

CAS Supports International Non-proprietary Names (INN) Submissions

CAS Registry ServicesSM

About CAS

Who we are

- Founded in 1907 as a division of the American Chemical Society
- Our experts collect, harmonize, organize, and connect the world's scientific information
- Our proprietary ontologies, lexicons, and thesauri enable and accelerate insights
- We develop and license technologies to access our content

CAS DATA:

- CAS Registry Numbers®
- Chemical structures and reactions
- Commercial sources
- Physicochemical properties
- Regulatory status
- Toxicological and regulatory data (the GHS)

About CAS

Who we are

Our experts serve industry and governments with data-enabled risk management services

- Determining chemical identity for regulatory compliance (nomenclature, CAS RN[®])
- Establishing and enhancing chemicals management systems
- Analyzing supply chains leveraging knowledge of best practices in industrial-scale production and emerging technologies



Today's topics



CAS REGISTRY® and CAS Registry Numbers



Using CAS Registry Services consultation to support WHO INN Submissions



Information for faster order processing

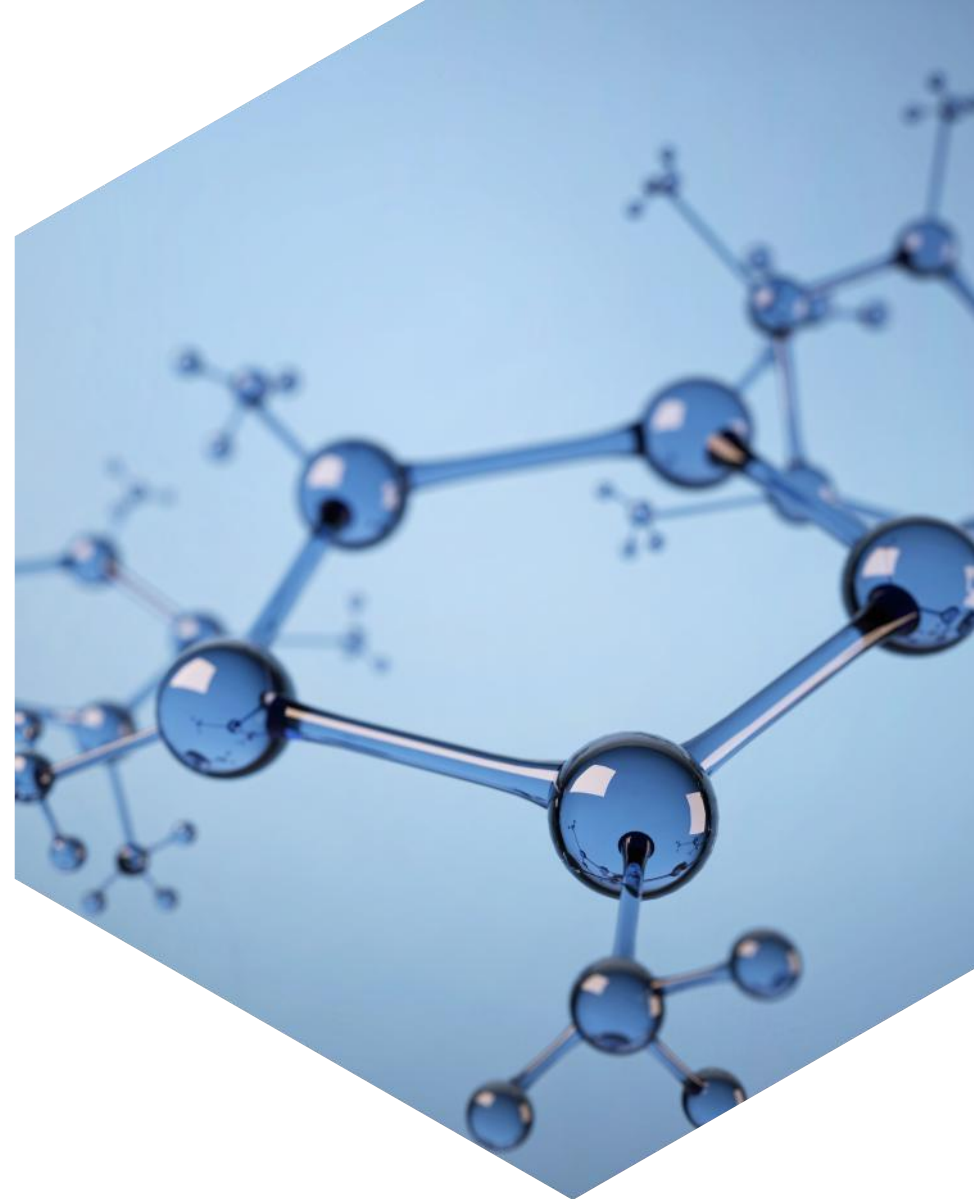


Questions

CAS REGISTRY

CAS substance collection

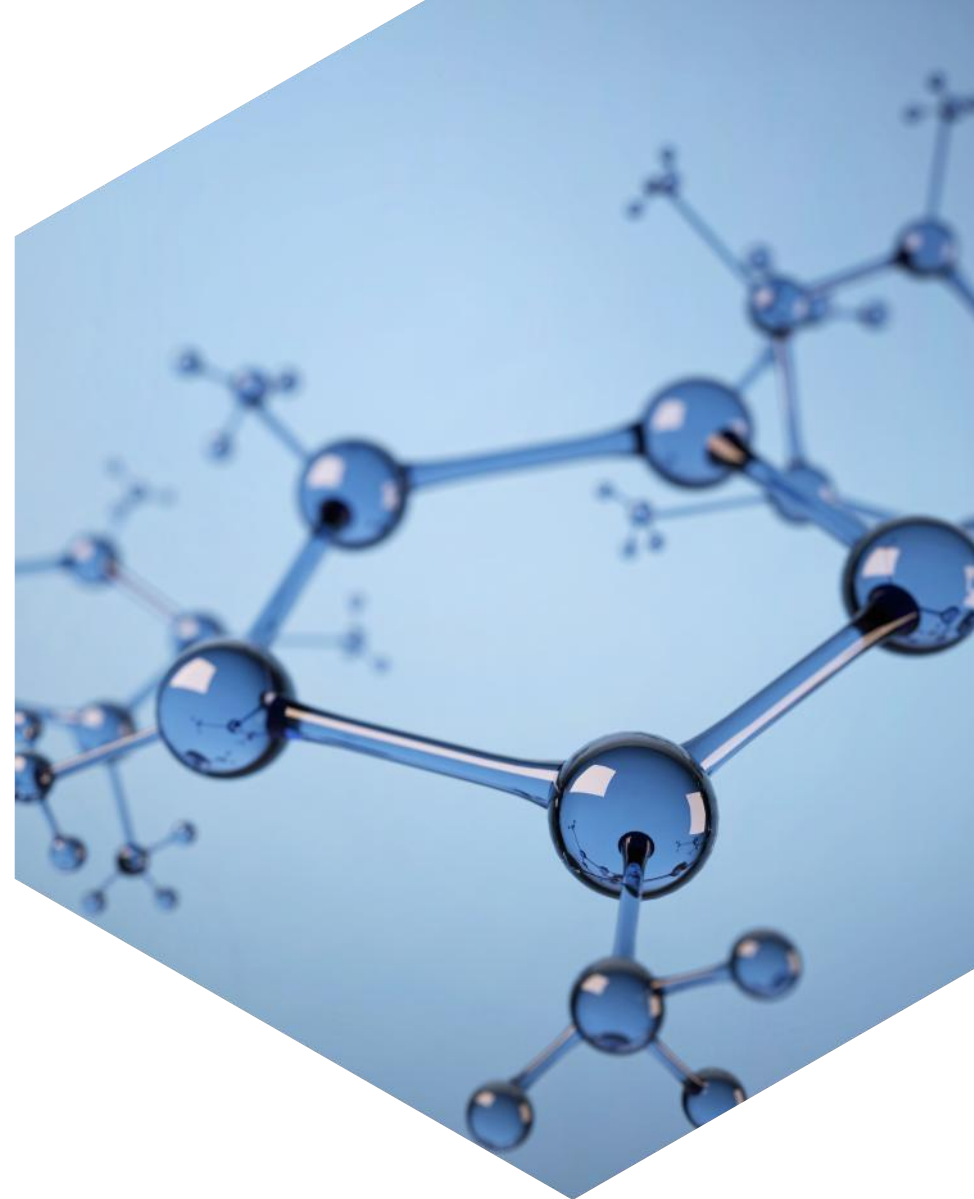
- Authoritative source for chemical names, structures, and CAS Registry Numbers (CAS RN)
- Contents include organic and inorganic substances, metals, alloys, minerals, polymers, salts, coordination compounds, protein and nucleic acid sequences, UVCBs
- Each unique CAS RN designates one substance



CAS Registry Numbers

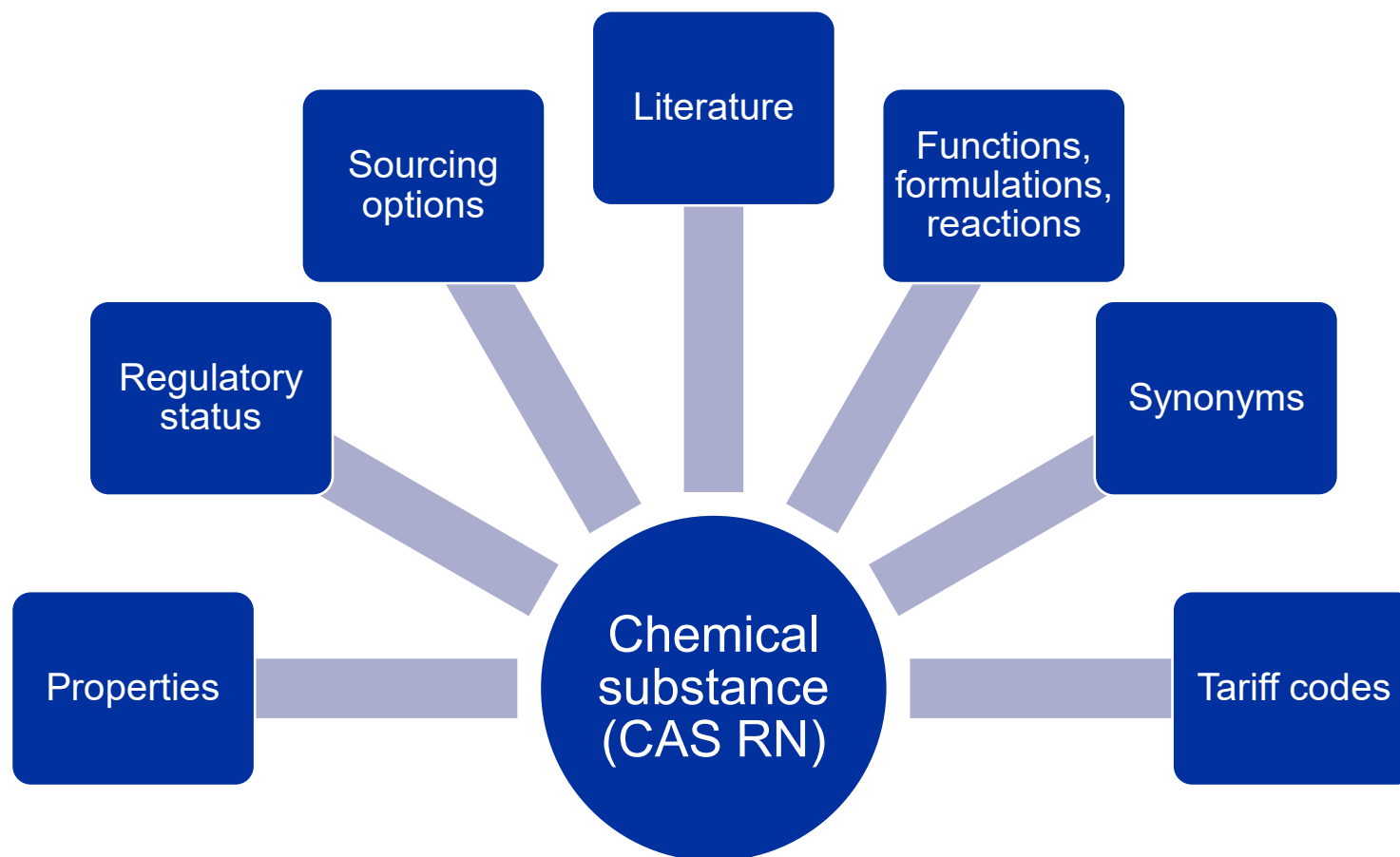
Unique substance identifiers

- A unique CAS Registry Number allows each chemical substance to be identified without the ambiguity of chemical nomenclature
- Serves as a link to information about that chemical substance
- Is a unique numeric identifier that designates only one substance
- Example:
 - 58-08-2 is the CAS RN for “caffeine”
 - 5426-85-7 is the CAS RN for a specific caffeine derivative “8-hexyl caffeine”



Data connections

Linking data, creating access to critical information



How CAS RNs and CA Index Names are assigned



CAS Registry Services



Team of chemists and
analysts



Three specialty
substance services:

- CAS Registry Services consultation
- CAS Registry lookup
- CAS Inventory Expert Service



CA Index Names and
CAS RNs

CAS Registry Services Consultation

CAS Registry Services consultation is...



A nomenclature and
registration service



Recommended for
International non-proprietary
name (INN) submitters



Confidential: all order
processing is strictly
confidential

Why use CAS Registry Services consultation?



Obtain a CA Index
Name



Obtain a CAS Registry
Number (CAS RN)



Use these items in
your INN submission

Order timeframes and pricing

CAS Registry Services consultation



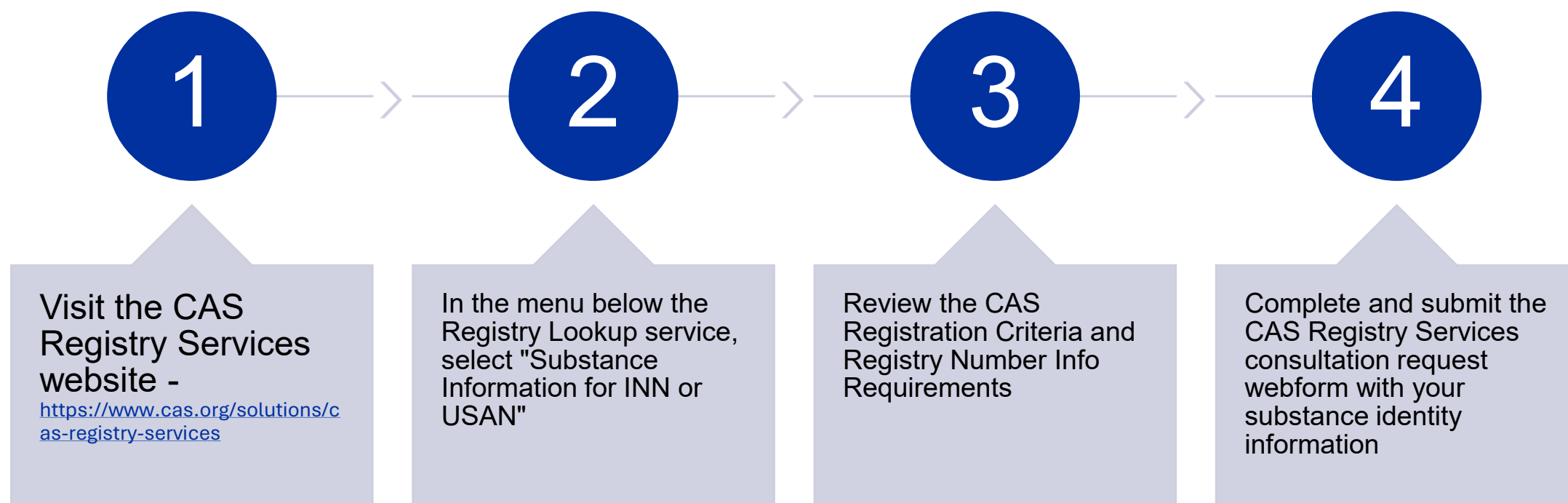
10 business days



Pricing is time and materials based

Order submission process

CAS Registry Services consultation



CAS Registry Service consultation

Select the results options that are best for you

CAS Registry Service consultation

Please check the appropriate option for your request*

- ☐ CA Index Name only – A CA Index Name will be provided in your results. If your substance matches an existing CAS Registry Number, it will also be provided. No new CAS Registry Number will be assigned.
- ☐ CAS Registry Number Assignment - A CA Index Name will be provided in your results. If your substance matches an existing CAS Registry Number, it will be provided. If none exists, then a new CAS Registry Number will be assigned.

Note: If you request assignment of a new CAS Registry number for a substance not already present in the CAS Registry system, that assignment will make your substance publicly available in CAS Registry®. Customer identity information will be kept confidential. If you wish to maintain confidentiality for your Substance's identity, you should request only a CA Index Name or retrieval of an existing CAS Registry number.

- If an existing CAS Registry Number is found, it will be provided in your results for both options.
- If you wish to maintain confidentiality of your substance when there is no existing CAS Registry Number, we suggest not selecting the "CAS Registry Number Assignment" option.

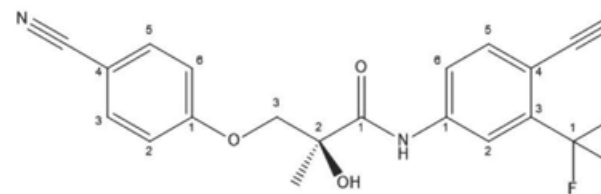
CAS Registry Services consultation

Simple organic substance submissions

Required substance information:

- Structure
- Molecular formula and/or chemically descriptive name
- Unique substance identifier (on webform)

Unique Substance Identifier - HID12345



(2S)-3-(4-Cyanophenoxy)-N-[4-cyano-3-(trifluoromethyl)phenyl]-2-hydroxy-2-methylpropanamide

CAS Registry Services consultation

Biologic substance submissions (RNA/DNA/protein)

Key information to include:

- Sequence
- Disulfide bridges
- Modifications or mutations

Ac-ASDEGCGGPT PGPKLEGPTT HTCTHPKQEF-OH

Disulfide bridge from 6th residue to 23rd residue

CAS Registry Services consultation

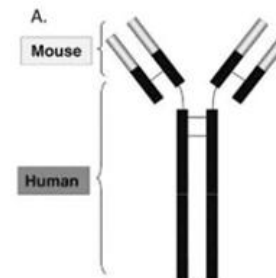
Biologic substance submissions (antibody)

Key information to include:

- Immunoglobulin and light chain information
- Antibody format
- Antigen information
- Source
- Expression system
- Drug-to-antibody ratio and attachment points
- Illustrations

Structure of HB1123

HB1123 is a chimeric antibody targeting PD-L1 and is comprised of a variable region derived from mouse anti-PD-L1 antibody V6, linked to human constant regions of IgG3 as indicated below:



The two heavy chains of HB1123 are composed of two chains with 400 amino acids and two light chains with 200 amino acids for a total of 1200 amino acids. Each chain is attached to the heavy chain by a disulfide bond.

Heavy Chain

VELKSSGTYP	KKLYPTYSQW	VELKSSGTYP	KKLYPTYSQW	VELKSSGTYP	50
KKLYPTYSQW	VELKSSGTYP	KKLYPTYSQW	VELKSSGTYP	KKLYPTYSQW	100
VELKSSGTYP	KKLYPTYSQW	VELKSSGTYP	KKLYPTYSQW	VELKSSGTYP	150
KKLYPTYSQW	VELKSSGTYP	KKLYPTYSQW	VELKSSGTYP	KKLYPTYSQW	200
VELKSSGTYP	KKLYPTYSQW	VELKSSGTYP	KKLYPTYSQW	VELKSSGTYP	250
KKLYPTYSQW	VELKSSGTYP	KKLYPTYSQW	VELKSSGTYP	KKLYPTYSQW	300
VELKSSGTYP	KKLYPTYSQW	VELKSSGTYP	VELKSSGTYP	KKLYPTYSQW	350
KKLYPTYSQW	VELKSSGTYP	KKLYPTYSQW	KKLYPTYSQW	VELKSSGTYP	400

Light Chain

VELKSSGTYP	KKLYPTYSQW	VELKSSGTYP	VELKSSGTYP	KKLYPTYSQW	50
KKLYPTYSQW	VELKSSGTYP	KKLYPTYSQW	KKLYPTYSQW	VELKSSGTYP	100
VELKSSGTYP	KKLYPTYSQW	VELKSSGTYP	VELKSSGTYP	KKLYPTYSQW	150
KKLYPTYSQW	VELKSSGTYP	KKLYPTYSQW	KKLYPTYSQW	VELKSSGTYP	200

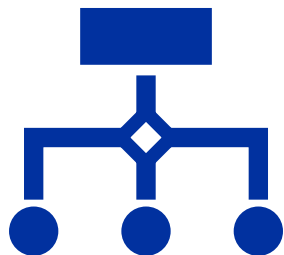
CAS Registry Service consultation

Select the results options that are best for you

Sequence suppression

- Option to not have sequence displayed in CAS REGISTRY at time of registration
- Sequence can be added later for an additional fee
- Request for sequence suppression must be included in submitted webform and substance information

Resources for order submissions



As needed, review the FAQs, CAS Registration Criteria, and/or CAS Registry Number Requirements for technical information regarding your specific submission

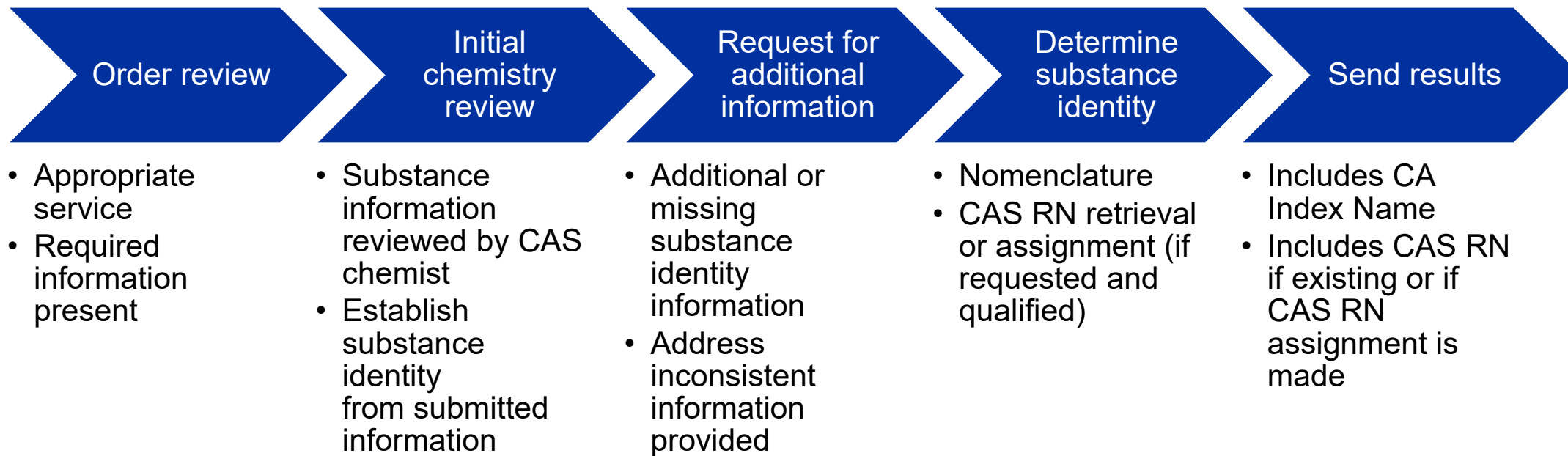


Questions – contact us at answers@cas.org

What To Expect During Order Processing

CAS Registry Services consultation

What happens during order processing



Requesting additional information or clarification

Chemist reviewing your order will reach out to the submitter on the following:

- Inconsistencies in substance identity information
- Additional information needed to establish your substance's chemical identity

Dear Mr. Johnson,

Thank you for your CAS Registry Services consultation order 123456. We have completed our initial review of your order and need additional information.

Your final product shows divinylbenzene as a monomer. However, your submitted starting materials does not include divinylbenzene. Is this substance part of your intended final product? If yes, please provide its CAS Registry Number.

Once we receive this information we will continue to process this request.

Best Regards,
Brad



Bradley Hutson
CAS Registry Services

+1 614.446.3600
cas.org



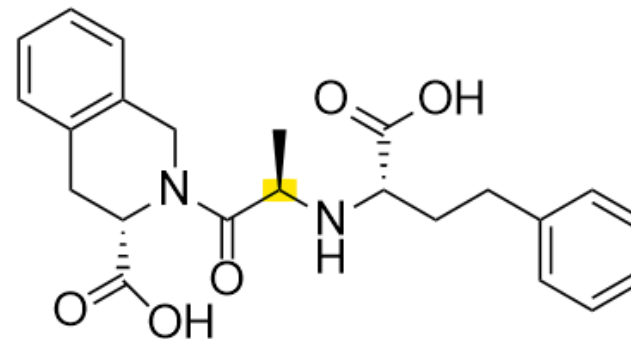
Additional information or clarification

Simple organic examples

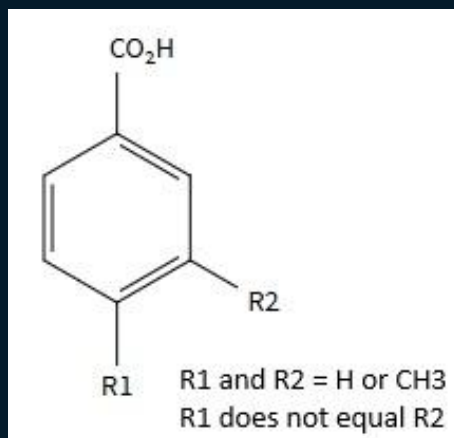
Molecular formula does not match structure



Name provided does not match stereo shown in structure



3-Isoquinolinecarboxylic acid, 2-[(2S)-2-[[[(1S)-1-carboxy-3-phenylpropyl]amino]-1-oxopropyl]-1,2,3,4-tetrahydro-, (3S)-



Product has specific molecular formula and variable structure

Additional information or clarification

Sequence examples

The DAR
is 4.0

What is the
average DAR
of your
substance?

There is one
mutation, the
231st residue is
a lysine.

Are there any
mutations in your
sequence and if so,
where are they
located?

It is removed
during post-
translational
modification

Is the C-terminal
lysine removed
during post-
translational
modification, or is
it absent at the
cDNA level?

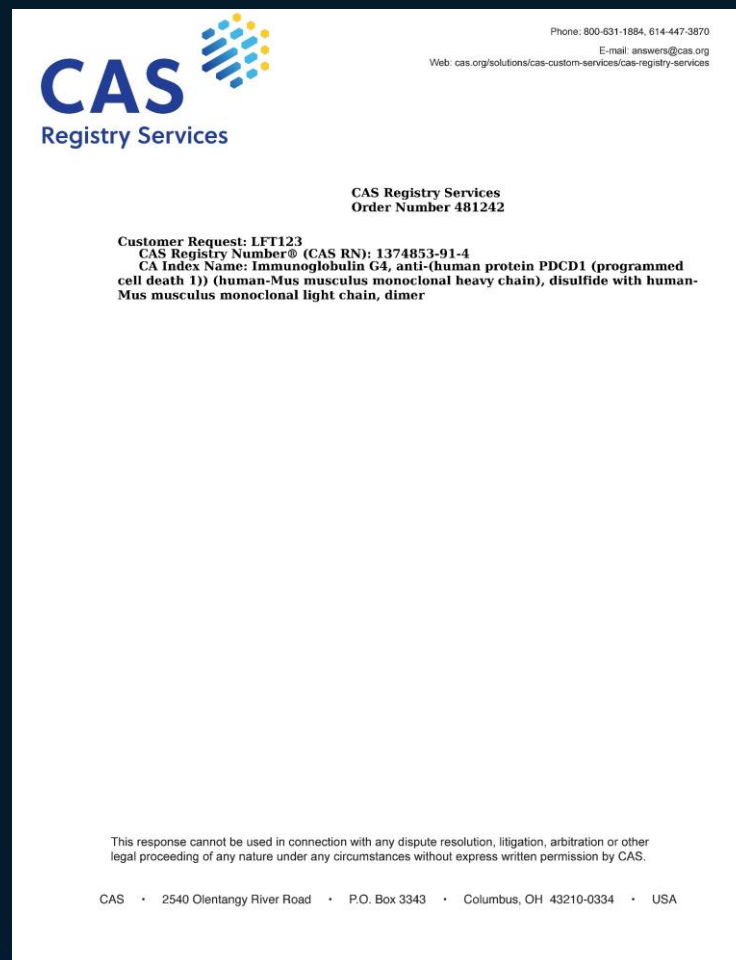
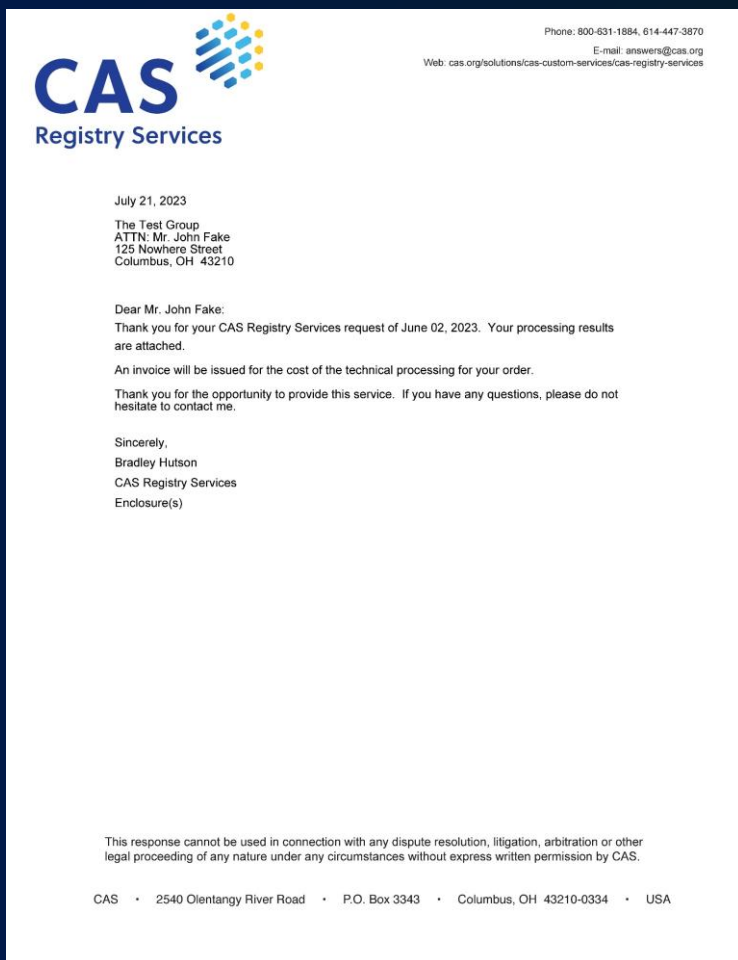
The
Isotype is
IgG2

What is the
Isotype of your
monoclonal
antibody

Order Results

CAS Registry Services consultation

What information is provided as order results?



Results include:

- Order number
- Your substance ID
- CAS RN (existing or new assignment)
- CA Index Name

All CA Index Names are assigned based on CAS nomenclature conventions

What will be displayed in CAS solutions?

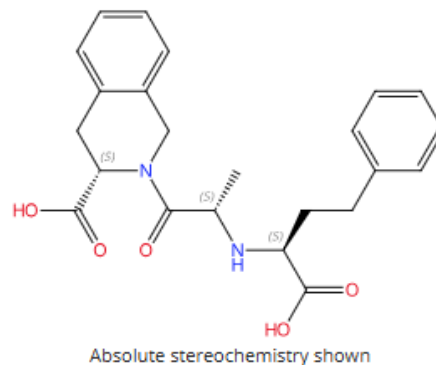
Organics substances

CAS Registry Number: 82768-85-2

310

15

39



C₂₃H₂₆N₂O₅

3-Isoquinolinecarboxylic acid, 2-[[[2S]-2-[[[1S]-1-carboxy-3-phenylpropyl]amino]-1-oxopropyl]-1,2,3,4-tetrahydro-, (3S)- (9CI, ACI)

What will be displayed in CAS solutions?

Sequences

 CAS Registry Number: 1374853-91-4

References (10K)

Reactions (2)

Suppliers (17)

Download icon

Image Not Available

Unspecified

Immunoglobulin G4, anti-(human protein PDCD1 (programmed cell death 1)) (human-Mus musculus monoclonal heavy chain), disulfide with human-Mus musculus monoclonal light chain, dimer (ACI)

Protein/Peptide Sequence
Sequence Length: 1330 (447, 447, 218, 218)
multichain; modified (modifications unspecified)

Other Names and Identifiers

8 Other Names for this Substance

h 409A11

Keytruda

Sequence Details

Sequence 1: Length 447; linear

1	QVQLVQSGVE	VKKPGASVKV	SCKASGYTFT	NYVMYWRQA	PGQGLEWMGG
51	INPSNGGTNF	NEKFKNRVTL	TTDSSTTTAY	MELKSLQFDD	TAVYYCARRD
101	YRFDMGFDYW	GQGTTTVTVSS	ASTKGPSVFP	LAPCSRSTSE	STAALGCLVK
151	DYFPEPVTVS	WNSGALTSGV	HTFPAVLQSS	GLYSLSSVVT	VPSSSLGTKT
201	YTCNVDHKPS	NTKVDKRVES	KYGPPCPPCP	APEFLGGPSV	FLFPPKPKDT
251	LMISRTPEVT	CVVVDVSQED	PEVQFNWYVD	GVEVHNAKTK	PREEQFNSTY
301	RVVSVLTVLH	QDWLNGKEYK	CKVSNKGLPS	SIEKTISKAK	GQPREPQVYT
351	LPPSQEEMTK	NQVSLTCLVK	GFYPSDIAVE	WESNGQPENN	YKTPPVLDL

Sequence Modifications

Type	Location	Description
bridge	chain 1 cysteine-22 to chain 1 cysteine-96	disulfide bridge
bridge	chain 1 cysteine-147 to chain 1 cysteine-203	disulfide bridge
bridge	chain 1 cysteine-261 to chain 1 cysteine-321	disulfide bridge
bridge	chain 1 cysteine-367 to chain 1 cysteine-425	disulfide bridge
bridge	chain 2 cysteine-22 to chain 2 cysteine-96	disulfide bridge
bridge	chain 2 cysteine-147 to chain 2 cysteine-203	disulfide bridge

CAS Registry Services consultation

Items to consider



Understand WHO's requirements for INN submissions prior to submitting your order



Please submit your order in timely a manner, relevant to upcoming WHO INN submission deadlines



CAS may need to request additional information to process your order. Processing will only resume upon receipt of your response.



FAQ and substance info requirements are available on the CAS.org website or contact us for additional support

Contact us



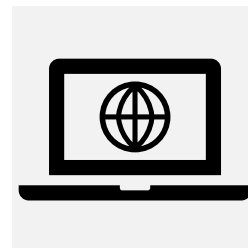
Email

answers@cas.org



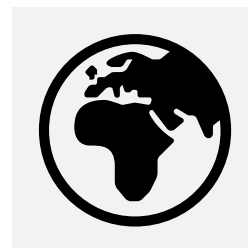
North America Toll-free

1-800-631-1884



Website

<https://www.cas.org/solutions/cas-registry-services>



Worldwide

614-447-3870

THANK YOU

CAS Registry Services

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