In-silico modelling of reaction networks involved in prebiotic chemistry to understand the origins of life

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Young Sci
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1
00:00:04,550 --> 00:00:02,710
hello everyone i am sidhan sharma a

2
00:00:05,910 --> 00:00:04,560
senior undergraduate from india

3
00:00:07,990 --> 00:00:05,920
and today through the medium of this

4
00:00:09,910 --> 00:00:08,000
wonderful app.con 2021

5
00:00:11,190 --> 00:00:09,920
i am going to be sharing with you an all

6
00:00:13,190 --> 00:00:11,200
undergraduate network

7
00:00:15,270 --> 00:00:13,200
that we did as a part of blue marble

8
00:00:17,029 --> 00:00:15,280
space and science young sciences program

9
00:00:18,870 --> 00:00:17,039
with our pi henderson james cleeve from

10
00:00:20,550 --> 00:00:18,880
our very own lc and all the wonderful

11
00:00:22,230 --> 00:00:20,560
collaborators as you can see here

12
00:00:23,990 --> 00:00:22,240
so we wanted to build the open source

13
00:00:25,670 --> 00:00:24,000

modifiable workflow where you can input

14
00:00:27,509 --> 00:00:25,680
a bunch of molecules and put a bunch of

15
00:00:28,790 --> 00:00:27,519
reactions and it can spit out a chemical

16
00:00:31,029 --> 00:00:28,800
reaction network

17
00:00:32,470 --> 00:00:31,039
and then it can further process for from

18
00:00:34,389 --> 00:00:32,480
network statistics or prebiotic

19
00:00:36,229 --> 00:00:34,399
relevance such as auto catalysis

20
00:00:38,069 --> 00:00:36,239
and we achieved that through the use of

21
00:00:39,030 --> 00:00:38,079
graph theory graph grammars graph

22
00:00:41,350 --> 00:00:39,040
databases

23
00:00:43,030 --> 00:00:41,360
along with getting our theoretical

24
00:00:44,790 --> 00:00:43,040
products of this reaction networks to

25
00:00:46,549 --> 00:00:44,800
experimental means such as comparing it

26
00:00:47,590 --> 00:00:46,559
with high resolution mass spectra data

27
00:00:49,830 --> 00:00:47,600
comparing it with

28
00:00:51,590 --> 00:00:49,840
a biological data biological databases

29
00:00:53,110 --> 00:00:51,600
of interest and comparing it with

30
00:00:55,110 --> 00:00:53,120
the structures that are experimentally

31
00:00:56,310 --> 00:00:55,120
reported in the literature so i hope you