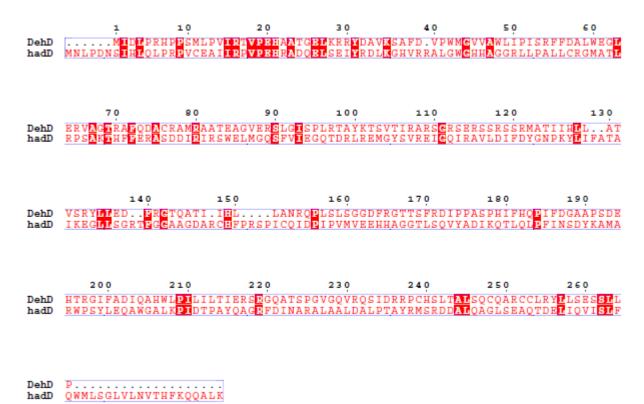
## **Supplementary Information**

**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	= -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			
rcoulomb	= 1.0		
vdwtype	= cut-off		
rvdw	= 1.4		
· -	= 4; Use 6, 8 or 10 when running in parallel		
_	= 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			
ref_p	= $1.0$ ; Generate velecities is on at 300 K.		
gen_vel	= yes		
gen_temp	= 300.0		
gen_seed	= 173529		

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

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

constraints	= all-bonds	sIntegrator = 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 To sourt	-	erendsen 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 velecities is on at 300 K.
gen_vel	= yes	
gen_temp	= 300.0	
gen_seed	= 173529	

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