

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

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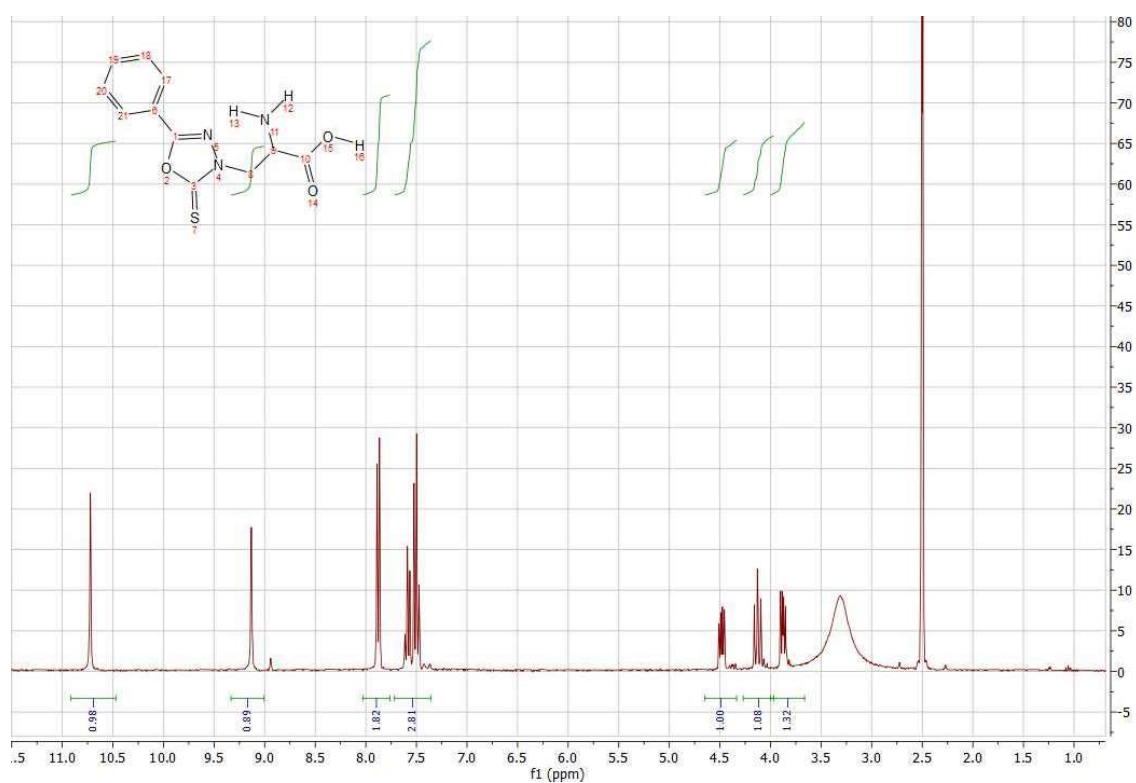


Figure S1. ^1H NMR spectral analysis of amino acid 5

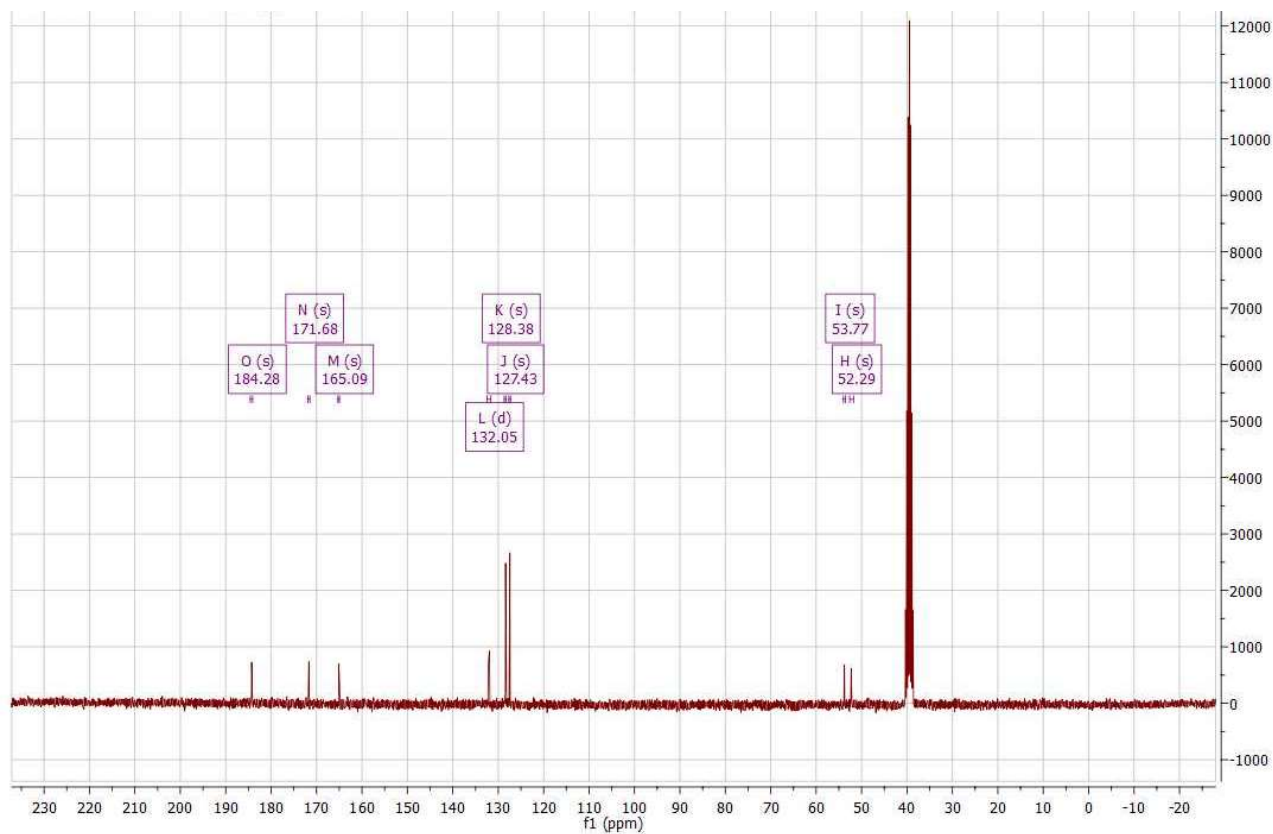
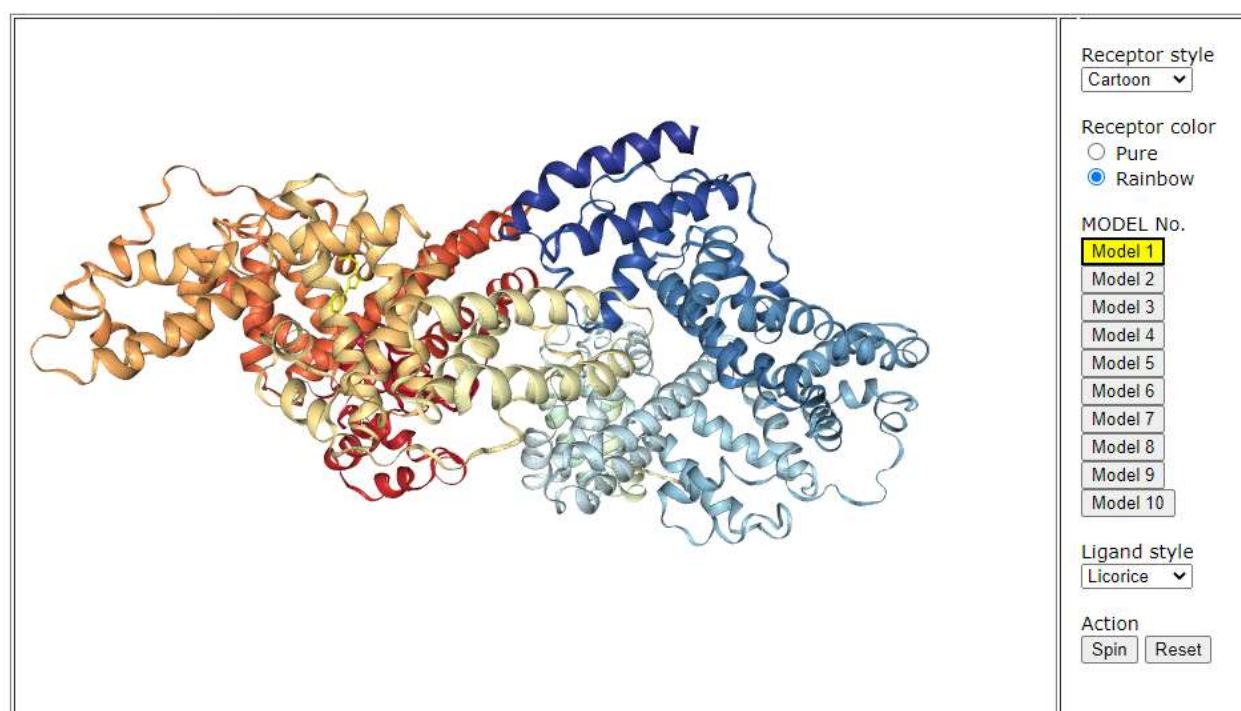


Figure S2. ^{13}C NMR spectral analysis of amino acid 5

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

Tab 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

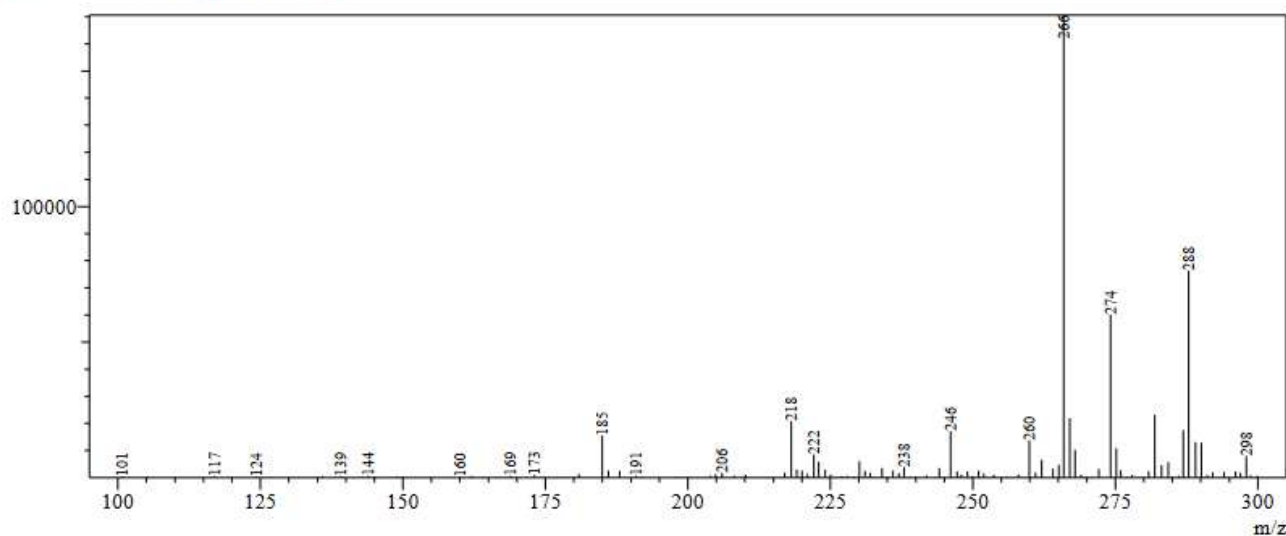
▼ Hydrogen Bonds —

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

Peak#:1 R.Time:0.761(Scan#:47)
 MassPeaks:129
 Spectrum Mode:Averaged 0.750-0.783(46-48)
 BG Mode:Calc Segment 1 - Event 1



MASS Peak Table TIC

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

Title	With ATR10	Comment	With ATR10	File Name	E-HS.SPA	Date	26 Apr 2024 13:42:12	Technique	Infrared
Spectral Region	IR	X Axis	Wavenumber (cm-1)	Y Axis	%Transmittance				
Spectrum Range	401.1936 - 4000.3645	Points Count	934	Data Spacing	3.8576				

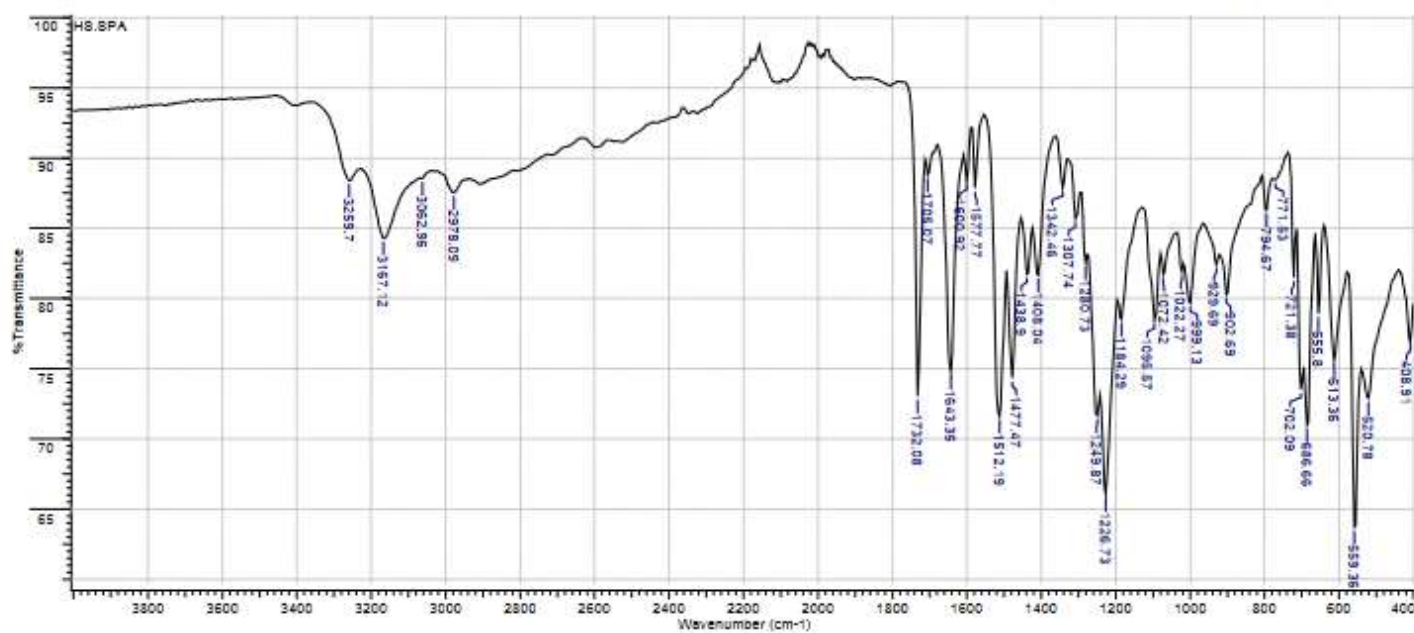
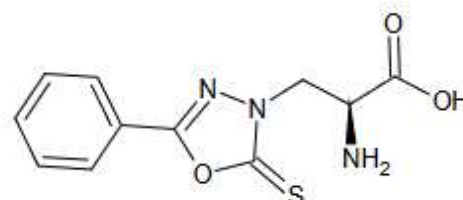


Figure S4. ESI MS (up) and IR (bottom) analysis of compound 5