

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 (V_i), macromolecule concentration (M_T), molar ratio (X_T/M_T), 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 (V_0), syringe concentration of ligand (X_0), 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
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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: X_T/M_T , Fit, ndh
where xxxxxxx is the input DAT files

OutputParSumm.txt: Text file containing $\Delta\phi C_p$, ΔxH° and ΔxS° along with errors