Figure S1. The binding mode of aspirin to the protein Exosome complex component RRP40 (EXOSC3). The overview and close-up view of the binding mode of aspirin to EXOSC3 were shown in the top and bottom panels, respectively. Secondary structural elements were colored from blue (N-terminus) to red (C-terminus). The compound aspirin is colored with green. The residues lying within 5 Å from atoms of the aspirin are shown as sticks. The H-bonds are shown by dashed yellow line.
Figure S2. The binding mode of aspirin to the protein Mitogen-activated protein kinase 12 (MAPK12). The overview and close-up view of the binding mode of aspirin to MAPK12 were shown in the top and bottom panels, respectively. Secondary structural elements were colored from blue (N-terminus) to red (C-terminus). The compound aspirin is colored with green. The residues lying within 5 Å from atoms of the aspirin are shown as sticks. The H-bonds are shown by dashed yellow line.
Figure S3. The binding mode of aspirin to the protein Integrin alpha-L (ITGAL). The overview and close-up view of the binding mode of aspirin to ITGAL were shown in the top and bottom panels, respectively. Secondary structural elements were colored from blue (N-terminus) to red (C-terminus). The compound aspirin is colored with green. The residues lying within 5 Å from atoms of the aspirin are shown as sticks. The H-bonds are shown by dashed yellow line.
Figure S4. The binding mode of aspirin to the protein Prostaglandin G/H synthase 2 (PTGS2). The overview and close-up view of the binding mode of aspirin to PTGS2 were shown in the top and bottom panels, respectively. Secondary structural elements were colored from blue (N-terminus) to red (C-terminus). The compound aspirin is colored with green. The residues lying within 5 Å from atoms of the aspirin are shown as sticks. The H-bonds are shown by dashed yellow line.
Figure S5. The binding mode of aspirin to the protein Prostaglandin G/H synthase 1 (PTGS1). The overview and close-up view of the binding mode of aspirin to PTGS1 were shown in the top and bottom panels, respectively. Secondary structural elements were colored from blue (N-terminus) to red (C-terminus). The compound aspirin is colored with green. The residues lying within 5 Å from atoms of the aspirin are shown as sticks. The H-bonds are shown by dashed yellow line.
**Figure S6.** The binding mode of aspirin to the protein Group X Secretory Phospholipase A2 (PLA2G10). The overview and close-up view of the binding mode of aspirin to PLA2G10 were shown in the top and bottom panels, respectively. Secondary structural elements were colored from blue (N-terminus) to red (C-terminus). The compound aspirin is colored with green. The residues lying within 5 Å from atoms of the aspirin are shown as sticks. The H-bonds are shown by dashed yellow line.
**Figure S7.** The binding mode of aspirin to the protein Fructose-1,6-bisphosphatase 1 (FBP1). The overview and close-up view of the binding mode of aspirin to FBP1 were shown in the top and bottom panels, respectively. Secondary structural elements were colored from blue (N-terminus) to red (C-terminus). The compound aspirin is colored with green. The residues lying within 5 Å from atoms of the aspirin are shown as sticks. The H-bonds are shown by dashed yellow line.
Figure S8. The binding mode of aspirin to the protein Cullin-4B (CUL4B). The overview and close-up view of the binding mode of aspirin to CUL4B were shown in the top and bottom panels, respectively. Secondary structural elements were colored from blue (N-terminus) to red (C-terminus). The compound aspirin is colored with green. The residues lying within 5 Å from atoms of the aspirin are shown as sticks. The H-bonds are shown by dashed yellow line.
Figure S9. The binding mode of aspirin to the protein Macrophage metalloelastase (MMP12). The overview and close-up view of the binding mode of aspirin to MMP12 were shown in the top and bottom panels, respectively. Secondary structural elements were colored from blue (N-terminus) to red (C-terminus). The compound aspirin is colored with green. The residues lying within 5 Å from atoms of the aspirin are shown as sticks. The H-bonds are shown by dashed yellow line.
Figure S10. The binding mode of aspirin to the protein Cyclin-dependent kinase 13 (CDK13). The overview and close-up view of the binding mode of aspirin to CDK13 were shown in the top and bottom panels, respectively. Secondary structural elements were colored from blue (N-terminus) to red (C-terminus). The compound aspirin is colored with green. The residues lying within 5 Å from atoms of the aspirin are shown as sticks. The H-bonds are shown by dashed yellow line.
Figure S11. The binding mode of aspirin to the protein Tumor necrosis factor-inducible protein TSG-6 (TNFAIP6). The overview and close-up view of the binding mode of aspirin to TNFAIP6 were shown in the top and bottom panels, respectively. Secondary structural elements were colored from blue (N-terminus) to red (C-terminus). The compound aspirin is colored with green. The residues lying within 5 Å from atoms of the aspirin are shown as sticks. The H-bonds are shown by dashed yellow line.
Figure S12. The binding mode of aspirin to the protein Group 3 secretory phospholipase A2 (PLA2G3). The overview and close-up view of the binding mode of aspirin to PLA2G3 were shown in the top and bottom panels, respectively. Secondary structural elements were colored from blue (N-terminus) to red (C-terminus). The compound aspirin is colored with green. The residues lying within 5 Å from atoms of the aspirin are shown as sticks. The H-bonds are shown by dashed yellow line.
Figure S13. The binding mode of aspirin to the protein MHC class I antigen (HLA-A). The overview and close-up view of the binding mode of aspirin to HLA-A were shown in the top and bottom panels, respectively. Secondary structural elements were colored from blue (N-terminus) to red (C-terminus). The compound aspirin is colored with green. The residues lying within 5 Å from atoms of the aspirin are shown as sticks. The H-bonds are shown by dashed yellow line.
Figure S14. The binding mode of aspirin to the protein Adenylyltransferase and sulfurtransferase MOCS3 (MOCS3). The overview and close-up view of the binding mode of aspirin to MOCS3 were shown in the top and bottom panels, respectively. Secondary structural elements were colored from blue (N-terminus) to red (C-terminus). The compound aspirin is colored with green. The residues lying within 5 Å from atoms of the aspirin are shown as sticks. The H-bonds are shown by dashed yellow line.
**Figure S15.** The binding mode of aspirin to the protein Axin interactor-dorsalization-associated protein (AIDA). The overview and close-up view of the binding mode of aspirin to AIDA were shown in the top and bottom panels, respectively. Secondary structural elements were colored from blue (N-terminus) to red (C-terminus). The compound aspirin is colored with green. The residues lying within 5 Å from atoms of the aspirin are shown as sticks. The H-bonds are shown by dashed yellow line.
Figure S16. The binding mode of aspirin to the protein ras-related C3 botulinum toxin substrate 1 isoform Rac1b (RAC1). The overview and close-up view of the binding mode of aspirin to RAC1 were shown in the top and bottom panels, respectively. Secondary structural elements were colored from blue (N-terminus) to red (C-terminus). The compound aspirin is colored with green. The residues lying within 5 Å from atoms of the aspirin are shown as sticks. The H-bonds are shown by dashed yellow line.
Figure S17. The binding mode of aspirin to the protein Calcium-dependent phospholipase A2 (PLA2G5). The overview and close-up view of the binding mode of aspirin to PLA2G5 were shown in the top and bottom panels, respectively. Secondary structural elements were colored from blue (N-terminus) to red (C-terminus). The compound aspirin is colored with green. The residues lying within 5 Å from atoms of the aspirin are shown as sticks. The H-bonds are shown by dashed yellow line.
Figure S18. The binding mode of aspirin to the protein Phospholipase A2 (PLA2G1B). The overview and close-up view of the binding mode of aspirin to PLA2G1B were shown in the top and bottom panels, respectively. Secondary structural elements were colored from blue (N-terminus) to red (C-terminus). The compound aspirin is colored with green. The residues lying within 5 Å from atoms of the aspirin are shown as sticks. The H-bonds are shown by dashed yellow line.
Figure S19. The binding mode of aspirin to the protein Phospholipase A2, membrane associated (PLA2G2A). The overview and close-up view of the binding mode of aspirin to PLA2G2A were shown in the top and bottom panels, respectively. Secondary structural elements were colored from blue (N-terminus) to red (C-terminus). The compound aspirin is colored with green. The residues lying within 5 Å from atoms of the aspirin are shown as sticks. The H-bonds are shown by dashed yellow line.
Figure S20. The binding mode of aspirin to the protein Tumor necrosis factor ligand superfamily member 14 (TNFSF14). The overview and close-up view of the binding mode of aspirin to TNFSF14 were shown in the top and bottom panels, respectively. Secondary structural elements were colored from blue (N-terminus) to red (C-terminus). The compound aspirin is colored with green. The residues lying within 5 Å from atoms of the aspirin are shown as sticks. The H-bonds are shown by dashed yellow line.
Figure S21. The binding mode of aspirin to the protein Pikachurin (EGFLAM). The overview and close-up view of the binding mode of aspirin to EGFLAM were shown in the top and bottom panels, respectively. Secondary structural elements were colored from blue (N-terminus) to red (C-terminus). The compound aspirin is colored with green. The residues lying within 5 Å from atoms of the aspirin are shown as sticks. The H-bonds are shown by dashed yellow line.
Figure S22. The binding mode of aspirin to the protein Group IID secretory phospholipase A2 (PLA2G2D). The overview and close-up view of the binding mode of aspirin to PLA2G2D were shown in the top and bottom panels, respectively. Secondary structural elements were colored from blue (N-terminus) to red (C-terminus). The compound aspirin is colored with green. The residues lying within 5 Å from atoms of the aspirin are shown as sticks. The H-bonds are shown by dashed yellow line.
**Figure S23.** The binding mode of aspirin to the protein Chitotriosidase-1 (CHIT1). The overview and close-up view of the binding mode of aspirin to CHIT1 were shown in the top and bottom panels, respectively. Secondary structural elements were colored from blue (N-terminus) to red (C-terminus). The compound aspirin is colored with green. The residues lying within 5 Å from atoms of the aspirin are shown as sticks. The H-bonds are shown by dashed yellow line.
Figure S24. The statistic of 23 putative binding pockets of aspirin. A) The size of the 22 binding pockets of aspirin. B) The frequency of residues in all binding pockets of aspirin. C) The frequency of residues involved in formation of H-bond in all binding pockets of aspirin.