Electronic Supplementary Material (ESI) for RSC Advances.

Computational Insights Into Substrate Binding and Catalytic Mechanism of the Glutaminase Domain of Glucosamine-6-Phosphate Synthase (GlmS)

Wanlei Wei,[1] Gerald Monard,[2] James W. Gauld[1]*

[1] Department of Chemistry and Biochemistry, University of Windsor, Windsor, Ontario N9B 3P4, Canada

[2] Université de Lorraine, UMR 7565 SRSMC, Boulevard des Aiguillettes B.P. 70239, F-54506 Vandoeuvre-les-Nancy

Supporting Information

(Figures S1 and S2; total pages 5)

*Author to whom correspondence should be addressed. Email: gauld@uwindsor.ca

Figure S1. The frequency of the key ${}_{\mathrm{Cys1}}\mathrm{S}^{-}\cdots{}_{\mathrm{His71}}\mathrm{N}_{\delta}$ Distance in the GlmS simulation with positively charged N-terminal amine.

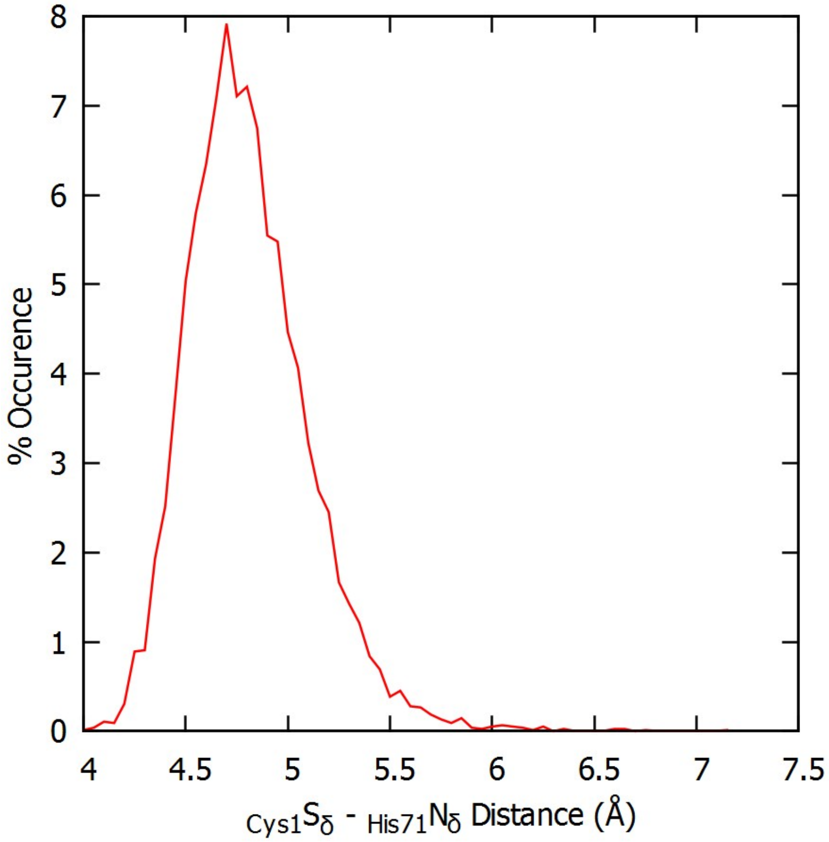
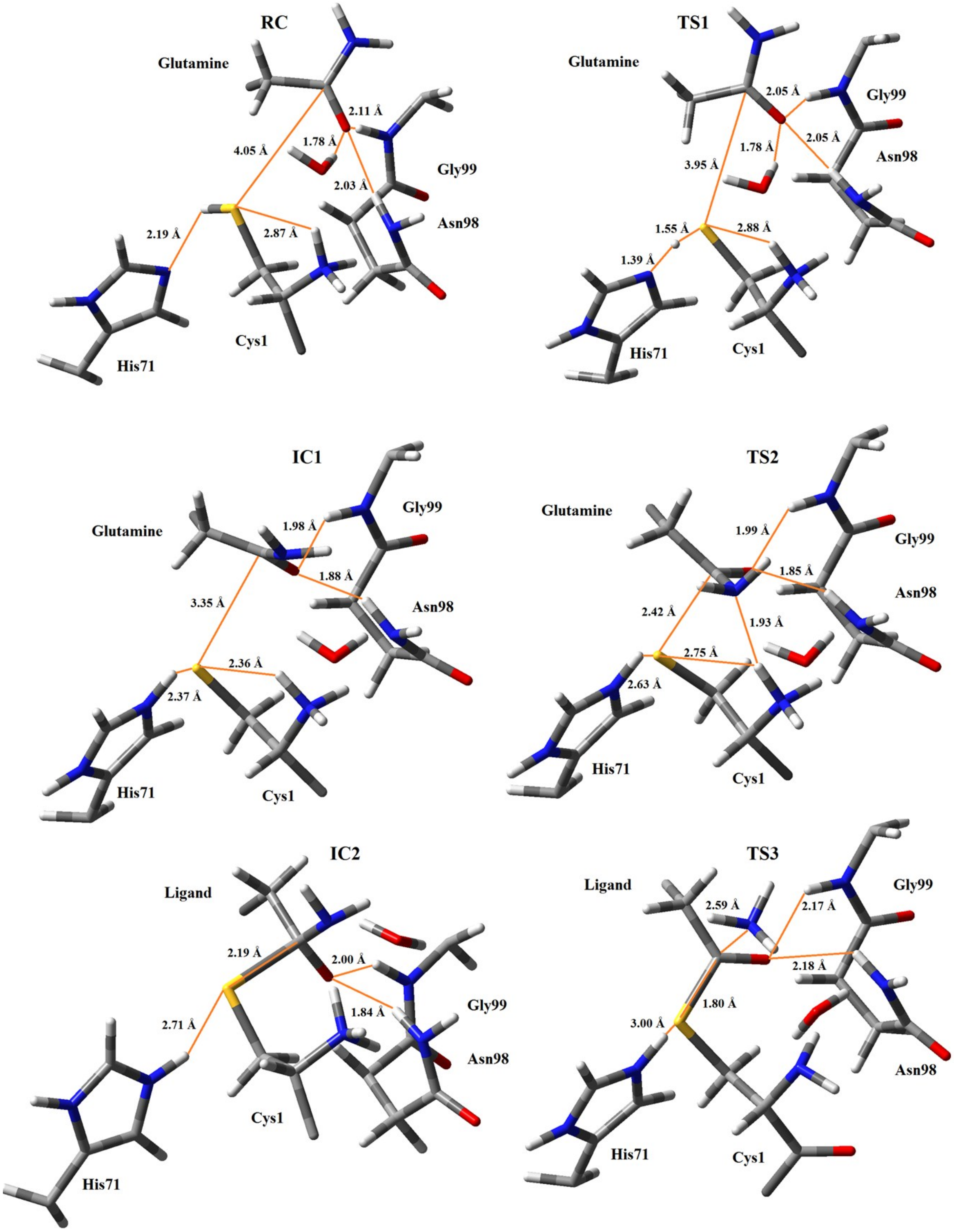
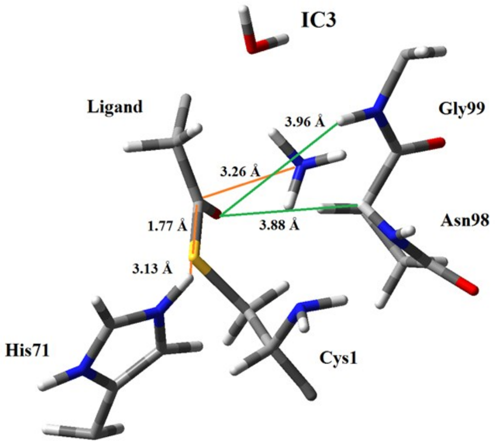


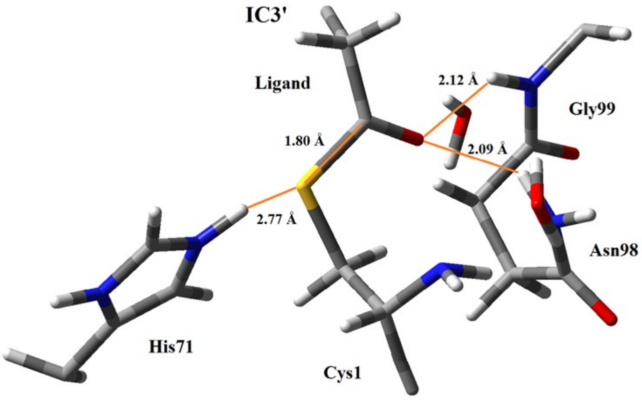
Figure S2. Optimized intermediates and transition state structures within the deamination site of the GlmS where the N-terminal amino group is positively charged, and a nearby His71 acts as a catalytic base.



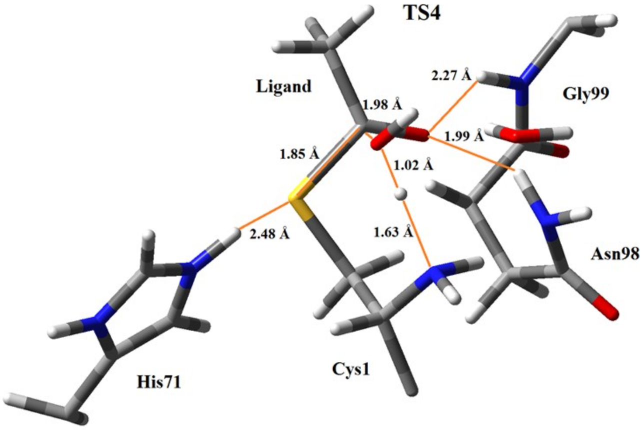
IC3



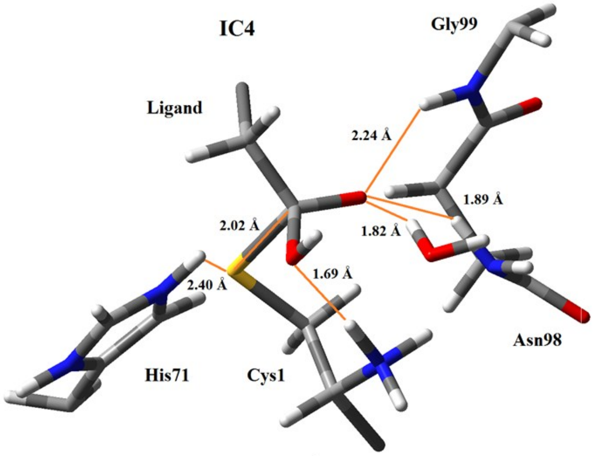
IC3'



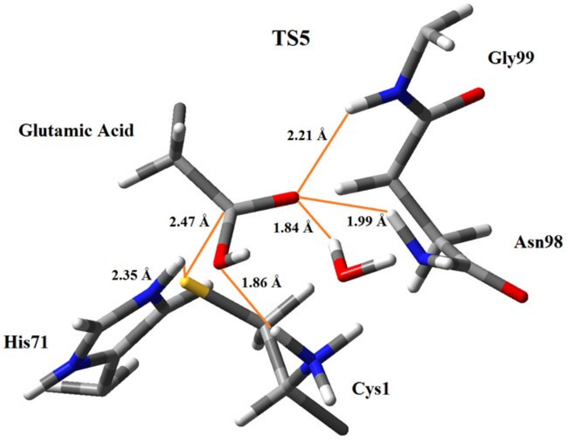
TS4



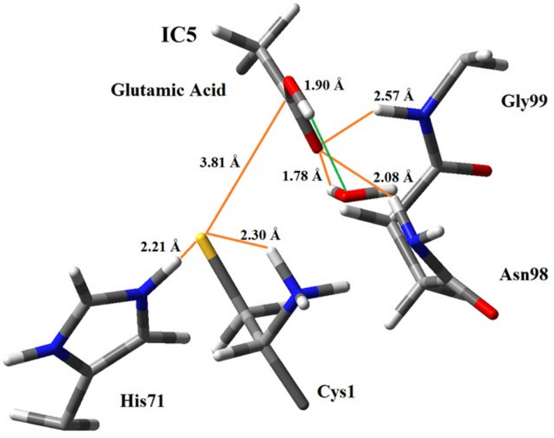
IC4

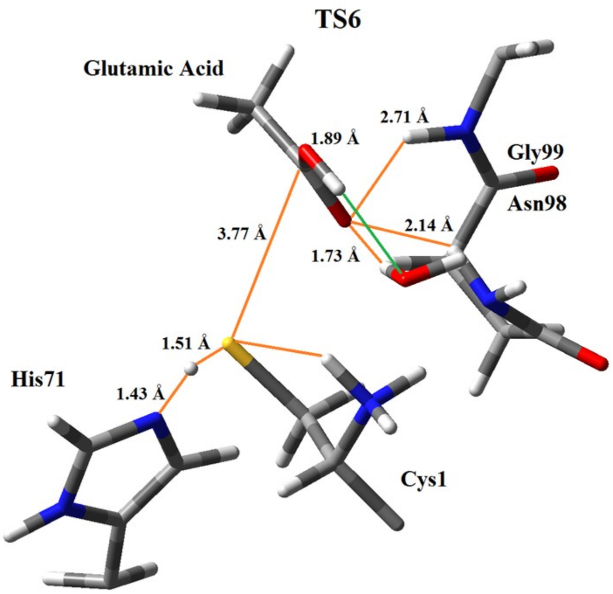


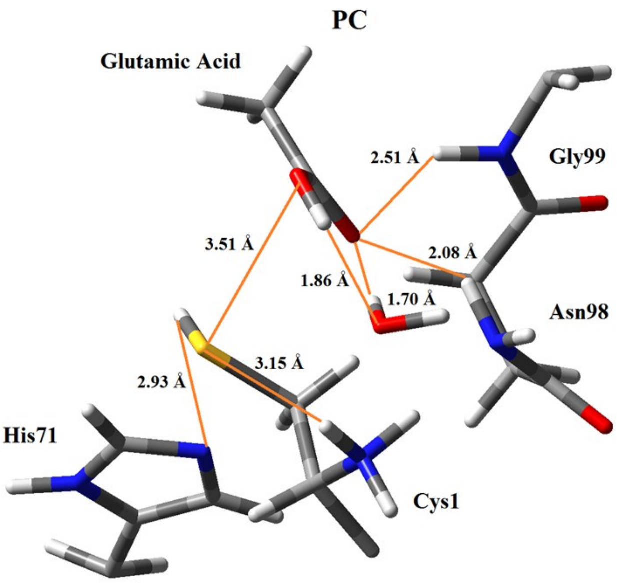
TS5



IC5




TS6
Glutamic Acid
2.71 Å
1.89 Å
Gly99
Asn98
3.77 Å
2.14 Å
1.73 Å
1.51 Å
His71
1.43 Å
Cys1


PC
Glutamic Acid
2.51 Å
Gly99
3.51 Å
2.08 Å
1.86 Å
1.70 Å
Asn98
3.15 Å
2.93 Å
His71
Cys1