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Supplementary material

Disruption of Irisin Dimerization by FDA-approved Drugs. A Computational Repurposing Approach for the Potential Treatment of Lipodystrophy Syndromes

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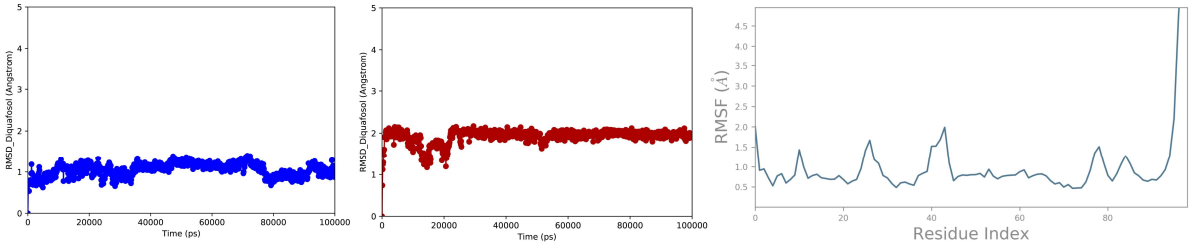
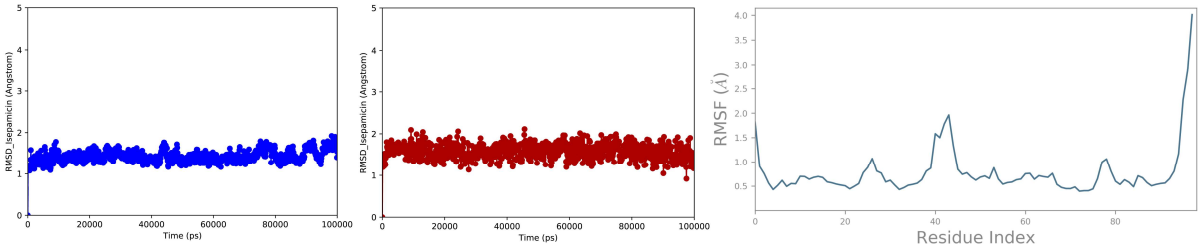
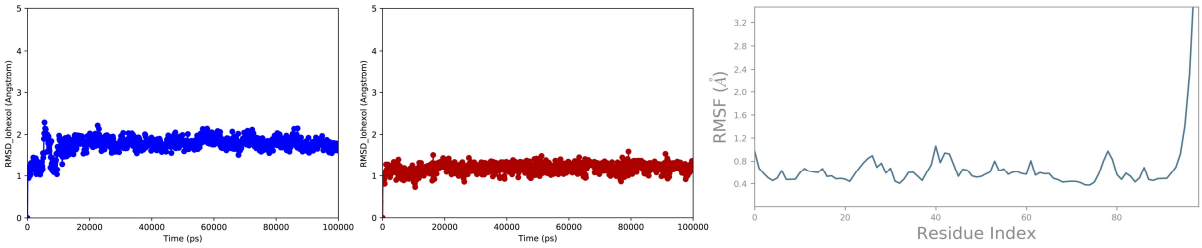
Irisin/Diquafosal



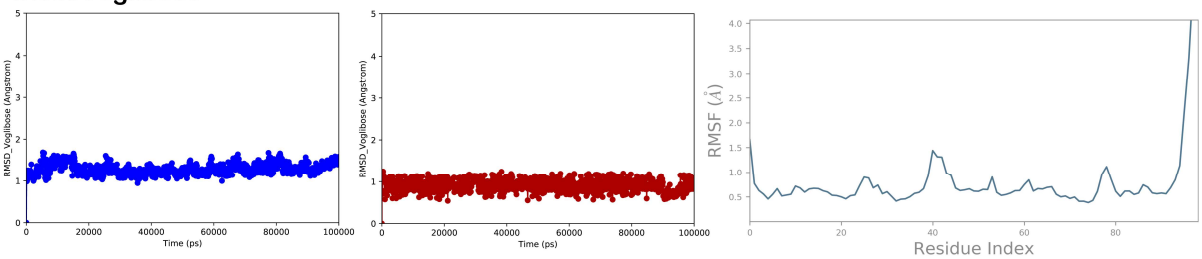
Irisin/Isepamicin



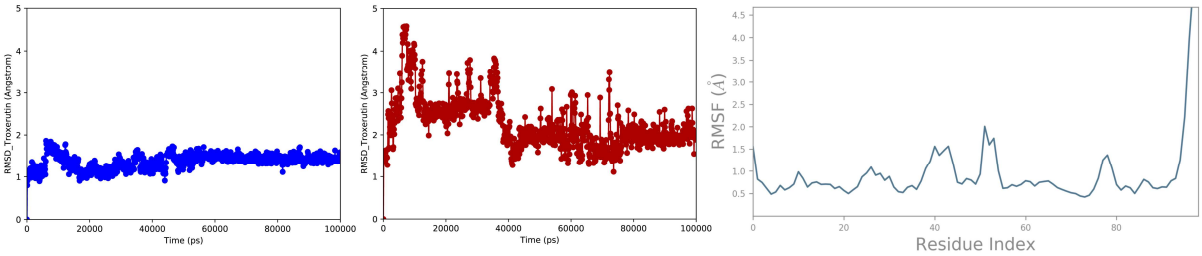
Irisin/Iohexol



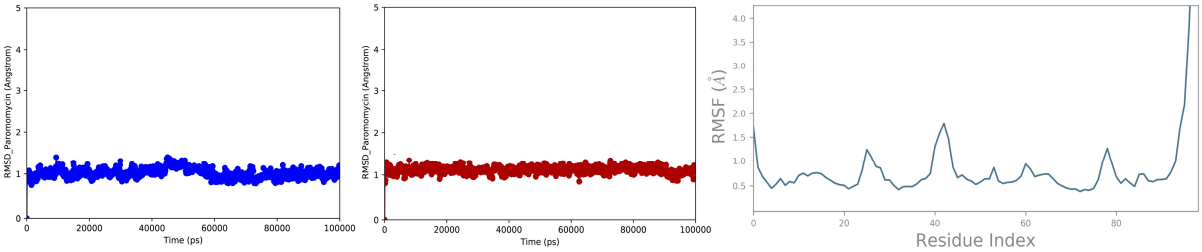
Irisin/Voglibose



Irisin/Troxerutin



Irisin/Paromomycin



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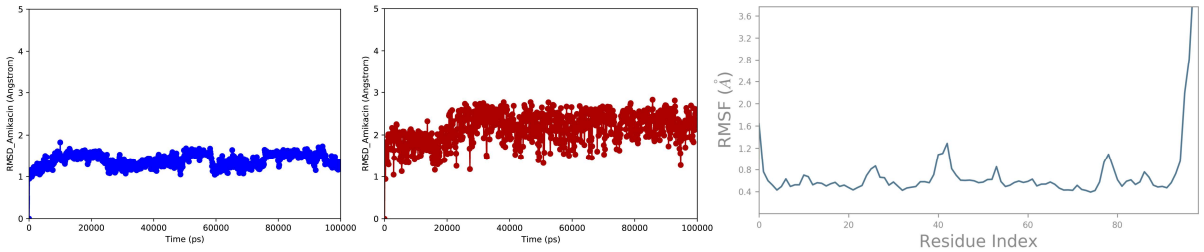
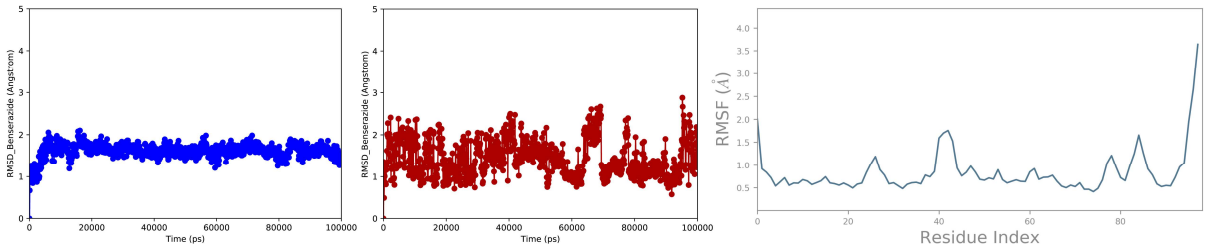
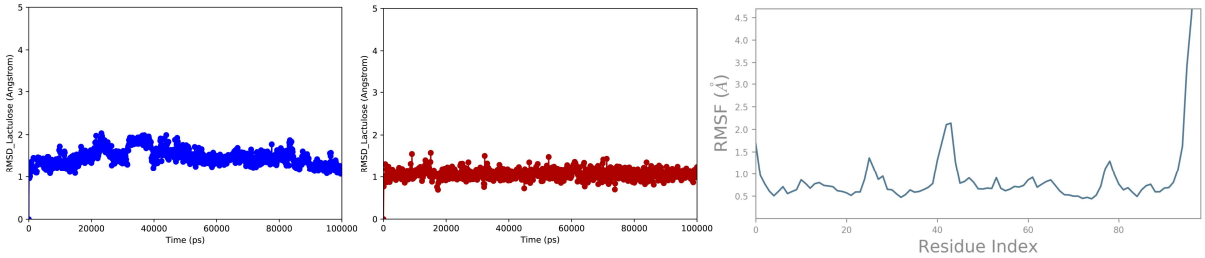
Irisin/Amikacin



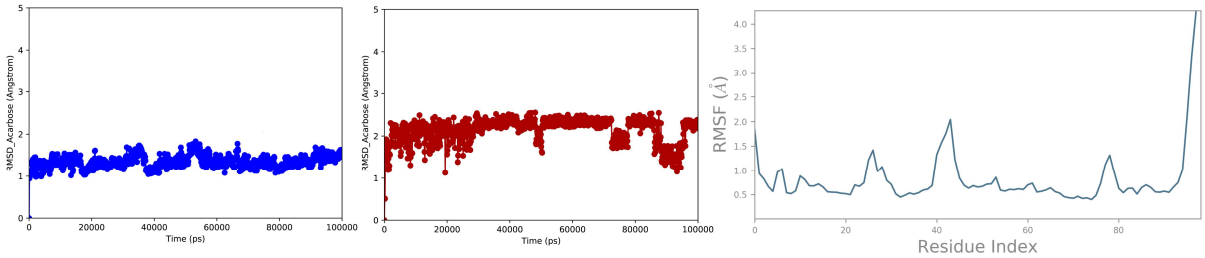
Irisin/Benserazide



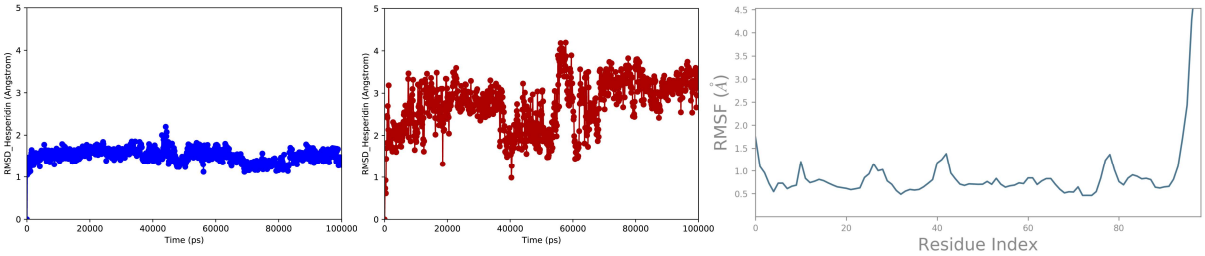
Irisin/Lactulose



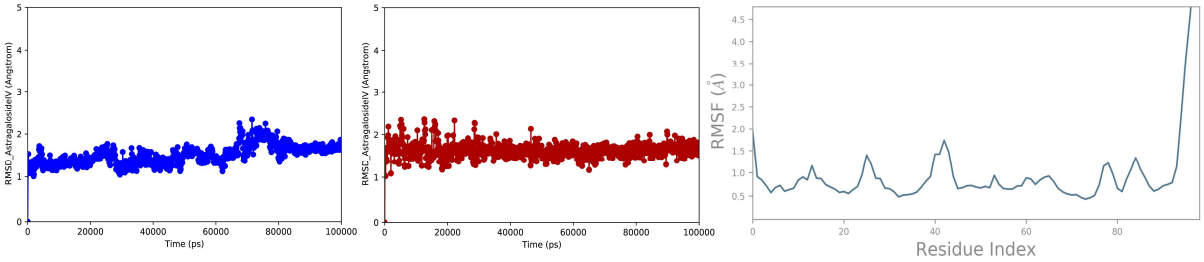
Irisin/Acarbose



Irisin/Hesperidin



Irisin/Astragaloside IV



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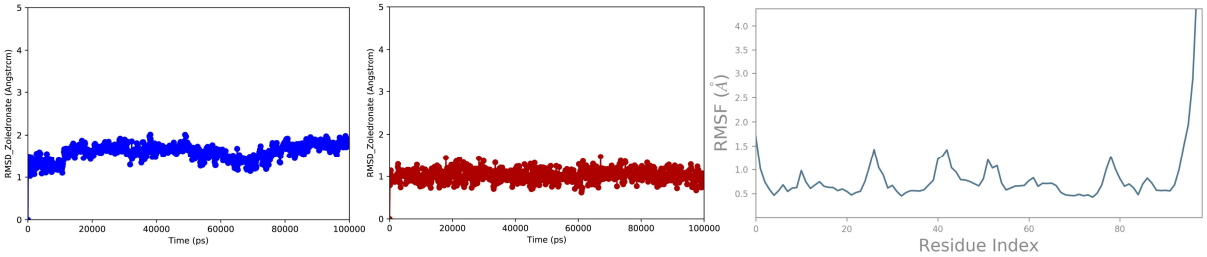
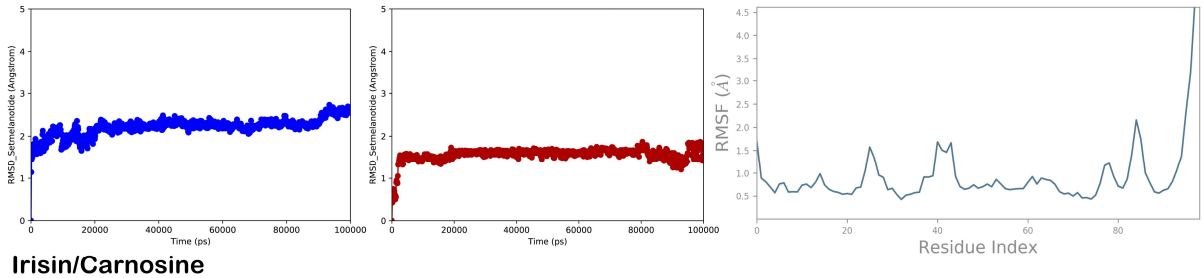
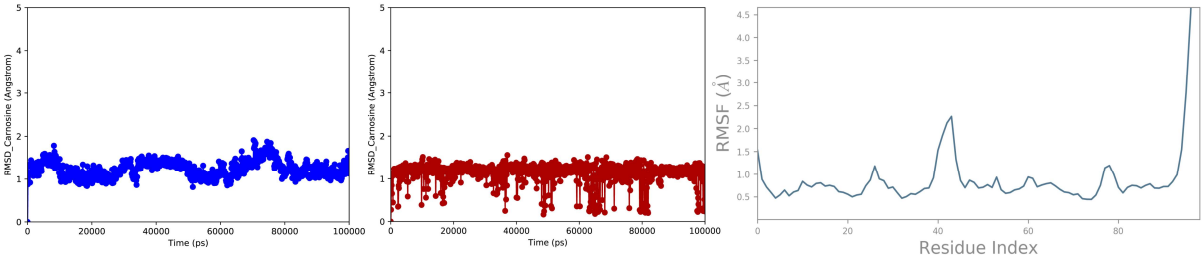
Irisin/Zoledronate



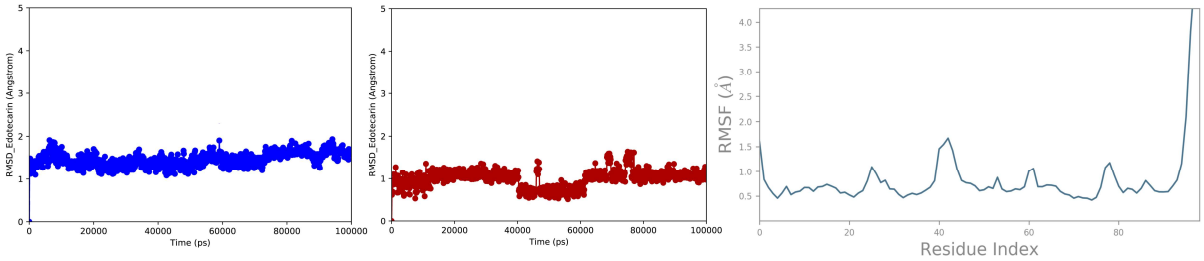
Irisin/Setmelanotide



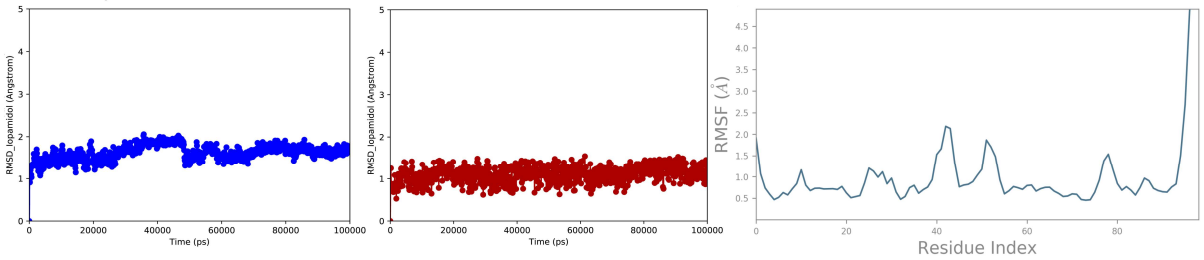
Irisin/Carnosine



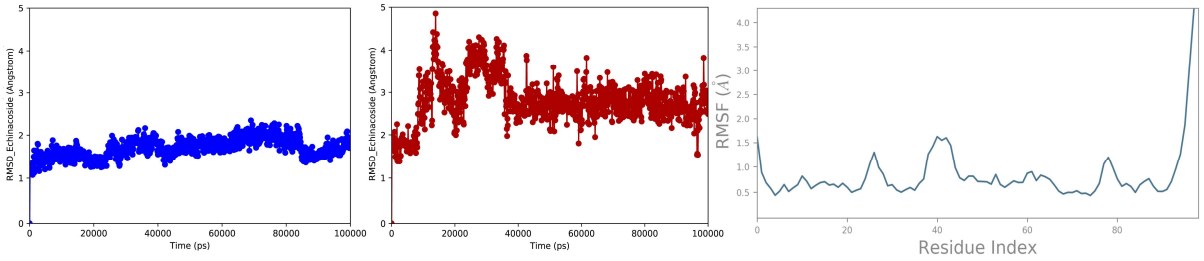
Irisin/Edotecarin



Irisin/Iopamidol



Irisin/Echinacoside



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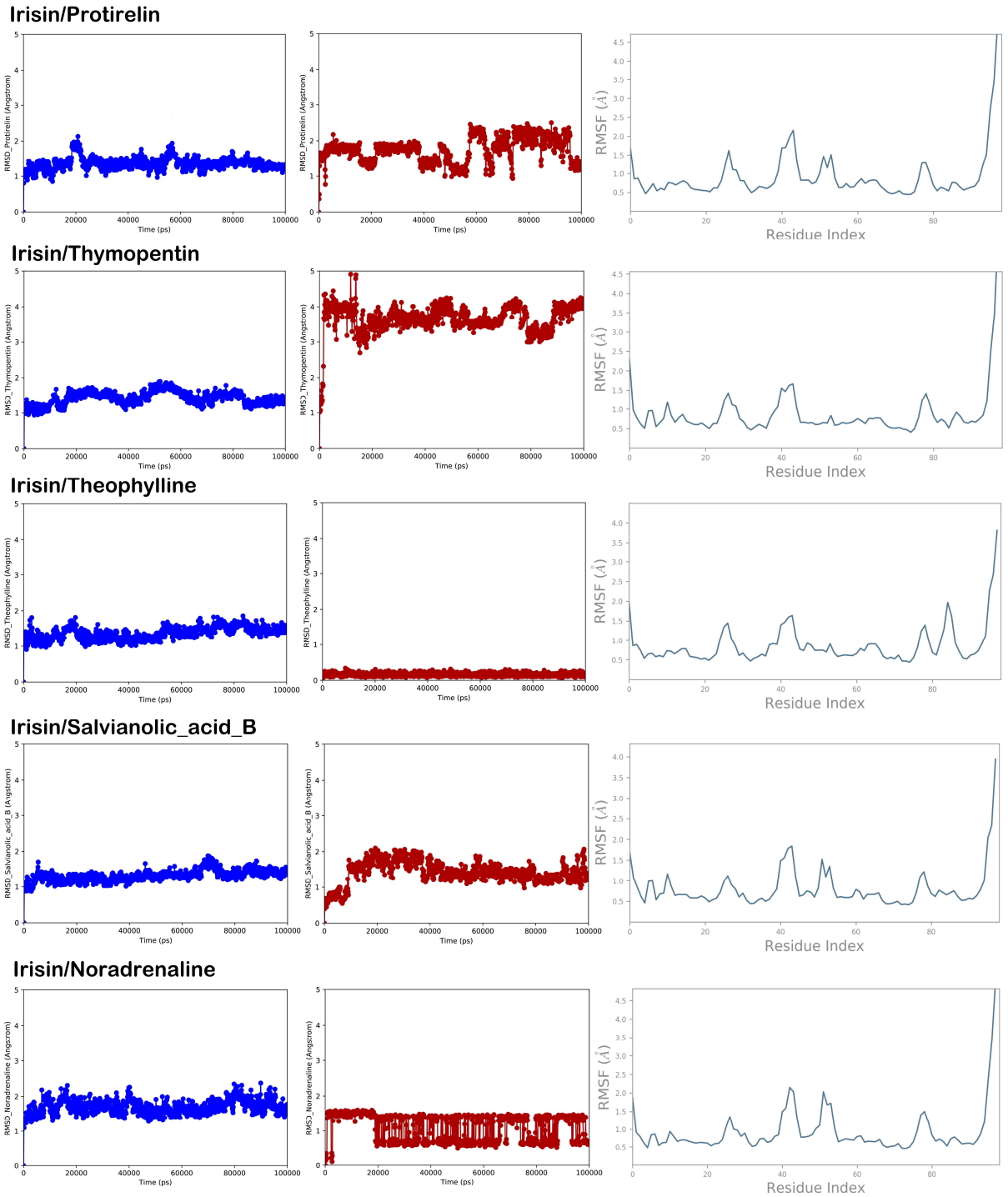

Figure S1. RMSD calculation (protein (blue line) and ligand (red line)) and RMSF evaluation for each complex, selected by docking studies, after 100 ns of MD simulation. Pictures were generated by Maestro (Maestro, Schrödinger LLC, release 2020-3).