植物芥酸合成代谢中关键酶脂肪酸延长酶的结构分析预测

组员：贾艳丽
张雪峰
王会
王杰

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背景及意义

- 芥酸在自然界中存在于十字花科芸薹属植物白芥(Brassica alba)种子脂肪及菜籽油中，含量颇高。芥酸是油菜籽中一种成分，是长链脂肪酸，人不易消化吸收，因此育种的一个目标就是降低菜籽中的芥酸含量，规定1%以下含量的菜籽为低芥酸菜籽，以低芥酸菜籽压榨的油为低芥酸菜籽油.

- 动物实验证明，大量摄入含芥酸高的菜籽油，动物心肌中脂肪积聚，并以甘油三酯的形式存在，可导致心肌纤维化。

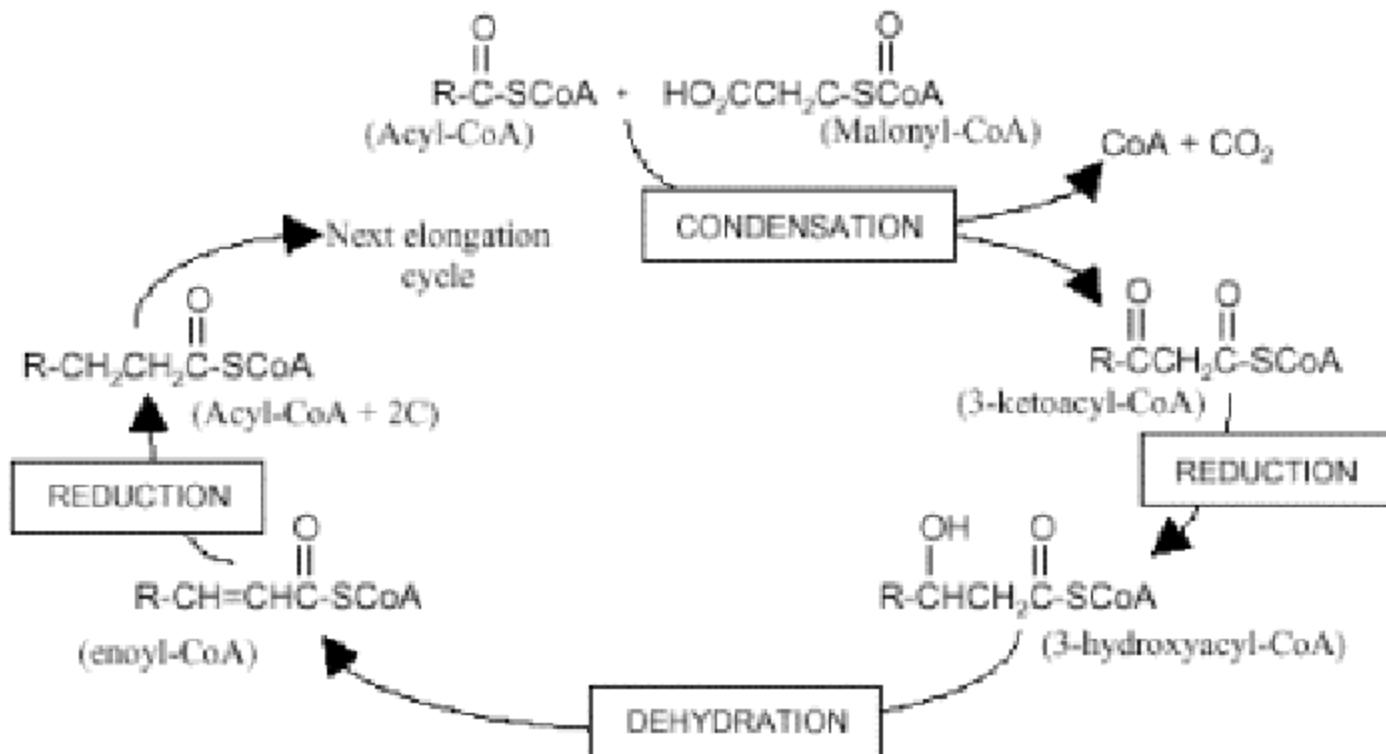- 油菜脂肪酸延长酶基因FAE1是广泛存在于植物中能催化脂肪酸碳链延长的酮脂酰CoA合成酶

Fig. 1 Reactions of fatty acid elongation

本研究拟通过学到的生物信息学知识对油菜脂肪酸延长酶基因**FAE1**进行一些分析，期待对其能有更深入的了解，为本课题组做这方面研究的老师及同学予以借鉴。

方法步骤

- 从Uniprot中得到FAE1基因的蛋白序列
- 在predictProtein中进行二级结构预测
- 用MEGA寻找 FAE1氨基酸保守序列

从Uniprot中得到FAE1基因的蛋白序列

>tr|Q8S3A0|Q8S3A0_BRANA 3-ketoacyl-CoA synthase OS=Brassica napus PE=3
SV=1
MTSINVKLLYHYVITNLFNLCFFPLTAIVAGKAYRLTIDDLHHLYYSYLQHNLITIAPLF
AFTVFGSVLYIATRPKPVYLVEYSCYLPPTHCRSSISKVMDIFYQVRKADPSRNGTCDDS
SWLDFLRKIQERSGLGDETHGPEGLLQVPPRKTFAAAREETEQVIIGALENLFKNTNVNP
KDIGILVVNSSMFNPTPSLSAMVVNTFKLRSNVRSFNLGGMGCSAGVIAIDLAKDLLHVH
KNTYALVVSTENITYNIYAGDNRSMMVSNCLFRVGGAAILLFNKPGDRRRSKYELVHTVR
THAGADDKSFRCVQQGDDENGKIGVSLSKDITDVAGRTVKKNIATLGPLILPLSEKLLFF
VTFMGKKLFKDKIKHYYVPDFKLAIDHFCIHAGGRAVIDVLEKNLALAPIDVEASRSTLH
RFGNTSSSSIWYELAYIEAKGRMKKGNKVWQIALGSGFKCNSAVWVALNNVKASTNSPWE
HCIDRYPVKIDSDSGKSETRAQNGRS

脂肪酸延长酶二级结构分析

- Protein molecular=2687
- Chairs=1
- AA Number=506

在*predictProtein*中进行二级结构预测
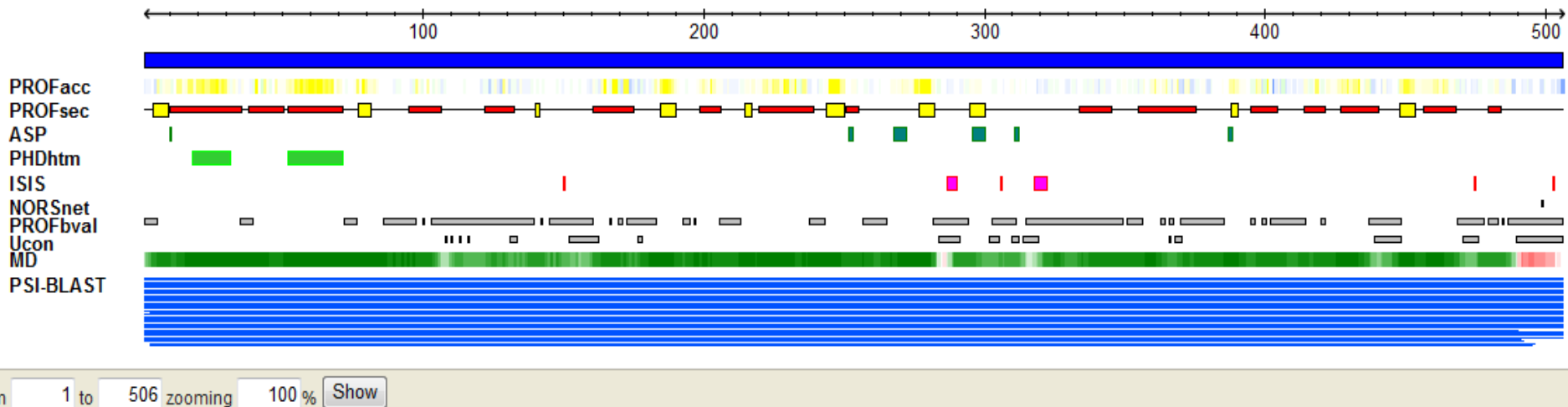
Sequence length	506
Secondary structure	Helix=41.9%, Strand=9.9%, Loop=48.2%

Transmembrane

PHDhtm summary

- **NHTM=2**
  PHDhtm detected 2 membrane helices for the **best** model.The second best model contained 1 helix.
- **TOP=in**
  PHDhtm predicted the topology in, i.e. the first loop region is in (Note: this prediction may be problematic when the sequence you sent starts or ends with a region predicted in a membrane helix!)
- Reliability of best model=1 (0 is low, 9 is high)
- Zscore for best model=0.707
- Difference of positive charges (K+R) inside - outside=-4.500 (the higher the value, the more reliable)
- Reliability of topology prediction =4 (0 is low, 9 is high)
- Details of the strength of each predicted membrane helix:
  (sorted by strength, strongest first)

N HTM	Total score	Best HTM	c-N
1	0.9476	0.8754	54 - 71
2	0.9594	0.6645	16 - 33

用MEGA寻找 FAE1氨基酸保守序列

- ## 方法：

Uniprot中查找FAE1（油菜）的氨基酸序列

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在NCBI的blastp中寻找相似序列

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高相似序列与 FAE1（油菜）在mega中作ClustalW

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找出保守序列

FAE1氨基酸保守序列寻找

结果： 在272-276部位保守性高

结果：在320-329部位保守性高

结果：在498-518部位保守性高

结果：在535-545部位保守性高

#	序列名	序列
1	Q8S3A0_BRANA_Brassica napu	K G N K V W Q I A L G S G F K C N S A V W V A L N N V K A S T N S - - - - - - P W E H C I D R Y P V K I D S D S G K
2	KCS9_ARATH	K G N R V W Q I A F G S G F K C N S A V W V A L N N V K P S V S S - - - - - - P W E H C I D R Y P V K L D F - - - -
3	KCS8_ARATH	E G D R I W Q I A L G S G F K C N S S V W V A L R D V K P S A N S - - - - - - P W E D C M D R Y P V E I D I - - - -
4	KCS7_ARATH	M G D K V W Q I G F G S G F K A N S A V W K C I S E I D S R G R N - - - - - - A W S D R I H L Y P V C G D T S S A L
5	KCS6_ARATH	R G D R V W Q I A F G S G F K C N S A V W K C N R T I K T P K D G - - - - - - P W S D C I D R Y P V F I P E V V K L
6	KCS5_ARATH	R N D R V W Q I A F G S G F K C N S A V W K C N R T I K T P T D G - - - - - - A W S D C I E R Y P V F I P E V V K L
7	KCS4_ARATH	R G N R V W Q I A F G S G F K C N S A I W E A L R H V K P S N N S - - - - - - P W E D C I D K Y P V T L S Y - - - -
8	KCS3_ARATH	R G D R V F M I S F G A G F K C N S C V W E V V R D L N V G E A V G N - - - V W N H C I N Q Y P P K S I L N P F F
9	KCS20_ARATH	K G D R V L Q I A F G S G F K C N S A V W R C I R K V E P N T E N - - - K W L D F I D S Y P V D V P D S T N I
10	KCS2_ARATH	K G N R V W Q I A F G S G F K C N S A V W V A L R N V E P S V N N - - - P W E H C I H R Y P V K I D L - - - -
11	KCS19_ARATH	R G D R T W Q I A F G S G F K C N S A V W K A L R T I D P M D E K - - - T N P W I D E I D D F P V Q V P R I T P I
12	KCS18_ARATH	K G N K A W Q I A L G S G F K C N S A V W V A L R N V K A S A N S - - - - - - P W Q H C I D R Y P V K I D S D L S K
13	KCS17_ARATH	R G D R T W Q I A F G S G F K C N S A V W R A L R T I D P S K E K K K T N P W I D E I H E F P V P V P R T S P V
14	KCS16_ARATH	K G D R I W Q I A L G S G F K C N S S V W V A L R N V K P S T N N - - - - - - P W E Q C L H K Y P V E I D I D L K E
15	KCS15_ARATH	R G D R V W Q I G F G S G F K C N S V V W K A L K N I D P P R H N - - - - - N P W N L - - - - - - - - - -
16	KCS14_ARATH	R G D R V W Q L A F G S G F K C N S I V W R A L R T I P A N E S L V G - - N P W G D S V H K Y P V H V T - - - -
17	KCS13_ARATH	R G D R V W Q L A F G S G F K C N S I V W R A L R T I P A N E S L V G - - N P W G D S V H K Y P V H V T - - - -
18	KCS12_ARATH	R G D R V F M I S F G A G F K C N S C V W E V V R D L T G G E S K G N - - - V W N H C I D D Y P P K S I L N P Y L
19	KCS11_ARATH	K G D R I W Q I A F G S G F K C N S S V W R A V R S V N P K K E K - - - N P W M D E I H E F P V E V P K V S T I
20	KCS10_ARATH	R G D R V W Q I A F G S G F K C N S V V W K A M R K V K K P T R N - - - N P W V D C I N R Y P V P L - - - -
21	KCS1_ARATH	A G D R L W Q I A F G S G F K C N S A V W K A L R P V S T - E E M T G - - N A W A G S I D Q Y P V K V V Q - - - -

结果与讨论

- 推测这些高保守序列与此酶的功能相关
- 该酶存在两个跨膜区段分别位于16-33,54-71，则可推测该酶定位于膜上

致谢

- 感谢罗老师课堂上对我们学习的精心指导
- 感谢农科院及北大给我们提供的宝贵学习机会