

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041823\
 Data File : VX035150.D
 Acq On : 19 Apr 2023 02:06
 Operator : JC/MD
 Sample : 02397-14
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 49 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMM6

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_X\Method\SFAMXML041823WMA.M
 Title : VOC Analysis

Signal : TIC: VX035150.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	24	28	42	rBV	68420	199414	0.24%	0.069%
2	1.367	42	46	58	rVB	245664	279049	0.34%	0.097%
3	1.672	91	96	105	rBV	180660	233280	0.28%	0.081%
4	2.306	194	200	210	rVV	454036	712150	0.86%	0.248%
5	2.386	210	213	220	rVB	3437	6509	0.01%	0.002%
6	2.520	231	235	240	rBV3	879	1240	0.00%	0.000%
7	2.794	274	280	282	rVV3	1901	3026	0.00%	0.001%
8	2.831	282	286	287	rVV4	1519	2452	0.00%	0.001%
9	2.867	287	292	299	rVV2	5658	12416	0.02%	0.004%
10	2.940	299	304	312	rVV2	1802	3845	0.00%	0.001%
11	3.105	325	331	341	rVB4	1335	2975	0.00%	0.001%
12	3.446	382	387	388	rBV3	847	1058	0.00%	0.000%
13	3.617	410	415	417	rBV3	607	1202	0.00%	0.000%
14	4.306	519	528	540	rVB2	24615	69115	0.08%	0.024%
15	4.458	543	553	578	rBV	120795	371025	0.45%	0.129%
16	4.873	619	621	626	rVB3	297	454	0.00%	0.000%
17	5.056	638	651	669	rBV	253815	802824	0.97%	0.280%
18	5.263	683	685	688	rVB2	476	457	0.00%	0.000%
19	5.379	702	704	708	rVV3	627	861	0.00%	0.000%
20	5.470	711	719	730	rVB4	8112	25411	0.03%	0.009%
21	5.550	730	732	733	rBV2	544	544	0.00%	0.000%
22	5.678	742	753	767	rVB2	32206	99644	0.12%	0.035%
23	5.836	776	779	782	rVV3	554	543	0.00%	0.000%
24	5.970	788	801	803	rBV3	685371	1579500	1.91%	0.550%
25	6.043	804	813	842	rVB	12547866	34711928	42.04%	12.093%
26	6.336	859	861	862	rBV2	867	689	0.00%	0.000%
27	6.519	890	891	893	rBV2	531	417	0.00%	0.000%
28	6.653	912	913	917	rBV2	420	467	0.00%	0.000%
29	6.696	917	920	921	rBV2	355	388	0.00%	0.000%
30	6.763	921	931	944	rBV	489345	1175914	1.42%	0.410%
31	7.007	969	971	975	rVB3	434	419	0.00%	0.000%
32	7.110	983	988	989	rBV4	2194	2495	0.00%	0.001%
33	7.305	1009	1020	1042	rBV	404828	917878	1.11%	0.320%
34	7.482	1044	1049	1053	rBV6	1270	2488	0.00%	0.001%
35	7.659	1072	1078	1084	rVB4	1462	2468	0.00%	0.001%
36	7.952	1119	1126	1130	rBV4	1463	3181	0.00%	0.001%

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37	8.116	1150	1153	1157	rVB3	1245	1749	0.00%	0.001%
38	8.153	1157	1159	1161	rBV2	480	427	0.00%	0.000%
39	8.324	1180	1187	1200	rBV	257857	420145	0.51%	0.146%
40	8.494	1211	1215	1217	rVV4	795	1322	0.00%	0.000%
41	8.513	1217	1218	1222	rVB2	890	778	0.00%	0.000%
42	8.647	1234	1240	1249	rBV	1076634	1677712	2.03%	0.584%
43	8.720	1249	1252	1262	rVV3	4969	9885	0.01%	0.003%
44	8.848	1271	1273	1275	rVB3	546	399	0.00%	0.000%
45	8.951	1284	1290	1301	rBV	183634	271364	0.33%	0.095%
46	9.061	1306	1308	1310	rVV2	840	759	0.00%	0.000%
47	9.104	1313	1315	1317	rVB2	553	401	0.00%	0.000%
48	9.275	1338	1343	1349	rVB2	11141	15464	0.02%	0.005%
49	9.384	1355	1361	1373	rBV	583154	817934	0.99%	0.285%
50	9.543	1385	1387	1390	rVB2	1337	1189	0.00%	0.000%
51	9.744	1416	1420	1423	rBV4	293	471	0.00%	0.000%
52	10.092	1465	1477	1483	rBV	44027850	82576580	100.00%	28.769%
53	10.896	1608	1609	1614	rVB3	573	499	0.00%	0.000%
54	11.189	1652	1657	1669	rBV	660177	881764	1.07%	0.307%
55	11.317	1674	1678	1681	rVV4	723	1005	0.00%	0.000%
56	11.366	1681	1686	1692	rVV	14472	18066	0.02%	0.006%
57	11.457	1697	1701	1707	rVV	7538	10594	0.01%	0.004%
58	11.579	1717	1721	1723	rBV2	346	531	0.00%	0.000%
59	11.707	1739	1742	1748	rVB6	864	1517	0.00%	0.001%
60	11.762	1748	1751	1756	rVB4	632	863	0.00%	0.000%
61	11.969	1780	1785	1790	rBV	4279905	5168666	6.26%	1.801%
62	12.049	1790	1798	1803	rBV	41506381	63556236	76.97%	22.142%
63	12.219	1823	1826	1834	rVB4	5968	8898	0.01%	0.003%
64	12.341	1837	1846	1851	rBV	34174979	47871689	57.97%	16.678%
65	12.707	1901	1906	1911	rVB	9933	13837	0.02%	0.005%
66	12.811	1920	1923	1927	rVB5	1492	2024	0.00%	0.001%
67	12.872	1929	1933	1936	rVV3	11085	13526	0.02%	0.005%
68	12.920	1936	1941	1949	rVB	401839	482243	0.58%	0.168%
69	13.061	1958	1964	1969	rBV	136567	276248	0.33%	0.096%
70	13.109	1969	1972	1980	rVV2	93703	128182	0.16%	0.045%
71	13.195	1981	1986	1995	rVV	212337	267001	0.32%	0.093%
72	13.262	1995	1997	2002	rVB3	975	1110	0.00%	0.000%
73	13.298	2002	2003	2005	rBV3	461	395	0.00%	0.000%
74	13.329	2007	2008	2010	rBV2	487	495	0.00%	0.000%
75	13.384	2012	2017	2024	rVB	30630	42167	0.05%	0.015%
76	13.499	2032	2036	2038	rVB4	585	781	0.00%	0.000%

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Peak Location: TOP

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77	13.591	2045	2051	2056	rBV	24316404	30862170	37.37%	10.752%
78	13.774	2078	2081	2085	rVB	7199	8850	0.01%	0.003%
79	13.963	2106	2112	2127	rVB	6532377	8424996	10.20%	2.935%
80	14.207	2149	2152	2157	rVB4	1341	1910	0.00%	0.001%
81	14.268	2157	2162	2165	rBV4	3838	5400	0.01%	0.002%
82	14.341	2169	2174	2175	rVV3	1972	2154	0.00%	0.001%
83	14.377	2175	2180	2185	rVB5	6394	11653	0.01%	0.004%
84	14.475	2193	2196	2198	rVB2	538	577	0.00%	0.000%
85	14.511	2198	2202	2203	rBV4	692	749	0.00%	0.000%
86	14.542	2203	2207	2211	rVV2	6902	8174	0.01%	0.003%
87	14.585	2211	2214	2217	rVV	7810	9827	0.01%	0.003%
88	14.627	2217	2221	2226	rVB	10440	13539	0.02%	0.005%
89	14.780	2234	2246	2255	rBV	360813	559357	0.68%	0.195%
90	14.920	2266	2269	2273	rVV4	3432	3958	0.00%	0.001%
91	15.005	2280	2283	2286	rBV5	592	969	0.00%	0.000%
92	15.249	2316	2323	2338	rVB	934160	1300672	1.58%	0.453%
93	15.432	2351	2353	2355	rBV3	639	487	0.00%	0.000%
94	15.481	2360	2361	2365	rVB3	645	617	0.00%	0.000%
95	15.591	2376	2379	2384	rBV3	497	875	0.00%	0.000%
96	16.084	2458	2460	2463	rBV2	522	603	0.00%	0.000%
97	16.401	2510	2512	2513	rBV2	966	543	0.00%	0.000%
98	16.505	2522	2529	2537	rBV3	21360	41916	0.05%	0.015%
99	16.590	2542	2543	2546	rVB3	535	550	0.00%	0.000%
100	16.712	2562	2563	2567	rVB4	616	582	0.00%	0.000%

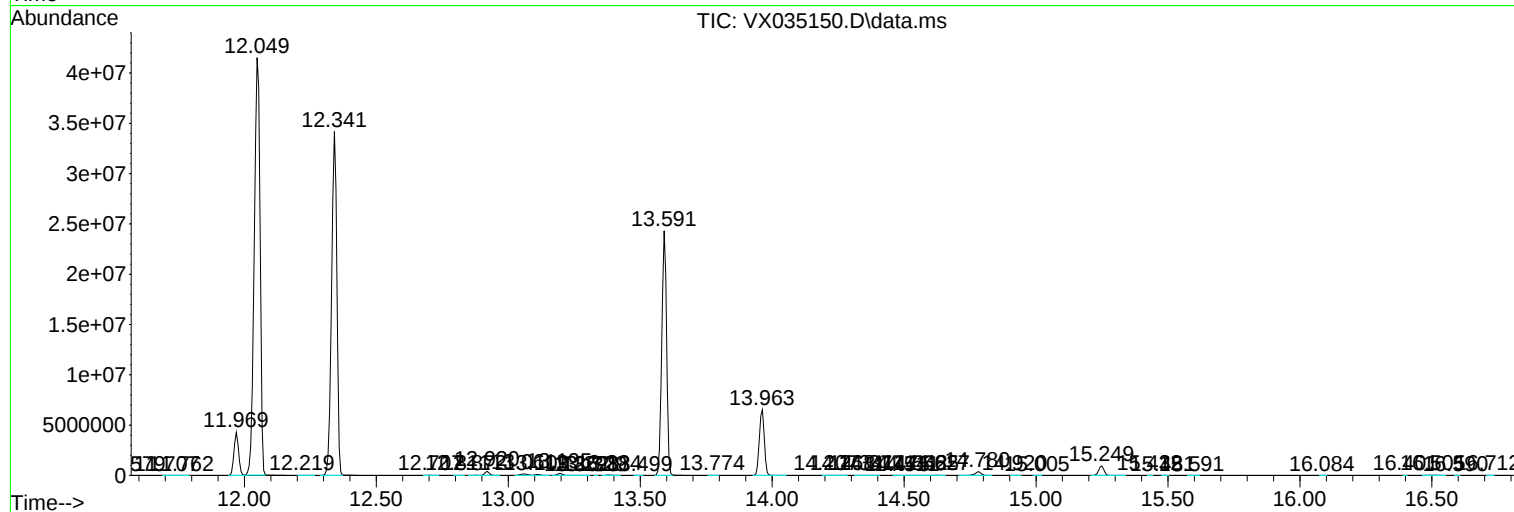
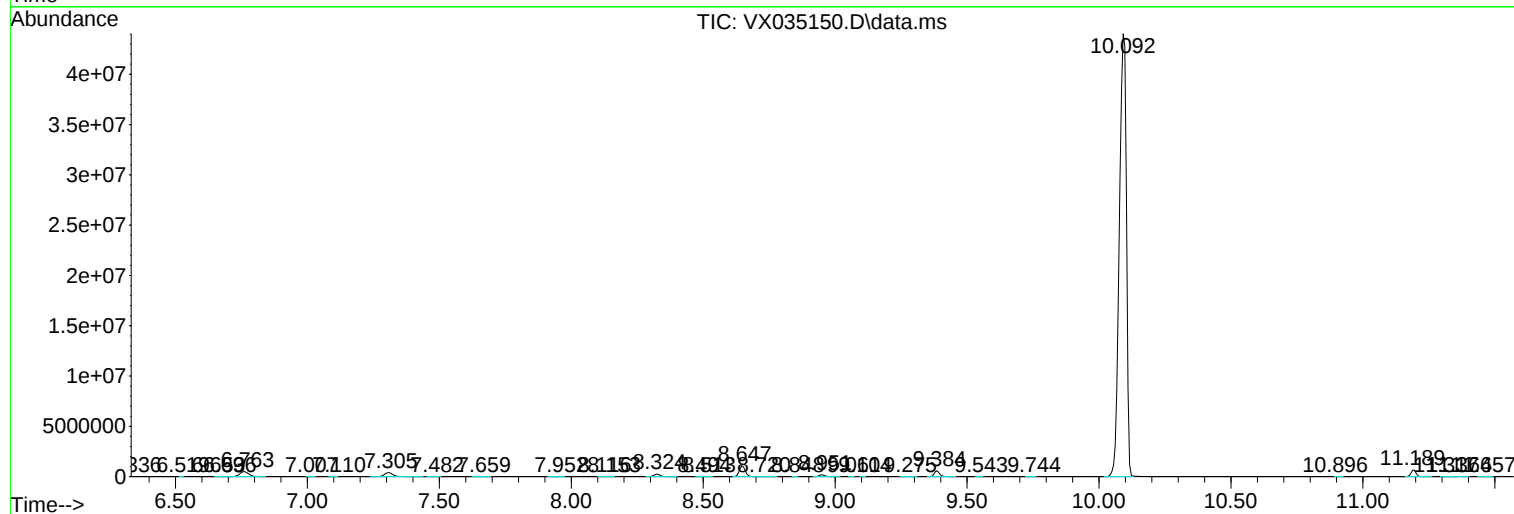
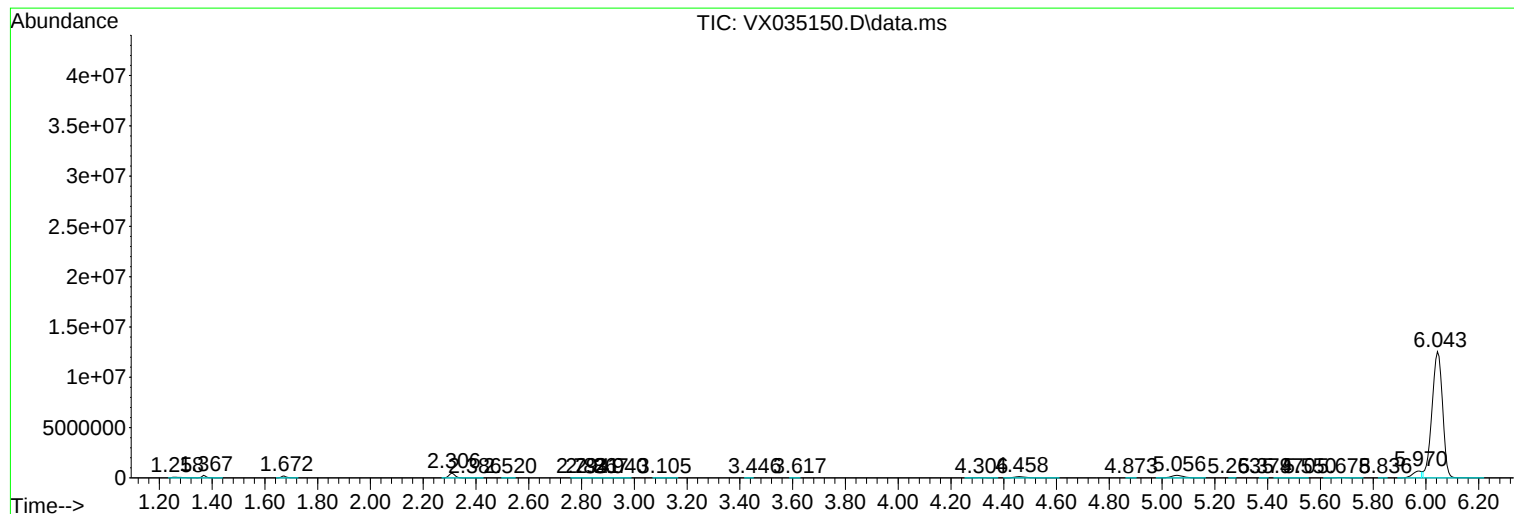
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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



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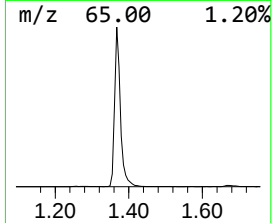
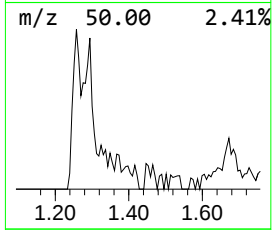
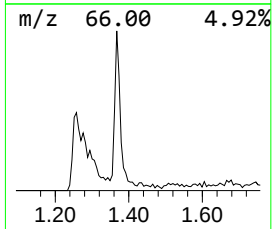
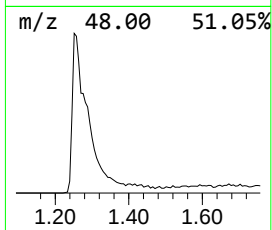
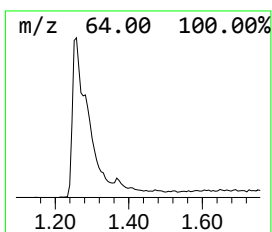
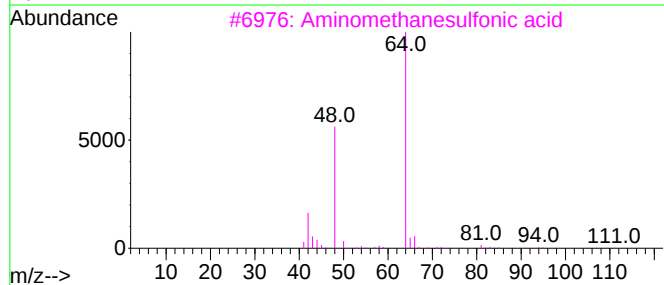
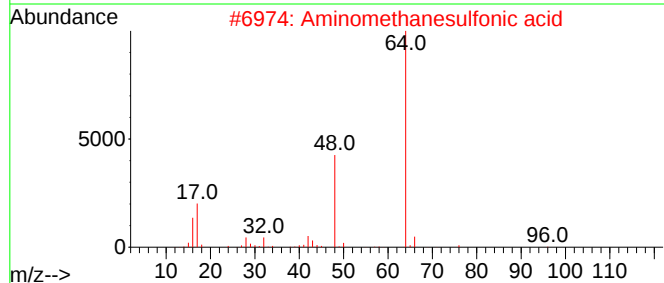
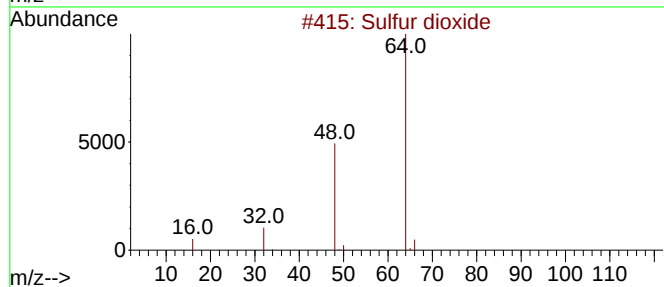
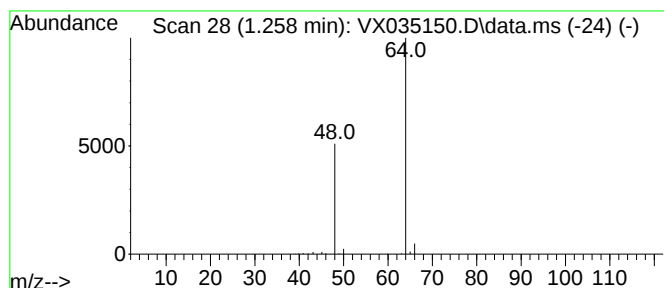
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.258	8.48 ug/L	199414	1,4-Difluorobenzene	6.763

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	74
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



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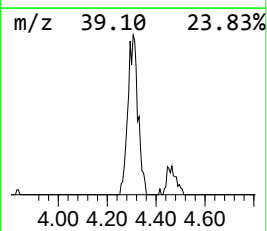
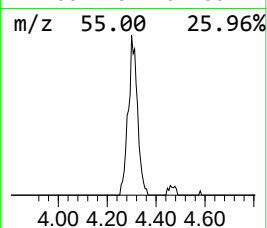
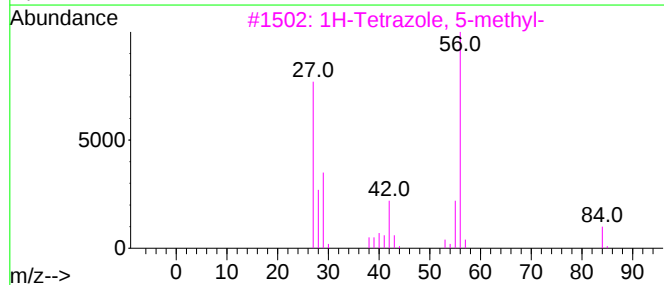
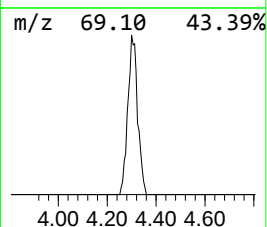
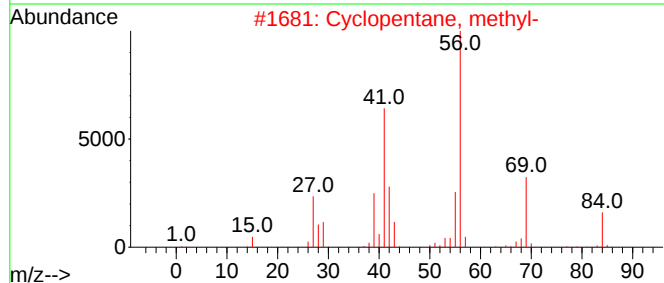
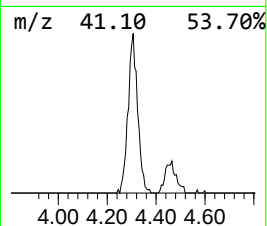
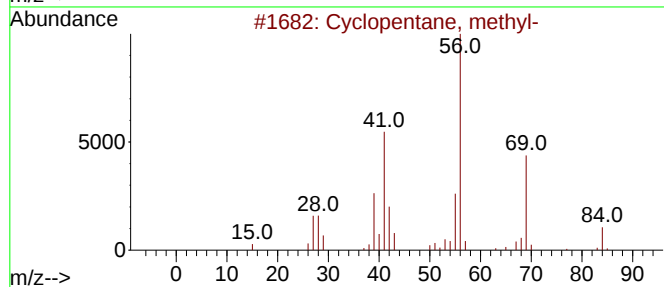
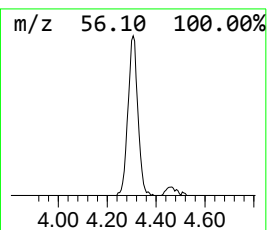
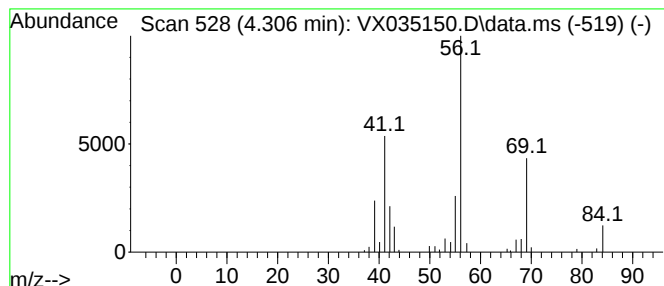
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TIC Integration Parameters: LSCINT.P

Peak Number 2 (DEL) Alkane: Cyclic4.306 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	2.94 ug/L	69115	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
3			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
4			Cyclopentane, methyl-	84	C6H12	000096-37-7	78
5			Cyclopentane, methyl-	84	C6H12	000096-37-7	56



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.258	8.5	ug/L	199414	1	6.763	1175910	50.0
(DEL) Alkane: C...	4.306	2.9	ug/L	69115	1	6.763	1175910	50.0