

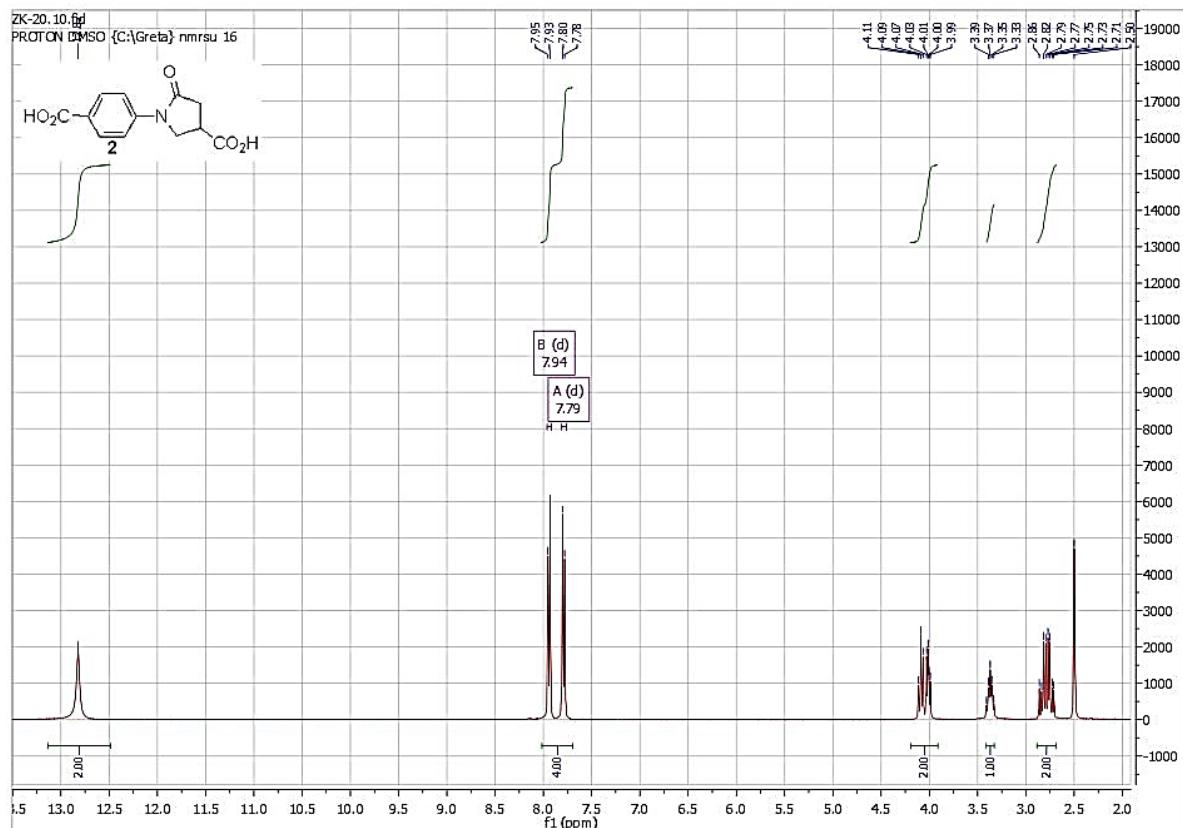
**Synthesis and antibacterial activity of new azole, diazole and triazole derivatives
based on *p*-aminobenzoic acid**

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SUPPORTING INFORMATION

- ❖ NMR Spectra (2-24) (All in DMSO-*d*₆)
- ❖ Bacteria strains used in the biological evaluation

Synthesis of 5-oxopyrrolidine derivatives 2-13
1-(4-Carboxyphenyl)-5-oxopyrrolidine-3-carboxylic acid 2



Methyl 1-[4-(methoxycarbonyl)phenyl]-5-oxopyrrolidine-3-carboxylate 3

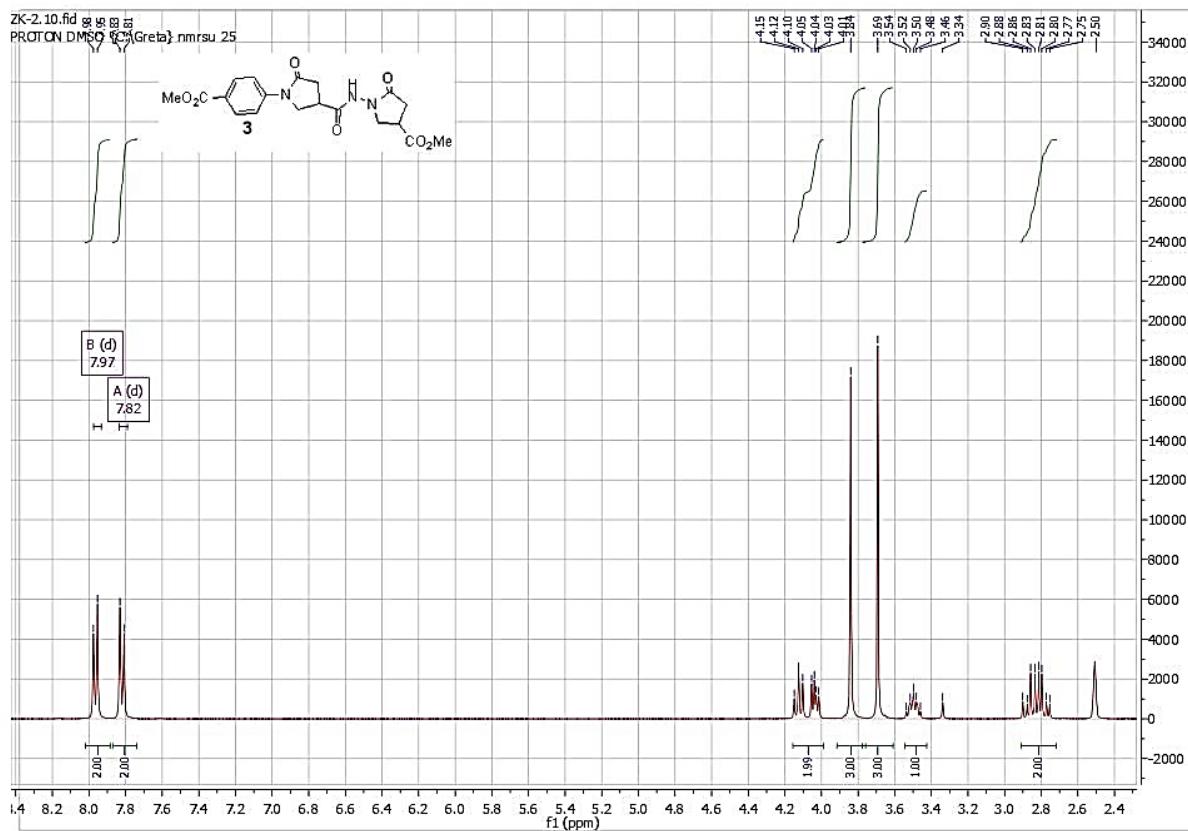


Figure S3: ^1H NMR of compound 3

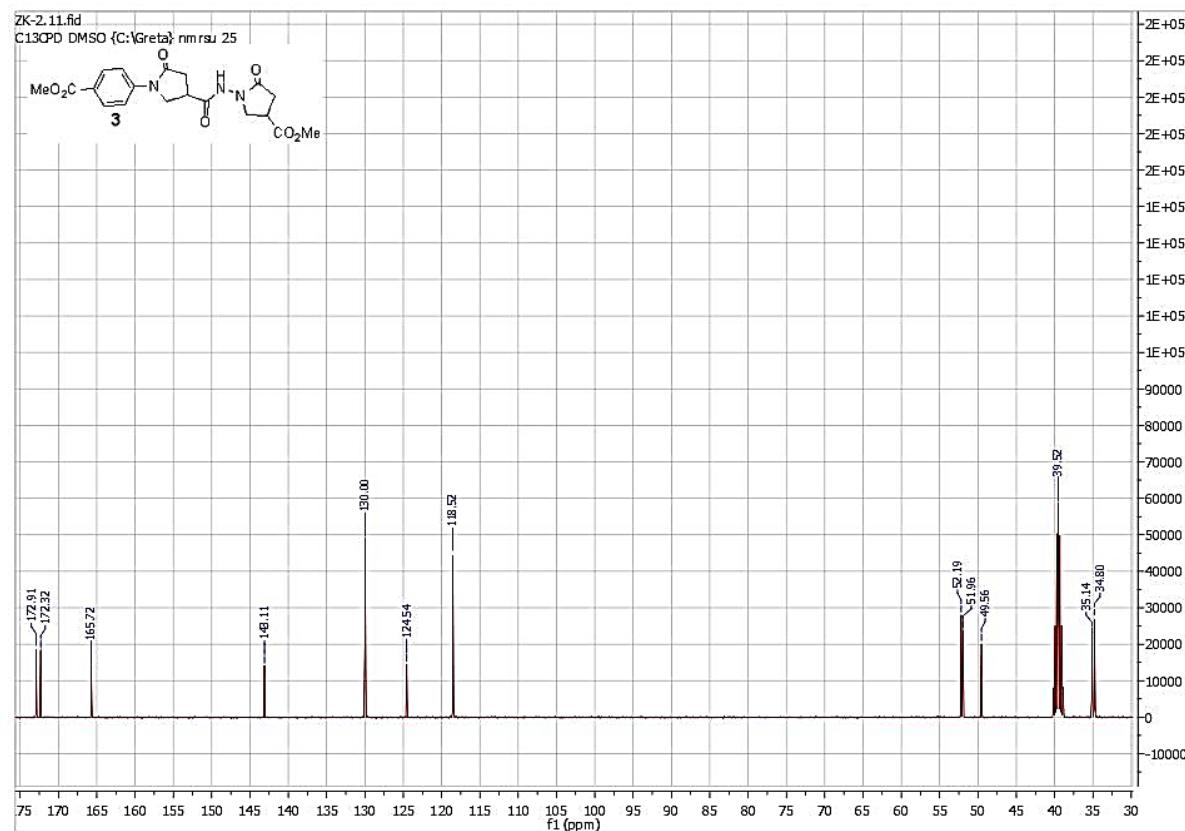


Figure S4: ^{13}C NMR of compound 3

Methyl 4-[3-(hydrazinocarbonyl)-5-oxopyrrolidin-1-yl]benzoate 4

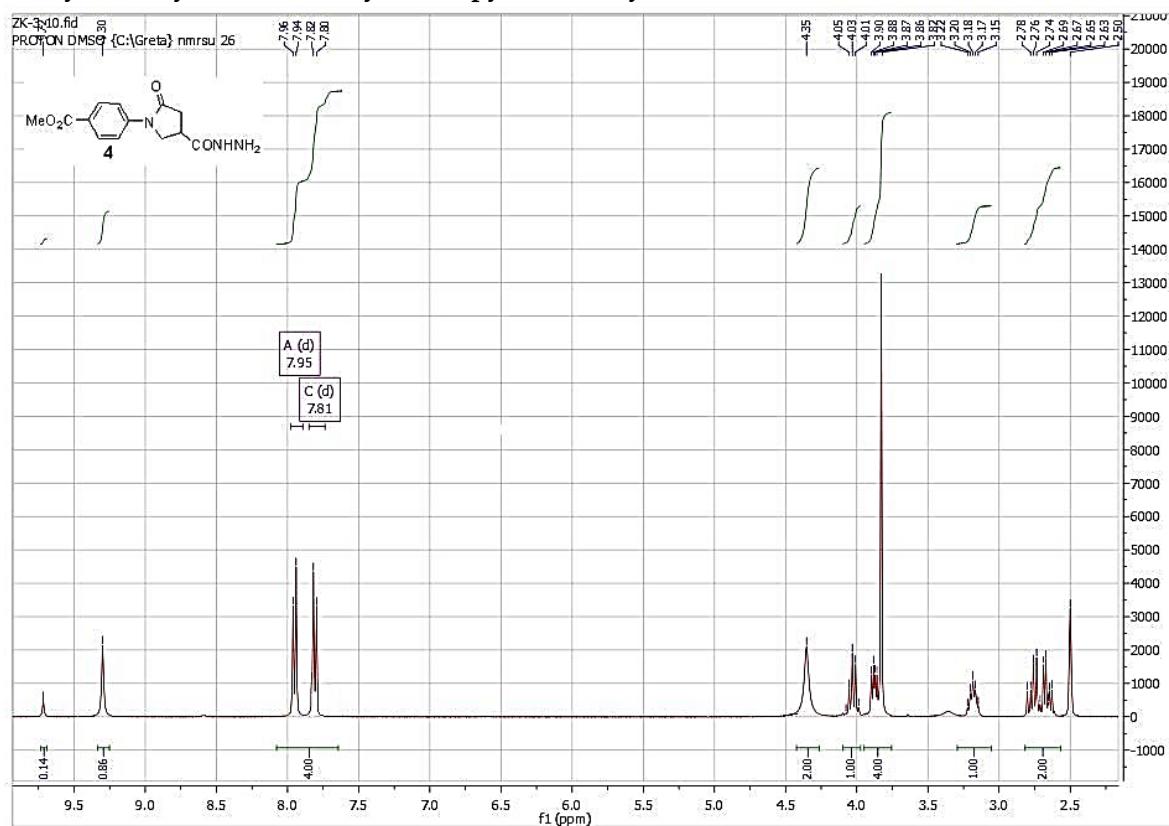


Figure S5: ¹H NMR of compound 4

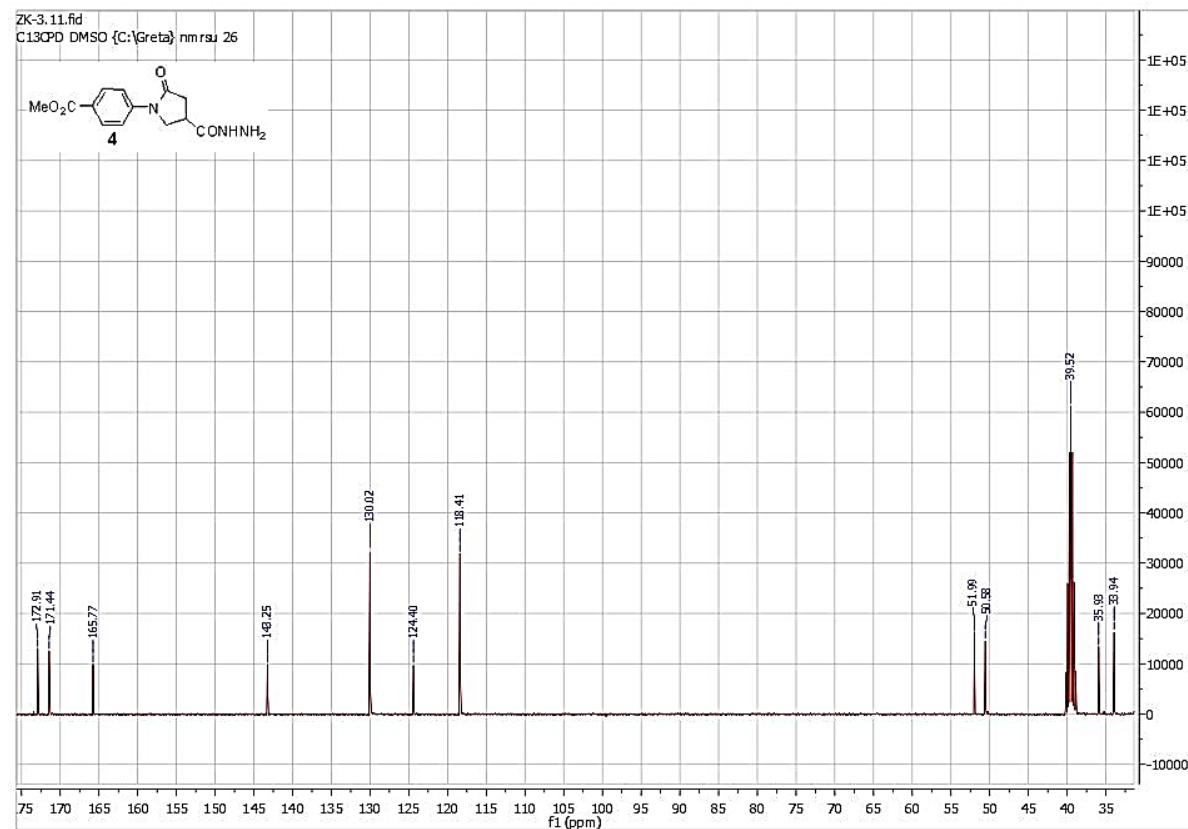


Figure S6: ¹³C NMR of compound 4

Methyl 4-(4-(3,5-dimethyl-1H-pyrazole-1-carbonyl)-2-oxopyrrolidin-1-yl)benzoate 5

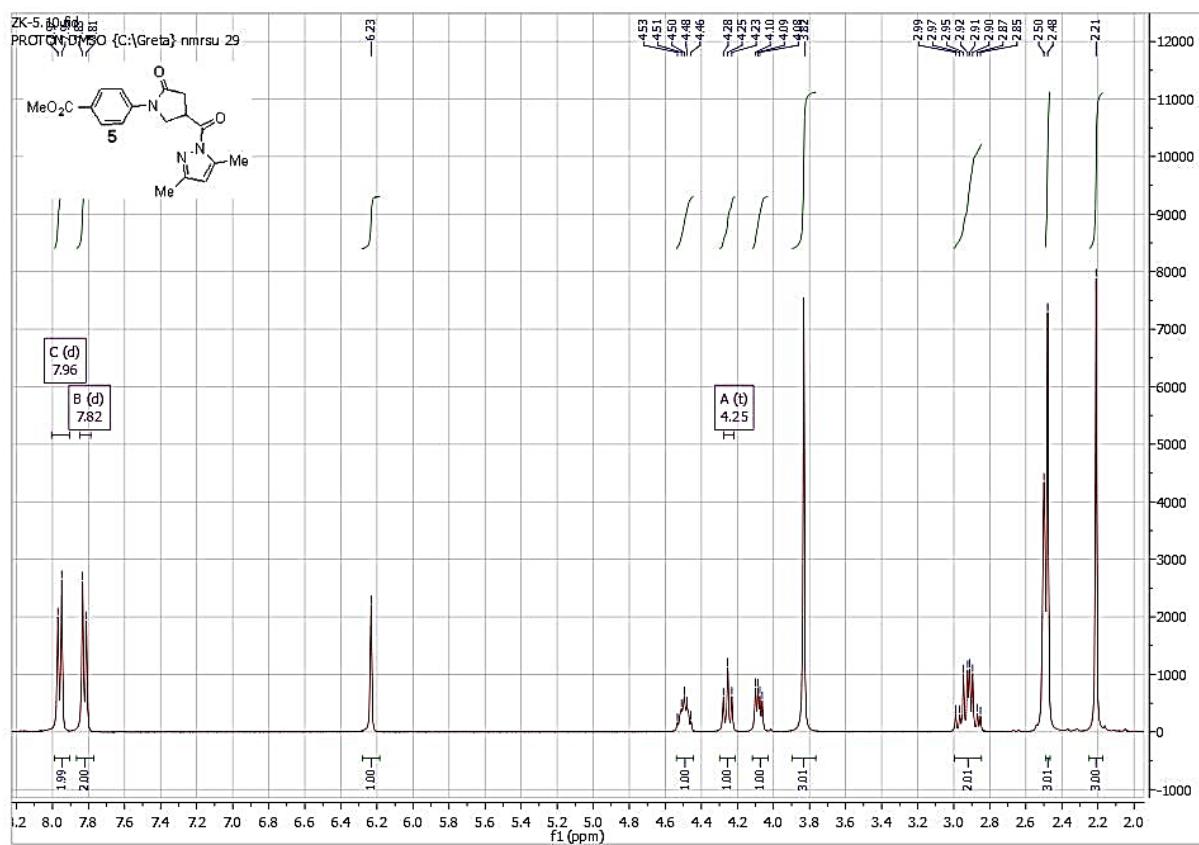


Figure S7: ¹H NMR of compound 5

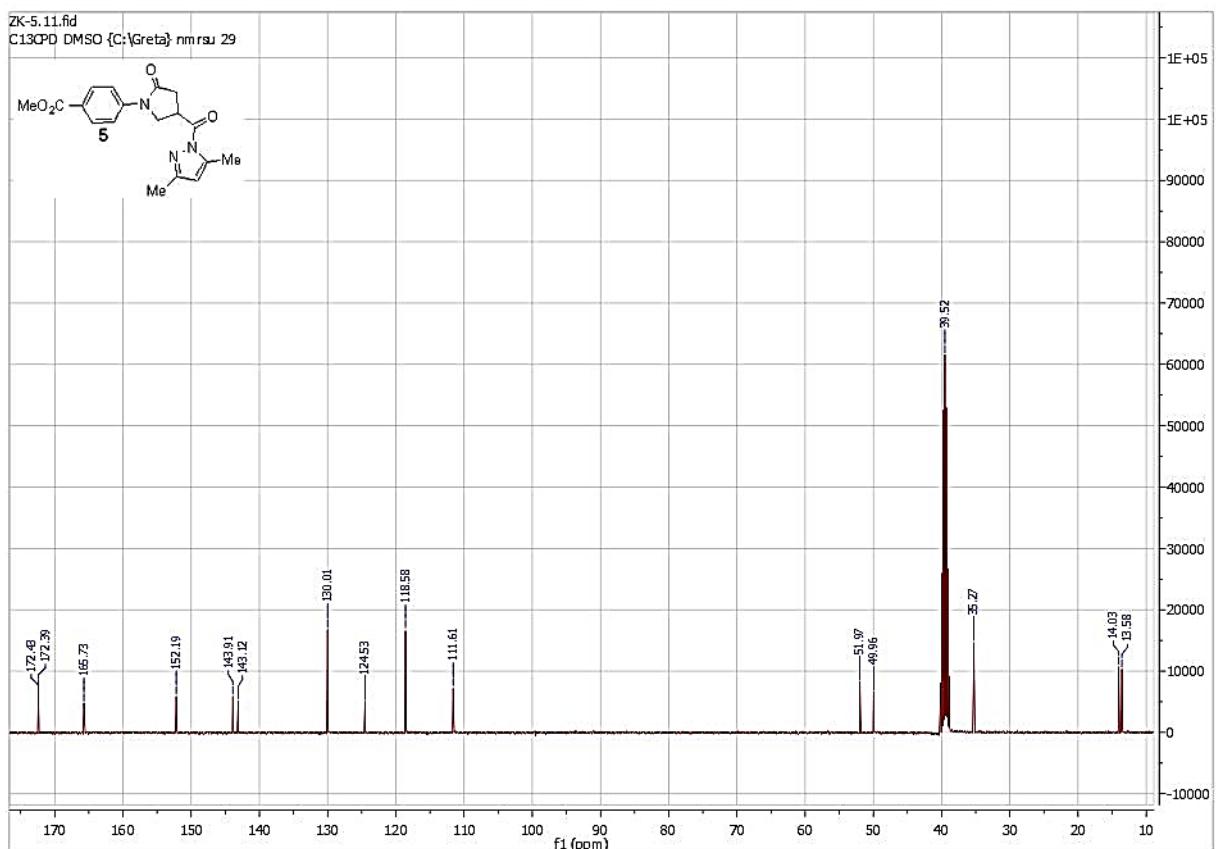


Figure S8: ¹³C NMR of compound 5

Methyl 4-((2,5-dimethyl-1H-pyrrol-1-yl)carbamoyl)-2-oxopyrrolidin-1-yl)benzoate 6

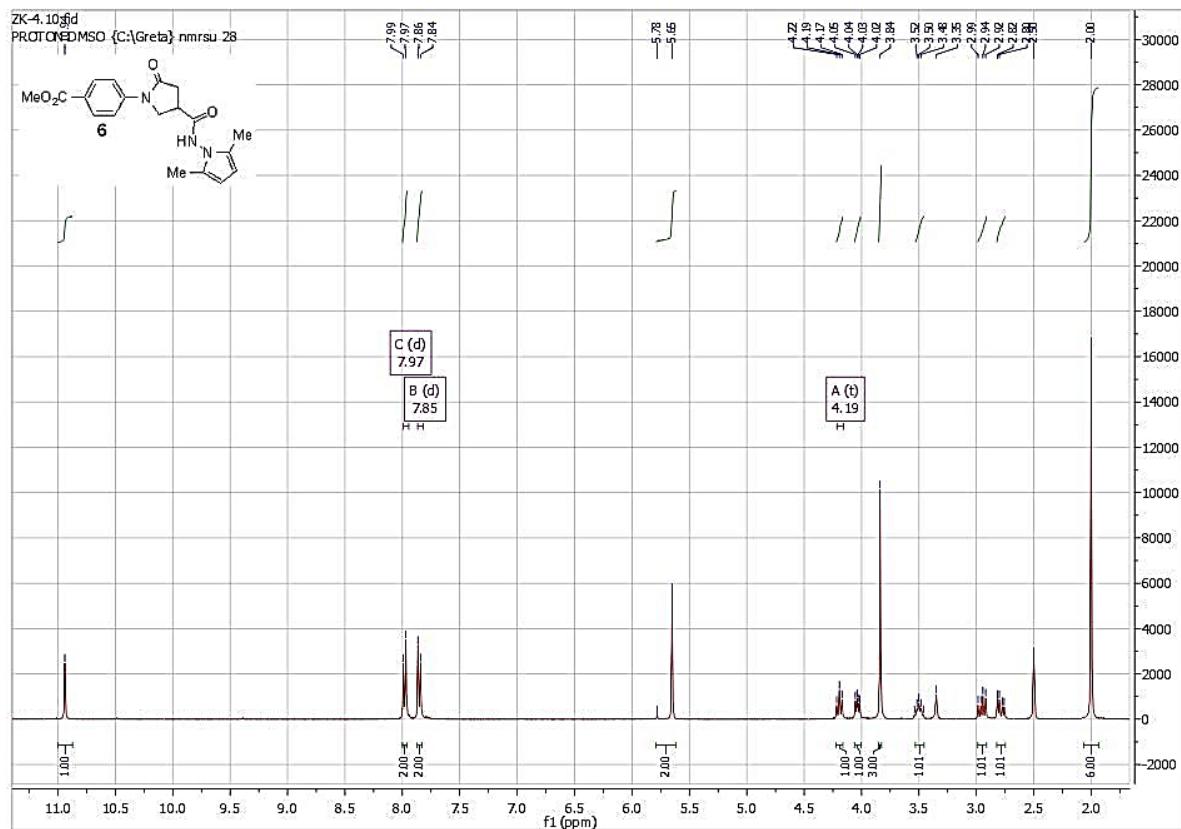


Figure S9: ¹H NMR of compound 6

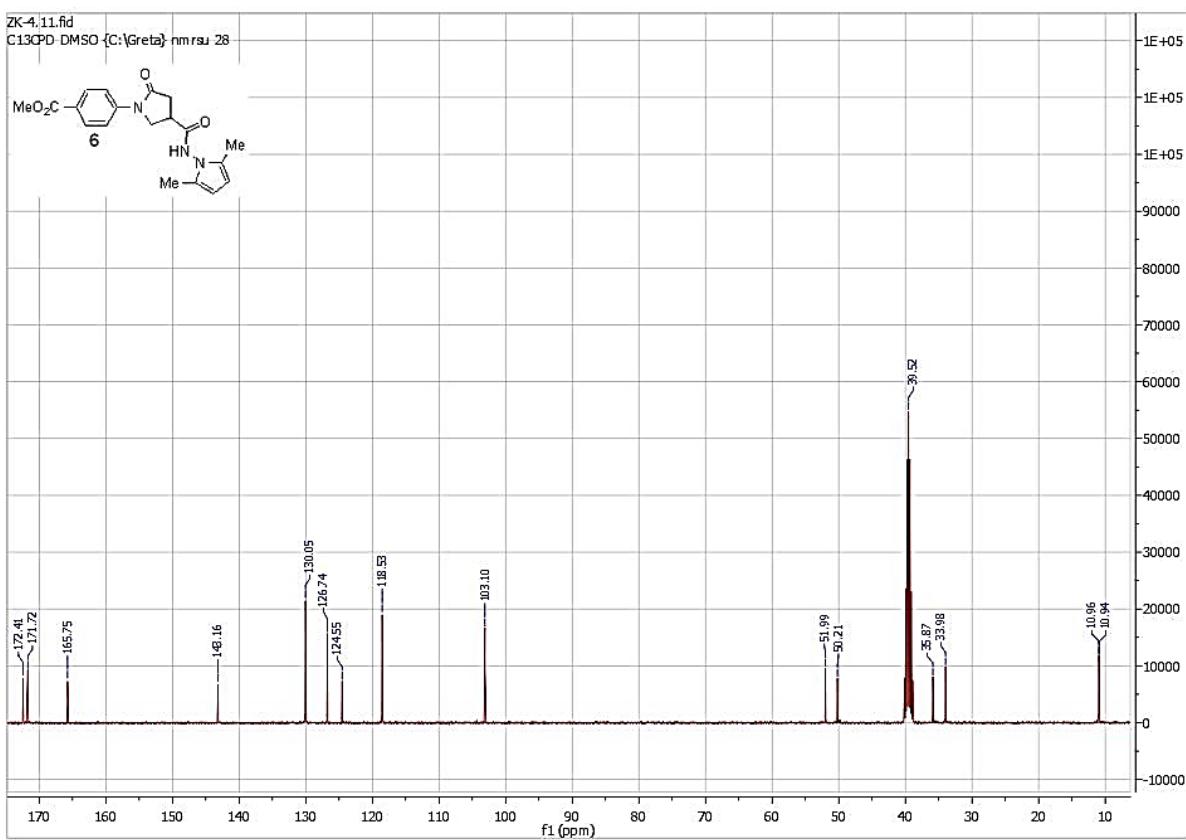


Figure S10: ¹³C NMR of compound 6

Methyl 4-(4-(2-benzylidenehydrazine-1-carbonyl)-2-oxopyrrolidin-1-yl)benzoate 7a

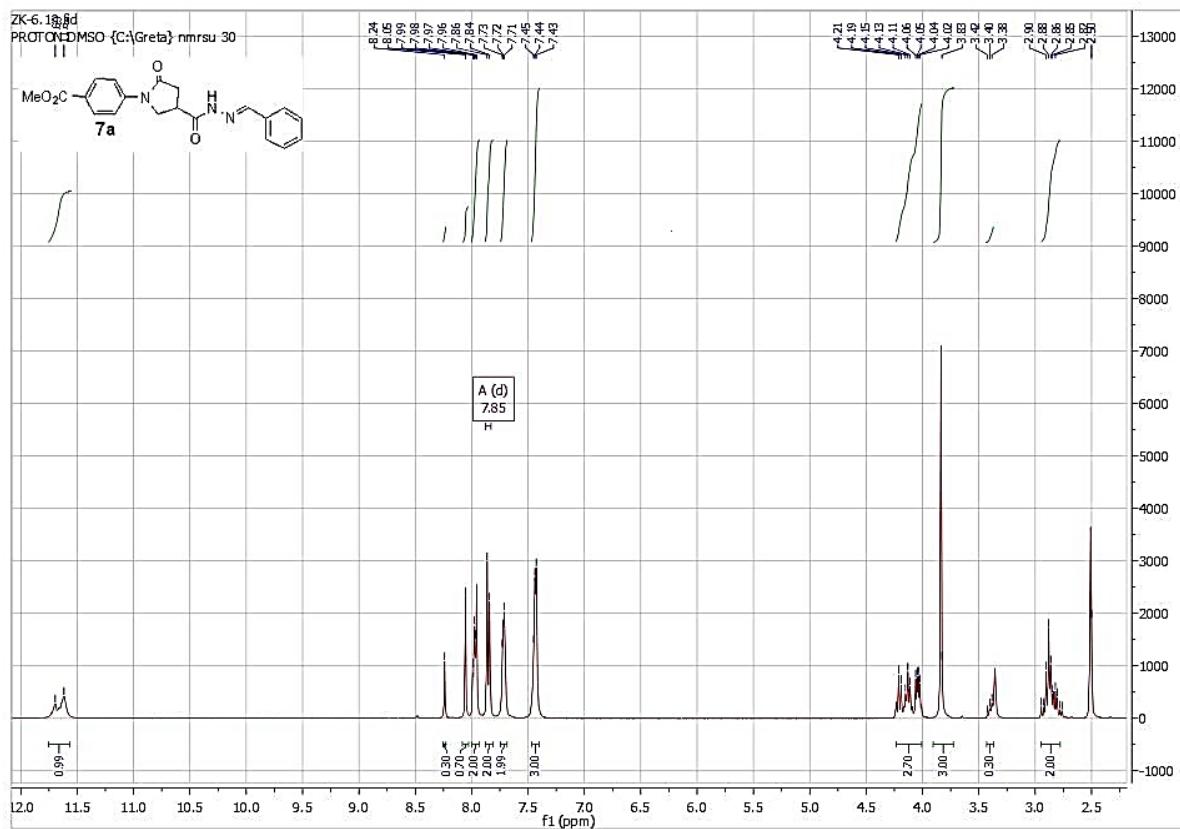


Figure S11: ¹H NMR of compound 7a

Methyl 4-(4-(2-(4-methoxybenzylidene)hydrazine-1-carbonyl)-2-oxopyrrolidin-1-yl)benzoate 7b

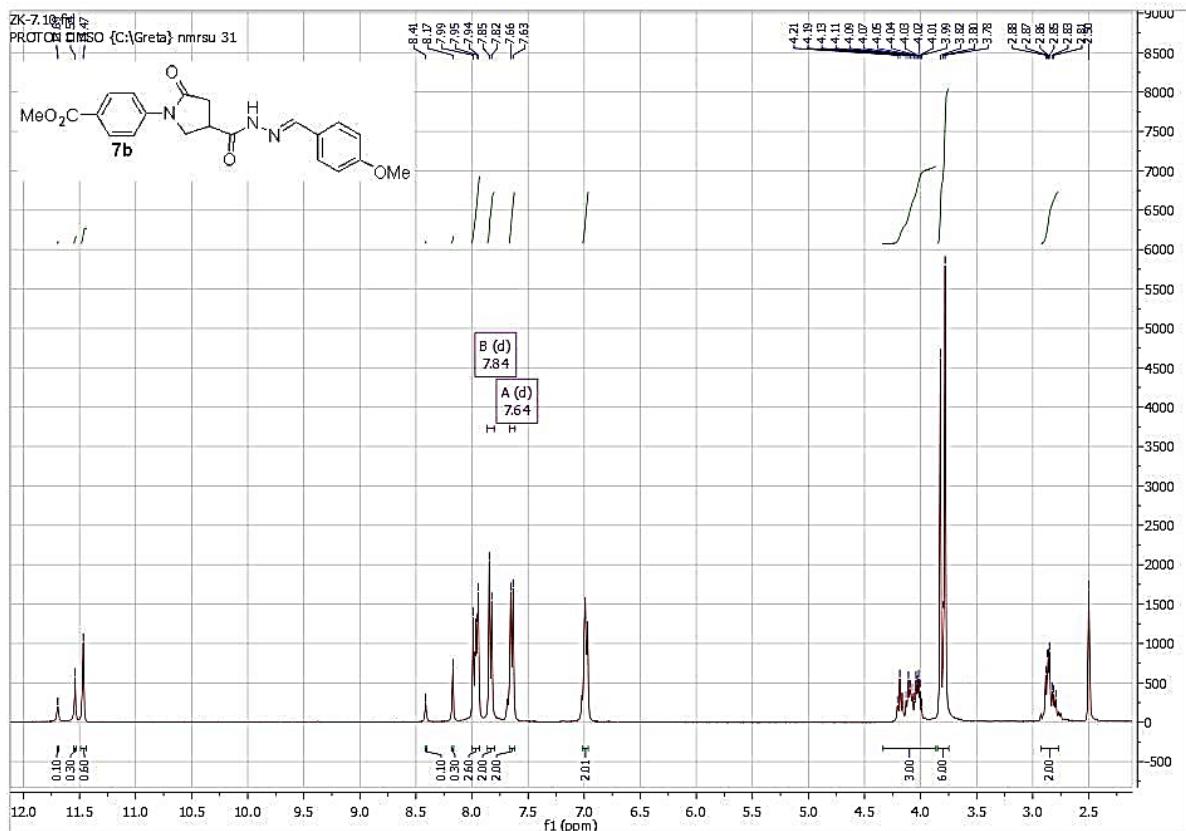


Figure S12: ¹H NMR of compound 7b

Methyl 4-(4-(2-(4-(dimethylamino)benzylidene)hydrazine-1-carbonyl)-2-oxopyrrolidin-1-yl)benzoate 7c

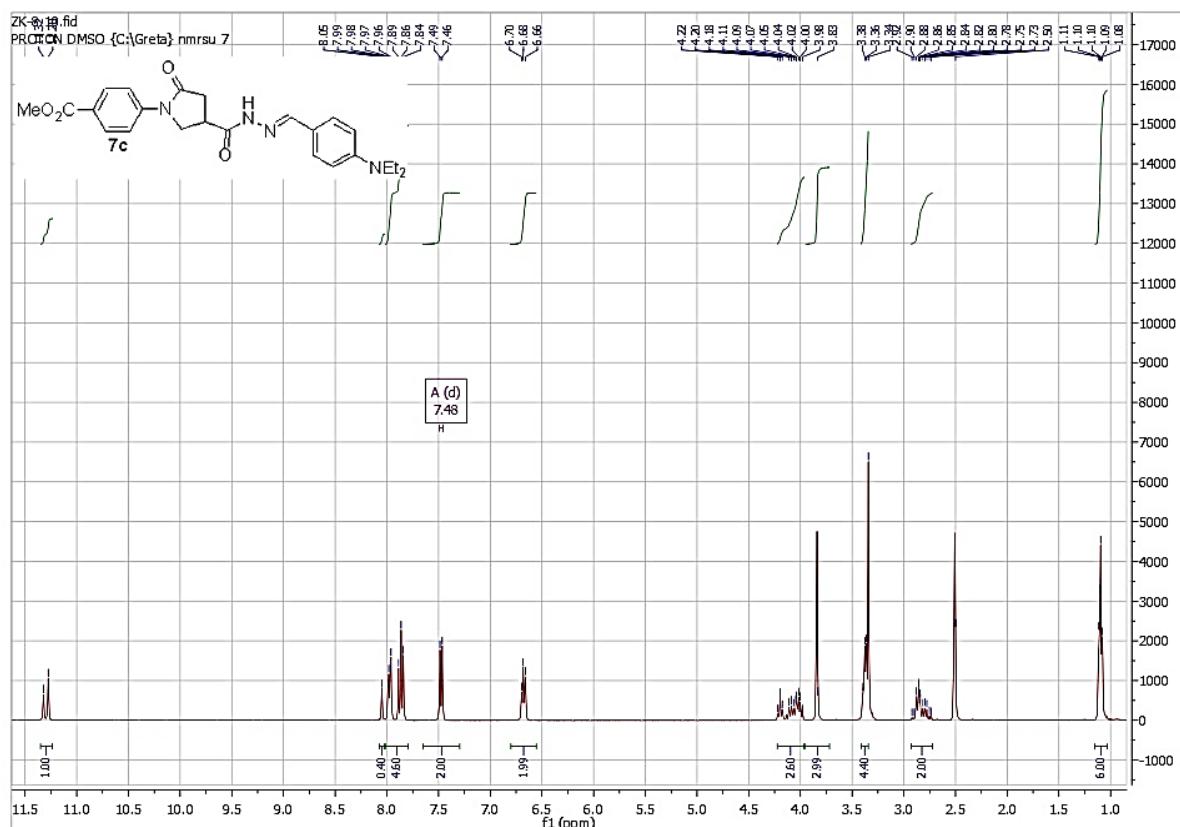


Figure S13: ^1H NMR of compound 7c

1-(1-(4-(Methoxycarbonyl)phenyl)-5-oxopyrrolidine-3-carboxamido)-5-oxopyrrolidine-3-carboxylic acid 8

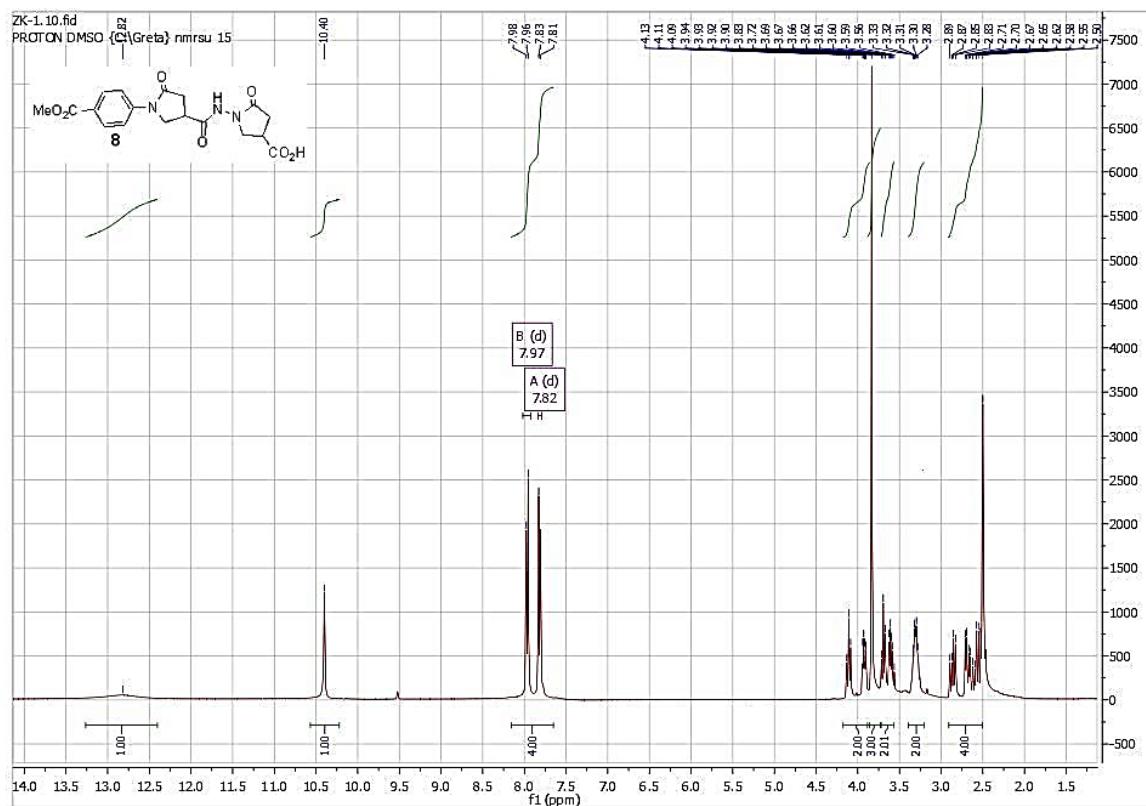


Figure S14: ¹H NMR of compound 8

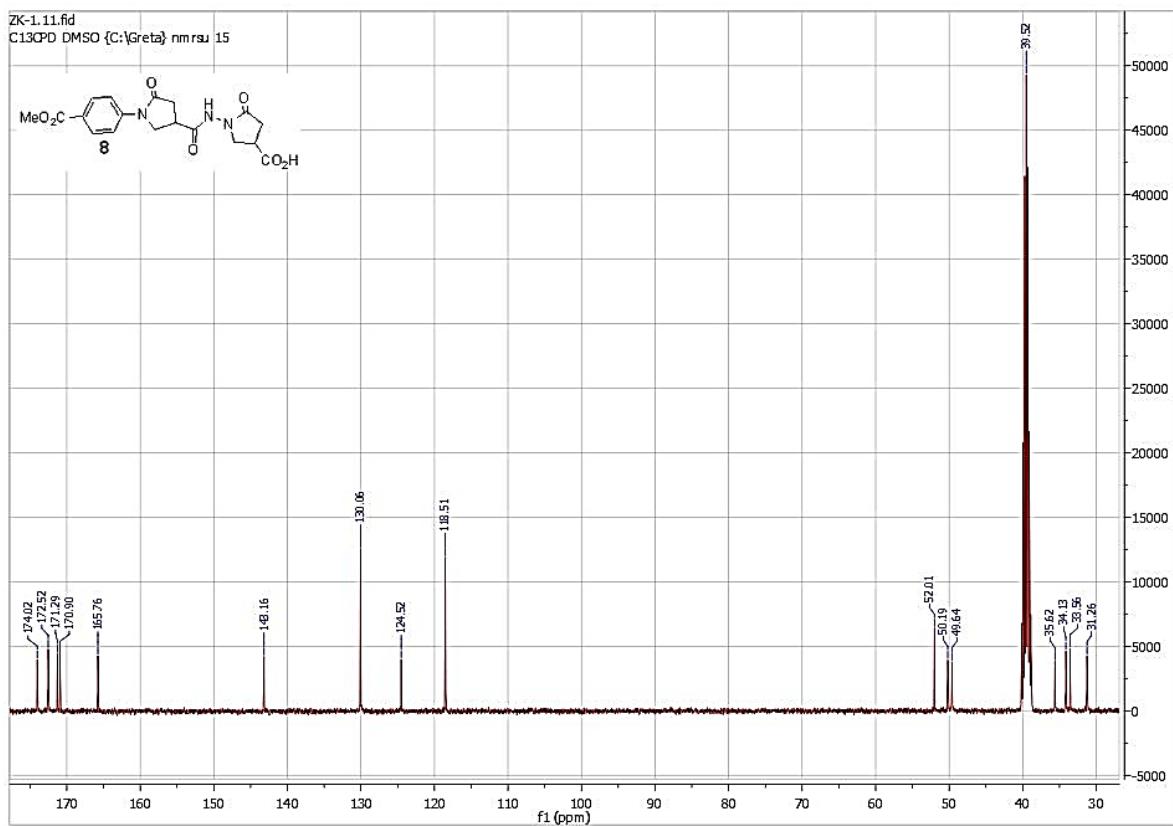


Figure S15: ¹³C NMR of compound 8

Methyl 4-(4-(2-benzoylhydrazine-1-carbonyl)-2-oxopyrrolidin-1-yl)benzoate 9

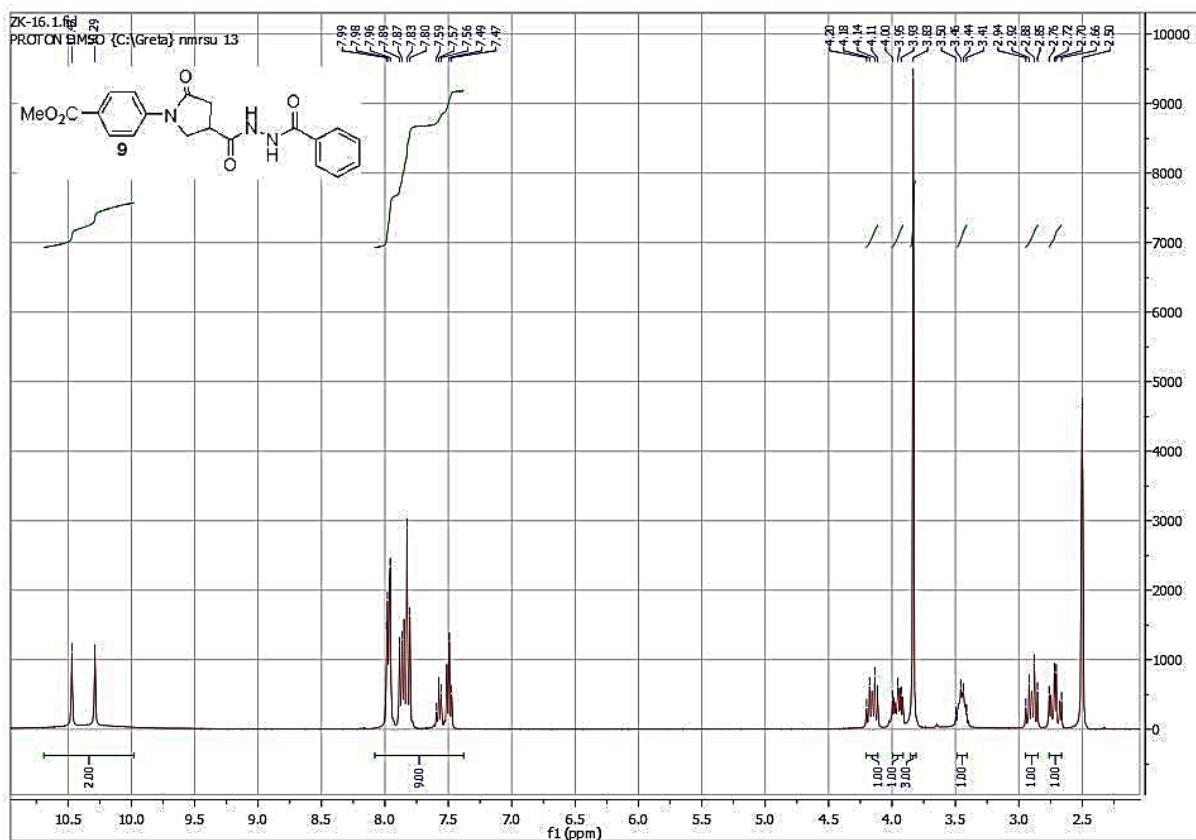


Figure S16: ¹H NMR of compound 9

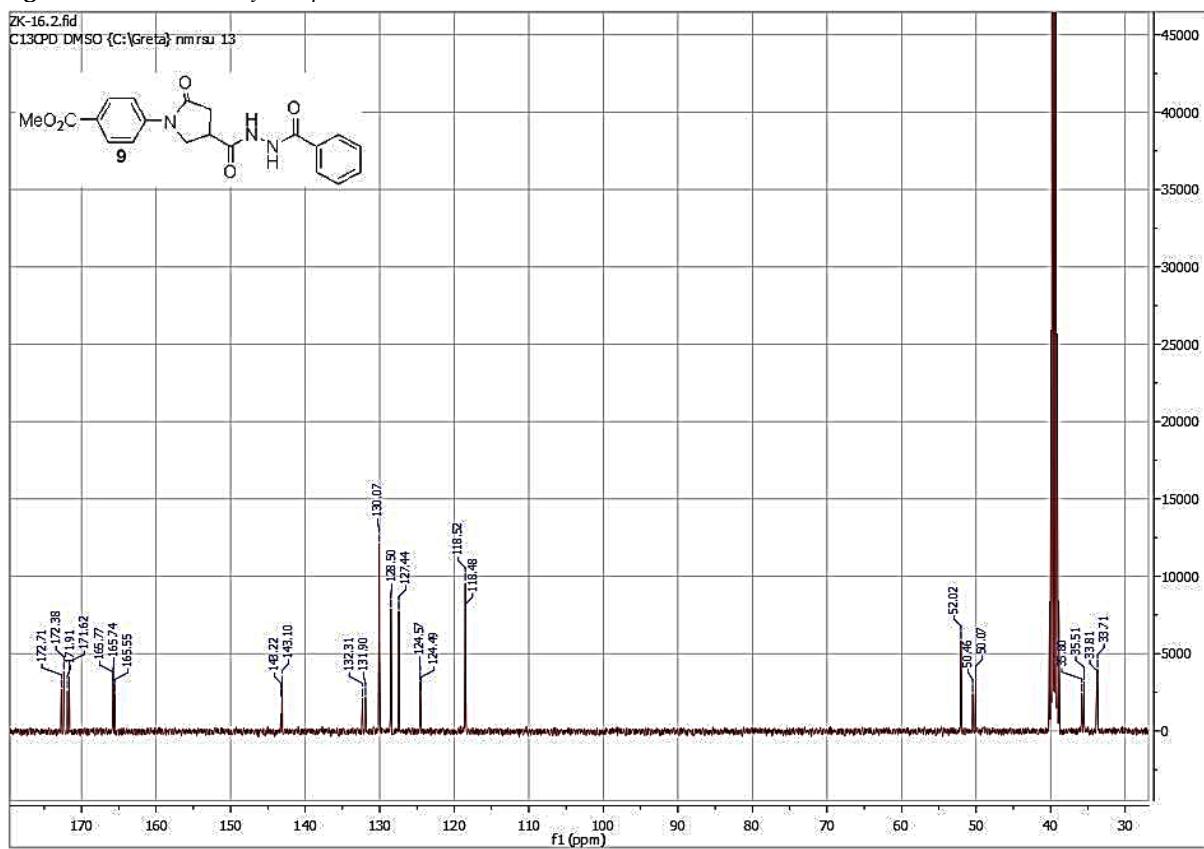


Figure S17: ¹³C NMR of compound 9

1-(4-(Hydrazinecarbonyl)phenyl)-5-oxopyrrolidine-3-carbohydrazide 10

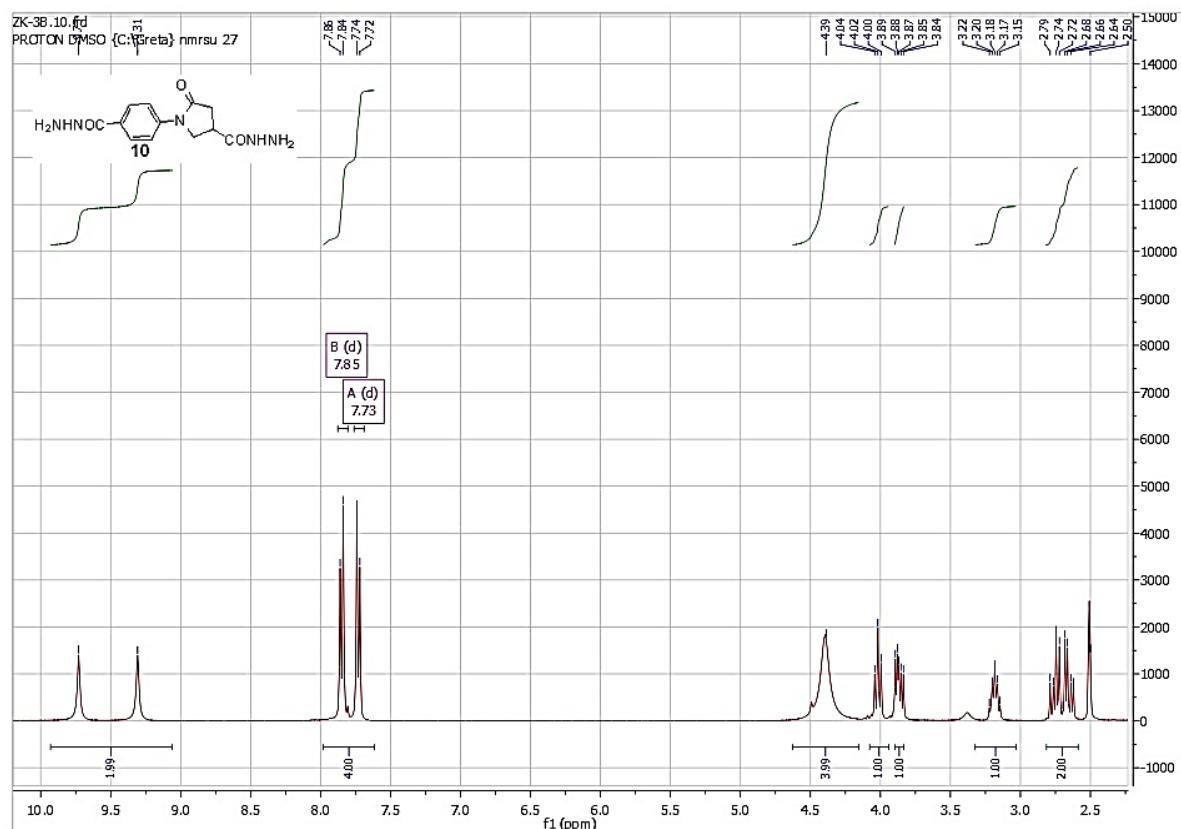


Figure S18: ¹H NMR of compound 10

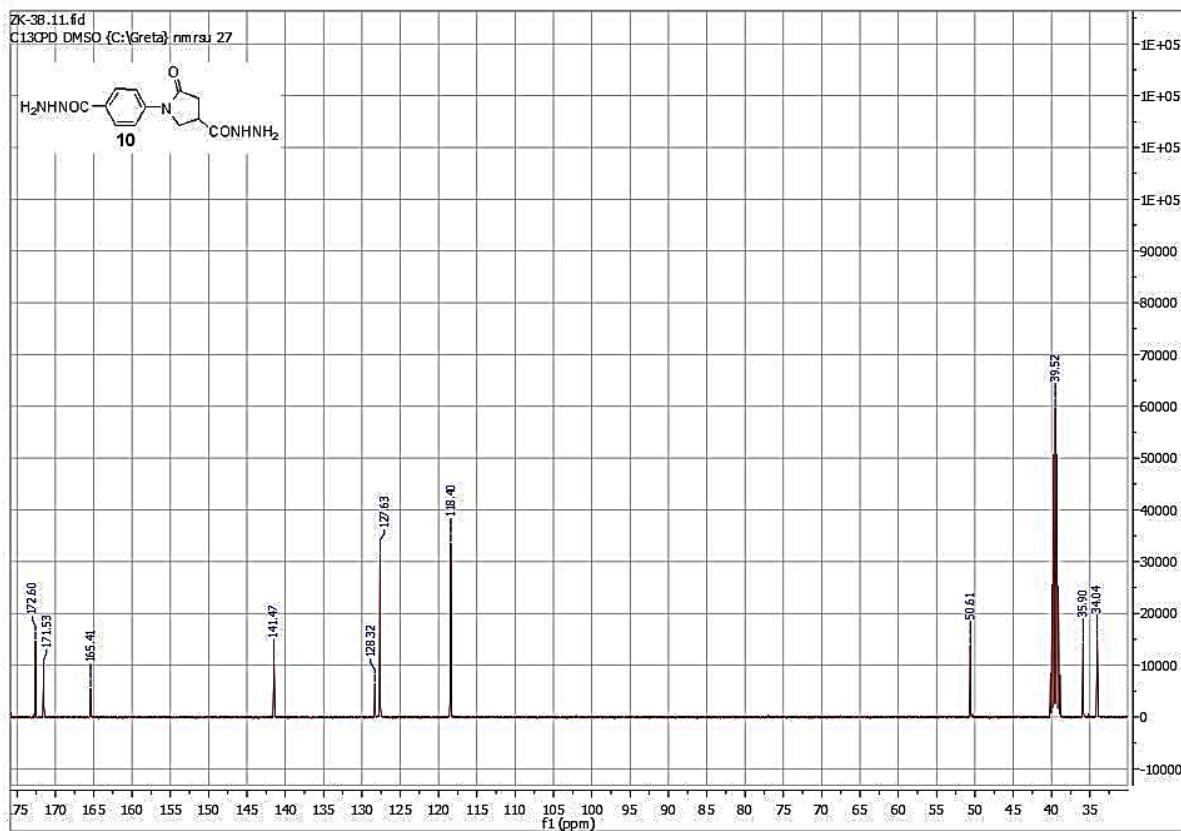


Figure S19: ¹³C NMR of compound 10

N-(4-nitrobenzylidene)-1-[4-[2-(4-nitrobenzylidenehydrazinocarbonyl)]phenyl]-5-oxopyrrolidine-3-carbohydrazide 11a

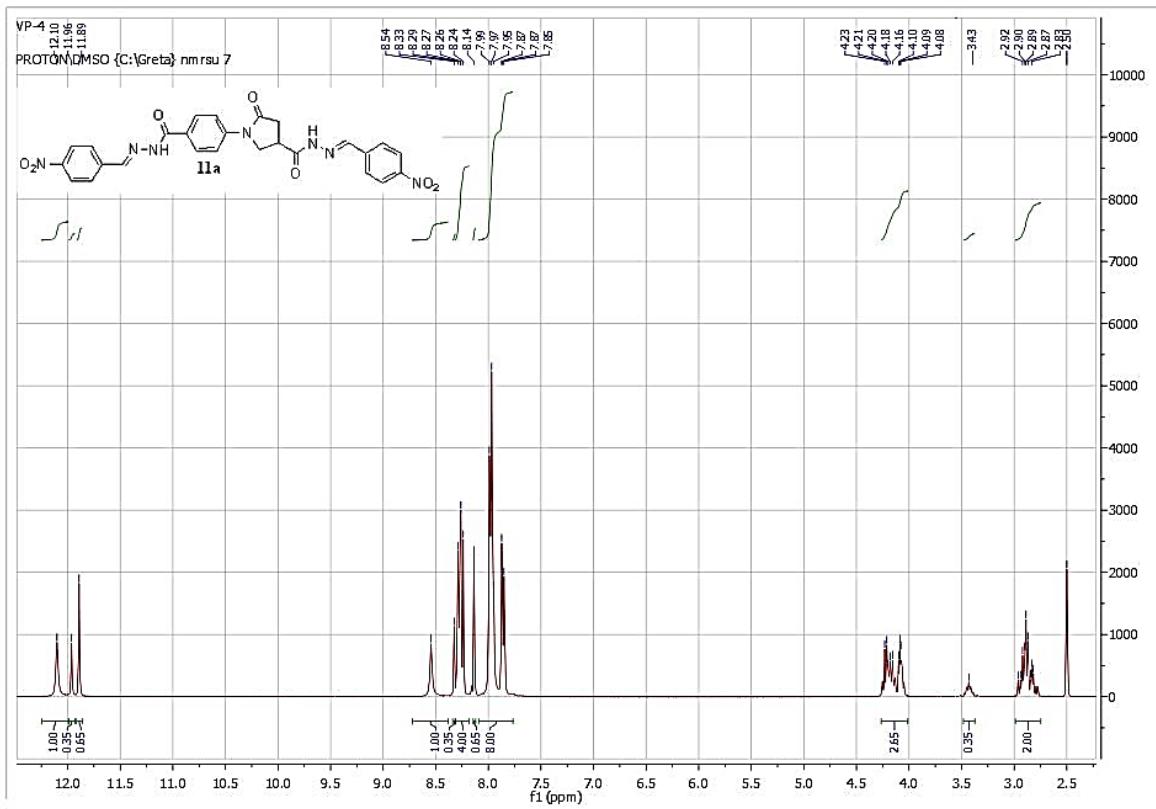


Figure S20: ¹H NMR of compound 11a
N-(4-chlorobenzylidene)-1-[4-[2-(4-chlorobenzylidenehydrazinocarbonyl)]phenyl]-5-oxopyrrolidine-3-carbohydrazide 11b

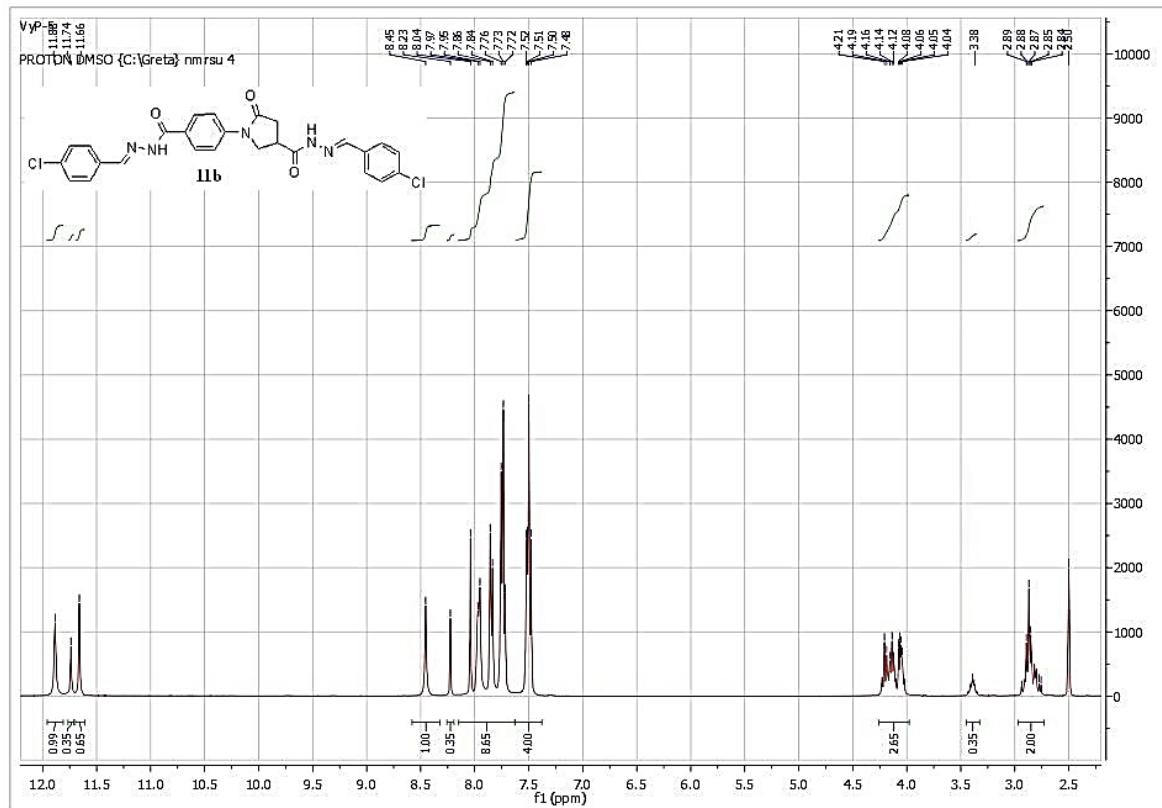


Figure S21: ¹H NMR of compound 11b

1-[[5-Oxo-1-(4-[(phenylcarbamoylthioamino)carbamoyl]pyrrolidin-3-carbonyl]-3-phenylthiocarbamide 12

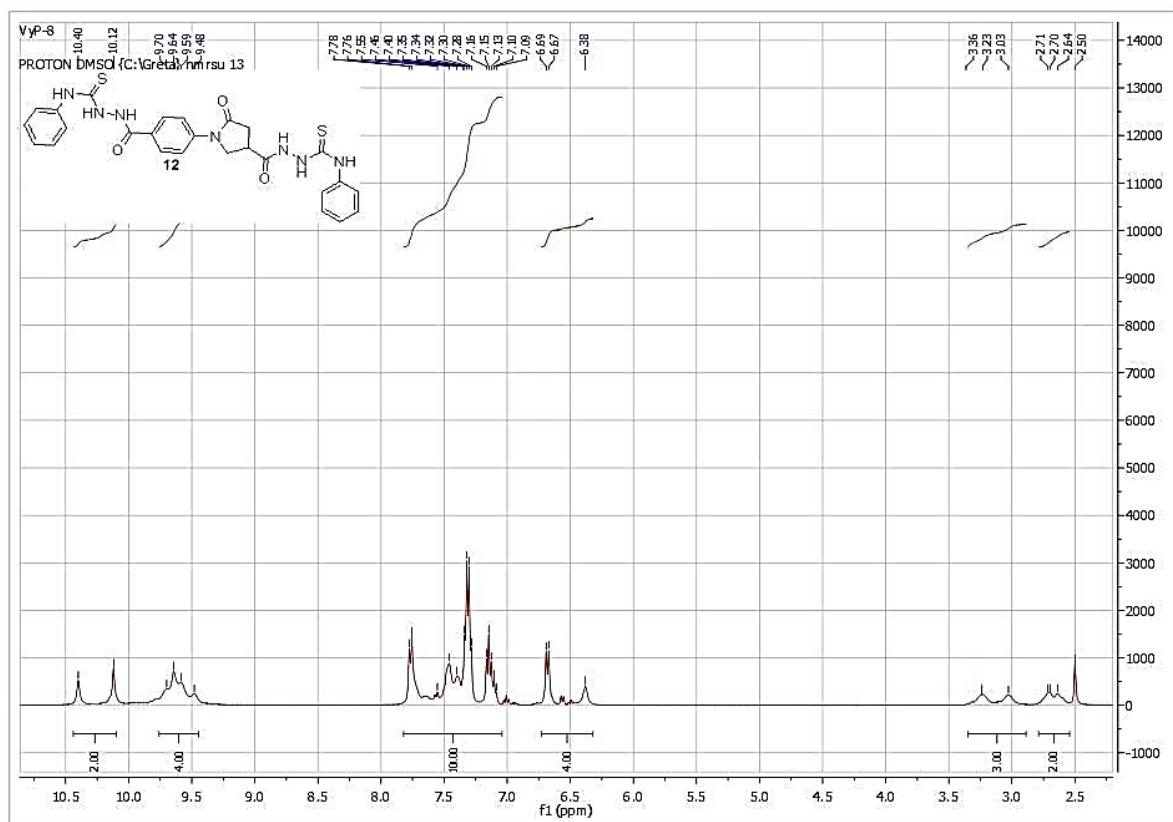


Figure S22: ¹H NMR of compound 12

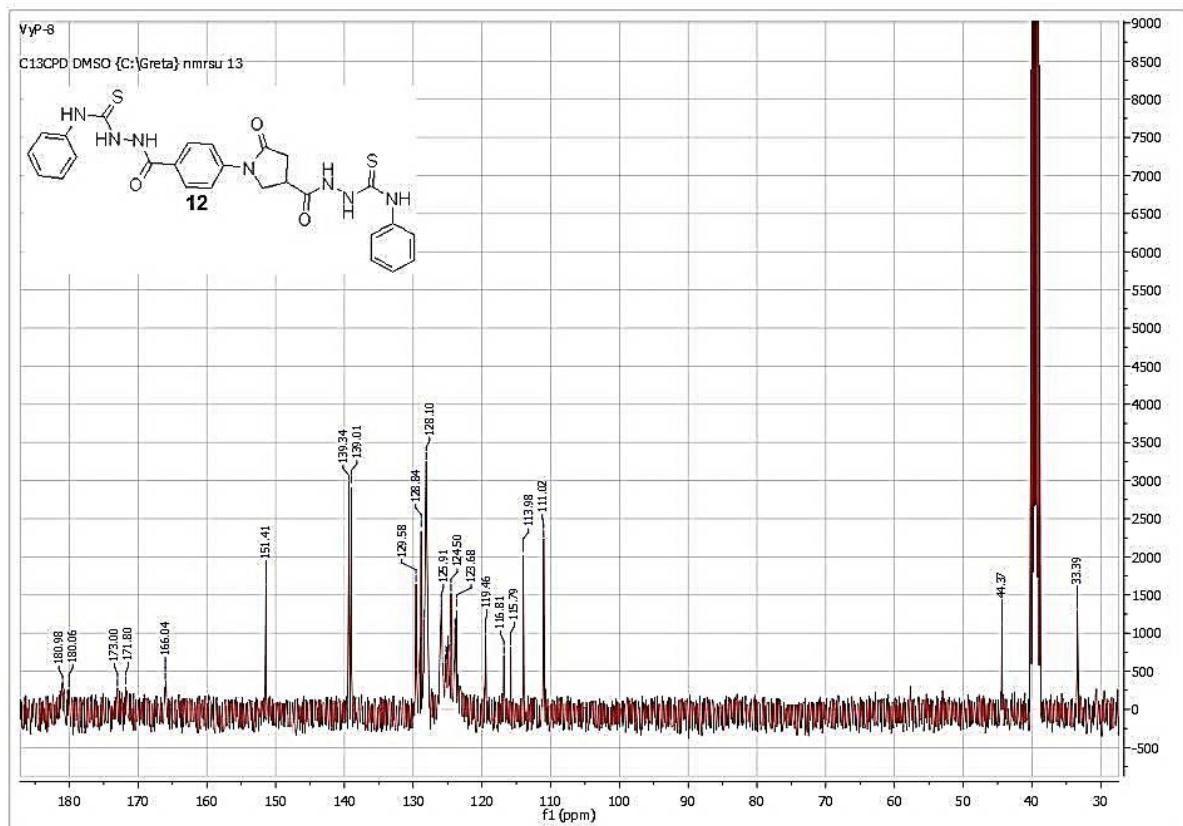


Figure S23: ¹³C NMR of compound 12

4-(4-phenyl-5-thioxo-4,5-dihydro-1H-1,2,4-triazol-3-yl)-1-(4-(4-phenyl-5-thioxo-4,5-dihydro-1H-1,2,4-triazol-3-yl)phenyl)pyrrolidin-2-one 13

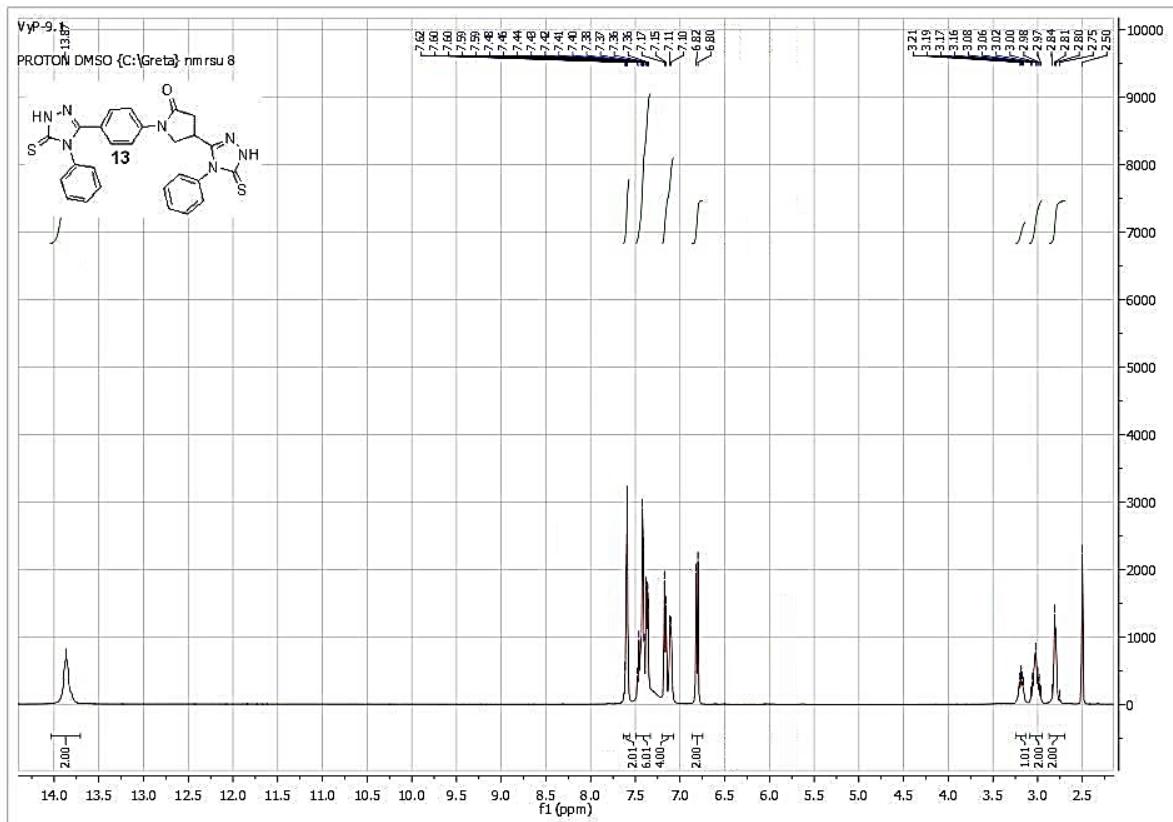


Figure S24: ^1H NMR of compound 13

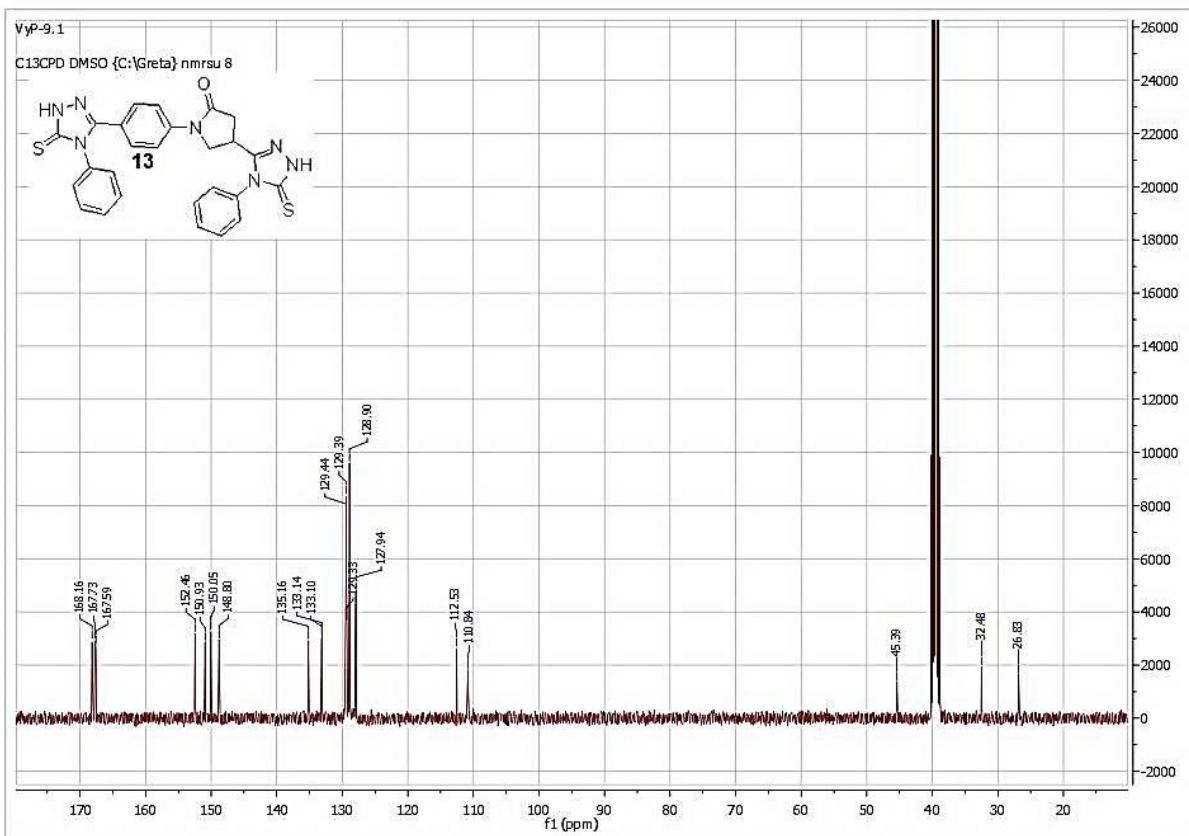


Figure S25: ^{13}C NMR of compound 13

Synthesis of benzimidazoles 14-18

3-(1H-benzimidazol-2-yl)-1-[4-(1H-benzimidazol-2-yl)phenyl]pyrrolidin-5-one 14

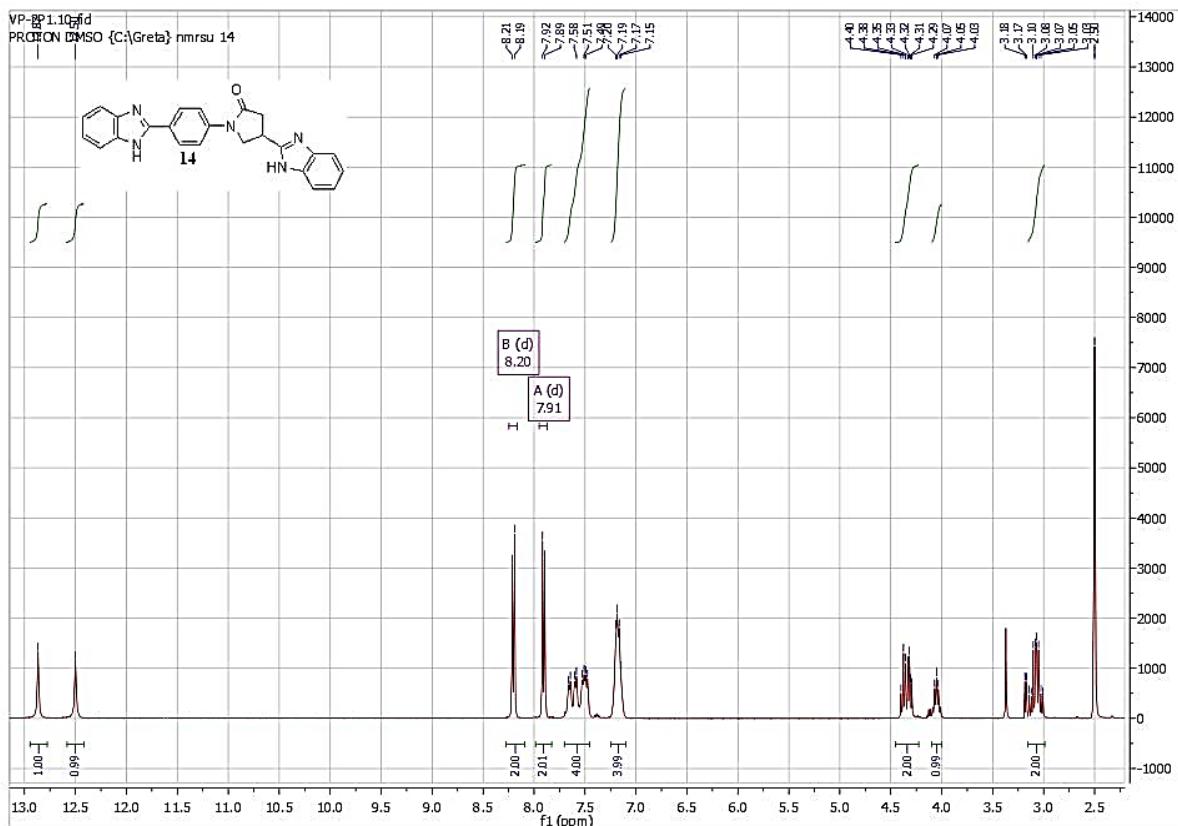


Figure S26: ¹H NMR of compound 14

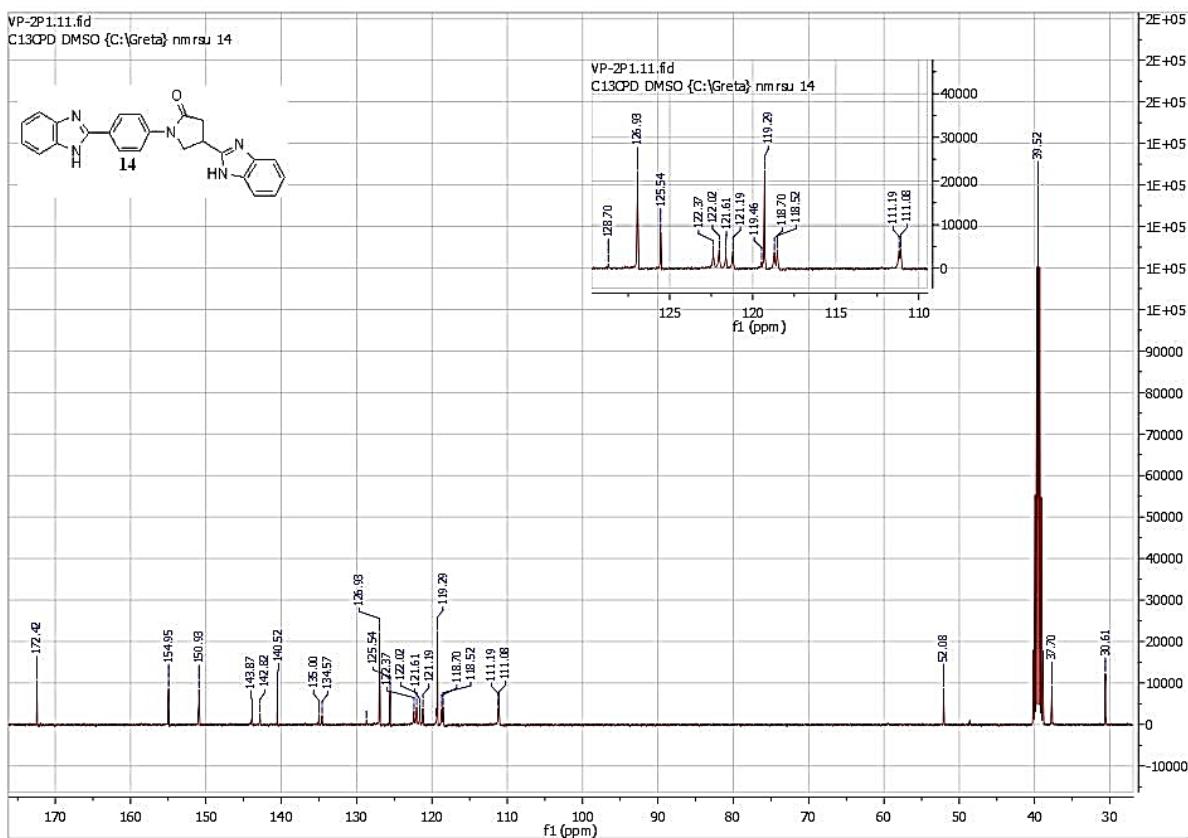


Figure S27: ¹³C NMR of compound 14

**3-(6-methyl-1H-benzimidazol-2-yl)-1-[4-(6-methyl-1H-benzimidazol-2-yl)phenyl]pyrrolidin-5-one
15**

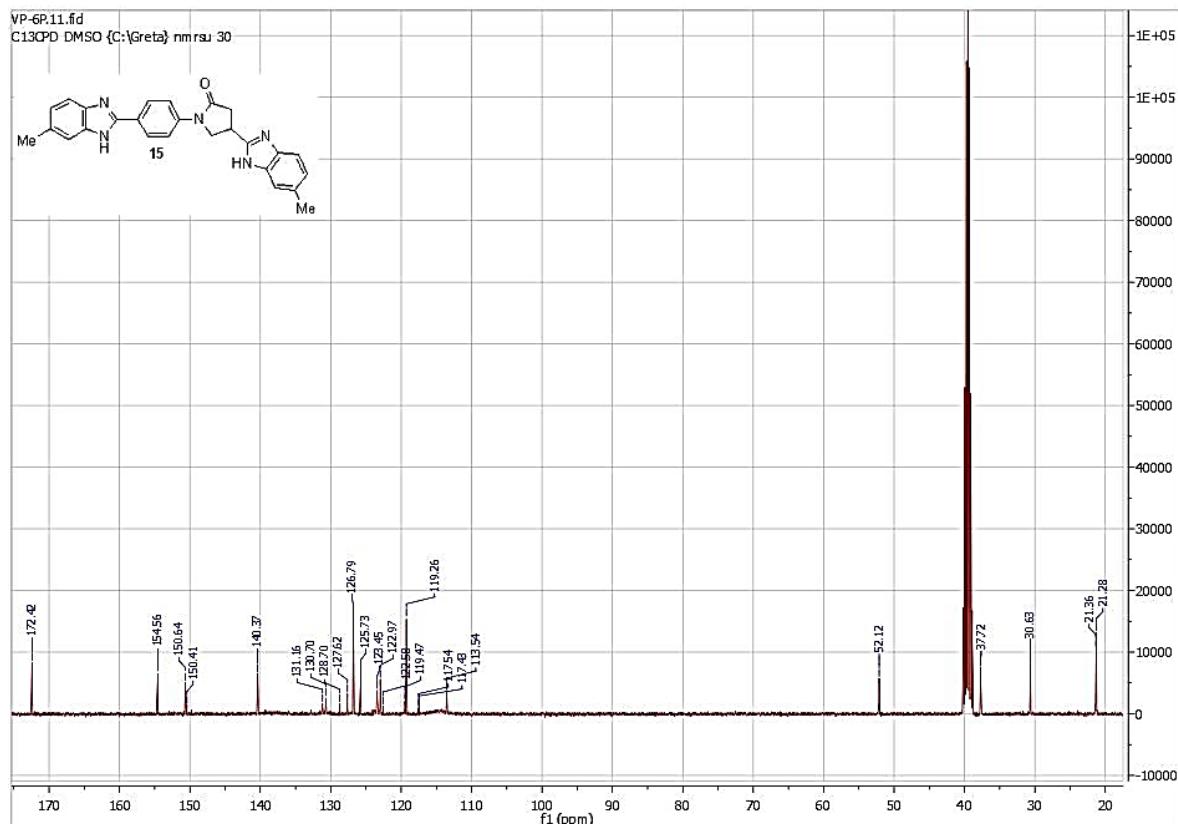
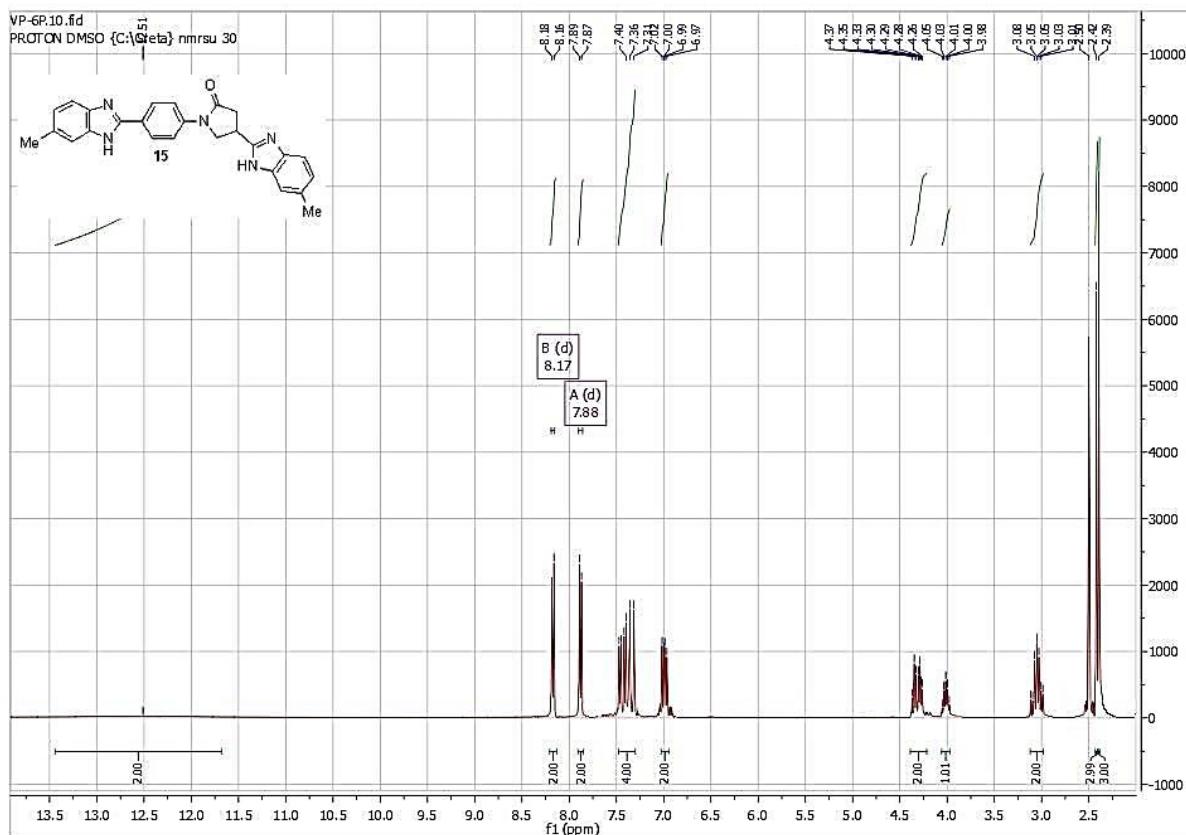


Figure S29: ^{13}C NMR of compound 15

3-(1H-benzimidazol-2-yl)-4-[4-(1H-benzimidazol-2-yl)anilino]butanoic acid 16

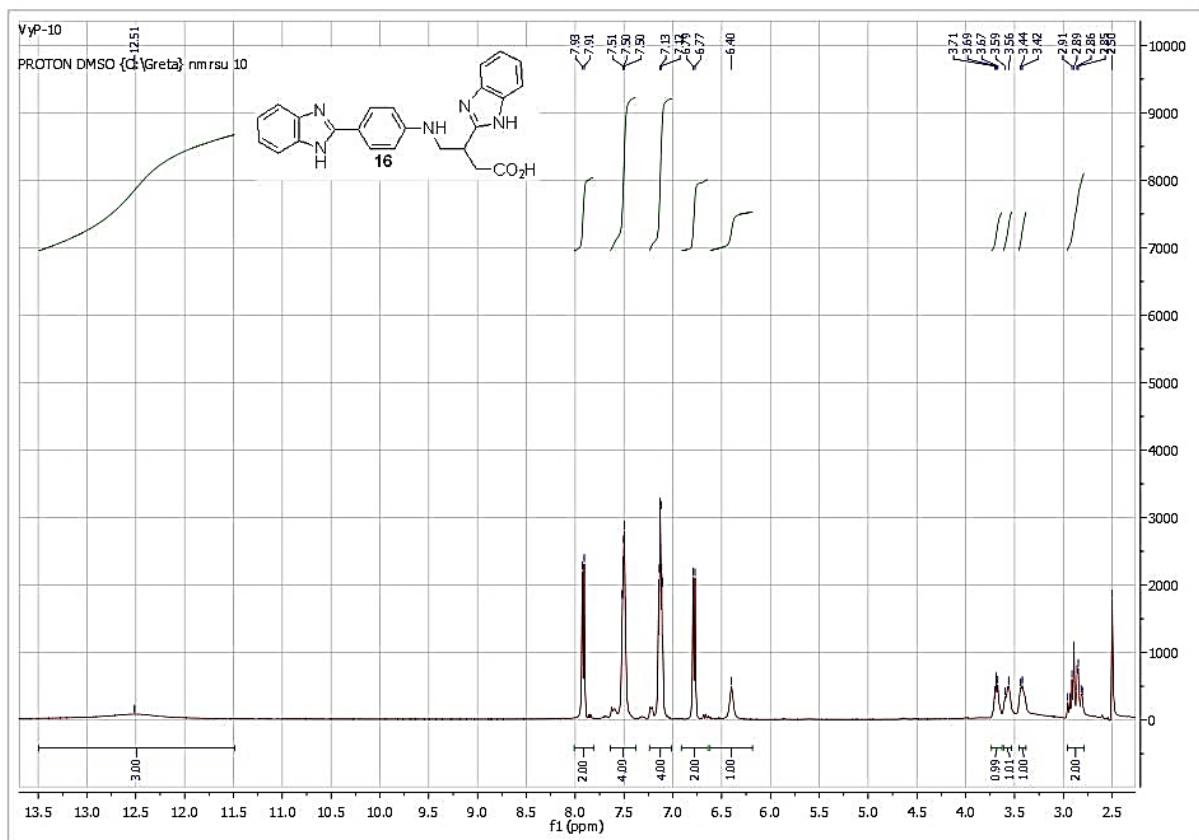


Figure S30: ¹H NMR of compound 16

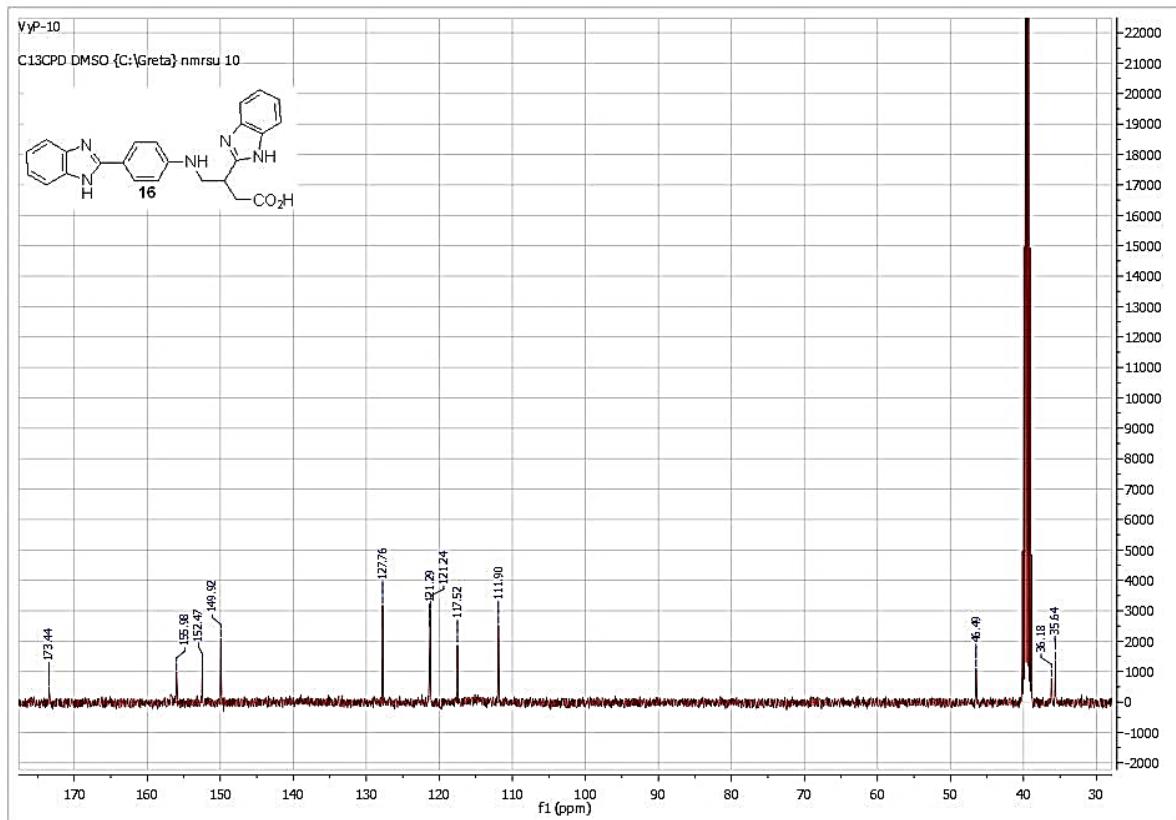


Figure S13: ¹³C NMR of compound 16

4-((4-(1H-benzimidazol-2-yl)phenyl)amino)-3-(1H-benzimidazol-2-yl)butanehydrazide 17

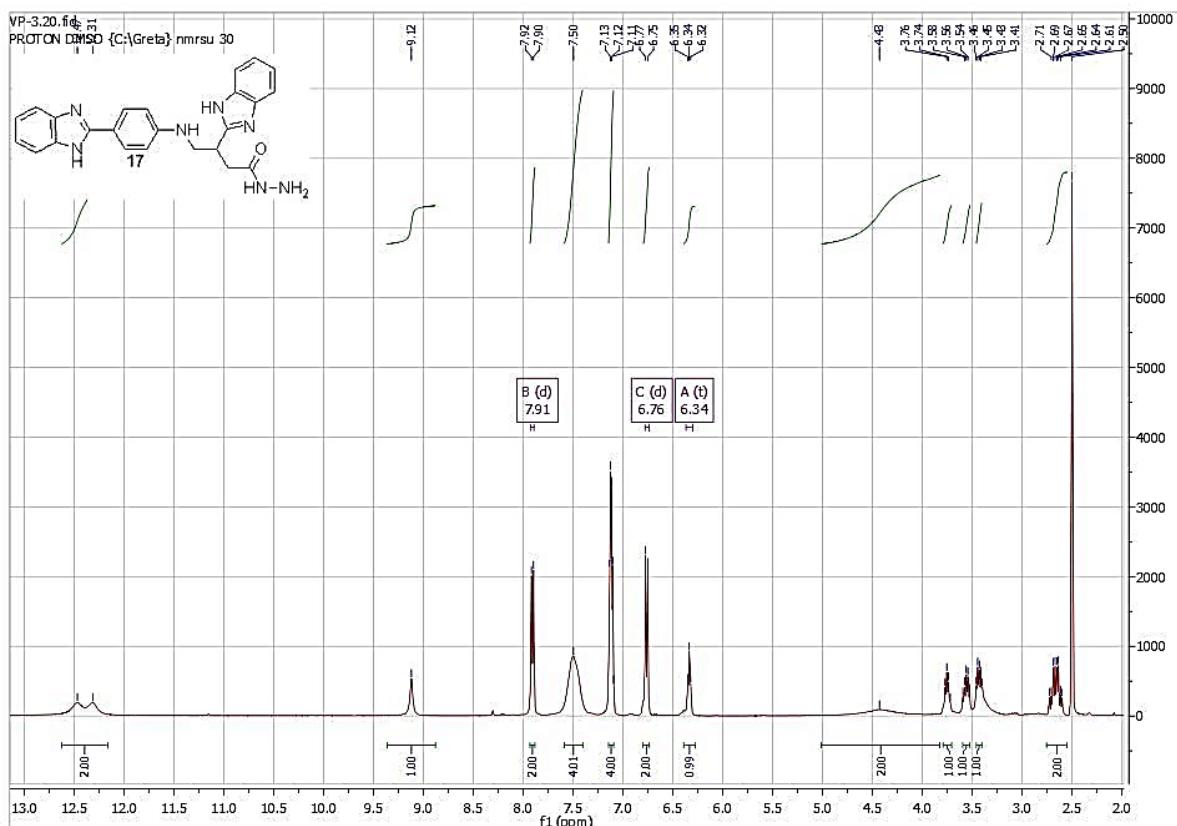


Figure S32: ¹H NMR of compound 17

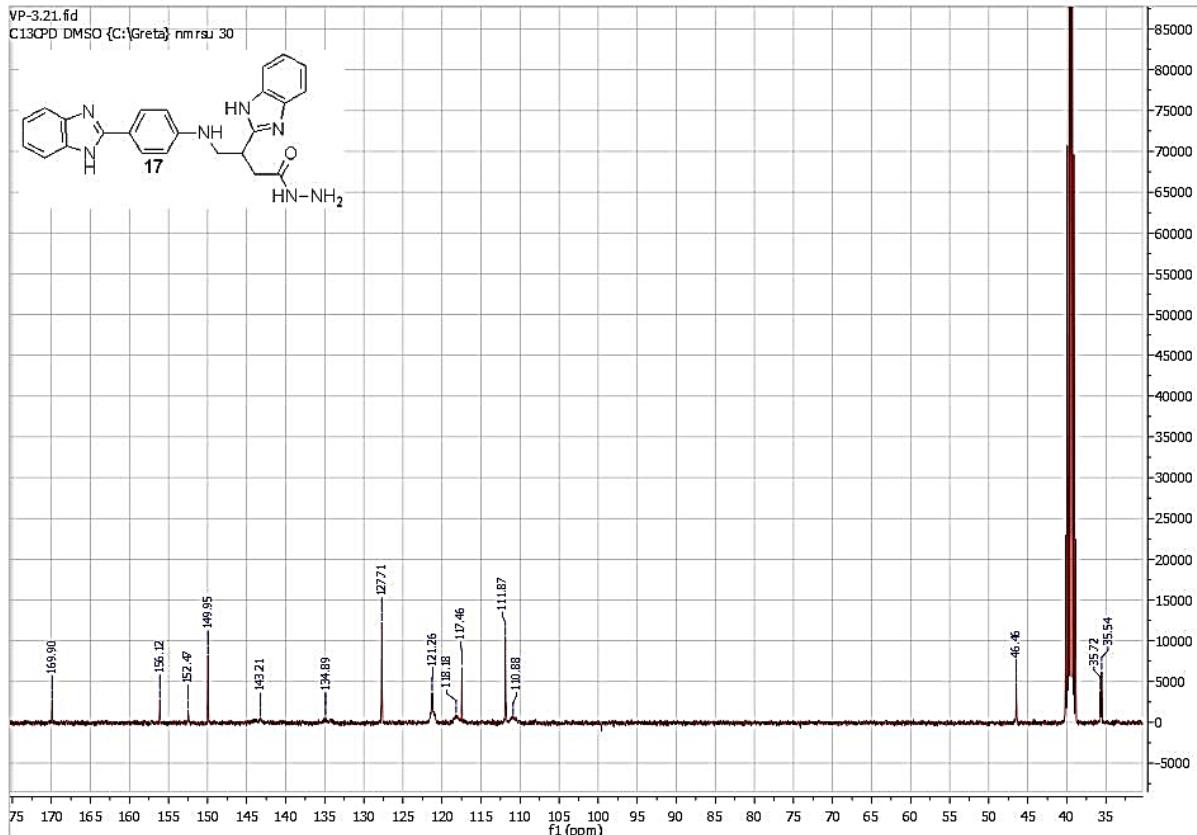


Figure S33: ¹³C NMR of compound 17

4-((4-(1H-benzimidazol-2-yl)phenyl)amino)-3-(1H-benzimidazol-2-yl)-N-(2,5-dimethyl-1H-pyrrol-2-yl)butanamide 18

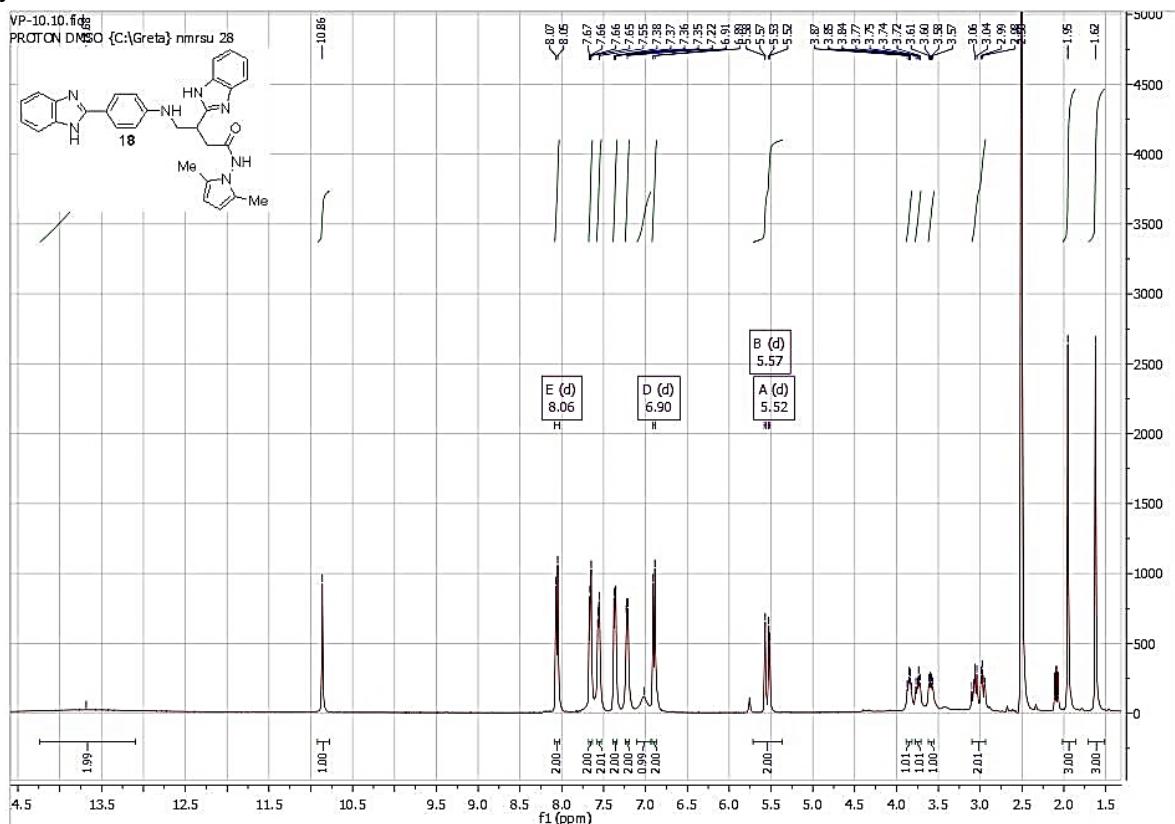


Figure S34: ^1H NMR of compound 18

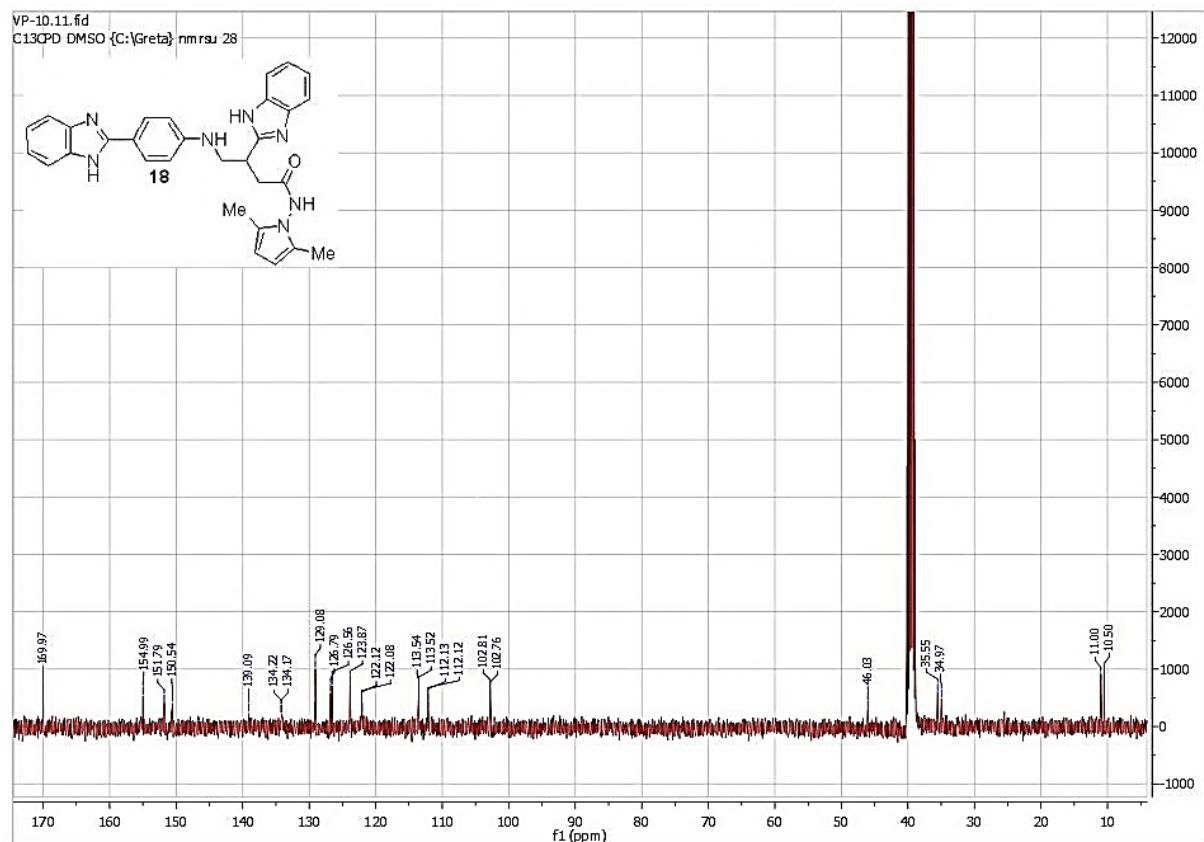


Figure S35: ^{13}C NMR of compound 18

Synthesis of bisbenzimidazoles 19-24

Ethyl 2-(2-(4-(1-(2-ethoxy-2-oxoethyl)-1H-benzimidazol-2-yl)-2-oxopyrrolidin-1-yl)phenyl)-1H-benzimidazol-1-yl)acetate 19

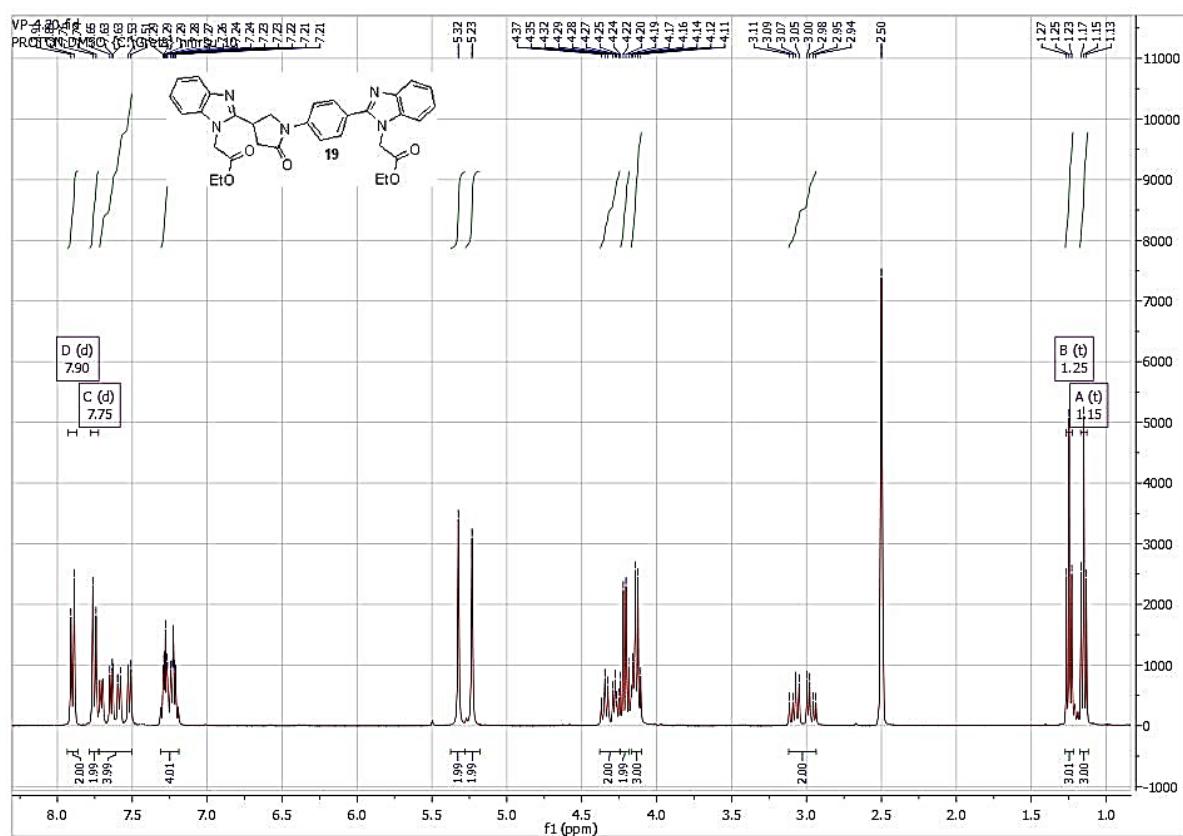


Figure S36: ^1H NMR of compound 19

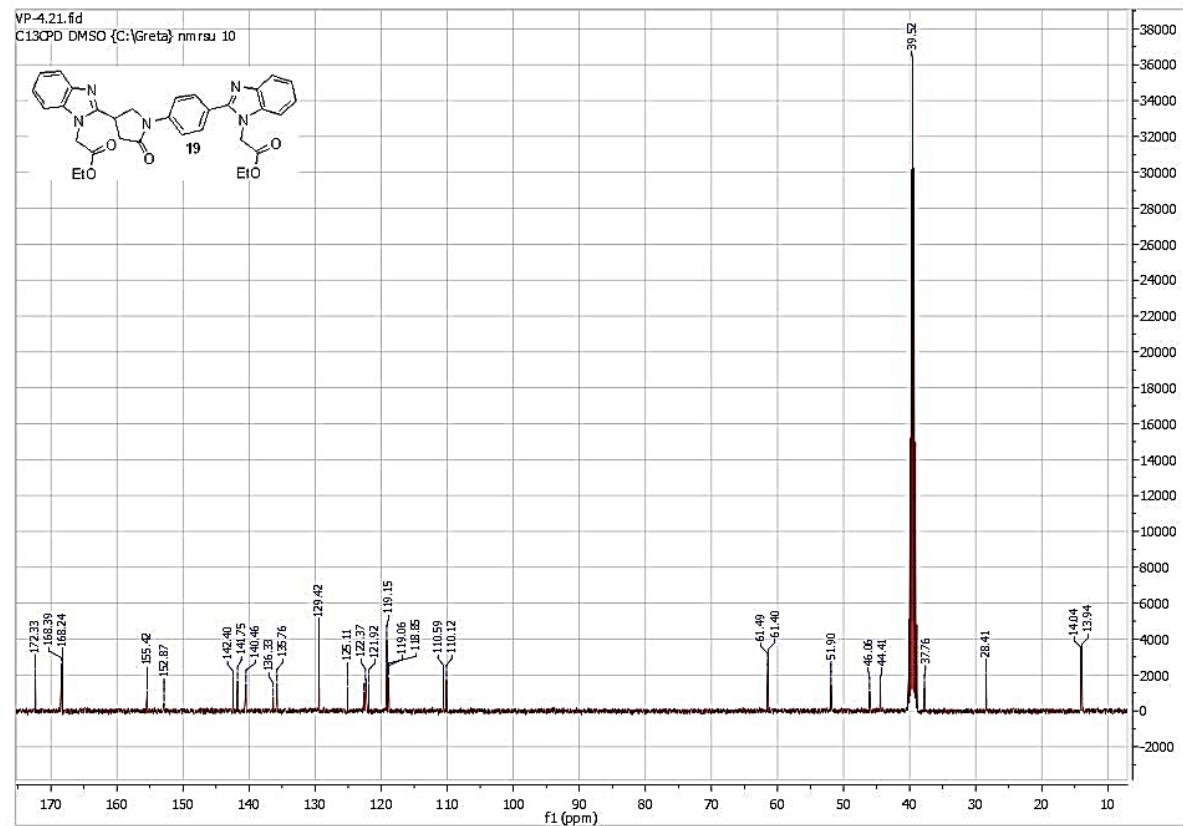


Figure S37: ^{13}C NMR of compound 19

2-(2-(4-(1-(2-hydrazinyl-2-oxoethyl)-1H-benzimidazol-2-yl)-2-oxopyrrolidin-1-yl)phenyl)-1H-benzimidazol-1-ylacetohydrazide 20

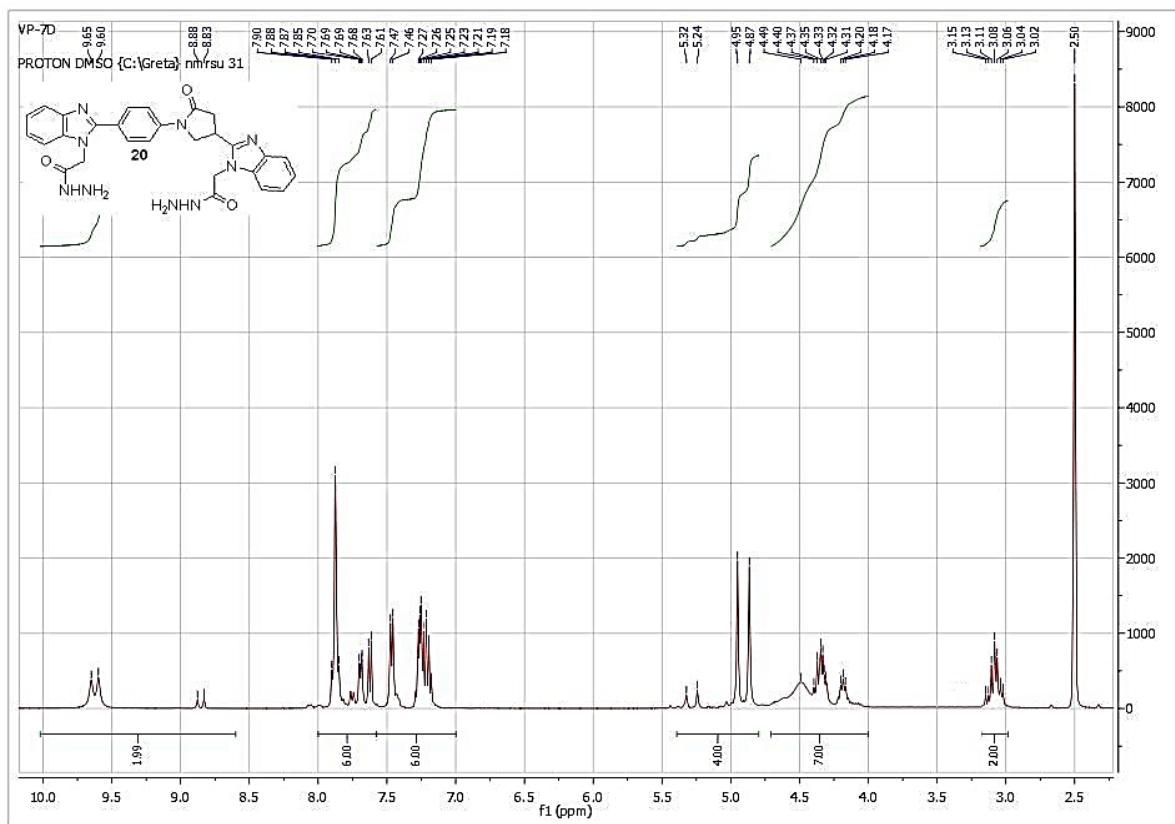


Figure S38: ¹H NMR of compound 20

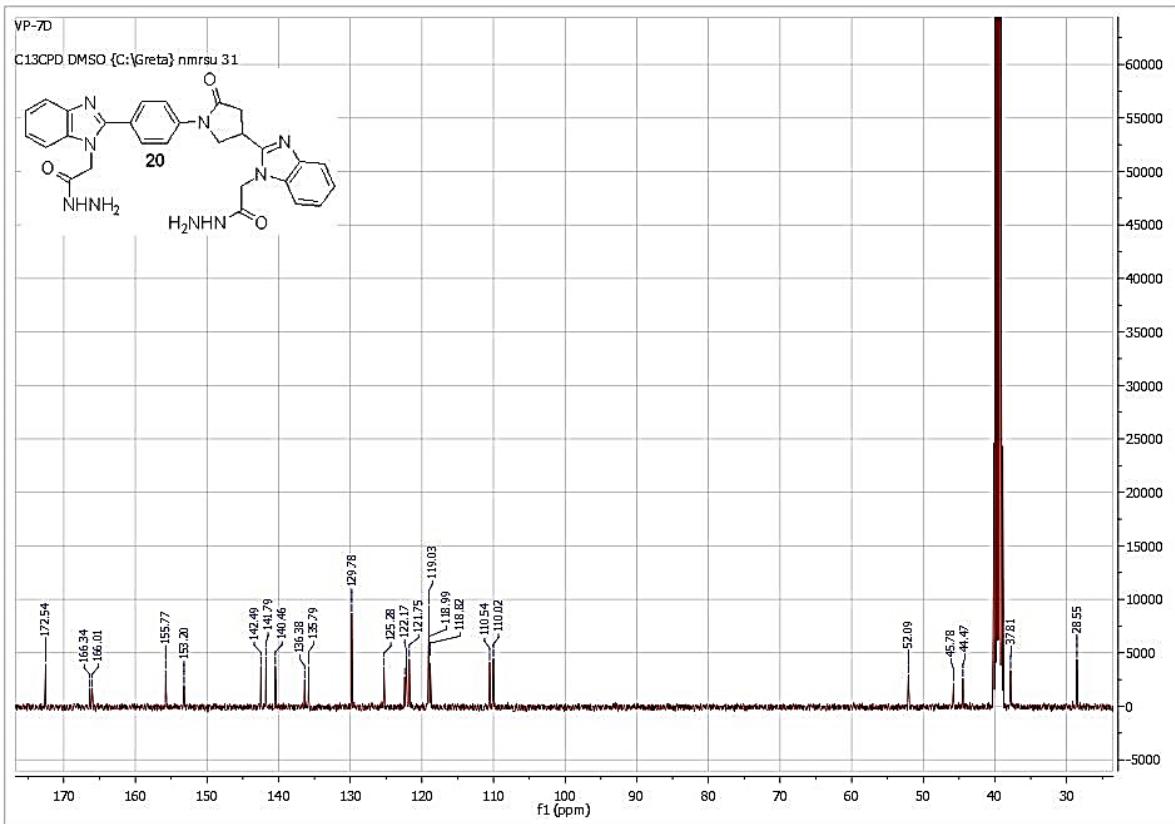


Figure S39: ¹³C NMR of compound 20

4-(1-(2-(3,5-dimethyl-1H-pyrazol-1-yl)-2-oxoethyl)-1H-benzimidazol-2-yl)-1-(4-(1-(3,5-dimethyl-1H-pyrazol-1-yl)-2-oxoethyl)-1H-benzimidazol-2-yl)phenylpyrrolidin-2-one 21

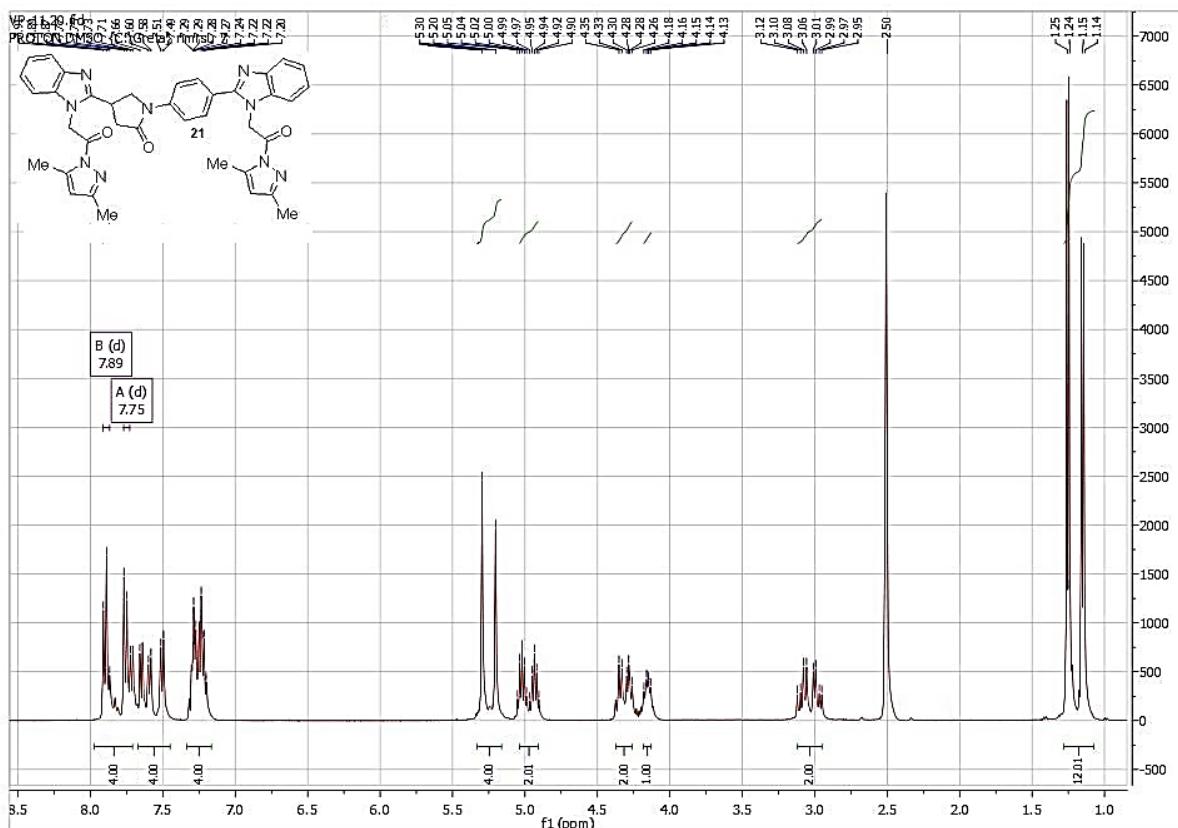


Figure S40: ¹H NMR of compound 21

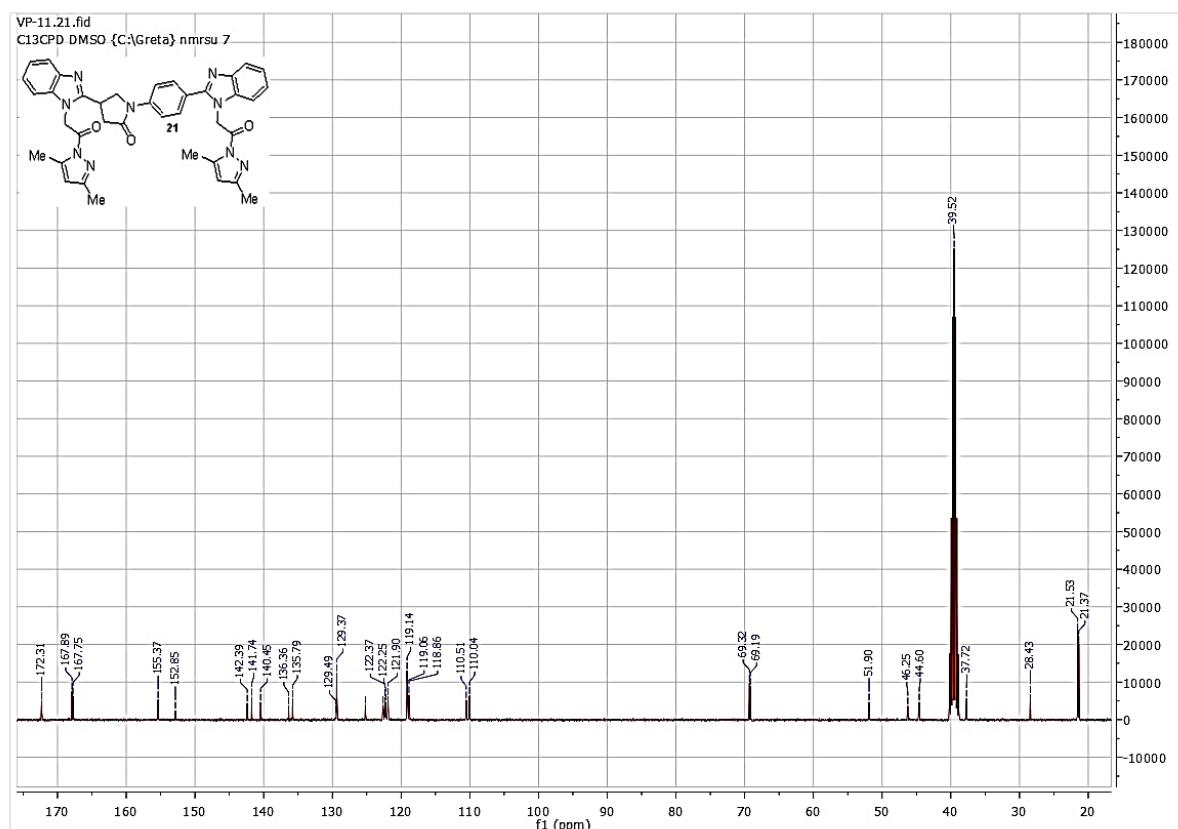


Figure S41: ¹³C NMR of compound 21

4-(1-((5-thioxo-4,5-dihydro-1,3,4-oxadiazol-2-yl)methyl)-1H-benzo[d]imidazol-2-yl)-1-(4-((5-thioxo-4,5-dihydro-1,3,4-oxadiazol-2-yl)methyl)-1H-benzo[d]imidazol-2-yl)phenyl)pyrrolidin-2-one
22

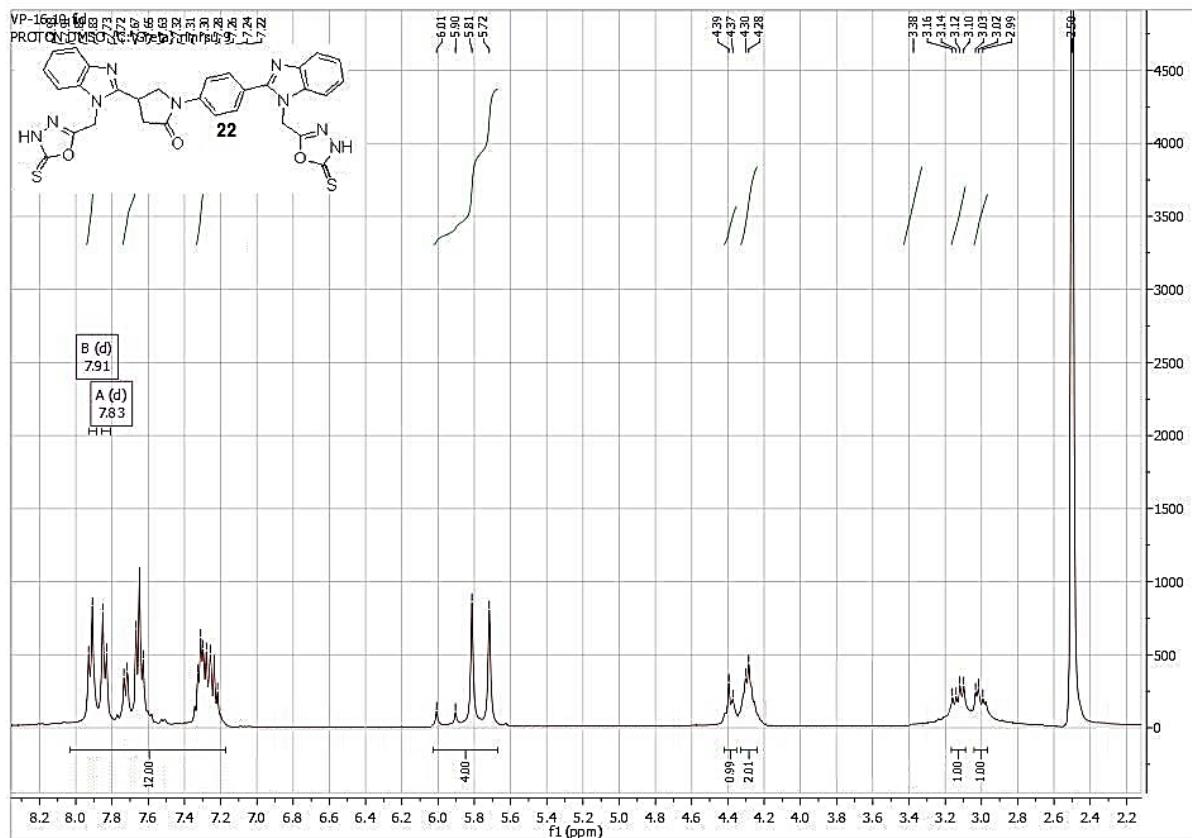


Figure S42: ¹H NMR of compound 22

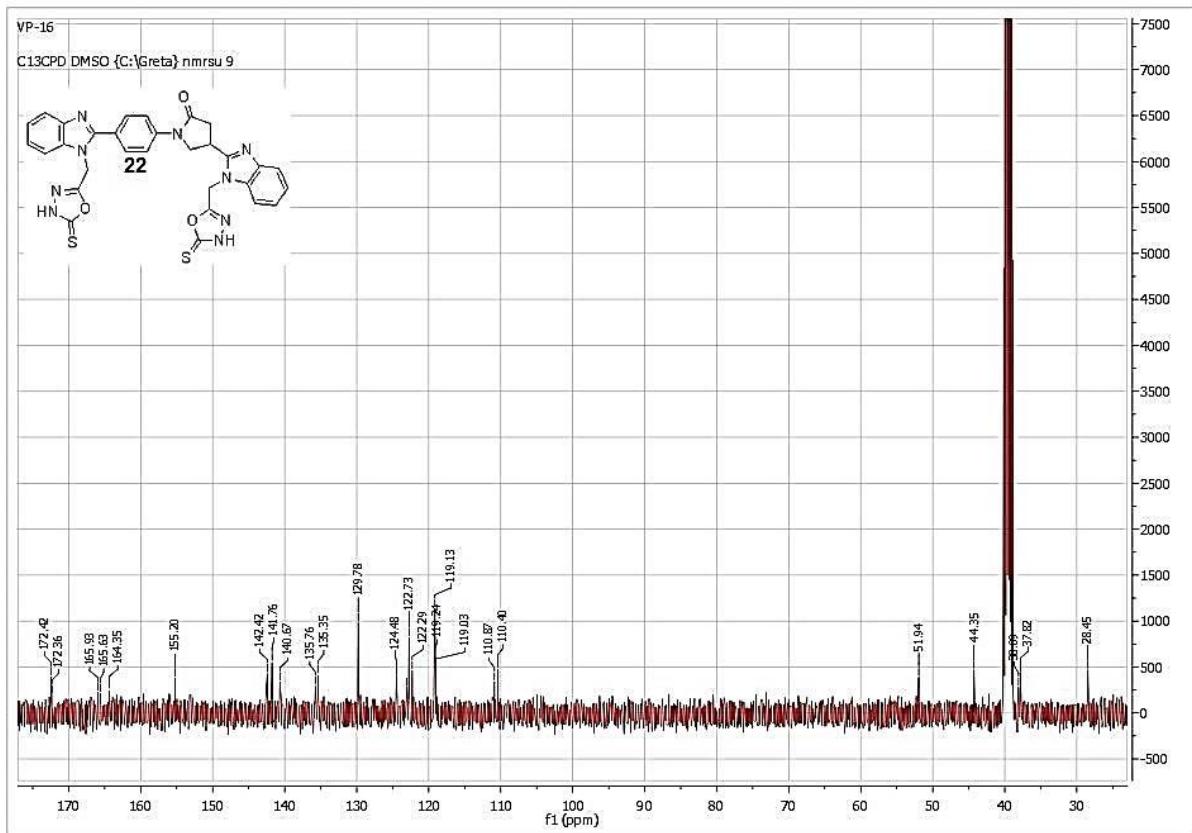


Figure S43: ¹³C NMR of compound 22

2-(2-(2-(5-oxo-1-(4-(1-(2-oxo-2-(2-(phenylcarbamothioyl)hydrazinyl)ethyl)-1H-benzimidazol-2-yl)phenyl)pyrrolidin-3-yl)-1H-benzimidazol-1-yl)acetyl)-N-phenylhydrazin-1-carbothioamide 23

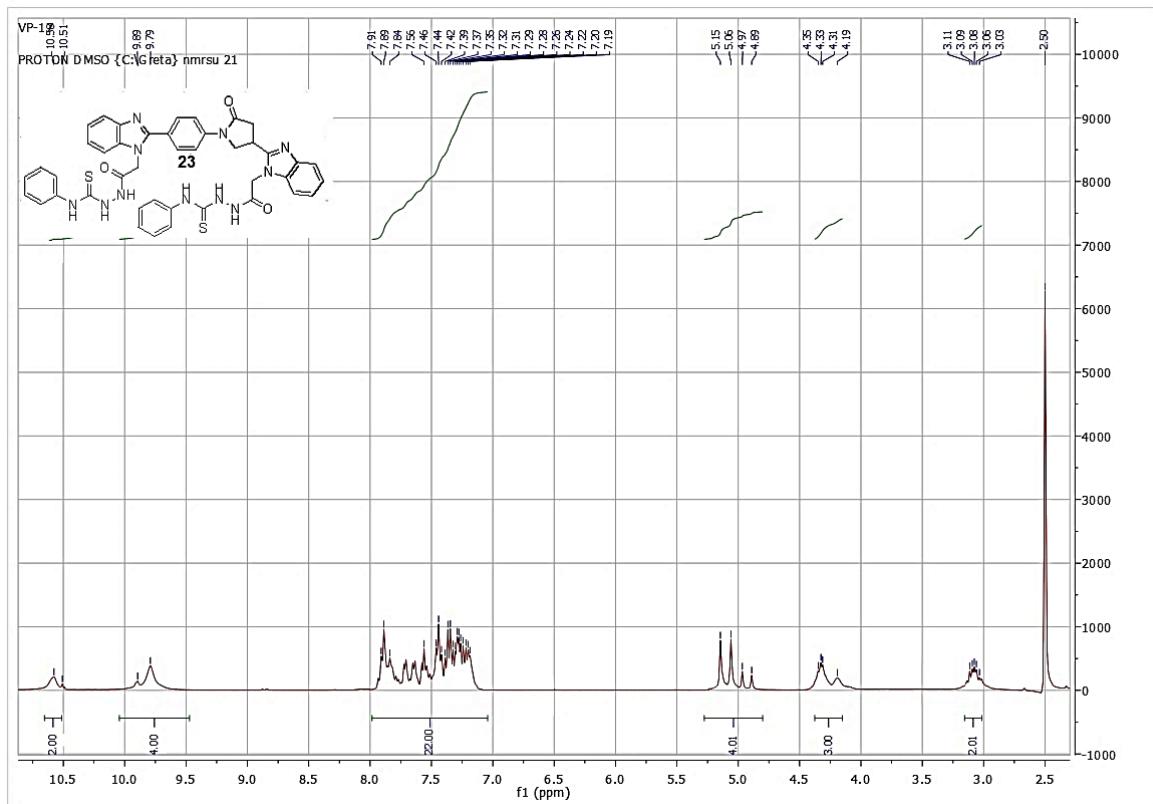


Figure S44: ^1H NMR of compound 23

N'-benzylidene-2-(2-(4-(1-(2-(benzylidene)hydrazinyl)-2-oxoethyl)-1H-benzo[d]imidazol-2-yl)-2-oxopyrrolidin-1-yl)phenyl)-1H-benzo[d]imidazol-1-ylacetohydrazide 24a

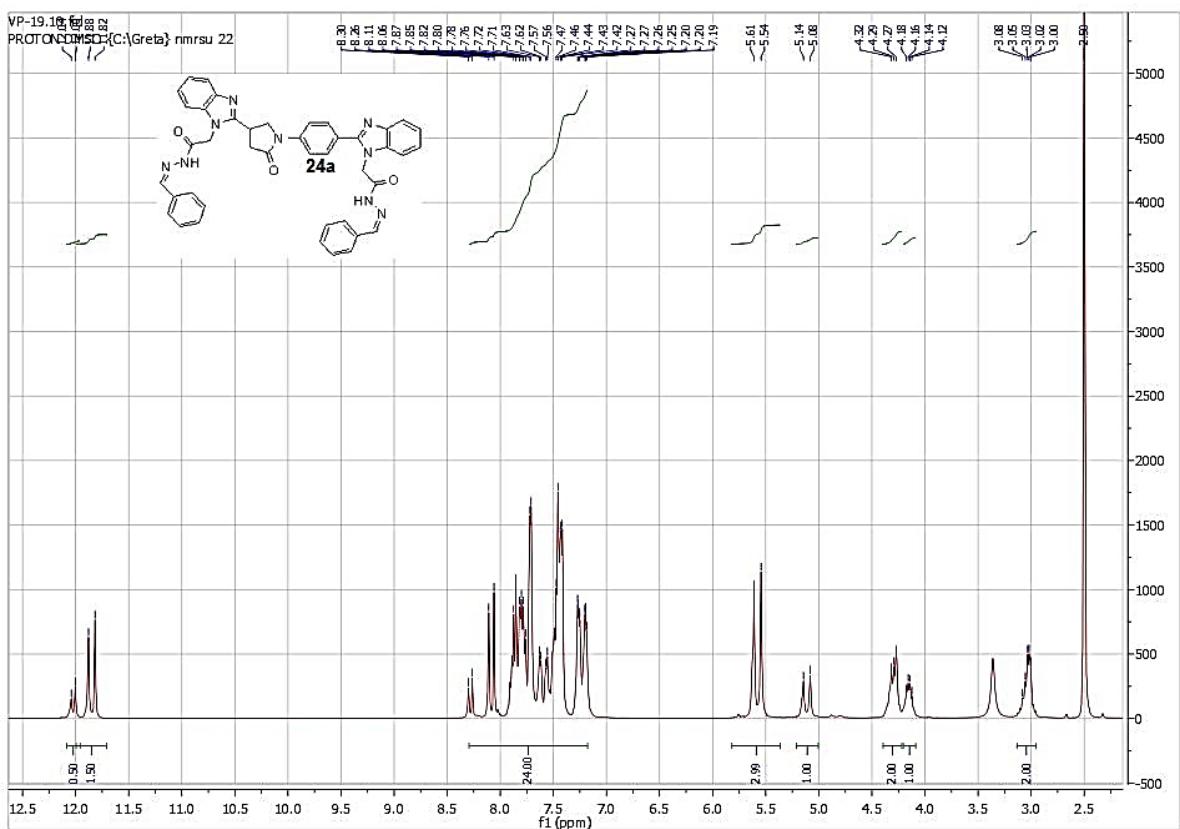


Figure S45: ^1H NMR of compound 24a

N'-4-nitrobenzylidene-2-(2-(4-(1-(2-(4-nitrobenzylidene)hydrazinyl)-2-oxoethyl)-1H-benzo[d]imidazol-2-yl)-2-oxopyrrolidin-1-yl)phenyl)-1H-benzo[d]imidazol-1-yl)acetohydrazide 24b

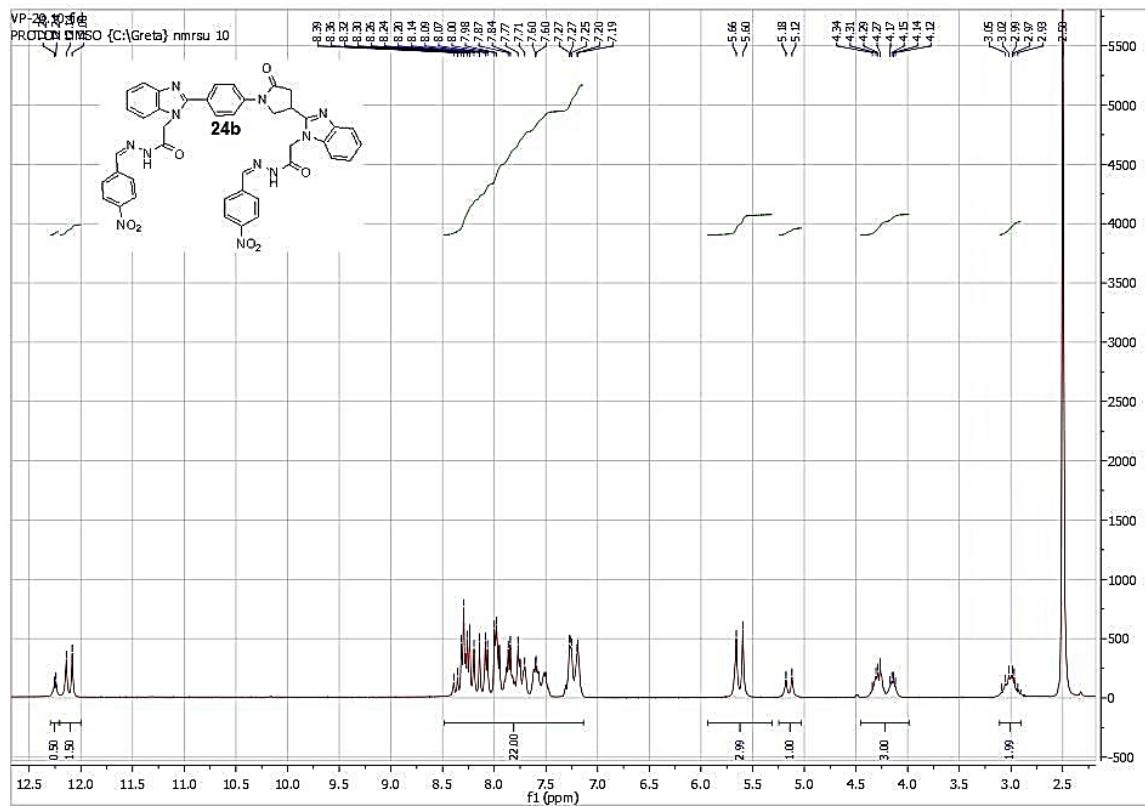


Figure S46: ^1H NMR of compound 24b

N'-(4-fluorobenzylidene)-2-(2-(4-(1-(2-(4-fluorobenzylidene)hydrazinyl)-2-oxoethyl)-1H-benzo[d]imidazol-2-yl)-2-oxopyrrolidin-1-yl)phenyl)-1H-benzo[d]imidazol-1-yl)acetohydrazide 24c

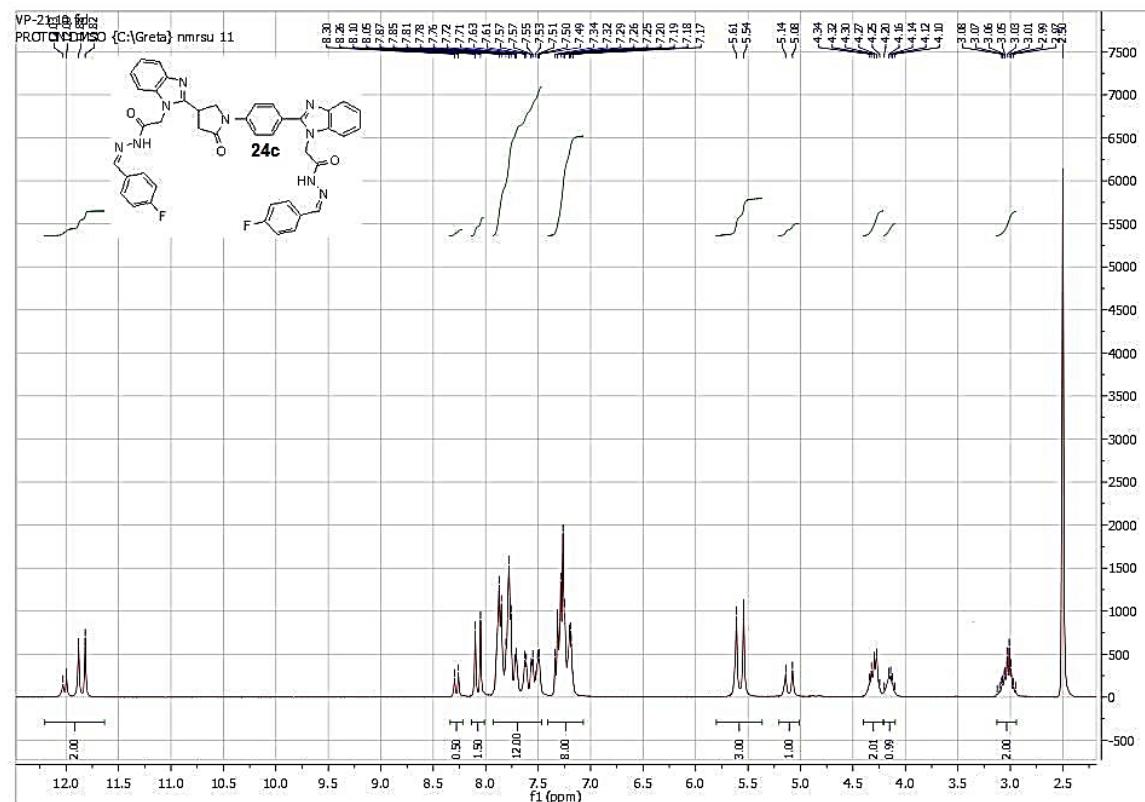


Figure S47: ^1H NMR of compound 24c

N'-3-chlorobenzylidene)-2-(2-(4-(1-(2-(3-chlorobenzylidene)hydrazinyl)-2-oxoethyl)-1H-benzo[d]imidazol-2-yl)-2-oxopyrrolidin-1-yl)phenyl)-1H-benzo[d]imidazol-1-yl)acetohydrazide 24d

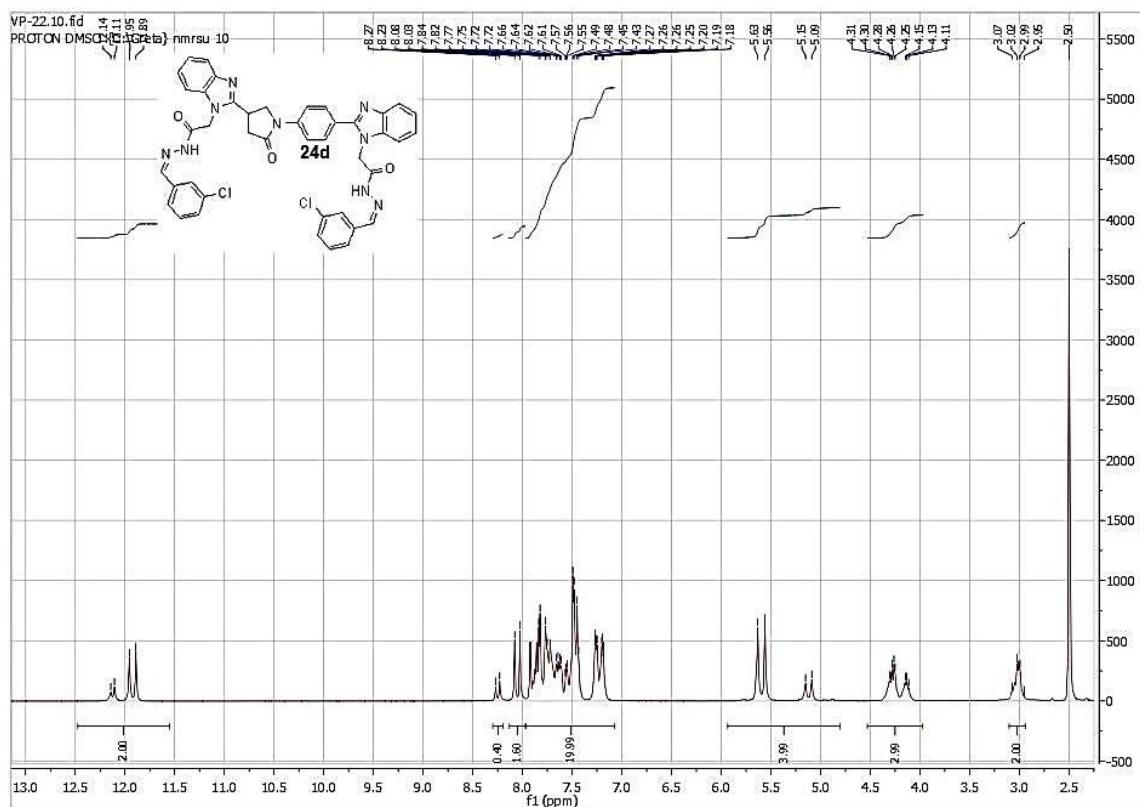


Figure S48: ¹H NMR of compound 24d

N'-(2,3-dimethoxybenzylidene)-2-(2-(4-(1-(2-(2,3-dimethoxybenzylidene)hydrazinyl)-2-oxoethyl)-1H-benzo[d]imidazol-2-yl)-2-oxopyrrolidin-1-yl)phenyl)-1H-benzo[d]imidazol-1-yl)acetohydrazide 24e

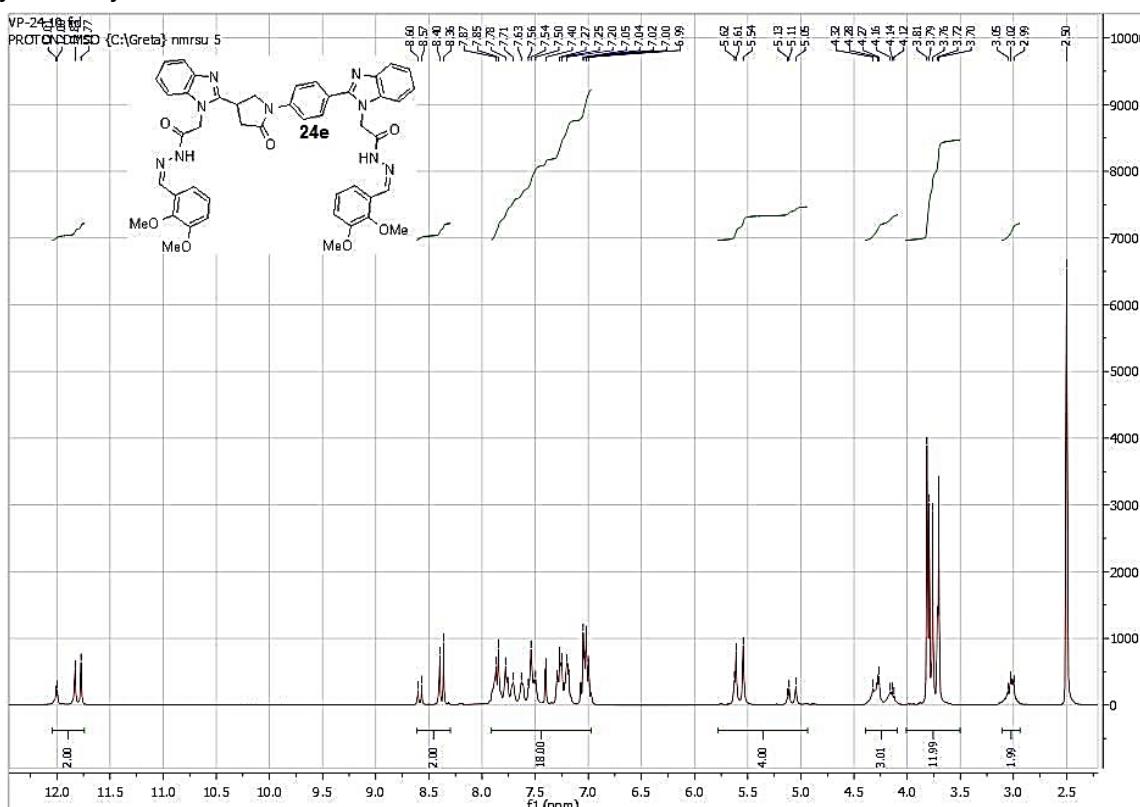


Figure S49: ¹H NMR of compound 24e

Supplementary table 1

Bacteria strains used in the biological evaluation

Organism	Strain number	Source
<i>Staphylococcus aureus</i>	ATCC 9144	ATCC ¹
<i>Listeria monocytogenes</i>	ATCC 7644	ATCC ¹
<i>Bacillus cereus</i>	ATCC 11778	ATCC ¹
<i>Escherichia coli</i>	ATCC 8739	ATCC ¹
<i>Pseudomonas aeruginosa</i>	NCTC 6750	NCTC ²
<i>Salmonella enteritidis</i>	ATCC 13076	ATCC ¹

^{1.} American Type Culture Collection.^{2.} National Collection of Type Cultures.