

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD022222\
 Data File : VD072062.D
 Acq On : 22 Feb 2022 17:29
 Operator : VA/SY
 Sample : N1628-01
 Misc : 4.71G/5.00ml/MSVOA_D/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 BP-3

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_D\Method\82D021822S.M
 Title : SW846 8260

Signal : TIC: VD072062.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.126	31	35	43	rBV3	5392	10676	1.91%	1.120%
2	7.908	1011	1018	1023	rBV3	10461	21453	3.83%	2.252%
3	7.973	1023	1029	1037	rVB2	14177	29165	5.21%	3.061%
4	8.320	1082	1088	1099	rVV4	13028	26678	4.76%	2.800%
5	8.861	1171	1180	1188	rBV2	21819	45035	8.04%	4.727%
6	10.332	1425	1430	1436	rBV	31233	53546	9.56%	5.620%
7	11.638	1647	1652	1659	rVB	34698	60770	10.85%	6.378%
8	12.626	1813	1820	1824	rVB2	25738	42726	7.63%	4.484%
9	13.396	1946	1951	1954	rVV4	2903	5709	1.02%	0.599%
10	13.567	1974	1980	1987	rVB3	28795	53914	9.63%	5.659%
11	13.761	1998	2013	2029	rBV4	144046	559990	100.00%	58.773%
12	14.332	2107	2110	2117	rVV8	5494	11169	1.99%	1.172%
13	14.585	2149	2153	2154	rBV2	6091	6113	1.09%	0.642%
14	15.767	2341	2354	2356	rBV6	10121	25852	4.62%	2.713%

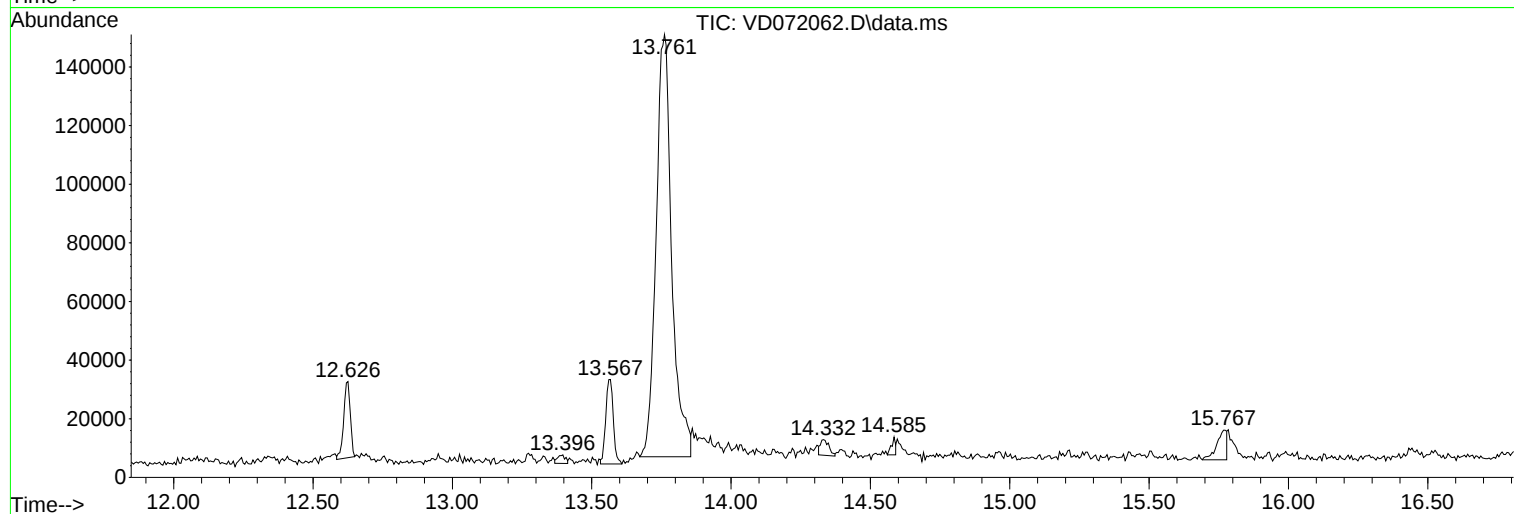
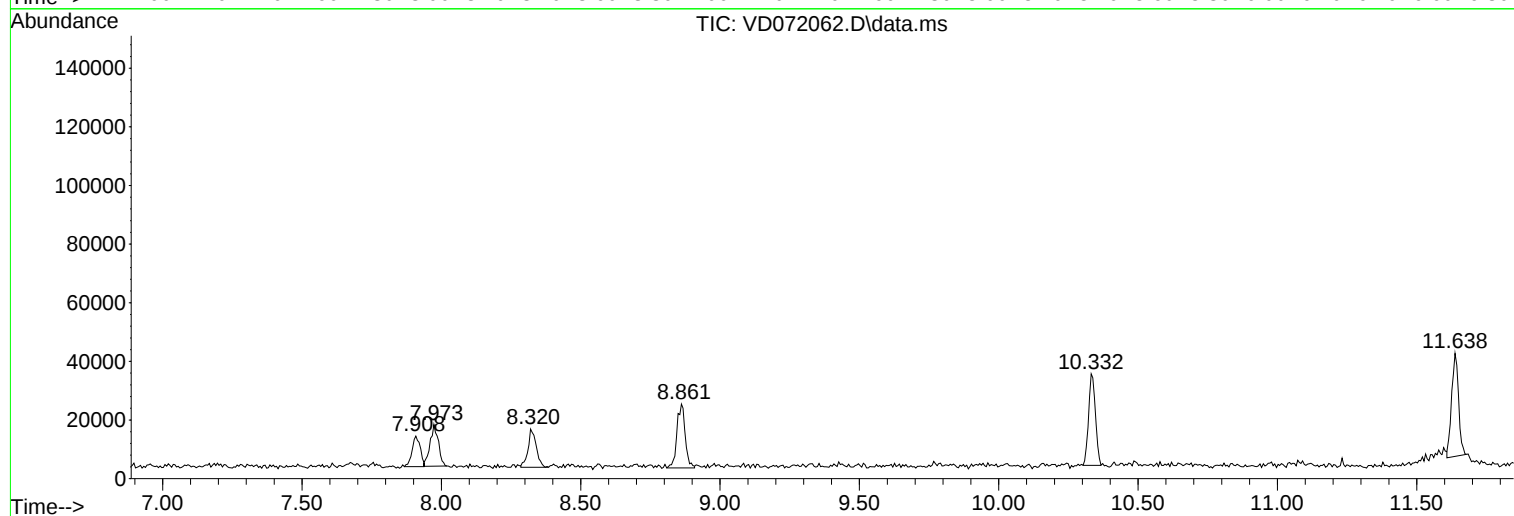
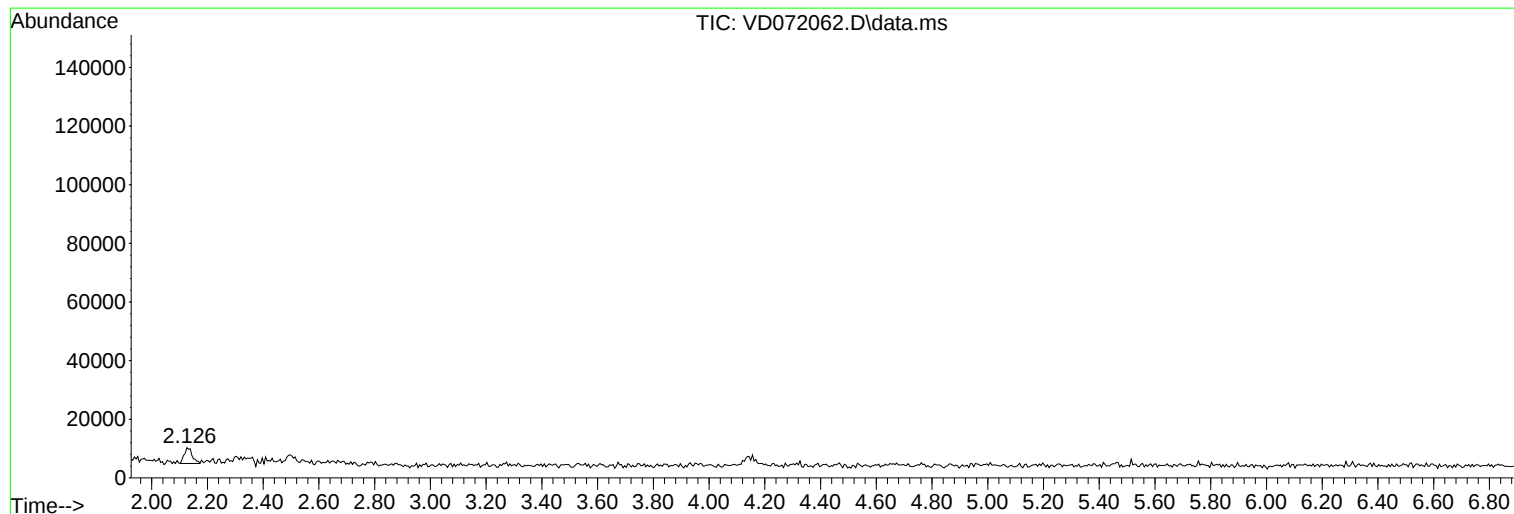
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D021822S.M
Quant Title : SW846 8260

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



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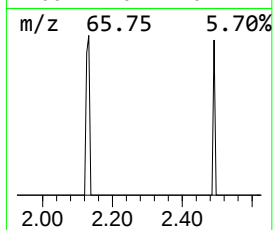
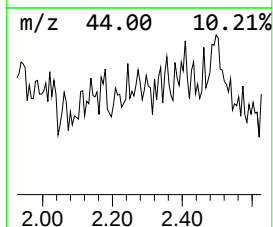
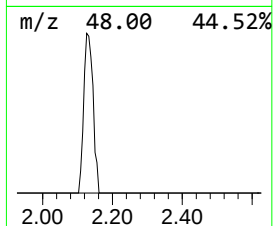
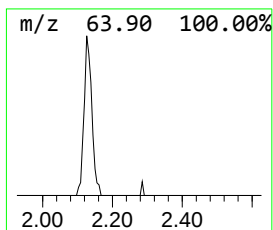
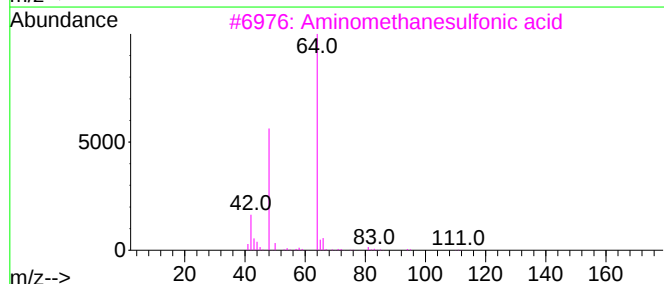
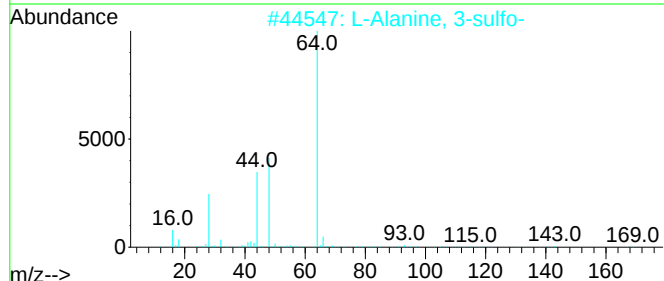
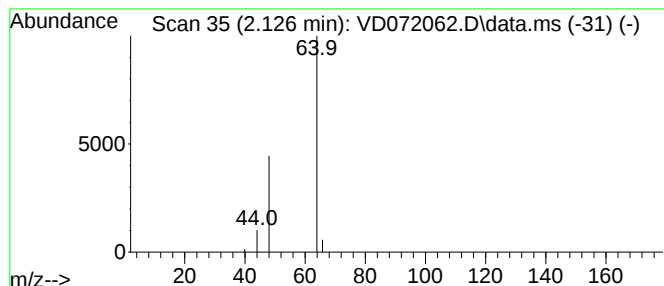
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Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.126	18.30 ug/l	10676	Pentafluorobenzene	7.973

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
2			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			Ethyl Chloride	64	C2H5Cl	000075-00-3	3
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	3



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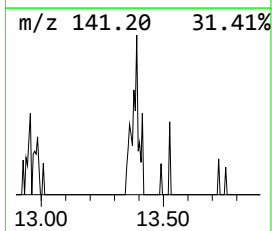
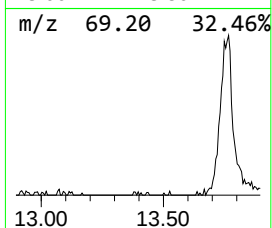
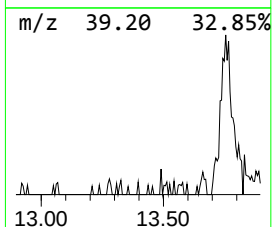
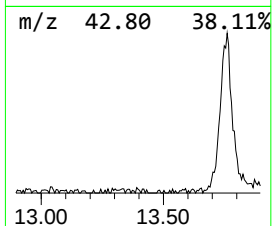
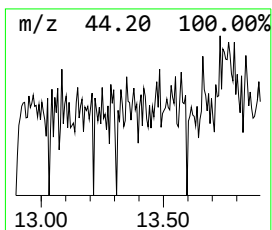
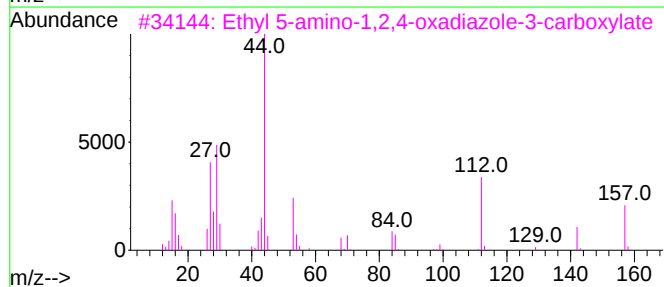
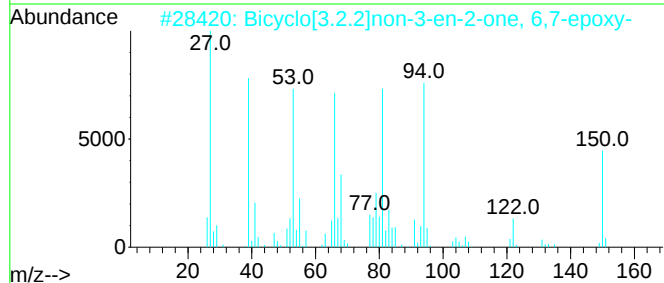
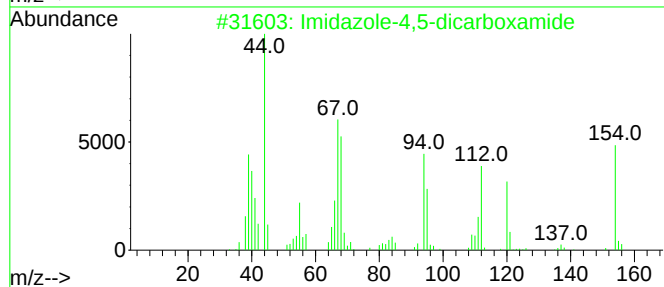
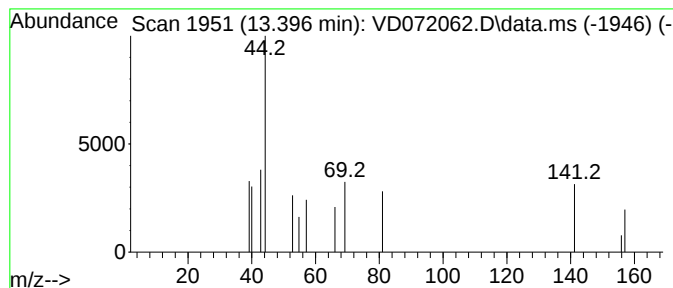
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Peak Number 2 unknown13.396 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.396	5.29 ug/l	5709	1,4-Dichlorobenzene-d4	13.567

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Imidazole-4,5-dicarboxamide	154	C5H6N4O2	000083-39-6	36
2			Bicyclo[3.2.2]non-3-en-2-one, 6,...	150	C9H10O2	1000155-95-4	25
3			Ethyl 5-amino-1,2,4-oxadiazole-3...	157	C5H7N3O3	144167-51-1	9
4			6H-Pyrazolo[1,2-a][1,2,4,5]tetra...	156	C7H16N4	070517-50-9	7
5			1H-Pyrazole-3-carboxylic acid, 4...	157	C4H3N3O4	005334-40-7	5



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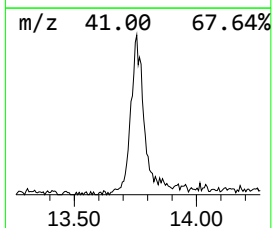
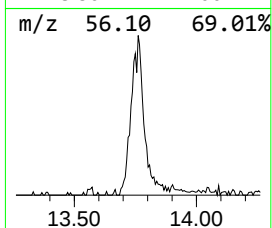
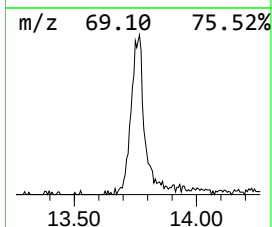
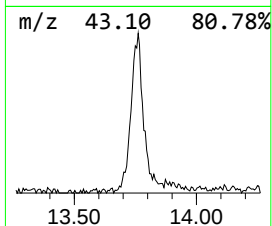
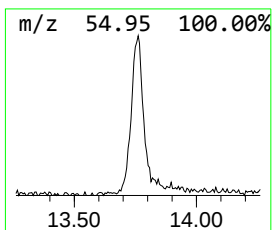
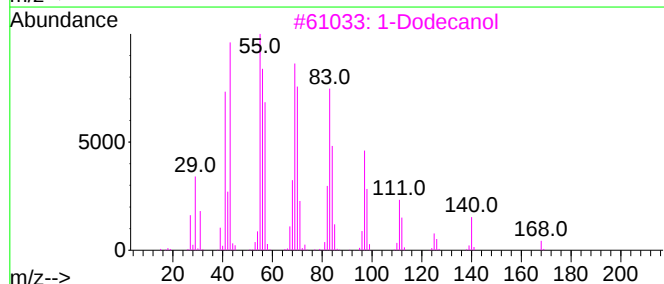
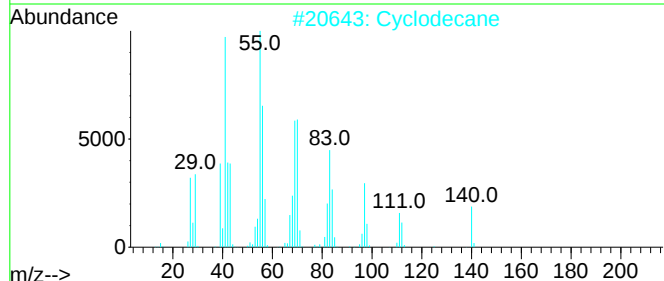
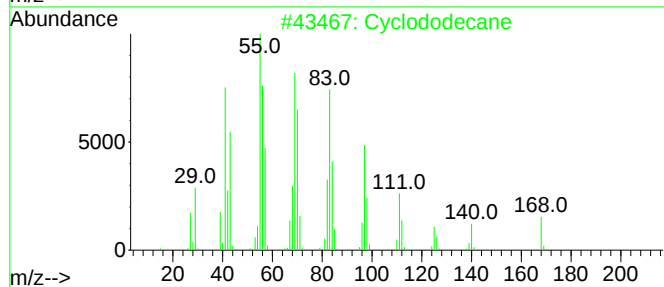
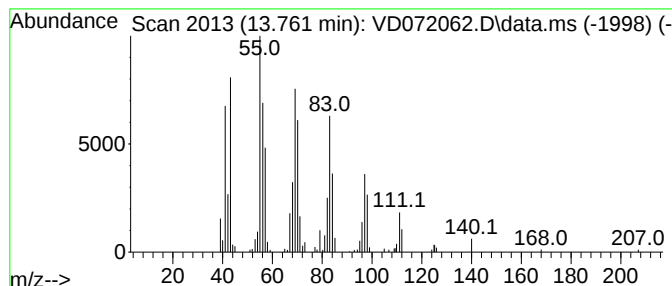
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Peak Number 3 Cyclododecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.761	519.34 ug/l	559990	1,4-Dichlorobenzene-d4	13.567

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclododecane	168	C12H24	000294-62-2	97
2			Cyclodecane	140	C10H20	000293-96-9	93
3			1-Dodecanol	186	C12H26O	000112-53-8	91
4			Cyclopropane, nonyl-	168	C12H24	074663-85-7	91
5			1-Tetradecanol	214	C14H30O	000112-72-1	91



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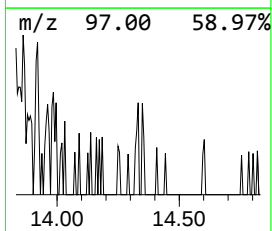
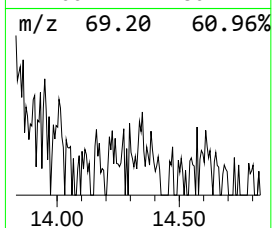
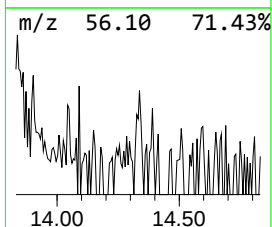
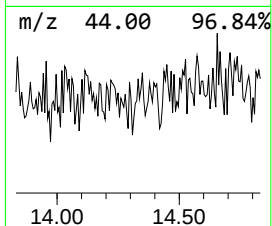
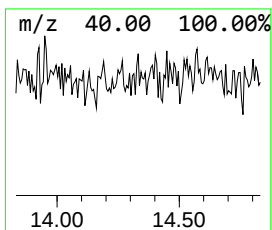
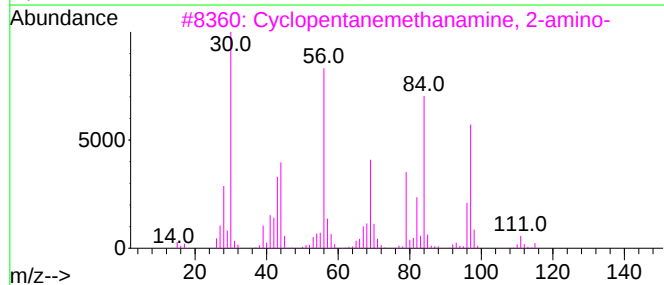
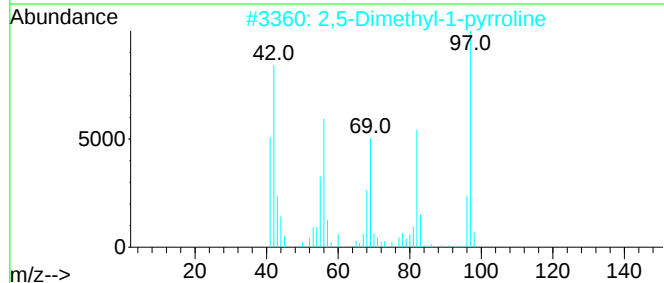
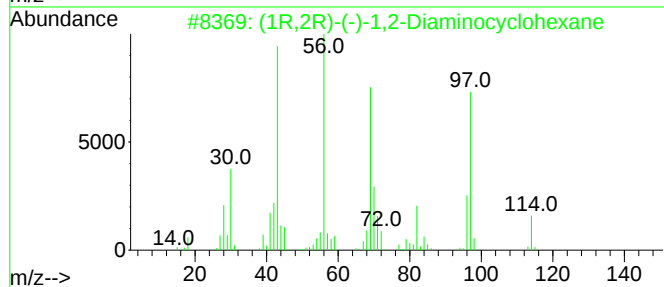
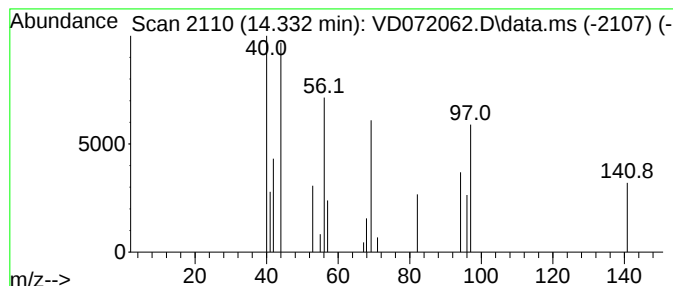
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown14.332 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.332	10.36 ug/l	11169	1,4-Dichlorobenzene-d4	13.567

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1R,2R)-(-)-1,2-Diaminocyclohexane	114	C6H14N2	020439-47-8	27		
2	2,5-Dimethyl-1-pyrroline	97	C6H11N	000822-64-0	25		
3	Cyclopentanemethanamine, 2-amino-	114	C6H14N2	021544-02-5	12		
4	1-Azabicyclo[2.2.2]octan-3-one	125	C7H11NO	003731-38-2	12		
5	Aziridine, 1-(2-methyl-1-propenyl)-	97	C6H11N	080839-93-6	9		



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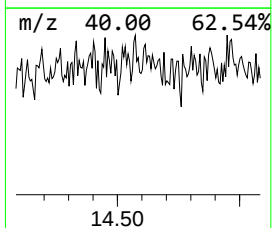
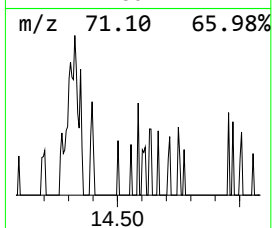
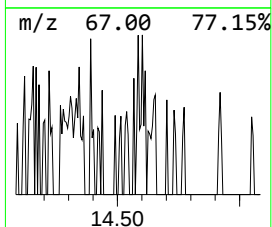
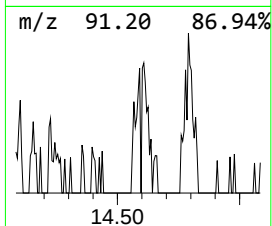
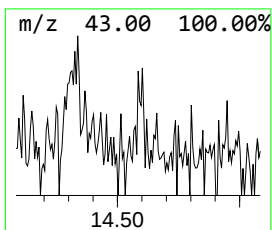
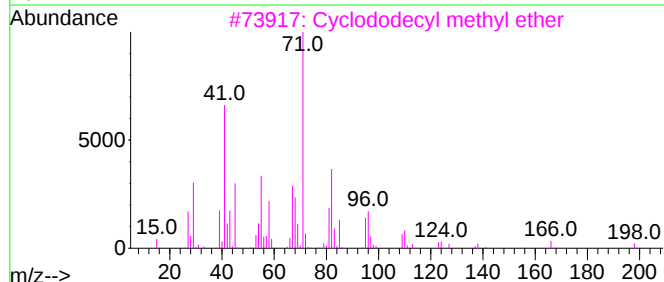
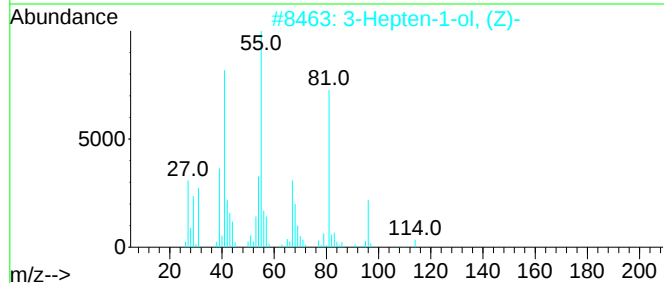
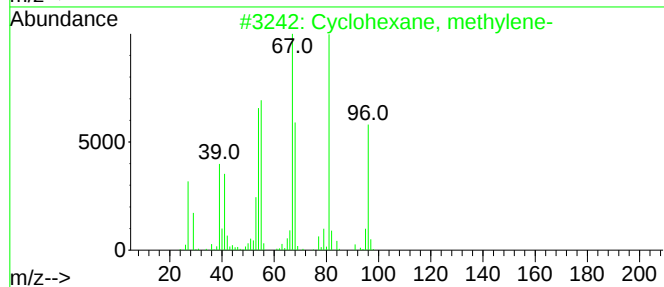
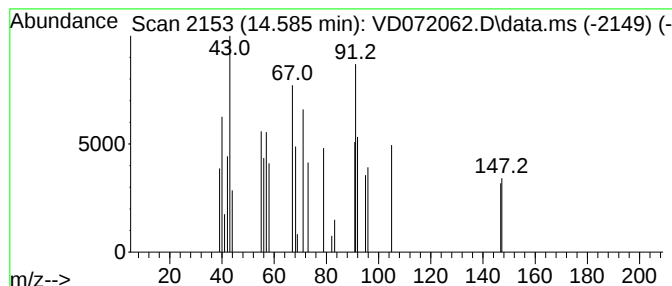
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Peak Number 5 unknown14.585 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.585	5.67 ug/l	6113	1,4-Dichlorobenzene-d4	13.567

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, methylene-	96	C7H12	001192-37-6	27
2			3-Hepten-1-ol, (Z)-	114	C7H14O	001708-81-2	25
3			Cyclododecyl methyl ether	198	C13H26O	002986-54-1	23
4			9-Decen-1-ol, pentafluoropropionate	302	C13H19F5O2	1000352-65-6	17
5			Cyclooctene, 3-methyl-	124	C9H16	013152-05-1	17



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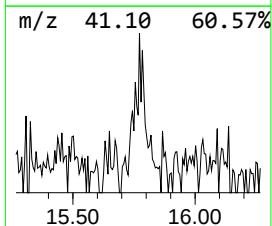
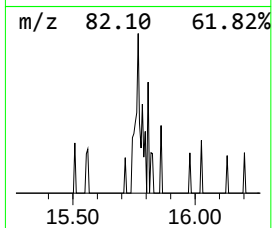
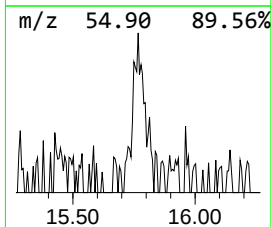
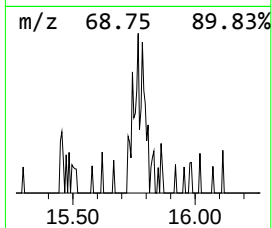
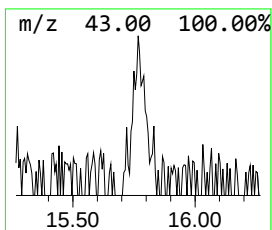
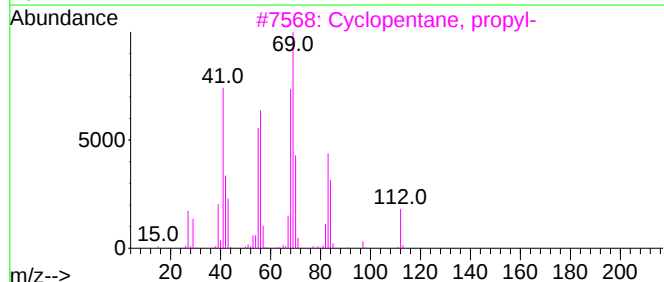
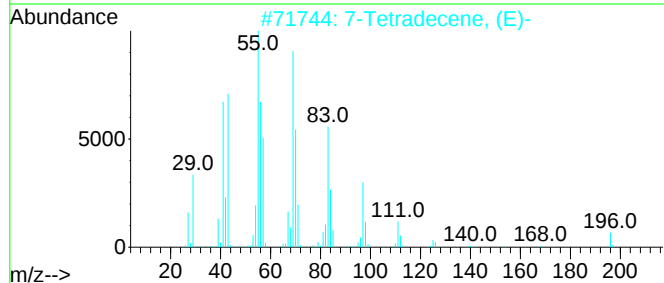
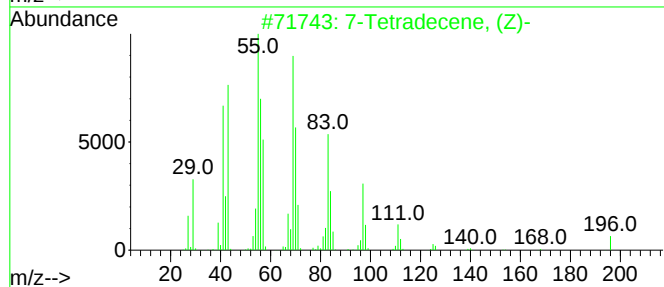
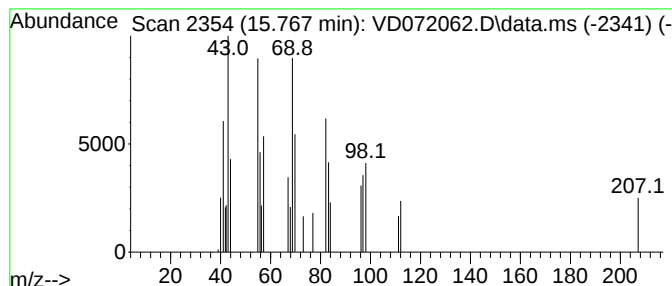
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 7-Tetradecene, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.767	23.98 ug/l	25852	1,4-Dichlorobenzene-d4	13.567

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Tetradecene, (Z)-	196	C14H28	041446-60-0	50
2			7-Tetradecene, (E)-	196	C14H28	041446-63-3	47
3			Cyclopentane, propyl-	112	C8H16	002040-96-2	46
4			4-Heptafluorobutyroxytetradecane	410	C18H29F7O2	1000245-49-9	43
5			1H-Imidazole, 2-ethyl-4,5-dihydr...	112	C6H12N2	000931-35-1	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD022222\
Data File : VD072062.D
Acq On : 22 Feb 2022 17:29
Operator : VA/SY
Sample : N1628-01
Misc : 4.71G/5.00ml/MSVOA_D/SOIL
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
BP-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D021822S.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
Sulfur dioxide	2.126	18.3	ug/l	10676	1	7.973	29165	50.0
unknown13.396	13.396	5.3	ug/l	5709	4	13.567	53914	50.0
Cyclododecane	13.761	519.3	ug/l	559990	4	13.567	53914	50.0
unknown14.332	14.332	10.4	ug/l	11169	4	13.567	53914	50.0
unknown14.585	14.585	5.7	ug/l	6113	4	13.567	53914	50.0
7-Tetradecene, ...	15.767	24.0	ug/l	25852	4	13.567	53914	50.0