LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU091918\
Data File : VU026894.D
Acq On : 19 Sep 2018 12:37
Operator : MD/SY
Sample : J4865-20ME
Misc : 4.59g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DB3P8ME

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\SOMULM091718WMA.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	1.392	62	68	87	rVB	60838	84965	1.74%	0.586%
2	2.234	320	330	354	rBV	135502	218601	4.48%	1.507%
3	2.344	355	364	403	rVB	38257	92098	1.89%	0.635%
4	2.620	440	450	490	rVB	282045	558872	11.46%	3.854%
5	3.090	594	596	602	rVB	299	205	0.00%	0.001%
6	3.186	613	626	637	rBV5	3049	6774	0.14%	0.047%
7	3.244	642	644	646	rVB5	184	71	0.00%	0.000%
8	3.257	646	648	649	rBV	210	76	0.00%	0.001%
9	3.295	658	660	661	rBV	254	76	0.00%	0.001%
10	3.398	690	692	695	rVB	179	75	0.00%	0.001%
11	3.446	701	707	710	rBV	274	248	0.01%	0.002%
12	3.466	711	713	716	rVB	214	100	0.00%	0.001%
13	3.553	738	740	742	rBV	192	93	0.00%	0.001%
14	3.665	772	775	780	rVB2	141	129	0.00%	0.001%
15	3.739	795	798	801	rBV2	765	647	0.01%	0.004%
16	3.967	864	869	872	rBV	208	166	0.00%	0.001%
17	4.061	895	898	901	rVB	125	79	0.00%	0.001%
18	4.192	924	939	960	rBV	49549	171424	3.51%	1.182%
19	4.546	1044	1049	1053	rBV	88	94	0.00%	0.001%
20	4.643	1062	1079	1107	rBV	123915	314712	6.45%	2.170%
21	4.807	1119	1130	1148	rBV3	7457	17934	0.37%	0.124%
22	4.926	1164	1167	1176	rBV2	209	265	0.01%	0.002%
23	4.983	1183	1185	1187	rVB2	149	79	0.00%	0.001%
24	5.167	1235	1242	1245	rBV	70	101	0.00%	0.001%
25	5.331	1270	1293	1331	rBV2	259948	759889	15.58%	5.240%
26	5.472	1333	1337	1342	rBV2	129	98	0.00%	0.001%
27	5.601	1367	1377	1386	rBV2	850	1776	0.04%	0.012%
28	5.636	1386	1388	1390	rVV	136	95	0.00%	0.001%
29	5.665	1393	1397	1406	rVB2	428	456	0.01%	0.003%
30	5.739	1418	1420	1424	rBV2	165	120	0.00%	0.001%
31	5.765	1424	1428	1430	rBV	685	605	0.01%	0.004%
32	5.884	1448	1465	1490	rBV	263724	549529	11.27%	3.789%
33	6.064	1514	1521	1522	rBV	385	365	0.01%	0.003%
34	6.147	1539	1547	1549	rBV	99	119	0.00%	0.001%

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Integrator: RTE
Smoothing : OFF Filtering: 5
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Stop Thrs : 0 Peak Location: TOP

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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091718WMA.M
Title : VOC Analysis

35	6.163	1549	1552	1554	rBV2	367	266	0.01%	0.002%
36	6.331	1589	1604	1625	rBV	171539	365142	7.49%	2.518%
37	6.456	1635	1643	1644	rBV2	778	818	0.02%	0.006%
38	6.549	1668	1672	1676	rBV2	187	164	0.00%	0.001%
39	6.620	1690	1694	1697	rBV	312	189	0.00%	0.001%
40	6.668	1706	1709	1713	rVB	105	75	0.00%	0.001%
41	6.707	1718	1721	1725	rVB	108	75	0.00%	0.001%
42	6.733	1725	1729	1731	rBV	93	74	0.00%	0.001%
43	6.761	1736	1738	1745	rVB2	187	154	0.00%	0.001%
44	6.810	1749	1753	1756	rBV	151	97	0.00%	0.001%
45	6.871	1761	1772	1789	rBV6	5169	13689	0.28%	0.094%
46	7.038	1821	1824	1827	rVV	154	107	0.00%	0.001%
47	7.228	1871	1883	1907	rBV	80108	159660	3.27%	1.101%
48	7.388	1928	1933	1937	rBV3	290	327	0.01%	0.002%
49	7.446	1949	1951	1954	rVB	174	82	0.00%	0.001%
50	7.478	1955	1961	1962	rBV3	735	685	0.01%	0.005%
51	7.565	1974	1988	2011	rBV	297727	540995	11.09%	3.730%
52	7.736	2038	2041	2047	rVB2	356	237	0.00%	0.002%
53	7.765	2047	2050	2052	rBV	218	119	0.00%	0.001%
54	7.800	2059	2061	2063	rBV2	221	94	0.00%	0.001%
55	7.855	2065	2078	2104	rVV2	56586	116963	2.40%	0.806%
56	7.999	2121	2123	2125	rBV2	159	99	0.00%	0.001%
57	8.060	2137	2142	2145	rBV2	264	300	0.01%	0.002%
58	8.105	2152	2156	2159	rBV2	175	163	0.00%	0.001%
59	8.183	2173	2180	2189	rBV3	1524	2470	0.05%	0.017%
60	8.327	2212	2225	2256	rBV	239876	450096	9.23%	3.104%
61	8.578	2301	2303	2308	rBV2	273	150	0.00%	0.001%
62	8.604	2308	2311	2313	rBV2	258	151	0.00%	0.001%
63	8.633	2313	2320	2329	rVB4	3020	4933	0.10%	0.034%
64	8.691	2330	2338	2343	rBV4	1137	1421	0.03%	0.010%
65	8.729	2348	2350	2354	rBV	157	112	0.00%	0.001%
66	8.797	2368	2371	2372	rBV	278	104	0.00%	0.001%
67	8.922	2407	2410	2412	rBV2	210	119	0.00%	0.001%
68	9.006	2432	2436	2440	rVB	171	128	0.00%	0.001%
69	9.093	2450	2463	2490	rBV	393893	704931	14.45%	4.861%
70	9.237	2505	2508	2509	rBV	173	89	0.00%	0.001%
71	9.324	2534	2535	2540	rVB2	413	235	0.00%	0.002%

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Instrument : MSVOA_U
ClientSampleId : DB3P8ME

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091718WMA.M
Title : VOC Analysis

72	9.382	2545	2553	2562	rVB2	4074	6167	0.13%	0.043%
73	9.585	2614	2616	2619	rBB	167	72	0.00%	0.000%
74	9.617	2623	2626	2630	rVV2	193	165	0.00%	0.001%
75	9.732	2660	2662	2666	rBB2	161	139	0.00%	0.001%
76	9.810	2684	2686	2688	rBV	248	135	0.00%	0.001%
77	10.002	2740	2746	2756	rVB5	3423	5062	0.10%	0.035%
78	10.051	2756	2761	2765	rVB2	205	164	0.00%	0.001%
79	10.096	2773	2775	2778	rBV	191	112	0.00%	0.001%
80	10.154	2778	2793	2816	rBV	3000528	4877266	100.00%	33.630%
81	10.311	2834	2842	2850	rBV7	2636	3818	0.08%	0.026%
82	10.437	2860	2881	2901	rBV	358303	586323	12.02%	4.043%
83	10.562	2917	2920	2921	rBV	123	75	0.00%	0.001%
84	10.610	2926	2935	2945	rVB2	2150	3350	0.07%	0.023%
85	10.652	2945	2948	2951	rBV	161	85	0.00%	0.001%
86	10.826	2988	3002	3035	rBV	966849	1588632	32.57%	10.954%
87	11.137	3086	3099	3104	rBV3	7649	13799	0.28%	0.095%
88	11.228	3125	3127	3129	rBV2	220	115	0.00%	0.001%
89	11.298	3140	3149	3160	rVB5	10996	15863	0.33%	0.109%
90	11.433	3176	3191	3198	rBV2	63832	102975	2.11%	0.710%
91	11.488	3198	3208	3233	rVV2	501540	914456	18.75%	6.305%
92	11.597	3233	3242	3255	rVB3	16488	26433	0.54%	0.182%
93	11.774	3291	3297	3305	rVB4	3867	5579	0.11%	0.038%
94	11.864	3312	3325	3344	rBV	410633	660939	13.55%	4.557%
95	12.028	3368	3376	3388	rVB3	13541	18692	0.38%	0.129%
96	12.144	3405	3412	3420	rBV4	7185	9941	0.20%	0.069%
97	12.327	3464	3469	3473	rBV5	771	841	0.02%	0.006%
98	12.600	3547	3554	3572	rVB3	6943	12162	0.25%	0.084%
99	12.973	3668	3670	3671	rBV3	317	139	0.00%	0.001%
100	14.649	4174	4191	4225	rBV	296289	502755	10.31%	3.467%

Sum of corrected areas: 14502703

LSC Report - Integrated Chromatogram

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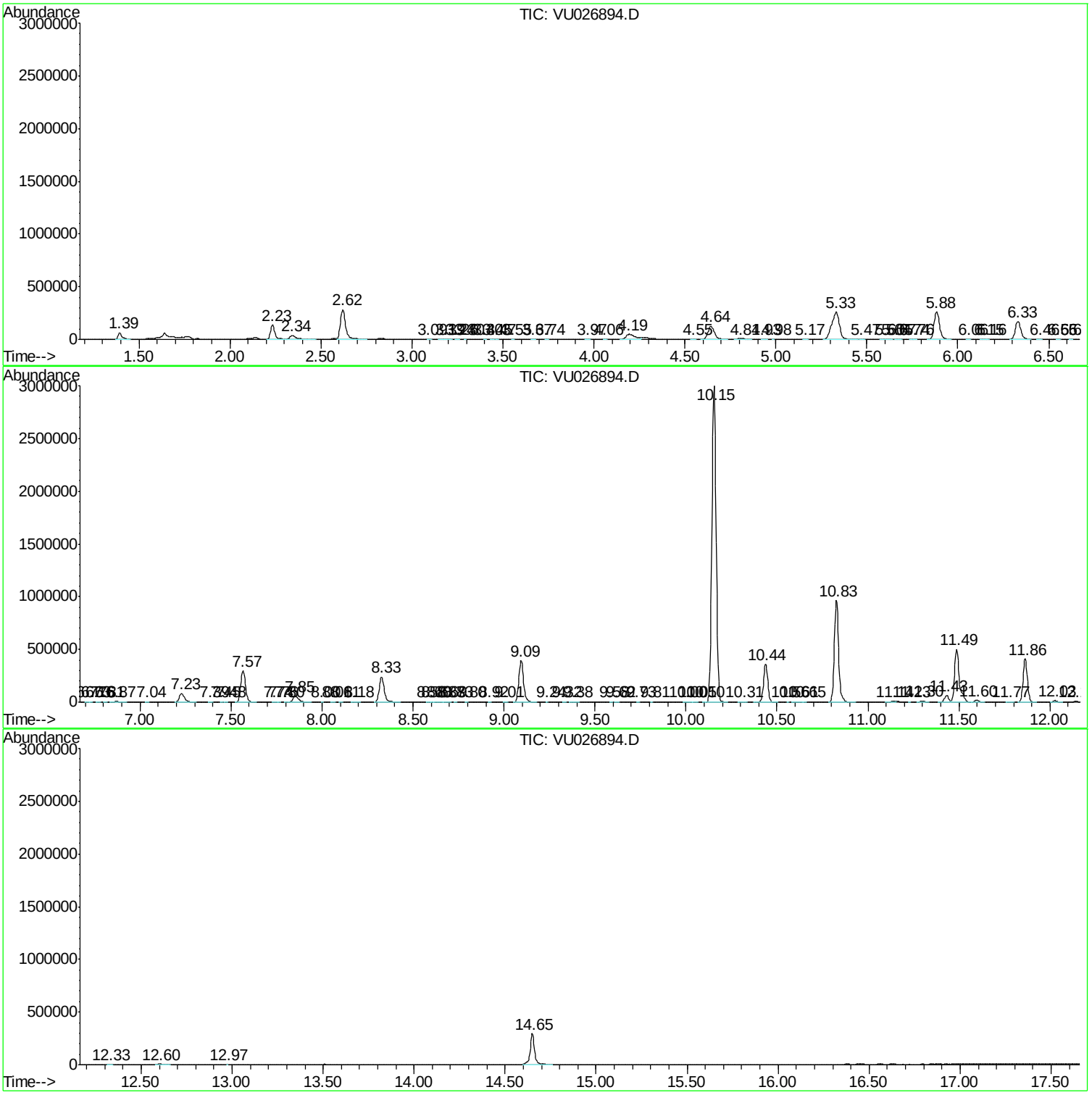
Instrument : MSVOA_U
ClientSampleId : DB3P8ME

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091718WMA.M
Quant Title : VOC Analysis

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



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ClientSampleId : DB3P8ME

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091718WMA.M
Quant Title : VOC Analysis

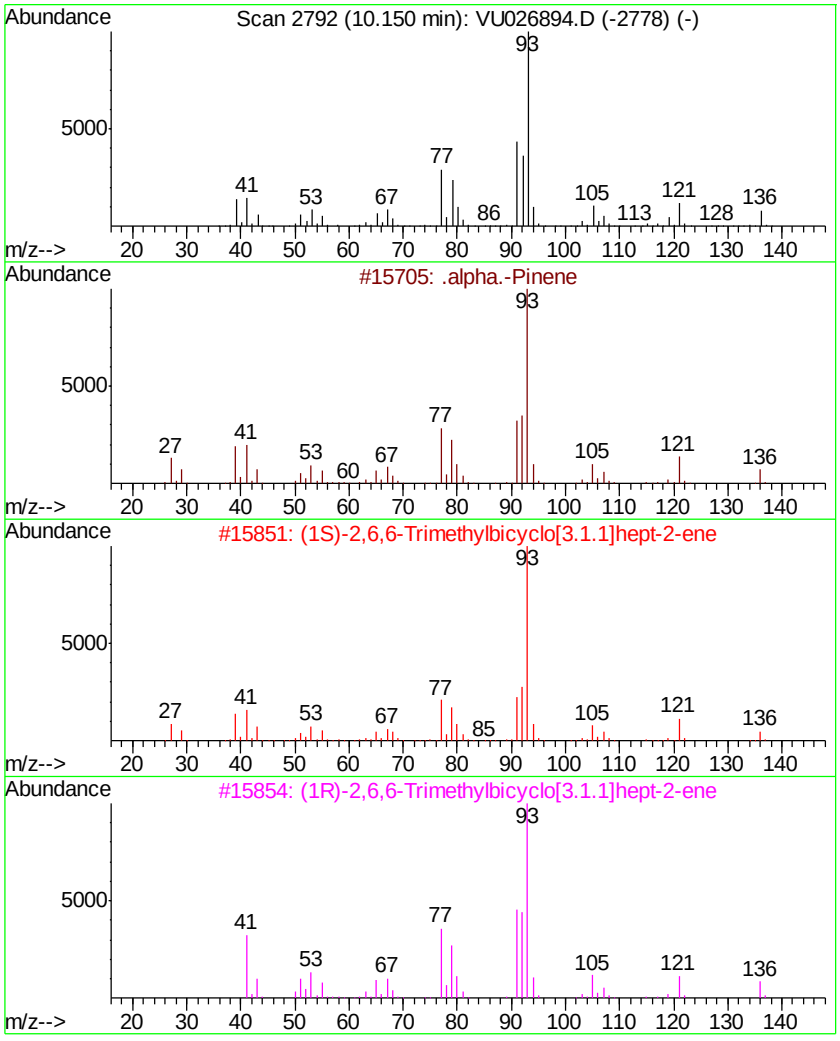
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

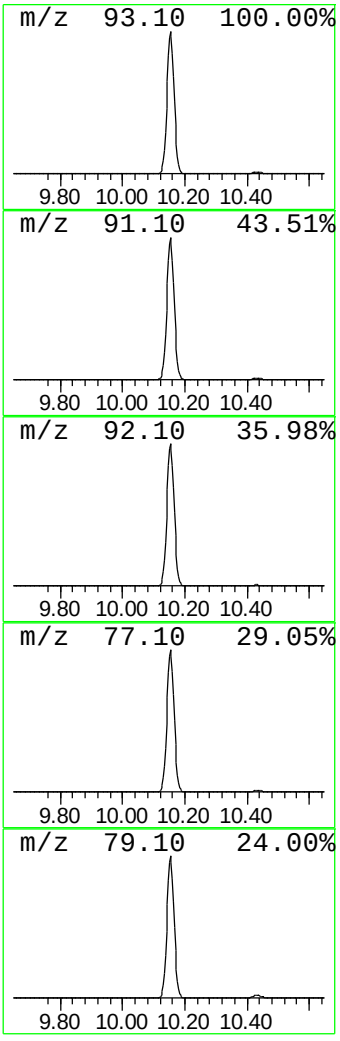
****

Peak Number 2 .alpha.-Pinene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.15	345.94 ug/L	4877270	Chlorobenzene-d5	9.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Pinene	136	C10H16	000080-56-8	97
2	(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	97
3	(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	94
4	(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	94
5	.alpha.-Pinene	136	C10H16	000080-56-8	91





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ClientSampleId : DB3P8ME

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091718WMA.M
Quant Title : VOC Analysis

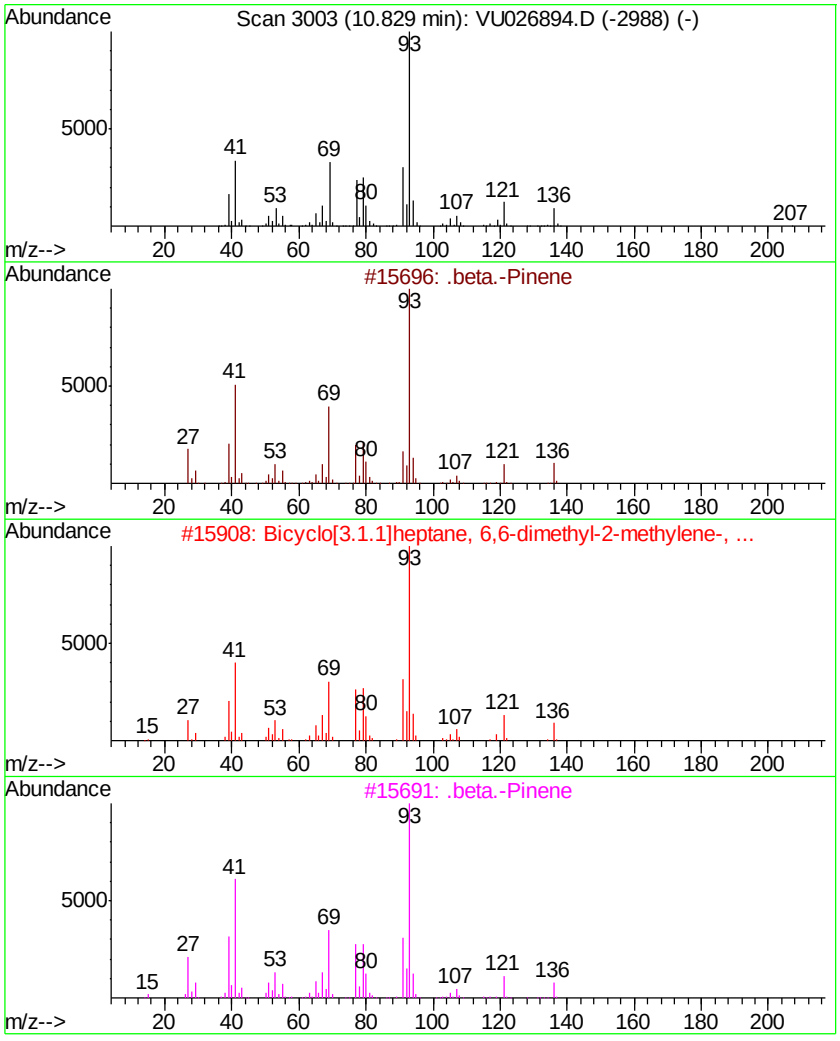
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

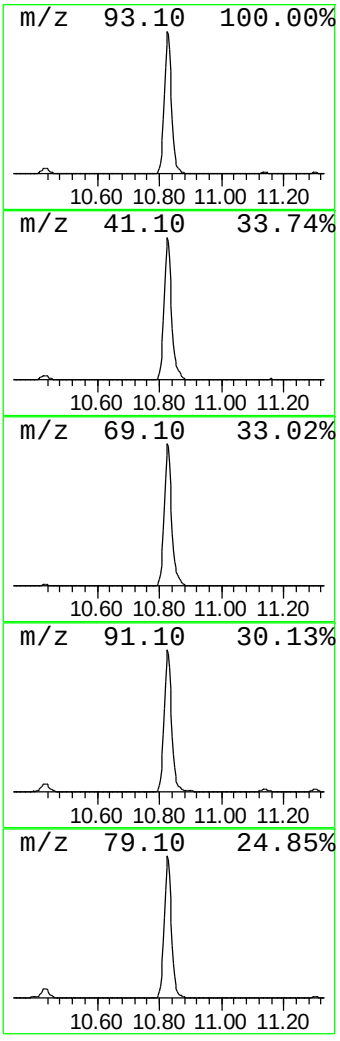
****

Peak Number 3 .beta.-Pinene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.83	86.86 ug/L	1588630	1,4-Dichlorobenzene-d4	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Pinene	136	C10H16	000127-91-3	97
2	Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	96
3	.beta.-Pinene	136	C10H16	000127-91-3	96
4	.beta.-Pinene	136	C10H16	000127-91-3	95
5	.alpha.-Pinene	136	C10H16	000080-56-8	93





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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091718WMA.M
Quant Title : VOC Analysis

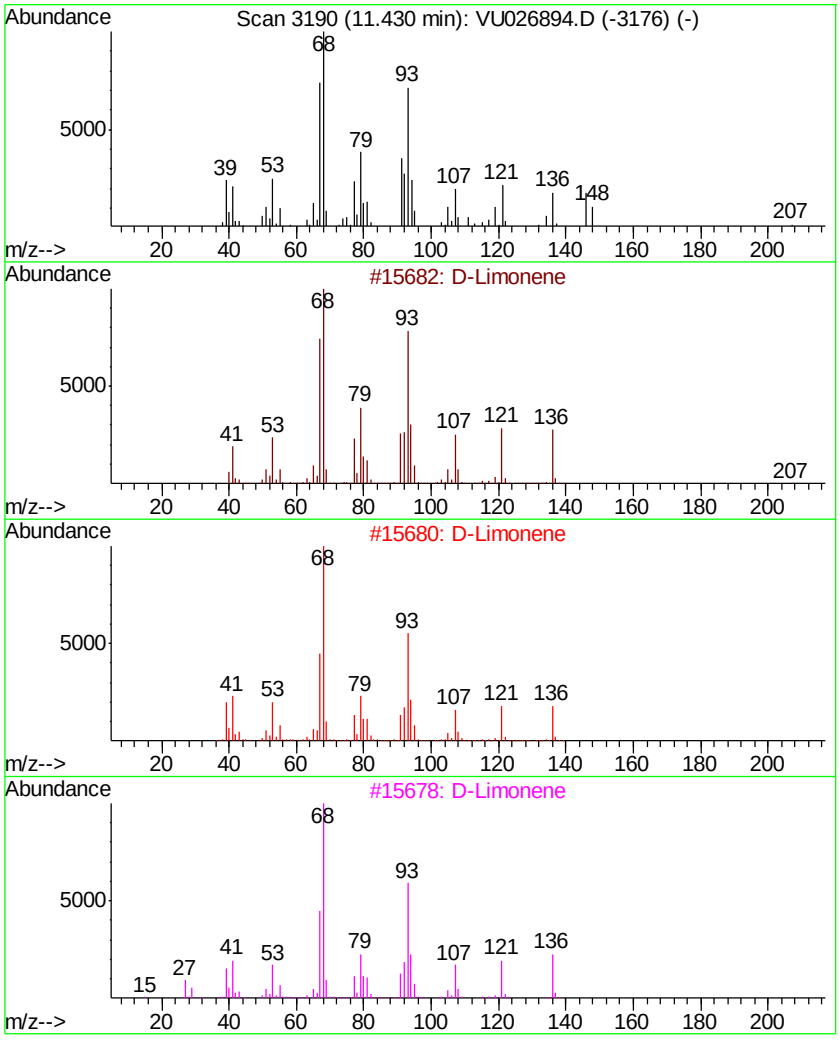
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

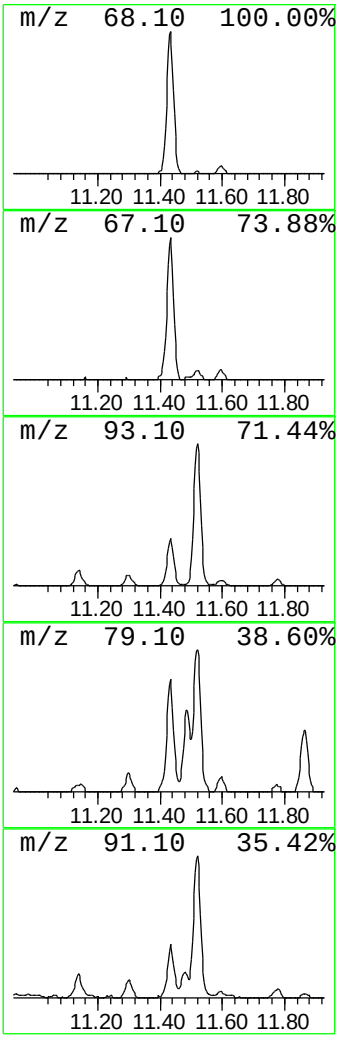
****

Peak Number 4 D-Limonene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.43	5.63 ug/L	102975	1,4-Dichlorobenzene-d4	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Limonene	136	C10H16	005989-27-5	97
2	D-Limonene	136	C10H16	005989-27-5	94
3	D-Limonene	136	C10H16	005989-27-5	93
4	D-Limonene	136	C10H16	005989-27-5	93
5	Limonene	136	C10H16	000138-86-3	90





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Quant Title : VOC Analysis

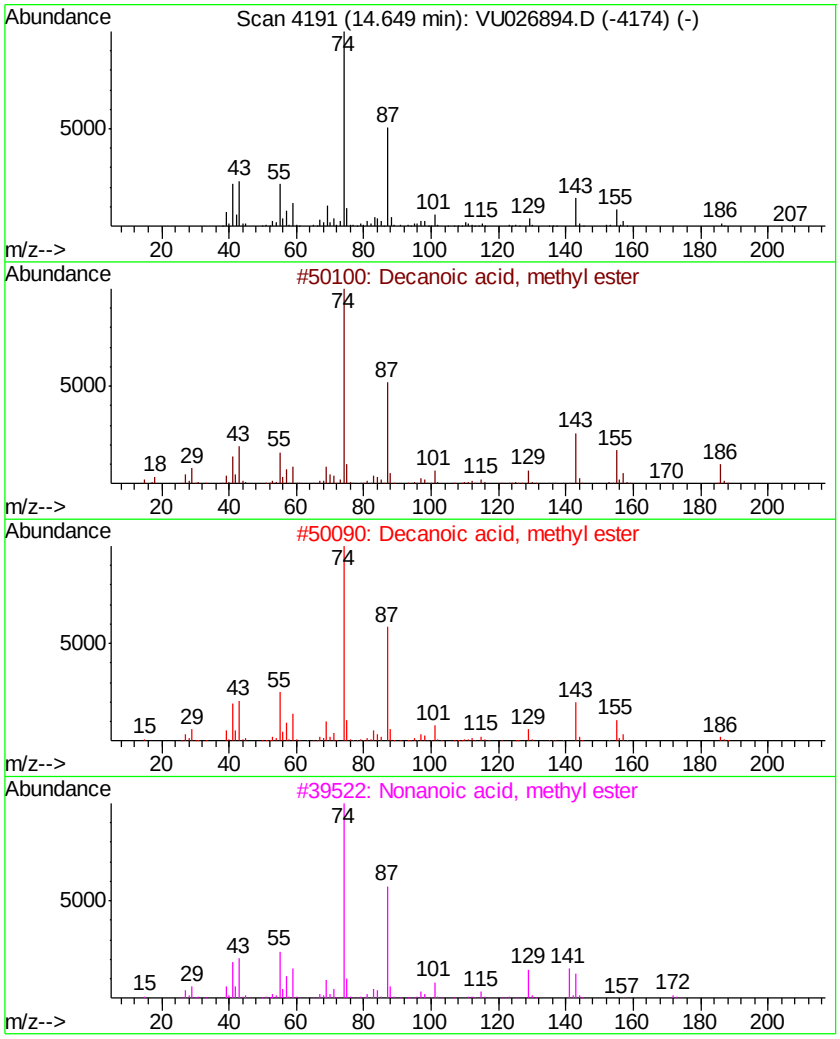
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

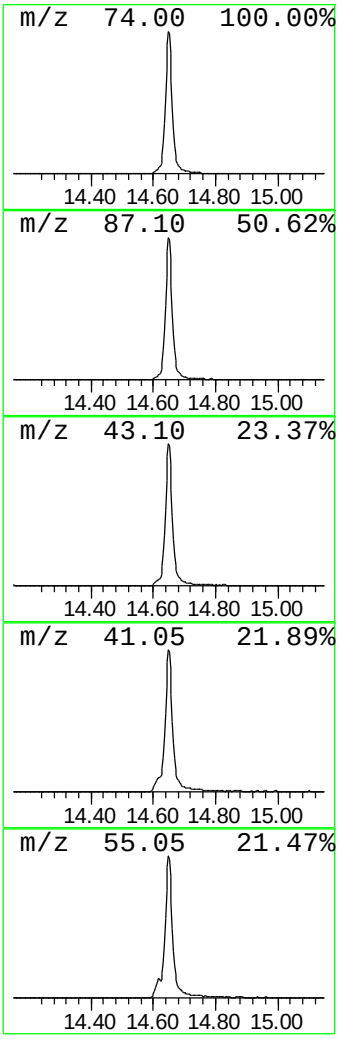
****

Peak Number 5 Decanoic acid, methyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	27.49 ug/L	502755	1,4-Dichlorobenzene-d4	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	97
2	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	96
3	Nonanoic acid, methyl ester	172	C10H20O2	001731-84-6	78
4	Nonanoic acid, methyl ester	172	C10H20O2	001731-84-6	78
5	Nonanoic acid, methyl ester	172	C10H20O2	001731-84-6	78





Tentatively Identified Compound (LSC) summary

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ClientSampleId : DB3P8ME

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091718WMA.M
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
.alpha.-Pinene	10.15	345.9	ug/L	4877270	2	9.10	704931	50.0
.beta.-Pinene	10.83	86.9	ug/L	1588630	3	11.49	914456	50.0
D-Limonene	11.43	5.6	ug/L	102975	3	11.49	914456	50.0
Decanoic acid, me...	14.65	27.5	ug/L	502755	3	11.49	914456	50.0