

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD061523\
 Data File : VD076443.D
 Acq On : 15 Jun 2023 17:36
 Operator : KP/SY
 Sample : 03236-13
 Misc : 5.12G/10.00ml/MSVOA_D/SOIL
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 YBTZ6

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\SFAMDLM061523SMA.M
 Title : SFAM01.0

Signal : TIC: VD076443.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.687	10	17	20	rBV	451322	719901	84.04%	14.432%
2	1.728	20	24	35	rVB	529047	856636	100.00%	17.174%
3	2.269	111	116	121	rVB	41726	60225	7.03%	1.207%
4	2.793	200	205	213	rVB	38287	69808	8.15%	1.400%
5	3.299	288	291	292	rBV2	1432	1065	0.12%	0.021%
6	3.481	321	322	325	rBV	1288	1049	0.12%	0.021%
7	3.552	333	334	337	rVB2	1681	966	0.11%	0.019%
8	3.716	360	362	364	rVB	864	710	0.08%	0.014%
9	3.805	374	377	378	rBV2	818	753	0.09%	0.015%
10	3.828	378	381	383	rVV2	1087	1204	0.14%	0.024%
11	3.911	386	395	406	rVV3	36813	96300	11.24%	1.931%
12	4.105	426	428	432	rVB2	856	967	0.11%	0.019%
13	4.187	441	442	446	rBV	1228	1295	0.15%	0.026%
14	4.258	452	454	455	rBV2	863	623	0.07%	0.012%
15	4.581	506	509	510	rBV2	513	634	0.07%	0.013%
16	4.628	513	517	521	rVB2	666	1169	0.14%	0.023%
17	4.663	521	523	527	rBV	945	881	0.10%	0.018%
18	4.799	536	546	556	rBV6	7156	23127	2.70%	0.464%
19	4.958	571	573	575	rBV2	1017	1001	0.12%	0.020%
20	5.069	590	592	595	rVV2	1155	797	0.09%	0.016%
21	5.263	623	625	628	rBV2	1117	945	0.11%	0.019%
22	5.369	641	643	645	rVB	1413	1035	0.12%	0.021%
23	5.510	665	667	669	rBV	683	645	0.08%	0.013%
24	5.575	676	678	680	rBV	732	689	0.08%	0.014%
25	5.728	701	704	708	rBV3	891	1121	0.13%	0.022%
26	5.905	730	734	737	rBV2	1509	1798	0.21%	0.036%
27	5.957	740	743	744	rBV2	921	1022	0.12%	0.020%
28	6.116	769	770	775	rVB	606	666	0.08%	0.013%
29	6.275	794	797	799	rBV2	617	686	0.08%	0.014%
30	6.352	807	810	815	rBV2	992	1150	0.13%	0.023%
31	6.393	815	817	822	rVB2	1296	1473	0.17%	0.030%
32	6.452	826	827	829	rBV2	1014	758	0.09%	0.015%
33	6.540	840	842	845	rVB	653	765	0.09%	0.015%
34	6.569	845	847	850	rVB2	891	801	0.09%	0.016%
35	6.605	850	853	856	rBV	1026	1241	0.14%	0.025%
36	6.987	908	918	925	rBV2	32054	90734	10.59%	1.819%

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Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM061523SMA.M
 Title : SFAM01.0

37	7.216	955	957	958	rVB	1178	612	0.07%	0.012%
38	7.252	961	963	966	rVB	1410	1284	0.15%	0.026%
39	7.281	966	968	970	rBV	1035	1176	0.14%	0.024%
40	7.563	1006	1016	1028	rBV	65472	165797	19.35%	3.324%
41	7.740	1045	1046	1048	rBV2	1164	711	0.08%	0.014%
42	8.204	1115	1125	1141	rBV3	128142	409435	47.80%	8.208%
43	8.322	1144	1145	1147	rBV	1024	716	0.08%	0.014%
44	8.404	1156	1159	1163	rBV2	700	1285	0.15%	0.026%
45	8.663	1200	1203	1204	rBV2	873	645	0.08%	0.013%
46	8.775	1214	1222	1232	rBV2	118854	246012	28.72%	4.932%
47	8.887	1237	1241	1243	rBV2	1256	1929	0.23%	0.039%
48	9.028	1259	1265	1274	rVB3	24430	46332	5.41%	0.929%
49	9.134	1279	1283	1285	rBV2	575	688	0.08%	0.014%
50	9.204	1287	1295	1306	rVV2	98736	214033	24.99%	4.291%
51	9.304	1310	1312	1317	rVV2	1903	1877	0.22%	0.038%
52	9.351	1317	1320	1322	rVB	1132	1046	0.12%	0.021%
53	9.593	1360	1361	1362	rBV	1598	960	0.11%	0.019%
54	9.651	1368	1371	1372	rBV	1184	1252	0.15%	0.025%
55	9.769	1389	1391	1394	rBV2	813	983	0.11%	0.020%
56	9.869	1406	1408	1409	rBV	912	645	0.08%	0.013%
57	9.981	1418	1427	1434	rVV	61043	117553	13.72%	2.357%
58	10.034	1434	1436	1440	rVB2	941	1109	0.13%	0.022%
59	10.110	1448	1449	1453	rBV2	867	936	0.11%	0.019%
60	10.157	1455	1457	1459	rVB	839	707	0.08%	0.014%
61	10.269	1468	1476	1484	rBV	163527	299022	34.91%	5.995%
62	10.522	1512	1519	1527	rVB	47715	83534	9.75%	1.675%
63	10.663	1538	1543	1547	rBV3	5301	8431	0.98%	0.169%
64	10.804	1563	1567	1573	rVB6	6384	10260	1.20%	0.206%
65	10.875	1573	1579	1587	rBV	113108	201106	23.48%	4.032%
66	10.963	1592	1594	1595	rBV	1201	692	0.08%	0.014%
67	11.028	1601	1605	1611	rVB3	11612	18389	2.15%	0.369%
68	11.216	1635	1637	1639	rBV	721	777	0.09%	0.016%
69	11.334	1655	1657	1660	rBV2	969	1212	0.14%	0.024%
70	11.469	1678	1680	1681	rVV	1342	683	0.08%	0.014%
71	11.581	1692	1699	1710	rVB	191482	322486	37.65%	6.465%
72	11.998	1768	1770	1773	rVB	1135	727	0.08%	0.015%
73	12.045	1776	1778	1782	rVV2	728	607	0.07%	0.012%
74	12.316	1822	1824	1825	rBV	823	672	0.08%	0.013%
75	12.416	1839	1841	1842	rVB2	1161	811	0.09%	0.016%
76	12.581	1865	1869	1874	rBV4	4455	6226	0.73%	0.125%

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 Title : SFAM01.0

77	12.651	1874	1881	1888	rVB	139876	226395	26.43%	4.539%
78	12.810	1906	1908	1912	rBV	694	774	0.09%	0.016%
79	12.845	1912	1914	1915	rBV2	919	748	0.09%	0.015%
80	12.904	1920	1924	1929	rBV2	1445	2866	0.33%	0.057%
81	13.139	1961	1964	1966	rBV3	862	1216	0.14%	0.024%
82	13.163	1966	1968	1973	rVV3	1324	1443	0.17%	0.029%
83	13.516	2022	2028	2037	rVB	193483	314565	36.72%	6.306%
84	13.610	2042	2044	2047	rVB2	1766	1966	0.23%	0.039%
85	13.816	2072	2079	2087	rBV	181225	301356	35.18%	6.042%
86	13.945	2099	2101	2104	rBV	1139	1010	0.12%	0.020%
87	13.986	2106	2108	2109	rBV2	1102	667	0.08%	0.013%
88	14.045	2116	2118	2124	rVB5	2768	3736	0.44%	0.075%
89	14.181	2139	2141	2145	rBV3	1364	1902	0.22%	0.038%
90	14.381	2172	2175	2176	rVB2	1412	1018	0.12%	0.020%
91	14.463	2187	2189	2190	rVB	1676	905	0.11%	0.018%
92	14.498	2190	2195	2198	rBV3	1114	1681	0.20%	0.034%
93	14.592	2208	2211	2212	rBV2	1521	1392	0.16%	0.028%
94	14.969	2273	2275	2276	rBV2	1431	803	0.09%	0.016%
95	15.098	2296	2297	2300	rVB3	1870	1358	0.16%	0.027%
96	15.151	2304	2306	2308	rBV2	1772	1119	0.13%	0.022%
97	15.257	2323	2324	2325	rBV	1678	993	0.12%	0.020%
98	15.375	2343	2344	2345	rBV	1281	614	0.07%	0.012%
99	15.563	2374	2376	2377	rBV	1362	662	0.08%	0.013%
100	16.180	2479	2481	2482	rBV	1726	877	0.10%	0.018%

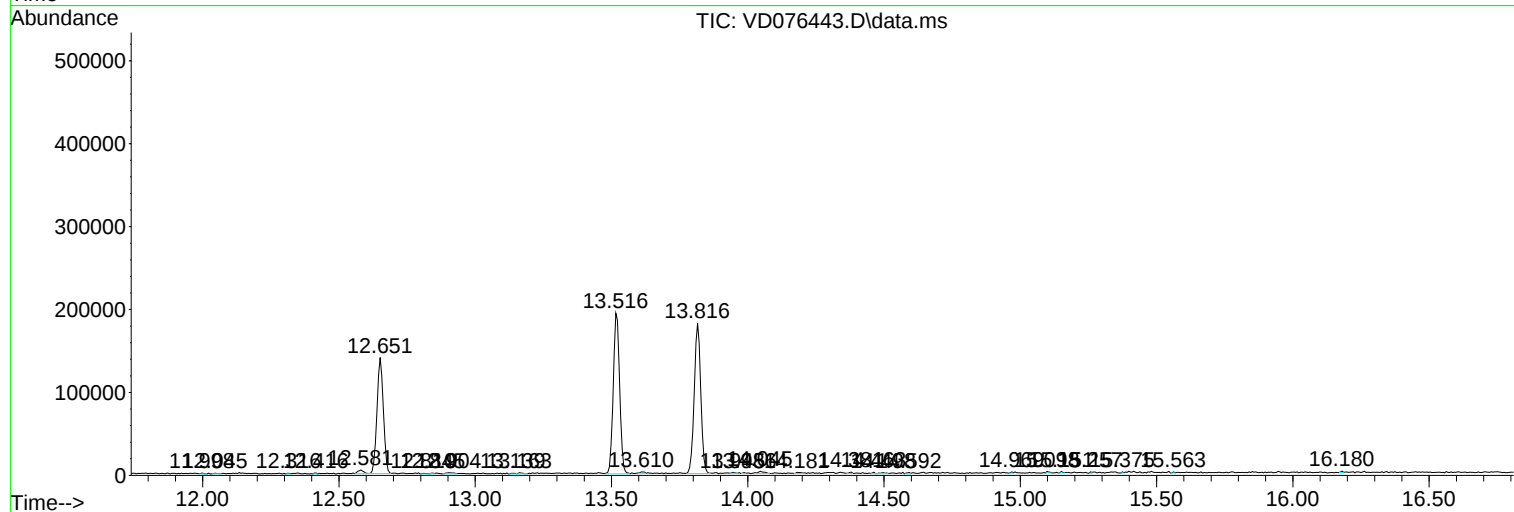
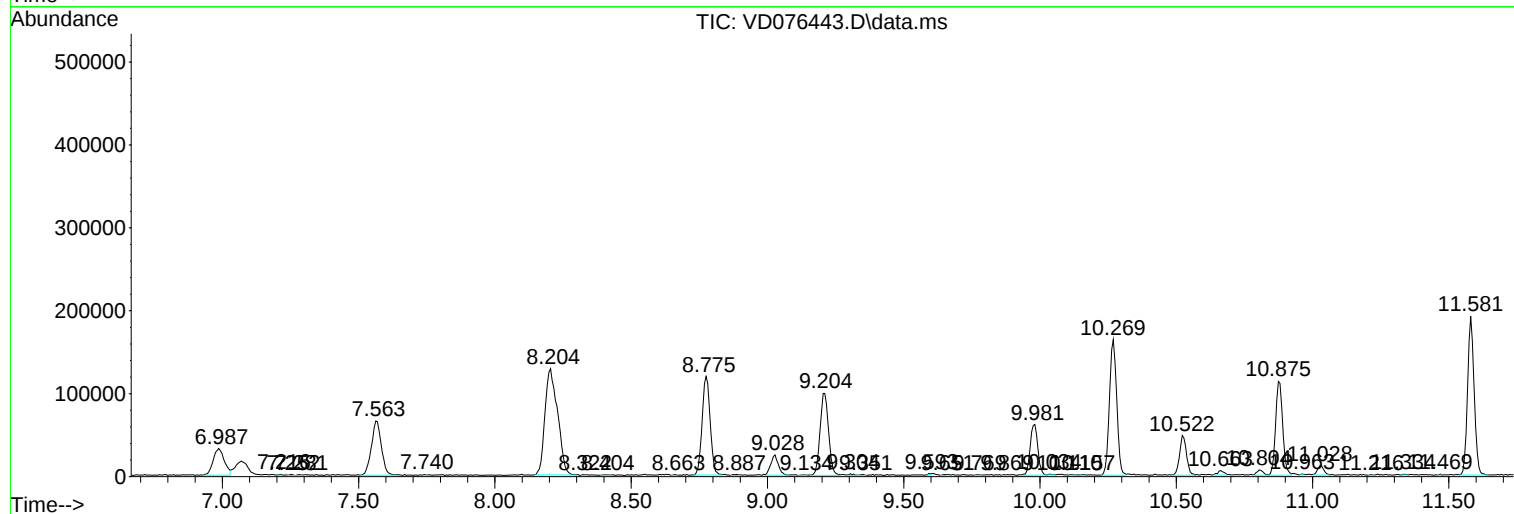
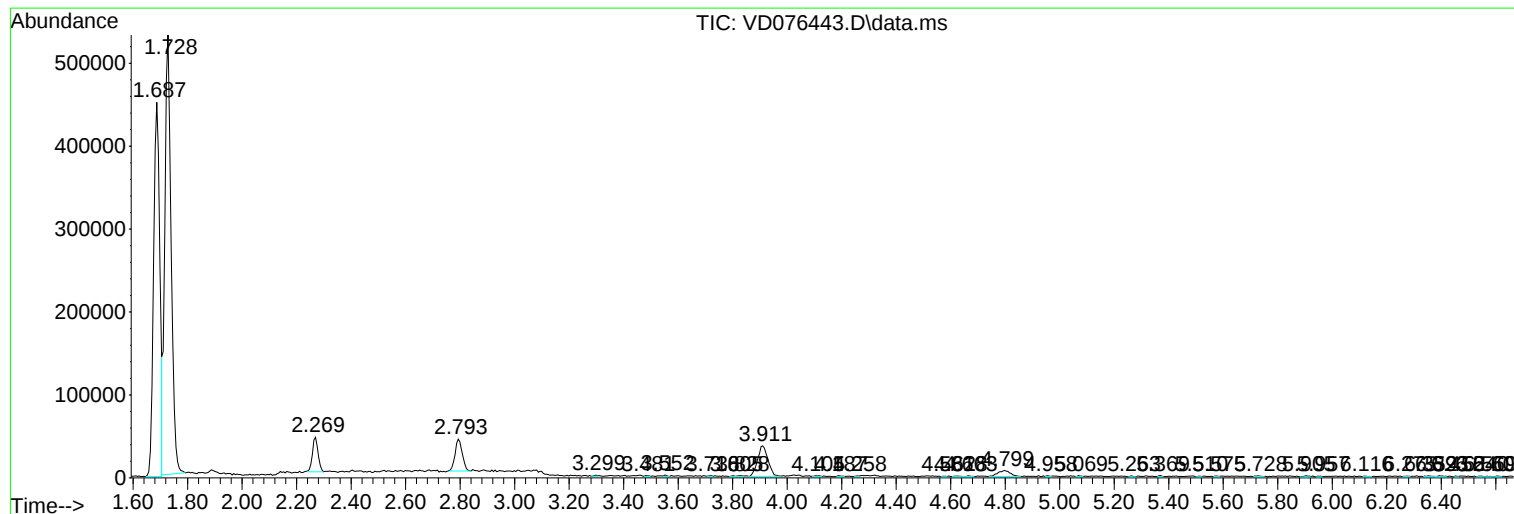
Sum of corrected areas: 4988064

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM061523SMA.M
Quant Title : SFAM01.0

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



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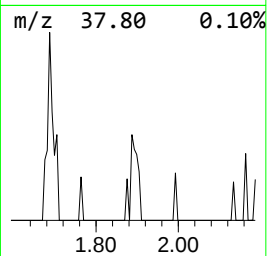
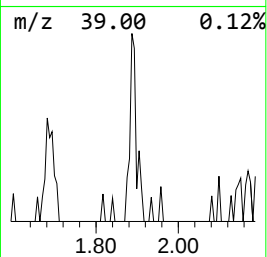
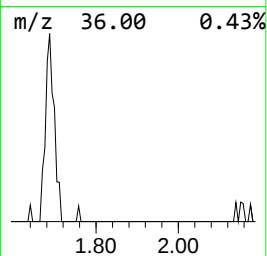
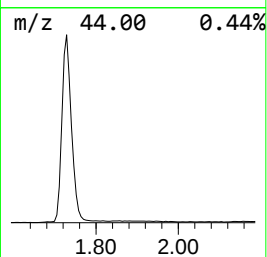
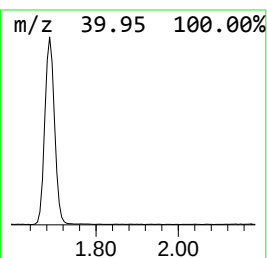
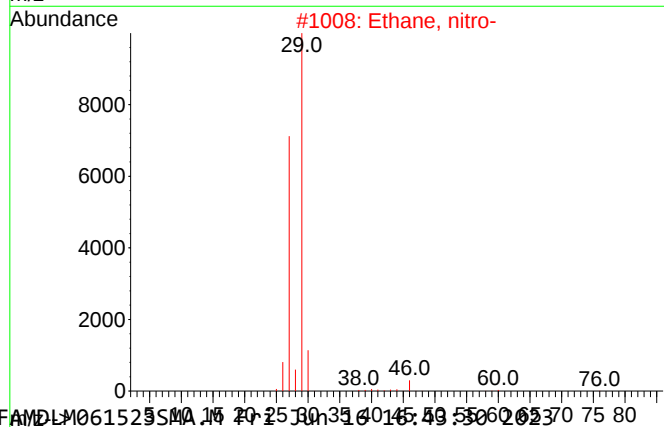
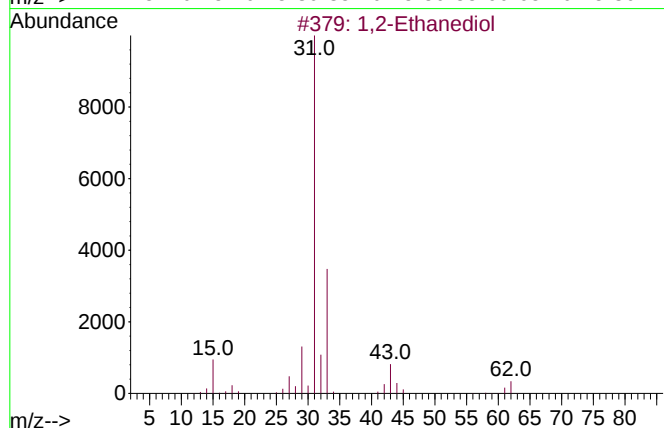
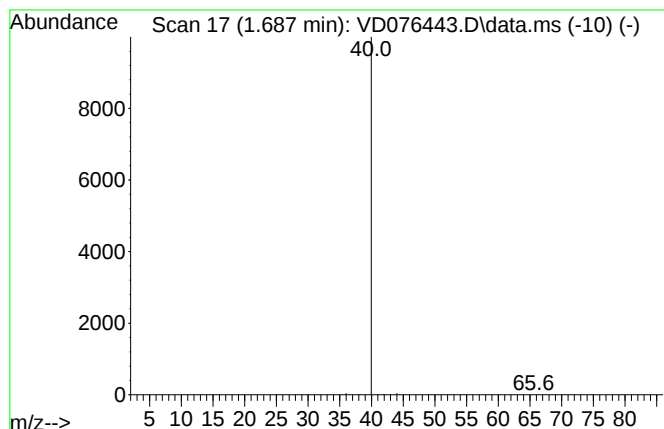
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM061523SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.687	73.16 ug/L	719901	1,4-Difluorobenzene	8.775

Hit#	of	2	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Ethanediol			62	C2H6O2	000107-21-1	1
2	Ethane, nitro-			75	C2H5NO2	000079-24-3	1



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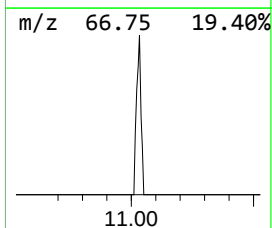
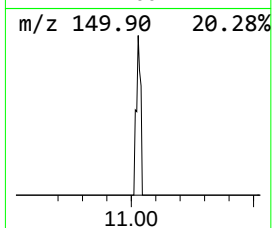
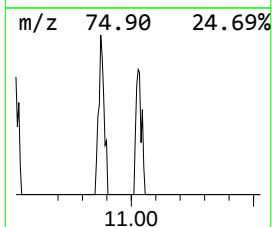
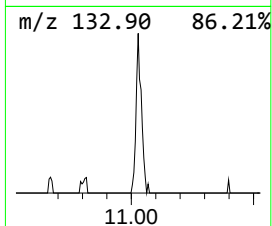
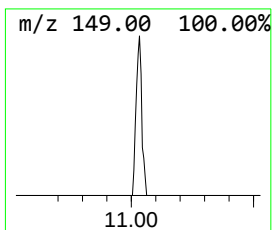
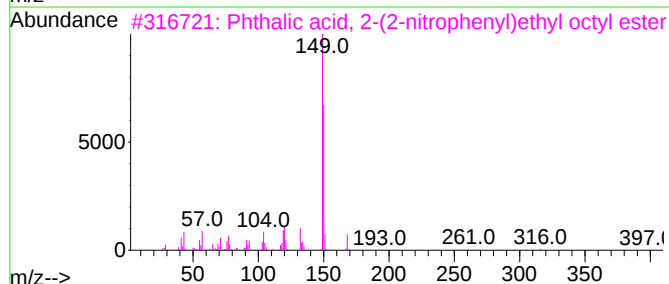
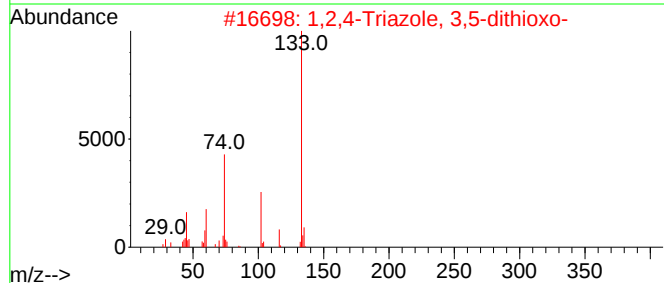
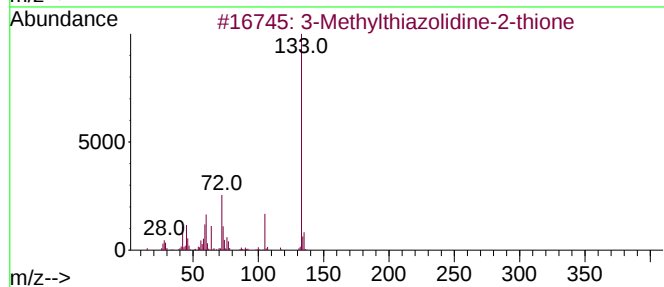
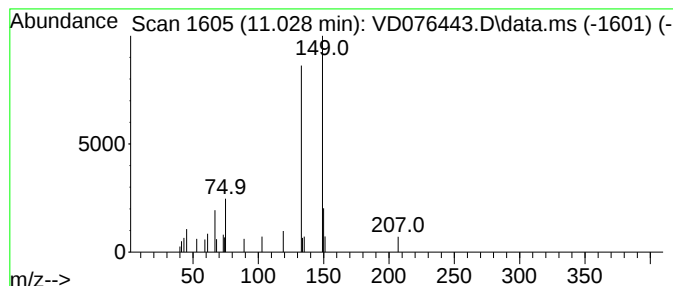
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM061523SMA.M
Quant Title : SFAM01.0

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

Peak Number 4 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.028	1.43 ug/L	18389	Chlorobenzene-d5	11.581

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Methylthiazolidine-2-thione	133	C4H7NS2	001908-87-8	22
2			1,2,4-Triazole, 3,5-dithio-	133	C2H3N3S2	005650-03-3	22
3			Phthalic acid, 2-(2-nitrophenyl)...	427	C24H29NO6	1000377-99-8	12
4			(2-Methyl[1,3]dithian-2-yl)methanol	164	C6H12OS2	1000191-37-4	10
5			4-Hydrazinobenzonitrile	133	C7H7N3	017672-27-4	10



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Quant Title : SFAM01.0

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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.687	73.2	ug/L	719901	1	8.775	246012	25.0
unknown-02	11.028	1.4	ug/L	18389	2	11.581	322486	25.0