

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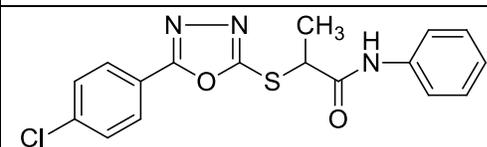
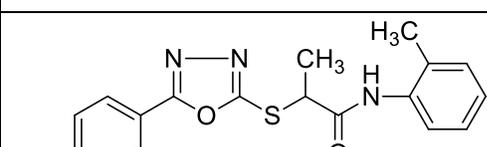
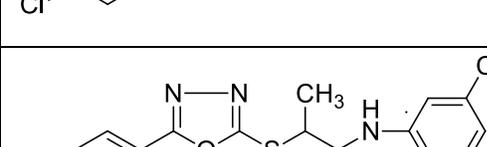
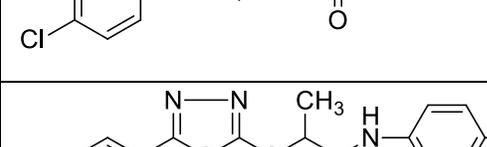
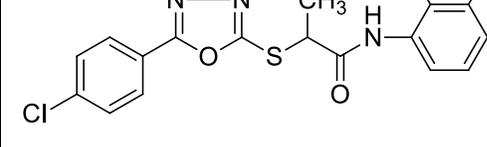
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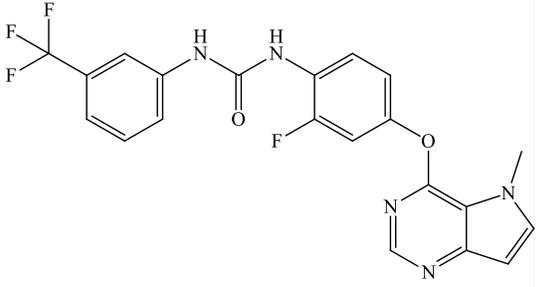
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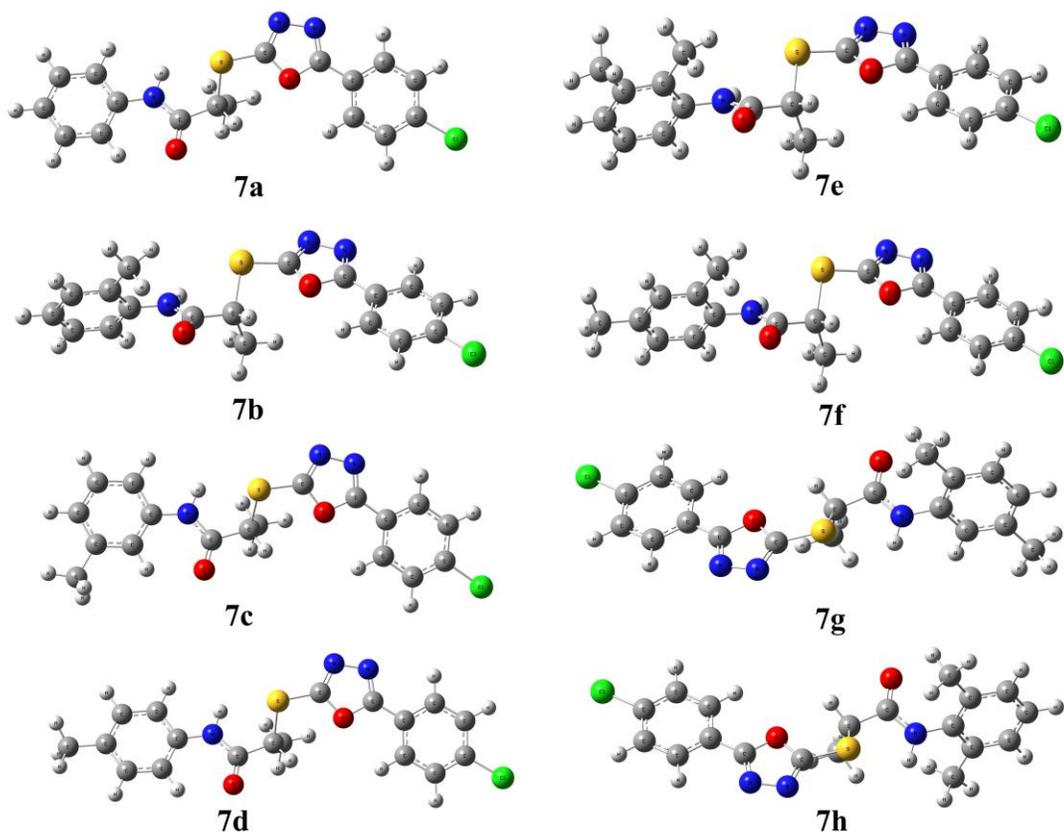
**Table S1:** Chemical structures of oxadiazoles with IUPAC names.

	Solubility	Substituted 1,3,4-oxadiazoles-	Molecular Formula/ Molecular Mass	IUPAC NAME
1	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
2	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
3	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
4	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
5	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
6	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

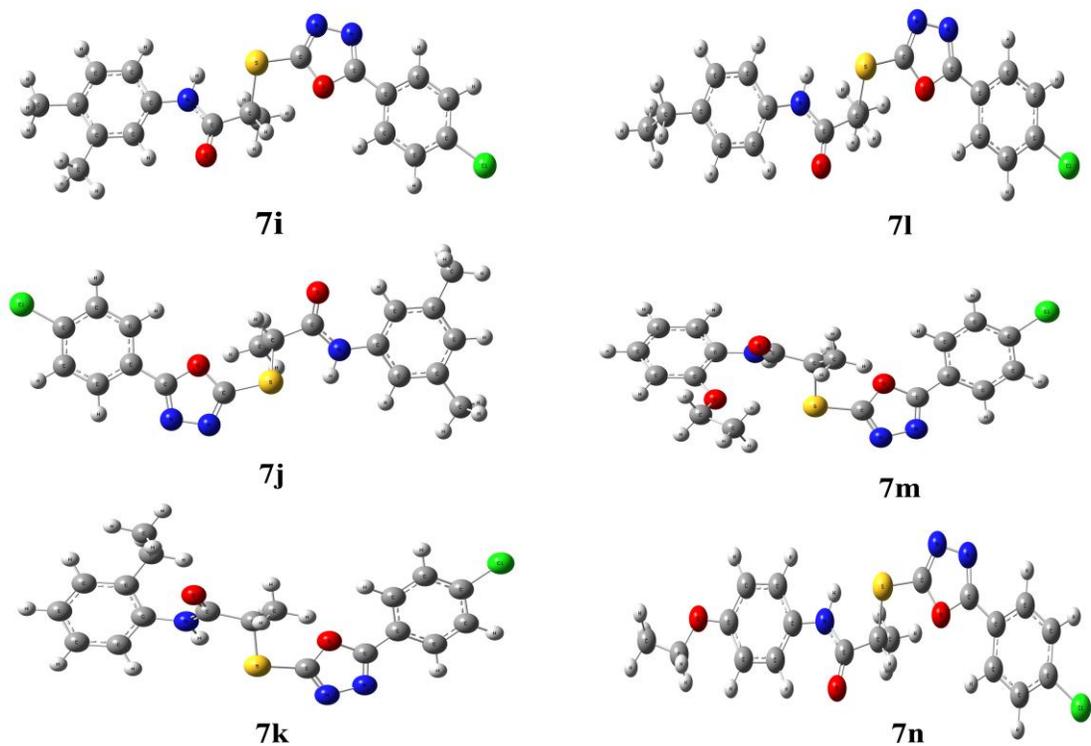
<b>Vegfr ligand</b>				1-(2-fluoro-4-[(5-methyl-5H-pyrrolo[3,2-d]pyrimidin-4-yl)oxy]phenyl)-3-(3-(trifluoromethyl)phenyl)urea

## Optimized Structures

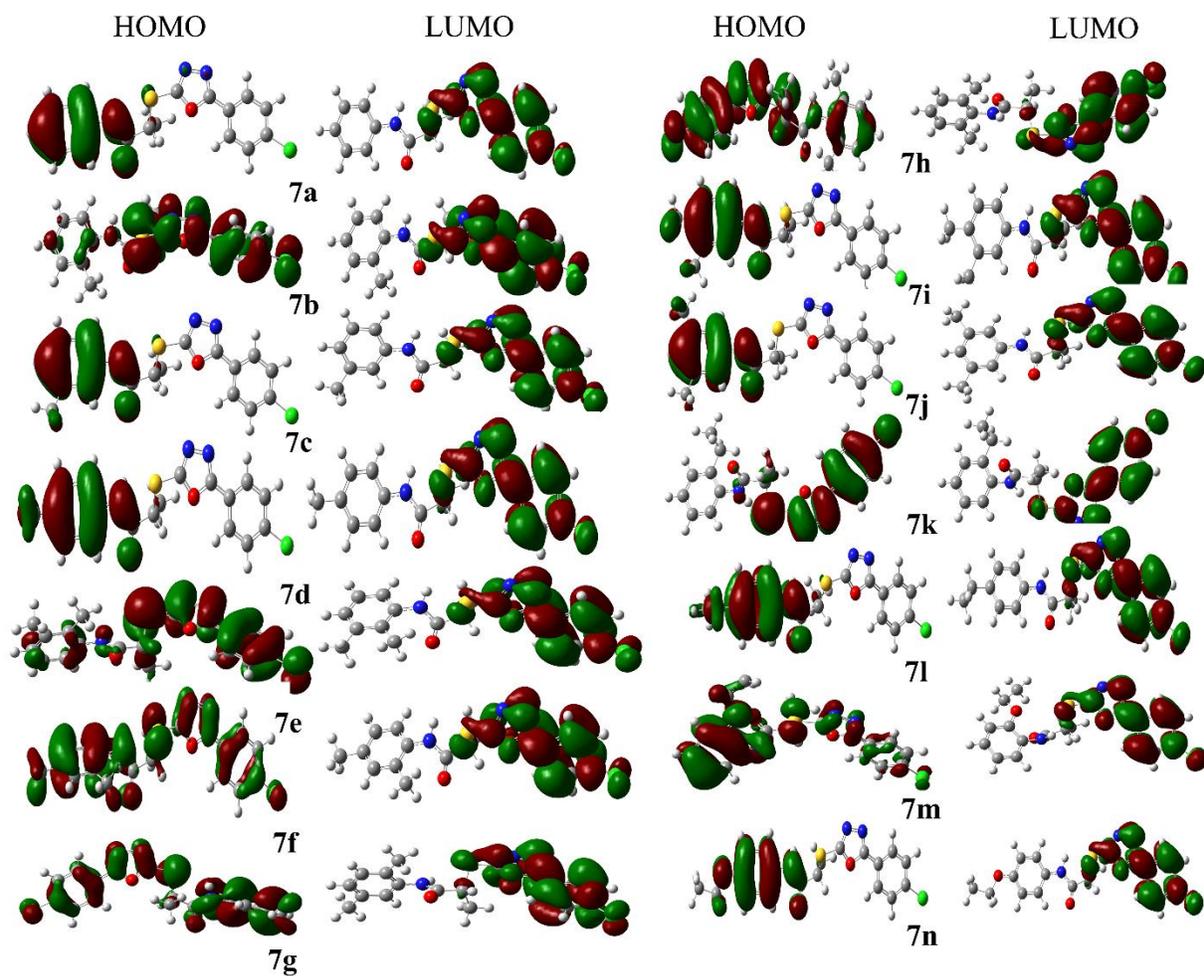


**Figure S1:** Optimized structures of the oxadiazoles derivatives (**7a-7h**) in gas phase.

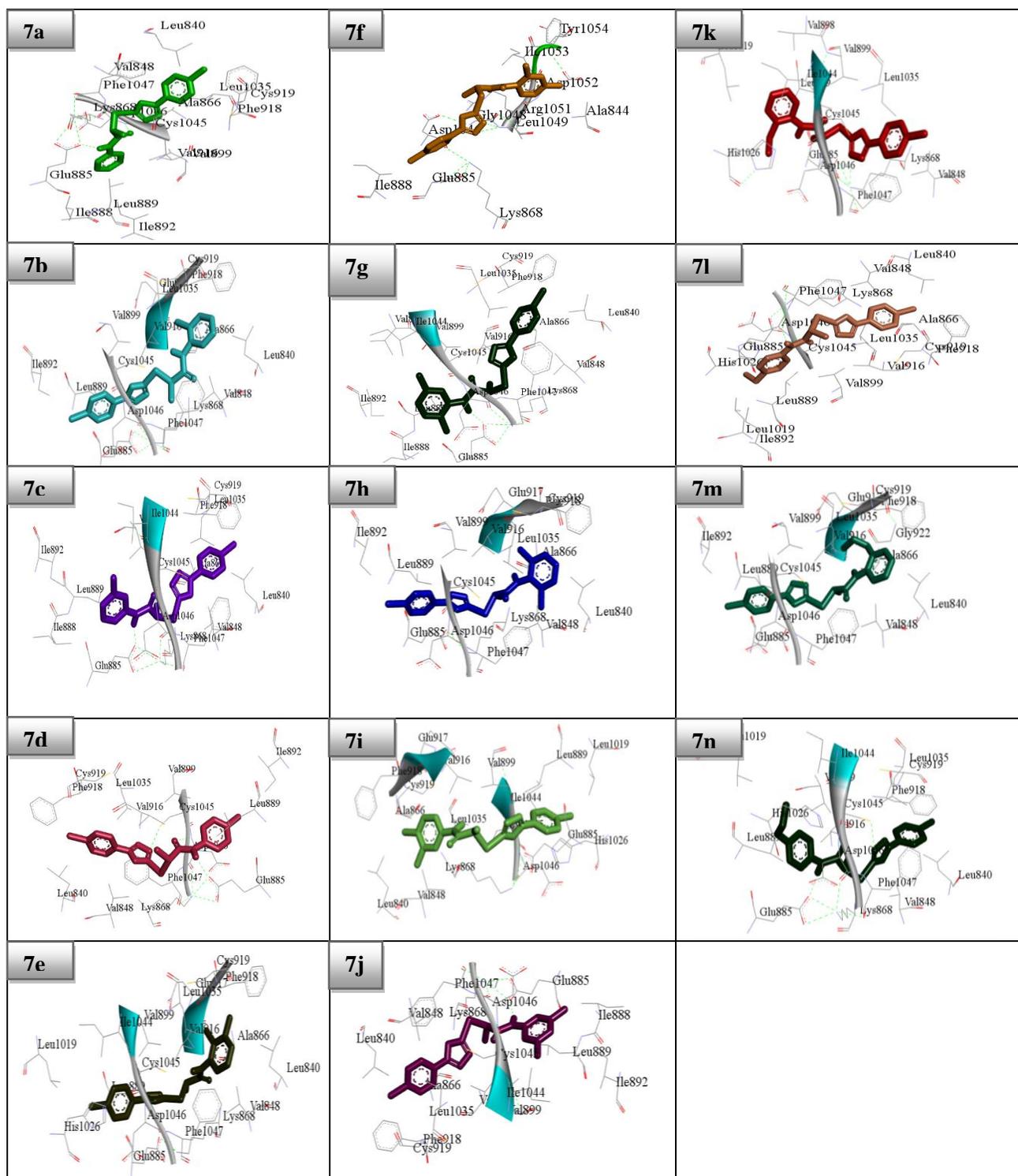
### Optimized Structures



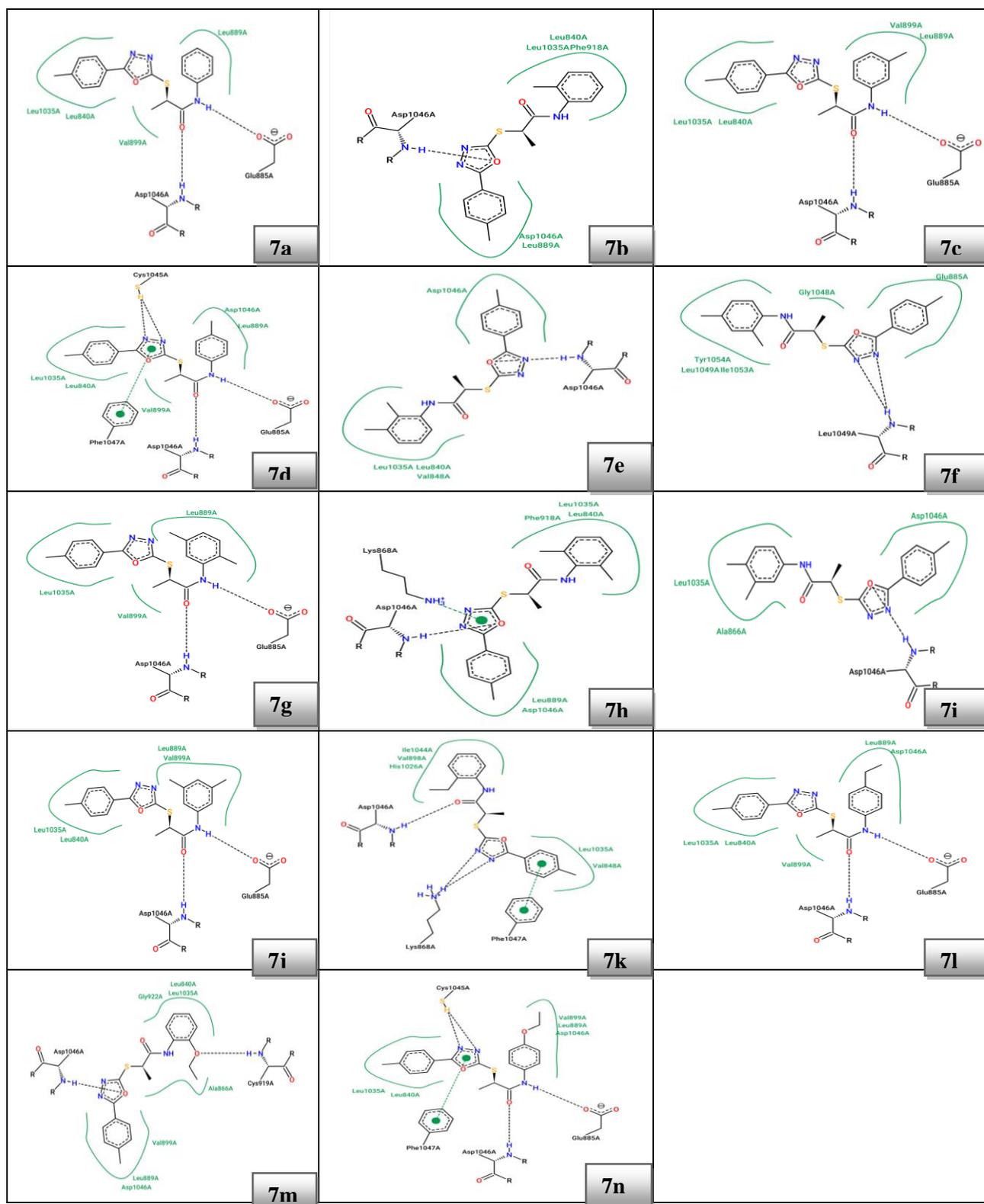
**Figure S2:** Optimized structures of the oxadiazoles derivatives (**7i-7n**) in gas phase.



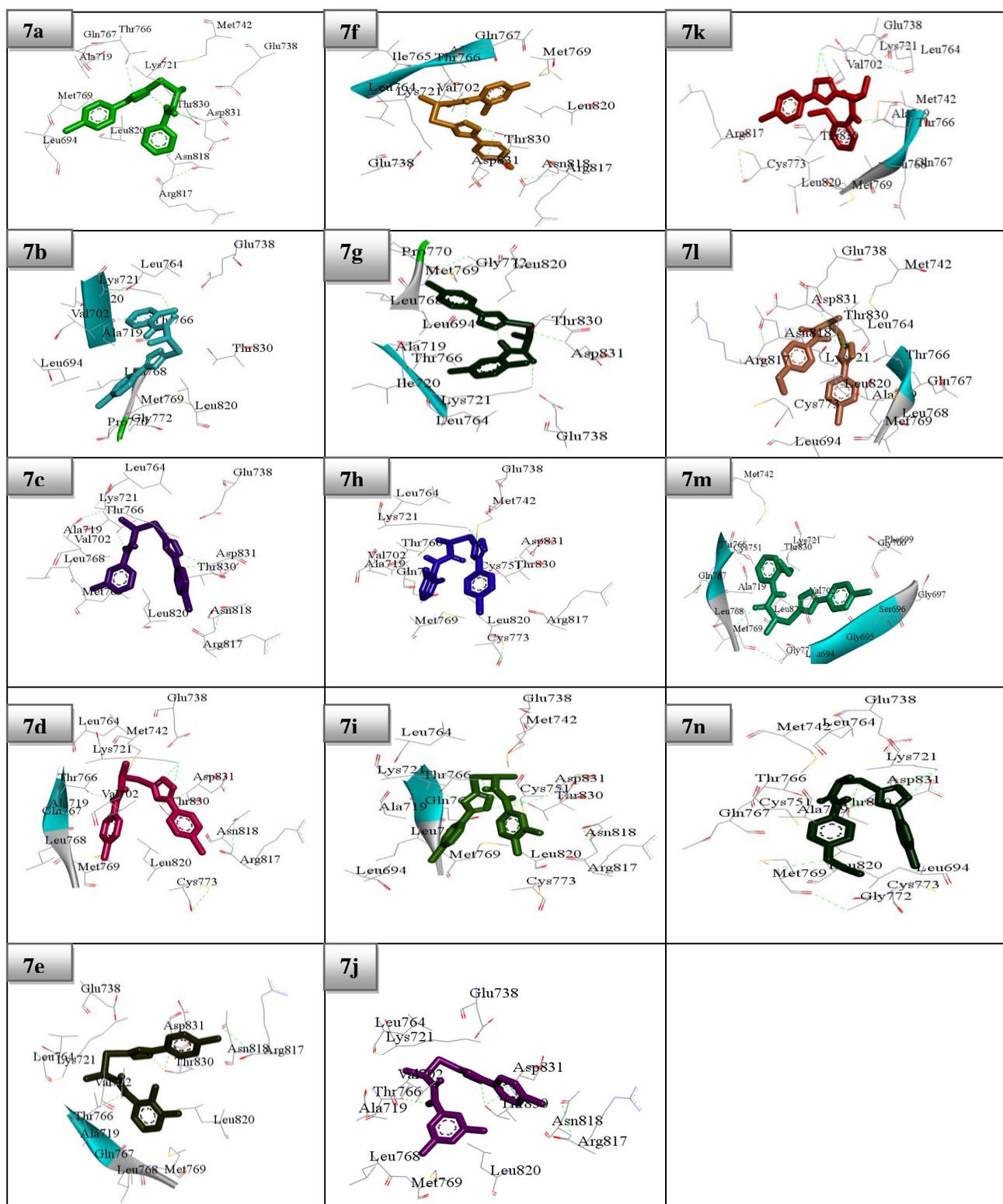
**Figure S3:** HOMO and LUMO structures of all the oxadiazoles derivatives in gas phase.



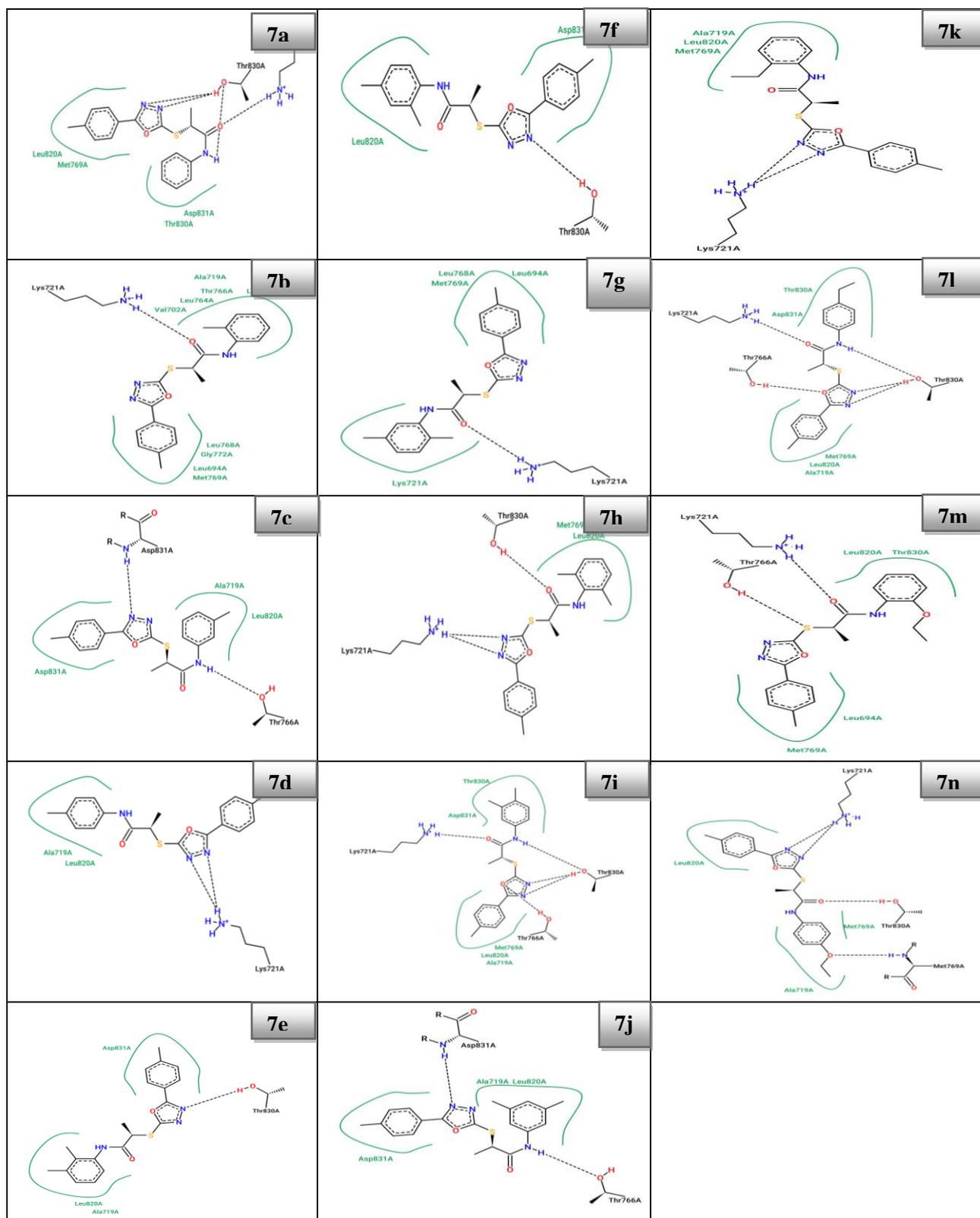
**Figure S4:** 3D binding interactions of all compounds with VEGFR



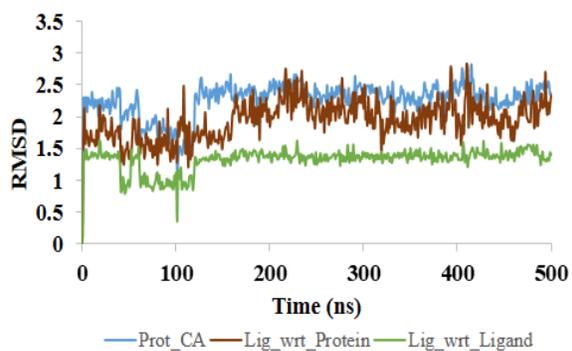
**Figure S5:** 2D binding interactions of all compounds with VEGFR



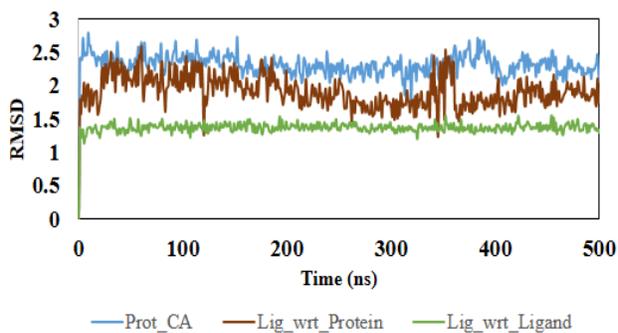
**Figure S6:** 3D binding interactions of all compounds with EGFR



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

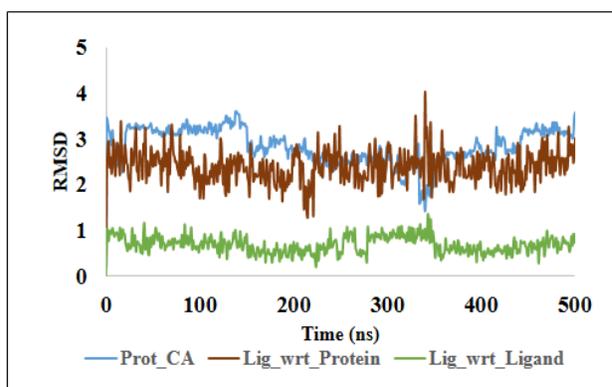


A

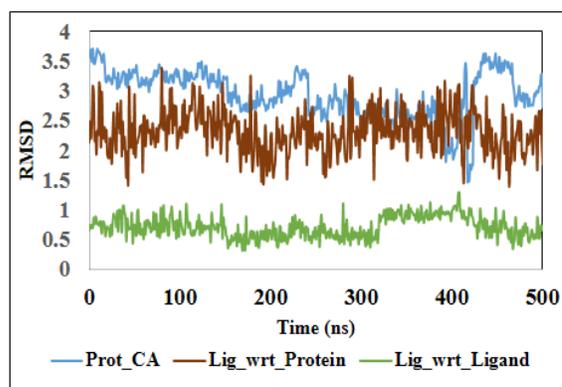


B

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



A



B

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