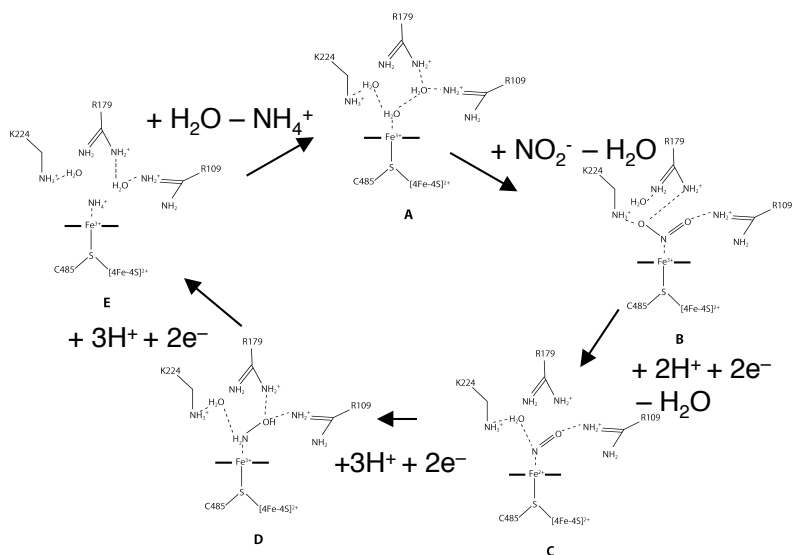
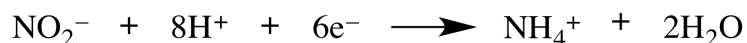


同化型亜硝酸還元酵素(aNiR)の高次機能の理論的解明

○庄司光男¹、實本英之²、鴨志田良和³

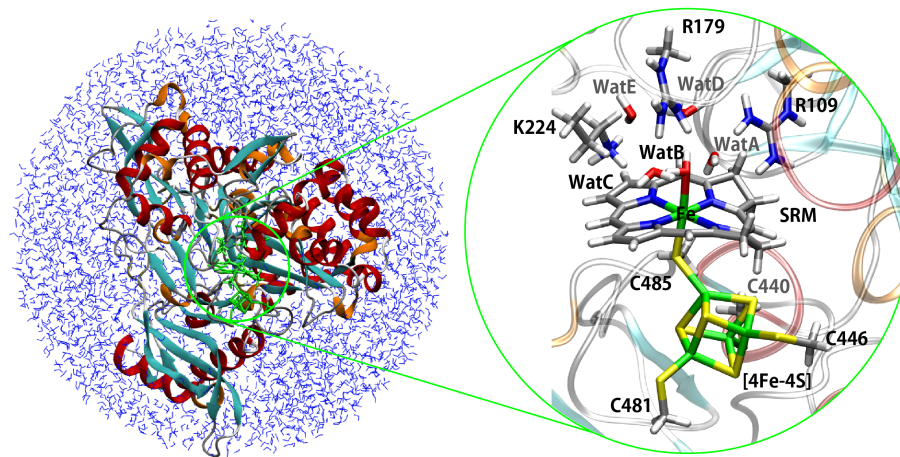
¹筑波大・数理 ²東大・情報基盤セ ²DeNA

aNiRの反応



S. Nakano, et al, *Proteins* 80, 2035 (2012).

- reaction mechanism
double electron transfer ?
- proton transfer steps
- reaction energy profile



Method: QM/MM: UB3LYP/AMBER99
 Basis: 6-31G* basis sets (1000 basis sets)
 Program: NWChem
 Computer: FX10
 #QM:120, #MM(els, vdw) :2,200
 #Total : 26,000 (PDB-ID: 3VKR)
 #Atoms in Opt. :500
 Water droplet, short relaxation MD

これまでのJHPCNによる研究成果(H24,25,26年度)

- [1] M. Shoji et al, *CPL*, DOI: 10.1016/j.cplett.2014.05.063, 2014.
- [2] M. Shoji, Y. Kamoshida et al, *JACS*, 136, 4525, 2014.
- [3] K.Hanaoka, M.Shoji et al, *J. Biomol. Struct. Dyn.*, 2013.
- [4] M. Shoji, et al, *Mol. Phys*, 112, 3-4, 393, 2013.