Supporting Information

Extra Binding Region Induced by Non-Zinc Chelating Inhibitors into the S_1' Subsite of Matrix Metalloproteinase 8 (MMP-8)

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Content

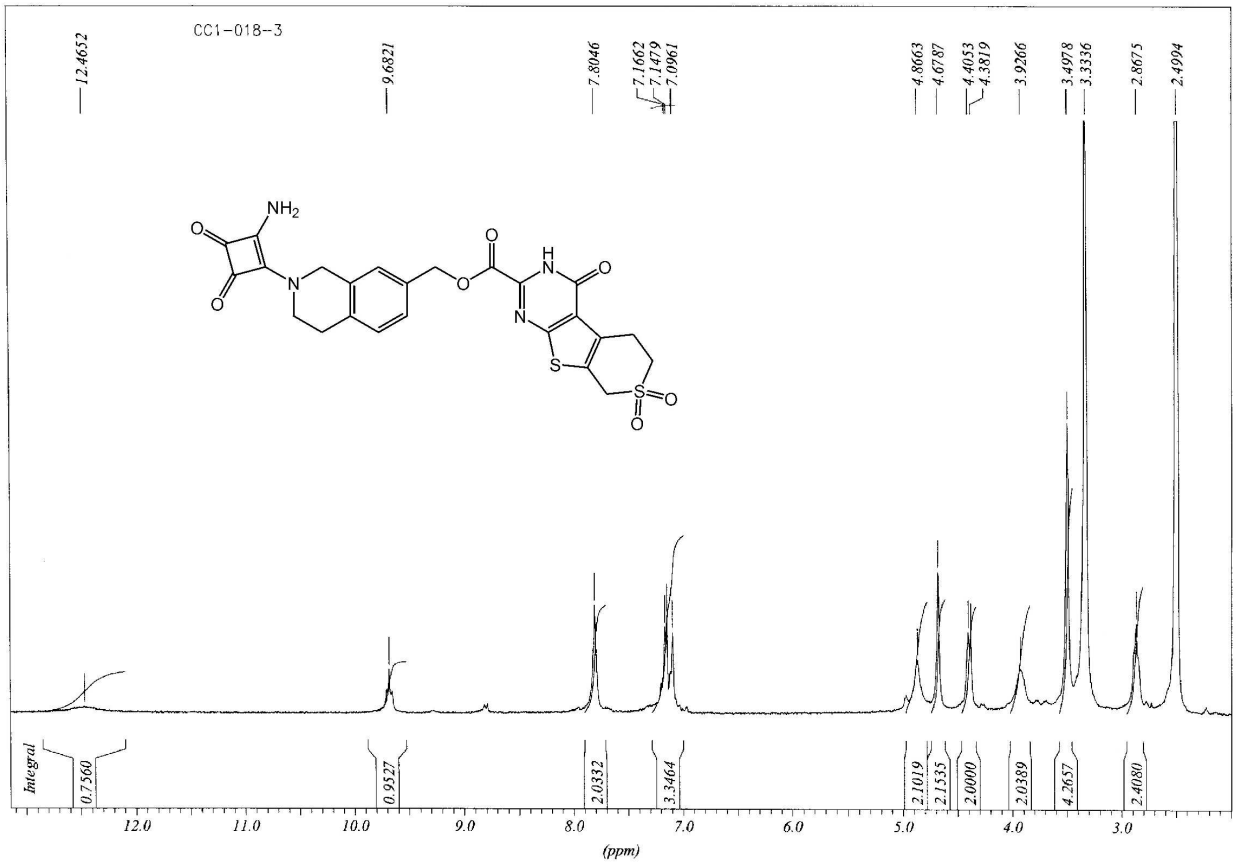
Table S1. C^{α} distances (Å) at the S_1' loop region between the uninhibited MMP-8 and the inhibited complexes MMP-8:**1** (first raw), MMP-8:(*S*)**-2** (second raw). The sequences 86-218 and 230-242 of the enzyme backbones were overlapped. The S_1' loop region was considered between the invariant Y219 and L229. For comparison, the rms differences between the C^{α} of chains 86-218 and 230-242 of uninhibited and the two complexed enzymes, respectively are 0.37 and 0.40 Å.

Y219	A220	F221	R222	E223	T224	S225	N226	Y227	S228	L229
0.39	0.71	0.16	2.01	1.61	5.82	5.30	1.51	0.69	0.14	0.45
0.39	0.79	0.59	2.23	3.19	6.30	5.37	3.73	0.98	0.58	0.40

Elemental analyses.

Compound	**Calculated**				**Found**			
	C%	**H%**	**N%**	**S%**	**C%**	**H%**	**N%**	**S%**
1	53.42	3.92	16.98	11.89	53.82	3.78	16.95	11.85
2	56.52	4.53	14.98	6.86	56.50	4.49	15.03	6.89

^{1}H NMR (DMSO-d_6) spectra of compound 1.



^{1}H NMR (DMSO-d_6) spectra of compound 2.