

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW092024\
 Data File : VW030184.D
 Acq On : 20 Sep 2024 18:50
 Operator : SY/MD
 Sample : P4109-20
 Misc : 4.93g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 A4EW2

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\SFAMWLM091624SMA.M
 Title : SFAM01.0

Signal : TIC: VW030184.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.174	40	47	52	rBV6	2222	5337	0.41%	0.065%
2	2.369	72	79	92	rVB	66914	159839	12.22%	1.953%
3	2.899	157	166	179	rBV	50871	153778	11.76%	1.879%
4	3.247	221	223	224	rBV2	351	339	0.03%	0.004%
5	3.302	230	232	238	rVB5	720	1203	0.09%	0.015%
6	3.381	241	245	246	rBV2	1187	1392	0.11%	0.017%
7	3.527	264	269	272	rBV3	326	628	0.05%	0.008%
8	3.625	281	285	286	rVB2	287	308	0.02%	0.004%
9	3.661	286	291	292	rBV2	317	412	0.03%	0.005%
10	3.734	297	303	304	rBV4	611	909	0.07%	0.011%
11	3.844	319	321	324	rBV3	287	386	0.03%	0.005%
12	3.881	324	327	329	rBV	420	405	0.03%	0.005%
13	4.021	338	350	360	rBV2	140005	432342	33.05%	5.281%
14	4.119	361	366	378	rVB	38964	109827	8.40%	1.342%
15	4.301	394	396	397	rVB2	368	243	0.02%	0.003%
16	4.393	403	411	416	rBV3	2168	6154	0.47%	0.075%
17	4.625	446	449	452	rVV	292	317	0.02%	0.004%
18	4.692	453	460	462	rVV2	326	609	0.05%	0.007%
19	4.923	488	498	511	rBV4	5682	22591	1.73%	0.276%
20	5.076	520	523	525	rBV2	248	234	0.02%	0.003%
21	5.143	530	534	535	rVV	389	478	0.04%	0.006%
22	5.185	538	541	543	rVB2	325	334	0.03%	0.004%
23	5.423	578	580	584	rBV	223	285	0.02%	0.003%
24	5.795	631	641	652	rVB3	3176	10770	0.82%	0.132%
25	5.947	657	666	676	rBV7	2335	6968	0.53%	0.085%
26	6.155	699	700	704	rBV	201	239	0.02%	0.003%
27	6.325	726	728	730	rBV	331	287	0.02%	0.004%
28	6.508	754	758	760	rBV2	211	319	0.02%	0.004%
29	6.722	791	793	795	rVB	434	287	0.02%	0.004%
30	6.838	809	812	816	rVB2	267	282	0.02%	0.003%
31	6.905	816	823	824	rBV3	1559	2615	0.20%	0.032%
32	7.075	842	851	861	rBV	41960	123136	9.41%	1.504%
33	7.167	861	866	885	rVB2	16354	49410	3.78%	0.604%
34	7.386	899	902	904	rVB3	227	253	0.02%	0.003%
35	7.447	910	912	917	rVB2	241	309	0.02%	0.004%
36	7.496	917	920	921	rBV	358	356	0.03%	0.004%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM091624SMA.M
 Title : SFAM01.0

37	7.648	934	945	957	rBV	220863	547066	41.82%	6.683%
38	7.965	994	997	999	rVB3	456	371	0.03%	0.005%
39	8.075	1014	1015	1019	rVB	360	304	0.02%	0.004%
40	8.276	1037	1048	1064	rBV2	449076	1308039	100.00%	15.979%
41	8.386	1064	1066	1068	rVB3	435	358	0.03%	0.004%
42	8.496	1082	1084	1086	rBV	267	335	0.03%	0.004%
43	8.551	1090	1093	1094	rVV	655	707	0.05%	0.009%
44	8.587	1098	1099	1103	rVV2	433	514	0.04%	0.006%
45	8.630	1103	1106	1107	rVB	366	311	0.02%	0.004%
46	8.843	1131	1141	1157	rVV2	513843	1039289	79.45%	12.696%
47	9.051	1169	1175	1176	rBV5	744	1335	0.10%	0.016%
48	9.276	1203	1212	1221	rBV	286632	594105	45.42%	7.258%
49	9.422	1234	1236	1241	rVB3	560	451	0.03%	0.006%
50	9.532	1251	1254	1257	rVB2	240	296	0.02%	0.004%
51	9.587	1260	1263	1264	rBV	223	236	0.02%	0.003%
52	9.660	1271	1275	1276	rBV2	903	1041	0.08%	0.013%
53	9.965	1315	1325	1328	rBV5	742	1531	0.12%	0.019%
54	10.032	1328	1336	1348	rBV	135562	248385	18.99%	3.034%
55	10.136	1348	1353	1357	rBV3	705	1240	0.09%	0.015%
56	10.215	1363	1366	1373	rVB4	569	940	0.07%	0.011%
57	10.319	1373	1383	1392	rBV	493793	896385	68.53%	10.950%
58	10.502	1409	1413	1418	rVB5	1282	2206	0.17%	0.027%
59	10.575	1418	1425	1435	rBV	80126	139943	10.70%	1.710%
60	10.697	1439	1445	1451	rVB2	8713	15316	1.17%	0.187%
61	10.800	1460	1462	1464	rVB3	257	259	0.02%	0.003%
62	10.837	1464	1468	1469	rBV4	935	1137	0.09%	0.014%
63	10.922	1475	1482	1497	rBV	171125	292562	22.37%	3.574%
64	11.154	1515	1520	1521	rBV3	1157	1884	0.14%	0.023%
65	11.172	1521	1523	1526	rVV4	1643	1817	0.14%	0.022%
66	11.227	1530	1532	1537	rVB4	1163	1432	0.11%	0.017%
67	11.288	1537	1542	1543	rBV4	540	543	0.04%	0.007%
68	11.306	1543	1545	1546	rBV	394	272	0.02%	0.003%
69	11.349	1549	1552	1553	rBV2	558	576	0.04%	0.007%
70	11.404	1558	1561	1567	rVB6	1181	1852	0.14%	0.023%
71	11.471	1567	1572	1577	rBV2	2396	4330	0.33%	0.053%
72	11.544	1581	1584	1586	rBV2	325	333	0.03%	0.004%
73	11.629	1590	1598	1607	rBV	459132	777173	59.42%	9.494%
74	11.837	1624	1632	1650	rVB9	5166	13498	1.03%	0.165%
75	12.038	1661	1665	1667	rBV4	480	754	0.06%	0.009%
76	12.056	1667	1668	1671	rVB3	503	375	0.03%	0.005%

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 Title : SFAM01.0

77	12.087	1671	1673	1675	rBV3	489	402	0.03%	0.005%
78	12.105	1675	1676	1677	rBV	668	458	0.04%	0.006%
79	12.142	1678	1682	1683	rBV3	944	1159	0.09%	0.014%
80	12.245	1696	1699	1705	rVB6	1286	2362	0.18%	0.029%
81	12.343	1710	1715	1717	rVV5	1396	2525	0.19%	0.031%
82	12.385	1720	1722	1723	rVB2	567	342	0.03%	0.004%
83	12.471	1728	1736	1739	rBV5	2656	4972	0.38%	0.061%
84	12.532	1744	1746	1748	rVB3	732	393	0.03%	0.005%
85	12.568	1749	1752	1753	rBV3	1328	1402	0.11%	0.017%
86	12.599	1753	1757	1762	rVB	11654	19280	1.47%	0.236%
87	12.690	1765	1772	1779	rVV	163116	270629	20.69%	3.306%
88	12.867	1797	1801	1803	rBV3	3465	5165	0.39%	0.063%
89	12.928	1807	1811	1818	rVV4	10607	20654	1.58%	0.252%
90	13.032	1822	1828	1834	rVV	22016	36853	2.82%	0.450%
91	13.160	1846	1849	1850	rBV3	2307	2810	0.21%	0.034%
92	13.275	1859	1868	1881	rVB2	60468	128650	9.84%	1.572%
93	13.403	1885	1889	1894	rVB	10422	16461	1.26%	0.201%
94	13.556	1908	1914	1919	rBV	205021	340046	26.00%	4.154%
95	13.641	1926	1928	1936	rVB	12059	17039	1.30%	0.208%
96	13.757	1942	1947	1954	rVB6	8323	16702	1.28%	0.204%
97	13.849	1955	1962	1968	rBV	147353	244207	18.67%	2.983%
98	14.050	1990	1995	2001	rBV2	19426	37894	2.90%	0.463%
99	14.513	2068	2071	2079	rVB4	7544	11728	0.90%	0.143%
100	15.123	2167	2171	2174	rBV6	6015	10820	0.83%	0.132%

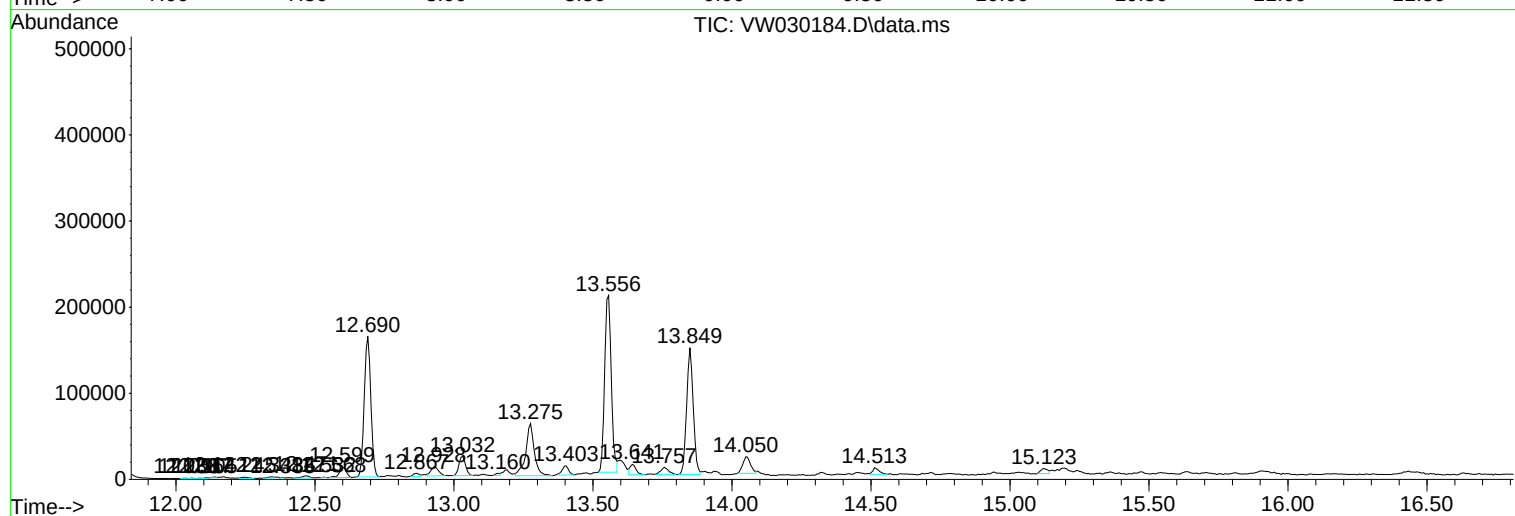
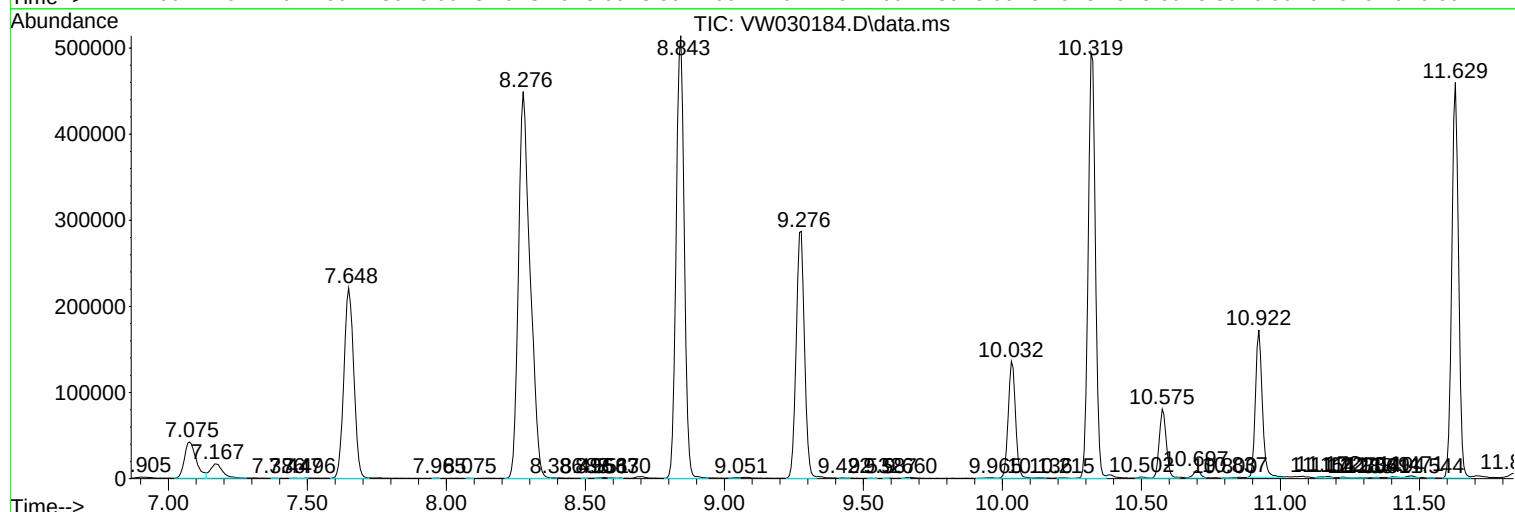
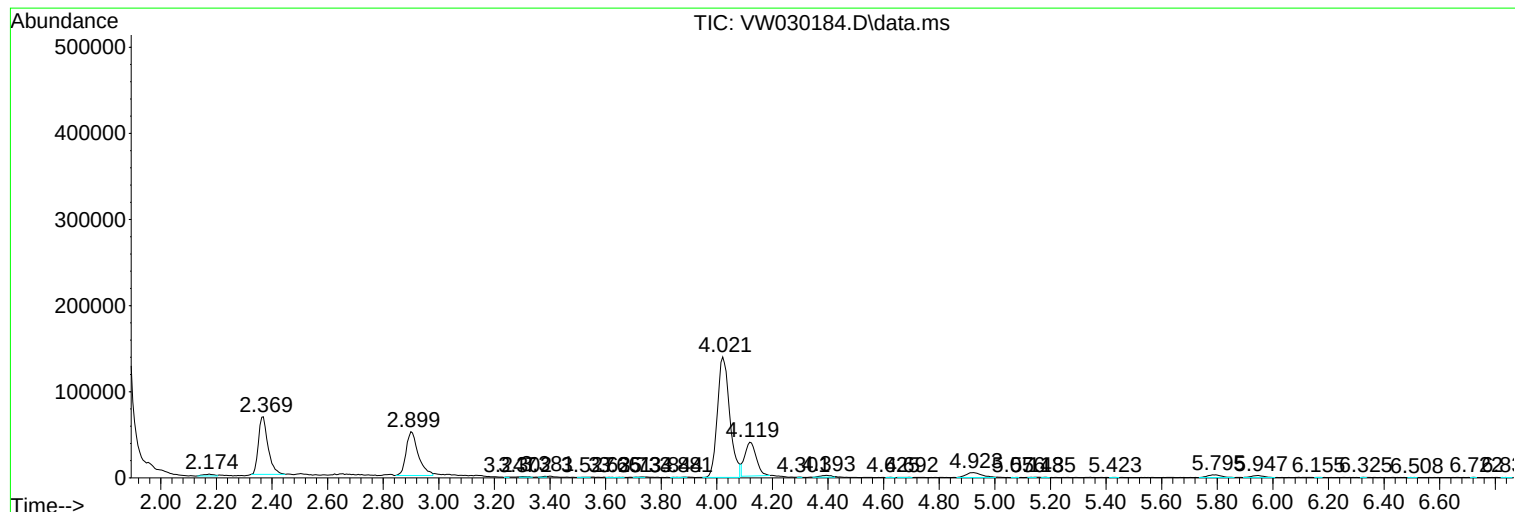
Sum of corrected areas: 8186035

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MSVOA_W
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM091624SMA.M
Quant Title : SFAM01.0

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



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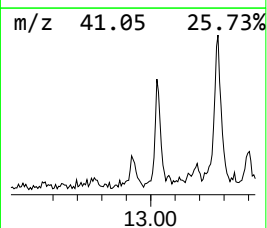
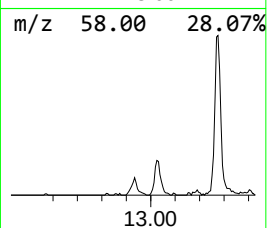
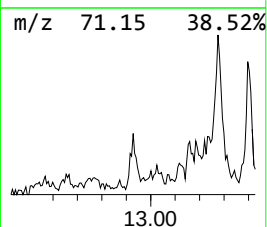
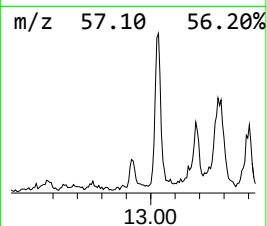
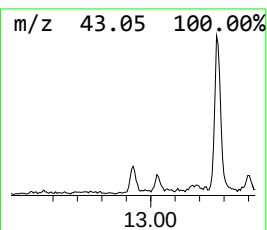
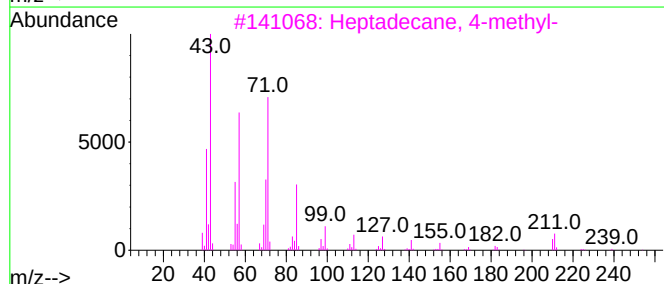
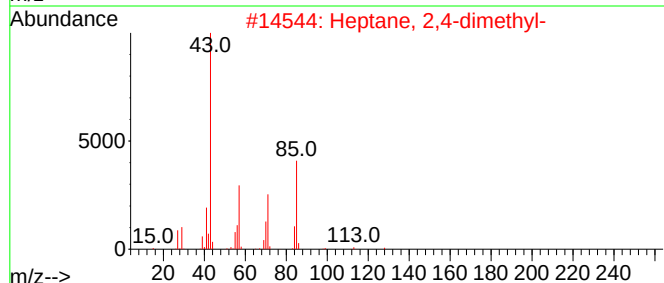
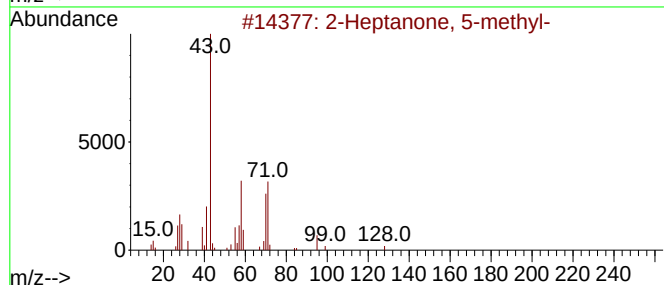
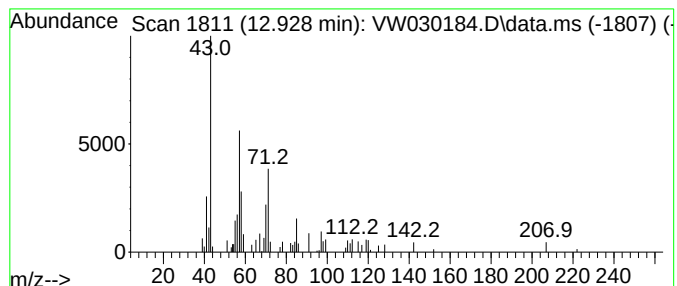
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM091624SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 2-Heptanone, 5-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.928	1.52 ug/L	20654	1,4-Dichlorobenzene-d4	13.550

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Heptanone, 5-methyl-	128	C8H16O	018217-12-4	58
2		Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	49
3		Heptadecane, 4-methyl-	254	C18H38	026429-11-8	47
4		Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	46
5		Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	43



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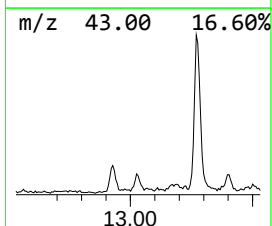
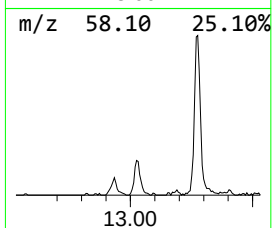
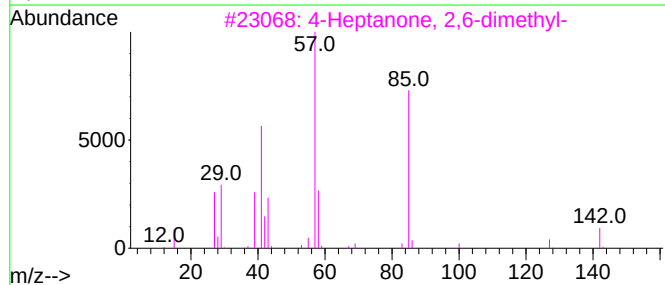
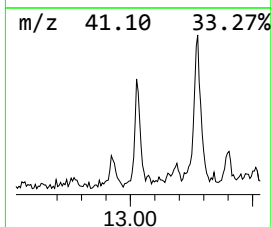
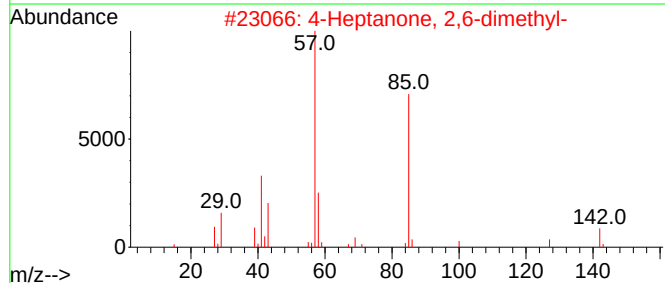
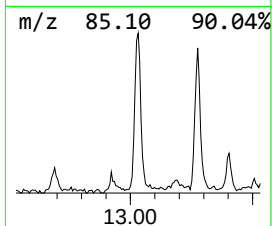
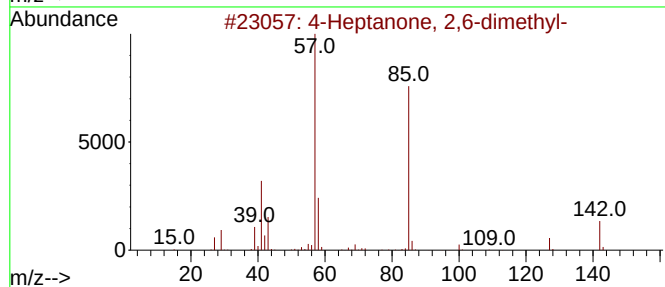
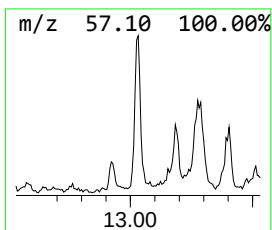
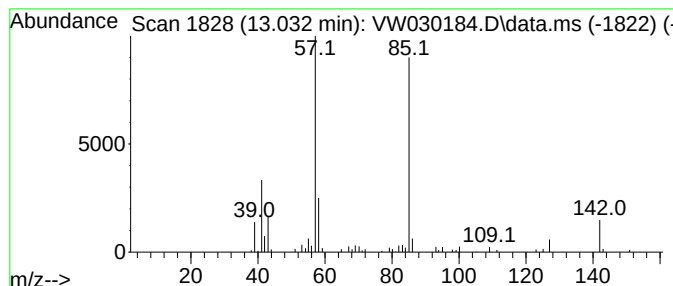
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM091624SMA.M
Quant Title : SFAM01.0

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

Peak Number 4 4-Heptanone, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.032	2.71 ug/L	36853	1,4-Dichlorobenzene-d4	13.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	91
2			4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	91
3			4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	90
4			4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	87
5			4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	64



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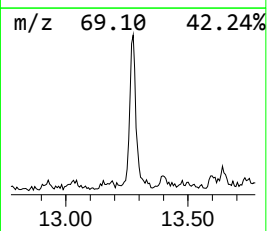
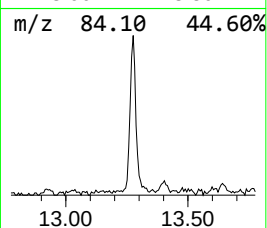
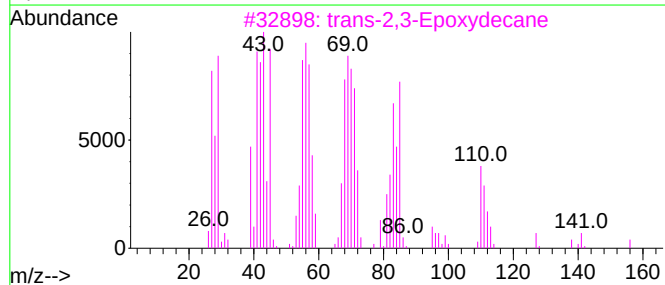
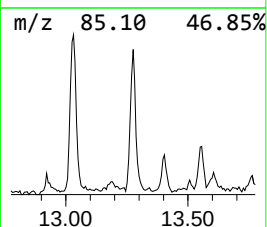
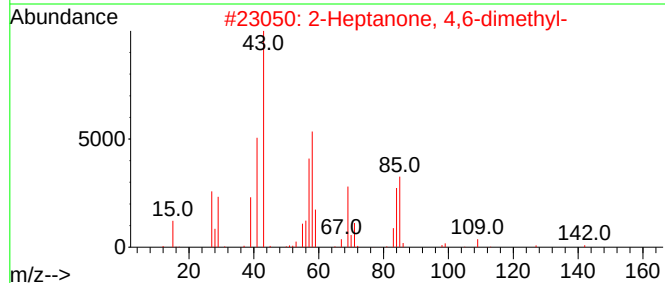
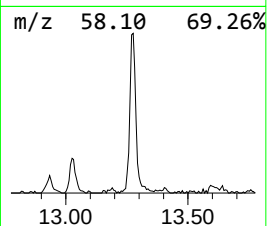
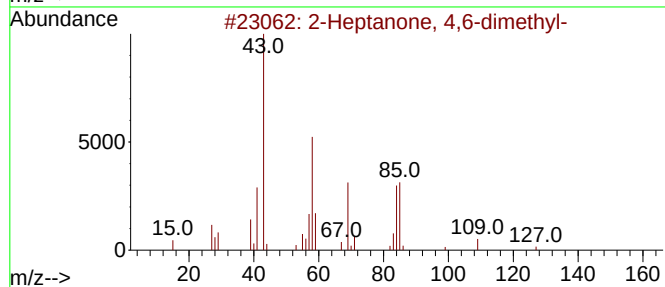
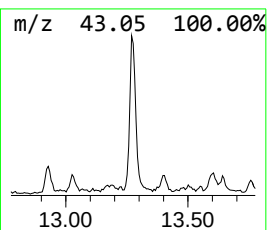
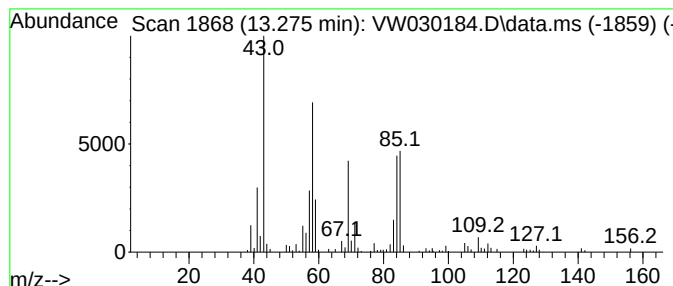
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM091624SMA.M
Quant Title : SFAM01.0

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

Peak Number 5 2-Heptanone, 4,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.275	9.46 ug/L	128650	1,4-Dichlorobenzene-d4	13.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptanone, 4,6-dimethyl-	142	C9H18O	019549-80-5	90
2			2-Heptanone, 4,6-dimethyl-	142	C9H18O	019549-80-5	87
3			trans-2,3-Epoxydecane	156	C10H20O	054125-39-2	46
4			Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	38
5			Octane, 3,4-dimethyl-	142	C10H22	015869-92-8	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW092024\
Data File : VW030184.D
Acq On : 20 Sep 2024 18:50
Operator : SY/MD
Sample : P4109-20
Misc : 4.93g/10mL/MSVOA_W/SOIL/A
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
A4EW2

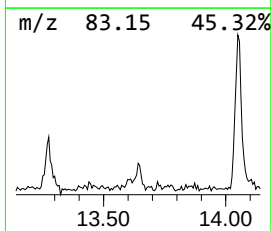
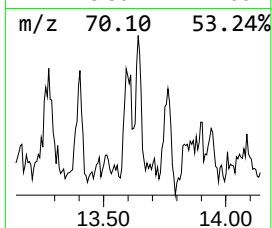
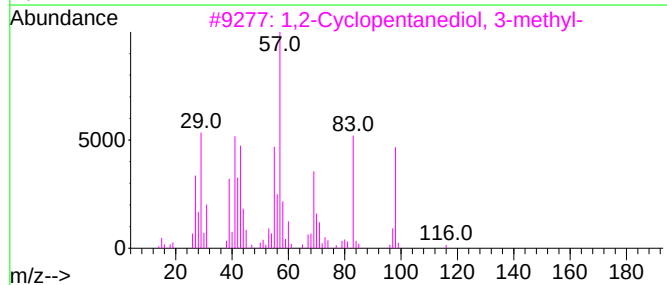
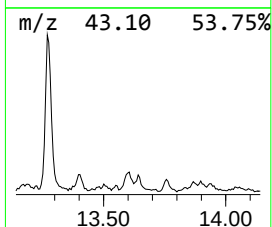
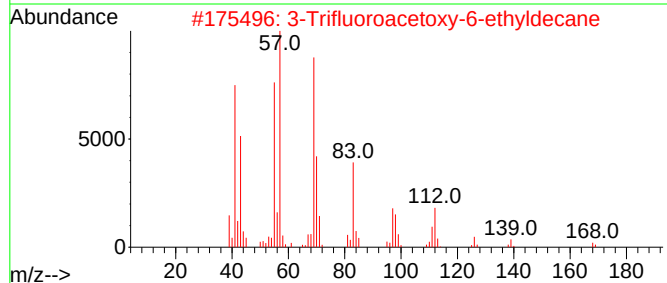
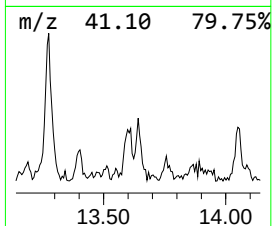
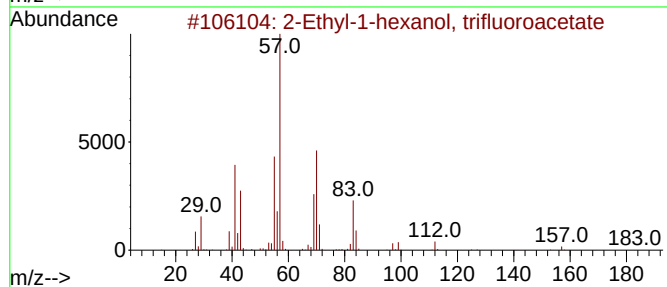
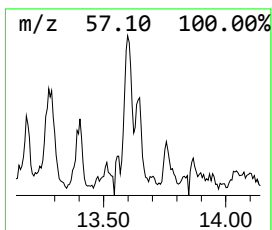
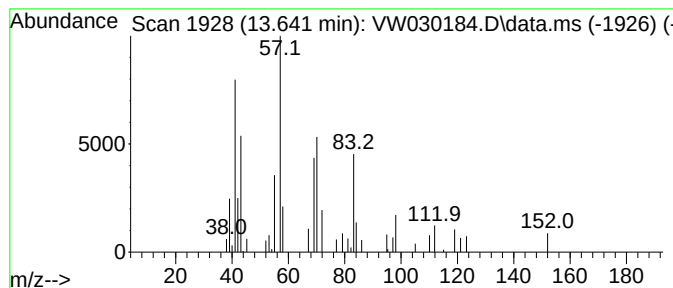
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Quant Title : SFAM01.0

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

Peak Number 6 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.641	1.25 ug/L	17039	1,4-Dichlorobenzene-d4	13.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Ethyl-1-hexanol, trifluoroacetate	226	C10H17F3O2	053800-08-1	40
2			3-Trifluoroacetoxy-6-ethyldecane	282	C14H25F3O2	116436-59-0	38
3			1,2-Cyclopentanediol, 3-methyl-	116	C6H12O2	027583-37-5	38
4			Octane, 2-chloro-	148	C8H17Cl	000628-61-5	32
5			3-Hexene, 2,2,5,5-tetramethyl-, ...	140	C10H20	000692-47-7	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW092024\
Data File : VW030184.D
Acq On : 20 Sep 2024 18:50
Operator : SY/MD
Sample : P4109-20
Misc : 4.93g/10mL/MSVOA_W/SOIL/A
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
A4EW2

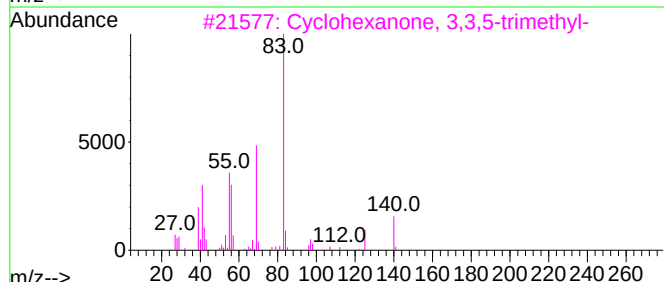
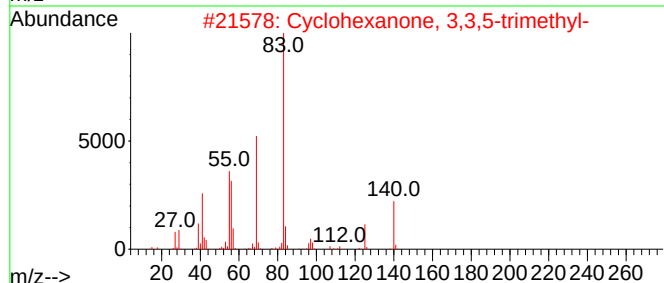
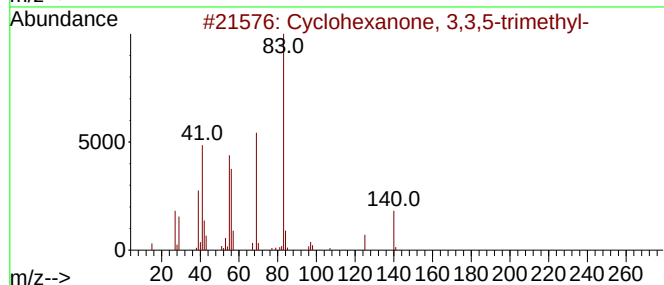
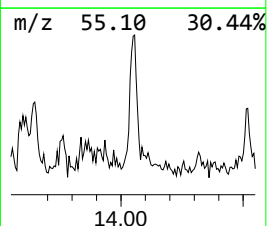
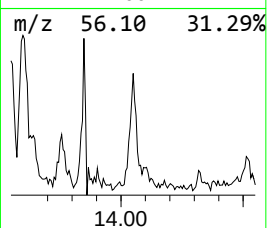
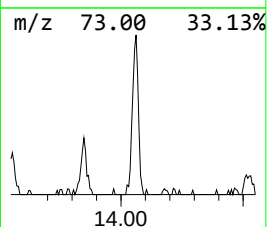
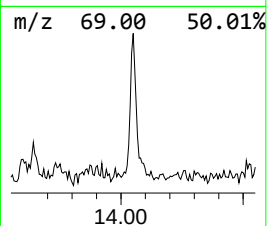
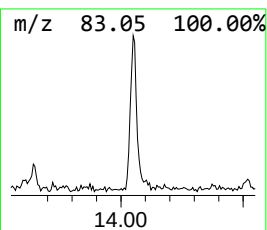
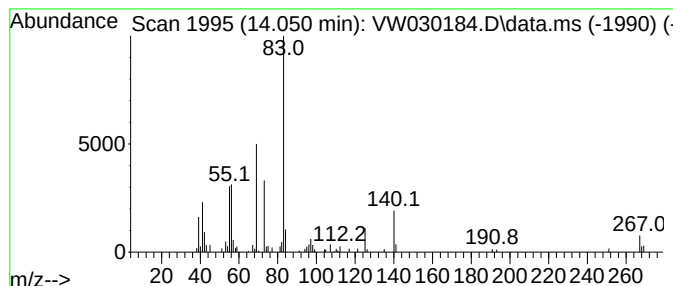
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Quant Title : SFAM01.0

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

Peak Number 7 Cyclohexanone, 3,3,5-trimet... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.050	2.79 ug/L	37894	1,4-Dichlorobenzene-d4	13.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	81
2			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	81
3			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	81
4			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	74
5			1H-1,2,4-Triazole, 3-(2-methylpr...	125	C6H11N3	040515-29-5	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW092024\
Data File : VW030184.D
Acq On : 20 Sep 2024 18:50
Operator : SY/MD
Sample : P4109-20
Misc : 4.93g/10mL/MSVOA_W/SOIL/A
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
A4EW2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM091624SMA.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
2-Heptanone, 5-...	12.928	1.5	ug/L	20654	3	13.550	340046	25.0
4-Heptanone, 2,...	13.032	2.7	ug/L	36853	3	13.550	340046	25.0
2-Heptanone, 4,...	13.275	9.5	ug/L	128650	3	13.550	340046	25.0
unknown-01	13.641	1.3	ug/L	17039	3	13.550	340046	25.0
Cyclohexanone, ...	14.050	2.8	ug/L	37894	3	13.550	340046	25.0