LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY010924\
Data File : VY016960.D
Acq On : 09 Jan 2024 19:41
Operator : SY/MD
Sample : P1085-07
Misc : 5.06g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
TP-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_Y\methods\82Y010224S.M
Title : SW846 8260

Signal : TIC: VY016960.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.119	46	49	50	rBV2	726	769	2.74%	0.499%
2	2.137	50	52	53	rVV	442	438	1.56%	0.284%
3	2.229	65	67	69	rBV3	481	503	1.79%	0.326%
4	2.272	73	74	78	rVV3	717	674	2.40%	0.437%
5	2.326	81	83	85	rVB2	745	740	2.64%	0.480%
6	7.734	965	970	975	rBV4	1455	2831	10.08%	1.837%
7	7.807	977	982	991	rVB2	3170	5989	21.33%	3.886%
8	8.161	1029	1040	1045	rBV5	1956	4950	17.63%	3.212%
9	8.551	1100	1104	1106	rVB3	359	486	1.73%	0.315%
10	8.606	1110	1113	1115	rVB3	511	487	1.73%	0.316%
11	8.703	1124	1129	1135	rBV2	5237	10116	36.03%	6.564%
12	8.770	1138	1140	1143	rVV4	425	392	1.40%	0.254%
13	8.825	1146	1149	1152	rVB3	565	849	3.02%	0.551%
14	8.862	1152	1155	1158	rBV3	498	762	2.71%	0.494%
15	9.002	1176	1178	1181	rVB4	578	441	1.57%	0.286%
16	9.148	1197	1202	1203	rBV4	603	795	2.83%	0.516%
17	9.173	1203	1206	1207	rVV2	484	499	1.78%	0.324%
18	9.270	1218	1222	1223	rBV3	506	458	1.63%	0.297%
19	9.356	1232	1236	1238	rBV4	405	506	1.80%	0.328%
20	9.404	1242	1244	1247	rBV4	488	675	2.40%	0.438%
21	9.496	1257	1259	1261	rBV3	621	710	2.53%	0.461%
22	9.581	1270	1273	1274	rBV3	694	632	2.25%	0.410%
23	9.691	1289	1291	1293	rBV2	509	560	1.99%	0.363%
24	9.813	1308	1311	1316	rBV7	937	1165	4.15%	0.756%
25	9.862	1318	1319	1323	rBV4	609	789	2.81%	0.512%
26	9.959	1333	1335	1337	rVB3	864	660	2.35%	0.428%
27	10.038	1342	1348	1350	rBV7	1267	2252	8.02%	1.461%
28	10.057	1350	1351	1357	rBV6	1309	2172	7.74%	1.409%
29	10.118	1357	1361	1363	rBV4	1040	1688	6.01%	1.095%
30	10.197	1368	1374	1379	rBV2	7620	15002	53.43%	9.735%
31	10.270	1383	1386	1388	rBV4	1118	1604	5.71%	1.041%
32	10.380	1402	1404	1406	rBV3	1157	879	3.13%	0.570%
33	10.685	1452	1454	1456	rVB3	1813	1115	3.97%	0.724%
34	10.825	1475	1477	1480	rBV4	1716	1252	4.46%	0.812%
35	11.508	1585	1589	1595	rVB3	7840	14896	53.05%	9.666%
36	12.495	1748	1751	1753	rBV4	4756	5339	19.02%	3.465%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY010924\
Data File : VY016960.D
Acq On : 09 Jan 2024 19:41
Operator : SY/MD
Sample : P1085-07
Misc : 5.06g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
TP-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_Y\methods\82Y010224S.M
Title : SW846 8260

37	13.251	1867	1875	1876	rBV8	10183	21106	75.17%	13.696%
38	15.330	2212	2216	2217	rBV4	2660	3912	13.93%	2.539%
39	15.531	2242	2249	2260	rVB5	9264	28077	100.00%	18.220%
40	15.745	2279	2284	2289	rBV8	2533	6818	24.28%	4.424%
41	16.123	2344	2346	2348	rBV3	1333	1680	5.98%	1.090%
42	16.367	2384	2386	2394	rVB9	2006	4155	14.80%	2.696%
43	16.428	2394	2396	2398	rVV3	942	642	2.29%	0.417%
44	16.482	2402	2405	2408	rBV5	838	1270	4.52%	0.824%
45	16.537	2413	2414	2416	rVB2	1149	715	2.55%	0.464%
46	16.598	2422	2424	2425	rBV2	1366	917	3.27%	0.595%
47	16.720	2442	2444	2445	rBV2	1349	736	2.62%	0.478%

Sum of corrected areas: 154103

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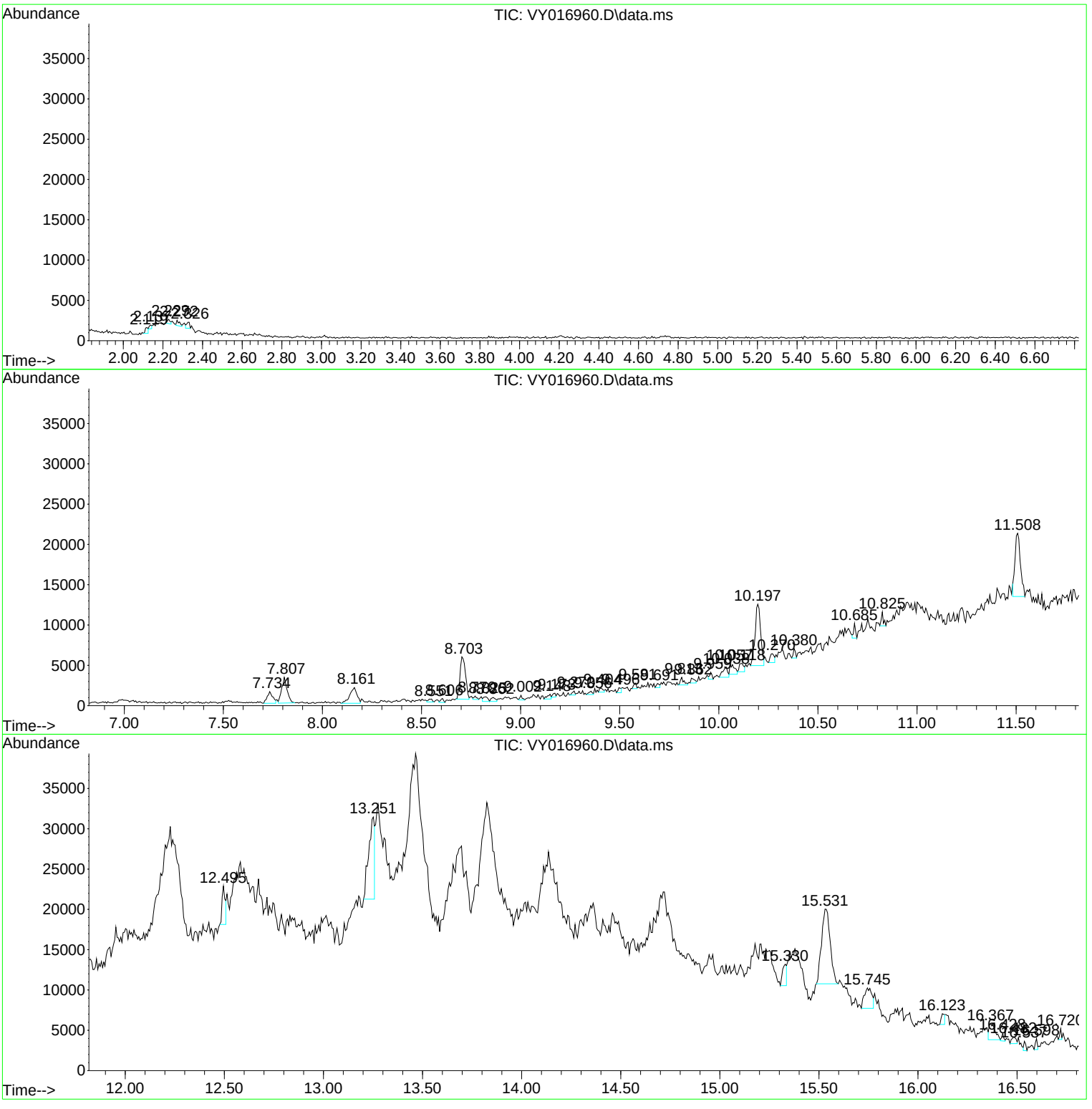
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
TP-4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010224S.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY010924\
Data File : VY016960.D
Acq On : 09 Jan 2024 19:41
Operator : SY/MD
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MSVOA_Y
ClientSampleId :
TP-4

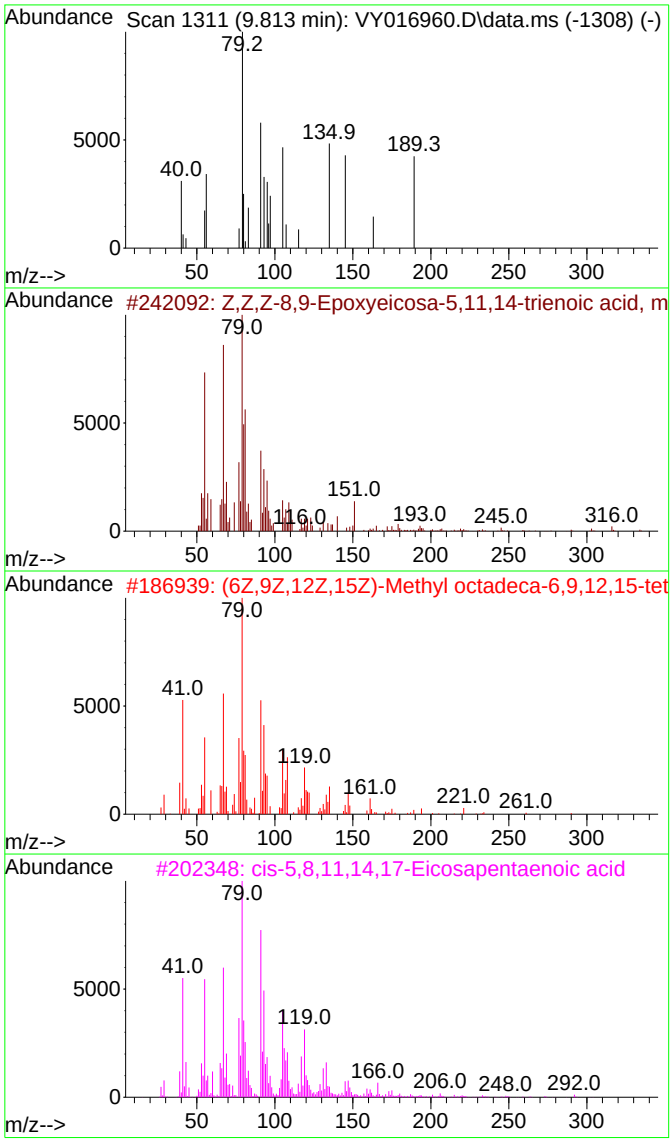
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010224S.M
Quant Title : SW846 8260

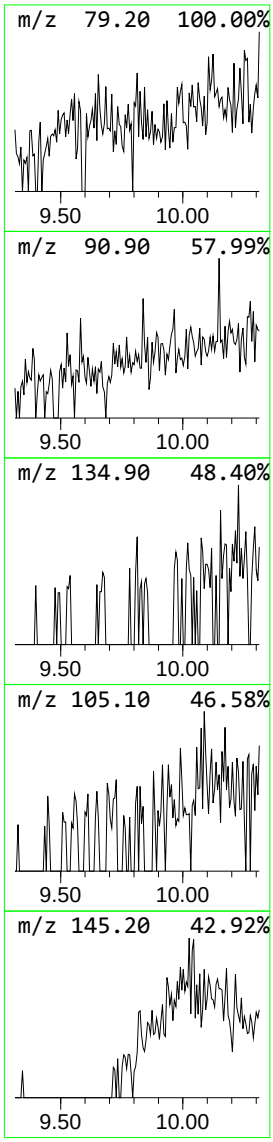
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 unknown9.813 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.813	5.76 ug/l	1165	1,4-Difluorobenzene	8.703

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Z,Z,Z-8,9-Epoxyeicosa-5,11,14-tr...	334	C21H34O3	1010368-68-2	12
2	(6Z,9Z,12Z,15Z)-Methyl octadeca-...	290	C19H30O2	073097-00-4	12
3	cis-5,8,11,14,17-Eicosapentaenoi...	302	C20H30O2	010417-94-4	9
4	Ethanol, 2-bromo-	124	C2H5BrO	000540-51-2	9
5	Butyraldehyde, 4-(methylenecyclo...	124	C8H12O	1000156-86-5	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY010924\
Data File : VY016960.D
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Operator : SY/MD
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Misc : 5.06g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
TP-4

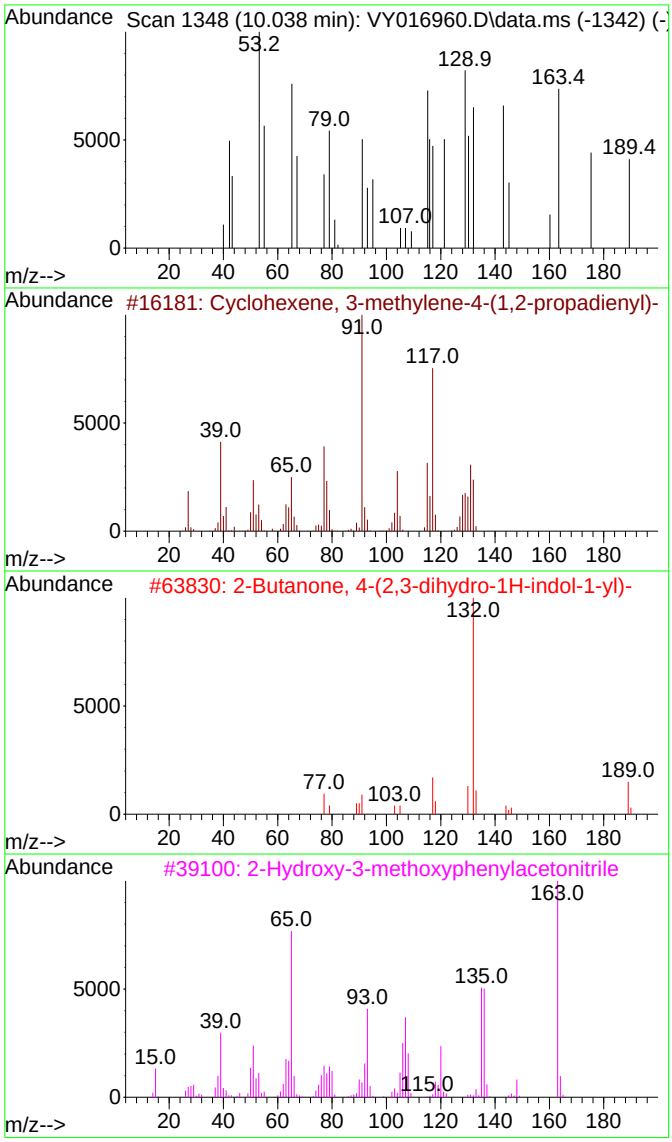
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010224S.M
Quant Title : SW846 8260

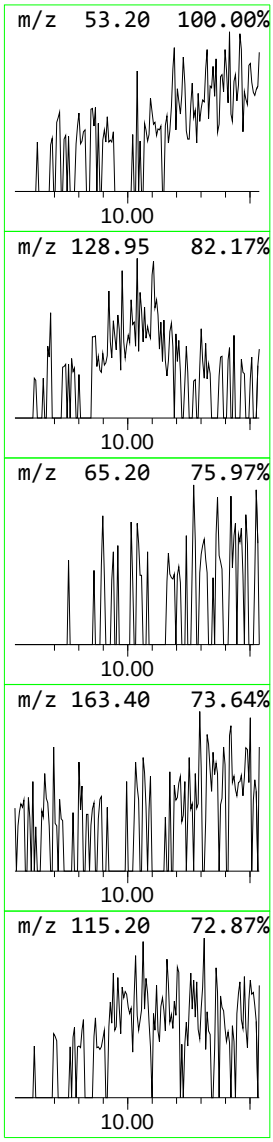
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 unknown10.038 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.038	11.13 ug/l	2252	1,4-Difluorobenzene	8.703

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 3-methylene-4-(1,2-...	132	C10H12	068377-81-1	10
2	2-Butanone, 4-(2,3-dihydro-1H-in...	189	C12H15NO	040135-92-0	10
3	2-Hydroxy-3-methoxyphenylacetoni...	163	C9H9NO2	042973-56-8	10
4	Dimethyl(phenylethynyl)silane	160	C10H12Si	1000434-27-7	9
5	Pyrrolidin-5-one, 2,3-dedihydro-...	129	C4H3NO4	1000124-44-1	9





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Data File : VY016960.D
Acq On : 09 Jan 2024 19:41
Operator : SY/MD
Sample : P1085-07
Misc : 5.06g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
TP-4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010224S.M
Quant Title : SW846 8260

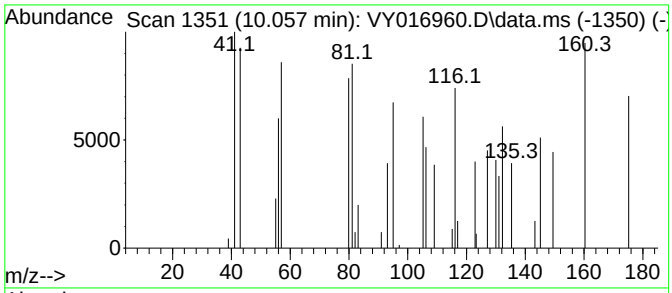
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

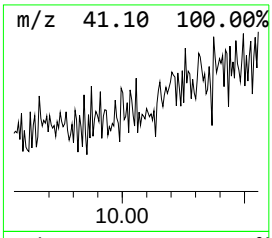
****

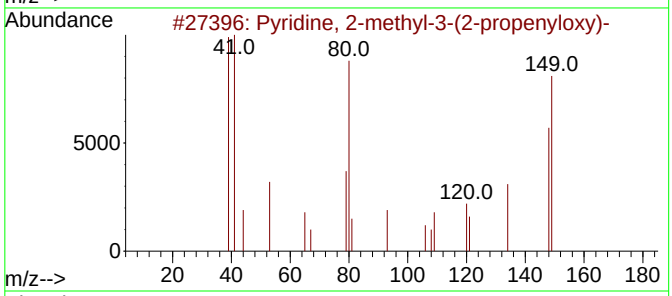
Peak Number 5 unknown10.057 Concentration Rank 5

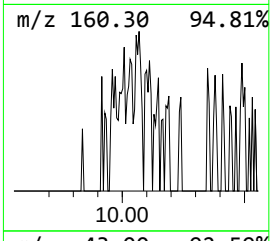
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.057	10.74 ug/l	2172	1,4-Difluorobenzene	8.703

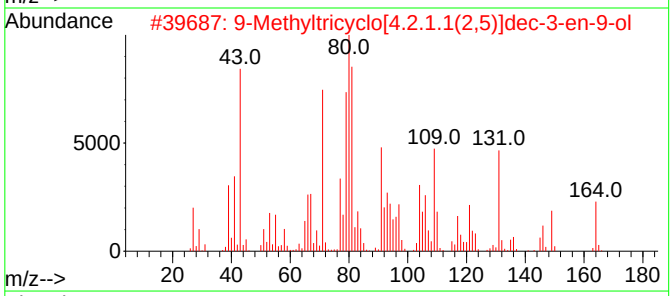
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine, 2-methyl-3-(2-propenyl...	149	C9H11NO	069022-75-9	25
2	9-Methyltricyclo[4.2.1.1(2,5)]de...	164	C11H16O	070220-94-9	16
3	1H-Pyrrole, 1-butyl-	123	C8H13N	000589-33-3	16
4	(-)-.beta.-Bourbonene	204	C15H24	005208-59-3	12
5	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	001985-59-7	9

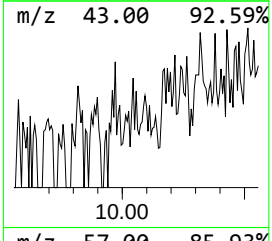


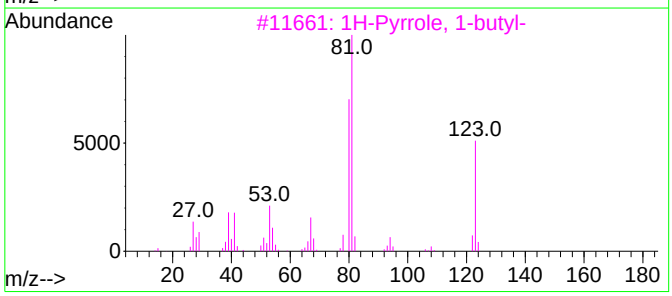


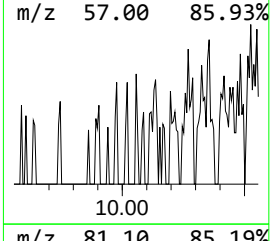


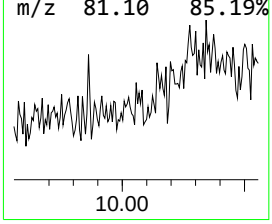












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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
TP-4

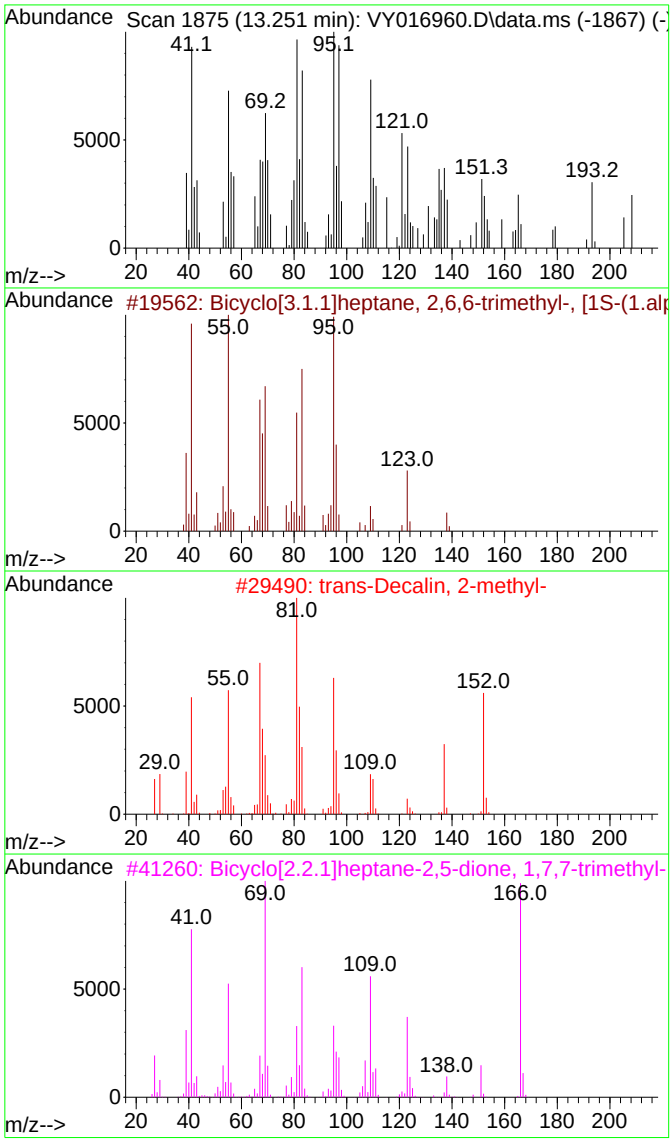
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010224S.M
Quant Title : SW846 8260

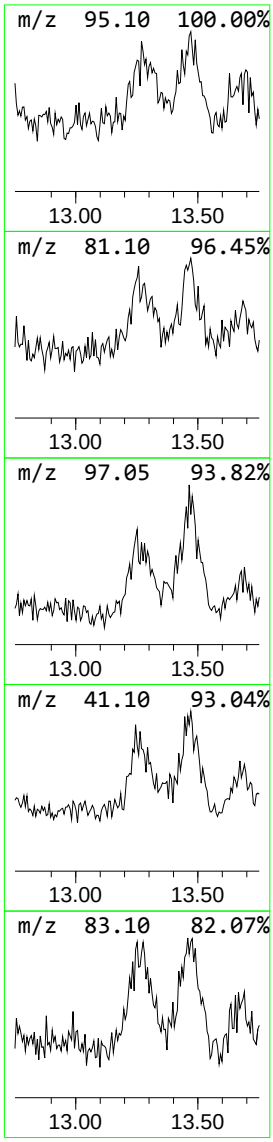
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 unknown13.251 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.251	50.00 ug/l	21106	1,4-Dichlorobenzene-d4	13.434

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	004755-33-3	42
2	trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	41
3	Bicyclo[2.2.1]heptane-2,5-dione,...	166	C10H14O2	004230-32-4	38
4	Naphthalene, decahydro-2,6-dimet...	166	C12H22	001618-22-0	30
5	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	004863-59-6	30





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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
TP-4

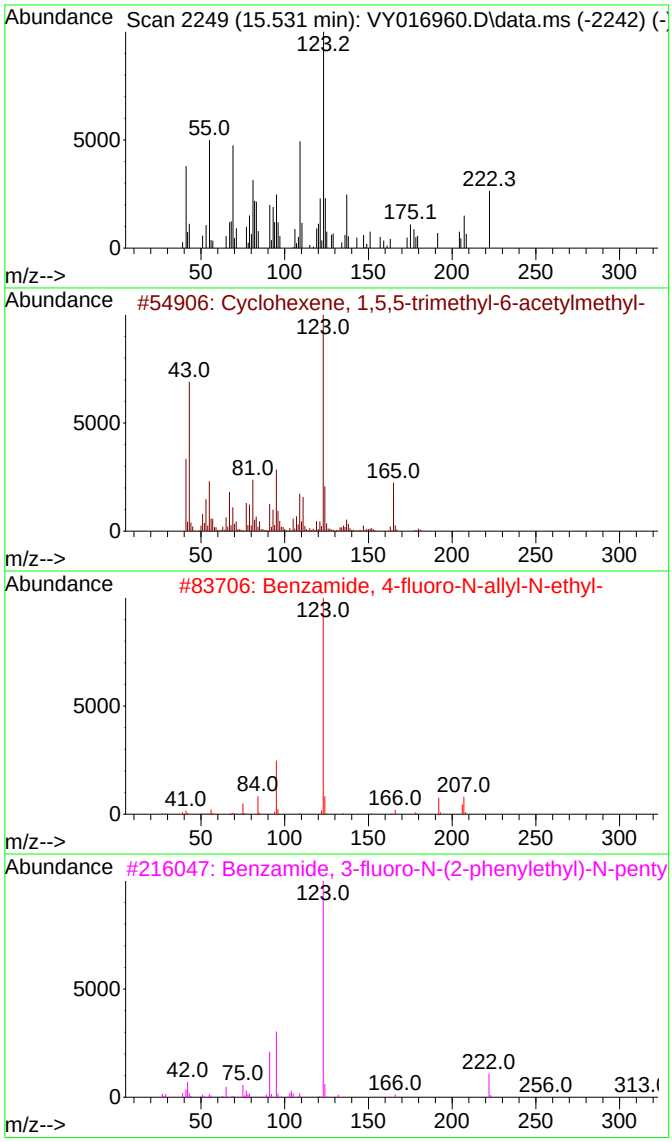
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010224S.M
Quant Title : SW846 8260

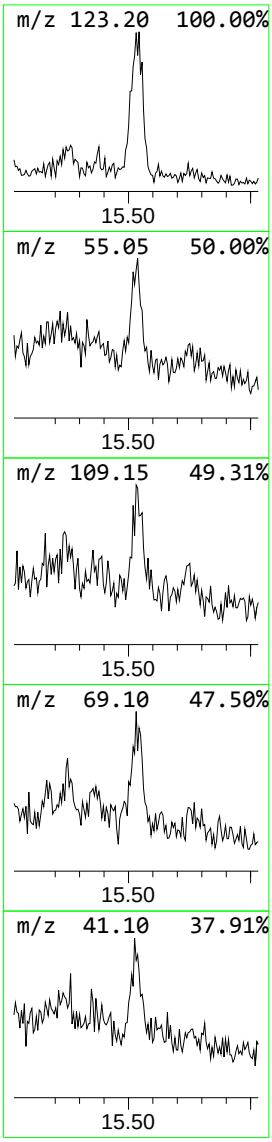
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 unknown15.531 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.531	66.51 ug/l	28077	1,4-Dichlorobenzene-d4	13.434

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 1,5,5-trimethyl-6-a...	180	C12H20O	211563-96-1	43
2	Benzamide, 4-fluoro-N-allyl-N-et...	207	C12H14FNO	1000446-42-7	38
3	Benzamide, 3-fluoro-N-(2-phenyle...	313	C20H24FNO	1000451-30-5	37
4	1-Trimethylsilylpent-1-en-4-yne	138	C8H14Si	079516-25-9	35
5	butanoic acid, (1-ethenyl-1H-imi...	194	C10H14N2O2	1000395-99-5	35





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MSVOA_Y
ClientSampleId :
TP-4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010224S.M
Quant Title : SW846 8260

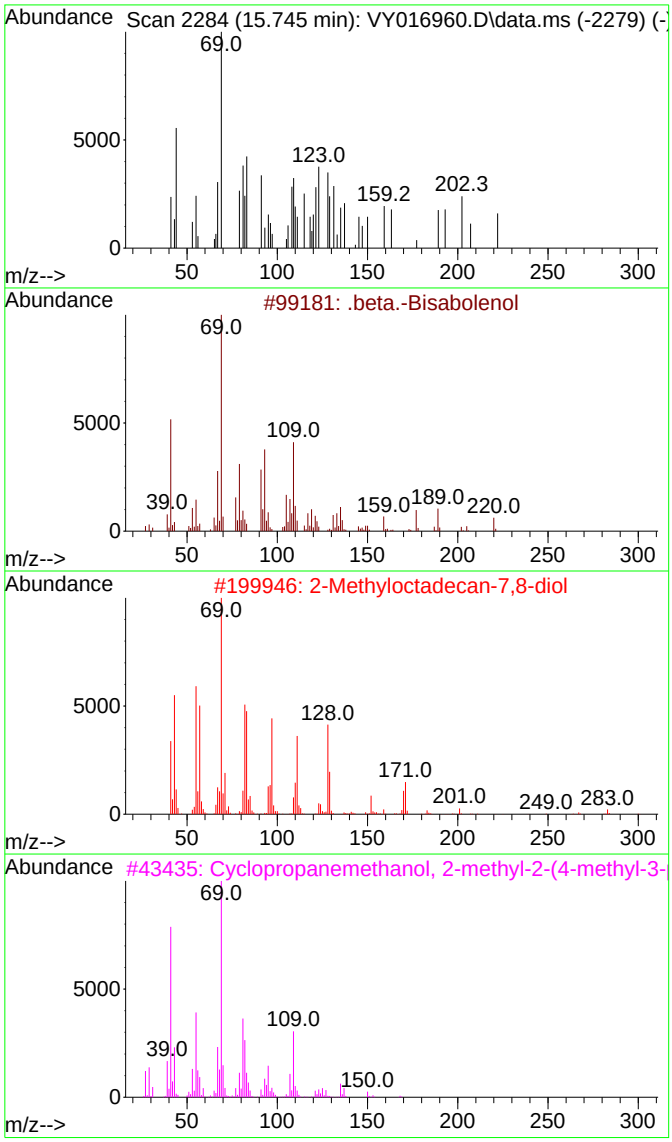
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

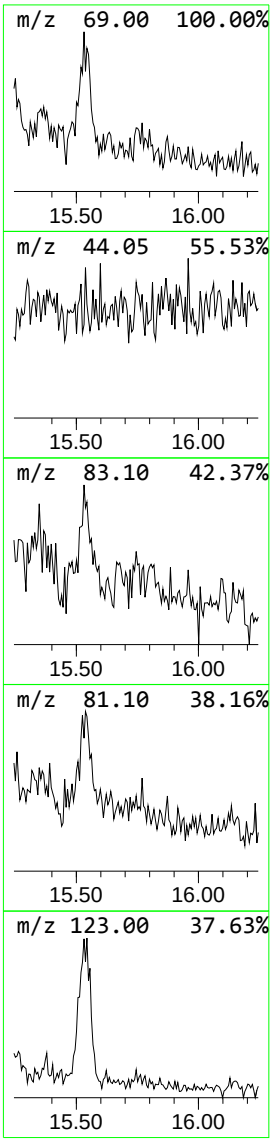
****

Peak Number 9 unknown15.745 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.745	16.15 ug/l	6818	1,4-Dichlorobenzene-d4	13.434

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Bisabolenol	220	C15H24O	147126-90-7	25
2	2-Methyloctadecan-7,8-diol	300	C19H40O2	1000130-91-8	23
3	Cyclopropanemethanol, 2-methyl-2...	168	C11H20O	098678-70-7	22
4	1,6,10,14,18,22-Tetracosahexaen-...	426	C30H50O	097232-74-1	22
5	(1R,4R)-1-methyl-4-(6-Methylhept...	222	C15H26O	058334-55-7	17





Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY010924\
Data File : VY016960.D
Acq On : 09 Jan 2024 19:41
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Sample : P1085-07
Misc : 5.06g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
TP-4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010224S.M
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TIC Integration Parameters: LSCINT.P

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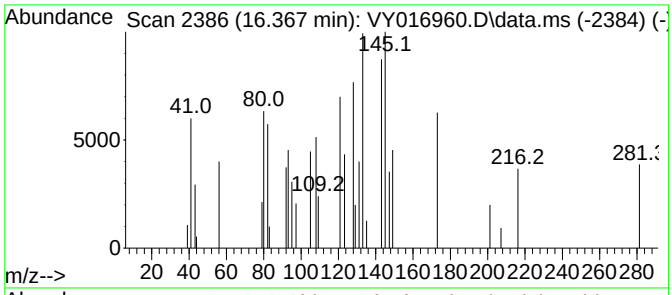
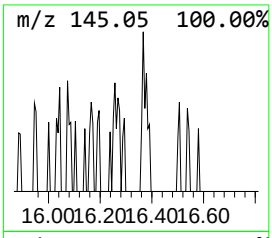
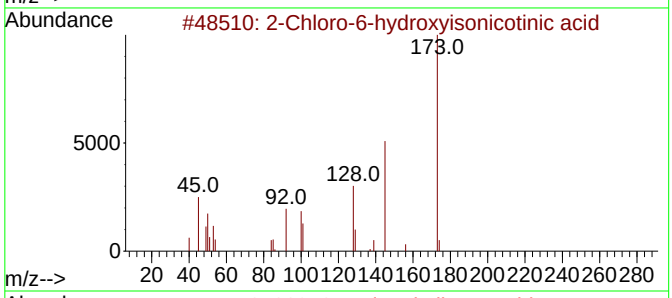
Peak Number 10 unknown16.366 Concentration Rank 6

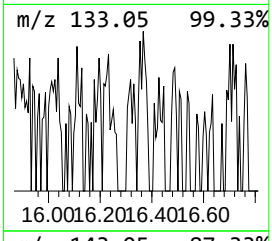
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.366	9.84 ug/l	4155	1,4-Dichlorobenzene-d4	13.434

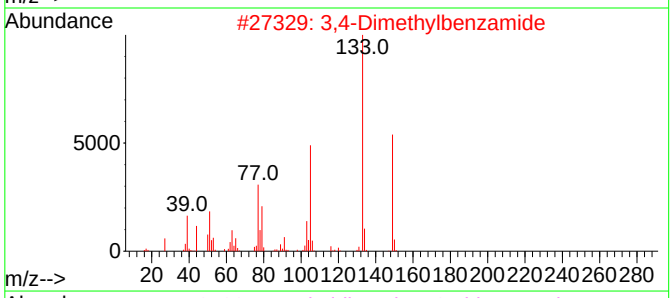
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chloro-6-hydroxyisonicotinic acid	173	C6H4ClNO3	006313-51-5	22
2	3,4-Dimethylbenzamide	149	C9H11NO	005580-33-6	10
3	5-Pyrimidinamine, 2-chloro-4-eth...	173	C6H8ClN3O	054484-70-7	9
4	Ethanone, 1-(3,4-dihydro-1H-isoq...	289	C13H15N5OS	1000304-30-0	9
5	Benzenepropanol, 2,4,6-trimethyl-	178	C12H18O	027645-07-4	9

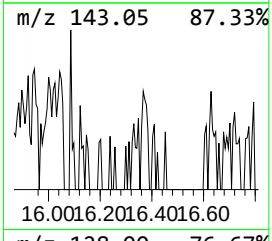


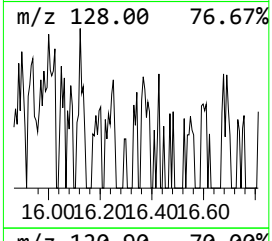


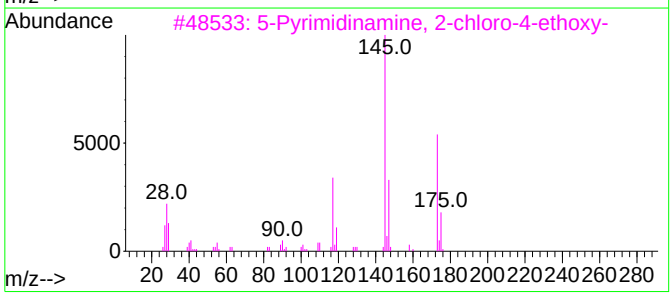


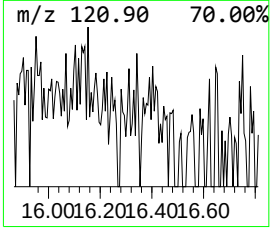












Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY010924\
Data File : VY016960.D
Acq On : 09 Jan 2024 19:41
Operator : SY/MD
Sample : P1085-07
Misc : 5.06g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
TP-4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y010224S.M
Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown9.813	9.813	5.8	ug/l	1165	2	8.703	10116	50.0
unknown10.038	10.038	11.1	ug/l	2252	2	8.703	10116	50.0
unknown10.057	10.057	10.7	ug/l	2172	2	8.703	10116	50.0
unknown13.251	13.251	50.0	ug/l	21106	4	13.434	21106	50.0
unknown15.531	15.531	66.5	ug/l	28077	4	13.434	21106	50.0
unknown15.745	15.745	16.1	ug/l	6818	4	13.434	21106	50.0
unknown16.366	16.366	9.8	ug/l	4155	4	13.434	21106	50.0