**The electronic Supporting Information**

###### A study of 1-benzyl-3-phenyl-2-thiourea as an effective steel corrosion inhibitor in 1.0 M HCl solution

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**List of supporting information**

**Table S1** Optimized structure of BPTU in gas phase using B3LYP/6-311G(d,p).

|  |  |
| --- | --- |
| **Stable Neutral form** | **C6H5-CH2-NH-CS-NH-C6H5** |
|  0 1 S 1.05906600 2.32988900 -0.82310800 N -0.82361100 0.51388000 -0.45888100 N 1.29373600 -0.28744700 -0.10290300 C -1.48510000 -0.74117700 -0.10557800 C -2.97262600 -0.53196500 0.07170100 C -3.45036200 0.26264500 1.12003700 C -3.88631500 -1.11711300 -0.80623200 C 2.69898200 -0.37703700 0.06598600 C 0.51064700 0.78615500 -0.43980000 C -4.81690500 0.46274600 1.28667700 C -5.25624600 -0.92037200 -0.63821800 C -5.72342900 -0.13036100 0.40811600 C 3.31529400 -1.57367300 -0.31687600 C 3.46372100 0.63349500 0.65497100 C 4.67889000 -1.76010500 -0.11669300 C 4.82930500 0.44021500 0.84053800 C 5.44507700 -0.75016600 0.45956000 H -1.31750500 -1.50783300 -0.87465400 H -1.05803400 -1.11560200 0.83307600 H -1.39756200 1.27821100 -0.78001600 H -2.74732400 0.72613300 1.80424000 H -3.52578400 -1.72947400 -1.62626900 H 0.84073900 -1.18884800 -0.12786000 H -5.17548500 1.07848100 2.10363800 H -5.95529100 -1.38162700 -1.32647900 H 2.72444200 -2.35551200 -0.78438800 H 2.99348100 1.55811300 0.95262000 H -6.78820600 0.02450000 0.53962100 H 5.14100900 -2.69234500 -0.42085400 H 5.41476000 1.23185500 1.29428300 H 6.50924700 -0.88903400 0.61013200 |

**Table S2** Optimized structure of URO in gas phase using B3LYP/6-311G(d,p).

|  |  |
| --- | --- |
| **Stable Neutral form** | **C6H12N4** |
|  N -0.14247900 -0.31384100 -1.46433000 N -0.80388200 -0.98517500 0.80452600 N -0.50247400 1.39311500 0.26563100 N 1.44937200 -0.09428800 0.39455800 C -0.91942800 -1.26176200 -0.64133800 C -0.62716800 1.04827800 -1.16453800 C 1.26922700 -0.39589900 -1.03960500 C -1.26883600 0.39647700 1.03992000 C 0.62655600 -1.04880400 1.16421300 C 0.91920300 1.26191000 0.64105800 H -1.97235200 -1.20408500 -0.93087600 H -0.56483900 -2.27731100 -0.83817500 H -0.05339100 1.76772700 -1.75526300 H -1.67777600 1.12457100 -1.45817200 H 1.64253700 -1.40386600 -1.24063400 H 1.85896300 0.31179400 -1.62879200 H -2.32481000 0.46786900 0.76507200 H -1.17572100 0.62603400 2.10502600 H 0.73517100 -0.83231200 2.23059100 H 0.99408600 -2.06239200 0.98146900 H 1.50693000 1.98287900 0.06606500 H 1.03011600 1.49923000 1.70273000 |

**Table S3** Optimized structures of protonated BPTU (pBPTU) and URO (pURO) in gas phase using B3LYP/6-311G(d,p)

|  |  |
| --- | --- |
| **Protonated form** | **pBPTU-N2** |
| 1 1 S 0.91293900 2.47255500 -0.23889800 N -0.83600800 0.46244800 -0.55487800 N 1.39398600 -0.22241400 -0.29436000 C -1.56377500 -0.07232900 0.70406200 C -3.01871200 -0.27388100 0.40890100 C -3.91799600 0.78882300 0.56247400 C -3.48441900 -1.51563000 -0.03996100 C 2.79952300 -0.37596200 -0.09882100 C 0.62082500 0.86872300 -0.35981100 C -5.26471100 0.61139200 0.26127800 C -4.83220000 -1.68985700 -0.33928400 C -5.72058600 -0.62591700 -0.19155500 C 3.26478700 -1.69802400 -0.11996700 C 3.68692200 0.68299500 0.10553800 C 4.61380300 -1.96163600 0.06277400 C 5.03865600 0.39949200 0.28699800 C 5.50743500 -0.91053200 0.26745100 H -1.05754600 -0.99609800 0.98218900 H -1.38107300 0.68152500 1.46922000 H -0.95465700 -0.20785800 -1.32378000 H -3.57226900 1.74798400 0.93584100 H -2.80197700 -2.35521100 -0.13377500 H 0.93715200 -1.11844800 -0.41389000 H -5.95876600 1.43286400 0.39024600 H -5.19042300 -2.65508500 -0.67575700 H 2.57286300 -2.52019400 -0.28027400 H 3.34096400 1.70347800 0.12279000 H -6.77073100 -0.76399000 -0.41912600 H 4.96636700 -2.98540400 0.04475800 H 5.72788000 1.21993300 0.44499500 H 6.56150200 -1.11394200 0.40998800 H -1.30946300 1.32340100 -0.84685500 |
| **Protonated form** | **pBPTU-N3** |
| 1 1 S 1.16659400 3.21153800 0.60365900 N -0.43698700 1.11740600 0.06137800 N 1.71300400 1.09086200 -0.97664300 C -0.90392300 -0.11421300 -0.63321500 C -2.33982100 -0.39484400 -0.26816600 C -2.63805400 -1.25645100 0.79158200 C -3.38004500 0.22541500 -0.96792000 C 2.37293700 -0.14712500 -0.44613800 C 0.70239600 1.79035500 -0.06088800 C -3.96293800 -1.49491000 1.14734300 C -4.70371400 -0.01391300 -0.61042000 C -4.99509300 -0.87340300 0.44752000 C 2.50735600 -1.23273700 -1.30172200 C 2.87328000 -0.14338600 0.84878300 C 3.16489900 -2.36839400 -0.83320300 C 3.52418000 -1.28908200 1.30076000 C 3.66998500 -2.39534400 0.46494500 H -0.81878500 0.03594000 -1.71584500 H -0.26288500 -0.94985700 -0.34567800 H -1.11460300 1.55417600 0.67610200 H -1.83705400 -1.74747600 1.33463100 H -3.15875700 0.88867400 -1.79818000 H 2.41822400 1.81708100 -1.14918100 H -4.18880300 -2.16826200 1.96538200 H -5.50580200 0.46365500 -1.16009900 H 2.11846600 -1.20612900 -2.31467700 H 2.76573300 0.72202600 1.49047600 H -6.02586400 -1.06267400 0.72235100 H 3.28128300 -3.22517000 -1.48490900 H 3.92228500 -1.31014000 2.30752300 H 4.18120900 -3.27943500 0.82543500 H 1.27906100 0.87331200 -1.88057800 |
| **Protonated form** | **pBPTU-S** |
| 1 1 S 1.10948700 2.23902300 -0.01828200 N -0.83435600 0.46383000 -0.06415000 N 1.27783500 -0.47492500 -0.05895900 C -1.57743400 -0.82264700 -0.04275300 C -3.06215200 -0.56246200 -0.00796600 C -3.72055600 -0.40685800 1.21605800 C -3.78494400 -0.45219000 -1.19998200 C 2.72489200 -0.47346100 -0.01474600 C 0.48398900 0.59689500 -0.05403100 C -5.08701100 -0.14289700 1.24628100 C -5.15154800 -0.18799400 -1.16734800 C -5.80218100 -0.03261200 0.05510300 C 3.44325800 -0.51560000 -1.20997000 C 3.37105800 -0.49309400 1.22137600 C 4.83461100 -0.55977400 -1.16176000 C 4.76231800 -0.53639300 1.25592500 C 5.49123100 -0.56912900 0.06780000 H -1.31200900 -1.39543500 -0.93736100 H -1.26592400 -1.38733700 0.84171600 H -1.40199700 1.30069900 -0.09832200 H -3.16990400 -0.50384100 2.14626400 H -3.28462500 -0.58509500 -2.15390400 H 0.82725100 -1.38060200 -0.11010600 H -5.59384000 -0.03170600 2.19727900 H -5.70822900 -0.11197200 -2.09359600 H 2.92053600 -0.51652800 -2.15937700 H 2.79327500 -0.47659400 2.13800000 H -6.86682900 0.16684000 0.07980500 H 5.40220700 -0.59253000 -2.08354900 H 5.27453500 -0.55081400 2.21006900 H 6.57334300 -0.60682100 0.10050700 H 2.40288400 1.87433400 -0.14708700 |
| **Protonated form** | **pURO-N** |
| 1 1 N -0.52573500 0.79013200 -1.15691800 N -0.52672900 0.59533100 1.26742400 N 1.46855400 0.02062200 0.00238100 N -0.49563400 -1.40691000 -0.11312700 C -1.01851000 1.37140000 0.10970900 C 0.90290400 0.83789500 -1.19435400 C -0.98748300 -0.61047000 -1.25711600 C 0.90148500 0.63657900 1.31370700 C -0.98768300 -0.80368900 1.14324600 C 0.93355700 -1.43551700 -0.11541200 H -0.68546800 2.40746900 0.19333900 H -2.10767500 1.35904400 0.10848300 H 1.29952300 0.38707300 -2.10519600 H 1.27715200 1.85741200 -1.09018600 H -2.07653800 -0.62768900 -1.26200600 H -0.63159000 -1.04908100 -2.19108300 H 1.27603800 1.65946400 1.37415000 H 1.29705600 0.04534900 2.14084100 H -0.63070400 -1.38544700 1.99497800 H -2.07668900 -0.82227200 1.14547600 H 1.32951800 -1.84659800 -1.04522100 H 1.32985500 -1.99162300 0.73547500 H 2.49071200 0.03548700 0.00395800 |