

# Organic Process Research & Development

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## *Editorial*

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### Cost Estimates for New Molecules

A question I am often asked by emerging pharmaceutical companies or virtual pharma is to estimate the cost of making a new drug substance. Often the only information available is a medicinal chemistry synthesis with its associated yields. The company itself may have already done the calculation based on “catalogue company” prices and may be horrified at how expensive the drug substance appears to be. I can usually allay their fears that the drug will be too expensive by using more realistic numbers, based on bulk prices for raw materials and reagents, and then making projections based on a better, more convergent synthesis with lower-cost reagents and optimized yields. Once this has been carried out, the projected cost/kilogram for the new drug substance (if only raw material costs and no manufacturing/overhead/labour costs are considered) may well come down by a factor of 10 or even 100, and this is often more acceptable to management trying to make strategic decisions about potential profitability. I am often worried that my estimates may not turn out to be correct, but on the one or two occasions when a drug has gone “all the way”, I have been surprised how close such rough calculations can be.

Of course many people in the fine chemicals industry, who are bidding to make late-stage intermediates for the increasingly complex molecules that emanate from discovery departments these days, have to do these cost projections on a daily basis, to give price quotes. Their company’s profit (or loss) may depend on the accuracy of their estimates. Nevertheless, a certain amount of contingency is built in to their quote, and this hopefully leads to a reasonable profit.

The main difficulty with these calculations is to get accurate bulk chemical prices. The price of raw materials, intermediates, or reagents is notoriously fluid, being dependent on supplier, amount purchased, quality, lead time, and (often the big imponderable) currency exchange rate. Whereas the bulk prices of commodity chemicals are known and listed each week in *Chemical Marketing Reporter*, no such listing exists for fine chemicals.

What the industry needs is a “bulk” equivalent of the “Aldrich Catalogue” where the kilogram or tonne prices of thousands of raw materials, reagents, and intermediates are regularly listed. Ballpark figures would be adequate for the needs of most people. Chemists would then be able to quickly price a variety of paper synthetic route options and decide which is the best low-cost option. Is any publisher prepared to commission such a compendium or compile such a database? Perhaps one exists already—let me know if you are already using one.

At present, I still have to rely on the familiar equation

$$\text{bulk price} = \frac{\text{catalogue company price}}{x}$$

where  $x$  is an integer from 2 to 10, to make my estimates.

Such an equation (particularly when  $x = 10$ ) tends to make the catalogue company prices appear excessively large, but the high inventory (leading to fast delivery of lab and sometimes kilogram quantities), wastage (as partially opened drums of sensitive materials allow deterioration), and the need to upgrade materials justify the prices charged. And one must remember that these companies have to make profits, too, to stay in business.

### Special Issues

Our planned special issue on Biopharmaceuticals will not be appearing, at least not in 2005. This is being replaced by a Crystallisation and Polymorphism special issue for which contributions are keenly requested. The last issue of 2005 will, of course, be the regular Safety special feature, and we welcome submissions for this issue, too.

### Absence of Highlights from the Patents

Now to another topic. I must apologise that there are no patent highlights in this issue. Keith Turner, the author of

Highlights from the Patents, was unable to submit his usual contribution, owing to a sudden, and very serious, illness in the family. We look forward to seeing the patent highlights in the following issue—perhaps it may even be double its usual length. We send our good wishes to Keith and his

family in these difficult circumstances and hope the outcome will be a good one.

Trevor Laird  
*Editor*

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