LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042623\
Data File : VX035316.D
Acq On : 26 Apr 2023 16:20
Operator : JC/MD
Sample : 02419-09ME
Misc : 5.01g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW924ME

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: VX035316.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	26	29	33	rBV3	1705	1708	0.14%	0.017%
2	1.368	42	46	52	rBV	54233	81634	6.81%	0.806%
3	1.672	86	96	101	rBV	25959	51869	4.33%	0.512%
4	2.288	190	197	211	rBV	210563	347406	28.97%	3.430%
5	2.715	264	267	271	rBV	708	937	0.08%	0.009%
6	2.782	271	278	290	rBV3	3908	8613	0.72%	0.085%
7	3.422	377	383	385	rBV3	1149	1824	0.15%	0.018%
8	4.483	548	557	579	rBV	60989	230044	19.19%	2.271%
9	4.751	599	601	606	rVB3	482	563	0.05%	0.006%
10	5.056	638	651	671	rBV	139995	444545	37.08%	4.389%
11	5.306	687	692	694	rBV4	1338	2266	0.19%	0.022%
12	5.550	729	732	733	rBV2	915	865	0.07%	0.009%
13	5.964	788	800	819	rBV2	405786	1162295	96.94%	11.476%
14	6.361	859	865	874	rBV4	2480	7116	0.59%	0.070%
15	6.757	920	930	949	rBV	452401	1078758	89.97%	10.651%
16	7.013	969	972	973	rBV3	591	725	0.06%	0.007%
17	7.110	982	988	990	rBV3	3630	6579	0.55%	0.065%
18	7.214	999	1005	1012	rBV4	4091	9165	0.76%	0.090%
19	7.305	1012	1020	1042	rVB	243575	533590	44.50%	5.268%
20	7.970	1121	1129	1139	rVB9	3821	10574	0.88%	0.104%
21	8.324	1180	1187	1201	rBV	131628	216695	18.07%	2.140%
22	8.494	1212	1215	1216	rBV	854	642	0.05%	0.006%
23	8.647	1233	1240	1251	rBV	616009	958901	79.98%	9.468%
24	8.744	1254	1256	1258	rBV2	607	661	0.06%	0.007%
25	8.817	1267	1268	1273	rVB2	701	594	0.05%	0.006%
26	8.952	1284	1290	1302	rBV	88604	139643	11.65%	1.379%
27	9.110	1313	1316	1319	rBV3	1136	1264	0.11%	0.012%
28	9.220	1330	1334	1337	rBV2	378	600	0.05%	0.006%
29	9.275	1338	1343	1350	rVB3	9031	14848	1.24%	0.147%
30	9.390	1356	1362	1363	rBV	106621	131901	11.00%	1.302%
31	9.421	1364	1367	1382	rVB	182781	326781	27.25%	3.227%
32	9.616	1395	1399	1404	rVB	4035	5903	0.49%	0.058%
33	9.829	1430	1434	1437	rBV4	798	951	0.08%	0.009%
34	9.903	1442	1446	1449	rVB2	590	691	0.06%	0.007%
35	10.006	1458	1463	1465	rBV4	491	772	0.06%	0.008%
36	10.055	1465	1471	1489	rBV	839709	1198996	100.00%	11.838%

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Misc : 5.01g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW924ME

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

37	10.299	1504	1511	1516	rVB8	1354	3051	0.25%	0.030%
38	10.360	1519	1521	1525	rVB2	794	819	0.07%	0.008%
39	10.457	1533	1537	1543	rVB4	1199	2095	0.17%	0.021%
40	10.561	1550	1554	1556	rBV3	557	717	0.06%	0.007%
41	10.585	1556	1558	1563	rVB3	906	1167	0.10%	0.012%
42	10.671	1568	1572	1574	rBV4	809	1072	0.09%	0.011%
43	10.780	1583	1590	1594	rBV3	2667	4055	0.34%	0.040%
44	10.829	1595	1598	1602	rVV5	710	1184	0.10%	0.012%
45	10.896	1604	1609	1613	rBV2	3719	4975	0.41%	0.049%
46	10.945	1613	1617	1621	rVB3	2244	3136	0.26%	0.031%
47	11.000	1623	1626	1628	rBV3	585	609	0.05%	0.006%
48	11.030	1628	1631	1633	rBV2	1252	1428	0.12%	0.014%
49	11.079	1634	1639	1642	rBV3	2806	4813	0.40%	0.048%
50	11.195	1652	1658	1672	rBV	351258	540915	45.11%	5.341%
51	11.311	1675	1677	1684	rVV5	764	1722	0.14%	0.017%
52	11.366	1684	1686	1687	rVV2	756	665	0.06%	0.007%
53	11.390	1687	1690	1693	rVV4	1649	2400	0.20%	0.024%
54	11.433	1693	1697	1701	rVV	25184	32386	2.70%	0.320%
55	11.475	1701	1704	1710	rVV3	9293	12742	1.06%	0.126%
56	11.518	1710	1711	1715	rVB3	1370	1128	0.09%	0.011%
57	11.634	1726	1730	1734	rVB4	2589	3727	0.31%	0.037%
58	11.683	1734	1738	1740	rBV3	2705	3792	0.32%	0.037%
59	11.713	1740	1743	1746	rBV	7425	8035	0.67%	0.079%
60	11.841	1758	1764	1766	rBV5	1743	2973	0.25%	0.029%
61	11.872	1766	1769	1770	rVV2	1826	2221	0.19%	0.022%
62	11.890	1770	1772	1776	rVB5	2636	3329	0.28%	0.033%
63	11.969	1782	1785	1788	rVB5	1816	2251	0.19%	0.022%
64	12.024	1789	1794	1805	rVV	930496	1184052	98.75%	11.691%
65	12.158	1812	1816	1821	rVB7	5130	8073	0.67%	0.080%
66	12.238	1825	1829	1833	rBV5	2550	3587	0.30%	0.035%
67	12.323	1837	1843	1853	rBV	667666	854552	71.27%	8.438%
68	12.420	1856	1859	1863	rBV2	8761	10988	0.92%	0.108%
69	12.524	1875	1876	1878	rBV2	1121	1083	0.09%	0.011%
70	12.579	1882	1885	1891	rVB5	2612	4675	0.39%	0.046%
71	12.628	1891	1893	1898	rVB5	1358	1672	0.14%	0.017%
72	12.683	1898	1902	1908	rBV5	3597	5069	0.42%	0.050%
73	12.768	1912	1916	1920	rVV4	2886	4118	0.34%	0.041%
74	12.878	1929	1934	1935	rBV3	4232	4990	0.42%	0.049%
75	12.945	1942	1945	1947	rBV4	1682	1831	0.15%	0.018%
76	13.042	1957	1961	1965	rVB7	2424	3285	0.27%	0.032%

LSC Area Percent Report

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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW924ME

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	13.091	1965	1969	1974	rBV7	1584	3436	0.29%	0.034%
78	13.268	1994	1998	2002	rBV	17086	22129	1.85%	0.218%
79	13.341	2008	2010	2013	rBV4	1142	1285	0.11%	0.013%
80	13.384	2013	2017	2021	rBV	15441	20406	1.70%	0.201%
81	13.701	2063	2069	2073	rBV6	8758	15251	1.27%	0.151%
82	13.798	2082	2085	2088	rVB4	5886	7032	0.59%	0.069%
83	13.841	2088	2092	2095	rVB2	7671	9201	0.77%	0.091%
84	13.987	2113	2116	2119	rBV5	3034	4561	0.38%	0.045%
85	14.036	2121	2124	2129	rVV	19915	23736	1.98%	0.234%
86	14.103	2131	2135	2138	rVV4	5967	9173	0.77%	0.091%
87	14.134	2138	2140	2144	rVB4	6914	8269	0.69%	0.082%
88	14.414	2184	2186	2193	rVB8	3804	6107	0.51%	0.060%
89	14.615	2216	2219	2221	rBV4	6147	6449	0.54%	0.064%
90	14.755	2238	2242	2245	rBV2	14061	15365	1.28%	0.152%
91	14.883	2260	2263	2267	rVB3	5795	7158	0.60%	0.071%
92	14.932	2267	2271	2275	rBV5	3230	6029	0.50%	0.060%
93	15.133	2301	2304	2307	rVB2	5651	6949	0.58%	0.069%
94	15.206	2311	2316	2321	rVB3	11865	20288	1.69%	0.200%
95	15.414	2345	2350	2357	rVB2	57834	86940	7.25%	0.858%
96	15.493	2360	2363	2368	rVB3	7522	9513	0.79%	0.094%
97	15.639	2383	2387	2395	rVB4	11632	21545	1.80%	0.213%
98	15.822	2414	2417	2420	rBV5	2675	3608	0.30%	0.036%
99	15.981	2437	2443	2448	rBV	49374	88667	7.40%	0.875%
100	16.670	2554	2556	2566	rVB9	3790	8619	0.72%	0.085%

Sum of corrected areas: 10128017

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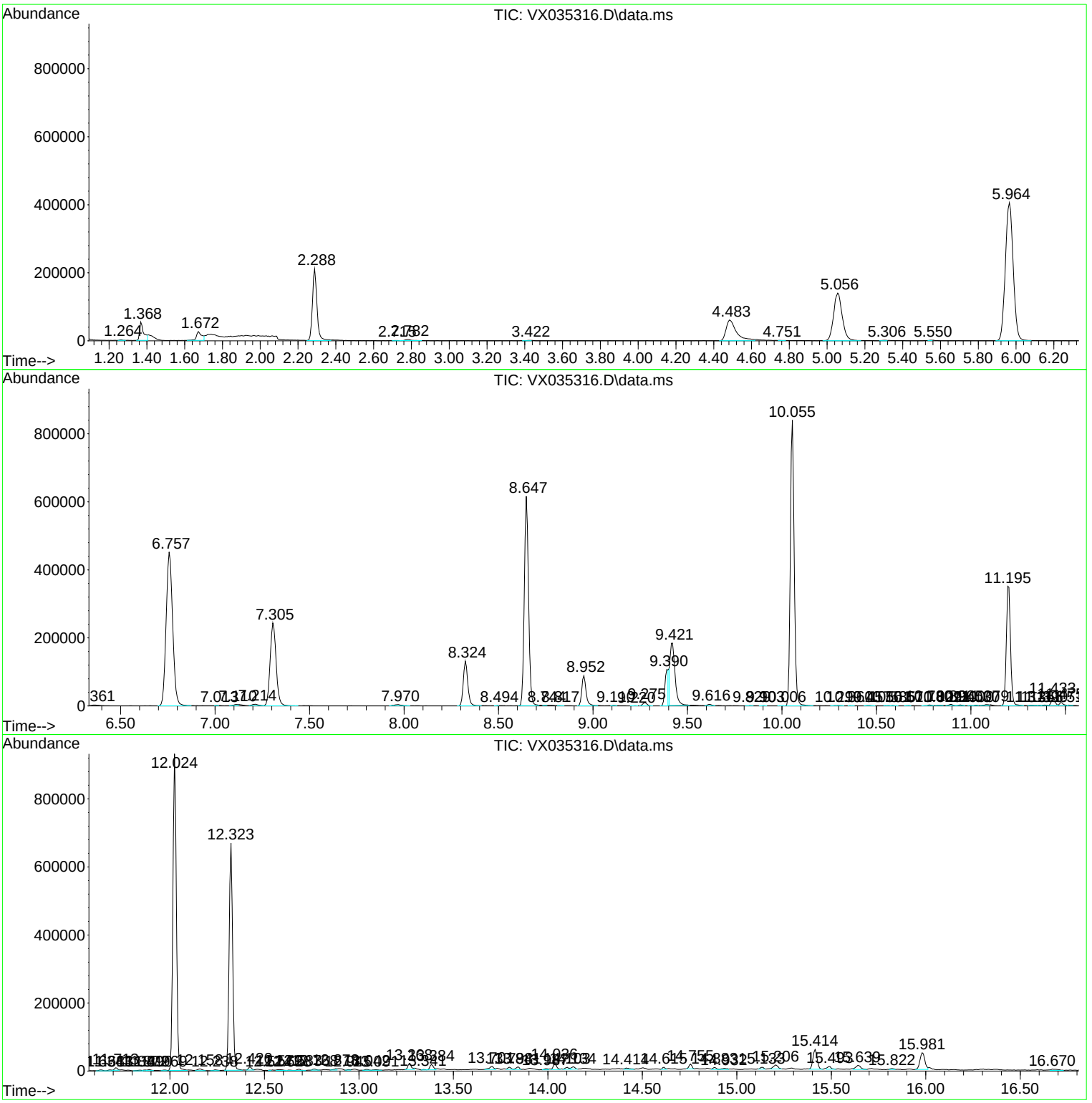
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041823WMA.M
Quant Title : VOC Analysis

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



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

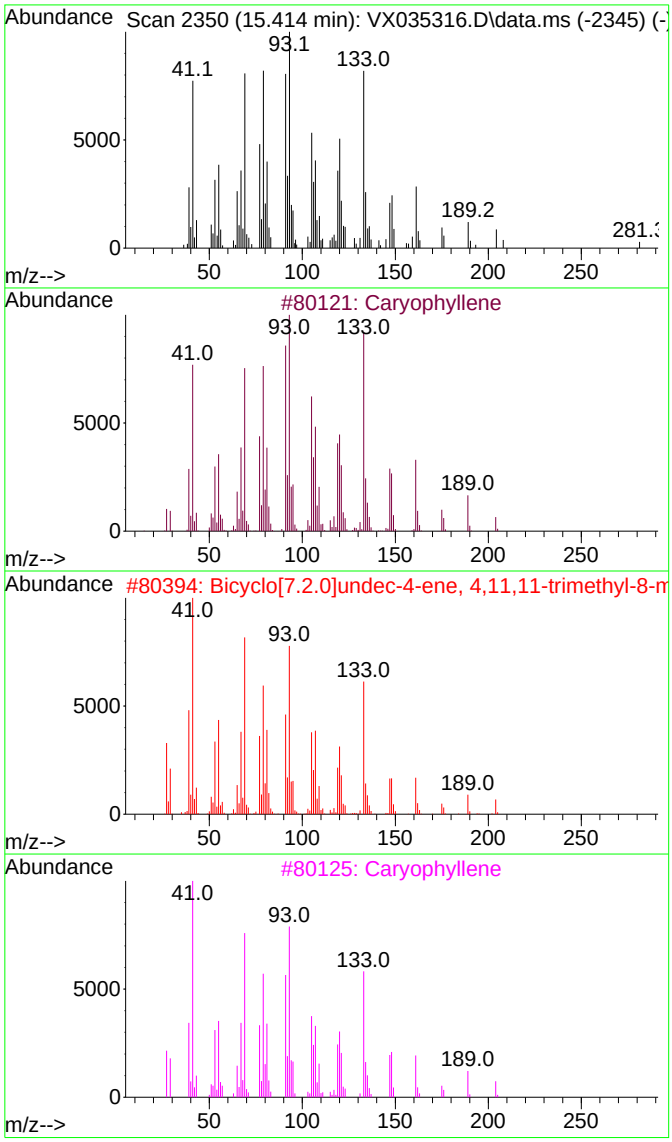
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

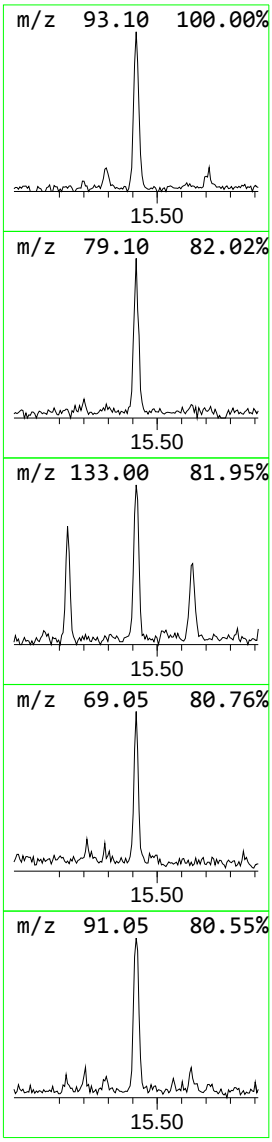
****

Peak Number 2 Caryophyllene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.414	3.67 ug/L	86940	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caryophyllene	204	C15H24	000087-44-5	99
2	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	96
3	Caryophyllene	204	C15H24	000087-44-5	93
4	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	013877-93-5	93
5	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	93





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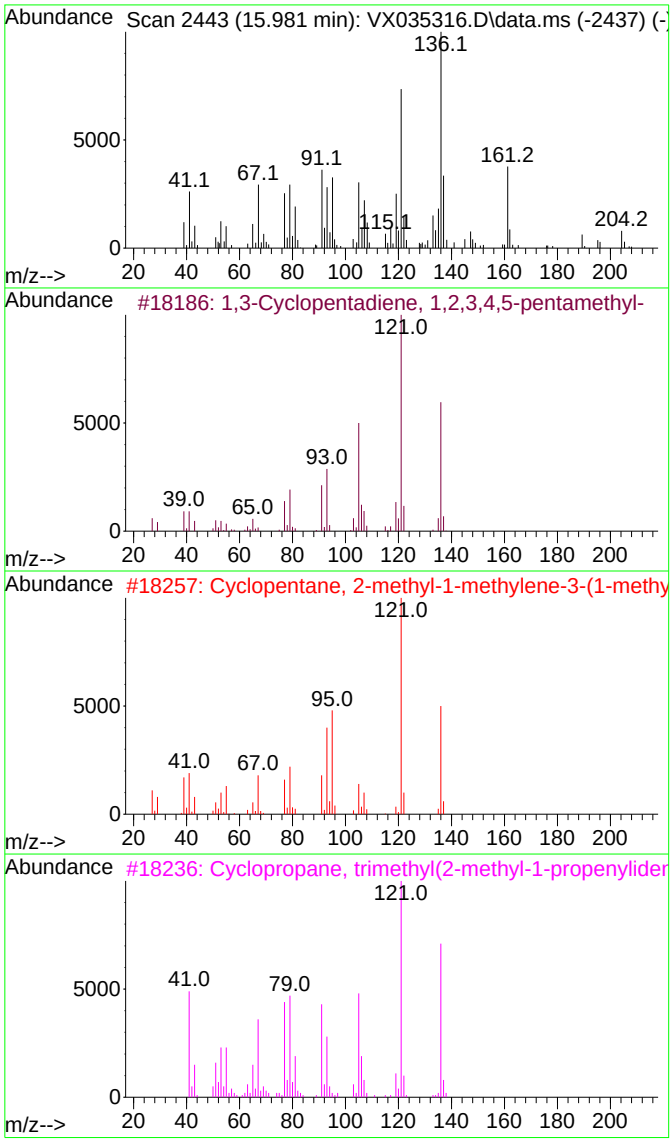
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041823WMA.M
Quant Title : VOC Analysis

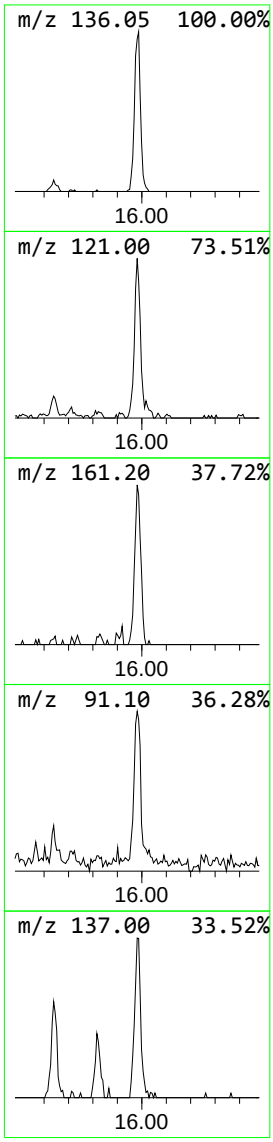
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1,3-Cyclopentadiene, 1,2,3,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.981	3.74 ug/L	88667	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentadiene, 1,2,3,4,5-p...	136	C10H16	004045-44-7	83
2	Cyclopentane, 2-methyl-1-methyle...	136	C10H16	056710-83-9	70
3	Cyclopropane, trimethyl(2-methyl...	136	C10H16	014803-30-6	64
4	1,3-Cyclopentadiene, 1,2,3,4,5-p...	136	C10H16	004045-44-7	58
5	2,4-Dimethylanisole	136	C9H12O	006738-23-4	52





Tentatively Identified Compound (LSC) summary

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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
Caryophyllene	15.414	3.7	ug/L	86940	3	12.024	1184050	50.0
1,3-Cyclopentad...	15.981	3.7	ug/L	88667	3	12.024	1184050	50.0