

The Hydrolysis Rate of Paraxonase-1 Q vs R Isoenzymes:

An *in silico* Study Based on *in vitro* Data

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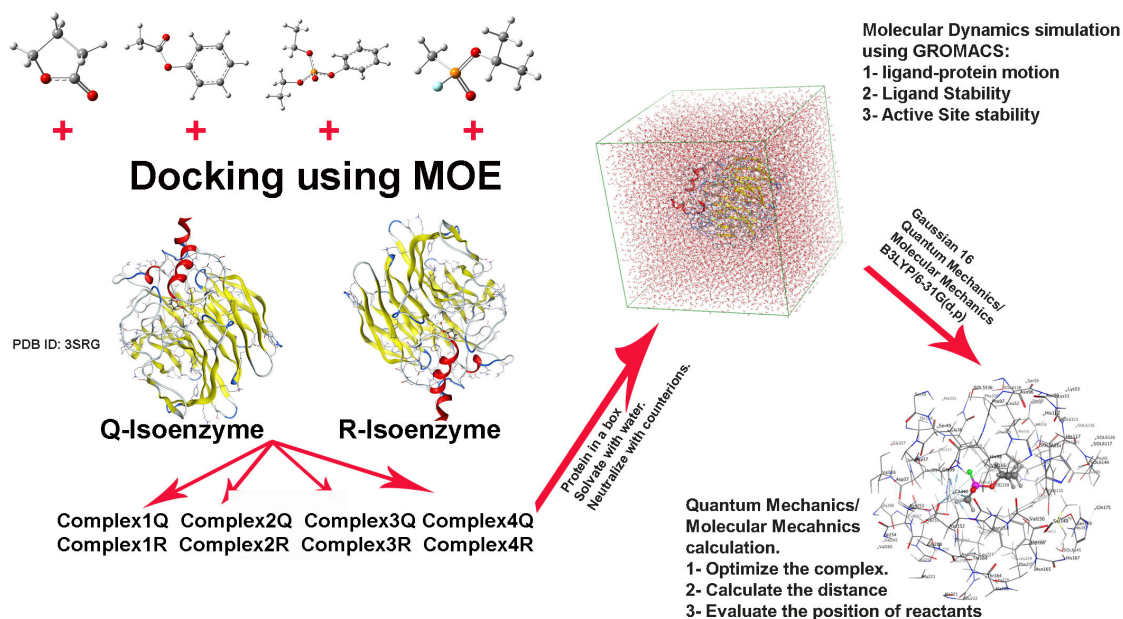


Figure S1. Schematic illustration of the enzyme-substrate complex modeling strategy used in this study.

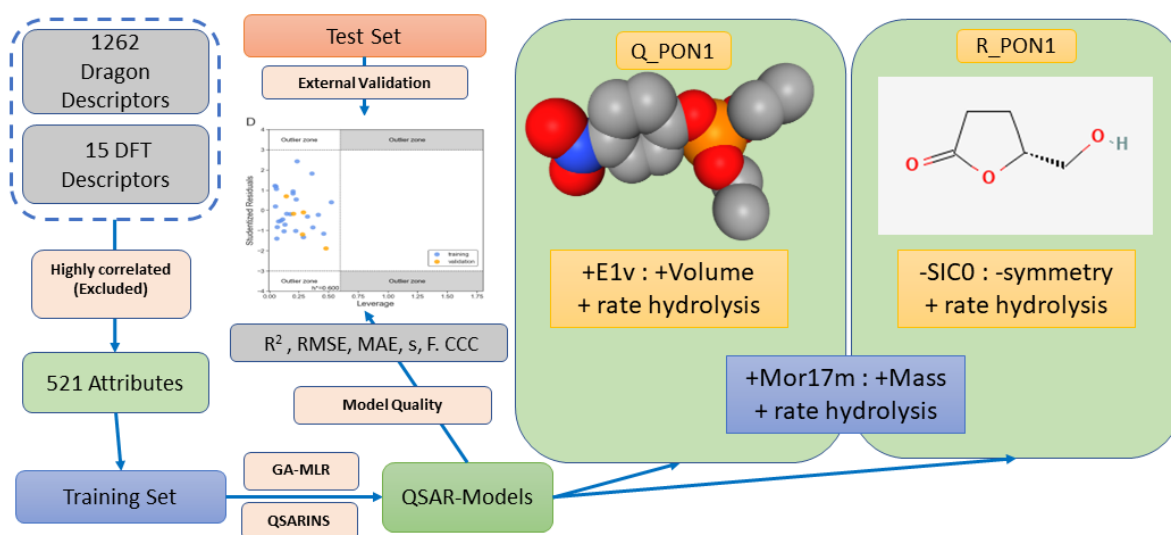
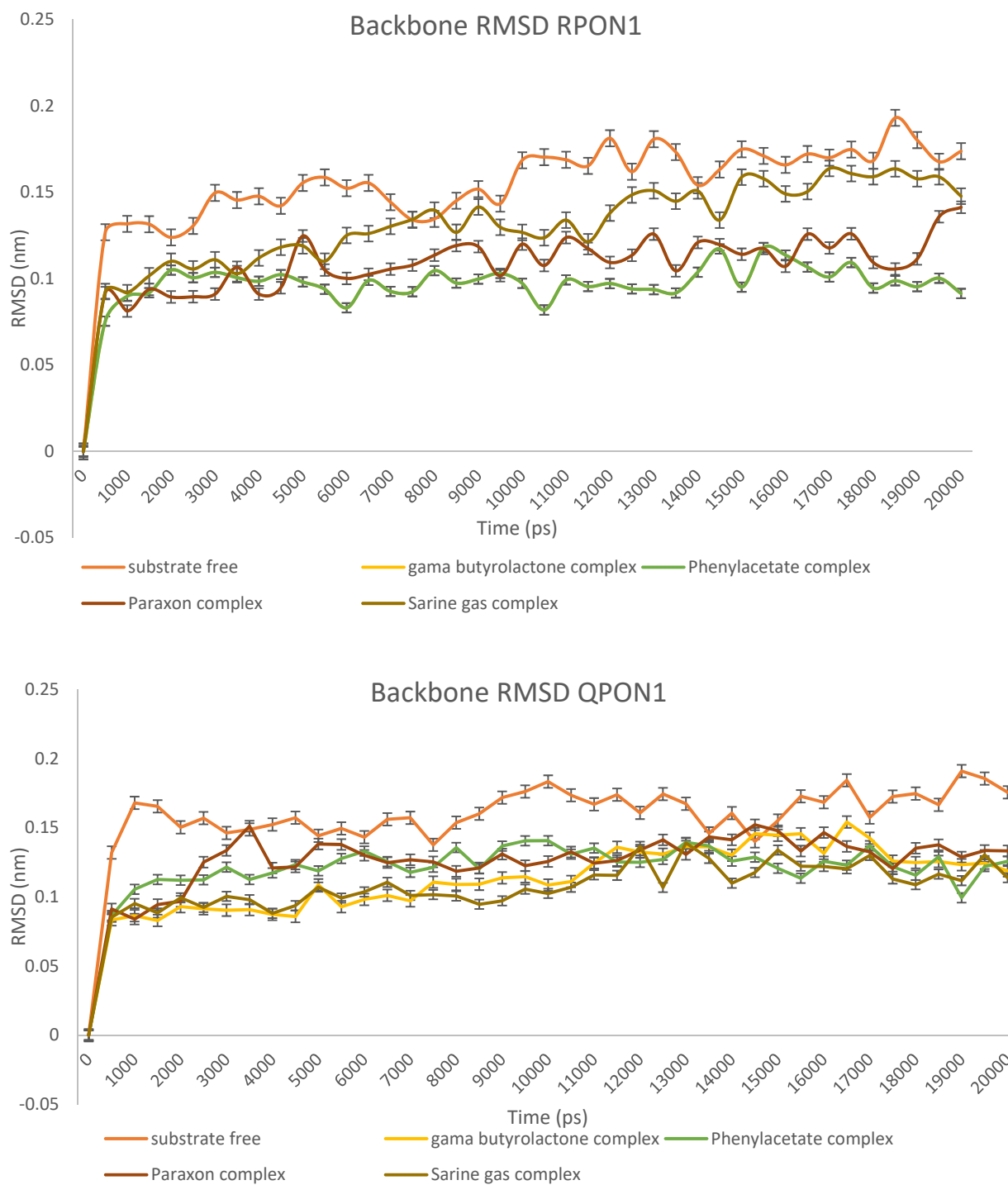
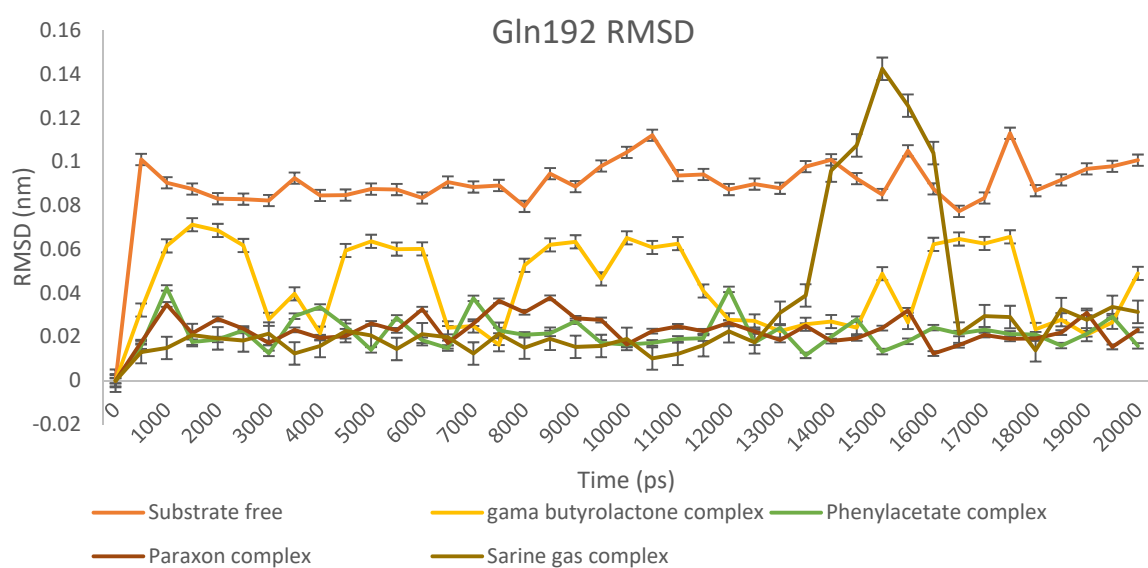
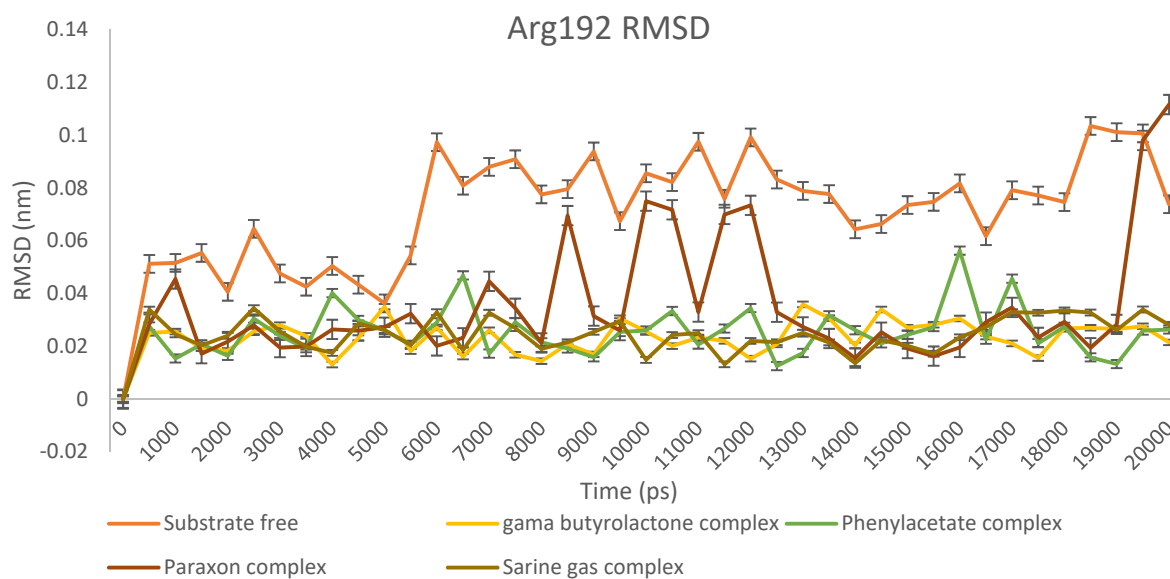


Figure S2. Schematic illustration of the QSAR modelling steps including descriptor generation, training and test sets created and GA-MLR modelling.

Figure S3A. Backbone RMSD, Gln192/Arg192 RMSD, and Ligands RMSD from MD results of the four complexes, γ -Butyrolactone, Phenylacetate, Paraoxon, Sarine gas, and substrate free complexes, including.





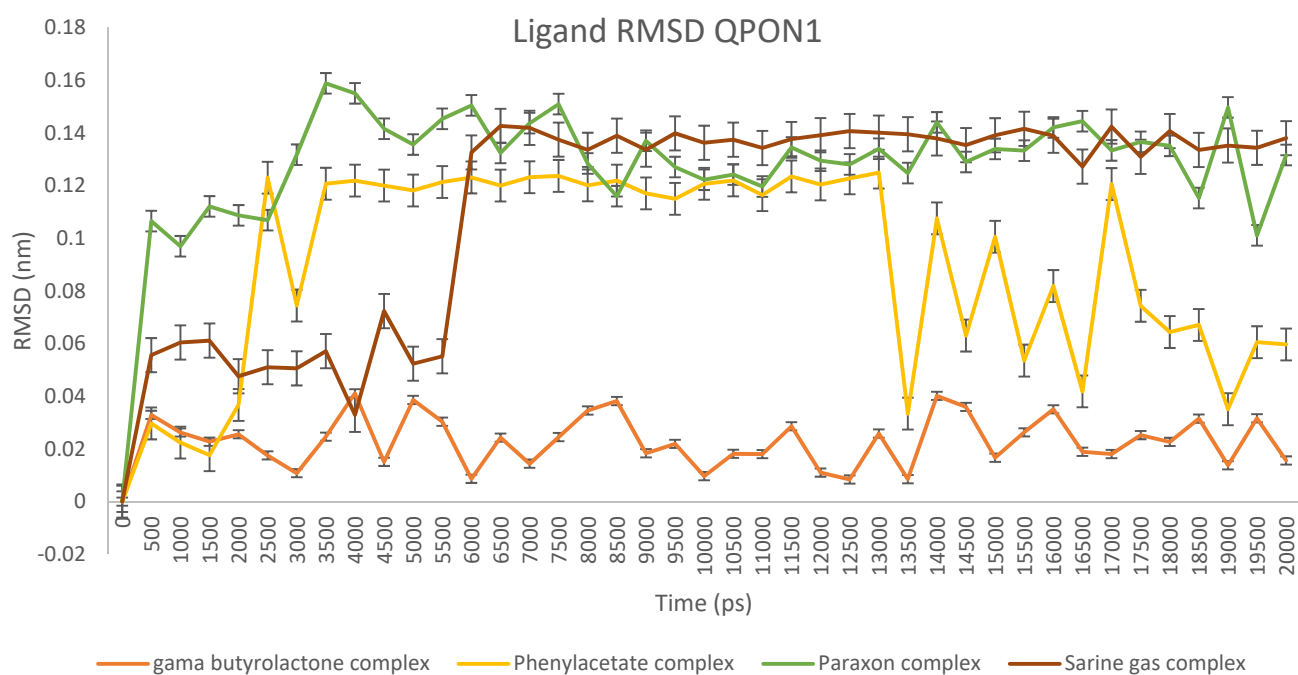
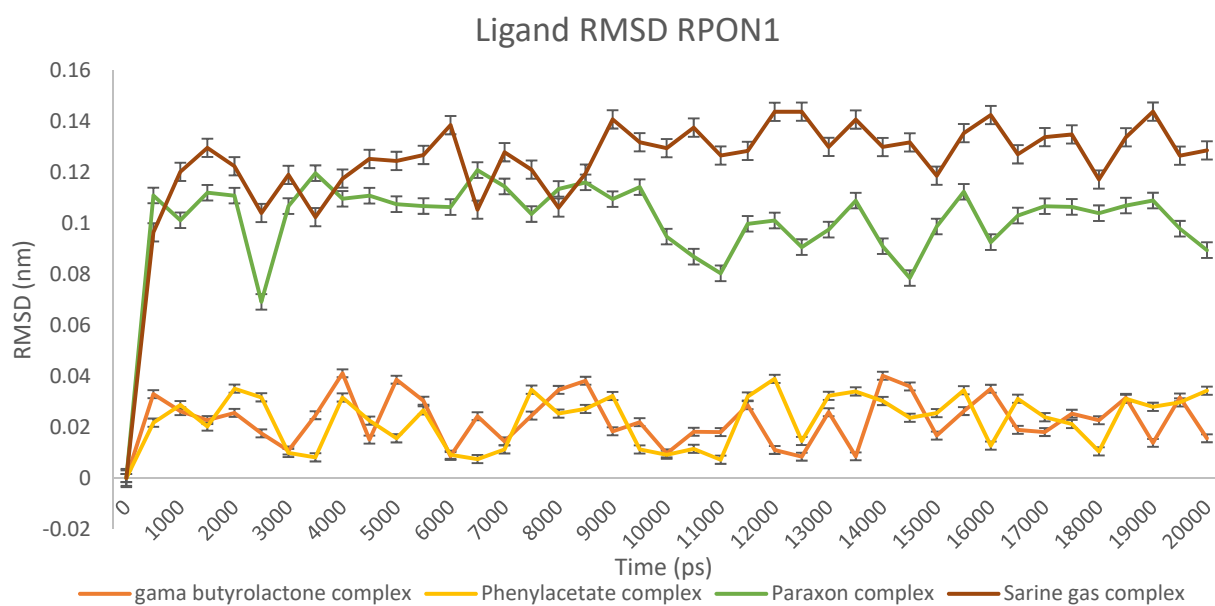


Figure S3B. Gln192/Arg192- Ca^{2+} ion distance from MD results of the four complexes, γ -Butyrolactone, Phenylacetate, Paraoxon, Sarine gas, and substrate free complexes.

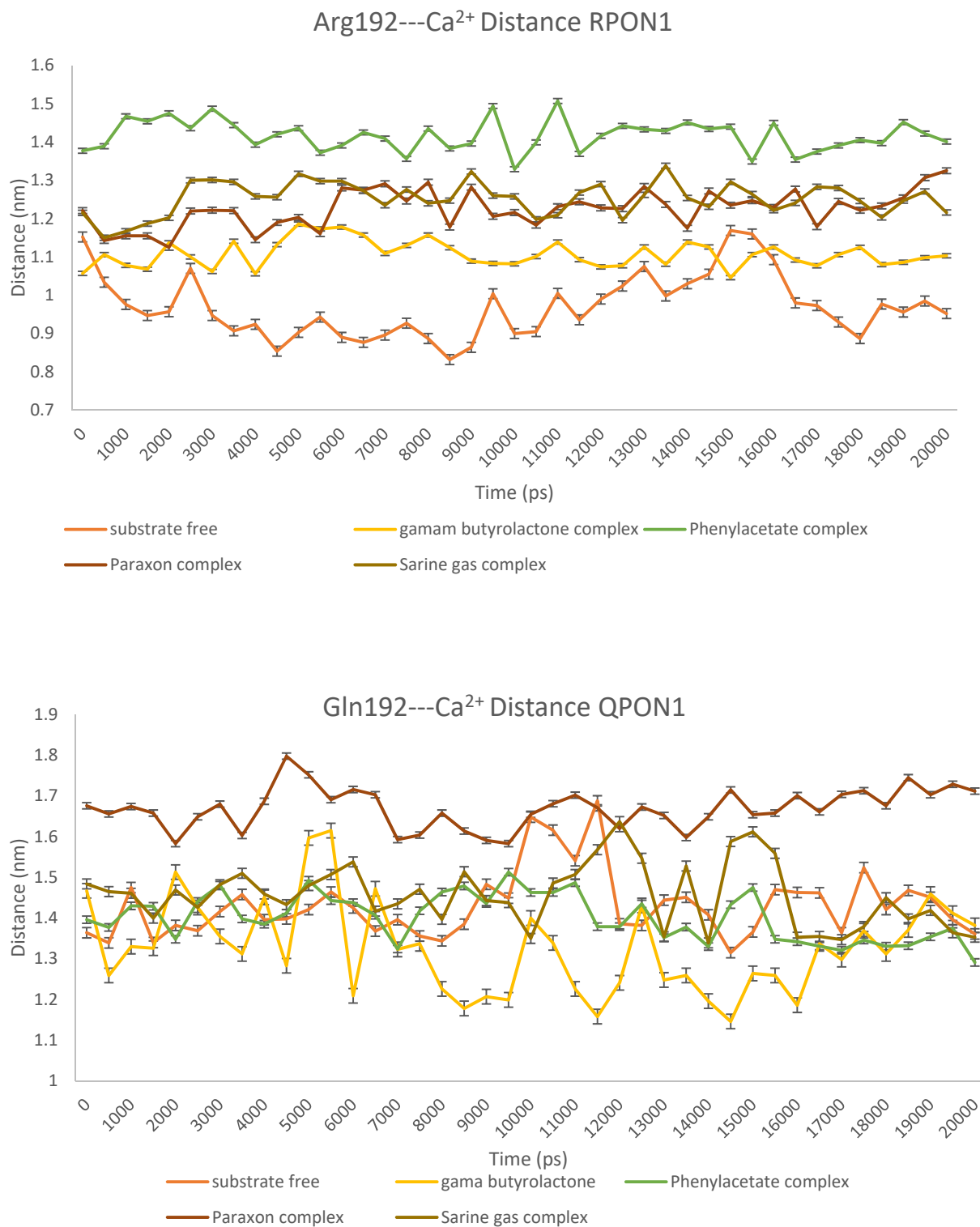
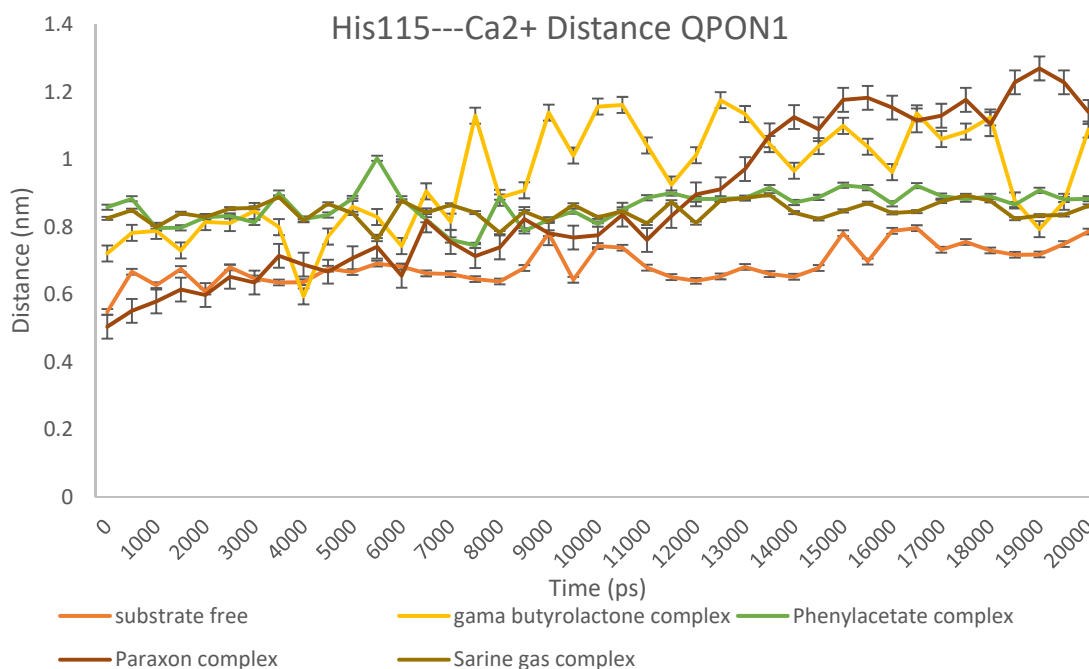
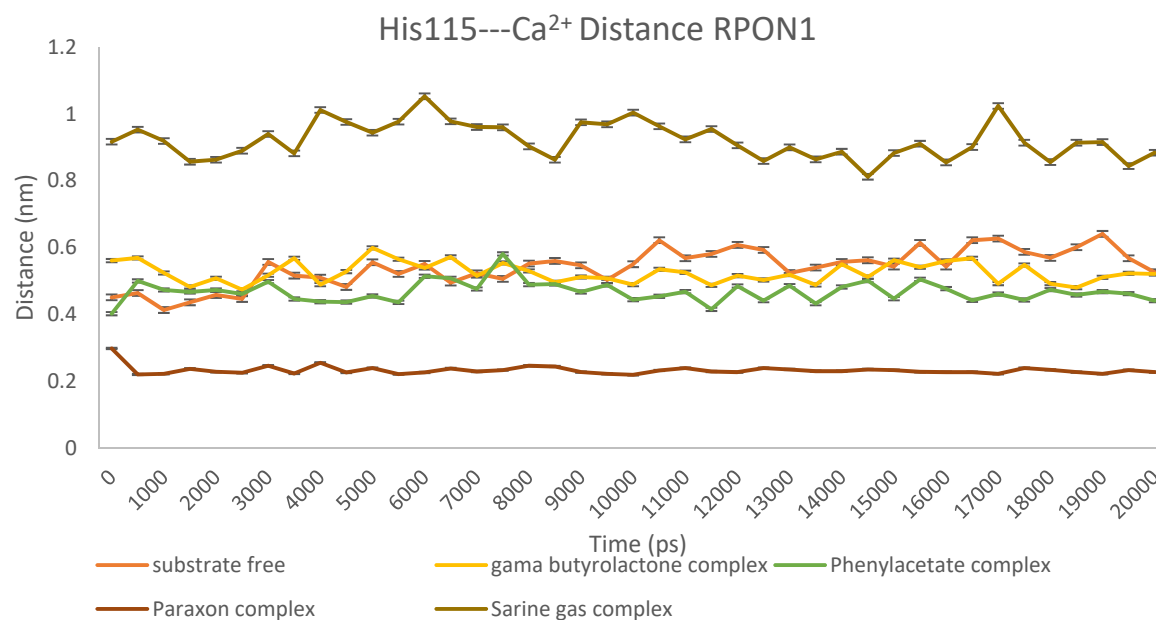


Figure S3C. His115-Ca²⁺ ion distance from MD results of the four complexes, γ -Butyrolactone, Phenylacetate, Paraoxon, Sarine gas, and substrate free complexes.



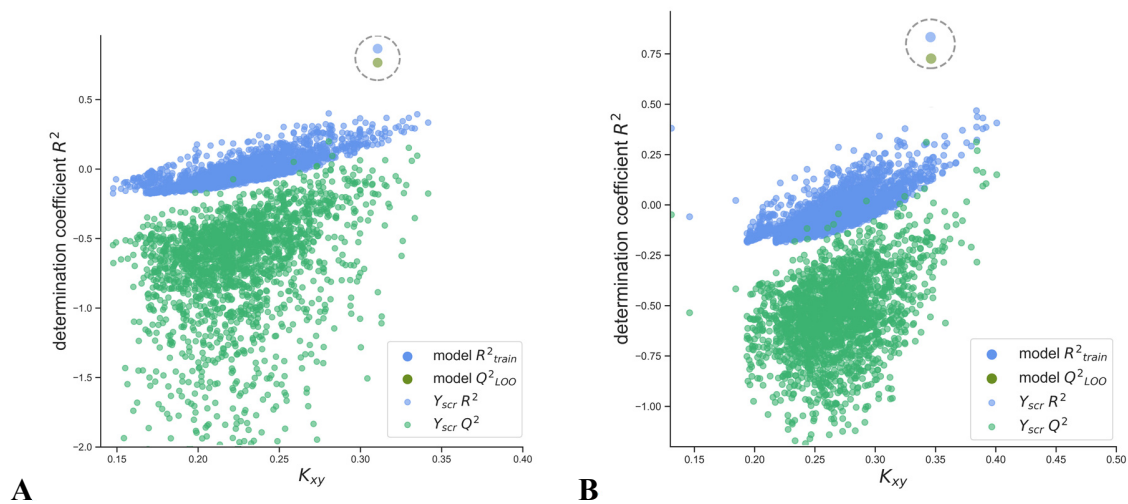


Figure S4. Y-scrambling test resulting graphs for QPON1 model, eq. 3 (A), and RPON1 model, eq. 4 (B)

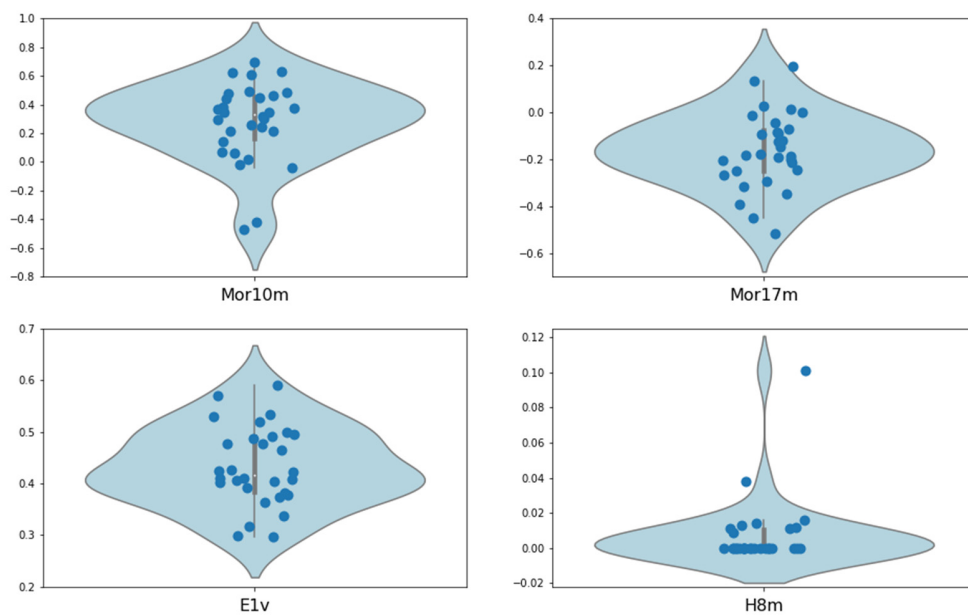


Figure S5. Density distribution of the descriptors values for each variable in a violin plot for the QPON1 model.

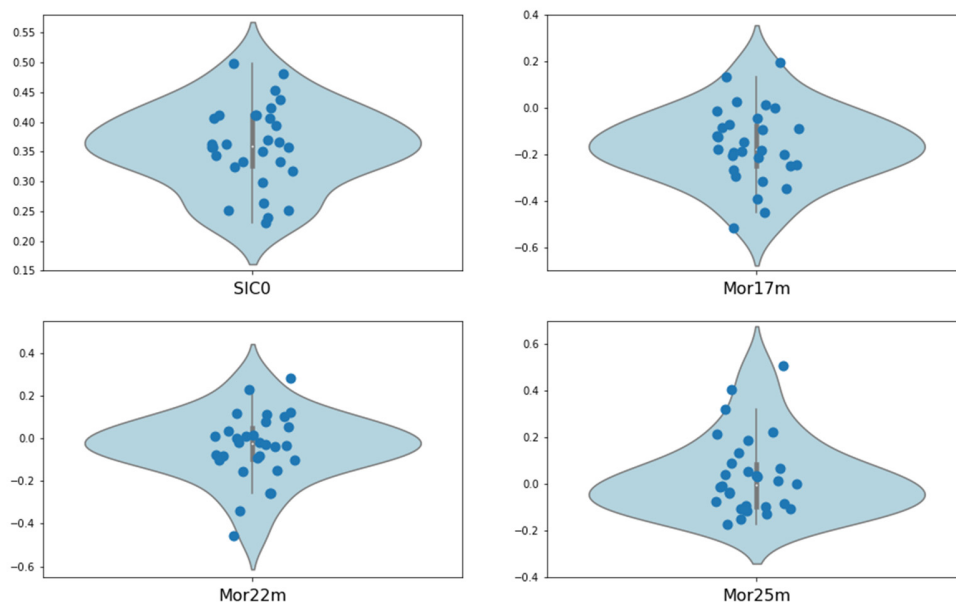


Figure S6. Density distribution of the descriptors values for each variable in the RPON1 model (Plot generated using matplotlib and seaborn library of Python).

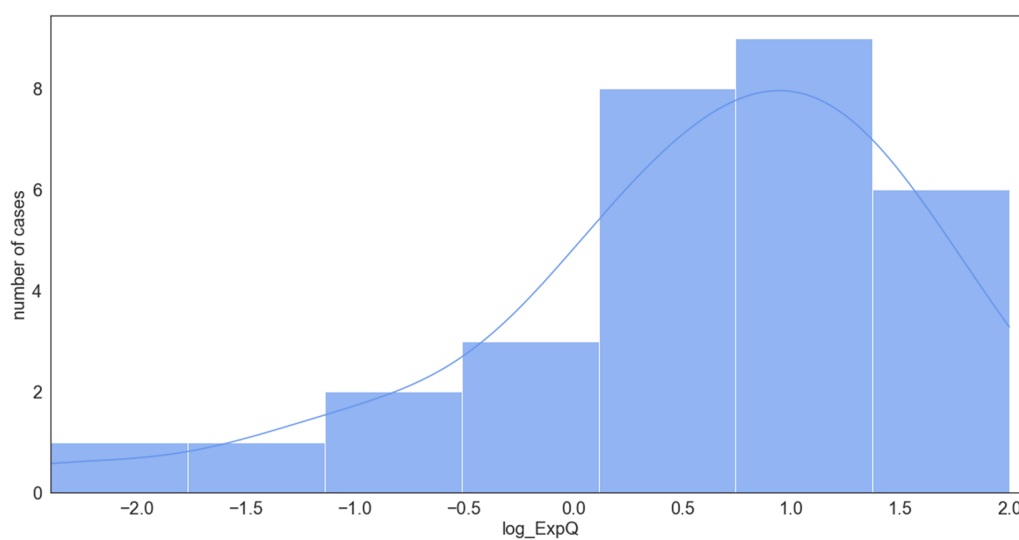


Figure S7. Histogram distribution for QPON1 model based on response variable (rate of reaction).

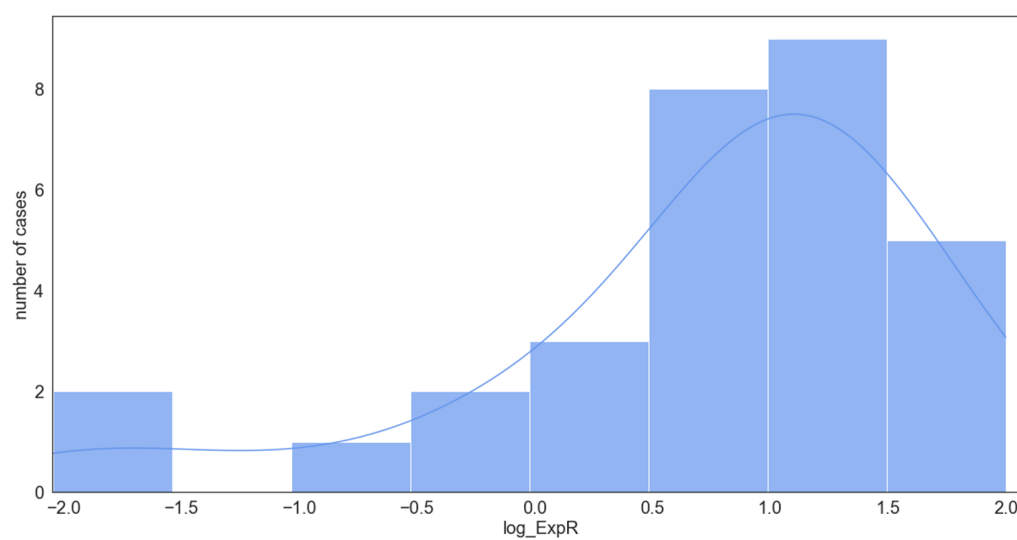


Figure S8. Histogram distribution for RPON1 model based on response variable (rate of reaction).