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

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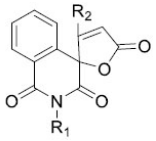
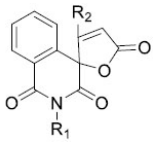
Content



**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- | $(CH_2)_2CH_3$ | -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 |

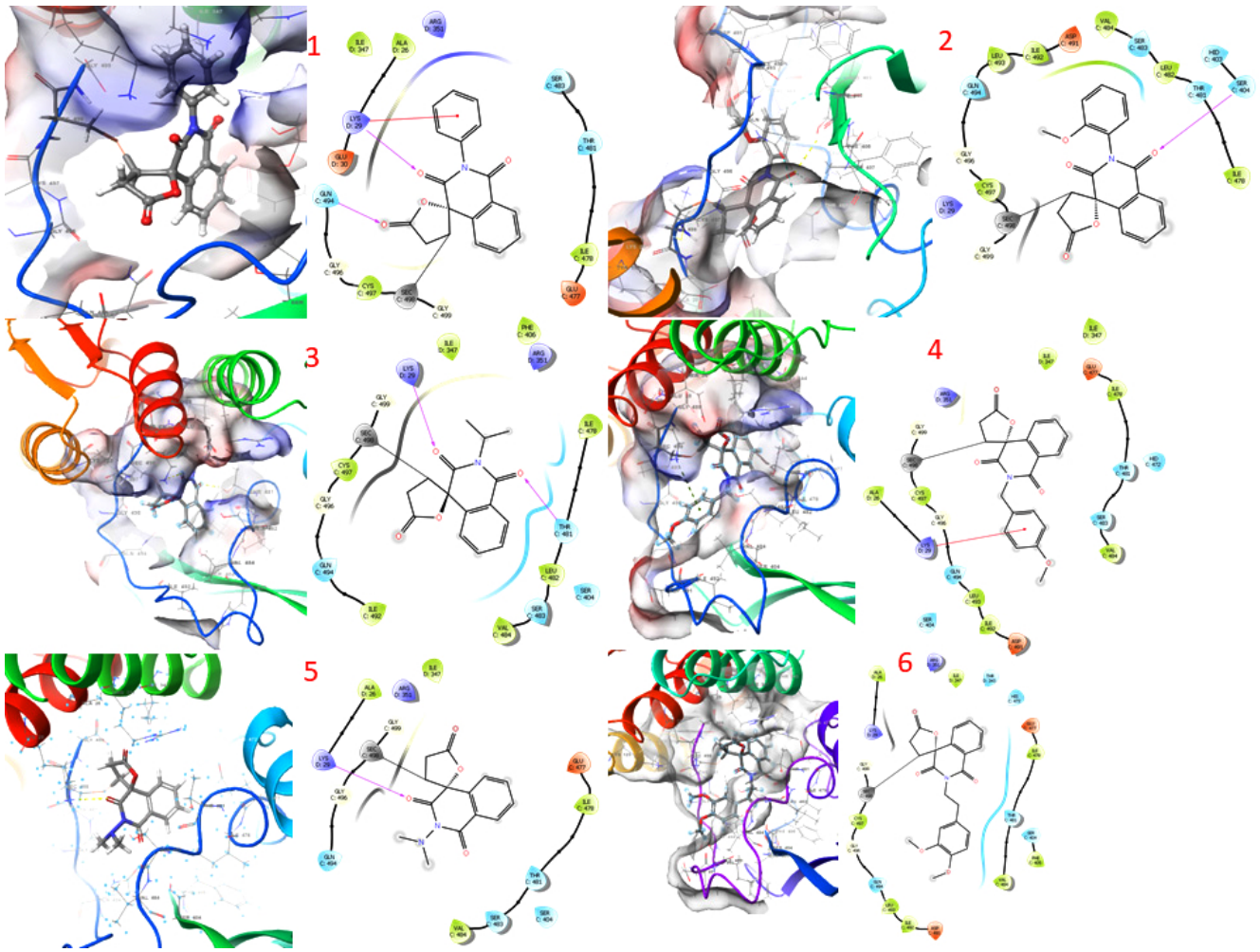



**Fig. (1).** Visualization of docking results.