

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122123\
 Data File : VX039425.D
 Acq On : 21 Dec 2023 13:33
 Operator : JC/MD
 Sample : 05835-20ME
 Misc : 3.06g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 12 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\SFAMXLM120523WMA.M
 Title : VOC Analysis

Signal : TIC: VX039425.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.368	43	46	60	rBV	74399	126731	11.57%	1.420%
2	1.648	89	92	99	rBV	25332	39047	3.56%	0.438%
3	2.288	191	197	209	rBV	199299	332704	30.37%	3.728%
4	2.715	260	267	276	rBV	22831	47491	4.33%	0.532%
5	2.849	284	289	295	rVB	4813	9154	0.84%	0.103%
6	2.947	298	305	315	rVV	6861	17419	1.59%	0.195%
7	3.093	327	329	330	rBV2	428	269	0.02%	0.003%
8	3.123	330	334	337	rVB4	413	557	0.05%	0.006%
9	3.434	381	385	387	rBV	237	343	0.03%	0.004%
10	3.605	408	413	415	rBV2	297	541	0.05%	0.006%
11	4.379	538	540	543	rBV2	274	343	0.03%	0.004%
12	4.477	547	556	585	rBV2	61470	288461	26.33%	3.233%
13	5.056	637	651	673	rBV	128381	430299	39.27%	4.822%
14	5.312	692	693	697	rBV2	309	271	0.02%	0.003%
15	5.544	729	731	734	rVV3	383	395	0.04%	0.004%
16	5.964	788	800	825	rBV2	374178	1095645	100.00%	12.278%
17	6.672	911	916	917	rBV2	387	435	0.04%	0.005%
18	6.757	921	930	947	rBV	210035	523926	47.82%	5.871%
19	7.111	980	988	995	rBV5	1729	4444	0.41%	0.050%
20	7.306	1011	1020	1040	rBV	223209	506529	46.23%	5.676%
21	7.489	1047	1050	1053	rBV4	451	581	0.05%	0.007%
22	7.824	1103	1105	1109	rVB2	208	274	0.03%	0.003%
23	7.958	1125	1127	1129	rVV	434	452	0.04%	0.005%
24	8.055	1142	1143	1147	rBV2	360	431	0.04%	0.005%
25	8.226	1166	1171	1174	rBV2	233	483	0.04%	0.005%
26	8.263	1174	1177	1181	rVB3	406	579	0.05%	0.006%
27	8.324	1181	1187	1204	rBV	137879	239644	21.87%	2.685%
28	8.501	1215	1216	1218	rBV2	431	339	0.03%	0.004%
29	8.647	1233	1240	1249	rBV	510942	832125	75.95%	9.325%
30	8.952	1284	1290	1309	rBV	97343	158626	14.48%	1.778%
31	9.165	1321	1325	1327	rBV	428	555	0.05%	0.006%
32	9.244	1334	1338	1340	rBV2	295	367	0.03%	0.004%
33	9.281	1340	1344	1346	rBV2	645	580	0.05%	0.006%
34	9.397	1356	1363	1375	rBV	337645	653425	59.64%	7.322%
35	9.714	1412	1415	1421	rBV4	1012	1327	0.12%	0.015%
36	10.055	1465	1471	1488	rBV	431332	646929	59.05%	7.250%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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

37	10.317	1511	1514	1518	rBV3	729	870	0.08%	0.010%
38	10.579	1555	1557	1561	rVB2	197	262	0.02%	0.003%
39	10.646	1564	1568	1569	rBV	582	428	0.04%	0.005%
40	10.829	1592	1598	1601	rVB3	735	1066	0.10%	0.012%
41	10.878	1604	1606	1611	rBV2	254	401	0.04%	0.004%
42	10.945	1611	1617	1624	rBV	55080	77161	7.04%	0.865%
43	11.085	1638	1640	1643	rBV2	202	256	0.02%	0.003%
44	11.134	1643	1648	1652	rVV	37426	54761	5.00%	0.614%
45	11.195	1653	1658	1668	rVV	425803	546557	49.88%	6.125%
46	11.311	1674	1677	1681	rVV2	1461	1832	0.17%	0.021%
47	11.488	1698	1706	1716	rVV	121087	176390	16.10%	1.977%
48	11.701	1737	1741	1742	rBV2	2543	2886	0.26%	0.032%
49	11.732	1743	1746	1748	rVV3	8269	11226	1.02%	0.126%
50	11.774	1749	1753	1762	rVB	117378	157123	14.34%	1.761%
51	11.860	1764	1767	1771	rVB5	1280	1794	0.16%	0.020%
52	11.939	1776	1780	1781	rVV3	2835	4017	0.37%	0.045%
53	11.969	1781	1785	1788	rVV	31383	40074	3.66%	0.449%
54	12.024	1788	1794	1803	rVV	531142	733434	66.94%	8.219%
55	12.104	1803	1807	1813	rVB7	3151	4511	0.41%	0.051%
56	12.232	1825	1828	1832	rVB4	860	1036	0.09%	0.012%
57	12.323	1837	1843	1860	rVV	584645	773799	70.62%	8.671%
58	12.500	1868	1872	1874	rBV2	2997	4138	0.38%	0.046%
59	12.524	1874	1876	1882	rVB2	4283	4254	0.39%	0.048%
60	12.591	1886	1887	1891	rVB2	639	629	0.06%	0.007%
61	12.671	1896	1900	1904	rVB4	2054	2884	0.26%	0.032%
62	12.762	1910	1915	1919	rBV2	5625	7903	0.72%	0.089%
63	12.823	1922	1925	1928	rBV3	448	495	0.05%	0.006%
64	12.878	1928	1934	1937	rBV4	1363	1895	0.17%	0.021%
65	13.036	1955	1960	1965	rVB2	384	748	0.07%	0.008%
66	13.073	1965	1966	1968	rBV2	292	266	0.02%	0.003%
67	13.402	2015	2020	2027	rVB	8223	10170	0.93%	0.114%
68	13.457	2027	2029	2033	rVV3	435	508	0.05%	0.006%
69	13.591	2046	2051	2058	rVB2	11025	14858	1.36%	0.167%
70	13.689	2064	2067	2069	rBV	435	445	0.04%	0.005%
71	13.737	2073	2075	2077	rVB	328	272	0.02%	0.003%
72	13.774	2079	2081	2086	rVV2	622	813	0.07%	0.009%
73	13.835	2087	2091	2093	rVV3	496	585	0.05%	0.007%
74	13.926	2103	2106	2108	rBV3	970	957	0.09%	0.011%
75	13.963	2108	2112	2117	rVB4	4567	5701	0.52%	0.064%
76	14.128	2131	2139	2145	rBV2	7483	10205	0.93%	0.114%

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Integrator: RTE

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

77	14.426	2185	2188	2193	rVV2	1019	1586	0.14%	0.018%
78	14.676	2225	2229	2233	rVB2	5508	5858	0.53%	0.066%
79	14.786	2244	2247	2249	rBV2	564	621	0.06%	0.007%
80	14.859	2256	2259	2262	rVB2	329	410	0.04%	0.005%
81	14.926	2265	2270	2276	rVV	45326	66197	6.04%	0.742%
82	15.048	2286	2290	2296	rVB2	12328	16262	1.48%	0.182%
83	15.127	2299	2303	2306	rBV4	3751	5054	0.46%	0.057%
84	15.249	2319	2323	2325	rVV4	2397	3443	0.31%	0.039%
85	15.292	2326	2330	2331	rVV3	2989	4438	0.41%	0.050%
86	15.316	2331	2334	2339	rVV4	5074	7401	0.68%	0.083%
87	15.414	2341	2350	2355	rVB5	9496	17669	1.61%	0.198%
88	15.548	2368	2372	2375	rBV3	3477	5866	0.54%	0.066%
89	15.676	2392	2393	2395	rBV2	273	262	0.02%	0.003%
90	15.737	2395	2403	2414	rVB9	8093	19647	1.79%	0.220%
91	15.810	2414	2415	2417	rBV2	395	318	0.03%	0.004%
92	15.853	2417	2422	2426	rBV4	9426	15020	1.37%	0.168%
93	15.908	2426	2431	2437	rVB	28280	45107	4.12%	0.505%
94	15.981	2438	2443	2446	rBV4	15058	24209	2.21%	0.271%
95	16.024	2447	2450	2456	rVB2	20964	32295	2.95%	0.362%
96	16.091	2456	2461	2464	rBV3	8666	12484	1.14%	0.140%
97	16.182	2471	2476	2477	rBV4	1032	1254	0.11%	0.014%
98	16.261	2483	2489	2495	rVB7	5620	11248	1.03%	0.126%
99	16.402	2507	2512	2517	rVB5	3969	6477	0.59%	0.073%
100	16.463	2517	2522	2525	rBV4	643	1182	0.11%	0.013%

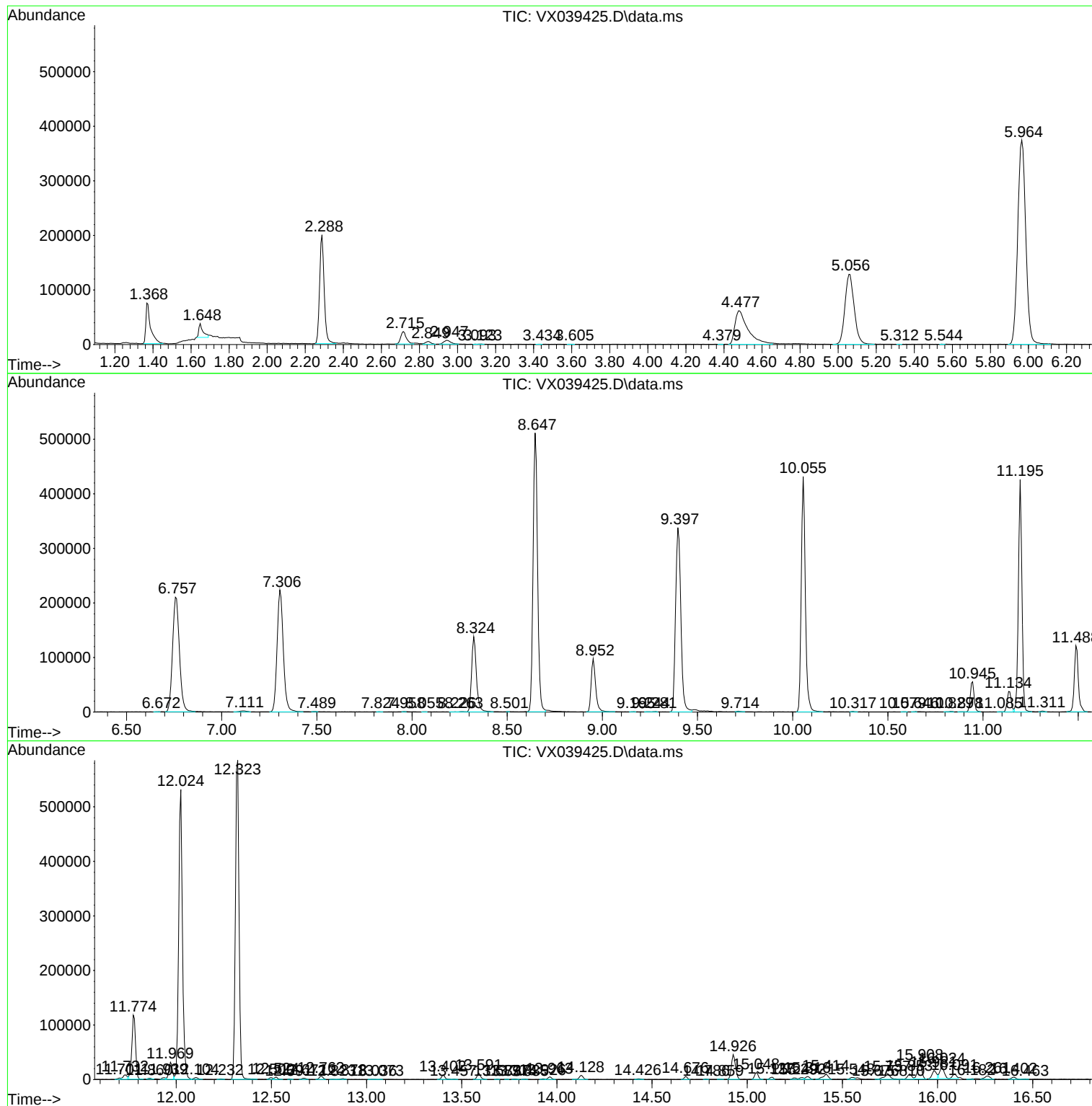
Sum of corrected areas: 8923639

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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COB24ME

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

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



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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0B24ME

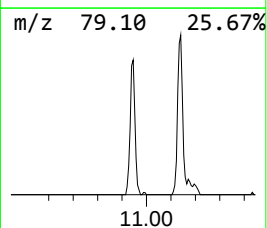
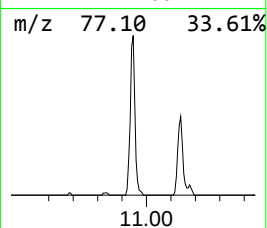
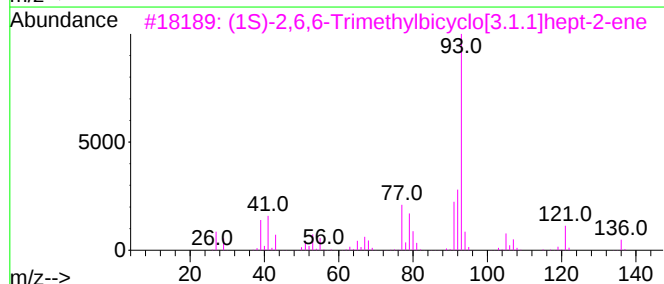
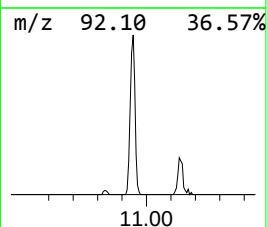
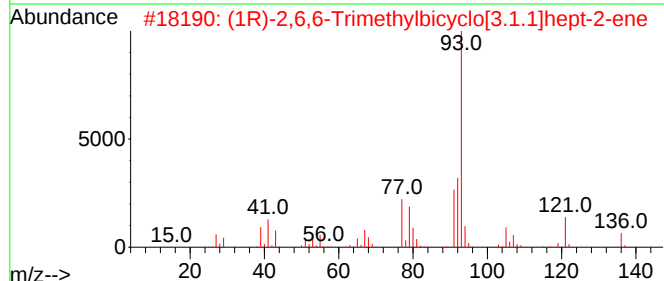
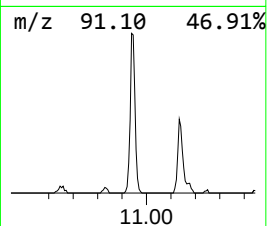
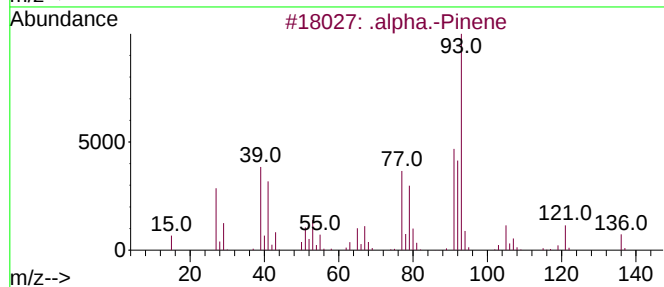
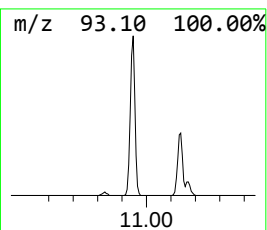
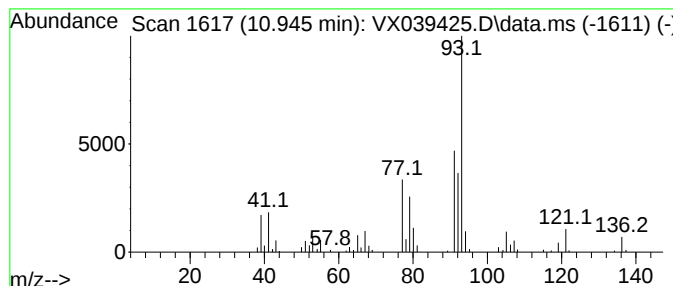
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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.
10.945	5.96 ug/L	77161	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.alpha.-Pinene	136	C10H16	000080-56-8	95
2			(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-70-8	94
3			(1S)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-26-4	91
4			Bicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-	136	C10H16	004889-83-2	91
5			(+)-3-Carene	136	C10H16	000498-15-7	91



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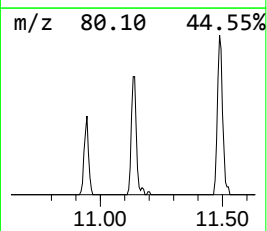
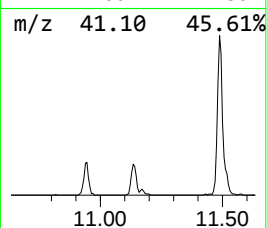
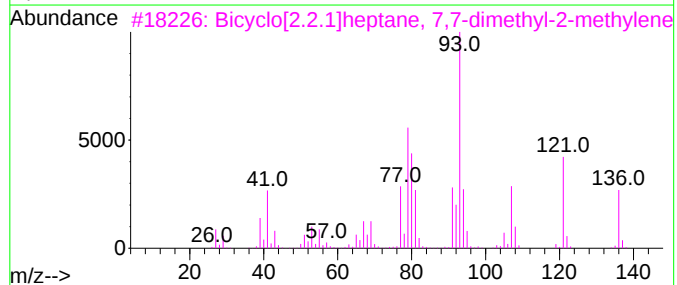
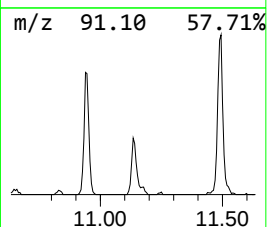
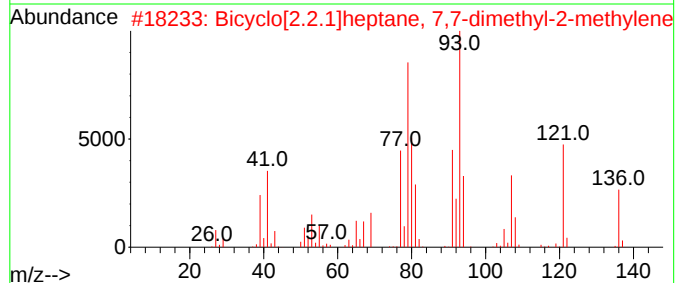
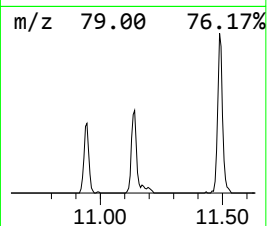
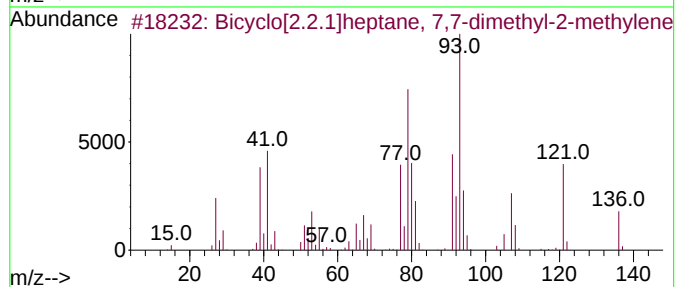
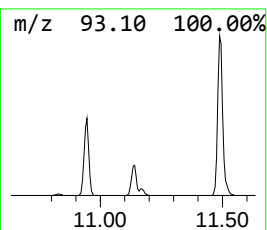
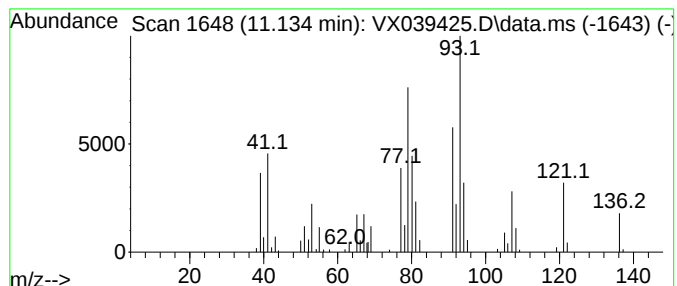
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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.
11.134	3.73 ug/L	54761	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	97
2			Bicyclo[2.2.1]heptane, 7,7-dimet...	136	C10H16	000471-84-1	97
3			Bicyclo[2.2.1]heptane, 7,7-dimet...	136	C10H16	000471-84-1	94
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	91



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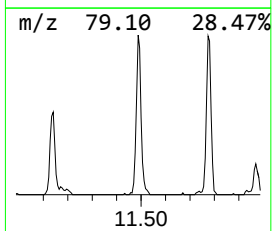
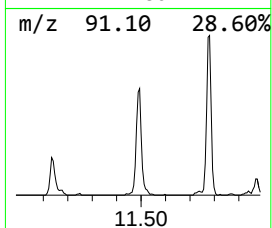
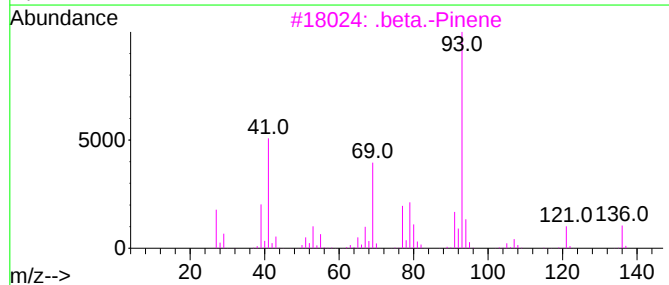
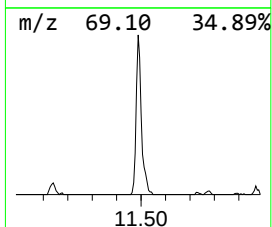
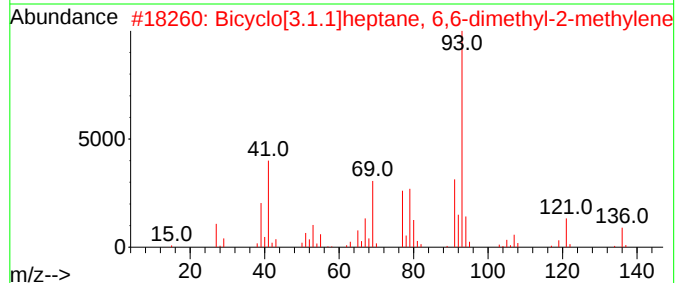
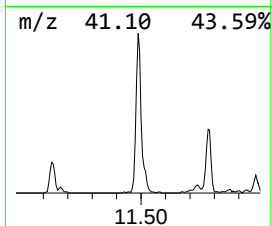
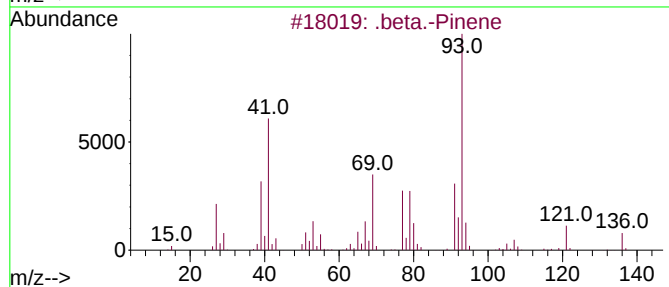
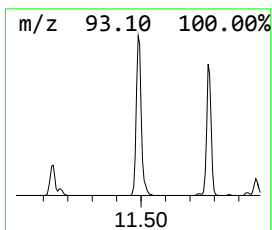
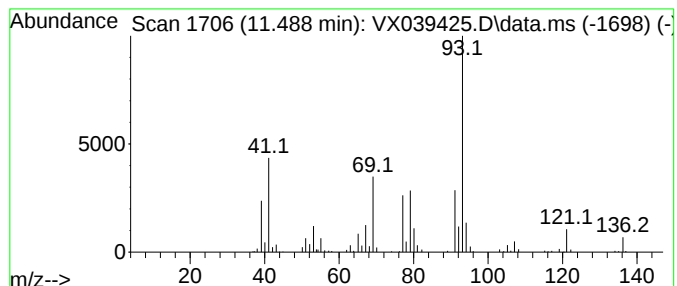
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Quant Title : VOC Analysis

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

Peak Number 4 .beta.-Pinene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.488	12.02 ug/L	176390	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.beta.-Pinene	136	C10H16	000127-91-3	96
2			Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	94
3			.beta.-Pinene	136	C10H16	000127-91-3	91
4			Cyclohexene, 4-methylene-1-(1-me...	136	C10H16	000099-84-3	91
5			Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122123\
Data File : VX039425.D
Acq On : 21 Dec 2023 13:33
Operator : JC/MD
Sample : 05835-20ME
Misc : 3.06g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COB24ME

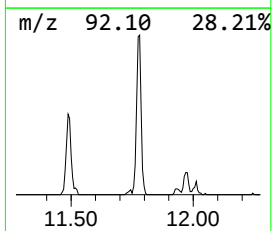
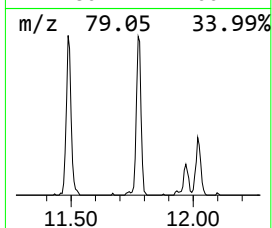
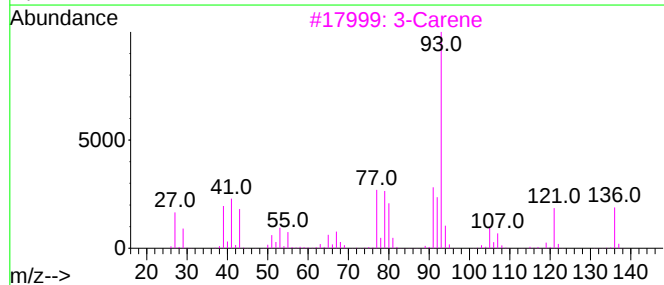
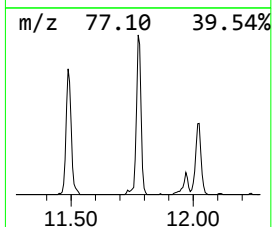
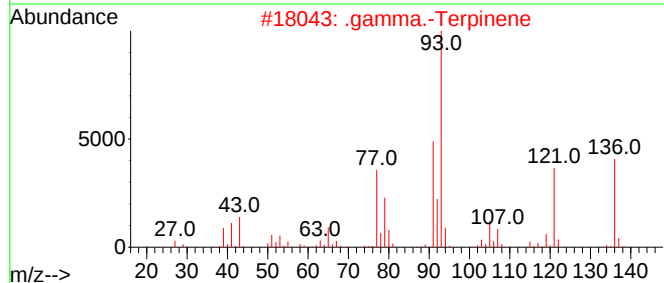
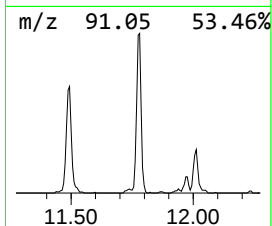
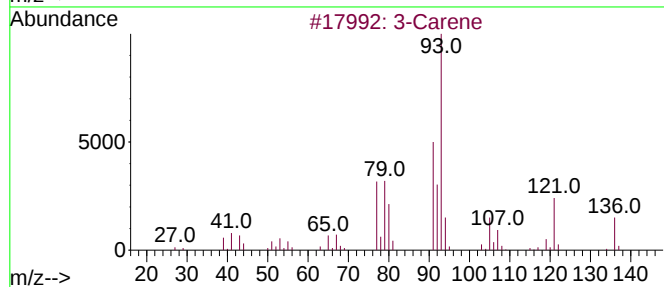
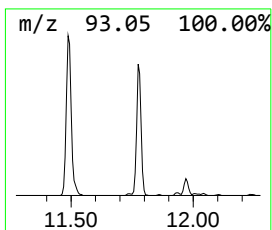
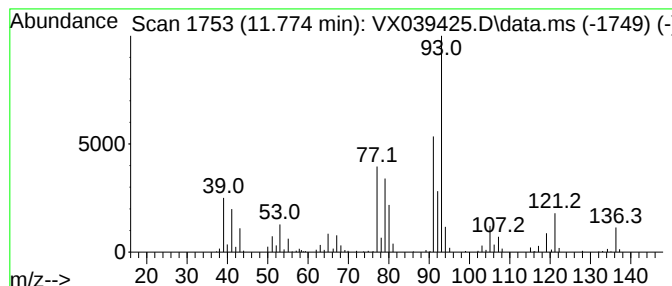
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Quant Title : VOC Analysis

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	10.71 ug/L	157123	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Carene	136	C10H16	013466-78-9	97
2			.gamma.-Terpinene	136	C10H16	000099-85-4	94
3			3-Carene	136	C10H16	013466-78-9	94
4			Cyclopropane, 1,1-dimethyl-2-(3-...	136	C10H16	068998-21-0	91
5			.gamma.-Terpinene	136	C10H16	000099-85-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122123\
Data File : VX039425.D
Acq On : 21 Dec 2023 13:33
Operator : JC/MD
Sample : 05835-20ME
Misc : 3.06g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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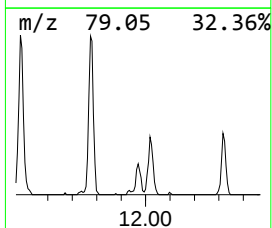
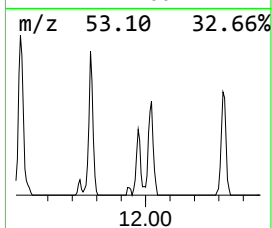
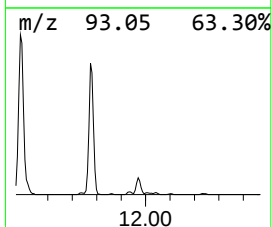
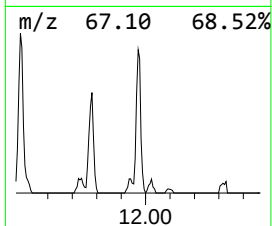
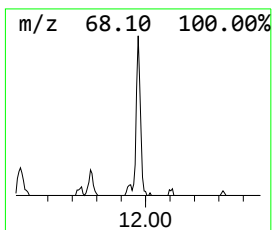
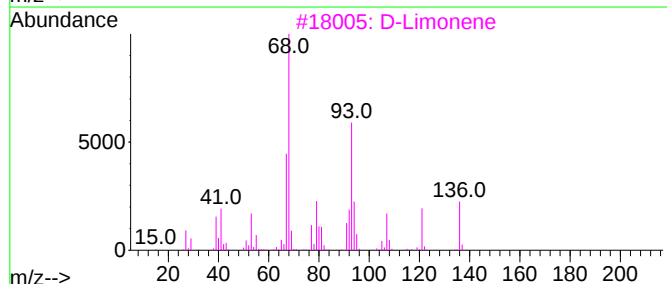
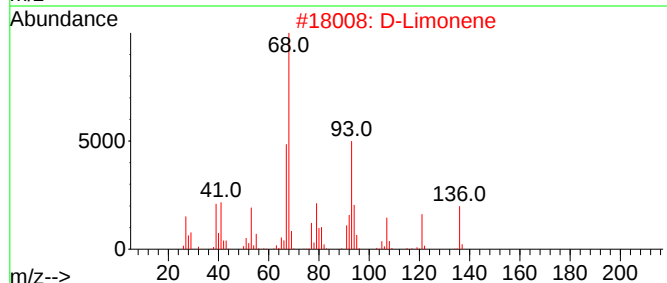
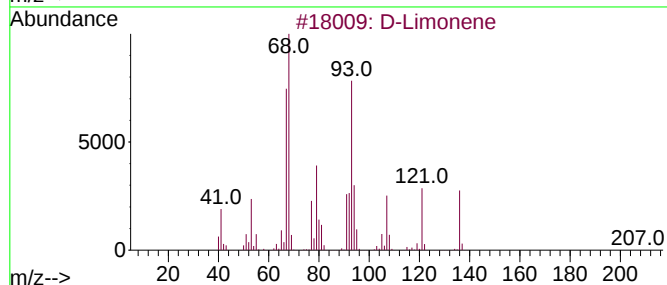
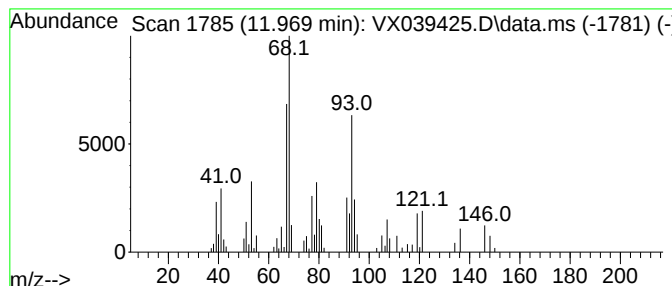
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Quant Title : VOC Analysis

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

Peak Number 6 D-Limonene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.969	2.73 ug/L	40074	1,4-Dichlorobenzene-d4	12.024

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	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122123\
Data File : VX039425.D
Acq On : 21 Dec 2023 13:33
Operator : JC/MD
Sample : 05835-20ME
Misc : 3.06g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COB24ME

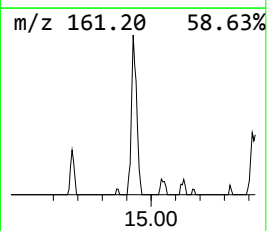
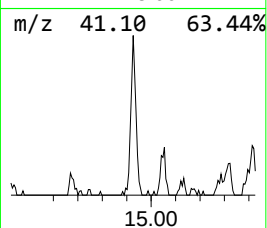
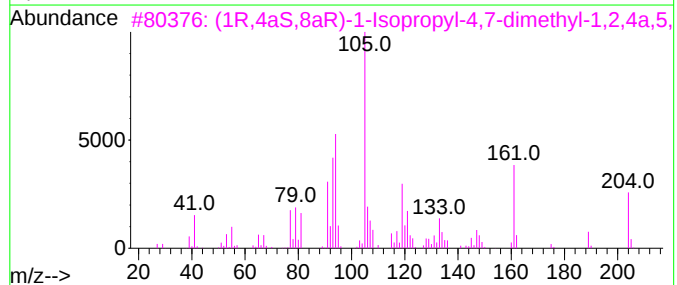
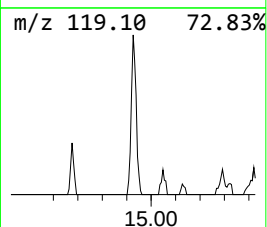
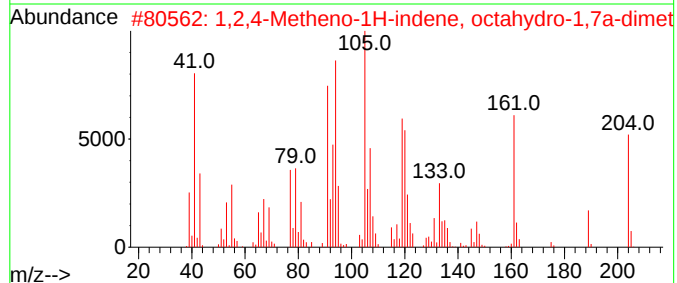
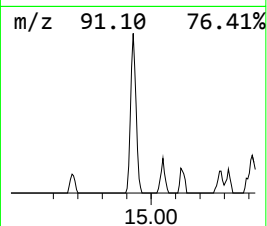
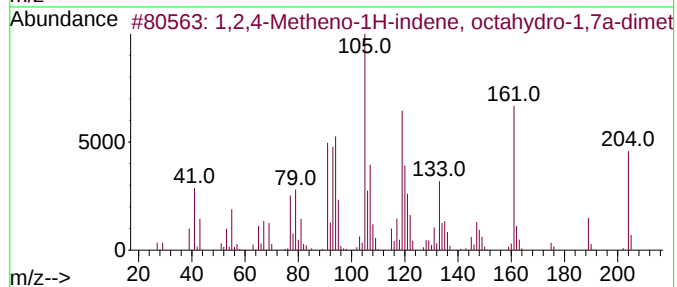
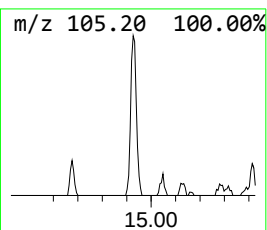
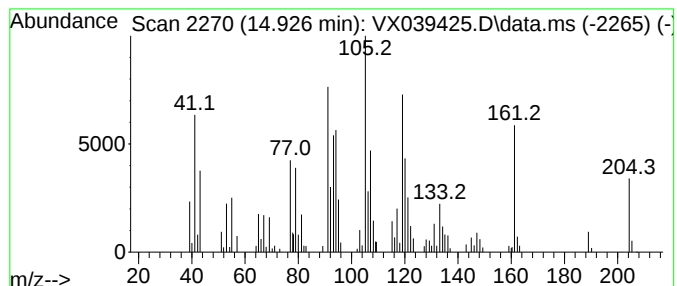
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Quant Title : VOC Analysis

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	4.51 ug/L	66197	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	93		
2	1,2,4-Metheno-1H-indene, octahyd...	204	C15H24	022469-52-9	91		
3	(1R,4aS,8aR)-1-Isopropyl-4,7-dim...	204	C15H24	020085-19-2	90		
4	8,8,9,9-Tetramethyl-3,4,5,6,7,8-...	204	C15H24	026783-22-2	64		
5	(1S,4aR,8aS)-1-Isopropyl-7-methy...	204	C15H24	006980-46-7	64		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122123\
Data File : VX039425.D
Acq On : 21 Dec 2023 13:33
Operator : JC/MD
Sample : 05835-20ME
Misc : 3.06g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0B24ME

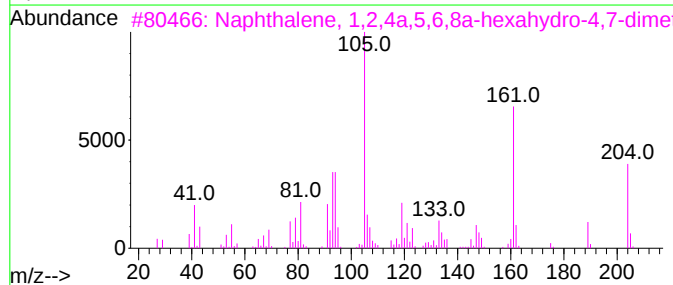
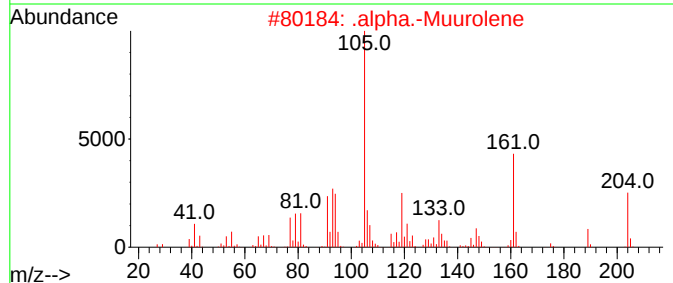
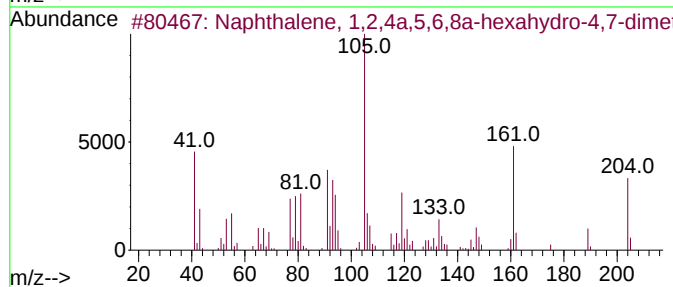
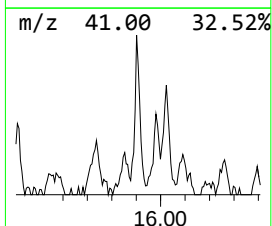
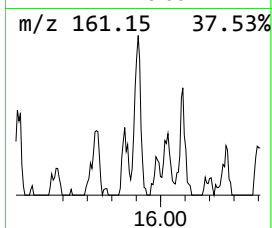
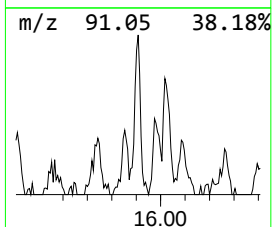
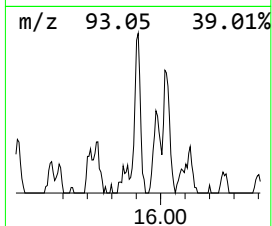
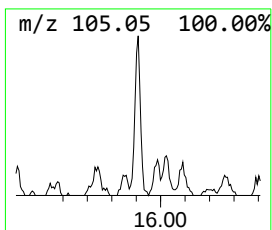
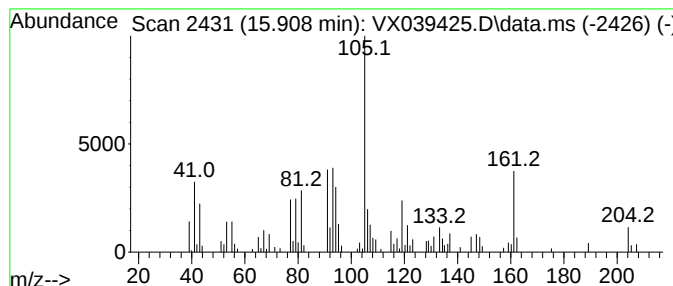
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Quant Title : VOC Analysis

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

Peak Number 8 Naphthalene, 1,2,4a,5,6,8a-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.908	3.08 ug/L	45107	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,4a,5,6,8a-hexah...	204	C15H24	031983-22-9	98
2			.alpha.-Muurolene	204	C15H24	010208-80-7	97
3			Naphthalene, 1,2,4a,5,6,8a-hexah...	204	C15H24	031983-22-9	95
4			Naphthalene, 1,2,4a,5,6,8a-hexah...	204	C15H24	031983-22-9	95
5			Naphthalene, 1,2,4a,5,6,8a-hexah...	204	C15H24	000483-75-0	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122123\
Data File : VX039425.D
Acq On : 21 Dec 2023 13:33
Operator : JC/MD
Sample : 05835-20ME
Misc : 3.06g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 12 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	10.945	6.0	ug/L	77161	2	10.055	646929	50.0
Bicyclo[2.2.1]h...	11.134	3.7	ug/L	54761	3	12.024	733434	50.0
.beta.-Pinene	11.488	12.0	ug/L	176390	3	12.024	733434	50.0
3-Carene	11.774	10.7	ug/L	157123	3	12.024	733434	50.0
D-Limonene	11.969	2.7	ug/L	40074	3	12.024	733434	50.0
1,2,4-Metheno-1...	14.926	4.5	ug/L	66197	3	12.024	733434	50.0
Naphthalene, 1,...	15.908	3.1	ug/L	45107	3	12.024	733434	50.0