

## **Supplementary File**

### **Computational Investigation of 1, 3, 4 oxadiazole derivatives as Lead Inhibitors of VEGFR 2 in comparison with EGFR: Density Functional Theory, Molecular docking and Molecular Dynamic Simulation Studies**

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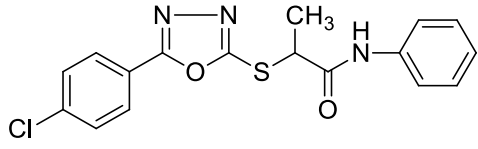
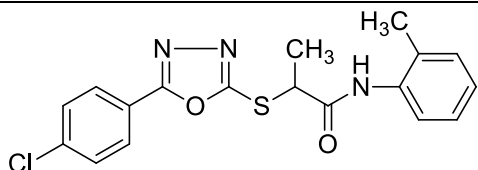
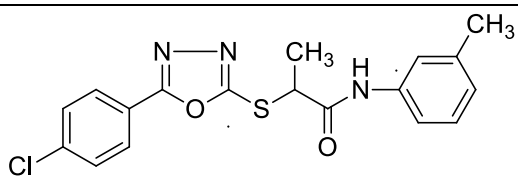
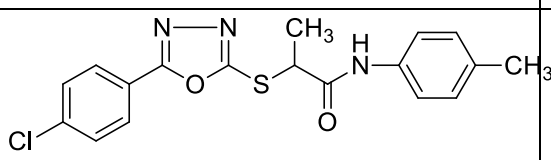
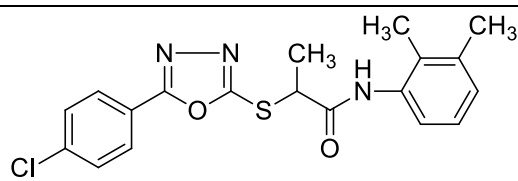
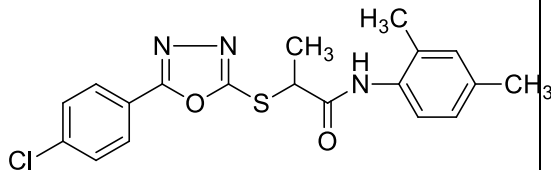
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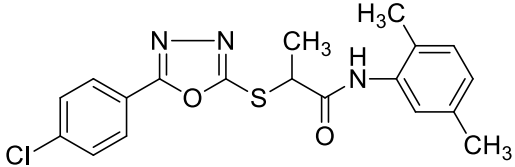
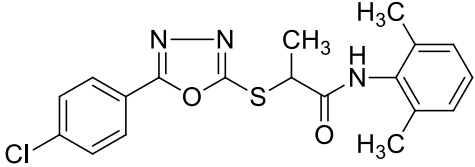
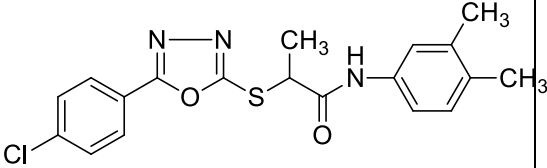
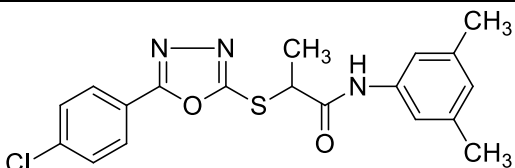
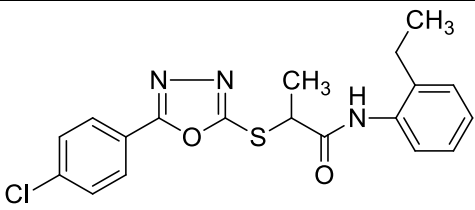
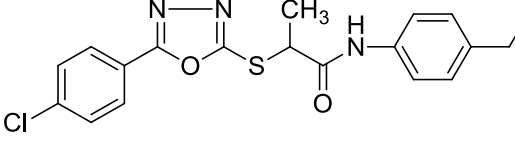
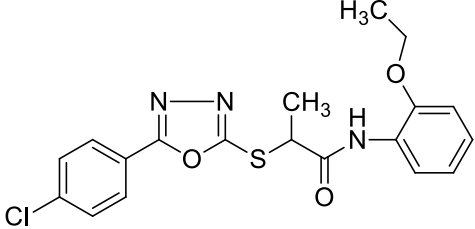
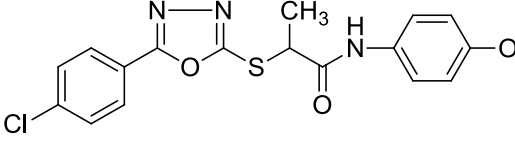
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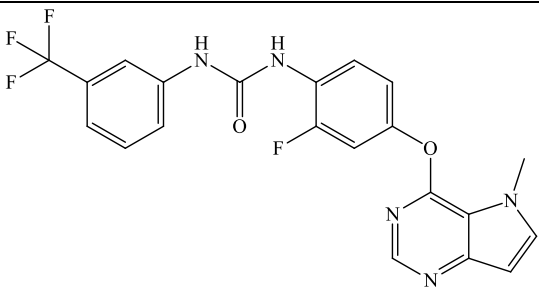
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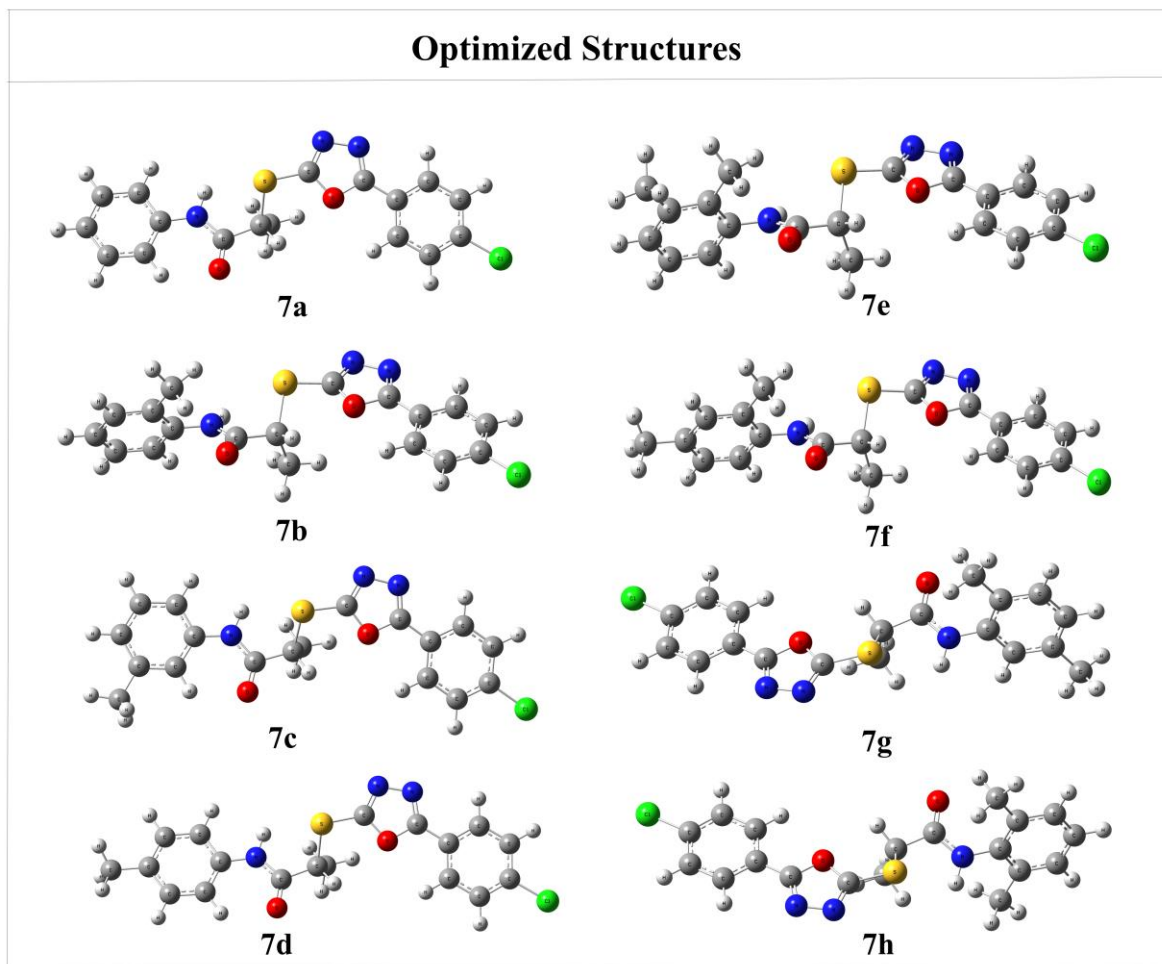
Dr. Syeda Abida Ejaz; *Department of Pharmaceutical Chemistry, Faculty of Pharmacy, The Islamia University of Bahawalpur, Pakistan., Postal Code 63100, Pakistan* Tel: +92-062-9250245 Fax: +92-062-9250245, E-Mail: abida.ejaz@iub.edu.pk; abidaejaz2010@gmail.com

**Table S1:** Chemical structures of oxadiazoles with IUPAC names.

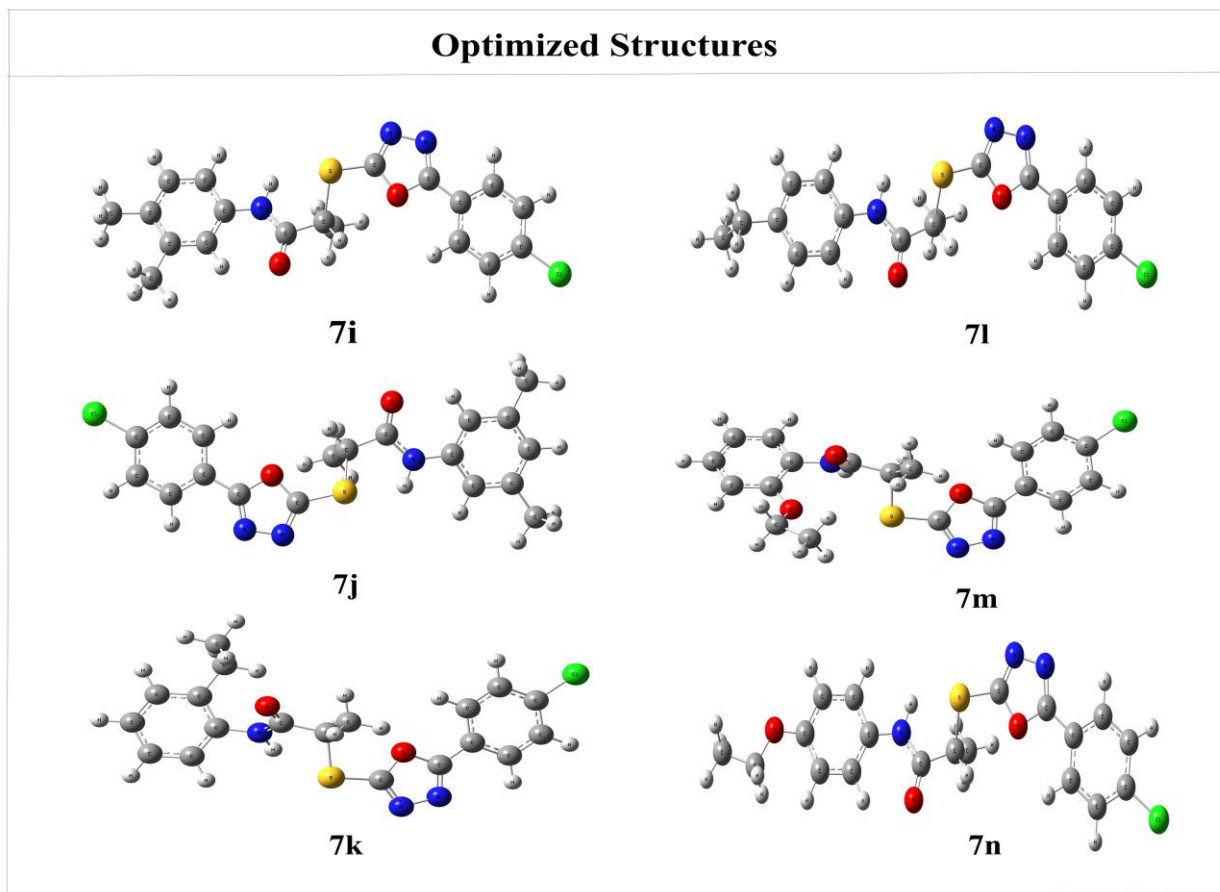
	Solubility	Substituted 1,3,4-Oxadiazoles-	Molecular Formula/ Molecular Mass	IUPAC NAME
<b>1</b>	CH <sub>3</sub> OH		C <sub>17</sub> H <sub>14</sub> ClN <sub>3</sub> O <sub>2</sub> S/359.05	2-((5-(4-chlorophenyl)-1,3,4-oxadiazol-2-yl)thio)-N-phenylpropanamide
<b>2</b>	CH <sub>3</sub> OH		C <sub>18</sub> H <sub>16</sub> ClN <sub>3</sub> O <sub>2</sub> S/373.07	2-((5-(4-chlorophenyl)-1,3,4-oxadiazol-2-yl)thio)-N-(o-tolyl)propanamide
<b>3</b>	CH <sub>3</sub> OH		C <sub>18</sub> H <sub>16</sub> ClN <sub>3</sub> O <sub>2</sub> S/373.07	2-((5-(4-chlorophenyl)-1,3,4-oxadiazol-2-yl)thio)-N-(m-tolyl)propanamide
<b>4</b>	CH <sub>3</sub> OH		C <sub>18</sub> H <sub>16</sub> ClN <sub>3</sub> O <sub>2</sub> S/373.07	2-((5-(4-chlorophenyl)-1,3,4-oxadiazol-2-yl)thio)-N-(p-tolyl)propanamide
<b>5</b>	CH <sub>3</sub> OH		C <sub>19</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>2</sub> S/387.08	2-((5-(4-chlorophenyl)-1,3,4-oxadiazol-2-yl)thio)-N-(2,3-dimethylphenyl)propanamide
<b>6</b>	CH <sub>3</sub> OH		C <sub>19</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>2</sub> S/387.08	2-((5-(4-chlorophenyl)-1,3,4-oxadiazol-2-yl)thio)-N-(2,4-dimethylphenyl)propanamide

7	CH <sub>3</sub> OH		C <sub>19</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>2</sub> S/387.08	2-((5-(4-chlorophenyl)-1,3,4-oxadiazol-2-yl)thio)-N-(2,5-dimethylphenyl)propanamide
8	CH <sub>3</sub> OH		C <sub>19</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>2</sub> S/387.08	2-((5-(4-chlorophenyl)-1,3,4-oxadiazol-2-yl)thio)-N-(2,6-dimethylphenyl)propanamide
9	CH <sub>3</sub> OH		C <sub>19</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>2</sub> S/387.08	2-((5-(4-chlorophenyl)-1,3,4-oxadiazol-2-yl)thio)-N-(3,4-dimethylphenyl)propanamide
10	CH <sub>3</sub> OH		C <sub>19</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>2</sub> S/387.08	2-((5-(4-chlorophenyl)-1,3,4-oxadiazol-2-yl)thio)-N-(3,5-dimethylphenyl)propanamide
11	CH <sub>3</sub> OH		C <sub>19</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>2</sub> S/387.08	2-((5-(4-chlorophenyl)-1,3,4-oxadiazol-2-yl)thio)-N-(2-ethylphenyl)propanamide
12	CH <sub>3</sub> OH		C <sub>19</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>2</sub> S/387.08	2-((5-(4-chlorophenyl)-1,3,4-oxadiazol-2-yl)thio)-N-(4-ethylphenyl)propanamide
13	CH <sub>3</sub> OH		C <sub>19</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>3</sub> S/403.08	2-((5-(4-chlorophenyl)-1,3,4-oxadiazol-2-yl)thio)-N-(2-ethoxyphenyl)propanamide
14	CH <sub>3</sub> OH		C <sub>19</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>3</sub> S/403.08	2-((5-(4-chlorophenyl)-1,3,4-oxadiazol-2-yl)thio)-N-(4-ethoxyphenyl)propanamide

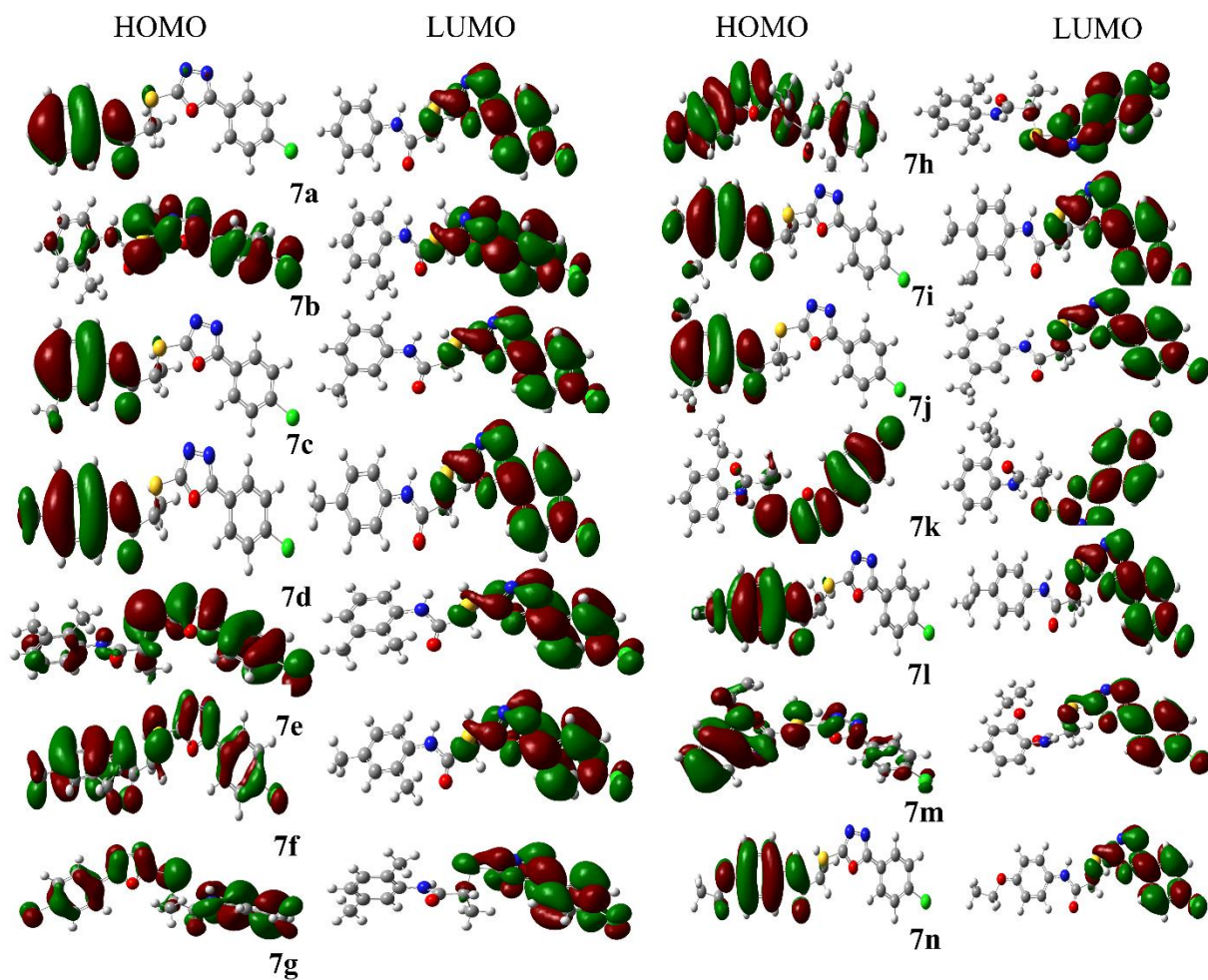
<b>Vegfr ligand</b>				1-{2-fluoro-4-[(5-methyl-5H-pyrrolo[3,2-d]pyrimidin-4-yl)oxy]phenyl}-3-[3-(trifluoromethyl)phenyl]urea



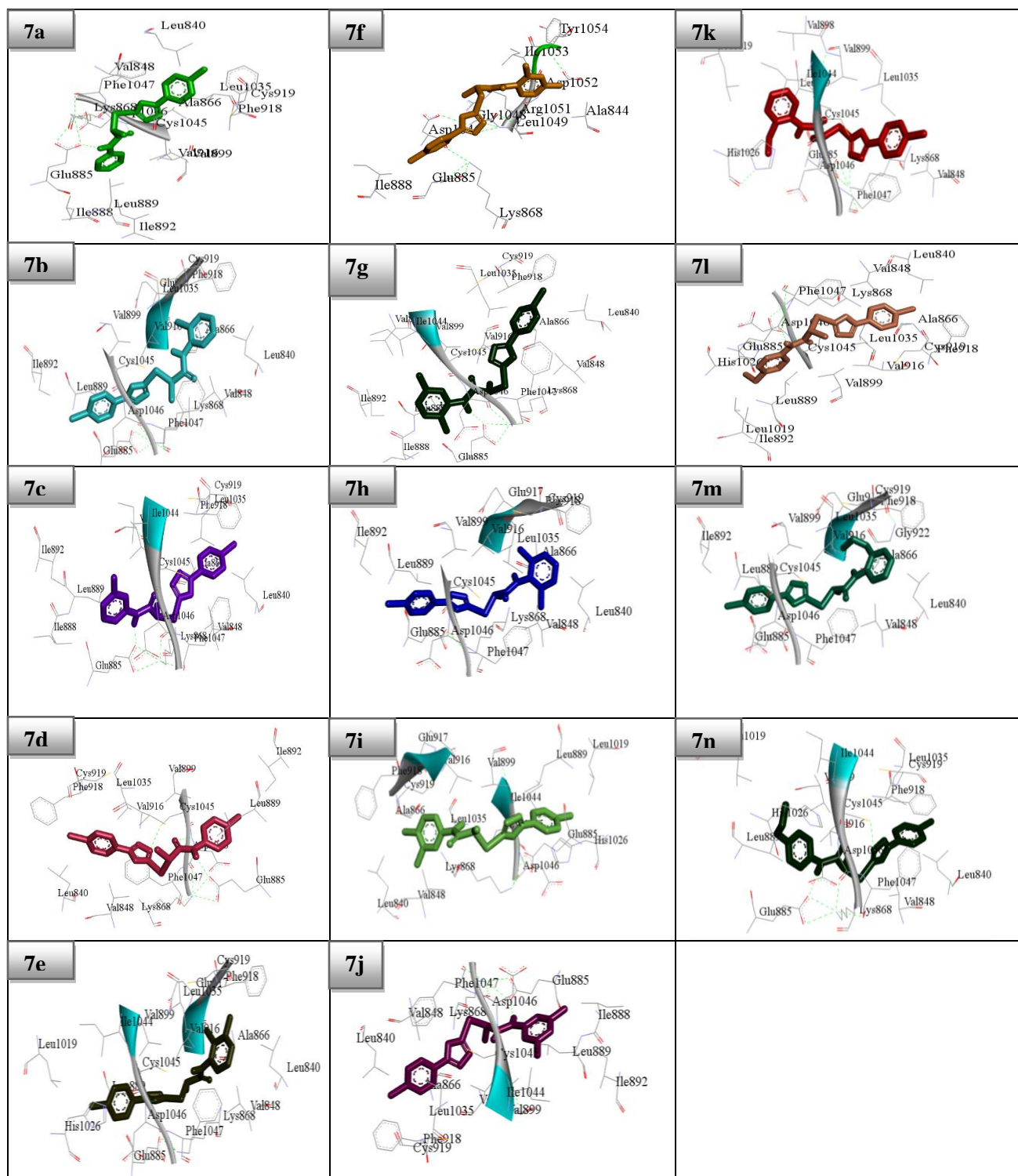
**Figure S1:** Optimized structures of the oxadiazoles derivatives (**7a-7h**) in gas phase.



**Figure S2:** Optimized structures of the oxadiazoles derivatives (**7i-7n**) in gas phase.

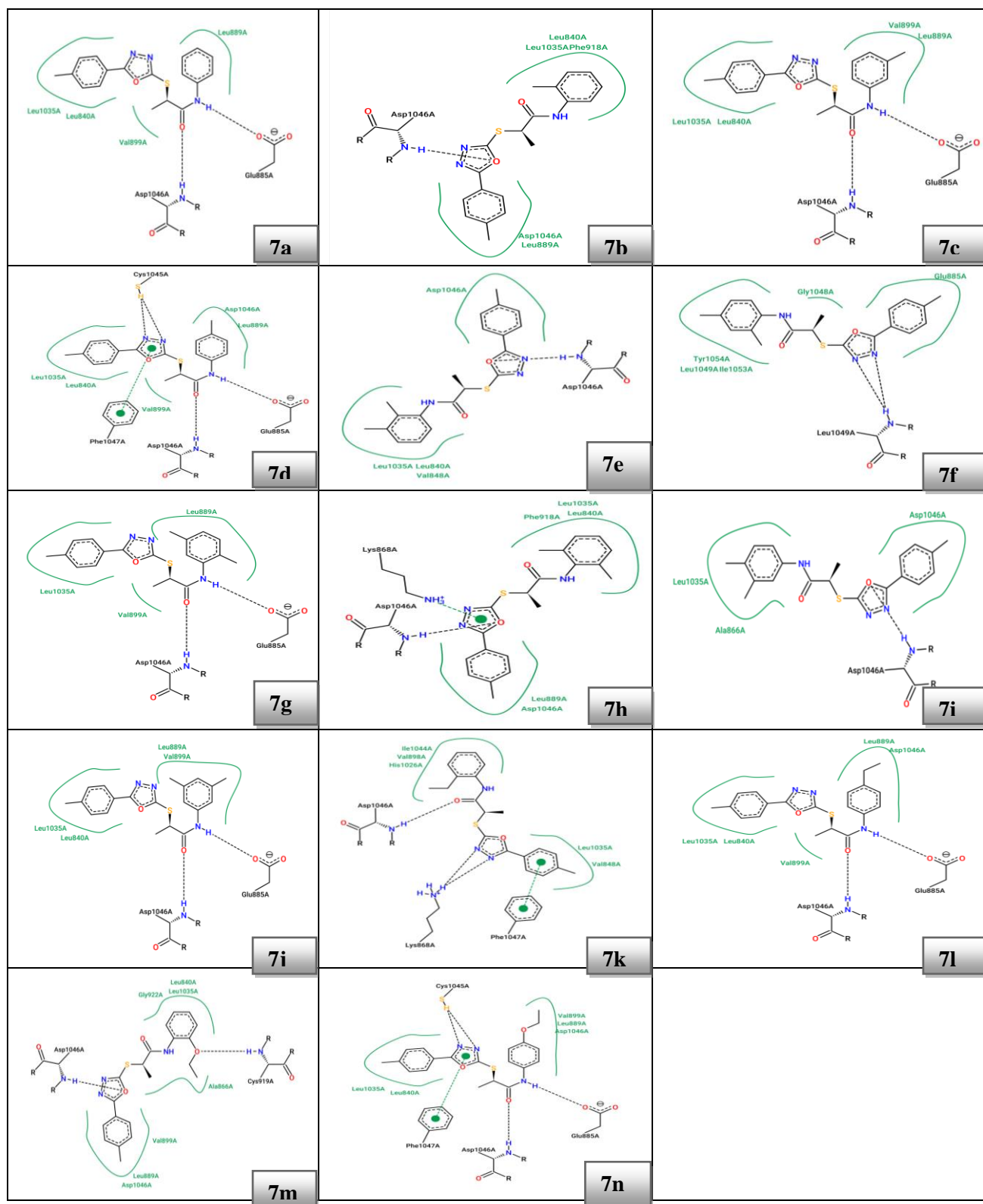


**Figure S3:** HOMO and LUMO structures of all the oxadiazoles derivatives in gas phase.

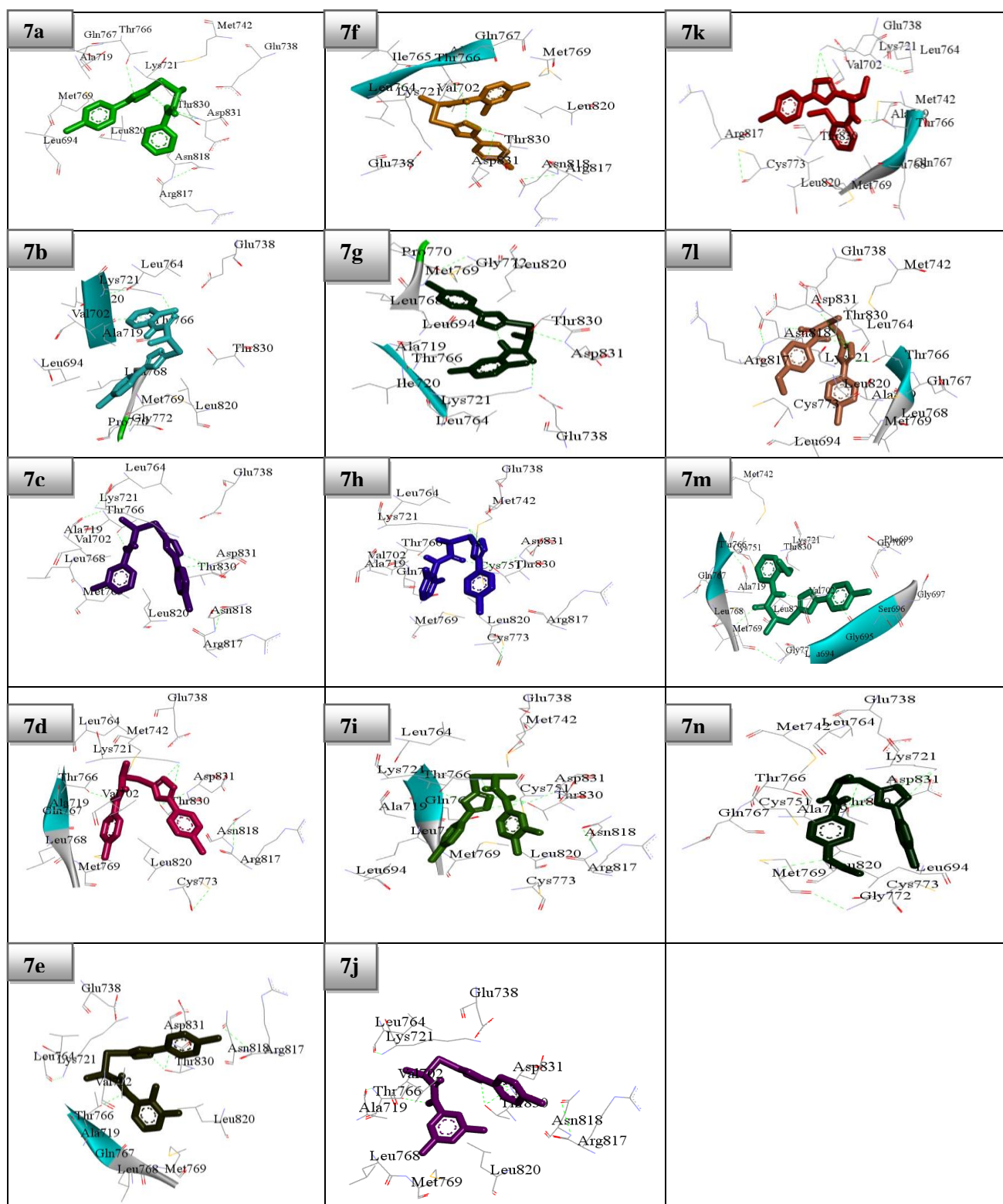


**Figure S4:** 3D binding interactions of all compounds with VEGFR

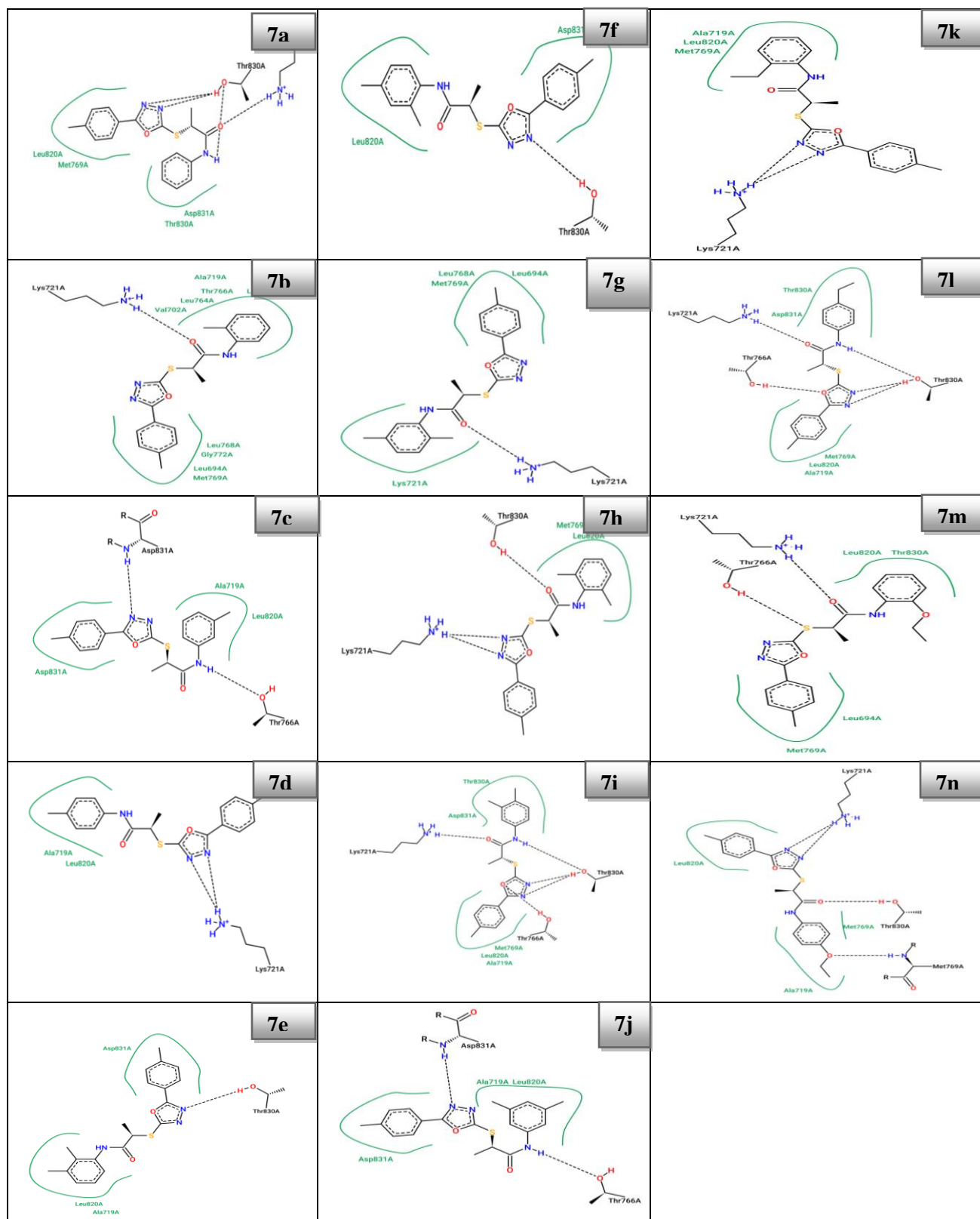




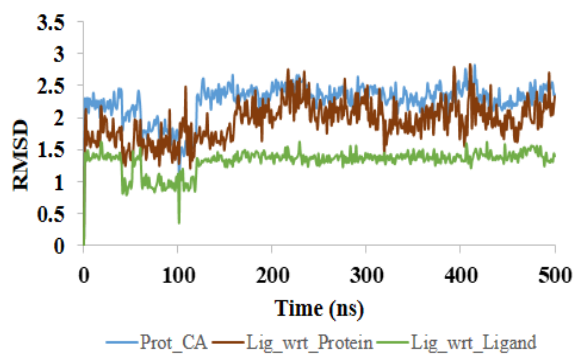
**Figure S5:** 2D binding interactions of all compounds with VEGFR



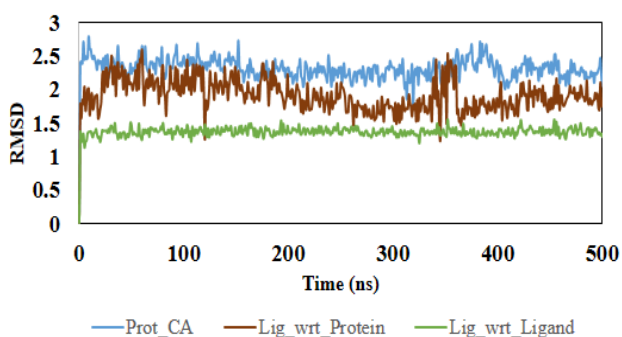
**Figure S6:** 3D binding interactions of all compounds with EGFR



**Figure S7:** 2D binding interactions of all compounds with EGFR

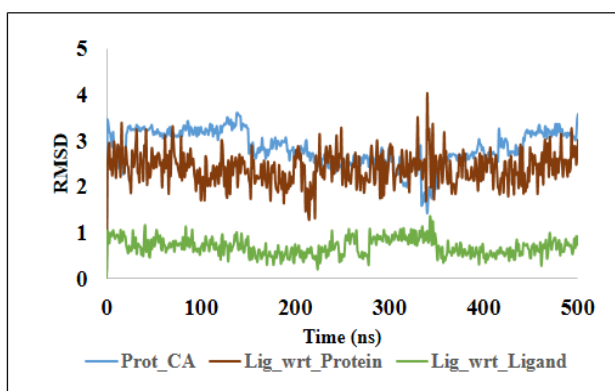


A

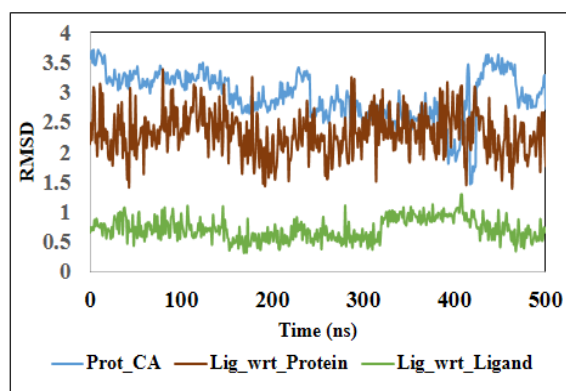


B

**Figure S8:** Simulation replicate of Vegfr-7j Complex



A



B

**Figure S9:** Simulation replicate of Egfr-7j Complex