

Supporting Information

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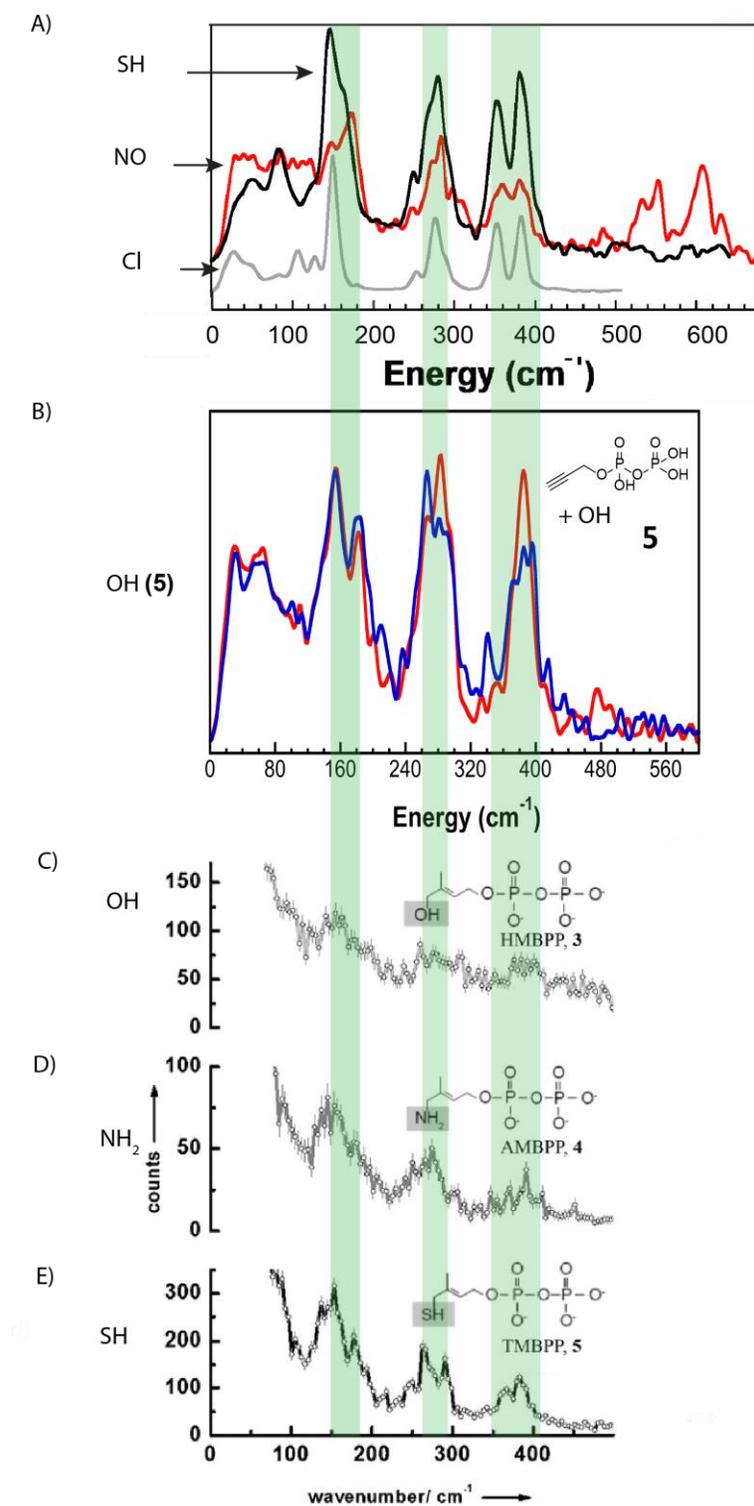
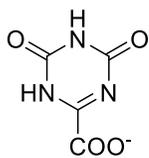
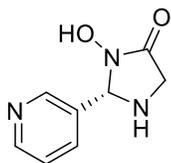


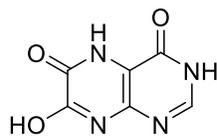
Figure S1. IspH and model compound NRVS spectra comparisons. A) Spectra from Figure 1B in the Text. B) Spectra from Figure 1C in the Text. C)-E) Spectra from Reference 16 in the Text. The frequency axes are all scaled to be the same and the green bands have been added to show that the 3 main features are present in each system. The ligand atoms bound to the 4th Fe are indicated on the left.



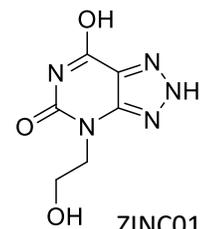
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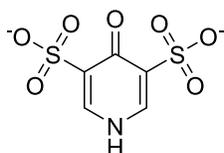
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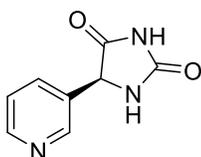
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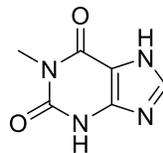
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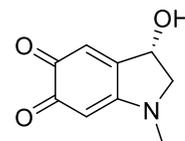
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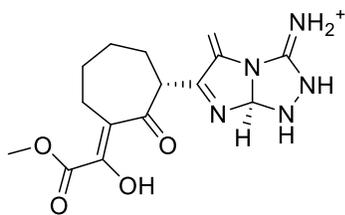
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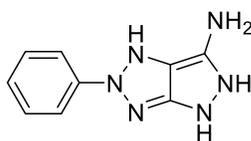
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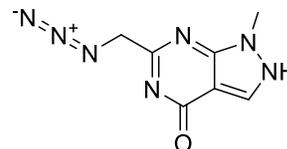
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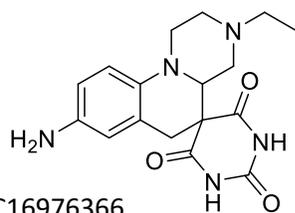
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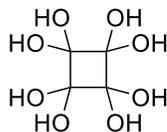
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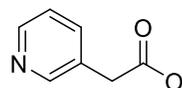
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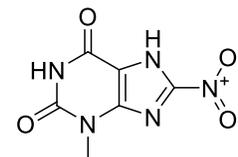
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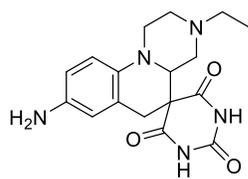


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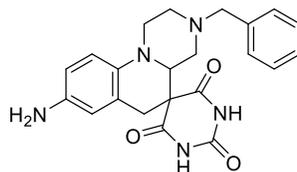


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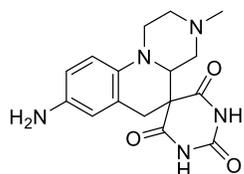
Figure S2. Structures of compounds from the *in silico* screen that were tested for IspH inhibition activity.



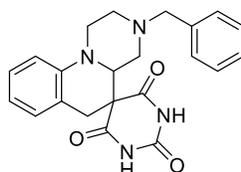
(CAS: 919735-08-3) **8**, IC₅₀ = 22 μM



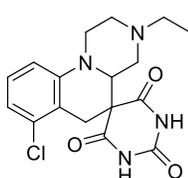
(CAS: 921163-37-3) **9**, IC₅₀ = 23 μM



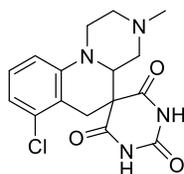
(CAS: 879578-61-7) IC₅₀ = 65 μM



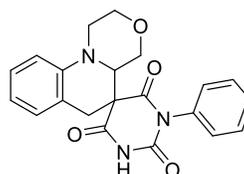
(CAS: 879578-61-7) IC₅₀ = 113 μM



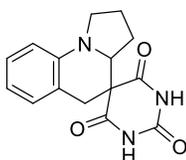
(CAS: 879454-42-9)
No effect at 0.4 mM



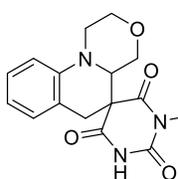
(CAS: 896674-96-7)
No effect at 0.4 mM



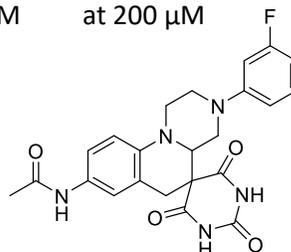
(CAS: 879457-44-0) No effect
at 200 μM



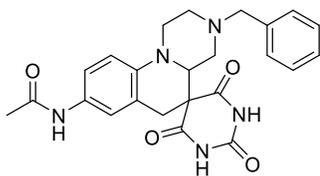
(CAS: 878489-40-8)
No effect at 100 μM



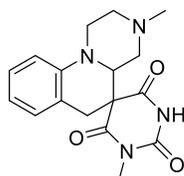
(CAS: 879459-40-2)
No effect at 100 μM



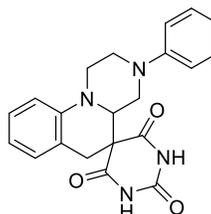
(PHAR112843) No effect at 0.4 mM



(CAS: 879432-98-1)
No effect at 0.4 mM



(CAS: 879570-28-2)
No effect at 0.4 mM



(CAS: 859128-43-1)
No effect at 0.4 mM

Figure S3. Structures of analogs of **8** that were tested for IspH inhibition activity.