

Data Path : Z:\VOASRV\HPCHEM1\MSVOA Y\DATA\VY070720\
 Data File : VY003129.D
 Acq On : 07 Jul 2020 16:14
 Operator : SY/MD
 Sample : L3217-04
 Misc : 5.09G/5ML/MSVOA Y/SOIL
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 E3-41-VAT

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\82Y062920S.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	2.365	85	103	119	rBV	2271395	7455240	100.00%	37.801%
2	2.688	153	156	160	rBV3	927256	757356	10.16%	3.840%
3	2.761	166	168	171	rBV2	779655	432070	5.80%	2.191%
4	2.816	173	177	178	rBV2	1694968	1567331	21.02%	7.947%
5	2.828	178	179	183	rVV3	1329508	979164	13.13%	4.965%
6	2.865	183	185	196	rVB5	861370	731600	9.81%	3.710%
7	2.944	196	198	204	rBV3	915211	697245	9.35%	3.535%
8	2.987	204	205	213	rVB2	473395	334051	4.48%	1.694%
9	3.151	228	232	234	rBV3	1015315	1051005	14.10%	5.329%
10	3.200	238	240	243	rBV3	1155236	820660	11.01%	4.161%
11	8.285	1060	1074	1085	rBV2	320801	866260	11.62%	4.392%
12	8.529	1107	1114	1119	rBV	36658	84869	1.14%	0.430%
13	8.596	1119	1125	1137	rVB	63701	162367	2.18%	0.823%
14	9.035	1189	1197	1205	rBV	325031	648337	8.70%	3.287%
15	10.351	1404	1413	1428	rBV	497194	927713	12.44%	4.704%
16	10.687	1461	1468	1478	rVB2	90268	176543	2.37%	0.895%
17	11.376	1575	1581	1588	rVB	43850	78471	1.05%	0.398%
18	11.571	1605	1613	1624	rBV	396064	695126	9.32%	3.525%
19	12.522	1758	1769	1781	rVB2	359853	633304	8.49%	3.211%
20	13.442	1914	1920	1929	rVB	406668	623593	8.36%	3.162%

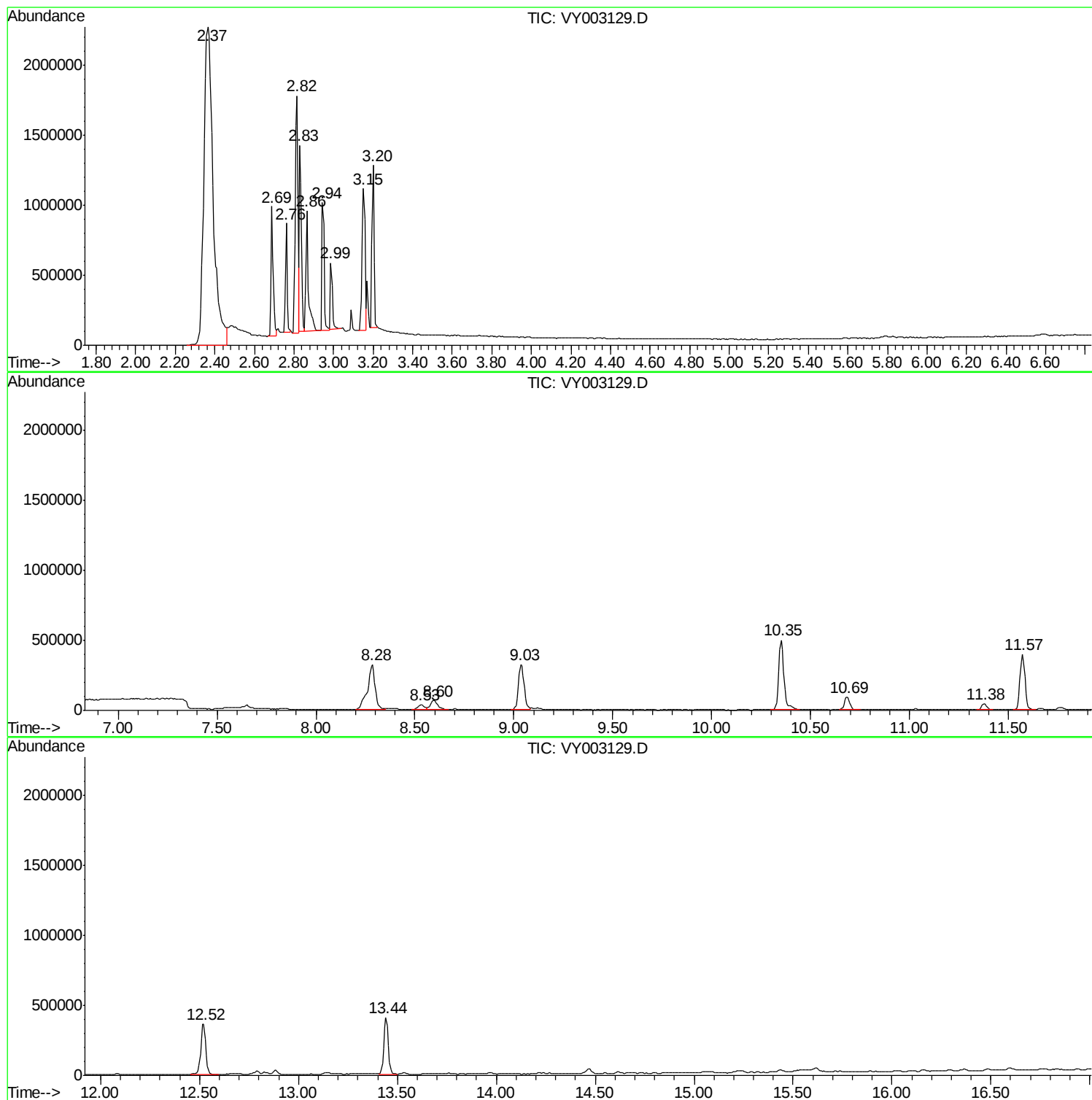
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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
E3-41-VAT

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_Y\METHODS\82Y062920S.M
Quant Title : SW846 8260

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



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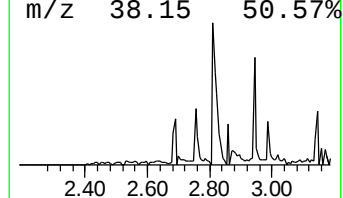
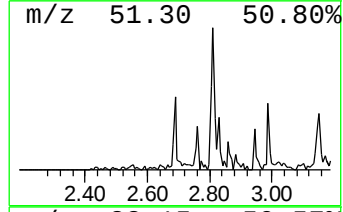
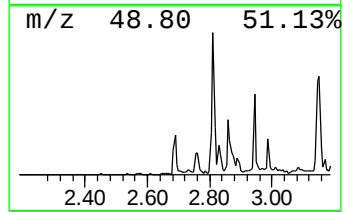
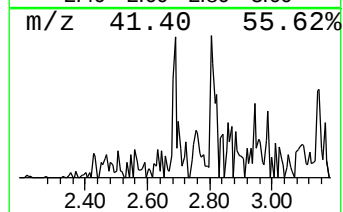
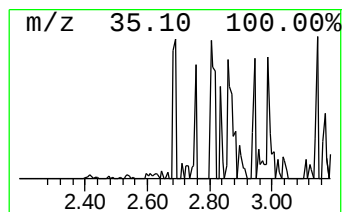
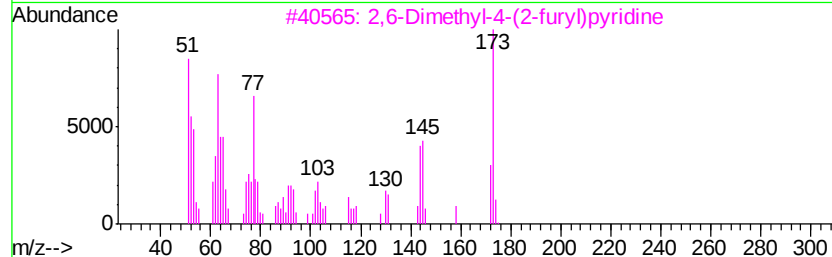
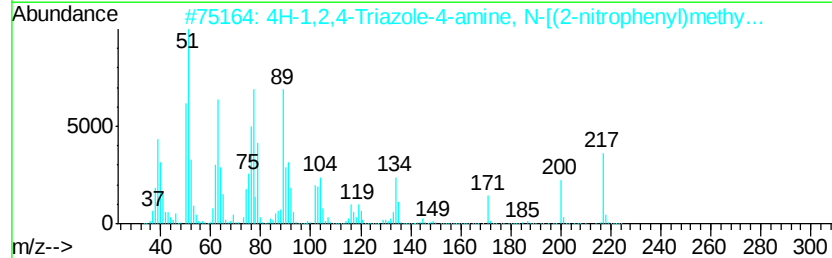
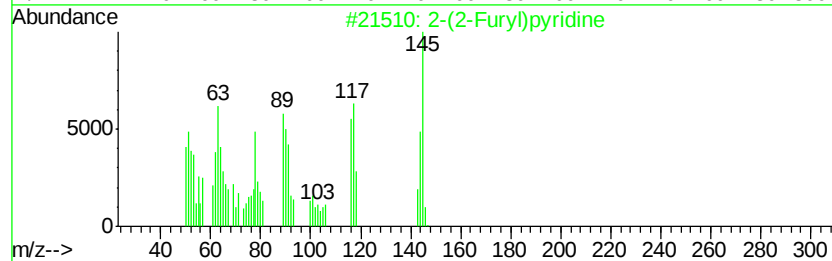
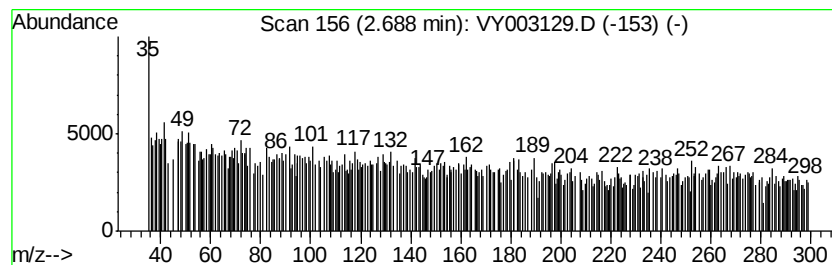
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_Y\METHODS\82Y062920S.M
Quant Title : SW846 8260

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

Peak Number 2 2-(2-Furyl)pyridine Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.69	43.71 ug/l	757356	Pentafluorobenzene	8.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-(2-Furyl)pyridine	145	C9H7NO	055484-03-2	90
2		4H-1,2,4-Triazole-4-amine, N-[(2-...	217	C9H7N5O2	035548-91-5	58
3		2,6-Dimethyl-4-(2-furyl)pyridine	173	C11H11NO	078563-66-3	55
4		(2,2-Dichlorovinyl)dimethylchlor...	188	C4H7Cl3Si	091455-15-1	48
5		Phenol, 4-nitro-2-(1,2,4-triazol...	233	C9H7N5O3	202118-42-1	45



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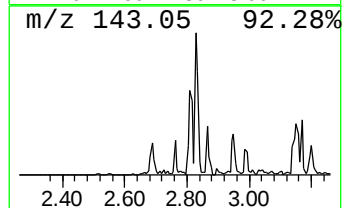
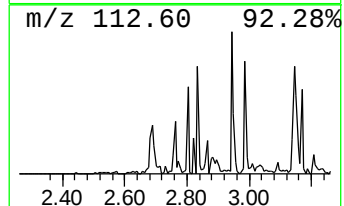
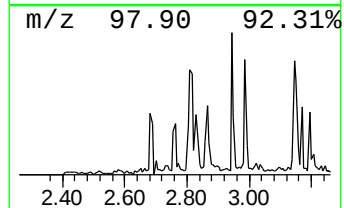
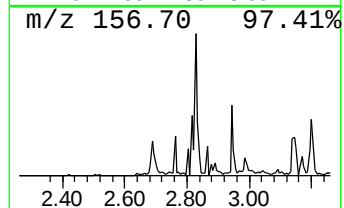
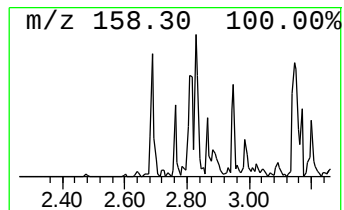
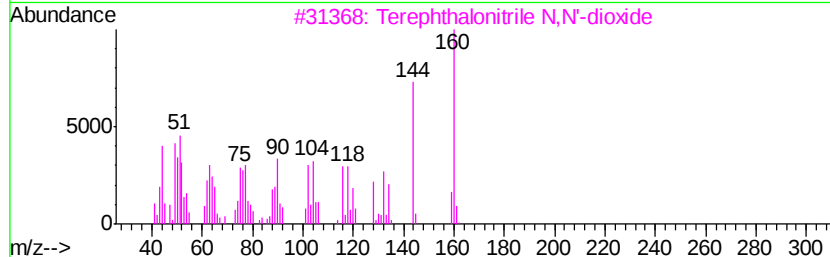
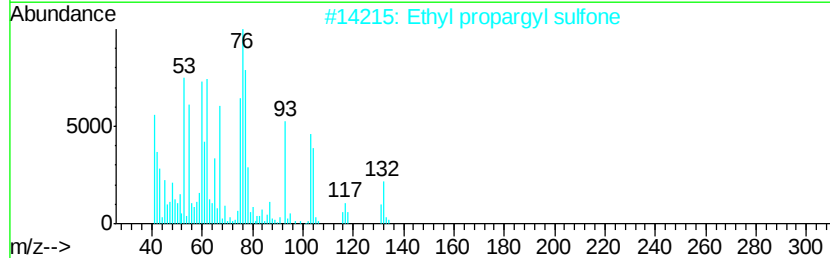
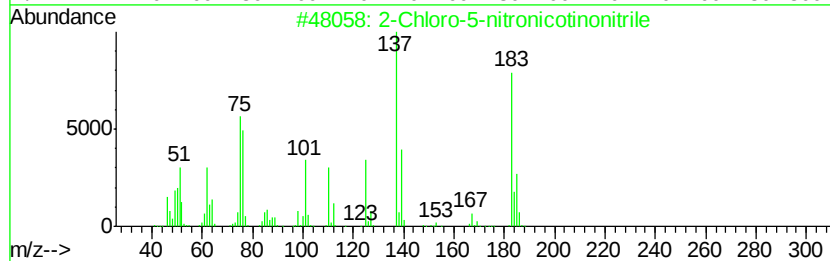
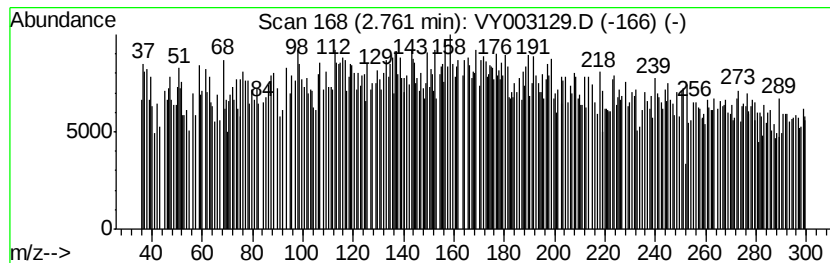
Instrument :
MSVOA_Y
ClientSampleId :
E3-41-VAT

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_Y\METHODS\82Y062920S.M
Quant Title : SW846 8260

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

Peak Number 3 2-Chloro-5-nitronicotinonit... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.		
2.76	24.94 ug/l	432070	Pentafluorobenzene	8.28		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Chloro-5-nitronicotinonitrile	183	C6H2ClN3O2	031309-08-7	64
2		Ethyl propargyl sulfone	132	C5H8O2S	013603-87-7	58
3		Terephthalonitrile N,N'-dioxide	160	C8H4N2O2	003729-34-8	55
4		Benzenecarboximidoyl chloride, N...	185	C8H8ClNO2	1000362-64-9	46
5		4-Methyl-6-phenyl-3-thioxo-3,4-d...	219	C10H9N3OS	022936-87-4	44



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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
E3-41-VAT

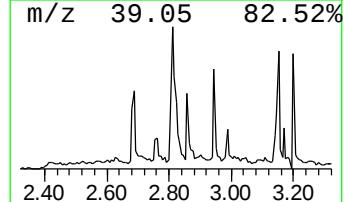
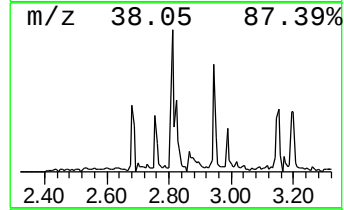
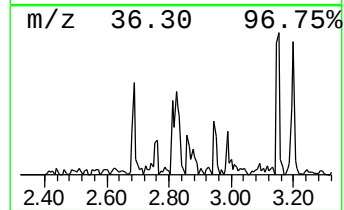
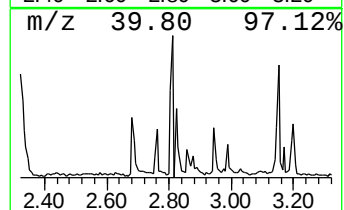
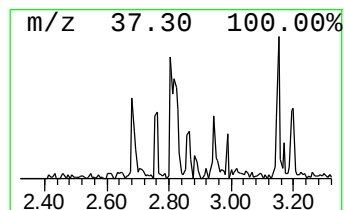
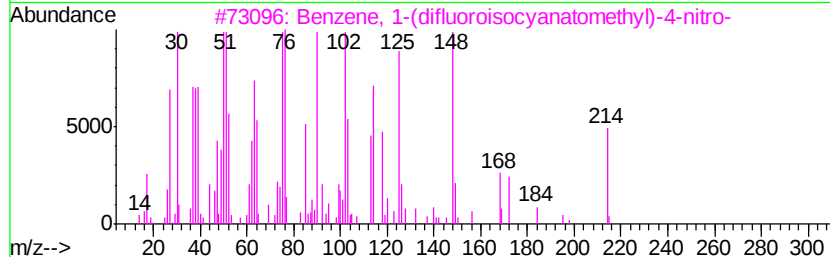
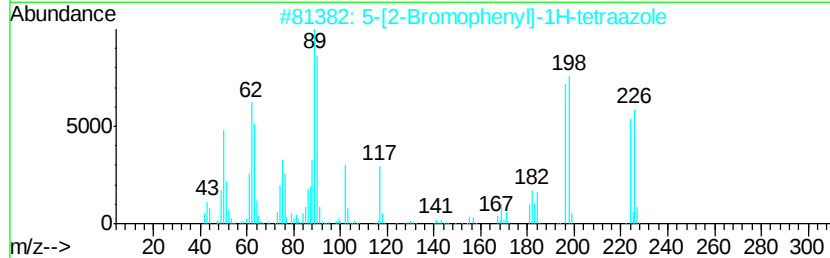
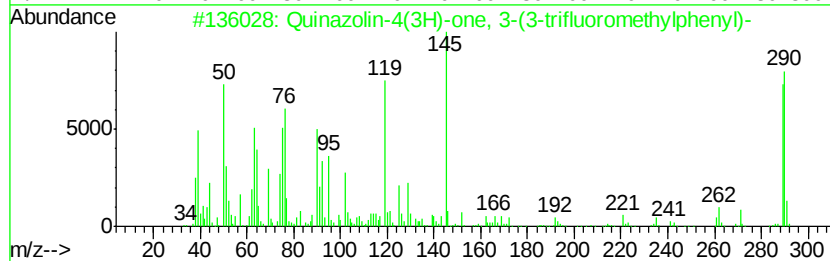
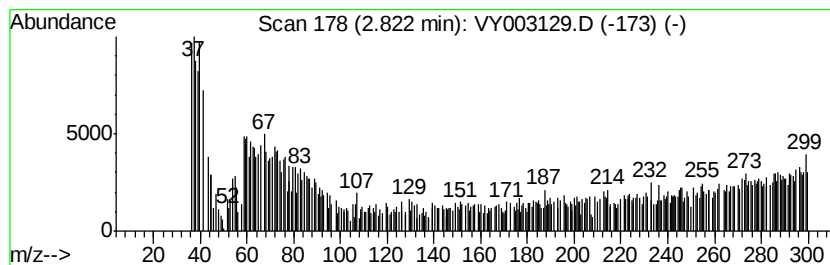
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown2.82 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.82	90.47 ug/l	1567330	Pentafluorobenzene	8.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Quinazolin-4(3H)-one, 3-(3-trifl...	290	C15H9F3N2O	024122-28-9	44
2		5-[2-Bromophenyl]-1H-tetraazole	224	C7H5BrN4	073096-42-1	41
3		Benzene, 1-(difluoroisocyanatome...	214	C8H4F2N2O3	055669-96-0	38
4		1H-1,2,3-Triazol-1-amine, 4-(4-m...	278	C16H14N4O	113261-44-2	30
5		Spiro[benzofuran-2(3H),2'-oxiran...	298	C17H14O5	035405-27-7	30



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Misc : 5.09G/5ML/MSVOA Y/SOIL
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
E3-41-VAT

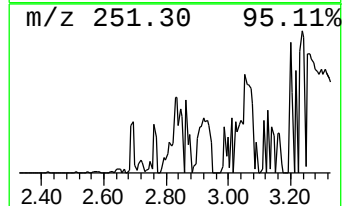
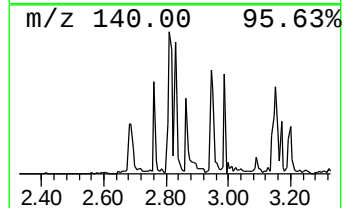
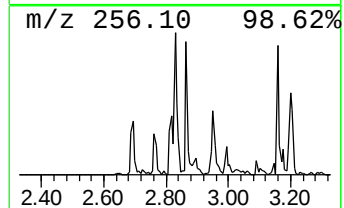
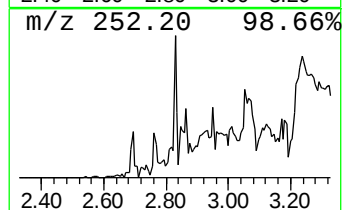
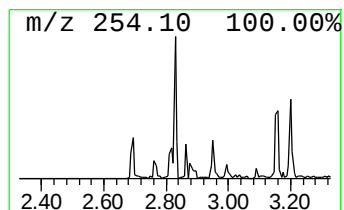
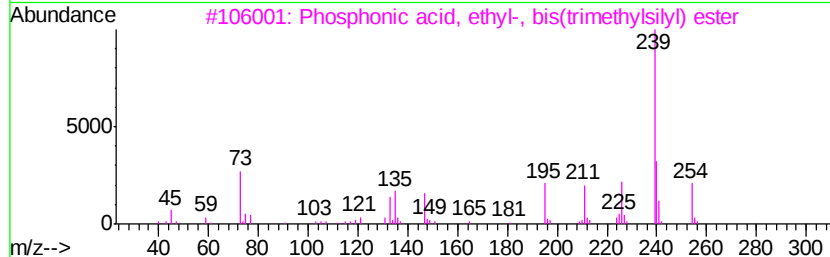
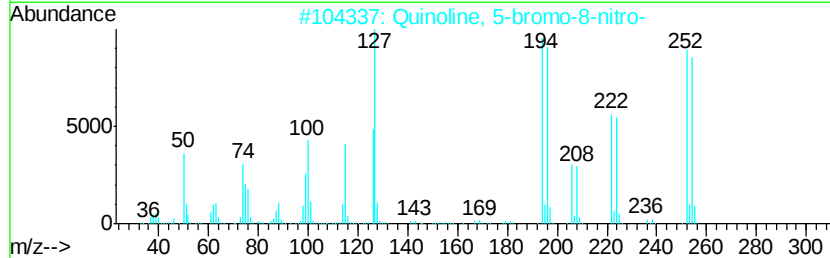
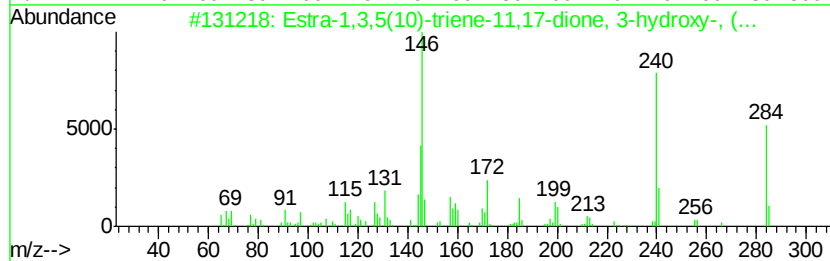
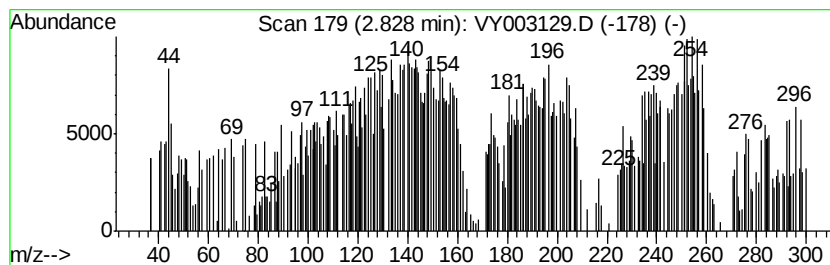
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown2.83 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.83	56.52 ug/l	979164	Pentafluorobenzene	8.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Estra-1,3,5(10)-triene-11,17-dio...	284	C18H20O3	017391-44-5	25
2		Quinoline, 5-bromo-8-nitro-	252	C9H5BrN2O2	176967-80-9	15
3		Phosphonic acid, ethyl-, bis(tri...	254	C8H23O3PSi2	001641-57-2	11
4		4-Isopropyl-9-chloro-acridine	255	C16H14ClN	055751-63-8	11
5		4-Oxy-5-phenyl-1,3-dihydro-benzo...	252	C15H12N2O2	003967-09-7	11



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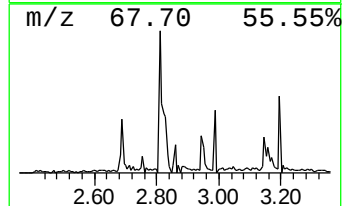
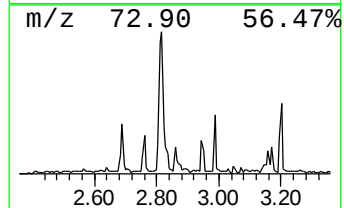
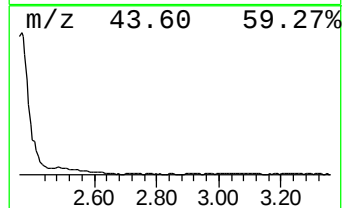
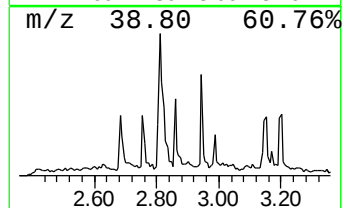
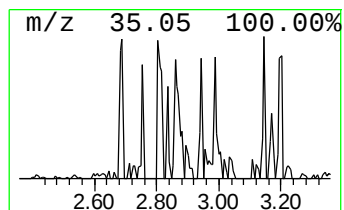
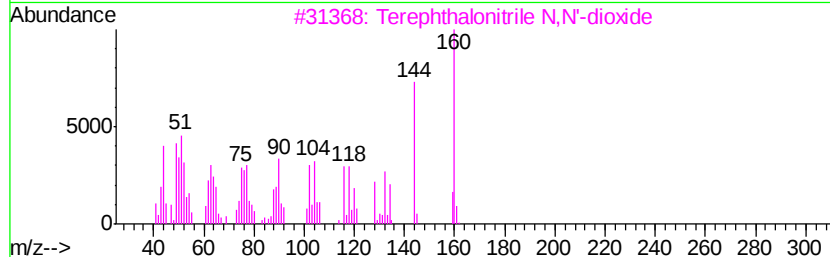
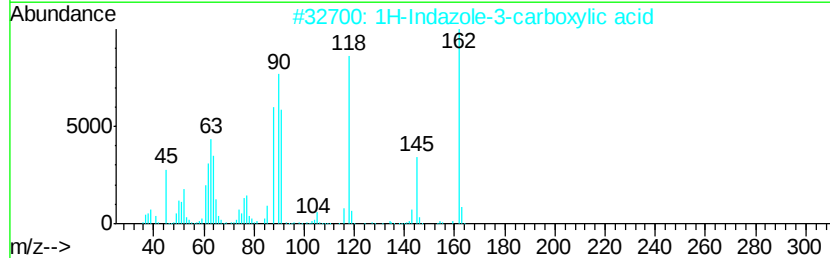
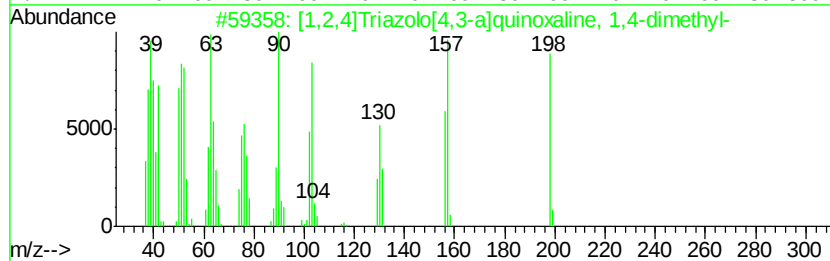
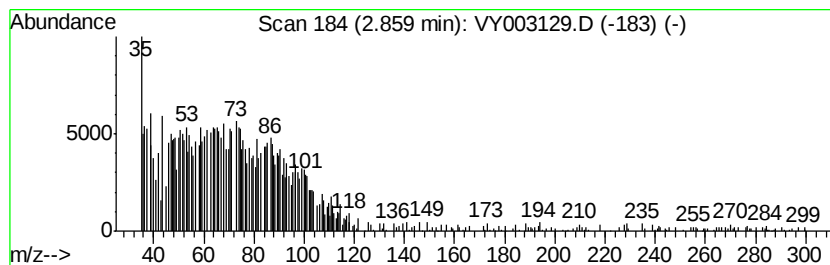
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown2.86 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.86	42.23 ug/l	731600	Pentafluorobenzene	8.28

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		[1,2,4]Triazolo[4,3-a]quinoxalin...	198	C11H10N4	1000362-67-9	48
2		1H-Indazole-3-carboxylic acid	162	C8H6N2O2	004498-67-3	47
3		Terephthalonitrile N,N'-dioxide	160	C8H4N2O2	003729-34-8	46
4		Quinazolin-4(3H)-one, 3-methyl-2...	263	C16H13N3O	337351-99-2	44
5		Quinazolin-4(3H)-one, 2-[2-(hydr...	278	C17H14N2O2	050830-07-4	42



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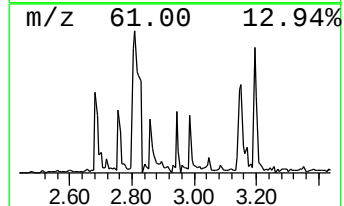
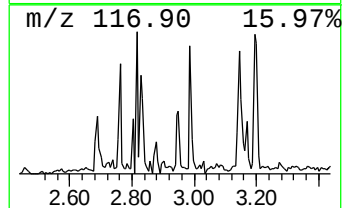
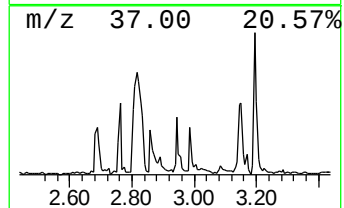
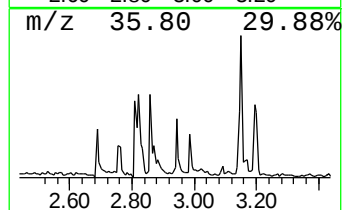
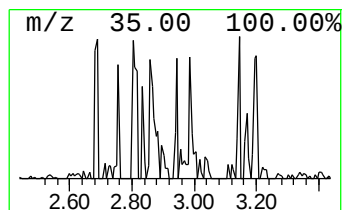
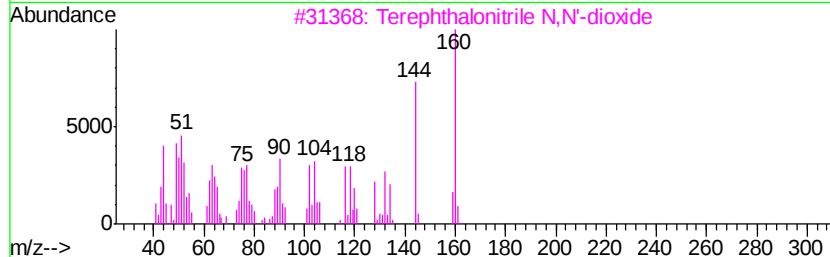
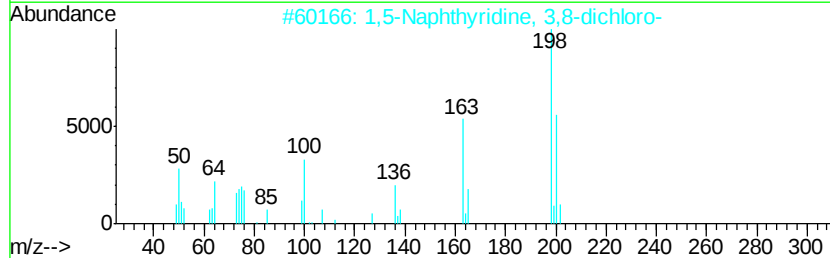
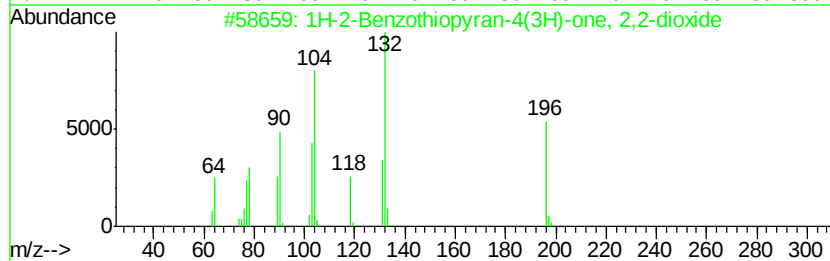
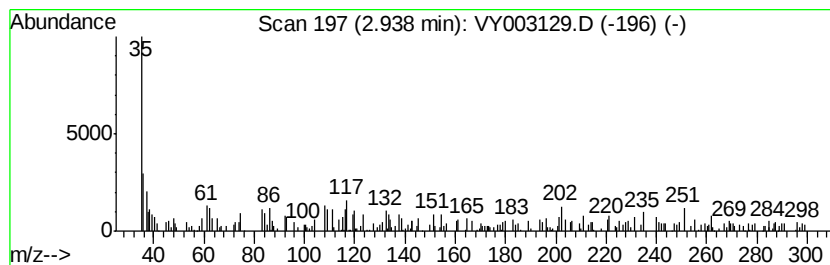
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Quant Title : SW846 8260

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

Peak Number 7 unknown2.94 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.94	40.24 ug/l	697245	Pentafluorobenzene	8.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-2-Benzothiopyran-4(3H)-one, 2...	196	C9H8O3S	016723-58-3	38
2		1,5-Naphthyridine, 3,8-dichloro-	198	C8H4Cl2N2	028252-81-5	35
3		Terephthalonitrile N,N'-dioxide	160	C8H4N2O2	003729-34-8	30
4		3H-Imidazo(4,5-f)quinoline, 2-am...	198	C11H10N4	076180-96-6	25
5		4-Chloropyridine-3-sulfonic acid	193	C5H4ClNO3S	1000306-80-4	25



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA Y\DATA\VY070720\
Data File : VY003129.D
Acq On : 07 Jul 2020 16:14
Operator : SY/MD
Sample : L3217-04
Misc : 5.09G/5ML/MSVOA Y/SOIL
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
E3-41-VAT

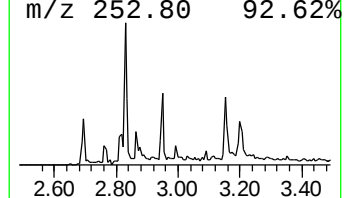
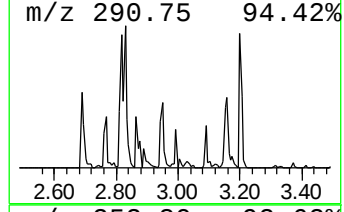
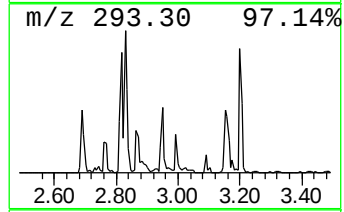
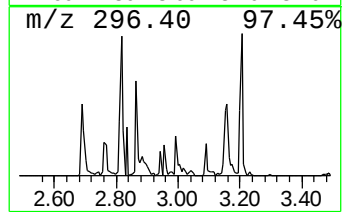
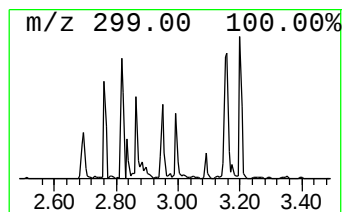
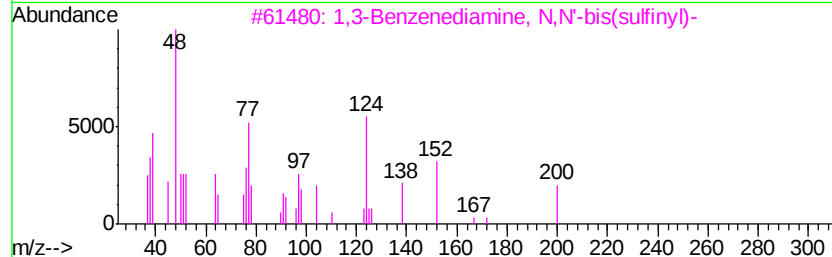
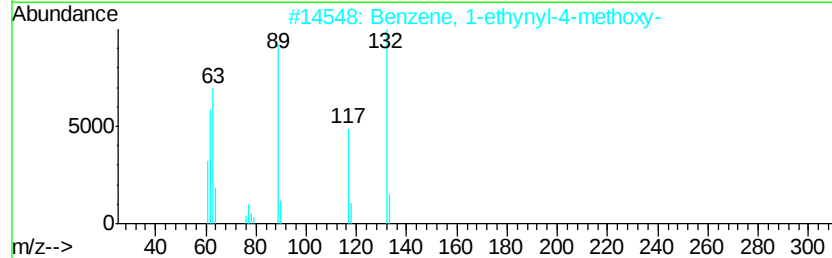
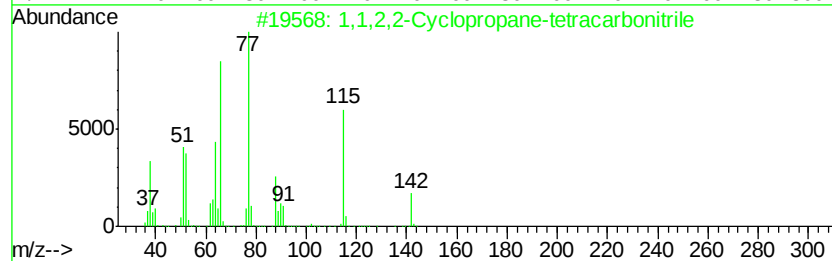
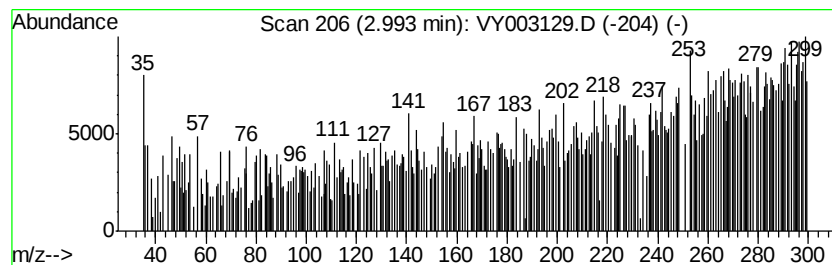
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Quant Title : SW846 8260

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

Peak Number 8 unknown2.99 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	19.28 ug/l	334051	Pentafluorobenzene	8.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,1,2,2-Cyclopropane-tetracarbon...	142	C7H2N4	002424-32-0	38
2		Benzene, 1-ethynyl-4-methoxy-	132	C9H8O	000768-60-5	30
3		1,3-Benzenediamine, N,N'-bis(sul...	200	C6H4N2O2S2	017420-01-8	15
4		3-Amino-4-acetyl-5-methylene-pyr...	152	C7H8N2O2	092220-23-0	15
5		Bicyclo[4.1.0]heptan-2-one, 1-me...	124	C8H12O	014845-40-0	15



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA Y\DATA\VY070720\
Data File : VY003129.D
Acq On : 07 Jul 2020 16:14
Operator : SY/MD
Sample : L3217-04
Misc : 5.09G/5ML/MSVOA Y/SOIL
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampled :
E3-41-VAT

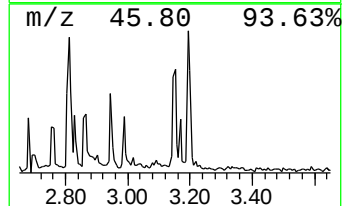
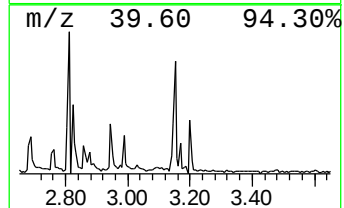
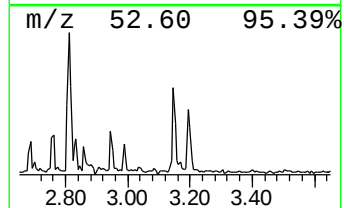
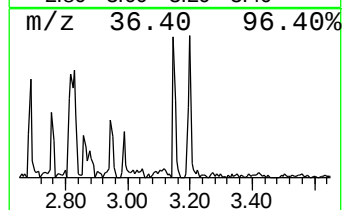
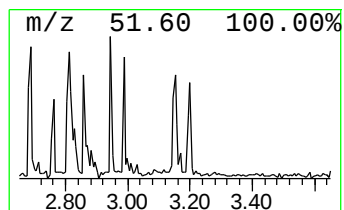
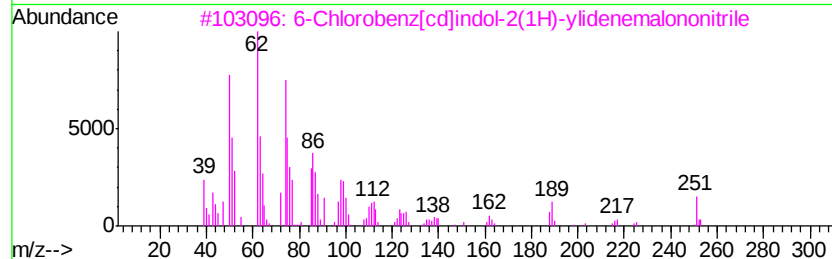
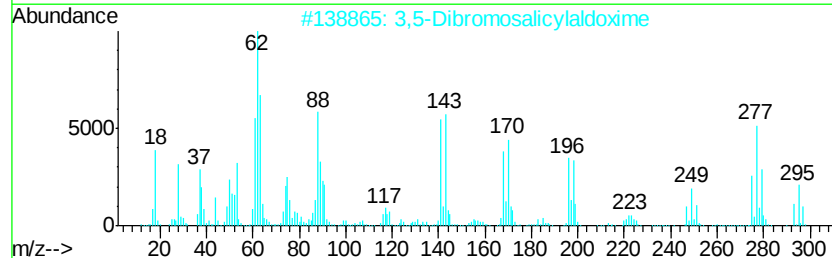
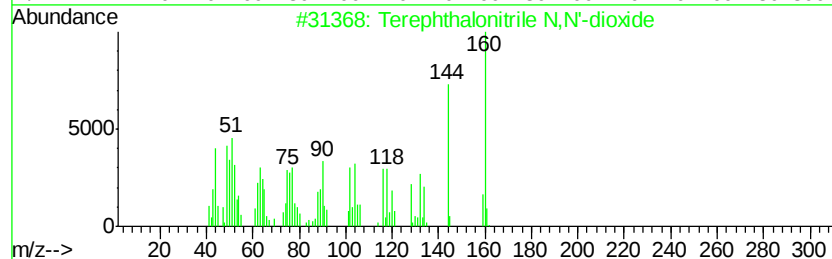
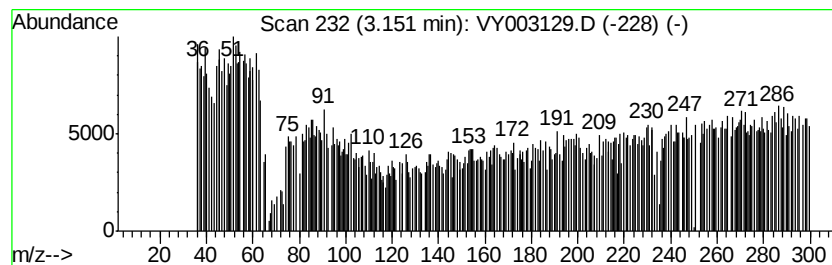
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Quant Title : SW846 8260

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

Peak Number 9 Terephthalonitrile N,N'-dio... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.15	60.66 ug/l	1051010	Pentafluorobenzene	8.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Terephthalonitrile N,N'-dioxide	160	C8H4N2O2	003729-34-8	91
2		3,5-Dibromosalicylaldehyde	293	C7H5Br2NO2	021386-43-6	47
3		6-Chlorobenz[cd]indol-2(1H)-ylid...	251	C14H6ClN3	331464-93-8	45
4		5-Bromo-7-methylisatin	239	C9H6BrNO2	077395-10-9	42
5		2,6-Dinitro-1-methoxy-benzene	198	C7H6N2O5	003535-67-9	41



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA Y\DATA\VY070720\
Data File : VY003129.D
Acq On : 07 Jul 2020 16:14
Operator : SY/MD
Sample : L3217-04
Misc : 5.09G/5ML/MSVOA Y/SOIL
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
E3-41-VAT

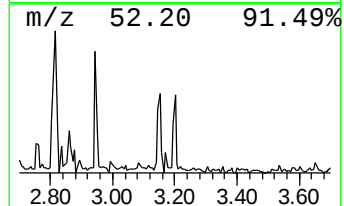
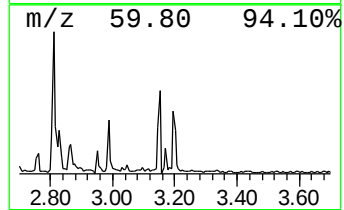
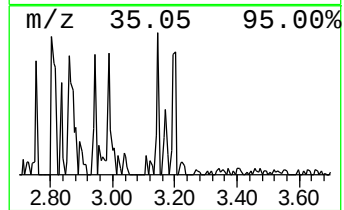
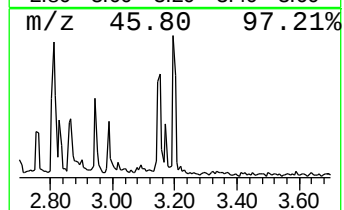
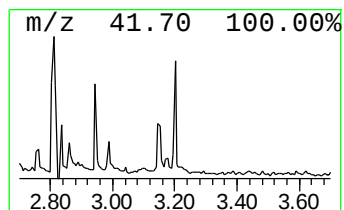
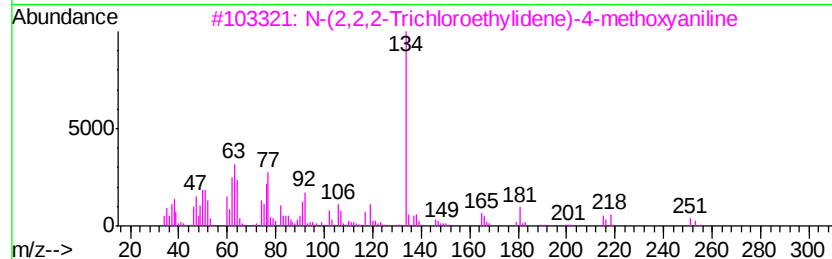
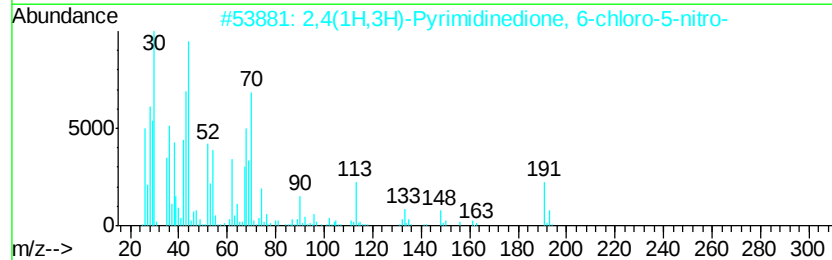
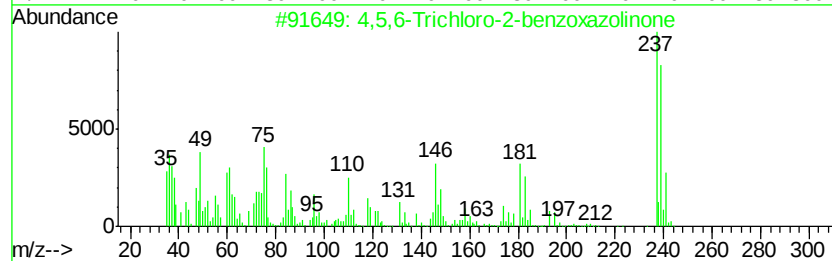
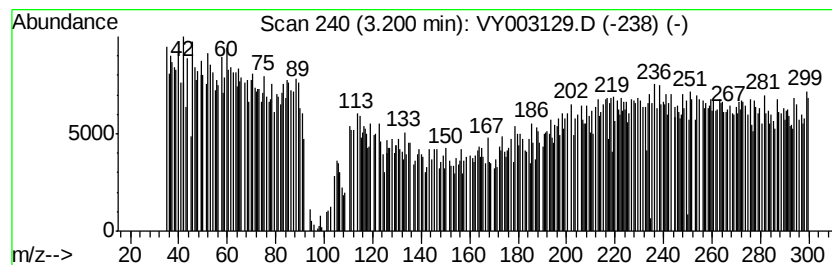
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_Y\METHODS\82Y062920S.M
Quant Title : SW846 8260

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

Peak Number 10 4,5,6-Trichloro-2-benzoxazo... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.20	47.37 ug/l	820660	Pentafluorobenzene	8.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4,5,6-Trichloro-2-benzoxazolinone	237	C7H2Cl3NO2	050995-94-3	84
2		2,4(1H,3H)-Pyrimidinedione, 6-ch...	191	C4H2ClN3O4	006630-30-4	47
3		N-(2,2,2-Trichloroethylidene)-4-...	251	C9H8Cl3NO	083320-59-6	45
4		4-Chloropyridine-3-sulfonic acid	193	C5H4ClN03S	1000306-80-4	44
5		1,3-Benzenediamine, N,N'-bis(sul...	200	C6H4N2O2S2	017420-01-8	41



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_Y\DATA\VY070720\
Data File : VY003129.D
Acq On : 07 Jul 2020 16:14
Operator : SY/MD
Sample : L3217-04
Misc : 5.09G/5ML/MSVOA_Y/SOIL
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
E3-41-VAT

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_Y\METHODS\82Y062920S.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-(2-Furyl)pyridine	2.69	43.7	ug/l	757356	1	8.28	866260	50.0
2-Chloro-5-nitron...	2.76	24.9	ug/l	432070	1	8.28	866260	50.0
unknown2.82	2.82	90.5	ug/l	1567330	1	8.28	866260	50.0
unknown2.83	2.83	56.5	ug/l	979164	1	8.28	866260	50.0
unknown2.86	2.86	42.2	ug/l	731600	1	8.28	866260	50.0
unknown2.94	2.94	40.2	ug/l	697245	1	8.28	866260	50.0
unknown2.99	2.99	19.3	ug/l	334051	1	8.28	866260	50.0
Terephthalonitril...	3.15	60.7	ug/l	1051010	1	8.28	866260	50.0
4,5,6-Trichloro-2...	3.20	47.4	ug/l	820660	1	8.28	866260	50.0