

図 2-17 結合したGlcNAcと硫酸イオンの  
 $|F_{obs}| - |F_{calc}|$ 電子密度マップ(3 $\sigma$ )。  
 GlcNAc(-1)は $\beta$ -アノマー型のみ見られる。GlcNAc(+1)は  
 $\alpha$ -アノマーと $\beta$ -アノマーの混在が見られる。

GlcNAc(-1)の $\alpha$ -アノマー側には、GlcNAc複合体構造で  
 はCl<sup>-</sup>、GlcNAc-SO<sub>4</sub>複合体構造では硫酸イオンの結合が  
 見られた。

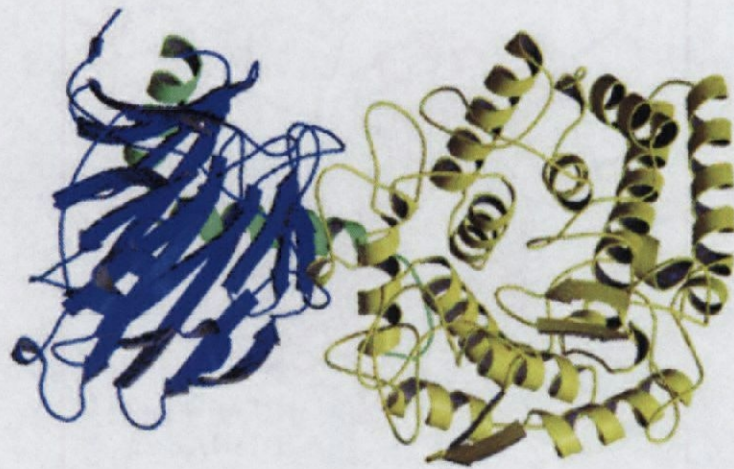
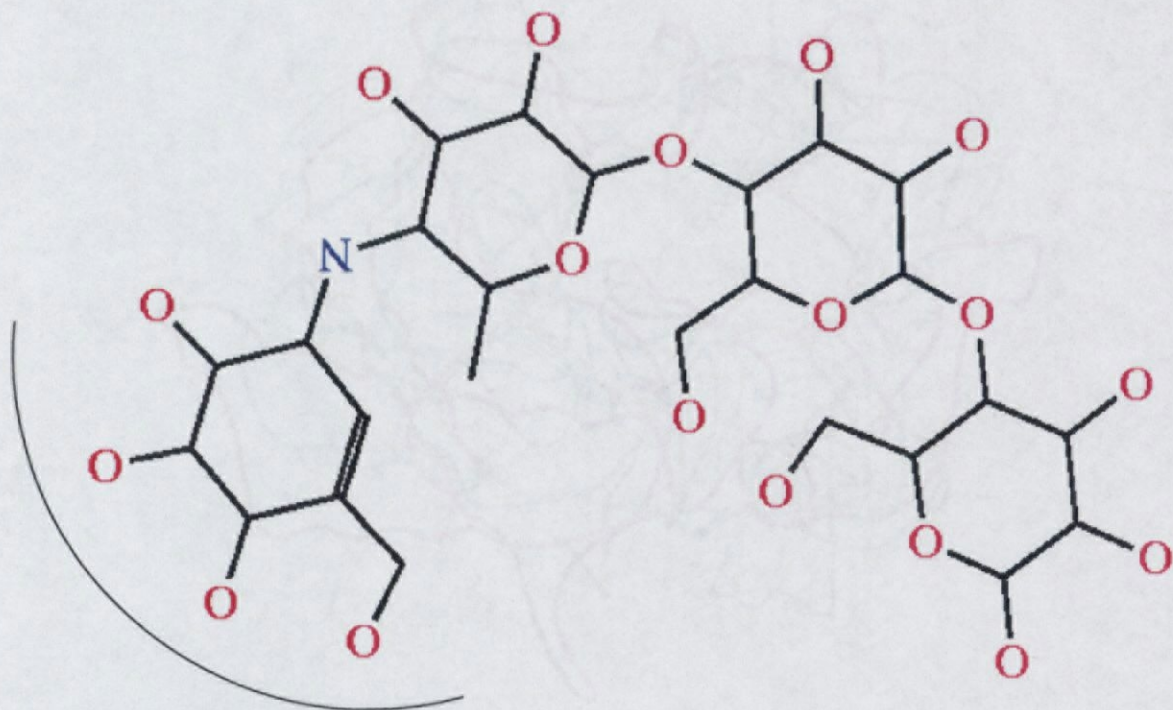


図 2-18a 細菌 *Thermoanaerobacterium thermosaccharolyticum* 由来グルコアミラーゼ (bGA: GH-15)。N末端の  $\beta$ -サンドイッチドメイン、リンカーヘリックス、 $\alpha$ -バレルドメインからなる。



図 2-18b *Lactobacillus brevis* 由来マルトースホスホリラーゼ (MalP: GH-15)。N末端の  $\beta$ -サンドイッチドメイン、リンカーヘリックス、 $\alpha$ -バレルドメイン、C末端の  $\beta$ -シートドメインからなる。



Valienamine基

図 2-19  $\alpha$ -グリコシダーゼの阻害剤アカボースの構造

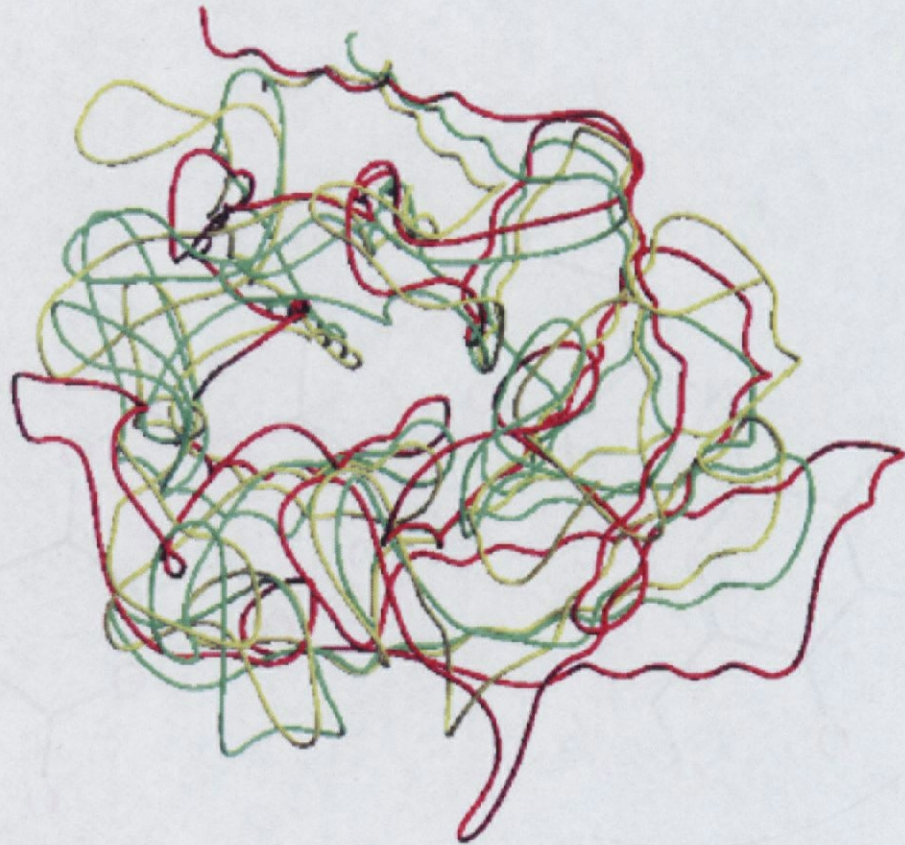
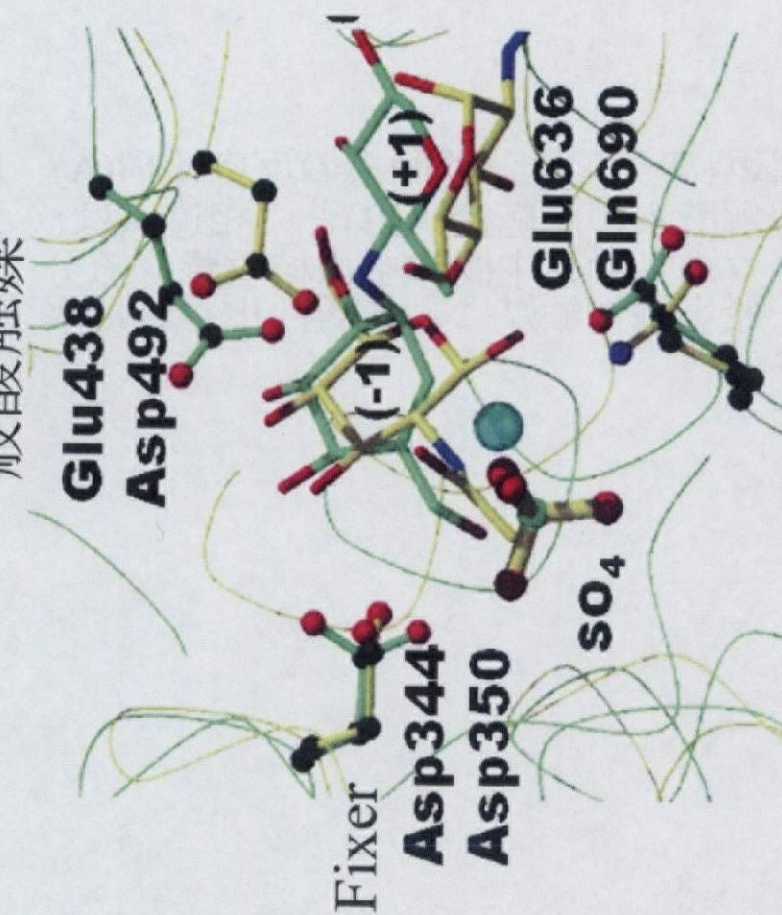


図 2-20 ChBP(黄色:残基番号310-724)、bGA(緑色:残基番号295-684)、MalP(赤色:残基番号316-683)の $\alpha$ -バレルドメインの重ね合わせ。

一般酸触媒



一般塩基性触媒(bGA)

図 2-21a ChBP と bGA の活性中心部位の重ね合わせ。残基番号は bGA/ChBP の順番。

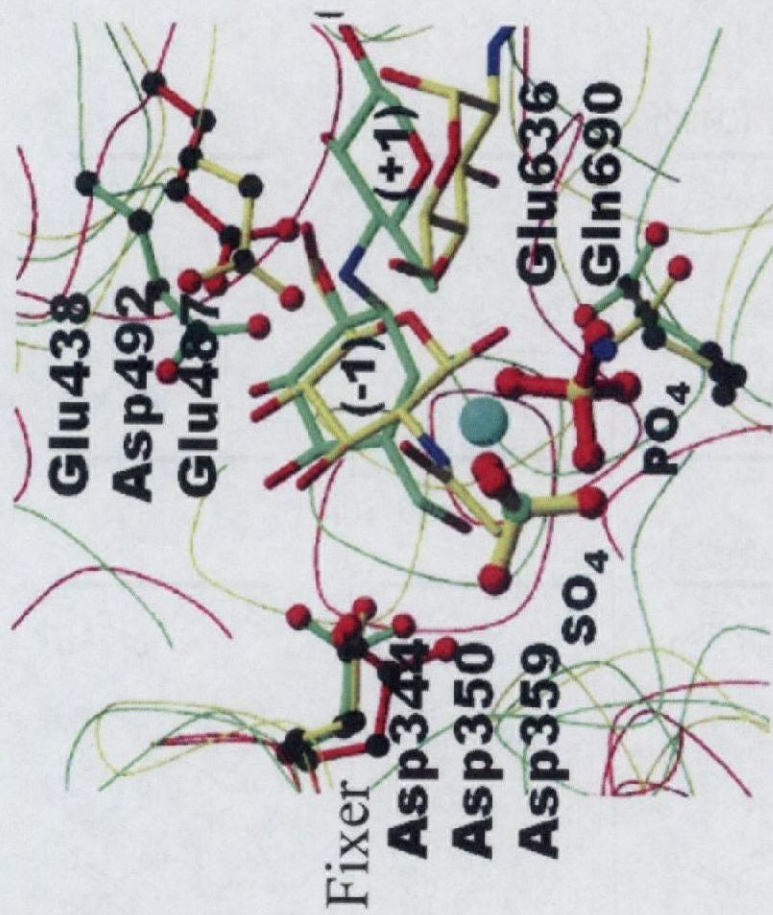


図 2-21b ChBP、bGA、MalP の活性中心部位の重ね合わせ。残基番号は bGA/ChBP/MalP の順番。bGA の Glu636、ChBP の Gln690 に相当する残基は MalP には見られない。

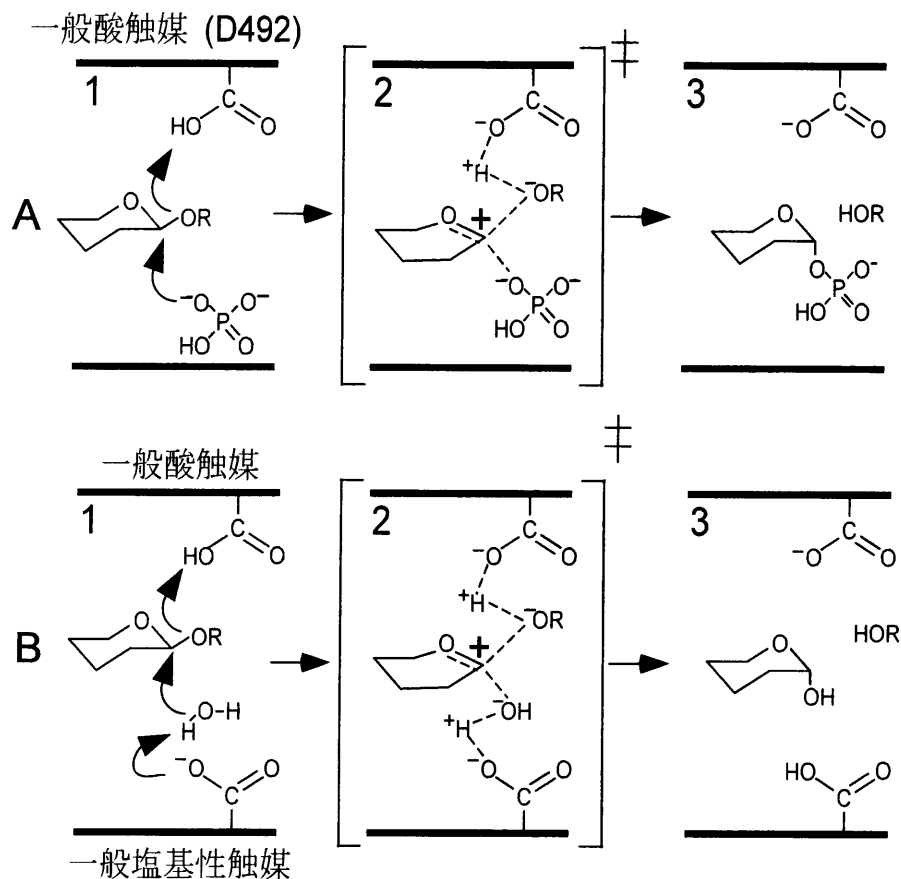


図 2-22 反転型加リン酸分解酵素の反応機構(A)。反転型加水分解酵素の反応機構(B)との相違点は、オキソカルボニウムイオン中間体を求核攻撃する分子がリン酸、一般塩基性触媒により活性化された水分子の違いのみ。

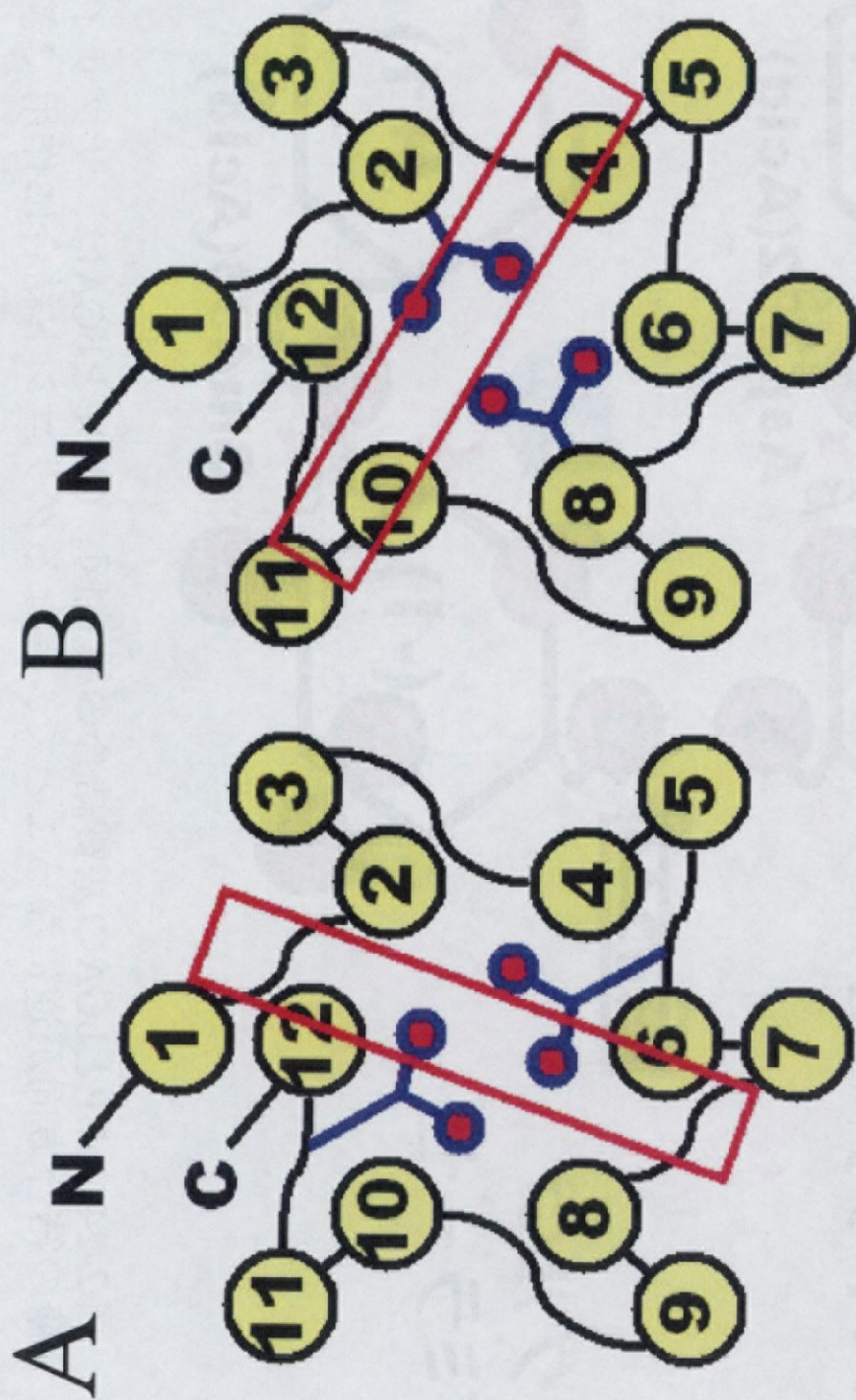


図 2-23 Clan GH-L と GH-M のトポロジ。Clan GH-L は  $\alpha$ -グリコシド結合に作用する GH-15、GH-65。Clan GH-M は  $\beta$ -グリコシド結合に作用する GH-8、GH-18 が分類される。Clan GH-L (A の図) は  $\alpha$ -ヘリックス 5-6、11-12 間に触媒残基がある。Clan GH-M (B の図) は  $\alpha$ -ヘリックス 2、8 に触媒残基がある。また、基質の結合方向 (赤色の四角で表した) も異なる。このように、 $\alpha$ -グリコシド結合に作用する酵素と  $\beta$ -グリコシド結合に作用する酵素は異なる構造のトポロジをとる。しかし  $\beta$ -グリコシド結合に作用する ChBP は Clan GH-L と同様のトポロジを持つ。

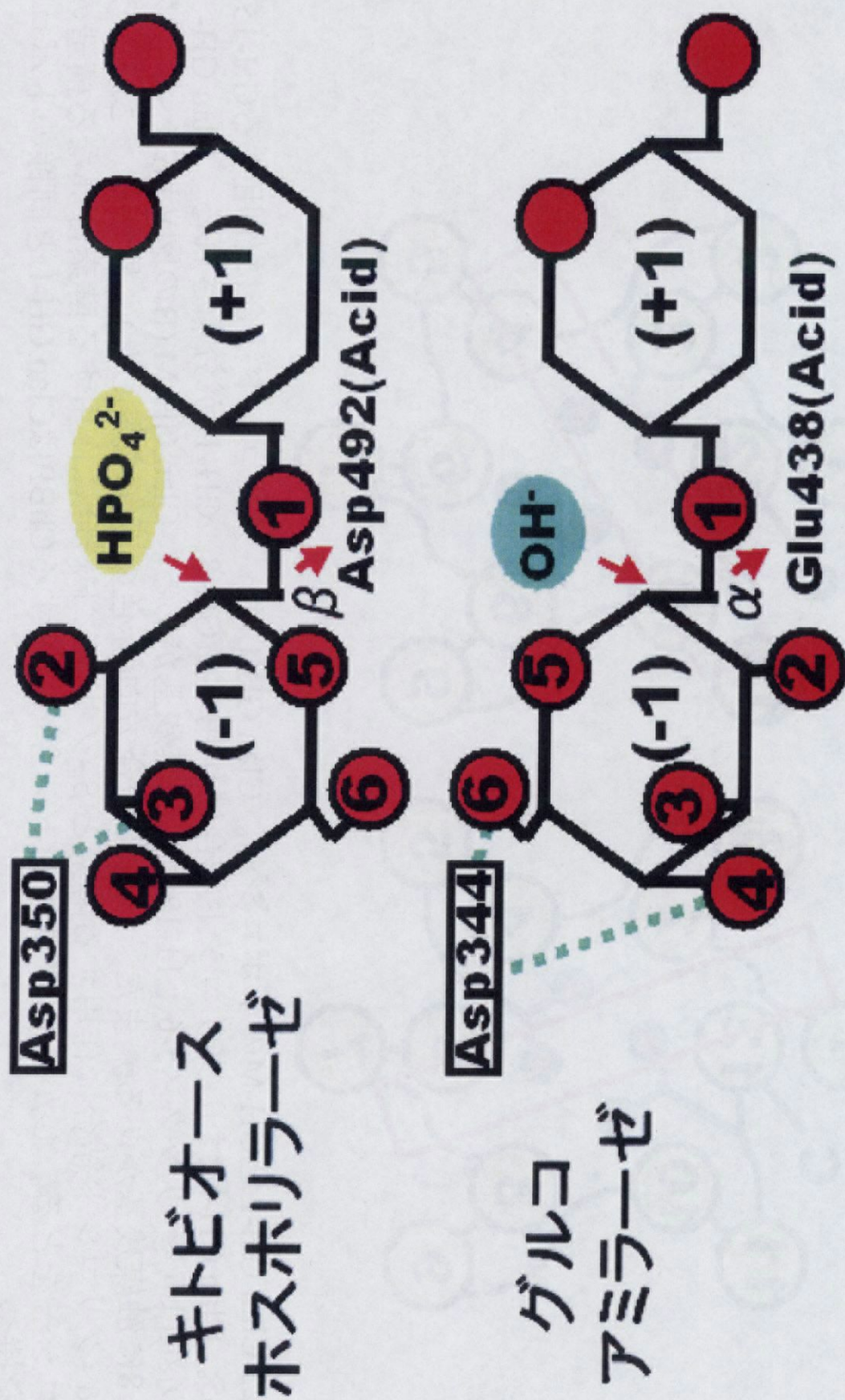


図2-24 ChBPとbGAの基質結合の模式図。ChBPとbGAは、サブサイト(-1)の糖の結合方向が逆になることで、異なるグリコシド結合に作用できる。



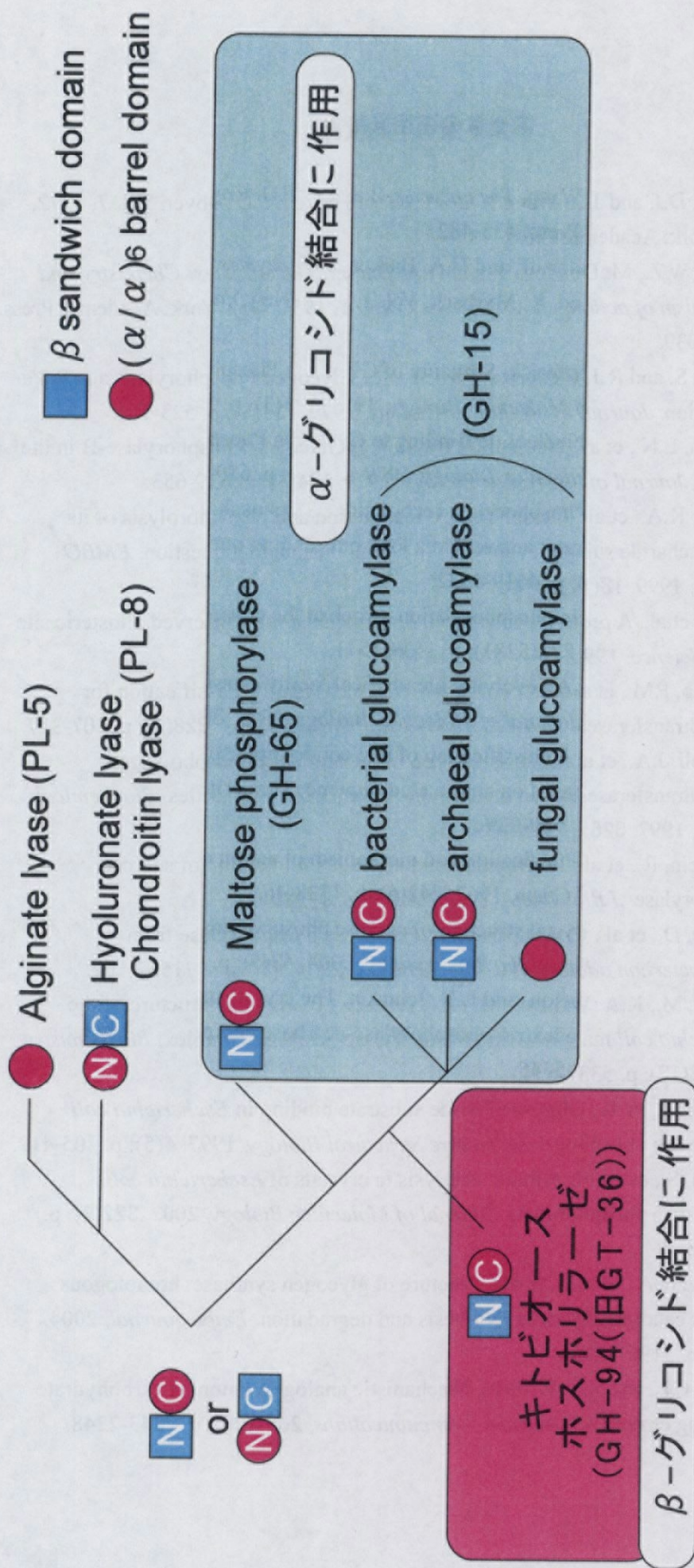


図 2-25  $(\alpha/\alpha)_6$ バレルフォールドの分子進化モデル。  
 Aleshin[29]により提唱されている進化モデルにChBPを加えた

## 第 2 章の引用文献

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