PMID- 19071200
OWN - NLM
STAT- MEDLINE
DCOM- 20090220
LR - 20090116
IS - 1879-0038 (Electronic)
IS - 0378-1119 (Linking)
VI - 431
IP - 1-2
DP - 2009 Feb 15
TI - Identification of two suites of cyclotide precursor genes from metallophyte Vio
baoshanensis: cDNA sequence variation, alternative RNA splicing and potential
cyclotide diversity.
PG - 23-32
LID - 10.1016/j.gene.2008.11.005 [doi]
AB - Cyclotides are a novel family of plant-derived defense peptides that are
biosynthetically produced via the processing of cyclotide precursor (CP) prote
containing one, two or three cyclotide domains. By screening a cDNA library of
Viola baoshanensis roots and using RACE and RT-PCR methods, 23 cDNA clones were
identified and then used to deduce full CP proteins containing one (VbCP1S-5),
two (VbCP6S), or three (VbCP7S) cyclotide domains. RT-PCR and sequence analyse
suggested that VbCP6S were resulted from the alternative splicing of VbCP7S RNA
The significance of VbCP7S RNA splicing is that it provides a mechanism for
increasing the diversity of cyclotide expression via the recombination of
N-terminal repeat (NTR) regions and cyclotide domains. After analyzing the ful
endoplasmic reticulum (ER) signals of known and novel CPs associated with RT-PC
tests, three primers encoding the conserved sequence ALVLIATFA, AAFALPA-LA and
AAFALPA-AFA were proposed to be more efficient in cloning CP genes than the
well-applied primer encoding AAFALPA. Cyclotide sequence analyses indicated tha
the cDNA clones encoded a variety of Möbius and bracelet cyclotides, which were
likely involved in the known bioactivities of cyclotides, and also might play a
previously unreported role in mediating the metal tolerance of V. baoshanensis
Overall, this study shows that CP genes are varied in V. baoshanensis and
cyclotide expression is subject to transcriptional and post-transcriptional
regulation in this plant.
FAU - Zhang, Jun
AU - Zhang J
AD - State Key Laboratory of Biocontrol, School of Life Sciences, Sun Yat-sen
(Zhongshan) University, Guangzhou 510006, China.
FAU - Liao, Bin
AU - Liao B
FAU - Craik, David J
AU - Craik DJ
FAU - Li, Jin-Tian
AU - Li JT
FAU - Hu, Min
AU - Hu M
FAU - Shu, Wen-Sheng
AU - Shu WS
LA - eng

PT - Journal Article
PT - Research Support, Non-U.S. Gov't
DEP - 20081119
PL - Netherlands
TA - Gene
JT - Gene
JID - 7706761
RN - 0 (Cyclotides)
RN - 0 (DNA, Complementary)
RN - 0 (RNA, Plant)
SB - IM
MH - Alternative Splicing/*genetics
MH - Amino Acid Sequence
MH - Base Sequence
MH - Cyclotides/chemistry/*genetics
MH - DNA, Complementary/*genetics
MH - Evolution, Molecular
MH - Gene Expression Profiling
MH - Gene Expression Regulation, Plant
MH - *Genes, Plant
MH - *Genetic Variation
MH - Molecular Sequence Data
MH - Multigene Family
MH - Phylogeny
MH - RNA, Plant/genetics
MH - Sequence Alignment
MH - Sequence Analysis, DNA
MH - Viola/*genetics
EDAT- 2008/12/17 09:00
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PHST- 2008/08/17 00:00 [revised]
PHST- 2008/11/04 00:00 [accepted]
PHST- 2008/12/17 09:00 [entrez]
PHST- 2008/12/17 09:00 [pubmed]
PHST- 2009/02/21 09:00 [medline]
AID - S0378-1119(08)00589-1 [pii]
AID - 10.1016/j.gene.2008.11.005 [doi]
PST - ppublish
SO - Gene. 2009 Feb 15;431(1-2):23-32. doi: 10.1016/j.gene.2008.11.005. Epub 2008 N
19.

PMID- 33787269
OWN - NLM
STAT- MEDLINE
DCOM- 20210514
LR - 20210514
IS - 1520-5207 (Electronic)
IS - 1520-5207 (Linking)
VI - 125

IP - 14
DP - 2021 Apr 15
TI - Molecular Dynamics Simulation Study on Interactions of Cycloviolacin with Different Phospholipids.
PG - 3476-3485
LID - 10.1021/acs.jpcb.0c10513 [doi]
AB - Cyclotides are disulfide-rich cyclic peptides isolated from plants, which are extremely stable against thermal and proteolytic degradation, with a variety o biological activities including antibacterial, hemolytic, anti-HIV, and anti-tumor. Most of these bioactivities are related to their preference for binding to certain types of phospholipids and subsequently disrupt lipid membranes. In the present study, we use a cyclotide, cycloviolacin O2 (cyO2), a a model system to investigate its interactions with three lipid bilayers 1-palmitoyl-2-oleoylphosphatidylethanolamine (POPE), 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphoglycerol (POPG)-doped POPE, and 1-palmitoyl-2-oleoylphosphatidylcholine (POPC), to help understand its potentia mechanism of action toward the membranes at the molecular level using molecula dynamics simulations. In our simulations, cyO2 repeatedly forms stable binding complexes with the POPE-containing bilayers, while within the same simulation time scale, it "jumps" back and forth on the surface of the POPC bilayer witho a strong binding. Detailed analyses reveal that the electrostatic attraction i the main driving force for the initial bindings between cyO2 and the lipids, b with strikingly different strengths in different bilayers. For the POPE-containing bilayers, the charged residues of cyO2 attract both POPE amino and phosphate head groups favorably; meanwhile, its hydrophobic residues are deeply inserted into the lipid hydrophobic tails (core) of the membrane, thus forming stable binding complexes. In contrast, POPC lipids with three methyl groups on the amino head group create a steric hindrance when interacting with cyO2, thus resulting in a relatively difficult binding of cyO2 on POPC compare to POPE. Our current findings provide additional insights for a better understanding of how cyO2 binds to the POPE-containing membrane, which should shed light on the future cyclotide-based antibacterial agent design.
FAU - Lei, Xiaotong
AU - Lei X
AD - Institute of Quantitative Biology and Medicine, State Key Laboratory of Radiat Medicine and Protection, School of Radiation Medicine and Protection, Collaborative Innovation Center of Radiation Medicine of Jiangsu Higher Educat Institutions, Soochow University, Suzhou 215123, China.
FAU - Liu, Shengtang
AU - Liu S
AD - Institute of Quantitative Biology and Medicine, State Key Laboratory of Radiat Medicine and Protection, School of Radiation Medicine and Protection, Collaborative Innovation Center of Radiation Medicine of Jiangsu Higher Educat Institutions, Soochow University, Suzhou 215123, China.
FAU - Zhou, Ruhong
AU - Zhou R
AUID- ORCID: 0000-0001-8624-5591
AD - Department of Chemistry, Columbia University, New York, New York 10027, United States.
FAU - Meng, Xuan-Yu
AU - Meng XY

AUID- ORCID: 0000-0003-1644-6552
AD - Institute of Quantitative Biology and Medicine, State Key Laboratory of Radiat Medicine and Protection, School of Radiation Medicine and Protection, Collaborative Innovation Center of Radiation Medicine of Jiangsu Higher Educat Institutions, Soochow University, Suzhou 215123, China.
LA - eng
PT - Journal Article
PT - Research Support, Non-U.S. Gov't
DEP - 20210331
PL - United States
TA - J Phys Chem B
JT - The journal of physical chemistry. B
JID - 101157530
RN - 0 (Lipid Bilayers)
RN - 0 (Peptides, Cyclic)
RN - 0 (Phosphatidylcholines)
RN - 0 (Phospholipids)
SB - IM
MH - Hydrophobic and Hydrophilic Interactions
MH - Lipid Bilayers
MH - *Molecular Dynamics Simulation
MH - Peptides, Cyclic
MH - Phosphatidylcholines
MH - *Phospholipids
EDAT- 2021/04/01 06:00
MHDA- 2021/05/15 06:00
CRDT- 2021/03/31 12:57
PHST- 2021/04/01 06:00 [pubmed]
PHST- 2021/05/15 06:00 [medline]
PHST- 2021/03/31 12:57 [entrez]
AID - 10.1021/acs.jpcb.0c10513 [doi]
PST - ppublish
SO - J Phys Chem B. 2021 Apr 15;125(14):3476-3485. doi: 10.1021/acs.jpcb.0c10513. E 2021 Mar 31.

PMID- 29522493
OWN - NLM
STAT- MEDLINE
DCOM- 20180918
LR - 20181114
IS - 1422-0067 (Electronic)
IS - 1422-0067 (Linking)
VI - 19
IP - 3
DP - 2018 Mar 9
TI - Coupling Plant-Derived Cyclotides to Metal Surfaces: An Antibacterial and Antibiofilm Study.
LID - 10.3390/ijms19030793 [doi]
LID - 793
AB - Modification of metal surfaces with antimicrobial peptides is a promising approach to reduce bacterial adhesion. Here, cyclic peptides or cycloids,

possessing remarkable stability and antimicrobial activities, were extracted a
purified from Viola philippica Cav., and identified using mass spectrometry.
Cyclotides were subsequently utilized to modify stainless steel surfaces via
polydopamine-mediated coupling. The resulting cyclotide-modified surfaces were
characterized by Fourier transform infrared (FTIR) spectroscopy and contact an
analysis. The antibacterial capacity of these cyclotides against Staphylococcu
aureus was assessed by Alamar blue assay. The antibiofilm capacity of the
modified surfaces was assessed by crystal violet assay, and scanning electron
microscopy (SEM). A composite of Kalata b1, Varv A, Viba 15 and Viba 17 (P1);
Varv E (P2); and Viphi G (P3) were isolated and identified. FTIR analysis of t
modified surfaces demonstrated that cyclotides bound to the surfaces and induc
reduction of contact angles. Antimicrobial effects showed an order P3 > P1 and
P2, with P3-treated surfaces demonstrating the strongest antibiofilm capacity.
SEM confirmed reduced biofilm formation for P3-treated surfaces. This study
provides novel evidence for cyclotides as a new class for development of
antibacterial and antibiofilm agents.

FAU - Cao, Pan
AU - Cao P
AD - School of Energy and Power Engineering, Wuhan University of Technology, Wuhan
430063, China. caop@whut.edu.cn.
AD - Institute for Science and Technology in Medicine, Keele University,
Stoke-on-Trent ST4 7QB, UK. caop@whut.edu.cn.
FAU - Yang, Ying
AU - Yang Y
AD - Institute for Science and Technology in Medicine, Keele University,
Stoke-on-Trent ST4 7QB, UK. y.yang@keele.ac.uk.
FAU - Uche, Fidelia Ijeoma
AU - Uche FI
AD - Institute for Science and Technology in Medicine, Keele University,
Stoke-on-Trent ST4 7QB, UK. f.i.uche@keele.ac.uk.
FAU - Hart, Sarah Ruth
AU - Hart SR
AUID- ORCID: 0000-0003-0521-6284
AD - Institute for Science and Technology in Medicine, Keele University,
Stoke-on-Trent ST4 7QB, UK. s.r.hart@keele.ac.uk.
FAU - Li, Wen-Wu
AU - Li WW
AUID- ORCID: 0000-0002-3706-6068
AD - Institute for Science and Technology in Medicine, Keele University,
Stoke-on-Trent ST4 7QB, UK. w.li@keele.ac.uk.
FAU - Yuan, Chengqing
AU - Yuan C
AUID- ORCID: 0000-0002-1056-6433
AD - School of Energy and Power Engineering, Wuhan University of Technology, Wuhan
430063, China. ycq@whut.edu.cn.

LA - eng
PT - Journal Article
DEP - 20180309
PL - Switzerland
TA - Int J Mol Sci
JT - International journal of molecular sciences

JID - 101092791
RN - 0 (Anti-Bacterial Agents)
RN - 0 (Cyclotides)
RN - 0 (Indoles)
RN - 0 (Metals)
RN - 0 (Plant Extracts)
RN - 0 (Plant Proteins)
RN - 0 (Polymers)
RN - 0 (polydopamine)
SB - IM
MH - Amino Acid Sequence
MH - Anti-Bacterial Agents/chemistry/*pharmacology
MH - Biofilms/*drug effects
MH - Cyclotides/chemistry/isolation & purification/*pharmacology
MH - Indoles/chemistry
MH - Metals/*chemistry
MH - Microscopy, Electron, Scanning
MH - Plant Extracts/chemistry/*pharmacology
MH - Plant Proteins/chemistry/isolation & purification/pharmacology
MH - Polymers/chemistry
MH - Staphylococcus aureus/drug effects/physiology
MH - Viola/*chemistry
PMC - PMC5877654
OTO - NOTNLM
OT - antibacterial
OT - antibiofilm
OT - cyclotides
OT - polydopamine
OT - surface modification
COIS- The authors declare no conflict of interest.
EDAT- 2018/03/10 06:00
MHDA- 2018/09/19 06:00
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AID - ijms19030793 [pii]
AID - ijms-19-00793 [pii]
AID - 10.3390/ijms19030793 [doi]
PST - epublish
SO - Int J Mol Sci. 2018 Mar 9;19(3):793. doi: 10.3390/ijms19030793.

PMID- 30277068
OWN - NLM
STAT- MEDLINE
DCOM- 20191114
LR - 20191114
IS - 1520-6904 (Electronic)

IS - 0022-3263 (Linking)
VI - 83
IP - 22
DP - 2018 Nov 16
TI - Enzymatic On-Resin Peptide Cleavage and in Situ Cyclization One-Pot Strategy f
the Synthesis of Cyclopeptide and Cyclotide.
PG - 14078-14083
LID - 10.1021/acs.joc.8b02032 [doi]
AB - A one-pot strategy combining sortase A mediated on-resin peptide cleavage and
situ cyclization was developed for the synthesis of cyclic peptides. This
strategy was applied to synthesize head-to-tail cyclic antibacterial bovine
lactoferricin peptide LFcinB(20-35) in a yield of 67%. The one-pot strategy wa
compatible with an oxidative folding reaction, and complex cyclotides containi
one or two disulfide bonds, such as sunflower trypsin inhibitors-1 and
α-conotoxin MII, were successfully synthesized in one pot in a yield of 77% an
61%, respectively.
FAU - Cheng, Xiaozhong
AU - Cheng X
AD - Key Laboratory of Carbohydrate Chemistry & Biotechnology, Ministry of Educatio
School of Biotechnology , Jiangnan University , Wuxi 214122 , China.
FAU - Hong, Haofei
AU - Hong H
AD - Key Laboratory of Carbohydrate Chemistry & Biotechnology, Ministry of Educatio
School of Biotechnology , Jiangnan University , Wuxi 214122 , China.
FAU - Zhou, Zhifang
AU - Zhou Z
AD - Key Laboratory of Carbohydrate Chemistry & Biotechnology, Ministry of Educatio
School of Biotechnology , Jiangnan University , Wuxi 214122 , China.
FAU - Wu, Zhimeng
AU - Wu Z
AUID- ORCID: 0000-0001-7583-7268
AD - Key Laboratory of Carbohydrate Chemistry & Biotechnology, Ministry of Educatio
School of Biotechnology , Jiangnan University , Wuxi 214122 , China.
LA - eng
PT - Journal Article
PT - Research Support, Non-U.S. Gov't
DEP - 20181105
PL - United States
TA - J Org Chem
JT - The Journal of organic chemistry
JID - 2985193R
RN - 0 (Acrylic Resins)
RN - 0 (Cyclotides)
RN - 0 (Enzymes)
RN - 0 (Peptides)
RN - 0 (Peptides, Cyclic)
RN - 0 (poly(acryloyl-bis(aminopropyl)polyethylene glycol))
RN - 3WJQ0SDW1A (Polyethylene Glycols)
SB - IM
MH - Acrylic Resins
MH - Amino Acid Sequence

MH - Cyclotides/*chemical synthesis
MH - Enzymes/chemistry/*metabolism
MH - Peptides/*chemistry
MH - Peptides, Cyclic/*chemical synthesis
MH - Polyethylene Glycols
MH - Protein Conformation
EDAT- 2018/10/03 06:00
MHDA- 2019/11/15 06:00
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PHST- 2018/10/03 06:00 [pubmed]
PHST- 2019/11/15 06:00 [medline]
PHST- 2018/10/03 06:00 [entrez]
AID - 10.1021/acs.joc.8b02032 [doi]
PST - ppublish
SO - J Org Chem. 2018 Nov 16;83(22):14078-14083. doi: 10.1021/acs.joc.8b02032. Epub 2018 Nov 5.

PMID- 25756919
OWN - NLM
STAT- MEDLINE
DCOM- 20160204
LR - 20200930
IS - 1618-1328 (Electronic)
IS - 0176-1617 (Linking)
VI - 178
DP - 2015 Apr 15
TI - Transcriptomic screening for cyclotides and other cysteine-rich proteins in the metallophyte Viola baoshanensis.
PG - 17-26
LID - S0176-1617(15)00040-1 [pii]
LID - 10.1016/j.jplph.2015.01.017 [doi]
AB - Cysteine (Cys)-rich proteins (CRPs) are frequently associated with plant defen and stress resistance. Viola baoshanensis is a cadmium (Cd) hyper-accumulating plant whose CRPs-based defense systems are so far poorly understood. Next generation sequencing (NGS) techniques and a specialist searching tool, CrpExc were employed for identifying CRPs in V. baoshanensis. The transcriptome sequences of V. baoshanensis were assembled primarily from 454FLX/Hiseq2000 rea of plant cDNA sequencing libraries. CrpExcel was then used to search the ORFs a 9687 CRPs were identified, and included zinc finger (ZF) proteins, lipid trans proteins, thaumatins and cyclotide precursors. Real-time PCR results showed tha all CRP genes tested are constitutively expressed, but the genes of defensive peptides showed greater up-regulated expression than those of ZF-proteins in C and/or wounding (Wd) treatments of V. baoshanensis seedlings. The NGS-derived sequences of cyclotide precursor genes were verified by RT-PCR and ABI3730 sequencing studies, and 32 novel cyclotides were identified in V. baoshanensis In general, the metal-binding sites of ZF-containing CRPs also represented the potential vulnerable targets of toxic metals. This study provides broad insigh into CRPs-based defense systems and stress-vulnerable targets in V. baoshanens It now brings the number of cyclotide sequences in V. baoshanensis to 53 and based on projections from this work, the number of cyclotides in the Violaceae now conservatively estimated to be >30000.

FAU - Zhang, Jun
AU - Zhang J
AD - Guangdong Pharmaceutical University, School of Biosciences and Biopharmaceutic Guangdong Province Key Laboratory for Biotechnology Drug Candidates, Guangzhou 510006, China; Sun Yat-sen University, School of Life Sciences, State Key Laboratory of Biocontrol, Guangzhou 510006, China. Electronic address: zhangj80@aliyun.com.
FAU - Li, Jintian
AU - Li J
AD - Sun Yat-sen University, School of Life Sciences, State Key Laboratory of Biocontrol, Guangzhou 510006, China. Electronic address: lijtian@mail.sysu.edu.cn.
FAU - Huang, Zebo
AU - Huang Z
AD - Guangdong Pharmaceutical University, School of Biosciences and Biopharmaceutic Guangdong Province Key Laboratory for Biotechnology Drug Candidates, Guangzhou 510006, China. Electronic address: zebohuang@gdpu.edu.cn.
FAU - Yang, Bing
AU - Yang B
AD - Sun Yat-sen University, School of Life Sciences, State Key Laboratory of Biocontrol, Guangzhou 510006, China. Electronic address: andyang@tom.com.
FAU - Zhang, Xiaojie
AU - Zhang X
AD - Guangdong Pharmaceutical University, School of Biosciences and Biopharmaceutic Guangdong Province Key Laboratory for Biotechnology Drug Candidates, Guangzhou 510006, China. Electronic address: zhangxiaojie9205@163.com.
FAU - Li, Dehua
AU - Li D
AD - Guangdong Pharmaceutical University, School of Biosciences and Biopharmaceutic Guangdong Province Key Laboratory for Biotechnology Drug Candidates, Guangzhou 510006, China. Electronic address: dehuali_25@163.com.
FAU - Craik, David J
AU - Craik DJ
AD - The University of Queensland, Institute for Molecular Bioscience, Brisbane 407 QLD, Australia. Electronic address: d.craik@imb.uq.edu.au.
FAU - Baker, Alan J M
AU - Baker AJ
AD - The University of Melbourne, School of Botany, Parkville 3010, VIC, Australia. Electronic address: ajmb@unimelb.edu.au.
FAU - Shu, Wensheng
AU - Shu W
AD - Sun Yat-sen University, School of Life Sciences, State Key Laboratory of Biocontrol, Guangzhou 510006, China. Electronic address: shuws@mail.sysu.edu.c
FAU - Liao, Bin
AU - Liao B
AD - Sun Yat-sen University, School of Life Sciences, State Key Laboratory of Biocontrol, Guangzhou 510006, China. Electronic address: lsslb@mail.sysu.edu.c
LA - eng
PT - Journal Article
PT - Research Support, Non-U.S. Gov't

DEP - 20150226
PL - Germany
TA - J Plant Physiol
JT - Journal of plant physiology
JID - 9882059
RN - 0 (Cyclotides)
RN - 0 (Plant Proteins)
RN - K848JZ4886 (Cysteine)
SB - IM
MH - Amino Acid Sequence
MH - Cyclotides/*genetics/metabolism
MH - Cysteine/genetics/metabolism
MH - Gene Expression Profiling/*methods
MH - *Gene Expression Regulation, Plant
MH - Phylogeny
MH - Plant Proteins/*genetics/metabolism
MH - Real-Time Polymerase Chain Reaction
MH - *Transcriptome
MH - Viola/*genetics/metabolism
OTO - NOTNLM
OT - CrpExcel
OT - Cyclotides
OT - Cysteine-rich proteins
OT - Transcriptome profiles
OT - Viola baoshanensis
EDAT- 2015/03/11 06:00
MHDA- 2016/02/05 06:00
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PHST- 2015/03/11 06:00 [entrez]
PHST- 2015/03/11 06:00 [pubmed]
PHST- 2016/02/05 06:00 [medline]
AID - S0176-1617(15)00040-1 [pii]
AID - 10.1016/j.jplph.2015.01.017 [doi]
PST - ppublish
SO - J Plant Physiol. 2015 Apr 15;178:17-26. doi: 10.1016/j.jplph.2015.01.017. Epub 2015 Feb 26.

PMID- 19106016
OWN - NLM
STAT- MEDLINE
DCOM- 20090708
LR - 20200930
IS - 1618-1328 (Electronic)
IS - 0176-1617 (Linking)
VI - 166
IP - 8
DP - 2009 May 15
TI - A transcriptional profile of metallophyte Viola baoshanensis involved in genera

and species-specific cadmium-defense mechanisms.
PG - 862-70
LID - 10.1016/j.jplph.2008.11.003 [doi]
AB - Viola baoshanensis Shu, Liu et Lan is a newly identified metallophyte, and its defensive strategies against heavy metals are still unclear. In the present study, we firstly constructed a root cDNA library of the plant subjected to 300muM Cd for 48h by using suppression subtractive hybridization (SSH), and 43 unique cDNA fragments were further isolated from the library. Sequence homology analysis showed that half of the identified genes were involved in general stre defense, such as antioxidative enzymes, protein degradation and stress signal transduction. After RT-PCR and RACE analysis, a Cd-responsive gene Vb40 was identified, which could deduce a novel cysteine-rich mini-protein. Meanwhile, five cyclotide precursor genes (VbCP1-VbCP5) were also identified. The Vb40 and the VbCP1-VbCP5 were further investigated by yeast expression analysis, and the could improve copper (Cu) tolerance in hosted yeast, indicating that these species-specific genes possibly functioned in V. baoshanensis heavy metals tolerance. Our results suggested that heavy metal tolerance in V. baoshanensis relied on both general and species-specific defense.
FAU - Zhang, Jun
AU - Zhang J
AD - State Key Laboratory of Biocontrol, School of Life Sciences, Sun Yat-sen (Zhongshan) University, Guangzhou 510006, PR China.
FAU - Hu, Min
AU - Hu M
FAU - Li, Jin-Tian
AU - Li JT
FAU - Guan, Jian-Ping
AU - Guan JP
FAU - Yang, Bin
AU - Yang B
FAU - Shu, Wen-Sheng
AU - Shu WS
FAU - Liao, Bin
AU - Liao B
LA - eng
PT - Journal Article
PT - Research Support, Non-U.S. Gov't
DEP - 20081221
PL - Germany
TA - J Plant Physiol
JT - Journal of plant physiology
JID - 9882059
RN - 0 (DNA, Complementary)
RN - 0 (Plant Proteins)
RN - 00BH33GNGH (Cadmium)
RN - 789U1901C5 (Copper)
SB - IM
MH - Adaptation, Physiological/drug effects
MH - Amino Acid Sequence
MH - Cadmium/metabolism/*toxicity
MH - Copper/toxicity

MH - DNA, Complementary/genetics
MH - *Gene Expression Profiling
MH - Gene Expression Regulation, Plant/*drug effects
MH - Genes, Plant
MH - Molecular Sequence Data
MH - Plant Proteins/chemistry/genetics/metabolism
MH - Plant Roots/drug effects/genetics/metabolism
MH - Saccharomyces cerevisiae/cytology/drug effects/metabolism
MH - Species Specificity
MH - Transcription, Genetic/*drug effects
MH - Viola/*drug effects/*genetics/immunology
EDAT- 2008/12/25 09:00
MHDA- 2009/07/09 09:00
CRDT- 2008/12/25 09:00
PHST- 2008/08/29 00:00 [received]
PHST- 2008/11/05 00:00 [revised]
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PHST- 2008/12/25 09:00 [entrez]
PHST- 2008/12/25 09:00 [pubmed]
PHST- 2009/07/09 09:00 [medline]
AID - S0176-1617(08)00339-8 [pii]
AID - 10.1016/j.jplph.2008.11.003 [doi]
PST - ppublish
SO - J Plant Physiol. 2009 May 15;166(8):862-70. doi: 10.1016/j.jplph.2008.11.003. Epub 2008 Dec 21.

PMID- 26399495
OWN - NLM
STAT- MEDLINE
DCOM- 20160909
LR - 20220310
IS - 1535-3907 (Electronic)
IS - 1535-3893 (Print)
IS - 1535-3893 (Linking)
VI - 14
IP - 11
DP - 2015 Nov 6
TI - Peptidomics of Circular Cysteine-Rich Plant Peptides: Analysis of the Diversity of Cyclotides from Viola tricolor by Transcriptome and Proteome Mining.
PG - 4851-62
LID - 10.1021/acs.jproteome.5b00681 [doi]
AB - Cyclotides are plant-derived mini proteins. They are genetically encoded as precursor proteins that become post-translationally modified to yield circular cystine-knotted molecules. Because of this structural topology cyclotides resi enzymatic degradation in biological fluids, and hence they are considered as promising lead molecules for pharmaceutical applications. Despite ongoing effo to discover novel cyclotides and analyze their biodiversity, it is not clear h many individual peptides a single plant specimen can express. Therefore, we investigated the transcriptome and cyclotide peptidome of Viola tricolor. Transcriptome mining enabled the characterization of cyclotide precursor architecture and processing sites important for biosynthesis of mature peptide

The cyclotide peptidome was explored by mass spectrometry and bottom-up proteomics using the extracted peptide sequences as queries for database searching. In total 164 cyclotides were discovered by nucleic acid and peptide analysis in V. tricolor. Therefore, violaceous plants at a global scale may be the source to as many as 150 000 individual cyclotides. Encompassing the diversity of V. tricolor as a combinatorial library of bioactive peptides, thi commercially available medicinal herb may be a suitable starting point for fut bioactivity-guided screening studies.

FAU - Hellinger, Roland
AU - Hellinger R
AD - Center for Physiology and Pharmacology, Medical University of Vienna , Schwarzspanierstrasse 17, 1090 Vienna, Austria.
FAU - Koehbach, Johannes
AU - Koehbach J
AD - Center for Physiology and Pharmacology, Medical University of Vienna , Schwarzspanierstrasse 17, 1090 Vienna, Austria.
AD - School of Biomedical Sciences, The University of Queensland , St. Lucia, Queensland 4072, Australia.
FAU - Soltis, Douglas E
AU - Soltis DE
AD - Florida Museum of Natural History, University of Florida , Gainesville, Florid 32611, United States.
FAU - Carpenter, Eric J
AU - Carpenter EJ
AD - Department of Biological Sciences, University of Alberta , Edmonton, Alberta T 2E9, Canada.
FAU - Wong, Gane Ka-Shu
AU - Wong GK
AD - Department of Biological Sciences, University of Alberta , Edmonton, Alberta T 2E9, Canada.
AD - Department of Medicine, University of Alberta , Edmonton, Alberta T6G 2E1, Canada.
AD - BGI-Shenzhen, Beishan Industrial Zone, Yantian District, Shenzhen 518083, Chin
FAU - Gruber, Christian W
AU - Gruber CW
AD - Center for Physiology and Pharmacology, Medical University of Vienna , Schwarzspanierstrasse 17, 1090 Vienna, Austria.
AD - School of Biomedical Sciences, The University of Queensland , St. Lucia, Queensland 4072, Australia.

LA - eng
PT - Journal Article
PT - Research Support, Non-U.S. Gov't
DEP - 20151008
PL - United States
TA - J Proteome Res
JT - Journal of proteome research
JID - 101128775
RN - 0 (Cyclotides)
RN - 0 (Plant Extracts)
RN - 0 (Plant Proteins)
RN - 0 (Proteome)

SB - IM
MH - Chromatography, High Pressure Liquid
MH - Cyclotides/*chemistry/genetics/isolation & purification/metabolism
MH - Cystine Knot Motifs/genetics
MH - Data Mining
MH - *Gene Expression Regulation, Plant
MH - Gene Library
MH - Liquid-Liquid Extraction
MH - Models, Molecular
MH - Molecular Sequence Data
MH - Plant Components, Aerial/chemistry
MH - Plant Extracts/chemistry
MH - Plant Proteins/chemistry/*genetics/isolation & purification/metabolism
MH - *Protein Processing, Post-Translational
MH - Proteome/genetics/metabolism
MH - Proteomics/methods
MH - Sequence Alignment
MH - Spectrometry, Mass, Matrix-Assisted Laser Desorption-Ionization
MH - *Transcriptome
MH - Violaceae/*genetics/metabolism
PMC - PMC4642221
OTO - NOTNLM
OT - 1kp
OT - Violaceae
OT - circular peptides
OT - cystine-knot
OT - mass spectrometry
OT - natural products
OT - peptidomics
OT - ribosomally synthesized and post-translationally modified peptides
OT - transcriptome
EDAT- 2015/09/25 06:00
MHDA- 2016/09/10 06:00
CRDT- 2015/09/25 06:00
PHST- 2015/09/25 06:00 [entrez]
PHST- 2015/09/25 06:00 [pubmed]
PHST- 2016/09/10 06:00 [medline]
AID - 10.1021/acs.jproteome.5b00681 [doi]
PST - ppublish
SO - J Proteome Res. 2015 Nov 6;14(11):4851-62. doi: 10.1021/acs.jproteome.5b00681. Epub 2015 Oct 8.

PMID- 25528148
OWN - NLM
STAT- MEDLINE
DCOM- 20151222
LR - 20181113
IS - 1432-2048 (Electronic)
IS - 0032-0935 (Linking)
VI - 241
IP - 4

DP - 2015 Apr
TI - Two Blast-independent tools, CyPerl and CyExcel, for harvesting hundreds of nov
cyclotides and analogues from plant genomes and protein databases.
PG - 929-40
LID - 10.1007/s00425-014-2229-5 [doi]
AB - Two high-throughput tools harvest hundreds of novel cyclotides and analogues i
plants. Cyclotides are gene-encoded backbone-cyclized polypeptides displaying a
diverse range of bioactivities associated with plant defense. However,
genome-scale or database-scale evaluations of cyclotides have been rare so far
Here, a novel time-efficient Perl program, CyPerl, was developed for searching
cyclotides from predicted ORFs of 34 available plant genomes and existing plant
protein sequences from Genbank databases. CyPerl-isolated sequences were furthe
analyzed by removing repeats, evaluating their cysteine-distributed regions
(CDRs) and comparing with CyBase-collected cyclotides in a user-friendly Excel
(Microsoft Office) template, CyExcel. After genome-screening, 186 ORFs contain
145 unique cyclotide analogues were identified by CyPerl and CyExcel from 30
plant genomes tested from 10 plant families. Phaseolus vulgaris and Zea mays we
the richest two species containing cyclotide analogues in the plants tested.
After screening protein databases, 266 unique cyclotides and analogues were
identified from seven plant families. By merging with 288 unique CyBase-listed
cyclotides, 510 unique cyclotides and analogues were obtained from 13 plant
families. In total, seven novel plant families containing cyclotide analogues a
202 novel cyclotide analogues were identified in this study. This study has
established two Blast-independent tools for screening cyclotides from plant
genomes and protein databases, and has also significantly widened the plant
distribution and sequence diversity of cyclotides and their analogues.
FAU - Zhang, Jun
AU - Zhang J
AD - School of Biosciences and Biopharmaceutics, Guangdong Province Key Laboratory f
Biotechnology Drug Candidates, Guangdong Pharmaceutical University, Guangzhou,
510006, China, zhangj80@aliyun.com.
FAU - Hua, Zhengshuang
AU - Hua Z
FAU - Huang, Zebo
AU - Huang Z
FAU - Chen, QiZhu
AU - Chen Q
FAU - Long, Qingyun
AU - Long Q
FAU - Craik, David J
AU - Craik DJ
FAU - Baker, Alan J M
AU - Baker AJ
FAU - Shu, Wensheng
AU - Shu W
FAU - Liao, Bin
AU - Liao B
LA - eng
PT - Journal Article
PT - Research Support, Non-U.S. Gov't
DEP - 20141221

PL - Germany
TA - Planta
JT - Planta
JID - 1250576
RN - 0 (Cyclotides)
RN - 0 (Plant Proteins)
SB - IM
MH - Amino Acid Sequence
MH - Cyclotides/*genetics
MH - *Databases, Nucleic Acid
MH - *Databases, Protein
MH - Genome, Plant/*genetics
MH - Magnoliopsida/*genetics/metabolism
MH - Models, Molecular
MH - Molecular Sequence Data
MH - Plant Proteins/genetics
MH - Sequence Alignment
MH - Sequence Analysis
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PHST- 2014/12/22 06:00 [entrez]
PHST- 2014/12/22 06:00 [pubmed]
PHST- 2015/12/23 06:00 [medline]
AID - 10.1007/s00425-014-2229-5 [doi]
PST - ppublish
SO - Planta. 2015 Apr;241(4):929-40. doi: 10.1007/s00425-014-2229-5. Epub 2014 Dec

PMID- 31187974
OWN - NLM
STAT- MEDLINE
DCOM- 20200601
LR - 20200601
IS - 1520-4995 (Electronic)
IS - 0006-2960 (Linking)
VI - 58
IP - 27
DP - 2019 Jul 9
TI - Recombinant Butelase-Mediated Cyclization of the p53-Binding Domain of the Oncoprotein MdmX-Stabilized Protein Conformation as a Promising Model for Structural Investigation.
PG - 3005-3015
LID - 10.1021/acs.biochem.9b00263 [doi]
AB - Cyclization of the polypeptide backbone has proven to be a powerful strategy fo enhancing protein stability for fundamental research and pharmaceutical application. The use of such an approach is restricted by how well a targeted polypeptide can be efficiently ligated. Recently, an Asx-specific peptide liga identified from a tropical cyclotide-producing plant and named butelase 1 exhibited excellent cyclization kinetics that cannot be matched by other known

ligases, including intein, PATG, PCY1, and sortase A. In this work, we aimed to examine whether butelase 1 facilitated protein conformational stability for structural investigation. First, we successfully expressed recombinant butelase (rBTase) in the yeast Pichia pastoris. Next, rBTase was shown to be highly efficient in the cyclization of the p53-binding domain (N-terminal domain) of murine double minute X (N-MdmX), an important target for designing anticancer drugs. The cyclized N-MdmX (cMdmX) exhibited increased conformational stability and improved interaction with the ligand compared with those of noncyclized N-MdmX. Importantly, the thermal melting process was completely reversible, contrary to noncyclized N-MdmX, and the melting temperature (T(m)) of cMdmX was increased to 47 from 43 °C. This stable conformation of cMdmX was further confirmed by (15)N-(1)H heteronuclear single-quantum coherence nuclear magnetic resonance (NMR) spectroscopy. The complex of cMdmX and the ligand was tested for protein crystallization, and several promising findings were revealed. Therefore, our work not only provides a recombinant version of butelase 1 but also suggests a conventional approach for preparing stable protein samples for both protein crystallization and NMR structural investigation.

FAU - Pi, Ni
AU - Pi N
AD - Key Laboratory of Industrial Fermentation (Ministry of Education), Hubei Key Laboratory of Industrial Microbiology and National "111" Center for Cellular Regulation and Molecular Pharmaceutics , Hubei University of Technology , Wuhan 430068 , China.
FAU - Gao, Meng
AU - Gao M
AD - Key Laboratory of Industrial Fermentation (Ministry of Education), Hubei Key Laboratory of Industrial Microbiology and National "111" Center for Cellular Regulation and Molecular Pharmaceutics , Hubei University of Technology , Wuhan 430068 , China.
FAU - Cheng, Xiyao
AU - Cheng X
AD - Key Laboratory of Industrial Fermentation (Ministry of Education), Hubei Key Laboratory of Industrial Microbiology and National "111" Center for Cellular Regulation and Molecular Pharmaceutics , Hubei University of Technology , Wuhan 430068 , China.
AD - Wuhan Amersino Biodevelop Inc. , B1-Building, Biolake Park , Wuhan 430075 , China.
FAU - Liu, Huili
AU - Liu H
AD - National Center for Magnetic Resonance in Wuhan, State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics , Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences , Wuhan , Hubei 430071 China.
FAU - Kuang, Zhengkun
AU - Kuang Z
AD - Key Laboratory of Industrial Fermentation (Ministry of Education), Hubei Key Laboratory of Industrial Microbiology and National "111" Center for Cellular Regulation and Molecular Pharmaceutics , Hubei University of Technology , Wuhan 430068 , China.
FAU - Yang, Zixin
AU - Yang Z
AD - Key Laboratory of Industrial Fermentation (Ministry of Education), Hubei Key

Laboratory of Industrial Microbiology and National "111" Center for Cellular Regulation and Molecular Pharmaceutics , Hubei University of Technology , Wuha 430068 , China.
FAU - Yang, Jing
AU - Yang J
AD - Key Laboratory of Industrial Fermentation (Ministry of Education), Hubei Key Laboratory of Industrial Microbiology and National "111" Center for Cellular Regulation and Molecular Pharmaceutics , Hubei University of Technology , Wuha 430068 , China.
FAU - Zhang, Bailing
AU - Zhang B
AD - Key Laboratory of Industrial Fermentation (Ministry of Education), Hubei Key Laboratory of Industrial Microbiology and National "111" Center for Cellular Regulation and Molecular Pharmaceutics , Hubei University of Technology , Wuha 430068 , China.
FAU - Chen, Yao
AU - Chen Y
AD - Key Laboratory of Industrial Fermentation (Ministry of Education), Hubei Key Laboratory of Industrial Microbiology and National "111" Center for Cellular Regulation and Molecular Pharmaceutics , Hubei University of Technology , Wuha 430068 , China.
FAU - Liu, Sen
AU - Liu S
AD - Key Laboratory of Industrial Fermentation (Ministry of Education), Hubei Key Laboratory of Industrial Microbiology and National "111" Center for Cellular Regulation and Molecular Pharmaceutics , Hubei University of Technology , Wuha 430068 , China.
FAU - Huang, Yongqi
AU - Huang Y
AD - Key Laboratory of Industrial Fermentation (Ministry of Education), Hubei Key Laboratory of Industrial Microbiology and National "111" Center for Cellular Regulation and Molecular Pharmaceutics , Hubei University of Technology , Wuha 430068 , China.
AD - Wuhan Amersino Biodevelop Inc. , B1-Building, Biolake Park , Wuhan 430075 , China.
FAU - Su, Zhengding
AU - Su Z
AUID- ORCID: 0000-0003-3558-001X
AD - Key Laboratory of Industrial Fermentation (Ministry of Education), Hubei Key Laboratory of Industrial Microbiology and National "111" Center for Cellular Regulation and Molecular Pharmaceutics , Hubei University of Technology , Wuha 430068 , China.
AD - Wuhan Amersino Biodevelop Inc. , B1-Building, Biolake Park , Wuhan 430075 , China.
LA - eng
PT - Journal Article
PT - Research Support, Non-U.S. Gov't
DEP - 20190620
PL - United States
TA - Biochemistry
JT - Biochemistry

JID - 0370623
RN - 0 (Mdm4 protein, mouse)
RN - 0 (Proto-Oncogene Proteins)
RN - 0 (Recombinant Proteins)
RN - 0 (Tumor Suppressor Protein p53)
RN - EC 6.- (Ligases)
SB - IM
MH - Amino Acid Sequence
MH - Animals
MH - Crystallization/methods
MH - Crystallography, X-Ray/methods
MH - Cyclization
MH - Fabaceae/*enzymology
MH - Ligases/*chemistry
MH - Mice
MH - Models, Molecular
MH - Protein Binding
MH - Protein Conformation
MH - Protein Domains
MH - Protein Stability
MH - Proto-Oncogene Proteins/*chemistry/metabolism
MH - Recombinant Proteins/chemistry
MH - Tumor Suppressor Protein p53/metabolism
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PHST- 2020/06/02 06:00 [medline]
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AID - 10.1021/acs.biochem.9b00263 [doi]
PST - ppublish
SO - Biochemistry. 2019 Jul 9;58(27):3005-3015. doi: 10.1021/acs.biochem.9b00263. E
2019 Jun 20.

PMID- 29755968
OWN - NLM
STAT- PubMed-not-MEDLINE
LR - 20201001
IS - 2296-2646 (Print)
IS - 2296-2646 (Electronic)
IS - 2296-2646 (Linking)
VI - 6
DP - 2018
TI - Exploring the Interaction Mechanism Between Cyclopeptide DC3 and Androgen
Receptor Using Molecular Dynamics Simulations and Free Energy Calculations.
PG - 119
LID - 10.3389/fchem.2018.00119 [doi]
LID - 119
AB - Androgen receptor (AR) is a key target in the discovery of anti-PCa (Prostate
Cancer) drugs. Recently, a novel cyclopeptide Diffusa Cyclotide-3 (DC3), isola
from Hedyotisdiffusa, has been experimentally demonstrated to inhibit the

AB - survival and growth of LNCap cells, which typically express T877A-mutated AR, most frequently detected point mutation of AR in castration-resistant prostate cancer (CRPC). But the interaction mechanism between DC3 and AR is not clear. Here in this study we aim to explore the possible binding mode of DC3 to T877A-mutated AR from molecular perspective. Firstly, homology modeling was employed to construct the three-dimensional structure of the cyclopeptide DC3 using 2kux.1.A as the template. Then molecular docking, molecular dynamics (MD simulations, and molecular mechanics/generalized Born surface area (MM-GBSA) methods were performed to determine the bind site and explore the detailed interaction mechanism of DC3-AR complex. The obtained results suggested that t site formed by H11, loop888-893, and H12 (site 2) was the most possible positi of DC3 binding to AR. Besides, hydrogen bonds, hydrophobic, and electrostatic interactions play dominant roles in the recognition and combination of DC3-AR complex. The essential residues dominant in each interaction were specifically revealed. This work facilitates our understanding of the interaction mechanism DC3 binding to AR at the molecular level and contributes to the rational cyclopeptide drug design for prostate cancer.

FAU - Zhang, Huimin
AU - Zhang H
AD - School of Pharmacy, Lanzhou University, Lanzhou, China.
FAU - Song, Tianqing
AU - Song T
AD - School of Pharmacy, Lanzhou University, Lanzhou, China.
FAU - Yang, Yizhao
AU - Yang Y
AD - College of Chemistry and Chemical Engineering, Lanzhou University, Lanzhou, China.
FAU - Fu, Chenggong
AU - Fu C
AD - School of Pharmacy, Lanzhou University, Lanzhou, China.
FAU - Li, Jiazhong
AU - Li J
AD - School of Pharmacy, Lanzhou University, Lanzhou, China.
LA - eng
PT - Journal Article
DEP - 20180419
PL - Switzerland
TA - Front Chem
JT - Frontiers in chemistry
JID - 101627988
PMC - PMC5932393
OTO - NOTNLM
OT - Cyclopeptide DC3
OT - androgen receptor
OT - homology modeling
OT - molecular docking
OT - molecular dynamics simulations
OT - protein drug interaction
EDAT- 2018/05/15 06:00
MHDA- 2018/05/15 06:01
CRDT- 2018/05/15 06:00

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PHST- 2018/05/15 06:00 [entrez]
PHST- 2018/05/15 06:00 [pubmed]
PHST- 2018/05/15 06:01 [medline]
AID - 10.3389/fchem.2018.00119 [doi]
PST - epublish