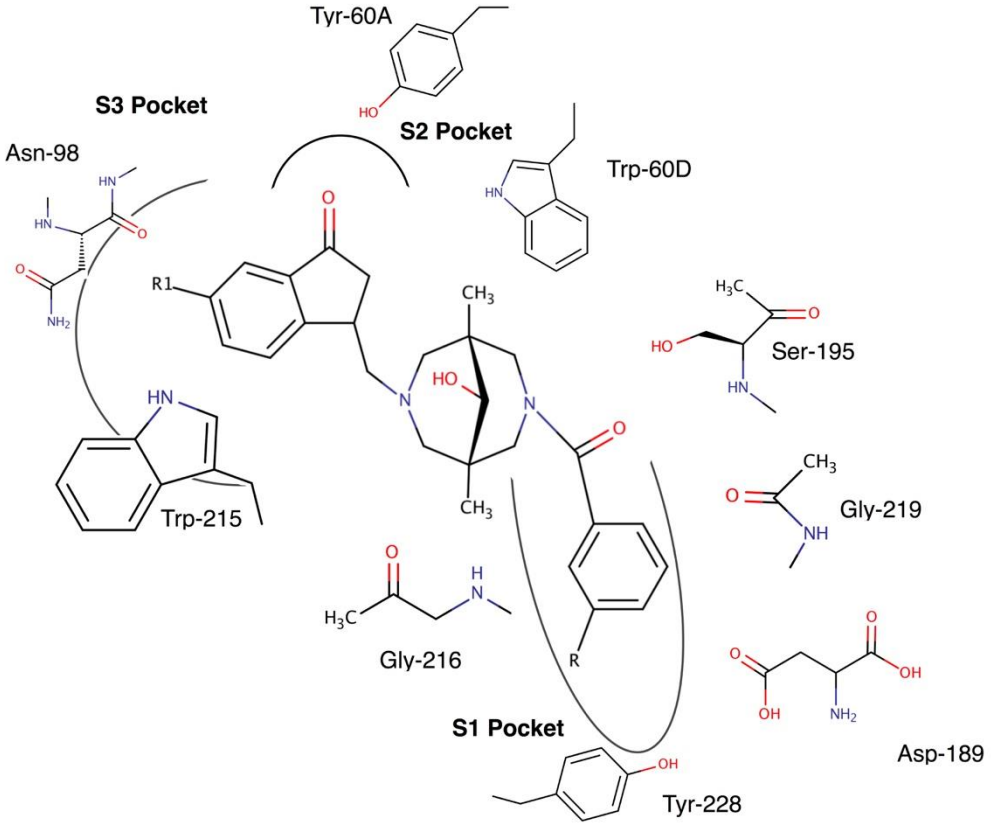
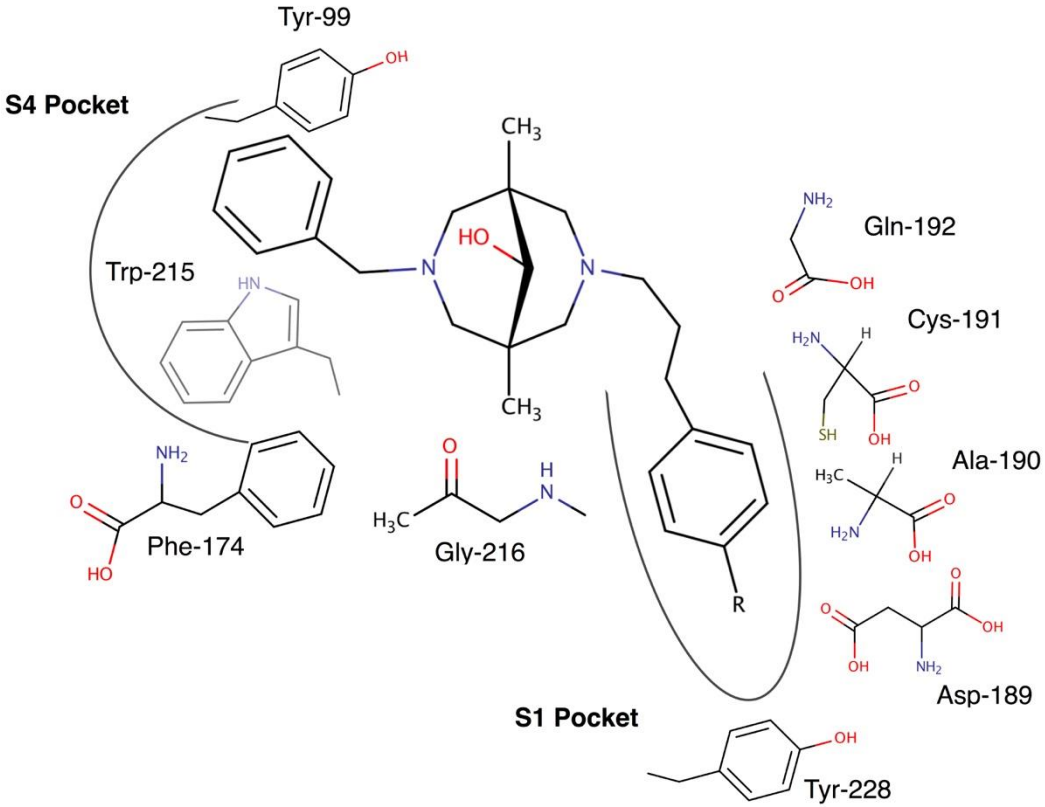
Electronic supplementary materials *Mendeleev Commun.*, 2016, **26**, 212−213

Computer modeling of ferrocene-substituted 3,7-diazabicyclo[3.3.1]nonanes as serine protease inhibitors

Sergey Z. Vatsadze, Dmitry A. Shulga, Yulia D. Loginova, Irina A. Vatsadze, Li Wang, Haojie Yu and Konstantin V. Kudryavtsev

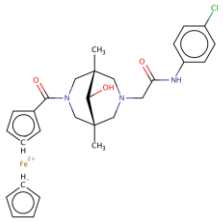
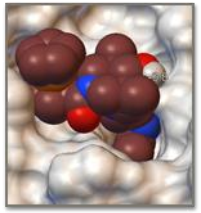
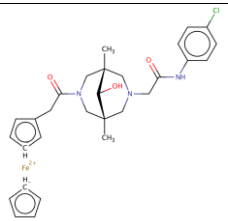
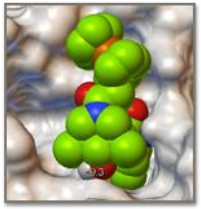
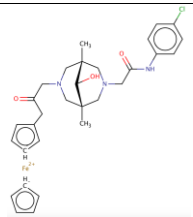
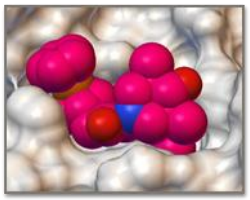


Thrombin binding site with ligand from our library (R=F, Cl, Br; R_1=F, Cl, Br).

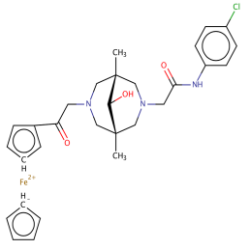
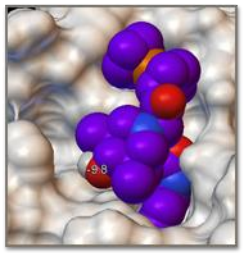
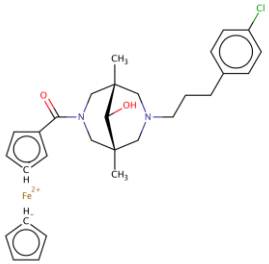
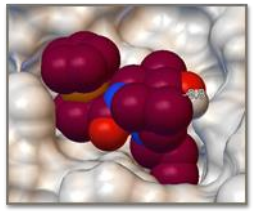
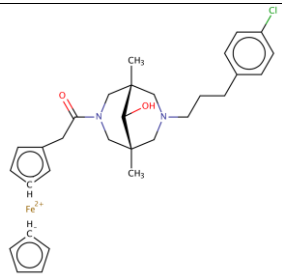
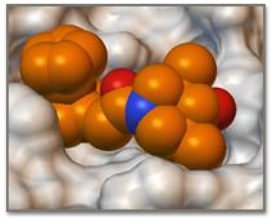
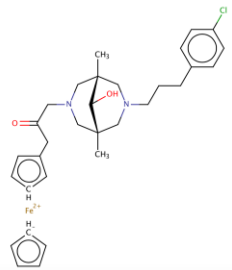
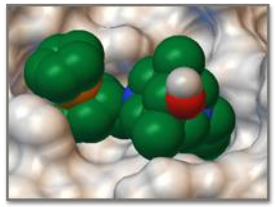


Factor Xa binding site with ligand from our library. (R=F, Cl, Br)

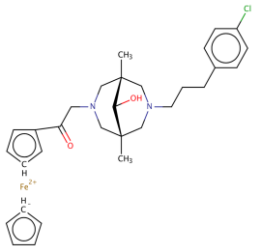
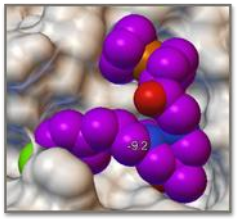
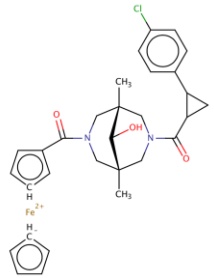
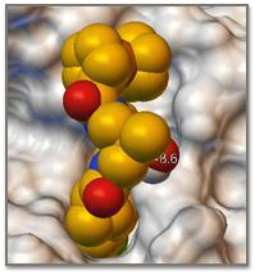
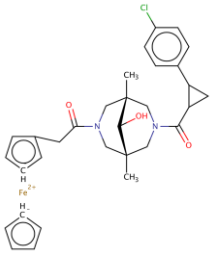
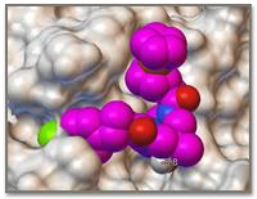
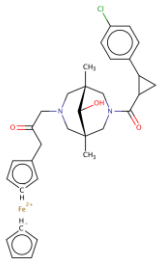
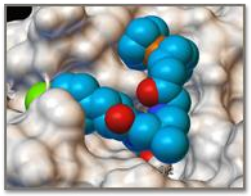
Results of the molecular docking of the ligands.

#	Compound	View	E_{vina}	K_{vina}, μM	N atoms	LE
Factor Xa						
1			-9.8	0.072	36	0.27
2			-9.3	0.166	37	0.25
3			-9.3	0.166	38	0.24

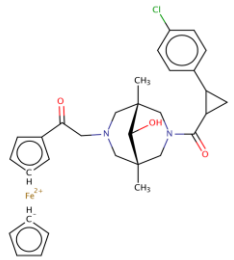
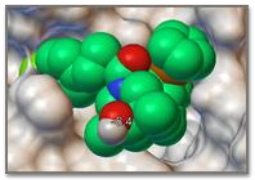
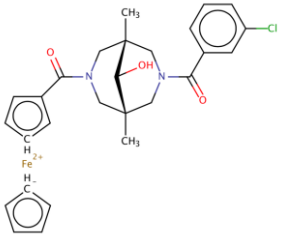
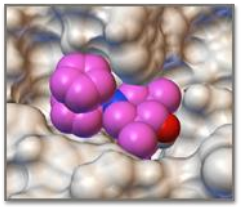
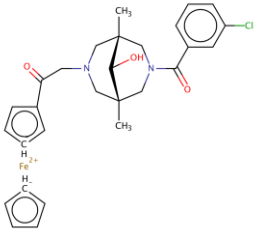
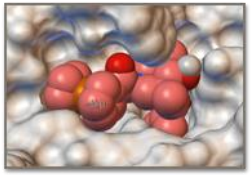
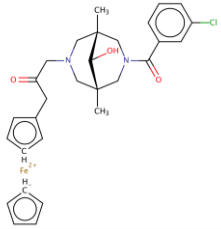
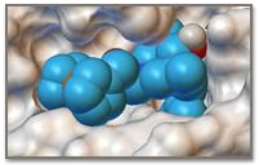
Results of the molecular docking of the ligands.

#	Compound	View	E_{vina}	K_{vina}, μM	N atoms	LE
4			-9.8	0.072	37	0.26
5			-9.8	0.072	35	0.28
6			-10.5	0.022	36	0.29
7			-8.9	0.326	37	0.24

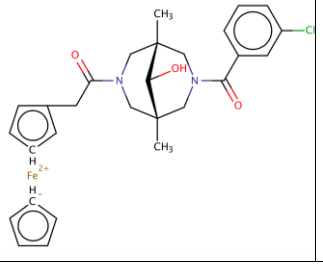
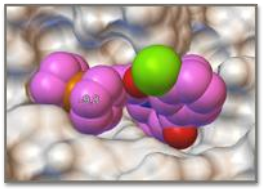
Results of the molecular docking of the ligands.

#	Compound	View	E_{vina}	K_{vina}, μM	N atoms	LE
8			-9.2	0.197	36	0.26
9			-8.6	0.539	37	0.23
10			-8.8	0.385	38	0.23
11			-9.2	0.197	39	0.24

Results of the molecular docking of the ligands.

#	Compound	View	E_{vina}	K_{vina}, μM	N atoms	LE
12			-8.4	0.753	38	0.22
Thrombin						
13			-10.4	0.026	34	0.31
14			-11.0	0.010	35	0.31
15			-10.2	0.037	36	0.28

Results of the molecular docking of the ligands.

#	Compound	View	E_{vina}	K_{vina}, μM	N atoms	LE
16			-9.8	0.072	35	0.28