Understanding molecules by exploring crystal structures

Chemistry, Physics
Target age group: High school/A-Level/University students (16+ y.o.)

Description: This learning module exposes students to the structures of molecules by allowing them to explore common chemicals through crystal structures contained in the Cambridge Structural Database (CSD). Students will be able to visualize 3D chemical structures as a way to understand concepts of bonding, chirality and isomerism. These activities can be run in series as part of a science learning day event or can be incorporated into classroom activities.

Expected Outcomes

- Familiarity with the Cambridge Structural Database (CSD)
- Ability to relate 2D chemical diagram to 3D molecular structure
- Understanding the nature of chirality (right- and left-handed molecules)
- Understanding the nature of isomerism (same chemical formula, different connectivity)
- Understanding the nature of common chemicals found in everyday objects
- Understanding differences between model kits and experimental data

Materials

Required

- Printed hand-outs
- Examples of everyday objects
    - Lemon, sugar, chocolate, mothballs, aspirin
- Computer with internet access
- Molecular model kit

Optional

- 3D printed models of compounds

Unit Outline

1. Investigate chemical compounds in everyday items; select one for further investigation
2. Search on-line database for crystal structures of selected compound
3. Visualize 3D representation of the molecule on the computer and via 3D print and/or VR goggles if available.
4. Build model of molecule from kit; compare 3D crystal structure with model structure.
5. Learn about special properties of compounds
6. Discussion

Section descriptions

Section 1 - Investigate chemical compounds in everyday items; select one for further investigation

Instructor activities

- Present common objects and the specific chemical compound found in each item.
  - Chocolate –
    - Cocoa butter (JEMSAW) – fatty acid, double bonds
  - Lemon
    - Citric acid (CITRACT10) – acid, double bonds (to O atoms)
  - Sugar cube
    - Sucrose (SUCROS01) – chirality
  - Aspirin
    - Aspirin (ACSALA) – aromatic bonds, medicine
  - Mothballs
    - Camphor (UGAHUF) – chirality
- Discuss each molecule's interesting features
  - Listed above
- Introduce X-ray crystallography as a technique used by scientists to determine the 3D shape of chemical compounds. Discuss discovery of the structure of DNA and how this was helped by X-ray crystallography. https://en.wikipedia.org/wiki/X-ray_crystallography for information.

Student activities

- Choose compound to investigate.

Section 2 - Search on-line database for crystal structures of selected compound

Instructor activities:

- Present concept of the CSD (https://www.ccdc.cam.ac.uk/solutions/csd-system/components/csd/):
  - Database of 1 million experimental crystal structures
  - Contributed by researchers all over the world
  - Each structure has its own identifier: REFCODE
- Let students choose a molecule to investigate / For classroom activity, divide students into small groups of 2-3 and assign molecules to investigate (or let groups choose).
- Assist students with searching the CSD
  - Name search vs. refcode?

Student activities:

- Search CSD for compound via refcode or by name
- Draw 2D diagram on handout.
- Write the common name of the molecule on the handout.
- Write down where you might find this compound in every day life.

Section 3 - Visualize 3D representation of the molecule

Instructor activities

- Assist students with 3D visualization; manipulating the molecule on the screen
    - Help students understand different bonding representations
- Provide 3D printed model

Student activities

- Look at 3D representation(s), notice differences between2D and 3D representations

Section 4 - Build model from kit; compare 3D crystal structure with model structure

Instructor activities

- Assist students with building models and comparisons
- Help students see differences in geometry, bond type, chirality

Student activities

- Construct model of the molecule using a 3D model kit.
- Compare the model to the 3D representation on the computer or 3D printed model

Section 5 - Learn about special properties of compounds

Instructor activities

- Explain concepts of chirality, bonding, and acidity to students.

Student activities

- Review chosen molecules and identify which special properties exist.

Section 6 – Discussion

Instructor activities

- Discuss with students what they learned about chemicals in every-day objects, crystallography, 3D representations of molecules and special properties of molecules. If age-appropriate, ask each student/group to present some information about their molecule
- Key points/questions for discussion:
    - What did you notice about all the molecules we studied?
        - They are all comprised of the same elements (C, H, N, O)
        - They have very different shapes
        - Explore similarities between "chemicals" (i.e. pharmaceutical compounds, synthetic compounds) and natural compounds (i.e. sugar, citric acid). Point out that a molecule is the same whether it is made by a plant or animal naturally or whether it is made in a laboratory by a chemist. It will always have the same properties.

- What did you learn about X-ray crystallography?
    - How scientists can determine structures of molecules.
    - What crystals are and why they are important
    - How diffraction works (for advanced students)
    - Important discoveries made possible by X-ray diffraction
- What did you learn about the CSD?
    - Collection of structures
    - Important for understanding what is known and what could be known
- What differences did you notice between the 3D crystal structure and the model you built? Explain those differences.
    - 3D crystal structure is real experimental data; model is generalized and averaged over many observations
    - Model is more flexible in arrangement (rotatable torsions); 3D structure is rigid, but varied (bond ranges, valence angles)
- What special properties did you learn about?
    - Chirality is important because it can cause different effects (smells/tastes, drug/poison)
    - Different bonds are represented differently (single, double, aromatic).

Using this activity in the classroom:

This activity was originally designed as part of The Cambridge University Science Festival. If you are interested in using this as part of your course curriculum, please see below for some places where this might fit into your classroom.

Guide to Science Curriculum from Ontario, Canada:

http://www.edu.gov.on.ca/eng/curriculum/secondary/2009science11_12.pdf

Areas where this activity might fit in your courses:

Grade 11 (University Prep Course) - Overall Expectations

By the end of this course, students will:

B1. analyse the properties of commonly used chemical substances and their effects on human health and the environment, and propose ways to lessen their impact; (pg 94)

B2. investigate physical and chemical properties of elements and compounds, and use various methods to visually represent them; (pg 94)

B2.6 build molecular models, and write structural formulae, for molecular compounds containing single and multiple bonds (e.g., CO2, H2O, C2H4), and for ionic crystalline structures (e.g., NaCl) (pg. 96)

Grade 12 (University Prep Course) - Overall Expectations

By the end of this course, students will:

B2. investigate organic compounds and organic chemical reactions, and use various methods to represent the compounds; (pg 108)

B3. demonstrate an understanding of the structure, properties, and chemical behaviour of compounds within each class of organic compounds. (pg 108)

B2.3 build molecular models for a variety of simple organic compounds (pg 108)

B3.5 explain the concept of isomerism in organic compounds, and how variations in the properties of isomers relate to their structural and molecular formulae (pg. 109)

C3. demonstrate an understanding of atomic structure and chemical bonding, and how they relate to the physical properties of ionic, molecular, covalent network, and metallic substances. (pg 110)

C3.5 describe a Canadian contribution to the field of atomic and molecular theory (e.g., the work of Richard F.W. Bader of McMaster University on electronic density in small molecules; the work of Robert J. LeRoy of the University of Waterloo on the mathematical technique to determine the atomic radius of molecules known as the LeRoy Radius; **the work of Ronald J. Gillespie of McMaster University on the VSEPR model)** (pg. 111)

Keep in touch:

We'd love to learn more about your experiences using this activity in your classroom or science festival. Please share your feedback with us at teaching@ccdc.cam.ac.uk

Thanks!
- The CCDC Education Team

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Workshop.

Pick a recode answer sheet

STEP 1 Pick a refcode and write it down.

STEP 2 From 1 million crystal structures find your chosen refcode using 1 of the 4 options on the "Pick a refcode" workshop sheet.

STEP 3 Write down the compound name of your structure.

STEP 4 Find the 3D printed molecule and draw it in the space below.

STEP 5 Find and write down the common name of your structure.

STEP 6 Where might you find your structure in everyday life?

STEP 7 Build 3D molecule of the structure using the model kits.

STEP 8 View your structure using the VR headsets. Can you see 3D hologram?

STEP 9 Collect your sticker and chocolate.

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Workshop.

Pick a refcode?

- UGAHUF
- RERXOB
- RERXIV
- ACSALA
- SUCROS01
- CITRAC10
- JEMSAW

Choose one of the **4** following options to identify your compound...

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Workshop.

1 QR Code

Identify your compound using the QR code app.

UGAHUF

RERXOB

RERXIV

ACSALA

SUCROS01

CITRAC10

JEMSAW

Write down your compound name on your answer sheet.

UGAHUF : 1,7,7-Trimethylbicyclo(2.2.1)heptan-2-one
Space Group: P 2_1 2_1 2_1 (19), **Cell:** *a* 8.9277(2)Å *b* 27.0359(5)Å *c* 7.3814(1)Å, *α* 90° *β* 90° *γ* 90°

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Workshop.

2 Access Structures

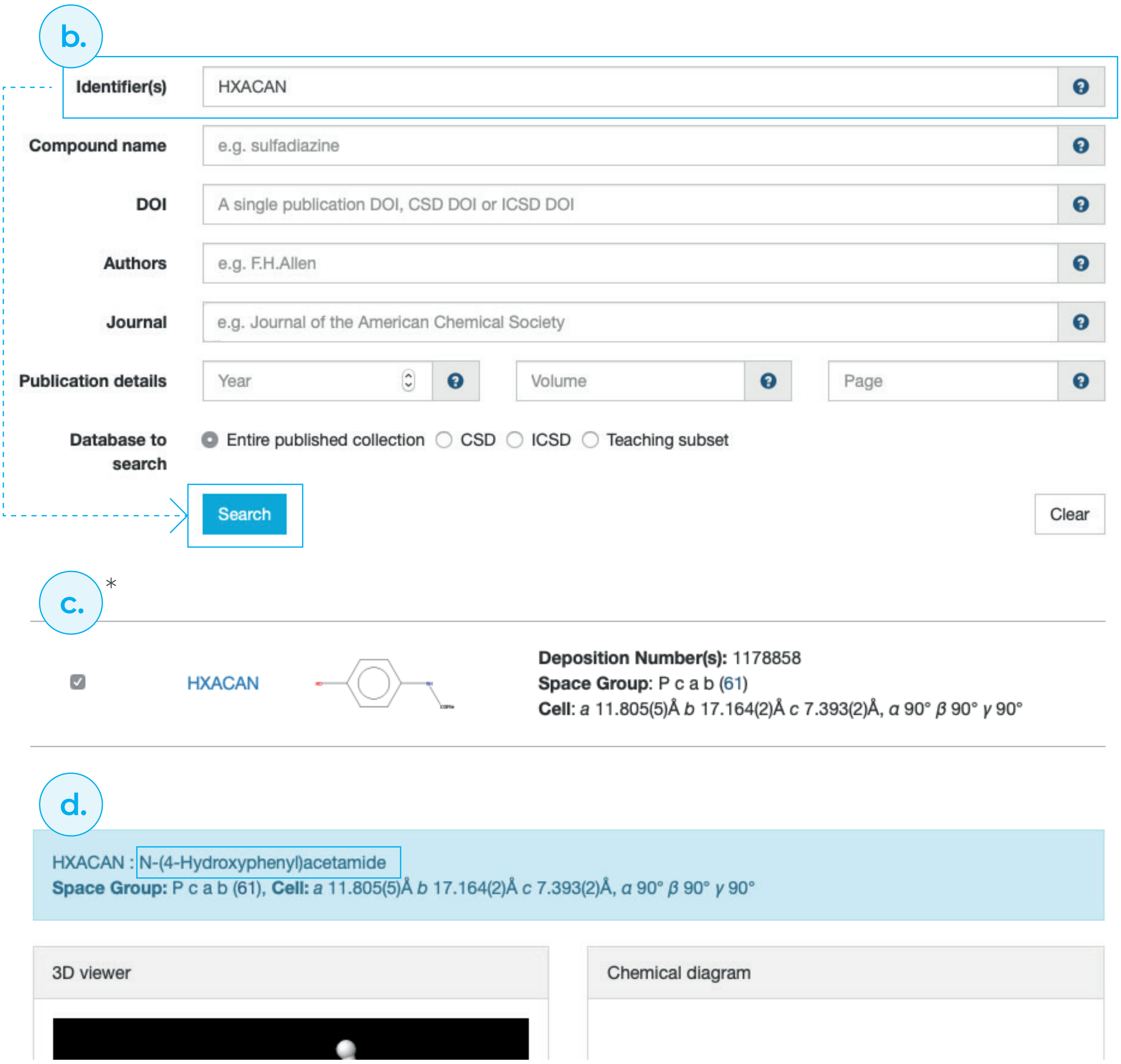
Identify your compound using Access Structures.

a. On your phone or laptop go to: www.ccdc.cam.ac.uk/structures

b. Type your refcode into the Identifier(s) section and click Search.

c. Click on your refcode (this only applies to ACSALA & JEMSAW)*.

d. Write down your compound name on your answer sheet.



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Workshop.

3 ConQuest

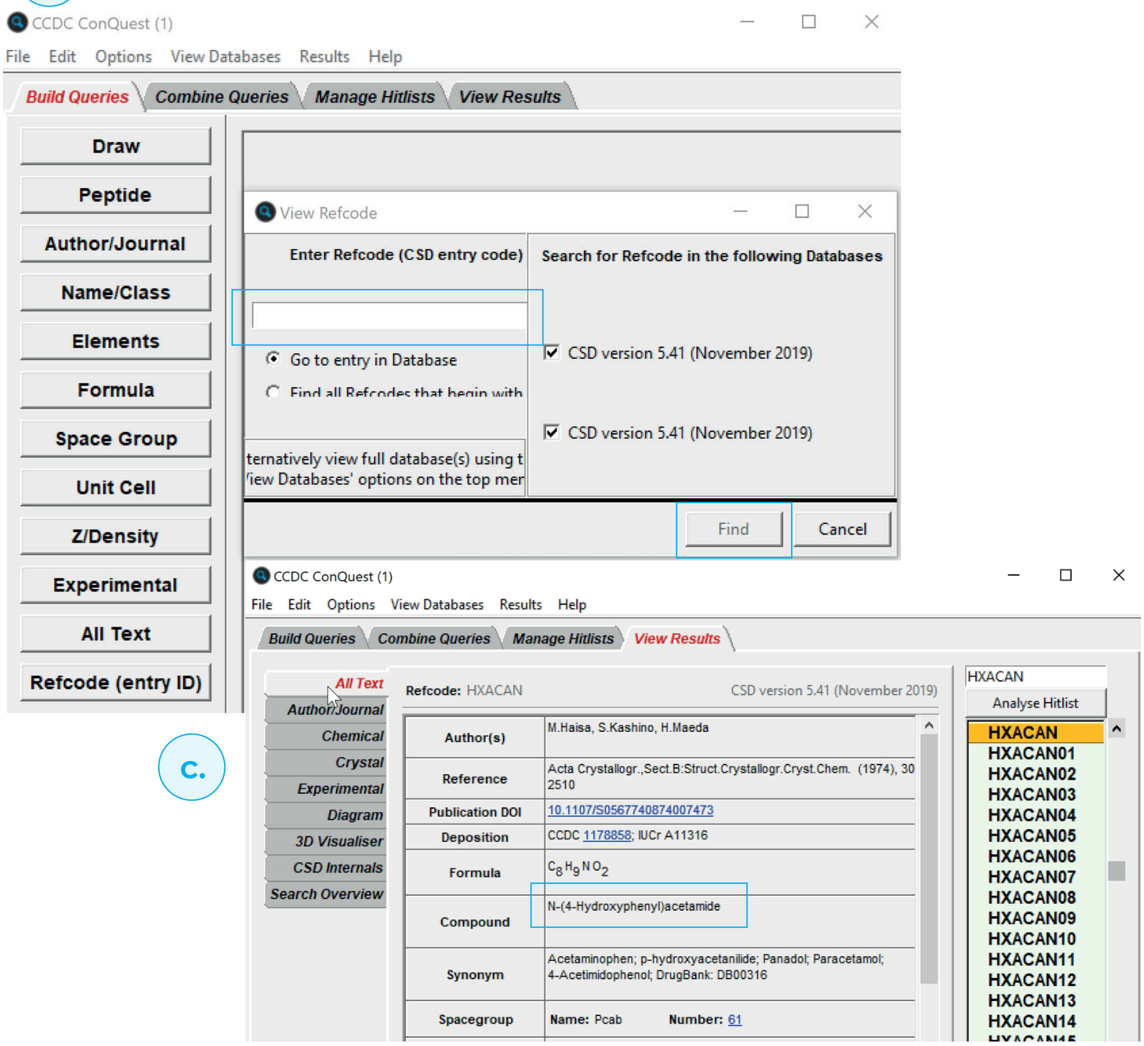
Identify your compound using ConQuest.

a. Open ConQuest on the computer.

b. Click on **Refcode (entry ID)** button, type your refcode in the View Refcode window and click **Find**.

c. Click on **All Text** and write down the compound name for your selected refcode on your answer sheet.

b.



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Workshop.

4 Mercury

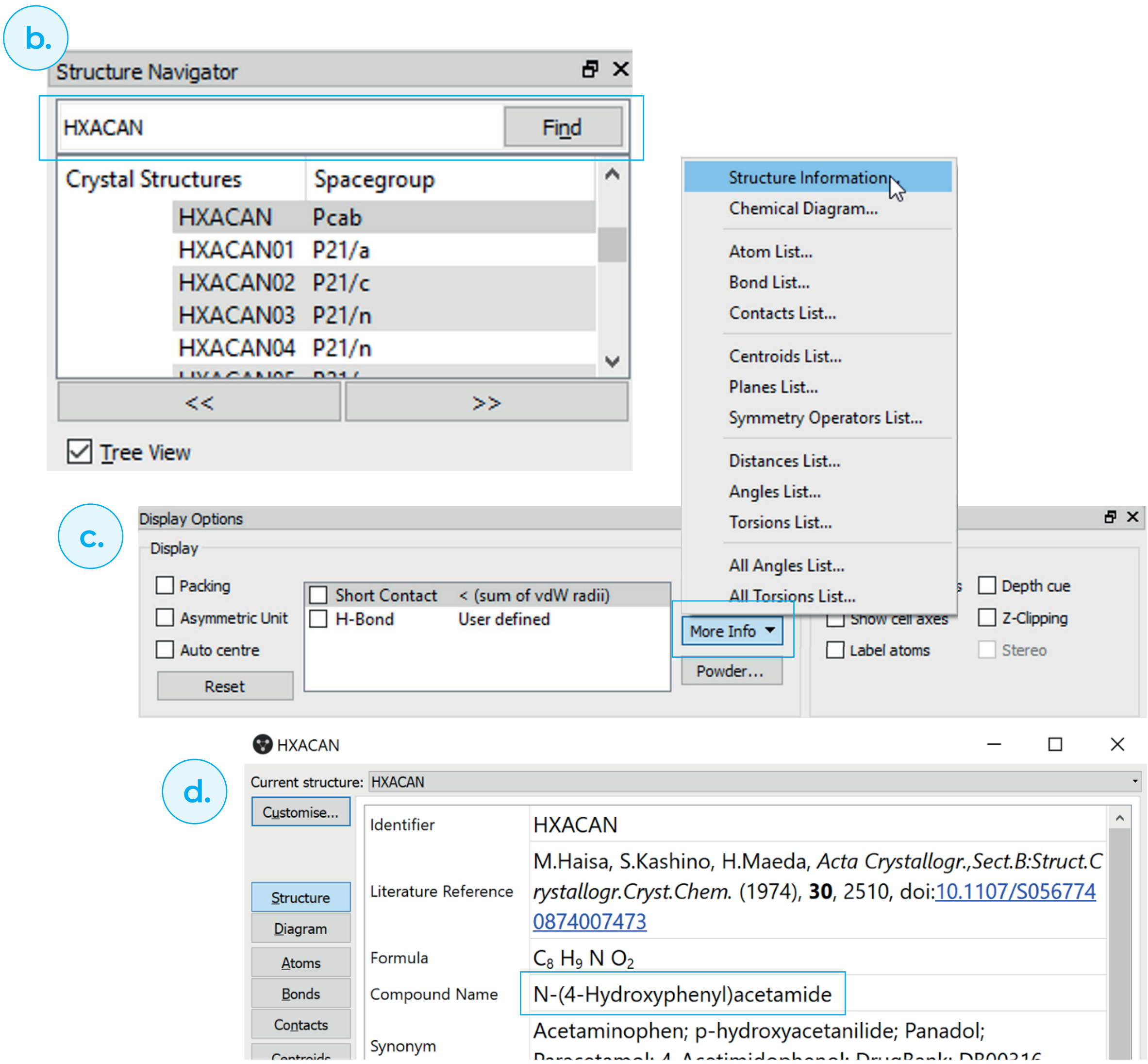
Identify your compound using Mercury

a. Open Mercury on the computer.

b. In the **Structure Navigator** window, type your refcode and click **Find**.

c. Select **More Info** button, then **Structure information...**

d. Write down your compound name on you answer sheet.



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Aspirin.

Compound name:
2-acetoxybenzoic acid

Compound name:
Aspirin

Found in:
Pain relief medication

Aspirin is used mainly as a pain relief medication but has a number of other appliations such as:

- Reducing swelling and inflammation for conditions such as arthritis.
- Reduce the impact of a fever by blocking certain natural substances in your body.
- Due to these applications aspirin is classed as a nonsteroidal anti-inflammatory drug (NSAID).
- Aspirin as we know it came about in the late 1890's when chemist Felix Hoffmann used it to alleviate his father's rheumatism.

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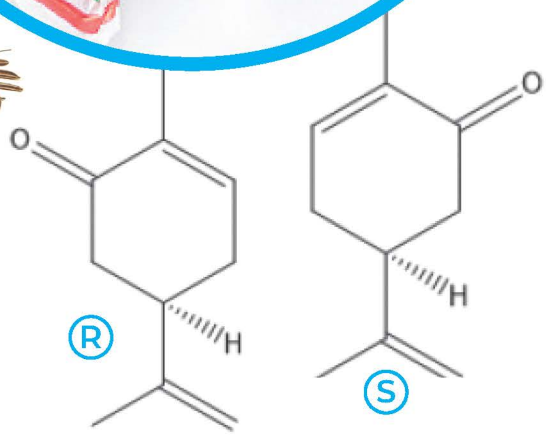
Carvone.

Compound name:
2-Methyl-5-(1-methylethenyl)-2-cyclohexen-1-one

Compound name:
Carvone

Found in:
Toothpaste, cumin, caraway and spearmint sweets



Carvone has 2 different isomers; there's a different spatial arrangement of their atoms. This difference results in different chemical properties.

(R)-stereoisomer

- In the "R" isomer when the H atom is pointing back into the plane of the paper, with the "O" to the left as you see it.
- R-Carvone has a strong spearmint smell and is used for flavouring both mint sweets and toothpaste.
- Uses: mosquito repellent.

(S)-stereoisomer

- In the "S" isomer when the H atom is pointing back into the plane of the paper, the "O" atom is to the right as you see it.
- S-Carvone is present in cumin and caraway seeds and many spices used since roman times.
- Uses: prevents potatoes sprouting during storage.

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Chocolate.

Compound name:
Bahia β6 cocoa butter

Compound name:
heobroma oil,
cocoa butter

Found in:
Makes various forms of chocolate

Cocoa butter is a pale-yellow, edible vegetable fat extracted from the cocoa bean. It is used to make chocolate, as well as some ointments and toiletries.

- Cocoa butter has a cocoa flavour and aroma.
- The melting point of the form of cocoa butter used in chocolate is just below human body temperature which means it melts in the mouth when you eat it
- The earliest known use of cocoa beans is dated at around 1750 BC.
- Cocoa butter has at least 6 different polymorphs (crystal forms)

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Citric Acid.

Compound name:
2-hydroxypropane-1,2,3-tricarboxylic acid

Compound name:
Citric acid

Found in:
Citrus fruit, flavourings, bath bombs, cleaning fluid

Citric acid can be found naturally in citrus fruit such as oranges and lemons but can be produced artificially and has been found to have many applications such as:

- It is used in strong flavourings as it is one of the stongest edible acids.
- It is used a lot in soft and fizzy drinks.
- Citric acid is great for creating the fizz in bath bombs.
- It is also used in cleaning fluids because it kills bacteria, mould, mildew and is a great disinfectant.

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Sucrose.

Compound name:
β-D-Fructofuranosyl-α-D-glucopyranoside

Compound name:
Sugar

Found in:
Flavouring and preservatives

Sucrose is the chemical name of table sugar and has been used since ancient times as both a flavouring and preservative.

- Generally it is used to make food sweeter and add flavour to bland meals.
- The two main sources or sugar are from sugar cane and sugar beet where sucrose is naturally produced.
- About 178 million tonnes of sugar were produced worldwide in 2019.

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