

Covalent Docking for Novel Series of Spiro-butenolides on Trx R1 for QSAR Modelling



Veronika Yudina^{1,*} , Alexander Zozulya¹ , Evgeny Chupakhin¹  and Dmitry Dar In² 

¹Immanuel Kant Baltic Federal University, ESC «MedBio», Kaliningrad 236016, Russian Federation, Universitetskaya 2

²Institute of Chemistry, Saint Petersburg State University, Saint Petersburg 199034 Russia, Universitetskii Prospect 26, Peterhoff

© 2024 The Author(s). Published by Bentham Open.

This is an open access article distributed under the terms of the Creative Commons Attribution 4.0 International Public License (CC-BY 4.0), a copy of which is available at: <https://creativecommons.org/licenses/by/4.0/legalcode>. This license permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.



*Address correspondence to this author at the Immanuel Kant Baltic Federal University, ESC «MedBio», Kaliningrad 236016, Russian Federation, Universitetskaya 2; E-mail: anohovaveronika@yandex.ru

Cite as: Yudina V, Zozulya A, Chupakhin E, In D. Covalent Docking for Novel Series of Spiro-butenolides on Trx R1 for QSAR Modelling. Open Med Chem J, 2024; 18: e18741045322069. <http://dx.doi.org/10.2174/0118741045322069240730073553>

Published: September 05, 2024



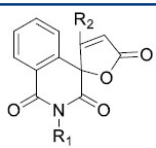
Send Orders for Reprints to reprints@benthamscience.net

Content

1. Structure for modelling
2. Visualization of docking results

Table 1. Structure for modeling.

#	R ₁	R ₂	R ₃	R ₄
1	4-F-Ph-	-H	-H	-H
2	Ph-	-H	-H	-H
3	CH ₃ -	-H	-H	-H
4	4-Me-Ph-	-H	-H	-H
5	4-OMe-Ph	-H	-H	-H
6	3-CF ₃ -Ph	-H	-H	-H
7	2-OMe-Ph	-H	-H	-H
8	(CH ₃) ₂ -CH-	-H	-H	-H
9	4-OMe-Ph-CH ₂	-H	-H	-H
10	(CH ₃) ₂ N-	-H	-H	-H
11	3,4-(OMe) ₂ -Ph-CH ₂ -CH ₂	-H	-H	-H
12	4-Cl-Ph-	-H	-F	-H
13	Ph-	-H	-Cl	-H
14	Ph	Me	-H	-H
15	Ph-	Ph-	-H	-H
16	Ph-	(CH ₂) ₂ CH ₃	-H	-H

				
#	R ₁	R ₂	R ₃	R ₄
17	Ph	Me	-H	-F
18	4-F-Ph	4-F-Ph	-H	-H
19	4-Me-Ph	4-OMe-Ph	-H	-H
20	(CH ₃) ₂ -CH-	2-Cl-Ph	-H	-H

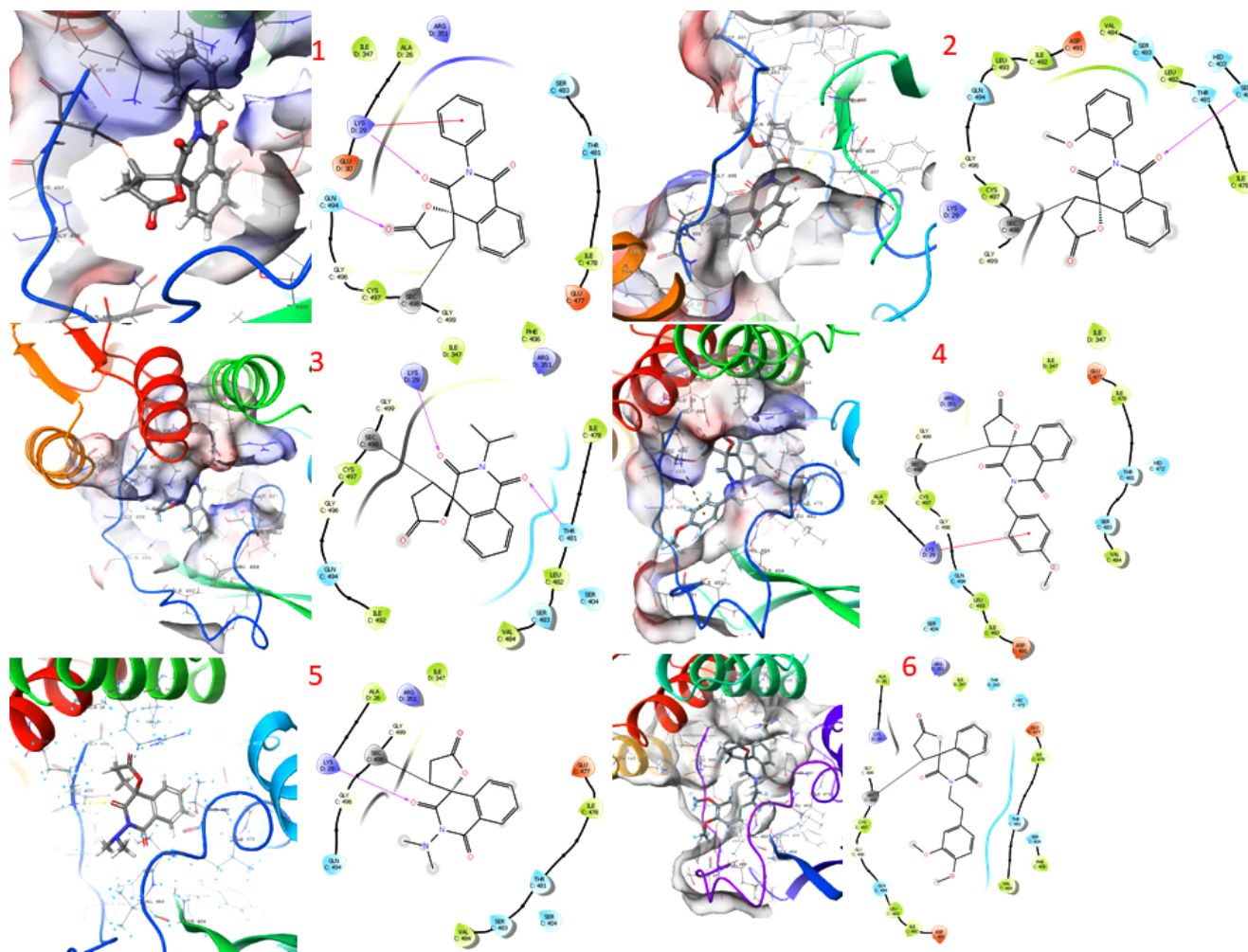


Fig. (1). Visualization of docking results.