

## Supplementary materials

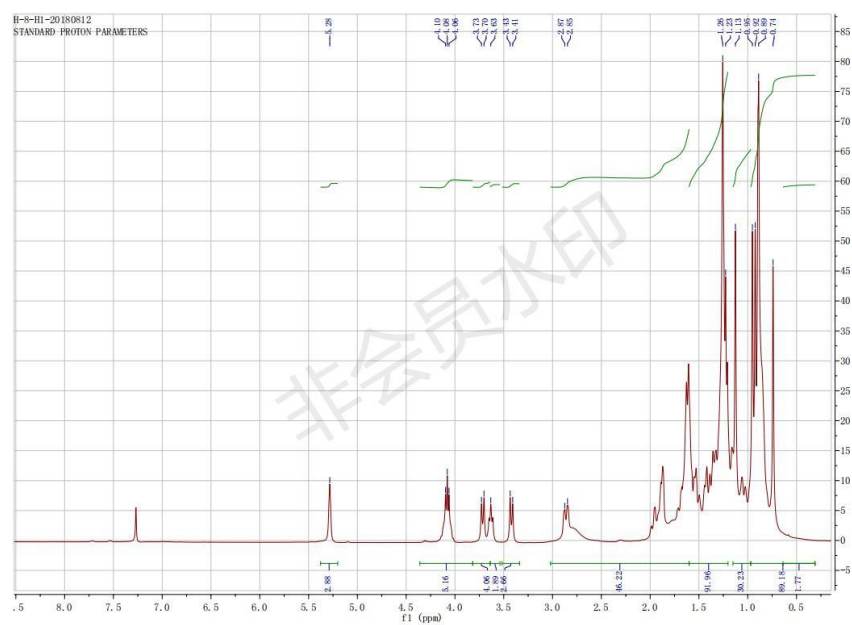
**Table S1.** Docking score, GLIDE score and GLIDE Emodel of ethyl caffeate, caffeic acid and isovanillin isolated from *Lonicera fulvotomentosa* Hsu et S. C. Cheng towards HIV protease.

Compounds	HIV protease		
	Docking score	GLIDE score	GLIDE Emodel (Kal/mol)
<b>Ethyl caffeate</b>			
Pose 1	-5.841	-5.844	-44.875
Pose 2	-5.573	-5.576	-44.431
Pose 3	-5.470	-5.473	-44.139
Pose 4	-5.311	-5.314	-44.925
Pose 5	-5.248	-5.251	-46.826
<b>Caffeic acid</b>			
Pose 1	-5.576	-5.576	-39.332
Pose 2	-5.505	-5.505	-41.301
Pose 3	-5.447	-5.447	-39.747
Pose 4	-5.222	-5.222	-37.197
Pose 5	-5.090	-5.090	-36.156
<b>Isovanillin</b>			
Pose 1	-6.109	-6.112	-34.995
Pose 2	-6.015	-6.019	-33.160
Pose 3	-5.986	-5.989	-34.585
Pose 4	-5.537	-5.540	-34.236
Pose 5	-5.507	-5.540	-31.349

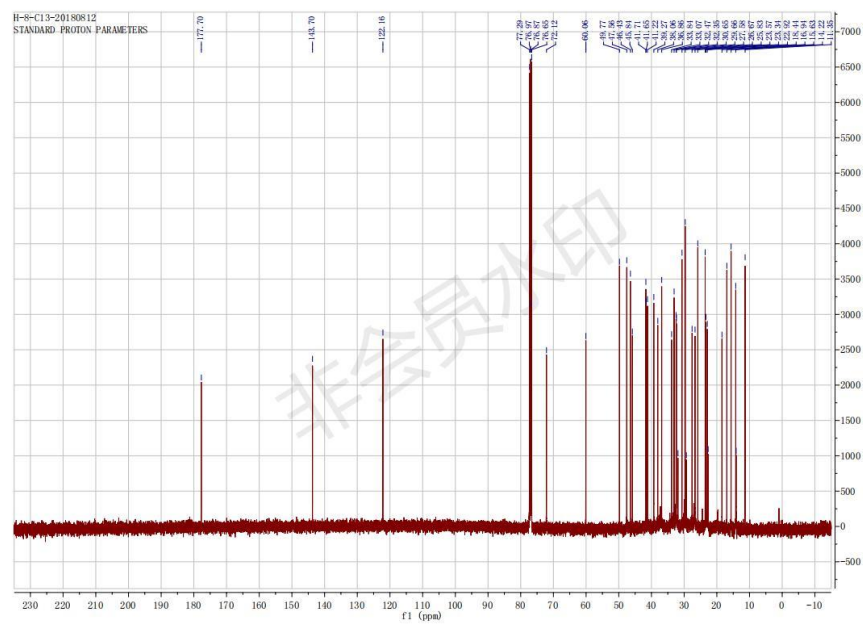
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Figure S1. Characterization of Compound 4

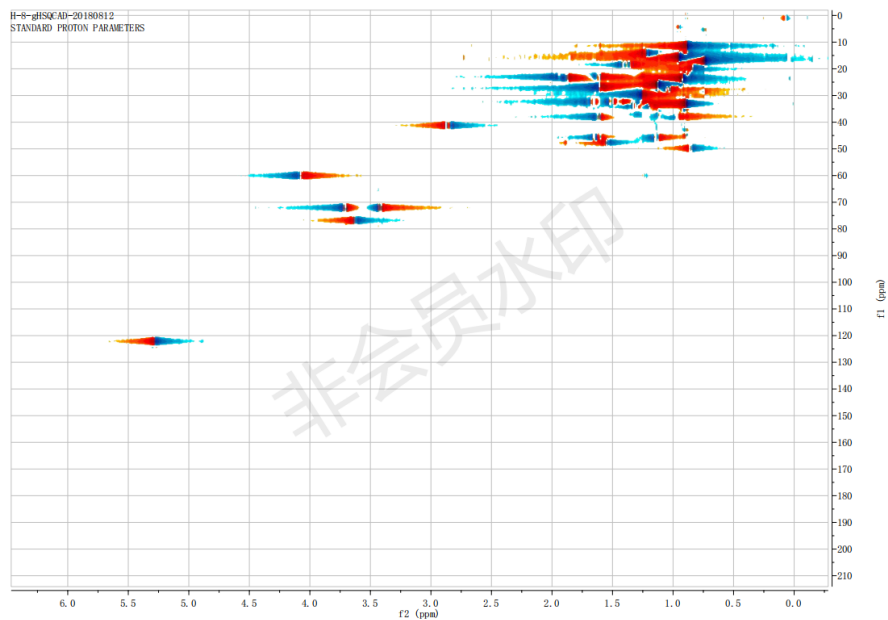
## $^1\text{H-NMR}$



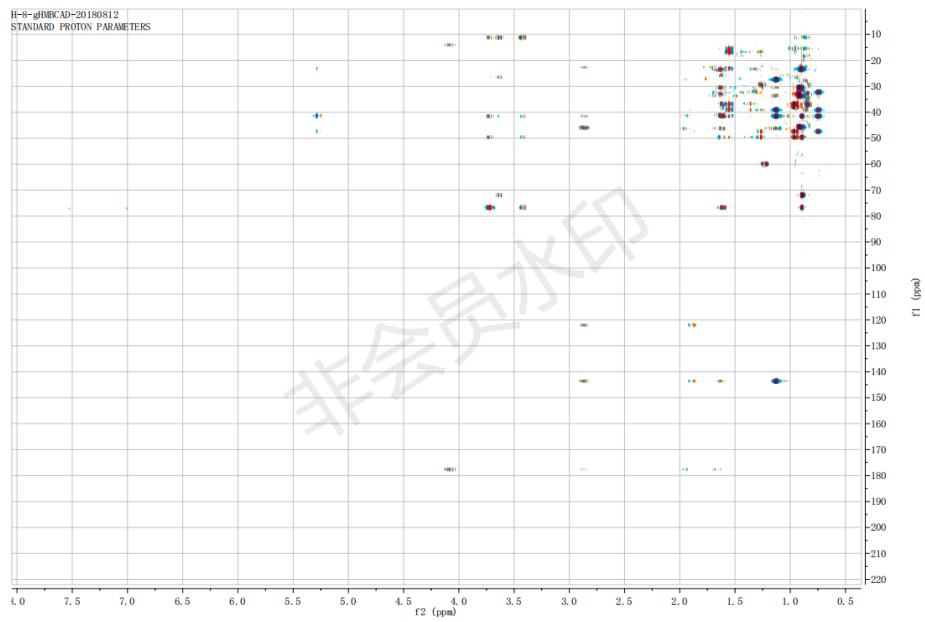
## $^{13}\text{C-NMR}$



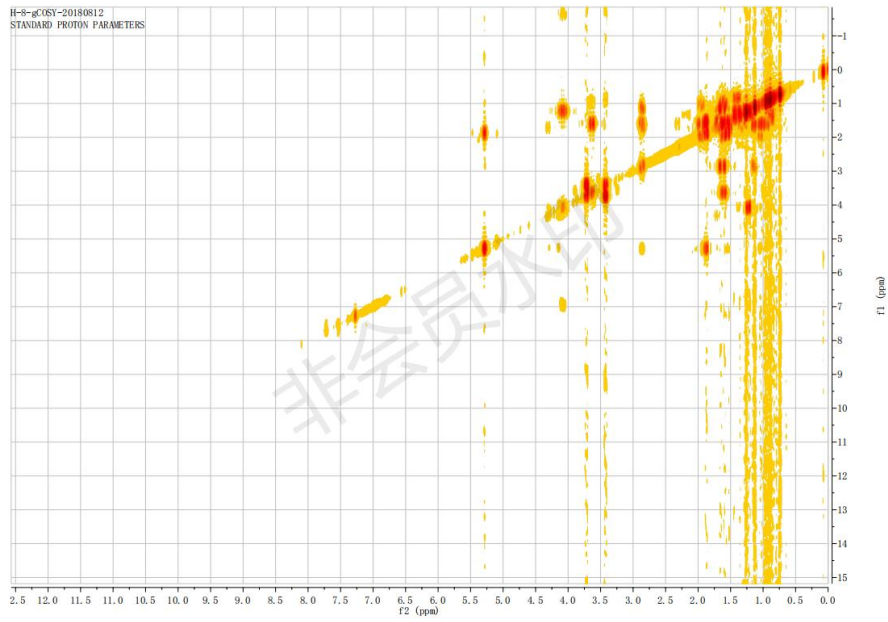
# HMQC



# HMBC



# GCOSY



# HR-MS

H-8\_180724153013 #123 RT: 0.57 AV: 1 NL: 2.06E8  
T: FTMS + p ESI Full ms (320.0000-1200.0000)

