**Supporting Information**

**Prediction of Matrix Metal Proteinases-12 Inhibitors by** **Machine Learning Approaches**

Bingke Li,[a] Li Hu,[a] Ying Xue,[b] Min Yang,[a] Long Huang,[a] Zhentao Zhang, [c,d] Jialei Liu,\*[c,d] Guowei Deng\*\*[a]

[a] College of Chemistry and Life Science, Institute of Functional Molecules, Chengdu Normal University, Chengdu 611130, People’s Republic of China

[b] College of Chemistry, Key Lab of Green Chemistry and Technology in Ministry of Education, Sichuan University, Chengdu 610064, People’s Republic of China

[c] Beijing Key Laboratory of ThermalScience and Technology, Beijing, China

[d]Technical Institute of Physics andChemistry, CAS Key Laboratory ofCryogenics, Beijing, China

\* Corresponding author.

\*\* Corresponding author.

E-mail addresses: liujialei@mail.ipc.ac.cn (J. Liu), guoweideng86@163.com (G. Deng)

**Contents**

**Table S1.** The MMP-12 inhibitors in the training set.

**Table S2.** The MMP-12 non-inhibitors in the training set.

**Table S3.** The MMP-12 inhibitors in the testing set.

**Table S4.** The MMP-12 non-inhibitors in the testing set.

**Table S5.** Description of 189 molecular descriptors.

**Table S6.** The MMP-12 inhibitors in the external independent evaluation set.