Supplemental Materials (Molecular Mechanics Parameter Development)

```
##########################################################################
##  Parameters for Mn2+ and Fosfomycin taken from Amber Parameter Database  ##
##          Website - http://pharmacy.man.ac.uk/amber/                    ##
##########################################################################
```

Mn^{2+} vdw parameters (from Concanavalin A study by G.M. Bradbrook et al.)

```
MASS
MN      55.00   0.00

NONB
MN      1.6900  0.0140
```

Manganese parameters (cont.)

```
mn.prp
MNG  INT  0
CHANGE OMIT DU  BEG
 0.0
   1 DUMM  DU  M  0  -1  -2  0.000     0.000   0.000   0.000
   2 DUMM  DU  M  1   0  -1  1.000     0.000   0.000   0.000
   3 DUMM  DU  M  2   1   0  1.000    90.000   0.000   0.000
   4 MN    MN  M             29.683   127.561 -18.450   2.000

DONE
STOP
```

Fosfomycin parameters (calix[4]arenes: PhD Thesis of Marc Baaden - 250800)

```
MASS

BOND
CT-P    331.       1.82

ANGLE
CT-P -O2     60.        104.6      angles from gopt / force const. (Baaden)
CT-CT-P      35.        113.1              "                 "
OS-CT-P      50.        124.3              "                 "
P -CT-H2     60.        127.3              "                 "

DIHEDRAL
X -CT-P -X    9           3.51           0.       3.   tpl - JPC 94

NONBOND
```

```
##########################################################################
##  Parameters for Fosfomycin and Glutathione (ILG) developed in collaboration   ##
##          with the research group of Professor Terry Lybrand                   ##
##########################################################################
```

Fosfomycin parameters (cont.)

```
fos.prp
FCN  INT  0
 CORRECT  OMIT  DU  BEG
 0.0
  1 DU1   DU   M     0   0   0   0.000    0.000    0.000
  2 DU2   DU   M     1   0   0   1.000    0.000    0.000
  3 DU3   DU   M     2   1   0   1.000   90.000    0.000
  4 C1    CT   M     3   2   1   0.559  119.220  156.267   -0.0043
  5 H11   HC   E     4   3   2   1.090  126.907  305.732   -0.0119
  6 H12   HC   E     4   3   2   1.092  119.722   97.641   -0.0119
  7 H13   HC   E     4   3   2   1.091   73.080  203.685   -0.0119
  8 C2    CT   M     4   3   2   1.511   33.238   14.929    0.0434
  9 H2    H1   E     8   4   3   1.083  116.259  184.228   -0.0280
 10 O3    OS   M     8   4   3   1.469  114.639   49.091   -0.4633
 11 C4    CT   M    10   8   4   1.518   59.584  247.771    0.0872
 12 H4    H2   E    11  10   8   1.082  108.886  253.746   -0.0113
 13 P     P    M    11  10   8   1.877  124.338  116.285    1.0550
 14 O2P   O2   E    13  11  10   1.504  103.349   74.682   -0.8810
 15 O3P   O2   E    13  11  10   1.519  104.574  313.185   -0.8810
 16 O1P   O2   E    13  11  10   1.508   98.477  194.010   -0.8810

LOOP
C2   C4

DONE
STOP
```

ILG - amino-terminal γ-glutamyl residue from glutathione (GSH)

```
ILG.prp
ILG  INT  0
 CORRECT  OMIT  DU  BEG
 0.0
  1 DU1  DU   M     0   0   0   0.000    0.000    0.000
  2 DU2  DU   M     1   0   0   1.000    0.000    0.000
  3 DU3  DU   M     2   1   0   1.000   90.000    0.000
  4 N    N3   M     3   2   1   1.262  149.168  315.313   -0.8689
  5 H1   H    E     4   3   2   1.005  133.615  120.590    0.3395
  6 H2   H    E     4   3   2   1.110   83.034  220.761    0.3395
  7 H3   H    E     4   3   2   1.007  111.441  327.265    0.3395
  8 CA   CT   M     4   3   2   1.480   29.196   65.498    0.2825
  9 HA   HP   E     8   4   3   1.085  107.123  107.881    0.0238
 10 C    C    B     8   4   3   1.536  107.353  354.046    0.6306
 11 O    O2   E    10   8   4   1.339  113.413   20.621   -0.5382
 12 OXT  O2   E    10   8   4   1.203  123.852  198.954   -0.5382
 13 CB   CT   M     8   4   3   1.533  113.868  229.142    0.0122
 14 HB2  HC   E    13   8   4   1.081  108.878  311.188    0.0095
 15 HB3  HC   E    13   8   4   1.085  109.375   68.078    0.0095
 16 CG   CT   M    13   8   4   1.533  113.389  190.403   -0.0498
 17 HG2  HC   E    16  13   8   1.078  110.008  294.996    0.0086
 18 HG3  HC   E    16  13   8   1.088  109.915   53.520    0.0086
 19 CD   C    M    16  13   8   1.519  110.542  171.884    0.5449
 20 OD   O    E    19  16  13   1.222  122.434  343.497   -0.5536

DONE
STOP
```

References from Supplemental Materials:

M. Baaden*, G. Wipff, F. Berny; *Laboratory of Molecular Biophysics, University of Oxford
M. Baaden, G. Wipff, M. R. Yaftian, M. Burgard and D. Matt (2000) Cation coordination by calix(*1*)arenes bearing amide and/or phosphine oxide pendant groups: how many arms are needed to bind Li+ vs Na+ ? A combined NMR and molecular dynamics study. *J. chem. Soc., Perkin Trans. 2*., 1315.

Bradbrook GM, Gleichmann T, Harrop SJ, Habash J, Raftery J, Kalb J, Yariv J, Hillier IH, Helliwell JR (1998) X-ray and molecular dynamics studies of concanavalin-A glucoside and mannoside complexes - Relating structure to thermodynamics of binding. *Journal of the Chemical Society-Faraday Transactions*. 94,1603.

Ewing, T.J.A. and Lybrand, T.P. (1994) A Comparison of Perturbation Methods and Poisson-Boltzmann Electrostatics Calculations for Estimation of Relative Solvation Free Energies. *J Phys Chem* **98**:1748-1752.

D.A. Pearlman, D.A. Case, J.W. Caldwell, W.S. Ross, T.E. Cheatham, III, S. DeBolt, D. Ferguson, G. Seibel, and P. Kollman. AMBER, a package of computer programs for applying molecular mechanics, normal mode analysis, molecular dynamics and free energy calculations to simulate the structural and energetic properties of molecules. Comp. Phys. Commun.91,1-41 (1995).