

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080422\
 Data File : VX030407.D
 Acq On : 04 Aug 2022 21:21
 Operator : JC/MD
 Sample : N4003-19
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 F5D89

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\SFAMXML080422WMA.M
 Title : VOC Analysis

Signal : TIC: VX030407.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	41	47	59	rVB	1673381	1824182	46.32%	12.280%
2	1.666	91	95	103	rVB	127334	153358	3.89%	1.032%
3	1.746	104	108	117	rVB2	16899	23488	0.60%	0.158%
4	1.953	139	142	150	rVB3	8137	13288	0.34%	0.089%
5	2.306	194	200	210	rBV	275897	431197	10.95%	2.903%
6	2.392	211	214	217	rBV2	2694	4076	0.10%	0.027%
7	2.709	263	266	270	rBV3	615	1096	0.03%	0.007%
8	2.776	270	277	280	rBV2	8616	18024	0.46%	0.121%
9	2.825	281	285	290	rVB2	18608	34356	0.87%	0.231%
10	2.977	306	310	311	rBV3	697	551	0.01%	0.004%
11	3.093	320	329	343	rBV3	125176	280984	7.13%	1.892%
12	3.416	379	382	383	rBV3	527	447	0.01%	0.003%
13	3.599	410	412	415	rVV2	416	339	0.01%	0.002%
14	3.648	419	420	425	rBV2	482	614	0.02%	0.004%
15	3.867	452	456	459	rVB2	584	678	0.02%	0.005%
16	3.940	465	468	470	rBV2	489	600	0.02%	0.004%
17	3.971	470	473	474	rVV2	452	372	0.01%	0.003%
18	4.184	505	508	509	rBV2	458	389	0.01%	0.003%
19	4.312	520	529	544	rVB2	17054	47628	1.21%	0.321%
20	4.495	545	559	583	rBV2	1425834	3938633	100.00%	26.515%
21	5.068	641	653	669	rBV	155683	493326	12.53%	3.321%
22	5.257	683	684	690	rVB4	410	522	0.01%	0.004%
23	5.379	699	704	708	rBV3	896	1654	0.04%	0.011%
24	5.483	713	721	729	rVB4	10299	29418	0.75%	0.198%
25	5.806	772	774	775	rBV	429	397	0.01%	0.003%
26	5.848	775	781	790	rVV5	2751	8440	0.21%	0.057%
27	5.976	790	802	826	rVV2	418064	1272059	32.30%	8.563%
28	6.159	827	832	841	rVV8	5475	16558	0.42%	0.111%
29	6.257	843	848	857	rVV3	5068	14224	0.36%	0.096%
30	6.361	857	865	874	rVB6	6352	17128	0.43%	0.115%
31	6.470	881	883	886	rBV2	445	621	0.02%	0.004%
32	6.537	892	894	899	rBV2	419	608	0.02%	0.004%
33	6.611	905	906	908	rBV2	451	322	0.01%	0.002%
34	6.647	910	912	920	rVB3	587	1112	0.03%	0.007%
35	6.769	920	932	944	rBV	266837	651033	16.53%	4.383%
36	7.117	980	989	1000	rBV4	12093	31659	0.80%	0.213%

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37	7.238	1007	1009	1012	rBV2	566	643	0.02%	0.004%
38	7.312	1012	1021	1028	rBV	255895	563233	14.30%	3.792%
39	7.488	1046	1050	1053	rVB3	851	1336	0.03%	0.009%
40	7.592	1064	1067	1072	rBV3	525	1214	0.03%	0.008%
41	7.659	1074	1078	1083	rVB4	2816	4858	0.12%	0.033%
42	7.744	1089	1092	1097	rBV	411	593	0.02%	0.004%
43	7.866	1110	1112	1113	rBV2	484	457	0.01%	0.003%
44	8.330	1181	1188	1200	rBV	169489	282968	7.18%	1.905%
45	8.500	1214	1216	1220	rBV3	515	451	0.01%	0.003%
46	8.537	1220	1222	1223	rVB	555	334	0.01%	0.002%
47	8.653	1234	1241	1249	rBV	644632	979345	24.87%	6.593%
48	8.952	1285	1290	1300	rBV	124240	185590	4.71%	1.249%
49	9.128	1316	1319	1321	rVB3	505	593	0.02%	0.004%
50	9.275	1340	1343	1348	rVB3	1454	1869	0.05%	0.013%
51	9.317	1348	1350	1353	rBV2	454	569	0.01%	0.004%
52	9.391	1356	1362	1375	rBV	461560	681545	17.30%	4.588%
53	9.592	1392	1395	1396	rBV2	845	646	0.02%	0.004%
54	9.726	1415	1417	1421	rVB2	438	434	0.01%	0.003%
55	9.775	1424	1425	1428	rBV	591	552	0.01%	0.004%
56	9.805	1428	1430	1432	rBV	477	541	0.01%	0.004%
57	9.872	1437	1441	1444	rBV2	414	630	0.02%	0.004%
58	10.055	1465	1471	1483	rBV	555972	742610	18.85%	4.999%
59	10.201	1492	1495	1499	rVB4	2666	3555	0.09%	0.024%
60	10.238	1499	1501	1505	rVV3	808	1306	0.03%	0.009%
61	10.311	1508	1513	1517	rVB3	3874	5741	0.15%	0.039%
62	10.537	1548	1550	1555	rBV3	479	590	0.01%	0.004%
63	10.598	1558	1560	1563	rBV	334	349	0.01%	0.002%
64	10.646	1563	1568	1571	rVV2	1451	2008	0.05%	0.014%
65	10.677	1571	1573	1578	rVB2	421	442	0.01%	0.003%
66	10.823	1595	1597	1600	rBV2	292	328	0.01%	0.002%
67	10.890	1606	1608	1610	rBV	403	361	0.01%	0.002%
68	10.969	1619	1621	1624	rVB2	502	376	0.01%	0.003%
69	11.128	1646	1647	1652	rBV2	294	464	0.01%	0.003%
70	11.195	1652	1658	1668	rBV	460344	570725	14.49%	3.842%
71	11.323	1677	1679	1682	rBV2	426	511	0.01%	0.003%
72	11.433	1694	1697	1701	rVB2	814	1124	0.03%	0.008%
73	11.463	1701	1702	1704	rBV2	677	539	0.01%	0.004%
74	11.713	1739	1743	1745	rBV3	648	813	0.02%	0.005%
75	11.750	1745	1749	1755	rVB4	428	716	0.02%	0.005%
76	11.799	1755	1757	1761	rVB2	326	330	0.01%	0.002%

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77	11.890	1769	1772	1774	rBV	878	801	0.02%	0.005%
78	12.024	1789	1794	1804	rBV	566180	678734	17.23%	4.569%
79	12.128	1809	1811	1814	rBV2	589	641	0.02%	0.004%
80	12.183	1818	1820	1823	rVB3	647	480	0.01%	0.003%
81	12.225	1824	1827	1831	rVB4	854	1115	0.03%	0.008%
82	12.323	1837	1843	1856	rBV	639160	806344	20.47%	5.428%
83	12.542	1876	1879	1885	rVB	1245	1878	0.05%	0.013%
84	12.792	1919	1920	1924	rBV2	396	417	0.01%	0.003%
85	12.963	1945	1948	1949	rBV	367	354	0.01%	0.002%
86	12.981	1949	1951	1954	rVV2	666	566	0.01%	0.004%
87	13.012	1954	1956	1959	rVV3	483	560	0.01%	0.004%
88	13.701	2066	2069	2074	rBV3	505	866	0.02%	0.006%
89	13.786	2081	2083	2088	rVB3	866	1033	0.03%	0.007%
90	13.951	2108	2110	2112	rBV3	427	392	0.01%	0.003%
91	14.042	2124	2125	2127	rBV2	518	446	0.01%	0.003%
92	14.188	2147	2149	2150	rVV	599	391	0.01%	0.003%
93	14.225	2153	2155	2158	rBV2	477	363	0.01%	0.002%
94	14.396	2180	2183	2184	rBV	611	607	0.02%	0.004%
95	14.670	2227	2228	2230	rBV	567	518	0.01%	0.003%
96	14.859	2257	2259	2260	rBV2	798	634	0.02%	0.004%
97	15.353	2338	2340	2341	rBV2	725	355	0.01%	0.002%
98	15.371	2341	2343	2347	rBV	743	949	0.02%	0.006%
99	15.645	2385	2388	2389	rBV2	823	902	0.02%	0.006%
100	15.688	2393	2395	2398	rVB3	780	583	0.01%	0.004%

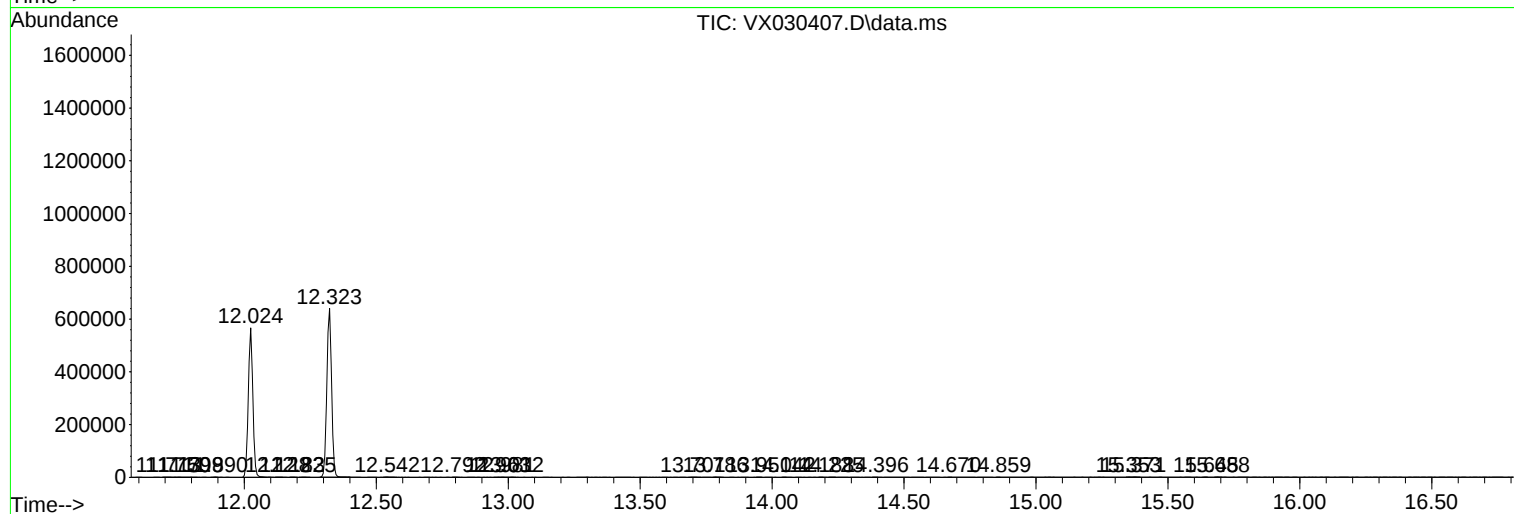
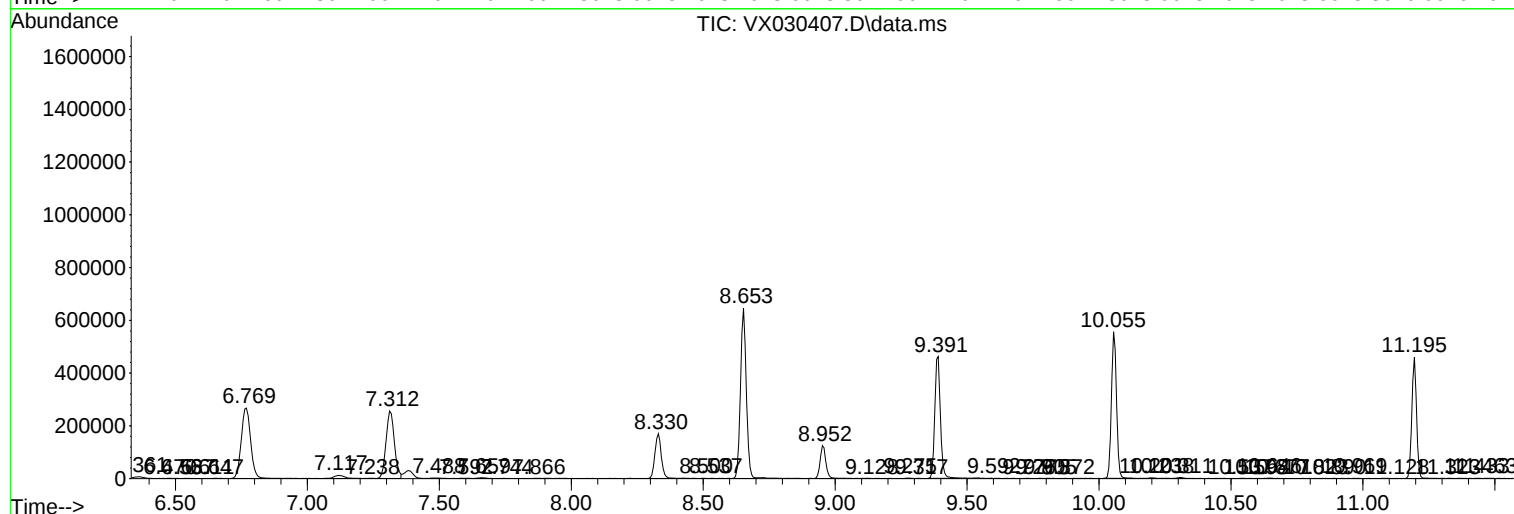
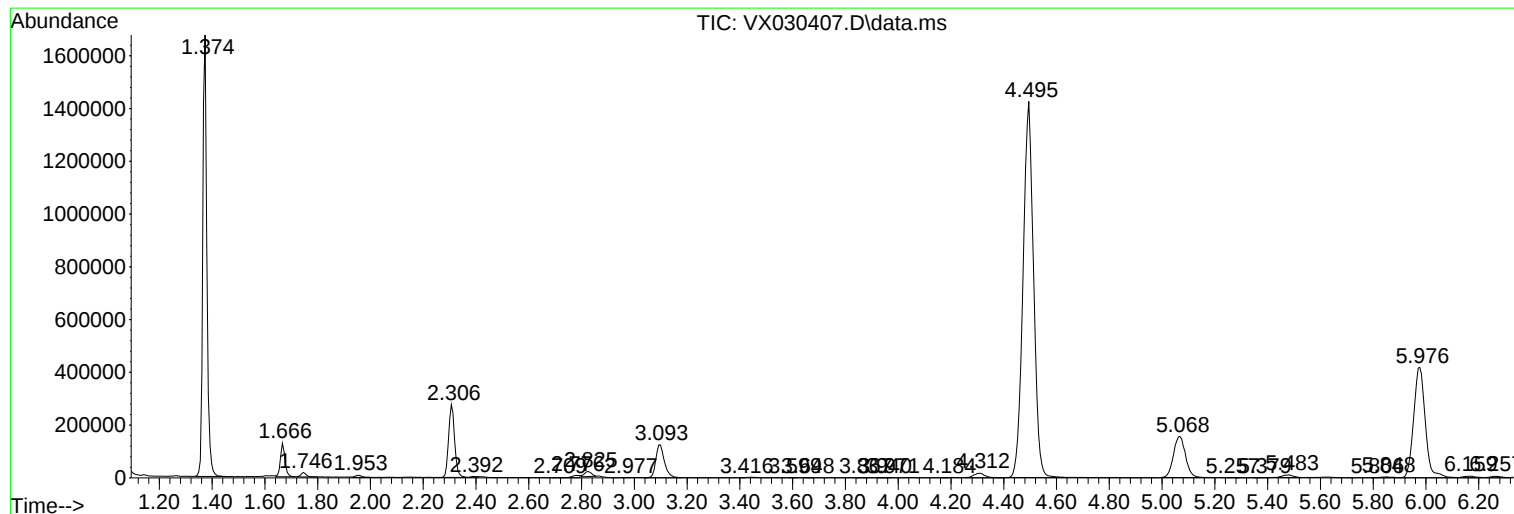
Sum of corrected areas: 14854599

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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



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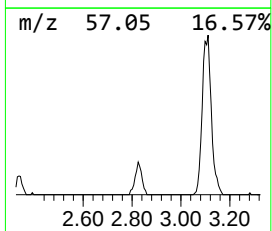
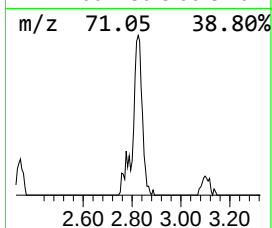
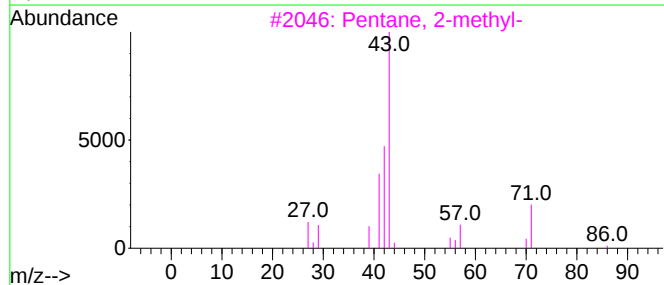
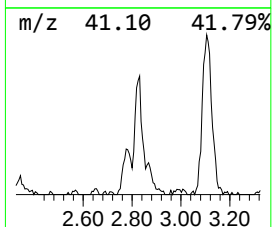
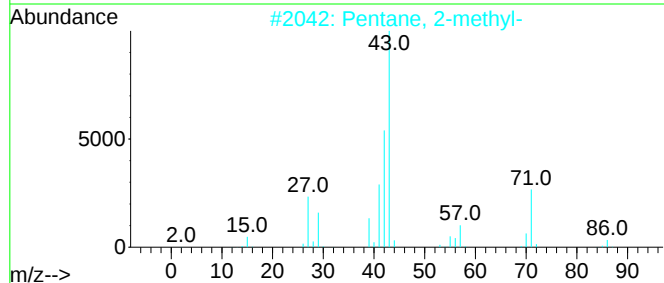
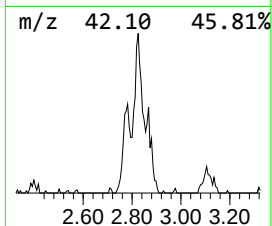
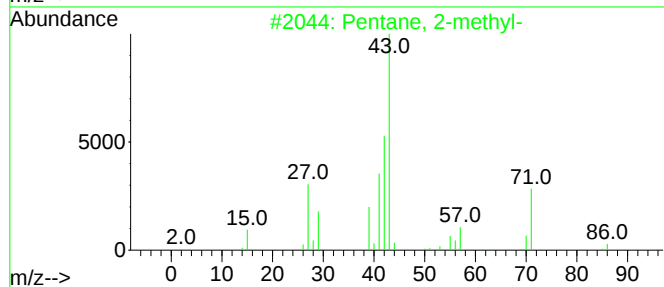
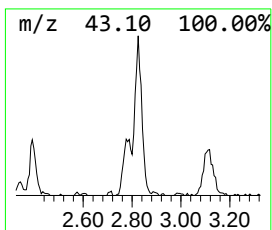
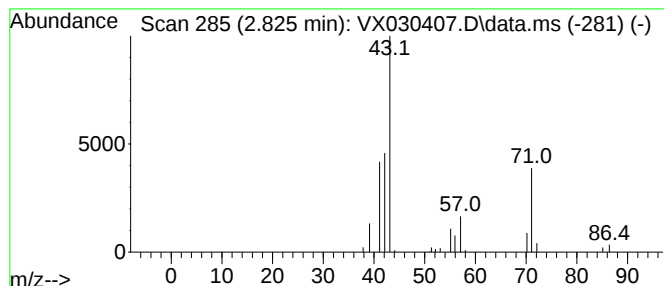
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.825	2.64 ug/L	34356	1,4-Difluorobenzene	6.769

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentane, 2-methyl-	86	C6H14	000107-83-5	87
2		Pentane, 2-methyl-	86	C6H14	000107-83-5	86
3		Pentane, 2-methyl-	86	C6H14	000107-83-5	83
4		Pentane, 2-methyl-	86	C6H14	000107-83-5	78
5		Pentane, 2-methyl-	86	C6H14	000107-83-5	56



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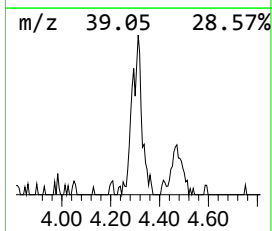
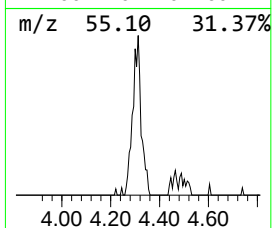
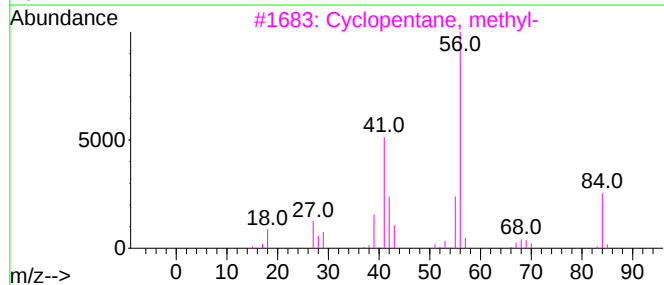
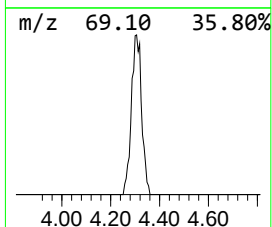
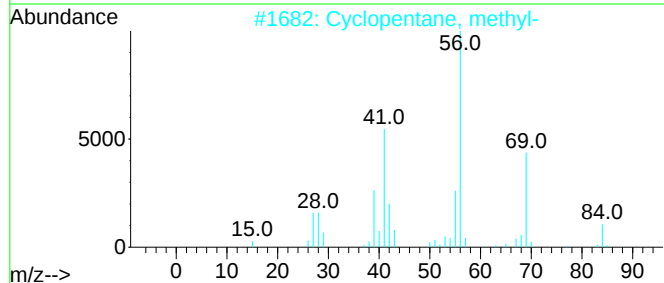
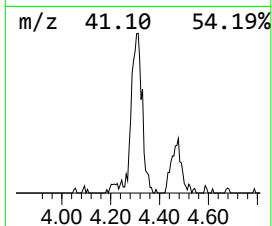
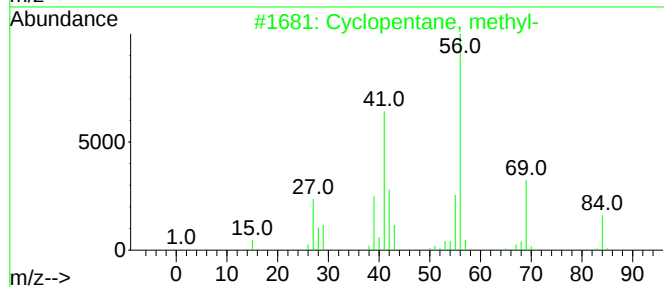
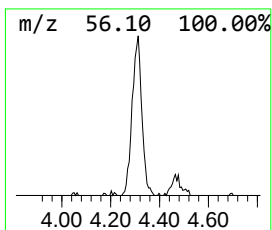
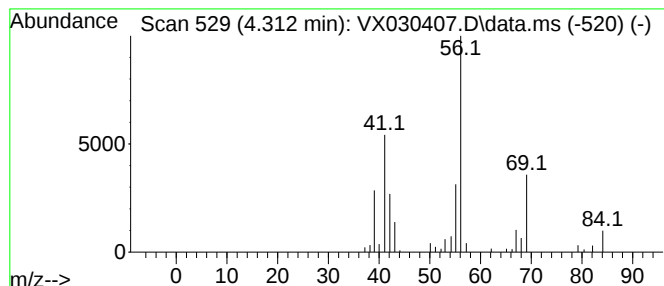
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Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Cyclic4.312 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.312	3.66 ug/L	47628	1,4-Difluorobenzene	6.769

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2		Cyclopentane, methyl-	84	C6H12	000096-37-7	72
3		Cyclopentane, methyl-	84	C6H12	000096-37-7	72
4		Cyclopentane, methyl-	84	C6H12	000096-37-7	72
5		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	2.825	2.6	ug/L	34356	1	6.769	651033	50.0
(DEL) Alkane: C...	4.312	3.7	ug/L	47628	1	6.769	651033	50.0