

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW122322\
 Data File : VW025203.D
 Acq On : 23 Dec 2022 17:43
 Operator : SY/MD
 Sample : N6171-07RE
 Misc : 7.13g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 GBQC5RE

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\SFAMWLM120822SMA.M
 Title : SFAM01.0

Signal : TIC: VW025203.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.172	39	44	50	rVB	40152	56297	0.08%	0.064%
2	2.349	67	73	83	rVB2	145482	242018	0.33%	0.276%
3	2.495	91	97	117	rVB	61327	133907	0.18%	0.153%
4	2.660	117	124	126	rBV6	3328	7708	0.01%	0.009%
5	2.806	145	148	152	rVV	3815	5692	0.01%	0.006%
6	2.885	153	161	171	rVB	75280	160317	0.22%	0.183%
7	3.019	176	183	193	rBV	28490	63863	0.09%	0.073%
8	3.196	210	212	216	rVB2	1056	1148	0.00%	0.001%
9	3.385	233	243	257	rBV	251207	584135	0.79%	0.666%
10	4.013	333	346	357	rBV	200845	591598	0.80%	0.675%
11	4.123	357	364	376	rVB	50257	134088	0.18%	0.153%
12	4.379	399	406	414	rVV3	2935	8562	0.01%	0.010%
13	4.666	446	453	454	rBV2	989	1301	0.00%	0.001%
14	4.915	482	494	520	rVB5	16475	78742	0.11%	0.090%
15	5.434	569	579	589	rBV5	5718	18948	0.03%	0.022%
16	5.787	624	637	649	rBV	11667	39232	0.05%	0.045%
17	5.940	652	662	674	rVB3	10479	31632	0.04%	0.036%
18	6.104	685	689	691	rBV3	1177	1650	0.00%	0.002%
19	6.220	697	708	718	rVB2	6939	19951	0.03%	0.023%
20	6.903	809	820	828	rBV2	8575	27001	0.04%	0.031%
21	6.982	829	833	839	rVV4	4292	9745	0.01%	0.011%
22	7.080	839	849	857	rVV	103604	290870	0.39%	0.332%
23	7.171	857	864	880	rVB2	88541	248715	0.34%	0.284%
24	7.537	919	924	927	rBV3	816	1442	0.00%	0.002%
25	7.647	931	942	955	rBV	306459	750581	1.02%	0.856%
26	7.872	969	979	985	rBV2	11966	31466	0.04%	0.036%
27	8.031	999	1005	1007	rBV3	1095	1901	0.00%	0.002%
28	8.153	1016	1025	1033	rBV5	3282	7603	0.01%	0.009%
29	8.275	1035	1045	1061	rBV2	574988	1801197	2.44%	2.055%
30	8.494	1079	1081	1084	rBV3	1507	1969	0.00%	0.002%
31	8.549	1084	1090	1101	rVB6	12593	32746	0.04%	0.037%
32	8.622	1101	1102	1107	rVB3	1107	1368	0.00%	0.002%
33	8.707	1107	1116	1125	rBV4	14436	36423	0.05%	0.042%
34	8.842	1129	1138	1150	rBV	574920	1135935	1.54%	1.296%
35	9.092	1167	1179	1196	rBV	629341	1234019	1.67%	1.408%
36	9.274	1200	1209	1217	rBV	422090	866310	1.17%	0.988%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM120822SMA.M
 Title : SFAM01.0

37	9.409	1225	1231	1243	rVB	13052	28346	0.04%	0.032%
38	9.512	1243	1248	1256	rVB4	1856	4104	0.01%	0.005%
39	9.604	1256	1263	1268	rBV2	1278	2675	0.00%	0.003%
40	9.659	1268	1272	1280	rBV5	3666	7526	0.01%	0.009%
41	9.890	1305	1310	1315	rBV4	755	1710	0.00%	0.002%
42	9.957	1315	1321	1325	rBV5	1785	3873	0.01%	0.004%
43	10.037	1326	1334	1341	rBV	212251	386673	0.52%	0.441%
44	10.122	1346	1348	1355	rVB3	3171	5218	0.01%	0.006%
45	10.219	1360	1364	1368	rVB4	924	1836	0.00%	0.002%
46	10.323	1372	1381	1388	rBV	654067	1163439	1.58%	1.327%
47	10.384	1388	1391	1397	rVB	21176	35386	0.05%	0.040%
48	10.500	1404	1410	1416	rVB7	4305	9073	0.01%	0.010%
49	10.579	1416	1423	1429	rBV	132009	239576	0.32%	0.273%
50	10.701	1438	1443	1449	rVB3	13715	22811	0.03%	0.026%
51	10.756	1449	1452	1455	rBV4	990	1267	0.00%	0.001%
52	10.866	1460	1470	1477	rBV	38598124	73735065	100.00%	84.128%
53	10.921	1477	1479	1495	rVV	355148	563358	0.76%	0.643%
54	11.073	1499	1504	1516	rVV2	20499	47089	0.06%	0.054%
55	11.170	1518	1520	1527	rVB4	2656	4284	0.01%	0.005%
56	11.402	1552	1558	1565	rVB9	3594	7837	0.01%	0.009%
57	11.506	1570	1575	1579	rBV6	1331	2301	0.00%	0.003%
58	11.628	1588	1595	1605	rVB	519711	859879	1.17%	0.981%
59	11.731	1605	1612	1619	rBV	14371	24278	0.03%	0.028%
60	11.841	1625	1630	1633	rBV4	4238	6604	0.01%	0.008%
61	11.939	1643	1646	1656	rVB6	4907	8961	0.01%	0.010%
62	12.097	1669	1672	1677	rBV5	769	1330	0.00%	0.002%
63	12.158	1677	1682	1690	rVB9	2515	5474	0.01%	0.006%
64	12.335	1707	1711	1722	rVB5	7819	13442	0.02%	0.015%
65	12.451	1727	1730	1733	rBV4	763	1162	0.00%	0.001%
66	12.603	1749	1755	1760	rVB2	19961	31413	0.04%	0.036%
67	12.688	1760	1769	1777	rBV	374885	616094	0.84%	0.703%
68	12.749	1777	1779	1783	rVB4	1162	1783	0.00%	0.002%
69	12.798	1783	1787	1792	rVB7	1178	2001	0.00%	0.002%
70	12.877	1797	1800	1804	rBV5	1226	1862	0.00%	0.002%
71	12.932	1804	1809	1814	rVV4	5407	8686	0.01%	0.010%
72	13.048	1822	1828	1835	rBV7	2221	5478	0.01%	0.006%
73	13.158	1840	1846	1848	rBV6	867	1509	0.00%	0.002%
74	13.182	1848	1850	1856	rVV4	1746	2611	0.00%	0.003%
75	13.268	1858	1864	1875	rVB	12029	27395	0.04%	0.031%
76	13.396	1880	1885	1892	rBV5	6594	12771	0.02%	0.015%

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 Title : SFAM01.0

77	13.499	1893	1902	1906	rBV	36426	60132	0.08%	0.069%
78	13.554	1906	1911	1922	rVV	244381	400283	0.54%	0.457%
79	13.646	1922	1926	1931	rVB4	8687	14071	0.02%	0.016%
80	13.755	1938	1944	1947	rBV6	2788	4532	0.01%	0.005%
81	13.847	1953	1959	1965	rBV	199005	348742	0.47%	0.398%
82	13.902	1965	1968	1973	rVV2	16363	24478	0.03%	0.028%
83	13.944	1973	1975	1980	rVB4	5045	7038	0.01%	0.008%
84	14.005	1982	1985	1989	rBV5	2459	4285	0.01%	0.005%
85	14.066	1990	1995	2000	rVB2	11799	17971	0.02%	0.021%
86	14.322	2030	2037	2042	rBV8	7209	14495	0.02%	0.017%
87	14.493	2062	2065	2067	rBV4	1755	2456	0.00%	0.003%
88	14.517	2067	2069	2074	rVB6	3602	4335	0.01%	0.005%
89	14.688	2093	2097	2099	rBV4	5336	7379	0.01%	0.008%
90	14.719	2099	2102	2107	rVB4	7517	10154	0.01%	0.012%
91	14.987	2144	2146	2148	rVV3	1399	1694	0.00%	0.002%
92	15.249	2186	2189	2193	rVB4	3566	4409	0.01%	0.005%
93	15.395	2208	2213	2221	rVB	52806	86725	0.12%	0.099%
94	15.481	2221	2227	2233	rBV	14227	28820	0.04%	0.033%
95	15.590	2243	2245	2252	rVB6	2872	4480	0.01%	0.005%
96	15.670	2256	2258	2260	rBV3	1693	1659	0.00%	0.002%
97	15.755	2269	2272	2273	rBV2	1766	2185	0.00%	0.002%
98	15.792	2273	2278	2284	rVB5	11376	20319	0.03%	0.023%
99	15.956	2298	2305	2311	rBV10	3211	8448	0.01%	0.010%
100	16.084	2323	2326	2328	rBV3	1246	1357	0.00%	0.002%

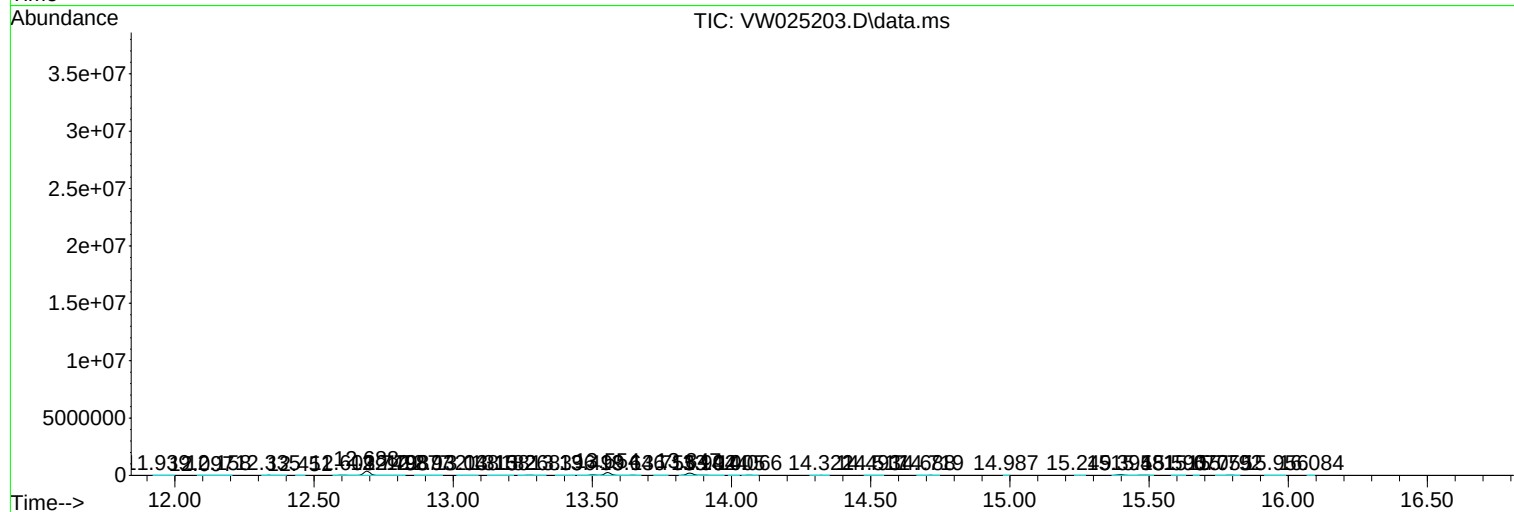
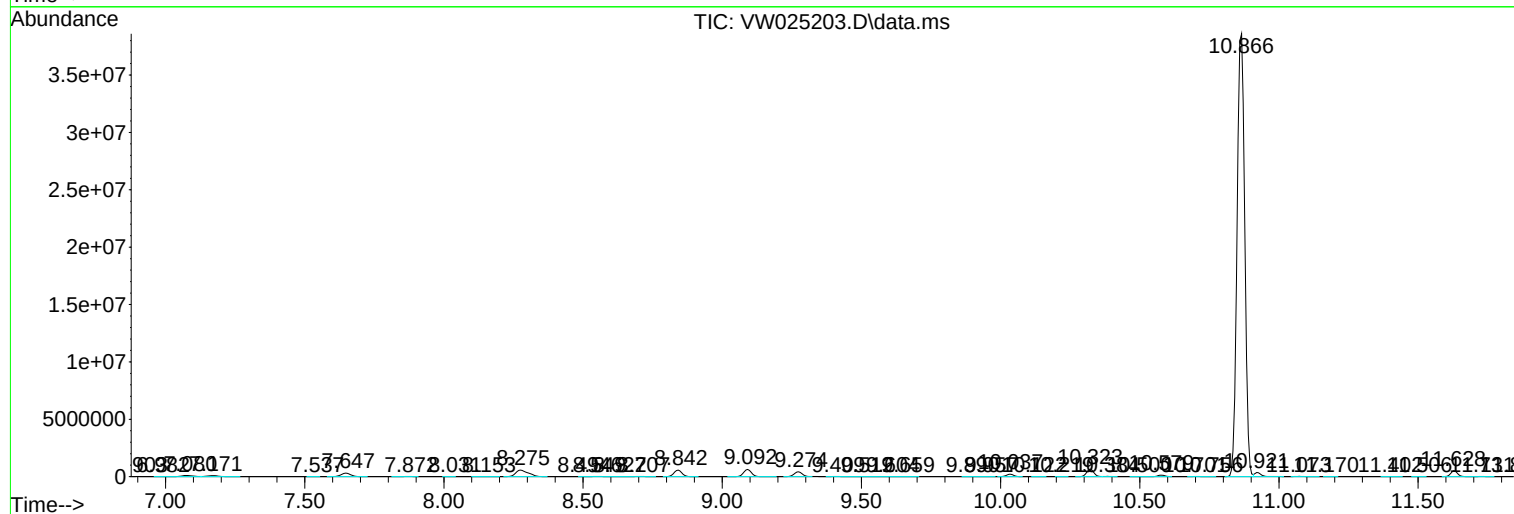
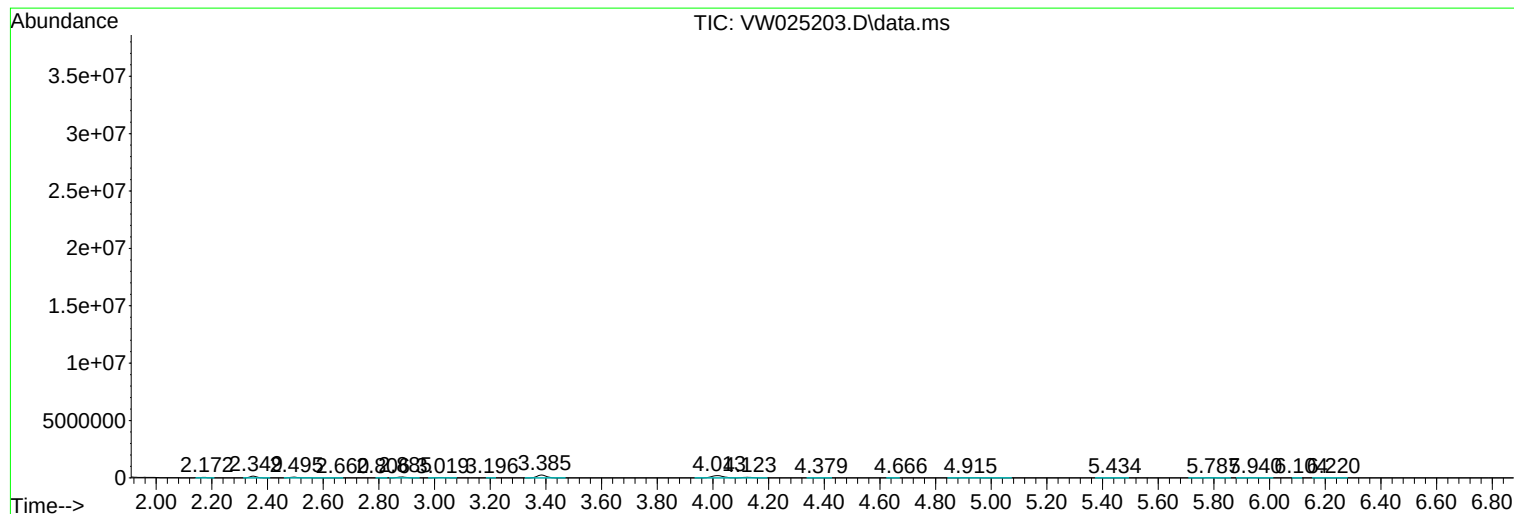
Sum of corrected areas: 87646707

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM120822SMA.M
Quant Title : SFAM01.0

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



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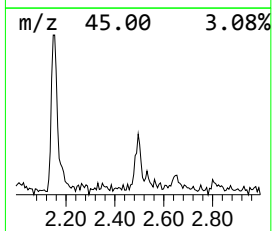
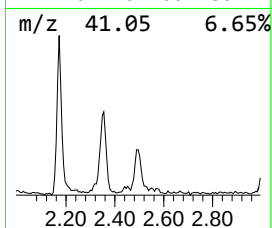
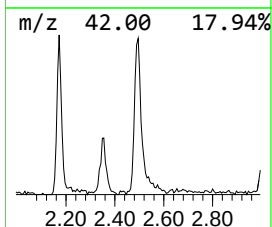
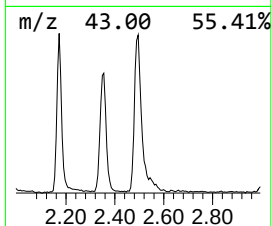
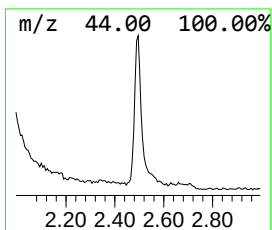
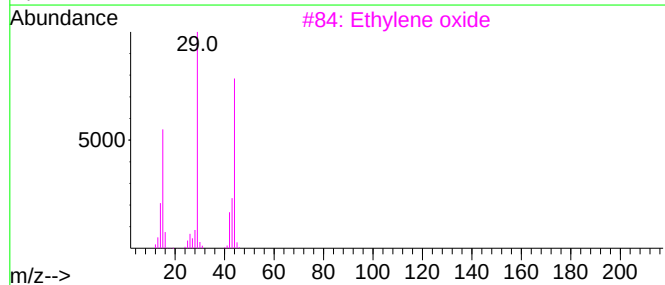
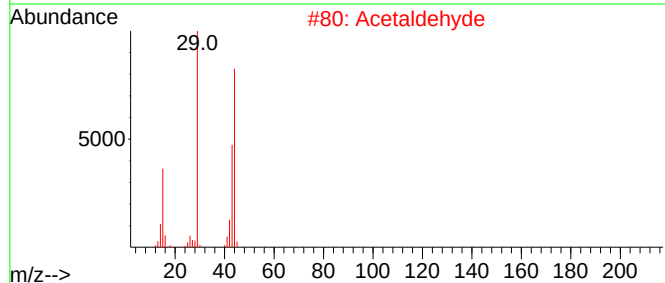
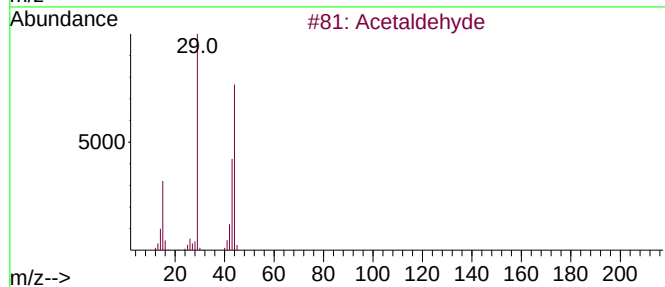
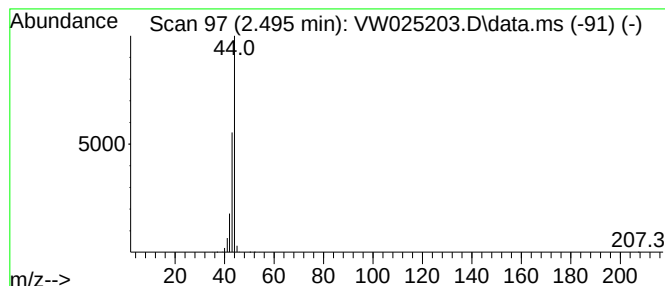
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM120822SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 Acetaldehyde Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.495	2.95 ug/L	133907	1,4-Difluorobenzene	8.842

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	64
2			Acetaldehyde	44	C2H4O	000075-07-0	64
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			Ethylene oxide	44	C2H4O	000075-21-8	5
5			Ethylene oxide	44	C2H4O	000075-21-8	5



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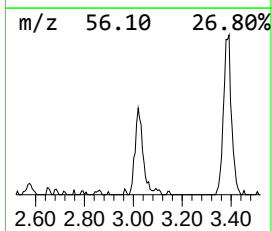
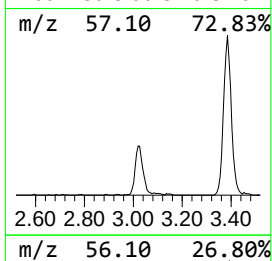
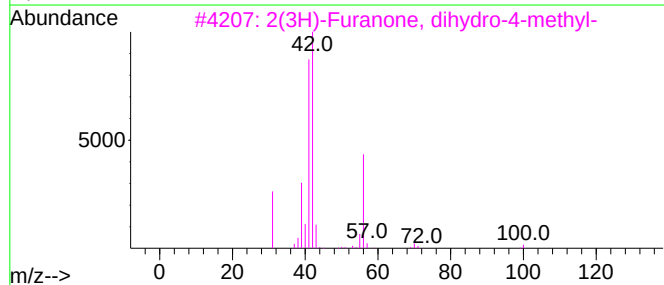
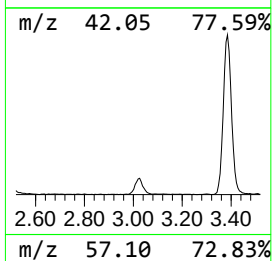
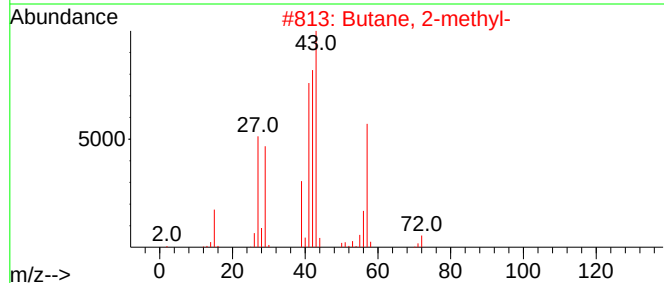
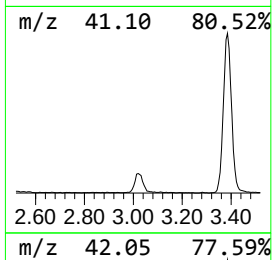
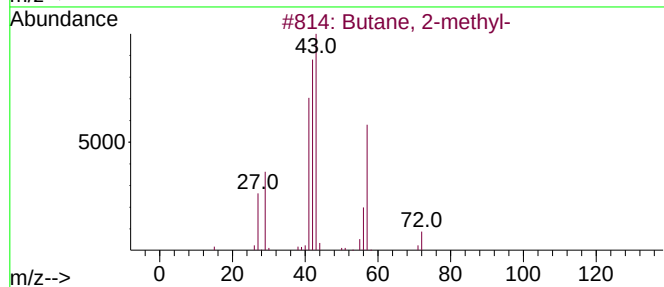
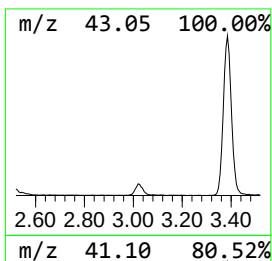
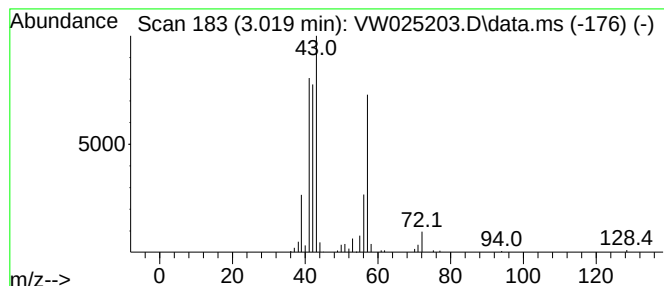
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM120822SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.019	1.41 ug/L	63863	1,4-Difluorobenzene	8.842

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methyl-	72	C5H12	000078-78-4	86
2		Butane, 2-methyl-	72	C5H12	000078-78-4	86
3		2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	53
4		Pentane	72	C5H12	000109-66-0	45
5		Oxirane, trimethyl-	86	C5H10O	005076-19-7	42



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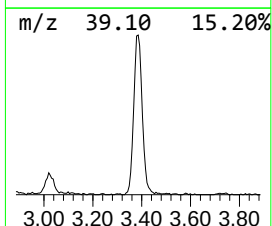
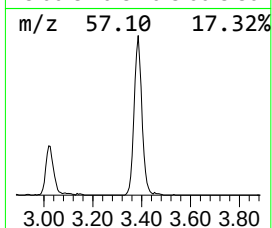
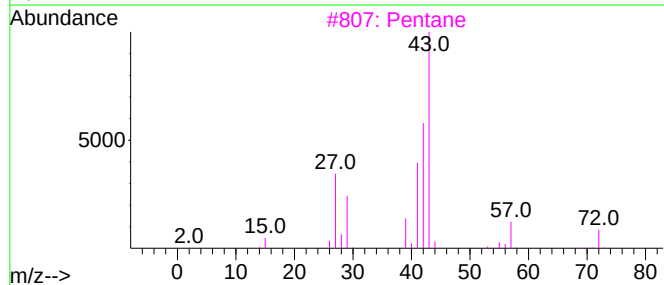
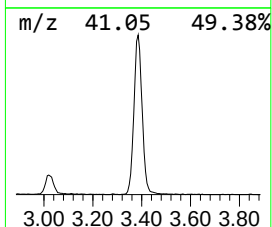
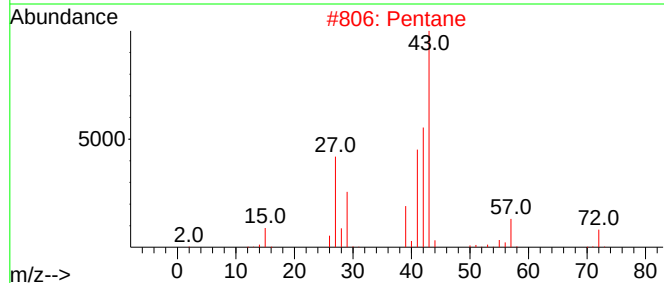
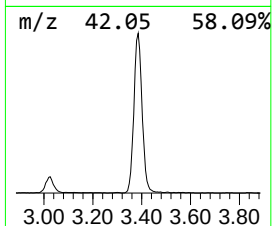
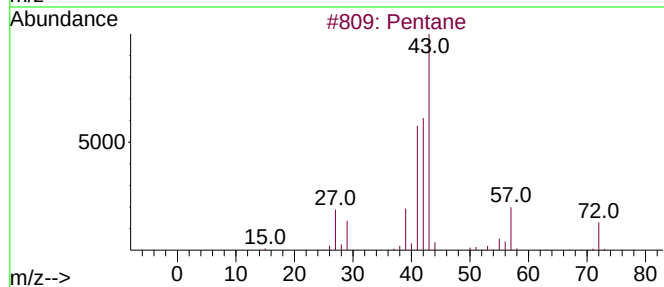
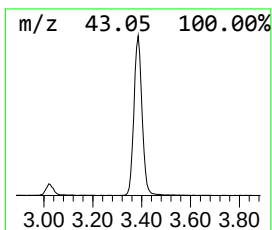
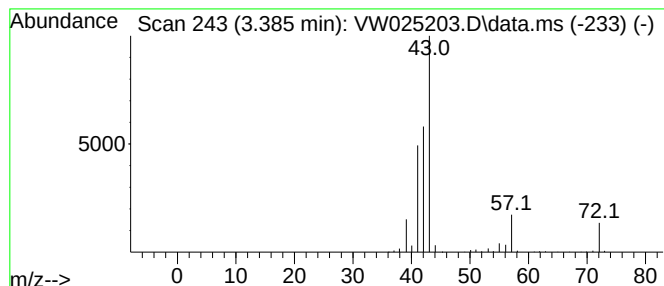
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM120822SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.385	12.86 ug/L	584135	1,4-Difluorobenzene	8.842

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane		72	C5H12	000109-66-0	91
2	Pentane		72	C5H12	000109-66-0	86
3	Pentane		72	C5H12	000109-66-0	86
4	Pentane		72	C5H12	000109-66-0	86
5	Pentane		72	C5H12	000109-66-0	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW122322\
Data File : VW025203.D
Acq On : 23 Dec 2022 17:43
Operator : SY/MD
Sample : N6171-07RE
Misc : 7.13g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
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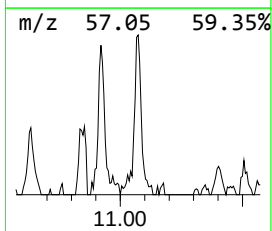
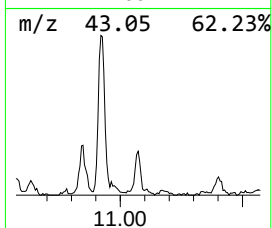
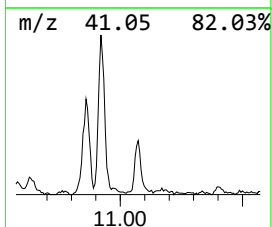
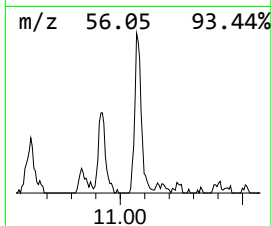
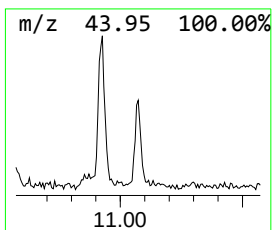
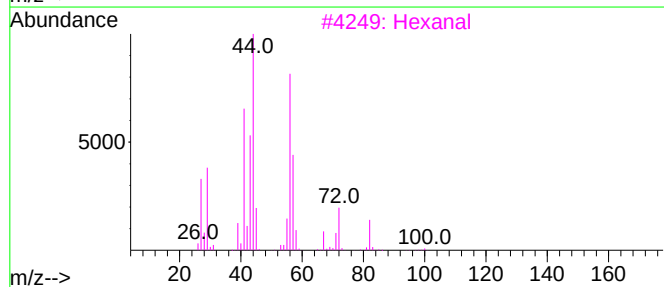
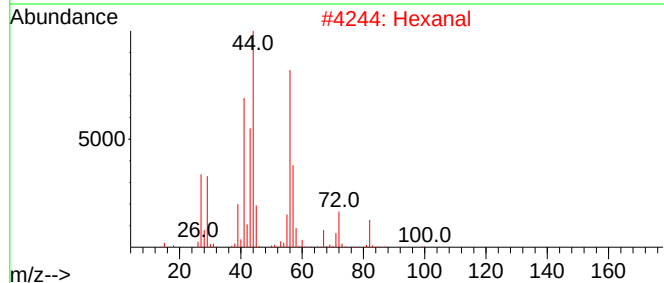
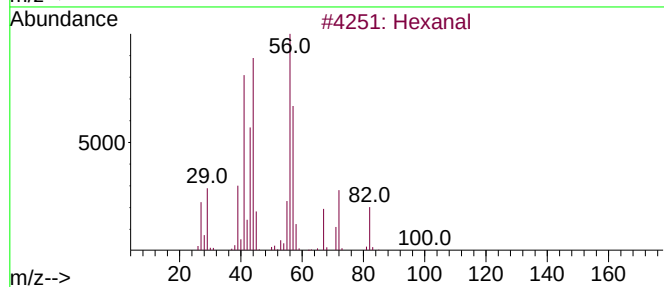
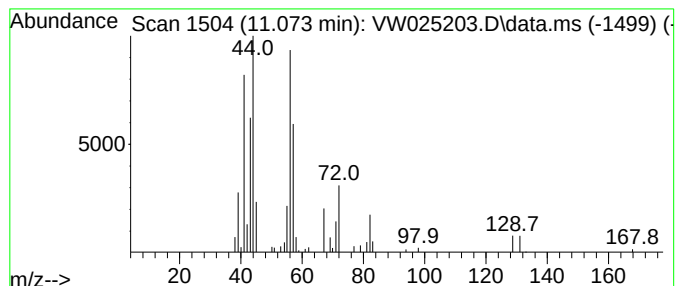
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Quant Title : SFAM01.0

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

Peak Number 6 Hexanal Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.073	1.37 ug/L	47089	Chlorobenzene-d5	11.628

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	78
2	Hexanal			100	C6H12O	000066-25-1	78
3	Hexanal			100	C6H12O	000066-25-1	64
4	Hexanal			100	C6H12O	000066-25-1	50
5	Hexanal			100	C6H12O	000066-25-1	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW122322\
Data File : VW025203.D
Acq On : 23 Dec 2022 17:43
Operator : SY/MD
Sample : N6171-07RE
Misc : 7.13g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
GBQC5RE

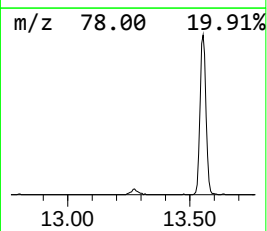
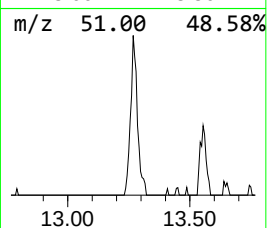
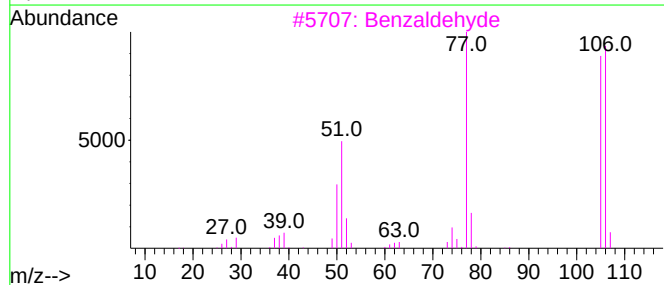
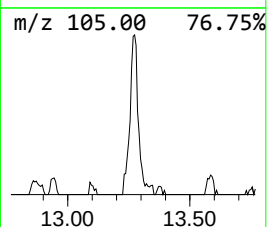
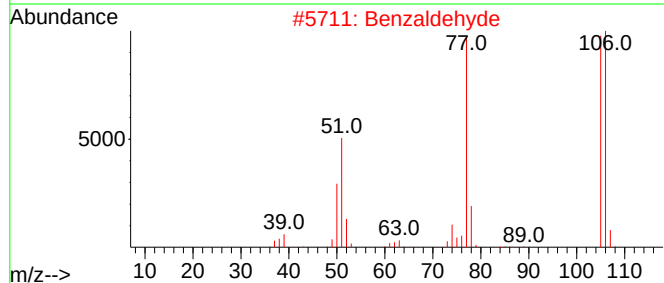
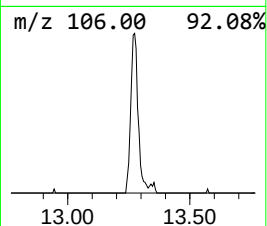
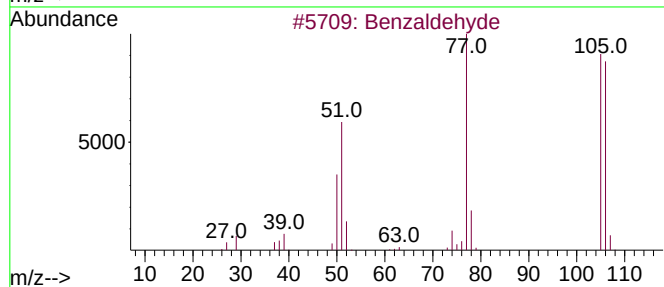
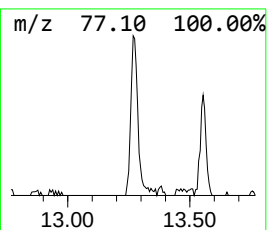
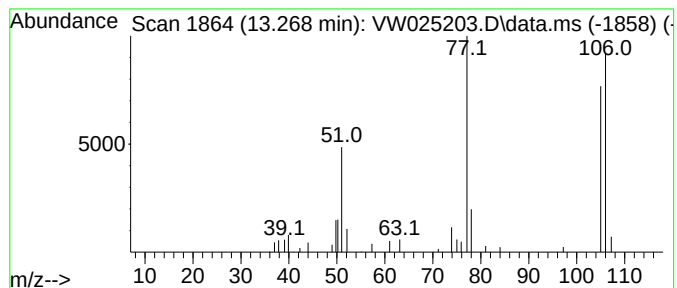
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Quant Title : SFAM01.0

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

Peak Number 8 Benzaldehyde Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.268	1.71 ug/L	27395	1,4-Dichlorobenzene-d4	13.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzaldehyde	106	C7H6O	000100-52-7	97
2			Benzaldehyde	106	C7H6O	000100-52-7	97
3			Benzaldehyde	106	C7H6O	000100-52-7	94
4			Benzaldehyde	106	C7H6O	000100-52-7	91
5			Benzaldehyde	106	C7H6O	000100-52-7	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW122322\
Data File : VW025203.D
Acq On : 23 Dec 2022 17:43
Operator : SY/MD
Sample : N6171-07RE
Misc : 7.13g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
GBQC5RE

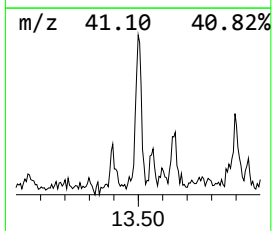
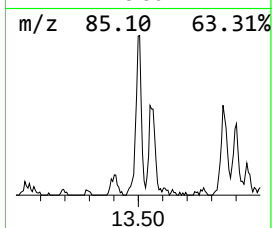
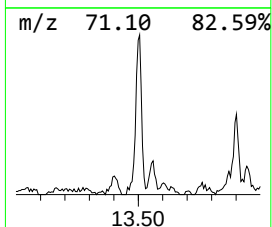
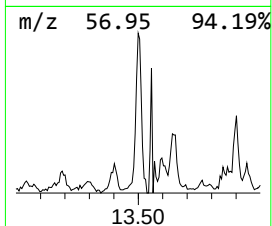
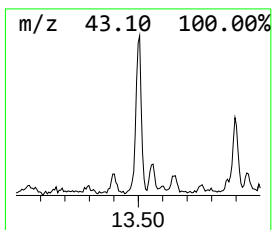
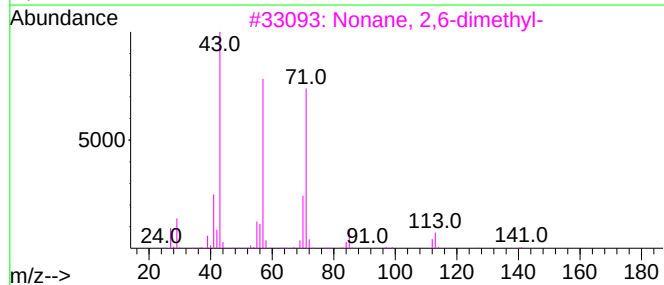
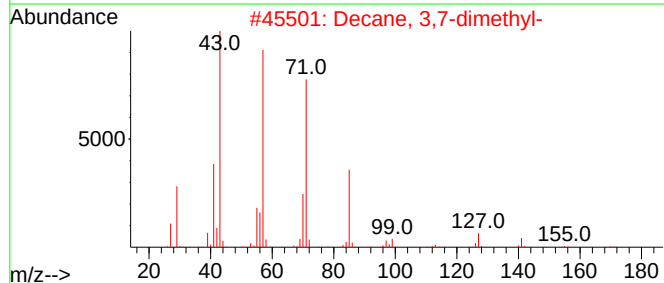
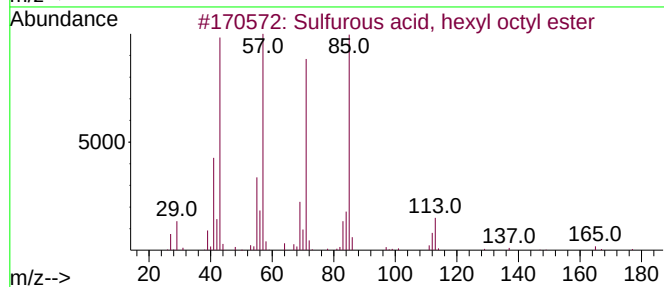
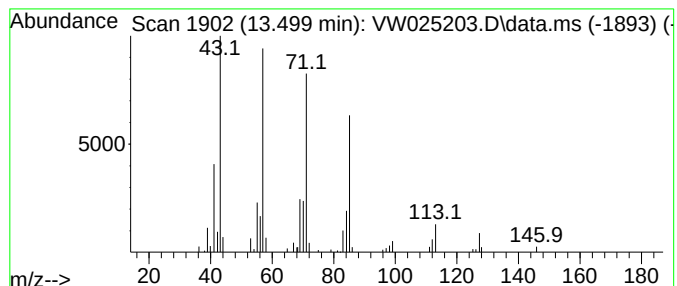
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Quant Title : SFAM01.0

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

Peak Number 9 Sulfurous acid, hexyl octyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.499	3.76 ug/L	60132	1,4-Dichlorobenzene-d4	13.554

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	64
2		Decane, 3,7-dimethyl-	170	C12H26	017312-54-8	53
3		Nonane, 2,6-dimethyl-	156	C11H24	017302-28-2	50
4		Octane, 2,3,6-trimethyl-	156	C11H24	062016-33-5	50
5		Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW122322\
Data File : VW025203.D
Acq On : 23 Dec 2022 17:43
Operator : SY/MD
Sample : N6171-07RE
Misc : 7.13g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
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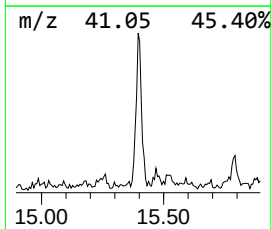
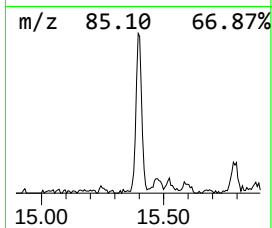
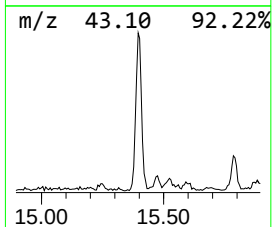
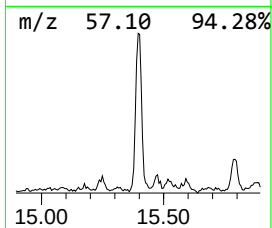
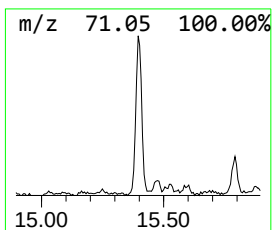
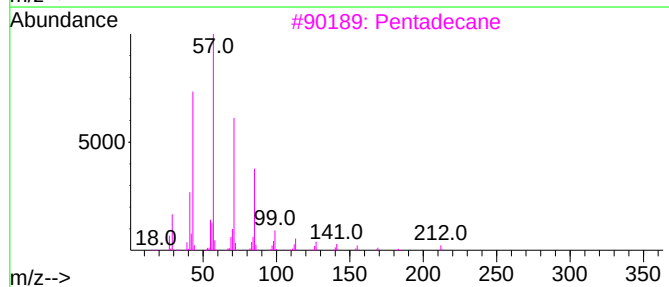
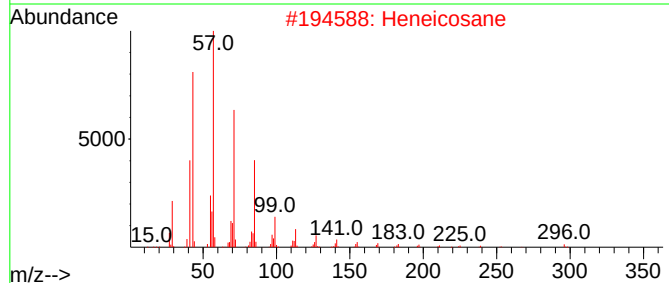
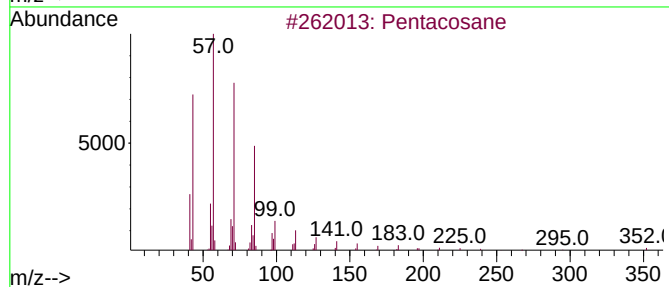
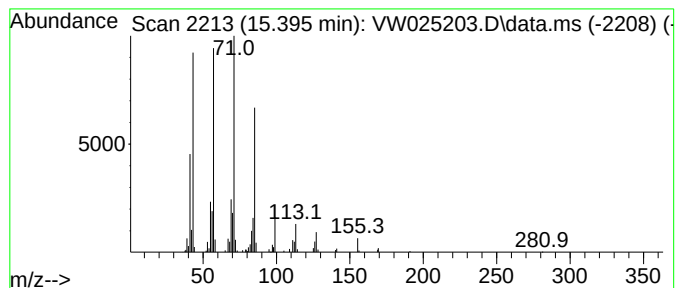
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Quant Title : SFAM01.0

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

Peak Number 10 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.395	5.42 ug/L	86725	1,4-Dichlorobenzene-d4	13.554

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentacosane	352	C25H52	000629-99-2	87
2		Heneicosane	296	C21H44	000629-94-7	72
3		Pentadecane	212	C15H32	000629-62-9	72
4		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	72
5		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW122322\
Data File : VW025203.D
Acq On : 23 Dec 2022 17:43
Operator : SY/MD
Sample : N6171-07RE
Misc : 7.13g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
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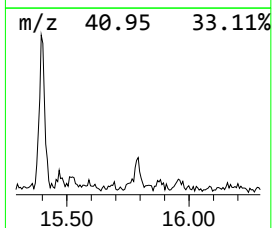
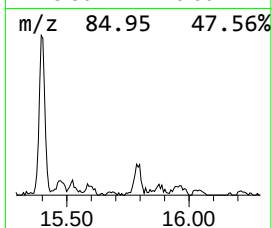
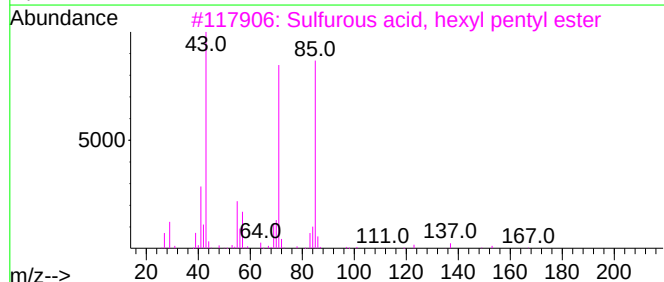
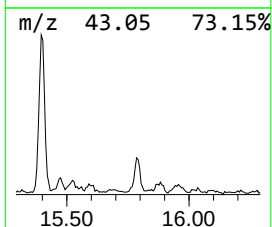
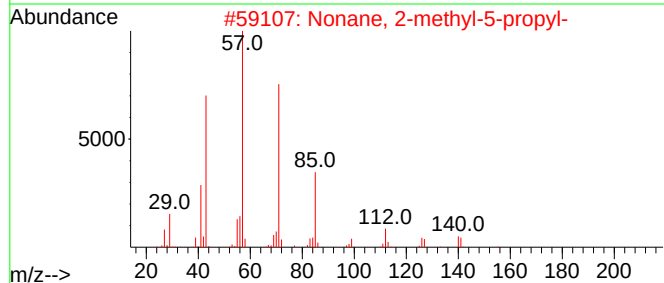
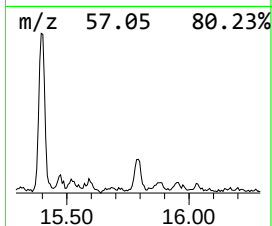
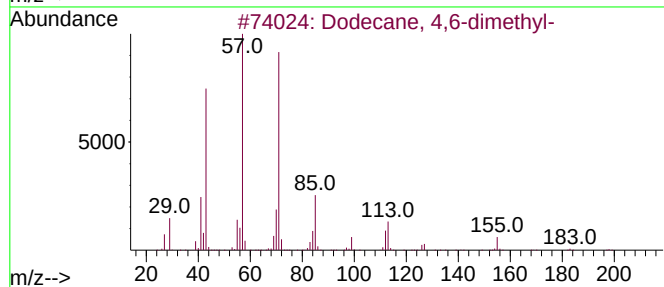
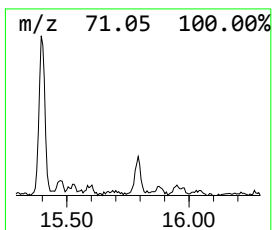
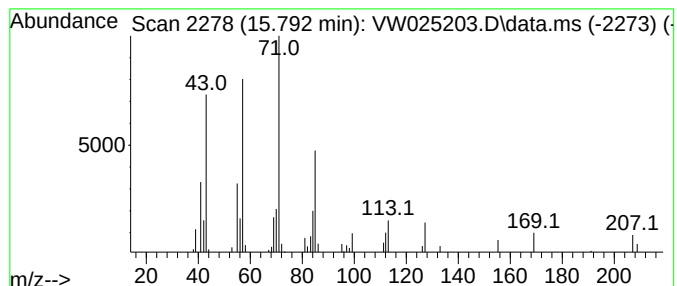
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Quant Title : SFAM01.0

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

Peak Number 12 (DEL) Alkane: Straight-Chai... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.792	1.27 ug/L	20319	1,4-Dichlorobenzene-d4	13.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	64
2			Nonane, 2-methyl-5-propyl-	184	C13H28	031081-17-1	53
3			Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	52
4			Undecane, 3,8-dimethyl-	184	C13H28	017301-30-3	50
5			Tetradecane, 4-ethyl-	226	C16H34	055045-14-2	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW122322\
Data File : VW025203.D
Acq On : 23 Dec 2022 17:43
Operator : SY/MD
Sample : N6171-07RE
Misc : 7.13g/10mL/MSVOA_W/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
GBQC5RE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM120822SMA.M
Quant Title : SFAM01.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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(DEL) Alkane: S...	3.019	1.4	ug/L	63863	1	8.842	1135940	25.0
(DEL) Alkane: S...	3.385	12.9	ug/L	584135	1	8.842	1135940	25.0
Hexanal	11.073	1.4	ug/L	47089	2	11.628	859879	25.0
Benzaldehyde	13.268	1.7	ug/L	27395	3	13.554	400283	25.0
Sulfurous acid,...	13.499	3.8	ug/L	60132	3	13.554	400283	25.0
(DEL) Alkane: S...	15.395	5.4	ug/L	86725	3	13.554	400283	25.0
(DEL) Alkane: S...	15.792	1.3	ug/L	20319	3	13.554	400283	25.0