*Article*

# Synthesis, Physicochemical Characterization, Biological Evaluation, In Silico and Molecular Docking Studies of Pd(II) Complexes with P, S-Donor Ligands

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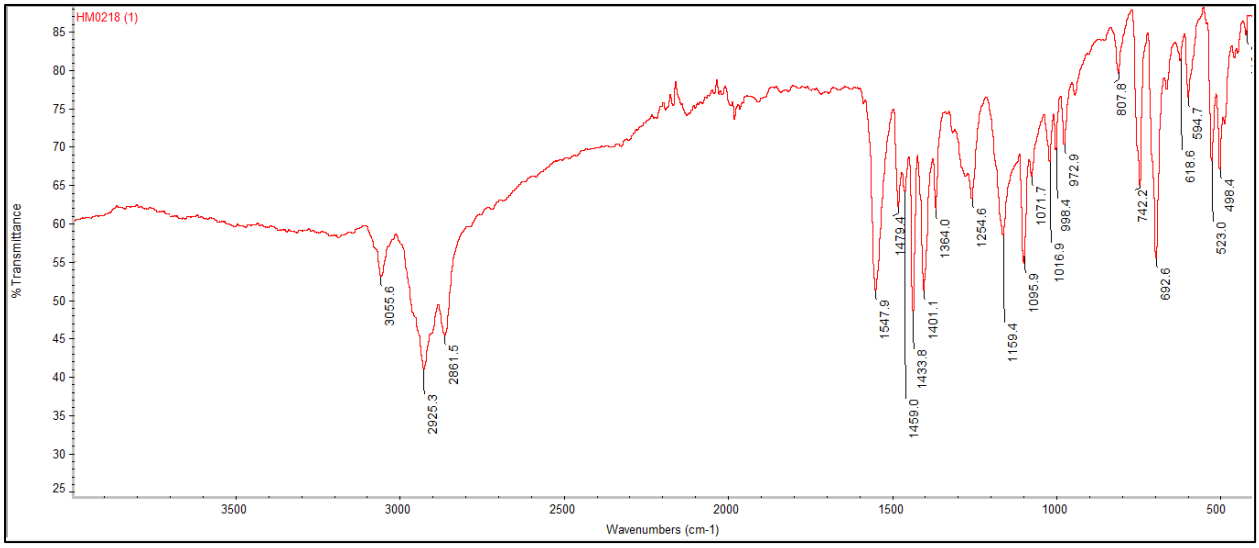


**Figure S1.** FTIR spectrum of complex **2**.

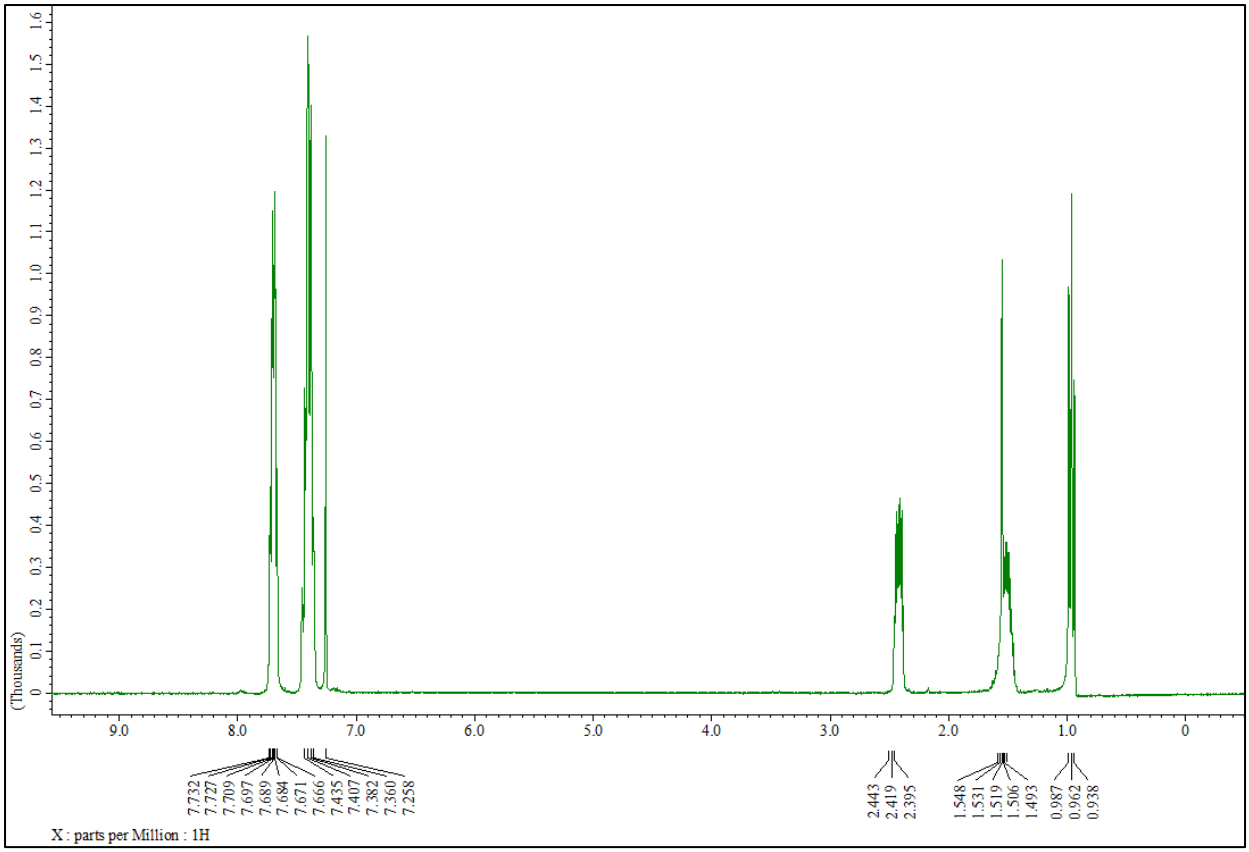


**Figure S2.** $^{1}$H NMR of complex **1**.

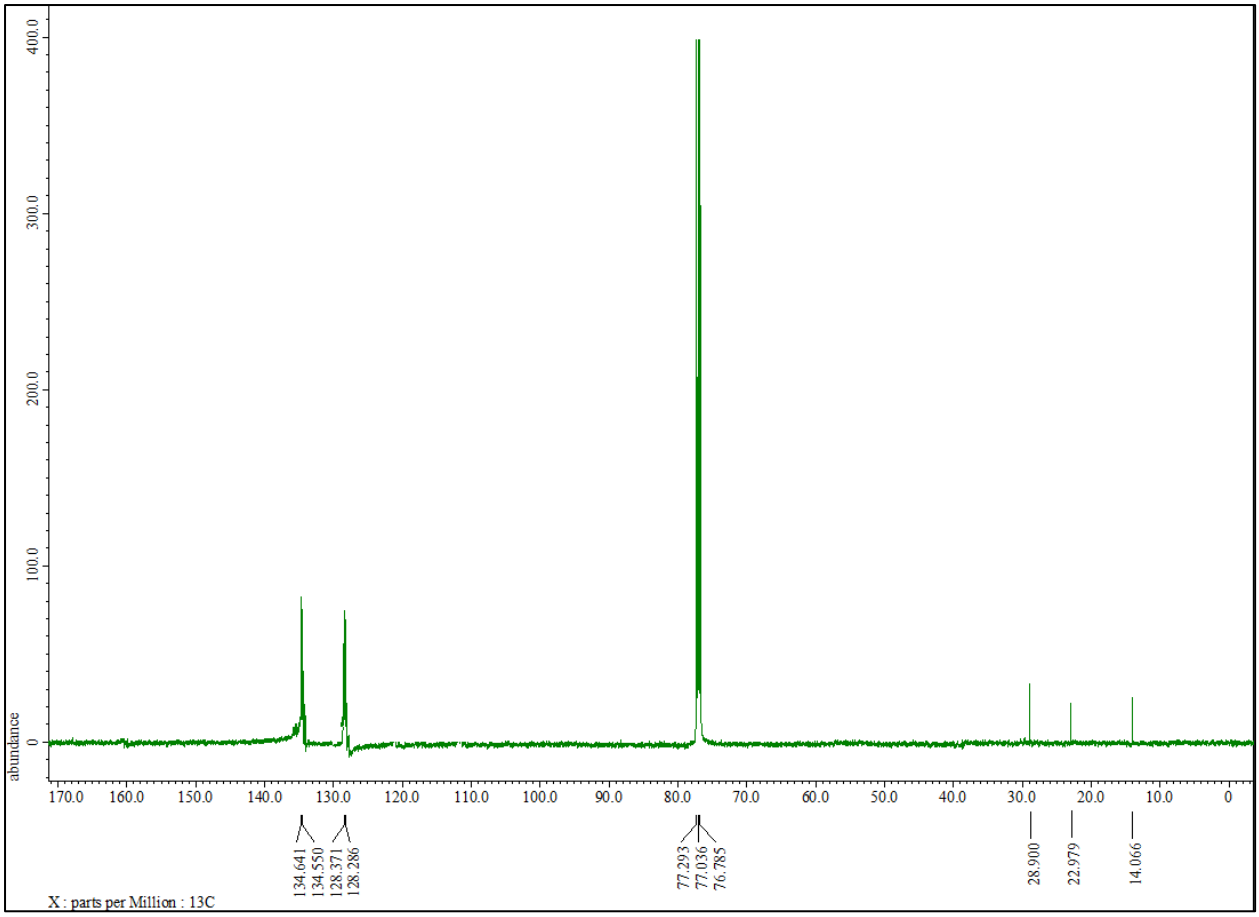


**Figure S3.** $^{13}C$ NMR of complex **1**.

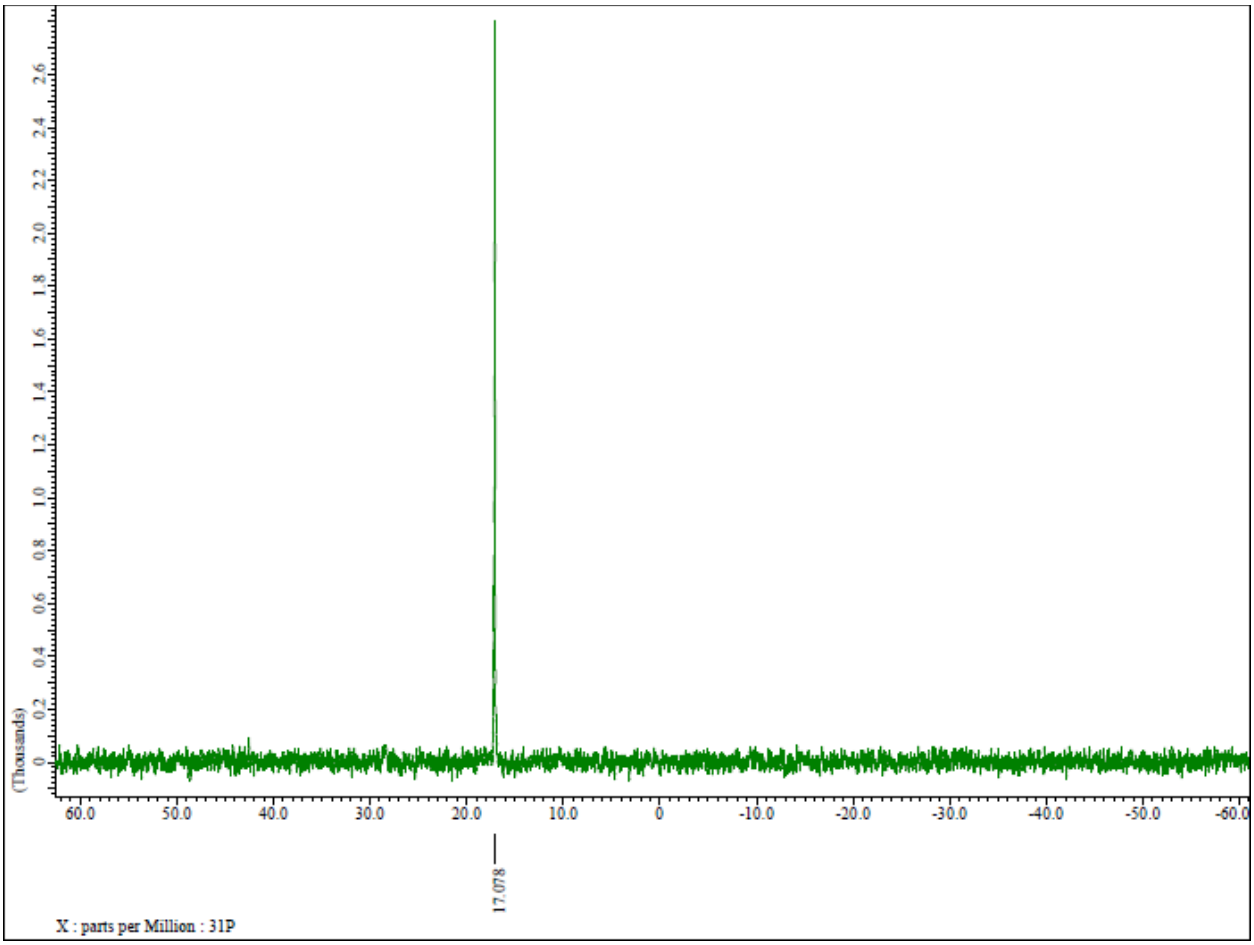


**Figure S4.** $^{31}P$ NMR of complex **1**.

**Table S1.** Binding energy score of starting organophosphorous Pd precursors with the receptor.

| Receptor | Ligand | Binding Affinity (kcal/mol) |
|---|---|---|
| *E. coli* (PDB_ID: 6G9S) | potassium dimethylcarbamodithioate | -4.4988 |
| | $(PR_3)_2PdCl_2$ where $PR_3$ = diphenyl-p-tolylphosphine | -6.3463 |
| | $(PR_3)_2PdCl_2$ where $PR_3$ = diphenyl-2-ethoxyphenyl phosphine | -4.6034 |
| | $(PR_3)_2PdCl_2$ where $PR_3$ = diphenyl-p-tolylphosphine | -6.8335 |
| *K. pneumonia* (PDB_ID: 4EXS) | potassium dimethylcarbamodithioate | -4.0926 |
| | $(PR_3)_2PdCl_2$ where $PR_3$ = diphenyl-p-tolylphosphine | -4.9375 |
| | $(PR_3)_2PdCl_2$ where $PR_3$ = diphenyl-2-ethoxyphenyl phosphine | -5.3247 |
| | $(PR_3)_2PdCl_2$ where $PR_3$ = diphenyl-p-tolylphosphine | -5.0306 |
| *S. aureus* (PDB_ID: 5ZH8) | potassium dimethylcarbamodithioate | -4.3260 |
| | $(PR_3)_2PdCl_2$ where $PR_3$ = diphenyl-p-tolylphosphine | -5.4957 |
| | $(PR_3)_2PdCl_2$ where $PR_3$ = diphenyl-2-ethoxyphenyl phosphine | -6.1572 |
| | $(PR_3)_2PdCl_2$ where $PR_3$ = diphenyl-p-tolylphosphine | -6.0522 |
| DR5 (PDB_ID: 1DU3) | potassium dimethylcarbamodithioate | -4.3843 |
| | $(PR_3)_2PdCl_2$ where $PR_3$ = diphenyl-p-tolylphosphine | -6.4459 |
| | $(PR_3)_2PdCl_2$ where $PR_3$ = diphenyl-2-ethoxyphenyl phosphine | -7.1002 |

| | | |
|---|---|---|
| | $(PR_3)_2PdCl_2$ where $PR_3$ = diphenyl-p-tolylphosphine | -6.9220 |

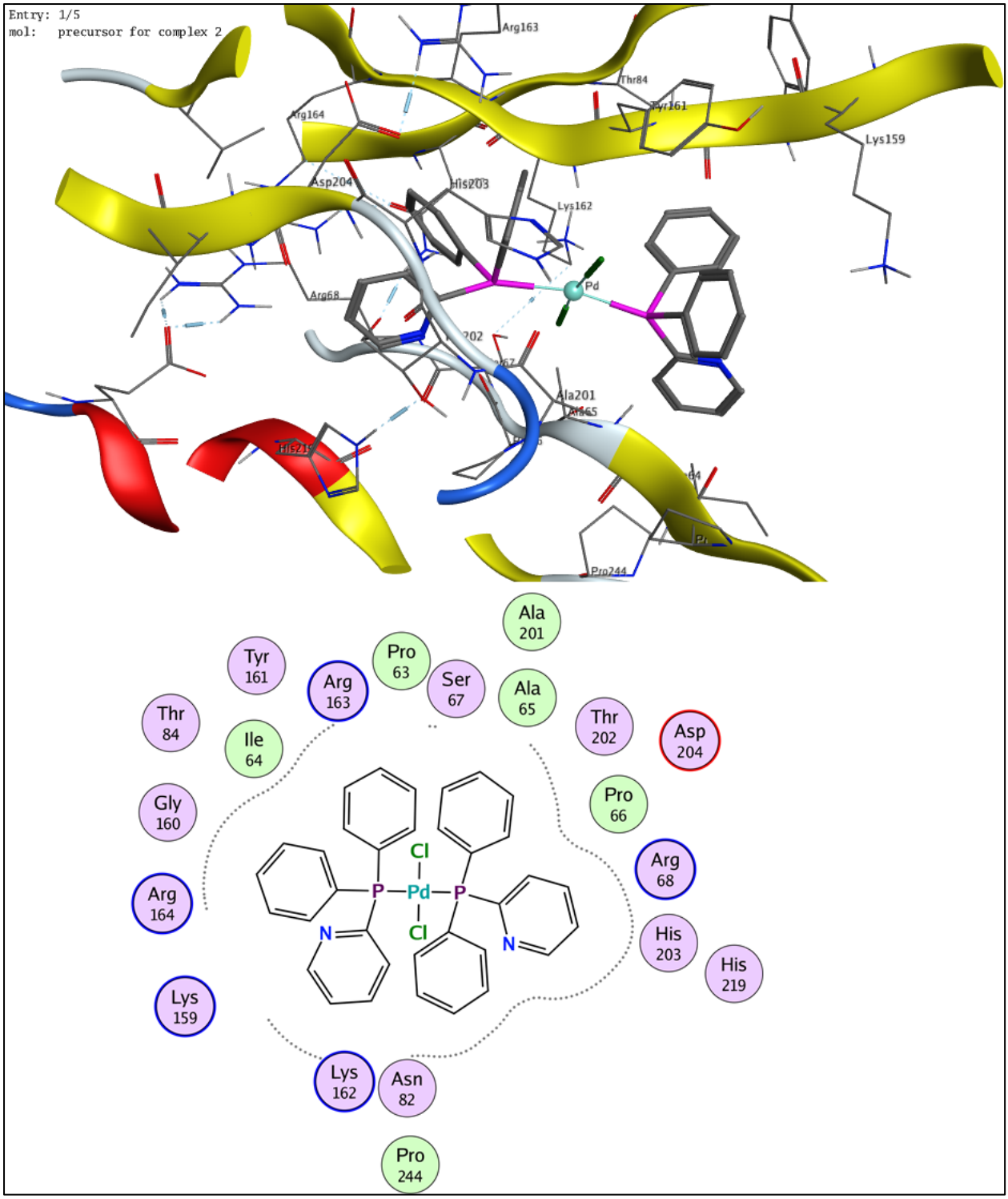


**Figure S5.** (A) Computed and (B) 2D interaction of $(PR_3)_2PdCl_2$ where $PR_3$ = diphenyl-p-tolylphosphine precursor with *E. coli* (PDB_ID: 6G9S).

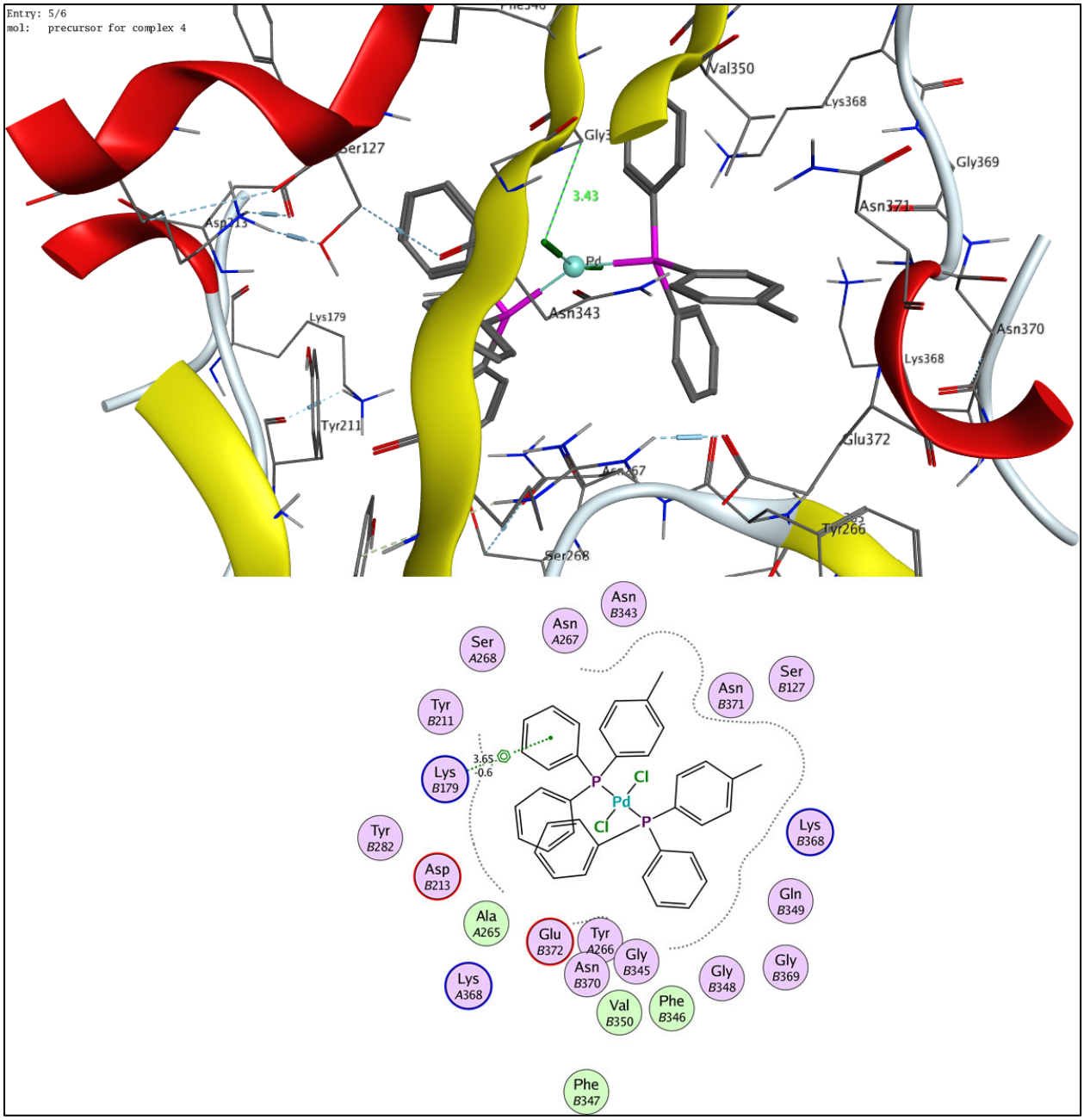


**Figure S6.** (A) Computed and (B) 2D interaction of $(PR_3)_2PdCl_2$ where $PR_3$ = diphenyl-p-tolylphosphine precursor with S. aureus (PDB_ID: 5ZH8)

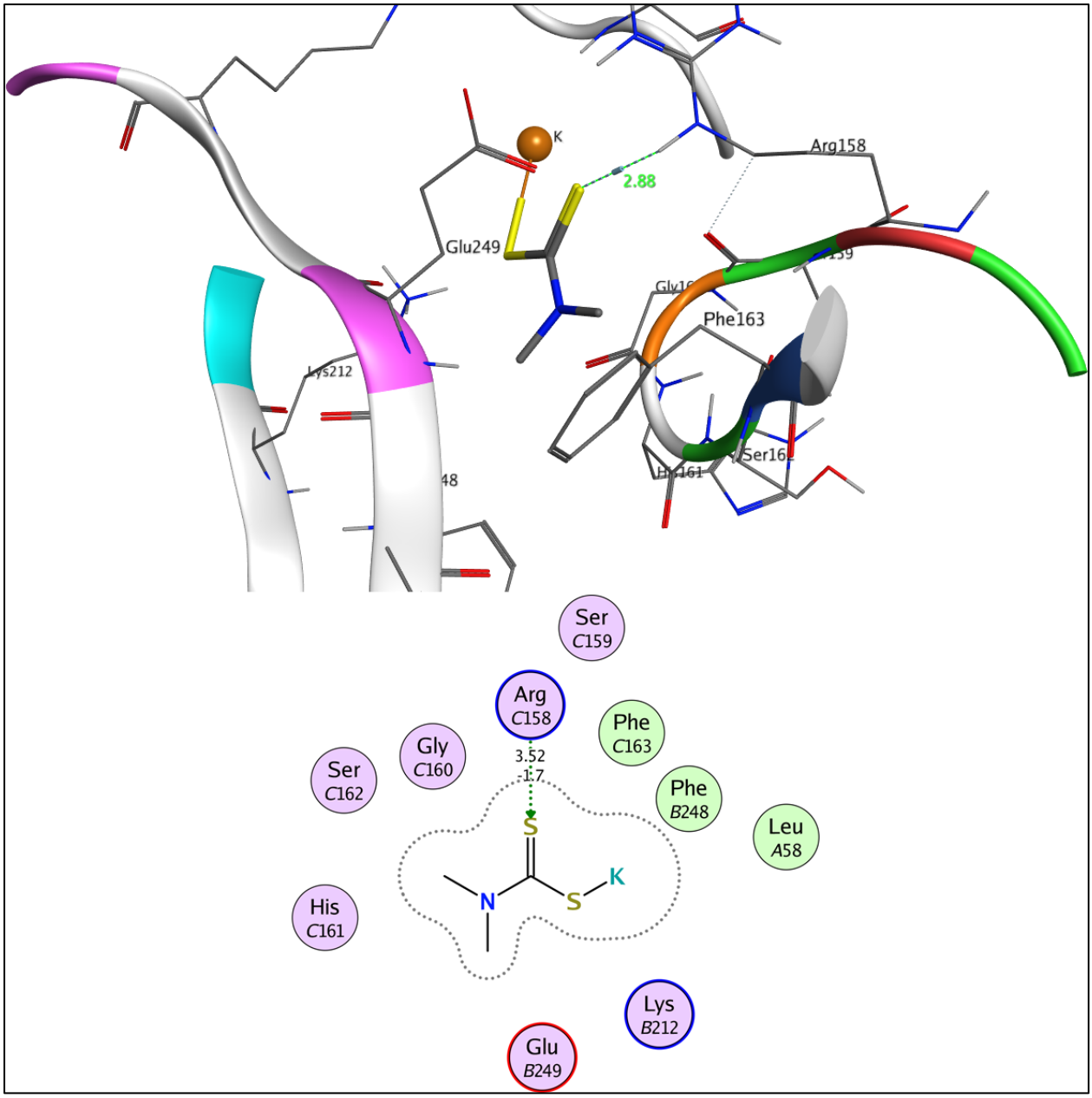


**Figure S7.** (A) Computed and (B) 2D interaction of potassium dimethylcarbamodithioate with DR5 (1DU3).

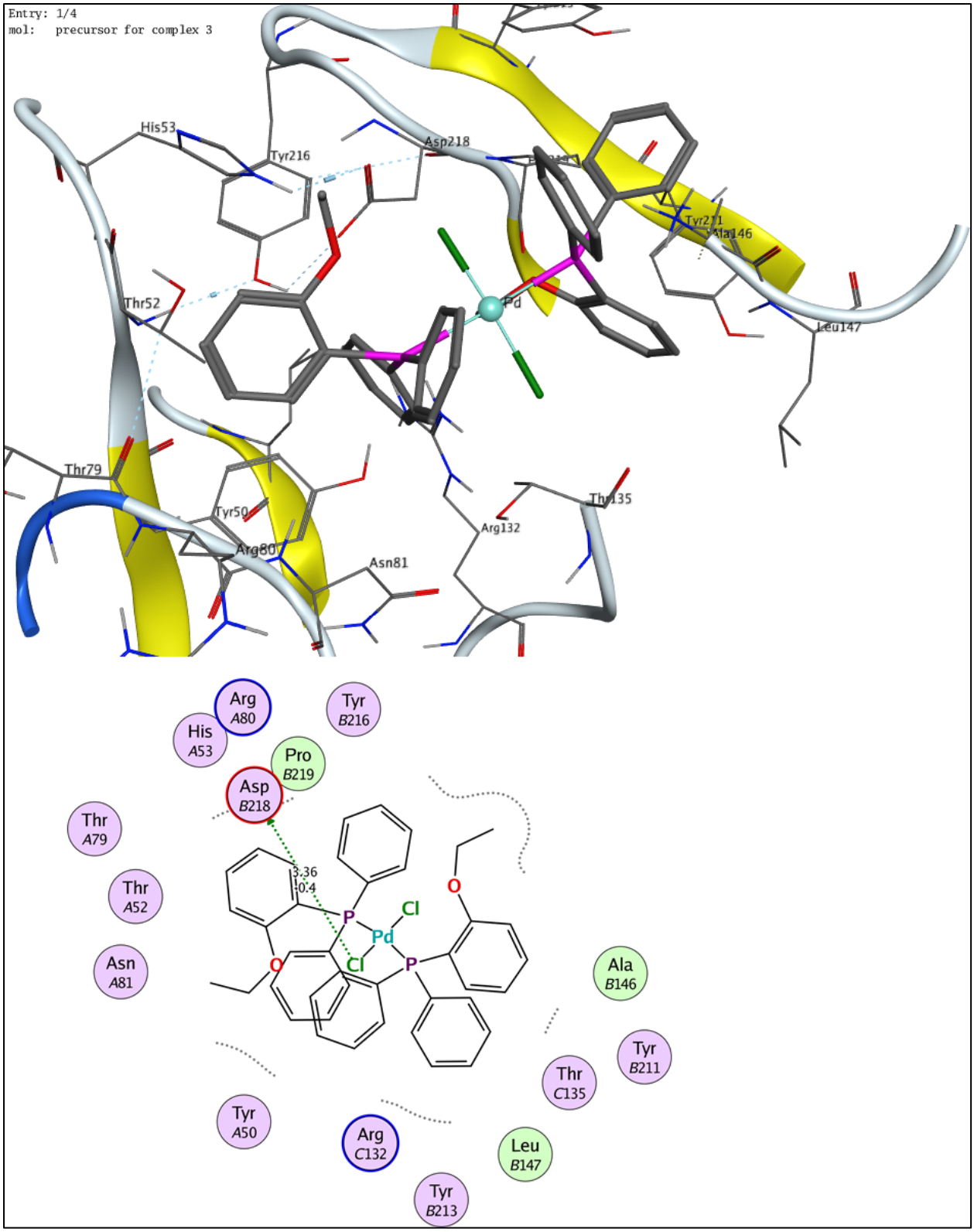


**Figure S8.** (A) Computed and (B) 2D interaction of $(PR_3)_2PdCl_2$ where $PR_3$ = diphenyl-p-tolylphosphine precursor with DR5 (1DU3).