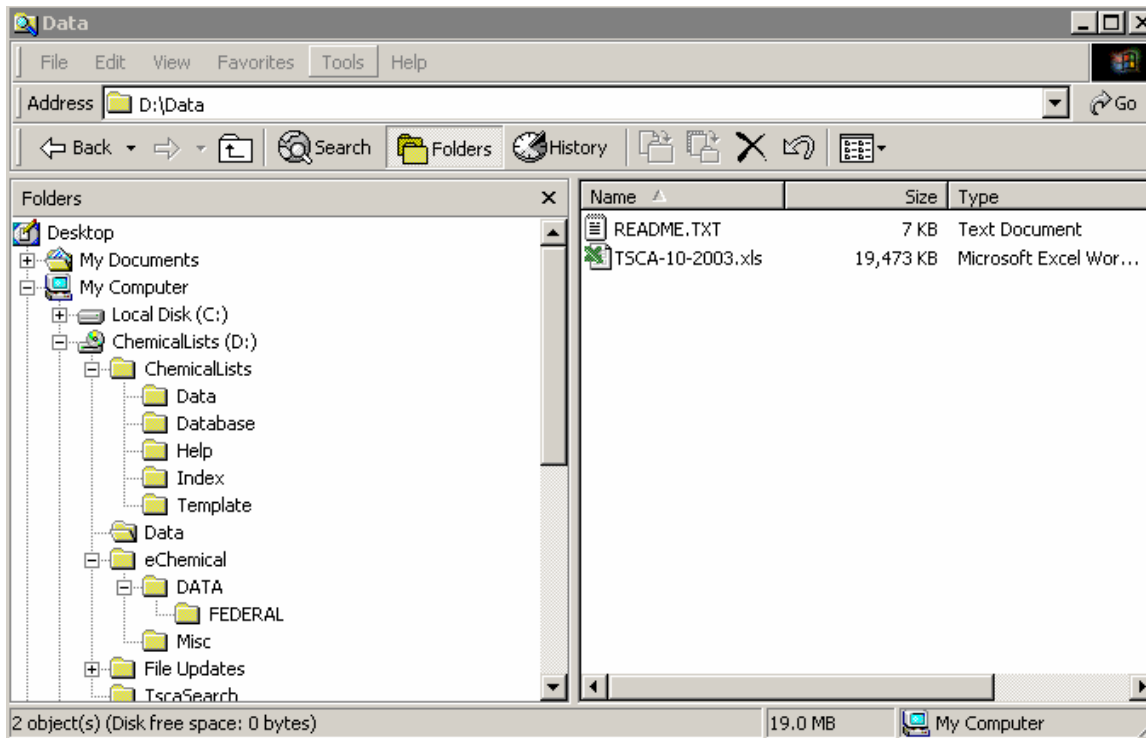
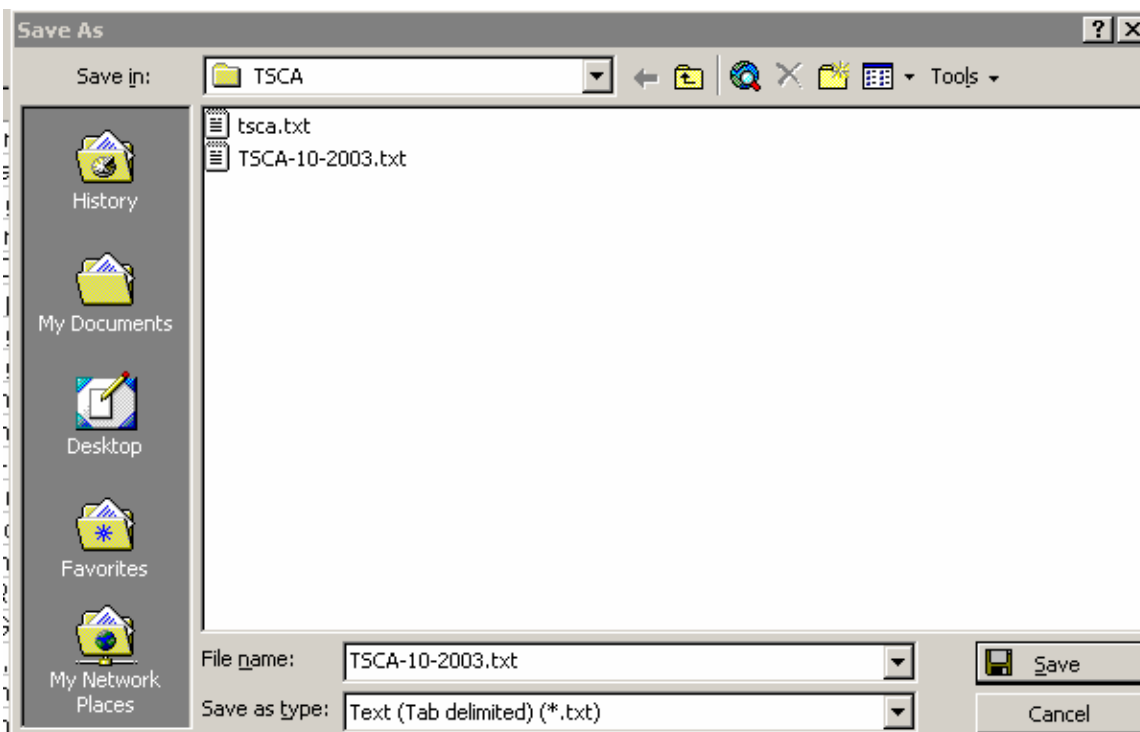


Conversion of File on Solutions, Software Corp. TSCA CD (May 2004)

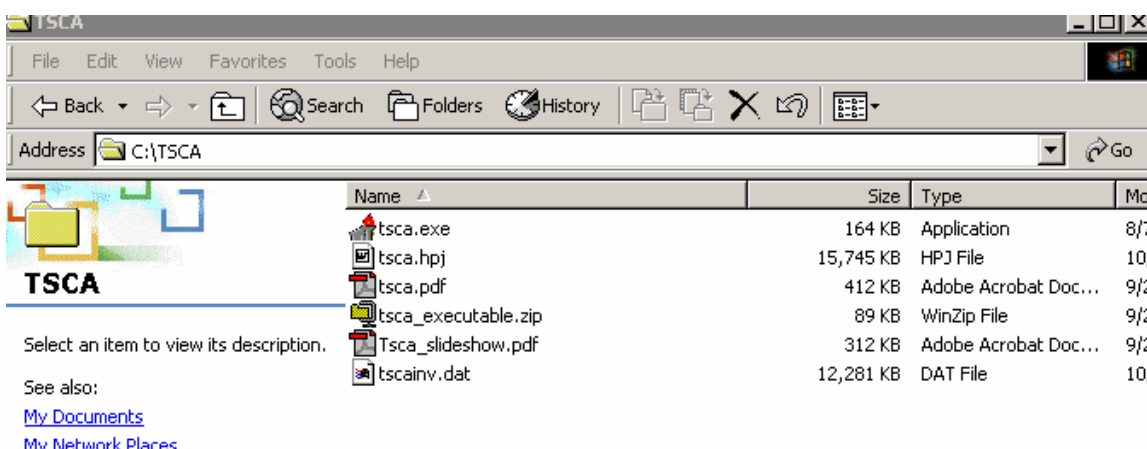
They have changed the distribution format of the files on their CD. First find the



Tsca-10-2003.xls file (date attached will change every time). Open it and save as a Text (tab delimited file) to the C:\tsca folder which contains the tsca.exe program.



Then rename the tscA-10-2003.txt to tscainv.dat.



Then run the tscA.exe. It should convert the tscainv.dat to a tscA.hpj file in a few minutes. A log file, tscA.txt will be created with information on the records converted. The following log info was noted in the current conversion.

TSCA DATA RUN ON 10/28/2003

Total exported: 40021

Total polymers: 14272

Total Complex: 13238

Total unspecified MF: 10685

Total examined: 64978

The only problem with this approach is that some name records will have “ appended to the end of their name. Somehow this occurs when the .xls file is saved to a tab delimited file which puts the undesired “ before and after the name. Fortunately, the tsca.exe program is not bothered by the “ before the name. Examples of a record field and its conversion are noted below. The following record is from the original tsca-10-2003.xls file:

					FN: 420-13-3; 14317-32-9; 15827-40-4; 87667-20-7; 94369-44-5; 106946-18-3; 139693-44-0; 143504-22-7	MF:		
RN: 50-01-1	IN: Guanidine, monohydrochloride	SN:	DF:			CH5N3.CIH	UV:	FL:

The IN field is changed to the following format in the Text (tab delimited) file created from Save As command:

```
RN: 50-01-1 "IN: Guanidine, monohydrochloride"SN: DF: FN: 420-13-3; 14317-32-9; 15827-40-4; 87667-20-7; 94369-44-5; 106946-18-3; 139693-44-0; 143504-22-7
MF: CH5N3.CIH UV: FL:
```

The IN field is then converted into the ##CAS Name field in the final tsca.hpj file with the residual “ noted at the end of the field:

```
##TITLE=Library Entry 1 in TSCA
##JCAMPDX=Revision 4.10
##DATA TYPE=MASS SPECTRUM
##SAMPLE DESCRIPTION= TSCA Listing
##NAMES=
##CAS NAME=Guanidine, monohydrochloride"
```

The tsca.hpj file is converted into a NIST library binary folder and associated files using the Lib2Niste.exe utility program supplied by NIST. The libraries thus created are searchable by MW, CAS number, MF, etc using the NIST library search software.