CULGI

Chemistry Unified Language Interface

Solutions for Chemical Modelling

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# A Fragment-based Computational Approach to Study the Phase Behavior of Bio(polymers) and Drug Excipients

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## AUTOMATED FRAGMENTATION ENGINE

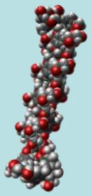
- Map from atoms to coarse-grained particles, and vice versa
- Can handle in principle any molecular architecture
- Based on a customizable scoring function (nr. of heavy atoms, bonding pattern, mass, etc.)

## CASE STUDY I. LIGNIN OLIGOMERS

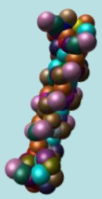
*"Bio-inspired polymers via extraction of natural compounds from renewable resources"*

BIO-MIMETIC Inspired by natural processes

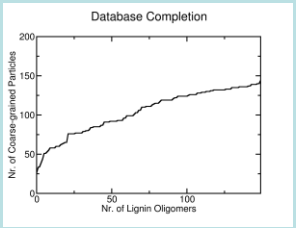
www.biomimetic-eu-project.eu



Atomic structure (493 atoms)



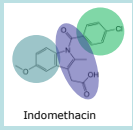
Coarse-grained structure (102 particles)



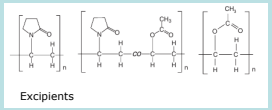

## CASE STUDY II. DRUG/EXCIPIENT INTERACTIONS

Lilly

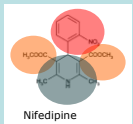
- Drug/Excipient phase behavior
- Compare computational methods



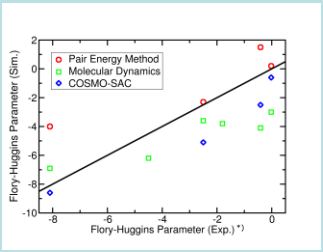
Indomethacin



Excipients



Nifedipine




*) Sun et al., *J. Pharm. Sci.* **2010**, 99, 4023

## CONCLUSIONS

- Fragmentation algorithm tested on database of >50.000 molecules (>99% success rate)
- Number of unique coarse-grained particles is limited to few thousands
- Coupled with quantum-based parameterization scheme to get to thermodynamics

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Culgi offers a suite of modeling and simulation algorithms from both thermodynamics and informatics, within an unique common interface. Our molecular modeling library includes all well-established simulation and chemical informatics methodologies

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