Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

Theoretical Study of the Hydrolysis Mechanism of Dihydrocoumarin Catalyzed by Serum Paraoxonase 1 (PON1): Different Roles of Glu53 and His115 for Catalysis

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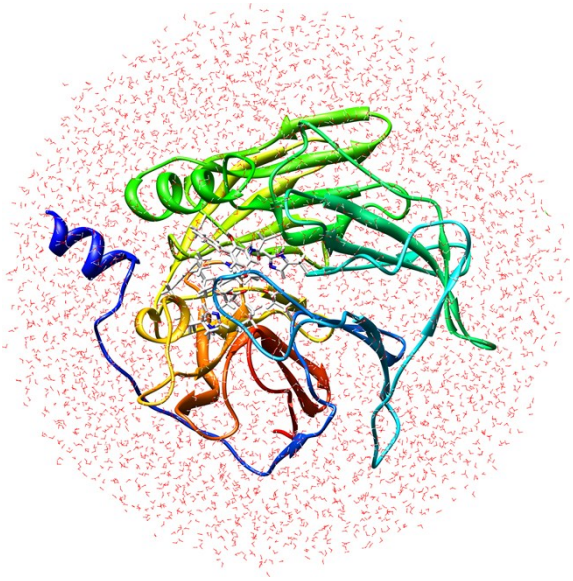

Figure S1. The constructed solvation model for the MD simulation.

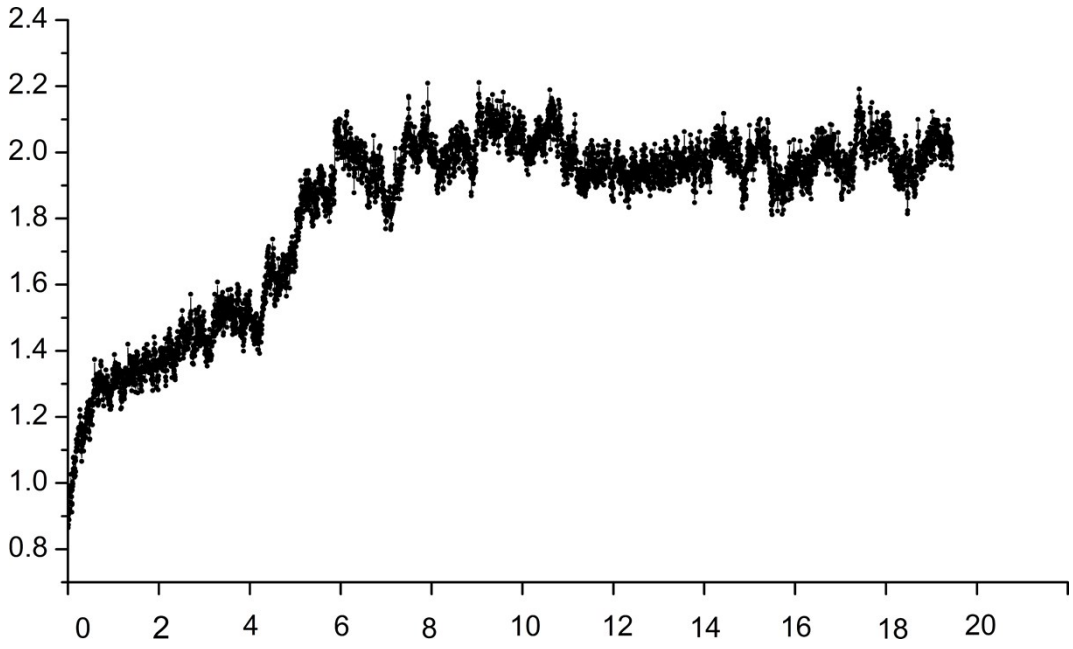

Figure S2. Time dependencies of the root-mean-square deviation (RMSD) for the backbone atoms of PON1.

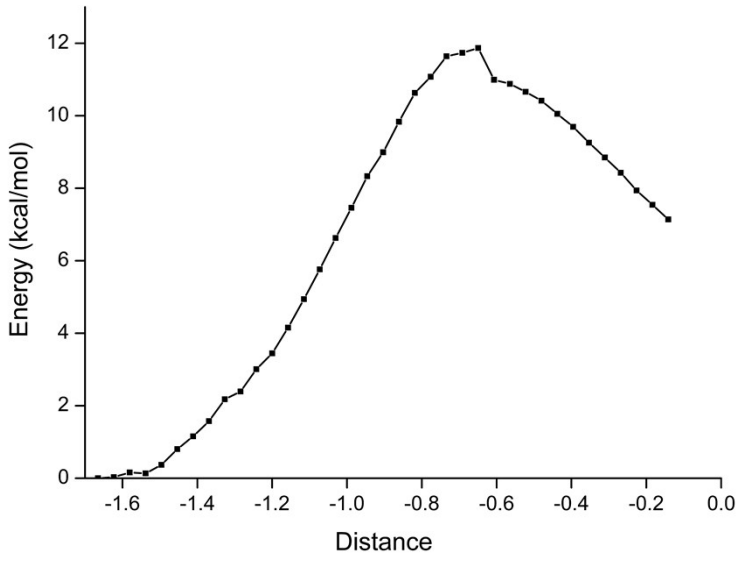

Figure S3. Energy profile for the scanning of the second step in path_a . X-axis refers to the distances of scanning radius (R). $R = R_{C1\text{-}O5} - R_{O2\text{-}H4} - R_{C1\text{-}O6}$.

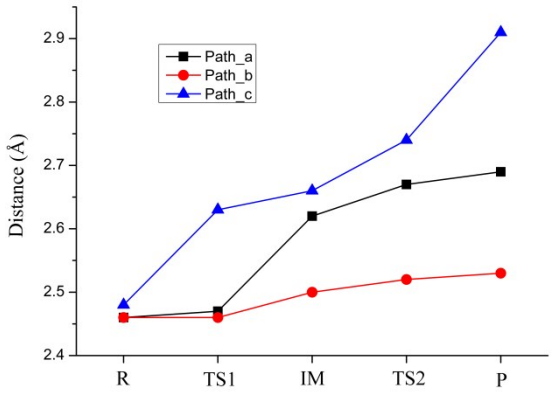

Figure S4. Distances between Ca^{2+} and the carboxyl oxygen of Glu53 in Path_a, Path_b and Path_c.

Table S1 Natural Population Atomic Charges of selected atoms in species for PON1-substrate complex in Path_a calculated at B3LYP/6-31++G(2d,2 p) level.

	R	TS1	IM	TS2	P
Ca^{2+}	1.85	1.84	1.84	1.84	1.84
O1	-0.97	-0.89	-0.83	-0.80	-0.82
H1	0.49	0.52	0.49	0.49	0.52
H2	0.49	0.53	0.52	0.53	0.54
O2	-0.93	-0.90	-0.88	-0.88	-0.81
N1	-0.57	-0.57	-0.52	-0.51	-0.57
O3	-0.68	-0.72	-0.73	-0.78	-0.85
O4	-0.72	-0.72	-0.71	-0.77	-0.79
H3	0.51	0.52	0.53	0.53	0.53
O5	-0.73	-0.81	-0.98	-0.85	-0.74
O6	-0.56	-0.56	-0.60	-0.69	-0.75
C1	0.90	0.89	0.89	0.88	0.91

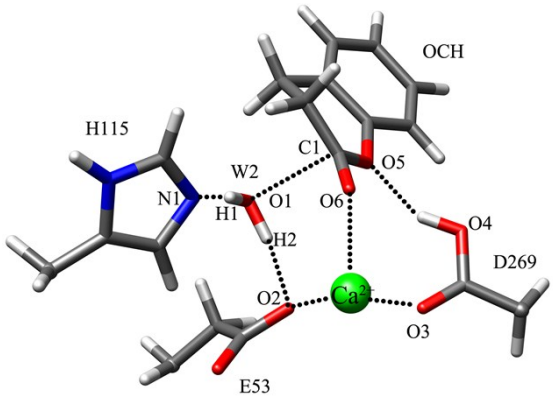

Table S2 Natural Population Atomic Charges of selected atoms in species for PON1-substrate complex in Path_b calculated at B3LYP/6-31++G(2d,2 p) level.

	R	TS1	IM	TS2	P
Ca^{2+}	1.85	1.84	1.84	1.85	1.84
O1	-0.97	-0.88	-0.83	-0.83	-0.69
H1	0.49	0.52	0.52	0.52	0.49
H2	0.49	0.53	0.53	0.53	0.53
O2	-0.93	-0.90	-0.84	-0.82	-0.87
N1	-0.57	-0.58	-0.57	-0.57	-0.52
O3	-0.68	-0.72	-0.74	-0.80	-0.85
O4	-0.72	-0.72	-0.71	-0.77	-0.79
H3	0.51	0.52	0.52	0.53	0.52
O5	-0.73	-0.87	-0.99	-0.88	-0.83
O6	-0.56	-0.56	-0.60	-0.69	-0.76
C1	0.90	0.89	0.90	0.89	0.92

Table S3 Natural Population Atomic Charges of selected atoms in species for PON1-substrate complex in Path_c calculated at B3LYP/6-31++G(2d,2 p) level.

	R	TS1	IM	TS2	P
Ca^{2+}	1.84	1.82	1.82	1.82	1.82
O1	-1.09	-1.09	-0.90	-0.87	-0.87
H1	0.52	0.49	0.49	0.49	0.49
H2	0.51	0.49	0.52	0.55	0.52
O2	*	*	*	*	*
N1	-0.59	-0.53	-0.53	-0.52	-0.52
O3	-0.71	-0.74	-0.76	-0.82	-0.77
O4	-0.70	-0.71	-0.71	-0.76	-0.70
H3	0.51	0.52	0.52	0.52	0.53
O5	-0.67	-0.78	-0.94	-0.75	-0.76
O6	-0.54	-0.57	-0.61	-0.72	-0.75
C1	0.90	0.89	0.88	0.84	0.83

Table S4 Natural Population Atomic Charges of selected atoms in species for PON1-substrate complex in Path_d calculated at B3LYP/6-31++G(2d,2 p) level.

	R	TS1	IM	TS2	P
Ca^{2+}	1.82	1.82	1.82	1.83	1.82
O1	-1.00	-0.88	-0.83	-0.83	-0.69
H1	0.48	0.52	0.52	0.52	0.49
H2	0.51	0.53	0.53	0.53	0.53
O2	-0.89	-0.84	-0.80	-0.78	-0.74
N1	*	*	*	*	*
O3	-0.66	-0.70	-0.72	-0.77	-0.85
O4	-0.75	-0.74	-0.72	-0.73	-0.79
H3	0.52	0.52	0.52	0.52	0.53
O5	-0.72	-0.88	-0.96	-0.80	-0.74
O6	-0.54	-0.58	-0.62	-0.76	-0.77
C1	0.91	0.89	0.90	0.89	0.91