39 二次代謝物データベースKNApSAcK family DBの開発とデータサイエンス

○金谷 重彦（奈良先端科学技術大）、森田 晶（奈良先端科学技術大）、有田 正規（遺伝研）、時松 敏明（遺伝研）、児玉 悠一（遺伝研）、藤澤 貴智（遺伝研）、荒 武（京都大）、高橋 みき子（理研）、長崎 英樹（かずさ研）、櫻井 望（遺伝研）、平川 英樹（かずさ研）

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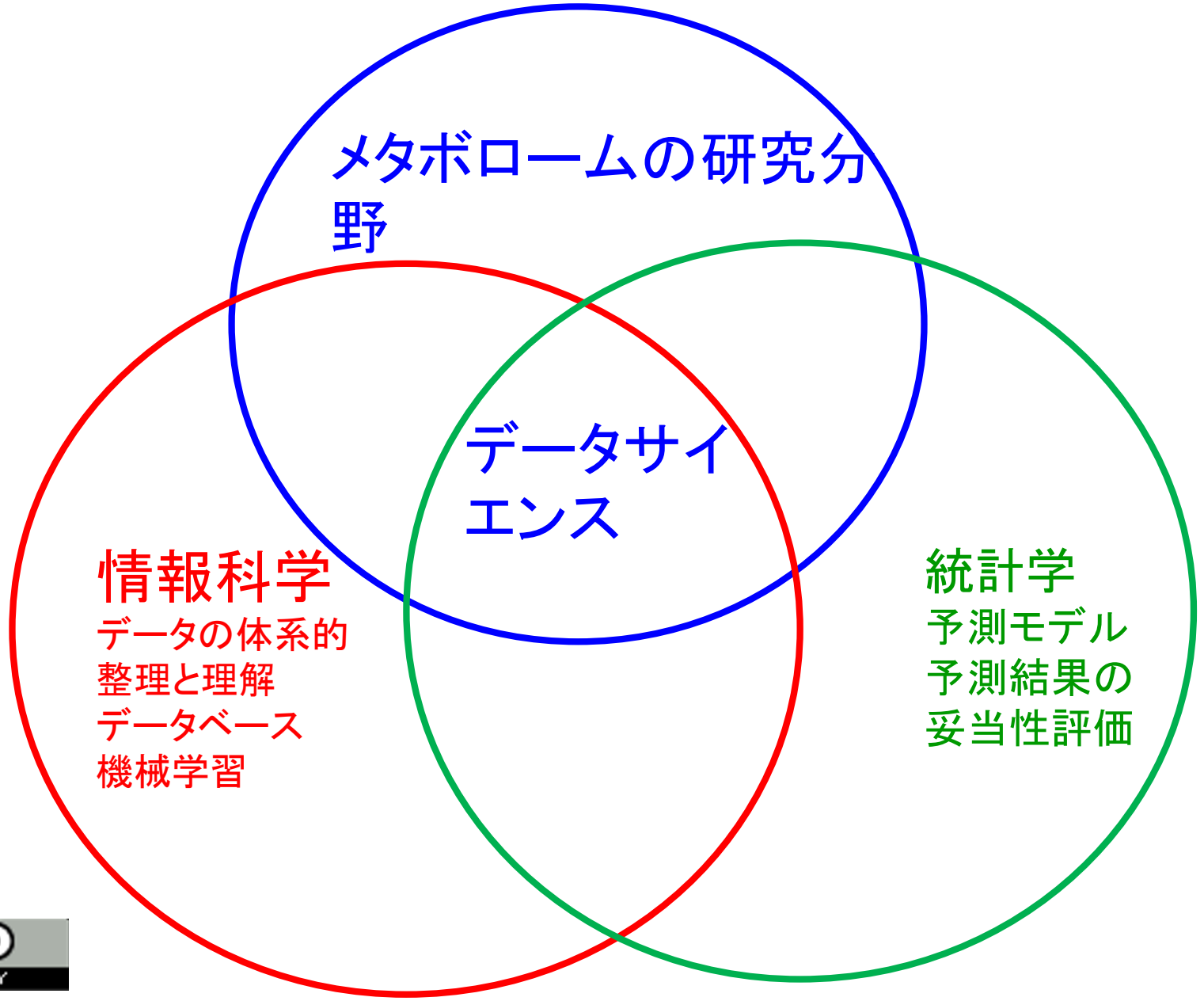
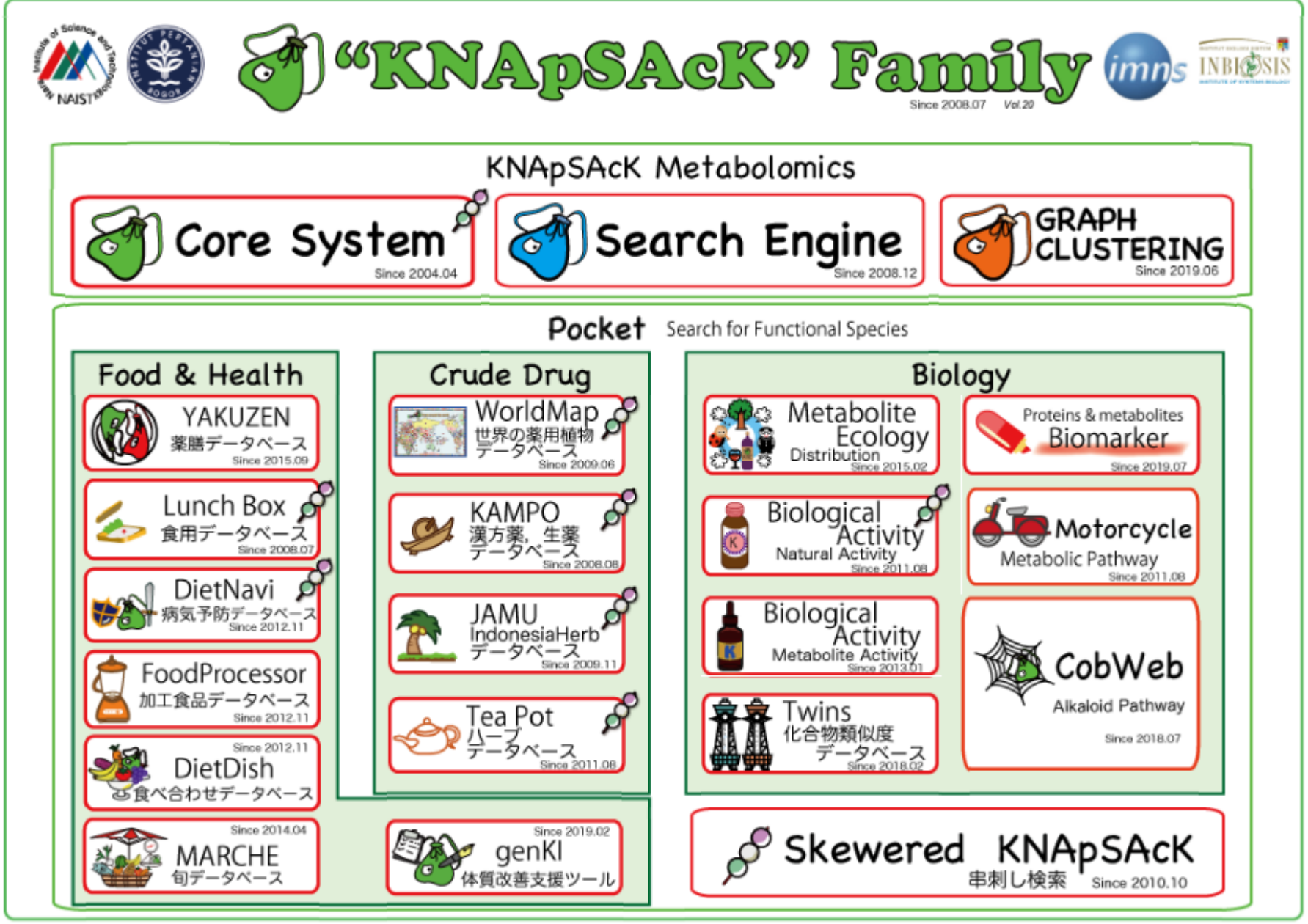
[1]さあはじめよう、データサイエンス！
データベースをつくろう！KNApSAcK family DB
[2] Application of Graph Convolution Neural Networks to chemical structures

2004

Last update	2022/09/22
metabolite	62,646 entries
metabolite-species pair	157,144 entries
species	24,704 entries

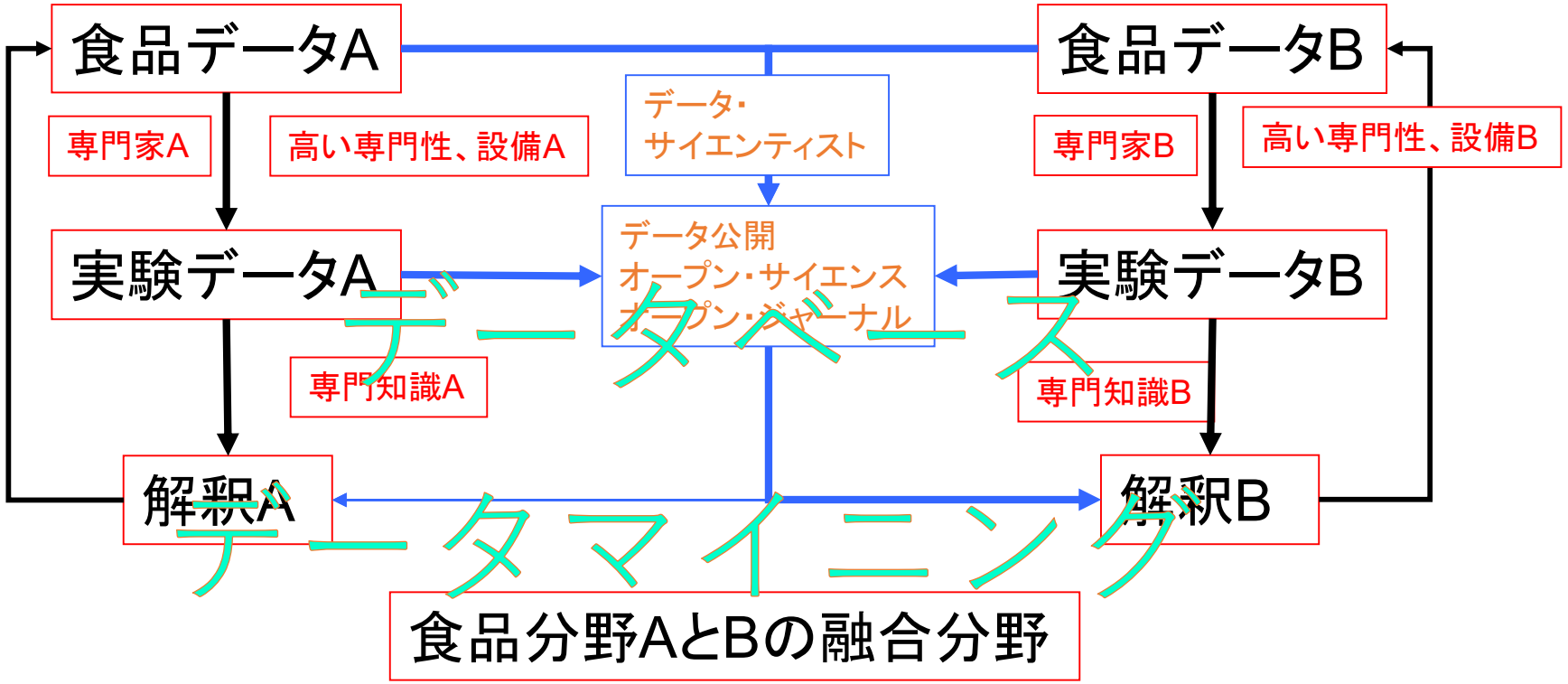
Plant Cell Physiol.53, e1(1-12) (2012)
1%-citation Paper, 2013 PCP paper awards


メタボローム
の研究分野
データサイ
エンス
情報科学
データの体系的
整理と理解
データベース
機械学習
統計学
予測モデル
予測結果の
妥当性評価



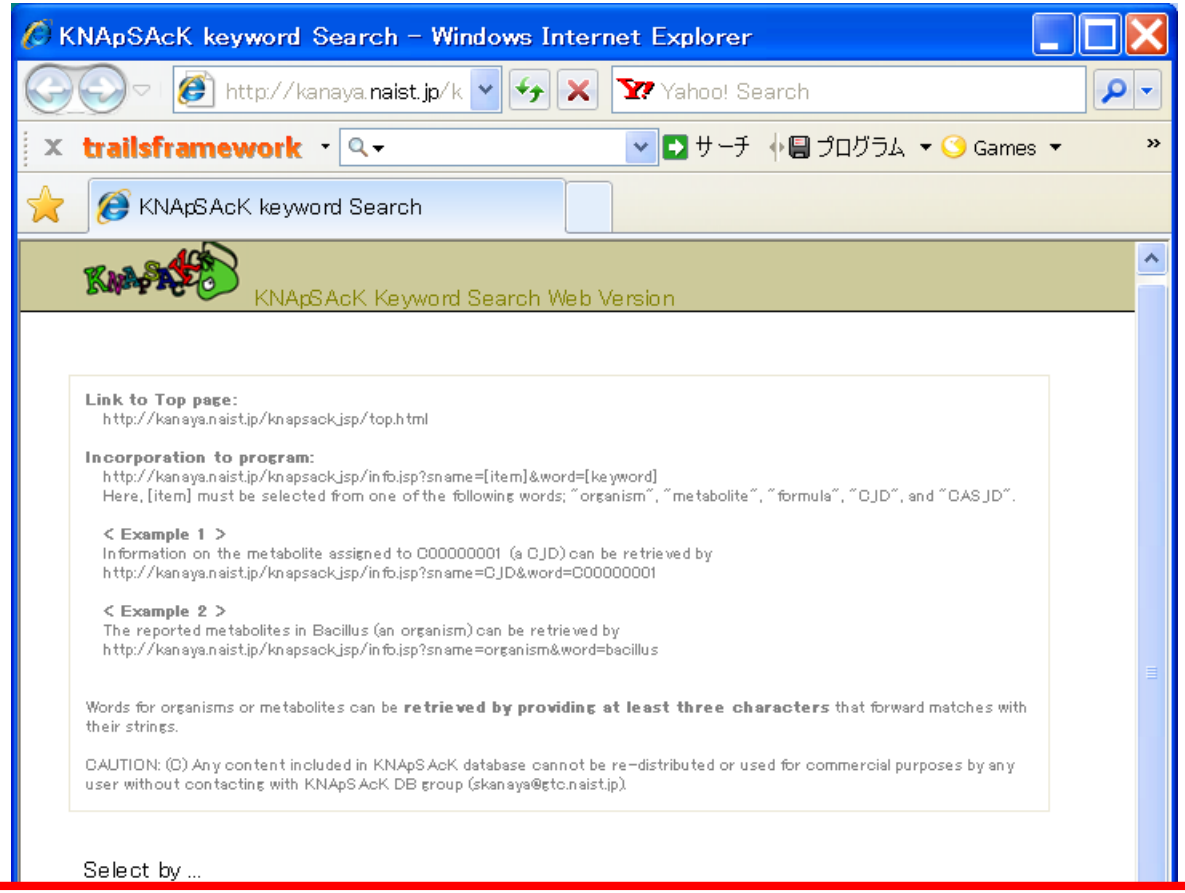
2013 days

データ・サイエンスとは



「縦つながり」から「横つながり」へ

5



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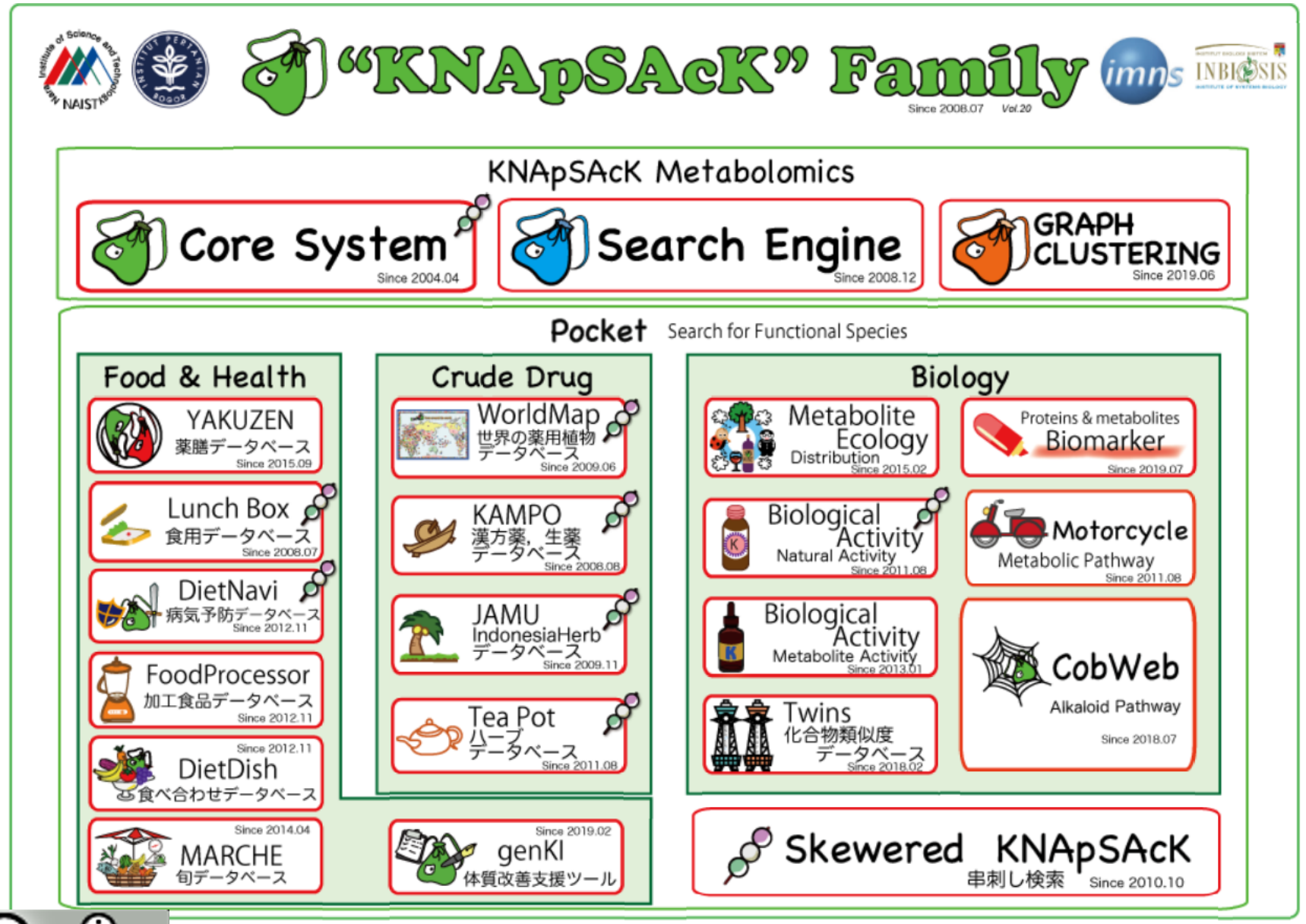
metabolite 62,646 entries
metabolite-species pair 157,144 entries
species 24,704 entries Plant Cell Physiol.53, e1(1-12) (2012)
1%-citation Paper, 2013 PCP paper awards

Input “KNApSAcK Family” in Google

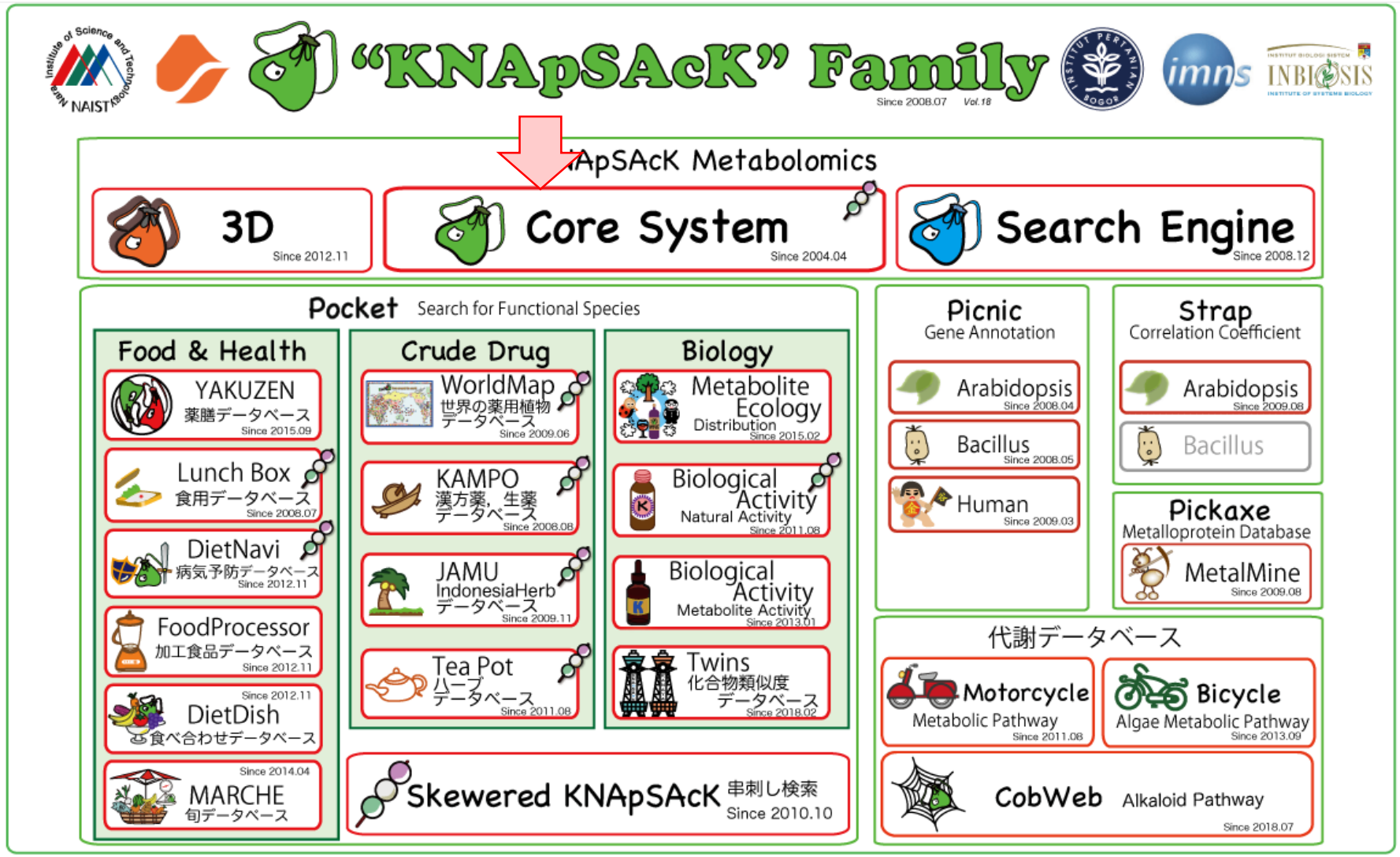
Main window



Japanese) Instruction Manual(English) Terms of service(Japanese)

2782 days left!

Let's enjoy species-metabolites information



Plant Cell Physiol.53, e1(1-12) (2012)
(the highest 1% citted paper, 2012PCP Papar Award)

Link to Top page:
http://kanaya.naist.jp/knapsack_jsp/top.ht

Incorporation to program:
http://kanaya.naist.jp/knapsack_jsp/info.jsp?sname=[item]&word=[keyword]
Here, [item] must be selected from one of the following words; "organism", "metabolite", "formula", "C_ID", and "CAS_ID".

< Example 1 >
Information on the metabolite assigned to C00000001 (a C_ID) can be retrieved by
http://kanaya.naist.jp/knapsack_jsp/info.jsp?sname=C_ID&word=C00000001

< Example 2 >
The reported metabolites in Bacillus (an organism) can be retrieved by
http://kanaya.naist.jp/knapsack_jsp/info.jsp?sname=organism&word=bacillus

Words for organisms or metabolites can be **retrieved by providing at least three characters** that forward matches with their strings.

CAUTION: (C) Any content included in KNApSAcK database cannot be re-distributed or used for commercial purposes by any user without contacting with KNApSAcK DB group (skanaya@gtc.naist.jp).

Instruction Manual(Japanese) Instruction Manual(English)

Select by ...
○ ALL Types ○ Organism ● Metabolite ○ Molecular formula
○ C_ID ○ CAS_ID ○ INCHI-KEY

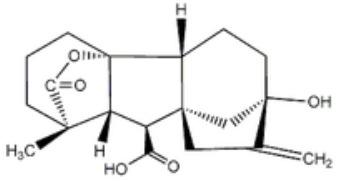
Gibberellin A20 List Clear

input word = C00000020

Metabolite Information

Name	Gibberellin A20 GA20
Formula	C19H24O5
Mw	332.16237388
CAS RN	19143-87-4
C_ID	C00000020 3D
InChIKey	OXFPYCSNYOFUCH-RWGJJKMUNA-N

Structural formula



zoom in

Kingdom	Family	Species	Reference
Bacteria	Bacillaceae	Bacillus licheniformis	Ref.
Bacteria	Bacillaceae	Bacillus pumilus	Ref.
Fungi	Nectriaceae	Gibberella fujikuroi	Ref.
Plantae	Agavaceae	Polianthes tuberosa	Ref.
Plantae	Alliaceae	Allium cepa	Ref.
Plantae	Alstroemeriaceae	Alstroemeria hybrida	Ref.
Plantae	Anacardiaceae	Mangifera indica	Ref.
Plantae	Araliaceae	Aralia cordata	Ref.
Plantae	Asteraceae	Carthamus tinctorius	Ref.
Plantae	Asteraceae	Chrysanthemum x morifolium	Ref.
Plantae	Asteraceae	Helianthus annuus	Ref.
Plantae	Asteraceae	Lactuca sativa	Ref.
Plantae	Asteraceae	Stevia rebaudiana	Ref.
Plantae	Begoniaceae	Begonia x cheimantha	Ref.
Plantae	Betulaceae	Alnus tenuifolia	Ref.
Plantae	Betulaceae	Betula pendula	Ref.
Plantae	Caryophyllaceae	Agrostemma githago	Ref.
Plantae	Caryophyllaceae	Silene armeria	Ref.
Plantae	Cbotiaceae/Dicksoniaceae	Cibotium glaucum	Ref.
Plantae	Chenopodiaceae	Spinacia oleracea	Ref.
Plantae	Convolvulaceae	Ipomoea batatas	Ref.
Plantae	Convolvulaceae	Ipomoea nil	Ref.
Plantae	Convolvulaceae	Ipomoea reptans	Ref.
Plantae	Cruciferae	Brassica campestris	Ref.

2 Bacteria
1 Fungi

83 Plants

Co-evolution of metabolic pathways between microorganisms and plants!

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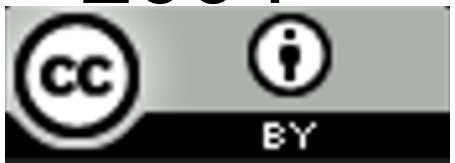

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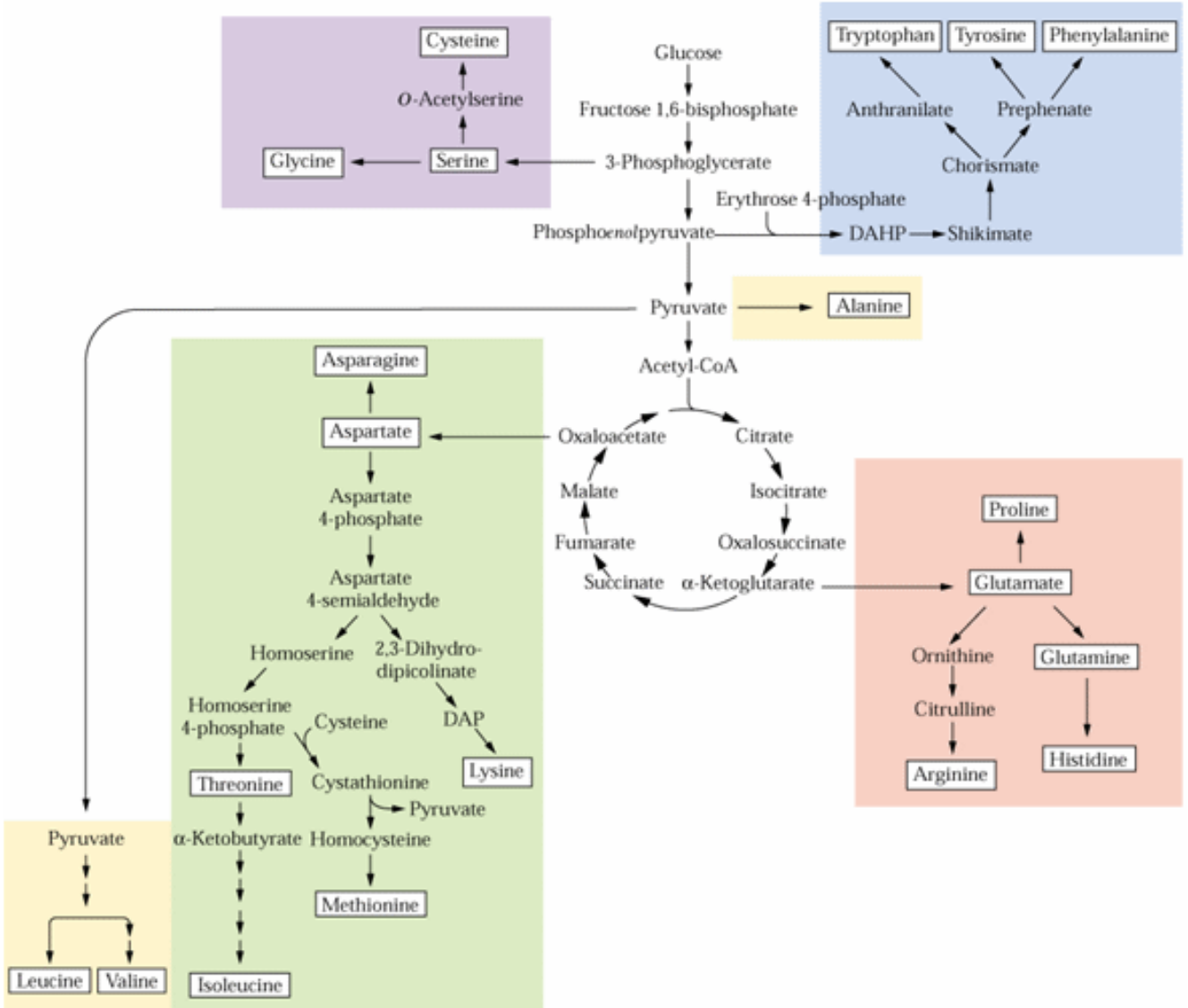
Plant Cell Physiol.53, e1(1-12) (2012)
1%-citation Paper, 2013 PCP paper awards

(a) Prediction of starting materials from alkaloids

Primary Metabolic pathway: directly involved in normal growth, development, and reproduction



Select by ...

◉ ALL Types ○ Organism ○ Metabolite ○ Molecular formula

○ C_ID ○ CAS_ID ○ INCHI-KEY

Streptomyces × List Clear

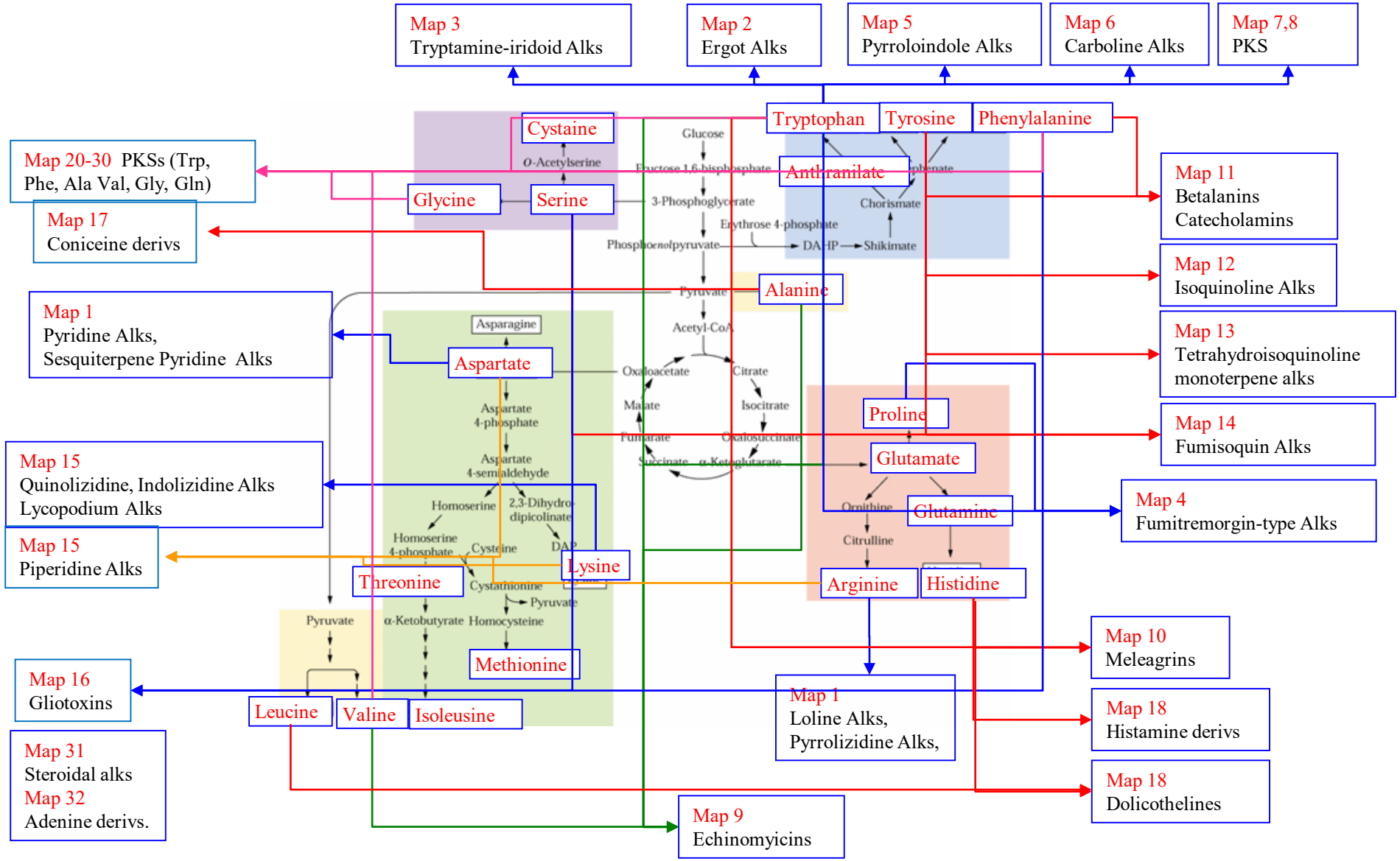
input type = all , input word = Streptomyces

Number of matched data : 2001

2001エントリー

C_ID	CAS ID	Metabolite	Molecular formula	Mw	Organism or InChIKey
C00000108	879-37-8	Indole-3-acetamide	C10H10N2O	174.07931296	Streptomyces atroolivaceus
C00000108	879-37-8	Indole-3-acetamide	C10H10N2O	174.07931296	Streptomyces mutabilis
C00000109	2591-98-2	Indole-3-acetaldehyde	C10H9NO	159.06841392	Streptomyces atroolivaceus
C00000112	487-89-8	Indole-3-carboxaldehyde	C9H7NO	145.05276385	Streptomyces sp. M491
C00000112	487-89-8	Indole-3-carboxaldehyde	C9H7NO	145.05276385	Streptomyces staurosporeus
C00000114	526-55-6	Indole-3-ethanol	C10H11NO	161.08406398	Streptomyces atroolivaceus
C00000114	526-55-6	Indole-3-ethanol	C10H11NO	161.08406398	Streptomyces mutabilis
C00000146	84453-40-7	(+)-Bottrospicatol	C10H16O2	168.11502976	Streptomyces bottropensis
C00000334	98-89-5	Cyclohexylcarboxylic acid	C7H12O2	128.08372963	Streptomyces collinus
C00000336	636-82-8	1-Cyclohexenylcarboxylic acid	C7H10O2	126.06807956	Streptomyces collinus
C00000339	82189-03-5	Ansatrienin A	C36H48N2O8	636.34106652	Streptomyces collinus
C00000339	82189-03-5	Ansatrienin A	C36H48N2O8	636.34106652	Streptomyces rishiriensis
C00000340	170591-54-5	U-106305	C28H41NO	407.31881494	Streptomyces sp. UC11136
C00000368	124753-55-5	IM-2	C9H16O4	188.104859	Streptomyces sp. strain FRI-5
C00000369	109075-62-9	Virginiae butanolide C	C11H20O4	216.13615913	Streptomyces virginiae
C00000370	125654-65-1	Virginiae butanolide E	C11H20O4	216.13615913	Streptomyces virginiae
C00000371	109215-47-6	Virginiae butanolide A	C12H22O4	230.15180919	Streptomyces antibioticus
C00000371	109215-47-6	Virginiae butanolide A	C12H22O4	230.15180919	Streptomyces bikiniensis
C00000371	109215-47-6	Virginiae butanolide A	C12H22O4	230.15180919	Streptomyces cyaneofuscatus
C00000371	109215-47-6	Virginiae butanolide A	C12H22O4	230.15180919	Streptomyces virginiae
C00000372	125761-52-6	Virginiae butanolide D	C12H22O4	230.15180919	Streptomyces virginiae

Secondary Metabolism: are not absolutely required for the survival of the organism. Alkaloids are biosynthesized by primary metabolites such as amino acids nucleotide, steroids, and secondary metabolites such as terpenoids..



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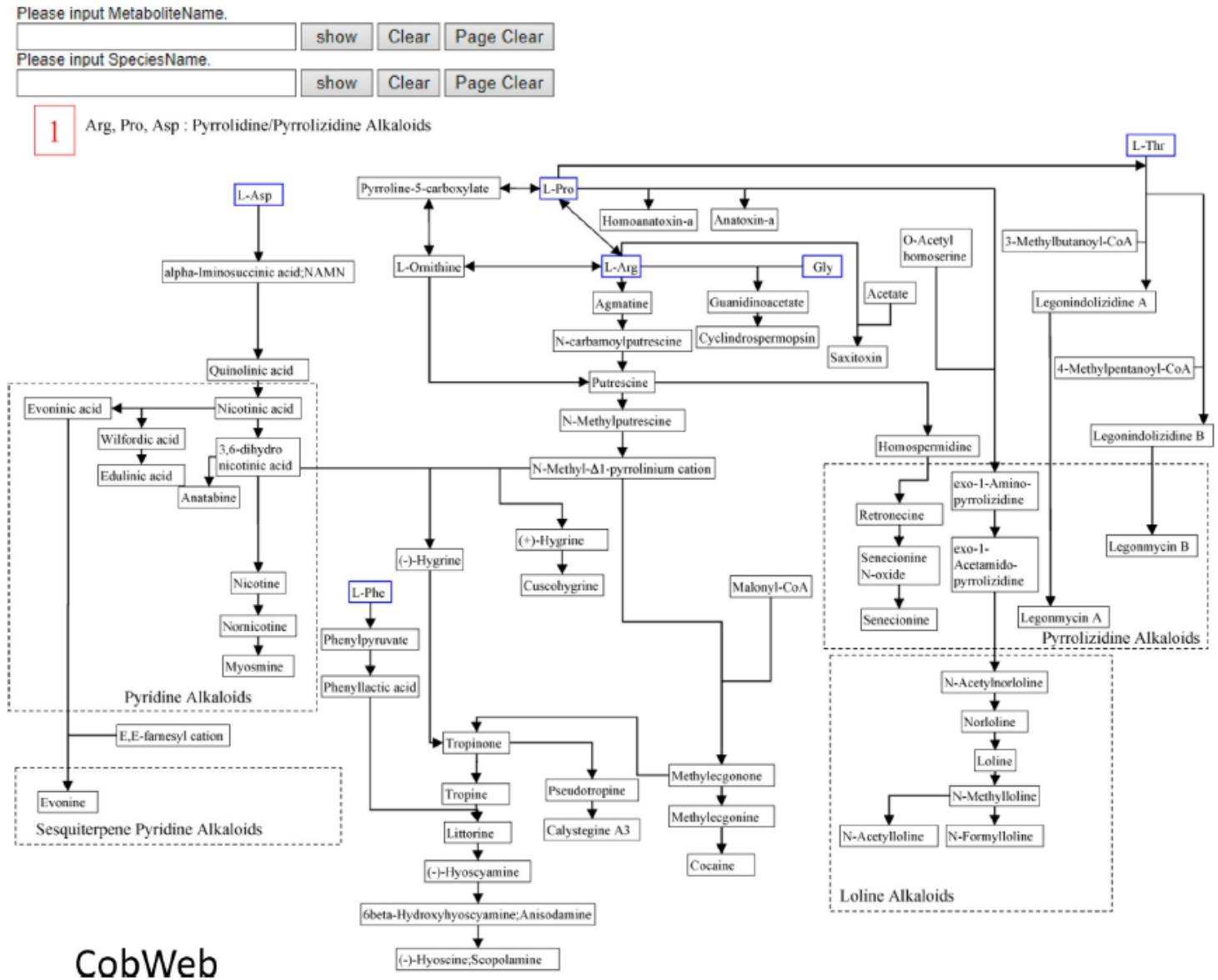
Example of metabolic pathway for alkaloids

metabolite

Species



CobWeb

Select by ...

◉ ALL Types ○ Organism ○ Metabolite ○ Molecular formula

○ C_ID ○ CAS_ID ○ INCHI-KEY

Streptomyces × List Clear

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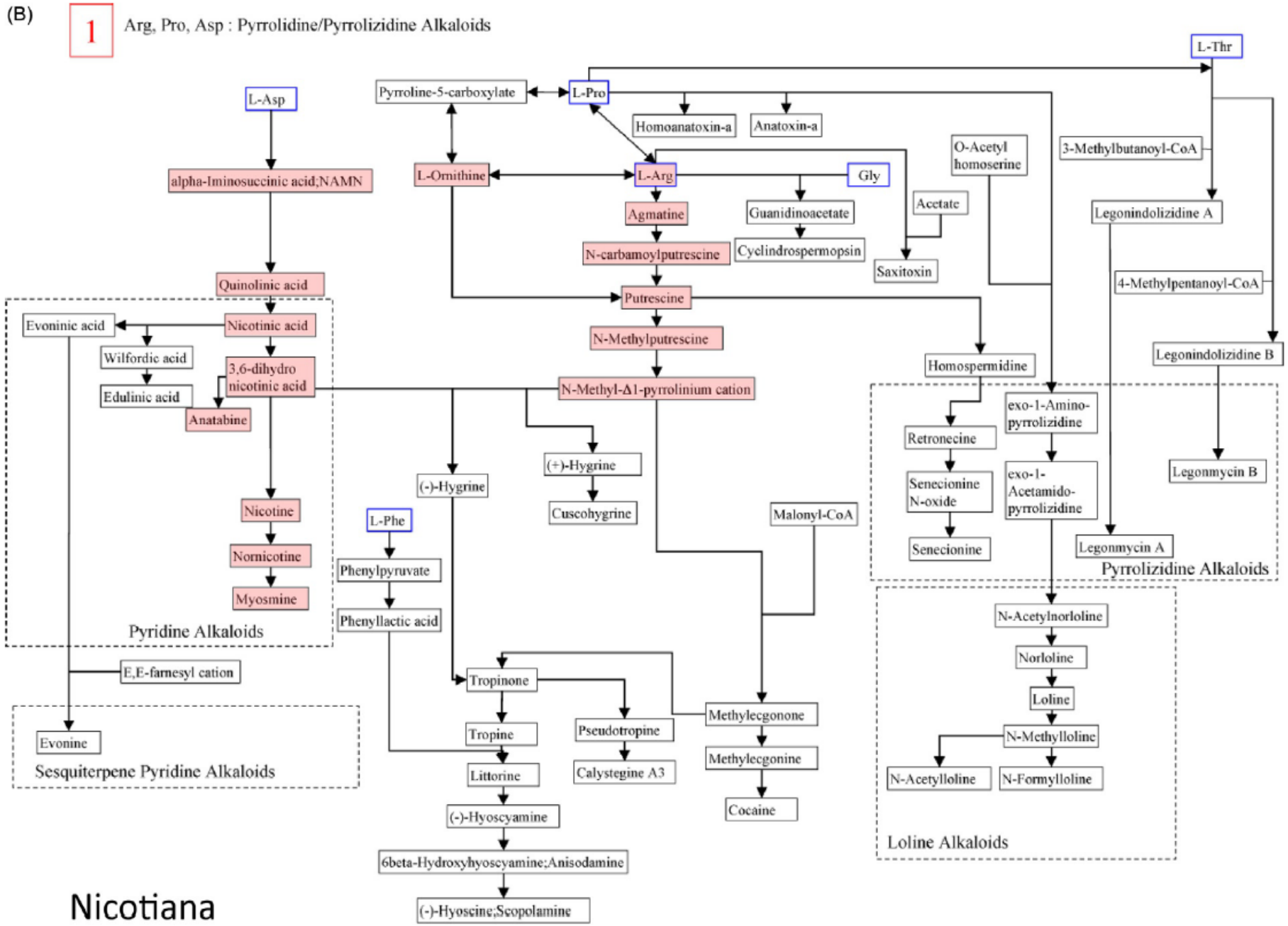
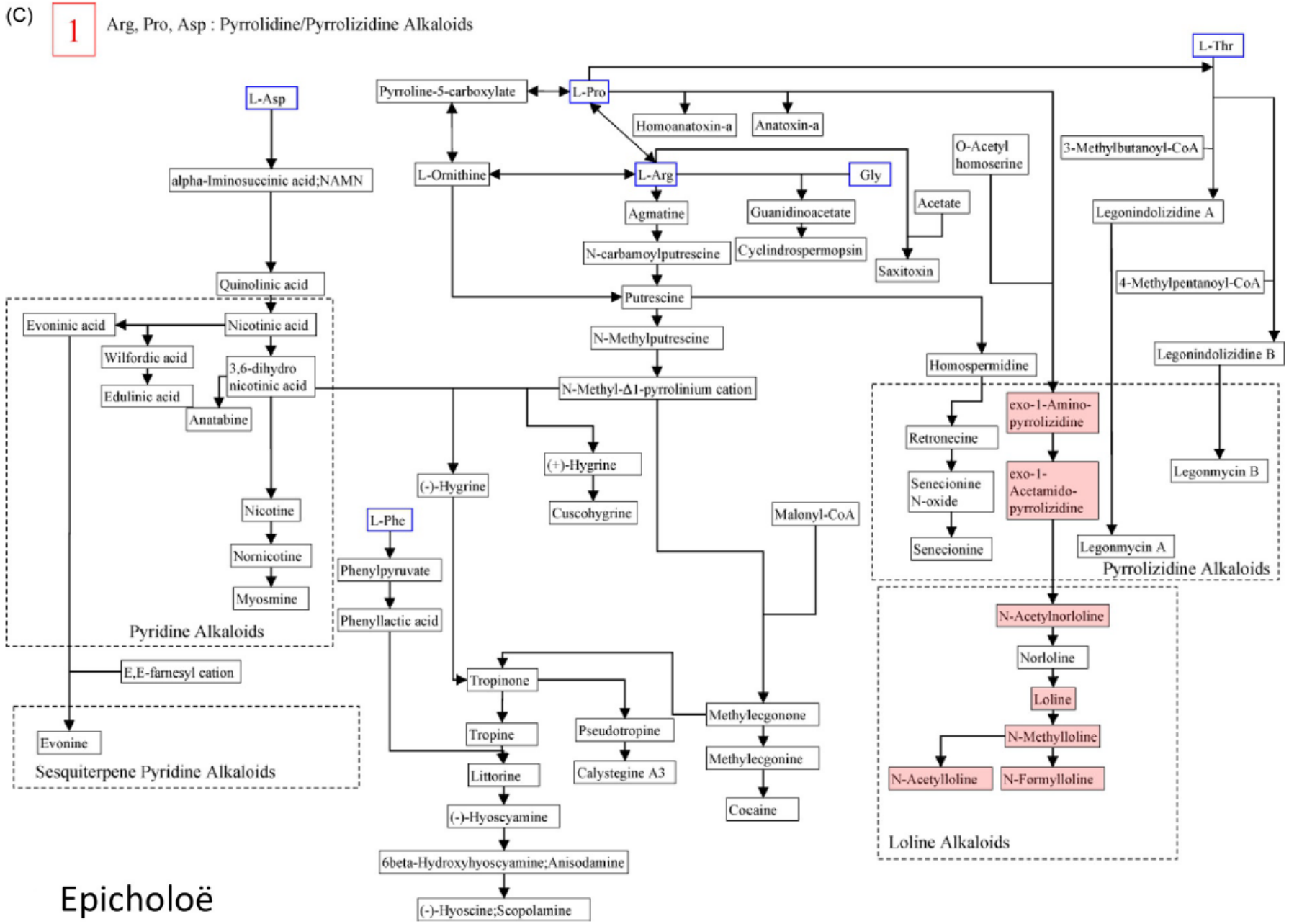
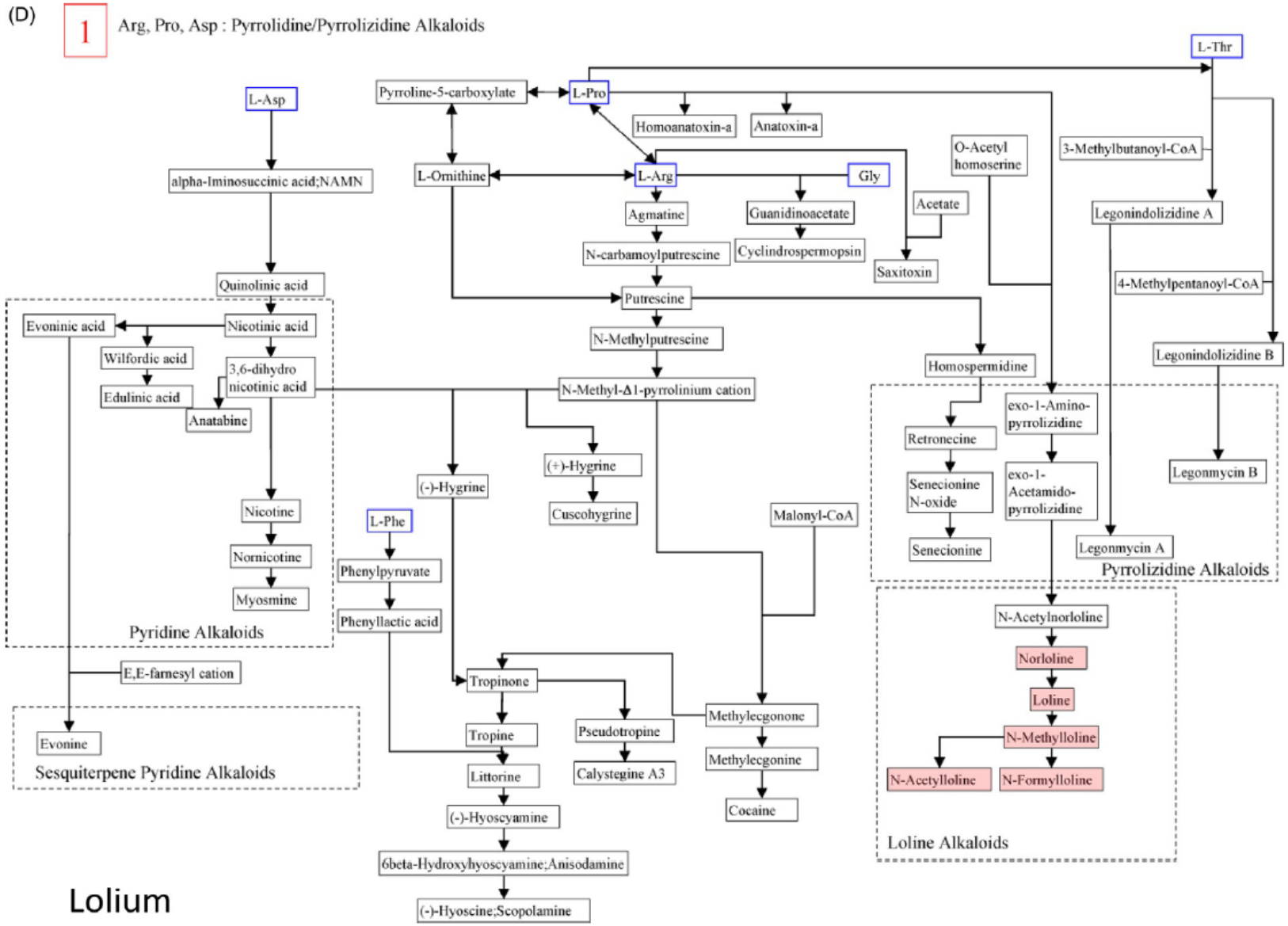
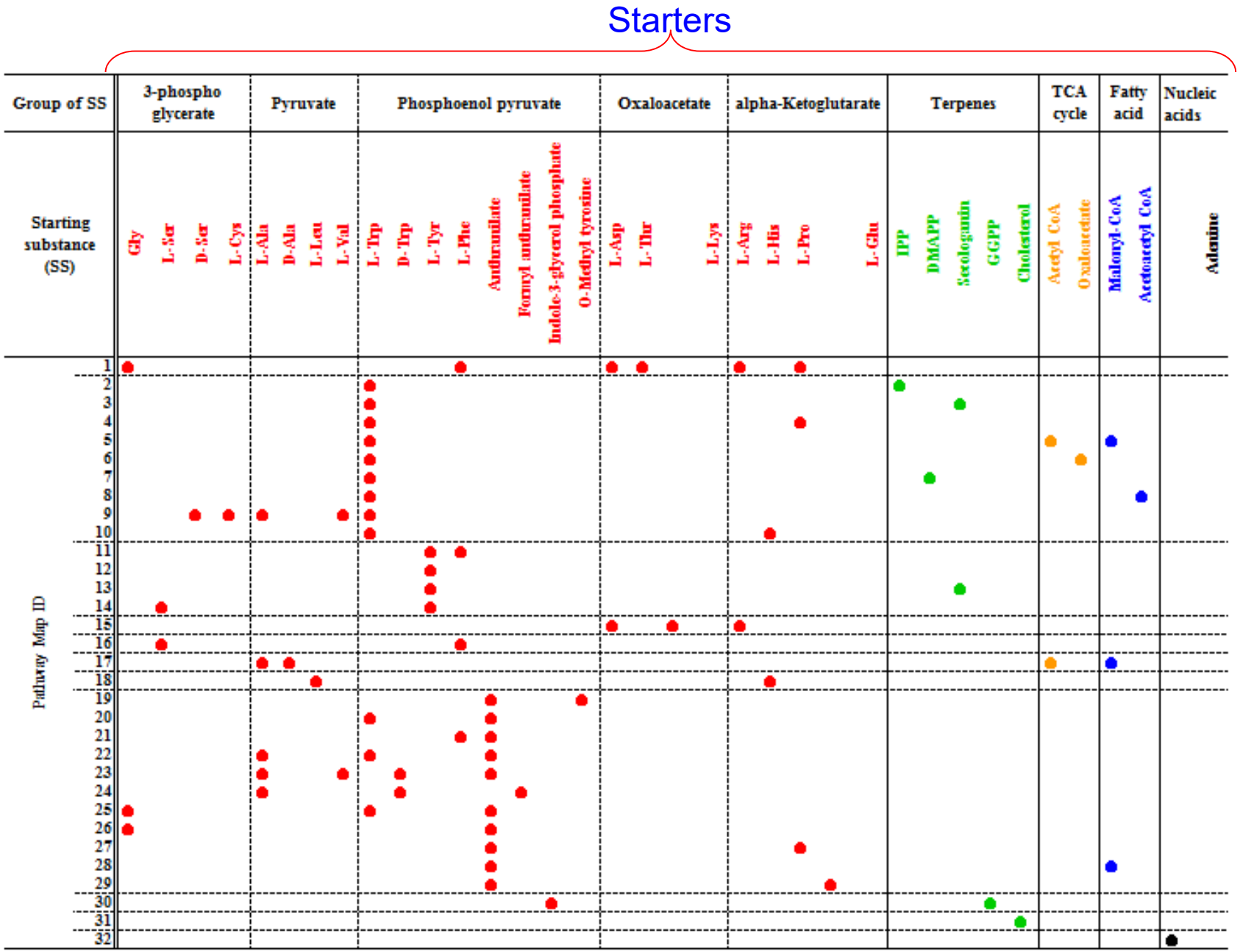

(B)
1
Arg, Pro, Asp : Pyrrolidine/Pyrrolizidine Alkaloids
L-Thr
L-Asp
Pyrroline-5-carboxylate
L-Pro
Homoanatoxin-a
Anatoxin-a
O-Acetyl homoserine
3-Methylbutanoyl-CoA
alpha-Iminosuccinic acid;NAMN
L-Ornithine
L-Arg
Gly
Acetate
Legonindolizidine A
Agmatine
Guanidinoacetate
N-carbamoylputrescine
Cyclindrospermopsin
Saxitoxin
Quinolinic acid
Putrescine
4-Methylpentanoyl-CoA
Evoninic acid
Nicotinic acid
N-Methylputrescine
Legonindolizidine B
Wilfordic acid
3,6-dihydro nicotinic acid
Homospermidine
Edulinic acid
N-Methyl-Δ1-pyrrolinium cation
exo-1-Amino-pyrrolizidine
Anatabine
Retronecine
(+)-Hygrine
Legonmycin B
(-)-Hygrine
Senecionine N-oxide
exo-1-Acetamido-pyrrolizidine
Nicotine
L-Phe
Malonyl-CoA
Cuscohygrine
Senecionine
Legonmycin A
Pyrrolizidine Alkaloids
Normicotine
Phenylpyruvate
Myosmine
Phenyllactic acid
N-Acetylnorloline
Pyridine Alkaloids
Norloline
E,E-farnesyl cation
Tropinone
Loline
Methylecgonone
Tropine
Pseudotropine
N-Methylloline
Evonine
Methylecgonine
N-Acetylloline
N-Formylloline
Sesquiterpene Pyridine Alkaloids
Littorine
Calystegine A3
Cocaine
(-)-Hyoscyamine
Loline Alkaloids
6beta-Hydroxyhyoscyamine;Anisodamine
(-)-Hyoscine;Scopolamine
Nicotiana


(C)
1
Arg, Pro, Asp : Pyrrolidine/Pyrrolizidine Alkaloids
L-Asp
alpha-Iminosuccinic acid;NAMN
Quinolinic acid
Evoninic acid
Nicotinic acid
Wilfordic acid
3,6-dihydro nicotinic acid
Edulinic acid
Anatabine
Nicotine
Nornicotine
Myosmine
Pyridine Alkaloids
E,E-farnesyl cation
Evonine
Sesquiterpene Pyridine Alkaloids
Pyrroline-5-carboxylate
L-Pro
Homoanatoxin-a
Anatoxin-a
L-Ornithine
L-Arg
Gly
Agmatine
Guanidinoacetate
N-carbamoylputrescine
Cyclindrospermopsin
Saxitoxin
Putrescine
N-Methylputrescine
N-Methyl-Δ1-pyrrolinium cation
(-)-Hygrine
(+)-Hygrine
Cuscohygrine
L-Phe
Phenylpyruvate
Phenyllactic acid
Malonyl-CoA
Tropinone
Tropine
Pseudotropine
Calystegine A3
Littorine
(-)-Hyoscyamine
6beta-Hydroxyhyoscyamine;Anisodamine
(-)-Hyoscine;Scopolamine
Methylecgonone
Methylecgonine
Cocaine
L-Thr
O-Acetyl homoserine
3-Methylbutanoyl-CoA
Acetate
Legonindolizidine A
4-Methylpentanoyl-CoA
Legonindolizidine B
Homospermidine
Retronecine
Senecionine N-oxide
Senecionine
exo-1-Amino-pyrrolizidine
exo-1-Acetamido-pyrrolizidine
Legonmycin B
Legonmycin A
Pyrrolizidine Alkaloids
N-Acetylnorloline
Norloline
Loline
N-Methylloline
N-Acetylloline
N-Formylloline
Loline Alkaloids

Epicholoë


(D)
1
Arg, Pro, Asp : Pyrrolidine/Pyrrolizidine Alkaloids
L-Thr
L-Asp
Pyrroline-5-carboxylate
L-Pro
Homoanatoxin-a
Anatoxin-a
O-Acetyl homoserine
3-Methylbutanoyl-CoA
alpha-Iminosuccinic acid;NAMN
L-Ornithine
L-Arg
Gly
Agmatine
Guanidinoacetate
Acetate
Legonindolizidine A
N-carbamoylputrescine
Cyclindrospermopsin
Saxitoxin
Quinolinic acid
4-Methylpentanoyl-CoA
Putrescine
Evoninic acid
Nicotinic acid
N-Methylputrescine
Homospermidine
Legonindolizidine B
Wilfordic acid
3,6-dihydro nicotinic acid
N-Methyl-Δ1-pyrrolinium cation
exo-1-Amino-pyrrolizidine
Edulinic acid
Retronecine
(+)-Hygrine
Legonmycin B
Anatabine
(-)-Hygrine
Senecionine N-oxide
exo-1-Acetamido-pyrrolizidine
Nicotine
L-Phe
Malonyl-CoA
Cuscohygrine
Senecionine
Legonmycin A
Nornicotine
Phenylpyruvate
Pyrrolizidine Alkaloids
Myosmine
Phenyllactic acid
N-Acetylnorloline
Pyridine Alkaloids
Norloline
E,E-farnesyl cation
Tropinone
Loline
Methylecgonone
Tropine
Pseudotropine
N-Methylloline
Evonine
Methylecgonine
N-Acetylloline
N-Formylloline
Sesquiterpene Pyridine Alkaloids
Littorine
Calystegine A3
Cocaine
Loline Alkaloids
(-)-Hyoscyamine
6beta-Hydroxyhyoscyamine;Anisodamine
(-)-Hyoscine;Scopolamine
Lolium

Starters for alkaloids from Scientific Literature Survey



Select by ...

◉ ALL Types ○ Organism ○ Metabolite ○ Molecular formula

○ C_ID ○ CAS_ID ○ INCHI-KEY

Streptomyces × List Clear

input type = all , input word = Streptomyces

Number of matched data : 2001

2001エントリー

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C00000146	84453-40-7	(+)-Bottrospicatol	C10H16O2	168.11502976	Streptomyces bottropensis
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C00000336	636-82-8	1-Cyclohexenylcarboxylic acid	C7H10O2	126.06807956	Streptomyces collinus
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C00000340	170591-54-5	U-106305	C28H41NO	407.31881494	Streptomyces sp. UC11136
C00000368	124753-55-5	IM-2	C9H16O4	188.104859	Streptomyces sp. strain FRI-5
C00000369	109075-62-9	Virginiae butanolide C	C11H20O4	216.13615913	Streptomyces virginiae
C00000370	125654-65-1	Virginiae butanolide E	C11H20O4	216.13615913	Streptomyces virginiae
C00000371	109215-47-6	Virginiae butanolide A	C12H22O4	230.15180919	Streptomyces antibioticus
C00000371	109215-47-6	Virginiae butanolide A	C12H22O4	230.15180919	Streptomyces bikiniensis
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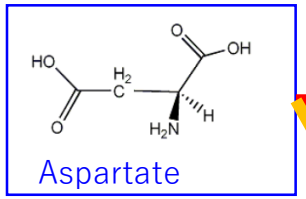
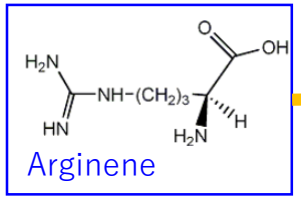
C00000372	125761-52-6	Virginiae butanolide D	C12H22O4	230.15180919	Streptomyces virginiae

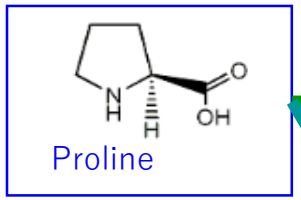
Examples of Sterters to produce alkaloids

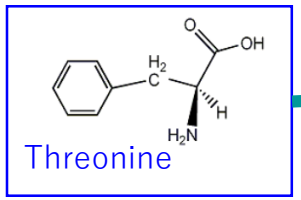
Starters

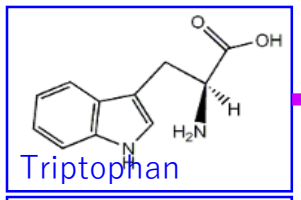
Biosynthesized alkaloids

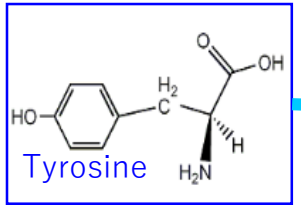


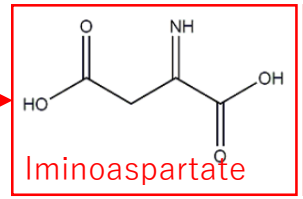


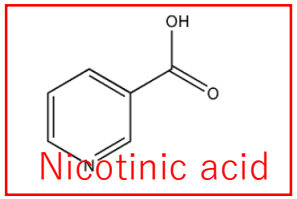


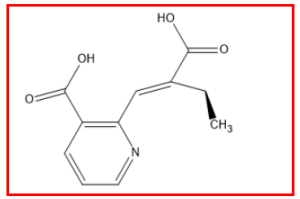


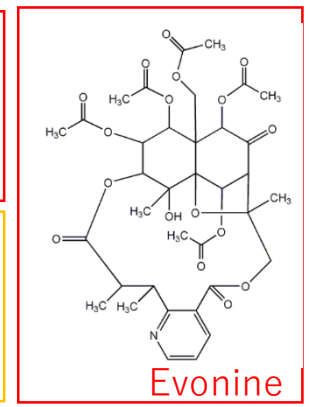


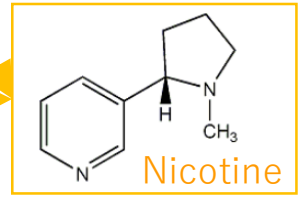


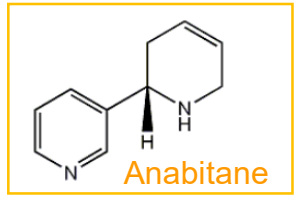


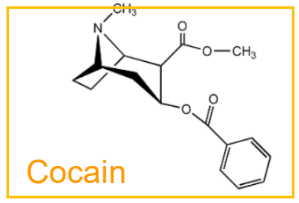


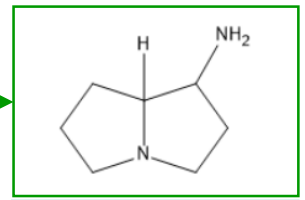


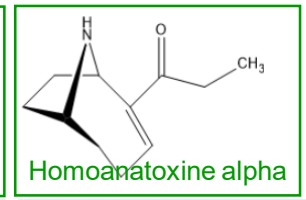


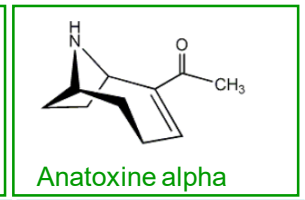


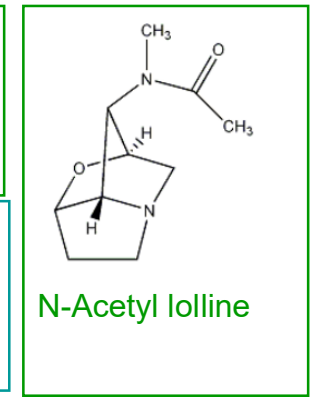


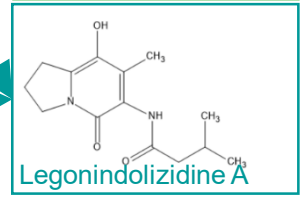


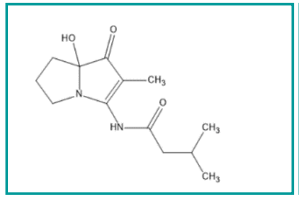


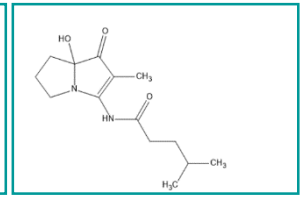


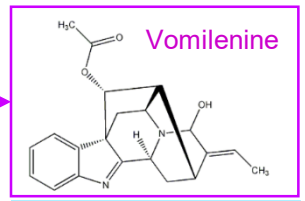


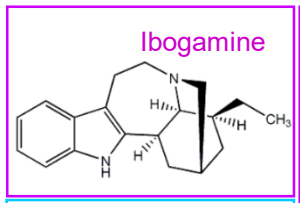


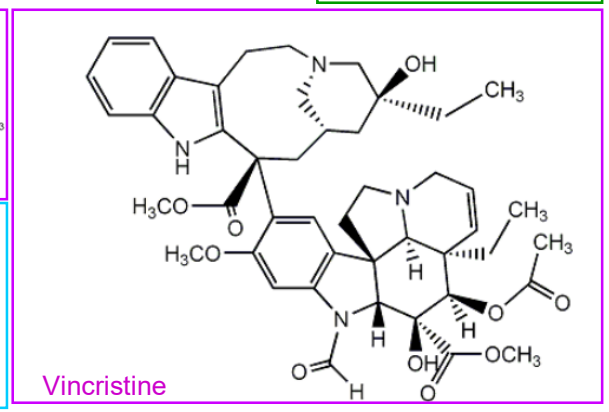


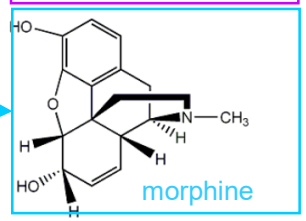


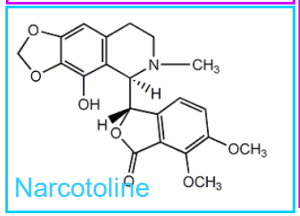












Select by ...

◉ ALL Types ○ Organism ○ Metabolite ○ Molecular formula

○ C_ID ○ CAS_ID ○ INCHI-KEY

Streptomyces × List Clear

input type = all , input word = Streptomyces

Number of matched data : 2001

2001エントリー

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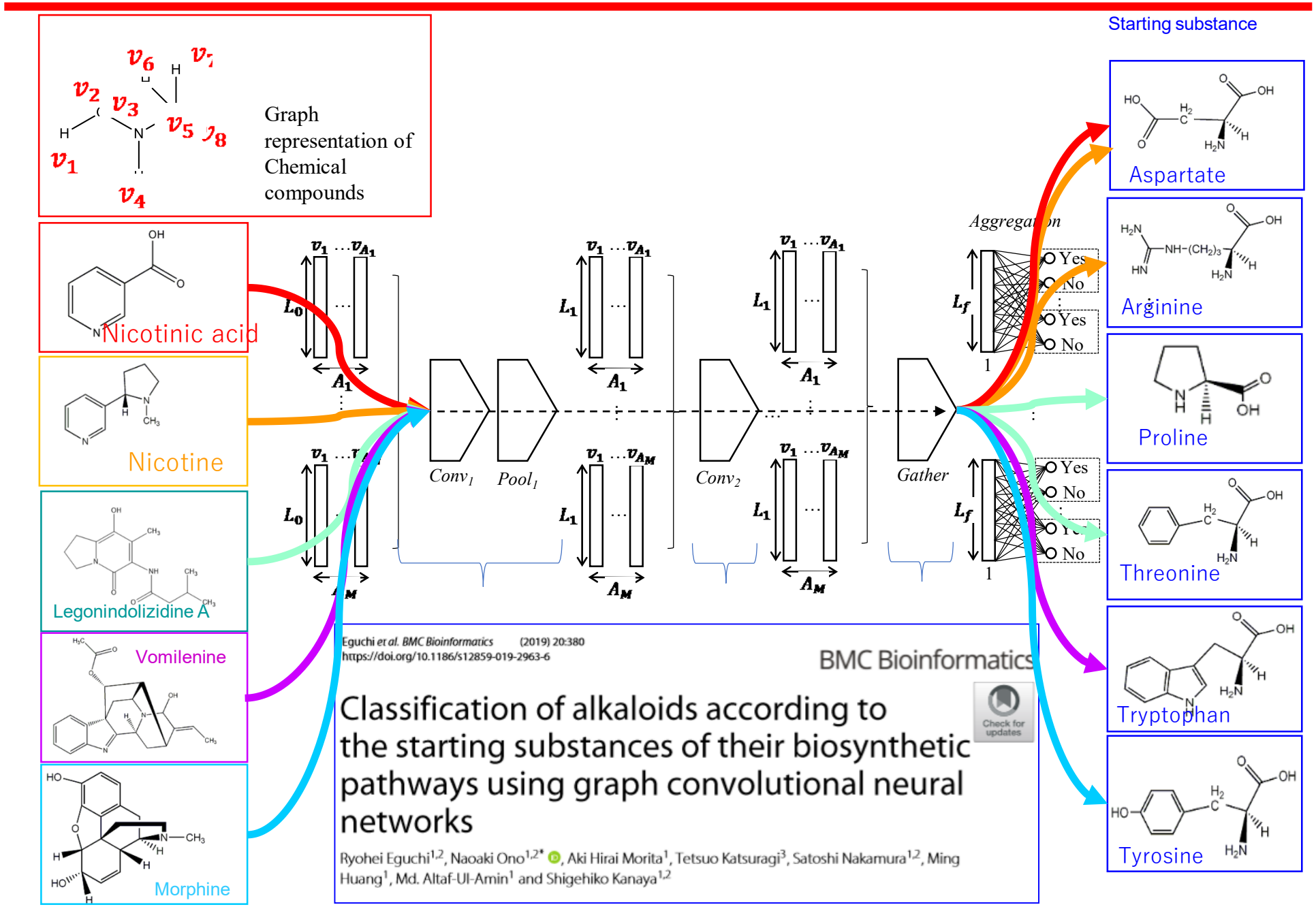
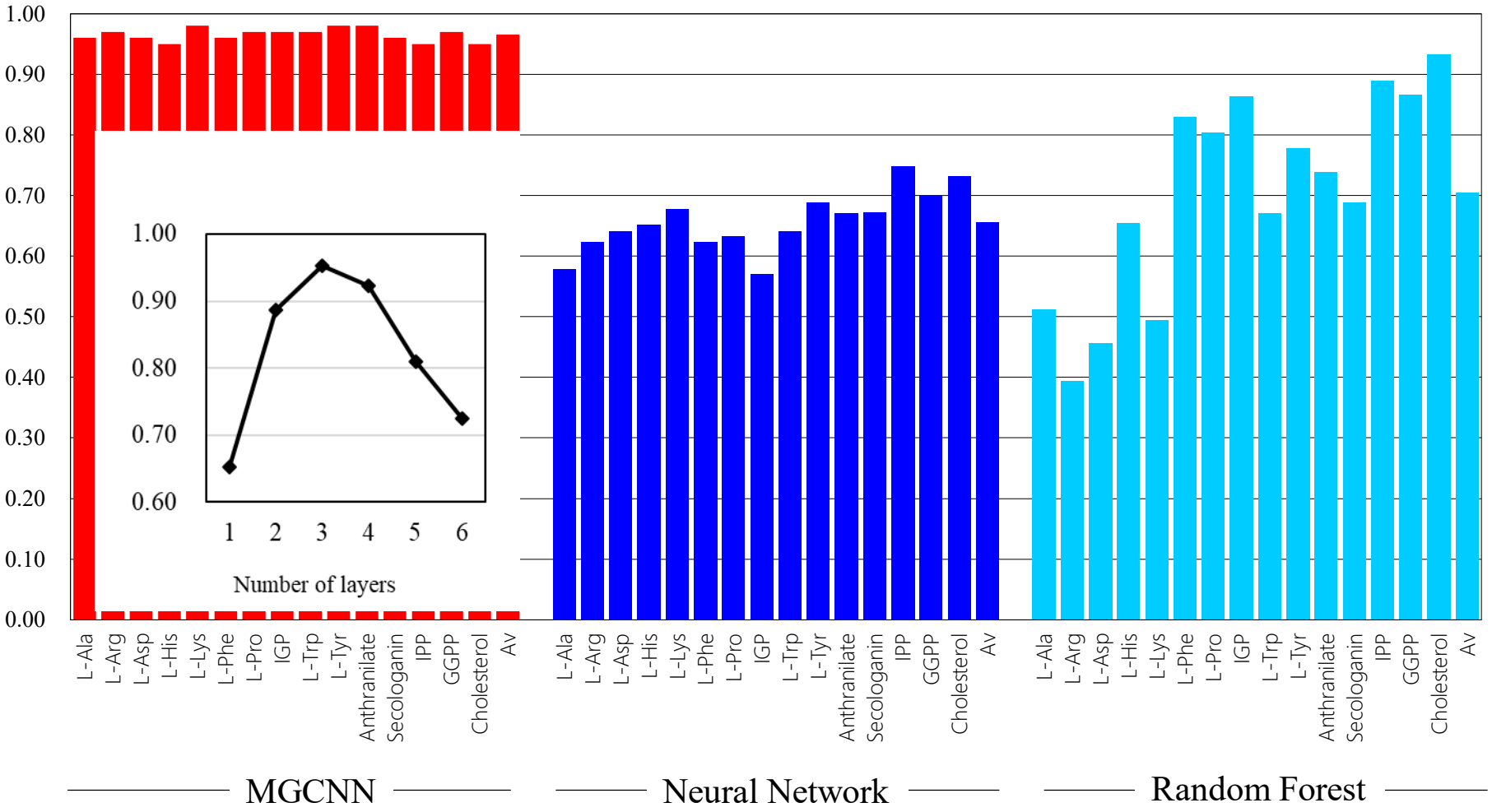
GCNN can learn the neighboring relationships of atoms in chemical graph.



Accuracy for GCNN, Neural Network, and Random Forest



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MGCNN can classify alkaloids into Starters in the highest recognition levels.