SUPPORTING INFORMATION

AN *IN SILICO* PHARMACOKINETIC INVESTIGATION OF ORGANIC LUMINOGENS: UNDERSTANDING THE NIR AIEGENS AND THEIR INTERACTIONS WITH SERUM ALBUMINS

Harun Nalçakan[1], Gülbin Kurtay[2,*], Dilara Tuğçe Özdil[1], Züleyha Yılmaz[1]

[1]Ankara University, Faculty of Sciences, Department of Chemistry, 06100, Ankara, Turkey

[2]Hacettepe University, Faculty of Sciences, Department of Chemistry, 06800, Ankara, Turkey

****Corresponding author: kurtay@science.ankara.edu.tr***

Content

Figure S1. Molecular structures of the studied dye molecules

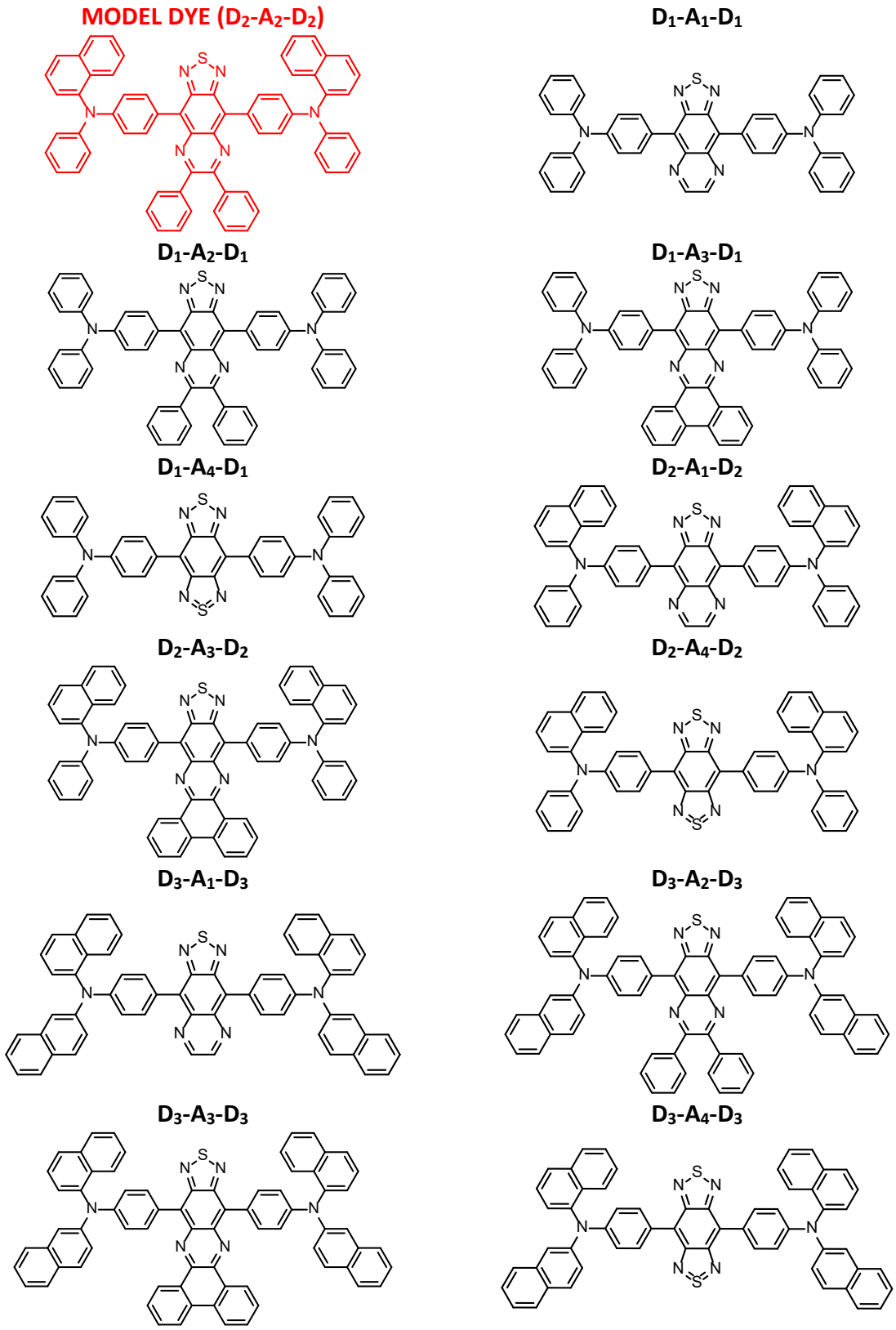
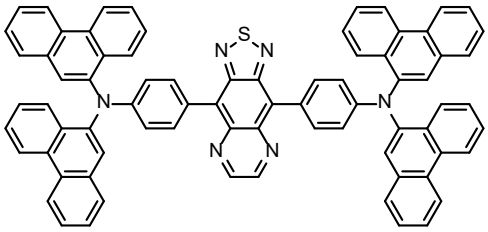


Figure S1. (*cont.*) Molecular structures of the studied dye molecules

D_4-A_1-D_4



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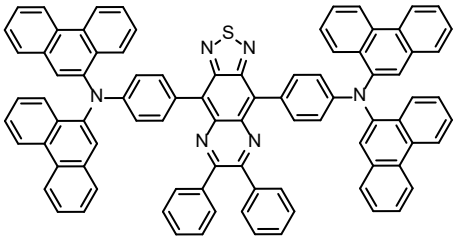

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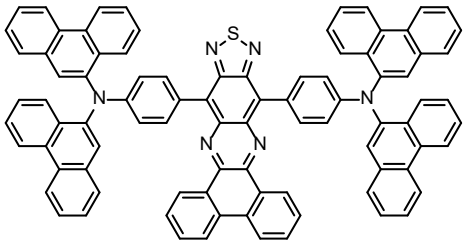

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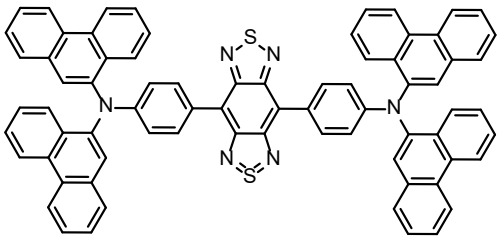

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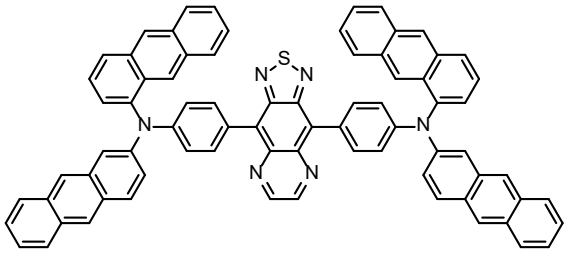

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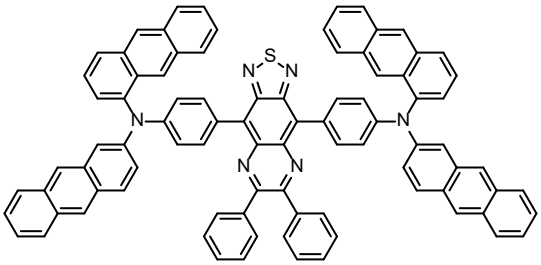

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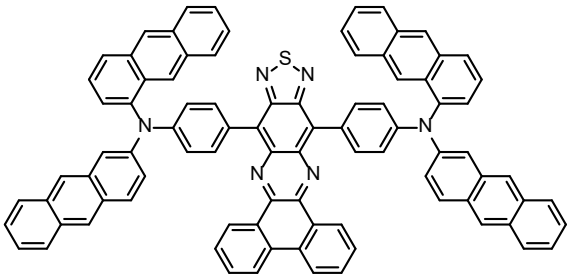

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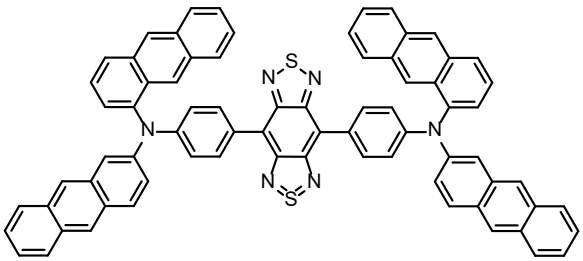


Figure S2. Geometry optimized structures of the studied dye molecules [B3LYP/6-31g(d,p)]

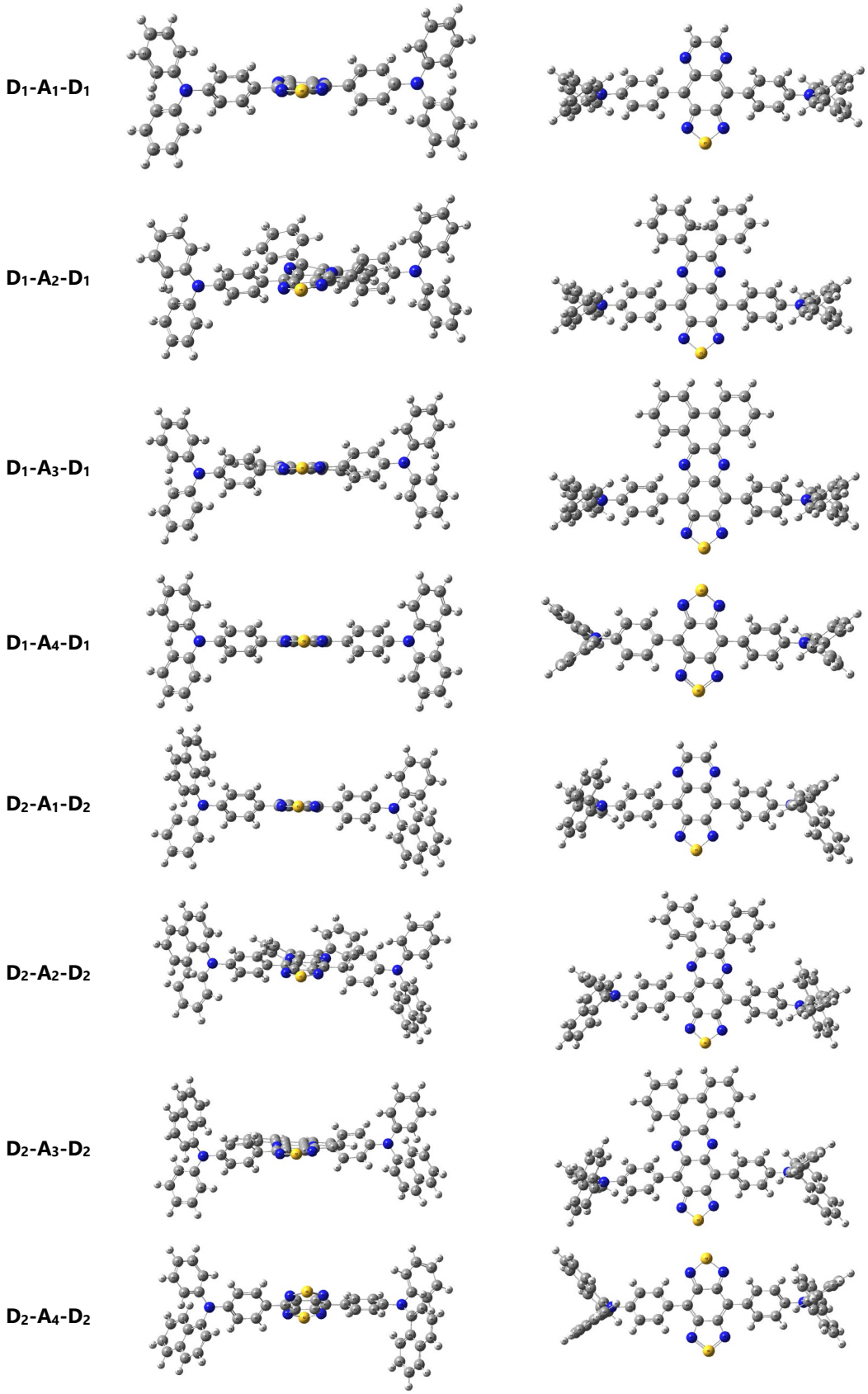


Figure S2. (*cont.*) Geometry optimized structures of the studied dye molecules [B3LYP/6-31g(d,p)]

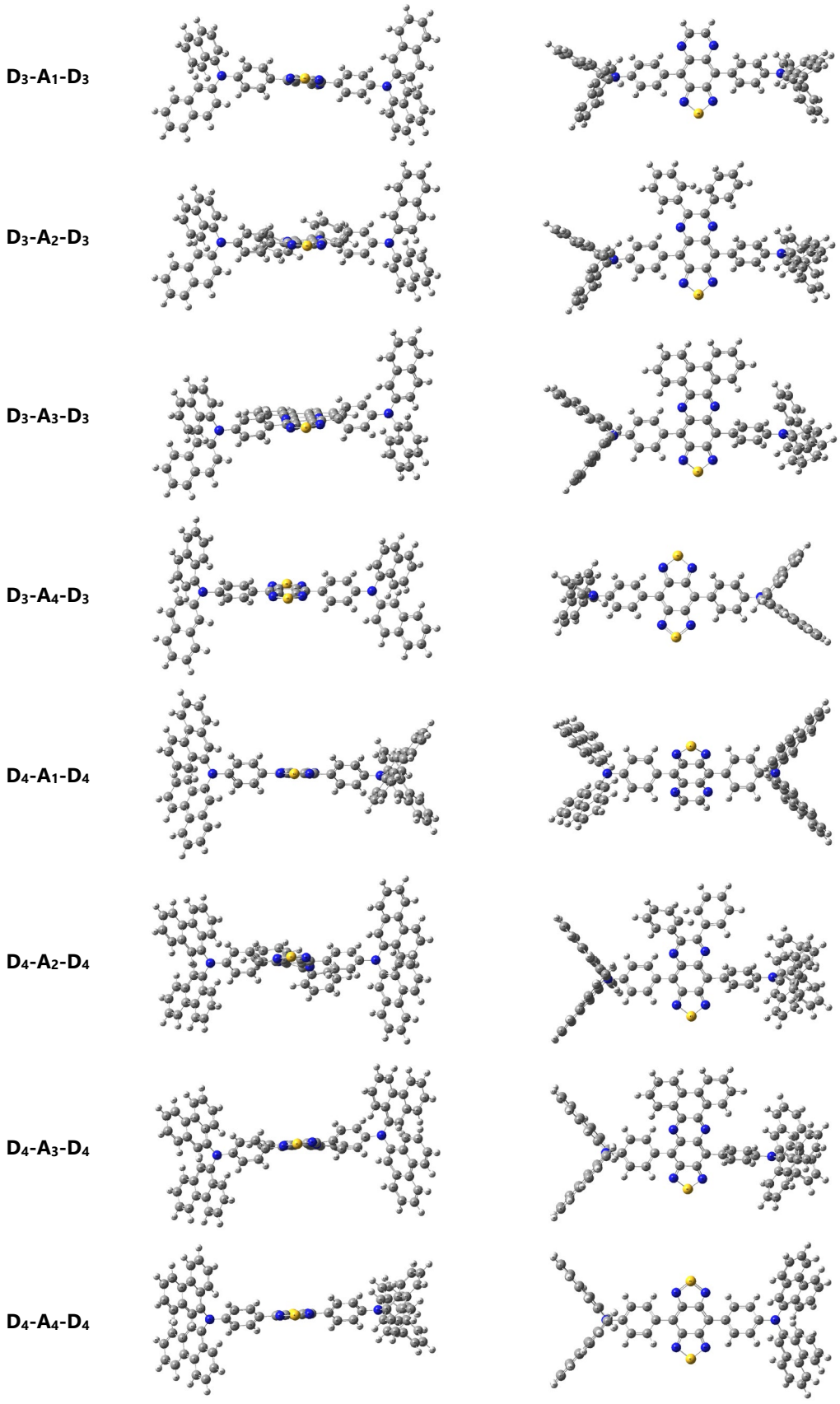


Figure S2. (*cont.*) Geometry optimized structures of the studied dye molecules [B3LYP/6-31g(d,p)]

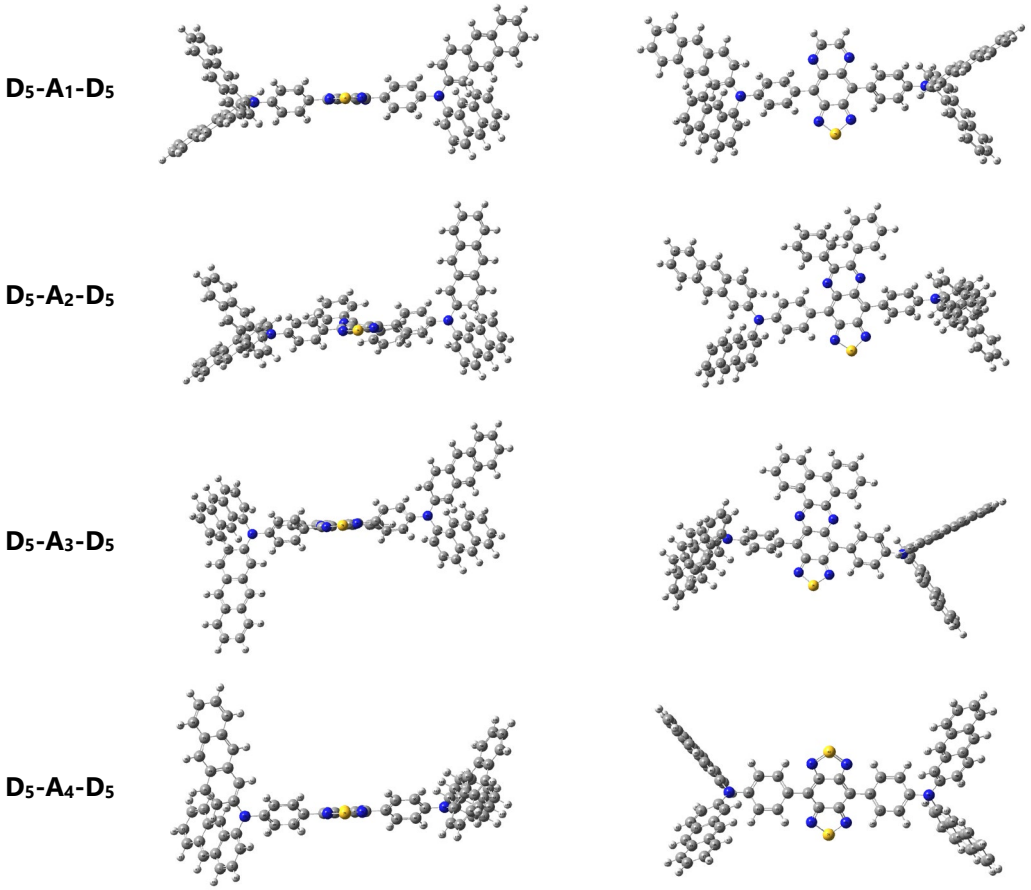


Figure S3. Frontier orbitals' contour plots (threshold of contours: ±0.02 au) [B3LYP/6-31g(d,p)]

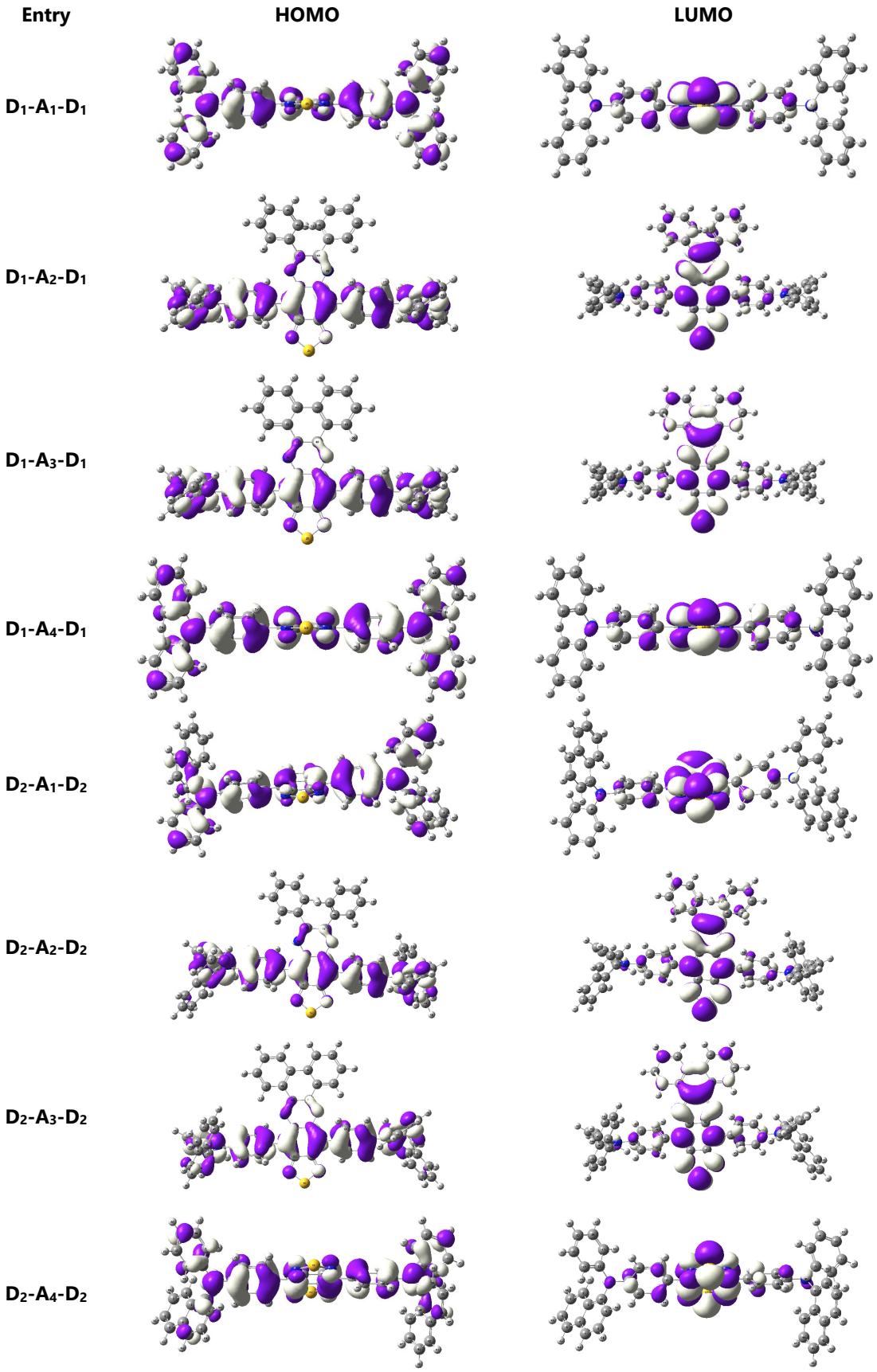


Figure S3. (*cont.*) Frontier orbitals' contour plots (threshold of contours: ±0.02 au) [B3LYP/6-31g(d,p)]

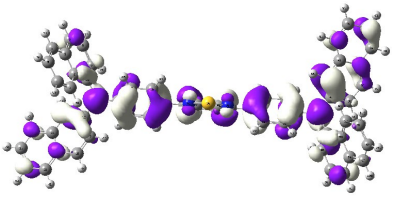
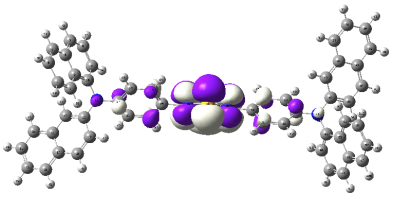
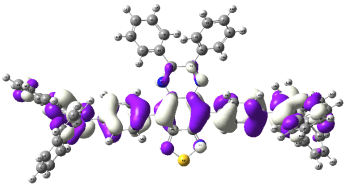
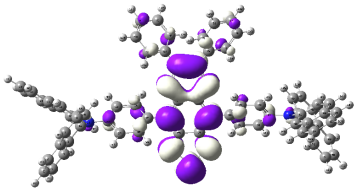
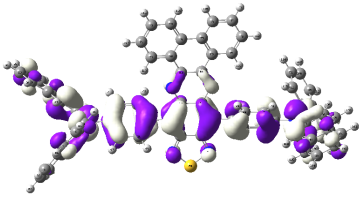
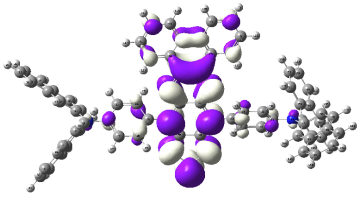
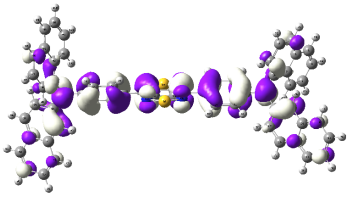
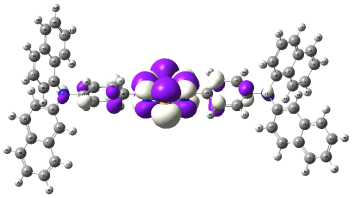
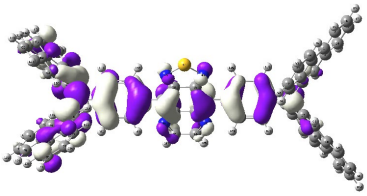
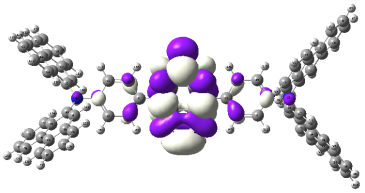
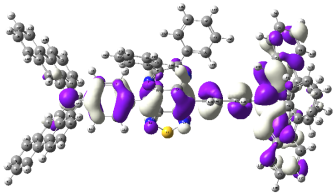
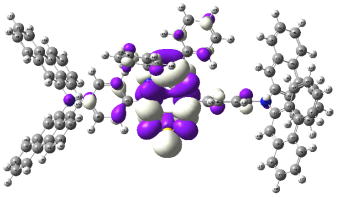
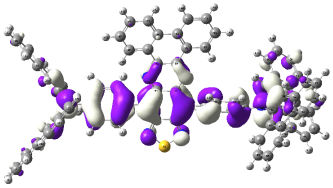
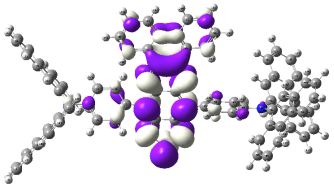
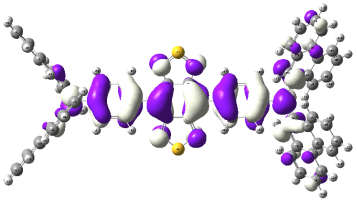
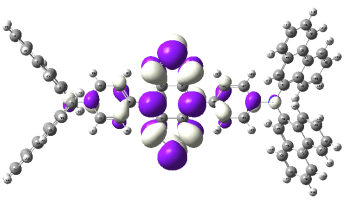
Entry	HOMO	LUMO
D_3-A_1-D_3		
D_3-A_2-D_3		
D_3-A_3-D_3		
D_3-A_4-D_3		
D_4-A_1-D_4		
D_4-A_2-D_4		
D_4-A_3-D_4		
D_4-A_4-D_4		

Figure S3. (*cont.*) Frontier orbitals' contour plots (threshold of contours: ±0.02 au) [B3LYP/6-31g(d,p)]

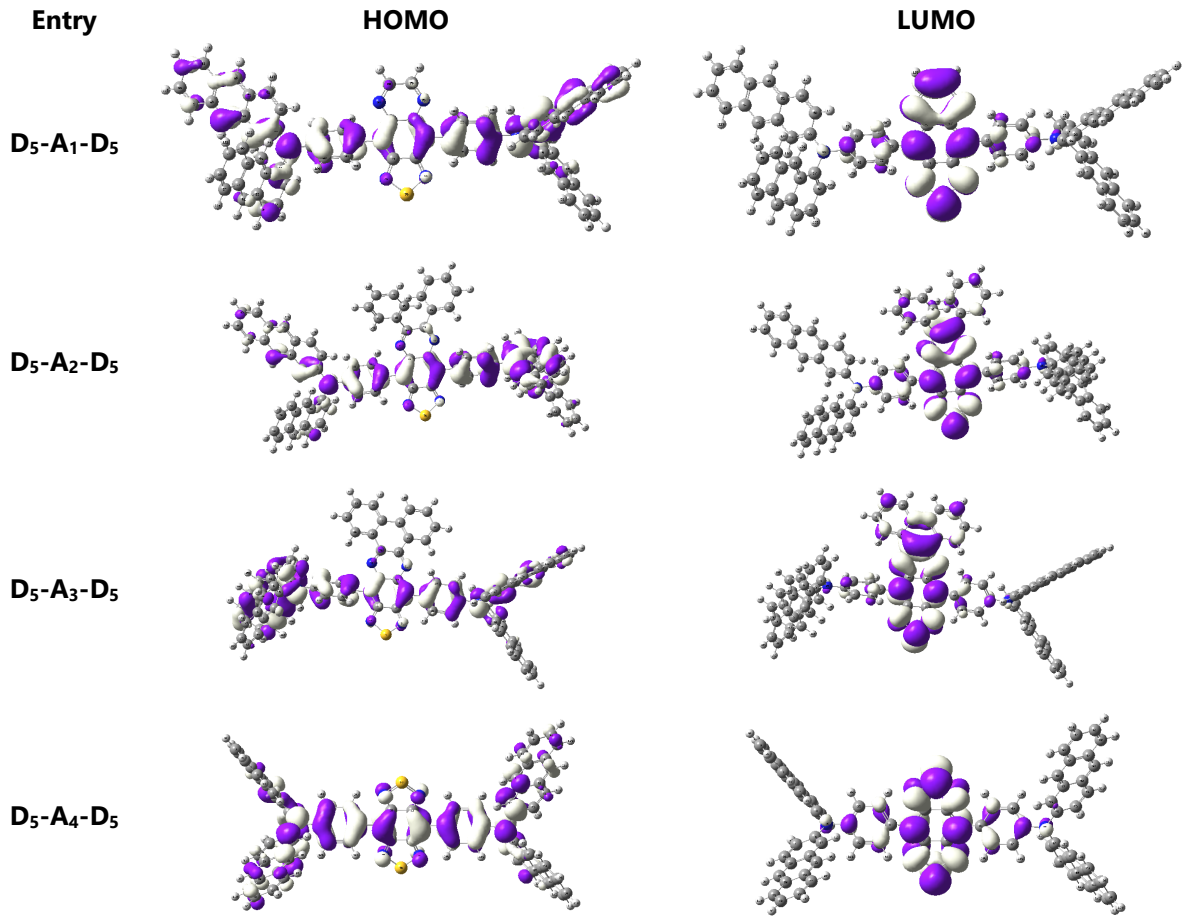


Figure S4. Bioavailability radar plots of the studied ligands

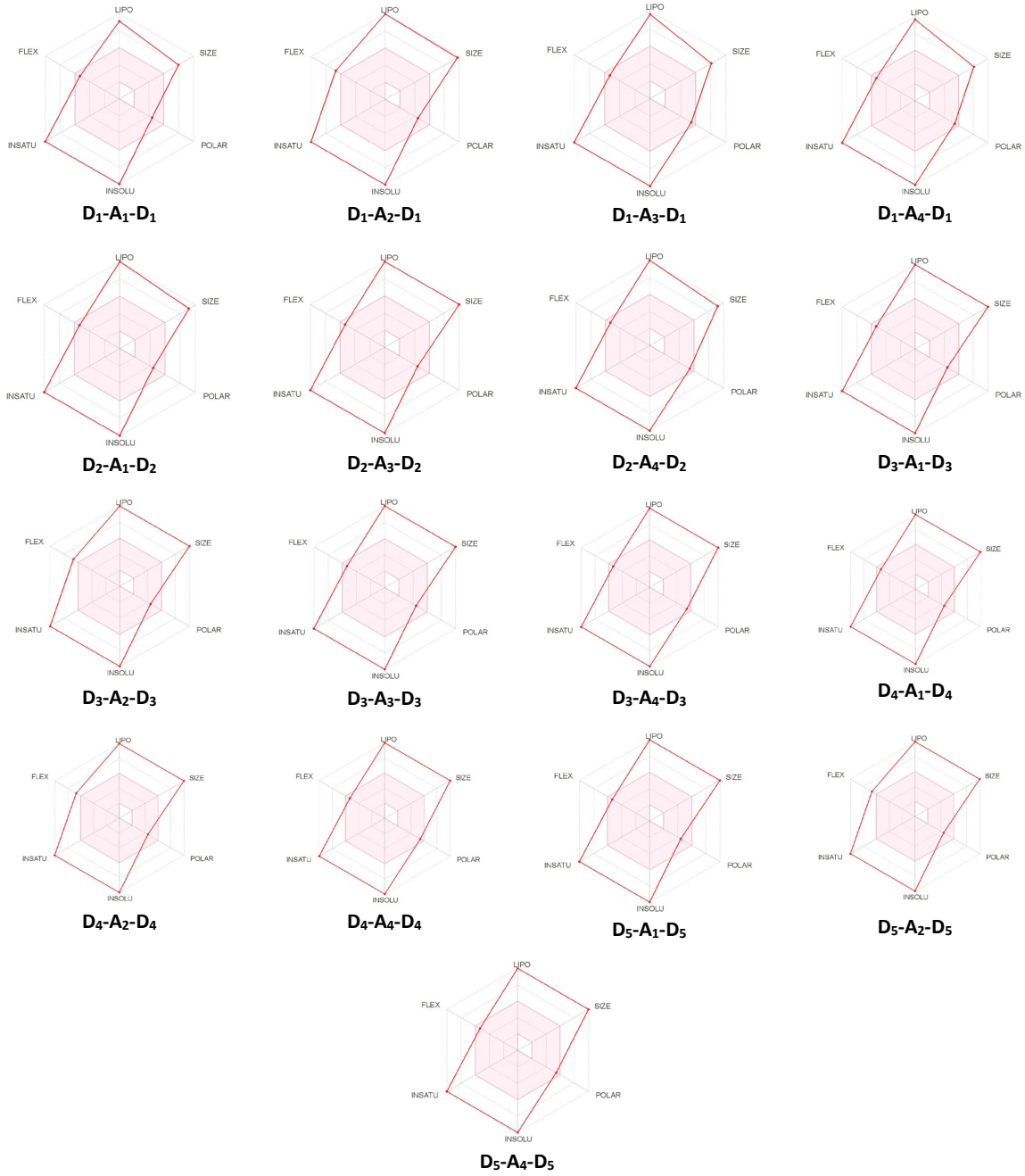


Table S1. Docking scores and interaction data of the studied ligands with BSA (PDB ID: 4F5S)

Ligands	Docking Scores	Distance	Category	Type of Interactions	Residue Information
MODEL DYE D_2-A_2-D_2	-10.7	4.09960	E	Pi-Ca	LYS136
		4.42061	E	Pi-Ca	LYS136
		3.37246	E	Pi-Ca	LYS136
		3.85040	HB; E	Pi-Ca; Pi-Do HB	ARG143
		3.02554	E	Pi-An	GLU125
		3.52817	E	Pi-An	GLU125
		4.10177	E	Pi-An	GLU140
		5.77772	Hyd	Pi-Pi T	UNK - UNK1
		5.35012	Hyd	Pi-Al	PRO113
		4.76700	Hyd	Pi-Al	PRO35
		4.41328	Hyd	Pi-Al	PRO35
		5.48517	Hyd	Pi-Al	LYS136
		3.82610	Hyd	Pi-Al	LYS136
		3.78178	Hyd	Pi-Al	LYS136
		4.64077	Hyd	Pi-Al	PRO35
D_1-A_1-D_1	-8.5	2.24665	HB	Carbon HB	LYS159
		3.43576	HB	Carbon HB	TYR155
		4.09694	E	Pi-Ca	LYS159
		3.61719	E	Pi-An	GLU166
		3.20849	E	Pi-An	GLU284
		3.45135	E	Pi-An	GLU284
		5.43703	Hyd	Pi-Al	LYS159
		5.41983	Hyd	Pi-Al	LEU283
		5.25644	Hyd	Pi-Al	PRO281
		4.5926	Hyd	Pi-Al	LYS159
		4.15577	Hyd	Pi-Al	LYS159
		4.986	Hyd	Pi-Al	LEU282
D_1-A_2-D_1	-10.3	3.08564	HB	CHB	GLU130
		4.60030	E	Pi-Ca	LYS131
		3.64052	E	Pi-Ca	LYS131
		4.54981	E	Pi-An	GLU17
		4.00051	E	Pi-An	GLU130
		3.37551	E	Pi-An	GLU284
		3.33344	E	Pi-An	GLU284
		5.37486	Other	Pi-S	PHE126
		5.78941	Hyd	Pi-Pi T	-
		4.77899	Hyd	Pi-Al	LYS131
		5.15997	Hyd	Pi-Al	LYS131
D_1-A_3-D_1	-9.6	4.83885	E	Pi-Ca	LYS136
		3.15007	E	Pi-An	GLU125
		4.89160	E	Pi-An	GLU140
		4.86105	E	Pi-An	GLU140
		2.48258	Hyd	Pi-Sg	LEU122
		5.41009	Hyd	Pi-Pi-St	PHE133
		5.38065	Hyd	Pi-Al	PRO113
		4.85549	Hyd	Pi-Al	PRO113
		4.19560	Hyd	Pi-Al	PRO113
		5.32119	Hyd	Pi-Al	LYS136
		3.72777	Hyd	Pi-Al	LYS136
		5.39605	Hyd	Pi-Al	PRO35
		4.83885	E	Pi-Ca	LYS136
		3.15007	E	Pi-An	GLU125
		4.89160	E	Pi-An	GLU140
		4.86105	E	Pi-An	GLU140

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

Table S1. (*cont.*) Docking scores and interaction data of the studied ligands with BSA (PDB ID: 4F5S)

Ligands	Docking Scores	Distance	Category	Type of Interactions	Residue Information
D_1-A_4-D_1	-8.5	2.53706	HB	HB	ARG144
		3.22289	HB	HB	GLU140
		4.47232	E	E	ARG143
		3.75016	HB; E	HB; E	ARG143
		3.48990	E	E	GLU140
		4.13250	E	E	GLU140
		3.48173	E	E	GLU140
		5.03873	Hyd	Hyd	PRO113
		5.45320	Hyd	Hyd	LEU115
		5.10274	Hyd	Hyd	LYS136
		5.35322	Hyd	Hyd	PRO35
		4.35676	Hyd	Hyd	PRO35
		4.59077	Hyd	Hyd	LEU122
		3.96488	Hyd	Hyd	LYS136
D_2-A_1-D_2	-11.3	3.38237	HB	CHB	GLU140
		3.72692	HB; E	Pi-Ca; Pi-Do; HB	ARG143
		3.57000	E	Pi-An	GLU140
		4.95931	E	Pi-An	GLU140
		3.74844	E	Pi-An	GLU140
		4.98078	Hyd	Pi-Al	PRO113
		5.41840	Hyd	Pi-Al	LEU115
		5.44346	Hyd	Pi-Al	LYS136
		4.91524	Hyd	Pi-Al	PRO35
		4.10509	Hyd	Pi-Al	PRO35
		5.41986	Hyd	Pi-Al	CYS34
		4.31307	Hyd	Pi-Al	PRO35
		3.98334	Hyd	Pi-Al	LYS136
		5.02908	Hyd	Pi-Al	LYS136
		5.49290	Hyd	Pi-Al	LEU115
D_2-A_3-D_2	-11.8	4.00532	HB; E	Pi-Ca; Pi-Do; HB	ARG217
		3.89822	E	Pi-Ca	ARG217
		3.98391	E	Pi-Ca	ARG217
		2.59383	HB; E	Pi-Ca; Pi-Do; HB	LYS294
		2.91618	HB; E	Pi-Ca; Pi-Do; HB	LYS294
		3.89130	E	Pi-An	ASP450
		5.13664	Hyd	Am-Pi-St	ALA290, GLU291
		4.96803	Hyd	Am-Pi-St	ALA290, GLU291
		4.88308	Hyd	Pi-Al	ALA290
		3.74132	Hyd	Pi-Al	ALA290
		5.37551	Hyd	Pi-Al	LYS187
D_2-A_4-D_2	-10.5	2.41573	HB	CHB	ARG144
		4.72488	E	Pi-Ca	ARG143
		3.96655	HB; E	Pi-Ca; Pi-Do; HB	ARG143
		3.67507	E	Pi-An	GLU140
		4.27159	E	Pi-An	GLU140
		3.57602	E	Pi-An	GLU140
		2.54242	Hyd	Pi-Sg	LEU122
		5.20487	Hyd	Pi-Pi-St	PHE133
		4.73603	Hyd	Pi-Pi-St	PHE133
		5.03694	Hyd	Pi-Al	PRO113
		5.49081	Hyd	Pi-Al	LEU115
		5.12436	Hyd	Pi-Al	LYS136
		4.14532	Hyd	Pi-Al	PRO35
		3.78349	Hyd	Pi-Al	LYS136
		4.76566	Hyd	Pi-Al	LYS136

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

Table S1. (*cont.*) Docking scores and interaction data of the studied ligands with BSA (PDB ID: 4F5S)

Ligands	Docking Scores	Distance	Category	Type of Interactions	Residue Information
D_3-A_1-D_3	-12.7	4.67331	E	Pi-Ca	ARG143
		3.93726	HB; E	Pi-Ca; Pi-Do; HB	ARG143
		4.89095	E	Pi-An	GLU125
		3.70142	E	Pi-An	GLU140
		4.47421	E	Pi-An	GLU140
		4.59194	E	Pi-An	GLU140
		4.03012	E	Pi-An	GLU140
		4.81839	Hyd	Pi-Al	PRO113
		5.07782	Hyd	Pi-Al	PRO35
		4.07857	Hyd	Pi-Al	PRO35
		5.31487	Hyd	Pi-Al	CYS34
		4.50306	Hyd	Pi-Al	PRO35
		3.94541	Hyd	Pi-Al	LYS136
		5.30614	Hyd	Pi-Al	LEU115
		4.71569	Hyd	Pi-Al	LYS136
		5.22555	Hyd	Pi-Al	LEU122
D_3-A_2-D_3	-11.9	3.43523	E	Pi-Ca	LYS136
		3.58600	HB; E	Pi-Ca; Pi-Do; HB	ARG143
		4.53191	E	Pi-An	GLU125
		3.46995	E	Pi-An	GLU125
		4.83408	E	Pi-An	GLU140
		3.92036	E	Pi-An	GLU140
		4.74834	Hyd	Pi-Al	PRO113
		5.20080	Hyd	Pi-Al	LEU115
		5.46252	Hyd	Pi-Al	LEU122
		5.06091	Hyd	Pi-Al	LYS136
		5.42119	Hyd	Pi-Al	LEU122
		4.59342	Hyd	Pi-Al	LYS136
		5.16133	Hyd	Pi-Al	PRO35
		4.25133	Hyd	Pi-Al	PRO35
		5.21973	Hyd	Pi-Al	CYS34
		4.59015	Hyd	Pi-Al	PRO35
		3.43523	E	Pi-Ca	LYS136
D_3-A_3-D_3	-12.6	3.88581	E	Pi-Ca	LYS136
		3.50371	HB; E	Pi-Ca; Pi-Do; HB	ARG143
		4.50431	E	Pi-An	GLU125
		3.46376	E	Pi-An	GLU125
		4.89227	E	Pi-An	GLU140
		3.82847	E	Pi-An	GLU140
		4.77588	Hyd	Pi-Al	PRO113
		5.19945	Hyd	Pi-Al	LEU115
		5.41398	Hyd	Pi-Al	LEU122
		5.13422	Hyd	Pi-Al	LYS136
		5.35539	Hyd	Pi-Al	LEU122
		4.56857	Hyd	Pi-Al	LYS136
		5.16934	Hyd	Pi-Al	PRO35
		4.2538	Hyd	Pi-Al	PRO35
		5.32532	Hyd	Pi-Al	CYS34
		4.58438	Hyd	Pi-Al	PRO35

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

Table S1. (*cont.*) Docking scores and interaction data of the studied ligands with BSA (PDB ID: 4F5S)

Ligands	Docking Scores	Distance	Category	Type of Interactions	Residue Information
D_3-A_4-D_3	-13.2	3.30625	HB	CHB	GLU140
		3.5509	HB; E	Pi-Ca; Pi-Do; HB	ARG143
		3.18925	E	Pi-An	GLU125
		3.28458	E	Pi-An	GLU125
		3.6103	E	Pi-An	GLU140
		3.79431	E	Pi-An	GLU140
		4.88075	Hyd	Pi-Al	PRO113
		5.49796	Hyd	Pi-Al	LYS136
		5.08673	Hyd	Pi-Al	PRO35
		4.23714	Hyd	Pi-Al	PRO35
		5.27199	Hyd	Pi-Al	CYS34
		4.58917	Hyd	Pi-Al	PRO35
		4.79039	Hyd	Pi-Al	LEU115
		5.32398	Hyd	Pi-Al	PRO117
		5.08274	Hyd	Pi-Al	LEU122
		3.82194	Hyd	Pi-Al	LYS136
		3.69733	Hyd	Pi-Al	LYS136
D_4-A_1-D_4	-13.9	3.64366	HB; E	Pi-Ca; Pi-Do; HB	ARG143
		4.77098	E	Pi-An	ASP118
		4.33625	E	Pi-An	GLU125
		3.37164	E	Pi-An	GLU125
		3.83026	E	Pi-An	GLU140
		2.70524	Hyd	Pi-Sg	LEU115
		4.69355	Hyd	Pi-Pi-St	PHE133
		4.50701	Hyd	Pi-Al	PRO113
		5.15654	Hyd	Pi-Al	LEU122
		5.2764	Hyd	Pi-Al	LYS136
		4.92341	Hyd	Pi-Al	PRO117
		4.86959	Hyd	Pi-Al	LEU122
		5.4456	Hyd	Pi-Al	LEU122
		4.24633	Hyd	Pi-Al	LYS136
		5.31115	Hyd	Pi-Al	PRO35
		4.0904	Hyd	Pi-Al	PRO35
		5.09072	Hyd	Pi-Al	CYS34
		4.50145	Hyd	Pi-Al	PRO35
		4.63316	Hyd	Pi-Al	PRO35
D_4-A_2-D_4	-13.9	2.28629	HB	CHB	ARG144
		3.07174	HB	CHB	GLU140
		2.91183	Other	S-X	ARG144
		4.16687	E	Pi-Ca	LYS136
		4.94323	E	Pi-Ca	LYS136
		4.57704	E	Pi-Ca	LYS136
		3.34109	HB; E	Pi-Ca; Pi-Do; HB	ARG143
		4.99211	E	Pi-Ca	ARG143
		3.78773	E	Pi-An	ASP111
		4.52326	E	Pi-An	ASP111
		3.18217	E	Pi-An	GLU125
		3.28467	E	Pi-An	GLU125
		4.095	E	Pi-An	GLU125
		4.96824	E	Pi-An	GLU125

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

Table S1. (*cont.*) Docking scores and interaction data of the studied ligands with BSA (PDB ID: 4F5S)

Ligands	Docking Scores	Distance	Category	Type of Interactions	Residue Information
D_4-A_3-D_4	-15.1	2.69091	HB	CHB	PHE36:HN
		3.98273	E	Pi-An	GLU125
		3.33594	E	Pi-An	GLU125
		2.46074	Hyd	Pi-Sg	LEU115
		5.11598	Hyd	Pi-Pi-St	PHE133
		4.98359	Hyd	Pi-Al	PRO113
		4.15882	Hyd	Pi-Al	PRO113
		5.10783	Hyd	Pi-Al	PRO113
		4.16257	Hyd	Pi-Al	PRO113
		5.28027	Hyd	Pi-Al	PRO35
		4.32822	Hyd	Pi-Al	PRO35
		4.99576	Hyd	Pi-Al	CYS34
		4.49389	Hyd	Pi-Al	PRO35
		5.09389	Hyd	Pi-Al	PRO35
		5.35035	Hyd	Pi-Al	LEU122
		5.4627	Hyd	Pi-Al	LYS136
		4.97415	Hyd	Pi-Al	PRO117
		5.07437	Hyd	Pi-Al	LEU122
		5.35386	Hyd	Pi-Al	LEU122
		4.32841	Hyd	Pi-Al	LYS136
D_4-A_4-D_4	-13.8	2.69754	HB	CHB	ARG144
		3.6959	HB; E	Pi-Ca; Pi-Do; HB	ARG143
		4.78974	E	Pi-An	ASP118
		4.34041	E	Pi-An	GLU125
		3.37275	E	Pi-An	GLU125
		3.88212	E	Pi-An	GLU140
		2.71506	Hyd	Pi-Sg	LEU115
		4.69102	Hyd	Pi-Pi-St	PHE133
		4.80615	Hyd	Pi-Al	PRO113
		5.17399	Hyd	Pi-Al	LEU122
		5.23951	Hyd	Pi-Al	LYS136
		4.96263	Hyd	Pi-Al	PRO117
		4.86538	Hyd	Pi-Al	LEU122
		5.4828	Hyd	Pi-Al	LEU122
		4.20984	Hyd	Pi-Al	LYS136
		5.08558	Hyd	Pi-Al	PRO35
		4.01862	Hyd	Pi-Al	PRO35
		5.08562	Hyd	Pi-Al	CYS34
		4.56283	Hyd	Pi-Al	PRO35
		4.5268	Hyd	Pi-Al	PRO35

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

Table S1. (*cont.*) Docking scores and interaction data of the studied ligands with BSA (PDB ID: 4F5S)

Ligands	Docking Scores	Distance	Category	Type of Interactions	Residue Information
D_5-A_1-D_5	-14.0	4.46759	E	Pi-Ca	LYS136
		4.35123	E	Pi-Ca	LYS136
		3.09717	HB; E	Pi-Ca; Pi-Do; HB	LYS136
		4.24007	E	Pi-Ca	ARG143
		3.27448	E	Pi-An	GLU125
		3.0983	E	Pi-An	GLU125
		4.02071	E	Pi-An	GLU140
		2.63487	Hyd	Pi-Sg	LYS136
		2.81554	Hyd	Pi-Sg	LYS136
		5.7687	Hyd	Pi-Pi T	-
		5.25073	Hyd	Pi-Al	PRO113
		5.12445	Hyd	Pi-Al	PRO35
		4.11911	Hyd	Pi-Al	PRO35
		5.142	Hyd	Pi-Al	CYS34
		4.35114	Hyd	Pi-Al	PRO35
		4.87012	Hyd	Pi-Al	LYS136
		3.59654	Hyd	Pi-Al	LYS136
		5.49644	Hyd	Pi-Al	LYS136
		4.94347	Hyd	Pi-Al	LEU115
		5.44165	Hyd	Pi-Al	PRO117
		4.33589	Hyd	Pi-Al	LEU122
		4.05246	Hyd	Pi-Al	LEU115
		5.2347	Hyd	Pi-Al	PRO117
		5.16019	Hyd	Pi-Al	LEU122
		4.34606	Hyd	Pi-Al	LEU115
D_5-A_2-D_5	-12.3	3.48519	E	Pi-Ca	LYS136
		3.39939	HB; E	Pi-Ca; Pi-Do; HB	ARG143
		3.55023	E	Pi-An	GLU125
		3.57866	E	Pi-An	GLU125
		4.94679	E	Pi-An	GLU125
		3.20874	E	Pi-An	GLU125
		3.37136	E	Pi-An	GLU125
		4.72823	E	Pi-An	GLU140
		3.88622	E	Pi-An	GLU140
		4.8654	E	Pi-An	GLU140
		5.40666	Hyd	Pi-Pi-St	-
		4.83488	Hyd	Pi-Al	PRO113
		5.46291	Hyd	Pi-Al	LEU115
		4.71732	Hyd	Pi-Al	LYS136
		3.64022	Hyd	Pi-Al	LYS136
		5.37325	Hyd	Pi-Al	LYS132
		3.84982	Hyd	Pi-Al	LYS136
		4.92688	Hyd	Pi-Al	PRO35
		4.29062	Hyd	Pi-Al	PRO35
		4.45906	Hyd	Pi-Al	PRO35
		5.17839	Hyd	Pi-Al	PRO35

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

Table S1. (*cont.*) Docking scores and interaction data of the studied ligands with BSA (PDB ID: 4F5S)

Ligands	Docking Scores	Distance	Category	Type of Interactions	Residue Information
D_5-A_3-D_5	-13.2	4.8285	E	Pi-An	ASP111
		3.93144	E	Pi-An	GLU125
		3.55408	E	Pi-An	GLU125
		3.09831	E	Pi-An	GLU125
		3.45528	E	Pi-An	GLU125
		4.86597	E	Pi-An	GLU140
		5.87653	Hyd	Pi-Pi T	-
		4.79708	Hyd	Pi-Al	PRO113
		4.05755	Hyd	Pi-Al	PRO113
		5.01173	Hyd	Pi-Al	PRO113
		4.18824	Hyd	Pi-Al	PRO113
		5.24399	Hyd	Pi-Al	PRO113
		5.41135	Hyd	Pi-Al	PRO35
		4.31787	Hyd	Pi-Al	PRO35
		4.40429	Hyd	Pi-Al	PRO35
		5.44292	Hyd	Pi-Al	LEU115
		5.00834	Hyd	Pi-Al	LYS136
		3.75122	Hyd	Pi-Al	LYS136
		5.35708	Hyd	Pi-Al	LYS132
		3.71921	Hyd	Pi-Al	LYS136
D_5-A_4-D_5	-13.7	3.47153	HB; E	Pi-Ca; Pi-Do; HB	ARG143
		4.87553	E	Pi-Ca	ARG143
		3.60143	E	Pi-An	GLU125
		3.47281	E	Pi-An	GLU125
		3.30574	E	Pi-An	GLU125
		3.29729	E	Pi-An	GLU125
		4.99514	E	Pi-An	GLU125
		4.49224	E	Pi-An	GLU140
		4.03593	E	Pi-An	GLU140
		4.69109	E	Pi-An	GLU140
		4.72329	Hyd	Pi-Al	PRO113
		4.94289	Hyd	Pi-Al	PRO35
		4.4199	Hyd	Pi-Al	LYS136
		3.50405	Hyd	Pi-Al	LYS136
		5.41484	Hyd	Pi-Al	LYS132
		3.95626	Hyd	Pi-Al	LYS136
		4.29337	Hyd	Pi-Al	PRO35
		4.25569	Hyd	Pi-Al	PRO35
		5.31805	Hyd	Pi-Al	PRO35
		3.47153	HB; E	Pi-Ca; Pi-Do; HB	ARG143

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

Figure S5. Binding poses and residue interactions of the investigated ligands with BSA (PDB ID: 4F5S)

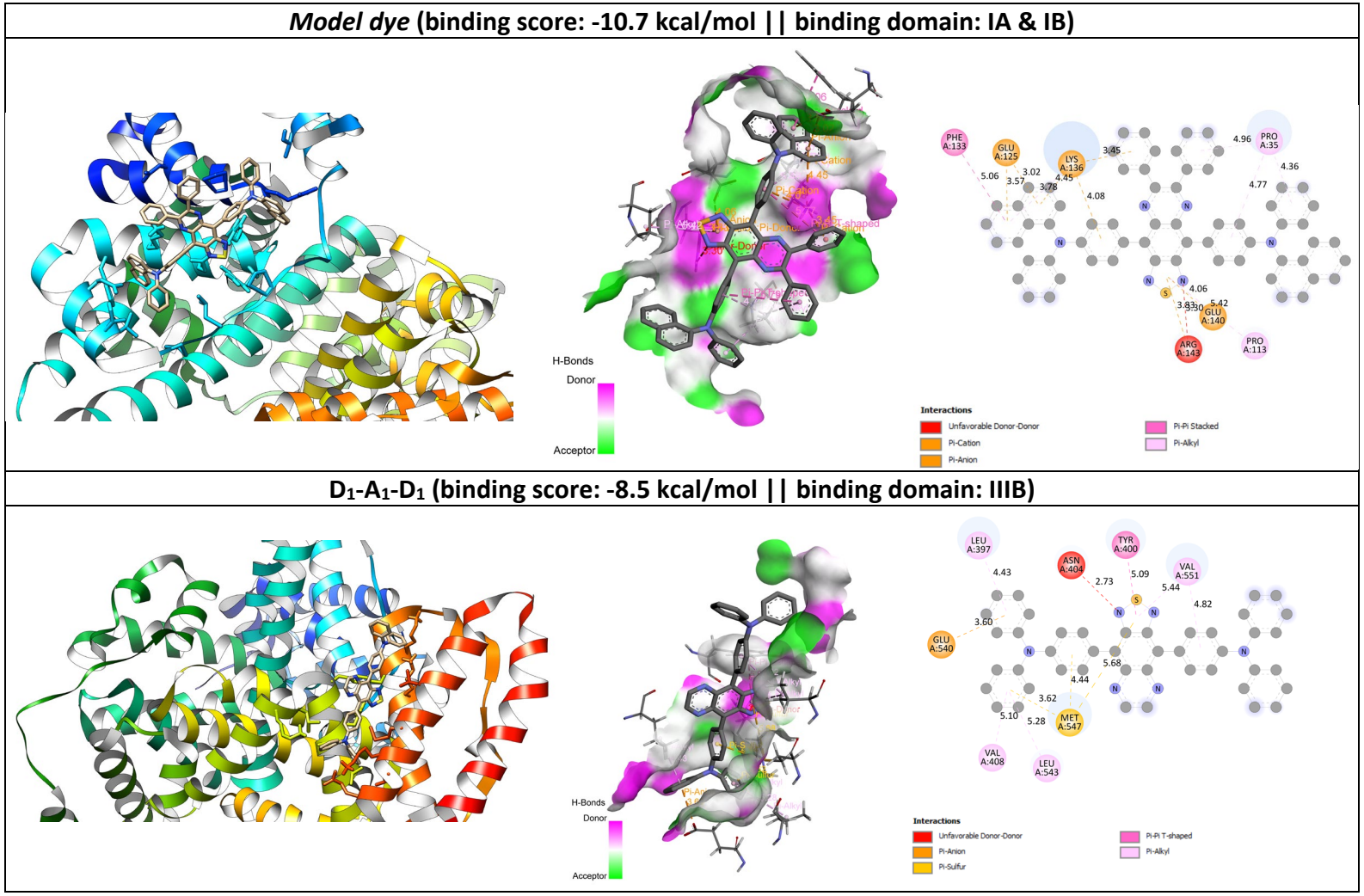
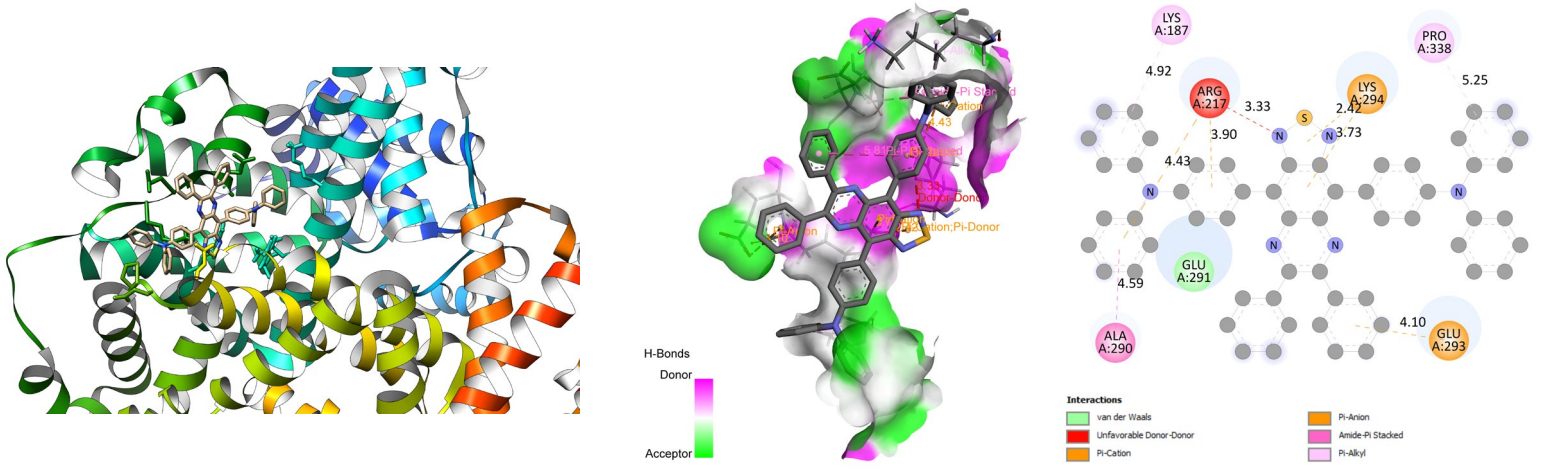


Figure S5. (*cont.*) Binding poses and residue interactions of the investigated ligands with BSA (PDB ID: 4F5S)

D_1-A_2-D_1 (binding score: -10.3 kcal/mol || binding domain: IB & IIA & IIIA)



D_1-A_3-D_1 (binding score: -9.6 kcal/mol || binding domain: IB & IIA & IIIA)

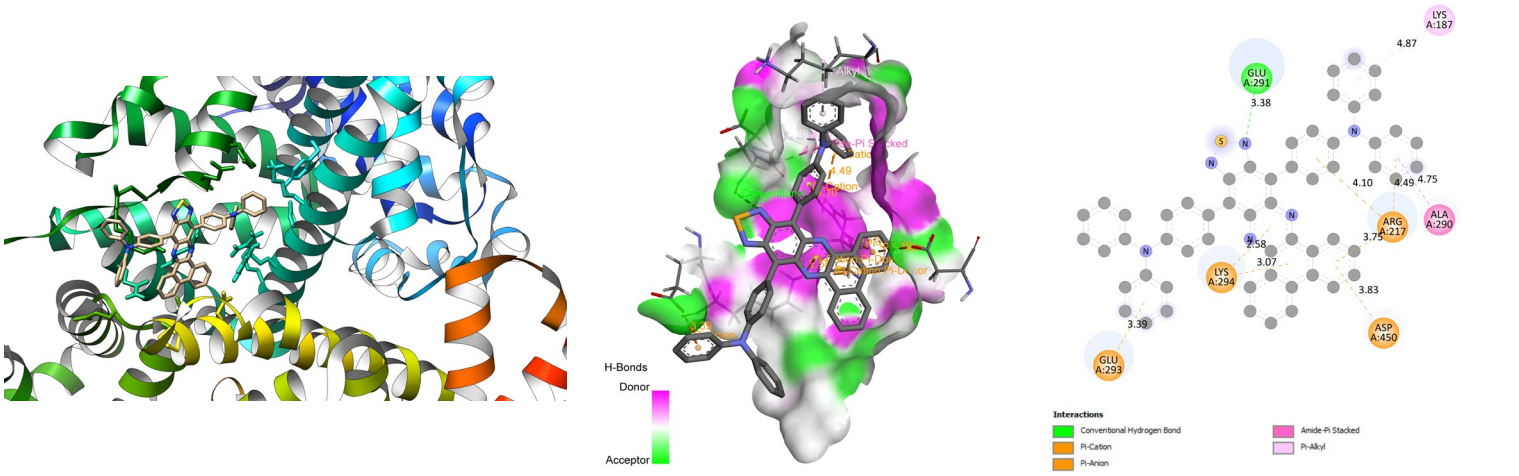


Figure S5. (*cont.*). Binding poses and residue interactions of the investigated ligands with BSA (PDB ID: 4F5S)

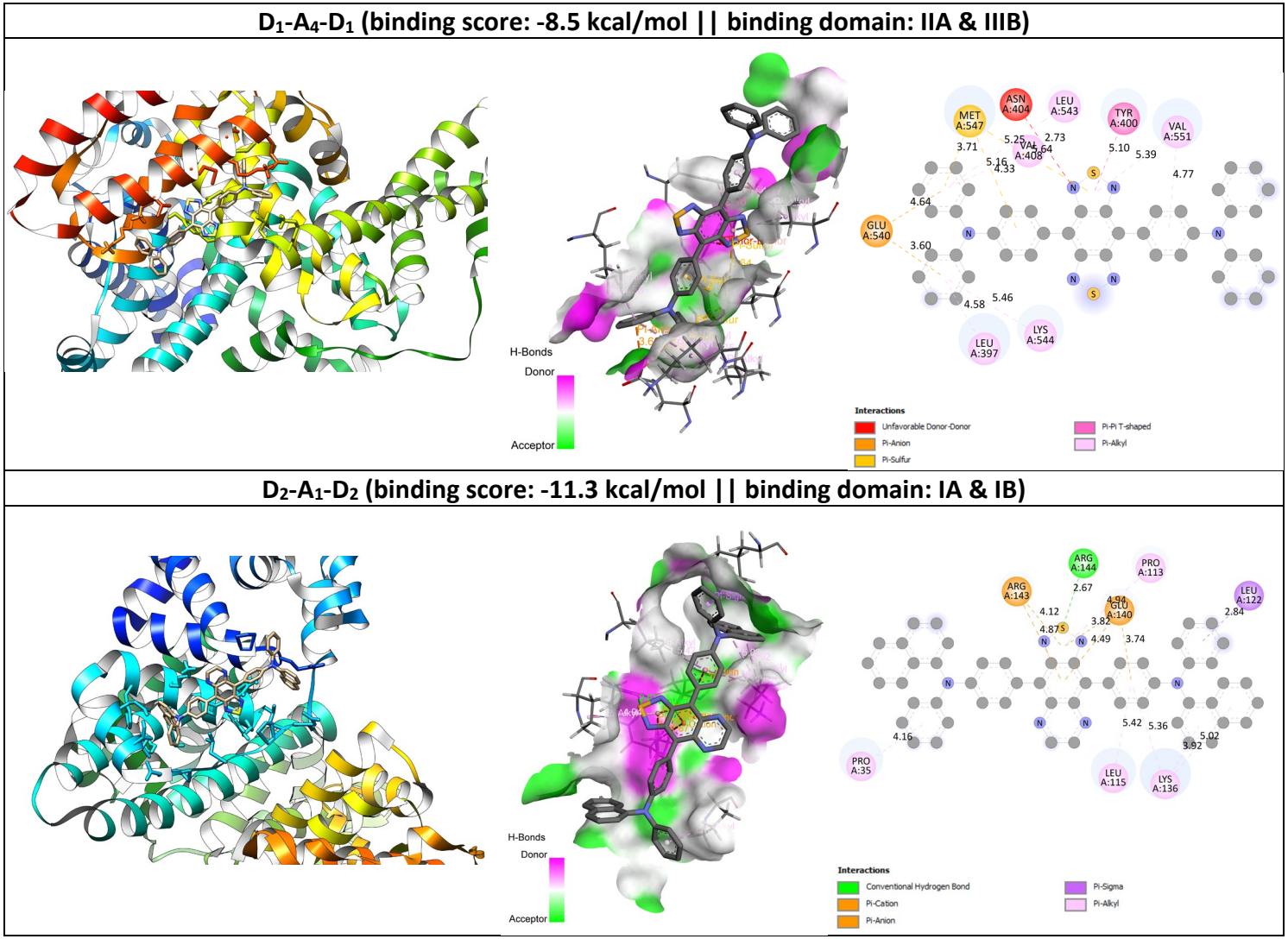
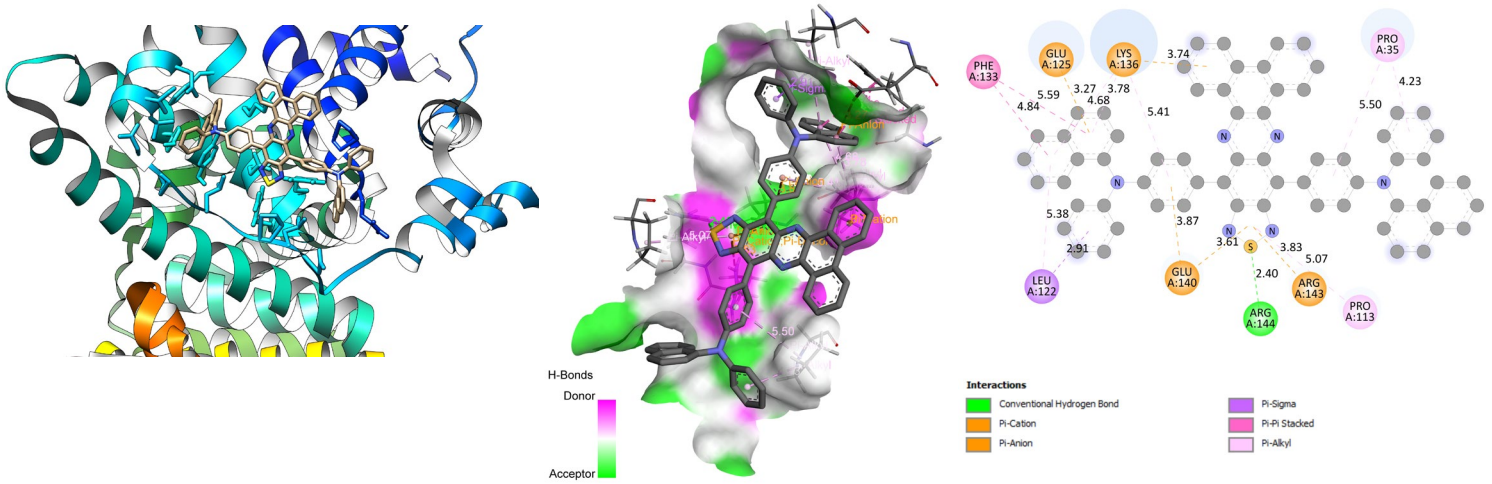


Figure S5. (*cont.*). Binding poses and residue interactions of the investigated ligands with BSA (PDB ID: 4F5S)

D_2-A_3-D_2 (binding score: -11.8 kcal/mol || binding domain: IA & IB)



D_2-A_4-D_2 (binding score: -10.5 kcal/mol || binding domain: IA & IB)

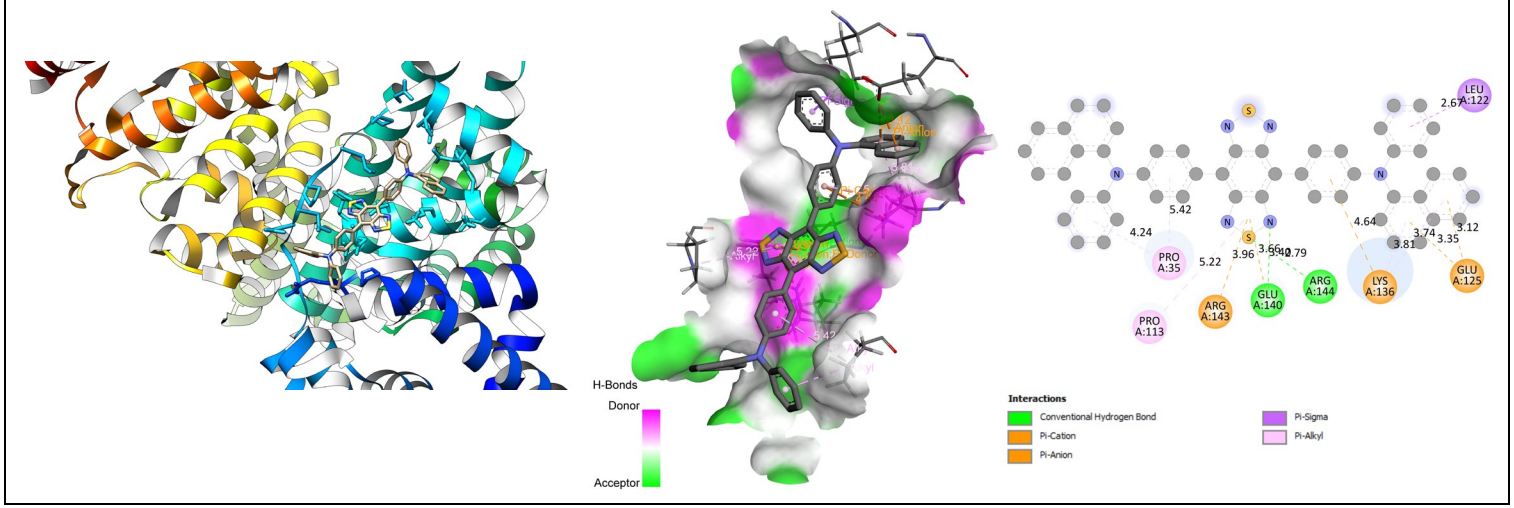
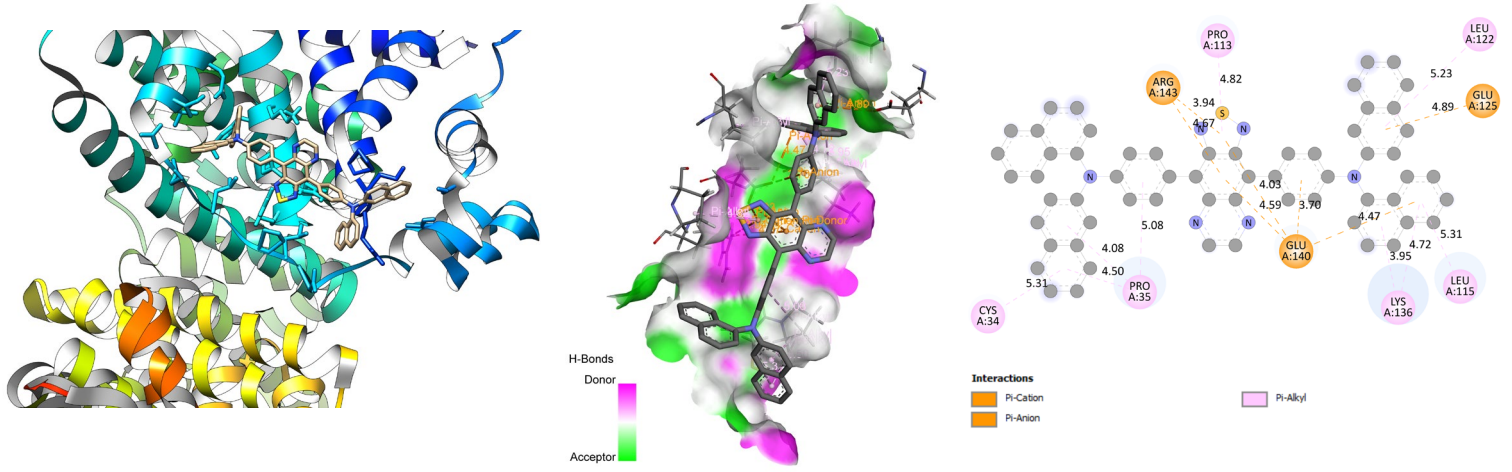


Figure S5. (*cont.*). Binding poses and residue interactions of the investigated ligands with BSA (PDB ID: 4F5S)

D_3-A_1-D_3 (binding score: -12.7 kcal/mol || binding domain: IA & IB)



D_3-A_2-D_3 (binding score: -11.9 kcal/mol || binding domain: IA & IB)

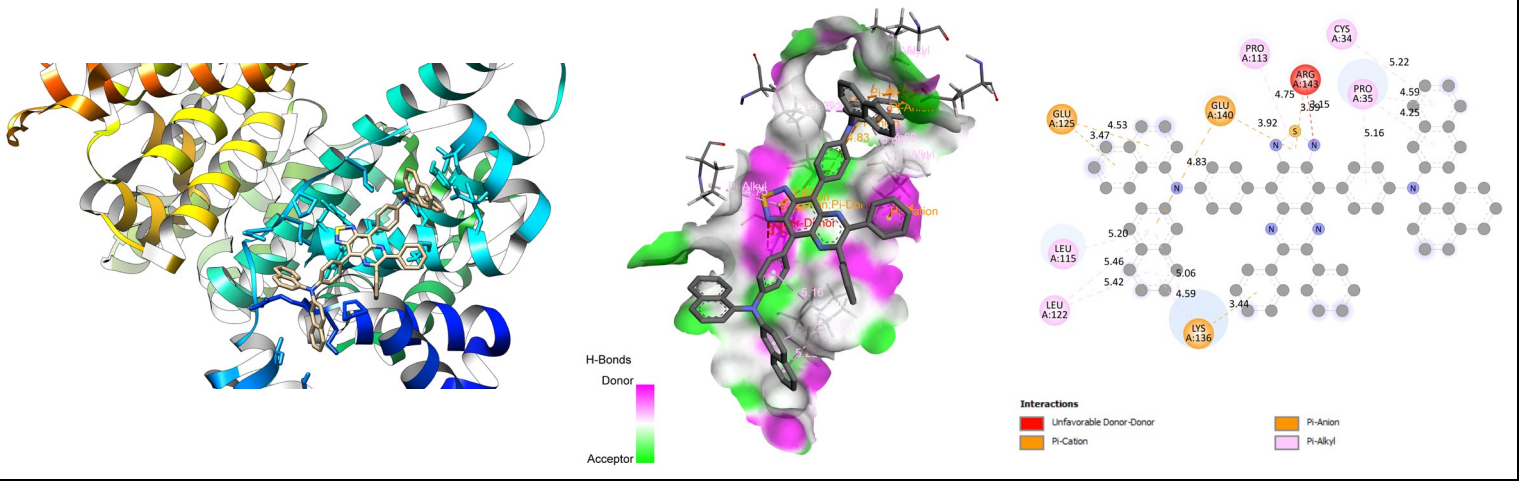


Figure S5. (*cont.*). Binding poses and residue interactions of the investigated ligands with BSA (PDB ID: 4F5S)

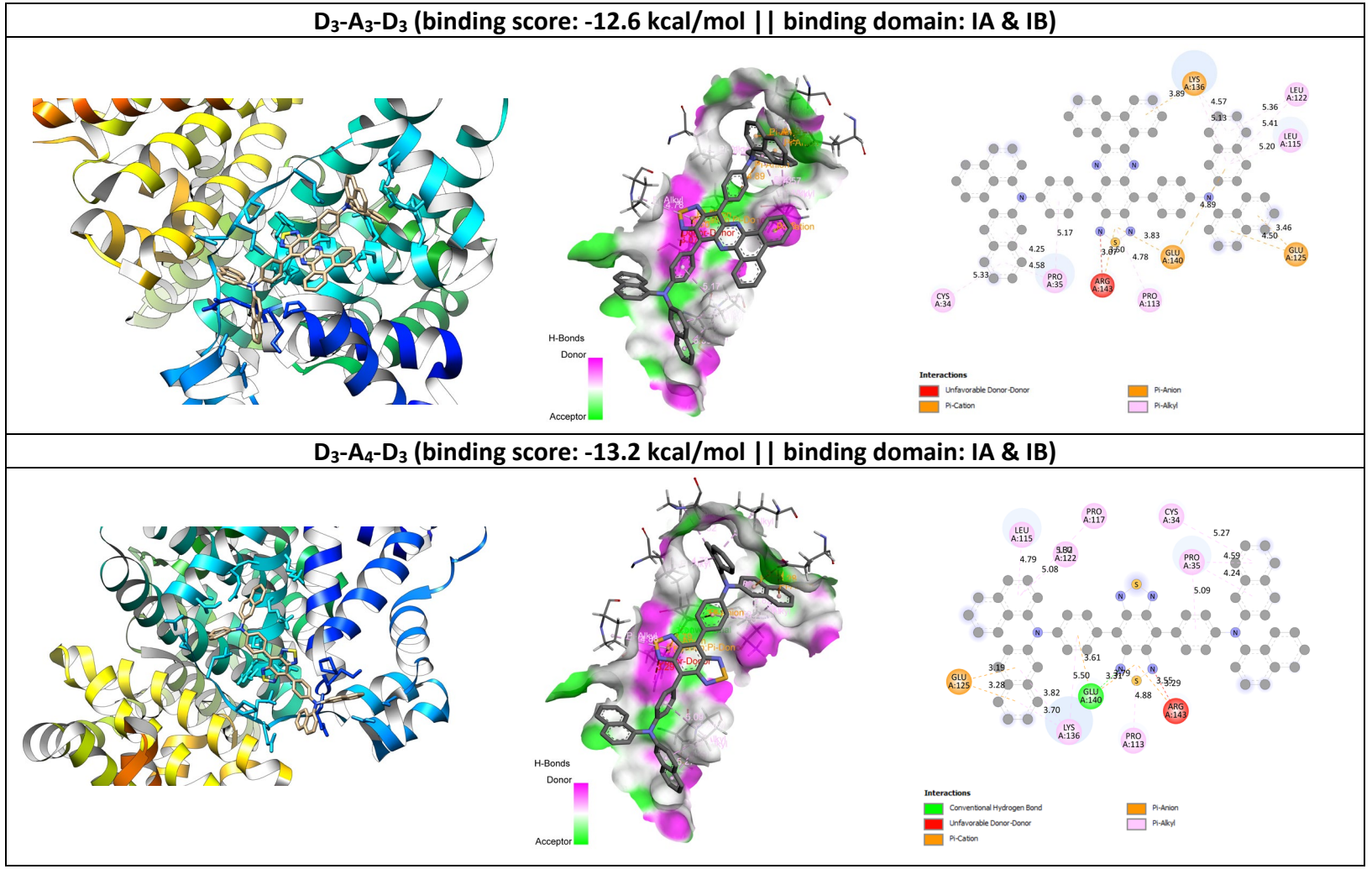
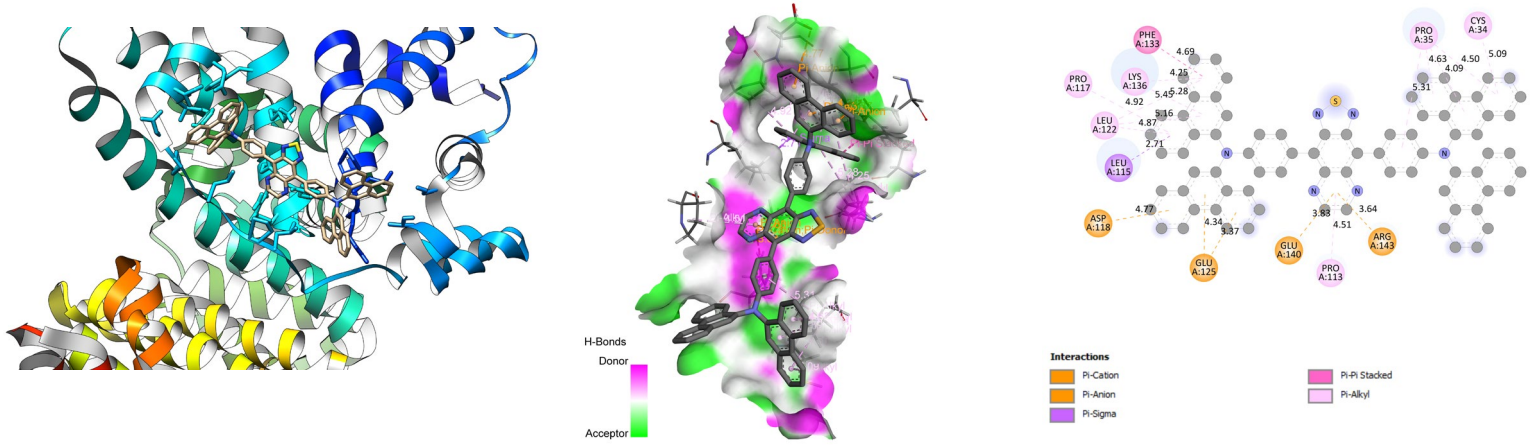


Figure S5. (*cont.*). Binding poses and residue interactions of the investigated ligands with BSA (PDB ID: 4F5S)

D_4-A_1-D_4 (binding score: -13.9 kcal/mol || binding domain: IA & IB)



D_4-A_2-D_4 (binding score: -13.9 kcal/mol || binding domain: IA & IB)

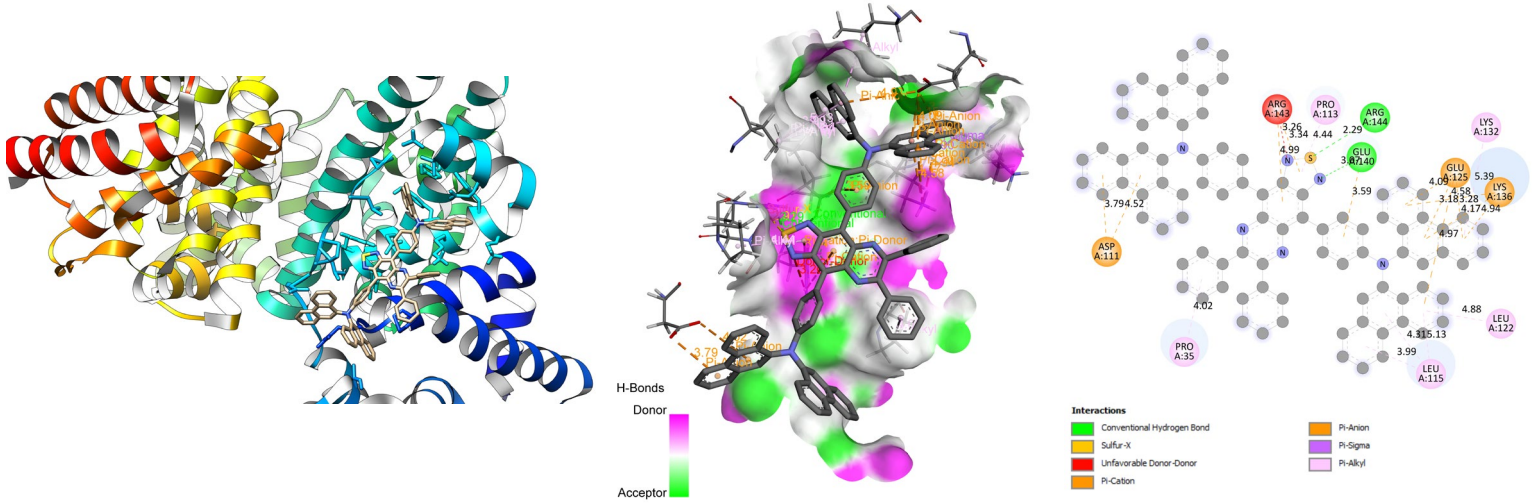


Figure S5. (*cont.*). Binding poses and residue interactions of the investigated ligands with BSA (PDB ID: 4F5S)

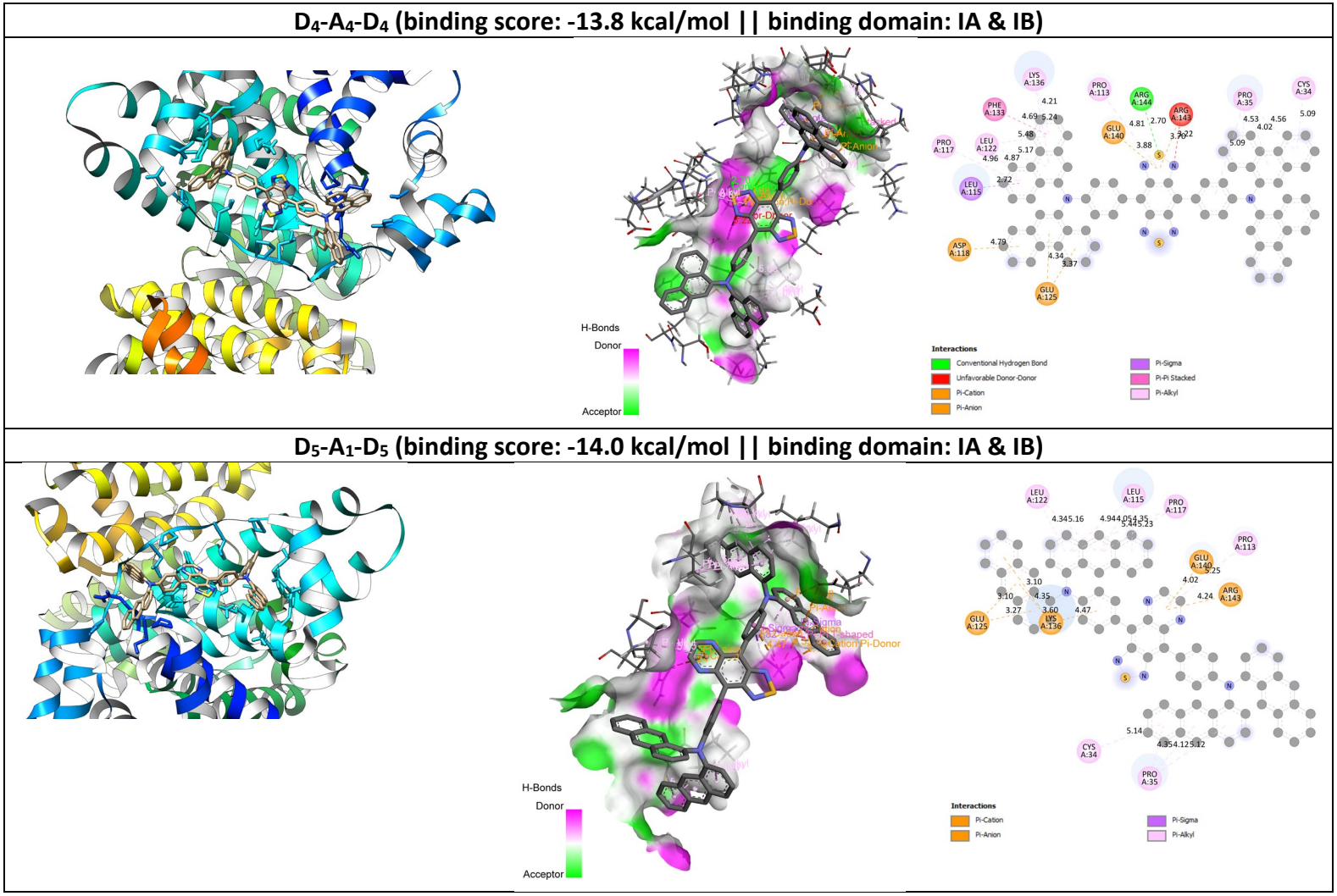


Figure S5. (*cont.*). Binding poses and residue interactions of the investigated ligands with BSA (PDB ID: 4F5S)

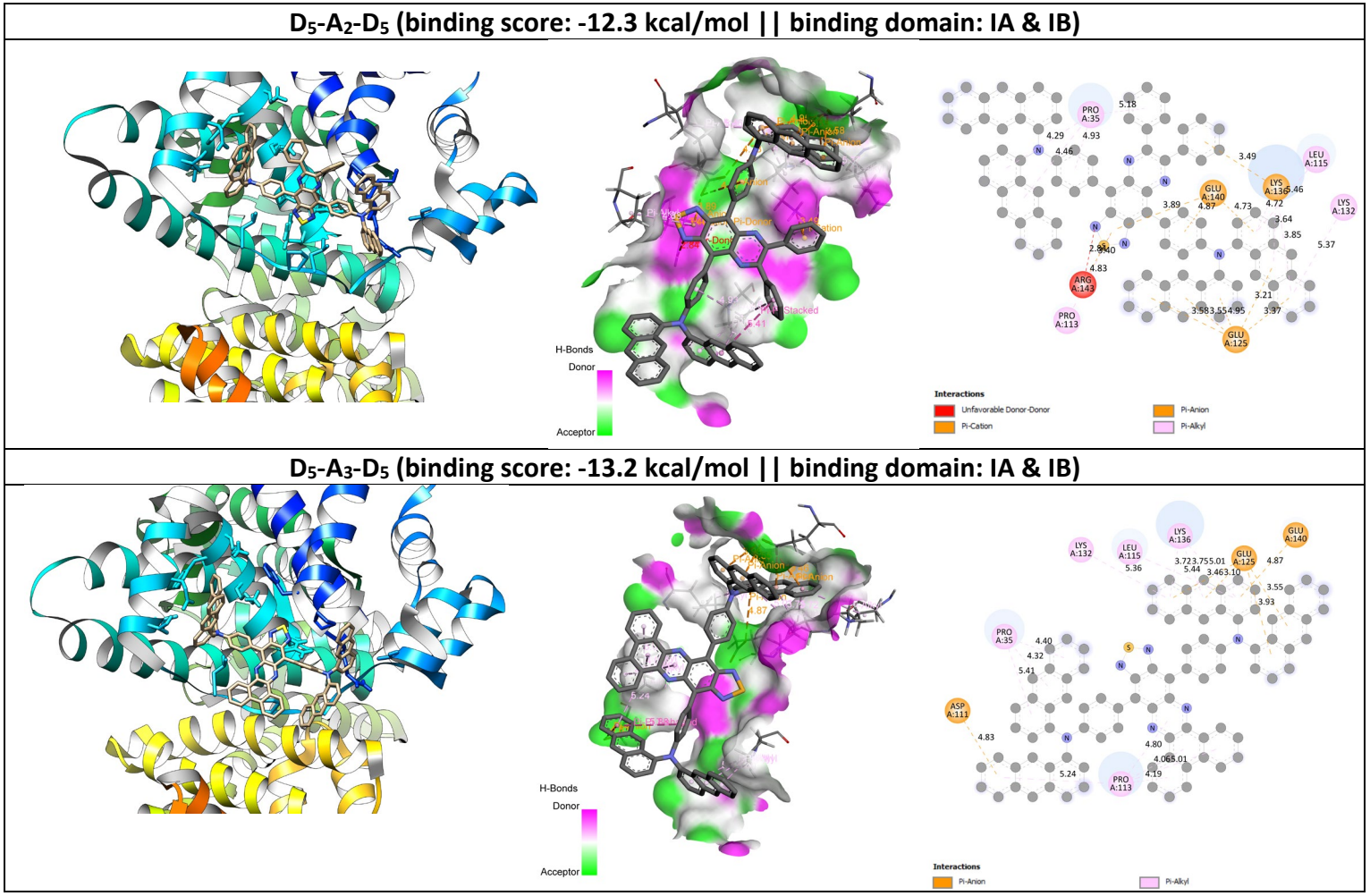


Figure S5. (*cont.*). Binding poses and residue interactions of the investigated ligands with BSA (PDB ID: 4F5S)

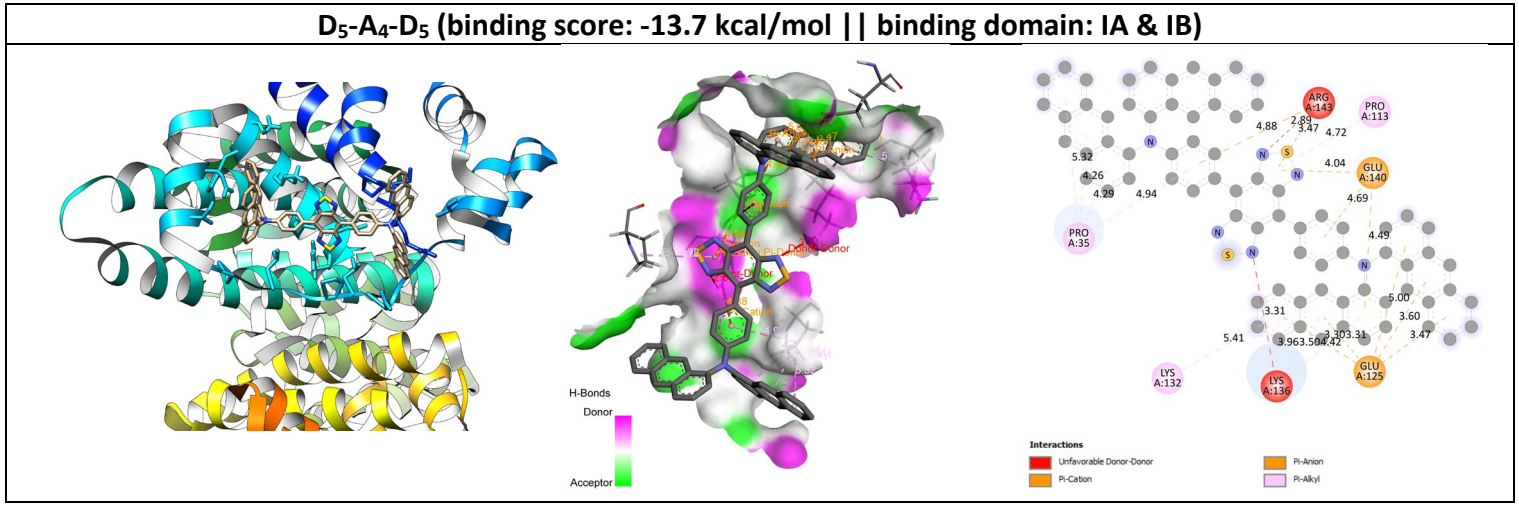


Table S2. Docking scores and interaction data of the studied ligands with HSA (PDB ID: 4L9Q)

Ligands	Docking Scores	Distance	Category	Type of Interactions	Residue Information
MODEL DYE (D_2-A_2-D_2)	-11.8	4.5782	E	Pi-Ca	LYS195
		3.86860	E	Pi-Ca	LYS195
		4.07402	E	Pi-Ca	ARG218
		3.57327	E	Pi-Ca	ARG218
		4.40034	E	Pi-Ca	LYS436
		4.20377	E	Pi-Ca	LYS436
		2.61458	HB; E	Pi-Ca; Pi-Do HB	LYS444
		5.51109	Other	Pi-S	CYS448
		5.55997	Hyd	Pi-Pi T	HIS440
		5.05842	Hyd	Pi-Al	PRO447
		5.13047	Hyd	Pi-Al	LYS444
		4.18031	Hyd	Pi-Al	PRO447
		4.33174	Hyd	Pi-Al	LYS195
		5.46594	Hyd	Pi-Al	VAL455
		5.42618	Hyd	Pi-Al	LYS195
		4.44020	Hyd	Pi-Al	LYS195
		3.90097	Hyd	Pi-Al	LYS444
		4.65552	Hyd	Pi-Al	ALA443
		4.62502	Hyd	Pi-Al	LYS444
		5.41997	Hyd	Pi-Al	PRO441
		4.0096	Hyd	Pi-Al	LYS444
		5.02679	Hyd	Pi-Al	LYS444
D_1-A_1-D_1	-10.0	2.38923	HB	CHB	ASN872
		4.36157	E	Pi-Ca	LYS772
		4.12125	E	Pi-Ca	ARG795
		3.59928	E	Pi-Ca	ARG795
		4.27303	E	Pi-Ca	LYS1013
		4.44600	Hyd	Am-Pi-St	ALA1020, LYS1021
		4.85941	Hyd	Pi-Al	PRO1024
		4.12289	Hyd	Pi-Al	PRO1024
		4.92971	Hyd	Pi-Al	LYS1021
		4.46685	Hyd	Pi-Al	LYS772
		4.39777	Hyd	Pi-Al	LYS772
		5.37313	Hyd	Pi-Al	VAL1032
		3.84331	Hyd	Pi-Al	LYS1021
		5.35913	Hyd	Pi-Al	PRO916
		4.59239	Hyd	Pi-Al	ALA1020
		4.60294	Hyd	Pi-Al	LYS1021
D_1-A_2-D_1	-12.6	4.49847	E	Pi-Ca	LYS772
		4.18537	E	Pi-Ca	ARG795
		3.61559	E	Pi-Ca	ARG795
		4.44621	E	Pi-Ca	LYS1013
		2.55789	HB; E	Pi-Ca; Pi-Do HB	LYS1021
		5.15594	Other	Pi-S	CYS1025
		5.27895	Hyd	Pi-Pi T	HIS1017
		4.37819	Hyd	Am-Pi-St	ALA1020, LYS1021
		4.95830	Hyd	Am-Pi-St	PRO1024, CYS1025
		4.95962	Hyd	Pi-Al	PRO1024
		5.11742	Hyd	Pi-Al	LYS1021
		4.14796	Hyd	Pi-Al	PRO1024
		4.30377	Hyd	Pi-Al	LYS772
		5.46202	Hyd	Pi-Al	VAL1032
		4.42765	Hyd	Pi-Al	LYS772
		5.26817	Hyd	Pi-Al	VAL1032
		3.82317	Hyd	Pi-Al	LYS1021
		4.64771	Hyd	Pi-Al	ALA1020
		4.50305	Hyd	Pi-Al	LYS1021
		5.37273	Hyd	Pi-Al	PRO916
		4.93560	Hyd	Pi-Al	LYS1021

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-Al: Pi-Al, Pi-Pi T-Shaped: Pi-Pi T, Am-Pi-St, Pi-Pi Stacked: Pi-Pi-St, Pi-Sulfur: Pi-S, Pi-Sigma: Pi-Sg, Sulfur-X: S-X

Table S2. (*cont.*). Docking scores and interaction data of the studied ligands with HSA (PDB ID: 4L9Q)

Ligands	Docking Scores	Distance	Category	Type of Interactions	Residue Information
D_1-A_3-D_1	-12.7	4.63599	E	Pi-Ca	LYS772
		3.92437	E	Pi-Ca	ARG795
		3.51655	E	Pi-Ca	ARG795
		4.14155	E	Pi-Ca	LYS1013
		3.17164	HB; E	Pi-Ca; Pi-Do; HB	LYS1021
		5.44295	Hyd	Pi-Al	LYS1021
		5.42499	Hyd	Pi-Al	PRO1024
		5.23545	Hyd	Pi-Al	LYS1021
		4.36935	Hyd	Pi-Al	PRO1024
		4.9103	Hyd	Pi-Al	LYS772
		4.59174	Hyd	Pi-Al	LYS772
		4.41816	Hyd	Pi-Al	LYS1021
		4.53758	Hyd	Pi-Al	PRO916
D_1-A_4-D_1	-10.1	4.03458	E	Pi-Ca	ARG795
		3.66550	E	Pi-Ca	ARG795
		4.40196	E	Pi-Ca	LYS1013
		4.70803	Hyd	Am-Pi-St	ALA1020, LYS1021
		5.27224	Hyd	Pi-Al	LYS1021
		5.12262	Hyd	Pi-Al	PRO1024
		4.24852	Hyd	Pi-Al	PRO1024
		4.87444	Hyd	Pi-Al	LYS1021
		3.88471	Hyd	Pi-Al	LYS1021
		4.53744	Hyd	Pi-Al	LYS772
		5.48259	Hyd	Pi-Al	VAL1032
		4.96443	Hyd	Pi-Al	LYS772
		4.55533	Hyd	Pi-Al	ALA1020
D_2-A_1-D_2	-12.3	2.68953	Other	S-X	PHE133
		4.58233	E	Pi-Ca	ARG185
		3.85315	E	Pi-Ca	ARG185
		5.96053	Other	Pi-S	MET122
		3.83301	Other	Pi-S	PHE133
		5.87263	Other	Pi-S	TYR137
		4.76413	Other	Pi-S	TYR160
		5.8058	Hyd	Pi-Pi-St	PHE133
		4.40236	Hyd	Pi-Pi-St	PHE133
		5.15813	Hyd	Pi-Pi T	TYR137
		4.86949	Hyd	Pi-Al	LYS136
		4.73836	Hyd	Pi-Al	PRO117
		4.59234	Hyd	Pi-Al	LYS136
		5.17693	Hyd	Pi-Al	ALA125
		4.2076	Hyd	Pi-Al	LYS136
		4.67286	Hyd	Pi-Al	LEU114
		5.24163	Hyd	Pi-Al	ILE141
		4.72396	Hyd	Pi-Al	ARG185
		5.41355	Hyd	Pi-Al	LEU181
		4.87133	Hyd	Pi-Al	ARG185
		5.43585	Hyd	Pi-Al	LEU114
		4.57351	Hyd	Pi-Al	ARG116
		4.07469	Hyd	Pi-Al	ALA125

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-Al: Pi-Al, Pi-Pi T-Shaped: Pi-Pi T, Am-Pi-St, Pi-Pi Stacked: Pi-Pi-St, Pi-Sulfur: Pi-S, Pi-Sigma: Pi-Sg, Sulfur-X: S-X

Table S2. (*cont.*). Docking scores and interaction data of the studied ligands with HSA (PDB ID: 4L9Q)

Ligands	Docking Scores	Distance	Category	Type of Interactions	Residue Information
D_2-A_3-D_2	-12.8	3.84536	E	Pi-Ca	LYS772
		3.96768	E	Pi-Ca	ARG795
		3.67853	E	Pi-Ca	ARG795
		4.44871	E	Pi-Ca	LYS1013
		4.24203	E	Pi-Ca	LYS1013
		3.05733	HB; E	Pi-Ca; Pi-Do HB	LYS1021
		5.31996	Hyd	Pi-Al	LYS1021
		5.34444	Hyd	Pi-Al	PRO1024
		5.12944	Hyd	Pi-Al	LYS1021
		4.26996	Hyd	Pi-Al	PRO1024
		4.53031	Hyd	Pi-Al	LYS772
		5.43903	Hyd	Pi-Al	VAL1032
		5.02826	Hyd	Pi-Al	LYS772
		4.84894	Hyd	Pi-Al	LYS772
		4.09846	Hyd	Pi-Al	LYS1021
		5.19825	Hyd	Pi-Al	ALA1020
		5.06319	Hyd	Pi-Al	LYS1021
		5.48162	Hyd	Pi-Al	PRO1018
		4.36384	Hyd	Pi-Al	LYS1021
D_2-A_4-D_2	-12.3	2.92338	Other	S-X	PHE133
		4.57296	E	Pi-Ca	ARG185
		3.74845	E	Pi-Ca	ARG185
		5.91986	Other	Pi-S	MET122
		3.89424	Other	Pi-S	PHE133
		4.96495	Other	Pi-S	TYR160
		5.78783	Hyd	Pi-Pi-St	PHE133
		4.40792	Hyd	Pi-Pi-St	PHE133
		5.16908	Hyd	Pi-Pi T	TYR137
		5.07412	Hyd	Pi-Al	LYS136
		4.67271	Hyd	Pi-Al	LYS136
		4.51298	Hyd	Pi-Al	PRO117
		4.68138	Hyd	Pi-Al	LEU114
		5.24221	Hyd	Pi-Al	ILE141
		4.69564	Hyd	Pi-Al	ARG185
		5.41505	Hyd	Pi-Al	LEU181
		4.85335	Hyd	Pi-Al	ARG185
		5.47278	Hyd	Pi-Al	LEU114
		4.64857	Hyd	Pi-Al	ARG116
		4.8706	Hyd	Pi-Al	ALA125
		4.61951	Hyd	Pi-Al	LYS136
		3.98003	Hyd	Pi-Al	ALA125

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-Al: Pi-Al, Pi-Pi T-Shaped: Pi-Pi T, Am-Pi-St, Pi-Pi Stacked: Pi-Pi-St, Pi-Sulfur: Pi-S, Pi-Sigma: Pi-Sg, Sulfur-X: S-X

Table S2. (*cont.*). Docking scores and interaction data of the studied ligands with HSA (PDB ID: 4L9Q)

Ligands	Docking Scores	Distance	Category	Type of Interactions	Residue Information
D_3-A_1-D_3	-13.9	1.89962	HB	CHB	ASN295
		4.36328	E	Pi-Ca	LYS195
		3.84671	E	Pi-Ca	LYS195
		3.6214	E	Pi-Ca	ARG218
		4.82138	E	Pi-An	GLU294
		2.64878	Hyd	Pi-Sg	LYS195
		4.95596	Hyd	Pi-Pi-St	TYR452
		3.91059	Hyd	Pi-Pi-St	TYR452
		5.2876	Hyd	Pi-Al	LYS444
		4.79912	Hyd	Pi-Al	PRO447
		4.14713	Hyd	Pi-Al	PRO447
		4.67148	Hyd	Pi-Al	LYS444
		5.31558	Hyd	Pi-Al	PRO339
		4.00159	Hyd	Pi-Al	LYS444
		5.39295	Hyd	Pi-Al	PRO339
		5.11878	Hyd	Pi-Al	LYS444
		5.48107	Hyd	Pi-Al	PRO441
		4.36002	Hyd	Pi-Al	ALA443
		5.22772	Hyd	Pi-Al	LYS444
		5.45839	Hyd	Pi-Al	CYS448
		4.57044	Hyd	Pi-Al	LYS195
		5.2985	Hyd	Pi-Al	VAL455
		5.46654	Hyd	Pi-Al	LYS195
		5.22407	Hyd	Pi-Al	LYS195
		5.28131	Hyd	Pi-Al	ALA191
		5.09574	Hyd	Pi-Al	LYS436
D_3-A_2-D_3	-13.2	4.49165	E	Pi-Ca	LYS195
		3.57086	E	Pi-Ca	ARG218
		4.6726	E	Pi-An	ASP451
		2.50358	Hyd	Pi-Sg	ASP451
		4.88067	Other	Pi-S	MET298
		5.2887	Other	Pi-S	CYS437
		5.53194	Hyd	Pi-Pi-St	TYR452
		4.09169	Hyd	Pi-Pi-St	TYR452
		4.72829	Hyd	Pi-Al	PRO447
		4.77652	Hyd	Pi-Al	LYS195
		5.40321	Hyd	Pi-Al	VAL455
		5.39138	Hyd	Pi-Al	LYS195
		5.26598	Hyd	Pi-Al	LYS436
		5.31069	Hyd	Pi-Al	CYS448
		4.94523	Hyd	Pi-Al	LYS444
		4.53168	Hyd	Pi-Al	PRO339
		4.58218	Hyd	Pi-Al	PRO339

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-Al: Pi-Al, Pi-Pi T-Shaped: Pi-Pi T, Am-Pi-St, Pi-Pi Stacked: Pi-Pi-St, Pi-Sulfur: Pi-S, Pi-Sigma: Pi-Sg, Sulfur-X: S-X

Table S2. (*cont.*). Docking scores and interaction data of the studied ligands with HSA (PDB ID: 4L9Q)

Ligands	Docking Scores	Distance	Category	Type of Interactions	Residue Information
D_3-A_3-D_3	-14.3	4.31893	E	Pi-Ca	LYS195
		4.20106	E	Pi-Ca	ARG218
		3.55512	E	Pi-Ca	ARG218
		4.81104	E	Pi-An	ASP451
		2.61973	Hyd	Pi-Sg	ASP451
		4.95943	Other	Pi-S	MET298
		5.54001	Other	Pi-S	CYS437
		5.80657	Hyd	Pi-Pi-St	TYR452
		4.24736	Hyd	Pi-Pi-St	TYR452
		4.86741	Hyd	Pi-Al	PRO447
		5.20185	Hyd	Pi-Al	LYS444
		4.63833	Hyd	Pi-Al	PRO339
		4.57355	Hyd	Pi-Al	PRO339
		5.40055	Hyd	Pi-Al	ALA191
		5.42861	Hyd	Pi-Al	LYS195
		5.28923	Hyd	Pi-Al	LYS436
		4.66063	Hyd	Pi-Al	LYS195
		5.45125	Hyd	Pi-Al	VAL455
		4.31893	E	Pi-Ca	LYS195
		4.20106	E	Pi-Ca	ARG218
		3.55512	E	Pi-Ca	ARG218
		4.81104	E	Pi-An	ASP451
		2.61973	Hyd	Pi-Sg	ASP451
		4.95943	Other	Pi-S	MET298
D_3-A_4-D_3	-13.7	2.92539	Other	S-X	PHE134
		3.48753	E	Pi-Ca	ARG186
		4.4318	E	Pi-Ca	ARG186
		3.95074	E	Pi-An	GLU37
		2.57252	Hyd	Pi-Sg	ARG186
		5.95415	Other	Pi-S	MET123
		3.89595	Other	Pi-S	PHE134
		4.89832	Other	Pi-S	TYR161
		5.78891	Hyd	Pi-Pi-St	PHE134
		4.42812	Hyd	Pi-Pi-St	PHE134
		5.15912	Hyd	Pi-Al	LYS137
		4.7191	Hyd	Pi-Al	LYS137
		4.45427	Hyd	Pi-Al	PRO118
		4.76923	Hyd	Pi-Al	LEU115
		5.26777	Hyd	Pi-Al	LEU115
		4.53294	Hyd	Pi-Al	ARG186
		5.44799	Hyd	Pi-Al	ILE142
		4.5069	Hyd	Pi-Al	ARG186
		4.52713	Hyd	Pi-Al	ILE142
		4.84076	Hyd	Pi-Al	ALA126
		4.72545	Hyd	Pi-Al	LYS137
		4.05942	Hyd	Pi-Al	ALA126
		3.86608	Hyd	Pi-Al	ALA126

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-Al: Pi-Al, Pi-Pi T-Shaped: Pi-Pi T, Am-Pi-St, Pi-Pi Stacked: Pi-Pi-St, Pi-Sulfur: Pi-S, Pi-Sigma: Pi-Sg, Sulfur-X: S-X

Table S2. (*cont.*). Docking scores and interaction data of the studied ligands with HSA (PDB ID: 4L9Q)

Ligands	Docking Scores	Distance	Category	Type of Interactions	Residue Information
D_4-A_1-D_4	-12.6	4.27854	E	Pi-Ca	LYS195
		3.00074	HB; E	Pi-Ca; Pi-Do HB	LYS195
		4.92347	E	Pi-Ca	LYS444
		4.49514	E	Pi-An	GLU294
		4.47865	E	Pi-An	GLU294
		5.02834	Other	Pi-S	MET298
		5.12834	Hyd	Pi-Al	LYS444
		4.84859	Hyd	Pi-Al	LYS195
		4.51751	Hyd	Pi-Al	LYS195
		5.43266	Hyd	Pi-Al	VAL455
		4.63288	Hyd	Pi-Al	ALA191
		5.35586	Hyd	Pi-Al	LYS195
		5.26333	Hyd	Pi-Al	PRO339
		4.23449	Hyd	Pi-Al	PRO339
D_4-A_2-D_4	-12.9	4.2777	E	Pi-Ca	LYS195
		4.69492	E	Pi-Ca	ARG218
		3.53122	E	Pi-An	GLU294
		5.43298	Other	Pi-S	MET298:SD
		4.96243	Hyd	Pi-Pi T	TYR452
		5.17658	Hyd	Pi-Pi T	UNK1 - UNK1
		5.43298	Hyd	Pi-Al	LYS444
		4.92541	Hyd	Pi-Al	LYS444
		4.69058	Hyd	Pi-Al	LYS195
		5.22916	Hyd	Pi-Al	LYS444
		4.74401	Hyd	Pi-Al	PRO339
		4.1627	Hyd	Pi-Al	PRO339
D_4-A_3-D_4	-13.5	4.25027	E	Pi-Ca	LYS195
		4.27921	E	Pi-Ca	LYS195
		4.67228	E	Pi-Ca	ARG218
		4.4065	E	Pi-An	GLU294
		3.59632	E	Pi-An	GLU294
		5.02913	Hyd	Pi-Pi T	TYR452
		5.22111	Hyd	Pi-Al	LYS444
		4.91504	Hyd	Pi-Al	LYS444
		5.40181	Hyd	Pi-Al	PRO447
		4.78942	Hyd	Pi-Al	LYS195
		5.11503	Hyd	Pi-Al	LYS444
		4.56432	Hyd	Pi-Al	PRO339
		5.36107	Hyd	Pi-Al	MET298
		4.15669	Hyd	Pi-Al	PRO339

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-Al: Pi-Al, Pi-Pi T-Shaped: Pi-Pi T, Am-Pi-St, Pi-Pi Stacked: Pi-Pi-St, Pi-Sulfur: Pi-S, Pi-Sigma: Pi-Sg, Sulfur-X: S-X

Table S2. (*cont.*). Docking scores and interaction data of the studied ligands with HSA (PDB ID: 4L9Q)

Ligands	Docking Scores	Distance	Category	Type of Interactions	Residue Information
D_4-A_4-D_4	-13.1	4.64237	E	Pi-Ca	ARG218
		4.10682	E	Pi-An	GLU292
		3.65307	E	Pi-An	GLU292
		2.78592	Hyd	Pi-Sg	LYS195
		5.25121	Other	Pi-S	MET298
		5.32452	Hyd	Pi-Pi T	TYR452
		5.34658	Hyd	Pi-Al	LYS444
		5.22297	Hyd	Pi-Al	LYS444
		5.31352	Hyd	Pi-Al	PRO339
		4.93854	Hyd	Pi-Al	PRO339
		5.17976	Hyd	Pi-Al	LYS444
		5.06417	Hyd	Pi-Al	PRO339
		4.88176	Hyd	Pi-Al	ALA291
		4.90784	Hyd	Pi-Al	LYS436
D_5-A_1-D_5	-14.4	3.7174	E	Pi-Ca	ARG186
		3.37596	E	Pi-Ca	ARG186
		4.16379	E	Pi-Ca	ARG186
		4.78789	Hyd	Pi-Pi T	TYR138
		4.39917	Hyd	Pi-Al	PRO118
		4.91017	Hyd	Pi-Al	MET123
		5.12495	Hyd	Pi-Al	LEU115
		4.92303	Hyd	Pi-Al	VAL116
		4.7516	Hyd	Pi-Al	PRO118
		4.15614	Hyd	Pi-Al	ALA126
		4.01382	Hyd	Pi-Al	ALA126
		3.94796	Hyd	Pi-Al	LEU115
		5.48076	Hyd	Pi-Al	ARG117
		4.97149	Hyd	Pi-Al	LEU115
		5.46617	Hyd	Pi-Al	ILE142
		4.55144	Hyd	Pi-Al	ARG186
		5.37621	Hyd	Pi-Al	LEU182
		4.62062	Hyd	Pi-Al	LEU185
		5.22864	Hyd	Pi-Al	ARG186
		5.19354	Hyd	Pi-Al	ARG114
D_5-A_2-D_5	-14.0	3.95453	E	Pi-Ca	LYS195
		3.53461	E	Pi-Ca	ARG218
		4.27653	E	Pi-Ca	LYS274
		4.23036	E	Pi-Ca	LYS444
		2.93403	HB; E	Pi-Ca; Pi-Do HB	LYS444
		3.60448	E	Pi-An	GLU294
		4.64049	E	Pi-An	ASP451
		5.79221	Hyd	Pi-Pi T	UNK1 - UNK1
		5.45063	Hyd	Pi-Al	LYS444
		4.53031	Hyd	Pi-Al	PRO447
		4.33427	Hyd	Pi-Al	LYS195
		5.38476	Hyd	Pi-Al	VAL455
		4.7923	Hyd	Pi-Al	LYS195
		5.36439	Hyd	Pi-Al	ARG218
		4.77931	Hyd	Pi-Al	LYS436
		5.38798	Hyd	Pi-Al	PRO339
		4.26999	Hyd	Pi-Al	LYS444
		4.97418	Hyd	Pi-Al	PRO339
		5.46728	Hyd	Pi-Al	PRO339

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-Al: Pi-Al, Pi-Pi T-Shaped: Pi-Pi T, Am-Pi-St, Pi-Pi Stacked: Pi-Pi-St, Pi-Sulfur: Pi-S, Pi-Sigma: Pi-Sg, Sulfur-X: S-X

Table S2. (*cont.*). Docking scores and interaction data of the studied ligands with HSA (PDB ID: 4L9Q)

Ligands	Docking Scores	Distance	Category	Type of Interactions	Residue Information
D_5-A_3-D_5	-15.9	3.94745	E	Pi-Ca	ARG218
		3.2849	E	Pi-Ca	ARG218
		3.56898	E	Pi-Ca	ARG218
		4.15674	E	Pi-Ca	LYS274
		4.87886	E	Pi-Ca	LYS444
		4.13618	E	Pi-Ca	LYS444
		2.77412	HB; E	Pi-Ca; Pi-Do; HB	LYS444
		4.13244	E	Pi-An	GLU292
		4.3746	E	Pi-An	GLU292
		4.14727	E	Pi-An	GLU294
		3.45505	E	Pi-An	GLU294
		2.43452	Hyd	Pi-Sg	LYS444
		5.20925	Hyd	Pi-Al	PRO447
		4.10316	Hyd	Pi-Al	PRO447
		4.0703	Hyd	Pi-Al	ALA191
		4.30579	Hyd	Pi-Al	ALA191
		4.73594	Hyd	Pi-Al	LYS436
		4.23771	Hyd	Pi-Al	LYS444
		3.7819	Hyd	Pi-Al	LYS444
		5.20688	Hyd	Pi-Al	PRO441
		5.22938	Hyd	Pi-Al	LYS444
		5.20496	Hyd	Pi-Al	PRO339
D_5-A_4-D_5	-14.7	2.24815	HB	CHB	VAL116
		3.02928	Other	S-X	TYR161
		4.69	E	Pi-Ca	LYS137
		3.61579	E	Pi-Ca	ARG186
		3.23592	E	Pi-Ca	ARG186
		2.75397	Hyd	Pi-Sg	LYS137
		5.2637	Other	Pi-S	MET123
		5.45453	Other	Pi-S	TYR161
		5.44498	Hyd	Pi-Pi T	TYR138
		4.54616	Hyd	Am-Pi-St	LEU185, ARG186
		4.60499	Hyd	Am-Pi-St	LEU185, ARG186
		5.4475	Hyd	Pi-Al	LYS137
		4.71506	Hyd	Pi-Al	LEU115
		5.25628	Hyd	Pi-Al	VAL116
		4.57003	Hyd	Pi-Al	LYS137
		5.07207	Hyd	Pi-Al	LEU182
		5.01805	Hyd	Pi-Al	LEU115
		4.92247	Hyd	Pi-Al	LEU182
		5.49834	Hyd	Pi-Al	LEU185
		4.79374	Hyd	Pi-Al	ARG186
		5.30738	Hyd	Pi-Al	ILE142
		3.8833	Hyd	Pi-Al	ARG186
		4.86894	Hyd	Pi-Al	ILE142
		4.22524	Hyd	Pi-Al	ARG186
		5.47436	Hyd	Pi-Al	LYS190
		5.2754	Hyd	Pi-Al	LYS137
		5.39769	Hyd	Pi-Al	VAL122
		4.68647	Hyd	Pi-Al	ALA126

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-Al: Pi-Al, Pi-Pi T-Shaped: Pi-Pi T, Am-Pi-St, Pi-Pi Stacked: Pi-Pi-St, Pi-Sulfur: Pi-S, Pi-Sigma: Pi-Sg, Sulfur-X: S-X

Figure S6. Binding poses and residue interactions of the investigated ligands with HSA (PDB ID: 4L9Q)

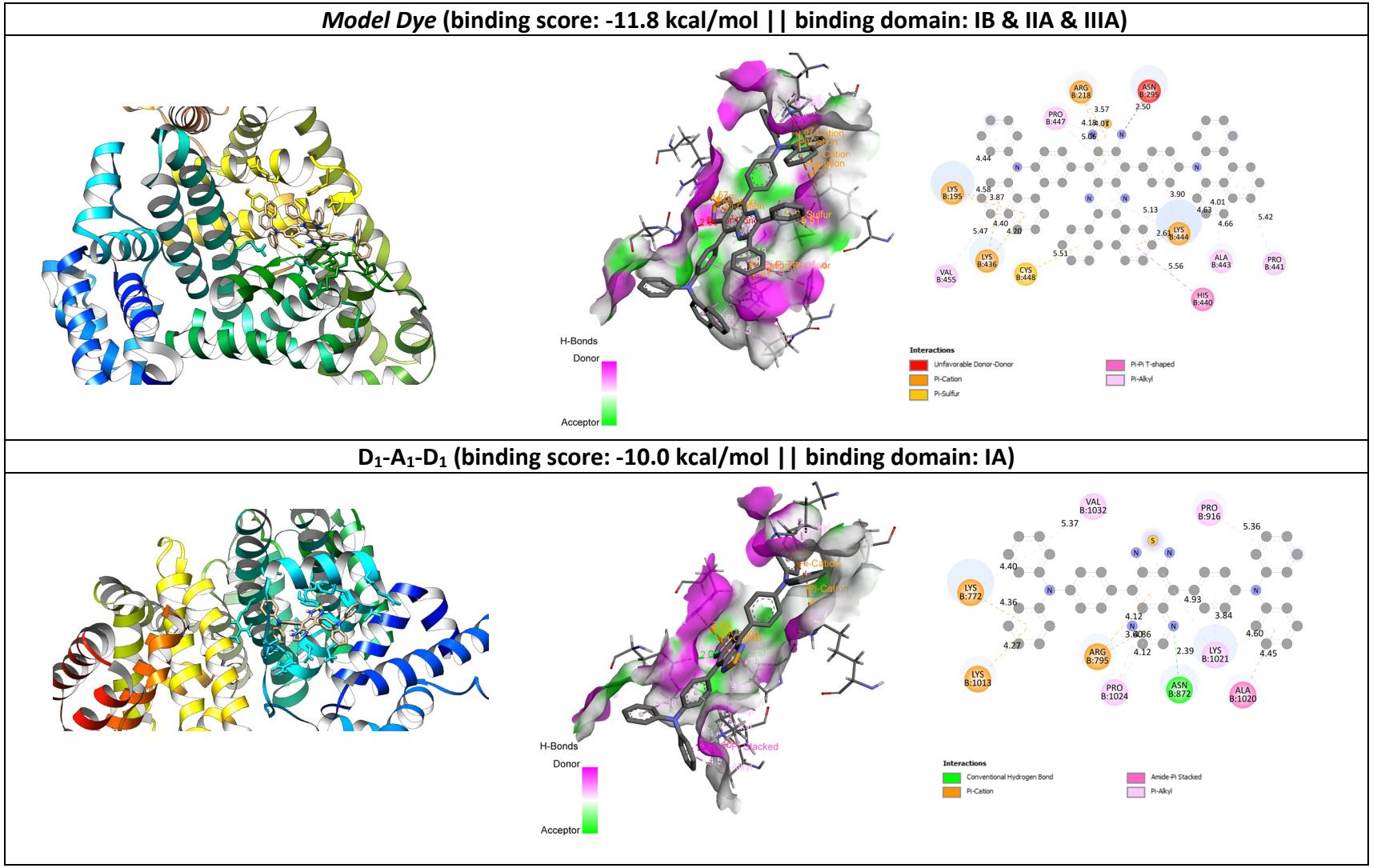
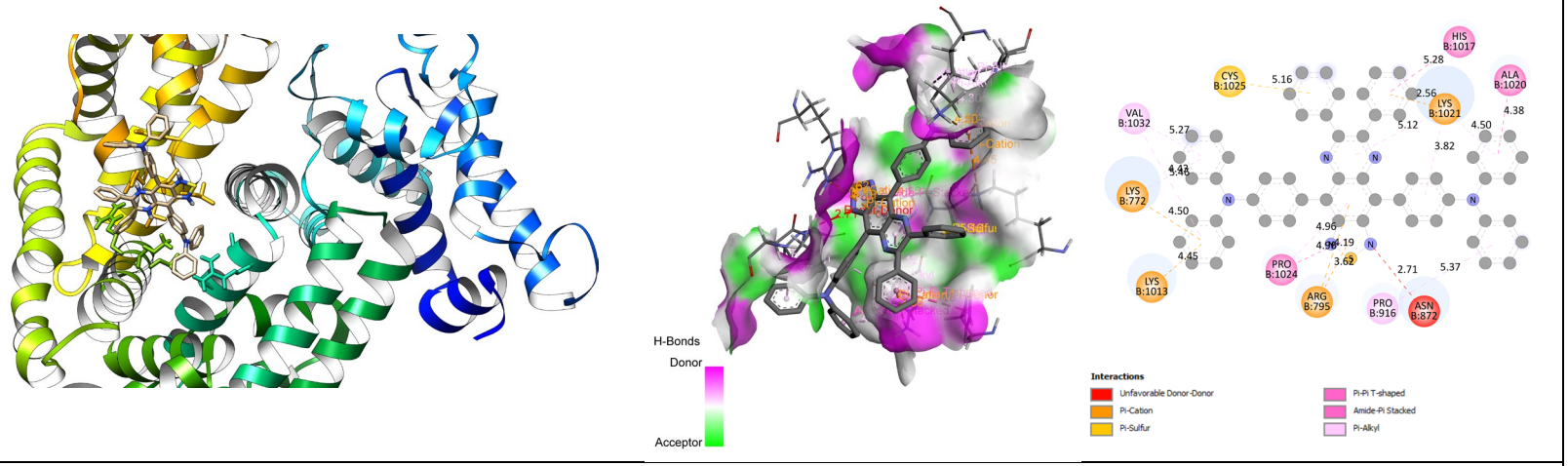


Figure S6. (*cont.*). Binding poses and residue interactions of the investigated ligands with HSA (PDB ID: 4L9Q)

D_1-A_2-D_1 (binding score: -12.6 kcal/mol || binding domain: IIB & IIIA)



D_1-A_3-D_1 (binding score: -12.7 kcal/mol || binding domain: IB & IIA & IIIA)

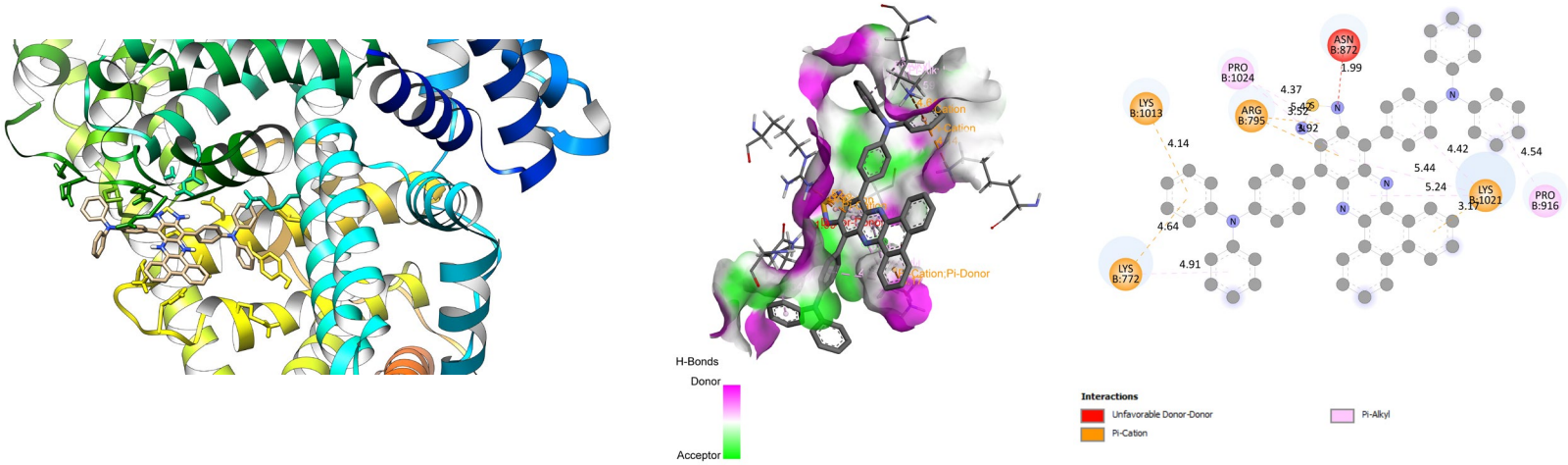
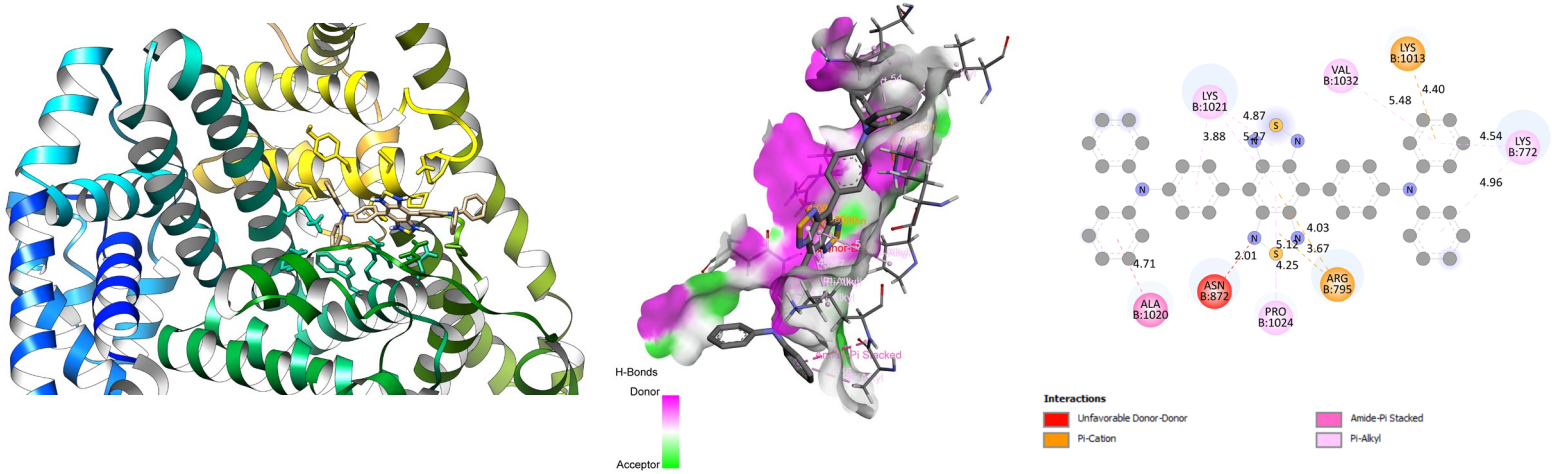


Figure S6. (*cont.*). Binding poses and residue interactions of the investigated ligands with HSA (PDB ID: 4L9Q)

D_1-A_4-D_1 (binding score: -10.1 kcal/mol || binding domain: IIA & IIIA)



D_2-A_1-D_2 (binding score: -12.3 kcal/mol || binding domain: IB)

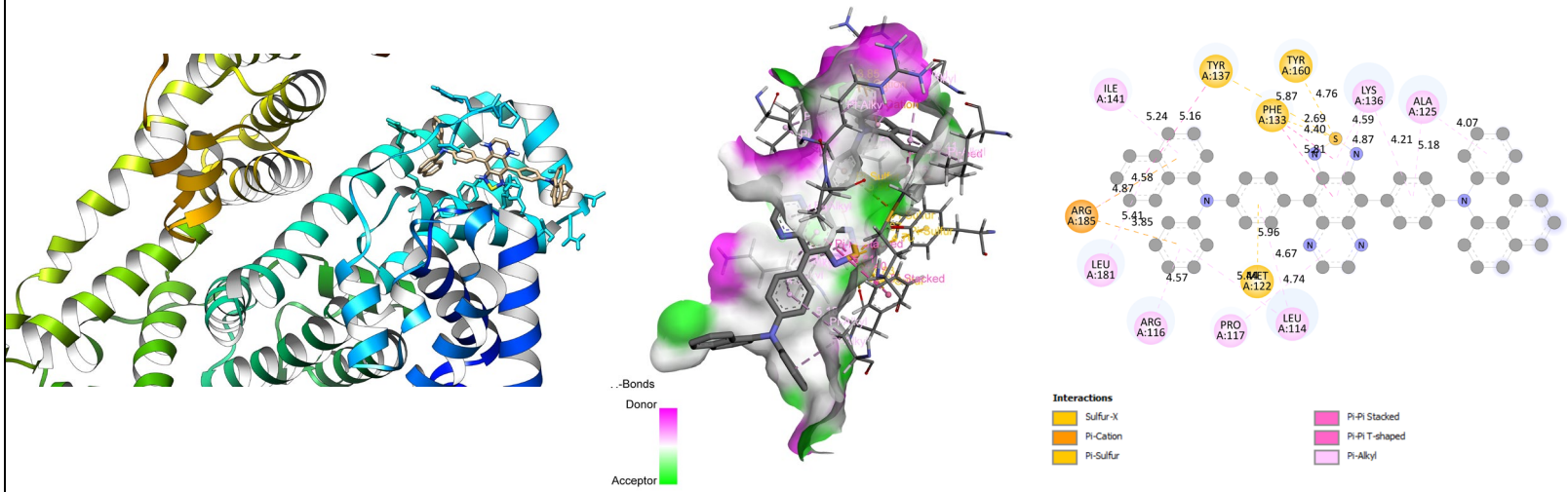
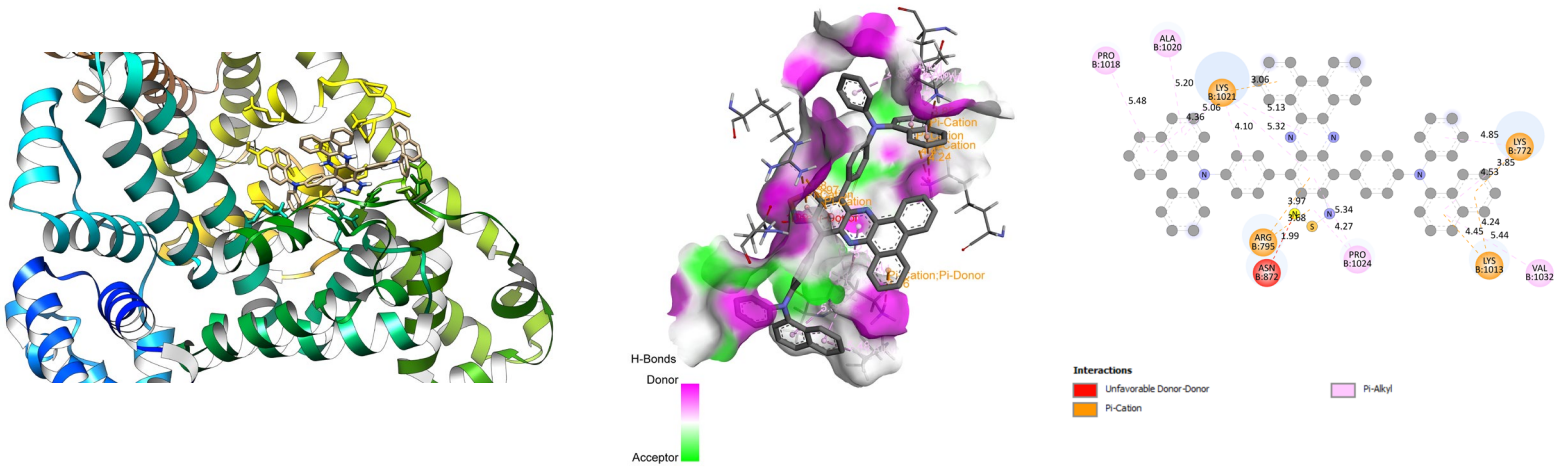


Figure S6. (*cont.*). Binding poses and residue interactions of the investigated ligands with HSA (PDB ID: 4L9Q)

D_2-A_3-D_2 (binding score: -12.8 kcal/mol || binding domain: IB & IIA & IIIA)



D_2-A_4-D_2 (binding score: -12.3 kcal/mol || binding domain: IA & IB)

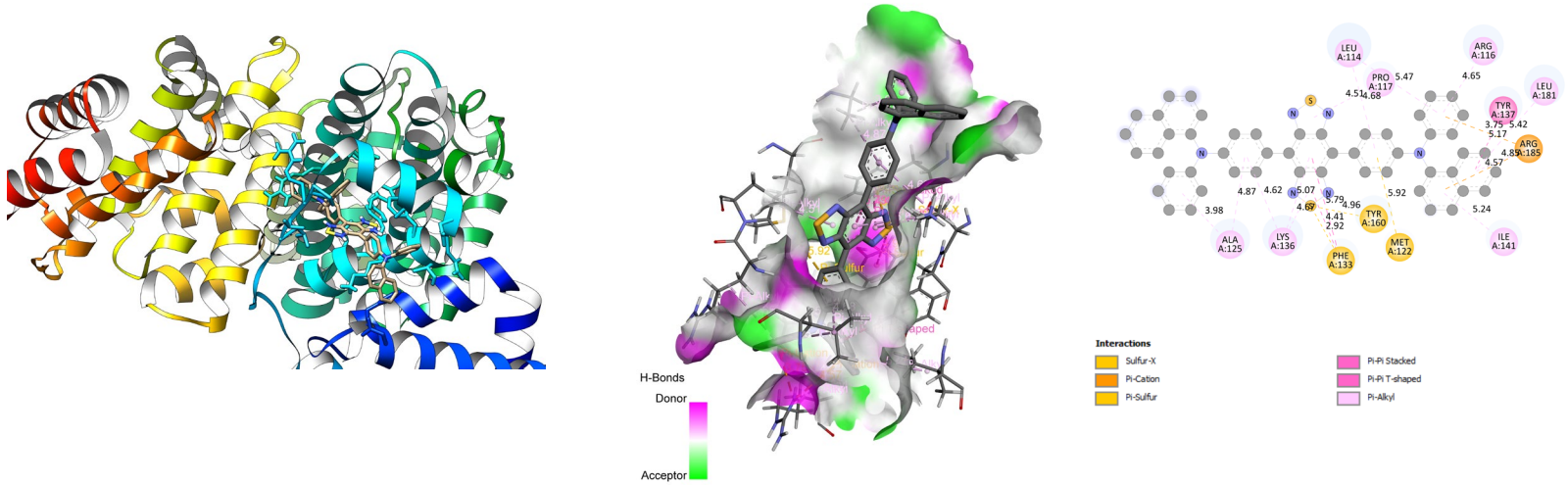
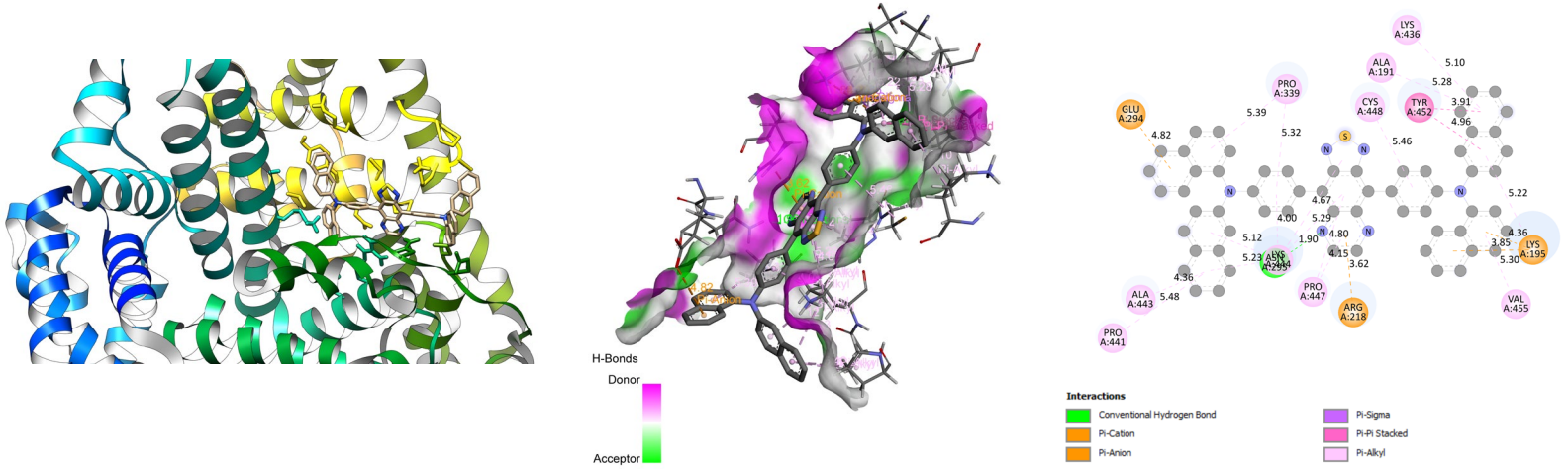


Figure S6. (*cont.*). Binding poses and residue interactions of the investigated ligands with HSA (PDB ID: 4L9Q)

D_3-A_1-D_3 (binding score: -13.9 kcal/mol || binding domain: IB & IIA & IIIA)



D_3-A_2-D_3 (binding score: -13.2 kcal/mol || binding domain: IB & IIA & IIIA)

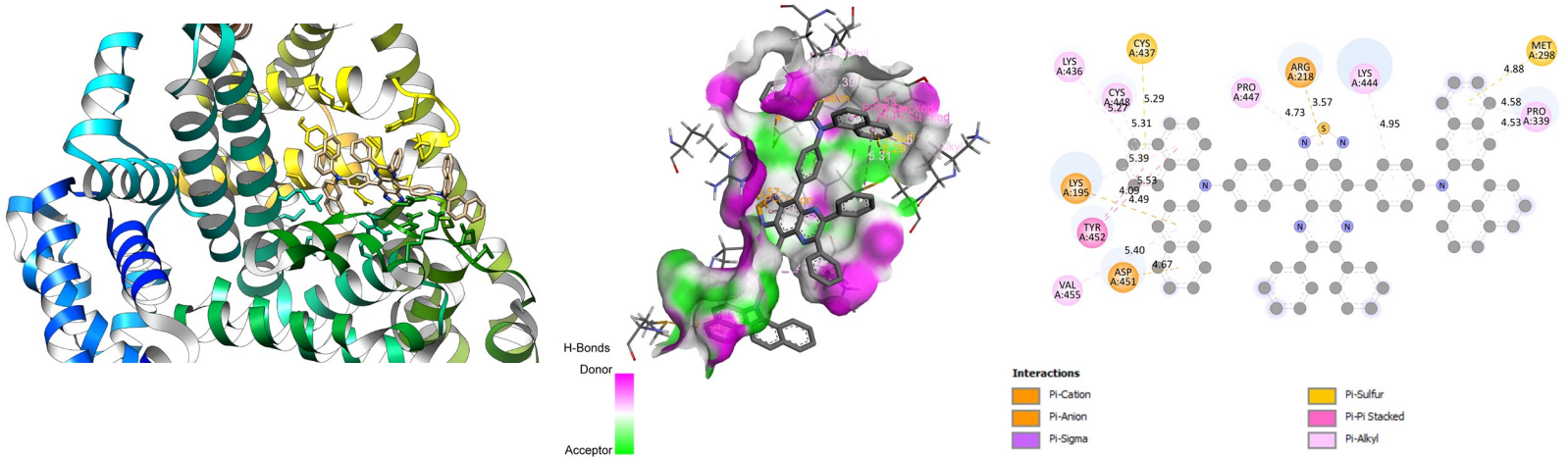


Figure S6. (*cont.*). Binding poses and residue interactions of the investigated ligands with HSA (PDB ID: 4L9Q)

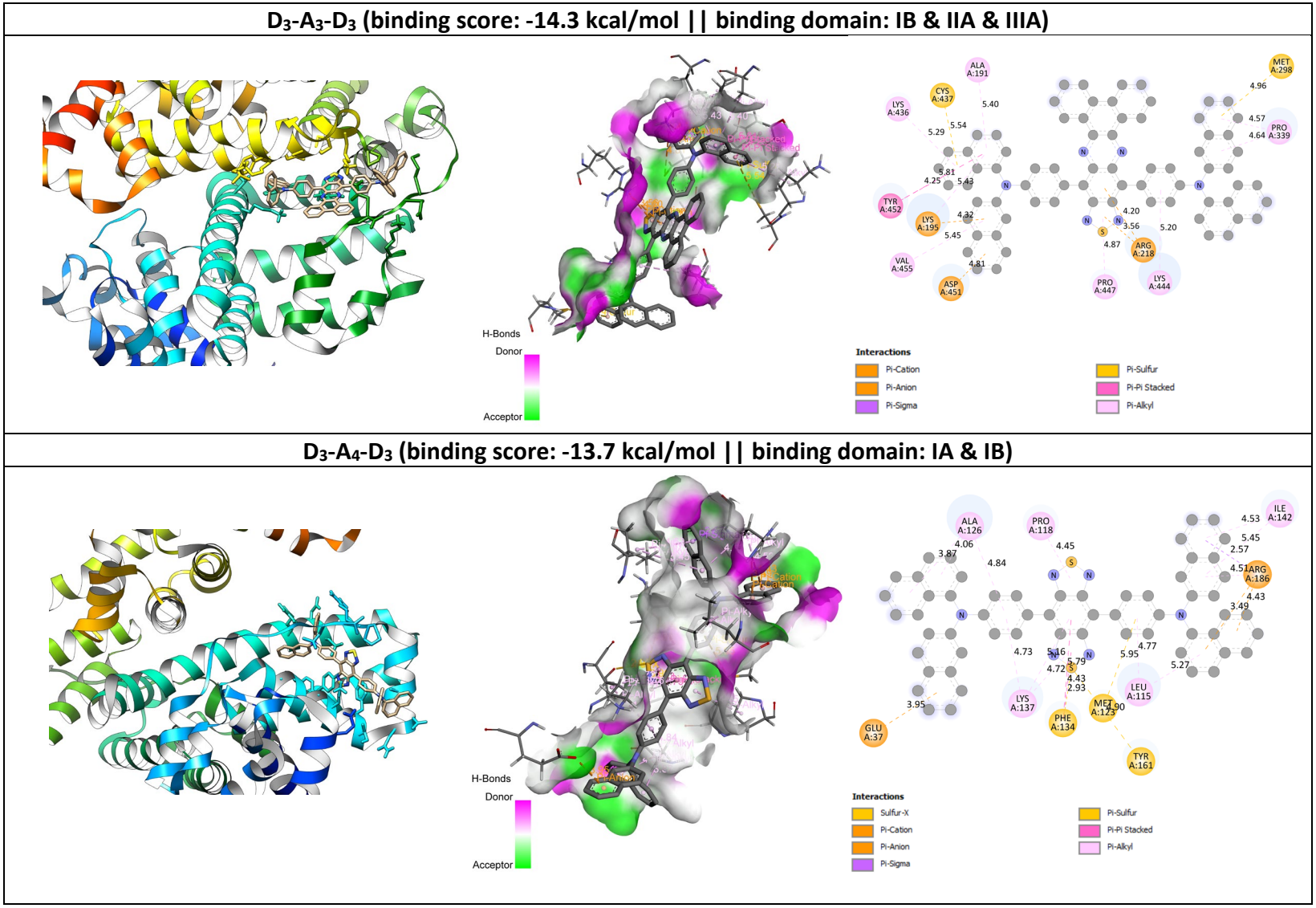
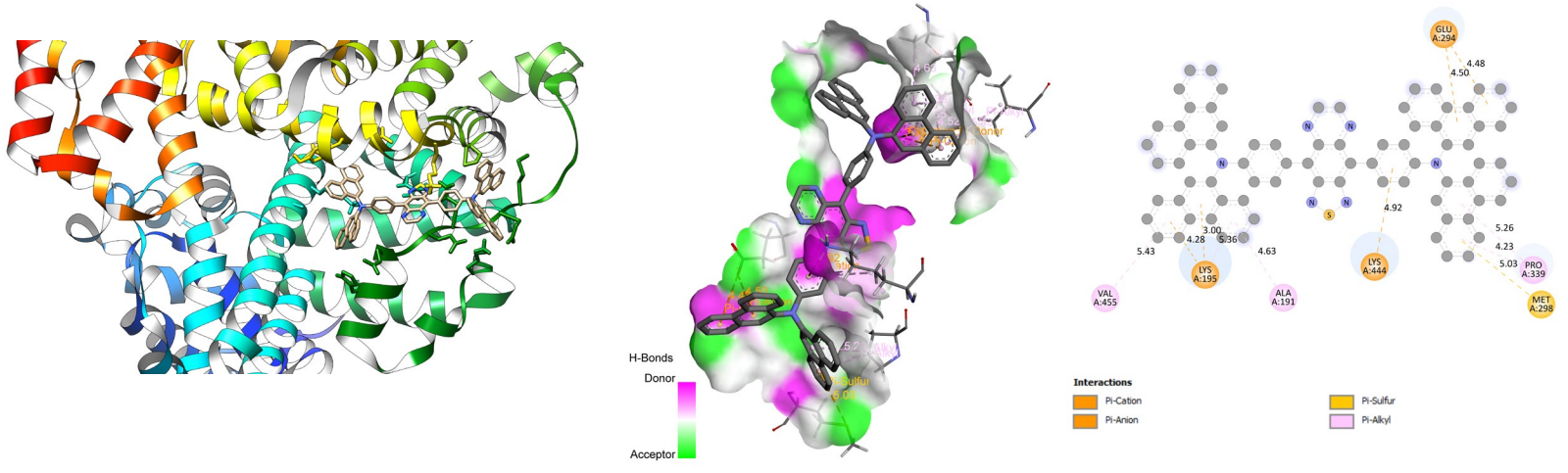


Figure S6. (*cont.*). Binding poses and residue interactions of the investigated ligands with HSA (PDB ID: 4L9Q)

D_4-A_1-D_4 (binding score: -12.6 kcal/mol || binding domain: IB & IIA & IIIA)



D_4-A_2-D_4 (binding score: -12.9 kcal/mol || binding domain: IB & IIA & IIIA)

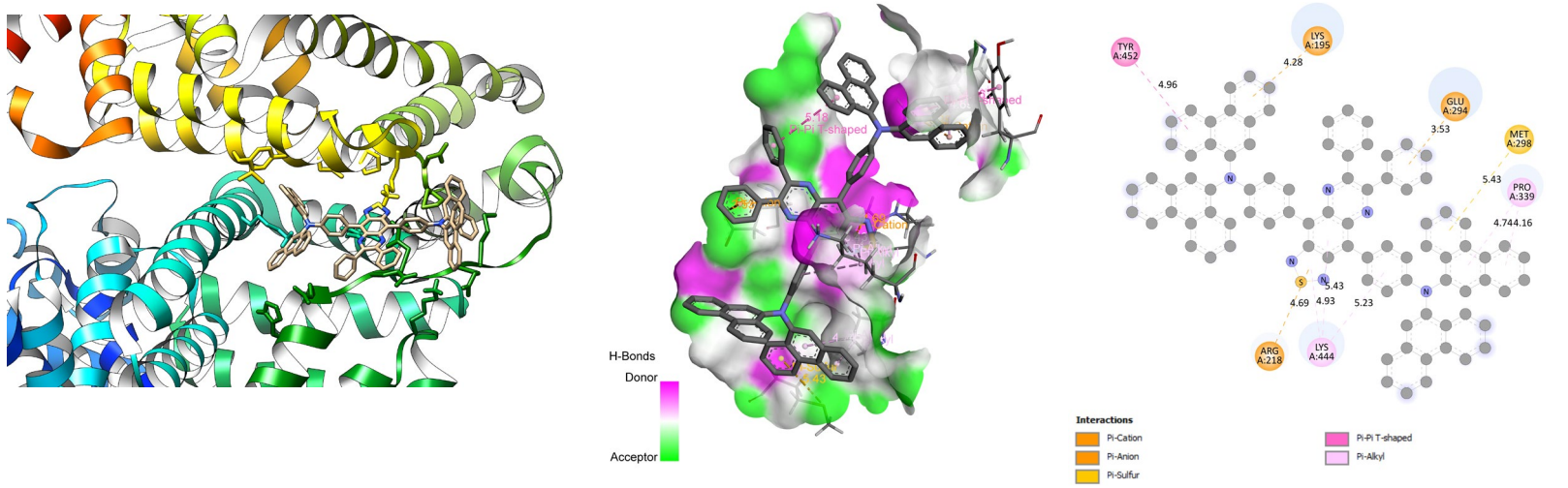


Figure S6. (*cont.*). Binding poses and residue interactions of the investigated ligands with HSA (PDB ID: 4L9Q)

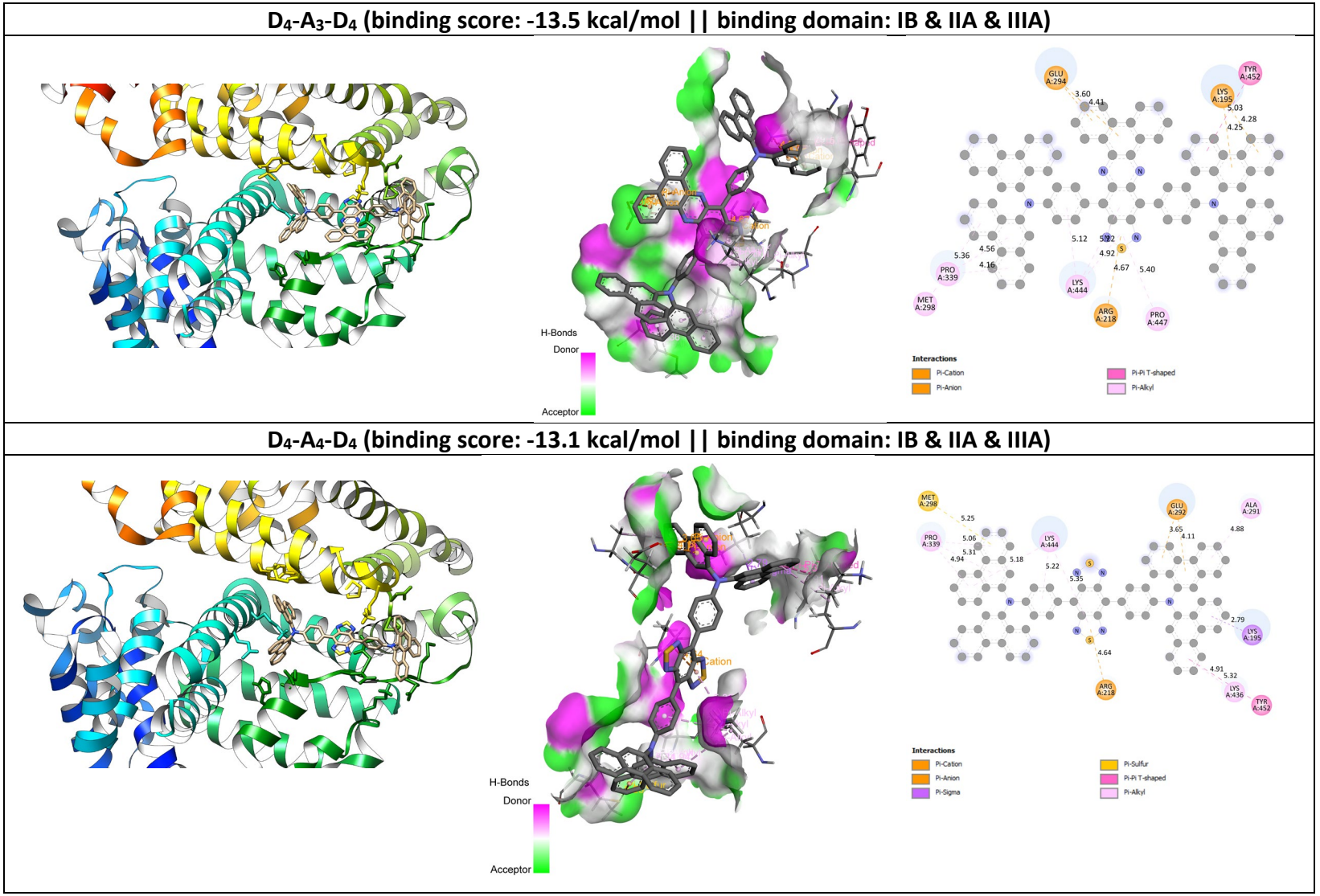


Figure S6. (*cont.*). Binding poses and residue interactions of the investigated ligands with HSA (PDB ID: 4L9Q)

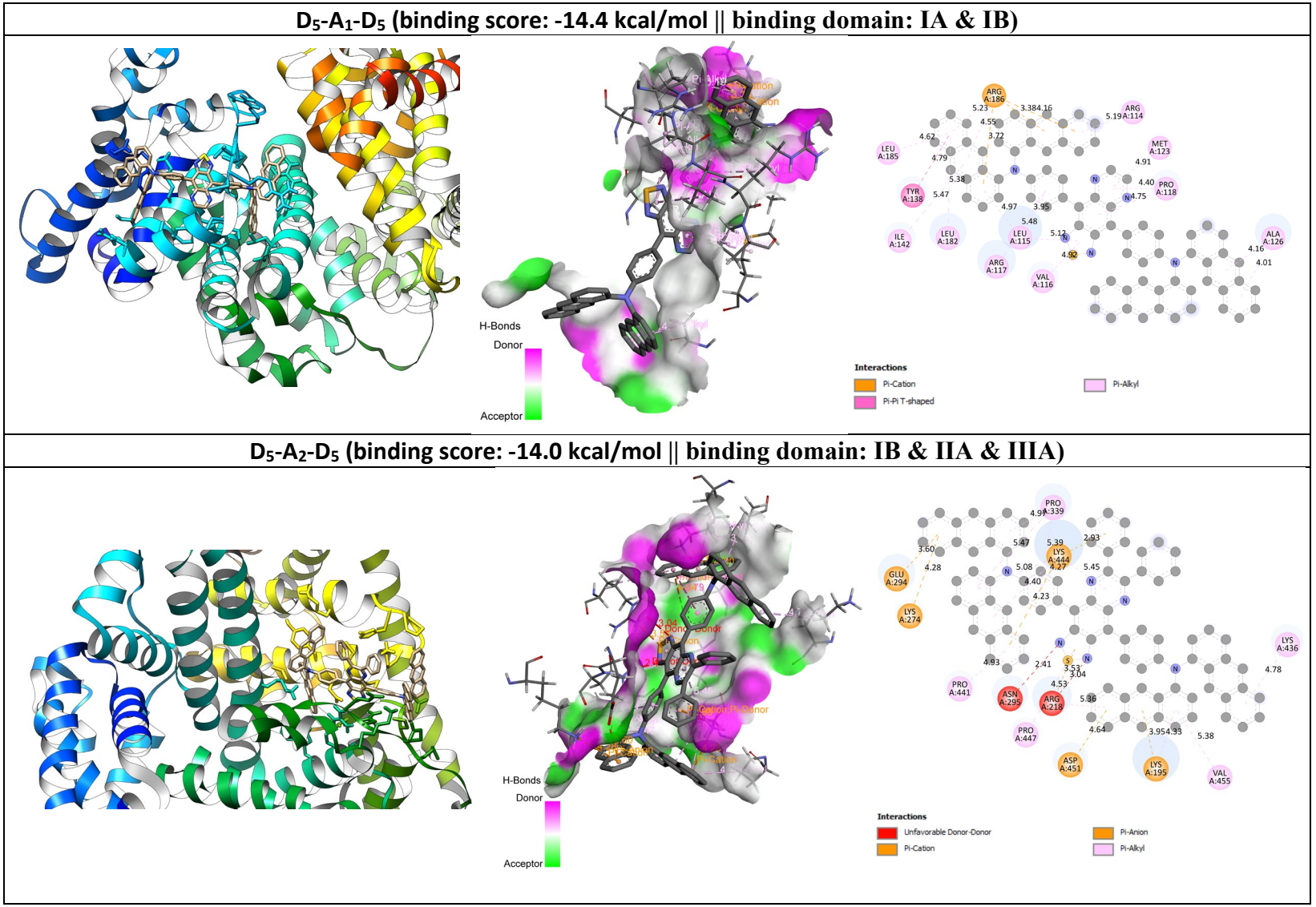


Figure S6. (*cont.*). Binding poses and residue interactions of the investigated ligands with HSA (PDB ID: 4L9Q)

D_5-A_4-D_5 (binding score: -14.7 kcal/mol || binding domain: IA & IB)