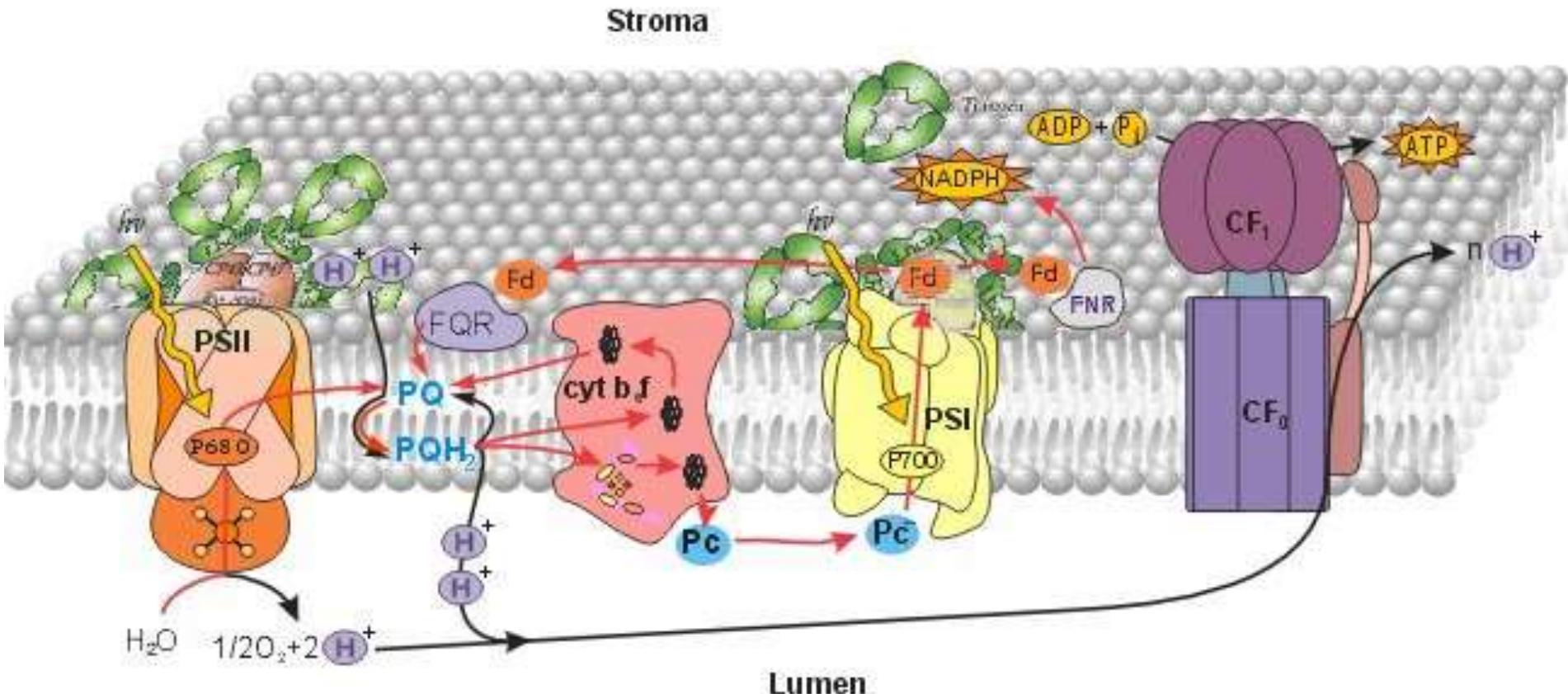


Энерго-преобразующие мембранны



Модели первичных процессов фотосинтеза

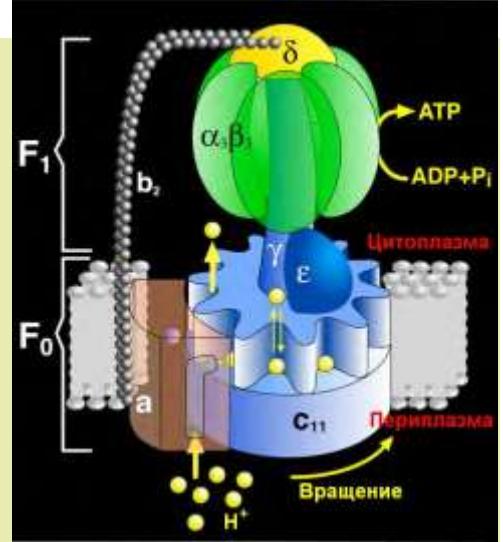
Нано-электростанции в живой клетке

- Дыхание
- Митохондрии
- Производство энергии

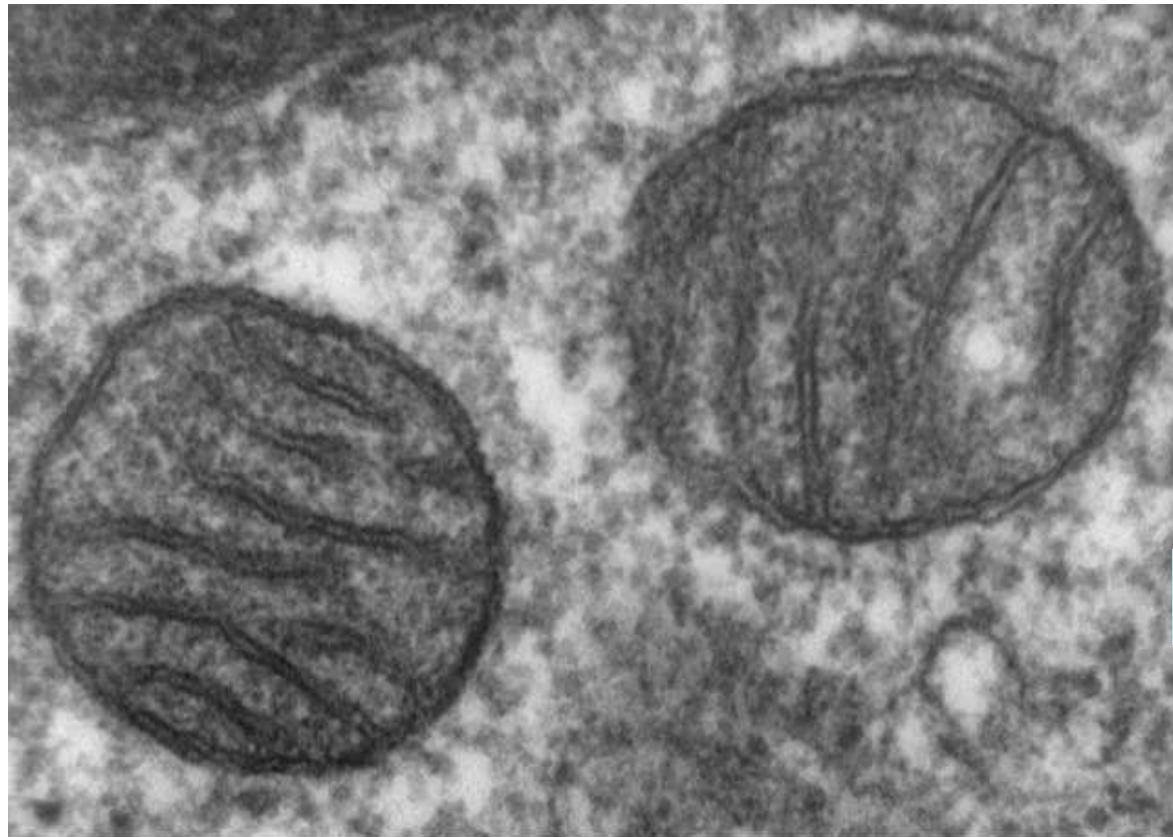
АТФ из энергии солнечного света

- Хлоропласти (зеленые растения и водоросли)

и хроматофоры (бактерии)



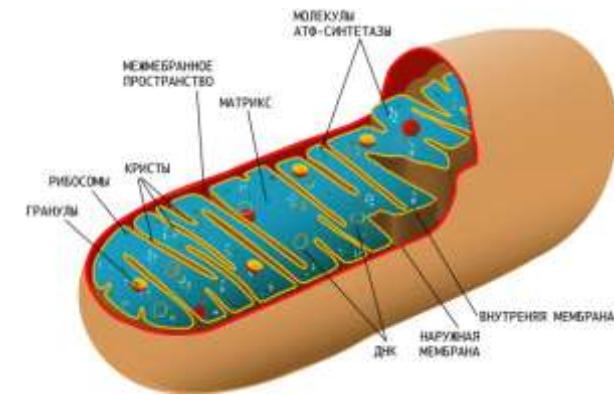
Производство энергии осуществляется в субклеточных системах



50 nm

08LungTEM

1/7/0 REMF



Митохондрия

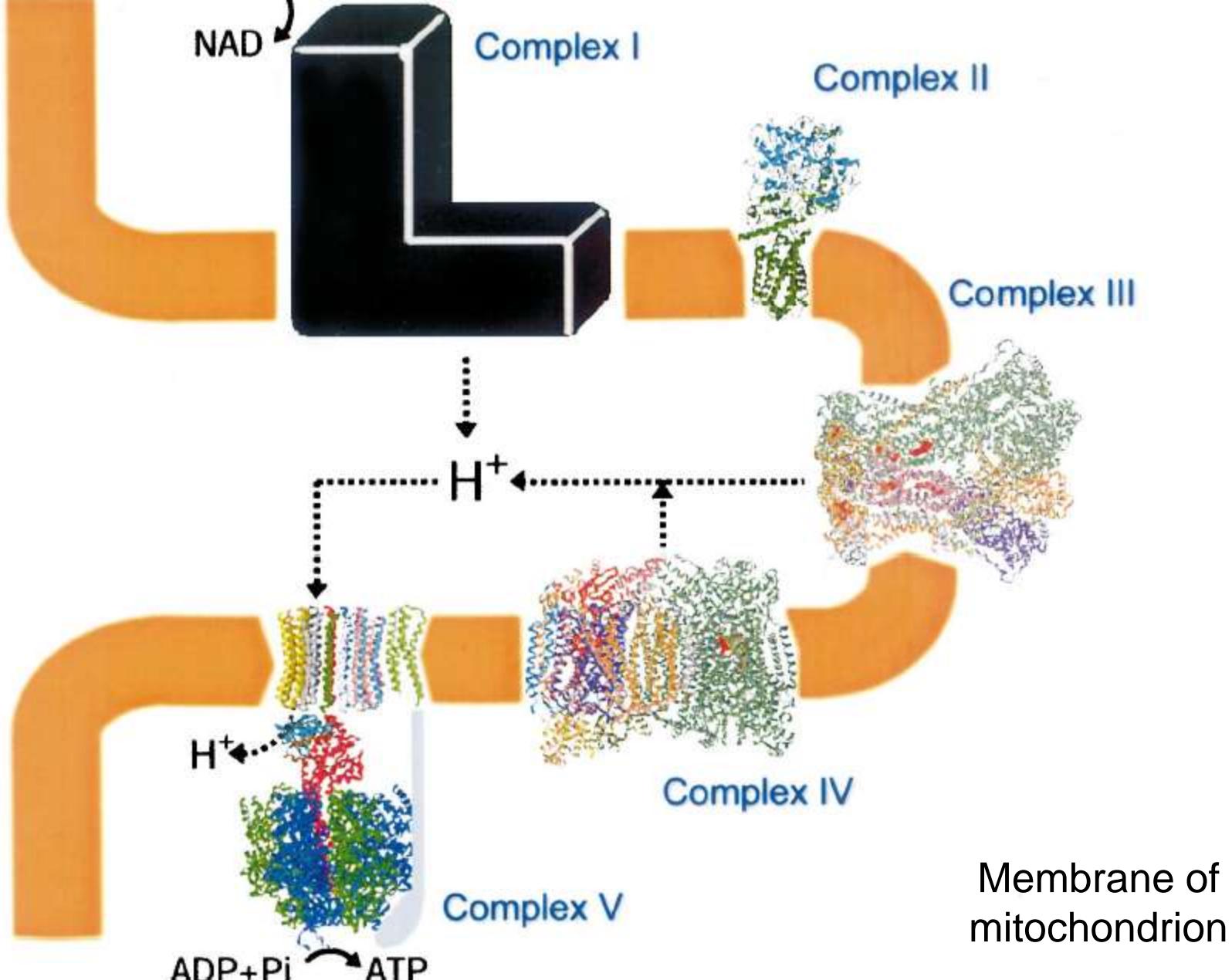
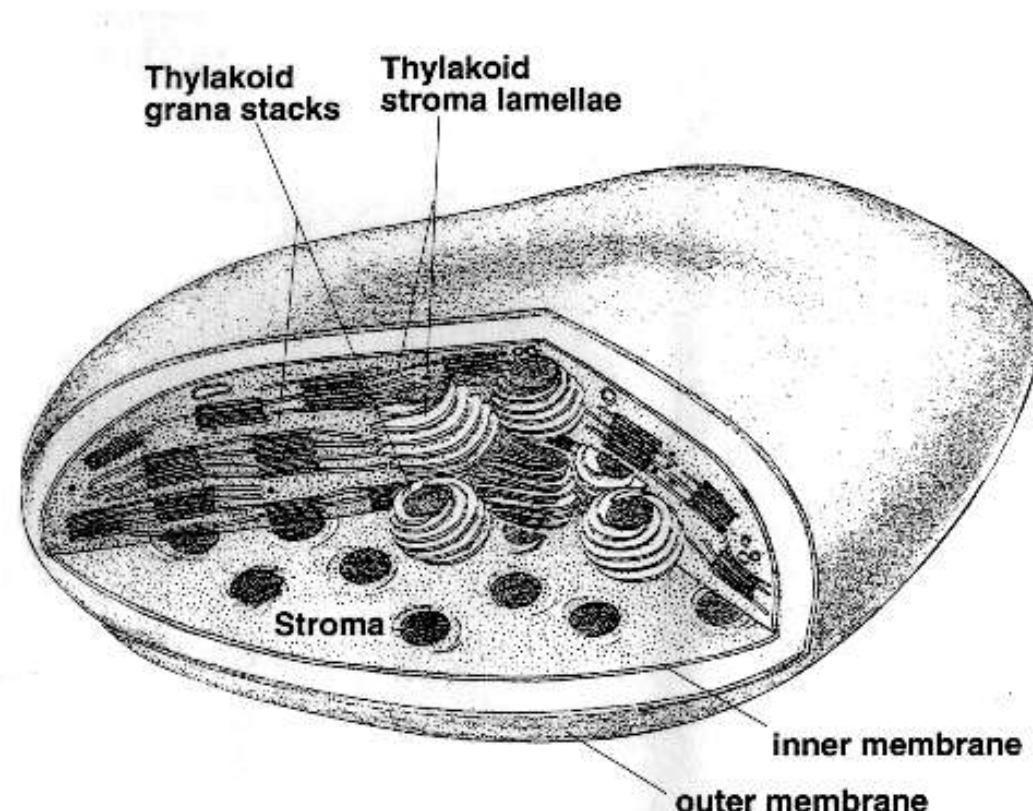
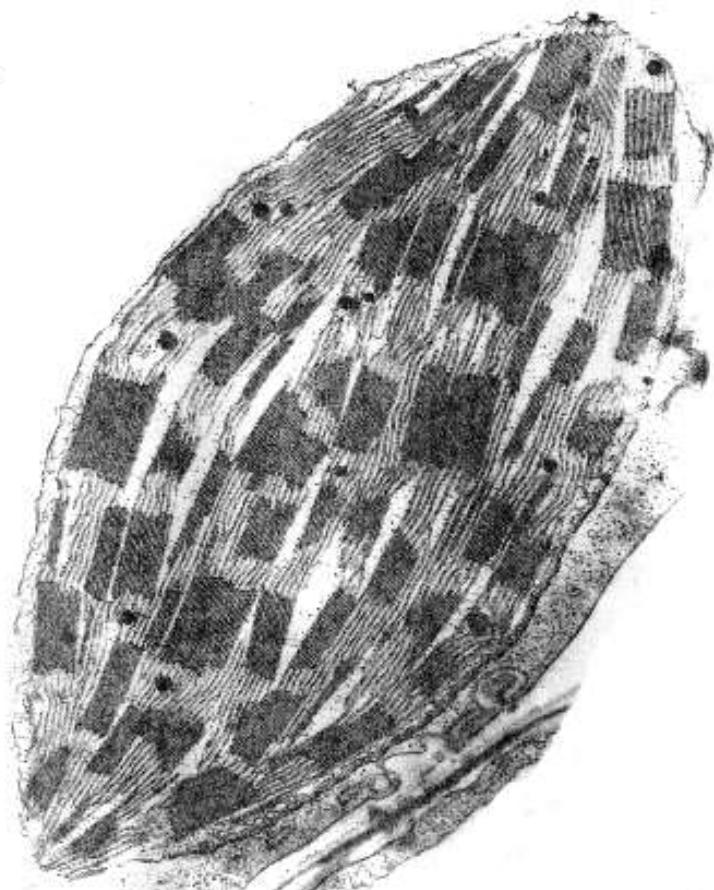
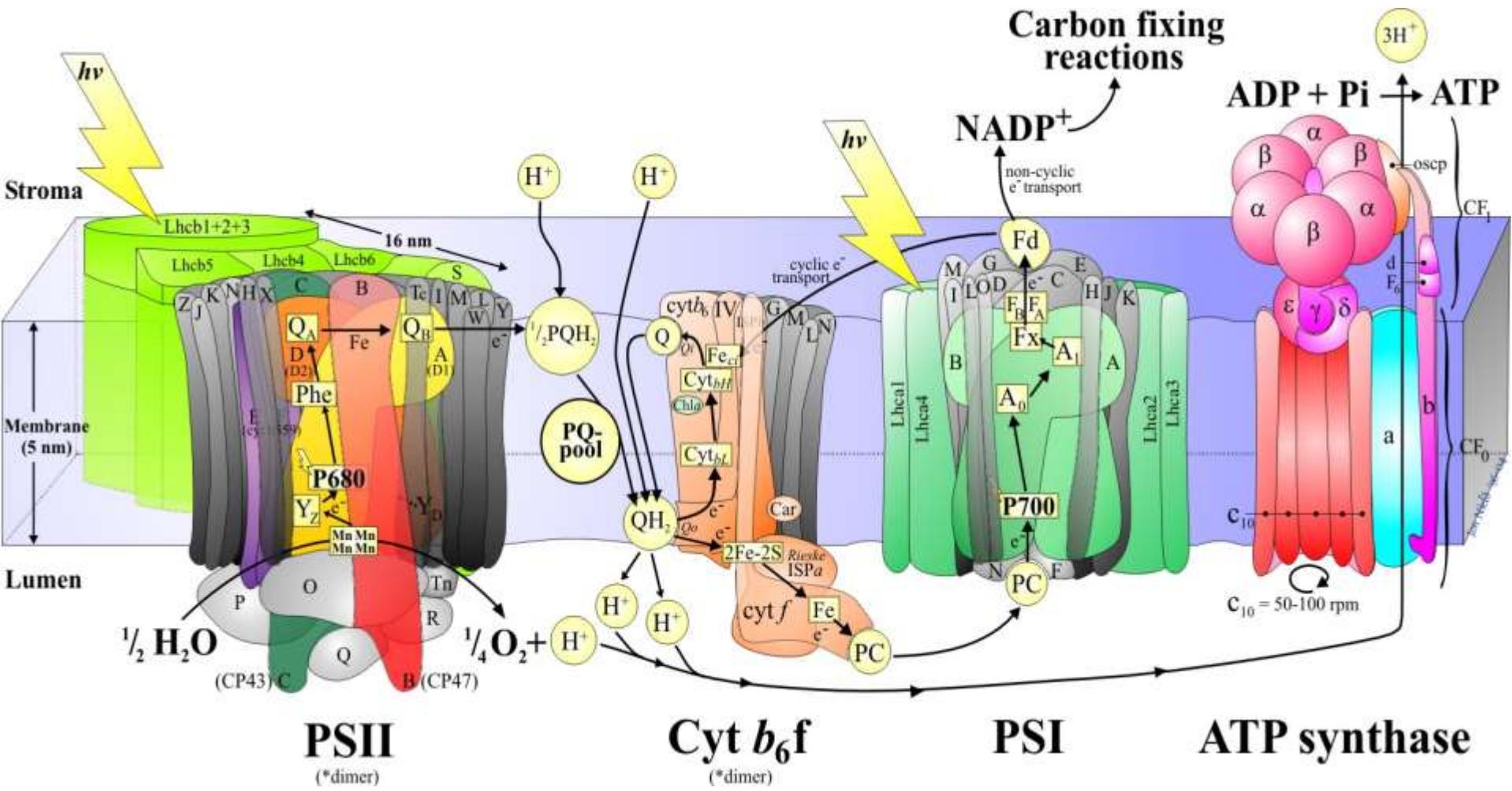


Fig. 1. A schematic representation of the oxidative phosphorylation system. The three-dimensional structures of the individual complexes were obtained from the PDB database. The coordinates used are as follows: complex II, 1FUM, as represented by fumarate reductase; complex III, 1BCC, 1BE3, and 1QCR; complex IV, 2OCC. Ribbon

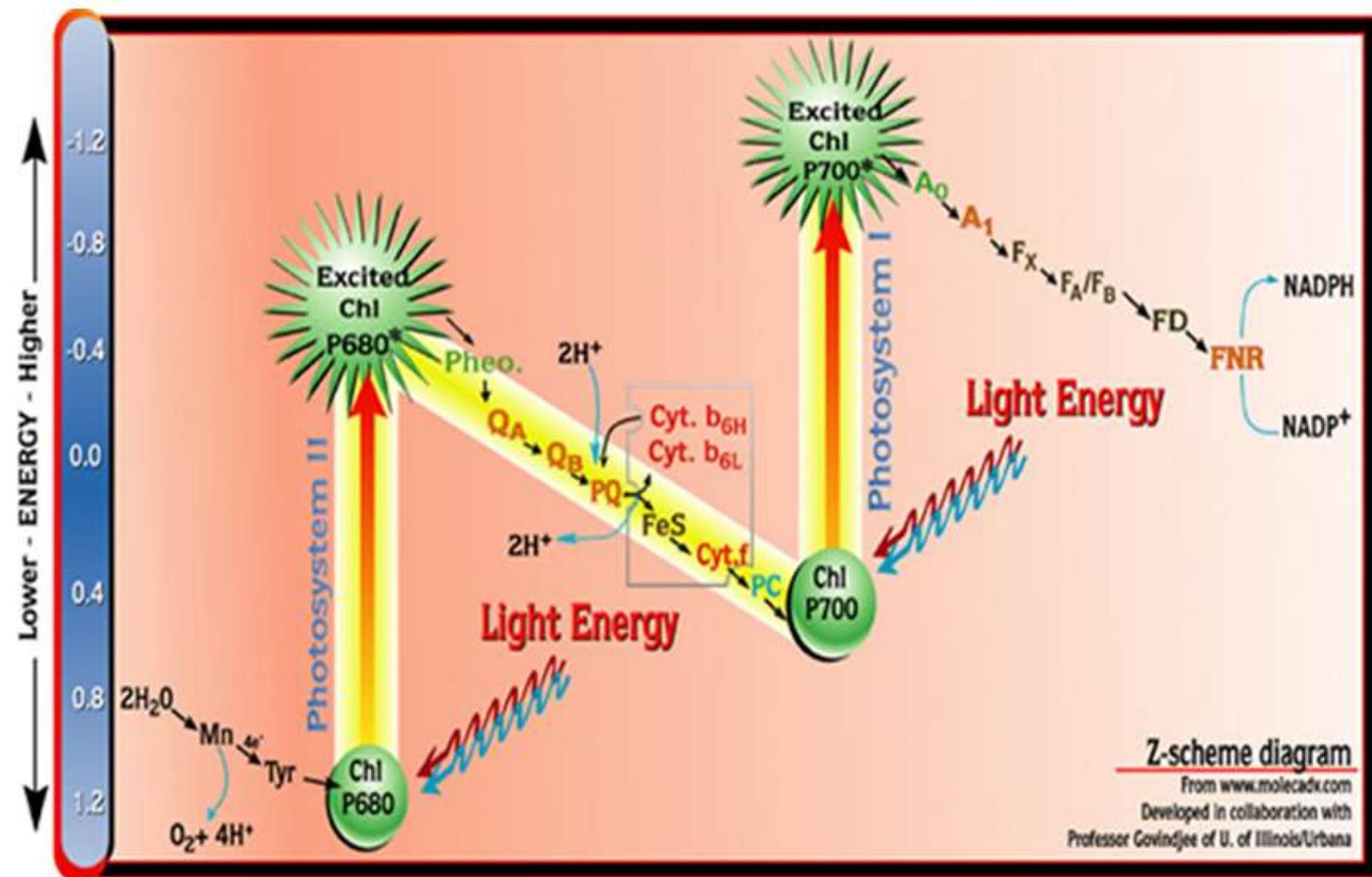
Хлоропласти. Микрофотография и схема



Структура мультиферментных комплексов



Z-схема фотосинтеза



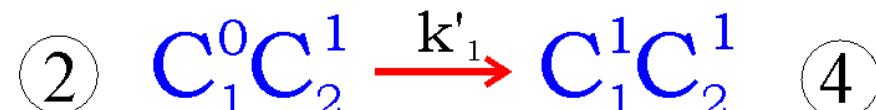
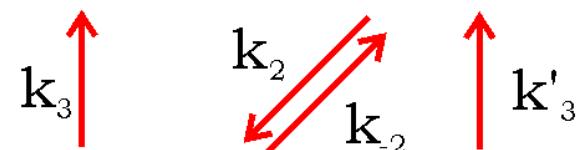
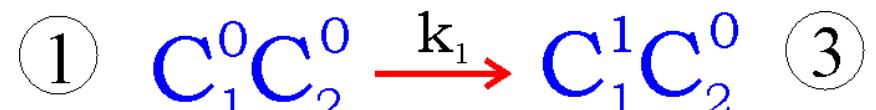
Description of the states of complex C_1C_2

X_i - concentration of i -th metabolite.

Probabilities
of the electron carriers C_i states

$$\frac{dp_i}{dt} = \sum_{j=1}^l (p_j k_{ji} - p_i k_{ij}),$$

The initial probabilities
 $p_i(0) = b_i$, $i = 1, \dots, l$.



$$\dot{p}_1 = k_3 p_2 - k_1 p_1$$

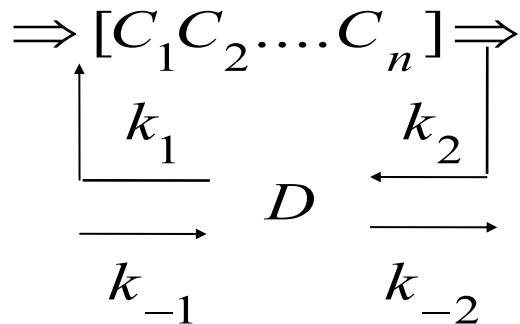
$$\dot{p}_2 = k_2 p_3 - (k'_1 + k_3 + k_{-2}) p_2$$

$$\dot{p}_3 = k_1 p_1 + k'_3 p_4 + k_{-2} p_2 - k_2 p_3$$

$$\dot{p}_4 = k'_1 p_2 - k'_3 p_4$$

$$p_1 + p_2 + p_3 + p_4 = 1$$

Interaction of the complex with the mobile electron carrier D



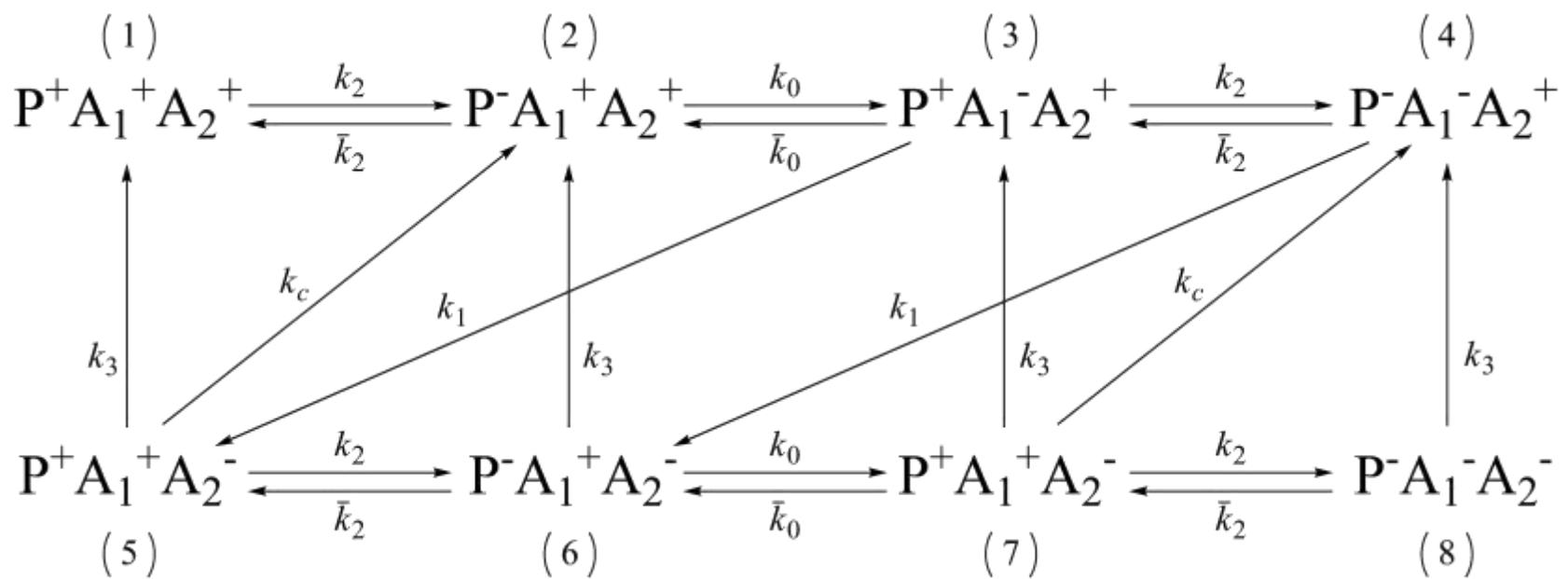
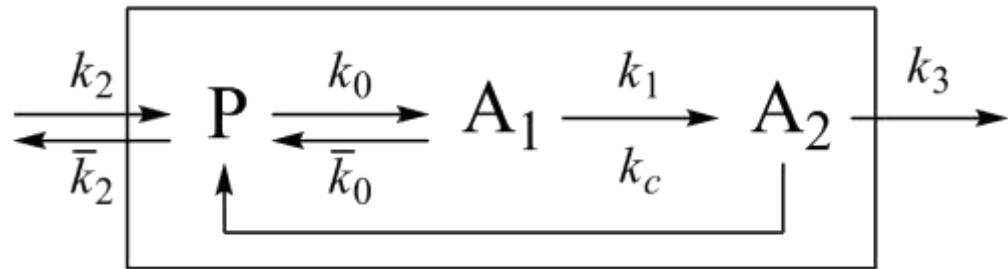
$$\frac{d[D^-]}{dt} = k_2[C_n^-][D^+] - k_{-2}[D^-][C_n^+] - k_1[D^-][C_1^+] + k_{-1}[C_1^-][D^+]$$

$[D^+]$, $[D^-]$ - concentrations of the mobile carrier in the oxidized and reduced forms;

$[C_1^+]$, $[C_1^-]$, $[C_n^+]$, $[C_n^-]$ - concentrations of the components of complex;

k_i - bimolecular rate constants.

Комплекс из трех переносчиков



Кинетические уравнения для вероятностей состояний ФСII имеют вид:

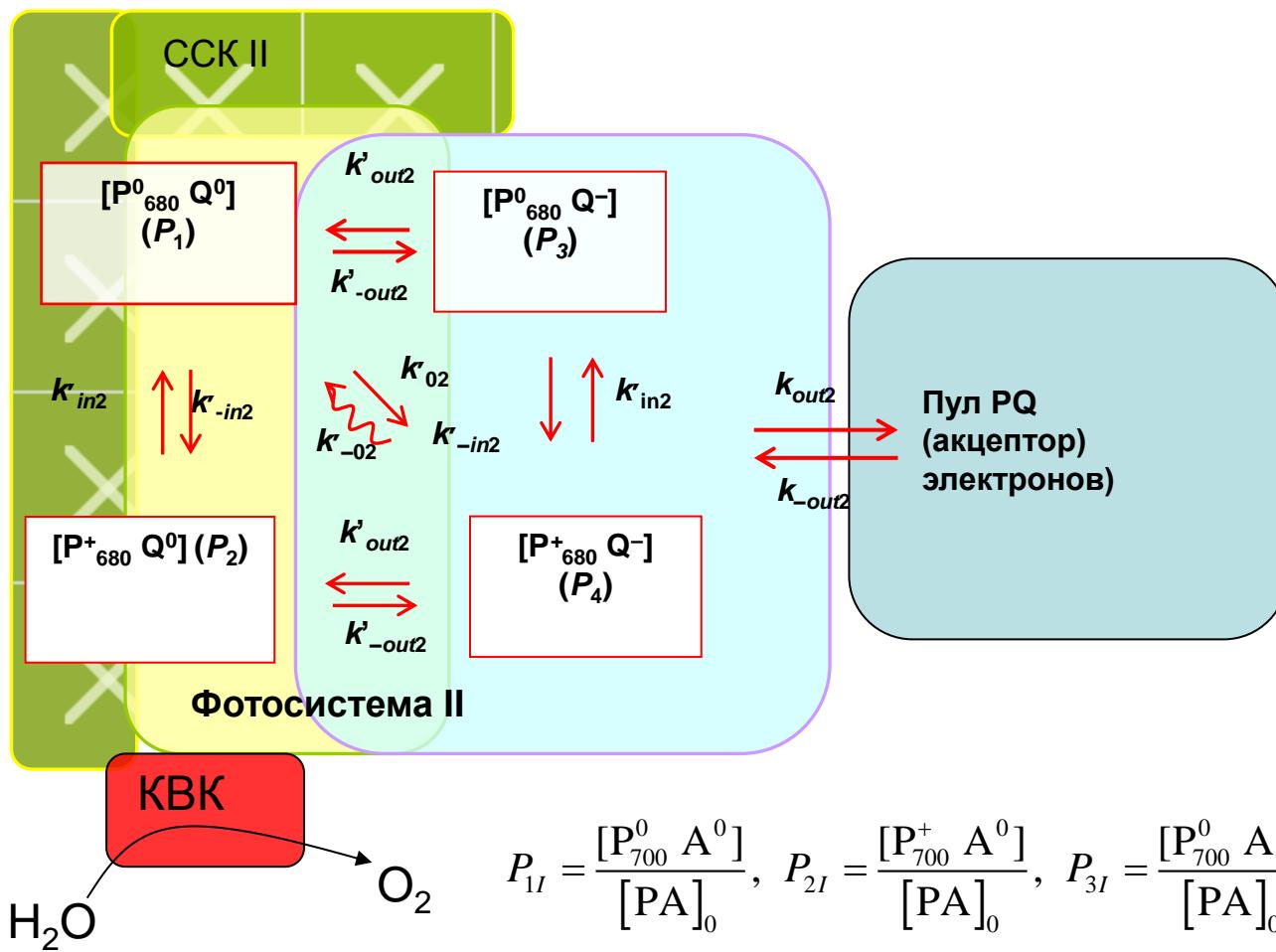
$$\frac{dP_{1II}}{dt} = -(k'_{-out2} + k'_{-in2} + k'_{02})P_{1II} + k'_{in2}P_{1II} + k'_{out2}P_{3II} + k'_{-02}P_{4II},$$

$$\frac{dP_{2II}}{dt} = k'_{-in2} \cdot P_{1II} - (k'_{in2} + k'_{-out2})P_{2II} + k'_{out2}P_{4II},$$

$$\frac{dP_{3II}}{dt} = k'_{-out2}P_{1II} - (k'_{out2} + k'_{-in2})P_{3II} + k'_{in2}P_{4II}$$

$$\frac{dP_{4II}}{dt} = k'_{02}P_{1II} + k'_{-out2}P_{2II} + k'_{-in2} \cdot P_{3II} - (k'_{in2} + k'_{-02} + k'_{out2})P_{4II}.$$

Фотосистема 2



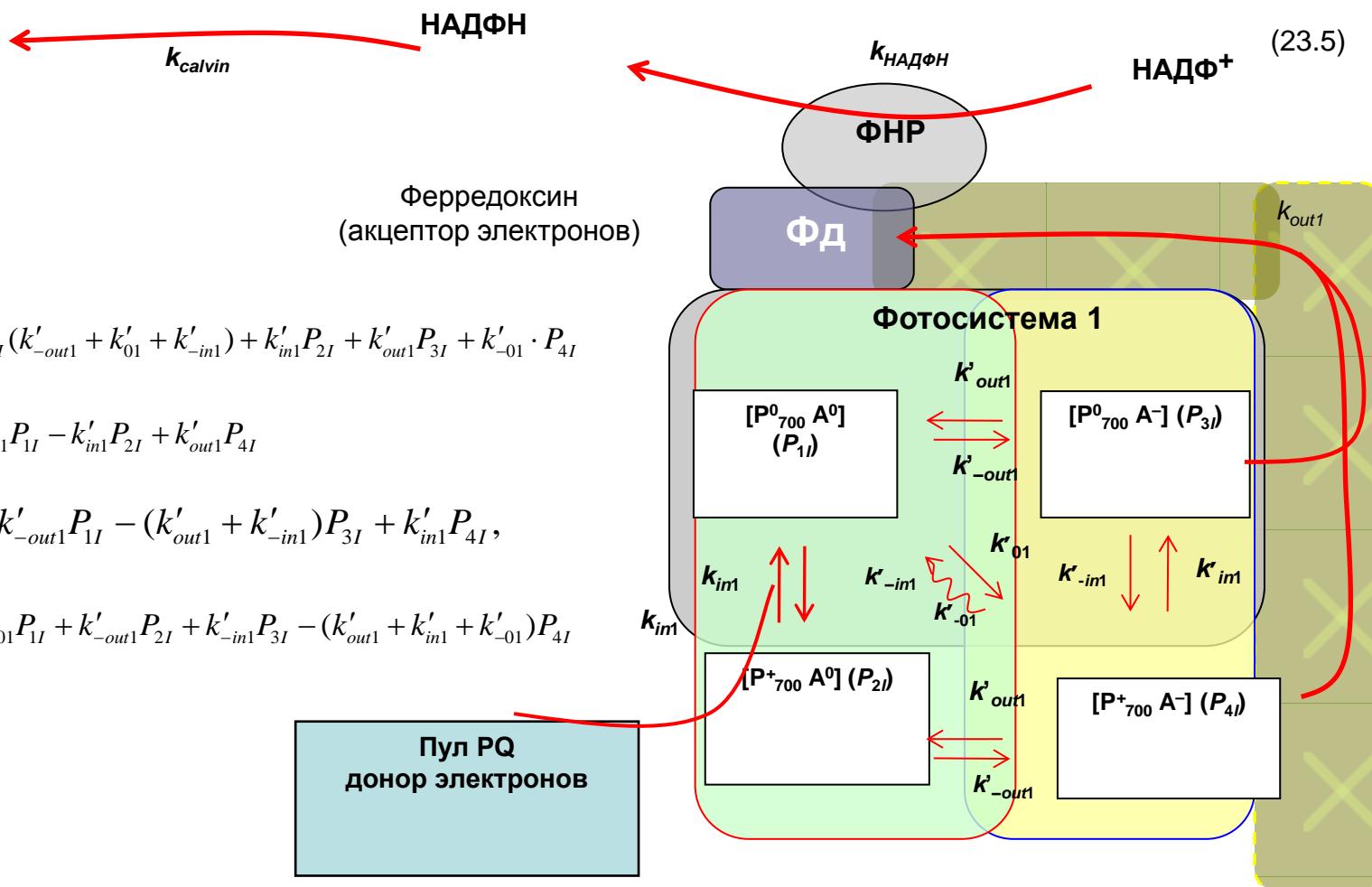
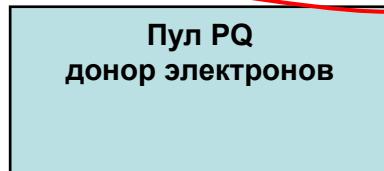
Фотосистема 1

$$\frac{dP_{1I}}{dt} = -P_{1I}(k'_{-out1} + k'_{01} + k'_{-in1}) + k'_{in1}P_{2I} + k'_{out1}P_{3I} + k'_{-01} \cdot P_{4I}$$

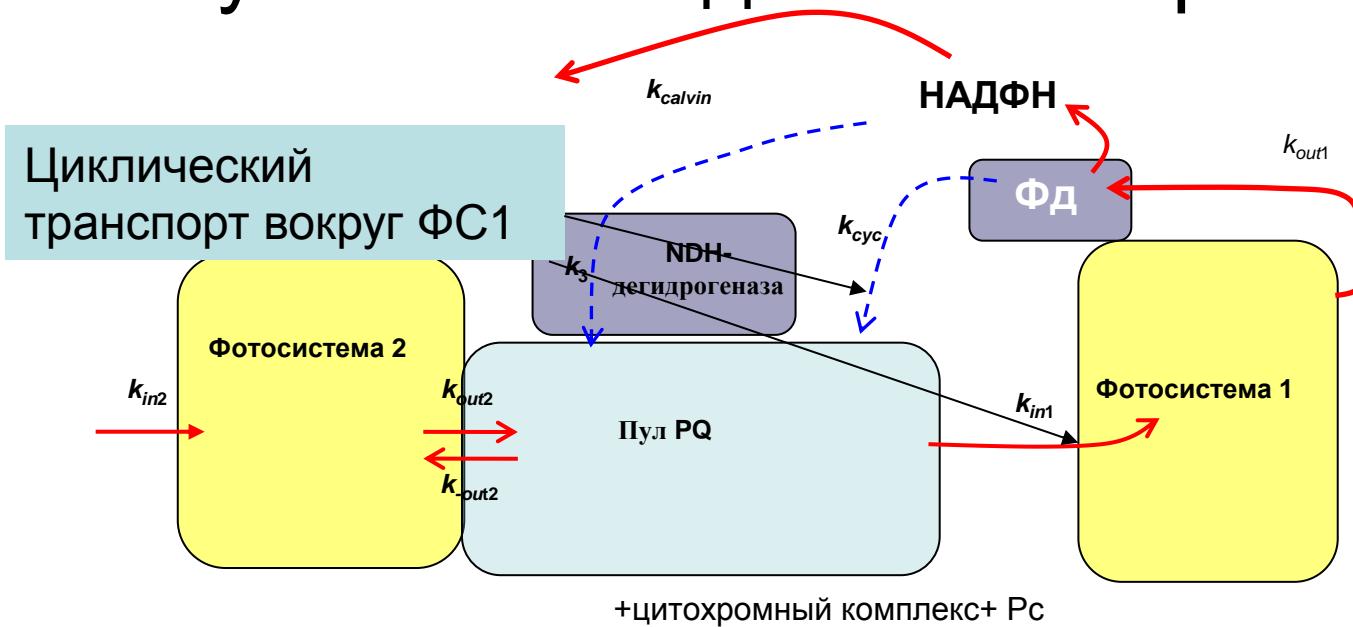
$$\frac{dP_{2I}}{dt} = k'_{-in1}P_{1I} - k'_{in1}P_{2I} + k'_{out1}P_{4I}$$

$$\frac{dP_{3I}}{dt} = k'_{-out1}P_{1I} - (k'_{out1} + k'_{-in1})P_{3I} + k'_{in1}P_{4I},$$

$$\frac{dP_{4I}}{dt} = k_{01}P_{1I} + k'_{-out1}P_{2I} + k'_{-in1}P_{3I} - (k'_{out1} + k'_{in1} + k'_{-01})P_{4I}$$



Взаимодействие двух фотосистем с участием подвижных переносчиков



$$\frac{d[\text{PQ}^-]}{dt} = k_{out2} \cdot (P_{3II} + P_{4II}) \cdot [\text{P}_{680}] \cdot [\text{PQ}] + k_3 \cdot [\text{НАДФН}] \cdot [\text{PQ}] + k_{cyc} \cdot [\Phi_D^-] [\text{PQ}^-] - \\ - (k_{in1} \cdot (P_{1I} + P_{3I}) \cdot [\text{P}_{700}] + k_{out2} \cdot (P_{1II} + P_{2II}) \cdot [\text{P}_{680}]) [\text{PQ}^-],$$

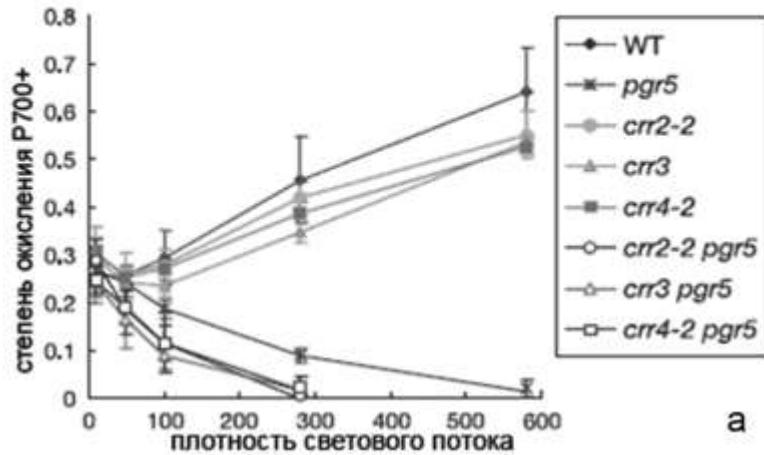
$$\frac{d[\Phi_D^-]}{dt} = k_{out1} (P_{3I} + P_{4I}) [\text{P}_{700}] \cdot [\Phi_D] + k_{-NAUDFH} [\text{НАДФН}] \cdot [\Phi_D] - \\ - (k_{NAUDFH} [\text{НАДФ}^+] + k_{cyc} [\text{PQ}] + k_{-out1} (P_{1I} + P_{2I}) [\text{P}_{700}]) [\Phi_D^-],$$

$$\frac{d[\text{НАДФН}]}{dt} = k_{NAUDFH} [\Phi_D^-] [\text{НАДФ}^+] - (k_{-NAUDFH} [\Phi_D] + k_3 [\text{PQ}] - k_{calvin}) [\text{НАДФН}].$$

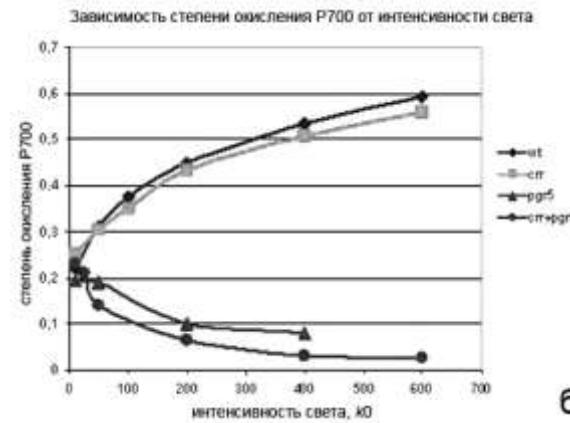
Изучение влияния мутаций

PGR progesterone receptor

Зависимость степени окисления P700 в зависимости от интенсивности освещения
у дикого типа и мутантов *Arabidopsis Thaliana*



а



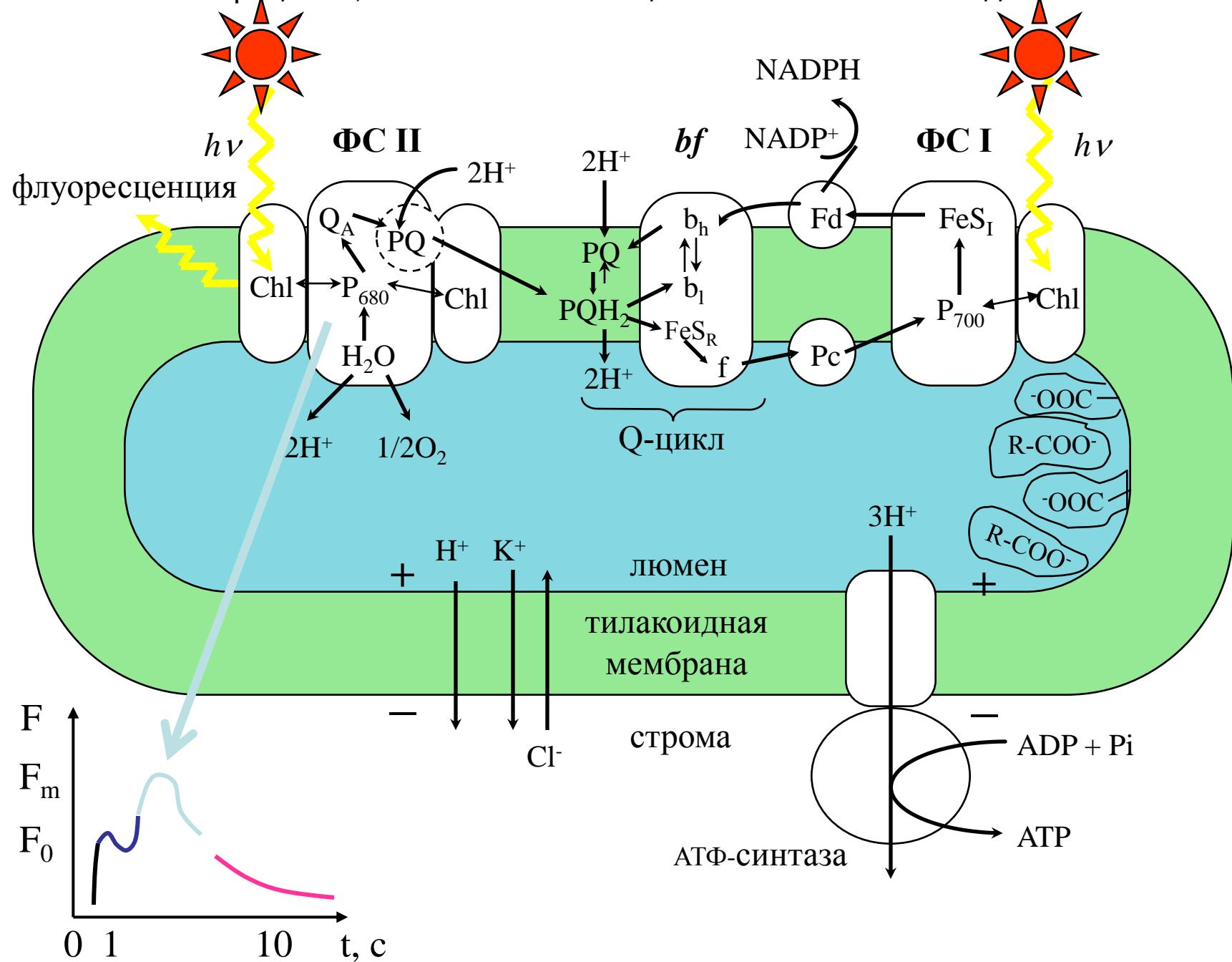
б

эксперимент

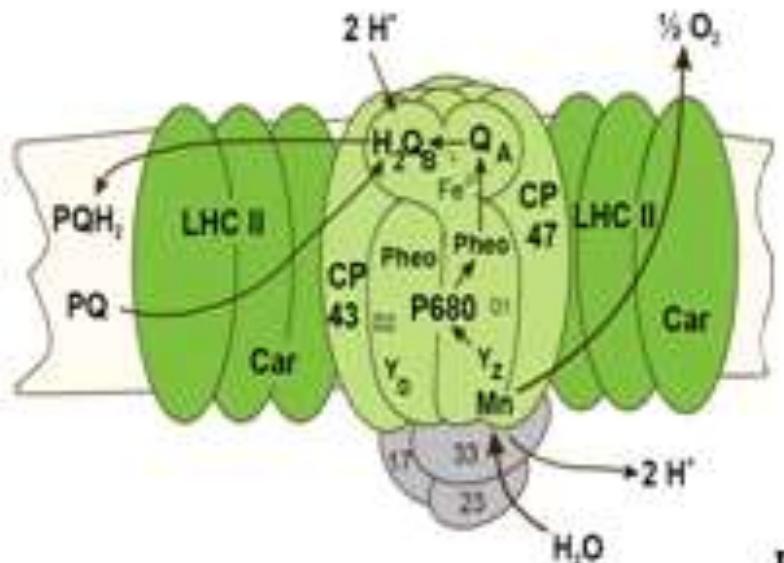
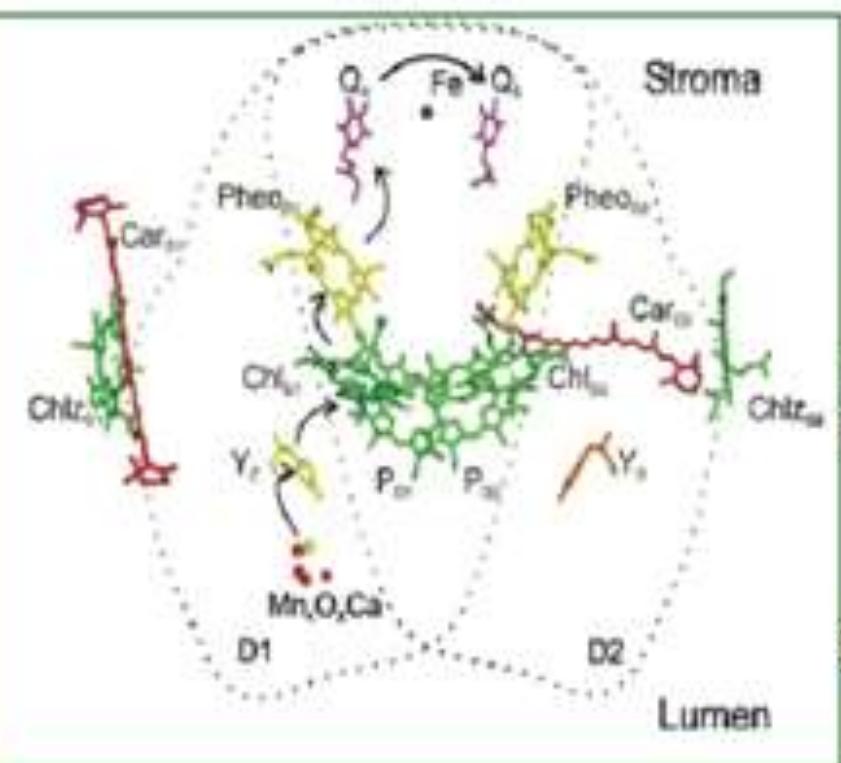
модель

у *crr*-мутантов подавлен только *NDH*-зависимый электронный транспорт, а у *pgr5*-мутантов подавлен как циклический *Fd*-зависимый электронный транспорт, так и электронный поток в акцепторной части ФСI.

Процессы, описанные в обобщенной кинетической модели

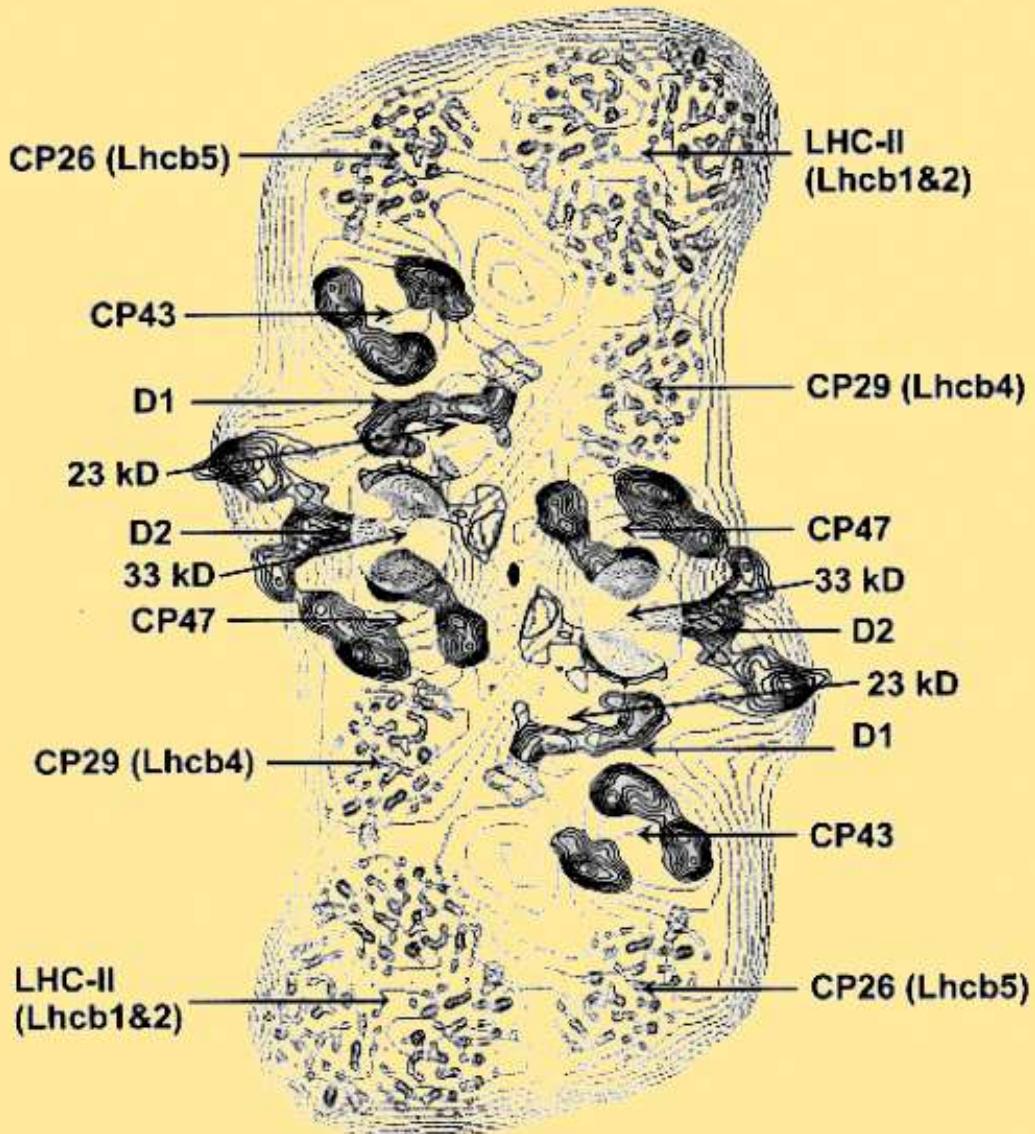
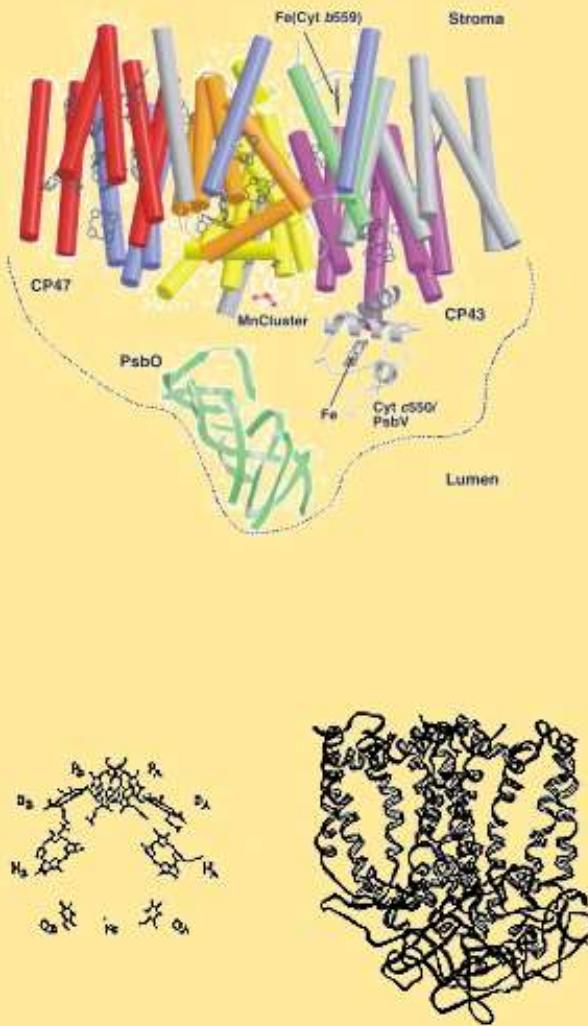


Photosystem II – the source of fluorescence

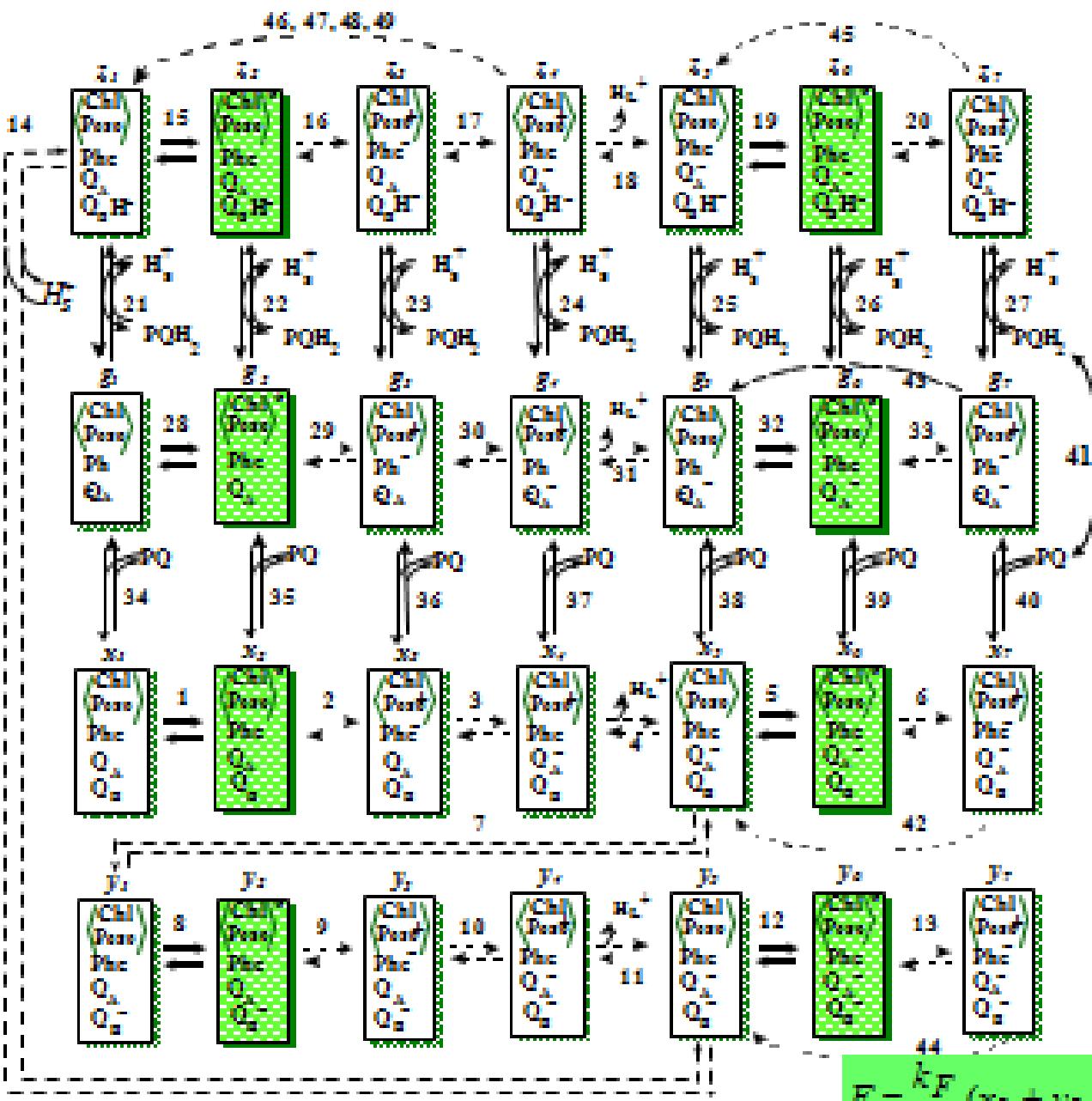


Chl, PSII chlorophyll, P680 - photoactive pigments; Phe, pheophytin; Q_A and Q_B , primary and secondary quinone acceptors; PQ, plastoquinone; PQH_2 , plastoquinol; H_L^+ and H_s^+ protons in lumen and stroma,

Комплекс Фотосистемы 2. Подробности.



Scheme of PSII states



Energy relaxation
processes

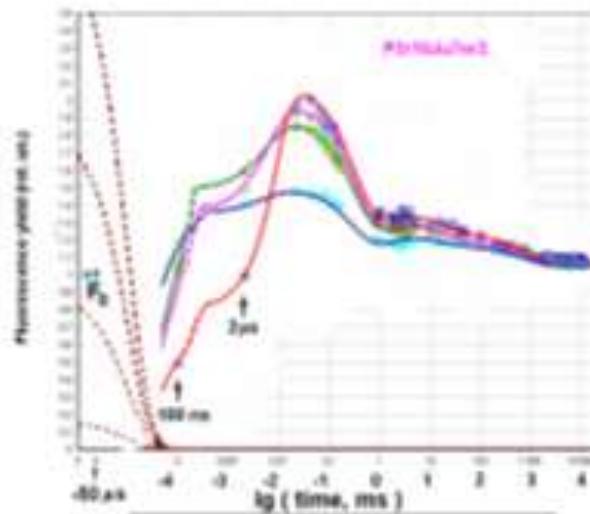
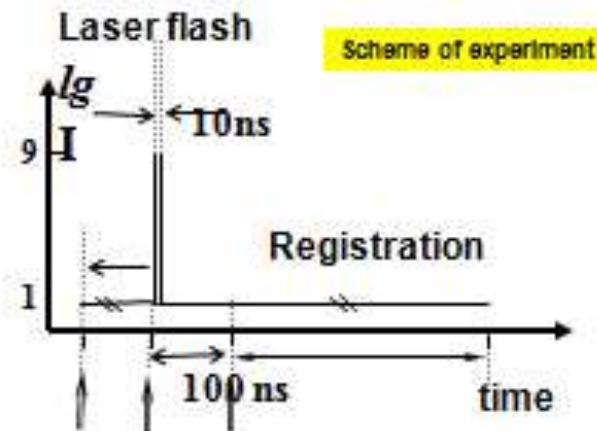
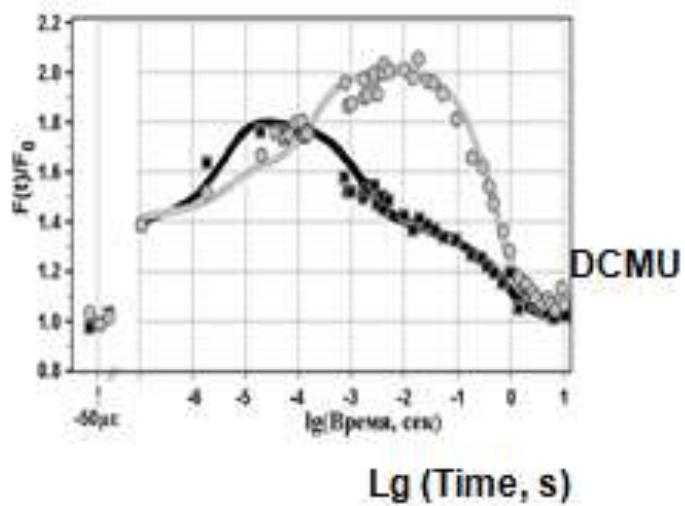
Fluorescence yield

$$F = \frac{k_F}{k_L} (x_2 + y_2 + z_2 + g_2 + x_6 + y_6 + z_6 + g_6)$$

Моделирование отклика системы на короткую вспышку

Experiment (dots) and simulation (solid lines). Fluorescence induction curves after the saturating 10 ns laser flash, cells of thermophilic *Chlorella pyrenoidosa* Chick.

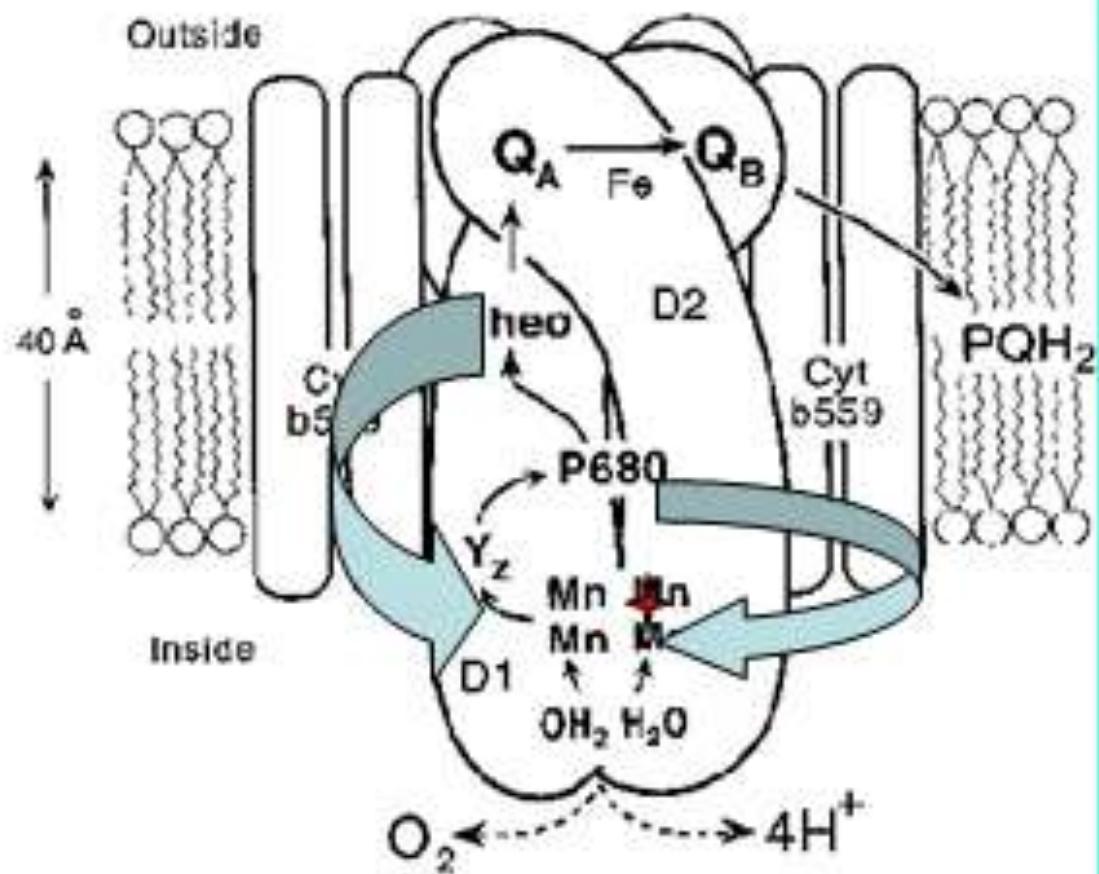
lab. Prof. G.Renger (Berlin)



Belyaeva, Renger et al., Phot.Res.
2008-2016

laser energies: $7.5 \cdot 10^{15}$ ph/cm² flash (dark blue), $6.2 \cdot 10^{15}$ ph/cm² flash (magenta), $3.0 \cdot 10^{15}$ ph/cm² flash (beige);
 $5.4 \cdot 10^{14}$ ph/cm² flash (light-green).

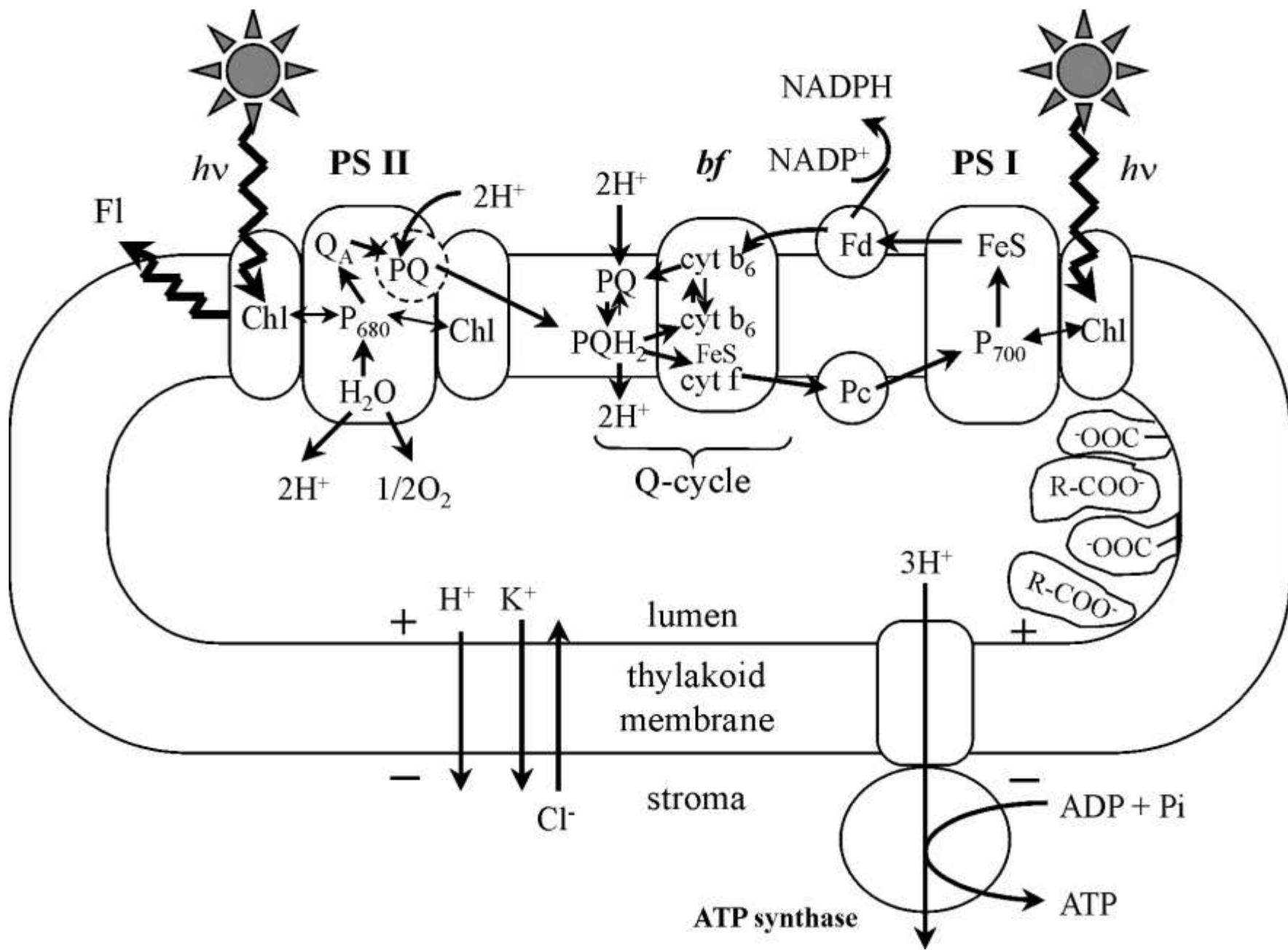
PSII



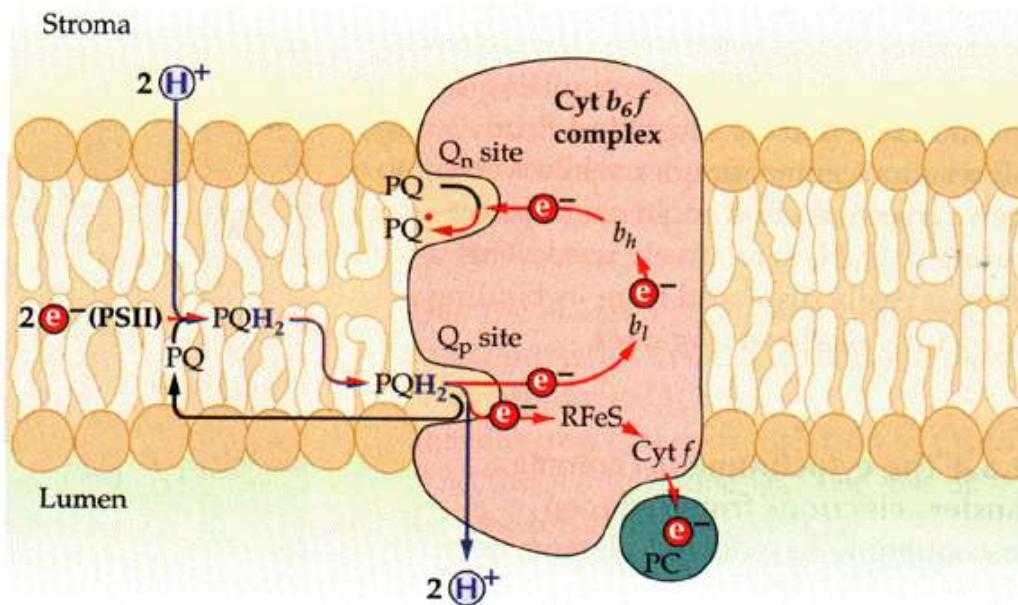
Electron transport in PSII

Arrows – the processes of non-radiation relaxation

Rate constants of this processes can be evaluated only by simulation (not directly in experiment)



(A) First turnover



(B) Second turnover

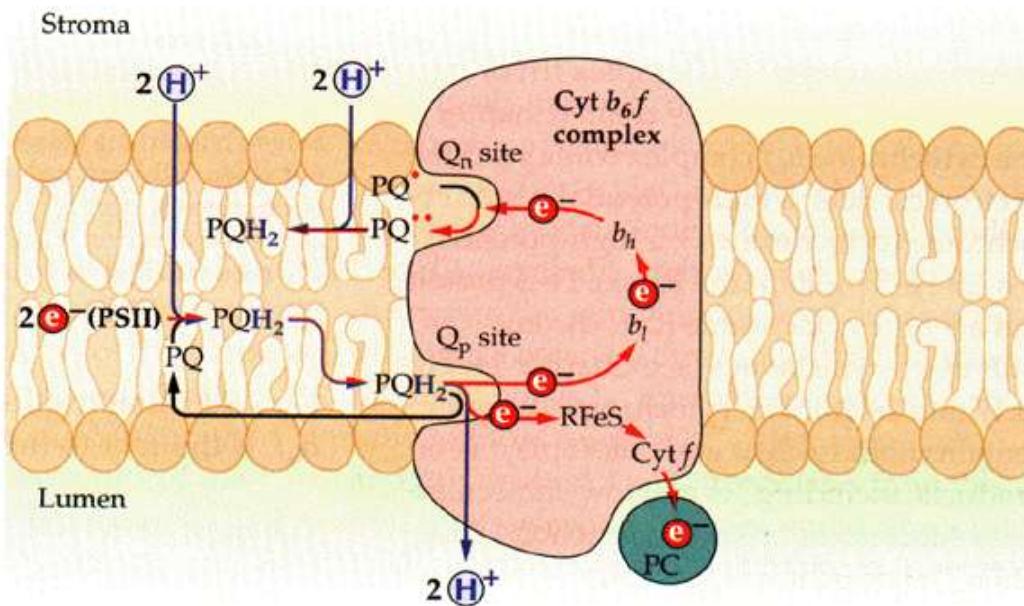
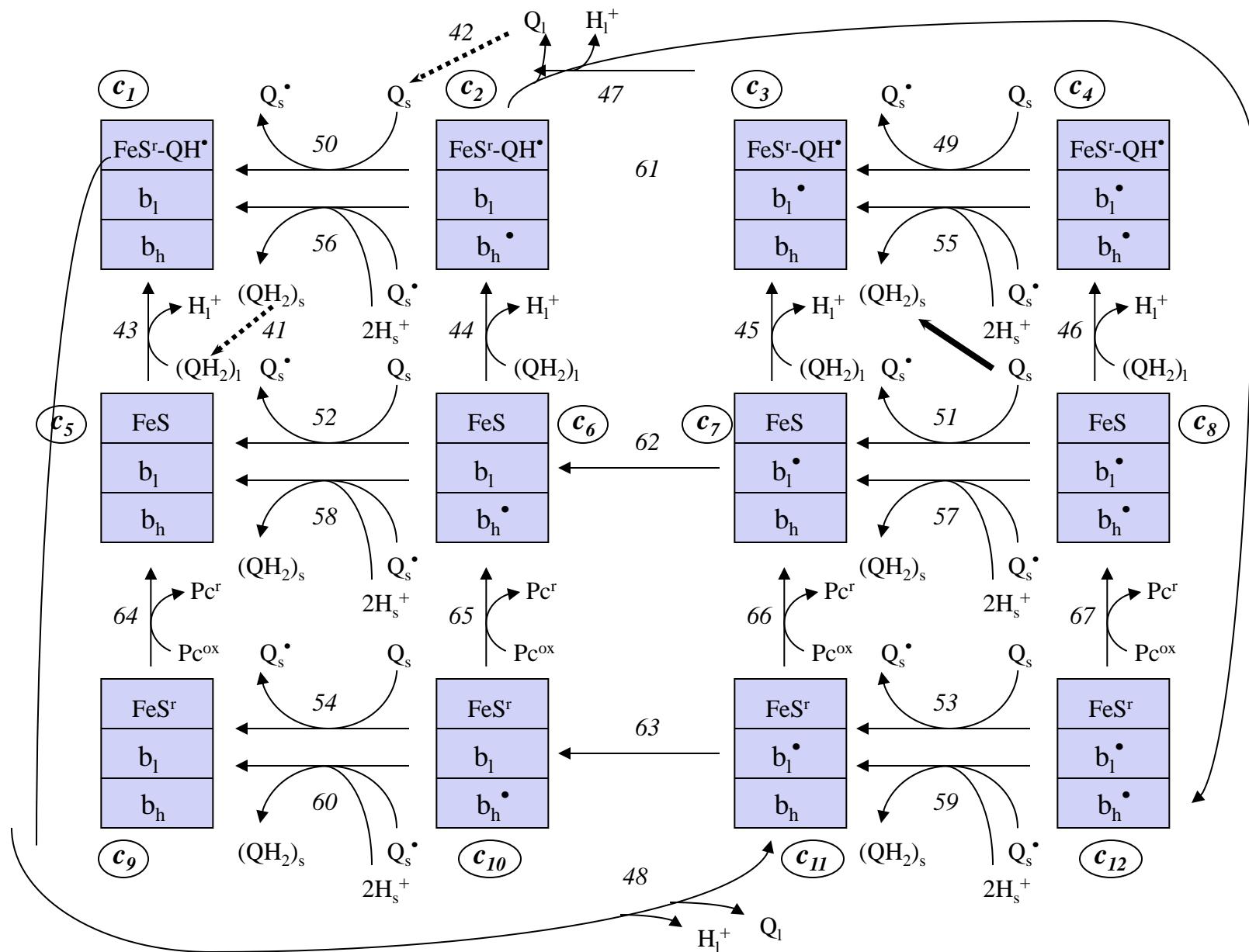
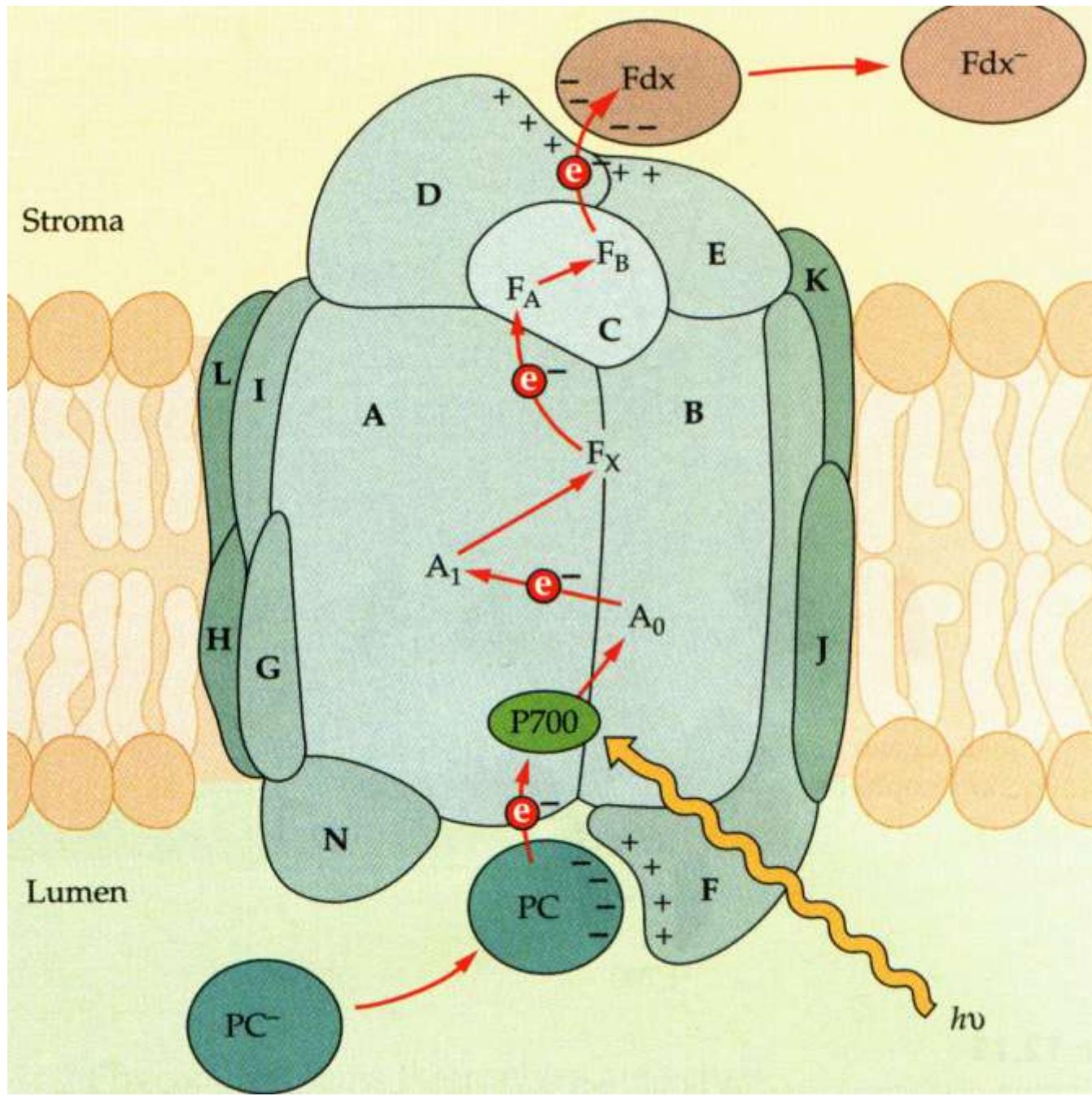


Схема Митчела
функционирования
цитохромного
комплекса.

Сопряжение
электронного
транспорта и
трансмембранного
переноса протонов

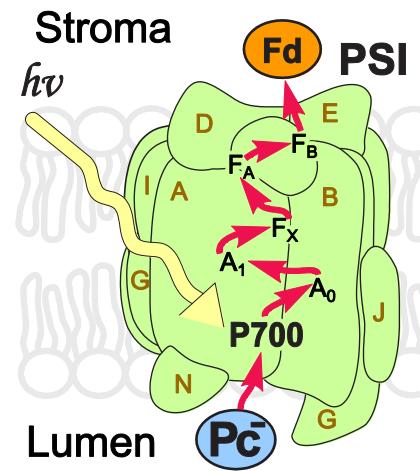
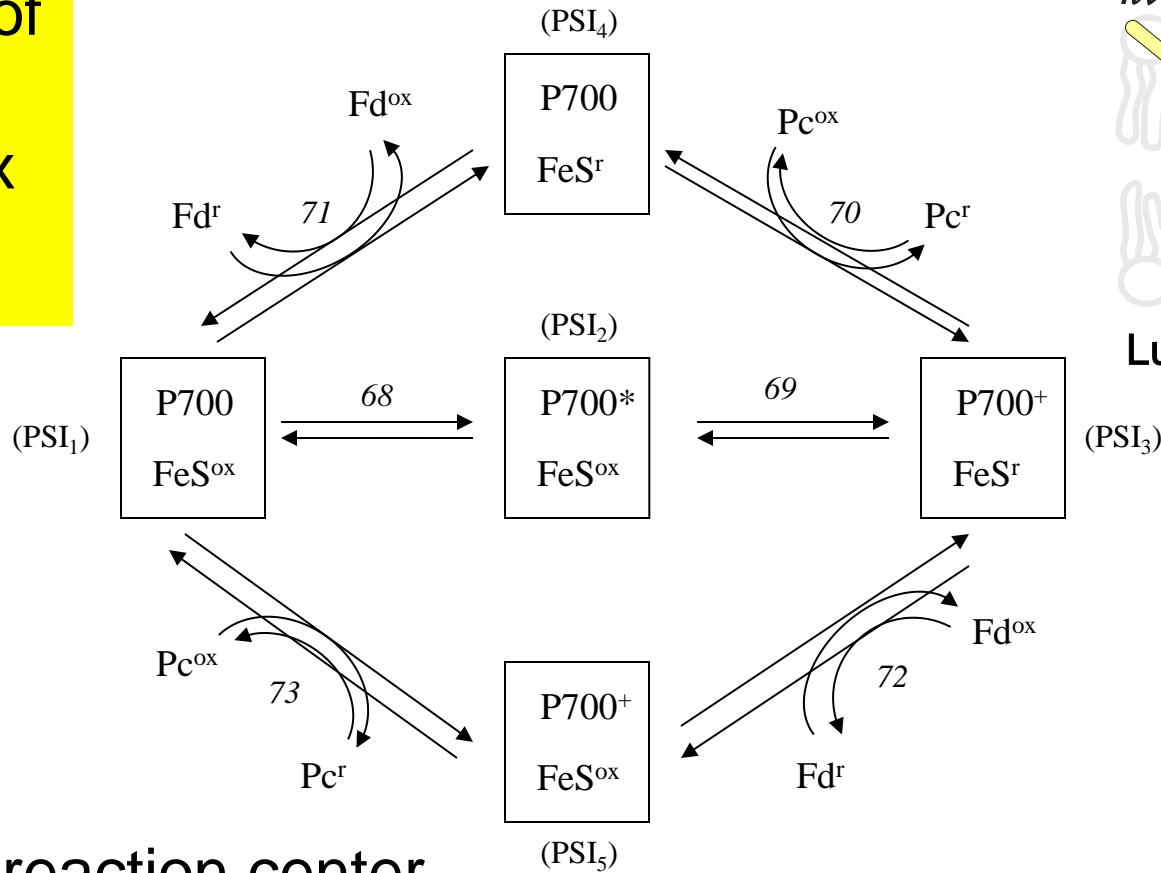
States of the Cytochrome complex





Комплекс
ФОТО-
реакционного
центра
Фотосистемы I

Scheme of PS1 Complex States



P700 - the reaction center
chlorophyll,

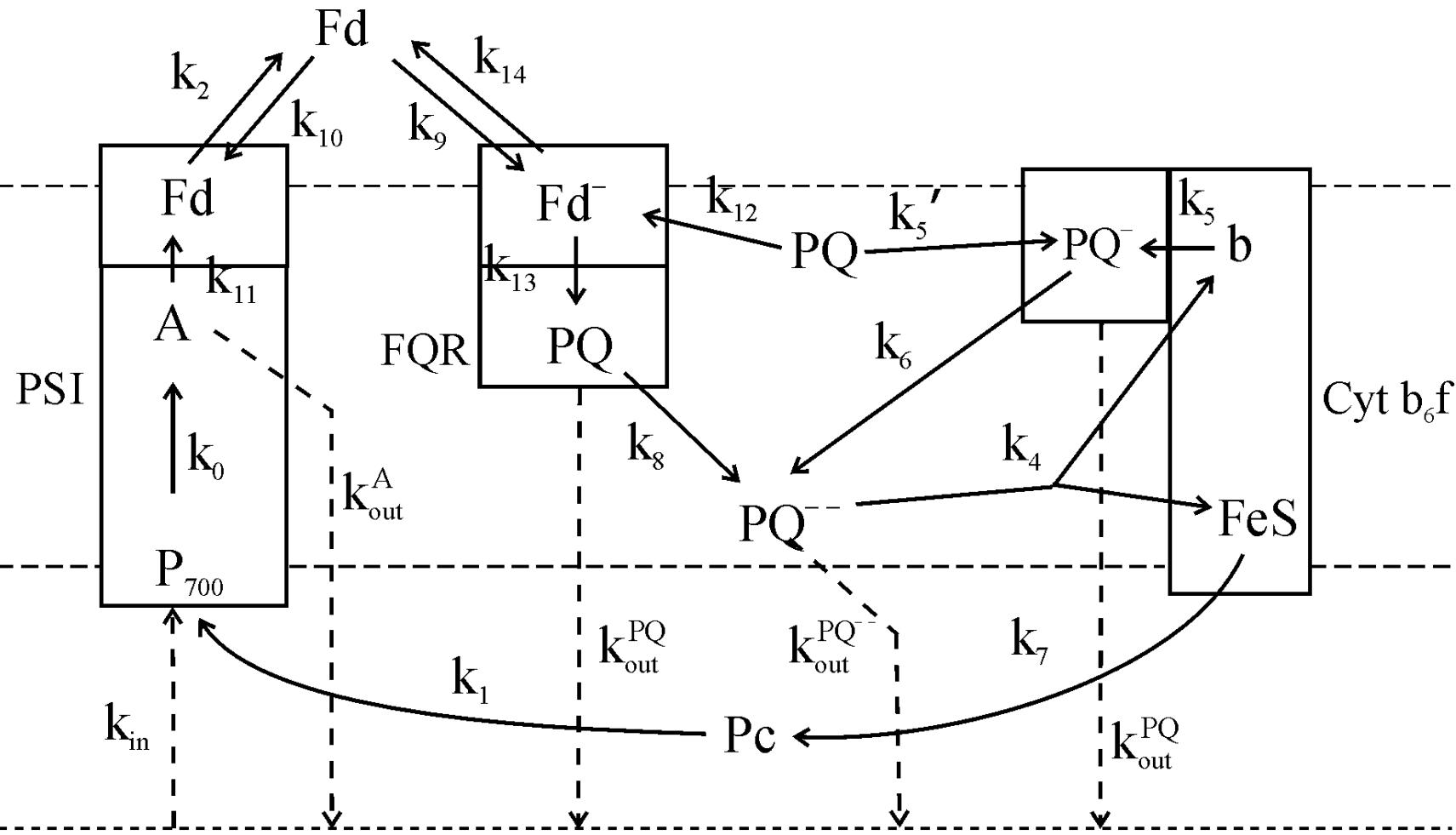
FeS - the entire acceptor
complex;

Fd, ferredoxin;

Pc, plastocyanin;

superscripts mark
the reduced (r)
and oxidized (ox) states.

Схема процессов в ФС1 и циклических потоков вокруг ФС1



Pool of non-specific electron donors and acceptors

General kinetic model. Fluorescence induction curves simulation

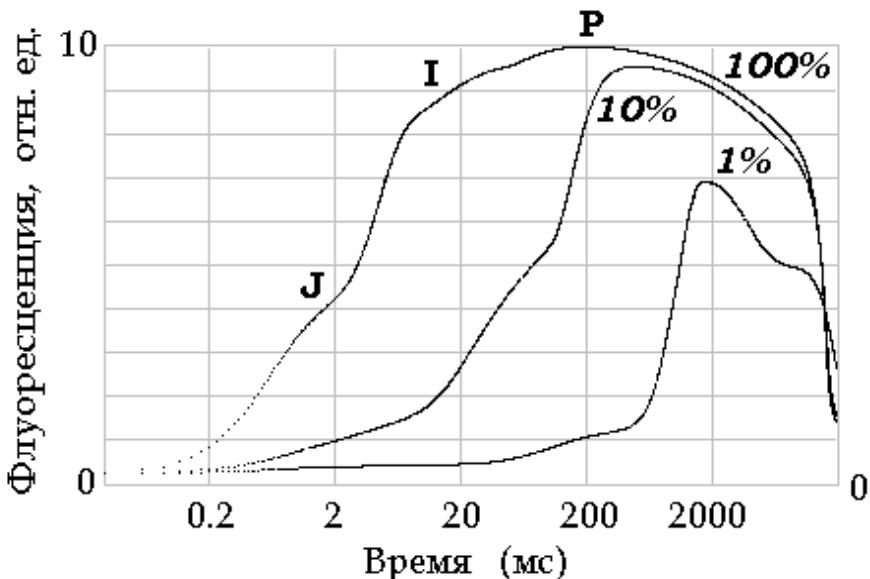
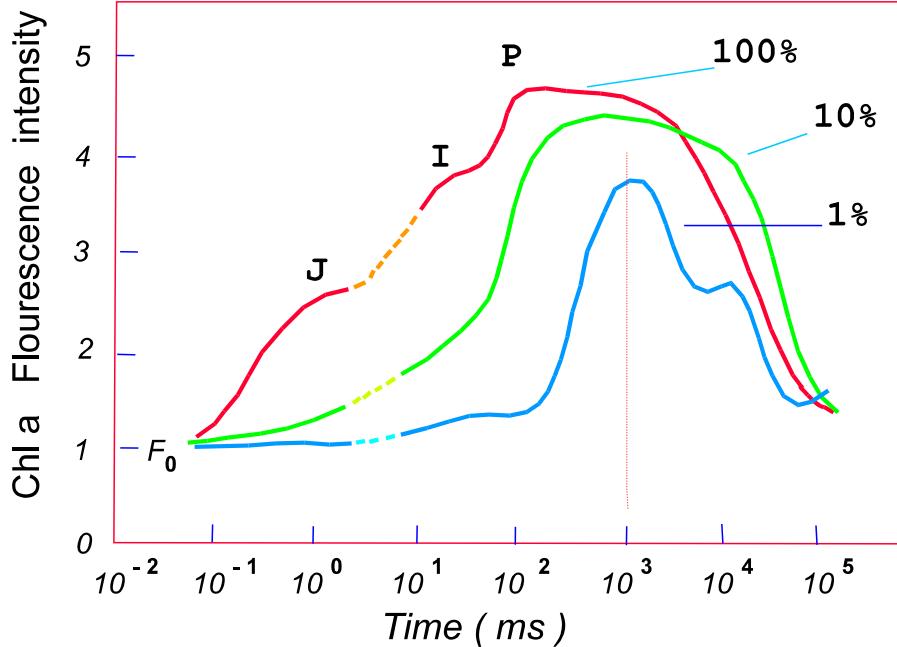
Experiment

Red light (650 nm) Intensity
600 (100%), 60 (10%) and 6
(1%) $W \cdot m^{-2}$.

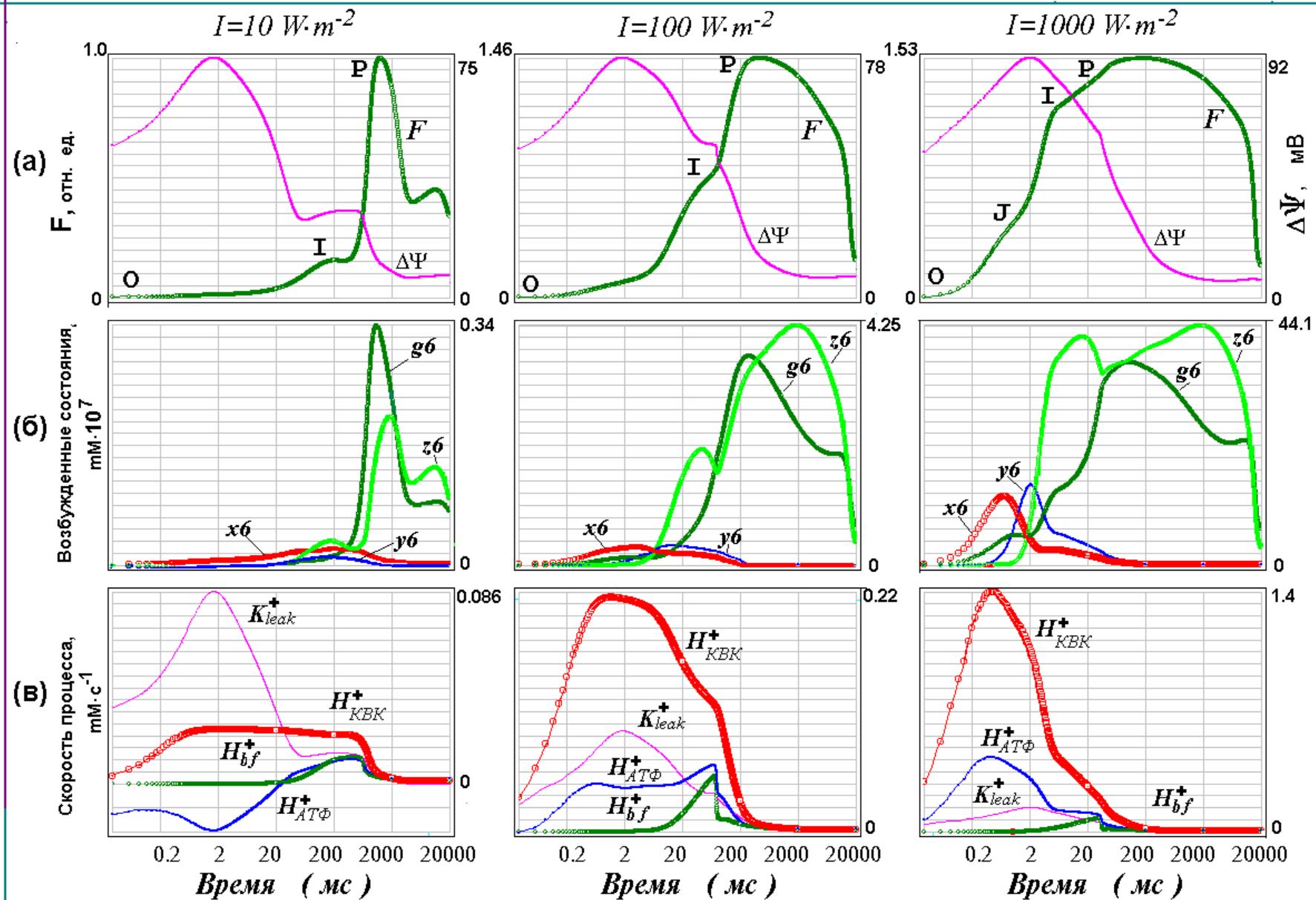
Strasser R.J., Srivastava A.,
Govindjee // Photochemistry
and Photobiology. 1995. V.61.
P.32-42 44.

Model

Light constants:
 $1500, 150 \text{ u } 15 \text{ c}^{-1}$.

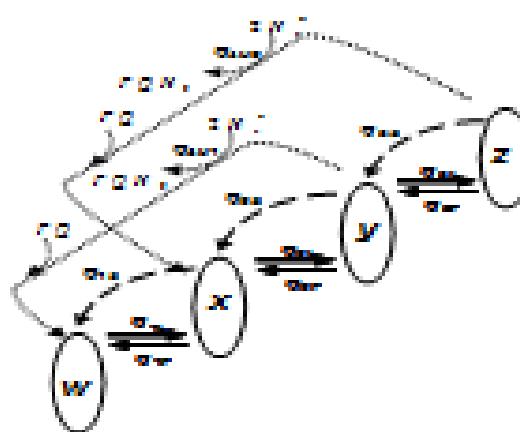
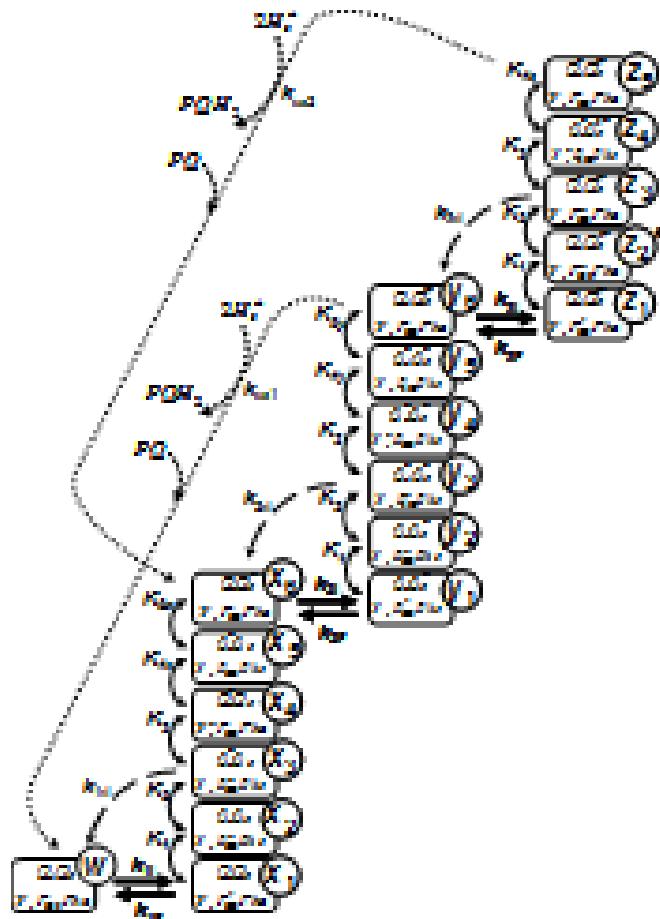


Kinetic curves of variables of the model



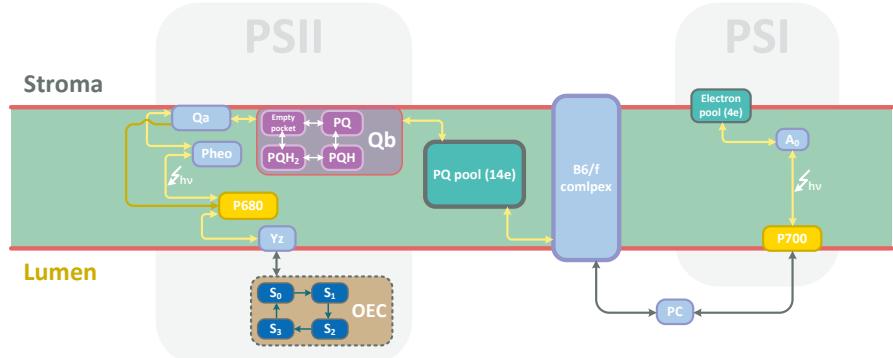
Как использовать кинетические модели

- Фитирование экспериментальных кривых и оценка параметров. Не определяемых экспериментально (параметры безызлучательной релаксации в ФРЦ)
Оценка параметров фотосинтетической цепи в разных условиях : для разных видов, в ходе роста культуры, при разных режимах культивирования и режимах освещения, при стрессе



Monte-Carlo model

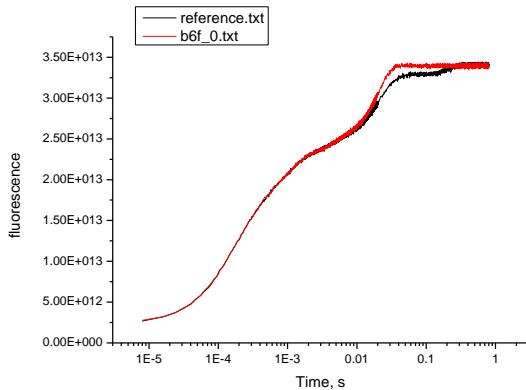
P700 redox transformations



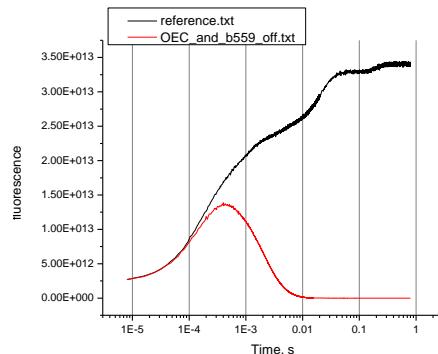
[Yellow] - light dependent electron carrier

[Blue] - electron carrier

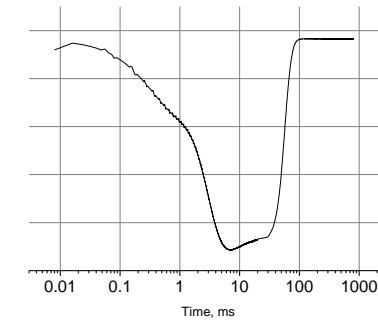
[Teal] - electron pool



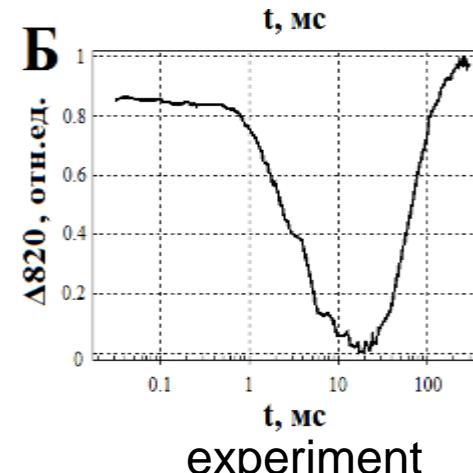
Fluorescence, red - DCMU



Fluorescence,
red – heat stress



simulation



t, мс

experiment

Maslakov, Antal et al., 2016

Недостатки кинетических моделей

- Трудности в описании пространственной гетерогенности
- Несвободная диффузия подвижных переносчиков
- Невозможность проследить судьбу отдельного участника процесса

