

Table S1. The distances between docked acetylenic sulfamoylquinoline derivatives and heme-iron center in active sites of CYP1A1 (PDB ID: 4I8V) and CYP1B1 (PDB ID: 3PM0).

Compound	CYP1A1		CYP1B1	
	Ligand Group	Closest Atom Distance to Fe (Å)	Ligand Group	Closest Atom Distance to Fe (Å)
2a	sulfamoyl	3.34	sulfamoyl	3.11
2b	sulfamoyl	3.18	sulfamoyl	3.52
2c	sulfamoyl	3.50	sulfamoyl	3.50
2d	sulfamoyl	3.61	sulfamoyl	3.53
2e	sulfamoyl	3.29	sulfamoyl	3.30
2f	sulfamoyl	3.02	sulfamoyl	3.46
5a	sulfamoyl	3.58	sulfamoyl	4.02
5b	thiopropargyl	3.64	thiopropargyl	3.94
5c	sulfamoyl	3.15	sulfamoyl	3.43
5d	sulfamoyl	4.43	sulfamoyl	3.36
5e	thiopropargyl	4.33	thiopropargyl	4.28
5f	thiopropargyl	3.19	sulfamoyl	3.56
6a	selenopropargyl	4.18	sulfamoyl	4.10
6b	sulfamoyl	3.36	sulfamoyl	3.48
6c	sulfamoyl	3.22	sulfamoyl	4.10
6d	sulfamoyl	3.05	sulfamoyl	3.41
6e	sulfamoyl	4.02	sulfamoyl	3.49
6f	sulfamoyl	2.92	sulfamoyl	3.48
11	quinoline moiety	3.68	thiopropargyl	4.33
12	sulfamoyl	3.01	sulfamoyl	3.39
13	sulfamoyl	3.38	sulfamoyl	3.54

Table S2. Amino acid residues of CYP1A1 (PDB ID: 4I8V) which formed a favorable interactions with acetylenic sulfamoylquinolines during docking simulation.

Ligand	Hydrophobic interactions					Hydrogen bonds		Others		
	π - π Stacked	π - π T-shaped	Amide- π Stacked	π -Alkyl	π -Sigma	Alkyl	Classic	Carbon	π -Sulfur	Halogen
2a	Phe224(2x)	no contact	Leu312/Asp313, Gly316/Ala317	Phe224, Ala317	no contact	Val382, Leu496	no contact	no contact	Phe123	no contact
2b	Phe224(2x)	no contact	Gly316/Ala317(2x)	Phe224, Phe258, Ala317(2x), Phe319	no contact	Val382, Le386, Leu496	no contact	no contact	no contact	no contact
2c	Phe224(2x)	no contact	Gly316/Ala317(2x)	Phe224, Leu312, Ala317	Gly316	Val382, Leu496	no contact	Ala317	Phe123	no contact
2d	Phe224(2x)	Phe258	Gly316/Ala317(2x)	Phe224, Leu312, Ala317, Phe319	Gly316	Val382, Leu496	no contact	Asp313, Ala317	Phe123	no contact
2e	Phe224(2x)	no contact	Gly316/Ala317(2x)	Phe224, Ala317(2x), Phe319	no contact	Val382, Le386, Leu496	no contact	Ala317	no contact	no contact
2f	Phe224(2x)	no contact	Gly316/Ala317(2x)	Phe224, Ala317(2x)	Phe123	Val382, Leu496	no contact	no contact	no contact	no contact
5a	Phe224(2x)	no contact	Gly316/Ala317(2x)	Ala317	no contact	Leu312, Val382, Leu496	no contact	Ser122	Phe123	no contact
5b	Phe224	Phe123(2x)	Gly316/Ala317	Phe224, Phe258, Ala317, Phe319	Phe123, Ala317	Val382, Leu496	no contact	Leu312	no contact	no contact
5c	Phe224(2x)	no contact	Gly316/Ala317(2x)	Ala317	no contact	Ile115, Leu312, Val382, Ile386, Leu496	no contact	no contact	Phe123	no contact
5d	Phe224(2x)	Phe258	Gly316/Ala317(2x)	Phe123	no contact	Ala317, Val382, Ile386, Leu496	no contact	Ala317	Phe123	no contact
5e	Phe224(2x)	Phe123(2x)	Gly316/Ala317	Phe224, Phe258, Ala317, Phe319	Phe123, Ala317	Val382	no contact	Leu312	no contact	no contact
5f	Phe224	Phe123(2x)	Gly316/Ala317	Phe258, Ala317	Ala317	Leu312, Val382	no contact	no contact	Phe123	no contact
6a	Phe224(2x)	Phe258	Gly316/Ala317	Phe123, Ala317	no contact	Ile115, Val382, Leu496	Thr321	no contact	no contact	no contact
6b	Phe224(2x)	no contact	Gly316/Ala317(2x)	Phe224, Phe258, Ala317, Phe319	no contact	Val382, Leu496	no contact	no contact	Phe123	no contact
6c	Phe224	Phe123(2x)	Gly316/Ala317(2x)	Phe224, Ala317	Phe123, Ala317	Val382, Leu496(2x)	no contact	no contact	no contact	no contact
6d	Phe224(2x)	no contact	Gly316/Ala317(2x)	Phe258, Ala317	no contact	Leu312, Val382, Leu496	no contact	no contact	no contact	no contact
6e	Phe224(2x)	Phe123	Gly316/Ala317	Ile115, Phe224, Leu312, Ala317, Phe319	Phe123	Leu496	Ser122	no contact	no contact	no contact
6f	Phe224(2x)	no contact	Gly316/Ala317(2x)	Phe258, Ala317(2x)	no contact	Leu312, Val382	no contact	no contact	no contact	no contact
11	Phe224	Phe123(2x)	Gly316/Ala317	Phe224, Phe258, Ala317, Phe319	Phe123, Ala317	Leu254, Val382	Ser122	no contact	Phe224	no contact
12	Phe224(2x)	no contact	Gly316/Ala317(2x)	Phe123, Ala317	no contact	Ile115, Val382	no contact	Gly316, Leu312(2x), Asn225	Phe258	no contact
13	Phe224(2x)	Phe123	Gly316/Ala317(2x)	Phe224, Phe258, Ala317	Ala317	Val382	no contact	no contact	no contact	no contact

Table S3. Amino acid residues of CYP1A1 (PDB ID: 3PM0) which formed a favorable interactions witch acetylenic sulfamoylquinolines during docking simulation.

Ligand	Hydrophobic interactions					Hydrogen bonds		Others		
	π - π Stacked	π - π T-Shaped	Amide- π STACKED	π -Alkyl	π -Sigma	Alkyl	Classic	Carbon	π -Sulfur	Halogen
2a	Phe231(2x)	no contact	Gly329/Ala330(2x)	Phe231, Ala330(2x)	no contact	Val395, Ile399, Leu509(2x)	no contact	no contact	no contact	Asp333
2b	Phe231(2x)	Phe134	Gly329/Ala330(2x)	Ala133, Phe268	Ala330	Val395, Leu509	no contact	no contact	no contact	no contact
2c	Phe231(2x)	no contact	Gly329/Ala330(2x)	Phe231, Ala330	no contact	Val395, Leu509	no contact	Asp326, Ala330	Phe134	Asp333
2d	Phe231(2x)	no contact	Gly329/Ala330(2x)	Phe231, Ala330	no contact	Val395, Leu509	no contact	no contact	Phe134	no contact
2e	Phe231(2x)	no contact	Gly329/Ala330(2x)	Phe231, Ala330(2x)	no contact	Val395, Ile399, Leu509	no contact	no contact	no contact	no contact
2f	Phe231(2x)	no contact	Gly329/Ala330(2x)	Phe231, Phe268, Ala330(2x)	no contact	Val395, Leu509	no contact	no contact	Phe134	no contact
5a	Phe231(2x)	Phe268	Gly329/Ala330(2x)	Ala330	no contact	Val126, Val395, Leu509	no contact	Gln332, Asp333	Phe134(2x)	no contact
5b	Phe231	Phe134(2x)	Gly329/Ala330(2x)	Ala133, Phe231, Ala330	Ala330	Val395, Leu509	no contact	Asn265, Gly329	no contact	no contact
5c	Phe231(2x)	no contact	Gly329/Ala330(2x)	Ala330	no contact	Val126, Val395, Ile399, Leu509	no contact	no contact	Phe134	no contact
5d	Phe231	Phe134	Gly329/Ala330(2x)	Ala133, Phe231, Phe268, Ala330	Ala330	Leu264, Val395, Leu509	no contact	Asp326, Ala330, Asp333	Phe134	no contact
5e	Phe231	Phe134	Gly329/Ala330(2x)	Ala133, Phe231, Ala330	Ala330	Val395, Leu509	no contact	Asn265, Gly329	Phe134	no contact
5f	Phe231(2x)	no contact	Gly329/Ala330(2x)	Ala330(2x)	no contact	Val126, Val395, Ile399, Leu509	no contact	Asp326	Phe134, Phe268	no contact
6a	Phe231(2x)	Phe268	Gly329/Ala330(2x)	Ala330(2x)	no contact	Ala133, Ala330, Val395, Leu509	no contact	Gln332, Asp333	Phe134(2x)	no contact
6b	Phe231(2x)	no contact	Gly329/Ala330(2x)	Val126, Phe231, Ala330	no contact	Leu264, Val395, Ile399, Leu509	no contact	no contact	Phe134	no contact
6c	Phe231(2x)	Phe268	Gly329/Ala330(2x)	Ala330	no contact	Ala133, Ala330, Val395, Leu509	no contact	no contact	Phe134	no contact
6d	Phe231(2x)	no contact	Gly329/Ala330(2x)	Phe231, Phe268, Ala330	no contact	Leu264, Val395, Leu509	no contact	Asp326	Phe134	no contact
6e	Phe231(2x)	no contact	Gly329/Ala330(2x)	Val126, Phe231, Ala330	no contact	Ala133, Leu264, Ala330	no contact	Asn228, Asp326	Phe134	no contact
6f	Phe231(2x)	no contact	Gly329/Ala330(2x)	Ala133, Phe231, Phe268, Ala330(2x)	no contact	Leu264, Val395, Leu509	no contact	no contact	Phe134	no contact
11	no contact	Phe134	Gly329/Ala330	Ala133(2x), Phe231, Phe268	Ala330(2x)	Val395, Ile399, Leu509	no contact	Asp326	Phe134	no contact
12	Phe231(2x)	Phe134(2x)	Gly329/Ala330	Ala133, Phe231, Ala330	Ala330	Val395, Ile399, Leu509	no contact	Asn265, Asp326(2x), Gly329	no contact	no contact
13	Phe231	Phe134	Gly329/Ala330(2x)	Ala133, Phe231, Phe268	Ala330	Leu264, Val395, Leu509	no contact	Asp326	no contact	no contact