Electronic Supporting Information

In Search of SARS CoV-2 Replication Inhibitors: Virtual Screening, Molecular Dynamics Simulations and ADMET Analysis

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Table of Contents

1. 2-D diagrams of Identified Hit Molecules

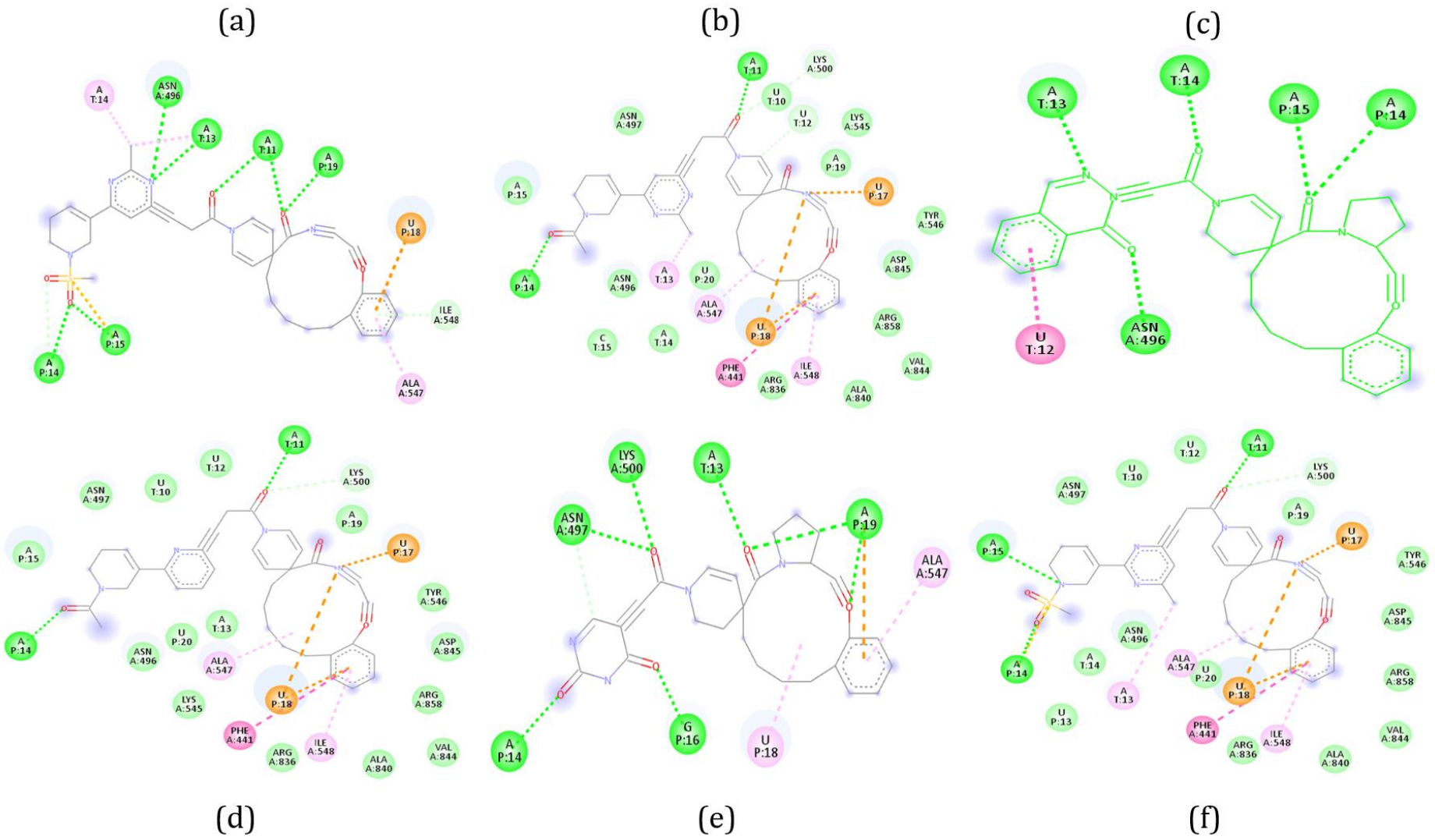

Figure S1. 2-D interactions of ligands **2** (a), **3** (b), **4** (c), **5** (d), **6** (e) and **7** (f) complexed with RdRp. Poses have been generated using Biovia Discovery Studio 2020.[1]

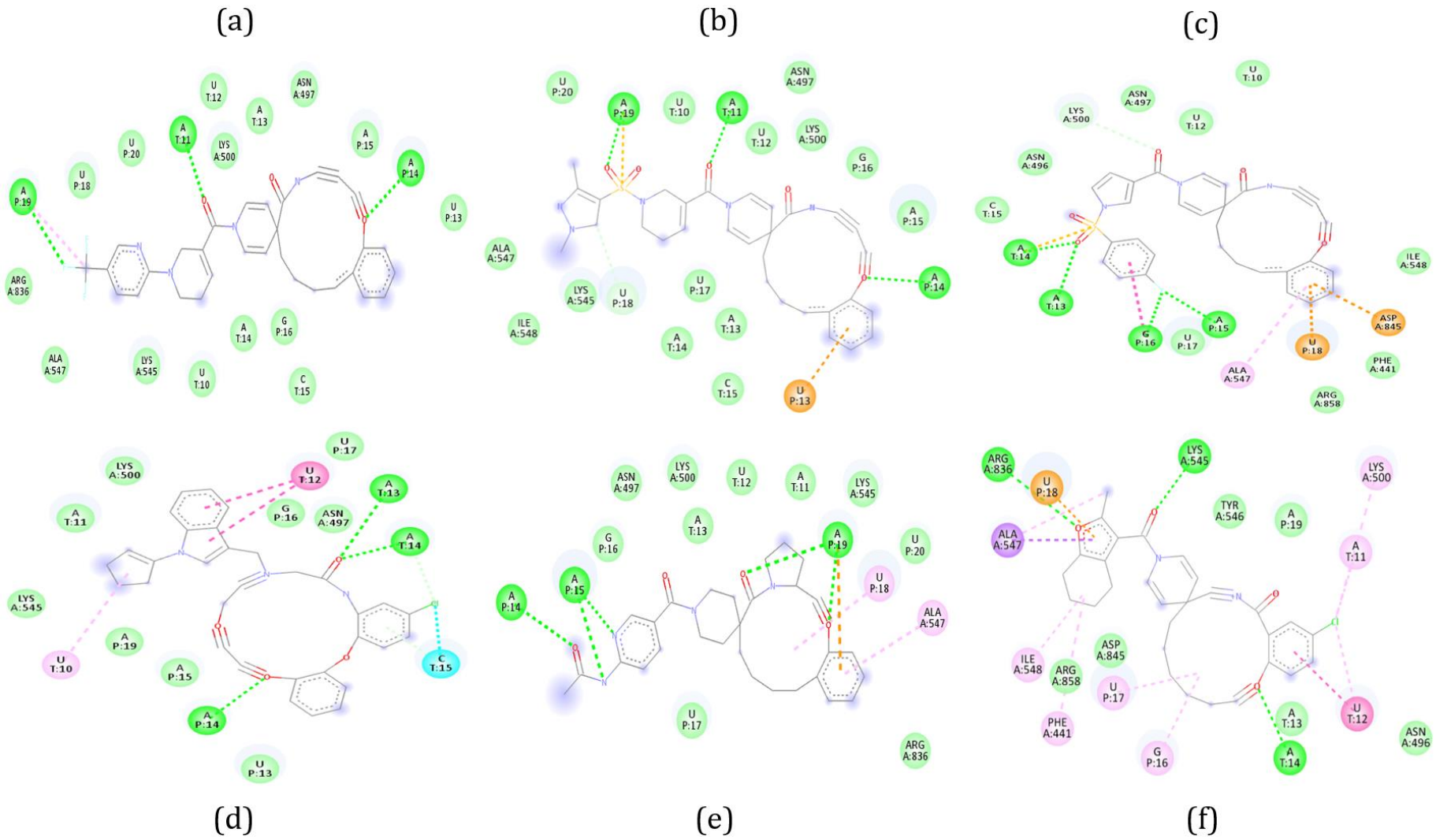

Figure S2. 2-D interactions of ligands **8** (a), **9** (b), **10** (c), **11** (d), **12** (e) and **13** (f) with RdRp (PDB ID: 7BV2). Interactive poses of hits have been generated using Biovia Discovery Studio 2020.[1]

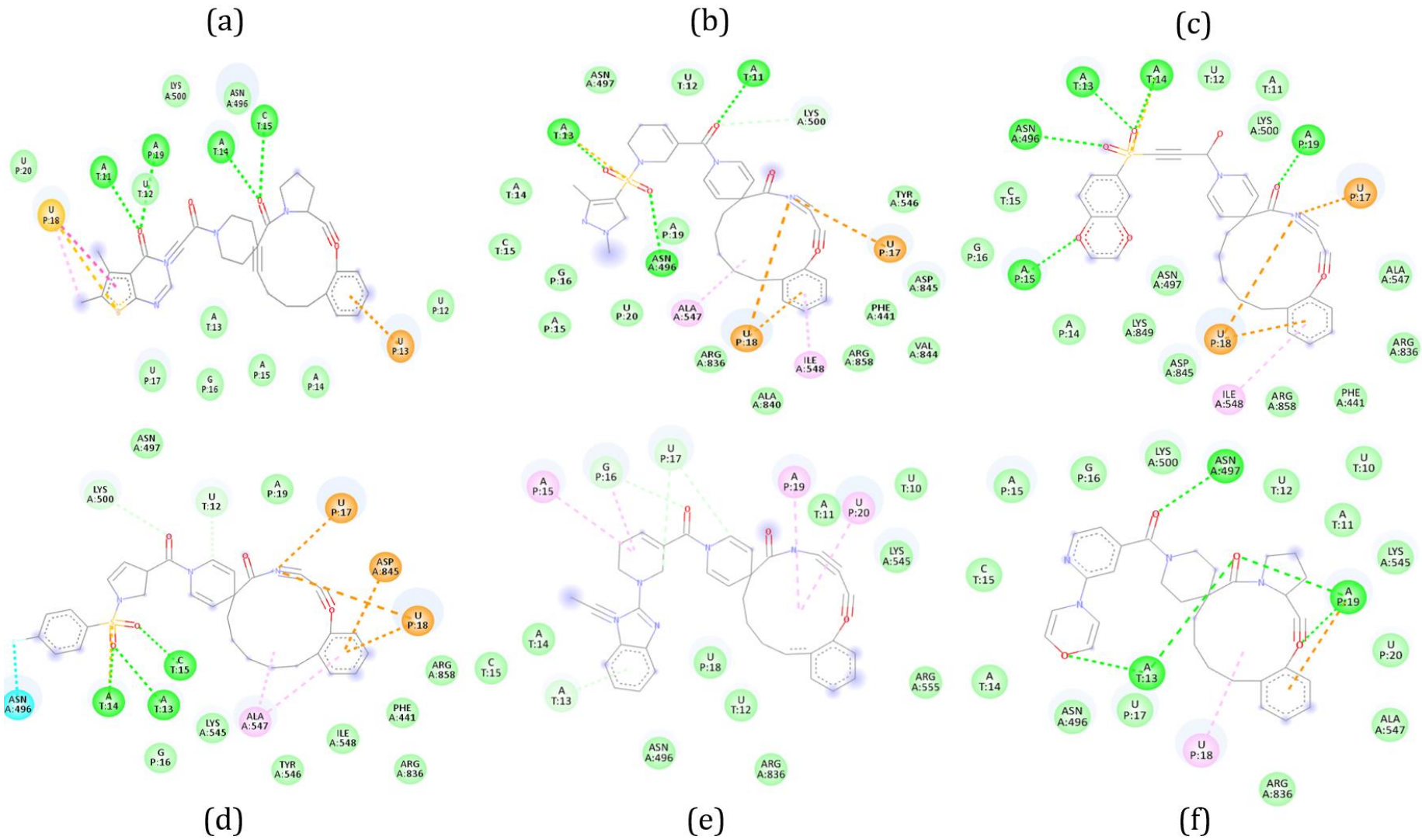

Figure S3. 2-D interactions of ligands compound **14** (a), compound **15** (b), compound **16** (c), compound **17** (d), compound **18** (e) and compound **19** (f) with 7BV2. Poses have been generated using Biovia Discovery Studio 2020.[1]

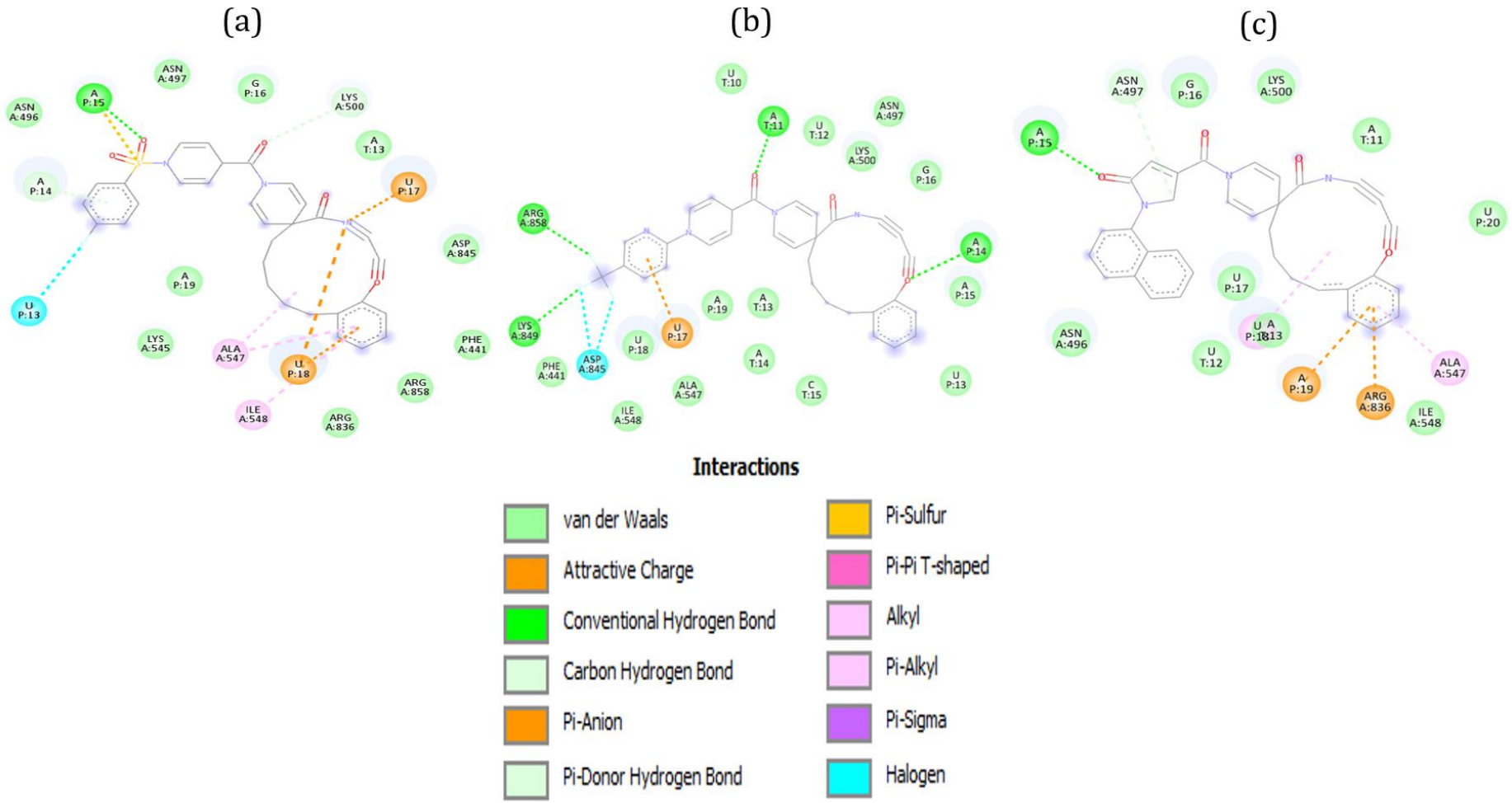

Figure S4. 2-D interactions of ligands **20** (a), **21** (b) and **22** (c) with 7BV2 (RdRp). Poses have been generated using Biovia Discovery Studio 2020.[1]

2. MD Simulations

Systems of MD simulation were assessed for their equilibration in terms of energy (kcal/mol), pressure (bar) and temperature (K) and were found to be equilibrated satisfactorily as these values were found to have consistency over the run time of the 10 ns (

Figure **S5**, and Figure S6 for compounds **2** and **3**, respectively). For the complex of **2** with RdRp, average energy, pressure and temperature were observed -1378180 kJ/mol, 1.082 bar and 300.011 K, respectively. Similarly, for the complex of **3** with RdRp, average energy, pressure and temperature were estimated -1378250 kJ/mol, 0.822 bar and 300.005 K, respectively.

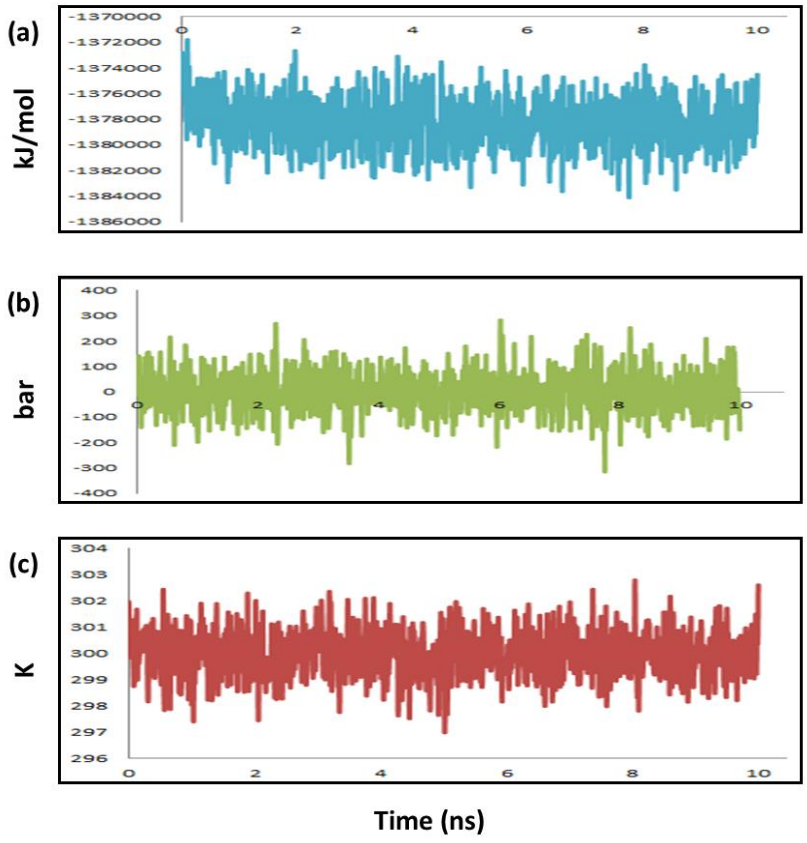

Figure S5. Energy equilibria (a), pressure equilibria (b) and temperature equilibria (c) of trajectory of complex of compound **2** with RdRp.

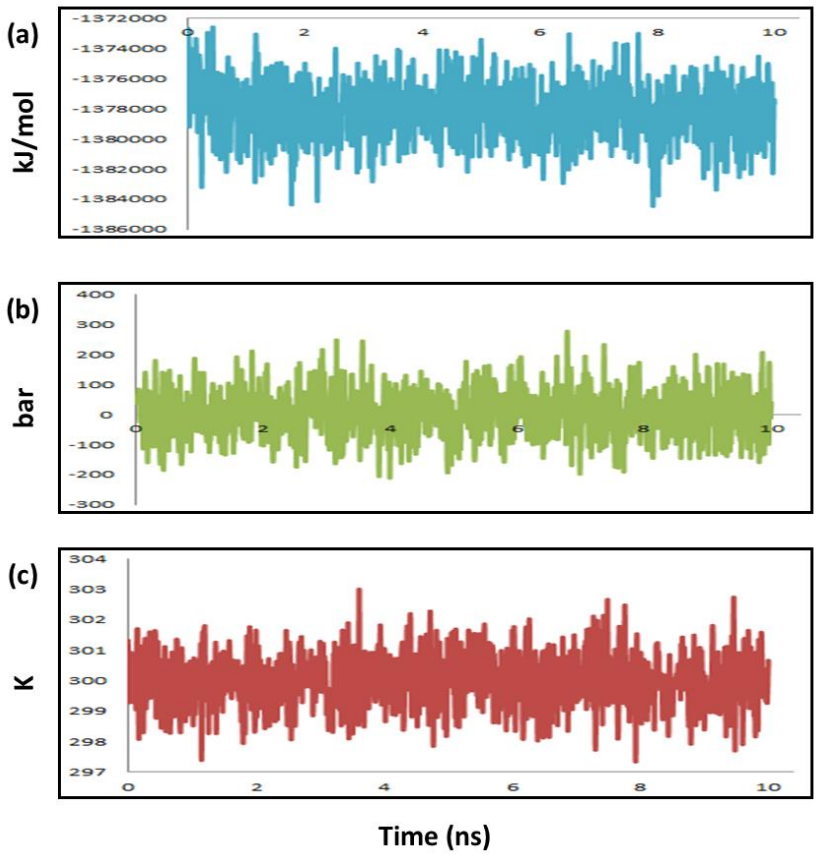

Figure S6. Energy equilibria (a), pressure equilibria (b) and temperature equilibria (c) of trajectory of complex of compound **3** with RdRp.

3. Reference

(1) Dassault Systèmes BIOVIA, BIOVIA Workbook, Release 2021; BIOVIA DS Visualizer, Release 2021, San Diego: Dassault Systèmes, 2021.