

New (N<sup>5</sup>) **Formelherstellung (8/25/09)**

(**change from the previous versions:** from version N<sup>3</sup> to N<sup>4</sup> only the preexponential terms in k<sup>+</sup> and k<sup>-</sup> of charge; from N<sup>4</sup> to N<sup>5</sup> the packing parameters (“curvature”) of the lipids.

The state equation stays the same:

$$\frac{dC_{iv}^j}{dt} = k_{fi} k_{fadj} [C_{im}^j] S_v - k_{bi} \cdot k_{badj} \cdot C_{iv}^j$$

**forward:**

Unsaturation forward:

$$un_f = 2^{stdev(un_v)}$$

Charge Forward

$$ch_f = 60^{-(\overline{ch_v} \cdot ch_m)}$$

Curvature Forward

$$cu_f = 10^{stdev(|\log(cu_v)|)}$$

Length Forward

$$l_f = 3^{stdev(l_v)}$$

Complex Formation 1 (CF1; formerly umbrella)

$$CF1_f = 1$$

$$k_{fadj} = un_f \cdot ch_f \cdot cu_f \cdot l_f \cdot CF1_f$$

**backward:**

unsaturation backward:

$$un_b = 10^{|3.5 - \overline{un_v} - 3.5 - un_m|}$$

Charge backward:



Doron the **Lancer**  
Commander of New **GARD**



**Raphael bin Musa**  
Commander of Z **GARD**

$$ch_f = 60^{-(\overline{ch_v} \cdot ch_m)}$$

Curvature backward

$$cub = 4^{|\log(cuv) - \log(cum)|}$$

Length backward

$$lb = 3.2^{|\overline{l_v} - l_m|}$$

Complex Formation 1 (CF1) backward

$$CF1_b = 1.5^{(CF1_v \cdot CF1_m - |CF1_v \cdot CF1_m|)}$$

$$k_{badj} = unb \cdot ch_b \cdot cub \cdot lb \cdot CF1_b$$

**The starting parameters** ( $k_f = M^{-1}s^{-1}$ ;  $k_b = s^{-1}$ )

PC:	$k_f = 3.7 \times 10^6$ ;	$k_b = 2 \times 10^{-5}$
PE:	$k_f = 2.3 \times 10^6$ ;	$k_b = 1 \times 10^{-5}$
PS:	$k_f = 3.7 \times 10^6$ ;	$k_b = 1.25 \times 10^{-5}$
SM:	$k_f = 3.7 \times 10^6$ ;	$k_b = 3.1 \times 10^{-3} s^{-1}$
CHOL:	$k_f = 5 \times 10^8$ ;	$k_b = 2.8 \times 10^{-4}$

$k_f$ (PC) taken from Nichols85; **weakness**: NBD-PC; no unlabeled  $k_+$  found.

$k_f$ (PE) taken from Abreu04; NBD-PE

$k_f$ (PS) and  $k_f$ (SM) assumed same as  $k_f$ (PC)

$k_f$ (CHOL) is **weak** – basically guessed from  $k_f$ (NBD-lysoPE) in Sampaio05 and  $k_f$ (PC); try adjustments, probably decrease

$k_b$ (PC) is taken from Wimley90 – radioactive label; LUV, 30° C.

Then, Nichols82 with C6-NBD-PC and other headgroups was used to determine *ratios* of  $k_b$ (PC) with other headgroups, and  $k_b$  for other headgroups assigned accordingly.  $k_b$ (PS) was assumed to be the same as  $k_b$ (PG) given by Nichols82 (also ratio from  $k_b$ (PC)).

$k_b$ (SM) is taken from  $k_b$ (PC) of Wimley90 (radioactive), and then a ratio of  $k_b$ (PC)/ $k_b$ (SM) taken from Bai97: = 34/2.2 = 15.45;  $2.0 \times 10^{-4} \times 15.45 = 3.1 \times 10^{-3} s^{-1}$ .

$k_b$ (CHOL) taken from Jones90 (radioactive; POPC LUV; 37°).

### Curvature:

PE = 1.33 (Kumar91)

CHOL = 1.21 (Kumar91)

PC=0.8 (Kumar91)

SM=0.8 (assumed by rz same as PC)

PS=1 (no refs so far; should be close to unity; rz)

**Charge:**

PS = -1

**CF1**

SM = 3; PC = 2; CHOL = -1

Initial concentrations:

$1 \times 10^{-10}$  M; gamma distributed with stdev =  $10^{-10}$