FORMULATION TOXICITY

ITT5

Tom Pennington and Tsoogii Saizmaa

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PROBLEM RECAP

		AI	AI	AI	Solvent	Solvent	Solvent	Surfactant	Surfactant	Surfactant	Anti-foam	Anti-foam	Anti-foam
		1	2	3	4	5	6	7	8	9	10	11	12
Formulation	1	■			■				■		■		
Formulation	2	■				■		■					
Formulation	3	■			■		■						
Formulation	4		■			■							
Formulation	5		■			■						■	
Formulation	6		■				■						
Formulation	7		■		■				■				
Formulation	8			■	■								
Formulation	9			■		■							■
Formulation	10			■		■		■					
Formulation	11			■			■					■	
Formulation	12			■			■						
Formulation	13			■						■			
Formulation	14			■									

We know formulation toxicities and compositions.
Some knowledge (interval data) of ingredient toxicity.

Assuming additivity, how can we find toxicity of component ingredients?

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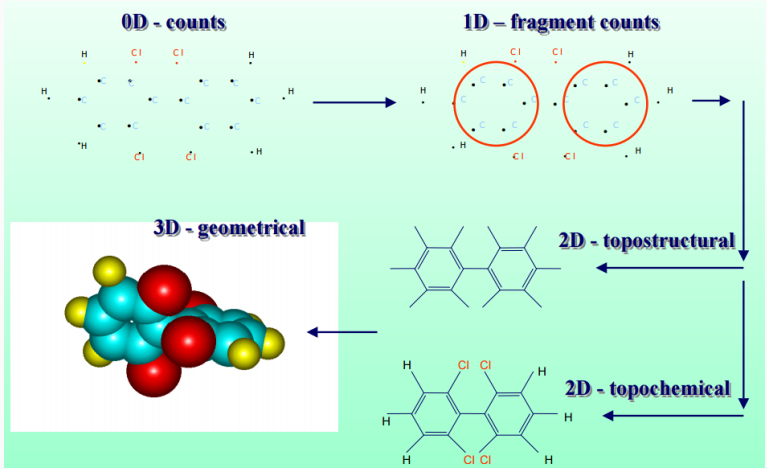
4. Prediction of toxicity from chemical structure...

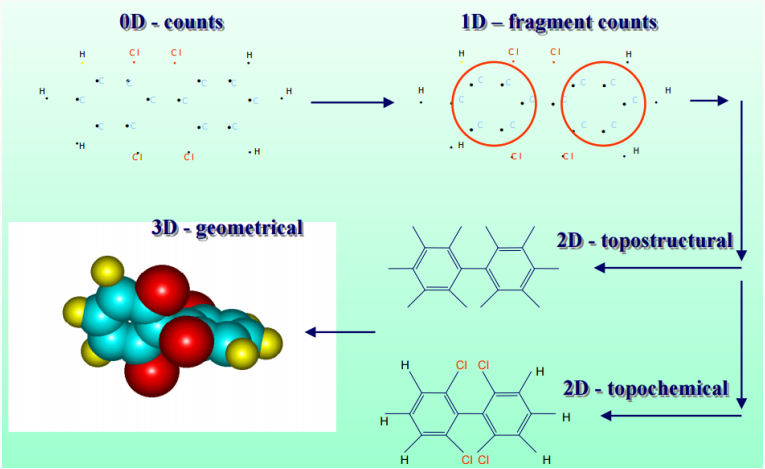
SEARCH FOR SMOOTH CHEMICAL SPACE

- Chemical Space vs Activity.



SEARCH FOR SMOOTH CHEMICAL SPACE

- Chemical Space vs Activity.
  - Non-smooth



SEARCH FOR SMOOTH CHEMICAL SPACE

- Chemical Space vs Activity.
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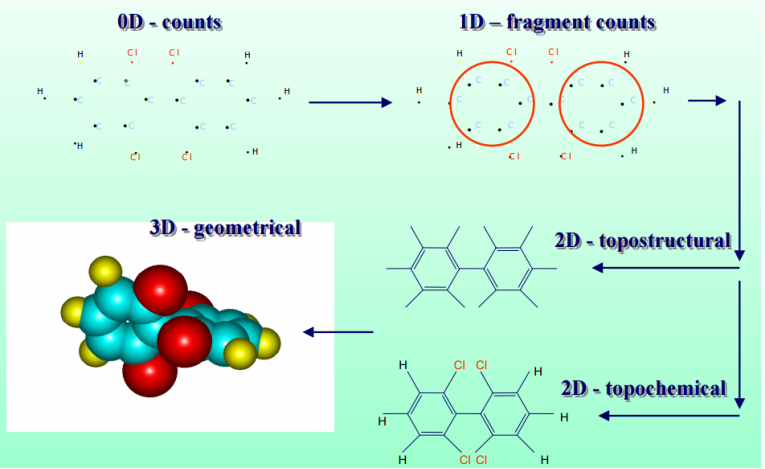

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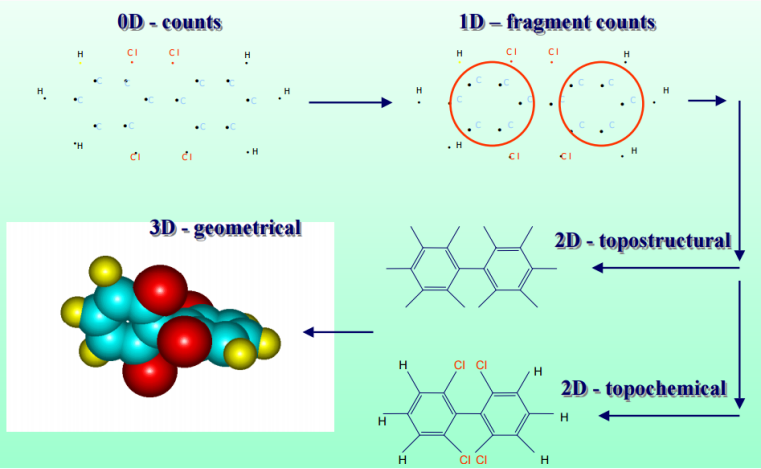
- Non-smoothness?
  - “Similar compounds” should resemble similar activity.



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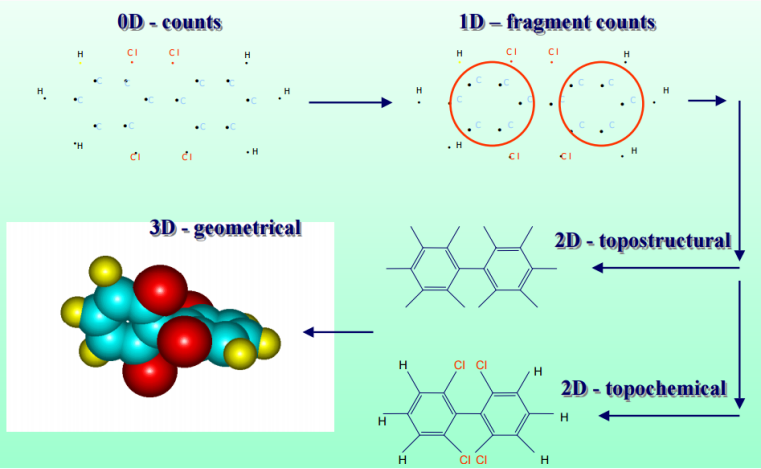

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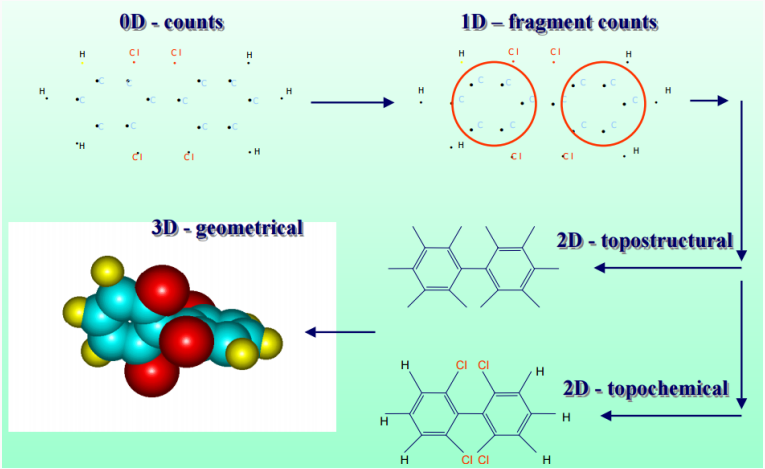

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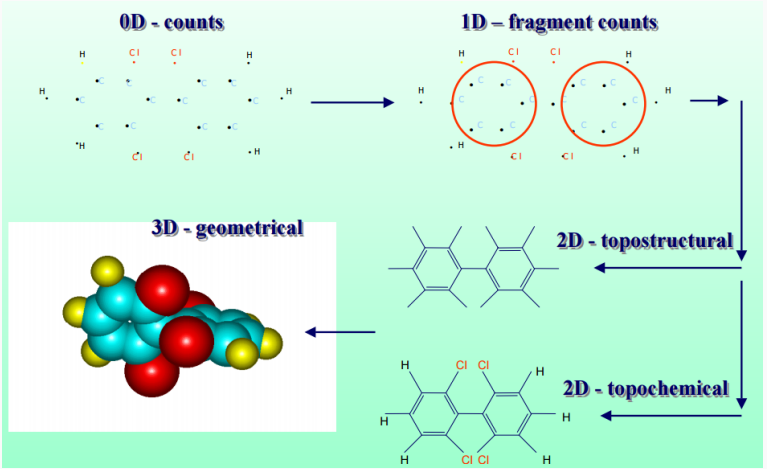

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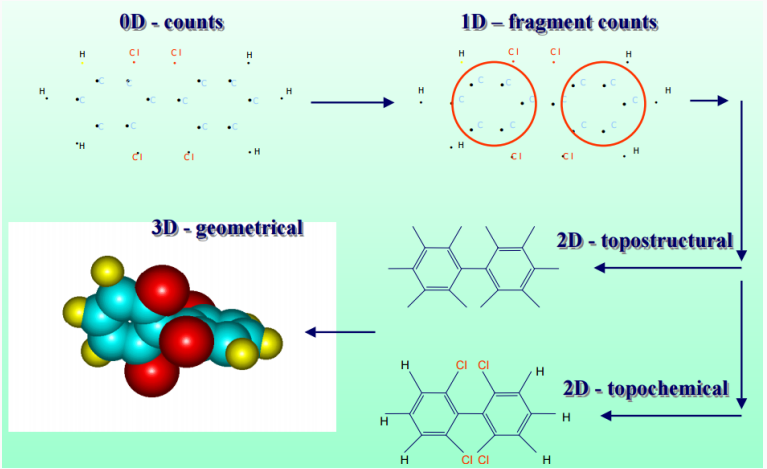

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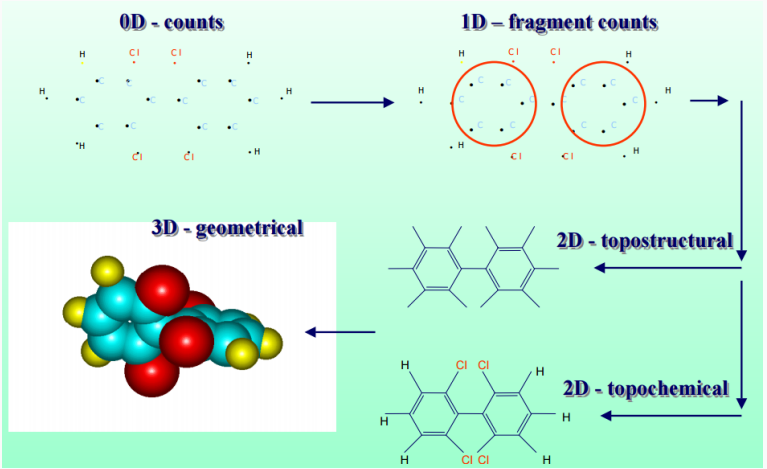

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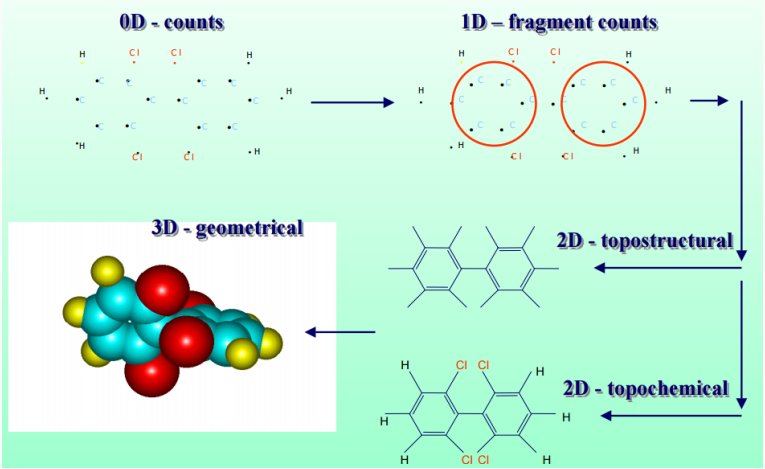
- Possible ways to search for smooth directions



Thanks for listening!