Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Kinetic Basis for Activation of Human Cyclooxygenase-2 Rather Than Cyclooxygenase-1 by Nitric Oxide

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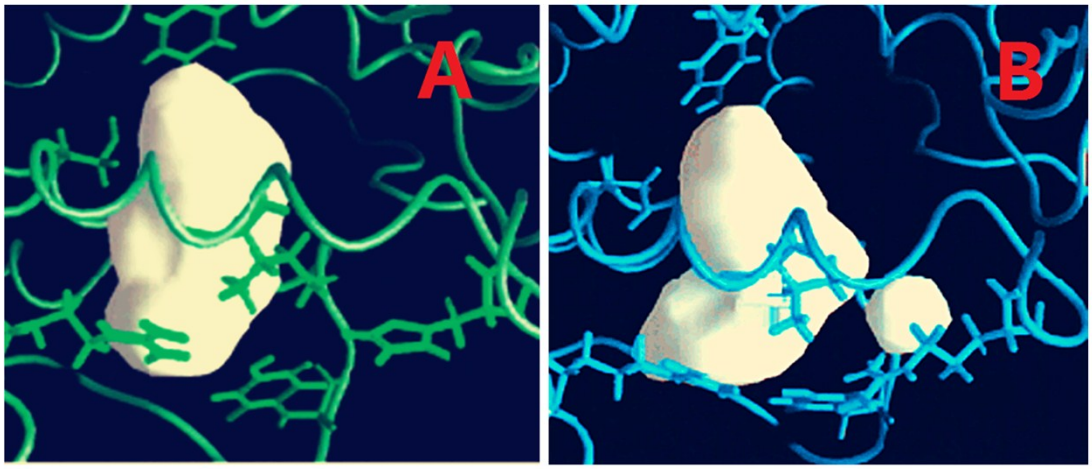

Figure S1. Comparison of solvent-accessible space (white) in the cyclooxygenase active sites of (A) human COX-1 (PDB id: 1DIY) and (B) human COX-2 (PDB id: 3HS5).

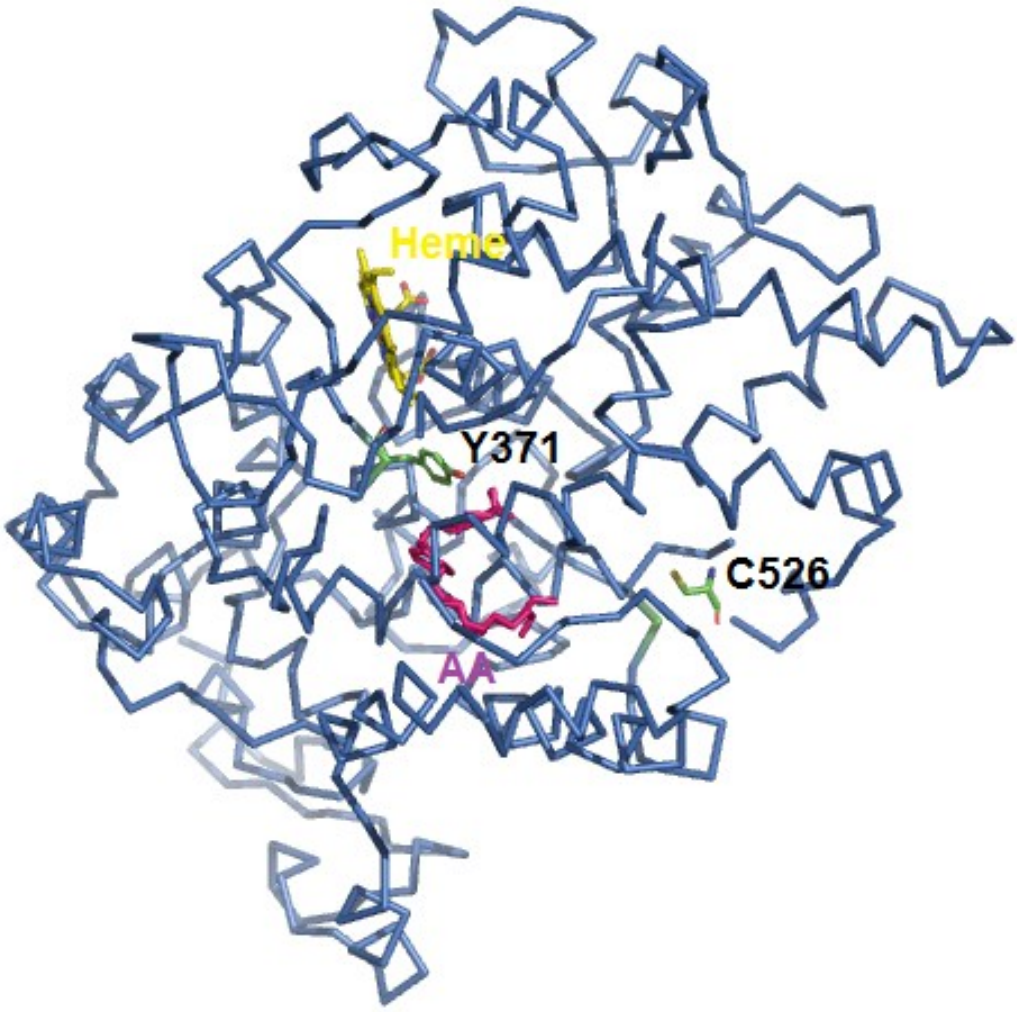

Figure S2. Structure of human COX-2 with AA bound to its active site (PDB id: 3HS5). The putative S-nitrosylated cysteine 526 located at a high hydrophobic region as far as 30 Å away from the heme prosthetic group.

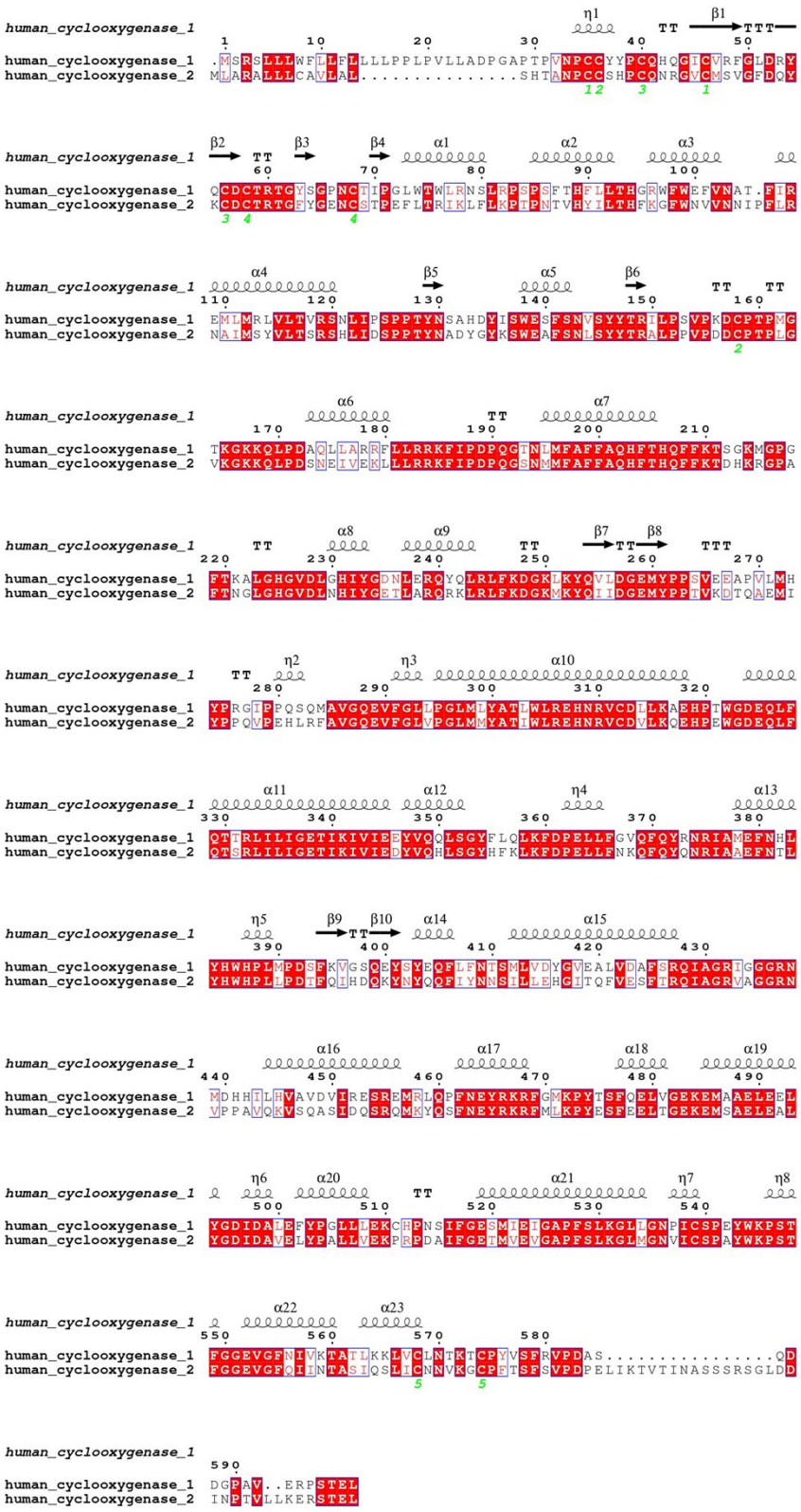

Figure S3. Sequence alignment of human COX-1 and COX-2 indicates that several cysteine residues can putatively be S-nitrosylated in both enzymes. The protein sequences are obtained from pubmed. The Cys526 in COX-2, which is suggested responsible for the activity enhancement by S-nitrosylation, is corresponding to Cys540 in COX-1.

Table S1. The maximum Soret absorbance of COX-1 and COX-2 with/without NO

	COX-1	COX-1 + NO	COX-2	COX-2 + NO
Maximum Soret absorbance	0.855	0.901	0.655	0.661

Notes: The experiments were carried out at the condition used in reference 4. COX-1 and COX-2 (5 μM) were incubated with NO (50 μM) in 100 mM Tris, pH 8.0.

Table S2. Quantitative analysis of CD data

Treatment	α-helix	β-sheet	turns & random coil
COX-1	37.3	0	62.6
S-nitrosylated COX-1	21.1	35.6	43.3
COX-2	40.0	1.2	58.8
S-nitrosylated COX-2	22.4	44.1	33.5