25 years in Pharma: What has changed in the industry since 1991?

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25 years is almost a full career for a scientist, but before looking to the future, we should ask what is really new in the last 25 years, i.e. since 1991? Surprisingly little! Most of techniques routinely today were introduced in the 1980s (many techniques have been re-invented since; the collective memory of the literature seems to be under 10 years and falling). The biggest revolution in computational chemistry was not new techniques, but computer power and data availability. We can now remove of the necessary short-cuts, refine our parameters, and validate using data sets of appropriate statistically power. We can now talk about our results with an estimate of error. If only we understood water and free energy!

The other paradigm shift has been in the holistic view of drug design. We are not here to improve, say, affinity, but also to factor in solubility, bioavaility, clearance, stability and many other issues that affect the success of a project. Although fundamental scientific progress has been slow, the opportunities for CADD scientists to really impact projects is at its highest.