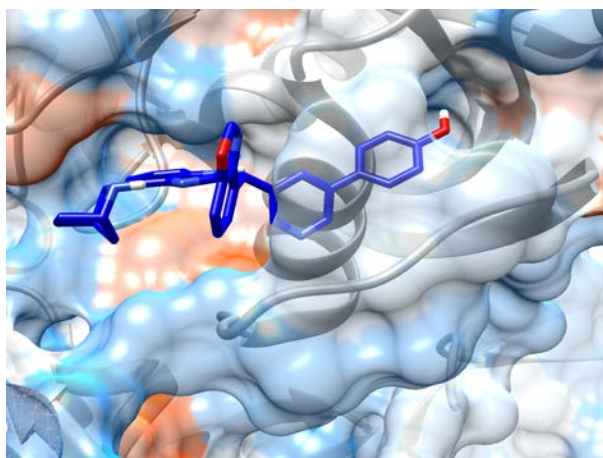
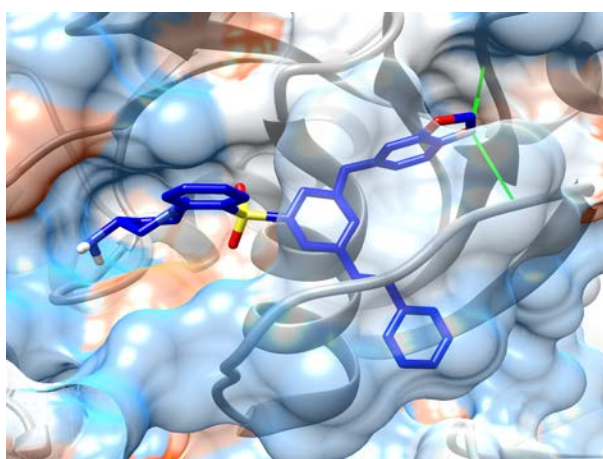


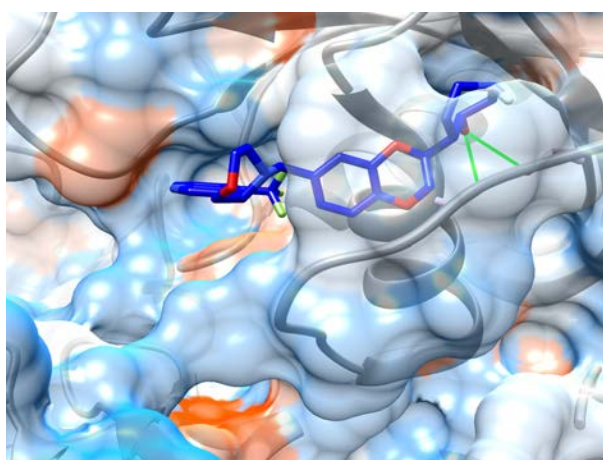
## Supplementary Materials



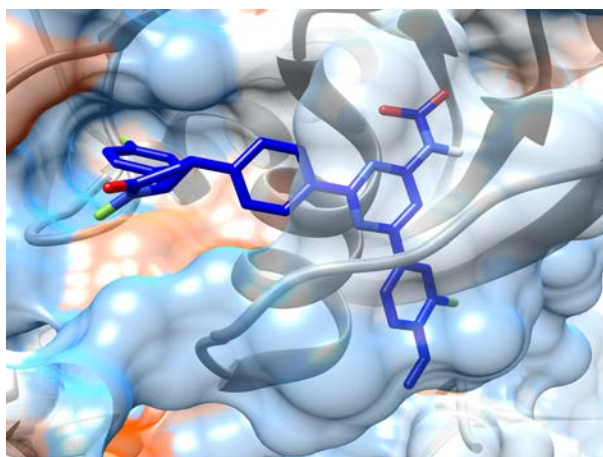
**Figure S1.** Visualization of the first candidate molecule binding into specific pocket in chain A of K-Ras.



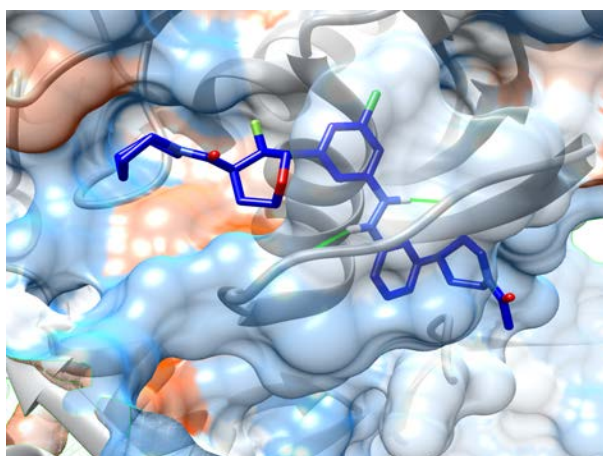
**Figure S2.** Visualization of the second candidate molecule binding into specific pocket in chain A of K-Ras. Hydrogen bonds are highlighted by green lines.



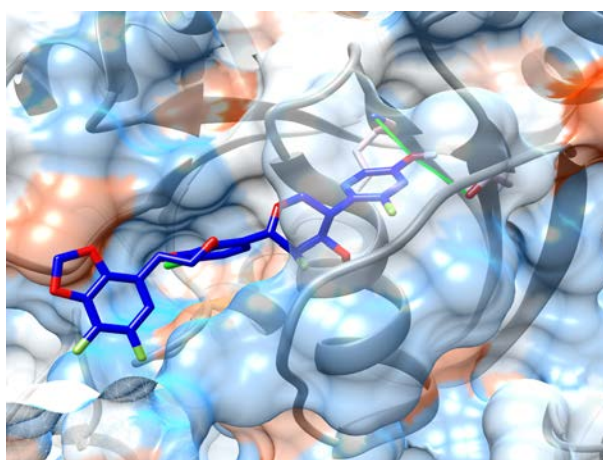
**Figure S3.** Visualization of the third candidate molecule binding into specific pocket in chain A of K-Ras. Hydrogen bonds are highlighted by green lines.



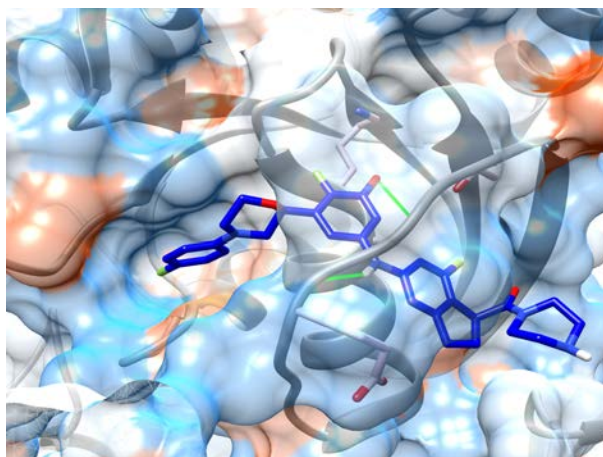
**Figure S4.** Visualization of the fourth candidate molecule binding into specific pocket in chain A of K-Ras. Hydrogen bonds are highlighted by green lines.



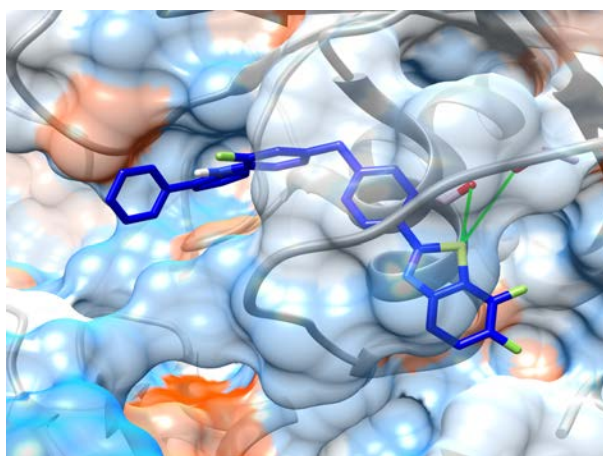
**Figure S5.** Visualization of the fifth candidate molecule binding into specific pocket in chain A of K-Ras. Hydrogen bonds are highlighted by green lines.



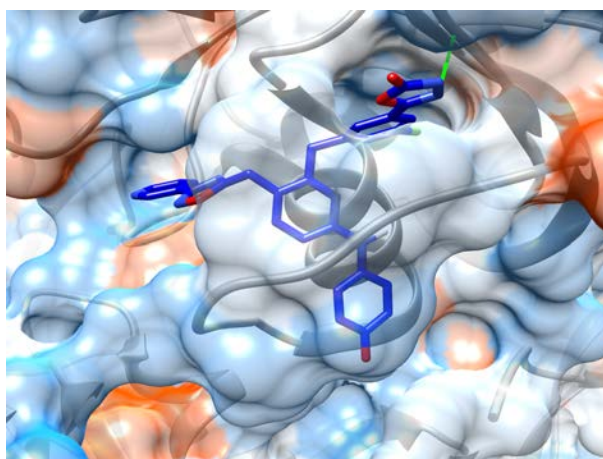
**Figure S6.** Visualization of the sixth candidate molecule binding into specific pocket in chain A of K-Ras. Hydrogen bonds are highlighted by green lines.



**Figure S7.** Visualization of the seventh candidate molecule binding into specific pocket in chain A of K-Ras. Hydrogen bonds are highlighted by green lines.

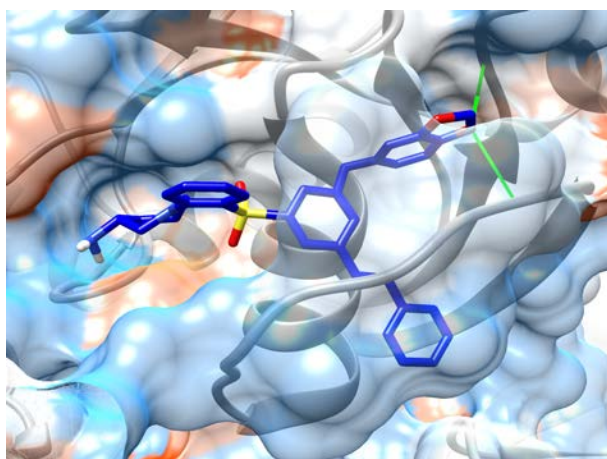


**Figure S8.** Visualization of the eighth candidate molecule binding into specific pocket in chain A of K-Ras. Hydrogen bonds are highlighted by green lines.



**Figure S9.** Visualization of the ninth candidate molecule binding into specific pocket in chain A of K-Ras. Hydrogen bonds are highlighted by green lines.





**Figure S10.** Visualization of the tenth candidate molecule binding into specific pocket in chain A of K-Ras. Hydrogen bonds are highlighted by green lines.