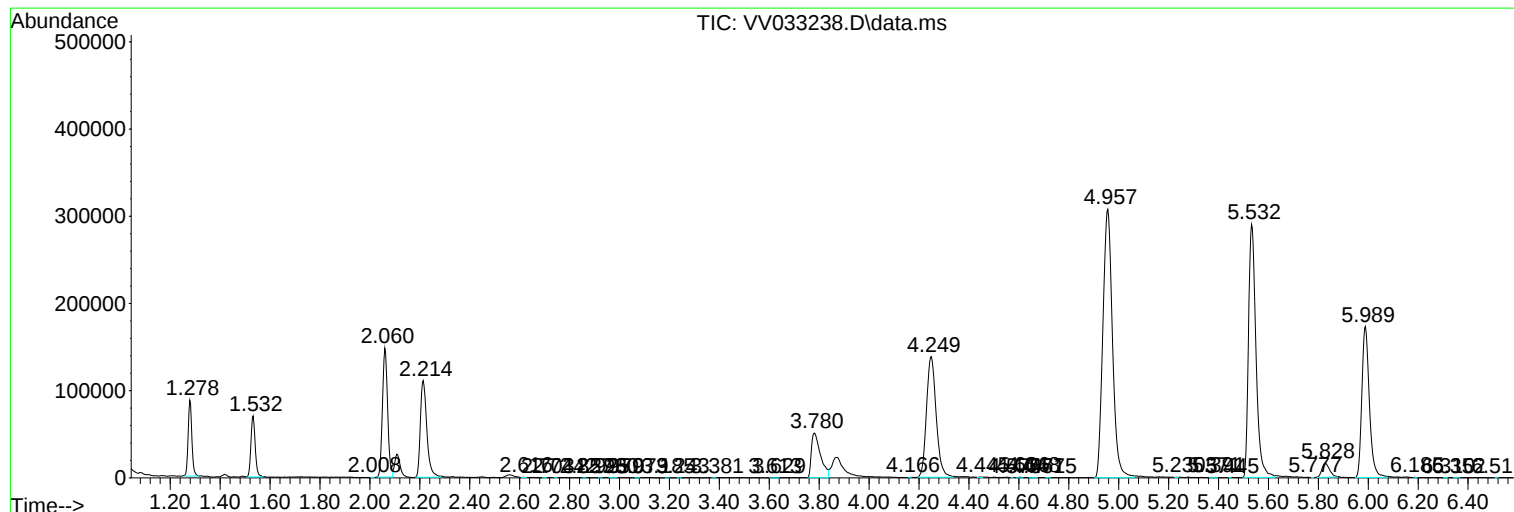
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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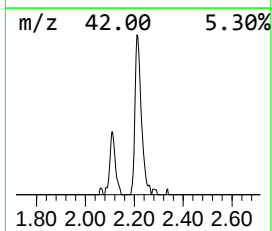
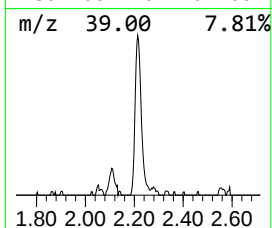
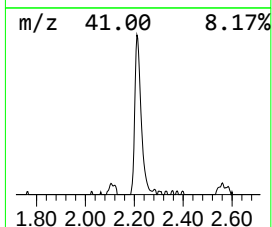
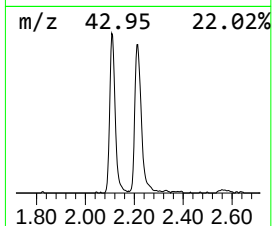
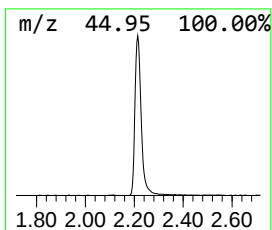
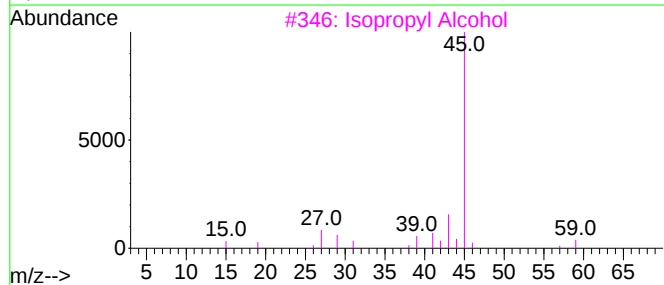
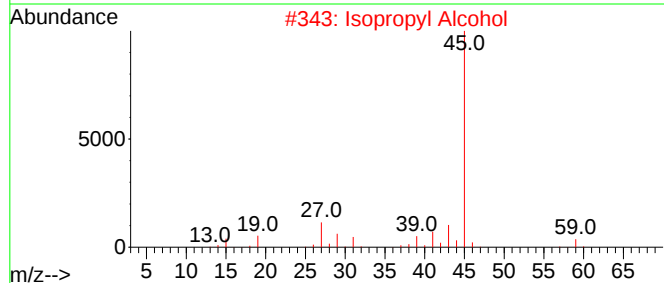
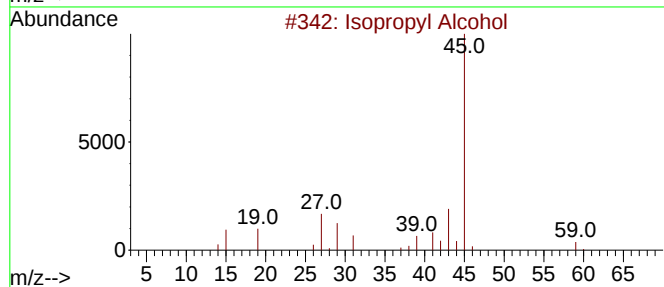
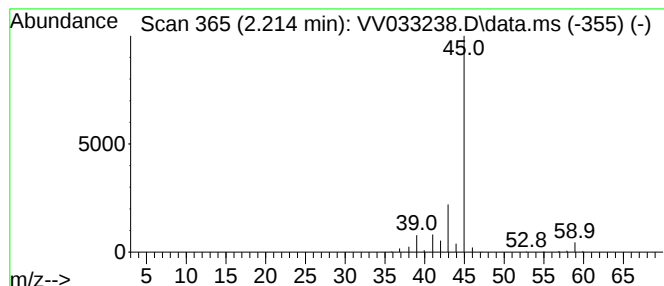
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.214	16.32 ug/L	196331	1,4-Difluorobenzene	5.532

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
4			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
5			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9



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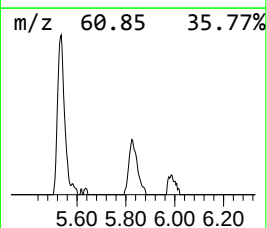
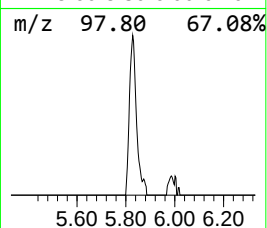
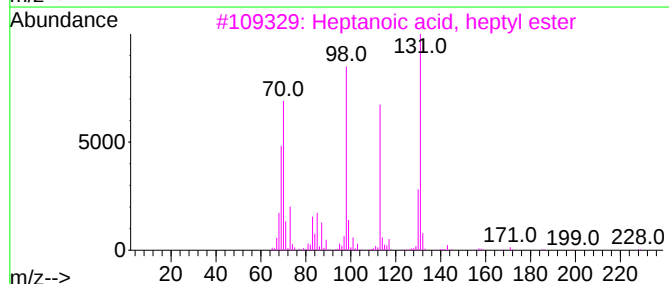
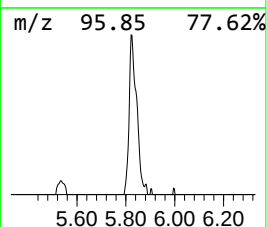
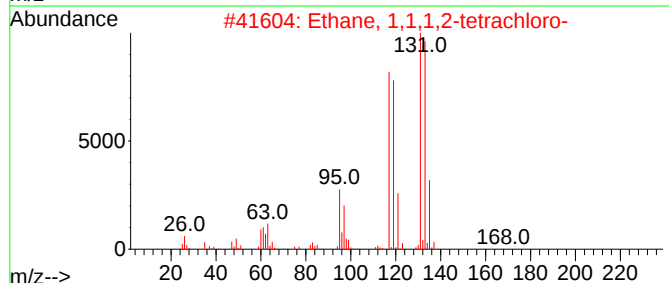
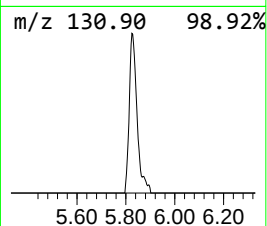
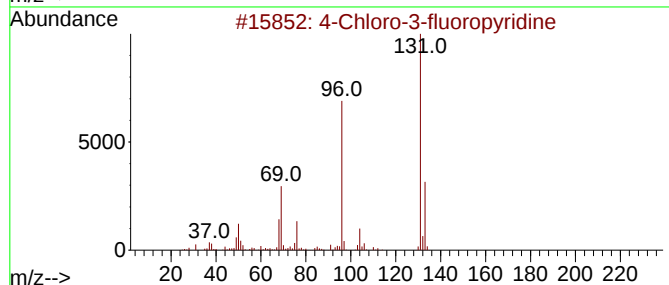
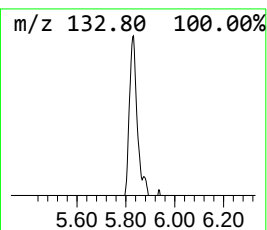
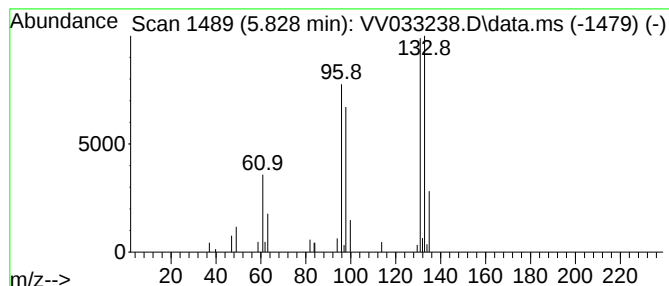
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Quant Title : VOC Analysis

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

Peak Number 2 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.828	2.90 ug/L	34904	1,4-Difluorobenzene	5.532

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	38
2			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	17
3			Heptanoic acid, heptyl ester	228	C14H28O2	000624-09-9	12
4			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	12
5			2-Chloro-5-methylthiazole	133	C4H4ClNS	033342-65-3	12



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl Alcohol	2.214	16.3	ug/L	196331	1	5.532	601467	50.0
unknown-01	5.828	2.9	ug/L	34904	1	5.532	601467	50.0