

Embedding Chemical Equations into Word with Automatic Numbering

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Not many convenient solutions exist for the chemistry student who wants to embed chemical equations into their written works. Those solutions that do exist are, based on my experience, cumbersome to implement. During my thesis writing I came up with this solution, which I thought was convenient and practical once the technique was learned. It embeds chemical equations into a table, with captions for each entity in the equation, so that you can move around chemicals during the writing process and have Word automatically update the numbering. This guide offers instruction in the use of this technique. This guide is long because it's thorough (and because it's full of screenshots), and because I've spelled out exactly how to do things, but not because it's a complex process.

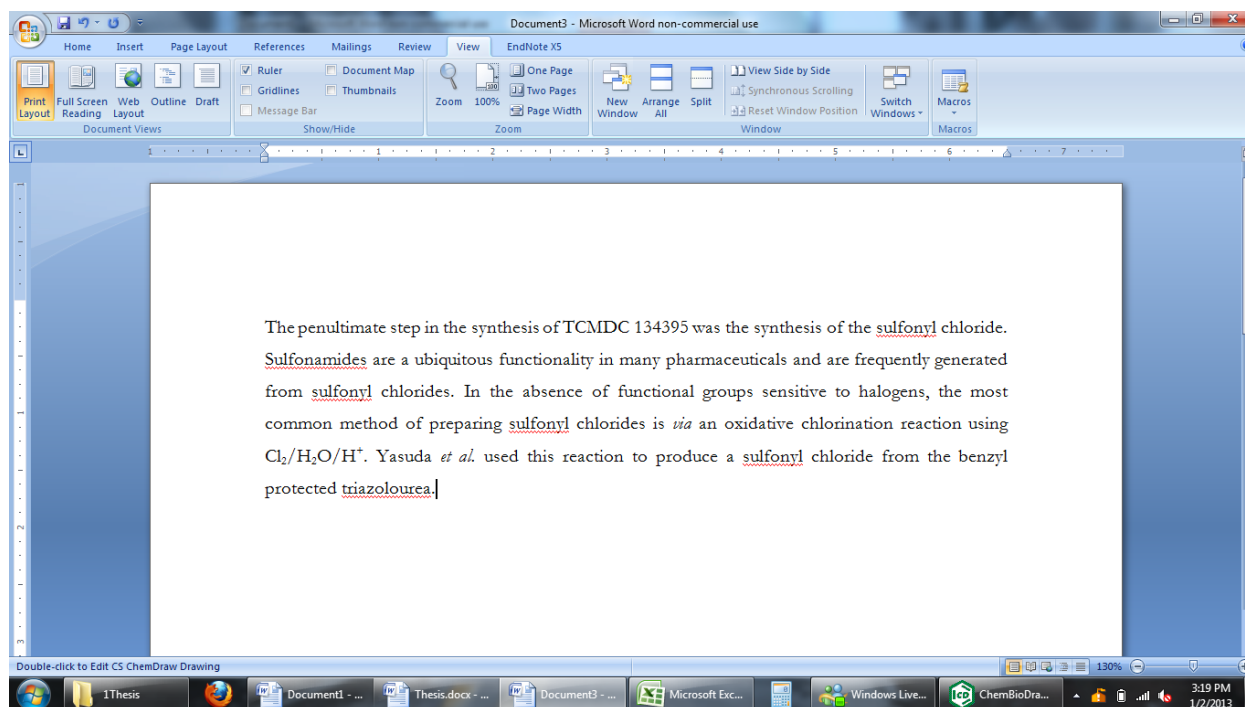
But why? The key advantages:

- Automatic sequential numbering of compounds. Word will ensure the numbers appear in sequential order even when you move those compound numbers around your document.
- Edit-as-you-go functionality. Never again will you copy and paste a scheme from ChemDraw only to realize that it's a tad too big for your page. Now, that scheme will be there as you write, affording you the ability to edit as you go.

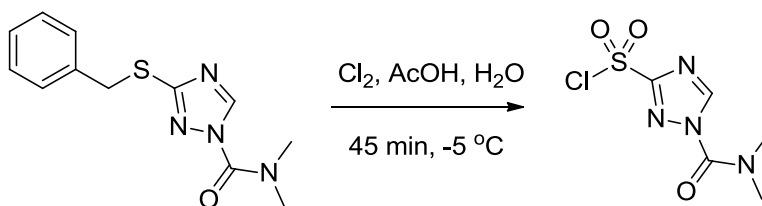
To be fair, there are disadvantages to the more conventional method:

- You have to learn this technique, which will take up a good 10 minutes of your time.
- You will have to select a style (in ChemDraw) at the beginning, and stick with it (unless you enjoy manual editing).
- Some bits can be a bit fiddly.

So you're writing your thesis in word and the time has come to insert a chemical equation. You've written something along the following lines:



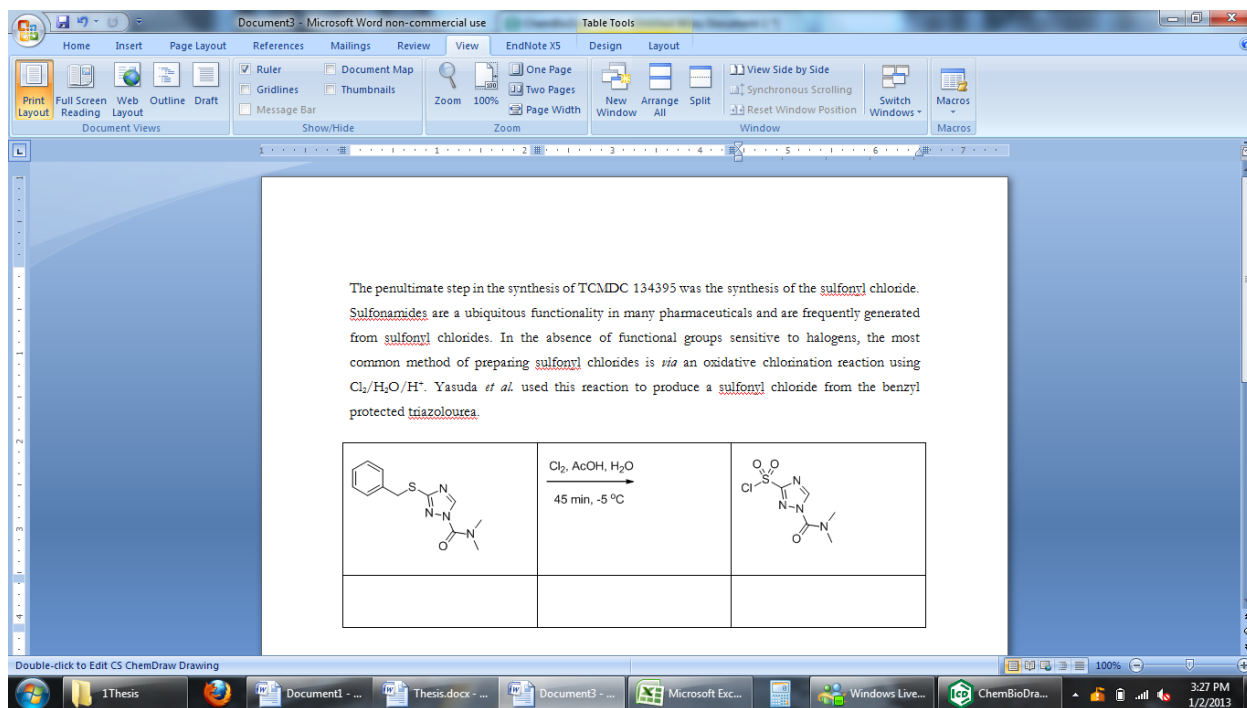
This paragraph would be spicier with a chemical equation that explains how Yasuda *et al.* made their sulfonyl chloride. The relevant chemical equation is:



Ordinarily, you'd just copy and paste this into Word and let the rest of your thesis rip. On the night before hand-in, you insert textboxes with numbers like a madman and shed a lump of hair by the morning. Instead: insert a table with 2 rows, and a number of columns corresponding to the number of horizontal entries there are in your chemical equation. In the above case, there are three horizontal entries: the leftmost chemical, the reaction arrow, and the rightmost chemical. Observe:

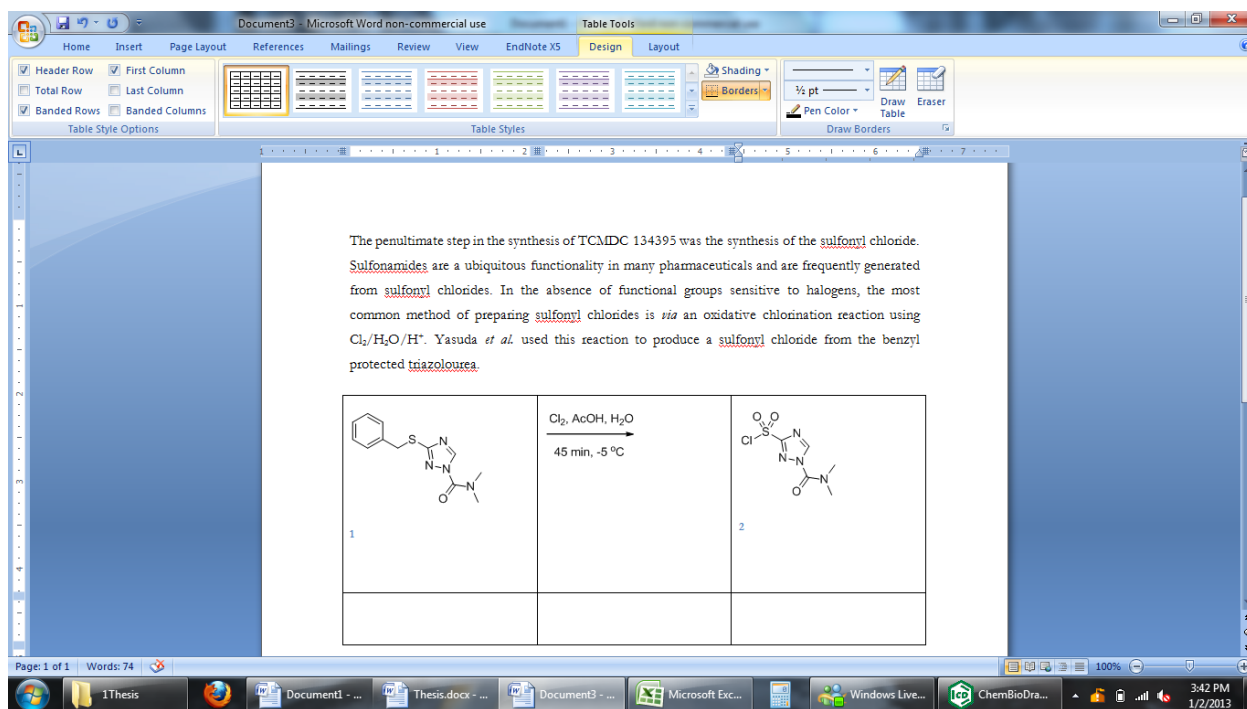
The penultimate step in the synthesis of TCMD 134395 was the synthesis of the sulfonyl chloride. Sulfonamides are a ubiquitous functionality in many pharmaceuticals and are frequently generated from sulfonyl chlorides. In the absence of functional groups sensitive to halogens, the most common method of preparing sulfonyl chlorides is *via* an oxidative chlorination reaction using $\text{Cl}_2/\text{H}_2\text{O}/\text{H}^+$. Yasuda *et al.* used this reaction to produce a sulfonyl chloride from the benzyl protected triazolone.

You've already done the drawings in ChemDraw. Copy & paste each horizontal entity into the corresponding column, so you have something like this:



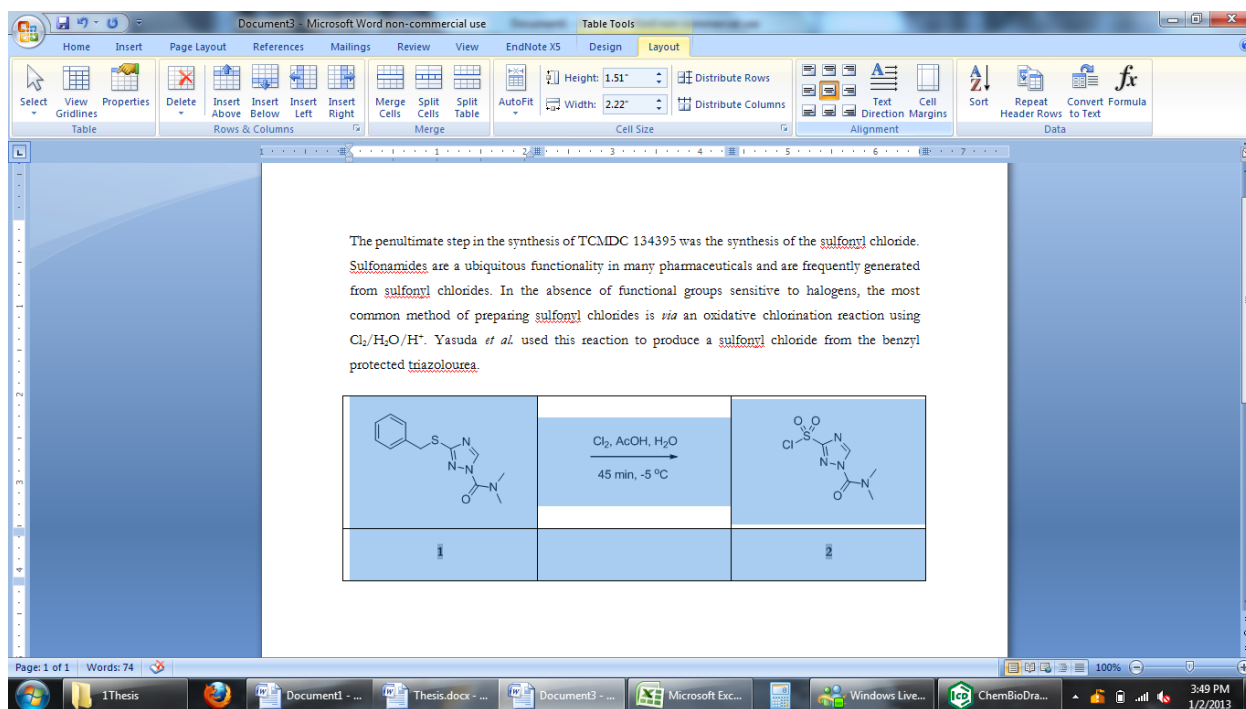
Right click one of the chemicals – it doesn't matter which – and then select "Insert caption". Since you're numbering your first chemical, you'll need to define the new chemical label (as opposed to defining it as a table, or a figure). Select "New label" and call the new label whatever you like. I'm calling it "chemical". Press "OK". Now, tick the "Exclude label from caption" checkbox. Press "OK". You have successfully numbered your first chemical.

Thankfully, the task becomes easier hereafter. You'll want to label the other chemicals now. Right click the next chemical you want to number and select "Insert caption". Under "Options", ensure that the field next to "Label" corresponds to "Chemical" (or whatever you decided to call it earlier). Ensure that the "Exclude label from caption" box is checked, and press OK. You have successfully numbered your second chemical. You should see something like this:

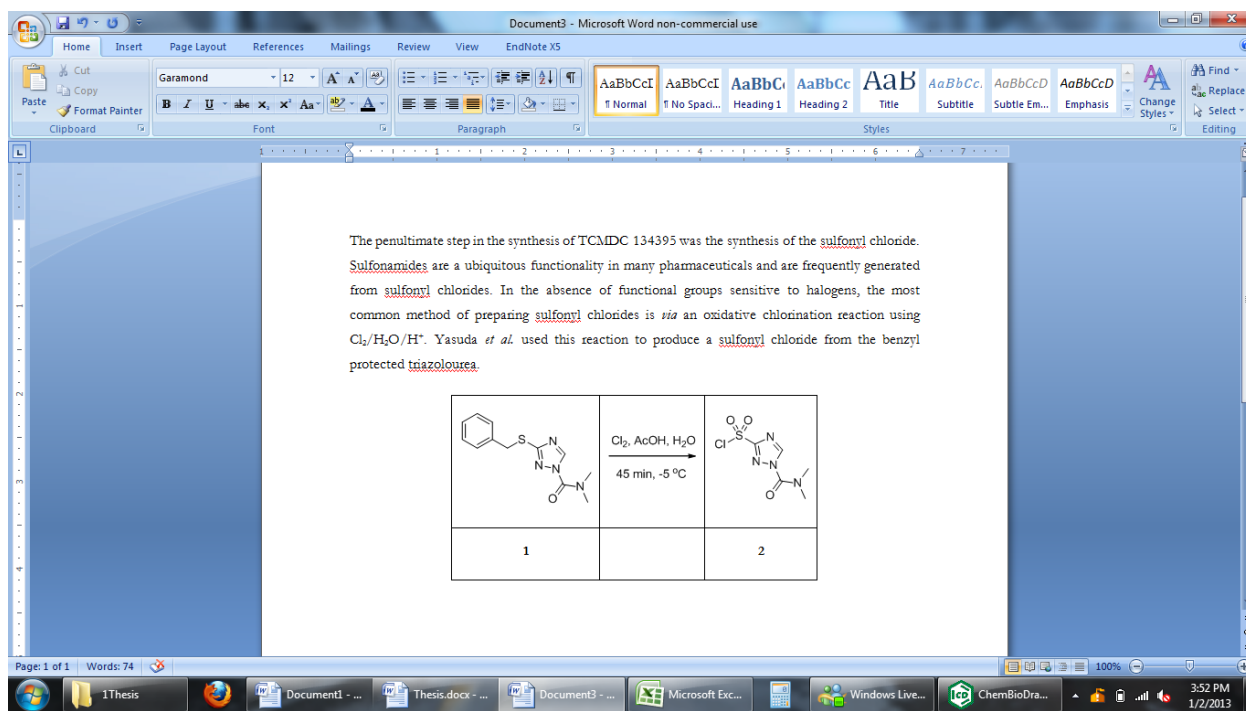


We put that second row in the table for a reason. Using cut & paste, move the newly formed labels "1" and "2" into the second row. Delete any superfluous relic spaces that Word has left in the table after the cut & paste job. Once you've done

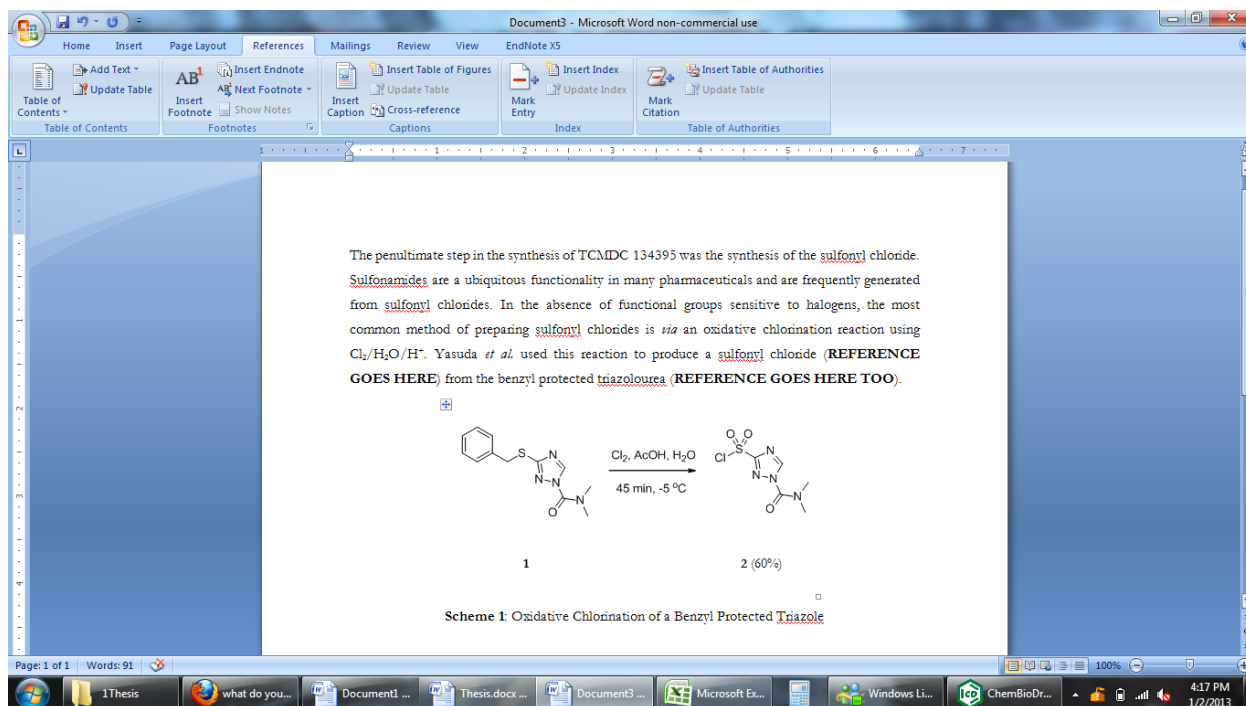
that, you can format these labels in one go by highlighting the entire row and formatting these labels according to your requirements. To align the table entries properly, select the entire table and align the horizontal and vertical axes to centre alignment. The whereabouts of this option is shown here (orange highlighted box, top right/centre):



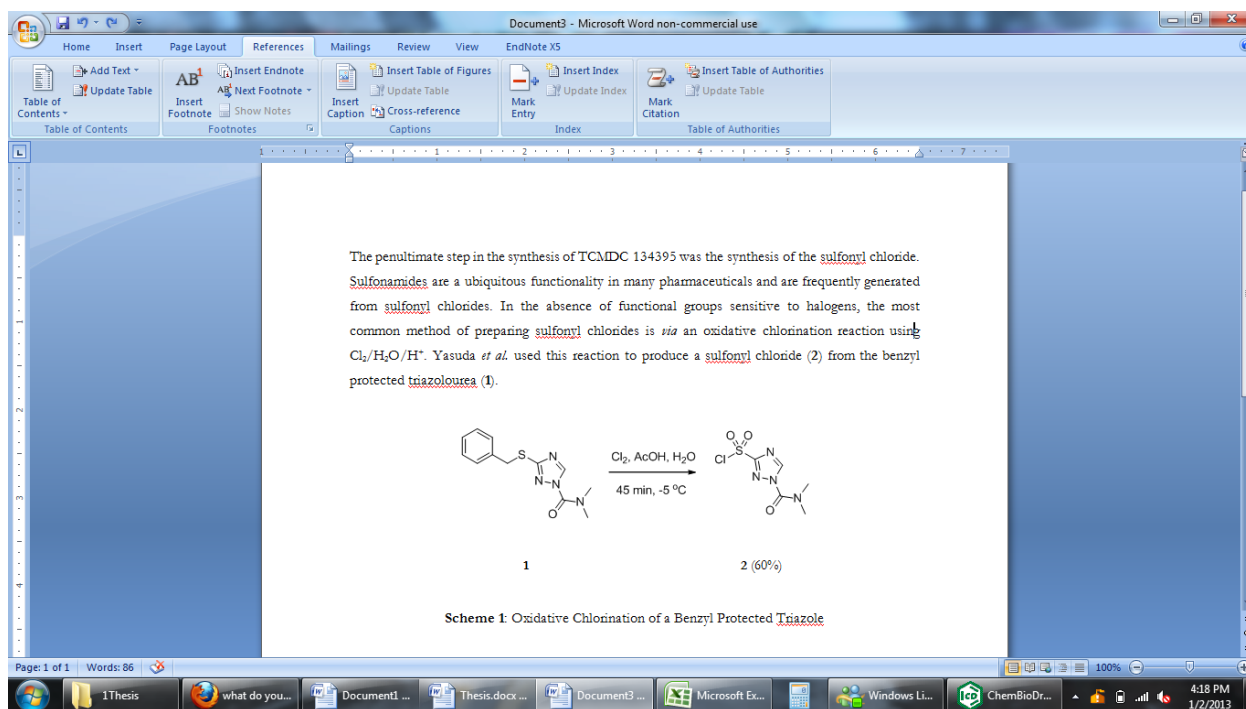
Last, you will need to adjust the column widths to obtain a “chemical equation” that looks the part. Select the entire table, and from “Table tools”, select “Layout”. Under “AutoFit”, select “AutoFit contents”. Move the entire table to the centre of the screen in the usual way (select the entire table and then, under “Paragraph”, choose centre alignment). You should now have a table that looks like this:



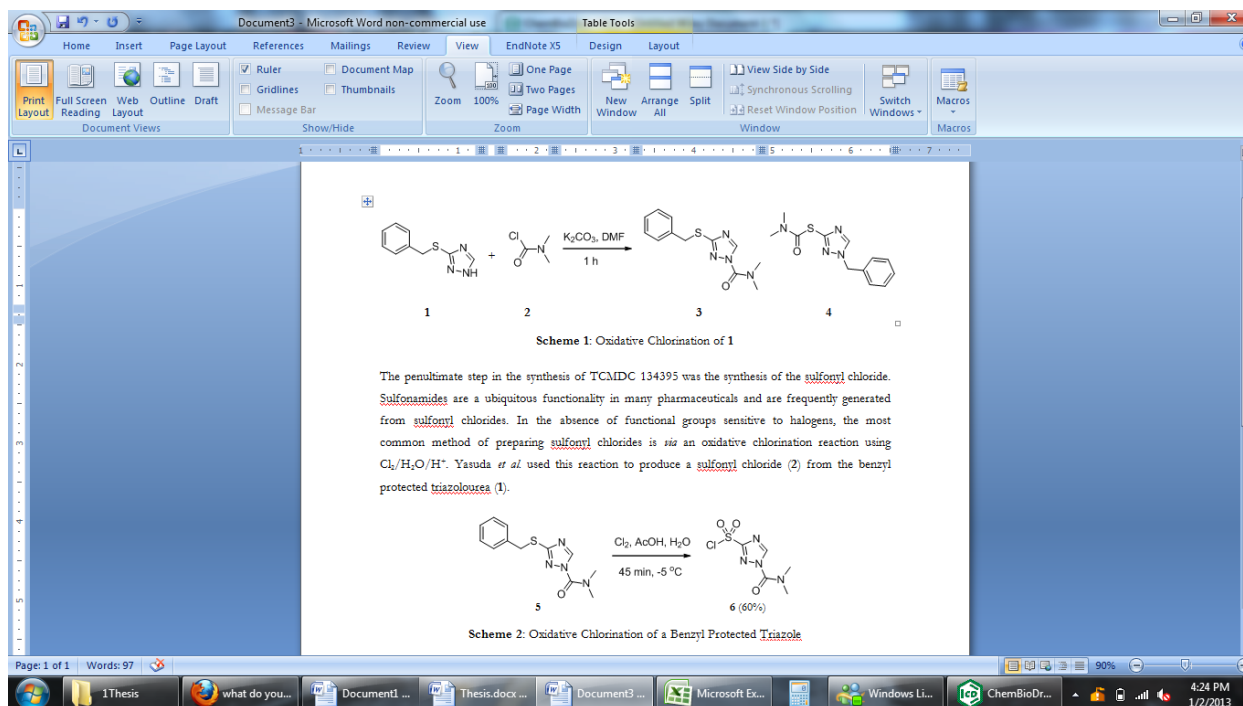
Those lines are unsightly, and you don’t need them now. Select the entire table and from “Table tools” select “Borders” and choose the “No borders” option. You should have something that looks like this:



To do so, place the text cursor (the little blinking “|”) in a spot in the document corresponding to where you want the reference to appear. In my case, it will be within the set of parentheses containing the text “**REFERENCE GOES HERE**”. From the “References” tab, select “Cross-reference”. Under “Reference type”, select “Chemical” (or whatever you called it earlier). Select whichever number corresponds to the chemical you wish to make reference to. Ensure that the drop-down box under “Insert reference to” is set to “Only label and number”. If you specified yields, it will make identification of the correct number simpler. Click “Insert”. Your reference is complete. Make reference to any and all chemicals in a similar fashion. You’ll notice that the formatting is retained from the caption, such that the reference in my case is also in bold:



Now I want to insert another chemical equation but in this case, before this block of text. In the manner described earlier, I have done so, and the document looks like this now:



The numbers have updated themselves: Great! But the references in the text are now wrong. That's easily remedied, albeit by using a fairly odd trick. Press "Print preview", and then "Close print preview". The references will now have corrected themselves. It's not necessary to do this until you're ready for publishing, but it can't hurt. A similar phenomenon will occur if you cut & paste the entire table entry to an earlier or later point in the document.

Some Important Points

The anchor to which all the references are tied is the caption, not the chemical image itself. Deleting the image makes no difference however, if you delete the caption then you will muck up all references to this (now non-existent) caption. If you delete the caption, then refresh the document with "Print preview" then all references to the (now non-existent) caption will now read **Error! Reference source not found.**

From this, you might assume that anything (such as text) can act as the anchor. Not so. In my experience, if you try to label a piece of text with a caption then everything seems to be working. But when you attempt to insert a reference to this caption then, as long as there is text that precedes the label in the sentence, then the reference will contain all of this preceding text.

There is – as far as I'm aware – no way to format all the chemical drawings in your document at once (not if you're using ChemDraw). The implication of this is that you will need to pick a style at the beginning of your document and stick with it, unless you want to put up with changing the style of chemical drawings manually for each drawing. It's probably beneficial to use a smaller "chemical font", such as the ACS setting in ChemDraw.

When messing around with tables in Word, you will likely find that Word will leave seemingly random spaces into the table, such that the entries in some cells are aligned differently to others. If that occurs, then the first thing to do is remove any and all superfluous spaces and paragraphs. This should tidy things up.

It is likely that you will want to conserve as much space in your document as possible. To that end, I recommend removing all "padding" from your tables. To do so, select all the cells in your table, and then from the "Home" tab, select "Paragraph". Set "Spacing" for both "Before" and "After" to 0 pt, and ensure that "Line spacing" is set to "Single". The contents of your table will now have effectively no padding between the table lines and the data within each cell.

I developed this technique when I was writing my thesis because I didn't want to learn LaTeX, and because I didn't want to experience the horror of night-before labeling. This technique was a good solution for me, but there are probably advanced possibilities that I'm not as yet aware of. If you've got any feedback, or you know a new trick, then send it to me at jcro3392@uni.sydney.edu.au and feel free to distribute this to your friends and colleagues. I thought it was a pretty nifty trick.