VCell Tutorial

PH-GFP binding to PIP2 and IP3

Create a biomodel and 3D spatial (PDE) application to simulate pleckstrin homology domain (PH-GFP) reporter of PIP_2 to IP_3 conversion.

In this tutorial...

- Create a biomodel with reactions involving membrane and volume species.
- Create a compartmental (ODE) application that uses events to include time-dependent triggers.
- Create a spatial deterministic (PDE) application of a model using analytic equations to create a 3D geometry
- Define initial concentrations that are non-uniform in space and create timed events in spatial models using Boolean expressions
- Create output functions for more complex analysis of simulation results, e.g. to sum all fluorescent species in a compartment.

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BIOMODEL: PIP2toIP3Tutorial (Wed Jul 08 16:37	7:27 EDT 2015) VCell 6.0 (build 3)	
File View Server Tools Help		
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BIOMODEL: PIP2toIP3Tutorial (Wed Jul 08 16:	37:27 EDT 2015) VCell 6.0 (build 3)	
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BIOMODEL: PIP2toIP3Tutorial (Wed Jul 08 16:37:27 EDT 2015) VCell 6.0 (build 3)										
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-BIOMODEL: PIP2IB3Tutorial (Thu Jul 09 11:57:01 EDT 2015) -- VCell 6.0 (build 4)

File View Server Tools Help

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BIOMODEL: PIP2IB3Tutorial (Thu Jul 09 11:57:01 EDT 2015) -- VCell 6.0 (build 4) File View Server Tools Help P Cimulati Structures (5) 23 Results for Simulation Simulation0 Species (6) X Axis: Molecules (0) IP3_PHGF... PH_GFP_Cyt_PIP2_PHG... t IP3_Cyt PIP2_PM Observables (0) 63 t • 0 0.1 120000 Applications (2) tatus 2.261572... 0.99999906 Y Axis: 2.261576... 9.999977... 3.256668.... 120000 d/dt Spatial = yes Display Options: 2.315854... 0.09976882 2.311801... 0.99904207 3.3330934 119996.67 对 Geometry Other 9.694619... 3.126403... 3.053806... 0.98719854 44.705844 119955.29 💕 Specifications Reactions 1.655835... 8.532420... 1.467579.... 0.93519956 229.88749 119770.11 Protocols Species 4.175484.... 6.870576... 3.129423... 0.84884602 549.71481 119450.29 A² Simulations d/dt Steady State 5.379743... 4.620256... 0.75208447 7.510314... 925.11965 119074.88 Act.delay 对 Geometry 0.10845145 4.398917... 5.601082... 0.67049821 1254.3163 118745.68 Act.triggerFunction 💕 Specifications 0.14179974 3.739349.... 6.260650.... 0.60066669 1544.3359 118455.66 Inact.delay Protocols 0.17514804 6.709782... 0.54027292 1800.7223 118199.28 3.290217... 🔏 Simulations 3_Cyt 2.22783835 2.853362... 7.146637... 0.46019728 2147.9391 117852.06 \land Parameter Estima P3 PHGFP Cvt 2.602782... 7.397217... 0.38693164 2472.4661 0.28786529 117527.53 AV J IP3PH VCell DB BioModels.net Pathway 0.34789223 Simultaneously hold down on "ctrl" on your keyboard J_PIP2_PH 0.407919 MathModels Geometr J_r2 and click "IP3 Cyt", "IP3 PHGFP Cyt", "PH GFP Cyt", BioModels KFlux_PM_Cyt 0.49192994 Search "PIP2 PHGFP PM", and "PIP2 PM". Kr_IP3PH 0.59192594 📃 Biological Models My BioModels (astfh234) (9) 192994 2.991073... 7.008926... 0.1549261 3554.3254 116445.67 GFP_Cyt 3.234741... 0.79192994 0.13267299 3667.5606 116332.44 PIP2 PHGFP_PM 6.765258.... E Public BioModels (514) PIP2_PM 0.89192994 3.481850.... 6.518149... 0.11675496 3751.8989 116248.1 🗄 🧰 Tutorials (5) 0.10530523 0.99192994 3.722828... 6.277171... 3815.463 116184.54 Education (33) UnitFactor_uM_um3_molecules_neg_1 🗄 💼 Tutorial VCell 6.0 (Rule-base 1.0919299 3.951689.... 6.048310... 9.701402... 3863.9855 116136.01 9.096095... 1.1919299 4.164900.... 5.835099... 3901.5253 116098.47 1.2919299 5.639348.... 8.649892... 116069.03 4.360651.... 3930.9673 1.3919299 4.538349.... 5.461650... 8.317285... 3954.3715 116045.63 1.4919299 0.04698234 0.05301766 8.066254... 3973.2174 116026.78 1.5919299 4.841088.... 5.158911... 7.874238... 3988.5756 116011.42 1.6919299 4.968027... 5.031972... 7.725304... 4001.228 115998.77

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-BIOMODEL: PIP2IB3Tutorial (Thu Jul 09 11:57:01 EDT 2015) -- VCell 6.0 (build 4) File View Server Tools Help A Simulations 🐋 Geometry Specifications Protocols 💮 Structures (5) 💿 Species (6) Simulations Output Functions Generated Math Molecules (0) Observables (0) 63 Applications (2) End Time Output Option Solver **Running Status** Results Name ⊨ d/_{dt} Spatial 对 Geometry 💕 Specifications Go to simulations and click Protocols the add simulation icon. 𝗚 Simulations d/dt Steady State 🐹 Geometry 🕼 Specifications Protocols A Simulations Parameter Estimation AV VCell DB BioModels.net Pathway Comm Sabio BioModels MathModels Geometries 🕀 Search 🛅 Biological Models Shared BioModels (0) Public BioModels (514) Tutorials (5) Education (33) Tutorial VCell 6.0 (Rule-based) (7) AV Object Properties Problems (0 Errors, 1 Warnings) Network Generation Status Select only one object (e.g. species, reaction, simulation) to view/edit properties.



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File View Server Tools Help

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BIOMODEL: PIP2IB3Tutorial (Thu Jul 09 13:29:23 EDT 2015) -- VCell 6.0 (build 4)





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