Meet the Molecules in Chocolate: Informal Opportunities for Building Thematic Molecular Models with Children

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Since their first use by Dalton ca. 1810 *(1),* physical molecular models have been employed by chemists to enhance visualization and understanding of the molecular world. Many descriptions have been reported of molecular modelling activities *(2–6)* together with research and reflections on their use *(7–11)* and relation to computational modelling *(12–15).* Furthermore, giant molecular models have been used to enhance public spaces, such as Jones' Molecules Matter project[1] *(18)* and, most grandly, the Atomium in Brussels, Belgium *(19).*

We have developed the molecular model building activity described here over a number of years' participation in science festivals and science clubs.[2] The initial impetus derived from our observation that the festival visitors could not resist handling and playing with the molecular models we had in our earlier displays. We also observed that another presenters' model bridge building exercise using toy construction kits held its young participants in rapt activity until they had completed the assigned task.[3] We found further encouragement in Laszlo's reflections on Playing with Molecular Models *(9).*

Benefits and Adaptability of This Activity

We shaped the content and experiences of this activity so that participants can meet these pedagogical objectives:

1. Recognize that chemistry is all around us and that everyday items are composed of chemicals
2. Become aware that the properties of everyday items—e.g., chocolate—reflect the chemicals they contain and that particular properties can be ascribed to specific chemicals
3. Discover that chemical structures are well defined and can be represented in a systematic and an aesthetically pleasing manner
4. Perceive that the chemical properties of compounds relate to the three-dimensional structures of their molecules
5. Encounter (some) diverse molecular structures

For classroom use, the pedagogical objectives can be linked to particular curriculum areas. The chocolate molecules may be used as examples of the class of organic chemicals being studied: for example, the triglyceride when studying fats and oils; phenylethylamine and vanillin when studying arenes; and the pyrazines, caffeine and theobromine, when studying heterocycles.

We have run the activity principally at science festivals and science clubs, and we have also used it successfully as a classroom activity for pupils ages 9–12 years, augmented by other practical activities as mentioned above. Because molecular model building is always popular in the classroom, it should be straightforward to adapt it to run with other age groups, with the objectives described above. In order to extend the activity or provide additional challenge for older pupils, it could be run competitively as described by Myers *(3)* or the 3D molecule representations could be omitted, using display or skeletal formulas alone.

Building the Models

Our activity was presented on a set of laminated sheets of paper depicting the key molecules found in chocolate that are imperative to making chocolate a unique, pleasurable eating experience; a sample set of these sheets is available in the online supplement and a selection is depicted below. Each sheet illustrates one molecule as a Chem3D *(20)* "ball and stick" model, and provides an accompanying structural line drawing, molecular formula, and brief description of its association with chocolate (see Figure 1). Participants were challenged to build a model of a molecule, using Molymod molecular model kits

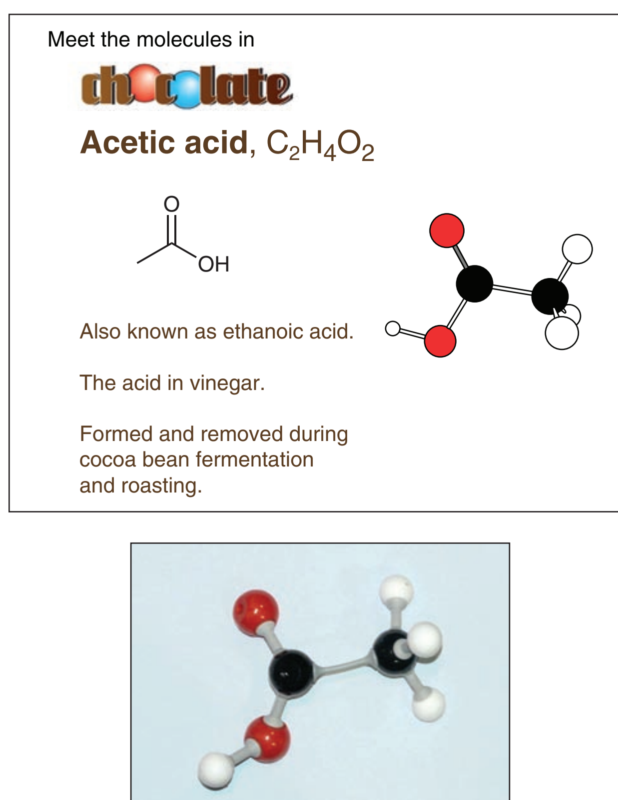

Figure 1. (Top) Acetic acid information handout given to participants; (Bottom) Acetic acid model built by a 3-year-old participant.

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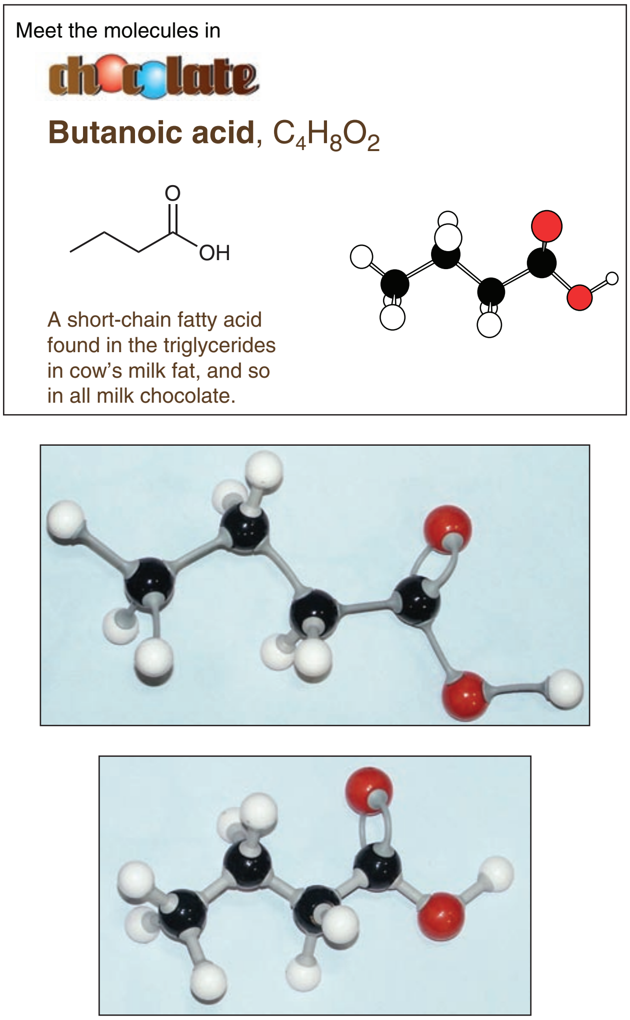

Figure 2. (Top) Butanoic acid information handout given to participants; (Center) Butanoic acid model built by a 10-year-old participant; (Bottom) Butanoic acid model built by a presenter.

(21) with the incentive being the reward of a piece of chocolate on completion of the task to the satisfaction of one of our presenters. We chose these particular model kits because they are pleasant to handle and easy to use. We ensured that the colors of the "balls" (model atoms) matched closely between the handout sheets and the model kits, and that only the requisite "balls" (atoms) were available. We provided further information in the form of additional sheets with molecular modelling instructions, posters, and leaflets describing the chemistry of chocolate in some detail; these resources also served as prompts for our presenters.

The molecules used were chosen both to include the key molecules in chocolate and to provide a range of challenge. Thus the simplest molecule included was acetic acid (Figure 1), which forms during cacoa bean fermentation and is largely removed during roasting *(22)*. The largest molecule included was a triglyceride;[4] successfully modelling this requires teamwork and perseverance (cf Figure 2). We took inspiration for our style of presentation, as well as information on the molecules, from Atkins' beautiful *Molecules* book *(25)*.

Additional detailed information on the molecules in chocolate, and the history and manufacture of chocolate, was obtained from work by Beckett *(22)* and Coultate *(24)*. Useful overviews of the chemistry of chocolate have been provided by Gaskell *(26)*, most thoroughly by Tannenbaum in this *Journal (27)*, and its "chemical charm[s]" summarized by Thakerar *(28)*. The presence in chocolate of the somewhat contentious "bliss molecules" is debated by Di Marzo, Sepe, and co-workers and Beltramo and Piomelli *(29–31)*, and its implications for "chocoholism" is discussed by Rogers and Smit *(32)*. Finally, the recently discovered potential of theobromine (Figure 3) as a lead ingredient for cough medicine—which attracted widespread media attention—was reported by Belvisi and co-workers *(33)*.

To control the variety of molecules the participants could question us about, we selected our chocolate carefully and chose brands with few ingredients. Additional molecules of interest were introduced by selecting flavored chocolates, for example capsaicin from chili-flavored chocolate, zingerone from ginger-flavored chocolate, and piperine from pepper-flavored chocolate[5] *(24, 25, 34)*. Recently, there has been much discussion of the possible health benefits of the flavanols present in cocoa *(35)*, however we have not yet addressed this developing area in our activity.

Although we have not run this activity competitively, it could be adapted following Myers' rules for The Molecular Model Game *(3)*. We have extended the activity to include the well-known chromatographic separation of food colorants in Smarties, M&Ms, and other candies (Meet the Molecules on Chocolate) *(22, 36)*, and a demonstration of the Maillard reaction *(22, 24)*. Further additions, such as melting or crystallizing *(22, 36)* and taste testing *(37, 38)* could be appended. We have also run slightly modified versions as classroom activities. Our further reflections on running this activity are reported below.

Potential Problems and Possible Solutions

We have found that participants in this activity can readily assemble quite complex molecular models by referring to the 3D representation of the molecules provided. However, all but the most chemically literate participants encountered the following problems, mainly problems of perspective perception:

1. *Obscured Atoms:* Care was needed in the orientation of our molecular representations on the sheets as atoms not clearly visible (being obscured by other parts of the structure "nearer the front") were ignored by participants and not included in their models. (Few participants referred to the structural line drawings or molecular formulas unless prompted).
2. *Misinterpretation of Depth Cues (13, 39):* This gave rise to requests for balls of different sizes, especially to represent larger and smaller hydrogen atoms, "near the front", and "back", respectively. Both these problems with perspective were alleviated by the use of sample models, PCs running a looping presentation of the 3D models rotating, and software permitting the participants to manipulate molecular models on screen and change the viewing perspective. Nevertheless, some of the molecules (e.g., sucrose), remain extremely challenging for the novice to build without expert assistance.

3. *Representation of Double Bonds:* This appeared confusing for many participants, primarily due to our use of Chem3D's default "cylindrical bonds" model display setting. This uses shading to represent double bonds, whereas the model kits use two flexible bonds. Such confusion could be alleviated by using Chem3D's "ball and stick" setting (or other software) to produce the 3D representations. Alternatively, photographs of pre-constructed models could be used. The use of space-filling models could also have been used to circumvent this problem, but we avoided these because it is difficult to convert a 2D representation of such models into 3D because much of the structure and the connections between atoms are obscured.
4. *Representation of Geometric Conformation:* The nitrogen atoms in caffeine, theobromine, and pyrazines are in aromatic rings so are trigonal, but the holes in the nitrogen "balls" in the model kits are arranged tetrahedrally. Rather than modify the balls we solved this problem by permitting the use of flexible "stick" bonds (see Figure 3).

All these difficulties arose from the participants' lack of experience in molecular visualization *(7, 12, 13)* and were overcome by guidance from presenters. We observed that those participants who progressed to construct further models gained some of the requisite expertise. The majority of the molecules included in this activity do not contain stereocenters and we chose not to emphasise stereochemistry. Nevertheless, as noted by George and co-workers, model building is an excellent way to understand stereoisomerism *(4)*.

We judged the activity to be successful by the number, range (age and scientific expertise), and enthusiasm of the participants and the duration of their participation. Participants' questions and comments also led us to conclude that the pedagogical objectives were demonstrably achieved. An important factor in ensuring this success is that the activity is founded in both the cognitive and psychomotor domains. Encouragingly, the activity served as a prompt for numerous chemistry conversations, initiated by the participants' questions, such as these. "So there are chemicals in chocolate?" "How much caffeine is there in chocolate?" "Is chocolate addictive?" (see ref *32*) "Why is it called theobromine when there is no bromine in it?" "What have I made?" (prompted by playful exploration of new structures). "Where can I buy these model kits?" (see ref *21*).

Summary

We have described the development and use of a molecular model building activity with a chocolate theme. We have found that the activity meets our pedagogical objectives, drawing in and engaging a wide variety of participants at science festivals; it can also be used successfully in the classroom. We consider the key features to the success of the activity to be carefully presented instruction sheets (with different levels of model complexity and hence challenge), an incentive to complete the model construction, tactile model kits, enthusiastic presenters, and an over-arching link between the models and an area of chemistry of general interest (i.e., the theme). Furthermore, we ascribe the success of the activities to our provision of a molecular playground that harnesses the playful model building instincts of children and adults, enabling them to learn about the delights of the molecular world *(9, 40)*.

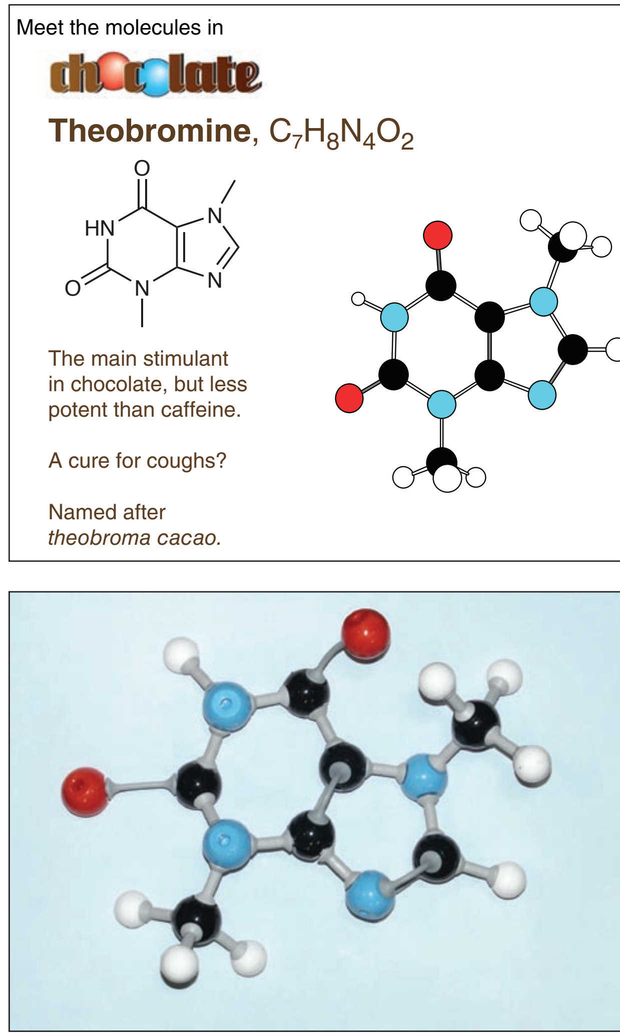

Figure 3. (Top) Theobromine information handout given to participants; (Bottom) Theobromine model built by an 11-year-old participant.

Acknowledgments

We wish to thank all the student presenters who have assisted in this activity; the organizers of the events at which we have presented this activity (*Scientriffic*, Wrexham Science Festival; UWB Science Fun Days; Careers Wales North West / Chemistry at Work; Catalyst Science Discovery Centre; Manchester Museum of Science and Industry); Sue Assinder; Peter Hollamby; Lorrie Murphy; Barnabas and Jonathan Fletcher.

Notes

1. In 2002, Jones and co-workers set the world record for the largest DNA model *(16)*. The *Guinness World Records 2007* book lists a record for the largest carbon nanotube model, built by students and staff at Rice University *(17)*.

2. We have also presented it in the medium of Welsh, Dewch i Gyfarfod y Moleciwlau Mewn Siocled.

3. During the preparation of this manuscript, Jones and co-workers have produced a similar activity, with the incentive of a

print-out of a digital photograph of the modeler and their completed model *(18)*.

4. The relatively small variety of triglycerides present in cocoa butter account for chocolate's sharp melting point of 34 °C, which is just below body temperature, 37 °C; a change in the crystalline form of the triglycerides results in chocolate bloom *(23–24)*.

5. We found suitable brands of chocolate to be: Divine Chocolate (*http://www.divinechocolate.com/* [accessed Jul 2008]), Green and Black's (*http://www.greenandblacks.com/* [accessed Jul 2008]), whose Maya Gold chocolate bar provides an instructive historical link to the origins of chocolate, and, for unusual flavored varieties, Rococo Chocolates (*http://www.rococochocolates.com/* [accessed Jul 2008]). Nevertheless these chocolate bars generally contain soya lecithin as an emulsifier. We did not discuss this in our resources as it is a mixture of structurally somewhat-complicated phosphoglycerides *(22)*.

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Structures of many of the molecules discussed in this article, including caffeine and theobromine, are available in fully manipulable Jmol format in the *JCE* Digital Library at *http://www.JCE.DivCHED.org/JCEWWW/Features/MonthlyMolecules/*.