

Supplementary Materials: Bioactivation and Regioselectivity of Pig Cytochrome P450 3A29 towards Aflatoxin B₁

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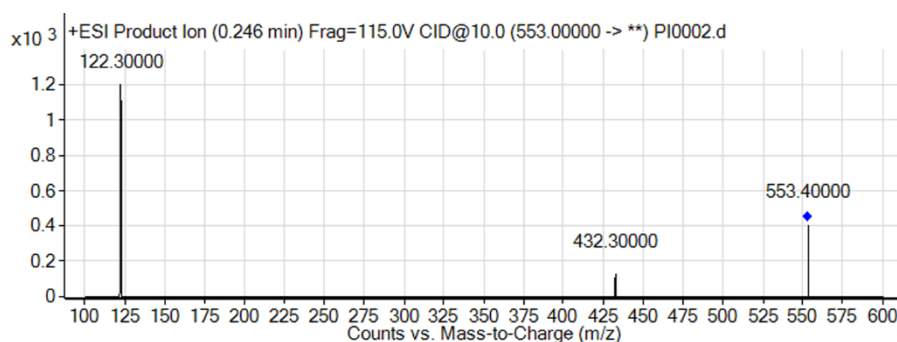


Figure S1. The identification of metabolite by LC-MS/MS.

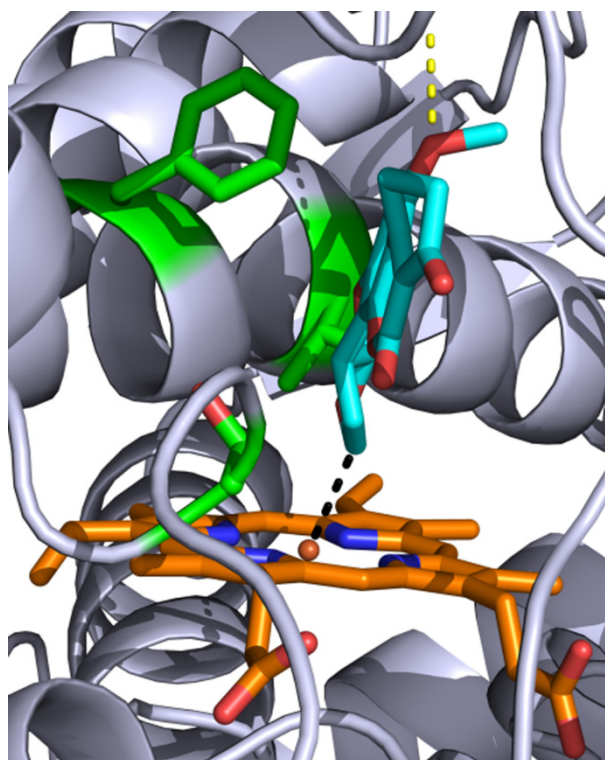


Figure S2. The side view of docking model.

Table S1. The relative quantification of metabolic activities of CYP3A29 and its mutants to AFB₁.

| Enzymes | Dihydrodiol-Tris | AFG ₁ | Dihydrodiol-Tris/AFG ₁ | Normalized Values * |
|---------|------------------|------------------|-----------------------------------|---------------------|
| WT1 | 1,775,720 | 19,910,728 | 0.089 | - |
| WT2 | 1,970,378 | 20,402,016 | 0.097 | - |
| WT3 | 1,600,007 | 18,956,344 | 0.084 | 1.00 (0.090) |
| S119A1 | 403,518 | 21,918,143 | 0.018 | - |
| S119A2 | 1,319,961 | 19,772,791 | 0.067 | - |
| S119A3 | 504,333 | 12,758,786 | 0.040 | 0.46 (0.042) |
| F304A1 | 3,506,055 | 15,406,563 | 0.23 | - |
| F304A2 | 4,335,512 | 19,841,307 | 0.22 | - |
| F304A3 | 3,913,793 | 18,719,767 | 0.21 | 2.42 (0.22) |
| T309A1 | 120,478 | 5,361,935 | 0.022 | - |
| T309A2 | 467,321 | 20,436,934 | 0.023 | - |
| T309A3 | 456,039 | 20,808,153 | 0.022 | 0.25 (0.0224) |

* The values in brackets represent the average of three repeats.