

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU051120\
 Data File : VU038109.D
 Acq On : 11 May 2020 16:20
 Operator : JC/MD
 Sample : L2578-02DL 20X
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFSF1DL

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM043020WMA.M
 Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.613	77	85	98	rBV	323899	343755	13.02%	1.360%
2	1.928	174	183	199	rVB	280087	371631	14.07%	1.470%
3	2.507	361	363	364	rBV2	1042	422	0.02%	0.002%
4	2.591	376	389	406	rBV2	494271	835966	31.66%	3.308%
5	2.781	439	448	451	rBV4	3247	4350	0.16%	0.017%
6	2.928	489	494	497	rBV3	662	705	0.03%	0.003%
7	3.073	530	539	540	rBV4	1438	1727	0.07%	0.007%
8	3.141	555	560	564	rBV4	605	650	0.02%	0.003%
9	3.211	570	582	595	rVV4	9145	21229	0.80%	0.084%
10	3.305	607	611	615	rVB2	570	513	0.02%	0.002%
11	3.353	619	626	630	rBV5	828	1148	0.04%	0.005%
12	3.478	663	665	670	rVB3	714	546	0.02%	0.002%
13	3.838	775	777	781	rVB3	856	537	0.02%	0.002%
14	3.909	781	799	822	rBV3	175653	427156	16.18%	1.690%
15	4.028	828	836	837	rBV6	4113	4938	0.19%	0.020%
16	4.433	957	962	965	rVB4	611	535	0.02%	0.002%
17	4.504	978	984	986	rBV	569	522	0.02%	0.002%
18	4.658	1013	1032	1058	rBV	356410	872123	33.03%	3.451%
19	4.980	1130	1132	1139	rVB4	913	708	0.03%	0.003%
20	5.015	1139	1143	1145	rBV3	594	457	0.02%	0.002%
21	5.102	1151	1170	1195	rBV	462125	1014882	38.43%	4.016%
22	5.215	1201	1205	1214	rVB6	1055	1311	0.05%	0.005%
23	5.263	1218	1220	1226	rVB3	730	607	0.02%	0.002%
24	5.353	1230	1248	1277	rBV	750968	1687061	63.89%	6.675%
25	5.542	1303	1307	1308	rBV4	499	410	0.02%	0.002%
26	5.581	1316	1319	1322	rBV	661	516	0.02%	0.002%
27	5.658	1340	1343	1349	rVB4	653	575	0.02%	0.002%
28	5.758	1349	1374	1404	rBV2	972837	2640672	100.00%	10.448%
29	6.002	1447	1450	1454	rVB5	756	589	0.02%	0.002%
30	6.028	1454	1458	1461	rBV2	952	781	0.03%	0.003%
31	6.141	1490	1493	1505	rVB5	1426	1928	0.07%	0.008%
32	6.279	1521	1536	1570	rBV	981629	1883100	71.31%	7.451%
33	6.427	1579	1582	1589	rBV3	858	894	0.03%	0.004%
34	6.562	1611	1624	1631	rBV4	10401	21379	0.81%	0.085%

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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM043020WMA.M
 Title : VOC Analysis

35	6.719	1657	1673	1691	rBV	629517	1232822	46.69%	4.878%
36	6.822	1701	1705	1706	rBV3	1416	899	0.03%	0.004%
37	6.880	1719	1723	1728	rBV3	794	584	0.02%	0.002%
38	6.941	1731	1742	1756	rVB3	23065	45490	1.72%	0.180%
39	7.124	1796	1799	1803	rVB2	596	430	0.02%	0.002%
40	7.166	1808	1812	1816	rBV3	509	452	0.02%	0.002%
41	7.205	1816	1824	1832	rBV4	5158	8955	0.34%	0.035%
42	7.362	1862	1873	1887	rBV2	20165	35958	1.36%	0.142%
43	7.430	1890	1894	1898	rVB2	691	495	0.02%	0.002%
44	7.539	1915	1928	1933	rBV2	31342	52156	1.98%	0.206%
45	7.591	1933	1944	1961	rVB	354636	614855	23.28%	2.433%
46	7.739	1972	1990	2006	rVB4	20144	43182	1.64%	0.171%
47	7.816	2008	2014	2021	rVB3	2124	2833	0.11%	0.011%
48	7.922	2029	2047	2083	rBV	1159725	2099677	79.51%	8.308%
49	8.198	2118	2133	2155	rBV	248136	411217	15.57%	1.627%
50	8.275	2155	2157	2163	rVV3	464	429	0.02%	0.002%
51	8.423	2200	2203	2211	rVB3	1127	1168	0.04%	0.005%
52	8.488	2216	2223	2226	rBV3	1027	1228	0.05%	0.005%
53	8.571	2245	2249	2256	rVB4	1131	1353	0.05%	0.005%
54	8.652	2261	2274	2319	rBV	973198	1780823	67.44%	7.046%
55	9.382	2497	2501	2504	rBV2	587	497	0.02%	0.002%
56	9.436	2504	2518	2540	rBV	1371662	2361751	89.44%	9.345%
57	9.587	2559	2565	2568	rBV5	725	949	0.04%	0.004%
58	9.703	2593	2601	2603	rBV4	1878	2118	0.08%	0.008%
59	9.732	2608	2610	2613	rVV3	853	469	0.02%	0.002%
60	9.848	2643	2646	2648	rBV	665	430	0.02%	0.002%
61	9.976	2684	2686	2689	rVV	766	411	0.02%	0.002%
62	10.025	2697	2701	2706	rBV2	595	659	0.02%	0.003%
63	10.057	2708	2711	2716	rVB2	835	794	0.03%	0.003%
64	10.083	2716	2719	2722	rBV	519	403	0.02%	0.002%
65	10.118	2726	2730	2731	rBV3	758	517	0.02%	0.002%
66	10.279	2766	2780	2800	rBV	141274	274012	10.38%	1.084%
67	10.481	2841	2843	2846	rBV2	935	742	0.03%	0.003%
68	10.568	2860	2870	2875	rBV6	4832	7460	0.28%	0.030%
69	10.645	2892	2894	2897	rBV3	704	420	0.02%	0.002%
70	10.661	2897	2899	2900	rBV2	1108	516	0.02%	0.002%
71	10.771	2919	2933	2950	rVV	874258	1411471	53.45%	5.585%

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 Title : VOC Analysis

72	10.896	2963	2972	2973	rBV6	3055	3615	0.14%	0.014%
73	10.944	2984	2987	2996	rVB6	1901	2471	0.09%	0.010%
74	11.044	2998	3018	3033	rBV	239126	408225	15.46%	1.615%
75	11.127	3038	3044	3053	rBV8	3754	5663	0.21%	0.022%
76	11.205	3061	3068	3075	rVB5	3226	4010	0.15%	0.016%
77	11.243	3075	3080	3086	rVB5	2301	2924	0.11%	0.012%
78	11.298	3094	3097	3101	rBV2	1191	999	0.04%	0.004%
79	11.346	3105	3112	3118	rBV4	1623	2078	0.08%	0.008%
80	11.423	3132	3136	3143	rBV4	1291	1675	0.06%	0.007%
81	11.488	3148	3156	3162	rVV5	1895	2890	0.11%	0.011%
82	11.526	3166	3168	3174	rVB2	503	430	0.02%	0.002%
83	11.639	3198	3203	3205	rBV5	1101	1063	0.04%	0.004%
84	11.722	3223	3229	3236	rBV8	1327	2113	0.08%	0.008%
85	11.751	3236	3238	3243	rVV3	1107	794	0.03%	0.003%
86	11.822	3247	3260	3279	rBV	1462004	2307641	87.39%	9.131%
87	11.980	3306	3309	3313	rBV3	598	429	0.02%	0.002%
88	12.105	3340	3348	3357	rVB7	9215	13885	0.53%	0.055%
89	12.205	3365	3379	3397	rVV	1204569	1960717	74.25%	7.758%
90	12.320	3412	3415	3417	rBV2	746	416	0.02%	0.002%
91	12.468	3458	3461	3466	rBV3	474	457	0.02%	0.002%
92	12.516	3473	3476	3479	rVB4	937	625	0.02%	0.002%
93	12.536	3479	3482	3486	rBV3	488	511	0.02%	0.002%
94	12.880	3585	3589	3601	rVB3	1331	1693	0.06%	0.007%
95	12.983	3618	3621	3625	rBV3	886	789	0.03%	0.003%
96	13.111	3658	3661	3663	rVB2	748	416	0.02%	0.002%
97	13.166	3675	3678	3680	rBV	898	538	0.02%	0.002%
98	13.860	3890	3894	3898	rBV5	1280	1377	0.05%	0.005%
99	14.098	3964	3968	3970	rBV3	1169	1040	0.04%	0.004%
100	15.301	4340	4342	4347	rBV3	977	1070	0.04%	0.004%

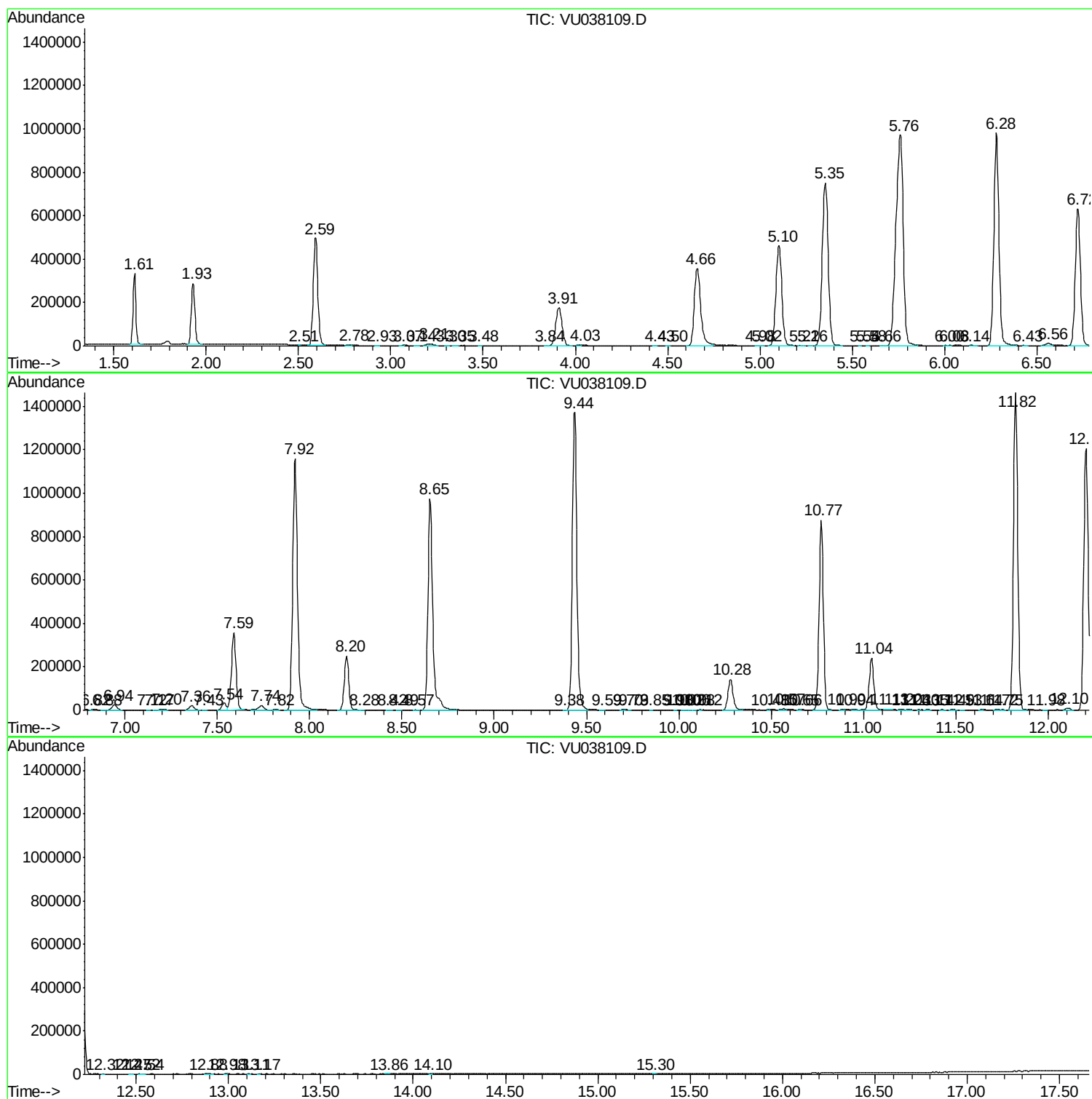
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM043020WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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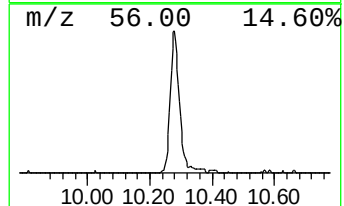
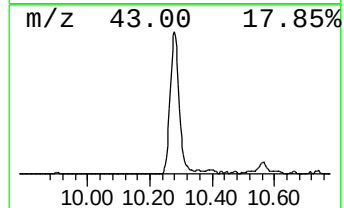
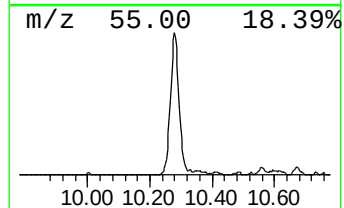
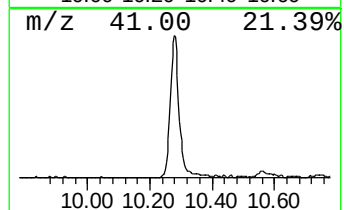
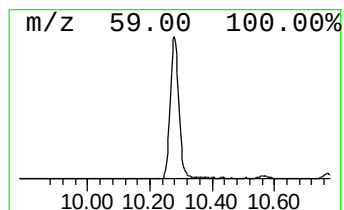
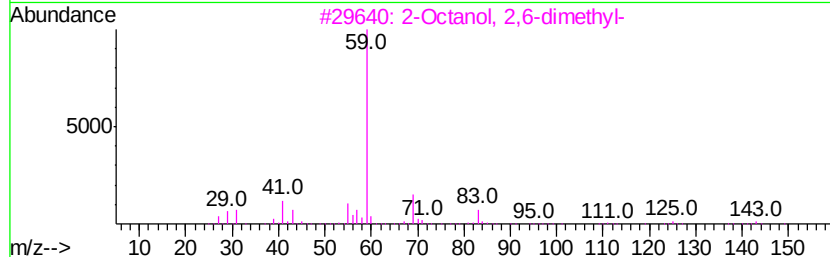
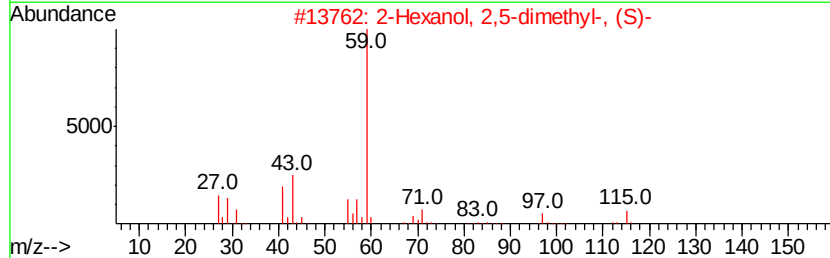
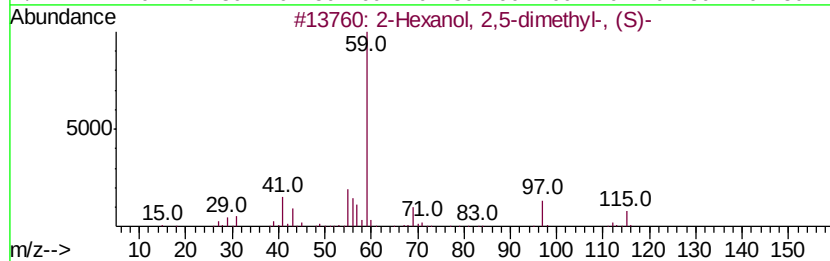
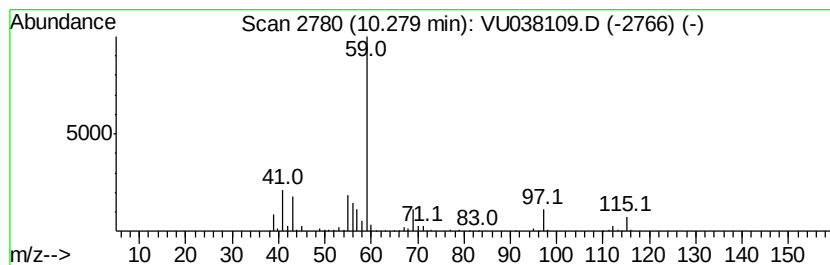
Instrument :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM043020WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.28	5.80 ug/L	274012	Chlorobenzene-d5	9.44	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	90
2	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	72
3	2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	50
4	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	42
5	2-Hexanol, methyl ether	116	C7H16O	1000333-92-0	42



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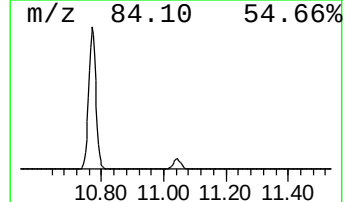
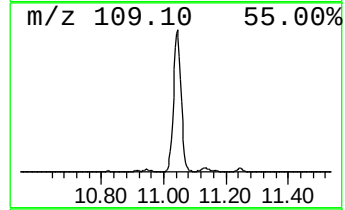
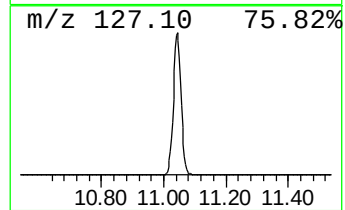
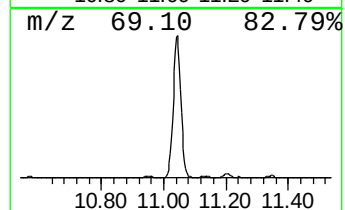
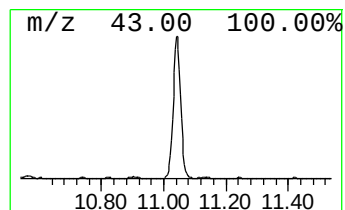
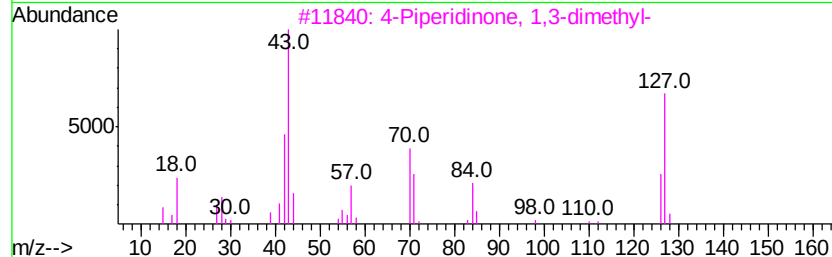
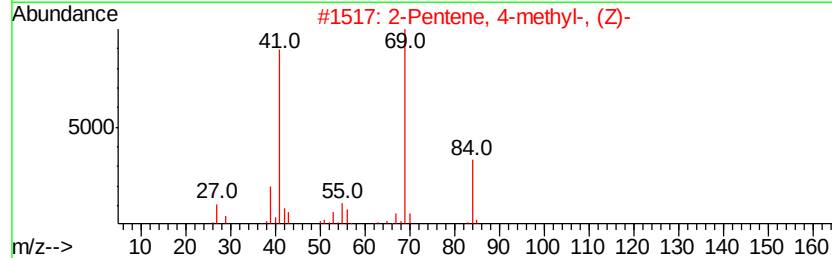
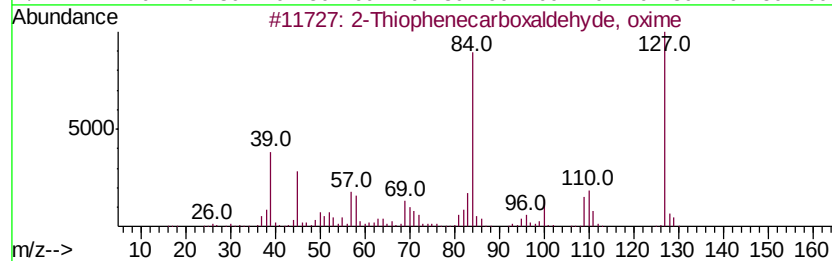
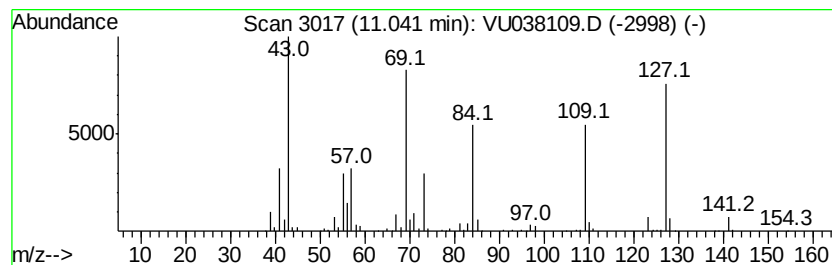
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.04	8.85 ug/L	408225	1,4-Dichlorobenzene-d4	11.82	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Thiophenecarboxaldehyde, oxime	127	C5H5NOS	029683-84-9	32
2	2-Pentene, 4-methyl-, (Z)-	84	C6H12	000691-38-3	27
3	4-Piperidinone, 1,3-dimethyl-	127	C7H13NO	004629-80-5	27
4	Furan, 2,3-dihydro-3-methyl-	84	C5H8O	001708-27-6	27
5	Cyclopropane, (1,2-dimethylpropyl)-	112	C8H16	006976-27-8	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Hexanol, 2,5-di...	10.28	5.8	ug/L	274012	2	9.44	2361750	50.0
unknown-01	11.04	8.8	ug/L	408225	3	11.82	2307640	50.0