



NOVAMECHANICS

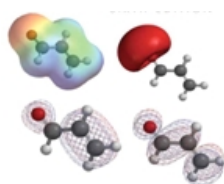
Chemoinformatics & Bioinformatics Solutions

[www.novamechanics.com](http://www.novamechanics.com)

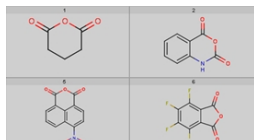
email: [info@novamechanics.com](mailto:info@novamechanics.com)

### Nano Chemo informatics Workflows

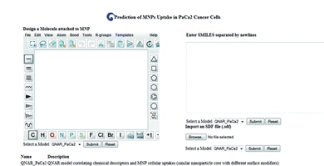
#### Advanced Modeling & Simulation Techniques



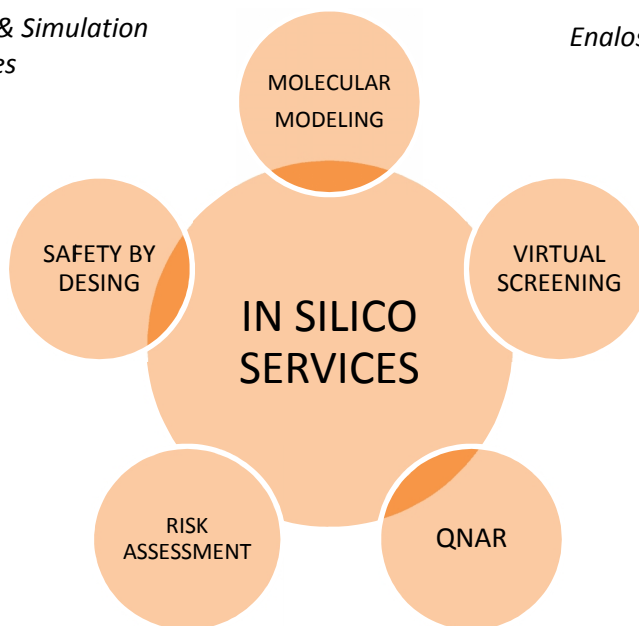
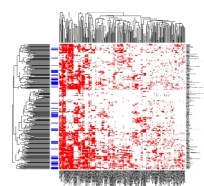
#### Data Mining Chemical Space Search



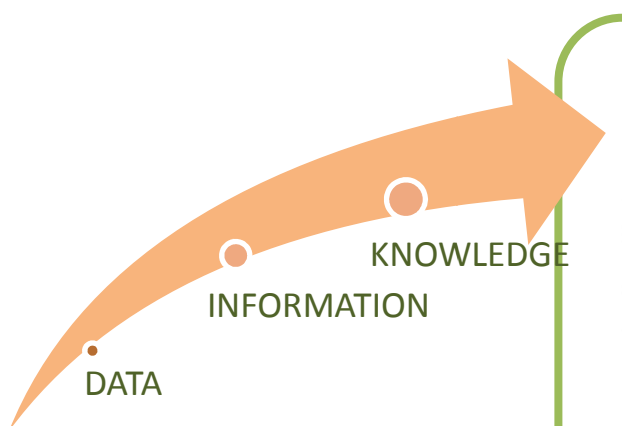
#### Enalos In Silico Nanopatform



#### Read Across



#### Computer aided nanoparticle design



### PREDICTIVE MODELS RELEASED ONLINE THROUGH ENALOS INSILICONANO PLATFORM



- ✓ Ready-to-use applications
- ✓ User friendly environment

1) Online decision support tool for the virtual screening of cellular uptake of nanoparticles with different surface modification<sup>1</sup>

[http://enalos.insilicotox.com/QNAR\\_PaCa2/](http://enalos.insilicotox.com/QNAR_PaCa2/)

2) Online predictive classification model for the toxicological assessment of iron oxide nanoparticles with different core, coating and surface modification<sup>2</sup>

[http://enalos.insilicotox.com/QNAR\\_IronOxide\\_Toxicity/](http://enalos.insilicotox.com/QNAR_IronOxide_Toxicity/)

1. G.Melagraki, A. Afantitis, RSC Adv., 2014, 4:50713-50725
2. G.Melagraki, A. Afantitis, Curr Top Med Chem. 2015, DOI: 10.2174/1568026615666150506144536

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