

## **Supplementary Information**

### **SAR Monitoring of Evolving Compound Data Sets Using Activity Landscapes**

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<sup>#</sup>The contributions of these authors should be considered equal.

### **Supplementary Figures S1-S3**

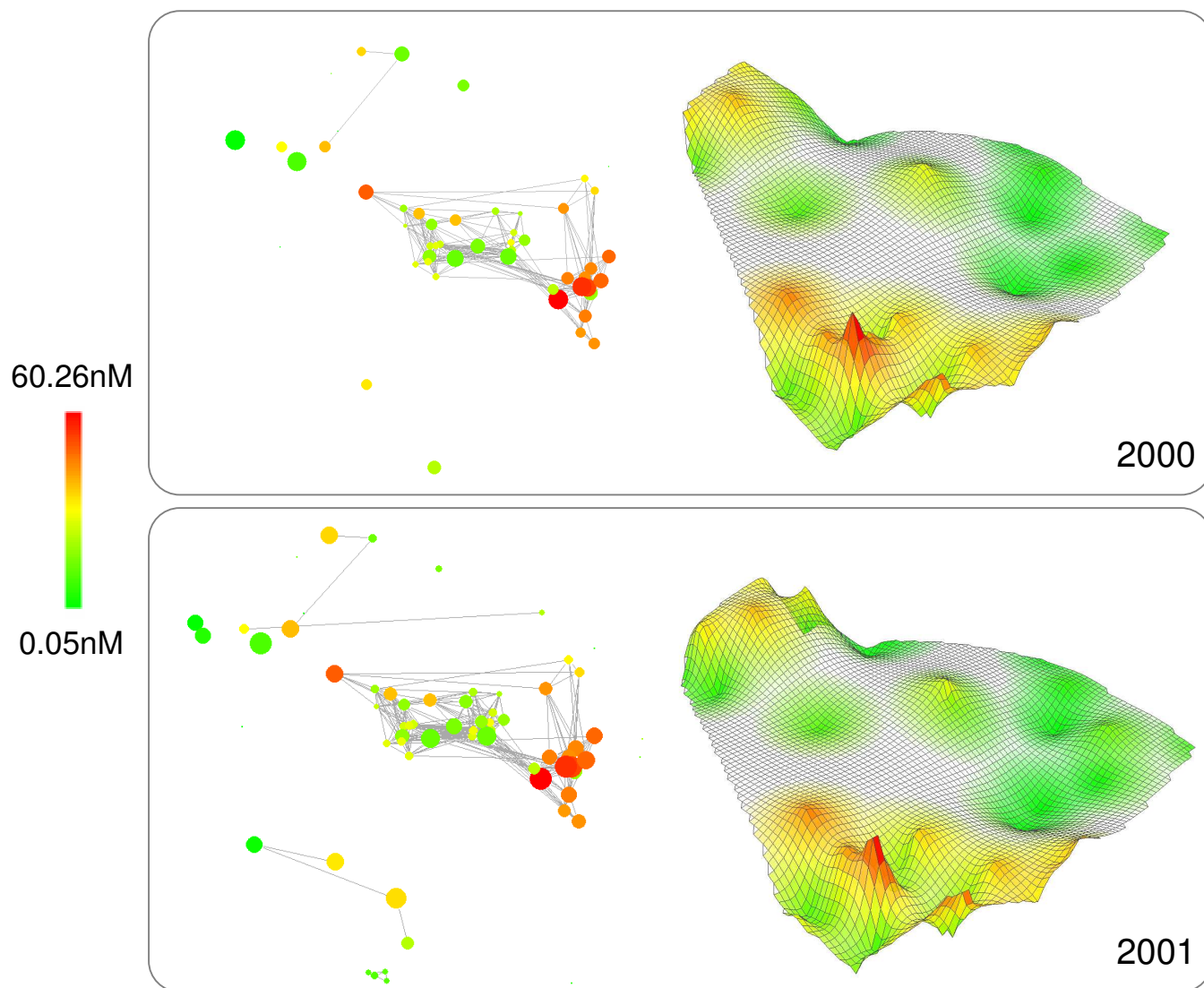
## Supplementary Figure Legends

**Figure S1. Activity landscape representations of the AA2 data set.** NSGs and 3D activity landscapes are shown for each year from 2000 to 2007. These activity landscapes are representative of the evolution of the data set between 2000 and 2007. For landscape display, the potency color code was adjusted to the potency range covered by all three data sets (shown on the left), which provided a constant node color scheme for all activity landscape representations.

**Figure S2. Activity landscape representations of the LCK data set.** NSGs and 3D activity landscapes are shown for each year from 2000 to 2007. These activity landscapes are representative of the evolution of the data set between 2000 and 2007. For landscape display, the potency color code was adjusted to the potency range covered by all three data sets (shown on the left), which provided a constant node color scheme for all activity landscape representations.

**Figure S3. Activity landscape representations of the MOR data set.** NSGs and 3D activity landscapes are shown for each year from 2003 to 2007. These activity landscapes are representative of the evolution of the data set between 2003 and 2007. For landscape display, the potency color code was adjusted to the potency range covered by all three data sets (shown on the left), which provided a constant node color scheme for all activity landscape representations.

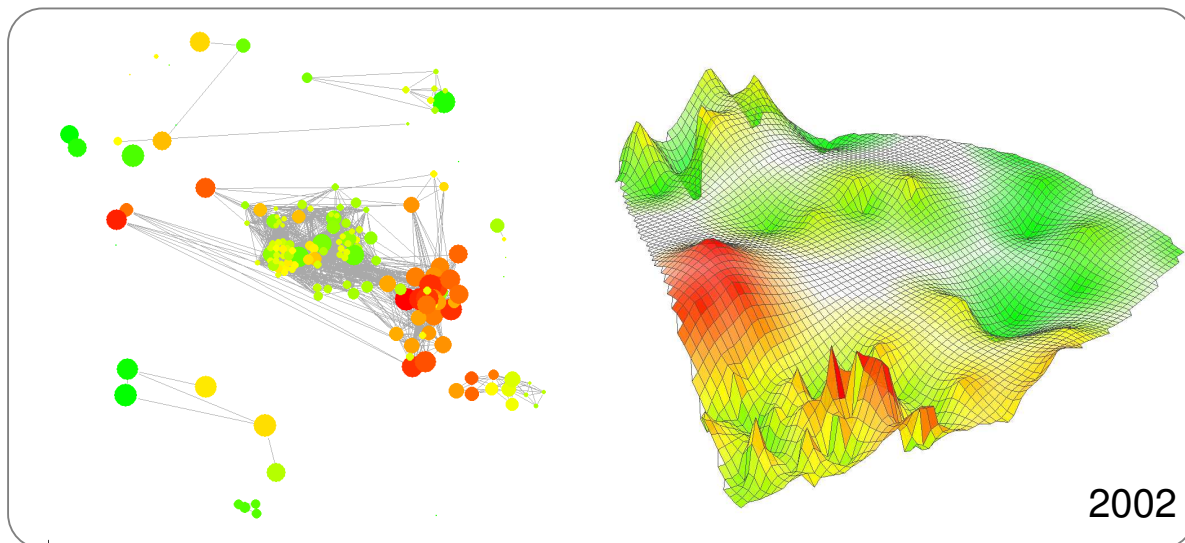
**Figure S1**



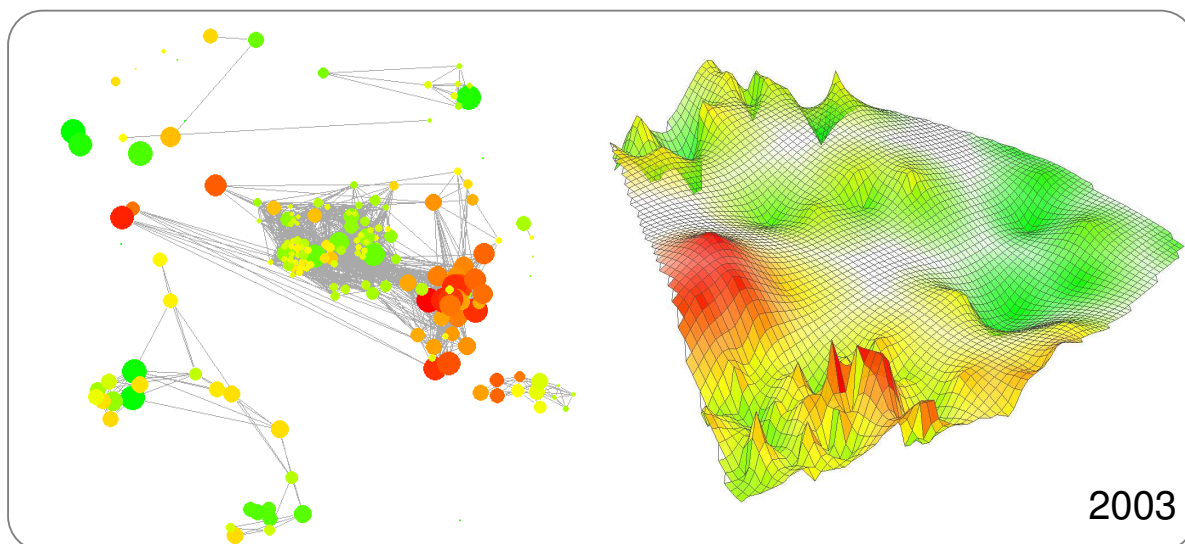
60.26nM



0.05nM



2002

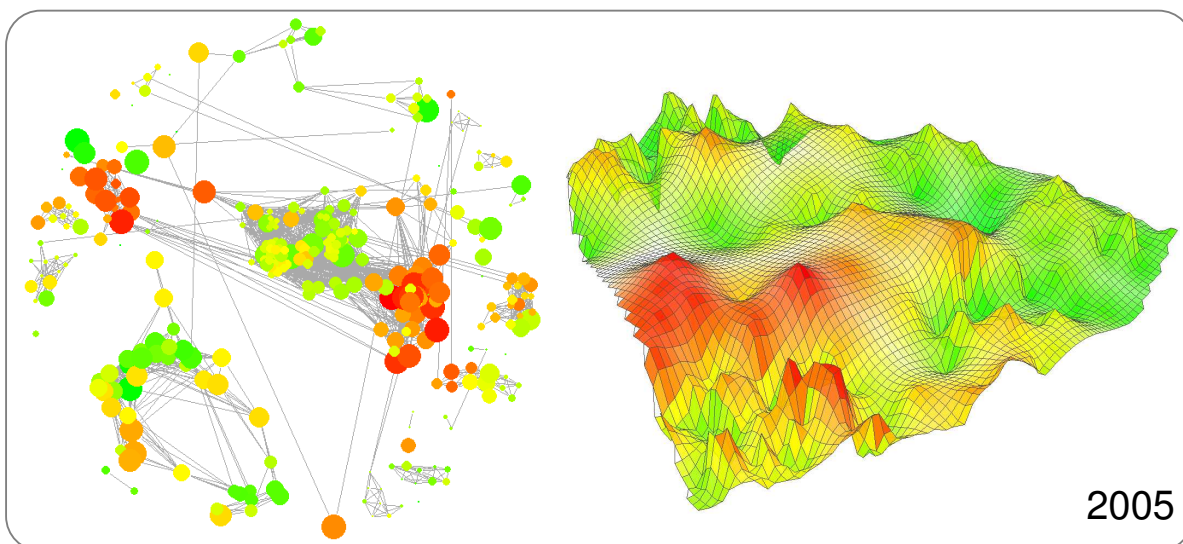
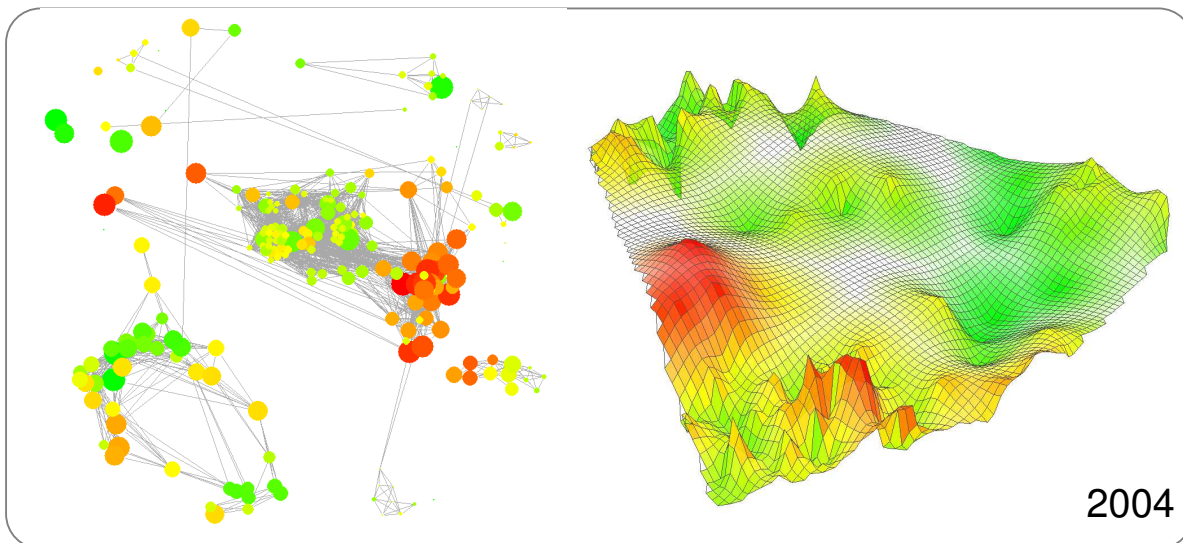


2003

60.26nM



0.05nM

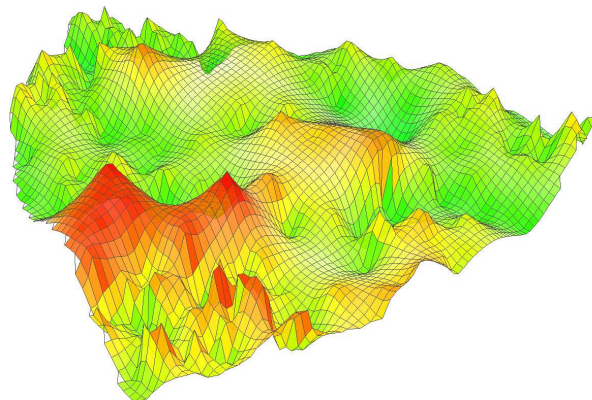
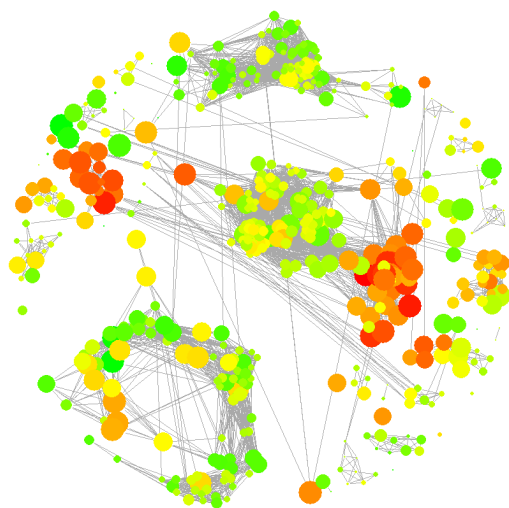




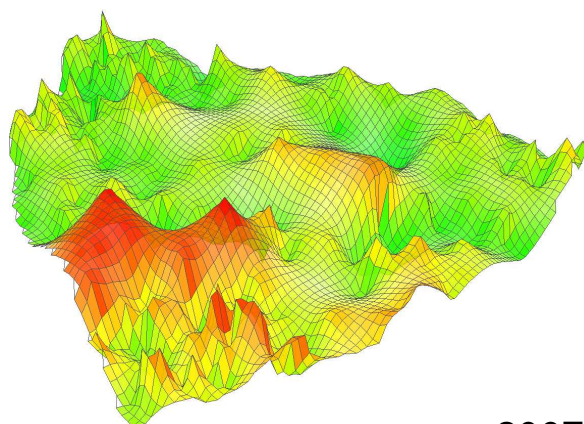
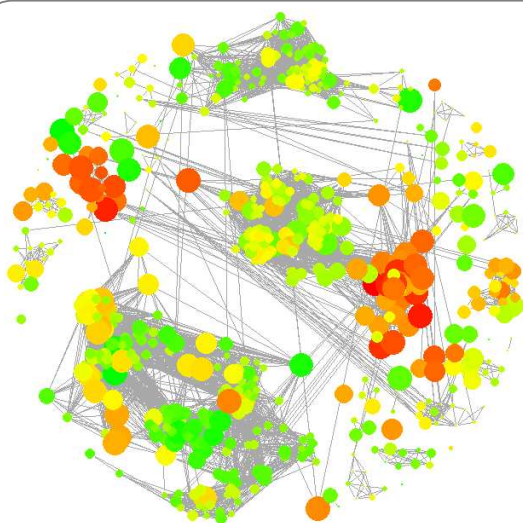
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0.05nM

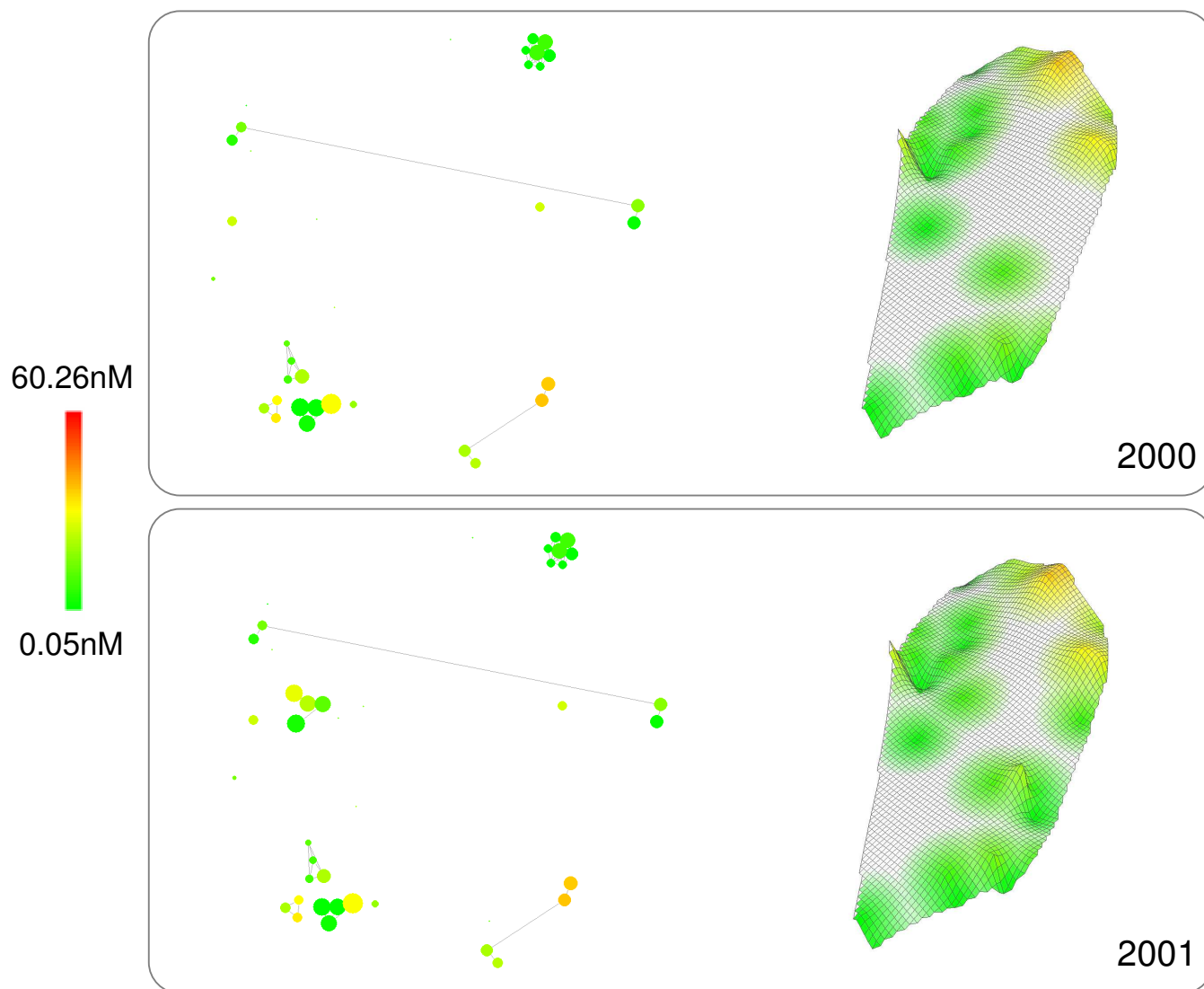


2006



2007

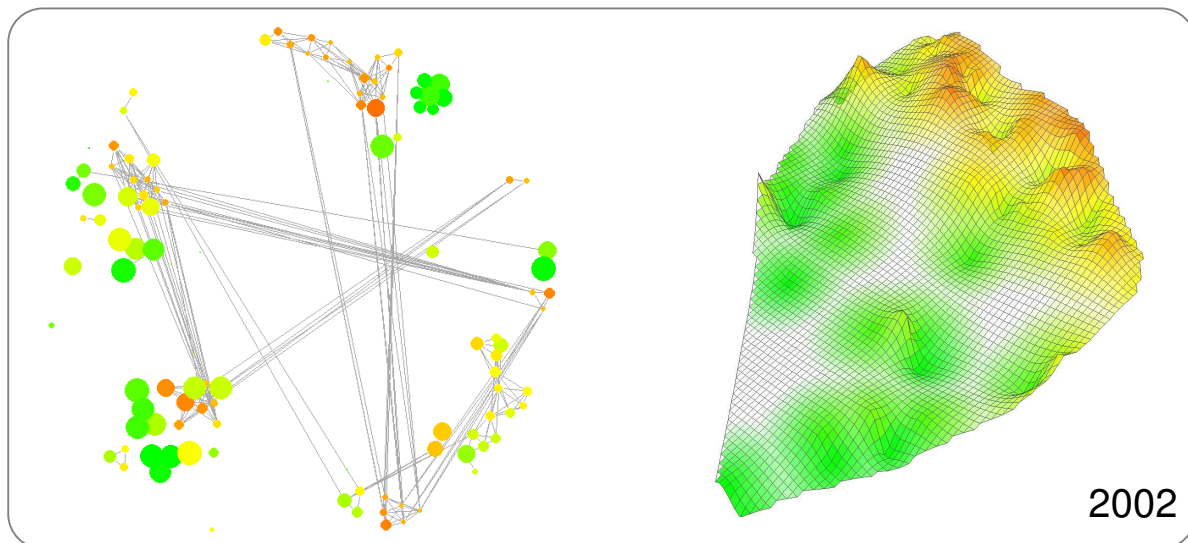
Figure S2



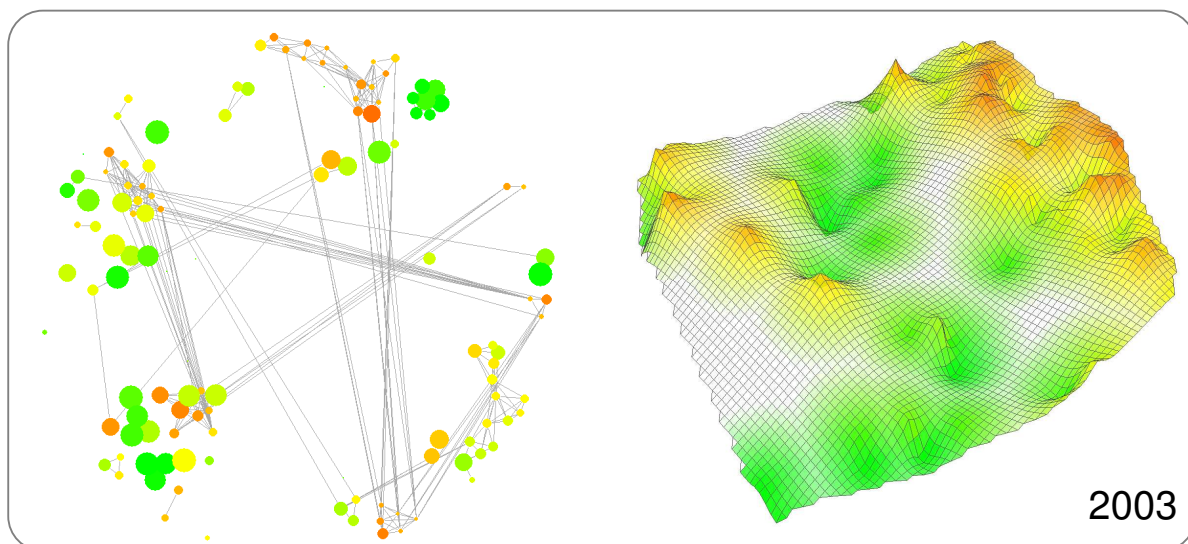
60.26nM



0.05nM



2002



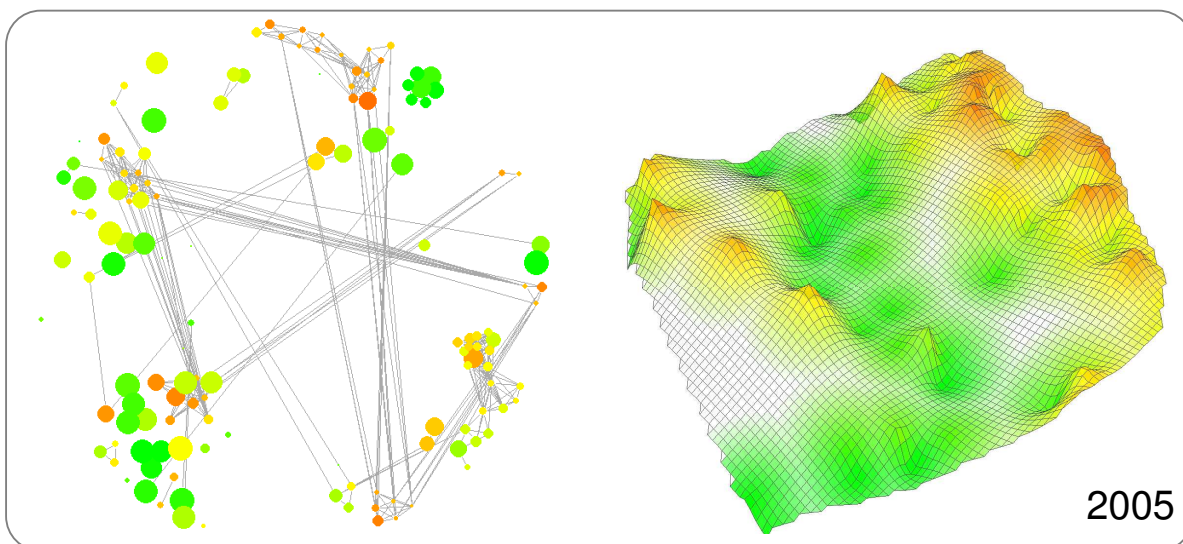
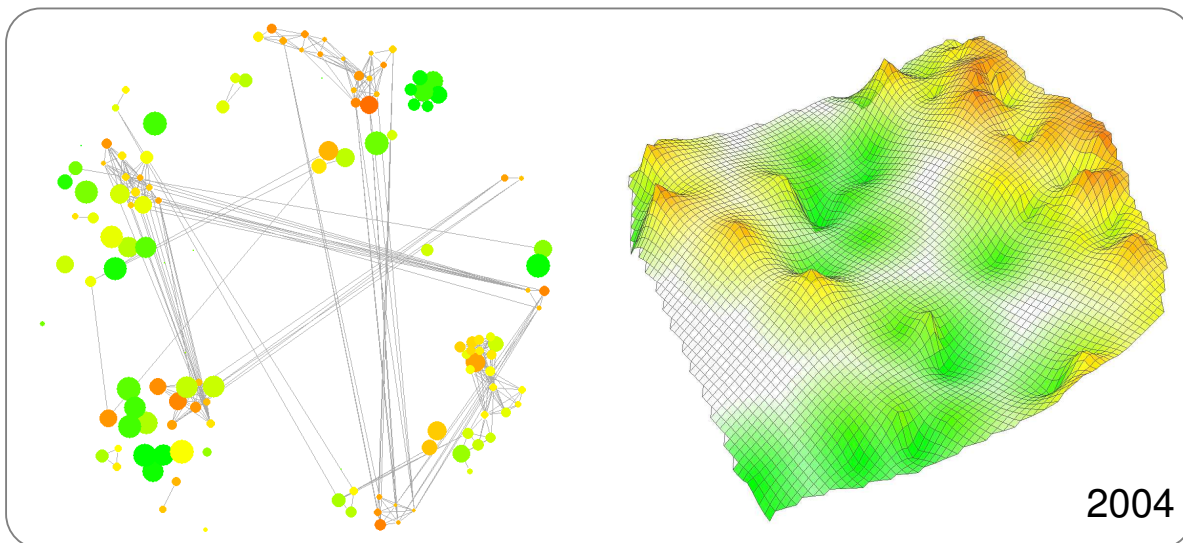
2003



60.26nM



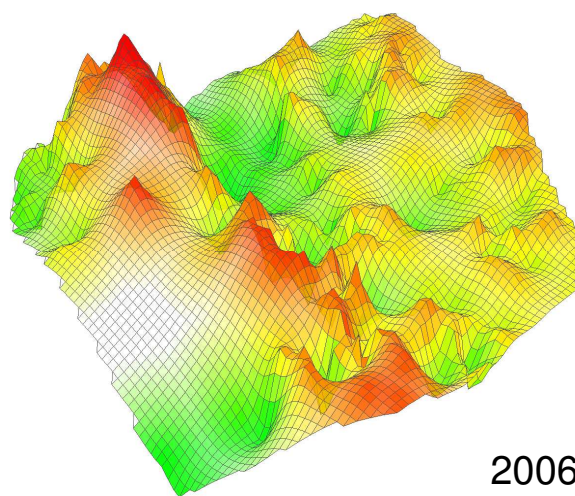
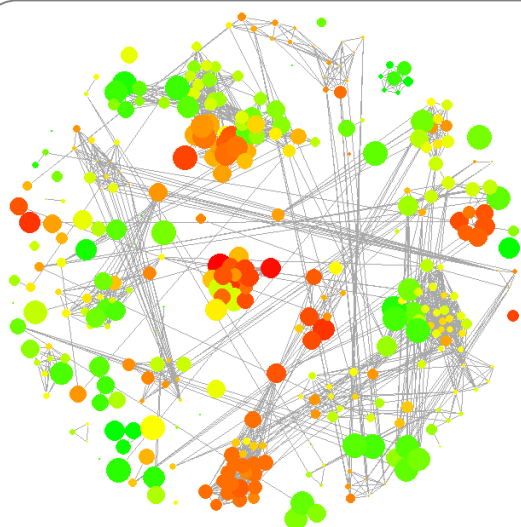
0.05nM



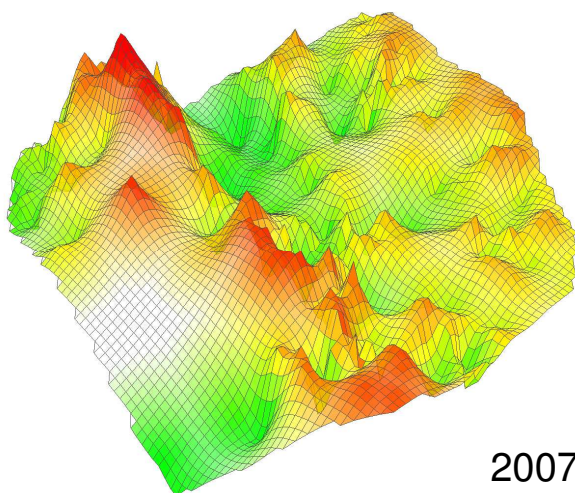
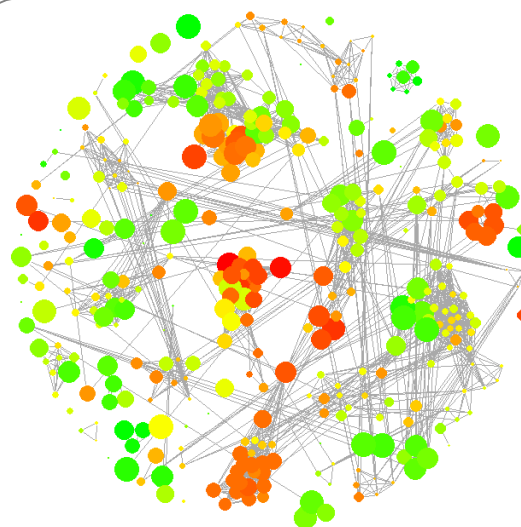
60.26nM



0.05nM

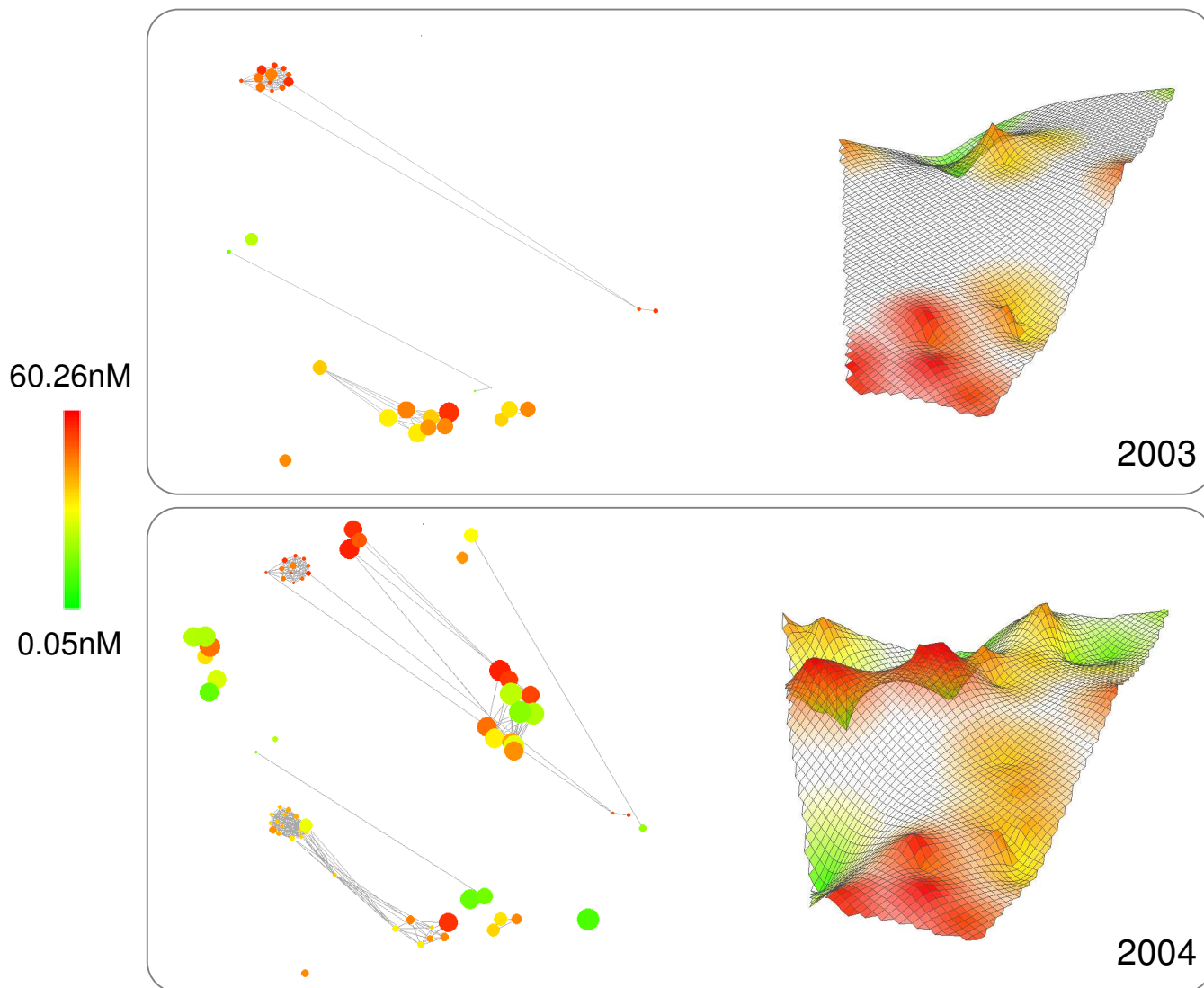


2006



2007

**Figure S3**

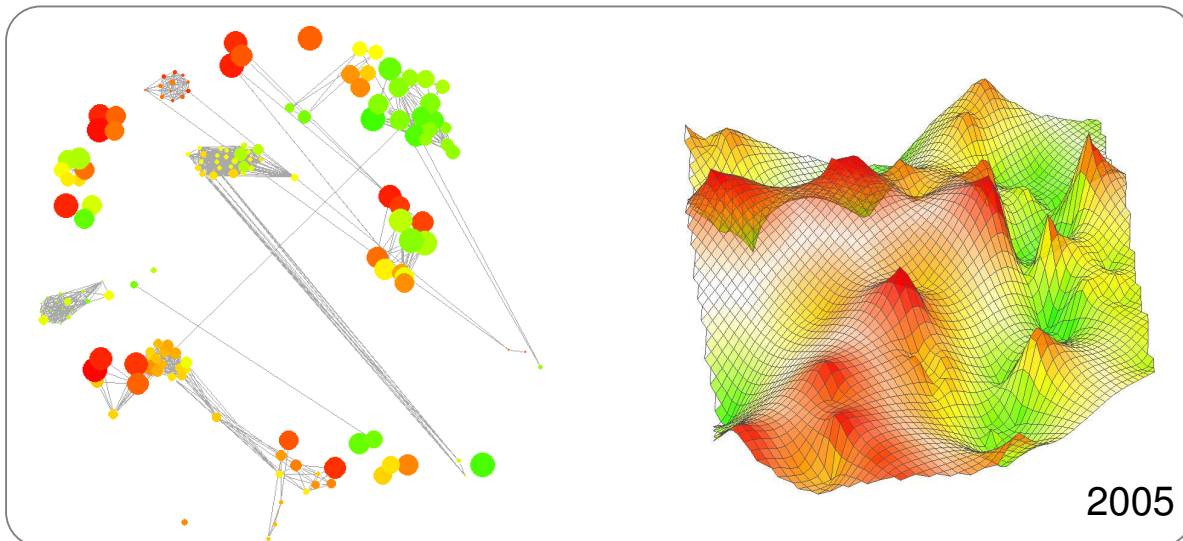




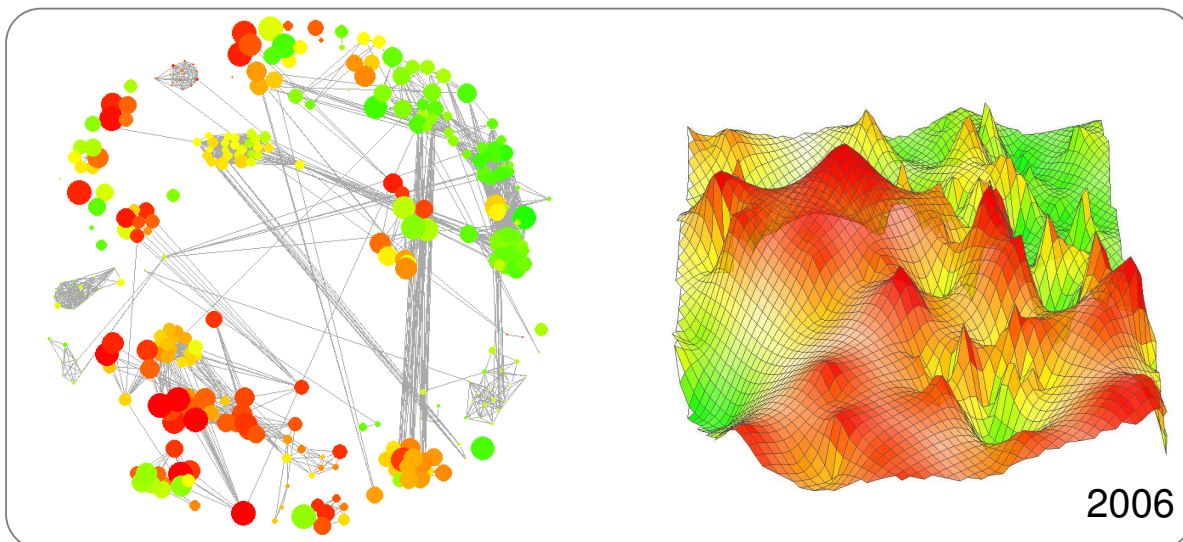
60.26nM



0.05nM



2005

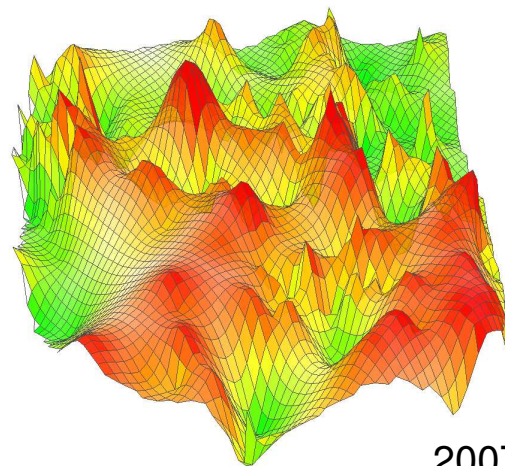
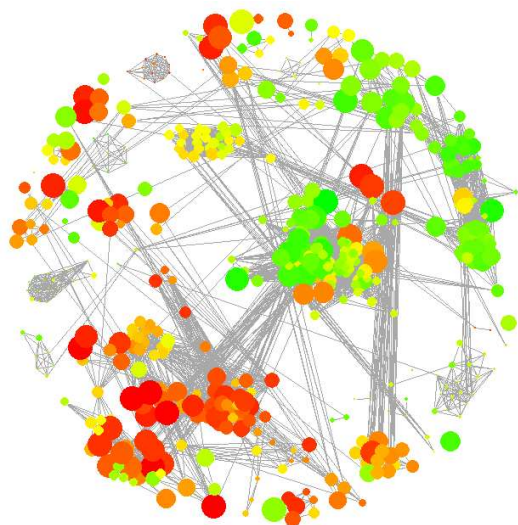


2006

60.26nM



0.05nM



2007