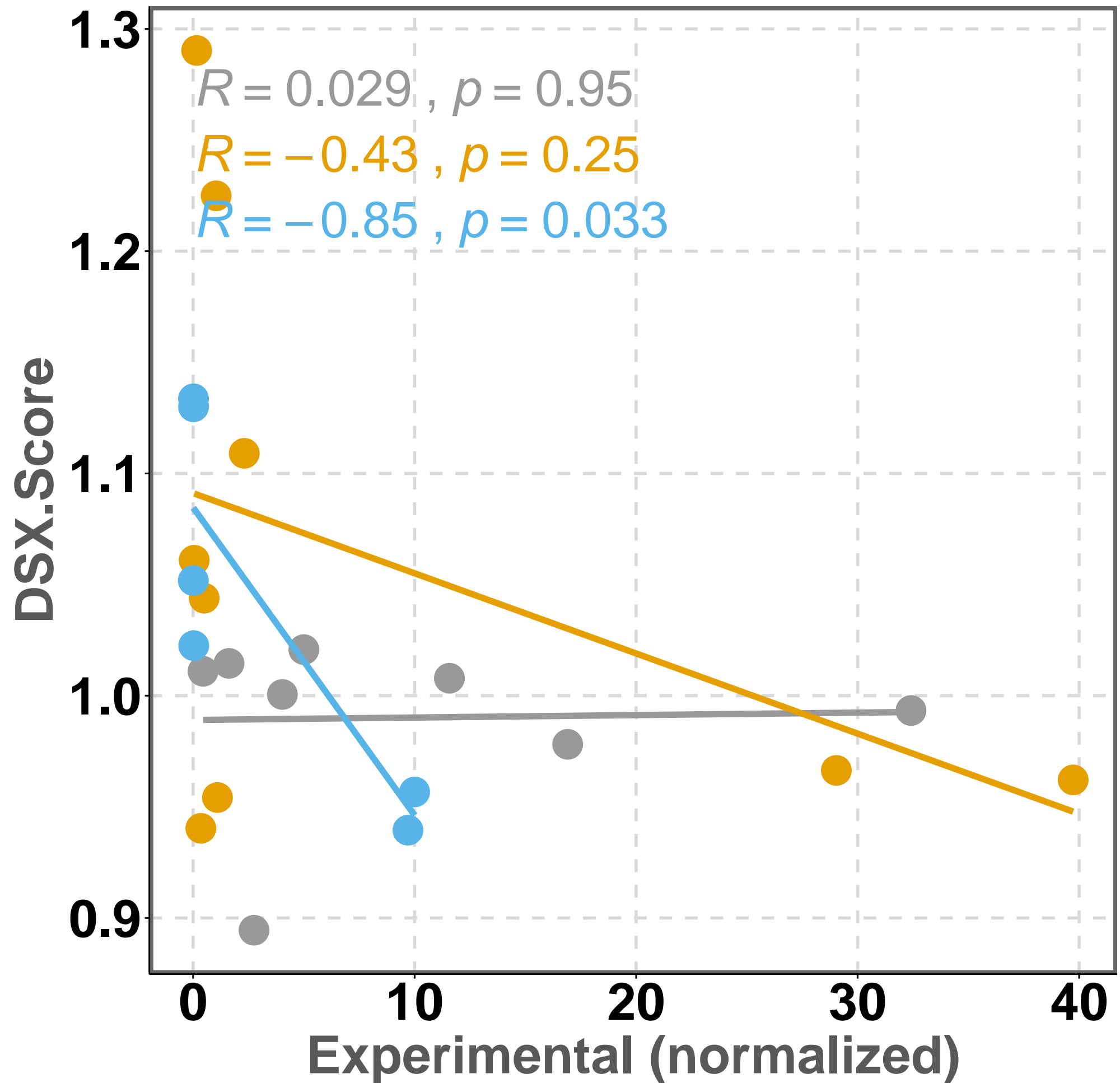
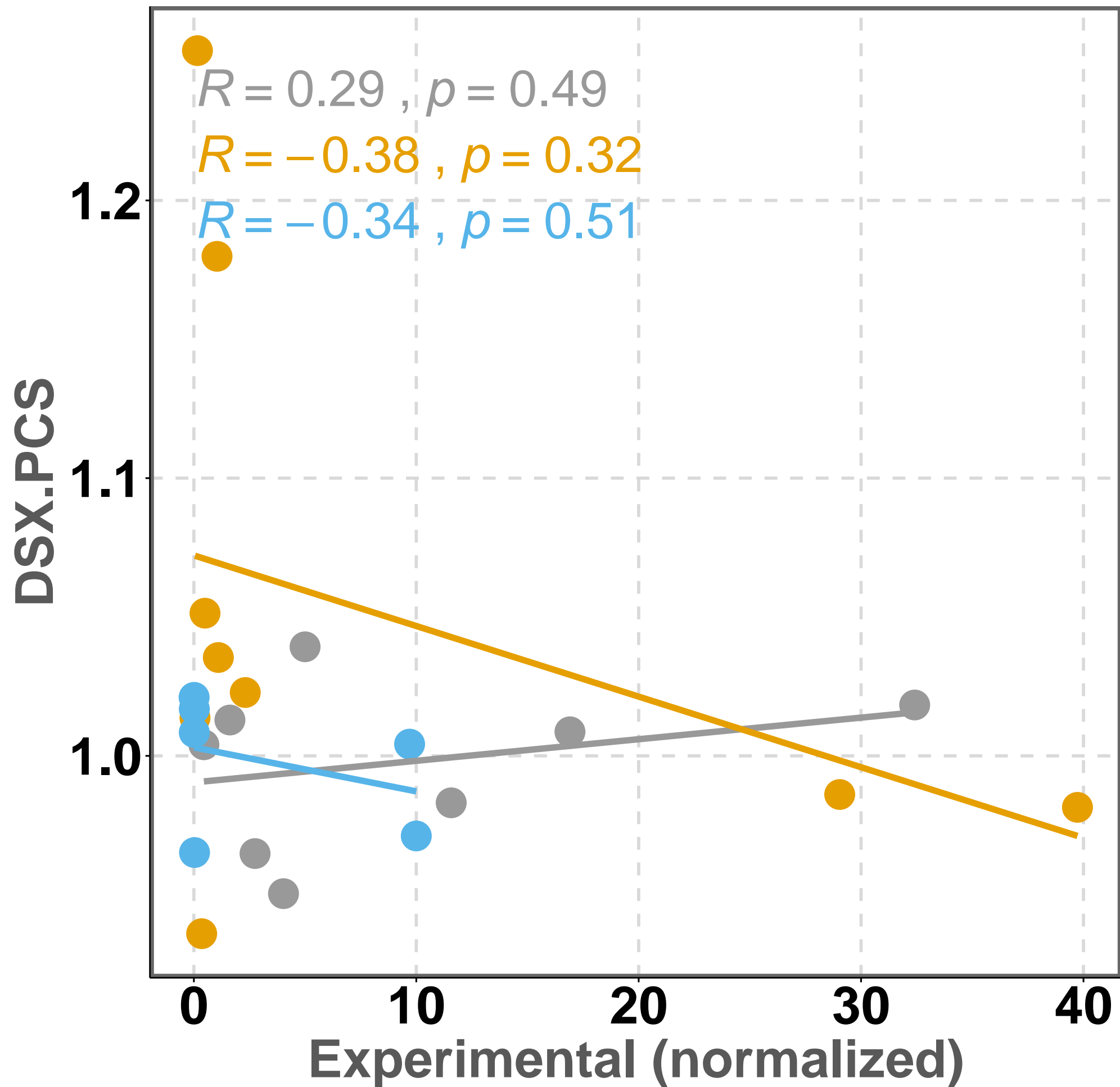


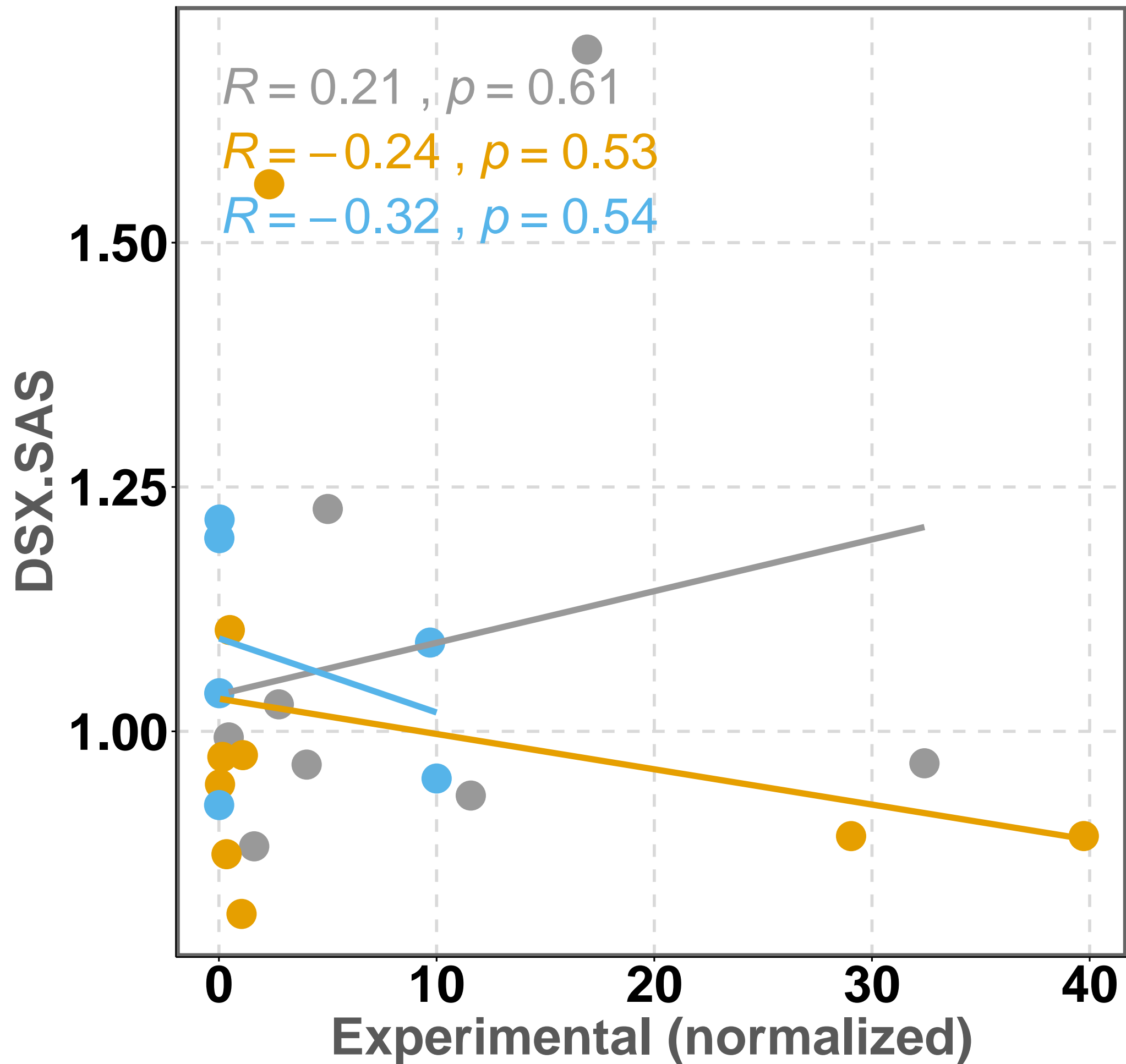
kinetics IC50 Kd Ki



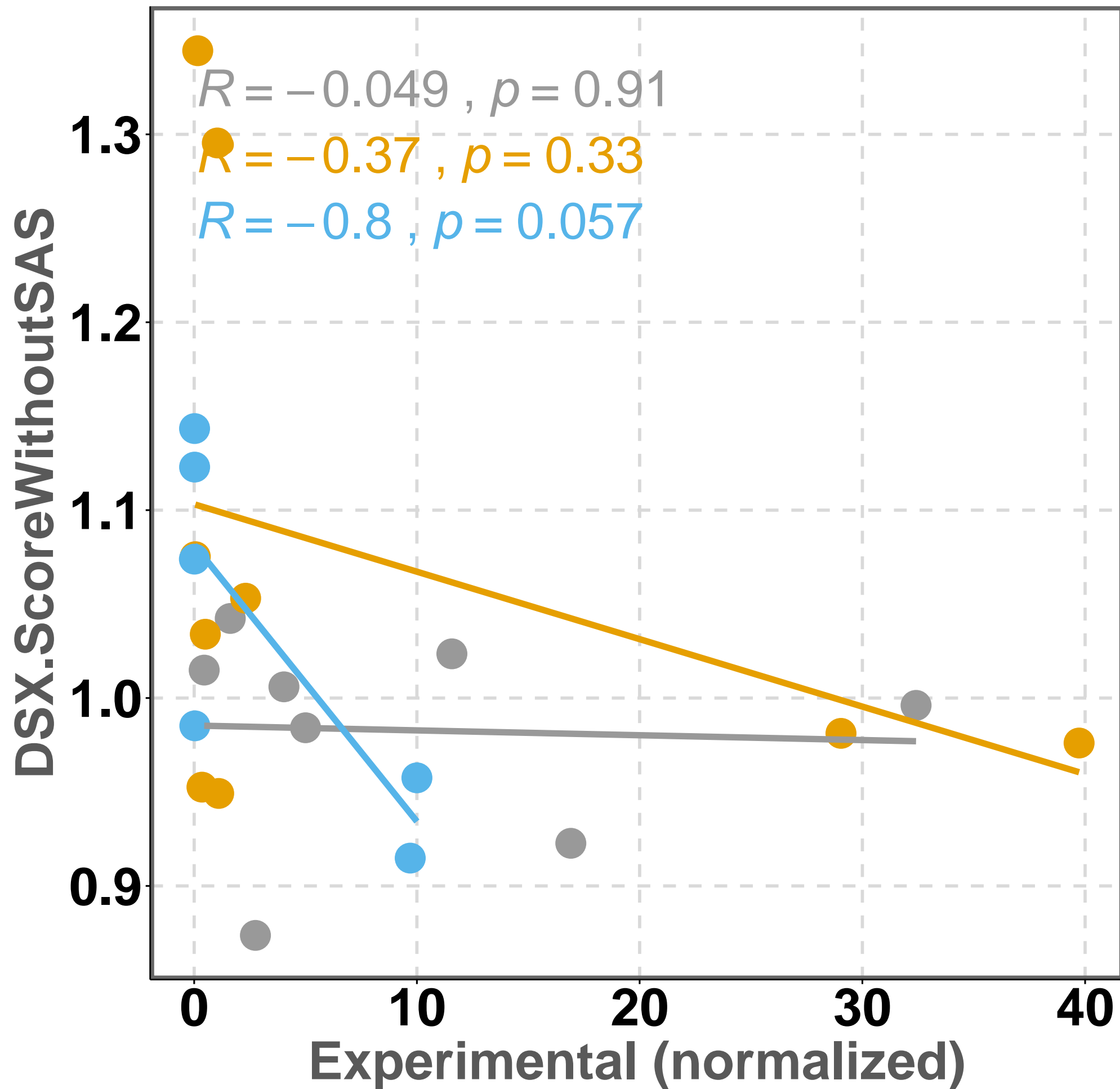
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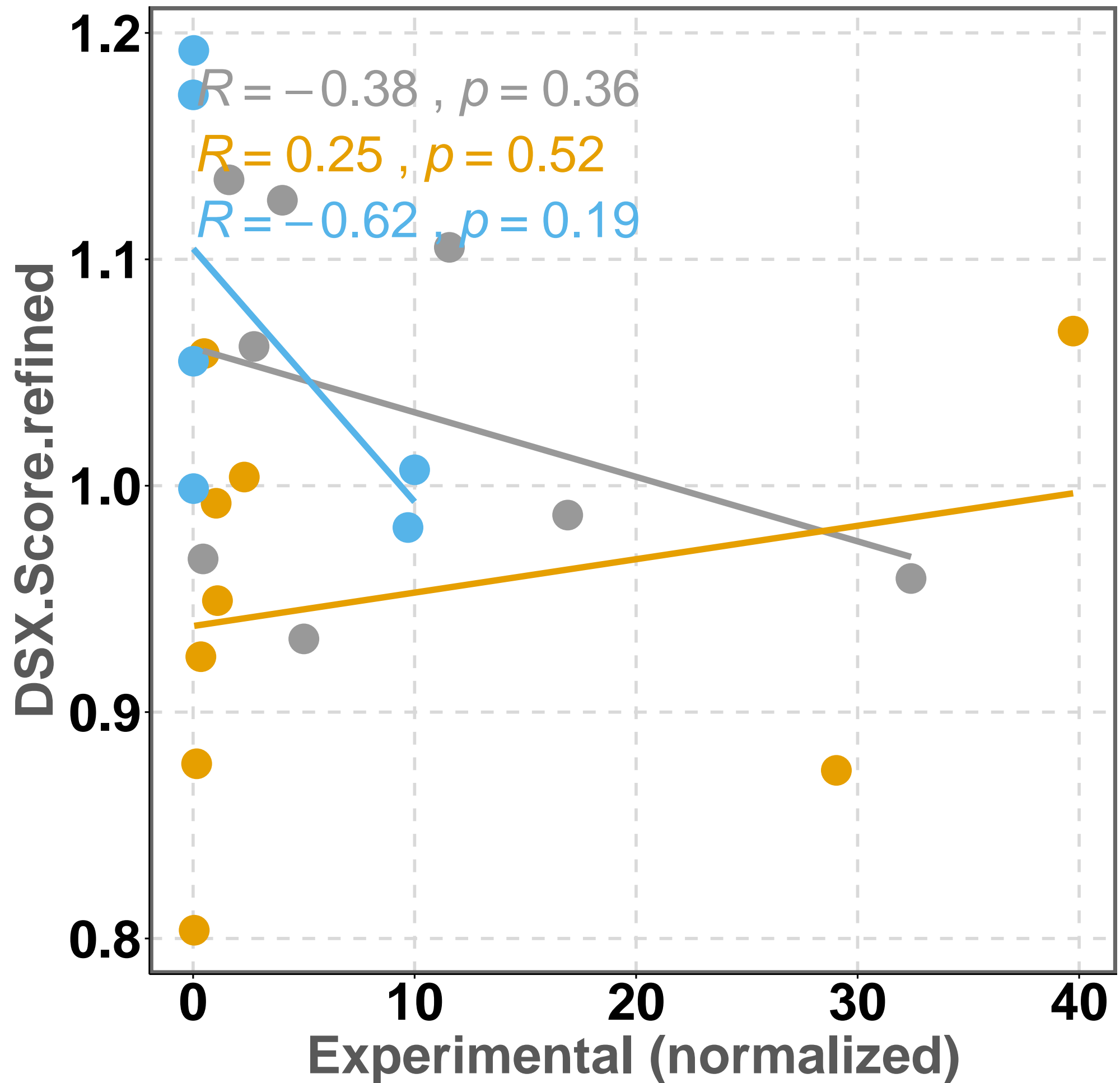
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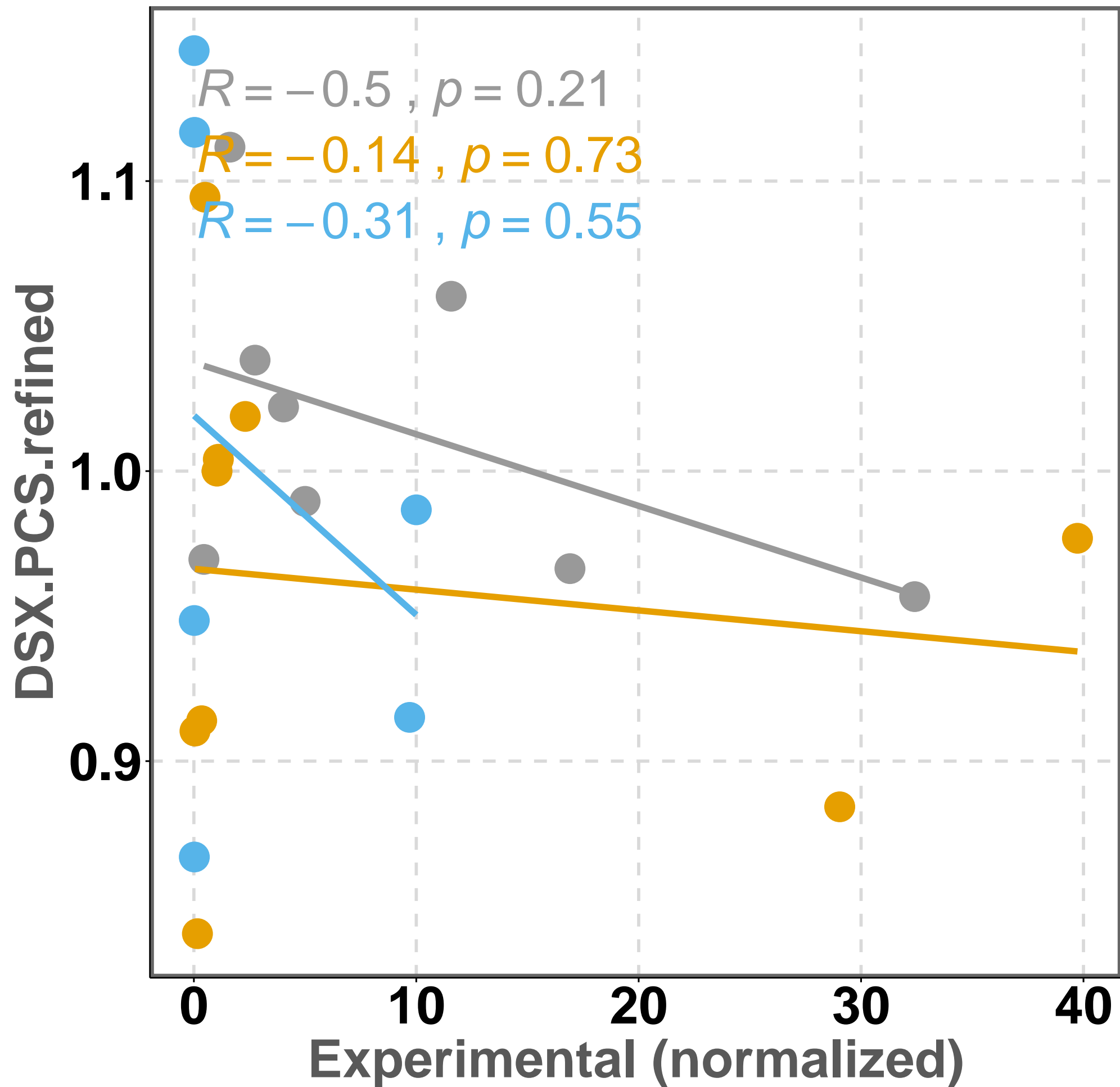
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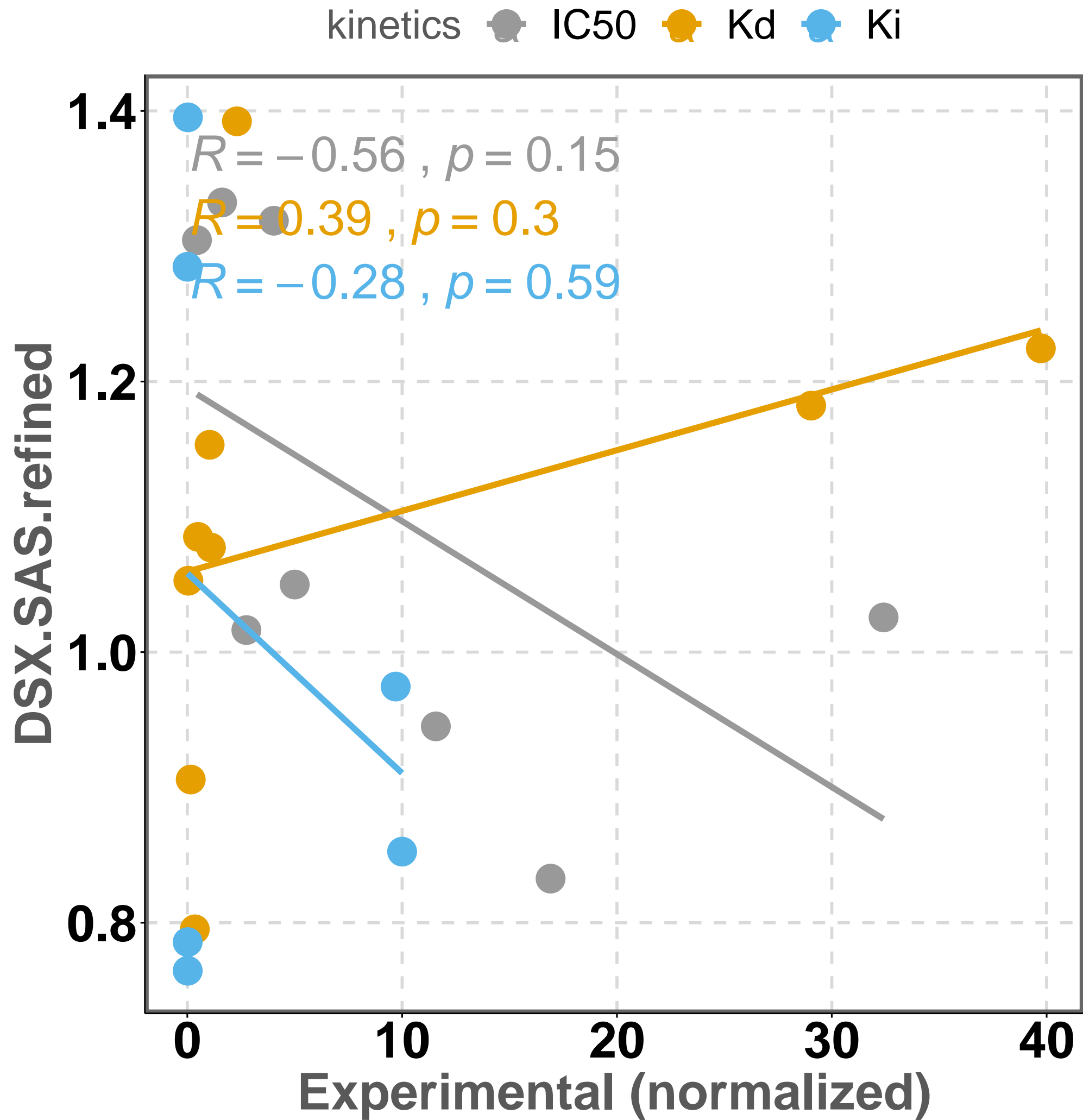


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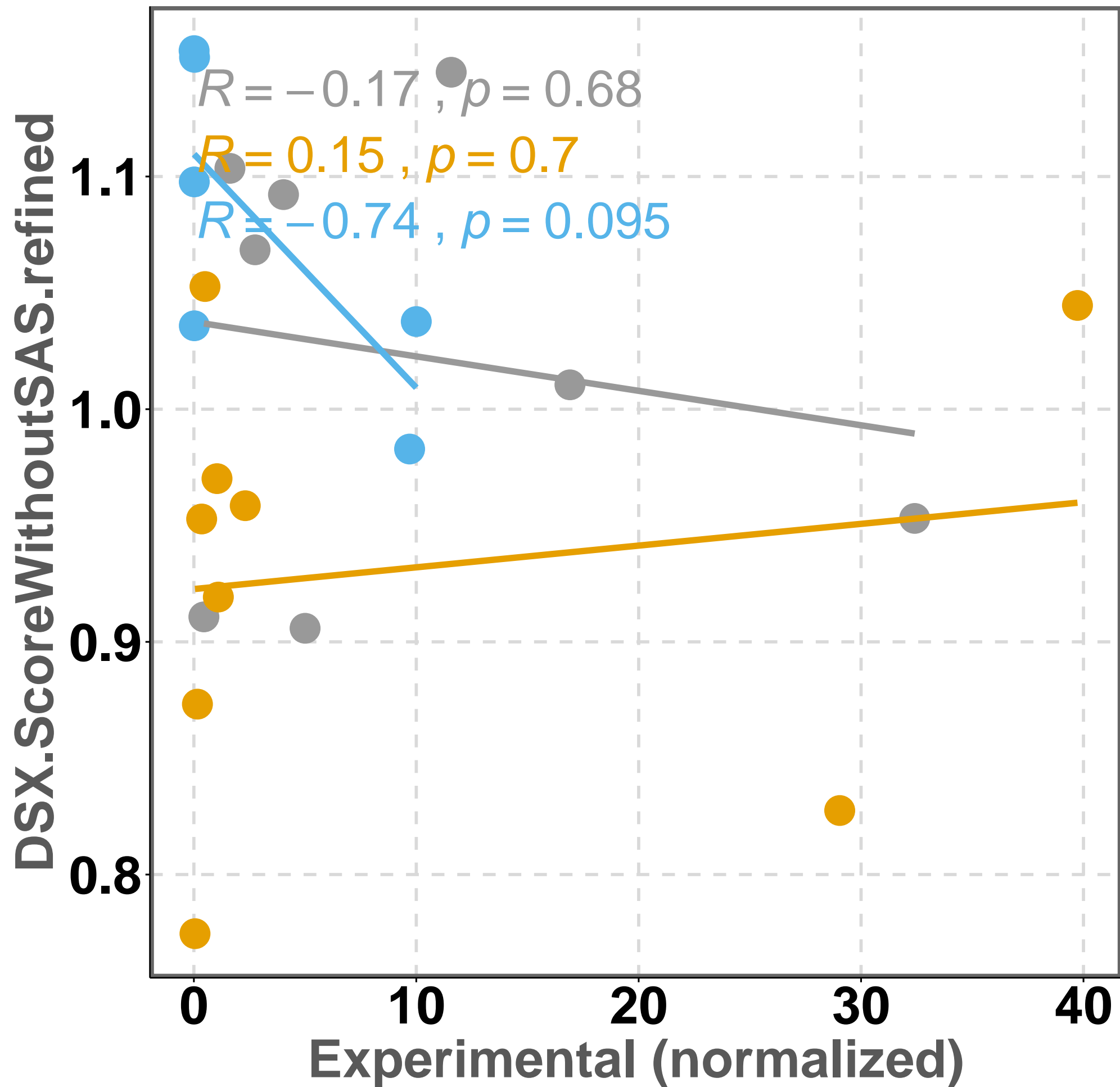


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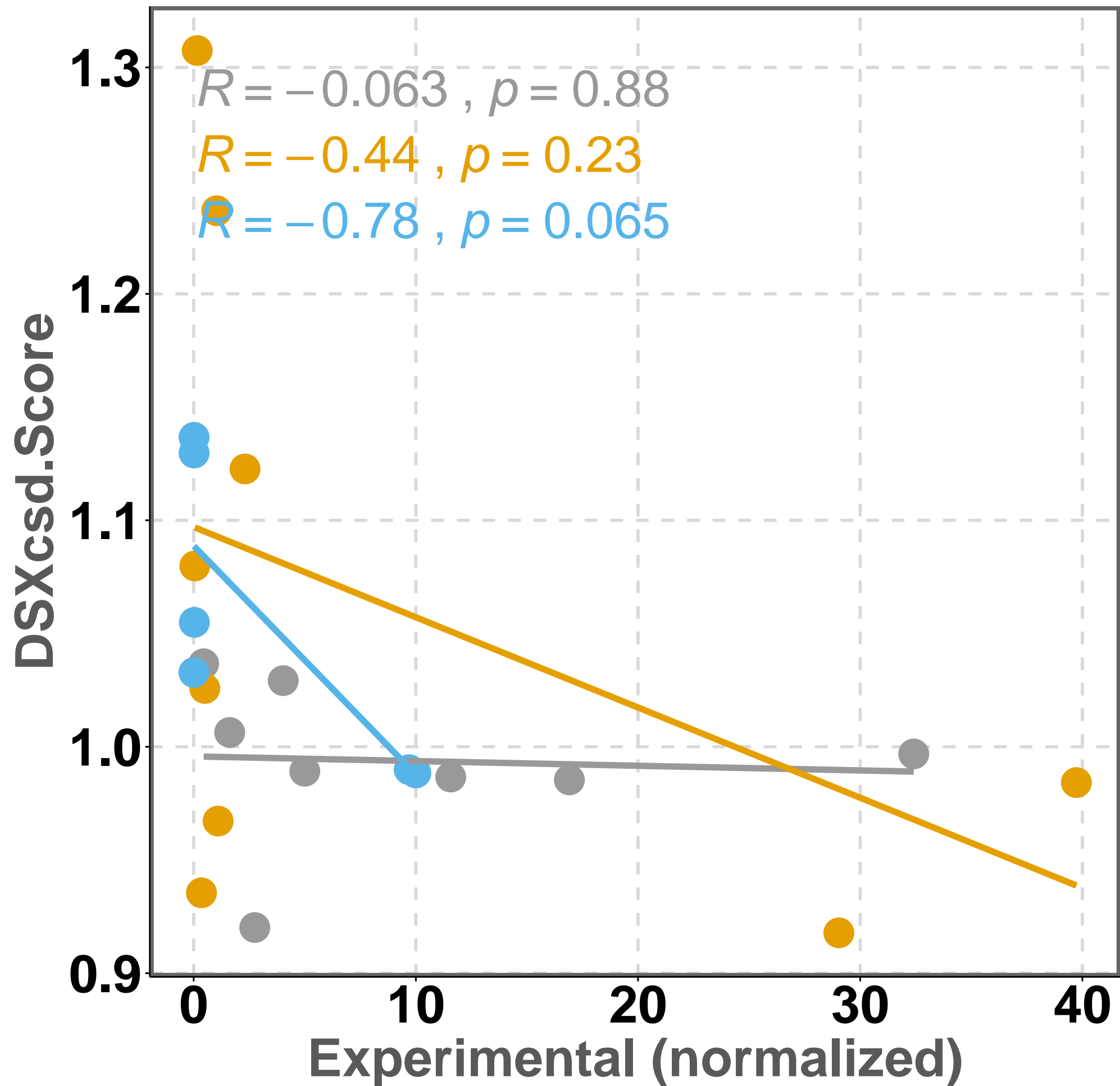


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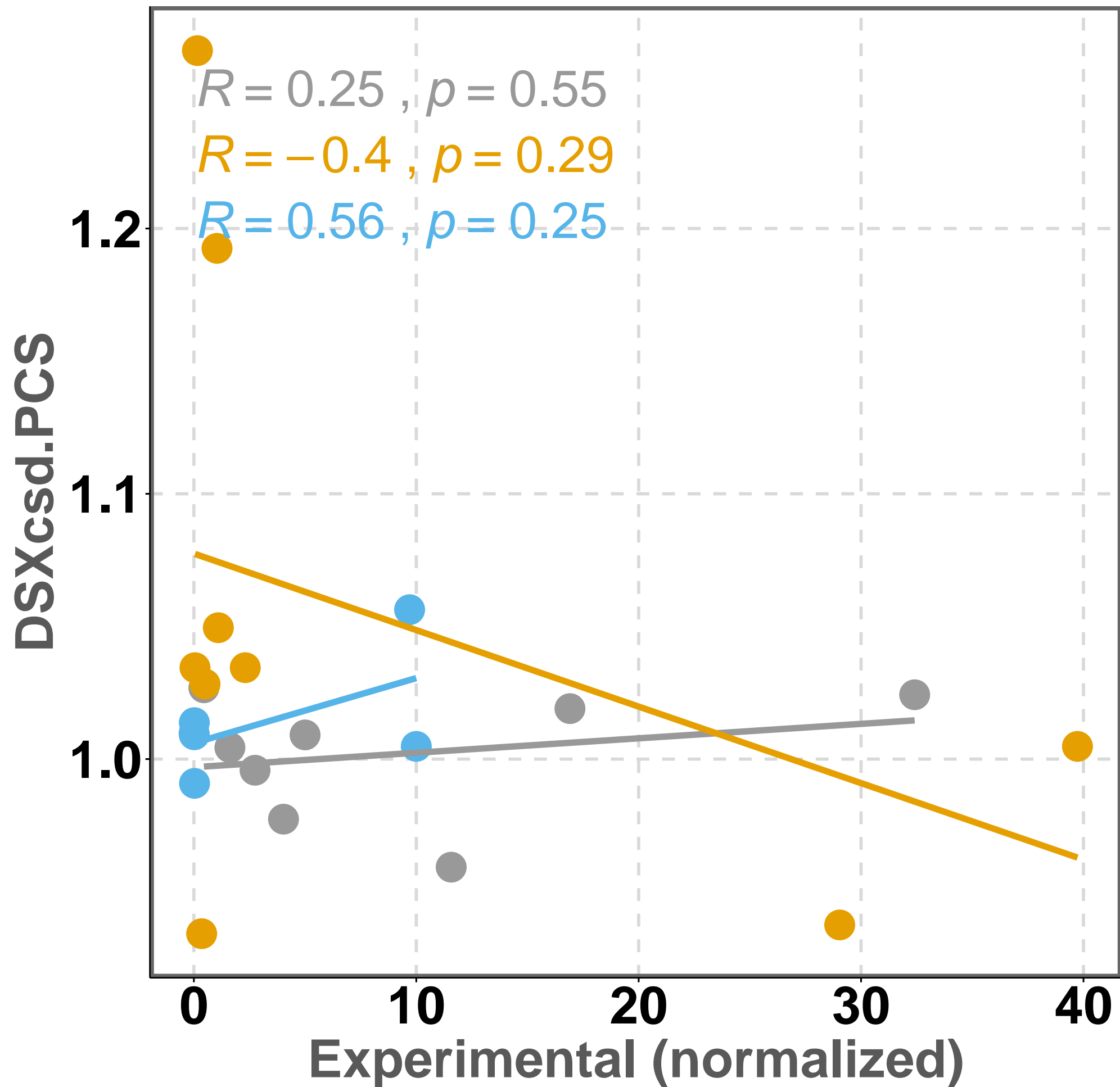


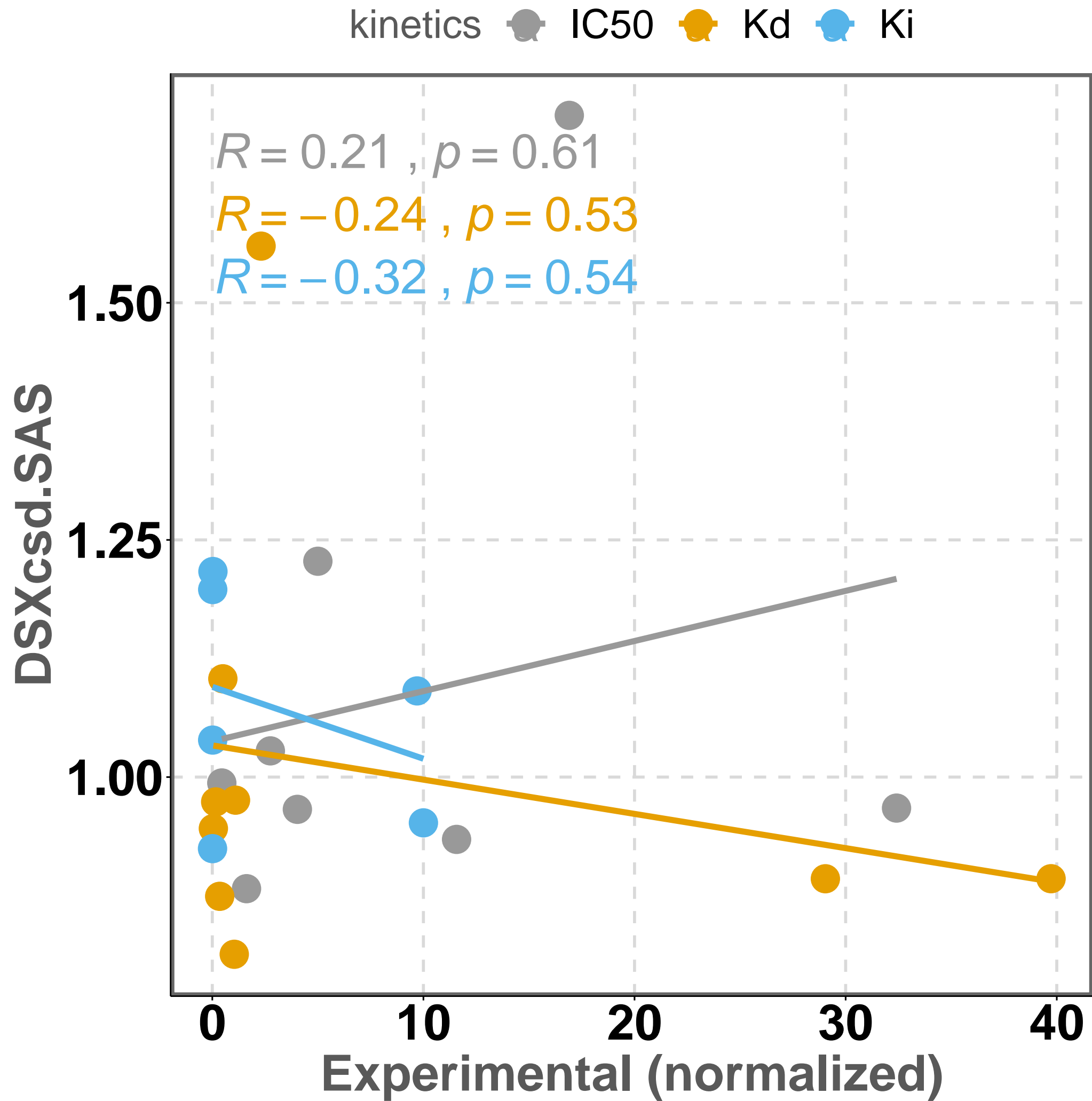


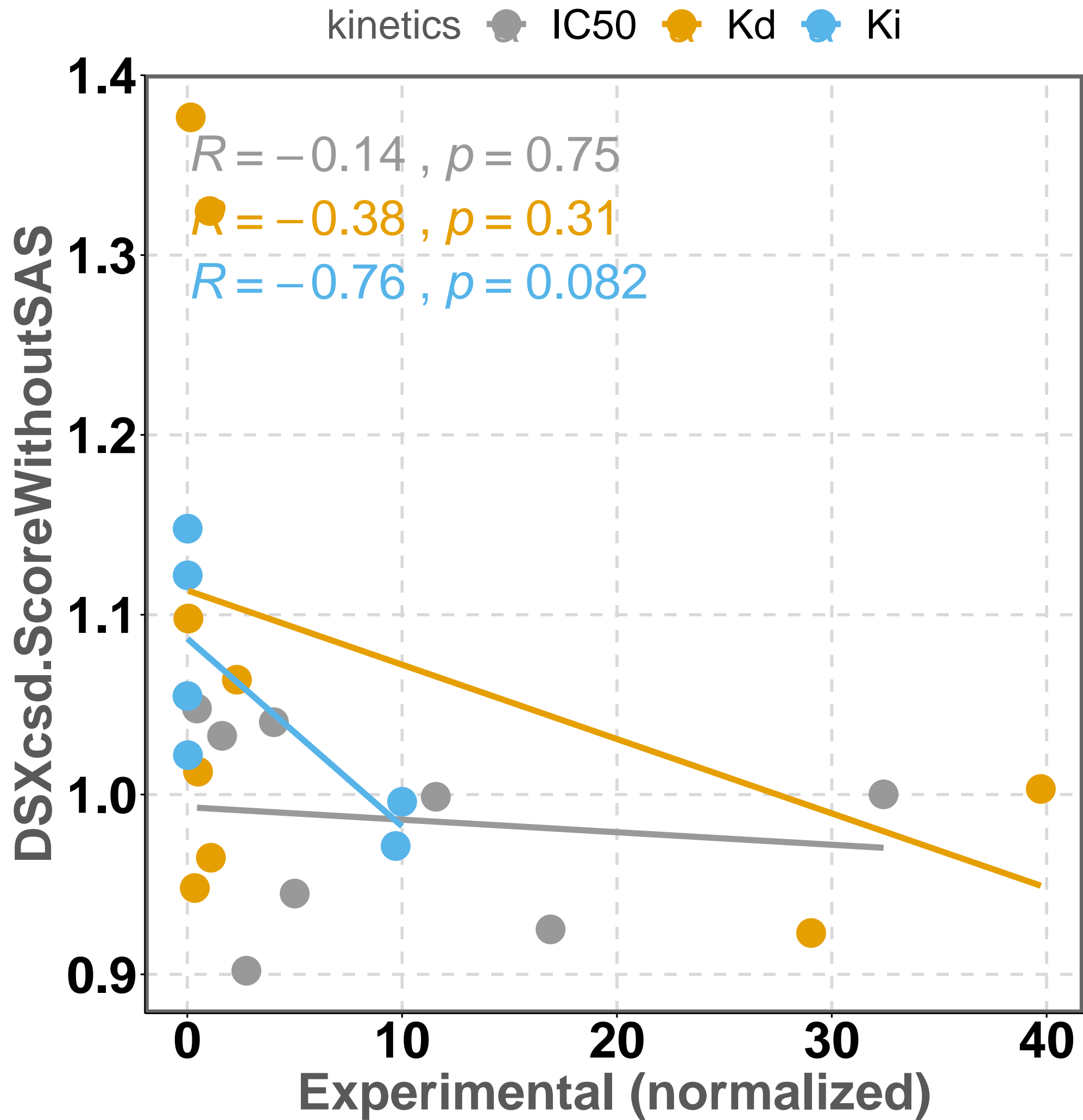
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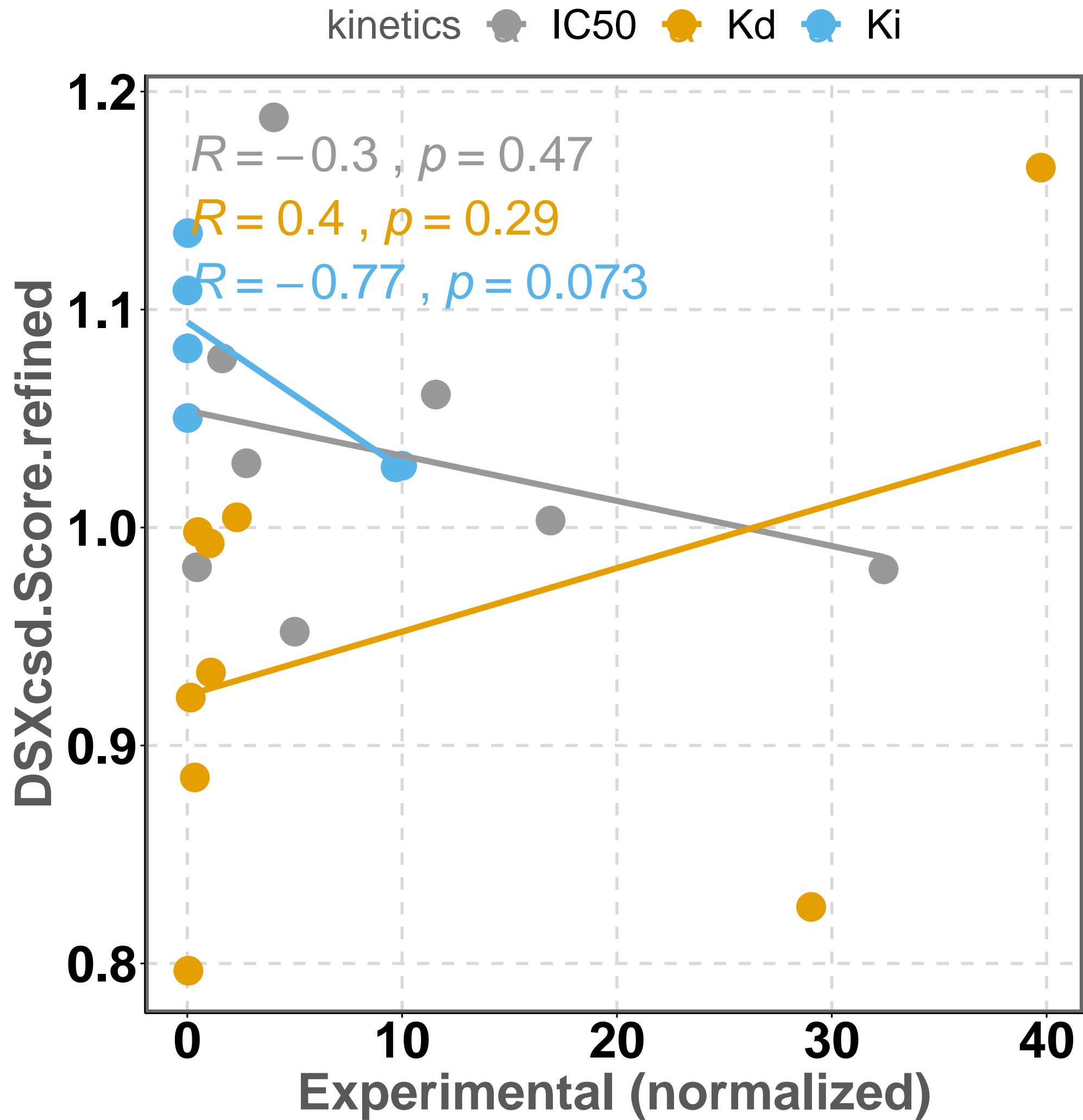


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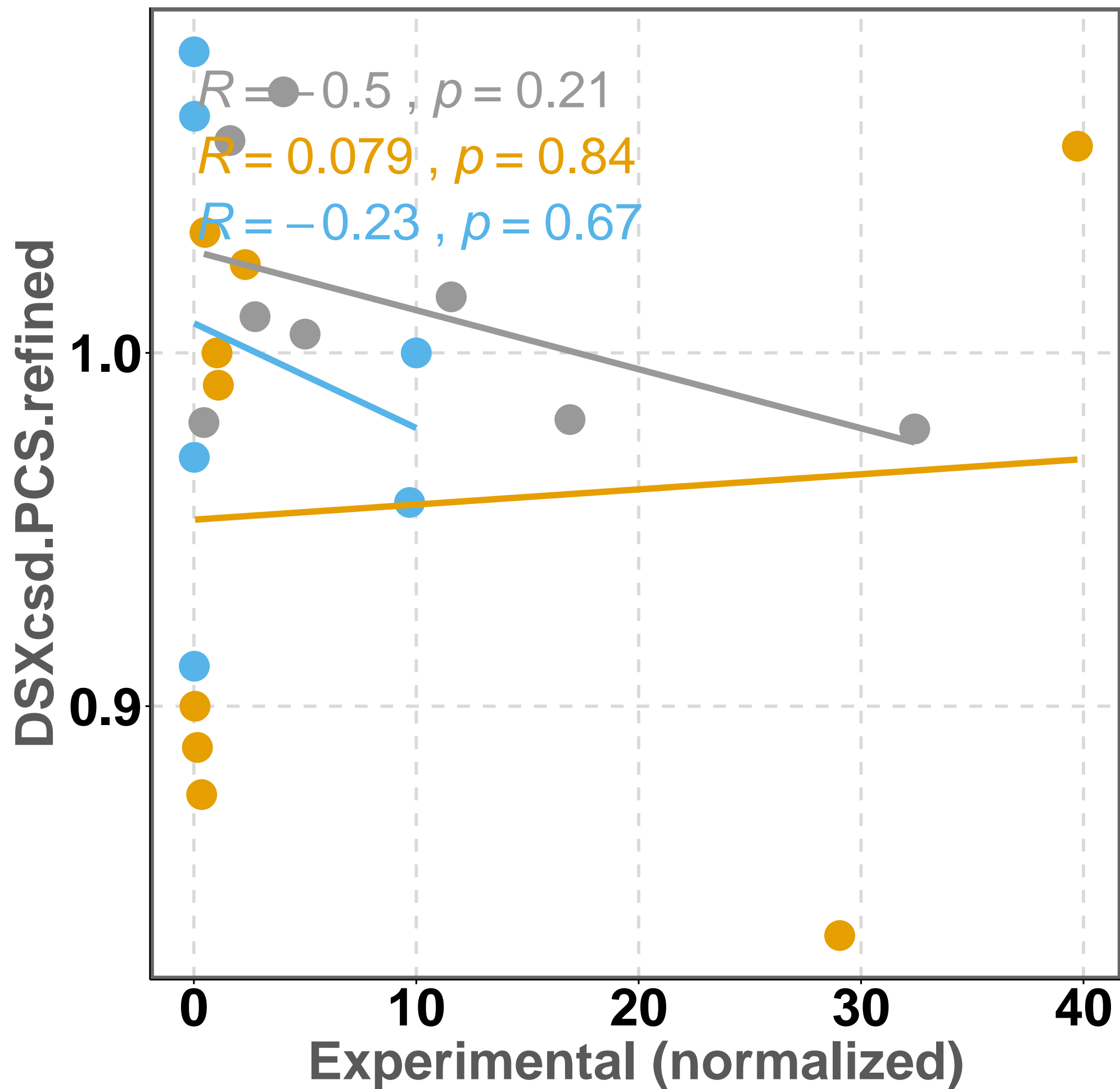


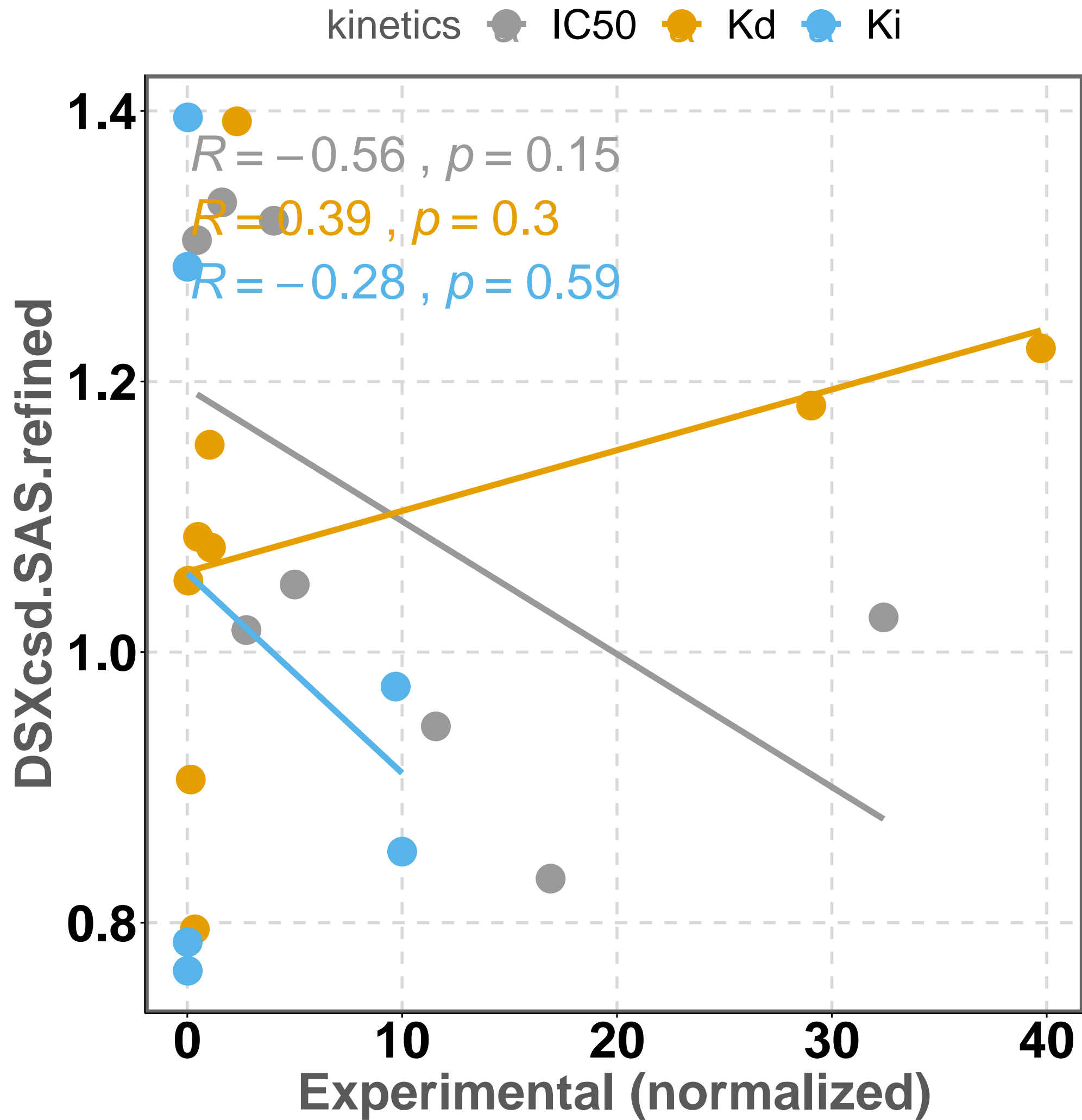




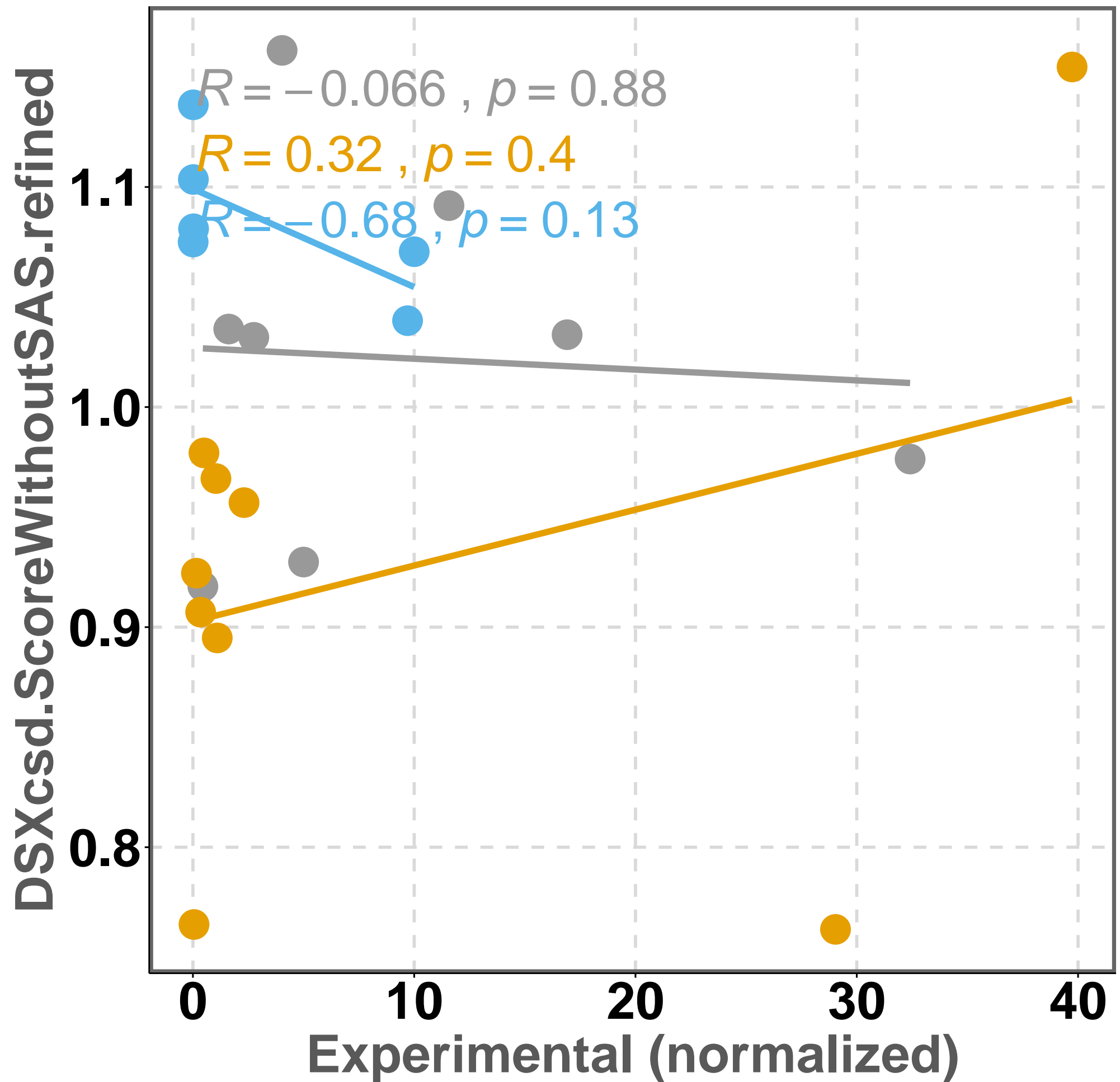


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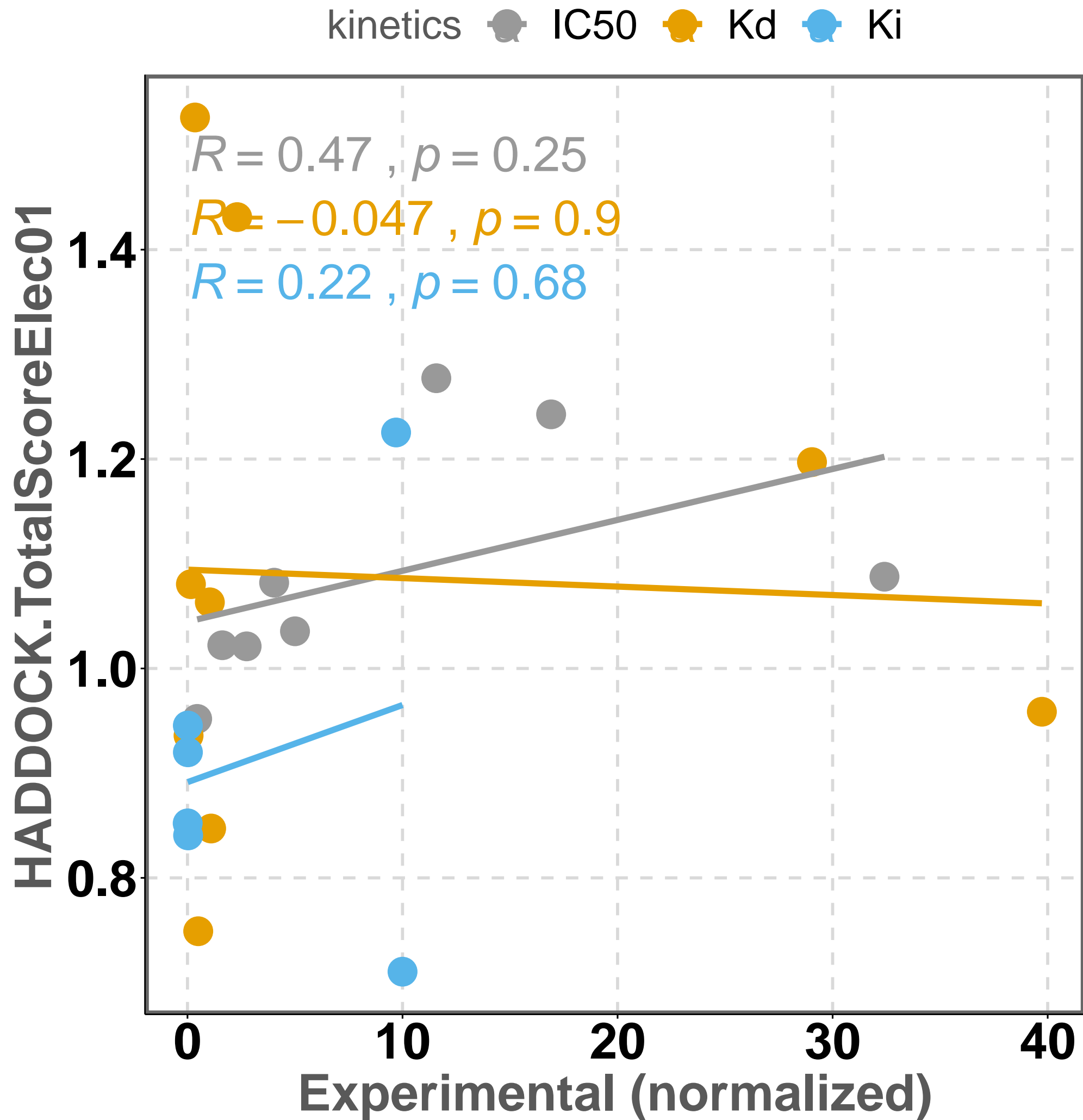


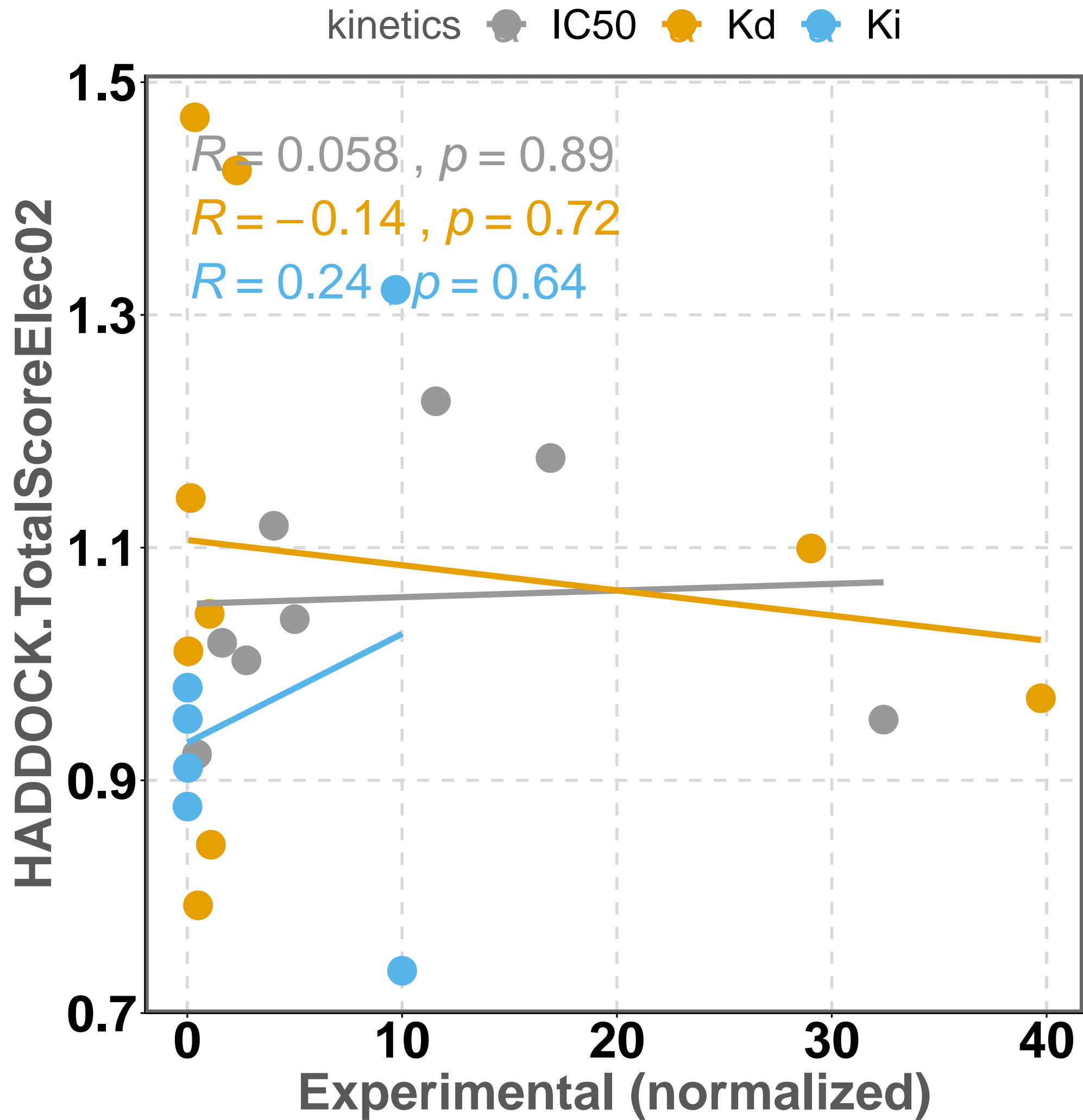


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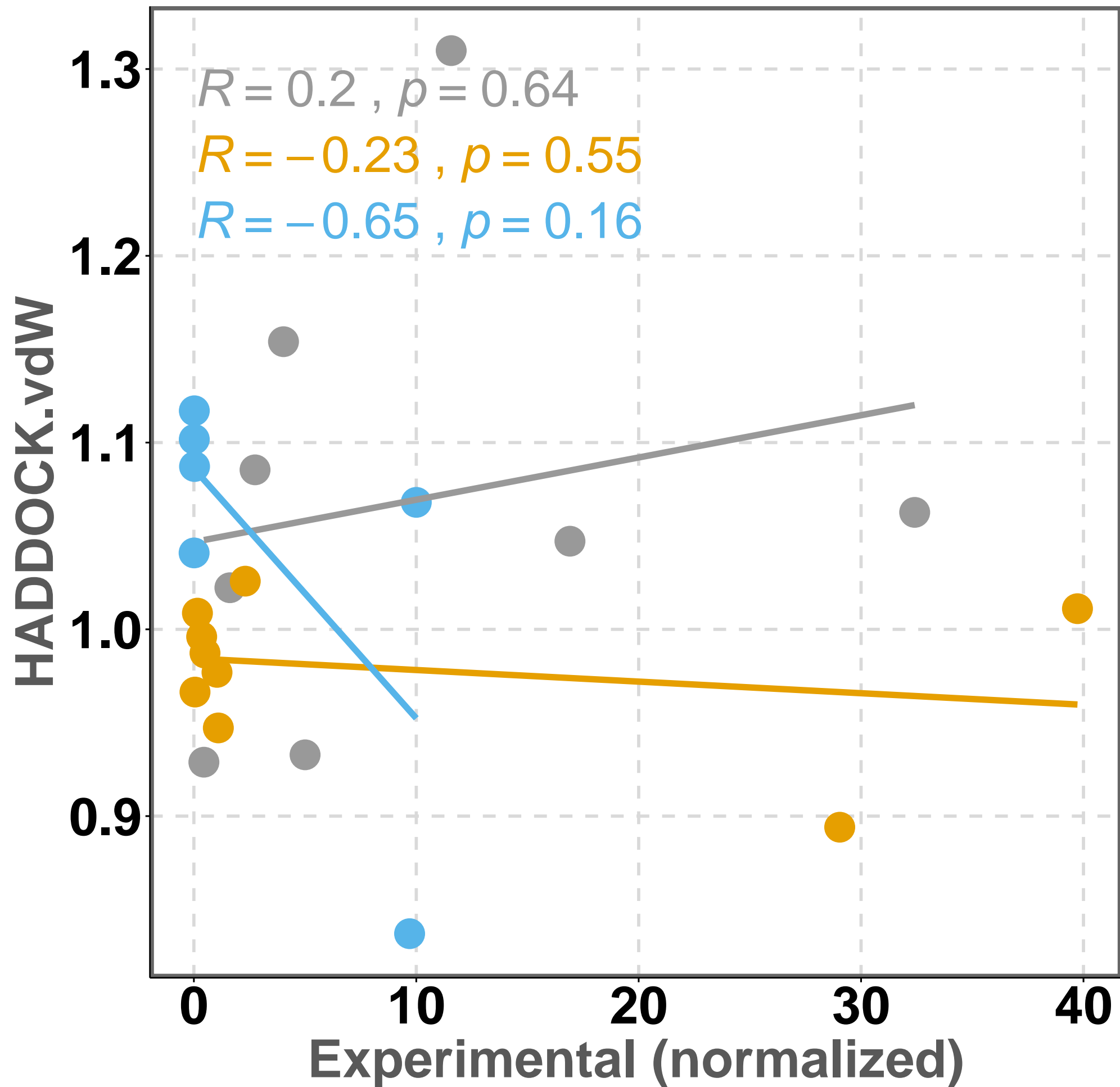




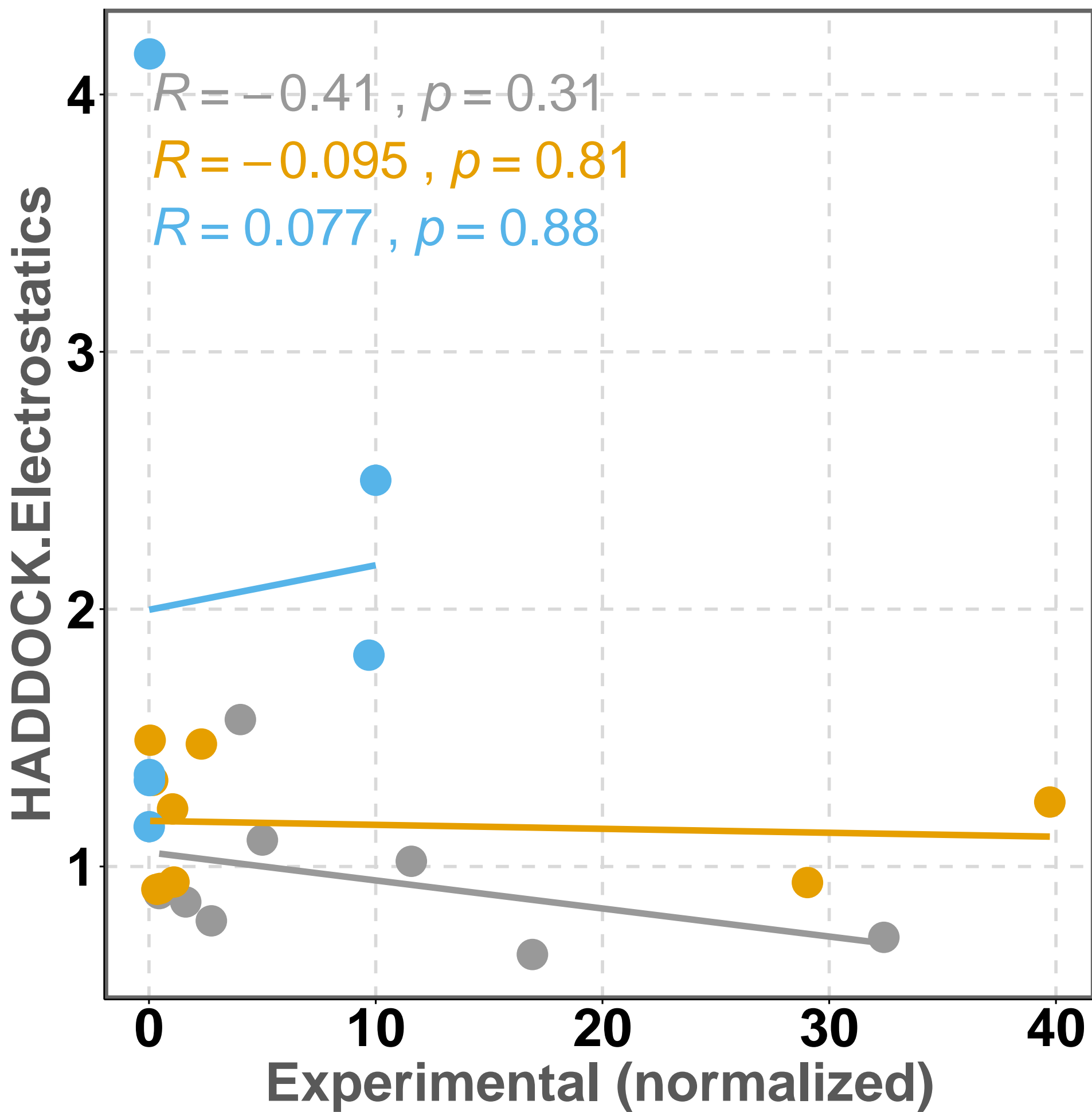


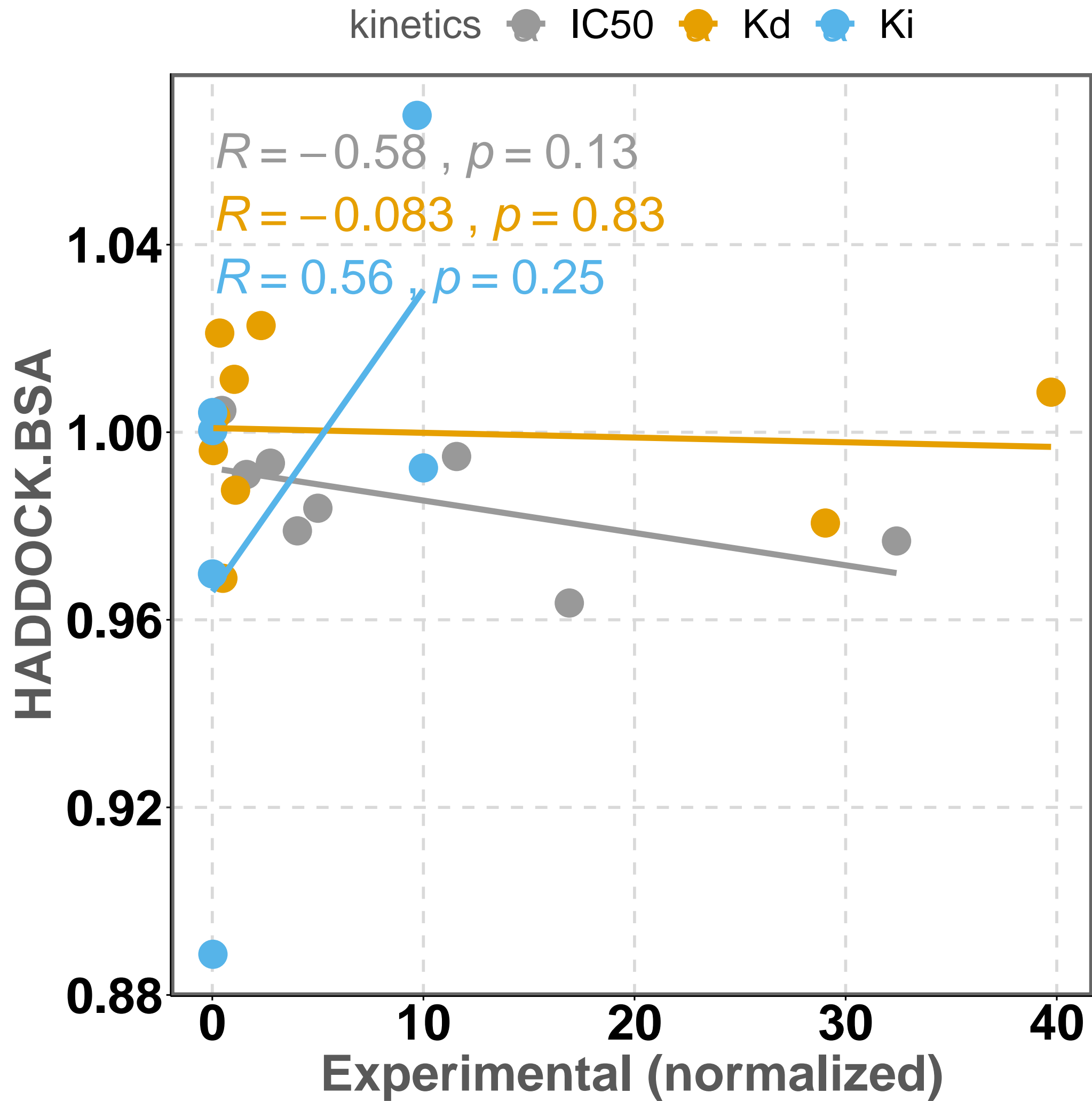


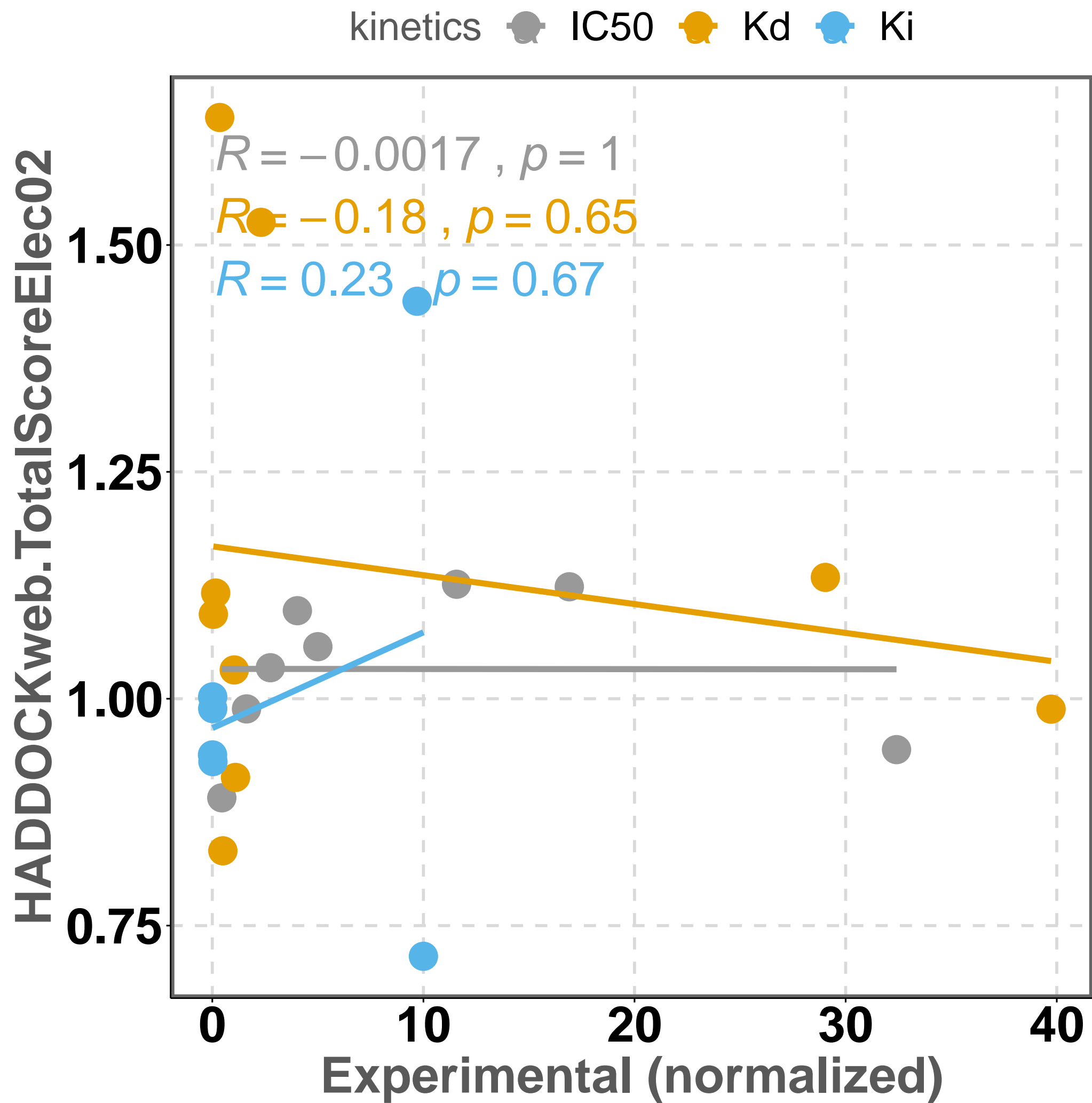
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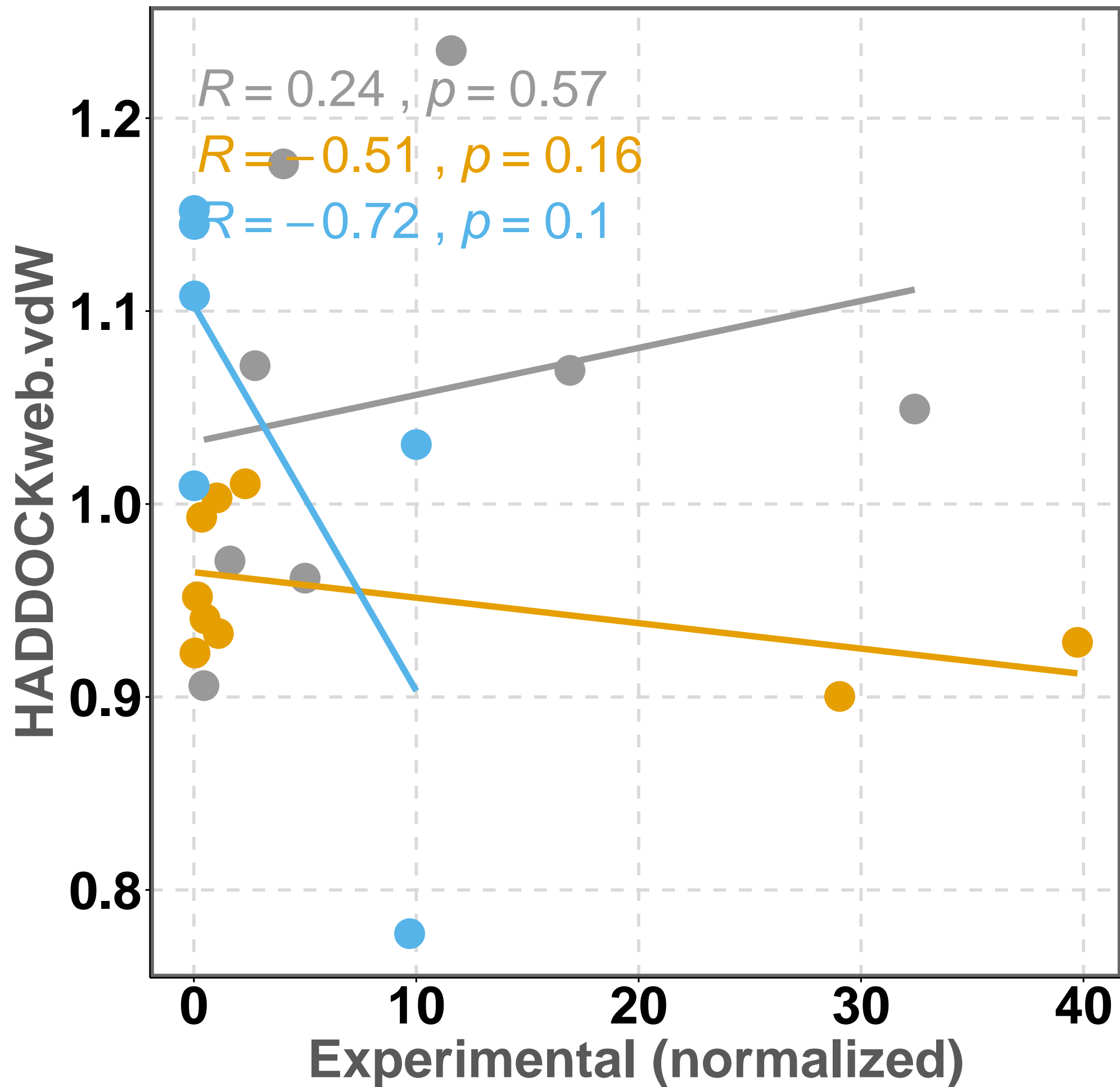
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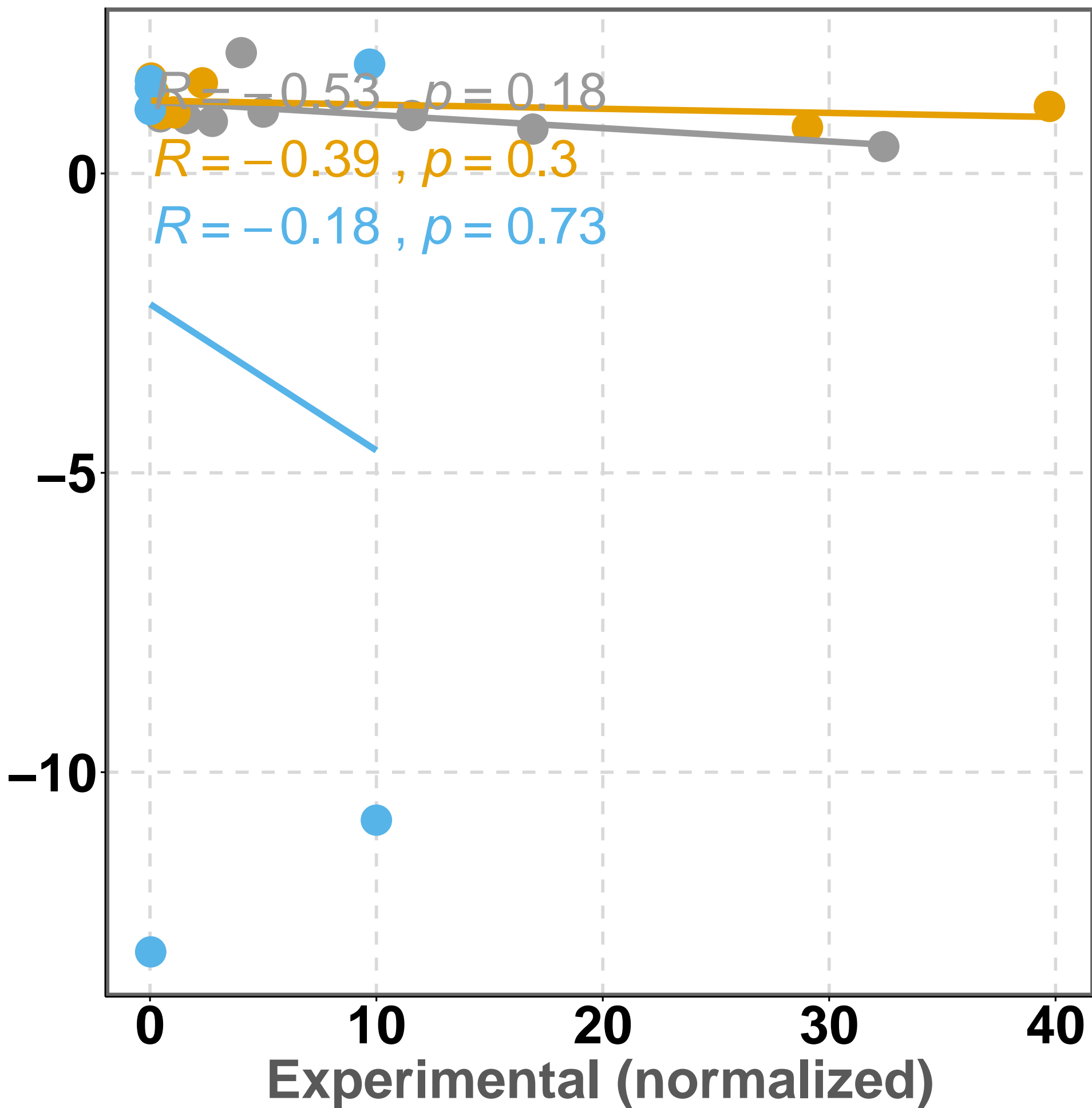


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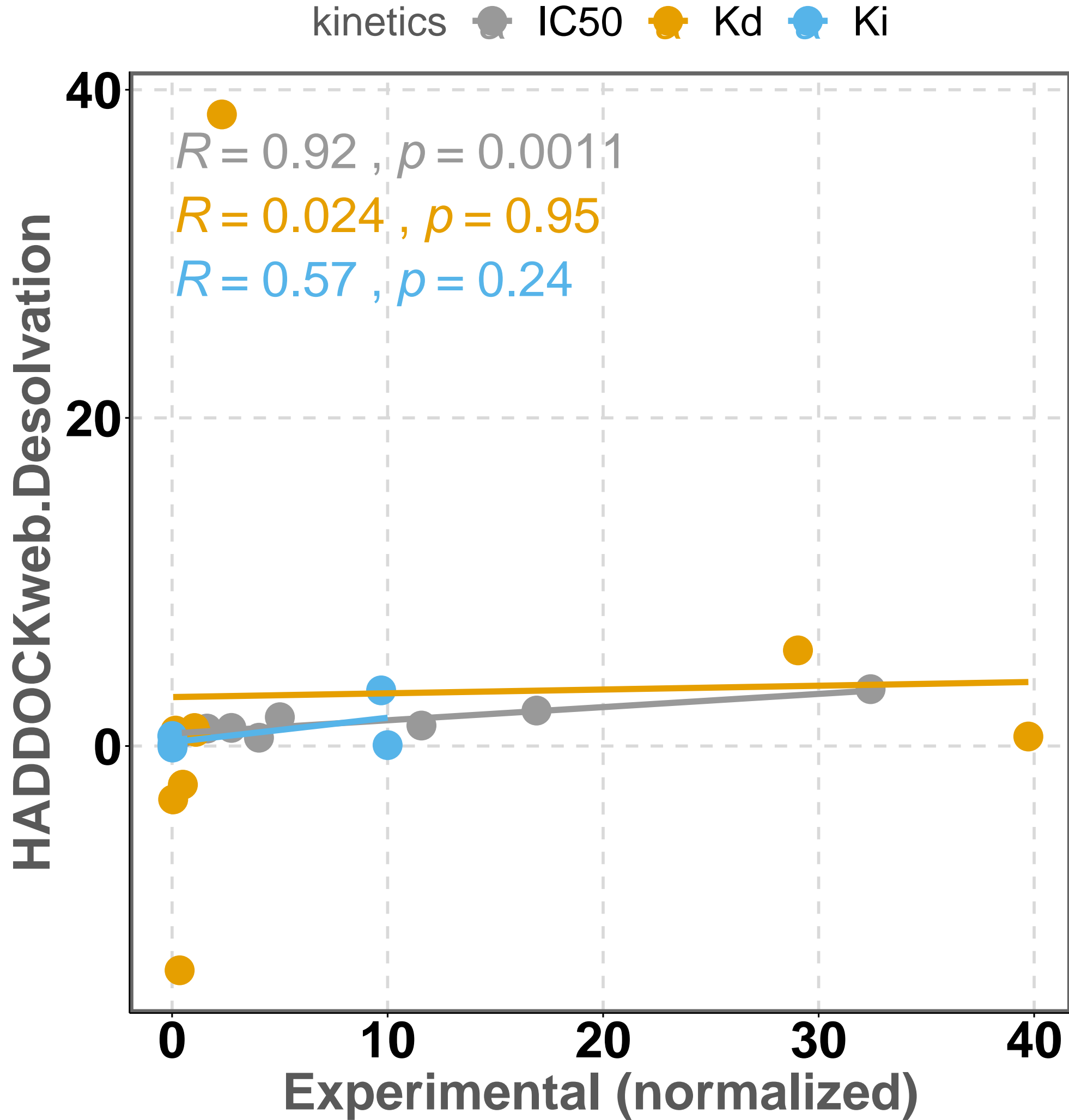


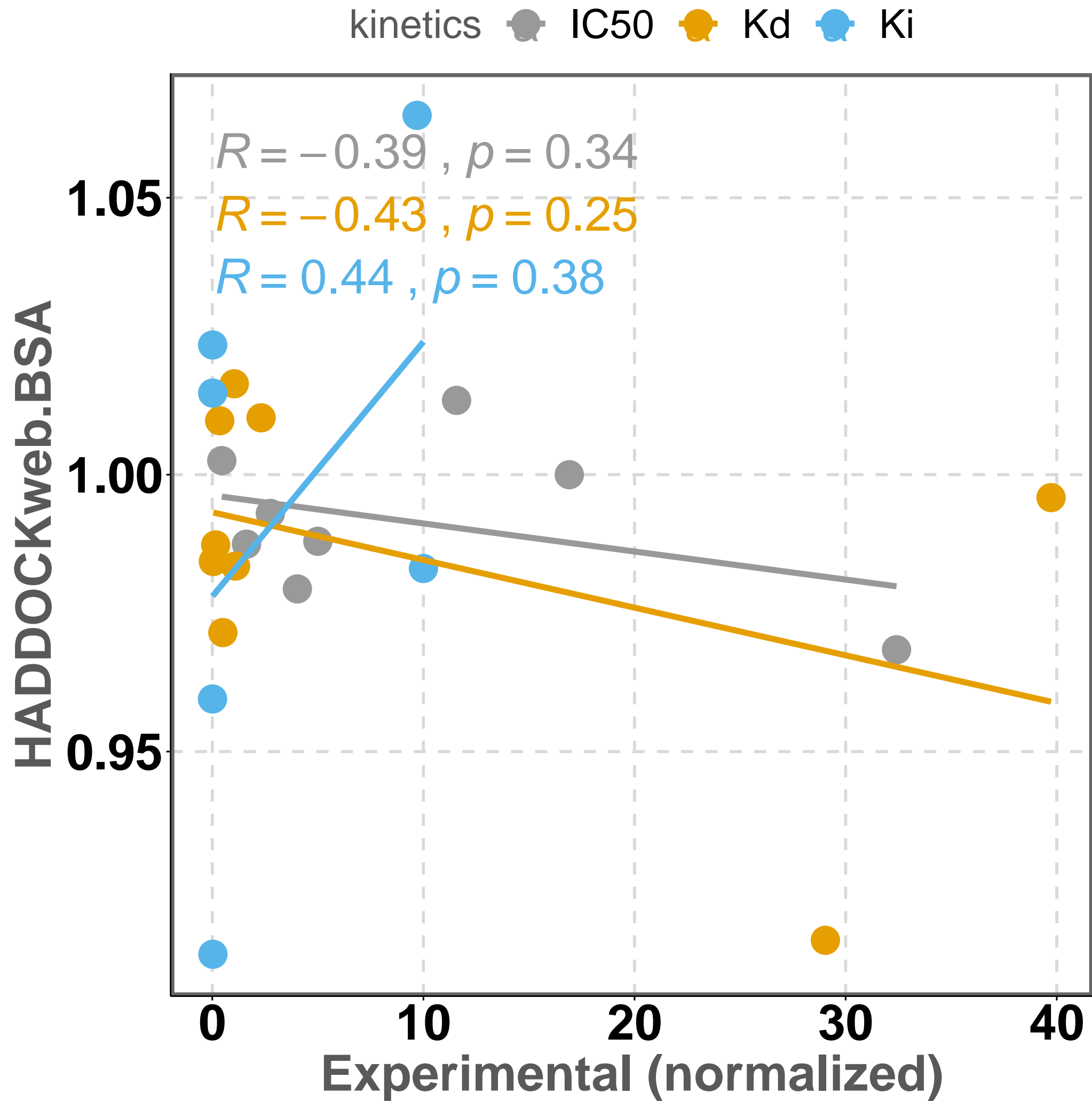
HADDOCKweb.Electrostatics

kinetics IC50 Kd Ki

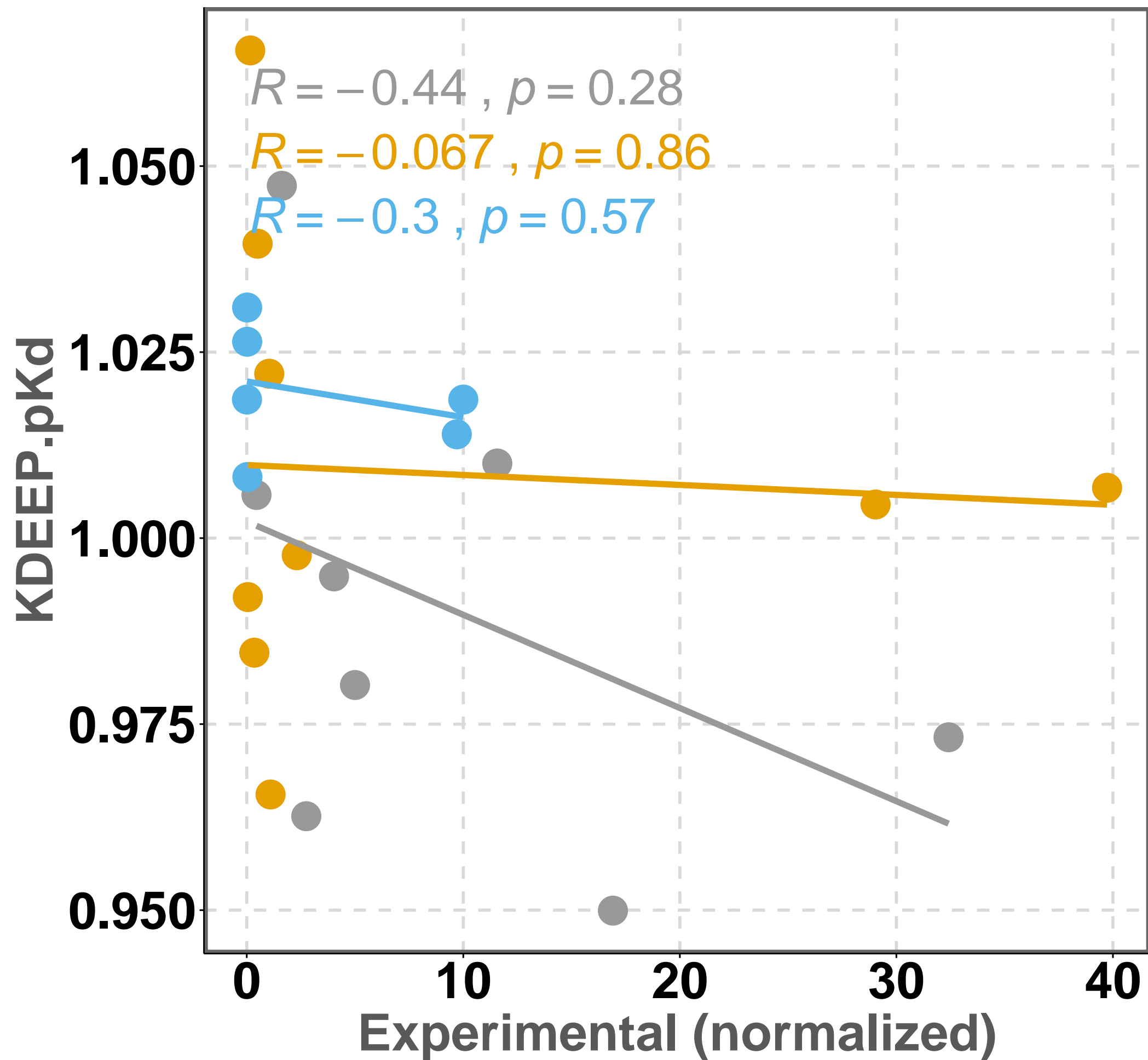




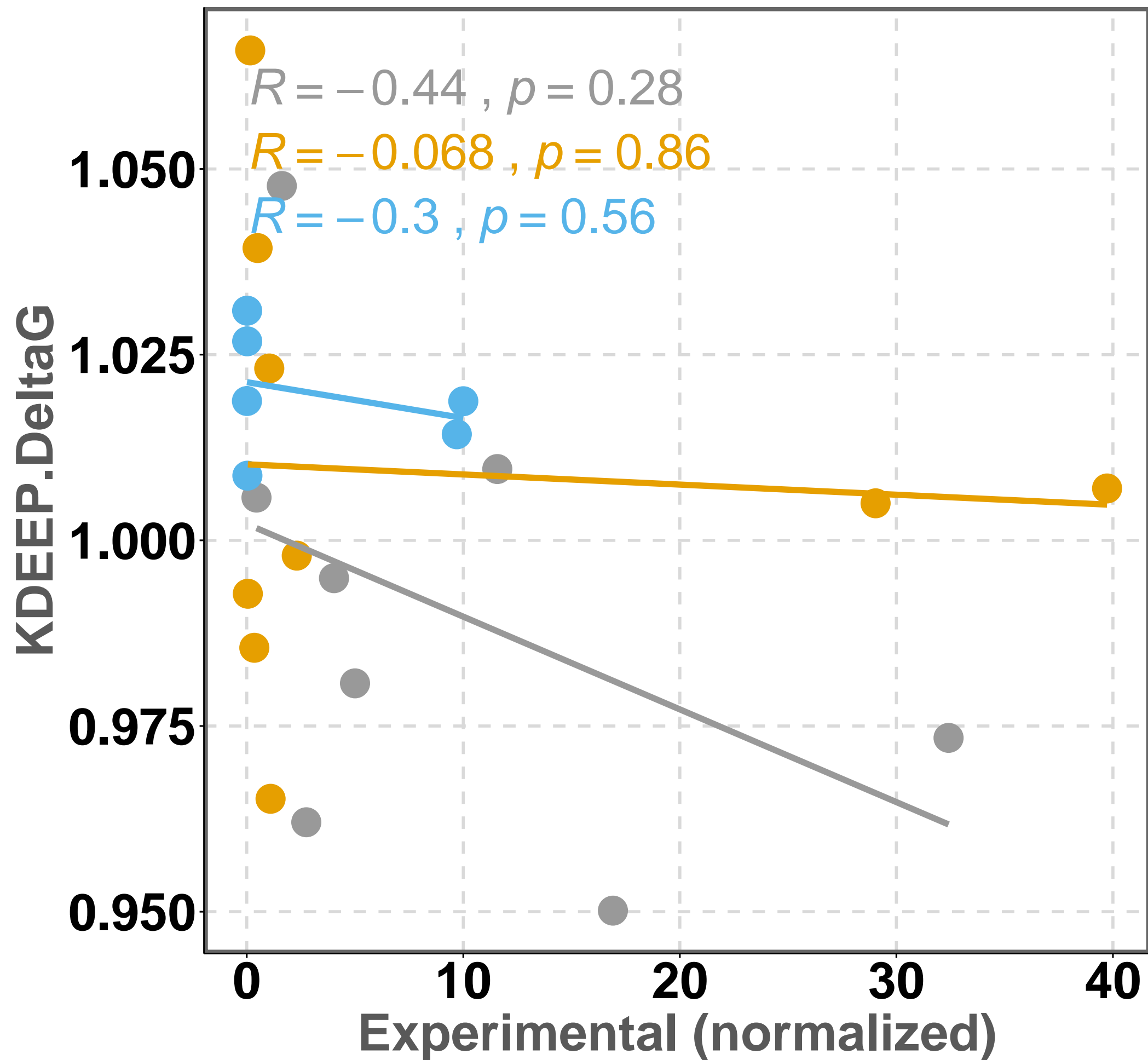


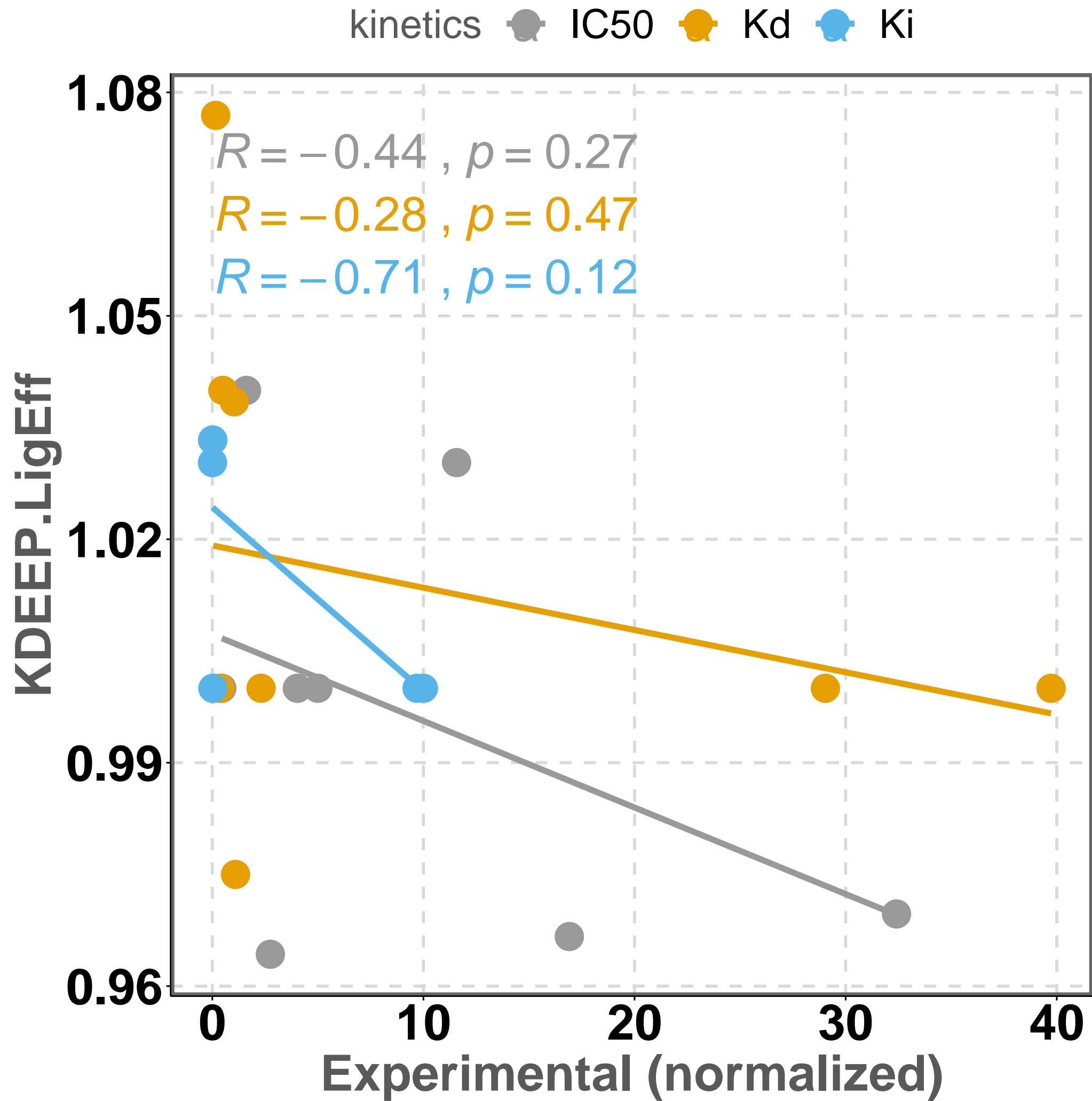


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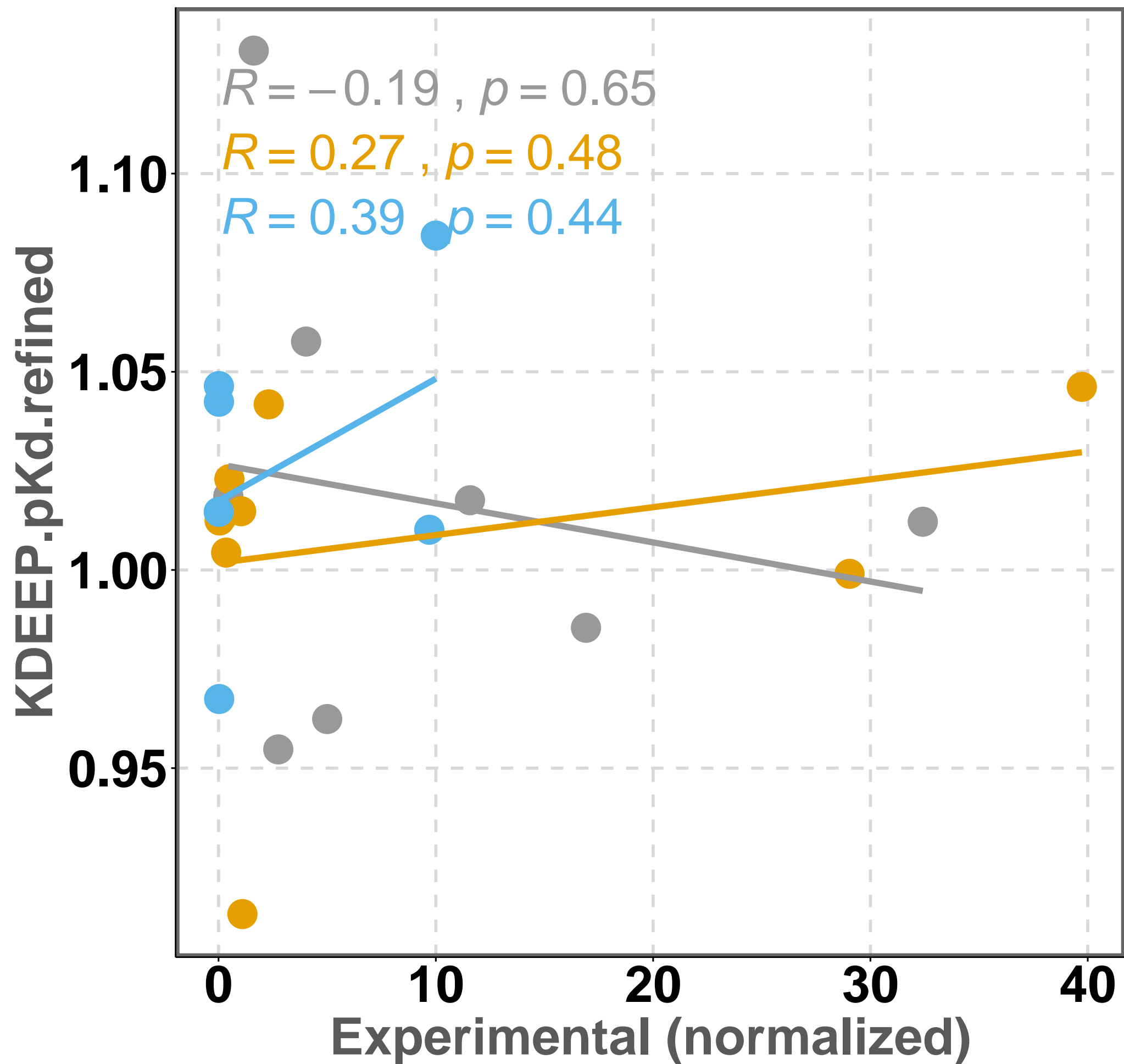


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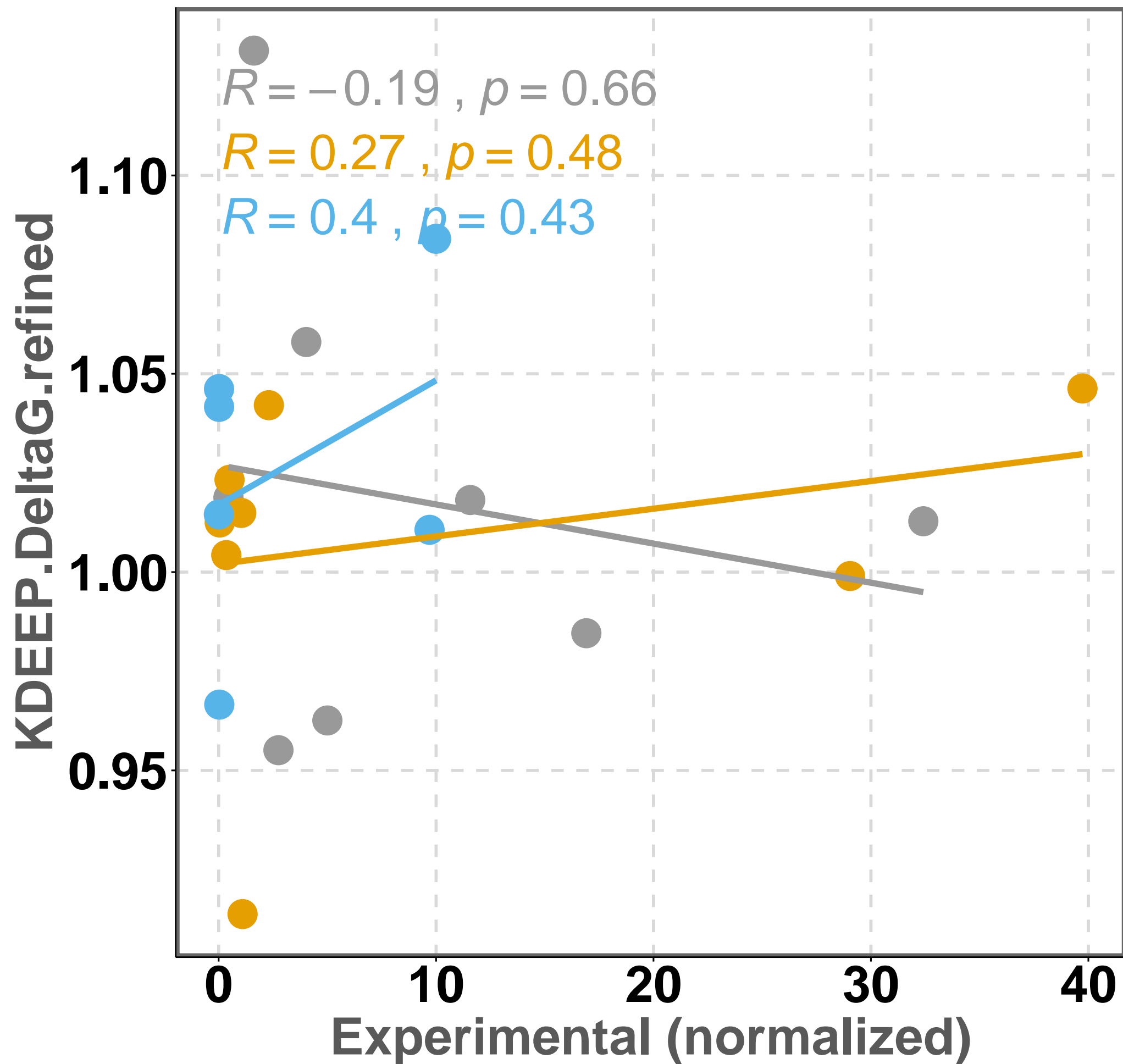


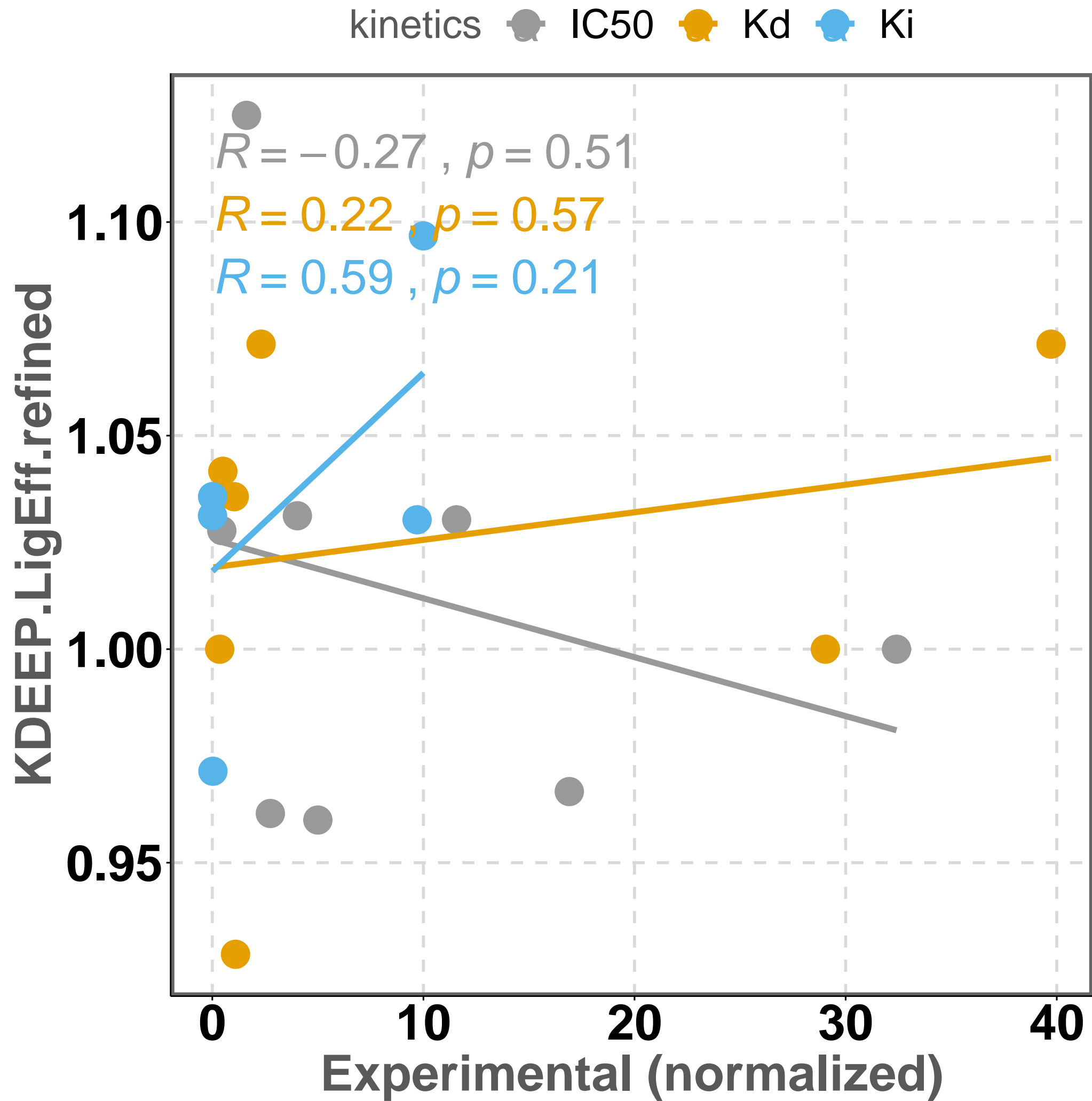


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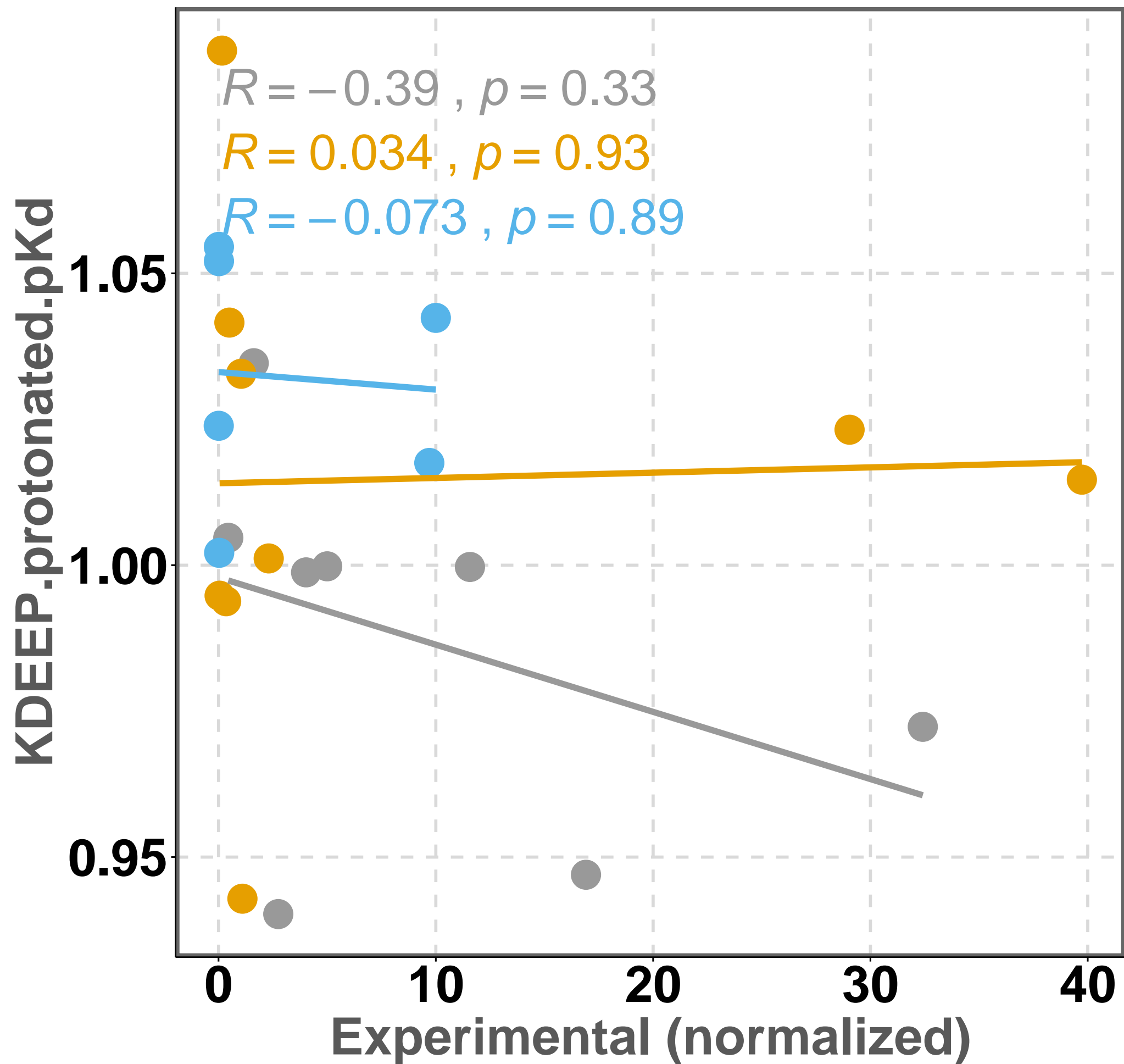
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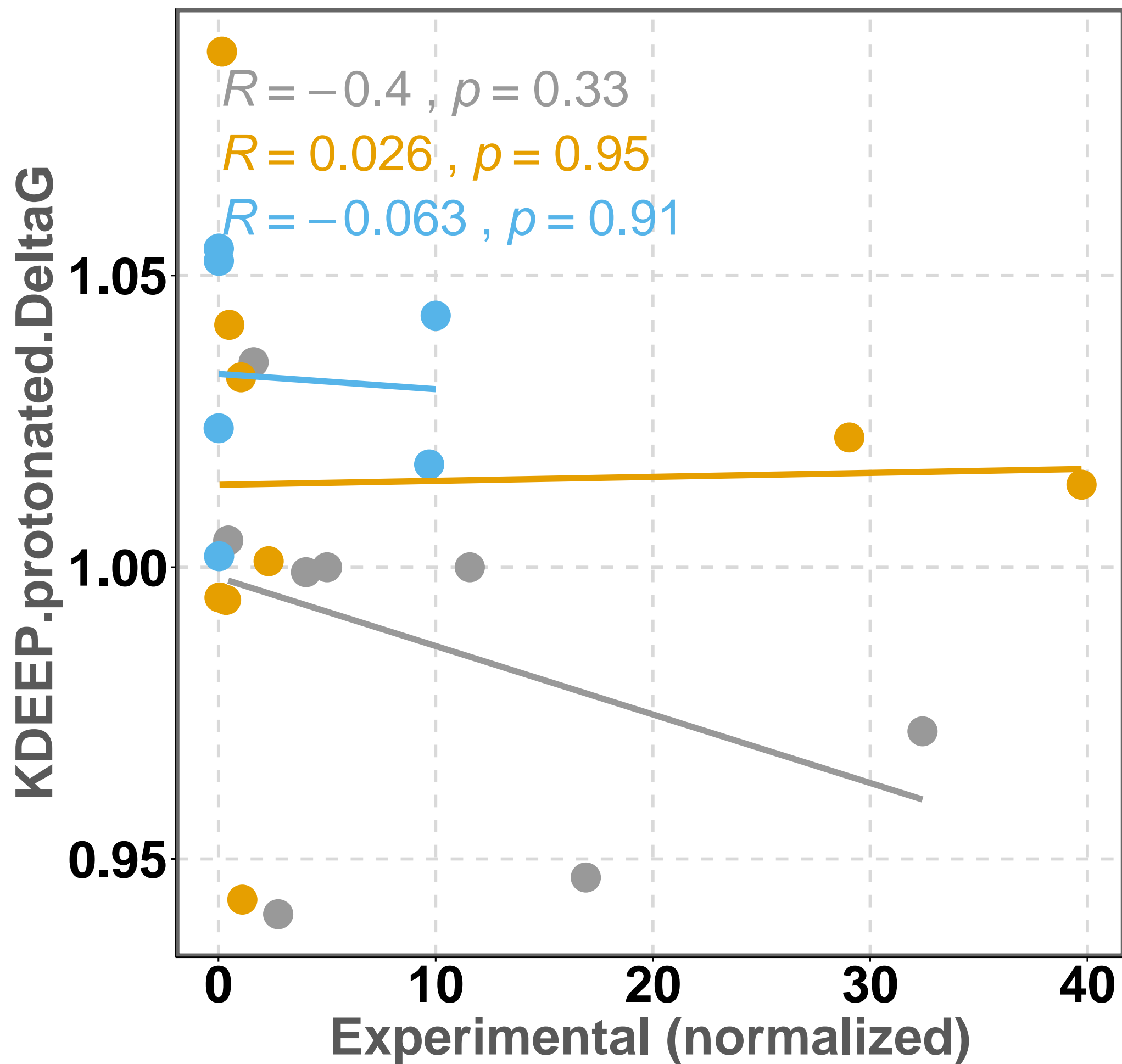


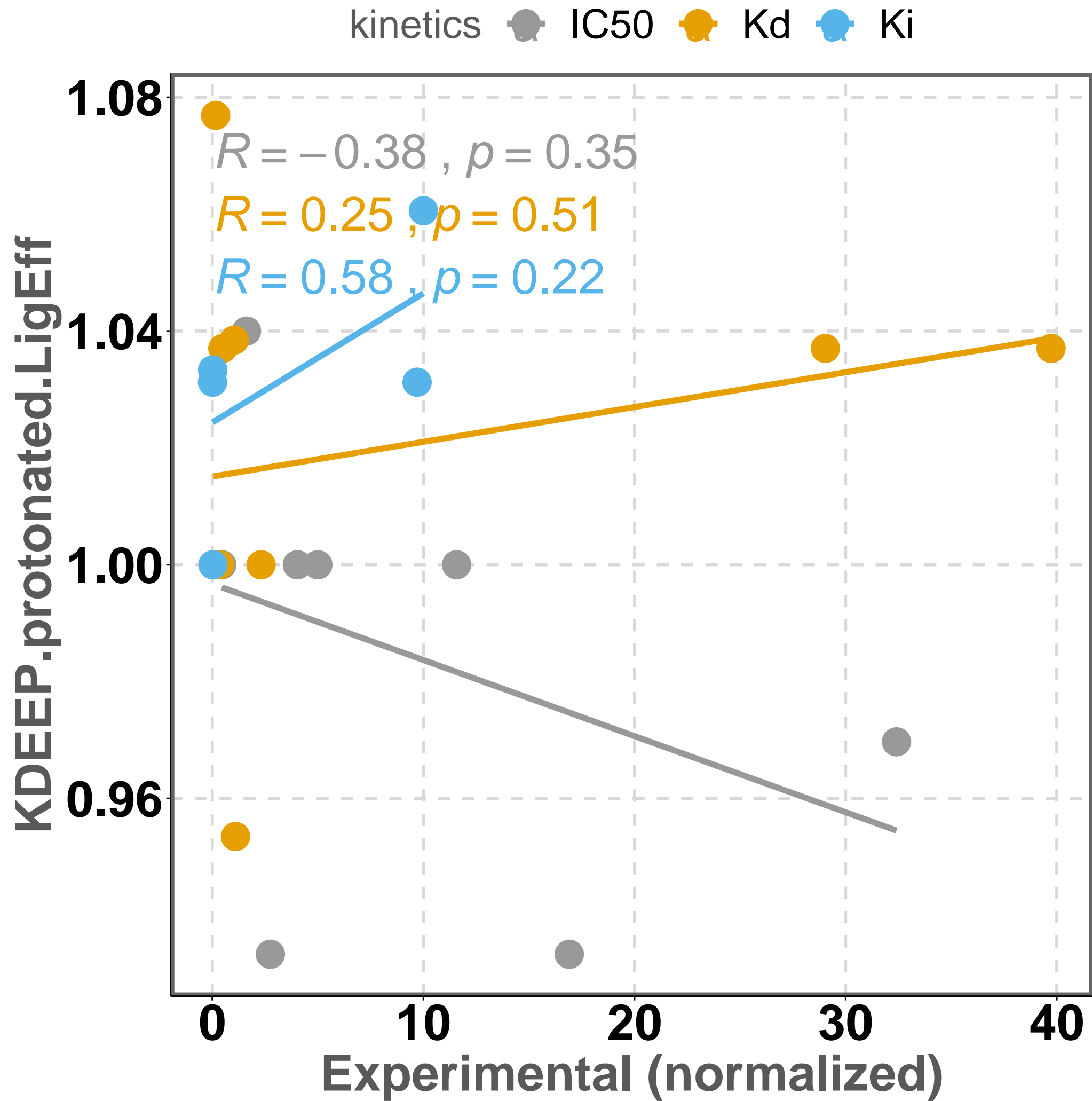


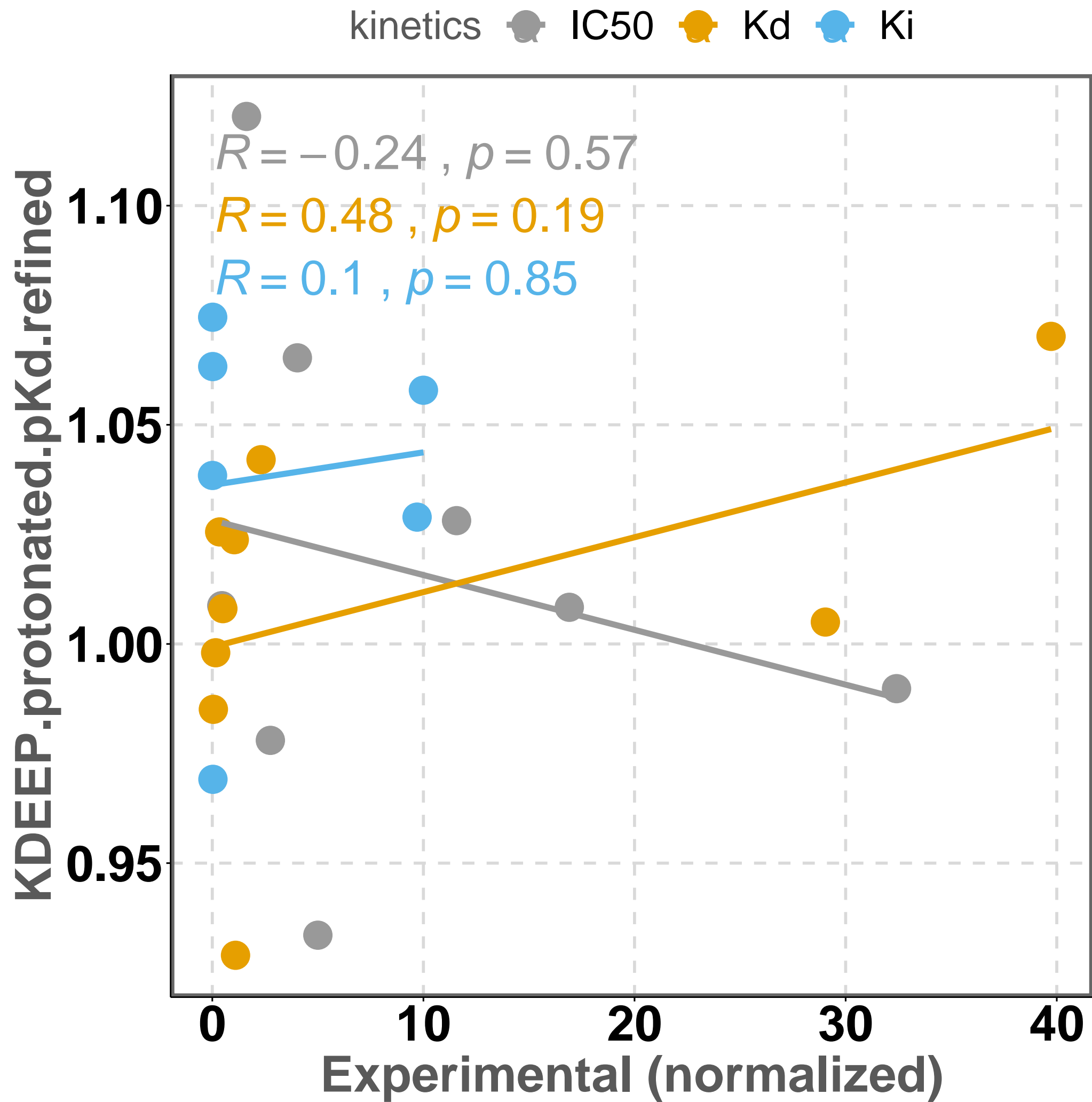
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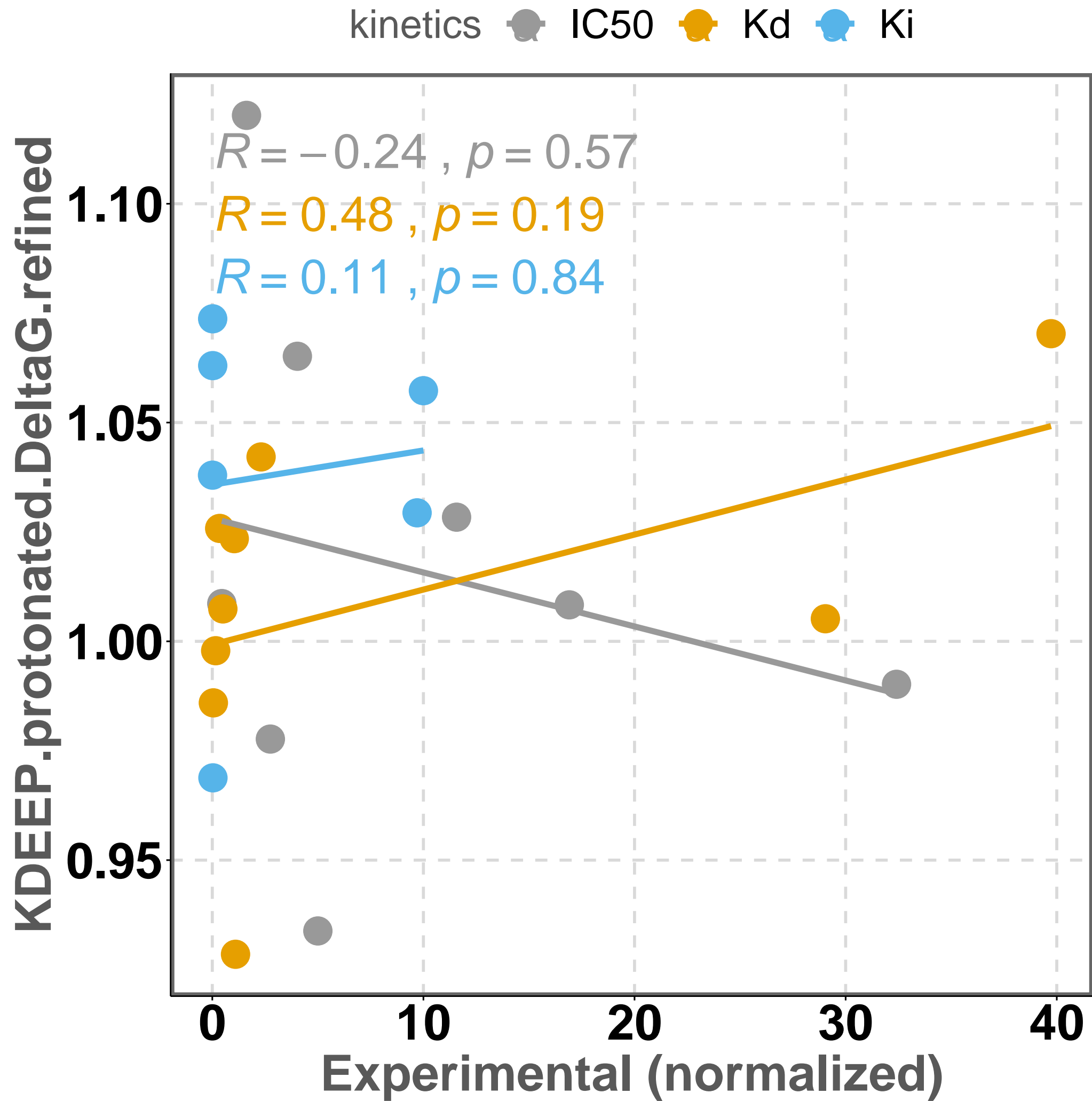


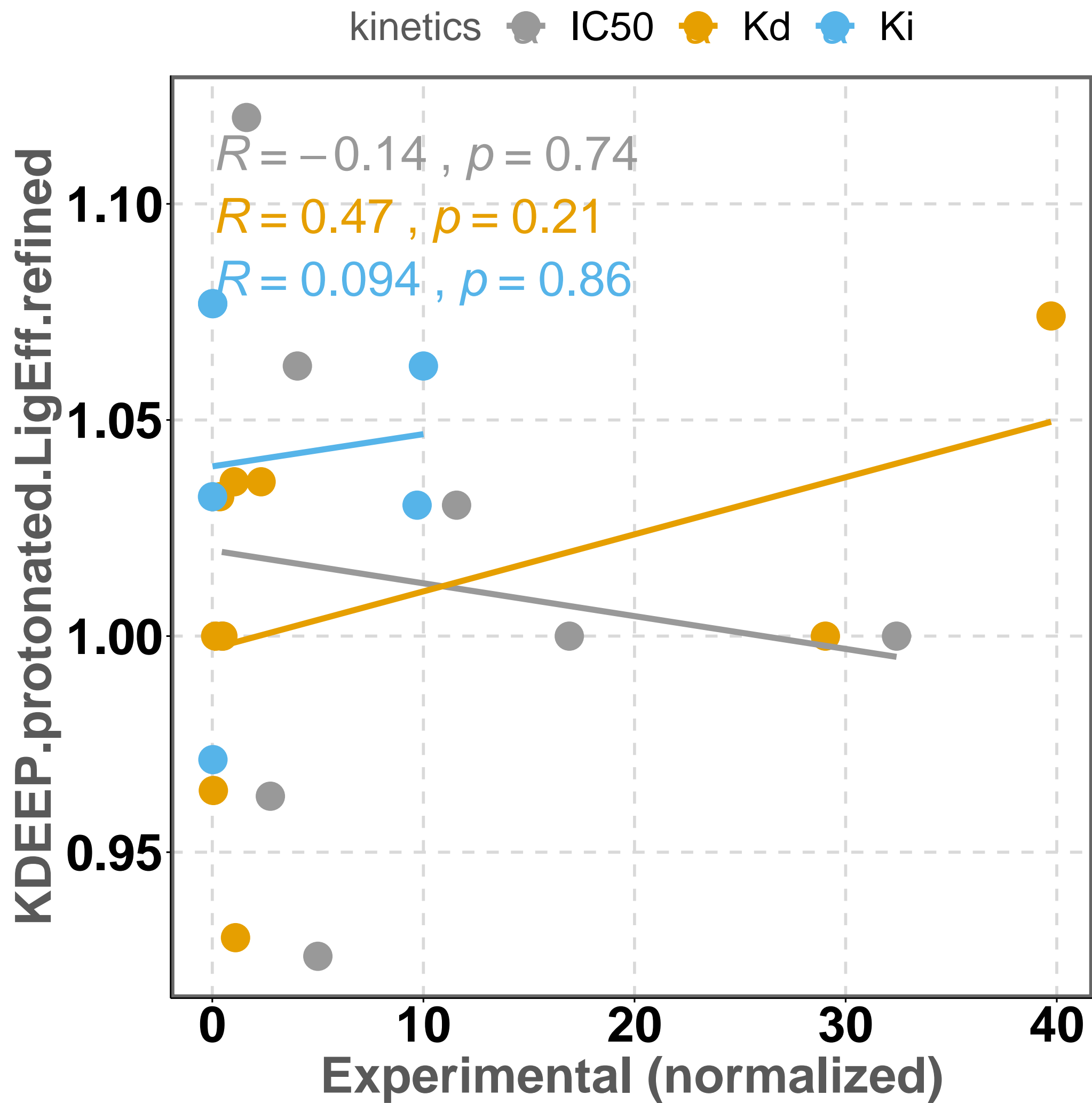
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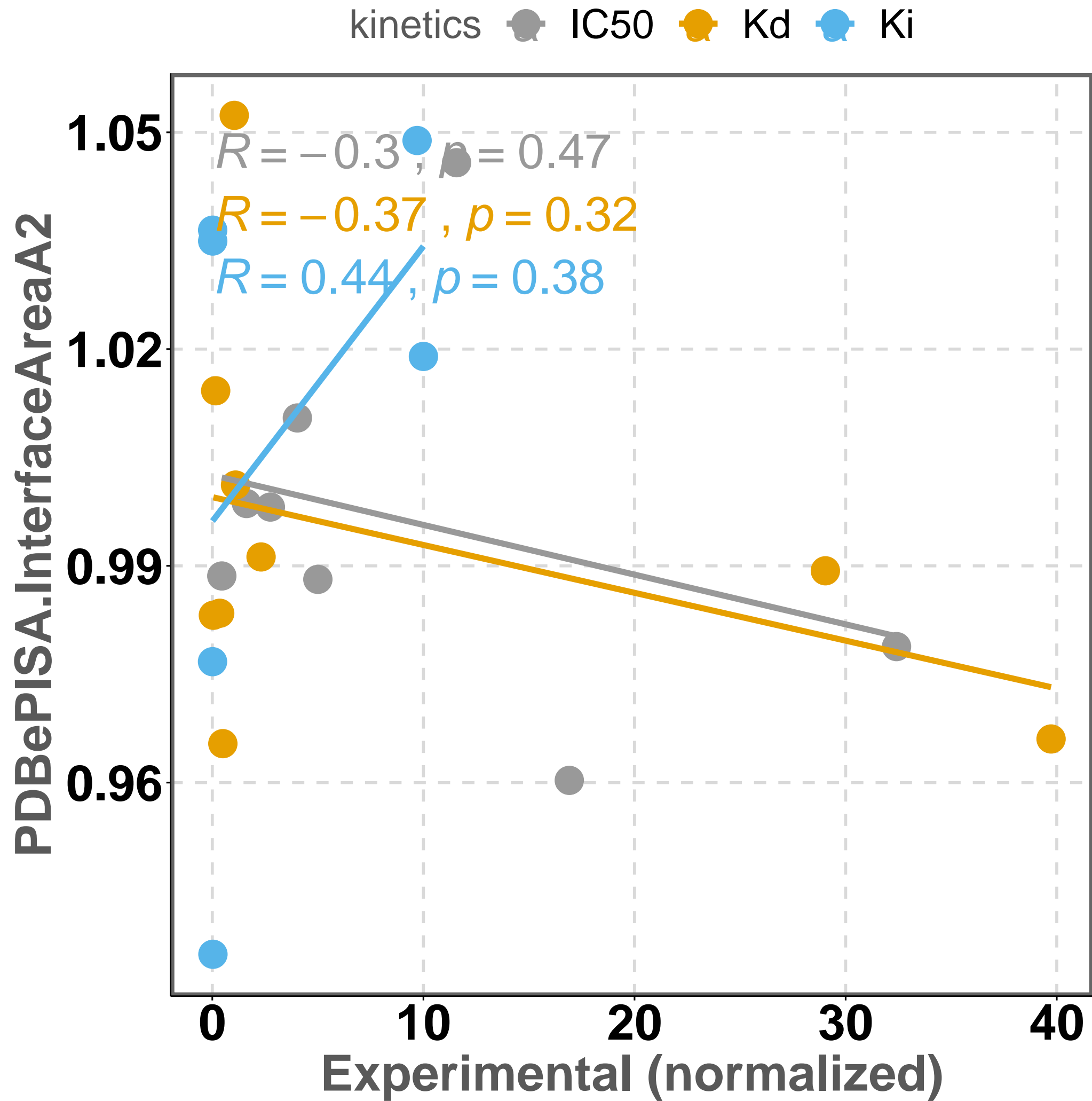


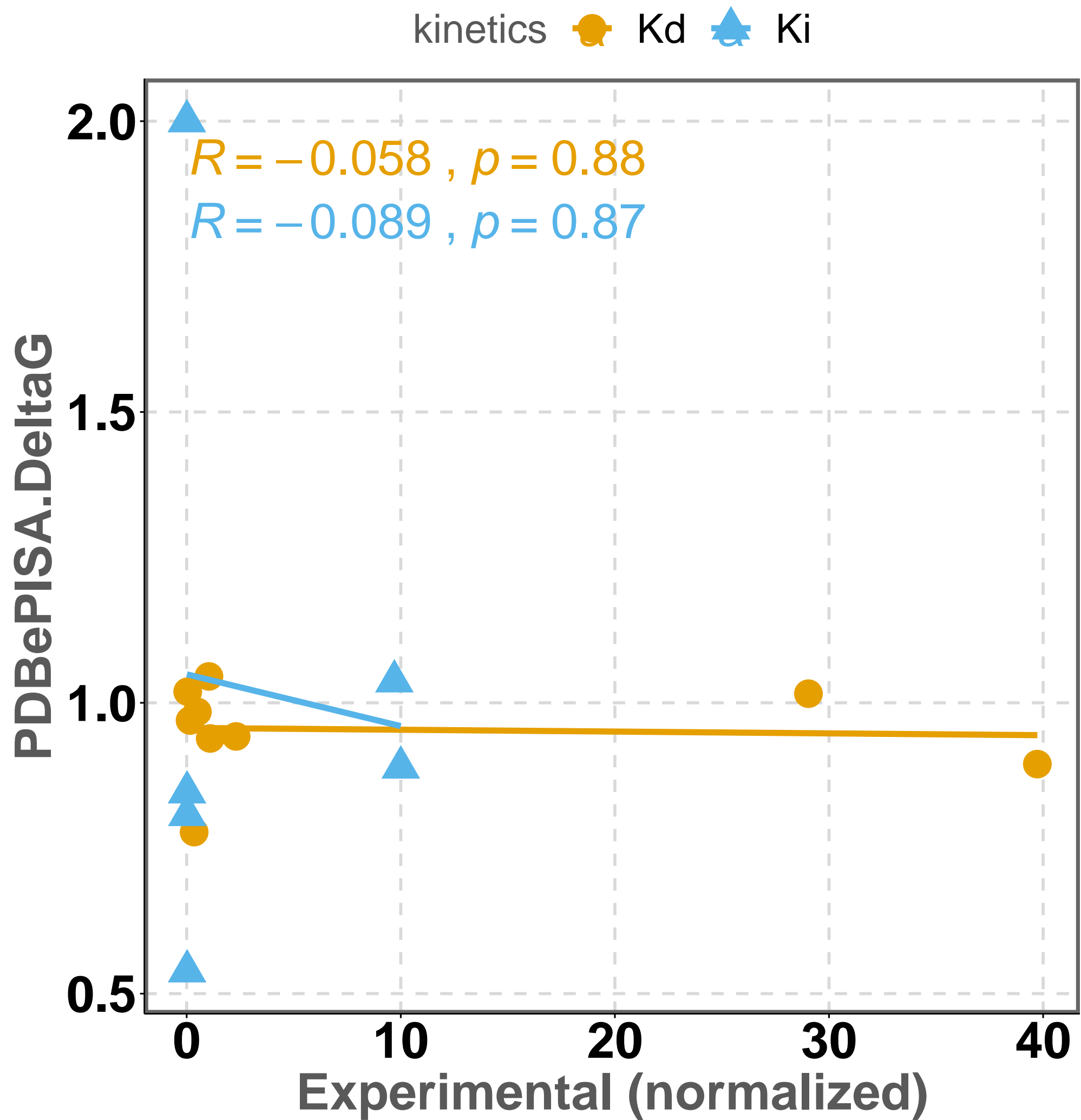






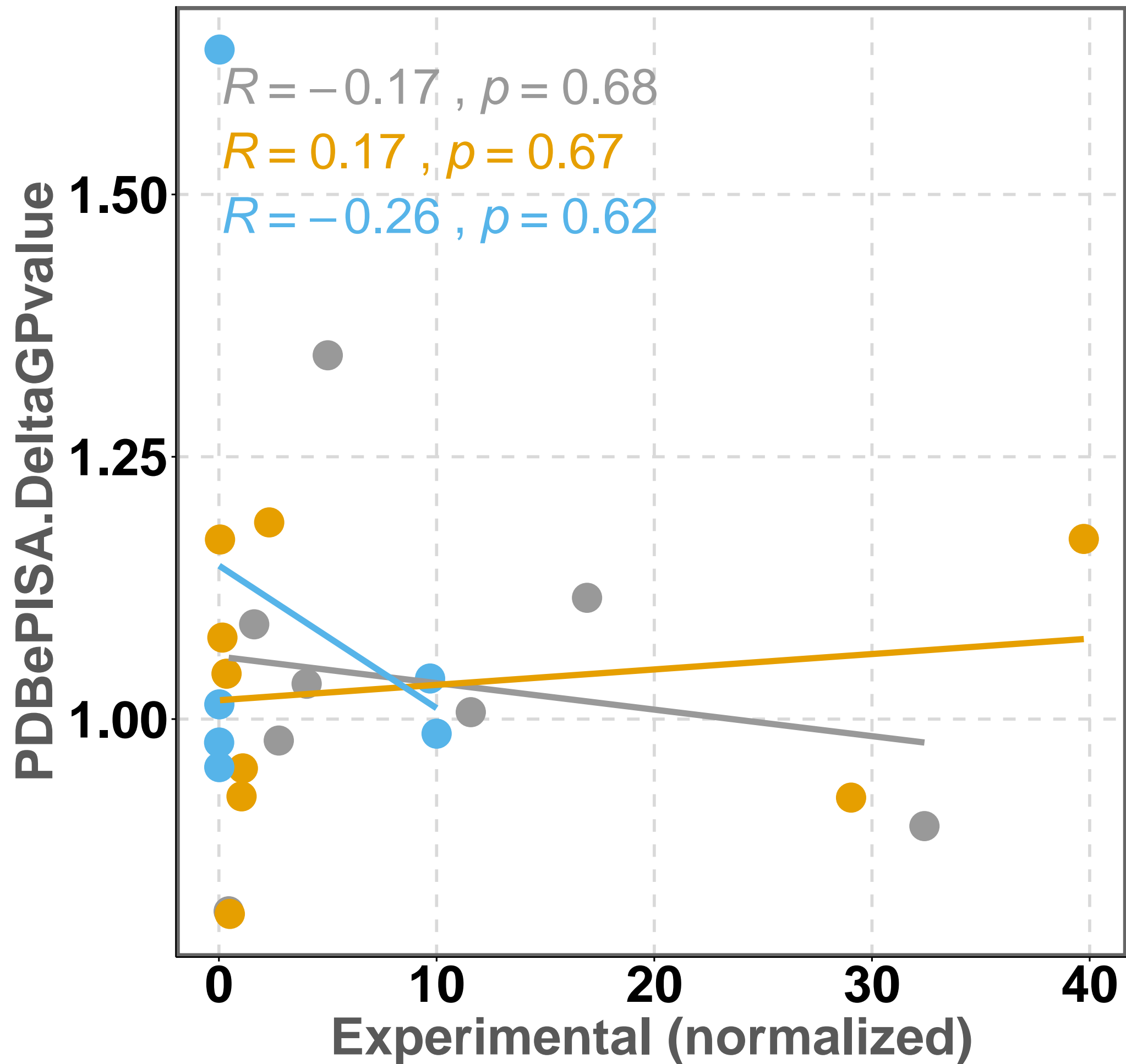


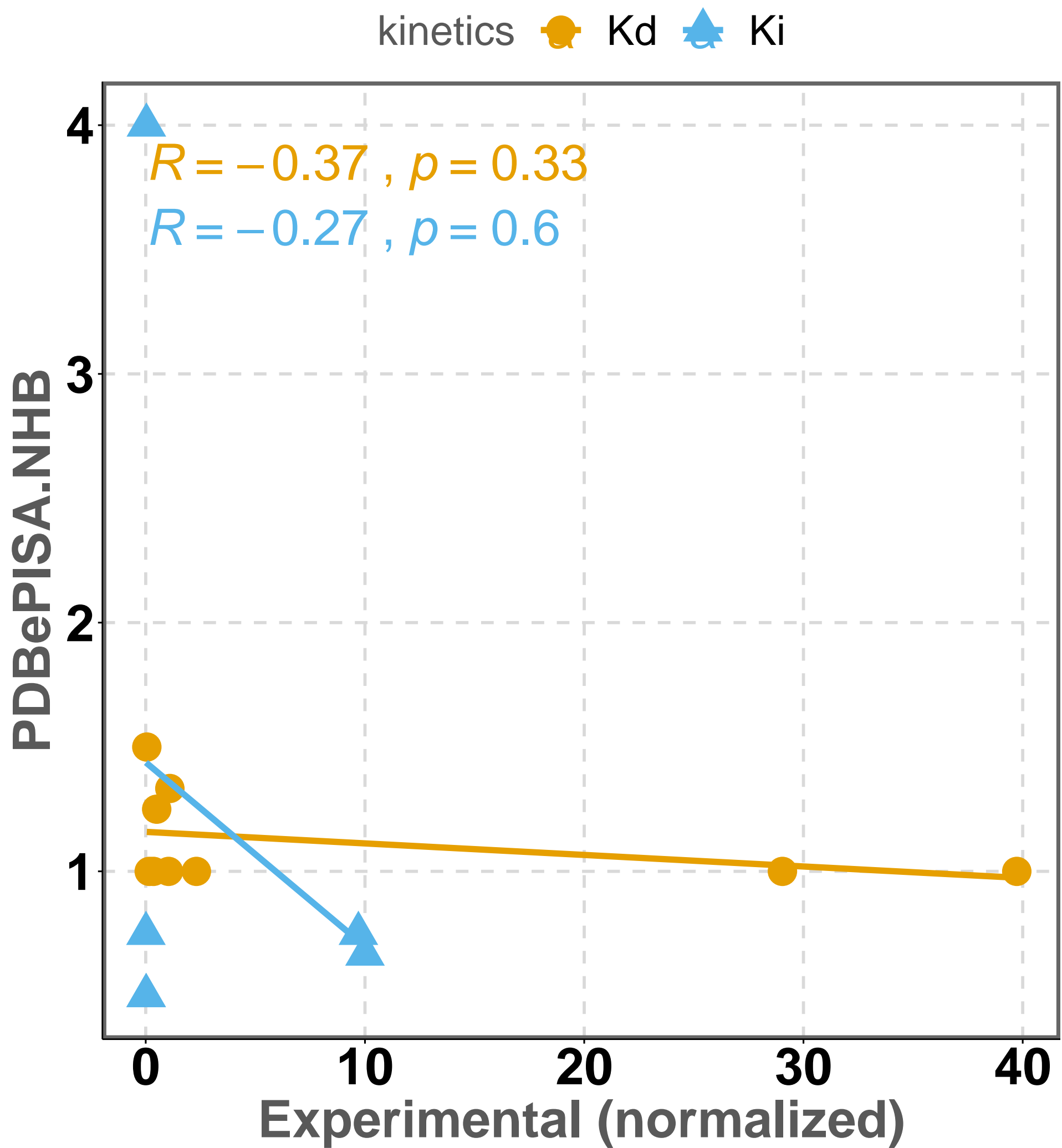


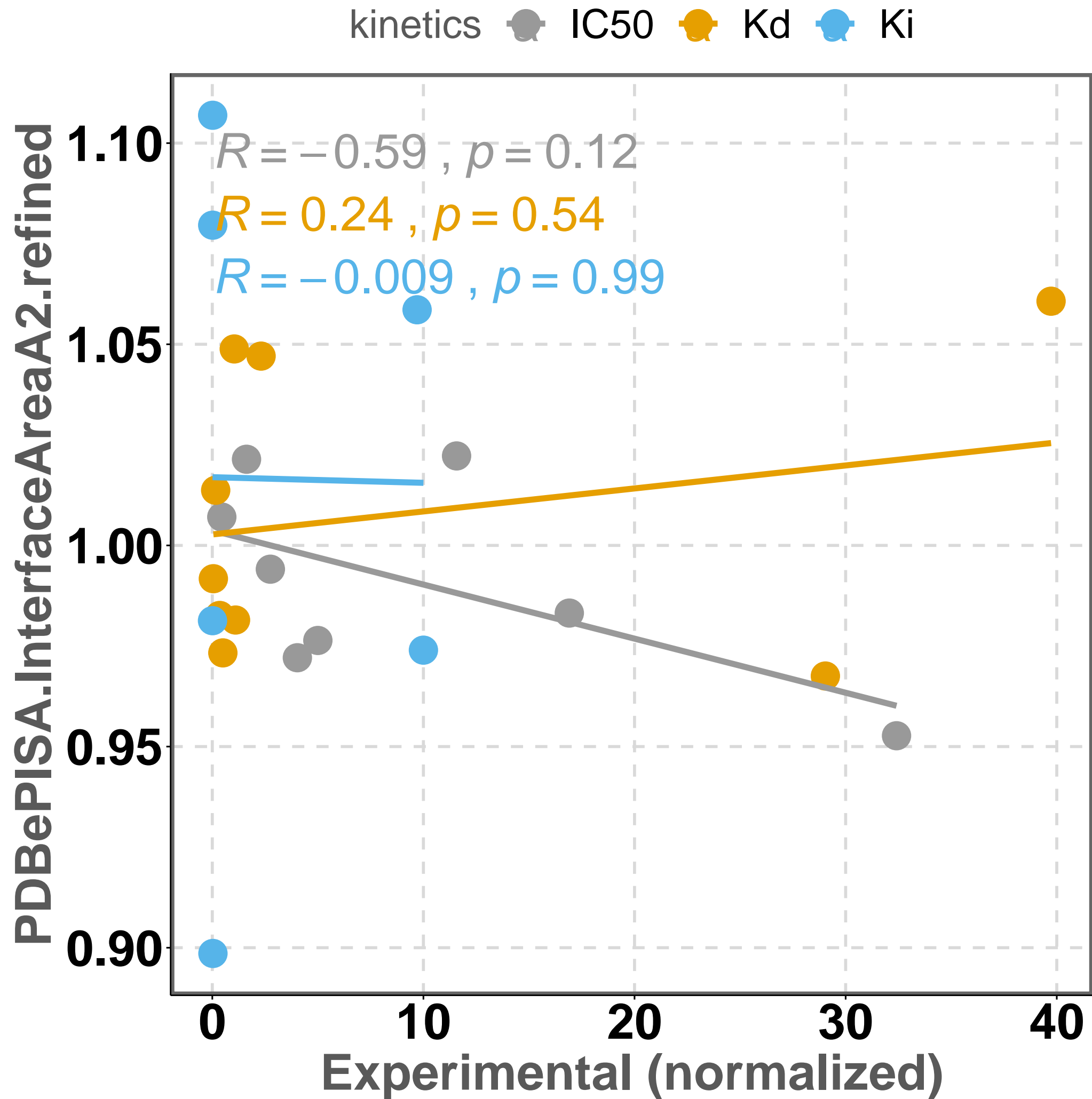




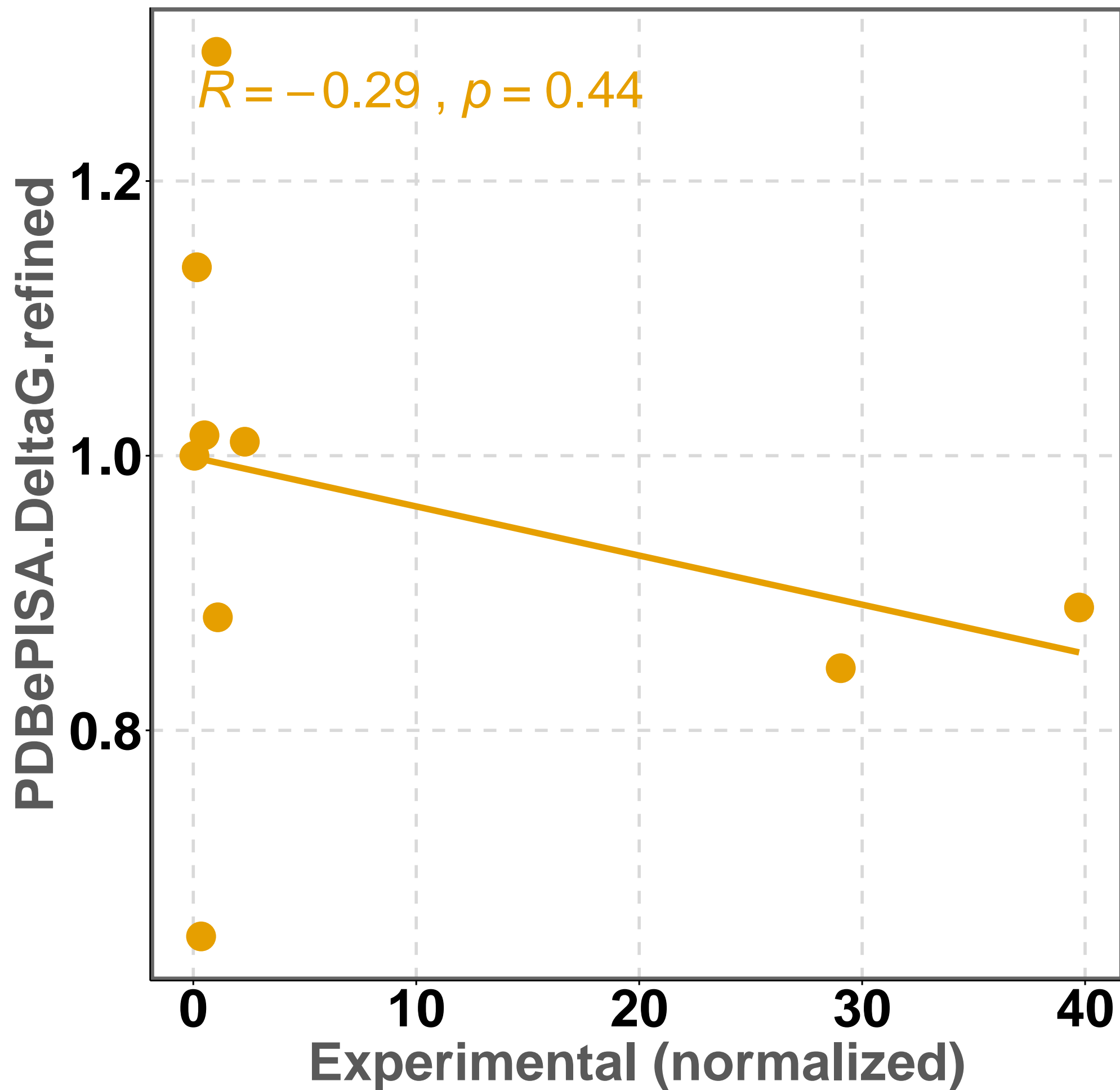
kinetics IC50 Kd Ki







kinetics  Kd



PDBePISA.DeltaG<sub>value.refined</sub>

kinetics IC50 Kd Ki

$R = 0.18$  ,  $p = 0.67$

$R = 0.23$  ,  $p = 0.56$

$R = -0.59$  ,  $p = 0.21$

0

10

20

30

40

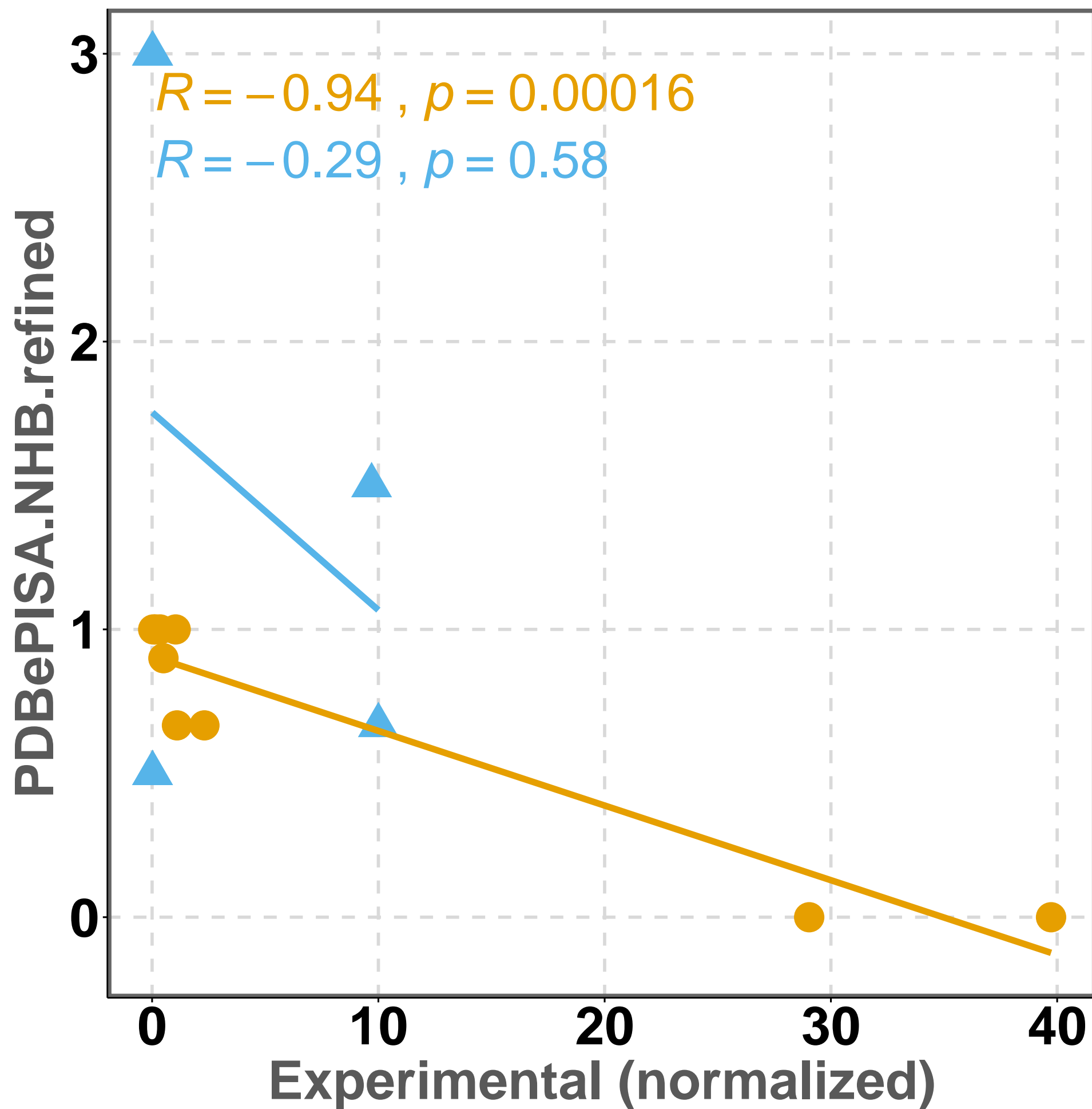
Experimental (normalized)

1.5

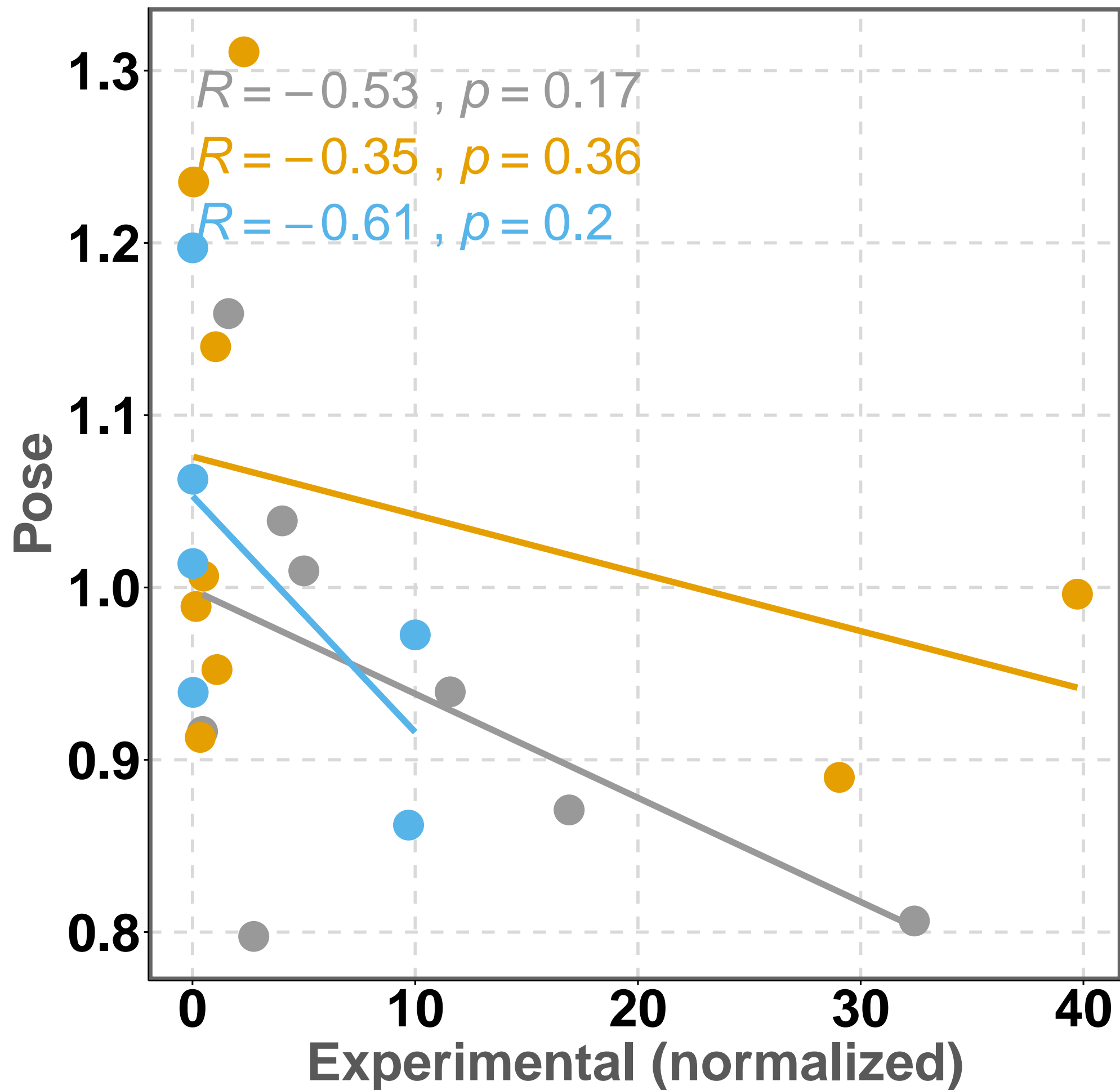
1.2

0.9

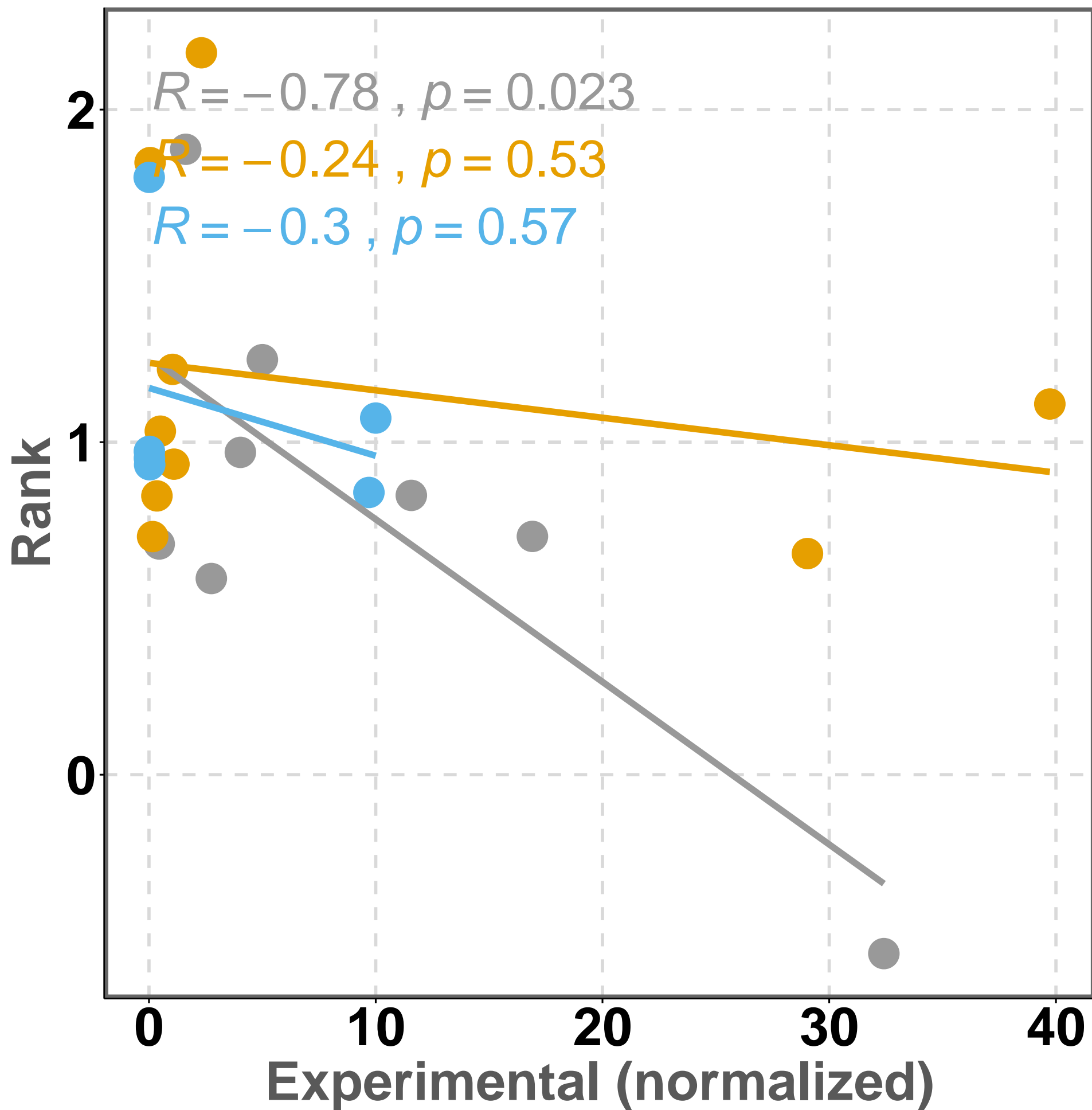
kinetics  Kd  Ki



kinetics IC50 Kd Ki

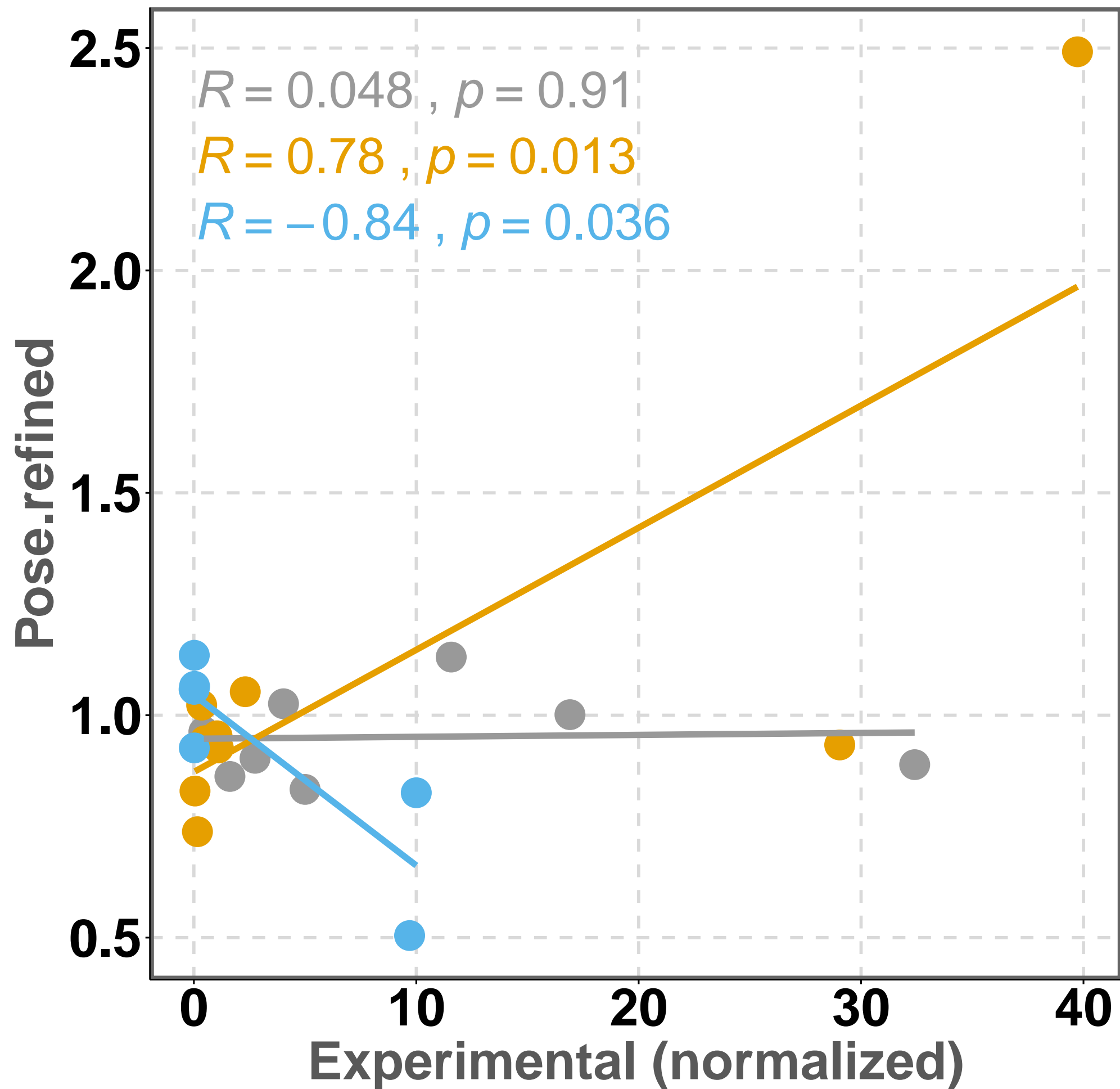


kinetics    IC50    Kd    Ki

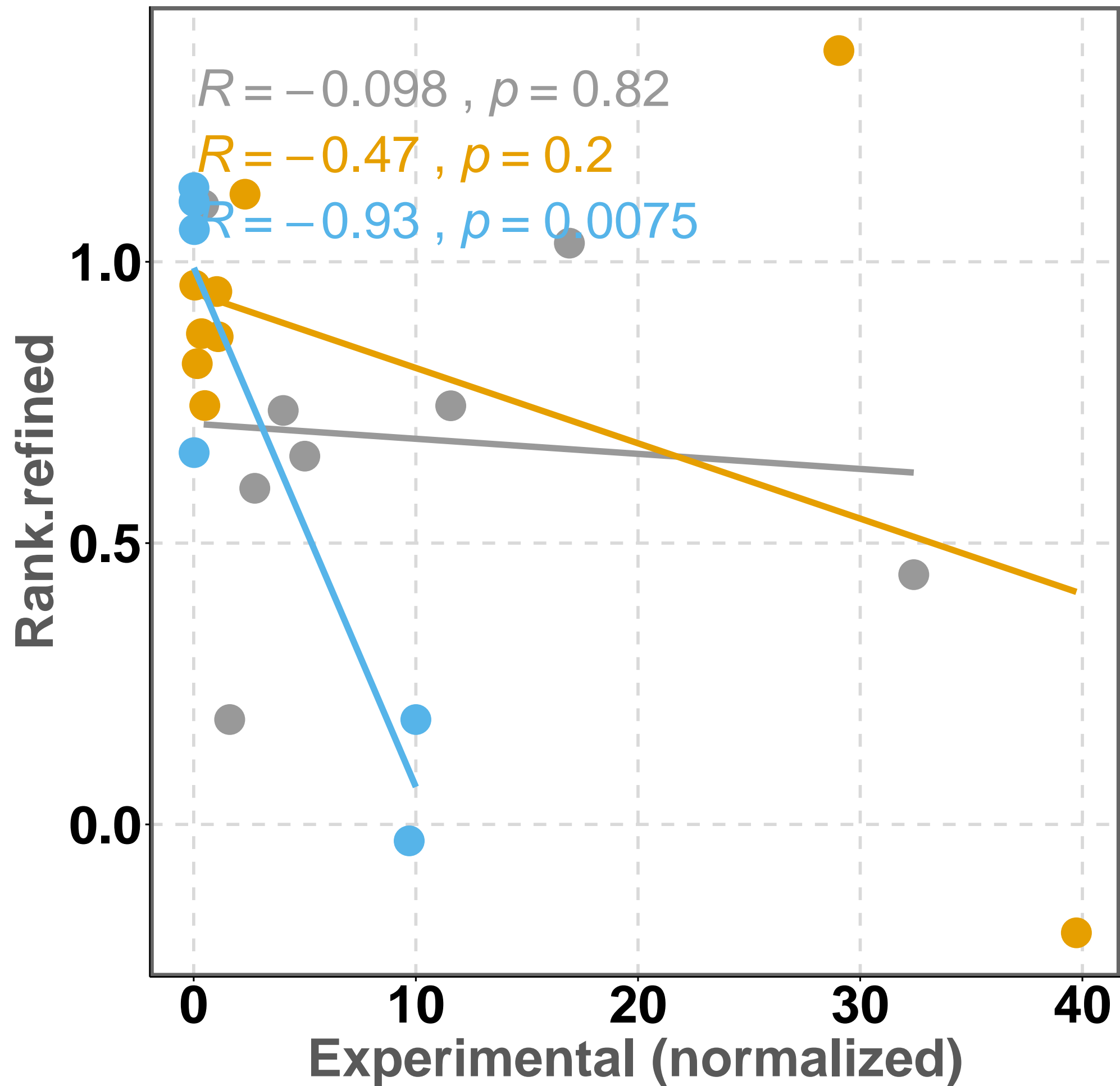




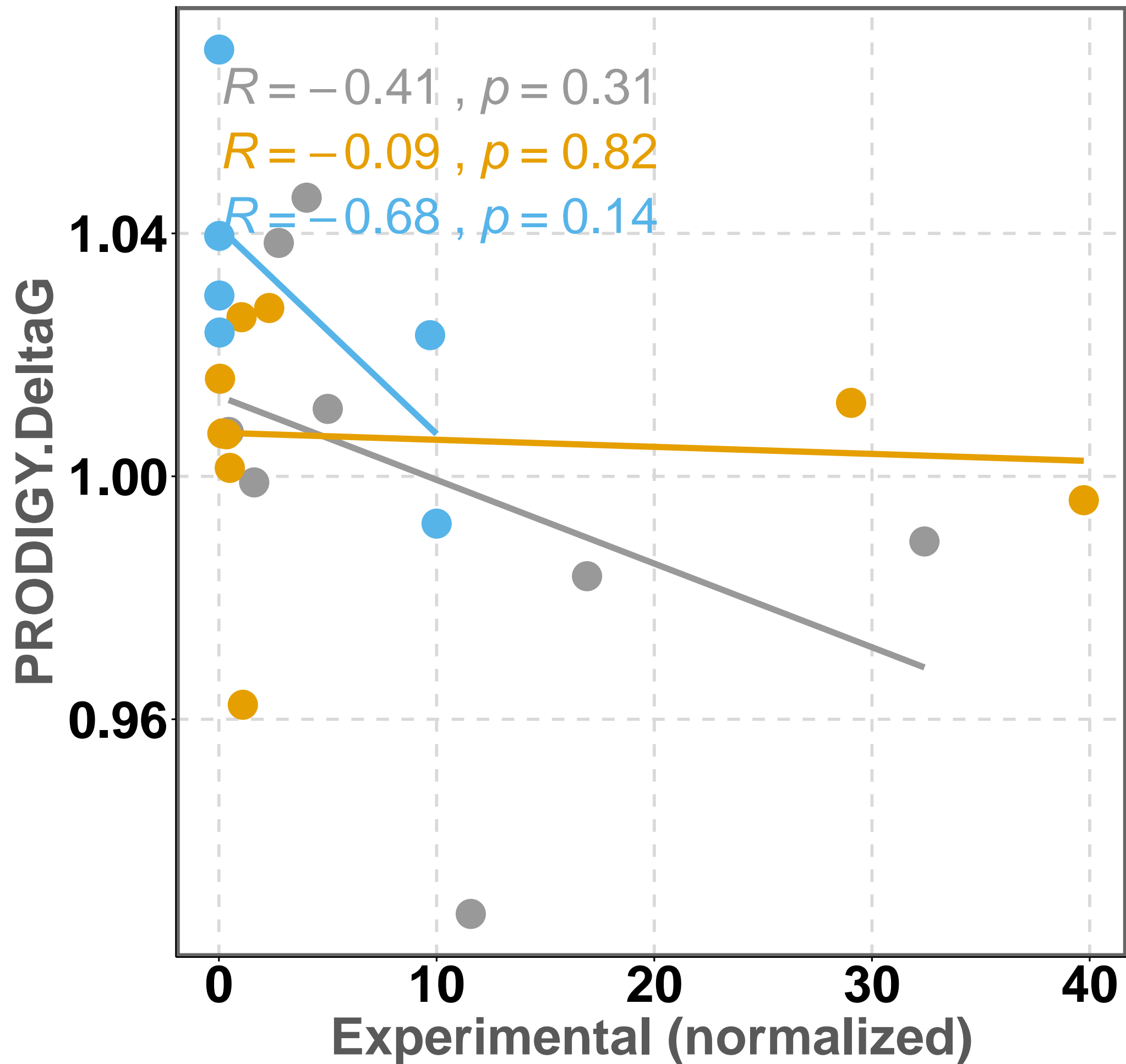
kinetics IC50 Kd Ki



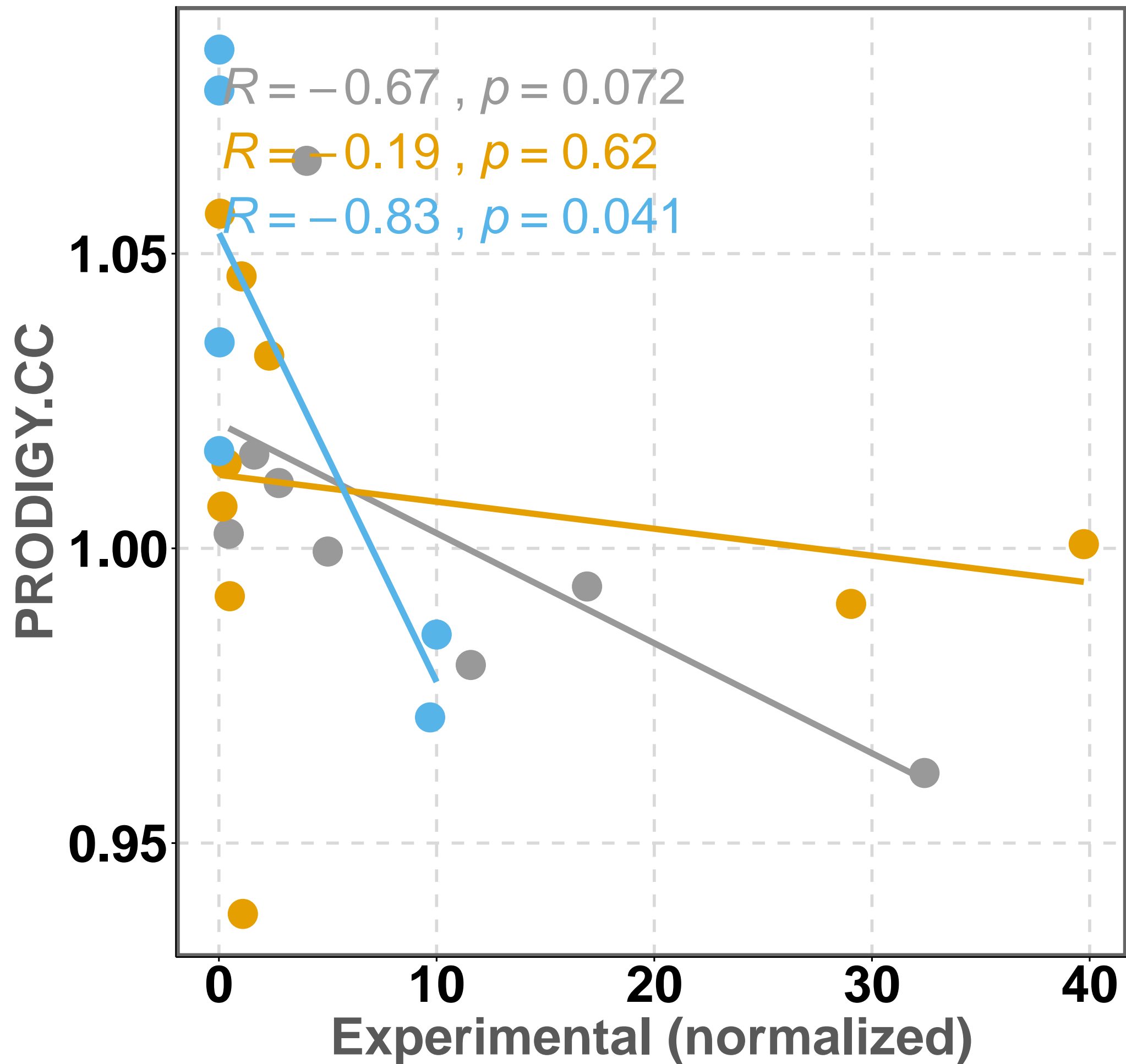
kinetics IC50 Kd Ki

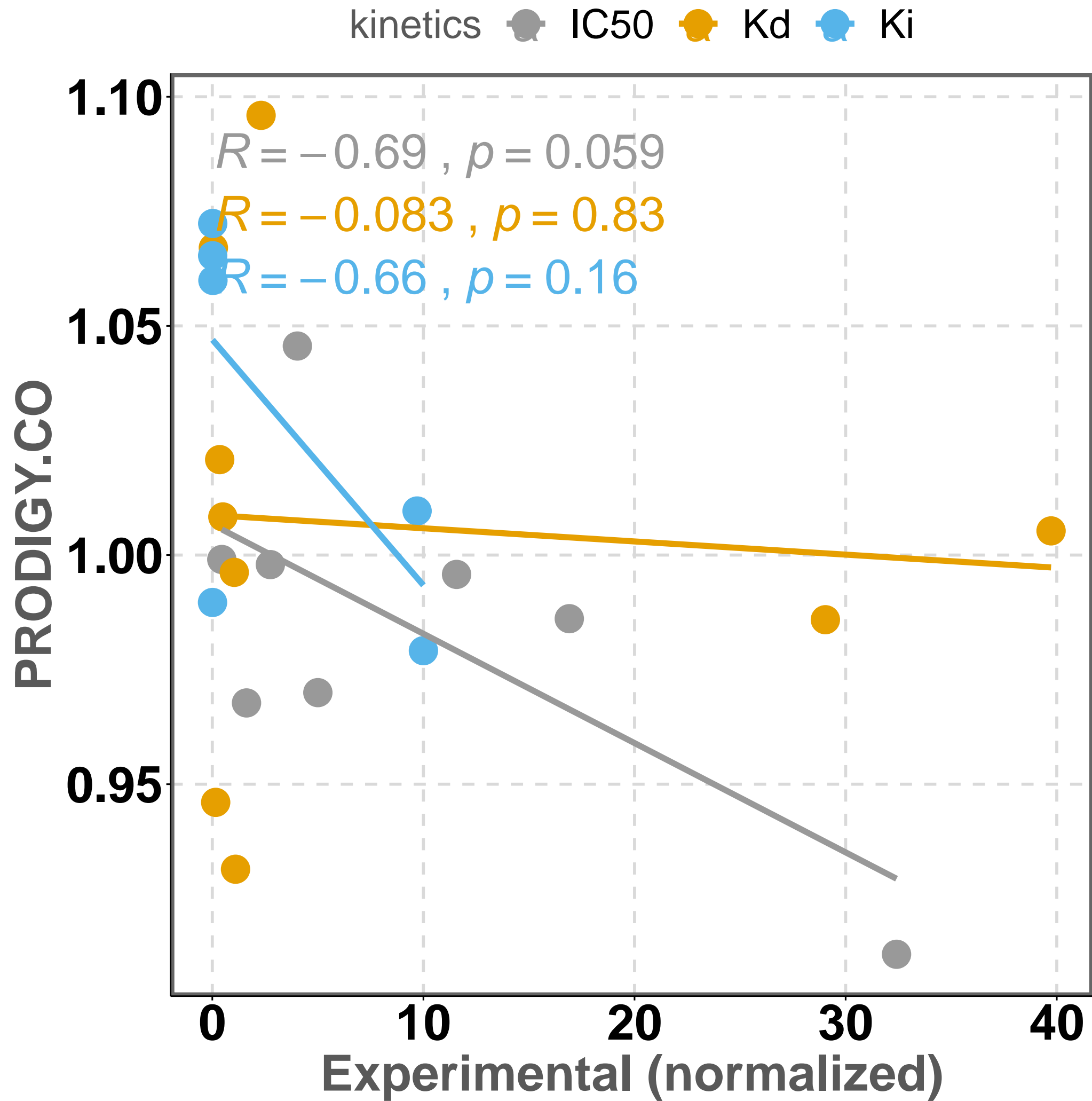


kinetics IC50 Kd Ki

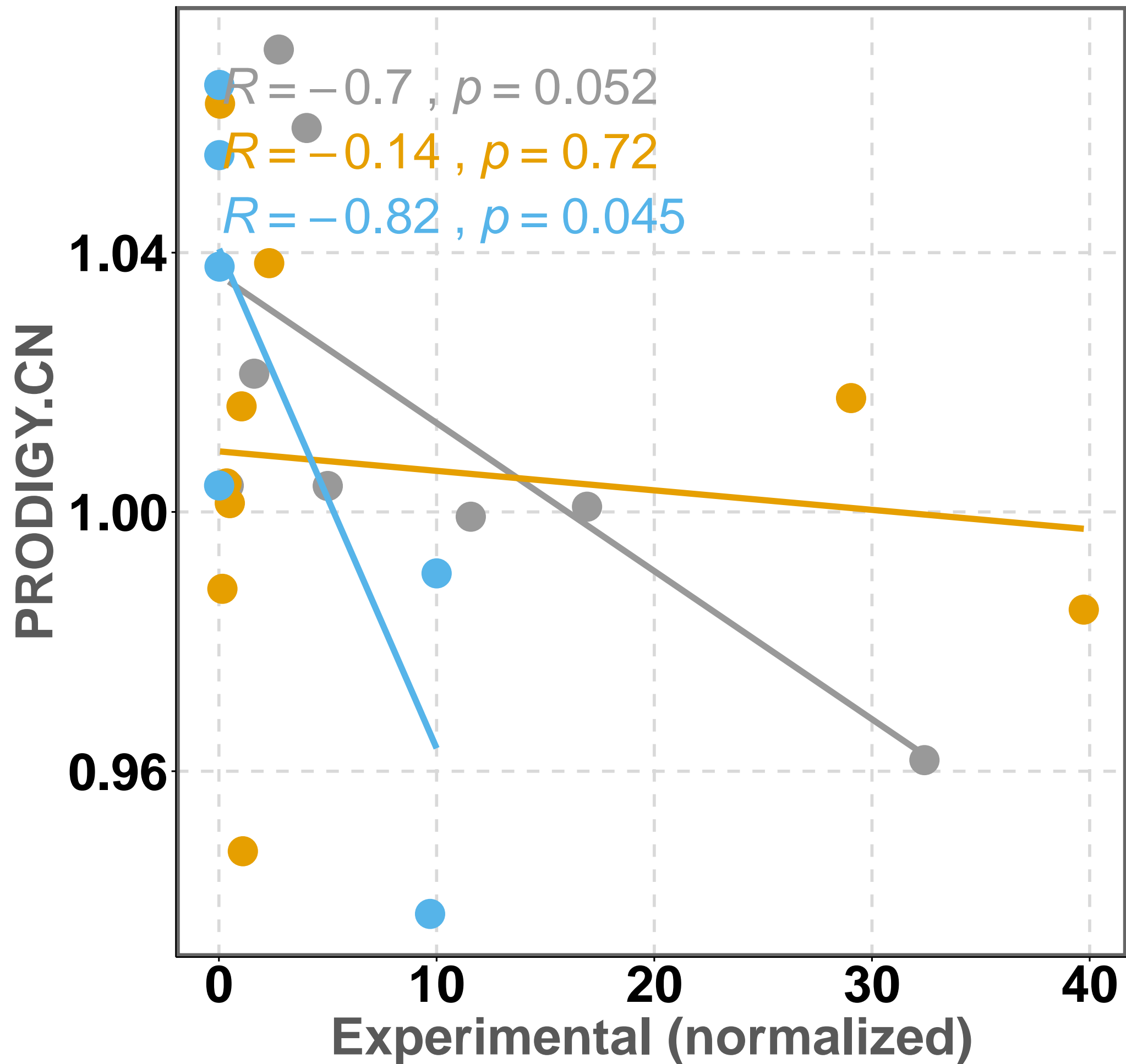


kinetics IC50 Kd Ki

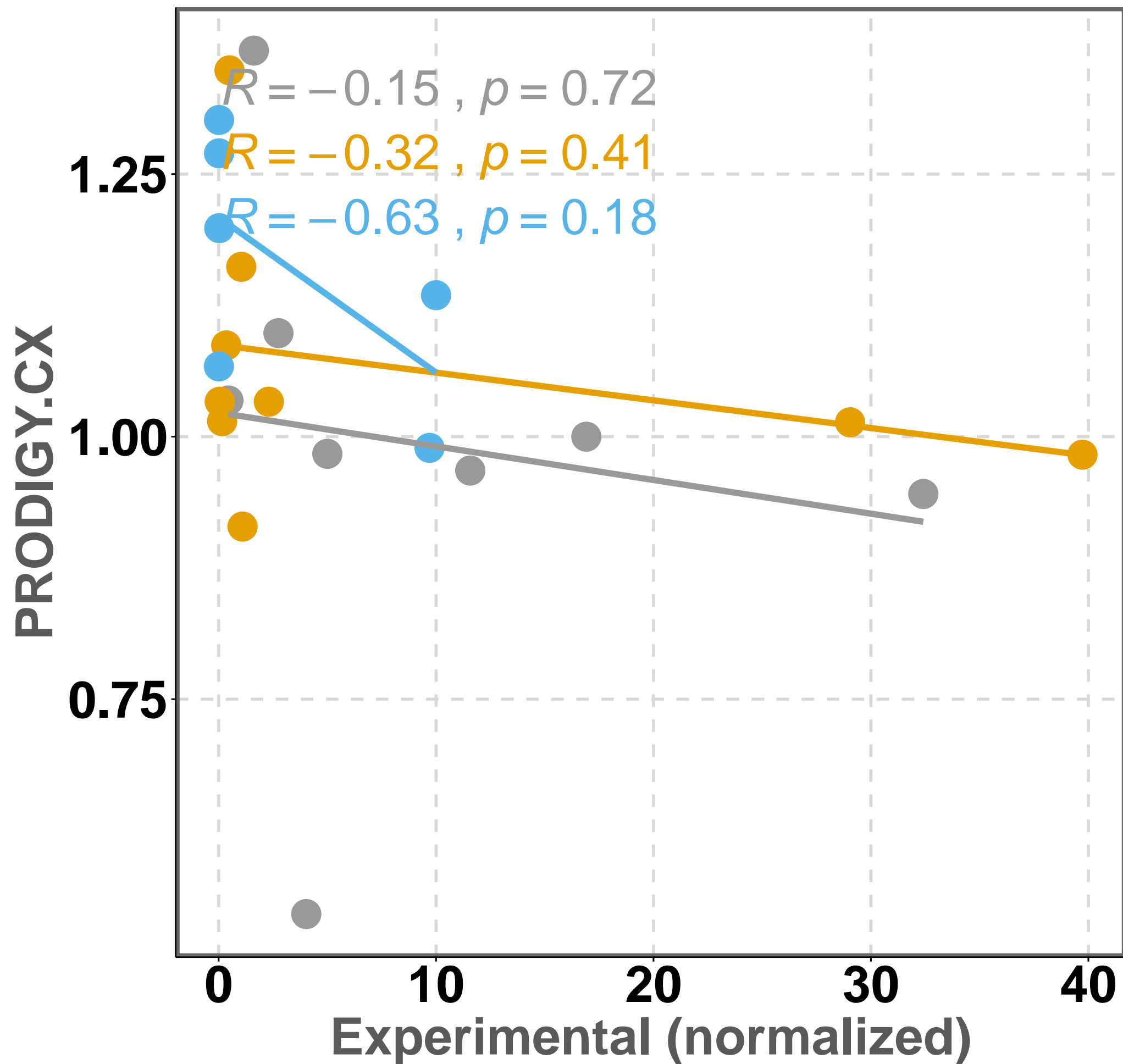




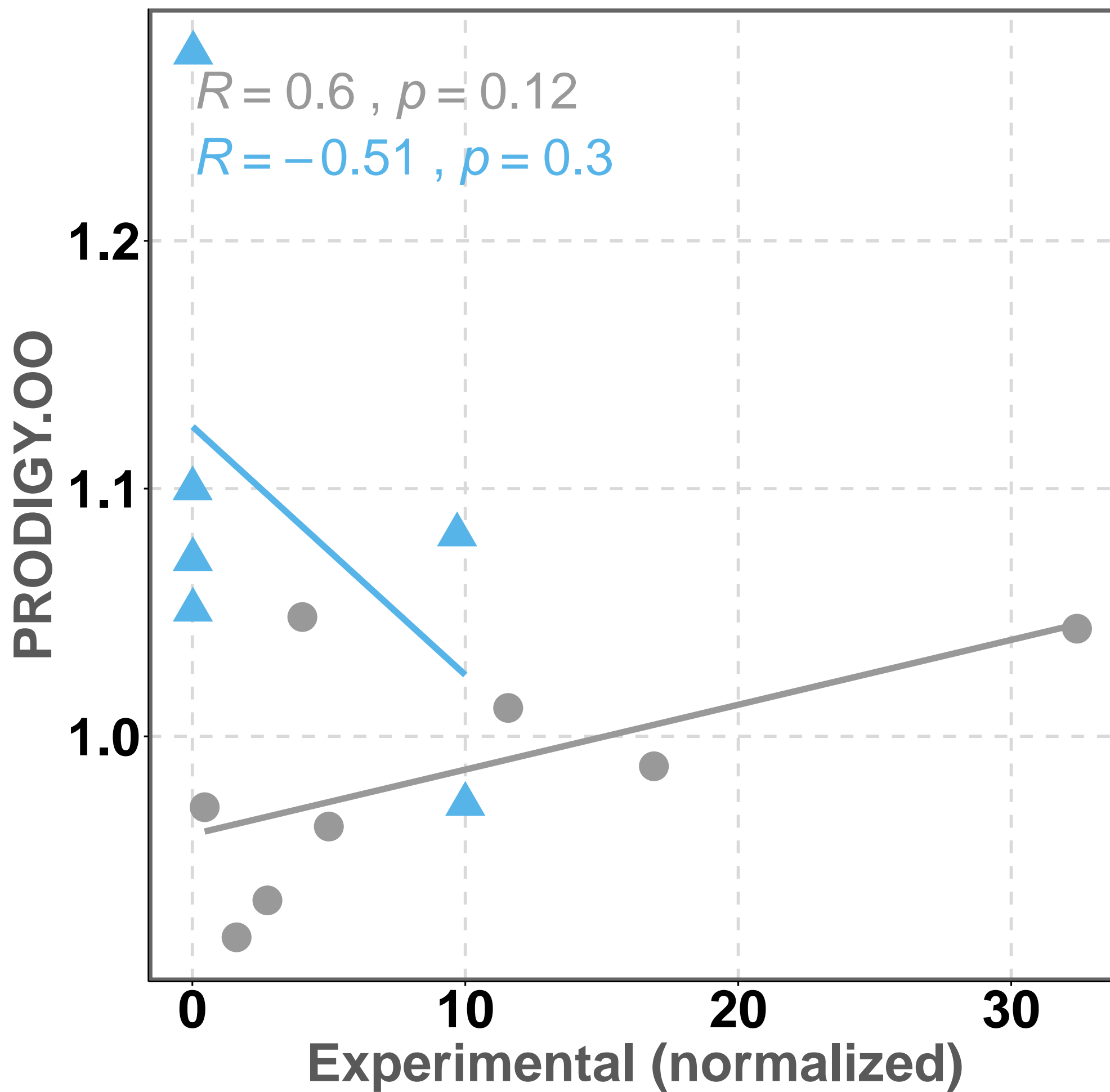
kinetics IC50 Kd Ki



kinetics IC50 Kd Ki

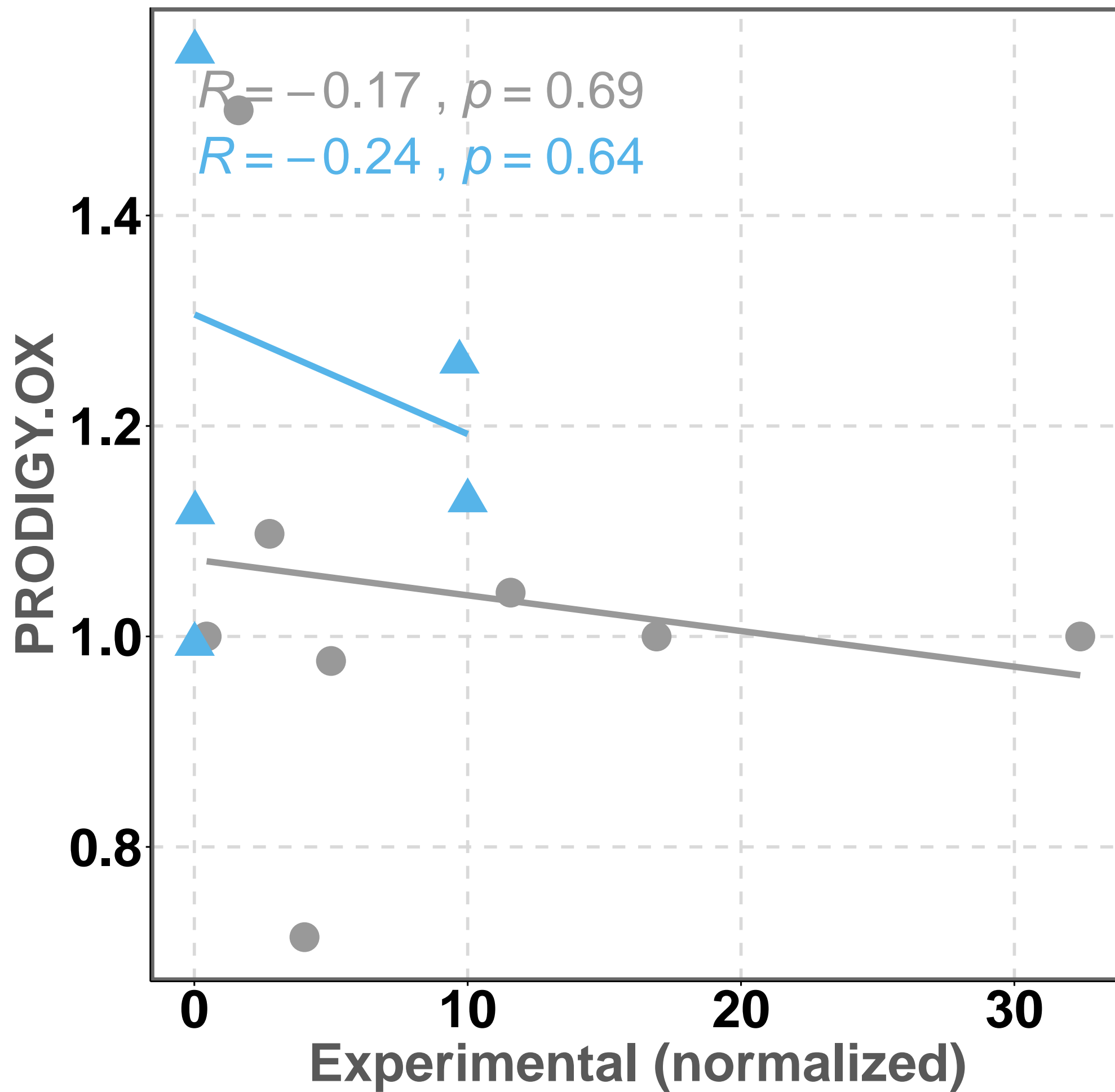


kinetics IC50 Ki

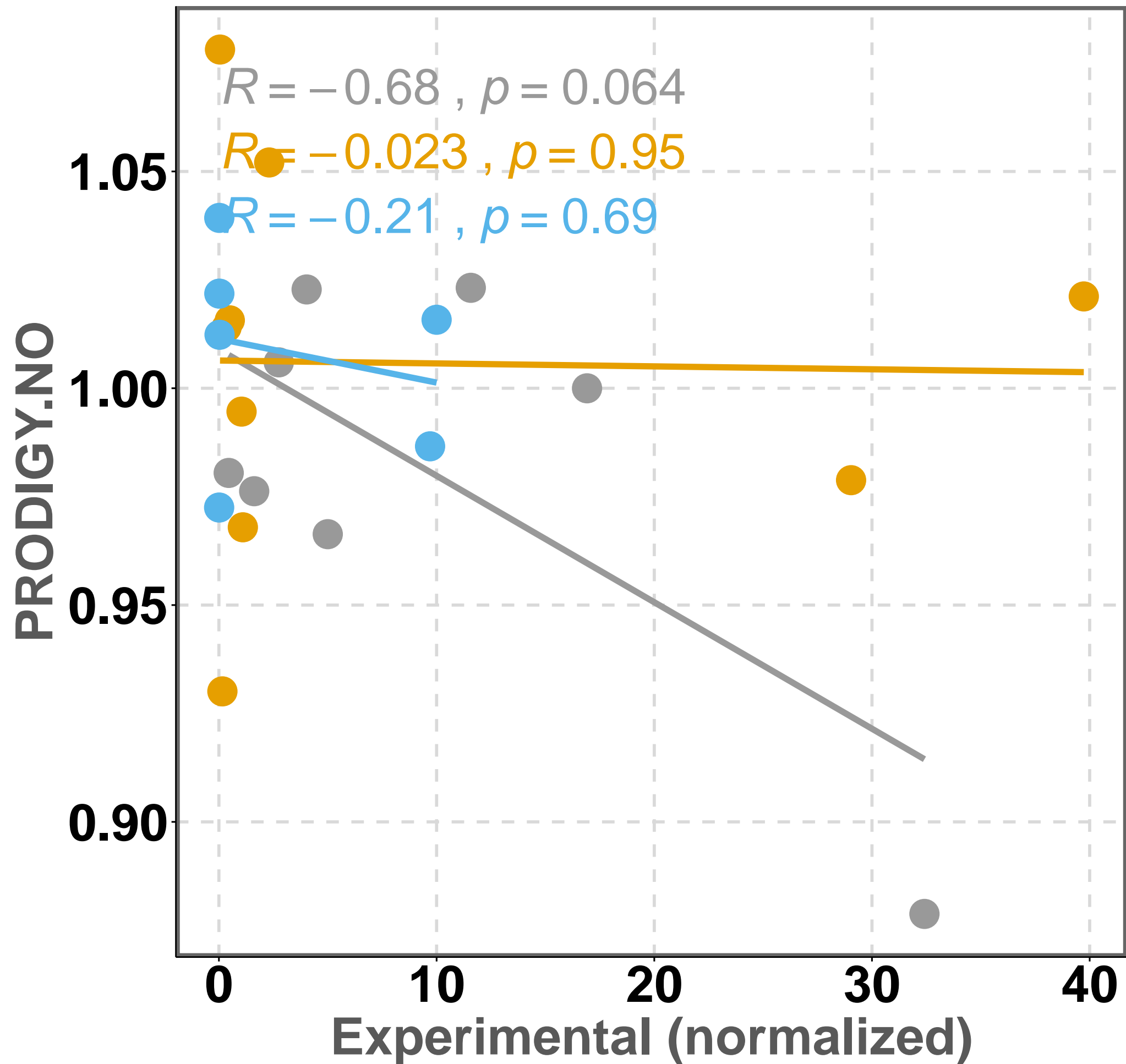




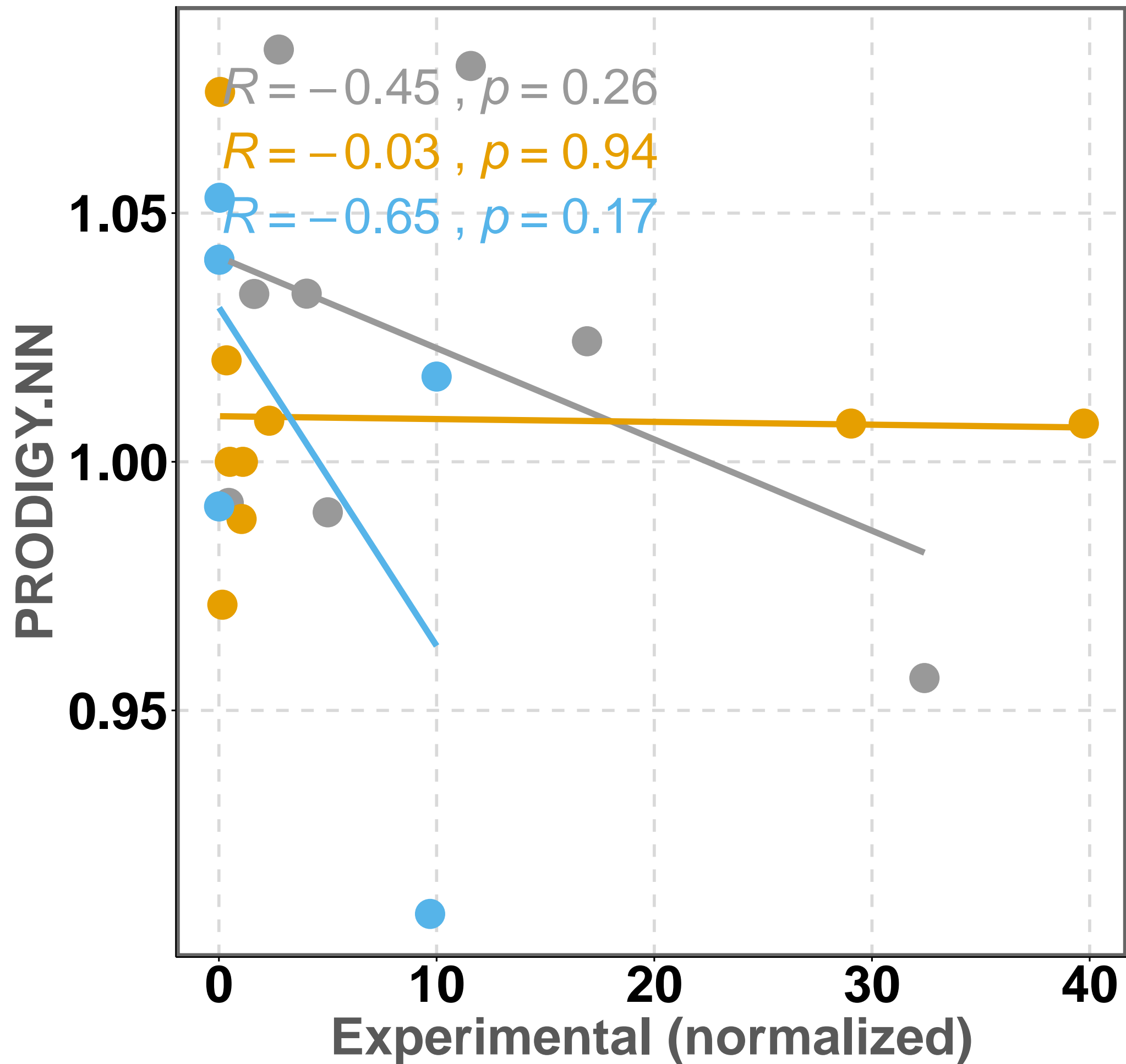
kinetics IC50 Ki



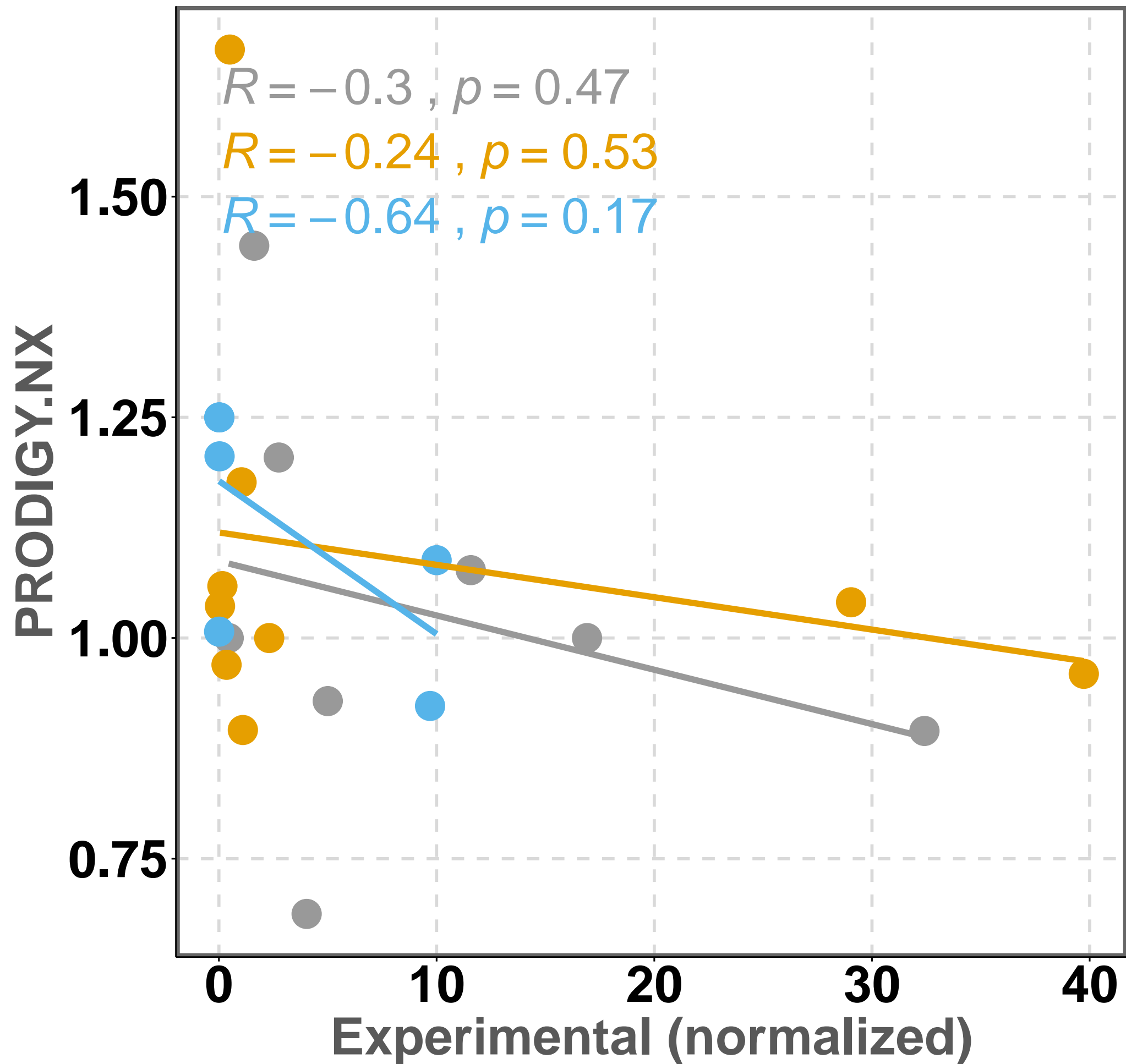
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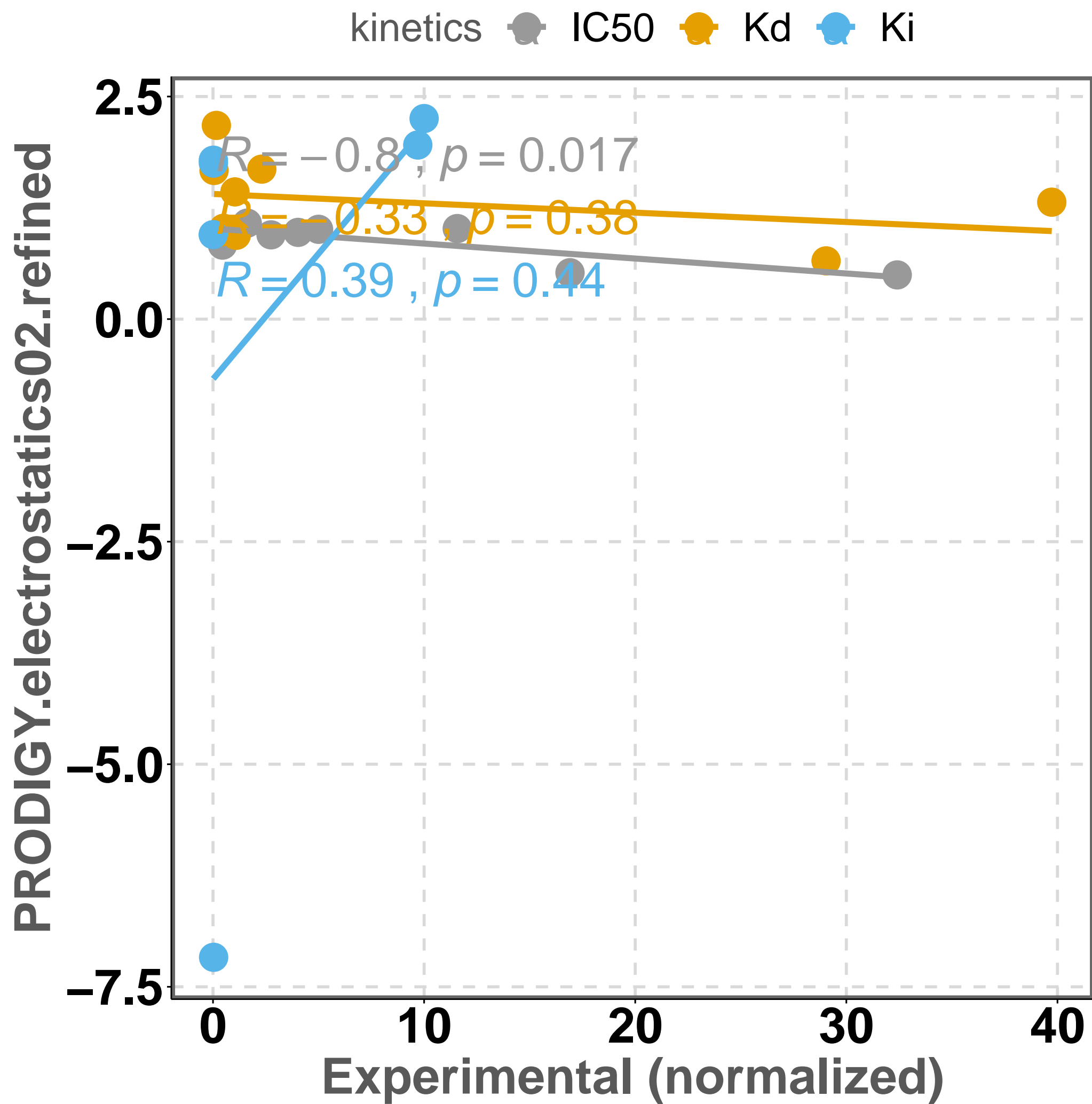


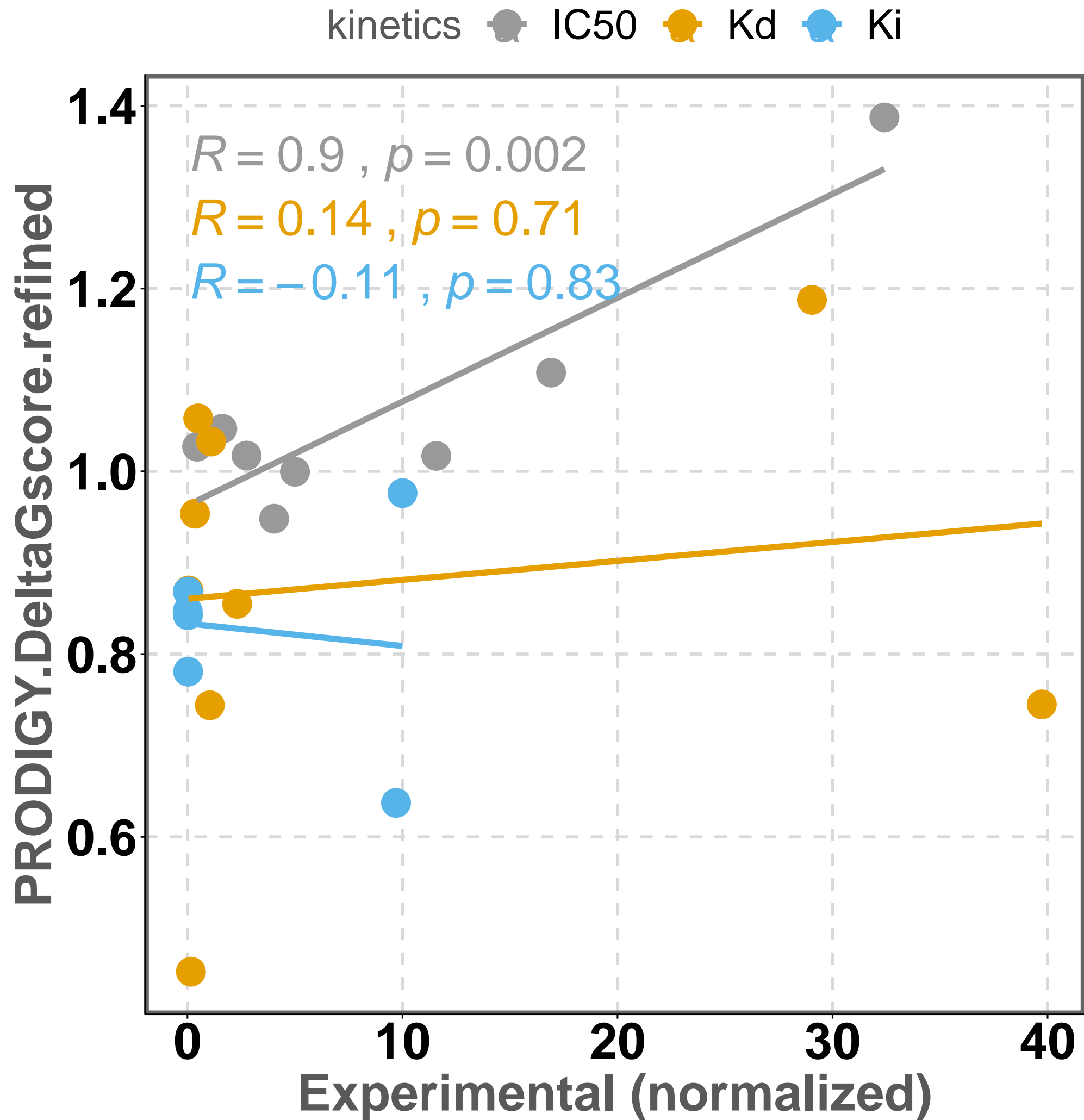
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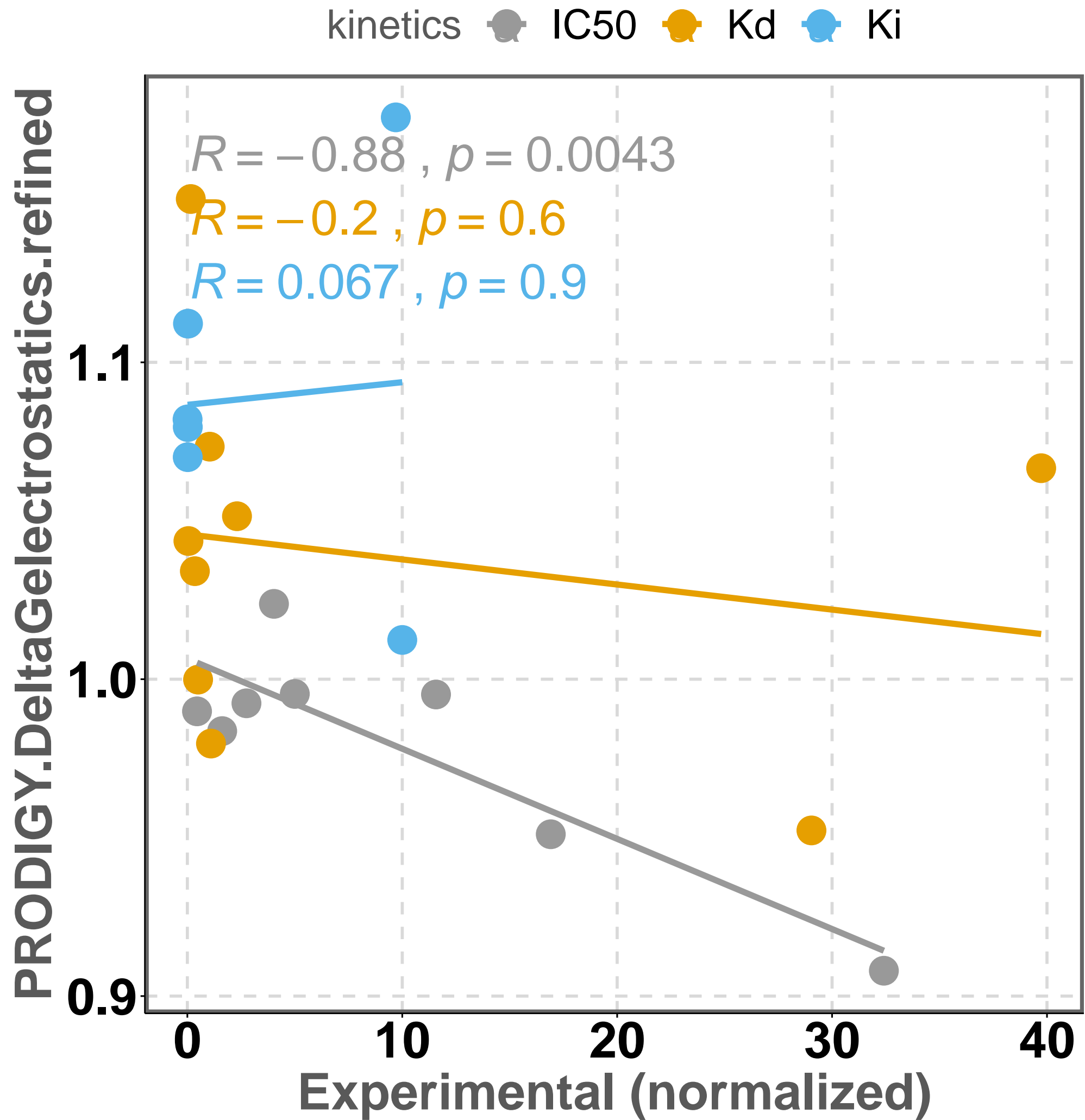


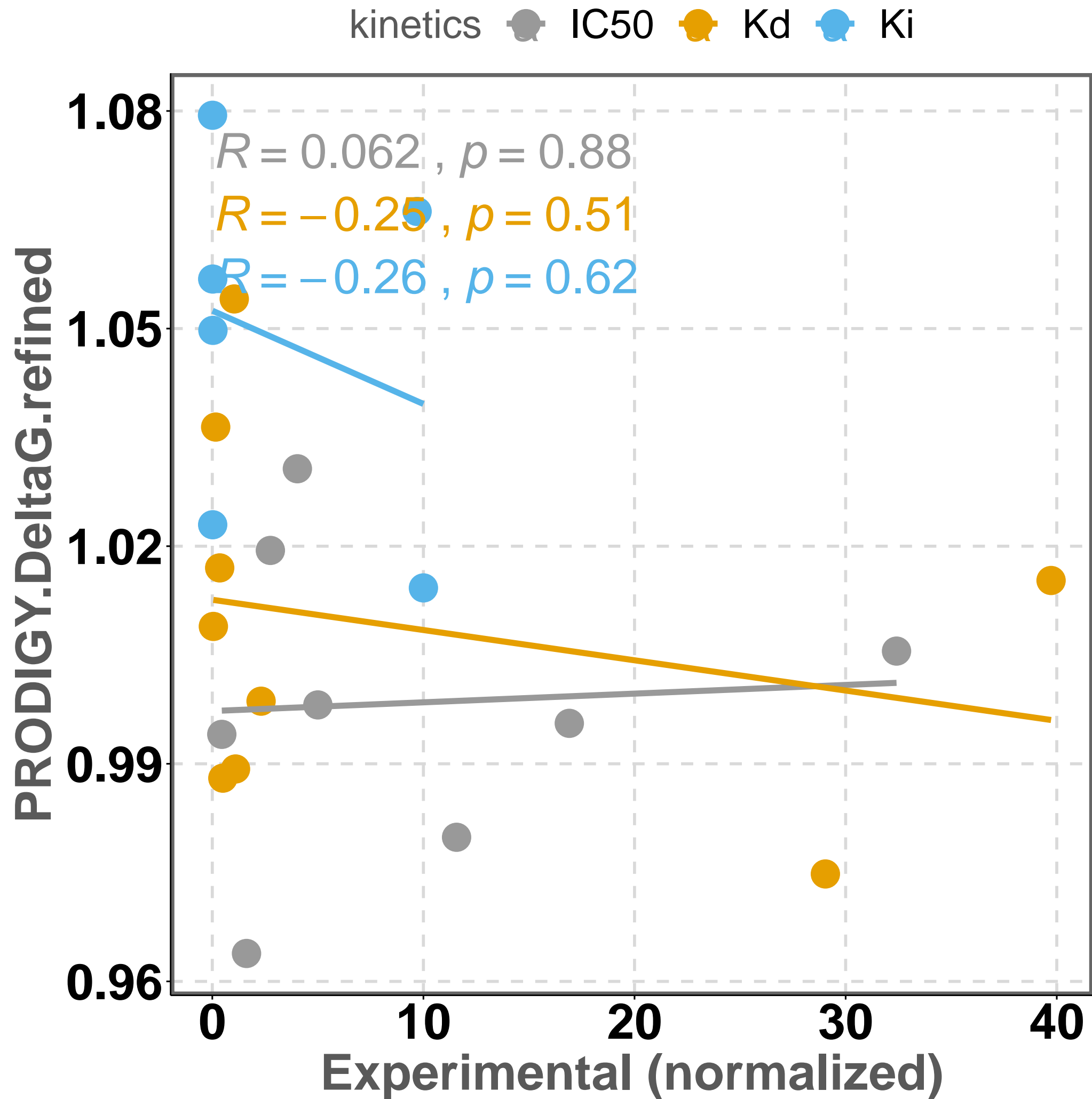
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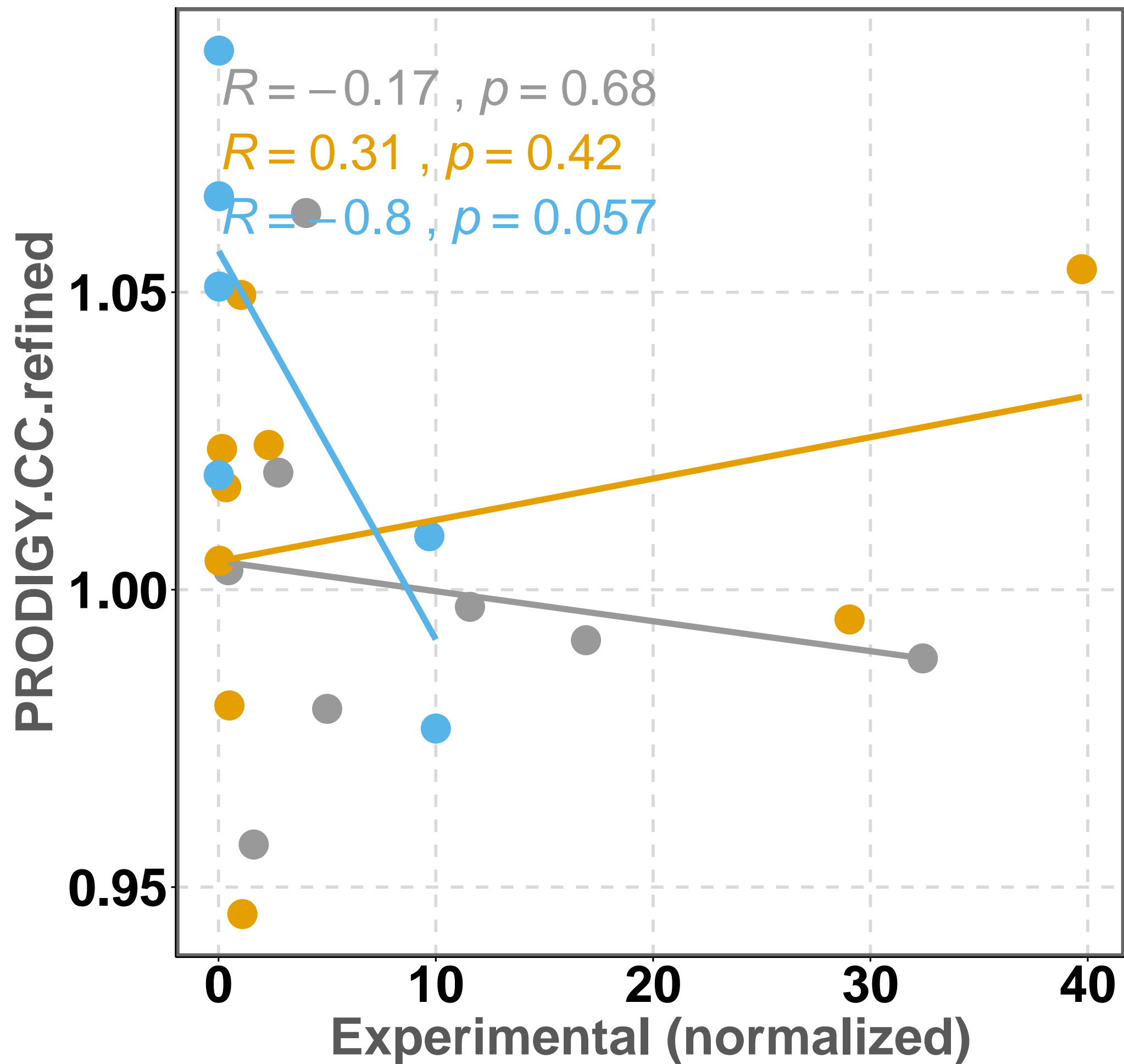


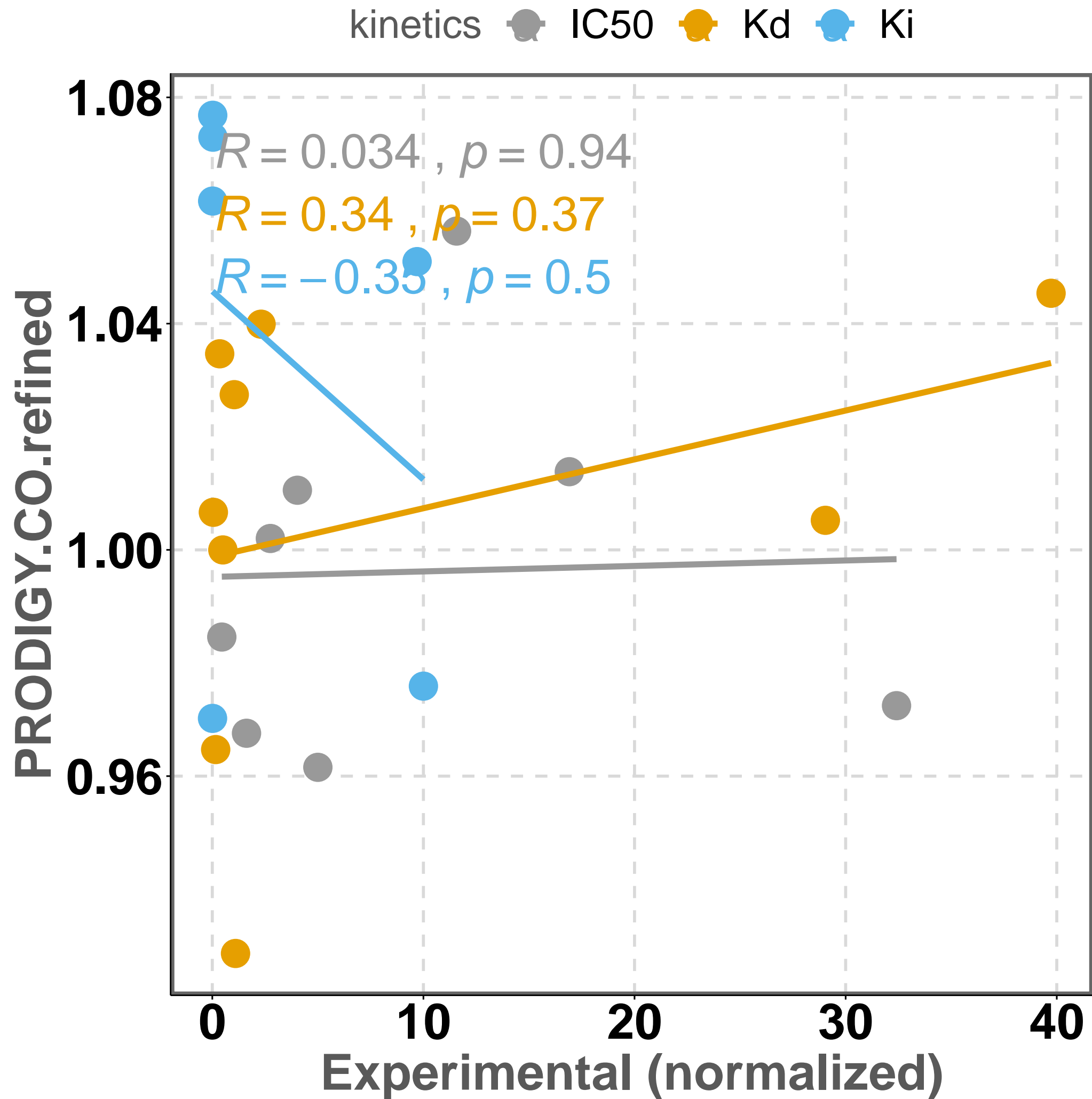


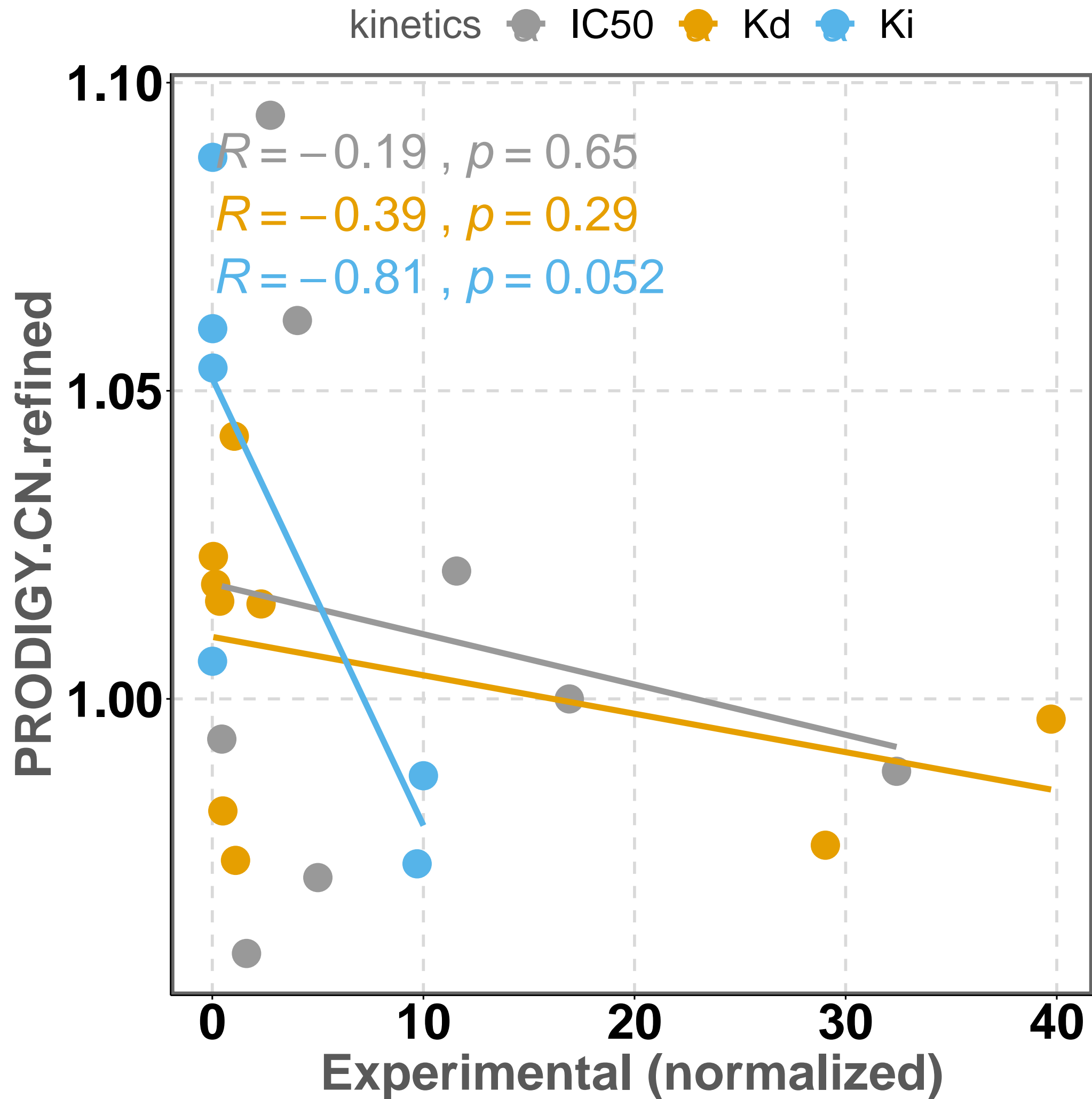




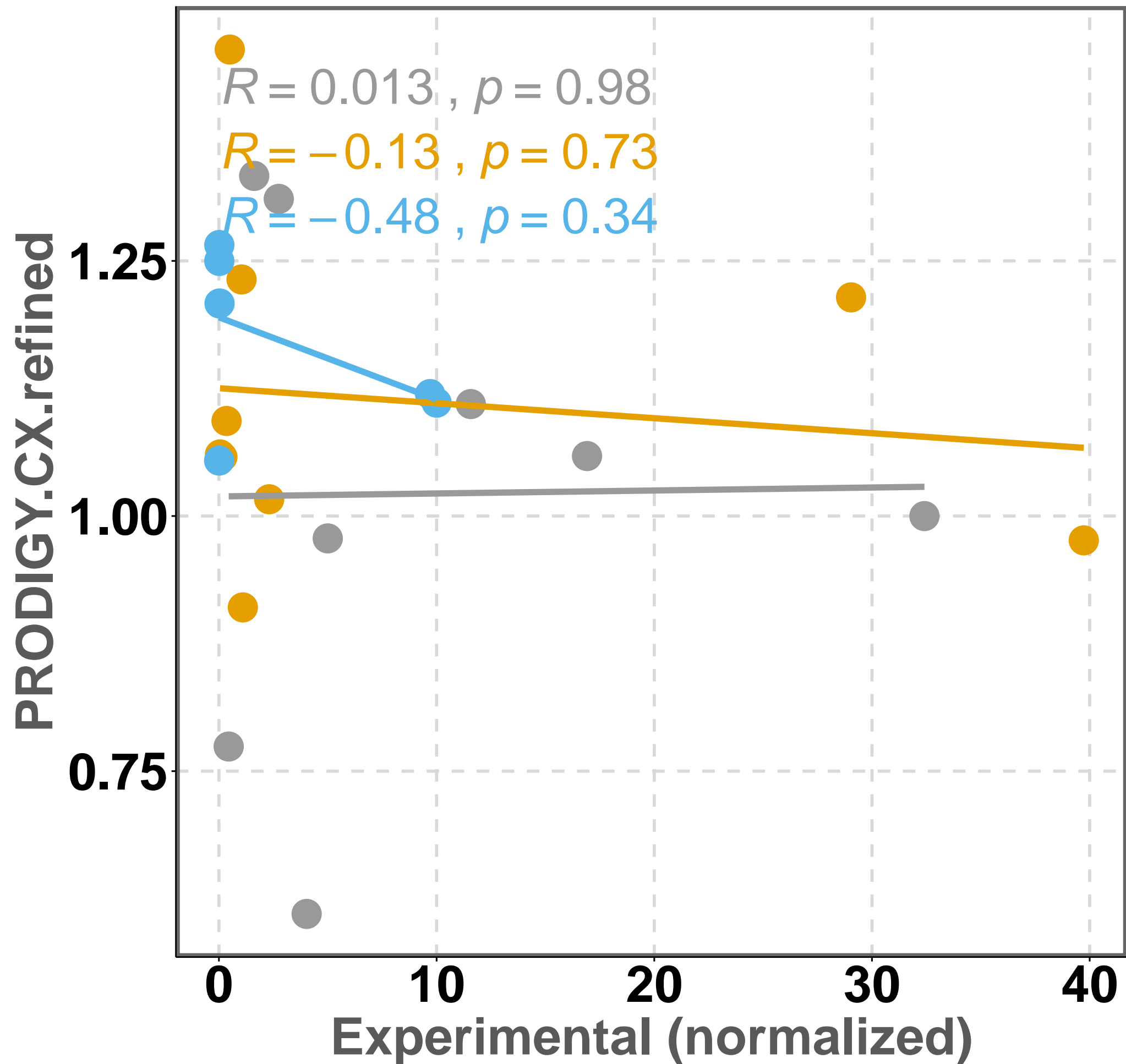
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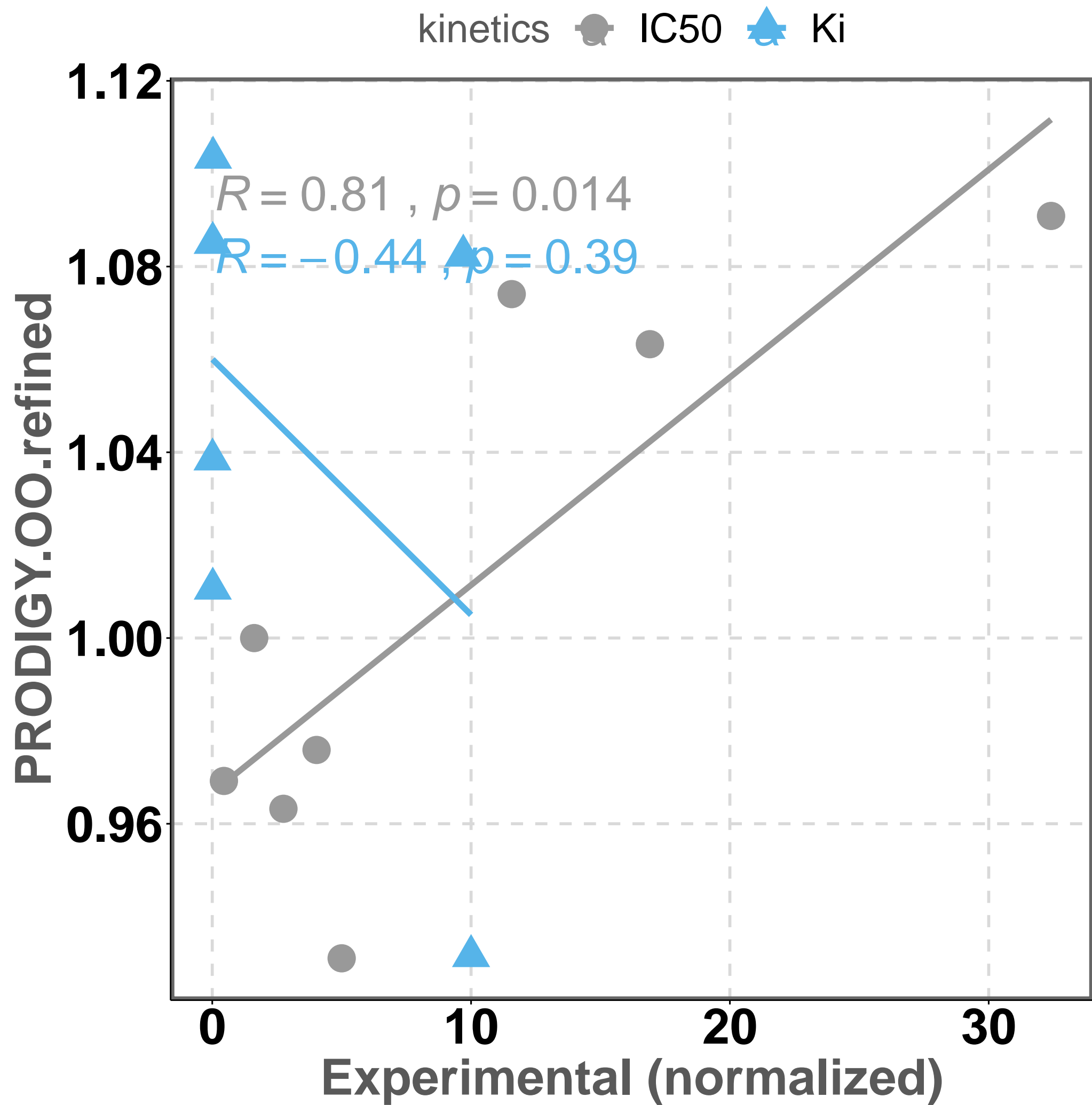




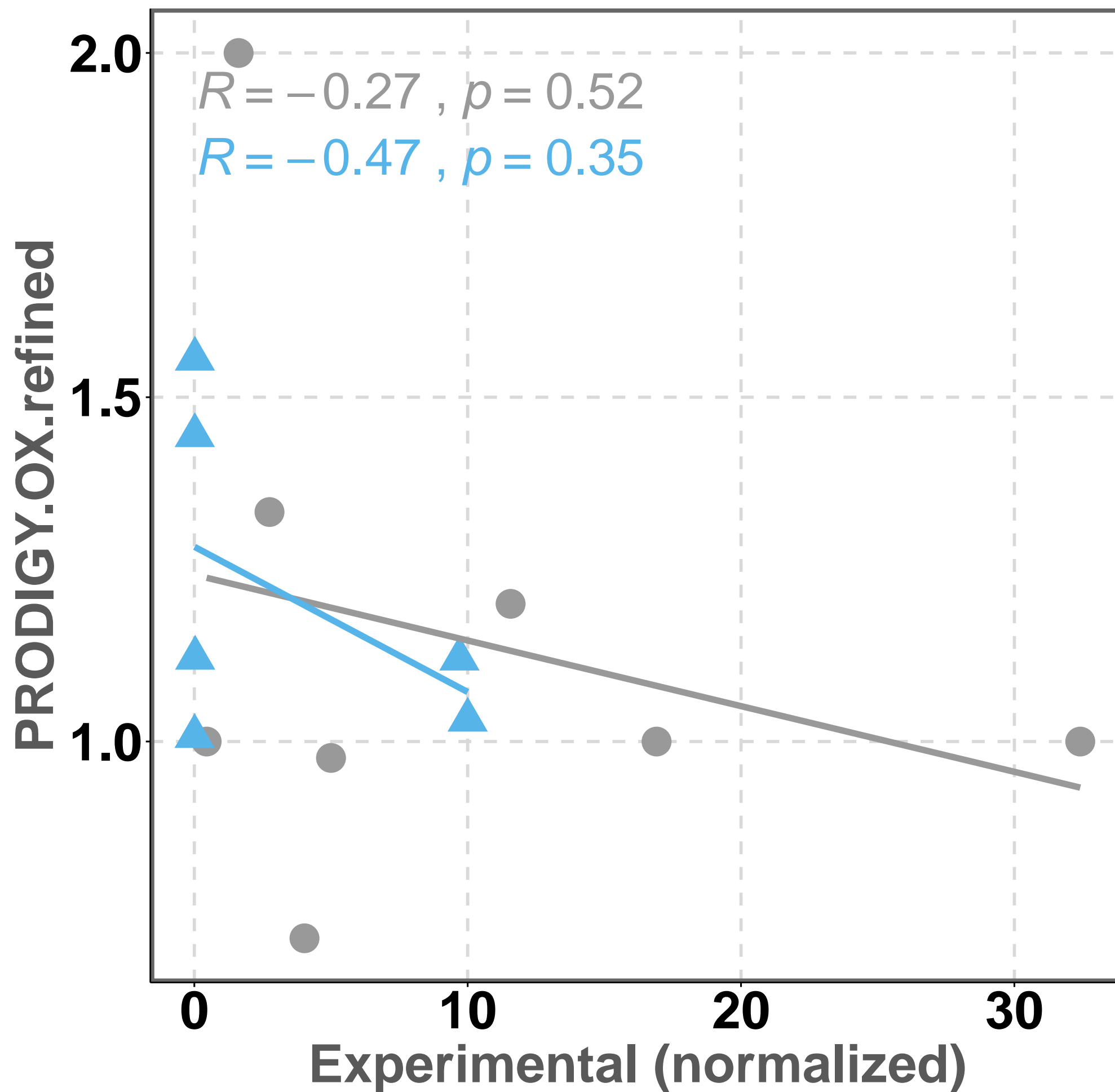


kinetics IC50 Kd Ki





kinetics IC50 Ki



kinetics IC50 Kd Ki

