

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU071318\
 Data File : VU025397.D
 Acq On : 13 Jul 2018 17:29
 Operator : MD/SY
 Sample : J3984-04
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DB177

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	0.667	20	24	25	rBV4	897	545	0.00%	0.001%
2	0.805	64	67	70	rBV3	648	612	0.00%	0.002%
3	1.085	145	154	169	rBV	1863105	2099410	8.20%	5.405%
4	1.156	171	176	184	rBV	41825	49323	0.19%	0.127%
5	1.400	246	252	267	rVB2	162212	183733	0.72%	0.473%
6	1.561	296	302	308	rBV	168956	168937	0.66%	0.435%
7	1.680	333	339	354	rVB	97485	133041	0.52%	0.343%
8	2.275	515	524	549	rVB2	222757	424924	1.66%	1.094%
9	2.378	551	556	568	rVB2	9104	13628	0.05%	0.035%
10	2.484	583	589	595	rBV2	5367	8941	0.03%	0.023%
11	2.995	738	748	787	rVB	91829	288378	1.13%	0.742%
12	3.458	889	892	896	rVB3	805	596	0.00%	0.002%
13	3.619	939	942	945	rBV3	701	447	0.00%	0.001%
14	3.644	945	950	958	rVV7	794	1032	0.00%	0.003%
15	3.812	997	1002	1004	rVV4	971	625	0.00%	0.002%
16	4.014	1063	1065	1068	rVB3	785	482	0.00%	0.001%
17	4.046	1073	1075	1083	rVB5	414	466	0.00%	0.001%
18	4.230	1091	1132	1191	rBV	10029641	25589899	100.00%	65.886%
19	4.651	1249	1263	1289	rVB	189797	450688	1.76%	1.160%
20	5.075	1392	1395	1398	rVV3	709	497	0.00%	0.001%
21	5.127	1408	1411	1412	rBV3	709	417	0.00%	0.001%
22	5.342	1454	1478	1499	rBV2	359304	1080580	4.22%	2.782%
23	5.532	1533	1537	1541	rVB6	894	784	0.00%	0.002%
24	5.644	1570	1572	1575	rVB2	921	536	0.00%	0.001%
25	5.670	1575	1580	1582	rBV3	755	714	0.00%	0.002%
26	5.715	1591	1594	1599	rVB4	1035	972	0.00%	0.003%
27	5.786	1610	1616	1618	rBV6	1107	913	0.00%	0.002%
28	5.815	1622	1625	1628	rVB2	893	562	0.00%	0.001%
29	5.834	1628	1631	1634	rBV4	471	430	0.00%	0.001%
30	5.889	1634	1648	1665	rBV	392924	769101	3.01%	1.980%
31	6.188	1728	1741	1760	rBV	229450	444514	1.74%	1.144%
32	6.332	1772	1786	1803	rBV	237817	482870	1.89%	1.243%
33	6.496	1833	1837	1843	rBV6	804	1023	0.00%	0.003%
34	6.529	1843	1847	1854	rVB8	1303	1320	0.01%	0.003%

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35	6.574	1854	1861	1866	rBV5	1647	2231	0.01%	0.006%
36	6.615	1867	1874	1883	rVB4	4251	7446	0.03%	0.019%
37	6.712	1898	1904	1907	rBV6	1061	1155	0.00%	0.003%
38	6.776	1920	1924	1928	rBV6	758	744	0.00%	0.002%
39	6.828	1938	1940	1942	rBV2	649	406	0.00%	0.001%
40	6.857	1947	1949	1952	rVB2	1021	529	0.00%	0.001%
41	6.911	1962	1966	1968	rBV2	836	709	0.00%	0.002%
42	6.950	1972	1978	1979	rVV3	681	613	0.00%	0.002%
43	7.120	2029	2031	2037	rVB4	611	473	0.00%	0.001%
44	7.230	2052	2065	2088	rVB	137827	242500	0.95%	0.624%
45	7.329	2092	2096	2098	rBV4	800	680	0.00%	0.002%
46	7.448	2130	2133	2134	rVV2	884	447	0.00%	0.001%
47	7.464	2134	2138	2149	rVB7	2622	3789	0.01%	0.010%
48	7.513	2149	2153	2156	rBV3	885	716	0.00%	0.002%
49	7.567	2156	2170	2187	rBV	499554	879128	3.44%	2.263%
50	7.767	2226	2232	2242	rVB7	1359	2553	0.01%	0.007%
51	7.850	2245	2258	2271	rBV	94967	159605	0.62%	0.411%
52	7.921	2277	2280	2282	rBV3	790	450	0.00%	0.001%
53	7.937	2284	2285	2296	rVB8	1500	1510	0.01%	0.004%
54	8.001	2303	2305	2311	rBV6	649	411	0.00%	0.001%
55	8.075	2323	2328	2331	rBV5	750	764	0.00%	0.002%
56	8.098	2331	2335	2336	rBV3	486	403	0.00%	0.001%
57	8.178	2352	2360	2363	rBV4	3597	4518	0.02%	0.012%
58	8.230	2363	2376	2390	rVV	839361	1436001	5.61%	3.697%
59	8.310	2391	2401	2431	rVB	340388	606990	2.37%	1.563%
60	8.461	2446	2448	2455	rVV4	861	732	0.00%	0.002%
61	8.503	2458	2461	2468	rVB5	723	642	0.00%	0.002%
62	8.574	2480	2483	2494	rVB7	979	1439	0.01%	0.004%
63	8.702	2520	2523	2525	rVB3	705	408	0.00%	0.001%
64	8.721	2525	2529	2531	rBV4	704	425	0.00%	0.001%
65	8.908	2584	2587	2594	rVB4	597	703	0.00%	0.002%
66	8.934	2594	2595	2600	rBV3	851	503	0.00%	0.001%
67	9.014	2615	2620	2622	rBV5	950	711	0.00%	0.002%
68	9.091	2631	2644	2673	rBV	539125	903674	3.53%	2.327%
69	9.249	2685	2693	2698	rBV7	1773	2360	0.01%	0.006%
70	9.345	2717	2723	2726	rBV3	914	912	0.00%	0.002%
71	9.374	2726	2732	2733	rBV2	2310	1845	0.01%	0.005%

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72	9.557	2786	2789	2795	rBV6	734	703	0.00%	0.002%
73	9.918	2894	2901	2911	rVB6	2500	3674	0.01%	0.009%
74	9.963	2911	2915	2918	rVB2	807	630	0.00%	0.002%
75	10.435	3050	3062	3080	rVV	347177	554936	2.17%	1.429%
76	10.609	3108	3116	3129	rBV2	4668	7954	0.03%	0.020%
77	10.763	3161	3164	3169	rBV3	707	715	0.00%	0.002%
78	11.146	3276	3283	3285	rBV6	1958	2152	0.01%	0.006%
79	11.284	3322	3326	3327	rBV2	661	427	0.00%	0.001%
80	11.487	3376	3389	3404	rBV	554282	858379	3.35%	2.210%
81	11.564	3409	3413	3422	rVB6	1945	2969	0.01%	0.008%
82	11.606	3422	3426	3429	rBV2	659	412	0.00%	0.001%
83	11.683	3447	3450	3454	rBV4	514	407	0.00%	0.001%
84	11.863	3493	3506	3522	rBV	521693	829442	3.24%	2.136%
85	11.953	3531	3534	3536	rBV2	786	557	0.00%	0.001%
86	11.985	3536	3544	3554	rVV4	4446	8331	0.03%	0.021%
87	12.072	3567	3571	3580	rVB7	2272	3095	0.01%	0.008%
88	12.130	3586	3589	3593	rBV3	547	412	0.00%	0.001%
89	12.184	3599	3606	3608	rBV4	577	646	0.00%	0.002%
90	12.361	3657	3661	3668	rBV3	475	612	0.00%	0.002%
91	12.483	3692	3699	3705	rVV8	2680	4033	0.02%	0.010%
92	12.570	3716	3726	3739	rBV2	43197	65477	0.26%	0.169%
93	12.863	3811	3817	3819	rBV4	999	931	0.00%	0.002%
94	12.905	3826	3830	3831	rBV2	882	616	0.00%	0.002%
95	13.007	3860	3862	3865	rBV2	777	437	0.00%	0.001%
96	13.052	3868	3876	3886	rVV8	3703	7527	0.03%	0.019%
97	13.329	3954	3962	3966	rBV8	7322	11384	0.04%	0.029%
98	13.779	4099	4102	4109	rVB9	1444	1583	0.01%	0.004%
99	13.876	4129	4132	4133	rBV2	755	455	0.00%	0.001%
100	14.798	4417	4419	4421	rBV3	877	417	0.00%	0.001%

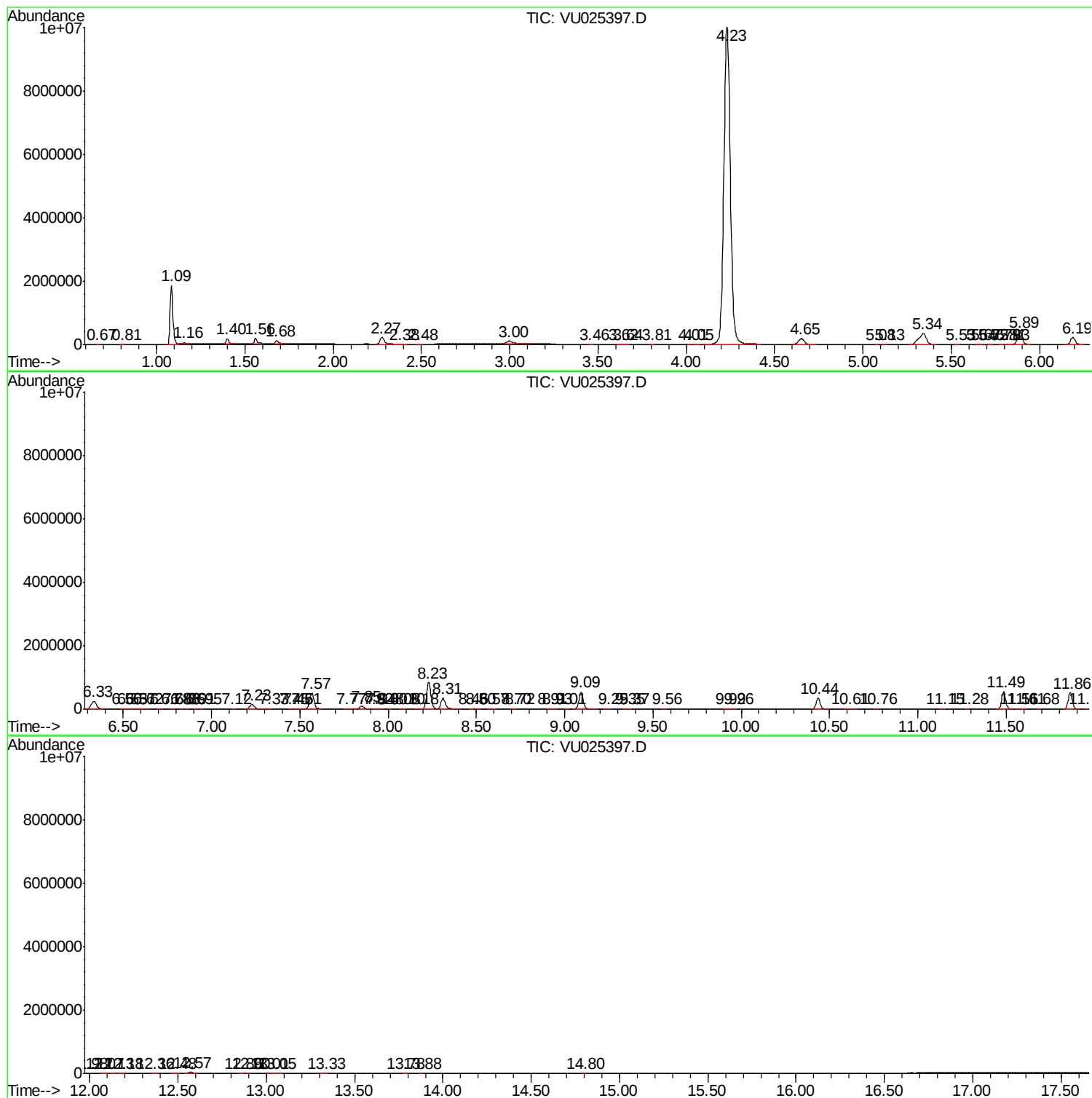
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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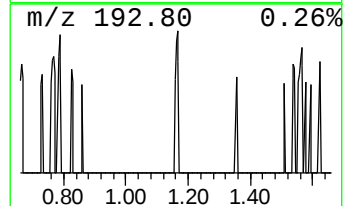
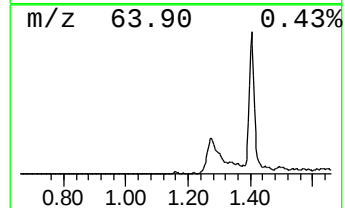
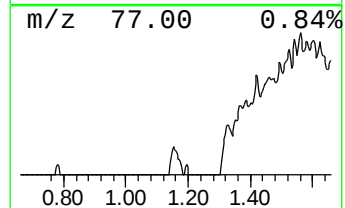
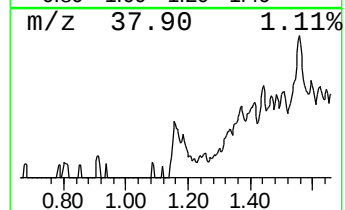
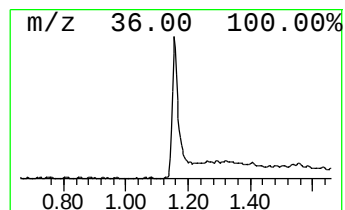
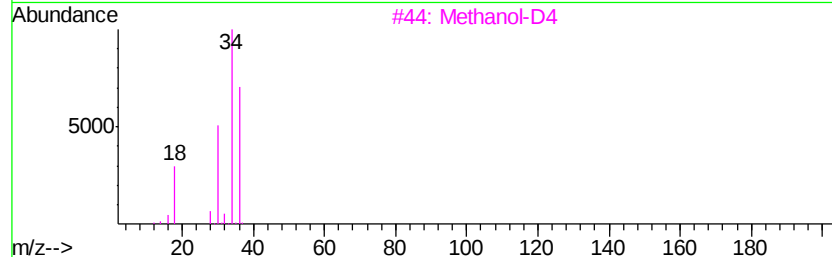
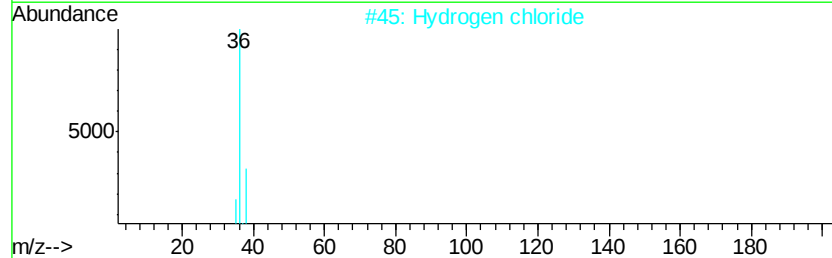
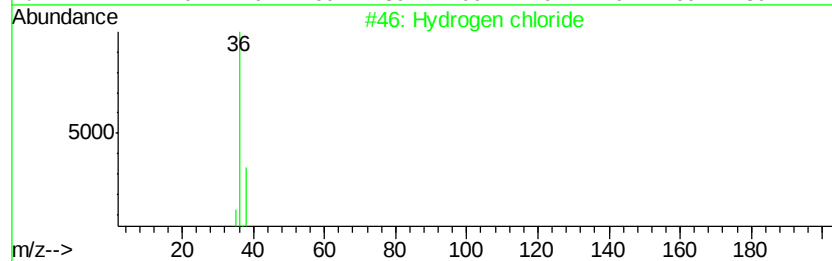
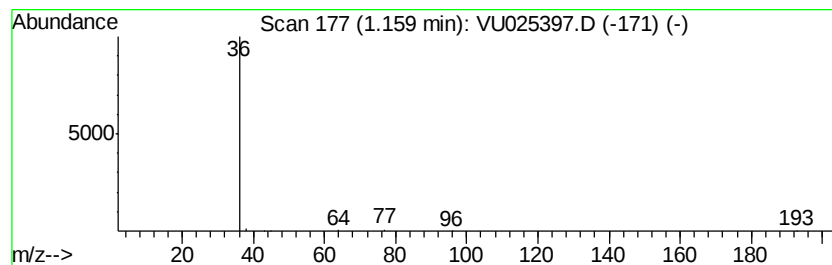
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM062918WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.16	3.21 ug/L	49323	1,4-Difluorobenzene	5.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hydrogen chloride	36	ClH	007647-01-0	2
2		Hydrogen chloride	36	ClH	007647-01-0	2
3		Methanol-D4	36	CD4O	000811-98-3	2
4		1H-Imidazole-1-ethanol, .alpha.-...	126	C6H10N2O	037788-55-9	1
5		Ammonium Chloride	53	ClH4N	012125-02-9	1



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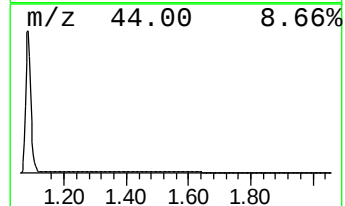
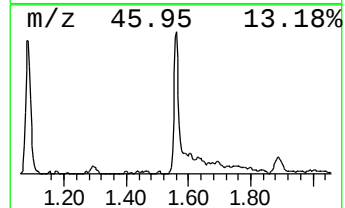
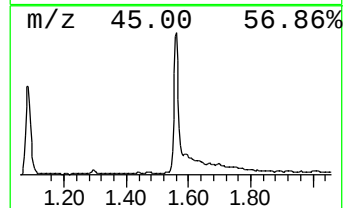
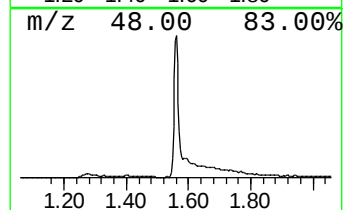
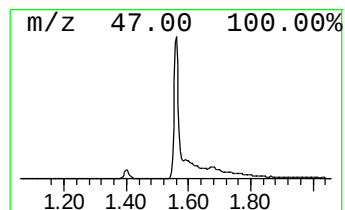
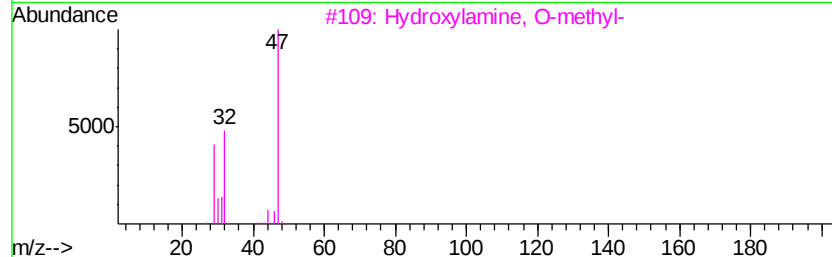
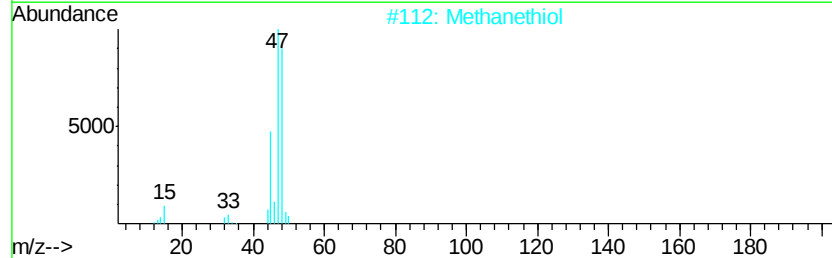
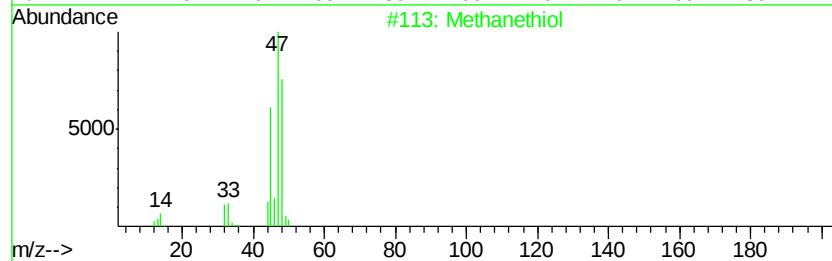
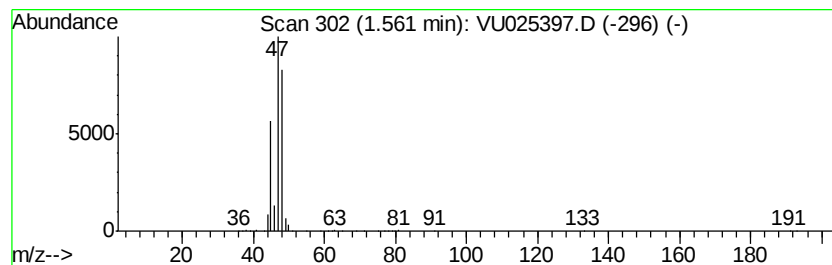
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Methanethiol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.56	10.98 ug/L	168937	1,4-Difluorobenzene	5.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methanethiol	48	CH4S	000074-93-1	90
2		Methanethiol	48	CH4S	000074-93-1	90
3		Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
4		Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
5		Methane, nitroso-	45	CH3NO	000865-40-7	5



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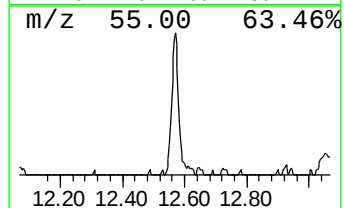
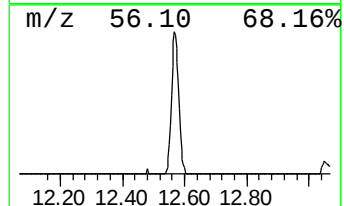
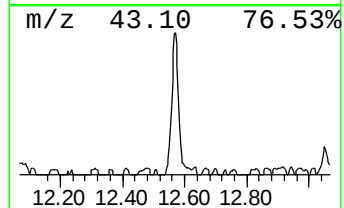
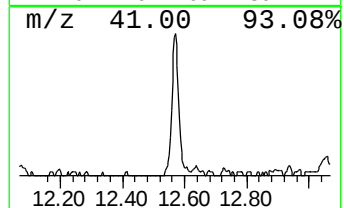
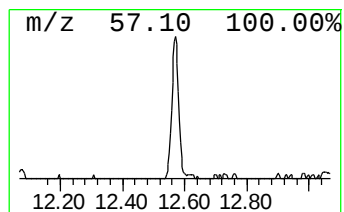
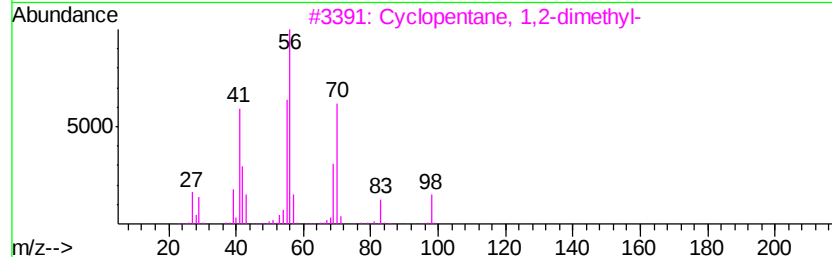
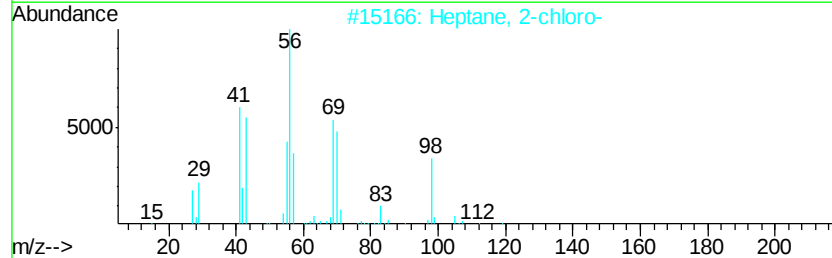
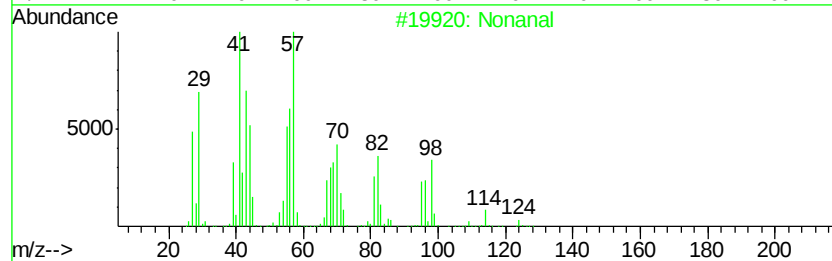
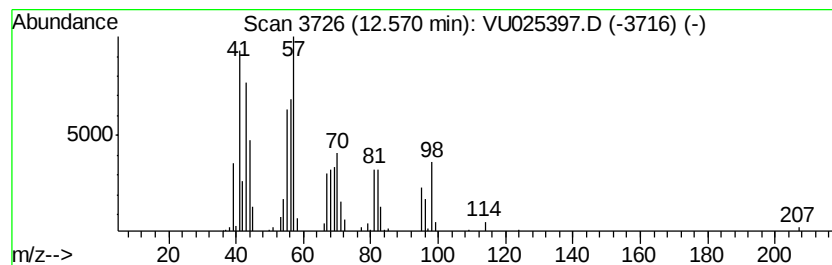
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Peak Number 5 Nonanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	3.81 ug/L	65477	1,4-Dichlorobenzene-d4	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonanal	142	C9H18O	000124-19-6	78
2		Heptane, 2-chloro-	134	C7H15Cl	001001-89-4	27
3		Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	27
4		2-Propen-1-amine, N-2-propenyl-	97	C6H11N	000124-02-7	25
5		2,3-Dimethyl-aziridine	71	C4H9N	002549-68-0	22



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU071318\
Data File : VU025397.D
Acq On : 13 Jul 2018 17:29
Operator : MD/SY
Sample : J3984-04
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DB177

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

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.16	3.2	ug/L	49323	1	5.89	769101	50.0
Methanethiol	1.56	11.0	ug/L	168937	1	5.89	769101	50.0
Nonanal	12.57	3.8	ug/L	65477	3	11.49	858379	50.0