

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121923\
 Data File : VX039355.D
 Acq On : 19 Dec 2023 14:48
 Operator : JC/MD
 Sample : 05835-20
 Misc : 3.06g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0B24ME

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\SFAMXML120523WMA.M
 Title : VOC Analysis

Signal : TIC: VX039355.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	43	47	65	rVB	68768	119850	14.20%	1.650%
2	1.648	89	92	100	rBV	23877	36851	4.36%	0.507%
3	2.288	191	197	211	rBV	180497	291963	34.58%	4.019%
4	2.715	261	267	276	rBV	22131	47170	5.59%	0.649%
5	2.843	285	288	295	rVB2	5136	9223	1.09%	0.127%
6	2.947	298	305	311	rVV	4185	8110	0.96%	0.112%
7	3.447	383	387	388	rBV	225	282	0.03%	0.004%
8	3.995	474	477	478	rBV2	281	288	0.03%	0.004%
9	4.038	482	484	488	rVB2	246	318	0.04%	0.004%
10	4.483	547	557	579	rBV	41830	194716	23.06%	2.680%
11	5.062	640	652	672	rBV2	101484	326698	38.70%	4.497%
12	5.513	724	726	731	rBV2	210	392	0.05%	0.005%
13	5.666	749	751	754	rBB2	220	287	0.03%	0.004%
14	5.964	789	800	817	rBV2	293163	844284	100.00%	11.622%
15	6.159	830	832	833	rBV2	228	244	0.03%	0.003%
16	6.281	851	852	857	rVB3	285	303	0.04%	0.004%
17	6.659	911	914	917	rBV2	262	433	0.05%	0.006%
18	6.757	921	930	949	rBV	197839	499182	59.12%	6.871%
19	7.117	984	989	994	rVB4	1359	2589	0.31%	0.036%
20	7.214	1001	1005	1007	rBV	287	473	0.06%	0.007%
21	7.232	1007	1008	1011	rVB	298	252	0.03%	0.003%
22	7.306	1011	1020	1038	rBV	165387	376958	44.65%	5.189%
23	7.482	1044	1049	1050	rBV2	497	593	0.07%	0.008%
24	8.324	1181	1187	1203	rBV	101391	184248	21.82%	2.536%
25	8.458	1208	1209	1213	rVB3	290	296	0.04%	0.004%
26	8.586	1227	1230	1231	rBV2	214	239	0.03%	0.003%
27	8.647	1234	1240	1256	rBV	413268	656340	77.74%	9.035%
28	8.952	1284	1290	1304	rBV	71660	119317	14.13%	1.642%
29	9.397	1357	1363	1375	rBV	238145	447995	53.06%	6.167%
30	9.671	1407	1408	1411	rVB3	353	347	0.04%	0.005%
31	9.714	1411	1415	1419	rBV3	681	1037	0.12%	0.014%
32	9.897	1442	1445	1447	rBV2	223	300	0.04%	0.004%
33	9.945	1451	1453	1455	rBV2	230	237	0.03%	0.003%
34	10.055	1465	1471	1483	rBV	414090	609929	72.24%	8.396%
35	10.208	1492	1496	1500	rVB2	532	635	0.08%	0.009%
36	10.311	1509	1513	1516	rBV3	426	626	0.07%	0.009%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120523WMA.M
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37	10.646	1565	1568	1576	rBV2	489	777	0.09%	0.011%
38	10.774	1587	1589	1594	rBV2	214	250	0.03%	0.003%
39	10.835	1594	1599	1601	rBV2	694	1029	0.12%	0.014%
40	10.939	1611	1616	1625	rVB	50144	72319	8.57%	0.996%
41	11.140	1643	1649	1652	rVV	35671	51912	6.15%	0.715%
42	11.195	1653	1658	1669	rVB	289390	379432	44.94%	5.223%
43	11.488	1698	1706	1720	rVB	112900	163886	19.41%	2.256%
44	11.701	1738	1741	1742	rVV2	2601	2873	0.34%	0.040%
45	11.732	1742	1746	1748	rVV3	8128	11995	1.42%	0.165%
46	11.774	1748	1753	1763	rVV	110618	149322	17.69%	2.055%
47	11.854	1763	1766	1771	rVV5	1781	3167	0.38%	0.044%
48	11.933	1775	1779	1781	rVV2	3107	3786	0.45%	0.052%
49	11.969	1781	1785	1788	rVV2	27486	36978	4.38%	0.509%
50	12.024	1788	1794	1803	rVV	485787	686703	81.34%	9.453%
51	12.104	1803	1807	1811	rVB4	3041	3930	0.47%	0.054%
52	12.238	1825	1829	1832	rVV6	1392	1831	0.22%	0.025%
53	12.323	1837	1843	1855	rVV	415847	562313	66.60%	7.740%
54	12.494	1868	1871	1873	rVV3	2918	3355	0.40%	0.046%
55	12.524	1873	1876	1880	rVB4	4251	5488	0.65%	0.076%
56	12.597	1885	1888	1890	rBV3	599	716	0.08%	0.010%
57	12.670	1896	1900	1905	rVB3	2159	3077	0.36%	0.042%
58	12.762	1910	1915	1920	rVV2	1623	2081	0.25%	0.029%
59	12.817	1923	1924	1927	rBV2	380	334	0.04%	0.005%
60	12.872	1930	1933	1938	rVV3	1216	1678	0.20%	0.023%
61	13.036	1958	1960	1964	rVB2	252	331	0.04%	0.005%
62	13.292	1999	2002	2004	rBV2	237	303	0.04%	0.004%
63	13.402	2016	2020	2025	rBV2	8940	10582	1.25%	0.146%
64	13.463	2028	2030	2034	rVB2	527	651	0.08%	0.009%
65	13.585	2045	2050	2058	rVB2	8273	11507	1.36%	0.158%
66	13.676	2063	2065	2071	rBV2	445	689	0.08%	0.009%
67	13.780	2078	2082	2086	rBV2	608	800	0.09%	0.011%
68	13.829	2086	2090	2093	rVB2	574	782	0.09%	0.011%
69	13.871	2093	2097	2098	rBV	264	271	0.03%	0.004%
70	13.932	2102	2107	2108	rBV	740	999	0.12%	0.014%
71	13.957	2108	2111	2117	rVB4	3248	4573	0.54%	0.063%
72	14.128	2136	2139	2145	rVB	1935	2772	0.33%	0.038%
73	14.426	2184	2188	2192	rBV3	1140	1823	0.22%	0.025%
74	14.524	2202	2204	2208	rVB	275	264	0.03%	0.004%
75	14.573	2211	2212	2215	rBV3	266	266	0.03%	0.004%
76	14.676	2226	2229	2233	rVB2	2995	3547	0.42%	0.049%

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 Title : VOC Analysis

77	14.786	2245	2247	2251	rBV3	487	586	0.07%	0.008%
78	14.926	2265	2270	2277	rVB2	40361	62049	7.35%	0.854%
79	14.993	2280	2281	2285	rBV	299	348	0.04%	0.005%
80	15.048	2285	2290	2295	rVB3	11414	15189	1.80%	0.209%
81	15.127	2299	2303	2308	rBV4	3414	4032	0.48%	0.056%
82	15.176	2308	2311	2315	rBV3	454	595	0.07%	0.008%
83	15.255	2320	2324	2326	rVV3	1298	2047	0.24%	0.028%
84	15.286	2326	2329	2331	rVV4	2671	3646	0.43%	0.050%
85	15.316	2331	2334	2338	rVV3	5217	6708	0.79%	0.092%
86	15.353	2338	2340	2342	rVV	379	243	0.03%	0.003%
87	15.414	2342	2350	2357	rVB5	7583	14678	1.74%	0.202%
88	15.548	2367	2372	2381	rBV8	3252	8231	0.97%	0.113%
89	15.737	2394	2403	2413	rVB8	8356	18716	2.22%	0.258%
90	15.816	2413	2416	2417	rBV2	405	484	0.06%	0.007%
91	15.853	2417	2422	2426	rVV4	9066	14537	1.72%	0.200%
92	15.908	2426	2431	2437	rVB3	27486	44970	5.33%	0.619%
93	15.981	2438	2443	2446	rVV4	14954	24581	2.91%	0.338%
94	16.024	2447	2450	2456	rVB3	21374	33580	3.98%	0.462%
95	16.091	2456	2461	2471	rVB6	8633	17574	2.08%	0.242%
96	16.176	2473	2475	2477	rBV3	811	921	0.11%	0.013%
97	16.261	2484	2489	2497	rVB6	5820	11227	1.33%	0.155%
98	16.395	2506	2511	2517	rBV5	3656	6394	0.76%	0.088%
99	16.475	2520	2524	2526	rVV3	441	540	0.06%	0.007%
100	16.609	2544	2546	2549	rBV2	301	312	0.04%	0.004%

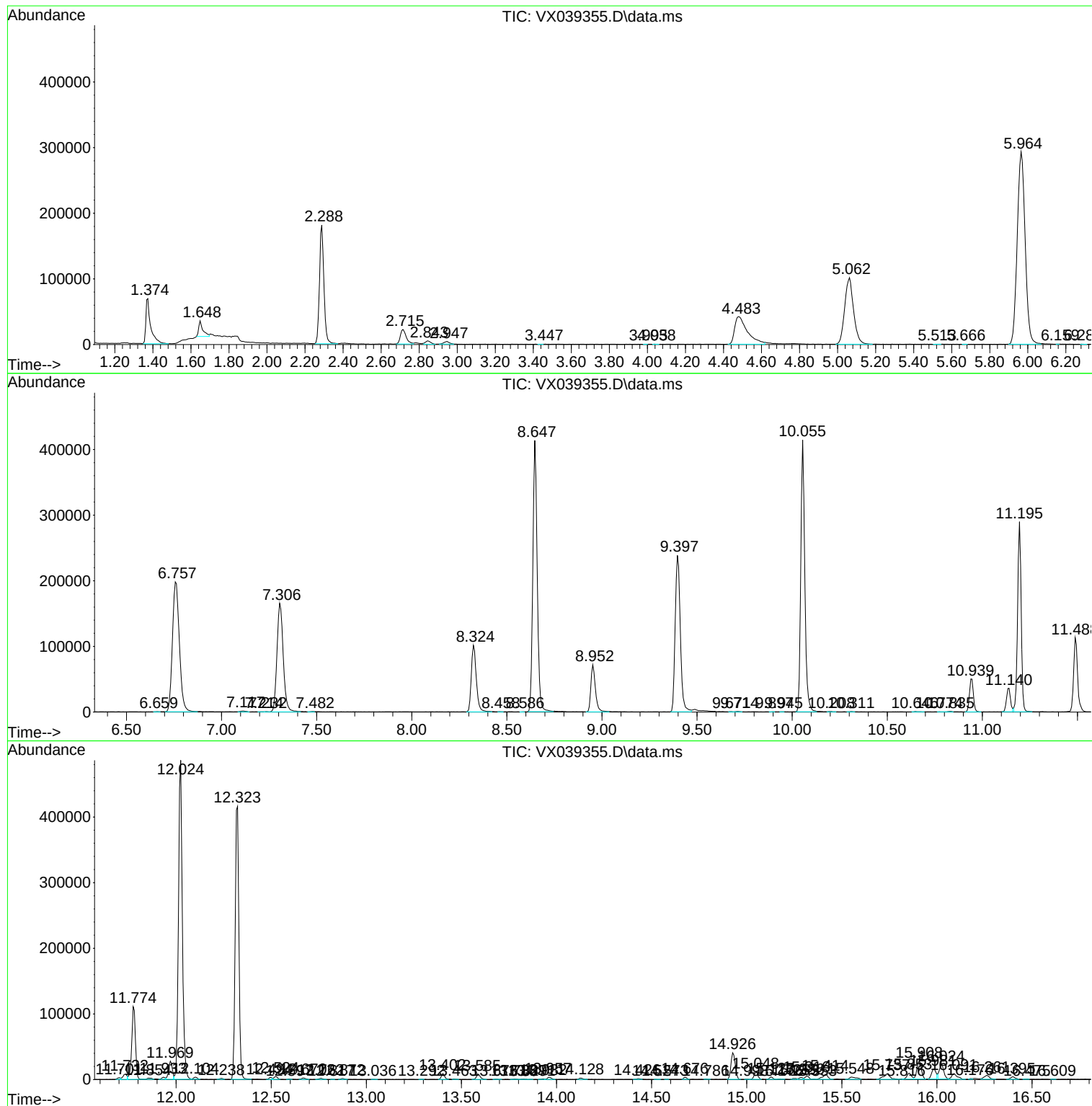
Sum of corrected areas: 7264585

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Instrument :
MSVOA_X
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_X
ClientSampleId :
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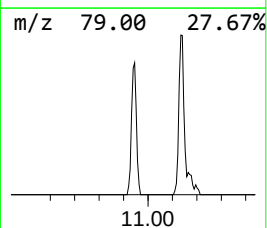
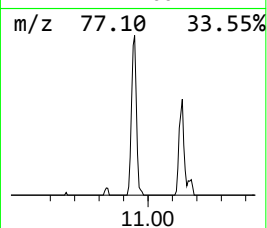
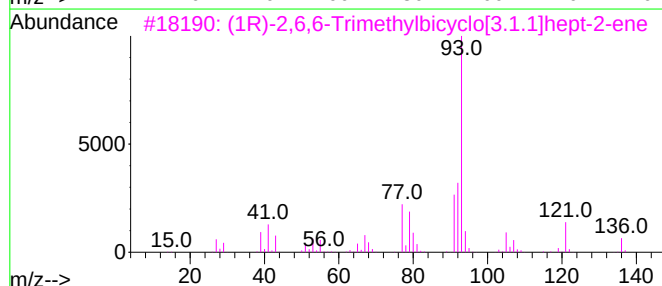
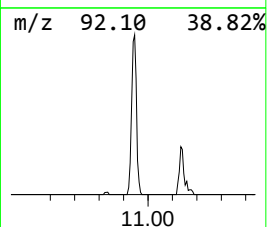
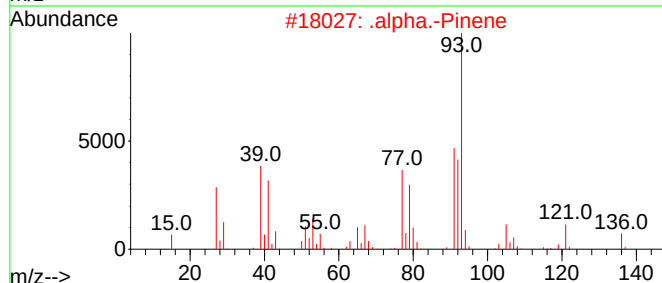
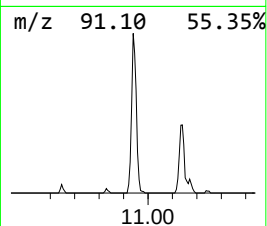
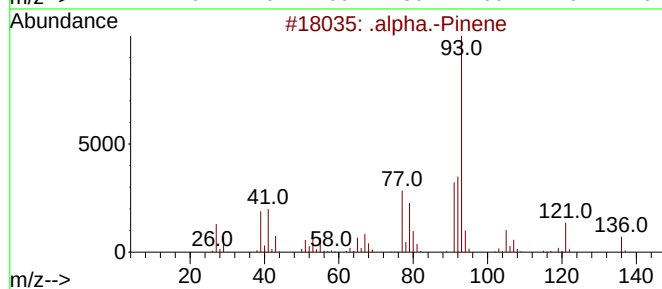
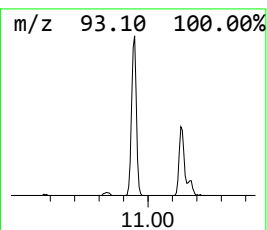
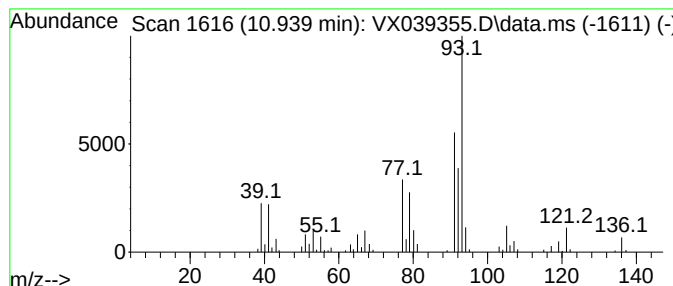
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 .alpha.-Pinene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.939	5.93 ug/L	72319	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.		.alpha.-Pinene	136	C10H16	000080-56-8	97
2	.		.alpha.-Pinene	136	C10H16	000080-56-8	95
3	(1R)-2,6,6-Trimethylbicyclo[3.1....			136	C10H16	007785-70-8	94
4	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...			136	C10H16	004889-83-2	91
5	.		.alpha.-Pinene	136	C10H16	000080-56-8	90



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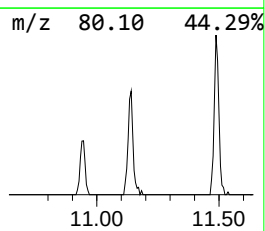
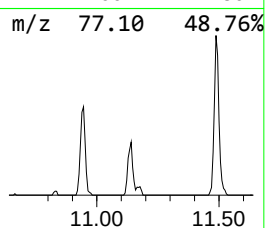
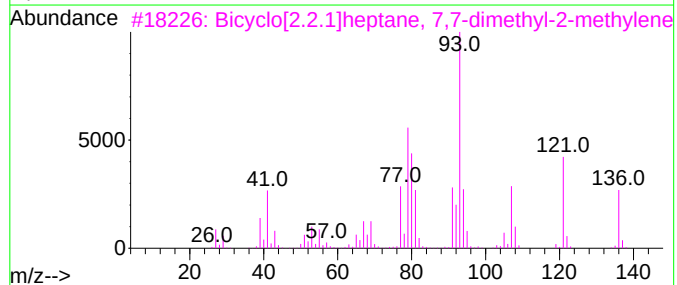
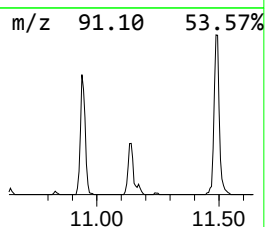
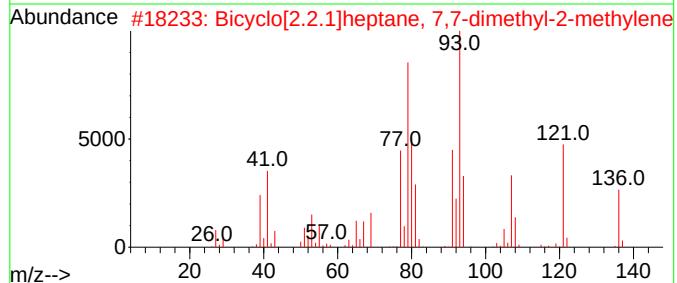
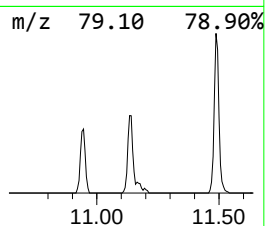
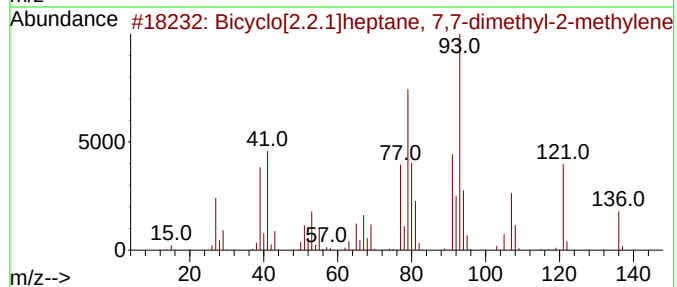
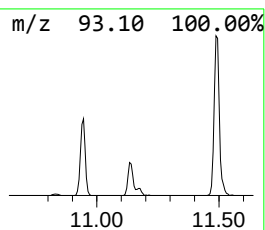
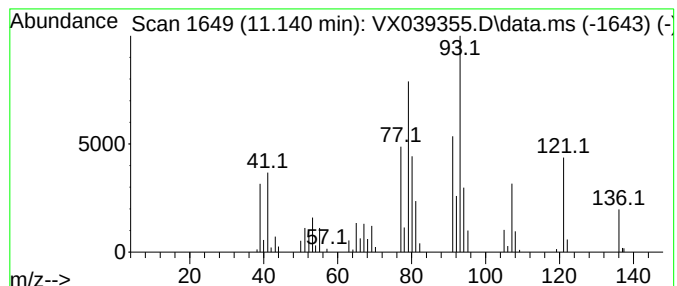
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Bicyclo[2.2.1]heptane, 7,7-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.140	3.78 ug/L	51912	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[2.2.1]heptane, 7,7-dimet...	136	C10H16	000471-84-1	98
2			Bicyclo[2.2.1]heptane, 7,7-dimet...	136	C10H16	000471-84-1	96
3			Bicyclo[2.2.1]heptane, 7,7-dimet...	136	C10H16	000471-84-1	93
4			Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	005794-03-6	91
5			Bicyclo[2.2.1]heptane, 7,7-dimet...	136	C10H16	000471-84-1	90



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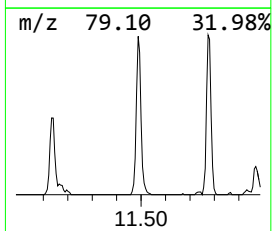
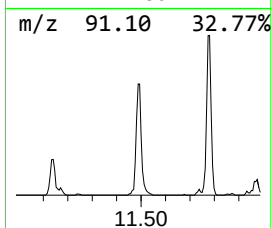
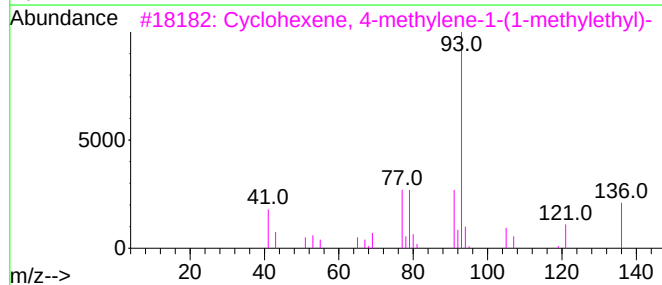
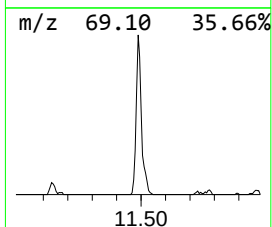
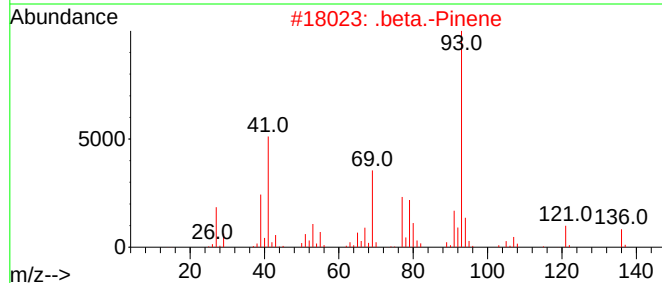
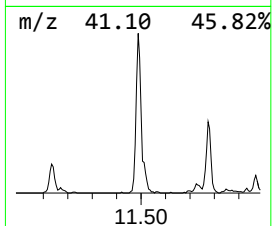
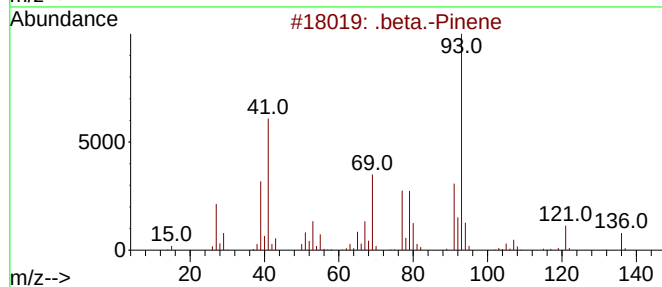
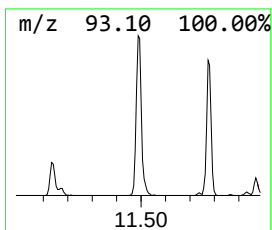
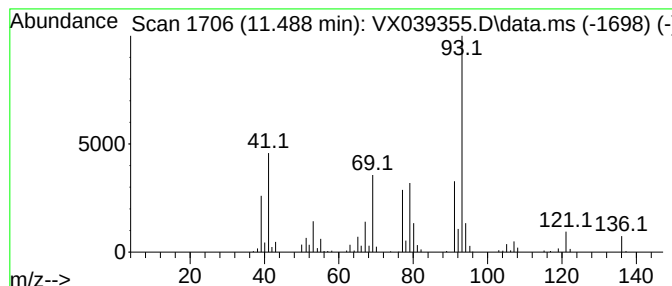
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 .beta.-Pinene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.488	11.93 ug/L	163886	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.beta.-Pinene	136	C10H16	000127-91-3	91
2			.beta.-Pinene	136	C10H16	000127-91-3	91
3			Cyclohexene, 4-methylene-1-(1-me...	136	C10H16	000099-84-3	91
4			.alpha.-Pinene	136	C10H16	000080-56-8	87
5			.beta.-Pinene	136	C10H16	000127-91-3	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121923\
Data File : VX039355.D
Acq On : 19 Dec 2023 14:48
Operator : JC/MD
Sample : 05835-20
Misc : 3.06g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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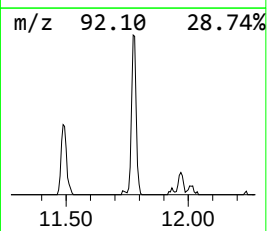
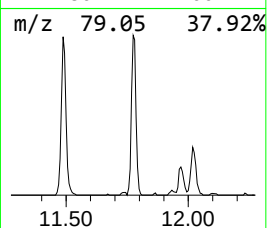
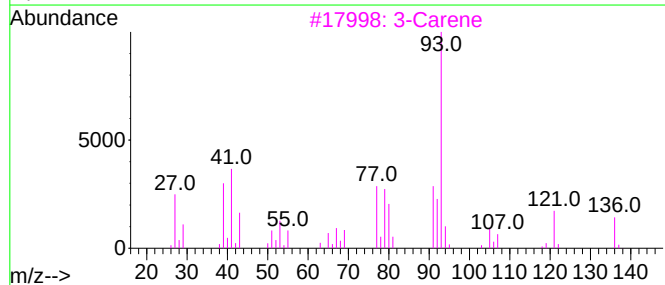
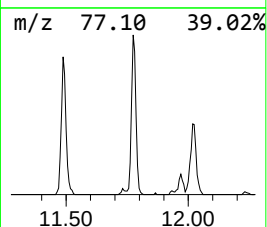
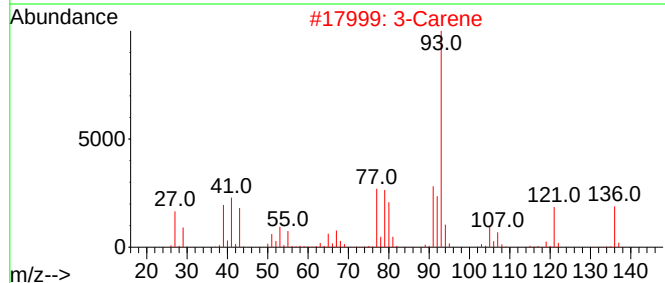
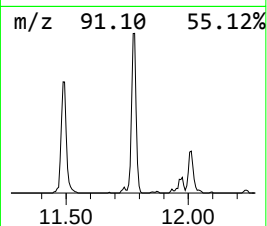
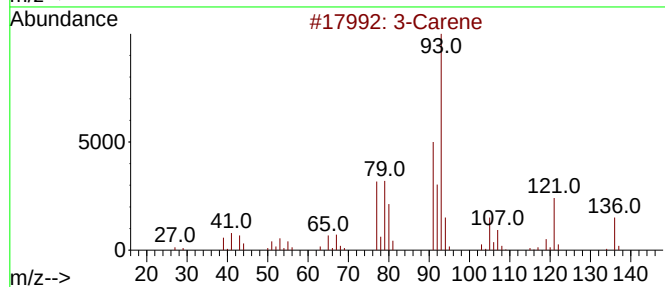
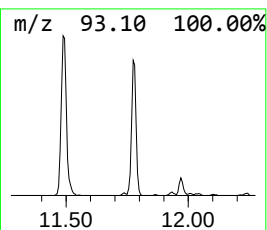
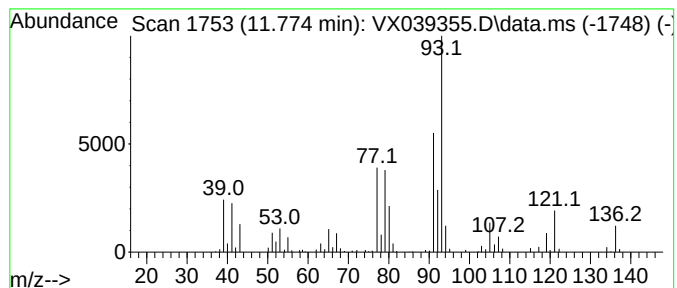
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Quant Title : VOC Analysis

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

Peak Number 5 3-Carene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.774	10.87 ug/L	149322	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Carene	136	C10H16	013466-78-9	95
2			3-Carene	136	C10H16	013466-78-9	95
3			3-Carene	136	C10H16	013466-78-9	94
4			(1R)-2,6,6-Trimethylbicyclo[3.1...	136	C10H16	007785-70-8	91
5			Cyclopropane, 1,1-dimethyl-2-(3-...	136	C10H16	068998-21-0	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121923\
Data File : VX039355.D
Acq On : 19 Dec 2023 14:48
Operator : JC/MD
Sample : 05835-20
Misc : 3.06g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0B24ME

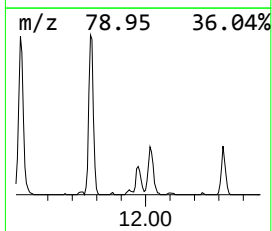
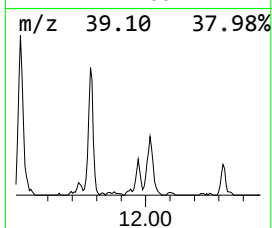
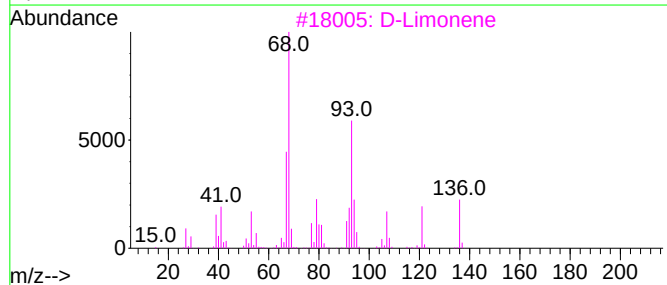
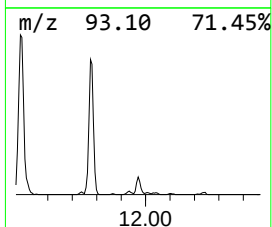
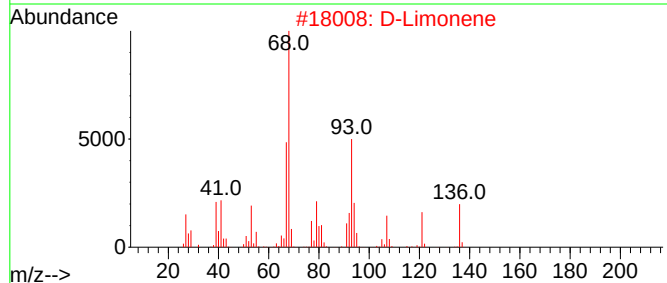
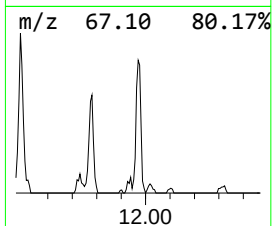
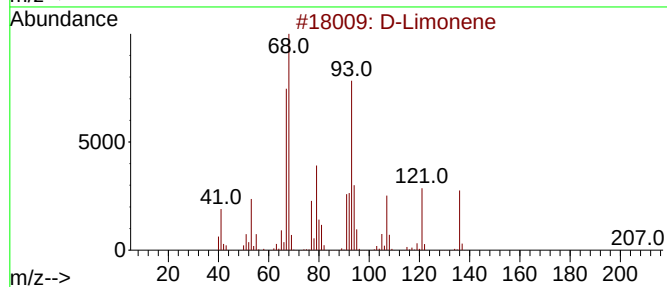
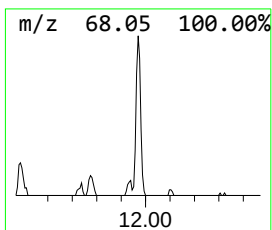
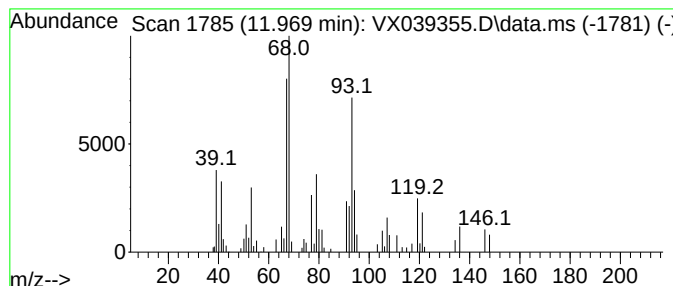
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Quant Title : VOC Analysis

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

Peak Number 6 D-Limonene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.969	2.69 ug/L	36978	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	93
3			D-Limonene	136	C10H16	005989-27-5	93
4			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	005989-54-8	93
5			Cyclohexene, 1-methyl-5-(1-methy...	136	C10H16	013898-73-2	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121923\
Data File : VX039355.D
Acq On : 19 Dec 2023 14:48
Operator : JC/MD
Sample : 05835-20
Misc : 3.06g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0B24ME

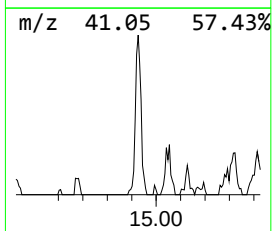
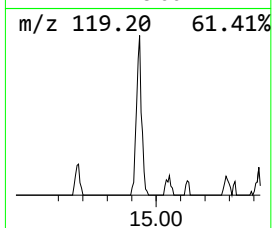
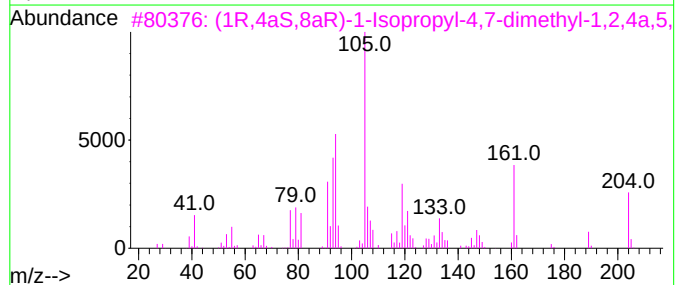
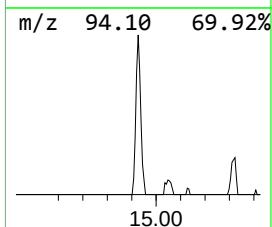
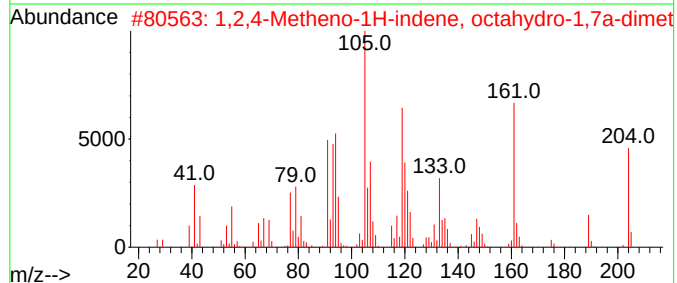
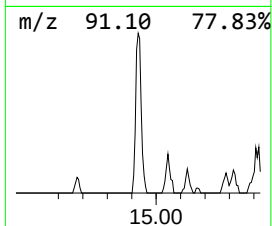
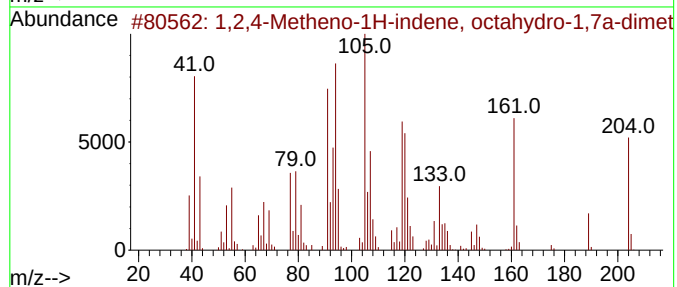
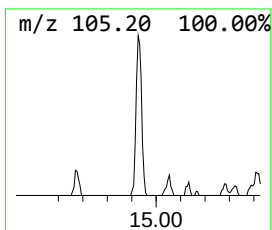
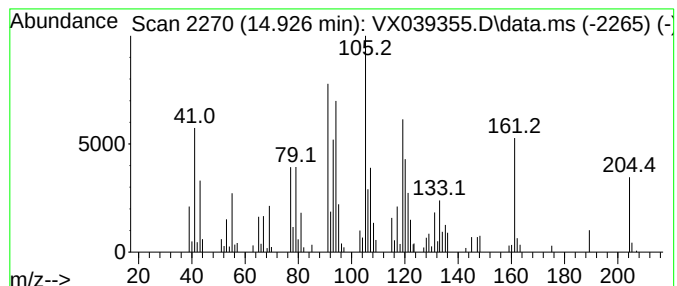
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Quant Title : VOC Analysis

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

Peak Number 7 1,2,4-Metheno-1H-indene, oc... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.926	4.52 ug/L	62049	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2,4-Metheno-1H-indene, octahyd...	204	C15H24	022469-52-9	95
2			1,2,4-Metheno-1H-indene, octahyd...	204	C15H24	022469-52-9	94
3			(1R,4aS,8aR)-1-Isopropyl-4,7-dim...	204	C15H24	020085-19-2	78
4			Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	010219-75-7	70
5			Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121923\
Data File : VX039355.D
Acq On : 19 Dec 2023 14:48
Operator : JC/MD
Sample : 05835-20
Misc : 3.06g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0B24ME

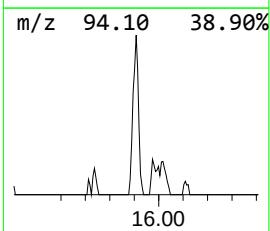
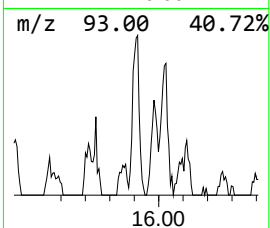
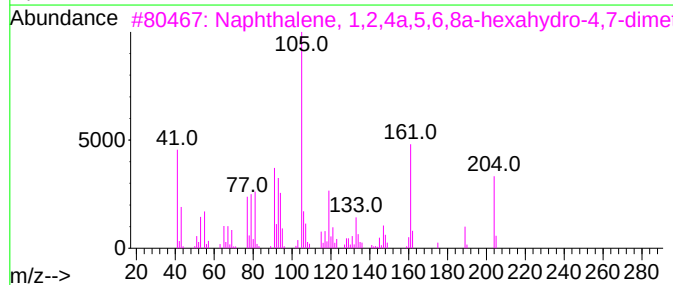
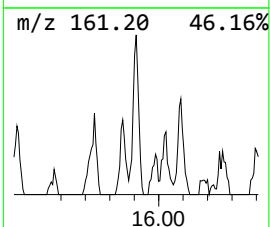
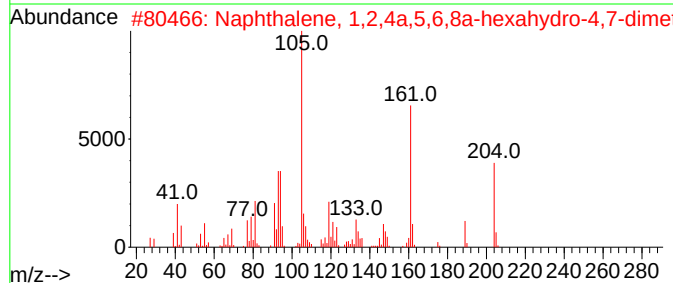
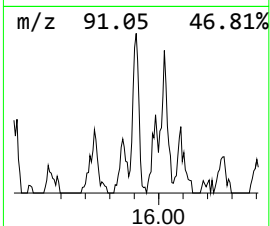
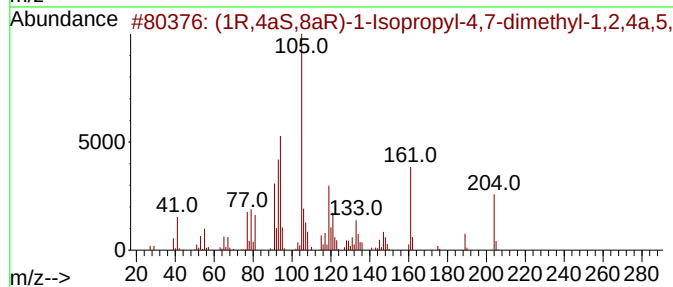
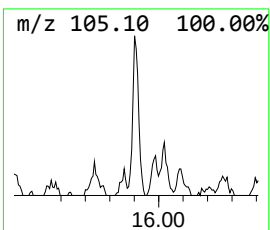
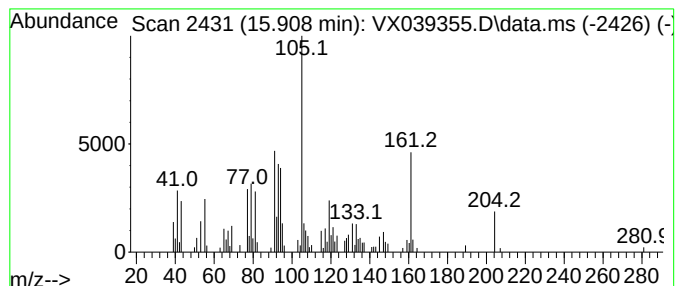
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Quant Title : VOC Analysis

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

Peak Number 8 (1R,4aS,8aR)-1-Isopropyl-4,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.908	3.27 ug/L	44970	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(1R,4aS,8aR)-1-Isopropyl-4,7-dim...	204	C15H24	020085-19-2	93
2			Naphthalene, 1,2,4a,5,6,8a-hexah...	204	C15H24	031983-22-9	93
3			Naphthalene, 1,2,4a,5,6,8a-hexah...	204	C15H24	031983-22-9	90
4			.alpha.-Muurolene	204	C15H24	010208-80-7	83
5			.alpha.-Muurolene	204	C15H24	010208-80-7	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121923\
Data File : VX039355.D
Acq On : 19 Dec 2023 14:48
Operator : JC/MD
Sample : 05835-20
Misc : 3.06g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0B24ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120523WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
.alpha.-Pinene	10.939	5.9	ug/L	72319	2	10.055	609929	50.0
Bicyclo[2.2.1]h...	11.140	3.8	ug/L	51912	3	12.024	686703	50.0
.beta.-Pinene	11.488	11.9	ug/L	163886	3	12.024	686703	50.0
3-Carene	11.774	10.9	ug/L	149322	3	12.024	686703	50.0
D-Limonene	11.969	2.7	ug/L	36978	3	12.024	686703	50.0
1,2,4-Metheno-1...	14.926	4.5	ug/L	62049	3	12.024	686703	50.0
(1R,4aS,8aR)-1-...	15.908	3.3	ug/L	44970	3	12.024	686703	50.0