

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW092024\
 Data File : VW030183.D
 Acq On : 20 Sep 2024 18:26
 Operator : SY/MD
 Sample : P4109-19
 Misc : 5.20g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 A4EW1

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: VW030183.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.155	39	44	47	rBV3	2226	4740	0.36%	0.065%
2	2.363	72	78	94	rVB	72353	165771	12.74%	2.273%
3	2.899	158	166	184	rBV	54795	162360	12.48%	2.226%
4	3.296	230	231	236	rVB4	470	462	0.04%	0.006%
5	3.393	241	247	255	rVB5	1663	4036	0.31%	0.055%
6	3.466	257	259	263	rVB2	182	239	0.02%	0.003%
7	3.509	265	266	268	rBV	481	361	0.03%	0.005%
8	3.667	289	292	293	rBV	370	293	0.02%	0.004%
9	3.734	298	303	309	rVB6	538	1236	0.10%	0.017%
10	3.777	309	310	313	rVB	446	309	0.02%	0.004%
11	3.820	313	317	318	rBV2	369	248	0.02%	0.003%
12	3.875	323	326	329	rBV3	252	349	0.03%	0.005%
13	4.021	336	350	363	rBV	147495	456911	35.12%	6.264%
14	4.314	397	398	404	rVB3	306	474	0.04%	0.006%
15	4.387	407	410	412	rBV2	436	440	0.03%	0.006%
16	4.503	425	429	430	rBV	218	268	0.02%	0.004%
17	4.545	434	436	438	rBV2	282	294	0.02%	0.004%
18	4.606	438	446	447	rBV2	2199	3620	0.28%	0.050%
19	4.917	488	497	513	rBV4	5195	19025	1.46%	0.261%
20	5.124	527	531	533	rVB2	251	237	0.02%	0.003%
21	5.765	632	636	638	rBV3	373	588	0.05%	0.008%
22	5.783	638	639	643	rVB4	285	362	0.03%	0.005%
23	5.941	657	665	676	rVV5	2216	7189	0.55%	0.099%
24	6.057	680	684	685	rVV	150	208	0.02%	0.003%
25	6.094	688	690	692	rBV2	216	240	0.02%	0.003%
26	6.179	702	704	707	rVB	174	201	0.02%	0.003%
27	6.234	709	713	715	rBV2	234	215	0.02%	0.003%
28	6.289	719	722	728	rVV3	482	1002	0.08%	0.014%
29	6.380	734	737	739	rBV2	272	209	0.02%	0.003%
30	6.423	739	744	746	rBV	207	333	0.03%	0.005%
31	6.685	786	787	791	rBV2	272	256	0.02%	0.004%
32	6.844	810	813	816	rBV	171	234	0.02%	0.003%
33	6.905	816	823	835	rBV4	1548	5004	0.38%	0.069%
34	7.075	843	851	859	rBV2	24493	81480	6.26%	1.117%
35	7.246	875	879	881	rVB3	419	552	0.04%	0.008%
36	7.392	902	903	906	rBV	317	263	0.02%	0.004%

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

37	7.435	906	910	911	rBV3	288	328	0.03%	0.004%
38	7.459	911	914	915	rVV3	317	306	0.02%	0.004%
39	7.478	915	917	918	rVB2	409	290	0.02%	0.004%
40	7.496	918	920	923	rBV3	183	213	0.02%	0.003%
41	7.648	934	945	958	rBV	216803	551405	42.38%	7.560%
42	7.740	958	960	962	rVB2	320	315	0.02%	0.004%
43	7.874	978	982	983	rVB2	175	201	0.02%	0.003%
44	7.929	989	991	994	rBV	264	298	0.02%	0.004%
45	7.984	999	1000	1006	rVB2	208	307	0.02%	0.004%
46	8.087	1015	1017	1019	rBV2	341	320	0.02%	0.004%
47	8.276	1038	1048	1063	rBV2	429039	1301026	100.00%	17.837%
48	8.502	1083	1085	1087	rBV3	317	293	0.02%	0.004%
49	8.526	1087	1089	1092	rVB3	243	203	0.02%	0.003%
50	8.697	1111	1117	1126	rVB5	1352	3284	0.25%	0.045%
51	8.758	1126	1127	1128	rBV	454	266	0.02%	0.004%
52	8.843	1132	1141	1156	rBV	508502	1007901	77.47%	13.818%
53	8.977	1162	1163	1166	rVB3	397	318	0.02%	0.004%
54	9.038	1167	1173	1175	rVV3	1059	1631	0.13%	0.022%
55	9.075	1175	1179	1180	rVV4	1320	1897	0.15%	0.026%
56	9.112	1184	1185	1189	rVV	557	306	0.02%	0.004%
57	9.270	1202	1211	1221	rBV	290642	587156	45.13%	8.050%
58	9.374	1226	1228	1230	rVB3	478	372	0.03%	0.005%
59	9.453	1239	1241	1244	rVB3	364	318	0.02%	0.004%
60	9.599	1262	1265	1268	rVB2	269	402	0.03%	0.006%
61	9.636	1268	1271	1272	rBV	230	234	0.02%	0.003%
62	9.660	1272	1275	1284	rVV7	1035	2582	0.20%	0.035%
63	9.721	1284	1285	1287	rVB	342	221	0.02%	0.003%
64	9.758	1289	1291	1296	rBV3	354	459	0.04%	0.006%
65	9.825	1298	1302	1304	rVB2	488	625	0.05%	0.009%
66	9.855	1304	1307	1308	rBV	271	246	0.02%	0.003%
67	9.874	1308	1310	1313	rVB	264	241	0.02%	0.003%
68	9.922	1317	1318	1321	rVB2	281	230	0.02%	0.003%
69	9.947	1321	1322	1324	rBV2	319	213	0.02%	0.003%
70	9.971	1324	1326	1327	rBV	275	259	0.02%	0.004%
71	10.032	1327	1336	1345	rBV	77452	144260	11.09%	1.978%
72	10.124	1349	1351	1359	rVB5	730	1434	0.11%	0.020%
73	10.319	1375	1383	1392	rBV	442008	800653	61.54%	10.977%
74	10.459	1405	1406	1407	rBV	451	229	0.02%	0.003%
75	10.575	1419	1425	1433	rBV	51451	89127	6.85%	1.222%
76	10.697	1438	1445	1452	rBV	9824	16531	1.27%	0.227%

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 Title : SFAM01.0

77	10.776	1456	1458	1463	rVB2	342	381	0.03%	0.005%
78	10.843	1464	1469	1470	rBV4	1288	1832	0.14%	0.025%
79	10.922	1476	1482	1496	rBV4	57592	138332	10.63%	1.897%
80	11.075	1503	1507	1513	rVB8	1116	2417	0.19%	0.033%
81	11.160	1519	1521	1528	rVB4	1410	1795	0.14%	0.025%
82	11.312	1544	1546	1547	rBV	704	518	0.04%	0.007%
83	11.410	1558	1562	1567	rVB6	1282	2509	0.19%	0.034%
84	11.471	1569	1572	1579	rVB3	2697	4510	0.35%	0.062%
85	11.629	1589	1598	1609	rBV	399129	668709	51.40%	9.168%
86	11.837	1622	1632	1637	rBV5	5369	11977	0.92%	0.164%
87	12.081	1670	1672	1674	rBV3	847	995	0.08%	0.014%
88	12.330	1711	1713	1714	rBV2	811	520	0.04%	0.007%
89	12.465	1731	1735	1742	rBV6	3154	5506	0.42%	0.075%
90	12.599	1754	1757	1763	rVB2	8359	12800	0.98%	0.175%
91	12.690	1766	1772	1779	rVB	142917	229970	17.68%	3.153%
92	12.861	1796	1800	1803	rBV3	4666	7868	0.60%	0.108%
93	12.928	1807	1811	1818	rVB4	8682	16869	1.30%	0.231%
94	13.025	1823	1827	1835	rVB	27500	45010	3.46%	0.617%
95	13.275	1860	1868	1880	rVB2	72199	158467	12.18%	2.173%
96	13.556	1908	1914	1920	rBV	155597	263694	20.27%	3.615%
97	13.641	1926	1928	1933	rVB3	12616	16105	1.24%	0.221%
98	13.849	1956	1962	1968	rBV	109965	186971	14.37%	2.563%
99	14.050	1990	1995	2009	rVB2	27512	65120	5.01%	0.893%
100	15.123	2167	2171	2174	rBV6	7601	14159	1.09%	0.194%

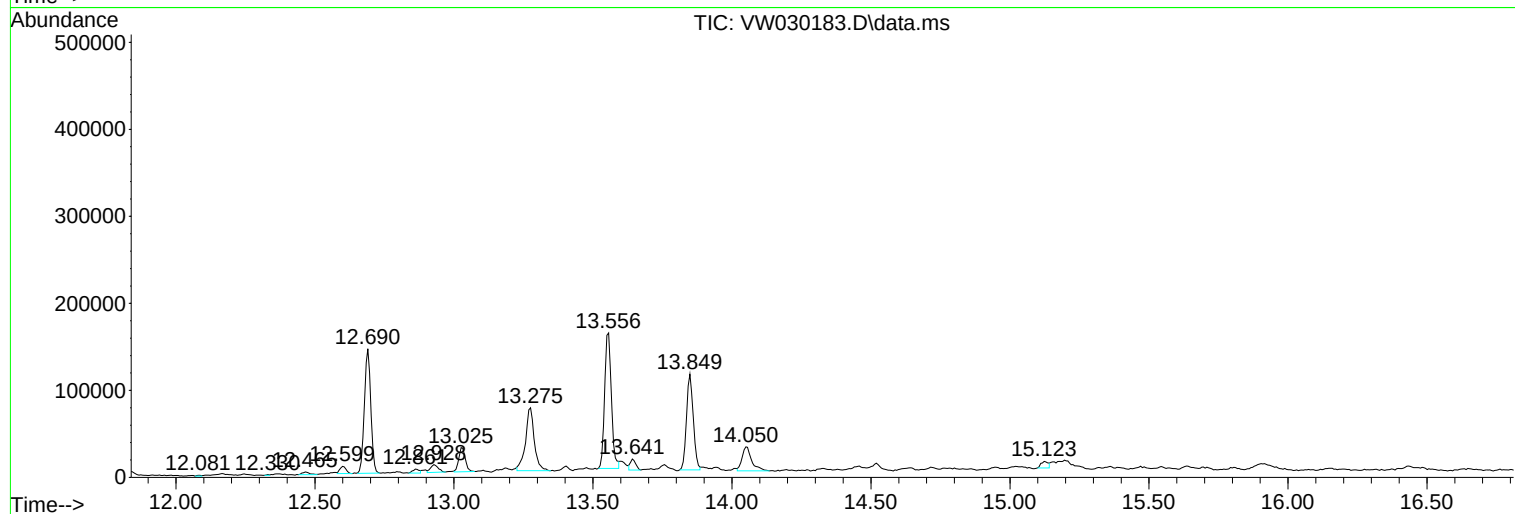
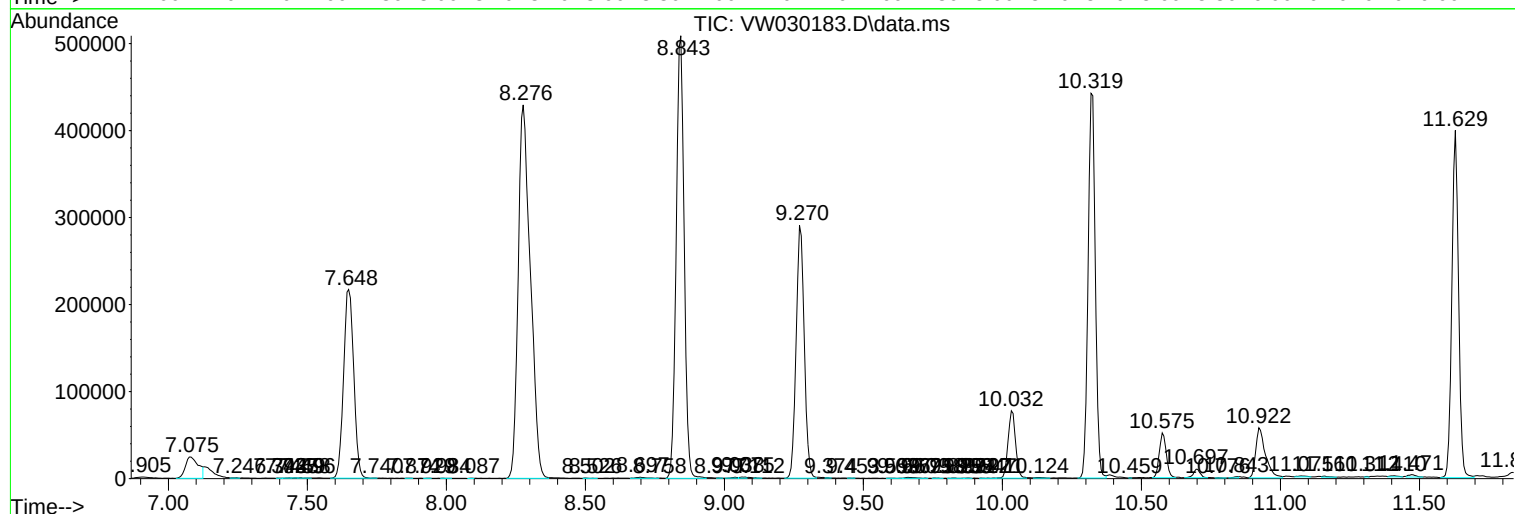
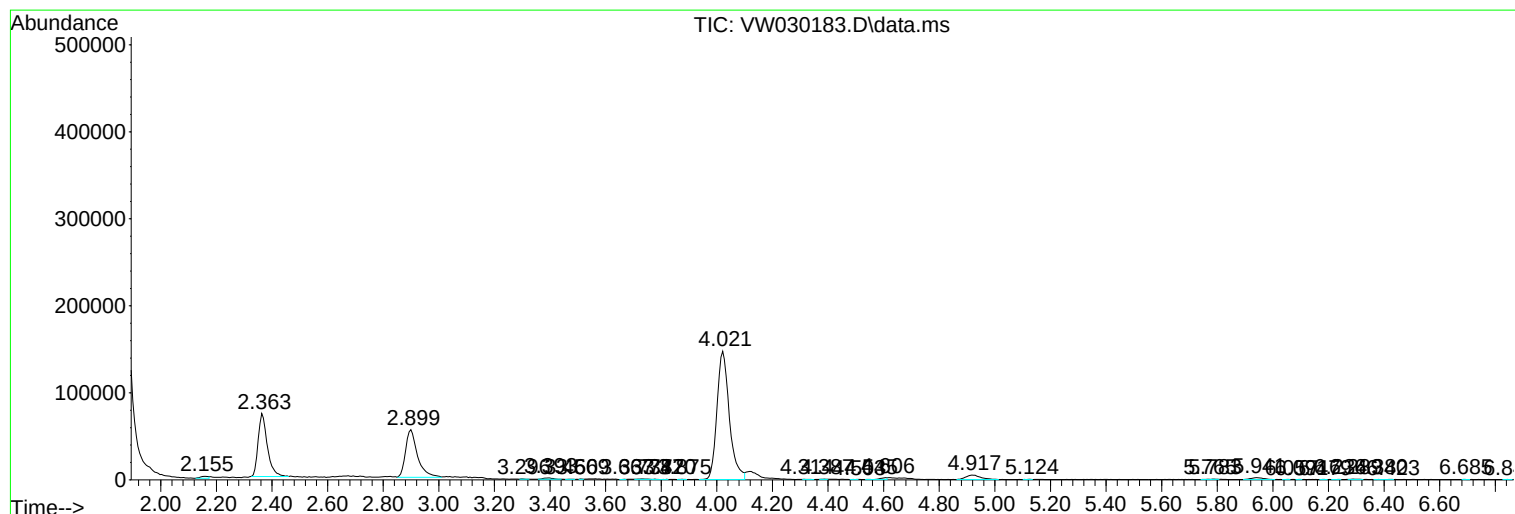
Sum of corrected areas: 7293943

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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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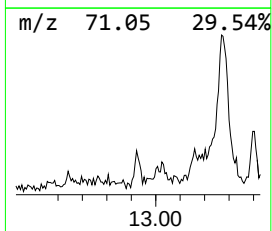
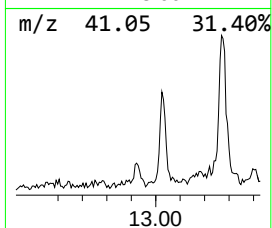
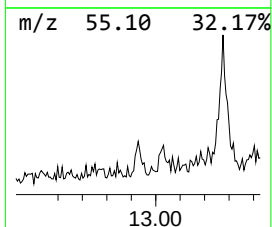
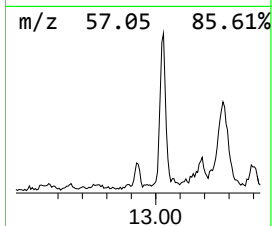
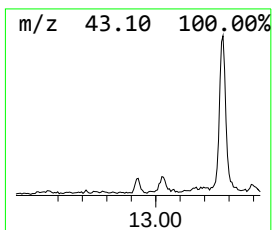
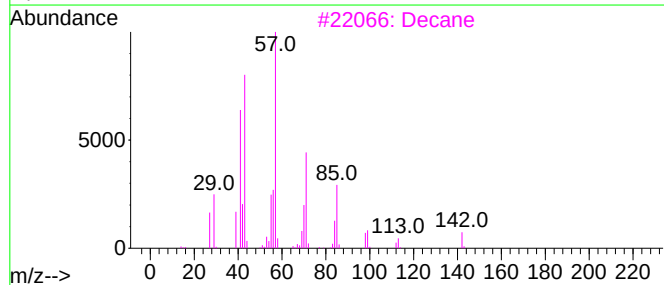
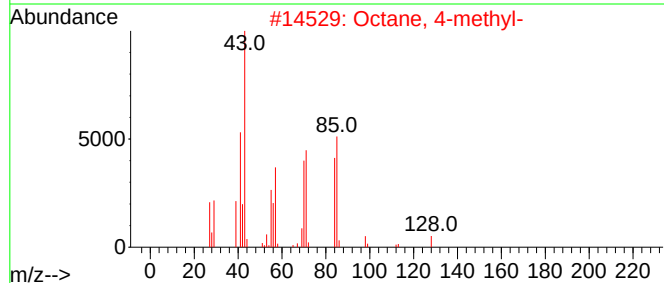
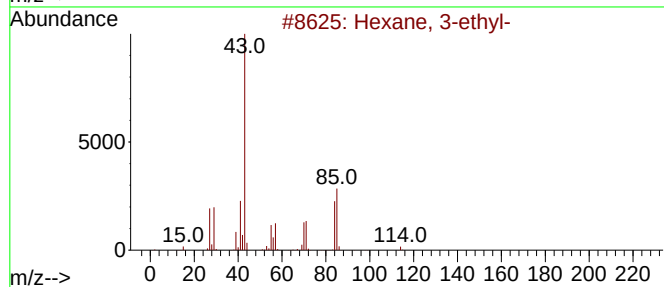
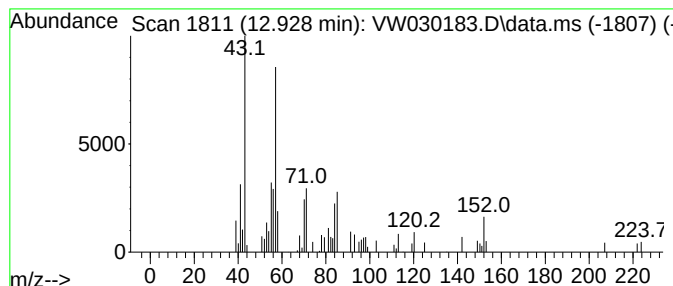
Instrument :
MSVOA_W
ClientSampleId :
A4EW1

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 2 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.928	1.60 ug/L	16869	1,4-Dichlorobenzene-d4		13.550	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexane, 3-ethyl-		114	C8H18	000619-99-8	47
2	Octane, 4-methyl-		128	C9H20	002216-34-4	47
3	Decane		142	C10H22	000124-18-5	47
4	1-Octanol, 2-butyl-		186	C12H26O	003913-02-8	47
5	1-Decanol, 2-ethyl-		186	C12H26O	021078-65-9	43



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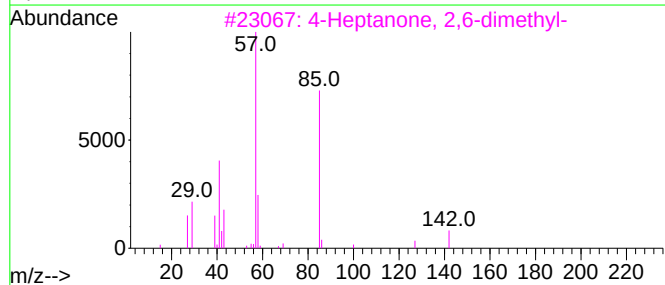
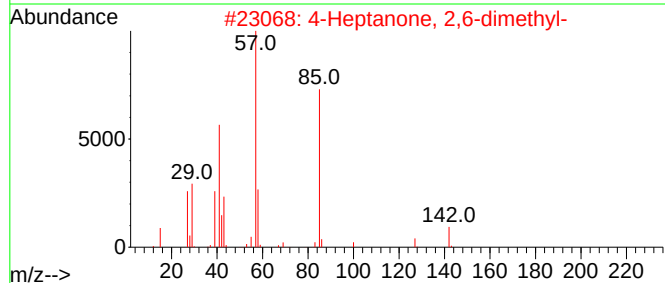
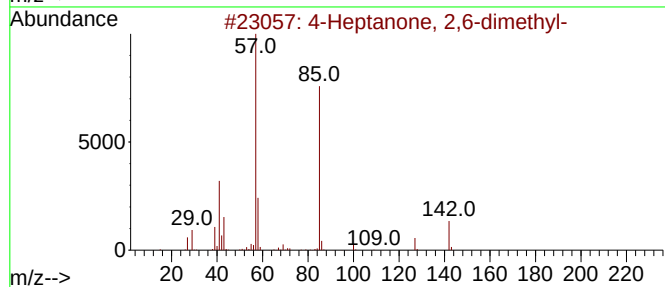
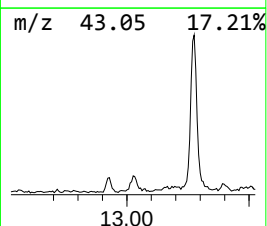
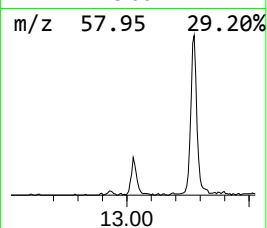
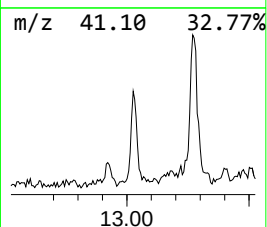
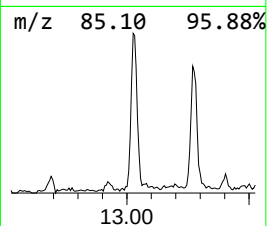
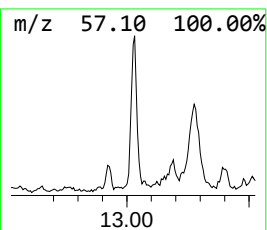
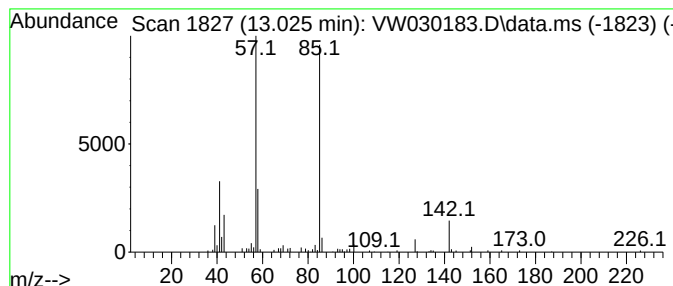
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM091624SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 4-Heptanone, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.025	4.27 ug/L	45010	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	94
2			4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	91
3			4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	91
4			4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	91
5			4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	90



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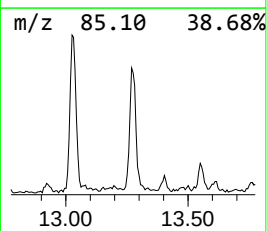
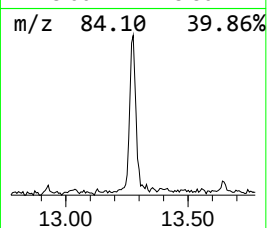
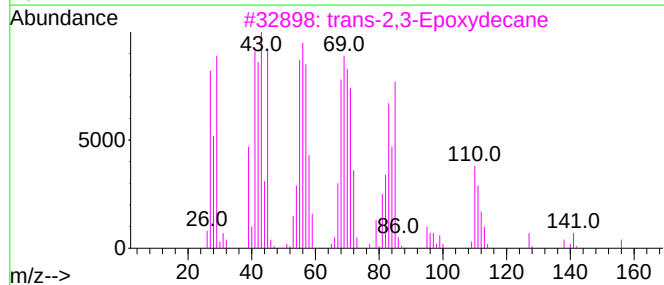
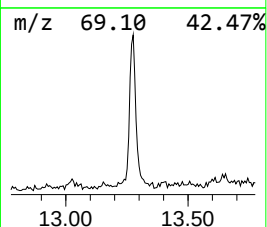
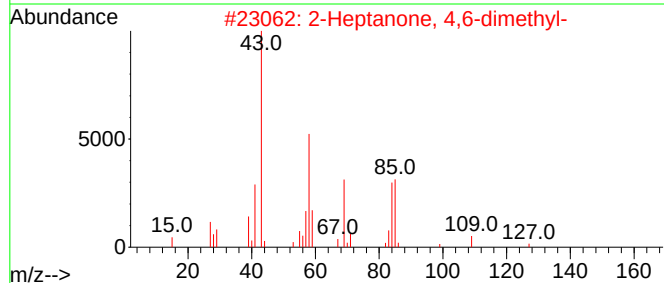
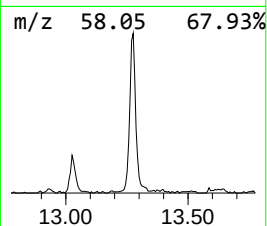
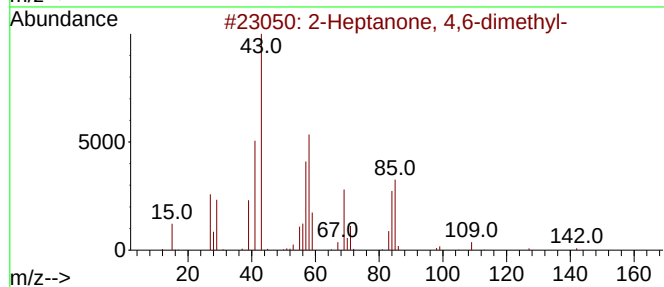
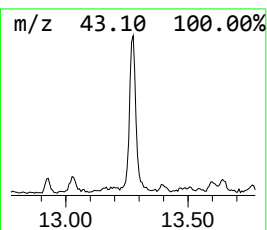
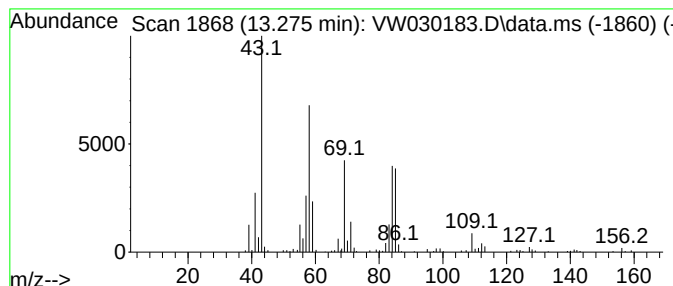
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM091624SMA.M
Quant Title : SFAM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.275	15.02 ug/L	158467	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	91
2			2-Heptanone, 4,6-dimethyl-	142	C9H18O	019549-80-5	86
3			trans-2,3-Epoxydecane	156	C10H20O	054125-39-2	43
4			2-Nonanone, 9-[(tetrahydro-2H-py...	242	C14H26O3	054699-41-1	43
5			Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW092024\
Data File : VW030183.D
Acq On : 20 Sep 2024 18:26
Operator : SY/MD
Sample : P4109-19
Misc : 5.20g/10mL/MSVOA_W/SOIL/A
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
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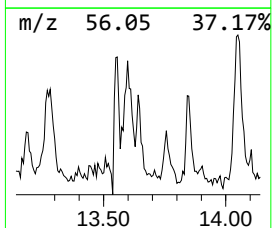
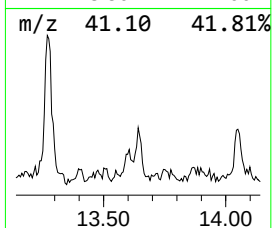
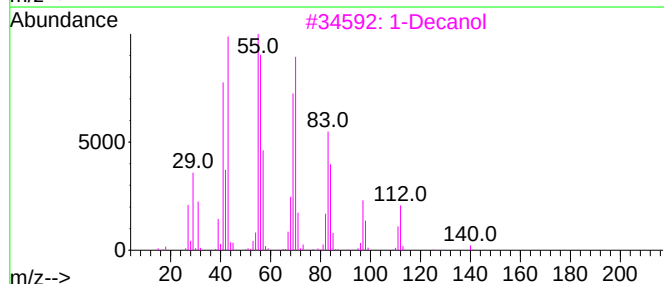
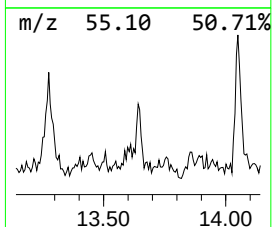
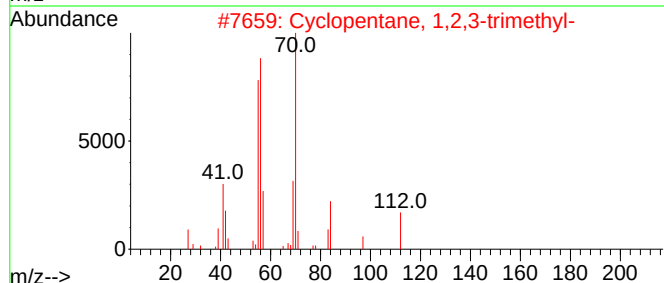
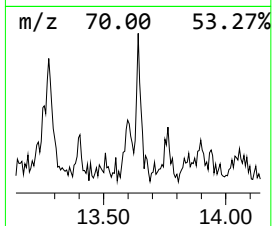
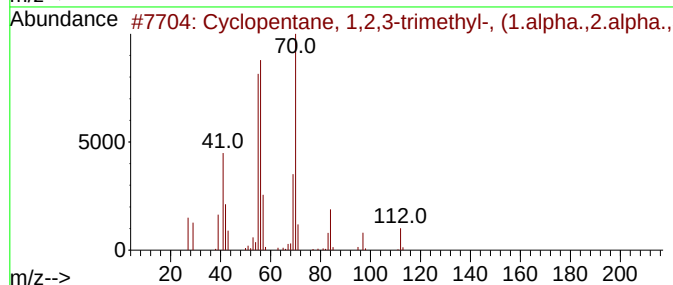
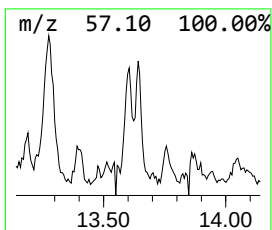
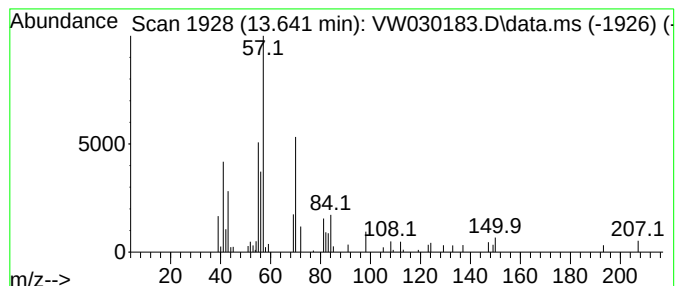
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Quant Title : SFAM01.0

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

Peak Number 5 (DEL) Alkane: Cyclic13.641 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.641	1.53 ug/L	16105	1,4-Dichlorobenzene-d4	13.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	015890-40-1	49
2			Cyclopentane, 1,2,3-trimethyl-	112	C8H16	002815-57-8	47
3			1-Decanol	158	C10H22O	000112-30-1	43
4			Formic acid, 2-ethylhexyl ester	158	C9H18O2	1000368-94-7	42
5			1-Hexanethiol, 2-ethyl-	146	C8H18S	007341-17-5	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW092024\
Data File : VW030183.D
Acq On : 20 Sep 2024 18:26
Operator : SY/MD
Sample : P4109-19
Misc : 5.20g/10mL/MSVOA_W/SOIL/A
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
A4EW1

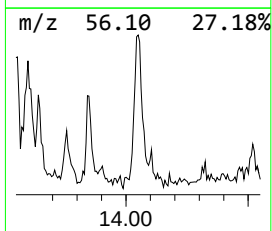
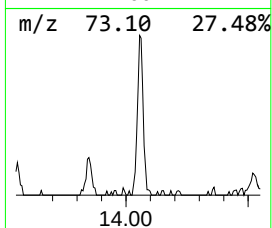
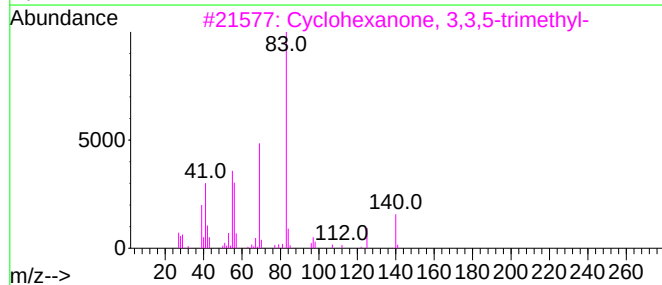
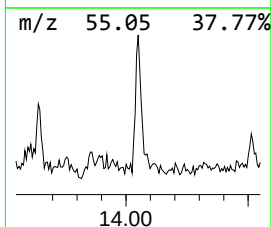
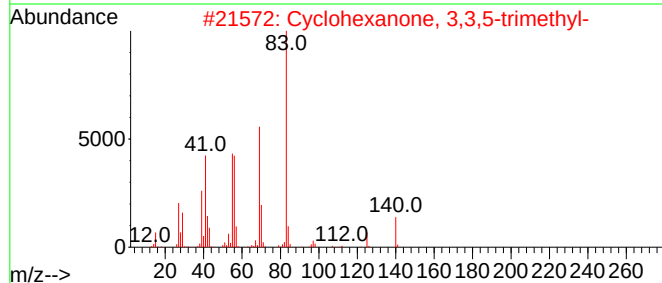
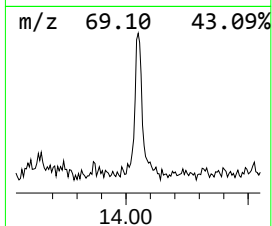
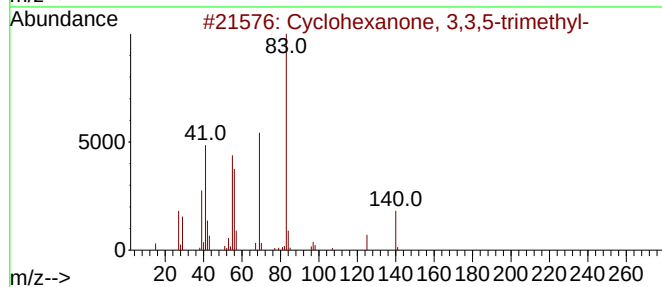
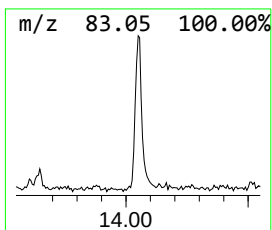
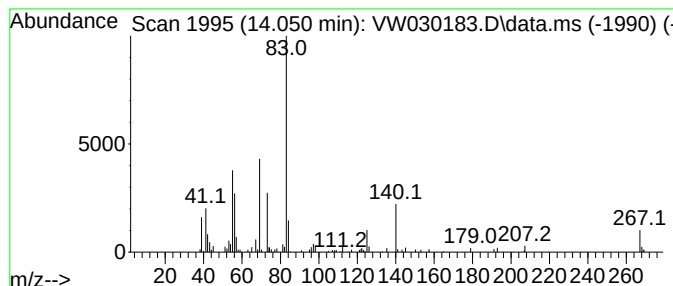
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Quant Title : SFAM01.0

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

Peak Number 6 Cyclohexanone, 3,3,5-trimet... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.050	6.17 ug/L	65120	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	74
3			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	68
4			2,4,6-Trimethyl-3-heptene	140	C10H20	1000113-56-9	40
5			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW092024\
Data File : VW030183.D
Acq On : 20 Sep 2024 18:26
Operator : SY/MD
Sample : P4109-19
Misc : 5.20g/10mL/MSVOA_W/SOIL/A
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
A4EW1

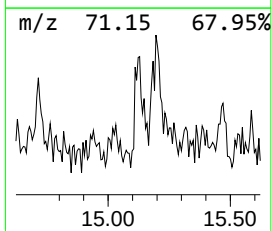
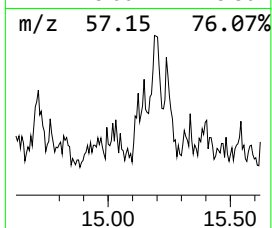
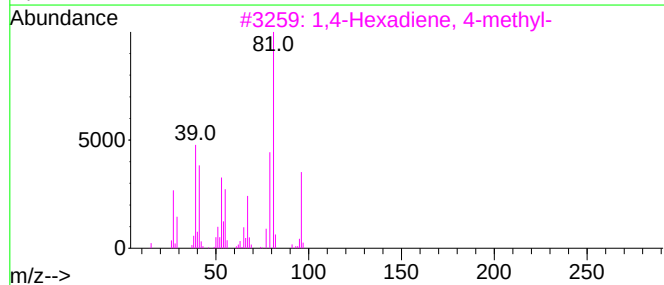
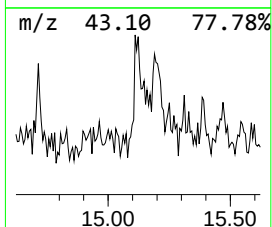
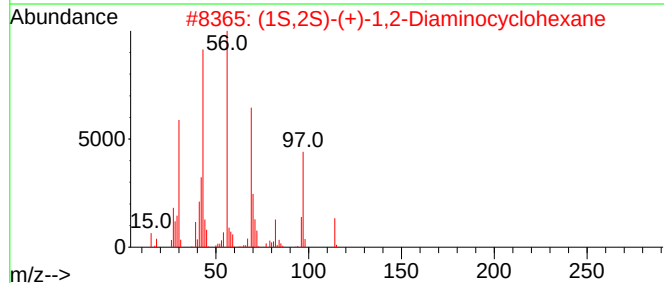
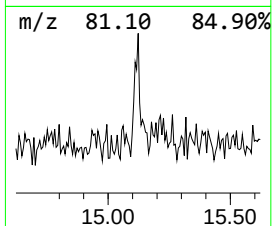
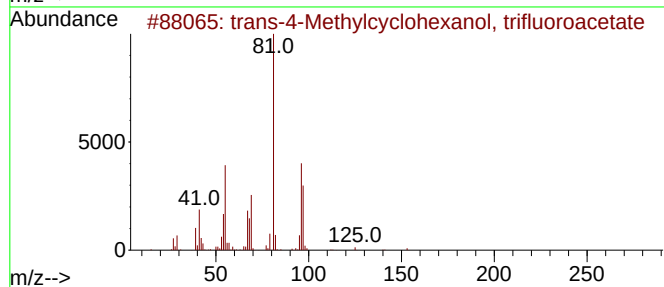
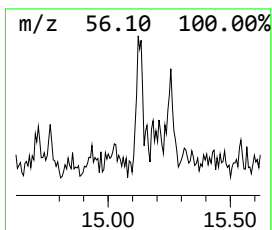
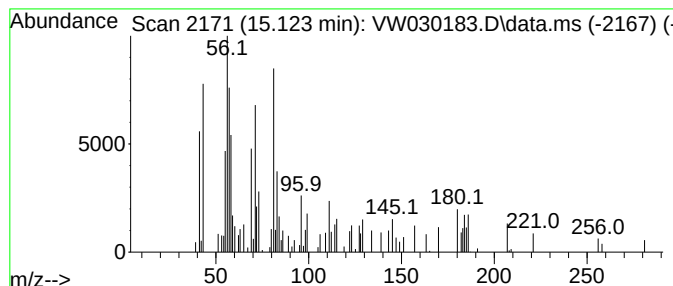
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Quant Title : SFAM01.0

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

Peak Number 7 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.123	1.34 ug/L	14159	1,4-Dichlorobenzene-d4	13.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-4-Methylcyclohexanol, trif...	210	C9H13F3O2	1000364-13-8	22
2			(1S,2S)-(+)-1,2-Diaminocyclohexane	114	C6H14N2	021436-03-3	22
3			1,4-Hexadiene, 4-methyl-	96	C7H12	001116-90-1	22
4			Cyclopentene, 4,4-dimethyl-	96	C7H12	019037-72-0	22
5			2,4-Hexadiene, 3-methyl-	96	C7H12	028823-42-9	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW092024\
Data File : VW030183.D
Acq On : 20 Sep 2024 18:26
Operator : SY/MD
Sample : P4109-19
Misc : 5.20g/10mL/MSVOA_W/SOIL/A
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
A4EW1

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
(DEL) Alkane: S...	12.928	1.6	ug/L	16869	3	13.550	263694	25.0
4-Heptanone, 2,...	13.025	4.3	ug/L	45010	3	13.550	263694	25.0
2-Heptanone, 4,...	13.275	15.0	ug/L	158467	3	13.550	263694	25.0
(DEL) Alkane: C...	13.641	1.5	ug/L	16105	3	13.550	263694	25.0
Cyclohexanone, ...	14.050	6.2	ug/L	65120	3	13.550	263694	25.0
unknown-01	15.123	1.3	ug/L	14159	3	13.550	263694	25.0