

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY031722\
 Data File : VY007888.D
 Acq On : 17 Mar 2022 20:36
 Operator : SY/MD
 Sample : N1875-11
 Misc : 1.30g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 SB-10C

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\82Y031722S.M

Title : SW846 8260

Signal : TIC: VY007888.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.058	36	39	41	rBV4	1700	2097	1.28%	0.449%
2	2.131	44	51	52	rBV5	7317	13463	8.24%	2.880%
3	2.442	99	102	104	rBV4	1398	1787	1.09%	0.382%
4	2.503	109	112	116	rBV5	4391	5366	3.28%	1.148%
5	2.662	135	138	142	rVB4	2233	2880	1.76%	0.616%
6	2.906	174	178	179	rBV4	1497	1706	1.04%	0.365%
7	3.265	234	237	240	rVB5	1182	1683	1.03%	0.360%
8	3.649	295	300	302	rVB5	1278	1912	1.17%	0.409%
9	3.820	323	328	330	rVB6	1290	2255	1.38%	0.482%
10	3.948	344	349	353	rVB7	1458	2899	1.77%	0.620%
11	4.302	404	407	410	rBV4	1986	2230	1.36%	0.477%
12	4.491	434	438	441	rBV6	1467	2133	1.31%	0.456%
13	5.911	668	671	674	rBV5	1581	2359	1.44%	0.505%
14	7.710	960	966	972	rVV5	5713	15651	9.58%	3.347%
15	7.789	973	979	986	rVV2	10592	24287	14.86%	5.195%
16	8.136	1030	1036	1043	rVB2	7940	18243	11.16%	3.902%
17	8.685	1119	1126	1133	rBV	15759	33733	20.64%	7.215%
18	9.728	1293	1297	1299	rVB4	1335	1872	1.15%	0.400%
19	9.764	1299	1303	1304	rBV3	1300	1692	1.04%	0.362%
20	10.106	1355	1359	1363	rVB6	1345	2214	1.35%	0.474%
21	10.179	1365	1371	1380	rVB	24514	44589	27.29%	9.537%
22	10.465	1415	1418	1421	rVV5	1478	1860	1.14%	0.398%
23	10.581	1430	1437	1445	rBV3	6900	14127	8.65%	3.022%
24	10.679	1450	1453	1456	rBV5	1662	2207	1.35%	0.472%
25	11.489	1579	1586	1593	rBV	23860	39939	24.44%	8.542%
26	12.026	1672	1674	1679	rVB5	1437	2021	1.24%	0.432%
27	12.489	1742	1750	1758	rBV2	91799	163412	100.00%	34.951%
28	12.672	1777	1780	1785	rVB6	1429	2549	1.56%	0.545%
29	12.855	1805	1810	1812	rVB6	1341	1811	1.11%	0.387%
30	12.965	1826	1828	1833	rVB5	1341	2080	1.27%	0.445%
31	13.422	1899	1903	1911	rVV2	14048	24269	14.85%	5.191%
32	13.574	1926	1928	1932	rBV5	1387	2006	1.23%	0.429%
33	13.965	1985	1992	1996	rVV3	9258	16134	9.87%	3.451%
34	14.135	2016	2020	2024	rVB6	1185	1674	1.02%	0.358%
35	14.379	2056	2060	2062	rVV4	1333	1755	1.07%	0.375%
36	14.489	2076	2078	2081	rVV4	1743	2523	1.54%	0.540%

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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\82Y031722S.M
Title : SW846 8260

37	14.660	2103	2106	2109	rVV5	1411	1888	1.16%	0.404%
38	16.586	2418	2422	2423	rBV3	1335	2238	1.37%	0.479%

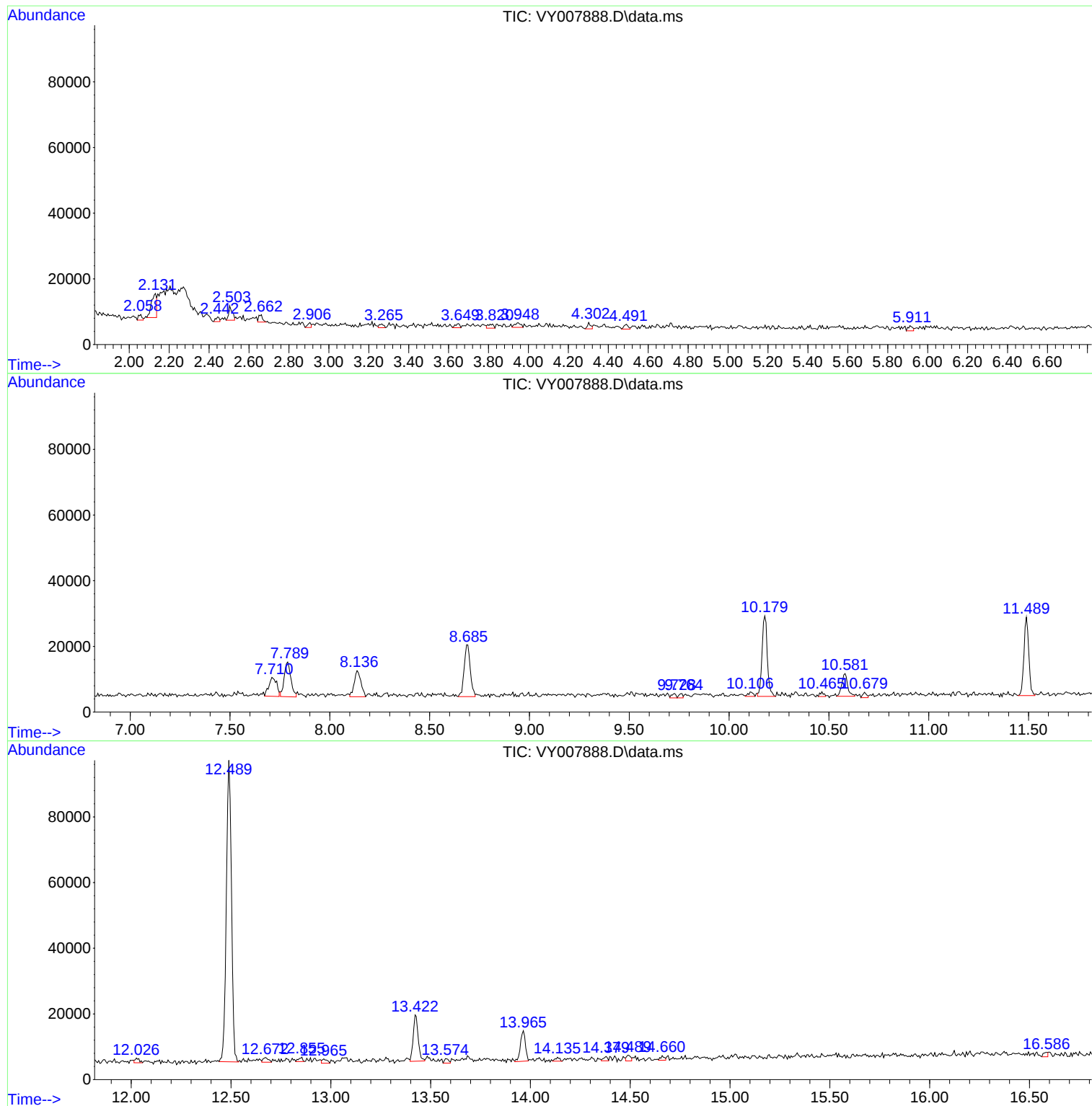
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y031722S.M
Quant Title : SW846 8260

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



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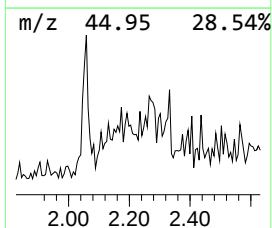
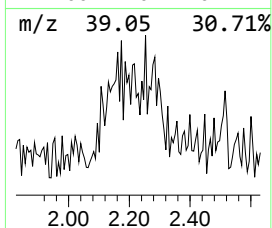
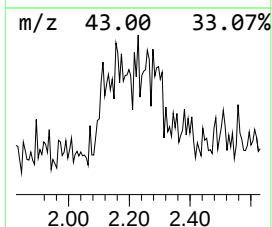
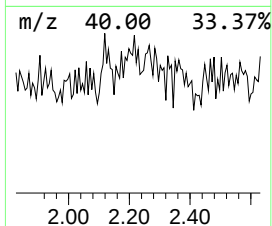
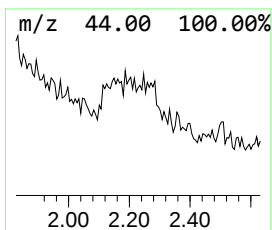
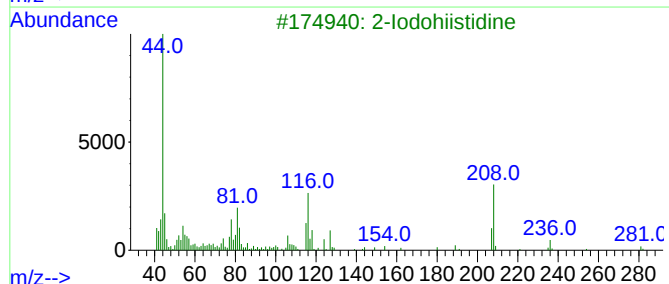
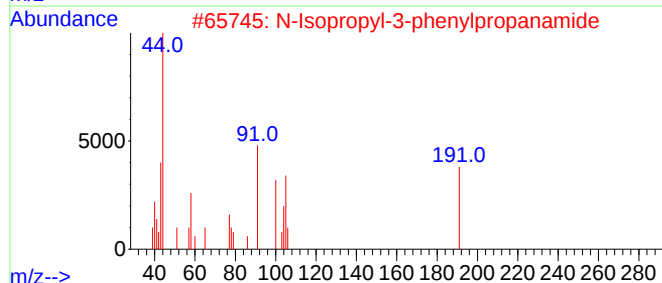
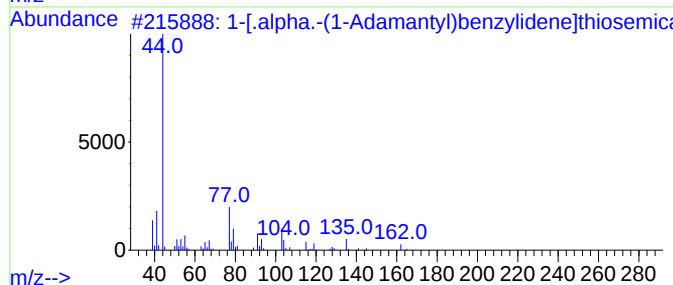
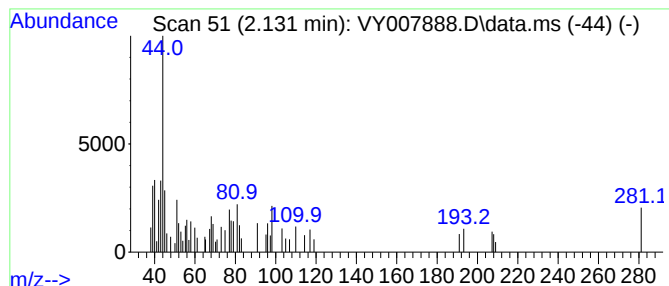
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y031722S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.131	27.72 ug/l	13463	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1		[.alpha.-(1-Adamantyl)benzylidene]thiosemicarbazide	313	C18H23N3S	1000222-83-3	35
2			N-Isopropyl-3-phenylpropanamide	191	C12H17NO	056146-87-3	35
3			2-Iodothiostidine	281	C6H8IN3O2	006996-15-2	28
4			4,6-dimethyl-2-propyl-1,3,5-dithiazine	191	C8H17NS2	1000365-92-6	25
5			(-)-Norephedrine	151	C9H13NO	000492-41-1	25



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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-10C

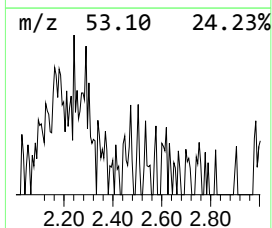
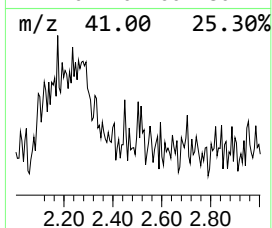
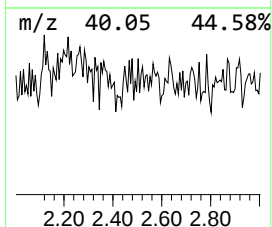
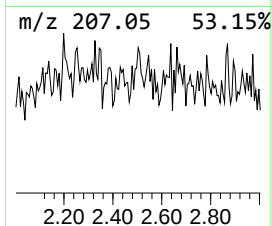
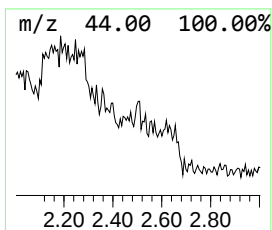
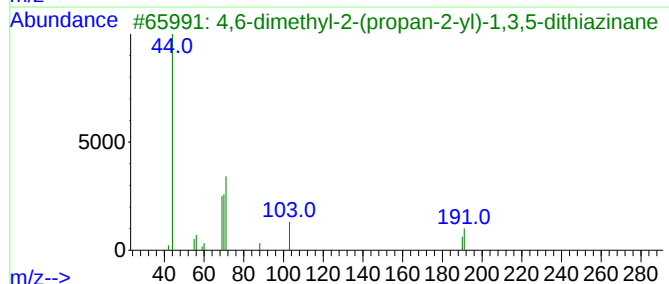
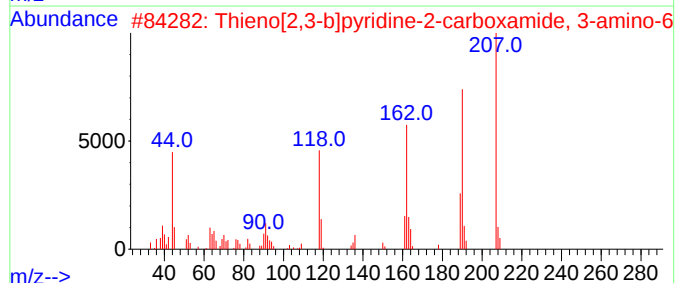
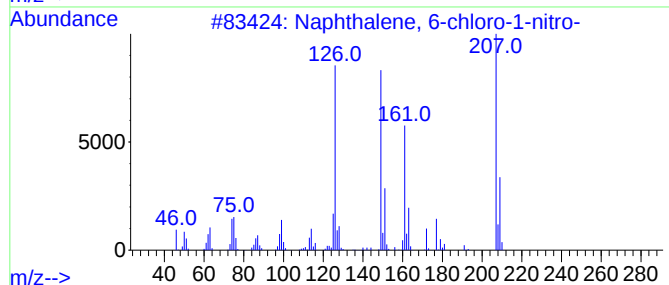
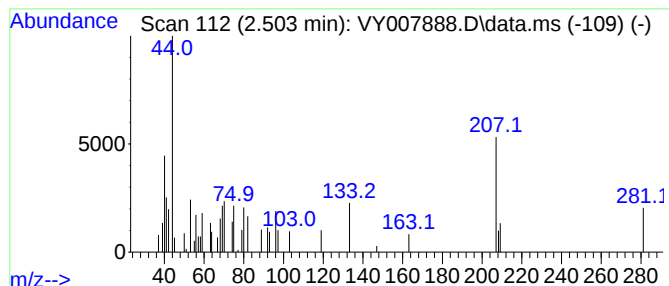
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y031722S.M
Quant Title : SW846 8260

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

Peak Number 2 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.503	11.05 ug/l	5366	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 6-chloro-1-nitro-	207	C10H6ClNO2	038396-29-1	16
2			Thieno[2,3-b]pyridine-2-carboxam...	207	C9H9N3OS	1000351-59-9	12
3			4,6-dimethyl-2-(propan-2-yl)-1,3...	191	C8H17NS2	104691-40-9	12
4			Corydaldine	207	C11H13NO3	000493-49-2	11
5			Cyclopropyl carbinol	72	C4H8O	002516-33-8	10



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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-10C

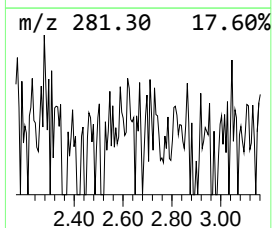
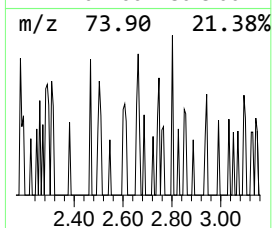
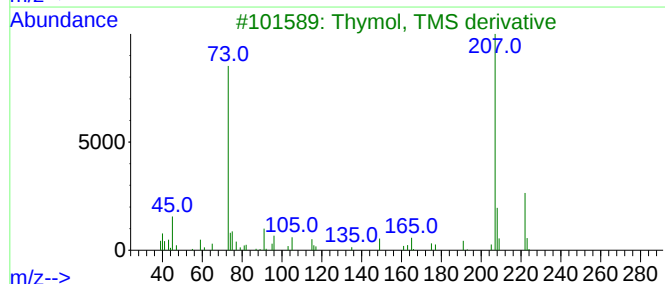
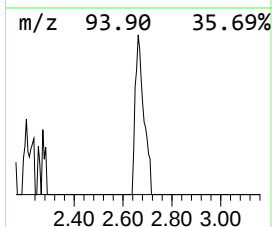
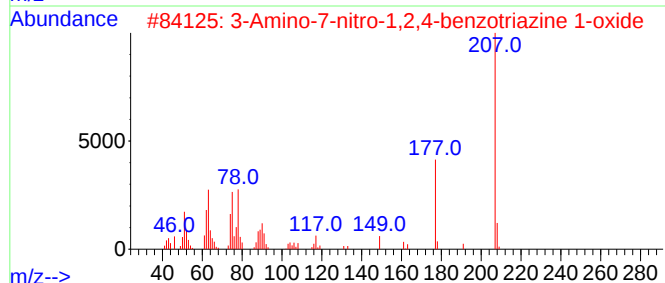
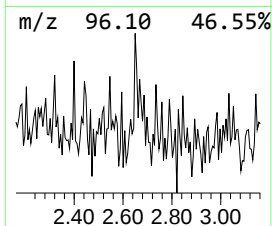
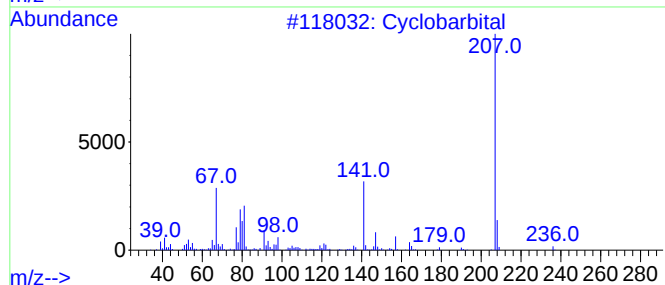
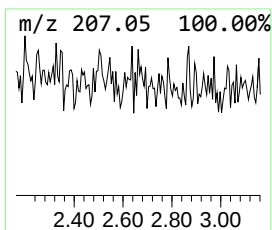
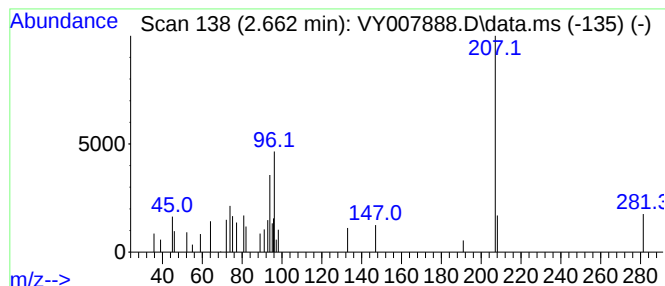
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y031722S.M
Quant Title : SW846 8260

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

Peak Number 3 unknown-03 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.662	5.93 ug/l	2880	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclobarbitol	236	C12H16N2O3	000052-31-3	38
2			3-Amino-7-nitro-1,2,4-benzotriaz...	207	C7H5N5O3	1010256-54-1	35
3			Thymol, TMS derivative	222	C13H22OSi	055012-80-1	35
4			1,2,5-Oxadiazol-3-amine, 4-(4-me...	207	C9H9N3O3	1000351-72-7	35
5			(E)-3-(3,4-Dimethoxyphenyl)prop...	207	C11H13NO3	130973-10-3	32



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Instrument :
MSVOA_Y
ClientSampleId :
SB-10C

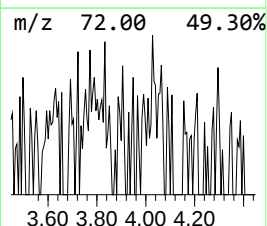
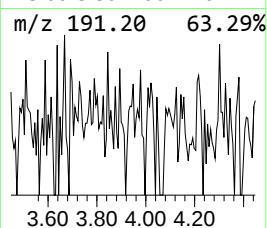
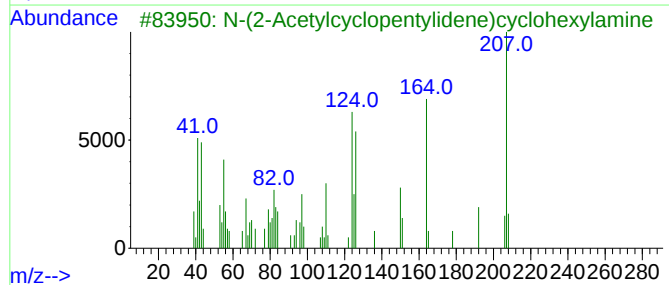
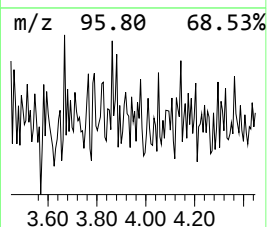
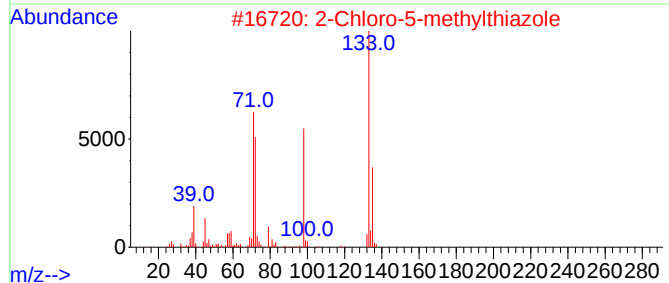
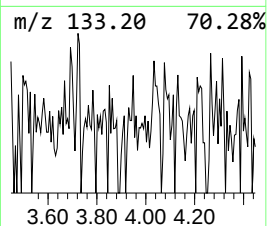
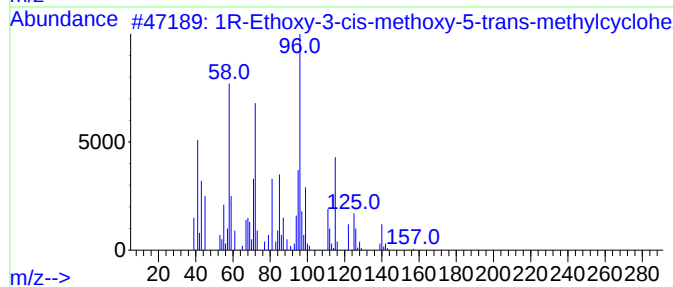
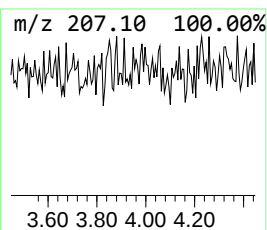
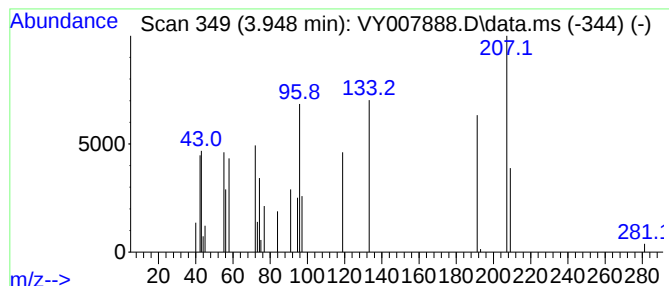
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y031722S.M
Quant Title : SW846 8260

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

Peak Number 4 unknown-04 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.948	5.97 ug/l	2899	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1R-Ethoxy-3-cis-methoxy-5-trans-...	172	C10H20O2	059013-93-3	12
2			2-Chloro-5-methylthiazole	133	C4H4ClNS	033342-65-3	9
3			N-(2-Acetylcyclopentylidene)cycl...	207	C13H21NO	1000100-48-5	9
4			4H-1,2,4-triazole-3,5-diamine, N...	207	C9H10FN5	1000396-10-8	9
5			3-Methylindole-2-carboxylic acid...	207	C12H17NO2	037945-37-2	9



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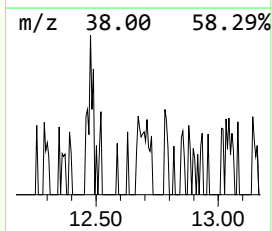
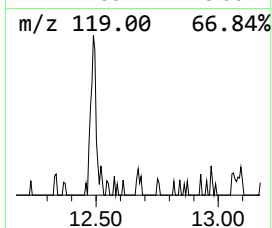
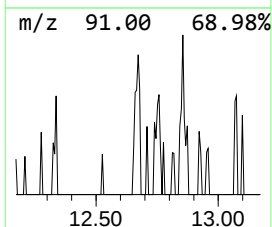
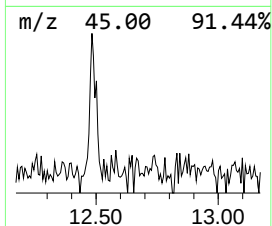
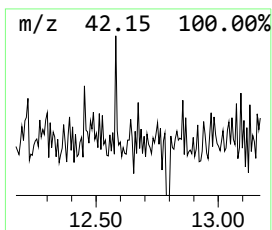
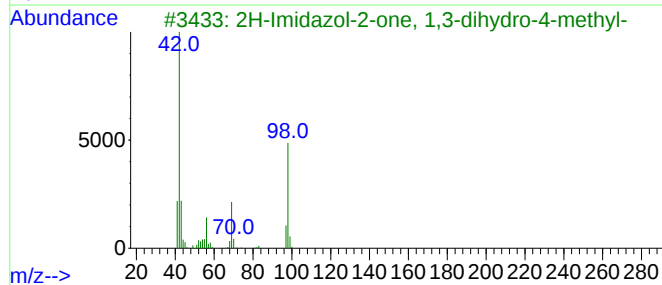
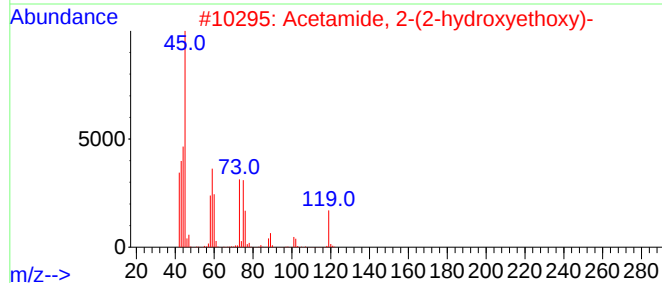
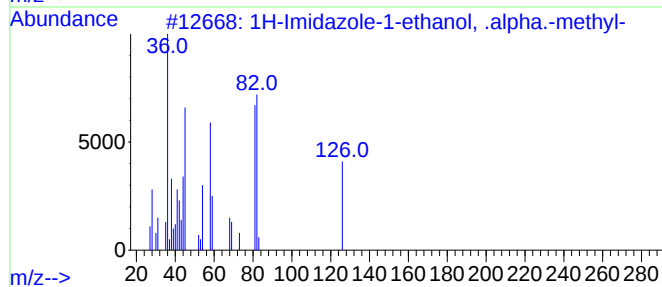
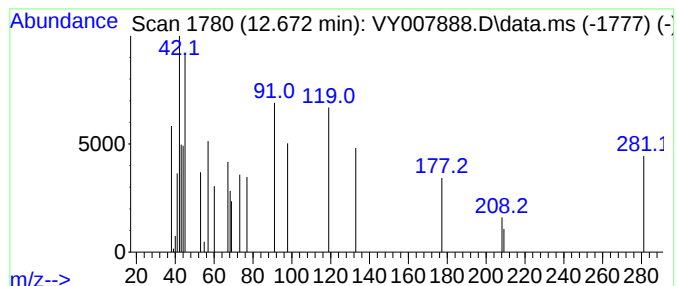
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y031722S.M
Quant Title : SW846 8260

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

Peak Number 6 unknown-05 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.672	5.25 ug/l	2549	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Imidazole-1-ethanol, .alpha.-...	126	C6H10N2O	037788-55-9	32
2			Acetamide, 2-(2-hydroxyethoxy)-	119	C4H9NO3	000123-85-3	17
3			2H-Imidazol-2-one, 1,3-dihydro-4...	98	C4H6N2O	001192-34-3	10
4			Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	9
5			(2Z)-3-Amino-3-[(2-hydroxyethyl)...	208	C8H8N4O5	1000327-07-8	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY031722\
Data File : VY007888.D
Acq On : 17 Mar 2022 20:36
Operator : SY/MD
Sample : N1875-11
Misc : 1.30g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-10C

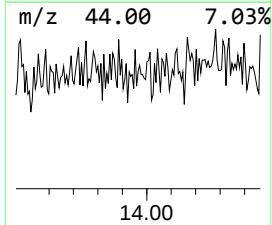
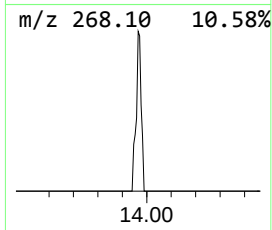
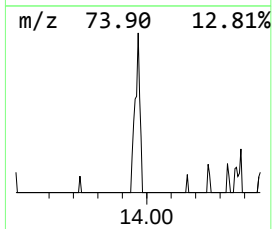
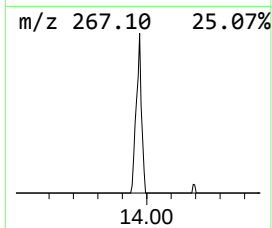
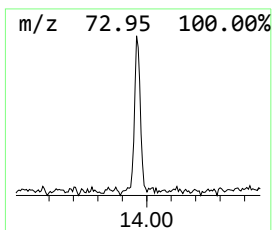
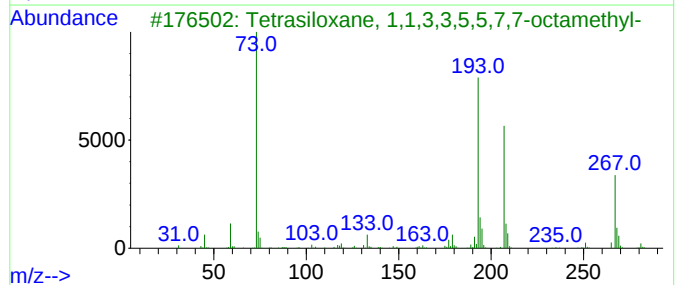
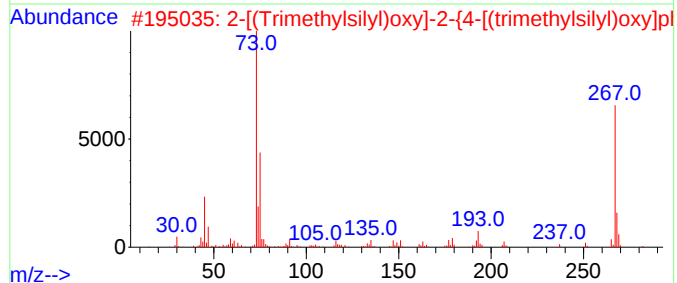
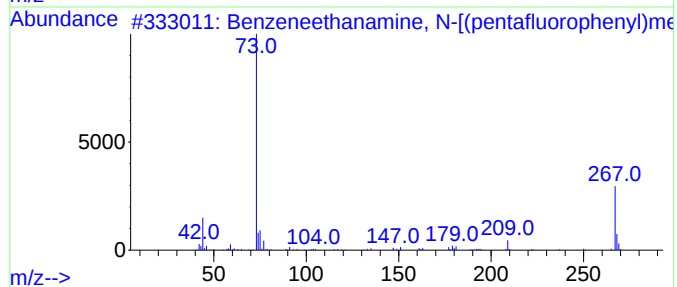
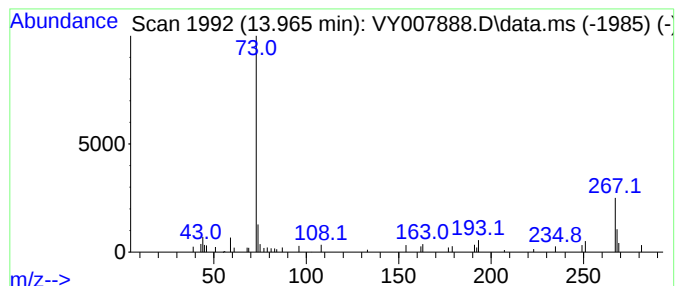
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Quant Title : SW846 8260

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

Peak Number 7 unknown-06 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.965	33.24 ug/l	16134	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzeneethanamine, N-[(pentafluoro...]	475	C21H26F5NO2Si2	055429-85-1	42
2			2-[(Trimethylsilyl)oxy]-2-{4-[(t...]	297	C14H27NO2Si2	1000473-27-9	39
3			Tetrasiloxane, 1,1,3,3,5,5,7,7-o...	282	C8H26O3Si4	001000-05-1	39
4			Salicylic acid, 2TMS derivative	282	C13H22O3Si2	003789-85-3	39
5			4'-hydroxy-[1,1'-biphenyl]-4-car...	267	C16H17NOSi	1000458-49-5	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY031722\
Data File : VY007888.D
Acq On : 17 Mar 2022 20:36
Operator : SY/MD
Sample : N1875-11
Misc : 1.30g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-10C

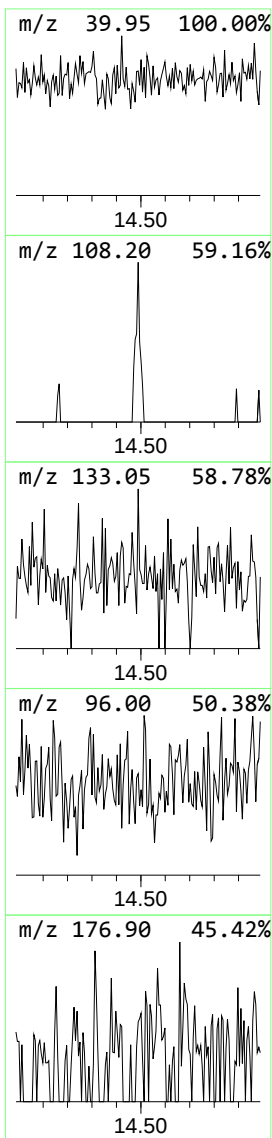
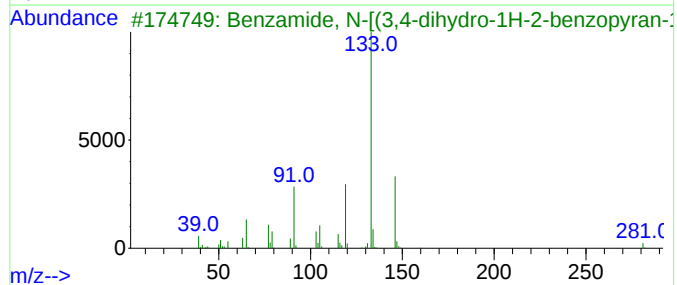
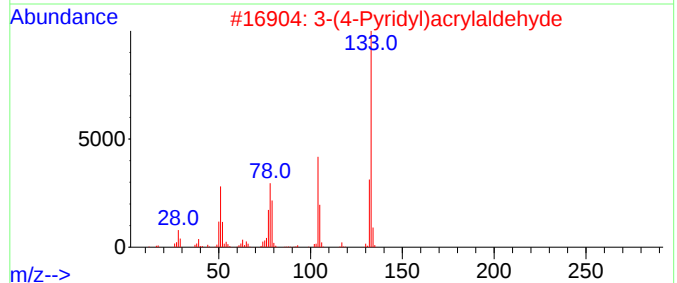
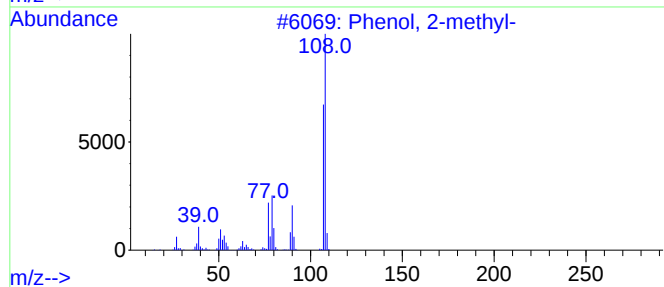
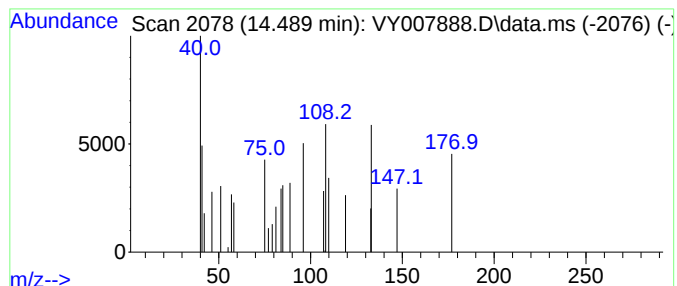
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Quant Title : SW846 8260

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

Peak Number 8 unknown-07 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.489	5.20 ug/l	2523	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-methyl-	108	C7H8O	000095-48-7	10
2			3-(4-Pyridyl)acrylaldehyde	133	C8H7NO	026505-36-2	9
3			Benzamide, N-[(3,4-dihydro-1H-2-...	281	C18H19NO2	1000320-15-7	9
4			Carbamic acid, methyl-, 3-methyl...	165	C9H11NO2	001129-41-5	9
5			4-Ethylbenzoic acid, 6-ethyl-3-o...	290	C19H30O2	1000293-32-3	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY031722\
Data File : VY007888.D
Acq On : 17 Mar 2022 20:36
Operator : SY/MD
Sample : N1875-11
Misc : 1.30g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB-10C

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y031722S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	2.131	27.7	ug/l	13463	1	7.789	24287	50.0
unknown-02	2.503	11.1	ug/l	5366	1	7.789	24287	50.0
unknown-03	2.662	5.9	ug/l	2880	1	7.789	24287	50.0
unknown-04	3.948	6.0	ug/l	2899	1	7.789	24287	50.0
unknown-05	12.672	5.3	ug/l	2549	4	13.428	24269	50.0
unknown-06	13.965	33.2	ug/l	16134	4	13.428	24269	50.0
unknown-07	14.489	5.2	ug/l	2523	4	13.428	24269	50.0