biomolecules

MDPI

Supplementary Information

BSA binding and aggregate formation of a synthetic amino acid with potential for promoting fibroblast proliferation: an in silico, CD spectroscopic, DLS, and cellular study

Hayarpi Simonyan[1#], Rosanna Palumbo[2#], Satenik Petrosyan[1], Anna Mkrtchyan[1], Armen Galstyan[3], Ashot Saghyan[1], Pasqualina Liana Scognamiglio[4], Caterina Vicidomini[2], Marta Fik-Jaskolka[5], Giovanni N. Roviello[2*]

[1] Institute of Pharmacy, Yerevan State University, 1 Alex Manoogian Str., Yerevan 0025, Armenia
[2] Institute of Biostructures and Bioimaging, Italian National Council for Research (IBB-CNR), Area di Ricerca Site and Headquarters, Via Pietro Castellino 111, 80131 Naples, Italy
[3] Department of Chemistry, Yerevan State University, 1 Alex Manoogian Str., Yerevan 0025, Armenia
[4] Department of Sciences, University of Basilicata, Via dell'Ateneo Lucano 10, 85100 Potenza, Italy
[5] Faculty of Chemistry, Adam Mickiewicz University in Poznań, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland

* Correspondence: giovanni.roviello@cnr.it; +390812203415
[#]these authors contributed equally to this work

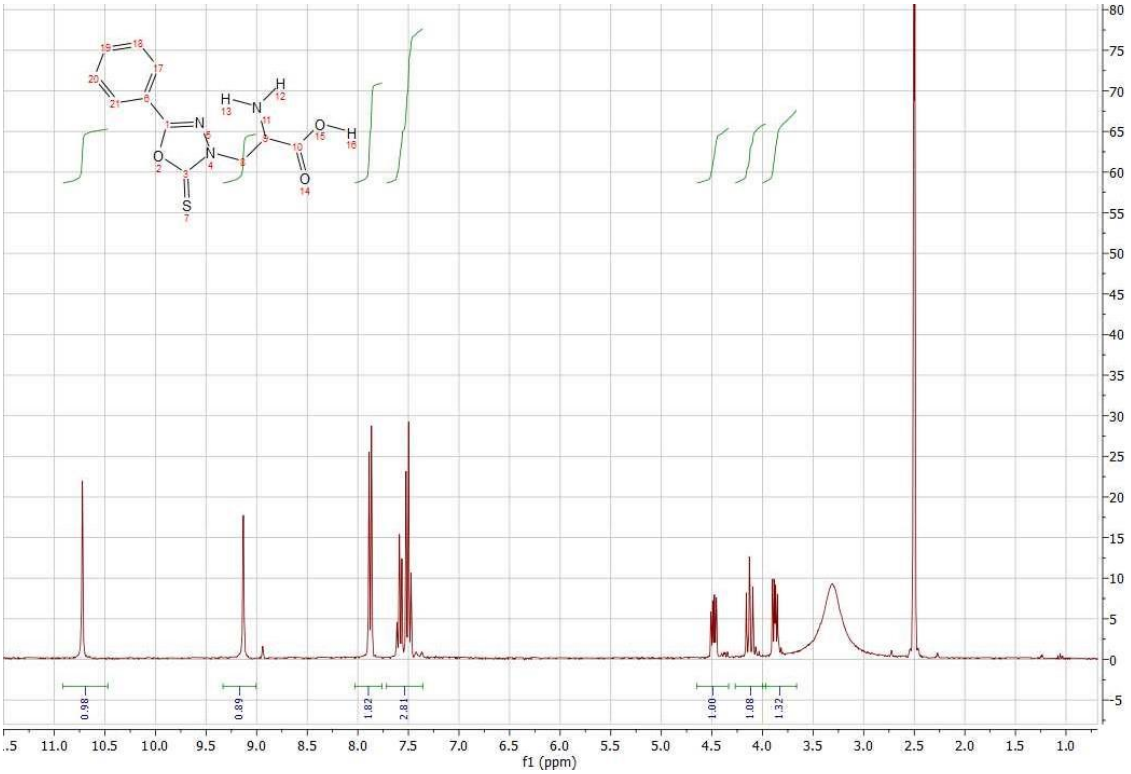


Figure S1. [1]H NMR spectral analysis of amino acid 5

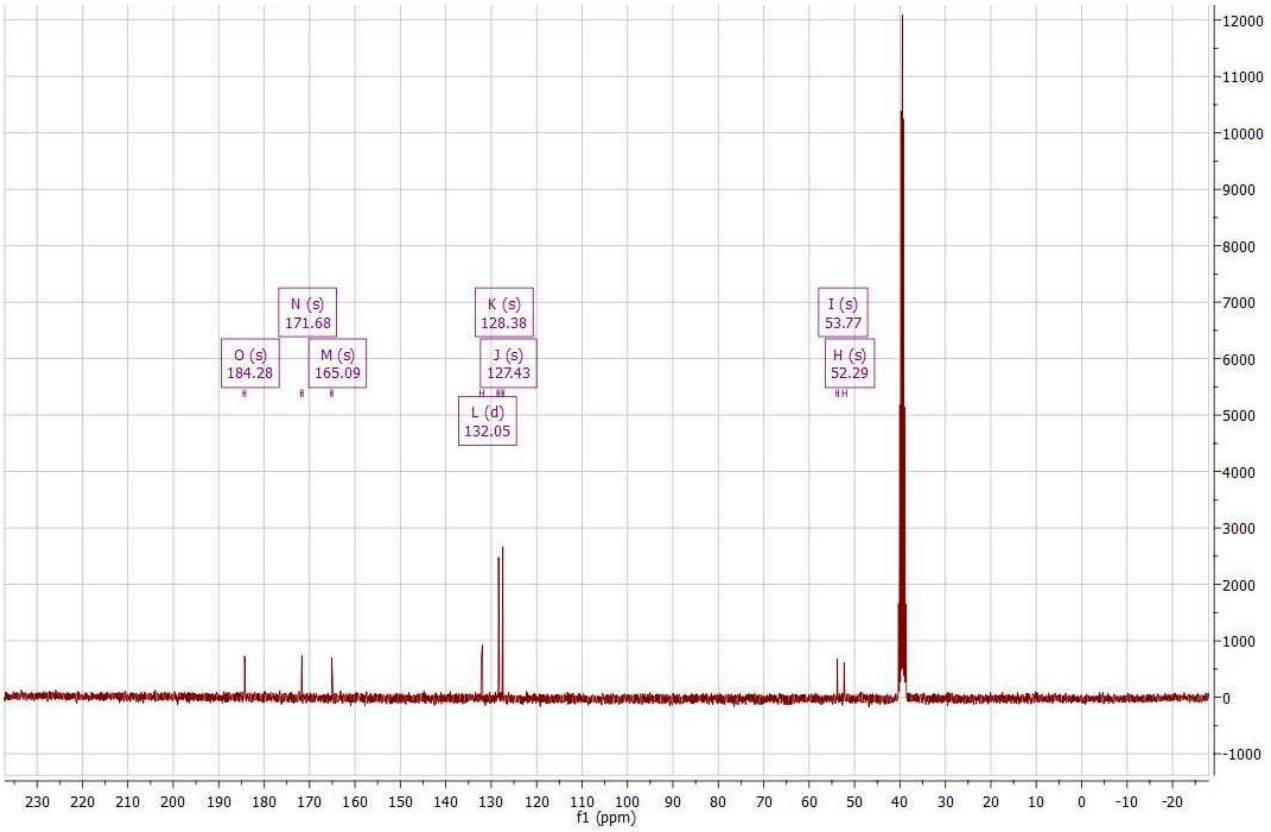
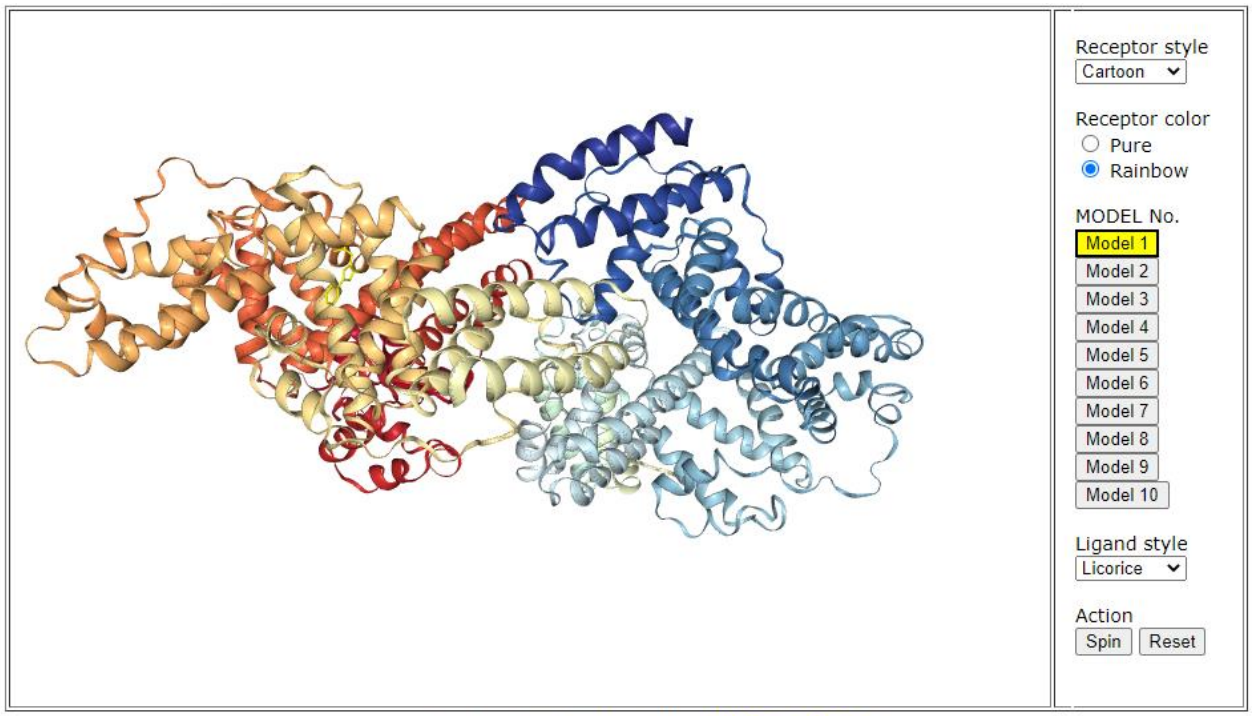


Figure S2. [13]C NMR spectral analysisi of amino acid 5



Complex Template Information (Click to Show)

Summary of the Top 10 Models

Rank	1	2	3	4	5	6	7	8	9	10
Docking Score	-140.91	-137.59	-135.39	-131.18	-130.79	-125.06	-121.99	-118.09	-118.06	-117.52

Figure S3. Three-dimensional view of the complex of 5 with BSA for the model 1 corresponding to the top-1 pose. Notice the variation in docking scores, which range from -117.52 to -140.91, with the top-1 pose corresponding to the model with the best HDOCK score (-140.91).

Table S1: Interface residues (type and number) and distances from the ligand for both A and B chain of BSA for the top-1, top-2 and top-3 poses. Notice how comp 1 binds chain A at level of the subdomain IIIA

LEU 386A 4.099 -140.91
ILE 387A 3.834
ASN 390A 3.293
CYS 391A 1.865
PHE 394A 4.986
PHE 402A 3.559
LEU 406A 4.290
ARG 409A 3.910
TYR 410A 3.203
SER 428A 4.653
LEU 429A 1.853
GLY 430A 4.084
LYS 431A 4.398

VAL 432A 2.064
GLY 433A 2.931
THR 434A 4.821
CYS 436A 4.096
CYS 437A 1.635
THR 448A 2.959
LEU 452A 3.823
SER 488A 3.322

LEU 386B 3.710 -137.59
ILE 387B 3.883
ASN 390B 2.817
CYS 391B 1.995
PHE 394B 4.663
PHE 402B 3.100
LEU 406B 4.594
ARG 409B 3.469
TYR 410B 3.429
LYS 413B 4.247
SER 428B 4.543
LEU 429B 1.804
GLY 430B 4.037
LYS 431B 4.743
VAL 432B 2.169
GLY 433B 2.868
THR 434B 4.932
CYS 436B 4.635
CYS 437B 1.864
THR 448B 3.933
LEU 452B 3.249
SER 488B 3.451

PHE 501A 3.070 -135.39
PHE 506A 3.342
PHE 508A 3.893
ALA 527A 4.141
LEU 528A 4.859
LEU 531A 3.376
HIS 534A 2.670
LYS 535A 2.751
VAL 546A 4.352

PHE 550A 3.254
LEU 574A 3.572
VAL 575A 1.908
VAL 576A 4.774
THR 578A 3.031
GLN 579A 2.910
LEU 582A 4.388

Table S2: Interaction between the target protein and compound 5 for the top-1 pose as visualized by PLIP software

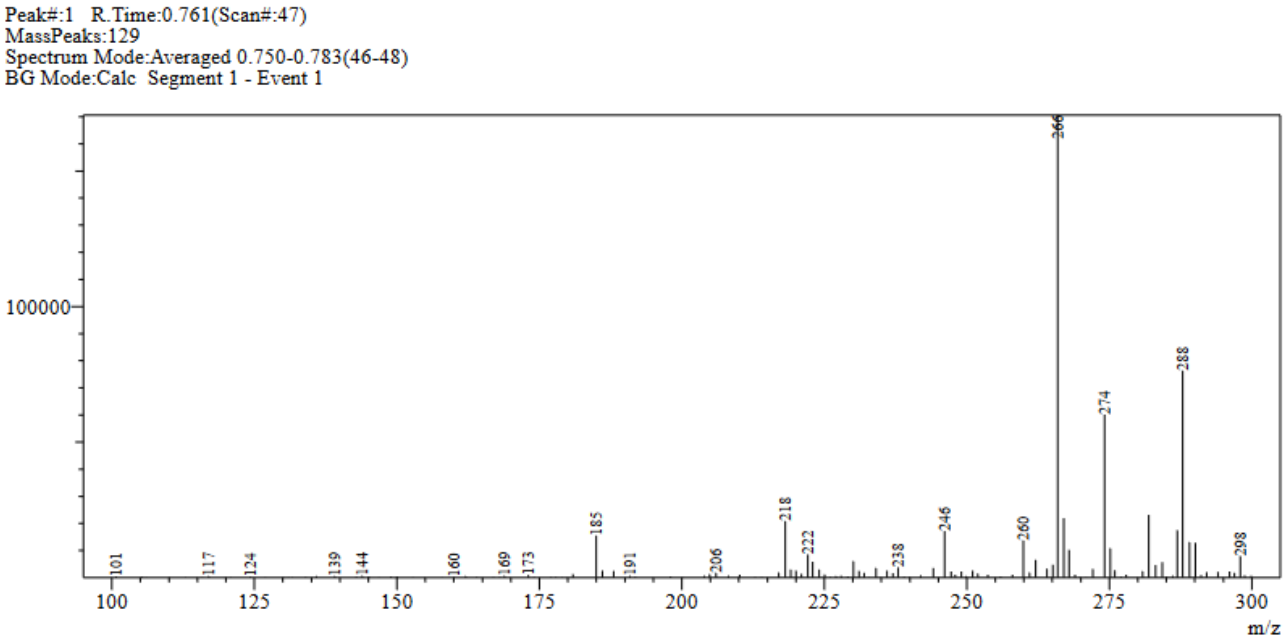
Hydrophobic Interactions ····

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	410A	TYR	3.40	9322	3305
2	429A	LEU	3.99	9321	3454

Hydrogen Bonds —

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Side chain	Donor Atom	Acceptor Atom
1	448A	THR	2.17	2.96	132.56	×	✓	9309 [N3]	3593 [O3]

···· *Hydrophobic Interaction*
— *Hydrogen Bond*



MASS Peak Table TIC

Peak#	Ret. Time	Area	Base Peak m/z
1	0.761	11187839	265.95
Total		11187839	

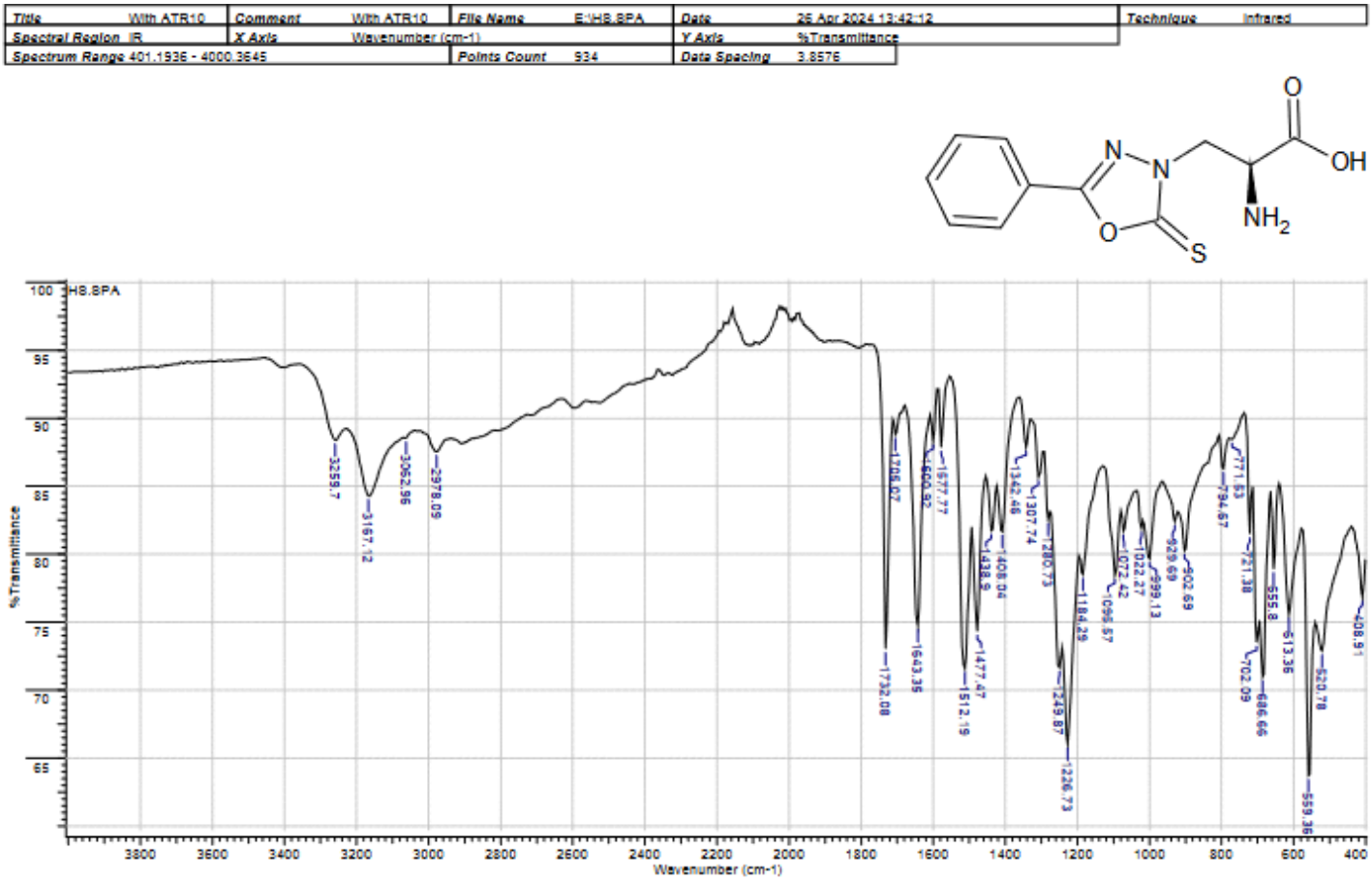


Figure S4. ESI MS (up) and IR (bottom) analysis of compound 5