SUPPORTING INFORMATION

Influence of geometric isomerism on the binding of platinum anticancer agents with phospholipids

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S1: Scientist Model: Reaction of 1,1/*c,c* with DHPA (1:5 mol ratio) (Scheme 1)
// MicroMath Scientist Model File
//11cc with DHPA treating as monomer (Scheme 1)
IndVars: T
DepVars: A, B, C, D,E, L,Cl
Params: KAB,KBA,KBC,KCB,KBE,KEB,KCD,KDC
A'=-KAB*A+KBA*B*Cl
B'=KAB*A-KBA*B*Cl-KBC*B*L+KCB*C-B*KBE*L+E*KEB
C'=KBC*B*L-KCB*C-C*KCD+D*KDC
D'=C*KCD-D*KDC
E'=B*KBE*L-E*KEB
L'=-B*KBC*L+C*KCB-B*KBE*L+E*KEB
Cl'=KAB*A-KBA*B*Cl
// A=Pt-Cl, B=Pt-H2O, Cl=Chloride, C = Pt-DHPA(C), D = Pt-DHPA(D), L=DHPA
// E=Pt-PO4
// Initial Conditions
T=2080.2
A=0.0018102
B=5.2712E-5
C=1.7086E-5
D=0.0
E=0.0
L=0.0046829
Cl=6.9798E-5