Supporting information for

"Mechanism for Isopenicillin N Synthase from Density-functional Modeling Highlights the Similarities with Other Enzymes in the 2-His-1-carboxylate Family"

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Electronic energies for all stationary points using the 6-31G(d) basis set. Optimized geometries are submitted as xyz files.

File Name	Energy (h)
Model_A_1_reactant_septet .xyz	-3296.778831
Model_A_1_reactant_quintet.xyz	-3296.771832
Model_A_2_int_septet.xyz	-3296.772963
Model_A_2_int_quintet.xyz	-3296.772379
Model_A_2_int_triplet.xyz	-3296.771994
Model_A_3_ts_septet.xyz	-3296.734486
Model_A_3_ts_quintet.xyz	-3296.742989
Model_A_3_ts_triplet.xyz	-3296.729280
Model_A_4_int_septet.xyz	-3296.756756
Model_A_4_int_quintet.xyz	-3296.782729
Model_A_4_int_triplet.xyz	-3296.759834
Model_A_5_int_quintet.xyz	-3296.789523
Model_A_6_ts_quintet.xyz	-3296.771202
Model_A_7_int_quintet.xyz	-3296.773430
Model_A_8_ts_quintet.xyz	-3296.769593
Model_A_9_int_quintet.xyz	-3296.821564
Model_B_9_int_quintet.xyz	-3108.820698
Model_B_10_ts_quintet.xyz	-3108.788748
Model_B_11_int_quintet.xyz	-3108.789463
Model_B_12_ts_quintet.xyz	-3108.781384
Model_B_13_int_quintet.xyz	-3108.820761
Model_C_13_int_quintet.xyz	-3032.394370
Model_C_14_int_quintet.xyz	-3032.394835
Model_C_15_ts_quintet.xyz	-3032.355163
Model_C_16_int_quintet.xyz	-3032.379847
Model_C_17_ts_quintet.xyz	-3032.369862
Model_C_17H_ts_quintet.xyz	-3032.365023
Model_C_18_product_quintet.xyz	-3032.419342
Model_C_18H_product_quintet.xyz	-3032.426611