LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042623\
Data File : VX035322.D
Acq On : 26 Apr 2023 18:39
Operator : JC/MD
Sample : 02419-09ME
Misc : 5.01g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 25 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: VX035322.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	26	28	33	rBV2	2047	2171	0.18%	0.022%
2	1.368	42	46	66	rVB	56862	115277	9.82%	1.190%
3	1.642	88	91	92	rBV2	1284	1219	0.10%	0.013%
4	1.673	92	96	101	rBV	27160	52859	4.50%	0.546%
5	2.172	177	178	183	rVB5	1333	1078	0.09%	0.011%
6	2.288	191	197	212	rBV	205773	333993	28.45%	3.448%
7	2.703	263	265	267	rBV	736	752	0.06%	0.008%
8	2.782	272	278	283	rBV2	3610	6980	0.59%	0.072%
9	2.941	301	304	306	rVV	529	532	0.05%	0.005%
10	3.434	378	385	391	rBV5	1485	3234	0.28%	0.033%
11	4.483	549	557	572	rBV	60860	227418	19.37%	2.348%
12	5.056	636	651	668	rBV	146528	461495	39.30%	4.764%
13	5.294	684	690	692	rBV3	1170	1906	0.16%	0.020%
14	5.538	726	730	731	rBV2	650	713	0.06%	0.007%
15	5.964	787	800	818	rBV2	409107	1174171	100.00%	12.121%
16	6.123	824	826	830	rVB3	467	556	0.05%	0.006%
17	6.355	858	864	865	rBV3	2107	2970	0.25%	0.031%
18	6.757	919	930	944	rBV	374572	889348	75.74%	9.181%
19	7.013	969	972	981	rVB5	1172	2346	0.20%	0.024%
20	7.123	981	990	998	rBV6	3735	12001	1.02%	0.124%
21	7.208	998	1004	1012	rVV3	4016	10479	0.89%	0.108%
22	7.306	1012	1020	1035	rVB	250150	547723	46.65%	5.654%
23	7.470	1045	1047	1050	rVV3	737	961	0.08%	0.010%
24	7.964	1120	1128	1135	rBV7	3163	8915	0.76%	0.092%
25	8.251	1171	1175	1181	rBV3	4860	7545	0.64%	0.078%
26	8.324	1181	1187	1197	rBV	131919	219629	18.71%	2.267%
27	8.440	1203	1206	1210	rVB3	1102	1375	0.12%	0.014%
28	8.495	1210	1215	1226	rBV3	1006	2459	0.21%	0.025%
29	8.647	1233	1240	1254	rVV	605354	935054	79.64%	9.653%
30	8.757	1256	1258	1259	rVV2	1588	1417	0.12%	0.015%
31	8.775	1259	1261	1270	rVB5	1461	3430	0.29%	0.035%
32	8.952	1284	1290	1305	rVV	90241	144425	12.30%	1.491%
33	9.104	1311	1315	1321	rBV6	677	1287	0.11%	0.013%
34	9.275	1338	1343	1351	rVB2	9549	15305	1.30%	0.158%
35	9.391	1357	1362	1363	rBV	104088	127540	10.86%	1.317%
36	9.421	1363	1367	1381	rVB	195804	393644	33.53%	4.064%

LSC Area Percent Report

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Operator : JC/MD
Sample : 02419-09ME
Misc : 5.01g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 25 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

37	9.616	1395	1399	1405	rBV3	3863	6190	0.53%	0.064%
38	9.744	1416	1420	1426	rVB5	479	746	0.06%	0.008%
39	9.903	1444	1446	1450	rBV2	411	575	0.05%	0.006%
40	10.055	1465	1471	1483	rBV	696305	992512	84.53%	10.246%
41	10.165	1488	1489	1491	rVV3	755	754	0.06%	0.008%
42	10.214	1494	1497	1500	rVV4	653	913	0.08%	0.009%
43	10.275	1503	1507	1508	rVV4	773	1020	0.09%	0.011%
44	10.299	1508	1511	1519	rVV4	1652	2646	0.23%	0.027%
45	10.366	1519	1522	1525	rVB2	1098	1234	0.11%	0.013%
46	10.458	1534	1537	1542	rVB4	1646	2002	0.17%	0.021%
47	10.580	1551	1557	1562	rVB6	701	1695	0.14%	0.017%
48	10.671	1567	1572	1574	rBV2	975	1413	0.12%	0.015%
49	10.781	1582	1590	1593	rBV4	3045	4316	0.37%	0.045%
50	10.836	1593	1599	1600	rBV4	1156	1727	0.15%	0.018%
51	10.897	1605	1609	1613	rVB	3529	4858	0.41%	0.050%
52	10.945	1613	1617	1621	rVB3	3243	4515	0.38%	0.047%
53	10.994	1621	1625	1626	rBV	890	718	0.06%	0.007%
54	11.031	1628	1631	1634	rVB2	1461	1556	0.13%	0.016%
55	11.079	1634	1639	1642	rBV7	2976	5895	0.50%	0.061%
56	11.201	1650	1659	1667	rBV	375857	568008	48.38%	5.864%
57	11.311	1674	1677	1679	rBV3	1210	1408	0.12%	0.015%
58	11.372	1684	1687	1688	rBV3	1006	1142	0.10%	0.012%
59	11.390	1688	1690	1693	rVV4	1786	1616	0.14%	0.017%
60	11.433	1693	1697	1701	rVV2	23216	29901	2.55%	0.309%
61	11.476	1701	1704	1709	rVB3	8381	10566	0.90%	0.109%
62	11.634	1727	1730	1735	rVB4	2525	3209	0.27%	0.033%
63	11.683	1735	1738	1740	rBV3	2400	3069	0.26%	0.032%
64	11.713	1740	1743	1746	rBV3	8346	9957	0.85%	0.103%
65	11.829	1758	1762	1763	rBV4	1016	1293	0.11%	0.013%
66	11.872	1766	1769	1770	rBV3	1884	2376	0.20%	0.025%
67	11.970	1782	1785	1789	rBV5	1997	2488	0.21%	0.026%
68	12.024	1789	1794	1804	rBV	757488	981422	83.58%	10.131%
69	12.159	1811	1816	1825	rVB8	5611	10607	0.90%	0.109%
70	12.238	1825	1829	1834	rBV5	3764	5927	0.50%	0.061%
71	12.323	1837	1843	1854	rVV	674829	873007	74.35%	9.012%
72	12.421	1856	1859	1864	rVV	10817	16502	1.41%	0.170%
73	12.463	1864	1866	1872	rVB5	3814	7058	0.60%	0.073%
74	12.585	1882	1886	1890	rVB6	2862	4710	0.40%	0.049%
75	12.628	1890	1893	1898	rVB5	1887	2738	0.23%	0.028%
76	12.683	1898	1902	1906	rBV5	4587	6688	0.57%	0.069%

LSC Area Percent Report

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Misc : 5.01g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 25 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

77	12.762	1913	1915	1919	rVB3	3467	3771	0.32%	0.039%
78	12.884	1931	1935	1937	rBV4	4652	6916	0.59%	0.071%
79	12.945	1942	1945	1946	rBV2	1205	1458	0.12%	0.015%
80	13.042	1957	1961	1965	rBV6	2412	3985	0.34%	0.041%
81	13.268	1994	1998	2001	rBV	16411	19991	1.70%	0.206%
82	13.341	2008	2010	2011	rBV	1582	980	0.08%	0.010%
83	13.384	2013	2017	2021	rBV2	15005	19130	1.63%	0.197%
84	13.701	2066	2069	2074	rBV4	7078	7283	0.62%	0.075%
85	13.798	2081	2085	2088	rBV6	5821	7183	0.61%	0.074%
86	13.841	2089	2092	2095	rVB3	8786	10960	0.93%	0.113%
87	13.987	2114	2116	2119	rBV4	2509	2994	0.25%	0.031%
88	14.036	2121	2124	2128	rVV	19146	22799	1.94%	0.235%
89	14.097	2132	2134	2137	rVV3	5560	6725	0.57%	0.069%
90	14.134	2137	2140	2144	rVB5	6582	9756	0.83%	0.101%
91	14.615	2216	2219	2222	rBV4	5630	5963	0.51%	0.062%
92	14.756	2239	2242	2245	rBV2	13405	15265	1.30%	0.158%
93	14.878	2260	2262	2268	rVB4	5197	7295	0.62%	0.075%
94	14.932	2268	2271	2274	rBV5	3496	4650	0.40%	0.048%
95	15.207	2311	2316	2320	rVB4	10746	16508	1.41%	0.170%
96	15.414	2345	2350	2356	rVB2	62020	91309	7.78%	0.943%
97	15.640	2383	2387	2395	rVB3	12304	20359	1.73%	0.210%
98	15.902	2428	2430	2433	rBV3	1984	2401	0.20%	0.025%
99	15.981	2438	2443	2457	rVB3	52572	106098	9.04%	1.095%
100	16.676	2555	2557	2559	rBV3	2104	1996	0.17%	0.021%

Sum of corrected areas: 9686959

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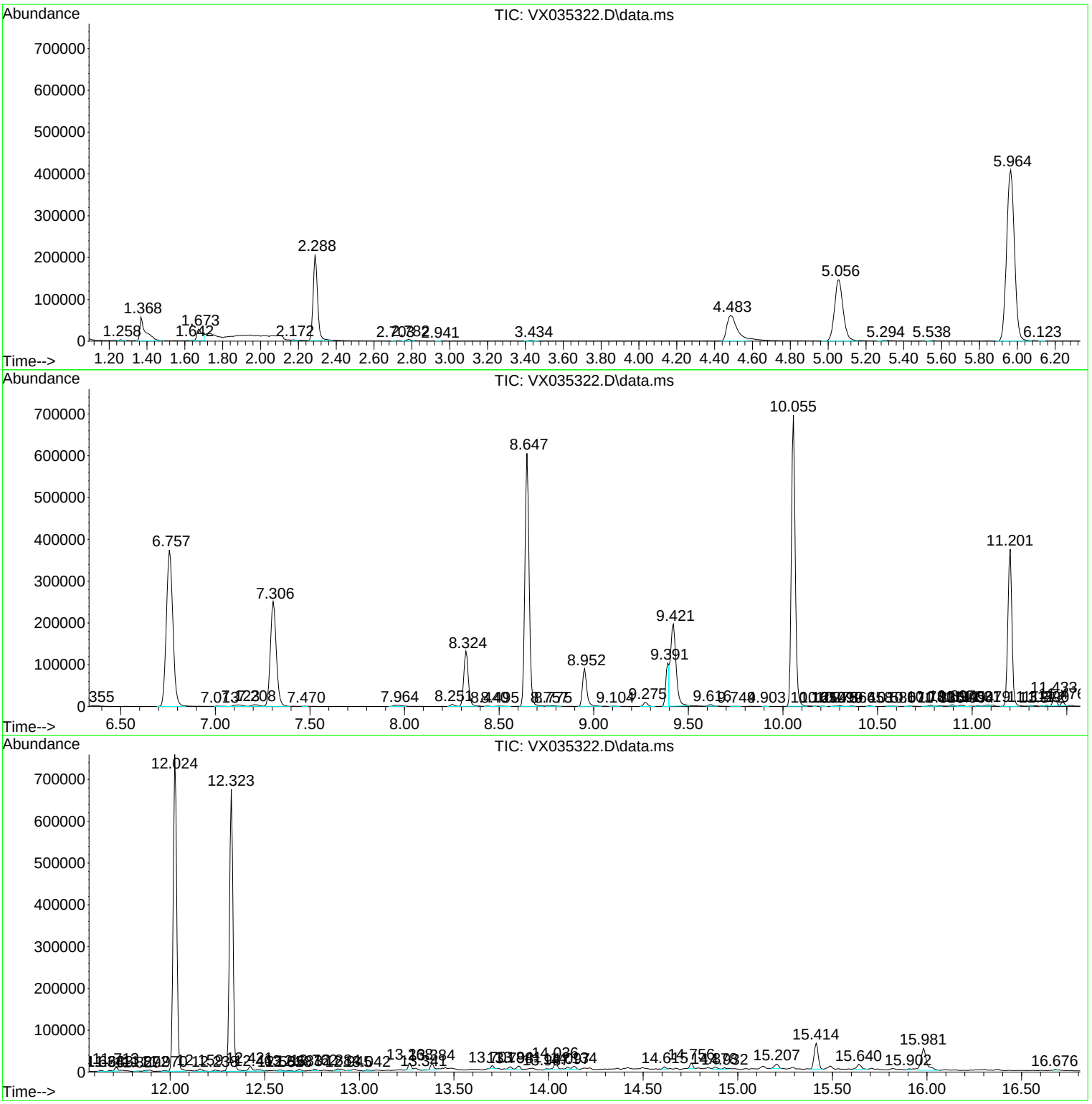
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW924ME

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042623\
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Instrument :
MSVOA_X
ClientSampleId :
EW924ME

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

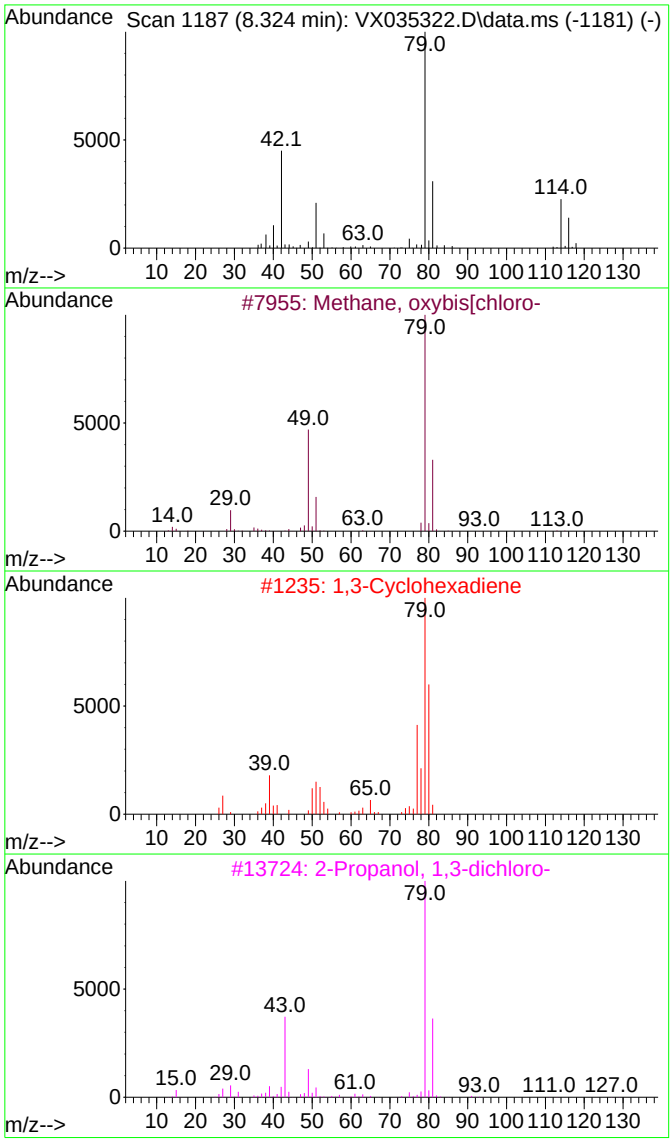
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

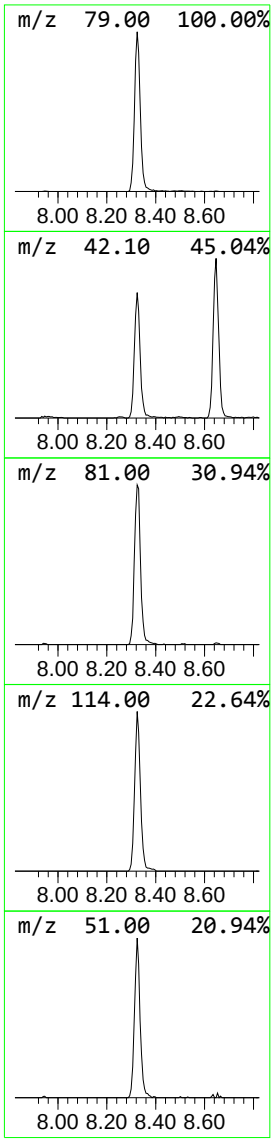
****

Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.324	12.35 ug/L	219629	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	37
2	1,3-Cyclohexadiene	80	C6H8	000592-57-4	25
3	2-Propanol, 1,3-dichloro-	128	C3H6Cl2O	000096-23-1	23
4	3-Thiatricyclo[3.1.1.0(2,4)]heptane	112	C6H8S	1000221-37-0	9
5	2-Propanol, 1,3-dichloro-	128	C3H6Cl2O	000096-23-1	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042623\
Data File : VX035322.D
Acq On : 26 Apr 2023 18:39
Operator : JC/MD
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ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW924ME

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

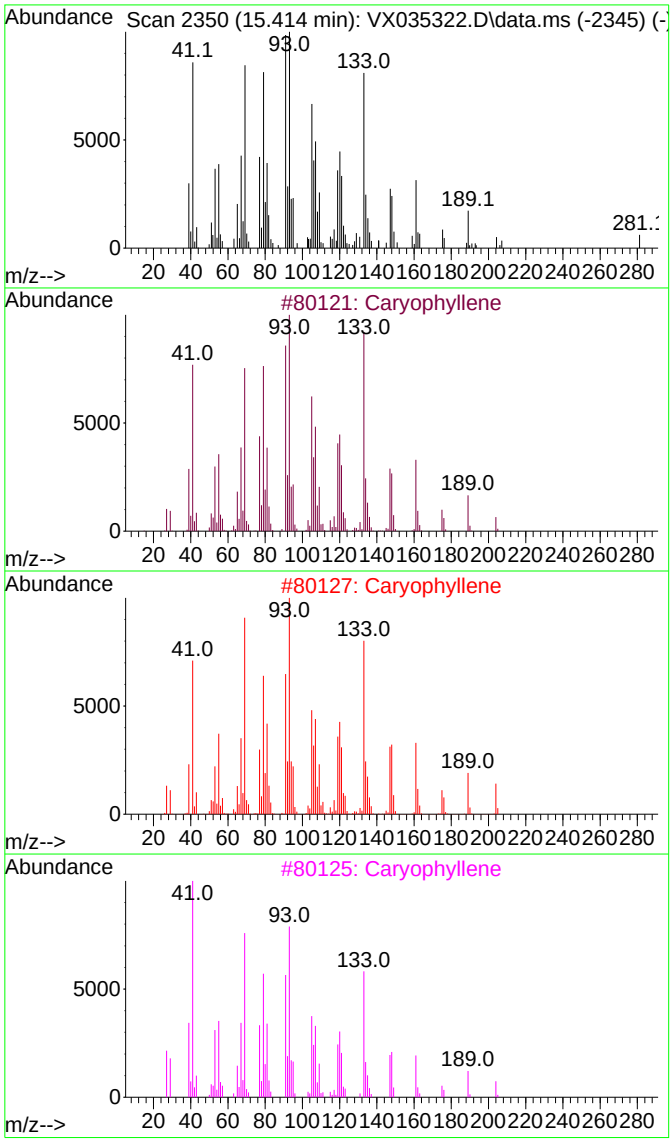
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

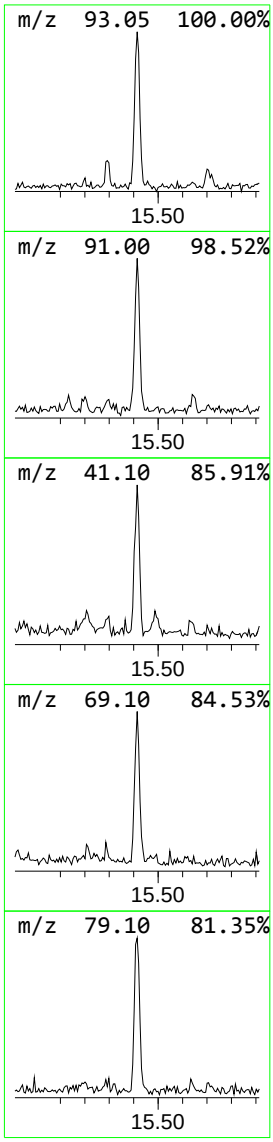
****

Peak Number 2 Caryophyllene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.414	4.65 ug/L	91309	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caryophyllene	204	C15H24	000087-44-5	99
2	Caryophyllene	204	C15H24	000087-44-5	96
3	Caryophyllene	204	C15H24	000087-44-5	94
4	Bicyclo[5.2.0]nonane, 2-methylen...	204	C15H24	242794-76-9	93
5	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	91





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ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW924ME

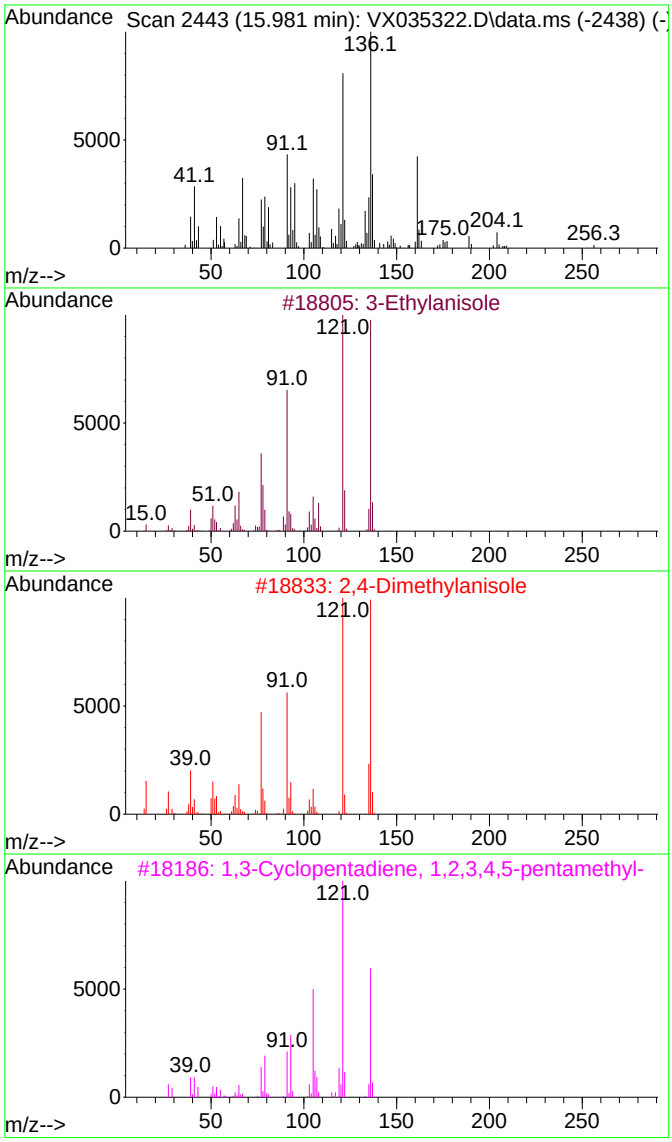
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041823WMA.M
Quant Title : VOC Analysis

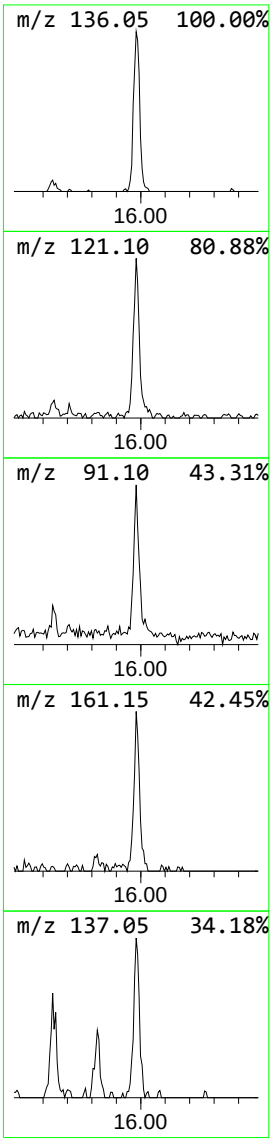
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 3-Ethylanisole Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.981	5.41 ug/L	106098	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Ethylanisole	136	C9H12O	010568-38-4	60
2	2,4-Dimethylanisole	136	C9H12O	006738-23-4	60
3	1,3-Cyclopentadiene, 1,2,3,4,5-p...	136	C10H16	004045-44-7	60
4	Cyclopentane, 2-methyl-1-methyle...	136	C10H16	056710-83-9	58
5	Phenol, 2,3,6-trimethyl-	136	C9H12O	002416-94-6	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042623\
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ALS Vial : 25 Sample Multiplier: 1

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown-01	8.324	12.4	ug/L	219629	1	6.757	889348	50.0
Caryophyllene	15.414	4.7	ug/L	91309	3	12.024	981422	50.0
3-Ethylanisole	15.981	5.4	ug/L	106098	3	12.024	981422	50.0