

## Supporting Information

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### Design, synthesis, characterization and bioassay of novel carboxamide derivatives of Celecoxib

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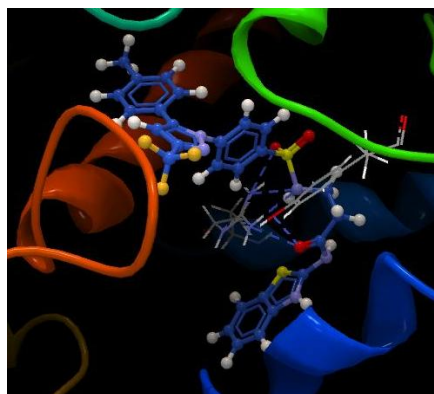
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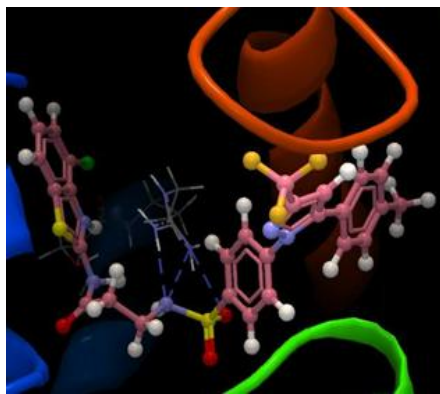
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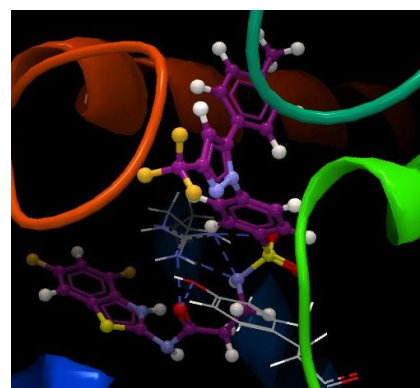
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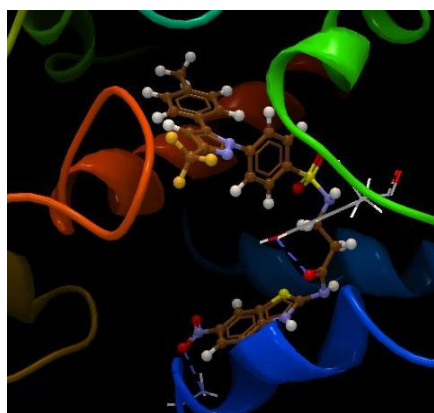
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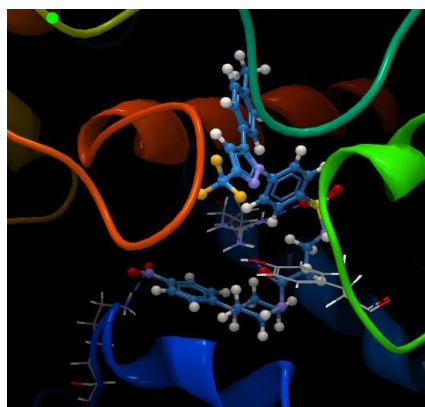
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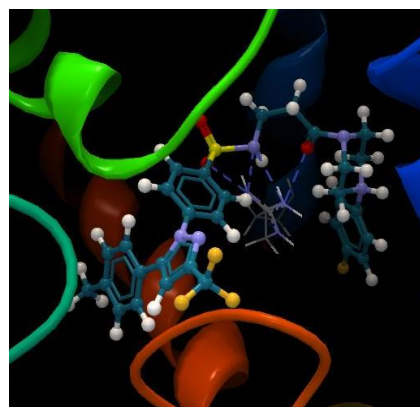
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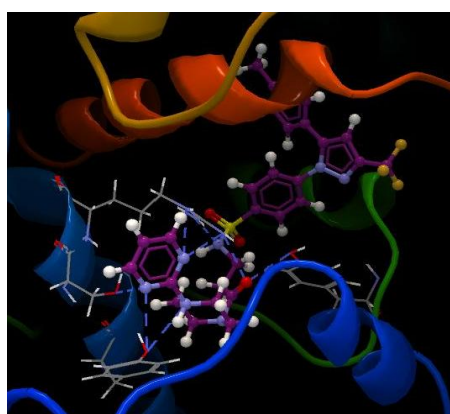
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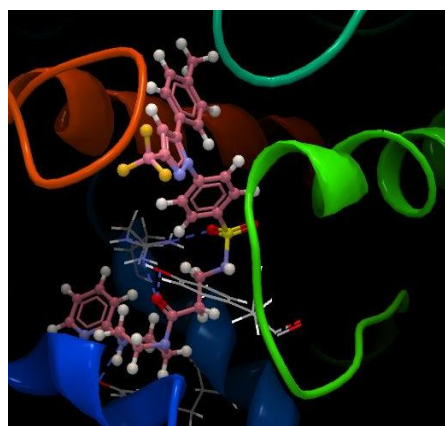
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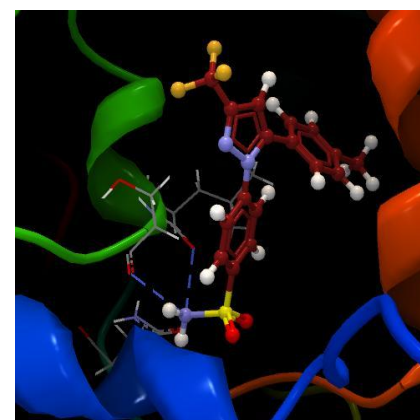
4f



4g



4h



Celecoxib

**Figure 4. Docking Results**

**Table 4.** Docking interactions (score) of the synthesized amide derivatives of celecoxib at COX-2 enzyme

Name of the ligand	CLC docking score	No. of hydrogen bonds	Amino acid involved in protein ligand interaction	(amino acid)-(ligand) Bonding
S58	-75.07	2	SER 353 LEU 352	O – N O – N
4a	-90.96	4	GLY 192 TYR 355 ARG 120	OC <sub>1</sub> – N H – O NH <sub>2</sub> – O NH <sub>1</sub> – N
4b	-91.70	4	ARG 120	NH <sub>1</sub> – O NH <sub>2</sub> – N NH <sub>1</sub> – N NH <sub>1</sub> – O
4c	-95.03	4	SER 119 TYR 355 ARG 120	OG – N OH – O NH <sub>2</sub> – N NH <sub>1</sub> – N NH <sub>1</sub> – O
4d	-86.69	2	LYS 83 TYR 355	N <sub>2</sub> – N OH – O
4e	-79.49	3	ARG 120 TYR 355 LYS 83	NH <sub>1</sub> – O OH – O N <sub>2</sub> – O
4f	-86.81	4	ARG 120	NH <sub>2</sub> – O NH <sub>2</sub> – N NH <sub>1</sub> – N NH <sub>1</sub> – O
4g	-80.16	5	ARG 120	NH <sub>2</sub> – N NH <sub>1</sub> – N NH <sub>1</sub> – O OH – N
4h	-80.00	4	TYR 115 TYR 355 ARG 120	OH – O NH <sub>2</sub> – O NE – N OH – N OH – O
Celecoxib	-75.64	3	GLN 192 LEU 352 SER 353	OE <sub>1</sub> – N O – N O – N