

Composition & General Info

Write nomenclature, structure, general properties, structure elucidation and the drug product composition, with molecular weight, CAS number, elemental analysis, salt factor and unit weight checked by calculation.

WRITES

3.2.S.1.1

3.2.S.1.2

3.2.S.1.3

3.2.S.3.1

3.2.P.1

PRODUCT TYPE

Small molecule

GUIDANCE IT FOLLOWS

ICH M4Q(R1) 3.2.S.1,
3.2.S.3.1, 3.2.P.1; ICH
Q6A; FDA Inactive
Ingredient
Database

TIME TO LEARN

About 20 minutes
with the example

Open the tool at <https://app.cmcfy.com/app/composition-studio.html>. This guide is also online at <https://cmcfy.com/guides/composition-studio.html>

1. What this module does

This is usually the first module you open for a new product. It writes the identity sections of the drug substance (3.2.S.1.1 to 3.2.S.1.3 and 3.2.S.3.1) and the description and composition of the drug product (3.2.P.1).

Every number a reviewer can recalculate is recalculated: the molecular weight from the formula (IUPAC atomic weights), the CAS check digit, the elemental analysis against theory, the salt-to-free-base factor, the sum of the composition against the target unit weight, and the active quantity against the label strength.

What you get

- Word or PDF files for 3.2.S.1.1 Nomenclature, 3.2.S.1.2 Structure, 3.2.S.1.3 General properties, 3.2.S.3.1 Elucidation of structure and 3.2.P.1 Description and composition.
- A summary file for the QOS Composer & Dossier Assembler and the Process & Controls Writer (it reads the composition as the unit formula).

2. Before you start

Have these ready. You can still start with the example data and replace it piece by piece.

- INN or USAN, company code, IUPAC name and CAS number.
- Molecular formula of the salt and of the free base, and the molecular weight you state in the dossier.
- Stereochemistry, and the techniques that confirm structure and configuration (NMR, MS, IR, X-ray, optical rotation).
- Elemental analysis results (found %), if you have them.
- The composition per unit with function and quality standard of each component, the strength, the target unit weight and the container closure.

Your data stays on your computer. The bar under the title counts every network request the page makes; it stays at 0 because your data never leaves your computer. [Download offline](#) [copy](#) saves a single file that opens from your own computer with all network access blocked, for air-gapped PCs.

3. Step by step with the example

Open the tool at app.cmcfy.com/app/composition-studio.html. The example is loaded when the page opens, so every panel already has realistic data. Follow the steps to see how it works, then replace the example with your own data.

1 Choose what to write

In panel 1 choose [Sections to write](#): both drug substance and drug product, or only one of them. The panels you do not need are hidden. Set [Submission region](#) to US, EU or both.

CMCfy Composition & General Info Projects All modules Training Security Runs entirely on this device Training guide

PROJECTS Keep this work in a project, with version history and your company logo on every report. Choose projects folder Keep in this browser

- Network requests since load: 0**
Counted live by your browser. Your data never leaves this device.
- Works offline**
Everything the tool needs is inside this page.
- Locked offline copy**
Save a single file that opens from your own computer with all network access blocked.

3.2.S.1.1 3.2.S.1.2 3.2.S.1.3 3.2.S.3.1 3.2.P.1 Save project Open project Start blank Load example

Write the nomenclature, structure, properties, structure elucidation and drug product composition sections. Molecular weight, elemental analysis, CAS check digit, unit weight and salt correction are all checked by calculation.

Guidance: ICH M4Q(R1) 3.2.S.1, 3.2.S.3.1, 3.2.P.1; ICH Q6A; FDA Inactive Ingredient Database

1 · SCOPE

Sections to write Submission region

Drug substance and drug product US: FDA (NDA, ANDA, BL)

Drug product name

CMX-101 Tablets, 50 mg

2 · DRUG SUBSTANCE: NOMENCLATURE AND STRUCTURE

INN or USAN Company code

Cimexafen hydrochloride CMX-101

Chemical name (IUPAC)

4-[(3S)-3-(4-fluorophenyl)piperidin-1-yl]-N-methyl-2-oxo-1

CAS registry number Molecular formula (salt)

RESULT

Drug substance and drug product information

C22H23FN3O2Cl, 415.89 g/mol calculated from IUPAC atomic weights.

MOLECULAR WEIGHT (CALCULATED)	SALT FACTOR	UNIT WEIGHT (SUM)
415.89 g/mol	1.0961	340.27 mg
ACTIVE PER UNIT		
55.07 mg		

ELEMENTAL ANALYSIS AGAINST THEORY

ELEMENT	FOUND (%)	CALCULATED (%)	DIFFERENCE
C	63.41	63.54	-0.13
H	5.61	5.57	+0.04

The tool opens with the example product CMX-101 Tablets, 50 mg already loaded.

2 Enter nomenclature and structure

Fill the INN, code, chemical name, CAS number and both molecular formulas. Write the formula as you would in the dossier, for example C22H22FN3O2.Cl. Type the molecular weight you state; the tool calculates its own and compares them.

3 Read the result

The result panel shows the formula as calculated (C22H23FN3O2Cl), the molecular weight from IUPAC atomic weights (415.89 g/mol), the salt factor (1.0961), the sum of the composition (340.27 mg) and the active quantity per unit (55.07 mg).

RESULT

Drug substance and drug product information

C22H23FN3O2Cl, 415.89 g/mol calculated from IUPAC atomic weights.

MOLECULAR WEIGHT
(CALCULATED)
415.89 g/mol

SALT FACTOR
1.0961

UNIT WEIGHT (SUM)
340.27 mg

ACTIVE PER UNIT
55.07 mg

Calculated molecular weight, salt factor, unit weight and active per unit.

4 Check elemental analysis and composition tables

The tables under the result compare each element found with theory, and list the composition with the total. A difference of more than 0.4% absolute in elemental analysis, or a total that does not match the target unit weight, raises an alert.

ELEMENTAL ANALYSIS AGAINST THEORY

ELEMENT	FOUND (%)	CALCULATED (%)	DIFFERENCE
C	63.41	63.54	-0.13
H	5.61	5.57	+0.04
N	10.02	10.10	-0.08

Elemental analysis against theory.

5 Resolve alerts

The example has no blocking alerts in US mode. Switch the region to EU and alerts appear for each excipient whose quality standard cites USP/NF only: add the Ph. Eur. reference to fix them.

ALERTS TO RESOLVE

No alerts. The data meets every rule checked.

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Preview and download

Under **Preview and download by CTD section**, press **Preview** next to 3.2.S.1.1 to see the document with its review, then download Word or PDF. Press **Download summary for QOS** to save the summary file.

Preview and review before download Close

Review
Checked on this device: gaps in the data, gaps in the report against ICH and regional expectations, and differences from the protocol.

No open gaps

No open gaps: the data, the report and the protocol (if given) match every rule checked, or you accepted the rest. Read the preview before you sign.

Compare with the protocol
Load or paste the approved protocol. Every requirement and acceptance criterion in it is looked for in the report.

Paste the protocol text here, or load the file.

Load protocol file **Compare**

AI review against guidance
AI reads the report, the protocol and the data against the ICH, FDA or EMA requirements for these sections, and lists gaps with the guideline it applies, protocol and data mismatches, and how to fix them. You see exactly what is sent before anything leaves this device. Results and pass/fail are not changed.

Run AI review

3.2.S.1.1 Nomenclature
CMX-101 Tablets, 50 mg - US (FDA)

Recommended INN / USAN	Cimexafen hydrochloride
Chemical name	4-[(3S)-3-(4-fluorophenyl)piperidin-1-yl]-N-methyl-2-oxo-1,2-dihydroquinoline-6-carboxamide hydrochloride
CAS registry number	2412345-67-4
Company code	CMX-101

Draft prepared with CMCfy Composition & General Info on 2026-10-29. Guidance applied: ICH M4Q(R1) 3.2.S.1, 3.2.S.3.1, 3.2.P.1; ICH Q6A; FDA Inactive Ingredient Database. To be reviewed and approved by a qualified person before submission.

Download Word (.docx) **Download PDF**

Each section opens in a preview with the gap review on the left.

4. Field reference

Every input in the tool, panel by panel. Tables accept rows pasted straight from Excel, comma-separated text, or a loaded file; check the columns after loading a file. Fields marked “when it applies” appear only for the choices that need them.

1 - Scope

FIELD	WHAT TO ENTER
Sections to write	Choose one: Drug substance and drug product; Drug substance only (3.2.S.1, 3.2.S.3.1); Drug product only (3.2.P.1).
Submission region	Choose one: US: FDA (NDA, ANDA, BLA, IND); EU: EMA and national agencies (MAA); Both US and EU.
Drug product name	Type it in.

2 · Drug substance: nomenclature and structure shown when it applies

FIELD	WHAT TO ENTER
INN or USAN	Type it in.
Company code	Type it in.
Chemical name (IUPAC)	Type it in.
CAS registry number	Type it in.
Molecular formula (salt)	For a salt, write the salt formula with a middle dot, for example C22H22FN3O2·HCl. Type it in.
Molecular formula (free base, if a salt)	Type it in.
Molecular weight stated (g/mol)	The value you will state in the dossier; the tool compares it with its own calculation. Type a number.
Stereochemistry	Type it in.
General properties	A table. Columns: Property Value. Paste rows from Excel, type comma-separated rows, or press Load file (Excel, CSV, Word, PDF or a scan).

3 · Drug substance: structure elucidation (3.2.S.3.1) shown when it applies

FIELD	WHAT TO ENTER
Techniques	A table. Columns: Technique Result or conclusion Batch. Paste rows from Excel, type comma-separated rows, or press Load file (Excel, CSV, Word, PDF or a scan).
Elemental analysis	A table. Columns: Element Found (%). Paste rows from Excel, type comma-separated rows, or press Load file (Excel, CSV, Word, PDF or a scan).

4 · Drug product: description and composition (3.2.P.1) shown when it applies

FIELD	WHAT TO ENTER
Dosage form	Type it in.
Strength (mg)	Type a number.

FIELD	WHAT TO ENTER
Strength expressed as	Says whether the label strength is expressed as free base or as the salt. Choose one: Free base; Salt as is.
Target unit weight (mg)	Type a number.
Description of the dosage form	Type it in.
Composition per unit	Give the active ingredient the function "Active ingredient" so the strength check can find it. A table. Columns: Component Function Quality standard mg per unit IID maximum for the route (mg, optional). Paste rows from Excel, type comma-separated rows, or press Load file (Excel, CSV, Word, PDF or a scan).
Container closure system	Type it in.

5. Checks and alerts

Calculations and pass/fail outcomes always come from fixed rules, never from AI. The tool checks:

- Molecular weight calculated from the formula and compared with the stated value; formulas that cannot be read are flagged.
- CAS number check digit.
- Stereochemistry described; for a chiral molecule, at least one technique that confirms the configuration (X-ray, chiral HPLC, optical rotation or VCD).
- Elemental analysis: each element must be in the formula, and found must be within 0.4% of calculated.
- Composition adds up to the target unit weight; an active ingredient is present; the active quantity matches the label strength after salt correction.
- Every component has a function and a quality standard; quantities above the FDA Inactive Ingredient Database maximum you enter are flagged.
- EU: excipients with a known effect (for example lactose) are listed for the labelling annex.

How to resolve alerts

- **Critical** alerts block the download and must be fixed in the data. A failing result can instead be linked to an investigation: type the investigation reference and outcome and press [Record](#).
- **Major** alerts block the download until you fix them or type a justification and press [Accept justification](#).

- **Minor** alerts do not block anything. They are listed in the documents so the reviewer sees them.
- Some alerts have an **Apply fix** button that makes the change for you. **Reopen** undoes a justification.

Narratives

This module writes: General properties (3.2.S.1.3); Elucidation of structure (3.2.S.3.1); Description and composition (3.2.P.1). Each narrative is written by fixed rules from your data. You can edit it in the box.

Rewrite with AI (where your plan includes AI) rewrites it in regulatory style; every number in the text is checked against your data, and a number that does not match is flagged under the box and blocks the download until you correct it. **Reset to rule-based text** brings back the original.

6. Preview, gap review and download

1. Press **Preview** next to a section, or **Preview and download all**. The document opens in a preview window, exactly as the Word file will read.
2. The left side lists the review, run on your device: **gaps in the data** (missing values, open alerts), **gaps in the report** (missing content the guidance expects, placeholders such as [site] or TBD left in the text) and, if you load the approved protocol under **Compare with the protocol**, **differences from the protocol** (requirements, criteria, batches or time points it plans that the report does not show).
3. Click a finding to jump to the place in the preview. Fix it in the tool, then preview again.
4. Optional **AI review**: a second read for contradictions, claims without data and vague wording. The report text is sent to Claude only when you press it, and only where your plan includes AI. Check every AI finding; AI can be wrong.
5. Press **Download Word (.docx)** or **Download PDF**. With several documents open, **All as Word (.zip)** and **All as PDF (.zip)** download the set. The download buttons stay disabled while a blocking alert is open; the preview still works.

Documents this module produces

SECTION	DOCUMENT
3.2.S.1.1	Nomenclature
3.2.S.1.2	Structure
3.2.S.1.3	General properties
3.2.S.3.1	Elucidation of structure and other characteristics
3.2.P.1	Description and composition of the drug product

Use **Save project** to keep your work as a file on your computer, and **Open project** to continue later. **Start blank** clears every field; **Load example** brings the example back. Nothing is stored on CMCfy servers.

7. US and EU submissions

The sections are the same in both regions (ICH M4Q). In EU mode, compendial references are expected as Ph. Eur., so a quality standard that cites only USP/NF raises a minor alert, and excipients with a known effect are named as the EU excipients guideline requires. In US mode the FDA Inactive Ingredient Database limits are used when you enter them.

Choose **Both US and EU** to write one set of sections that cites both pharmacopoeias.

8. Working with other modules

- Save the summary and add it in the Process & Controls Writer under **Composition from Composition & General Info**: the unit formula is filled for you.
 - The QOS Composer & Dossier Assembler compares the active quantity here with the batch formula in 3.2.P.3.2 and flags any difference.
 - Excipient quality standards are written in more depth in the Excipients Writer module.
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9. Common pitfalls

- Writing the free-base formula in the salt field. The molecular weight then looks wrong by the weight of the counter-ion.
 - Stating the strength as free base but entering the salt quantity in the composition without choosing **Free base** under **Strength expressed as**.
 - Rounding the stated molecular weight differently from the certificate of analysis. Use the same value everywhere.
 - Leaving the container closure empty: 3.2.P.1 must name it, even though the detail goes in 3.2.P.7.
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10. Practice exercises

Each exercise starts from the example (press **Load example** to reset). We run these on every update of this guide, so the result you see should match.

1. Catch a molecular weight error

Change **Molecular weight stated (g/mol)** from 415.90 to 420.

EXPECTED RESULT

A major alert says the stated molecular weight 420 differs from the value calculated from the formula.

2. Catch a mistyped CAS number

Change the last digit of the CAS registry number from 4 to 5 (2412345-67-5).

EXPECTED RESULT

A major alert says the CAS number fails the check-digit test.

3. See the EU pharmacopoeia check

Set **Submission region** to EU.

EXPECTED RESULT

Minor alerts appear for excipients whose quality standard cites USP/NF only.

Guide updated 28 October 2026 for the current version of the tool. CMCfy drafts are for review by a qualified person before use in a submission.