

Supplementary Information

Figure S1. Amino acid sequence alignment of DehD and HadD. An alignment with the consensus greater than 50% is shown in red blocks with white characters. The interacting residues of DehD are shown by black stars.



Data S1. em.mdp file for Molecular dynamic simulation.

```
define          = -DFLEXIBLE
constraints      = none
integrator       = steep
dt              = 0.002 ; ps!
nsteps          = 400
nstlist         = 10
ns_type         = grid
rlist           = 1.0
coulombtype     = PME
rcoulomb        = 1.0
vdwtype         = cut-off
rvdw            = 1.4
optimize_fft    = yes; ;Energy minimizing stuff;
Emtol           = 1000.0
Emstep         = 0.01
```

Date S2. pr.mdp file for Molecular dynamic simulation.

```

define                = -DPOSRES
constraints            = all bonds
Integrator            = md
dt                    = 0.002      ; ps!
nsteps                = 25000      ; total 50.0 ps
nstcomm               = 10
nstxout                = 250        ; collect data every 0.5 ps
nstvout               = 1000
nstfout               = 0
nstlog                = 10
nstenergy             = 10
nstlist               = 10
ns_type               = grid
rlist                 = 1.0
coulombtype           = PME
rcoulomb              = 1.0
vdwtype               = cut-off
rvdw                  = 1.4
pme_order              = 4          ; Use 6, 8 or 10 when running in parallel
ewald_rtol            = 1e-5
optimize_fft          = yes
DispCorr              = no         ; Berendsen temperature coupling is on
Tcoupl                = v-rescale
taut_t                = 0.1        0.1
tc-grps               = protein    non-protein
ref_t                 = 300        300 ; Pressure coupling is on
Pcoupl                = parrinello-rahman
Pcoupltype            = isotropic
tau_p                 = 0.5
compressibility        = 4.5e-5
ref_p                 = 1.0        ; Generate velocities is on at 300 K.
gen_vel               = yes
gen_temp               = 300.0
gen_seed              = 173529

```

Date S3. md.mdp file for Molecular dynamic simulation.

```

constraints            = all-bondsIntegrator      = md
dt                    = 0.002      ; ps!
nsteps                = 500000     ; total 1000 ps
nstcomm               = 10
nstxout                = 500        ; collect data every 1 ps
nstvout               = 0
nstfout               = 0
nstlist               = 10
ns_type               = grid
rlist                 = 1.0
coulombtype           = PME
rcoulomb              = 1.0
vdwtype               = cut-off
rvdw                  = 1.4
pme_order              = 4          ; Use 6, 8 or 10 when running in parallel
ewald_rtol            = 1e-5
optimize_fft          = yes

```

Date S3. Cont.

DispCorr = no ; Berendsen temperature coupling is on
 Tcoupl = v-rescale
 taut_t = 0.1 0.1
 tc-grps = protein non-protein
 ref_t = 300 300 ; Pressure coupling is on
 Pcoupl = parrinello-rahman
 Pcoupltype = isotropic
 tau_p = 0.5
 compressibility = 4.5e-5
 ref_p = 1.0 ; Generate velocities is on at 300 K.
 gen_vel = yes
 gen_temp = 300.0
 gen_seed = 173529

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