

Supplementary Information

Characterizing the interaction between methyl ferulate and human serum albumin by saturation transfer difference NMR technique

Wenjing Wang^a, Qiaomei Sun^{*,a}, Na Gan^a, Yuanming Zhai^{*,b}, Hongzhao Xiang^a,
Hui Li^a

^a School of Chemical Engineering, Sichuan University, Chengdu 610065, China

^b Analytical & Testing Center, Sichuan University, Chengdu 610065, China

*Corresponding author:

Dr. Qiaomei Sun, E-mail address: qiaomeisun@163.com. Phone: +86 18200261093.

Address: School of Chemical Engineering, Sichuan University, Chengdu, Sichuan,
China

Dr. Yuanming Zhai, E-mail address: yuanmingzhai@scu.edu.cn. Phone: +86
13709089605. Address: Analytical & Testing Center, Sichuan University, Chengdu,
Sichuan, China

Table S1 $\eta(t_{sat})$ values for each ligand proton of MF (1.3×10^{-3} M) for its interaction with HSA

proton	0.5s	0.75s	1.0s	1.5s	2s	5s
H1	0.134	0.195	0.227	0.316	0.355	0.424
H2	0.133	0.182	0.254	0.320	0.360	0.433
H3	0.123	0.188	0.231	0.280	0.315	0.363
H4	0.155	0.201	0.267	0.338	0.396	0.449
H5	0.147	0.207	0.273	0.354	0.393	0.450
H6	0.119	0.164	0.198	0.272	0.300	0.339
H8	0.126	0.184	0.234	0.288	0.327	0.378

Values obtained by scaling the off-resonance spectrum to the difference spectrum.

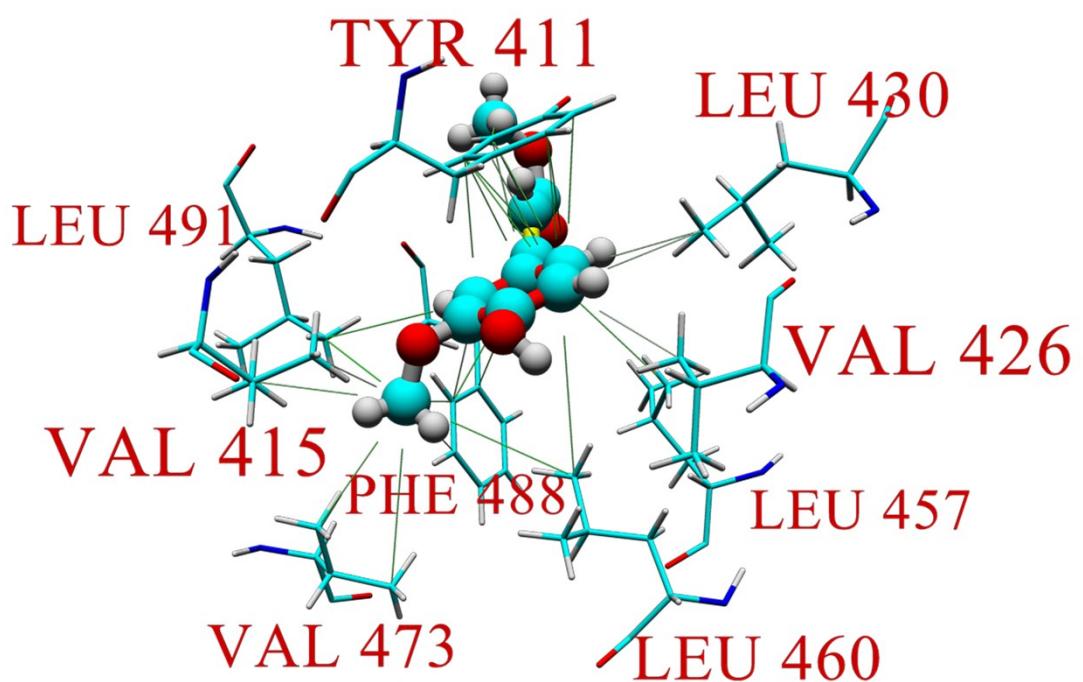


Figure S1 3D diagram of amino acid residues that interact with MF. Green line represents hydrophobic force.