

SUPPLEMENTARY MATERIAL

2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5*H*-pyrrolo[3,4-*b*]pyridin-5-one

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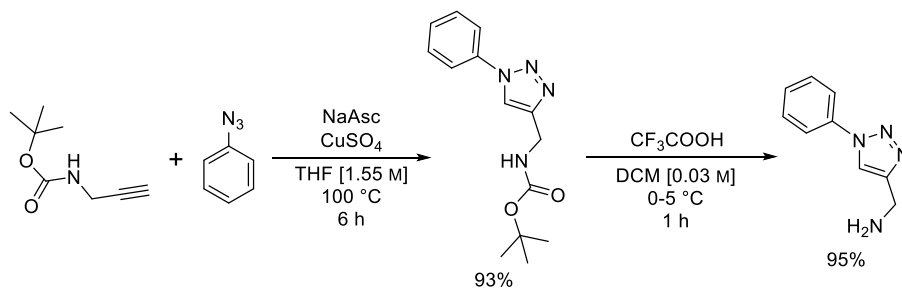
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TABLE OF CONTENTS

Content	Page
Synthesis of (1-phenyl-1 <i>H</i> -1,2,3-triazol-4-yl)methanamine (1)	S3
¹ H-NMR spectrum of (1-phenyl-1 <i>H</i> -1,2,3-triazol-4-yl)methanamine (1)	S3
¹³ C-NMR spectrum of (1-phenyl-1 <i>H</i> -1,2,3-triazol-4-yl)methanamine (1)	S4
Synthesis of 2-isocyano-1-morpholino-3-phenylpropan-1-one (3)	S4
¹ H-NMR spectrum of 2-isocyano-1-morpholino-3-phenylpropan-1-one (3)	S5
¹³ C-NMR spectrum of 2-isocyano-1-morpholino-3-phenylpropan-1-one (3)	S5
¹ H-NMR spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1 <i>H</i> -1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5 <i>H</i> -pyrrolo[3,4- <i>b</i>]pyridin-5-one (5)	S6
¹³ C-NMR spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1 <i>H</i> -1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5 <i>H</i> -pyrrolo[3,4- <i>b</i>]pyridin-5-one (5)	S7
2D-NMR (COSY-part I) spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1 <i>H</i> -1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5 <i>H</i> -pyrrolo[3,4- <i>b</i>]pyridin-5-one (5)	S8
2D-NMR (COSY-part II) spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1 <i>H</i> -1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5 <i>H</i> -pyrrolo[3,4- <i>b</i>]pyridin-5-one (5)	S8
2D-NMR (COSY-part III) spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1 <i>H</i> -1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5 <i>H</i> -pyrrolo[3,4- <i>b</i>]pyridin-5-one (5)	S9
2D-NMR (HSQC- part I) spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1 <i>H</i> -1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5 <i>H</i> -pyrrolo[3,4- <i>b</i>]pyridin-5-one (5)	S9
2D-NMR (HSQC- part II) spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1 <i>H</i> -1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5 <i>H</i> -pyrrolo[3,4- <i>b</i>]pyridin-5-one (5)	S10
2D-NMR (HSQC- part III) spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1 <i>H</i> -1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5 <i>H</i> -pyrrolo[3,4- <i>b</i>]pyridin-5-one (5)	S11
2D-NMR (HMBC-part I) spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1 <i>H</i> -1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5 <i>H</i> -pyrrolo[3,4- <i>b</i>]pyridin-5-one (5)	S12
2D-NMR (HMBC-part II) spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1 <i>H</i> -1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5 <i>H</i> -pyrrolo[3,4- <i>b</i>]pyridin-5-one (5)	S13
2D-NMR (HMBC-part III) spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1 <i>H</i> -1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5 <i>H</i> -pyrrolo[3,4- <i>b</i>]pyridin-5-one (5)	S14
2D-NMR (HMBC-part IV) spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1 <i>H</i> -1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5 <i>H</i> -pyrrolo[3,4- <i>b</i>]pyridin-5-one (5)	S15
¹⁵ N-NMR spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1 <i>H</i> -1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5 <i>H</i> -pyrrolo[3,4- <i>b</i>]pyridin-5-one (5)	S16
HRMS spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1 <i>H</i> -1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5 <i>H</i> -pyrrolo[3,4- <i>b</i>]pyridin-5-one (5)	S17
FT-IR spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1 <i>H</i> -1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5 <i>H</i> -pyrrolo[3,4- <i>b</i>]pyridin-5-one (5)	S17

For the synthesis of the (1-phenyl-1*H*-1,2,3-triazol-4-yl)methanamine (**1**), the commercially available *N*-Boc protected propargylamine was reacted with azidobenzene to obtain the corresponding *tert*-butyl((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)carbamate. Then, using trifluoroacetic acid, the later one is deprotected just before being used to give the (1-phenyl-1*H*-1,2,3-triazol-4-yl)methanamine (**1**) (**Scheme S1**). The overall yield was 88%.



Scheme S1. Synthesis of (1-phenyl-1*H*-1,2,3-triazol-4-yl)methanamine (**1**)

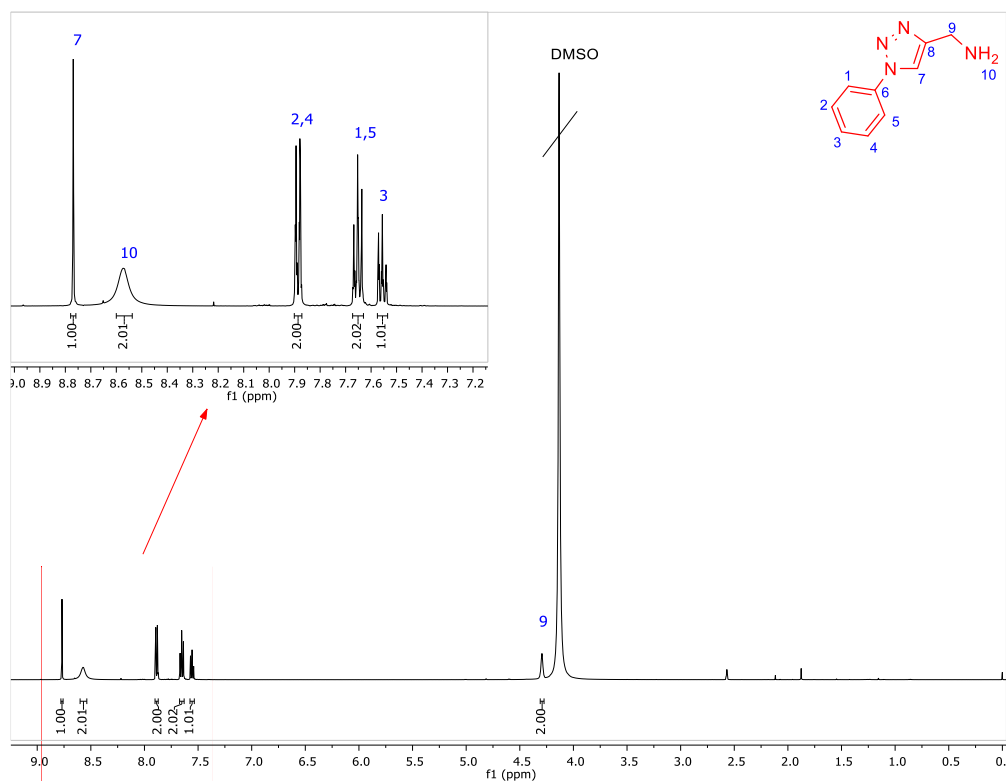


Figure S1. ¹H NMR (500 MHz, DMSO) spectrum of (1-phenyl-1*H*-1,2,3-triazol-4-yl)methanamine (**1**)

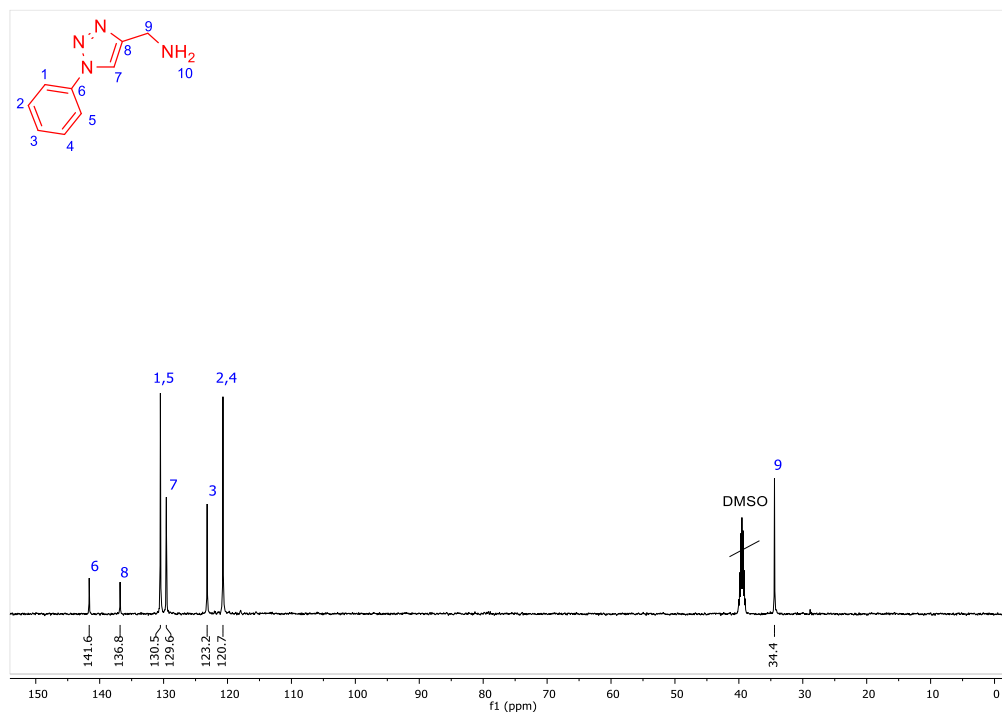
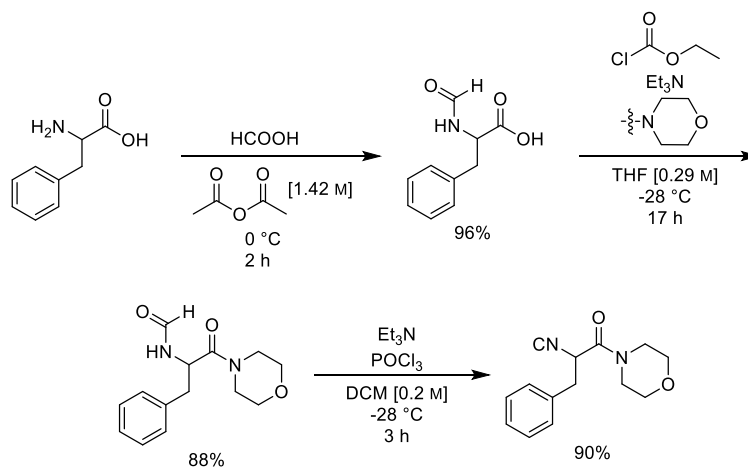


Figure S2. ^{13}C NMR (125 MHz, DMSO) spectrum of (1-phenyl-1H-1,2,3-triazol-4-yl)methanamine (**1**)

The preparation of the 2-isocyano-1-morpholino-3-phenylpropan-1-one (**3**) was carried out by formylation of racemic phenylalanine in formic acid and acetic anhydride, followed by a peptide coupling with morpholine using ethyl chloroformate as coupling agent in anhydrous THF at low temperature, and finally an Ugi-type dehydration with POCl_3 also at low temperature (**Scheme S2**). The overall yield was 76%.



Scheme S2. Synthesis of 2-isocyano-1-morpholino-3-phenylpropan-1-one (**3**)

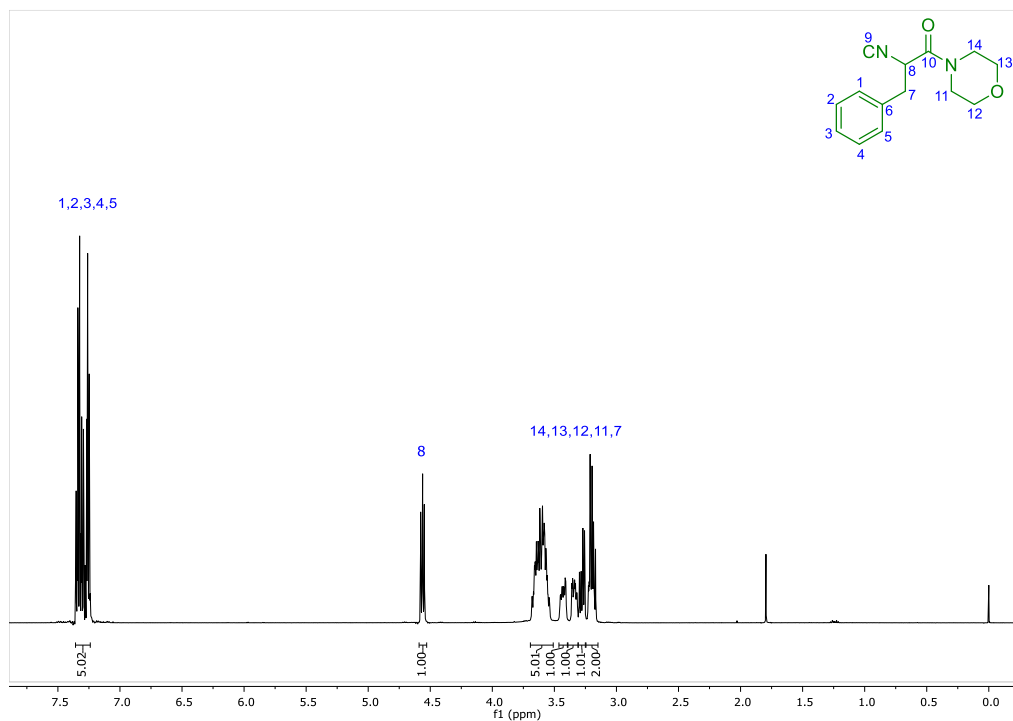


Figure S3. ¹H NMR (500 MHz, CDCl₃) spectrum of 2-isocyano-1-morpholino-3-phenylpropan-1-one (3)

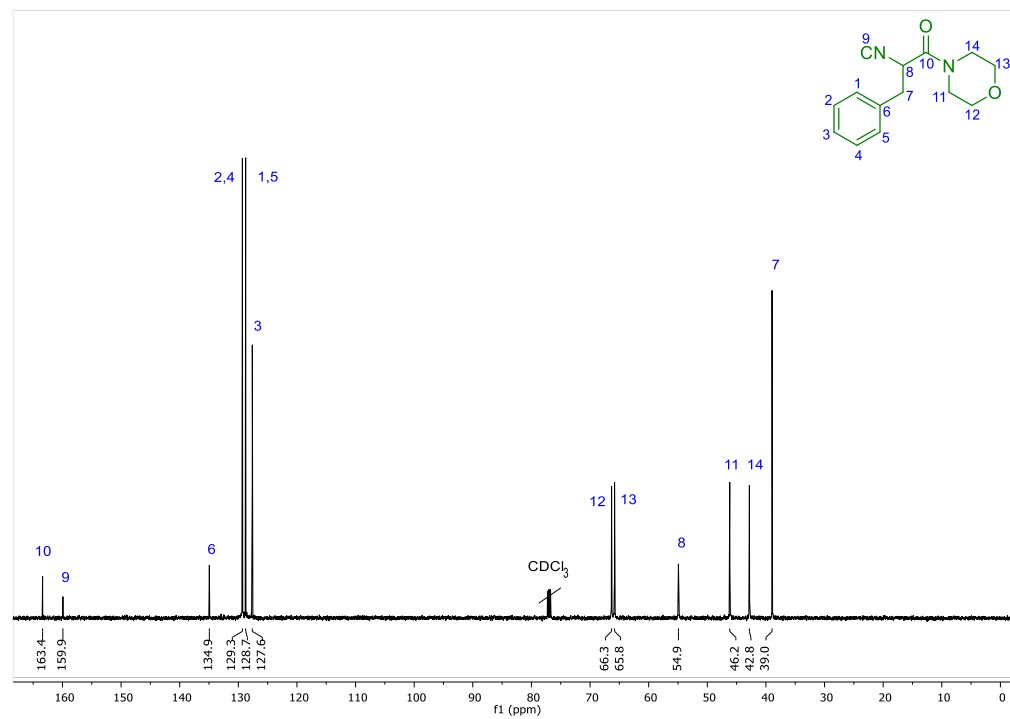


Figure S4. ¹³C NMR (125 MHz, CDCl₃) spectrum of 2-isocyano-1-morpholino-3-phenylpropan-1-one (3)

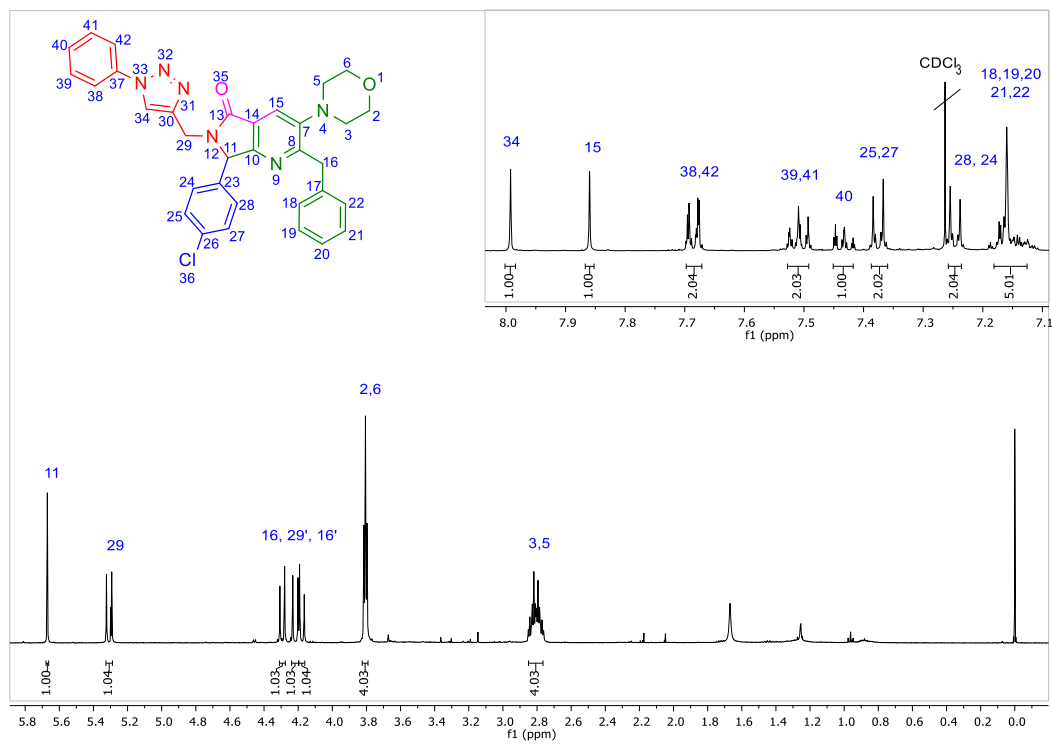


Figure S5. ¹H NMR (500 MHz, CDCl₃) spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5*H*-pyrrolo[3,4-*b*]pyridin-5-one (5)

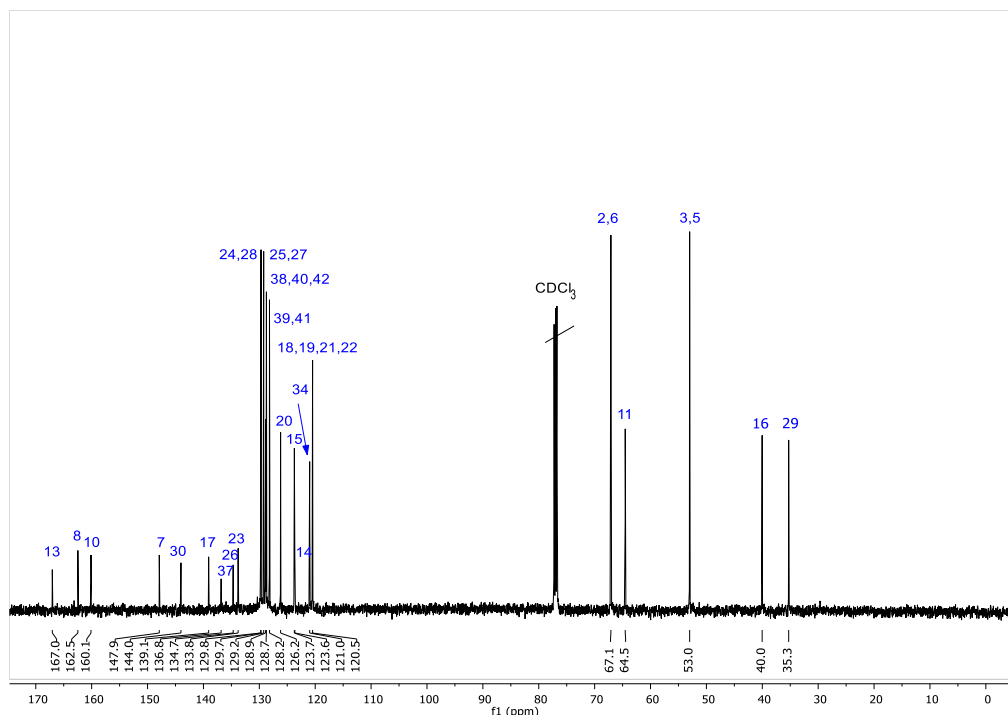
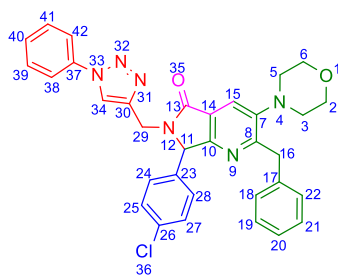


Figure S6. ^{13}C NMR (125 MHz, CDCl_3) spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1H-1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5H-pyrrolo[3,4-b]pyridin-5-one (5)

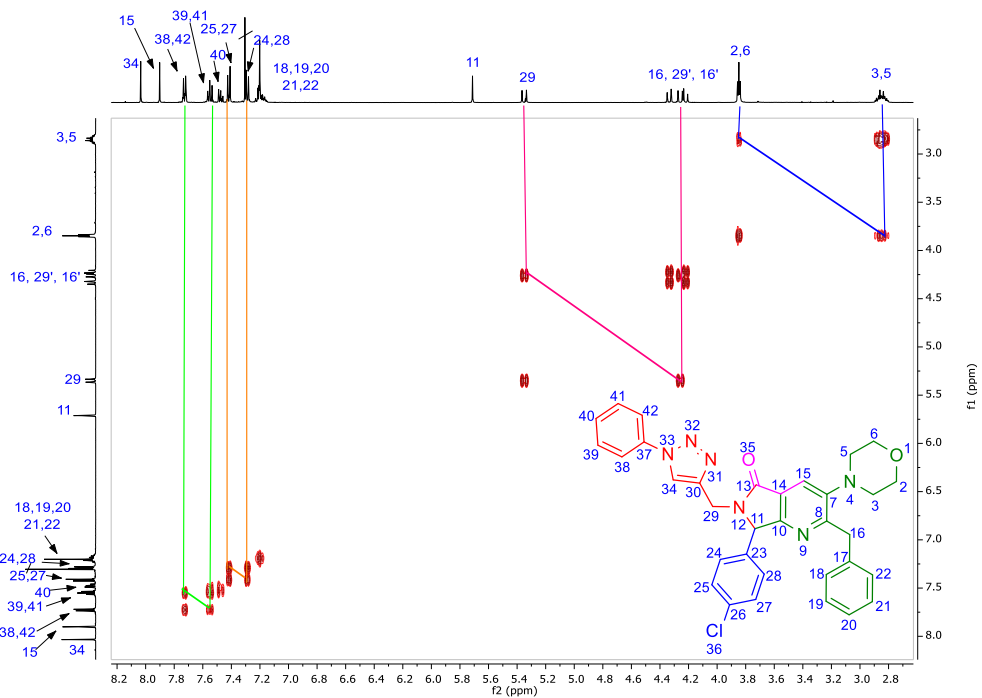


Figure S7. 2D-NMR (COSY-part I) spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5*H*-pyrrolo[3,4-*b*]pyridin-5-one (**5**)

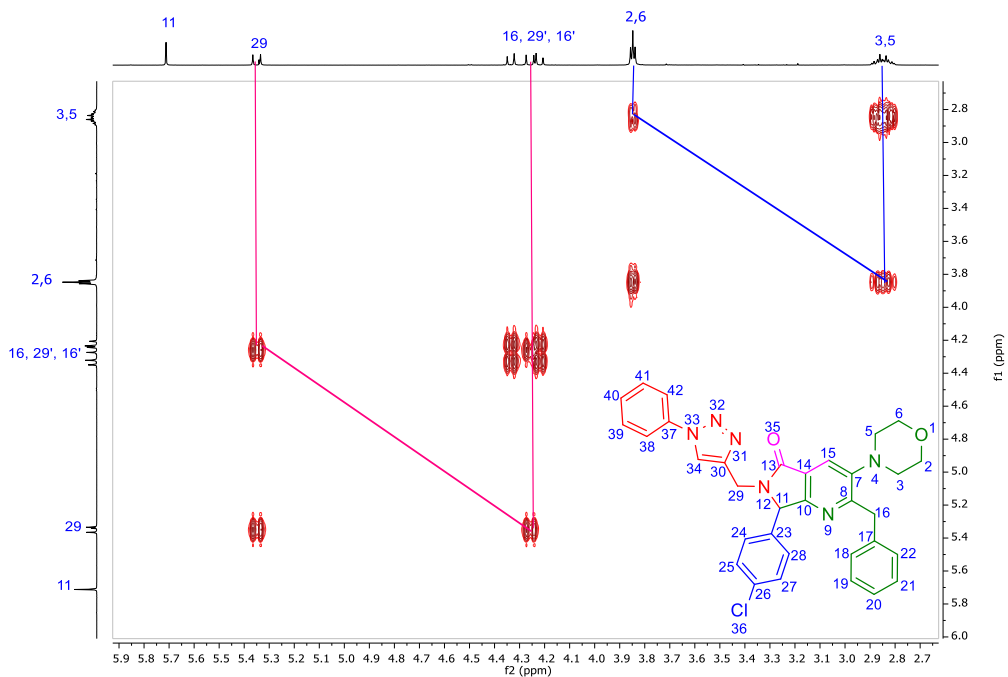


Figure S8. 2D-NMR (COSY-part II) spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5*H*-pyrrolo[3,4-*b*]pyridin-5-one (**5**)

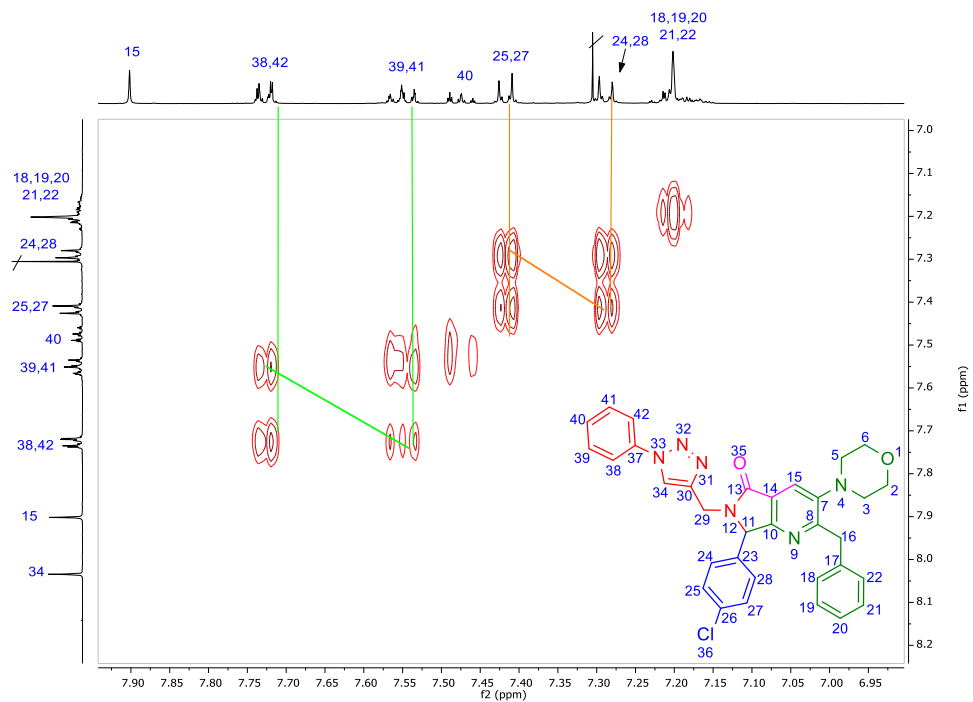


Figure S9. 2D-NMR (COSY-part III) spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5*H*-pyrrolo[3,4-*b*]pyridin-5-one (**5**)

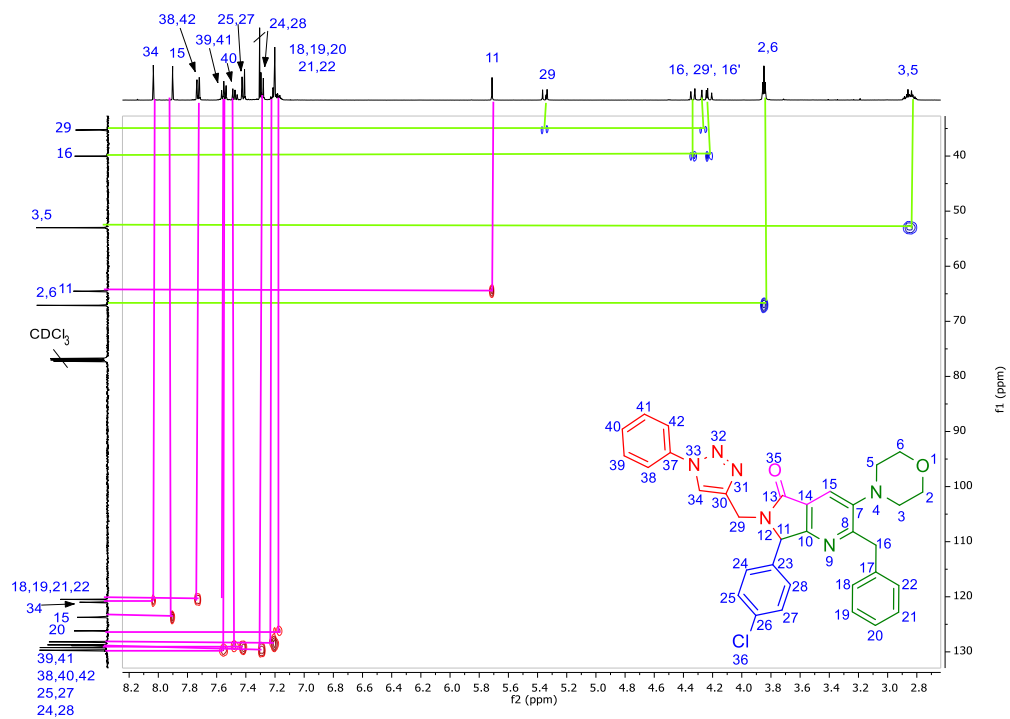


Figure S10. 2D-NMR (HSQC-part I) spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5*H*-pyrrolo[3,4-*b*]pyridin-5-one (**5**)

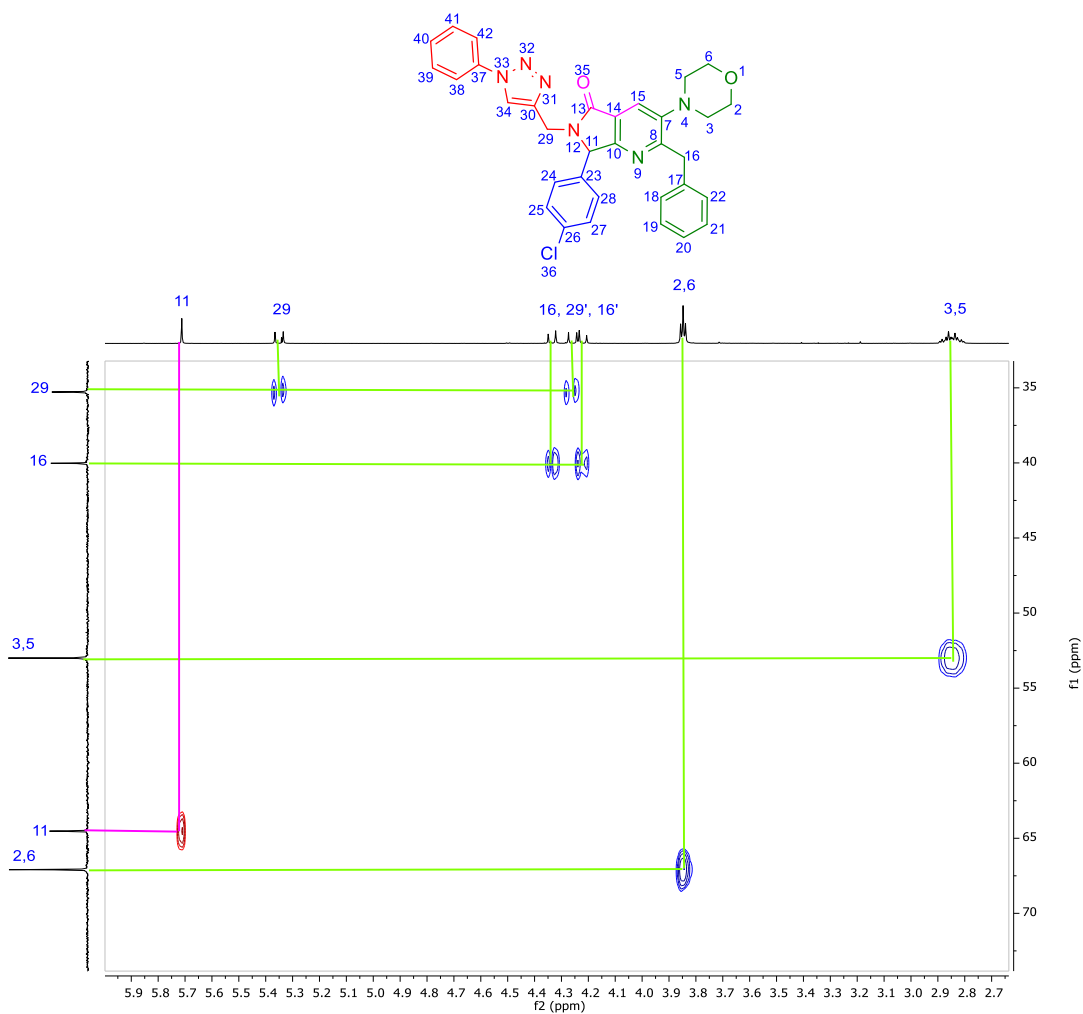


Figure S11. 2D-NMR (HSQC-part II) spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5*H*-pyrrolo[3,4-*b*]pyridin-5-one (5)

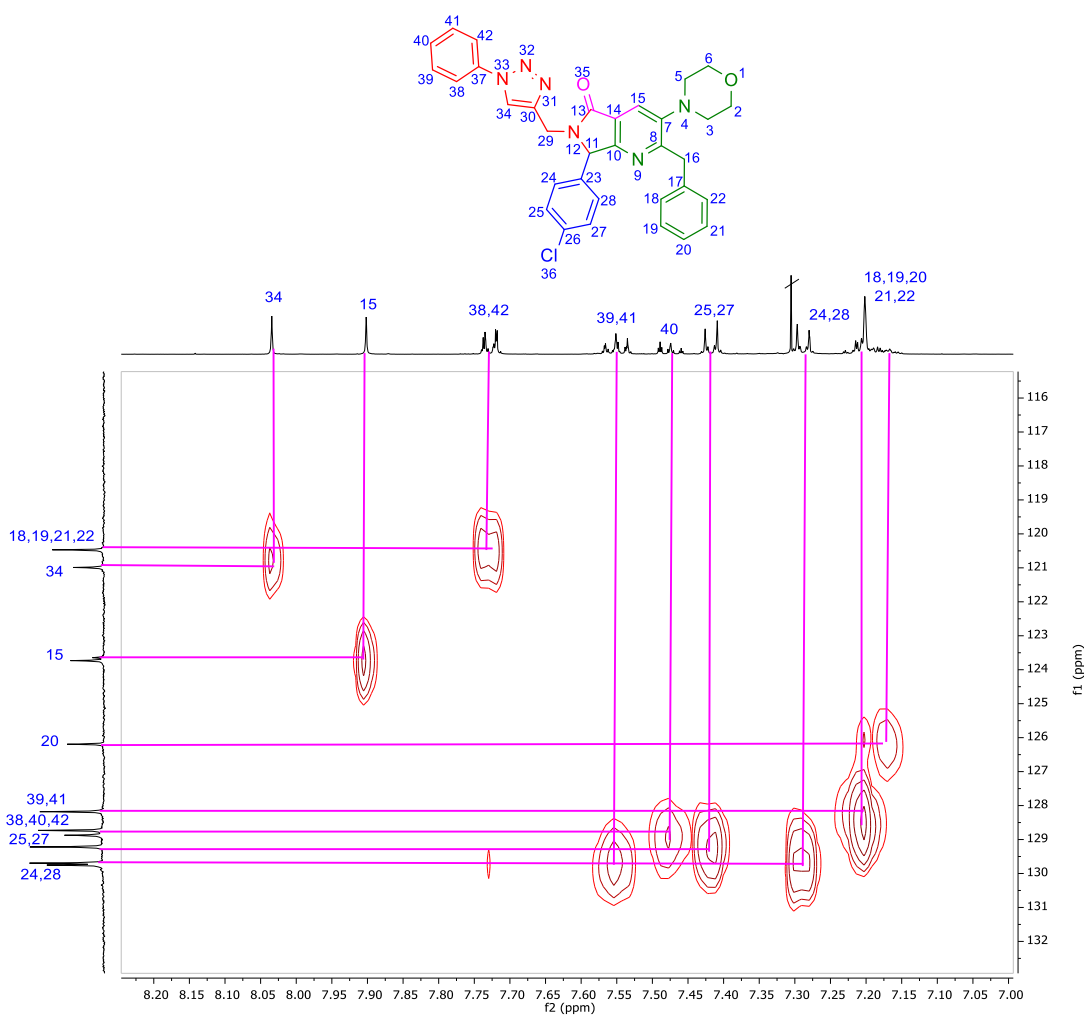


Figure S12. 2D-NMR (HSQC-part III) spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5*H*-pyrrolo[3,4-*b*]pyridin-5-one (**5**)

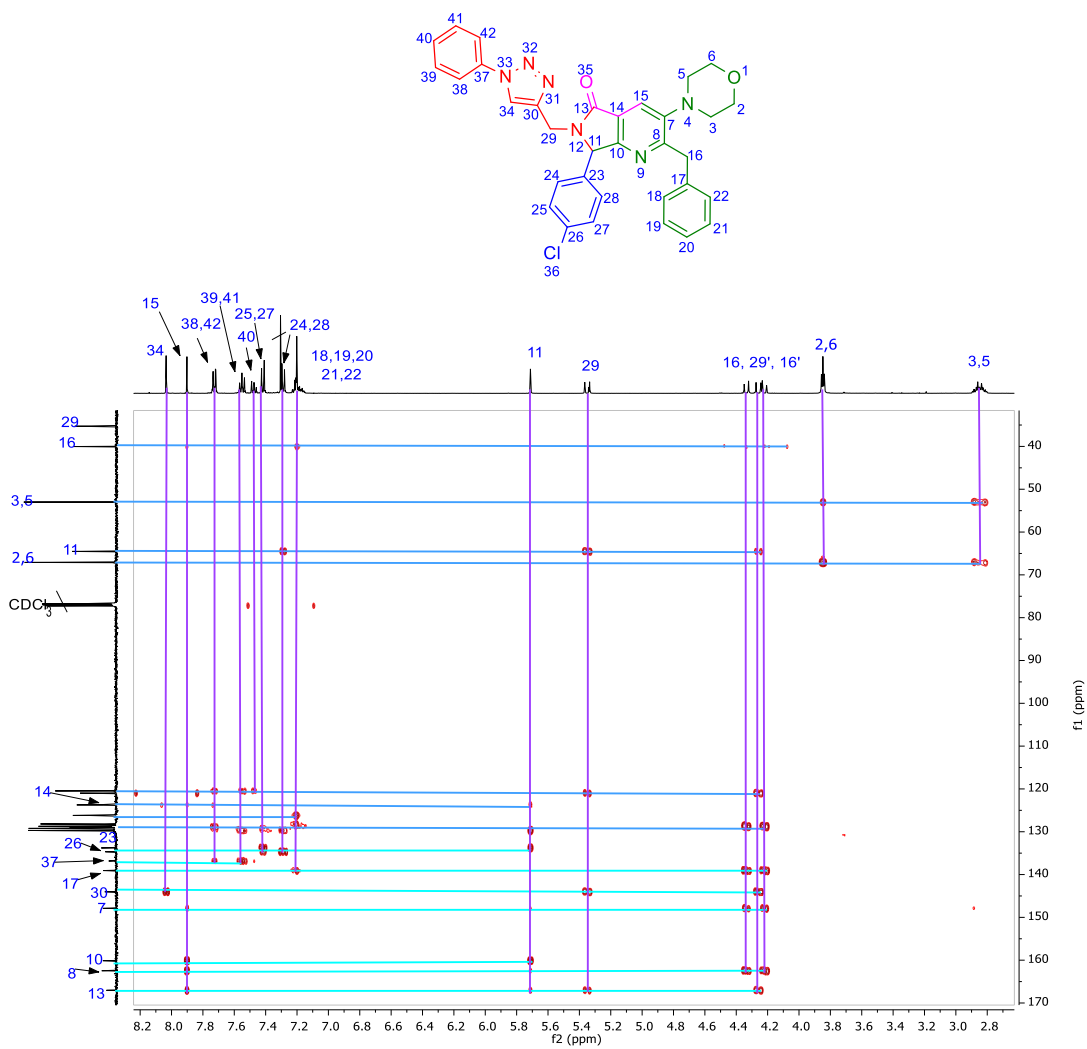


Figure S13. 2D-NMR (HMBC-part I) spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1H-1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5H-pyrrolo[3,4-b]pyridin-5-one (5)

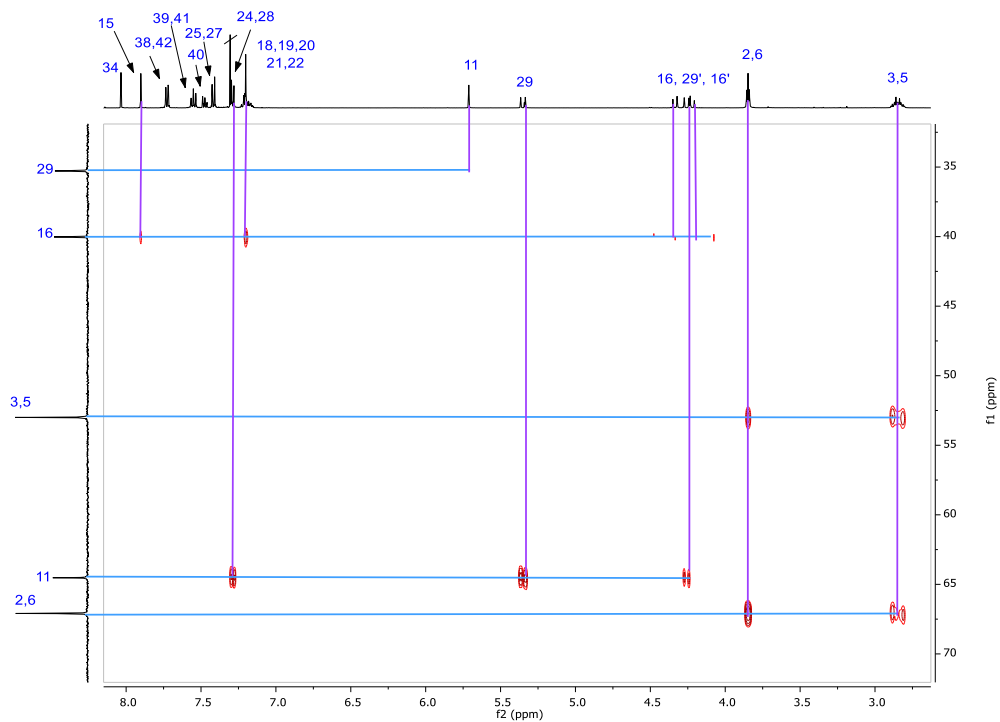
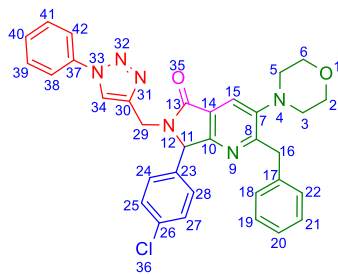


Figure S14. 2D-NMR (HMBC-part II) spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5*H*-pyrrolo[3,4-*b*]pyridin-5-one (**5**)

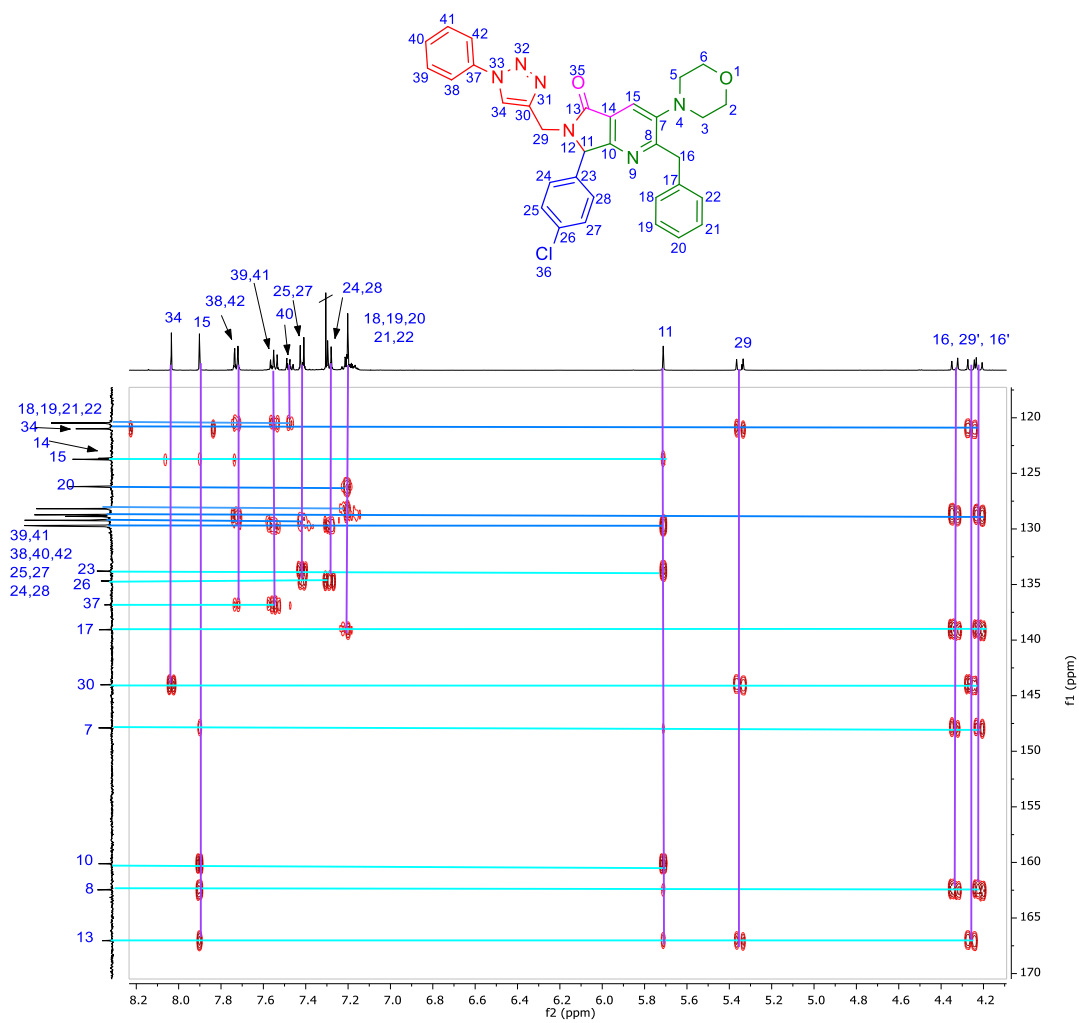


Figure S15. 2D-NMR (HMBC-part III) spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1H-1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5H-pyrrolo[3,4-b]pyridin-5-one (**5**)

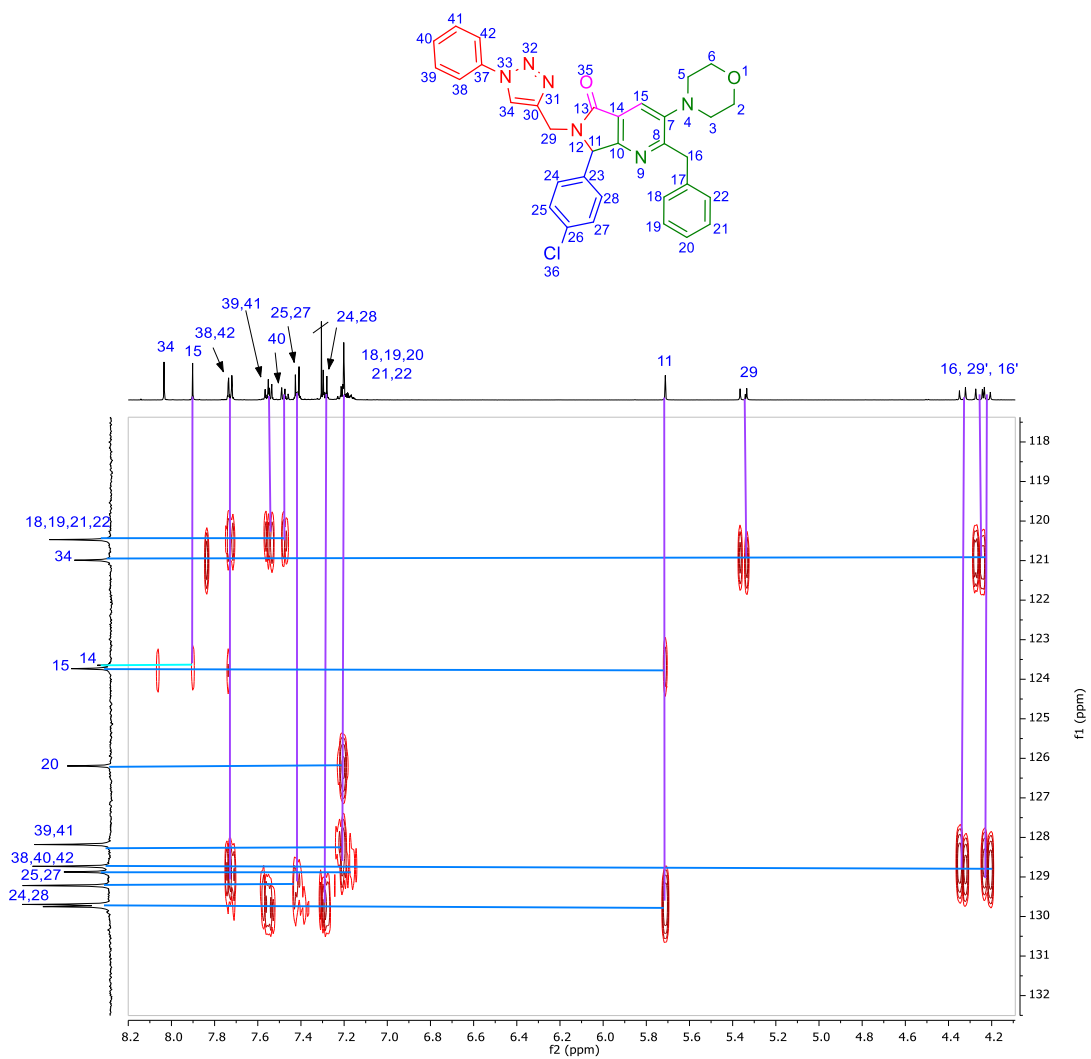


Figure S16. 2D-NMR (HMBC-part IV) spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1H-1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5H-pyrrolo[3,4-b]pyridin-5-one (5)

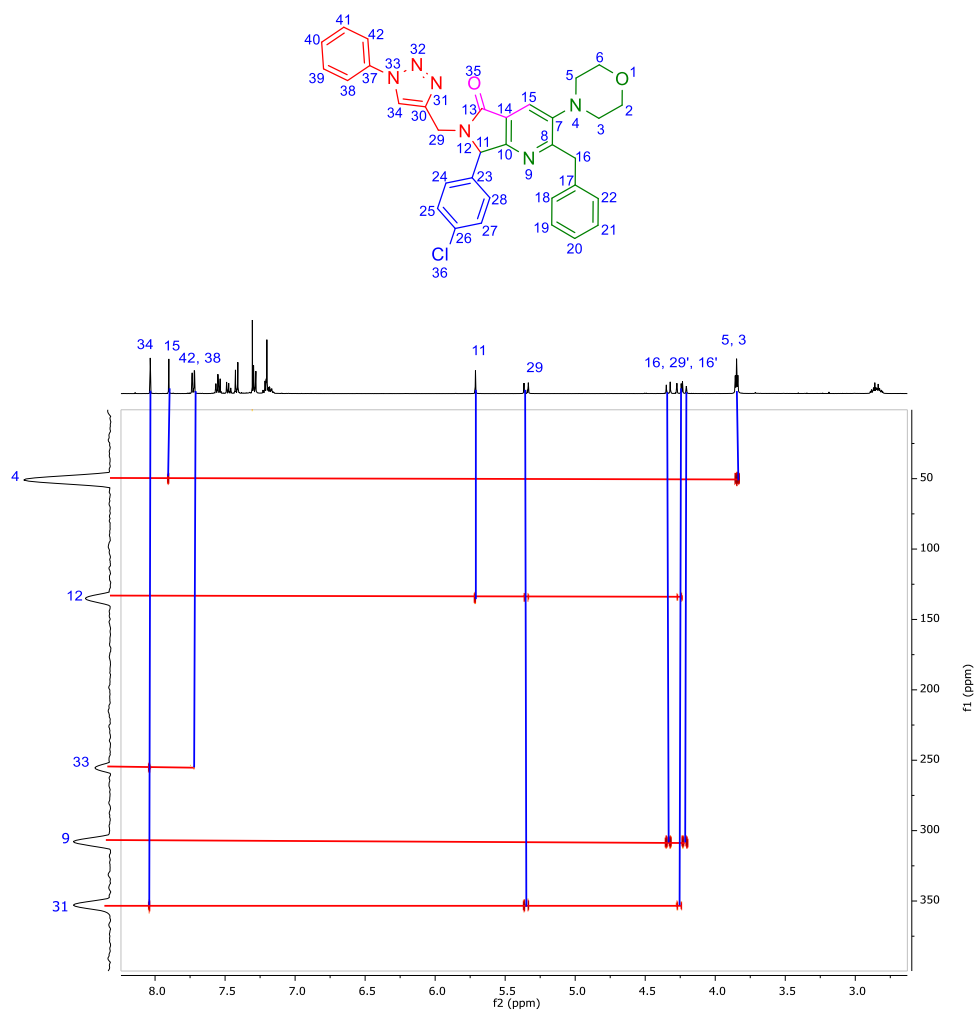


Figure S17. ^{15}N NMR HMBC spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5*H*-pyrrolo[3,4-*b*]pyridin-5-one (5)

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	150 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

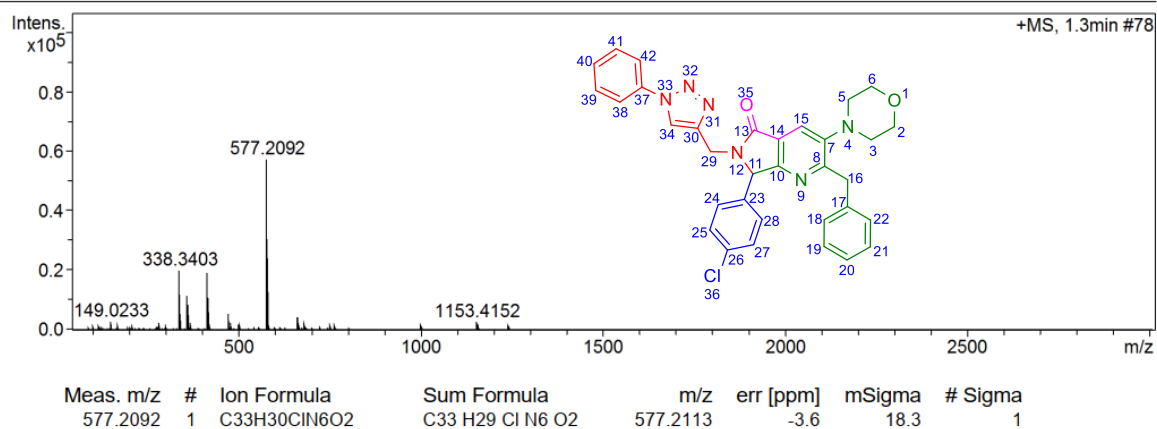


Figure S18. HRMS (ESI⁺-TOF) spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5*H*-pyrrolo[3,4-*b*]pyridin-5-one (5)

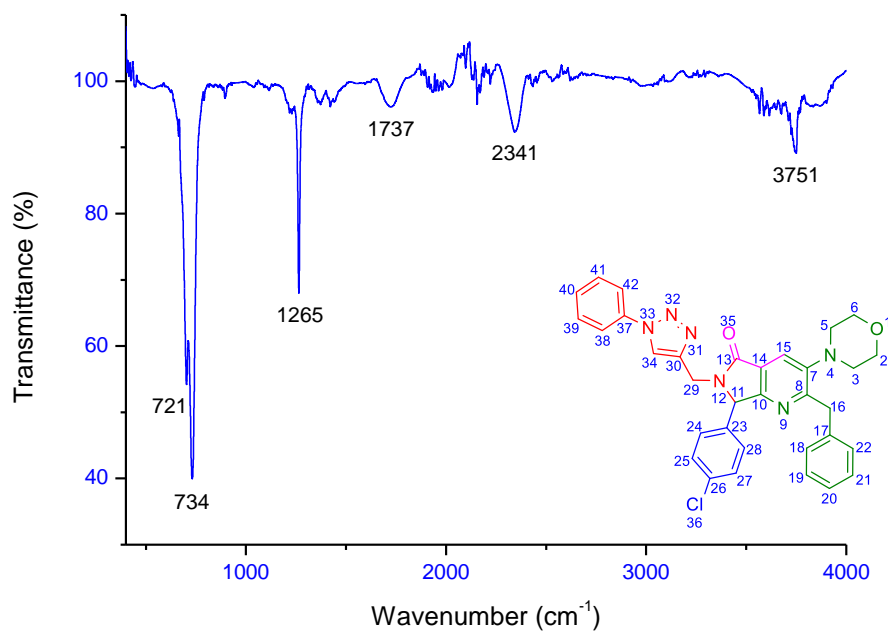


Figure S19. FT-IR (ATR) spectrum of 2-benzyl-7-(4-chlorophenyl)-3-morpholino-6-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)-6,7-dihydro-5*H*-pyrrolo[3,4-*b*]pyridin-5-one (5)