

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD112223\
 Data File : VD077664.D
 Acq On : 22 Nov 2023 12:19
 Operator : JC/SY
 Sample : 05459-14
 Misc : 4.30G/10ml/MSVOA_D/SOIL
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 COAK0

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_D\Method\SFAMDLM110923SMA.M
 Title : SFAM01.0

Signal : TIC: VD077664.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.740	20	26	34	rVB	169892	301972	100.00%	39.134%
2	2.069	79	82	84	rBV3	1216	1491	0.49%	0.193%
3	3.111	257	259	261	rBV	1315	1161	0.38%	0.150%
4	3.140	261	264	266	rVB2	830	1092	0.36%	0.142%
5	3.216	275	277	279	rBV2	1098	888	0.29%	0.115%
6	3.269	282	286	288	rVB	854	1091	0.36%	0.141%
7	3.293	288	290	293	rBV2	890	1130	0.37%	0.146%
8	3.322	293	295	297	rVV2	1127	750	0.25%	0.097%
9	3.358	299	301	304	rBV2	1129	1435	0.48%	0.186%
10	3.440	312	315	317	rBV	1106	1214	0.40%	0.157%
11	3.481	319	322	325	rBV	833	1279	0.42%	0.166%
12	3.505	325	326	329	rVB	998	773	0.26%	0.100%
13	3.546	329	333	338	rBV	1443	2356	0.78%	0.305%
14	3.628	344	347	349	rVB2	1278	1130	0.37%	0.146%
15	3.722	361	363	364	rVB	1180	693	0.23%	0.090%
16	3.746	364	367	369	rBV	1287	1638	0.54%	0.212%
17	3.840	381	383	385	rVB	1661	950	0.31%	0.123%
18	3.916	390	396	398	rBV4	5804	10362	3.43%	1.343%
19	4.011	410	412	413	rBV	1212	892	0.30%	0.116%
20	4.058	416	420	423	rVV3	1220	1848	0.61%	0.239%
21	4.252	451	453	454	rBV	1294	728	0.24%	0.094%
22	4.310	461	463	465	rVV2	1127	1043	0.35%	0.135%
23	4.769	538	541	542	rBV	986	1031	0.34%	0.134%
24	4.799	544	546	549	rVV4	2534	2152	0.71%	0.279%
25	4.875	557	559	563	rBV2	637	922	0.31%	0.119%
26	5.075	591	593	596	rVB	1156	1065	0.35%	0.138%
27	5.252	622	623	626	rVB2	1242	983	0.33%	0.127%
28	5.281	626	628	629	rBV2	765	712	0.24%	0.092%
29	5.428	652	653	656	rBV	782	804	0.27%	0.104%
30	5.516	665	668	672	rBV2	1065	1697	0.56%	0.220%
31	5.746	705	707	709	rBV2	975	832	0.28%	0.108%
32	6.122	768	771	772	rBV	1603	1438	0.48%	0.186%
33	6.140	772	774	775	rVV	1350	1069	0.35%	0.139%
34	6.169	778	779	781	rVV	2047	991	0.33%	0.128%
35	6.193	781	783	785	rVV2	956	818	0.27%	0.106%
36	6.299	800	801	803	rBV	1053	754	0.25%	0.098%

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Integrator: RTE

Smoothing : OFF

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Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM110923SMA.M
 Title : SFAM01.0

37	6.334	805	807	809	rVB2	879	695	0.23%	0.090%
38	6.575	847	848	851	rVV	910	740	0.25%	0.096%
39	6.652	859	861	864	rVB3	1185	884	0.29%	0.115%
40	6.875	897	899	902	rVB2	923	805	0.27%	0.104%
41	6.916	902	906	907	rBV2	836	936	0.31%	0.121%
42	6.952	910	912	913	rBV2	911	661	0.22%	0.086%
43	7.175	948	950	953	rVB	1460	929	0.31%	0.120%
44	7.204	953	955	959	rBV	963	1158	0.38%	0.150%
45	7.246	961	962	965	rBV	1403	1452	0.48%	0.188%
46	7.440	993	995	996	rBV	1104	692	0.23%	0.090%
47	7.481	1000	1002	1005	rVB2	875	794	0.26%	0.103%
48	7.516	1005	1008	1009	rBV2	604	664	0.22%	0.086%
49	7.569	1009	1017	1025	rVB	10192	27355	9.06%	3.545%
50	7.716	1038	1042	1045	rVB2	824	1250	0.41%	0.162%
51	7.740	1045	1046	1049	rVB2	1338	977	0.32%	0.127%
52	7.763	1049	1050	1052	rBV2	1043	682	0.23%	0.088%
53	7.834	1060	1062	1064	rVB	1019	883	0.29%	0.114%
54	7.969	1082	1085	1089	rVB	1435	1559	0.52%	0.202%
55	7.999	1089	1090	1091	rBV	1182	630	0.21%	0.082%
56	8.069	1099	1102	1103	rVB2	1210	896	0.30%	0.116%
57	8.081	1103	1104	1107	rBV2	1302	1255	0.42%	0.163%
58	8.210	1117	1126	1136	rBV6	18347	59550	19.72%	7.717%
59	8.716	1210	1212	1215	rBV2	1142	1630	0.54%	0.211%
60	8.775	1216	1222	1229	rVB3	17212	35113	11.63%	4.550%
61	8.881	1238	1240	1242	rVV	892	708	0.23%	0.092%
62	8.963	1252	1254	1256	rVV	832	641	0.21%	0.083%
63	9.016	1261	1263	1265	rVB	1135	713	0.24%	0.092%
64	9.104	1274	1278	1281	rVB	966	1657	0.55%	0.215%
65	9.151	1284	1286	1289	rBV	980	1213	0.40%	0.157%
66	9.216	1290	1297	1306	rVB4	14572	32228	10.67%	4.177%
67	9.287	1306	1309	1311	rBV2	1363	1733	0.57%	0.225%
68	9.398	1325	1328	1331	rBV2	805	1105	0.37%	0.143%
69	9.887	1409	1411	1413	rBV	833	658	0.22%	0.085%
70	9.975	1421	1426	1434	rVB4	7303	13239	4.38%	1.716%
71	10.269	1469	1476	1483	rVB3	18883	37541	12.43%	4.865%
72	10.416	1499	1501	1504	rBV2	1309	1454	0.48%	0.188%
73	10.528	1515	1520	1526	rBV4	6222	11734	3.89%	1.521%
74	10.593	1529	1531	1532	rVB	1189	624	0.21%	0.081%
75	10.745	1555	1557	1558	rBV2	1154	641	0.21%	0.083%
76	10.875	1575	1579	1585	rBV2	11511	21934	7.26%	2.843%

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 Title : SFAM01.0

77	10.945	1589	1591	1595	rBV	1008	1148	0.38%	0.149%
78	11.098	1615	1617	1621	rBV2	968	1180	0.39%	0.153%
79	11.210	1634	1636	1638	rVB	1068	640	0.21%	0.083%
80	11.381	1663	1665	1666	rBV	1362	807	0.27%	0.105%
81	11.422	1670	1672	1676	rVB2	731	1020	0.34%	0.132%
82	11.581	1694	1699	1707	rVB	26948	45185	14.96%	5.856%
83	11.634	1707	1708	1710	rBV	1029	1015	0.34%	0.132%
84	12.204	1803	1805	1807	rBV2	888	847	0.28%	0.110%
85	12.475	1849	1851	1852	rBV	1152	802	0.27%	0.104%
86	12.528	1859	1860	1863	rVB2	1091	730	0.24%	0.095%
87	12.575	1867	1868	1872	rVV2	1164	1079	0.36%	0.140%
88	12.651	1876	1881	1887	rVB2	14546	25076	8.30%	3.250%
89	12.887	1919	1921	1922	rBV	1071	950	0.31%	0.123%
90	13.328	1994	1996	1997	rBV	1367	928	0.31%	0.120%
91	13.463	2017	2019	2023	rVV2	1154	1766	0.58%	0.229%
92	13.522	2023	2029	2036	rVB2	16995	31261	10.35%	4.051%
93	13.639	2047	2049	2051	rBV2	1101	993	0.33%	0.129%
94	13.692	2055	2058	2059	rVV2	1416	995	0.33%	0.129%
95	13.739	2064	2066	2068	rBV3	945	902	0.30%	0.117%
96	13.822	2074	2080	2085	rVB3	15355	26935	8.92%	3.491%
97	14.016	2111	2113	2114	rBV2	1047	719	0.24%	0.093%
98	14.057	2119	2120	2124	rVB2	1282	1345	0.45%	0.174%
99	14.086	2124	2125	2129	rBV3	976	1278	0.42%	0.166%
100	16.675	2563	2565	2568	rBV2	2752	2842	0.94%	0.368%

Sum of corrected areas: 771640

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Instrument :
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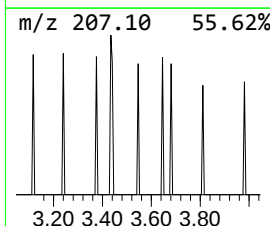
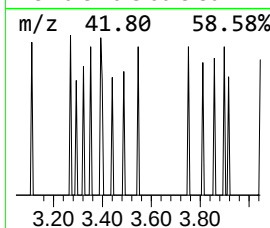
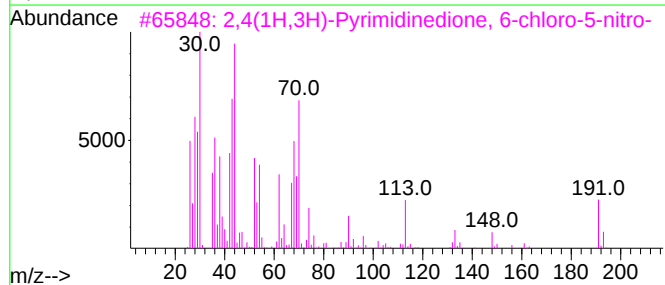
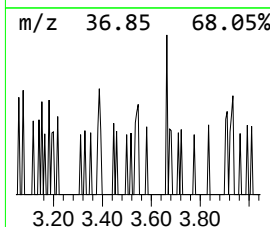
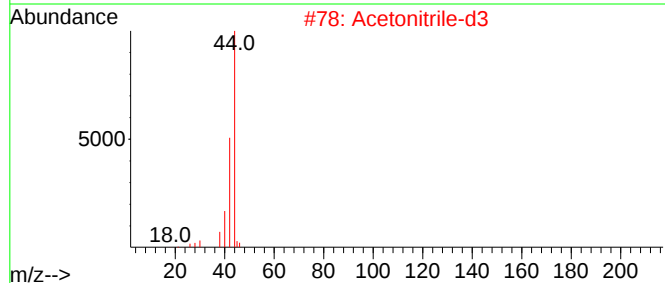
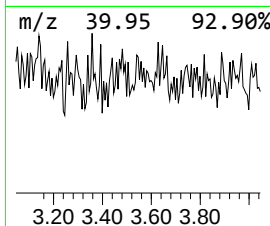
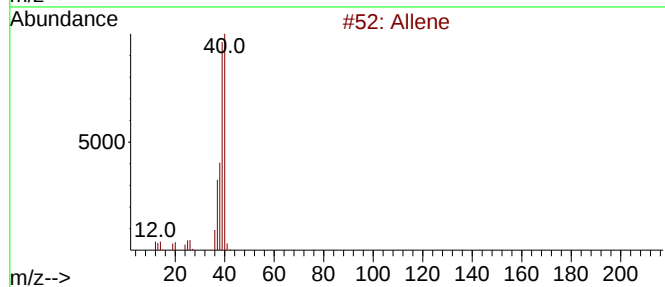
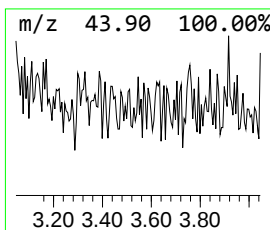
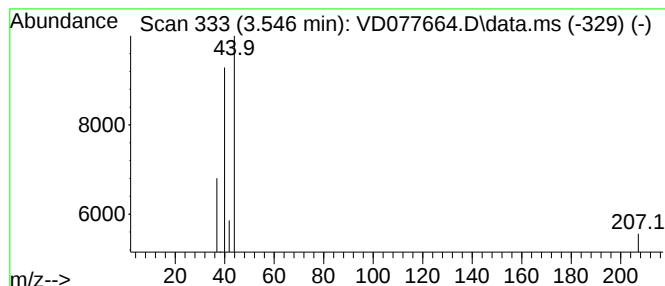
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM110923SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.546	1.68 ug/L	2356	1,4-Difluorobenzene	8.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Allene	40	C3H4	000463-49-0	5
2			Acetonitrile-d3	44	C2D3N	002206-26-0	4
3			2,4(1H,3H)-Pyrimidinedione, 6-ch...	191	C4H2ClN3O4	006630-30-4	4
4			Cyclohexane-1,3-dione, 2-allylam...	207	C12H17NO2	104926-37-6	2
5			6-Nitro-8-methoxy-2H-chromene	207	C10H9NO4	062063-07-4	2



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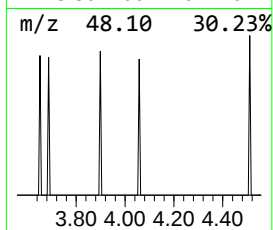
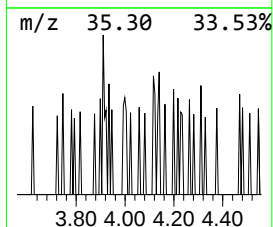
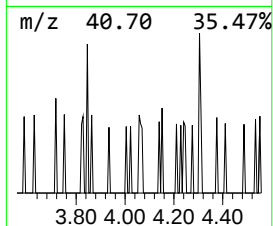
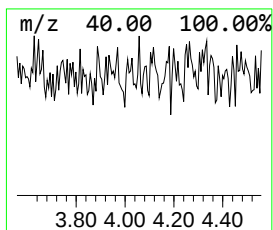
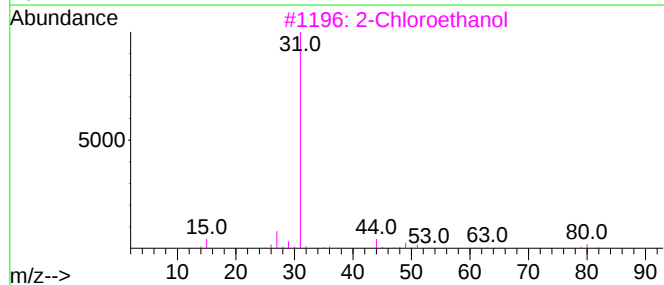
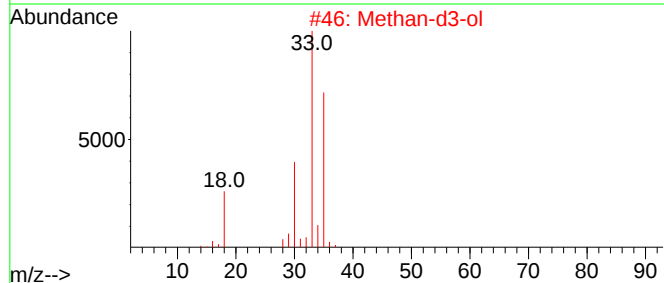
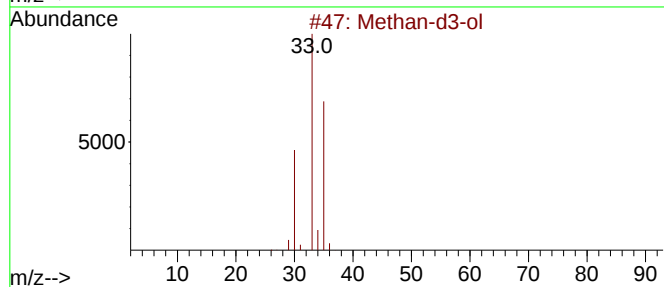
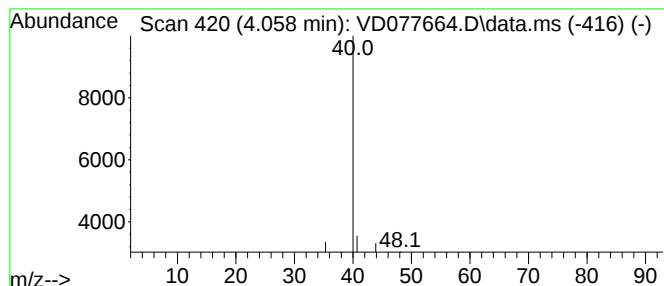
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM110923SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 unknown-02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.058	1.32 ug/L	1848	1,4-Difluorobenzene	8.775

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Methan-d3-ol	35	CHD3O	001849-29-2	3
2		Methan-d3-ol	35	CHD3O	001849-29-2	3
3		2-Chloroethanol	80	C2H5ClO	000107-07-3	1
4		Nitrosyl chloride	65	ClNO	002696-92-6	1
5		2-Chloroethylamine	79	C2H6ClN	000689-98-5	1



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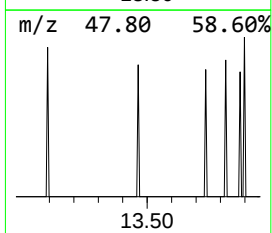
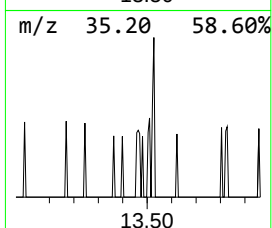
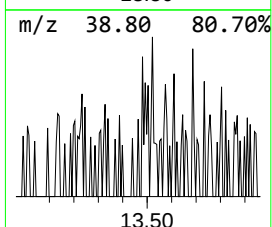
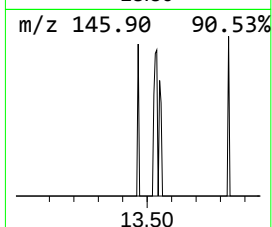
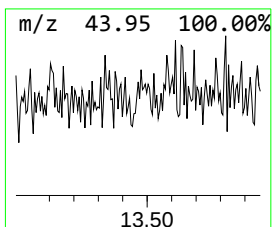
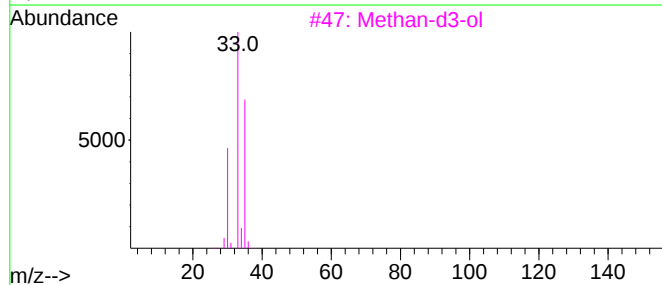
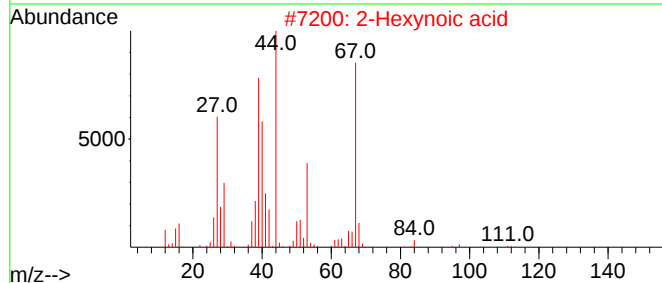
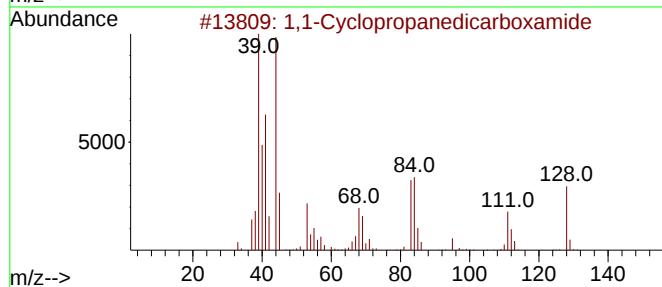
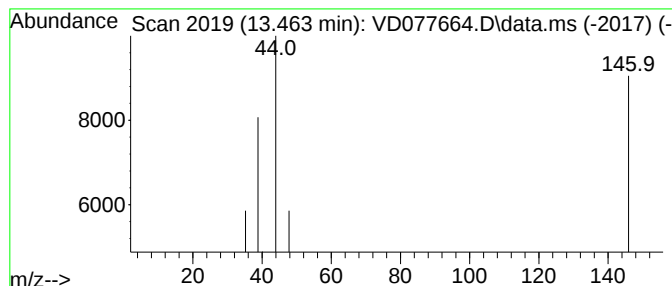
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM110923SMA.M
Quant Title : SFAM01.0

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

Peak Number 5 unknown-03 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.463	1.41 ug/L	1766	1,4-Dichlorobenzene-d4	13.522

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,1-Cyclopropanedicarboxamide	128	C5H8N2O2	005813-85-4	4
2			2-Hexynoic acid	112	C6H8O2	000764-33-0	4
3			Methan-d3-ol	35	CHD3O	001849-29-2	3
4			Methan-d3-ol	35	CHD3O	001849-29-2	3
5			Propane	44	C3H8	000074-98-6	3



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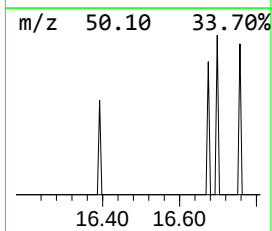
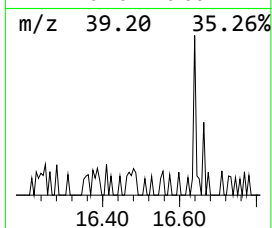
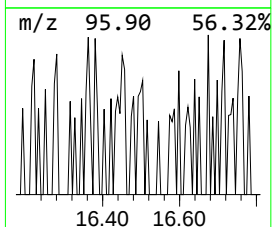
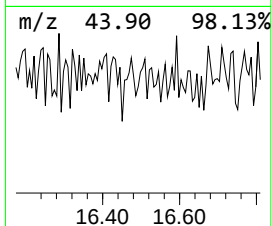
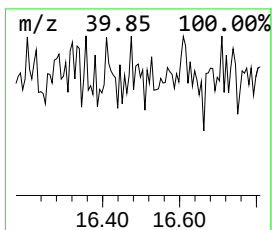
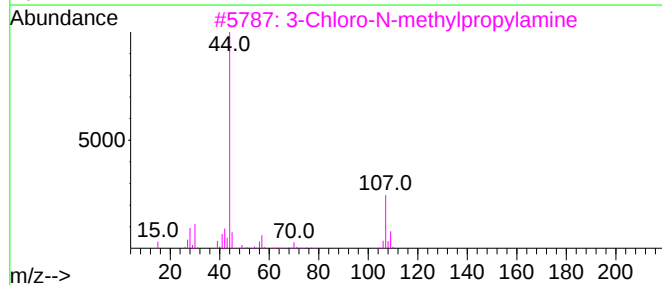
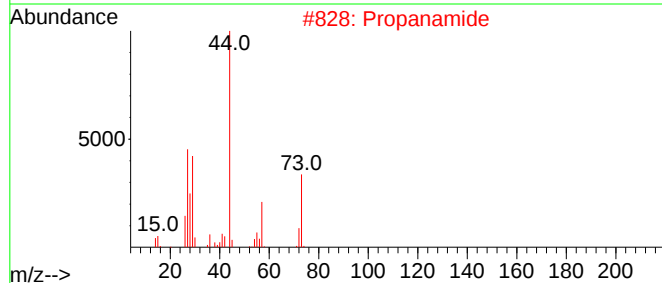
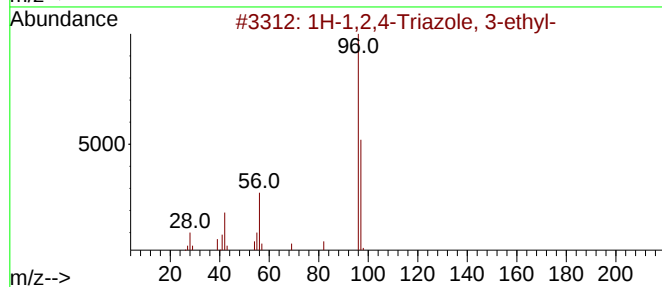
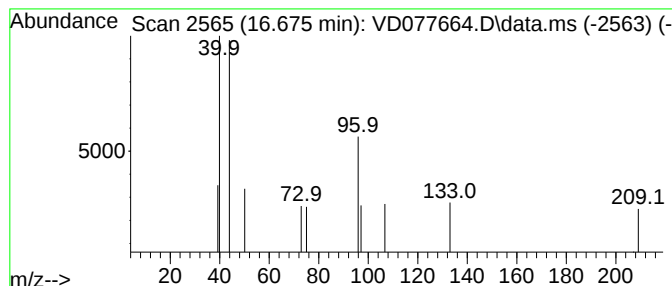
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Quant Title : SFAM01.0

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

Peak Number 6 unknown-04 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.675	2.27 ug/L	2842	1,4-Dichlorobenzene-d4	13.522

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-1,2,4-Triazole, 3-ethyl-	97	C4H7N3	007411-16-7	5
2			Propanamide	73	C3H7NO	000079-05-0	4
3			3-Chloro-N-methylpropylamine	107	C4H10ClN	065232-62-4	4
4			Propanamide	73	C3H7NO	000079-05-0	4
5			Pterin-6-carboxylic acid	207	C7H5N5O3	000948-60-7	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD112223\
Data File : VD077664.D
Acq On : 22 Nov 2023 12:19
Operator : JC/SY
Sample : 05459-14
Misc : 4.30G/10ml/MSVOA_D/SOIL
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
C0AK0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM110923SMA.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
unknown-01	3.546	1.7	ug/L	2356	1	8.775	35113	25.0
unknown-02	4.058	1.3	ug/L	1848	1	8.775	35113	25.0
unknown-03	13.463	1.4	ug/L	1766	3	13.522	31261	25.0
unknown-04	16.675	2.3	ug/L	2842	3	13.522	31261	25.0