

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW100824\
 Data File : VW030443.D
 Acq On : 08 Oct 2024 13:48
 Operator : SY/MD
 Sample : P4329-07
 Misc : 4.97g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 A4EN4

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM092724SMA.M
 Title : SFAM01.0

Signal : TIC: VW030443.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	72	79	92	rVB	25969	58712	10.06%	1.382%
2	2.503	99	101	107	rVB2	435	525	0.09%	0.012%
3	2.808	149	151	153	rBV	188	187	0.03%	0.004%
4	2.899	158	166	181	rBV2	15803	47370	8.12%	1.115%
5	3.088	196	197	199	rBV2	195	131	0.02%	0.003%
6	3.113	199	201	203	rVV	115	138	0.02%	0.003%
7	3.234	219	221	222	rBV	143	129	0.02%	0.003%
8	3.344	238	239	242	rBV	171	183	0.03%	0.004%
9	3.399	242	248	253	rVB3	381	812	0.14%	0.019%
10	3.490	260	263	264	rBV	154	153	0.03%	0.004%
11	3.509	264	266	269	rVB	190	227	0.04%	0.005%
12	3.576	273	277	280	rBV	236	357	0.06%	0.008%
13	3.704	295	298	299	rBV	152	165	0.03%	0.004%
14	3.740	302	304	306	rVB	267	212	0.04%	0.005%
15	3.808	311	315	317	rBV	98	169	0.03%	0.004%
16	4.027	340	351	361	rBV	78829	213722	36.62%	5.031%
17	4.314	396	398	400	rBB	134	126	0.02%	0.003%
18	4.387	402	410	411	rBV	1875	2949	0.51%	0.069%
19	4.612	446	447	451	rBB	137	149	0.03%	0.004%
20	4.685	454	459	461	rVB	143	242	0.04%	0.006%
21	4.765	469	472	473	rBV	123	162	0.03%	0.004%
22	5.057	517	520	522	rBB	161	149	0.03%	0.004%
23	5.265	551	554	555	rBV	191	166	0.03%	0.004%
24	5.447	582	584	586	rBV	121	127	0.02%	0.003%
25	5.630	613	614	617	rVB	138	119	0.02%	0.003%
26	5.777	633	638	639	rBV	492	517	0.09%	0.012%
27	5.899	655	658	661	rBB	136	134	0.02%	0.003%
28	5.947	662	666	671	rBB	382	504	0.09%	0.012%
29	6.161	698	701	703	rBB	95	121	0.02%	0.003%
30	6.283	717	721	724	rBB	160	227	0.04%	0.005%
31	6.453	747	749	752	rBB	134	140	0.02%	0.003%
32	6.606	772	774	777	rVB	106	135	0.02%	0.003%
33	6.673	783	785	788	rBV	132	148	0.03%	0.003%
34	6.862	811	816	818	rBB	167	180	0.03%	0.004%
35	6.886	818	820	823	rBB	132	145	0.02%	0.003%
36	7.081	844	852	860	rBV	10149	30095	5.16%	0.709%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM092724SMA.M
 Title : SFAM01.0

37	7.252	878	880	882	rVB	315	249	0.04%	0.006%
38	7.441	909	911	913	rBV	123	121	0.02%	0.003%
39	7.526	923	925	928	rBB	179	160	0.03%	0.004%
40	7.648	935	945	956	rBV	105547	255632	43.80%	6.018%
41	7.758	962	963	966	rVB	211	161	0.03%	0.004%
42	7.862	978	980	981	rBV	170	131	0.02%	0.003%
43	7.947	992	994	995	rBV	453	286	0.05%	0.007%
44	7.984	998	1000	1002	rVB	196	133	0.02%	0.003%
45	8.032	1003	1008	1012	rBV2	228	414	0.07%	0.010%
46	8.148	1025	1027	1030	rBV	340	375	0.06%	0.009%
47	8.173	1030	1031	1035	rVB	138	140	0.02%	0.003%
48	8.276	1038	1048	1070	rBB2	198383	583649	100.00%	13.740%
49	8.423	1070	1072	1075	rBB	183	221	0.04%	0.005%
50	8.471	1076	1080	1081	rBV	225	291	0.05%	0.007%
51	8.484	1081	1082	1084	rVB	324	200	0.03%	0.005%
52	8.563	1093	1095	1096	rBV	222	206	0.04%	0.005%
53	8.575	1096	1097	1102	rVB3	496	516	0.09%	0.012%
54	8.624	1103	1105	1109	rBB	200	245	0.04%	0.006%
55	8.703	1113	1118	1121	rBV3	349	559	0.10%	0.013%
56	8.843	1132	1141	1151	rVV	212552	422411	72.37%	9.944%
57	9.075	1176	1179	1180	rBV	198	180	0.03%	0.004%
58	9.276	1203	1212	1219	rBV	125851	253679	43.46%	5.972%
59	9.392	1227	1231	1234	rVB3	895	1404	0.24%	0.033%
60	9.422	1234	1236	1239	rBB	174	192	0.03%	0.005%
61	9.526	1250	1253	1256	rBB	141	163	0.03%	0.004%
62	9.569	1258	1260	1261	rVV	283	200	0.03%	0.005%
63	9.611	1262	1267	1271	rVB2	1033	1785	0.31%	0.042%
64	9.666	1275	1276	1280	rBB	127	153	0.03%	0.004%
65	9.752	1284	1290	1295	rVV3	1754	3377	0.58%	0.080%
66	9.806	1295	1299	1300	rVB	148	157	0.03%	0.004%
67	9.898	1309	1314	1318	rBV2	1419	2254	0.39%	0.053%
68	9.989	1325	1329	1330	rBV2	595	723	0.12%	0.017%
69	10.032	1330	1336	1348	rVV	58278	110049	18.86%	2.591%
70	10.209	1363	1365	1367	rBV	461	538	0.09%	0.013%
71	10.245	1369	1371	1376	rVB3	618	700	0.12%	0.016%
72	10.325	1376	1384	1401	rBV	270844	491141	84.15%	11.563%
73	10.440	1401	1403	1406	rBV3	528	537	0.09%	0.013%
74	10.508	1406	1414	1419	rVB6	2750	6387	1.09%	0.150%
75	10.581	1419	1426	1431	rBV	35693	61233	10.49%	1.442%
76	10.666	1436	1440	1443	rVV3	3247	5622	0.96%	0.132%

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Integration Parameters: LSCINT.P

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77	10.703	1443	1446	1451	rVB2	5709	7696	1.32%	0.181%
78	10.764	1451	1456	1459	rBV6	1824	2792	0.48%	0.066%
79	10.843	1465	1469	1474	rVB3	2464	4342	0.74%	0.102%
80	10.922	1474	1482	1493	rBV2	51726	93144	15.96%	2.193%
81	11.038	1496	1501	1509	rVB2	4070	8379	1.44%	0.197%
82	11.105	1509	1512	1515	rBV4	2360	3103	0.53%	0.073%
83	11.178	1520	1524	1527	rVV2	5064	8597	1.47%	0.202%
84	11.227	1527	1532	1538	rVB	16718	30429	5.21%	0.716%
85	11.331	1545	1549	1554	rBV3	7940	13499	2.31%	0.318%
86	11.434	1562	1566	1573	rVB2	8288	14965	2.56%	0.352%
87	11.507	1573	1578	1581	rBV2	3665	5885	1.01%	0.139%
88	11.629	1590	1598	1606	rBV	229111	379973	65.10%	8.945%
89	11.763	1616	1620	1623	rBV3	4407	7312	1.25%	0.172%
90	11.867	1633	1637	1642	rBV	12899	24341	4.17%	0.573%
91	11.971	1650	1654	1657	rBV3	5629	9123	1.56%	0.215%
92	12.135	1673	1681	1687	rBV5	21925	52252	8.95%	1.230%
93	12.251	1697	1700	1704	rVB	28727	38838	6.65%	0.914%
94	12.361	1704	1718	1729	rBV5	41286	157283	26.95%	3.703%
95	12.611	1754	1759	1765	rVB3	16342	32470	5.56%	0.764%
96	12.690	1765	1772	1777	rBV	79486	144199	24.71%	3.395%
97	12.861	1794	1800	1804	rBV6	16571	38617	6.62%	0.909%
98	13.556	1909	1914	1926	rVB	121157	211262	36.20%	4.974%
99	13.854	1958	1963	1970	rBV2	98502	236653	40.55%	5.571%
100	15.318	2199	2203	2210	rVB2	97559	156241	26.77%	3.678%

Sum of corrected areas: 4247696

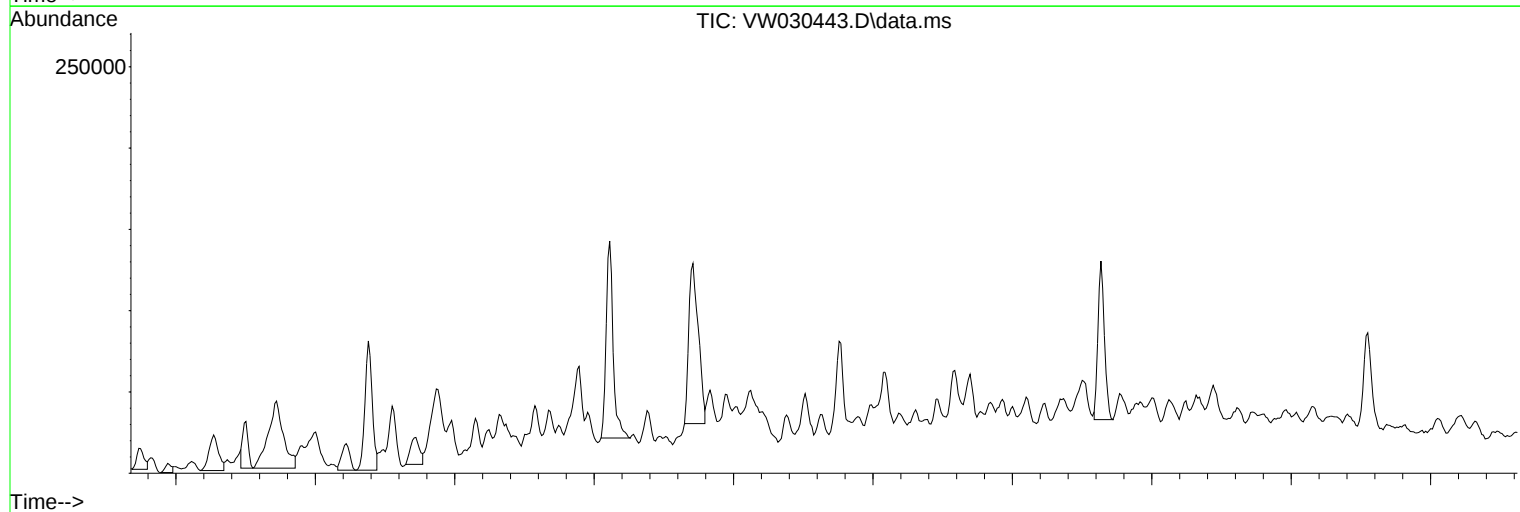
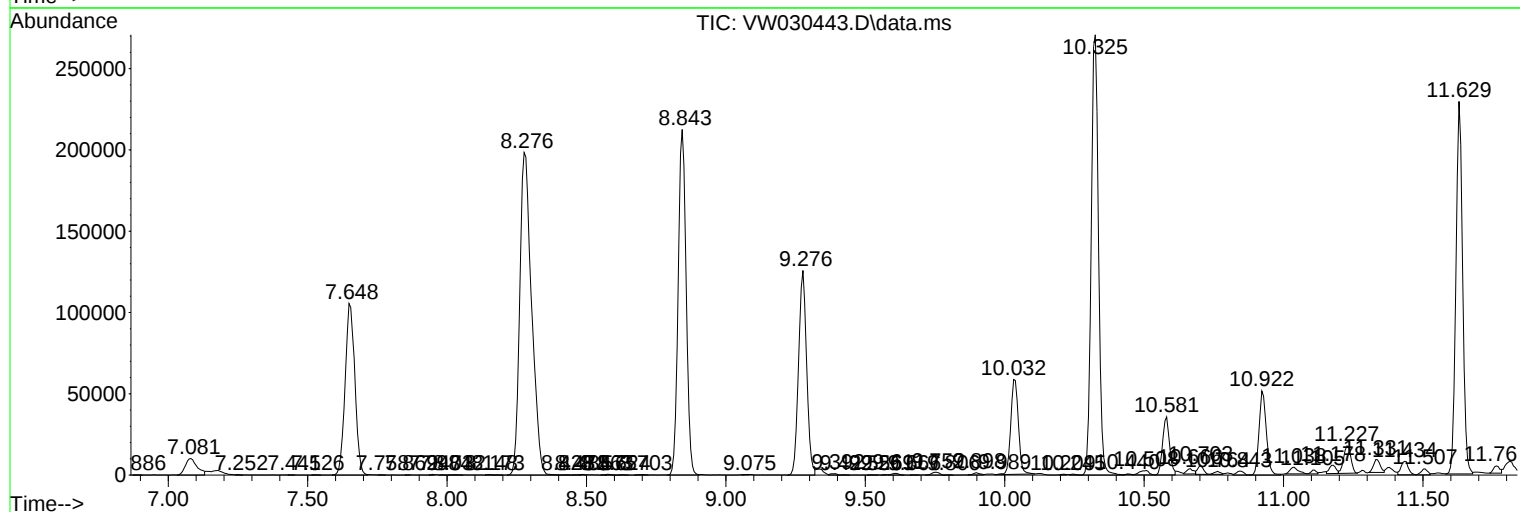
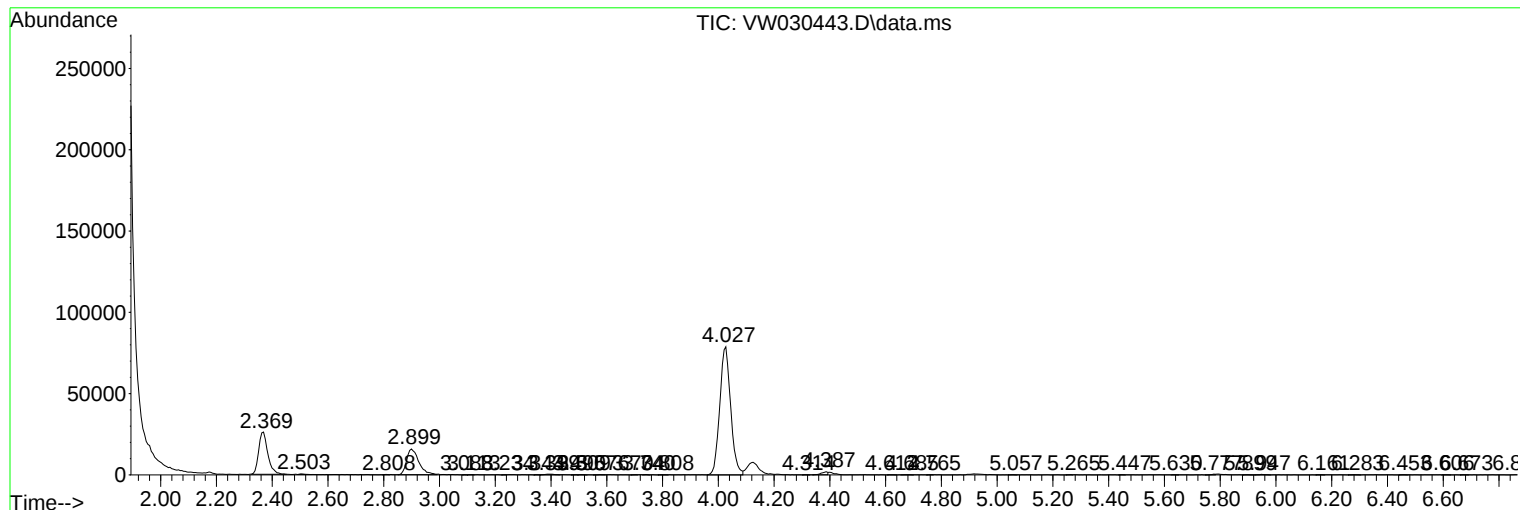
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM092724SMA.M
Quant Title : SFAM01.0

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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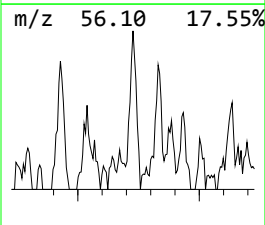
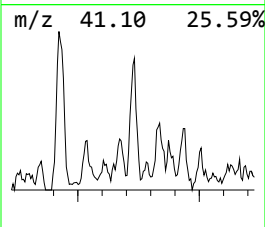
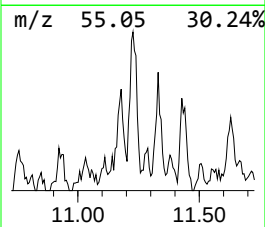
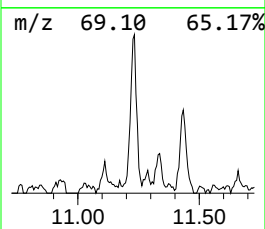
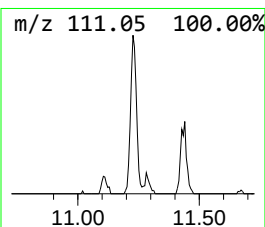
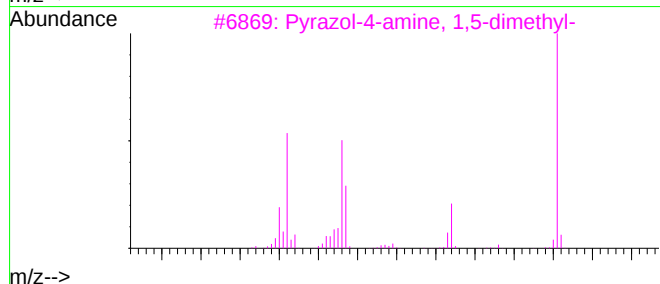
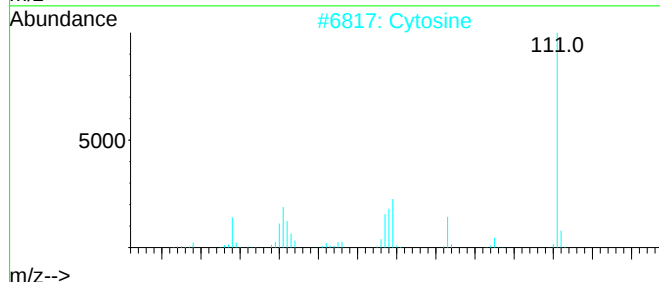
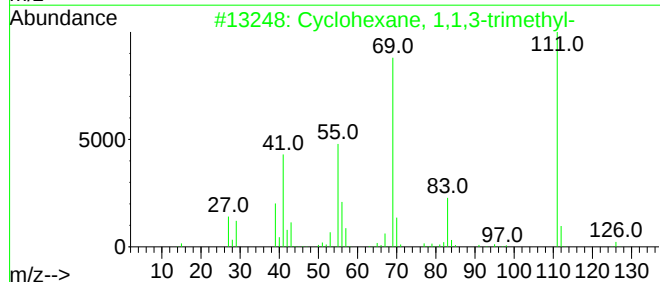
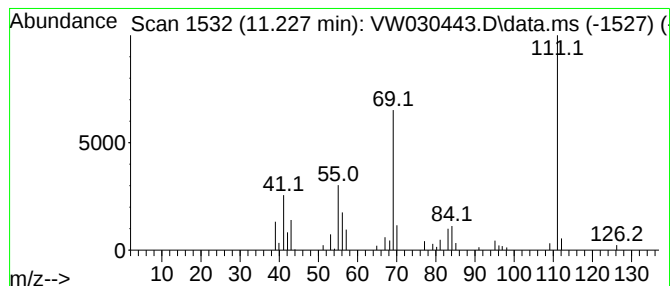
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM092724SMA.M
Quant Title : SFAM01.0

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 2 (DEL) Alkane: Cyclic11.227 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.227	2.00 ug/L	30429	Chlorobenzene-d5		11.629	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1,3-trimethyl-		126	C9H18	003073-66-3	72
2	Cytosine		111	C4H5N3O	000071-30-7	59
3	Pyrazol-4-amine, 1,5-dimethyl-		111	C5H9N3	121983-36-6	59
4	Cyclohexane, 1,1,3-trimethyl-		126	C9H18	003073-66-3	53
5	Cyclohexane, 1,1,3-trimethyl-		126	C9H18	003073-66-3	49



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Quant Title : SFAM01.0

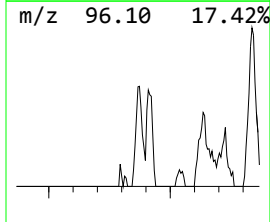
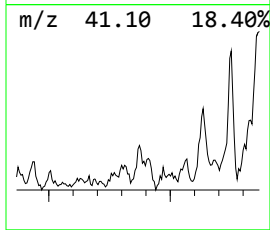
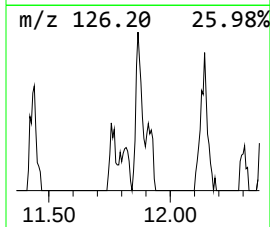
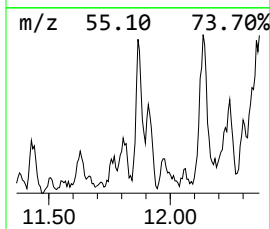
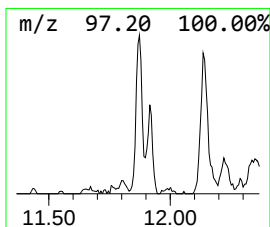
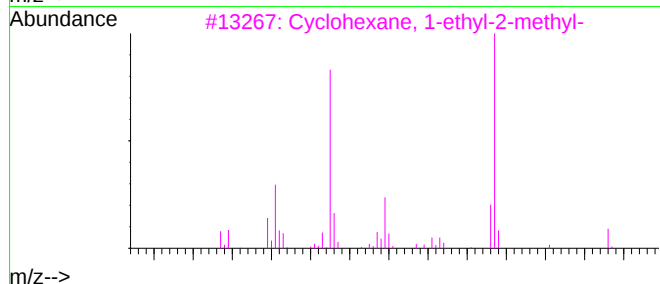
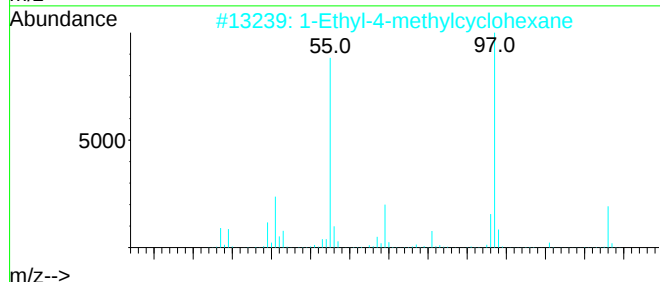
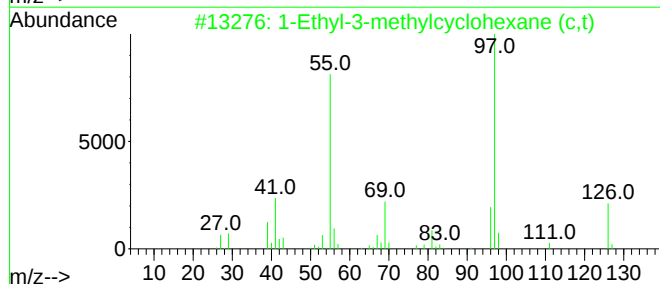
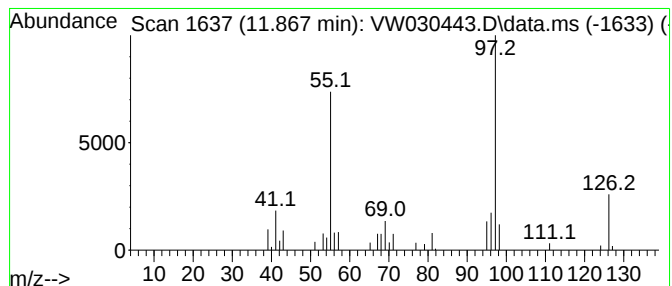
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 (DEL) Alkane: Cyclic11.867 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.867	1.60 ug/L	24341	Chlorobenzene-d5	11.629

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	90
2	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	90
3	Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	86
4	cis-1-Ethyl-3-methyl-cyclohexane	126	C9H18	019489-10-2	80
5	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	64



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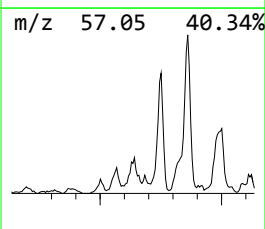
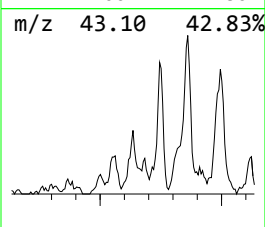
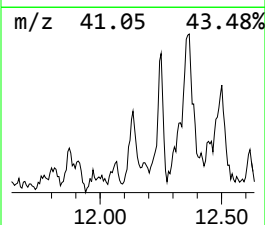
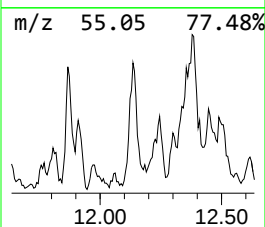
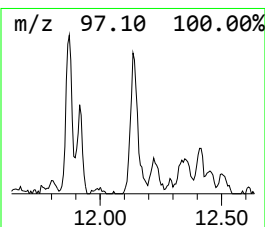
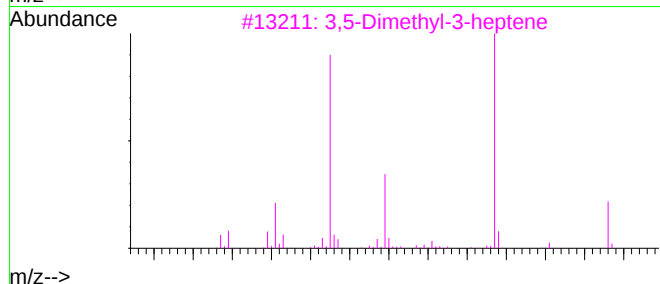
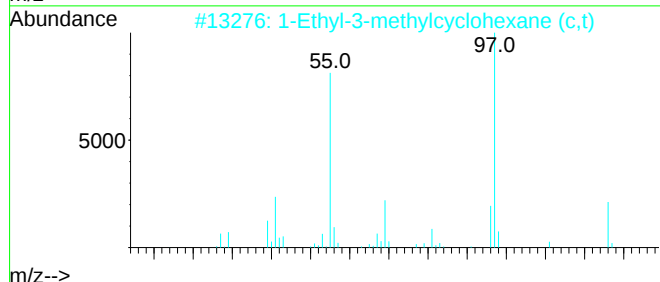
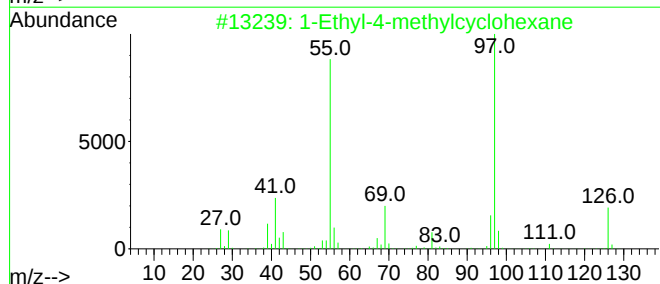
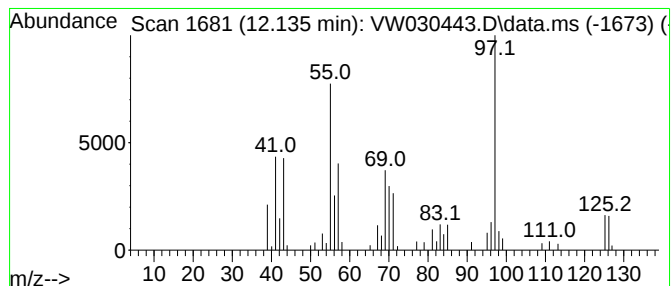
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM092724SMA.M
Quant Title : SFAM01.0

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 (DEL) Alkane: Cyclic12.135 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.135	3.44 ug/L	52252	Chlorobenzene-d5	11.629	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	53
2	1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	49
3	3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	49
4	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	49
5	4-Octen-3-one	126	C8H14O	014129-48-7	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW100824\
Data File : VW030443.D
Acq On : 08 Oct 2024 13:48
Operator : SY/MD
Sample : P4329-07
Misc : 4.97g/10mL/MSVOA_W/SOIL/A
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
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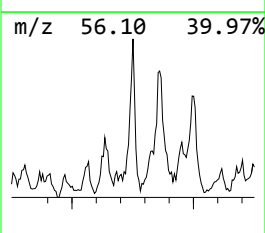
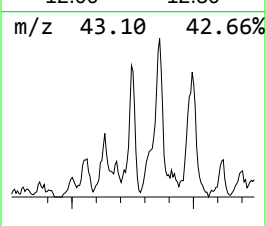
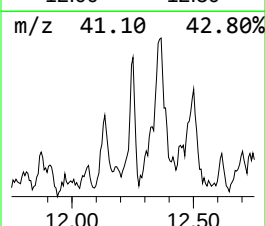
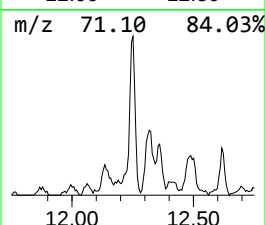
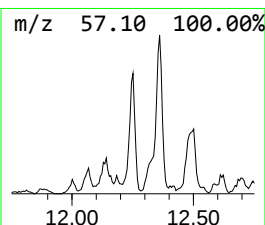
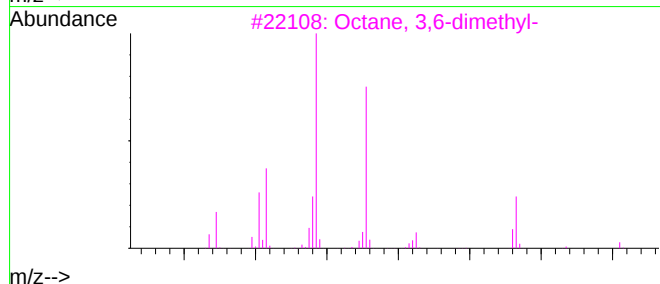
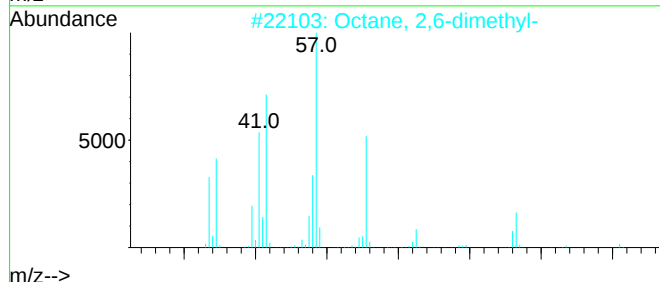
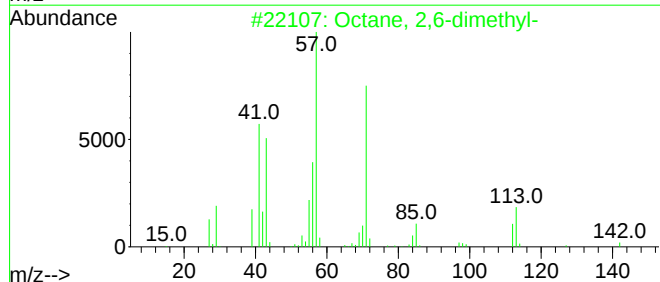
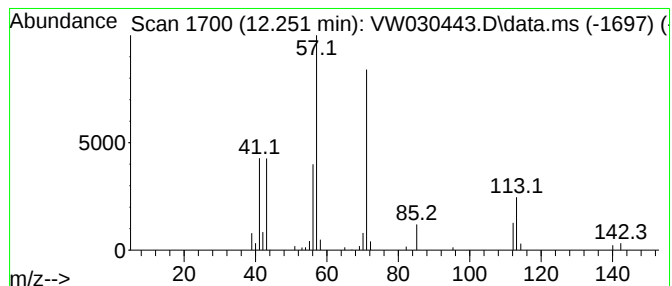
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Quant Title : SFAM01.0

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.251	2.56 ug/L	38838	Chlorobenzene-d5		11.629	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octane, 2,6-dimethyl-		142	C10H22	002051-30-1	91
2	Octane, 2,6-dimethyl-		142	C10H22	002051-30-1	91
3	Octane, 3,6-dimethyl-		142	C10H22	015869-94-0	87
4	Nonane, 3-methyl-		142	C10H22	005911-04-6	83
5	Nonane, 3-methyl-		142	C10H22	005911-04-6	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW100824\
Data File : VW030443.D
Acq On : 08 Oct 2024 13:48
Operator : SY/MD
Sample : P4329-07
Misc : 4.97g/10mL/MSVOA_W/SOIL/A
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM092724SMA.M
Quant Title : SFAM01.0

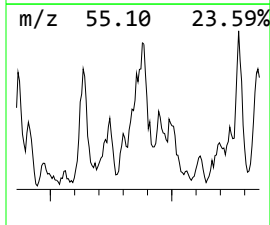
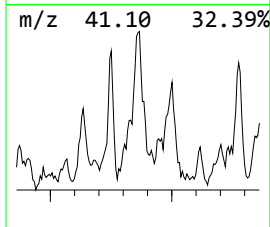
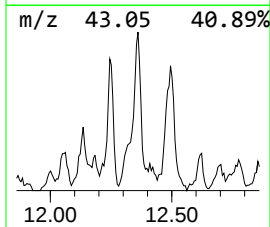
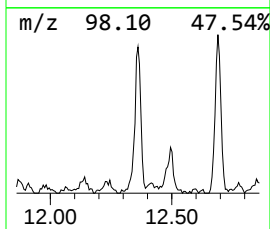
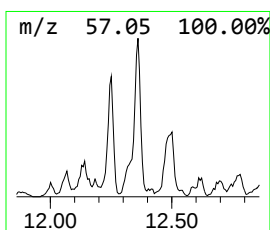
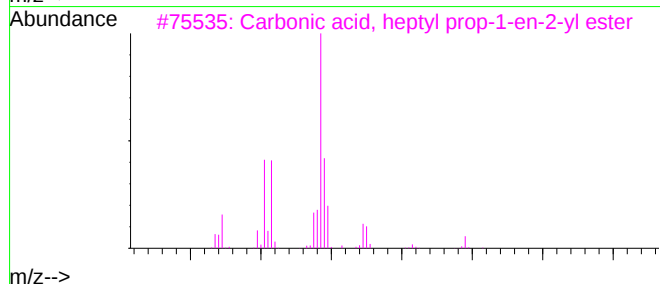
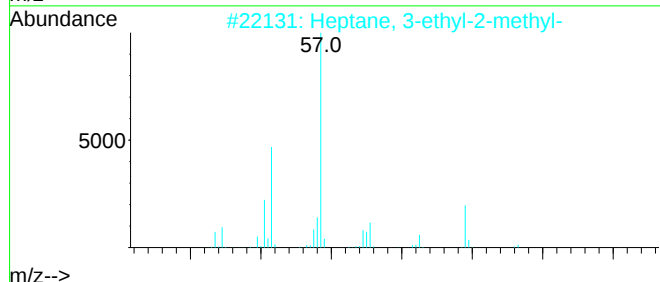
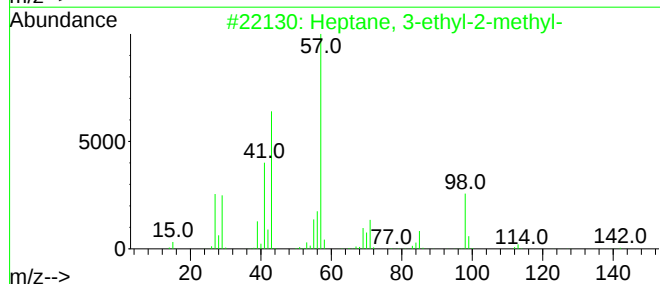
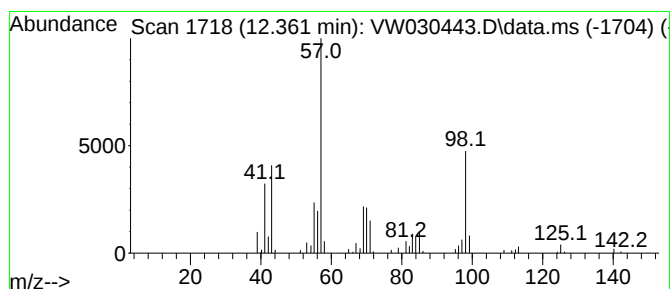
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.361	10.35 ug/L	157283	Chlorobenzene-d5	11.629

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	68
2	Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	50
3	Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	47
4	Heptane, 3-ethyl-	128	C9H20	015869-80-4	47
5	Ether, tert-butyl isopropylidene...	154	C10H18O	024524-56-9	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW100824\
Data File : VW030443.D
Acq On : 08 Oct 2024 13:48
Operator : SY/MD
Sample : P4329-07
Misc : 4.97g/10mL/MSVOA_W/SOIL/A
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
A4EN4

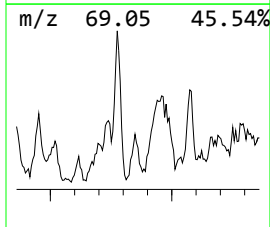
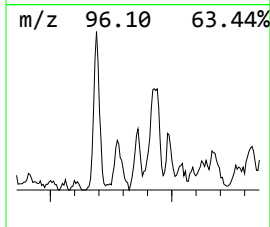
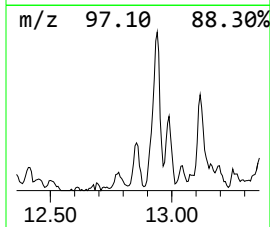
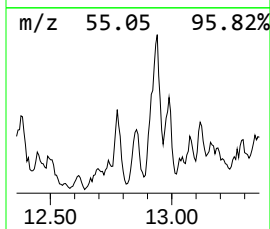
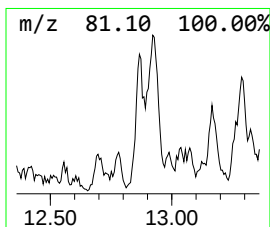
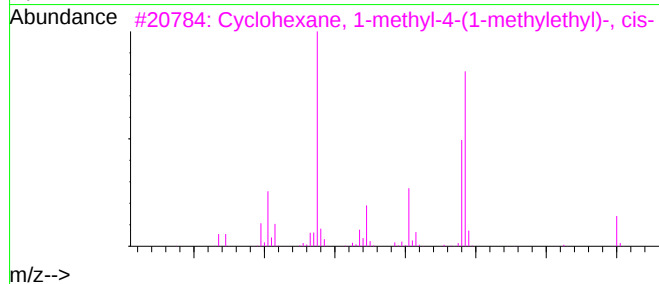
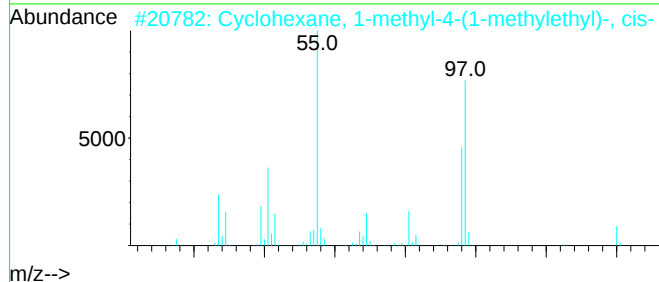
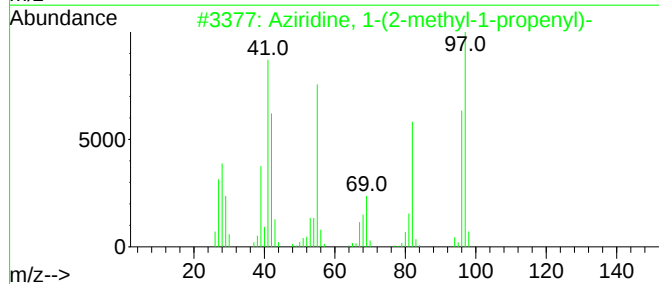
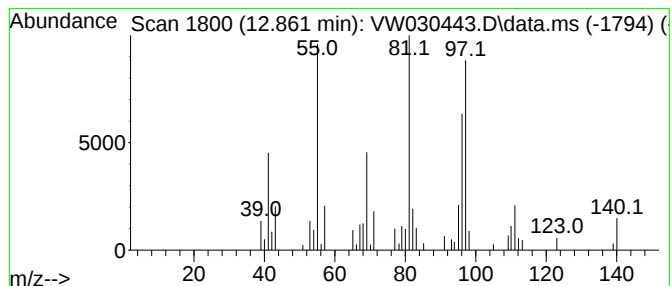
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Quant Title : SFAM01.0

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.861	4.57 ug/L	38617	1,4-Dichlorobenzene-d4		13.556	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Aziridine, 1-(2-methyl-1-propenyl)-		97	C6H11N	080839-93-6	46
2	Cyclohexane, 1-methyl-4-(1-methy...		140	C10H20	006069-98-3	43
3	Cyclohexane, 1-methyl-4-(1-methy...		140	C10H20	006069-98-3	43
4	Cyclohexane, 1-methyl-4-(1-methy...		140	C10H20	001678-82-6	43
5	Cyclohexane, 1-methyl-4-(1-methy...		140	C10H20	001678-82-6	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW100824\
Data File : VW030443.D
Acq On : 08 Oct 2024 13:48
Operator : SY/MD
Sample : P4329-07
Misc : 4.97g/10mL/MSVOA_W/SOIL/A
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
A4EN4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM092724SMA.M
Quant Title : SFAM01.0

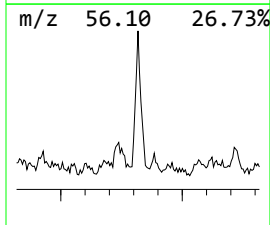
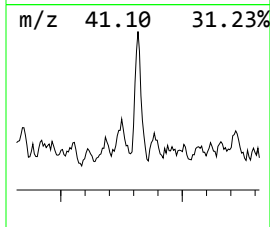
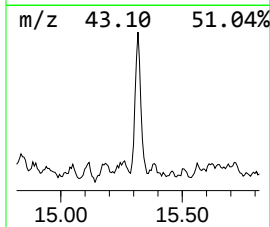
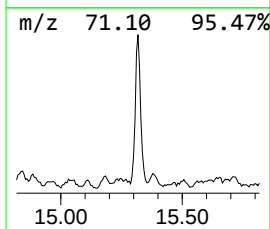
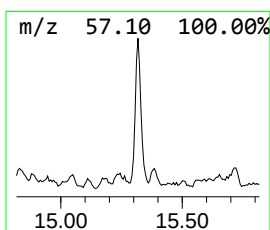
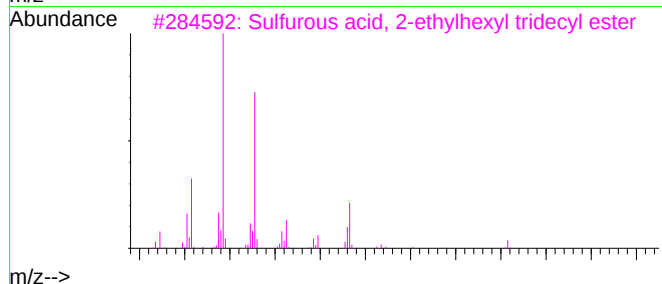
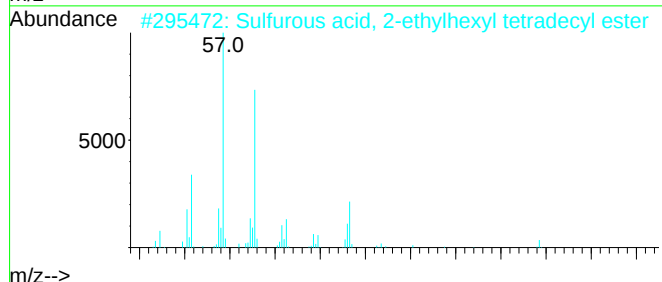
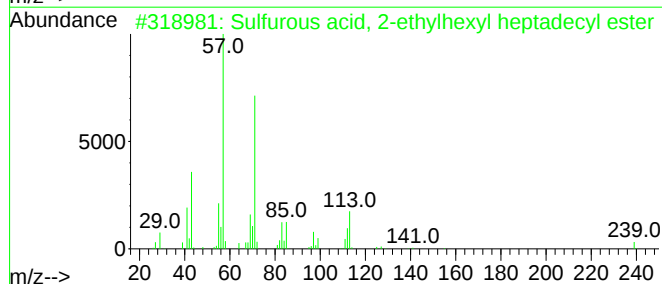
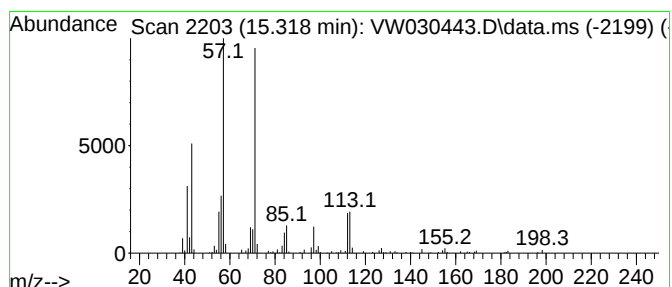
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 9 Sulfurous acid, 2-ethylhexy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.318	18.49 ug/L	156241	1,4-Dichlorobenzene-d4	13.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	78
2	Sulfurous acid, 2-ethylhexyl tet...	390	C22H46O3S	1000309-19-7	72
3	Sulfurous acid, 2-ethylhexyl tri...	376	C21H44O3S	1000309-19-6	72
4	Tridecane, 7-methyl-	198	C14H30	026730-14-3	72
5	Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW100824\
Data File : VW030443.D
Acq On : 08 Oct 2024 13:48
Operator : SY/MD
Sample : P4329-07
Misc : 4.97g/10mL/MSVOA_W/SOIL/A
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
A4EN4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM092724SMA.M
Quant Title : SFAM01.0

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

					--Internal Standard--			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: C...	11.227	2.0	ug/L	30429	2	11.629	379973	25.0
(DEL) Alkane: C...	11.867	1.6	ug/L	24341	2	11.629	379973	25.0
(DEL) Alkane: C...	12.135	3.4	ug/L	52252	2	11.629	379973	25.0
(DEL) Alkane: S...	12.251	2.6	ug/L	38838	2	11.629	379973	25.0
(DEL) Alkane: S...	12.361	10.4	ug/L	157283	2	11.629	379973	25.0
unknown-01	12.861	4.6	ug/L	38617	3	13.556	211262	25.0
Sulfurous acid,...	15.318	18.5	ug/L	156241	3	13.556	211262	25.0