

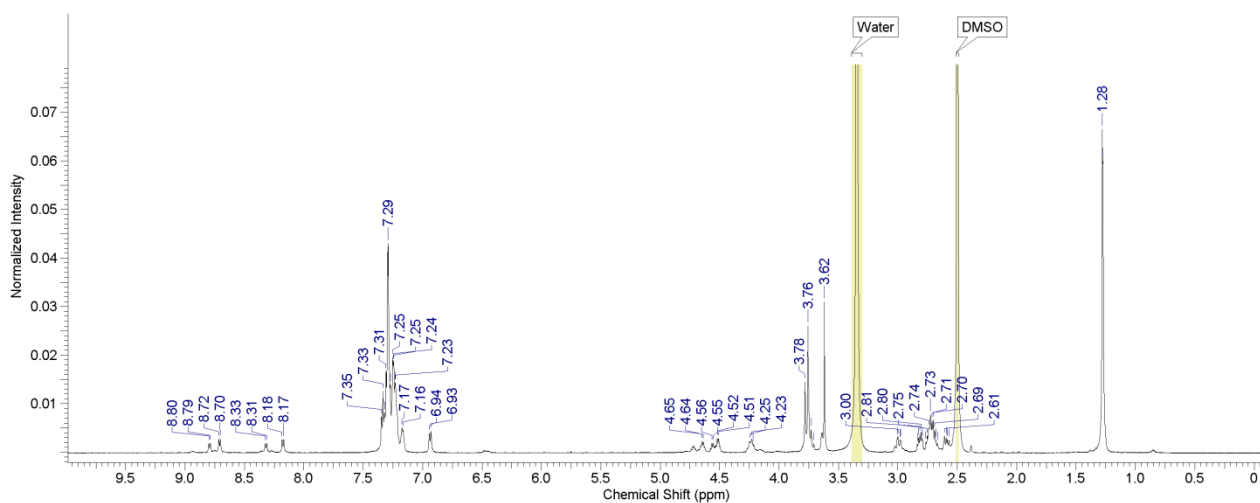
Tripeptide Consisting of Benzyl Protected di-Cysteine and Phenylalanine forms Spherical Assembly and Induces Cytotoxicity in Cancer Cell via Apoptosis

SUPPORTING INFORMATION

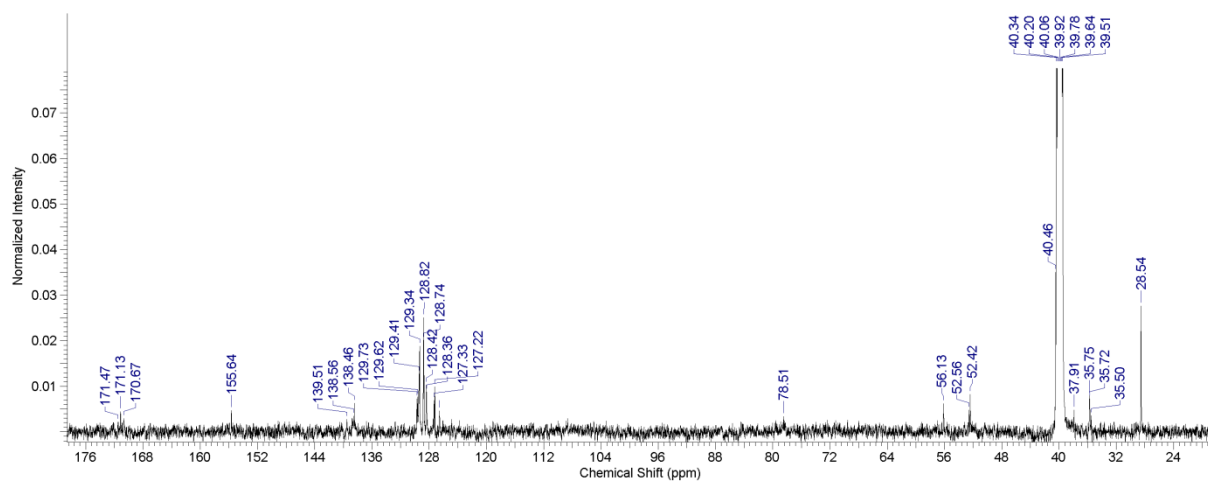
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Characterization of the tripeptide:

N-Boc-L-Phe-S-benzyl-L-Cys-S-benzyl-L-Cys methyl ester: White solid, R_f 0.40 (petroleum ether, ethyl acetate 2:1), ^1H NMR (600 MHz, DMSO-d_6): δ (in ppm) 1.28 (9H, s, CH_3 of tertiary butyl), 2.57-2.61 (1H, m, $-\text{CH}_2-\text{S}$), 2.67-2.76 (3H, m, $-\text{CH}_2-\text{S}$), 2.79-2.84 (1H, m, $-\text{CH}_2-\text{Ph}$), 2.98-3.03 (1H, m, $-\text{CH}_2-\text{Ph}$), 3.62 (3H, s, CH_3 of ester group), 3.73-3.78 (4H, m, $-\text{CH}_2-\text{Ph}$), 4.21-4.25 (1H, m, C_αH), 4.50-4.56 (1H, m, C_αH), 4.63-4.74 (1H, m, C_αH), 6.93 (1H, d, $J = 6$, NH of BOC group), 7.165 (1H, d, $J = 6$, Ar-H), 7.23-7.35 (14H, m, Ar-H), 8.17- 8.33 (1H, m, NH), 8.70 -8.80 (1H, m, NH); ^{13}C NMR (150 MHz, DMSO-d_6): δ (in ppm) 28.54, 35.50, 35.68, 35.72, 35.75, 37.91, 52.42, 52.56, 56.09, 56.13, 78.51, 126.58, 127.22, 127.33, 128.36, 128.42, 128.74, 128.82, 129.34, 129.41, 129.45, 129.62, 129.73, 138.46, 138.56, 139.51, 155.64, 170.67, 171.13, 171.47; IR (cm^{-1}) 3297, 3062, 3029, 2974, 2925, 1745, 1694, 1642, 1526, 1447, 1388, 1367, 1245, 1168, 701. IR (cm^{-1}) 3297, 3062, 3029, 2974, 2925, 1745, 1694, 1642, 1526, 1447, 1388, 1367, 1245, 1168, 701 cm^{-1} . Mass (ESI⁺): m/z 688.22 ($\text{M} + \text{Na}$)⁺



¹H NMR of tripeptide



¹³C NMR of tripeptide