Which of the following is **not** one of the principles of green chemistry?

a. Use of catalysis
b. Reduction of derivatization
c. Use of computational methods
d. Minimizing energy use

Though not one of the 12 Principles of Green Chemistry developed by Paul Anastas and John Warner[1] (see below), theoretical and computational methods can be used to examine the interactions within and between molecules in order to understand chemical reactivity and the relationship between structure and function in chemistry, biology and materials science.[2]

Computational models can be applied to the search for safer chemicals in a higher dimensional chemical space and computational toxicology has been recognized a very useful tool for the evaluation of green chemicals and processes since computational models allow for testing of the toxicity through means that do not involve humans or animal species.[3]

12 Principles of Green Chemistry[1]

1. Prevent waste: Design chemical syntheses to prevent waste, leaving no waste to treat or clean up.
2. Maximize atom economy: Design synthetic methods to maximize the incorporation of all materials used in the process into the final product.
3. Design less hazardous chemical syntheses: Design syntheses to use and generate substances with little or no toxicity to humans and the environment.
4. Design safer chemicals and products: Design chemical products to be fully effective, yet have little or no toxicity.
5. Use safer solvents and auxiliaries: Avoid using solvents, separation agents, or other auxiliary chemicals. If these chemicals are necessary, use innocuous chemicals.
6. Increase energy efficiency: Run chemical reactions at ambient temperature and pressure whenever possible.
7. Use renewable feedstocks: Use raw materials and feedstocks that are renewable rather than depleting. Renewable feedstocks are often made from agricultural products or are the wastes of other processes; depleting feedstocks are made from fossil fuels (petroleum, natural gas, or coal) or are mined.
8. Avoid chemical derivatives: Avoid using blocking or protecting groups or any temporary modifications if possible. Derivatives use additional reagents and generate waste.
9. Use catalysts, not stoichiometric reagents: Minimize waste by using catalytic reactions. Catalysts are used in small amounts and can carry out a single reaction many times. They are preferable to stoichiometric reagents, which are used in excess and work only once.
10. Design chemicals and products to degrade after use: Design chemical products to break down to innocuous substances after use so that they do not accumulate in the environment.
11. Analyze in real time to prevent pollution: Include in-process real-time monitoring and control during syntheses to minimize or eliminate the formation of by-products.
12. Minimize the potential for accidents: Design chemicals and their forms (solid, liquid, or gas) to minimize the potential for chemical accidents including explosions, fires, and releases to the environment.

[1] Anastas, P. T.; Warner, J. C. Green Chemistry: Theory and Practice, Oxford University Press: New York, 1998, p.30.

[2] http://sydney.edu.au/science/chemistry/research/honsproj-green-chemistry.shtml#anchorjordan

[3] https://www.linkedin.com/pulse/computational-modelling-green-chemistry-alfons-nonell-canals