Kinetics

(1) Starting from a series of 1D files:
    a. wrpa ***newname2*** (this will be your 2D file)
    b. re ***newname2***
        i. eda <return> parmode → 2D → Save (OK, OK)
        ii. eda <return> F1 → TD → number of FIDs → Save
        iii. edp <return> F1 → SI → 2^n > number of FIDs → Save
    c. fidtoser <return> (will get a list of questions)
        i. Enter name of 1D series (give the directory name of the original data)
        ii. Enter starting EXPNO: (what's the number of the first FID?)
        iii. Enter starting PROCNO: (usually 1)
        iv. Enter # of FIDs: (how many exnpo's did you run?)

(2) The file must contain a "vdlist" which contains the time points of your x-axis
    a. Copy the file "vdlist" from shared documents to the folder of the experiment number (data/directory owner/nmr/ ***newname2***/expno/vdlist)
    b. Create a list of time points (***e.g.*** origin, <ctrl>Q: 0+((i-1)*293), where zero is the starting value and 293 is the increment in seconds – use (ns+ds)*(aq+d1) to get the correct value for ***your*** data).
    c. Copy the list of time points into the vdlist file (open with notepad).

(3) xf2 <enter> (executes fourier transform of F2 dimension (FID) only)

(4) phase <enter> (select a row – middle mouse, mov (move) to windows 1-3, ph0, ph1, save & return)

(5) abs2 <enter> (automatic baseline correction (like abc/abs) using absg settings in F2 only)

(6) edt1 <enter> (fill in the table with the following)
    a. NUMPNTS (number of original 1D FIDs)
    b. FITTYPE (toggle between area and intensity)
    c. LISTTYP (vdlist)
    d. LISTINC (1)
    e. Cursor (2 , but it will choose it automatically . . .)
    f. DRIFT (20, this is the number of points left and right of the peak position for the computer to identify the peak)
    g. START (1, usually start with the first FID in the series)
    h. INC (1, increment each FID by one)
    i. FCTTYPE (linear)

    Save to exit

(7) rspc <enter> (replaces with 1D spectra. To return to the 2D view, change PARMOD in eda to 2D. Note that typing parmode <space> 2D <enter> will ***not*** work in this case – it's a bug.)

(8) utilities → define points → (middle mouse / append) → return

(9) integration → define integral areas → save & return

(10) edo <enter> CURPRIN (change to screen)

(11) t1/t2<enter> (goes to the graphing window called t1/t2)

(12) pd <enter> (calculates the **area** or **intensity** of the chosen peaks according to steps: 6b, 7, 9 – starts with the first peak #1, according to 6g)

(13) simfit <enter> (will put the results, including x-axis time points, y-axis intensities/areas, and linear fit, on the screen).
(14) To save the file:
    a. open D:\data\directory owner\nmr\ ***newname2***\1\pdata\1
    b. rename the file called simfit.txt
(15) in XWIN-NMR in the t1/t2 window, to get the results for peak #2
    a. type: nxtp <enter>
    b. simfit <enter>
    c. repeat step (14) to save the file