

# Identification and Dynamics Understanding of Novel Inhibitors of Peptidase Domain of Collagenase G from *Clostridium histolyticum*

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**Table S2:** Lipophilicity properties of the investigated compounds

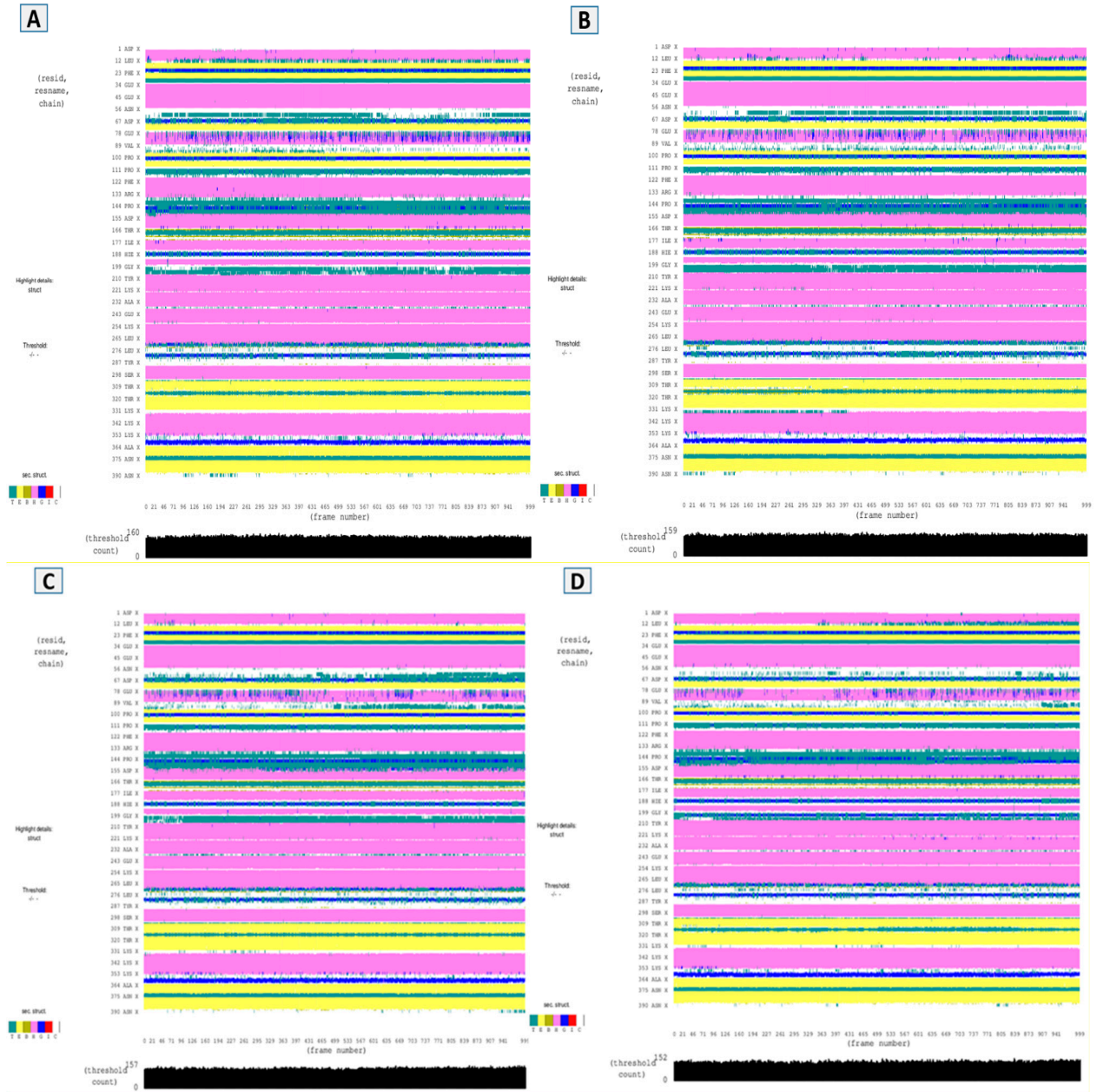
Lipophilicity Properties						
Compounds	Log $P_{o/w}$ (iLOGP)	Log $P_{o/w}$ (XLOGP3)	Log $P_{o/w}$ (WL OGP)	Log $P_{o/w}$ (ML OGP)	Log $P_{o/w}$ (SILICOS-IT)	Consensus Log $P_{o/w}$
MSID000001	4.22	7.78	7.54	5.73	6.91	6.44
MSID000002	5.24	9.44	8.73	7.01	8.20	7.72
MSID000003	4.17	5.59	5.50	4.62	5.07	4.990
Control	0.80	0.51	0.86	-0.64	0.66	0.44

**Table S3:** Physiochemical properties of the selected compounds

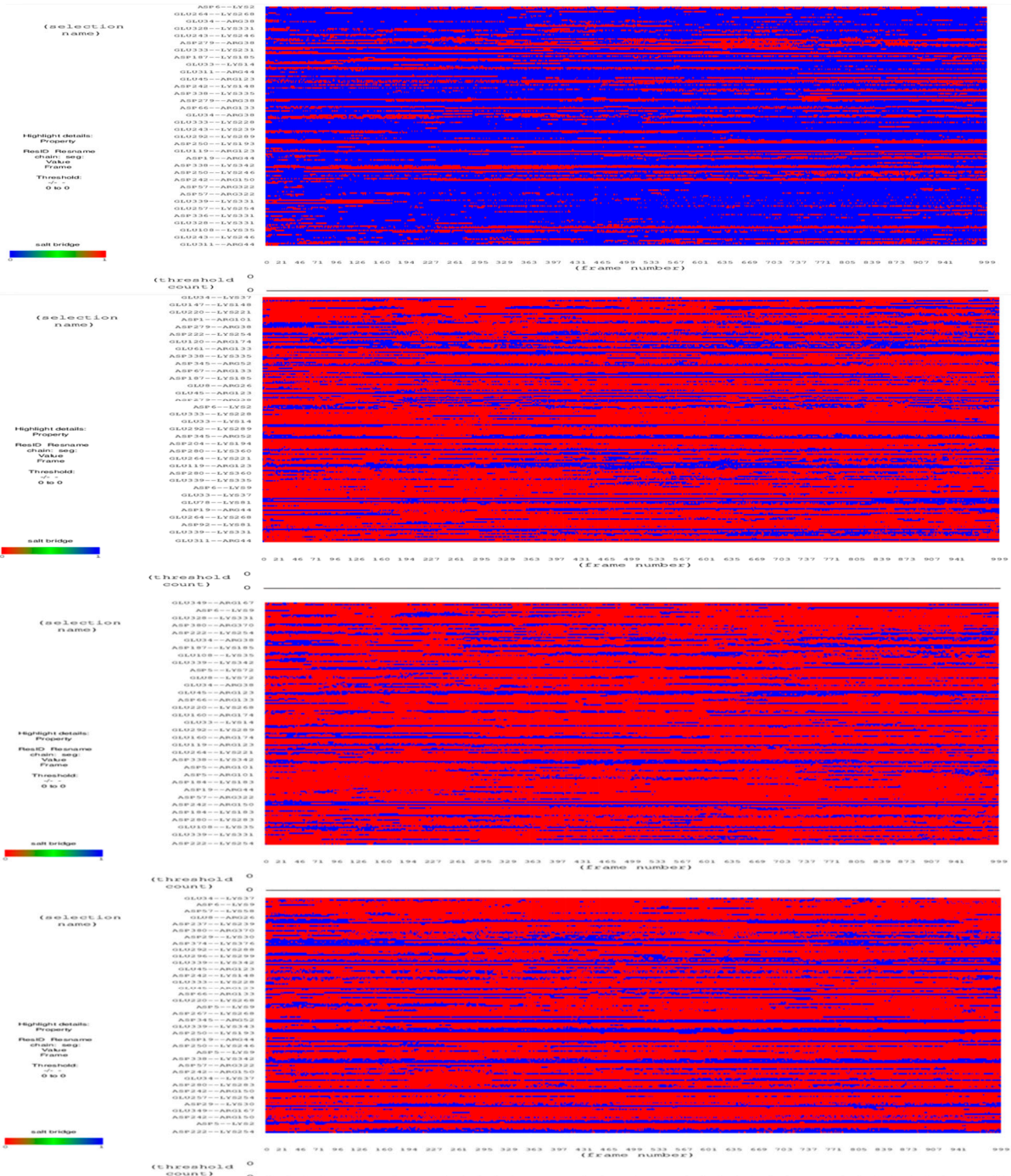
Physicochemical Properties								
Compounds	Formula	Molecular Weight	Num. heavy atoms	Num. arom.	Num. H-bond acceptors	Num. H-bond donors	Molar Refractivity	TPSA
MSID000001	C30H48O3	456.70 g/mol	33	0	3	2	138.81	57.53 Å <sup>2</sup>
MSID000002	C31H52O	440.74 g/mol	32	0	1	1	141.85	20.23 Å <sup>2</sup>
MSID000003	C28H46O3	430.66 g/mol	31	0	3	3	130.31	60.69 Å <sup>2</sup>
Control	C15H12O7	304.25 g/mol	22	12	7	5	74.76	127.45 Å <sup>2</sup>

**Table S4:** Drug-likeness of the studied compounds.

Drug-likeness										
Compounds	Ghose	Veber	Lipinski	Muegge	Egan	Bioavailability	PAINS	Brenk	Leadlikeness	Synthetic accessibility
<b>MSID000001</b>	Yes; 1 violation: MLOGP>4.15	No; 3 violations: WLOGP>5.6, MR>130, #atoms>70	Yes	No; 1 violation: WLOGP>5.88	No; 1 violation: XLOGP3>5	0.85	0 alert	1 alert: isolated_alkene	No; 2 violations: MW>350, XLOGP3>3.5	5.87
<b>MSID000002</b>	Yes; 1 violation: MLOGP>4.15	No; 3 violations: WLOGP>5.6, MR>130, #atoms>70	Yes	No; 1 violation: WLOGP>5.88	No; 2 violations: XLOGP3>5, Heteroatoms<2	0.55	0 alert	1 alert: isolated_alkene	No; 2 violations: MW>350, XLOGP3>3.5	6.19
<b>MSID000003</b>	Yes; 1 violation: MLOGP>4.15	No; 2 violations: MR>130, #atoms>70	Yes	Yes	No; 1 violation: XLOGP3>5	0.55	0 alert	1 alert: isolated_alkene	No; 2 violations: MW>350, XLOGP3>3.5	6.53
<b>Control</b>	Yes; 0 violation	Yes	Yes	Yes	Yes	0.55	1 alert: catechol_A	1 alert: catechol	Yes	3.49



**Figure S1.** The secondary structure of the top three complexes MSID000001 (A), MSID000002 (B), MSID000003 (C), and Control (D), respectively.



**Figure S2.** The salt bridges interaction of top three complexes MSID000001, MSID000002, MSID000003 and Control, respectively.