

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD070323\
 Data File : VD076684.D
 Acq On : 03 Jul 2023 11:28
 Operator : KP/SY
 Sample : 03444-07RE
 Misc : 4.31G/10.0ml/MSVOA_D/SOIL
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 A46Q1RE

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: VD076684.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	13	17	18	rBV	1758	2291	0.34%	0.051%
2	1.734	18	25	32	rVV	266873	500486	74.12%	11.247%
3	2.264	112	115	122	rVB	20121	29143	4.32%	0.655%
4	2.793	202	205	212	rVB	21065	33281	4.93%	0.748%
5	2.922	225	227	228	rBV2	2566	1932	0.29%	0.043%
6	3.293	287	290	291	rBV	1335	1128	0.17%	0.025%
7	3.387	303	306	307	rVB	1483	930	0.14%	0.021%
8	3.405	307	309	311	rBV2	1034	1096	0.16%	0.025%
9	3.487	319	323	326	rBV2	1593	2123	0.31%	0.048%
10	3.516	326	328	330	rVB2	1255	730	0.11%	0.016%
11	3.552	330	334	336	rVB2	843	872	0.13%	0.020%
12	3.575	336	338	340	rBV2	608	726	0.11%	0.016%
13	3.910	386	395	406	rVB2	21588	55452	8.21%	1.246%
14	4.016	406	413	414	rBV	14652	21130	3.13%	0.475%
15	4.087	423	425	427	rVV2	1703	1135	0.17%	0.026%
16	4.116	428	430	431	rVB	1865	1114	0.16%	0.025%
17	4.246	449	452	455	rBV3	1002	1737	0.26%	0.039%
18	4.381	473	475	478	rVB2	1103	1168	0.17%	0.026%
19	4.499	491	495	496	rVB	998	1050	0.16%	0.024%
20	4.522	496	499	502	rBV	1562	2141	0.32%	0.048%
21	4.552	502	504	507	rVB3	947	921	0.14%	0.021%
22	4.628	516	517	520	rBV	1105	984	0.15%	0.022%
23	4.746	535	537	538	rBV	1009	892	0.13%	0.020%
24	4.793	538	545	556	rVV3	10659	32260	4.78%	0.725%
25	4.981	576	577	582	rVB2	1432	1544	0.23%	0.035%
26	5.028	582	585	587	rBV2	1050	1093	0.16%	0.025%
27	5.228	613	619	620	rBV	949	1344	0.20%	0.030%
28	5.357	640	641	644	rVB2	2033	1446	0.21%	0.032%
29	5.399	644	648	650	rBV2	1064	1240	0.18%	0.028%
30	5.428	652	653	656	rBV	1221	984	0.15%	0.022%
31	5.546	671	673	675	rBV	1489	769	0.11%	0.017%
32	5.716	701	702	706	rVB	1059	988	0.15%	0.022%
33	5.763	706	710	713	rBV	948	1562	0.23%	0.035%
34	5.816	718	719	720	rVV	1606	813	0.12%	0.018%
35	5.834	720	722	727	rVV3	2266	3526	0.52%	0.079%
36	6.046	755	758	759	rVB2	1282	1214	0.18%	0.027%

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Integrator: RTE

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

37	6.081	762	764	766	rVB	931	711	0.11%	0.016%
38	6.122	766	771	775	rVB2	862	1377	0.20%	0.031%
39	6.193	781	783	784	rBV	748	740	0.11%	0.017%
40	6.340	806	808	813	rVB	983	1168	0.17%	0.026%
41	6.375	813	814	817	rVB	1411	984	0.15%	0.022%
42	6.416	817	821	822	rBV2	1305	1609	0.24%	0.036%
43	6.552	842	844	846	rBV	939	765	0.11%	0.017%
44	6.622	853	856	857	rBV	889	679	0.10%	0.015%
45	6.640	857	859	862	rBV	873	1095	0.16%	0.025%
46	6.693	866	868	871	rVV2	813	812	0.12%	0.018%
47	6.775	879	882	884	rBV2	929	1193	0.18%	0.027%
48	6.987	907	918	926	rBV2	23318	65882	9.76%	1.481%
49	7.081	928	934	941	rVB4	7639	19207	2.84%	0.432%
50	7.246	961	962	965	rBV	788	866	0.13%	0.019%
51	7.375	983	984	987	rVB2	1206	793	0.12%	0.018%
52	7.563	1006	1016	1027	rBV3	49090	125851	18.64%	2.828%
53	7.699	1034	1039	1041	rBV	1047	1348	0.20%	0.030%
54	7.775	1047	1052	1054	rBV	740	1158	0.17%	0.026%
55	7.810	1054	1058	1062	rVV	968	1372	0.20%	0.031%
56	7.893	1070	1072	1074	rVB	1033	834	0.12%	0.019%
57	8.057	1098	1100	1103	rBV2	750	940	0.14%	0.021%
58	8.093	1103	1106	1109	rVV2	1467	1670	0.25%	0.038%
59	8.204	1112	1125	1142	rBV4	74107	253588	37.56%	5.699%
60	8.675	1203	1205	1209	rBV2	1150	1187	0.18%	0.027%
61	8.775	1213	1222	1232	rBV2	138873	291133	43.12%	6.543%
62	9.093	1273	1276	1278	rBV2	816	1106	0.16%	0.025%
63	9.210	1287	1296	1303	rBV	69495	144638	21.42%	3.250%
64	9.369	1322	1323	1326	rBV2	1067	730	0.11%	0.016%
65	9.557	1352	1355	1356	rBV	1452	1513	0.22%	0.034%
66	9.645	1368	1370	1373	rVB2	1802	1343	0.20%	0.030%
67	9.698	1375	1379	1384	rBV	1758	3031	0.45%	0.068%
68	9.981	1420	1427	1435	rVB3	36873	71354	10.57%	1.604%
69	10.151	1455	1456	1458	rBV2	994	687	0.10%	0.015%
70	10.269	1469	1476	1483	rVV	93583	173802	25.74%	3.906%
71	10.322	1483	1485	1490	rVB3	2305	3885	0.58%	0.087%
72	10.528	1512	1520	1527	rBV	27960	48302	7.15%	1.085%
73	10.598	1531	1532	1536	rBV	1179	983	0.15%	0.022%
74	10.663	1539	1543	1548	rVB4	3039	4526	0.67%	0.102%
75	10.745	1555	1557	1558	rBV4	1024	837	0.12%	0.019%
76	10.881	1574	1580	1592	rVB2	79393	134624	19.94%	3.025%

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 Title : SFAM01.0

77	11.040	1605	1607	1610	rBV3	1096	1165	0.17%	0.026%
78	11.110	1617	1619	1620	rBV	1079	840	0.12%	0.019%
79	11.128	1620	1622	1624	rVV2	1996	1663	0.25%	0.037%
80	11.181	1628	1631	1637	rVV4	2085	3350	0.50%	0.075%
81	11.245	1640	1642	1644	rBV	787	697	0.10%	0.016%
82	11.281	1646	1648	1653	rBV3	2354	3545	0.53%	0.080%
83	11.340	1656	1658	1660	rVV	1475	1430	0.21%	0.032%
84	11.387	1664	1666	1668	rVB2	1184	783	0.12%	0.018%
85	11.451	1675	1677	1678	rBV	1147	793	0.12%	0.018%
86	11.516	1686	1688	1691	rBV2	1564	1324	0.20%	0.030%
87	11.581	1691	1699	1709	rBV	209264	362126	53.63%	8.138%
88	11.816	1737	1739	1740	rBV	1934	1286	0.19%	0.029%
89	11.922	1755	1757	1758	rBV	1196	1019	0.15%	0.023%
90	11.975	1764	1766	1772	rBV3	1523	2980	0.44%	0.067%
91	12.028	1772	1775	1781	rVB4	1888	3310	0.49%	0.074%
92	12.098	1782	1787	1789	rBV3	2433	4151	0.61%	0.093%
93	12.581	1863	1869	1872	rVB6	4263	8677	1.29%	0.195%
94	12.651	1875	1881	1888	rVV2	100692	169805	25.15%	3.816%
95	12.734	1892	1895	1902	rVB6	8801	17410	2.58%	0.391%
96	12.816	1902	1909	1913	rBV7	5829	13088	1.94%	0.294%
97	13.516	2022	2028	2035	rBV	214197	347159	51.41%	7.802%
98	13.816	2074	2079	2087	rBV	116677	259655	38.46%	5.835%
99	15.304	2328	2332	2339	rVB	319150	488814	72.39%	10.985%
100	16.257	2490	2494	2502	rVB2	388794	675215	100.00%	15.174%

Sum of corrected areas: 4449853

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Instrument :
MSVOA_D
ClientSampleId :
A46Q1RE

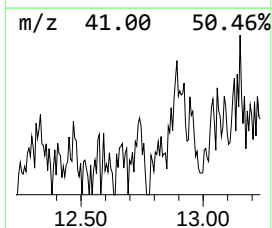
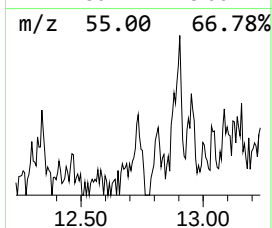
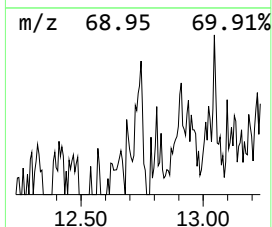
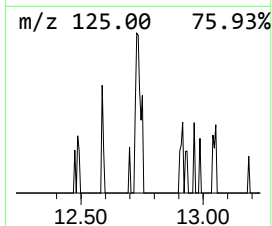
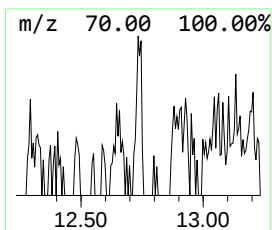
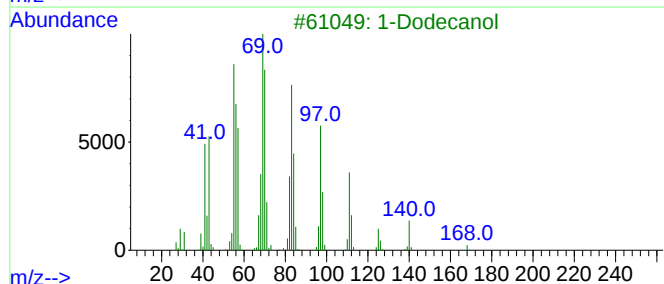
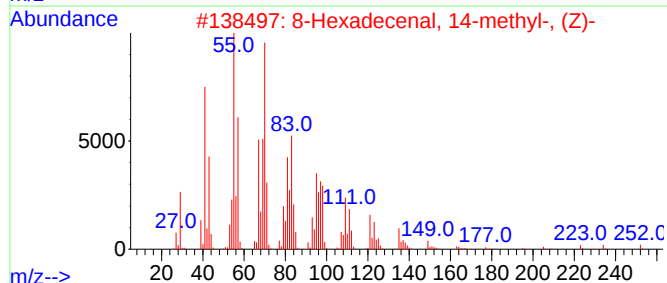
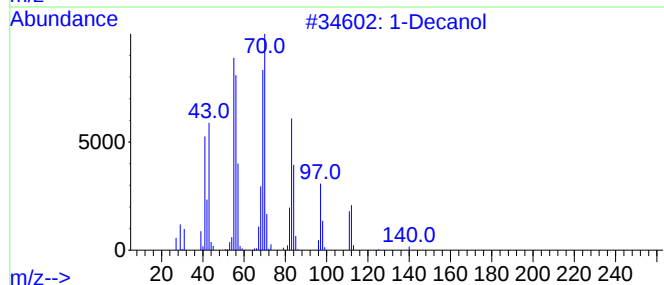
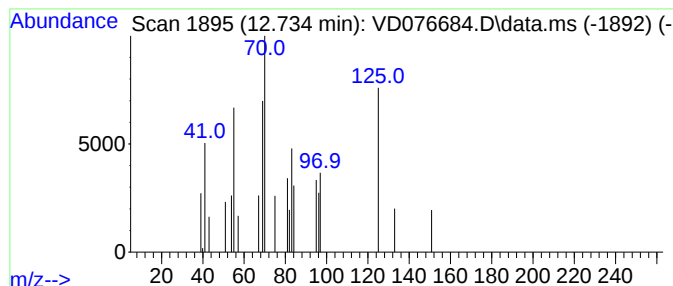
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM061523SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.734	1.25 ug/L	17410	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Decanol	158	C10H22O	000112-30-1	38
2			8-Hexadecenal, 14-methyl-, (Z)-	252	C17H32O	060609-53-2	37
3			1-Dodecanol	186	C12H26O	000112-53-8	35
4			2-Amino-4-hydroxy-6-methylpyrimi...	125	C5H7N3O	003977-29-5	30
5			Octane, 4-chloro-	148	C8H17Cl	000999-07-5	25



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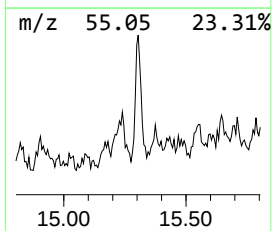
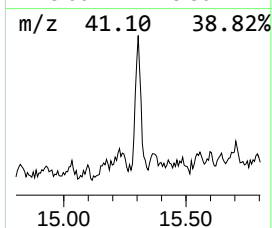
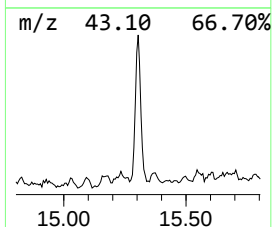
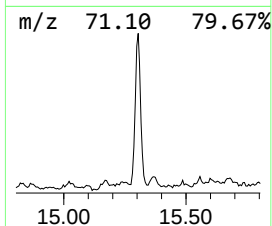
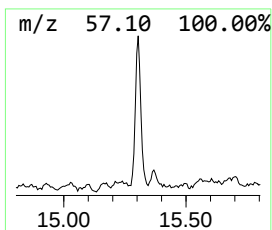
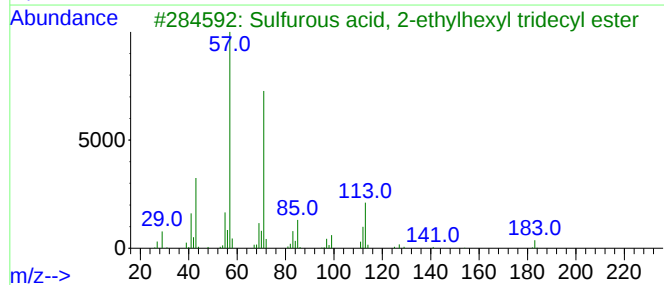
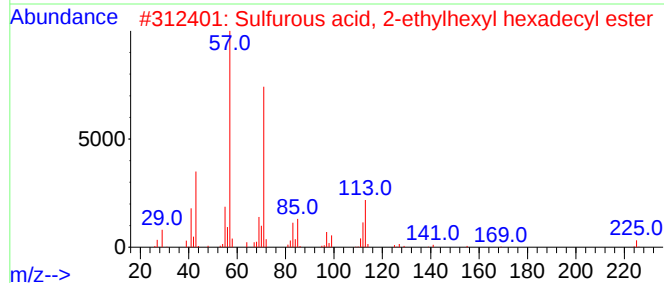
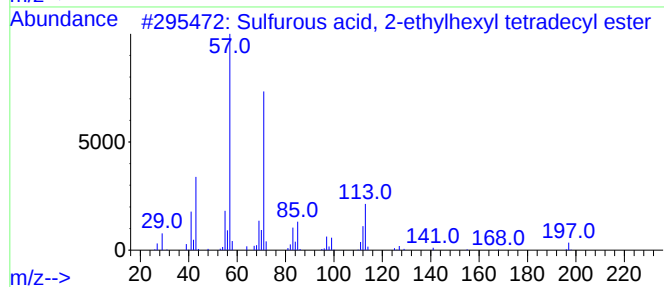
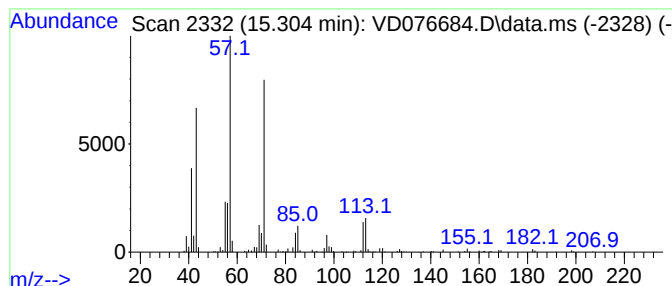
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM061523SMA.M
Quant Title : SFAM01.0

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

Peak Number 4 Sulfurous acid, 2-ethylhexy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.304	35.20 ug/L	488814	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, 2-ethylhexyl tet...	390	C22H46O3S	1000309-19-7	86
2			Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	86
3			Sulfurous acid, 2-ethylhexyl tri...	376	C21H44O3S	1000309-19-6	80
4			Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	80
5			Sulfurous acid, 2-ethylhexyl oct...	446	C26H54O3S	1000309-20-1	78



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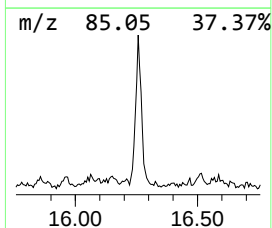
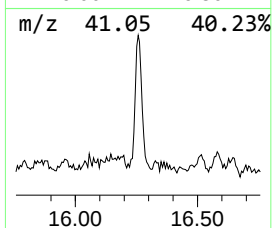
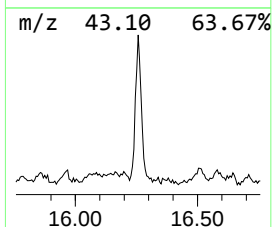
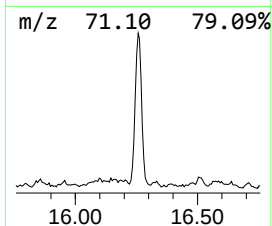
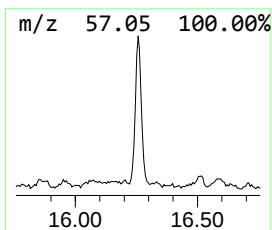
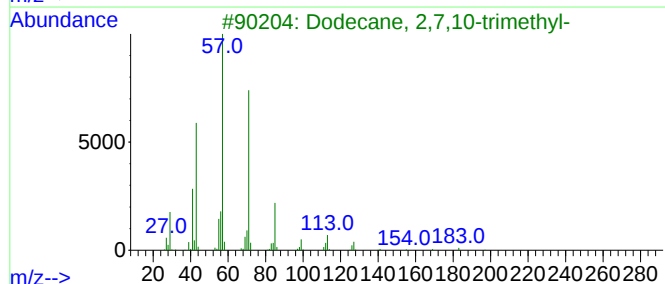
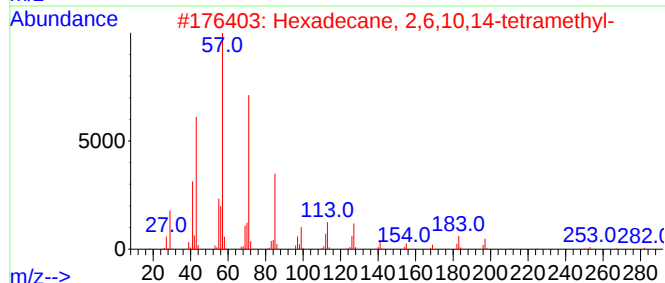
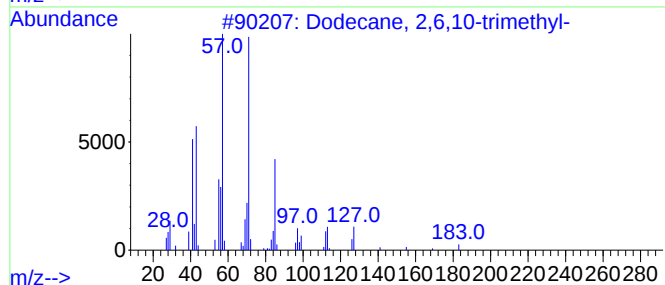
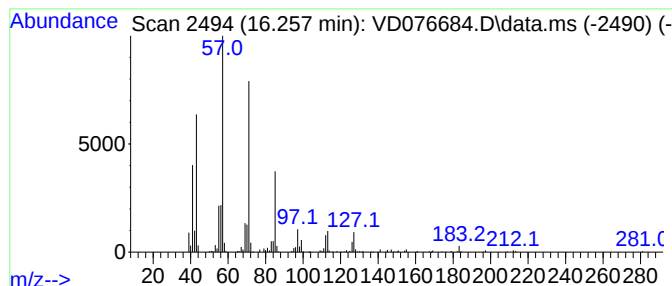
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM061523SMA.M
Quant Title : SFAM01.0

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.257	48.62 ug/L	675215	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	91
2			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	90
3			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
4			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	86
5			Octane, 2-methyl-	128	C9H20	003221-61-2	81



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Instrument :
MSVOA_D
ClientSampleId :
A46Q1RE

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	12.734	1.3	ug/L	17410	3	13.516	347159	25.0
Sulfurous acid,...	15.304	35.2	ug/L	488814	3	13.516	347159	25.0
(DEL) Alkane: S...	16.257	48.6	ug/L	675215	3	13.516	347159	25.0