

# Using the PubMed Abstract Sifter for Computational Modeling of Complex Biological Processes

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PRESENTATION TO IMAG – MSM WORKING GROUP

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*Does not necessarily represent US EPA policy.*

# Acknowledgments

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- Tom Knudsen and the Virtual Tissues Modeling project
- CCTE management and scientists

# The problem – lots of publications

**Aerosol  
transport  
modeling:  
2K PubMed  
citations**

ange and Aelurostrongylidosis in Two Domestic  
rasiticide products combining fipronil and (S)-m  
of Pesticide Exposures in Domestic Dogs and Th  
ile of fipronil and efficacy against flea and tick i  
ectoparasiticide purchases from veterinary clinic  
field study to assess the efficacy and safety of l  
ea Abundance on Black-Tailed Prairie Dogs: Pote  
v dose fipronil bait in reducing black-tailed prairie dog (*Cynomys ludovicianus*) fleas at reduced a  
ecticide-rodenticide product on ectoparasite and commensal rodent mortality.  
y flea products in widespread pesticide contamination of English rivers.  
ecommendations for ectoparasiticide

**Chagas disease:  
20K PubMed  
citations**

Recent Advancements in the Control of Cat Fleas.  
Does bathing affect tick and flea burdens and ectoparasiticide e  
Fleas infesting cats and dogs in Great Britain: spatial distribution  
Manag  
Investi  
Evalua  
Efficac  
Efficac  
Synerg  
Evalua  
Field Effectiveness and Safety of moxidectin plus sarolaner (Bravecto® Plus) against ticks and fleas: a European randomize  
Evaluation of an 11.2% spinetoram topical spot-on solution for the control of experimental and natural flea (*Ctenocephalid*

**Epiblast:  
33K PubMed  
citations**

**Chondrogenesis:  
9K PubMed  
citations**

les as ectopa  
y: Insight into  
ir Tick (Acari:  
moxidectin  
plus sarolaner for the control of fleas and ticks infesting cats in Japan.  
tors Against Larval Cat Fleas (Siphonaptera: Pulicidae).  
lack-Tailed Prairie Dogs: Encouraging Long-Term Results with Systemic O

Where to  
start?

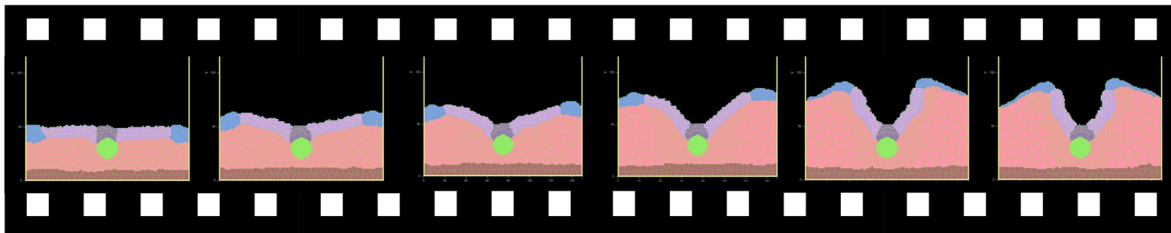
# Ontologies: *computational systems model for retinoic signaling during neurulation*

## Literature review

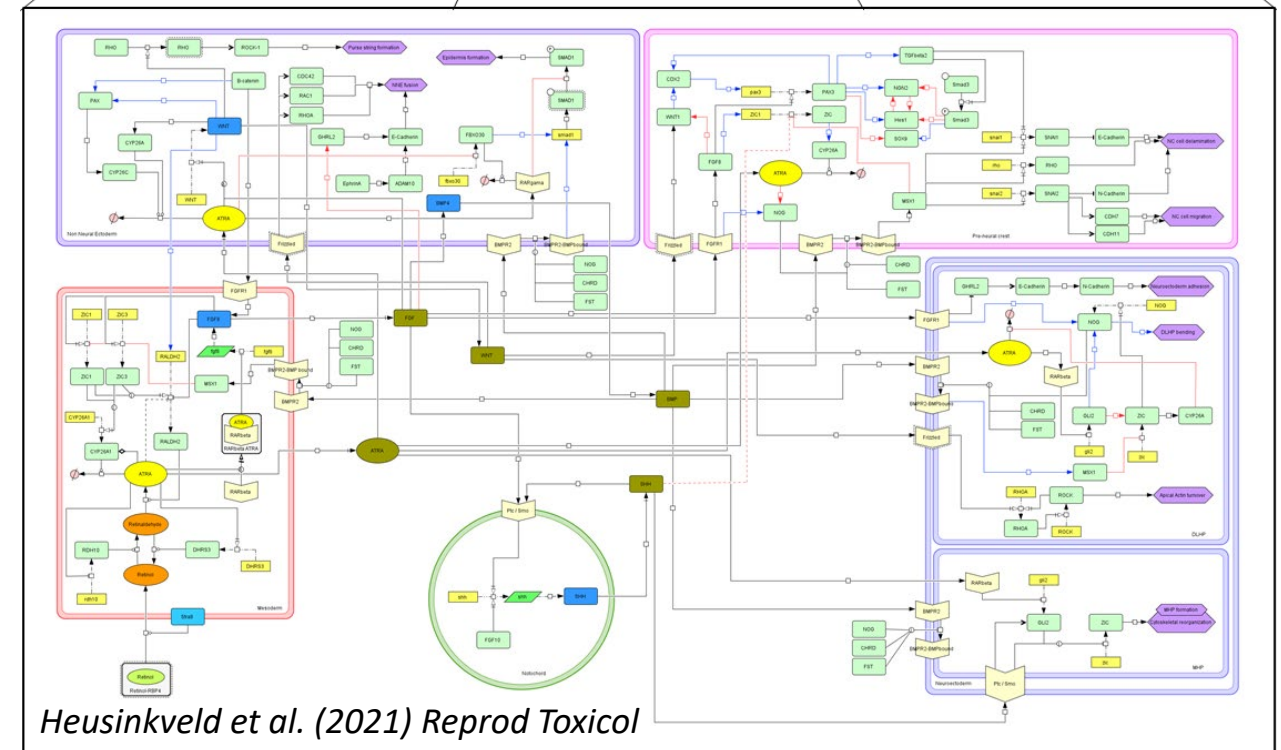
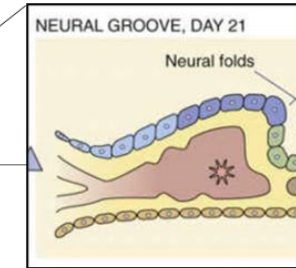
- Physiological information
- Cellular compartments
- Biochemical gradients
- Critical cell fate and behavior
- Reduced to the essence

## Systems biology map

- Useful for AOP elucidation
- Starting point for *in silico* simulation



Job Berkhout, RIVM (work in progress, [compucell3d.org](http://compucell3d.org) prototype)



Heusinkveld et al. (2021) *Reprod Toxicol*

# Today — information retrieval to support rapid model construction

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1. Show how with the Abstract Sifter you can take a biological corpus and explore the gene and protein players. (In an unbiased way)
2. Show how you can take a complex list of gene or protein players and find their relationships to each other, both in your biological context and outside it.
3. Show how you can take a set of genes or proteins of interest to your group and measure their occurrence in your biological corpus.
4. Show how you can find chemicals that perturb players in your network and investigate their downstream adverse effects.

# But first ...

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The PubMed Abstract Sifter is a free tool downloadable from the Comptox Chemicals Dashboard (CCD):

<https://comptox.epa.gov/dashboard/downloads>