LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041823\
Data File : VX035141.D
Acq On : 18 Apr 2023 22:38
Operator : JC/MD
Sample : 02397-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 40 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : C0ML7

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\SFAMXLM041823WMA.M
Title : VOC Analysis

Signal : TIC: VX035141.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	17	rVB4	1371	2083	0.00%	0.000%
2	1.276	25	31	42	rBV	39843	125296	0.04%	0.013%
3	1.368	42	46	58	rVB	257640	286023	0.08%	0.030%
4	1.489	65	66	69	rBV2	1011	1038	0.00%	0.000%
5	1.581	79	81	83	rBV3	1019	1073	0.00%	0.000%
6	1.624	83	88	90	rVV5	2092	3342	0.00%	0.000%
7	1.672	91	96	105	rVV	179480	239236	0.07%	0.025%
8	1.886	130	131	134	rBV2	971	930	0.00%	0.000%
9	1.977	144	146	149	rVB2	1037	1048	0.00%	0.000%
10	2.093	163	165	169	rVB4	1082	1251	0.00%	0.000%
11	2.136	169	172	179	rVB7	1915	4302	0.00%	0.000%
12	2.203	181	183	190	rVB6	1469	2592	0.00%	0.000%
13	2.306	194	200	208	rBV	487592	746078	0.22%	0.078%
14	2.386	208	213	225	rVB	84713	165191	0.05%	0.017%
15	2.508	230	233	237	rBV4	836	1129	0.00%	0.000%
16	2.562	237	242	244	rBV4	771	1199	0.00%	0.000%
17	2.782	273	278	282	rBV5	1544	3146	0.00%	0.000%
18	2.825	282	285	287	rVV3	1484	2120	0.00%	0.000%
19	2.873	290	293	297	rVB3	1631	2352	0.00%	0.000%
20	2.940	297	304	317	rVB	24721	55280	0.02%	0.006%
21	3.099	324	330	339	rVB5	2517	5644	0.00%	0.001%
22	3.440	381	386	393	rVB4	1964	3715	0.00%	0.000%
23	4.306	517	528	543	rBV	77023	218997	0.06%	0.023%
24	4.458	543	553	566	rBV	128008	396538	0.12%	0.041%
25	5.056	637	651	670	rBV	267239	796251	0.23%	0.083%
26	5.208	673	676	677	rVV3	814	783	0.00%	0.000%
27	5.385	698	705	708	rBV3	970	1984	0.00%	0.000%
28	5.470	708	719	732	rVV3	44508	141769	0.04%	0.015%
29	5.556	732	733	737	rVV2	638	854	0.00%	0.000%
30	5.672	739	752	765	rBV2	38562	115314	0.03%	0.012%
31	5.842	769	780	788	rBV9	2587	8319	0.00%	0.001%
32	5.970	788	801	807	rBV2	702857	2087724	0.61%	0.218%
33	6.037	807	812	827	rVV	384544	1011931	0.30%	0.106%
34	6.153	827	831	840	rVV6	3179	9098	0.00%	0.001%
35	6.257	840	848	856	rVB8	3085	8758	0.00%	0.001%
36	6.354	856	864	873	rVB4	4799	12585	0.00%	0.001%

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ALS Vial : 40 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : C0ML7

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\SFAMXLM041823WMA.M
Title : VOC Analysis

37	6.550	889	896	897	rBV2	528	804	0.00%	0.000%
38	6.617	900	907	912	rVB3	1281	2395	0.00%	0.000%
39	6.763	921	931	954	rBV	436729	1062209	0.31%	0.111%
40	7.116	981	989	997	rBV7	1900	4825	0.00%	0.001%
41	7.305	1010	1020	1029	rBV	414291	951549	0.28%	0.099%
42	7.482	1046	1049	1052	rBV3	849	1102	0.00%	0.000%
43	7.659	1069	1078	1085	rVB3	5667	12317	0.00%	0.001%
44	7.946	1121	1125	1128	rBV3	1581	2909	0.00%	0.000%
45	8.110	1147	1152	1158	rBV4	2813	5231	0.00%	0.001%
46	8.324	1180	1187	1201	rBV	261528	439135	0.13%	0.046%
47	8.494	1213	1215	1220	rBV5	592	927	0.00%	0.000%
48	8.653	1232	1241	1248	rBV	1040200	1719337	0.50%	0.179%
49	8.720	1248	1252	1261	rVV	44082	82546	0.02%	0.009%
50	8.952	1284	1290	1305	rBV	186155	284411	0.08%	0.030%
51	9.275	1338	1343	1352	rVB	28123	46808	0.01%	0.005%
52	9.390	1356	1362	1384	rBV	383845	885505	0.26%	0.092%
53	9.573	1391	1392	1398	rVB5	609	840	0.00%	0.000%
54	10.116	1466	1481	1491	rBV7	57984557	340802975	100.00%	35.564%
55	10.323	1511	1515	1520	rBV6	23463	58170	0.02%	0.006%
56	10.646	1566	1568	1574	rVB	7858	11069	0.00%	0.001%
57	10.963	1618	1620	1626	rVB6	2950	4311	0.00%	0.000%
58	11.030	1629	1631	1633	rBV2	806	887	0.00%	0.000%
59	11.195	1652	1658	1674	rVV2	860025	1209684	0.35%	0.126%
60	11.372	1682	1687	1693	rBV	53905	75011	0.02%	0.008%
61	11.421	1693	1695	1697	rVV3	2680	2983	0.00%	0.000%
62	11.463	1697	1702	1710	rVB	30398	47160	0.01%	0.005%
63	11.719	1740	1744	1748	rBV6	1419	2482	0.00%	0.000%
64	11.762	1748	1751	1756	rVB3	6974	8945	0.00%	0.001%
65	11.981	1780	1787	1793	rBV	28444718	47360640	13.90%	4.942%
66	12.067	1793	1801	1806	rVB	60366304	126962696	37.25%	13.249%
67	12.219	1822	1826	1831	rBV	89451	134573	0.04%	0.014%
68	12.372	1840	1851	1857	rBV5	62970776	271841869	79.77%	28.368%
69	12.713	1903	1907	1913	rVB	38933	52312	0.02%	0.005%
70	12.878	1929	1934	1937	rBV2	35541	46892	0.01%	0.005%
71	12.926	1937	1942	1953	rVV	1906322	2344510	0.69%	0.245%
72	13.000	1953	1954	1957	rVV3	3120	2516	0.00%	0.000%
73	13.061	1958	1964	1970	rVV	208012	379109	0.11%	0.040%
74	13.115	1970	1973	1979	rVB	43302	56095	0.02%	0.006%
75	13.201	1981	1987	1995	rVB	796555	1006268	0.30%	0.105%
76	13.292	2000	2002	2006	rVB5	3193	3842	0.00%	0.000%

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ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0ML7

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

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041823WMA.M
Title : VOC Analysis

77	13.390	2013	2018	2023	rVB	46605	64950	0.02%	0.007%
78	13.609	2045	2054	2059	rBV	59663441	116758886	34.26%	12.184%
79	13.780	2077	2082	2092	rVB	278002	345300	0.10%	0.036%
80	13.871	2094	2097	2102	rVB	9302	11941	0.00%	0.001%
81	13.969	2107	2113	2118	rBV	22417793	29070147	8.53%	3.034%
82	14.176	2145	2147	2148	rBV2	1740	1172	0.00%	0.000%
83	14.213	2150	2153	2159	rVB8	4570	8448	0.00%	0.001%
84	14.383	2174	2181	2189	rVB	40868	75024	0.02%	0.008%
85	14.469	2193	2195	2200	rBV6	1318	2276	0.00%	0.000%
86	14.542	2203	2207	2213	rVB2	19575	26434	0.01%	0.003%
87	14.633	2216	2222	2228	rVB2	44404	75881	0.02%	0.008%
88	14.786	2236	2247	2253	rBV	1202376	1894608	0.56%	0.198%
89	14.920	2262	2269	2277	rVB3	11054	17883	0.01%	0.002%
90	15.121	2299	2302	2304	rBV3	893	1102	0.00%	0.000%
91	15.249	2317	2323	2333	rVB	4057723	5514218	1.62%	0.575%
92	15.414	2346	2350	2353	rBV6	1179	1641	0.00%	0.000%
93	15.749	2403	2405	2408	rVB4	1321	1281	0.00%	0.000%
94	15.780	2408	2410	2412	rBV3	953	929	0.00%	0.000%
95	15.956	2437	2439	2440	rBV2	1305	1331	0.00%	0.000%
96	16.121	2462	2466	2467	rBV4	733	1131	0.00%	0.000%
97	16.249	2485	2487	2490	rVV4	671	847	0.00%	0.000%
98	16.279	2490	2492	2494	rVB3	982	796	0.00%	0.000%
99	16.511	2524	2530	2535	rVB5	9094	16477	0.00%	0.002%
100	16.700	2559	2561	2563	rBV3	768	787	0.00%	0.000%

Sum of corrected areas: 958276312

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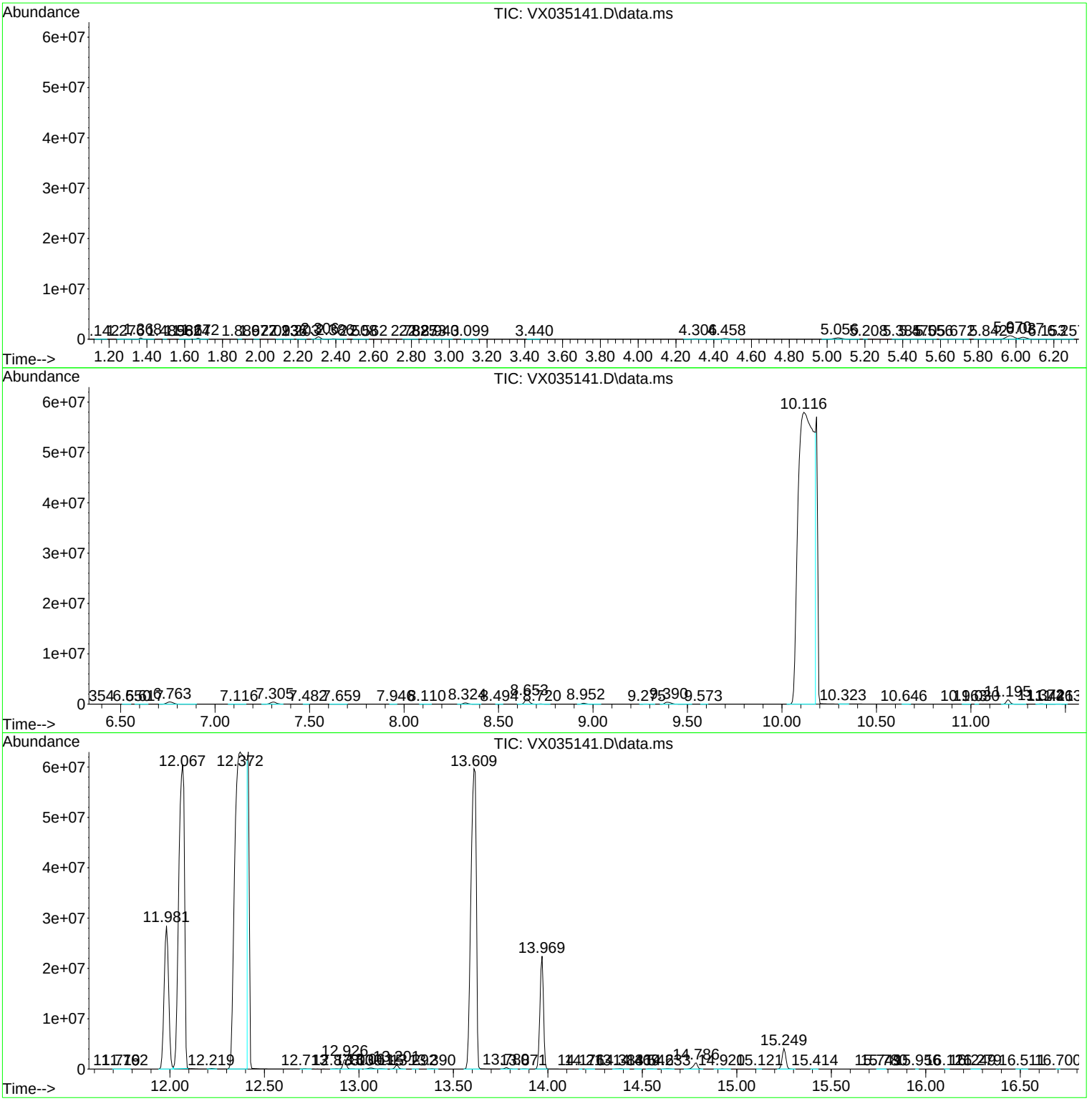
Instrument :
MSVOA_X
ClientSampleId :
C0ML7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041823WMA.M
Quant Title : VOC Analysis

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



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Sample : 02397-05
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ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0ML7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041823WMA.M
Quant Title : VOC Analysis

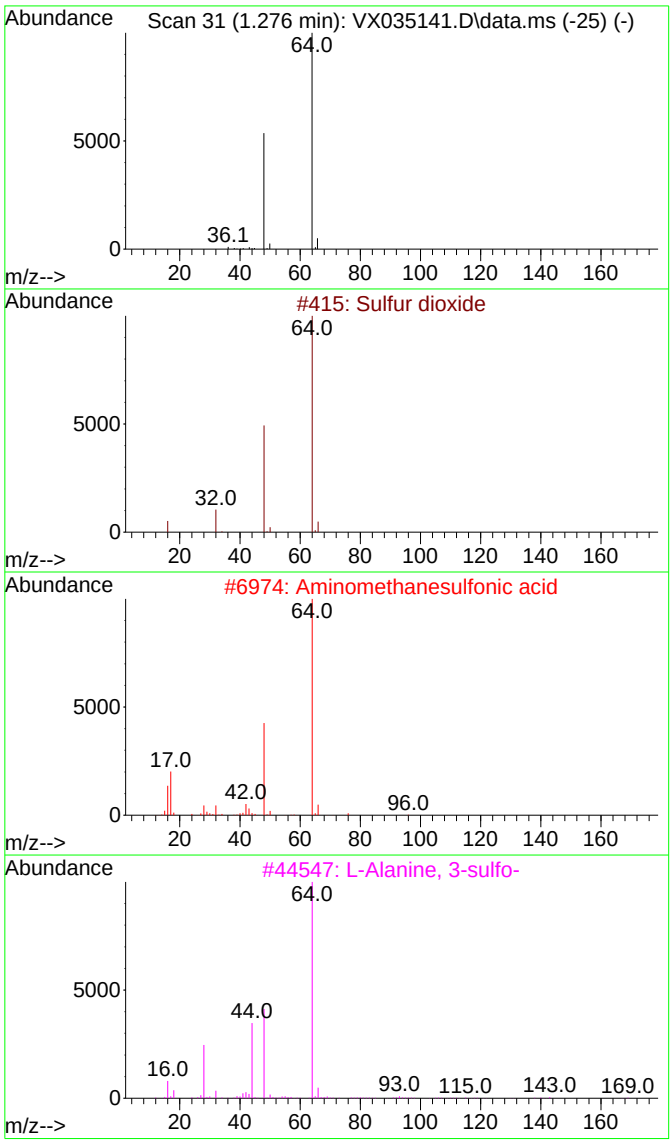
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

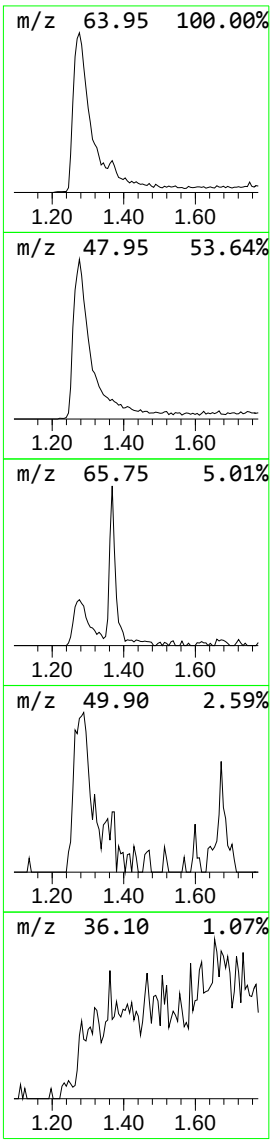
****

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.276	5.90 ug/L	125296	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4





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ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0ML7

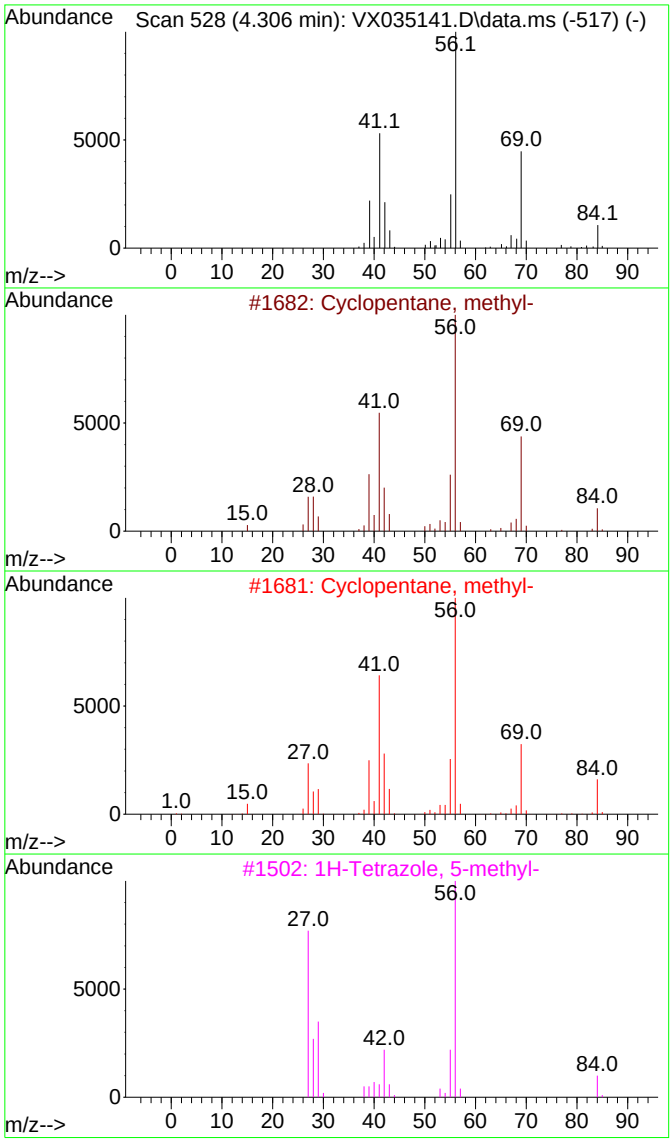
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041823WMA.M
Quant Title : VOC Analysis

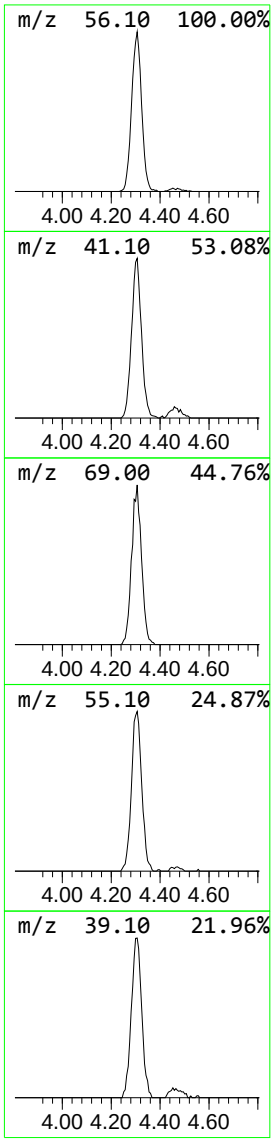
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	10.31 ug/L	218997	1,4-Difluorobenzene	6.763

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	86
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4	Cyclopentane, methyl-	84	C6H12	000096-37-7	72
5	Cyclohexane	84	C6H12	000110-82-7	64





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041823WMA.M
Quant Title : VOC Analysis

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Sulfur dioxide	1.276	5.9	ug/L	125296	1	6.763	1062210	50.0
(DEL) Alkane: C...	4.306	10.3	ug/L	218997	1	6.763	1062210	50.0