The Marine Cyanobacterial Metabolite Gallinamide A is a Potent and Selective Inhibitor of Human Cathepsin L

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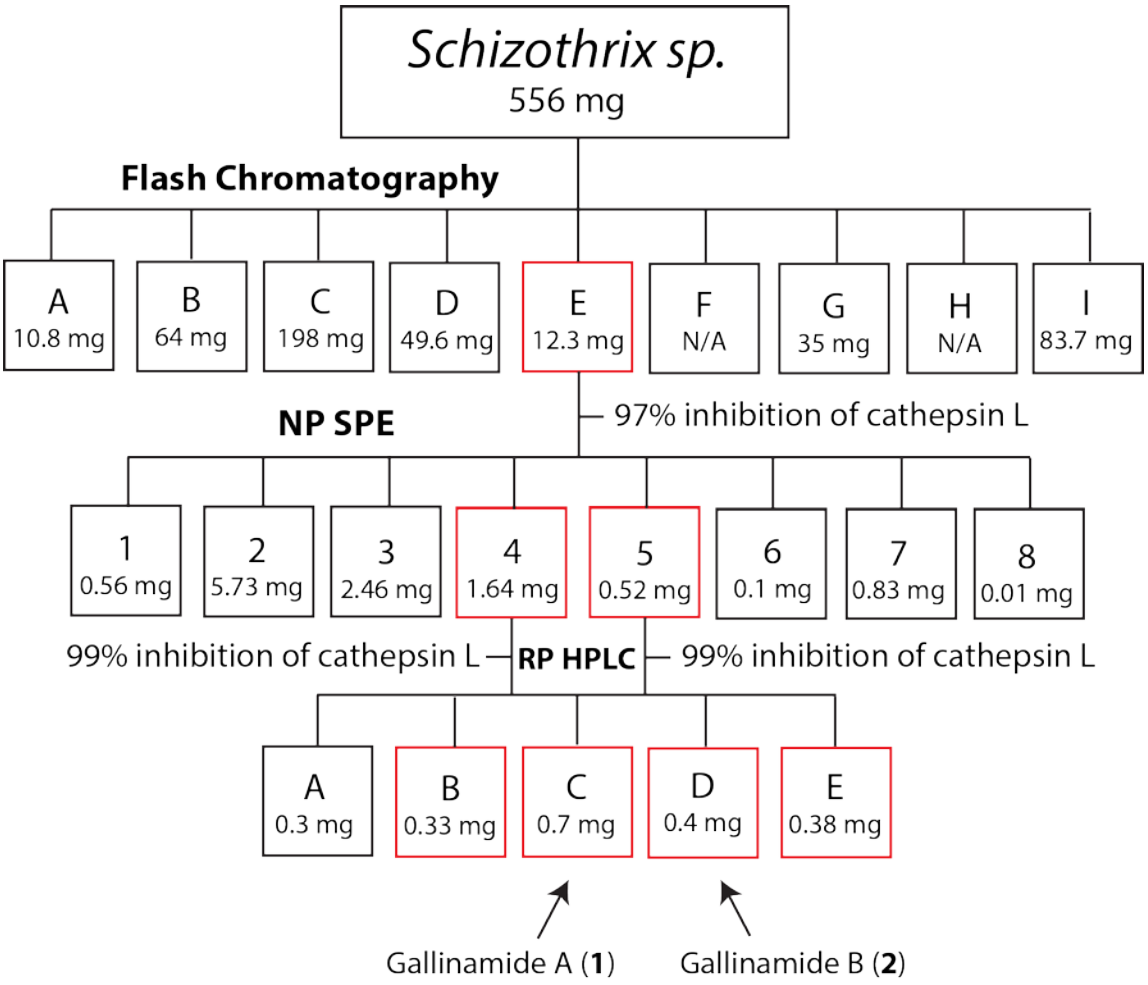
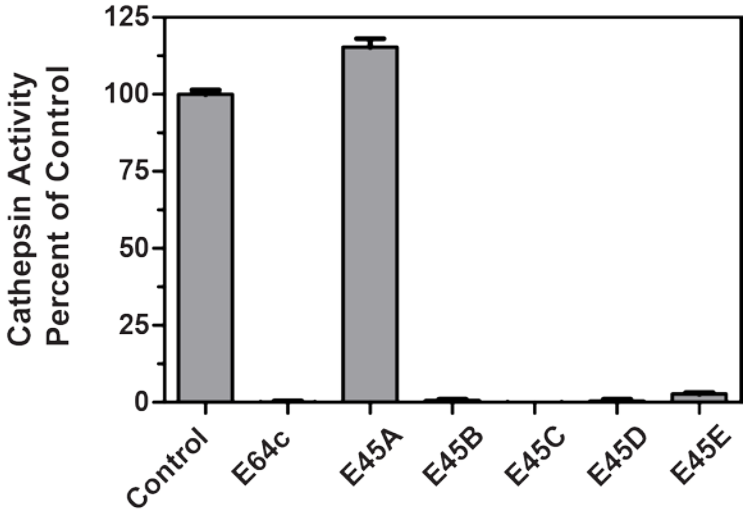
Supporting Information

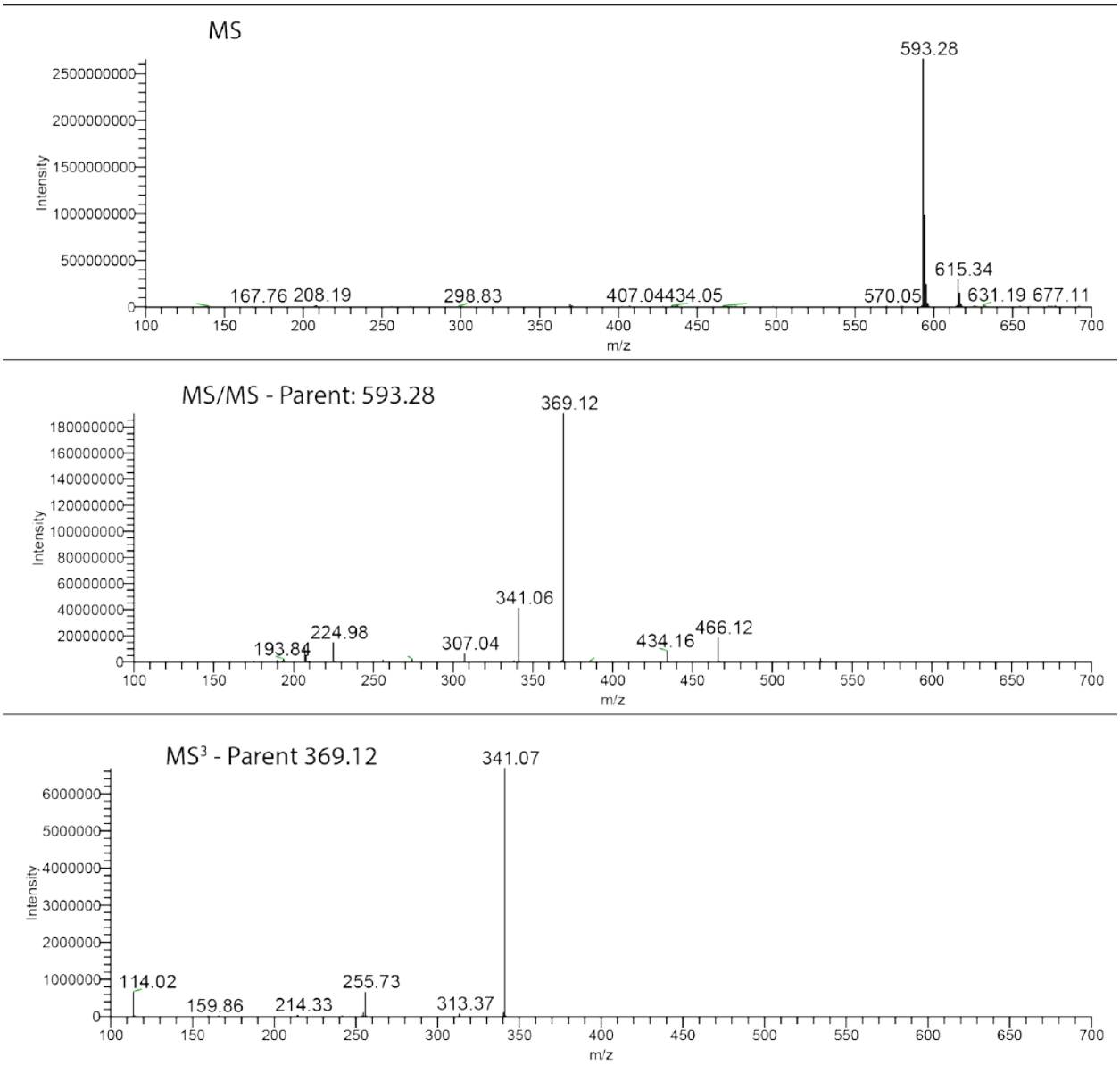
S1. Fractionation and isolation scheme



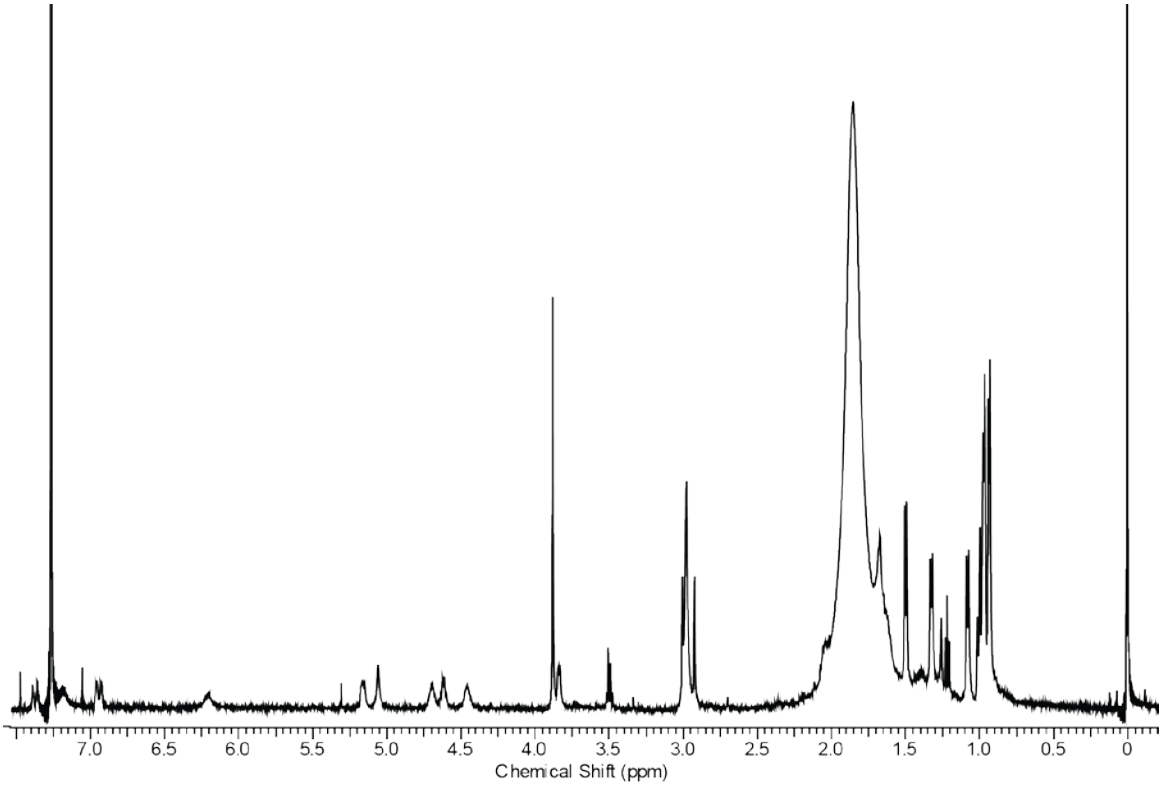
S2. Cathepsin L activity assay for HPLC collections



S3. ESI-MS/MS and MS^3 spectra of Gallinamide A (**1**)

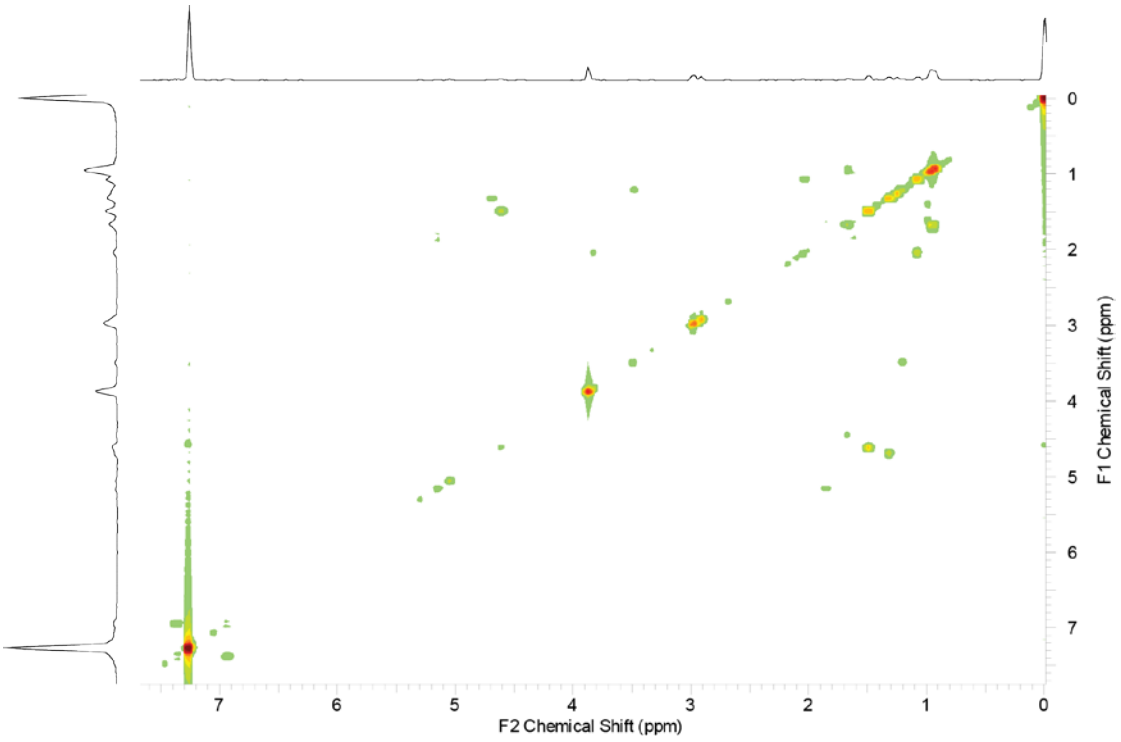


S4. ^{1}H NMR spectrum of gallinamide A (**1**) in $CDCl_3$ (500 MHz)



^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.42 (1H, d, *J* = 15.8 Hz, H-8), 7.14 (1H, brs, 13-NH), 6.94 (1H, dd, *J* = 15.8, 4.3 Hz, H-9), 6.21 (1H, brd, 10-NH), 5.16 (1H, dd, *J* = 9.3, 4.0 Hz, H-19), 5.05 (1H, s, H-2), 4.69 (1H, m, H-10), 4.61 (1H, q, *J* = 6.5 Hz, H-4), 4.45 (1H, brdd, H-13), 3.88 (3H, s, O-Me), 3.83 (1H, d, *J* = 5.9 Hz, H-25), 2.98 (6H, brs, H-30), 2.04 (1H, m, H-26), 1.84 (2H, m, H-20a), 1.67 (2H, m, H-14), 1.66 (1H, m, H-15), 1.63 (2H, m, H-20b), 1.62 (1H, m, H-21), 1.5 (3H, d, *J* = 6.5 Hz, H-5), 1.4 (2H, brm, H-27), 1.32 (3H, d, *J* = 6.5 Hz, H-11), 1.08 (3H, d, *J* = 6.5 Hz, H-29), 0.99 (3H, t, *J* = 7.3 Hz, H-28), 0.96 (3H, d, H-22), 0.96 (3H, d, *J* = 6.2 Hz, H-16), 0.93 (3H, d, *J* = 6.2 Hz, H-17), 0.92 (3H, d, *J* = 6.2 Hz, H-23)

S5. ^{1}H-^{1}H COSY spectrum of gallinamide A (**1**) in $CDCl_3$ (500 MHz)



S6. UV and HR-ESITOFMS of gallinamide A (**1**)

UV (MeOH) λ_{max} (log ε) 203 (3.96), 246 (3.63) nm; HR-ESITOFMS *m/z* $[M+H]^+$ 593.3908 (calcd for $C_{31}H_{53}N_4O_7$, 593.3914).