

Workshop.

Pick a refcode?



UGAHUF

RERXOB

RERXIV

ACSALA

SUCROS01

CITRAC10

JEMSAW



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

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 2₁ 2₁ 2₁ (19), Cell: a 8.9277(2) Å b 27.0359(5) Å c 7.3814(1) Å, α 90° β 90° γ 90°

Workshop.

2 Access Structures



Identify your compound using Access Structures.

- On your phone or laptop go to: www.ccdc.cam.ac.uk/structures
- Type your refcode into the Identifier(s) section and click Search.
- Click on your refcode (this only applies to ACSALA & JEMSAW)*.
- Write down your compound name on your answer sheet.

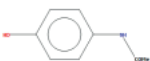
b.

Identifier(s)	HXACAN			?
Compound name	e.g. sulfadiazine			?
DOI	A single publication DOI, CSD DOI or ICSD DOI			?
Authors	e.g. F.H.Allen			?
Journal	e.g. Journal of the American Chemical Society			?
Publication details	Year	Volume	Page	?
Database to search	<input checked="" type="radio"/> Entire published collection <input type="radio"/> CSD <input type="radio"/> ICSD <input type="radio"/> Teaching subset			
	<input type="button" value="Search"/>			<input type="button" value="Clear"/>

c.

☒

HXACAN



Deposition Number(s): 1178858

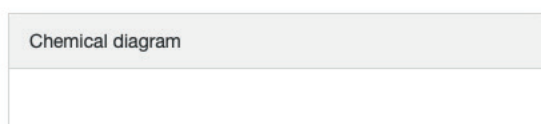
Space Group: P c a b (61)

Cell: a 11.805(5)Å b 17.164(2)Å c 7.393(2)Å, α 90° β 90° γ 90°

d.

HXACAN : N-(4-Hydroxyphenyl)acetamide

Space Group: P c a b (61), Cell: a 11.805(5)Å b 17.164(2)Å c 7.393(2)Å, α 90° β 90° γ 90°



Workshop.

3 ConQuest



Identify your compound using ConQuest.

- Open ConQuest on the computer.
- Click on **Refcode (entry ID)** button, type your refcode in the View Refcode window and click **Find**.
- Click on **All Text** and write down the compound name for your selected refcode on your answer sheet.

b.

CCDC ConQuest (1)

File Edit Options View Databases Results Help

Build Queries **Combine Queries** **Manage Hitlists** **View Results**

Draw

Peptide

Author/Journal

Name/Class

Elements

Formula

Space Group

Unit Cell

Z/Density

Experimental

All Text

Refcode (entry ID)

View Refcode

Enter Refcode (CSD entry code) Search for Refcode in the following Databases

☒ Go to entry in Database ☒ CSD version 5.41 (November 2019)

☐ Find all Refcodes that begin with ☒ CSD version 5.41 (November 2019)

alternatively view full database(s) using the 'View Databases' options on the top menu

Find **Cancel**

c.

CCDC ConQuest (1)

File Edit Options View Databases Results Help

Build Queries **Combine Queries** **Manage Hitlists** **View Results**

All Text

Author/Journal

Chemical

Crystal

Experimental

Diagram

3D Visualiser

CSD Internals

Search Overview

Refcode: HXACAN CSD version 5.41 (November 2019)

Author(s)	M. Haisa, S. Kashino, H. Maeda
Reference	Acta Crystallogr., Sect. B: Struct. Crystallogr. Cryst. Chem. (1974), 30, 2510
Publication DOI	10.1107/S0567740874007473
Deposition	CCDC 1178858; IUCr A11316
Formula	C ₈ H ₉ N ₂ O ₂
Compound	N-(4-Hydroxyphenyl)acetamide
Synonym	Acetaminophen; p-hydroxyacetanilide; Panadol; Paracetamol; 4-Acetimidophenol; DrugBank: DB00316
Spacegroup	Name: Pcab Number: 61

HXACAN

Analyse Hitlist

HXACAN

HXACAN01

HXACAN02

HXACAN03

HXACAN04

HXACAN05

HXACAN06

HXACAN07

HXACAN08

HXACAN09

HXACAN10

HXACAN11

HXACAN12

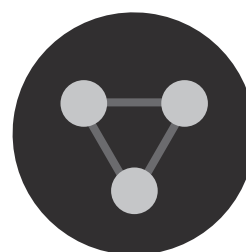
HXACAN13

HXACAN14

HXACAN15

Workshop.

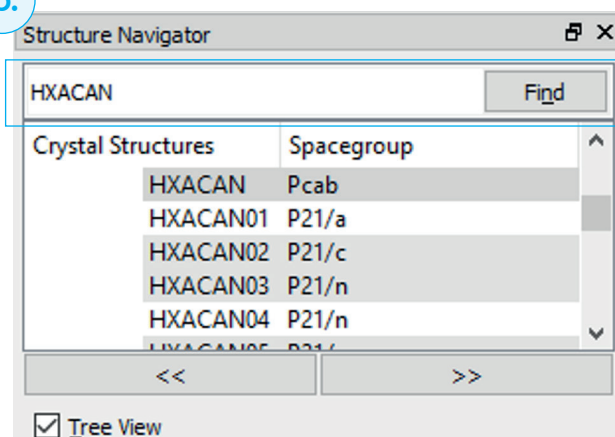
4 Mercury



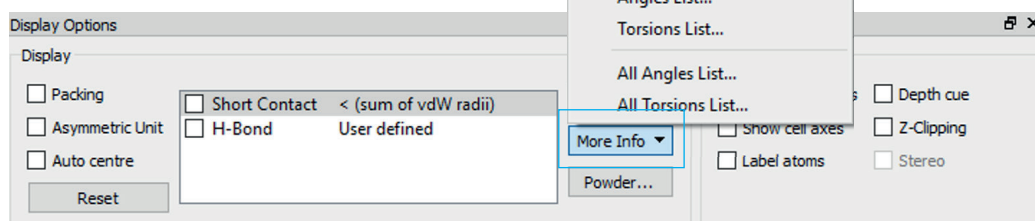
Identify your compound using Mercury

- Open Mercury on the computer.
- In the **Structure Navigator** window, type your refcode and click **Find**.
- Select **More Info** button, then **Structure information...**
- Write down your compound name on you answer sheet.

b.



c.



d.

