

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY010323\
 Data File : VY012046.D
 Acq On : 03 Jan 2023 14:58
 Operator : KP/MD
 Sample : 01001-01
 Misc : 5.06g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 TP-C2

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\82Y122022S.M
 Title : SW846 8260

Signal : TIC: VY012046.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.984	838	847	855	rBV4	1550	3901	4.29%	1.181%
2	7.795	973	980	982	rBV2	840	1580	1.74%	0.478%
3	8.136	1030	1036	1043	rVB5	759	1636	1.80%	0.495%
4	8.685	1121	1126	1133	rVB2	1283	2269	2.49%	0.687%
5	8.935	1162	1167	1174	rVB5	2168	4082	4.49%	1.236%
6	10.179	1367	1371	1379	rVB2	2979	5712	6.28%	1.729%
7	10.252	1379	1383	1385	rBV3	694	1070	1.18%	0.324%
8	10.892	1486	1488	1492	rBV4	620	983	1.08%	0.298%
9	10.965	1496	1500	1501	rBV4	780	951	1.05%	0.288%
10	11.264	1544	1549	1550	rBV4	1186	1533	1.69%	0.464%
11	11.331	1554	1560	1562	rVV6	1921	4273	4.70%	1.293%
12	11.489	1581	1586	1591	rVB4	2471	4754	5.23%	1.439%
13	11.886	1647	1651	1652	rBV4	954	1354	1.49%	0.410%
14	12.026	1672	1674	1677	rBV4	906	993	1.09%	0.301%
15	12.105	1677	1687	1688	rBV6	6789	16360	17.98%	4.952%
16	12.337	1723	1725	1728	rBV4	1403	1930	2.12%	0.584%
17	12.489	1748	1750	1753	rVB4	2004	1599	1.76%	0.484%
18	12.837	1801	1807	1809	rBV7	2073	3988	4.38%	1.207%
19	13.215	1854	1869	1881	rBV7	15256	90977	100.00%	27.536%
20	13.416	1898	1902	1919	rVB7	20605	74848	82.27%	22.655%
21	13.623	1926	1936	1937	rBV7	13036	27492	30.22%	8.321%
22	13.769	1956	1960	1961	rBV4	7489	9803	10.78%	2.967%
23	15.123	2179	2182	2188	rBV7	3989	7953	8.74%	2.407%
24	15.336	2210	2217	2222	rBV7	5454	15311	16.83%	4.634%
25	15.501	2237	2244	2255	rVB6	11544	38591	42.42%	11.680%
26	16.050	2332	2334	2336	rBV3	1127	1370	1.51%	0.415%
27	16.440	2396	2398	2400	rBV3	887	1006	1.11%	0.304%
28	16.464	2400	2402	2410	rVB9	2175	4070	4.47%	1.232%

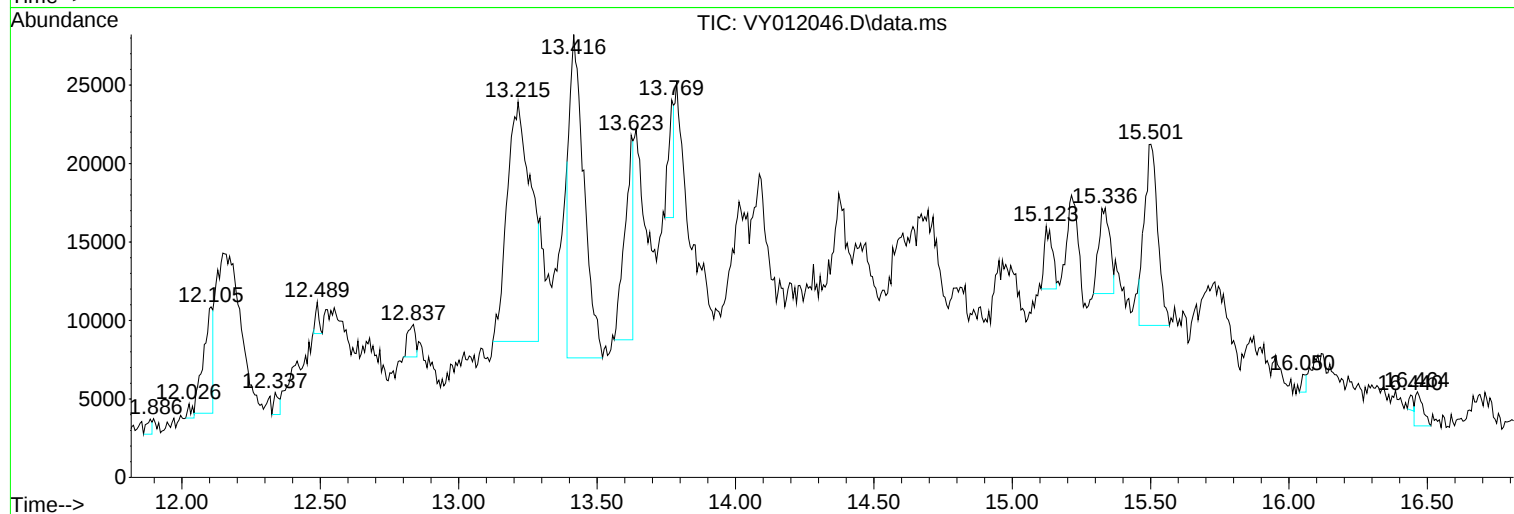
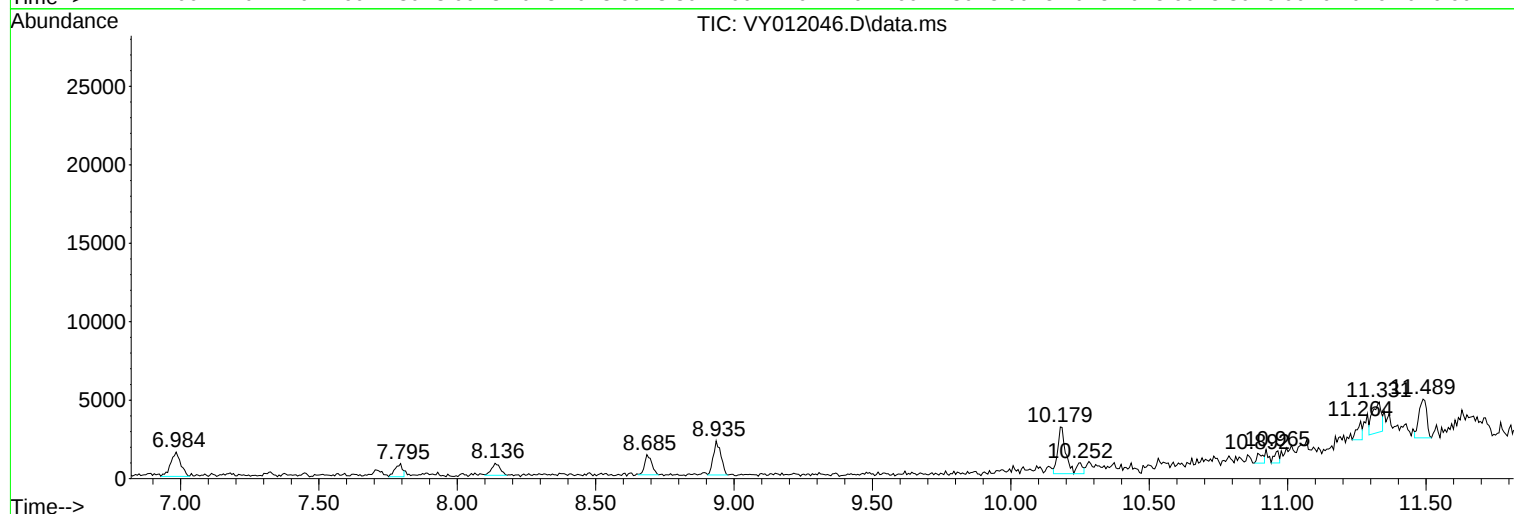
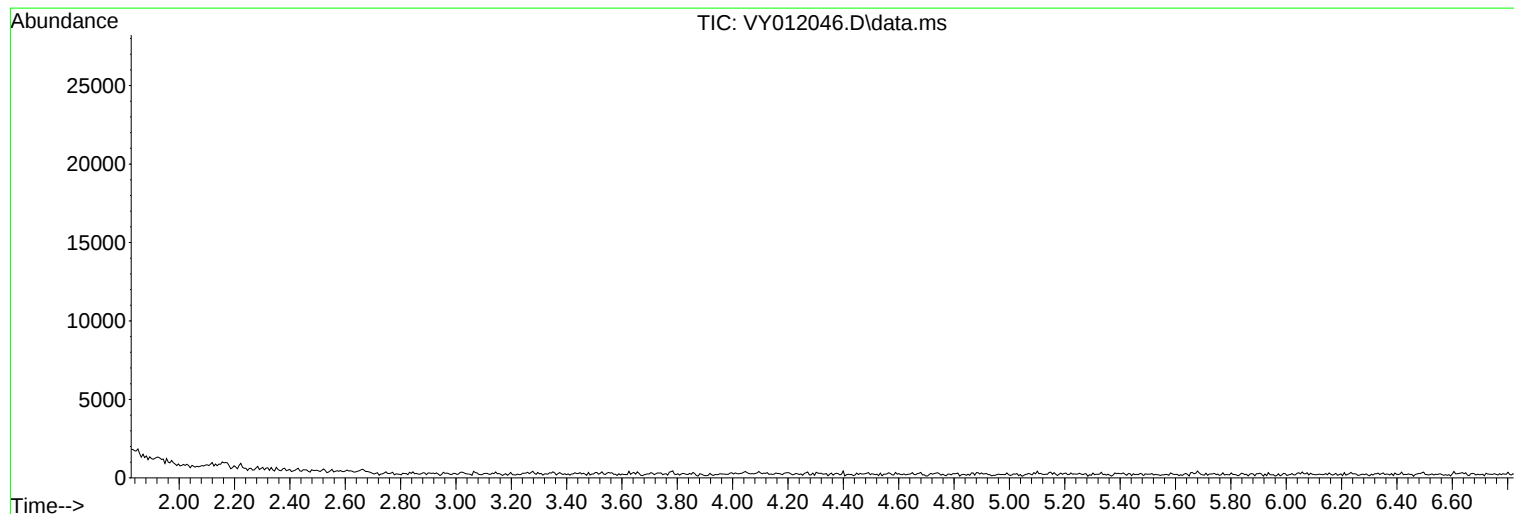
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Instrument :
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ClientSampleId :
TP-C2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y122022S.M
Quant Title : SW846 8260

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



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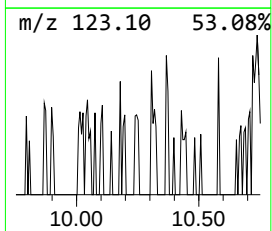
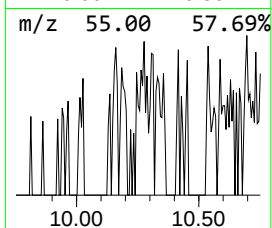
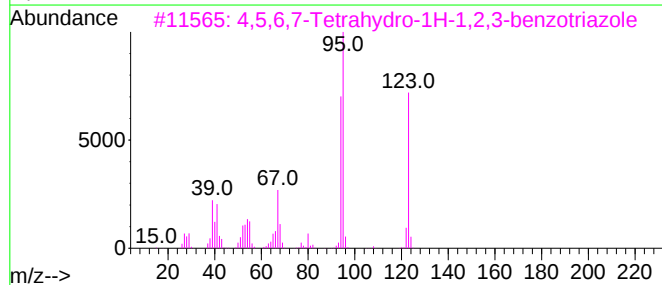
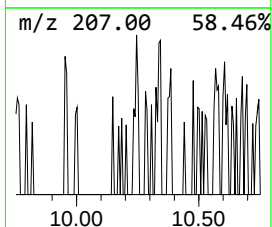
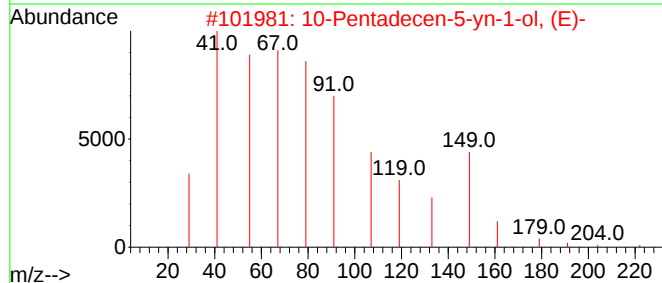
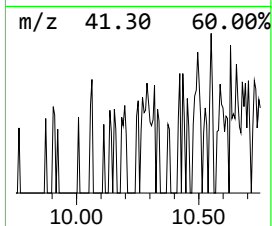
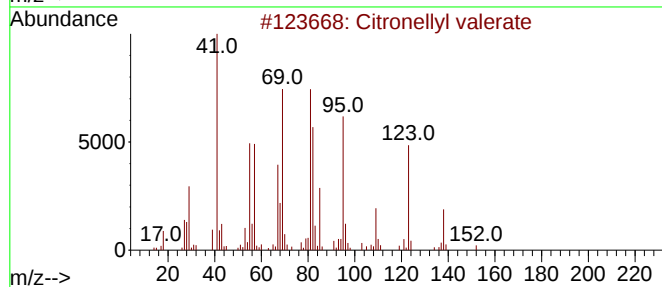
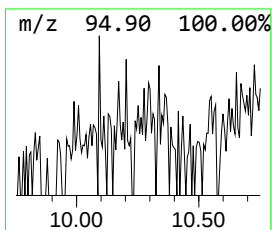
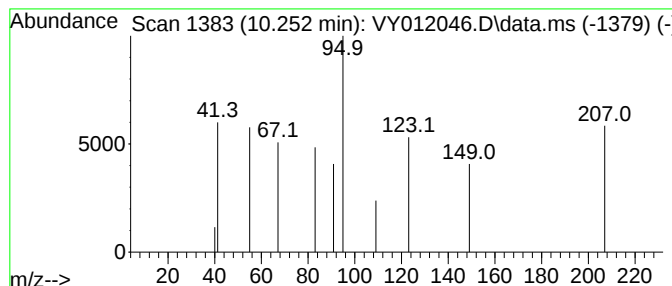
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y122022S.M
Quant Title : SW846 8260

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

Peak Number 1 unknown10.252 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.252	11.25 ug/l	1070	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Citronellyl valerate	240	C15H28O2	007540-53-6	28
2			10-Pentadecen-5-yn-1-ol, (E)-	222	C15H26O	064275-59-8	9
3			4,5,6,7-Tetrahydro-1H-1,2,3-benz...	123	C6H9N3	006789-99-7	5
4			2(1H)-Pyridinone, 1-ethyl-	123	C7H9NO	013337-79-6	5
5			Cyclohexane-1,3-dione, 2-allylam...	207	C12H17NO2	104926-37-6	5



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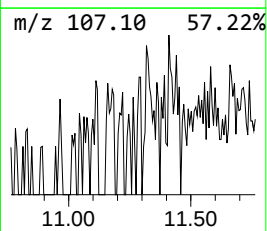
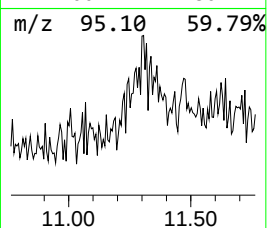
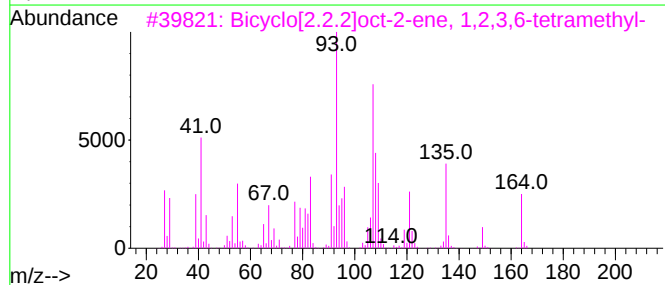
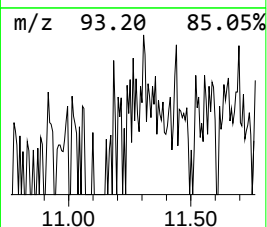
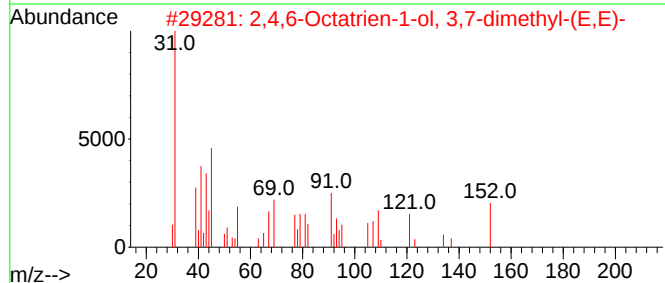
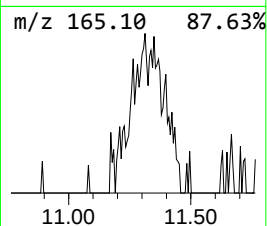
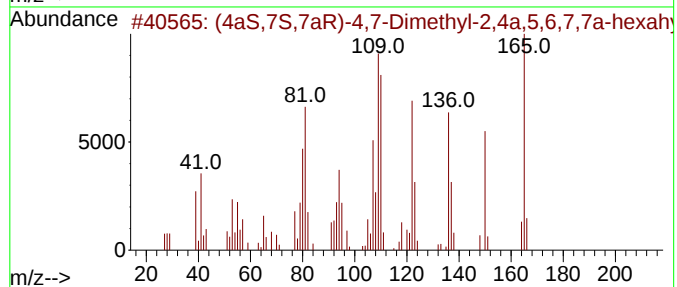
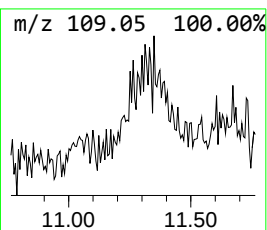
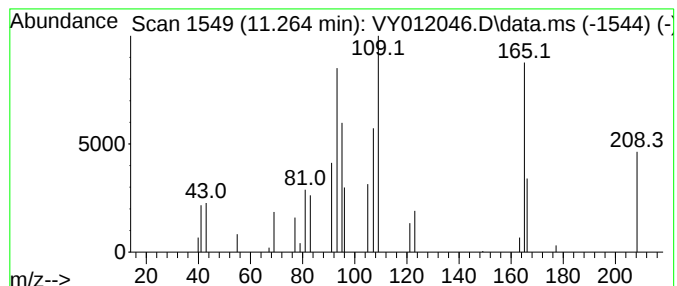
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y122022S.M
Quant Title : SW846 8260

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

Peak Number 2 unknown11.264 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.264	16.12 ug/l	1533	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(4aS,7S,7aR)-4,7-Dimethyl-2,4a,5...	165	C10H15NO	115421-73-3	32
2			2,4,6-Octatrien-1-ol, 3,7-dimeth...	152	C10H16O	089155-85-1	28
3			Bicyclo[2.2.2]oct-2-ene, 1,2,3,6...	164	C12H20	062376-14-1	27
4			1H-Indene, octahydro-2,3a,4-trim...	208	C15H28	031230-13-4	25
5			(Cyclopropyl)trivinylsilane	150	C9H14Si	1000109-93-8	12



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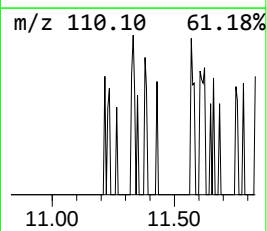
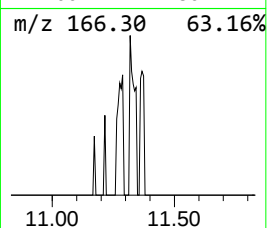
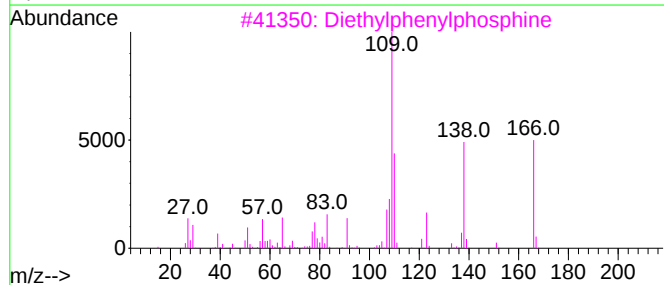
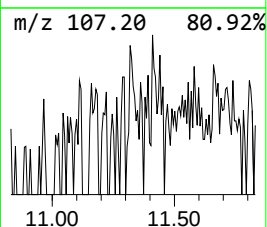
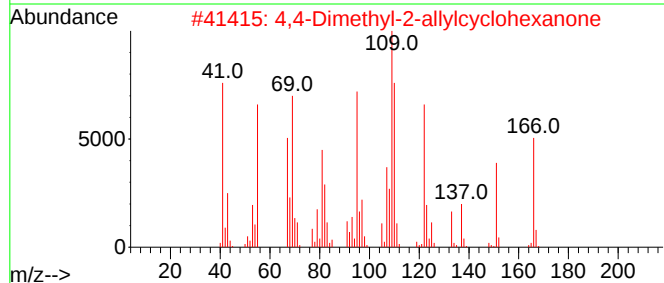
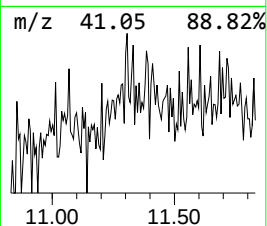
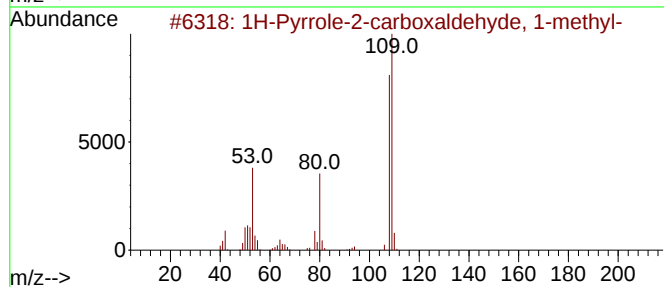
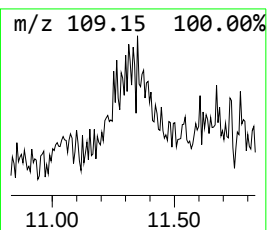
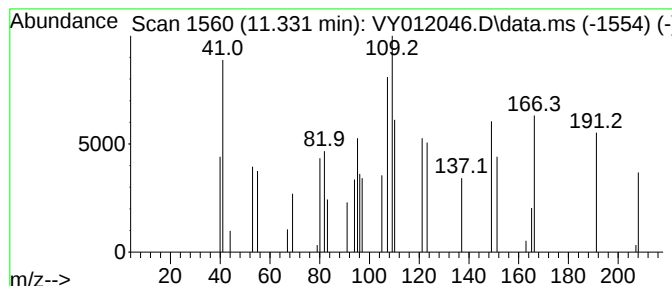
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y122022S.M
Quant Title : SW846 8260

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

Peak Number 3 unknown11.331 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.331	44.94 ug/l	4273	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Pyrrole-2-carboxaldehyde, 1-m...	109	C6H7NO	001192-58-1	27
2			4,4-Dimethyl-2-allylcyclohexanone	166	C11H18O	059077-96-2	27
3			Diethylphenylphosphine	166	C10H15P	001605-53-4	18
4			.alpha.-Farnesene	204	C15H24	000502-61-4	17
5			N-(5-Hydroxy-2-nitroso-phenyl)-f...	166	C7H6N2O3	1000317-47-3	16



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ALS Vial : 13 Sample Multiplier: 1

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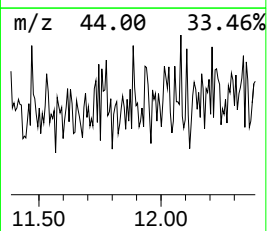
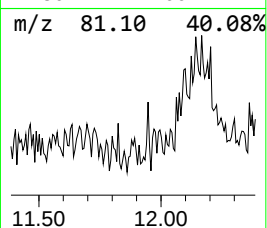
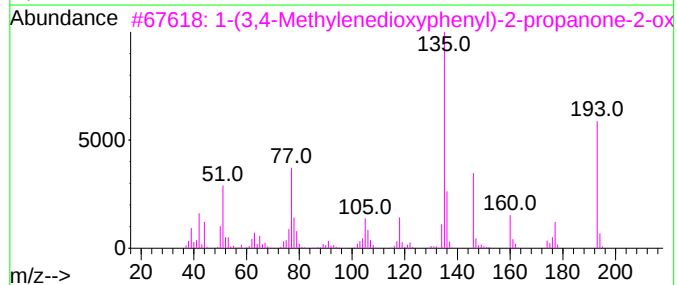
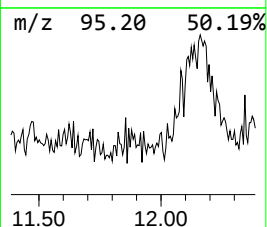
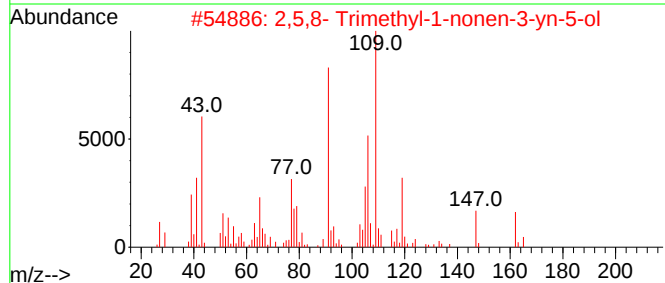
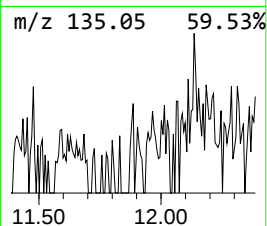
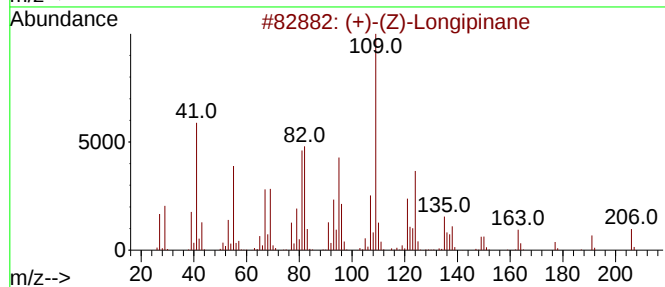
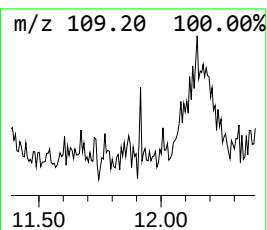
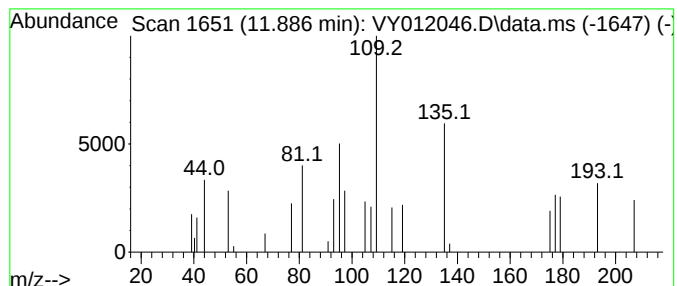
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown11.886 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	14.24 ug/l	1354	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-(Z)-Longipinane	206	C15H26	1000156-12-3	23		
2	2,5,8- Trimethyl-1-nonen-3-yn-5-ol	180	C12H20O	208173-17-5	10		
3	1-(3,4-Methylenedioxyphenyl)-2-p...	193	C10H11NO3	052271-42-8	9		
4	Piperidine, 1-(1-oxo-2,4-hexadie...	179	C11H17NO	019074-11-4	9		
5	1-Pyridin-3-yl-1,4-diazepane	177	C10H15N3	223796-20-1	9		



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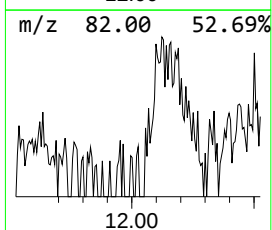
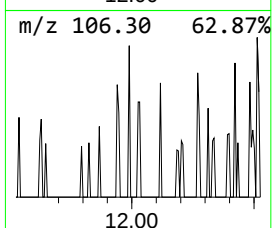
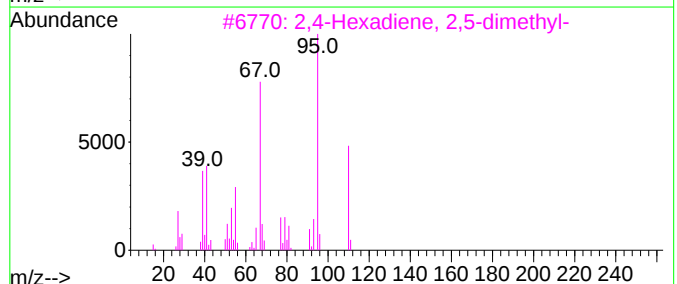
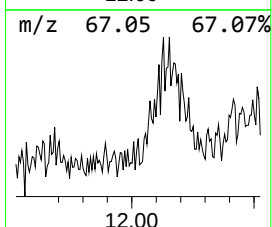
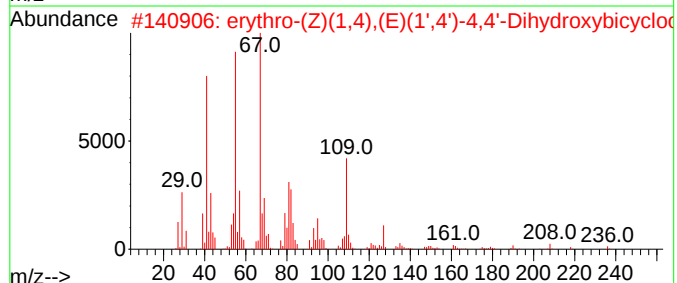
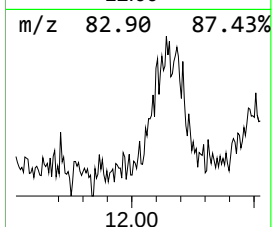
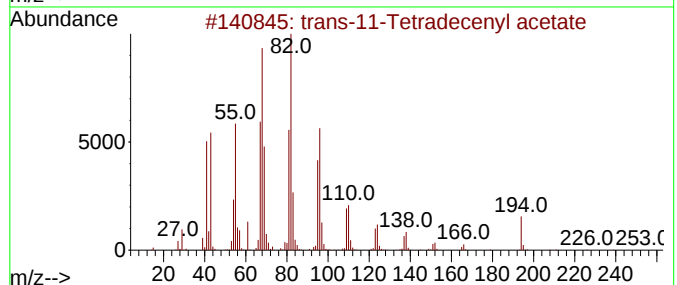
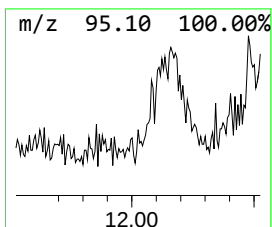
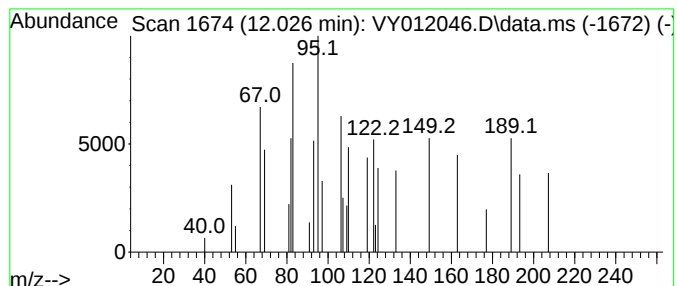
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Peak Number 5 unknown12.026 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.026	10.44 ug/l	993	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-11-Tetradecenyl acetate	254	C16H30O2	033189-72-9	23
2			erythro-(Z)(1,4),(E)(1',4')-4,4'...	254	C16H30O2	1000154-12-9	12
3			2,4-Hexadiene, 2,5-dimethyl-	110	C8H14	000764-13-6	11
4			R(-)-1-Cyano-2-methylpyrrolidine	110	C6H10N2	1000145-01-8	10
5			(E)-4-(2,4,6-Trimethylcyclohex-3...	192	C13H20O	1000498-55-5	10



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ClientSampleId :
TP-C2

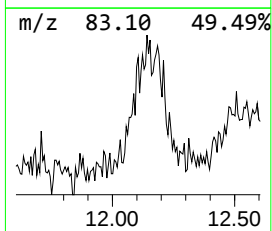
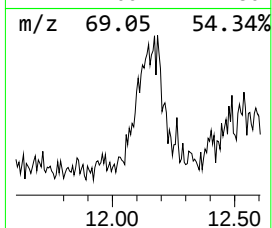
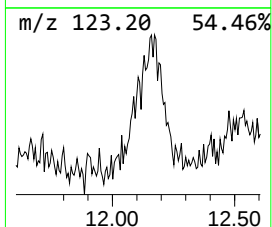
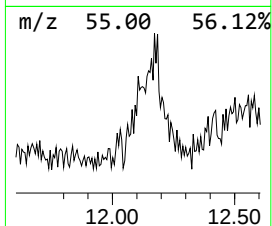
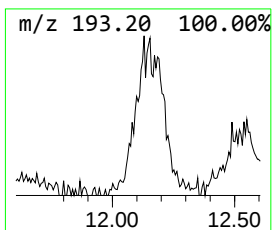
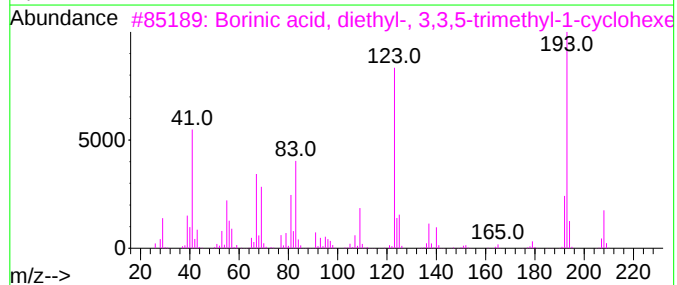
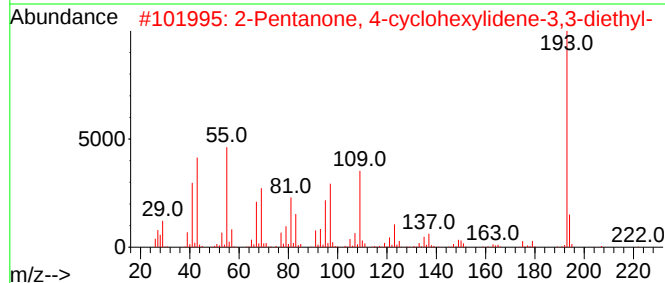
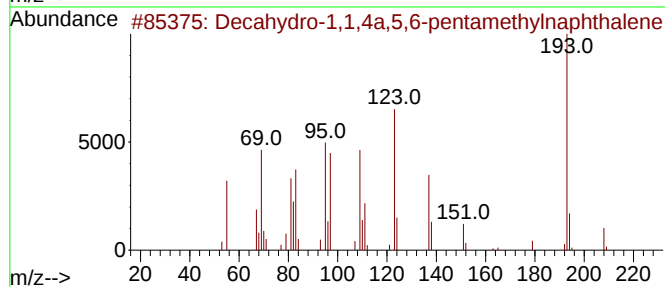
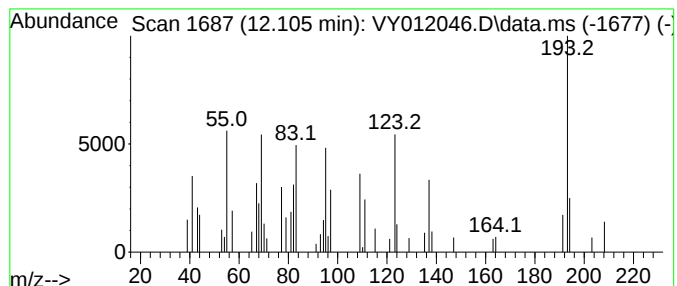
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Quant Title : SW846 8260

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

Peak Number 6 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.105	172.07 ug/l	16360	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	93
2			2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	43
3			Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	27
4			2-Phenylindolizine	193	C14H11N	025379-20-8	14
5			2-Anthracenamine	193	C14H11N	000613-13-8	14



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY010323\
Data File : VY012046.D
Acq On : 03 Jan 2023 14:58
Operator : KP/MD
Sample : 01001-01
Misc : 5.06g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
TP-C2

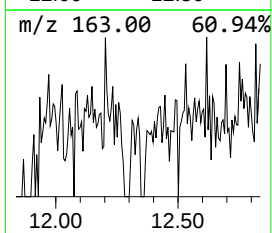
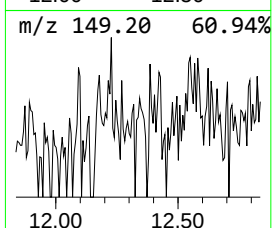
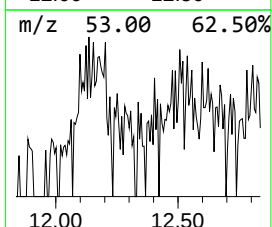
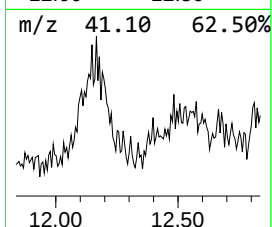
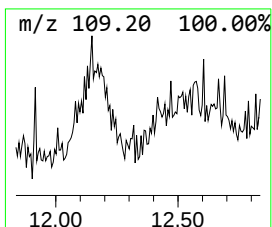
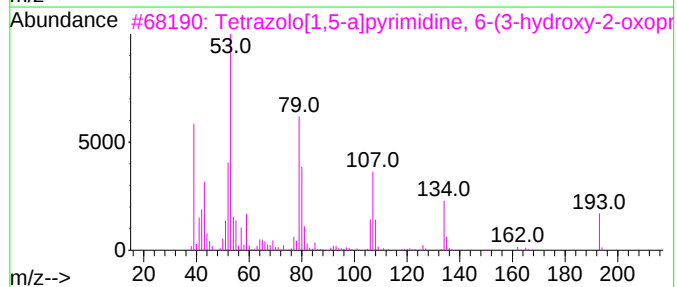
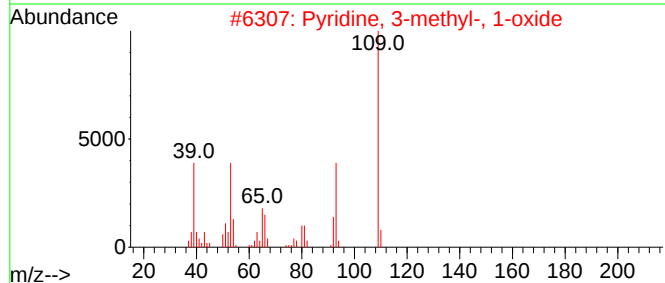
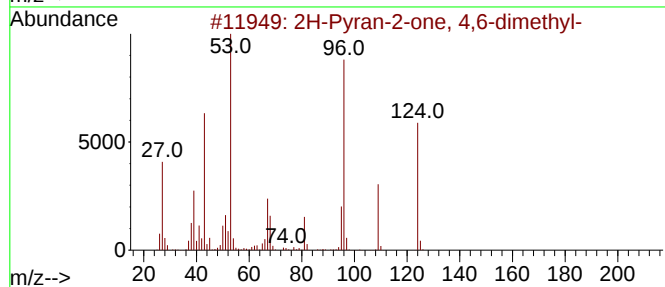
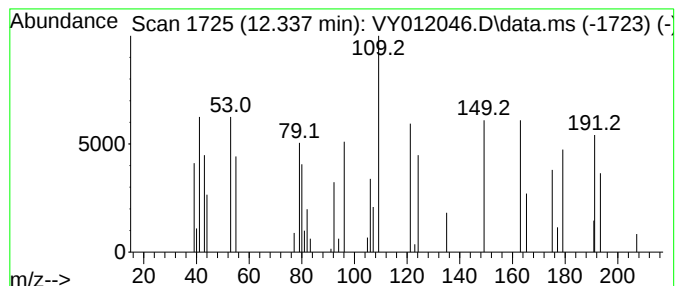
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Quant Title : SW846 8260

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

Peak Number 7 unknown12.337 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.337	20.30 ug/l	1930	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2H-Pyran-2-one, 4,6-dimethyl-	124	C7H8O2	000675-09-2	35
2			Pyridine, 3-methyl-, 1-oxide	109	C6H7NO	001003-73-2	25
3			Tetrazolo[1,5-a]pyrimidine, 6-(3...	193	C7H7N5O2	201053-52-3	12
4			2-(2-Cyanoethyl)-2,3-dihydro-3-o...	149	C7H7N3O	073535-74-7	10
5			3,5-Heptadien-2-one, 6-methyl-, ...	124	C8H12O	016647-04-4	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY010323\
Data File : VY012046.D
Acq On : 03 Jan 2023 14:58
Operator : KP/MD
Sample : 01001-01
Misc : 5.06g/5.0mL/MSVOA_Y/soil
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
TP-C2

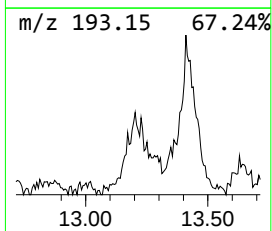
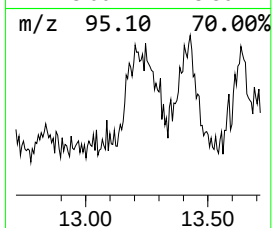
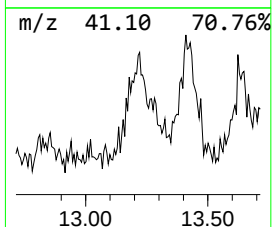
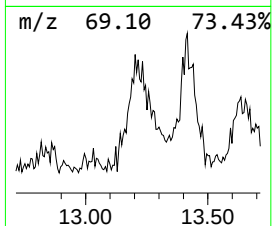
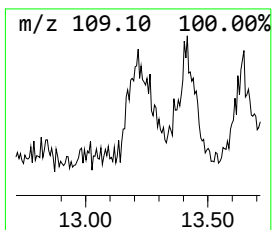
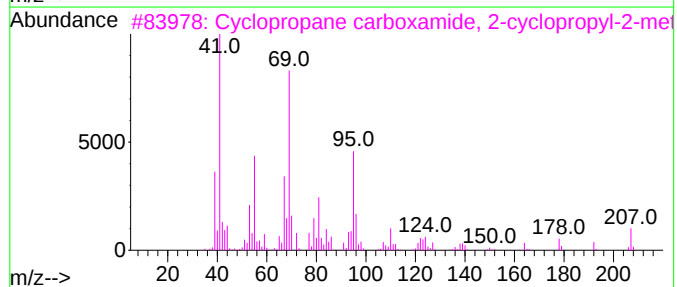
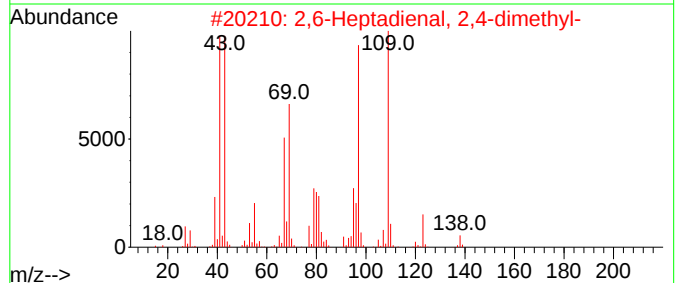
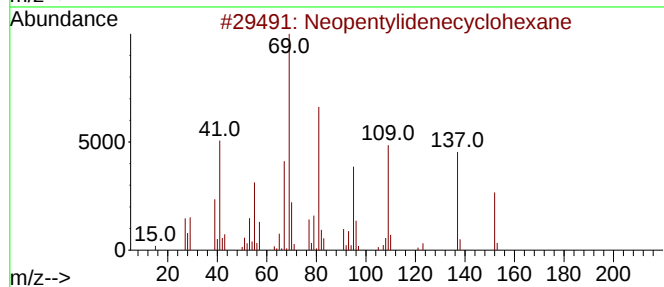
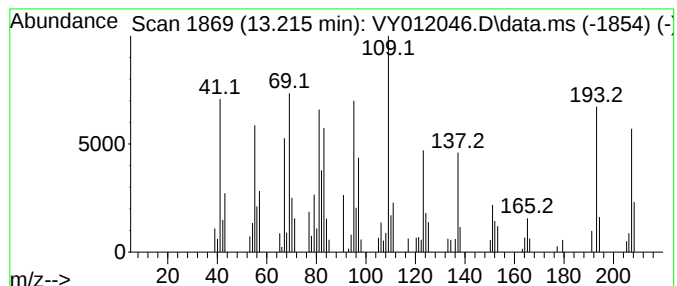
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Quant Title : SW846 8260

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

Peak Number 8 unknown13.215 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.215	60.77 ug/l	90977	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Neopentylidenecyclohexane	152	C11H20	039546-80-0	38
2			2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	38
3			Cyclopropane carboxamide, 2-cycl...	207	C13H21NO	331416-19-4	30
4			Bicyclo[3.1.1]heptan-2-one, 6,6-...	138	C9H14O	038651-65-9	25
5			Bicyclo[3.1.1]heptan-3-one, 2-et...	166	C11H18O	1000163-95-8	18



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY010323\
Data File : VY012046.D
Acq On : 03 Jan 2023 14:58
Operator : KP/MD
Sample : 01001-01
Misc : 5.06g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
TP-C2

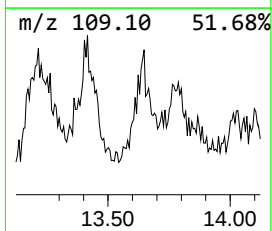
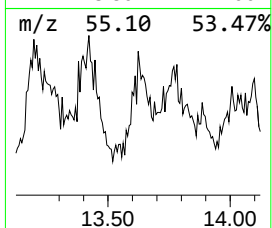
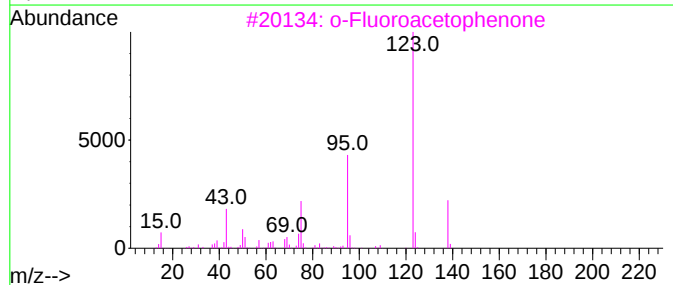
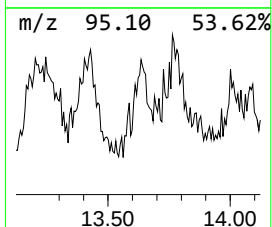
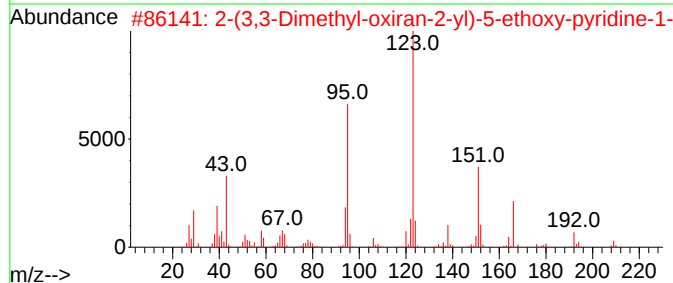
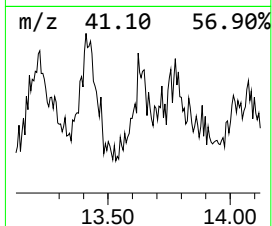
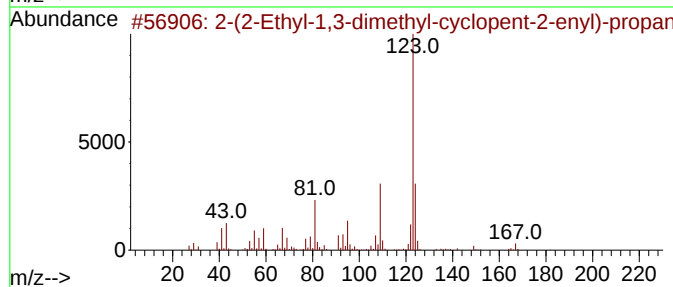
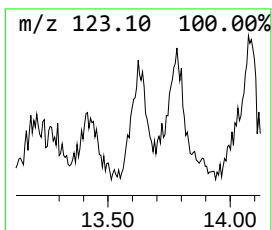
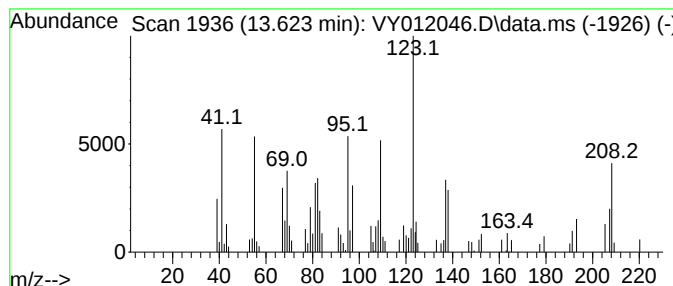
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Quant Title : SW846 8260

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

Peak Number 9 unknown13.623 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.623	18.37 ug/l	27492	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-Ethyl-1,3-dimethyl-cyclopent-2-enyl)-propan-2-ol	182	C12H22O	1000186-82-4	38		
2	2-(3,3-Dimethyl-oxiran-2-yl)-5-ethoxy-pyridine-1-oxide	209	C11H15NO3	1000194-95-4	38		
3	o-Fluoroacetophenone	138	C8H7FO	000445-27-2	35		
4	Ethanone, 1-(3-fluorophenyl)-	138	C8H7FO	000455-36-7	35		
5	Ethanone, 1-(4-fluorophenyl)-	138	C8H7FO	000403-42-9	35		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY010323\
Data File : VY012046.D
Acq On : 03 Jan 2023 14:58
Operator : KP/MD
Sample : 01001-01
Misc : 5.06g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
TP-C2

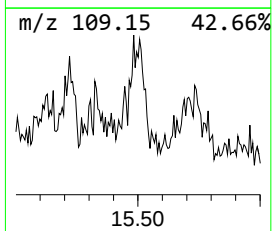
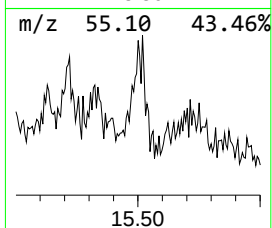
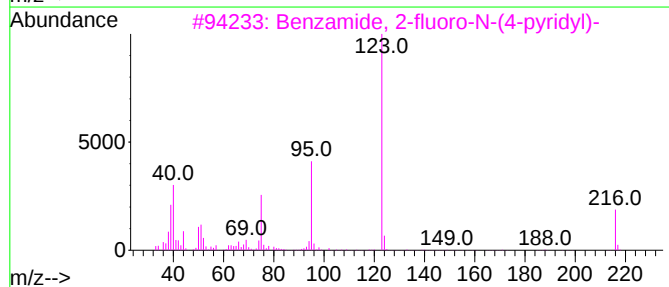
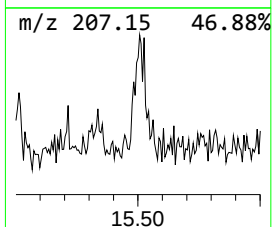
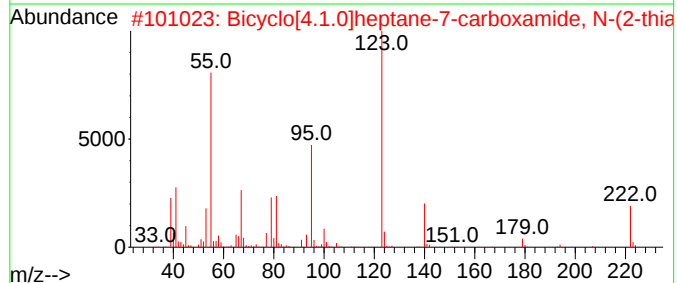
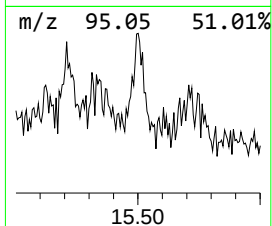
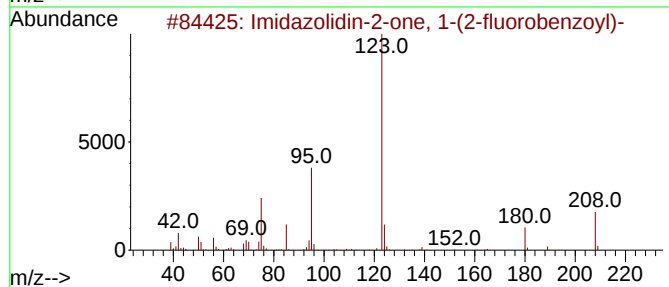
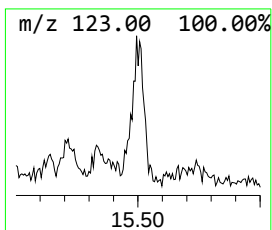
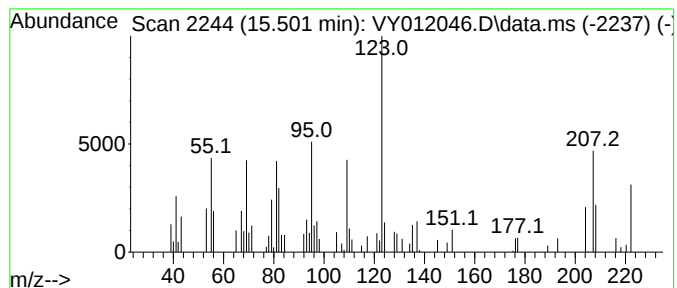
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y122022S.M
Quant Title : SW846 8260

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

Peak Number 10 unknown15.501 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.501	25.78 ug/l	38591	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Imidazolidin-2-one, 1-(2-fluorobenzoyl)-	208	C10H9FN2O2	1010310-62-2	43
2			Bicyclo[4.1.0]heptane-7-carboxamide, N-(2-thia	222	C11H14N2OS	329912-72-3	38
3			Benzamide, 2-fluoro-N-(4-pyridyl)-	216	C12H9FN2O	113204-23-2	38
4			Acetic acid, 2,2,2-trifluoro-, 4-	220	C9H7F3O3	005672-87-7	35
5			Bromo-4-fluoroacetophenone	216	C8H6BrFO	000403-29-2	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY010323\
Data File : VY012046.D
Acq On : 03 Jan 2023 14:58
Operator : KP/MD
Sample : 01001-01
Misc : 5.06g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
TP-C2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y122022S.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
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unknown11.264	11.264	16.1	ug/l	1533	3	11.496	4754	50.0
unknown11.331	11.331	44.9	ug/l	4273	3	11.496	4754	50.0
unknown11.886	11.886	14.2	ug/l	1354	3	11.496	4754	50.0
unknown12.026	12.026	10.4	ug/l	993	3	11.496	4754	50.0
Decahydro-1,1,4...	12.105	172.1	ug/l	16360	3	11.496	4754	50.0
unknown12.337	12.337	20.3	ug/l	1930	3	11.496	4754	50.0
unknown13.215	13.215	60.8	ug/l	90977	4	13.428	74848	50.0
unknown13.623	13.623	18.4	ug/l	27492	4	13.428	74848	50.0
unknown15.501	15.501	25.8	ug/l	38591	4	13.428	74848	50.0