AI Search

UV/Vis+ Photochemistry Database – User Guide

1 What the search does

The AI search answers questions written in plain language. Instead of entering search terms, you write the sentence you would say to a colleague.

> `are there temperature dependent absorption cross sections of SO2 in the gas phase?`

The classic text search remains available alongside it. It is still the better choice when you know exactly what you are looking for — a particular CAS number, for instance, or an author's name.

How an answer is produced

Your question is first translated into search conditions: substance, phase, spectral range, temperature, year. The application then searches a database built from all data sheets of the collection. This step is exact arithmetic, not guesswork.

Only at the end does a language model write a summary from the data sheets that were found. It may draw on those results and on nothing else.

> **Important when judging a result:** what counts is the list of matches, not the answer text. The list comes from the database and can be verified. The answer text is an assessment of the most relevant work and deliberately does not name every match.

Three separate collections

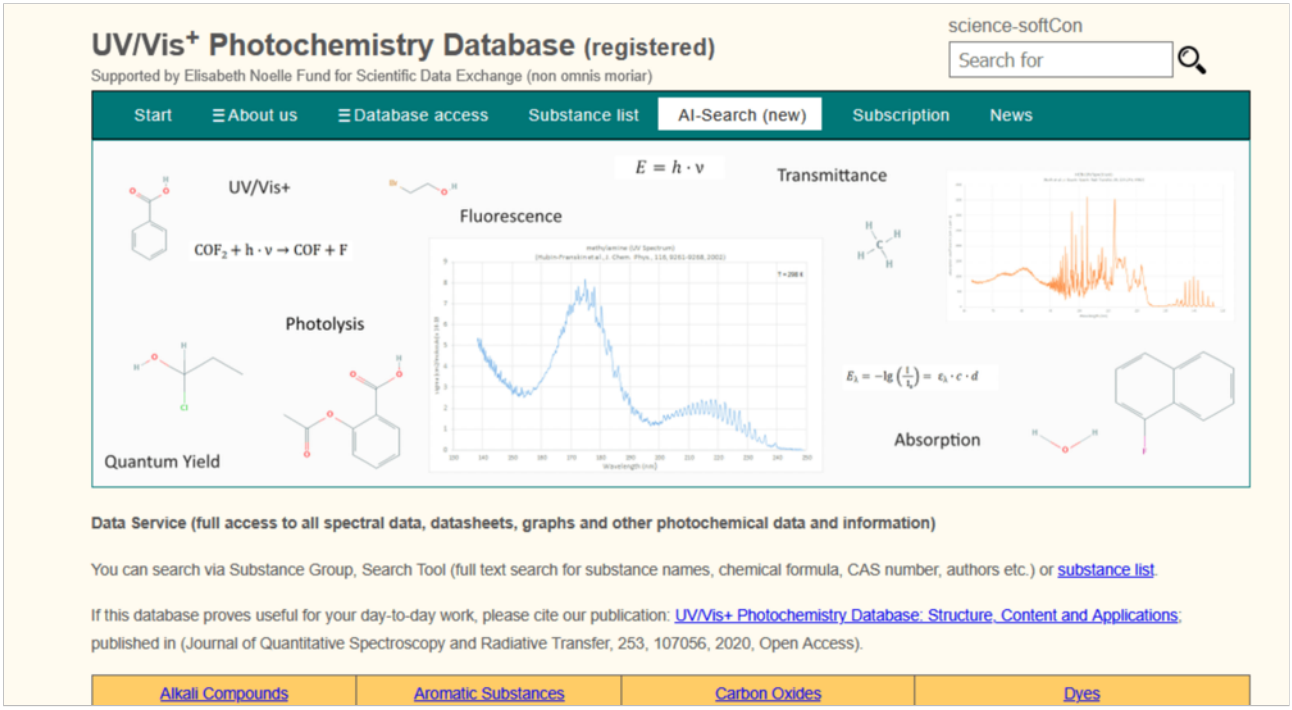
The search runs separately in each section of the site. Each one has its own index and sees only its own data sheets — a search in one section can never return matches from another.

The subscription section offers more than the public one: there, the measured values themselves are indexed, and they can be plotted. Section 4 describes this.

The public Literature Service has not been extended since January 2025. New substances are still entered in its substance list, but their spectra and photochemical information are held in the subscription sections. A question about such a substance is therefore answered in the public section by a note saying where the data are — see section 3.

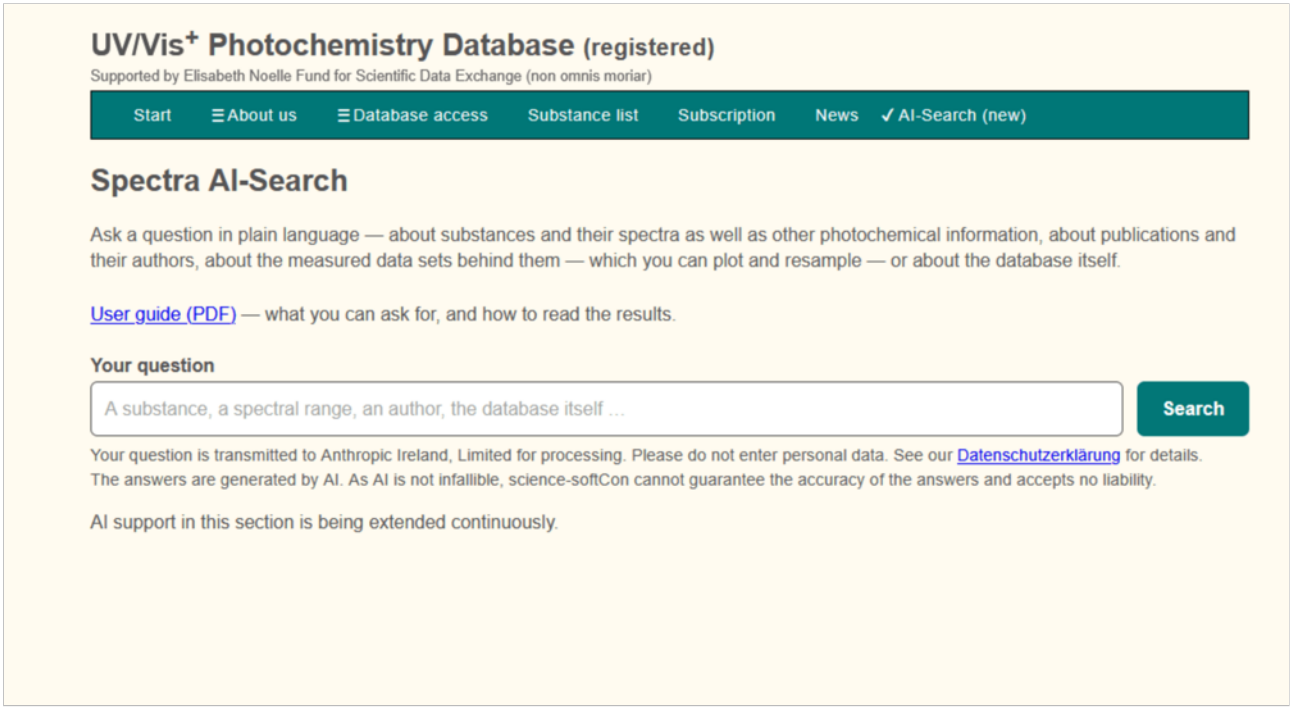
Finding the search

The search has its own entry in the menu bar of the database, **AI-Search (new)**. It sits alongside the classic routes — the substance groups, the substance list and the text search — and does not replace them.



The entry point: **AI-Search (new)** in the menu bar of the database.

The page itself holds one field. Below it stand the link to this guide, the note on data protection and the reminder that the answers are generated by AI.



The search page. One field, one button — everything else is explanation.

2 What you can ask for

Property	Examples in a question
Substance	name, synonym, formula or CAS number
Spectral range	as wavelength `between 200 and 300 nm`, as wavenumber `34000 to 41000 cm-1` or as energy `4 to 10 eV`

Property	Examples in a question
Spectral region	`uv`, `vuv`, `euv`, `vis`, `nir`, `ir`
Phase	`gas phase`, `vapor`, `vapour`, `liquid`, `in solution`, `solid`, `matrix`
Temperature	a single value `at 298 K`, a limit `below 100 K`, or `at room temperature`
Temperature dependence	`temperature dependent`
Type of measurement	`absorption`, `absorbance`, `cross sections`, `molar extinction coefficient`, `fluorescence`, `linear dichroism`, `photolysis`, `quantum yields`
Author	`papers by Moortgat`, or several names from one publication
Year	`since 2015`, `before 1990`
Measurement files	`with downloadable data files`
About the site	advisory group, company, subscription, contact

These can be combined freely. The answer is written in the language of your question; a single word or a name yields an English answer.

Asking about more than one substance

A question may name two or more substances: `acetic acid (CAS 64-19-7) and formic acid (CAS 64-18-6)` returns matches for both, and the answer covers both. The matches are not listed one substance after the other but mixed by year, and the answer is written from an even share of each — otherwise a substance with many publications would crowd out the other.

If you name authors from two different publications in such a question, no single data sheet can carry all of those names. The search then asks for any one of them instead of all, and the line below the status message says so.

A temperature is treated as a range, in the same way as a spectral range: `at 298 K` returns every work whose temperature range covers 298 K, including measurements made over a span such as 250–300 K. A study recorded at a single temperature is only matched by that exact figure, so if 298 K returns less than expected, try a narrow span such as `between 290 and 300 K`.

Units of the spectral range

In spectroscopy the wavelength in nanometres, the wavenumber in cm^{-1} and the energy in electronvolts are all in common use. All three may appear in a question; they are converted to nanometres before the search.

The conversions follow the usual relations: $\lambda\ [nm] = 10^7 / \tilde{\nu}\ [cm^{-1}]$ and $\lambda\ [nm] = 1239.84 / E\ [eV]$.

Wavelength	Wavenumber	Energy
120 nm	83,300 cm^{-1}	10.33 eV
200 nm	50,000 cm^{-1}	6.20 eV
300 nm	33,300 cm^{-1}	4.13 eV
500 nm	20,000 cm^{-1}	2.48 eV
1000 nm	10,000 cm^{-1}	1.24 eV

Note the reversal: a range from 200 to 300 nm corresponds to 50,000 down to 33,300 cm^{-1}. The limits swap places, which the search takes into account.

The data sheets themselves are inconsistent here — sometimes nanometres, sometimes cm^{-1} or eV with the nanometre value in brackets. This makes no difference to the search: everything is converted to nanometres when the database is built.

Naming a spectral region

Words such as `uv` or `ir` are treated as a range and do narrow the result. The boundaries are fixed:

Region	Range used
`euv`	10–121 nm
`vuv`	10–200 nm
`uv`	100–400 nm
`vis`	380–780 nm
`nir`	700–3000 nm
`ir`	from 700 nm

A question about `ir` spectra therefore excludes work in the UV, and a question about `uv` spectra excludes work in the near infrared. If you want every spectrum of a substance regardless of region, leave the word out. Explicit figures always take precedence over a region named in words.

Better and more difficult questions

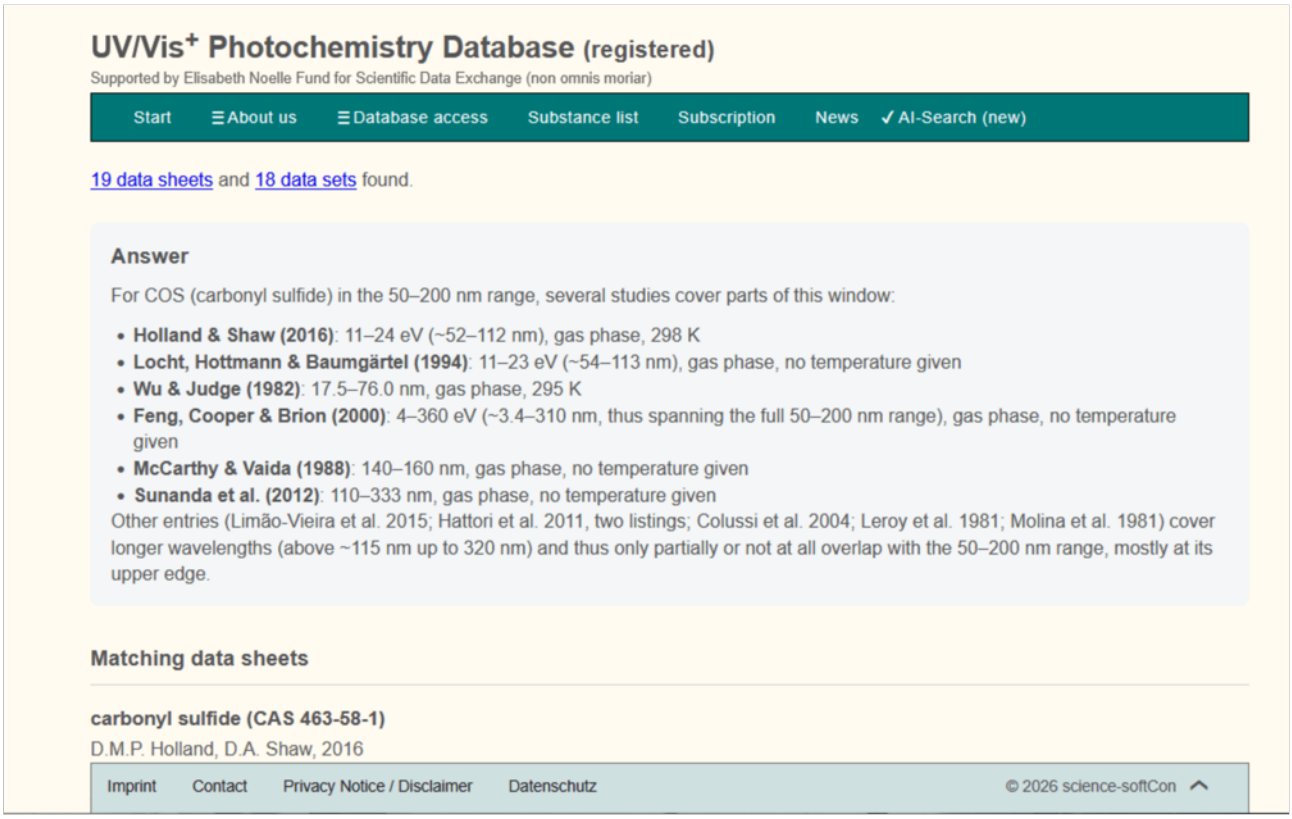
Works well	Why
`absorption cross sections of benzene in the gas phase between 200 and 280 nm`	Substance, phase and range are all stated.
`temperature dependent spectra of ozone`	Matches the field in the data sheet exactly.
`papers by Vandaele on SO2`	Author and substance together.

More difficult	Why
`uv spectrum of methane`	The word `uv` restricts the result to 100–400 nm and excludes measurements in the near infrared. Omit it, or give the range in figures.
`good data for chlorine`	"Good" is not a property recorded in the data sheets.
`everything about aromatics`	Too broad; at most 30 matches are shown.

3 What you see on the page

A result is built of the same parts every time, from the top down. Not all of them appear for every question: **From the website** only where the question touches the site itself, **Measured data sets** only in the subscription section.

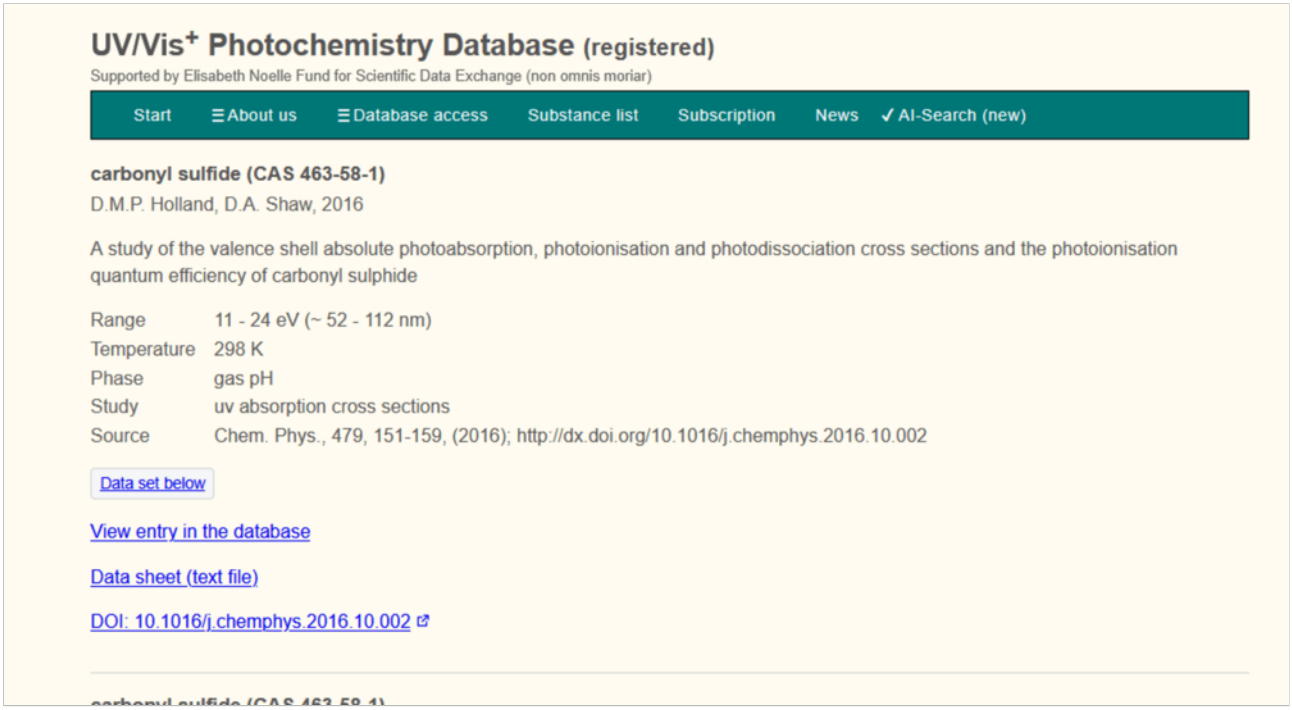
Section	Meaning
Available to registered users	Public section only. Appears when the question names a substance that the collection records but does not hold. It names the substance and links to the registration information and the subscription details.
Answer	A summary of the most relevant matches, one or two paragraphs.
From the website	Pages of this site that match your question — the advisory group, the company, subscription terms. The link jumps straight to the passage and highlights it.
Matching data sheets	The data sheets found, each with substance, authors, title, spectral range, temperature, phase and type of measurement.
Measured data sets	Subscription section only. The measurement series themselves, each with its spectral range, the quantity measured and the number of data points. See section 4.
What was actually searched for?	Expandable. Shows the search conditions derived from your question.



A result. The line at the top counts what was found and jumps to the two lists; the **Answer** orders the matches by what the question asked for.

The two figures in the first line are links. *19 data sheets* and *18 data sets* jump to the respective list — useful when the answer is long and the data sets sit several screens further down.

Every match carries two links. *View entry in the database* leads to the substance overview page, *Data sheet (text file)* to the data sheet itself.



One data sheet. Everything the collection records about the work — and, as a button, the jump to its measured values.

Where measured values belong to a match, a third line follows. *Data set below* — or *3 data sets below* — jumps to the matching entry under **Measured data sets**. Where a measurement file exists but is not listed there, the file is named directly, with a *Plot* link beside it. In the public section, where the measured values are not indexed, the line reads *Data file available* and is plain text.

In the public section a question may name a substance whose data are held in the subscription sections. The collection records it — the substance list carries the entry — but there is no data sheet for it here. The box **Available to registered users** then stands above the answer, names the substance and leads to the registration information and the subscription details.

If the question named *only* such substances, that box is the whole result. No answer is written and no data sheets are listed, because this collection holds none for the substance; the status line says *Found in the substance list, but not in the freely accessible section.* Words in the question that merely describe the substance — `uv absorption data for …` — are not searched for on their own, which would otherwise fill the page with unrelated work.

If the question named a second substance that this collection does hold, both happen at once: the box appears for the one, and answer and matches follow for the other.

4 Plotting measured data

> **Subscription required.** Everything in this section is available in the subscription section of the database only. The public section lists data sheets; it does not hold the measured values. Terms and access: https://science-softcon.de/spectra/sub_1.php

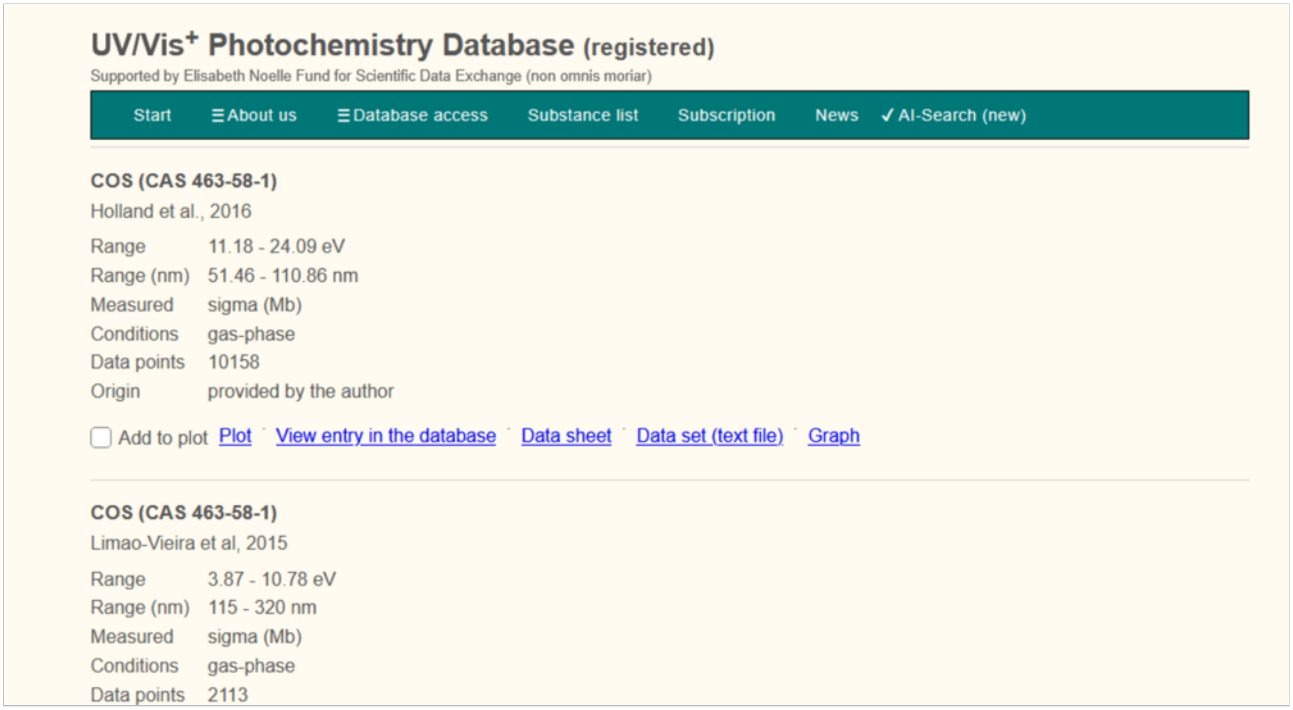
In the subscription section the measurement series are indexed in their own right — close to ten thousand data sets with some fifteen million data points. They appear under **Measured data sets**, below the list of data sheets, whenever your question names something concrete: a substance, an author, a quantity such as `cross sections`, or a keyword from the measurement conditions.

What each entry offers

Every data set carries three links: *Data sheet* for the record that describes the work, *Data set (text file)* for the measured values themselves, and *Graph* for a figure of those values. Almost every data set has one.

That figure was drawn for this database from the measured values. It is not the figure printed in the publication.

Next to them sit a checkbox *Add to plot* and a link *Plot*. The link draws that one data set. The checkbox collects several: tick two or more and a button appears above the list, offering to plot them together.

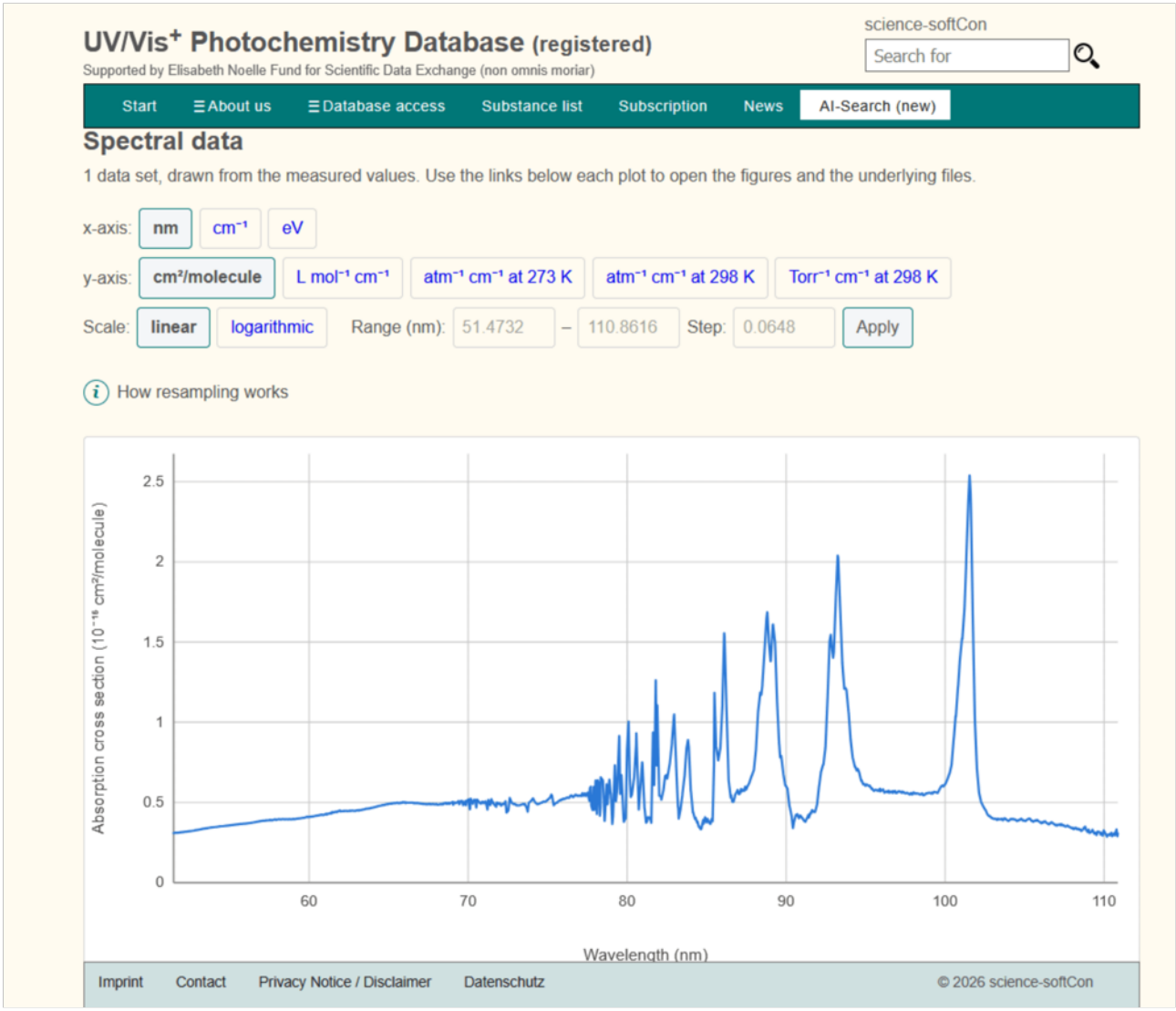


Two data sets of the same substance from different publications. *Range (nm)* appears because these works were recorded in electronvolts; *Data points* tells a swept spectrum from a handful of values.

The plot

A plot is drawn from the values in the file, not from the published figure. Above it sit the controls:

Control	What it does
x-axis	Switches the horizontal axis between nm, cm^{-1} and eV. The data are converted; nothing is re-measured.
y-axis	Switches the unit of the vertical axis, for instance from cm^2/molecule to L mol^{-1} cm^{-1}. Appears only where the quantity is one that can be converted.
Scale	Switches the vertical axis between linear and logarithmic. Useful where a band spans several orders of magnitude.
Range	Restricts the plot to a section of the horizontal axis. Enter the limits in the unit currently selected and press *Apply*; *Full range* returns to the whole spectrum.
Step	Puts the data on an even grid — see *Resampling* below. Leave it empty to see the values as measured.



The plot with its controls. The faint number in *Step* is not an entry but the usual spacing of the measured points.

The range is worth knowing about: a data set running from 200 to 600 nm shows little of a weak band at 250 nm, because the vertical scale is set by the strongest feature. Restrict the plot to 200–280 nm and the vertical scale follows the section, so the band becomes legible.

When you switch the horizontal unit, the section travels with it. A range of 200–280 nm becomes 35,710–50,000 cm^{-1} — note that the limits swap places, as they do everywhere in this database. A step, by contrast, is cleared when you switch: a grid of 1 nm has no fixed equivalent in cm^{-1}, because the spacing would depend on the wavelength.

Where a curve rests on fewer than ten points, each measured point is marked with a symbol — a circle, a triangle, a square. Each curve has its own shape, so the curves can still be told apart in a black-and-white print and by readers who distinguish colours poorly. A line through seven measured values looks like a spectrum that was swept; the symbols show where measurements were actually taken and where the line merely connects.

Units of the vertical axis

Absorption cross sections and molar extinction coefficients describe the same thing in different units, and the database holds both. The **y-axis** control converts between them, so that a cross section from one publication and an extinction coefficient from another can be drawn on one scale. Without it, the two would always end up in separate plots.

Unit	Factor from cm² molecule^{-1}
cm² molecule^{-1}	1
L mol^{-1} cm^{-1} (= M^{-1} cm^{-1})	× 6.02 · 10^{20}
atm^{-1} cm^{-1} at 273 K	× 2.69 · 10^{19}
atm^{-1} cm^{-1} at 298 K	× 2.46 · 10^{19}
Torr^{-1} cm^{-1} at 298 K	× 3.24 · 10^{16}

> **One assumption worth knowing:** these factors hold for two quantities taken in the *same* logarithmic base. Converting a cross section in base e into a decadic extinction coefficient would need a further factor of ln 10 = 2.303. The data sheets do not record the base, so the conversion keeps it, and a note under the plot says so.

Resampling: putting the data on an even grid

Measurement series come with the spacing their instrument produced — 0.09 nm here, 5 nm there, and often irregularly. The **Step** field puts a data set on an even grid, say every 1 nm. An *i* below the controls explains the method on the page itself; in short:

- Where your grid is **finer** than the measurement, values between measured points are interpolated. For absorption cross sections and extinction coefficients the interpolation runs on the logarithm of the value, because these quantities span orders of magnitude and a straight line in linear space reads systematically too high on a steep edge.
- Where your grid is **coarser**, values are averaged over each interval. Taking every n-th point instead would let a narrow band fall between two grid points — or be hit by chance and appear too strong.

Gaps are not bridged: where the next measured point is far away, the grid stays empty rather than drawing a straight line through nothing. A measured point that falls on a grid point is used as it stands, and no value carries more digits than the source file.

Resampled values are computed values, not measurements, and the plot says so. The legend then reads *100 grid points from 200 measured*, and the point symbols described above are omitted — they mean "measured here", which would not be true of a grid point.

Each resampled curve offers *Download resampled data set (text file)* in the legend. The file carries a header naming the source file, the authors, the step, the method and the date, and it asks that the original measurement be cited rather than the derived file. It is written in the same format as the data sets of the collection, so it can be read back with the same tools.

Comparing publications

Several data sets in one plot is the point of the exercise: measurements of the same substance drawn on one scale, with authors, year and conditions in the legend below. They may come from different publications, or from one work that measured the substance under several conditions — two temperatures, two solvents, two values of pH. Up to six curves can be shown at once — beyond that they can no longer be told apart.

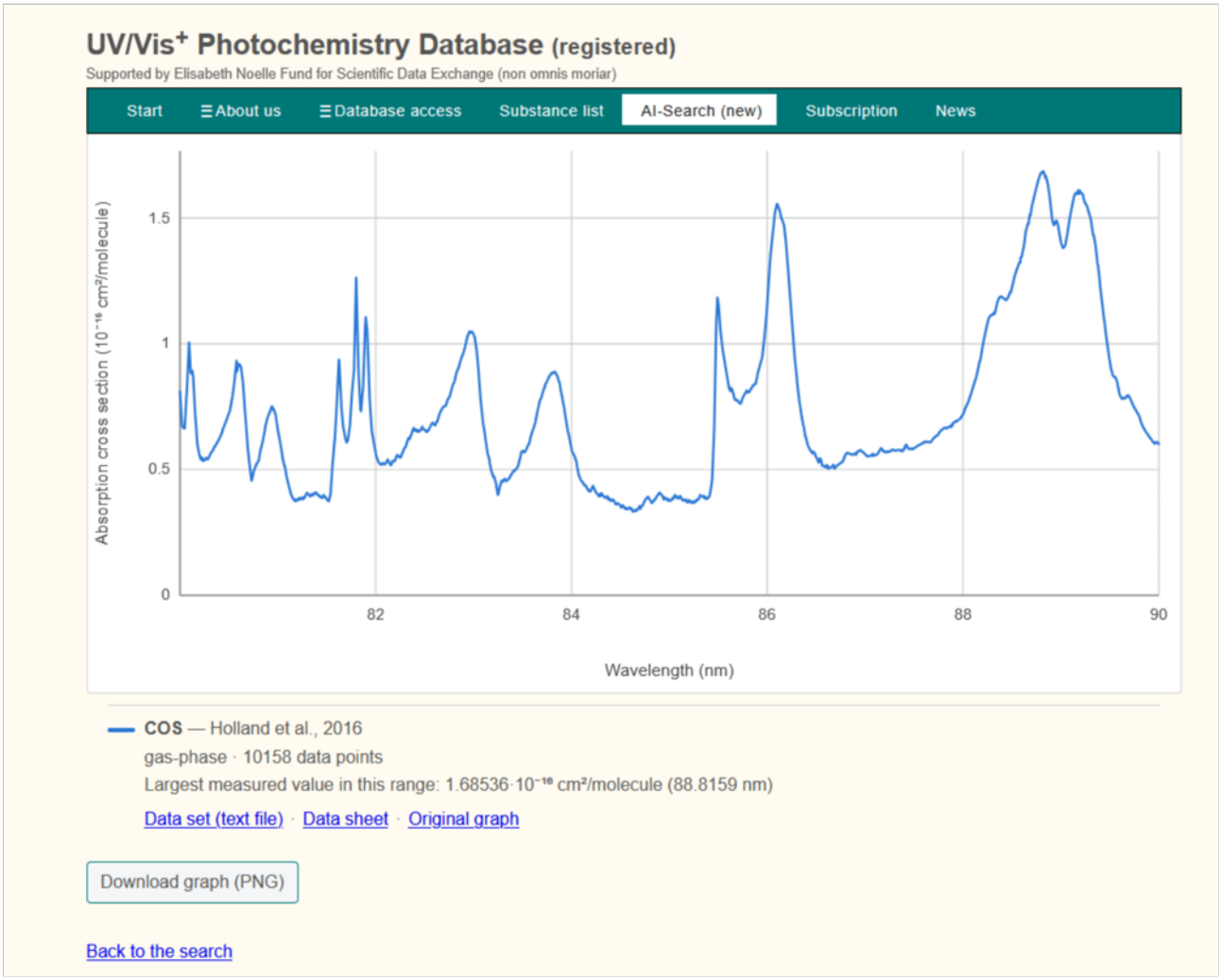
Curves are only combined when they measure the same quantity in the same unit. Absorption cross sections are brought to a common footing first, whether the file states them in megabarn, in cm²/molecule or scaled by a power of ten, and the axis is then labelled `Absorption cross section (10⁻¹⁸ cm²/molecule)` or whichever power suits the data. Where a reliable conversion is not possible, the data set is drawn in a plot of its own, with a note saying so.

The vertical axis names its quantity in words, not in the shorthand of the source file: `Optical density` rather than `OD`, `Polarized absorption` rather than `Eu`. Where the column heading of the file adds something the name does not carry — a unit, or the ion mass of a photoionisation measurement — that travels with it. Only a quantity the collection cannot classify keeps its heading unchanged, since nothing better is available.

Where two data sets differ only in the unit — a cross section and an extinction coefficient, say — they are also drawn separately at first, and a line under the controls points to the **y-axis** switch that brings them onto one scale.

Taking the plot with you

Below the legend sits **Download graph (PNG)**. It saves the figure as it stands — with the range, the units and the grid you chose — at twice the drawing size, on a white background whether or not your screen shows the page in a dark scheme.



Below the legend sits the button for the image. The legend above it names what the picture shows — in the file this information is set beneath the curves.

The picture carries a caption of its own, set beneath the curves: one line per curve with substance, authors, year and source file; a line naming the step where the data were resampled, with the reminder that these are computed values and that the original measurement is the thing to cite; a line for a change of unit; and the database, its address and the time the file was made.

That caption is not decoration. A figure leaves this page and turns up in a talk, an e-mail, a manuscript — where it stands without a legend, without an address and without anyone to ask. A curve with no provenance is a measurement that never happened, and a resampled curve with no note is a set of numbers nobody measured.

For numbers rather than a picture, use the text files: *Data set (text file)* for the measurement as recorded, and *Download resampled data set (text file)* for your own grid.

> **What a plot is and is not:** with the *Step* field empty it is a view of the measured values as they stand in the file. Nothing is smoothed or fitted. Where a curve is drawn from more points than the width of the plot can show, the highest and lowest value of each pixel column are kept, so no peak is lost. A step, or a change of the unit of either axis, replaces the measured numbers with computed ones; the plot then says which of the two you are looking at. For quantitative work, use the data file — the original one for measured values, the resampled one where you want them on your own grid.

5 Limits

The search knows only what the data sheets record

The database is built from the data sheets. What is not entered there cannot be found. If a measurement made at several temperatures lacks the *Temperature dependence* marker, it may not appear when you ask for temperature dependence.

Spelling errors in the fields have the same effect. Some are compensated for — the spelling `dicroism` that is common in the collection, and the abbreviations `LD`, `CD` and `MCD`. Others only come to light when an expected match is absent.

Translating the question is the delicate step

Search conditions are derived from your question, and conditions can arise that were not intended. This is exactly what the *What was actually searched for?* section is for.

The answer text does not name every match

The summary considers the twelve highest-ranked matches and highlights some of them. Where a question names several substances, those twelve are shared evenly between them. For the full picture, read the list.

Further limits

- At most 30 data sheets per search.
- The search evaluates what is *known about* a measurement — range, temperature, phase, source. It computes with the measured values only in the ways described in section 4: converting the units of either axis, and putting a data set on an even grid. It cannot normalise a spectrum, subtract one from another, integrate over a range or find peaks.
- For some data sets the unit of the axis or the quantity measured could not be read from the file header. They are listed and can be plotted, but a question that names a quantity may not reach them.
- To limit abuse, the number of queries per hour and visitor is capped.

6 If a match is missing or looks wrong

Before reporting a fault, three steps will usually explain what happened.

First: expand the section

What was actually searched for? shows the conditions that were derived. If something appears there that was not in your question — a phase, or a spectral range — that is the cause. Ask again without that word.

Second: read the line below the status message

If it says *Not applied: …*, a condition could not be applied and was dropped so that any matches at all could be shown. The list is then broader than your question.

One case occurs regularly: if no data sheet carries the substance name exactly as you wrote it, the name is matched as part of a longer name instead. Related compounds then appear in the list, and the line below says so.

A second case concerns the keywords. Where your question yields several words, a data sheet must normally carry all of them. One word that occurs nowhere in the database — a misspelling, or a term the collection does not use — would then empty the result, and a single missing word would decide the whole search. So if nothing is found that way, the words are weighed instead of required: sheets matching some of them are listed, the closest match first, and the line below says that this happened. Rare words count for much and common ones for little, so a misspelling no longer does damage; it simply contributes nothing.

If that still finds nothing and the question named a substance, the restriction to that name is dropped as well, and the line says so. The message is worth reading: nothing in the database carries the name you used. The substance may be recorded under another name, or it may not be there at all.

A third case concerns authors. Where several names are given, a data sheet must normally carry all of them — that is what makes `Watanabe and Jursa` find one publication rather than every paper by Watanabe. If the names belong to two different publications, no sheet can satisfy that, so any one name is then enough, and the line says so.

Third: rephrase the question

- Write the substance name as it appears in the data sheet, or use the CAS number.
- Drop restrictions that are not essential.
- Instead of `uv` or `ir`, give the range in nanometres — or give none at all.

If nothing is found at all

A line then offers the classic text search with a ready-made link. It works differently: it looks for words anywhere in the collection and finds phrasings that the conditions used here would filter out.

One case is not a failure of the search. If the question named a substance that the public collection records but does not hold, the box described in section 3 appears instead of that offer — the text search would only lead back to the same entry in the substance list.

What helps when reporting a fault

If a match is genuinely missing or genuinely wrong, three pieces of information make a report usable:

1. The question, word for word.
2. The content of *What was actually searched for?*.
3. Which data sheet you expected, with its path — for example `hyca/74-82-8_8.txt`.

With these three, it usually takes only a few minutes to establish whether the cause lies in the translation of the question, in the search itself, or in the data sheet.

7 Data protection

The question you enter is transmitted for processing to Anthropic Ireland, Limited, Dublin, which belongs to the Anthropic group based in San Francisco and uses sub-processors outside the

European Union. Your browser does not connect to Anthropic itself — the server makes that connection. Your IP address and other connection data are therefore not passed on.

Anthropic processes the data under a contract pursuant to Article 28 GDPR and has undertaken not to use the content for training AI models. Your question and the answer are deleted there within 30 days.

The measured values are a different matter: they are read, converted and drawn on this server. Nothing of their content is sent to the language model.

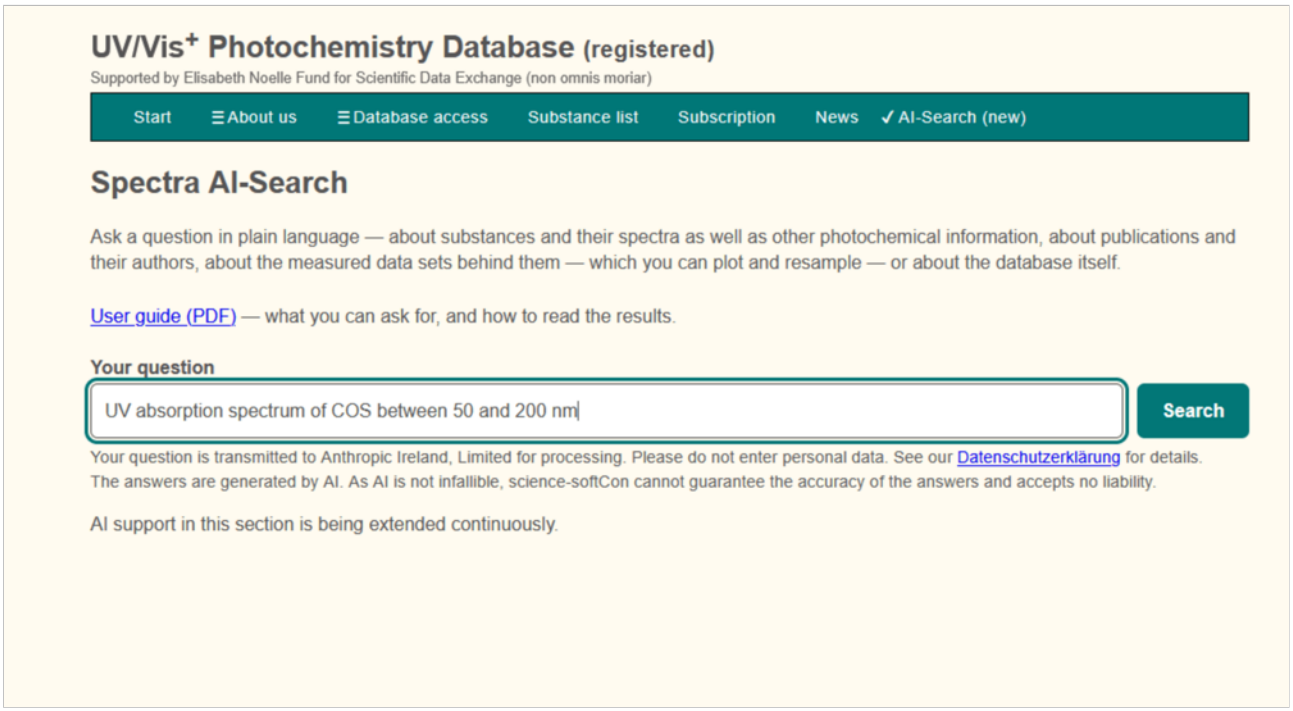
For this reason the note below the input field asks you not to enter personal data. Details are set out in the privacy policy of this site, which is available in English and in German; both are linked below the input field.

8 Appendix: working with a plot

This appendix follows one question — the UV spectrum of carbonyl sulfide — from the search box to a file on your disk. It uses every control of the plot once, in the order in which they are usually needed. Section 4 describes the same controls one by one; here they are shown working together. Everything in it needs the subscription section.

1 The question

```
UV absorption spectrum of COS between 50 and 200 nm
```



The question as it is typed. Plain language, no operators, no field names.

Nineteen data sheets and eighteen data sets come back. The answer sorts the publications by the window each one covers: those reaching into the range asked for stand first, with their ranges converted to nanometres, and the works that only touch its upper edge are named together at the end. COS is a case where this matters — several of these measurements are recorded in electronvolts, and the conversion is what makes them comparable at a glance.

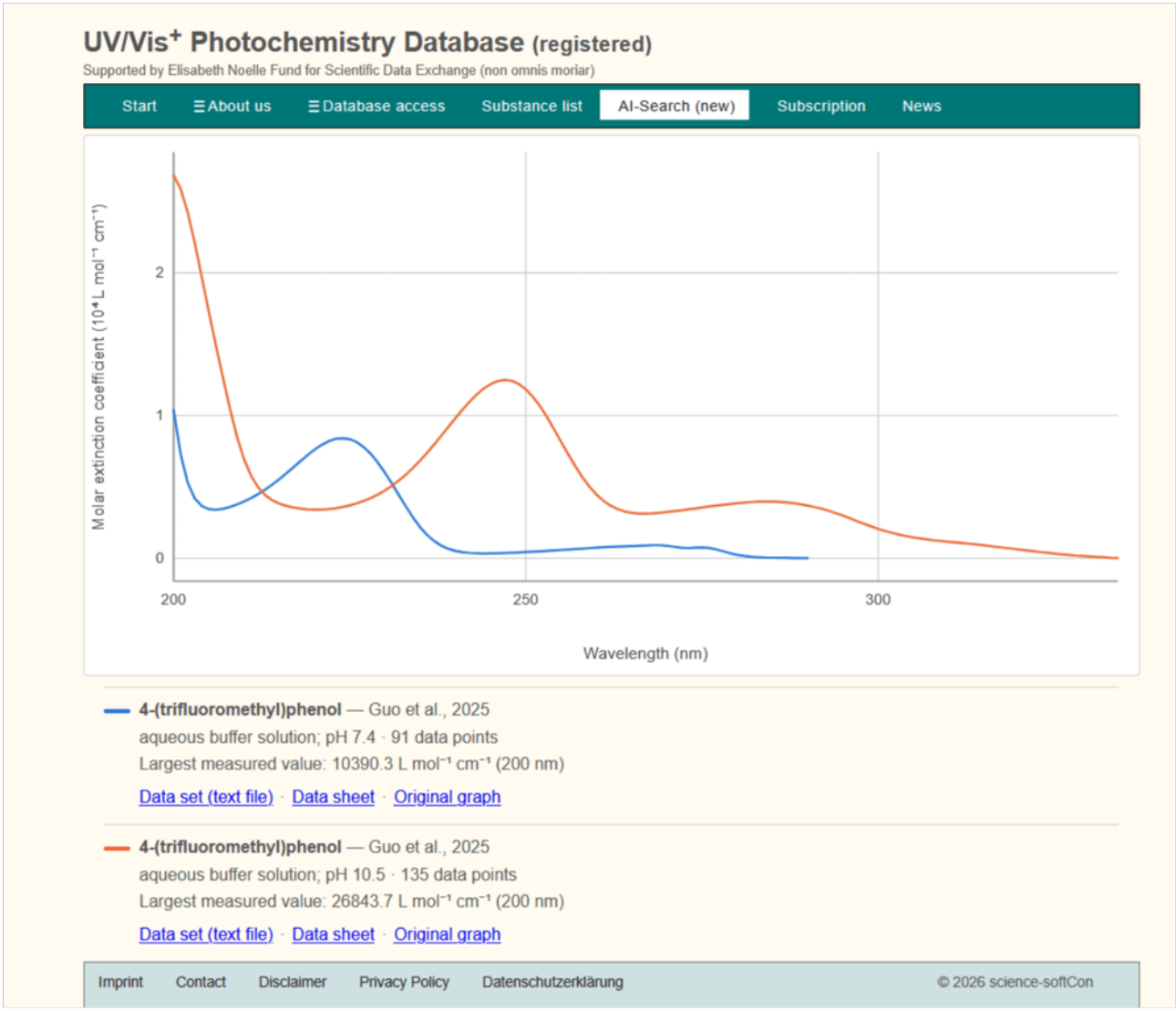
Below the matching data sheets, the block **Measured data sets** appears. Each entry carries the links *Data sheet*, *Data set (text file)* and *Graph* — the last of these a figure drawn for this database, not the one printed in the publication — together with a checkbox *Add to plot* and a link *Plot*.

The number next to *data points* is worth a glance: it tells you whether a measurement was swept densely or consists of a handful of values. Both occur in this collection, and the two behave differently in what follows.

2 Two results in one plot

Tick the checkbox of two data sets of the same substance, then use the button that appears above the list: **Plot 2 data sets together**.

The two need not come from different publications. One work often reports the same substance under several conditions — two temperatures, two solvents, two values of pH — and each of those is a data set of its own. Drawn together, the difference between them is the result.

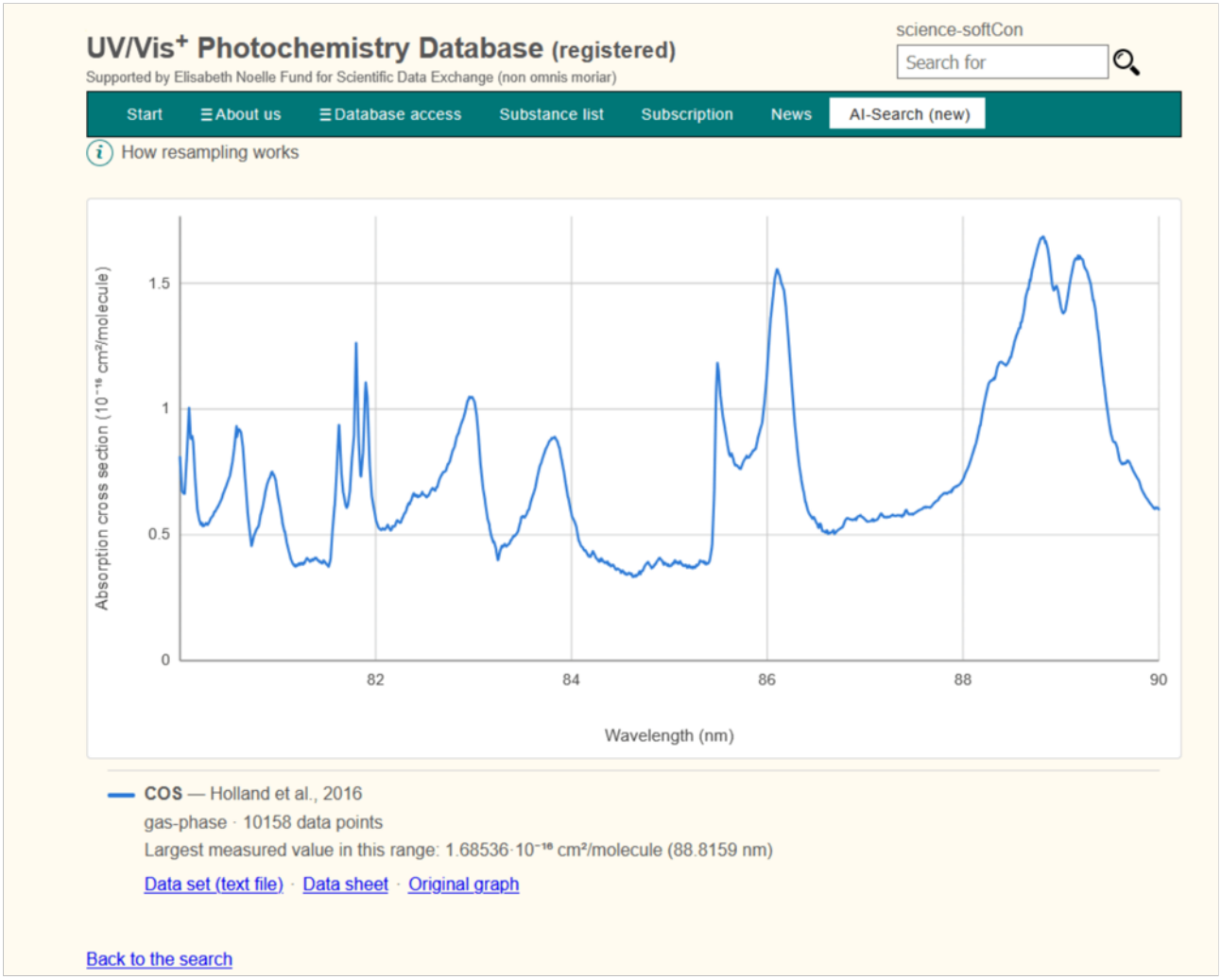


Two measurements of one substance from a single work, differing only in pH. The legend names the conditions of each curve — that is where the two are told apart.

Both curves are drawn on one scale, with authors, year and conditions in the legend below. This works even when the two files state their values differently — one in megabarn, the other scaled by a power of ten. They are brought to a common footing first, and the axis is labelled accordingly.

3 Narrowing the view

The data set runs from 51.5 to 110.9 nm, and at that width the fine structure above 80 nm is a thicket of lines. Enter a narrow section under **Range** — in the example the band structure between about `81` and `91` nm — and press *Apply*. The vertical scale follows the section, so what was pressed together becomes legible.



The same data set, restricted to ten nanometres. The legend now also names the largest measured value in the section and where it lies.

Now click **cm⁻¹** under *x-axis*. The section travels with you and reads roughly 110,000–123,000; note that the limits swap places. Click **nm** to return.

4 Changing the unit of the vertical axis

Click **L mol⁻¹ cm⁻¹** under *y-axis*. The curves are unchanged in substance; the axis now reads *Molar extinction coefficient*, and a line below the controls states what was used to convert and that both quantities are taken in the same logarithmic base.

The real gain shows when a cross section and a *measured* extinction coefficient of the same substance are selected together — recognisable in the list by `sigma` for one and `epsilon` for the other. Without the switch the two are necessarily drawn in separate plots, and a line under the controls points this out. One click puts them on one scale.

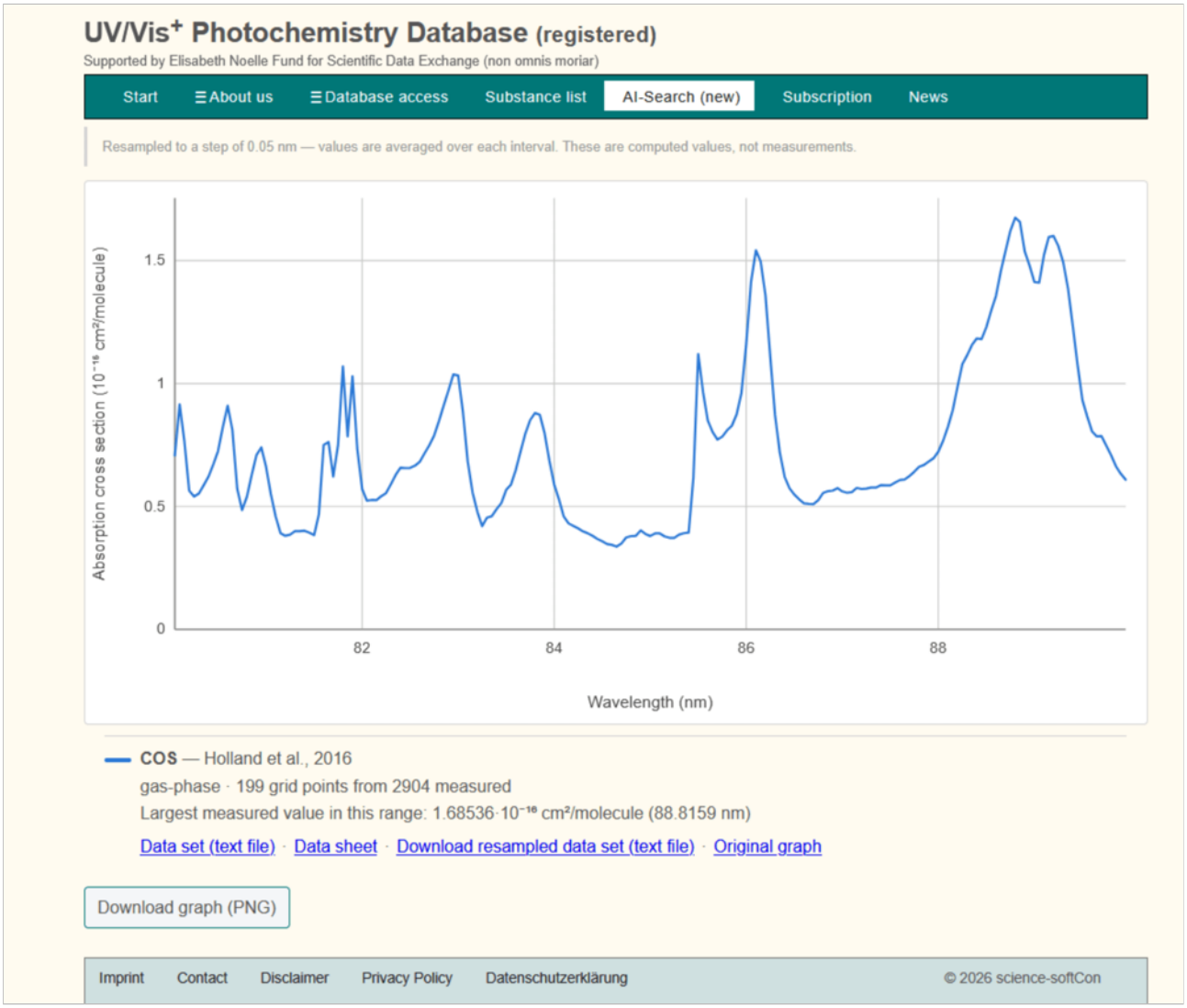
5 Putting the data on an even grid

Type `0.05` into the field **Step** and press *Apply*.

Before you typed, the empty field showed a faint number: the usual spacing of the measured points. That tells you whether your step is finer or coarser than the measurement, which decides what happens next. The line above the plot then says which of the two it was:

The line says	What was done
values are averaged over each interval	Your grid is coarser than the measurement. Each grid value is the mean over its interval, so a narrow band cannot fall between two grid points.
values between measured points are interpolated	Your grid is finer. For cross sections and extinction coefficients the interpolation runs on the logarithm of the value.

The legend changes with it. In this example it reads *199 grid points from 2904 measured* — the section held some three thousand measured values, and a step of 0.05 nm is coarser than that, so they were averaged.



After resampling. The line above the plot names the step and the method and states that these are computed values; the legend counts grid points against measured ones.

Try a much finer step on the same section — finer than the spacing of the measurement — and the page switches to interpolation and says so. The curve then carries more points than were ever measured, which is exactly the case the information panel below the controls warns about.

6 Reading what was done

Open the *i* below the controls: **How resampling works**. It sets out both cases, why cross sections are interpolated on the logarithm, that gaps in the measurement are not bridged, that a measured point falling on a grid point is used as it stands, and that no value carries more digits than the source file. It is worth reading before the first resampling rather than after, and the panel is there whether or not the field is filled.

7 Taking the numbers with you

In the legend, next to *Data set (text file)*, a second link has appeared: **Download resampled data set (text file)**. Its header names the source file, the authors, the measurement conditions, the step, the method and the date, and it asks that the original measurement be cited rather than the derived file.

```
# Derived from the UV/Vis Spectra Data Base, www.photochemistry.org
# Source file: <group>/<file>.txt
# COS; authors and conditions as recorded in the data sheet
# Generated 2026-10-23 11:40 UTC
#
# Resampled to a step of 0.05 nm
# Method: values averaged over each interval
# 199 grid points from 2904 measured values
# Computed values, not measurements. No more digits than the source.
# Please cite the original measurement, not this file.
#
wavelength (nm) Absorption cross section (cm2/molecule)
81.00   …
81.05   …
```

The last header line carries no hash mark on purpose: it is the column heading, so the file can be read back with the same tools as the data sets of the collection.

8 A second example: few measured points

Some measurements consist of a handful of values rather than a swept spectrum — again, the *data points* figure in the list shows this. Plot one of them.

Where a curve rests on fewer than ten points, each measured point is marked with a symbol, and each curve has a shape of its own, so the curves remain distinguishable in a black-and-white print. A line through seven measured values looks like a spectrum that was swept; the symbols show where measurements were actually taken and where the line merely connects.

Now enter a step. The symbols disappear — they mean "measured here", which would not be true of a grid point.

> **What to keep in mind.** With the *Step* field empty, the plot shows the measured values as they stand in the file. A step, or a change of the unit of either axis, replaces them with computed values; the plot says so, and so does the header of any file you download. For quantitative work take the original file where you need the measurement, and the resampled one where you need it on your own grid.

Version: October 2026, sixth edition — substances held only in the subscription sections are now recognised in the public section and answered with a note on where their data are (sections 1, 3 and 6).