LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA F\DATA\VF080418\
Data File : VF059874.D
Acq On : 4 Aug 2018 9:47
Operator : VA/AP
Sample : J4318-09
Misc : 4.30g/5mL/MSVOA F/SOIL
ALS Vial : 100 Sample Multiplier: 1

Instrument : MSVOA_F
ClientSampleId : BEEBEE-SITE-DEMO-4

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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_F\METHODS\82F080418S.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.102	56	58	60	rVB	6840	7089	5.59%	1.138%
2	1.279	74	76	77	rVB2	2090	2456	1.94%	0.394%
3	1.328	77	81	83	rBV2	2651	6449	5.08%	1.035%
4	1.604	105	109	113	rVB3	1775	4250	3.35%	0.682%
5	1.673	113	116	118	rVB2	2173	3434	2.71%	0.551%
6	1.821	129	131	134	rBV2	1795	3071	2.42%	0.493%
7	1.861	134	135	138	rVB3	1190	1627	1.28%	0.261%
8	2.245	170	174	176	rVV2	931	1787	1.41%	0.287%
9	2.294	176	179	181	rVB2	2047	3006	2.37%	0.483%
10	2.324	181	182	188	rVB2	1193	3032	2.39%	0.487%
11	2.423	190	192	194	rVB2	1663	2205	1.74%	0.354%
12	2.482	196	198	202	rVB2	1553	3495	2.76%	0.561%
13	2.541	202	204	205	rBV	944	1464	1.15%	0.235%
14	2.649	212	215	218	rBV	839	1889	1.49%	0.303%
15	2.738	223	224	226	rBV	8743	6261	4.94%	1.005%
16	3.122	260	263	266	rVV	1083	2311	1.82%	0.371%
17	3.211	268	272	274	rVV	1265	2133	1.68%	0.342%
18	3.300	280	281	284	rBV	1288	1960	1.55%	0.315%
19	3.349	284	286	290	rVV2	907	1486	1.17%	0.239%
20	3.458	294	297	298	rBV2	1369	2004	1.58%	0.322%
21	3.507	298	302	305	rBV2	1204	2624	2.07%	0.421%
22	3.674	316	319	322	rVB2	917	1693	1.33%	0.272%
23	3.763	325	328	330	rBV	1626	2412	1.90%	0.387%
24	4.039	354	356	358	rVB2	1035	1524	1.20%	0.245%
25	4.295	377	382	392	rVB3	10561	30530	24.07%	4.902%
26	4.601	410	413	415	rBV2	1106	1845	1.45%	0.296%
27	4.719	422	425	429	rBV2	1086	3059	2.41%	0.491%
28	4.867	439	440	442	rBV	1258	1753	1.38%	0.281%
29	5.045	451	458	465	rBV3	40336	126840	100.00%	20.366%
30	5.242	477	478	480	rBV	1665	1846	1.46%	0.296%
31	5.459	496	500	502	rBV2	1178	2101	1.66%	0.337%
32	5.537	502	508	512	rVV3	1924	6436	5.07%	1.033%
33	5.774	527	532	539	rVV	31123	83562	65.88%	13.417%
34	5.882	542	543	545	rVB	2231	1686	1.33%	0.271%

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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
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Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_F\METHODS\82F080418S.M
Title : SW846 8260

35	5.981	552	553	556	rVB	1235	1666	1.31%	0.268%
36	6.060	559	561	565	rBV3	1219	2412	1.90%	0.387%
37	6.306	583	586	588	rBV3	873	1895	1.49%	0.304%
38	6.444	598	600	604	rBV2	882	1734	1.37%	0.278%
39	6.543	607	610	613	rVB2	934	2034	1.60%	0.327%
40	6.612	613	617	620	rBV2	1381	2761	2.18%	0.443%
41	6.691	623	625	626	rBV2	1151	1477	1.16%	0.237%
42	6.779	632	634	635	rVB	3550	2513	1.98%	0.404%
43	7.055	657	662	665	rBV2	834	2239	1.77%	0.360%
44	7.174	673	674	678	rVB2	1353	2165	1.71%	0.348%
45	7.381	693	695	699	rVB2	1051	1861	1.47%	0.299%
46	7.479	703	705	708	rBV2	1217	2770	2.18%	0.445%
47	7.716	724	729	734	rBV3	24340	57009	44.95%	9.154%
48	7.883	744	746	749	rVB3	1438	2047	1.61%	0.329%
49	7.943	749	752	753	rBV2	1292	2385	1.88%	0.383%
50	8.179	774	776	778	rVB	1326	1677	1.32%	0.269%
51	8.248	778	783	784	rBV2	999	2032	1.60%	0.326%
52	8.495	806	808	809	rBV	1448	1529	1.21%	0.246%
53	8.554	813	814	818	rVV	970	1787	1.41%	0.287%
54	8.721	829	831	834	rVB2	1092	2161	1.70%	0.347%
55	8.830	841	842	845	rVB2	1046	1566	1.23%	0.251%
56	8.879	845	847	853	rBV3	1546	3670	2.89%	0.589%
57	9.116	870	871	875	rVV	1202	2367	1.87%	0.380%
58	9.175	875	877	879	rVV	1131	1879	1.48%	0.302%
59	9.224	879	882	885	rVV2	1374	2945	2.32%	0.473%
60	9.313	889	891	896	rBV2	1227	3342	2.63%	0.537%
61	9.441	901	904	906	rBV2	1445	2724	2.15%	0.437%
62	9.539	911	914	917	rVV2	728	1578	1.24%	0.253%
63	9.579	917	918	921	rVB2	1355	1952	1.54%	0.313%
64	9.628	921	923	924	rBV2	1286	2157	1.70%	0.346%
65	9.677	926	928	930	rVV2	929	1502	1.18%	0.241%
66	9.707	930	931	934	rVV3	934	1797	1.42%	0.289%
67	9.756	934	936	940	rVB	1354	2513	1.98%	0.404%
68	9.865	946	947	948	rVV	1348	1484	1.17%	0.238%
69	9.924	948	953	958	rVV	19541	45778	36.09%	7.350%
70	9.993	958	960	963	rVB	1708	2807	2.21%	0.451%
71	10.121	969	973	975	rBV3	1496	3364	2.65%	0.540%

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ClientSampleId : BEEBEE-SITE-DEMO-4

Integration Parameters: RTEINT.P
Integrator: RTE
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Start Thrs: 0.2 Max Peaks: 100
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Title : SW846 8260

72	10.160	975	977	979	rBV2	1194	1510	1.19%	0.242%
73	10.693	1030	1031	1035	rBV2	1583	3515	2.77%	0.564%
74	11.511	1111	1114	1119	rVV2	11990	19822	15.63%	3.183%
75	11.748	1134	1138	1141	rBV2	2099	5545	4.37%	0.890%
76	11.895	1151	1153	1155	rBV2	1000	1764	1.39%	0.283%
77	12.014	1162	1165	1166	rBV2	1439	1964	1.55%	0.315%
78	12.122	1173	1176	1177	rVB	1002	1638	1.29%	0.263%
79	12.309	1189	1195	1196	rBV2	1521	3990	3.15%	0.641%
80	12.546	1218	1219	1223	rVB2	1266	1638	1.29%	0.263%
81	12.635	1225	1228	1231	rBV3	12653	20976	16.54%	3.368%
82	12.842	1246	1249	1250	rBV2	1074	1646	1.30%	0.264%
83	12.921	1255	1257	1258	rVB2	1707	1775	1.40%	0.285%
84	12.970	1258	1262	1264	rBV	1594	3699	2.92%	0.594%
85	13.226	1286	1288	1289	rVV2	1108	1464	1.15%	0.235%
86	13.404	1305	1306	1309	rBV	1855	1950	1.54%	0.313%
87	13.650	1329	1331	1333	rBV2	1253	2263	1.78%	0.363%
88	13.758	1335	1342	1348	rVB5	2367	10120	7.98%	1.625%
89	13.867	1351	1353	1357	rVB2	1242	2474	1.95%	0.397%
90	14.074	1370	1374	1376	rBV2	1287	2333	1.84%	0.375%
91	14.113	1376	1378	1379	rVB2	1862	1729	1.36%	0.278%
92	14.172	1381	1384	1387	rBV2	1174	2830	2.23%	0.454%
93	14.281	1394	1395	1397	rBV2	1765	2764	2.18%	0.444%
94	14.596	1425	1427	1428	rBV	2247	1594	1.26%	0.256%
95	14.754	1441	1443	1444	rBV	1715	2290	1.81%	0.368%
96	14.823	1448	1450	1453	rBV2	1425	3529	2.78%	0.567%
97	14.872	1453	1455	1457	rVB2	1612	1803	1.42%	0.290%
98	15.079	1474	1476	1477	rBV	2286	2364	1.86%	0.380%
99	15.316	1498	1500	1503	rBV2	2062	2468	1.95%	0.396%
100	15.405	1507	1509	1510	rBV	1748	2439	1.92%	0.392%

Sum of corrected areas: 622795

LSC Report - Integrated Chromatogram

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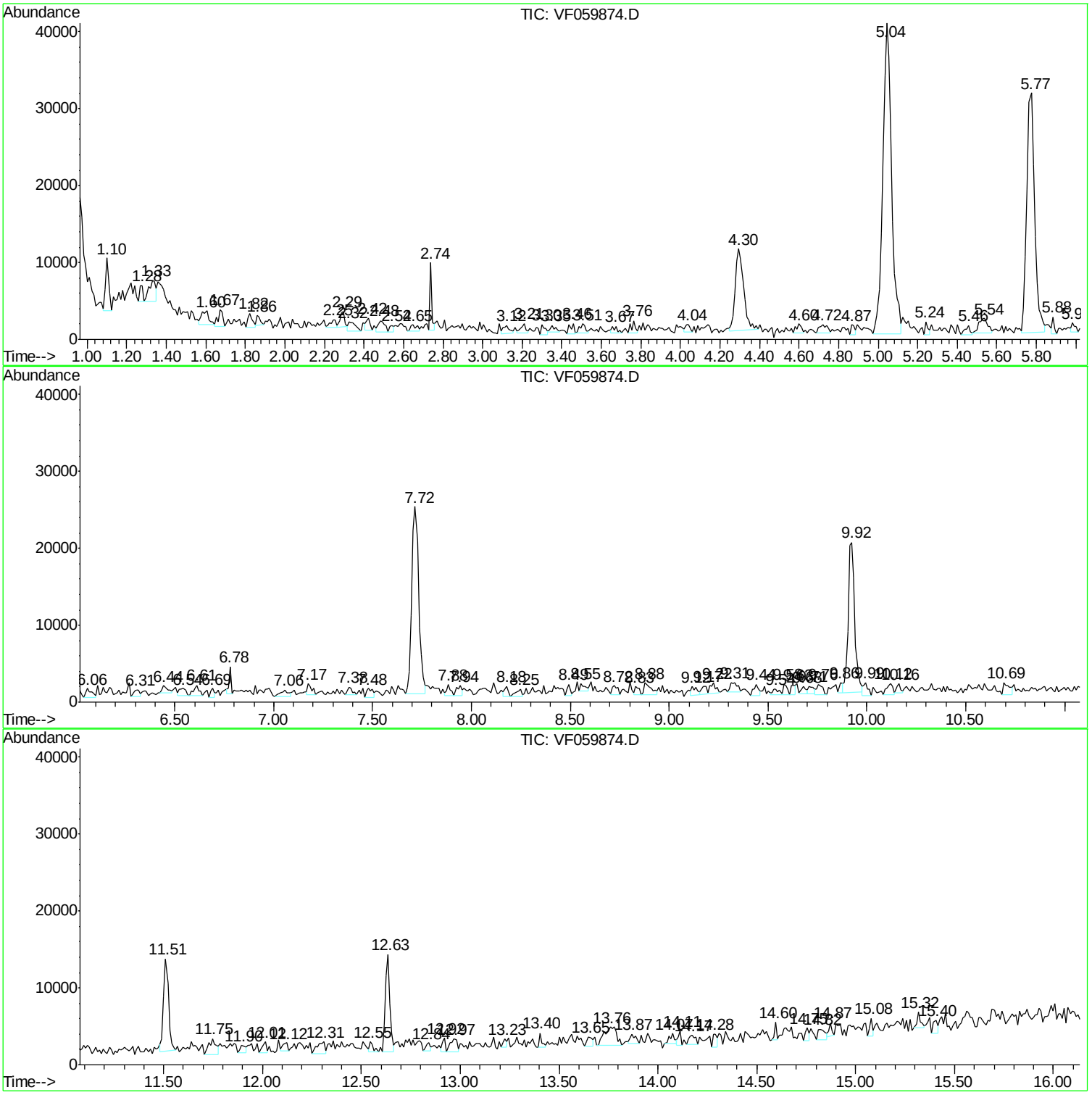
ALS Vial : 100 Sample Multiplier: 1

Instrument : MSVOA_F
ClientSampleId : BEEBEE-SITE-DEMO-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_F\METHODS\82F080418S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\VOASRV\HPCHEM1\MSVOA F\DATA\VF080418\
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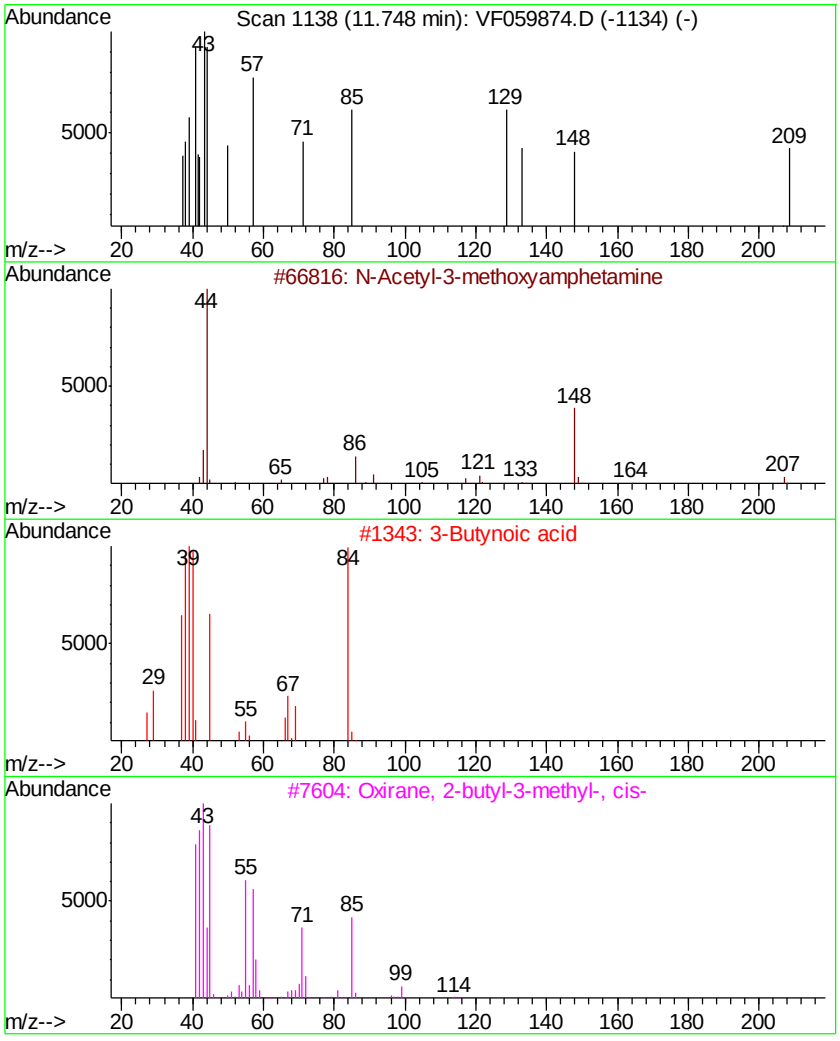
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

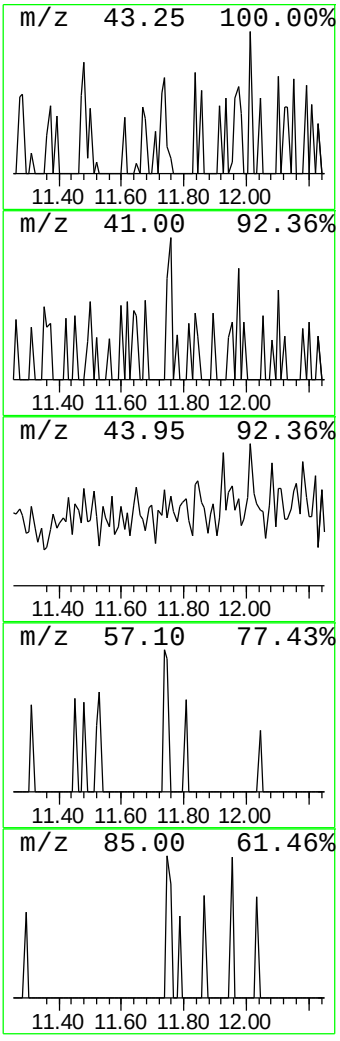
****

Peak Number 1 unknown11.75 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	13.22 ug/l	5545	1,4-Dichlorobenzene-d4	12.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-Acetyl-3-methoxyamphetamine	207	C12H17NO2	072687-67-3	9
2	3-Butynoic acid	84	C4H4O2	002345-51-9	9
3	Oxirane, 2-butyl-3-methyl-, cis-	114	C7H14O	056052-93-8	9
4	1H-1,2,4-Triazole-3-carboxylic a...	129	C3H3N3O3	1000327-51-1	9
5	1,2,4-Triazin-5(2H)-one, 3,4-dih...	129	C3H3N3OS	000626-08-4	5





Library Search Compound Report

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Sample : J4318-09
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ALS Vial : 100 Sample Multiplier: 1

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ClientSampleId : BEEBEE-SITE-DEMO-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_F\METHODS\82F080418S.M
Quant Title : SW846 8260

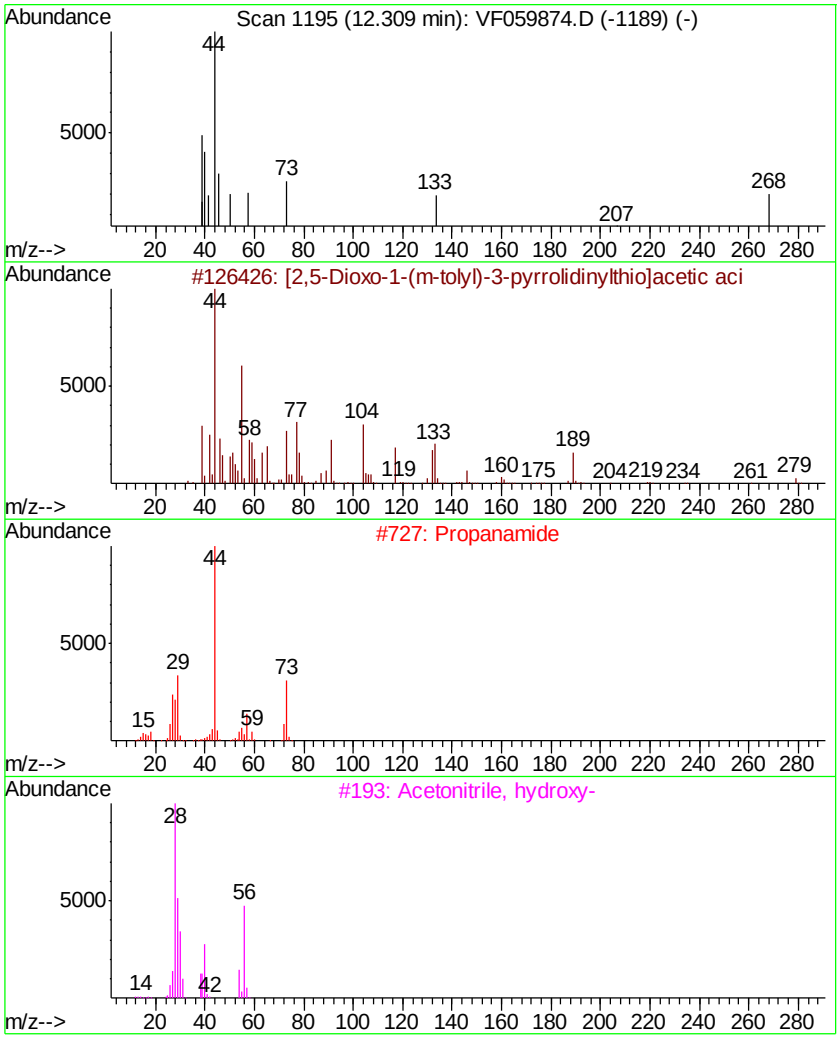
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

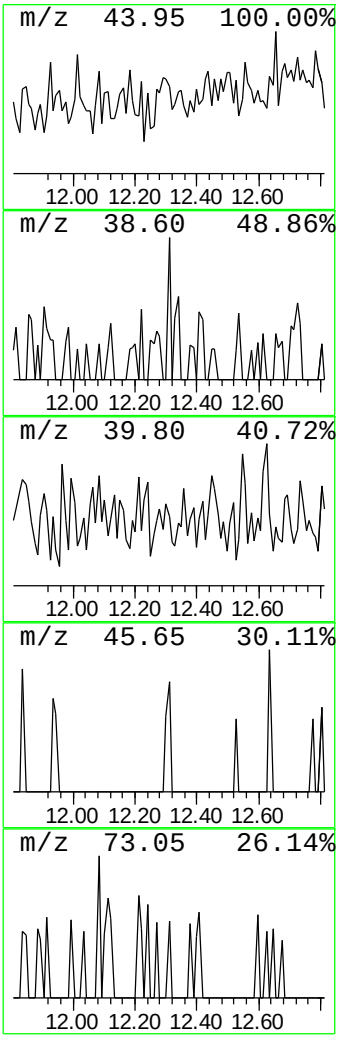
****

Peak Number 2 unknown12.31 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.31	9.51 ug/l	3990	1,4-Dichlorobenzene-d4	12.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	[2,5-Dioxo-1-(m-tolyl)-3-pyrroli...	279	C13H13NO4S	1000223-78-4	12
2	Propanamide	73	C3H7NO	000079-05-0	4
3	Acetonitrile, hydroxy-	57	C2H3NO	000107-16-4	4
4	Pterin-6-carboxylic acid	207	C7H5N5O3	000948-60-7	4
5	Acetaldehyde	44	C2H4O	000075-07-0	2





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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_F\METHODS\82F080418S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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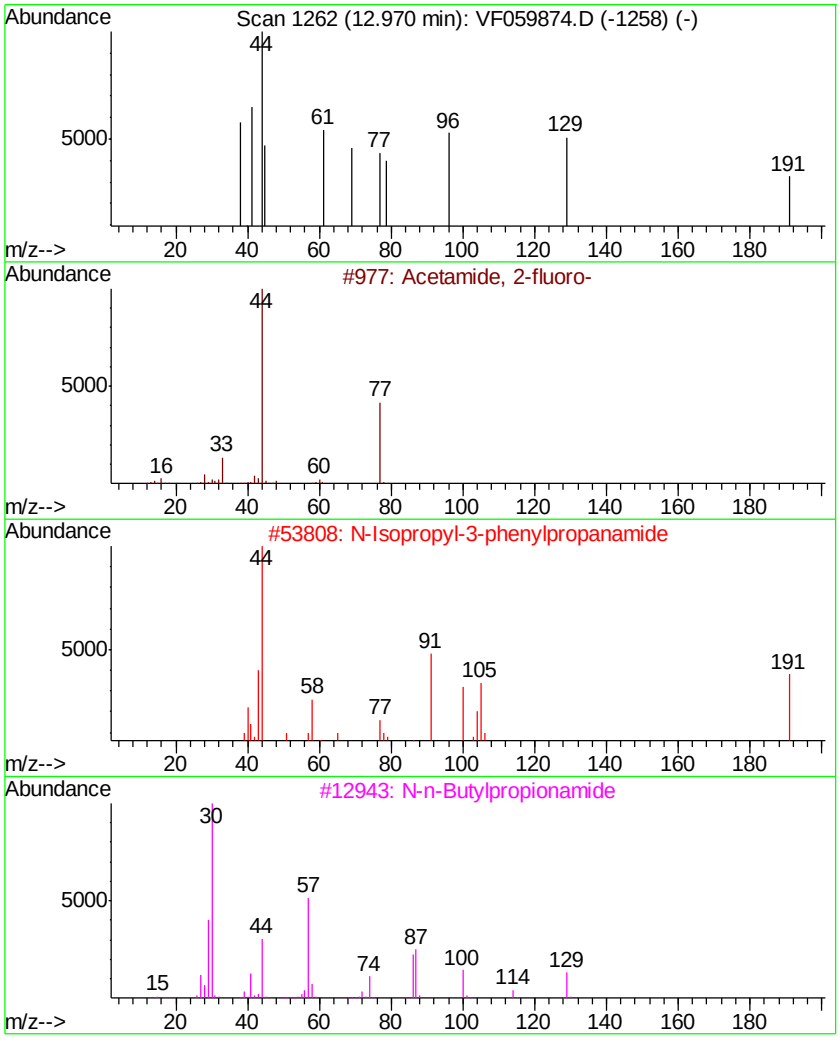
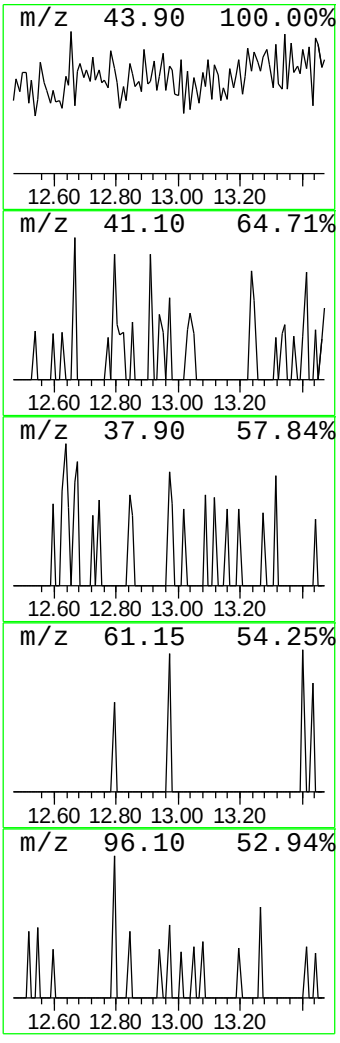
****

Peak Number 3 unknown12.97 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.97	8.82 ug/l	3699	1,4-Dichlorobenzene-d4	12.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, 2-fluoro-	77	C2H4FNO	000640-19-7	4
2	N-Isopropyl-3-phenylpropanamide	191	C12H17NO	056146-87-3	4
3	N-n-Butylpropionamide	129	C7H15NO	002955-67-1	4
4	Propane	44	C3H8	000074-98-6	4
5	Benzoxazol, 2,3-dihydro-2-thioxo...	260	C14H16N2OS	339064-71-0	4





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Quant Title : SW846 8260

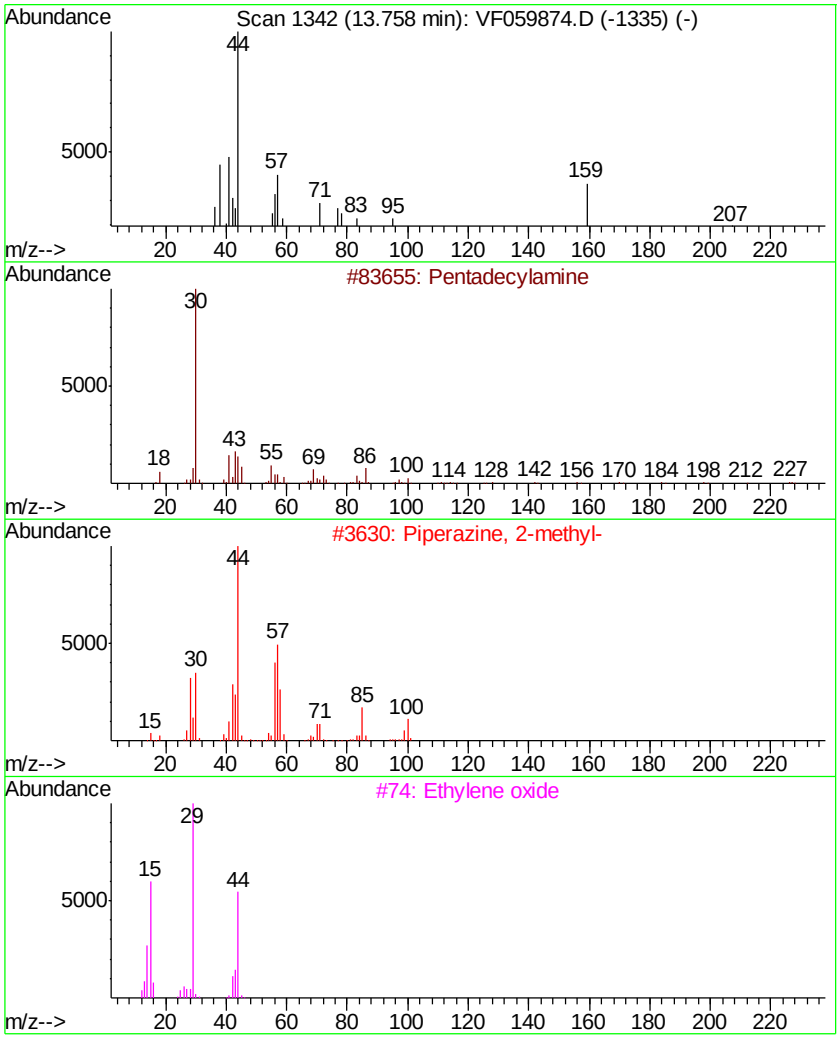
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

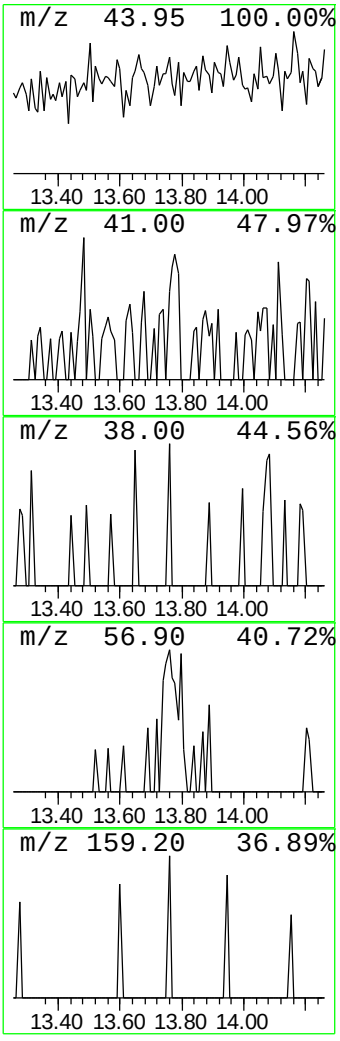
****

Peak Number 4 unknown13.76 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	24.12 ug/l	10120	1,4-Dichlorobenzene-d4	12.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecylamine	227	C15H33N	002570-26-5	9
2	Piperazine, 2-methyl-	100	C5H12N2	000109-07-9	9
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Benzaldehyde, 2-nitro-, diaminom...	207	C8H9N5O2	102632-31-5	4
5	Propane	44	C3H8	000074-98-6	4





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Instrument : MSVOA_F
ClientSampleId : BEEBEE-SITE-DEMO-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_F\METHODS\82F080418S.M
Quant Title : SW846 8260

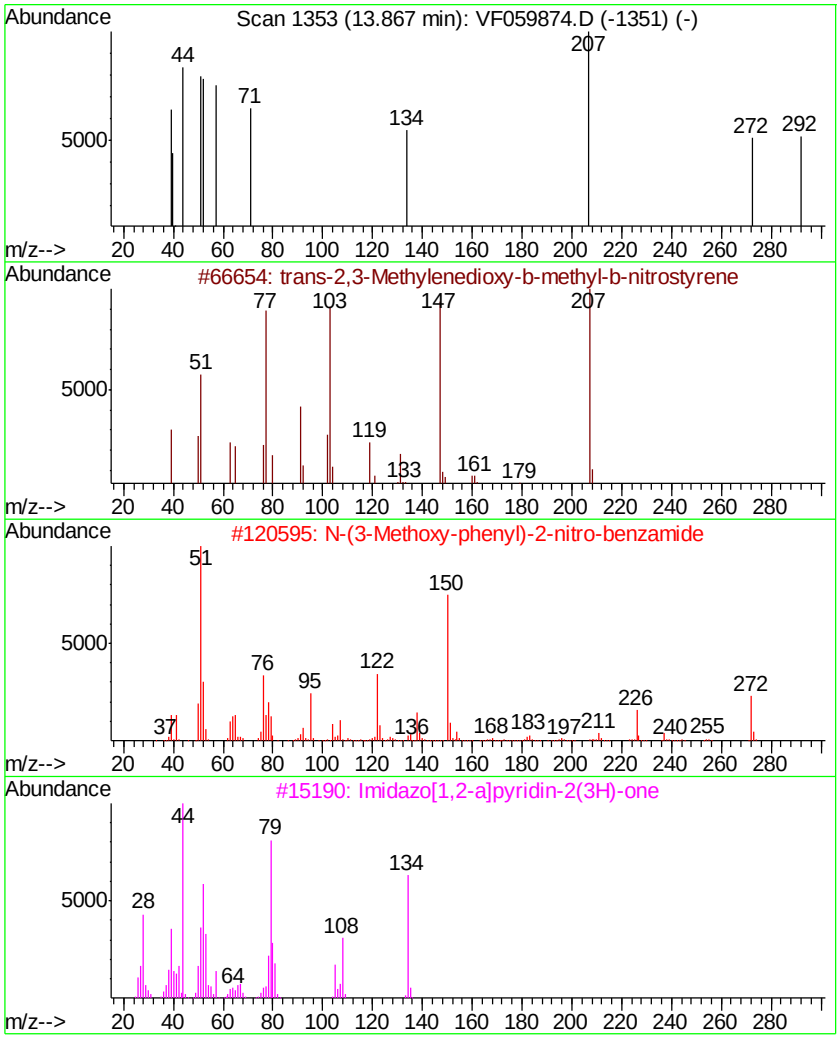
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

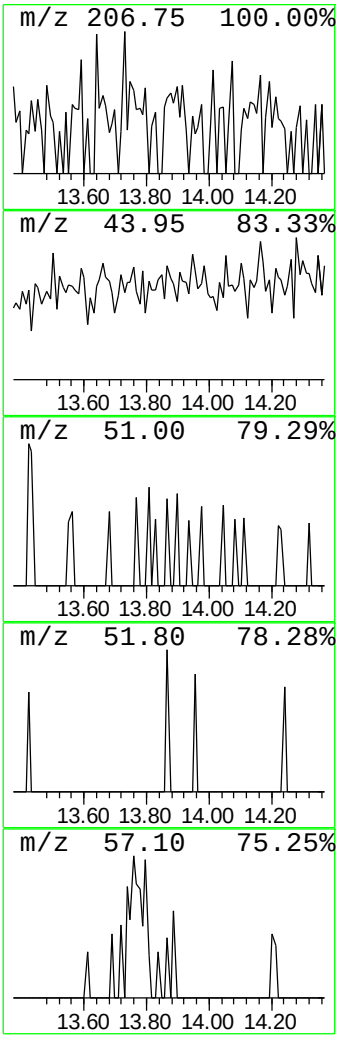
****

Peak Number 5 unknown13.87 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	5.90 ug/l	2474	1,4-Dichlorobenzene-d4	12.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-2,3-Methylenedioxy-b-methy...	207	C10H9NO4	086029-47-2	5
2	N-(3-Methoxy-phenyl)-2-nitro-ben...	272	C14H12N2O4	058495-04-8	5
3	Imidazo[1,2-a]pyridin-2(3H)-one	134	C7H6N2O	003999-06-2	5
4	[1,2,3,4]Tetrazolo[1,5-a]pyridin...	134	C6H6N4	1000338-33-0	4
5	[1,2,3,4]Tetrazolo[1,5-a]pyridin...	134	C6H6N4	1000338-32-8	4





Data Path : Z:\VOASRV\HPCHEM1\MSVOA F\DATA\VF080418\
Data File : VF059874.D
Acq On : 4 Aug 2018 9:47
Operator : VA/AP
Sample : J4318-09
Misc : 4.30g/5mL/MSVOA F/SOIL
ALS Vial : 100 Sample Multiplier: 1

Instrument : MSVOA_F
ClientSampleId : BEEBEE-SITE-DEMO-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_F\METHODS\82F080418S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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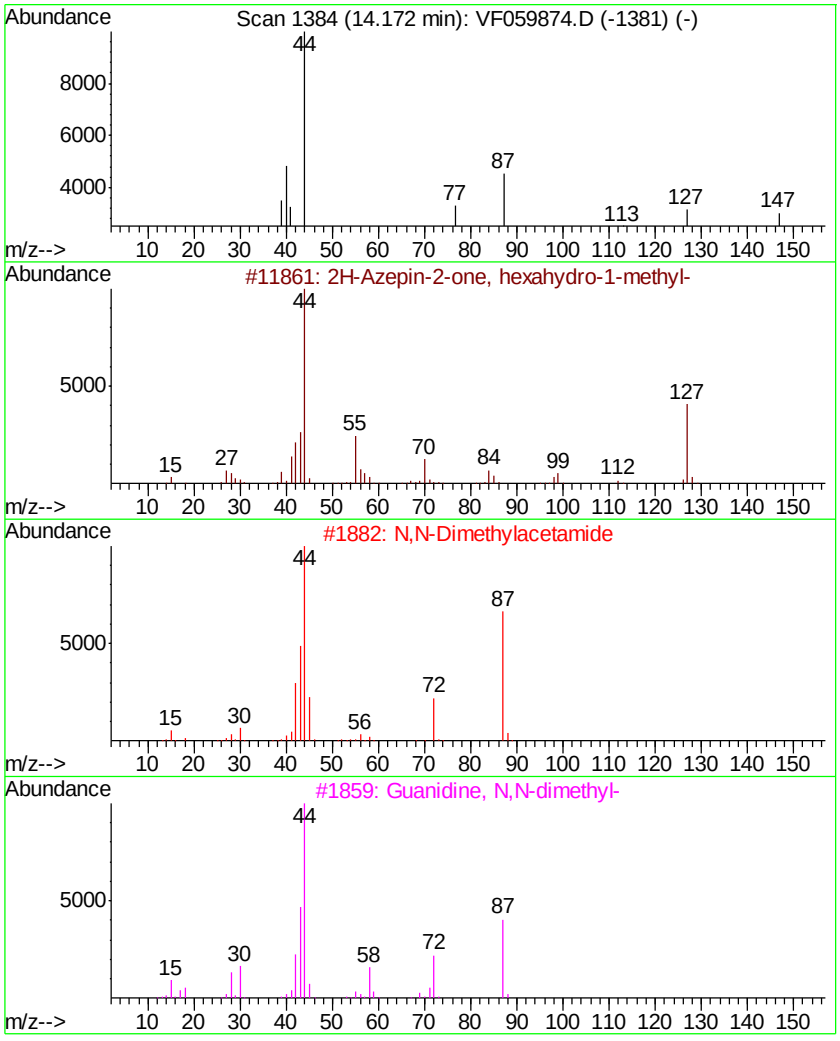
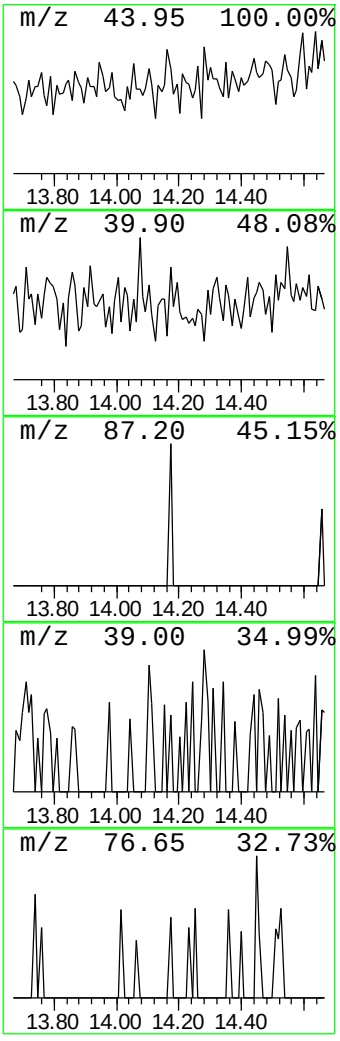
Peak Number 6 unknown14.17 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.17	6.75 ug/l	2830	1,4-Dichlorobenzene-d4	12.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Azepin-2-one, hexahydro-1-met...	127	C7H13NO	002556-73-2	5
2	N,N-Dimethylacetamide	87	C4H9NO	000127-19-5	5
3	Guanidine, N,N-dimethyl-	87	C3H9N3	006145-42-2	5
4	Piperidine, 3,5-dimethyl-	113	C7H15N	035794-11-7	4
5	Piperidine, 3-isopropyl-	127	C8H17N	013603-18-4	4





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Data File : VF059874.D
Acq On : 4 Aug 2018 9:47
Operator : VA/AP
Sample : J4318-09
Misc : 4.30g/5mL/MSVOA F/SOIL
ALS Vial : 100 Sample Multiplier: 1

Instrument : MSVOA_F
ClientSampleId : BEEBEE-SITE-DEMO-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_F\METHODS\82F080418S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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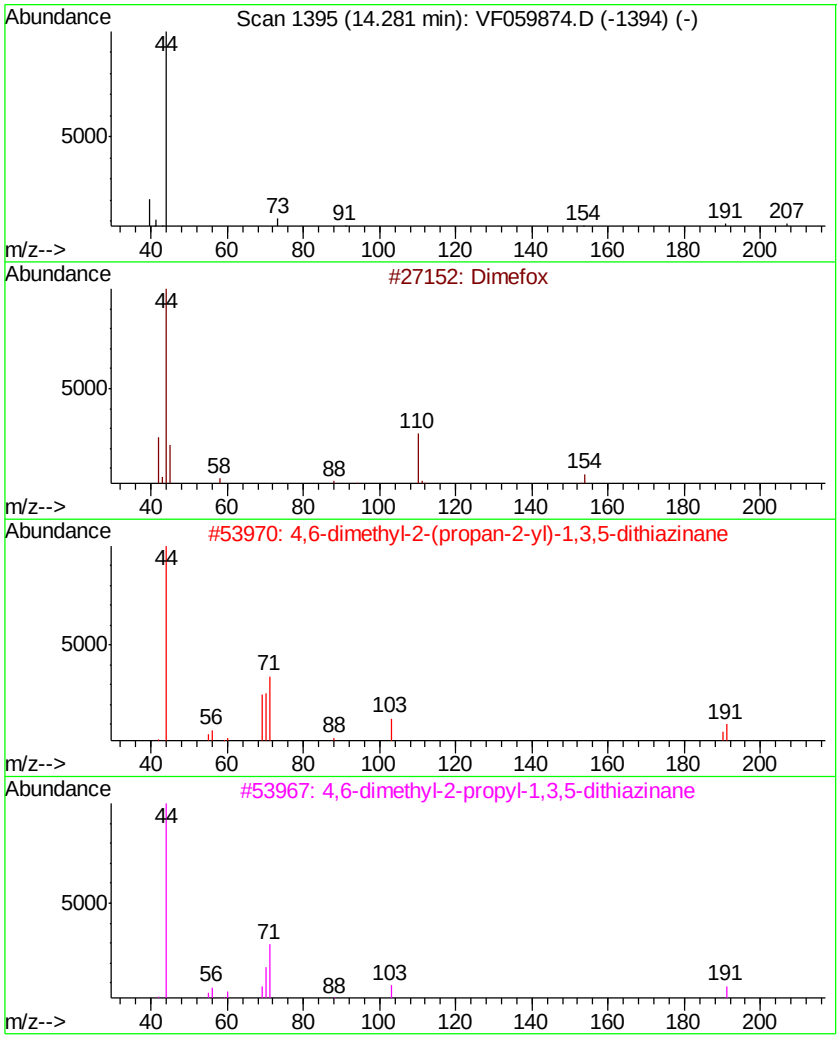
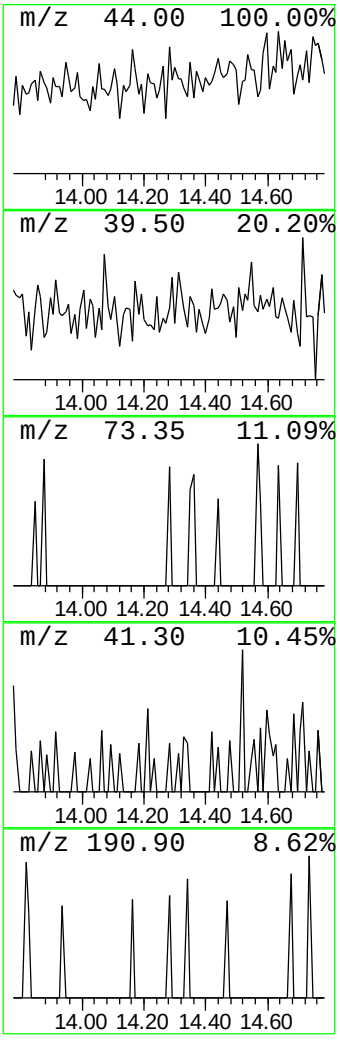
Peak Number 7 unknown14.28 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.28	6.59 ug/l	2764	1,4-Dichlorobenzene-d4	12.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimefox	154	C4H12FN2OP	000115-26-4	5
2	4,6-dimethyl-2-(propan-2-yl)-1,3...	191	C8H17NS2	104691-40-9	4
3	4,6-dimethyl-2-propyl-1,3,5-dith...	191	C8H17NS2	1000365-92-6	4
4	Ethyne, fluoro-	44	C2HF	002713-09-9	3
5	Benzaldehyde, 2-nitro-, diaminom...	207	C8H9N5O2	102632-31-5	3





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Data File : VF059874.D
Acq On : 4 Aug 2018 9:47
Operator : VA/AP
Sample : J4318-09
Misc : 4.30g/5mL/MSVOA F/SOIL
ALS Vial : 100 Sample Multiplier: 1

Instrument : MSVOA_F
ClientSampleId : BEEBEE-SITE-DEMO-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_F\METHODS\82F080418S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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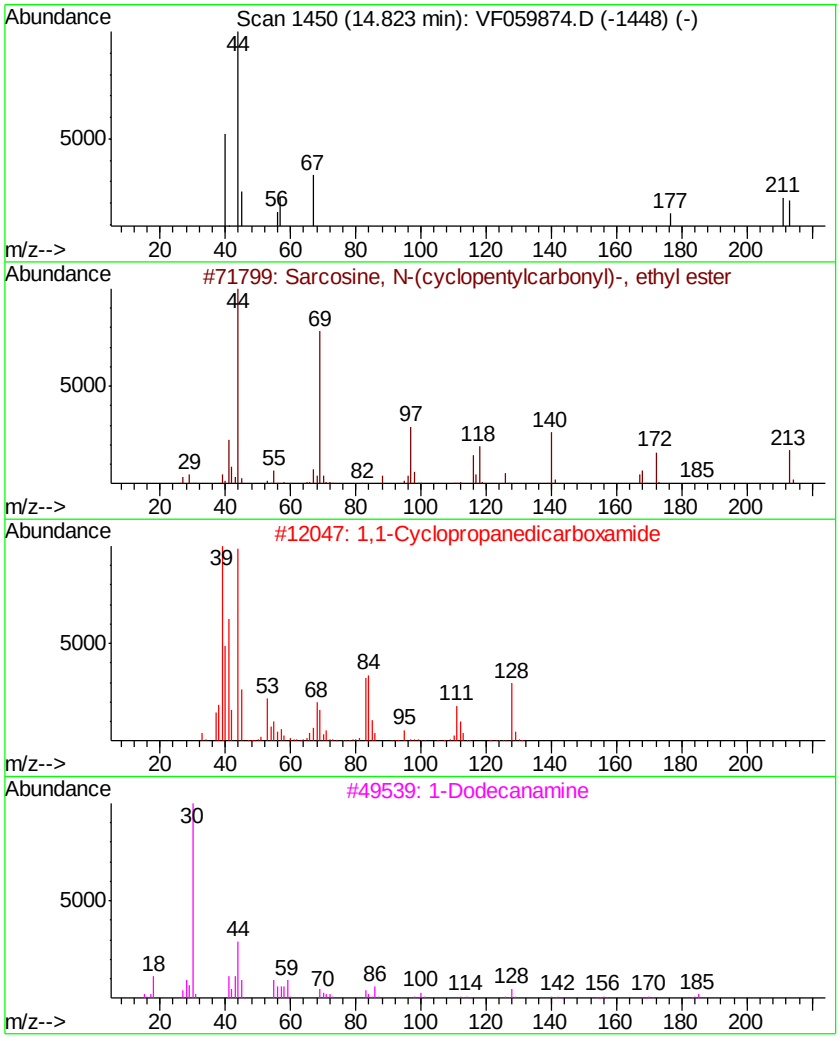
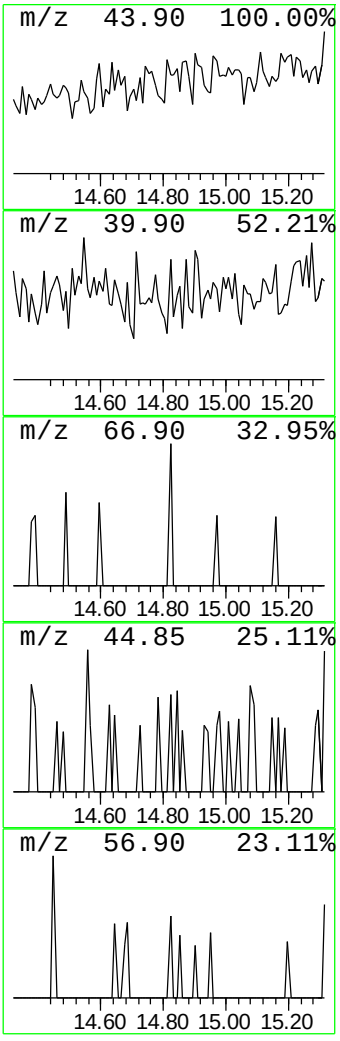
Peak Number 8 unknown14.82 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	8.41 ug/l	3529	1,4-Dichlorobenzene-d4	12.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sarcosine, N-(cyclopentylcarbonyl...	213	C11H19NO3	1000321-33-5	4
2	1,1-Cyclopropanedicarboxamide	128	C5H8N2O2	005813-85-4	4
3	1-Dodecanamine	185	C12H27N	000124-22-1	4
4	Acetaldehyde	44	C2H4O	000075-07-0	3
5	1-Tetradecanamine	213	C14H31N	002016-42-4	3





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Data File : VF059874.D
Acq On : 4 Aug 2018 9:47
Operator : VA/AP
Sample : J4318-09
Misc : 4.30g/5mL/MSVOA F/SOIL
ALS Vial : 100 Sample Multiplier: 1

Instrument : MSVOA_F
ClientSampleId : BEEBEE-SITE-DEMO-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_F\METHODS\82F080418S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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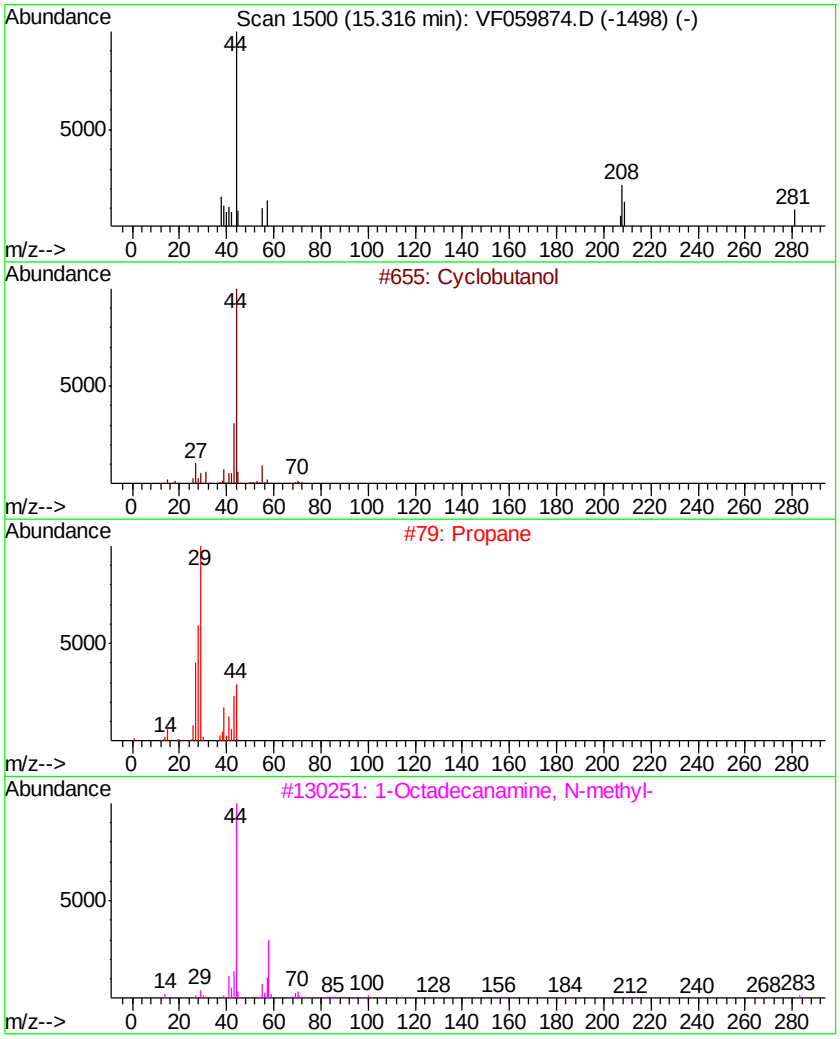
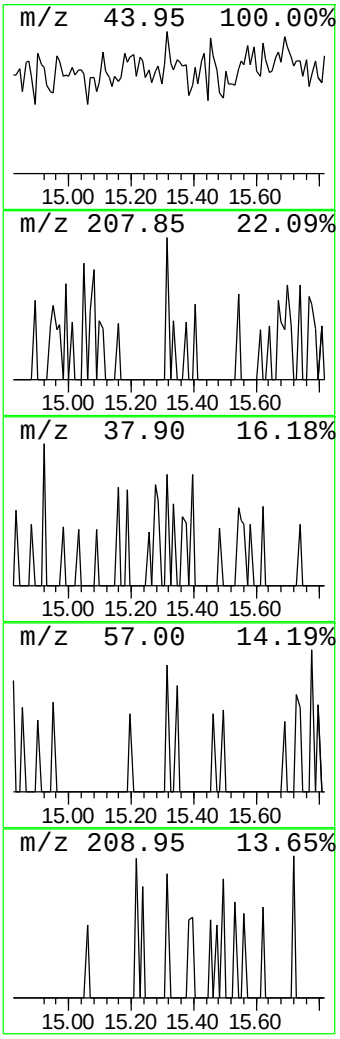
Peak Number 9 unknown15.32 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.32	5.88 ug/l	2468	1,4-Dichlorobenzene-d4	12.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutanol	72	C4H8O	002919-23-5	9
2	Propane	44	C3H8	000074-98-6	4
3	1-Octadecanamine, N-methyl-	283	C19H41N	002439-55-6	4
4	Propanamide	73	C3H7NO	000079-05-0	4
5	Propanamide, N-(1-cyclohexylethyl)-	183	C11H21NO	1000142-14-3	4





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Data File : VF059874.D
Acq On : 4 Aug 2018 9:47
Operator : VA/AP
Sample : J4318-09
Misc : 4.30g/5mL/MSVOA F/SOIL
ALS Vial : 100 Sample Multiplier: 1

Instrument : MSVOA_F
ClientSampleId : BEEBEE-SITE-DEMO-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_F\METHODS\82F080418S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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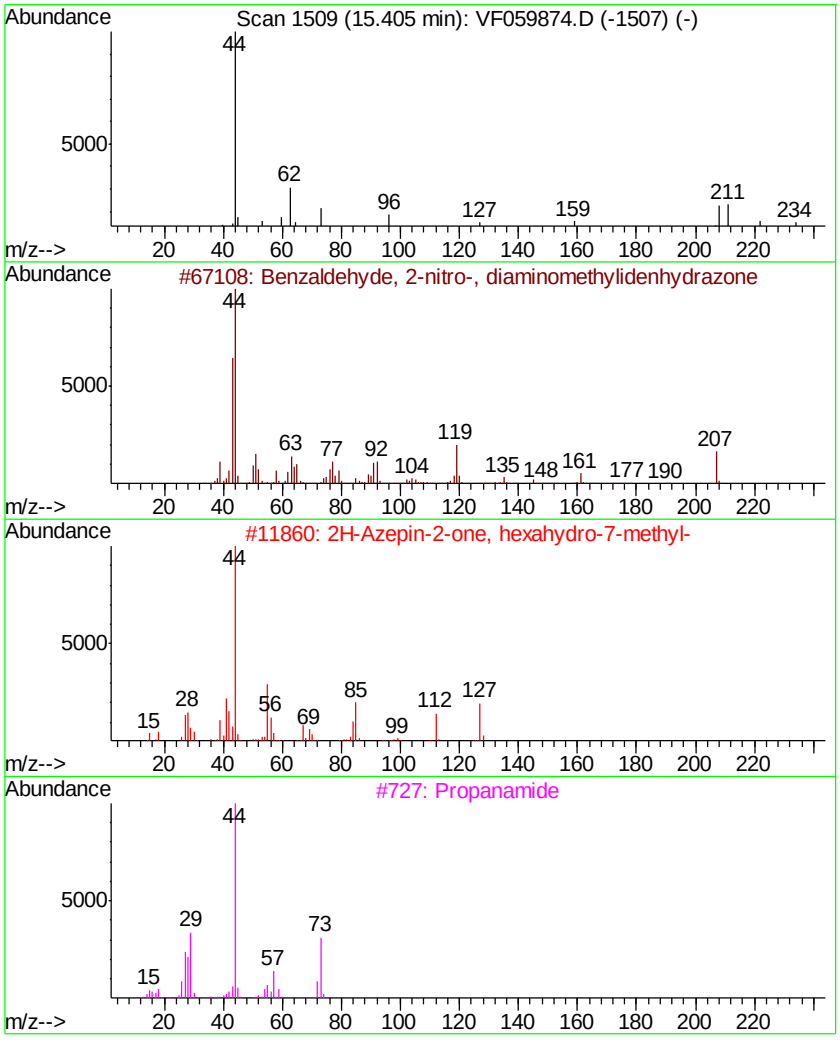
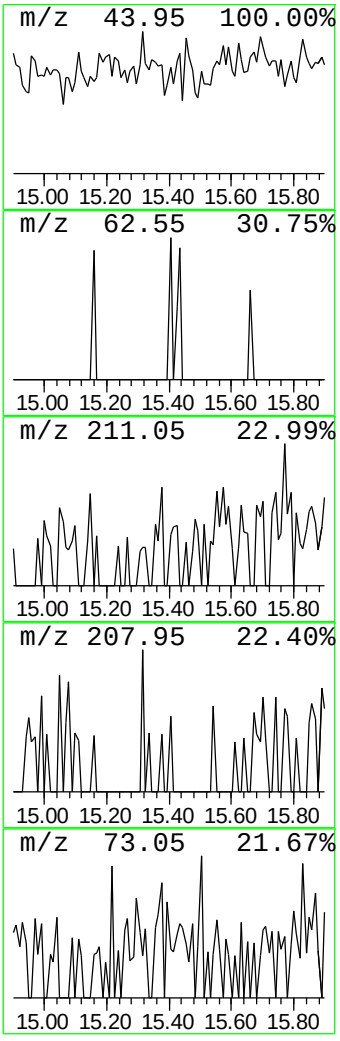
Peak Number 10 unknown15.40 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.40	5.81 ug/l	2439	1,4-Dichlorobenzene-d4	12.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 2-nitro-, diaminom...	207	C8H9N5O2	102632-31-5	7
2	2H-Azepin-2-one, hexahydro-7-met...	127	C7H13NO	001985-48-4	4
3	Propanamide	73	C3H7NO	000079-05-0	4
4	Chlorozotocin	313	C9H16ClN3O7	054749-90-5	4
5	Carbamic acid 2,3-dibromopropyl ...	259	C4H7Br2NO2	055190-46-0	4





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_F\DATA\VF080418\
Data File : VF059874.D
Acq On : 4 Aug 2018 9:47
Operator : VA/AP
Sample : J4318-09
Misc : 4.30g/5mL/MSVOA_F/SOIL
ALS Vial : 100 Sample Multiplier: 1

Instrument : MSVOA_F
ClientSampleId : BEEBEE-SITE-DEMO-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_F\METHODS\82F080418S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
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unknown12.31	12.31	9.5	ug/l	3990	4	12.63	20976	50.0
unknown12.97	12.97	8.8	ug/l	3699	4	12.63	20976	50.0
unknown13.76	13.76	24.1	ug/l	10120	4	12.63	20976	50.0
unknown13.87	13.87	5.9	ug/l	2474	4	12.63	20976	50.0
unknown14.17	14.17	6.8	ug/l	2830	4	12.63	20976	50.0
unknown14.28	14.28	6.6	ug/l	2764	4	12.63	20976	50.0
unknown14.82	14.82	8.4	ug/l	3529	4	12.63	20976	50.0
unknown15.32	15.32	5.9	ug/l	2468	4	12.63	20976	50.0
unknown15.40	15.40	5.8	ug/l	2439	4	12.63	20976	50.0