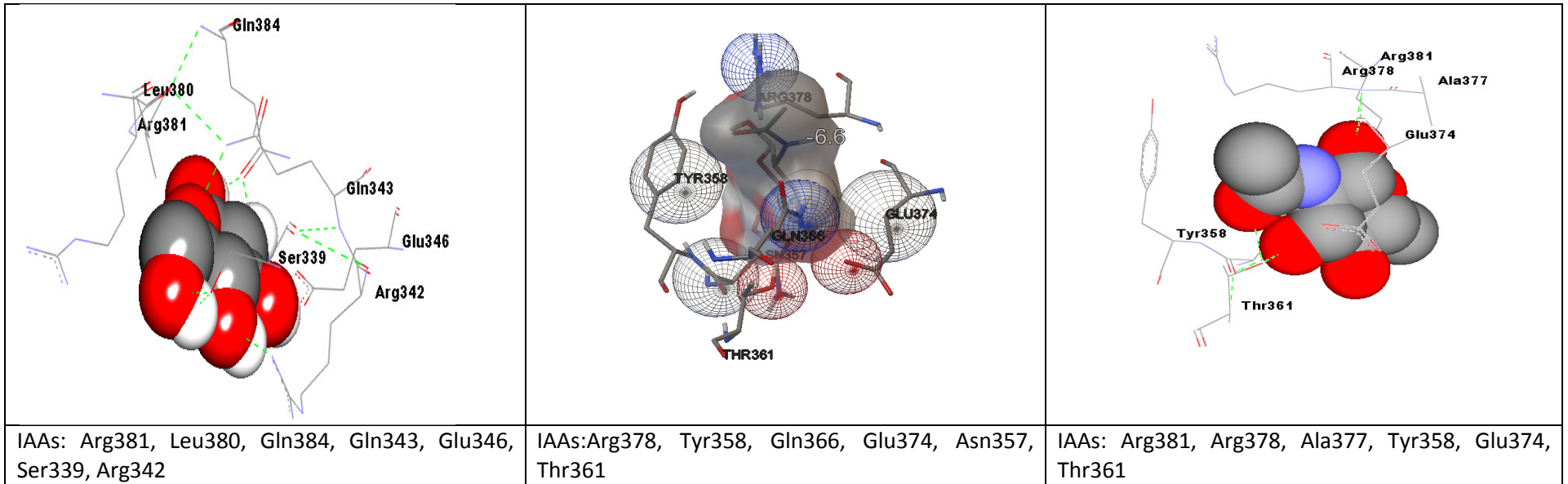
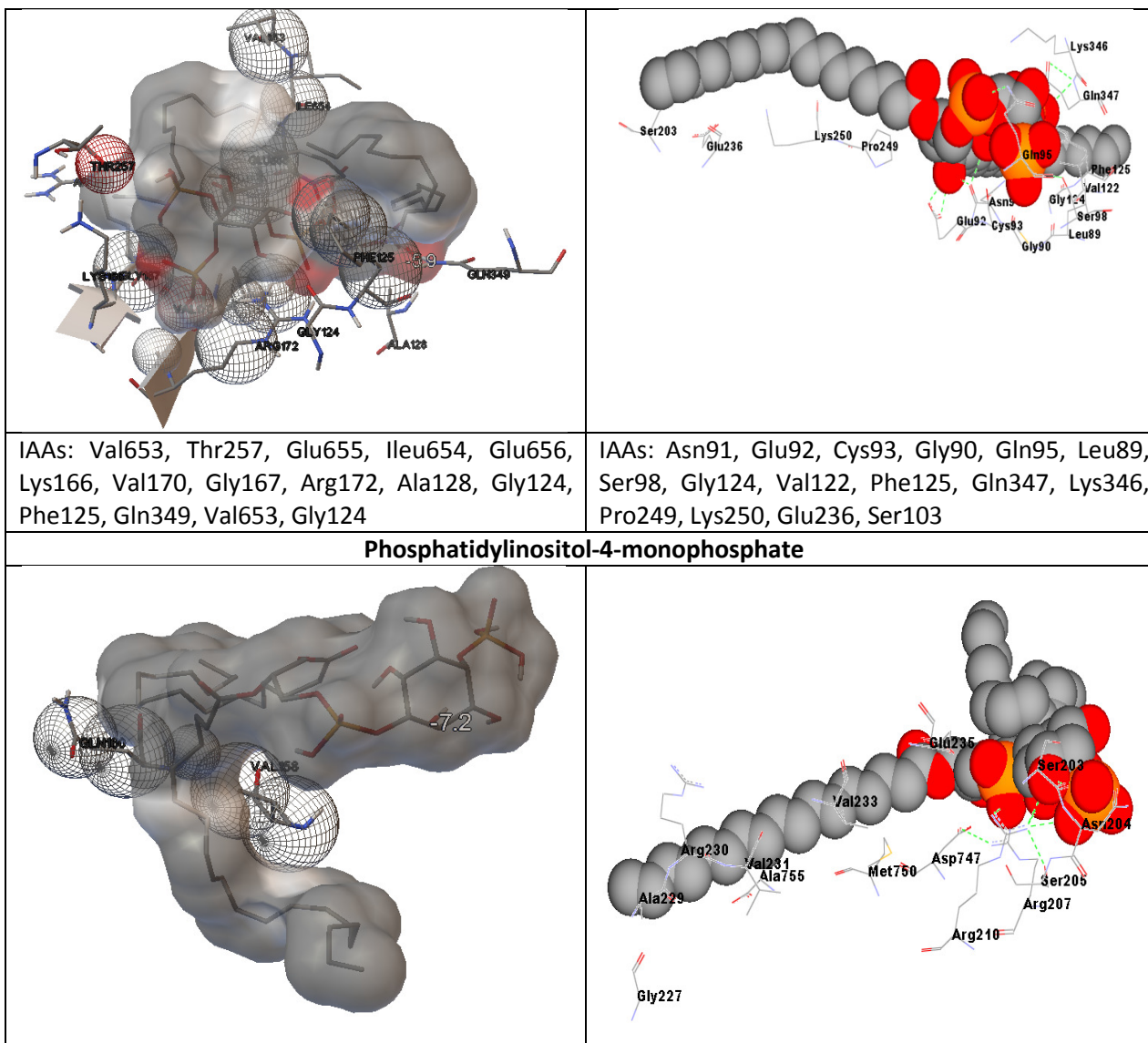


| A. Vimentin | | |
|--|--|--|
| AutoDock v4.2.6 | AutoDock vina | iGEMDOCK v2.1 |
| Acetate | | |
| | | |
| IAAs: Arg381, Arg378, Ala377, Glu374 | IAAs: Tyr358, Asn657, Thr361 | IAAs: Tyr383, Leu380, His379, Met376 |
| ATP | | |
| | | |
| IAAs: Gln384, Gln343, Ser339, Glu346, Arg342, Glu345, Asn357, Val353, Asn350, Arg381, Asp335 | IAAs: Glu375, Ala332, Gln343, Ser339, Glu346, Ala377, Arg381 | IAAs: Lys334, Asn337, Glu338, Glu341, Arg342, Arg345 |
| N-acetyl glucosamine | | |

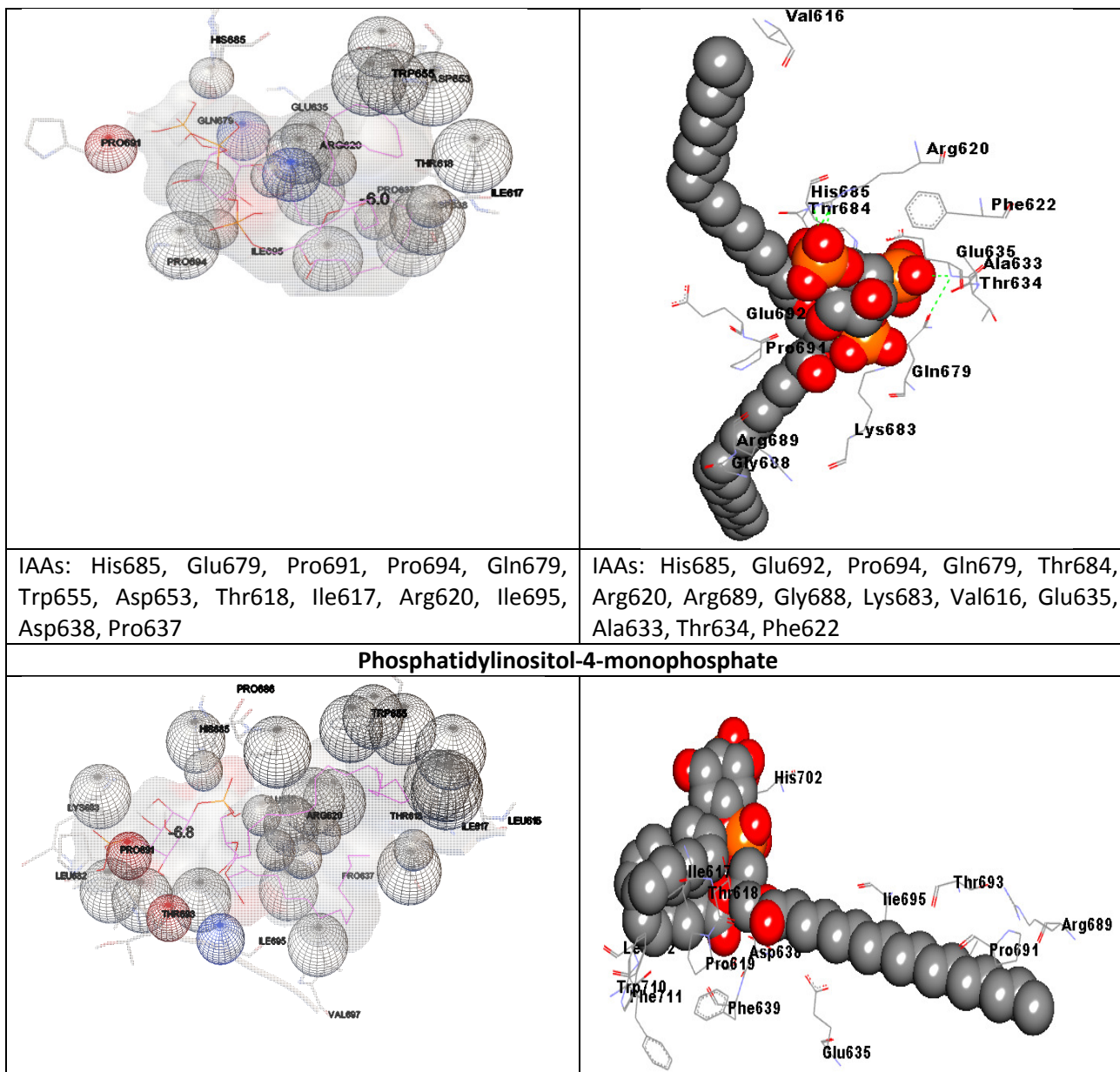


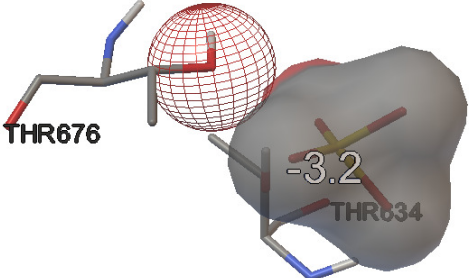
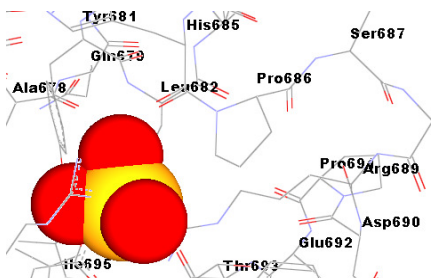
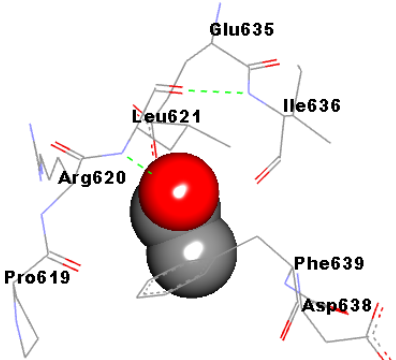
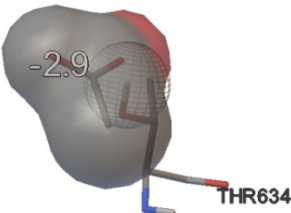
| B. Gelsolin | |
|---|---------------|
| AutoDock vina | iGEMDOCK v2.1 |
| Phosphatidylinositol (4,5)-bisphosphate | |

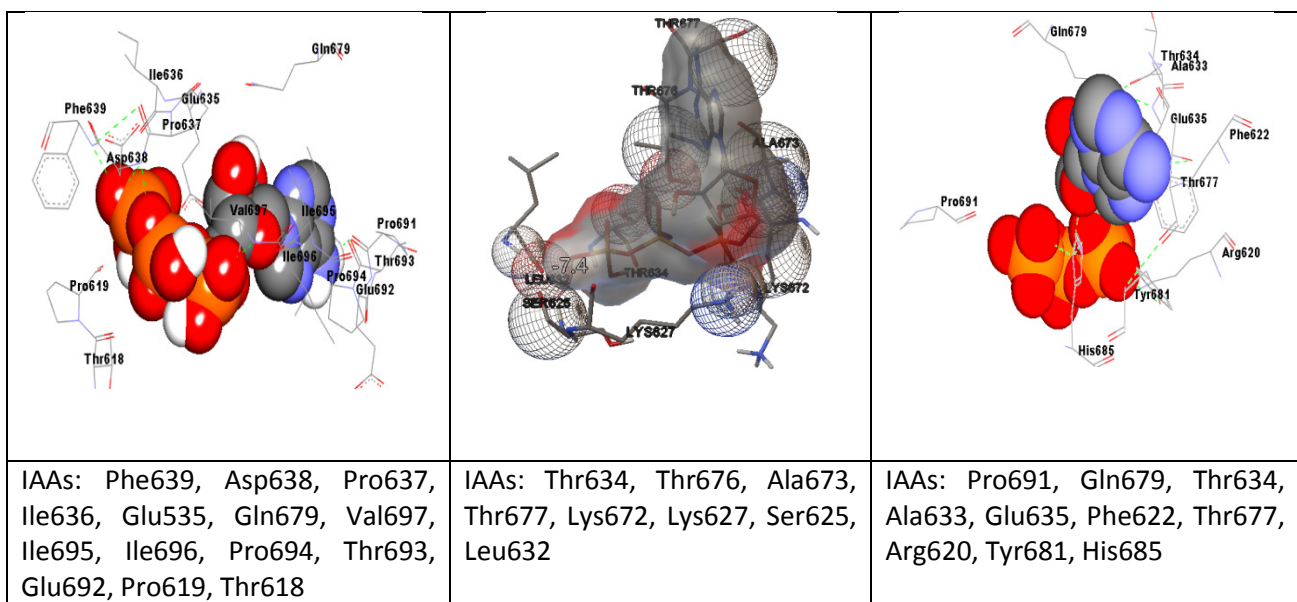


| | |
|--|--|
| IAAs: Gln160, Val158 | IAAs: Gly227, Ala229, Arg230, Val231, Ala755, Val233, Met750, Asp747, Glu235, Arg210, Arg207, Ser205, Ser203, Asn204, Ala755 |
| AutoDock v4.2.6 | iGEMDOCK v2.1 |
| ATP | |
| | |
| IAAs: Trp180, Leu247, Ser179, Lys142, Pro177, Val176, Gln164, Phe183, Glu181, Ser182 | IAAs: Met509, Glu504, Pro505, Ala506, Lys503, Asp678, Asn544, Ser545, Lys634, Lys631, Arg629, Glu587, Arg542, Ala543 |

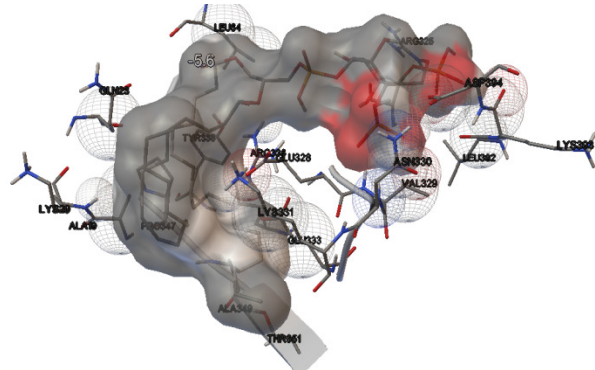
| | |
|--|----------------------|
| C. Villin | |
| AutoDock vina | iGEMDOCK v2.1 |
| Phosphatidylinositol (4,5)-bisphosphate | |



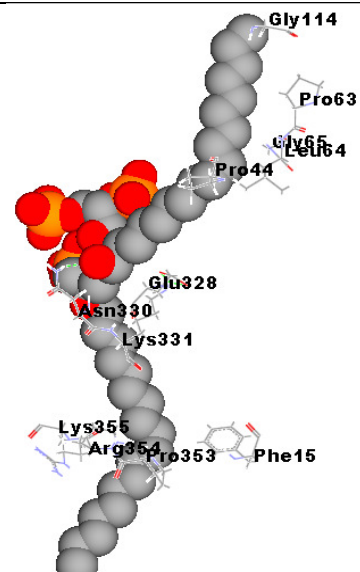
| | | | |
|--|----------------------|--|--|
| IAAs: Lys683, Leu682, Pro691, Thr693, Ile695, His685, Pro686, Glu635, Thr655, Arg620, Pro637, Thr618, Ile617, Leu615, Val697 | | IAAs: His702, Leu712, Phe711, Trp710, Thr648, Pro619, Arg689, Thr693, Leu682, Glu635, Phe639, Pro691, Asp638, Thr618, Thr693, Arg689, Ile695 | |
| Sulfate | | | |
|  | |  | |
| IAAs: Thr634, Thr676 | | IAAs: Arg620, Asp653, Tyr681, Arg689 | |
| AutoDock v4.2.6 | AutoDock vina | iGEMDOCK v2.1 | |
| Acetate | | | |
|  | |  | |
| IAAs: Pro619, Arg620, Leu621, Glu635, Ile636, Phe639, Asp538 | | IAAs: Thr634 | |
| | | IAAs: Arg689, Asp653, Tyr681, Pro686, Trp655 | |
| ATP | | | |
| | | | |



| D. Coronin-1A | |
|---|---------------|
| AutoDock vina | iGEMDOCK v2.1 |
| Phosphatidylinositol (4,5)-bisphosphate | |

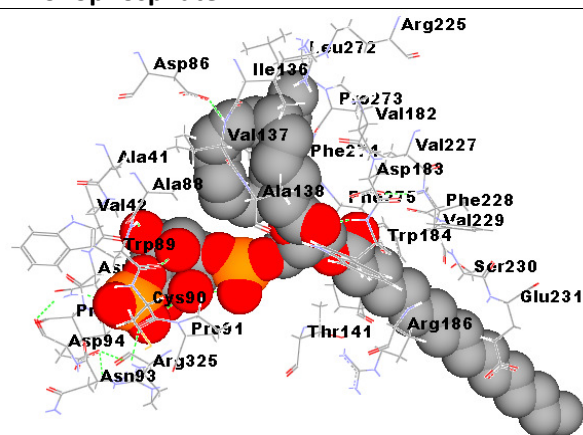
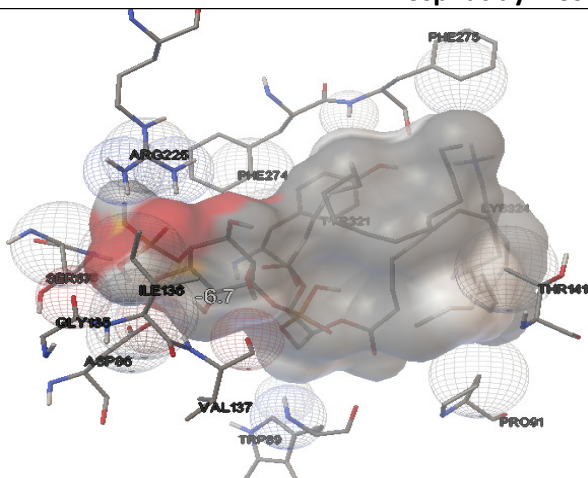


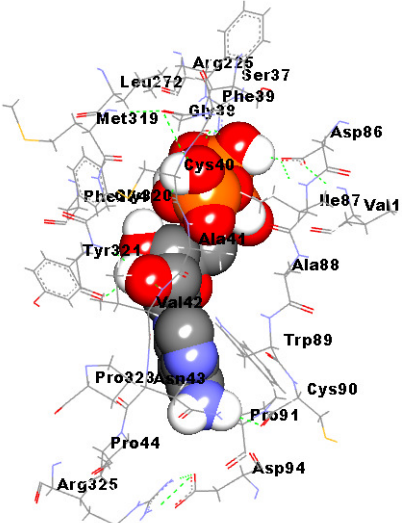
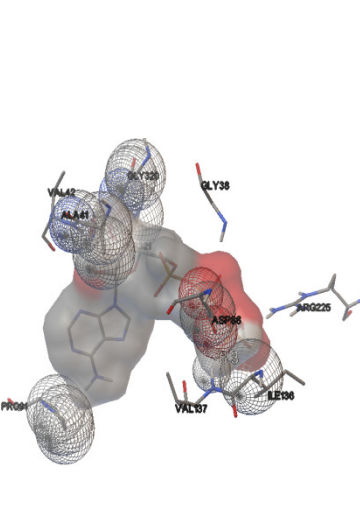
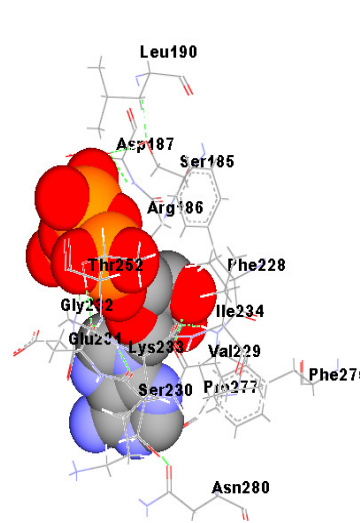
IAAs: Arg 325, Asp394, Leu392,Lys393, Val329, Leu64,Arg336,gln23, Tyr338, Lys20,Pro347,Thr351, Asn330, Val329, Glu328, Lys331, Glu333, Ala19, Pro347, Ala349, Thr351, Lys392

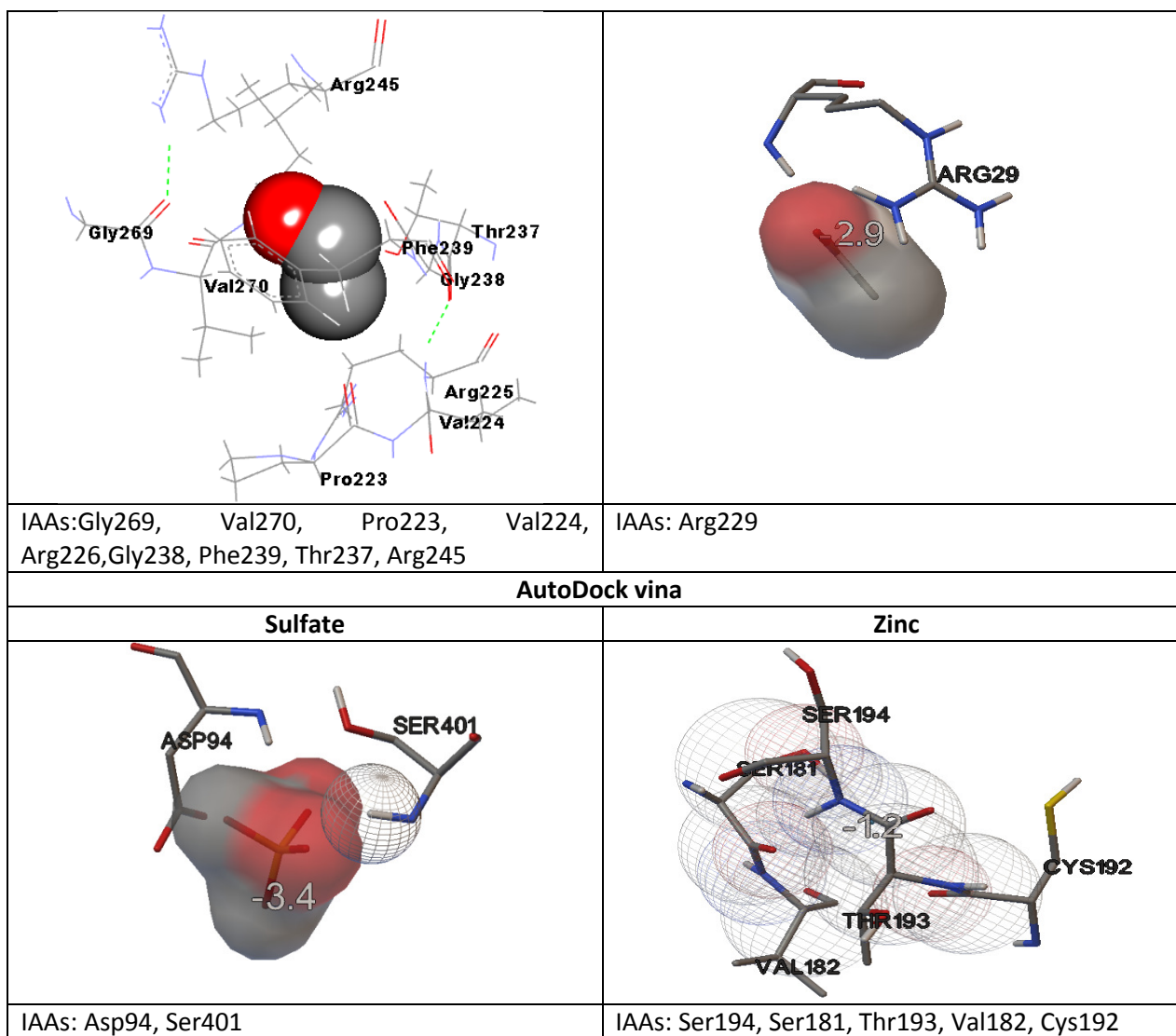


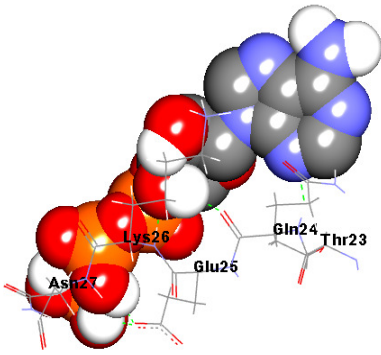
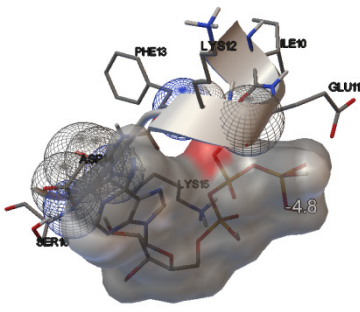
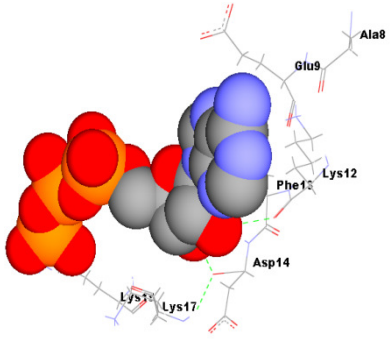
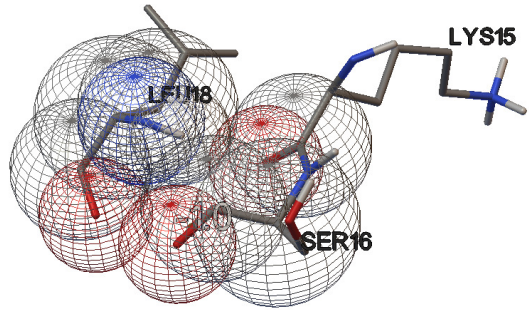
IAAs:Gly114,Pro63,Gly65,Leu64,Pro44,Glu328,Asn 330, Lys331, Lys355, Arg354, Pro353, Phe15

Phosphatidylinositol-4-monophosphate

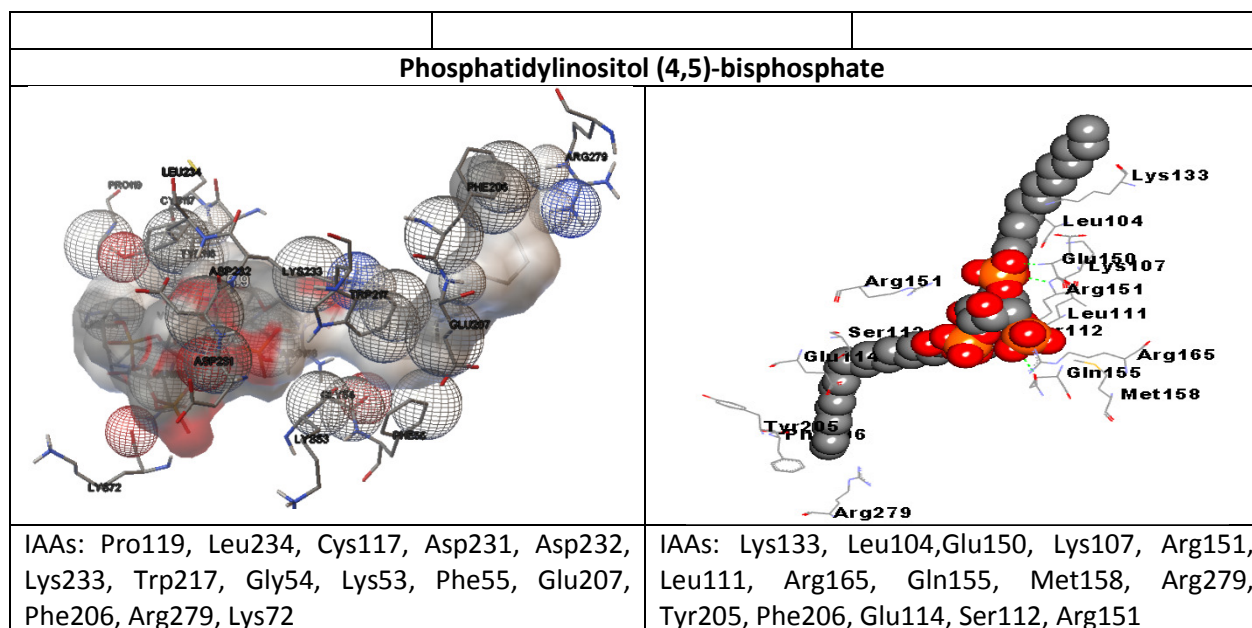


| | | |
|--|---|---|
| IAAs: Arg225, Phe274, Tyr321, Lys324, Thr141, Pro91, Trp89, Val137, Ileu136, Asp86, Gly135, Ser37, Phe275 | IAAs: Asn43, Trp89, Asp94, Asp183, Trp184, Pro91, Val137, Arg186, Arg225, Ser230, Glu231, Phe274, Phe275, Pro277, Pro44, Ala41, Asp86, Ileu136, Leu272, Pro273, Val182, Val227, Phe228, Cys90, Arg325, Asn93, Val42, Ala138, Ala88, Val229, Thr141, Val42 | |
| AutoDock v4.2.6 | AutoDock vina | iGEMDOCK v2.1 |
| ATP | | |
|  |  |  |
| IAAs: Arg226, Ser37, Phe39, Leu272, Met319, Gly38, Asp86, Ile97, Ala98, Trp89, Cys90, Pro91, Asp94, Arg325, Pro44, Pro323, Tyr321, Gly320, Phe275, | IAAs: Arg225, Ile136, Val137, Pro91, Asp86, Tyr321, Gly320, Val42, Ala41, Gly38 | IAAs: Leu190, Asp187, Ser185, Val229, Gly232, Lys233, Pro277, Asn280, Arg186, Phe228, Ser230, Glu231, Phe275, Ile234, Thr252, |
| AutoDock v4.2.6 | AutoDock vina | |
| Acetate | | |

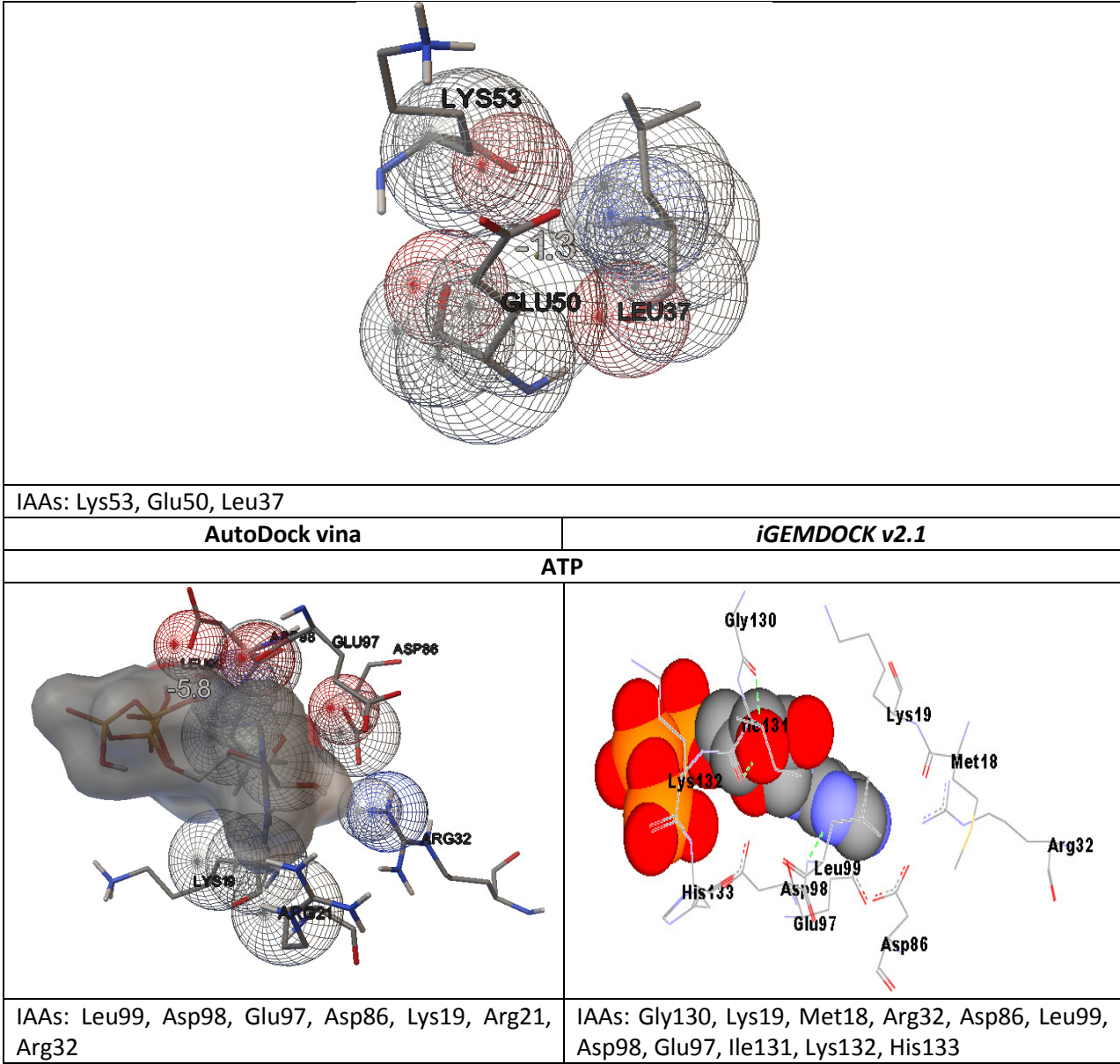


| E. Thymosin β -4 | | |
|---|--|---|
| AutoDock v4.2.6 | AutoDock vina | iGEMDOCK v2.1 |
| ATP | | |
|  |  |  |
| IAAs: Asn227, Lys26, Glu25, Gln24, Thr23 | IAAs: Phe13, Lys12, Ile10, Glu11, Asp14, Lys15, Ser16 | IAAs: Lys12, Lys13, Lys17, Lys19, Asp14, Glu9, Ala8, Phe13 |
| AutoDock vina | | |
| Calcium | | |
|  | | |
| IAAs: Leu18, Ser16, Lys15 | | |

| F. Ezrin | | |
|---|---|---|
| AutoDock vina | | |
| Sulfate | | |
| | | |
| IAAs: Gly202, Ile203 | | |
| AutoDock v4.2.6 | AutoDock vina | iGEMDOCK v2.1 |
| ATP | | |
| | | |
| IAAs: Thr 57, Pro56, Phe55, Gly54, Lys233, Trp217, Tyr205, Ile276, Arg275, Arg279 | IAAs: Gly202, Tyr85, Gly109, Gln105, Arg31, His481, Trp58, Asn204, Ile203 | IAAs: Arg8, Glu15, Arg165, Arg151, Leu163, Gln155, Met158, Asp159, His161 |



| |
|----------------------|
| G. Cofilin |
| AutoDock vina |
| Mg |
| |



Best docking poses for binding of physiological ligands to (A) Vimentin (B) Gelsolin (C) Villin (D) Coronin-1A (E) Thymosin β -4 (F) Ezrin (G) Cofilin. The poses were generated using AutoDock v4.2.6, AutoDock vina and iGEMDOCK v2.1.