

Supplementary Table 1

Interaction matchprints for 42 known thrombin inhibitors, labeled by PDB code, followed by the five new inhibitors from SLIDE screening, labeled by ZINC code. Interactions are highlighted in grey, showing the number of ligand interactions with the corresponding thrombin atom (for polar interactions) or side chain (for hydrophobic interactions).

LIGAND	PHE 40 sc	LEU 41 sc	CYS 42 sc	HIS 57 NE2	HIS 57 sc	CYS 58 sc	TYR 60A sc	TRP 60D sc	LYS 60F NZ	LYS 60F sc	LEU 99 sc	GLU 146 sc	ILE 174 sc	ASP 189 OD1	ASP 189 OD2	ALA 190 O	ALA 190 sc	CYS 191 O	CYS 191 sc	GLU 192 OE2	GLU 192 sc	GLY 193 N	SER 195 N	VAL 213 sc	SER 214 O	TRP 215 sc	GLY 216 N	GLY 216 O	GLU 217 OE2	GLU 217 sc	GLY 219 N	GLY 219 O	CYS 220 sc		
1a3b	0	0	0	1	1	0	3	3	0	0	4	0	1	1	1	1	1	0	0	0	0	1	1	1	1	5	1	1	0	0	0	1	0		
1a46	0	0	1	1	0	0	2	3	0	0	1	0	1	0	0	1	1	0	0	0	0	1	1	0	0	4	1	1	0	1	0	0	1	1	
1a4w	0	0	0	0	0	0	2	5	1	0	4	0	2	1	0	1	1	0	0	0	0	0	0	0	3	1	1	0	1	0	0	0	1		
1a5g	1	0	0	1	1	0	3	3	0	0	4	0	1	2	2	0	1	0	0	0	2	1	1	1	0	3	1	1	0	0	0	0	1	0	
1a61	0	0	1	1	0	0	2	3	0	0	4	0	1	2	1	1	1	0	0	0	0	1	0	1	0	3	1	1	0	0	0	0	1	0	
1abj	0	0	0	0	0	0	3	3	0	0	4	0	1	2	2	1	1	0	0	0	0	0	0	1	1	3	1	1	0	0	0	0	1	0	
1ae8	0	0	0	0	0	0	2	2	0	0	4	0	1	0	1	1	1	0	0	0	0	0	0	0	1	5	1	1	0	0	0	0	1	1	
1afe	0	0	0	0	0	0	3	3	0	0	1	0	2	0	0	1	1	0	0	0	0	0	0	0	1	2	1	0	0	2	0	1	2		
1awf	0	0	0	1	0	0	1	5	0	0	1	0	0	0	0	0	1	0	0	0	0	1	1	1	0	1	1	1	0	1	0	0	1		
1awh	0	0	0	0	0	0	0	4	0	0	1	0	0	0	0	0	1	0	0	0	0	1	1	1	0	1	0	0	0	0	0	0	0	1	
1ay6	0	0	0	0	1	0	4	4	0	0	4	0	1	2	2	0	1	0	0	0	0	1	1	1	1	4	1	0	0	1	0	1	0		
1b5g	0	0	1	0	1	0	2	4	0	1	1	0	0	2	2	0	1	0	0	0	0	1	1	1	0	1	1	1	0	2	0	1	0		
1ba8	0	0	0	0	0	0	1	3	0	0	3	0	2	1	1	0	1	0	0	0	0	1	1	1	1	5	0	0	0	1	0	1	0		
1bb0	0	0	0	0	0	0	2	3	0	0	2	0	2	1	1	0	0	0	0	0	0	1	1	1	1	5	0	0	0	1	0	1	1		
1bcu	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	1	2	0	0	1	0	0	0	0	0	0	0	0	0	1	
1bhx	0	0	0	0	1	0	1	3	0	0	2	0	2	1	1	1	1	0	0	0	0	0	0	1	0	5	1	0	0	1	0	1	0		
1bmm	0	0	0	0	0	0	2	5	0	0	4	0	1	1	1	0	1	0	0	0	0	0	0	0	1	5	1	0	0	0	0	0	1	0	
1bmn	0	0	0	0	0	0	3	4	0	0	4	0	2	0	0	1	1	0	0	0	0	0	0	1	1	6	1	0	0	1	0	2	1		
1ca8	0	0	0	1	0	0	2	2	0	0	2	0	2	1	1	0	0	0	0	0	0	0	0	1	1	5	1	0	0	1	0	1	1		
1dwc	0	0	0	0	0	0	3	5	0	0	1	0	1	1	0	0	1	0	0	0	0	0	0	0	0	5	1	1	0	0	0	0	1	1	
1dwd	0	0	0	0	1	0	5	5	0	0	4	0	1	1	1	1	1	0	0	0	0	0	0	1	0	4	1	0	0	0	0	0	0	1	1
1dwe	0	0	1	0	1	0	3	3	0	0	3	0	1	2	2	0	1	0	0	0	0	0	0	1	1	5	1	1	0	0	0	0	1	0	
1fpc	0	0	0	0	1	0	6	5	0	0	4	0	1	1	1	1	1	0	1	0	1	0	0	0	3	1	1	0	1	0	0	0	0	1	
1hai	0	0	1	0	1	0	4	2	0	0	4	0	1	2	2	1	1	0	0	0	0	0	1	1	1	5	1	1	0	0	0	0	1	0	
1hap	0	0	1	0	1	0	3	3	0	0	4	0	1	2	2	1	1	0	0	0	0	0	0	1	1	3	1	1	0	0	0	0	1	0	
1hdt	0	0	0	0	0	0	2	5	0	0	1	0	1	0	1	1	1	0	0	0	0	0	0	1	0	4	1	1	0	2	1	0	0	1	

Supplementary Table 1

1ht	0	0	0	0	0	0	3	2	0	0	3	0	1	2	2	0	1	0	0	0	0	0	0	0	1	1	5	1	1	0	0	0	1	0
1hc	0	0	0	0	1	0	3	3	0	0	3	0	1	1	1	0	1	0	0	0	0	0	1	1	1	1	5	1	1	0	0	0	1	0
1hd	0	0	0	0	1	0	3	3	0	0	4	0	1	0	0	1	0	0	0	0	0	1	1	0	1	5	1	1	0	0	0	1	1	
1he	0	0	0	0	1	0	3	3	0	0	4	0	1	1	1	1	1	0	0	0	0	1	1	1	1	5	1	1	0	0	0	1	0	
1nrr	0	0	1	0	1	0	3	3	0	0	3	0	1	2	2	0	1	0	0	0	0	0	1	1	1	5	1	1	0	0	0	1	0	
1ppb	0	0	1	0	0	1	3	3	0	0	4	0	1	2	2	0	1	0	0	0	0	0	0	1	1	3	1	1	0	0	0	1	0	
1tbz	0	0	1	0	1	0	3	3	0	1	4	0	1	2	2	0	1	0	0	0	0	1	1	1	0	4	1	1	0	0	0	1	0	
1tmt	0	0	0	2	0	0	3	3	0	0	4	0	1	2	2	1	1	0	0	0	0	1	1	1	0	5	1	1	0	0	0	1	0	
1tmu	0	0	0	0	1	0	3	3	0	0	4	0	1	2	2	0	1	0	0	0	0	0	0	1	1	5	1	1	0	0	0	0	0	
1tom	0	0	0	0	1	0	4	2	0	0	4	0	1	0	0	1	1	0	0	0	0	0	0	1	1	5	1	0	0	0	0	1	1	
1uma	0	0	0	0	0	0	0	3	0	0	0	0	0	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1
1uvu	0	0	0	0	1	0	3	3	0	0	1	0	0	1	1	1	1	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	1	0
2hpq	0	0	1	0	1	1	3	3	0	0	3	0	1	2	1	1	1	0	0	0	0	0	0	1	1	5	1	1	0	0	0	1	0	
3hat	0	0	0	0	1	0	3	3	0	0	1	0	4	1	1	0	1	0	0	0	0	0	0	1	1	3	1	0	0	2	0	1	0	
7kme	0	0	0	0	1	0	2	3	0	0	2	1	1	1	0	1	1	0	0	0	2	0	0	1	0	2	1	1	0	2	0	0	1	
8kme	0	0	0	0	0	0	3	3	0	0	0	0	2	1	1	1	1	0	0	0	1	0	0	1	0	4	0	1	1	2	0	1	1	
ZINC01627553	0	1	1	1	0	0	0	1	0	0	0	0	0	2	2	1	1	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	1	0
ZINC00393806	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	1	1	1	1	0	0	0	0	0	0	0	0	1	1
ZINC01692407	0	0	0	0	0	0	0	1	0	0	0	0	0	1	2	1	1	1	0	0	2	1	1	0	0	0	0	0	0	0	0	0	0	0
ZINC01694232	0	0	0	0	0	0	0	2	0	0	0	0	0	2	2	0	1	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	1	1
ZINC01280746	0	0	0	0	0	0	0	2	0	0	0	0	0	2	2	1	1	0	0	0	2	0	0	1	0	0	0	0	0	0	0	0	1	0

Supplementary Table 2

Interaction matchprints for 42 known thrombin inhibitors, labeled by PDB code, followed by 27 NCI compounds obtained for testing, labeled by their ZINC codes. \* denotes confirmed SLIDE inhibitors. Interactions are highlighted in grey, with the number of ligand interactions with the corresponding thrombin atom (for polar interactions) or side chain (for hydrophobic interactions) listed.

LIGAND

LIGAND	PHE 40 sc	LEU 41 sc	CYS 42 sc	HIS 57 NE2	HIS 57 sc	CYS 58 sc	TYR 60A sc	TRP 60D sc	LYS 60F NZ	LYS 60F sc	LEU 99 sc	GLU 146 sc	ILE 174 sc	ASP 189 OD1	ASP 189 OD2	ASP 189 sc	ALA 190 O	ALA 190 sc	CYS 191 O	CYS 191 sc	GLU 192 OE2	GLU 192 sc	GLY 193 N	SER 195 N	VAL 213 sc	SER 214 O	TRP 215 O	TRP 215 sc	GLY 216 N	GLY 216 O	GLU 217 OE2	GLU 217 sc	GLY 219 N	GLY 219 O	CYS 220 sc	PHE 227 N	PHE 227 O				
1a3b	0	0	0	1	1	0	3	3	0	0	4	0	1	1	1	0	1	1	0	0	0	0	1	1	1	1	0	5	1	1	0	0	0	1	0	0	0	0	0		
1a46	0	0	1	1	0	0	2	3	0	0	1	0	1	0	0	0	1	1	0	0	0	0	1	1	0	0	0	4	1	1	0	1	0	1	1	0	0	0	0		
1a4w	0	0	0	0	0	0	2	5	1	0	4	0	2	1	0	0	1	1	0	0	0	0	0	0	0	0	3	1	1	0	1	0	0	1	0	0	1	0	0	0	
1a5g	1	0	0	1	1	0	3	3	0	0	4	0	1	2	2	0	0	1	0	0	0	2	1	1	1	0	0	3	1	1	0	0	0	0	0	1	0	0	0	0	
1a61	0	0	1	1	0	0	2	3	0	0	4	0	1	2	1	0	1	1	0	0	0	0	1	0	1	0	0	3	1	1	0	0	0	0	1	0	0	0	0		
1abj	0	0	0	0	0	0	3	3	0	0	4	0	1	2	2	0	1	1	0	0	0	0	0	0	1	1	0	3	1	1	0	0	0	1	0	0	0	0	0		
1ae8	0	0	0	0	0	0	2	2	0	0	4	0	1	0	1	0	1	1	0	0	0	0	0	0	0	1	0	5	1	1	0	0	0	0	1	1	0	0	0		
1afe	0	0	0	0	0	0	3	3	0	0	1	0	2	0	0	0	1	1	0	0	0	0	0	0	0	1	0	2	1	0	0	2	0	1	2	0	0	0	0		
1awf	0	0	0	1	0	0	1	5	0	0	1	0	0	0	0	0	0	1	0	0	0	0	1	1	1	0	0	1	1	1	0	1	0	0	1	0	0	1	0	0	
1awh	0	0	0	0	0	0	0	4	0	0	1	0	0	0	0	0	0	1	0	0	0	0	1	1	1	0	0	1	0	0	0	0	0	0	0	0	1	0	0		
1ay6	0	0	0	0	1	0	4	4	0	0	4	0	1	2	2	0	0	1	0	0	0	0	1	1	1	1	0	4	1	0	0	1	0	1	0	1	0	0	0	0	
1b5g	0	0	1	0	1	0	2	4	0	1	1	0	0	2	2	0	0	1	0	0	0	0	1	1	1	0	0	1	1	1	0	2	0	1	0	1	0	0	0	0	
1ba8	0	0	0	0	0	0	1	3	0	0	3	0	2	1	1	0	0	1	0	0	0	0	1	1	1	1	0	5	0	0	0	1	0	1	0	1	0	0	0	0	
1bb0	0	0	0	0	0	0	2	3	0	0	2	0	2	1	1	0	0	0	0	0	0	0	1	1	1	1	0	5	0	0	0	1	0	1	0	1	1	0	0	0	
1bcu	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	1	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	
1bhx	0	0	0	0	1	0	1	3	0	0	2	0	2	1	1	0	1	1	0	0	0	0	0	0	1	0	0	5	1	0	0	1	0	1	0	1	0	0	0	0	
1bmm	0	0	0	0	0	0	2	5	0	0	4	0	1	1	1	0	0	1	0	0	0	0	0	0	0	1	0	5	1	0	0	0	0	0	0	1	0	0	0	0	
1bmn	0	0	0	0	0	0	3	4	0	0	4	0	2	0	0	0	1	1	0	0	0	0	0	0	1	1	0	6	1	0	0	1	0	2	1	0	0	0	0	0	
1ca8	0	0	0	1	0	0	2	2	0	0	2	0	2	1	1	0	0	0	0	0	0	0	0	0	0	1	1	5	1	0	0	1	0	1	0	1	1	0	0	0	
1dwc	0	0	0	0	0	0	3	5	0	0	1	0	1	1	0	0	0	1	0	0	0	0	0	0	0	0	5	1	1	0	0	0	0	0	1	1	0	0	0	0	
1dwd	0	0	0	0	1	0	5	5	0	0	4	0	1	1	1	0	1	1	0	0	0	0	0	0	1	0	4	1	0	0	0	0	0	0	1	1	0	0	1	0	0
1dwe	0	0	1	0	1	0	3	3	0	0	3	0	1	2	2	0	0	1	0	0	0	0	0	0	1	1	5	1	1	0	0	0	0	0	1	0	0	1	0	0	0
1fpc	0	0	0	0	1	0	6	5	0	0	4	0	1	1	1	0	1	1	0	0	0	0	0	0	0	0	3	1	1	0	1	0	0	0	0	1	0	0	1	0	0
1hai	0	0	1	0	1	0	4	2	0	0	4	0	1	2	2	0	1	1	0	0	0	0	0	1	1	1	5	1	1	0	0	0	0	0	1	0	0	0	0	0	

Supplementary Table 2

1hap	0	0	1	0	1	0	3	3	0	0	4	0	1	2	2	0	1	1	0	0	0	0	0	0	0	0	0	1	1	0	3	1	1	0	0	0	1	0	0	0			
1hdt	0	0	0	0	0	0	2	5	0	0	1	0	1	0	1	0	1	1	0	0	0	0	0	0	0	0	0	0	1	0	0	4	1	1	0	2	1	0	1	0	0		
1hlt	0	0	0	0	0	0	3	2	0	0	3	0	1	2	2	0	0	1	0	0	0	0	0	0	0	0	0	1	1	0	5	1	1	0	0	0	0	1	0	0	0		
1lhc	0	0	0	0	1	0	3	3	0	0	3	0	1	1	1	0	0	1	0	0	0	0	0	0	0	0	1	1	1	1	0	5	1	1	0	0	0	1	0	0	0		
1lhd	0	0	0	0	1	0	3	3	0	0	4	0	1	0	0	0	1	0	0	0	0	0	0	0	0	0	1	1	0	1	0	5	1	1	0	0	0	1	1	0	0		
1lhe	0	0	0	0	1	0	3	3	0	0	4	0	1	1	1	0	1	1	0	0	0	0	0	0	0	0	1	1	1	1	0	5	1	1	0	0	0	1	0	0	0		
1nrr	0	0	1	0	1	0	3	3	0	0	3	0	1	2	2	0	0	1	0	0	0	0	0	0	0	0	1	1	1	0	5	1	1	0	0	0	1	0	0	0			
1ppb	0	0	1	0	0	1	3	3	0	0	4	0	1	2	2	0	0	1	0	0	0	0	0	0	0	0	0	1	1	0	3	1	1	0	0	0	1	0	0	0			
1tbz	0	0	1	0	1	0	3	3	0	1	4	0	1	2	2	0	0	1	0	0	0	0	0	0	0	0	1	1	1	0	0	4	1	1	0	0	0	1	0	0	0		
1tmt	0	0	0	2	0	0	3	3	0	0	4	0	1	2	2	0	1	1	0	0	0	0	0	0	0	0	1	1	1	0	0	5	1	1	0	0	0	1	0	0	0		
1tmu	0	0	0	0	1	0	3	3	0	0	4	0	1	2	2	0	0	1	0	0	0	0	0	0	0	0	0	1	1	0	5	1	1	0	0	0	0	0	0	0	0		
1tom	0	0	0	0	1	0	4	2	0	0	4	0	1	0	0	0	1	1	0	0	0	0	0	0	0	0	0	1	1	0	5	1	0	0	0	0	0	1	1	0	0		
1uma	0	0	0	0	0	0	0	3	0	0	0	0	0	1	1	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0		
1uvu	0	0	0	0	1	0	3	3	0	0	1	0	0	1	1	0	1	1	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	1	0	0	0		
2hpq	0	0	1	0	1	1	3	3	0	0	3	0	1	2	1	0	1	1	0	0	0	0	0	0	0	0	0	1	1	0	5	1	1	0	0	0	1	0	0	0			
3hat	0	0	0	0	1	0	3	3	0	0	1	0	4	1	1	0	0	1	0	0	0	0	0	0	0	0	0	1	1	0	3	1	0	0	2	0	1	0	0	0			
7kme	0	0	0	0	1	0	2	3	0	0	2	1	1	1	0	0	1	1	0	0	0	0	2	0	0	0	1	0	0	2	1	1	0	2	0	0	1	0	0	0			
8kme	0	0	0	0	0	0	3	3	0	0	0	0	2	1	1	0	1	1	0	0	0	0	1	0	0	0	1	0	0	4	0	1	1	2	0	1	1	0	0	0			
* ZINC00393806	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0		
* ZINC01280746	0	0	0	0	0	0	0	2	0	0	0	0	0	2	2	0	1	1	0	0	0	0	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0		
* ZINC01627553	0	1	1	1	0	0	0	1	0	0	0	0	0	2	2	0	1	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0		
* ZINC01692407	0	0	0	0	0	0	0	1	0	0	0	0	0	1	2	0	1	1	1	0	0	0	2	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0		
* ZINC01694232	0	0	0	0	0	0	0	2	0	0	0	0	0	2	2	0	0	1	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	
ZINC00039096	0	0	0	0	1	0	5	3	0	0	2	0	0	1	1	1	0	1	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	2	0	0	0	
ZINC00040134	0	0	0	0	0	0	0	2	0	0	0	0	0	1	0	0	1	1	0	0	0	0	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	
ZINC00128262	0	0	0	0	0	0	0	1	0	0	0	0	0	1	2	0	1	1	1	0	0	0	0	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
ZINC00331108	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	1	1	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	
ZINC00334967	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	1	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0	
ZINC00388143	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	
ZINC00399488	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	1	0	0	1	0	
ZINC01571102	0	0	0	0	0	0	0	0	0	0	0	0	0	3	2	0	1	1	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0		
ZINC01571123	0	0	0	0	0	0	0	0	0	0	0	0	0	2	2	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0		
ZINC01578169	0	0	0	0	0	0	0	2	0	0	1	0	0	1	1	0	1	1	0	0	0	0	2	0	0	1	0	0	0	1	0	0	0	0	0	0	1	0	0	0	0		
ZINC01590788	0	0	0	0	0	0	0	2	0	0	0	0	0	1	1	0	0	1	0	0	0	0	2	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
ZINC01592422	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	1	1	1	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	
ZINC01620760	0	0	1	0	0	0	0	1	0	0	0	0	0	2	2	0	0	1	0	0	0	0	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0



Supplementary Table 3

Interaction matchprints for the 100 top-scoring candidates according to EON/1ppb. Interactions are highlighted in grey showing the number of ligand interactions with the corresponding thrombin atom (for polar interactions) or side chain (for hydrophobic interactions).

LIGAND	LEU 41 sc	CYS 42 sc	HIS 57 NE2	HIS 57 sc	TYR 60A sc	TRP 60D sc	LYS 60F sc	PHE 60H sc	LEU 99 sc	GLU 146 sc	ASP 189 OD1	ASP 189 OD2	ASP 189 sc	ALA 190 O	ALA 190 sc	CYS 191 O	CYS 191 sc	GLU 192 sc	GLY 193 N	ASP 194 sc	SER 195 N	VAL 213 sc	SER 214 O	TRP 215 sc	GLY 216 N	GLY 219 O	CYS 220 sc
ZINC00152886_2_0000	0	0	0	0	0	0	0	0	0	0	1	1	0	1	1	0	0	2	0	0	0	1	0	0	0	0	1
ZINC01709133_8_0000	0	0	0	0	0	2	0	0	0	0	1	1	1	0	1	0	0	1	0	0	0	0	0	1	0	0	1
ZINC02024829_17_0000	0	0	0	0	0	3	0	0	0	0	1	1	1	0	1	0	0	1	0	0	0	1	0	0	0	0	0
ZINC01694478_3_0001	0	0	0	0	0	1	0	0	0	1	2	1	0	1	1	0	2	2	0	0	0	0	0	0	0	2	1
ZINC01620761_4_0025	0	0	0	0	0	2	0	0	0	0	2	1	0	0	1	0	0	1	0	0	0	1	0	0	0	1	0
ZINC01697190_33_0024	0	0	0	0	2	3	0	0	1	0	2	1	0	0	1	0	0	2	0	0	0	0	0	0	0	2	1
ZINC01688454_7_0000	0	0	0	0	0	2	0	0	0	1	1	1	1	0	1	0	1	2	0	0	0	2	0	0	0	1	1
ZINC01668371_7_0001	0	0	0	0	0	0	0	0	0	0	1	1	0	1	1	0	0	0	1	0	1	1	0	1	0	0	0
ZINC01571124_1_0001	0	0	0	0	0	0	0	0	0	0	2	2	0	1	1	0	0	2	0	0	0	1	0	0	0	1	1
ZINC01694154_6_0001	0	0	0	0	0	3	0	0	0	0	2	2	0	1	1	0	0	0	0	0	0	1	0	1	0	1	0
ZINC01612663_5_0004	0	1	0	0	0	0	0	0	0	0	2	2	0	1	1	0	0	2	0	0	0	1	0	0	0	1	1
ZINC00040134_9_0000	0	0	0	0	0	2	0	0	0	0	1	0	0	1	1	0	0	1	1	0	1	1	0	0	0	0	1
ZINC01694232_1_0001	0	0	0	0	0	2	0	0	0	0	2	2	0	0	1	0	0	2	0	0	0	0	0	0	0	1	1
ZINC01590790_11_0000	0	0	1	0	0	2	0	0	0	0	1	1	0	0	1	0	0	0	1	0	1	2	0	0	0	0	1
ZINC01723906_2_0000	0	0	0	0	0	2	0	0	0	0	2	2	0	1	1	0	0	0	0	0	0	0	0	0	0	1	1
ZINC01666219_6_0002	0	0	0	0	0	3	0	0	0	0	2	2	0	1	1	0	0	1	0	0	0	0	0	0	0	1	1
ZINC01609953_31_0002	0	0	0	0	0	0	0	0	0	0	2	2	0	1	1	0	0	0	0	0	0	0	0	0	1	1	0
ZINC01703906_1_0009	0	1	0	0	0	2	0	0	0	0	2	3	0	0	0	0	0	2	0	0	0	0	0	0	0	1	1
ZINC01661211_18_0000	0	0	0	0	0	0	0	0	0	0	2	2	0	1	1	0	0	0	0	0	0	0	0	0	0	1	1
ZINC01576560_6_0000	0	0	0	0	0	0	0	0	0	0	1	1	0	1	1	0	0	2	0	0	0	1	0	0	0	0	1
ZINC01665520_2_0000	0	0	1	0	0	0	0	0	0	0	2	2	0	0	1	0	0	2	0	0	0	0	0	0	0	1	1
ZINC00161844_1_0000	0	0	0	0	0	0	0	0	0	0	1	1	0	0	1	0	0	2	1	0	0	0	0	0	0	0	0
ZINC01733126_1_0002	0	0	0	0	0	1	0	0	0	0	1	1	0	1	1	0	0	0	0	0	0	0	0	1	0	1	1
ZINC01564199_12_0002	0	0	0	0	0	3	0	0	0	0	2	2	0	1	1	0	0	1	0	0	0	0	0	0	0	1	1
ZINC01694230_2_0015	0	0	0	0	0	2	0	0	0	0	2	1	0	0	1	0	0	2	0	0	0	0	0	0	0	2	1
ZINC01702595_3_0000	0	0	0	0	0	0	0	0	0	0	2	1	0	0	1	0	0	0	0	0	0	0	0	0	0	2	0

Supplementary Table 3

ZINC01686494_2_0001	0	0	0	0	0	2	0	0	0	0	2	2	0	1	1	0	0	2	0	0	0	0	0	0	0	0	0	0	1	0	
ZINC01674367_1_0002	0	0	0	0	0	0	0	0	0	1	2	2	0	0	1	0	1	2	0	1	0	1	0	1	0	2	0	0	2	1	
ZINC01628143_8_0000	0	0	0	0	0	3	0	0	3	0	1	1	0	2	1	0	0	0	0	0	1	0	2	0	0	0	1	0	0	1	
ZINC01676782_12_0002	0	0	0	0	0	3	0	0	0	0	1	1	1	1	1	0	0	2	0	0	0	0	0	0	1	0	2	0	0	2	
ZINC01733113_2_0000	0	0	0	0	0	0	0	0	0	0	1	1	0	0	1	0	0	2	0	0	0	1	0	1	0	0	0	0	0	0	
ZINC01682931_17_0000	0	0	0	0	0	0	0	0	0	0	2	2	0	1	1	0	0	0	0	0	0	2	1	0	0	0	1	0	0	1	
ZINC01433164_3_0004	0	0	0	0	0	1	0	0	0	0	2	2	0	0	1	0	1	2	0	0	0	1	0	0	0	0	2	1	0	1	
ZINC01692407_1_0008	0	0	0	0	0	1	0	0	0	0	1	2	0	1	1	1	0	2	1	0	1	0	0	0	0	0	0	0	0	0	
ZINC01755965_11_0001	0	0	0	0	0	2	0	0	0	0	1	1	1	0	1	0	0	2	1	0	1	1	0	0	0	0	0	0	0	0	
ZINC01665216_6_0000	0	0	0	0	0	0	0	0	0	0	2	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	1	1		
ZINC01670550_6_0000	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	2	0	0	0	1	0	0	0	1	2	0	0	1	
ZINC01733125_5_0000	0	0	0	0	0	0	0	0	0	0	1	1	0	1	1	0	0	2	0	0	0	1	0	1	0	0	1	0	0	1	
ZINC01558074_5_0002	0	0	0	0	0	0	0	0	0	0	2	2	0	1	1	0	0	2	0	0	0	1	0	0	0	1	0	0	1	0	
ZINC01706327_19_0000	0	0	0	0	0	2	0	0	0	0	1	1	0	1	1	1	0	0	0	0	1	1	0	1	0	0	0	0	0	0	
ZINC01675036_9_0001	0	0	1	0	0	0	0	0	0	0	1	2	0	0	1	0	0	2	0	0	0	0	0	0	0	0	0	1	1		
ZINC01585277_3_0000	0	0	0	0	0	0	0	0	0	0	2	2	0	1	1	0	0	1	1	0	0	1	0	1	0	1	0	1	0	1	
ZINC01573859_16_0003	0	0	0	0	0	3	0	0	0	0	2	2	1	1	1	0	0	2	0	0	0	2	0	1	0	0	0	1	0	1	
ZINC01578169_8_0007	0	0	0	0	0	2	0	0	1	0	1	1	0	1	1	0	0	2	0	0	0	1	0	0	1	1	0	1	1	0	
ZINC01556651_3_0000	0	0	0	0	0	2	0	0	0	0	0	1	0	0	1	0	0	1	0	0	0	1	0	1	0	1	0	1	1	1	
ZINC00055120_1_0001	0	0	0	0	0	1	0	0	0	0	1	1	0	1	1	0	0	2	0	0	0	0	0	0	0	0	1	1	0	1	
ZINC01567454_1_0000	0	0	0	0	0	4	0	0	0	0	1	1	0	1	1	0	0	1	0	0	0	0	0	0	1	0	1	0	1	0	
ZINC01654079_4_0000	0	0	0	0	0	0	0	0	0	0	1	1	0	1	1	0	0	1	0	0	0	1	0	0	0	0	0	0	1	1	
ZINC01718790_1_0006	0	0	0	0	0	2	0	0	0	0	1	1	0	1	1	0	0	0	0	0	0	1	0	0	0	1	0	0	0	1	0
ZINC00396555_12_0000	0	0	0	0	0	3	0	0	0	0	1	1	1	0	1	0	0	2	1	0	0	1	0	0	0	0	0	0	0	0	0
ZINC00066085_7_0000	0	0	0	0	0	0	0	0	0	0	1	1	0	1	1	0	0	0	0	0	0	2	0	1	0	1	0	1	0	1	0
ZINC01706265_3_0003	0	0	1	0	0	2	0	0	0	0	2	2	0	1	1	0	0	2	0	0	0	1	0	0	0	1	1	0	0	1	1
ZINC01661214_9_0000	0	0	0	0	0	2	0	0	0	0	2	2	0	0	1	0	0	0	0	0	0	1	0	1	0	1	0	0	0	0	0
ZINC01571122_2_0001	0	0	0	0	0	0	0	0	0	0	2	1	0	1	1	0	0	2	0	0	0	1	0	0	0	0	0	1	0	0	1
ZINC00481176_6_0004	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	2	0	0	0	0	0	0	0	0	0	1	1	0	1
ZINC01688931_22_0002	0	0	0	0	0	0	0	0	0	0	1	1	0	1	1	1	0	0	1	0	1	1	0	0	0	0	0	0	0	0	0
ZINC01742147_13_0000	0	0	0	0	0	1	0	0	0	0	2	2	0	1	1	0	0	2	0	0	0	1	0	0	0	1	0	0	0	1	0
ZINC01750897_1_0004	0	0	1	0	0	2	0	0	0	0	2	2	0	0	1	0	0	2	0	0	0	1	0	0	0	1	0	0	0	1	1
ZINC01627553_11_0002	1	1	1	0	0	1	0	0	0	0	2	2	0	1	1	0	0	0	0	0	0	1	0	0	0	1	0	0	0	1	0
ZINC01620694_2_0000	0	0	0	0	0	0	0	0	0	0	2	2	0	0	0	0	0	2	0	1	0	1	0	0	0	2	1	0	0	2	1
ZINC01590788_9_0000	0	0	0	0	0	2	0	0	0	0	1	1	0	0	1	0	0	2	1	0	1	1	0	0	0	0	0	0	0	0	0
ZINC00055122_1_0001	0	0	0	0	0	0	0	0	0	1	1	1	0	1	1	0	0	2	0	0	0	0	0	0	0	0	0	1	1	0	1

Supplementary Table 3

ZINC01694515_4_0000	0	0	0	0	0	0	0	0	0	0	2	1	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	2	1	
ZINC00047610_3_0001	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	2	1	
ZINC01723503_1_0001	0	0	0	0	0	1	0	0	0	0	2	2	0	0	1	1	0	2	1	0	1	0	0	0	0	0	0	0	0	0
ZINC01745988_2_0001	0	0	0	0	0	2	0	0	0	0	2	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	1	
ZINC01722154_9_0000	0	0	0	0	0	2	0	0	0	0	1	1	0	1	1	0	0	2	0	0	0	1	0	0	0	0	0	1	1	
ZINC01693049_10_0000	0	0	0	0	0	2	0	0	0	0	2	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	1	
ZINC01697188_3_0001	0	0	1	0	0	0	0	0	0	0	2	2	0	0	1	0	0	0	0	0	0	0	1	1	0	0	1	0	0	
ZINC01703212_8_0000	0	0	0	0	0	2	0	0	0	0	2	2	0	1	1	0	0	2	0	0	0	0	0	0	0	0	0	1	1	
ZINC01682932_20_0003	0	0	0	0	0	0	0	0	1	0	2	2	0	0	1	0	0	0	0	0	0	0	0	0	1	0	1	1	0	
ZINC01697191_8_0000	0	0	0	0	0	0	0	0	0	0	2	2	0	1	1	0	0	2	1	0	0	0	1	1	0	1	1	0	0	
ZINC01620692_24_0002	0	0	0	0	0	2	0	0	0	0	2	2	0	0	1	0	0	1	0	0	0	0	0	0	1	0	2	1	0	
ZINC01665528_6_0006	0	0	0	0	0	0	0	0	0	0	2	2	0	1	1	0	0	1	0	0	0	1	0	0	0	0	1	0	0	
ZINC01871536_3_0000	0	0	0	0	0	0	0	0	0	1	2	2	0	0	1	0	1	2	0	0	0	1	0	1	0	1	0	1	2	
ZINC01620687_6_0007	0	1	0	0	0	0	0	0	0	0	2	1	0	1	1	0	0	2	0	0	0	0	0	0	0	0	2	0	0	
ZINC01587182_4_0006	0	0	0	0	0	2	0	0	0	0	2	2	1	0	1	0	0	2	0	0	0	1	0	0	0	0	1	2	0	
ZINC01718877_11_0003	0	0	0	0	0	2	0	0	0	0	2	2	0	0	1	0	0	2	0	0	1	1	0	0	1	0	0	0	0	
ZINC01592721_15_0001	0	0	0	0	0	2	0	0	0	0	0	1	0	1	1	0	0	0	0	0	0	1	0	0	0	0	1	0	0	
ZINC01723361_1_0002	0	0	0	0	0	0	0	0	0	0	2	1	0	0	1	0	0	2	0	0	0	1	0	1	0	1	0	2	0	
ZINC00039096_15_0000	0	0	0	1	5	3	0	0	2	0	1	1	1	0	1	0	0	0	0	0	0	1	0	1	0	1	0	0	2	
ZINC01655994_3_0009	0	0	0	0	0	3	0	0	1	0	1	1	0	1	1	0	0	0	1	0	1	1	0	0	0	0	1	0	0	
ZINC01604777_9_0000	0	0	0	0	0	0	0	0	0	0	2	2	0	1	1	0	0	0	0	0	1	1	0	1	0	1	0	1	0	
ZINC01735750_7_0000	0	0	0	0	0	0	0	0	0	0	2	2	0	1	1	0	1	2	0	0	0	0	0	0	0	0	1	1	0	
ZINC01280756_6_0002	0	1	0	0	0	2	0	0	0	0	2	1	0	0	0	0	0	2	0	0	0	0	0	0	0	0	2	1	0	
ZINC01723500_2_0000	0	0	1	0	0	0	0	0	0	0	2	2	0	0	1	0	0	2	0	0	0	1	1	0	0	1	0	1	0	
ZINC01280746_1_0008	0	0	0	0	0	2	0	0	0	0	2	2	0	1	1	0	0	2	0	0	0	1	0	0	0	1	0	1	0	
ZINC01573995_11_0001	1	1	1	0	0	1	1	2	0	0	2	2	0	0	1	0	0	2	1	0	0	1	0	0	0	1	0	1	0	
ZINC01593739_2_0000	0	0	0	0	0	0	0	0	0	0	2	2	0	1	1	0	0	2	0	0	0	1	0	0	0	0	1	1	0	
ZINC01693800_2_0001	0	0	1	0	0	0	0	0	0	0	2	2	0	0	1	0	0	2	0	0	0	0	0	0	0	0	1	1	0	
ZINC00128262_4_0001	0	0	0	0	0	1	0	0	0	0	1	2	0	1	1	1	0	0	1	0	1	1	0	0	0	0	0	0	0	
ZINC01736105_111_0006	0	1	0	0	0	2	1	0	0	0	2	2	0	1	1	0	0	0	0	0	0	1	0	0	0	0	1	0	0	
ZINC01620760_1_0010	0	1	0	0	0	1	0	0	0	0	2	2	0	0	1	0	0	2	0	0	0	1	0	0	0	0	1	0	0	
ZINC01697434_10_0000	0	0	0	0	0	0	0	0	0	0	2	2	0	1	1	0	0	2	0	0	0	0	0	0	0	0	1	0	0	
ZINC01694247_7_0000	0	0	0	0	0	0	0	0	0	0	2	2	0	1	1	0	0	2	0	0	0	0	0	0	1	0	1	0	0	
ZINC01571123_3_0002	0	0	0	0	0	0	0	0	0	0	2	2	0	0	1	0	0	0	0	0	0	1	0	0	0	2	0	0	0	
ZINC00251668_6_0001	0	0	0	0	0	2	0	0	0	0	0	0	0	0	1	0	0	2	0	0	0	0	0	0	0	0	1	1	0	
ZINC00271013_3_0000	0	0	0	0	0	0	0	0	0	0	1	1	0	0	1	0	0	1	1	0	0	0	0	0	0	0	1	1	0	



Supplementary Table 3

ZINC00240537_2_0000	0	0	0	0	0	0	0	0	0	0	1	1	0	0	1	0	0	2	0	0	0	0	0	0	0	1	0
ZINC01730267_1_0004	0	0	0	0	0	2	0	0	0	0	2	2	0	0	1	0	0	2	0	0	0	2	0	1	0	1	0

Supplementary Table 4

Interaction matchprints for the top-scoring 100 candidates according to EON/1a5g. Interactions are highlighted in grey, showing the number of ligand interactions with the corresponding thrombin atom (for polar interactions) or side chain (for hydrophobic interactions).

LIGAND	LEU 41 sc	CYS 42 sc	HIS 57 NE2	HIS 57 sc	CYS 58 sc	TYR 60A sc	TRP 60D sc	LYS 60F sc	PHE 60H sc	LEU 99 sc	GLU 146 sc	ASP 189 OD1	ASP 189 OD2	ASP 189 sc	ALA 190 O	ALA 190 sc	CYS 191 O	CYS 191 sc	GLU 192 sc	GLY 193 N	ASP 194 sc	SER 195 N	VAL 213 sc	SER 214 O	TRP 215 sc	GLY 216 N	GLY 216 O	GLY 219 O	CYS 220 sc	
ZINC01709133_8_0000	0	0	0	0	0	0	2	0	0	0	0	1	1	1	0	1	0	0	1	0	0	0	0	0	1	0	0	0	1	
ZINC00047608_1_0000	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	2	1
ZINC02024829_17_0000	0	0	0	0	0	0	3	0	0	0	0	1	1	1	0	1	0	0	1	0	0	0	1	0	0	0	0	0	0	0
ZINC01703905_2_0030	0	0	0	0	0	1	3	0	0	1	0	2	3	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	1
ZINC01620761_4_0025	0	0	0	0	0	0	2	0	0	0	0	2	1	0	0	1	0	0	1	0	0	0	0	1	0	0	0	0	1	0
ZINC00128284_4_0001	0	0	1	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	2	1
ZINC01697190_33_0024	0	0	0	0	0	2	3	0	0	1	0	2	1	0	0	1	0	0	2	0	0	0	0	0	0	0	0	0	2	1
ZINC01582976_1_0006	0	0	0	0	0	0	0	0	0	0	0	2	1	0	0	0	1	0	2	0	0	0	0	0	0	0	0	0	2	1
ZINC01694249_1_0003	0	0	0	0	0	0	0	0	0	0	0	2	2	0	0	1	0	0	2	0	0	0	0	0	0	0	0	0	2	1
ZINC01668371_7_0001	0	0	0	0	0	0	0	0	0	0	0	1	1	0	1	1	0	0	0	1	0	1	1	0	1	0	0	0	0	0
ZINC01571124_1_0001	0	0	0	0	0	0	0	0	0	0	0	2	2	0	1	1	0	0	2	0	0	0	1	0	0	0	0	1	1	
ZINC01694154_6_0001	0	0	0	0	0	0	3	0	0	0	0	2	2	0	1	1	0	0	0	0	0	0	1	0	1	0	0	1	0	
ZINC00040134_9_0000	0	0	0	0	0	0	2	0	0	0	0	1	0	0	1	1	0	0	1	1	0	1	1	0	0	0	0	0	0	1
ZINC01694232_1_0001	0	0	0	0	0	0	2	0	0	0	0	2	2	0	0	1	0	0	2	0	0	0	0	0	0	0	0	1	1	
ZINC01694516_1_0001	0	0	0	0	0	0	0	0	0	0	0	2	1	0	0	0	0	0	2	0	0	0	0	0	0	0	0	2	1	
ZINC01590790_11_0000	0	0	1	0	0	0	2	0	0	0	0	1	1	0	0	1	0	0	0	1	0	1	2	0	0	0	0	0	0	1
ZINC01723906_2_0000	0	0	0	0	0	0	2	0	0	0	0	2	2	0	1	1	0	0	0	0	0	0	0	0	0	0	0	1	1	
ZINC01666219_6_0002	0	0	0	0	0	0	3	0	0	0	0	2	2	0	1	1	0	0	1	0	0	0	0	0	0	0	0	1	1	
ZINC01609953_31_0002	0	0	0	0	0	0	0	0	0	0	0	2	2	0	1	1	0	0	0	0	0	0	0	0	0	1	0	1	0	
ZINC01703906_1_0009	0	1	0	0	0	0	2	0	0	0	0	2	3	0	0	0	0	0	2	0	0	0	0	0	0	0	0	1	1	
ZINC01661211_18_0000	0	0	0	0	0	0	0	0	0	0	0	2	2	0	1	1	0	0	0	0	0	0	0	0	0	0	0	1	1	
ZINC01665520_2_0000	0	0	1	0	0	0	0	0	0	0	0	2	2	0	0	1	0	0	2	0	0	0	0	0	0	0	0	1	1	
ZINC00161844_1_0000	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	1	0	0	2	1	0	0	0	0	0	0	0	0	0	0
ZINC01733126_1_0002	0	0	0	0	0	0	1	0	0	0	0	1	1	0	1	1	0	0	0	0	0	0	0	0	1	0	0	1	1	
ZINC01564199_12_0002	0	0	0	0	0	0	3	0	0	0	0	2	2	0	1	1	0	0	1	0	0	0	0	0	0	0	0	1	1	
ZINC01694230_2_0015	0	0	0	0	0	0	2	0	0	0	0	2	1	0	0	1	0	0	2	0	0	0	0	0	0	0	0	2	1	





Supplementary Table 5

Interaction matchprints for the top-scoring 100 candidates according to EON/1tbz. Interactions are highlighted in grey showing the number of ligand interactions with the corresponding thrombin atom (for polar interactions) or side chain (for hydrophobic interactions).

LIGAND	LEU 41 sc	CYS 42 sc	HIS 57 NE2	HIS 57 sc	TYR 60A sc	TRP 60D sc	LYS 60F NZ	LYS 60F sc	PHE 60H sc	LEU 99 sc	GLU 146 sc	ASP 189 OD1	ASP 189 OD2	ASP 189 sc	ALA 190 O	ALA 190 sc	CYS 191 O	CYS 191 sc	GLU 192 sc	GLY 193 N	ASP 194 sc	SER 195 N	VAL 213 sc	SER 214 O	TRP 215 sc	GLY 216 N	GLY 219 O	CYS 220 sc
ZINC00152886_2_0000	0	0	0	0	0	0	0	0	0	0	0	1	1	0	1	1	0	0	2	0	0	0	1	0	0	0	0	1
ZINC01709133_8_0000	0	0	0	0	0	2	0	0	0	0	0	1	1	1	0	1	0	0	1	0	0	0	0	0	1	0	0	1
ZINC02024829_17_0000	0	0	0	0	0	3	0	0	0	0	0	1	1	1	0	1	0	0	1	0	0	0	1	0	0	0	0	0
ZINC01694478_3_0001	0	0	0	0	0	1	0	0	0	0	1	2	1	0	1	1	0	2	2	0	0	0	0	0	0	0	2	1
ZINC01703905_2_0030	0	0	0	0	1	3	0	0	0	1	0	2	3	0	0	0	0	0	0	0	0	0	0	0	1	0	1	1
ZINC01620761_4_0025	0	0	0	0	0	2	0	0	0	0	0	2	1	0	0	1	0	0	1	0	0	0	1	0	0	0	1	0
ZINC01697190_33_0024	0	0	0	0	2	3	0	0	0	1	0	2	1	0	0	1	0	0	2	0	0	0	0	0	0	0	2	1
ZINC01582976_1_0006	0	0	0	0	0	0	0	0	0	0	0	2	1	0	0	0	1	0	2	0	0	0	0	0	0	0	2	1
ZINC01688454_7_0000	0	0	0	0	0	2	0	0	0	0	1	1	1	1	0	1	0	1	2	0	0	0	2	0	0	0	1	1
ZINC01694249_1_0003	0	0	0	0	0	0	0	0	0	0	0	2	2	0	0	1	0	0	2	0	0	0	0	0	0	0	2	1
ZINC01668371_7_0001	0	0	0	0	0	0	0	0	0	0	0	1	1	0	1	1	0	0	0	1	0	1	1	0	1	0	0	0
ZINC01571124_1_0001	0	0	0	0	0	0	0	0	0	0	0	2	2	0	1	1	0	0	2	0	0	0	1	0	0	0	1	1
ZINC01694154_6_0001	0	0	0	0	0	3	0	0	0	0	0	2	2	0	1	1	0	0	0	0	0	0	1	0	1	0	1	0
ZINC00040134_9_0000	0	0	0	0	0	2	0	0	0	0	0	1	0	0	1	1	0	0	1	1	0	1	1	0	0	0	0	1
ZINC01694232_1_0001	0	0	0	0	0	2	0	0	0	0	0	2	2	0	0	1	0	0	2	0	0	0	0	0	0	0	1	1
ZINC01694516_1_0001	0	0	0	0	0	0	0	0	0	0	0	2	1	0	0	0	0	0	2	0	0	0	0	0	0	0	2	1
ZINC01590790_11_0000	0	0	1	0	0	2	0	0	0	0	0	1	1	0	0	1	0	0	0	1	0	1	2	0	0	0	0	1
ZINC01723906_2_0000	0	0	0	0	0	2	0	0	0	0	0	2	2	0	1	1	0	0	0	0	0	0	0	0	0	0	1	1
ZINC01666219_6_0002	0	0	0	0	0	3	0	0	0	0	0	2	2	0	1	1	0	0	1	0	0	0	0	0	0	0	1	1
ZINC01609953_31_0002	0	0	0	0	0	0	0	0	0	0	0	2	2	0	1	1	0	0	0	0	0	0	0	0	0	1	1	0
ZINC01703906_1_0009	0	1	0	0	0	2	0	0	0	0	0	2	3	0	0	0	0	0	2	0	0	0	0	0	0	0	1	1
ZINC01661211_18_0000	0	0	0	0	0	0	0	0	0	0	0	2	2	0	1	1	0	0	0	0	0	0	0	0	0	0	1	1
ZINC01665520_2_0000	0	0	1	0	0	0	0	0	0	0	0	2	2	0	0	1	0	0	2	0	0	0	0	0	0	0	1	1
ZINC00161844_1_0000	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	1	0	0	2	1	0	0	0	0	0	0	0	0
ZINC01564199_12_0002	0	0	0	0	0	3	0	0	0	0	0	2	2	0	1	1	0	0	1	0	0	0	0	0	0	0	1	1
ZINC01694230_2_0015	0	0	0	0	0	2	0	0	0	0	0	2	1	0	0	1	0	0	2	0	0	0	0	0	0	0	2	1

Supplementary Table 5

ZINC01702595_3_0000	0	0	0	0	0	0	0	0	0	0	2	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	
ZINC01686494_2_0001	0	0	0	0	0	2	0	0	0	0	0	2	2	0	1	1	0	0	2	0	0	0	0	0	0	0	0	0	0	1	0
ZINC01674367_1_0002	0	0	0	0	0	0	0	0	0	0	1	2	2	0	0	1	0	1	2	0	1	0	1	0	1	0	1	0	2	1	
ZINC01628143_8_0000	0	0	0	0	0	3	0	0	0	3	0	1	1	0	2	1	0	0	0	0	0	0	1	0	2	0	0	0	1		
ZINC01676782_12_0002	0	0	0	0	0	3	0	0	0	0	0	1	1	1	1	1	0	0	2	0	0	0	0	0	0	0	1	0	2		
ZINC01733113_2_0000	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	1	0	0	2	0	0	0	0	0	0	0	0	1	0	0	
ZINC01682931_17_0000	0	0	0	0	0	0	0	0	0	0	2	2	0	1	1	0	0	0	0	0	0	0	2	1	0	0	0	1	0		
ZINC01433164_3_0004	0	0	0	0	0	1	0	0	0	0	0	2	2	0	0	1	0	1	2	0	0	0	1	0	0	0	0	2	1		
ZINC01692407_1_0008	0	0	0	0	0	1	0	0	0	0	0	1	2	0	1	1	1	0	2	1	0	1	0	0	0	0	0	0	0		
ZINC01755965_11_0001	0	0	0	0	0	2	0	0	0	0	0	1	1	1	0	1	0	0	2	1	0	1	1	0	0	0	0	0	0		
ZINC01665216_6_0000	0	0	0	0	0	0	0	0	0	0	0	2	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	1	1	
ZINC01670550_6_0000	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	2	0	0	0	1	0	0	0	0	1	2		
ZINC01733125_5_0000	0	0	0	0	0	0	0	0	0	0	0	1	1	0	1	1	0	0	2	0	0	0	1	0	1	0	0	0	1		
ZINC01558074_5_0002	0	0	0	0	0	0	0	0	0	0	0	2	2	0	1	1	0	0	2	0	0	0	1	0	0	0	0	1	0		
ZINC01706327_19_0000	0	0	0	0	0	2	0	0	0	0	0	1	1	0	1	1	1	0	0	0	0	1	1	0	1	0	0	0	0		
ZINC01675036_9_0001	0	0	1	0	0	0	0	0	0	0	0	1	2	0	0	1	0	0	2	0	0	0	0	0	0	0	0	0	1	1	
ZINC01585277_3_0000	0	0	0	0	0	0	0	0	0	0	0	2	2	0	1	1	0	0	1	1	0	0	1	0	1	0	1	0	1	0	
ZINC01573859_16_0003	0	0	0	0	0	3	0	0	0	0	0	2	2	1	1	1	0	0	2	0	0	0	2	0	1	0	0	0	1		
ZINC01578169_8_0007	0	0	0	0	0	2	0	0	0	1	0	1	1	0	1	1	0	0	2	0	0	0	1	0	0	1	1	0			
ZINC00128266_1_0001	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	2	1		
ZINC01602662_7_0000	0	0	0	0	0	0	0	0	0	0	0	2	1	0	0	1	0	0	2	0	0	0	0	0	0	0	0	0	1	1	
ZINC01556651_3_0000	0	0	0	0	0	2	0	0	0	0	0	0	1	0	0	1	0	0	1	0	0	0	1	0	1	0	1	1			
ZINC01568703_1_0001	0	1	0	0	0	2	0	0	0	0	0	2	1	0	0	1	0	0	2	0	0	0	0	0	0	0	0	1	1		
ZINC01654079_4_0000	0	0	0	0	0	0	0	0	0	0	0	1	1	0	1	1	0	0	1	0	0	0	1	0	0	0	0	0	1		
ZINC00396555_12_0000	0	0	0	0	0	3	0	0	0	0	0	1	1	1	0	1	0	0	2	1	0	0	1	0	0	0	0	0	0	0	
ZINC00240543_1_0001	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	2	1		
ZINC01735494_15_0000	0	0	1	0	0	2	0	0	0	0	0	1	1	1	1	1	0	0	0	0	0	0	1	0	1	0	0	0	1		
ZINC01661214_9_0000	0	0	0	0	0	2	0	0	0	0	0	2	2	0	0	1	0	0	0	0	0	0	1	0	1	0	0	0	0		
ZINC00481176_6_0004	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	2	0	0	0	0	0	0	0	0	1	1		
ZINC01742147_13_0000	0	0	0	0	0	1	0	0	0	0	0	2	2	0	1	1	0	0	2	0	0	0	1	0	0	0	0	1	0		
ZINC01750897_1_0004	0	0	1	0	0	2	0	0	0	0	0	2	2	0	0	1	0	0	2	0	0	0	1	0	0	0	0	1	1		
ZINC01627553_11_0002	1	1	1	0	0	1	0	0	0	0	0	2	2	0	1	1	0	0	0	0	0	0	1	0	0	0	0	1	0		
ZINC01620694_2_0000	0	0	0	0	0	0	0	0	0	0	0	2	2	0	0	0	0	0	2	0	1	0	1	0	0	0	0	2	1		
ZINC01590788_9_0000	0	0	0	0	0	2	0	0	0	0	0	1	1	0	0	1	0	0	2	1	0	1	1	0	0	0	0	0	0		
ZINC01694515_4_0000	0	0	0	0	0	0	0	0	0	0	0	2	1	0	0	0	0	0	2	0	0	0	0	0	0	0	0	2	1		
ZINC00047610_3_0001	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	2	1		
ZINC01723503_1_0001	0	0	0	0	0	1	0	0	0	0	0	2	2	0	0	1	1	0	2	1	0	1	0	0	0	0	0	0	0	0	











Supplementary Table 7

Interaction matchprints for the top-scoring 100 candidates according to AffiScore. Interactions are highlighted in grey, showing the number of ligand interactions with the corresponding thrombin atom (for polar interactions) or side chain (for hydrophobic interactions).

LIGAND	ARG 39 NH2	ARG 39 sc	LEU 41 sc	CYS 42 sc	HIS 57 NE2	HIS 57 sc	TYR 60A OH	TYR 60A sc	TRP 60D sc	ASP 60E sc	LYS 60F NZ	LYS 60F sc	PHE 60H sc	GLU 97A O	LEU 99 sc	GLU 146 sc	ILE 174 sc	ASP 189 OD1	ASP 189 OD2	ASP 189 sc	ALA 190 O	ALA 190 sc	CYS 191 O	CYS 191 sc	GLU 192 N	GLU 192 sc	GLY 193 N	SER 195 N	VAL 213 sc	SER 214 N	SER 214 O	TRP 215 N	TRP 215 O	TRP 215 sc	GLY 216 N	GLY 216 O	GLU 217 sc	GLY 219 N	GLY 219 O	CYS 220 sc	PHE 227 N	PHE 227 O	TYR 228 OH	TYR 228 sc					
ZINC01568009_4_0000	0	0	0	1	0	1	1	2	3	0	0	0	0	0	3	1	0	0	1	0	0	0	0	1	0	2	0	0	1	0	0	0	0	0	1	0	0	0	0	1	1	0	0	0	0	0			
ZINC01691684_1_0000	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	2	0	0	1	0	0	0	0	0	1	0	0	0	0	0	0	1	0	0	0	0		
ZINC01700146_3_0000	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	2	0	0	0	0	0	0	0	0	1	0	0	0	0	1	1	0	0	0	0	0		
ZINC01585807_3_0000	0	0	0	0	0	0	0	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	1	0	0	0	0	0		
ZINC01584235_1_0001	0	0	0	0	1	0	0	0	4	0	0	0	0	0	0	0	0	1	0	0	1	1	0	0	0	2	1	1	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0			
ZINC01671331_6_0000	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1	0	1	1	0	0	1	1	1	0	0	0	0	0	1	0	0	0	0	0	0	3	1	0	0	0	0	0	0	0	0	0	0		
ZINC01561701_16_0000	0	0	0	0	0	0	0	0	6	1	0	1	0	0	0	0	0	1	1	1	0	1	0	0	0	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0		
ZINC01741421_21_0001	0	0	0	1	0	0	0	0	4	0	0	0	0	0	0	0	0	0	1	0	1	1	0	0	0	2	0	0	2	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0		
ZINC01760748_1_0002	0	0	0	0	0	0	0	1	3	0	0	0	0	0	1	0	0	1	0	0	1	1	0	0	0	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0		
ZINC01739584_3_0000	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	1	0	0	1	1	0	0	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0		
ZINC01698107_1_0000	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	1	1	0	1	1	0	2	0	0	1	0	0	0	0	0	0	0	0	0	0	1	2	0	1	0	2	0		
ZINC01581897_5_0000	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	1	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	2	2	0	0	0	0	0		
ZINC01634714_5_0001	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	1	0	0	0	1	0	1	0	2	0	0	1	0	0	0	0	0	0	0	0	0	2	1	0	2	0	0	0	0	0		
ZINC01686077_12_0003	0	0	0	0	0	1	0	5	4	0	0	0	0	0	3	0	1	1	0	0	1	1	0	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0		
ZINC01633770_26_0014	0	0	0	0	0	0	0	0	3	0	0	0	0	0	1	0	0	0	1	0	1	1	0	0	0	1	0	0	1	0	0	0	0	0	0	3	0	0	0	0	1	1	0	0	0	0	0		
ZINC01576967_54_0000	0	0	0	0	0	0	0	0	3	0	1	0	0	0	0	0	0	0	1	0	1	1	0	0	0	1	0	0	2	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	1	5	0	0	
ZINC01611406_82_0000	0	0	0	0	0	1	0	5	1	0	0	0	0	0	2	0	0	0	1	0	1	1	1	0	0	0	1	1	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0	
ZINC01637269_20_0000	0	0	0	0	0	0	0	0	3	0	0	0	0	0	1	0	1	0	0	0	1	0	1	0	1	0	2	0	0	3	0	0	0	0	1	0	0	0	0	1	2	0	0	0	0	0	1	0	
ZINC00401809_1_0000	0	0	0	0	0	0	0	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	2	0	0	2	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	
ZINC01718925_41_0000	0	1	1	0	1	0	0	0	2	0	0	2	3	0	0	0	0	0	1	1	1	0	1	0	0	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	2	0	0	0	0	0	0	
ZINC01694598_15_0000	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	1	1	1	0	0	2	0	0	2	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	
ZINC01627315_84_0000	0	0	1	0	0	0	0	0	2	0	0	3	4	0	0	0	0	1	1	0	1	1	0	0	0	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	
ZINC01665959_3_0002	0	0	0	0	1	0	0	0	3	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ZINC01729108_3_0003	0	0	0	0	0	0	0	0	3	0	0	0	0	0	1	0	0	0	0	0	1	0	0	0	0	2	1	0	0	0	0	0	0	0	0	1	0	1	0	0	1	2	0	0	0	0	0	0	
ZINC01633756_15_0001	0	0	0	0	0	1	0	4	4	0	1	1	0	0	1	0	1	0	0	0	0	1	0	0	0	2	0	0	1	0	0	0	0	0	3	1	0	0	0	0	1	0	0	0	0	0	0	0	
ZINC00271076_4_0018	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	2	0	1	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	
ZINC01576053_10_0006	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	1	0	1	1	0	0	0	2	0	0	1	0	0	0	0	0	1	0	0	0	0	0	1	1	1	1	0	0	0	0	
ZINC01696478_2_0000	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	2	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	1	1	0	0	0	0	0	
ZINC00633601_2_0000	0	0	0	0	1	0	0	0	3	0	0	0	0	0	0	0	0	1	0	0	1	1	0	0	0	1	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	
ZINC01568448_19_0001	0	0	0	0	0	0	0	0	2	0	0	0	0	0	1	0	1	0	1	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	4	0	0	0	0	0	1	2	0	0	0	0	0	0	
ZINC01633094_8_0001	0	0	0	0	1	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	1	1	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ZINC01632847_1_0001	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	1	0	1	0	1	0	2	0	0	1	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	





Supplementary Table 8

Interaction matchprints for the top-scoring 100 candidates according to AffiScore/N. Interactions are highlighted in grey, showing the number of ligand interactions with the corresponding thrombin atom (for polar interactions) or side chain (for hydrophobic interactions).

LIGAND	HIS 57 NE2	TRP 60D sc	ASP 189 OD1	ASP 189 OD2	ASP 189 sc	ALA 190 N	ALA 190 O	ALA 190 sc	CYS 191 O	CYS 191 sc	GLU 192 sc	GLY 193 N	ASP 194 sc	SER 195 N	VAL 213 O	VAL 213 sc	SER 214 N	SER 214 O	TRP 215 O	TRP 215 sc	GLY 216 N	GLY 216 O	GLY 219 N	GLY 219 O	CYS 220 sc	PHE 227 N	PHE 227 O	TYR 228 sc	
ZINC01680040_79_0000	0	0	0	0	0	0	1	1	0	0	2	0	0	0	0	1	0	0	0	0	0	0	0	1	1	0	0	0	
ZINC00164581_4_0000	0	0	0	0	0	0	1	1	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	1	1	0	0	0
ZINC01682991_11_0000	0	0	0	0	1	1	1	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	2	0	0	0
ZINC01687467_13_0001	0	0	0	1	0	0	1	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	1	0	0	0	
ZINC01529428_12_0000	0	0	0	0	0	0	1	1	0	0	2	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0	
ZINC00152526_1_0000	0	0	0	0	0	0	1	0	0	1	2	1	0	1	0	0	0	0	0	0	0	0	0	1	2	0	0	0	
ZINC01706119_31_0000	0	0	0	1	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	
ZINC00153125_1_0000	0	0	0	1	0	0	1	1	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	1	0	0	0	1	
ZINC01722002_86_0000	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	2	0	0	0	
ZINC01666983_24_0000	0	0	0	0	0	0	1	1	0	0	0	1	0	1	0	1	0	0	0	0	0	0	0	1	1	0	0	0	
ZINC01665970_21_0000	0	0	0	1	0	0	1	1	1	0	0	1	0	1	0	2	0	0	0	0	0	0	0	1	0	0	0	0	
ZINC01680237_86_0004	0	2	0	1	0	0	1	1	0	0	2	0	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	
ZINC01706122_2_0000	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	1	0	0	0	
ZINC01595512_2_0000	0	0	0	1	0	0	1	1	0	0	0	0	0	0	0	2	0	0	0	0	1	1	0	1	1	0	0	3	
ZINC01702595_3_0000	0	0	2	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	
ZINC01571116_1_0001	0	0	0	1	0	0	1	1	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	1	1	0	0	0	
ZINC01577228_17_0000	0	0	0	1	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	
ZINC01640796_22_0000	0	0	0	0	0	0	1	1	0	0	2	0	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	
ZINC01577875_6_0000	0	0	0	0	0	0	1	1	0	0	2	0	0	0	0	0	0	0	0	0	0	1	1	2	1	0	0	0	
ZINC01679277_1_0002	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	2	1	0	0	0	
ZINC01665216_6_0000	0	0	2	2	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	1	0	0	0	
ZINC01561828_4_0000	0	0	0	0	0	0	0	1	0	2	1	0	0	0	0	0	0	0	0	0	0	0	0	1	2	0	0	0	
ZINC01706121_16_0000	0	0	0	1	0	0	1	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	
ZINC01648306_6_0000	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	1	0	0	0	4	
ZINC01711183_5_0000	0	0	1	0	0	0	1	1	0	0	0	0	0	0	1	2	0	0	0	0	0	0	0	0	1	0	0	0	
ZINC01688726_10_0000	0	0	0	1	0	0	1	1	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0	1	1	0	0	0	

Supplementary Table 8

ZINC00164447_1_0002	0	0	0	0	0	0	1	1	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	1	1	0	0	0
ZINC00393806_1_0008	0	0	0	0	0	0	1	1	0	0	1	1	0	1	0	0	0	0	0	0	0	0	0	1	1	0	0	0
ZINC01577152_26_0000	0	0	1	1	0	0	1	1	0	0	2	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0
ZINC01607457_2_0000	0	0	0	1	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	2	0	0	0	0
ZINC01693957_1_0000	0	0	0	1	0	0	1	1	0	0	0	0	1	1	0	1	0	0	0	0	0	0	0	1	0	0	0	0
ZINC01737500_2_0000	0	0	1	1	0	0	0	1	0	1	2	0	0	0	0	0	0	0	0	0	0	0	0	1	2	0	0	0
ZINC01711182_9_0001	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	2	0	0	1	0	0	0	0	1	1	0	1	0
ZINC01692483_3_0000	0	0	0	0	0	0	1	1	0	0	2	0	0	0	0	1	0	0	0	0	0	0	0	1	1	0	0	0
ZINC01571615_10_0000	0	0	0	1	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	1	1	0	0	0
ZINC00161624_7_0000	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	1	0	0	0	1	1	0	0	1	1	0	0	0
ZINC01571613_12_0000	0	0	0	0	0	0	1	1	1	0	0	0	1	1	0	2	0	0	0	0	0	0	0	1	0	0	0	0
ZINC01709927_10_0000	1	0	0	0	0	0	1	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	1	0	0	0
ZINC01699906_10_0000	0	2	0	1	0	0	1	1	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
ZINC01566606_2_0000	1	0	0	1	0	0	1	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0
ZINC01747839_31_0000	0	0	0	0	0	0	1	1	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0
ZINC01646545_1_0000	0	0	0	1	0	0	1	1	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	1	0	1	0	0
ZINC01723869_38_0000	0	0	0	0	0	0	1	1	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0
ZINC01628244_3_0000	0	0	1	1	0	0	1	1	0	0	0	0	0	0	0	2	0	0	1	0	0	0	0	1	0	1	1	0
ZINC00404295_8_0000	0	0	1	0	0	0	1	1	1	0	0	1	0	1	0	1	0	0	0	0	0	0	0	0	1	0	0	0
ZINC01716673_22_0000	0	0	1	1	0	0	2	1	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	1	0	0	0	0
ZINC01765761_16_0000	0	0	0	0	0	0	1	1	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0	1	1	0	0	0
ZINC00404411_1_0000	0	0	1	0	0	0	1	1	0	1	2	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0
ZINC01722003_83_0000	0	0	0	1	0	0	1	1	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0
ZINC00388437_1_0000	0	0	0	1	0	0	1	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	2	0	0	1	0
ZINC01613077_1_0000	0	0	0	0	0	0	1	1	1	0	0	1	0	1	0	0	0	0	0	0	0	0	0	1	1	0	0	0
ZINC00002500_1_0000	0	0	0	1	0	0	1	1	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	2	0	0	0	5
ZINC01699998_22_0000	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0
ZINC01724649_4_0000	0	0	0	1	0	0	1	1	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	1	0	1	0	0
ZINC01592422_16_0002	0	0	1	1	0	0	1	1	1	0	0	1	0	1	0	0	0	0	0	0	0	0	0	1	1	0	0	0
ZINC01598511_1_0000	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	1	1	0	0	0
ZINC01711184_2_0000	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	2	1	0	0	0	0	0	0	1	0	0	1	0
ZINC01755559_11_0000	0	0	0	0	0	0	1	1	0	0	0	0	1	1	0	1	0	0	0	0	0	0	0	1	1	0	0	0
ZINC01707886_17_0000	0	2	0	1	0	0	1	1	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0
ZINC00331108_5_0000	0	0	1	1	0	0	1	1	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0
ZINC01856592_2_0000	1	0	1	0	0	0	1	1	0	0	0	0	0	0	0	2	0	0	0	1	0	0	0	0	0	0	0	0
ZINC01595513_3_0000	0	0	0	1	0	0	1	1	0	0	0	0	0	0	0	2	0	0	0	0	1	1	0	1	1	0	0	3
ZINC01729706_27_0001	0	0	0	0	0	0	1	1	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0

Supplementary Table 8

ZINC01641410_24_0000	0	0	2	2	0	0	1	1	0	0	1	0	0	0	0	1	0	0	0	1	0	0	0	0
ZINC01643384_22_0000	0	0	0	0	0	0	1	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0
ZINC01765486_75_0000	0	0	0	0	0	0	1	1	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0
ZINC01696779_17_0001	0	0	0	0	0	0	1	1	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0
ZINC01690618_1_0000	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
ZINC01678023_38_0000	0	0	0	0	0	0	1	1	0	0	2	0	0	0	0	1	0	0	0	0	0	0	0	0
ZINC01577873_8_0000	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1	1	2
ZINC00389838_10_0000	0	0	0	1	0	0	1	1	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0
ZINC01634306_8_0000	0	0	0	1	1	0	1	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
ZINC01571612_9_0000	0	0	0	1	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0
ZINC01604103_10_0000	0	0	1	1	0	0	1	1	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0
ZINC00399488_3_0000	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	1
ZINC00388143_4_0000	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
ZINC00406951_5_0000	0	0	0	1	0	0	1	1	0	0	0	0	0	0	0	2	0	0	0	0	1	0	0	0
ZINC01666984_28_0000	0	0	1	0	0	0	1	1	0	0	2	0	0	0	0	2	0	0	0	0	0	0	0	0
ZINC01662386_7_0000	0	0	0	1	0	0	1	1	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0
ZINC01716672_19_0000	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0
ZINC01604777_9_0000	0	0	2	2	0	0	1	1	0	0	0	0	0	1	0	1	0	0	0	1	0	0	0	0
ZINC01760433_3_0000	0	0	0	1	0	0	1	1	1	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0
ZINC01571614_28_0000	0	0	0	0	0	0	1	1	1	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0
ZINC01716671_22_0000	0	0	1	1	0	0	2	1	0	0	1	0	0	0	0	1	0	0	0	0	0	0	0	0
ZINC01721653_9_0000	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	1	1	2	2
ZINC00334967_1_0000	0	0	1	1	0	0	1	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1
ZINC01648289_3_0000	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0
ZINC01577204_1_0000	0	0	0	0	0	0	1	1	0	0	0	1	0	0	2	0	0	0	1	0	0	0	0	0
ZINC01661205_15_0000	0	0	2	1	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0
ZINC01712621_17_0000	0	0	0	1	0	0	1	1	0	0	1	0	0	0	0	0	0	0	0	0	1	1	2	1
ZINC01606501_15_0000	0	0	2	2	0	0	1	1	0	0	1	0	0	0	0	0	0	0	0	0	0	1	1	1
ZINC01701838_24_0000	0	0	0	1	0	0	1	1	0	0	2	0	0	0	0	0	0	0	0	0	0	1	2	0
ZINC02022076_1_0000	0	0	0	1	0	0	0	1	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0
ZINC01653215_21_0000	0	0	0	0	0	0	1	1	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0
ZINC00391230_20_0000	0	0	0	1	0	0	0	1	1	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0
ZINC01555566_29_0001	0	0	0	1	0	0	1	1	1	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0
ZINC01670293_7_0000	0	0	0	1	0	0	1	1	0	1	2	0	0	0	0	0	0	0	0	0	0	0	0	0
ZINC01571102_2_0000	0	0	3	2	0	0	1	1	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0
ZINC01687319_3_0000	0	0	0	0	0	0	1	1	1	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0
ZINC00033882_8_0000	0	0	1	1	0	0	1	0	0	0	0	0	0	0	0	0	1	0	1	0	1	0	1	0



Supplementary Table 9

Interaction matchprints for the top-scoring 100 candidates according to GOLD score. Interactions are highlighted in grey, showing the number of ligand interactions with the corresponding thrombin atom (for polar interactions) or side chain (for hydrophobic interactions).

LIGAND	ARG 39 NE	ARG 39 sc	LEU 41 O	LEU 41 sc	CYS 42 sc	HIS 57 NE2	HIS 57 sc	CYS 58 sc	TYR 60A OH	TYR 60A sc	TRP 60D sc	ASP 60E sc	LYS 60F NZ	LYS 60F sc	PHE 60H sc	GLU 97A O	LEU 99 sc	ASN 143 ND2	GLU 146 sc	ILE 174 sc	ASP 189 OD1	ASP 189 OD2	ASP 189 sc	ALA 190 N	ALA 190 O	ALA 190 sc	CYS 191 O	CYS 191 sc	GLU 192 N	GLU 192 sc	GLY 193 N	ASP 194 sc	SER 195 N	VAL 213 sc	SER 214 N	SER 214 O	TRP 215 sc	GLY 216 N	GLY 216 O	GLU 217 sc	GLY 219 N	GLY 219 O	CYS 220 sc	ARG 221A N	ARG 221A sc	LYS 224 sc	PHE 227 N	PHE 227 O	TYR 228 OH	TYR 228 sc	
ZINC01563104_12_0000	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	1	0	0	0	2	1	0	0	0	3	0	0	0	0	0	1	1	0	0	0	0	0	2			
ZINC01574115_19_0001	0	0	1	0	1	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	1	2	0	0	0	0	0	3		
ZINC01692101_32_0000	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	2	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	3		
ZINC01561701_16_0000	0	0	0	0	0	0	0	0	0	0	6	1	0	0	0	0	0	0	0	0	0	1	1	1	0	0	1	0	0	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0		
ZINC01621077_5_0001	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	2	0	0	0	0	0	1	0	0	0	0	0	1	2	0	0	0	0	0	0		
ZINC01558276_9_0000	0	0	0	0	0	0	0	0	0	1	4	0	0	0	0	0	1	0	0	0	0	0	0	0	1	0	0	1	0	0	1	0	0	0	0	3	0	0	1	0	0	0	1	1	0	0	0	0	1		
ZINC01871513_51_0000	0	0	0	0	1	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	1	1	1	0	1	0	0	2	0	0	0	0	0	1	0	0	0	0	0	0	2	0	0	0	1	0	0	0		
ZINC01595840_5_0000	0	0	0	0	0	0	1	0	0	1	2	0	0	0	0	0	3	0	0	0	0	0	1	0	0	1	0	1	0	0	0	0	0	1	1	0	1	3	0	0	0	0	2	0	0	0	0	0	0		
ZINC01568061_2_0046	0	0	1	0	1	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	2	2	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0		
ZINC01688849_3_0001	0	0	0	0	0	0	0	0	0	4	5	0	0	0	0	0	1	0	0	0	0	0	1	1	0	1	1	0	0	0	0	0	0	1	1	0	0	0	1	0	0	0	1	1	0	0	0	0	0	0	
ZINC01720708_4_0002	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	2	0	0	0	1	0	0	0	2	0	0	0	0	1	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	
ZINC01624897_1_0000	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	2	1	0	0	0	0	0	2		
ZINC01686453_13_0000	0	0	0	0	0	0	1	0	0	3	3	0	0	0	0	0	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	2	0	0	1	0	0	0	0	0	1	0	0	0	0	0	2		
ZINC01613676_17_0000	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	2	0	0	0	0	2	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	2	
ZINC01735857_2_0000	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	1	0	0	1	1	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	2	1	0	0	0	0	0	
ZINC01601370_2_0000	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	1	1	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5		
ZINC01739338_14_0001	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	1	1	0	1	1	0	0	2	1	0	0	1	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	
ZINC01726994_2_0006	0	0	0	0	0	0	1	0	0	5	3	0	0	0	0	0	3	0	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	1	0	1	1	0	0	0	0	0	1	1	0	0	0	0	0	0	
ZINC01637216_5_0000	0	0	0	0	1	0	0	0	0	2	3	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	1	1	0	0	0	0	
ZINC01682715_80_0000	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0	3	0	0	0	0	0	1	1	0	0	0	0	0	1	5			
ZINC00123621_45_0000	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	2	0	1	2	0	0	0	0	
ZINC01708139_1_0000	0	0	0	0	1	1	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
ZINC00052703_10_0002	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	1	0	1	3	0	0	0	0	0	0	0	0	0	0	0	0	3		
ZINC01592542_8_0002	0	0	0	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	1	0	0	1	1	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	
ZINC01736496_210_0000	0	0	0	0	0	0	0	0	0	2	3	0	0	0	0	0	2	0	0	0	0	0	1	0	0	1	0	0	0	2	1	0	0	1	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	
ZINC00108625_21_0002	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	1	0	1	3	0	0	0	0	0	0	0	0	0	0	0	0	0	3	
ZINC01610993_3_0000	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	2	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
ZINC01670873_12_0000	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	3	
ZINC01596947_3_0001	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	1	1	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ZINC01692111_2_0000	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0	1	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5	
ZINC01698330_2_0000	0	0	0	0	0	1	0	0	0	4	2	0	1	0	0	0	3	0	0	0	0	0	1	0	0	1	0	0	0	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ZINC01671304_5_0000	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	1	0	0	1	1	0	0	2	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	5
ZINC01579585_1_0000	0	0	0	0	2	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	1	1	1	0	0	0	0	0	1	2	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	4	
ZINC01573137_2_0000	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	1	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
ZINC01620753_7_0001	0	0	0	0	0	1	0	0	0	4	5	0	0	0	0	0	0	0	0	0	0	1	1	0	0	1	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ZINC01706605_4_0005	0	0	0	0	0	0	1	0	0	5	3	0	0	0	0	0	1	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1	0																	







