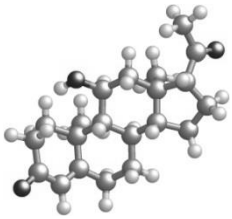

Chem!stry

Name: …… **( )**

Class: ……

Date: …… **/** …… **/** ……

Case #1: Deviant Data

You are engaged in the study of the substituent effects on the rates of reaction of a particular class of compounds. Based on a variety of considerations, you expect that the rate constant will vary linearly with the increasing polarity of the substituent. The graduate student doing the experiment comes in one day with a graph of rate constants versus polarity with the results of ten different systems plotted. Eight of the ten fall nicely on a straight line, but two points are well above the line. You are convinced that the two "deviant" points are in error. What should you do?

1. Do you tell the student to repeat the two "deviant" measurements?

2. Do you tell the student to repeat all of the experiments to make sure that the data is correct?

3. Do you publish the data omitting the two points that do not fall on the straight line?

Taken from Kovac, J. (2004). *The Ethical Chemist: Professionalism and Ethics in Science*.
New Jersey: Pearson Prentice Hall. ISBN: 0-13-141132-2

Commentary: Deviant Data

Judgements are always being made as to whether a particular measurement should be retained or thrown out. The variety of good reasons for rejecting a data point include instrument malfunction, presence of impurities and poor technique. Much good science is done right at the edge of the detection limit, so errors are common. The ethical question is whether the data point is being rejected because of good scientific judgement or because of wishful thinking.

Alternative two is the safest: going back and re-measuring everything. But this option might be wasteful, both in time and material. In some circumstances it might be essentially impossible. For example, the measurements might have been performed with an instrument to which you do not have ready access such as a synchrotron or a neutron beam. Deadlines might be pressing, making this option unattractive.

Alternative one can also be justified, depending on your relative confidence in the various measurements. It might be that the two “deviant” points were the hardest systems to work with. They might have been done on a day when the instrument was “acting-up.” Under these circumstances, re-measuring these two points alone can be justified.

Alternative three can also be justified under circumstances similar to those used to justify the second. The scientific reasons to doubt the validity of those two measurements may be very good, and it may be impossible or overly expensive to repeat them prior to publication. It might then be perfectly legitimate to throw them out.

After you have chosen one of the three alternatives, what is your responsibility to the scientific community as you write your paper? Must you reveal that you had to re-measure two points or that you threw them out? What should you disclose and what can you ethically leave out?