Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

The catalytic mechanism of mouse renin studied by QM/MM calculations

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Supporting Information

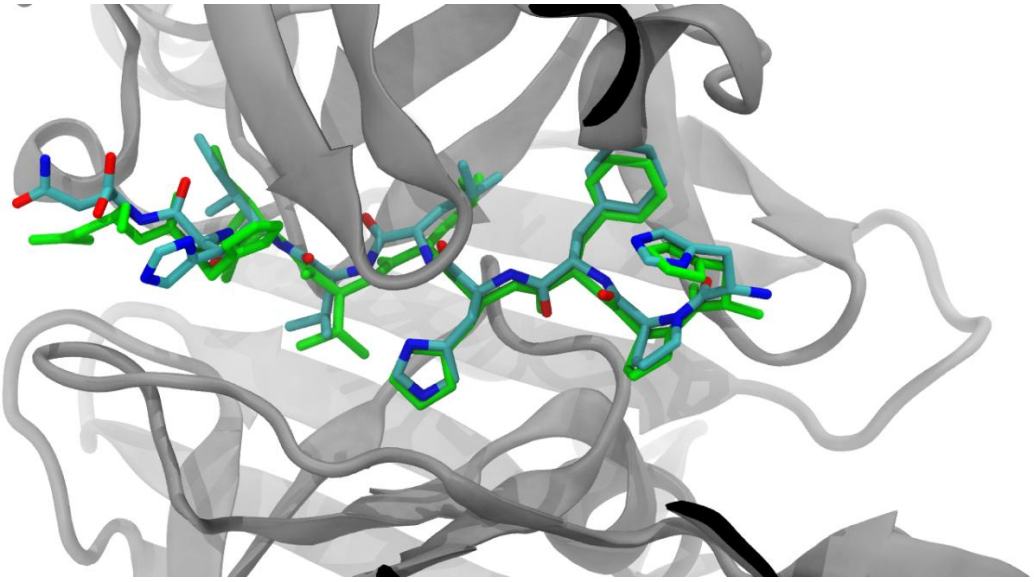

Figure SI-1 – The superposition of the modelled substrate (coloured by element and depicted ball and stick representation) and the recently crystallized human renin:angiotensinogen structure (pdb id: 2XOB coloured green and depicted ball and stick representation).

Table SI-1 – Activation and reaction energies obtained for the three mechanistic steps with the QM region treated at the B3LYP, B3LYP-D3, X3LYP, M06, B1B95, BMK, mPWB1K and B2PLY density functionals, using the 6-311+G(2d,2p) basis set and the electrostatic embedding scheme. The difference obtained with the B3LYP functional using either electrostatic (ee) or mechanical embedding (me) is also shown.

	TS1 ($\Delta H^{\ddagger}$)	**INT1**	**TS2 ($\Delta H^{\ddagger}$)**	**INT2**	**TS3 ($\Delta H^{\ddagger}$)**	**P (ΔH_R)**
B3LYP (ee)[1]	23.68	14.37	15.51	10.20	14.40	-0.61
B3LYP (ee)-B3LYP (me)[2]	-1.93	-0.99	-6.16	-6.06	-3.07	-4.70
B3LYP-D3	24.64	12.92	19.73	14.87	18.89	0.75
BMK	24.02	12.17	12.86	7.69	12.63	2.87
B1B95	22.62	11.93	13.02	8.33	12.78	1.73
X3LYP	23.36	13.94	14.98	9.70	13.97	-0.07
M06	23.88	11.82	12.76	8.84	12.24	4.05
mPWB1K	22.62	9.92	11.54	7.00	12.31	3.21
B2PLYP	23.71	13.70	14.61	9.43	13.78	1.37