

Singular code for analysing RPA in the esterified cholesterol concentration (E) in the cellular cholesterol CRN

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ring F =
  ↪(0,k1,k2,k3,k4,k5,k6,k7,k8,k9,k10,k11,k12,k13,k14,k15,k16,p1,p2,p3,mu,eta,
  theta,alpha),(Sp,C,P,R,Sr,Sh,H,HR,Ce,Cf,Sci,Cp,CL,E),(dp(11),dp(2));

poly f1 = mu - eta*Sci*C;
poly f2 = theta*Ce - eta*Sci*C;
poly f3 = k1*Sci - k2*Sr;
poly f4 = k1*Sci - k10*Sh;
poly f5 = p1*Sr - k11*R - k14*P*R;
poly f6 = k3*CL*R - k4*Cf;
poly f7 = k4*Cf - k5*Cp + k6*Ce;
poly f8 = k5*Cp - k6*Ce + k9*HR*H - k12*Ce - k7*Ce + k8*E;
poly f9 = k7*Ce - k8*E;
poly f10 = p2*Sh - k15*HR*Ce;
poly f11 = alpha - k9*HR*H;
poly f12 = k1*Sci - k13*Sp;
poly f13 = p3*Sp - k16*P;

ideal I = f1, f2, f3, f4, f5, f6, f7, f8, f9, f10, f11, f12, f13;
ideal GI = groebner (I);
GI;

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GI[1]=(k8*theta)*E+(-k7*mu)
GI[2]=(k5*theta)*Cp+(-k6*mu-k12*mu+theta*alpha)
GI[3]=(k1*k3*k13*k16*p1*theta)*Sci*CL+(-k1*k2*k12*k14*p3*mu+k1*k2*k14*p3*theta*alpha)*Sci+(-k2*k11*k12*k13*k16*mu+k2*k11*k13*k16*theta*alpha)
GI[4]=(k4*theta)*Cf+(-k12*mu+theta*alpha)
GI[5]=(theta)*Ce+(-mu)
GI[6]=(k10*k15*mu)*HR+(-k1*p2*theta)*Sci
GI[7]=(k2*k9*k11*k12*k13*k16*p2*mu-k2*k9*k11*k13*k16*p2*theta*alpha)*H+(-k3*k10*k13*k15*k16*p1*theta*alpha)*Ce*CL+(k2*k10*k12*k14*k15*p3*mu*alpha-k2*k10*k14*k15*p3*theta*alpha^2)*Ce
GI[8]=(k10)*Sh+(-k1)*Sci
GI[9]=(k2)*Sr+(-k1)*Sci
GI[10]=(k3)*R*CL+(-k12)*Ce+(alpha)

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GI[11]=(k13*k16)*P+(-k1*p3)*Sci
GI[12]=(k10*k15*mu*eta*alpha)*C+(-k1*k9*p2*mu*theta)*H
GI[13]=(p3)*Sp+(-k16)*P
GI[14]=(k1*k14*p3)*R*Sci+(k11*k13*k16)*R+(-k13*k16*p1)*Sr

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lift(I,GI[1]);
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_[1,1]=(-k7)
_[2,1]=(k7)
_[3,1]=0
_[4,1]=0
_[5,1]=0
_[6,1]=0
_[7,1]=0
_[8,1]=0
_[9,1]=(-theta)
_[10,1]=0
_[11,1]=0
_[12,1]=0
_[13,1]=0

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In this case, the RPA polynomial, ρ , explicitly comprises

$$\begin{aligned}
GI[1] &= (-k_7)f_1 + (k_7)f_2 - \theta f_9 \\
&= -k_7(\mu - \eta S_{ci}C) + k_7(\theta C_e - \eta S_{ci}C) - \theta(k_7Ce - k_8E),
\end{aligned}$$

from here the setpoint is computed as:

$$E^* = \frac{k_7\mu}{k_8\theta}.$$