Bioinformatic screening of polypheonl oxidases for theaflavi synthesis from the natural biological resources

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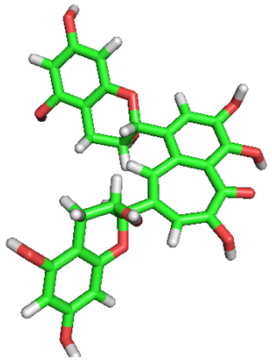
Introduction

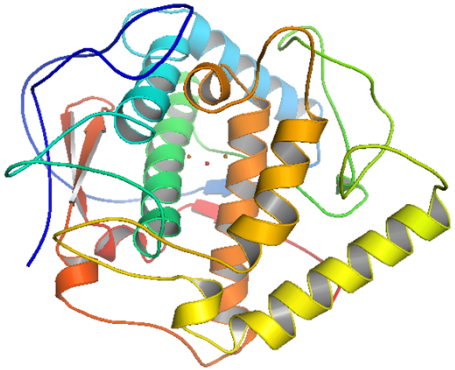


- **茶黄素（TFs）：** 红茶重要品质成分之一，具有多种保健功效。
- 红茶中含量较低（0.5%~3%），不利于提取。
- 主要制备途径：多酚氧化酶（PPO）体外酶促合成成为茶黄素的。
- PPO来源众多，活性不一；传统方法筛选PPO酶原具有盲目性，而且成本高，效率低。
- 本实验使用生物信息学方法筛选高效催化茶黄素合成的PPO酶源。比传统方法成本更低，效率更高。

Introduction

Homology modelling

Database

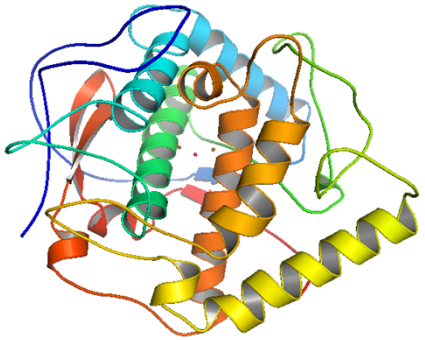


Template

>tr|A6N8J4|
A6N8J4_CAMSI_Polyphenol_oxidase_OS_Camellia_sinensis_PE_4_SV_1
APVTAPDLSKCGAADLPADAKPTNCCPPKTNKIIEFKLPPPSNILRVRPAAHLADEKYIA
KFSKALQLMKSLPDDDPRSFKQQSNIHCAYCEGAYHQVGFPSTELQVHNSWLFFPFHRFY
LYFFEKILGMLLDDPAFAIPFWNWDSPAGMKIPAMYADINSPLYNRLRDAKHQPPTLIDL
DYNLTDPKNVDEEKQKLRNLTIMYRQVVSGGKTPRLFLGSSYRAGDDPDPGAGSLENIPH
GPVHIWCGDRTQPNLEDMGNFYSAGRDPIFYGHHANVDRIWTVWKTLGGKRNDFKDSDCL
NSEFTFYDENAQLVTVKVKESLDHRKLGYVYQDVEIPWL

Amino acid sequence

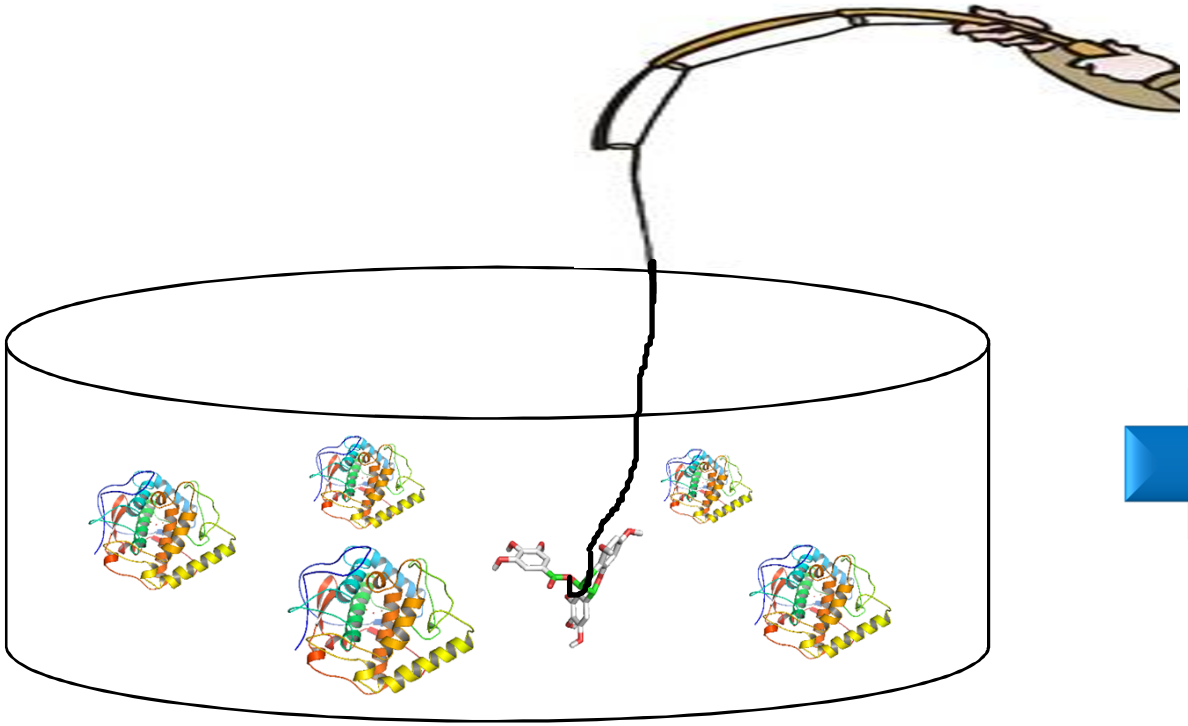
Modeller



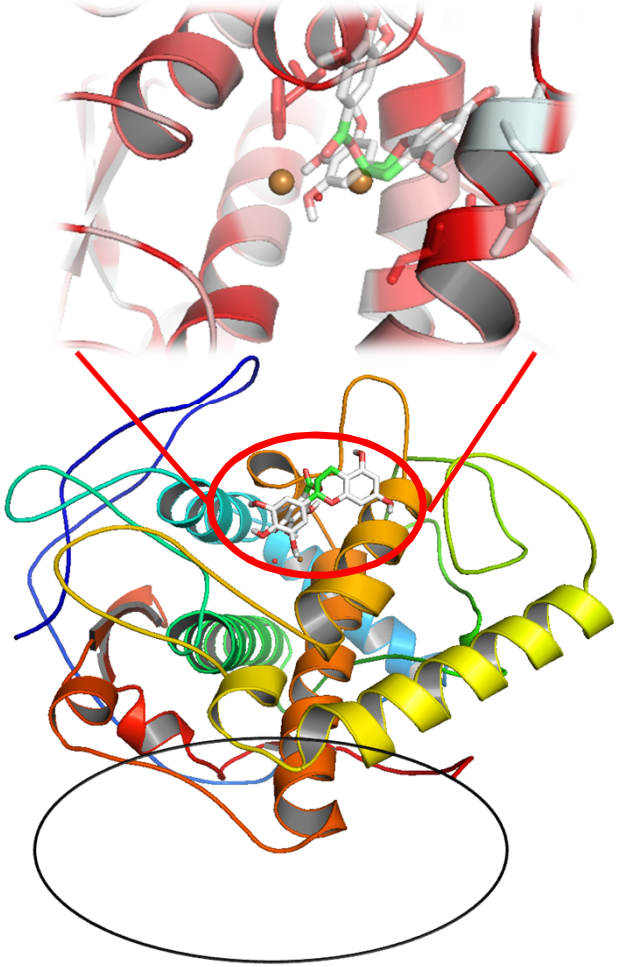
model

Introduction

Inverse virtual screening

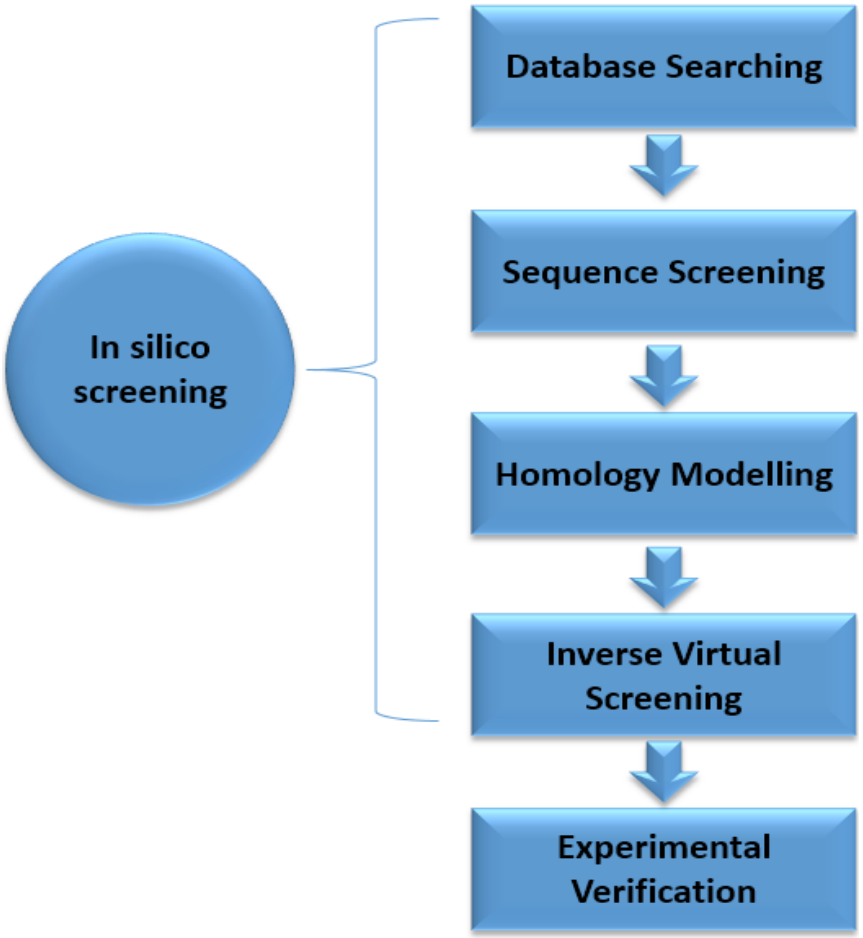


Structure database

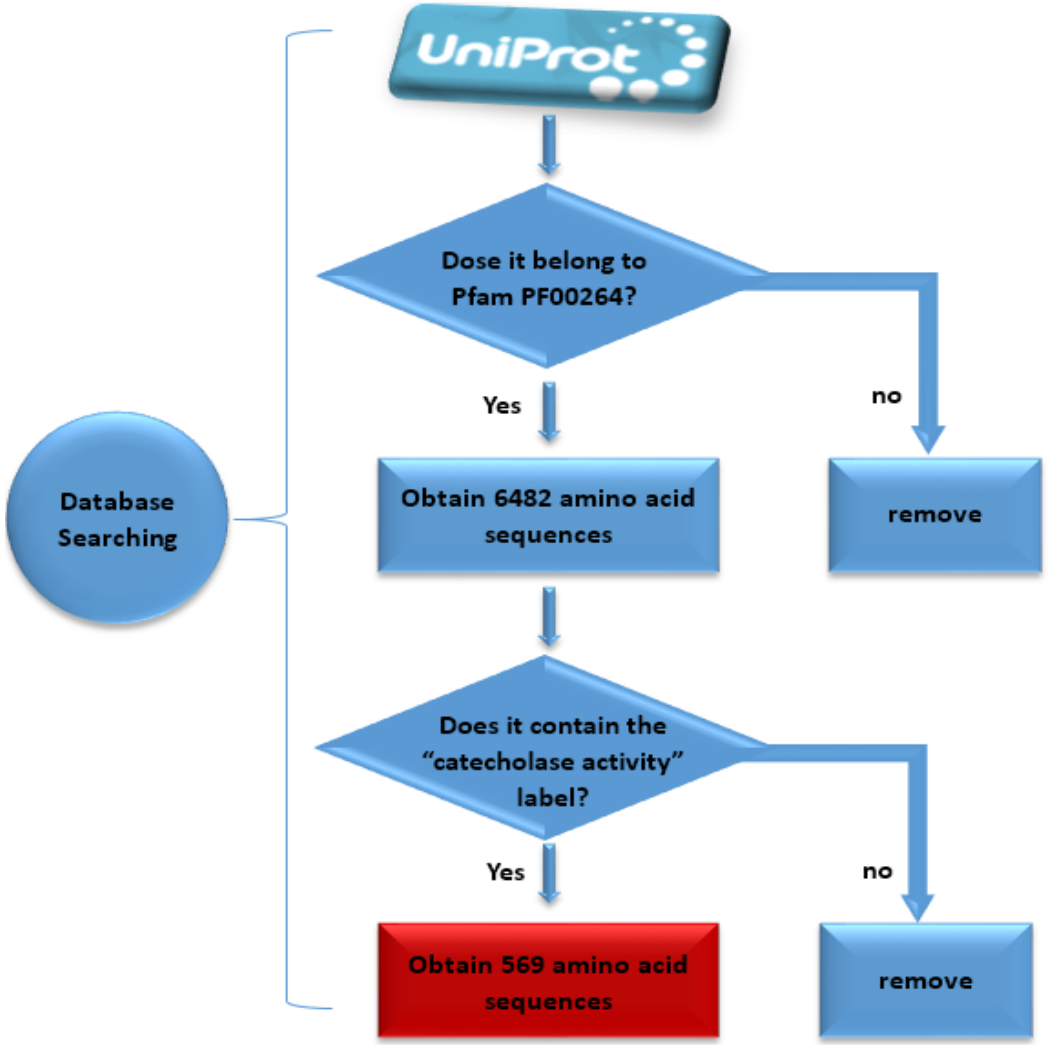


Best receptor

Methods

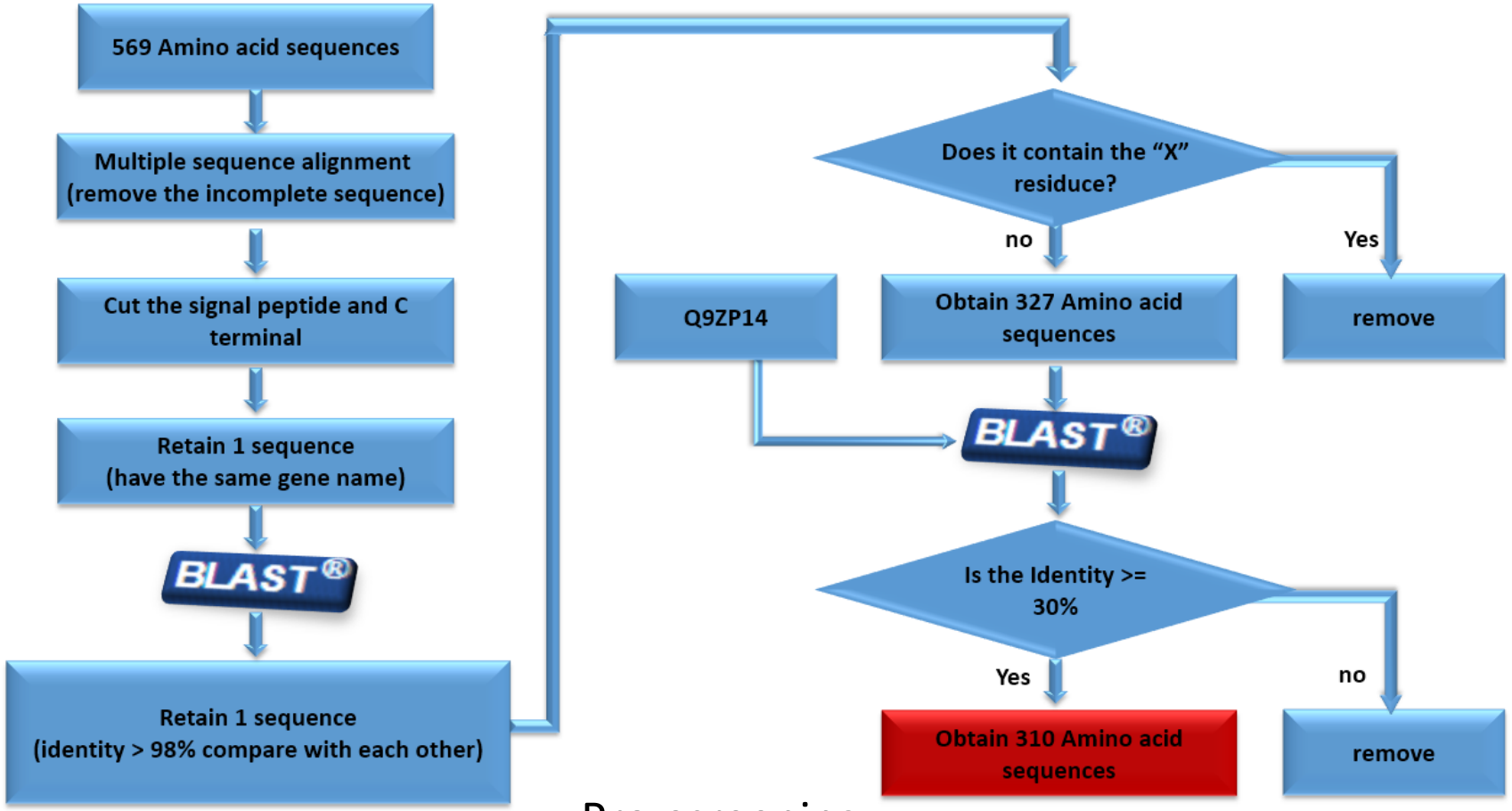

In silico screening
Database Searching
Sequence Screening
Homology Modelling
Inverse Virtual Screening
Experimental Verification

Methods



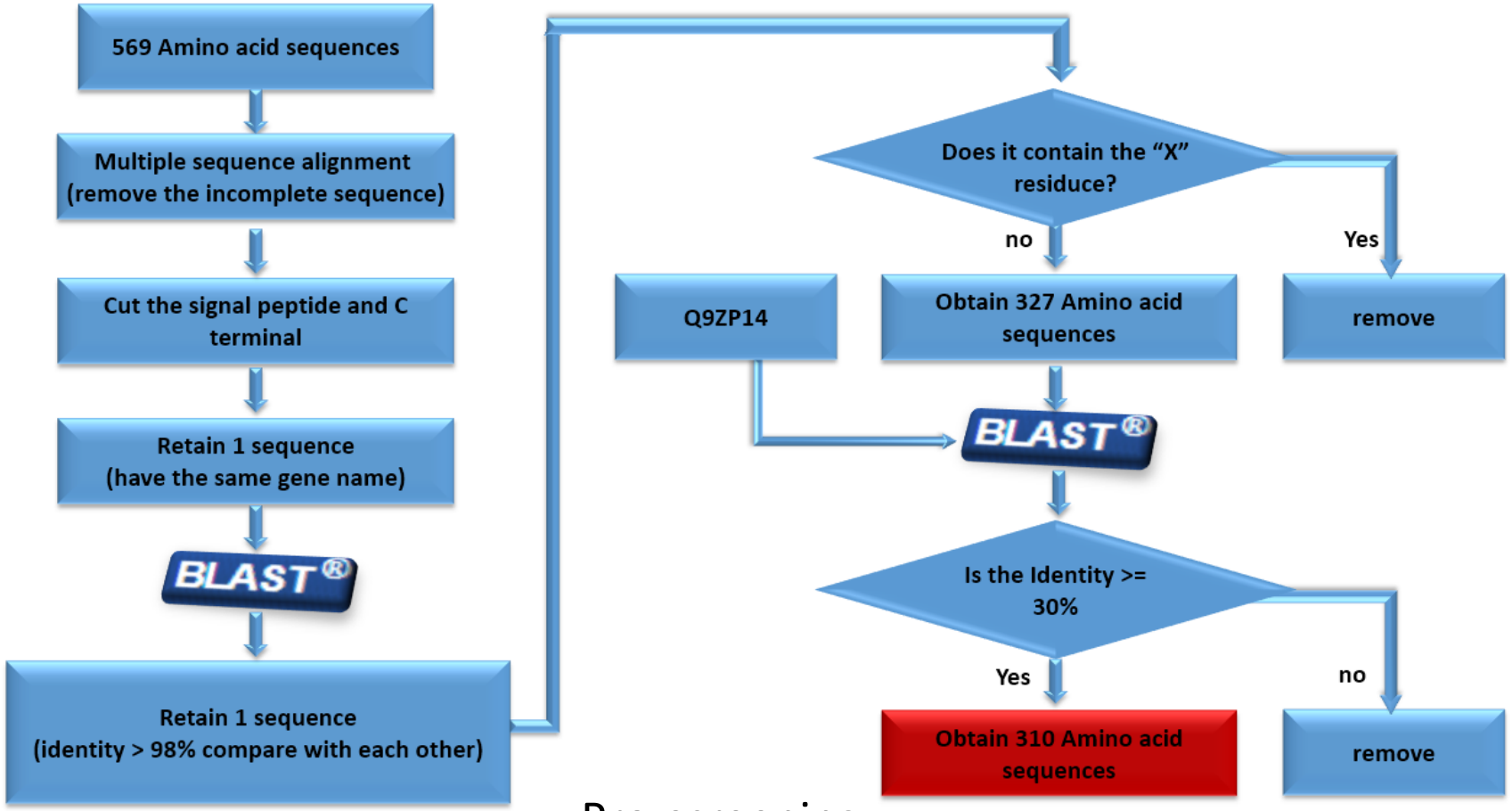
Database searching

Methods



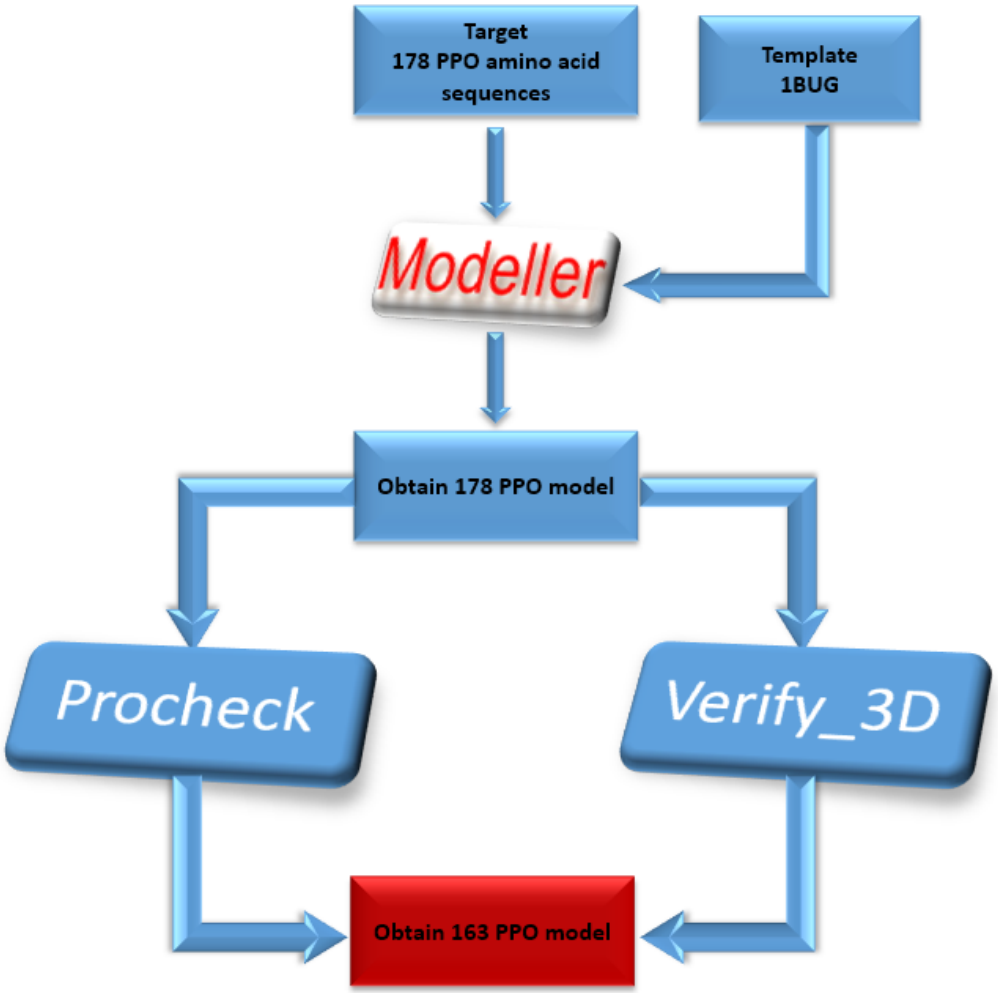
Pro-screening

Methods



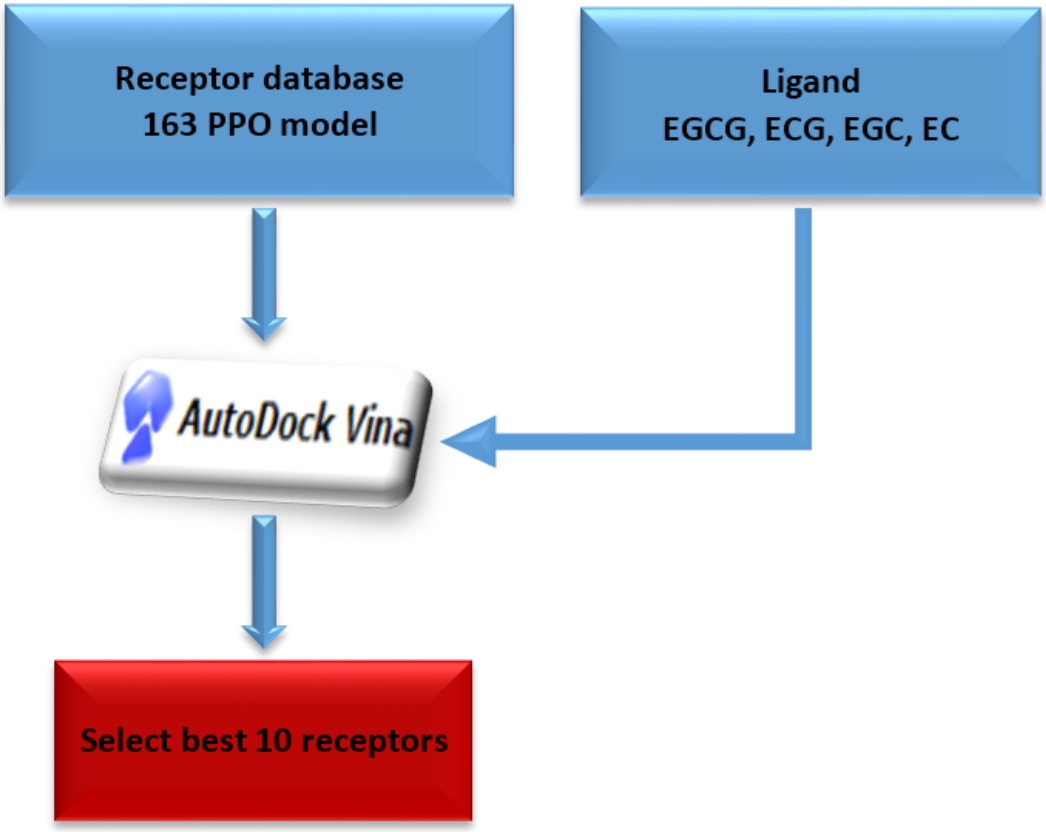
Pro-screening

Methods



Homology modelling

Methods



Inverse virtual screening

Table 1 Selected 10 PPO resources from 163 molecular docking results depended on the binding affinity, quantity of production, price and accessibility.

Uniprot Entry	Organism	BA_{final} (kcal/mol)	rank
W5VXS2	Musa acuminata AAA Group	-8.3	1
Q9ZP19	Ipomoea batatas	-8.035	3
Q6YHK7	Ananas comosus	-7.7775	7
M1BMR4	Solanum tuberosum	-7.77	9
I3WE67	Pyrus pyrifolia	-7.5225	14
K4CMI7	Solanum lycopersicum	-7.45	18
I1MEE6	Glycine max	-7.4375	19
P43309	Malus domestica	-7.4075	21
V7B2A0	Phaseolus vulgaris	-7.365	27
E5L9E4	Nelumbo nucifera	-7.34	28

Results and discussion

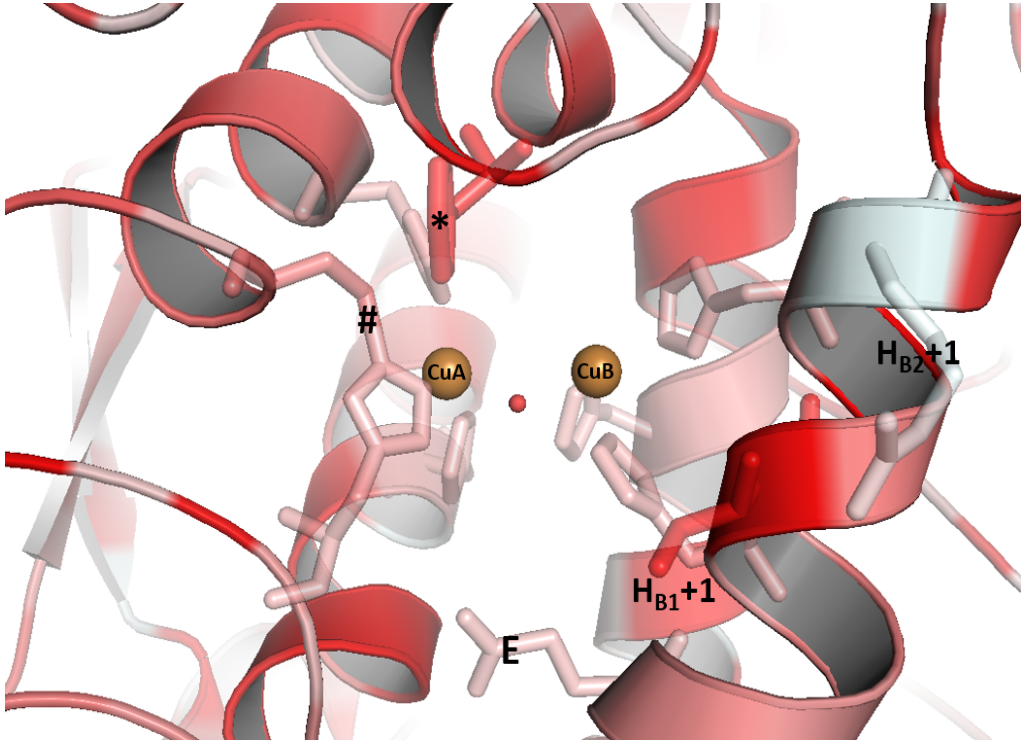


Fig. 1 Active side of *Ipomoea batatas* PPO (Q9ZP19)

- PPO is colored according to hydrophobicity (red, hydrophobic; white, hydrophilic) and shown in cartoon mode.
- * represents gate residue (phenylalanine);
- # represents the covalent cysteine-histidine thioether bond;
- gold spheres represents copper atoms; red sphere represents bound oxygen;
- E represents a highly conserved glutamic acid which is important for substrate deprotonation.
- H_{B1}+1 and H_{B2}+1 represent the residue next to the first histidine coordinated with CuB and the residue next to the second histidine coordinated with CuB, respectively.

Results and discussion

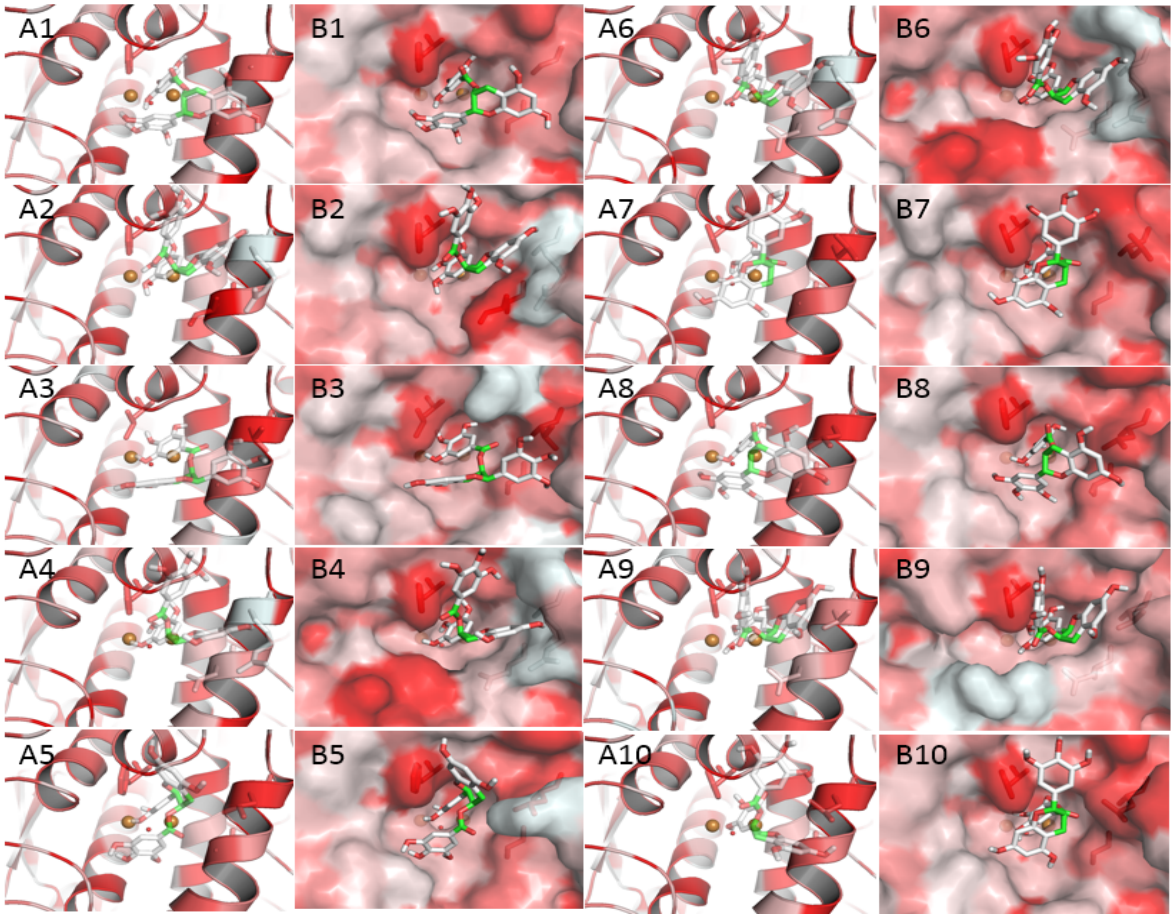


Fig. 3.4.2 Interactions between L-EGCG and best 10 PPOs