

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU071318\
 Data File : VU025396.D
 Acq On : 13 Jul 2018 16:37
 Operator : MD/SY
 Sample : J3984-03
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DB175

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\SOMULM062918WMA.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	0.696	28	33	35	rBV4	879	786	0.02%	0.005%
2	0.709	35	37	40	rVB3	881	483	0.01%	0.003%
3	0.764	51	54	57	rBV4	833	692	0.02%	0.005%
4	0.809	63	68	76	rBV8	939	1438	0.04%	0.009%
5	0.844	76	79	83	rVV4	895	608	0.02%	0.004%
6	0.915	96	101	102	rBV3	1125	875	0.02%	0.006%
7	1.085	145	154	172	rBV	3250051	3697200	100.00%	24.062%
8	1.404	245	253	268	rBV2	546227	611116	16.53%	3.977%
9	1.680	332	339	355	rVB	96975	126896	3.43%	0.826%
10	2.188	490	497	514	rVB2	38313	62755	1.70%	0.408%
11	2.275	514	524	534	rBV	227295	344334	9.31%	2.241%
12	2.481	580	588	595	rBV	6150	10910	0.30%	0.071%
13	2.982	737	744	757	rVB2	21192	39551	1.07%	0.257%
14	3.452	886	890	892	rBV2	805	585	0.02%	0.004%
15	3.484	895	900	903	rVV4	790	691	0.02%	0.004%
16	3.593	931	934	940	rVB4	915	982	0.03%	0.006%
17	4.024	1065	1068	1075	rVB7	793	789	0.02%	0.005%
18	4.085	1083	1087	1088	rBV3	928	597	0.02%	0.004%
19	4.175	1092	1115	1120	rBV	102405	232386	6.29%	1.512%
20	4.230	1123	1132	1161	rVB	382810	903689	24.44%	5.881%
21	4.522	1221	1223	1227	rVB5	917	575	0.02%	0.004%
22	4.561	1227	1235	1238	rBV7	1128	1699	0.05%	0.011%
23	4.651	1248	1263	1281	rVB	185409	433955	11.74%	2.824%
24	4.764	1295	1298	1302	rBV5	675	549	0.01%	0.004%
25	4.876	1329	1333	1338	rBV6	939	1100	0.03%	0.007%
26	4.973	1360	1363	1364	rBV2	968	624	0.02%	0.004%
27	4.985	1364	1367	1369	rVV3	851	605	0.02%	0.004%
28	5.342	1452	1478	1507	rBV2	354023	1093430	29.57%	7.116%
29	5.593	1553	1556	1560	rBV4	1186	1123	0.03%	0.007%
30	5.648	1571	1573	1579	rVB8	1147	852	0.02%	0.006%
31	5.677	1579	1582	1588	rVB5	1126	1141	0.03%	0.007%
32	5.751	1600	1605	1609	rBV6	546	507	0.01%	0.003%
33	5.889	1624	1648	1667	rBV	385248	787376	21.30%	5.124%
34	6.188	1728	1741	1767	rBV	491410	954680	25.82%	6.213%

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 Title : VOC Analysis

35	6.333	1773	1786	1806	rBV	240698	481340	13.02%	3.133%
36	6.509	1835	1841	1845	rBV8	1580	2635	0.07%	0.017%
37	6.616	1866	1874	1883	rVB2	7961	13258	0.36%	0.086%
38	6.940	1971	1975	1978	rVB4	817	732	0.02%	0.005%
39	6.973	1979	1985	1990	rVB7	959	1108	0.03%	0.007%
40	7.156	2039	2042	2046	rBV4	1054	649	0.02%	0.004%
41	7.230	2050	2065	2080	rVV	140134	247620	6.70%	1.612%
42	7.426	2123	2126	2129	rBV3	770	543	0.01%	0.004%
43	7.461	2133	2137	2139	rBV4	1024	836	0.02%	0.005%
44	7.567	2156	2170	2185	rBV	500293	879168	23.78%	5.722%
45	7.638	2187	2192	2202	rVB	23754	39068	1.06%	0.254%
46	7.747	2221	2226	2227	rBV5	1056	918	0.02%	0.006%
47	7.850	2245	2258	2273	rBV	99361	167883	4.54%	1.093%
48	8.114	2337	2340	2342	rBV4	821	518	0.01%	0.003%
49	8.181	2348	2361	2366	rBV2	8762	14506	0.39%	0.094%
50	8.230	2366	2376	2389	rVV	111586	188085	5.09%	1.224%
51	8.310	2389	2401	2433	rVV	343168	620815	16.79%	4.040%
52	8.468	2443	2450	2459	rVB8	3561	5462	0.15%	0.036%
53	8.619	2493	2497	2500	rVB5	726	535	0.01%	0.003%
54	8.641	2500	2504	2505	rBV3	907	682	0.02%	0.004%
55	8.680	2511	2516	2518	rBV2	703	555	0.02%	0.004%
56	8.831	2557	2563	2565	rBV6	929	1064	0.03%	0.007%
57	8.915	2584	2589	2592	rBV5	916	780	0.02%	0.005%
58	8.976	2600	2608	2610	rBV7	1275	1307	0.04%	0.009%
59	9.091	2629	2644	2675	rBV	519671	885422	23.95%	5.762%
60	9.252	2686	2694	2702	rBV	11139	16447	0.44%	0.107%
61	9.323	2713	2716	2717	rBV4	851	540	0.01%	0.004%
62	9.329	2717	2718	2722	rBV3	872	528	0.01%	0.003%
63	9.381	2725	2734	2743	rBV	13537	24107	0.65%	0.157%
64	9.542	2782	2784	2787	rBV2	637	476	0.01%	0.003%
65	9.689	2825	2830	2832	rBV2	860	715	0.02%	0.005%
66	9.783	2851	2859	2869	rVB3	11589	18285	0.49%	0.119%
67	9.869	2884	2886	2889	rBV4	580	490	0.01%	0.003%
68	9.918	2896	2901	2909	rVB5	2198	2790	0.08%	0.018%
69	10.169	2974	2979	2981	rBV3	899	774	0.02%	0.005%
70	10.310	3018	3023	3024	rBV4	1003	732	0.02%	0.005%
71	10.435	3050	3062	3085	rVB	346242	564800	15.28%	3.676%

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72	10.532	3089	3092	3095	rBV3	941	627	0.02%	0.004%
73	10.612	3103	3117	3127	rBV4	11662	21106	0.57%	0.137%
74	10.683	3135	3139	3142	rBV3	1003	756	0.02%	0.005%
75	10.773	3162	3167	3170	rBV2	988	983	0.03%	0.006%
76	10.866	3192	3196	3199	rBV4	853	666	0.02%	0.004%
77	10.911	3207	3210	3213	rBV3	745	550	0.01%	0.004%
78	10.976	3223	3230	3234	rBV5	1474	1928	0.05%	0.013%
79	11.017	3239	3243	3245	rBV3	654	504	0.01%	0.003%
80	11.156	3274	3286	3296	rVB7	7304	13134	0.36%	0.085%
81	11.259	3310	3318	3322	rBV5	2534	3737	0.10%	0.024%
82	11.339	3339	3343	3345	rBV4	724	583	0.02%	0.004%
83	11.368	3349	3352	3360	rVB6	1424	1753	0.05%	0.011%
84	11.487	3377	3389	3404	rBV	547212	849526	22.98%	5.529%
85	11.574	3410	3416	3426	rVB5	2829	4341	0.12%	0.028%
86	11.631	3431	3434	3437	rBV3	879	554	0.01%	0.004%
87	11.757	3469	3473	3477	rBV5	760	827	0.02%	0.005%
88	11.863	3493	3506	3527	rVB	527359	846986	22.91%	5.512%
89	11.979	3539	3542	3546	rBV3	1415	1285	0.03%	0.008%
90	12.072	3563	3571	3578	rBV6	2666	4083	0.11%	0.027%
91	12.143	3586	3593	3600	rBV7	1432	2363	0.06%	0.015%
92	12.268	3628	3632	3634	rBV3	573	510	0.01%	0.003%
93	12.416	3674	3678	3681	rBV4	564	546	0.01%	0.004%
94	12.455	3681	3690	3692	rBV7	7134	8519	0.23%	0.055%
95	12.570	3716	3726	3739	rVB2	39228	60430	1.63%	0.393%
96	13.056	3866	3877	3881	rBV9	4906	8451	0.23%	0.055%
97	13.111	3891	3894	3896	rBV3	1488	1220	0.03%	0.008%
98	13.281	3944	3947	3948	rBV3	918	487	0.01%	0.003%
99	13.342	3952	3966	3968	rBV3	9193	19005	0.51%	0.124%
100	14.281	4252	4258	4265	rBV2	6224	8334	0.23%	0.054%

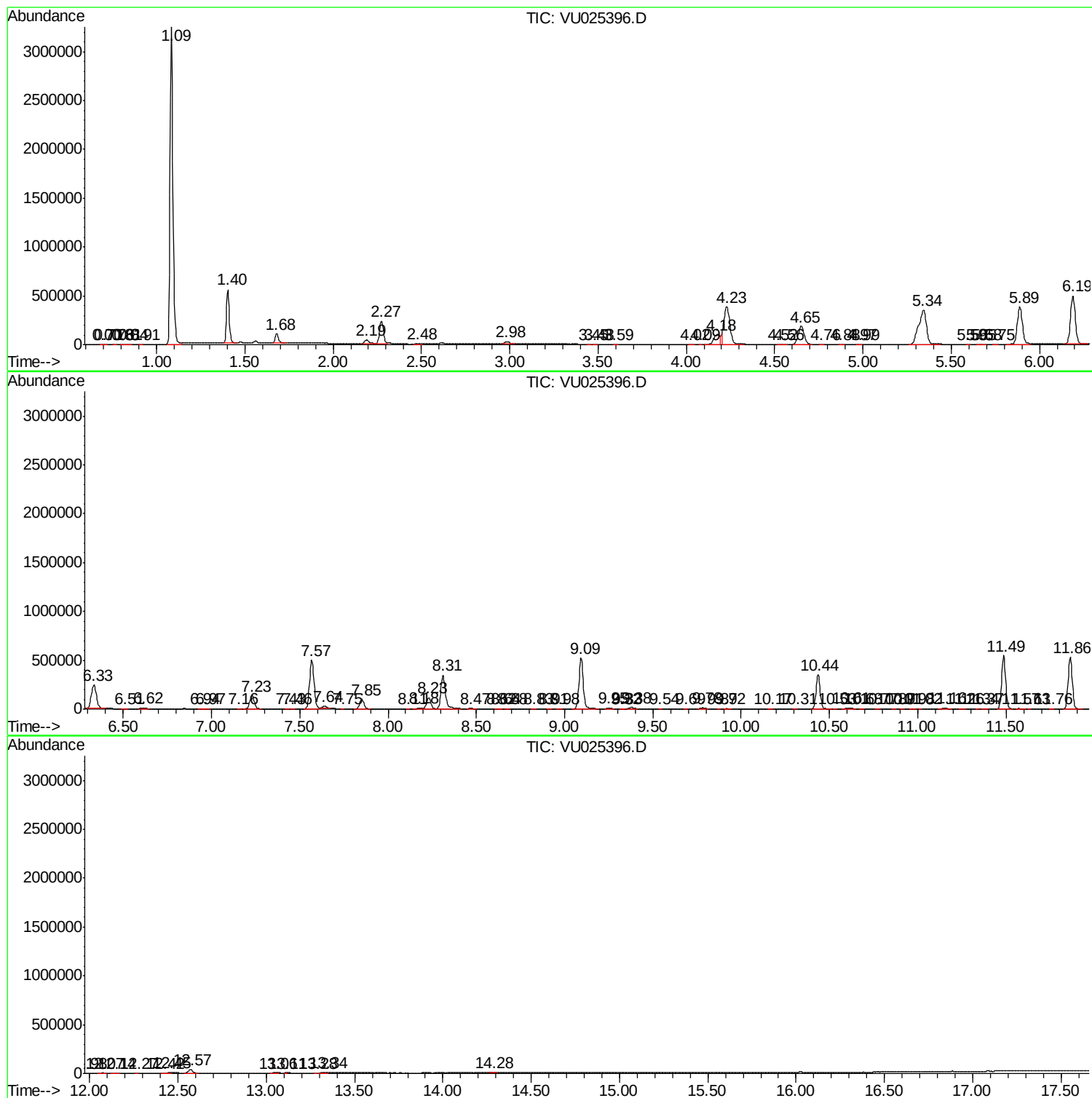
Sum of corrected areas: 15365546

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM062918WMA.M
Quant Title : VOC Analysis

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



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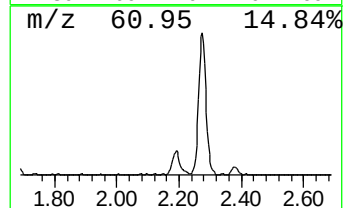
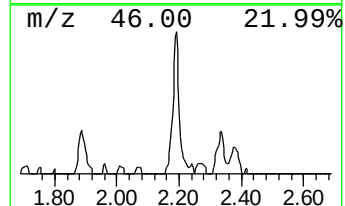
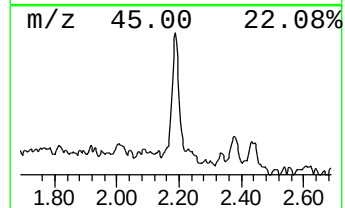
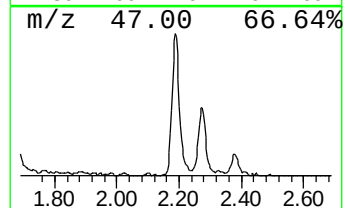
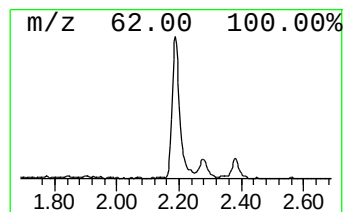
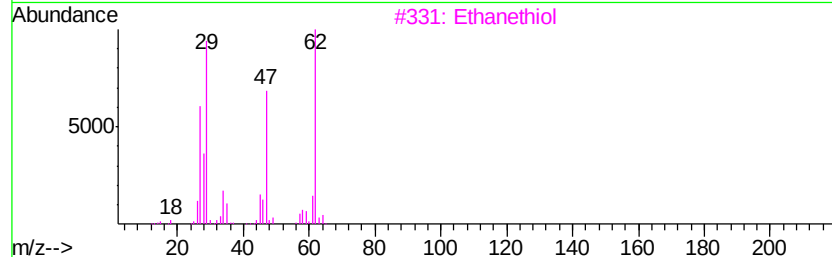
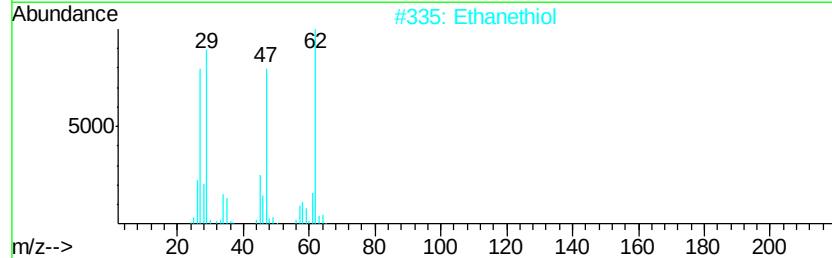
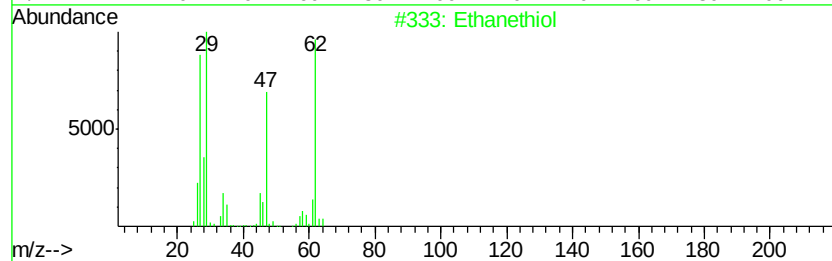
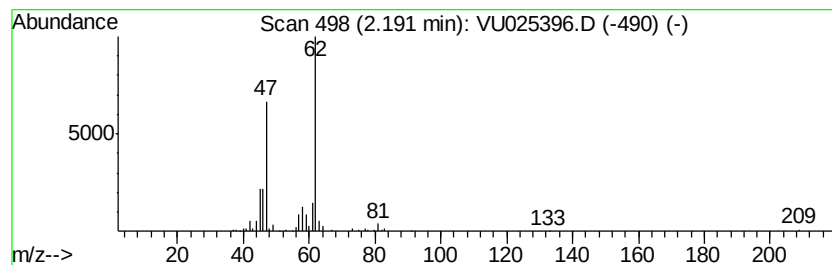
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM062918WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Ethanethiol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.19	3.99 ug/L	62755	1,4-Difluorobenzene	5.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanethiol	62	C2H6S	000075-08-1	87
2		Ethanethiol	62	C2H6S	000075-08-1	86
3		Ethanethiol	62	C2H6S	000075-08-1	78
4		Ethanethiol	62	C2H6S	000075-08-1	78
5		Ethanethiol	62	C2H6S	000075-08-1	78



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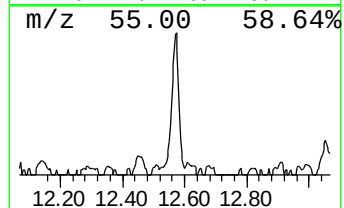
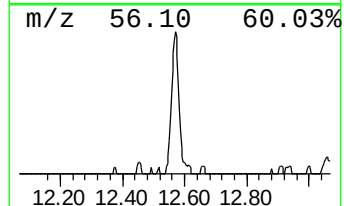
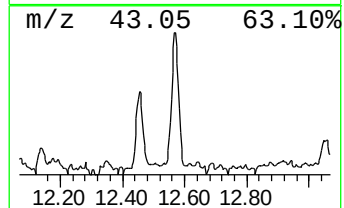
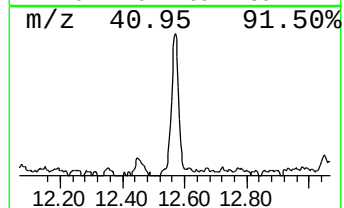
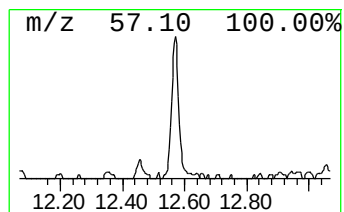
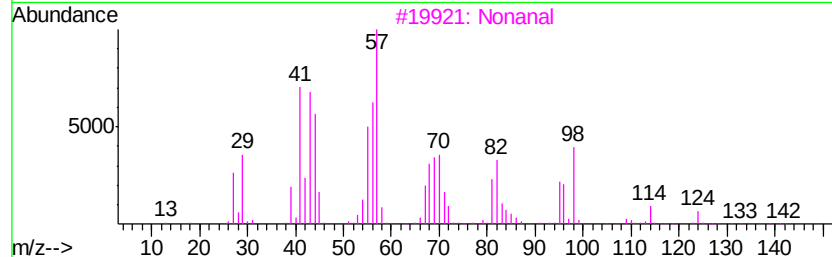
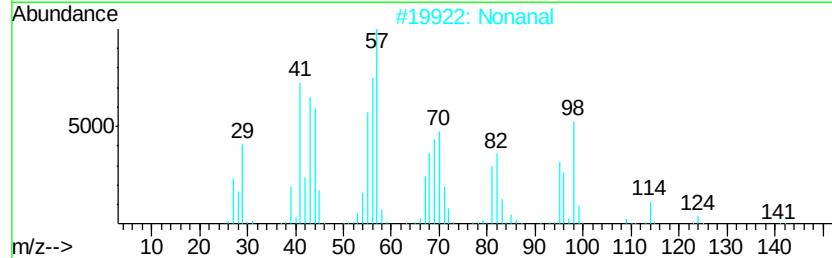
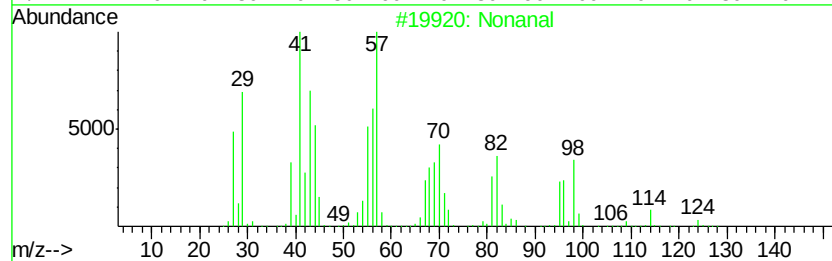
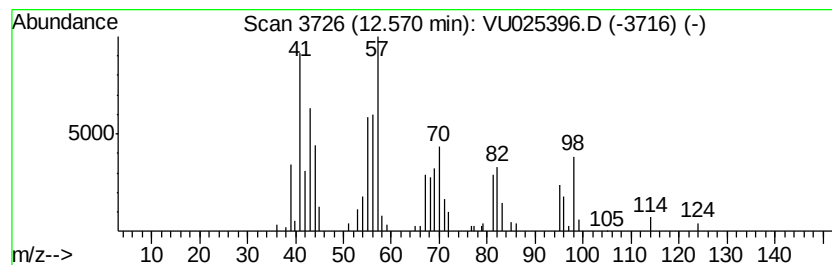
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Nonanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	3.56 ug/L	60430	1,4-Dichlorobenzene-d4	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonanal	142	C9H18O	000124-19-6	91
2		Nonanal	142	C9H18O	000124-19-6	90
3		Nonanal	142	C9H18O	000124-19-6	86
4		Cycloheptane	98	C7H14	000291-64-5	43
5		Cycloheptane	98	C7H14	000291-64-5	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanethiol	2.19	4.0	ug/L	62755	1	5.89	787376	50.0
Nonanal	12.57	3.6	ug/L	60430	3	11.49	849526	50.0