
AbSciCon
2019

1
00:00:00,790 --> 00:00:07,320
[Music]

2
00:00:11,459 --> 00:00:09,110
[Applause]

3
00:00:13,980 --> 00:00:11,469
good afternoon everyone my name is

4
00:00:16,920 --> 00:00:13,990
Fillie way in this talk I'm going to

5
00:00:19,380 --> 00:00:16,930
present our recent study modern a study

6
00:00:22,230 --> 00:00:19,390
on self-assembly of short peptides in

7
00:00:27,689 --> 00:00:22,240
memory and how they would mediate ion

8
00:00:31,230 --> 00:00:27,699
transport the transport of ionic cores

9
00:00:34,049 --> 00:00:31,240
memory is very important for biochemical

10
00:00:36,150 --> 00:00:34,059
functions however the insistence of

11
00:00:39,090 --> 00:00:36,160
permeation through the memory is not

12
00:00:42,119 --> 00:00:39,100
energetically favorable and an energy

13
00:00:44,820 --> 00:00:42,129

barrier can be kankakee culpable so you

14
00:00:48,030 --> 00:00:44,830
early you need some help you need either

15
00:00:50,009 --> 00:00:48,040
iron transporter or ion channels and it

16
00:00:52,560 --> 00:00:50,019
cannot only low the free energy barrier

17
00:00:55,350 --> 00:00:52,570
it can also provide selectivity and

18
00:00:58,049 --> 00:00:55,360
regulation however different designs are

19
00:01:00,869 --> 00:00:58,059
in the contemporary art channel which

20
00:01:04,380 --> 00:01:00,879
has very high sequency requirement and

21
00:01:07,560 --> 00:01:04,390
has very high ion selectivity we expect

22
00:01:09,719 --> 00:01:07,570
that EEE only our channel the lands and

23
00:01:12,210 --> 00:01:09,729
the secrecy requirement is rather

24
00:01:15,660 --> 00:01:12,220
minimum and the ANSI selectivity is

25
00:01:18,510 --> 00:01:15,670
rather weak so to understand the early

26
00:01:21,930 --> 00:01:18,520
on channel the formation of it we use a

27
00:01:25,080 --> 00:01:21,940
rather or model system the modern

28
00:01:28,230 --> 00:01:25,090
channel we try to use is called is

29
00:01:32,010 --> 00:01:28,240
formed by antimicrobial peptides it is

30
00:01:35,580 --> 00:01:32,020
rather short it has only 8 to 20 amino

31
00:01:39,330 --> 00:01:35,590
acids and it is and fulfilling peptides

32
00:01:43,020 --> 00:01:39,340
and loss of exam had found this type of

33
00:01:46,980 --> 00:01:43,030
peptides can polymerize membrane and

34
00:01:48,060 --> 00:01:46,990
have ions and some molecules and vesicle

35
00:01:51,990 --> 00:01:48,070
content leakage

36
00:01:54,200 --> 00:01:52,000
one of the well studied antimicrobial

37
00:01:57,090 --> 00:01:54,210
peptide formation of Valentino is this

38
00:02:01,260 --> 00:01:57,100

ala missing peptide it has a length of

39
00:02:03,830 --> 00:02:01,270
20 amino acid and it is longer enough to

40
00:02:06,810 --> 00:02:03,840
span the membrane and has well-defined

41
00:02:08,699 --> 00:02:06,820
conductance however we want studies on

42
00:02:11,339 --> 00:02:08,709
seeing even shorter so we are trying to

43
00:02:13,410 --> 00:02:11,349
understand he was a peptide is even is

44
00:02:19,830 --> 00:02:13,420
much shorter than al amazing channel can

45
00:02:22,460 --> 00:02:19,840
it immediate transpose remember so with

46
00:02:27,020 --> 00:02:22,470
the peptide we true to study is this

47
00:02:30,320 --> 00:02:27,030
called trikuti peptide it has only 10

48
00:02:34,790 --> 00:02:30,330
sequence e and most of it is hydrophobic

49
00:02:39,260 --> 00:02:34,800
or sto and it has few crises rescue on

50
00:02:41,930 --> 00:02:39,270
it and this pipe has is rather high for

51
00:02:44,810 --> 00:02:41,940
helical conformation in memory it can

52
00:02:46,730 --> 00:02:44,820
either increase memory state or can be

53
00:02:49,700 --> 00:02:46,740
in a surface bounded state and they are

54
00:02:52,520 --> 00:02:49,710
interconvertible and experiment has

55
00:02:56,810 --> 00:02:52,530
found that this peptide can immobilize

56
00:02:59,780 --> 00:02:56,820
membrane and at a certain type ID to the

57
00:03:02,390 --> 00:02:59,790
padishah and even iron transporter arc

58
00:03:06,710 --> 00:03:02,400
has been observed however the mechanism

59
00:03:08,930 --> 00:03:06,720
of our transport is very weak so people

60
00:03:11,840 --> 00:03:08,940
propose the various mechanisms such as

61
00:03:13,730 --> 00:03:11,850
deformation of memory due to the peptide

62
00:03:17,270 --> 00:03:13,740
maybe there are channel formation

63
00:03:19,280 --> 00:03:17,280

maybe that who are water defects so our

64
00:03:22,760 --> 00:03:19,290
studies many focused try to understand

65
00:03:25,310 --> 00:03:22,770
this we use modeling a method basically

66
00:03:28,040 --> 00:03:25,320
we use atomic molecular dynamic

67
00:03:31,280 --> 00:03:28,050
simulations and to a solution every see

68
00:03:33,530 --> 00:03:31,290
the process we also use a society there

69
00:03:35,570 --> 00:03:33,540
are simulation which can lower the free

70
00:03:40,390 --> 00:03:35,580
energy overall in the system so we can

71
00:03:44,570 --> 00:03:40,400
study a long time scale of the process

72
00:03:47,840 --> 00:03:44,580
so we first try to understand with even

73
00:03:50,900 --> 00:03:47,850
just one single peptide a monomers here

74
00:03:53,810 --> 00:03:50,910
how the effects the memory structure so

75
00:03:56,840 --> 00:03:53,820
we found that we with this trend are

76
00:03:59,150 --> 00:03:56,850
transmembrane orientation of this single

77
00:04:01,789 --> 00:03:59,160
peptide is already induced local

78
00:04:04,310 --> 00:04:01,799
memories in effects and introduce the

79
00:04:07,820 --> 00:04:04,320
water defects from both side and such

80
00:04:10,160 --> 00:04:07,830
deformation is shown to lower water on

81
00:04:12,289 --> 00:04:10,170
free energy crossing the membrane for

82
00:04:14,120 --> 00:04:12,299
one kcal per mole and the water

83
00:04:17,570 --> 00:04:14,130
transport through the memory is found

84
00:04:18,909 --> 00:04:17,580
highly favorable in the neighborhood of

85
00:04:22,900 --> 00:04:18,919
this peptide

86
00:04:25,340 --> 00:04:22,910
however to think about this whether such

87
00:04:29,860 --> 00:04:25,350
deformation can induce iron transporter

88
00:04:32,360 --> 00:04:29,870

the possibilities rather are low because

89
00:04:35,430 --> 00:04:32,370
for ion to transport easily in either

90
00:04:38,280 --> 00:04:35,440
much larger water pool so

91
00:04:40,560 --> 00:04:38,290
to continue to understand it what we do

92
00:04:43,200 --> 00:04:40,570
what we did is that we have more than

93
00:04:45,860 --> 00:04:43,210
one peptides on the surface memory as

94
00:04:48,660 --> 00:04:45,870
you see on the far right far left side

95
00:04:51,480 --> 00:04:48,670
that's our initial confusion when we

96
00:04:54,510 --> 00:04:51,490
study the study the simulation we have

97
00:04:57,300 --> 00:04:54,520
14 of the tributing peptides initially

98
00:04:59,160 --> 00:04:57,310
as a memory surface because we want

99
00:05:01,770 --> 00:04:59,170
studies and transport so we apply

100
00:05:04,020 --> 00:05:01,780
electric field across a membrane so with

101
00:05:07,010 --> 00:05:04,030
the simulation progressed we see that

102
00:05:09,780 --> 00:05:07,020
the peptides began some of them began to

103
00:05:12,740 --> 00:05:09,790
adopt it is transmembrane conformation

104
00:05:15,090 --> 00:05:12,750
and as he began to irrigate and various

105
00:05:16,200 --> 00:05:15,100
irrigation state has been found they can

106
00:05:18,870 --> 00:05:16,210
be time well actually there are two

107
00:05:21,480 --> 00:05:18,880
types of tangled it can be try more and

108
00:05:23,820 --> 00:05:21,490
the Tetra more and with even longer

109
00:05:26,340 --> 00:05:23,830
simulation we found a ependymal

110
00:05:28,770 --> 00:05:26,350
structure on the snapshot were taken

111
00:05:30,990 --> 00:05:28,780
from our simulation on the right sides

112
00:05:33,990 --> 00:05:31,000
in most the right side so this kind of a

113
00:05:36,480 --> 00:05:34,000

structure actually is well-defined if I

114
00:05:40,070 --> 00:05:36,490
check the cross section of this Panama

115
00:05:42,870 --> 00:05:40,080
structure as sure on the top it is

116
00:05:45,390 --> 00:05:42,880
actually behave as a better state model

117
00:05:48,720 --> 00:05:45,400
it has this cry seen which is higher

118
00:05:51,750 --> 00:05:48,730
slightly hydrophilic residues facing the

119
00:05:54,930 --> 00:05:51,760
lumen officer of the of the arguments

120
00:05:57,990 --> 00:05:54,940
structure and also there what for quince

121
00:06:00,590 --> 00:05:58,000
reserve polymer and we observed iron and

122
00:06:03,600 --> 00:06:00,600
conductance Tiffany's waterfall and

123
00:06:06,390 --> 00:06:03,610
however I have it were mentioned that on

124
00:06:09,690 --> 00:06:06,400
such original structure although a

125
00:06:12,360 --> 00:06:09,700
contact ions it rather present so not

126
00:06:14,910 --> 00:06:12,370
only it have formed and he was

127
00:06:18,120 --> 00:06:14,920
structured Ramos structure it can it can

128
00:06:20,760 --> 00:06:18,130
assembled back to its original disorder

129
00:06:28,350 --> 00:06:20,770
structure so it is than any chimera turn

130
00:06:31,230 --> 00:06:28,360
any caused aggregation so if we want how

131
00:06:32,910 --> 00:06:31,240
to understand little bit about how this

132
00:06:37,670 --> 00:06:32,920
organ was formed there was a mechanism

133
00:06:39,840 --> 00:06:37,680
for the formation of the ugly more so

134
00:06:42,420 --> 00:06:39,850
quantitatively there are two steps to

135
00:06:46,140 --> 00:06:42,430
for it formed on the right side on the

136
00:06:48,720 --> 00:06:46,150
left side you can see if I have two

137
00:06:51,720 --> 00:06:48,730
peptides

138
00:06:53,760 --> 00:06:51,730

in inserting in the memory and each of

139
00:06:59,010 --> 00:06:53,770
them can cause local or membrane

140
00:07:02,420 --> 00:06:59,020
deformation and to have to reduce the

141
00:07:04,410 --> 00:07:02,430
total free energy of this of the

142
00:07:07,200 --> 00:07:04,420
sophistic earth of the memory

143
00:07:11,040 --> 00:07:07,210
deformation all these two peptides is

144
00:07:12,840 --> 00:07:11,050
time to aggregate and such total free

145
00:07:15,000 --> 00:07:12,850
energy is depending on the surface

146
00:07:18,000 --> 00:07:15,010
tension is depend on the pending

147
00:07:19,890 --> 00:07:18,010
stiffness of witchly PDR you see it also

148
00:07:23,520 --> 00:07:19,900
depend on the membranes Martinez

149
00:07:26,400 --> 00:07:23,530
curvature of the LDP so the second step

150
00:07:29,970 --> 00:07:26,410
is that once the true pipe has get close

151
00:07:31,940 --> 00:07:29,980
enough they will adjust to each other

152
00:07:34,980 --> 00:07:31,950
and have a sequence II dependent

153
00:07:38,520 --> 00:07:34,990
Alchemist structure so in our case we

154
00:07:41,670 --> 00:07:38,530
have a guy see rest you will face in the

155
00:07:44,280 --> 00:07:41,680
looming officer pentamer or the elegance

156
00:07:48,110 --> 00:07:44,290
of limas structure and the soul which is

157
00:07:55,170 --> 00:07:52,530
so we found that actually there are more

158
00:07:58,430 --> 00:07:55,180
than just the only most structural have

159
00:08:03,090 --> 00:07:58,440
this arm channel like structure actually

160
00:08:08,400 --> 00:08:03,100
the lipid can also be I induced to have

161
00:08:11,270 --> 00:08:08,410
a free flop motion constantly so due to

162
00:08:15,090 --> 00:08:11,280
the water defects induced by this

163
00:08:17,310 --> 00:08:15,100

special peptide the head group of the

164
00:08:19,230 --> 00:08:17,320
deep heat can go through a free flow

165
00:08:21,570 --> 00:08:19,240
process coming from one side of

166
00:08:23,870 --> 00:08:21,580
remembering to the other side ideally

167
00:08:26,790 --> 00:08:23,880
this process is kind introduce a

168
00:08:29,130 --> 00:08:26,800
transient water power and through this

169
00:08:32,880 --> 00:08:29,140
transient world poor aren't a transport

170
00:08:35,880 --> 00:08:32,890
through the memory also so this is kind

171
00:08:40,160 --> 00:08:35,890
of similar as people have been long

172
00:08:43,589 --> 00:08:40,170
proposed as this hurdle hope for some

173
00:08:47,520 --> 00:08:43,599
activity of antimicrobial peptides so

174
00:08:52,470 --> 00:08:47,530
this kind of in confirm that is it is

175
00:08:55,830 --> 00:08:52,480
possible so exciti was what high people

176
00:08:59,630 --> 00:08:55,840
have been observed in the antimicrobial

177
00:09:02,870 --> 00:08:59,640
peptides that people do find some

178
00:09:05,210 --> 00:09:02,880
I don't handle like activity and people

179
00:09:08,319 --> 00:09:05,220
also through recent years people have

180
00:09:11,000 --> 00:09:08,329
been used as TM eg try to understand the

181
00:09:14,660 --> 00:09:11,010
structure of this poll however I

182
00:09:17,000 --> 00:09:14,670
recommend that because different than

183
00:09:20,240 --> 00:09:17,010
the contemporary handle that people can

184
00:09:22,910 --> 00:09:20,250
study the structures through x-ray or

185
00:09:25,250 --> 00:09:22,920
NMR because of dynamic nature of this

186
00:09:28,130 --> 00:09:25,260
short peptides so it's very extremely

187
00:09:33,980 --> 00:09:28,140
Challenger to capture the real structure

188
00:09:37,160 --> 00:09:33,990

of it why is interaction so in

189
00:09:39,590 --> 00:09:37,170
conclusion we have study the short

190
00:09:41,900 --> 00:09:39,600
peptides a sense of assembly in the

191
00:09:44,540 --> 00:09:41,910
membrane we follow it immediate an

192
00:09:47,569 --> 00:09:44,550
transpose through various ways and we

193
00:09:49,400 --> 00:09:47,579
found that the short peptides have

194
00:09:52,040 --> 00:09:49,410
formed Optimus different Oklahoma

195
00:09:54,889 --> 00:09:52,050
structures through the membrane mediated

196
00:09:58,509 --> 00:09:54,899
our formation or we found that translate

197
00:10:00,850 --> 00:09:58,519
what Paul can be formed through the

198
00:10:03,710 --> 00:10:00,860
pentamer structure and iron can be

199
00:10:06,410 --> 00:10:03,720
transverse research structure we also

200
00:10:10,189 --> 00:10:06,420
found that memory and structure can be

201
00:10:14,000 --> 00:10:10,199
disrupted by peptide induced repeat a

202
00:10:17,060 --> 00:10:14,010
flip-flop and also iron transfer can is

203
00:10:20,630 --> 00:10:17,070
observers to such process so what's the

204
00:10:22,790 --> 00:10:20,640
implication of how study so it shows

205
00:10:26,210 --> 00:10:22,800
that short and simple and fulfilling

206
00:10:29,509 --> 00:10:26,220
peptides is capable to polymerizing

207
00:10:33,350 --> 00:10:29,519
memory so it suggests that maybe select

208
00:10:35,870 --> 00:10:33,360
peptides or they can be a candidate for

209
00:10:40,030 --> 00:10:35,880
the precursors or for continuing

210
00:10:44,000 --> 00:10:40,040
contemporary ion channels so this is a

211
00:10:48,120 --> 00:10:44,010
some good indication for that that would

212
00:10:53,450 --> 00:10:48,130
be concluding my talk thank you

213
00:11:20,420 --> 00:10:55,890

Thank You China we have time for many

214
00:11:29,660 --> 00:11:26,629
okay so this down standard an acid is

215
00:11:33,120 --> 00:11:29,670
called amino ethyle

216
00:11:37,470 --> 00:11:33,130
periodic acid so it is from it has fungi

217
00:11:39,780 --> 00:11:37,480
nature so it is generate post the

218
00:11:48,420 --> 00:11:39,790
translational process for the standard

219
00:11:51,329 --> 00:11:48,430
amino acid so yeah kind of like that

220
00:11:54,660 --> 00:11:51,339
yeah so regarding whether we can

221
00:11:57,030 --> 00:11:54,670
substituted with other amino acid such

222
00:12:03,389 --> 00:11:57,040
as standard city it's a little bit hard

223
00:12:05,309 --> 00:12:03,399
to see because why is it positive answer

224
00:12:08,249 --> 00:12:05,319
is that it is possible to replace it

225
00:12:11,309 --> 00:12:08,259
with a hydrophobic the aldehyde to stand

226
00:12:14,189 --> 00:12:11,319
out hydrophobic peptides amino acid so

227
00:12:19,350 --> 00:12:14,199
because of me function of it is is

228
00:12:22,439 --> 00:12:19,360
hydrophobic property and the other side

229
00:12:24,929 --> 00:12:22,449
unique about this amino acid is that it

230
00:12:28,230 --> 00:12:24,939
is hydrophobic it is a helical

231
00:12:31,079 --> 00:12:28,240
conformation promoter so as you can see

232
00:12:35,160 --> 00:12:31,089
in this specific sequence II it has lots

233
00:12:38,370 --> 00:12:35,170
of for AIB residue it promotes a helical

234
00:12:42,030 --> 00:12:38,380
conformation of these peptides so when

235
00:12:44,220 --> 00:12:42,040
people be substituting with other for

236
00:12:46,710 --> 00:12:44,230
example hydrophobic residue this might

237
00:12:49,170 --> 00:12:46,720
take into account whether it can

238
00:13:06,370 --> 00:12:49,180

influence some summary the properties of

239
00:13:11,400 --> 00:13:10,480
okay Thank You 10 you our next speaker