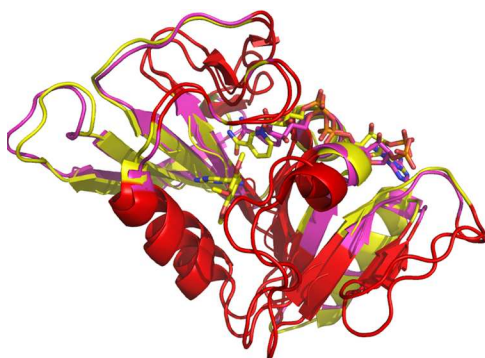


Supporting Information for:

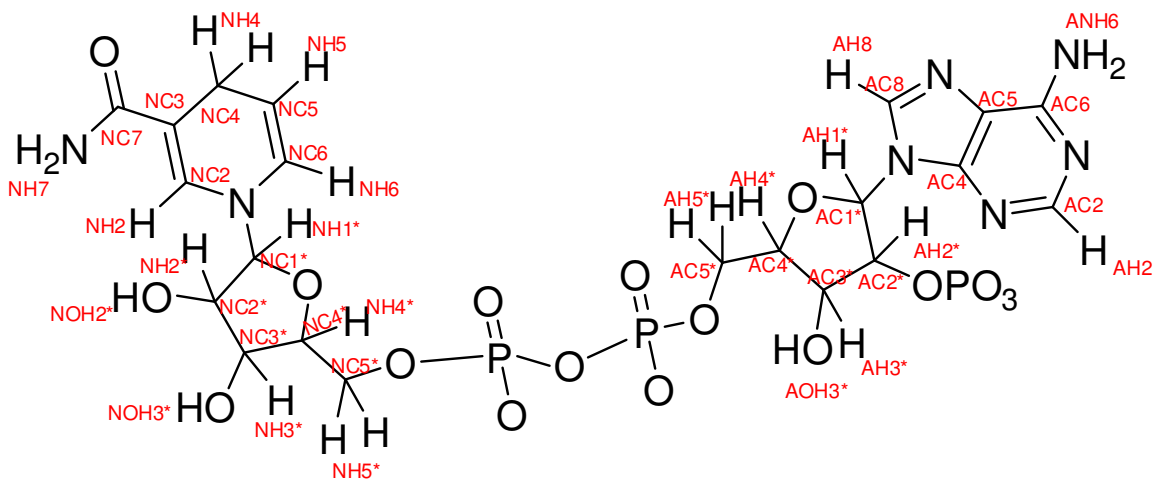
The Solution Structure of *Bacillus anthracis* Dihydrofolate Reductase Yields Insight into  
the Analysis of Structure-Activity Relationships for Novel Inhibitors

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**Figure S1:** Cartoon depiction of the solution structures of LcDHFR binary and ternary complexes. LcDHFR bound to NADPH is shown in magenta (PDB ID:2HQP) and LcDHFR bound to trimethoprim (PDB ID:1LUD) is shown in yellow. Trimethoprim and NADPH are shown in sticks. Regions that show significant shifts between the binary and ternary complexes are colored in red. Figure generated in PyMol.

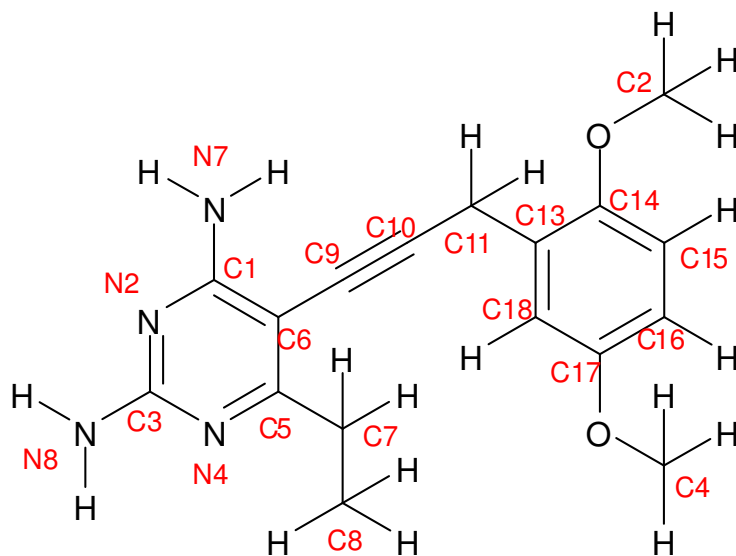
Table S1. Chemical shifts for NADPH (free ligand) in 20 mM TES pH 7.0



| Atom <sup>a</sup> | Shift  | Atom  | Shift     |
|-------------------|--------|-------|-----------|
| NH7               | -      | AC5*  | 65.2      |
| NC7               | 172.77 | AH5*  | 4.22,4.13 |
| NC3               |        | AC4*  | 82.5      |
| NC4               | 70.2   | AH4*  | 4.31      |
| NH4               | 4.13   | AC3*  | 69.8      |
| NC5               | 105.3  | AH3*  | 4.53      |
| NH5               | 4.74   | AOH3* | -         |
| NC6               | 123.8  | AC2*  | 75.9      |
| NH6               | 5.9    | AH2*  | 4.9       |
| NC2               | 138.35 | AC1*  | 86.9      |
| NH2               | 6.876  | AH1*  | 6.15      |
| NC1*              | 94.9   | AC4   |           |
| NH1*              | 4.71   | AC2   | 152.70    |
| NC2*              |        | AH2   | 8.176     |
| NH2*              |        | AC6   |           |
| NOH2*             | -      | ANH6  | -         |
| NC3*              |        | AC5   |           |
| NH3*              |        | AC8   | 140.09    |
| NOH3*             | -      | AH8   | 8.406     |
| NC4*              | 82.3   |       |           |
| NH4*              | 4.00   |       |           |
| NC5*              | 60.5   |       |           |
| NH5*              | 3.98   |       |           |

<sup>a</sup> Standard nomenclature for NADPH includes asterisks for the atoms in the ribose rings bound to the nicotinamide and adenine rings.

Table S2. Chemical shifts for UCP120B (free ligand) in 20 mM TES pH 7.0



| Atom | Shift | Atom | Shift  |
|------|-------|------|--------|
| C1   |       | C13  | 126.47 |
| C3   |       | C14  | 153.29 |
| C5   |       | C15  | 115.60 |
| C6   |       | H15  | 6.799  |
| C7   | 29.00 | C16  | 112.36 |
| H7   |       | H16  | 6.913  |
| C8   | 12.88 | C17  | 151.17 |
| H8   | 1.041 | C18  | 112.63 |
| NH7  |       | H18  | 6.945  |
| NH8  |       | C2   | 55.81  |
| C9   |       | H2   | 3.650  |
| C10  |       | C4   | 56.26  |
| C11  | 20.82 | H4   | 3.710  |
| H11  | 3.710 |      |        |

Table S3. NOE signals Involving Helix B or the Ligand (120B)

| Residue 1                 | Atom | Residue 2     | Atom |
|---------------------------|------|---------------|------|
| NOEs Involving Helix B    |      |               |      |
| 26                        | HG1  | 148           | HN   |
| 26                        | HG1  | 148           | HE*  |
| 26                        | HG1  | 148           | HG*  |
| 26                        | HG2  | 148           | HG*  |
| 26                        | HB2  | 149           | HD2* |
| 26                        | HB1  | 149           | HD2* |
| 26                        | HB2  | 148           | HG*  |
| 26                        | HG2  | 149           | HD2* |
| 26                        | HG1  | 149           | HD2* |
| 27                        | HN   | 148           | HG*  |
| 29                        | HD1* | Ligand (120B) | C7   |
| NOEs Involving the Ligand |      |               |      |
| 29                        | HD1* | 120B          | C7   |
| 29                        | HD2* | 120B          | C7   |
| 51                        | HA   | 120B          | C16  |
| 96                        | HN   | 120B          | HAD  |
| 96                        | HN   | 120B          | HAC  |