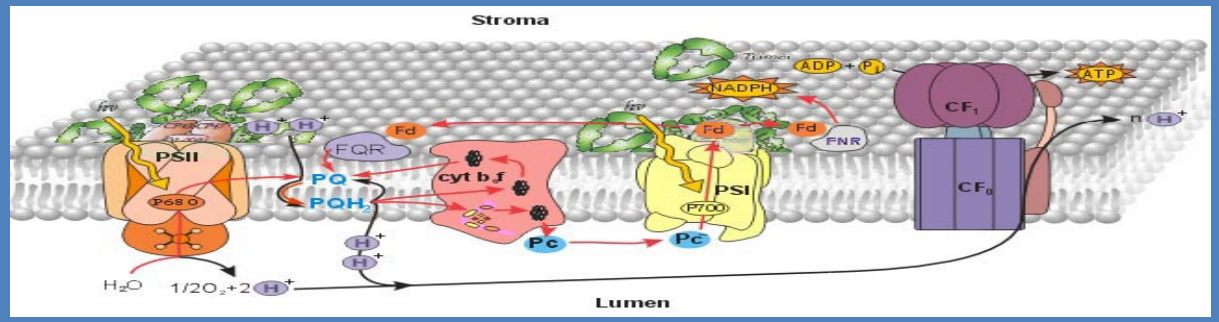

Достижения и некоторые нерешенные проблемы биофизики

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МГУ, Биологический факультет

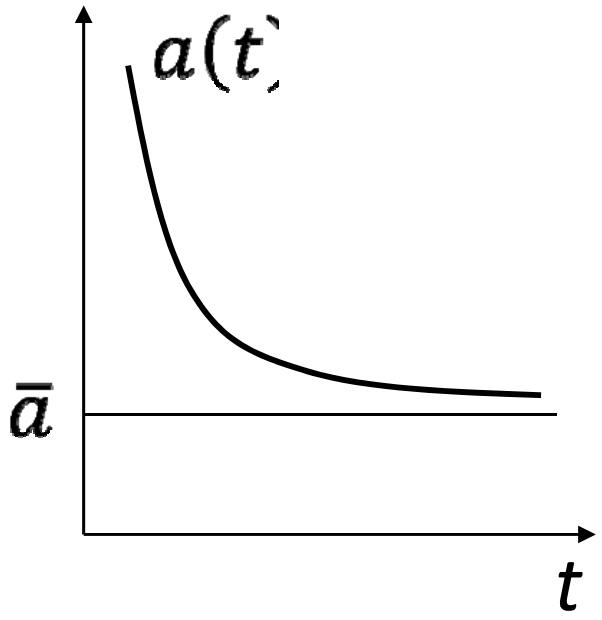
кафедра биофизики

The entire cell can be viewed as factory that contains an elaborate net work of interlocking assembly lines, each of which is composed of set large protein machines

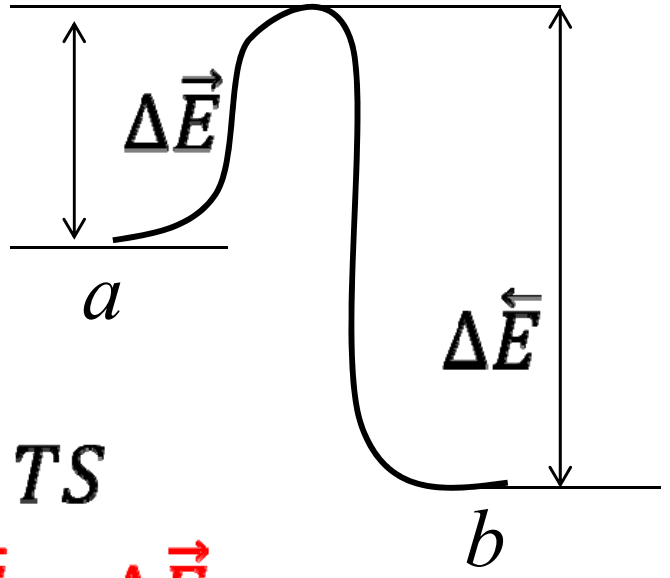
Modern machines comprised of subsystems from different "domains" (I.e., mechanical, electrical, fluid, thermal) are often analyzed by energy-based approach

Any real understanding of the function of a protein machine will require not only its resting structure in atomic detail, but also a knowledge of the kinetics and energetic of each of its reaction intermediates

Extracts from the paper by ***Bruce Alberts***
Cell, vol.92, 291 – 294, February, 1998



$$a \underset{\overleftarrow{k}}{\overset{\vec{k}}{\rightleftarrows}} b$$



$$G = U - TS$$

$$\Delta G = \Delta\overleftarrow{E} - \Delta\vec{E}$$

$$\vec{v} = \vec{k}a$$

$$\overleftarrow{v} = \overleftarrow{k}b$$

$$\vec{k} = k_0 e^{-\Delta\vec{E}/k_B T}$$

$$\overleftarrow{k} = k_0 e^{-\Delta\overleftarrow{E}/k_B T}$$

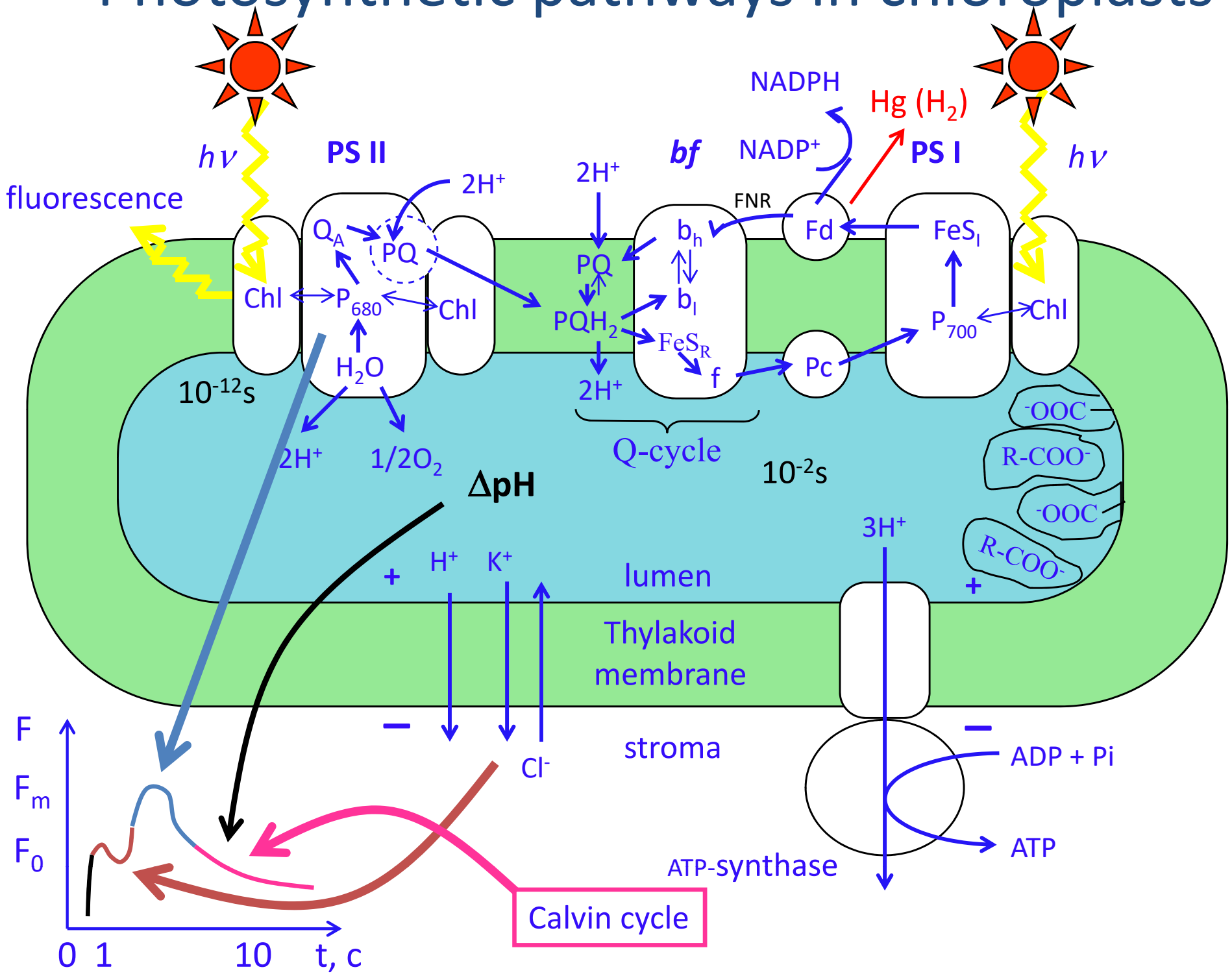
$$\vec{v} = \overleftarrow{v}$$

при $\vec{k}\bar{a} = \overleftarrow{k}\bar{b} \Rightarrow$

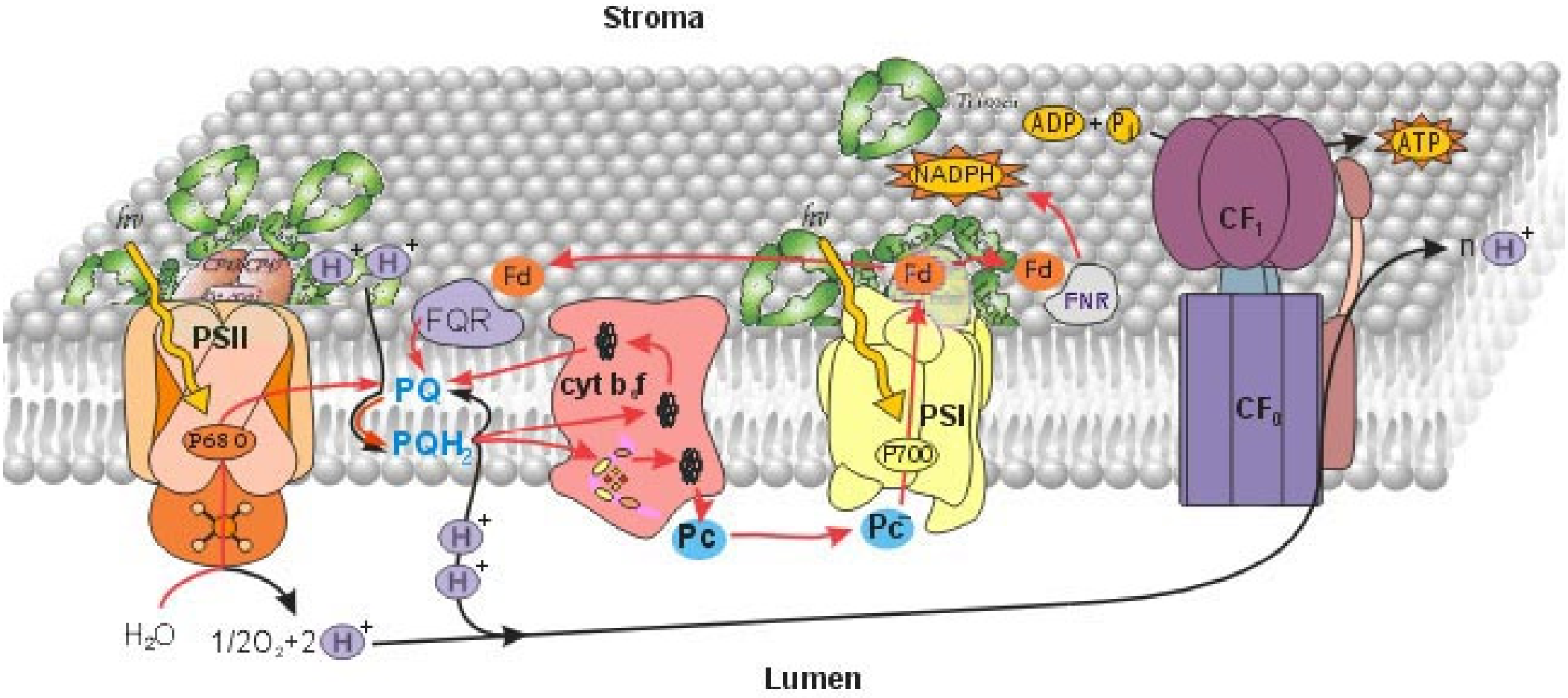
$$K(T) = \frac{\bar{b}}{\bar{a}} = \frac{\vec{k}}{\overleftarrow{k}} = k_0 e^{\Delta G/k_B T}$$

$$\Delta G = RT \ln K(T)$$

Photosynthetic pathways in chloroplasts

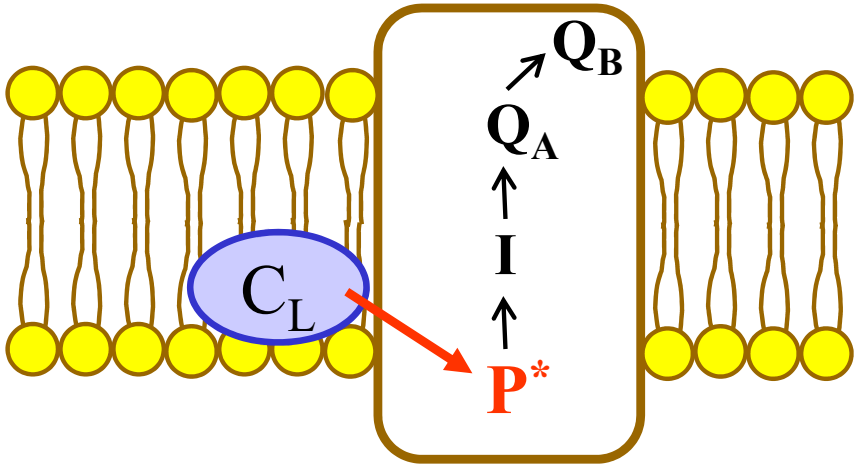


Space distribution of protein electron carriers in a membrane



Времена внутримолекулярных движений белка

Первичные процессы фотосинтеза и зрения	$10^{-13} – 10^{-12}$ с
Динамика атомов и групп атомов	$10^{-12} – 10^{-11}$ с
Динамика боковых цепей белков	$10^{-11} – 10^{-7}$ с
Движение доменов и субъединиц	$10^{-8} – 10^{-5}$ с
Лиганд-рецепторные взаимодействия	$10^{-6} – 10^{-3}$ с
Кинетика сворачивания белковой глобулы	$10^{-4} – 10^{2}$ с

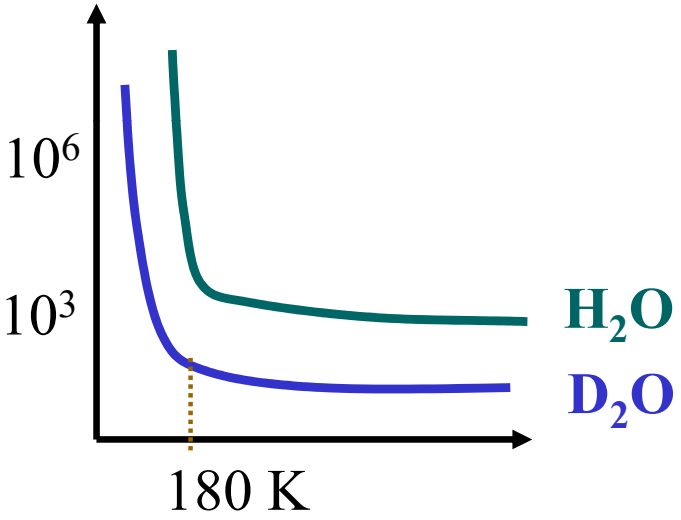


C_H, C_L → P^+ Mb - CO

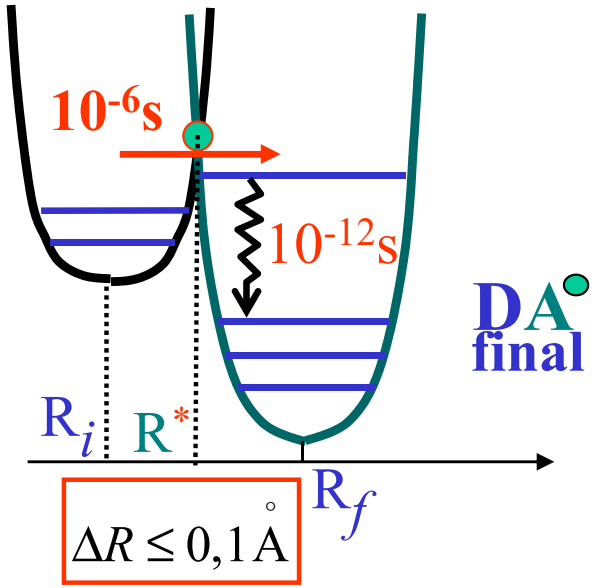
$P^* \rightarrow$ Bchl $\rightarrow$ Bpheo $\rightarrow Q_A$

$P^* \rightarrow$ Bpheo $\rightarrow Q_A \rightarrow Q_B$

$P_{700} \rightarrow A_0 \rightarrow A_1 \rightarrow F_X \rightarrow F_B \rightarrow F_A$



D A
init.

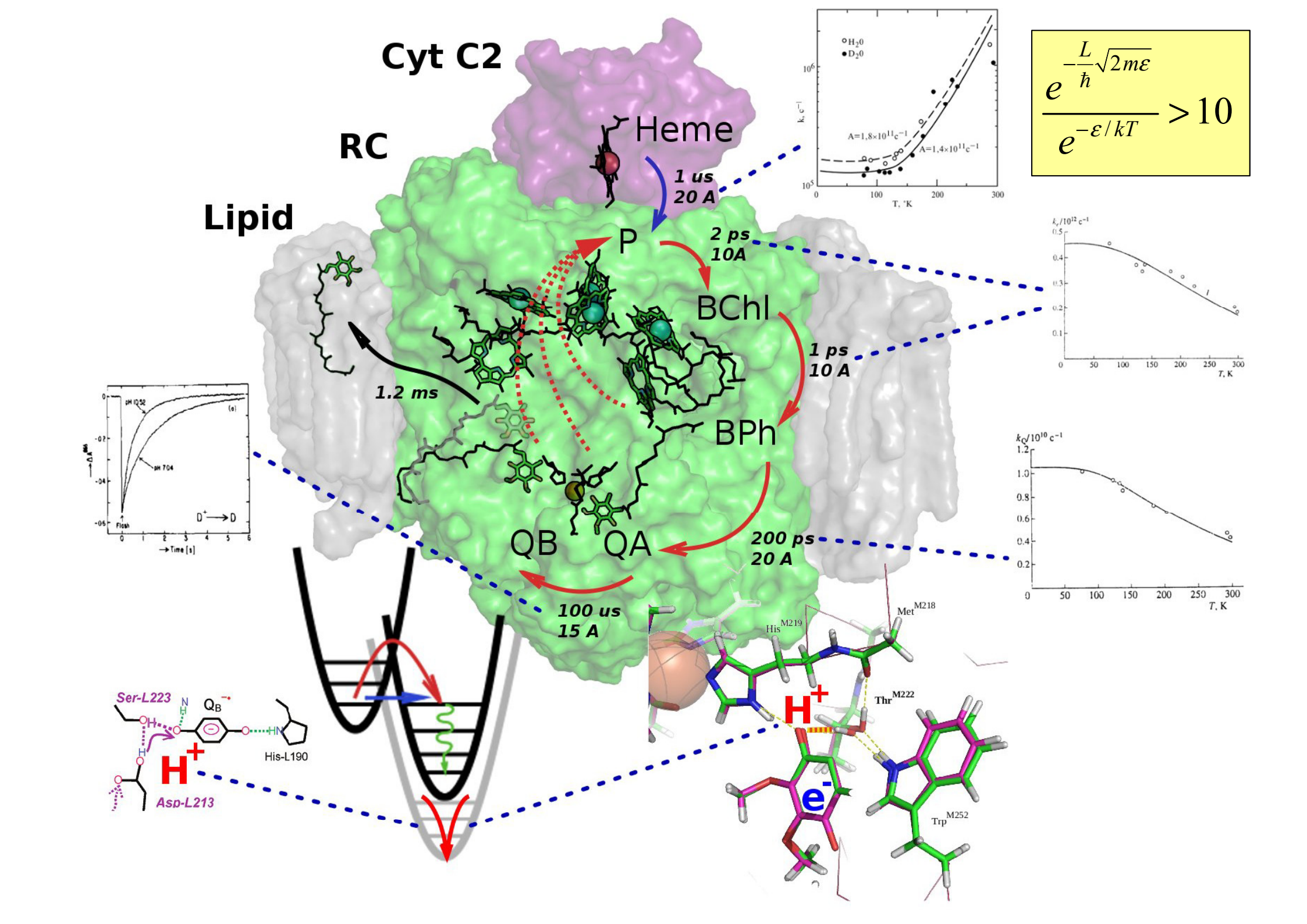


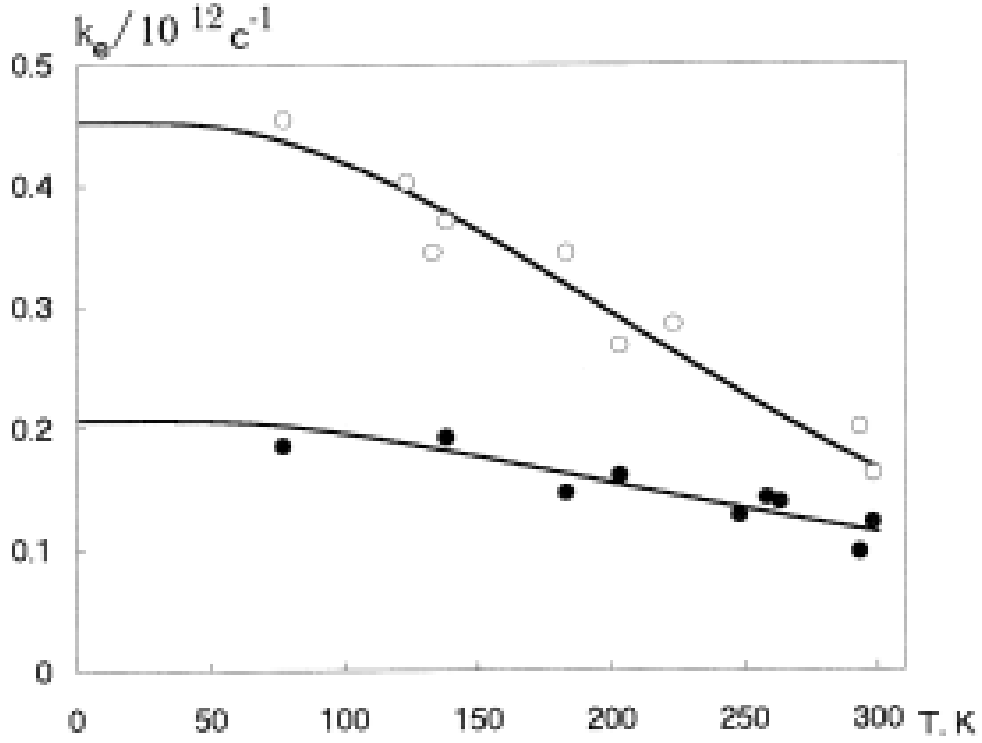
D A
final

$k_{tunn} > k_{act}$
at T<700K

$$\frac{e^{-\frac{L}{\hbar}\sqrt{2m\varepsilon}}}{e^{-\varepsilon/kT}} > 10$$

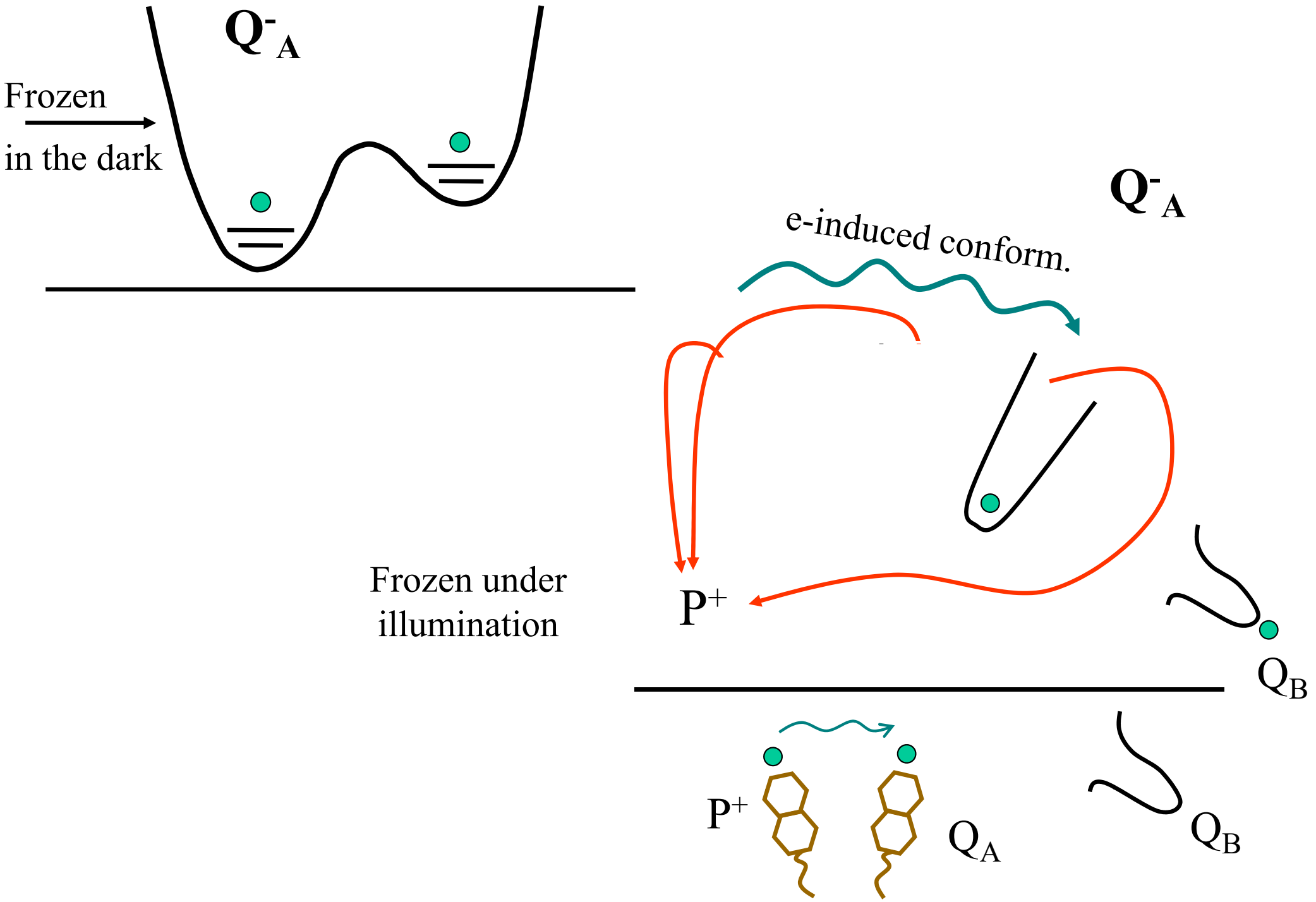
Electron tunneling in a reaction center


Cyt C2
RC
Lipid
Heme
1 us
20 A
P
2 ps
10A
BChl
1 ps
10 A
BPh
200 ps
20 A
QA
QB
100 us
15 A
1.2 ms
$\frac{e^{-\frac{L}{\hbar}\sqrt{2m\varepsilon}}}{e^{-\varepsilon/kT}} > 10$
H_2O
D_2O
A=1,8×10^11 c^-1
A=1,4×10^11 c^-1
T, °K
T, K
Ser-L223
$Q_B^{-\bullet}$
His-L190
Asp-L213
H^+
e^-
Met M218
His M219
Thr M222
Trp M252
D+ → D
Time [s]

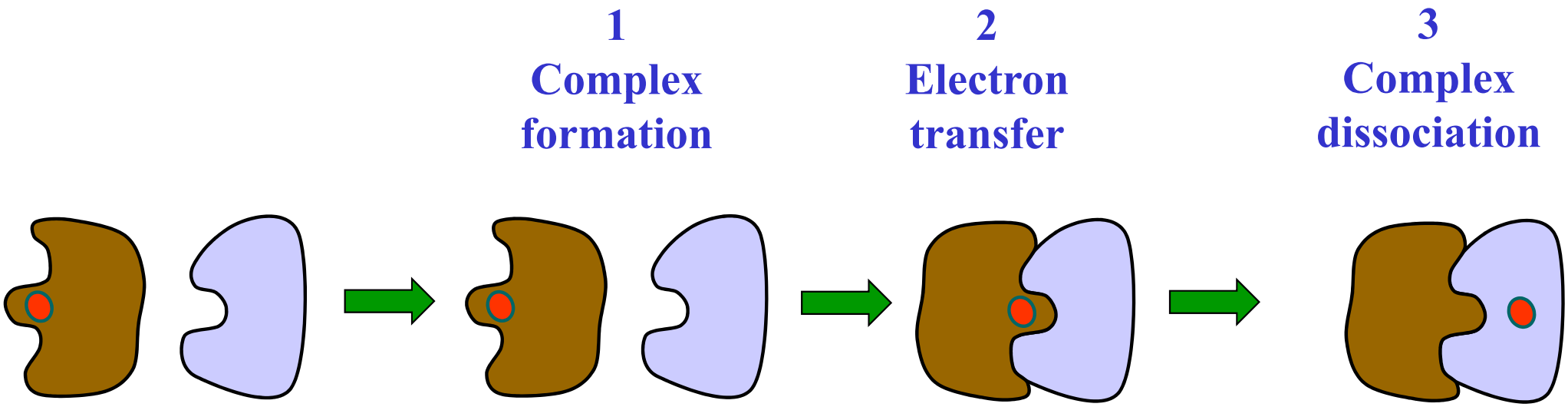


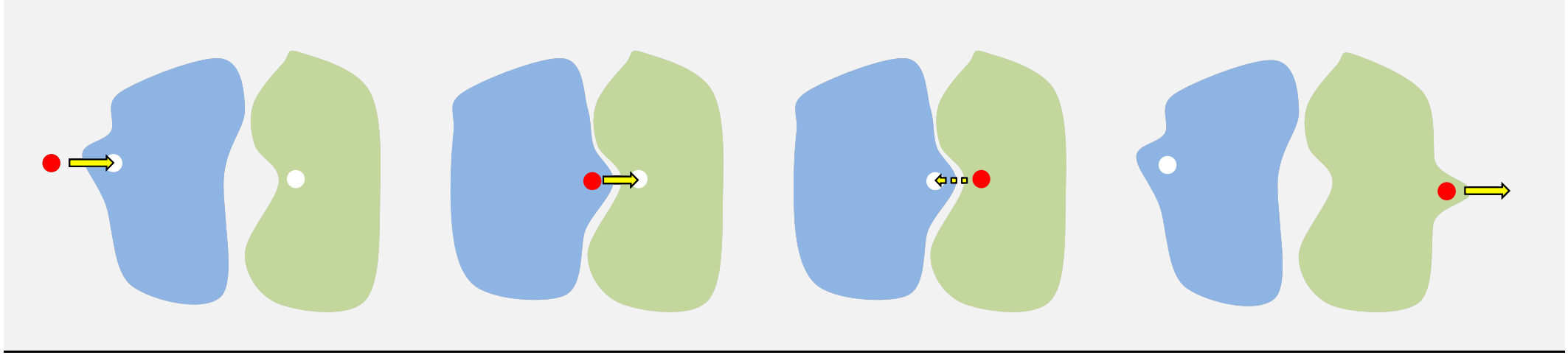
Температурная зависимость константы скорости разделения заряда в реакционном центре

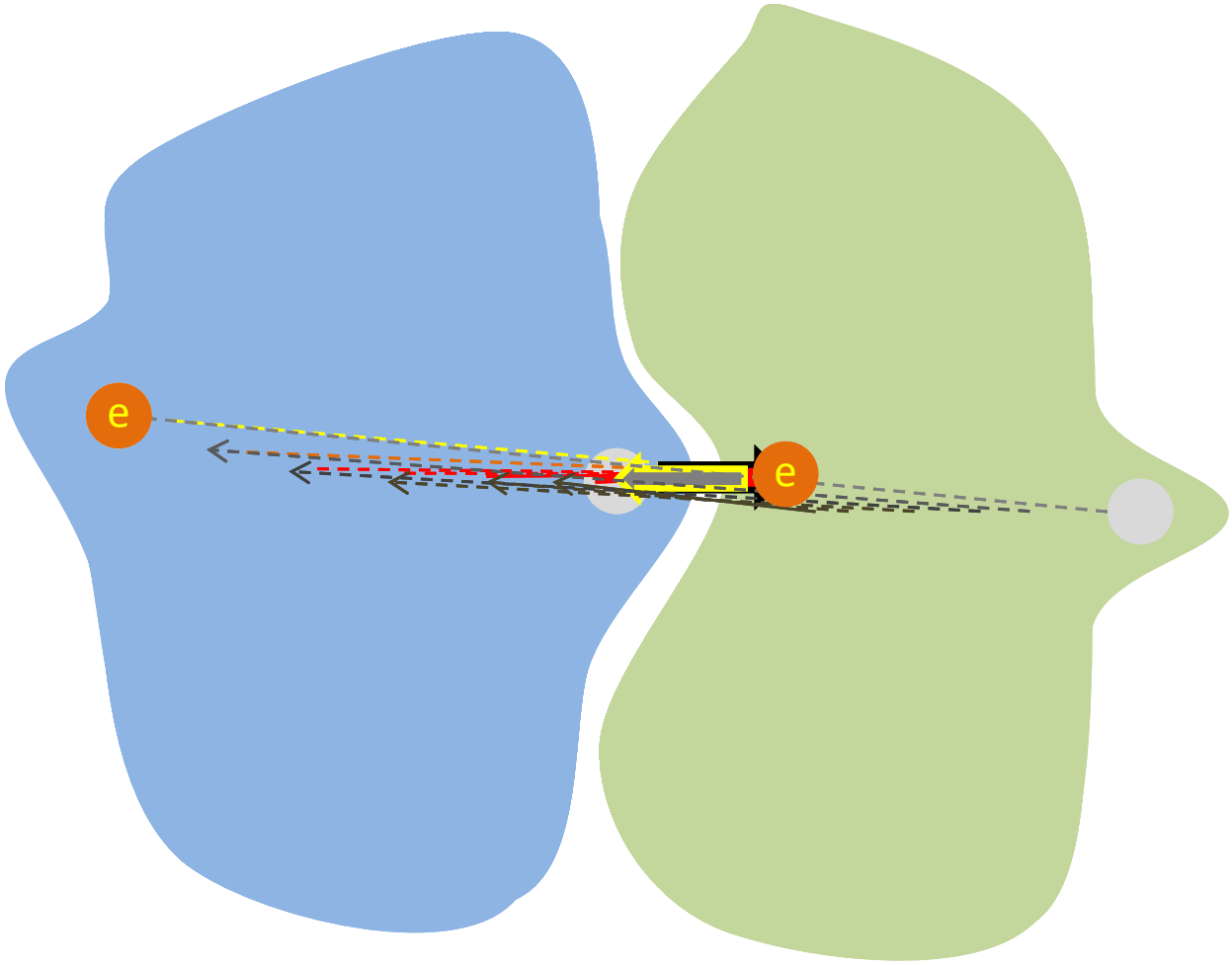
о: контроль, •: под действием DMSO.

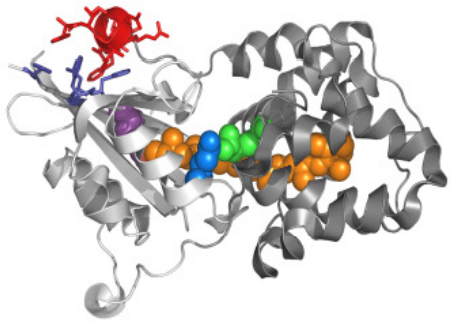

Q-A
Frozen
in the dark
Q-A
e-induced conform.
Frozen under
illumination
P+
QB
P+
QA
QB

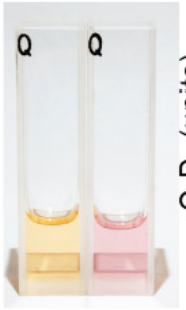
Protein Interaction

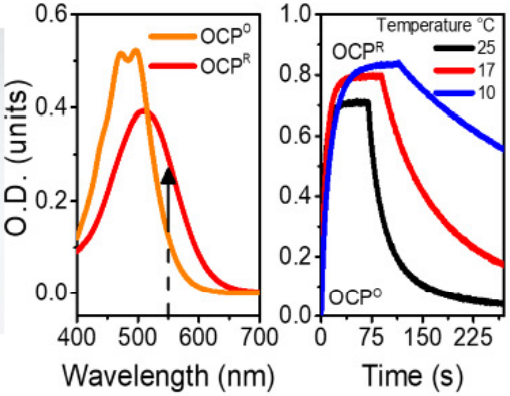




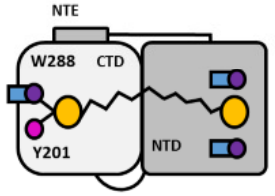

e
e





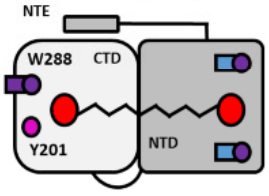


1. OCP^{O}
Inactive form



σF
>> (200 ns)$^{-1}$

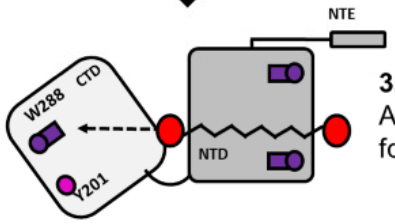
K_1
≈ (300 mks)$^{-1}$



2. OCP^{RI}
Red intermediate

Legend:
- Tryptophan
- Tyrosine
- Fluorescence
- Static quenching

K_2

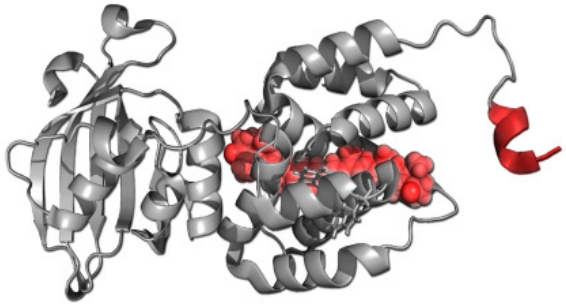


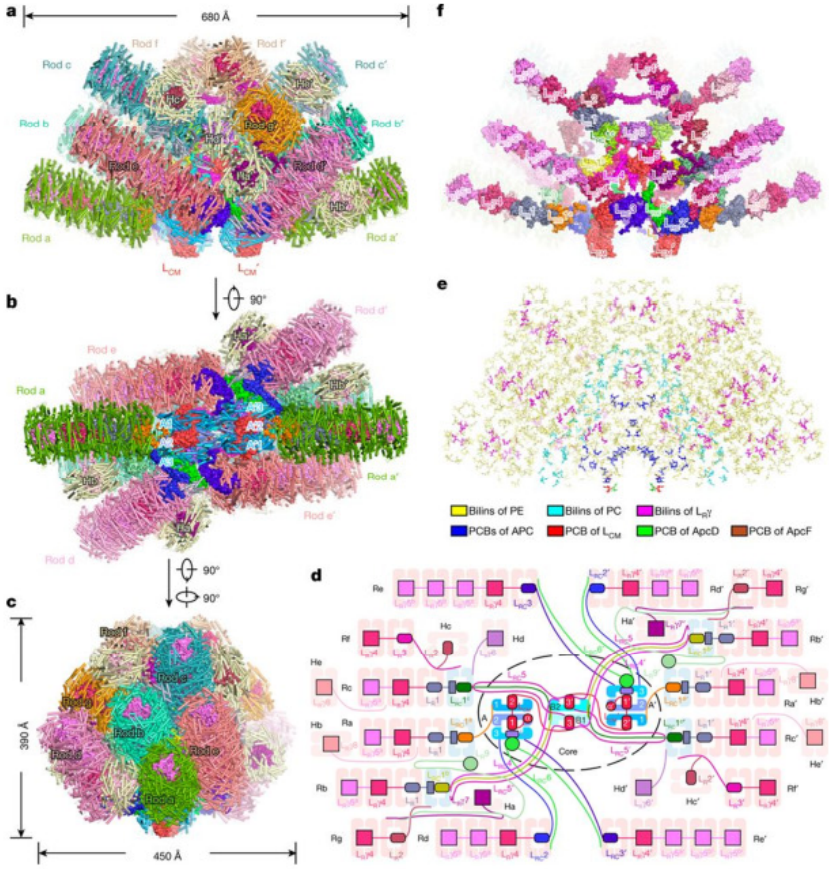
3. OCP^{R}
Active form

K_3
≈ (3 s)$^{-1}$

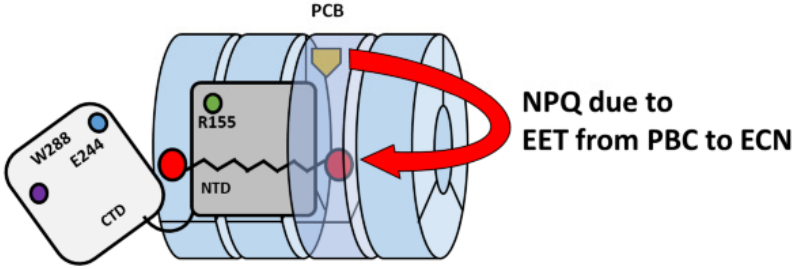
+PBs

kT



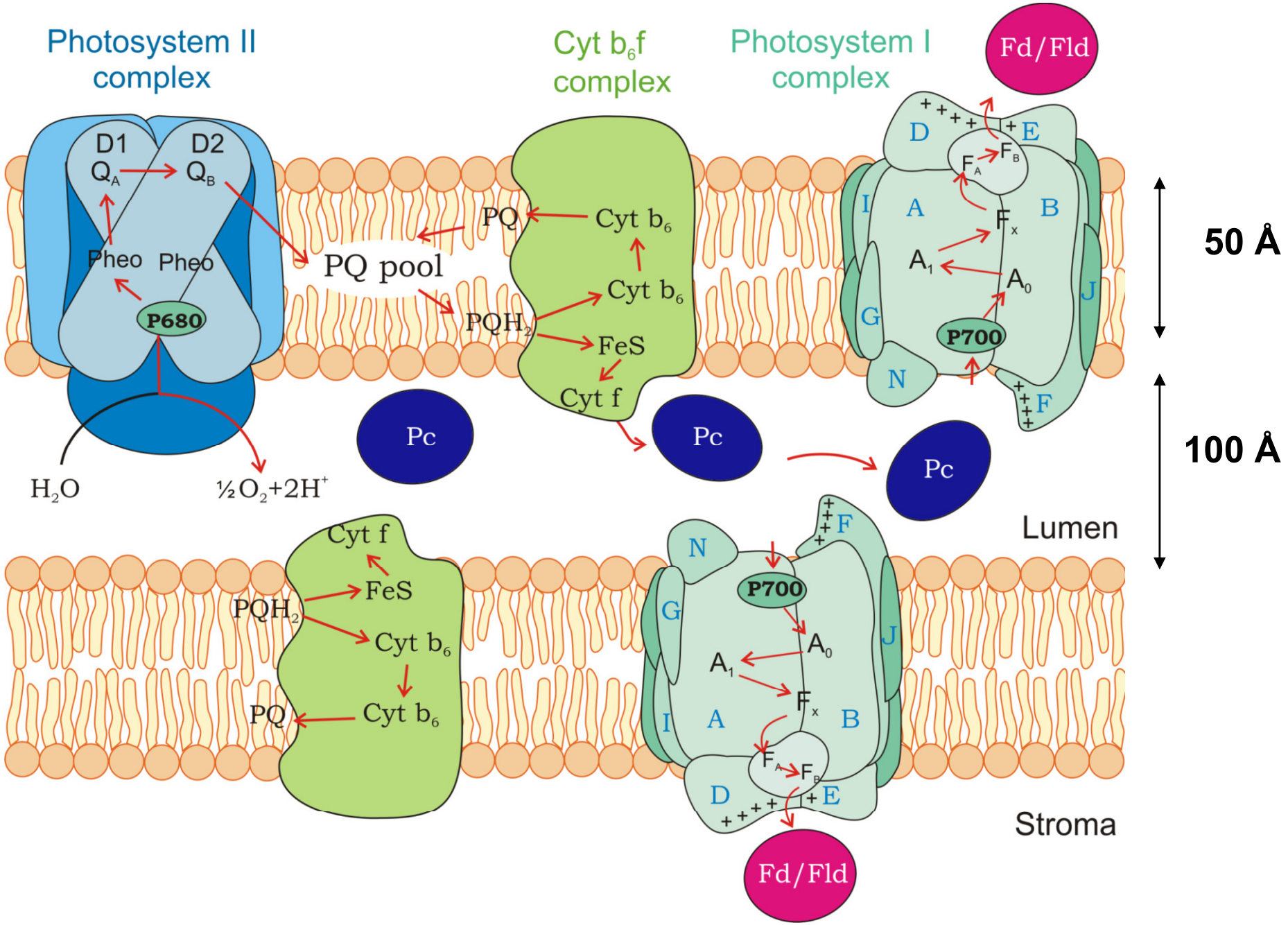


OCP^{R} + PBs

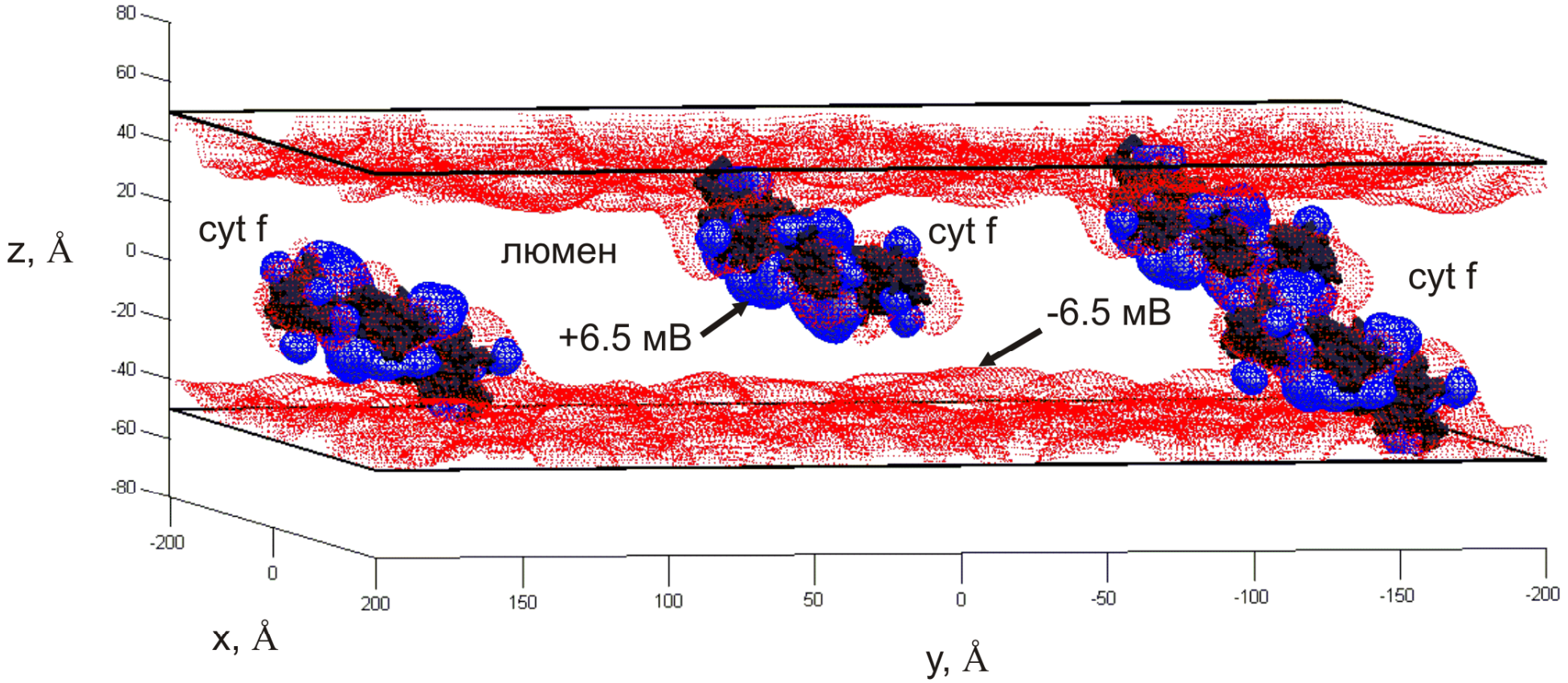


NPQ due to EET from PBC to ECN

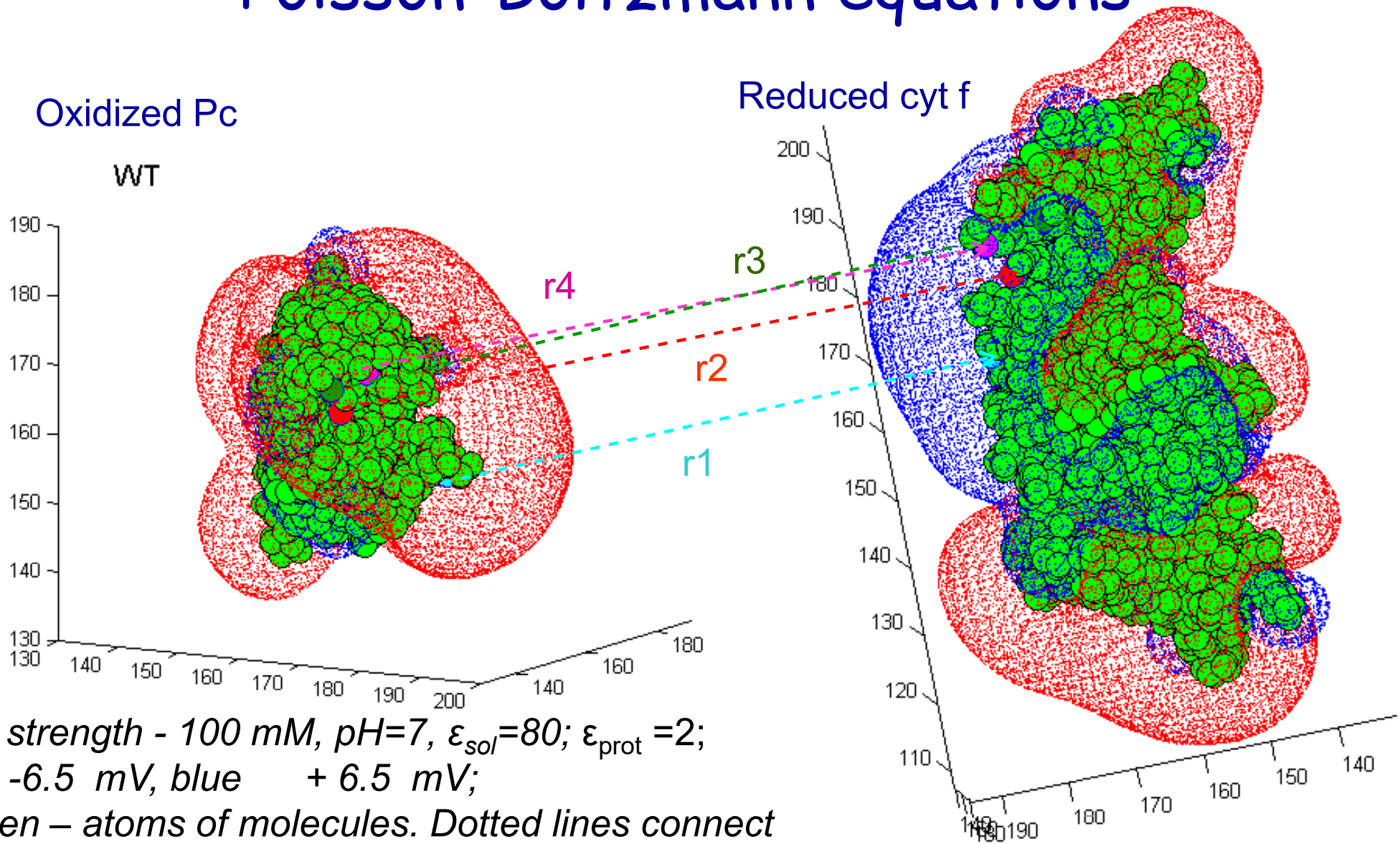
Thylakoid Membrane and Luminal Space



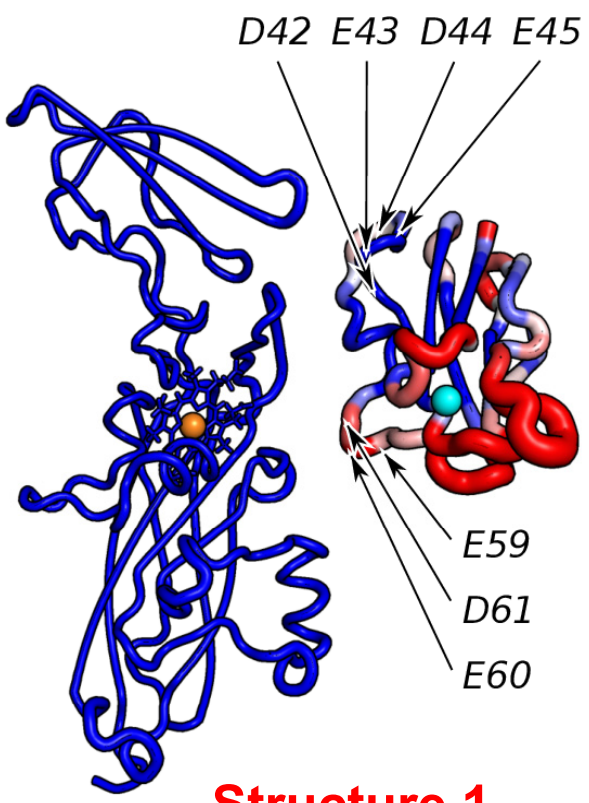
Эквипотенциальные поверхности (6.5 мВ) в люмене тилакоида хлоропласта, pH=7, I=100 моль/м^3, σ=-18 мКл/м^2



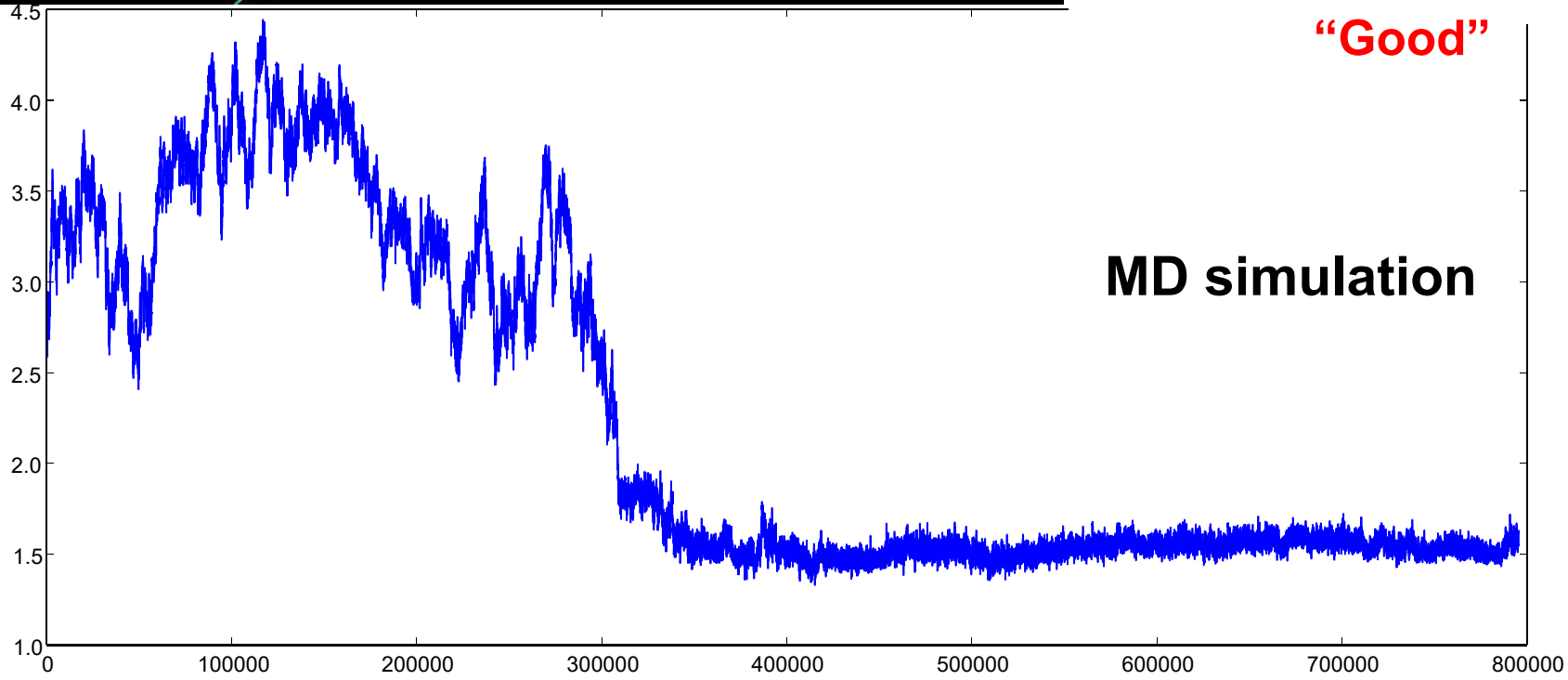
Equipotential surfaces calculated according to Poisson-Boltzmann equations



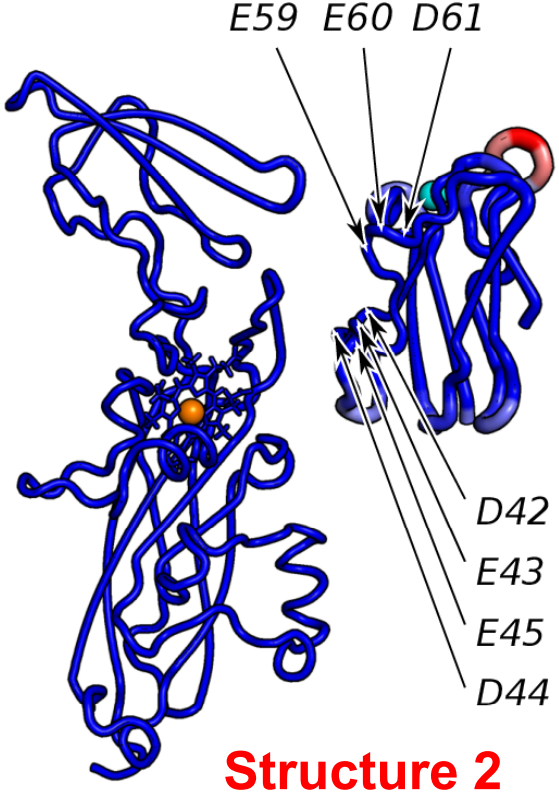
Ion strength - 100 mM, pH=7, ε_{sol}=80; ε_{prot} =2;
red -6.5 mV, blue + 6.5 mV;
green – atoms of molecules. Dotted lines connect residues on Pc and Cyt f that were used by simulation for calculation the distance between proteins



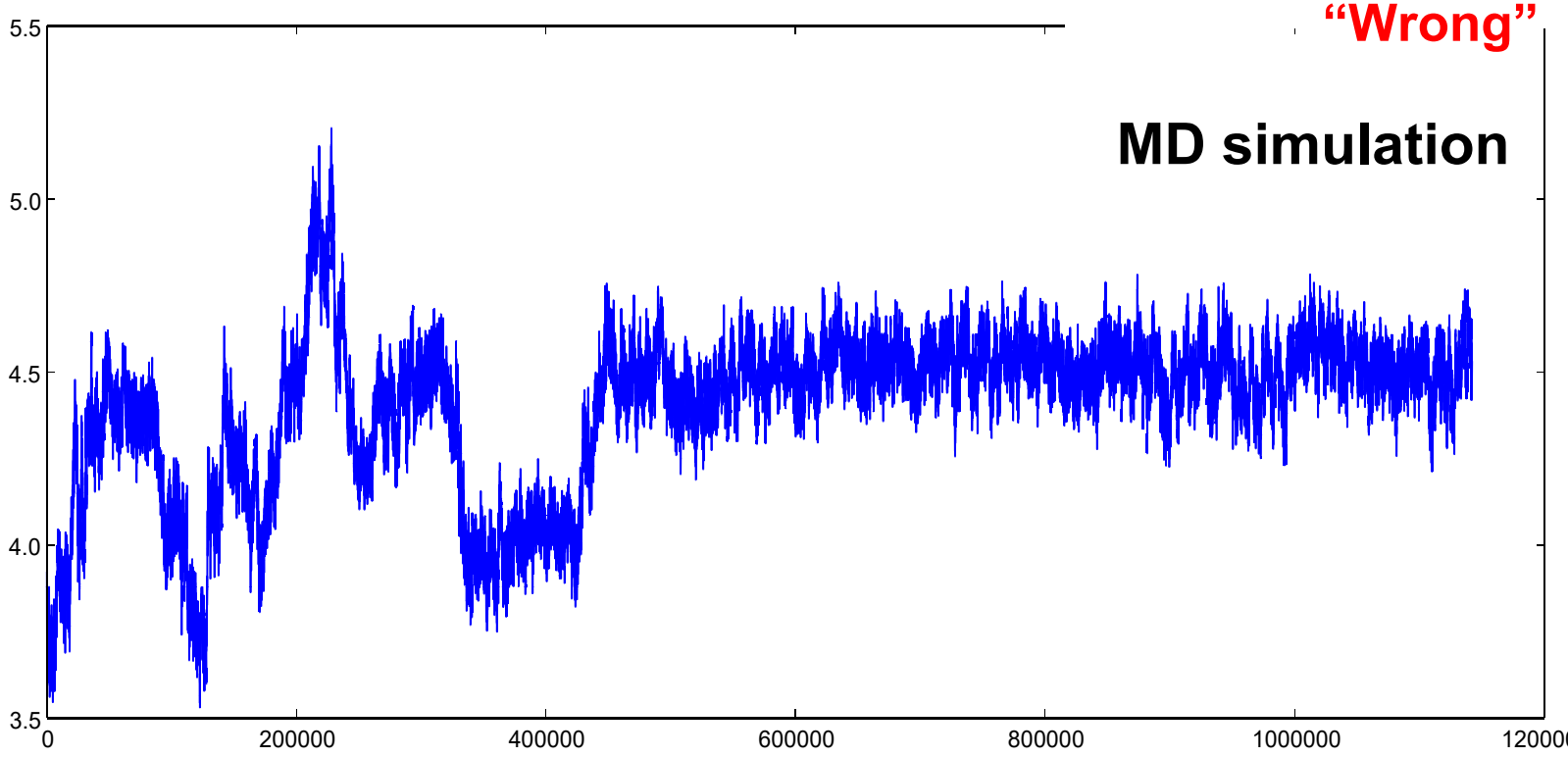
Structure 1
"Good"



MD simulation

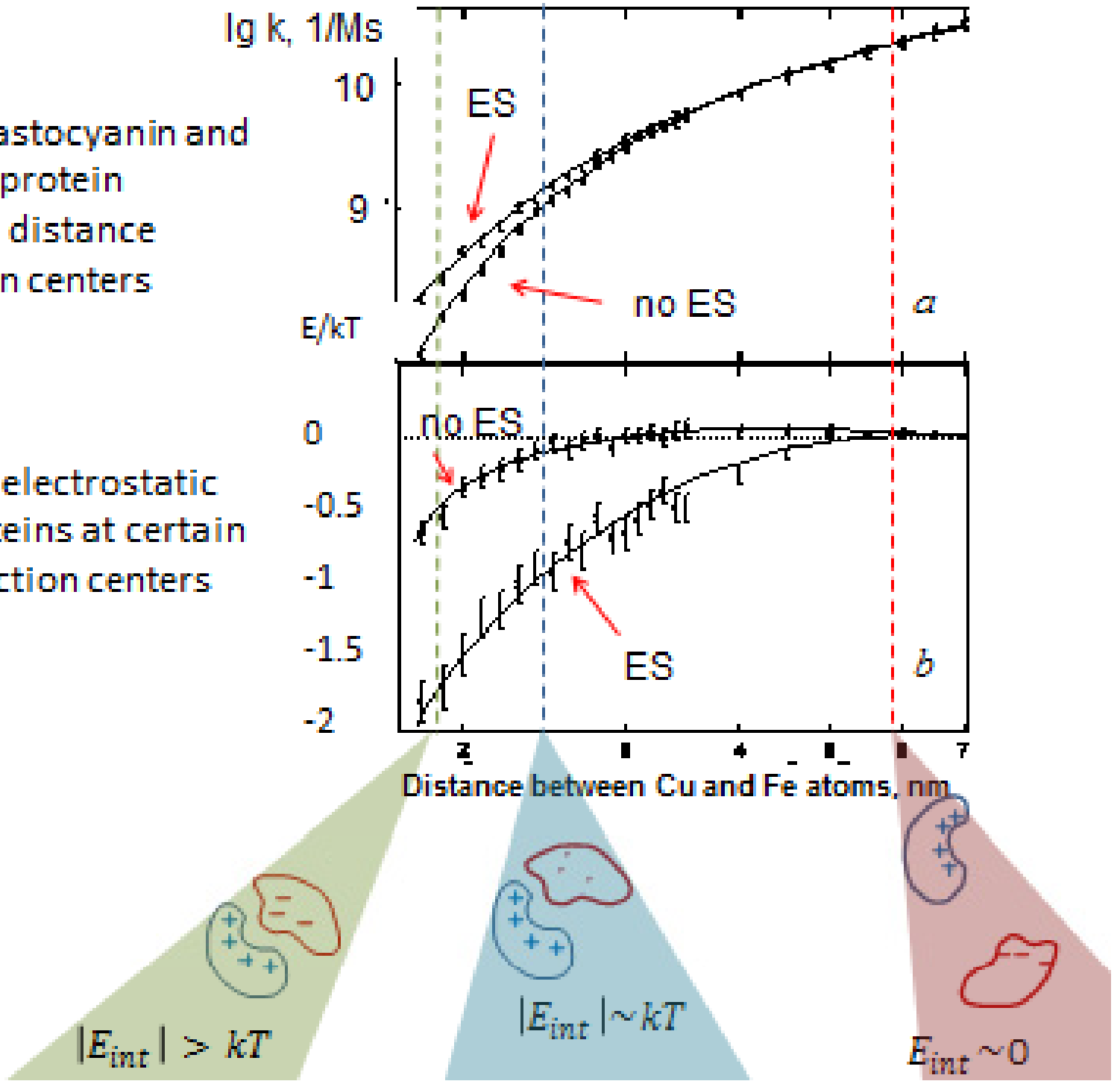


Structure 2
"Wrong"

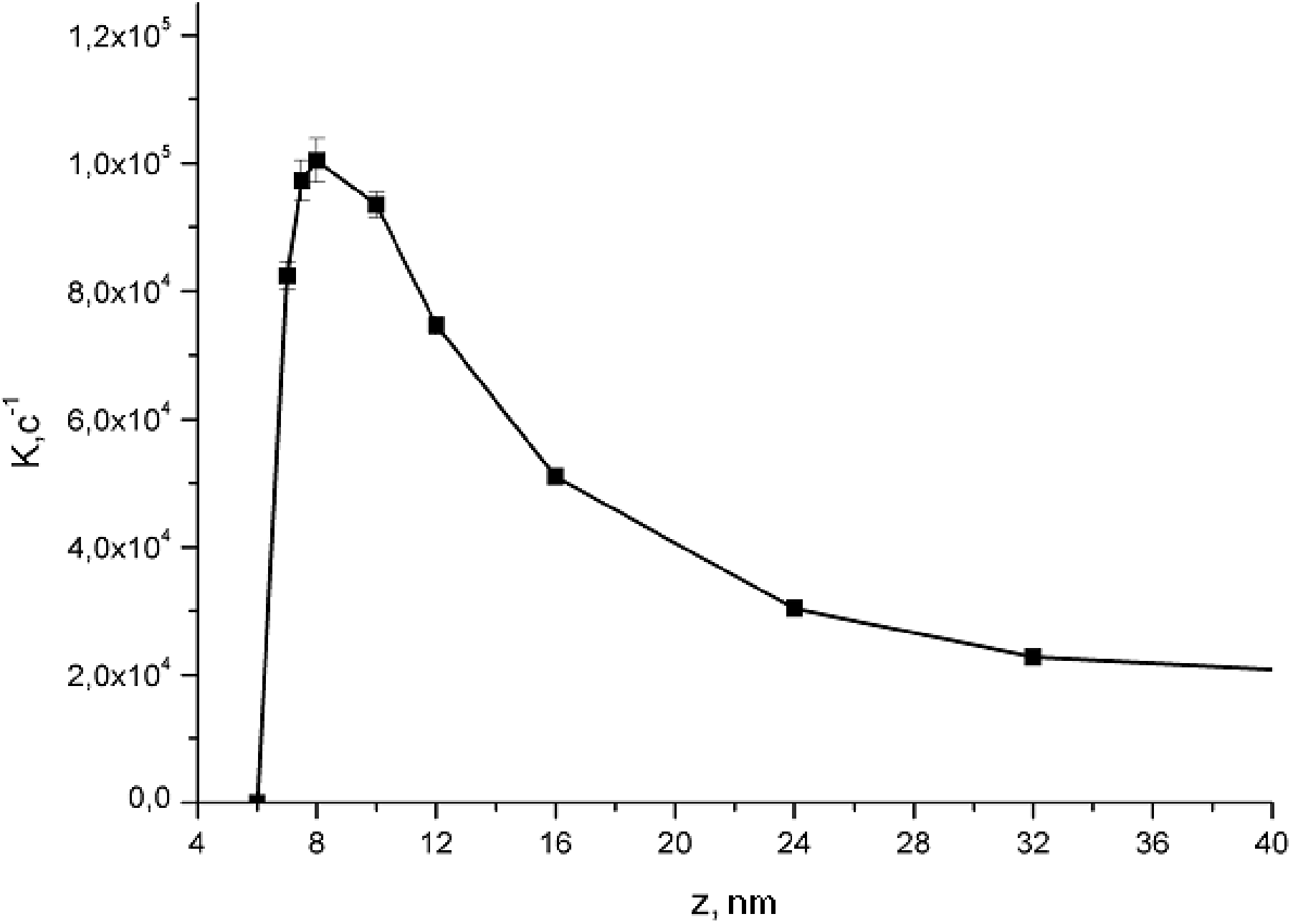


a – Dependence of plastocyanin and cytochrome f protein-protein encounter rate on the distance between their reaction centers

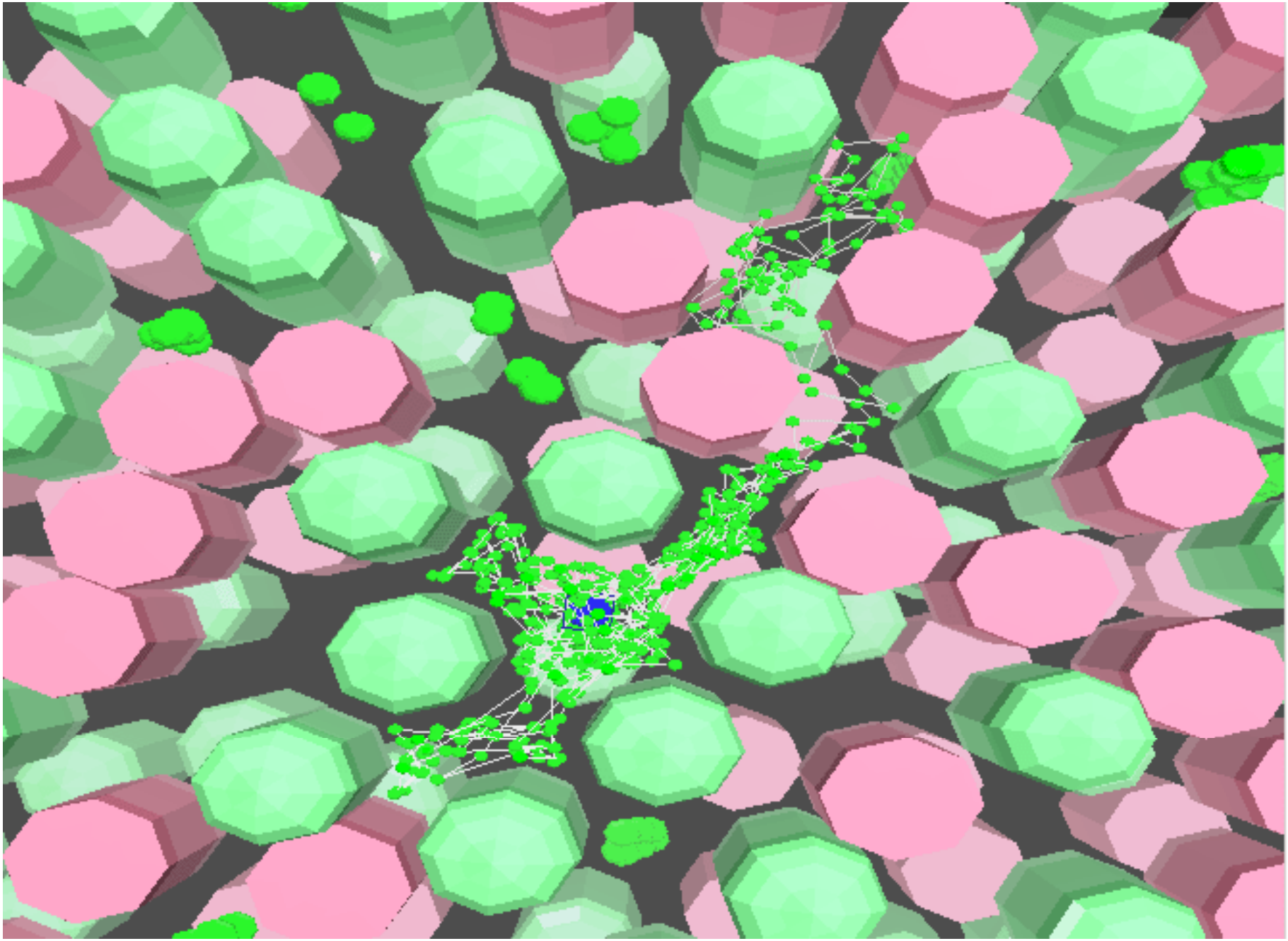
b – Average energy of electrostatic interaction of the proteins at certain distance between reaction centers



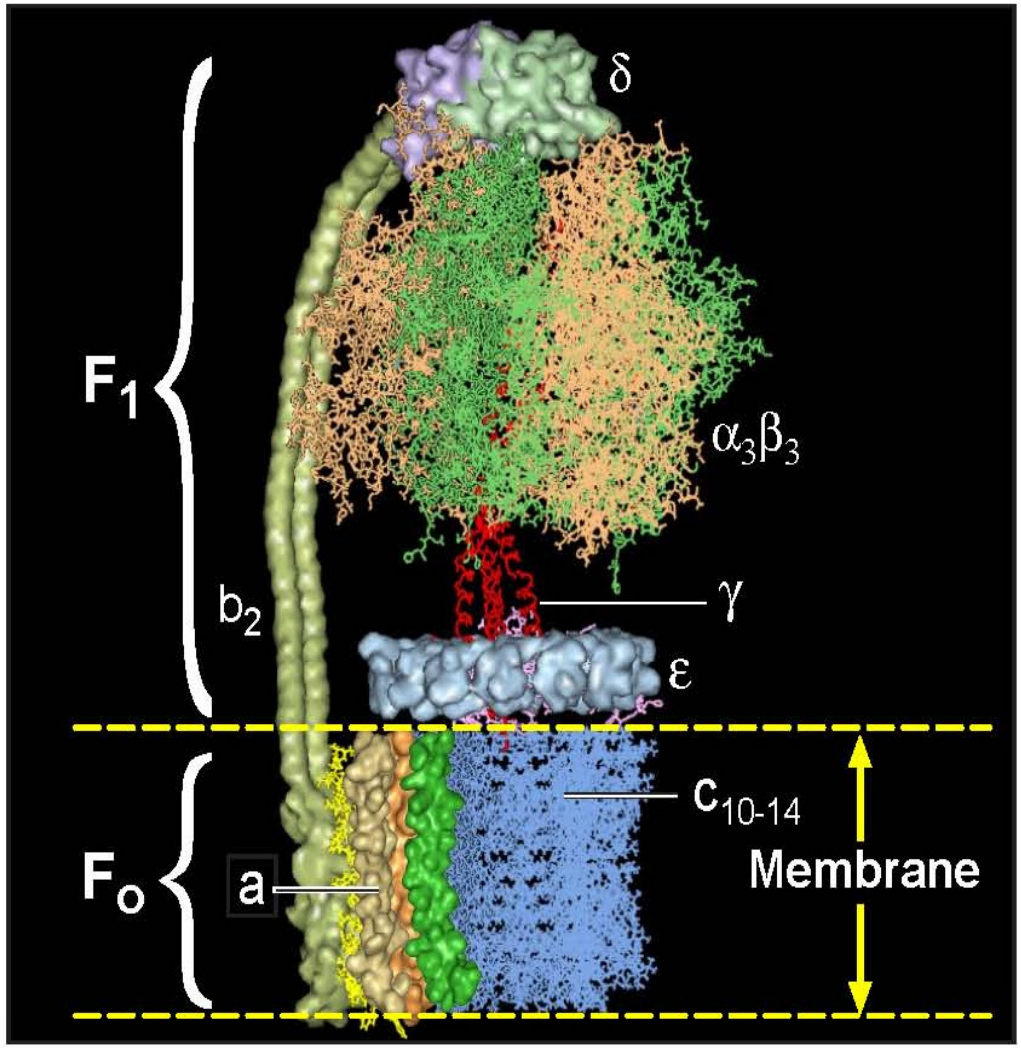
The dependence of Pc-Cyt *f* complex formation rate in lumen on the distance between thylakoid membranes

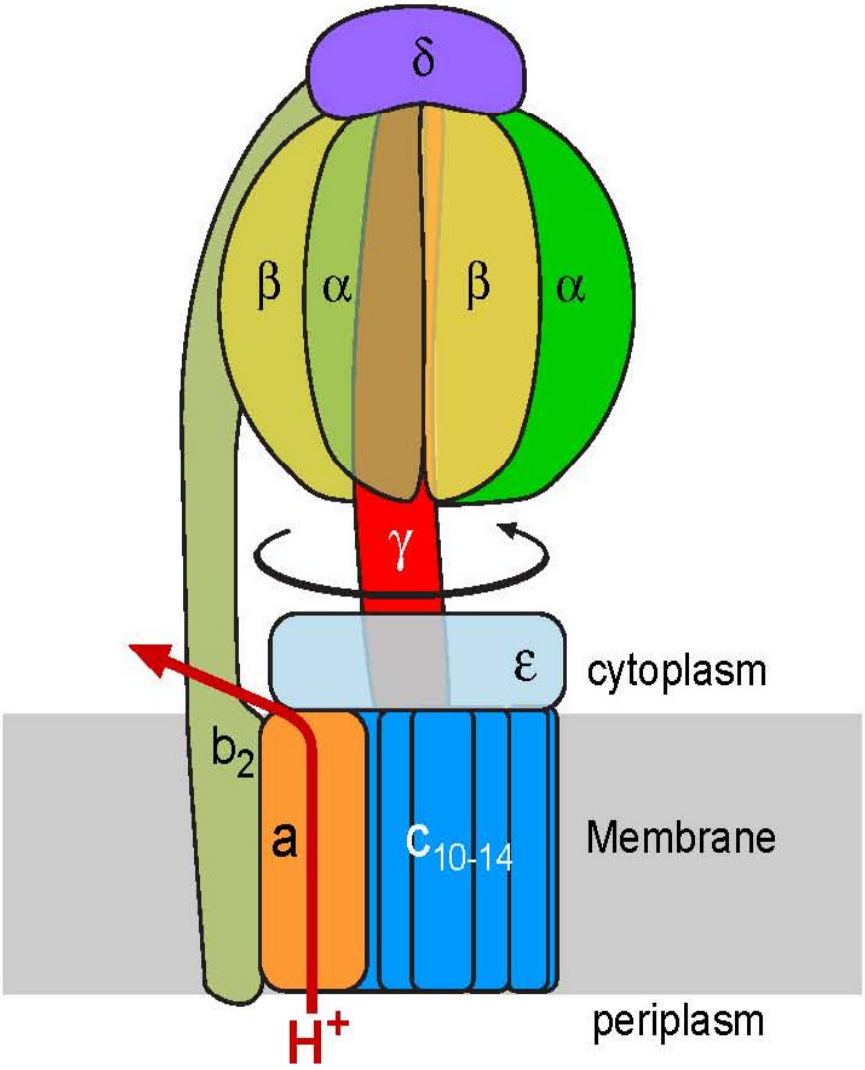


Plastoquinone trajectory in a thylakoid membrane



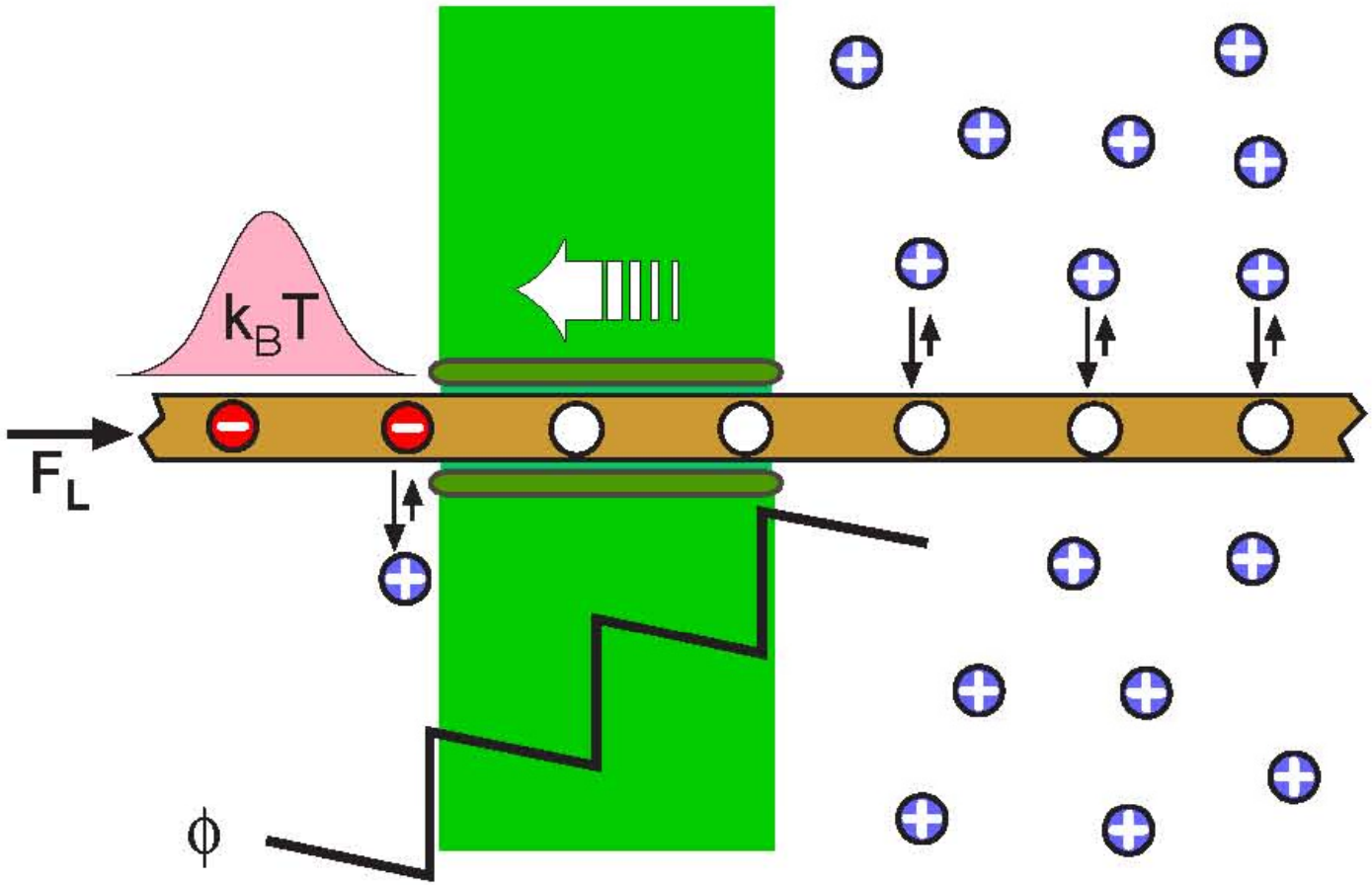
Структура АТФ-азы





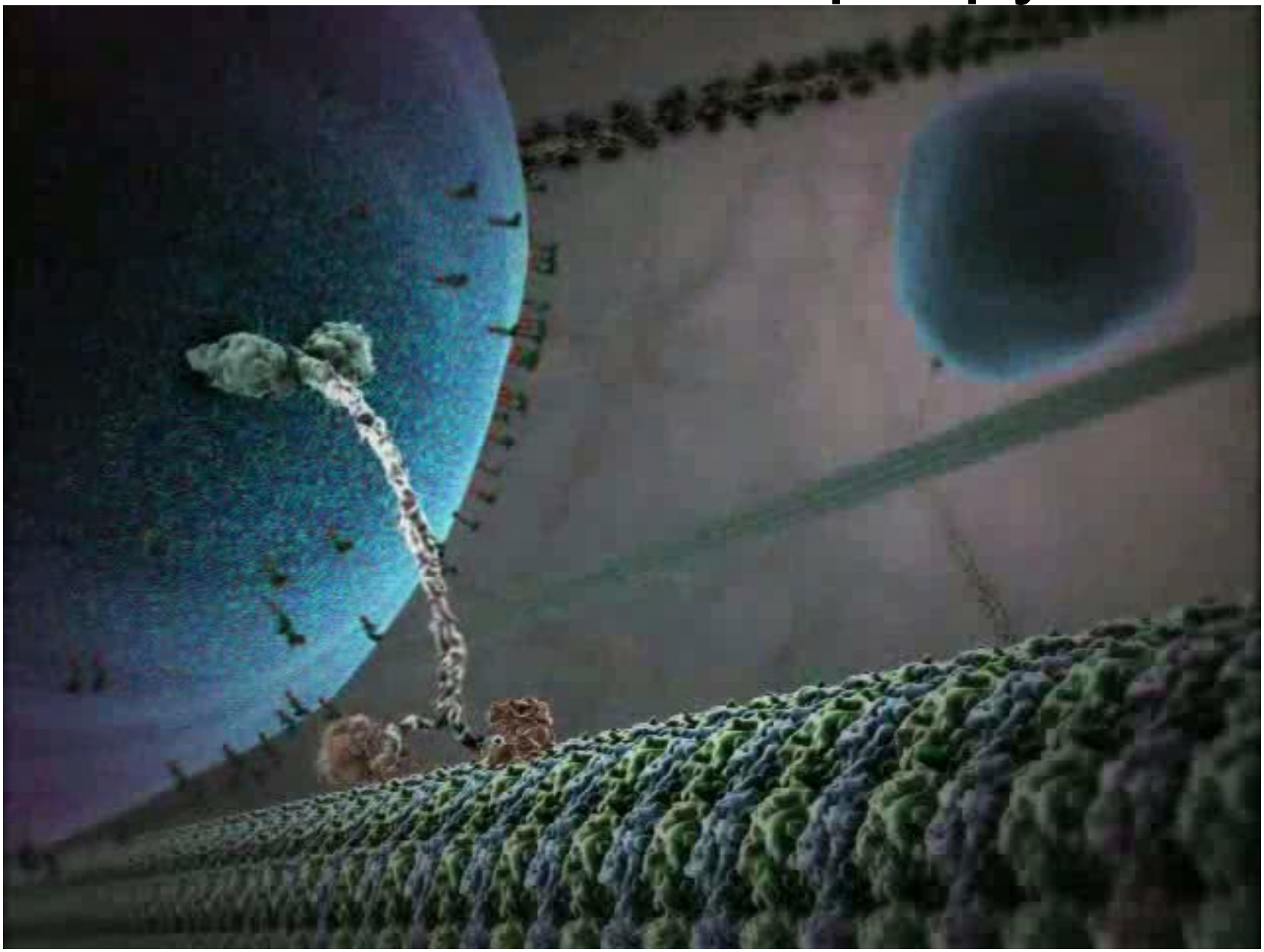
Oster/Wang
Figure 1

Общая схема работы митохондриальной АТФ-азы



(b)

Направленный перенос везикулы кинезином вдоль микротрубочки



Сворачивание белка

MET LEU SER ASP GLU ASP PHE LYS ALA VAL PHE GLY
MET THR ARG SER ALA PHE ALA ASN LEU PRO LEU TRP
LYS GLN GLN ASN LEU LYS LYS GLU LYS GLY LEU PHE