Supporting Information for:

Rates and equilibria for probe capture by an antibody with infinite affinity

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Key Mathematica instructions for solving Equations 1–4 to prepare for Figure 5.

Units for numerical calculation
First-order rate const: min-1; second-order rate const: conc-1 min-1, where all conc expressed in molecules/µ3
a+b->c   a+b->cc   c->d   c->a+b   cc->a+b
a=site concn   b=DOTA concn   c=reactive complex   cc=non-reactive complex
d=product

```
ka1 = .35; kd1 = .42; kirr =i; b0 = 600; a0 = 6000; fxn =j;

Do[Do[solution = NDSolve[{
    a'[t] == -ka1 a[t] b[t] + kd1 c[t] + kd1 cc[t],
    b'[t] == -ka1 a[t] b[t] + kd1 c[t] + kd1 cc[t],
    cc'[t] == (1. - j)*ka1 a[t] b[t] - kd1 cc[t],
    c'[t] == j*ka1 a[t] b[t] - i c[t] - kd1 c[t],
    d'[t] == i c[t],
    a[0] == a0, b[0] == b0, c[0] == 0, cc[0] == 0, d[0] == 0}, {a, b, c, cc,
    d}, {t, 0, 150}];

  modelf2d = Function[{t}, Evaluate[First[d[t] /. solution]]];
  data2 = {{1, 23}, {2, 30}, {4, 34}, {8, 45}, {16, 66}, {32, 85}, {64,
    95}, {96, 95}, {128, 98}};
  v1 = (modelf2d[1]*95/573 - 23)^2;
  v2 = (modelf2d[2]*95/573 - 30)^2;
  v4 = (modelf2d[4]*95/573 - 34)^2;
  v8 = (modelf2d[8]*95/573 - 45)^2;
  v16 = (modelf2d[16]*95/573 - 66)^2;
  v32 = (modelf2d[32]*95/573 - 85)^2;
  v64 = (modelf2d[64]*95/573 - 95)^2;
  v96 = (modelf2d[96]*95/573 - 95)^2;
  v128 = (modelf2d[128]*95/573 - 98)^2;
  sumv = v1 + v2 + v4 + v8 + v16 + v32 + v64 + v96 + v128;
  Print[i, "   ", j, "   ", sumv], {i, 0, 10, .1}], {j, 0, 1, .1}]
```

Key Mathematica instructions for solving Equations 5–9 to prepare for Figure 6.

u is AABD(Y) concn, c is free receptor concn , v is ligand-receptor reactive complex concn, vv is ligand-receptor non-reactive complex concn, w is covalent product concn.
radius of capillary=10μ, max radius of cord=110μ, time minutes, conc molecules/μ3

```
difco = 20000;
k1 = .35;
k2 = .42;
kir = 1.5; fxn = .2; preexp = i;
Do[solution =
  NDSolve[{D[u[r, t], t] ==
     difco*(D[u[r, t], r, r] + D[u[r, t], r]/r) - k1*c[r, t]*u[r, t] +
      k2*v[r, t] + k2*vv[r, t],
    D[c[r, t], t] == -k1*c[r, t]*u[r, t] + k2*v[r, t] + k2*vv[r, t],
    D[vv[r, t], t] == (1 - fxn)*k1*c[r, t]*u[r, t] - k2*vv[r, t],
    D[v[r, t], t] == fxn*k1*c[r, t]*u[r, t] - (k2 + kir)*v[r, t],
    D[w[r, t], t] == kir*v[r, t], u[r, 0] == i*Exp[-(r - 10)^2],
    u[10, t] == i*Exp[-0.12*t], (D[u[r, t], r] /. r -> 110) == 0,
    c[r, 0] == 28.2, vv[r, 0] == 0, vv[10, t] == 0, v[r, 0] == 0,
    v[10, t] == 0, w[r, 0] == 0, w[10, t] == 0}, {u, c, vv, v, w}, {r, 10,
    110}, {t, 0, 60},
   Method -> {"MethodOfLines",
     "SpatialDiscretization" -> {"TensorProductGrid",
       "DifferenceOrder" -> "Pseudospectral"}}];


 toall = Table[
   1.67*10^-4*
    NIntegrate[
     Evaluate[
      First[u[r, ti] /. solution]*r + First[vv[r, ti] /. solution]*r +
       First[v[r, ti] /. solution]*r + First[w[r, ti] /. solution]*r],
     {r, 10, 110}, WorkingPrecision -> 24, PrecisionGoal -> 10,
     MaxRecursion -> 40], {ti, 60}];
 sumvar = (toall[[1]]/.103256 - 3.8)^2 + (toall[[5]]/.103256 -
      5.2)^2 + (toall[[10]]/.103256 - 6.4)^2 + (toall[[20]]/.103256 -
      6.6)^2 + (toall[[30]]/.103256 - 6.7)^2 + (toall[[40]]/.103256 -
      7.5)^2 + (toall[[50]]/.103256 - 7.1)^2 + (toall[[60]]/.103256 - 7.7)^2;
 Print[i, "    ", sumvar, "    ", toall[[1]]/.103256, toall[[5]]/.103256,
   toall[[10]]/.103256, toall[[20]]/.103256, toall[[30]]/.103256,
   toall[[40]]/.103256, toall[[50]]/.103256, toall[[60]]]/.103256, {i, 0.05,
  0.7, .05}]
```