

Why plain QSAR is not enough for me...

Egon Willighagen 

Published September 16, 2007

Citation

Willighagen, E. (2007, September 16). Why plain QSAR is not enough for me... *Chem-bla-ics*.
<https://doi.org/10.59350/s8dts-h8t13>

Keywords

Qsar

Abstract

Amanda had a very nice post on Small molecules that modulate quorum sensing. It's the perfect read for a Sunday morning, when you have a view looking down on Strasbourg from a hill in the Black Forrest. Biology fascinates me, particularly when small molecules are involved. And the molecular signaling used by these bacteria is just delightful. Make sure to read up on the small squids in 96-well plates too! (And we are worried about varkensflats!)

Copyright

Copyright © Egon Willighagen 2007. Distributed under the terms of the [Creative Commons Attribution 4.0 International License](#), which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.

[Amanda](#) had a very nice post on [Small molecules that modulate quorum sensing](#). It's the perfect read for a Sunday morning, when you have a view looking down on Strasbourg from a hill in the [Black Forrest](#). Biology fascinates me, particularly when small molecules are involved. And the molecular signaling used by these bacteria is just delightful. Make sure to read up on the small squids in 96-well plates too! (And we are worried about [varkensflats](#)! That's put in perspective :) These very small squids have a symbiosis with bacteria that light up under certain conditions, and this squid species learned how to control that lightning. Nerdy facts like this adds that coolness factor that outliers in QSAR lack.

Small-molecule macroarrays

Another bit in Amanda's blog caught my eye too: the small-molecule macroarray. I had not seen that term before, and looked up the paper by Brown et al. *Rapid Identification of Antibacterial Agents Effective against Staphylococcus aureus Using Small-Molecule Macroarrays* (DOI:[10.1016/j.chembiol.2007.03.006](https://doi.org/10.1016/j.chembiol.2007.03.006)). Like the more famous (gene expression) microarray, this SMMs are arrays of wells where small molecules are connected to a planer cellulose support system, after which the antibacterial activity can be measure. Now, I do have to read up on this technology. For example, are the small-molecule inhibitors released into the assay medium at some point? That is, they will need to find their way to whatever protein it inhibits, as the protein will not go to the support system. Can anyone explain me how to inhibition takes place?