

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW061224\
 Data File : VW029104.D
 Acq On : 12 Jun 2024 14:03
 Operator : SY/MD
 Sample : P2776-20
 Misc : 4.73g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 A4C73

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_W\Method\SFAMWLM060324SMA.M
 Title : SFAM01.0

Signal : TIC: VW029104.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.363	72	78	93	rBV	99911	241210	13.93%	2.268%
2	2.899	159	166	184	rVB	76462	221842	12.81%	2.086%
3	3.942	335	337	338	rBV	401	378	0.02%	0.004%
4	4.027	339	351	376	rVV	171141	563318	32.54%	5.296%
5	4.618	440	448	454	rBV3	1769	4216	0.24%	0.040%
6	4.716	463	464	469	rVB4	559	606	0.04%	0.006%
7	4.759	469	471	474	rVB2	416	331	0.02%	0.003%
8	4.838	482	484	487	rBV2	444	420	0.02%	0.004%
9	4.923	487	498	517	rVV3	15561	61433	3.55%	0.578%
10	5.124	529	531	532	rBV2	527	470	0.03%	0.004%
11	5.179	539	540	544	rVB	973	788	0.05%	0.007%
12	5.283	555	557	561	rBV3	453	586	0.03%	0.006%
13	5.320	561	563	565	rBV3	458	447	0.03%	0.004%
14	5.393	573	575	576	rBV2	360	221	0.01%	0.002%
15	5.411	576	578	580	rVV3	350	307	0.02%	0.003%
16	5.460	584	586	587	rBV2	356	216	0.01%	0.002%
17	5.478	587	589	591	rBV3	321	249	0.01%	0.002%
18	5.588	605	607	610	rVB2	554	458	0.03%	0.004%
19	5.795	640	641	644	rBV2	461	582	0.03%	0.005%
20	5.874	652	654	655	rVV2	378	250	0.01%	0.002%
21	5.941	658	665	675	rVV7	3872	12279	0.71%	0.115%
22	6.027	678	679	682	rBV	412	270	0.02%	0.003%
23	6.069	684	686	688	rVB2	377	294	0.02%	0.003%
24	6.094	688	690	691	rBV2	626	359	0.02%	0.003%
25	6.124	693	695	696	rVB2	381	214	0.01%	0.002%
26	6.185	704	705	710	rBV3	332	447	0.03%	0.004%
27	6.386	736	738	739	rVB2	387	242	0.01%	0.002%
28	6.441	744	747	748	rBV	419	455	0.03%	0.004%
29	6.490	752	755	756	rBV3	325	281	0.02%	0.003%
30	6.514	757	759	762	rVB5	478	383	0.02%	0.004%
31	6.557	762	766	768	rVB4	326	361	0.02%	0.003%
32	6.581	768	770	771	rBV	310	235	0.01%	0.002%
33	6.673	782	785	786	rBV	522	445	0.03%	0.004%
34	6.740	792	796	797	rBV3	494	512	0.03%	0.005%
35	6.807	804	807	810	rBV3	455	539	0.03%	0.005%
36	6.880	817	819	820	rVB	449	245	0.01%	0.002%

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

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM060324SMA.M
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37	6.899	820	822	824	rBV2	447	455	0.03%	0.004%
38	6.935	826	828	830	rVB2	316	224	0.01%	0.002%
39	6.996	835	838	839	rBV2	594	478	0.03%	0.004%
40	7.075	843	851	870	rBV	58738	180158	10.41%	1.694%
41	7.319	889	891	895	rBV2	755	779	0.04%	0.007%
42	7.350	895	896	897	rVB	684	250	0.01%	0.002%
43	7.465	914	915	918	rBV3	678	444	0.03%	0.004%
44	7.648	933	945	959	rBV	297401	733466	42.36%	6.896%
45	7.898	984	986	989	rBV3	340	335	0.02%	0.003%
46	7.929	989	991	993	rVB	557	432	0.02%	0.004%
47	7.953	993	995	997	rBV	380	366	0.02%	0.003%
48	8.051	1009	1011	1012	rBV2	516	341	0.02%	0.003%
49	8.087	1014	1017	1021	rBV3	429	757	0.04%	0.007%
50	8.142	1025	1026	1028	rVB2	548	255	0.01%	0.002%
51	8.203	1034	1036	1037	rBV	424	343	0.02%	0.003%
52	8.276	1037	1048	1063	rBV2	592653	1731331	100.00%	16.277%
53	8.843	1132	1141	1154	rBV	502282	996636	57.56%	9.370%
54	9.276	1202	1212	1223	rBV	404367	832212	48.07%	7.824%
55	9.471	1242	1244	1249	rVB3	741	1016	0.06%	0.010%
56	9.508	1249	1250	1253	rBV3	575	509	0.03%	0.005%
57	9.618	1266	1268	1269	rBV3	293	220	0.01%	0.002%
58	9.660	1271	1275	1276	rBV3	1606	1870	0.11%	0.018%
59	9.788	1294	1296	1298	rVB2	451	407	0.02%	0.004%
60	9.928	1316	1319	1320	rBV2	241	271	0.02%	0.003%
61	10.032	1328	1336	1347	rBV	176621	325751	18.82%	3.062%
62	10.319	1375	1383	1394	rBV	677359	1172374	67.72%	11.022%
63	10.428	1397	1401	1406	rVV2	8589	14428	0.83%	0.136%
64	10.508	1409	1414	1418	rVV6	2791	5393	0.31%	0.051%
65	10.575	1419	1425	1436	rVV	112128	198956	11.49%	1.870%
66	10.697	1440	1445	1451	rVV2	8159	13423	0.78%	0.126%
67	10.843	1467	1469	1473	rVB5	750	713	0.04%	0.007%
68	10.922	1475	1482	1494	rBV	191633	337033	19.47%	3.169%
69	11.367	1553	1555	1557	rVB2	622	358	0.02%	0.003%
70	11.398	1557	1560	1564	rVB4	730	1047	0.06%	0.010%
71	11.446	1566	1568	1572	rVB4	515	490	0.03%	0.005%
72	11.483	1572	1574	1577	rBV4	384	400	0.02%	0.004%
73	11.629	1590	1598	1607	rBV	518046	874662	50.52%	8.223%
74	11.776	1621	1622	1627	rVB5	606	618	0.04%	0.006%
75	12.001	1657	1659	1660	rBV2	548	370	0.02%	0.003%
76	12.020	1660	1662	1665	rVB2	583	486	0.03%	0.005%

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 Title : SFAM01.0

77	12.050	1665	1667	1668	rBV2	477	396	0.02%	0.004%
78	12.081	1670	1672	1674	rBV3	642	720	0.04%	0.007%
79	12.184	1682	1689	1694	rBV8	1140	2676	0.15%	0.025%
80	12.465	1727	1735	1747	rBV	124325	214661	12.40%	2.018%
81	12.599	1751	1757	1763	rVB2	21543	38304	2.21%	0.360%
82	12.690	1764	1772	1782	rBV	250059	460645	26.61%	4.331%
83	12.879	1801	1803	1806	rVB3	667	446	0.03%	0.004%
84	12.922	1807	1810	1811	rBV2	764	735	0.04%	0.007%
85	12.958	1812	1816	1819	rVV5	2297	3570	0.21%	0.034%
86	13.019	1820	1826	1835	rVV	177389	298977	17.27%	2.811%
87	13.208	1852	1857	1868	rBV3	18899	37706	2.18%	0.354%
88	13.355	1877	1881	1885	rBV4	9154	13257	0.77%	0.125%
89	13.464	1894	1899	1907	rBV3	17407	30698	1.77%	0.289%
90	13.556	1907	1914	1924	rBV	298753	493852	28.52%	4.643%
91	13.848	1955	1962	1975	rBV	275475	455034	26.28%	4.278%
92	13.989	1983	1985	1990	rVB6	4349	6528	0.38%	0.061%
93	14.062	1993	1997	2002	rVB	8154	13349	0.77%	0.125%
94	14.318	2035	2039	2051	rVB10	3602	7003	0.40%	0.066%
95	14.513	2069	2071	2077	rVB5	4196	5519	0.32%	0.052%
96	14.684	2094	2099	2101	rBV6	2255	3820	0.22%	0.036%
97	14.873	2128	2130	2132	rBV2	501	423	0.02%	0.004%
98	14.897	2132	2134	2137	rVB2	646	537	0.03%	0.005%
99	15.476	2228	2229	2233	rVB3	1758	1773	0.10%	0.017%
100	15.751	2273	2274	2275	rBV	520	279	0.02%	0.003%

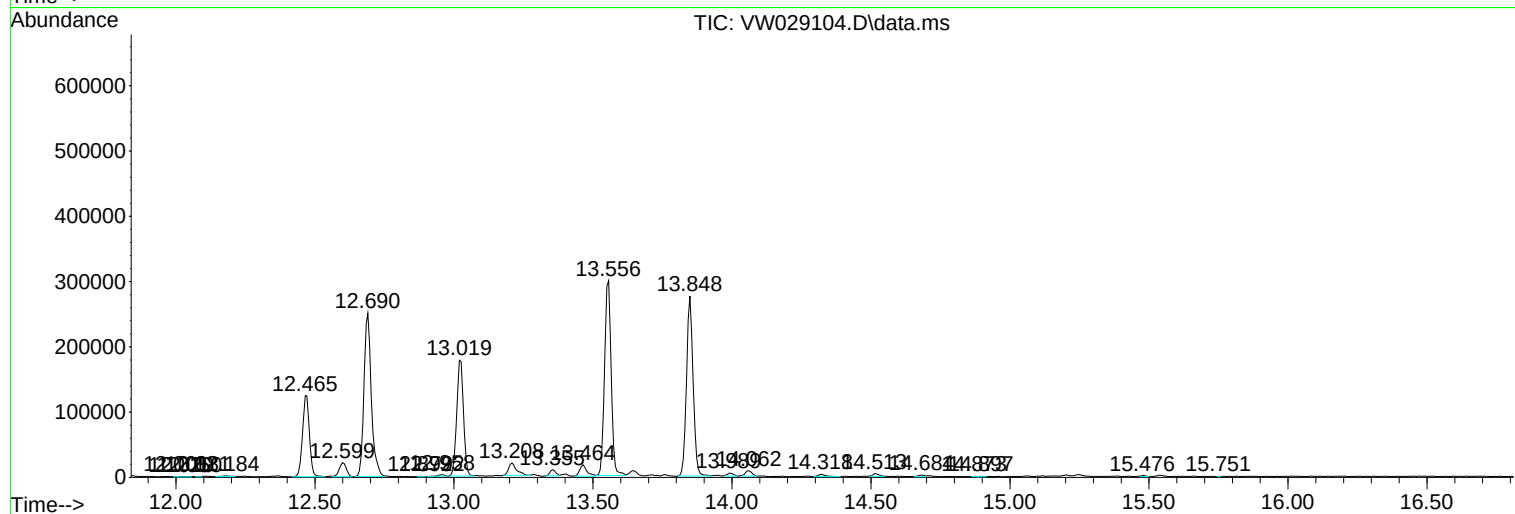
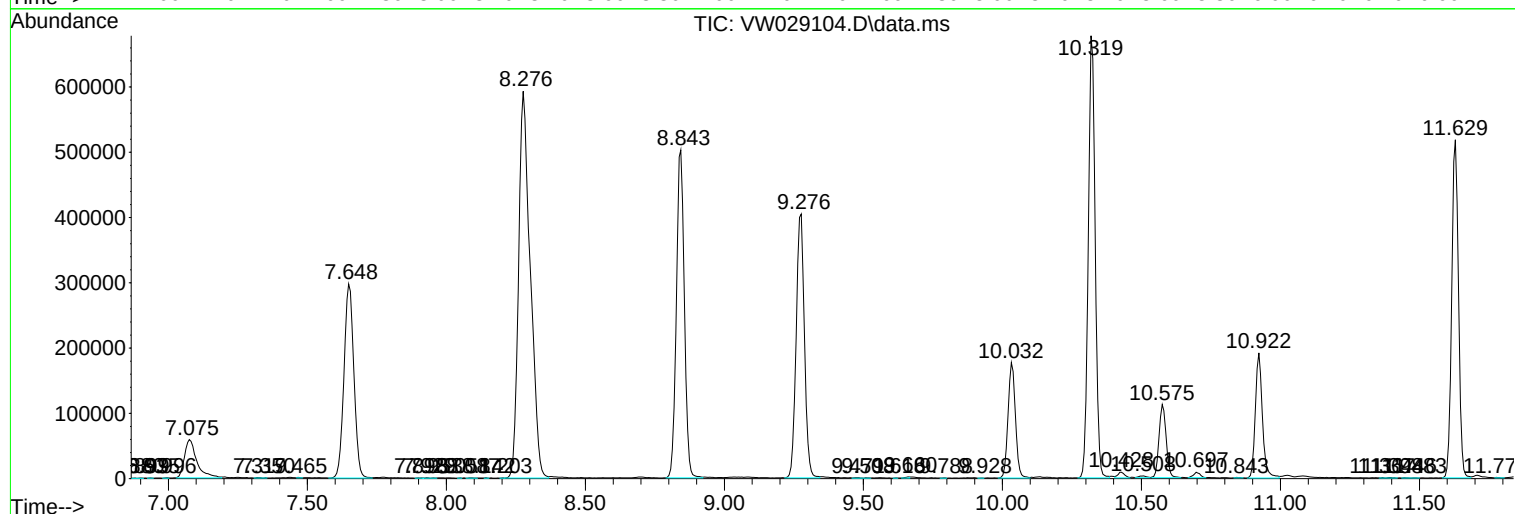
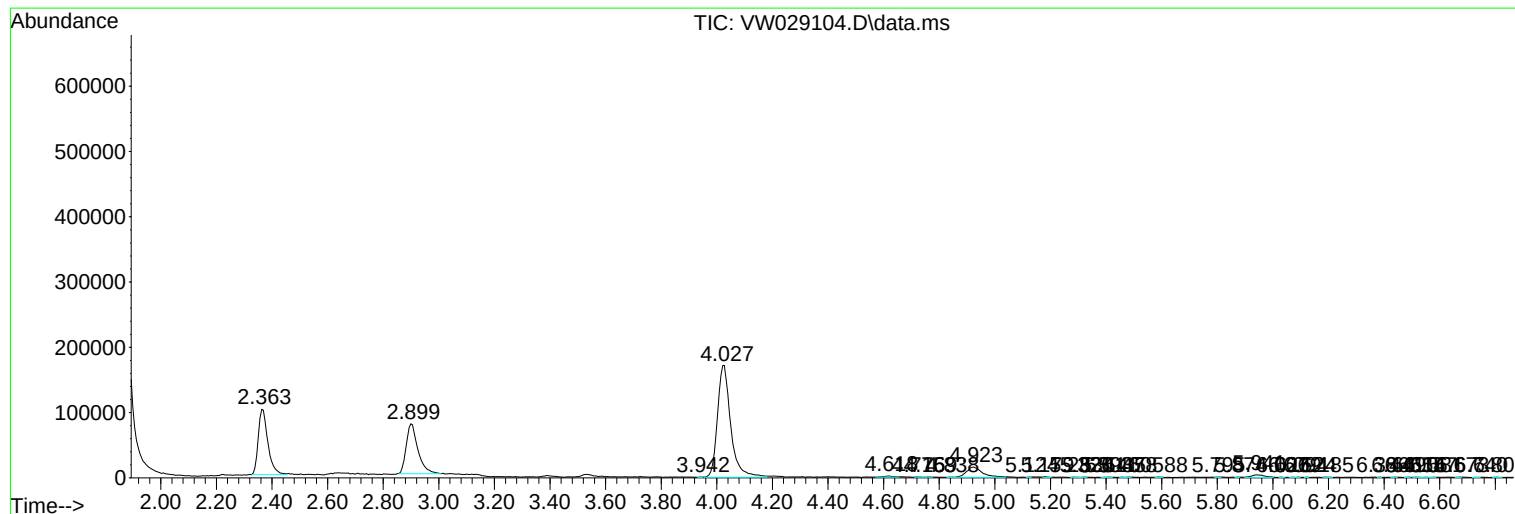
Sum of corrected areas: 10636854

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Instrument :
MSVOA_W
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM060324SMA.M
Quant Title : SFAM01.0

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



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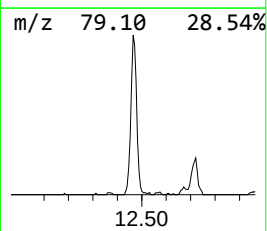
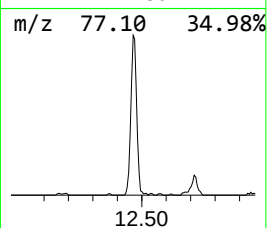
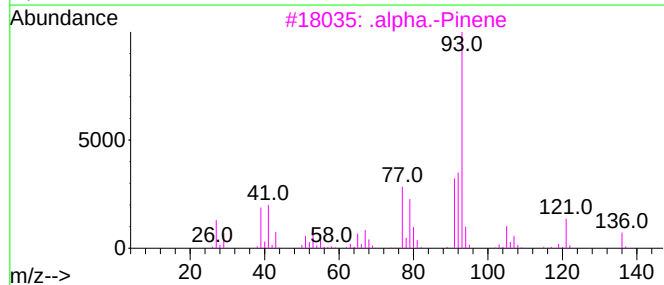
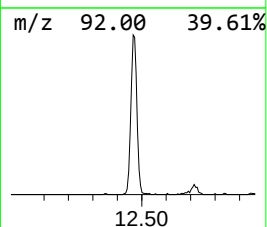
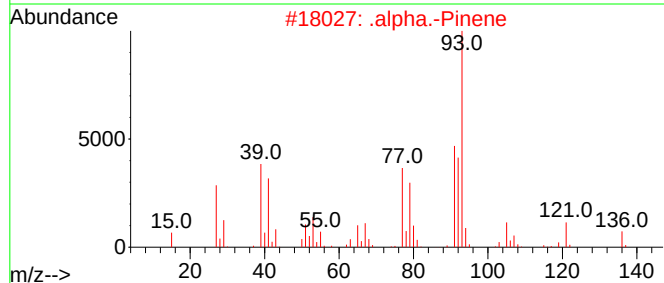
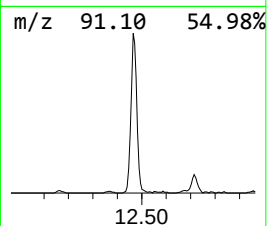
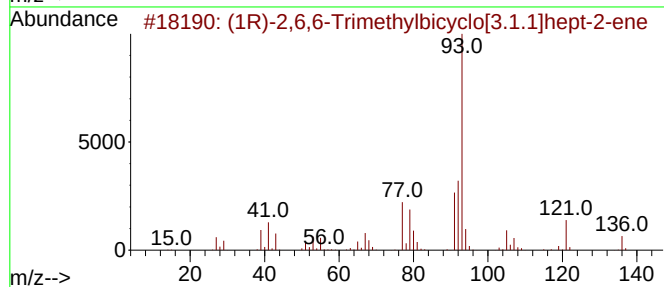
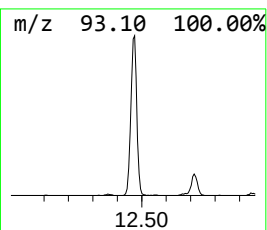
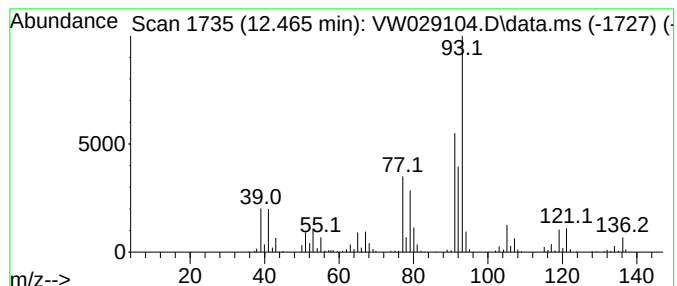
Instrument :
MSVOA_W
ClientSampleId :
A4C73

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM060324SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 (1R)-2,6,6-Trimethylbicyclo... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.465	6.14 ug/L	214661	Chlorobenzene-d5	11.629	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-70-8	94
2	.alpha.-Pinene	136	C10H16	000080-56-8	93
3	.alpha.-Pinene	136	C10H16	000080-56-8	93
4	Bicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-	136	C10H16	004889-83-2	91
5	(1S)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-26-4	90



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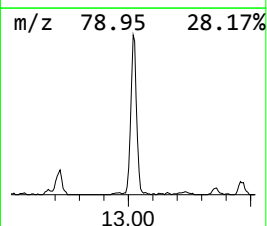
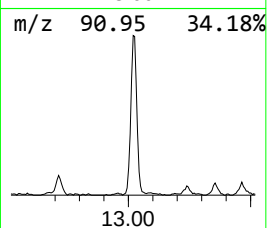
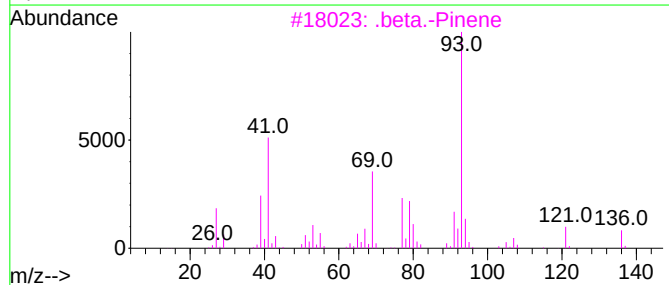
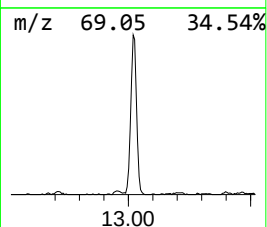
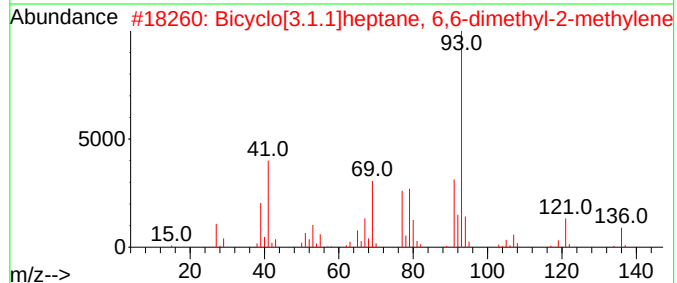
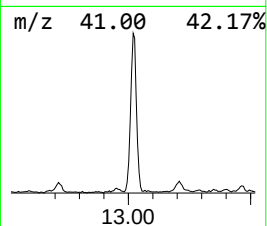
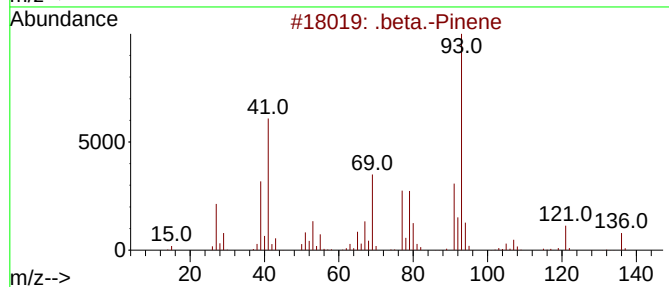
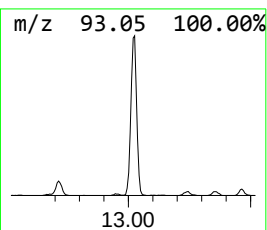
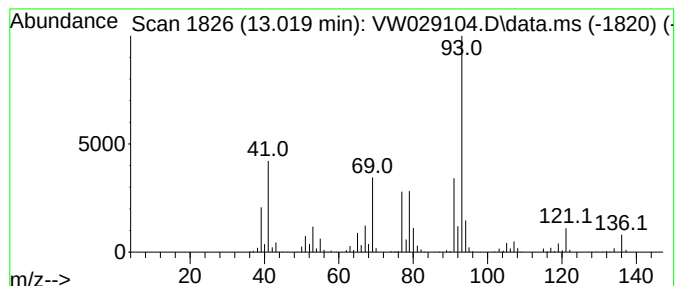
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM060324SMA.M
Quant Title : SFAM01.0

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

Peak Number 4 .beta.-Pinene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.019	15.13 ug/L	298977	1,4-Dichlorobenzene-d4	13.556

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	96		
3	.	beta.-Pinene	136	C10H16	000127-91-3	95	
4	Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	93		
5	Bicyclo[3.1.0]hexane, 4-methylen...	136	C10H16	003387-41-5	91		



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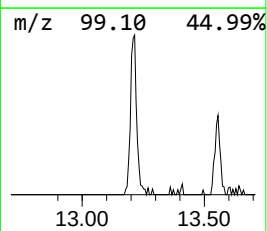
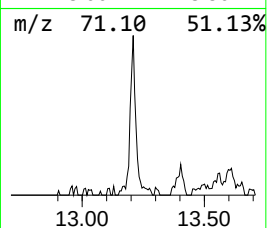
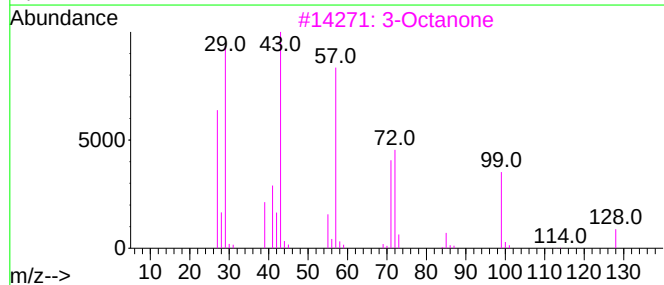
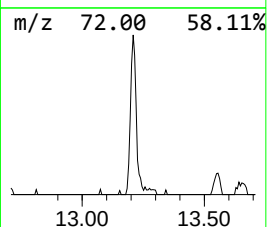
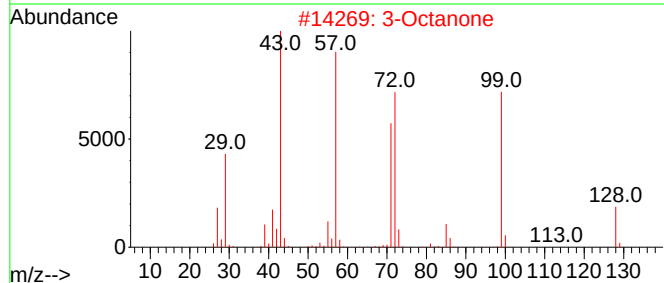
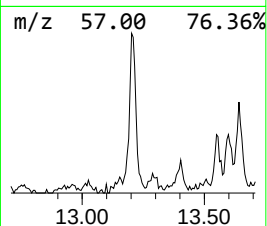
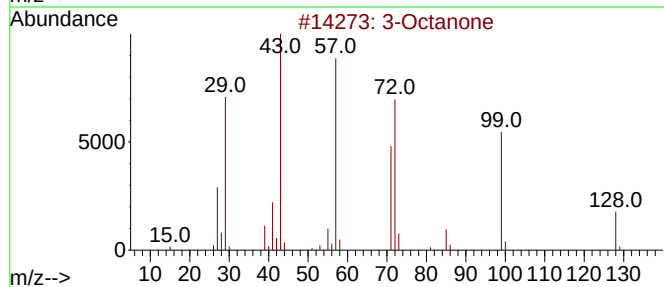
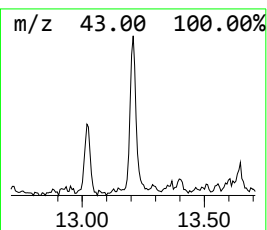
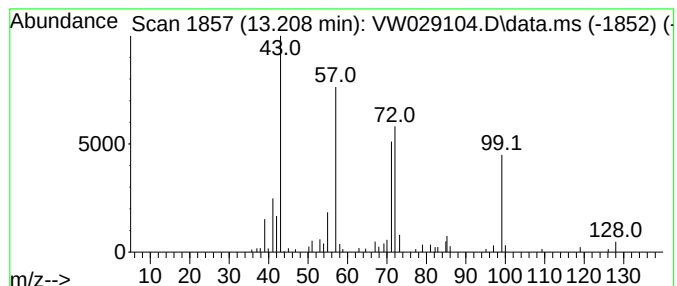
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM060324SMA.M
Quant Title : SFAM01.0

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

Peak Number 5 3-Octanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.208	1.91 ug/L	37706	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octanone			128	C8H16O	000106-68-3	91
2	3-Octanone			128	C8H16O	000106-68-3	90
3	3-Octanone			128	C8H16O	000106-68-3	83
4	Butanal, 2-ethyl-			100	C6H12O	000097-96-1	49
5	3-Octanone			128	C8H16O	000106-68-3	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW061224\
Data File : VW029104.D
Acq On : 12 Jun 2024 14:03
Operator : SY/MD
Sample : P2776-20
Misc : 4.73g/10mL/MSVOA_W/SOIL/A
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
A4C73

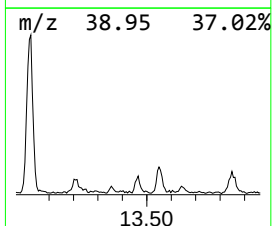
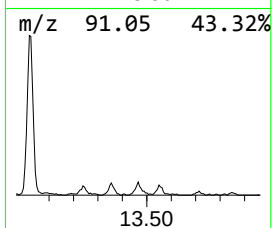
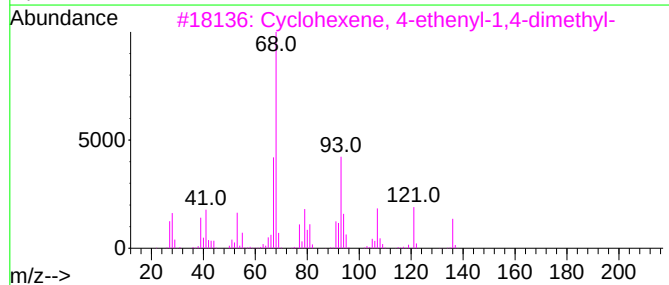
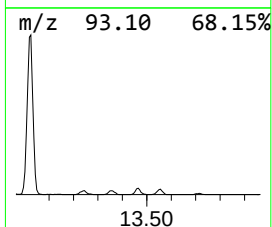
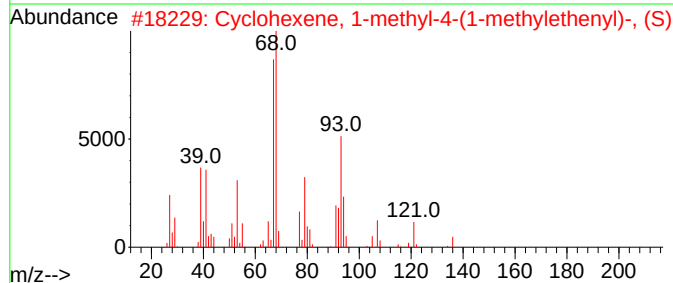
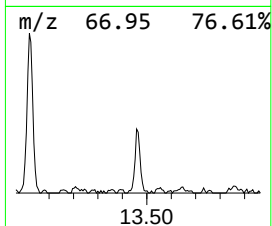
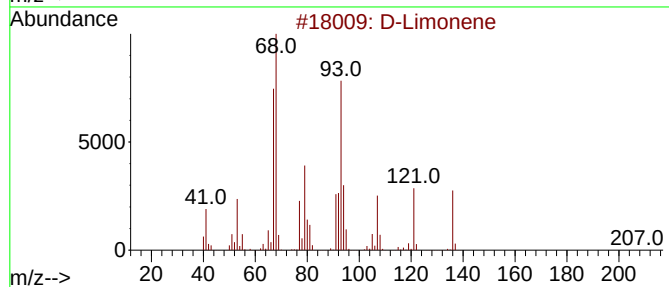
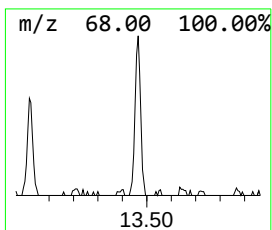
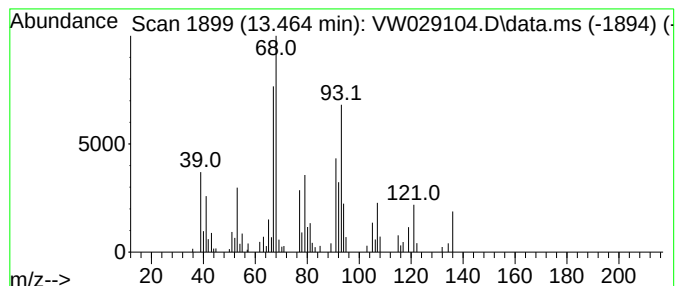
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Quant Title : SFAM01.0

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

Peak Number 6 D-Limonene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.464	1.55 ug/L	30698	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			D-Limonene	136	C10H16	005989-27-5	96
2			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	005989-54-8	93
3			Cyclohexene, 4-ethenyl-1,4-dimet...	136	C10H16	001743-61-9	76
4			Limonene	136	C10H16	000138-86-3	76
5			D-Limonene	136	C10H16	005989-27-5	76



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW061224\
Data File : VW029104.D
Acq On : 12 Jun 2024 14:03
Operator : SY/MD
Sample : P2776-20
Misc : 4.73g/10mL/MSVOA_W/SOIL/A
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
A4C73

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM060324SMA.M
Quant Title : SFAM01.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(1R)-2,6,6-Trim...	12.465	6.1	ug/L	214661	2	11.629	874662	25.0
.beta.-Pinene	13.019	15.1	ug/L	298977	3	13.556	493852	25.0
3-Octanone	13.208	1.9	ug/L	37706	3	13.556	493852	25.0
D-Limonene	13.464	1.6	ug/L	30698	3	13.556	493852	25.0