# PROTOCOL

1. At the end of an ITC experiment the user will initially integrate the heat released or absorbed in each injection.

2. Following integration, a text file should be saved in ASCII format containing data series for the injection volume (Vi), macromolecule concentration (MT), molar ratio (XT/MT), and heat of injection (ndh). E.g., 15C.DAT, 20C.DAT, 25C.DAT, 30C.DAT, 35C.DAT

3. The files generated in step 2, along with the active cell volume (V0), syringe concentration of ligand (X0), experiment temperature (T) and number of points to exclude (npd) are used as inputs into the Matlab fitting macro (Fcn\_Fit\_Cp\_Ndil.m). These above-mentioned values are read from a text file written in a tab separated format:

File\_name.DAT T V0 X0 npd

E.g. Listfile.txt,

15C.DAT 288 1427.47 0.3 2

20C.DAT 293 1427.47 0.3 1

25C.DAT 298 1427.47 0.3 1

30C.DAT 303 1427.47 0.3 2

35C.DAT 308 1427.47 0.3 1

## Global Fitting

Syntax: Fcn\_Fit\_Cp\_Ndil('list\_file\_text\_format\_from\_step\_3')

Example MATLAB command: **Fcn\_Fit\_Cp\_Ndil('Listfile.txt')**

INPUTS:

list\_file\_text\_format\_from\_step\_3: filename from step 3 ['Listfile.txt']

OUTPUTS:

Fit.xxxxxxx.dat: Tab separated file containing: XT/MT, Fit, ndh  
 where xxxxxxx is the input DAT files

OutputParSumm.txt: Text file containing ΔφCp, ΔxH° and ΔxS° along with errors