LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012925\
Data File : VX044763.D
Acq On : 29 Jan 2025 12:34
Operator : JC/MD
Sample : Q1190-17ME
Misc : 5.65g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44T7ME

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\SFAMXLM012825WMA.M
Title : VOC Analysis

Signal : TIC: VX044763.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	22	28	33	rBV2	11289	22114	0.51%	0.167%
2	1.368	43	46	49	rBV	74970	80863	1.88%	0.610%
3	2.276	189	195	211	rBV	214117	361771	8.40%	2.727%
4	2.941	297	304	314	rBV2	4186	11850	0.28%	0.089%
5	3.081	326	327	330	rVB2	815	600	0.01%	0.005%
6	3.129	330	335	336	rBV3	447	656	0.02%	0.005%
7	3.337	366	369	372	rVB3	464	504	0.01%	0.004%
8	3.843	450	452	455	rVV2	443	389	0.01%	0.003%
9	3.946	467	469	471	rBV2	300	364	0.01%	0.003%
10	4.001	475	478	482	rBV4	525	899	0.02%	0.007%
11	4.074	488	490	496	rVB2	534	839	0.02%	0.006%
12	4.135	499	500	503	rBV2	332	392	0.01%	0.003%
13	4.263	517	521	522	rBV2	438	390	0.01%	0.003%
14	4.398	541	543	546	rBV3	295	329	0.01%	0.002%
15	4.483	548	557	584	rBV2	45163	192554	4.47%	1.452%
16	5.056	637	651	665	rBV	130007	411379	9.56%	3.101%
17	5.166	668	669	672	rVB2	919	676	0.02%	0.005%
18	5.385	702	705	706	rBV	436	429	0.01%	0.003%
19	5.525	725	728	729	rBV2	593	628	0.01%	0.005%
20	5.544	729	731	742	rVB4	1027	2419	0.06%	0.018%
21	5.714	758	759	762	rVB2	516	349	0.01%	0.003%
22	5.806	771	774	776	rBV2	385	387	0.01%	0.003%
23	5.958	788	799	820	rBV2	381765	1093905	25.41%	8.246%
24	6.318	854	858	859	rBV2	278	378	0.01%	0.003%
25	6.385	865	869	871	rBV4	728	1248	0.03%	0.009%
26	6.470	879	883	885	rBV2	280	439	0.01%	0.003%
27	6.604	903	905	906	rBV	666	557	0.01%	0.004%
28	6.684	915	918	920	rBV3	500	609	0.01%	0.005%
29	6.757	920	930	949	rBV	266813	673113	15.64%	5.074%
30	6.958	962	963	967	rVB2	872	571	0.01%	0.004%
31	7.214	1000	1005	1006	rBV3	838	1231	0.03%	0.009%
32	7.306	1012	1020	1040	rBV	218974	497455	11.56%	3.750%
33	7.610	1068	1070	1072	rBV2	314	337	0.01%	0.003%
34	7.641	1072	1075	1078	rVB3	329	406	0.01%	0.003%
35	7.946	1122	1125	1126	rBV	404	386	0.01%	0.003%
36	8.080	1145	1147	1149	rVB	411	384	0.01%	0.003%

LSC Area Percent Report

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Acq On : 29 Jan 2025 12:34
Operator : JC/MD
Sample : Q1190-17ME
Misc : 5.65g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44T7ME

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\SFAMXLM012825WMA.M
Title : VOC Analysis

37	8.165	1157	1161	1164	rBV4	495	841	0.02%	0.006%
38	8.324	1181	1187	1208	rBV	154328	271807	6.31%	2.049%
39	8.647	1233	1240	1269	rBV	512538	908795	21.11%	6.851%
40	8.909	1280	1283	1284	rBV3	869	782	0.02%	0.006%
41	8.952	1284	1290	1303	rVV	104023	168921	3.92%	1.273%
42	9.269	1338	1342	1350	rBV2	11560	19203	0.45%	0.145%
43	9.391	1357	1362	1378	rBV	194400	380784	8.85%	2.870%
44	9.708	1410	1414	1420	rVB5	1619	2787	0.06%	0.021%
45	10.049	1465	1470	1491	rBV	537505	801637	18.62%	6.043%
46	10.195	1491	1494	1500	rVV3	2104	3937	0.09%	0.030%
47	10.305	1509	1512	1518	rBV4	2474	3916	0.09%	0.030%
48	10.445	1531	1535	1537	rBV2	465	406	0.01%	0.003%
49	10.506	1543	1545	1548	rVB	452	360	0.01%	0.003%
50	10.573	1553	1556	1558	rVB2	492	416	0.01%	0.003%
51	10.604	1558	1561	1564	rBV3	480	775	0.02%	0.006%
52	10.646	1564	1568	1570	rBV3	860	1071	0.02%	0.008%
53	10.823	1593	1597	1601	rVV4	2188	3382	0.08%	0.025%
54	10.896	1605	1609	1610	rBV2	279	381	0.01%	0.003%
55	10.939	1611	1616	1627	rVV	110088	153875	3.57%	1.160%
56	11.024	1628	1630	1633	rVB2	493	391	0.01%	0.003%
57	11.085	1638	1640	1641	rBV	619	355	0.01%	0.003%
58	11.189	1644	1657	1671	rVV2	360055	627023	14.57%	4.727%
59	11.305	1673	1676	1680	rVB2	999	1418	0.03%	0.011%
60	11.372	1684	1687	1688	rBV	678	621	0.01%	0.005%
61	11.384	1688	1689	1691	rBV2	666	404	0.01%	0.003%
62	11.433	1693	1697	1701	rBV	7234	10175	0.24%	0.077%
63	11.488	1701	1706	1716	rVB	68448	114753	2.67%	0.865%
64	11.683	1733	1738	1741	rBV3	619	884	0.02%	0.007%
65	11.744	1741	1748	1755	rVB6	3563	7473	0.17%	0.056%
66	11.969	1775	1785	1789	rBV	64852	85100	1.98%	0.642%
67	12.018	1789	1793	1802	rVV	589537	771863	17.93%	5.819%
68	12.103	1803	1807	1814	rVB2	19071	28142	0.65%	0.212%
69	12.317	1837	1842	1851	rBV	586082	744273	17.29%	5.611%
70	12.622	1890	1892	1894	rBV3	478	444	0.01%	0.003%
71	12.695	1900	1904	1905	rBV2	557	687	0.02%	0.005%
72	12.713	1905	1907	1910	rVV3	632	614	0.01%	0.005%
73	12.762	1911	1915	1921	rVB2	2013	2932	0.07%	0.022%
74	12.908	1934	1939	1943	rVB	7144	9955	0.23%	0.075%
75	13.128	1972	1975	1976	rBV	686	648	0.02%	0.005%
76	13.225	1985	1991	1994	rBV3	1171	1901	0.04%	0.014%

LSC Area Percent Report

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Data File : VX044763.D
Acq On : 29 Jan 2025 12:34
Operator : JC/MD
Sample : Q1190-17ME
Misc : 5.65g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44T7ME

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\SFAMXLM012825WMA.M
Title : VOC Analysis

77	13.268	1994	1998	2005	rVV5	1926	3128	0.07%	0.024%
78	13.335	2005	2009	2013	rVV3	659	882	0.02%	0.007%
79	13.512	2032	2038	2047	rVV	97936	138015	3.21%	1.040%
80	13.670	2060	2064	2073	rBV2	27261	39841	0.93%	0.300%
81	13.786	2080	2083	2086	rVB	1213	1285	0.03%	0.010%
82	13.841	2088	2092	2098	rVB4	1030	1975	0.05%	0.015%
83	13.908	2101	2103	2104	rBV2	827	589	0.01%	0.004%
84	14.036	2121	2124	2131	rVB5	3092	4349	0.10%	0.033%
85	14.128	2131	2139	2142	rBV4	2343	4253	0.10%	0.032%
86	14.268	2159	2162	2164	rBV3	570	654	0.02%	0.005%
87	14.335	2170	2173	2175	rBV2	380	418	0.01%	0.003%
88	14.396	2177	2183	2184	rBV	19816	21840	0.51%	0.165%
89	14.432	2184	2189	2211	rVB	3797852	4304289	100.00%	32.447%
90	14.676	2225	2229	2234	rVB6	4574	6375	0.15%	0.048%
91	14.755	2240	2242	2245	rBV3	1341	1264	0.03%	0.010%
92	14.847	2254	2257	2261	rVB2	1118	1569	0.04%	0.012%
93	14.987	2275	2280	2284	rBV4	1788	2524	0.06%	0.019%
94	15.127	2301	2303	2309	rVB5	2678	3184	0.07%	0.024%
95	15.280	2323	2328	2332	rBV	43772	61059	1.42%	0.460%
96	15.316	2332	2334	2339	rVB2	7983	10373	0.24%	0.078%
97	15.444	2350	2355	2361	rBV3	22233	32948	0.77%	0.248%
98	15.743	2401	2404	2408	rBV5	1637	2872	0.07%	0.022%
99	15.859	2417	2423	2433	rBV3	34738	70343	1.63%	0.530%
100	16.261	2483	2489	2500	rVB2	31758	55668	1.29%	0.420%

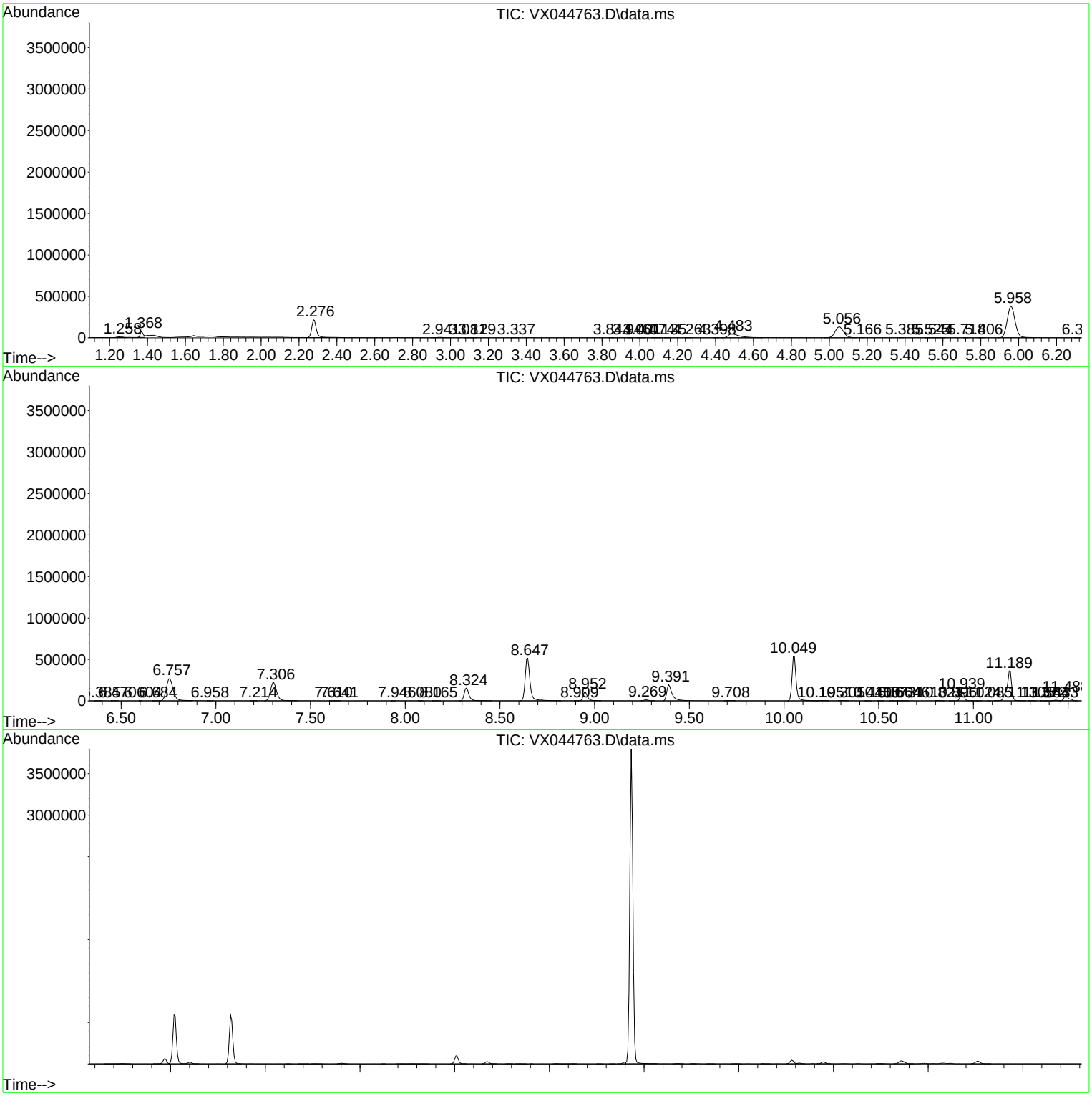
Sum of corrected areas: 13265629

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012925\
Data File : VX044763.D
Acq On : 29 Jan 2025 12:34
Operator : JC/MD
Sample : Q1190-17ME
Misc : 5.65g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44T7ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM012825WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012925\
Data File : VX044763.D
Acq On : 29 Jan 2025 12:34
Operator : JC/MD
Sample : Q1190-17ME
Misc : 5.65g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44T7ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM012825WMA.M
Quant Title : VOC Analysis

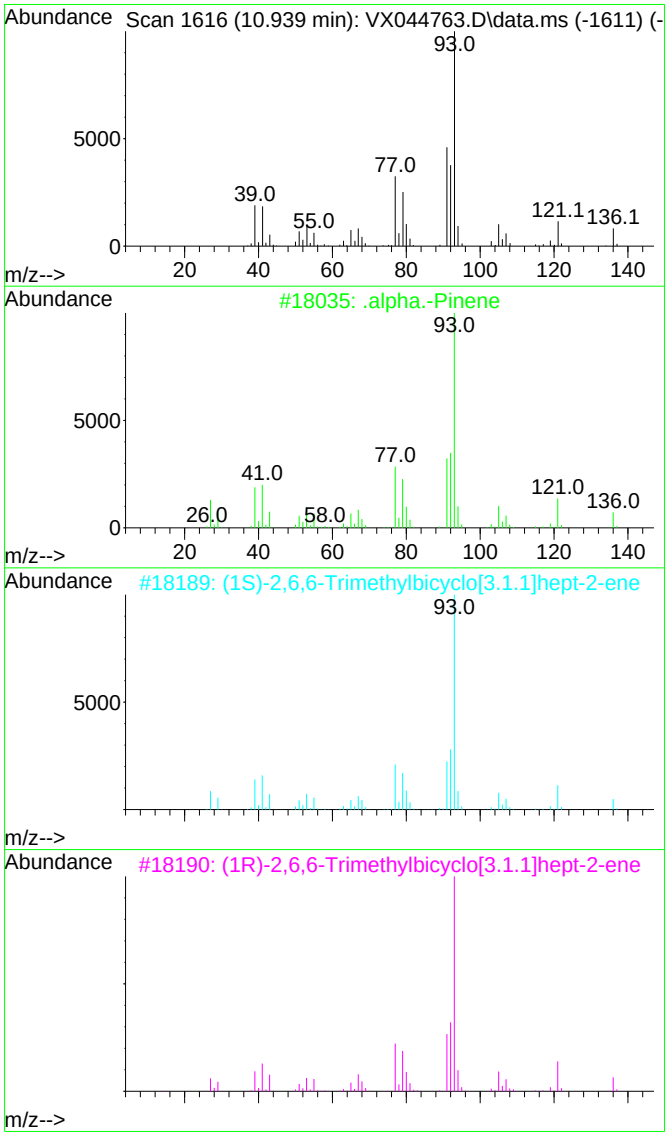
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

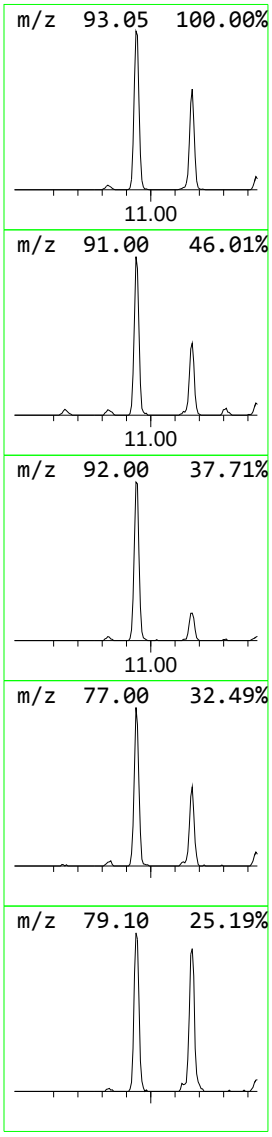
****

Peak Number 2 .alpha.-Pinene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.939	9.60 ug/L	153875	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Pinene	136	C10H16	000080-56-8	96
2	(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	95
3	(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	95
4	.alpha.-Pinene	136	C10H16	000080-56-8	95
5	.alpha.-Pinene	136	C10H16	000080-56-8	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012925\
Data File : VX044763.D
Acq On : 29 Jan 2025 12:34
Operator : JC/MD
Sample : Q1190-17ME
Misc : 5.65g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44T7ME

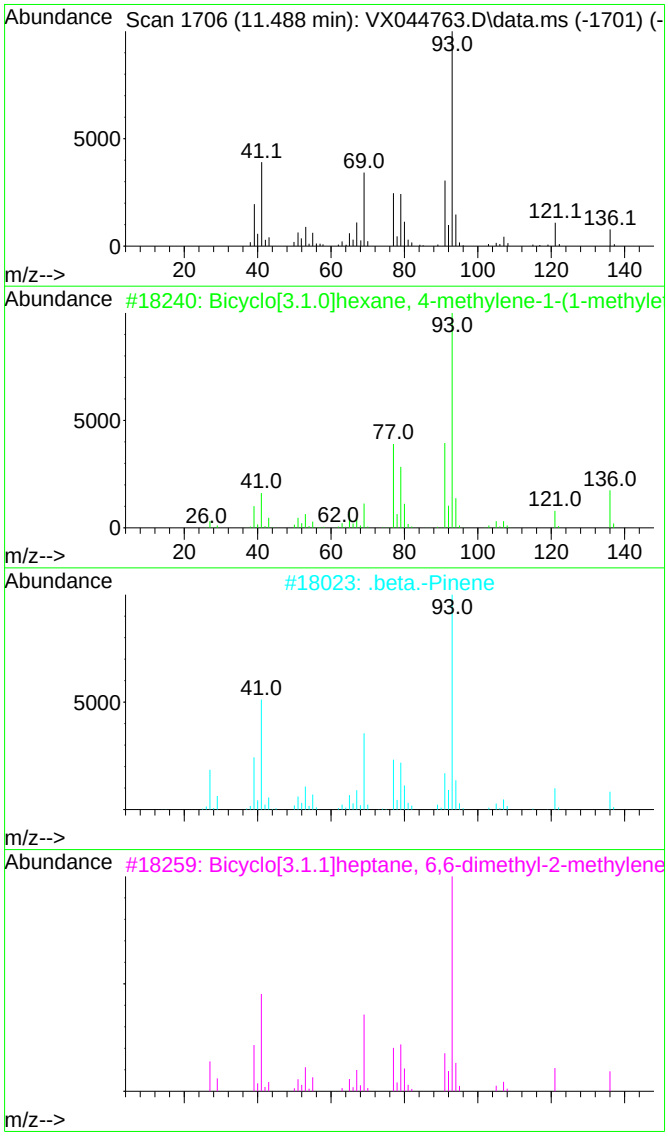
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM012825WMA.M
Quant Title : VOC Analysis

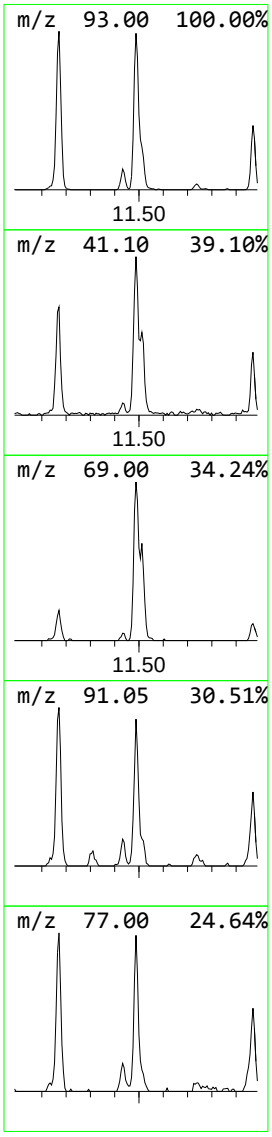
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Bicyclo[3.1.0]hexane, 4-met... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.488	7.43 ug/L	114753	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.0]hexane, 4-methylen...	136	C10H16	003387-41-5	94
2	.beta.-Pinene	136	C10H16	000127-91-3	91
3	Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	91
4	.beta.-Pinene	136	C10H16	000127-91-3	91
5	Cyclohexene, 4-methylene-1-(1-me...	136	C10H16	000099-84-3	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012925\
Data File : VX044763.D
Acq On : 29 Jan 2025 12:34
Operator : JC/MD
Sample : Q1190-17ME
Misc : 5.65g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44T7ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM012825WMA.M
Quant Title : VOC Analysis

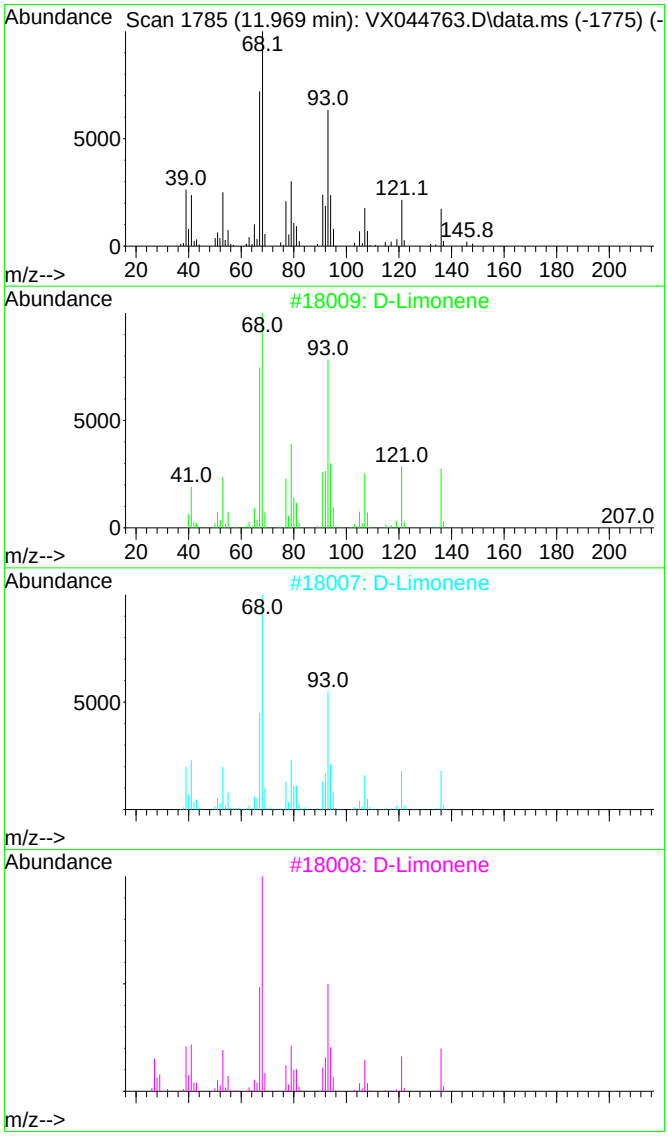
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

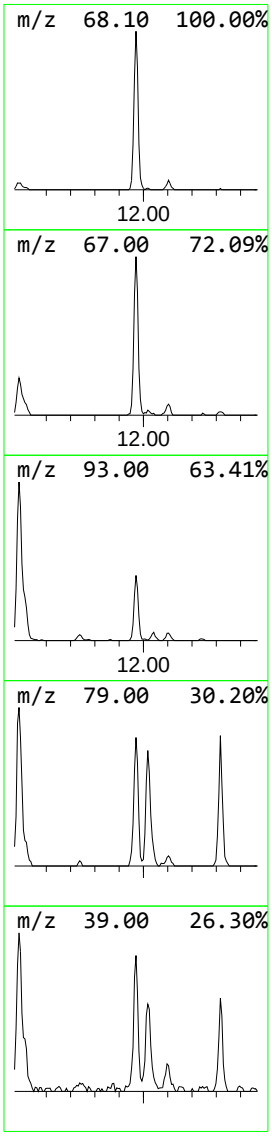
****

Peak Number 4 D-Limonene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.969	5.51 ug/L	85100	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Limonene	136	C10H16	005989-27-5	96
2	D-Limonene	136	C10H16	005989-27-5	95
3	D-Limonene	136	C10H16	005989-27-5	94
4	D-Limonene	136	C10H16	005989-27-5	93
5	Limonene	136	C10H16	000138-86-3	93





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012925\
Data File : VX044763.D
Acq On : 29 Jan 2025 12:34
Operator : JC/MD
Sample : Q1190-17ME
Misc : 5.65g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44T7ME

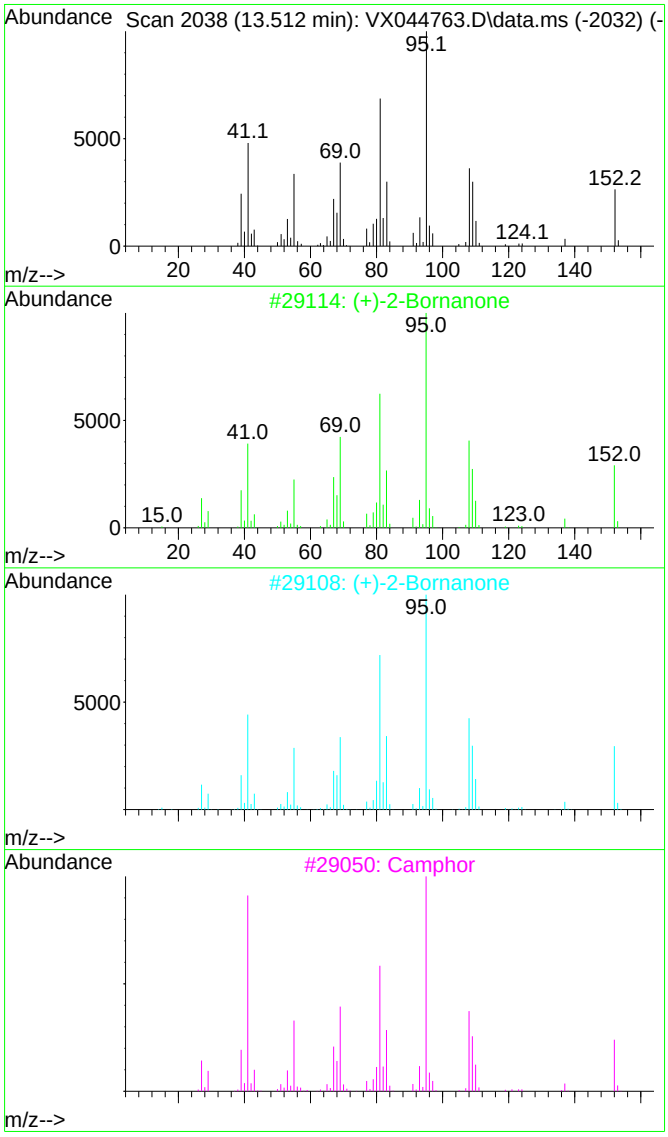
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM012825WMA.M
Quant Title : VOC Analysis

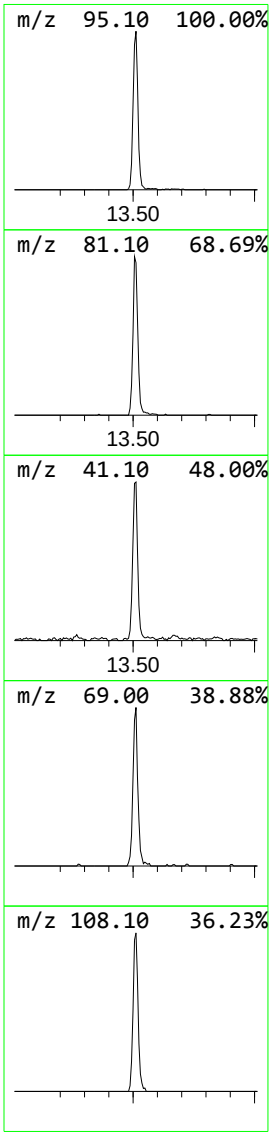
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (+)-2-Bornanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.512	8.94 ug/L	138015	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-2-Bornanone	152	C10H16O	000464-49-3	98
2	(+)-2-Bornanone	152	C10H16O	000464-49-3	98
3	Camphor	152	C10H16O	000076-22-2	98
4	(+)-2-Bornanone	152	C10H16O	000464-49-3	98
5	Camphor	152	C10H16O	000076-22-2	98





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012925\
Data File : VX044763.D
Acq On : 29 Jan 2025 12:34
Operator : JC/MD
Sample : Q1190-17ME
Misc : 5.65g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44T7ME

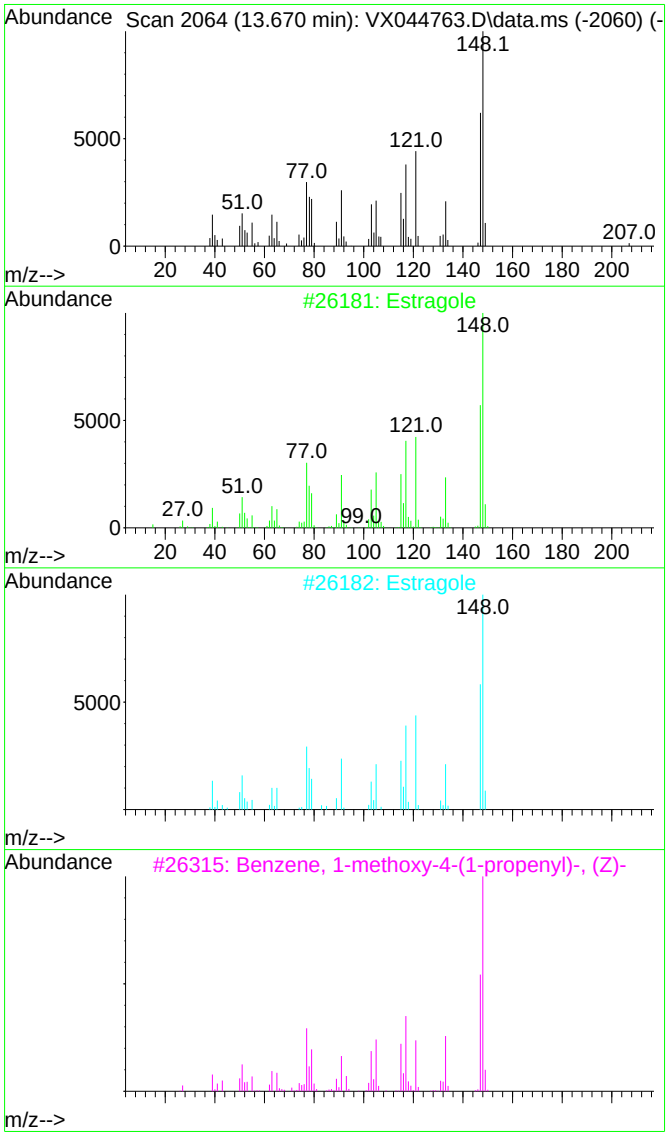
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM012825WMA.M
Quant Title : VOC Analysis

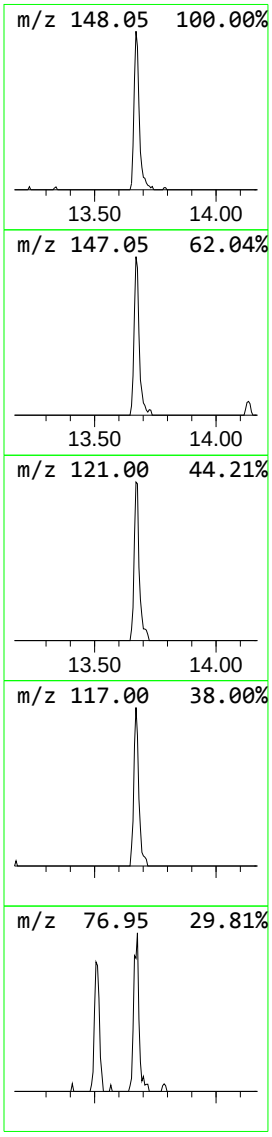
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Estragole Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.670	2.58 ug/L	39841	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Estragole	148	C10H12O	000140-67-0	98
2	Estragole	148	C10H12O	000140-67-0	98
3	Benzene, 1-methoxy-4-(1-propenyl...	148	C10H12O	025679-28-1	97
4	Estragole	148	C10H12O	000140-67-0	97
5	Estragole	148	C10H12O	000140-67-0	97





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012925\
Data File : VX044763.D
Acq On : 29 Jan 2025 12:34
Operator : JC/MD
Sample : Q1190-17ME
Misc : 5.65g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44T7ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM012825WMA.M
Quant Title : VOC Analysis

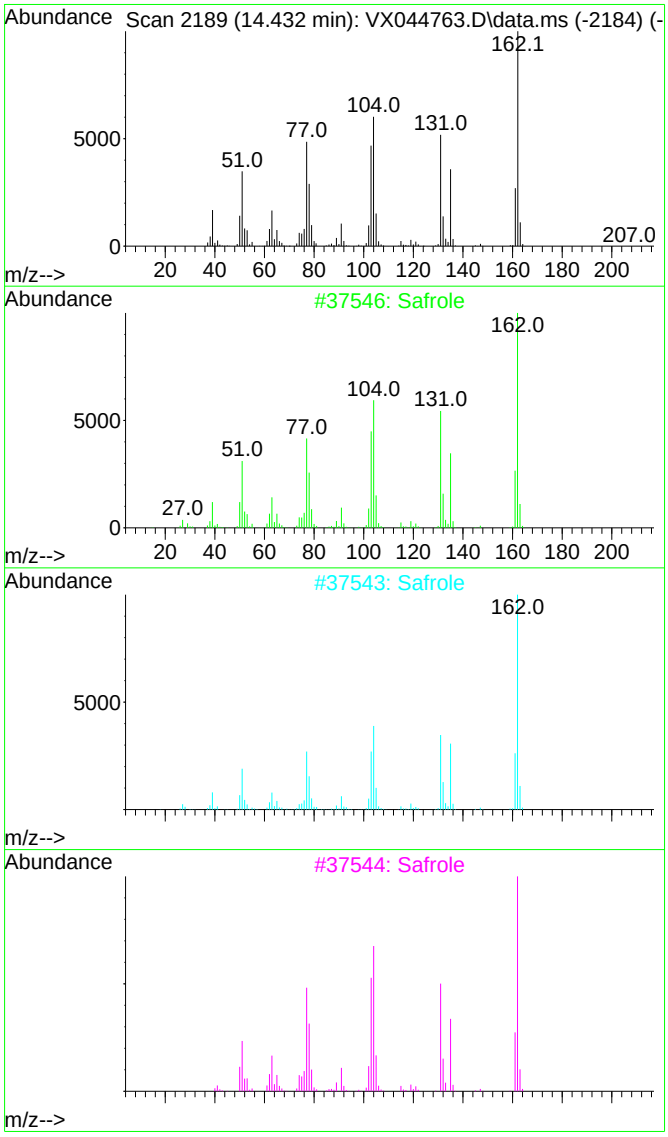
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

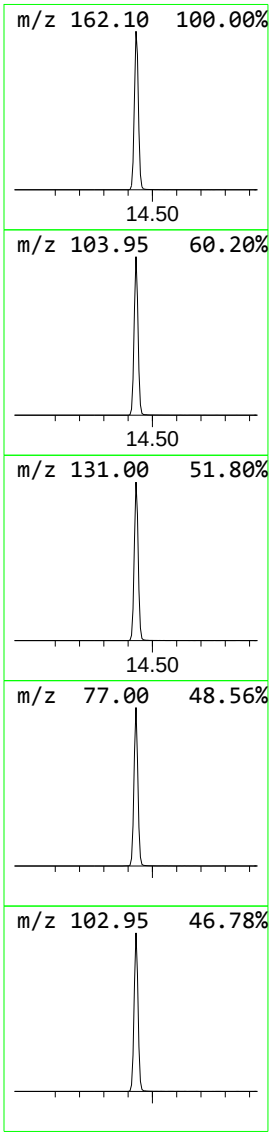
****

Peak Number 7 Safrole Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.432	278.82 ug/L	4304290	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Safrole	162	C10H10O2	000094-59-7	98
2	Safrole	162	C10H10O2	000094-59-7	98
3	Safrole	162	C10H10O2	000094-59-7	98
4	1,3-Benzodioxole, 5-(1-propenyl)-	162	C10H10O2	000120-58-1	97
5	Safrole	162	C10H10O2	000094-59-7	97





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012925\
Data File : VX044763.D
Acq On : 29 Jan 2025 12:34
Operator : JC/MD
Sample : Q1190-17ME
Misc : 5.65g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44T7ME

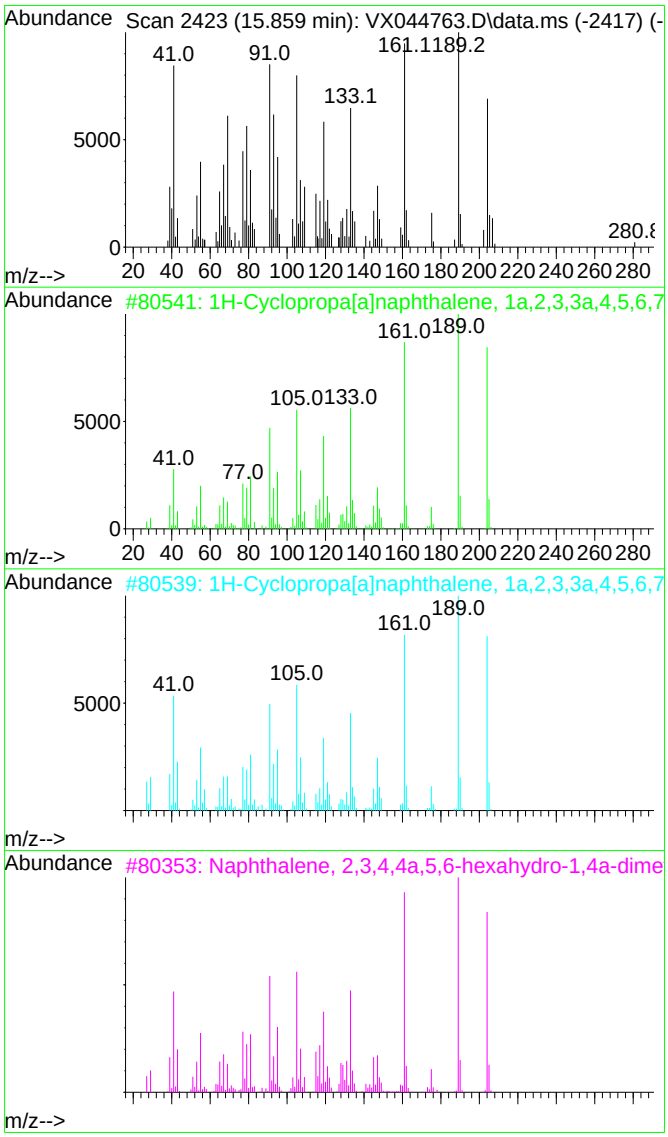
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM012825WMA.M
Quant Title : VOC Analysis

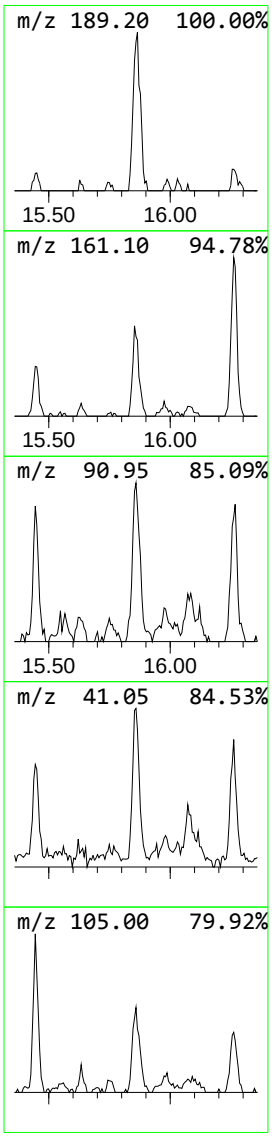
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1H-Cyclopropa[a]naphthalene... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.859	4.56 ug/L	70343	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	000489-29-2	98
2	1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	000489-29-2	97
3	Naphthalene, 2,3,4,4a,5,6-hexahy...	204	C15H24	000473-14-3	96
4	Naphthalene, 1,2,4a,5,8,8a-hexah...	204	C15H24	000523-47-7	96
5	Naphthalene, 1,2,4a,5,8,8a-hexah...	204	C15H24	005951-61-1	96





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012925\
Data File : VX044763.D
Acq On : 29 Jan 2025 12:34
Operator : JC/MD
Sample : Q1190-17ME
Misc : 5.65g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44T7ME

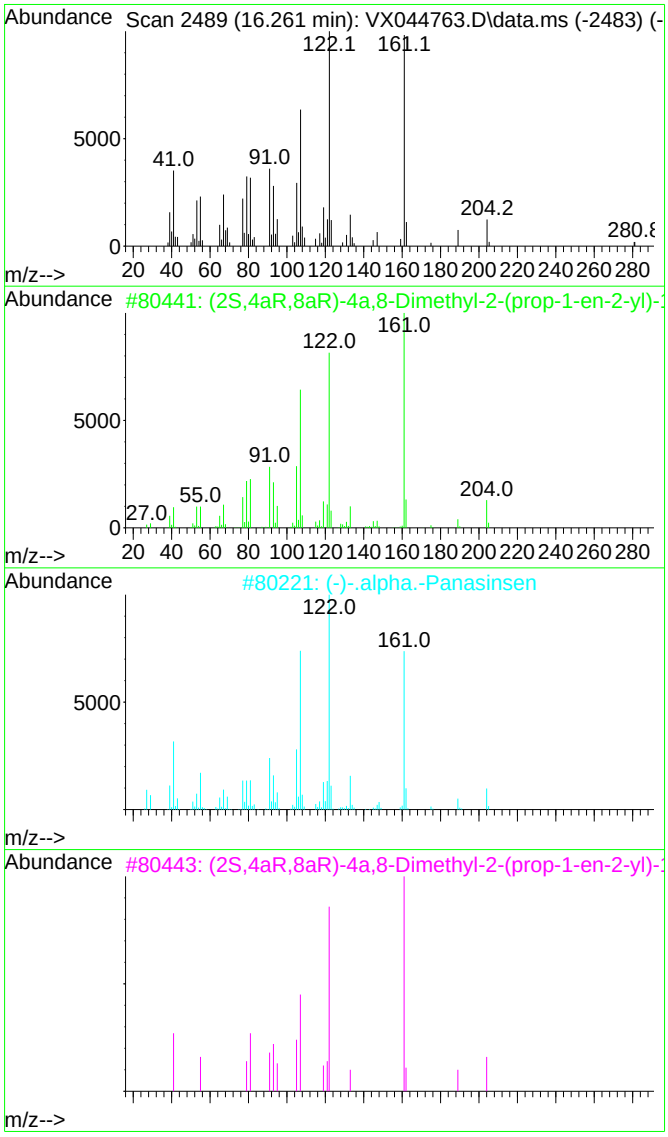
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM012825WMA.M
Quant Title : VOC Analysis

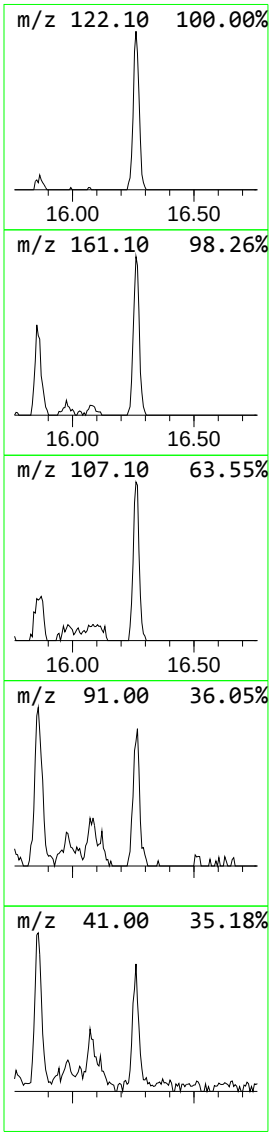
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 (2S,4aR,8aR)-4a,8-Dimethyl-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.261	3.61 ug/L	55668	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(2S,4aR,8aR)-4a,8-Dimethyl-2-(pr...	204	C15H24	123123-37-5	96
2	(-)-.alpha.-Panasinsen	204	C15H24	056633-28-4	96
3	(2S,4aR,8aR)-4a,8-Dimethyl-2-(pr...	204	C15H24	123123-37-5	96
4	.alpha.-Maaliene	204	C15H24	000489-28-1	91
5	cis-Muurola-4(15),5-diene	204	C15H24	157477-72-0	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012925\
Data File : VX044763.D
Acq On : 29 Jan 2025 12:34
Operator : JC/MD
Sample : Q1190-17ME
Misc : 5.65g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A44T7ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM012825WMA.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
.alpha.-Pinene	10.939	9.6	ug/L	153875	2	10.055	801637	50.0
Bicyclo[3.1.0]h...	11.488	7.4	ug/L	114753	3	12.024	771863	50.0
D-Limonene	11.969	5.5	ug/L	85100	3	12.024	771863	50.0
(+)-2-Bornanone	13.512	8.9	ug/L	138015	3	12.024	771863	50.0
Estragole	13.670	2.6	ug/L	39841	3	12.024	771863	50.0
Safrole	14.432	278.8	ug/L	4304290	3	12.024	771863	50.0
1H-Cyclopropa[a...	15.859	4.6	ug/L	70343	3	12.024	771863	50.0
(2S,4aR,8aR)-4a...	16.261	3.6	ug/L	55668	3	12.024	771863	50.0