New (N^7) **Formelherstellung (9/6/09)**

(***change from the previous versions***: from version N^3 to N^4 only the preexponential terms in k+ and k- of charge; from N^4 to N^5 the packing parameters ("curvature") of the lipids. From N^5 to N^6 only k+(CHOL) is made as 3.7 x 10^7 – x10 of most other lipids; from N^6 to N^7 CHOL k+ is changed to 5 x 10^7, from k+ for ergosterol from Estronca07)

The state equation stays the same:

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

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

forward:

Unsaturation forward:

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

Charge Forward

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

Curvature Forward

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

Length Forward

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

Complex Formation 1 (CF1; formerly umbrella)

$$CF1_f = 1$$
$$k_{fadj} = un_f \cdot ch_f \cdot cu_f \cdot l_f \cdot CF1_f$$

Raphael bin Musa
Commander of Z GARD

backward:

unsaturation backward:

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

Charge backward:

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

Curvature backward

$$cu_b = 4^{\left\|\log(cu_v)\right|-\left|\log(cu_m)\right\|}$$

Length backward

$$l_b = 3.2^{\left|\overline{l_v}-l_m\right|}$$

Complex Formation 1 (CF1) backward

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

$$k_{badj} = un_b\cdot ch_b\cdot cu_b\cdot l_b\cdot CF1_b$$

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: $k_f = 5.1 \times 10^7$; $k_b = 2.8 \times 10^{-4}$

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 taken from Estronca07, equal to that of dehydroergosterol.

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 x 10^{-10} M; gamma distributed with stdev = 10^{-10}