Supplementary File of "AutoDock Koto: A Gradient Boosting Differential Evolution for Molecule Docking"

A. Conversion between quaternions and three angles

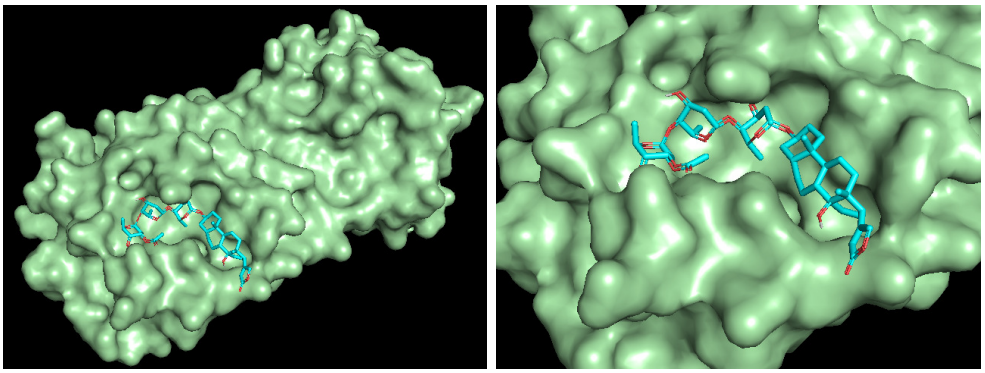
The conversion between quaternions and three angles is presented below. Given θ, α and β, the corresponding quaternion $\mathbf{q} = a + b\mathbf{i} + c\mathbf{j} + d\mathbf{k}$ can be calculated as follow:

$$\begin{aligned} a &= \cos\frac{\theta}{2}, \\ b &= \cos\beta\sin\alpha\cdot\sin\frac{\theta}{2}, \\ c &= \sin\beta\sin\alpha\cdot\sin\frac{\theta}{2}, \\ d &= \cos\alpha\cdot\sin\frac{\theta}{2}. \end{aligned} \tag{1}$$

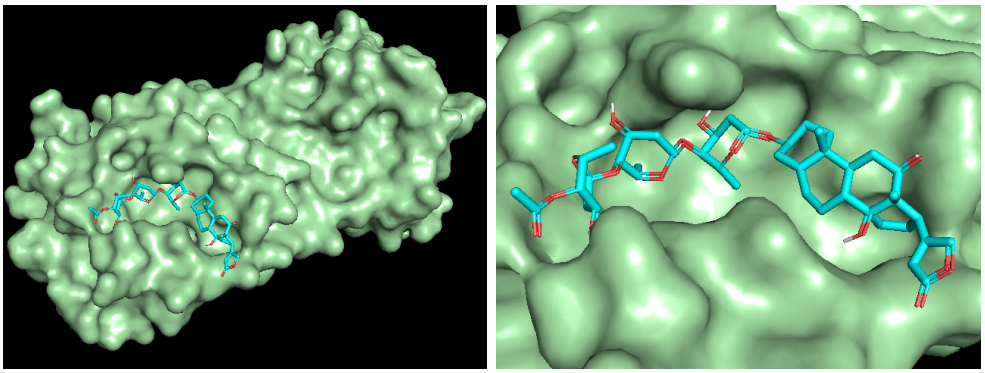
If a unit quaternion $\mathbf{q} = a + b\mathbf{i} + c\mathbf{j} + d\mathbf{k}$ is given, the corresponding angles are calculated by:

$$\begin{aligned} &\theta = 2\arccos a, \\ &\alpha = \arccos\frac{d}{\sin\frac{\theta}{2}}, \\ &\beta = \begin{cases} \arccos\frac{b}{\sin\frac{\theta}{2}\cdot\sin\alpha}, & \text{if } \frac{c}{\sin\frac{\theta}{2}\cdot\sin\alpha} > 0; \\ 2\pi - \arccos\frac{b}{\sin\frac{\theta}{2}\cdot\sin\alpha}, & \text{otherwise .} \end{cases} \end{aligned} \tag{2}$$

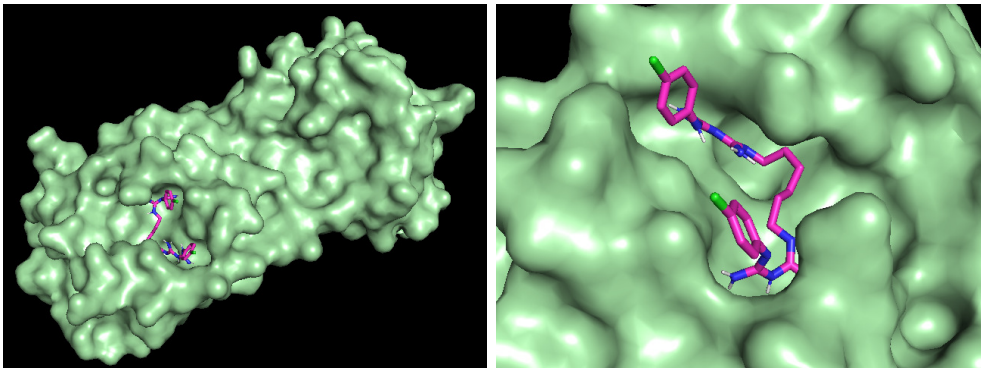
B. Supplementary Figures



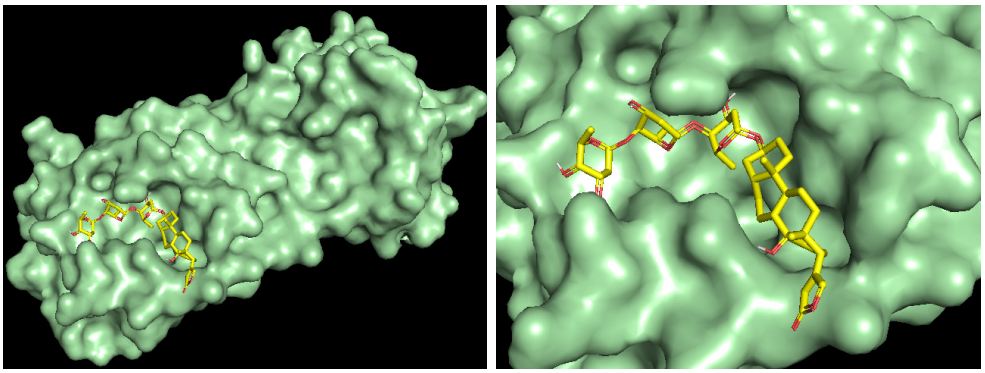
(a) Nilotinib



(b) Ergotamine

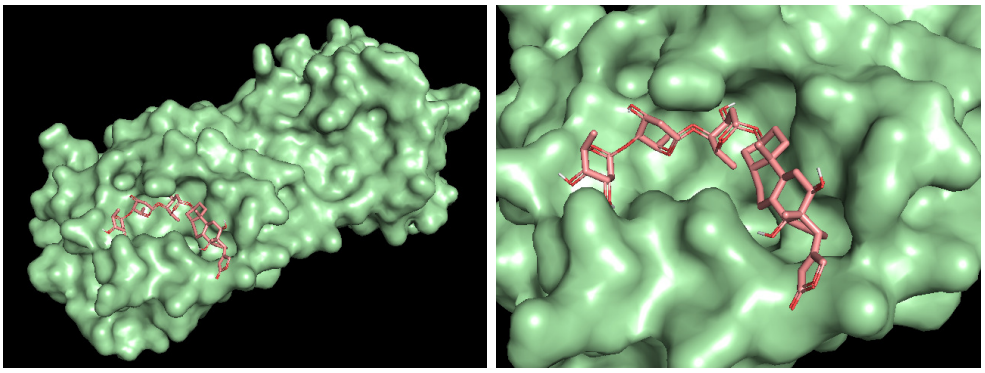


(c) Tirilazad

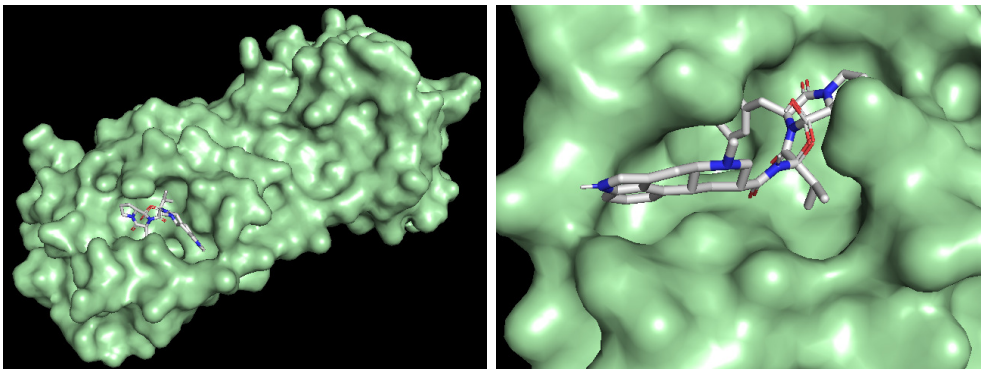


(d) Dihydroergotamine

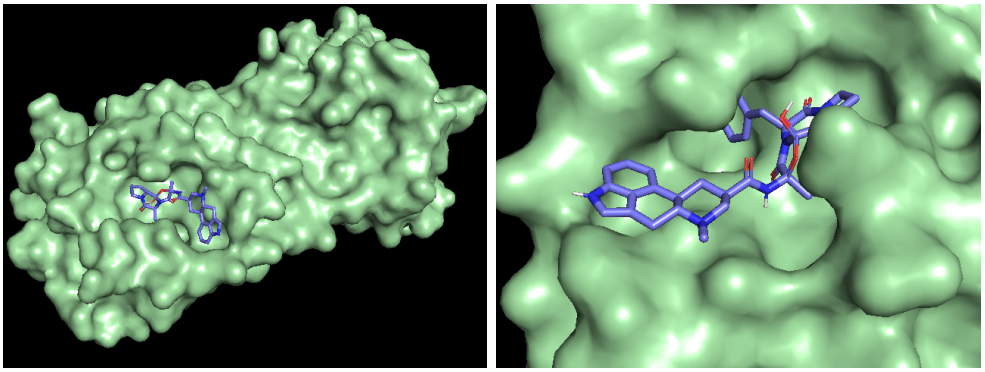
Fig.S. 1. Computational determined binding modes of nilotinib, ergotamine, tirilazad and dihydroergotamine predicted with AutoDock Koto. Surface of SARS-CoV-2 M^{pro} is given in green.



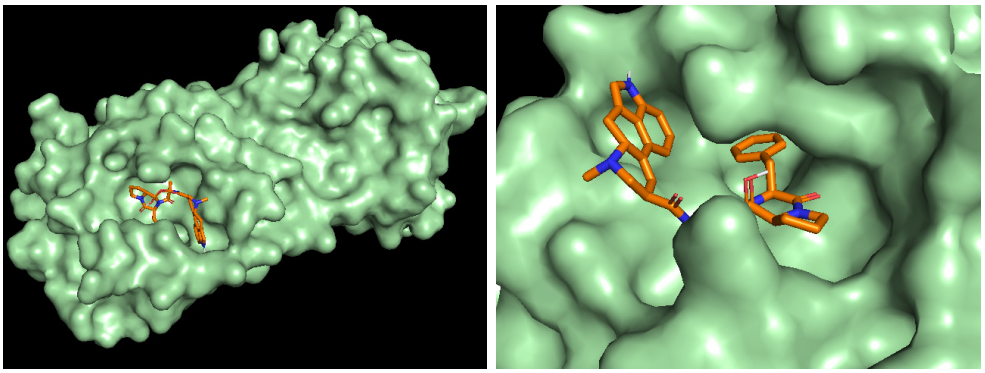
(a) Guamecycline



(b) Glecaprevir

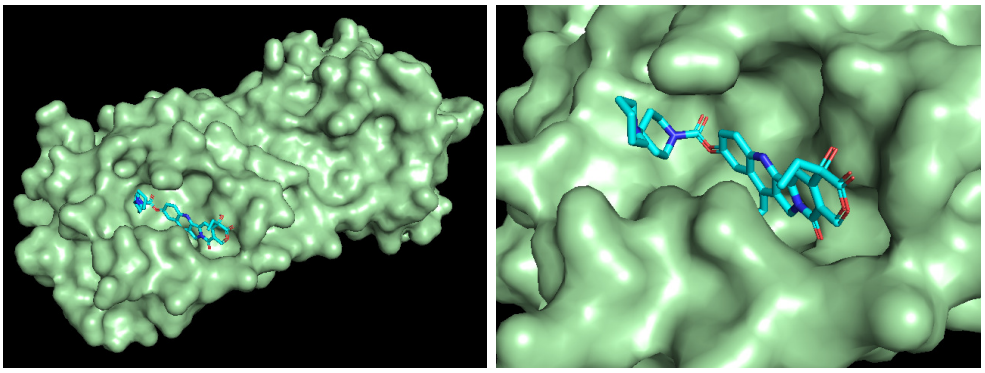


(c) Radotinib

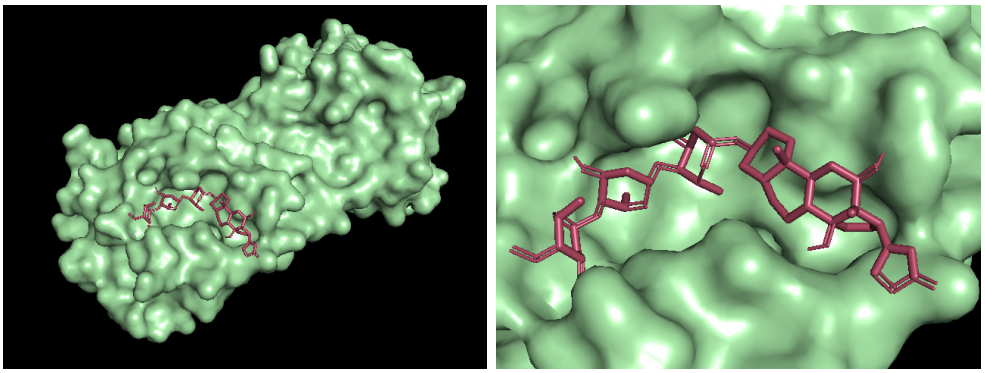


(d) Dihydroergocristine

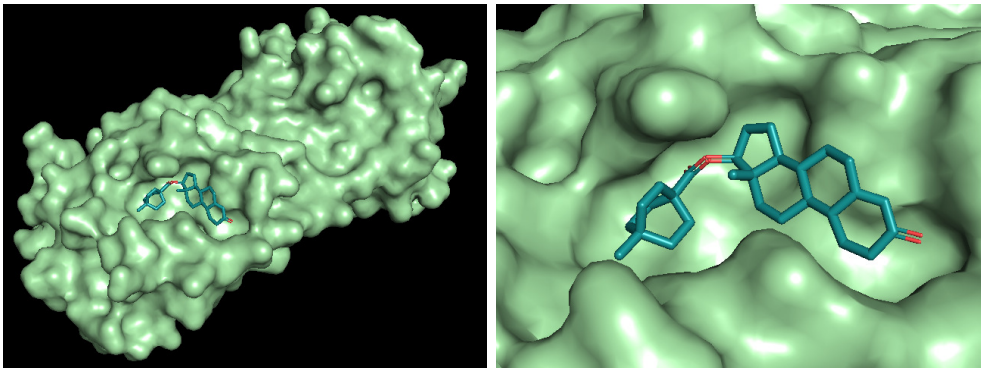
Fig.S. 2. Computational determined binding modes of guamecycline, glecaprevir, radotinib and dihydroergocristine predicted with AutoDock Koto. Surface of SARS-CoV-2 M^{pro} is given in green.



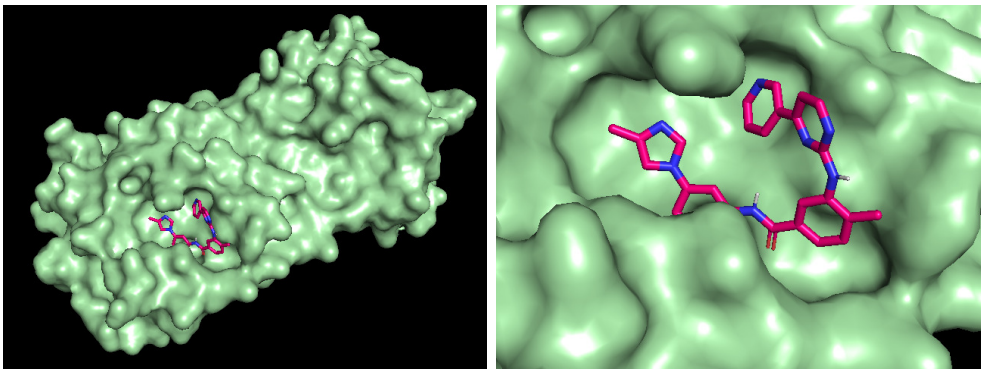
(a) Digitoxin



(b) Chlorhexidine

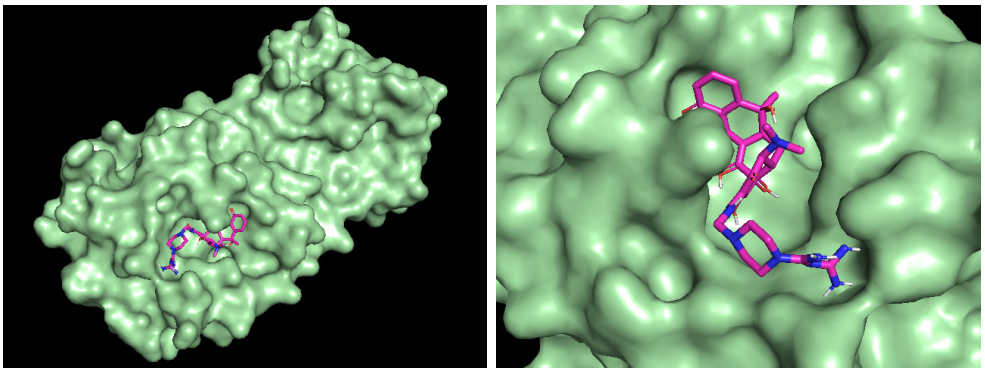


(c) Acetyldigitoxin

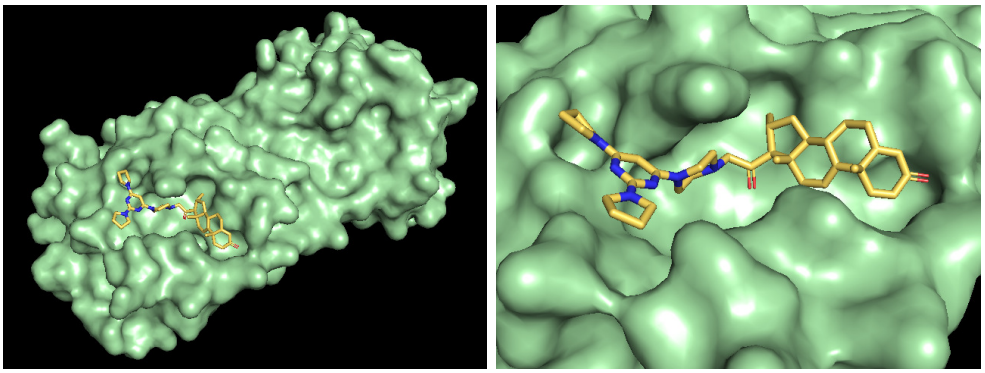


(d) Digoxin

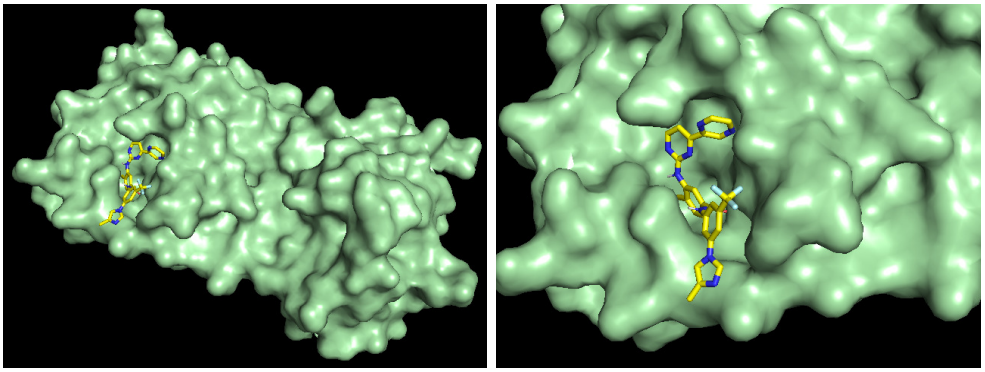
Fig.S. 3. Computational determined binding modes of digitoxin, chlorhexidine, acetyldigitoxin and digoxin predicted with AutoDock Koto. Surface of SARS-CoV-2 M^{pro} is given in green.



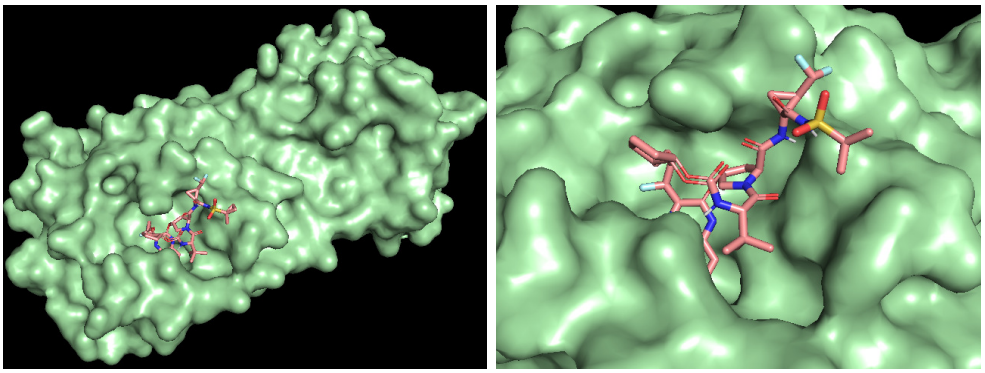
(a) Metildigoxin



(b) Acetyldigoxin



(c) Irinotecan



(d) Nandrolone cyclotate

Fig.S. 4. Computational determined binding modes of metildigoxin, acetyldigoxin, irinotecan and nandrolone cyclotate predicted with AutoDock Koto. Surface of SARS-CoV-2 M^{pro} is given in green.