

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW071322\
 Data File : VW023666.D
 Acq On : 13 Jul 2022 23:00
 Operator : SY/VA
 Sample : N3679-02
 Misc : 5.77g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 F5B42

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\SFAMWLM071322SMA.M
 Title : SFAM01.0

Signal : TIC: VW023666.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.343	68	72	80	rVB	48704	75231	25.52%	3.699%
2	4.007	333	345	354	rBV3	29287	80876	27.43%	3.976%
3	4.403	400	410	419	rBV9	4350	16550	5.61%	0.814%
4	4.586	438	440	442	rVB3	1256	1015	0.34%	0.050%
5	4.708	458	460	461	rBV2	941	740	0.25%	0.036%
6	4.781	468	472	473	rBV4	1346	1460	0.50%	0.072%
7	4.903	483	492	494	rBV5	9067	21733	7.37%	1.069%
8	5.001	505	508	510	rBV3	1123	1351	0.46%	0.066%
9	5.025	510	512	514	rVB3	1413	1119	0.38%	0.055%
10	5.062	514	518	519	rBV4	1399	1690	0.57%	0.083%
11	5.080	519	521	522	rBV2	1757	1456	0.49%	0.072%
12	5.403	572	574	575	rBV2	1946	1415	0.48%	0.070%
13	5.525	592	594	596	rVB3	1173	838	0.28%	0.041%
14	5.568	599	601	603	rVB3	1537	928	0.31%	0.046%
15	5.806	638	640	642	rBV3	1127	1041	0.35%	0.051%
16	5.885	651	653	654	rBV2	1253	1079	0.37%	0.053%
17	6.007	672	673	678	rVB5	1244	1511	0.51%	0.074%
18	6.056	678	681	685	rBV6	1206	1876	0.64%	0.092%
19	6.116	688	691	692	rBV3	1071	1174	0.40%	0.058%
20	6.171	697	700	701	rBV3	1856	1921	0.65%	0.094%
21	6.299	720	721	725	rBV4	1801	1629	0.55%	0.080%
22	6.537	759	760	762	rBV2	939	675	0.23%	0.033%
23	6.555	762	763	765	rVB2	1569	753	0.26%	0.037%
24	6.702	786	787	790	rBV3	885	727	0.25%	0.036%
25	6.787	800	801	803	rVB2	1105	735	0.25%	0.036%
26	6.811	803	805	806	rBV2	1159	1089	0.37%	0.054%
27	6.903	818	820	821	rBV	974	674	0.23%	0.033%
28	7.086	845	850	853	rBV	7479	15026	5.10%	0.739%
29	7.543	921	925	927	rBV4	1529	2423	0.82%	0.119%
30	7.647	934	942	953	rVB	50717	129782	44.02%	6.381%
31	7.775	959	963	964	rBV4	1618	1651	0.56%	0.081%
32	7.897	982	983	985	rBV2	1017	674	0.23%	0.033%
33	8.012	1000	1002	1005	rVB4	1413	1514	0.51%	0.074%
34	8.055	1005	1009	1012	rBV3	1466	2506	0.85%	0.123%
35	8.116	1017	1019	1021	rBV3	1642	1697	0.58%	0.083%
36	8.275	1033	1045	1060	rBV2	89976	294802	100.00%	14.494%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
 Title : SFAM01.0

37	8.592	1095	1097	1101	rBV5	1215	1665	0.56%	0.082%
38	8.683	1110	1112	1115	rBV4	1154	1347	0.46%	0.066%
39	8.842	1130	1138	1146	rBV	82671	163265	55.38%	8.027%
40	8.970	1157	1159	1160	rBV2	1244	926	0.31%	0.046%
41	9.037	1166	1170	1171	rBV4	1452	1670	0.57%	0.082%
42	9.201	1195	1197	1198	rBV	1501	1056	0.36%	0.052%
43	9.274	1202	1209	1218	rVB	63107	132552	44.96%	6.517%
44	9.470	1240	1241	1243	rBV2	1422	946	0.32%	0.047%
45	9.756	1286	1288	1290	rVB3	1419	982	0.33%	0.048%
46	9.811	1295	1297	1299	rBV2	1096	939	0.32%	0.046%
47	9.878	1304	1308	1309	rBV2	2295	2988	1.01%	0.147%
48	9.927	1315	1316	1319	rVB3	1258	800	0.27%	0.039%
49	9.957	1319	1321	1325	rVB5	1311	1531	0.52%	0.075%
50	10.030	1327	1333	1339	rBV2	25218	48199	16.35%	2.370%
51	10.201	1358	1361	1362	rBV3	1372	1553	0.53%	0.076%
52	10.323	1374	1381	1388	rBV	106144	194560	66.00%	9.566%
53	10.488	1404	1408	1412	rBV6	1031	2080	0.71%	0.102%
54	10.579	1417	1423	1428	rBV	17751	31818	10.79%	1.564%
55	10.701	1440	1443	1449	rVB3	6115	8675	2.94%	0.427%
56	10.927	1473	1480	1489	rBV	34031	65805	22.32%	3.235%
57	11.067	1496	1503	1508	rBV2	10237	20506	6.96%	1.008%
58	11.152	1515	1517	1519	rBV3	1026	1087	0.37%	0.053%
59	11.238	1528	1531	1532	rBV3	1504	1648	0.56%	0.081%
60	11.329	1543	1546	1549	rBV4	1858	2711	0.92%	0.133%
61	11.481	1568	1571	1573	rBV4	1047	1426	0.48%	0.070%
62	11.567	1583	1585	1588	rBV4	1566	1266	0.43%	0.062%
63	11.628	1588	1595	1603	rBV	112474	198761	67.42%	9.772%
64	11.817	1623	1626	1629	rBV5	1156	2020	0.69%	0.099%
65	12.152	1679	1681	1684	rBV4	1049	1385	0.47%	0.068%
66	12.219	1690	1692	1696	rBV5	859	1177	0.40%	0.058%
67	12.457	1729	1731	1733	rBV3	1156	934	0.32%	0.046%
68	12.603	1747	1755	1762	rBV7	7360	16032	5.44%	0.788%
69	12.695	1762	1770	1776	rBV	57607	102682	34.83%	5.048%
70	12.847	1792	1795	1800	rBV7	1083	2028	0.69%	0.100%
71	12.884	1800	1801	1803	rVV2	902	653	0.22%	0.032%
72	12.999	1818	1820	1821	rVB2	1398	983	0.33%	0.048%
73	13.030	1821	1825	1829	rVB6	984	1572	0.53%	0.077%
74	13.243	1858	1860	1864	rBV5	1858	2367	0.80%	0.116%
75	13.292	1866	1868	1874	rVB7	2745	4491	1.52%	0.221%
76	13.359	1877	1879	1881	rBV3	1275	1272	0.43%	0.063%

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77	13.475	1894	1898	1899	rBV4	1186	1252	0.42%	0.062%
78	13.554	1905	1911	1917	rBV	82630	142917	48.48%	7.027%
79	13.755	1940	1944	1948	rBV7	2927	5359	1.82%	0.263%
80	13.853	1953	1960	1967	rBV	88910	148636	50.42%	7.308%
81	14.066	1989	1995	2000	rBV4	4551	9778	3.32%	0.481%
82	14.188	2012	2015	2016	rBV2	1493	1622	0.55%	0.080%
83	14.237	2021	2023	2026	rBV3	1337	1694	0.57%	0.083%
84	14.292	2031	2032	2033	rBV	1082	655	0.22%	0.032%
85	14.615	2083	2085	2086	rBV2	982	641	0.22%	0.032%
86	14.859	2122	2125	2126	rBV3	1170	884	0.30%	0.043%
87	14.883	2126	2129	2133	rVV6	1672	2807	0.95%	0.138%
88	14.944	2133	2139	2143	rBV9	1681	3465	1.18%	0.170%
89	15.017	2149	2151	2153	rBV3	1255	962	0.33%	0.047%
90	15.103	2161	2165	2166	rBV4	844	1254	0.43%	0.062%
91	15.164	2174	2175	2177	rBV2	996	849	0.29%	0.042%
92	15.298	2194	2197	2199	rVB4	1154	1139	0.39%	0.056%
93	15.414	2214	2216	2217	rBV	1629	1380	0.47%	0.068%
94	15.664	2256	2257	2260	rBV3	1452	1694	0.57%	0.083%
95	15.846	2284	2287	2289	rBV4	881	910	0.31%	0.045%
96	15.932	2299	2301	2302	rVB2	1182	816	0.28%	0.040%
97	15.950	2302	2304	2309	rBV6	1138	2464	0.84%	0.121%
98	16.084	2325	2326	2328	rBV2	960	651	0.22%	0.032%
99	16.548	2400	2402	2404	rVB4	1067	770	0.26%	0.038%
100	16.718	2428	2430	2433	rBV3	1635	1653	0.56%	0.081%

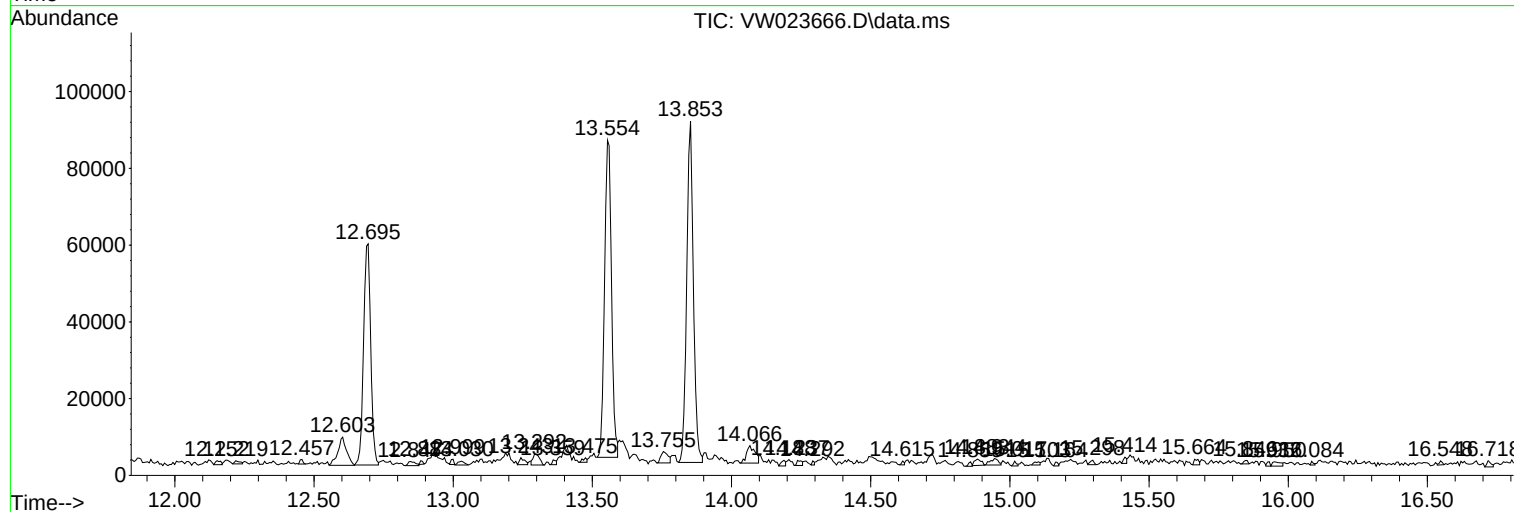
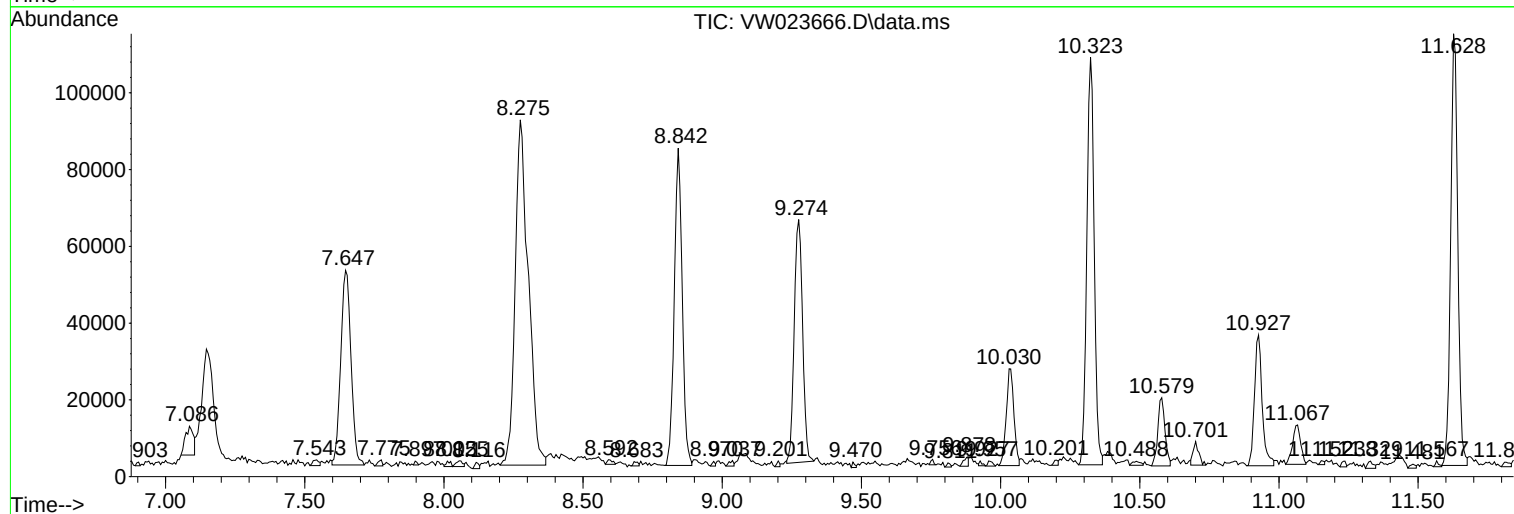
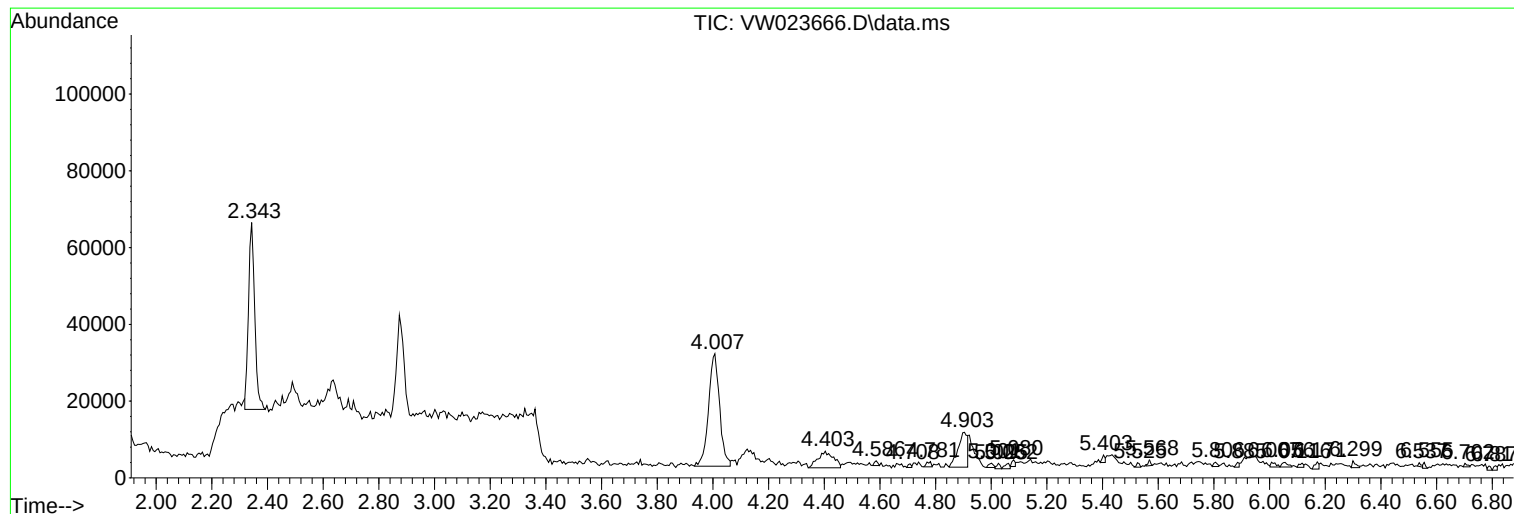
Sum of corrected areas: 2033971

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Instrument :
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F5B42

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
Quant Title : SFAM01.0

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



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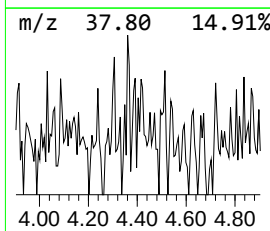
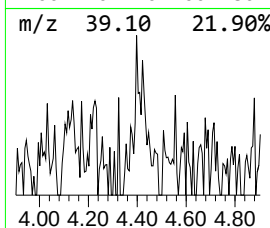
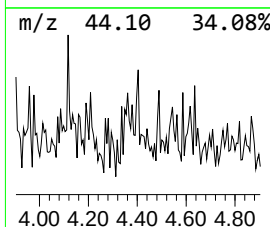
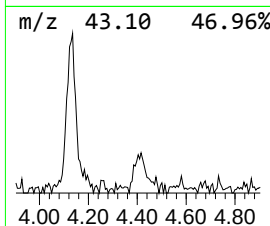
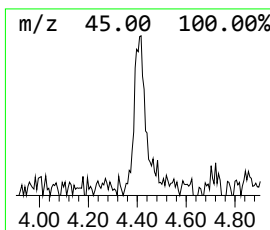
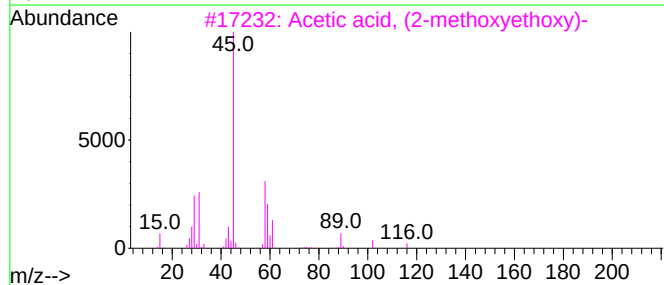
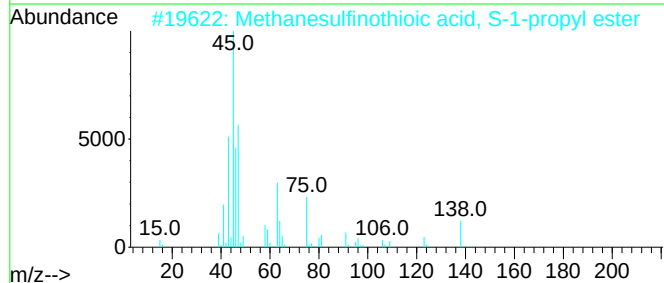
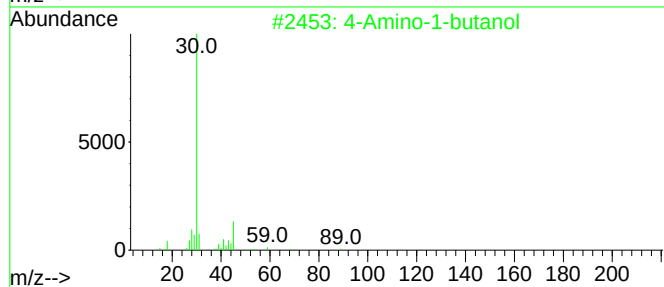
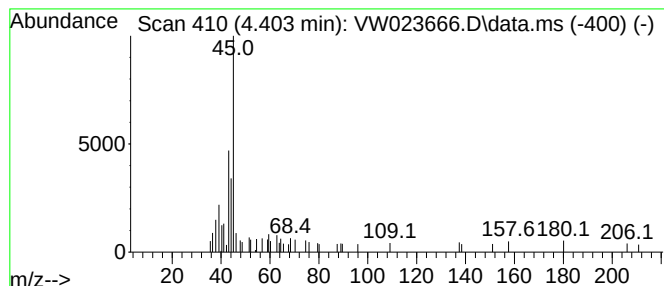
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.403	2.53 ug/L	16550	1,4-Difluorobenzene	8.842

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Amino-1-butanol	89	C4H11NO	013325-10-5	42
2			Methanesulfinothioic acid, S-1-p...	138	C4H10S2	1000322-32-0	33
3			Acetic acid, (2-methoxyethoxy)-	134	C5H10O4	016024-56-9	28
4			Methoxymethyl ethyl sulfone	138	C4H10O3S	1000288-88-3	9
5			Boronic acid, ethyl-	74	C2H7BO2	004433-63-0	9



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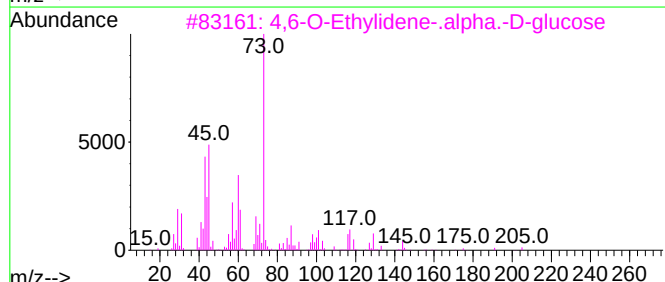
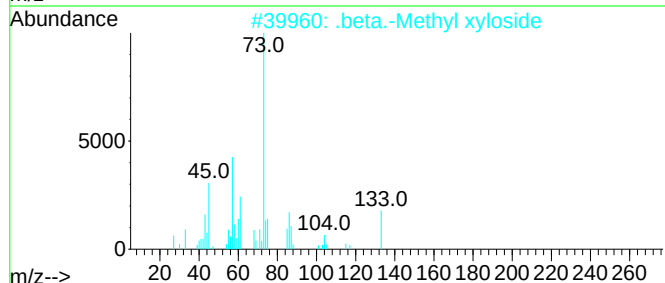
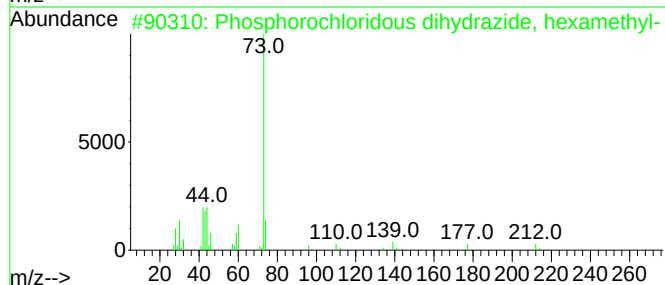
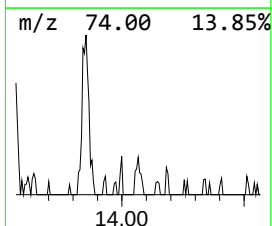
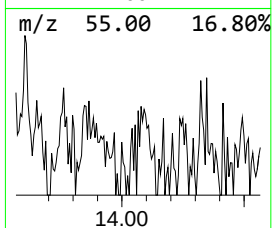
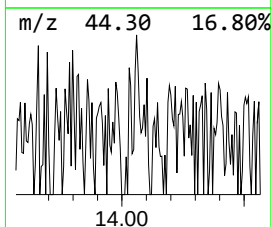
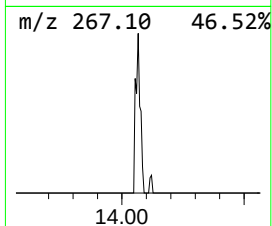
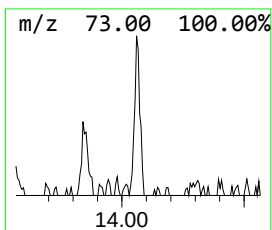
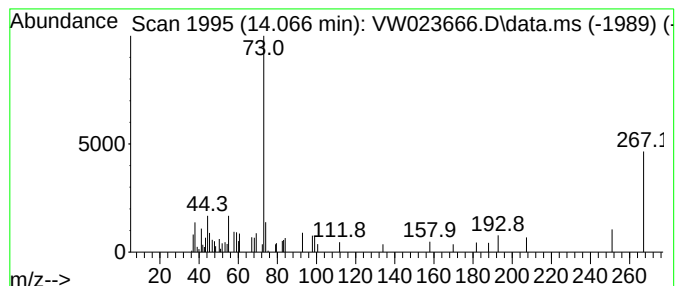
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
Quant Title : SFAM01.0

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

Peak Number 5 unknown-02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.066	1.71 ug/L	9778	1,4-Dichlorobenzene-d4	13.560

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phosphorochloridous dihydrazide,...	212	C6H18ClN4P	022692-22-4	10
2			.beta.-Methyl xyloside	164	C6H12O5	007473-45-2	10
3			4,6-O-Ethylidene-.alpha.-D-glucose	206	C8H14O6	013224-99-2	9
4			2-Chloro-N-(prop-2-en-1-yl)aceta...	205	C8H16ClNOSi	1000478-29-9	9
5			1-(t-Butyldimethylsilyl)-4-(2,2-...	308	C19H36OSi	095452-00-9	9



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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	4.403	2.5	ug/L	16550	1	8.842	163265	25.0
unknown-02	14.066	1.7	ug/L	9778	3	13.560	142917	25.0