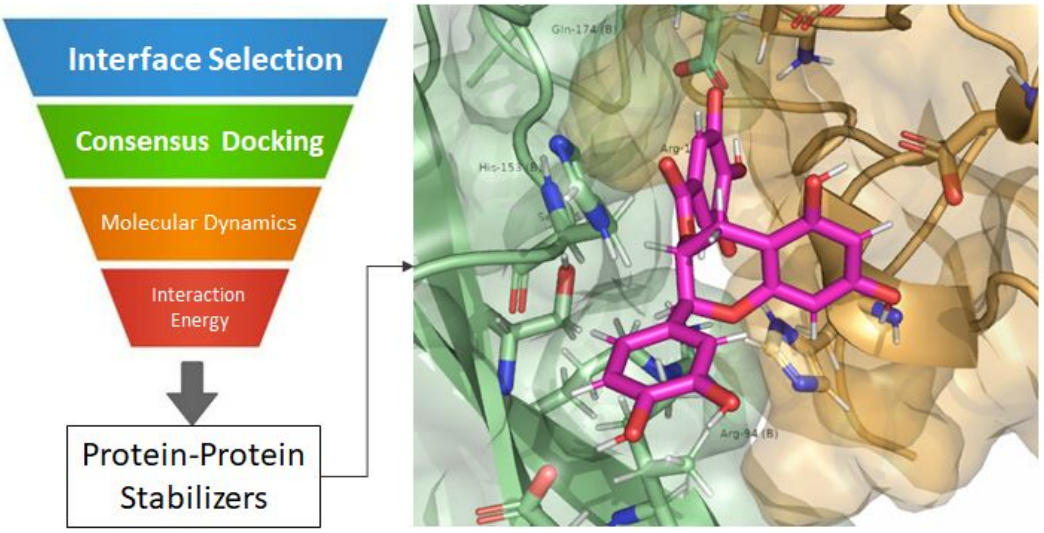
Supplementary Information



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Additional Information about the Methodology

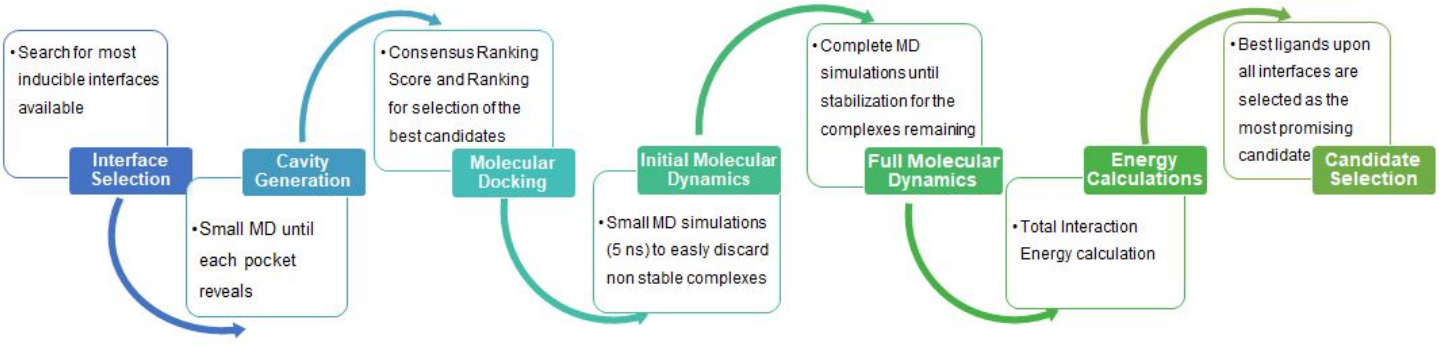

Figure S1. General scheme of the protocol developed for this research.

Interface Preparation

Dimers were subjected to a minimization, heating and NPT equilibration process in order to generate small cavities, where it is possible to locate a ligand that stabilizes. Thus, three dimers interfaces were obtained, which monomers are formed with residues 44-180 of the NTD N protein.

Molecular Docking Studies

Compounds from the DrugBank 5.1.16 database were screened against dimer interfaces. The protonation state of each ligand at pH 7.4 was based on analysis using FixpKa, included in QUACPAC 2.0.2.2 (QUACPAC 2.0.2.2: OpenEye Scientific Software, Santa Fe, NM. http://www.eyesopen.com) and its conformers were generated using Omega (Hawkins PCD *et al.* 2010) . Molecular docking was performed to find and score binding poses on interfaces by means of FRED software. Using Make Receptor tool, include in the OEDocking 3.4.0.2 suite, OpenEye (OEDOCKING 3.4.0.2: OpenEye Scientific Software, Santa Fe, NM. http://www.eyesopen.com.) a docking region was selected to include the dimer interface. Parameters were kept to their default value.

Based on the results, the Phenol-Explorer database (Neveu V. *et al.* 2010) was included to be treated with this same docking protocol.

Consensus Docking Score (CDS) was calculated with the following equation:

$$CDS = \frac{Score\ IF-1}{Average\ Score\ IF-1} + \frac{Score\ IF-2}{Average\ Score\ IF-2} + \frac{Score\ IF-3}{Average\ Score\ IF-3} + \frac{Score\ RNA}{Average\ Score\ RNA}$$

Molecular Dynamics (MD) Simulations

MD simulations were performed on complexes of the selected ligands and dimers. These systems have a positive net charge, chlorides were added as counterions with Leap module to achieve electroneutrality. The

neutralized complexes were immersed in a box of TIP3P waters which extended up to 15 Å from the complex. Dimers were described using the Amber14SB force field (Maier J. *et al.* 2015). Ligands were described using the Generalized Amber Force Field (GAFF) (Wang J. *et al.* 2004) with charges derived from RESP, which were calculated with Antechamber module and Gaussian03 (XX). Leap and Antechamber (Wang W. *et al.* 2006) are included in the package AmberTools 19.0 (D.A. Case *et. al.* 2019)

All MD simulations were run using the NAMD 2.13 software (Philips J. *et al.* 2005). The van der Waals interaction cutoff distances were set at 12 Å and long-range electrostatic forces were computed using the particle mesh Ewald summation method with a grid size set to 1.0 Å. The 1-4 contributions were multiplied by a factor of 0.83 to match the AMBER force field requirements. The complexes were submitted to a series of minimization stages (including hydrogens, waters, residue side chains and the complete system) of 100,000 maximum steps each, and heating from 0 to 310K. For equilibration/production simulations, constant temperature (310 K) was maintained using Langevin dynamics with a damping coefficient of 5 ps^{-1}, while pressure was kept constant at 1 atm through the Nosé-Hoover Langevin piston method with a decay period of 200 fs and a damping time constant of 100 fs. A time step of 1 fs was used along molecular mechanics. Bonds involving H atoms of waters were constrained using the SHAKE algorithm. Cationic Dummy Atom method (Pang Y. 2001) was used when the Zn^{2+} cation is included in the system.

Interaction energy calculations

With the intention to quantify the dimer stabilization exerted by the ligand, two stabilization components were considered: ligand-dimer and monomer-monomer interactions. The sum of these two components was called total interaction. These components were calculated using free energy decomposition analysis, which were performed using a pairwise energy decomposition scheme (idecomp option 3) with the MMPBSA.py module (Miller B. *et al.* 2012). In this scheme, interactions are decomposed by specific residue pairs by including only those interactions in which one atom from each of the analyzed residues is participating, following the work of Gohlke et al.(Gohlke C.K and Case D. 2003) A single trajectory based on 50 snapshots was taken from the last 5 ns portion (100 ps interval) of the MD production trajectories. The entropic change of the complexes was assumed constant to reduce computational cost. The solvation free energy (ΔGsolv) was separated into polar and non-polar contributions. The polar contribution to ΔGsolv was calculated using the generalized Born (GB) model implemented in MMPBSA.py module: igb=2/mbondi2 raddi sets and igb=8/mbondi3 radii sets as selected models for ligand-protein and monomer-monomer interactions, respectively. Further, this decomposition scheme allowed us to assign the percentage of the ligand-dimer interaction to each monomer, and thus ensure that there is a balanced distribution. CPPTRAJ (Cheatham T. and Roe D. 2013) and ParmEd programs, included in AmberTools, were used for trajectory handling.

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Compounds Structures

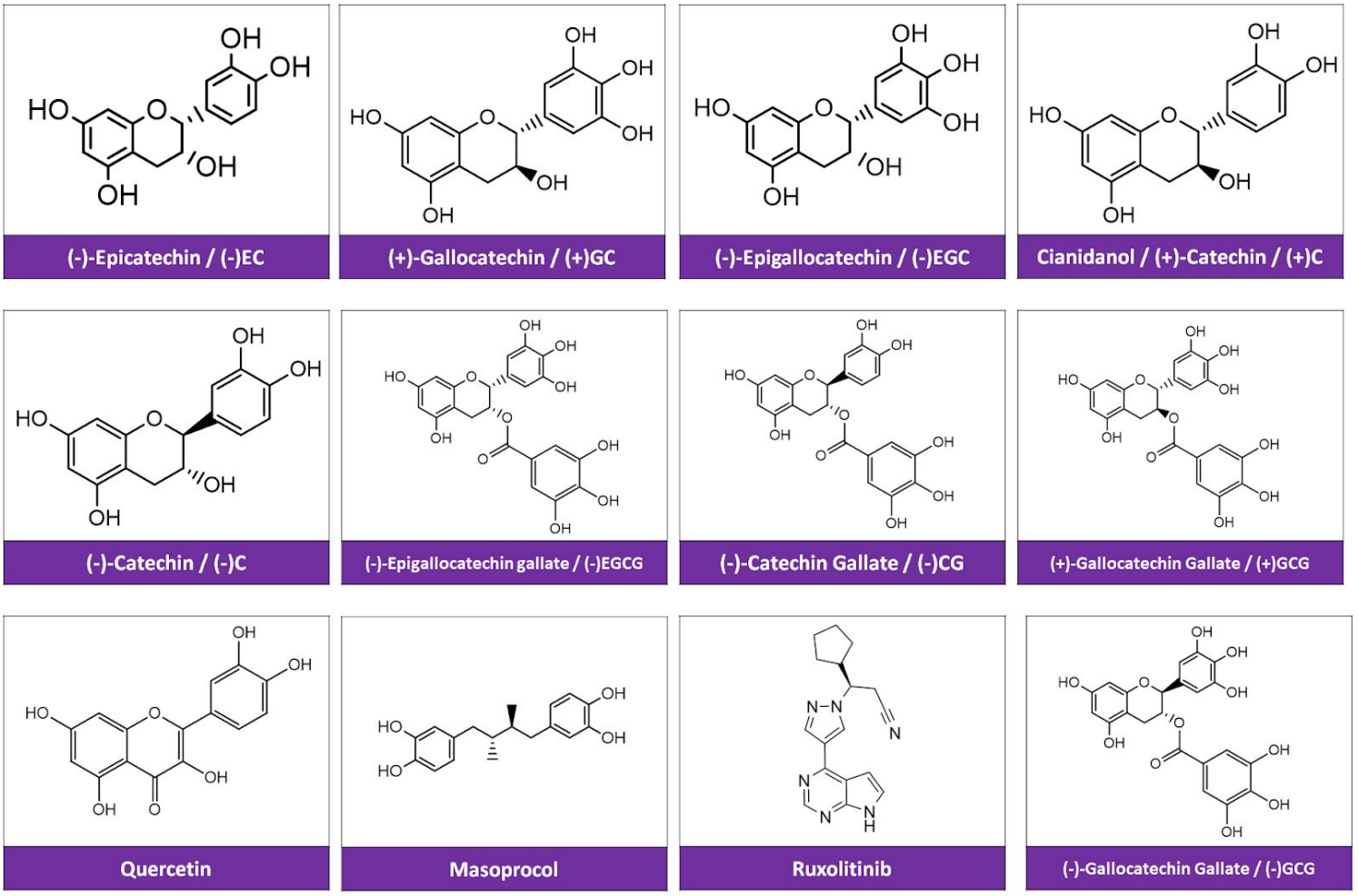


Figure S2. Structure of the compounds that stabilized at least two interfaces

Docking

Docking Results

Table S1. Summary of Docking Results. Compounds with the best consensus docking score of all three docked interfaces are displayed.

Molecule Name	Database	Score IF-1	Pos. IF-1	Score IF-2	Pos. IF-2	Score IF-3	Pos. IF-3	Score RNA	Pos. RNA	Position *Consensus* Docking
Rosmarinic acid	Polyphenol	-11,0	108	-11,6	312	-13,0	41	-8,5	1	1
Gallic acid 3-O-gallate	Polyphenol	-12,2	24	-12,4	75	-14,2	8	-6,4	151	2
Ignotine	Investigational	-12,3	21	-11,2	477	-10,9	437	-7,9	2	3
255734-04-4	Investigational	-11,0	116	-11,2	472	-13,3	23	-7,0	50	4
Butein	Polyphenol	-12,1	25	-11,8	195	-12,3	93	-6,4	164	5
4-Caffeoylquinic acid	Polyphenol	-11,4	59	-10,2	1334	-14,9	2	-6,2	253	6
Epigallocatechin	Investigational / Polyphenol	-11,2	83	-12,6	43	-12,4	82	-6,3	195	7
Tienamicina	Approved	-10,6	177	-11,9	182	-13,9	14	-6,2	245	8
1-Butylguanidinium	Polyphenol	-11,3	68	-9,3	2184	-14,0	13	-6,9	53	9
Cianidanol	Approved / Polyphenol	-12,2	23	-11,8	198	-12,8	52	-5,7	516	10
(+)-Gallocatechin 3-O-gallate	Polyphenol	-11,6	41	-12,9	21	-12,6	64	-5,5	650	11
(+)-Gallocatechin	Polyphenol	-11,7	37	-12,0	156	-12,9	46	-5,7	543	12
5-hidroxy-L-tryptophan	Approved	-11,8	35	-11,8	201	-10,5	596	-6,9	60	13
5-Br-2'-Deoxyuridine	Investigational	-12,0	30	-10,7	819	-10,7	503	-7,2	31	14
o6-bencylguaniane	Investigational	-12,5	18	-11,4	391	-10,8	462	-6,4	143	15
Diazepinomicin	Investigational	-9,0	760	-13,6	4	-10,7	525	-7,5	9	16
177975-08-5	Investigational	-9,7	414	-11,3	416	-13,1	33	-6,9	59	17
Ruxolitinib	Approved	-13,1	7	-9,9	1651	-11,1	346	-6,6	98	18
1-[Amino-(3,4-dichloroanilino)methylidene]-2-propan-2-ylguanidine	Investigational	-11,7	39	-11,1	550	-11,5	207	-6,6	97	19
Phenformin	Approved	-11,5	48	-10,9	673	-14,4	7	-5,4	830	20
Arbutamine	Approved	-9,6	482	-12,2	109	-12,9	47	-6,6	107	21
Arginin	Approved	-11,4	55	-11,4	380	-12,9	49	-5,9	386	22
Masoprocol	Approved	-12,1	26	-12,1	138	-13,2	28	-4,9	1359	23
Cyanidin	Polyphenol	-12,4	20	-11,1	541	-12,4	79	-5,6	607	24
3-Caffeoylquinic acid	Polyphenol	-10,5	198	-11,9	165	-13,4	21	-5,8	476	25
Feruloyl tartaric acid	Polyphenol	-10,5	199	-10,1	1403	-12,2	105	-7,2	21	26
(-)-Epicatechine	Investigational / Polyphenol	-11,6	46	-12,6	41	-12,2	112	-5,4	831	27
N-Butan-2-yl-1-(6-methyl-1H-benzimidazol-2-yl)piperidine-4-carboxamide	Investigational	-10,0	316	-11,7	266	-10,9	430	-7,4	15	28
Indalpine	Investigational	-10,2	272	-11,6	270	-11,9	138	-6,7	81	29
Etilevodapo	Investigational	-13,0	8	-11,4	396	-10,1	812	-6,0	315	30
ECGC	Investigational /	-8,6	1095	-11,6	320	-13,0	43	-7,1	32	31

	Polyphenol									
(-)-Catechin Gallate	Polyphenol	-8,9	798	-13,2	10	-12,4	83	-6,4	162	32
Caffeoyl tartaric acid	Investigational	-11,1	101	-11,0	619	-12,3	99	-6,1	259	33
Sedemetan	Investigational	-9,4	549	-11,3	454	-11,4	249	-7,4	13	34
Ceforanide	Approved	-10,3	245	-11,7	245	-10,3	731	-7,3	20	35
Vipadenant	Investigational	-10,0	339	-11,1	534	-11,6	195	-7,0	44	36
Valomaciclovir	Investigational	-11,3	70	-11,8	222	-13,1	29	-5,1	1090	37
Phloretin	Polyphenol	-10,2	269	-12,0	153	-10,8	460	-6,8	69	38
Solabegron	Investigational	-11,3	67	-11,3	421	-12,3	97	-5,7	509	39
Pexidartinib	Approved	-10,8	133	-10,5	984	-11,6	194	-6,7	82	40
Guanosina	Investigational	-11,5	47	-10,9	685	-10,2	795	-6,8	66	41
Vyvanse	Approved	-9,8	388	-12,2	107	-13,3	25	-5,6	569	42
Bendazac	Investigational	-11,2	89	-11,6	299	-9,7	1129	-6,9	54	43
5-Caffeoylquinic acid	Polyphenol	-10,0	323	-11,8	213	-11,5	223	-6,6	108	43
Debio-1347	Investigational	-9,7	445	-12,7	36	-11,2	296	-6,5	135	44
Procaterol	Investigational	-11,2	87	-11,8	214	-8,7	1957	-7,3	17	45
(-)-Catechin	Polyphenol	-11,2	75	-11,7	235	-12,2	108	-5,5	709	46
Triprolidine	Investigational	-10,6	179	-12,1	140	-10,5	592	-6,5	119	47
Polydatin	Approved	-8,7	1022	-12,2	113	-14,9	3	-5,4	787	48
Resveratrol 5-O-glucoside	Polyphenol	-8,7	1023	-12,2	114	-14,9	4	-5,4	788	49
Zolmitriptan	Approved	-10,8	139	-13,3	6	-11,7	185	-5,2	1000	51
(-)-Gallocatechin Gallate	Polyphenol	-7,4	2223	-13,2	11	-13,1	36	-6,3	131	55
Quercetina	Investigational	-10,9	124	-12,4	63	-11,2	310	-5,5	673	59
Brivudine	Approved	-13,8	1	-10,7	846	-9,9	1011	-5,1	1075	74
Trifluridine	Approved	-13,3	4	-10,1	1429	-11,4	241	-4,1	2262	165
Compounds selected for MD prior to Polyphenol database addition										
Catechins selected for MD prior to Polyphenol database addition										
Catechins selected for MD after Polyphenol database addition										

Correlation with previously reported activities

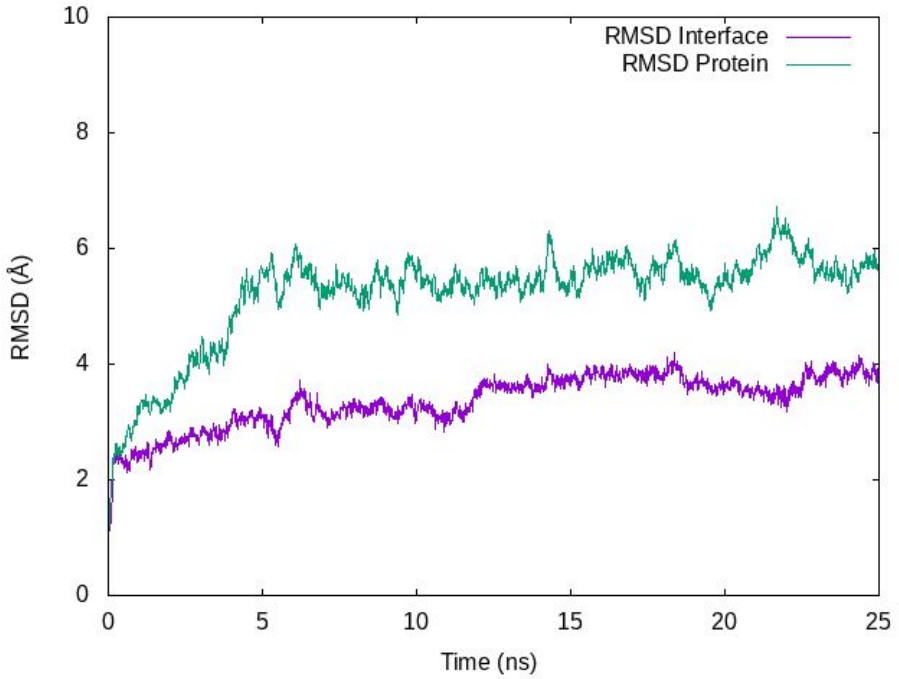
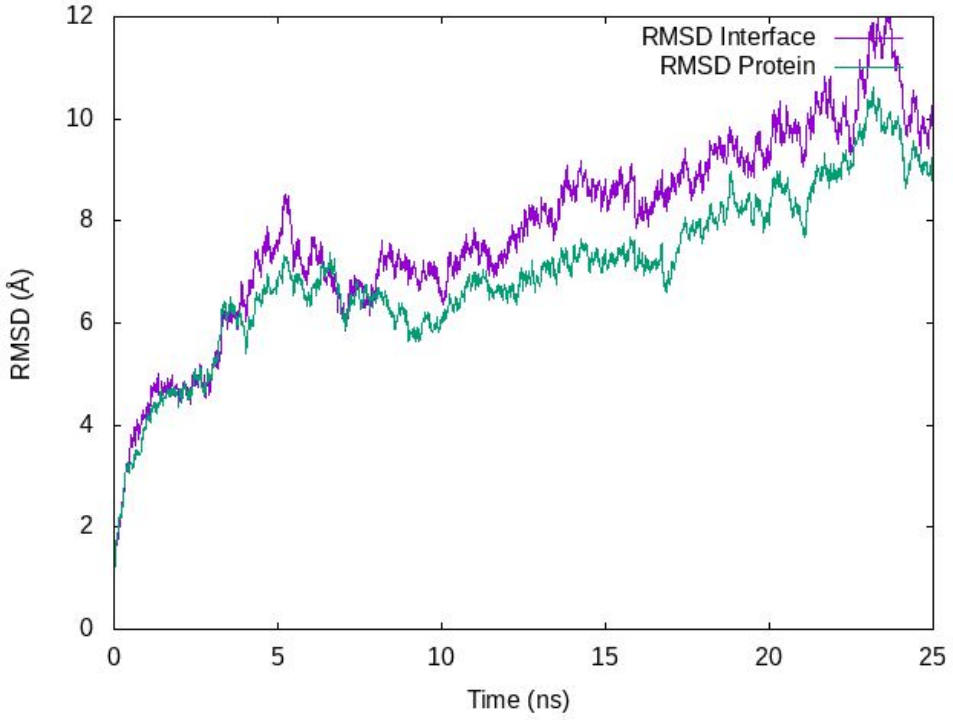
Table S2. Docking results of compounds included in Roh's work, where "Reported activity" classifies compounds according to their reported outcome.

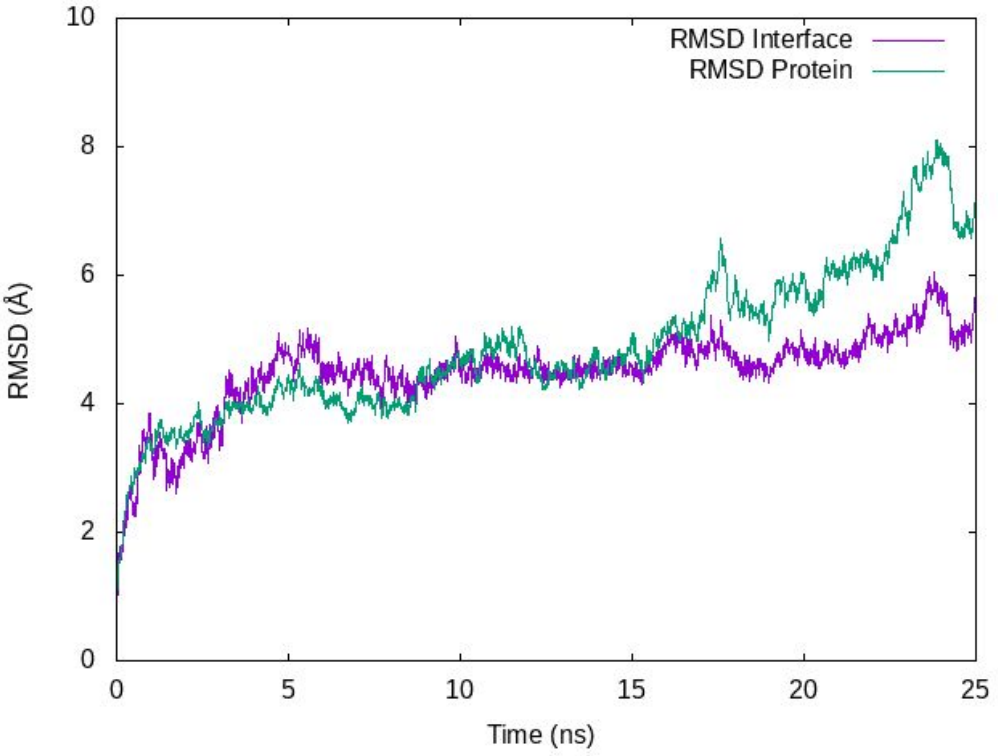
Molecule Name	Score IF-1	Position IF-1	Score IF-2	Position IF-2	Score IF-3	Position IF-3	Score RNA	Position RNA	Consensus Docking Position	Reported Activity
(-)-Catechin Gallate	-8,9	798	-13,2	10	-12,4	83	-6,4	162	32	Active
(-)-Galloatechin Gallate	-7,4	2223	-13,2	11	-13,1	36	-6,3	191	55	Active
Myricetin	-10,7	154	-12,5	55	-11,8	160	-5,2	976	63	Inactive
Quercetin	-10,9	125	-12,4	64	-11,2	311	-5,6	629	56	Inactive
(-)-Catechin	-11,2	75	-11,7	235	-12,2	108	-5,5	709	46	Inactive
Baicalein	-10,6	182	-11,5	355	-10,7	495	-5,8	455	112	Inactive
Glycitein	-7,4	2238	-11,1	523	-10,8	465	-4,3	2102	1275	Inactive
Kaempferol	-9,6	464	-10,8	706	-10,6	572	-5,2	1030	436	Inactive
Luteolin	-10,4	215	-10,8	707	-12,2	107	-5,5	683	104	Inactive
Morin	-10,3	251	-10,8	727	-10,7	508	-5,7	510	193	Inactive
Genistein	-10,8	145	-10,6	864	-11,0	376	-5,1	1155	248	Inactive
Rutin	-6,6	2973	-10,6	900	-7,0	3198	-4,1	2874	2763	Inactive
Naringenin	-9,2	657	-10,6	919	-11,1	358	-5,4	853	401	Inactive
Hesperidin	-5,9	3388	-10,0	1477	-7,6	2830	-3,5	2675	3085	Inactive
Daidzein	-9,5	515	-10,0	1558	-11,3	276	-4,5	1863	727	Inactive
Apigenin	-9,2	654	-9,5	2031	-10,8	479	-5,2	1058	719	Inactive
Naringin	-7,8	1921	-8,8	2645	-8,0	2577	-4,1	2301	2645	Inactive
Diosmin	-4,8	3717	-7,2	3474	-8,5	2099	-3,7	2570	3407	Inactive

Molecular Dynamics

Ligand-Free Interfaces

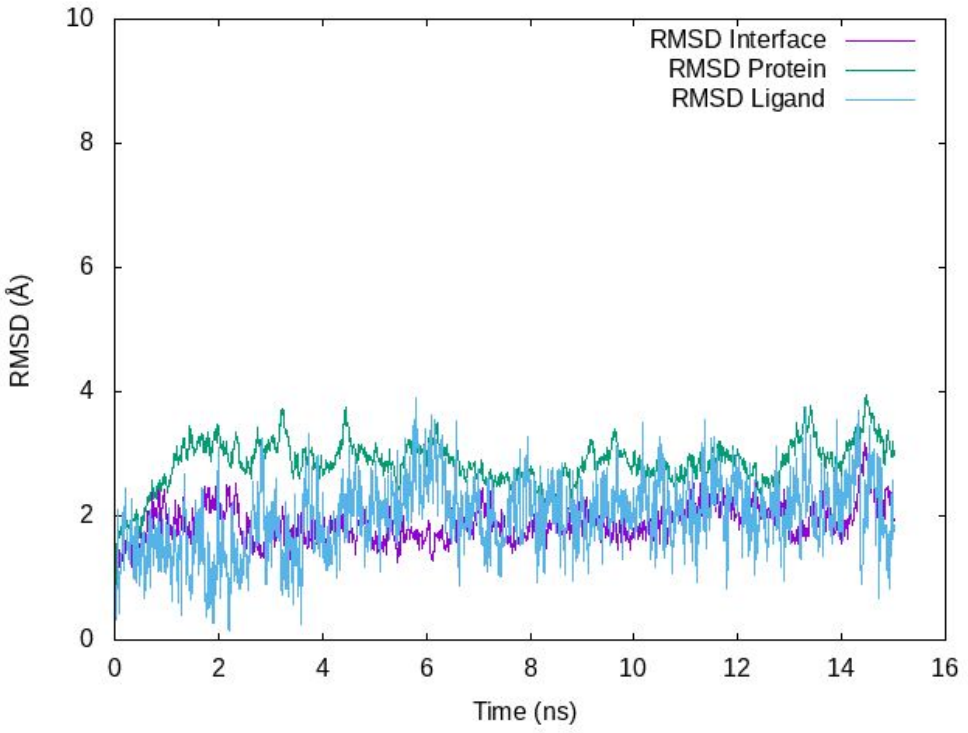
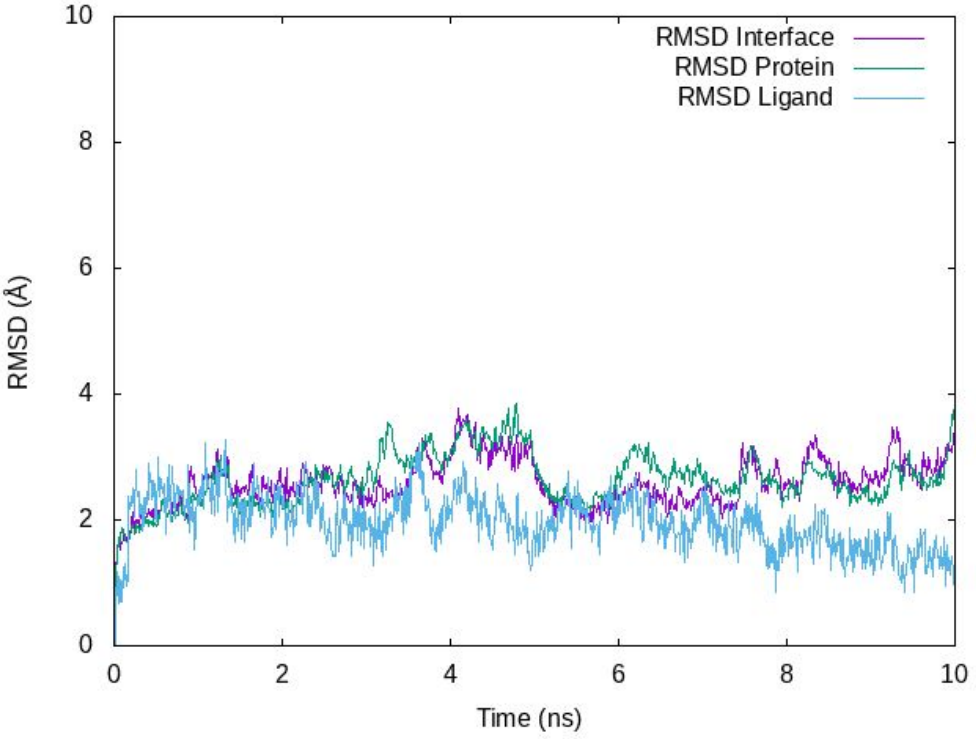
Table S3. RMSD profiles of the equilibration/production stage is shown for ligand-free interfaces. "RMSD Protein" was measured considering all residues in the complex aligned using the protein backbone. "RMSD Interface" were calculated aligning by the interface-forming residues and then measured using those same residues.

Ligand ID	**RMSD**
IF-1	
IF-2	

IF-3	 RMSD Interface RMSD Protein RMSD (Å) Time (ns) 0 2 4 6 8 10 0 5 10 15 20 25

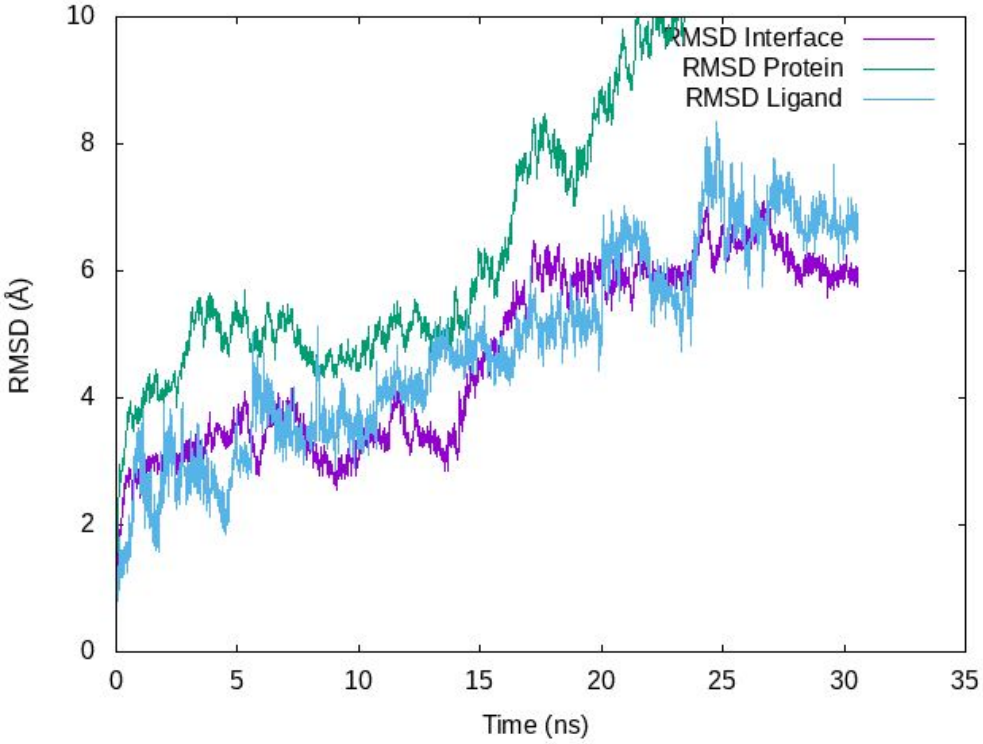
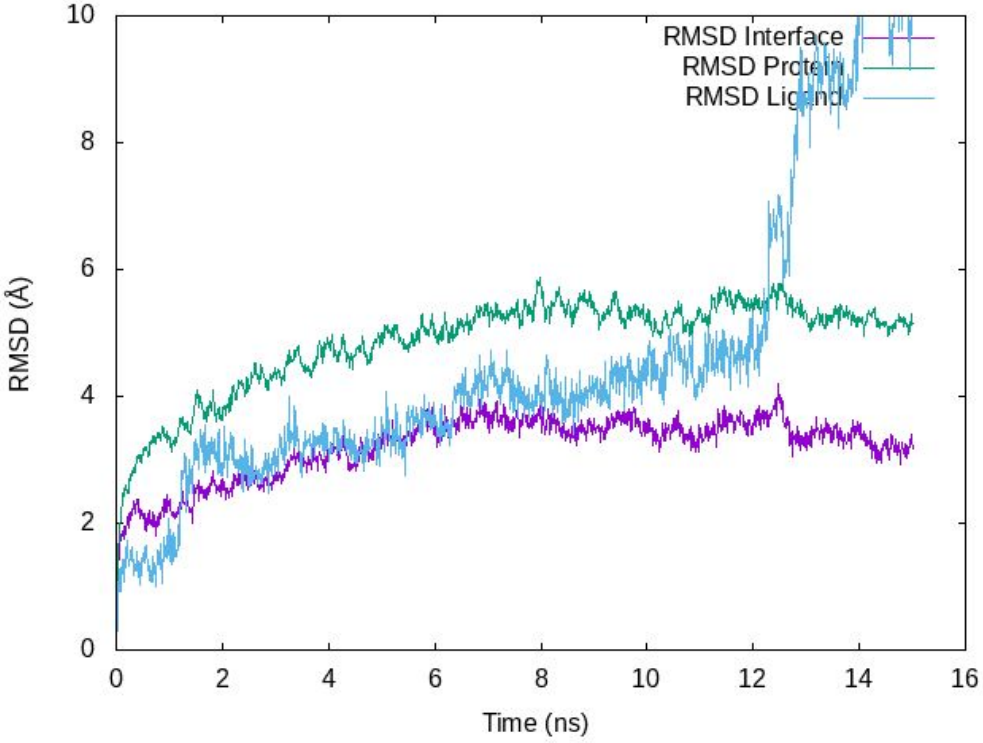
Interfaces and their Interaction with Zn

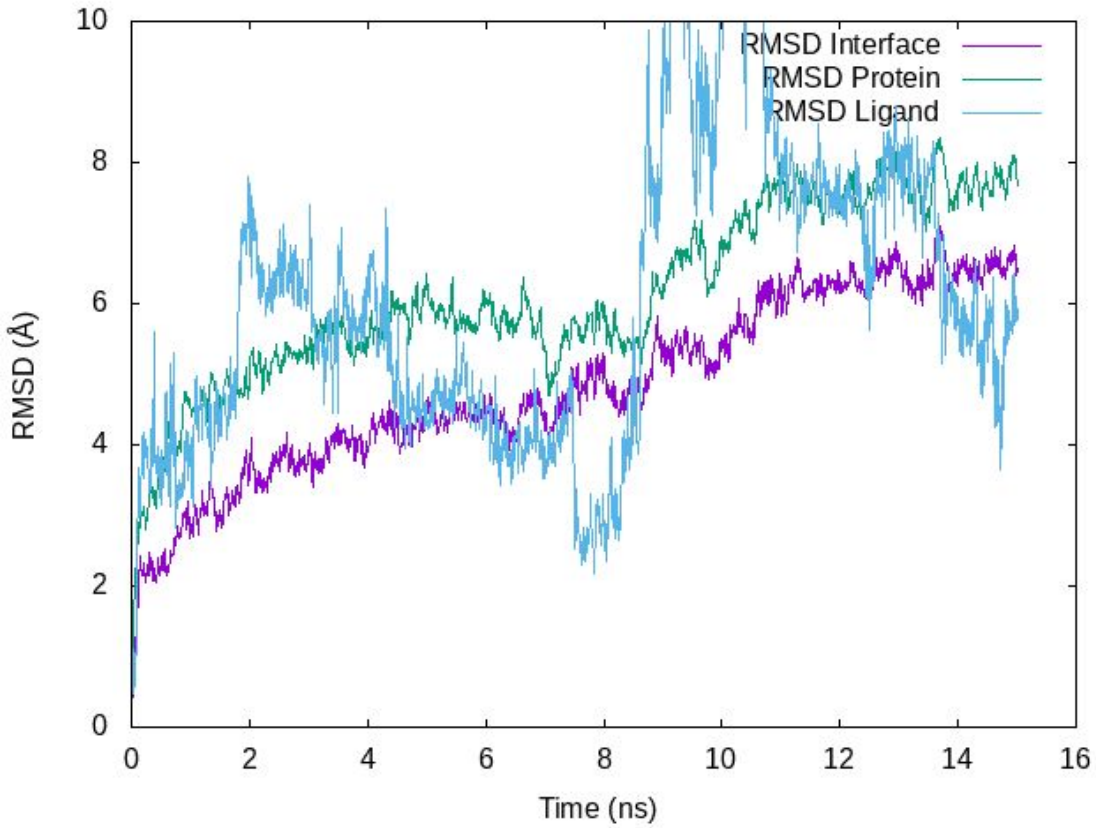
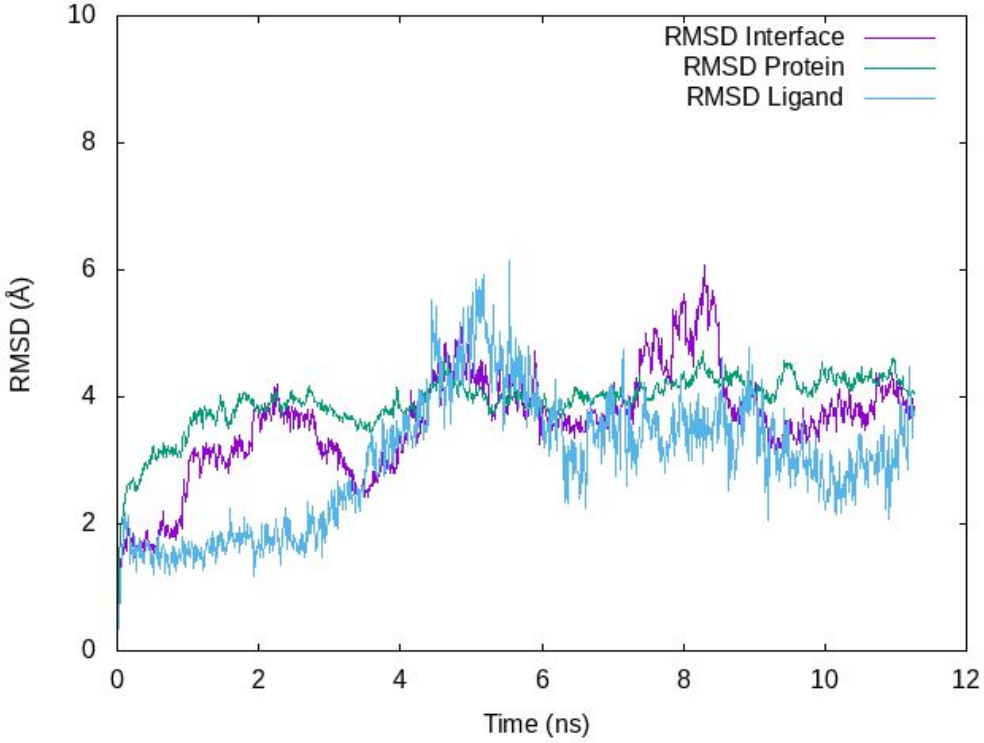
*Table S4. RMSD profiles of the equilibration/production stage is shown for **IF-1** and **IF-2** interacting with Zn. "RMSD Protein" was measured considering all residues in the complex aligned using the protein backbone. "RMSD Interface" and "RMSD Ligand" were calculated aligning by the interface-forming residues and then measured using those same residues and Zn^{2+}, respectively.*

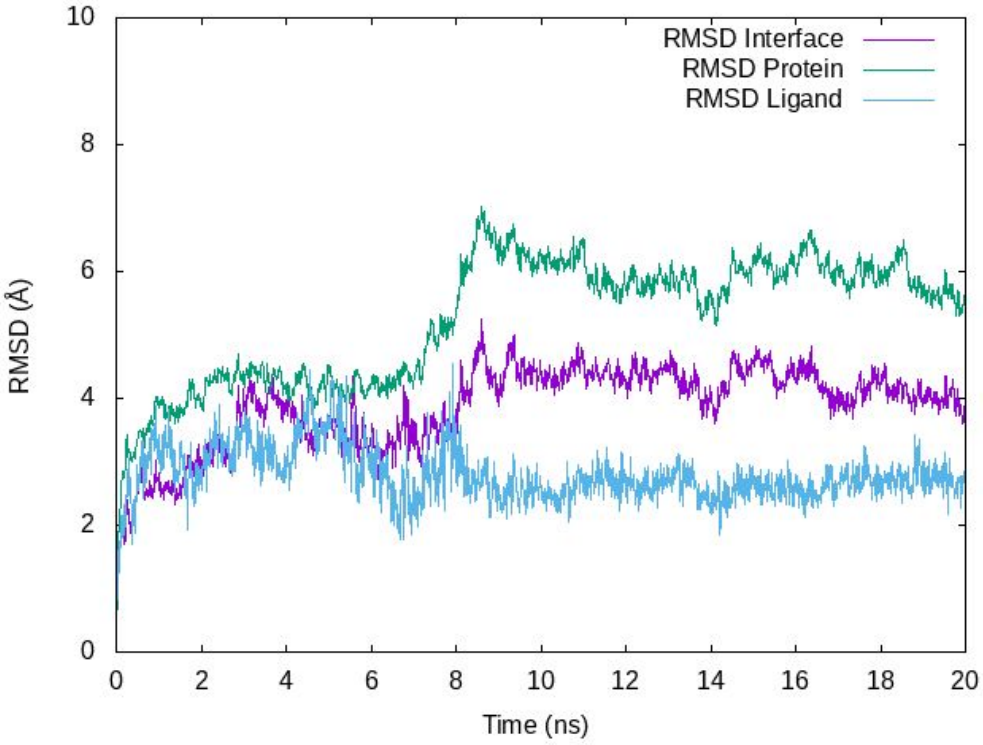
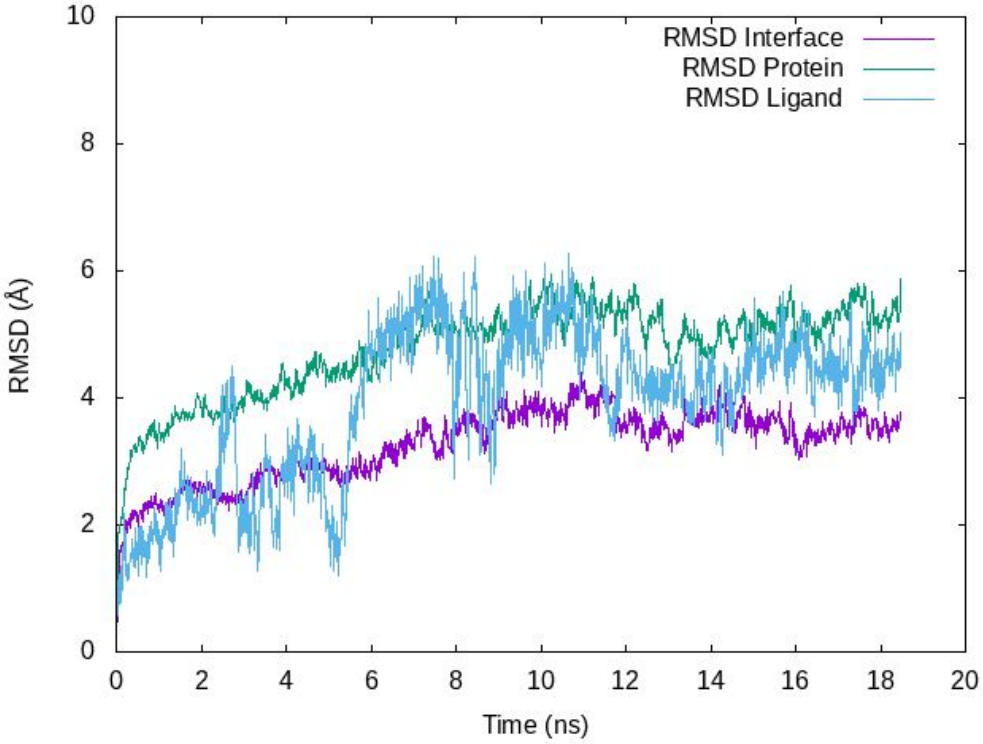
Ligand ID	RMSD
IF-1	
IF-2	

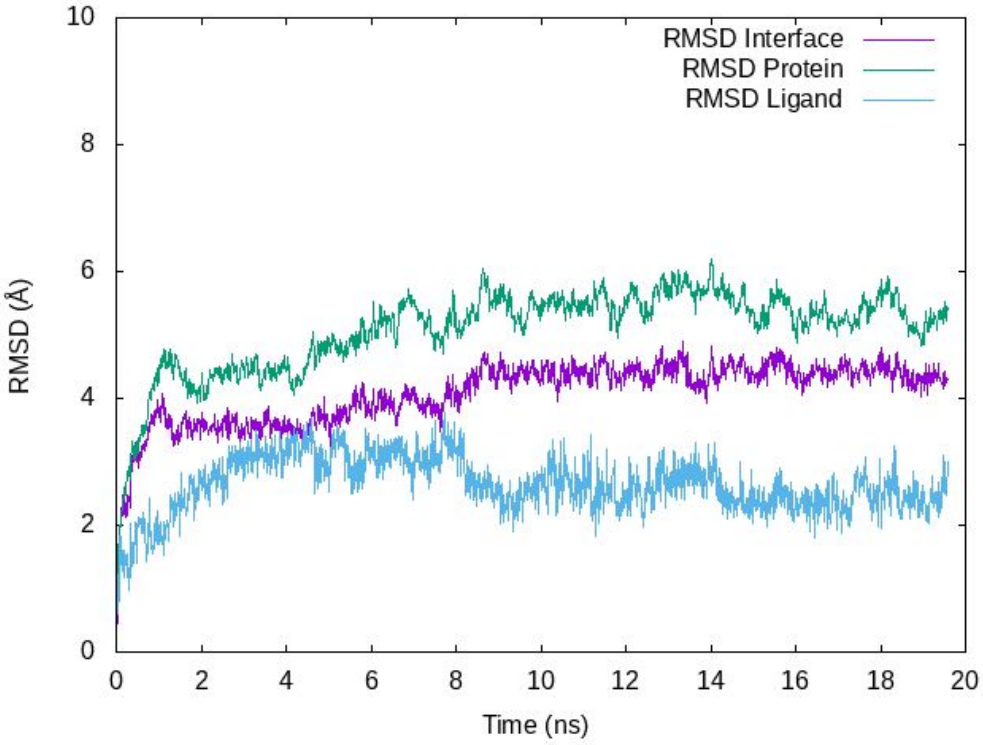
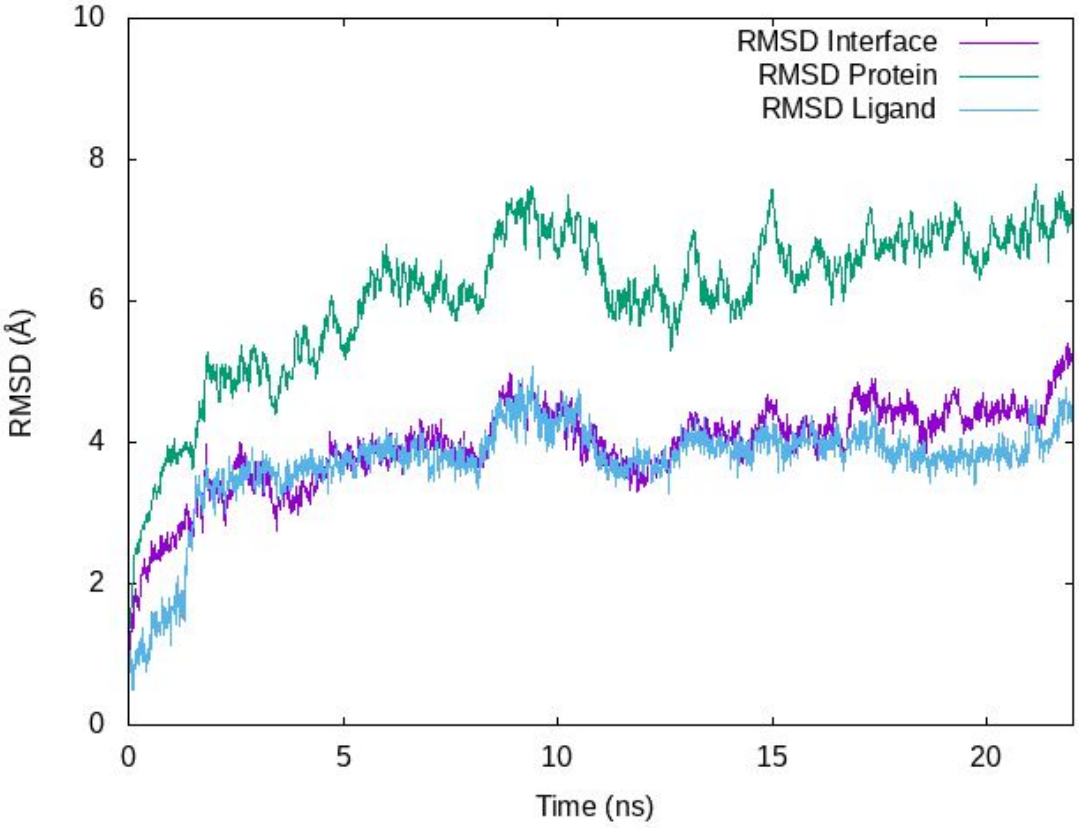
IF-1

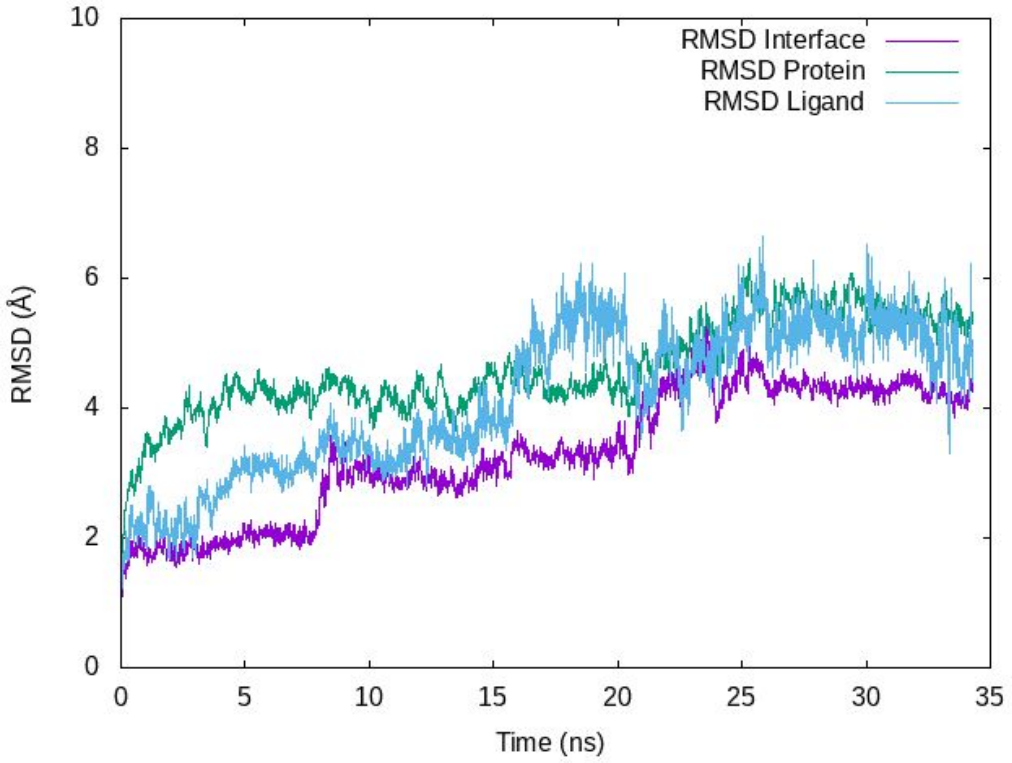
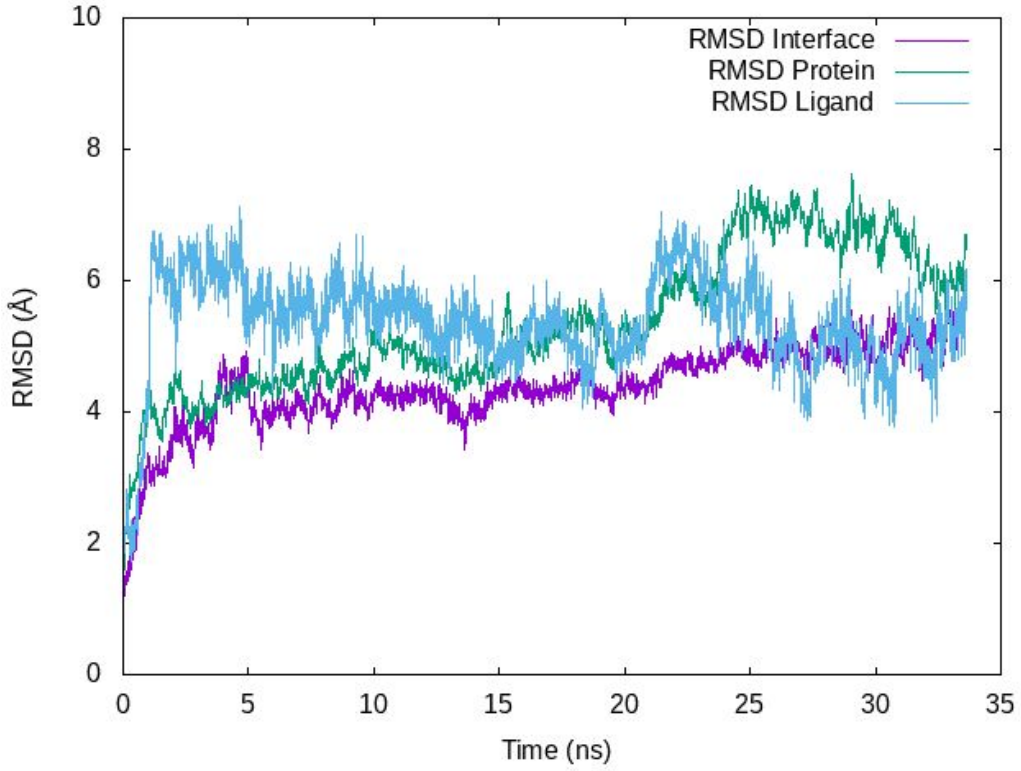
*Table S5. RMSD profiles of the equilibration/production stage is shown for each compound in **IF-1**. "RMSD Protein" was measured considering all residues in the complex aligned using the protein backbone. "RMSD Interface" and "RMSD Ligand" were calculated aligning by the interface-forming residues and then measured using those same residues and the ligand, respectively.*

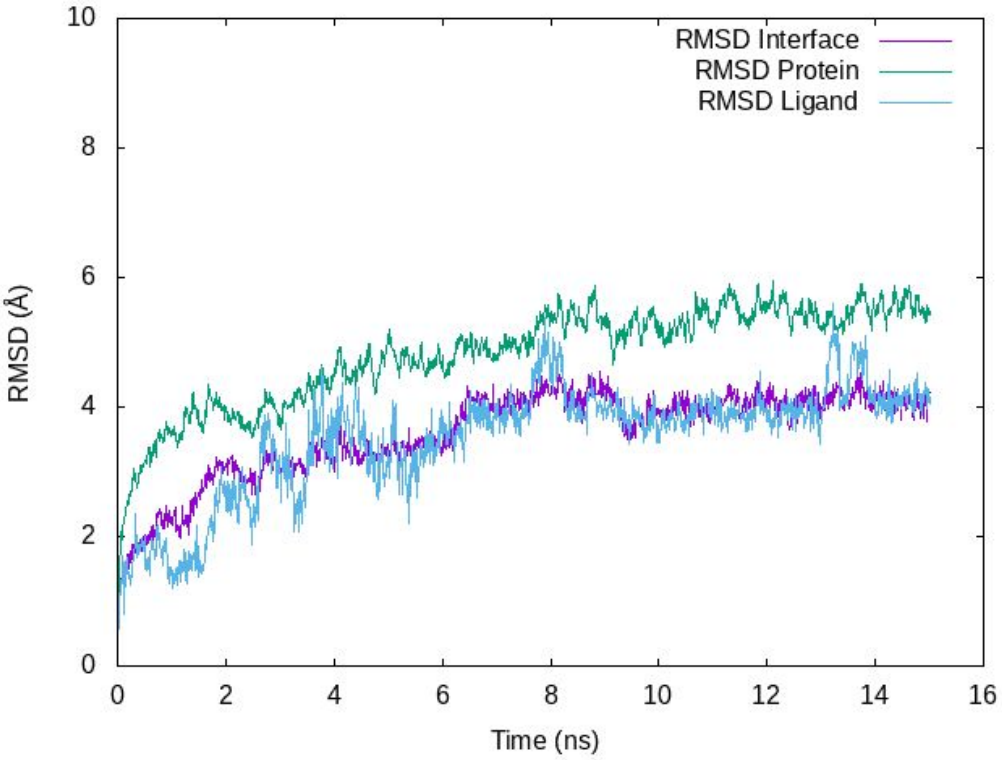
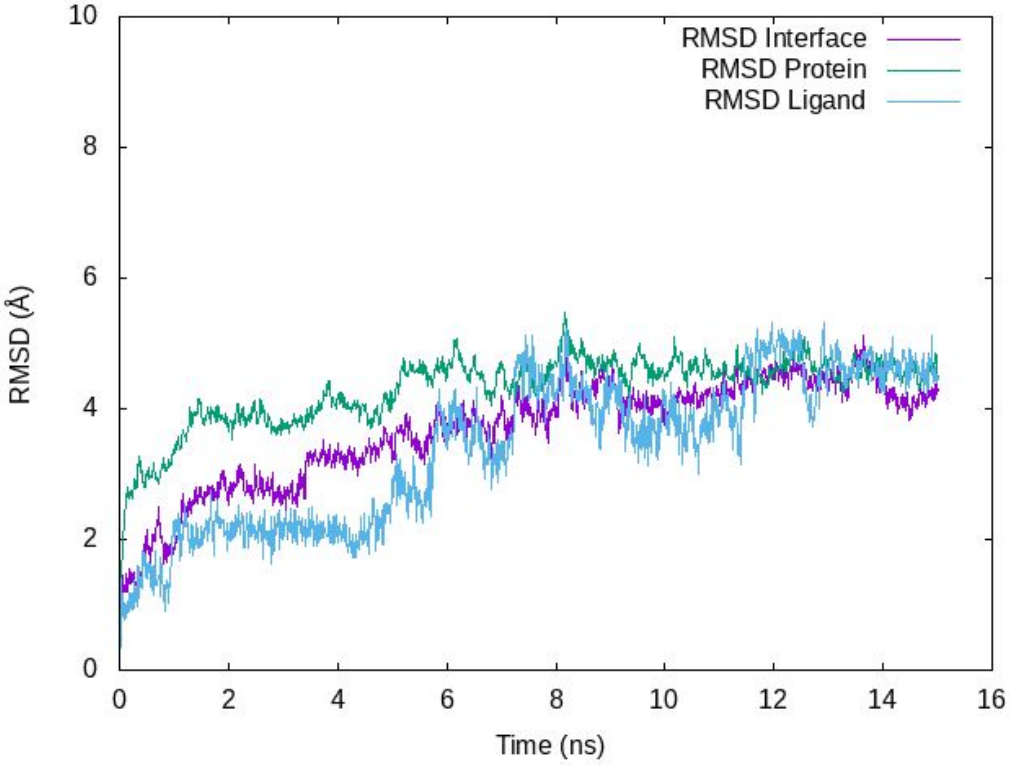
Ligand ID	RMSD
Masoprocol	
Trifluridine	

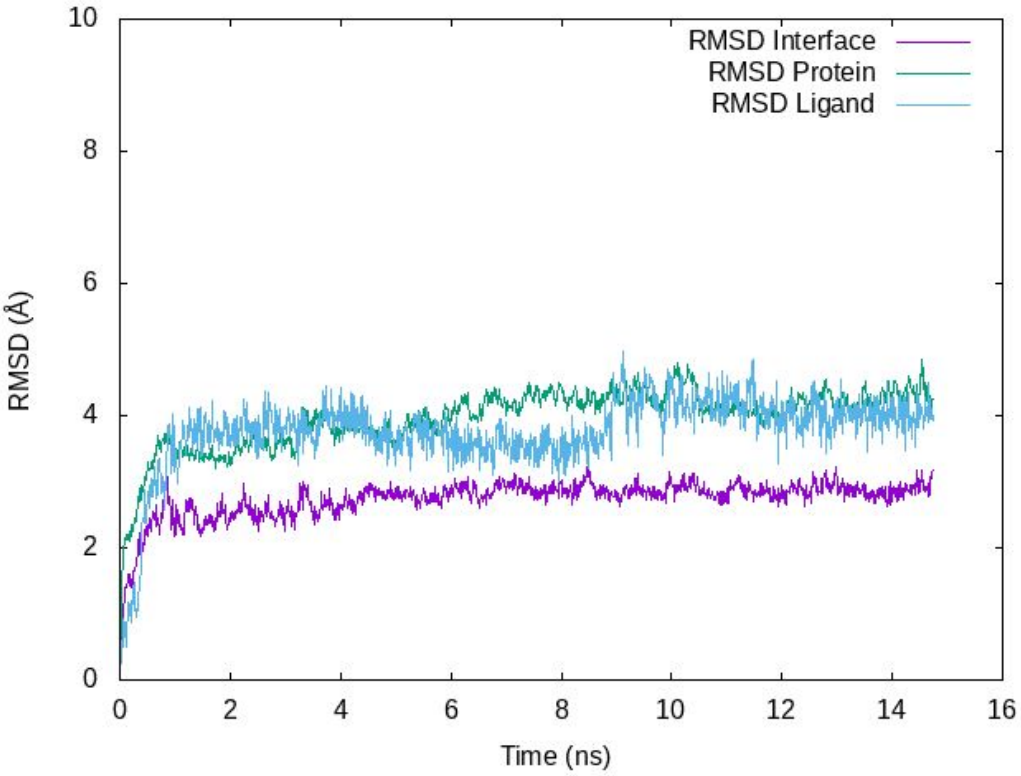
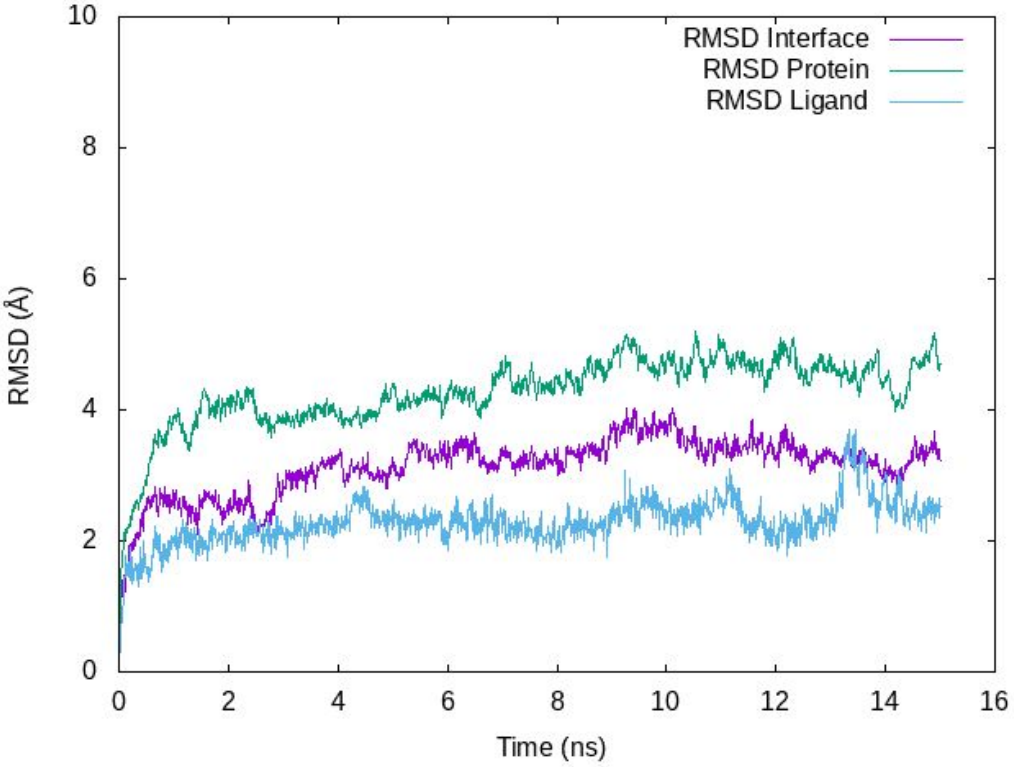
Brivudine	
(-)EGC	

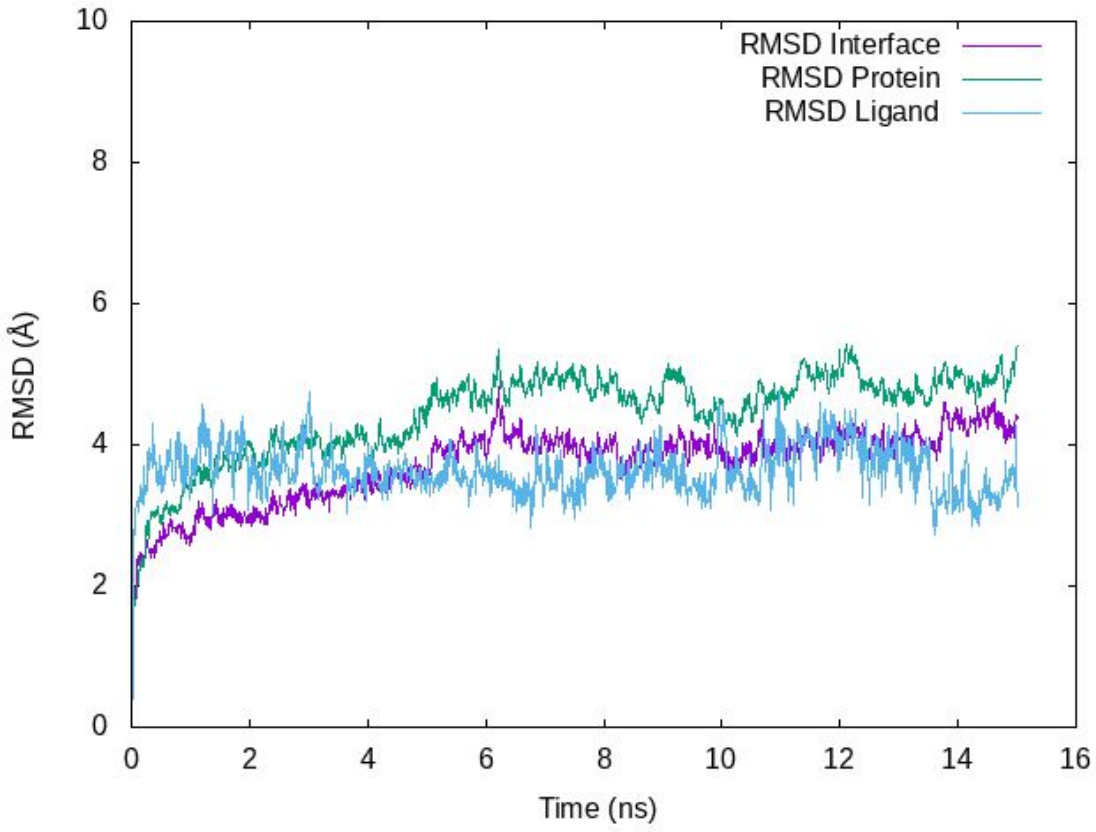
Quercetin	
Ruxolitinib	

(-)EC	 RMSD Interface RMSD Protein RMSD Ligand RMSD (Å) Time (ns) 0 2 4 6 8 10 0 2 4 6 8 10 12 14 16 18 20
(-)EGCG	 RMSD Interface RMSD Protein RMSD Ligand RMSD (Å) Time (ns) 0 2 4 6 8 10 0 5 10 15 20

Cianidanol	
Gallic acid 3-O-gallate	

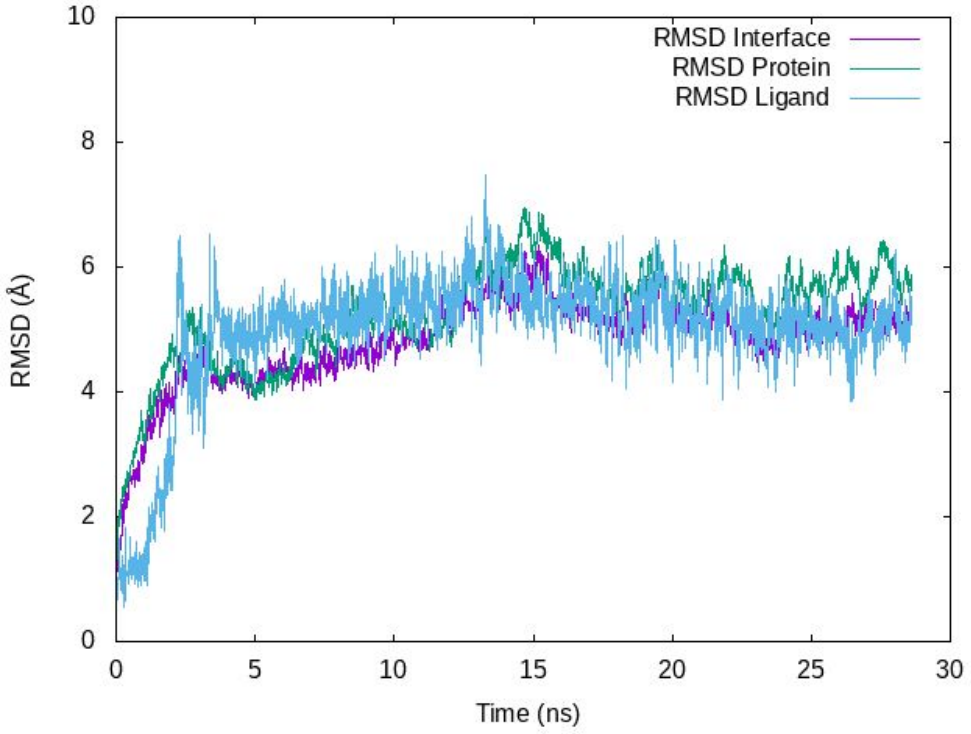
(+)GC	 RMSD Interface RMSD Protein RMSD Ligand RMSD (Å) Time (ns) 0 2 4 6 8 10 12 14 16
(+)GCG	 RMSD Interface RMSD Protein RMSD Ligand RMSD (Å) Time (ns) 0 2 4 6 8 10 12 14 16

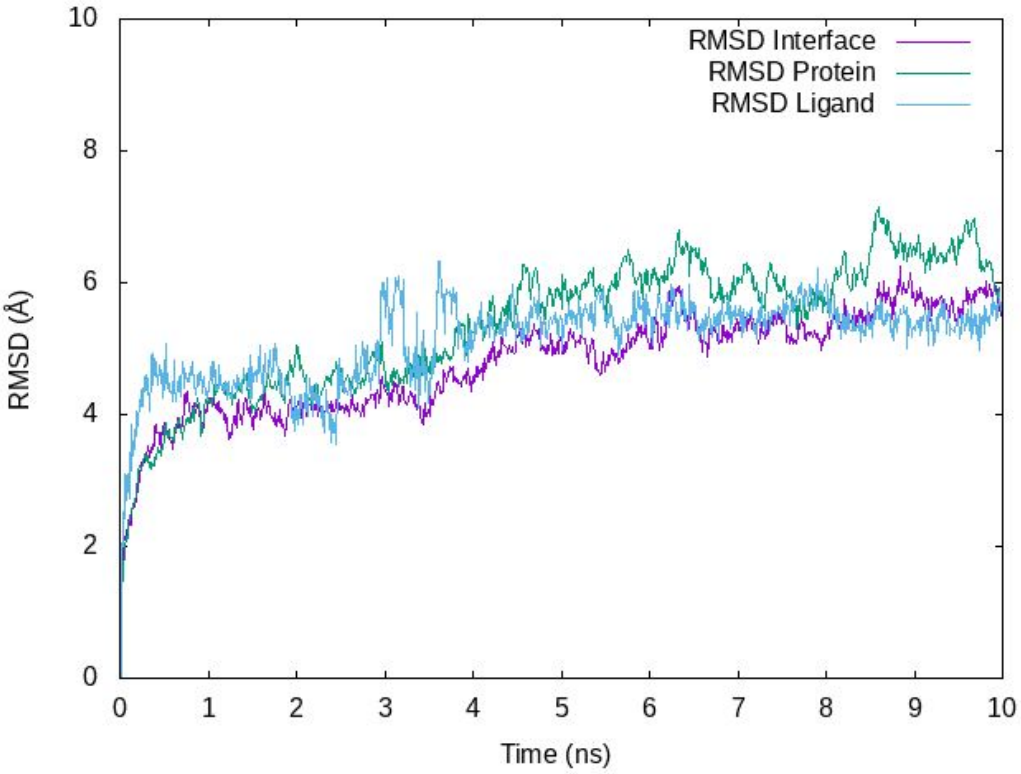
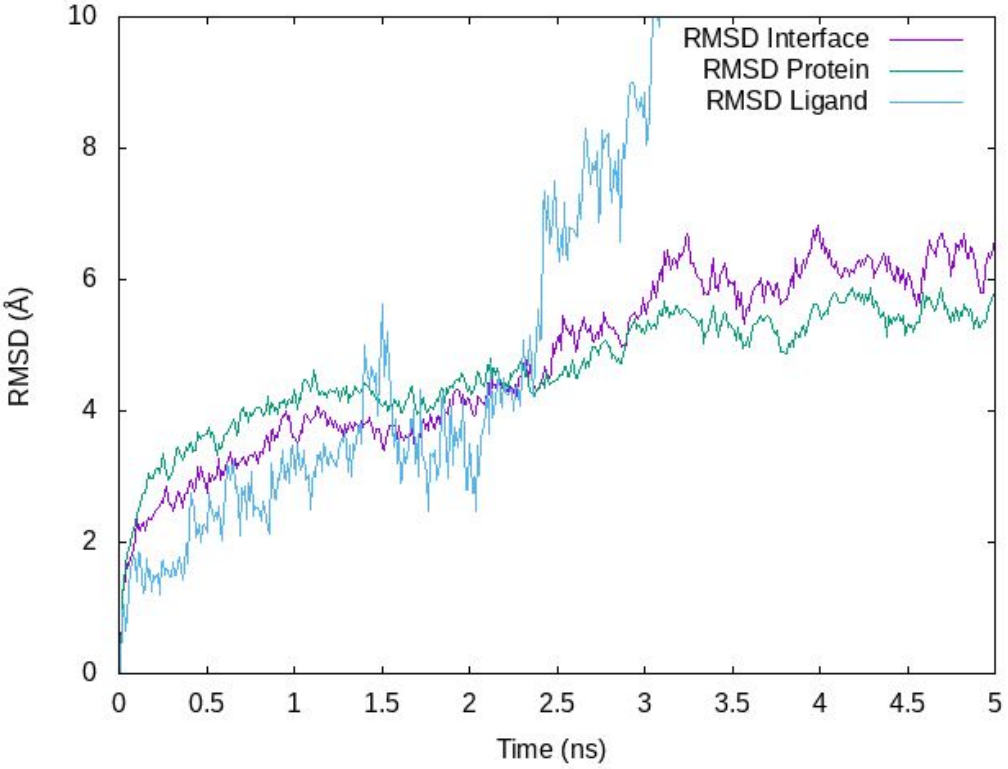
(-)C	 RMSD Interface RMSD Protein RMSD Ligand RMSD (Å) Time (ns) 0 2 4 6 8 10 12 14 16
(-)CG	 RMSD Interface RMSD Protein RMSD Ligand RMSD (Å) Time (ns) 0 2 4 6 8 10 12 14 16

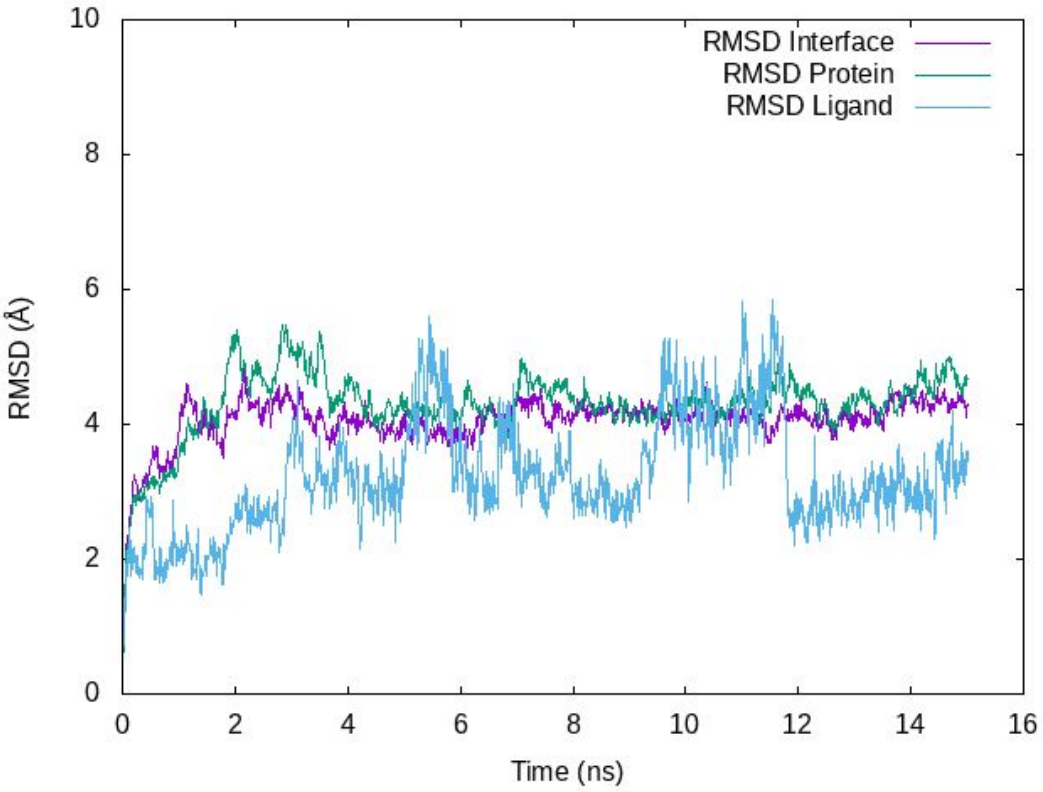
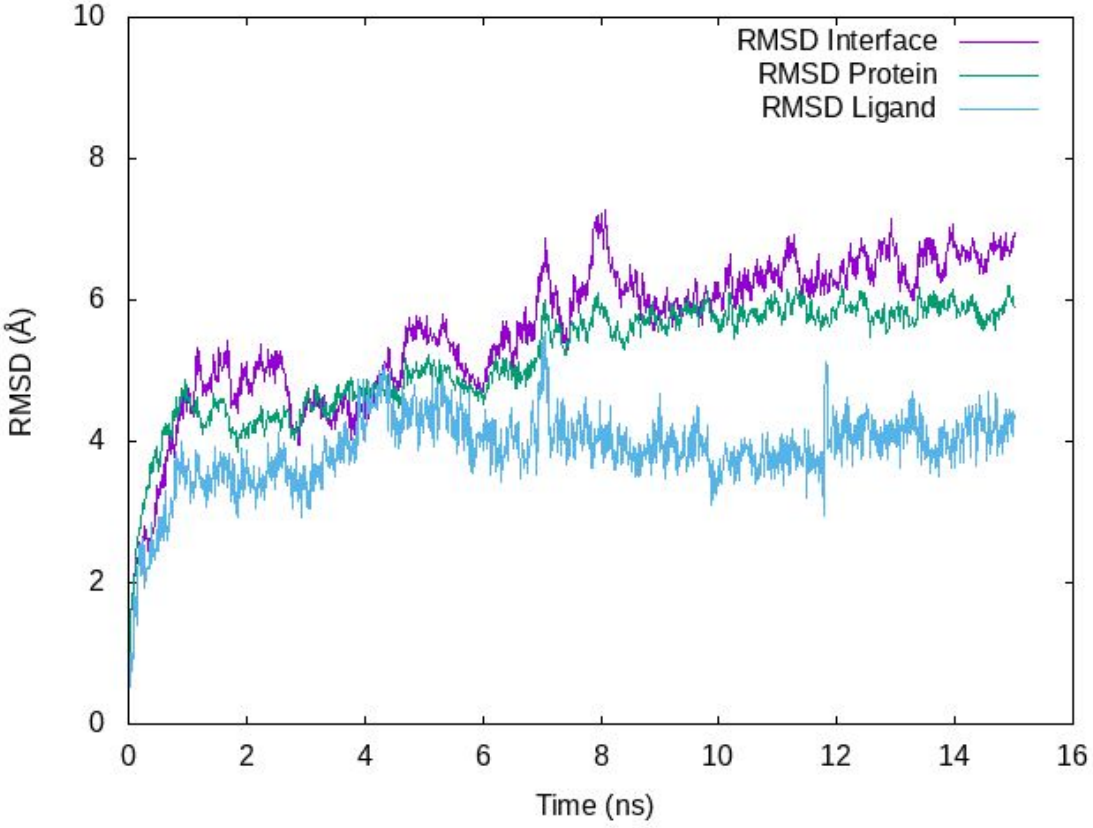
(-)GCG	

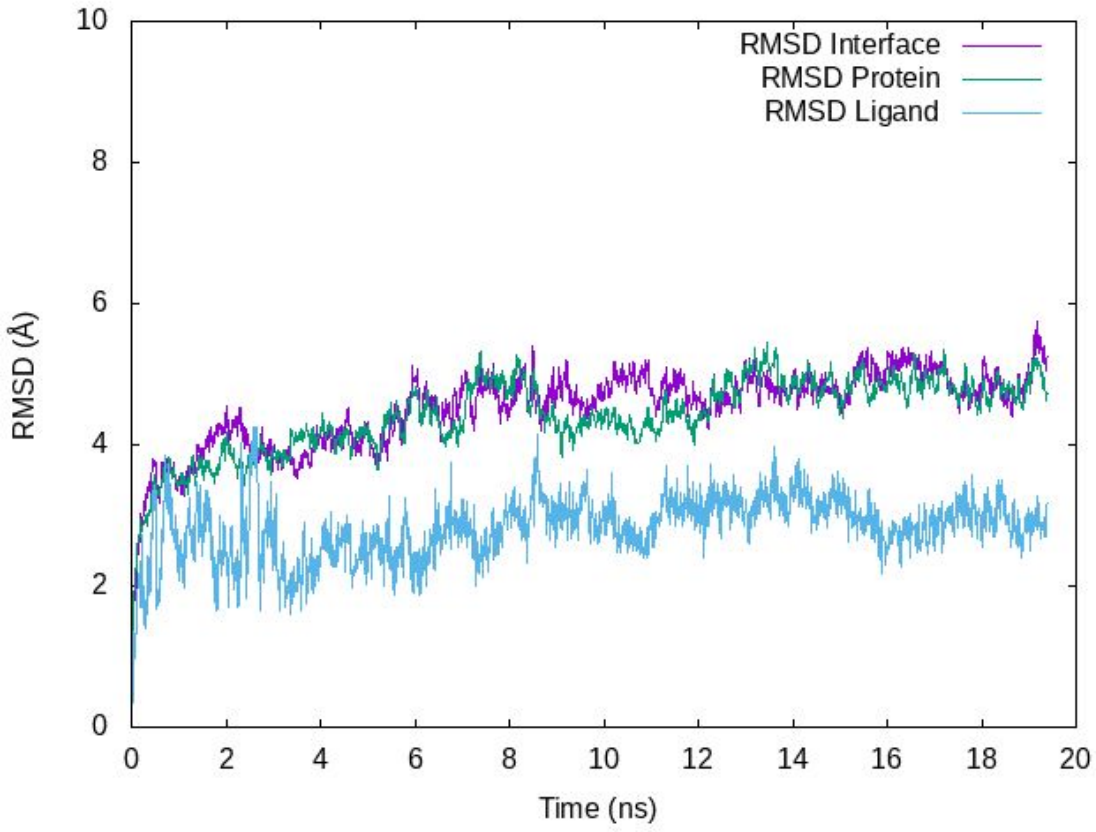
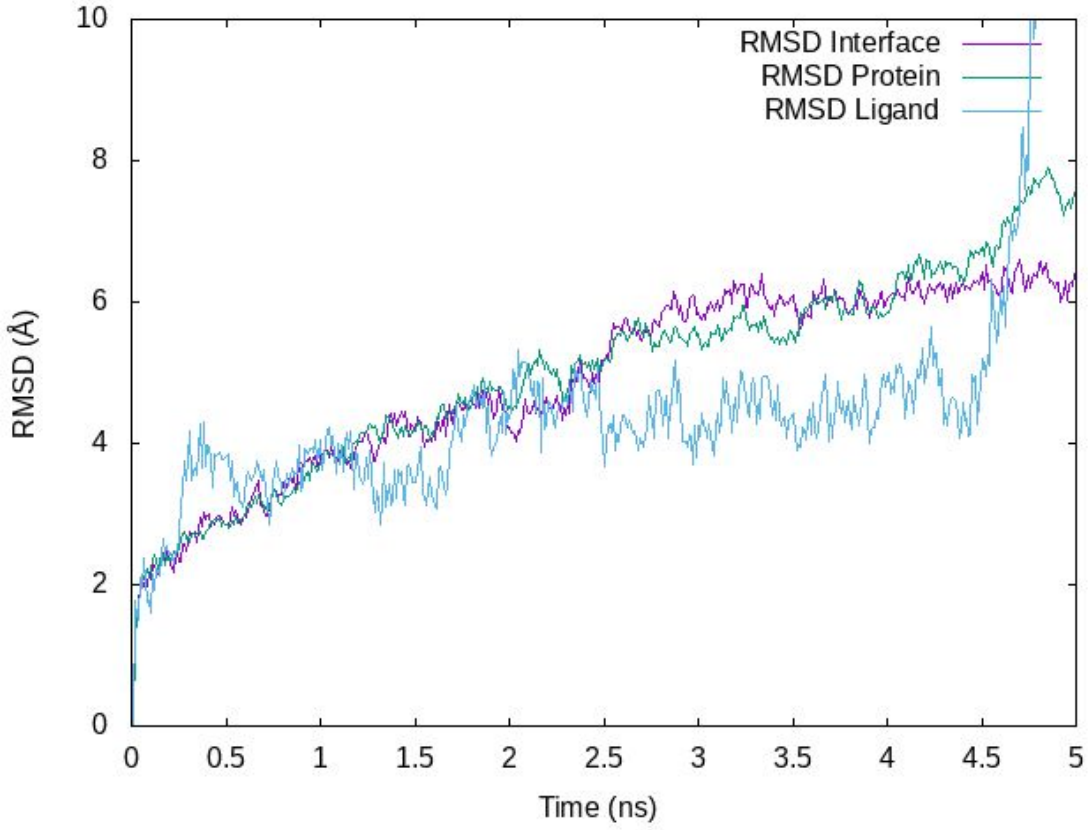
IF-2

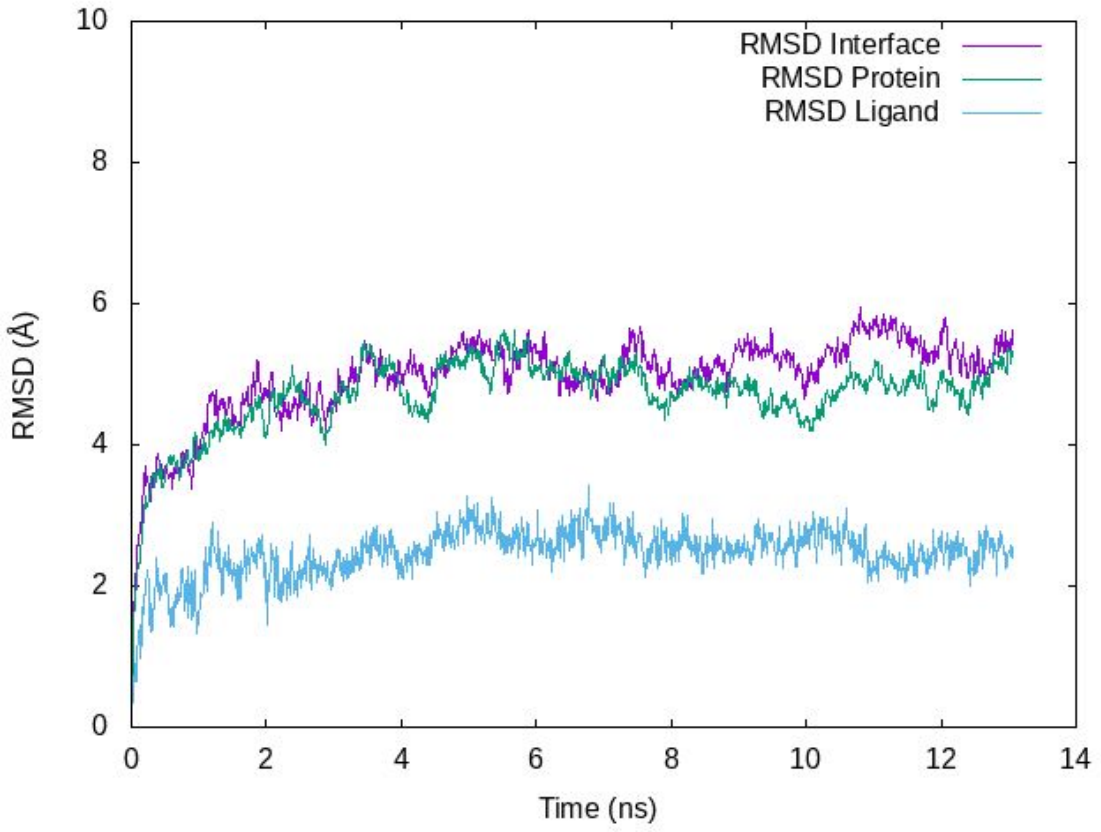
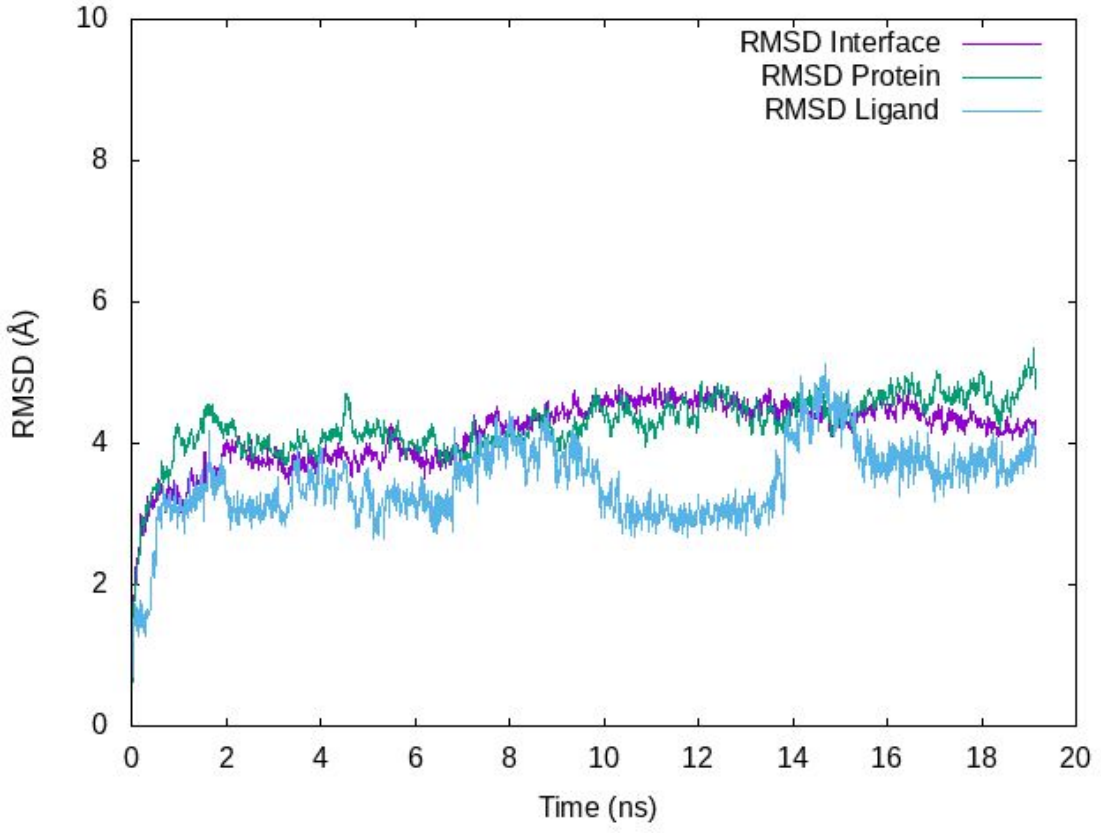
*Table S6. RMSD profiles of the equilibration/production stage is shown for each compound in **IF-2**. "RMSD Protein" was measured considering all residues in the complex aligned using the protein backbone. "RMSD Interface" and "RMSD Ligand" were calculated aligning by the interface-forming residues and then measured using those same residues and the ligand, respectively.*

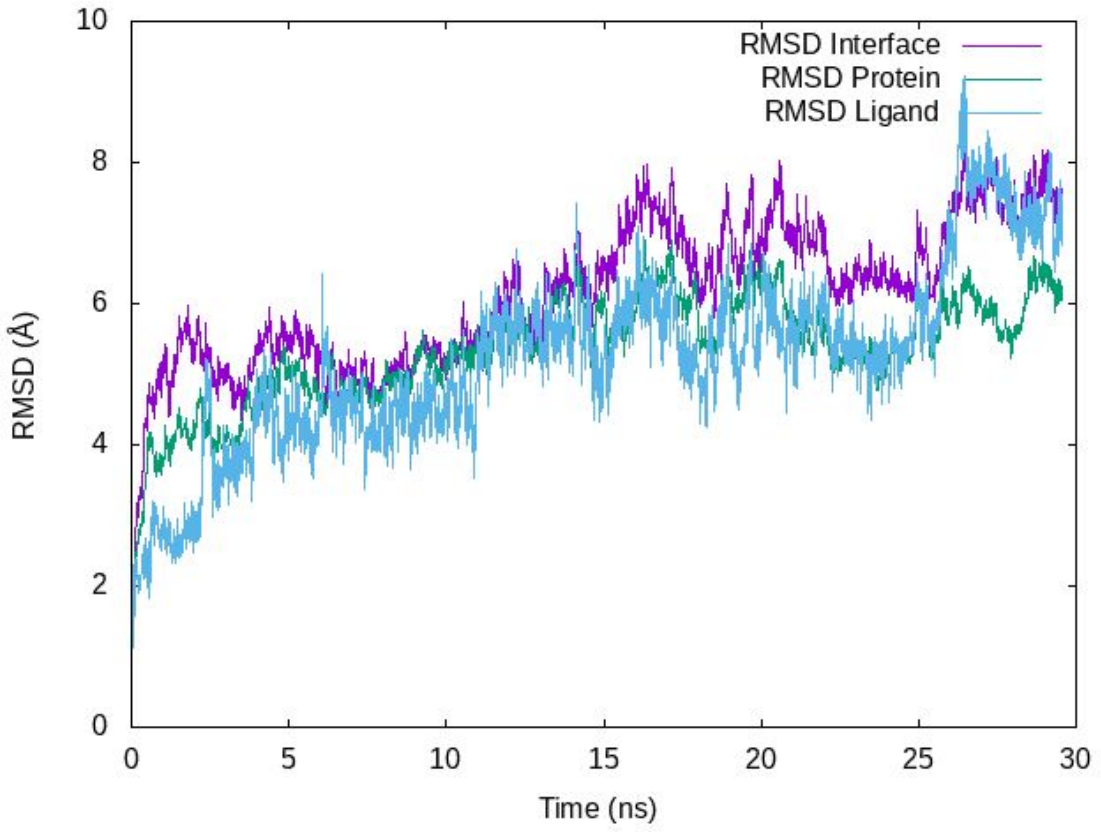
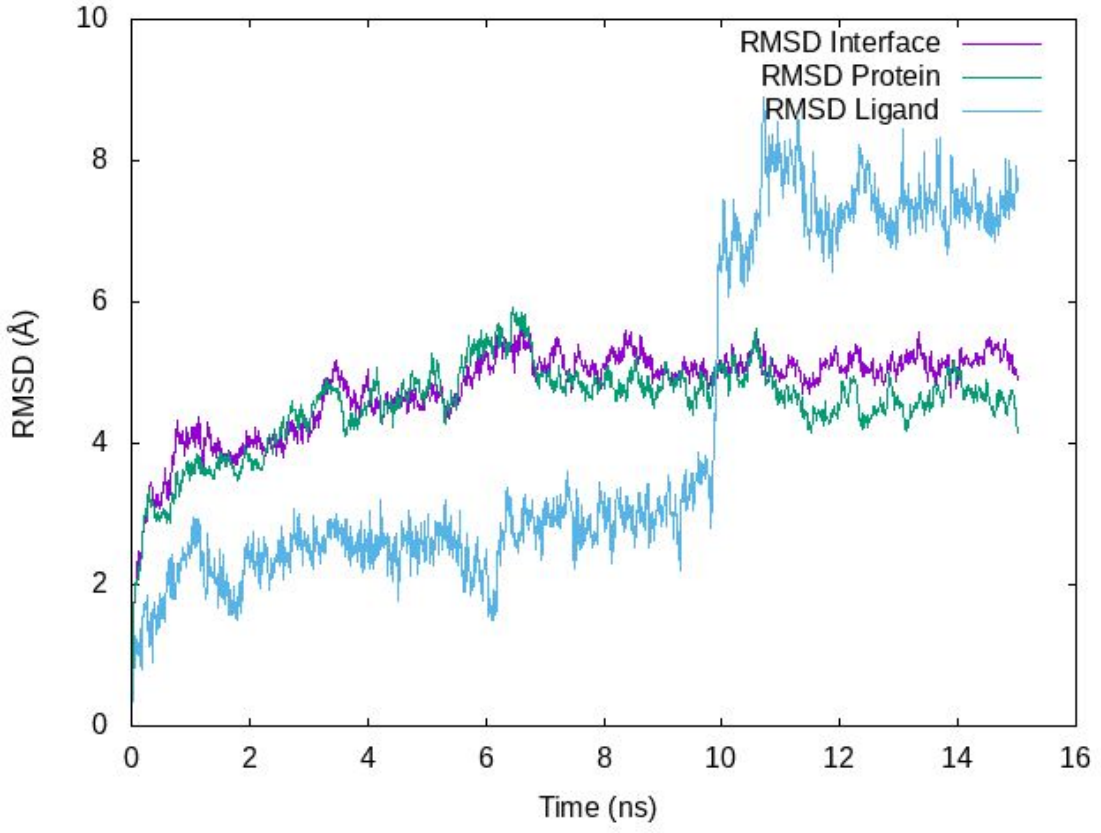
Ligand ID	RMSD
Masoprocol	

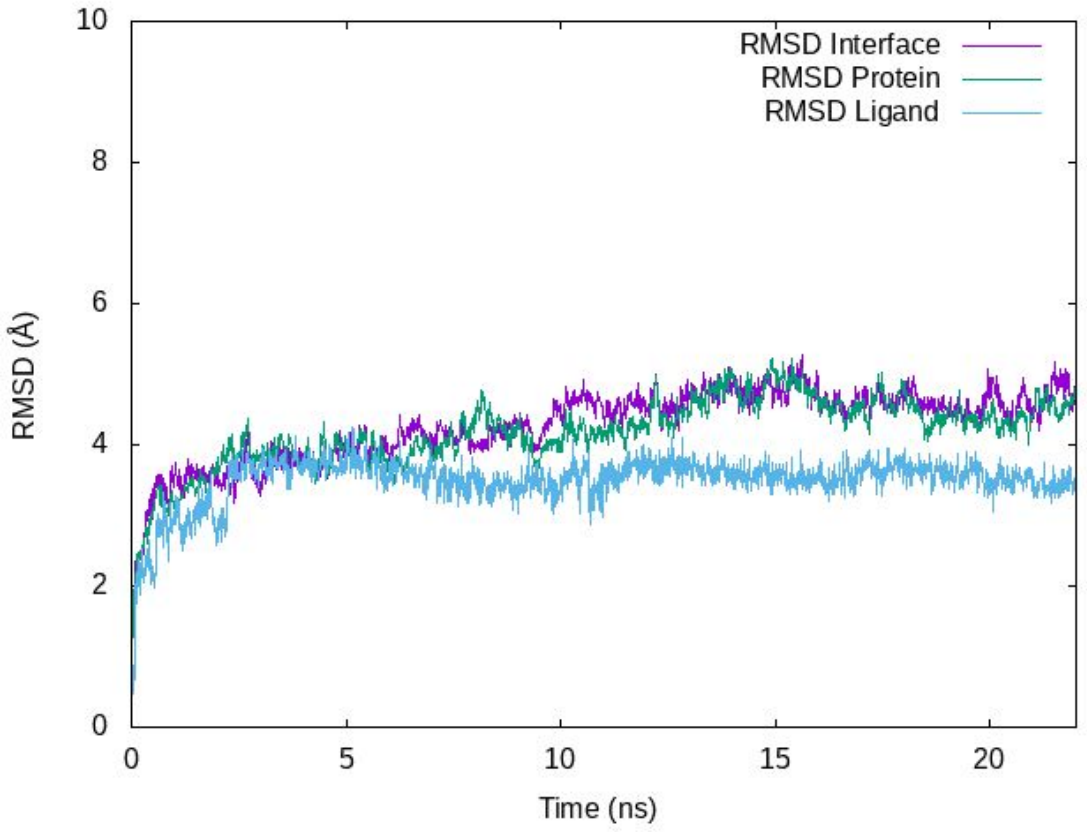
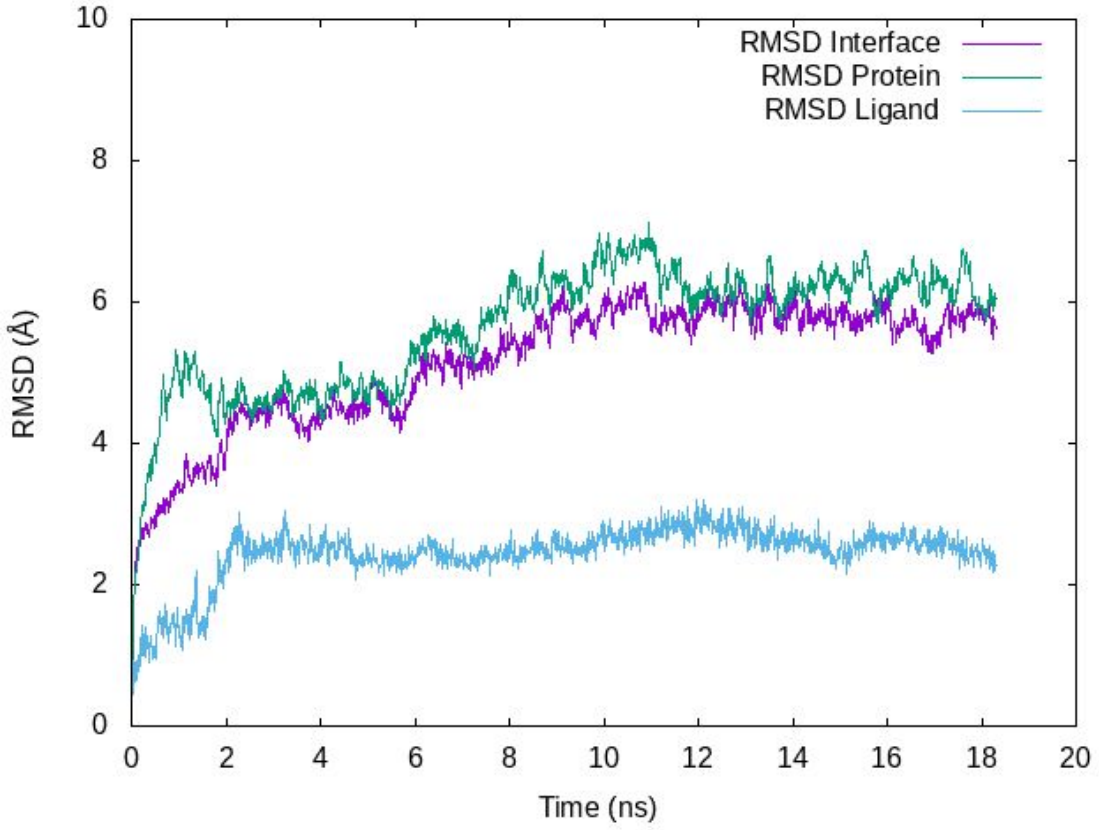
Phenformin	
2-iminobiotin e	

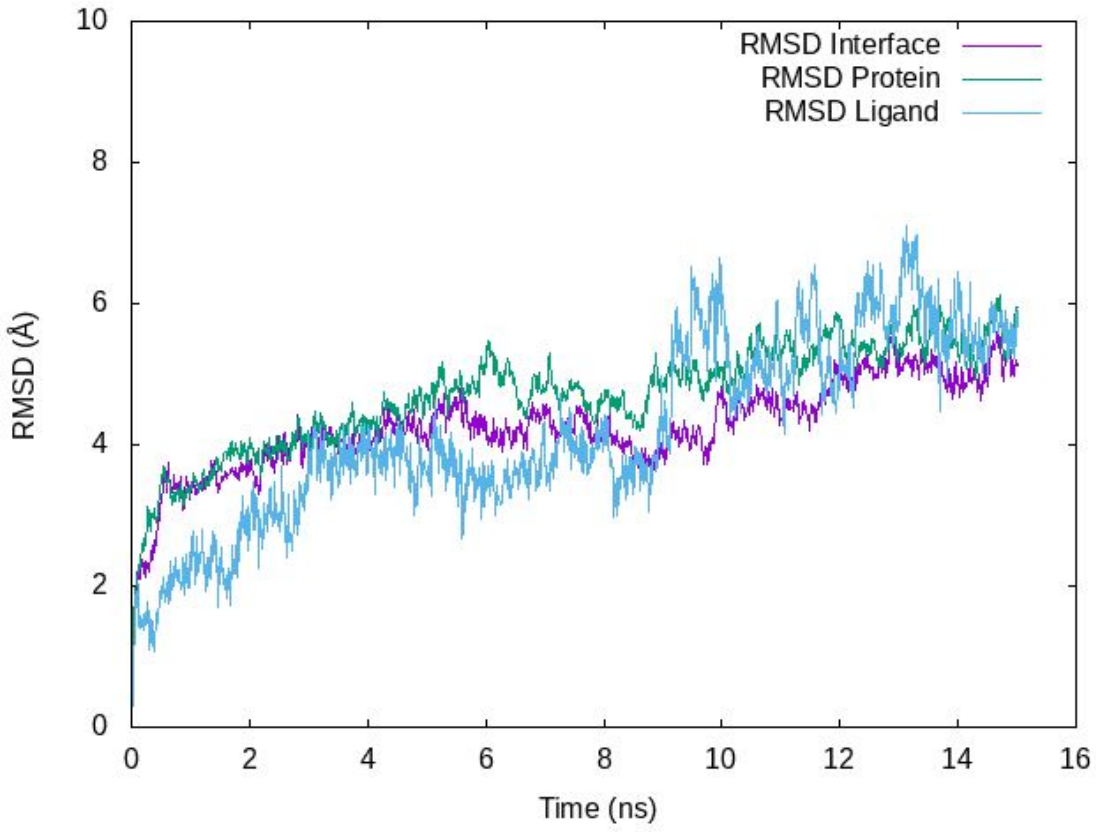
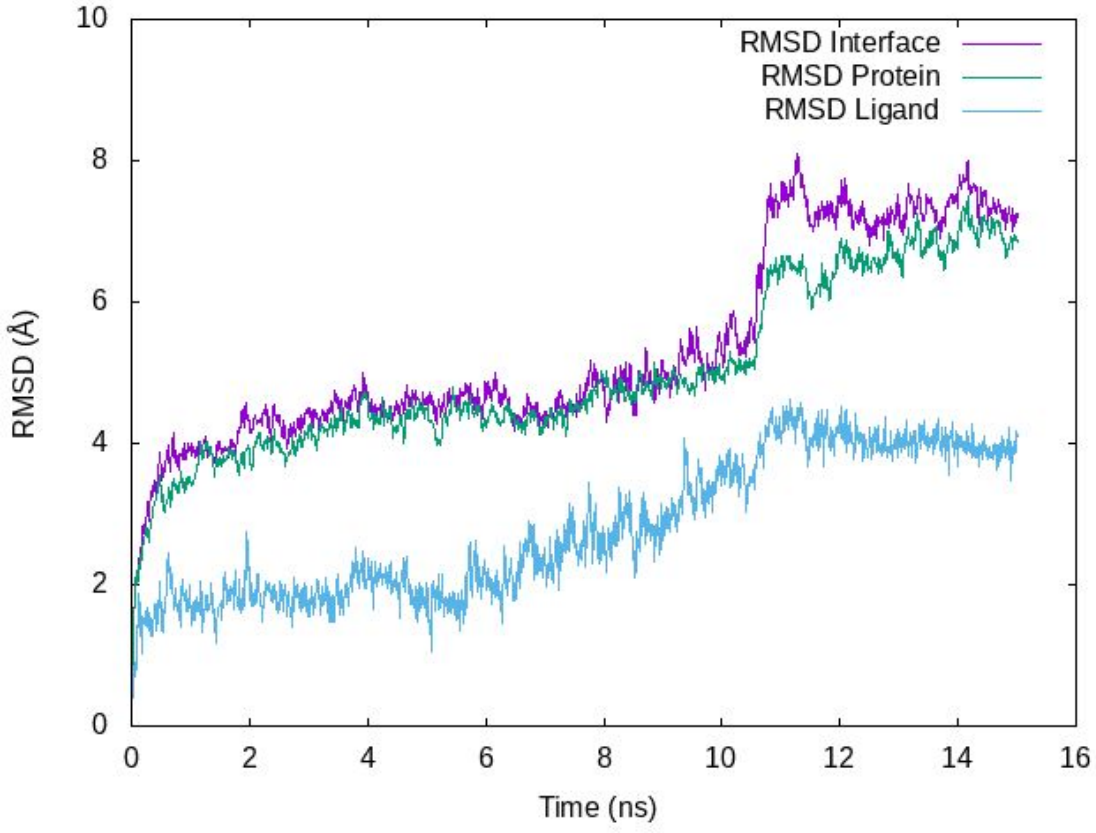
(-)EGC	
Quercetin	

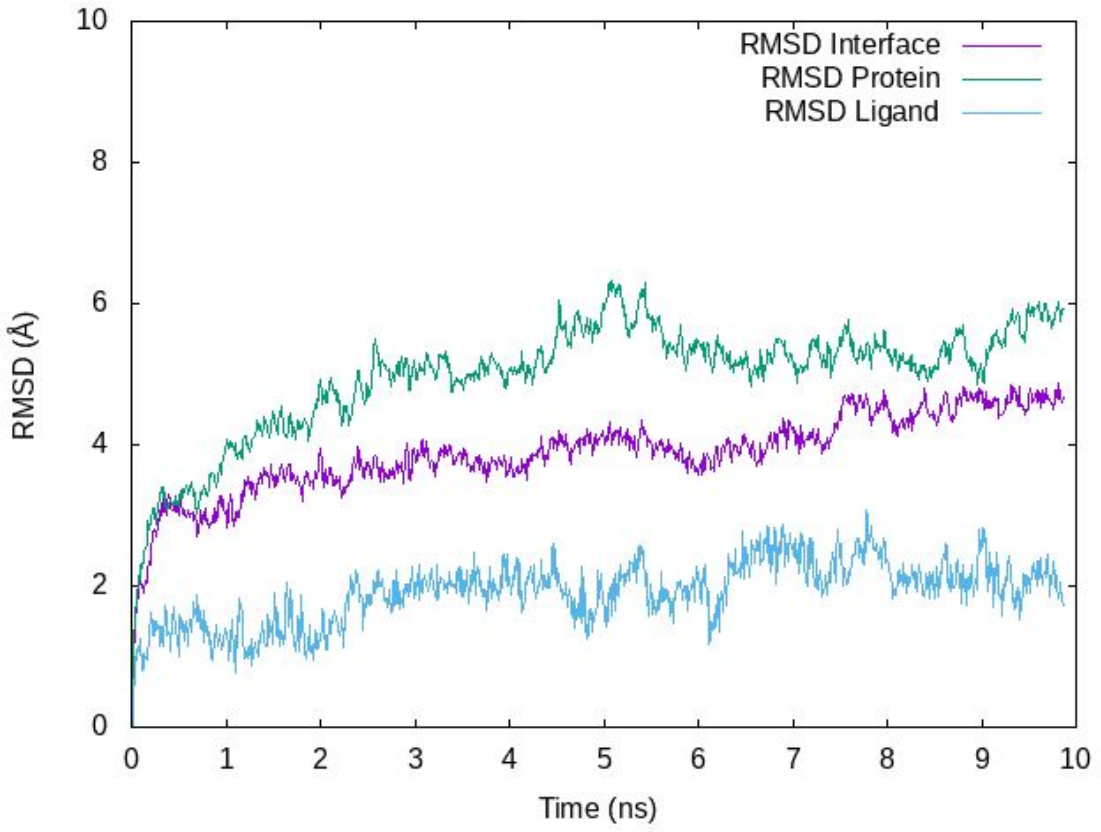
Ruxolitinib	
o6-bencylguaniane	

(-)EC	 RMSD Interface RMSD Protein RMSD Ligand RMSD (Å) Time (ns) 0 2 4 6 8 10 12 14
(-)EGCG	 RMSD Interface RMSD Protein RMSD Ligand RMSD (Å) Time (ns) 0 2 4 6 8 10 12 14 16 18 20

Cianidanol	
Gallic acid 3-O-gallate	

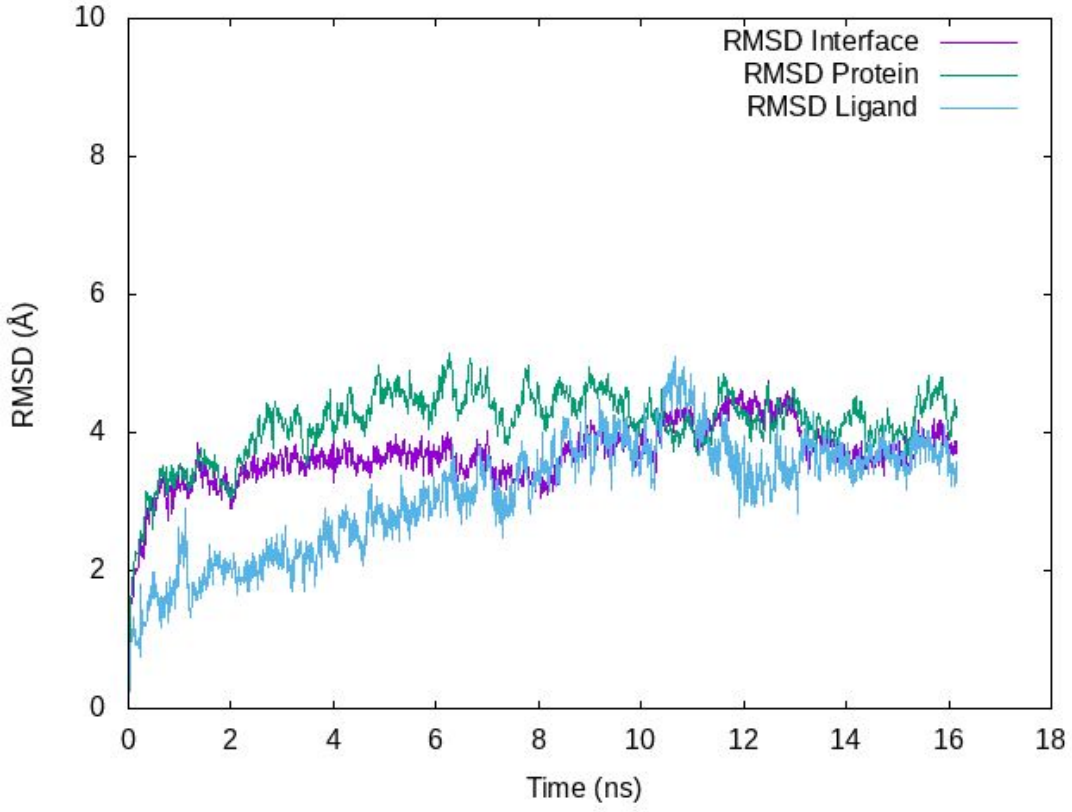
(+)GC	 RMSD Interface RMSD Protein RMSD Ligand RMSD (Å) Time (ns) 0 2 4 6 8 10 0 5 10 15 20
(+)GCG	 RMSD Interface RMSD Protein RMSD Ligand RMSD (Å) Time (ns) 0 2 4 6 8 10 0 2 4 6 8 10 12 14 16 18 20

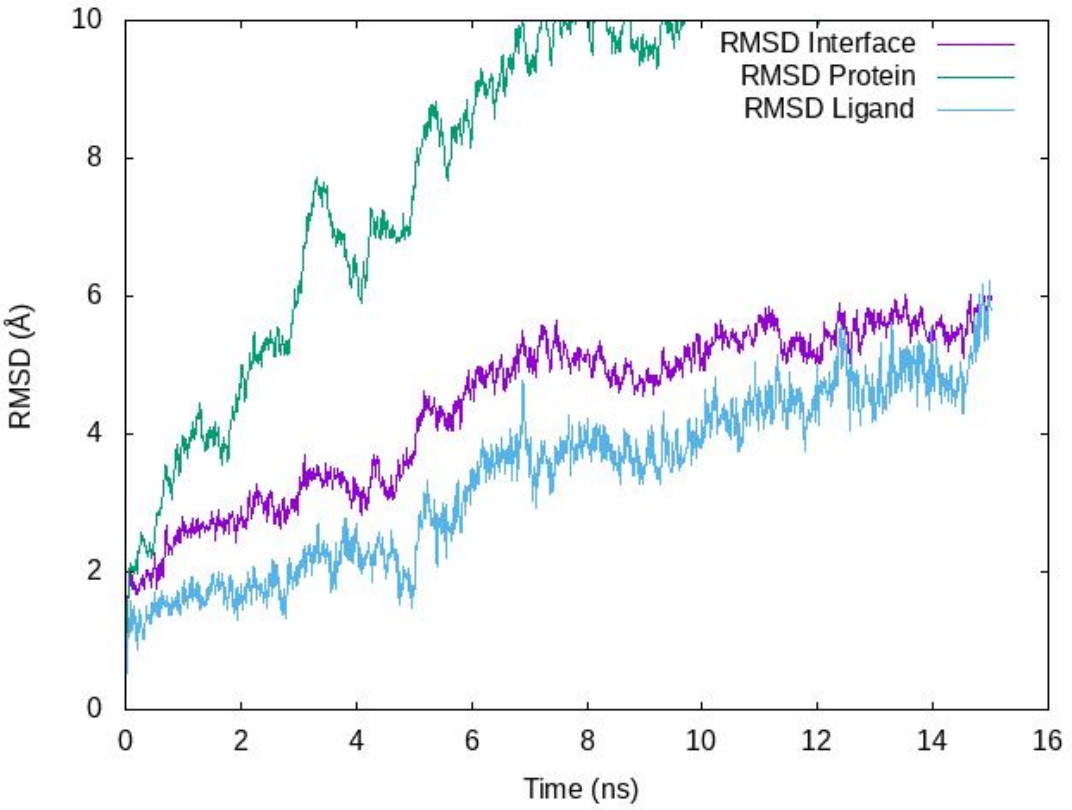
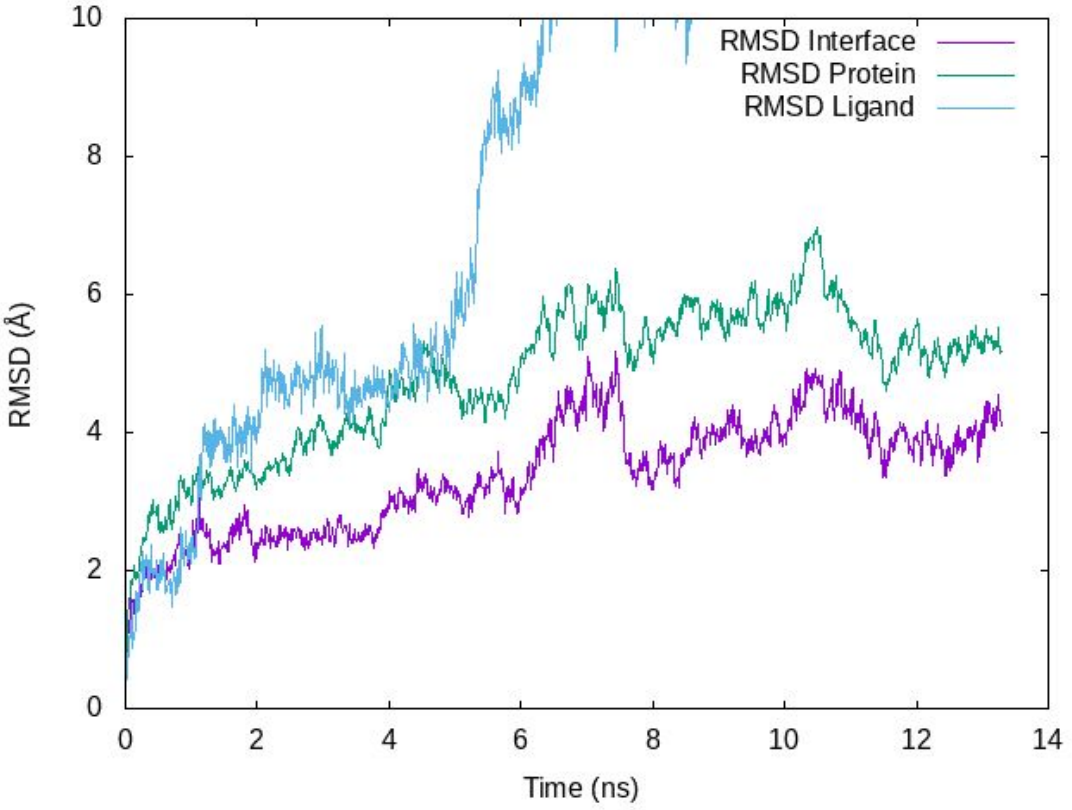
(-)C	 RMSD Interface RMSD Protein RMSD Ligand RMSD (Å) Time (ns) 0 2 4 6 8 10 12 14 16
(-)CG	 RMSD Interface RMSD Protein RMSD Ligand RMSD (Å) Time (ns) 0 2 4 6 8 10 12 14 16

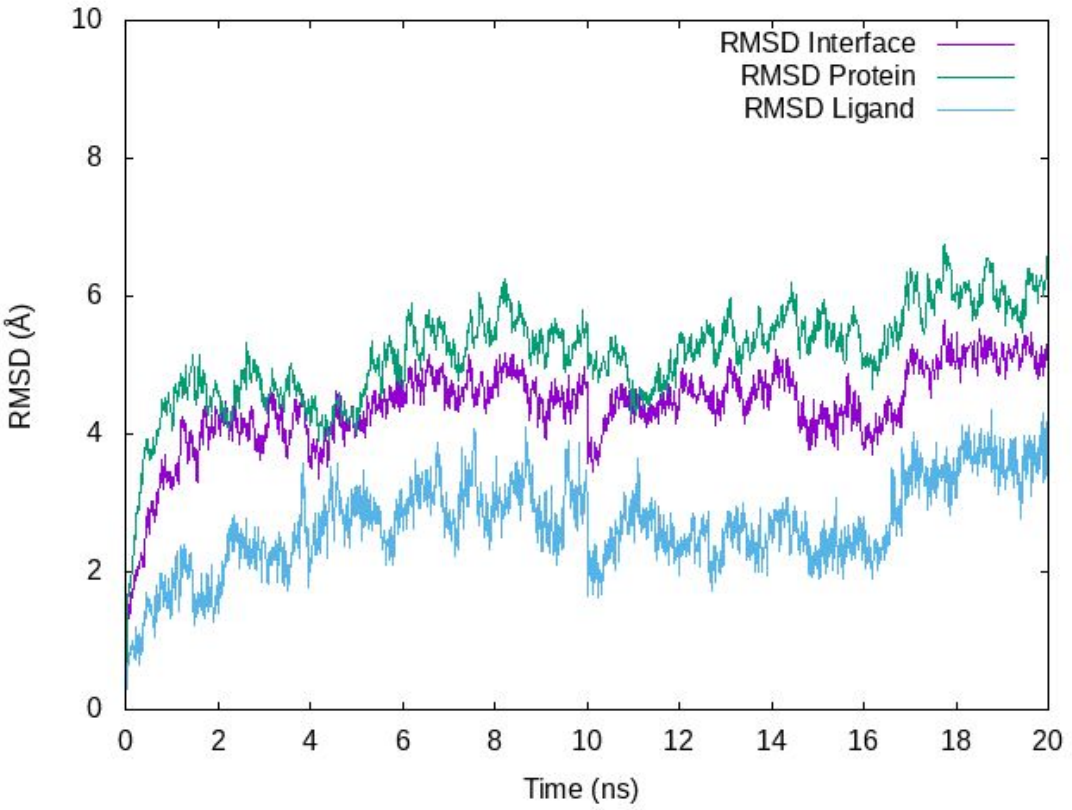
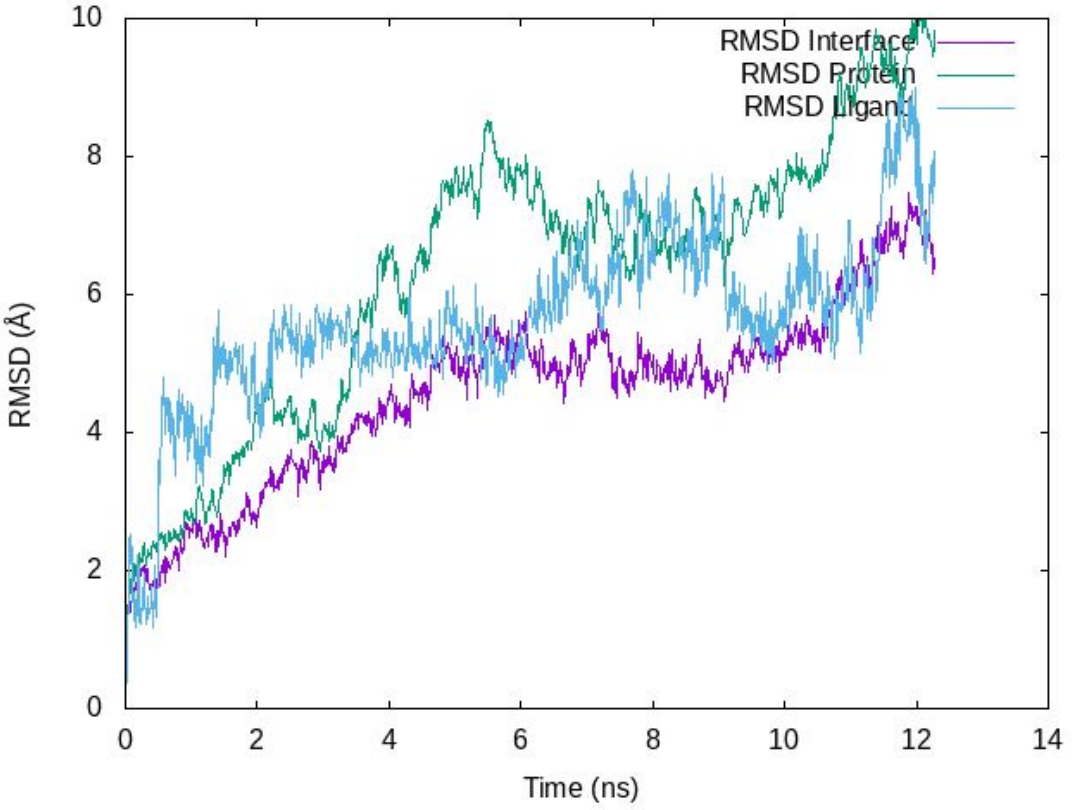
(-)GCG	 RMSD Interface RMSD Protein RMSD Ligand RMSD (Å) Time (ns) 0 2 4 6 8 10 0 1 2 3 4 5 6 7 8 9 10

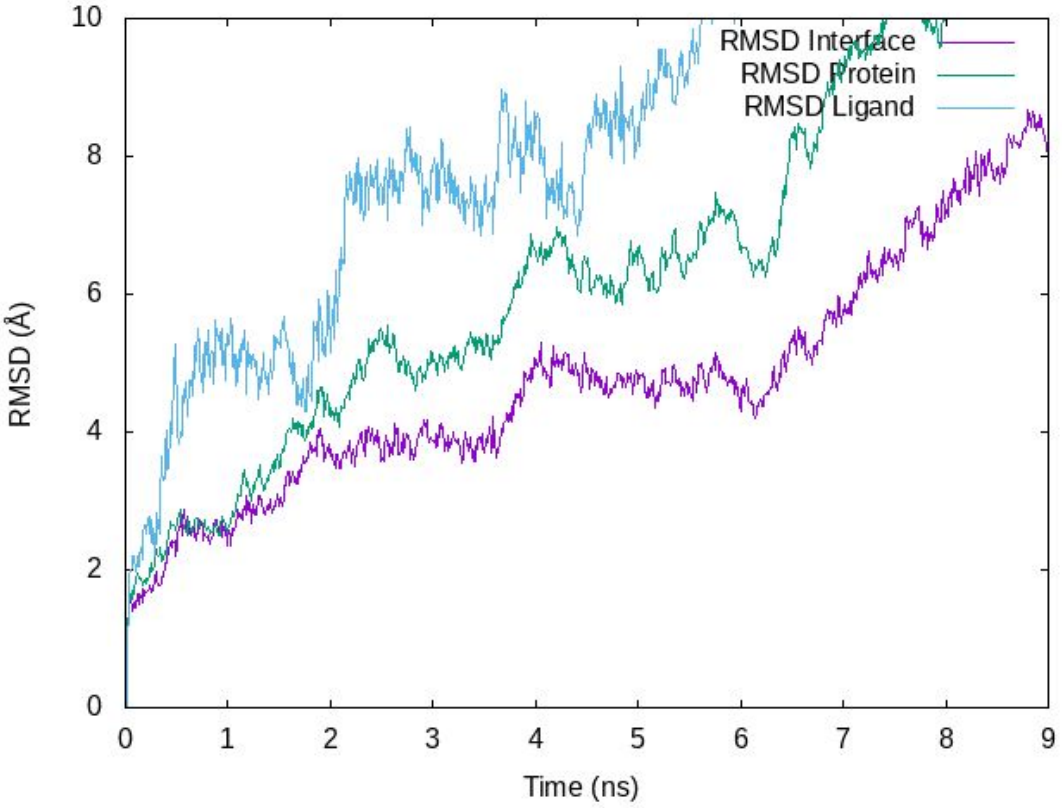
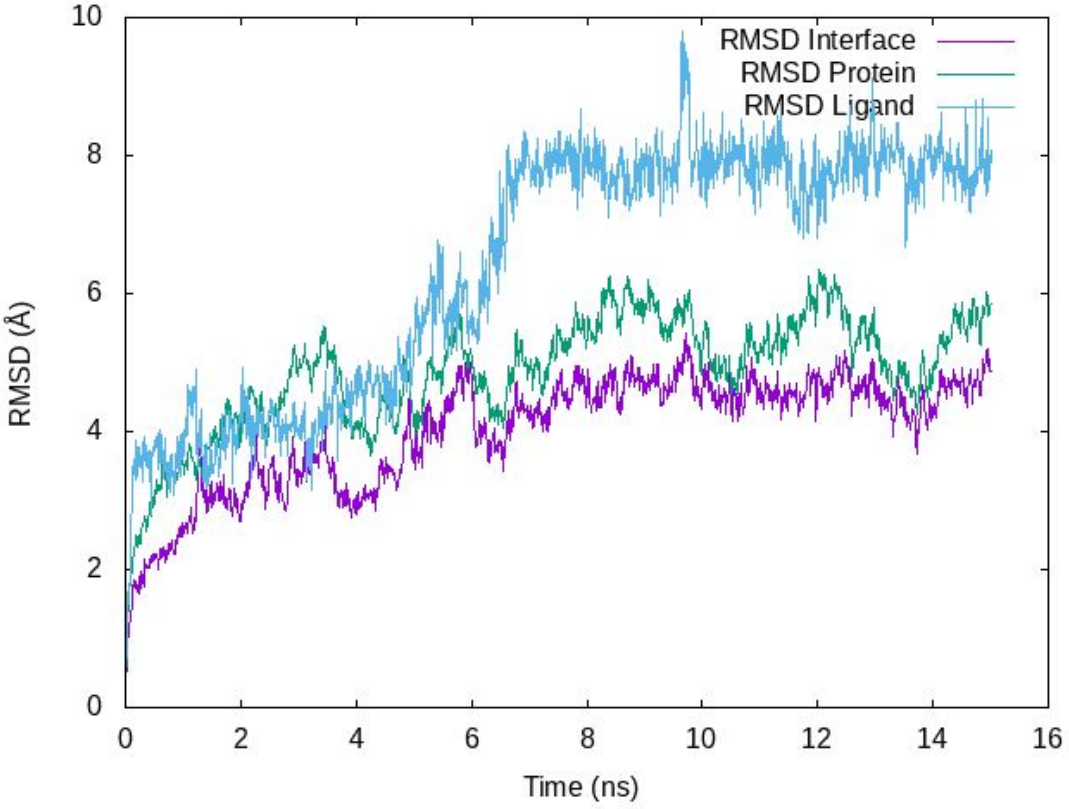
IF-3

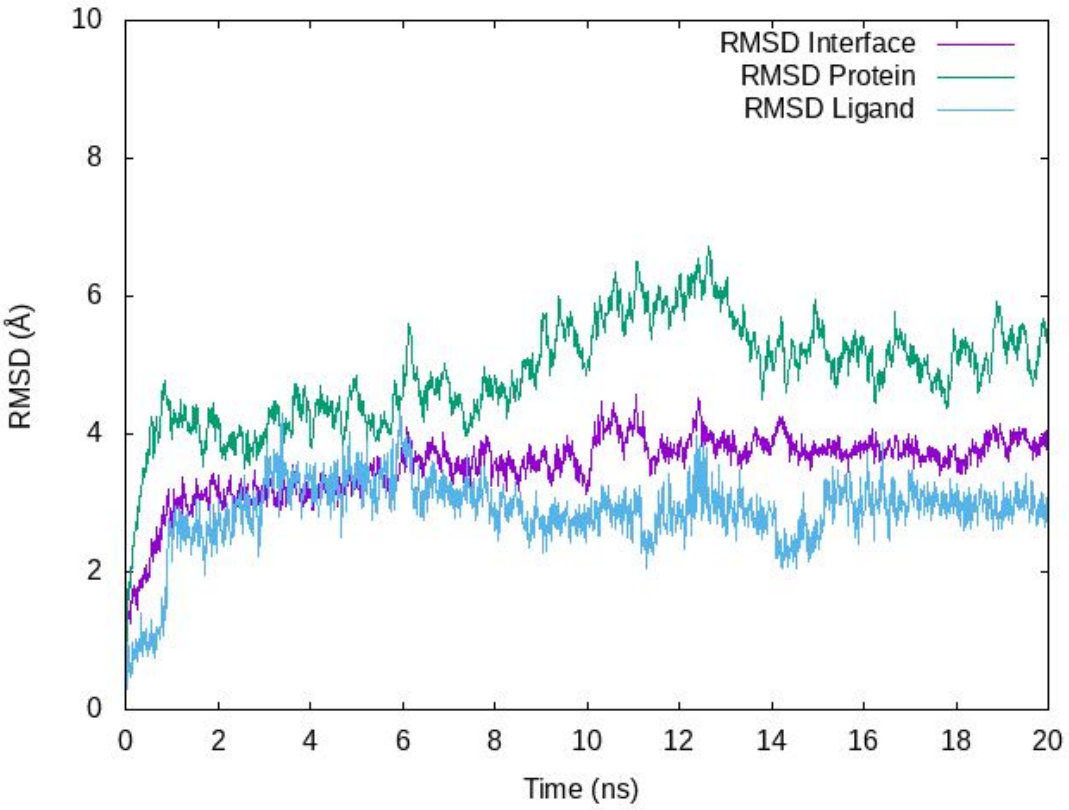
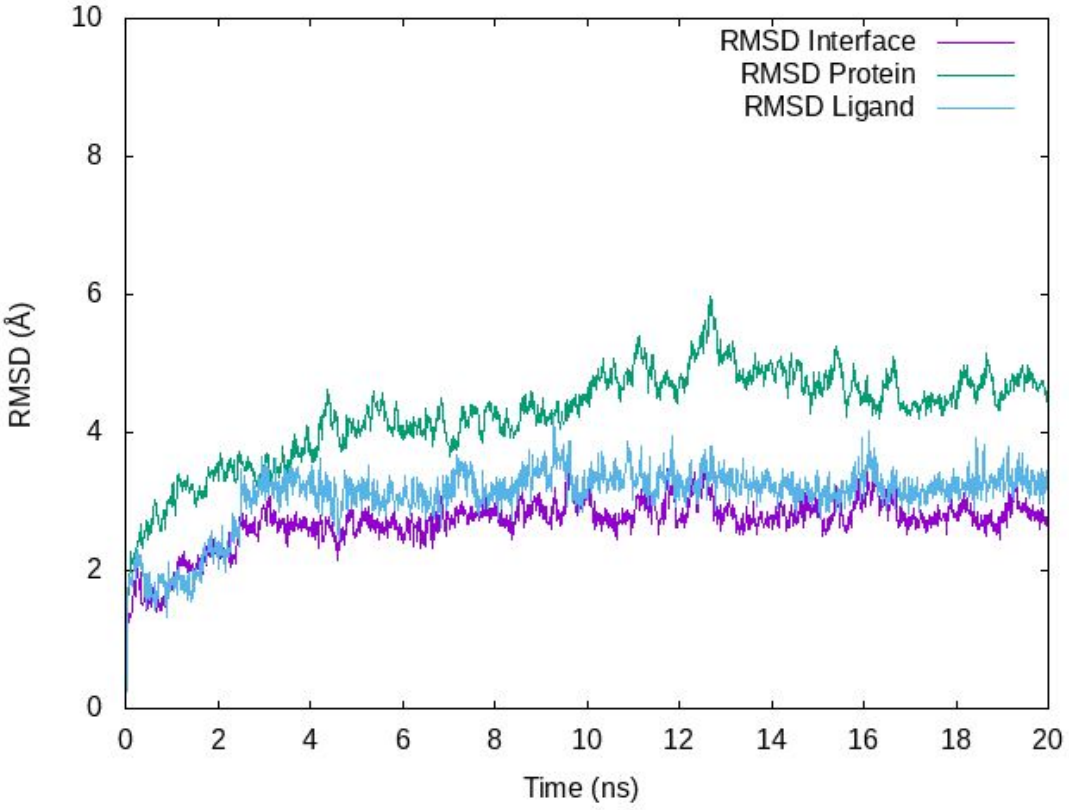
*Table S7. RMSD profiles of the equilibration/production stage is shown for each compound in **IF-3**. "RMSD Protein" was measured considering all residues in the complex aligned using the protein backbone. "RMSD Interface" and "RMSD Ligand" were calculated aligning by the interface-forming residues and then measured using those same residues and the ligand respectively.*

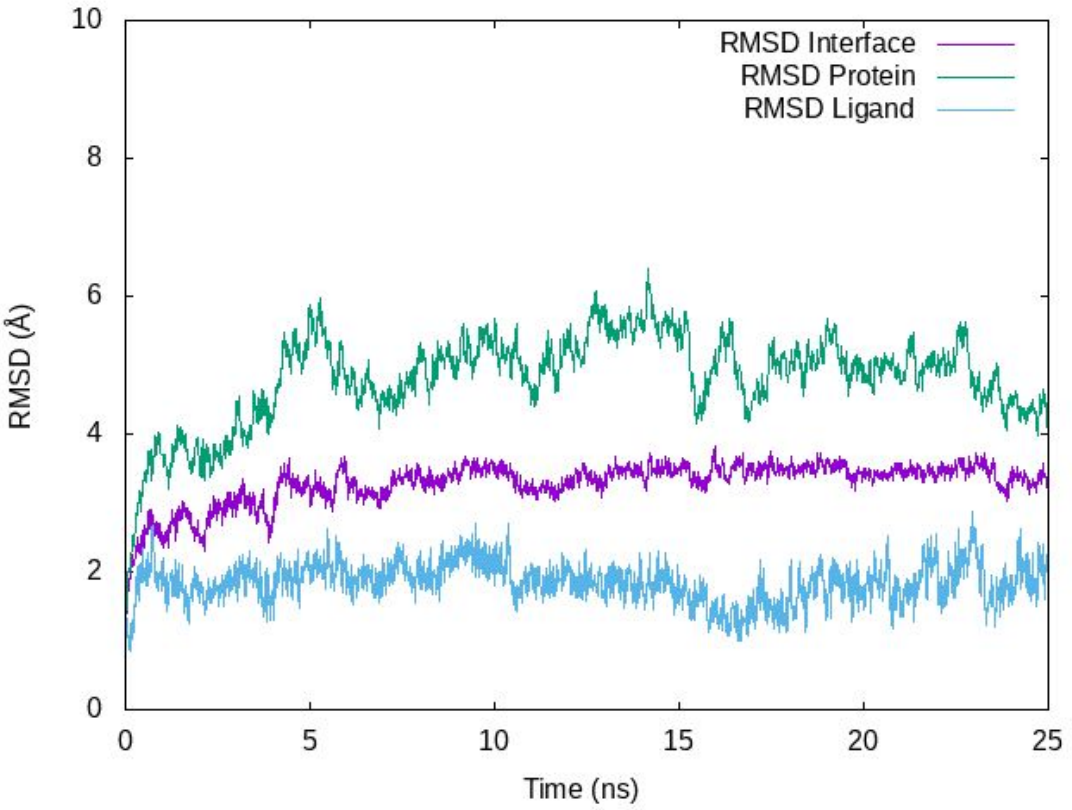
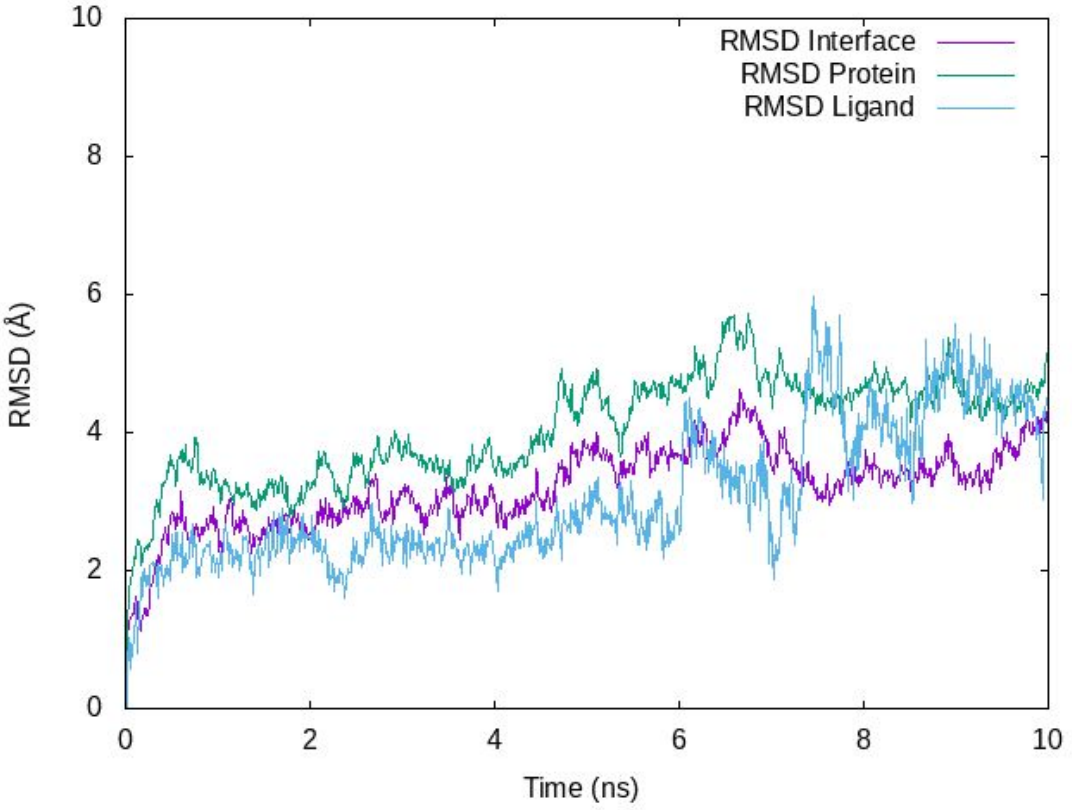
Ligand ID	RMSD
Masoprocol	

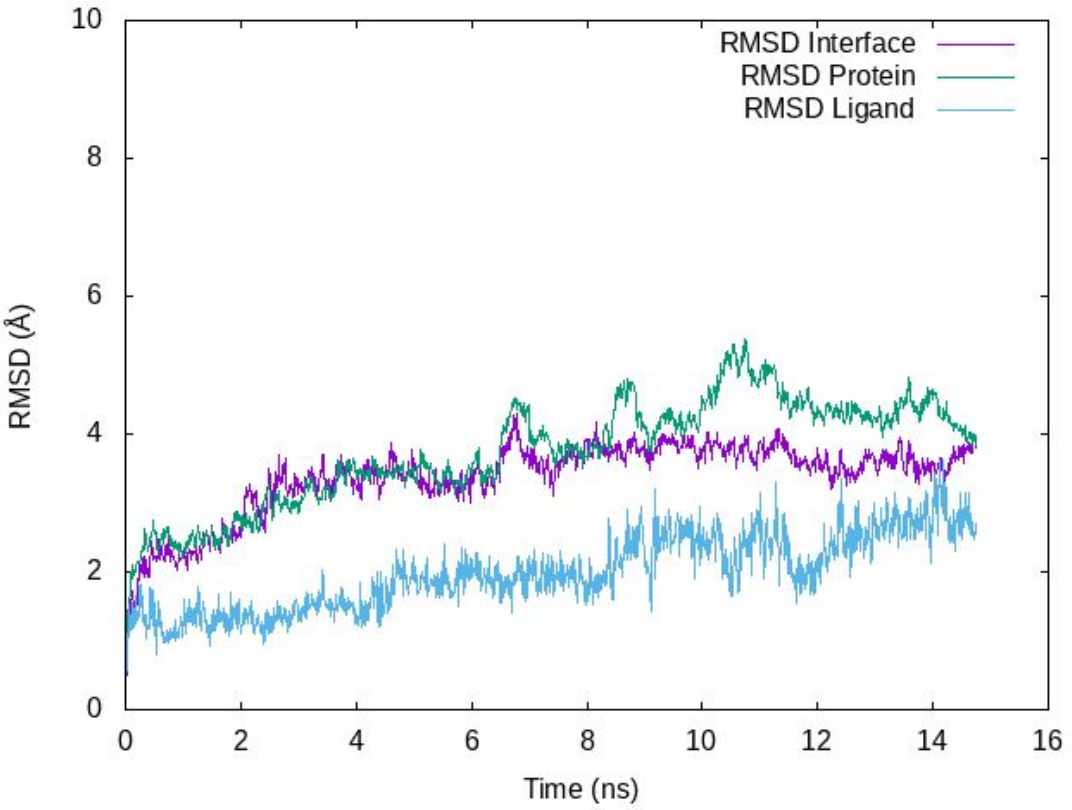
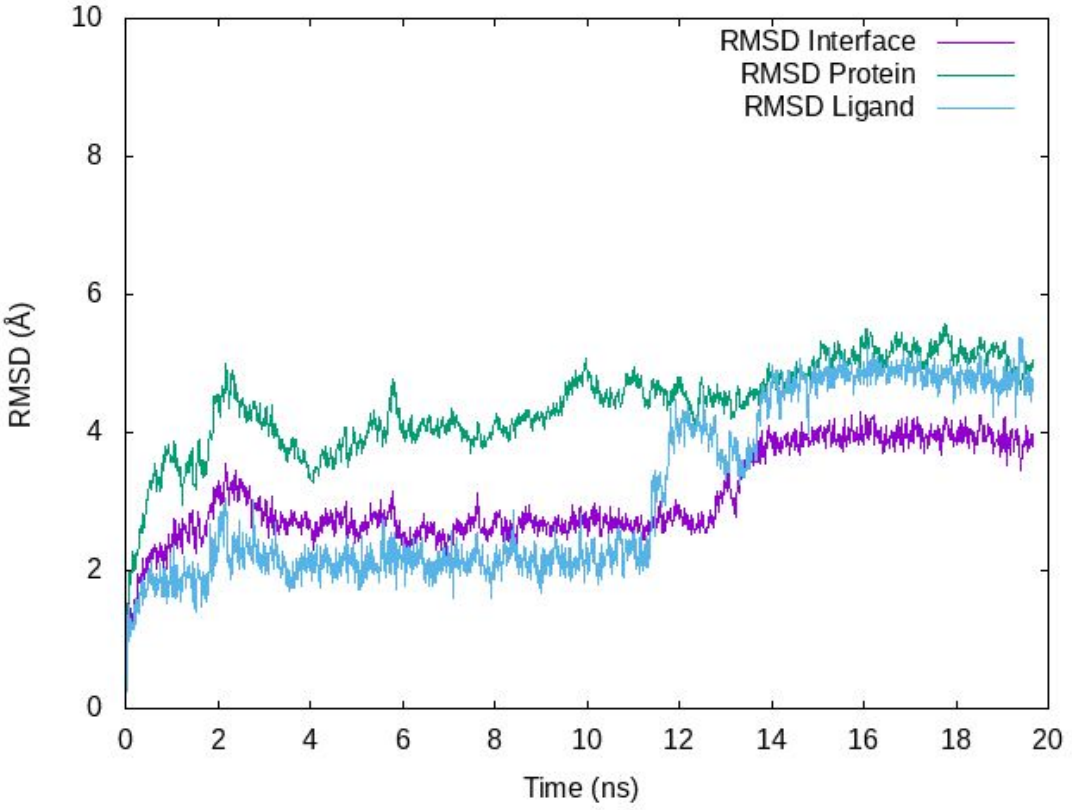
Phenformin	
Thienamycin	

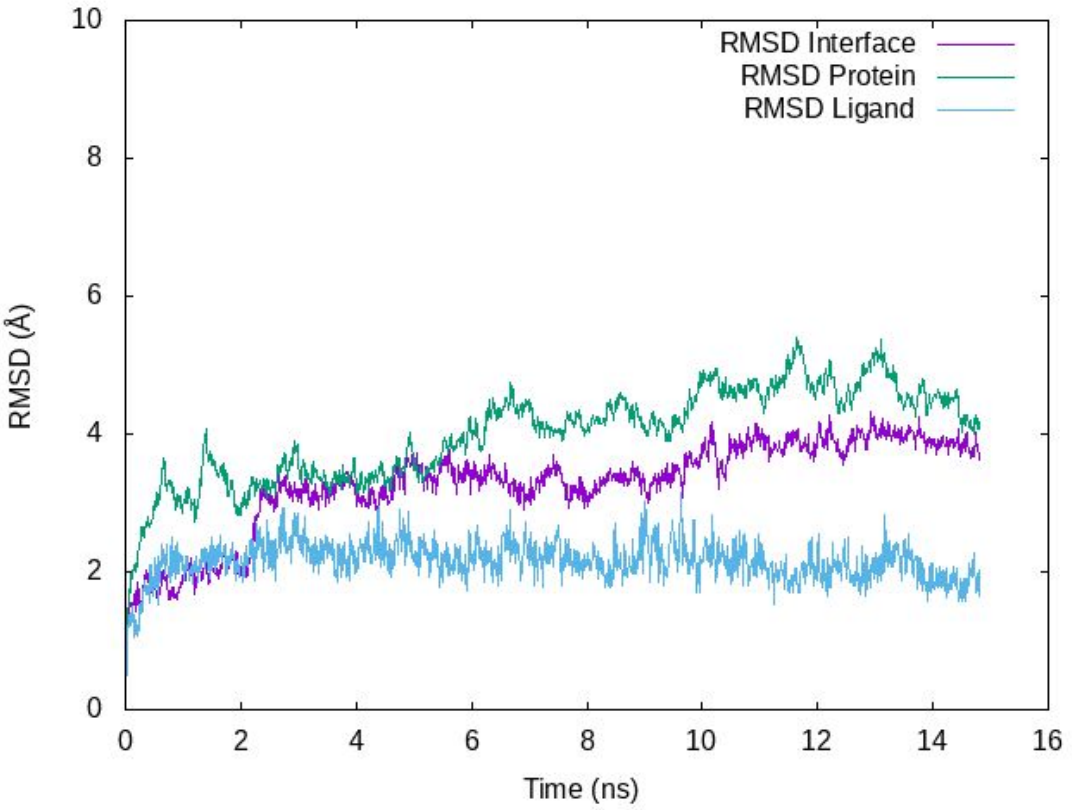
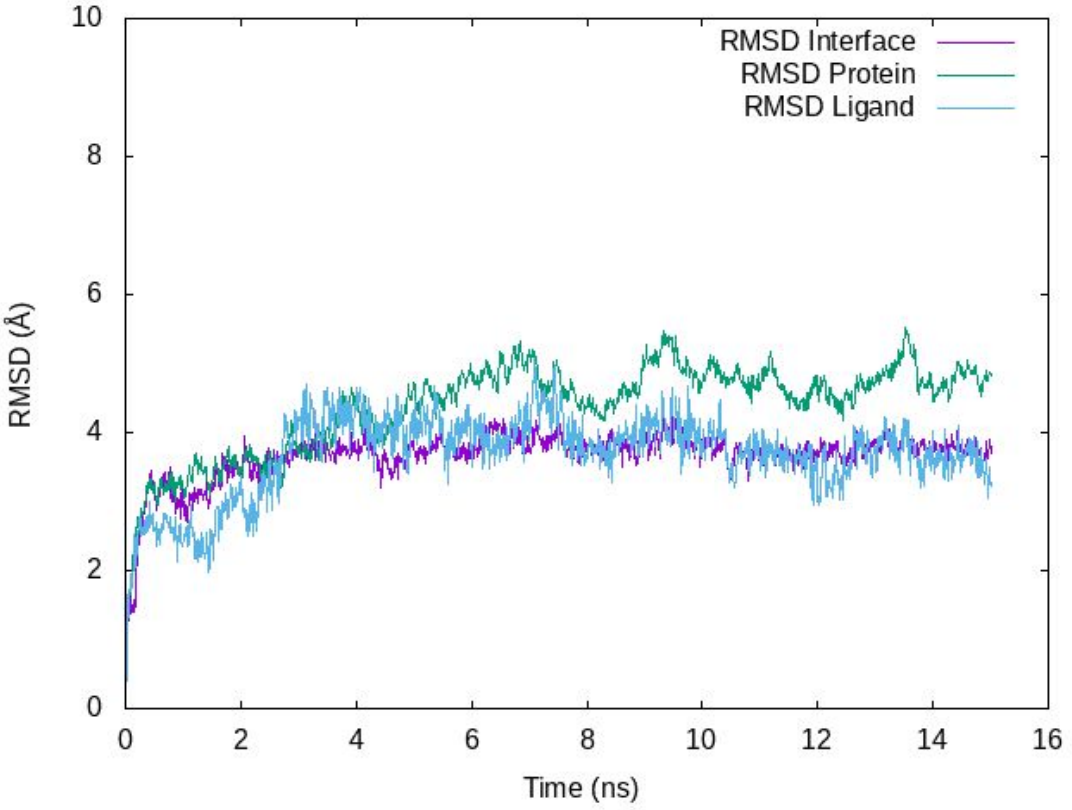
(-)EGC	
Quercetin	

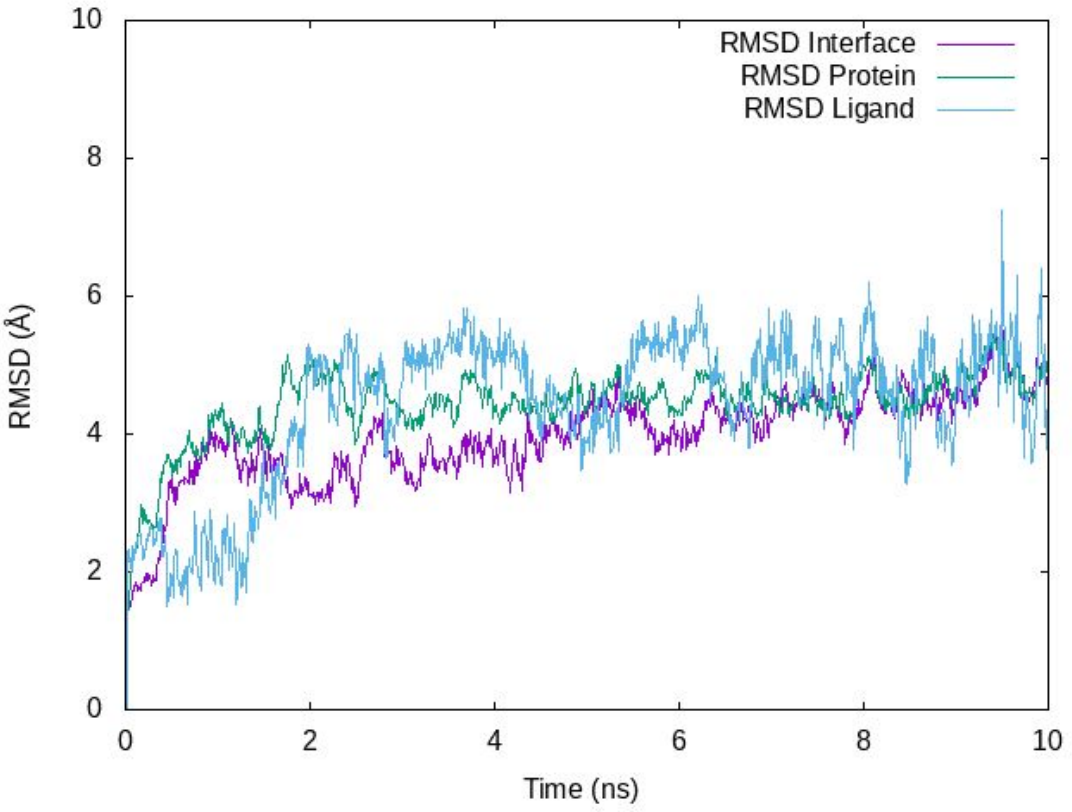
Ruxolitinib	
Polydatin	

(-)EC	 RMSD Interface RMSD Protein RMSD Ligand RMSD (Å) Time (ns) 0 2 4 6 8 10 0 2 4 6 8 10 12 14 16 18 20
(-)EGCG	 RMSD Interface RMSD Protein RMSD Ligand RMSD (Å) Time (ns) 0 2 4 6 8 10 0 2 4 6 8 10 12 14 16 18 20

Cianidanol	
Gallic acid 3-O-gallate	

(+)GC	 RMSD Interface RMSD Protein RMSD Ligand RMSD (Å) Time (ns) 0 2 4 6 8 10 12 14 16
(+)GCG	 RMSD Interface RMSD Protein RMSD Ligand RMSD (Å) Time (ns) 0 2 4 6 8 10 12 14 16 18 20

(-)C	 RMSD Interface RMSD Protein RMSD Ligand RMSD (Å) Time (ns) 0 2 4 6 8 10 12 14 16
(-)CG	 RMSD Interface RMSD Protein RMSD Ligand RMSD (Å) Time (ns) 0 2 4 6 8 10 12 14 16

(-)GCG	 RMSD Interface RMSD Protein RMSD Ligand RMSD (Å) Time (ns) 0 2 4 6 8 10

MMPBSA/MMGBSA Energy Calculations

Ligand Free Interfaces and Zn^{2+}-Dimer Interaction

Table S8. Energy estimations for the isolated homodimers and their Interaction with Zn^{2+}. Standard deviations are shown between parentheses.

Interface	Zn^{2+}-Protein Interaction (kcal/mol)	Monomer-Monomer Interaction (kcal/mol)	Total Interaction (kcal/mol)
IF-1	-	-37 (5)	-37 (5)
IF-2	-	-14 (5)	-14 (5)
IF-3	-	-17 (4)	-17 (4)
IF-1 + Zn^{2+}	-101 (4)	-57 (4)	-158 (6)
IF-2 + Zn^{2+}	-101 (5)	-41 (6)	-142 (7)

Ligand-Dimer Energy Calculations

Table S9. Interaction Energy calculations for each compound. Reported biological activity is mentioned, when available. Standard deviations are shown between parentheses.

Ligand	Interface	Lig-Monomer1 (kcal/mol)	Lig-Monomer2 (kcal/mol)	Lig-Dimer (kcal/mol)	Monomer-Monomer Interaction (kcal/mol)	Interaction Energy (kcal/mol)	Reported Activity
Cianidanol	MERS	-140 (7)	-51 (3)	-191 (7)	-50 (5)	-240 (8)	
(-)EGC	MERS	-61 (4)	-59 (3)	-120 (4)	-65 (4)	-185 (6)	
Masoprocol	MERS	-101 (5)	-28 (2)	-129 (5)	-56 (3)	-185 (6)	
(+)GCG	BC	-56 (3)	-22 (2)	-77 (3)	-89 (8)	-166 (8)	
(-)CG	BC	-45 (3)	-32 (2)	-78 (4)	-83 (7)	-162 (8)	Active
(-)EC	AB	-46 (2)	-15 (5)	-60 (6)	-94 (6)	-154 (8)	
(-)EC	MERS	-78 (5)	-18 (2)	-95 (5)	-55 (4)	-150 (6)	
(-)EGCG	BC	-30 (3)	-27 (3)	-57 (4)	-93 (4)	-150 (6)	
(-)GCG	AB	-31 (2)	-29 (3)	-60 (4)	84 (6)	-144 (7)	Active
Cianidanol	AB	-9 (2)	-23 (2)	-32 (3)	-110 (5)	-142 (6)	
(+)GC	AB	-32 (5)	-11 (3)	-42 (3)	-96 (6)	-139 (7)	
(+)GCG	AB	-39 (3)	-16 (6)	-55 (6)	-79 (9)	-134 (9)	
(-)GCG	BC	-45 (2)	-20 (2)	-63 (3)	-69 (7)	-133 (8)	Active
(-)CG	AB	-26 (2)	-35 (3)	-60 (4)	-69 (6)	-130 (6)	Active
(+)GCG	MERS	-36 (4)	-26 (2)	-61 (5)	-67 (4)	-129 (6)	
(-)C	AB	-48 (2)	-13 (1)	-60 (2)	-67 (5)	-127 (5)	Inactive
Quercetin	AB	-37 (4)	-12 (2)	-49 (4)	-77 (6)	-126 (6)	Inactive
(-)C	MERS	-31 (3)	-22 (2)	-53 (3)	-72 (4)	-125 (5)	Inactive
Gallic acid	AB	-22 (5)	-31 (2)	-52 (5)	-72 (7)	-124 (7)	

3-O-gallate							
(+)GC	BC	-31 (3)	-19 (2)	-50 (3)	-70 (4)	-120 (5)	
(-)EGCG	AB	-36 (4)	-37 (4)	-73 (6)	-45 (5)	-118 (7)	
(-)EGCG	MERS	-49 (2)	-20 (3)	-69 (3)	-47 (4)	-116 (5)	
Ruxolitinib	BC	-15 (1)	-30 (2)	-44 (2)	-70 (5)	-114 (5)	
(+)GC	MERS	-42 (5)	-16 (4)	-58 (5)	-55 (4)	-113 (6)	
(-)CG	MERS	-35 (3)	-25 (2)	-60 (3)	-53 (4)	-113 (5)	Active
(-)EC	BC	-30 (5)	-9 (2)	-37 (3)	-74 (5)	-110 (6)	
(-)EGC	BC	-37 (4)	-11 (3)	-48 (4)	-55 (6)	-103 (7)	
(-)C	BC	-22 (3)	-22 (2)	-44 (5)	-56 (6)	-100 (7)	Inactive
Scopletin	AB	-26 (1)	-4 (1)	-30 (1)	-69 (6)	-98 (6)	
(-)EGC	AB	-17 (2)	-28 (3)	-45 (4)	-52 (4)	-97 (6)	
Quercetin	BC	-25 (2)	-16 (1)	-38 (2)	-50 (4)	-88 (5)	Inactive
Cianidanol	BC	-18 (4)	-16 (2)	-34 (5)	-51 (4)	-84 (6)	
Ruxolitinib	AB	-15 (1)	-15 (2)	-30 (2)	-51 (4)	-81 (5)	
Masoprocol	BC	-18 (2)	-15 (2)	-33 (2)	-43 (4)	-76 (5)	
Scopletin	MERS	-14 (1)	-14 (3)	-28 (4)	-42 (4)	-70 (5)	
Scopletin	BC	-2 (2)	-17 (2)	-19 (3)	-7 (6)	-26 (7)	
2-iminobiotin	BC	Complex Not Stabilized					
Brivudine	AB	Complex Not Stabilized					
Dexlansoprazole	MERS	Complex Not Stabilized					
Gallic acid 3-O-gallate	MERS	Complex Not Stabilized					
Masoprocol	AB	Complex Not Stabilized					
(-)GCG	MERS	Complex Not Stabilized					Active
o6-bencylguaniane	BC	Complex Not Stabilized					
Phenformin	BC	Complex Not Stabilized					
Phenformin	MERS	Complex Not Stabilized					
Polydatin	MERS	Complex Not Stabilized					
Quercetin	MERS	Complex Not Stabilized					Inactive
Ruxolitinib	MERS	Complex Not Stabilized					
Thienamycin	MERS	Complex Not Stabilized					

Ligand-Dimer Interaction Visualization of the Most Stable Complexes

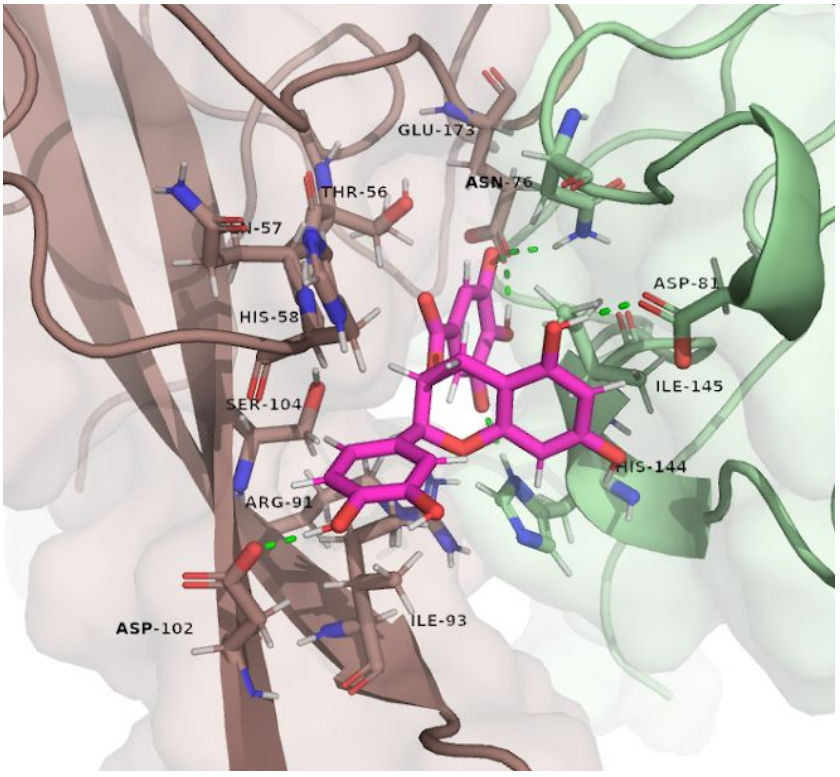


*Figure S3. (-)-Catechin Gallate in **IF-1***

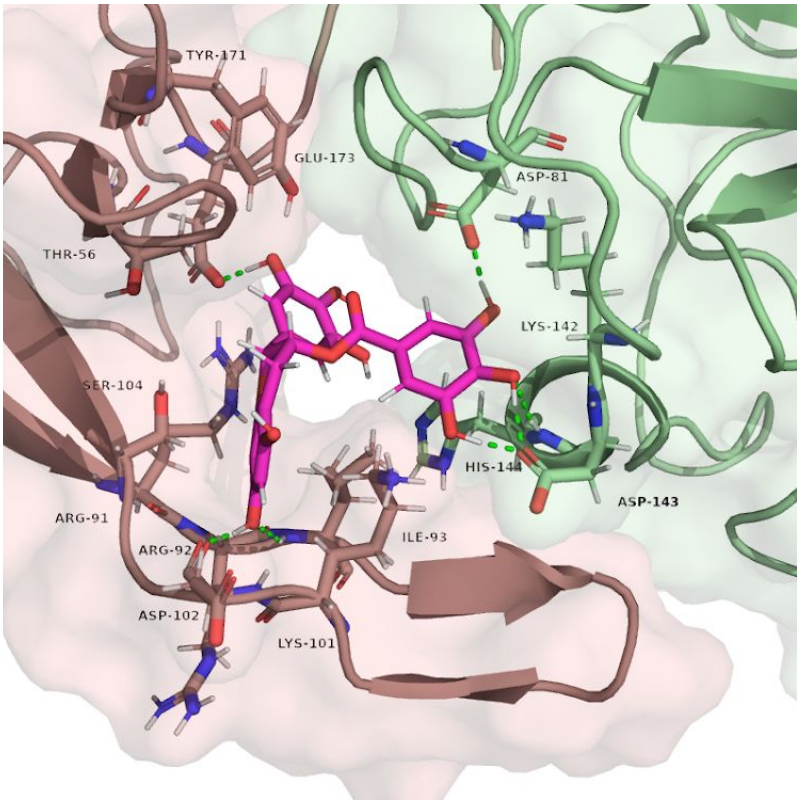


*Figure S4. (-)-Epigallocatechin Gallate in **IF-1***

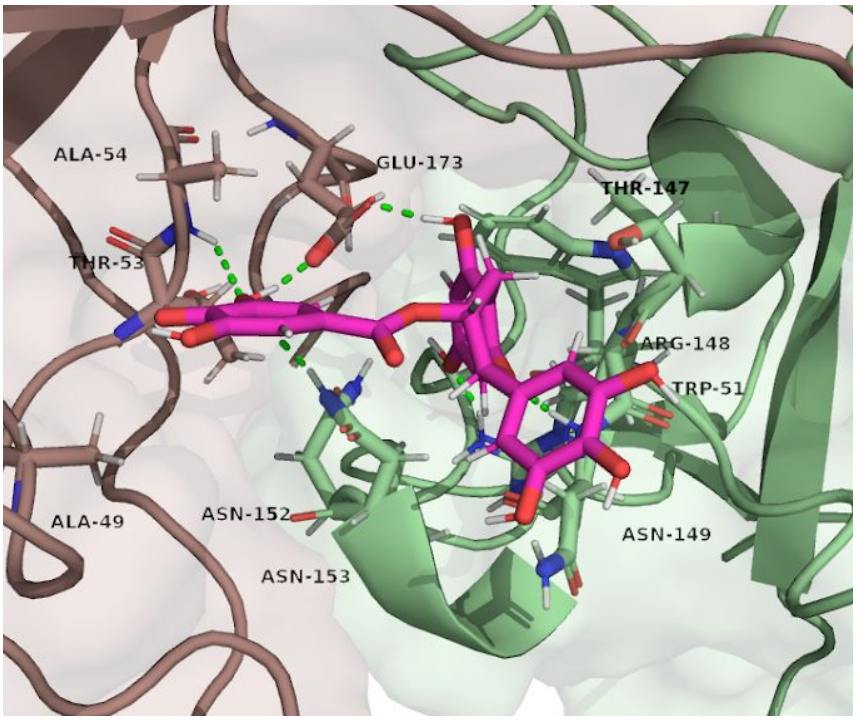


*Figure S5. (-)-Gallocatechin Gallate in **IF-1***

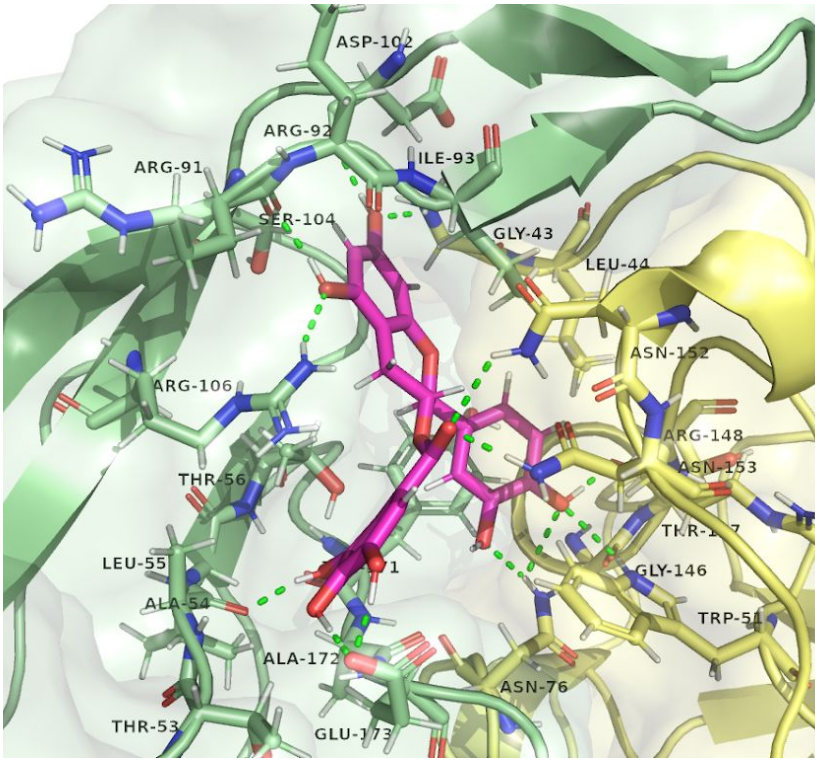


*Figure S6. (-)-Catechin Gallate in **IF-2***

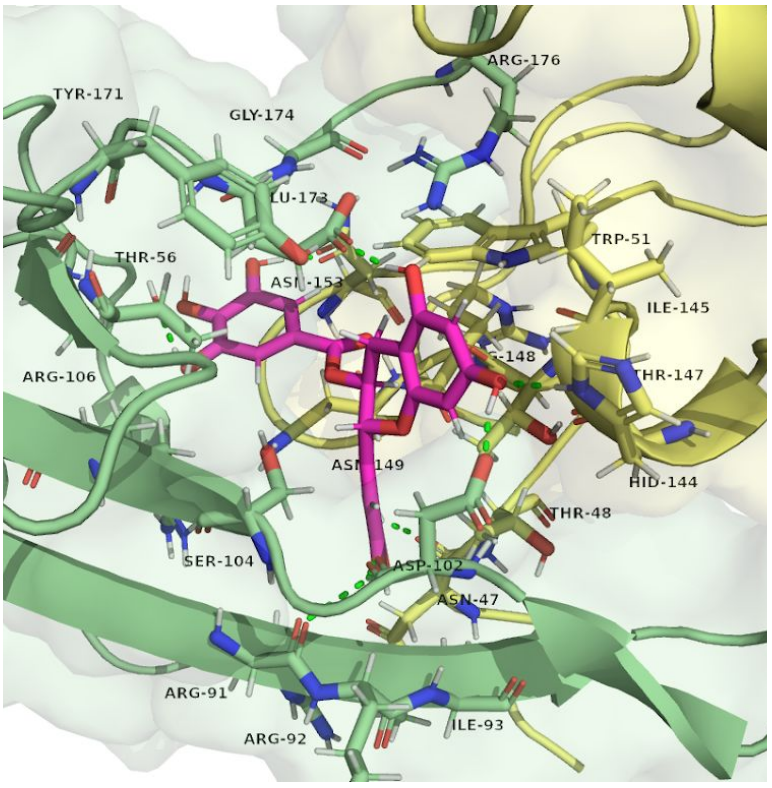


*Figure S7. (-)-Gallocatechin Gallate in **IF-2***

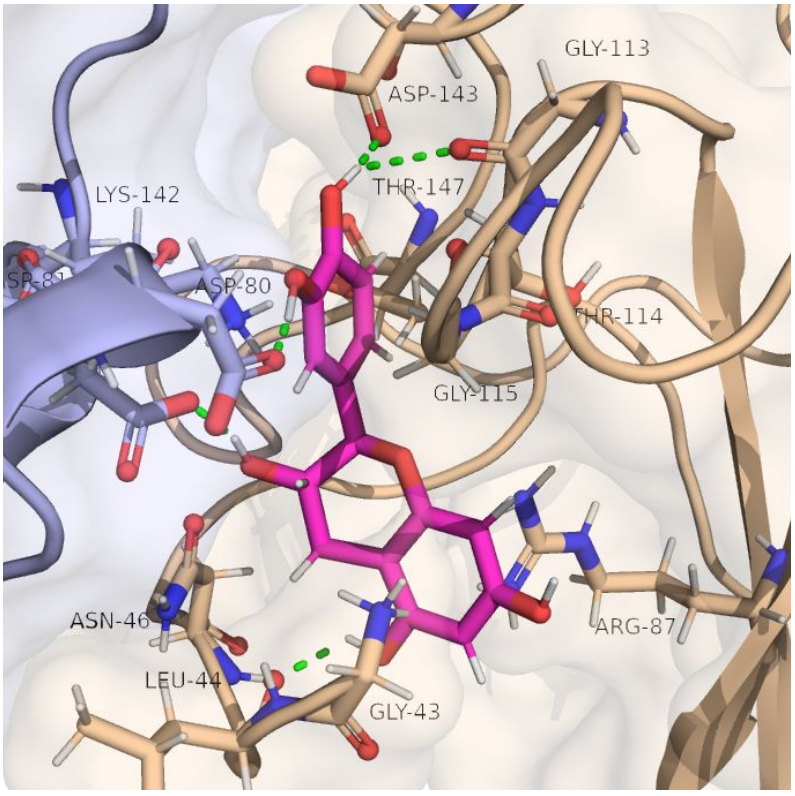


*Figure S8. Cianidanol in **IF-3***

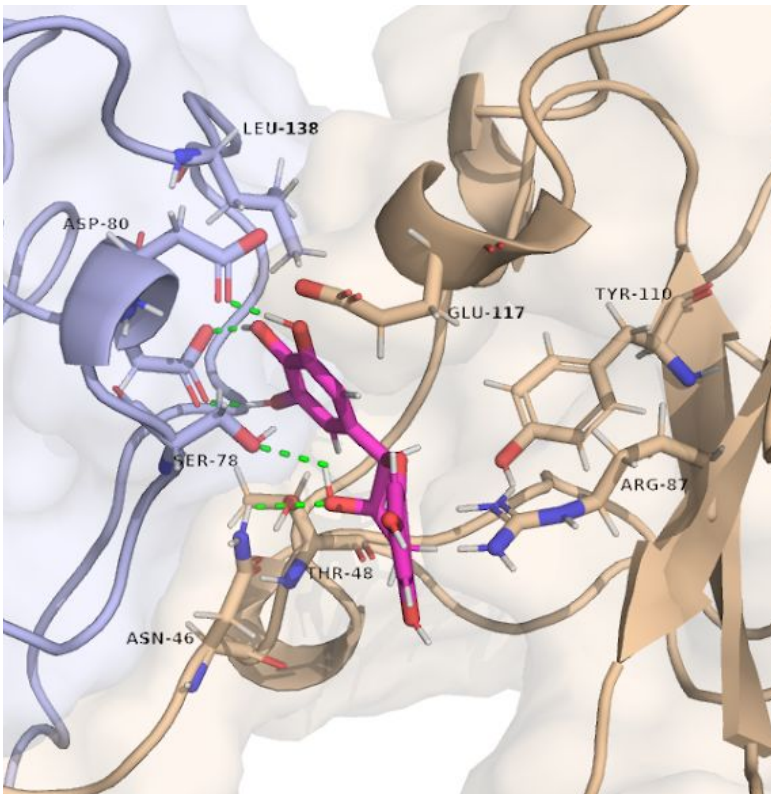


*Figure S9. (-)-Epigallocatechin in **IF-3***

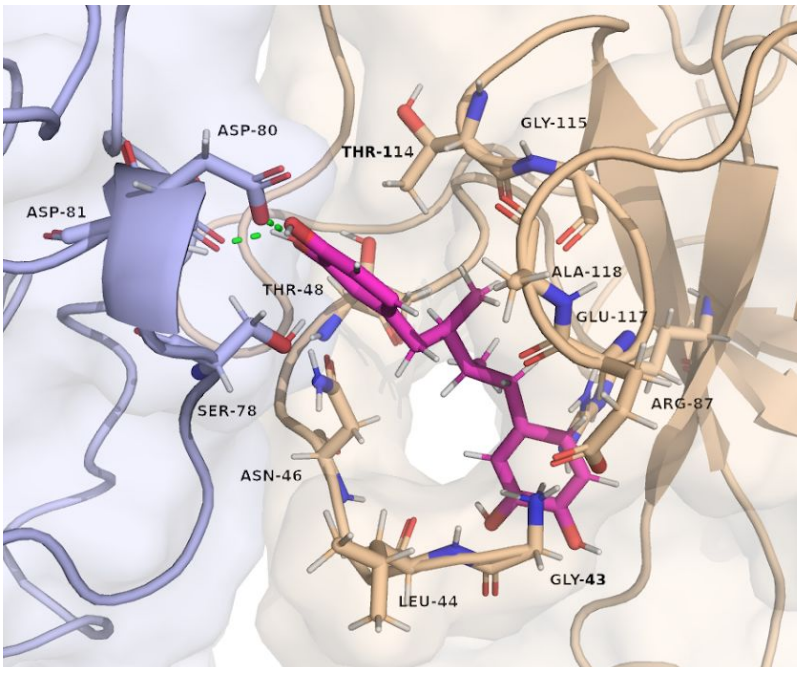


*Figure S10. Masoprocol in **IF-3***