Supporting Material

We included the CHARMM RTF files for the CH_3CH_2SH and $CH_3CH_2S^-$ molecules used in the calculations. They have been slightly modified (see comments in the file) based on entries from the top_all22_model.inp, which is a standard file distributed with CHARMM.

```
RESI ETSH        0.00 ! ethanethiol, Dzung Nguyen
GROUP
Atom h1   ha     0.09 !   H1  H4   H5
Atom h2   ha     0.09 !     \   \  /
Atom h3   ha     0.09 !  H2-CM1--CM2
Atom cm1  ct3   -0.27 !     /      \
GROUP                 !   H3        S3--H6
Atom h4   ha     0.09
Atom h5   ha     0.09
Atom cm2  ct2   -0.11
Atom s3   s     -0.23
Atom h6   hs     0.16
Bond cm1 h1  cm1 h2  cm1 h3
Bond cm1 cm2 cm2 h4  cm2 h5
bond cm2 s3  s3  h6


RESI ES1        -1.00 ! ethylthiolate, adm jr.
GROUP
ATOM S    S     -0.80 !  H21  H11 H12 (ORG: SS)
ATOM C1   CT2   -0.38 !     \   \  /  (ORG: CS)
ATOM C2   CT3   -0.27 ! H22--C2--C1
ATOM H21  HA     0.09 !     /      \
ATOM H22  HA     0.09 !  H23        S (-)
ATOM H23  HA     0.09
ATOM H11  HA     0.09
ATOM H12  HA     0.09
BOND  S  C1  C1 H11 C1 H12 C1 C2
BOND  C2 H21 C2 H22 C2 H23
```

Non-bonded parameters (from par_all22_prot.inp):

```
CT2     0.000000  -0.055000     2.175000   0.000000  -
0.010000     1.900000 ! ALLOW   ALI
               ! propane pure solvent properties, adm jr,
2/3/92

CT3     0.000000  -0.080000     2.060000   0.000000  -
0.010000     1.900000 ! ALLOW   ALI
```

HA 0.000000 -0.022000 1.320000 ! ALLOW PEP ALI POL SUL ARO PRO ALC
! methane/ethane a.i. and ethane pure solvent, adm jr, 2/3/92
HS 0.000000 -0.100000 0.450000 ! ALLOW SUL
! methanethiol pure solvent, adm jr., 6/22/92

S 0.000000 -0.450000 2.000000 ! ALLOW SUL ION
! adm jr., 3/3/92, methanethiol/ethylmethylsulfide pure solvent