

# molecular informatics

Supporting Information

## **A Computational Approach to Identify Potential Novel Inhibitors against the Coronavirus SARS-CoV-2**

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## Supporting Information

# A Computational Approach to Identify Potential Novel Inhibitors against the Coronavirus SARS- CoV-2

*Verena Battisti<sup>‡</sup>, Oliver Wieder<sup>‡</sup>, Arthur Garon<sup>‡</sup>, Thomas Seidel<sup>‡</sup>, Ernst Urban<sup>‡</sup>, Thierry Langer<sup>‡</sup>,\**

<sup>‡</sup>University of Vienna, Department of Pharmaceutical Chemistry, Althanstraße 14, A-1090 Vienna, Austria

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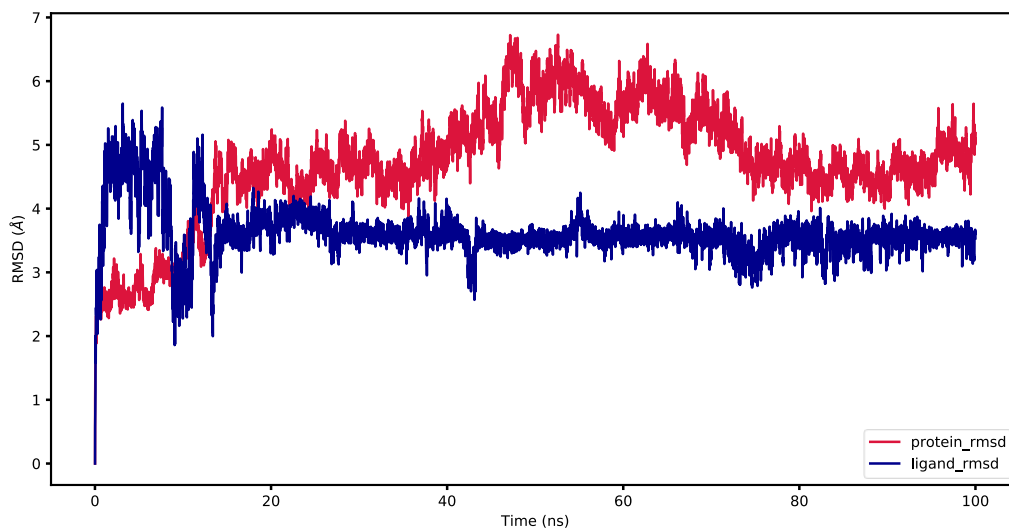
**Table S1. Details on the 10 Protein-Systems Used in the MD Simulations.**

<i>Protein-System</i>	<i>Box Size (Angstrom<sup>3</sup>)</i>	<i>Number of Water Molecules</i>	<i>Number of Cl<sup>-</sup> Ions</i>	<i>Number of K<sup>+</sup> Ions</i>	<i>Total Number of Atoms</i>
<i>QHD43421_0</i>	69	9961	31	27	32003
<i>QHD43415_5</i>	95	26196	73	75	83523
<i>QHD43415_7</i>	57	5618	14	14	18301
<i>QHD43415_9</i>	67	9134	31	25	29312
<i>QHD43415_10</i>	77	14042	40	39	44325
<i>QHD43415_11</i>	139	77437	219	229	247623
<i>QHD43415_12</i>	120	52501	162	148	167293
<i>QHD43415_13</i>	146	96920	279	275	299720
<i>QHD43415_14</i>	94	24826	69	79	80199
<i>QHD43415_15</i>	78	13821	40	37	46317

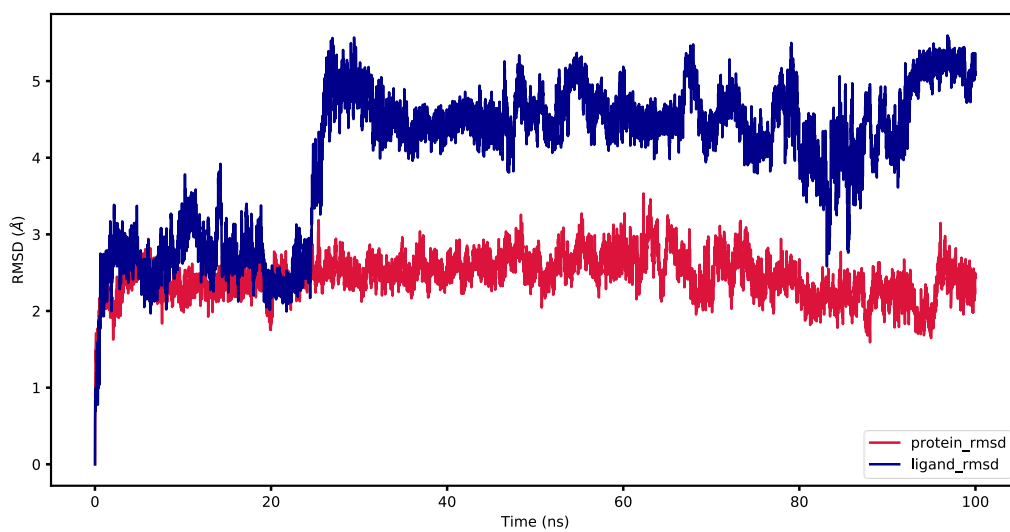
**Table S2. Plots of the RMSD for the Proteins and for their Ligand**

*Protein-System* | *RMSD Plot*

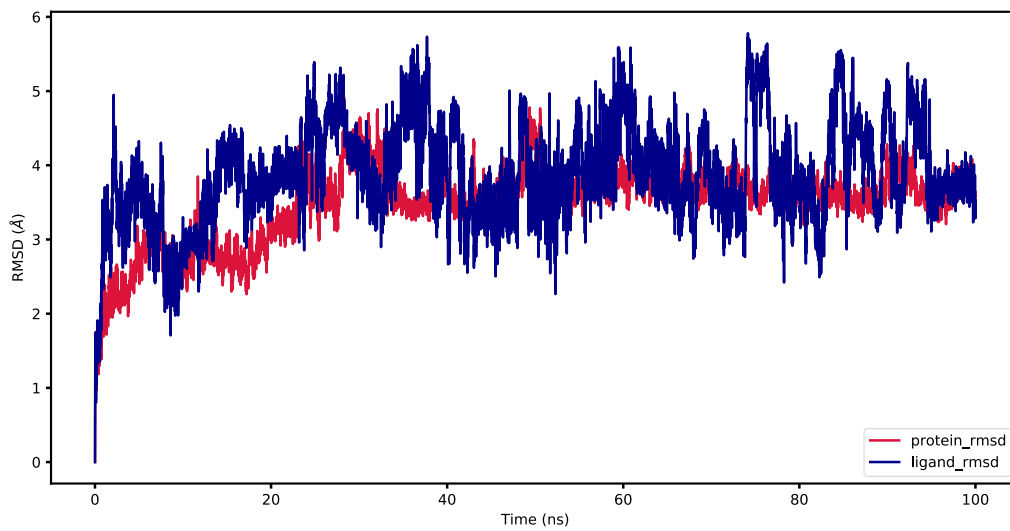
*QHD  
43421\_0*



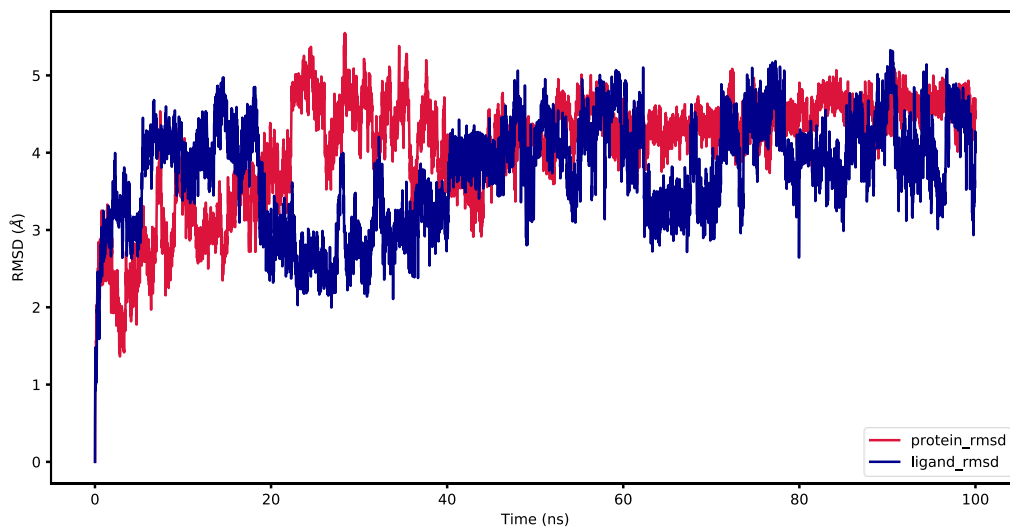
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43415\_5



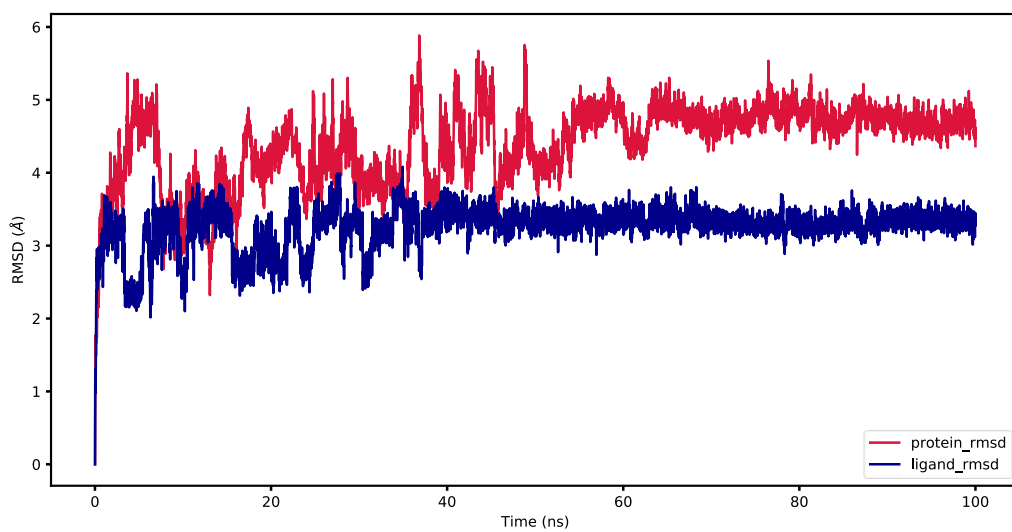
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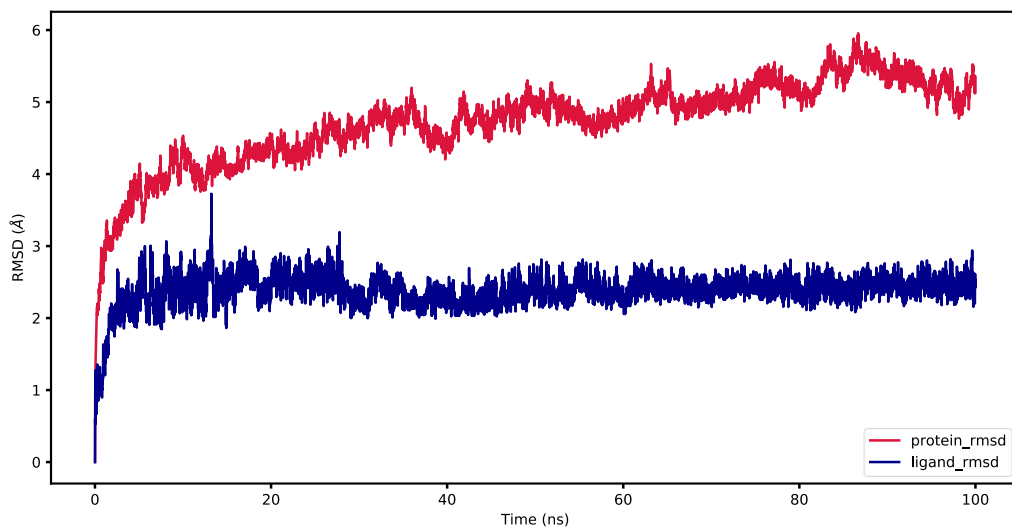
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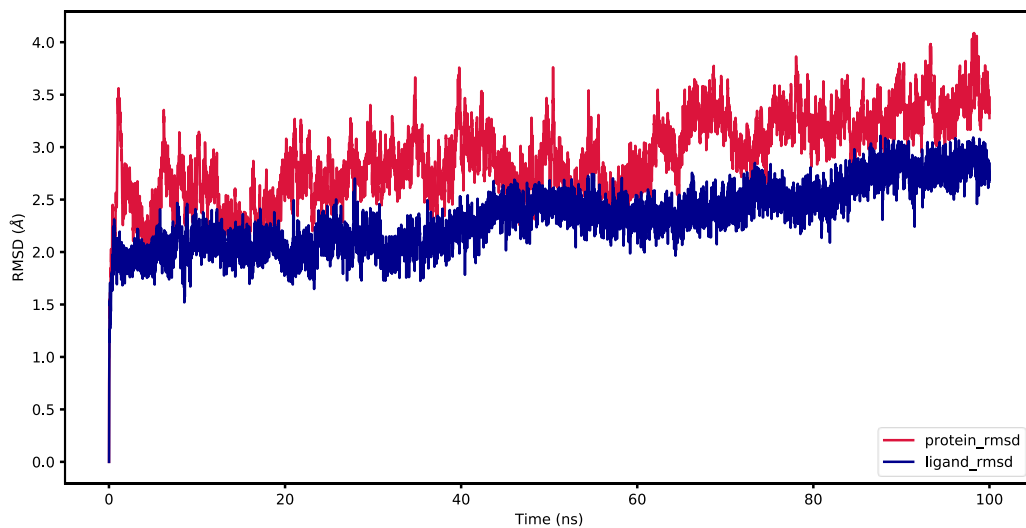
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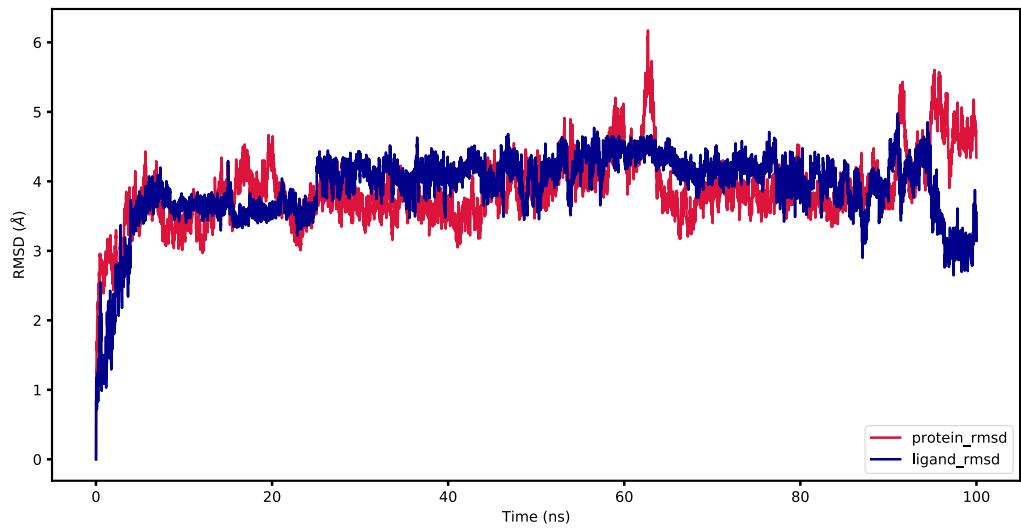
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43415\_11



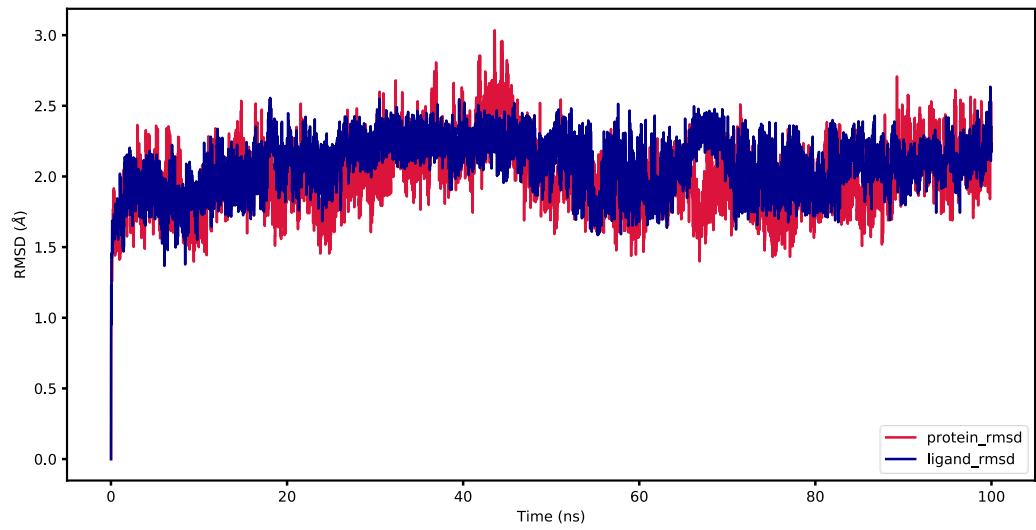
*QHD*  
43415\_12



*QHD*  
43415\_13



*QHD*  
43415\_14



*QHD*  
43415\_15

