SUPPORTING INFORMATION

Identification of Ligand Templates using Local Structure Alignment for Structure-based Drug Design

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Table S1. Structure information of the benchmark set and the best template ligand identified by G-LoSA. The best template was determined in terms of the best overlap ratio value among top 10 template ligands.

PDB ID	chain	ligand	best template	PDB ID	chain	ligand	best template
1GKC	A	BUM	2W15	1Q41	A	IXM	1V0O
1GPK	A	HUP	2DLC	1Q4G	A	BFL	1P3T
1HNN	A	SKF	3GE7	1R1H	A	BIR	1U4G
1HP0	A	AD3	3G5I	1R55	A	097	2I47
1HQ2	A	PH2	3DS6	1R58	A	AO5	1QXZ
1HVY	A	D16	2GQU	1R9O	A	FLP	1TDG
1HWW	A	SWA	2WYI	1S19	A	MC9	3GWX
1IA1	A	TQ3	2BLC	1S3V	A	TQD	3FQV
1IG3	A	VIB	3LM8	1SJ0	A	E4D	2W8Y
1J3J	A	CP6	3QLZ	1SQ5	A	PAU	2F3E
1JD0	A	AZM	3BXU	1SQN	A	NDR	2GPV
1JJE	A	BYS	1X8I	1T40	A	ID5	3HB6
1JLA	A	TNK	2A0C	1T46	A	STI	3HEC
1K3U	A	IAD	1WXJ	1TOW	A	CRZ	1EP3
1KE5	A	LS1	2GDO	1TT1	A	KAI	3OEN
1L2S	A	STC	3HUO	1U4D	A	DBQ	1ZLT
1L7F	A	BCZ	2F10	1UML	A	FR4	2PGR
1LPZ	B	CMB	2PKS	1UNL	A	RRC	3H9F
1LRH	A	NLA	1H1M	1UOU	A	CMU	2WIY
1M2Z	A	DEX	3HM1	1V0P	A	PVB	2F57
1MEH	A	MOA	1H7W	1V48	A	HA1	1ODI
1MMV	A	3AR	2CU0	1V4S	A	MRK	2ZT9
1MZC	B	BNE	3HXF	1VCJ	A	IBA	1L7H
1N1M	A	A3M	3IUQ	1W1P	A	GIO	2A3A
1N2J	A	PAF	3GUZ	1W2G	A	THM	1TMK
1N2V	A	BDI	1IT8	1X8X	A	TYR	2DLC
1N46	A	PFA	3FAL	1XM6	A	5RM	1UDT
1NAV	A	IH5	3FAL	1XOQ	A	ROF	2H44
1OF1	A	SCT	2VQS	1XOZ	A	CIA	1BGP
1OF6	A	DTY	3KW2	1Y6B	A	AAX	1PMQ
1OPK	A	P16	3EQR	1YGC	H	905	2PKS
1OQ5	A	CEL	1X8O	1YQY	A	915	2A8H
1OWE	A	675	1T32	1YV3	A	BIT	2WOV
1OYT	H	FSN	8GCH	1YVF	A	PH7	3BEN
1P2Y	A	NCT	3DOG	1YWR	A	LI9	2WOT
1P62	B	GEO	2JAQ	1Z95	A	198	2QH6
1PMN	A	984	3POZ	2BR1	A	PFP	3K5U
1Q1G	A	MTI	3DF9	2BSM	A	BSM	2ZDX