

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW091924\
 Data File : VW030152.D
 Acq On : 19 Sep 2024 16:58
 Operator : SY/MD
 Sample : P4083-17
 Misc : 4.94g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 A4EH0

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: VW030152.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.369	70	79	94	rBV	59428	149890	11.78%	1.818%
2	2.655	124	126	128	rVB	673	503	0.04%	0.006%
3	2.680	128	130	131	rBV	797	728	0.06%	0.009%
4	2.783	146	147	150	rBV3	559	606	0.05%	0.007%
5	2.899	157	166	182	rBV	45307	136087	10.70%	1.651%
6	3.033	186	188	192	rVB4	1174	1207	0.09%	0.015%
7	3.149	205	207	210	rVB3	777	784	0.06%	0.010%
8	3.173	210	211	216	rBV2	435	509	0.04%	0.006%
9	3.265	223	226	227	rBV3	332	426	0.03%	0.005%
10	3.307	230	233	235	rVV2	831	852	0.07%	0.010%
11	3.393	241	247	254	rVV4	1584	3630	0.29%	0.044%
12	3.539	269	271	274	rVB	328	219	0.02%	0.003%
13	3.728	296	302	306	rBV4	565	1044	0.08%	0.013%
14	3.826	316	318	320	rBV2	197	233	0.02%	0.003%
15	3.911	330	332	333	rVB	356	213	0.02%	0.003%
16	3.929	333	335	337	rBV	261	258	0.02%	0.003%
17	4.021	338	350	362	rBV	138546	421262	33.11%	5.110%
18	4.137	363	369	386	rVB2	29542	93847	7.38%	1.138%
19	4.332	400	401	403	rBV2	309	307	0.02%	0.004%
20	4.393	403	411	426	rVV	2909	10730	0.84%	0.130%
21	4.685	454	459	460	rBV2	184	241	0.02%	0.003%
22	4.795	476	477	482	rVB	374	343	0.03%	0.004%
23	4.923	486	498	512	rBV2	13336	48606	3.82%	0.590%
24	5.130	529	532	536	rVB2	185	309	0.02%	0.004%
25	5.234	544	549	550	rBV2	268	341	0.03%	0.004%
26	5.441	580	583	586	rBV3	221	218	0.02%	0.003%
27	5.569	602	604	606	rVB	267	230	0.02%	0.003%
28	5.795	631	641	646	rBV4	3060	9137	0.72%	0.111%
29	5.917	658	661	662	rVV2	1058	1243	0.10%	0.015%
30	5.941	662	665	675	rVB5	2330	5722	0.45%	0.069%
31	6.618	773	776	777	rVB2	280	262	0.02%	0.003%
32	6.758	796	799	803	rVB2	241	320	0.03%	0.004%
33	7.081	843	852	861	rBV	31565	90520	7.12%	1.098%
34	7.179	863	868	881	rVB2	14367	38909	3.06%	0.472%
35	7.313	887	890	892	rBV2	320	382	0.03%	0.005%
36	7.496	916	920	921	rBV	211	267	0.02%	0.003%

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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\SFAMWLM091624SMA.M
 Title : SFAM01.0

37	7.648	934	945	958	rBV	216877	535237	42.07%	6.493%
38	7.916	988	989	993	rBV2	198	262	0.02%	0.003%
39	7.953	993	995	998	rVB2	252	334	0.03%	0.004%
40	8.069	1011	1014	1017	rBV2	183	274	0.02%	0.003%
41	8.276	1036	1048	1066	rBV2	443545	1272188	100.00%	15.433%
42	8.538	1087	1091	1092	rBV	170	214	0.02%	0.003%
43	8.550	1092	1093	1096	rVV	248	247	0.02%	0.003%
44	8.624	1103	1105	1109	rBV2	373	517	0.04%	0.006%
45	8.703	1111	1118	1123	rBV6	1121	2585	0.20%	0.031%
46	8.843	1132	1141	1158	rBV	556310	1082897	85.12%	13.137%
47	9.044	1171	1174	1175	rBV2	311	317	0.02%	0.004%
48	9.075	1175	1179	1186	rVB5	1410	2457	0.19%	0.030%
49	9.270	1202	1211	1229	rBV	282971	580356	45.62%	7.041%
50	9.599	1260	1265	1267	rBV	227	267	0.02%	0.003%
51	9.660	1272	1275	1276	rBV	480	361	0.03%	0.004%
52	9.678	1276	1278	1280	rVB2	286	242	0.02%	0.003%
53	9.879	1306	1311	1313	rBV	374	656	0.05%	0.008%
54	9.940	1319	1321	1323	rBV2	277	304	0.02%	0.004%
55	10.032	1328	1336	1349	rBV	132066	238135	18.72%	2.889%
56	10.325	1374	1384	1392	rBV	500384	875603	68.83%	10.622%
57	10.507	1407	1414	1419	rBV7	921	1793	0.14%	0.022%
58	10.574	1419	1425	1438	rBV	74709	132306	10.40%	1.605%
59	10.696	1440	1445	1455	rVB3	9049	16825	1.32%	0.204%
60	10.782	1457	1459	1462	rVB2	353	347	0.03%	0.004%
61	10.812	1462	1464	1465	rBV	416	315	0.02%	0.004%
62	10.824	1465	1466	1468	rBV	360	267	0.02%	0.003%
63	10.922	1474	1482	1493	rBV	132476	231443	18.19%	2.808%
64	11.068	1502	1506	1507	rBV4	1546	1748	0.14%	0.021%
65	11.196	1521	1527	1530	rBV4	657	1225	0.10%	0.015%
66	11.227	1530	1532	1534	rVB2	322	311	0.02%	0.004%
67	11.263	1536	1538	1539	rBV2	438	240	0.02%	0.003%
68	11.330	1547	1549	1550	rBV2	766	554	0.04%	0.007%
69	11.404	1556	1561	1562	rBV2	546	690	0.05%	0.008%
70	11.416	1562	1563	1565	rVB2	572	389	0.03%	0.005%
71	11.513	1572	1579	1580	rBV2	442	844	0.07%	0.010%
72	11.629	1590	1598	1607	rBV	507358	843801	66.33%	10.236%
73	11.708	1608	1611	1619	rVB4	3257	5398	0.42%	0.065%
74	11.769	1619	1621	1622	rVB2	413	275	0.02%	0.003%
75	11.830	1623	1631	1635	rBV8	2591	6620	0.52%	0.080%
76	11.891	1637	1641	1648	rVB7	2741	5904	0.46%	0.072%

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 Title : SFAM01.0

77	11.971	1650	1654	1657	rBV3	2048	2944	0.23%	0.036%
78	12.025	1660	1663	1668	rVB6	1434	2383	0.19%	0.029%
79	12.068	1668	1670	1672	rVB3	504	347	0.03%	0.004%
80	12.117	1672	1678	1683	rBV4	6447	12139	0.95%	0.147%
81	12.190	1686	1690	1695	rBV9	1038	2618	0.21%	0.032%
82	12.275	1702	1704	1707	rBV2	375	286	0.02%	0.003%
83	12.330	1707	1713	1717	rBV6	4401	8892	0.70%	0.108%
84	12.440	1723	1731	1735	rBV5	7351	15128	1.19%	0.184%
85	12.562	1747	1751	1753	rBV4	1518	2577	0.20%	0.031%
86	12.598	1753	1757	1764	rVB2	7835	16322	1.28%	0.198%
87	12.690	1764	1772	1779	rBV	152086	259978	20.44%	3.154%
88	12.775	1779	1786	1792	rVB2	33293	59152	4.65%	0.718%
89	12.855	1793	1799	1800	rBV5	3780	5648	0.44%	0.069%
90	12.958	1808	1816	1822	rBV7	11838	35046	2.75%	0.425%
91	13.074	1830	1835	1841	rVB6	8322	15482	1.22%	0.188%
92	13.196	1850	1855	1860	rBV5	7876	15359	1.21%	0.186%
93	13.251	1861	1864	1869	rBV5	6323	10012	0.79%	0.121%
94	13.403	1880	1889	1893	rBV10	11257	36753	2.89%	0.446%
95	13.556	1908	1914	1925	rBV	229013	388958	30.57%	4.719%
96	13.690	1932	1936	1941	rVB3	15793	25916	2.04%	0.314%
97	13.848	1956	1962	1973	rVB	157531	277082	21.78%	3.361%
98	14.379	2045	2049	2053	rBV5	16709	30258	2.38%	0.367%
99	15.318	2199	2203	2209	rVB	51731	89792	7.06%	1.089%
100	16.275	2356	2360	2367	rVB2	34040	64877	5.10%	0.787%

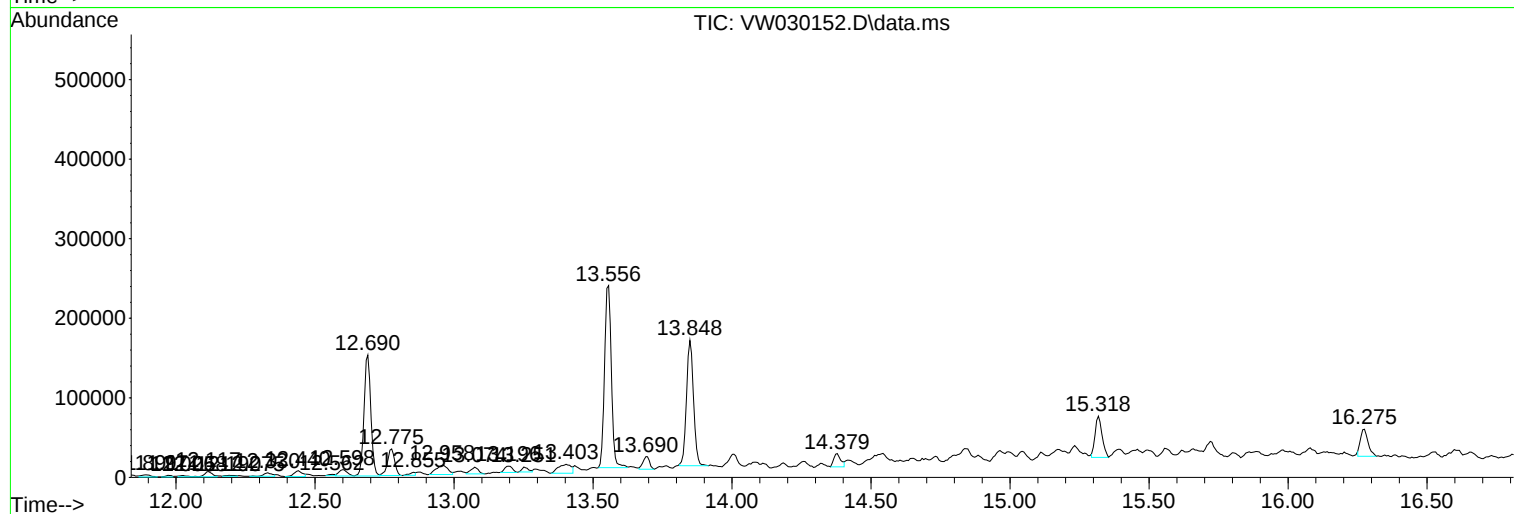
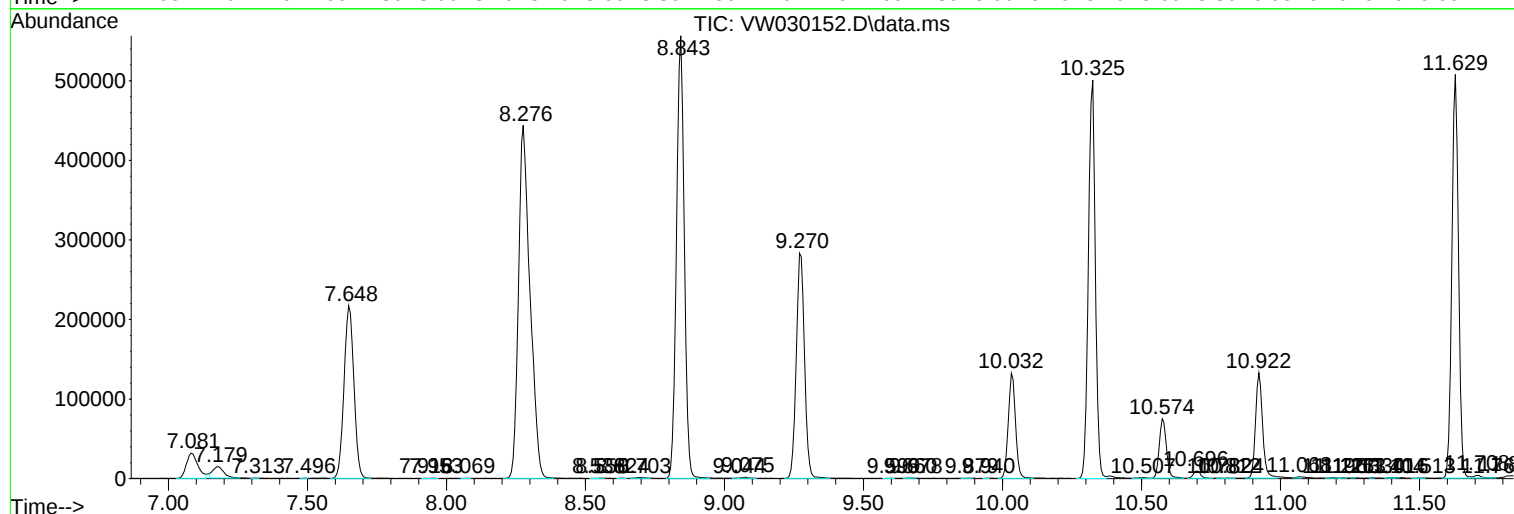
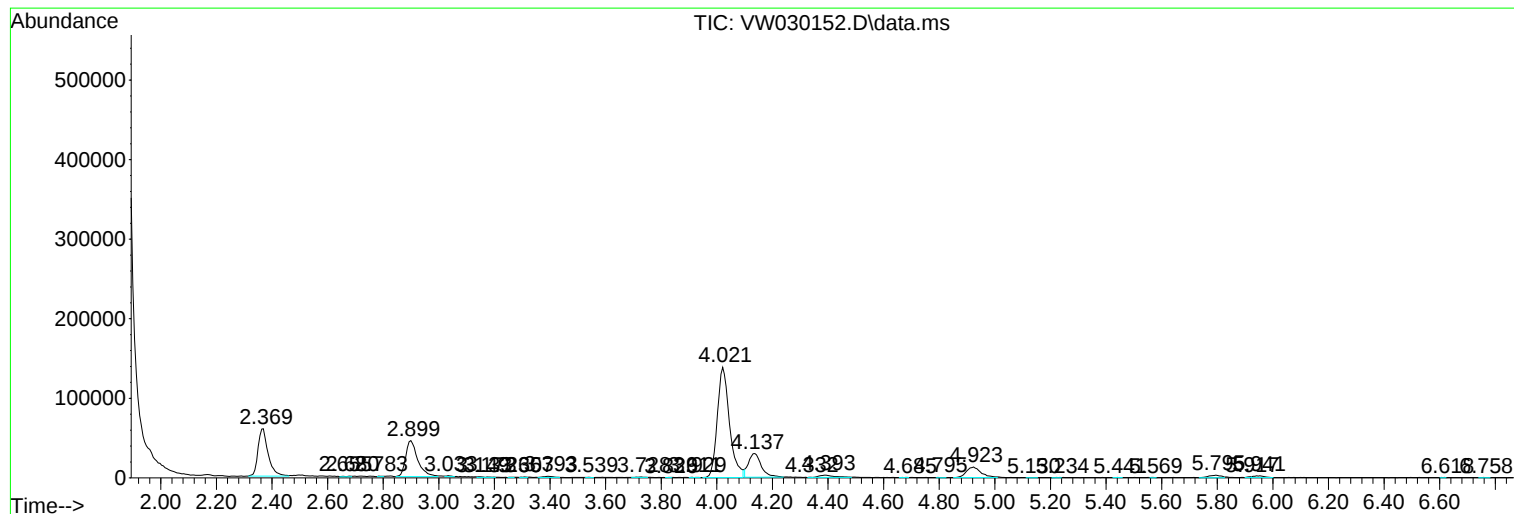
Sum of corrected areas: 8243082

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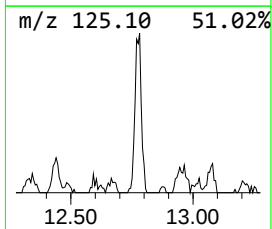
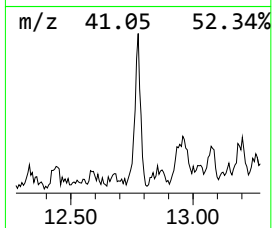
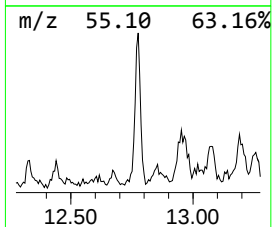
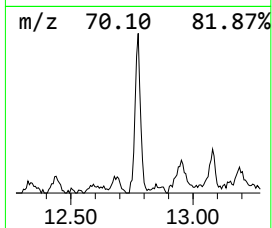
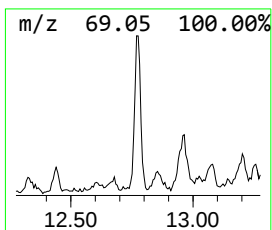
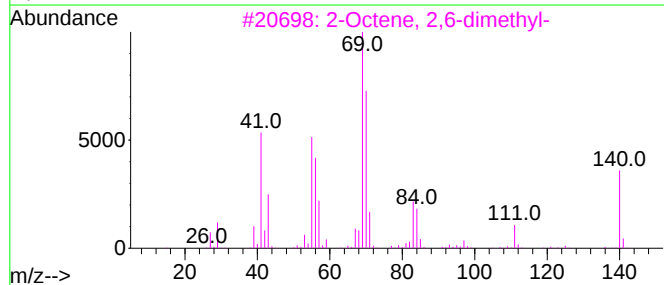
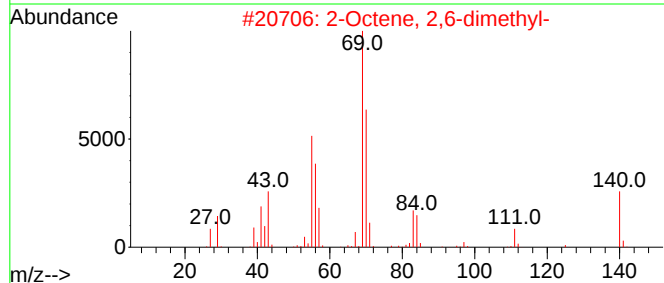
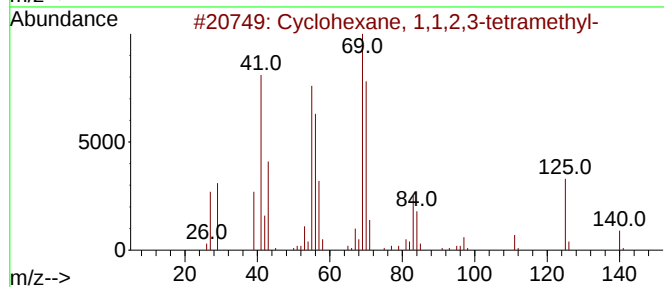
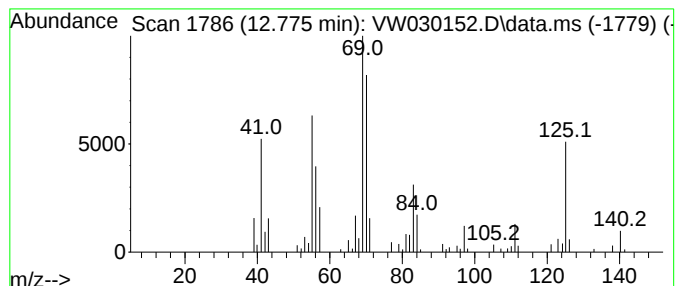
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM091624SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 (DEL) Alkane: Cyclic12.775 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.775	3.80 ug/L	59152	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,1,2,3-tetramethyl-	140	C10H20	006783-92-2	95
2			2-Octene, 2,6-dimethyl-	140	C10H20	004057-42-5	81
3			2-Octene, 2,6-dimethyl-	140	C10H20	004057-42-5	72
4			cis-1-Butyl-2-methylcyclopropane	112	C8H16	038851-69-3	50
5			Cyclooctane, 1-methyl-3-propyl-	168	C12H24	255885-37-1	47



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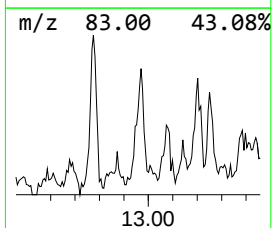
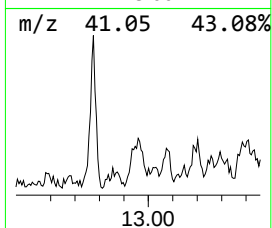
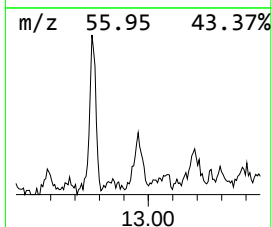
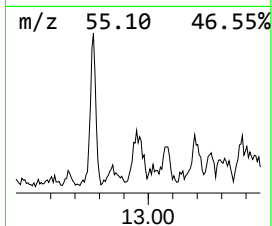
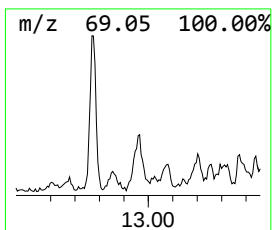
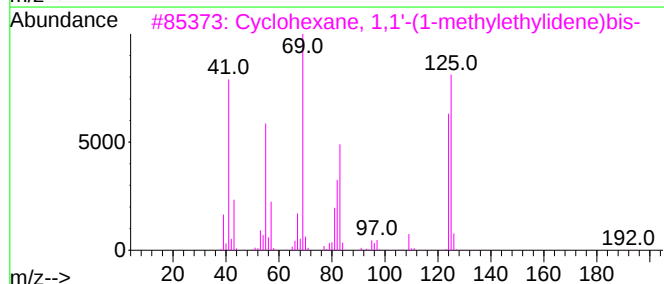
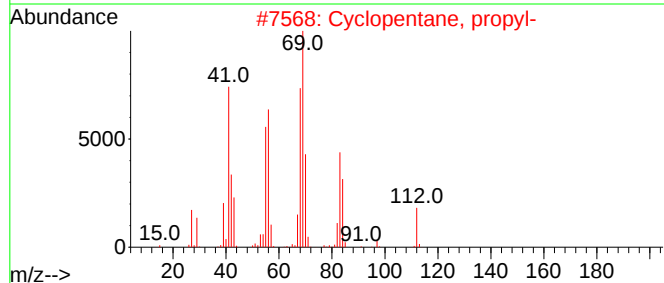
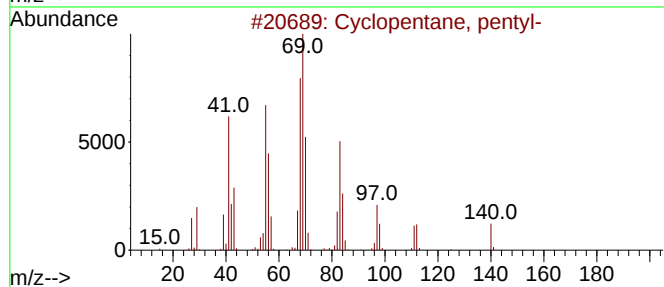
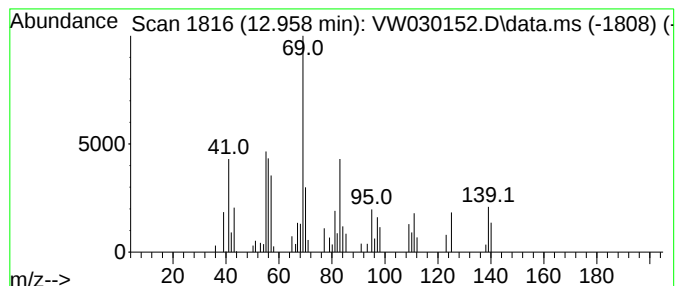
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM091624SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 (DEL) Alkane: Cyclic12.958 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.958	2.25 ug/L	35046	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, pentyl-	140	C10H20	003741-00-2	53
2			Cyclopentane, propyl-	112	C8H16	002040-96-2	49
3			Cyclohexane, 1,1'-(1-methylethyl...	208	C15H28	054934-90-6	43
4			1-Isopropyl-1,4,5-trimethylcyclo...	168	C12H24	219783-06-9	43
5			Cyclopentane, propyl-	112	C8H16	002040-96-2	43



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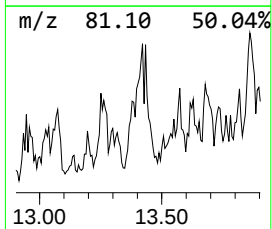
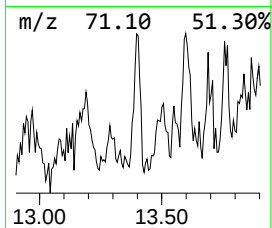
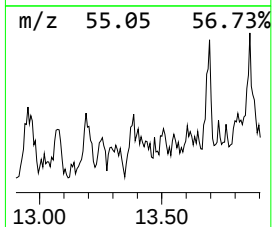
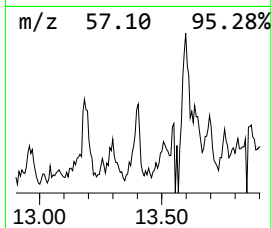
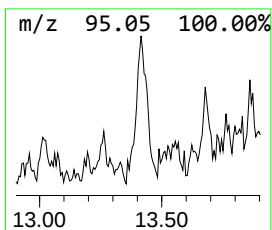
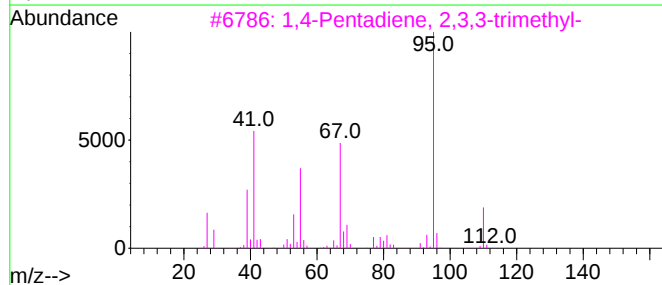
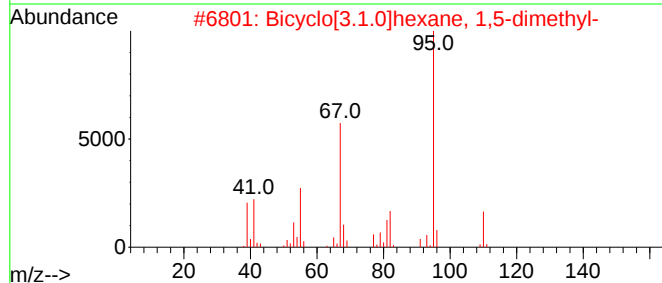
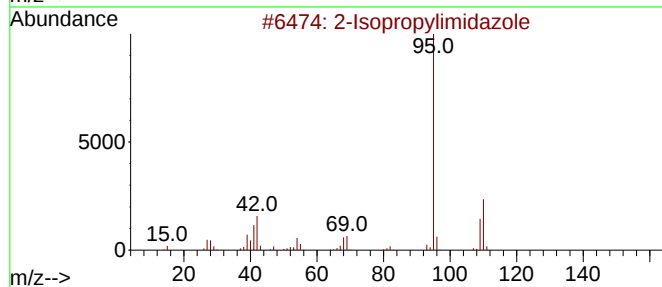
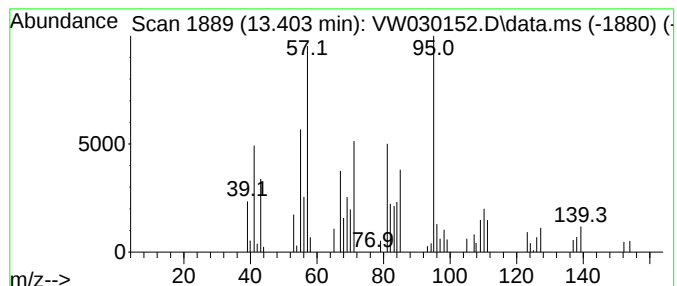
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM091624SMA.M
Quant Title : SFAM01.0

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

Peak Number 4 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.403	2.36 ug/L	36753	1,4-Dichlorobenzene-d4	13.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Isopropylimidazole	110	C6H10N2	036947-68-9	38
2		Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1010142-17-5	30
3		1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	30
4		Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	30
5		1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW091924\
Data File : VW030152.D
Acq On : 19 Sep 2024 16:58
Operator : SY/MD
Sample : P4083-17
Misc : 4.94g/10mL/MSVOA_W/SOIL/A
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
A4EH0

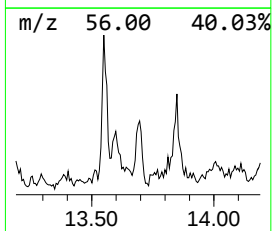
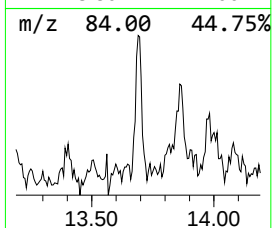
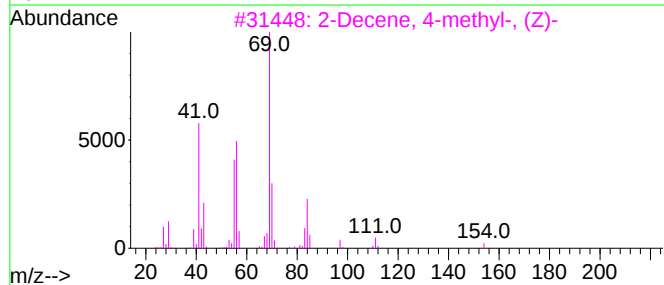
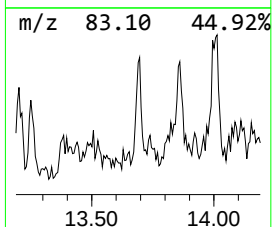
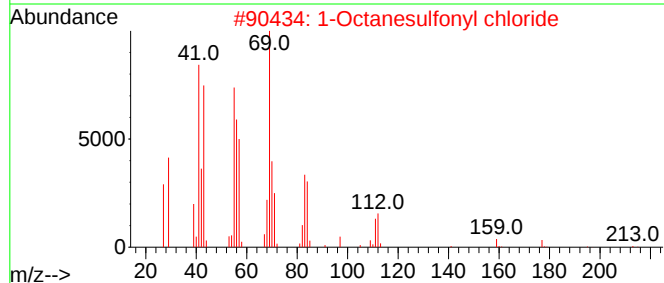
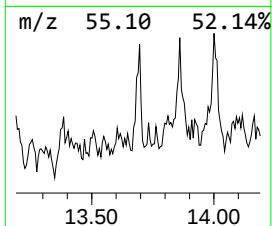
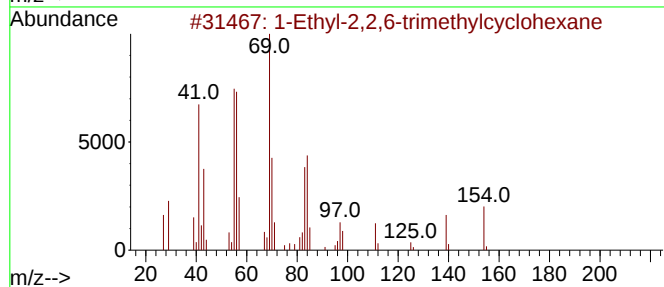
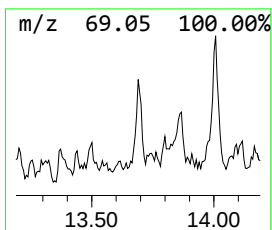
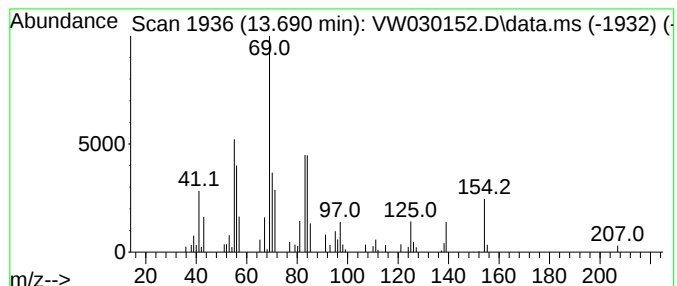
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Quant Title : SFAM01.0

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

Peak Number 5 (DEL) Alkane: Cyclic13.690 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.690	1.67 ug/L	25916	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Ethyl-2,2,6-trimethylcyclohexane	154	C11H22	071186-27-1	76
2			1-Octanesulfonyl chloride	212	C8H17ClO2S	007795-95-1	59
3			2-Decene, 4-methyl-, (Z)-	154	C11H22	074630-30-1	59
4			2,3-Dimethyl-3-heptene, (Z)-	126	C9H18	059643-73-1	49
5			1-Heptanol, 6-methyl-	130	C8H18O	001653-40-3	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW091924\
Data File : VW030152.D
Acq On : 19 Sep 2024 16:58
Operator : SY/MD
Sample : P4083-17
Misc : 4.94g/10mL/MSVOA_W/SOIL/A
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
A4EH0

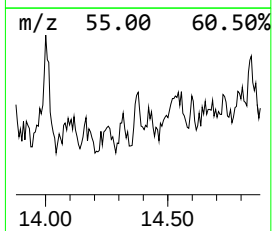
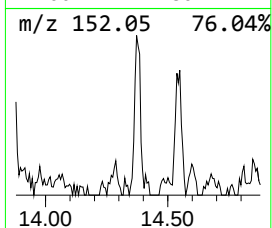
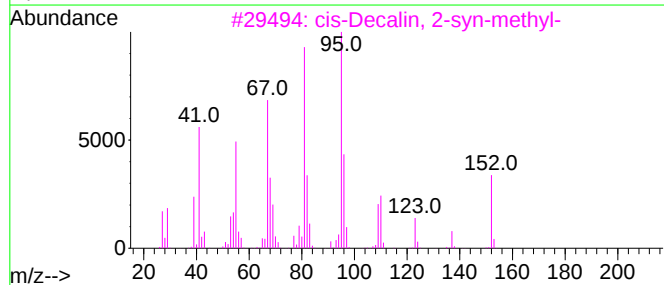
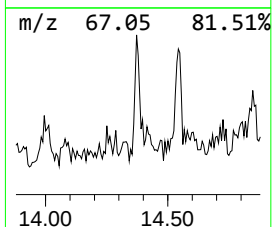
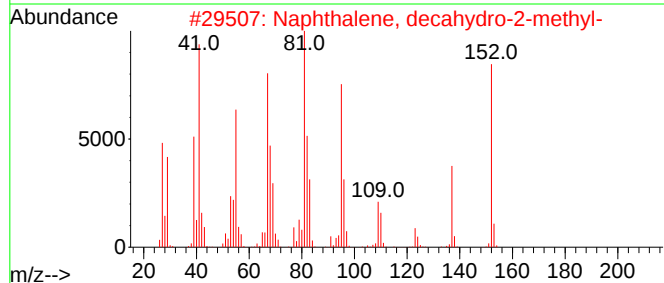
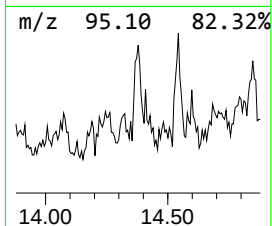
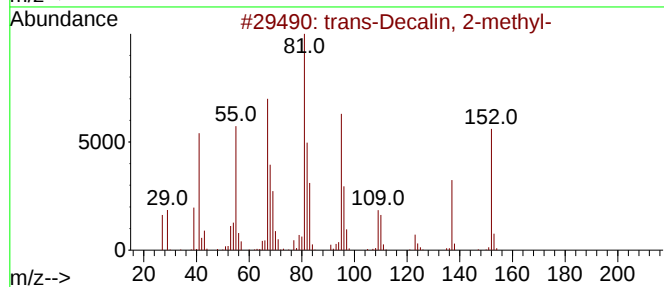
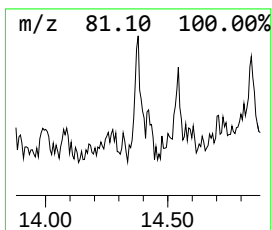
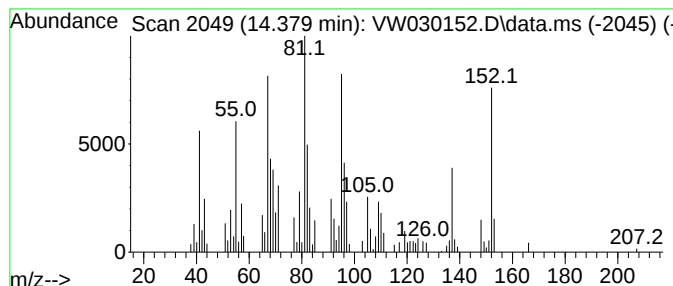
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Quant Title : SFAM01.0

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

Peak Number 6 trans-Decalin, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.379	1.94 ug/L	30258	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	94
2			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	93
3			cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	87
4			trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	86
5			9-Octadecyne	250	C18H34	035365-59-4	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW091924\
Data File : VW030152.D
Acq On : 19 Sep 2024 16:58
Operator : SY/MD
Sample : P4083-17
Misc : 4.94g/10mL/MSVOA_W/SOIL/A
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
A4EH0

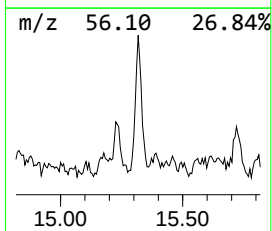
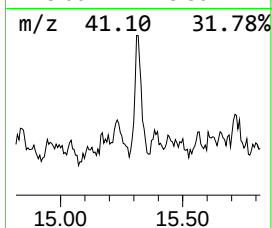
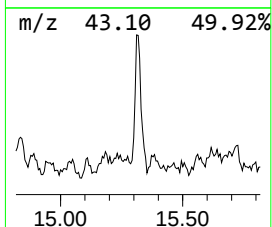
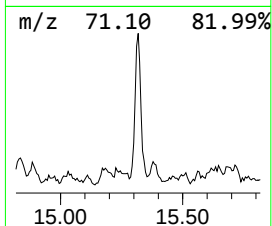
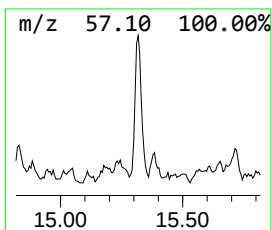
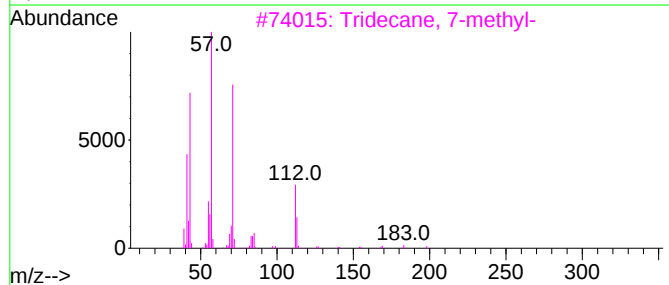
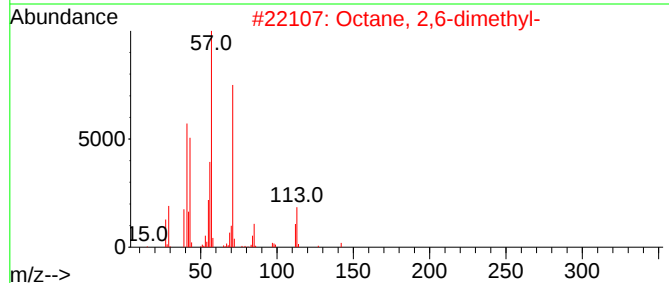
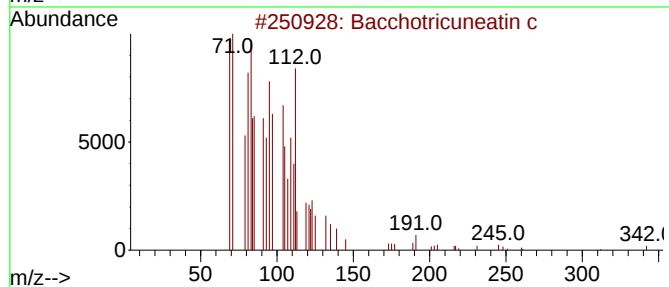
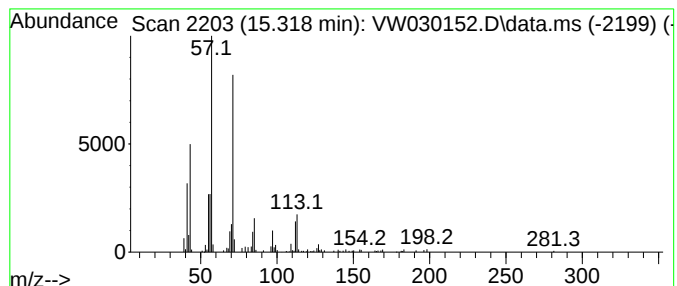
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Quant Title : SFAM01.0

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

Peak Number 7 Bacchotricuneatin c Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.318	5.77 ug/L	89792	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bacchotricuneatin c	342	C20H22O5	066563-30-2	80
2			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	78
3			Tridecane, 7-methyl-	198	C14H30	026730-14-3	76
4			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	72
5			Sulfurous acid, butyl octyl ester	250	C12H26O3S	1000309-17-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW091924\
Data File : VW030152.D
Acq On : 19 Sep 2024 16:58
Operator : SY/MD
Sample : P4083-17
Misc : 4.94g/10mL/MSVOA_W/SOIL/A
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
A4EH0

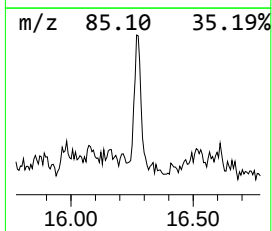
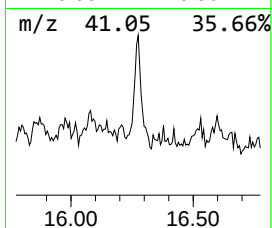
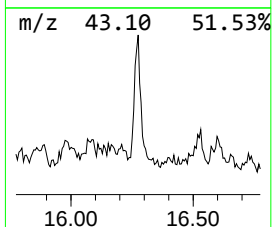
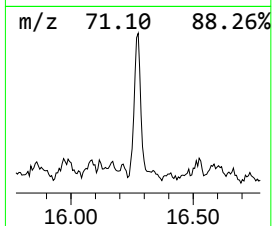
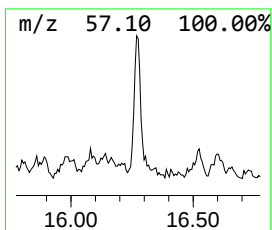
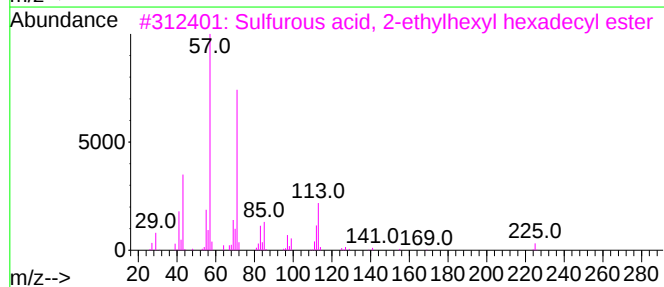
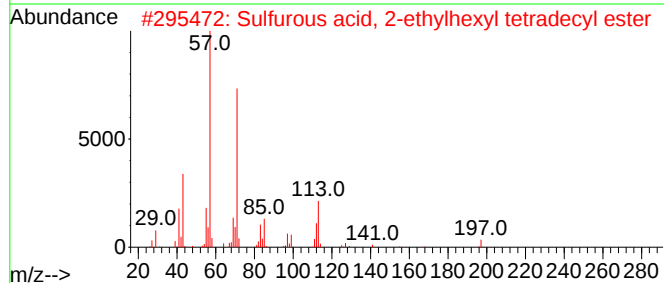
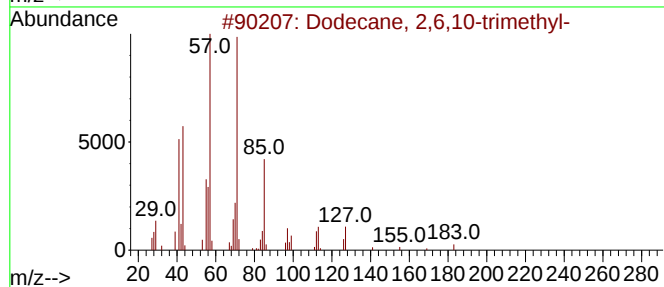
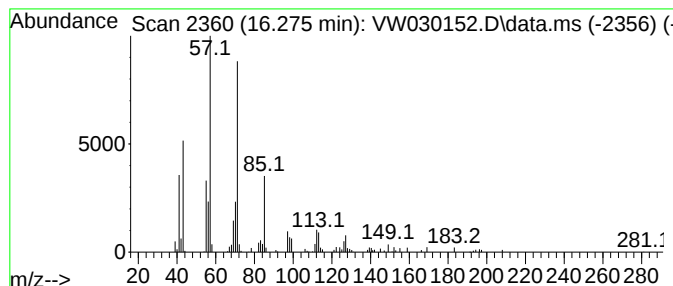
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Quant Title : SFAM01.0

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.275	4.17 ug/L	64877	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	91
2			Sulfurous acid, 2-ethylhexyl tet...	390	C22H46O3S	1000309-19-7	58
3			Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	53
4			Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	50
5			2-Decanone, 5,9-dimethyl-	184	C12H24O	033933-82-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW091924\
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Acq On : 19 Sep 2024 16:58
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Misc : 4.94g/10mL/MSVOA_W/SOIL/A
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
A4EH0

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: C...	12.775	3.8	ug/L	59152	3	13.556	388958	25.0
(DEL) Alkane: C...	12.958	2.3	ug/L	35046	3	13.556	388958	25.0
unknown-01	13.403	2.4	ug/L	36753	3	13.556	388958	25.0
(DEL) Alkane: C...	13.690	1.7	ug/L	25916	3	13.556	388958	25.0
trans-Decalin, ...	14.379	1.9	ug/L	30258	3	13.556	388958	25.0
Bacchotricuneat...	15.318	5.8	ug/L	89792	3	13.556	388958	25.0
(DEL) Alkane: S...	16.275	4.2	ug/L	64877	3	13.556	388958	25.0