Electronic Supplementary Material (ESI) for CrystEngComm.

Highly selective metallogel from 4-biphenylcarboxy capped diphenylalanine and $FeCl_3$

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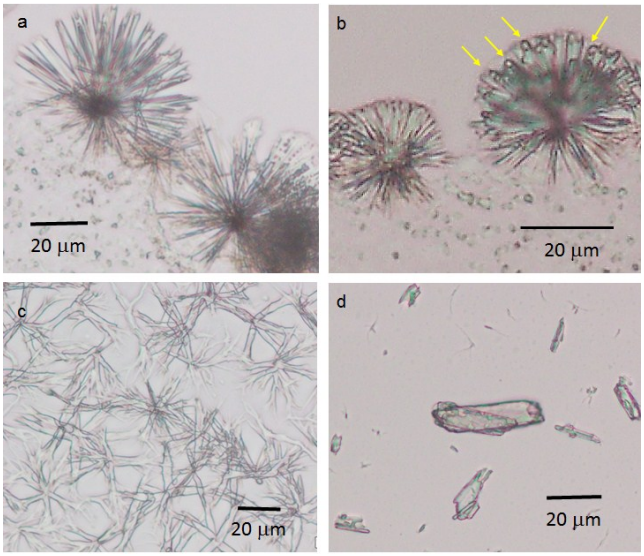
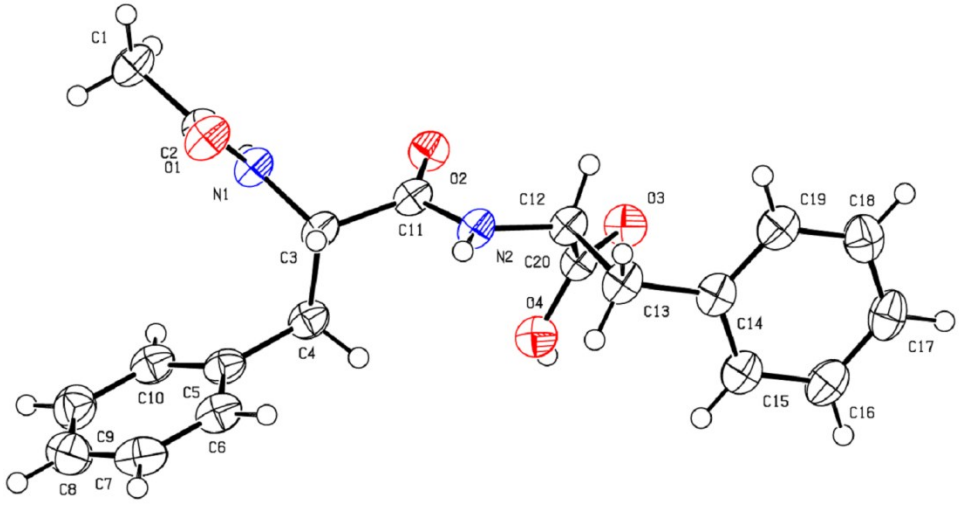


ESI Fig S1. POM images of compounds **1, 2** and **3** from methanol solution.



ESI Fig. S2: The ORTEP diagram of Ac-Phe-Phe-OH **2**. Ellipsoids are drawn at the 50% probability level.

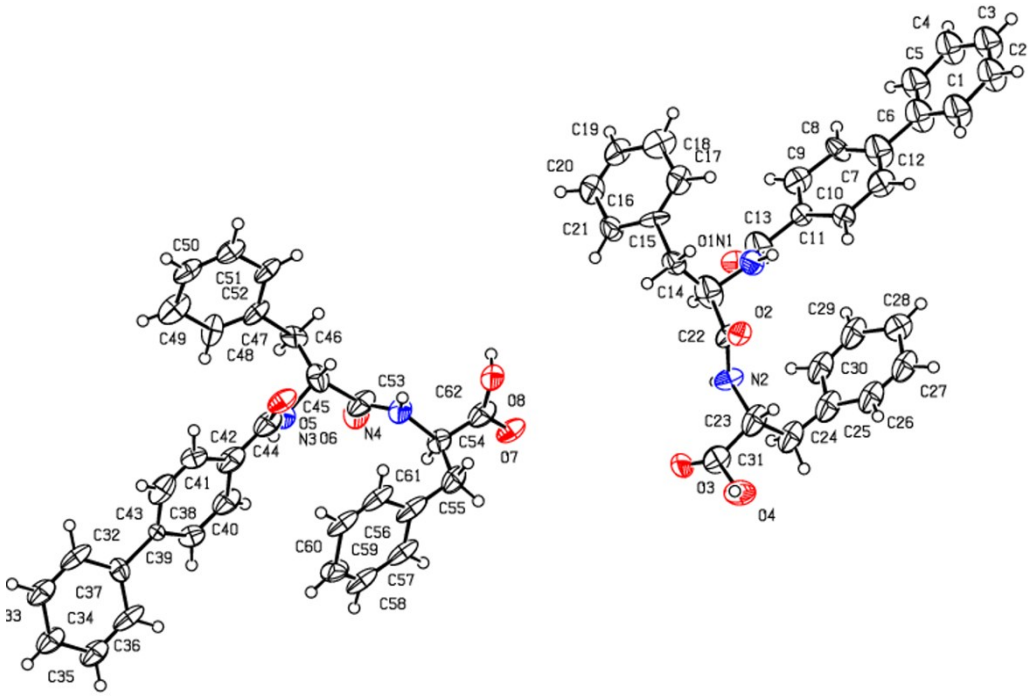
ESI Table 1. Selected backbone torsion angles (deg) for peptides **2** and **3**

Peptide 2					
C1-C2-N2-C3	-177.7	ω1	C3-C11-N2-C12	160.7	ω2
C2-N1-C3-C11	-115.6	ϕ1	C11-N2-C12-C20	-48.8	ϕ2
N1-C3-C11-N2	152.5	ψ1	N2-C12-C20-O4	46.6	ψ2
Peptide 3 A					
C10-C13-N1-C14	174.2	ω1	C14-C22-N2-C23	170.3	ω3
C13-N1-C14-C22	125.7	ϕ1	C22-N2-C23-C31	108.9	ϕ2
N1-C14-C22-N2	-103.3	ψ1	N2-C23-C31-O4	-176.8	ψ2
Peptide 3 B					
C41-C44-N3-C45	174.4	ω1	C45-C53-N4-C54	169.4	ω3
C44-N3-C45-C53	125.8	ϕ1	C53-N4-C54-C62	107.2	ϕ2
N3-C45-C53-N4	-99.5	ψ1	N4-C54-C62-O8	-32.8	ψ2

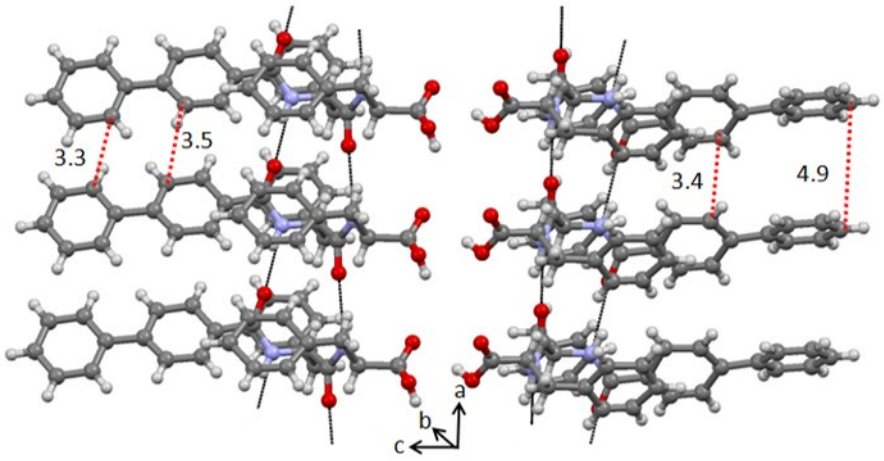
ESI Table 2. Hydrogen bonding parameters of peptides **2** and **3**[a]

D-H….A	D..H(Å)	H..A(Å)	D..A(Å)	D-H..A (°)
Peptide 2				
N1-H1….O3 [a]	0.86	2.04	2.881(6)	166
N2-H2….O1[b]	0.86	2.00	2.835(5)	162
O4-H4….O2[c]	0.82	1.82	2.620(6)	166
Peptide 3 A				
N1-H1….O1 [a]	0.86	2.05	2.800(6)	145
N2-H2….O2[b]	0.86	2.09	2.938(5)	166
Peptide 3 B				
N3-H3….O5 [a]	0.86	2.12	2.872(6)	145
N4-H4….O6[b]	0.86	2.11	2.966(5)	172

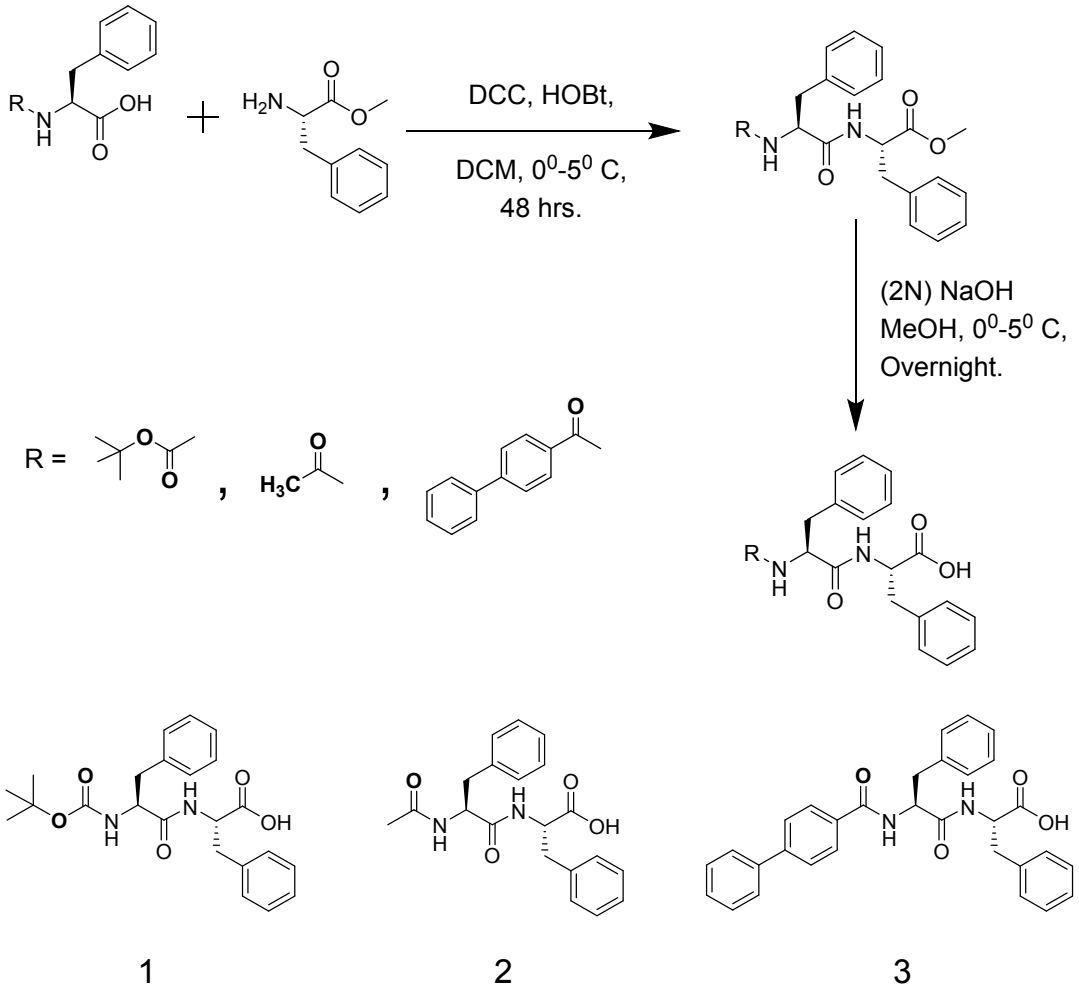
[a]Symmetry equivalent Peptide 2 *a*: 1-x, ½+y, -z, *b* = 1-x, 1/2+y, 1-z, *c* = 1-x, -1/2+y, -z.; Peptide 3 *a*: -1+x, y, z, *b* = 1+x, y, z.



ESI Fig. S3: The ORTEP diagram of Bi-Ph-Phe-Phe-OH **3**. Ellipsoids are drawn at the 50% probability level.



ESI Fig. S4: two supramolecular parallel-sheets form an antiparallel duplex of compound **3**.



Scheme 1: Schematic presentation of synthesis of compound**s 1, 2** and **3.**

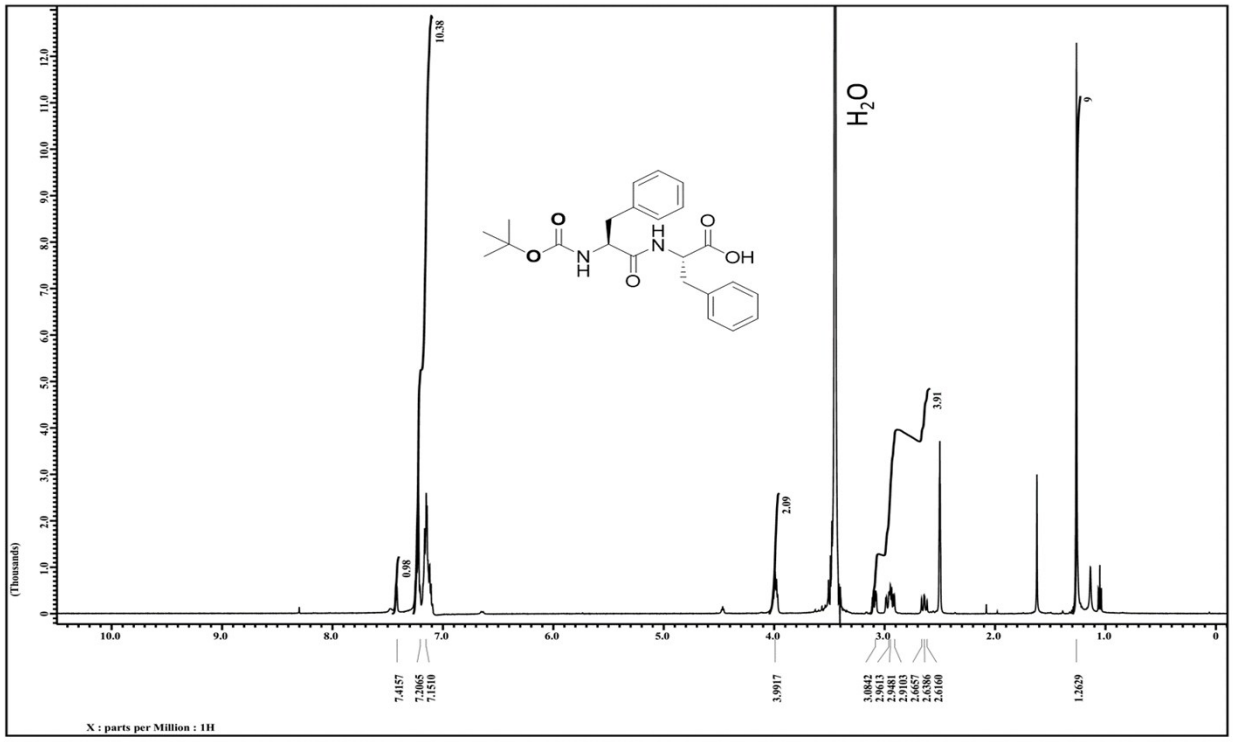


Figure S5: ^{1}H NMR (400 MHz, DMSO-d_6) spectra of Compound **1**.

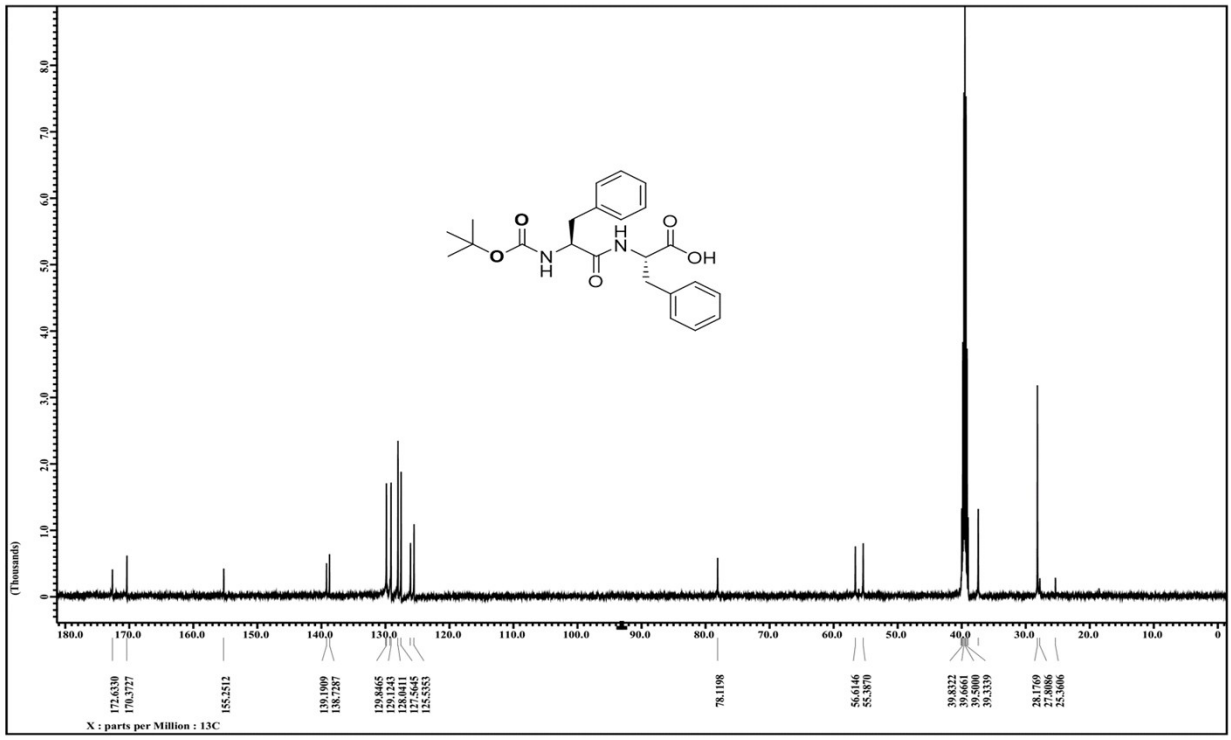


Figure S6: ^{13}C NMR (100 MHz, DMSO-d_6) spectra of Compound **1**.

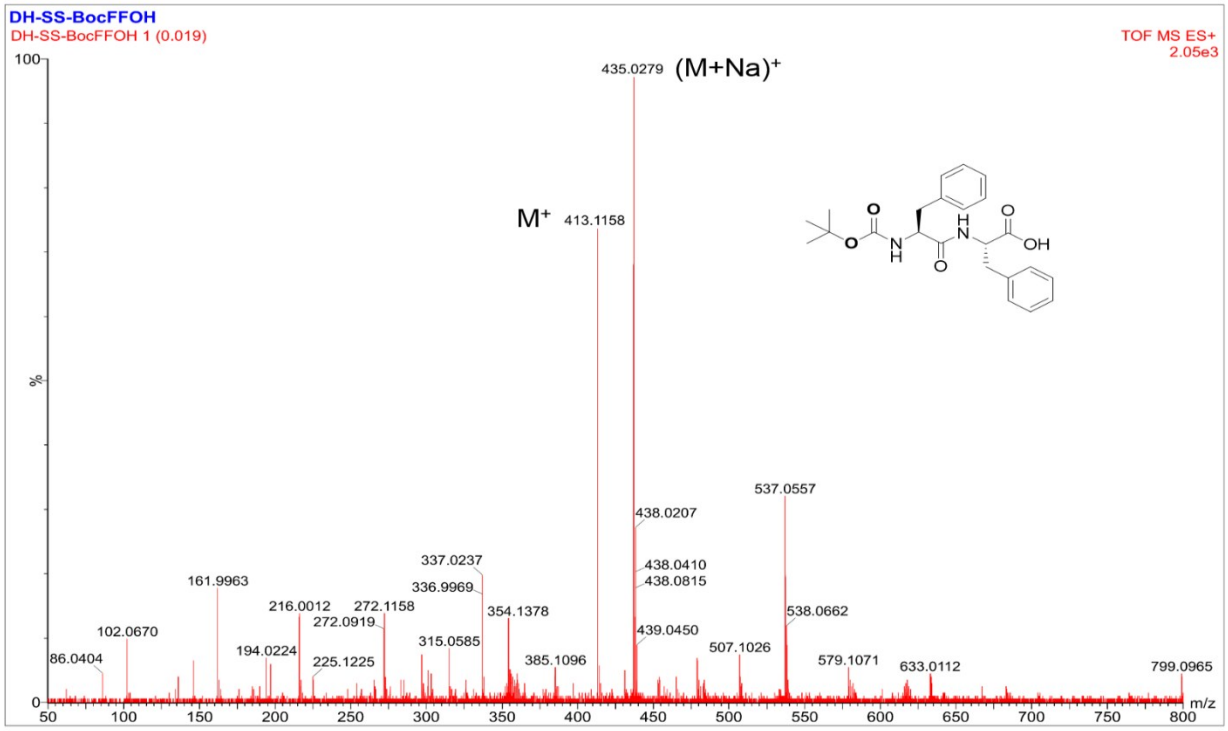


Figure S7: ESI-Mass Spectra of compound **1**.

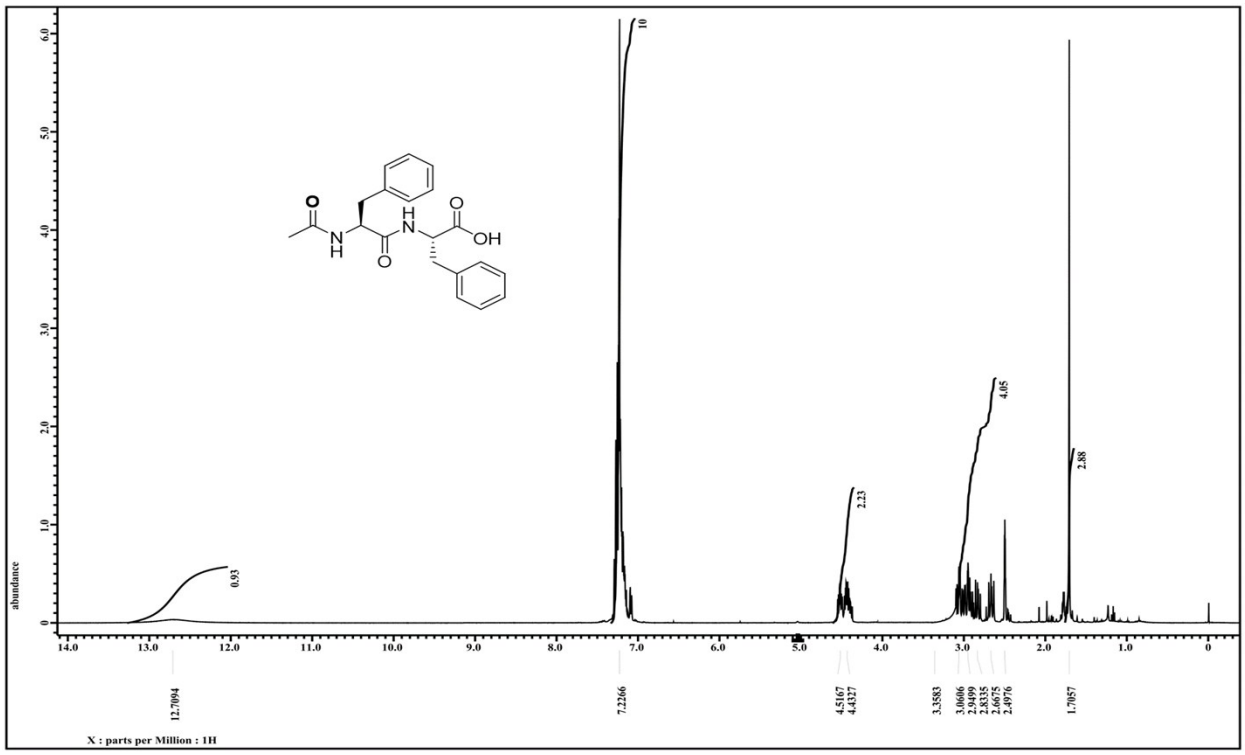


Figure S8: ^{1}H NMR (400 MHz, DMSO-d_6) spectra of Compound **2**.

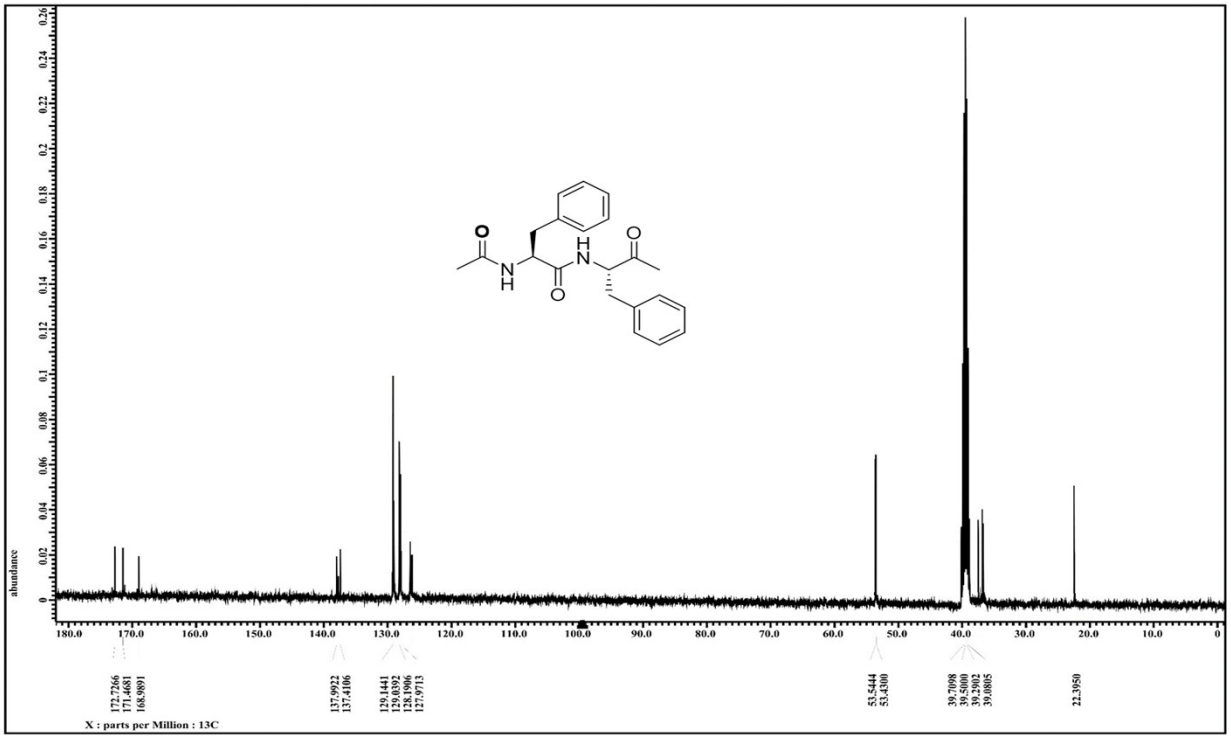


Figure S9: ^{13}C NMR (100 MHz, DMSO-d_6) spectra of Compound **2**.

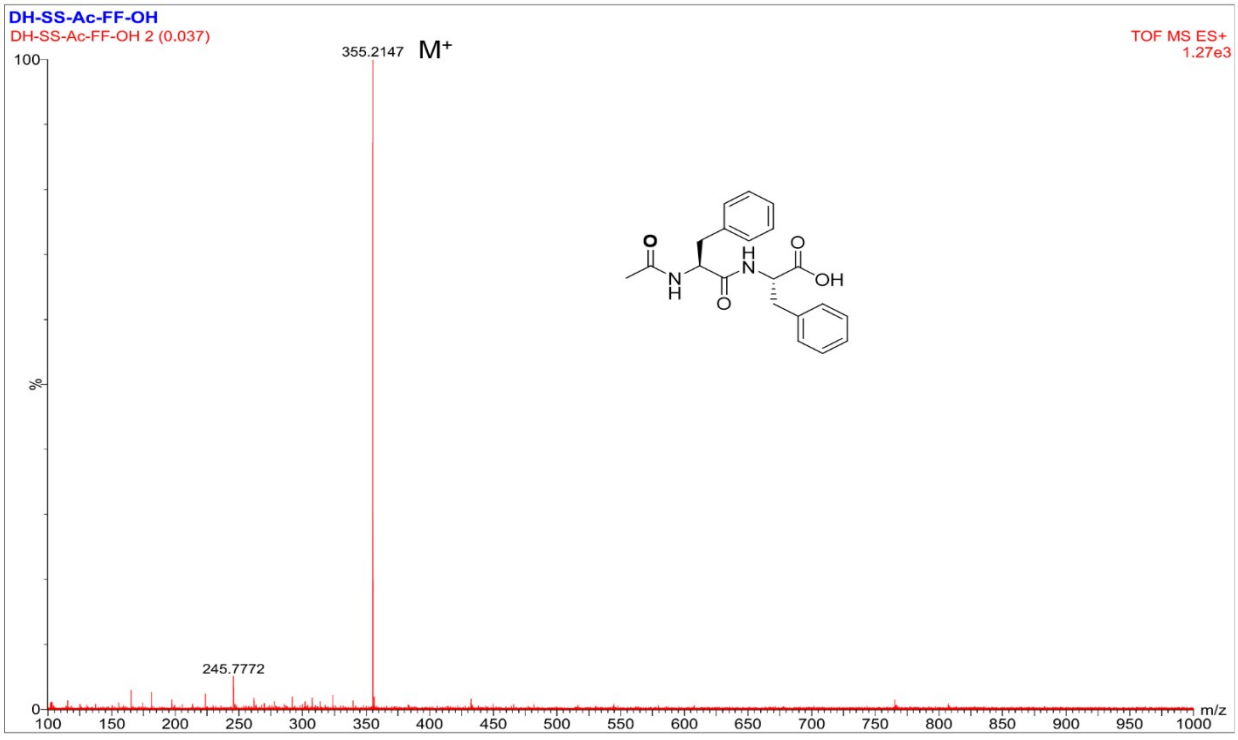


Figure S10: ESI-Mass Spectra of compound **2**.

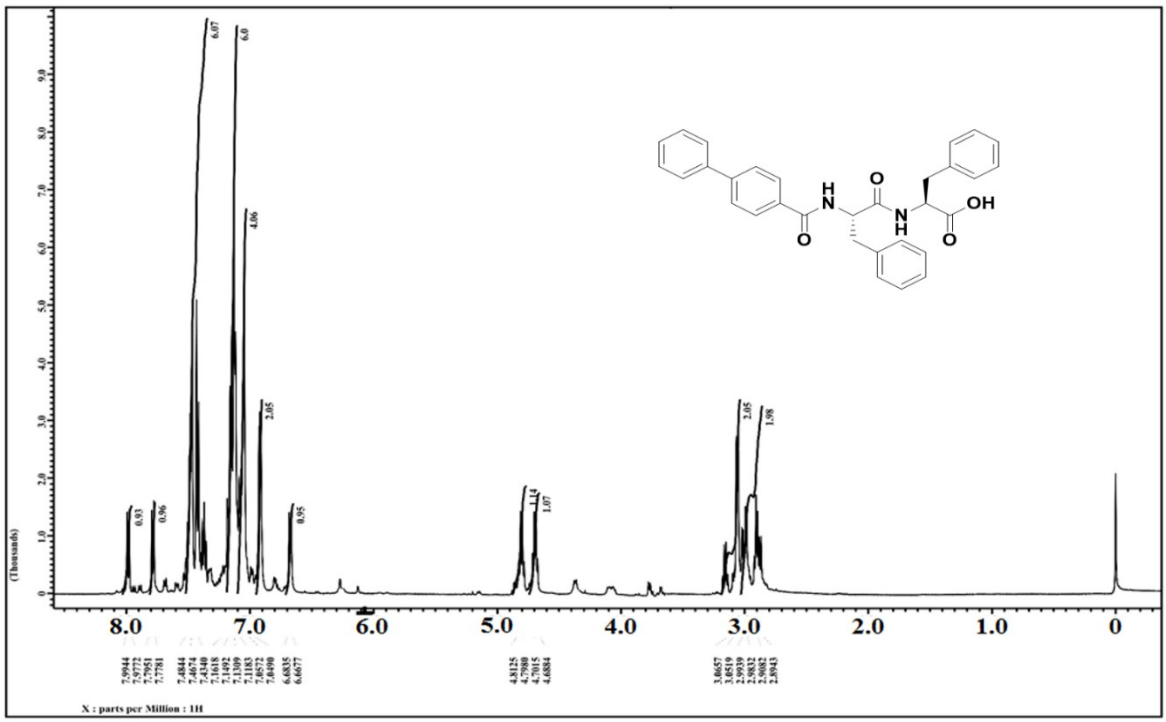


Figure S11: ^{1}H NMR (400 MHz, DMSO-d_6) spectra of Compound **3**.

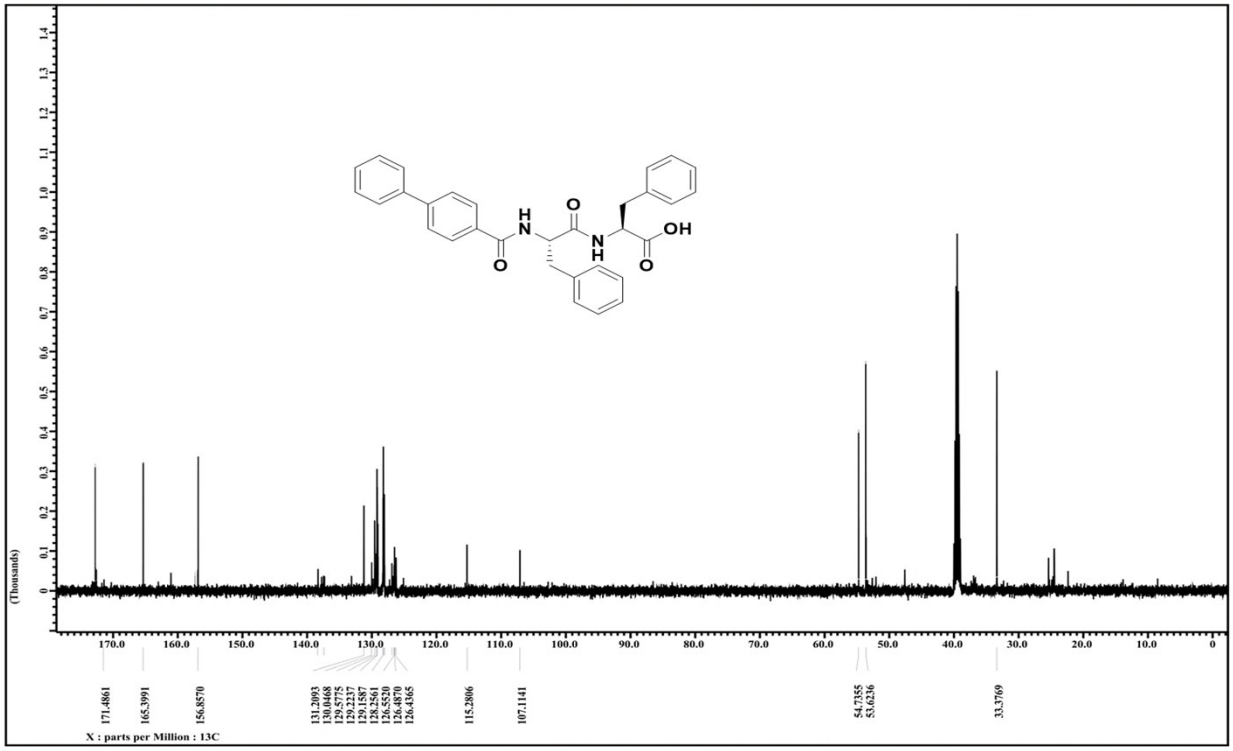


Figure S12: ^{13}C NMR (100 MHz, DMSO-d_6) spectra of Compound **3**.

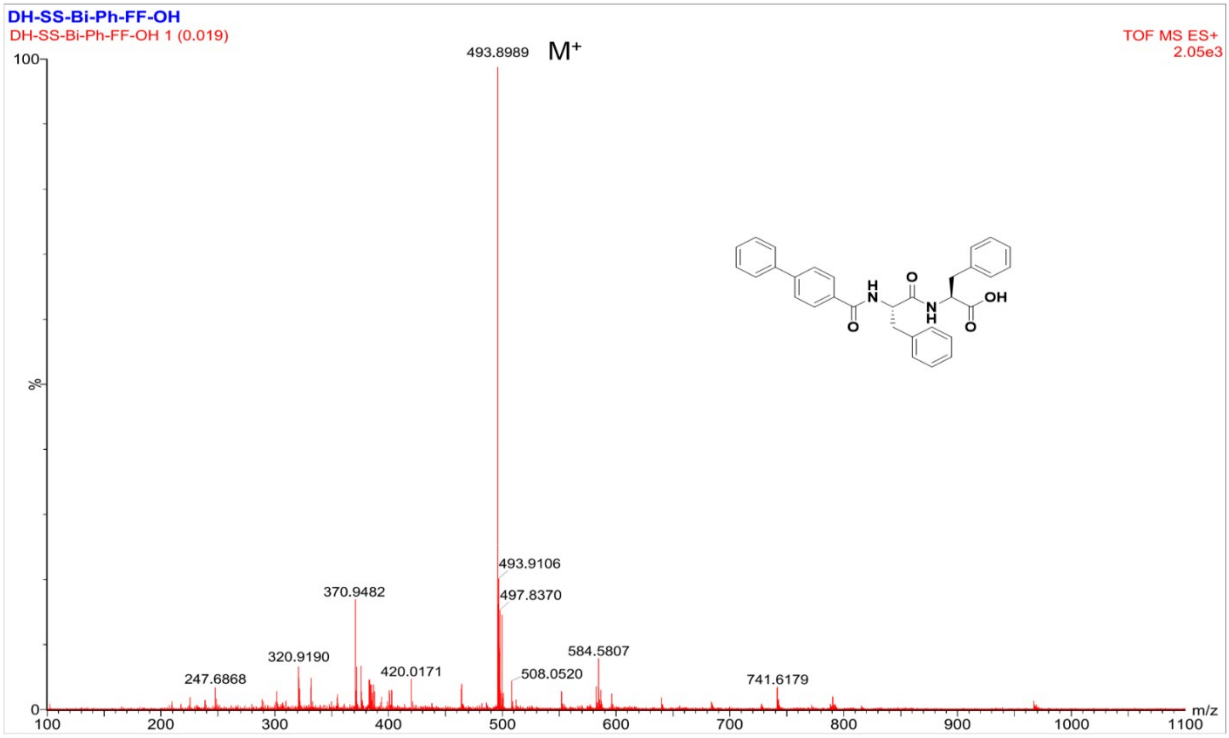


Figure S13: ESI-Mass Spectra of compound **3**.

Table 3: Crystallographic Parameters of Ac-Phe-Phe-OH **2**.

Identification code	AcFFOH
Empirical formula	$C_{20}H_{22}N_2O_4$
Formula weight	354.40
Temperature/K	99.94(15)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	10.2025(7)
b/Å	8.6320(6)
c/Å	10.5300(7)
α/°	90
β/°	96.701(6)

γ/°	90
Volume/Å^3	921.02(11)
Z	2
ρ_{calc}g/cm^3	1.278
μ/mm^{-1}	0.733
F(000)	376.0
Crystal size/mm^3	0.3158 × 0.2589 × 0.2569
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.454 to 132.228
Index ranges	-12 ≤ h ≤ 12, -9 ≤ k ≤ 10, -11 ≤ l ≤ 12
Reflections collected	5077
Independent reflections	2602 [R_{int} = 0.0212, R_{sigma} = 0.0248]
Data/restraints/parameters	2602/1/237
Goodness-of-fit on F^2	1.071
Final R indexes [I>=2σ (I)]	R_1 = 0.0335, wR_2 = 0.0869
Final R indexes [all data]	R_1 = 0.0344, wR_2 = 0.0883
Largest diff. peak/hole / e Å^{-3}	0.16/-0.21
Flack parameter	0.003(17)

Table 4: Crystallographic Parameters of Bi-Ph-Phe-Phe-OH **3**.

Empirical formula	$C_{62}H_{56}N_4O_8$
Formula weight	985.10
Temperature/K	100.00(10)
Crystal system	triclinic
Space group	P1

a/Å	4.9942(4)
b/Å	16.6717(12)
c/Å	19.0158(15)
α/°	99.361(6)
β/°	95.074(7)
γ/°	90.062(7)
Volume/Å^3	1555.9(2)
Z	1
ρ_{calc}g/cm^3	1.051
μ/mm^{-1}	0.561
F(000)	520.0
Crystal size/mm^3	0.1258 × 0.2589 × 0.3478
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.554 to 131.93
Index ranges	$-5 \leq h \leq 5$, $-19 \leq k \leq 19$, $-22 \leq l \leq 22$
Reflections collected	20475
Independent reflections	8560 [R_{int} = 0.0761, R_{sigma} = 0.0853]
Data/restraints/parameters	8560/3/435
Goodness-of-fit on F^2	1.260
Final R indexes [I>=2σ (I)]	R_1 = 0.1262, wR_2 = 0.3217
Final R indexes [all data]	R_1 = 0.1456, wR_2 = 0.3535
Largest diff. peak/hole / e Å^{-3}	0.73/-0.44
Flack parameter	-0.2(2)