SUPPORTING INFORMATION

Targeting LIMK1 in Alzheimer's Disease: A Multifaceted Computational Investigation Involving ADMET, Virtual Screening, Molecular Docking, and Molecular Dynamics

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Contents

Figure S1. Molecular structures of the investigated ligands

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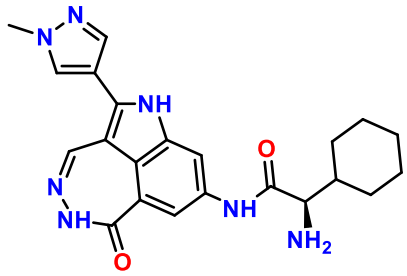	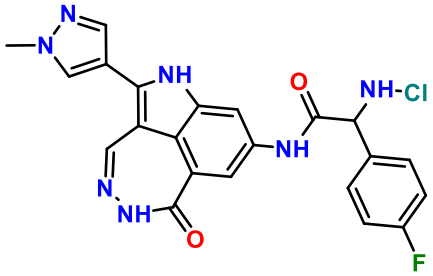	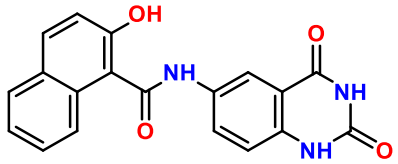
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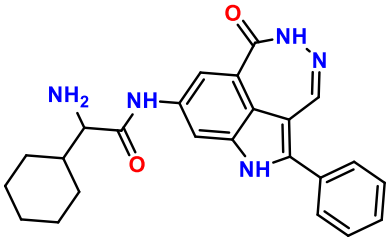	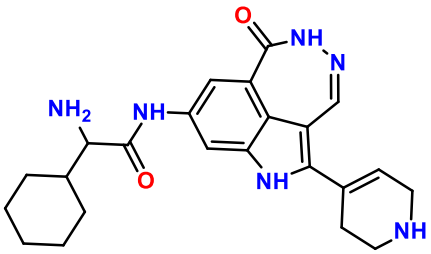	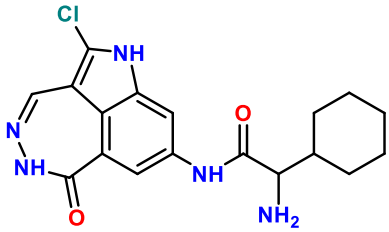
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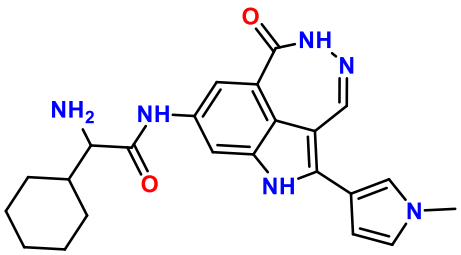	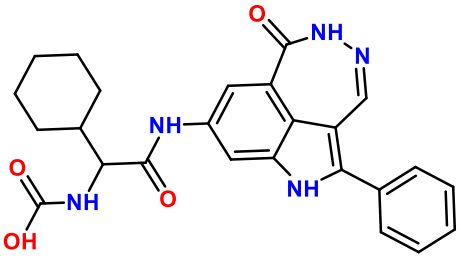	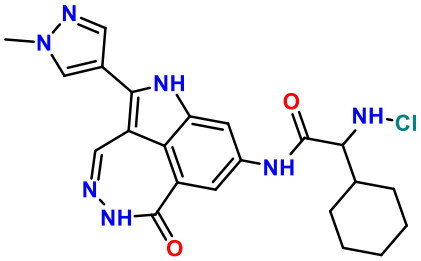
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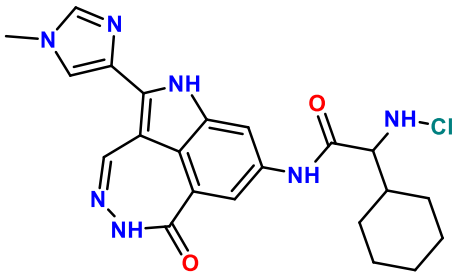	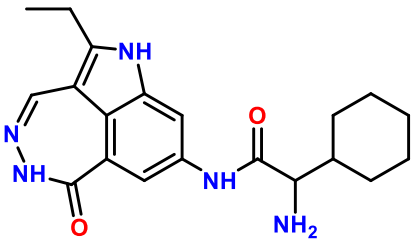	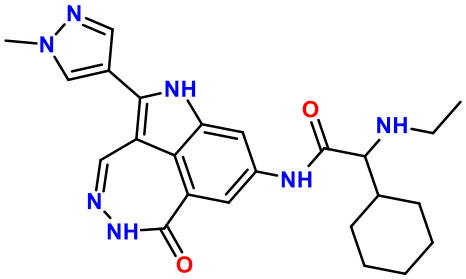
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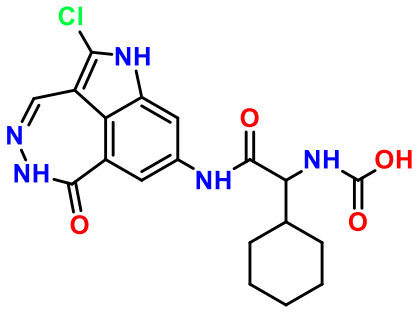	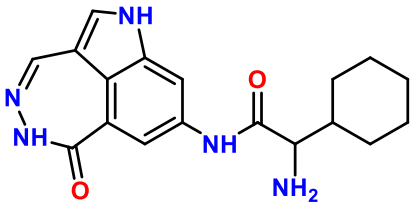	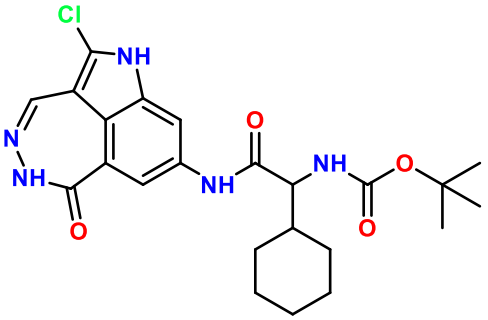

Figure S1. (*cont.*) Molecular structures of the investigated ligands

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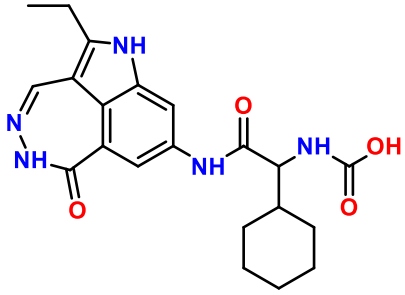	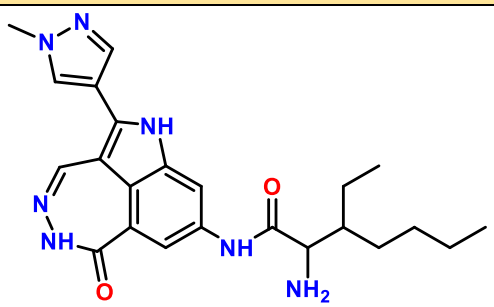	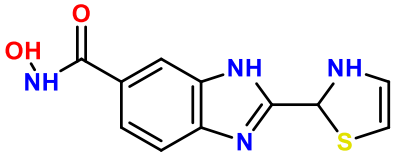
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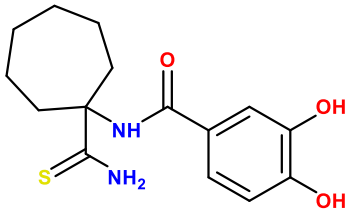	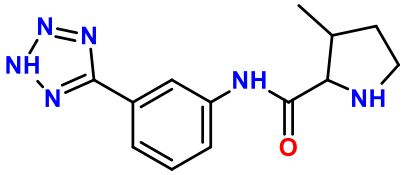	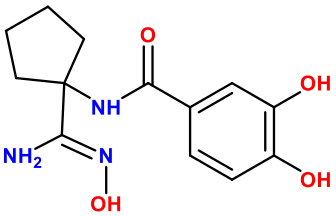
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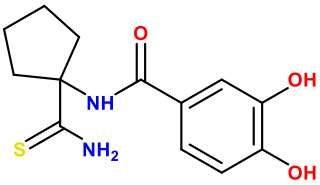	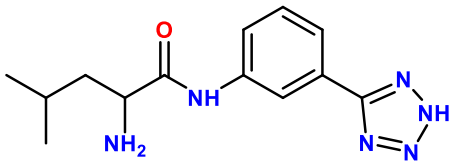	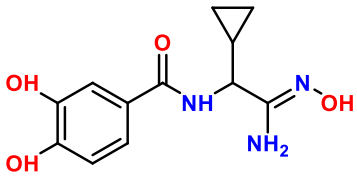
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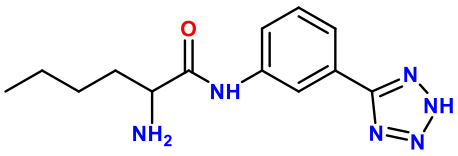	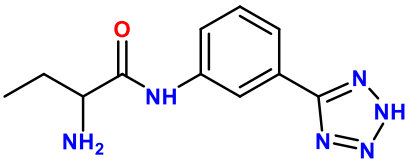	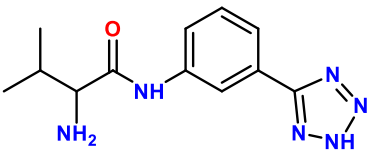
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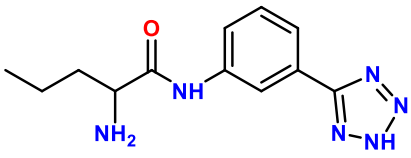	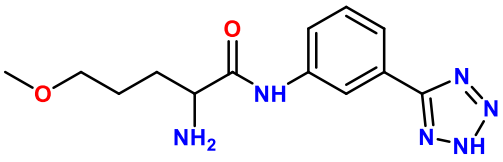	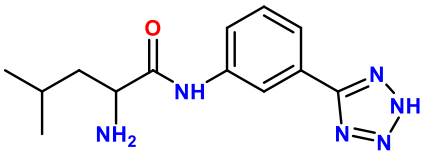
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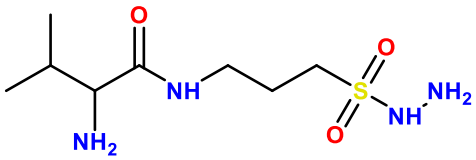		

Table S1. Docking scores of the investigated ligands

PubChem ID	Docking Scores (kcal/mol)	PubChem ID	Docking Scores (kcal/mol)
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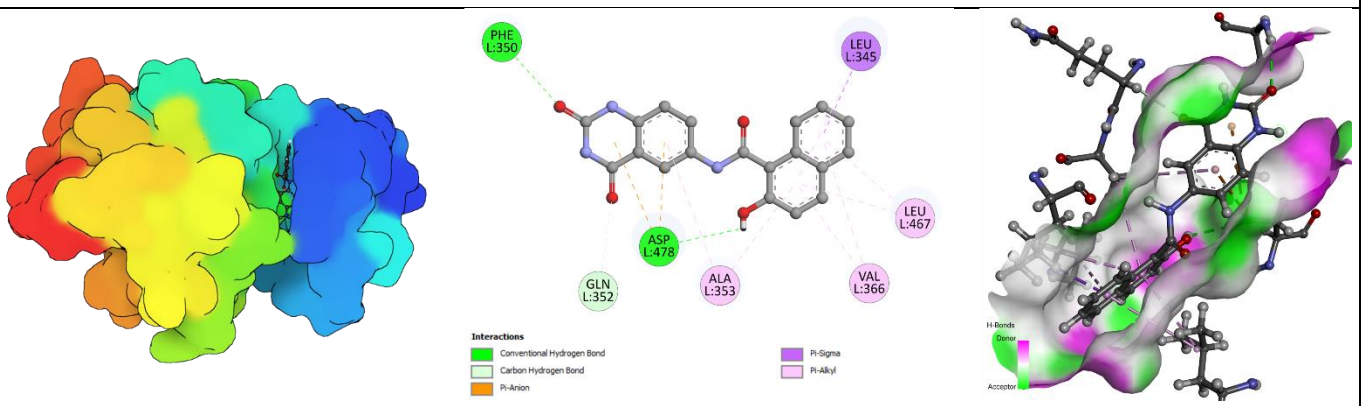
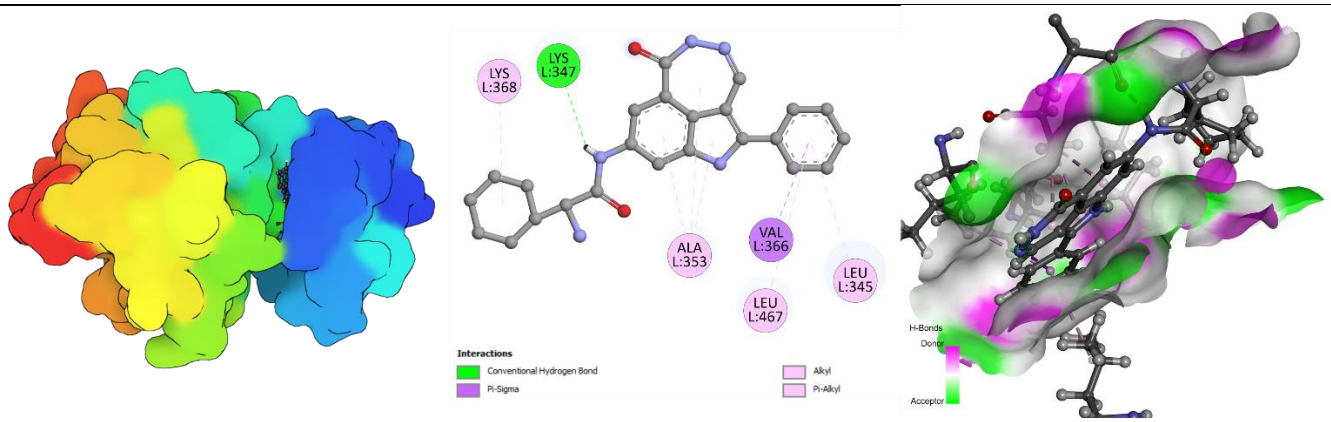
135774106	-9.10	**43712981**	-6.90
136141675	-9.10	**107728922**	-6.50
136181657	-8.90	**60854249**	-6.50
135794603	-8.80	**65813383**	-6.50
141608268	-8.30	**79013386**	-6.50
146582701	-7.50	**93269140**	-6.50
107728365	-7.40	**81071023**	-6.40
102778224	-7.30	**93041470**	-6.30
107728896	-7.00	**143275306**	-5.20

Figure S2. Binding poses and residue interactions of the investigated ligands with $LIMK_1$ (PDB ID: 5NXC)

PubChem-141609259: $LIMK_1$ complex || **Binding score: -10.10 kcal/mol**



PubChem-136141701: $LIMK_1$ complex || **Binding score: -10.00 kcal/mol**



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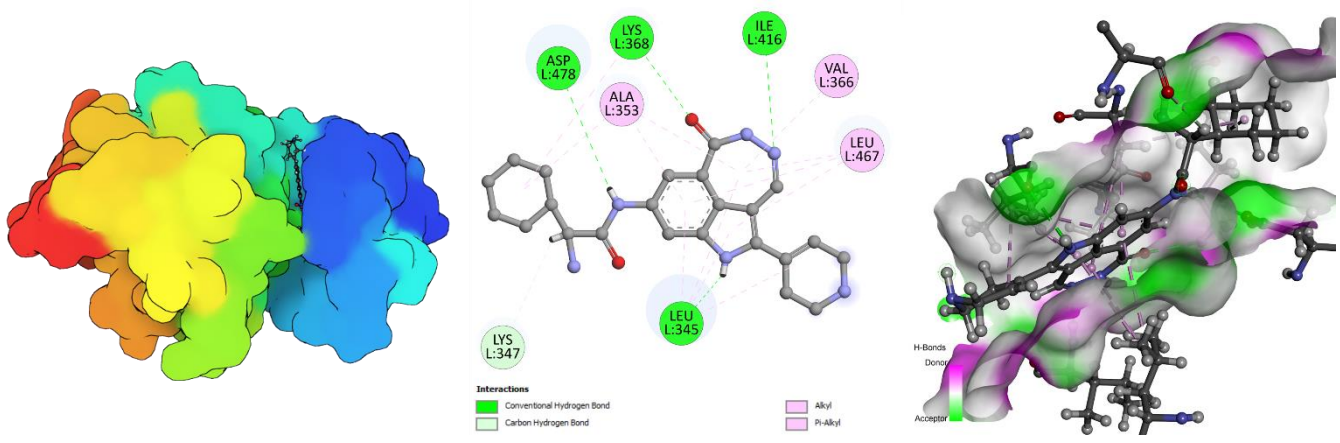

Figure S2. (*cont.*) Binding poses and residue interactions of the investigated ligands with $LIMK_1$ (PDB ID: 5NXC)

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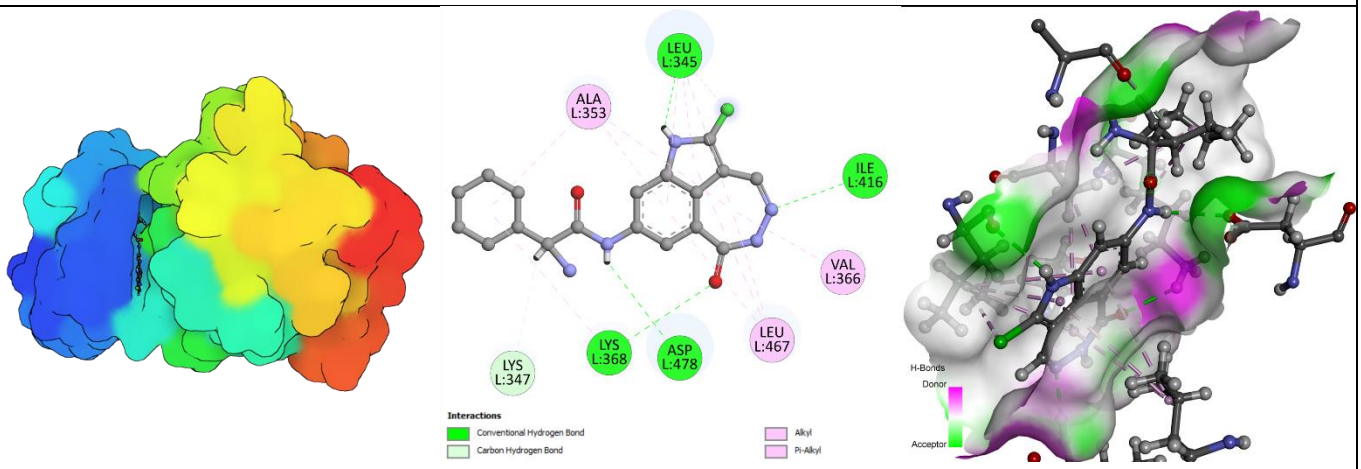
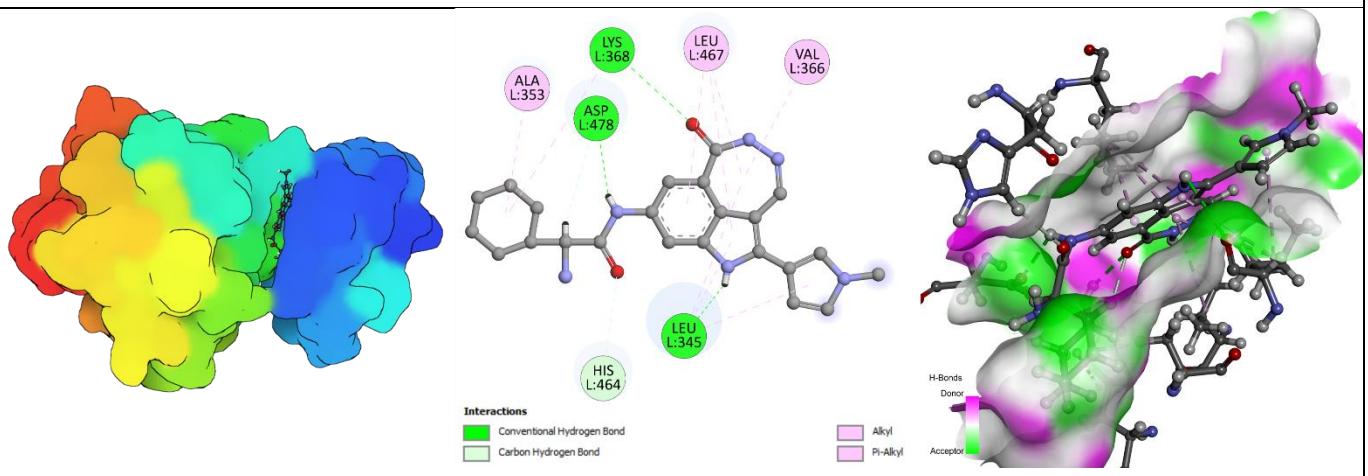


PubChem-135797427: $LIMK_1$ complex || **Binding score: -9.60 kcal/mol**



PubChem-136401905: $LIMK_1$ complex || **Binding score: -9.50 kcal/mol**

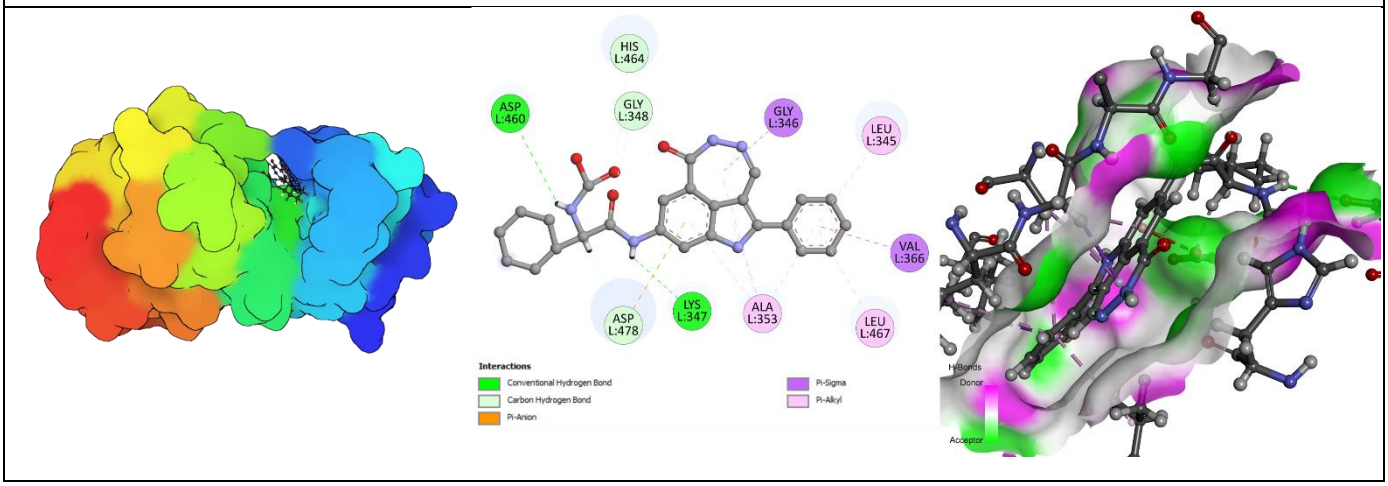


Figure S2. (*cont.*) Binding poses and residue interactions of the investigated ligands with $LIMK_1$ (PDB ID: 5NXC)

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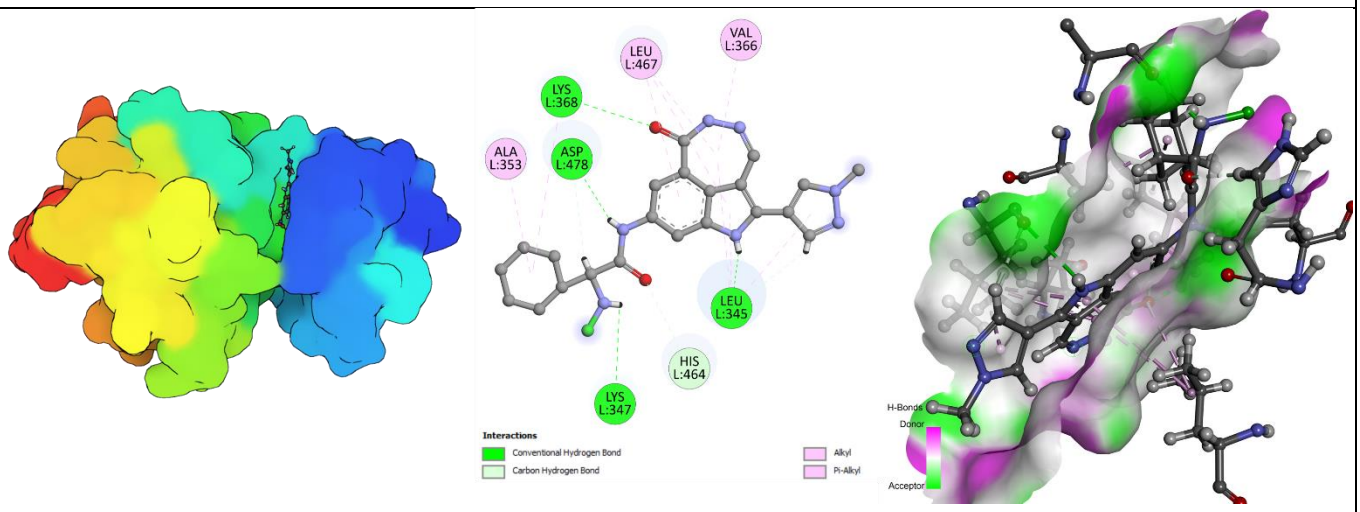

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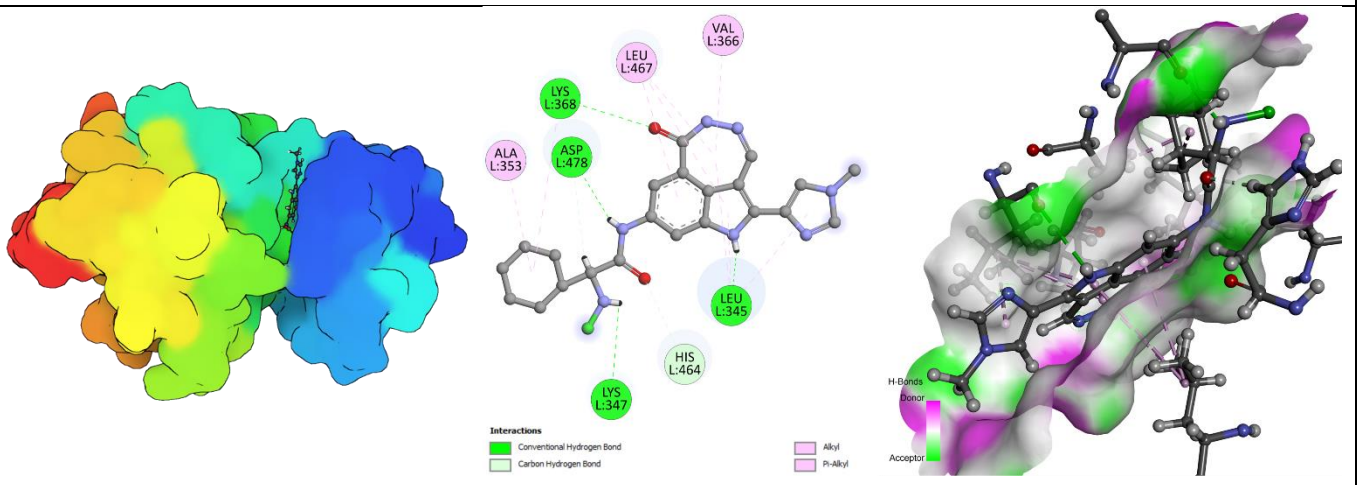

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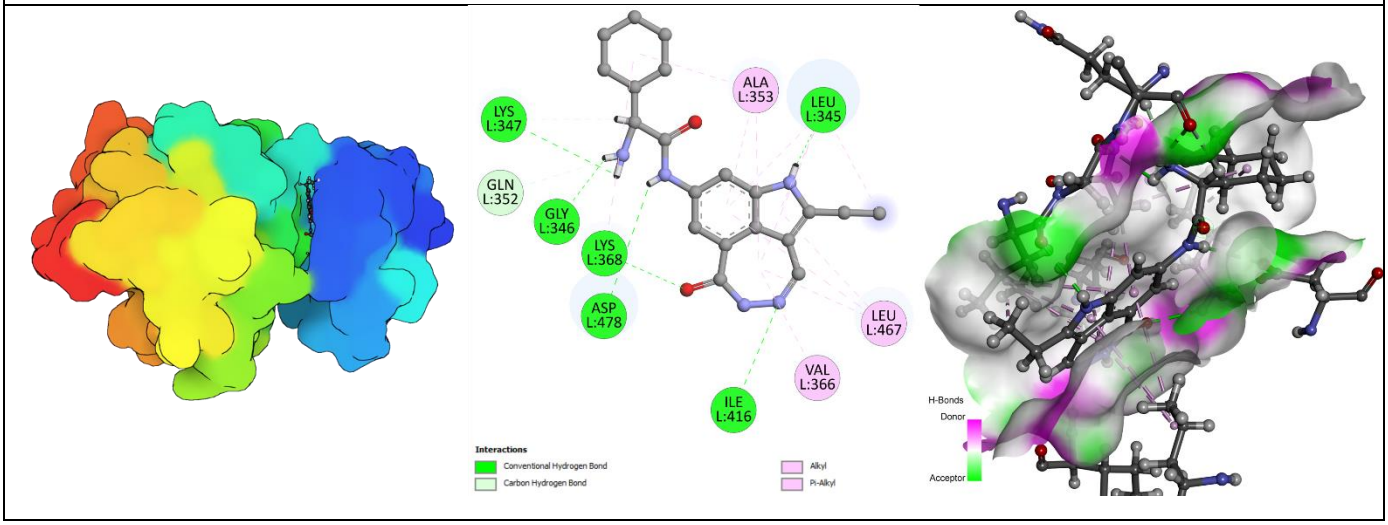

Figure S2. (*cont.*) Binding poses and residue interactions of the investigated ligands with $LIMK_1$ (PDB ID: 5NXC)

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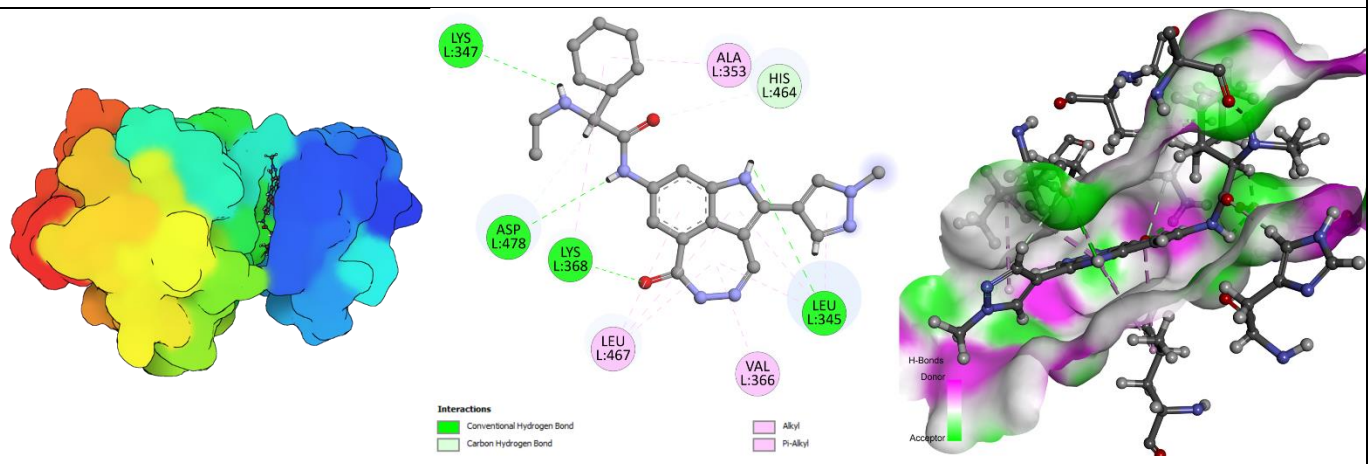

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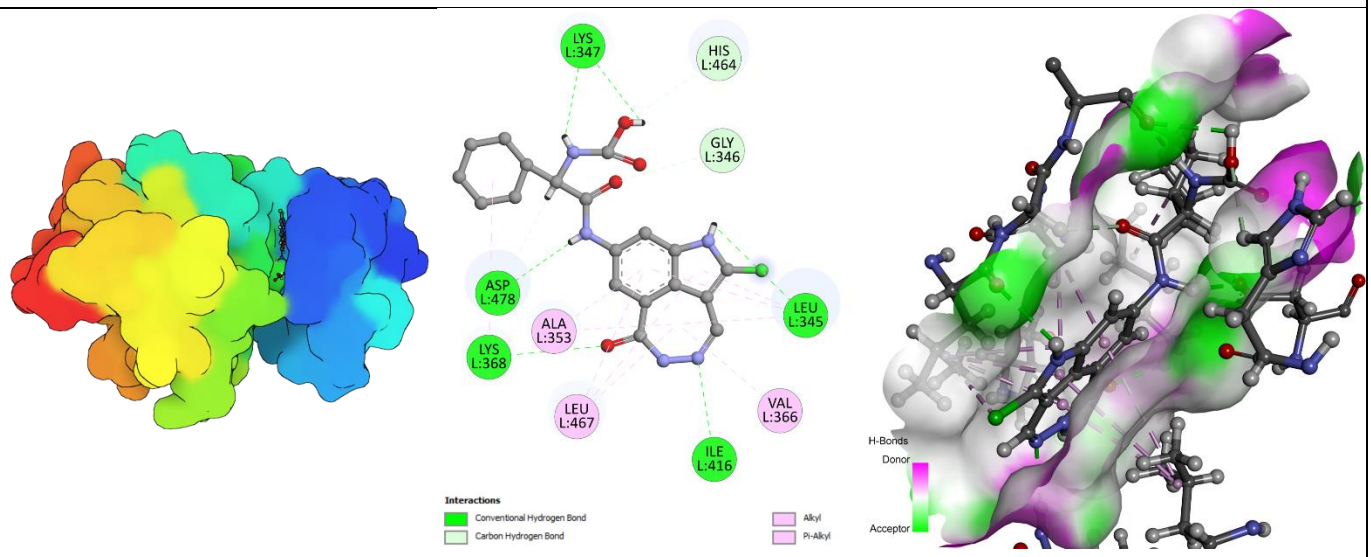

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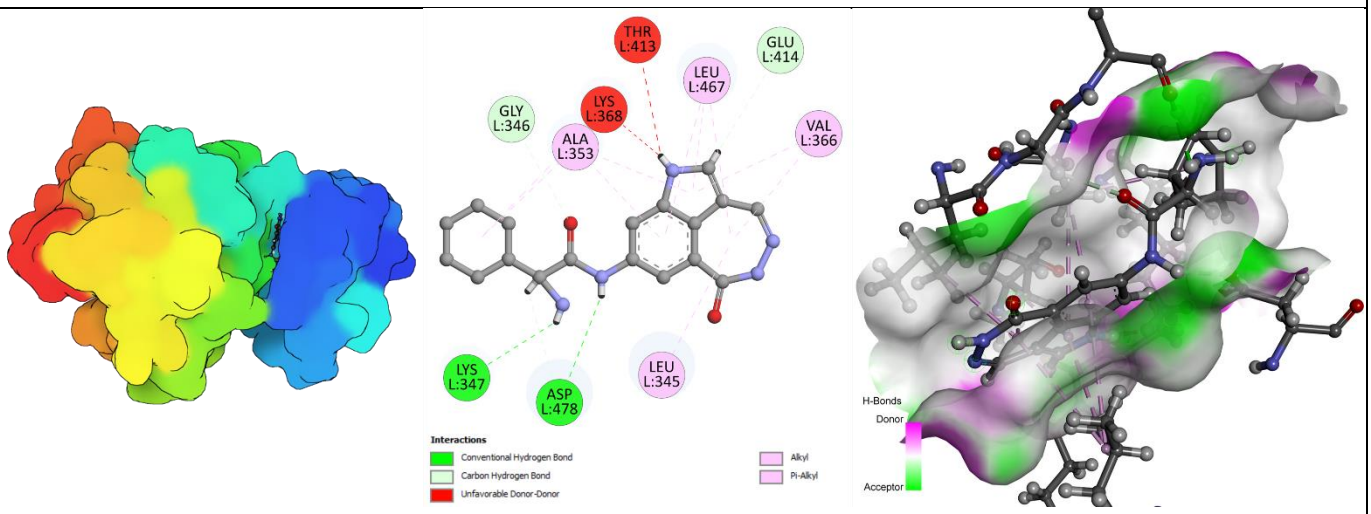

Figure S2. (*cont.*) Binding poses and residue interactions of the investigated ligands with $LIMK_1$ (PDB ID: 5NXC)

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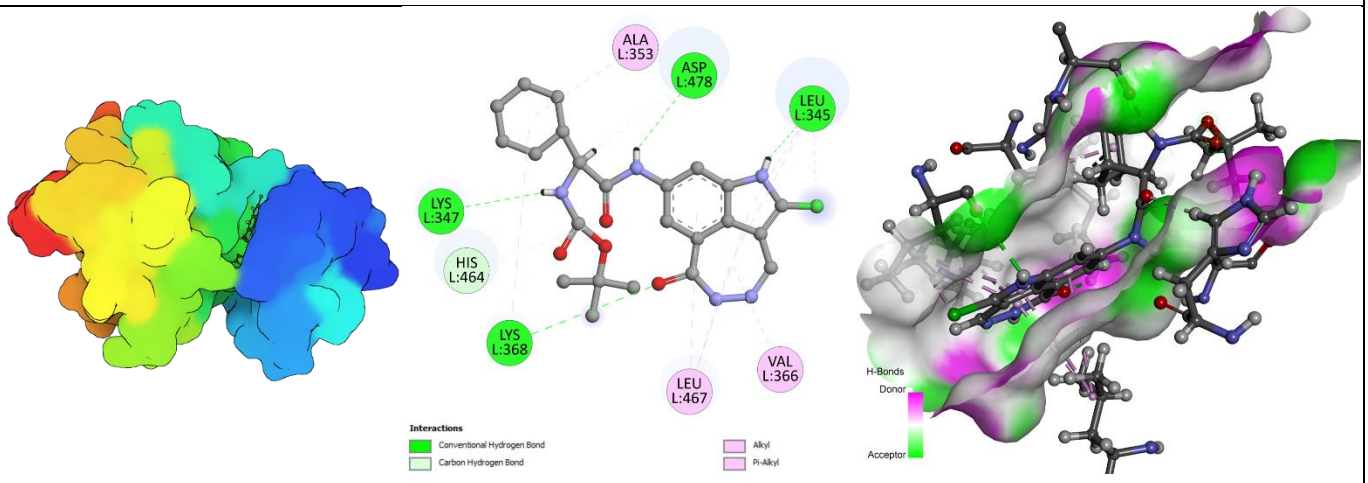

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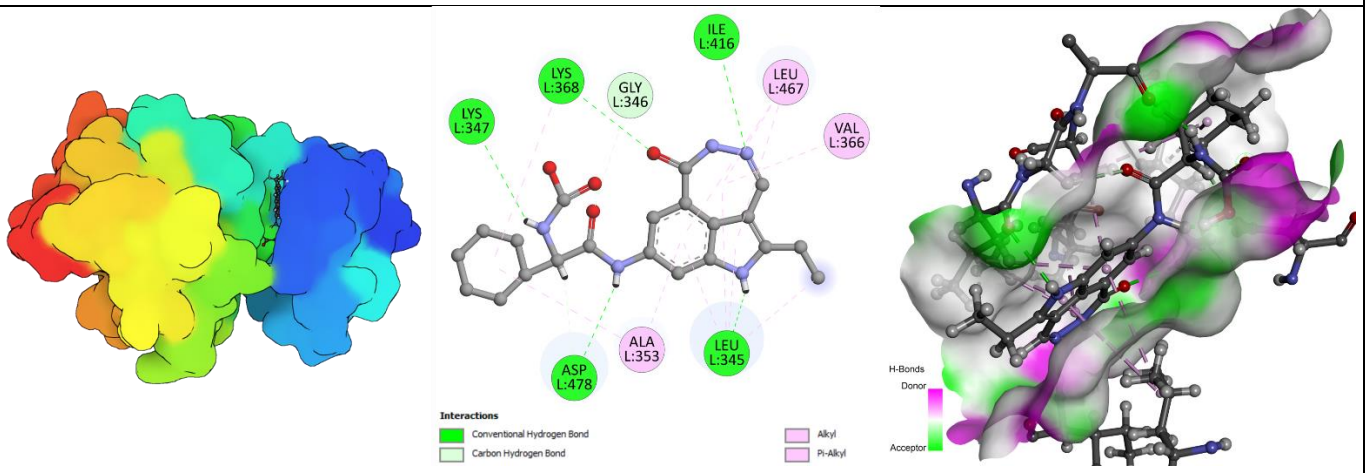

PubChem-141608268: $LIMK_1$ complex || **Binding score: -8.30 kcal/mol**

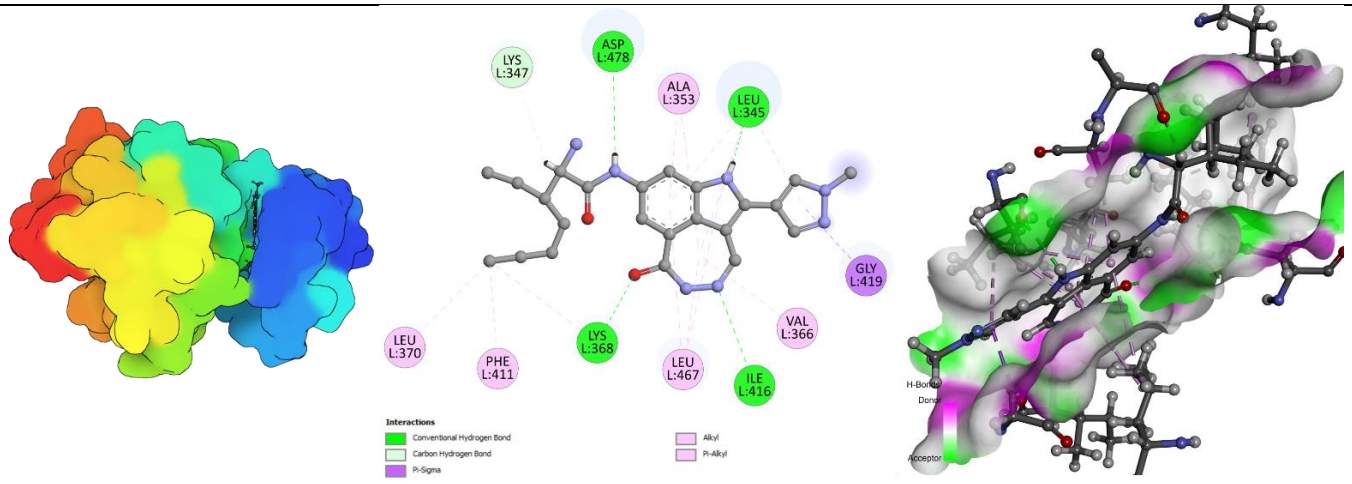

Figure S2. (*cont.*) Binding poses and residue interactions of the investigated ligands with $LIMK_1$ (PDB ID: 5NXC)

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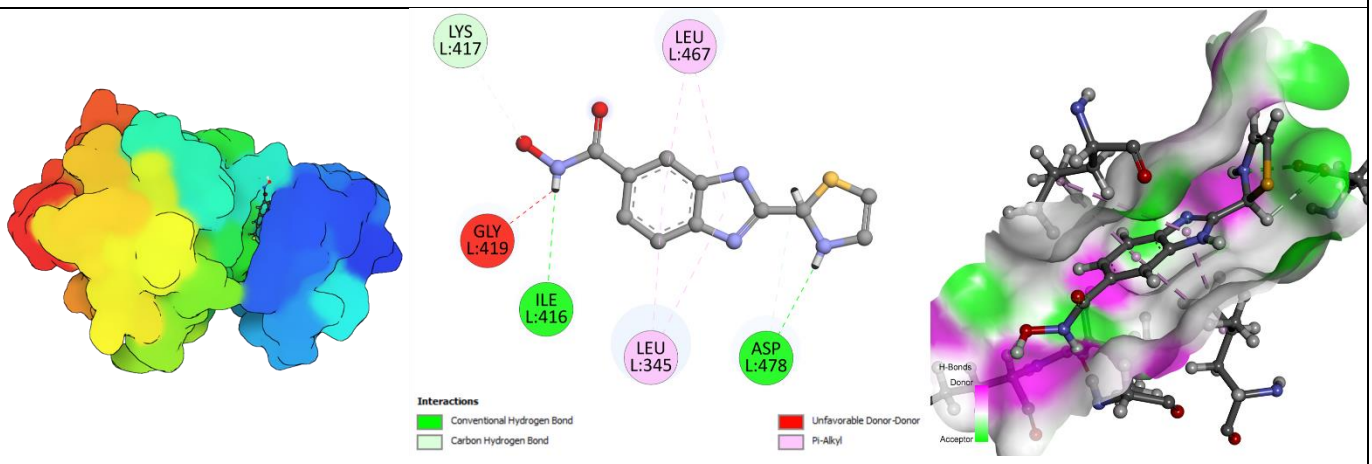

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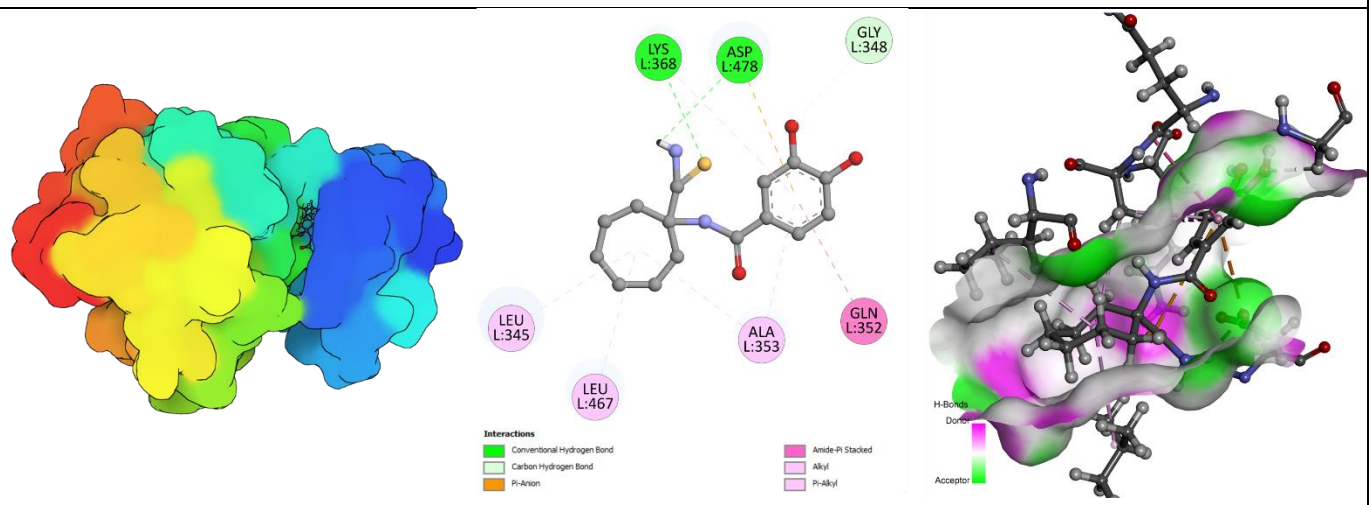

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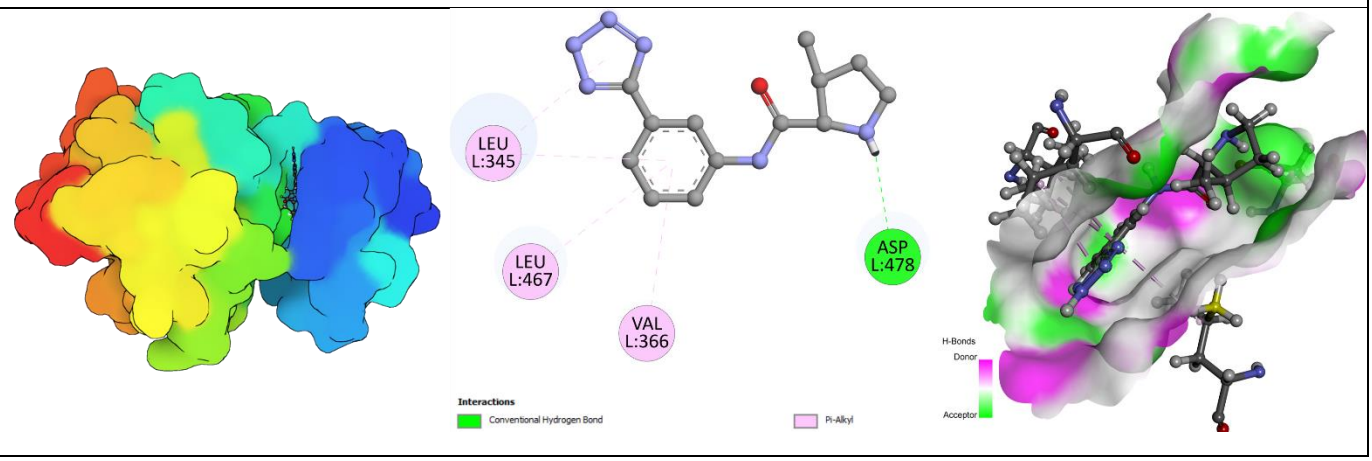
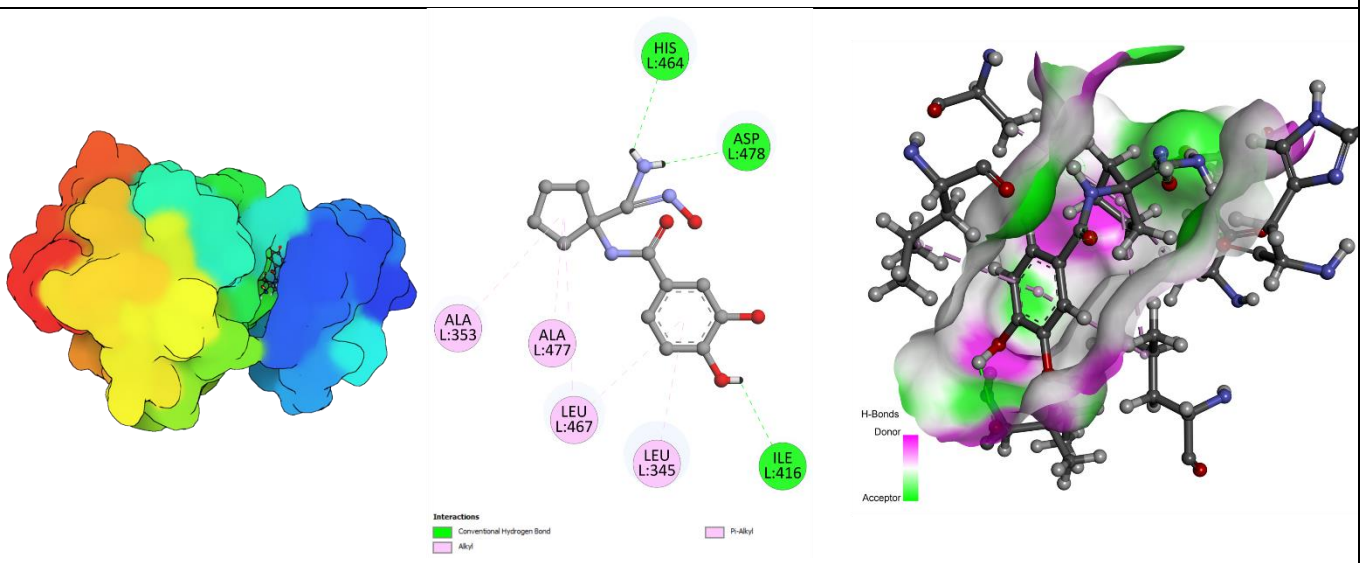
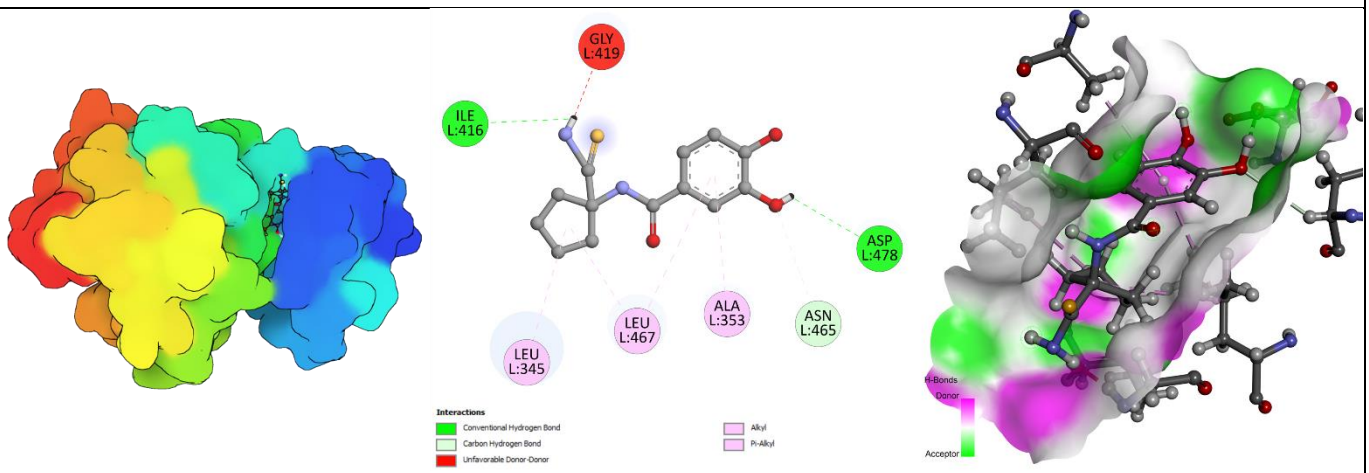


Figure S2. (*cont.*) Binding poses and residue interactions of the investigated ligands with $LIMK_1$ (PDB ID: 5NXC)

PubChem-107728896: $LIMK_1$ complex || **Binding score: -7.00 kcal/mol**



PubChem-107728362: $LIMK_1$ complex || **Binding score: -6.90 kcal/mol**



PubChem-43712981: $LIMK_1$ complex || **Binding score: -6.90 kcal/mol**

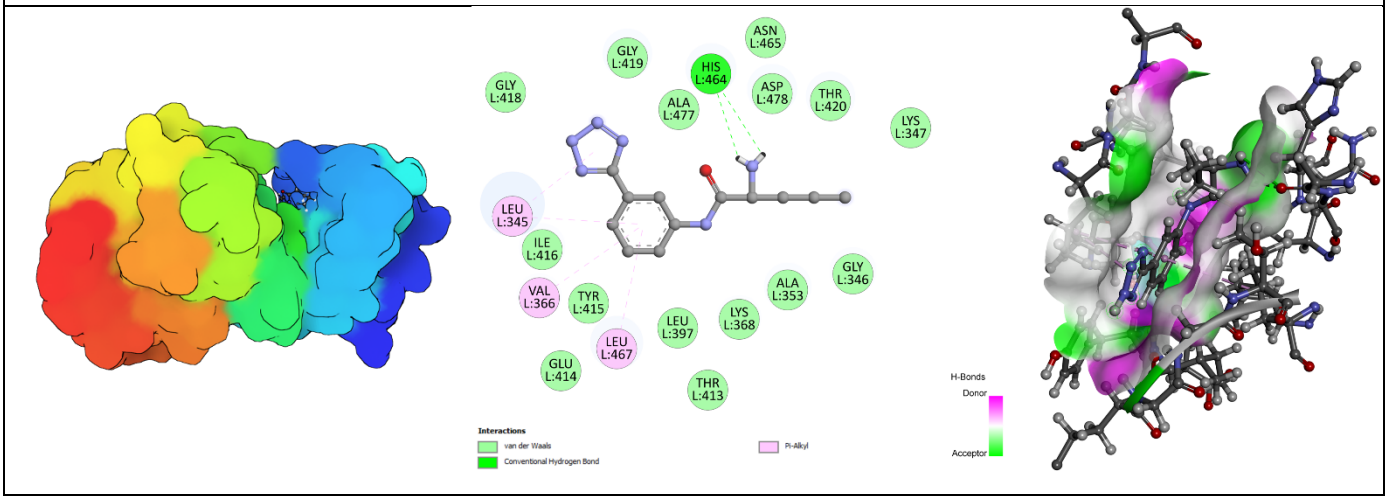
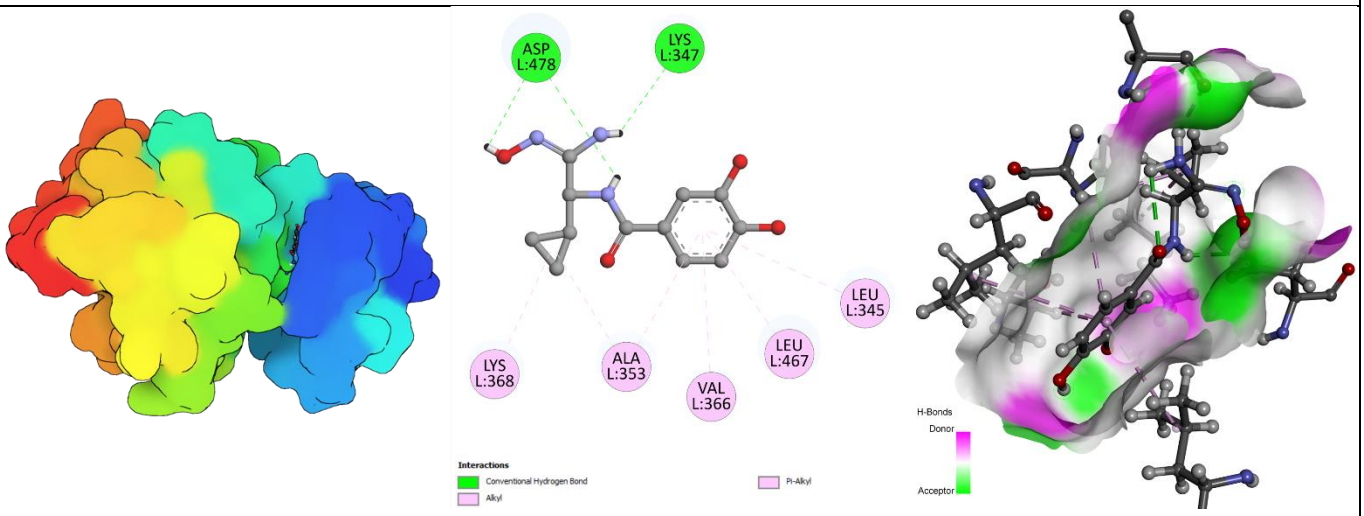
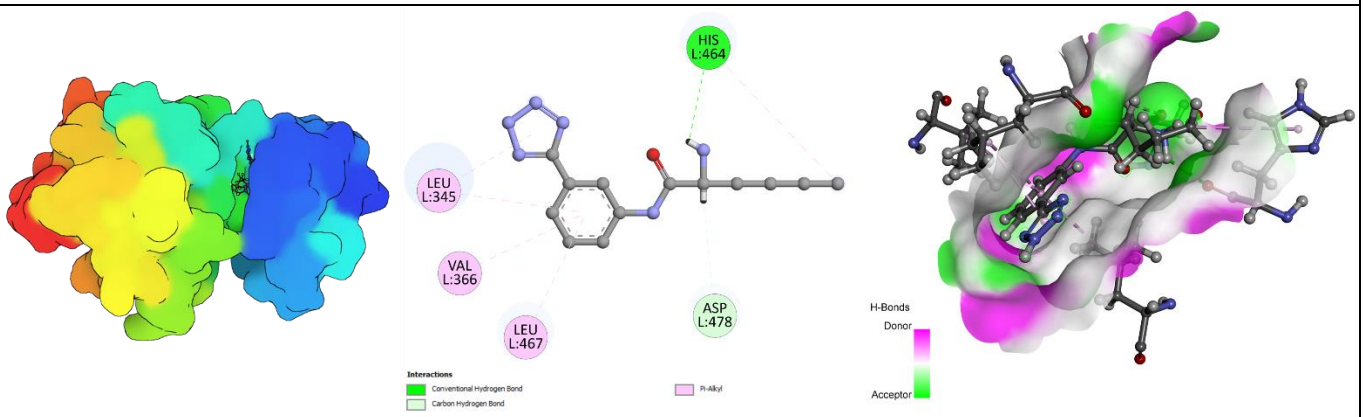


Figure S2. (*cont.*) Binding poses and residue interactions of the investigated ligands with $LIMK_1$ (PDB ID: 5NXC)

PubChem-107728922: $LIMK_1$ complex || **Binding score: -6.50 kcal/mol**



PubChem-60854249: $LIMK_1$ complex || **Binding score: -6.50 kcal/mol**



PubChem-65813383: $LIMK_1$ complex || **Binding score: -6.50 kcal/mol**

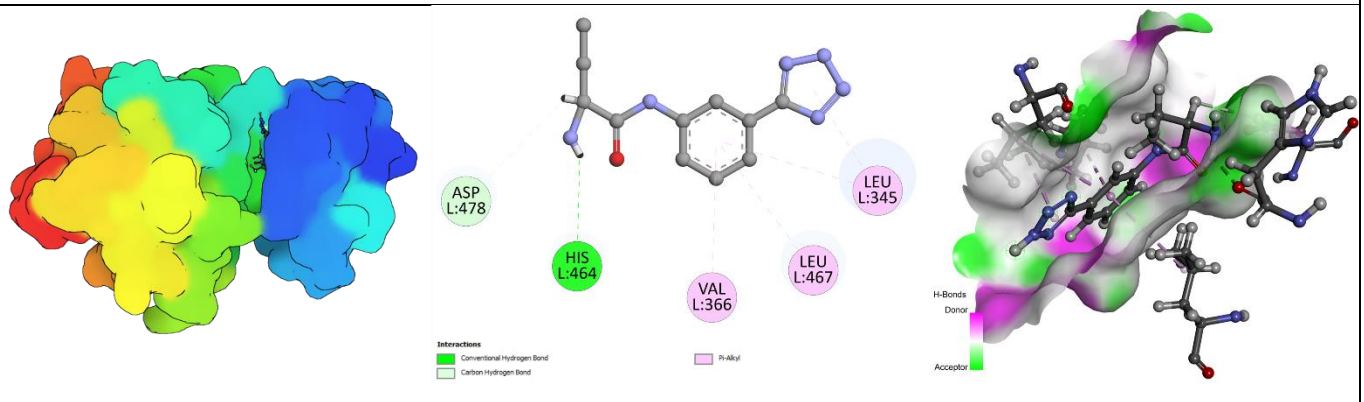
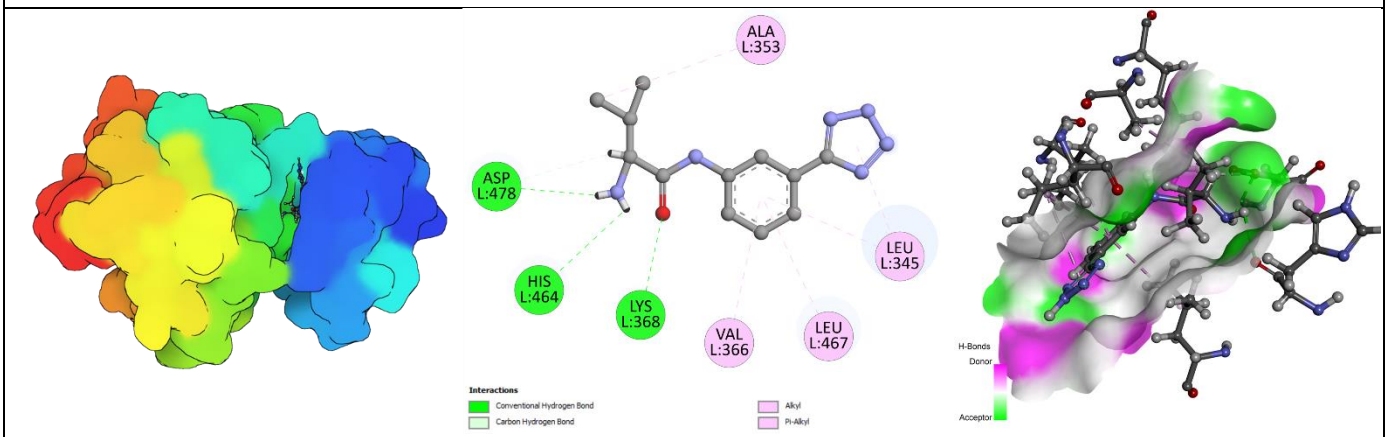
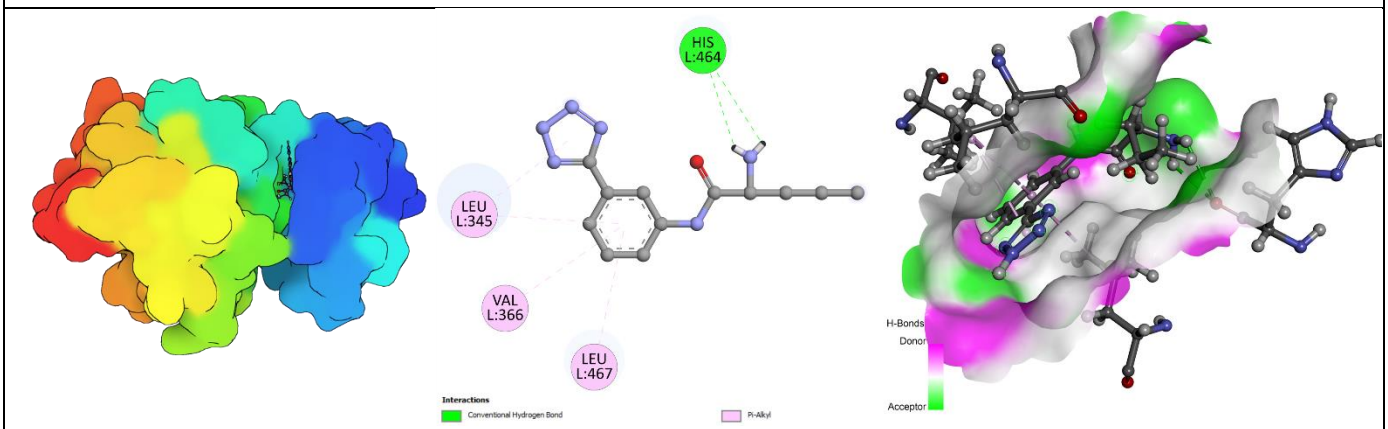


Figure S2. (*cont.*) Binding poses and residue interactions of the investigated ligands with $LIMK_1$ (PDB ID: 5NXC)

PubChem-79013386: $LIMK_1$ complex || **Binding score: -6.50 kcal/mol**



PubChem-93269140: $LIMK_1$ complex || **Binding score: -6.50 kcal/mol**



PubChem-81071023: $LIMK_1$ complex || **Binding score: -6.40 kcal/mol**

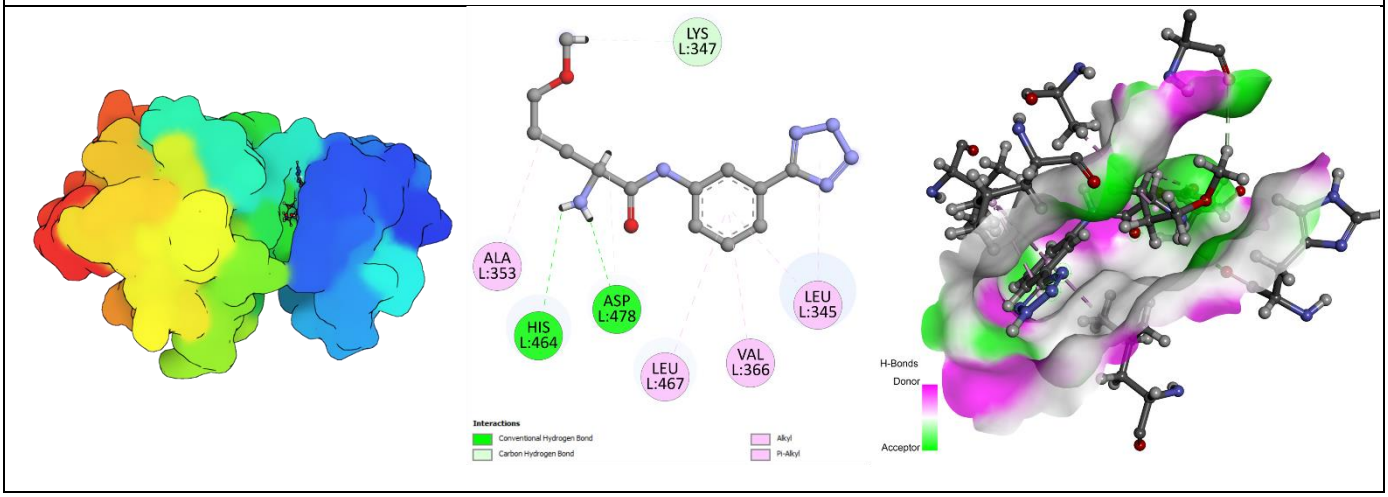
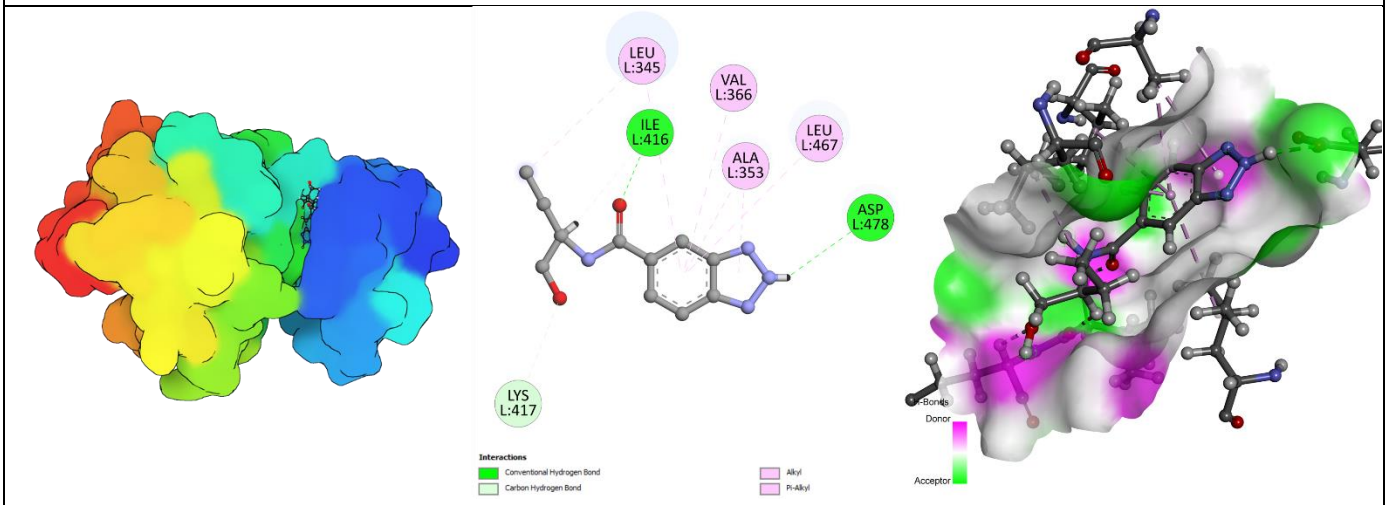


Figure S2. (*cont.*) Binding poses and residue interactions of the investigated ligands with $LIMK_1$ (PDB ID: 5NXC)

PubChem-93041470: $LIMK_1$ complex || **Binding score: -6.30 kcal/mol**



PubChem-143275306: $LIMK_1$ complex || **Binding score: -5.20 kcal/mol**

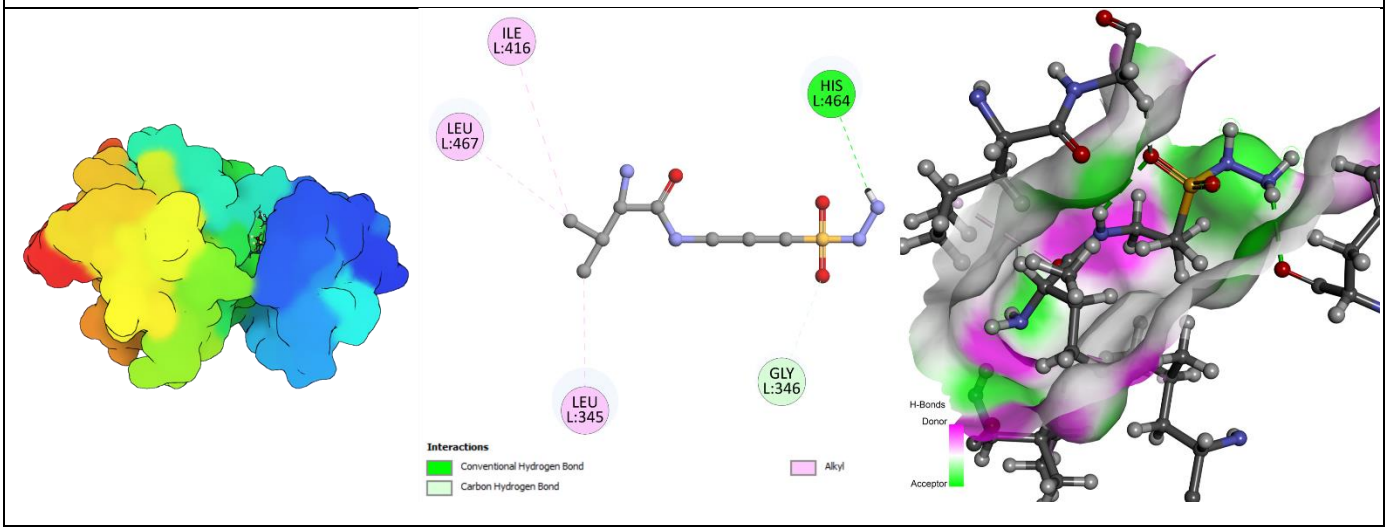


Table S2. SwissADME properties of the investigated ligands

PubChem ID	[a]MW (g/mol)	[b]HBA	[c]HBD	[d]nROTB	[e]TPSA	[f]GI abs.	[g]BBB	[h]clog$P_{o/w}$	Solubility	Violation
136931641	447.53	5	4	7	120.49	High	No	2.78	MS	0
135774106	417.85	5	5	6	139.97	Low	No	2.47	MS	0
136141675	339.39	4	4	4	116.66	High	No	1.95	S	0
136181657	473.95	5	4	8	128.97	Low	No	3.69	MS	0
135794603	411.45	5	5	7	139.97	Low	No	2.47	S	0
141608268	435.52	5	4	9	134.48	High	No	2.67	MS	0
136141701	415.49	4	4	5	116.66	High	No	3.31	MS	0
107728365	308.40	3	4	4	127.67	High	No	1.98	S	0
102778224	272.31	5	3	4	95.59	High	No	1.04	S	0
107728896	279.29	5	5	4	128.17	High	No	0.91	S	0
107728362	280.34	3	4	4	127.67	High	No	1.36	S	0
43712981	274.32	5	3	6	109.58	High	No	1.26	S	0
107728922	265.27	5	5	5	128.17	High	No	0.33	VS	0
60854249	274.32	5	3	7	109.58	High	No	1.27	S	0
65813383	246.27	5	3	5	109.58	High	No	0.65	VS	0
79013386	260.30	5	3	5	109.58	High	No	0.9	S	0
93269140	260.30	5	3	6	109.58	High	No	0.98	VS	0
81071023	290.32	6	3	8	118.81	High	No	0.67	VS	0
93041470	274.32	5	3	6	109.58	High	No	1.29	S	0
143275306	252.33	6	4	8	135.69	High	No	-0.79	VS	0

Lipinski's Rule: [a]MW≤500 g/mol, [b]HBA≤10, [c]HBD≤5, [d]nROTB≤9, 20≤[e]TPSA≥130Å², [h]clog$P_{o/w}$≤5

Abbreviations: [a]MW: Molecular Weight, [b]HBA: Hydrogen Bond Acceptor, [c]HBD: Hydrogen Bond Donor, [d]nROTB: Number of Rotatable Bonds, [e]TPSA: Topological Polar Surface Area, [f]GI abs: Gastrointestinal absorption [g]BBB: Blood-brain Barrier Permeability, [h]clog$P_{o/w}$: Consensus log$P_{o/w}$, IS: Insoluble, PS: Poorly Soluble, MS: Moderately Soluble, S: Soluble, HS: Highly Soluble

Table S3. PreADMET results of the candidate drug molecules

PubChem ID	BBB[a] ([brain]/[blood])	HIA[c] (%)	PPB[e] (%)
136931641	0.30	85.43	66.82
135774106	0.17	78.07	83.17
136141675	0.15	78.61	35.35
136181657	0.62	85.18	85.48
135794603	0.23	73.75	82.74
141608268	0.23	83.47	67.80
146582701	0.10	76.26	30.96
107728365	0.19	86.84	81.43
102778224	0.01	87.61	18.62
107728896	0.14	49.31	57.90
107728362	0.83	85.85	92.24
43712981	0.04	83.95	17.20
107728922	0.10	46.96	56.47
60854249	0.03	83.97	20.60
65813383	0.01	79.89	11.67
79013386	0.01	81.99	14.66
93269140	0.02	82.02	15.52
81071023	0.03	77.91	17.03
93041470	0.04	83.95	17.20
143275306	0.22	44.70	0.00

Abbreviations: [a]BBB: Blood-brain barrier, [c]HIA: Passive gastrointestinal absorption, [e]PPB: Plasma-protein binding
The rule for BBB permeability: <0.1 low absorption by CNS, between 0.1 and 0.2 moderate absorption, >0.2 high absorption

Figure S3. Bioavailability radar representations of the investigated ligands

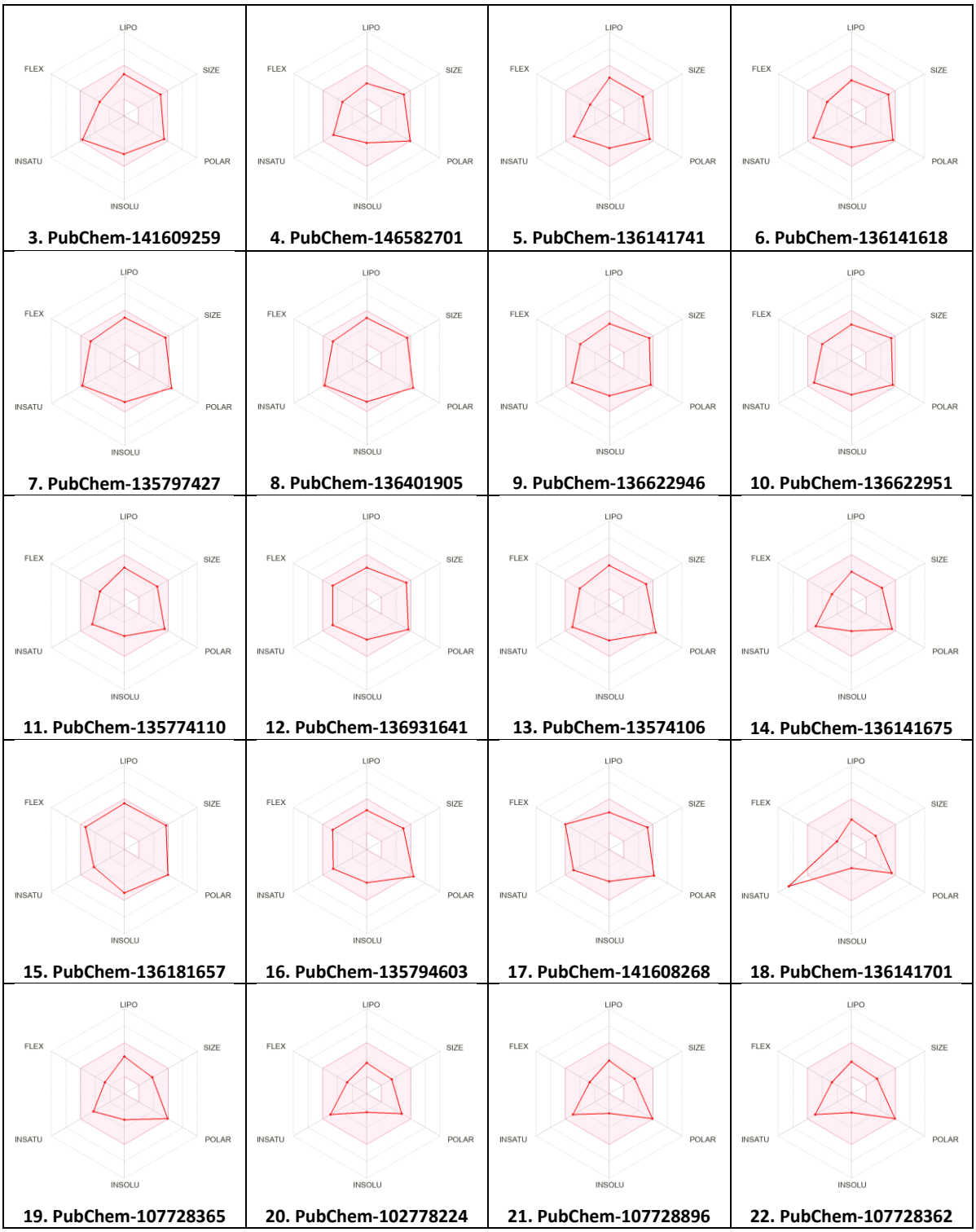
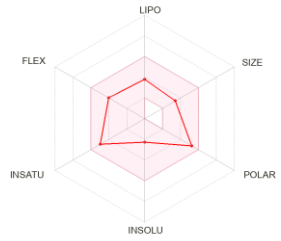
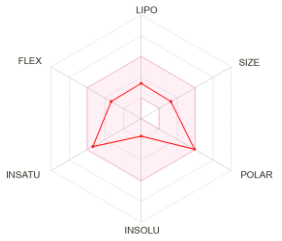


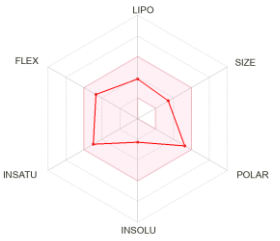
Figure S3. ***(cont.)*** Bioavailability radar representations of the investigated ligands



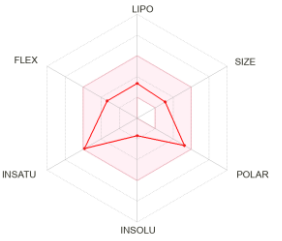
23. PubChem-43712981



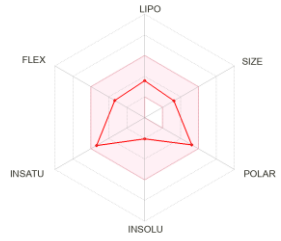
24. PubChem-107728922



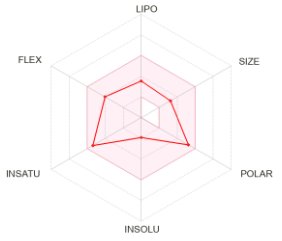
25. PubChem-60854249



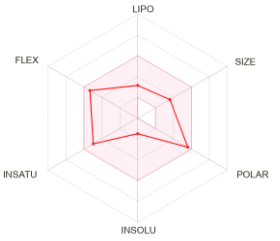
26. PubChem-65813383



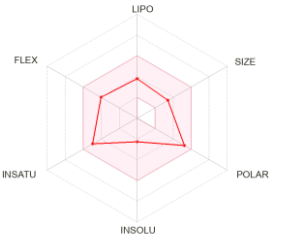
27. PubChem-79013386



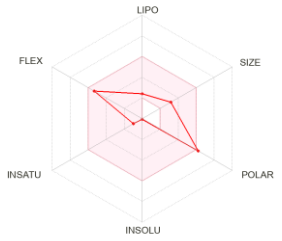
28. PubChem-93269140



29. PubChem-81071023



30. PubChem-93041470



31. PubChem-143275306

Table S4. Toxicity risk assessment of the investigated ligands

PubChem ID	Mut	Tum	Irr	Rep. E.	d	ds
136931641	🟢	🔴	🟢	🟢	+3.92	0.33
135774106	🟡	🔴	🔴	🟡	+3.22	0.13
136141675	🟢	🔴	🟢	🟢	+0.27	0.34
136181657	🟢	🔴	🟢	🟢	-52.96	0.13
135794603	🟡	🔴	🔴	🟡	+3.40	0.13
141608268	🟢	🔴	🟡	🔴	+0.36	0.13
146582701	🔴	🟢	🟢	🟢	+2.77	0.55
107728365	🟢	🟢	🟢	🟢	-1.95	0.48
102778224	🟢	🟢	🟢	🟢	+1.41	0.78
107728896	🟢	🟢	🟢	🟢	+0.52	0.75
107728362	🟢	🟢	🟢	🟢	+0.41	0.73
43712981	🟢	🟢	🟢	🟢	-12.19	0.42
107728922	🟢	🟢	🟢	🟢	+3.62	0.93
60854249	🟢	🟢	🟢	🟢	-9.79	0.42
65813383	🟢	🟢	🟢	🟢	-1.81	0.51
79013386	🟢	🟢	🟢	🟢	-7.86	0.44
93269140	🟢	🟢	🟢	🟢	-5.84	0.43
81071023	🟢	🟢	🟢	🟢	-6.74	0.44
93041470	🟢	🟢	🟢	🟢	-12.19	0.42
143275306	🟢	🟢	🟢	🟢	-7.74	0.49

Abbreviations: Mut: Mutagenic, Tum: Tumorgenic, Irr: Irritant, Rep. E: Reproductive effectiveness, d: Druglikeness, ds: Drug Score

🟢 **No detectable toxicitiy** 🟡 **Moderate toxicity** 🔴 **High toxicity**

Table S5. Bioactivity data of the investigated ligands | Molinspiration

PubChem ID	GPCR	ICM	KI	NRL	PI	EI
136931641	0.02	-0.18	0.29	-0.92	-0.13	0.09
135774106	0.19	0.07	0.17	-0.52	0.18	0.26
136141675	0.04	-0.01	0.36	-0.70	0.07	0.25
136181657	0.14	0.15	0.14	-0.47	0.23	0.24
135794603	0.08	-0.03	0.09	-0.52	0.11	0.22
141608268	0.05	-0.14	0.34	-0.81	-0.01	0.20
146582701	-0.05	-0.27	-0.07	-0.53	0.47	0.48
107728365	-0.04	-0.25	-0.18	-0.13	-0.06	0.05
102778224	0.46	0.24	0.13	-0.64	0.37	0.24
107728896	0.00	-0.29	-0.17	-0.01	0.24	0.24
107728362	-0.12	-0.28	-0.25	-0.18	-0.13	0.09
43712981	0.42	0.20	0.12	-0.54	0.38	0.22
107728922	0.02	-0.13	-0.13	-0.32	0.20	0.22
60854249	0.43	0.15	0.14	-0.56	0.28	0.24
65813383	0.30	0.13	0.04	-0.78	0.13	0.15
79013386	0.28	-0.01	0.08	-0.80	0.26	0.16
93269140	0.39	0.15	0.10	-0.66	0.22	0.23
81071023	0.37	0.07	0.18	-0.59	0.27	0.17
93041470	0.42	0.20	0.12	-0.54	0.38	0.22
143275306	-0.18	-0.14	-0.66	-0.84	0.48	0.08

Table S6. ADME results of the investigated ligands | Molinspiration

PubChem ID	miLogP[a]	TPSA[b]	nAtoms[c]	nON[d]	nOHNH[e]	nROTB[f]	Volume	Violation
136931641	2.54	120.50	33	9	4	6	409.98	0
135774106	3.94	139.97	29	9	5	4	347.97	0
136141675	1.20	116.67	25	7	5	3	306.32	0
136181657	5.75	128.97	33	9	4	6	415.13	1
135794603	3.94	139.97	30	9	5	5	367.80	0
141608268	2.15	134.49	32	9	5	8	402.67	0
146582701	0.34	90.04	18	6	4	2	212.20	0
107728365	1.56	95.58	21	5	5	3	277.09	0
102778224	1.17	95.59	20	7	3	3	244.74	0
107728896	0.65	128.17	20	7	6	3	246.90	1
107728362	0.55	95.58	19	5	5	3	243.48	0
43712981	1.04	109.59	20	7	4	5	254.22	0
107728922	0.04	128.17	19	7	6	4	230.45	1
60854249	1.33	109.59	20	7	4	6	254.44	0
65813383	0.26	109.59	18	7	4	4	220.83	0
79013386	0.51	109.59	19	7	4	4	237.42	0
93269140	0.82	109.59	19	7	4	5	237.63	0
81071023	-0.09	118.82	21	8	4	7	263.42	0
93041470	1.04	109.59	20	7	4	5	254.22	0
143275306	-1.78	127.31	16	7	6	7	227.62	1

Abbreviations: [a]milogP: Partition coefficient between n-octanol and water ($logP_{o/w}$), [b]TPSA: Topological polar surface area, [c]nAtoms: Number of atoms, [d]nON: Number of hydrogen bond acceptors (HBA), [e]nOHNH: Number of hydrogen bond donors (HBD), [f]nROTB: Number of rotatable bonds

Table S7. Syntelly toxicity results of the investigated ligands

PubChem ID	M.O LD_{50} (mg/kg)	Rep. Tox.	Hpt.	Crd.	Crn.	Tox	Phys	Bio	Eco
136931641	861.00	T	NT	NT	NT	🟡	🟢	🟢	🟢
135774106	1690.00	T	T	NT	T	🟢	🟢	🟢	🟢
136141675	1250.00	T	NT	NT	NT	🟡	🟢	🔴	🟢
136181657	1280.00	T	T	NT	NT	🟡	🟢	🔴	🟢
135794603	1730.00	T	T	NT	T	🟢	🟢	🟢	🟢
141608268	1200.00	T	NT	NT	NT	🟡	🟢	🟢	🟢
146582701	1260.00	T	T	NT	NT	🟡	🟢	🟢	🔴
107728365	1860.00	T	NT	NT	NT	🟢	🟢	🟢	🔴
102778224	1090.00	T	T	NT	NT	🟡	🟢	🔴	🔴
107728896	864.00	T	NT	NT	NT	🟡	🟢	🟢	🔴
107728362	1730.00	T	NT	NT	NT	🟢	🟢	🔴	🔴
43712981	1080.00	T	T	NT	NT	🟡	🟢	🟢	🟢
107728922	878.00	T	NT	NT	NT	🟡	🟢	🟢	🔴
60854249	1380.00	T	T	NT	NT	🟢	🟢	🔴	🟢
65813383	1390.00	T	T	NT	NT	🟡	🟢	🟢	🔴
79013386	1070.00	T	T	NT	NT	🟡	🟢	🔴	🔴
93269140	1350.00	T	T	NT	NT	🟢	🟢	🟢	🟢
81071023	1620.00	T	T	NT	NT	🟡	🟢	🟢	🟢
93041470	1080.00	T	T	NT	NT	🟡	🟢	🟢	🟢
143275306	1460.00	T	NT	NT	NT	🟡	🟢	🟢	🔴

Abbreviations: M.O. LD_{50}: Mouse oral LD_{50}, Rep. Tox: Reproductive toxicity, Hpt: Hepatotoxicity, Crd: Cardiotoxicity, Crn: Carcinogenicity, T: Toxic, NT: Non-toxic,

Table S8. Interaction data of the investigated ligands with $LIMK_1$ (PDB ID: 5NXC)

PubChem ID	Residue Information	Distance	Category	Type of Interactions
329823760 (*Reference)*	L:9DB701:H - L:LEU345:O	2,53937	HB	CHB
	L:9DB701:H - L:ASP478:OD2	2,37334	HB	CHB
	L:9DB701:H - L:LYS347:O	2,98533	HB	CHB
	L:9DB701:H - L:LYS347:O	2,9145	HB	Carbon HB
	L:LEU467:CD1 - L:9DB701	3,93692	Hyd	Pi-Sg
	L:ALA353 - L:9DB701	5,46324	Hyd	Alkyl
	L:LYS368 - L:9DB701	4,72629	Hyd	Alkyl
	L:9DB701 - L:LEU345	5,09628	Hyd	Pi-Al
	L:9DB701 - L:LEU345	4,25185	Hyd	Pi-Al
	L:9DB701 - L:LEU467	5,38461	Hyd	Pi-Al
	L:9DB701 - L:LEU345	5,26779	Hyd	Pi-Al
	L:9DB701 - L:ALA353	4,0369	Hyd	Pi-Al
	L:9DB701 - L:LEU467	5,4436	Hyd	Pi-Al
	L:9DB701 - L:LEU345	4,41523	Hyd	Pi-Al
	L:9DB701 - L:ALA353	5,44588	Hyd	Pi-Al
	L:9DB701 - L:VAL366	4,82584	Hyd	Pi-Al
136621040	L:LYS368:HZ1 - A:UNK1:O1	2,01535	HB	CHB
	L:THR413:HG1 - A:UNK1:O1	2,77087	HB	CHB
	L:ILE416:HN - A:UNK1:N3	2,03829	HB	CHB
	A:UNK1:H7 - L:GLU414:O	2,24315	HB	CHB
	A:UNK1:H10 - L:ASP478:OD2	2,10057	HB	CHB
	A:UNK1:H16 - L:LYS347:O	2,16743	HB	CHB
	L:GLY346:HA2 - A:UNK1:O2	2,65385	HB	Carbon HB
	L:LYS368:HE1 - A:UNK1:O1	2,98373	HB	Carbon HB
	A:UNK1:H5 - L:ILE416:O	2,40205	HB	Carbon HB
	A:UNK1:H6 - L:ILE416:O	2,65091	HB	Carbon HB
	A:UNK1:H11 - L:ASP478:OD2	2,27026	HB	Carbon HB
	L:GLN352:O - A:UNK1:F1	3,38585	Halogen	Halogen (F)
	L:GLU369:O - A:UNK1:F1	3,50815	Halogen	Halogen (F)
141609259	L:PHE350:HN - :UNL1:O	2,58498	HB	CHB
	:UNL1:H - L:ASP478:OD1	2,41757	HB	CHB
	L:GLN352:HA - :UNL1:O	2,70668	HB	Carbon HB
	L:ASP478:OD2 - :UNL1	3,49744	E	Pi-An
	L:ASP478:OD2 - :UNL1	4,33544	E	Pi-An
	L:LEU345:HD13 - :UNL1	2,90056	Hyd	Pi-Sg
	:UNL1 - L:ALA353	5,25876	Hyd	Pi-Al
	:UNL1 - L:VAL366	5,35882	Hyd	Pi-Al
	:UNL1 - L:LEU467	4,89242	Hyd	Pi-Al
	:UNL1 - L:LEU345	5,44768	Hyd	Pi-Al
	:UNL1 - L:ALA353	4,85227	Hyd	Pi-Al

Abbreviations: Electrostatic: E, Hydrogen Bond: HB, Conventional Hydrogen Bond: CHB, Hydrophobic: Hyd, Pi-Cation: Pi-Ca, Pi-Anion: Pi-An, Pi-Donor: Pi-Do, Pi-Alkyl: Pi-Al, Pi-Pi T-Shaped: Pi-Pi-T, Pi-Pi Stacked: Pi-Pi-St, Pi-Sulfur: Pi-S, Pi-Sigma: Pi-Sg, Fluorine: F

Table S8 *(cont.)*. Interaction data of the investigated ligands with $LIMK_1$ (PDB ID: 5NXC)

PubChem ID	Residue Information	Distance	Category	Type of Interactions
136141701	:UNL1:H - L:LYS347:O	1,73883	HB	CHB
	L:VAL366:HG21 - :UNL1	2,84352	Hyd	Pi-Sg
	L:LYS368 - :UNL1	4,91264	Hyd	Alkyl
	:UNL1 - L:ALA353	4,4352	Hyd	Pi-Al
	:UNL1 - L:ALA353	3,86021	Hyd	Pi-Al
	:UNL1 - L:ALA353	5,37598	Hyd	Pi-Al
	:UNL1 - L:LEU345	5,41968	Hyd	Pi-Al
	:UNL1 - L:LEU467	4,58746	Hyd	Pi-Al
136141741	L:LYS368:HZ1 - :UNL1:O	2,68738	HB	CHB
	L:ILE416:HN - :UNL1:N	2,6857	HB	CHB
	:UNL1:H - L:LEU345:O	2,63885	HB	CHB
	:UNL1:H - L:ASP478:OD2	2,50355	HB	CHB
	:UNL1:H - L:LYS347:O	2,91624	HB	Carbon HB
	L:ALA353 - :UNL1	5,49086	Hyd	Alkyl
	L:LYS368 - :UNL1	4,73239	Hyd	Alkyl
	:UNL1 - L:LEU345	4,77609	Hyd	Alkyl
	:UNL1 - L:LEU345	5,31975	Hyd	Pi-Al
	:UNL1 - L:ALA353	4,05518	Hyd	Pi-Al
	:UNL1 - L:LEU467	5,43611	Hyd	Pi-Al
	:UNL1 - L:LEU345	4,33933	Hyd	Pi-Al
	:UNL1 - L:LEU467	5,39388	Hyd	Pi-Al
	:UNL1 - L:LEU345	4,34836	Hyd	Pi-Al
	:UNL1 - L:ALA353	5,41286	Hyd	Pi-Al
	:UNL1 - L:VAL366	4,87121	Hyd	Pi-Al
	:UNL1 - L:LEU467	4,72023	Hyd	Pi-Al
136141618	L:LYS368:HZ1 - :UNL1:O	2,66211	HB	CHB
	L:ILE416:HN - :UNL1:N	2,4774	HB	CHB
	:UNL1:H - L:LEU345:O	2,48785	HB	CHB
	:UNL1:H - L:ASP478:OD2	2,46591	HB	CHB
	:UNL1:H - L:LYS347:O	3,01302	HB	Carbon HB
	L:ALA353 - :UNL1	5,37339	Hyd	Alkyl
	L:LYS368 - :UNL1	4,45183	Hyd	Alkyl
	:UNL1:CL - L:LEU345	4,31965	Hyd	Alkyl
	:UNL1 - L:LEU345	5,27673	Hyd	Pi-Al
	:UNL1 - L:ALA353	3,99498	Hyd	Pi-Al
	:UNL1 - L:LEU467	5,3906	Hyd	Pi-Al
	:UNL1 - L:LEU345	4,20013	Hyd	Pi-Al
	:UNL1 - L:LEU467	5,36694	Hyd	Pi-Al
	:UNL1 - L:LEU345	4,42175	Hyd	Pi-Al

Abbreviations: Electrostatic: E, Hydrogen Bond: HB, Conventional Hydrogen Bond: CHB, Hydrophobic: Hyd, Pi-Cation: Pi-Ca, Pi-Anion: Pi-An, Pi-Donor: Pi-Do, Pi-Alkyl: Pi-Al, Pi-Pi T-Shaped: Pi-Pi-T, Pi-Pi Stacked: Pi-Pi-St, Pi-Sulfur: Pi-S, Pi-Sigma: Pi-Sg, Fluorine: F

Table S8 ***(cont.)*****.** Interaction data of the investigated ligands with $LIMK_1$ (PDB ID: 5NXC)

PubChem ID	Residue Information	Distance	Category	Type of Interactions
135797427	L:LYS368:HZ1 - :UNL1:O	2,54816	HB	CHB
	:UNL1:H - L:LEU345:O	3,01932	HB	CHB
	:UNL1:H - L:ASP478:OD2	2,49268	HB	CHB
	L:LYS368:HE1 - :UNL1:O	3,02608	HB	Carbon HB
	L:HIS464:HD2 - :UNL1:O	2,43902	HB	Carbon HB
	:UNL1:H - L:ASP478:OD2	2,31924	HB	Carbon HB
	L:ALA353 - :UNL1	3,82327	Hyd	Alkyl
	L:LYS368 - :UNL1	5,01089	Hyd	Alkyl
	:UNL1 - L:LEU345	4,54227	Hyd	Pi-Al
	:UNL1 - L:LEU467	5,27341	Hyd	Pi-Al
	:UNL1 - L:LEU345	4,49705	Hyd	Pi-Al
	:UNL1 - L:VAL366	5,03421	Hyd	Pi-Al
	:UNL1 - L:LEU467	4,6069	Hyd	Pi-Al
	:UNL1 - L:LEU467	4,91433	Hyd	Pi-Al
	:UNL1 - L:LEU345	4,45606	Hyd	Pi-Al
136401937	L:LYS368:HZ1 - :UNL1:O	2,60181	HB	CHB
	L:ILE416:HN - :UNL1:N	2,55814	HB	CHB
	:UNL1:H - L:LEU345:O	2,49959	HB	CHB
	:UNL1:H - L:ASP478:OD2	2,40408	HB	CHB
	L:GLN352:HA - :UNL1:N	2,90722	HB	Carbon HB
	:UNL1:H - L:LYS347:O	2,91833	HB	Carbon HB
	L:ALA353 - :UNL1	5,4586	Hyd	Alkyl
	L:LYS368 - :UNL1	4,72462	Hyd	Alkyl
	:UNL1:CL - L:LEU345	4,38363	Hyd	Alkyl
	:UNL1 - L:LEU345	5,30617	Hyd	Pi-Al
	:UNL1 - L:ALA353	4,01817	Hyd	Pi-Al
	:UNL1 - L:LEU467	5,43545	Hyd	Pi-Al
	:UNL1 - L:LEU345	4,24368	Hyd	Pi-Al
	:UNL1 - L:LEU467	5,388	Hyd	Pi-Al
	:UNL1 - L:LEU345	4,4303	Hyd	Pi-Al
	:UNL1 - L:ALA353	5,43529	Hyd	Pi-Al
	:UNL1 - L:VAL366	4,80728	Hyd	Pi-Al

Abbreviations: Electrostatic: E, Hydrogen Bond: HB, Conventional Hydrogen Bond: CHB, Hydrophobic: Hyd, Pi-Cation: Pi-Ca, Pi-Anion: Pi-An, Pi-Donor: Pi-Do, Pi-Alkyl: Pi-Al, Pi-Pi T-Shaped: Pi-Pi-T, Pi-Pi Stacked: Pi-Pi-St, Pi-Sulfur: Pi-S, Pi-Sigma: Pi-Sg, Fluorine: F

Table S8 *(cont.)*. Interaction data of the investigated ligands with $LIMK_1$ (PDB ID: 5NXC)

PubChem ID	Residue Information	Distance	Category	Type of Interactions
136401905	:UNL1:H - L:LYS347:O	2,86265	HB	CHB
	:UNL1:H - L:ASP460:OD2	2,55774	HB	CHB
	L:GLY348:HA2 - :UNL1:O	2,19525	HB	Carbon HB
	L:HIS464:HD2 - :UNL1:O	2,81736	HB	Carbon HB
	:UNL1:H - L:ASP478:OD2	2,29939	HB	Carbon HB
	L:ASP478:OD2 - :UNL1	3,87796	E	Pi-An
	L:GLY346:HA2 - :UNL1	2,83916	Hyd	Pi-Sg
	L:VAL366:HG21 - :UNL1	2,91507	Hyd	Pi-Sg
	:UNL1 - L:ALA353	4,26458	Hyd	Pi-Al
	:UNL1 - L:ALA353	3,64485	Hyd	Pi-Al
	:UNL1 - L:ALA353	5,2345	Hyd	Pi-Al
	:UNL1 - L:LEU345	5,30297	Hyd	Pi-Al
	:UNL1 - L:ALA353	5,27997	Hyd	Pi-Al
	:UNL1 - L:LEU467	4,64049	Hyd	Pi-Al
136622946	L:LYS368:HZ1 - :UNL1:O	2,54822	HB	CHB
	:UNL1:H - L:LEU345:O	2,95924	HB	CHB
	:UNL1:H - L:ASP478:OD2	2,44802	HB	CHB
	:UNL1:H - L:LYS347:O	2,49576	HB	CHB
	L:LYS368:HE1 - :UNL1:O	3,08622	HB	Carbon HB
	L:HIS464:HD2 - :UNL1:O	2,55701	HB	Carbon HB
	:UNL1:H - L:LEU345:O	2,8069	HB	Carbon HB
	:UNL1:H - L:ASP478:OD2	2,25915	HB	Carbon HB
	L:ALA353 - :UNL1	3,9554	Hyd	Alkyl
	L:LYS368 - :UNL1	5,00239	Hyd	Alkyl
	:UNL1 - L:LEU345	4,49277	Hyd	Pi-Al
	:UNL1 - L:LEU467	5,29786	Hyd	Pi-Al
	:UNL1 - L:LEU345	4,46585	Hyd	Pi-Al
	:UNL1 - L:VAL366	4,99197	Hyd	Pi-Al
	:UNL1 - L:LEU467	4,64036	Hyd	Pi-Al
	:UNL1 - L:LEU467	4,94154	Hyd	Pi-Al
136622951	L:LYS368:HZ1 - :UNL1:O	2,52285	HB	CHB
	:UNL1:H - L:LEU345:O	3,0052	HB	CHB
	:UNL1:H - L:ASP478:OD2	2,4701	HB	CHB
	:UNL1:H - L:LYS347:O	2,3662	HB	CHB
	L:LYS368:HE1 - :UNL1:O	3,03392	HB	Carbon HB
	L:HIS464:HD2 - :UNL1:O	2,45068	HB	Carbon HB
	:UNL1:H - L:ASP478:OD2	2,36058	HB	Carbon HB
	L:ALA353 - :UNL1	3,88069	Hyd	Alkyl
	L:LYS368 - :UNL1	5,00788	Hyd	Alkyl
	:UNL1 - L:LEU345	4,56499	Hyd	Pi-Al

Abbreviations: Electrostatic: E, Hydrogen Bond: HB, Conventional Hydrogen Bond: CHB, Hydrophobic: Hyd, Pi-Cation: Pi-Ca, Pi-Anion: Pi-An, Pi-Donor: Pi-Do, Pi-Alkyl: Pi-Al, Pi-Pi T-Shaped: Pi-Pi-T, Pi-Pi Stacked: Pi-Pi-St, Pi-Sulfur: Pi-S, Pi-Sigma: Pi-Sg, Fluorine: F

Table S8 *(cont.)*. Interaction data of the investigated ligands with $LIMK_1$ (PDB ID: 5NXC)

PubChem ID	Residue Information	Distance	Category	Type of Interactions
135774110	L:LYS368:HZ1 - :UNL1:O	2,63345	HB	CHB
	L:ILE416:HN - :UNL1:N	2,51942	HB	CHB
	:UNL1:H - L:LEU345:O	2,58453	HB	CHB
	:UNL1:H - L:ASP478:OD2	2,48357	HB	CHB
	:UNL1:H - L:LYS347:O	2,70259	HB	CHB
	:UNL1:H - L:GLY346:O	2,7976	HB	CHB
	L:GLN352:HA - :UNL1:N	2,86804	HB	Carbon HB
	:UNL1:H - L:LYS347:O	2,93399	HB	Carbon HB
	L:ALA353 - :UNL1	5,45069	Hyd	Alkyl
	L:LYS368 - :UNL1	4,70606	Hyd	Alkyl
	:UNL1:C - L:LEU345	4,25925	Hyd	Alkyl
	:UNL1 - L:LEU345	4,2643	Hyd	Pi-Al
	:UNL1 - L:LEU467	5,34254	Hyd	Pi-Al
	:UNL1 - L:LEU345	4,42803	Hyd	Pi-Al
	:UNL1 - L:ALA353	5,45841	Hyd	Pi-Al
	:UNL1 - L:VAL366	4,79535	Hyd	Pi-Al
	:UNL1 - L:LEU467	4,67953	Hyd	Pi-Al
	:UNL1 - L:LEU345	5,27291	Hyd	Pi-Al
	:UNL1 - L:ALA353	4,01202	Hyd	Pi-Al
	:UNL1 - L:LEU467	5,43248	Hyd	Pi-Al
136931641	L:LYS368:HZ1 - :UNL1:O	2,50613	HB	CHB
	:UNL1:H - L:LEU345:O	2,96951	HB	CHB
	:UNL1:H - L:ASP478:OD2	2,50164	HB	CHB
	:UNL1:H - L:LYS347:O	2,39752	HB	CHB
	L:LYS368:HE1 - :UNL1:O	3,04189	HB	Carbon HB
	L:HIS464:HD2 - :UNL1:O	2,41854	HB	Carbon HB
	:UNL1:H - L:LEU345:O	2,733	HB	Carbon HB
	:UNL1:H - L:ASP478:OD2	2,33095	HB	Carbon HB
	L:ALA353 - :UNL1	3,87897	Hyd	Alkyl
	L:LYS368 - :UNL1	5,01569	Hyd	Alkyl
	:UNL1 - L:LEU467	4,95445	Hyd	Pi-Al
	:UNL1 - L:LEU345	4,56011	Hyd	Pi-Al
	:UNL1 - L:LEU467	5,28478	Hyd	Pi-Al
	:UNL1 - L:LEU345	4,54546	Hyd	Pi-Al
	:UNL1 - L:VAL366	5,02959	Hyd	Pi-Al
	:UNL1 - L:LEU467	4,59806	Hyd	Pi-Al
	:UNL1 - L:LEU345	4,4395	Hyd	Pi-Al

Abbreviations: Electrostatic: E, Hydrogen Bond: HB, Conventional Hydrogen Bond: CHB, Hydrophobic: Hyd, Pi-Cation: Pi-Ca, Pi-Anion: Pi-An, Pi-Donor: Pi-Do, Pi-Alkyl: Pi-Al, Pi-Pi T-Shaped: Pi-Pi-T, Pi-Pi Stacked: Pi-Pi-St, Pi-Sulfur: Pi-S, Pi-Sigma: Pi-Sg, Fluorine: F

Table S8 *(cont.)*. Interaction data of the investigated ligands with $LIMK_1$ (PDB ID: 5NXC)

PubChem ID	Residue Information	Distance	Category	Type of Interactions
135774106	L:LYS368:HZ1 - :UNL1:O	2,77234	HB	CHB
	L:ILE416:HN - :UNL1:N	2,7435	HB	CHB
	:UNL1:H - L:ASP478:OD2	2,18783	HB	CHB
	:UNL1:H - L:LEU345:O	2,71481	HB	CHB
	:UNL1:H - L:LYS347:O	2,18292	HB	CHB
	:UNL1:H - L:LYS347:O	2,73755	HB	CHB
	L:GLY346:HA2 - :UNL1:O	2,88871	HB	Carbon HB
	L:HIS464:HD2 - :UNL1:O	2,96407	HB	Carbon HB
	:UNL1:H - L:ASP478:OD2	2,18227	HB	Carbon HB
	L:LYS368 - :UNL1	4,51607	Hyd	Alkyl
	:UNL1:CL - L:LEU345	4,40572	Hyd	Alkyl
	:UNL1 - L:LEU345	5,39109	Hyd	Pi-Al
	:UNL1 - L:ALA353	4,35623	Hyd	Pi-Al
	:UNL1 - L:LEU467	5,251	Hyd	Pi-Al
	:UNL1 - L:LEU345	4,31486	Hyd	Pi-Al
	:UNL1 - L:LEU467	5,39715	Hyd	Pi-Al
	:UNL1 - L:LEU345	4,26908	Hyd	Pi-Al
	:UNL1 - L:ALA353	5,43502	Hyd	Pi-Al
	:UNL1 - L:VAL366	4,92767	Hyd	Pi-Al
	:UNL1 - L:LEU467	4,76018	Hyd	Pi-Al
136141675	:UNL1:H - L:ASP478:OD2	2,53117	HB	CHB
	:UNL1:H - L:LYS347:O	2,54062	HB	CHB
	L:GLY346:HA2 - :UNL1:O	2,54946	HB	Carbon HB
	:UNL1:H - L:GLU414:O	2,58046	HB	Carbon HB
	:UNL1:H - L:ASP478:OD2	2,30008	HB	Carbon HB
	L:ALA353 - :UNL1	4,66471	Hyd	Alkyl
	L:LYS368 - :UNL1	4,2115	Hyd	Alkyl
	:UNL1 - L:ALA353	4,27599	Hyd	Pi-Al
	:UNL1 - L:LEU467	4,95171	Hyd	Pi-Al
	:UNL1 - L:ALA353	4,98921	Hyd	Pi-Al
	:UNL1 - L:VAL366	4,19981	Hyd	Pi-Al
	:UNL1 - L:LEU467	4,72693	Hyd	Pi-Al
	:UNL1 - L:LEU345	4,10651	Hyd	Pi-Al
	:UNL1 - L:VAL366	5,33749	Hyd	Pi-Al
	:UNL1 - L:LEU467	4,80181	Hyd	Pi-Al

Abbreviations: Electrostatic: E, Hydrogen Bond: HB, Conventional Hydrogen Bond: CHB, Hydrophobic: Hyd, Pi-Cation: Pi-Ca, Pi-Anion: Pi-An, Pi-Donor: Pi-Do, Pi-Alkyl: Pi-Al, Pi-Pi T-Shaped: Pi-Pi-T, Pi-Pi Stacked: Pi-Pi-St, Pi-Sulfur: Pi-S, Pi-Sigma: Pi-Sg, Fluorine: F

Table S8 *(cont.)*. Interaction data of the investigated ligands with $LIMK_1$ (PDB ID: 5NXC)

PubChem ID	Residue Information	Distance	Category	Type of Interactions
136181657	L:LYS368:HZ1 - :UNL1:O	2,56038	HB	CHB
	:UNL1:H - L:ASP478:OD2	2,4783	HB	CHB
	:UNL1:H - L:LEU345:O	2,95244	HB	CHB
	:UNL1:H - L:LYS347:O	1,86801	HB	CHB
	L:LYS368:HE1 - :UNL1:O	3,02981	HB	Carbon HB
	L:HIS464:HD2 - :UNL1:O	2,42587	HB	Carbon HB
	:UNL1:H - L:ASP478:OD2	2,35479	HB	Carbon HB
	L:ALA353 - :UNL1	3,80335	Hyd	Alkyl
	L:LYS368 - :UNL1	4,958	Hyd	Alkyl
	:UNL1:CL - L:LEU345	4,10668	Hyd	Alkyl
	:UNL1 - L:LEU467	5,02189	Hyd	Pi-Al
	:UNL1 - L:LEU345	4,63794	Hyd	Pi-Al
	:UNL1 - L:LEU467	5,33683	Hyd	Pi-Al
	:UNL1 - L:LEU345	4,51337	Hyd	Pi-Al
	:UNL1 - L:VAL366	5,11118	Hyd	Pi-Al
	:UNL1 - L:LEU467	4,62405	Hyd	Pi-Al
135794603	L:LYS368:HZ1 - :UNL1:O	2,74169	HB	CHB
	L:ILE416:HN - :UNL1:N	2,5337	HB	CHB
	:UNL1:H - L:LEU345:O	2,69253	HB	CHB
	:UNL1:H - L:ASP478:OD2	2,22342	HB	CHB
	:UNL1:H - L:LYS347:O	2,28599	HB	CHB
	L:GLY346:HA2 - :UNL1:O	2,78809	HB	Carbon HB
	:UNL1:H - L:ASP478:OD2	2,3159	HB	Carbon HB
	L:ALA353 - :UNL1	5,27139	Hyd	Alkyl
	L:LYS368 - :UNL1	4,93543	Hyd	Alkyl
	:UNL1:C - L:LEU345	4,26968	Hyd	Alkyl
	:UNL1 - L:LEU345	4,26187	Hyd	Pi-Al
	:UNL1 - L:LEU467	5,32886	Hyd	Pi-Al
	:UNL1 - L:LEU345	4,34568	Hyd	Pi-Al
	:UNL1 - L:VAL366	4,87135	Hyd	Pi-Al
	:UNL1 - L:LEU467	4,70377	Hyd	Pi-Al
	:UNL1 - L:LEU345	5,26836	Hyd	Pi-Al
	:UNL1 - L:ALA353	4,26127	Hyd	Pi-Al
	:UNL1 - L:LEU467	5,2746	Hyd	Pi-Al

Abbreviations: Electrostatic: E, Hydrogen Bond: HB, Conventional Hydrogen Bond: CHB, Hydrophobic: Hyd, Pi-Cation: Pi-Ca, Pi-Anion: Pi-An, Pi-Donor: Pi-Do, Pi-Alkyl: Pi-Al, Pi-Pi T-Shaped: Pi-Pi-T, Pi-Pi Stacked: Pi-Pi-St, Pi-Sulfur: Pi-S, Pi-Sigma: Pi-Sg, Fluorine: F

Table S8 *(cont.)*. Interaction data of the investigated ligands with $LIMK_1$ (PDB ID: 5NXC)

PubChem ID	Residue Information	Distance	Category	Type of Interactions
141608268	L:LYS368:HZ1 - :UNL1:O	2,62735	HB	CHB
	L:ILE416:HN - :UNL1:N	2,55056	HB	CHB
	:UNL1:H - L:LEU345:O	2,58259	HB	CHB
	:UNL1:H - L:ASP478:OD2	2,80914	HB	CHB
	:UNL1:H - L:LYS347:O	2,48446	HB	Carbon HB
	L:GLY419:HA1 - :UNL1	2,68023	Hyd	Pi-Sg
	:UNL1:C - L:LYS368	3,79594	Hyd	Alkyl
	:UNL1:C - L:LEU370	5,1682	Hyd	Alkyl
	L:PHE411 - :UNL1:C	4,95073	Hyd	Pi-Al
	:UNL1 - L:LEU345	5,29773	Hyd	Pi-Al
	:UNL1 - L:ALA353	4,01089	Hyd	Pi-Al
	:UNL1 - L:LEU467	5,43371	Hyd	Pi-Al
	:UNL1 - L:LEU345	4,44562	Hyd	Pi-Al
	:UNL1 - L:ALA353	5,46188	Hyd	Pi-Al
	:UNL1 - L:VAL366	4,83095	Hyd	Pi-Al
	:UNL1 - L:LEU467	4,65306	Hyd	Pi-Al
	:UNL1 - L:LEU345	4,3054	Hyd	Pi-Al
	:UNL1 - L:LEU467	5,3428	Hyd	Pi-Al
146582701	:UNL1:H - L:ILE416:O	2,14104	HB	CHB
	:UNL1:H - L:ASP478:OD1	3,00613	HB	CHB
	L:LYS417:HA - :UNL1:O	2,61687	HB	Carbon HB
	:UNL1:H - L:ASP478:OD2	3,04246	HB	Carbon HB
	:UNL1 - L:LEU345	4,10669	Hyd	Pi-Al
	:UNL1 - L:LEU467	4,77109	Hyd	Pi-Al
	:UNL1 - L:LEU345	5,17586	Hyd	Pi-Al
	:UNL1 - L:LEU467	4,40846	Hyd	Pi-Al
107728365	L:LYS368:HZ1 - :UNL1:S	2,85806	HB	CHB
	:UNL1:H - L:ASP478:OD2	2,43979	HB	CHB
	L:GLY348:HA2 - :UNL1:O	2,76013	HB	Carbon HB
	L:ASP478:OD2 - :UNL1	4,05047	E	Pi-An
	:UNL1:S - :UNL1	5,49801	Other	Pi-S
	L:GLN352:C,O;ALA353:N - :UNL1	4,26403	Hyd	Amide-Pi Stacked
	L:LEU345 - :UNL1	4,78717	Hyd	Alkyl
	L:ALA353 - :UNL1	5,12962	Hyd	Alkyl
	L:LEU467 - :UNL1	4,83879	Hyd	Alkyl
	:UNL1 - L:ALA353	3,82158	Hyd	Pi-Al
	:UNL1 - L:LYS368	5,16532	Hyd	Pi-Al

Abbreviations: Electrostatic: E, Hydrogen Bond: HB, Conventional Hydrogen Bond: CHB, Hydrophobic: Hyd, Pi-Cation: Pi-Ca, Pi-Anion: Pi-An, Pi-Donor: Pi-Do, Pi-Alkyl: Pi-Al, Pi-Pi T-Shaped: Pi-Pi-T, Pi-Pi Stacked: Pi-Pi-St, Pi-Sulfur: Pi-S, Pi-Sigma: Pi-Sg, Fluorine: F

Table S8 *(cont.)*. Interaction data of the investigated ligands with $LIMK_1$ (PDB ID: 5NXC)

PubChem ID	Residue Information	Distance	Category	Type of Interactions
102778224	:UNL1:H - L:ASP478:OD2	1,86231	HB	CHB
	:UNL1 - L:LEU345	4,6344	Hyd	Pi-Al
	:UNL1 - L:VAL366	4,43966	Hyd	Pi-Al
	:UNL1 - L:LEU467	4,7059	Hyd	Pi-Al
	:UNL1 - L:LEU345	3,94921	Hyd	Pi-Al
107728896	:UNL1:H - L:ILE416:O	2,26813	HB	CHB
	:UNL1:H - L:HIS464:O	2,3022	HB	CHB
	:UNL1:H - L:ASP478:OD2	1,91687	HB	CHB
	L:ALA353 - :UNL1	4,61093	Hyd	Alkyl
	L:LEU467 - :UNL1	5,36967	Hyd	Alkyl
	L:ALA477 - :UNL1	5,04615	Hyd	Alkyl
	:UNL1 - L:LEU345	4,35591	Hyd	Pi-Al
	:UNL1 - L:LEU467	4,54141	Hyd	Pi-Al
107728362	:UNL1:H - L:ASP478:OD2	2,66179	HB	CHB
	:UNL1:H - L:ILE416:O	2,27435	HB	CHB
	L:ASN465:HA - :UNL1:O	3,05904	HB	Carbon HB
	L:LEU345 - :UNL1	4,69825	Hyd	Alkyl
	L:LEU467 - :UNL1	4,5441	Hyd	Alkyl
	:UNL1 - L:ALA353	4,40155	Hyd	Pi-Al
	:UNL1 - L:LEU467	5,05096	Hyd	Pi-Al
43712981	:UNL1:H - L:HIS464:O	2,59878	HB	CHB
	:UNL1:H - L:HIS464:O	2,66492	HB	CHB
	:UNL1 - L:LEU345	4,6844	Hyd	Pi-Al
	:UNL1 - L:VAL366	4,51764	Hyd	Pi-Al
	:UNL1 - L:LEU467	4,62641	Hyd	Pi-Al
	:UNL1 - L:LEU345	3,97864	Hyd	Pi-Al
107728922	:UNL1:H - L:ASP478:OD2	2,34907	HB	CHB
	:UNL1:H - L:ASP478:OD2	2,00969	HB	CHB
	:UNL1:H - :UNL1:O	2,85928	HB	CHB
	:UNL1:H - L:LYS347:O	2,24211	HB	CHB
	L:ALA353 - :UNL1	4,03964	Hyd	Alkyl
	L:LYS368 - :UNL1	4,23106	Hyd	Alkyl
	:UNL1 - L:LEU345	5,21912	Hyd	Pi-Al
	:UNL1 - L:ALA353	4,67145	Hyd	Pi-Al
	:UNL1 - L:VAL366	4,61499	Hyd	Pi-Al
	:UNL1 - L:LEU467	4,72846	Hyd	Pi-Al

Abbreviations: Electrostatic: E, Hydrogen Bond: HB, Conventional Hydrogen Bond: CHB, Hydrophobic: Hyd, Pi-Cation: Pi-Ca, Pi-Anion: Pi-An, Pi-Donor: Pi-Do, Pi-Alkyl: Pi-Al, Pi-Pi T-Shaped: Pi-Pi-T, Pi-Pi Stacked: Pi-Pi-St, Pi-Sulfur: Pi-S, Pi-Sigma: Pi-Sg, Fluorine: F

Table S8 *(cont.)*. Interaction data of the investigated ligands with $LIMK_1$ (PDB ID: 5NXC)

PubChem ID	Residue Information	Distance	Category	Type of Interactions
60854249	:UNL1:H - L:HIS464:O	2,35982	HB	CHB
	:UNL1:H - L:ASP478:OD2	3,08406	HB	Carbon HB
	L:HIS464 - :UNL1:C	4,79464	Hyd	Pi-Al
	:UNL1 - L:LEU345	4,67337	Hyd	Pi-Al
	:UNL1 - L:VAL366	4,5135	Hyd	Pi-Al
	:UNL1 - L:LEU467	4,63585	Hyd	Pi-Al
	:UNL1 - L:LEU345	3,98384	Hyd	Pi-Al
65813383	:UNL1:H - L:HIS464:O	2,384	HB	CHB
	:UNL1:H - L:ASP478:OD2	2,99863	HB	Carbon HB
	:UNL1 - L:LEU345	4,71875	Hyd	Pi-Al
	:UNL1 - L:VAL366	4,47766	Hyd	Pi-Al
	:UNL1 - L:LEU467	4,62968	Hyd	Pi-Al
	:UNL1 - L:LEU345	3,96406	Hyd	Pi-Al
79013386	L:LYS368:HZ1 - :UNL1:O	3,05694	HB	CHB
	:UNL1:H - L:HIS464:O	2,58673	HB	CHB
	:UNL1:H - L:ASP478:OD2	2,60384	HB	CHB
	:UNL1:H - L:ASP478:OD2	2,51489	HB	Carbon HB
	L:ALA353 - :UNL1:C	4,42092	Hyd	Alkyl
	:UNL1 - L:LEU345	4,46147	Hyd	Pi-Al
	:UNL1 - L:VAL366	4,6342	Hyd	Pi-Al
	:UNL1 - L:LEU467	4,71706	Hyd	Pi-Al
	:UNL1 - L:LEU345	4,20307	Hyd	Pi-Al
93269140	:UNL1:H - L:HIS464:O	2,59878	HB	CHB
	:UNL1:H - L:HIS464:O	2,66492	HB	CHB
	:UNL1 - L:LEU345	4,6844	Hyd	Pi-Al
	:UNL1 - L:VAL366	4,51764	Hyd	Pi-Al
	:UNL1 - L:LEU467	4,62641	Hyd	Pi-Al
	:UNL1 - L:LEU345	3,97864	Hyd	Pi-Al
81071023	:UNL1:H - L:ASP478:OD2	2,47412	HB	CHB
	:UNL1:H - L:HIS464:O	2,42412	HB	CHB
	:UNL1:H - L:ASP478:OD2	2,90665	HB	Carbon HB
	:UNL1:H - L:LYS347:O	2,8189	HB	Carbon HB
	L:ALA353 - :UNL1	5,1892	Hyd	Alkyl
	:UNL1 - L:LEU345	4,52917	Hyd	Pi-Al
	:UNL1 - L:VAL366	4,58174	Hyd	Pi-Al
	:UNL1 - L:LEU467	4,69396	Hyd	Pi-Al
	:UNL1 - L:LEU345	4,0267	Hyd	Pi-Al

Abbreviations: Electrostatic: E, Hydrogen Bond: HB, Conventional Hydrogen Bond: CHB, Hydrophobic: Hyd, Pi-Cation: Pi-Ca, Pi-Anion: Pi-An, Pi-Donor: Pi-Do, Pi-Alkyl: Pi-Al, Pi-Pi T-Shaped: Pi-Pi-T, Pi-Pi Stacked: Pi-Pi-St, Pi-Sulfur: Pi-S, Pi-Sigma: Pi-Sg, Fluorine: F

Table S8 *(cont.)*. Interaction data of the investigated ligands with $LIMK_1$ (PDB ID: 5NXC)

PubChem ID	Residue Information	Distance	Category	Type of Interactions
93041470	L:ILE416:HN - :UNL1:O	2,24055	HB	CHB
	:UNL1:H - L:ASP478:OD2	2,55547	HB	CHB
	L:LYS417:HA - :UNL1:O	2,85853	HB	Carbon HB
	:UNL1:H - L:ILE416:O	2,98214	HB	Carbon HB
	:UNL1:C - L:LEU345	4,08916	Hyd	Alkyl
	:UNL1 - L:LEU345	5,1877	Hyd	Pi-Al
	:UNL1 - L:ALA353	4,34213	Hyd	Pi-Al
	:UNL1 - L:VAL366	4,92689	Hyd	Pi-Al
	:UNL1 - L:LEU467	4,90941	Hyd	Pi-Al
	:UNL1 - L:ALA353	4,10648	Hyd	Pi-Al
143275306	:UNL1:H - :UNL1:O	2,53268	HB	CHB
	:UNL1:H - L:HIS464:O	2,31892	HB	CHB
	L:GLY346:HA2 - :UNL1:O	2,75099	HB	Carbon HB
	:UNL1:C - L:LEU345	3,87348	Hyd	Alkyl
	:UNL1:C - L:ILE416	5,14019	Hyd	Alkyl
	:UNL1:C - L:LEU467	3,71456	Hyd	Alkyl
Abbreviations: Electrostatic: E, Hydrogen Bond: HB, Conventional Hydrogen Bond: CHB, Hydrophobic: Hyd, Pi-Cation: Pi-Ca, Pi-Anion: Pi-An, Pi-Donor: Pi-Do, Pi-Alkyl: Pi-Al, Pi-Pi T-Shaped: Pi-Pi-T, Pi-Pi Stacked: Pi-Pi-St, Pi-Sulfur: Pi-S, Pi-Sigma: Pi-Sg, Fluorine: F				