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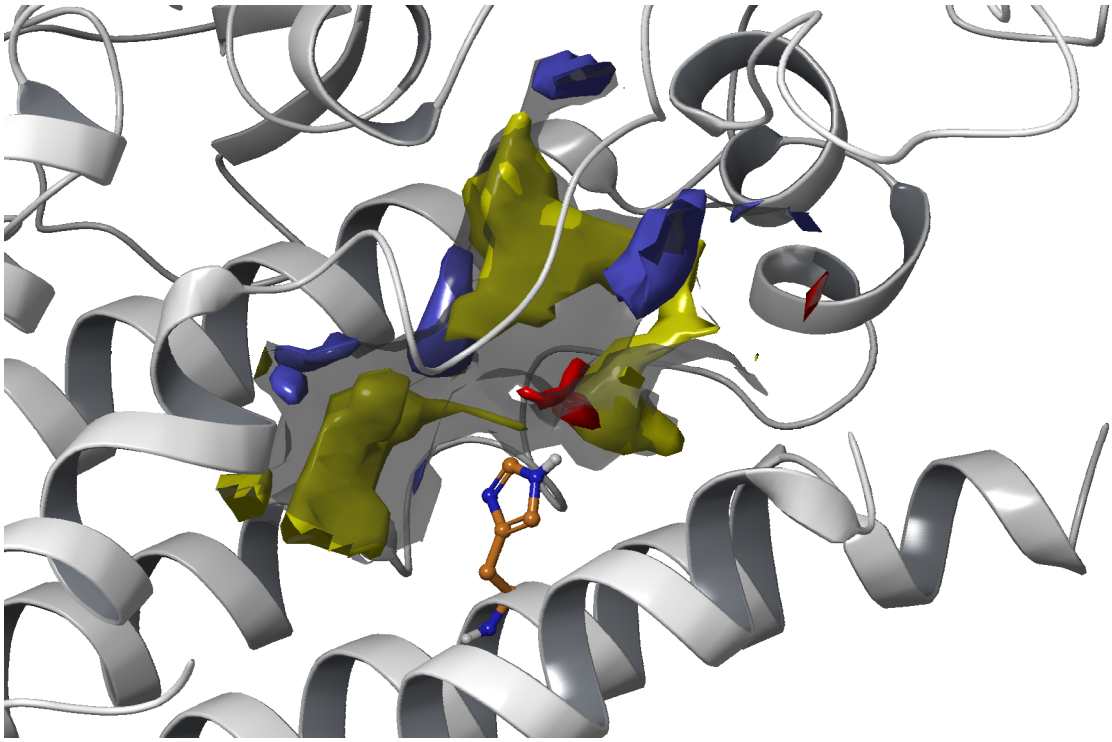


Figure S1. Binding site properties of the catalytic cleft in the IDO1 structure 6AZW. Solvent accessible surfaces are generated with SiteMap and color-coded according to total area (grey surface), hydrogen bond acceptor area (red surface), hydrogen bond donor area (violet surface), hydrophobic area (yellow surface).

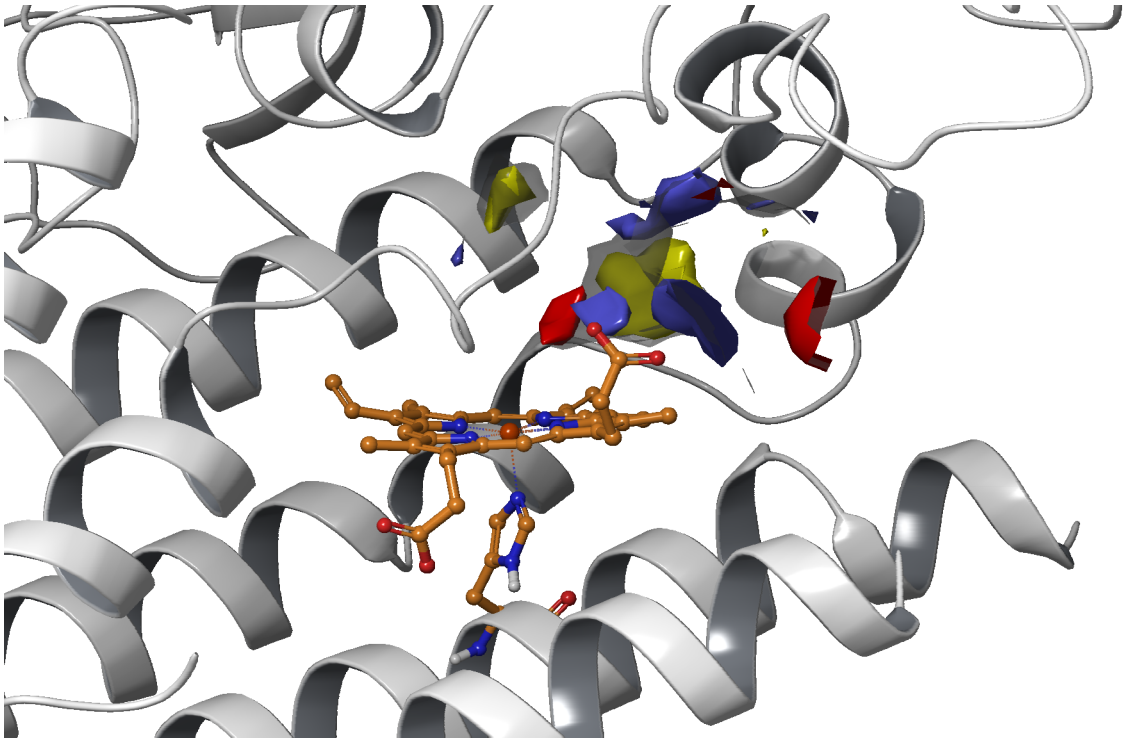


Figure S2. Binding site properties of the catalytic cleft in the IDO1 structure 6E45. Solvent accessible surfaces are generated with SiteMap and color-coded according to total area (grey surface), hydrogen bond acceptor area (red surface), hydrogen bond donor area (violet surface), hydrophobic area (yellow surface).

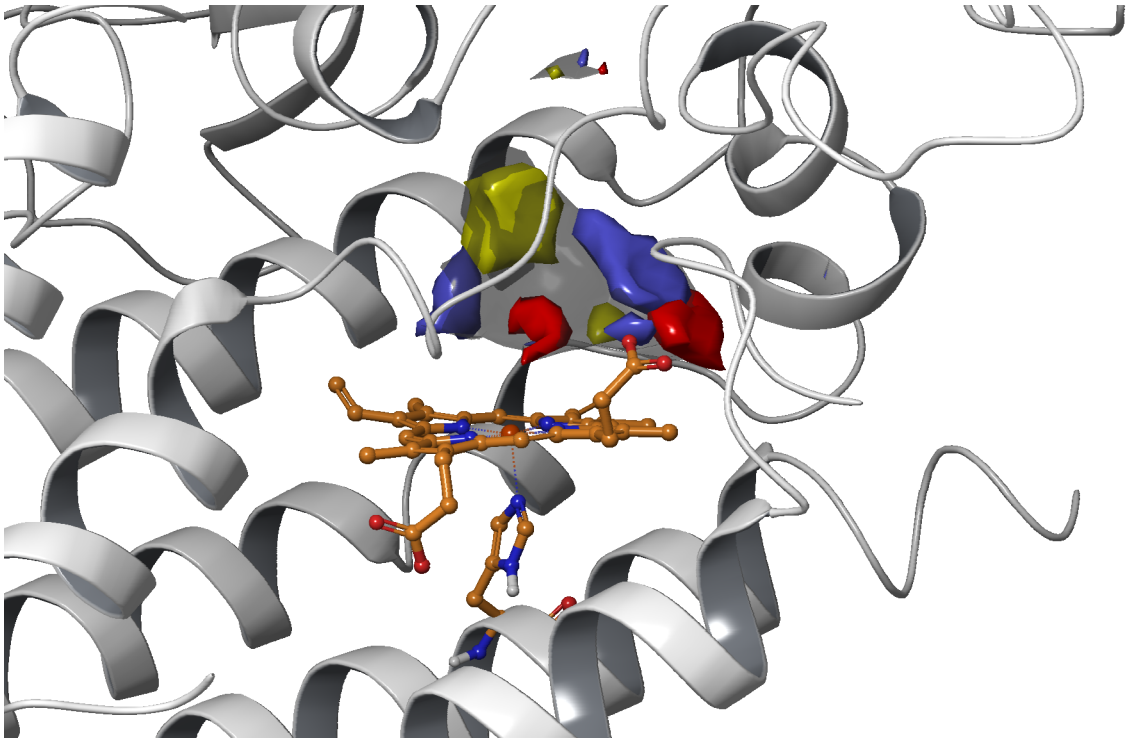
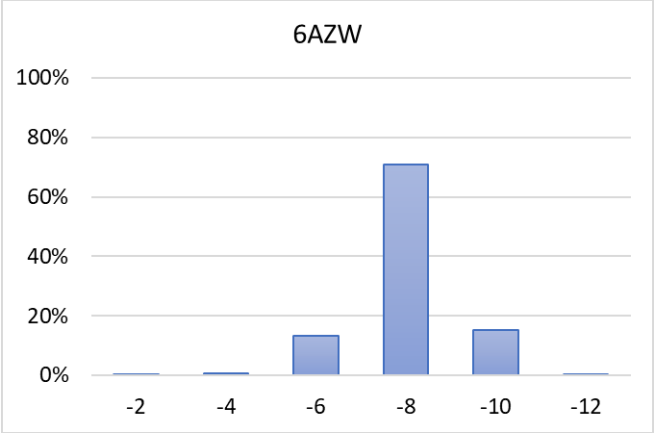


Figure S3. Binding site properties of the catalytic cleft in the IDO1 structure 6E46. Solvent accessible surfaces are generated with SiteMap and color-coded according to total area (grey surface), hydrogen bond acceptor area (red surface), hydrogen bond donor area (violet surface), hydrophobic area (yellow surface).

a



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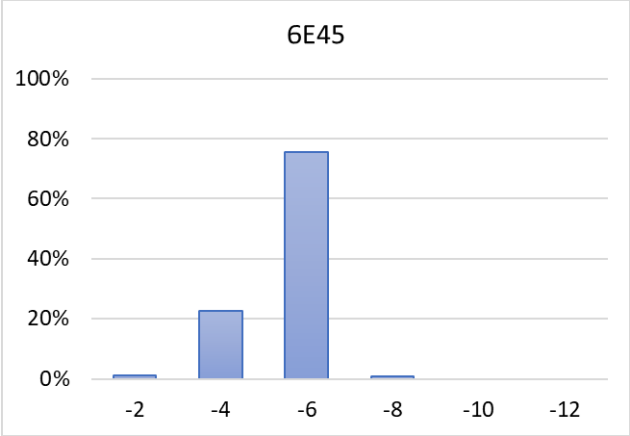

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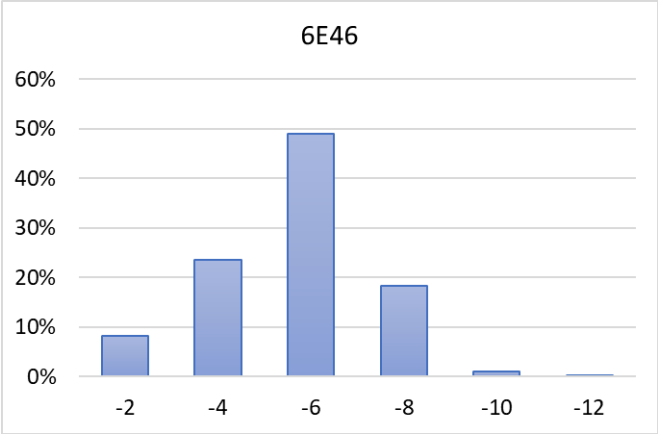

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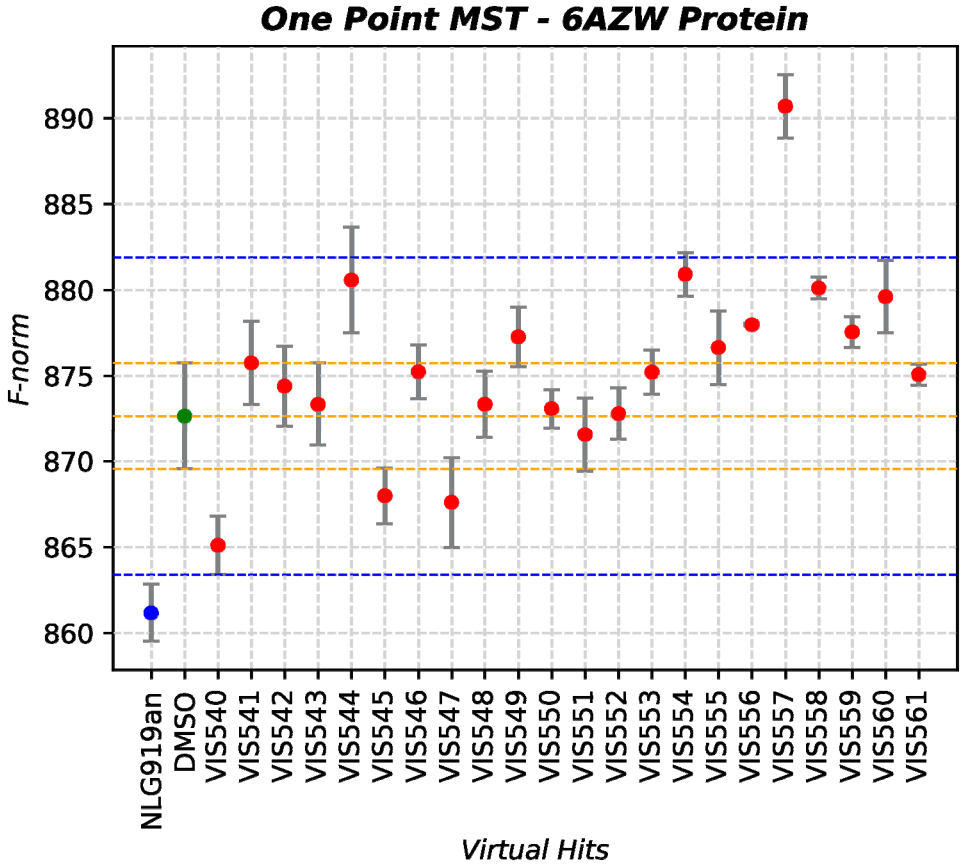


Figure S5. Single point assay of MST binding experiments of virtual hit compounds (set A) from IDO1 structure 6AZW. The blue filled circle shows the positive control (concentration of 250 µM), the green filled circle shows negative control (buffer vehicle).

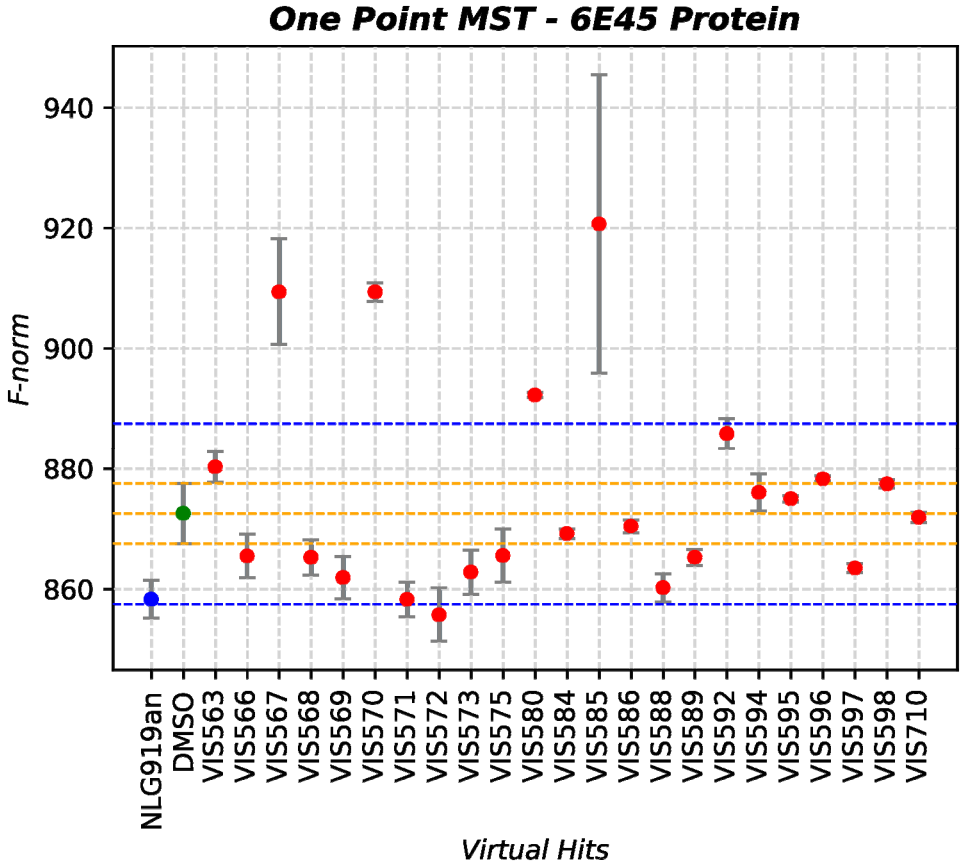


Figure S6. Single point assay of MST binding experiments of virtual hit compounds (set B) from IDO1 structure 6E45. The blue filled circle shows the positive control (concentration of 250 μM), the green filled circle shows negative control (buffer vehicle).

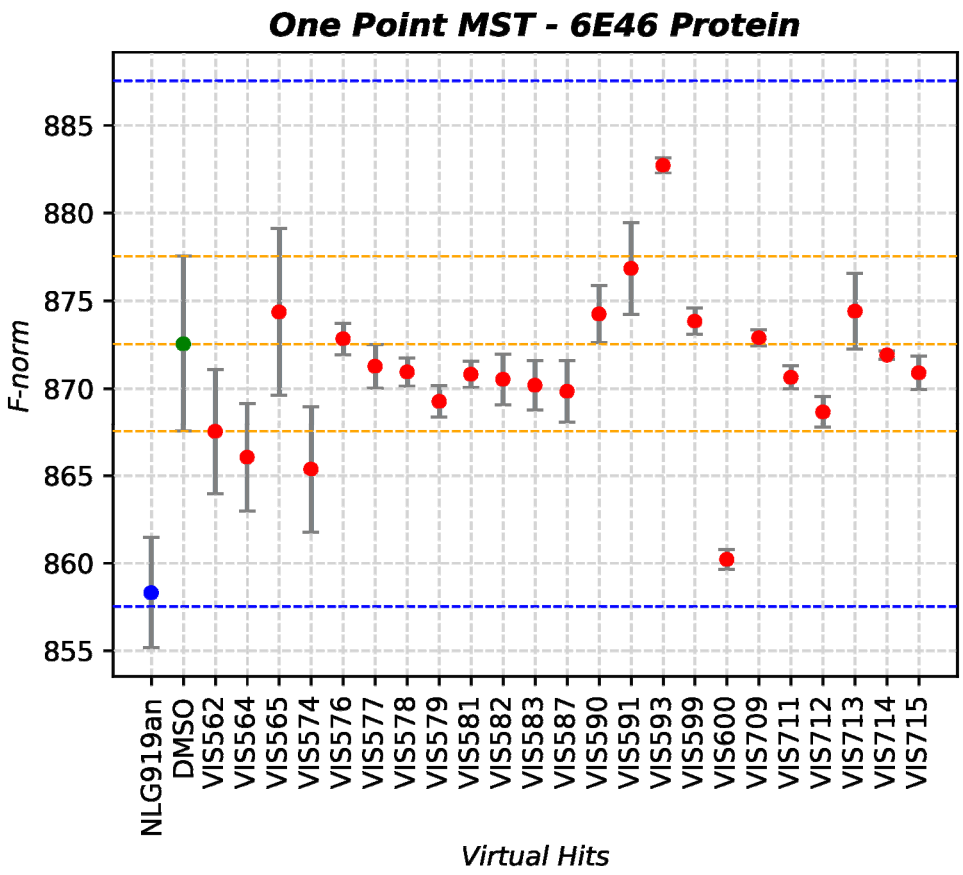
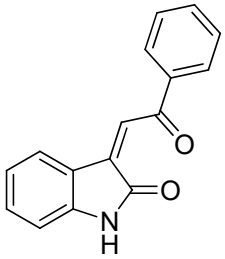


Figure S7. Single point assay of MST binding experiments of virtual hit compounds (set C) from IDO1 structure 6E46. The blue filled circle shows the positive control (concentration of 250 μM), the green filled circle shows negative control (buffer vehicle).



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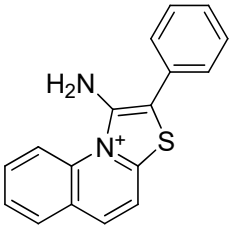

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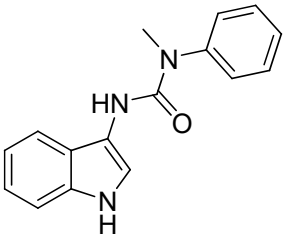

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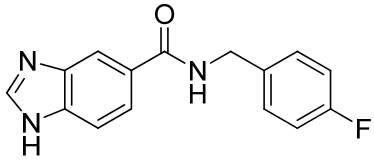

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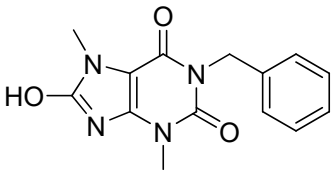

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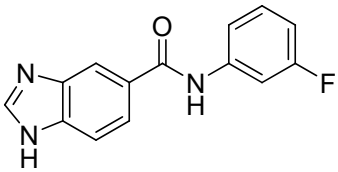

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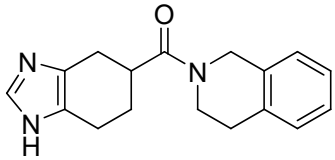

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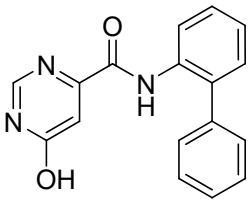

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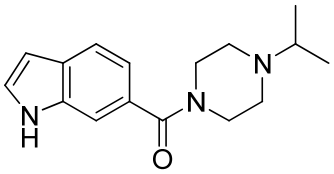

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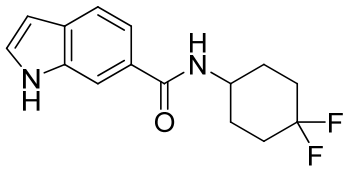

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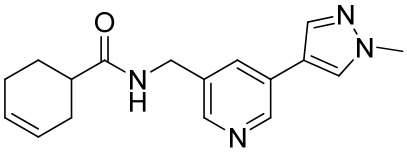

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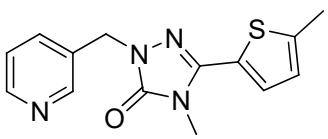

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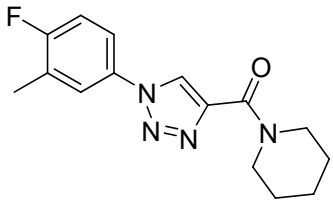

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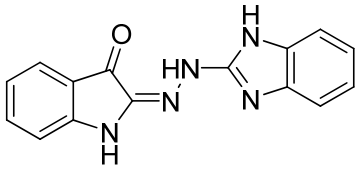
Figure S8. Chemical structures of n.13 binders from IDO1 structure 6AZW.



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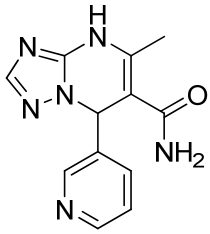

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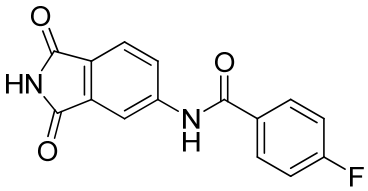

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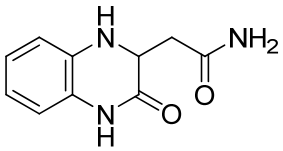

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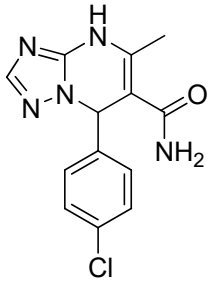

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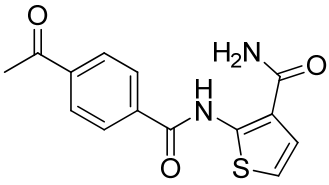

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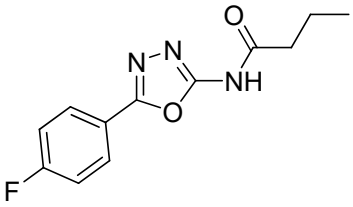

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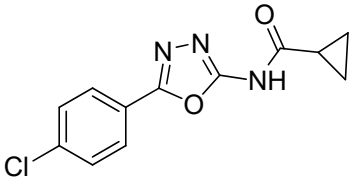

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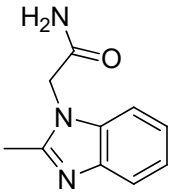

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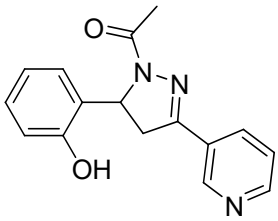

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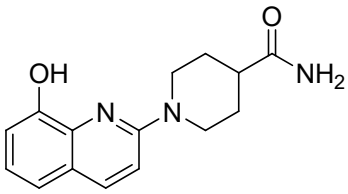

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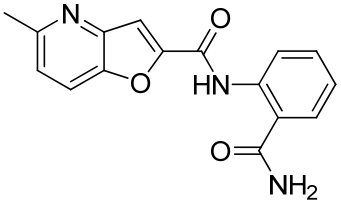

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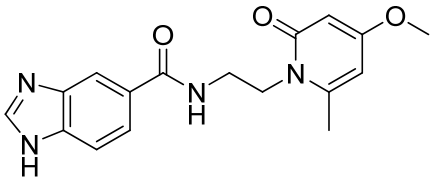

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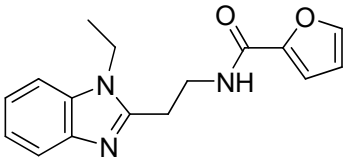

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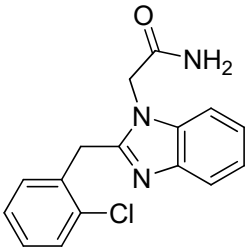

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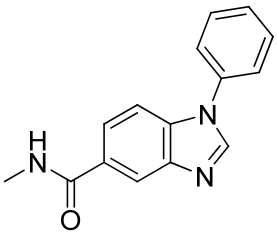

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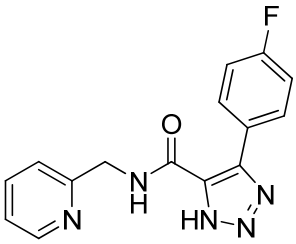

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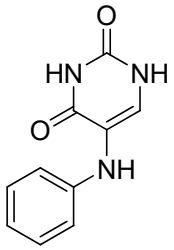
Figure S9. Chemical structures of n.17 binders from IDO1 structure 6E45.



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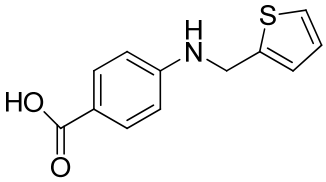

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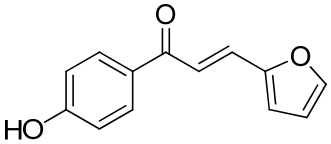

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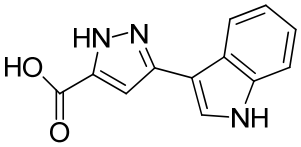

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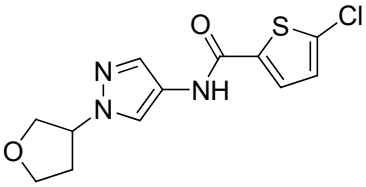

VIS600

Figure S10. Chemical structures of n.5 binders from IDO1 structure 6E46.