

Supplementary materials

Biological Evaluation and Molecular Docking Studies of Novel 1,3,4-Oxadiazole Derivatives of 4,6-Dimethyl-2-Sulfanylpuridine-3-Carboxamide

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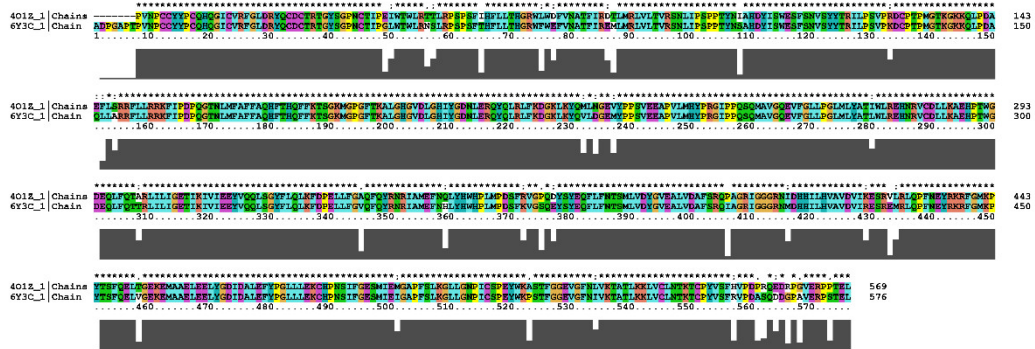
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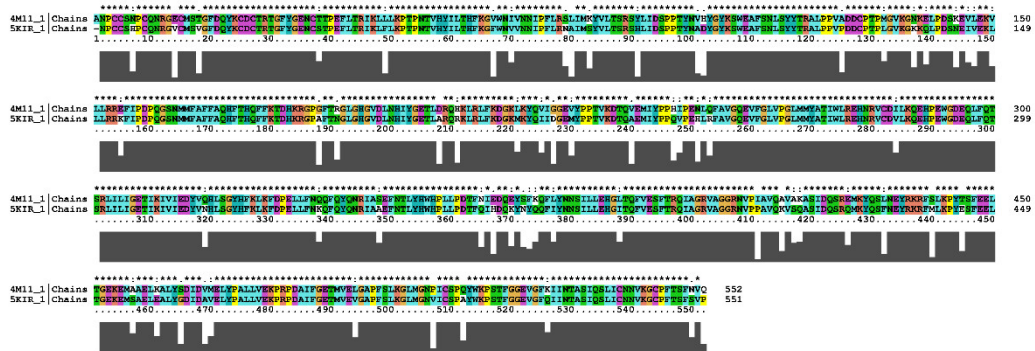
(a)

CLUSTAL 2.1 MULTIPLE SEQUENCE ALIGNMENT
Ovine COX-1 (401Z) vs. human COX-1 (6Y3C): 91% sequence similarity



(b)

CLUSTAL 2.1 MULTIPLE SEQUENCE ALIGNMENT
Murine COX-2 (4M11) vs. human COX-2 (5KIR): 88% sequence similarity



(c)

CLUSTAL 2.1 MULTIPLE SEQUENCE ALIGNMENT
Human COX-1 (6Y3C) vs. human COX-2 (5KIR): 66% sequence similarity

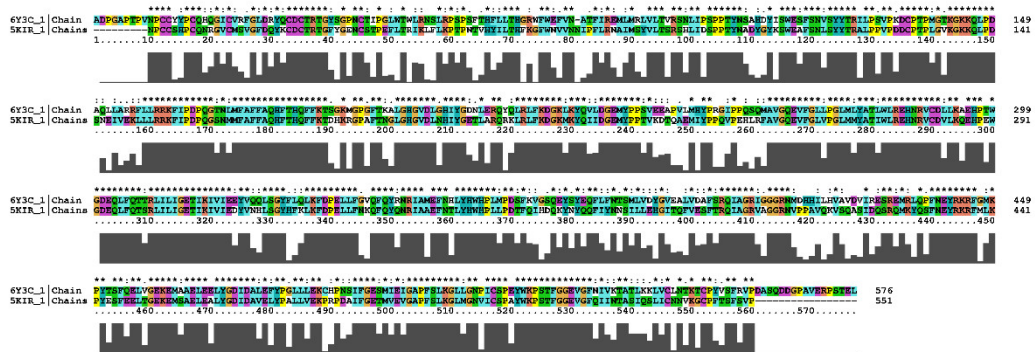


Figure S1. Sequence alignment of the proteins used in the study: (a) ovine COX-1 vs. human COX-1, (b) murine COX-2 vs. human COX-2, and (c) human COX-1 vs. human COX-2.

Table S1. The SCF energies for two series of examined compounds calculated at the ω B97XD/cc-pVDZ level of theory.

Total and relative energy of the structures				
Compound	SCF energy [kcal/mol]	Compound	SCF energy [kcal/mol]	Relative energy of E vs. S [kcal/mol]
4(E)	-1164210.45	4(S)	-1164209.94	-0.5
5(E)	-1333053.63	5(S)	-1333063.04	9.4
6(E)	-1395310.96	6(S)	-1395321.67	10.7
7(E)	-1357719.42	7(S)	-1357729.16	9.7
8(E)	-1607580.85	8(S)	-1607590.47	9.6
9(E)	-1390917.34	9(S)	-1390928.55	11.2
10(E)	-1621455.36	10(S)	-1621464.66	9.3
11(E)	-1544506.58	11(S)	-1544516.83	10.3
12(E)	-1621455.04	12(S)	-1621464.31	9.3
13(E)	-2947974.15	13(S)	-2947984.65	10.5

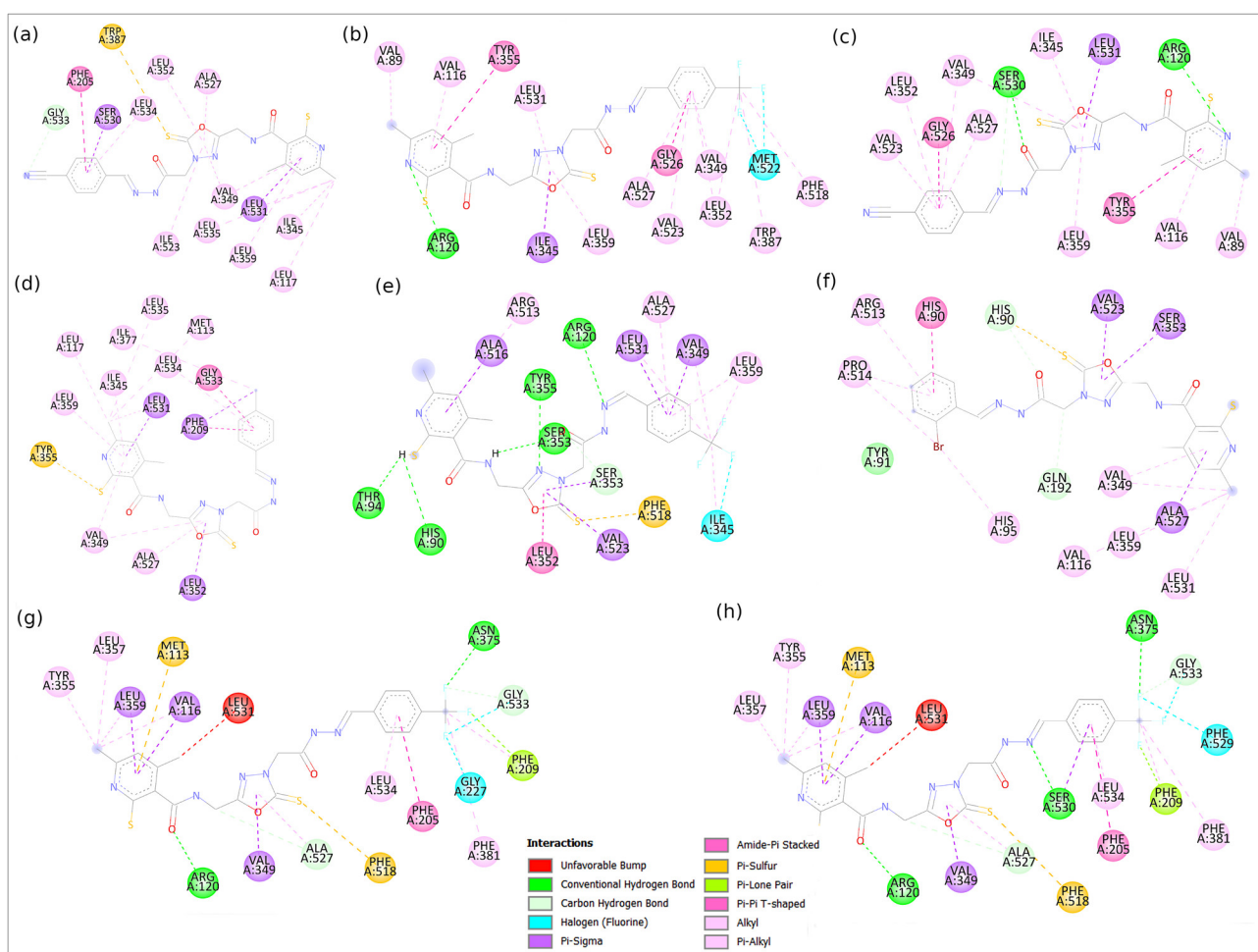


Figure S2. Non-covalent interactions 2D diagram for studied compounds in receptor binding sites: (a) **9(S)** in ovine COX1, (b) **11(E)** in murine COX2, (c) **9(S)** in murine COX2, (d) **7(E)** in ovine COX1, (e) **11(E)** in human COX2, (f) **13(S)** in human COX2, (g) **11(S)** in human COX1, (h) **11(E)** in human COX1.