

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV062024\
 Data File : VV036164.D
 Acq On : 20 Jun 2024 15:29
 Operator : SY/MD
 Sample : P2856-19
 Misc : 5.38g/10.0mL/MSVOA_V/SOIL/B
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0SJ5

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\SFAMVLM053024SMA.M

Title : VOC Analysis

Signal : TIC: VV036164.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.272	67	72	90	rVB	228157	249504	18.09%	2.596%
2	1.526	145	151	168	rVB	182509	215666	15.64%	2.244%
3	2.050	305	314	331	rBV	401540	570546	41.38%	5.937%
4	2.442	427	436	456	rVB	64954	111266	8.07%	1.158%
5	3.085	632	636	639	rBV3	358	300	0.02%	0.003%
6	3.108	641	643	646	rVB2	374	163	0.01%	0.002%
7	3.182	663	666	669	rBV3	465	298	0.02%	0.003%
8	3.204	669	673	678	rVB3	553	573	0.04%	0.006%
9	3.236	680	683	684	rBV3	242	145	0.01%	0.002%
10	3.333	711	713	719	rVB3	398	352	0.03%	0.004%
11	3.465	752	754	759	rVB2	205	151	0.01%	0.002%
12	3.625	802	804	809	rVB3	377	248	0.02%	0.003%
13	3.648	809	811	814	rBV2	295	137	0.01%	0.001%
14	3.670	814	818	821	rBV2	424	355	0.03%	0.004%
15	3.834	848	869	917	rBV4	66926	328907	23.85%	3.423%
16	4.243	981	996	1037	rBV2	225521	591847	42.92%	6.159%
17	4.657	1122	1125	1131	rVB7	404	412	0.03%	0.004%
18	4.799	1165	1169	1173	rVB3	644	561	0.04%	0.006%
19	4.828	1173	1178	1181	rBV3	582	544	0.04%	0.006%
20	4.886	1191	1196	1200	rBV2	389	388	0.03%	0.004%
21	4.953	1200	1217	1262	rBV2	531937	1378960	100.00%	14.350%
22	5.374	1346	1348	1353	rVB3	423	209	0.02%	0.002%
23	5.410	1356	1359	1362	rVB3	450	284	0.02%	0.003%
24	5.532	1386	1397	1427	rBV	297118	641006	46.48%	6.670%
25	5.825	1478	1488	1508	rBV2	24089	54239	3.93%	0.564%
26	5.985	1525	1538	1570	rBV	308578	646202	46.86%	6.724%
27	6.288	1629	1632	1634	rBV2	477	294	0.02%	0.003%
28	6.326	1641	1644	1646	rBV3	291	166	0.01%	0.002%
29	6.384	1660	1662	1666	rBV3	397	174	0.01%	0.002%
30	6.474	1686	1690	1694	rBV3	468	428	0.03%	0.004%
31	6.500	1694	1698	1702	rBV2	380	253	0.02%	0.003%
32	6.554	1711	1715	1717	rBV2	300	149	0.01%	0.002%
33	6.583	1722	1724	1725	rVV	298	152	0.01%	0.002%
34	6.606	1727	1731	1735	rVB3	302	241	0.02%	0.003%
35	6.632	1735	1739	1743	rBV3	448	269	0.02%	0.003%
36	6.683	1749	1755	1757	rBV2	403	412	0.03%	0.004%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM053024SMA.M
 Title : VOC Analysis

37	6.735	1769	1771	1776	rVB	488	295	0.02%	0.003%
38	6.757	1776	1778	1779	rBV	361	156	0.01%	0.002%
39	6.844	1802	1805	1806	rBV	297	146	0.01%	0.002%
40	6.853	1806	1808	1810	rVB	391	158	0.01%	0.002%
41	6.873	1810	1814	1816	rBV2	371	291	0.02%	0.003%
42	6.911	1816	1826	1859	rBV	133737	266576	19.33%	2.774%
43	7.124	1889	1892	1898	rBV2	307	390	0.03%	0.004%
44	7.172	1903	1907	1909	rBV4	499	372	0.03%	0.004%
45	7.239	1917	1928	1961	rBV	560635	1023576	74.23%	10.651%
46	7.554	2016	2026	2052	rBV	94795	183921	13.34%	1.914%
47	7.876	2116	2126	2133	rBV3	4624	8584	0.62%	0.089%
48	8.030	2166	2174	2212	rBV	97252	231250	16.77%	2.406%
49	8.358	2267	2276	2291	rBV2	22396	40131	2.91%	0.418%
50	8.628	2358	2360	2364	rVB	416	204	0.01%	0.002%
51	8.654	2364	2368	2370	rBV2	529	458	0.03%	0.005%
52	8.783	2393	2408	2435	rBV	514346	865903	62.79%	9.011%
53	9.066	2493	2496	2497	rBV3	484	229	0.02%	0.002%
54	9.104	2506	2508	2511	rBV4	574	342	0.02%	0.004%
55	9.172	2527	2529	2533	rBV4	540	423	0.03%	0.004%
56	9.194	2534	2536	2539	rVV2	381	243	0.02%	0.003%
57	9.284	2561	2564	2566	rBV2	686	367	0.03%	0.004%
58	9.329	2575	2578	2579	rBV2	458	261	0.02%	0.003%
59	9.390	2592	2597	2599	rBV2	341	330	0.02%	0.003%
60	9.548	2643	2646	2649	rBV	348	205	0.01%	0.002%
61	9.570	2649	2653	2657	rVV3	398	349	0.03%	0.004%
62	9.590	2657	2659	2664	rVV3	384	339	0.02%	0.004%
63	9.625	2667	2670	2671	rBV	334	151	0.01%	0.002%
64	9.673	2681	2685	2688	rBV3	335	312	0.02%	0.003%
65	9.693	2688	2691	2693	rVV2	431	254	0.02%	0.003%
66	9.728	2700	2702	2704	rBV2	270	135	0.01%	0.001%
67	9.773	2710	2716	2717	rBV2	417	368	0.03%	0.004%
68	9.943	2766	2769	2773	rBV4	287	243	0.02%	0.003%
69	10.046	2798	2801	2803	rBV	383	251	0.02%	0.003%
70	10.091	2810	2815	2819	rBV	479	508	0.04%	0.005%
71	10.152	2821	2834	2861	rVV	250842	405994	29.44%	4.225%
72	10.323	2880	2887	2896	rVB	6144	9401	0.68%	0.098%
73	10.464	2928	2931	2934	rBV2	357	275	0.02%	0.003%
74	10.480	2934	2936	2939	rVB3	592	269	0.02%	0.003%
75	10.506	2943	2944	2947	rBV2	468	316	0.02%	0.003%
76	10.525	2947	2950	2954	rBV4	673	540	0.04%	0.006%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Min Area: 0 % of largest Peak

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Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM053024SMA.M
 Title : VOC Analysis

77	10.580	2964	2967	2970	rVB2	405	240	0.02%	0.002%
78	10.606	2970	2975	2979	rVB3	491	444	0.03%	0.005%
79	10.638	2983	2985	2987	rBV	212	136	0.01%	0.001%
80	10.741	3012	3017	3019	rBV2	1151	1009	0.07%	0.010%
81	10.783	3028	3030	3037	rVB3	264	229	0.02%	0.002%
82	10.812	3037	3039	3041	rBV	268	148	0.01%	0.002%
83	10.914	3066	3071	3074	rBV2	480	461	0.03%	0.005%
84	11.021	3101	3104	3106	rBV	295	203	0.01%	0.002%
85	11.104	3127	3130	3131	rBV	328	185	0.01%	0.002%
86	11.181	3143	3154	3178	rBV	482480	765975	55.55%	7.971%
87	11.484	3239	3248	3261	rBV2	21236	47323	3.43%	0.492%
88	11.557	3261	3271	3296	rVB	577442	914562	66.32%	9.517%
89	12.069	3428	3430	3433	rBV2	326	149	0.01%	0.002%
90	12.194	3463	3469	3479	rVB3	6093	8834	0.64%	0.092%
91	12.577	3584	3588	3592	rBV4	1455	1633	0.12%	0.017%
92	12.824	3659	3665	3673	rVB6	2959	4143	0.30%	0.043%
93	12.908	3689	3691	3692	rBV2	417	144	0.01%	0.001%
94	12.937	3698	3700	3701	rBV	372	143	0.01%	0.001%
95	13.008	3719	3722	3725	rBV2	585	336	0.02%	0.003%
96	13.033	3728	3730	3732	rBV2	467	202	0.01%	0.002%
97	13.210	3780	3785	3790	rBV5	518	639	0.05%	0.007%
98	13.528	3881	3884	3886	rBV	503	291	0.02%	0.003%
99	13.683	3924	3932	3944	rVB	14862	21229	1.54%	0.221%
100	13.792	3960	3966	3969	rBV5	690	826	0.06%	0.009%

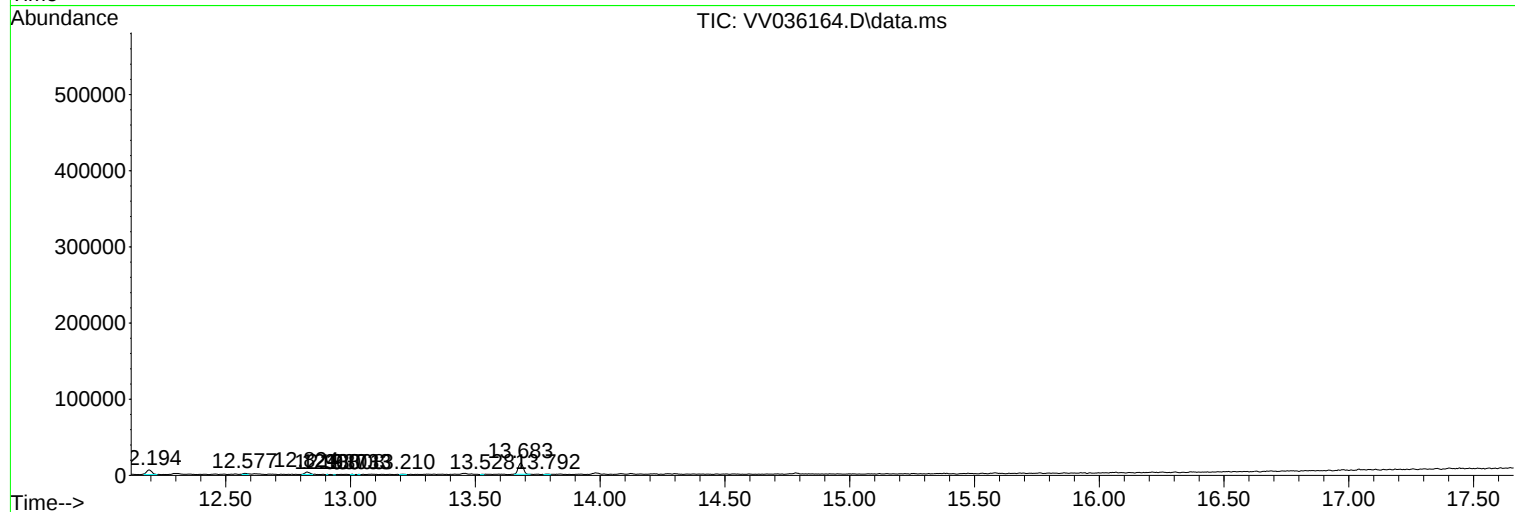
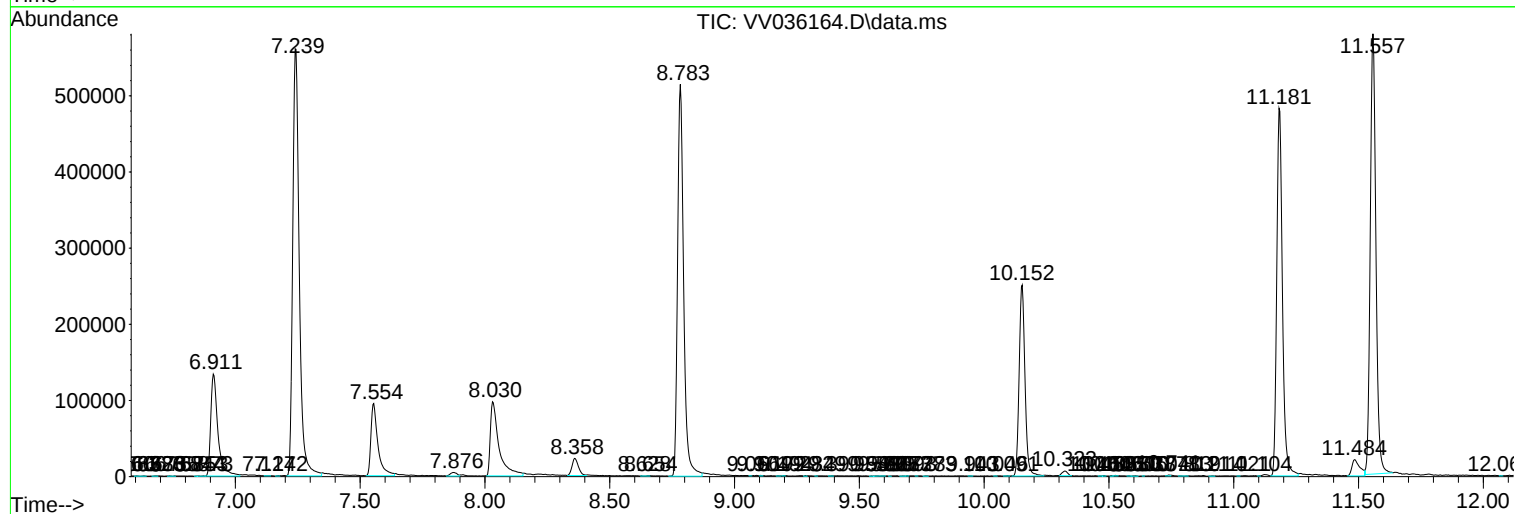
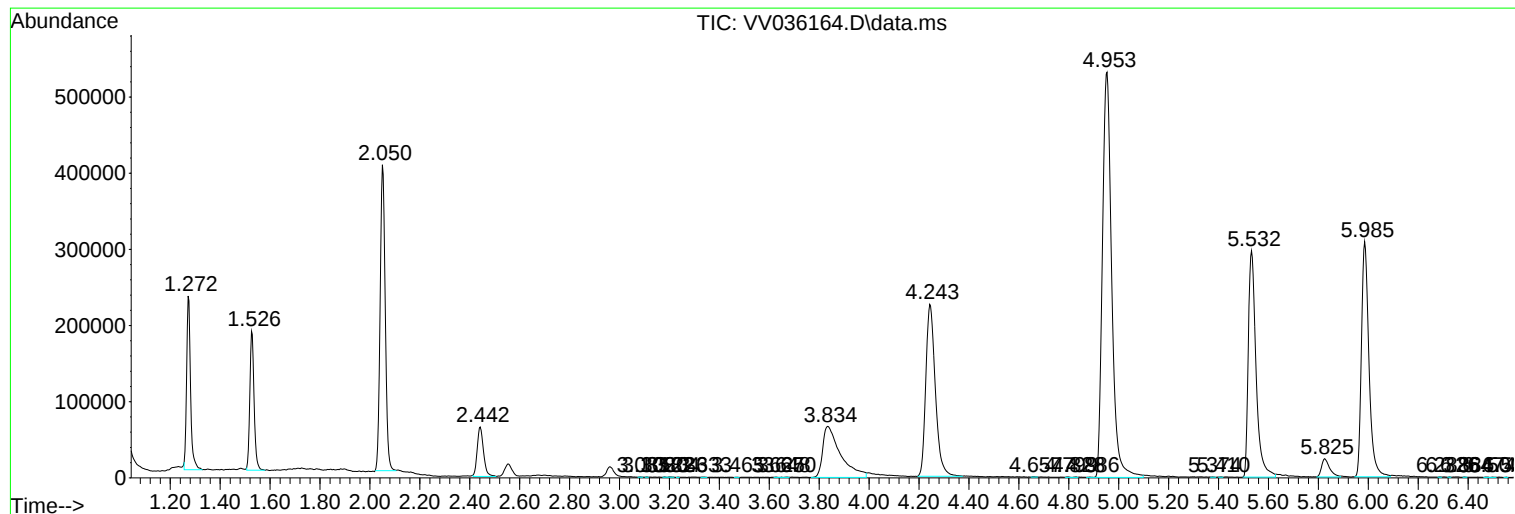
Sum of corrected areas: 9609801

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM053024SMA.M
Quant Title : VOC Analysis

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



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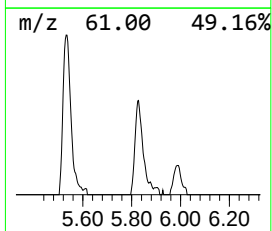
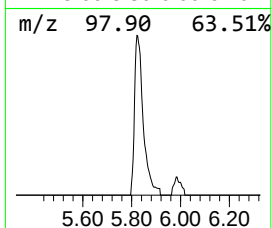
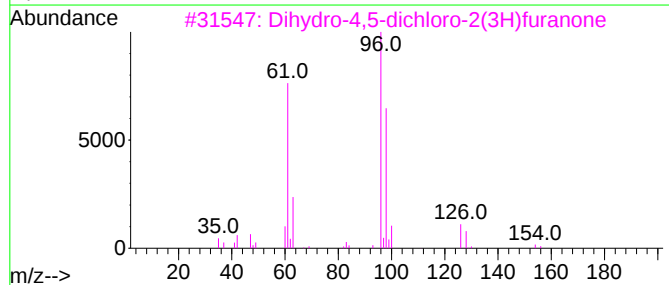
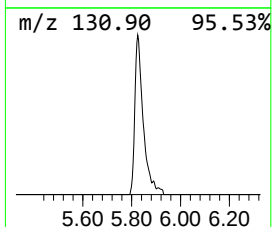
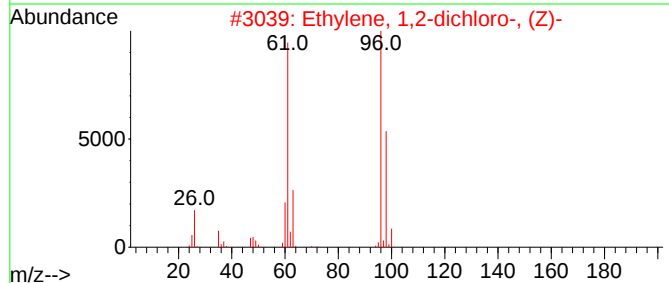
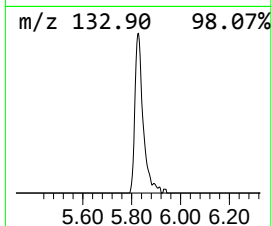
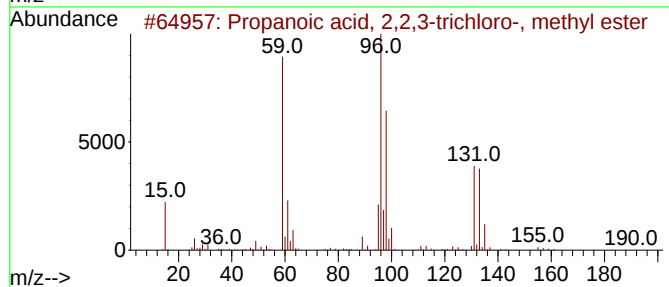
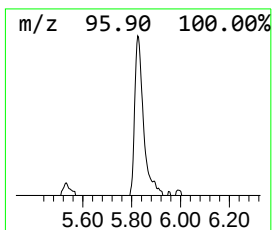
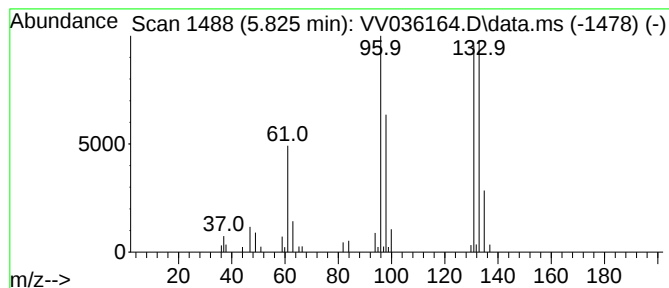
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM053024SMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Propanoic acid, 2,2,3-trich... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.825	2.12 ug/L	54239	1,4-Difluorobenzene	5.532

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	56
2			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
3			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	17
4			2-Chloro-5-methylthiazole	133	C4H4ClNS	033342-65-3	10
5			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	9



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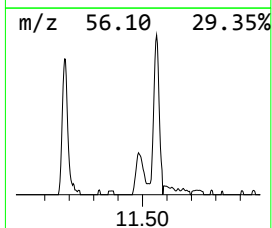
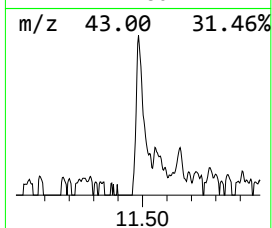
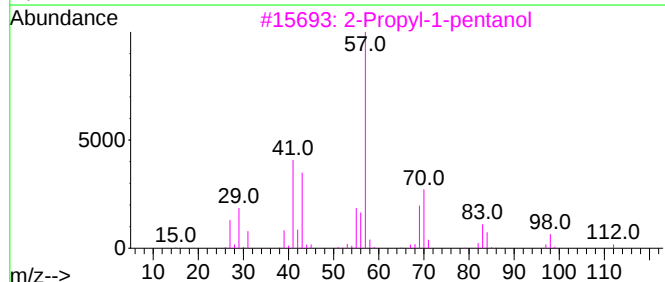
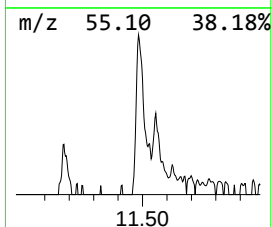
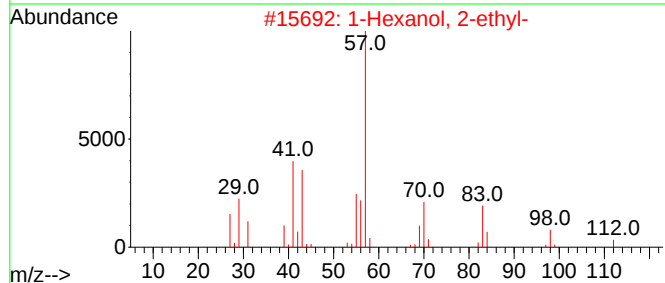
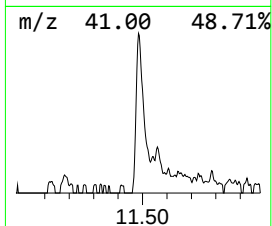
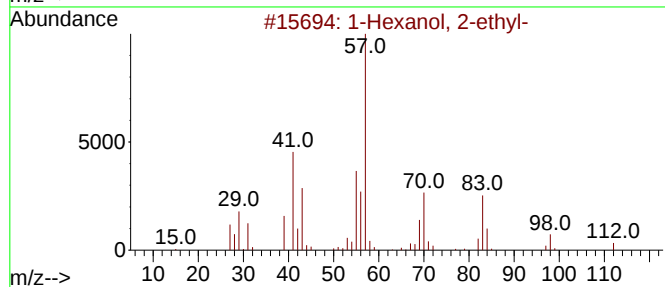
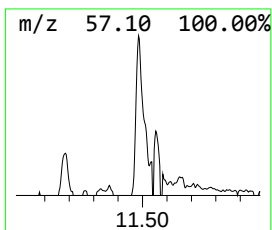
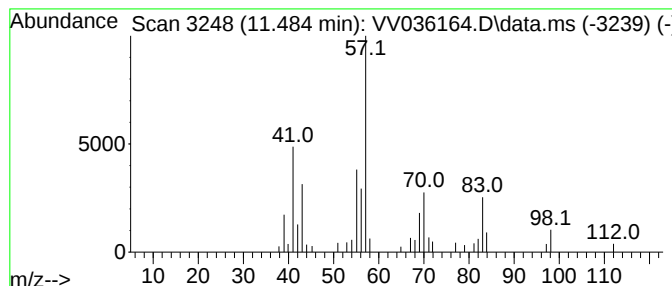
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Quant Title : VOC Analysis

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

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.483	1.54 ug/L	47323	1,4-Dichlorobenzene-d4	11.185

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	64
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	64



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	5.825	2.1	ug/L	54239	1	5.532	641006	25.0
1-Hexanol, 2-et...	11.483	1.5	ug/L	47323	3	11.185	765975	25.0