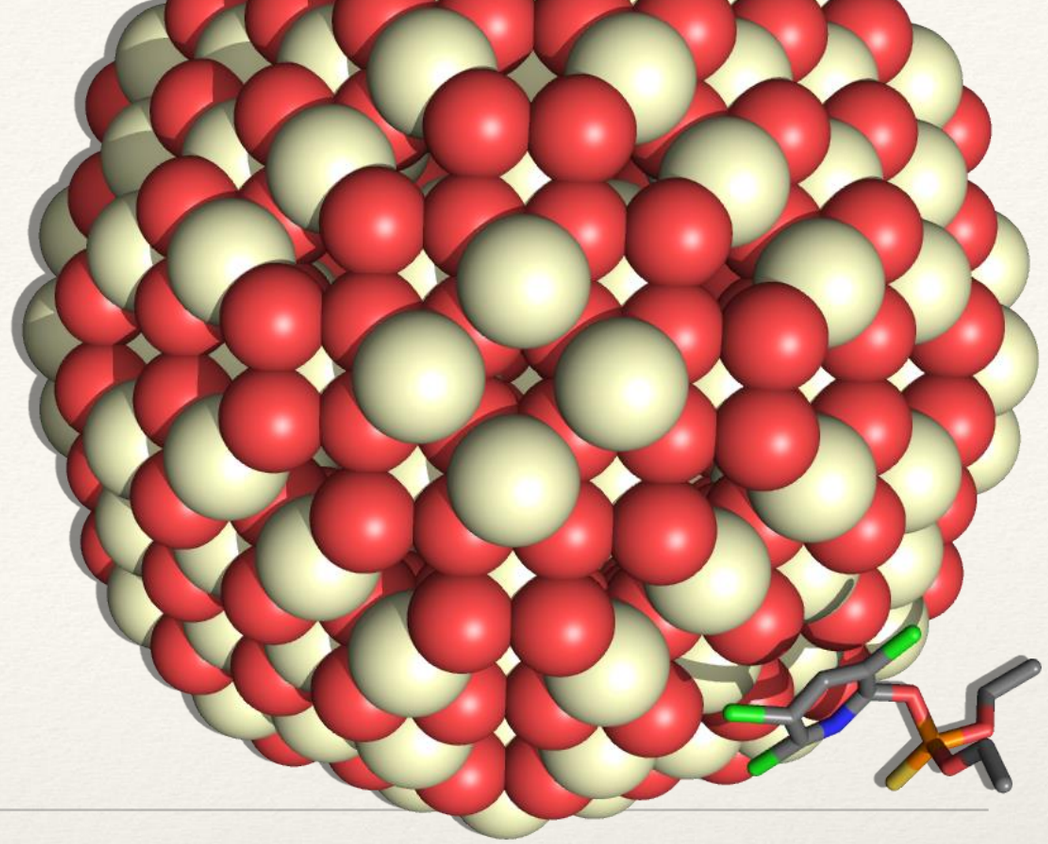

SNO 2016 Orlando, FL

Molecular Dynamic Screening for Nano Trojan Horses

Nick Geitner, PhD
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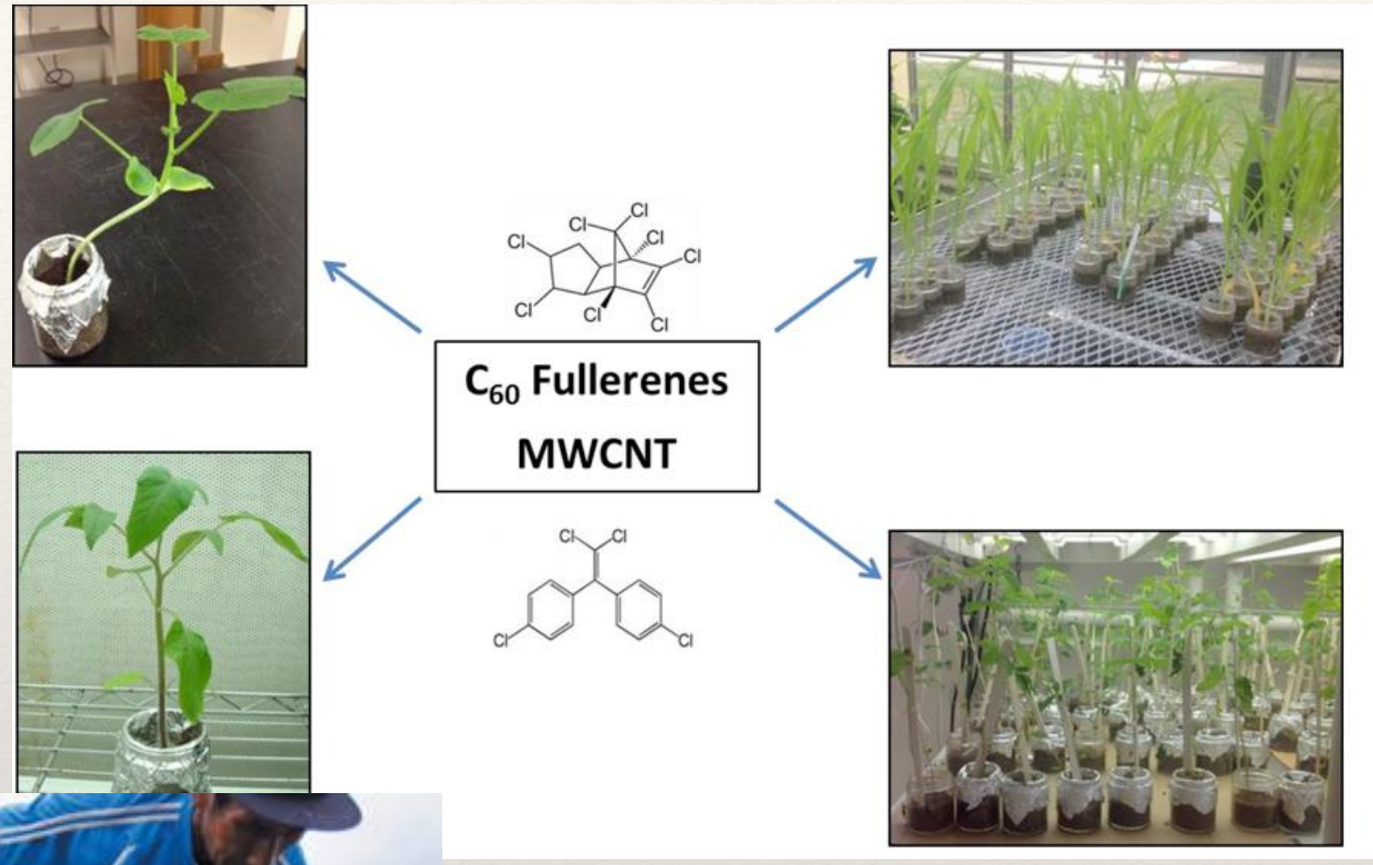
Importance of Nano in Agriculture



J White et al

Exposure Routes

Intentional

Pesticide Delivery

Soil Contaminant Remediation

Biomass Enhancement

Anti-Pathogen…

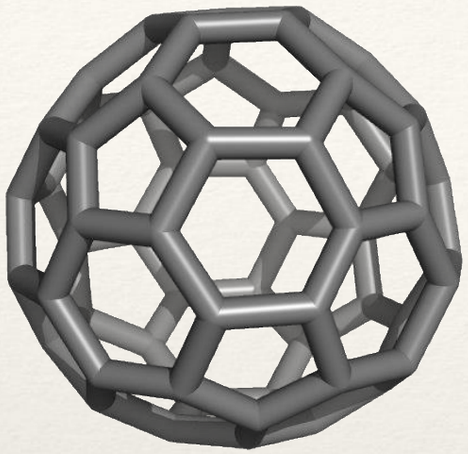
Incidental

Biochar

Air Deposition

Wastewater

A



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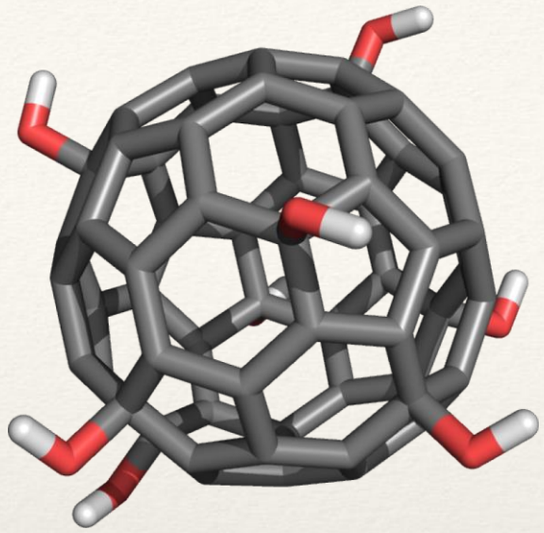

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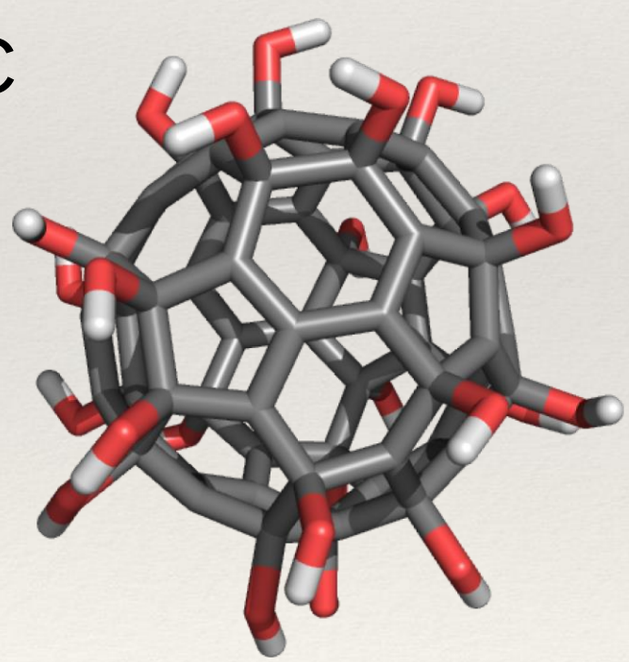
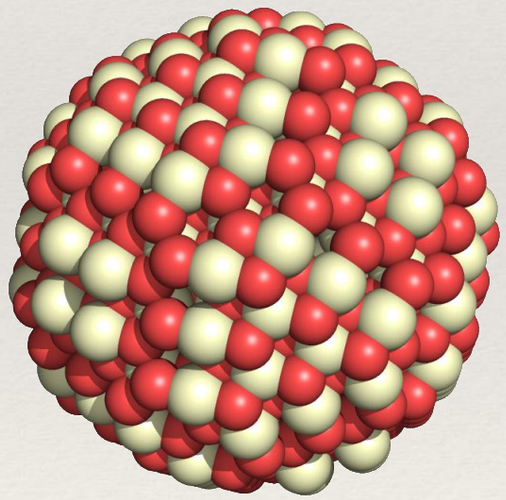
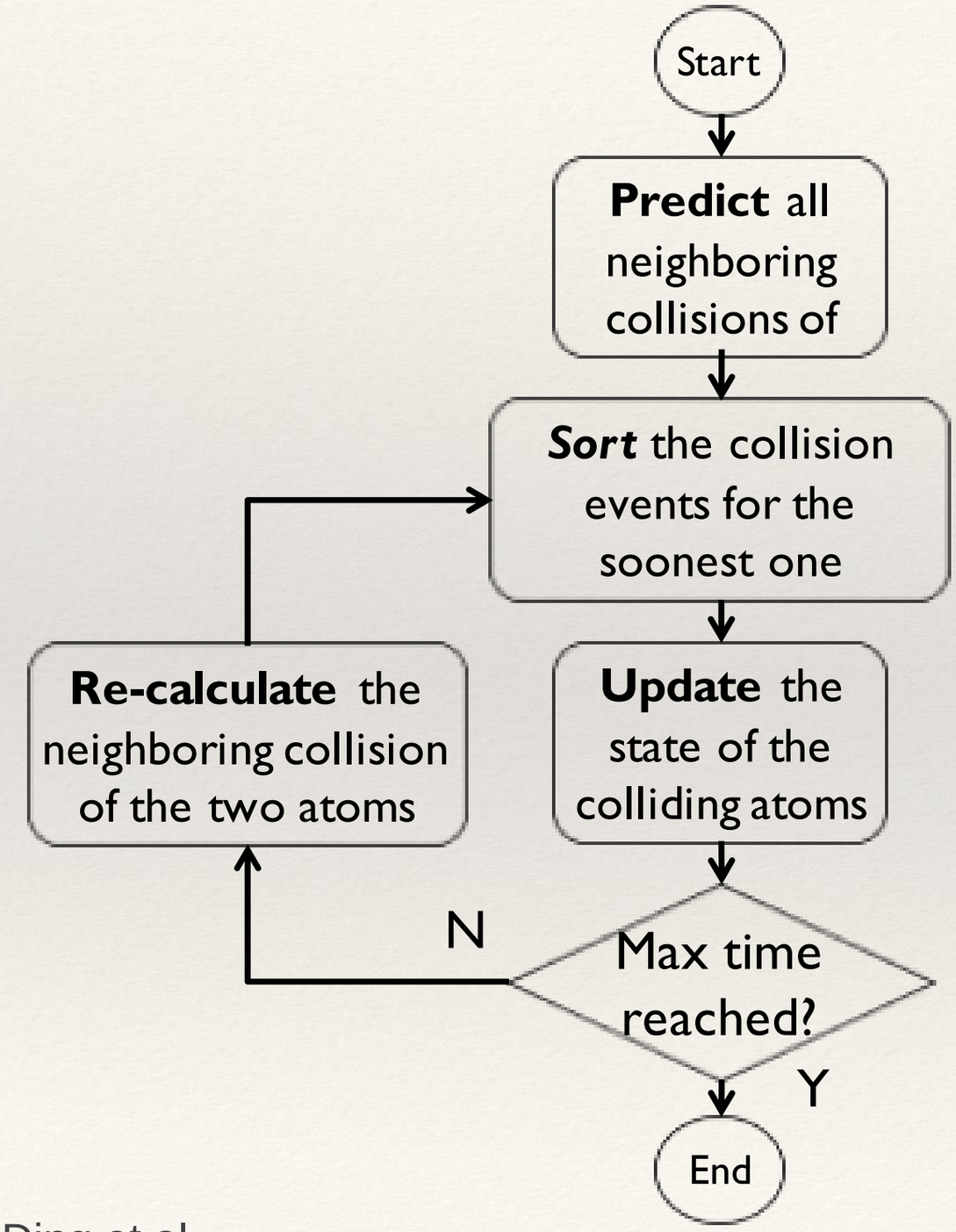


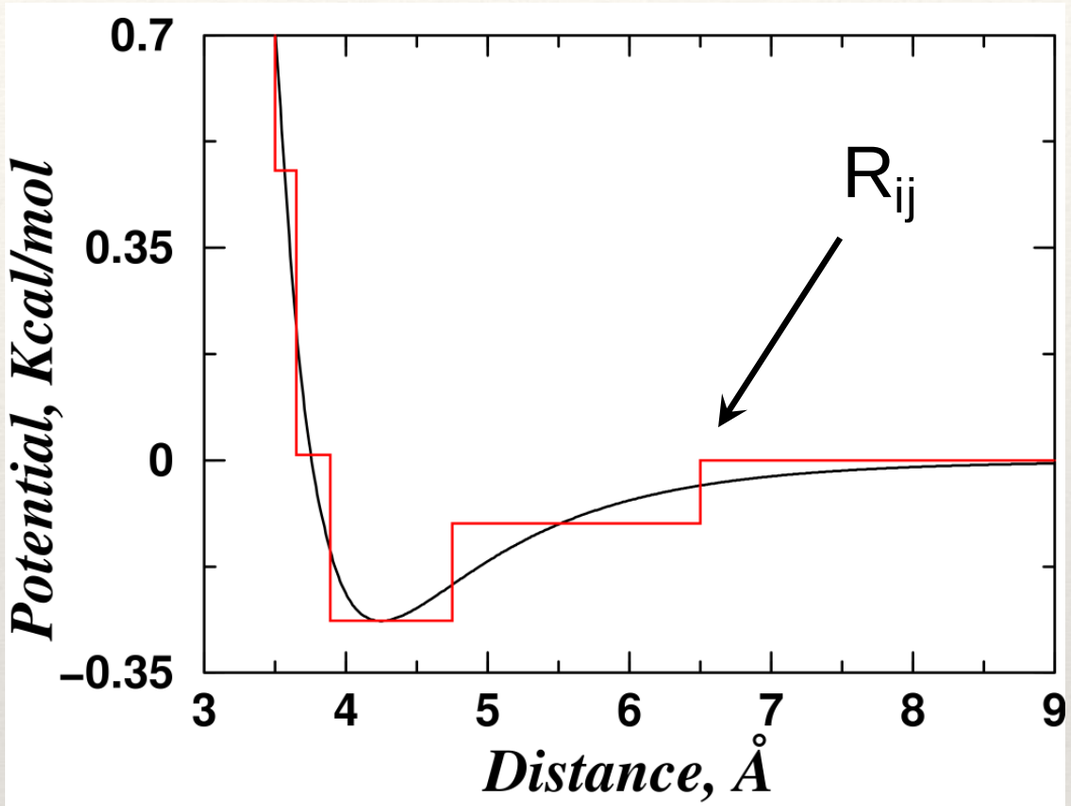
D

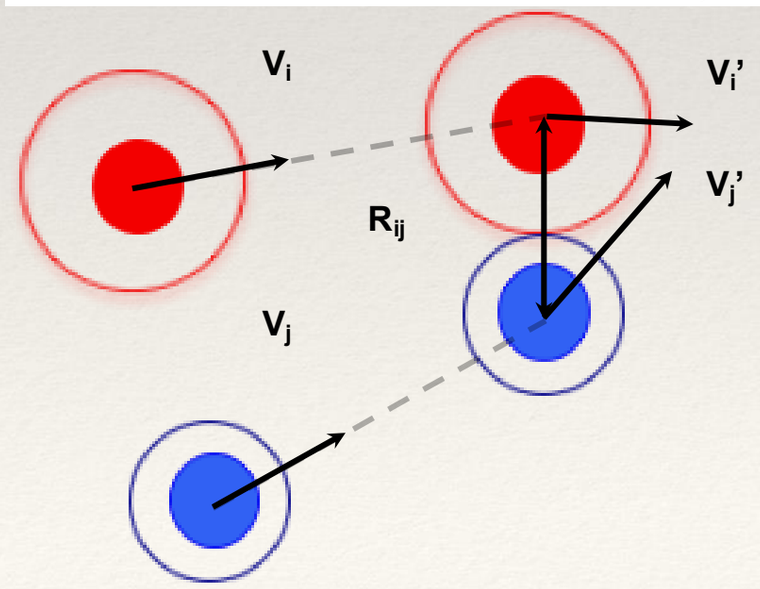


Name	MW (g/mol)	log K_{OW}
Aldicarb	190.26	1.13
Atrazine	215.69	2.61
Bifenthrin	422.87	6.00
Carbofuran	221.26	2.32
Chlordane	409.76	6.16
Chlorpyrifos	350.59	4.96
DDE	318.02	6.51
Dicamba	221.03	2.21
Glyphosate	169.07	-3.40
Imidacloprid	255.66	0.57
Methyldithiocarbamate	107.19	1.07
Metolachlor	283.80	3.13
Permethrin	391.29	6.50
Tefluthrin	418.74	6.40
Terbufos	288.42	4.48

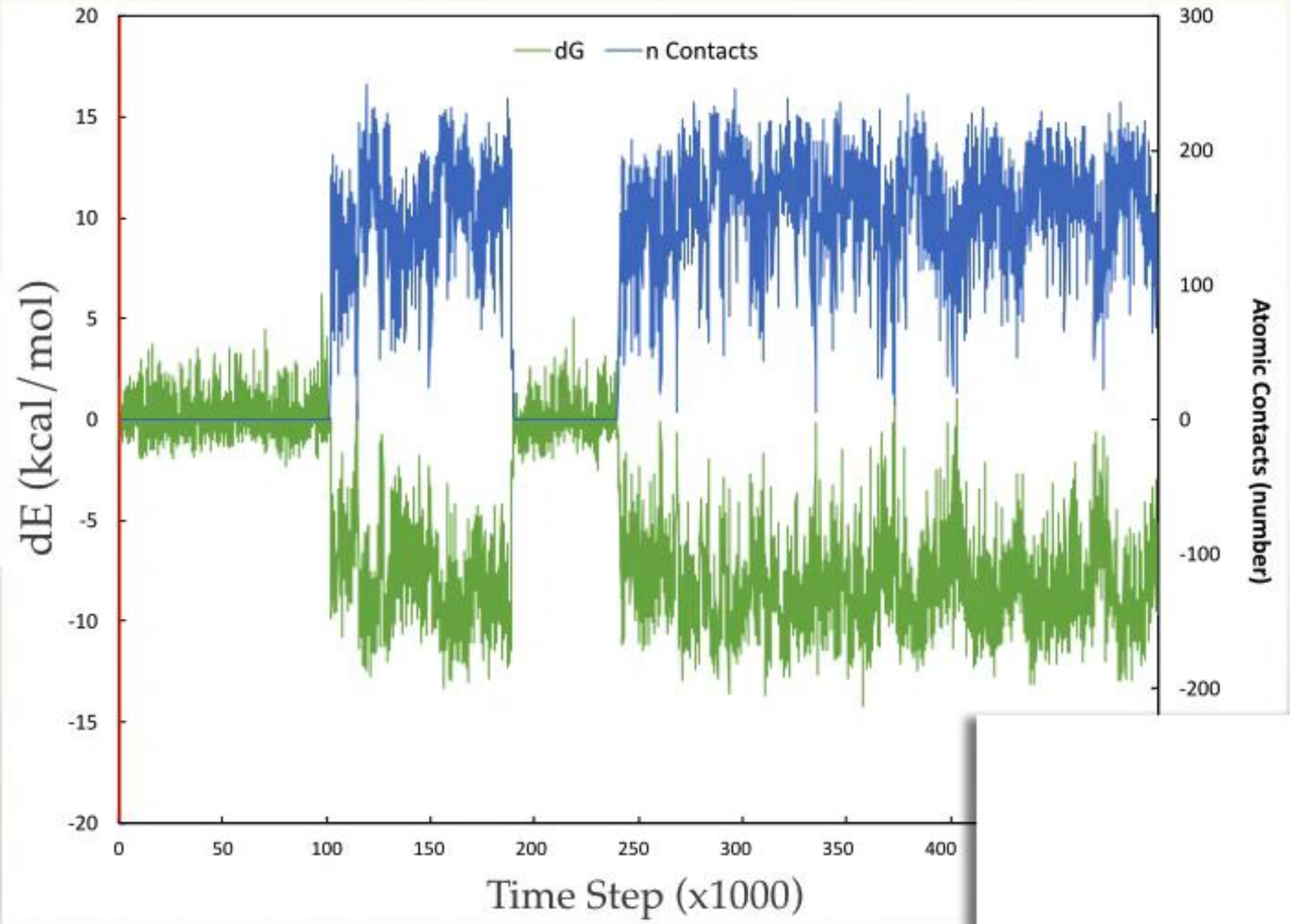
Discrete Molecular Dynamics







F Ding et al

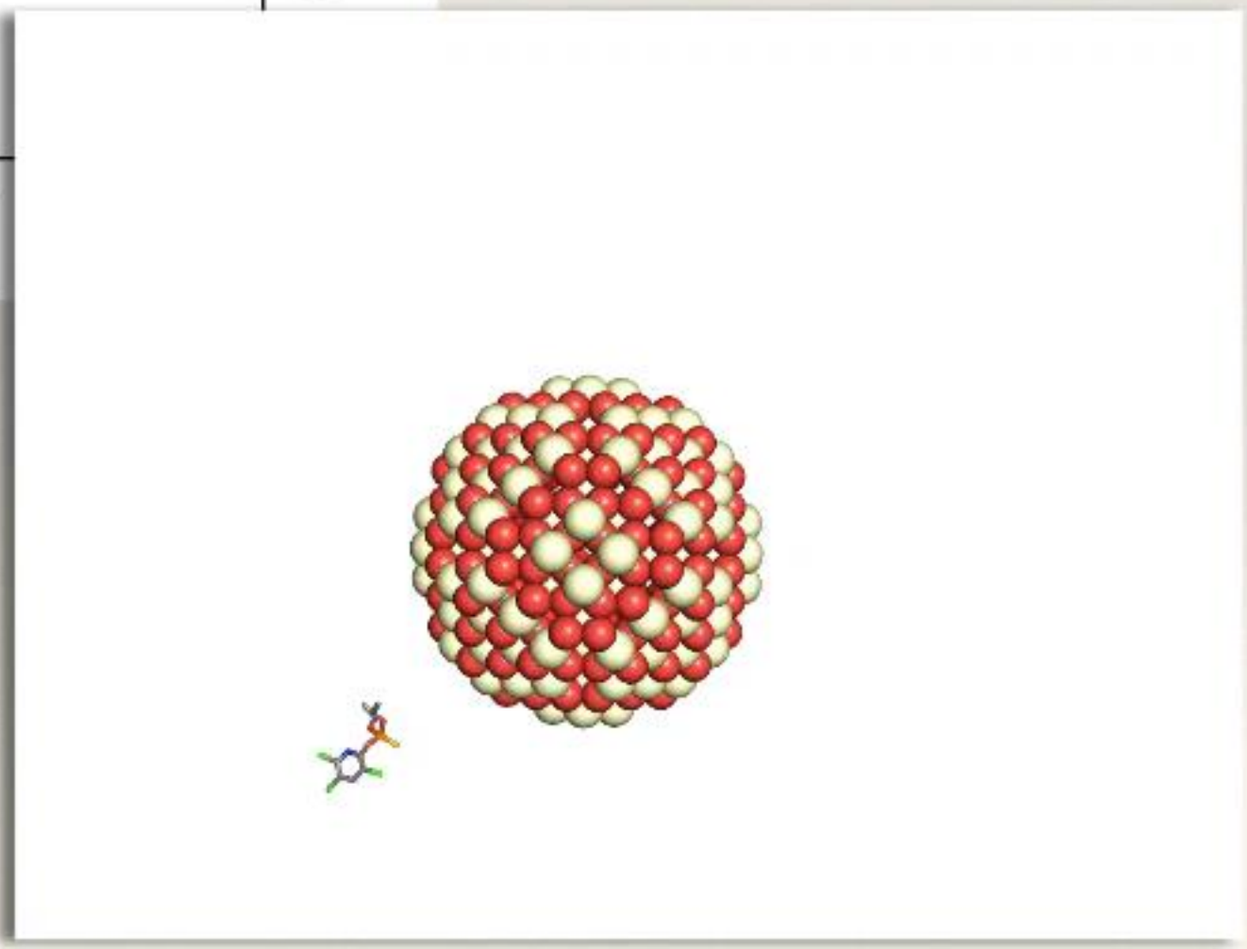


$$\Delta G = \Delta E - T\Delta S$$

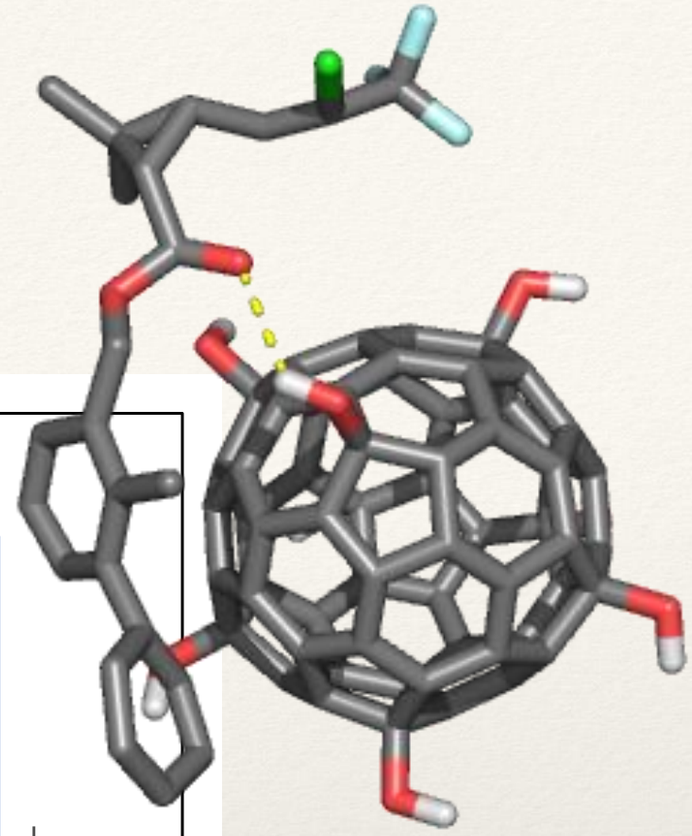
$$K_d = e^{\frac{-\Delta G}{k_B T}}$$

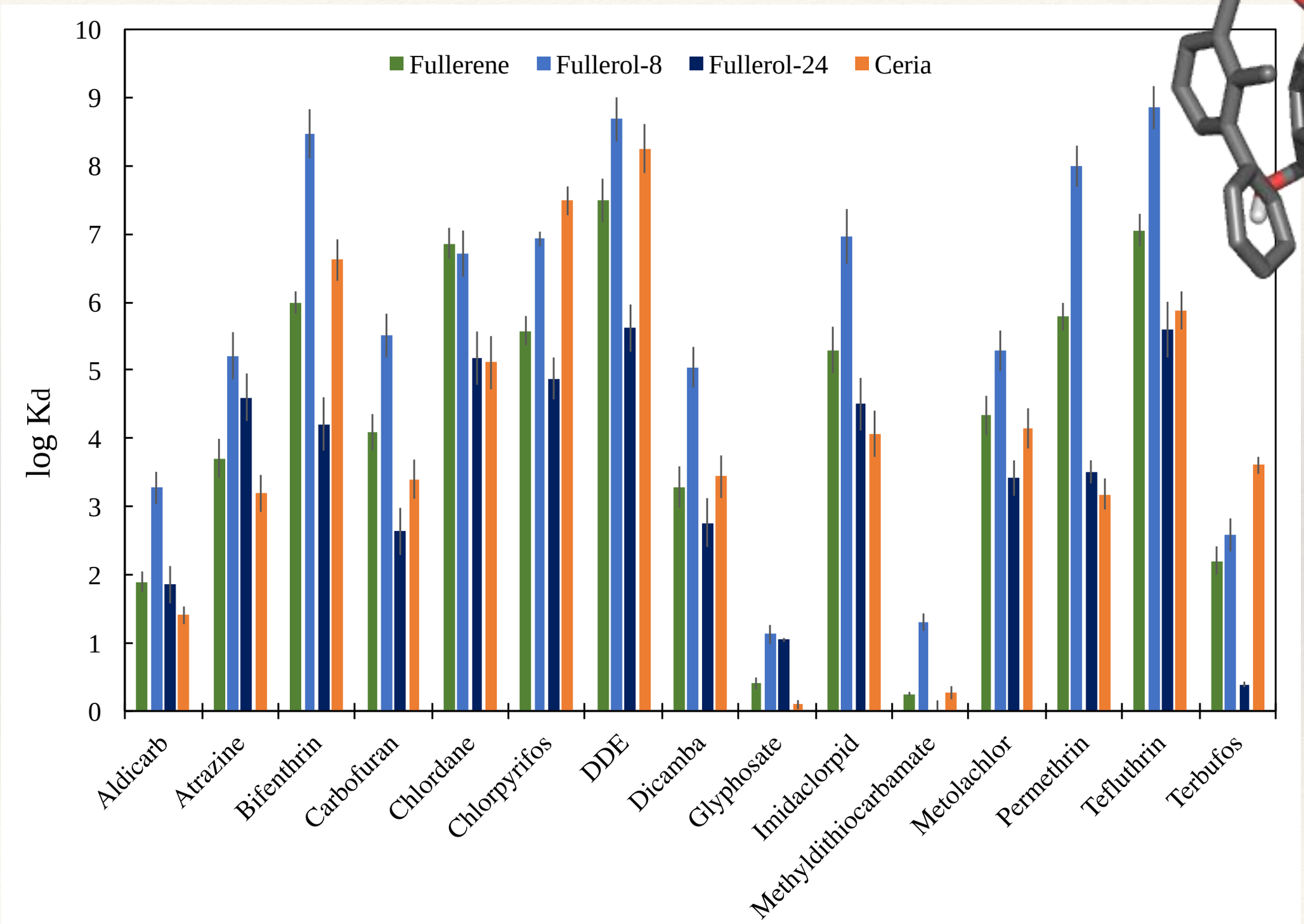
Includes:

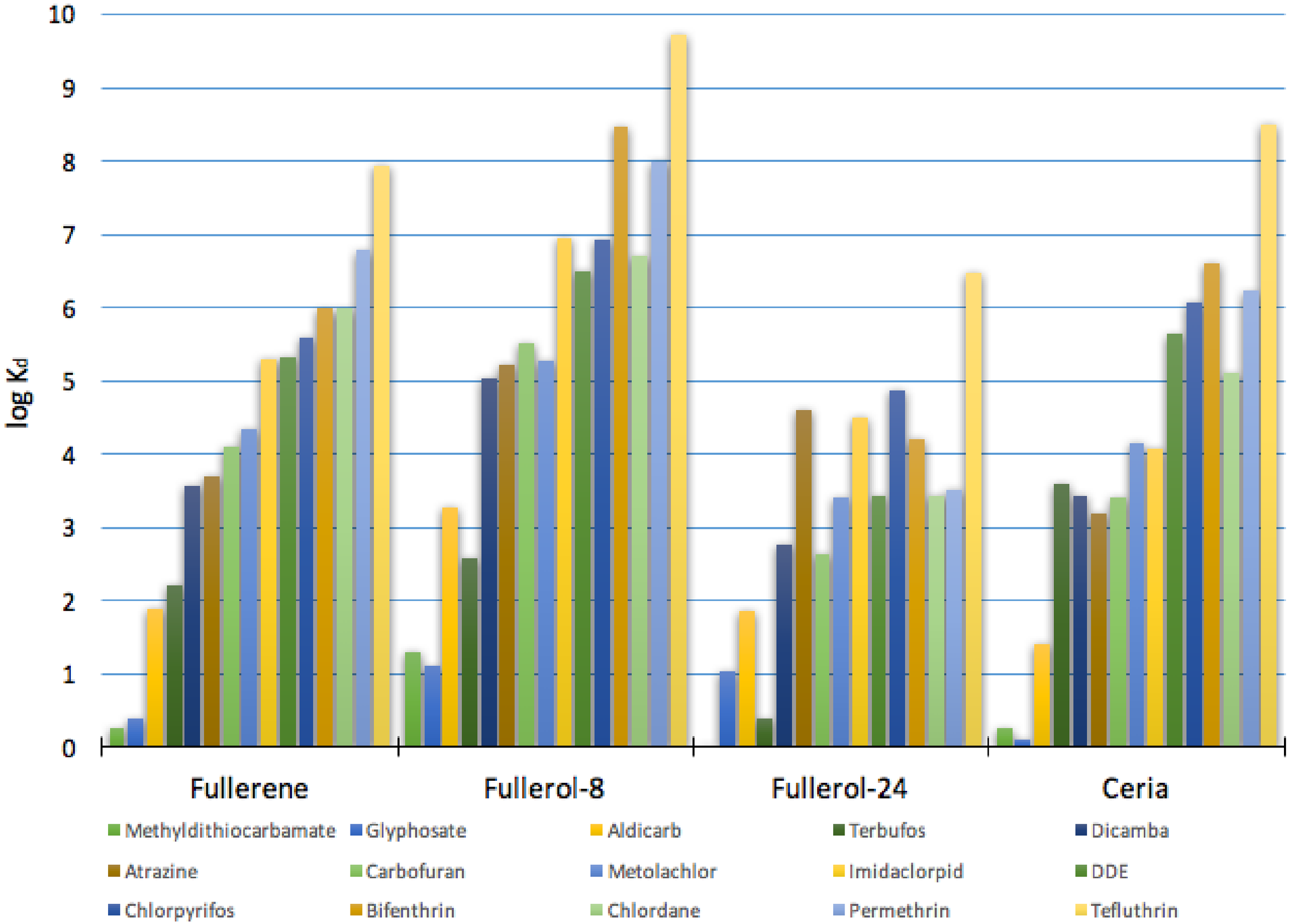
- Implicit Solvent
- Adjustable temperature
- Adjustable ionic strength
- Solvation energy
- van der Waals
- Electrostatics
- Hydrogen binding

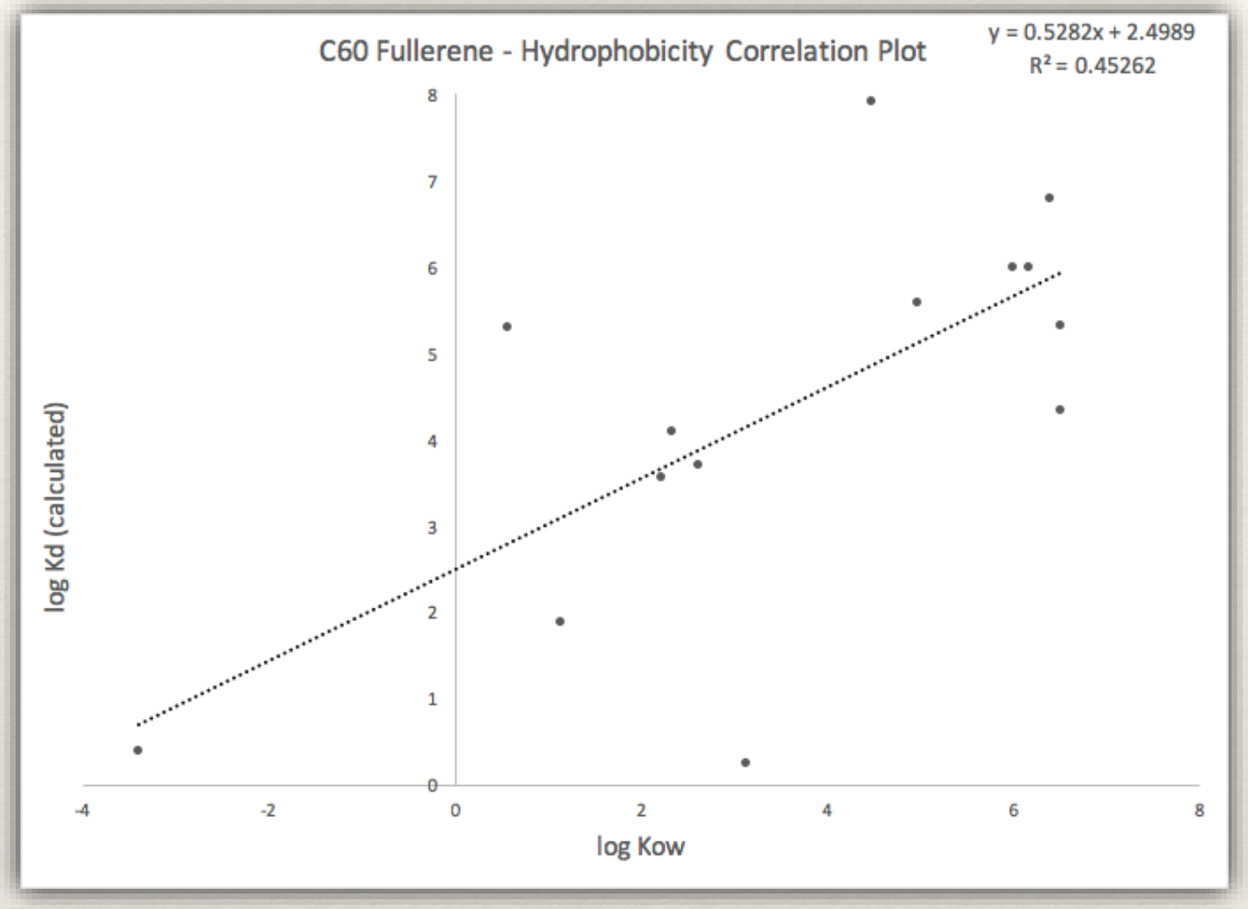


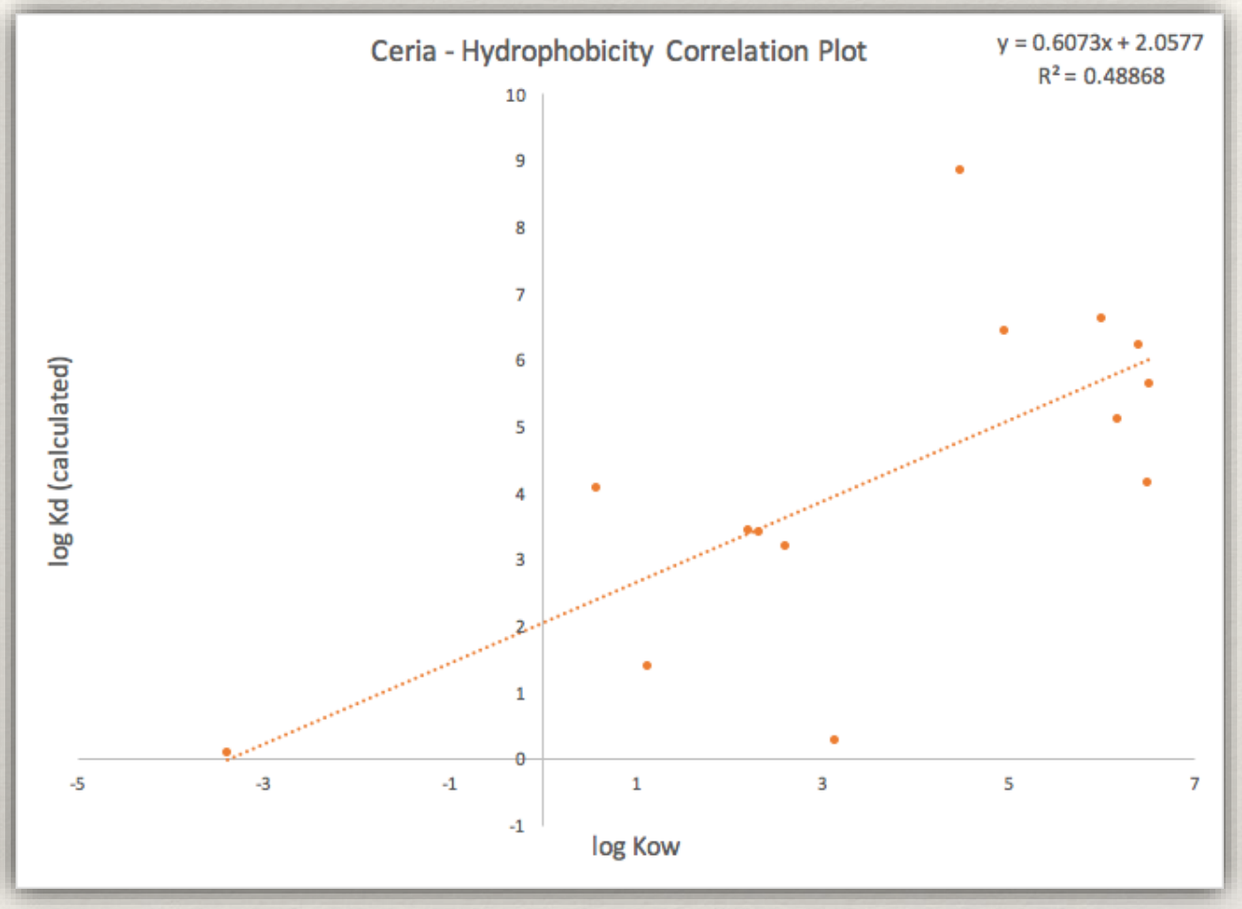
- Wide range of adsorption affinities
- In general, strongest to Fullerol-8

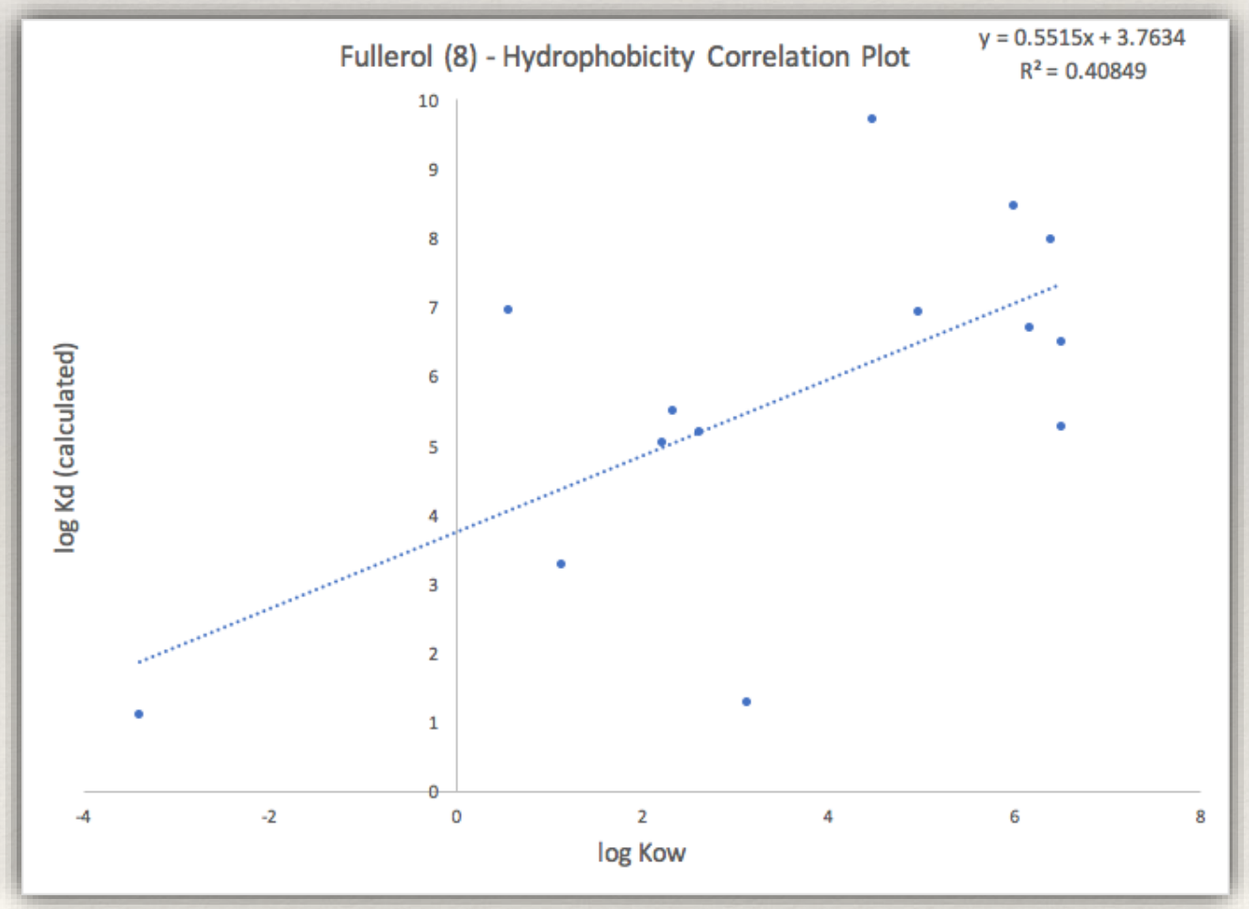


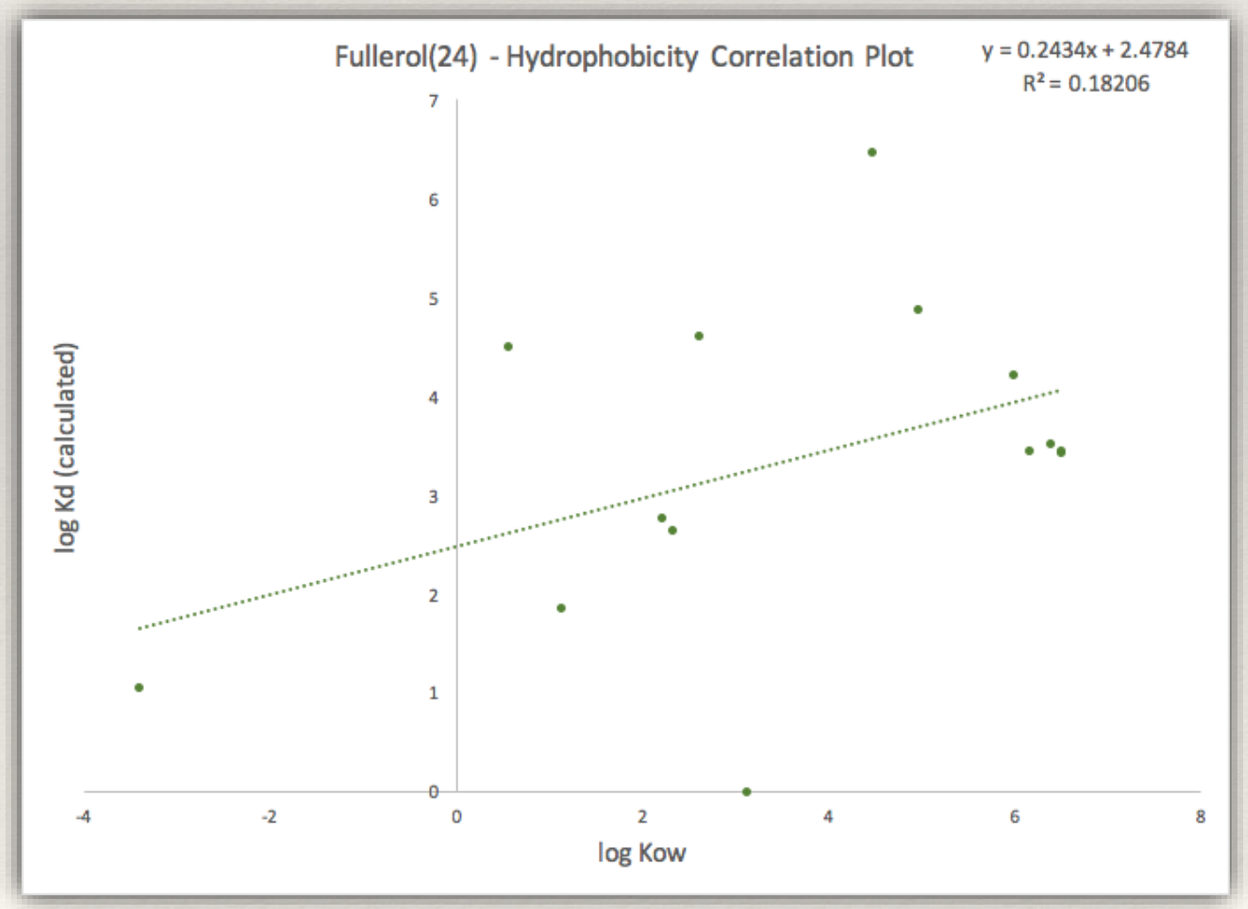


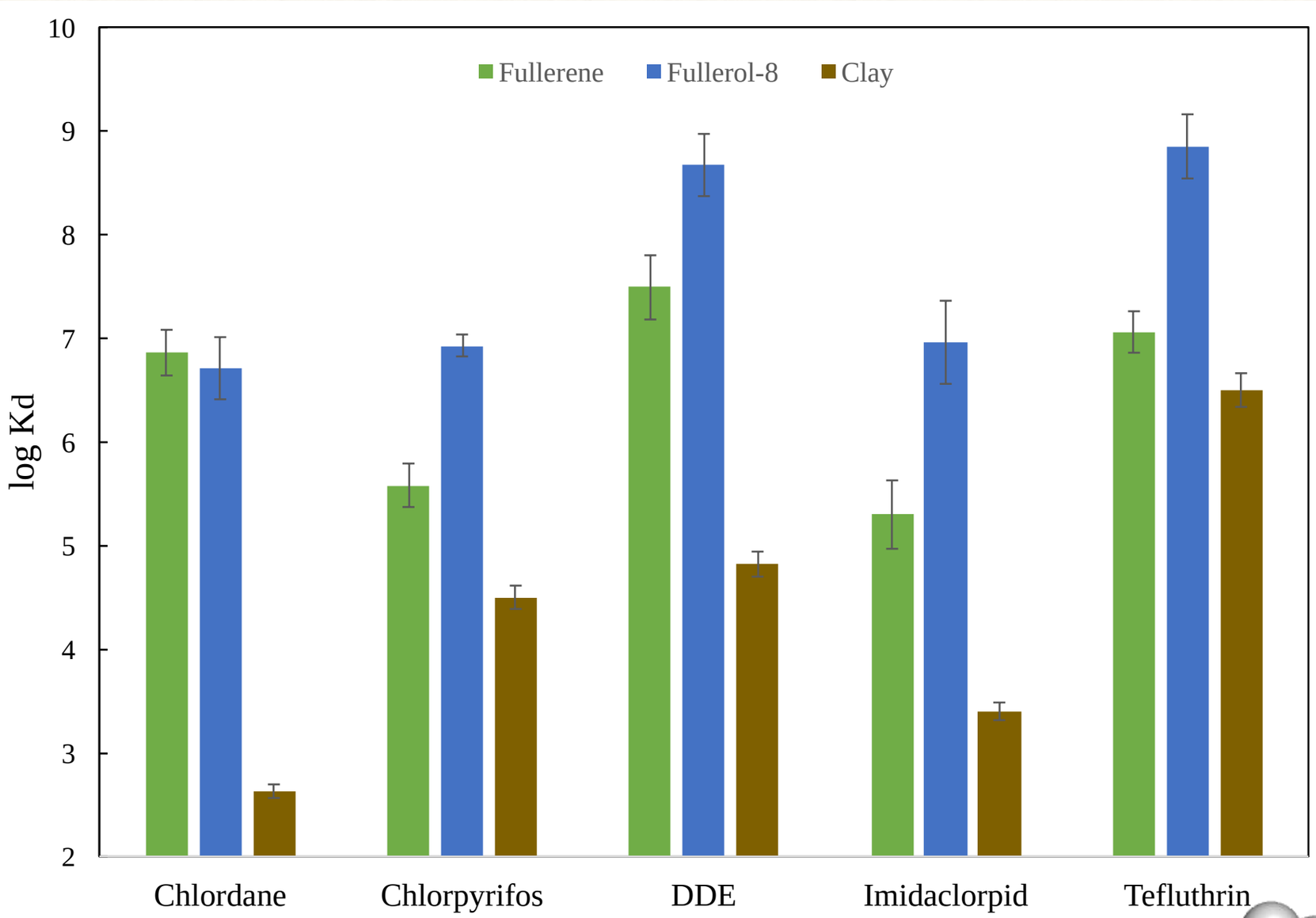

10
9
8
7
6
5
4
3
2
1
0
log K_d
Fullerene
Fullerol-8
Fullerol-24
Ceria
Methyldithiocarbamate
Glyphosate
Aldicarb
Terbufos
Dicamba
Atrazine
Carbofuran
Metolachlor
Imidaclorpid
DDE
Chlorpyrifos
Bifenthrin
Chlordane
Permethrin
Tefluthrin


C60 Fullerene - Hydrophobicity Correlation Plot
y = 0.5282x + 2.4989
R² = 0.45262
log Kd (calculated)
log Kow
8
7
6
5
4
3
2
1
0
-4
-2
0
2
4
6
8

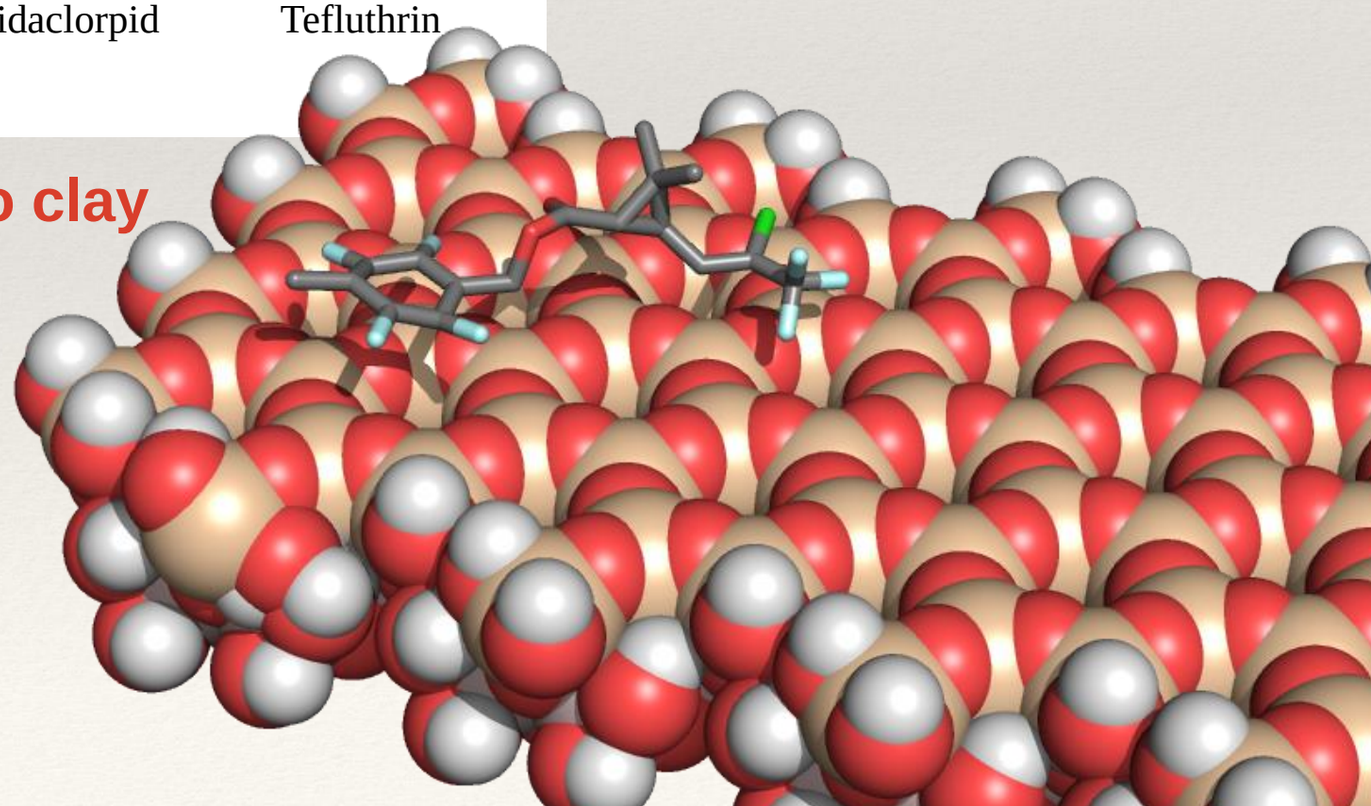

Ceria - Hydrophobicity Correlation Plot
y = 0.6073x + 2.0577
R² = 0.48868
log Kd (calculated)
log Kow
10
9
8
7
6
5
4
3
2
1
0
-1
-5
-3
-1
1
3
5
7

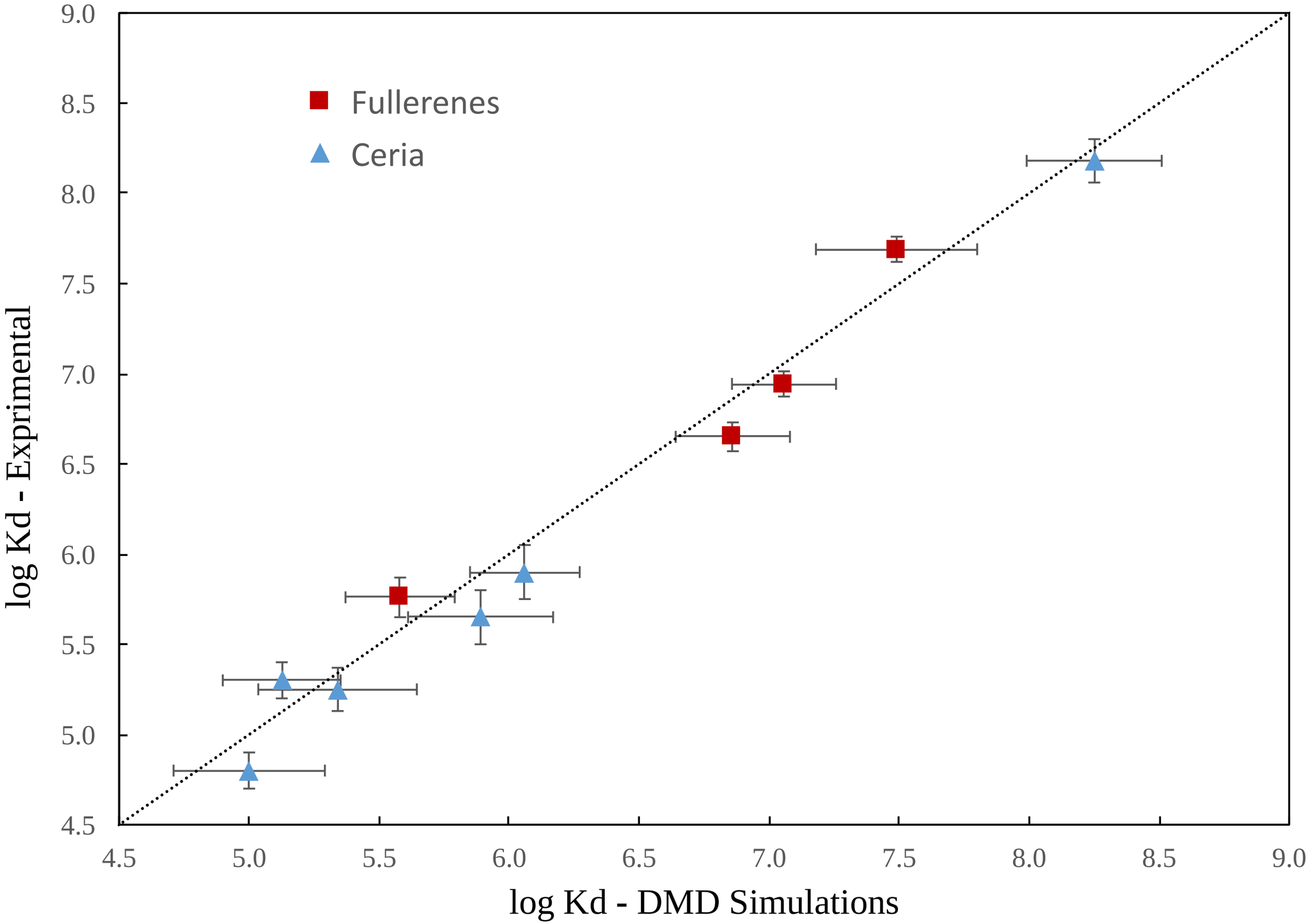

Fullerol (8) - Hydrophobicity Correlation Plot
y = 0.5515x + 3.7634
R² = 0.40849
log Kd (calculated)
log Kow
10
9
8
7
6
5
4
3
2
1
0
-4
-2
0
2
4
6
8


Fullerol(24) - Hydrophobicity Correlation Plot
y = 0.2434x + 2.4784
R² = 0.18206
log Kd (calculated)
log Kow
7
6
5
4
3
2
1
0
-4
-2
0
2
4
6
8



Orders of magnitude weaker adsorption to clay




Fullerenes
Ceria
log Kd - Exprimental
log Kd - DMD Simulations
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.5
5.0
5.5
6.0
6.5
7.0
7.5
8.0
8.5
9.0

Conclusions

- DMD produces rapid, accurate predictions of adsorption coefficients
  - Prediction stronger than K_{OW}, etc alone, with mechanistic insight
- Adsorption strongest to lightly hydroxylated carbon particles
- Many adsorb more strongly to particles than to clays

Future Directions

- Additional nanomaterial classes
- Shift from heuristic to situational understanding:
- Incorporation of multiple nanoparticles, competitive binding, and environmental biomolecules

Acknowledgements

- Dr Mark Wiesner, Duke University
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- Dr Wei Chen, Nankai University
- Duke Compute Cluster

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