

SEARCHING GENERICALLY CLAIMED SEQUENCES IN CAS STNEXT®

CAS STNext® Coffee Lecture

Jan Baur, CAS

Baseline situation

Patent with generically claimed sequence

52. An anti-inflammatory peptide (AIP) comprising an amino acid sequence of Formula II:

L-X2-X3-X4-X5-X6-K-L-X9-X10-X11-X12 (Formula II)

Wherein

X2 is A, Y, W, V, R, Q, M, L, K, I, H, or F;

X3 is L, W, or F;

X4 is L, W, N, or C;

X5 is A, W, or F;

X6 is P, Y, W, V, T, S, R, Q, N, M, L, I, H, G, F, D, C, or A;

X9 is L or W;

X10 is R or S;

X11 is R or Q; and

X12 is F, V, T, S, R, Q, P, N, K, I, G, E, D, C, or A.

Table 1. Peptide Sequences with Anti-inflammatory Activity

Peptide	Sequence	SEQ ID NO.
KBP63	KLAKRLLLSMNQ	1
KBP73	LALLAPKLLRRF	2
KBP82	FAVPAKQAKKTLT	3

Generic sequence claim and exemplified and claimed specific sequences in patent application WO2024054928

To which databases will these sequence types be added?

Generic sequence is added to MARPAT, specific sequence to CAS REGISTRY

52. An anti-inflammatory peptide (AIP) comprising an amino acid sequence of Formula II:

L-X2-X3-X4-X5-X6-K-L-X9-X10-X11-X12 (Formula II)

MARPAT

Indexing limits: NT<30 | AA<180

Table 1. Peptide Sequences with Anti-inflammatory Activity

Peptide	Sequence	SEQ ID NO.
KBP63	KLAKRLLLSMNQ	1
KBP73	LALLAPKLLRRF	2
KBP82	FAVPAKQAKKTLT	3

PatentPak markers are added too

CAS REGISTRY

and GENESEQ, USGENE, PATGENE

Search in CAS REGISTRY

Construct a motif query to capture all alternative AAs in REGISTRY

52. An anti-inflammatory peptide (AIP) comprising an amino acid sequence of Formula II:

L-X2-X3-X4-X5-X6-K-L-X9-X10-X11-X12 (Formula II)

↓
Encode claimed sequence
into motif query using
variability symbols

```
=> S L[AYWVRQMLKIH F][LWF][LWNC][AWF][PYWVTSRQNMLIHGFDCA]KL[LW][RS][RQ][FVTSRQPNKIGEDCA]/SQSP
L1          20 L[AYWVRQMLKIH F][LWF][LWNC][AWF][PYWVTSRQNMLIHGFDCA]KL[LW][RS][RQ][FVTSRQPNKIGEDCA]/SQSP
```

```
=> S L1 AND 12/SQ L
```

```
337996 12/SQ L
```

```
L2          20 L37 AND 12/SQ L
```

This motif yields 20 sequences with the exact length of 12

```
=> FIL CAPLUS
```

```
.....=> S L2
```

```
L3          1 L2
```

All 20 sequences were published in the WO patent we used as a starting point

Crossover to CAplus and display

=> FIL CAPLUS

=> S L2

L3 1 L2

=> D BIB AB HITPPAK

L3 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2025 ACS on STN
[PatentPak PDF](#) | [PatentPak PDF+](#) | [PatentPak Interactive](#)

AN 2024:570046 CAPLUS [Full-text](#)

DN 186:180878

TI Peptides with cytokine-releasing activity and methods for characterizing
 cytokine-releasing profiles of peptides

IN Lis, Ewa; Lindmeier, Lily Kang

PA Koliber Biosciences Inc., USA

UO KOLIBER BIOSCIENCES

UOS KOLIBER BIOSCIENCES

SO PCT Int. Appl., 65pp.

 CODEN: PIXXD2

DT Patent

LA English

CAS PatentPak shows location(s) of sequence indexing

PPPI

PATENT NO.	KIND	DATE	LANGUAGE	PatentPak
WO 2024054928	A1	20240314	English	PDF PDF+ Interactive

. . .

PSPI

PATENT NO.	KIND	STATUS	STATUS DATE
WO 2024054928	A1	Alive	20240321

OS MARPAT 186:180878

AB Disclosed herein are peptides that exhibit cytokine-releasing activity.

. . .

[PatentPak PDF](#) | [PatentPak PDF+](#) |

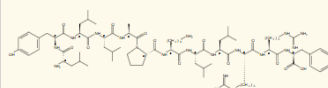
PPAK

3032316-74-5P, [Pg 38 Claim](#)

3032316-99-4P, [Pg 42 Claim](#)

. . .

CAS RN 3032316-99-4



Analyst Markup Locations (2)

page 42 - Claim

page 36

and A.

66. The AIP of claim 65, wherein X₁₂ is selected from F, K, E, D, and A.

67. The AIP of claims 65 or 66, wherein X₁₂ is F.

68. The AIP of claim 52, wherein the AIP comprises an amino acid sequence selected from any one of SEQ ID NOs 2 and 27-45.

These sequences were marked up in claim 68 and a table on page 36

How does the sequence look like in MARPAT?

MARPAT is a structure-searchable database!

52. An anti-inflammatory peptide (AIP) comprising an amino acid sequence of Formula II:

L-X2-X3-X4-X5-X6-K-L-X9-X10-X11-X12 (Formula II)

Wherein

X2 is A, Y, W, V, R, Q, M, L, K, I, H, or F;

X3 is L, W, or F;

X4 is L, W, N, or C;

X5 is A, W, or F;

X6 is P, Y, W, V, T, S, R, Q, N, M, L, I, H, G, F, D, C, or A;

X9 is L or W;

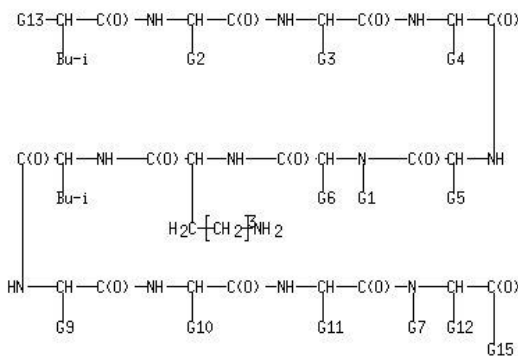
X10 is R or S;

X11 is R or Q; and

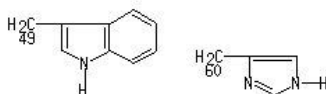
X12 is F, V, T, S, R, Q, P, N, K, I, G, E, D, C, or A.



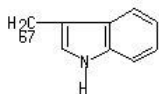
MSTR 2



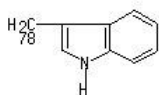
G1 = H
G2 = Me / CH₂C₆H₄OH-p / 49 / Pr-i / CH₂CH₂CH₂NHC(NH)NH₂ / CH₂CH₂CONH₂ / CH₂CH₂SMe / Bu-i / CH₂CH₂CH₂CH₂NH₂ / Bu-s / 60 / CH₂Ph



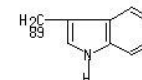
G3 = Bu-i / 67 / CH₂Ph



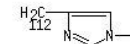
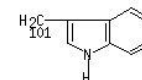
G4 = Bu-i / 78 / CH₂CONH₂ / CH₂SH



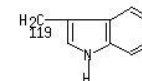
G5 = Me / 89 / CH₂Ph



G6 = CH₂C₆H₄OH-p / 101 / Pr-i / CH(OH)Me / CH₂OH / CH₂CH₂CH₂NHC(NH)NH₂ / CH₂CH₂CONH₂ / CH₂CONH₂ / CH₂CH₂SMe / Bu-i / Bu-s / 112 / H / CH₂Ph / CH₂CO₂H / CH₂SH / Me



G7 = H
G9 = Bu-i / 119



G10 = CH₂CH₂CH₂NHC(NH)NH₂ / CH₂OH
G11 = CH₂CH₂CH₂NHC(NH)NH₂ / CH₂CH₂CONH₂
G12 = CH₂Ph / Pr-i / CH(OH)Me / CH₂OH / CH₂CH₂CH₂NHC(NH)NH₂ / CH₂CH₂CONH₂ / CH₂CONH₂ / CH₂CH₂CH₂CH₂NH₂ / Bu-s / H / CH₂CH₂CO₂H / CH₂CO₂H / CH₂SH / Me
G13 = NH₂ / 135



G14 = R <"peptide residue">
G15 = OH / R <"peptide residue">
G1 + G6 = CH₂CH₂CH₂
G7 + G12 = CH₂CH₂CH₂
Patent location: claim 52

Tips for drawing sequence structures in CASDraw

3032316-74-5



Model structure using an existing RN

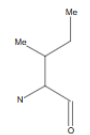


Structure
Templates

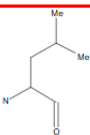
Templates

Leucin

Draw amino acids
using templates



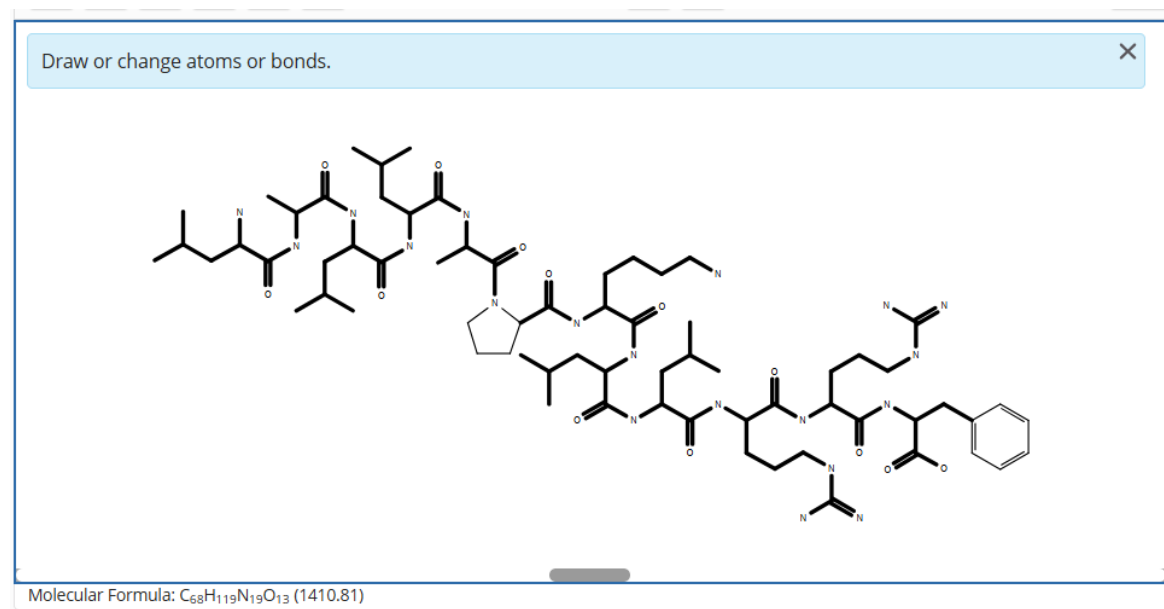
Isoleucine



Leucine

ChemDraw®

Transform sequence query into
structure using ChemDraw and
import into CASDraw



Search in MARPAT

Query template was SEQ ID NO 2 from claim 68

68. The AIP of claim 52, wherein the AIP comprises an amino acid sequence selected from any one of SEQ ID NOs 2 and 27-45.

Table 1. Peptide Sequences with Anti-inflammatory Activity

Peptide	Sequence	SEQ ID NO.
KBP63	KLAKRLLLSMNQ	1
KBP73	LALLAPKLLRRF	2

L4 STRUCTURE UPLOADED

=> S L4 CSS FULL

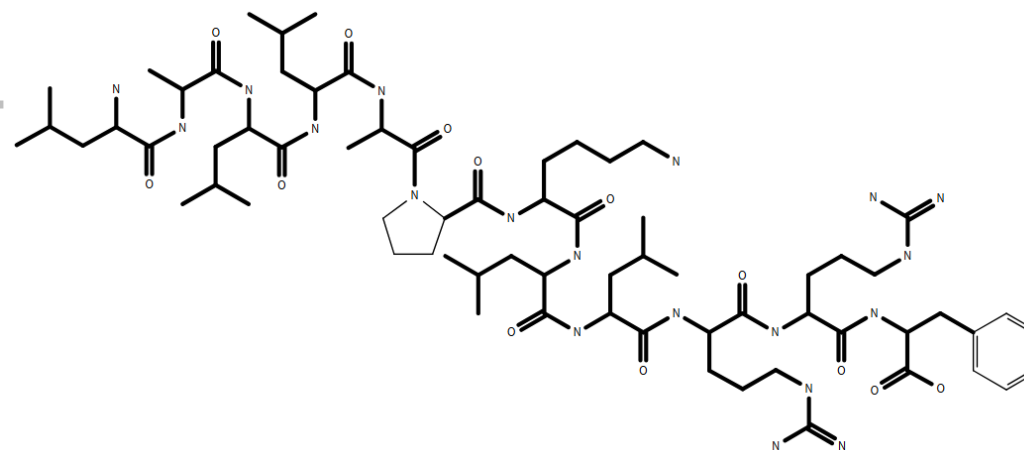
FULL SEARCH INITIATED 09:24:08

100.0% PROCESSED 61639 ITERATIONS

SEARCH TIME: 00.02.00

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**

L5 17 SEA CSS FUL L4



MARPAT display

FQHIT shows the first query hit assembled hit structure

=> D L5 BIB FQHIT 1-TOT

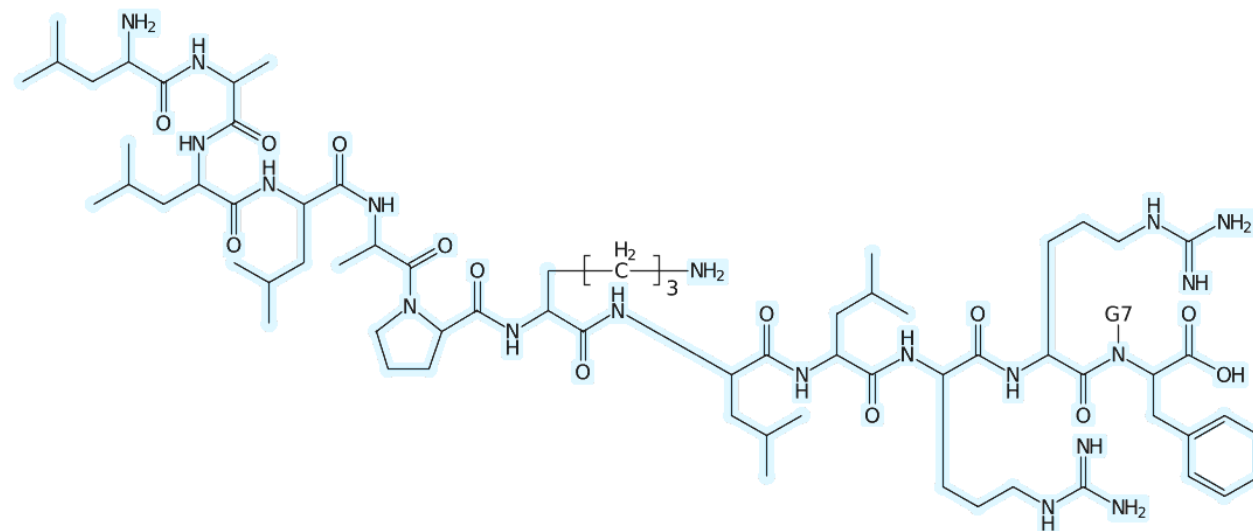
L5 ANSWER 1 OF 17 MARPAT COPYRIGHT 2025 ACS on STN
[PatentPak PDF](#) | [PatentPak PDF+](#) | [PatentPak Interactive](#)
AN 186:180878 MARPAT [Full-text](#)
TI Peptides with cytokine-releasing activity and methods
for characterizing
cytokine-releasing profiles of peptides
IN Lis, Ewa; Lindmeier, Lily Kang
PA Koliber Biosciences Inc., USA
UO KOLIBER BIOSCIENCES
SO PCT Int. Appl., 65pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1
PI

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2024054928	A1	20240314	WO 2023-US73665	20230907
PRAI US 2022-63405169		20220909		

PSPI

PATENT NO.	KIND	STATUS	STATUS DATE
WO 2024054928	A1	Alive	20240321

MSTR 2 Assembled



Patent location:

claim 52

If definitions of G Groups in the main structure shall be displayed, use **FQHITEXG** instead of FQHIT

Unify and contrast in CPlus

=> **FIL CAPLUS**

=> **S L2**

L6 1 L2 Crossover from
REGISTRY

=> **S L5**

L7 18 L5 Crossover from MARPAT

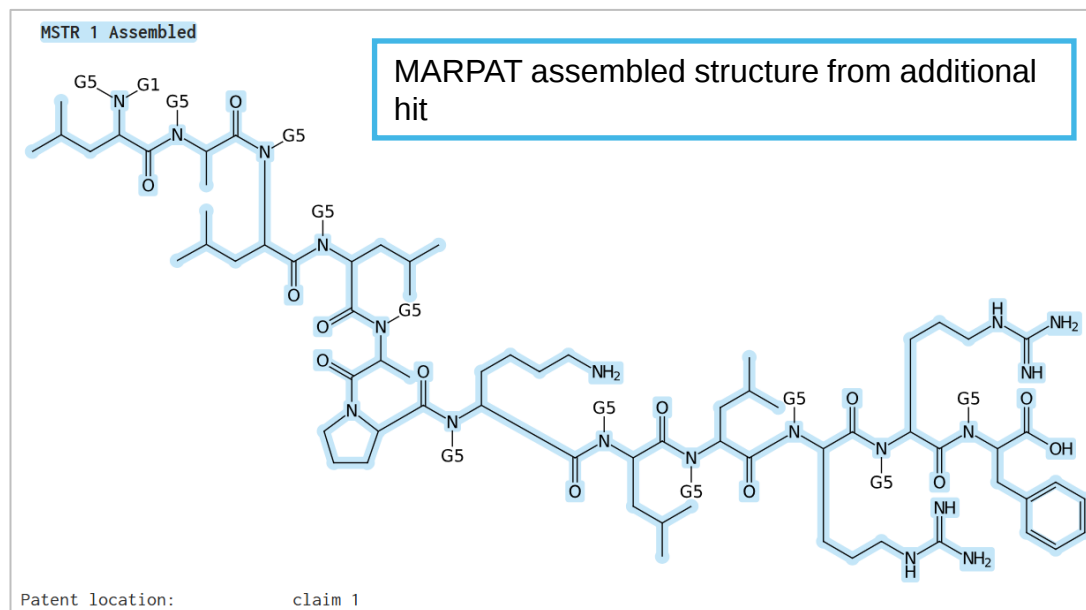
=> **S L7 AND INFLAMM?**

L8 4 L6 AND INFLAMM?

=> **S L8 NOT L3**

L9 3 L7 NOT L3

There are 3 more patents retrieved
via the Markush search when limited to
inflammation



1. A method of treating a patient having a neutrophil-driven inflammatory disease, the method comprising:
administering to the patient a multivalent structured polypeptide comprising at least one therapeutic peptide;
wherein the sequence of the therapeutic peptide consists of the sequence X₁-X₂-X₃-X₄-X₅-X₆-X₇-X₈-X₉-X₁₀-X₁₁-X₁₂ (SEQ ID NO: 9) with each of X₁, X₂, X₃, X₄, X₅, X₆, X₇, X₈, X₉, X₁₀, X₁₁, and X₁₂ independently being absent or any amino acid residue,
so long as the therapeutic peptide comprises at least 4 amino acid residues and at least one of X₁, X₂, X₃, X₄, X₅, X₆, X₇, X₈, X₉, X₁₀, X₁₁, and X₁₂ is Q.

CAS accelerates breakthroughs



Jan Baur

Manager, Customer Success Specialists, EMEA

jbaur@acs-i.org