LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU091518\
Data File : VU026749.D
Acq On : 14 Sep 2018 00:28
Operator : MD/SY
Sample : J4893-20
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C08K8

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\SOMULM091018WMA.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	1.292	33	37	45	rVB	3278	3324	0.00%	0.001%
2	1.395	62	69	87	rBV	90227	92261	0.05%	0.022%
3	1.556	112	119	125	rVB5	3004	4055	0.00%	0.001%
4	1.678	149	157	173	rVB	68258	86938	0.04%	0.021%
5	1.884	216	221	229	rBV4	2934	3615	0.00%	0.001%
6	2.167	306	309	310	rBV2	473	268	0.00%	0.000%
7	2.189	310	316	325	rVB3	1857	2724	0.00%	0.001%
8	2.273	331	342	353	rBV	143444	218242	0.11%	0.052%
9	2.440	384	394	412	rBV	17199	30856	0.02%	0.007%
10	2.614	444	448	457	rBV2	317	539	0.00%	0.000%
11	2.704	470	476	482	rBV3	867	1171	0.00%	0.000%
12	2.733	482	485	487	rBV	354	238	0.00%	0.000%
13	2.794	495	504	509	rBV3	1409	2347	0.00%	0.001%
14	2.836	514	517	525	rVB3	373	485	0.00%	0.000%
15	3.000	560	568	577	rBV4	1526	2824	0.00%	0.001%
16	3.070	585	590	599	rVB	98	137	0.00%	0.000%
17	3.305	659	663	668	rBV4	488	498	0.00%	0.000%
18	3.829	821	826	833	rVB	146	196	0.00%	0.000%
19	3.874	833	840	843	rBV	103	118	0.00%	0.000%
20	4.096	894	909	922	rBV2	10243	26446	0.01%	0.006%
21	4.180	922	935	956	rBV	49911	124234	0.06%	0.030%
22	4.386	988	999	1016	rVB2	3199	7372	0.00%	0.002%
23	4.504	1032	1036	1041	rVB	219	156	0.00%	0.000%
24	4.652	1064	1082	1109	rBV2	102585	277547	0.14%	0.067%
25	4.797	1126	1127	1132	rVB	171	105	0.00%	0.000%
26	4.877	1149	1152	1153	rBV	265	156	0.00%	0.000%
27	5.000	1178	1190	1207	rBV5	5092	11756	0.01%	0.003%
28	5.135	1217	1232	1249	rBV3	20550	46736	0.02%	0.011%
29	5.395	1273	1313	1374	rBV	10685088	22757822	11.58%	5.464%
30	5.890	1452	1467	1493	rVV	216711	424126	0.22%	0.102%
31	5.980	1493	1495	1500	rVB2	317	224	0.00%	0.000%
32	6.051	1513	1517	1522	rVB2	182	196	0.00%	0.000%
33	6.189	1555	1560	1561	rBV3	356	238	0.00%	0.000%
34	6.199	1561	1563	1568	rVB3	492	357	0.00%	0.000%

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Sample : J4893-20
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C08K8

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\SOMULM091018WMA.M
Title : VOC Analysis

35	6.334	1590	1605	1619	rBV	135950	267248	0.14%	0.064%
36	6.469	1645	1647	1651	rVB2	194	107	0.00%	0.000%
37	6.639	1696	1700	1705	rVB3	508	483	0.00%	0.000%
38	6.762	1732	1738	1740	rBV2	217	201	0.00%	0.000%
39	6.826	1752	1758	1764	rBV	122	169	0.00%	0.000%
40	6.861	1764	1769	1777	rBV3	454	657	0.00%	0.000%
41	6.980	1800	1806	1812	rVB	89	123	0.00%	0.000%
42	7.051	1823	1828	1831	rBV2	190	207	0.00%	0.000%
43	7.189	1866	1871	1872	rBV	176	115	0.00%	0.000%
44	7.228	1872	1883	1904	rVV	72463	128908	0.07%	0.031%
45	7.347	1915	1920	1924	rVB2	184	133	0.00%	0.000%
46	7.392	1929	1934	1935	rBV	202	161	0.00%	0.000%
47	7.443	1944	1950	1956	rBV	96	120	0.00%	0.000%
48	7.472	1956	1959	1973	rVB	335	318	0.00%	0.000%
49	7.569	1973	1989	2006	rBV	276812	477048	0.24%	0.115%
50	7.723	2035	2037	2040	rVB	255	109	0.00%	0.000%
51	7.852	2066	2077	2098	rBV	51770	86692	0.04%	0.021%
52	8.135	2159	2165	2169	rBV2	203	203	0.00%	0.000%
53	8.183	2169	2180	2188	rBV3	2773	6120	0.00%	0.001%
54	8.231	2188	2195	2206	rVV5	4990	8895	0.00%	0.002%
55	8.315	2210	2221	2244	rVV	165219	280840	0.14%	0.067%
56	8.479	2267	2272	2276	rVV4	774	620	0.00%	0.000%
57	8.508	2279	2281	2283	rVB	246	101	0.00%	0.000%
58	8.585	2302	2305	2310	rBV2	201	165	0.00%	0.000%
59	9.134	2448	2476	2521	rBV2	34481964	59679781	30.36%	14.329%
60	9.543	2599	2603	2607	rBV3	248	257	0.00%	0.000%
61	9.594	2616	2619	2622	rBV2	325	300	0.00%	0.000%
62	9.749	2665	2667	2669	rVB2	281	132	0.00%	0.000%
63	9.781	2674	2677	2678	rBV	234	155	0.00%	0.000%
64	9.964	2725	2734	2741	rBV4	613	1067	0.00%	0.000%
65	10.019	2747	2751	2757	rVB	90	105	0.00%	0.000%
66	10.089	2770	2773	2776	rBV	246	127	0.00%	0.000%
67	10.151	2787	2792	2795	rBV	110	105	0.00%	0.000%
68	10.167	2795	2797	2799	rBV	179	117	0.00%	0.000%
69	10.228	2810	2816	2820	rBV	112	128	0.00%	0.000%
70	10.433	2866	2880	2900	rVV	188087	326109	0.17%	0.078%
71	10.610	2926	2935	2943	rVV3	1958	2968	0.00%	0.001%

LSC Area Percent Report

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Sample : J4893-20
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C08K8

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\SOMULM091018WMA.M
Title : VOC Analysis

72	10.665	2943	2952	2962	rVB2	6709	9915	0.01%	0.002%
73	10.733	2971	2973	2977	rVB	197	103	0.00%	0.000%
74	10.778	2977	2987	2996	rBV2	2697	4192	0.00%	0.001%
75	11.224	3123	3126	3131	rBV	116	107	0.00%	0.000%
76	11.253	3131	3135	3139	rVB	150	136	0.00%	0.000%
77	11.308	3148	3152	3157	rBV	105	122	0.00%	0.000%
78	11.424	3173	3188	3200	rBV	5355959	8473238	4.31%	2.034%
79	11.533	3200	3222	3247	rVB3	55103359	101400975	51.59%	24.347%
80	11.752	3287	3290	3293	rBV3	957	745	0.00%	0.000%
81	11.922	3314	3343	3381	rBV4	77952327	196552067	100.00%	47.193%
82	12.572	3541	3545	3553	rVV5	906	1324	0.00%	0.000%
83	12.636	3554	3565	3578	rVB	59132	89908	0.05%	0.022%
84	12.732	3594	3595	3598	rBV2	356	196	0.00%	0.000%
85	12.816	3612	3621	3626	rBV4	11274	20410	0.01%	0.005%
86	12.861	3627	3635	3655	rVB	88691	153444	0.08%	0.037%
87	12.990	3664	3675	3688	rVB2	29875	47417	0.02%	0.011%
88	13.237	3746	3752	3757	rBV3	1582	1744	0.00%	0.000%
89	13.321	3771	3778	3785	rVB4	1352	1950	0.00%	0.000%
90	13.353	3785	3788	3793	rBV4	485	396	0.00%	0.000%
91	13.511	3821	3837	3867	rBV	12577423	19013545	9.67%	4.565%
92	13.990	3972	3986	4004	rBV	2717877	4207325	2.14%	1.010%
93	14.099	4017	4020	4023	rBV2	671	562	0.00%	0.000%
94	14.382	4099	4108	4123	rBV2	20473	33864	0.02%	0.008%
95	14.581	4166	4170	4173	rBV2	369	383	0.00%	0.000%
96	14.694	4201	4205	4214	rVB4	1461	1942	0.00%	0.000%
97	14.864	4255	4258	4266	rVB5	788	751	0.00%	0.000%
98	15.073	4306	4323	4340	rBV	192057	335725	0.17%	0.081%
99	15.559	4472	4474	4479	rVB2	609	409	0.00%	0.000%
100	15.649	4490	4502	4528	rBV	454670	735761	0.37%	0.177%

Sum of corrected areas: 416488057

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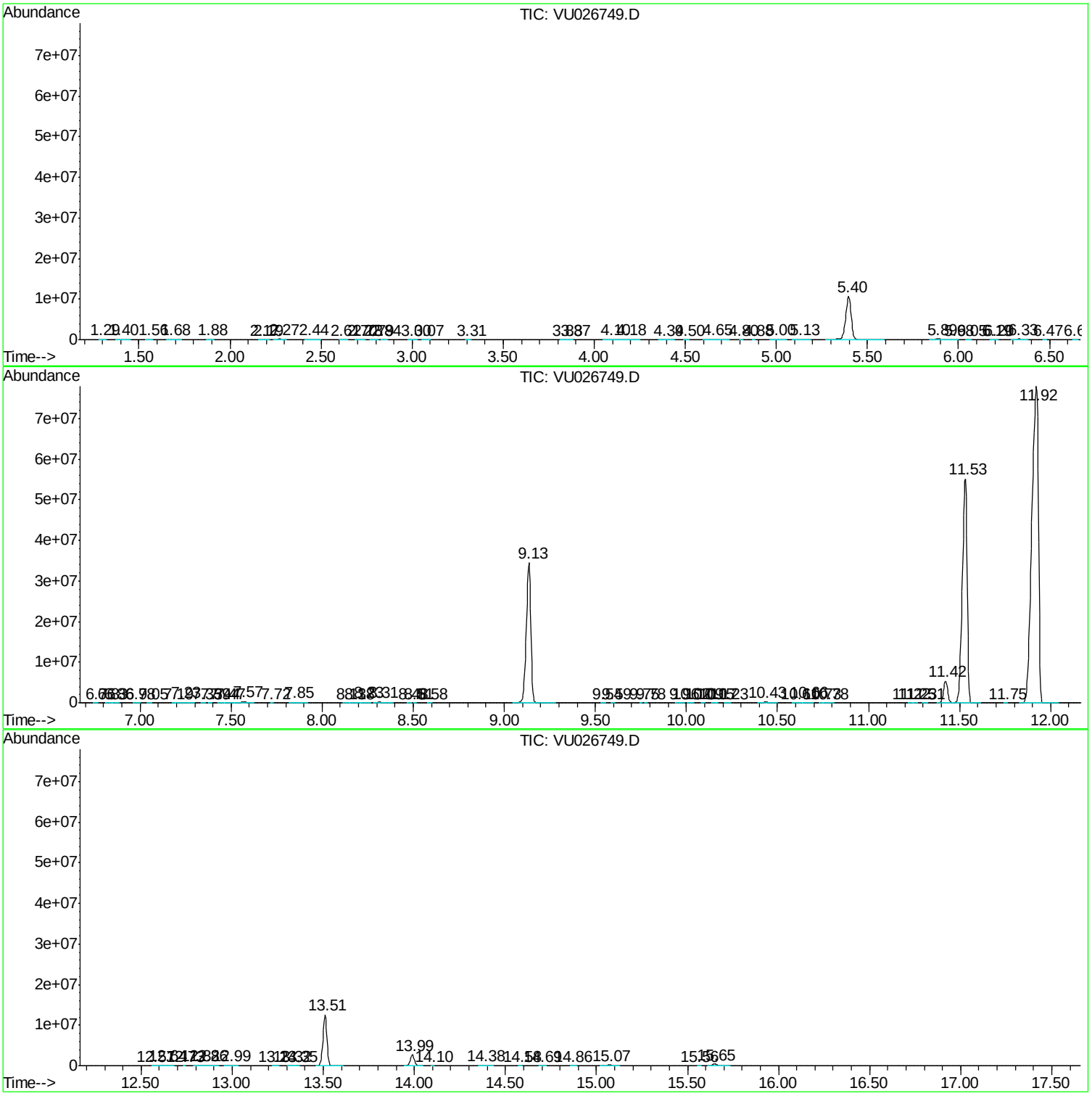
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C08K8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091018WMA.M
Quant Title : VOC Analysis

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU091518\
Data File : VU026749.D
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ClientSampleId : C08K8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091018WMA.M
Quant Title : VOC Analysis

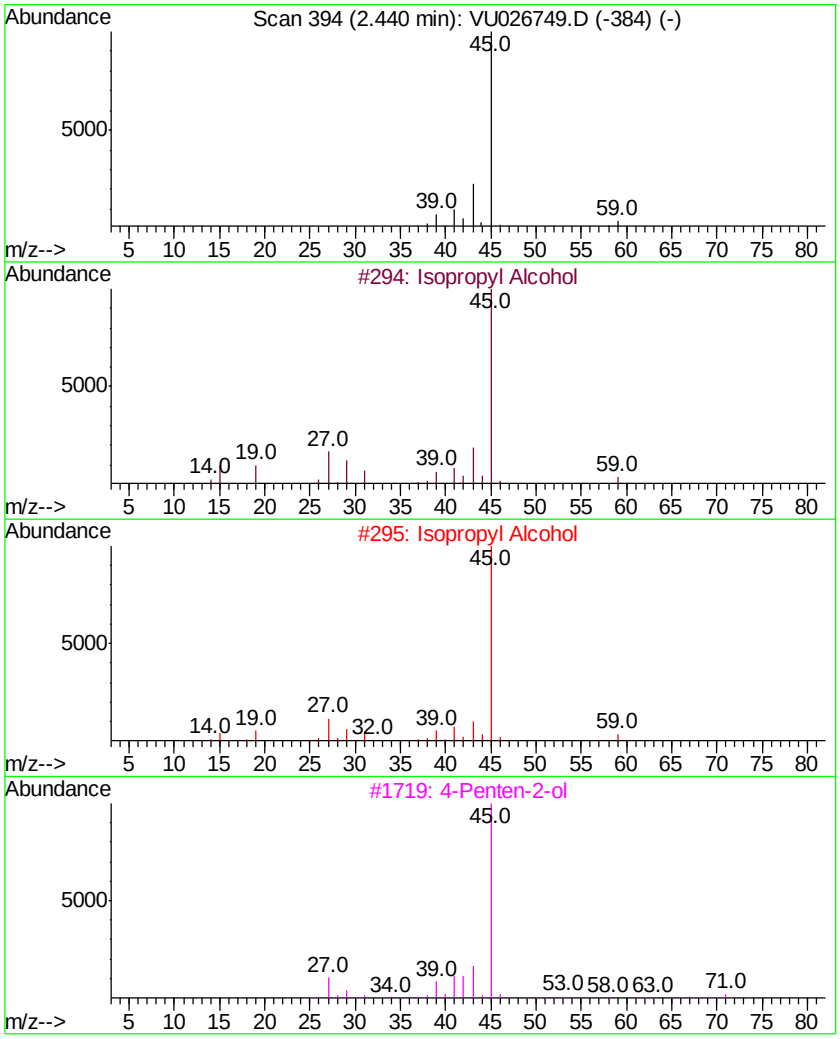
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

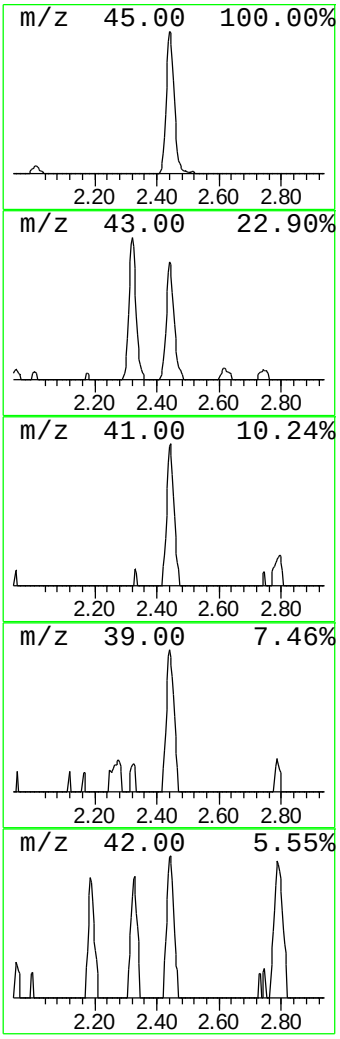
****

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.44	3.64 ug/L	30856	1,4-Difluorobenzene	5.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	43
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
3	4-Penten-2-ol	86	C5H10O	000625-31-0	9
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	Isopropyl Alcohol	60	C3H8O	000067-63-0	9





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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091018WMA.M
Quant Title : VOC Analysis

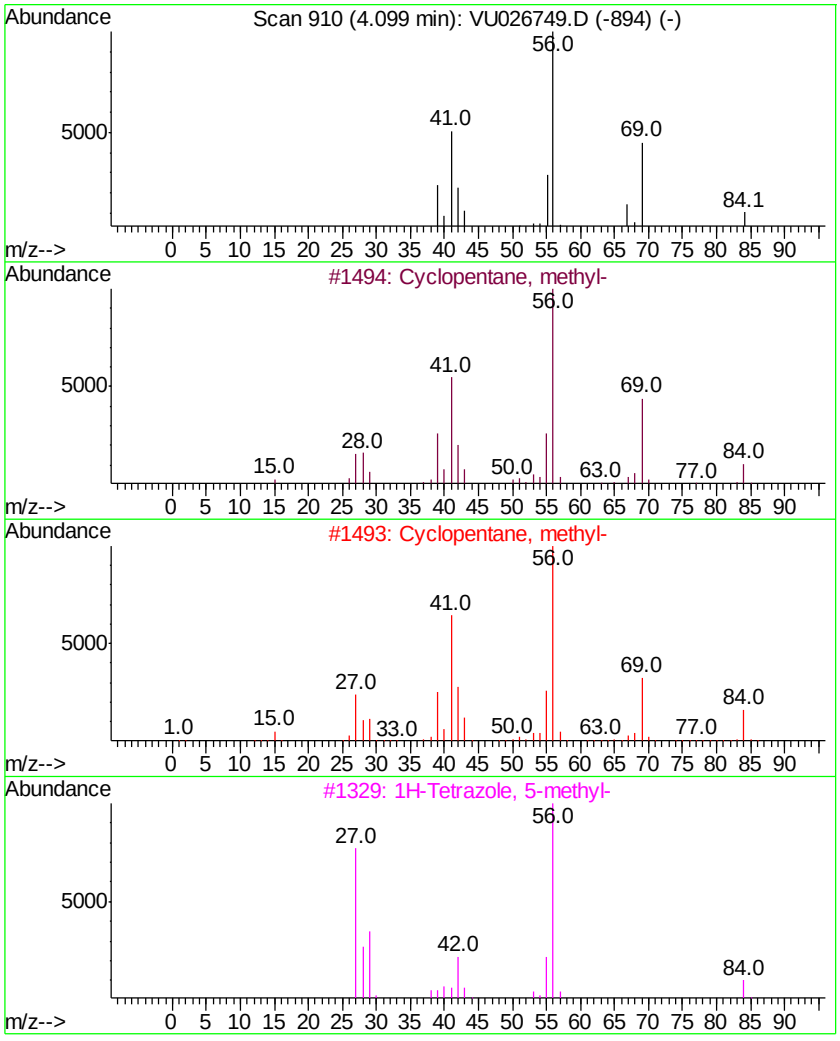
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

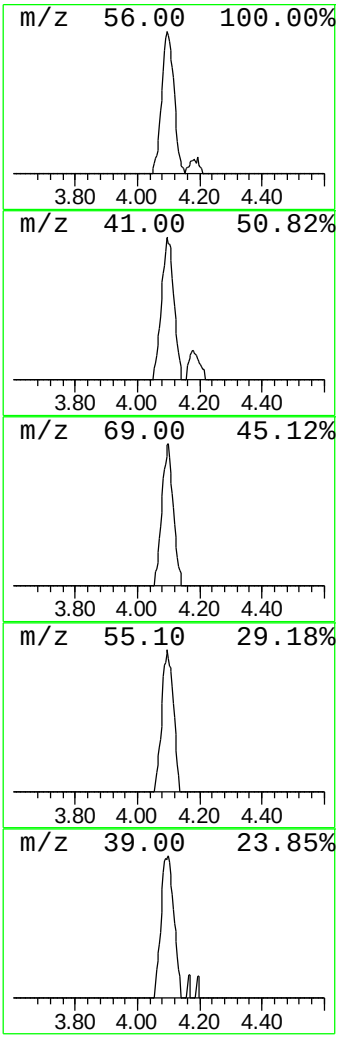
****

Peak Number 2 (DEL) Alkane: Cyclic4.10 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.10	3.12 ug/L	26446	1,4-Difluorobenzene	5.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	87
2	Cyclopentane, methyl-	84	C6H12	000096-37-7	80
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4	Cyclopentane, methyl-	84	C6H12	000096-37-7	72
5	Cyclobutane	56	C4H8	000287-23-0	49





Tentatively Identified Compound (LSC) summary

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Quant Title : VOC Analysis

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

						--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown-01	2.44	3.6	ug/L	30856	1	5.89	424126	50.0
(DEL) Alkane: Cyc...	4.10	3.1	ug/L	26446	1	5.89	424126	50.0