SUPPLEMENTARY INFORMATION

Global Analysis of Protein-Protein Interactions Reveals

Multiple CYP2E1–Reductase Complexes[†]

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CONTENTS

DynaFit Script and Experimental Data - Model Discrimination #1

```
;_____________________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR* ?

[components]

   P, R

[mechanism]

   P + R <===> P.R      :     Kpr    dissoc

[constants]

   Kpr = 0.1 ?

[responses]

   P.R = 10 ?

[concentrations]

[data]

    variable    P, R
    set           alldata

[output]

    directory  ./output/models-round-1

;_____________________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-P2R* ?

[mechanism]

   P + R <===> P.R              :     Kpr   dissoc
   P.R + P <===> P.P.R          :     Kppr  dissoc

[constants]
```

```
   Kpr = 0.1 ?
   Kppr = 0.1 ?

[responses]

   P.R = 10 ?
   P.P.R = 10 ?

;_____________________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-PR2* ?

[mechanism]

   P + R <===> P.R              :     Kpr   dissoc
   P.R + R <===> P.R.R          :     Kprr  dissoc

[constants]

   Kpr = 0.1 ?
   Kprr = 0.1 ?

[responses]

   P.R = 10 ?
   P.R.R = 10 ?

;_____________________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-PR2*-P2R* ?

[mechanism]

   P + R <===> P.R              :     Kpr   dissoc
   P.R + R <===> P.R.R          :     Kprr  dissoc
   P.R + P <===> P.P.R          :     Kppr  dissoc

[constants]

   Kpr = 0.1 ?
   Kprr = 0.1 ?
   Kppr = 0.1 ?

[responses]

   P.R = 10 ?
   P.R.R = 10 ?
   P.P.R = 10 ?
```

```
;_____________________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-P2R2* ?

[mechanism]

   P + R <===> P.R              :     Kpr   dissoc
   P.R + P.R <===> P.R.P.R      :     Kprpr  dissoc

[constants]

   Kpr = 0.1 ?
   Kprpr = 0.1 ?

[responses]

   P.R = 10 ?
   P.R.P.R = 10 ?
;_____________________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-P2R*-P2R2* ?

[mechanism]

   P + R <===> P.R              :     Kpr   dissoc
   P.R + P <===> P.P.R          :     Kppr  dissoc
   P.P.R + R <===> P.R.P.R      :     Kprpr  dissoc

[constants]

   Kpr = 0.1 ?
   Kppr = 0.1 ?
   Kprpr = 0.1 ?

[responses]

   P.R = 10 ?
   P.P.R = 10 ?
   P.R.P.R = 10 ?
;_____________________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-PR2*-P2R2* ?

[mechanism]
```

```
   P + R <===> P.R              :     Kpr   dissoc
   P.R + R <===> P.R.R          :     Kprr  dissoc
   P.R.R + P <===> P.R.P.R      :     Kprpr  dissoc

[constants]

   Kpr = 0.1 ?
   Kprr = 0.1 ?
   Kprpr = 0.1 ?

[responses]

   P.R = 10 ?
   P.R.R = 10 ?
   P.R.P.R = 10 ?
;_____________________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-P2R*-PR2*-P2R2* ?

[mechanism]

   P + R <===> P.R              :     Kpr   dissoc
   P.R + P <===> P.P.R          :     Kppr  dissoc
   P.R + R <===> P.R.R          :     Kprr  dissoc
   P.R.R + P <===> P.R.P.R      :     Kprpr  dissoc

[constants]

   Kpr = 0.1 ?
   Kppr = 0.1 ?
   Kprr = 0.1 ?
   Kprpr = 0.1 ?

[responses]

   P.R = 10 ?
   P.P.R = 10 ?
   P.R.R = 10 ?
   P.R.P.R = 10 ?
;_____________________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-P2 ?

[components]

   P, R

[mechanism]
```

```
   P + R <===> P.R      :     Kpr    dissoc
   P + P <===> P.P      :     Kpp    dissoc

[constants]

   Kpr = 0.1 ?
   Kpp = 0.1 ?

[responses]

   P.R = 10 ?

;_____________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-P2R*-P2 ?

[mechanism]

   P + R <===> P.R             :     Kpr   dissoc
   P.R + P <===> P.P.R         :     Kppr  dissoc
   P + P <===> P.P             :     Kpp    dissoc

[constants]

   Kpr = 0.1 ?
   Kppr = 0.1 ?
   Kpp = 0.1 ?

[responses]

   P.R = 10 ?
   P.P.R = 10 ?

;_____________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-PR2*-P2 ?

[mechanism]

   P + R <===> P.R             :     Kpr   dissoc
   P.R + R <===> P.R.R         :     Kprr  dissoc
   P + P <===> P.P           :     Kpp   dissoc

[constants]

   Kpr = 0.1 ?
   Kprr = 0.1 ?
   Kpp = 0.1 ?
```

```
[responses]

   P.R = 10 ?
   P.R.R = 10 ?

;_____________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-PR2*-P2R*-P2 ?

[mechanism]

   P + R <===> P.R              :     Kpr   dissoc
   P.R + R <===> P.R.R          :     Kprr  dissoc
   P.R + P <===> P.P.R          :     Kppr  dissoc
   P + P <===> P.P            :     Kpp   dissoc

[constants]

   Kpr = 0.1 ?
   Kprr = 0.1 ?
   Kppr = 0.1 ?
   Kpp = 0.1 ?

[responses]

   P.R = 10 ?
   P.R.R = 10 ?
   P.P.R = 10 ?
;_____________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-P2R2*-P2 ?

[mechanism]

   P + R <===> P.R              :     Kpr   dissoc
   P.R + P.R <===> P.R.P.R      :     Kprpr  dissoc
   P + P <===> P.P            :     Kpp   dissoc

[constants]

   Kpr = 0.1 ?
   Kprpr = 0.1 ?
   Kpp = 0.1 ?

[responses]

   P.R = 10 ?
   P.R.P.R = 10 ?
;_____________________________________________________________
```

```
[task]

   data = equilibria
   task = fit
   model = PR*-P2R*-P2R2*-P2 ?

[mechanism]

   P + R <===> P.R              :     Kpr   dissoc
   P.R + P <===> P.P.R          :     Kppr  dissoc
   P.P.R + R <===> P.R.P.R      :     Kprpr  dissoc
   P + P <===> P.P            :     Kpp   dissoc

[constants]

   Kpr = 0.1 ?
   Kppr = 0.1 ?
   Kprpr = 0.1 ?
   Kpp = 0.1 ?

[responses]

   P.R = 10 ?
   P.P.R = 10 ?
   P.R.P.R = 10 ?
;_____________________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-PR2*-P2R2*-P2 ?

[mechanism]

   P + R <===> P.R              :     Kpr   dissoc
   P.R + R <===> P.R.R          :     Kprr  dissoc
   P.R.R + P <===> P.R.P.R      :     Kprpr  dissoc
   P + P <===> P.P            :     Kpp   dissoc

[constants]

   Kpr = 0.1 ?
   Kprr = 0.1 ?
   Kprpr = 0.1 ?
   Kpp = 0.1 ?

[responses]

   P.R = 10 ?
   P.R.R = 10 ?
   P.R.P.R = 10 ?
;_____________________________________________________________________

[task]
```

```
   data = equilibria
   task = fit
   model = PR*-P2R*-PR2*-P2R2*-P2 ?

[mechanism]

   P + R <===> P.R              :     Kpr   dissoc
   P.R + P <===> P.P.R          :     Kppr  dissoc
   P.R + R <===> P.R.R          :     Kprr  dissoc
   P.R.R + P <===> P.R.P.R      :     Kprpr  dissoc
   P + P <===> P.P            :     Kpp   dissoc

[constants]

   Kpr = 0.1 ?
   Kppr = 0.1 ?
   Kprr = 0.1 ?
   Kprpr = 0.1 ?
   Kpp = 0.1 ?

[responses]

   P.R = 10 ?
   P.P.R = 10 ?
   P.R.R = 10 ?
   P.R.P.R = 10 ?
;_____________________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-R2 ?

[components]

   P, R

[mechanism]

   P + R <===> P.R      :     Kpr    dissoc
   R + R <===> R.R      :     Krr    dissoc

[constants]

   Kpr = 0.1 ?
   Krr = 0.1 ?

[responses]

   P.R = 10 ?

;_____________________________________________________________________

[task]

   data = equilibria
```

```
   task = fit
   model = PR*-P2R*-R2 ?

[mechanism]

   P + R <===> P.R              :     Kpr   dissoc
   P.R + P <===> P.P.R          :     Kppr  dissoc
   R + R <===> R.R              :     Krr    dissoc

[constants]

   Kpr = 0.1 ?
   Kppr = 0.1 ?
   Krr = 0.1 ?

[responses]

   P.R = 10 ?
   P.P.R = 10 ?

;_____________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-PR2*-R2 ?

[mechanism]

   P + R <===> P.R              :     Kpr   dissoc
   P.R + R <===> P.R.R          :     Kprr  dissoc
   R + R <===> R.R            :     Krr   dissoc

[constants]

   Kpr = 0.1 ?
   Kprr = 0.1 ?
   Krr = 0.1 ?

[responses]

   P.R = 10 ?
   P.R.R = 10 ?

;_____________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-PR2*-P2R*-R2 ?

[mechanism]

   P + R <===> P.R              :     Kpr   dissoc
   P.R + R <===> P.R.R          :     Kprr  dissoc
```

```
   P.R + P <===> P.P.R          :     Kppr  dissoc
   R + R <===> R.R            :     Krr   dissoc

[constants]

   Kpr = 0.1 ?
   Kprr = 0.1 ?
   Kppr = 0.1 ?
   Krr = 0.1 ?

[responses]

   P.R = 10 ?
   P.R.R = 10 ?
   P.P.R = 10 ?
;_____________________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-P2R2*-R2 ?

[mechanism]

   P + R <===> P.R              :     Kpr   dissoc
   P.R + P.R <===> P.R.P.R      :     Kprpr  dissoc
   R + R <===> R.R            :     Krr   dissoc

[constants]

   Kpr = 0.1 ?
   Kprpr = 0.1 ?
   Krr = 0.1 ?

[responses]

   P.R = 10 ?
   P.R.P.R = 10 ?
;_____________________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-P2R*-P2R2*-R2 ?

[mechanism]

   P + R <===> P.R              :     Kpr   dissoc
   P.R + P <===> P.P.R          :     Kppr  dissoc
   P.P.R + R <===> P.R.P.R      :     Kprpr  dissoc
   R + R <===> R.R            :     Krr   dissoc

[constants]

   Kpr = 0.1 ?
```

```
   Kppr = 0.1 ?
   Kprpr = 0.1 ?
   Krr = 0.1 ?

[responses]

   P.R = 10 ?
   P.P.R = 10 ?
   P.R.P.R = 10 ?
;_____________________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-PR2*-P2R2*-R2 ?

[mechanism]

   P + R <===> P.R              :     Kpr   dissoc
   P.R + R <===> P.R.R          :     Kprr  dissoc
   P.R.R + P <===> P.R.P.R      :     Kprpr  dissoc
   R + R <===> R.R            :     Krr   dissoc

[constants]

   Kpr = 0.1 ?
   Kprr = 0.1 ?
   Kprpr = 0.1 ?
   Krr = 0.1 ?

[responses]

   P.R = 10 ?
   P.R.R = 10 ?
   P.R.P.R = 10 ?
;_____________________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-P2R*-PR2*-P2R2*-R2 ?

[mechanism]

   P + R <===> P.R              :     Kpr   dissoc
   P.R + P <===> P.P.R          :     Kppr  dissoc
   P.R + R <===> P.R.R          :     Kprr  dissoc
   P.R.R + P <===> P.R.P.R      :     Kprpr  dissoc
   R + R <===> R.R            :     Krr   dissoc

[constants]

   Kpr = 0.1 ?
   Kppr = 0.1 ?
   Kprr = 0.1 ?
```

```
   Kprpr = 0.1 ?
   Krr = 0.1 ?

[responses]

   P.R = 10 ?
   P.P.R = 10 ?
   P.R.R = 10 ?
   P.R.P.R = 10 ?
;_____________________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-P2-R2 ?

[components]

   P, R

[mechanism]

   P + R <===> P.R      :     Kpr    dissoc
   P + P <===> P.P      :     Kpp    dissoc
   R + R <===> R.R      :     Krr    dissoc

[constants]

   Kpr = 0.1 ?
   Kpp = 0.1 ?
   Krr = 0.1 ?

[responses]

   P.R = 10 ?

;_____________________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-P2R*-P2-R2 ?

[mechanism]

   P + R <===> P.R             :     Kpr   dissoc
   P.R + P <===> P.P.R         :     Kppr  dissoc
   P + P <===> P.P             :     Kpp    dissoc
   R + R <===> R.R             :     Krr    dissoc

[constants]

   Kpr = 0.1 ?
   Kppr = 0.1 ?
   Kpp = 0.1 ?
```

```
   Krr = 0.1 ?

[responses]

   P.R = 10 ?
   P.P.R = 10 ?

;_____________________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-PR2*-P2-R2 ?

[mechanism]

   P + R <===> P.R              :     Kpr   dissoc
   P.R + R <===> P.R.R          :     Kprr  dissoc
   P + P <===> P.P            :     Kpp   dissoc
   R + R <===> R.R            :     Krr   dissoc

[constants]

   Kpr = 0.1 ?
   Kprr = 0.1 ?
   Kpp = 0.1 ?
   Krr = 0.1 ?

[responses]

   P.R = 10 ?
   P.R.R = 10 ?

;_____________________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-PR2*-P2R*-P2-R2 ?

[mechanism]

   P + R <===> P.R              :     Kpr   dissoc
   P.R + R <===> P.R.R          :     Kprr  dissoc
   P.R + P <===> P.P.R          :     Kppr  dissoc
   P + P <===> P.P            :     Kpp   dissoc
   R + R <===> R.R            :     Krr   dissoc

[constants]

   Kpr = 0.1 ?
   Kprr = 0.1 ?
   Kppr = 0.1 ?
   Kpp = 0.1 ?
   Krr = 0.1 ?
```

```
[responses]

   P.R = 10 ?
   P.R.R = 10 ?
   P.P.R = 10 ?
;_____________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-P2R2*-P2-R2 ?

[mechanism]

   P + R <===> P.R              :     Kpr   dissoc
   P.R + P.R <===> P.R.P.R      :     Kprpr  dissoc
   P + P <===> P.P            :     Kpp   dissoc
   R + R <===> R.R            :     Krr   dissoc

[constants]

   Kpr = 0.1 ?
   Kprpr = 0.1 ?
   Kpp = 0.1 ?
   Krr = 0.1 ?

[responses]

   P.R = 10 ?
   P.R.P.R = 10 ?
;_____________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-P2R*-P2R2*-P2-R2 ?

[mechanism]

   P + R <===> P.R              :     Kpr   dissoc
   P.R + P <===> P.P.R          :     Kppr  dissoc
   P.P.R + R <===> P.R.P.R      :     Kprpr  dissoc
   P + P <===> P.P            :     Kpp   dissoc
   R + R <===> R.R            :     Krr   dissoc

[constants]

   Kpr = 0.1 ?
   Kppr = 0.1 ?
   Kprpr = 0.1 ?
   Kpp = 0.1 ?
   Krr = 0.1 ?

[responses]
```

```
   P.R = 10 ?
   P.P.R = 10 ?
   P.R.P.R = 10 ?
;_____________________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-PR2*-P2R2*-P2-R2 ?

[mechanism]

   P + R <===> P.R              :     Kpr   dissoc
   P.R + R <===> P.R.R          :     Kprr  dissoc
   P.R.R + P <===> P.R.P.R      :     Kprpr  dissoc
   P + P <===> P.P            :     Kpp   dissoc
   R + R <===> R.R            :     Krr   dissoc

[constants]

   Kpr = 0.1 ?
   Kprr = 0.1 ?
   Kprpr = 0.1 ?
   Kpp = 0.1 ?
   Krr = 0.1 ?

[responses]

   P.R = 10 ?
   P.R.R = 10 ?
   P.R.P.R = 10 ?
;_____________________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-P2R*-PR2*-P2R2*-P2-R2 ?

[mechanism]

   P + R <===> P.R              :     Kpr   dissoc
   P.R + P <===> P.P.R          :     Kppr  dissoc
   P.R + R <===> P.R.R          :     Kprr  dissoc
   P.R.R + P <===> P.R.P.R      :     Kprpr  dissoc
   P + P <===> P.P            :     Kpp   dissoc
   R + R <===> R.R            :     Krr   dissoc

[constants]

   Kpr = 0.1 ?
   Kppr = 0.1 ?
   Kprr = 0.1 ?
   Kprpr = 0.1 ?
   Kpp = 0.1 ?
```

```
   Krr = 0.1 ?

[responses]

   P.R = 10 ?
   P.P.R = 10 ?
   P.R.R = 10 ?
   P.R.P.R = 10 ?

;_____________________________________________________________________

[set:alldata]

P_tot R_tot rate
======      ======      =======

; Constant [R] = 0.0075, variable [P]

0.0075      0.0075      0.00776
0.0150      0.0075      0.01392
0.0300      0.0075      0.01849
0.0600      0.0075      0.02508
0.1000      0.0075      0.02651
0.2000      0.0075      0.02994
0.3000      0.0075      0.03101
0.4000      0.0075      0.02843
0.0075      0.0075      0.00894
0.0150      0.0075      0.01624
0.0300      0.0075      0.02498
0.0600      0.0075      0.02820
0.1000      0.0075      0.03220
0.2000      0.0075      0.03354
0.3000      0.0075      0.03636
0.4000      0.0075      0.03444

; Constant [R] = 0.0150, variable [P]

0.0075      0.0150      0.01078
0.0150      0.0150      0.04981
0.0300      0.0150      0.08317
0.0600      0.0150      0.09133
0.1000      0.0150      0.10090
0.2000      0.0150      0.10750
0.3000      0.0150      0.10700
0.4000      0.0150      0.09316
0.0075      0.0150      0.01415
0.0150      0.0150      0.04119
0.0300      0.0150      0.07528
0.0600      0.0150      0.09700
0.1000      0.0150      0.10240
0.2000      0.0150      0.11680
0.3000      0.0150      0.11200
0.4000      0.0150      0.11050

; Constant [R] = 0.0300, variable [P]

0.0075      0.0300      0.02263
```

```
0.0150      0.0300      0.07508
0.0300      0.0300      0.12210
0.0600      0.0300      0.15240
0.1000      0.0300      0.18510
0.2000      0.0300      0.20000
0.3000      0.0300      0.19380
0.4000      0.0300      0.20000
0.0075      0.0300      0.02529
0.0150      0.0300      0.07633
0.0300      0.0300      0.12580
0.0600      0.0300      0.14090
0.1000      0.0300      0.17940
0.2000      0.0300      0.21380
0.3000      0.0300      0.19970
0.4000      0.0300      0.21780

; Constant [R] = 0.0600, variable [P]

0.0075      0.0600      0.02419
0.0150      0.0600      0.05593
0.0300      0.0600      0.17880
0.0600      0.0600      0.19190
0.1000      0.0600      0.38380
0.2000      0.0600      0.41980
0.3000      0.0600      0.40820
0.4000      0.0600      0.41400
0.0075      0.0600      0.02915
0.0150      0.0600      0.06719
0.0300      0.0600      0.17680
0.0600      0.0600      0.18680
0.1000      0.0600      0.37670
0.2000      0.0600      0.39840
0.3000      0.0600      0.38470
0.4000      0.0600      0.39150

; Constant [R] = 0.1000, variable [P]

0.0075      0.1000      0.03527
0.0150      0.1000      0.07973
0.0300      0.1000      0.24090
0.0600      0.1000      0.37680
0.1000      0.1000      0.58850
0.2000      0.1000      0.63490
0.3000      0.1000      0.60490
0.4000      0.1000      0.64860
0.0075      0.1000      0.04025
0.0150      0.1000      0.08718
0.0300      0.1000      0.22710
0.0600      0.1000      0.37440
0.1000      0.1000      0.49120
0.2000      0.1000      0.59710
0.3000      0.1000      0.58710
0.4000      0.1000      0.64880

; Constant [R] = 0.2000, variable [P]

0.0075      0.2000      0.04323
```

```
0.0150      0.2000      0.09872
0.0300      0.2000      0.27430
0.0600      0.2000      0.48950
0.1000      0.2000      0.80310
0.2000      0.2000      0.96650
0.3000      0.2000      1.17800
0.4000      0.2000      1.19700
0.0075      0.2000      0.04303
0.0150      0.2000      0.09348
0.0300      0.2000      0.25100
0.0600      0.2000      0.52360
0.1000      0.2000      0.79180
0.2000      0.2000      0.99280
0.3000      0.2000      1.10400
0.4000      0.2000      1.19100

; Constant [R] = 0.3000, variable [P]

0.0075      0.3000      0.04482
0.0150      0.3000      0.10260
0.0300      0.3000      0.28060
0.0600      0.3000      0.53340
0.1000      0.3000      0.67150
0.2000      0.3000      1.27700
0.3000      0.3000      1.35500
0.4000      0.3000      1.67600
0.0075      0.3000      0.04380
0.0150      0.3000      0.11200
0.0300      0.3000      0.28430
0.0600      0.3000      0.56690
0.1000      0.3000      0.70200
0.2000      0.3000      1.32400
0.3000      0.3000      1.40500
0.4000      0.3000      1.63600

; Constant [R] = 0.4000, variable [P]

0.0075      0.4000      0.04410
0.0150      0.4000      0.10570
0.0300      0.4000      0.28690
0.0600      0.4000      0.57520
0.1000      0.4000      0.75220
0.2000      0.4000      1.31700
0.3000      0.4000      1.83200
0.4000      0.4000      1.94900
0.0075      0.4000      0.04505
0.0150      0.4000      0.10760
0.0300      0.4000      0.27610
0.0600      0.4000      0.59340
0.1000      0.4000      0.80600
0.2000      0.4000      1.41100
0.3000      0.4000      1.78300
0.4000      0.4000      1.88000

[end]
```

Results - Model Discrimination #1

Minimum sum of squares = 0.17464

	model	nD	nP	SSrel	AICc	Δ AICc	weight
[1]	PR*	128	2	4.537	-23.6	175.6	0.000
[2]	PR*-P2R*	128	4	1.775	-139.4	59.8	0.000
[3]	PR*-PR2*	128	4	1.450	-165.3	33.9	0.000
[4]	PR*-PR2*-P2R*	128	6	1.188	-186.4	12.8	0.000
[5]	PR*-P2R2*	128	4	2.202	-111.8	87.3	0.000
[6]	PR*-P2R*-P2R2*	128	6	1.173	-188.0	11.2	0.001
[7]	PR*-PR2*-P2R2*	128	6	1.138	-191.8	7.3	0.007
[8]	PR*-P2R*-PR2*-P2R2*	128	8	1.056	-196.9	2.3	0.082
[9]	PR*-P2	128	3	2.293	-108.8	90.4	0.000
[10]	PR*-P2R*-P2	128	5	1.521	-157.0	42.1	0.000
[11]	PR*-PR2*-P2	128	5	1.451	-163.1	36.1	0.000
[12]	PR*-PR2*-P2R*-P2	128	7	1.116	-192.1	7.1	0.007
[13]	PR*-P2R2*-P2	128	5	1.094	-199.2	0.0	0.259
[14]	PR*-P2R*-P2R2*-P2	128	7	1.069	-197.6	1.6	0.116
[15]	PR*-PR2*-P2R2*-P2	128	7	1.064	-198.2	1.0	0.160
[16]	PR*-P2R*-PR2*-P2R2*-P2	128	9	1.044	-196.0	3.2	0.053
[17]	PR*-R2	128	3	4.538	-21.4	177.7	0.000
[18]	PR*-P2R*-R2	128	5	1.643	-147.1	52.1	0.000
[19]	PR*-PR2*-R2	128	5	1.431	-164.8	34.3	0.000
[20]	PR*-PR2*-P2R*-R2	128	7	1.167	-186.4	12.8	0.000
[21]	PR*-P2R2*-R2	128	5	2.808	-78.5	120.7	0.000
[22]	PR*-P2R*-P2R2*-R2	128	7	2.785	-75.1	124.1	0.000

[23]	PR*-PR2*-P2R2*-R2	128	7	1.137	-189.7	9.5	0.002
[24]	PR*-P2R*-PR2*-P2R2*-R2	128	9	1.053	-194.9	4.3	0.030
[25]	PR*-P2-R2	128	4	1.488	-162.0	37.2	0.000
[26]	PR*-P2R*-P2-R2	128	6	1.247	-180.2	19.0	0.000
[27]	PR*-PR2*-P2-R2	128	6	1.235	-181.4	17.8	0.000
[28]	PR*-PR2*-P2R*-P2-R2	128	8	1.071	-195.1	4.1	0.034
[29]	PR*-P2R2*-P2-R2	128	6	1.289	-176.0	23.2	0.000
[30]	PR*-P2R*-P2R2*-P2-R2	128	8	1.949	-118.5	80.7	0.000
[31]	PR*-PR2*-P2R2*-P2-R2	128	8	1.779	-130.1	69.1	0.000
[32]	PR*-P2R*-PR2*-P2R2*-P2-R2	128	10	1.000	-199.1	0.1	0.248

DynaFit Script and Experimental Data - Model Discrimination #2

```
;_____________________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-P2R2*-P2 ?

[components]

   P, R

[mechanism]

   P + R <===> P.R            :     Kpr   dissoc
   P.R + P.R <===> P.R.P.R      :     Kprpr  dissoc
   P + P <===> P.P            :     Kpp   dissoc

[constants]

   Kpr = 0.1 ?
   Kprpr = 0.1 ?
   Kpp = 0.1 ?

[responses]

   P.R = 10 ?
   P.R.P.R = 10 ?

[concentrations]

[data]

    variable    P, R
    set           alldata

[output]

    directory  ./users/Miller_GP/070510/output/fit-002d

[settings]

{Marquardt}
   IterationsPerParameter = 300

;_____________________________________________________________________

[task]
```

```
   data = equilibria
   task = fit
   model = PR*-P2R2-P2 ?

[mechanism]

   P + R <===> P.R            :     Kpr   dissoc
   P.R + P.R <===> P.R.P.R      :     Kprpr  dissoc
   P + P <===> P.P            :     Kpp   dissoc

[constants]

   Kpr = 0.1 ?
   Kprpr = 0.1 ?
   Kpp = 0.1 ?

[responses]

   P.R = 10 ?

;_____________________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-P2R*-P2R2*-P2 ?

[mechanism]

   P + R <===> P.R            :     Kpr   dissoc
   P.R + P <===> P.P.R          :     Kppr  dissoc
   P.P.R + R <===> P.R.P.R      :     Kprpr  dissoc
   P + P <===> P.P            :     Kpp   dissoc

[constants]

   Kpr = 0.1 ?
   Kppr = 0.1 ?
   Kprpr = 0.1 ?
   Kpp = 0.1 ?

[responses]

   P.R = 10 ?
   P.P.R = 10 ?
   P.R.P.R = 10 ?

;_____________________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-P2R*-P2R2-P2 ?

[mechanism]
```

```
   P + R <===> P.R            :     Kpr   dissoc
   P.R + P <===> P.P.R          :     Kppr  dissoc
   P.P.R + R <===> P.R.P.R      :     Kprpr  dissoc
   P + P <===> P.P            :     Kpp   dissoc

[constants]

   Kpr = 0.1 ?
   Kppr = 0.1 ?
   Kprpr = 0.1 ?
   Kpp = 0.1 ?

[responses]

   P.R = 10 ?
   P.P.R = 10 ?

;_____________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-P2R-P2R2*-P2 ?

[mechanism]

   P + R <===> P.R            :     Kpr   dissoc
   P.R + P <===> P.P.R          :     Kppr  dissoc
   P.P.R + R <===> P.R.P.R      :     Kprpr  dissoc
   P + P <===> P.P            :     Kpp   dissoc

[constants]

   Kpr = 0.1 ?
   Kppr = 0.1 ?
   Kprpr = 0.1 ?
   Kpp = 0.1 ?

[responses]

   P.R = 10 ?
   P.R.P.R = 10 ?

;_____________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-P2R-P2R2-P2 ?

[mechanism]

   P + R <===> P.R            :     Kpr   dissoc
   P.R + P <===> P.P.R          :     Kppr  dissoc
```

```
   P.P.R + R <===> P.R.P.R      :     Kprpr  dissoc
   P + P <===> P.P              :     Kpp   dissoc

[constants]

   Kpr = 0.1 ?
   Kppr = 0.1 ?
   Kprpr = 0.1 ?
   Kpp = 0.1 ?

[responses]

   P.R = 10 ?

;_____________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-PR2*-P2R2*-P2 ?

[mechanism]

   P + R <===> P.R              :     Kpr   dissoc
   P.R + R <===> P.R.R          :     Kprr  dissoc
   P.R.R + P <===> P.R.P.R      :     Kprpr  dissoc
   P + P <===> P.P              :     Kpp   dissoc

[constants]

   Kpr = 0.1 ?
   Kprr = 0.1 ?
   Kprpr = 0.1 ?
   Kpp = 0.1 ?

[responses]

   P.R = 10 ?
   P.R.R = 10 ?
   P.R.P.R = 10 ?

;_____________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-PR2*-P2R2-P2 ?

[mechanism]

   P + R <===> P.R              :     Kpr   dissoc
   P.R + R <===> P.R.R          :     Kprr  dissoc
   P.R.R + P <===> P.R.P.R      :     Kprpr  dissoc
   P + P <===> P.P              :     Kpp   dissoc
```

```
[constants]

   Kpr = 0.1 ?
   Kprr = 0.1 ?
   Kprpr = 0.1 ?
   Kpp = 0.1 ?

[responses]

   P.R = 10 ?
   P.R.R = 10 ?

;_____________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-PR2-P2R2*-P2 ?

[mechanism]

   P + R <===> P.R              :     Kpr   dissoc
   P.R + R <===> P.R.R          :     Kprr  dissoc
   P.R.R + P <===> P.R.P.R      :     Kprpr  dissoc
   P + P <===> P.P            :     Kpp   dissoc

[constants]

   Kpr = 0.1 ?
   Kprr = 0.1 ?
   Kprpr = 0.1 ?
   Kpp = 0.1 ?

[responses]

   P.R = 10 ?
   P.R.P.R = 10 ?

;_____________________________________________________________

[task]

   data = equilibria
   task = fit
   model = PR*-PR2-P2R2-P2 ?

[mechanism]

   P + R <===> P.R              :     Kpr   dissoc
   P.R + R <===> P.R.R          :     Kprr  dissoc
   P.R.R + P <===> P.R.P.R      :     Kprpr  dissoc
   P + P <===> P.P            :     Kpp   dissoc

[constants]

   Kpr = 0.1 ?
```

```
   Kprr = 0.1 ?
   Kprpr = 0.1 ?
   Kpp = 0.1 ?

[responses]

   P.R = 10 ?

;_____________________________________________________________

[set:alldata]

...
... AS ABOVE IN MODEL DISCRIMINATION #1
...

[end]
```

Results - Model Discrimination #2

Minimum sum of squares = 0.185593

	model	nD	nP	SSrel	AICc	Δ AICc	weight
[1]	PR*-P2R2*-P2	128	5	1.029	-199.2	3.4	0.058
[2]	PR*-P2R2-P2	128	4	1.028	-201.5	1.1	0.183
[3]	PR*-P2R*-P2R2*-P2	128	7	1.004	-197.9	4.8	0.030
[4]	PR*-P2R*-P2R2-P2	128	6	1.003	-200.2	2.4	0.095
[5]	PR*-P2R-P2R2*-P2	128	6	1.003	-200.2	2.4	0.095
[6]	PR*-P2R-P2R2-P2	128	5	1.002	-202.6	0.0	0.318
[7]	PR*-PR2*-P2R2*-P2	128	7	1.001	-198.3	4.4	0.036
[8]	PR*-PR2*-P2R2-P2	128	6	1.000	-200.6	2.0	0.118
[9]	PR*-PR2-P2R2*-P2	128	6	1.043	-195.2	7.4	0.008
[10]	PR*-PR2-P2R2-P2	128	5	1.028	-199.3	3.3	0.061