

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
 Data File : VU043733.D
 Acq On : 14 May 2021 05:01
 Operator : SY/MD
 Sample : M2350-04
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BG6L7

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_U\Method\SFAMULM051421WMA.M

Title : VOC Analysis

Signal : TIC: VU043733.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.485	38	45	59	rBV	26917	69987	3.85%	0.521%
2	1.604	75	82	91	rBV	243556	284789	15.66%	2.119%
3	1.912	170	178	195	rVB	173501	233224	12.82%	1.736%
4	2.571	370	383	397	rBV	384170	628963	34.58%	4.681%
5	2.764	429	443	463	rBV	64159	139369	7.66%	1.037%
6	3.054	528	533	540	rVB4	1783	2433	0.13%	0.018%
7	3.092	541	545	548	rBV2	398	294	0.02%	0.002%
8	3.186	556	574	595	rBV2	74779	182487	10.03%	1.358%
9	3.311	611	613	616	rVB	324	188	0.01%	0.001%
10	3.562	687	691	694	rBV2	322	315	0.02%	0.002%
11	3.633	710	713	716	rBV	253	161	0.01%	0.001%
12	3.649	716	718	724	rVB3	394	291	0.02%	0.002%
13	3.684	724	729	733	rBV2	289	280	0.02%	0.002%
14	3.838	772	777	780	rBV	341	282	0.02%	0.002%
15	3.874	780	788	789	rVV2	380	417	0.02%	0.003%
16	3.893	793	794	797	rVV	356	181	0.01%	0.001%
17	4.044	835	841	844	rBV2	216	216	0.01%	0.002%
18	4.462	966	971	973	rBV2	261	188	0.01%	0.001%
19	4.475	973	975	979	rVB	288	187	0.01%	0.001%
20	4.530	990	992	994	rBV	258	179	0.01%	0.001%
21	4.559	998	1001	1006	rVB2	241	180	0.01%	0.001%
22	4.626	1006	1022	1053	rBV	207314	496016	27.27%	3.691%
23	5.073	1140	1161	1182	rBV	315045	687836	37.81%	5.119%
24	5.266	1217	1221	1223	rBV	253	199	0.01%	0.001%
25	5.304	1223	1233	1234	rBV3	1457	2071	0.11%	0.015%
26	5.385	1249	1258	1266	rBV3	527	1022	0.06%	0.008%
27	5.485	1283	1289	1293	rBV2	304	324	0.02%	0.002%
28	5.732	1344	1366	1401	rBV2	685575	1818970	100.00%	13.536%
29	5.989	1443	1446	1451	rVB3	318	243	0.01%	0.002%
30	6.018	1451	1455	1458	rBV4	307	220	0.01%	0.002%
31	6.047	1458	1464	1465	rVV3	334	383	0.02%	0.003%
32	6.105	1479	1482	1485	rBV3	530	426	0.02%	0.003%
33	6.256	1510	1529	1547	rBV	468826	885486	48.68%	6.590%
34	6.529	1609	1614	1623	rBV5	1289	2055	0.11%	0.015%
35	6.700	1652	1667	1687	rBV	413591	814323	44.77%	6.060%
36	6.893	1723	1727	1731	rVB3	320	219	0.01%	0.002%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
 Title : VOC Analysis

37	6.973	1745	1752	1765	rVB5	1628	2759	0.15%	0.021%
38	7.054	1766	1777	1781	rBV3	788	1384	0.08%	0.010%
39	7.182	1809	1817	1819	rBV3	563	652	0.04%	0.005%
40	7.349	1860	1869	1874	rBV3	359	527	0.03%	0.004%
41	7.414	1883	1889	1891	rBV2	271	279	0.02%	0.002%
42	7.517	1915	1921	1924	rBV2	1356	1403	0.08%	0.010%
43	7.571	1926	1938	1957	rVB	211746	368921	20.28%	2.745%
44	7.668	1965	1968	1970	rBV2	344	215	0.01%	0.002%
45	7.687	1971	1974	1979	rVV2	588	473	0.03%	0.004%
46	7.803	2004	2010	2013	rBV3	450	336	0.02%	0.003%
47	7.906	2027	2042	2056	rBV	816305	1393084	76.59%	10.367%
48	8.076	2092	2095	2097	rBV2	446	292	0.02%	0.002%
49	8.185	2116	2129	2146	rBV	148429	249096	13.69%	1.854%
50	8.410	2196	2199	2202	rVB2	322	158	0.01%	0.001%
51	8.433	2202	2206	2208	rBV2	252	189	0.01%	0.001%
52	8.449	2208	2211	2214	rVV2	347	258	0.01%	0.002%
53	8.475	2217	2219	2224	rVB3	549	393	0.02%	0.003%
54	8.568	2245	2248	2253	rVB2	239	218	0.01%	0.002%
55	8.639	2253	2270	2304	rBV	565582	1001686	55.07%	7.454%
56	8.796	2316	2319	2325	rVB4	540	483	0.03%	0.004%
57	8.967	2368	2372	2379	rVB2	429	516	0.03%	0.004%
58	9.002	2379	2383	2385	rBV2	255	209	0.01%	0.002%
59	9.198	2441	2444	2447	rBV3	256	193	0.01%	0.001%
60	9.272	2463	2467	2470	rBV2	261	201	0.01%	0.001%
61	9.301	2470	2476	2479	rBV2	336	435	0.02%	0.003%
62	9.423	2497	2514	2538	rBV	657454	1079775	59.36%	8.035%
63	9.549	2551	2553	2557	rVB2	355	235	0.01%	0.002%
64	9.587	2557	2565	2570	rBV3	624	719	0.04%	0.005%
65	9.700	2592	2600	2607	rVB6	1096	1721	0.09%	0.013%
66	9.886	2653	2658	2661	rBV	283	255	0.01%	0.002%
67	9.906	2661	2664	2665	rBV2	265	163	0.01%	0.001%
68	10.079	2716	2718	2722	rVB2	341	210	0.01%	0.002%
69	10.102	2722	2725	2731	rBV2	508	594	0.03%	0.004%
70	10.198	2750	2755	2757	rBV	175	161	0.01%	0.001%
71	10.272	2769	2778	2781	rBV4	1653	2273	0.12%	0.017%
72	10.481	2840	2843	2847	rBV	255	162	0.01%	0.001%
73	10.558	2864	2867	2869	rBV	229	171	0.01%	0.001%
74	10.680	2897	2905	2911	rBV4	2076	2597	0.14%	0.019%
75	10.764	2918	2931	2951	rBV	570487	928103	51.02%	6.907%
76	10.867	2960	2963	2966	rVB2	338	209	0.01%	0.002%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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 Title : VOC Analysis

77	10.896	2966	2972	2973	rBV3	659	573	0.03%	0.004%
78	10.938	2983	2985	2989	rVB3	310	188	0.01%	0.001%
79	10.999	3000	3004	3008	rBV3	321	329	0.02%	0.002%
80	11.037	3008	3016	3024	rVB5	3927	5932	0.33%	0.044%
81	11.118	3037	3041	3044	rBV2	455	403	0.02%	0.003%
82	11.301	3094	3098	3101	rBV2	525	435	0.02%	0.003%
83	11.423	3133	3136	3138	rBV	384	272	0.01%	0.002%
84	11.442	3140	3142	3145	rVV2	367	262	0.01%	0.002%
85	11.465	3145	3149	3159	rVB4	1100	1750	0.10%	0.013%
86	11.700	3216	3222	3224	rBV4	877	825	0.05%	0.006%
87	11.758	3238	3240	3246	rVB2	322	193	0.01%	0.001%
88	11.819	3246	3259	3284	rBV	601113	941975	51.79%	7.010%
89	11.938	3294	3296	3302	rVB4	397	322	0.02%	0.002%
90	12.041	3325	3328	3330	rBV2	302	218	0.01%	0.002%
91	12.057	3331	3333	3336	rVV2	308	175	0.01%	0.001%
92	12.079	3337	3340	3343	rVV2	292	216	0.01%	0.002%
93	12.143	3356	3360	3362	rBV3	233	167	0.01%	0.001%
94	12.201	3363	3378	3398	rBV	733154	1185953	65.20%	8.825%
95	12.320	3412	3415	3419	rVB2	400	306	0.02%	0.002%
96	13.285	3712	3715	3717	rBV2	269	188	0.01%	0.001%
97	13.584	3806	3808	3813	rVB2	308	213	0.01%	0.002%
98	13.947	3917	3921	3924	rBV3	362	355	0.02%	0.003%
99	14.057	3952	3955	3957	rBV2	335	204	0.01%	0.002%
100	14.339	4040	4043	4045	rBV2	416	259	0.01%	0.002%

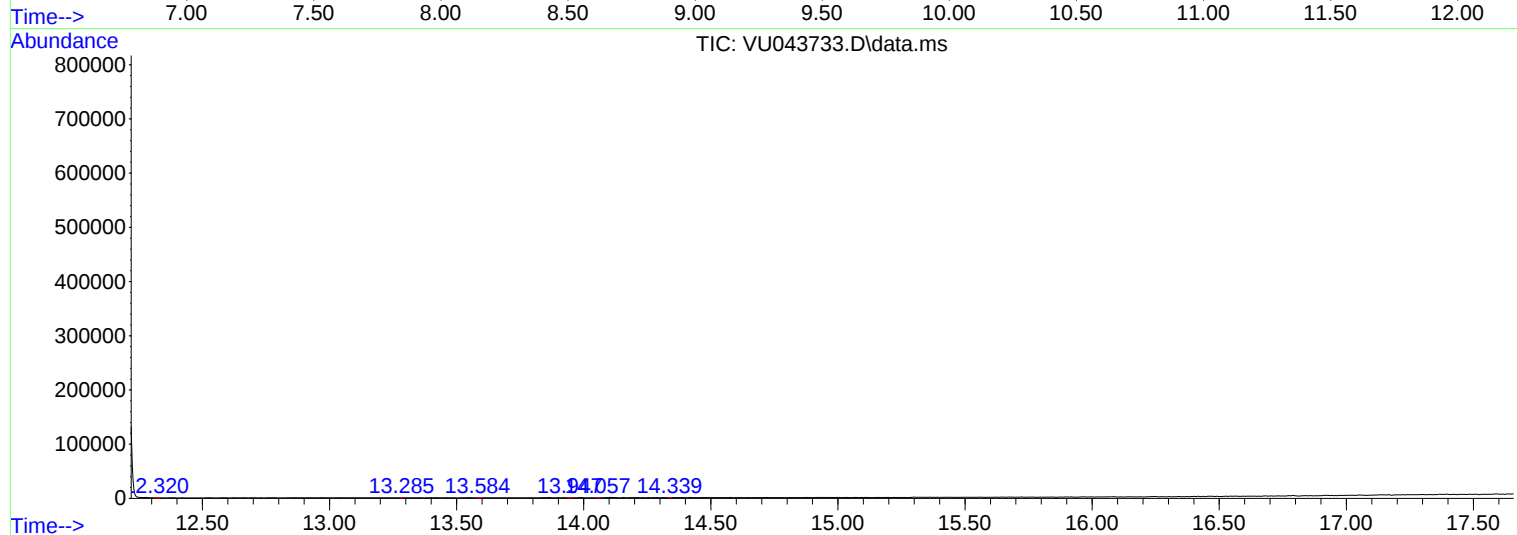
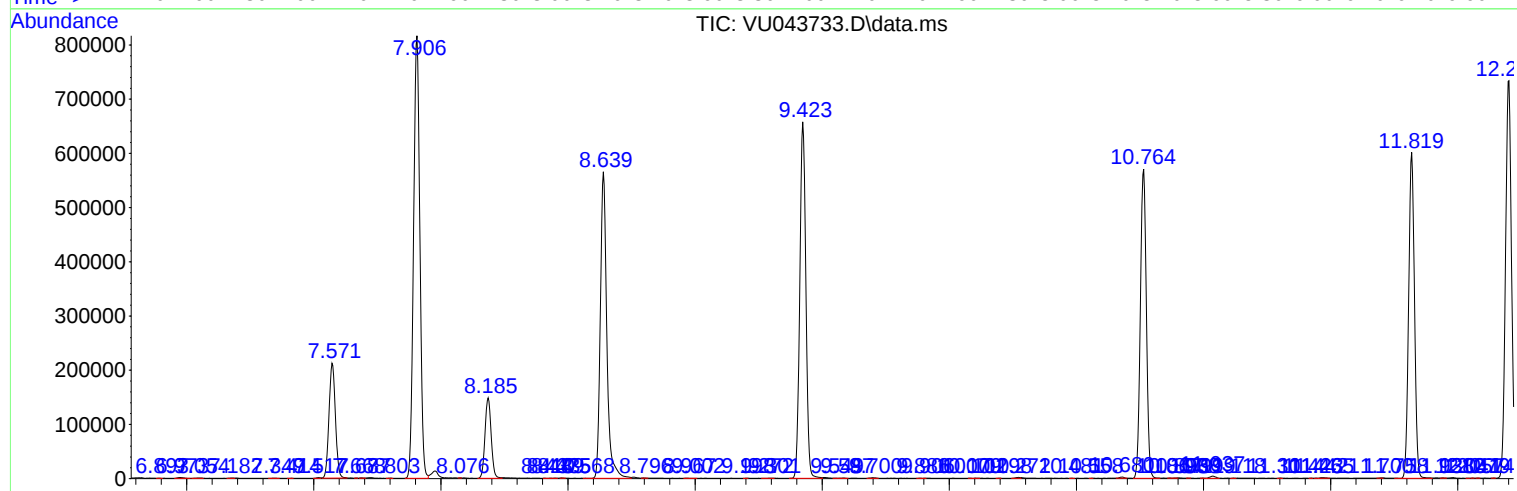
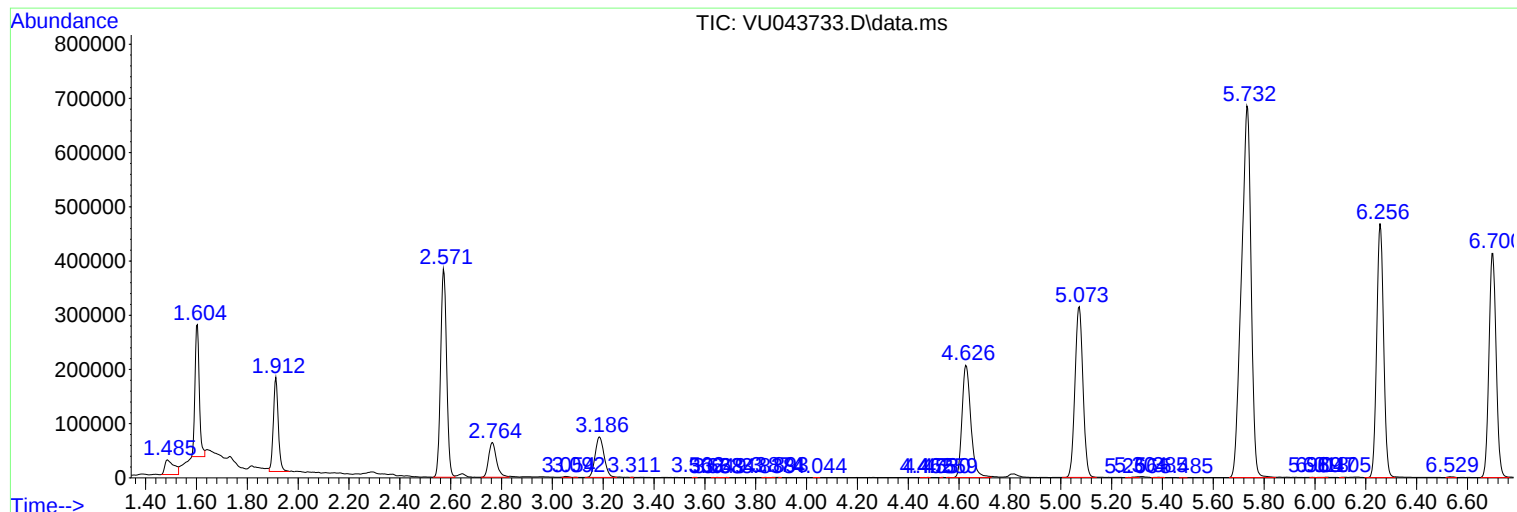
Sum of corrected areas: 13437825

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ALS Vial : 45 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.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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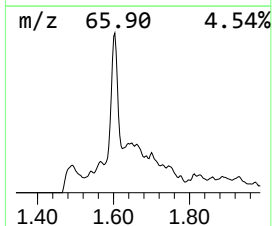
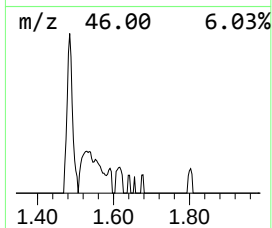
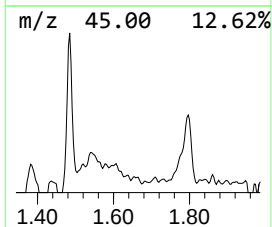
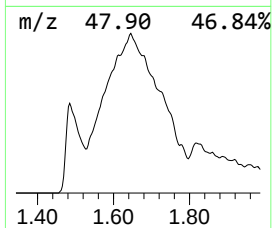
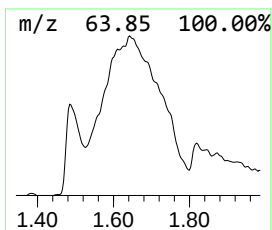
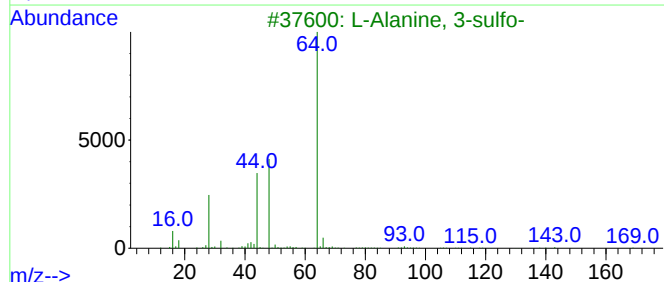
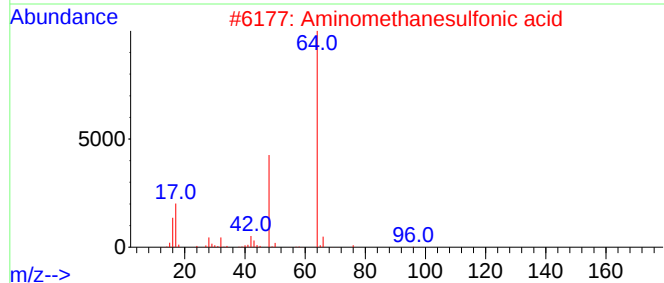
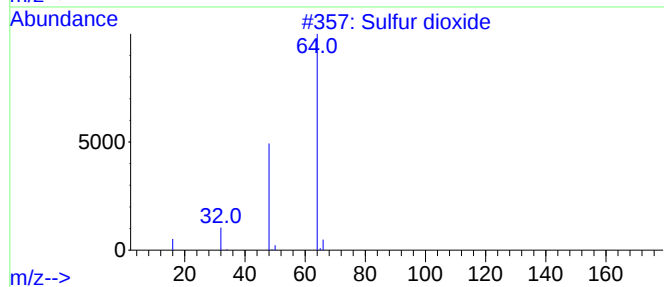
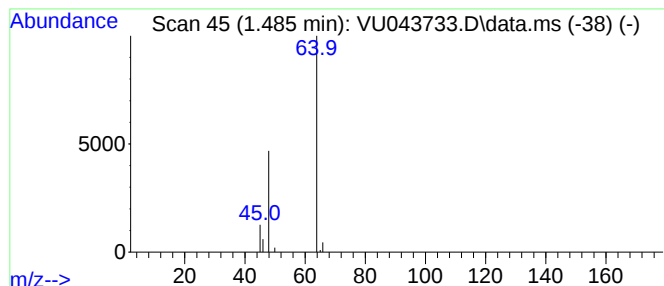
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.485	3.95 ug/L	69987	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	5
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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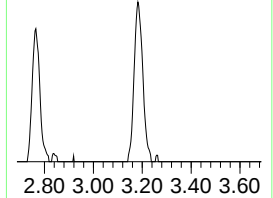
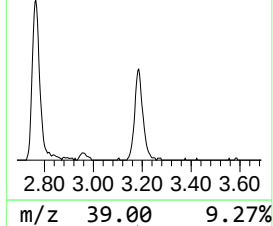
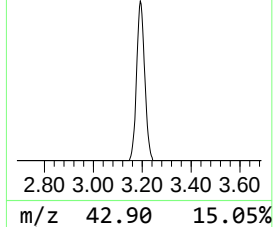
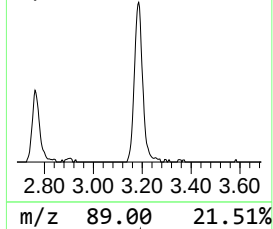
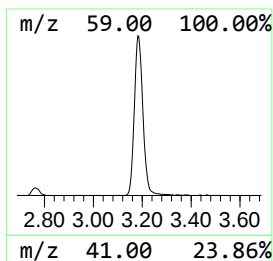
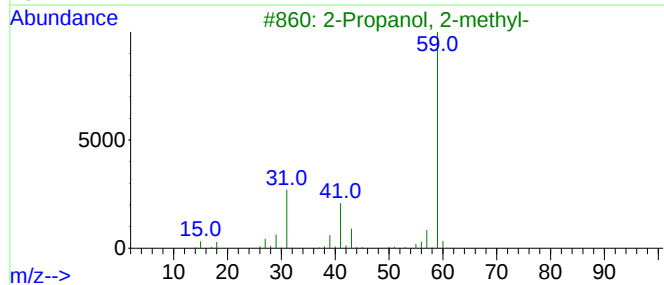
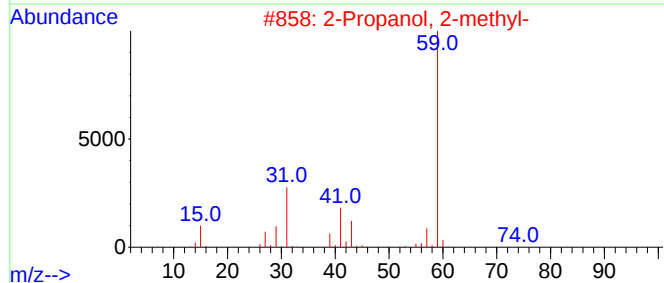
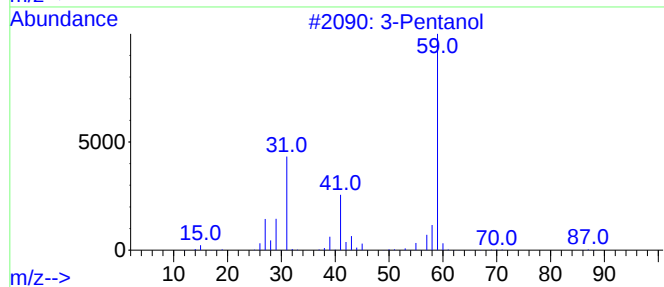
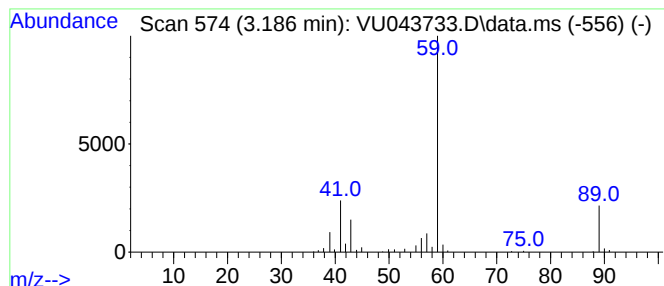
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Quant Title : VOC Analysis

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

Peak Number 2 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.186	10.30 ug/L	182487	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanol	88	C5H12O	000584-02-1	42
2			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	38
3			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	38
4			3-Pentanol	88	C5H12O	000584-02-1	36
5			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	36



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.485	4.0	ug/L	69987	1	6.256	885486	50.0
unknown-01	3.186	10.3	ug/L	182487	1	6.256	885486	50.0