Supplementary Information

Streamlined Synthesis of 6-((1*H*-1,2,3-Triazol-4-yl)methyl)-1*H*-pyrrolo [3,4-*d*]pyridazin-1-one System via Sequential N-Alkylation, CuAAC, and [4 + 2] Cyclization Reactions

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X-ray diffraction of single crystals

The crystallographic parameters for **3a** and **8a** and details of data collection and refinement are listed on Tables S1 and S4. Selected bond and angles are listed on Tables S2 and S5. Interplanar angles between molecular fragments are listed in Tables S3 and S6, respectively.

Table S1. Crystal data and structure refinement parameters for 1-(prop-2-yn-1-yl)-1*H*-pyrrole (**3a**)

Empirical formula		$C_{18}H_{15}NO_3$
Formula weight		293.31
T / K		293(2)
Radiation, λ / Å		1.54178
Crystal system, space group		monoclinic, *Cc*
Unit cell dimensions, *a*, *b*, *c* / Å		*a* = 10.3244(3)
		b = 19.9176(6)
		c = 8.2093(2)
α, *β*, *γ* / degree		*β* = 111.0900(10)
Volume / Å^3		1575.06(8)
Z, Calculated density / (g cm^{-3})		4, 1.237
Absorption coefficient / mm^{-1}		0.689
F(000)		616
Crystal size / mm		0.422 × 0.247 × 0.196
Theta range / degree		6.351 – 68.237
Index ranges		$-11 \le h \le 12$, $-16 \le k \le 23$, $-9 \le l \le 9$
Reflections collected		6152
Independent reflections		2375 [R_{int} = 0.0119]
Completeness to theta max.		95.1%
Max. and min. transmission		0.7531 and 0.7130
Refinement method		Full-matrix least-squares on F^2
Data / restraints / parameters		2375 / 2 / 203
Goodness-of-fit on F^2		1.087
Final *R* indices [$I > 2\sigma(I)$]		R_1 = 0.0312, wR_2 = 0.0882
R indices (all data)		R_1 = 0.0313, wR_2 = 0.0882
BASF	0.19207	
Extinction coeficient	0.033(5)	
Largest diff. peak and hole / (e Å^{-3})		0.234 and –0.099

Highest peak 0.234 (e Å^{-3}) at 0.8981 0.4918 0.2559 [0.98 Å from C(11)].

Deepest hole -0.099 (e Å^{-3}) at 0.5558 0.1040 0.0358 [0.74 Å from H(26)].

Table S2. Selected bond lengths and angles for 1-(prop-2-yn-1-yl)-1*H*-pyrrole (**3a**)

Bond distance / Å		Bond angle / degree	
C(2)-N(1)	1.396(2)	C(3)-C(2)-N(1)	106.62(17)
C(5)-N(1)	1.365(3)	C(2)-C(3)-C(4)	108.44(18)
C(2)-C(3)	1.370(3)	C(5)-C(4)-C(3)	106.95(19)
C(4)-C(5)	1.385(3)	N(1)-C(5)-C(4)	107.76(17)
C(3)-C(4)	1.427(3)	C(5)-N(1)-C(2)	110.22(17)
N(1)-C(11)	1.468(3)	O(311)-C(31)-O(32)	124.6(2)
C(11)-C(12)	1.466(3)	O(311)-C(31)-C(3)	124.8(2)
C(12)-C(13)	1.171(4)	O(32)-C(31)-C(3)	110.51(19)
C(3)-C(31)	1.483(3)	C(31)-O(32)-C(33)	115.8(3)
C(31)-O(311)	1.196(3)	O(411)-C(41)-C(4)	118.9(2)
C(31)-O(32)	1.330(3)	O(411)-C(41)-C(42)	119.6(3)
C(33)-O(32)	1.449(4)	C(4)-C(41)-C(42)	121.4(2)
C(4)-C(41)	1.471(3)	C(13)-C(12)-C(11)	178.4(3)
C(41)-O(411)	1.220(3)	N(1)-C(5)-C(51)	120.3(2)
C(41)-C42)	1.494(4)	C(4)-C(5)-C(51)	131.9(2)
		C(2)-N(1)-C(11)	124.38(17)

Table S3. Interplanar angles between molecular fragments of 1-(prop-2-yn-1-yl)-1*H*-pyrrole (**3a**)

Fragment	Interplanar angle with the central pyrrole ring / degree
Ethynyl H(13)C(13)C(12)C(11)-N(1)	80.0(2)
Phenyl C(26)-C(21)	44.61(7)
Methoxycarbonyl C(33)O(32)C(31)O(311)	76.7(10)
Acetyl C(42)C(41)(O411)	10.0(3)

Table S4. Crystal data and structure refinement parameters for 1-((1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrrole (**8a**)

Empirical formula	$C_{25}H_{24}N_4O_3$
Formula weight	428.48
T / K	100(2)
Radiation, λ / Å	0.56086
Crystal system, space group	triclinic, *P*(-1)
Unit cell dimensions, *a*, *b*, *c* / Å	*a* = 9.5258(4)
	b = 10.2250(4)
	c = 12.4371(5)
α, β, γ / degree	α = 107.5450(10)
	β = 91.3260(10)
	γ = 111.8490(10)
Volume / Å^3	1059.46(7)
Z, Calculated density / (g cm^{-3})	2, 1.343
Absorption coefficient / mm^{-1}	0.057
F(000)	452
Crystal size / mm	0.388 × 0.227 × 0.185
Theta range / degree	1.861 – 27.405
Index ranges	$-15 \le h \le 15$, $-16 \le k \le 16$, $-20 \le l \le 20$
Reflections collected	93896
Independent reflections	9793 [R_{int} = 0.0991]
Completeness to theta max.	99.8%
Max. and min. transmission	0.7145 and 0.7455
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9793 / 0 / 289
Goodness-of-fit on F^2	1.102
Final *R* indices [$I > 2\sigma(I)$]	R_1 = 0.0618, wR_2 = 0.1400
R indices (all data)	R_1 = 0.1290, wR_2 = 0.1680
Extinction coefficient	n/a
Largest diff. peak and hole / (e Å^{-3})	0.537 and –0.436

Highest peak 0.537 (e Å^{-3}) at 0.9386 0.3780 0.3553 [0.54 Å from H(41C)].

Deepest hole -0.436 (e Å^{-3}) at 0.9298 0.6827 0.3322 [1.10 Å from C(5)].

Table S5. Selected bond lengths and angles for 1-((1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrrole (**8a**)

Bond distance / Å		Bond angle / degree	
C(2)-N(1)	1.3811(17)	C(12)-C(16)	1.3738(18)
C(2)-C(3)	1.3854(17)	C(16)-N(15)	1.3530(17)
C(2)-C(21)	1.4808(18)	C(31)-O(311)	1.2178(15)
C(3)-C(4)	1.4381(18)	C(31)-O(32)	1.3379(15)
C(3)-C(31)	1.4661(18)	C(33)-O(32)	1.4504(17)
C(4)-C(5)	1.3832(18)	C(41)-O(412)	1.2234(17)
C(4)-C(41)	1.4775(18)	C(41)-C(411)	1.5118(19)
C(5)-N(1)	1.3782(17)	C(151)-N(15)	1.4740(17)
C(5)-C(51)	1.4883(19)	C(151)-C(152)	1.5100(19)
C(11)-N(1)	1.4575(17)	N(13)-N(14)	1.3209(17)
C(11)-C(12)	1.5007(18)	N(14)-N(15)	1.3444(17)
C(12)-N(13)	1.3603(17)		
N(1)-C(5)-C(51)	121.09(12)	C(4)-C(41)-C(411)	119.45(11)
C(4)-C(5)-C(51)	131.30(12)	N(15)-C(151)-C(152)	113.16(11)
N(1)-C(11)-C(12)	113.63(11)	C(5)-N(1)-C(2)	110.34(11)
N(13)-C(12)-C(16)	108.61(12)	C(5)-N(1)-C(11)	123.59(11)
N(13)-C(12)-C(11)	119.86(12)	C(2)-N(1)-C(11)	125.98(11)
C(16)-C(12)-C(11)	131.21(12)	N(14)-N(13)-C(12)	108.90(12)
N(15)-C(16)-C(12)	104.26(11)	N(13)-N(14)-N(15)	106.91(11)
O(311)-C(31)-O(32)	123.52(12)	N(14)-N(15)-C(16)	111.31(11)
O(311)-C(31)-C(3)	123.41(12)	N(14)-N(15)-C(151)	119.48(11)
O(32)-C(31)-C(3)	113.07(11)	C(16)-N(15)-C(151)	128.89(12)
O(412)-C(41)-C(4)	121.07(12)	C(31)-O(32)-C(33)	115.95(11)
O(412)-C(41)-C(411)	119.35(12)		

Table S6. Interplanar angles between molecular fragments of 1-((1*H*-1,2,3-triazol-4-yl)methyl)-1*H*-pyrrole (**8a**)

Fragment	Interplanar angle with the central pyrrole ring / degree
Triazole C(12)N(13)N(14)N(15)C(16)	82.26(5)
Phenyl C(26)-C(21)	60.43(6)
Methoxycarbonyl C(33)O(32)C(31)O(311)	25.58(7)
Acetyl C(411)C(41)(O412)	37.8(12)
Phenyl C(152)-C(157)	33.36(6)
	Interplanar angle with the triazole ring -C(12)N(13)N(14)N(15)C(16)
Phenyl C(152)-C(157)	74.85(5)

^{1}H and ^{13}C NMR spectra

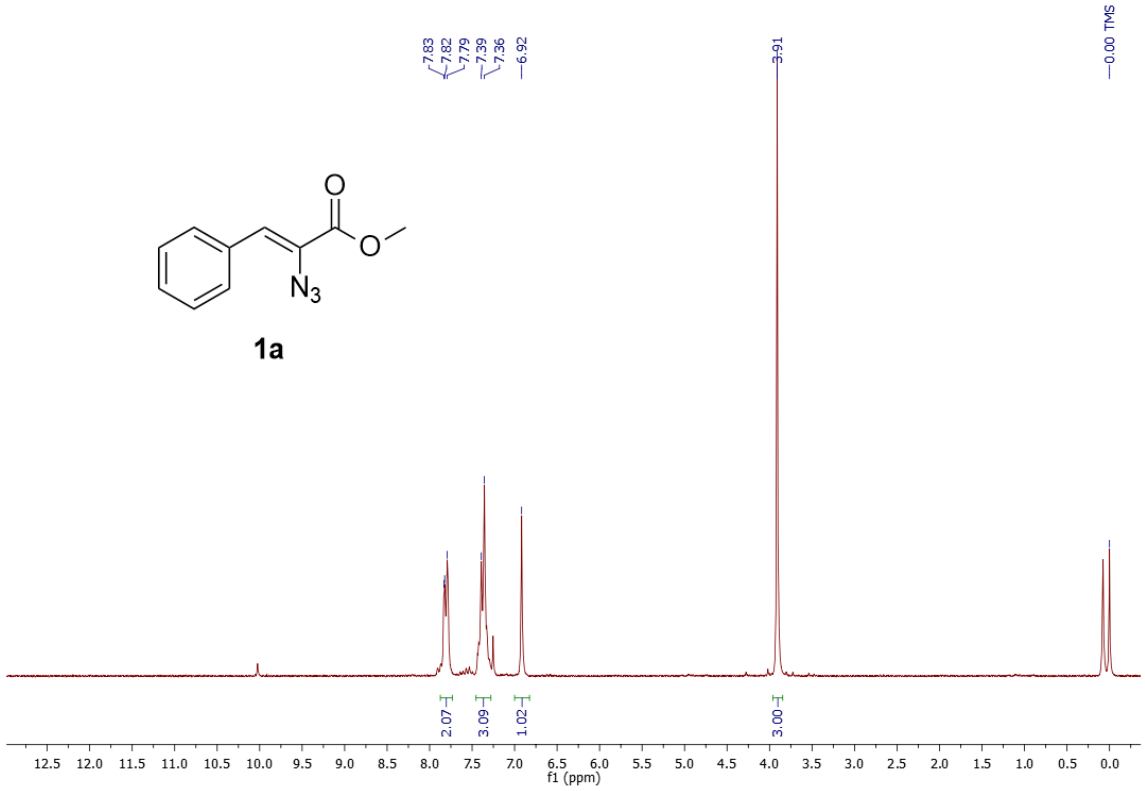


Figure S1. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **1a**.

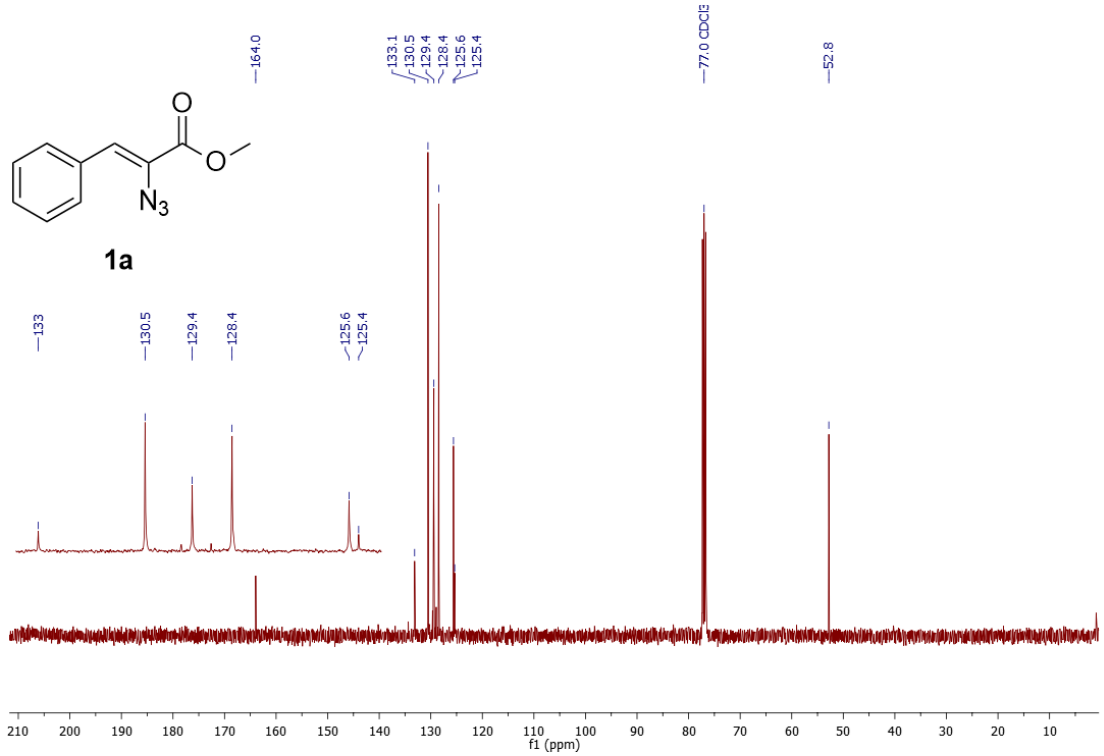


Figure S2. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **1a**.

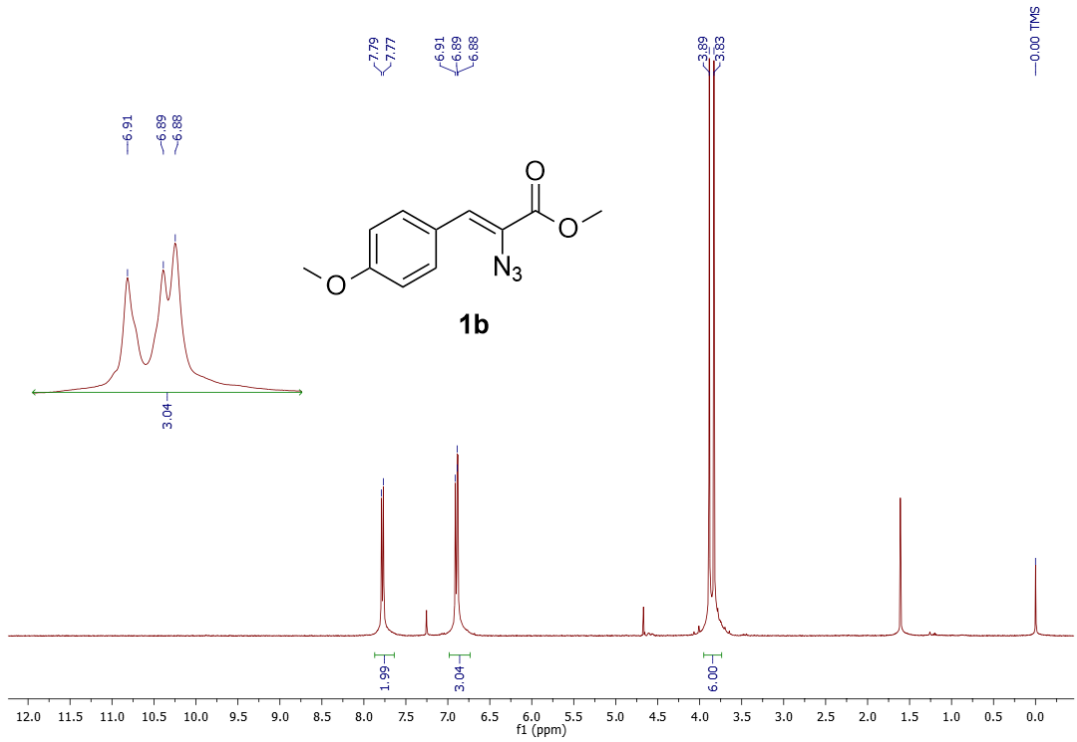


Figure S3. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **1b**.

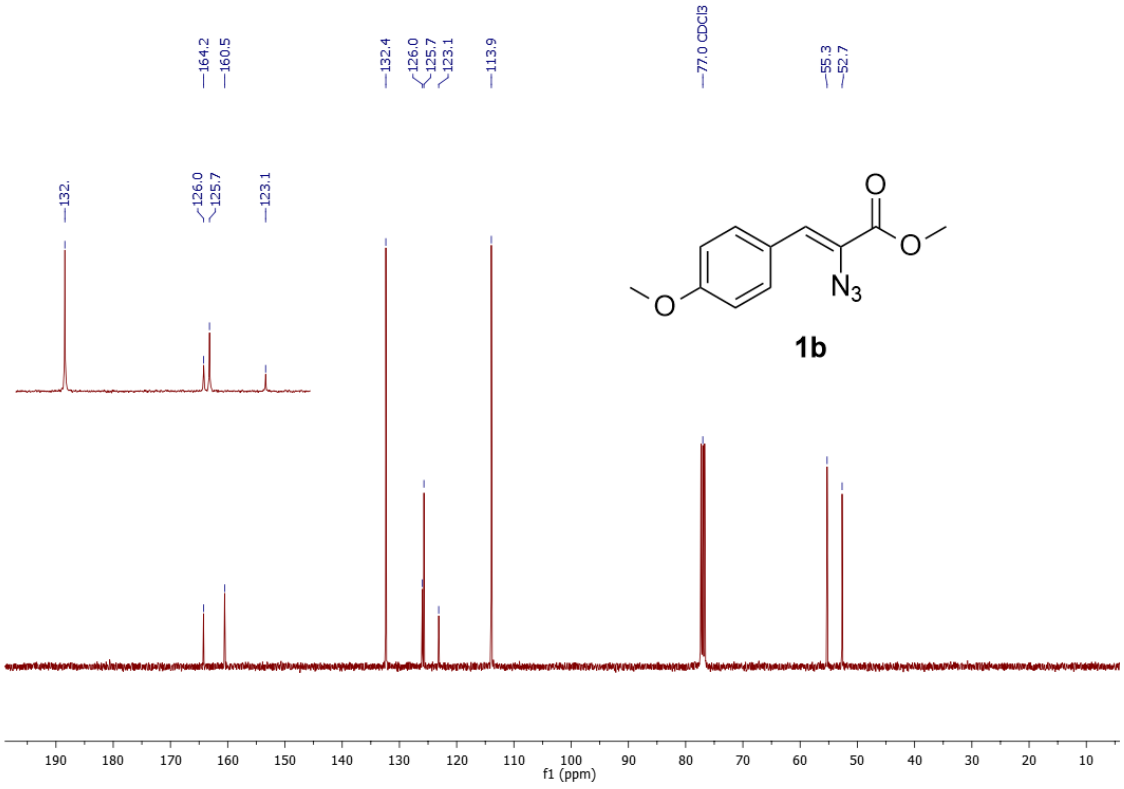


Figure S4. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **1b**.

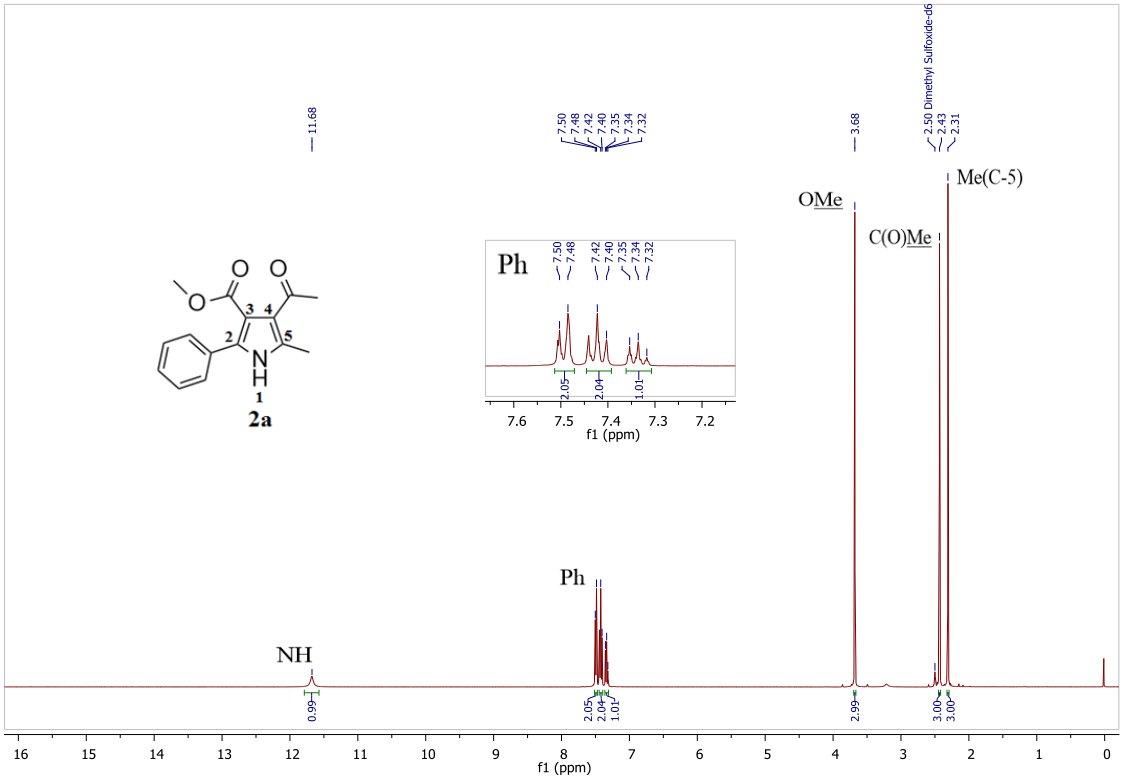


Figure S5. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of **2a**.

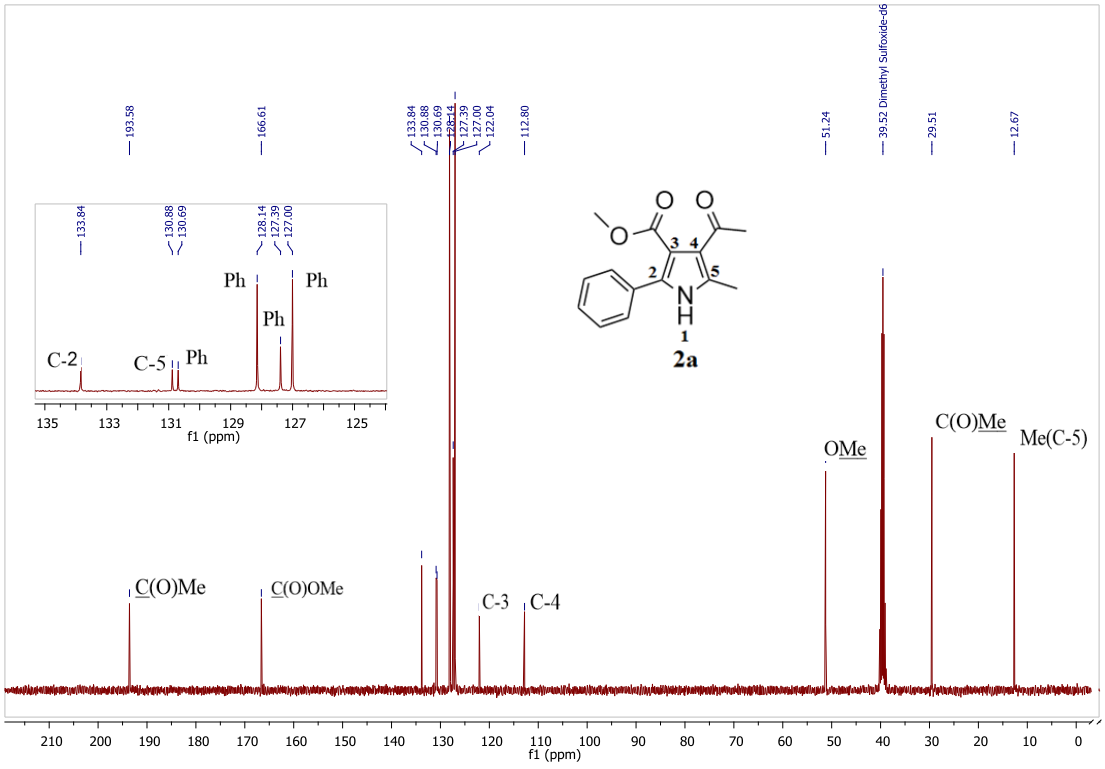


Figure S6. ^{13}C MNR spectrum (100 MHz, DMSO-d_6) of **2a**.

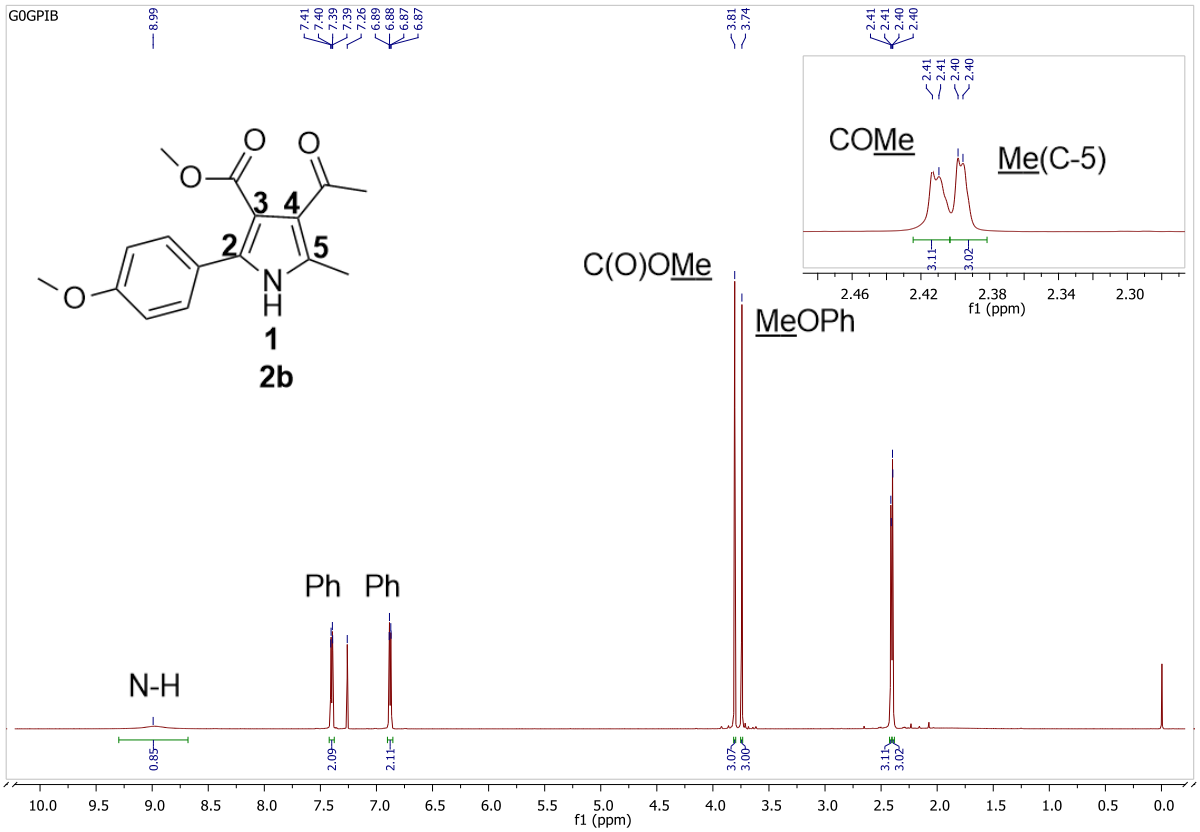


Figure S7. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **2b**.

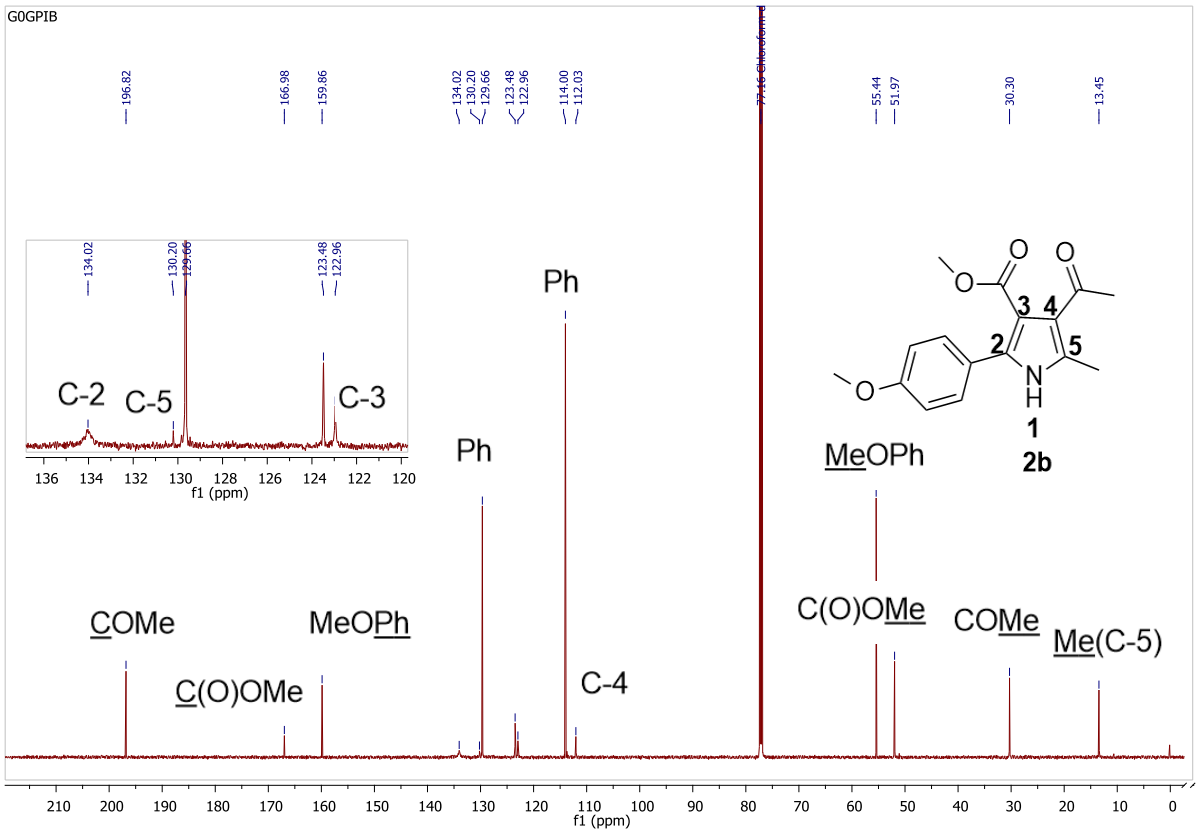


Figure S8. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **2b**.

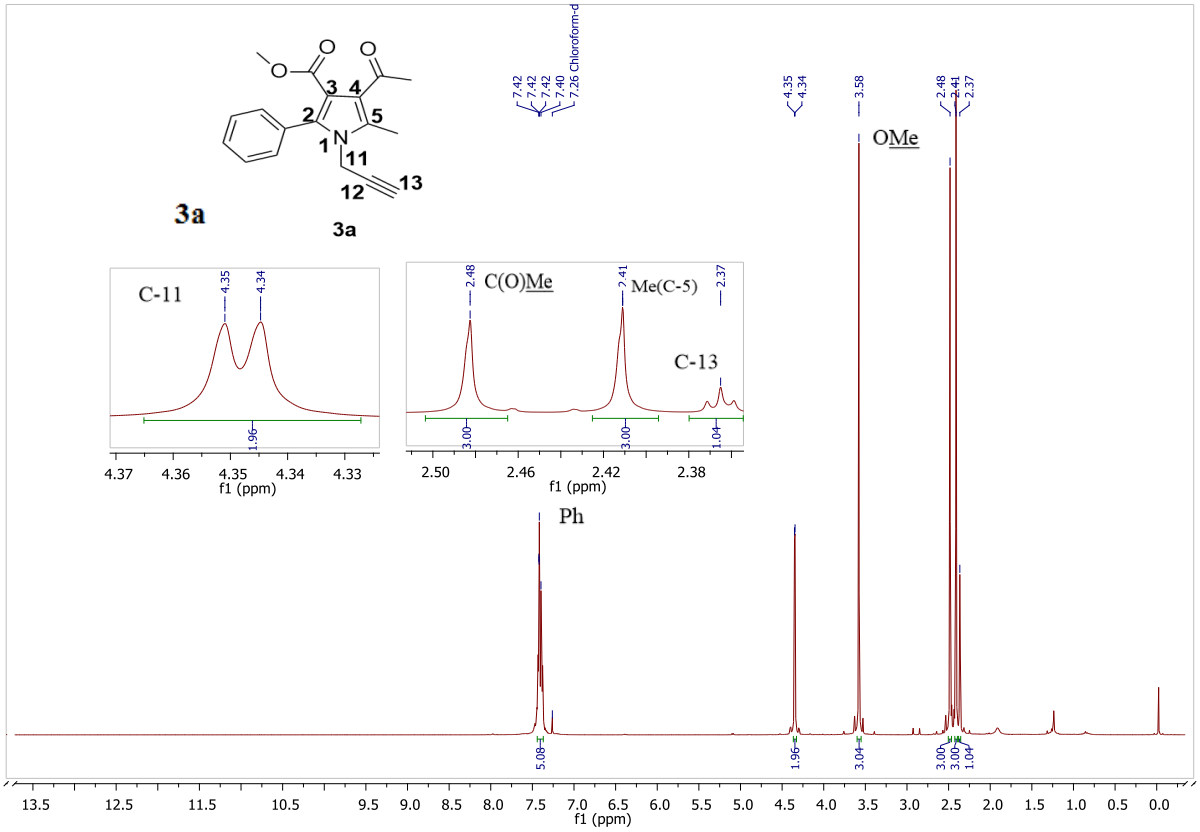


Figure S9. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3a**.

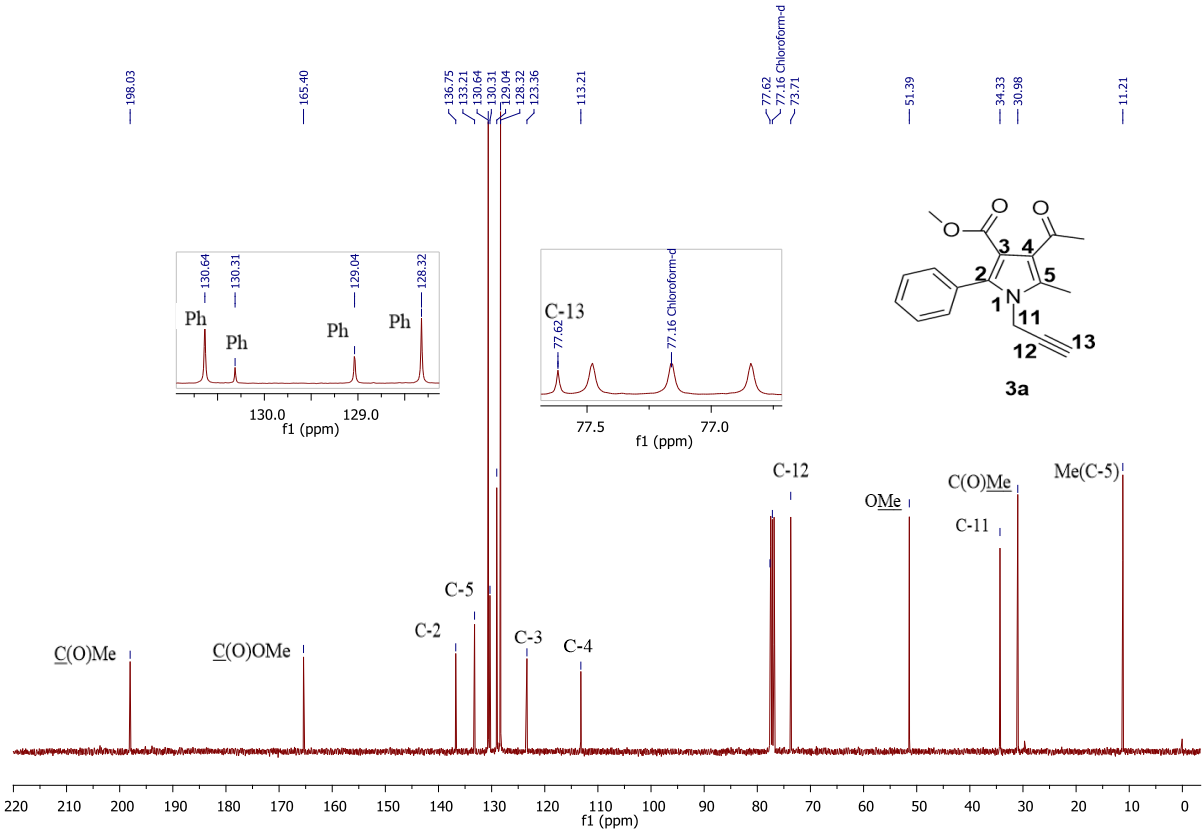


Figure S10. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **3a**.

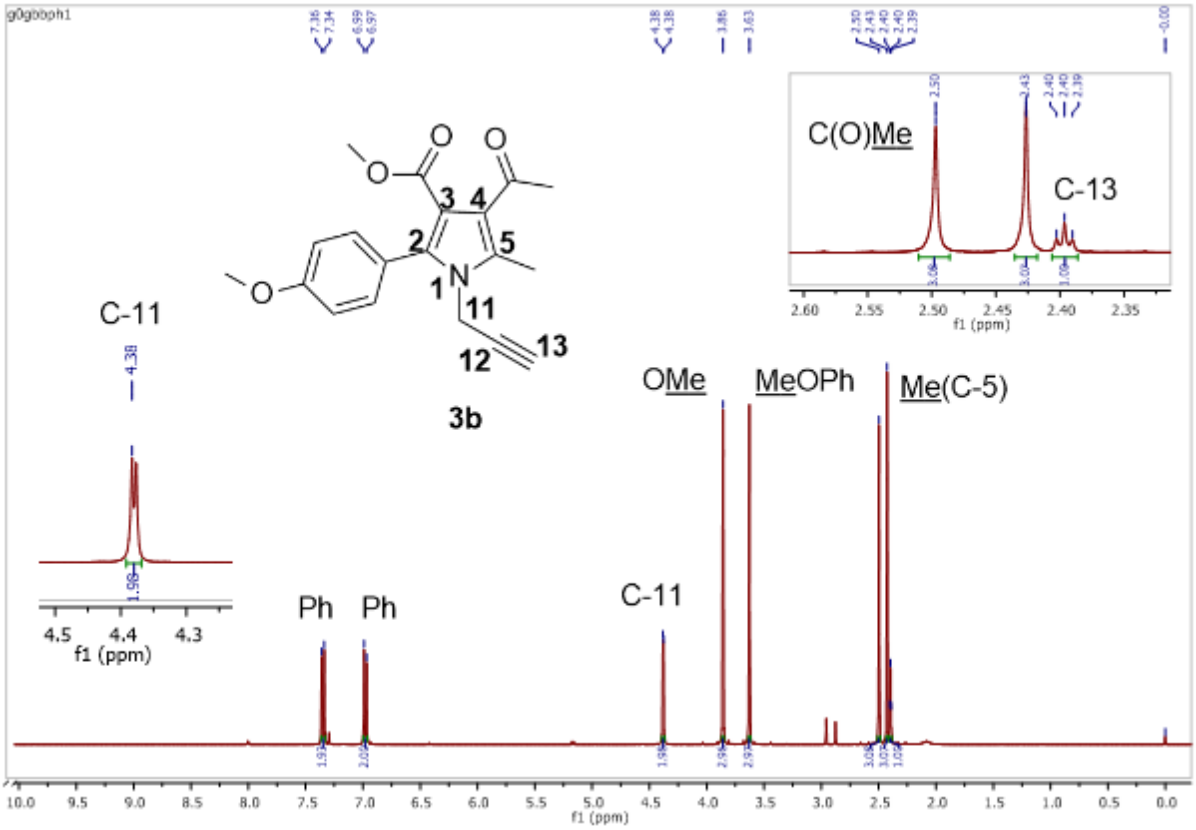


Figure S11. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **3b**.

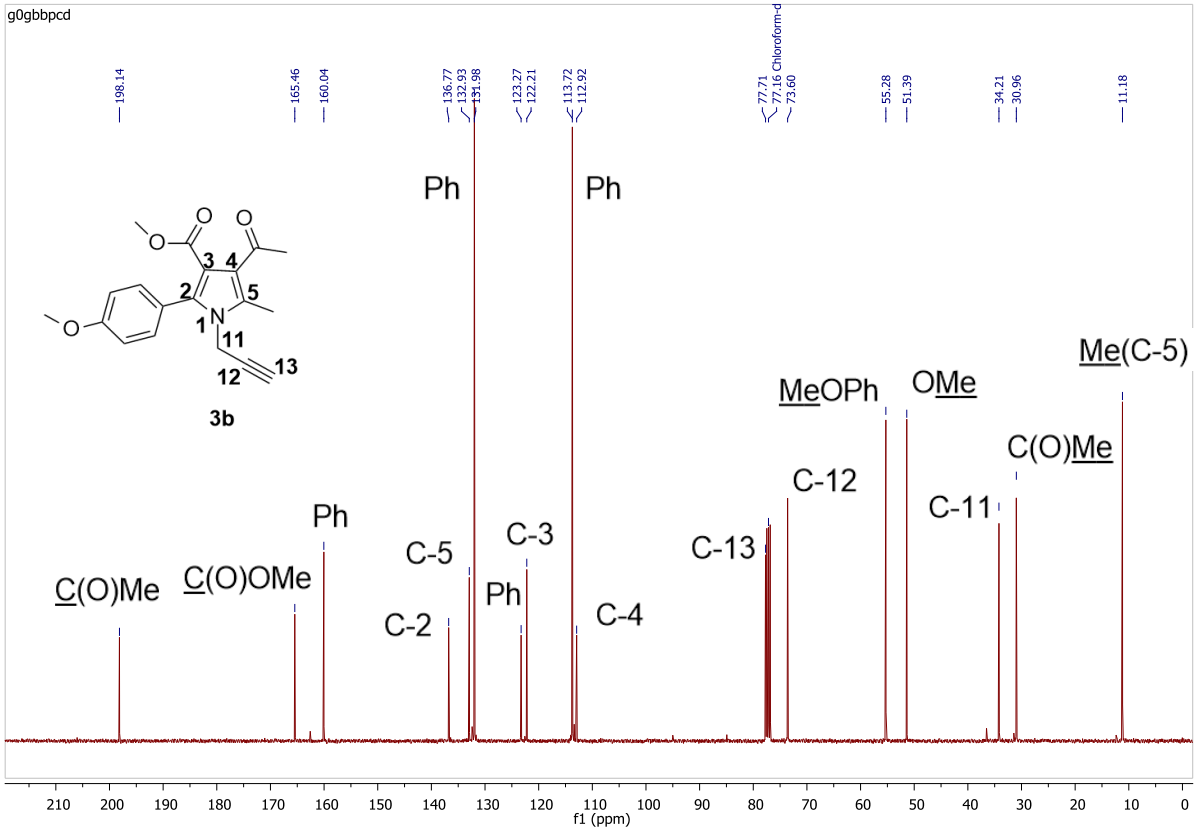


Figure S12. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **3b**.

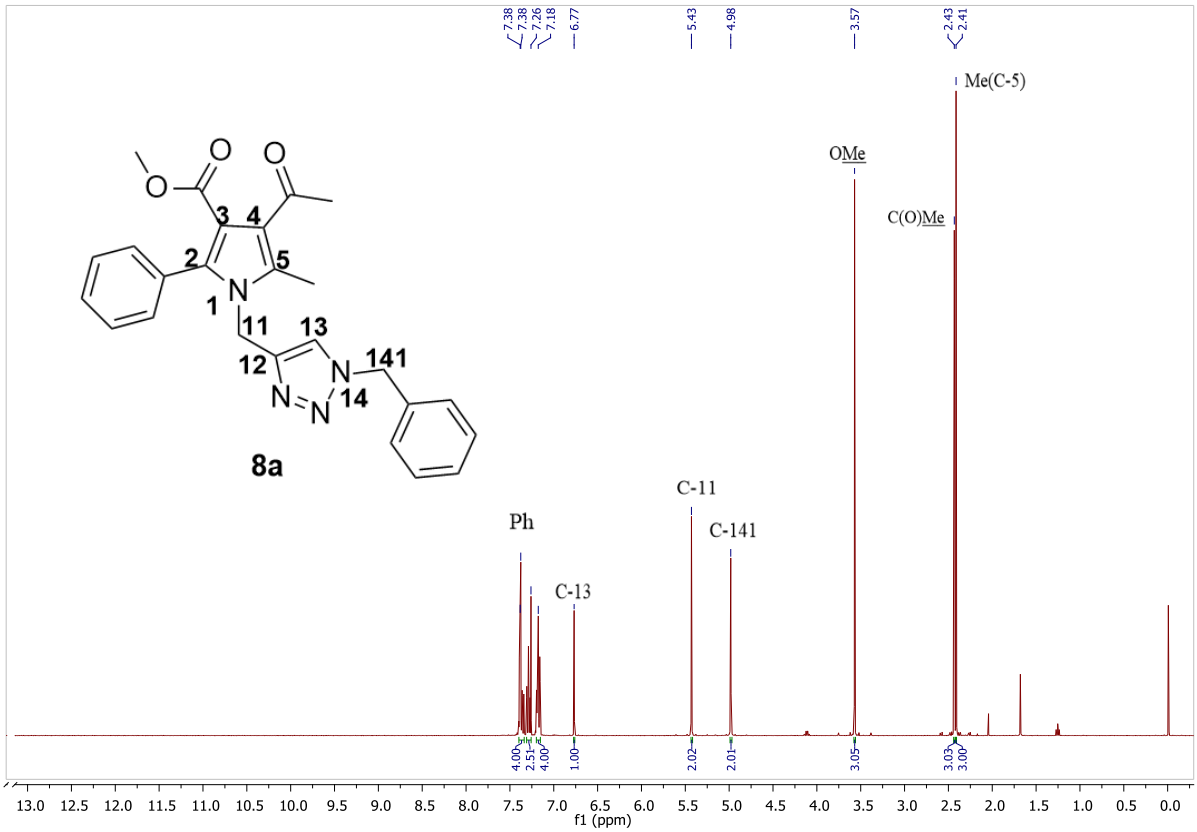


Figure S13. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **8a**.

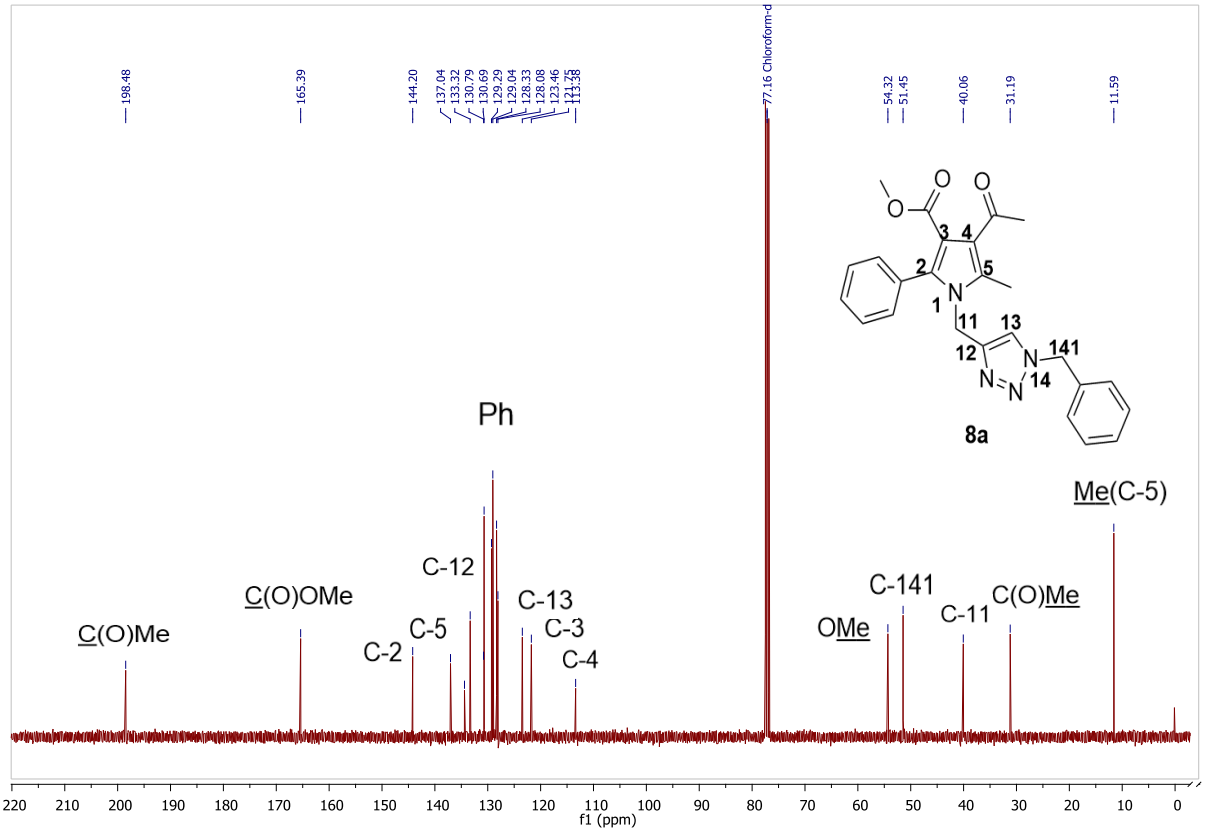


Figure S14. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **8a**.

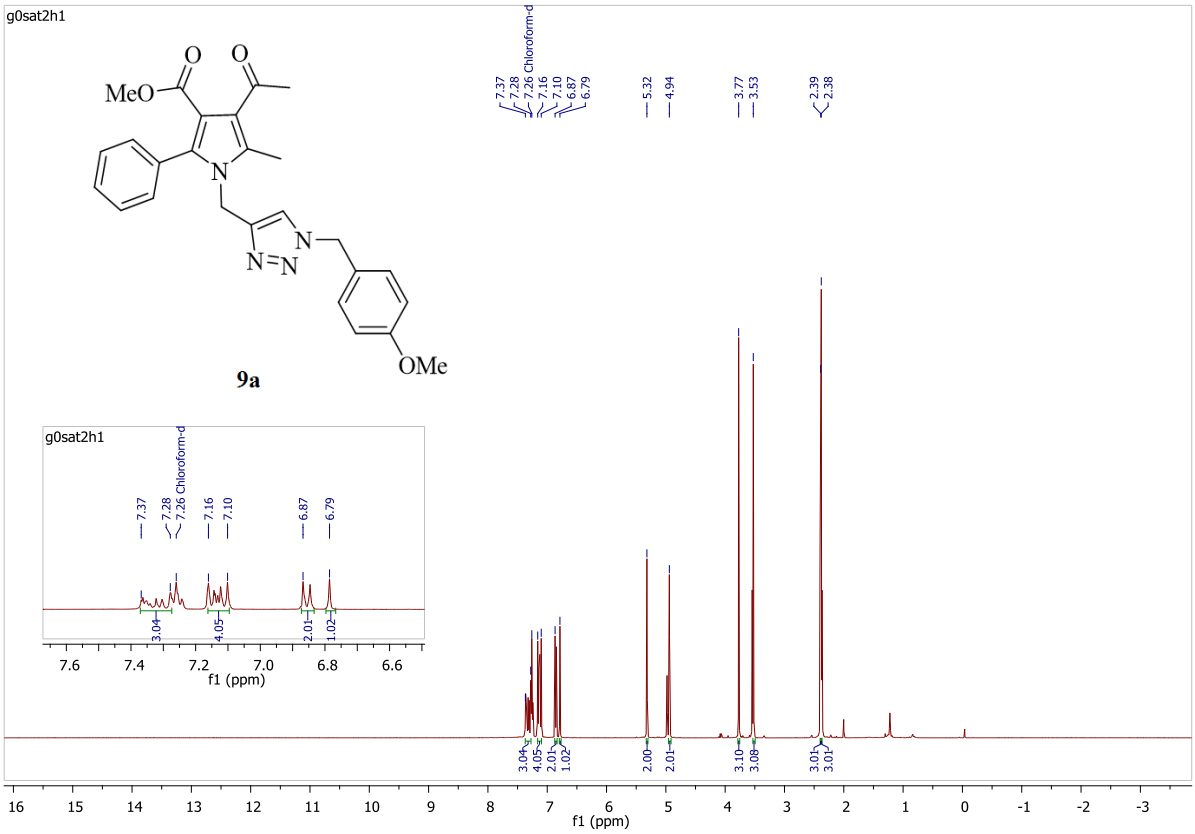


Figure S15. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **9a**.

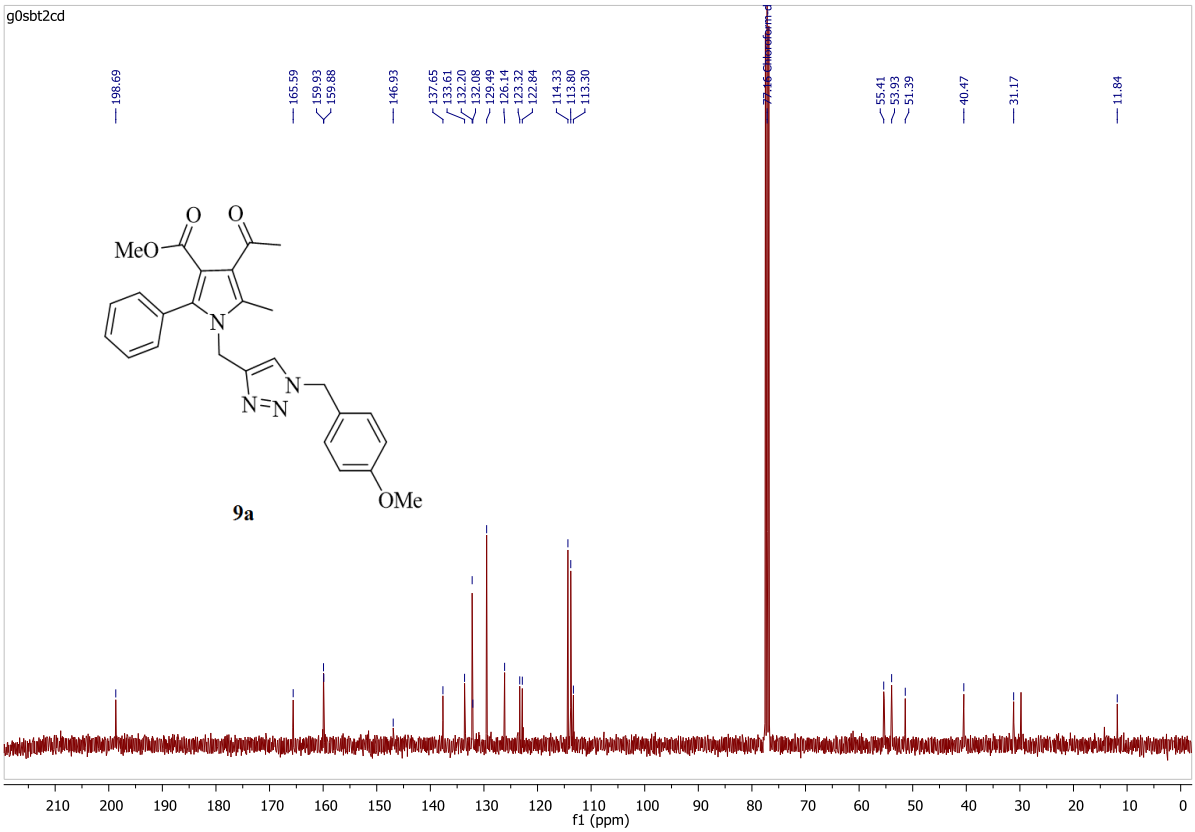


Figure S16. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **9a**.

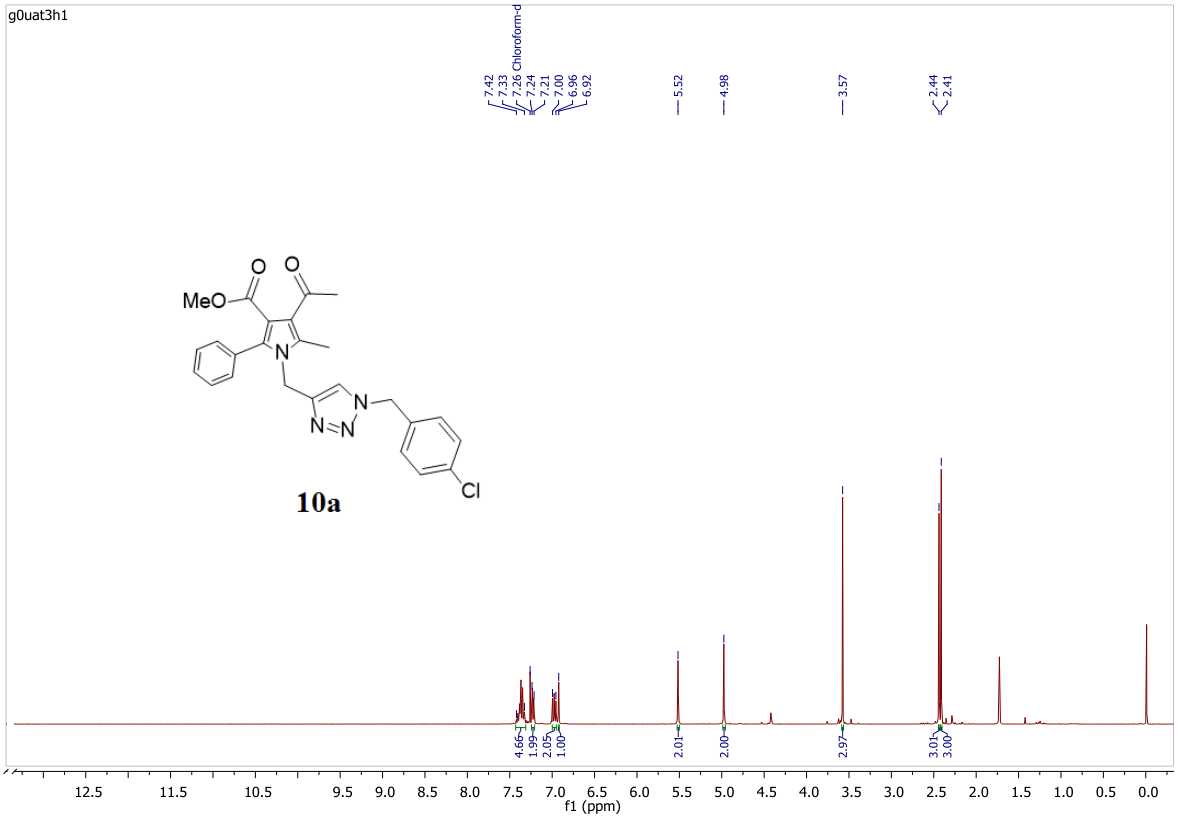


Figure S17. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **10a**.

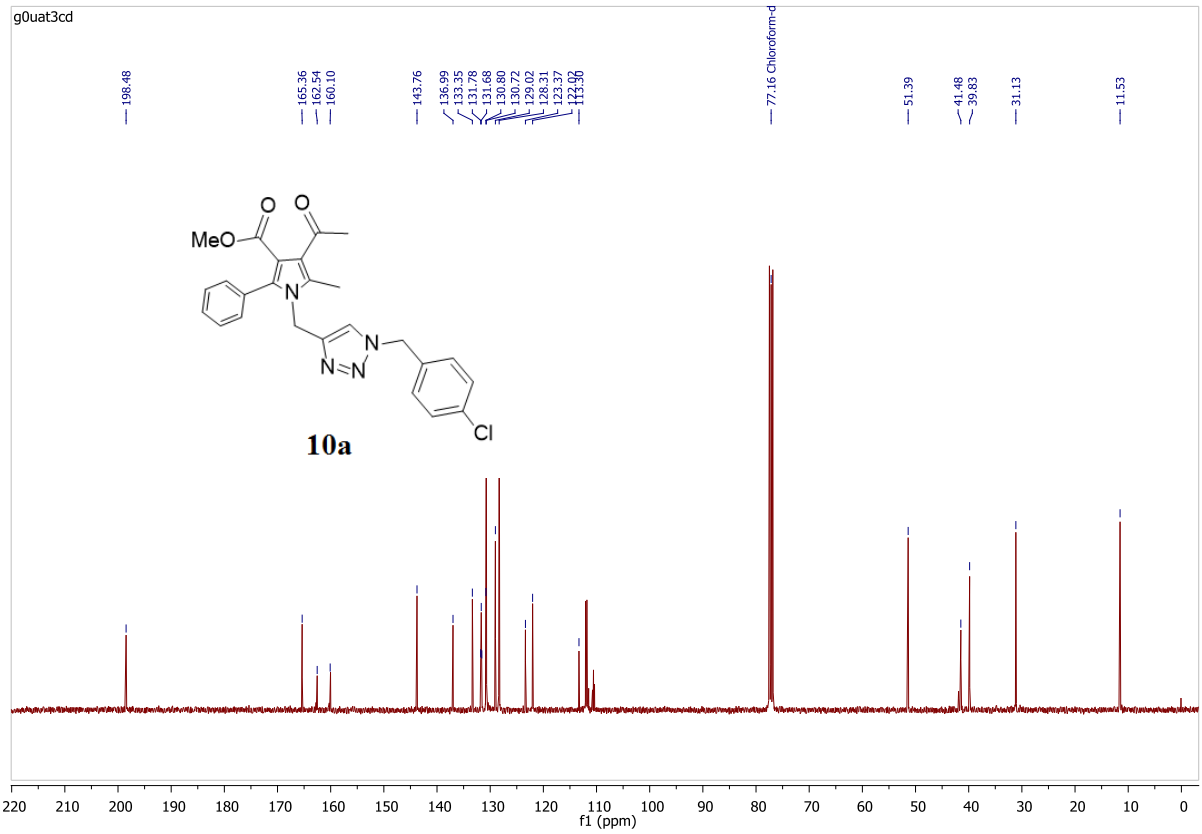


Figure S18. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **10a**.

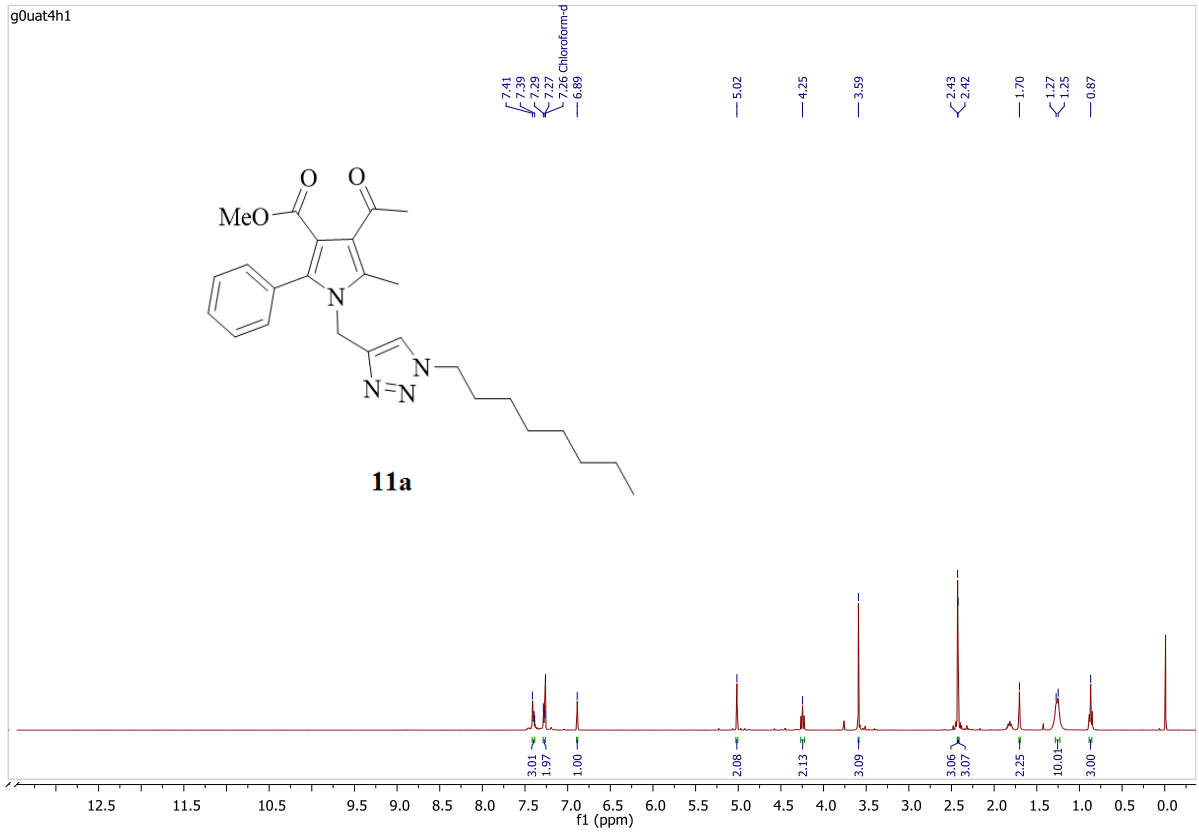


Figure S19. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **11a**.

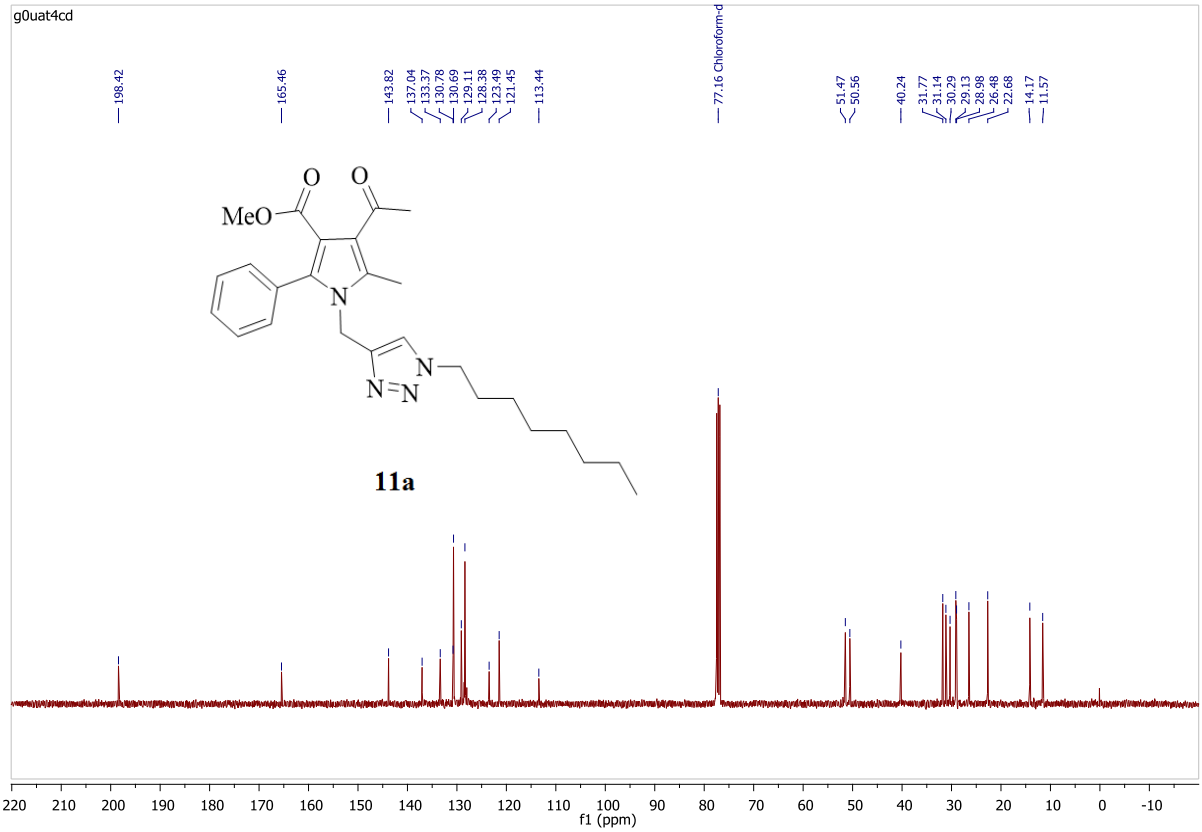


Figure S20. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **11a**.

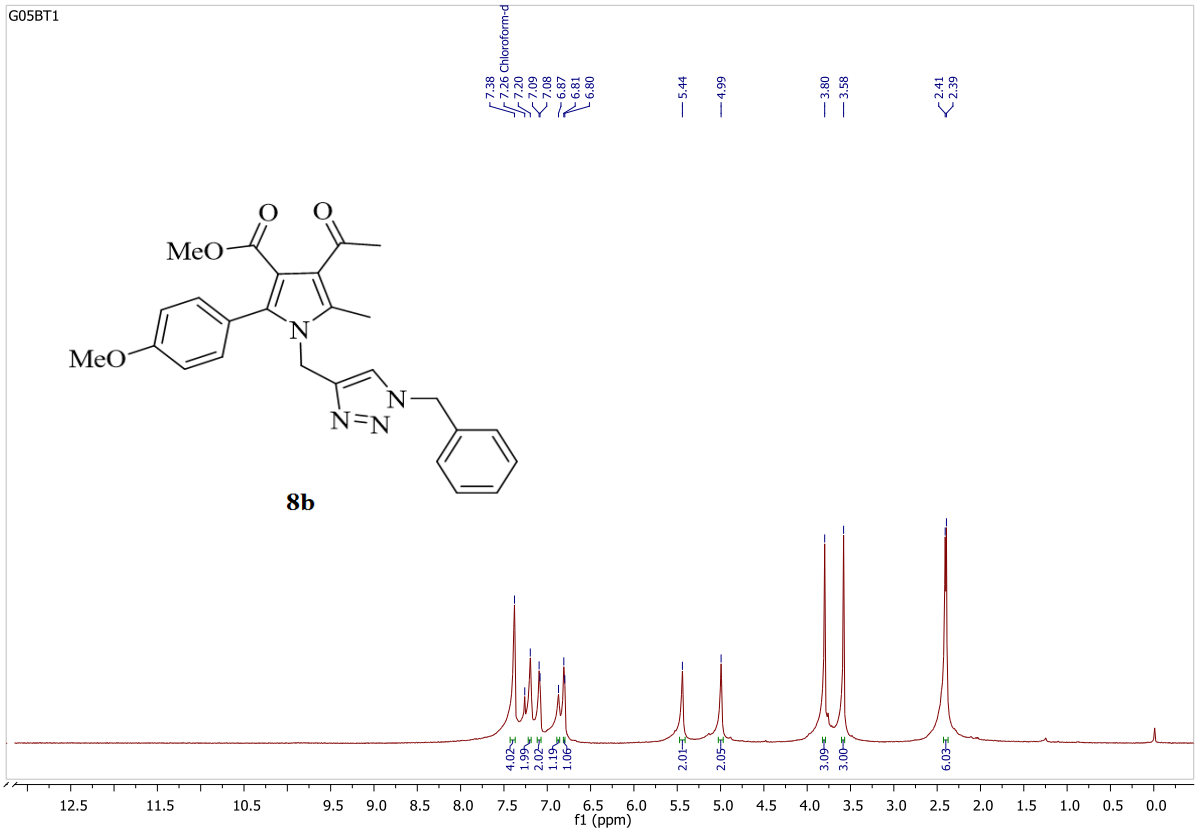


Figure S21. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **8b**.

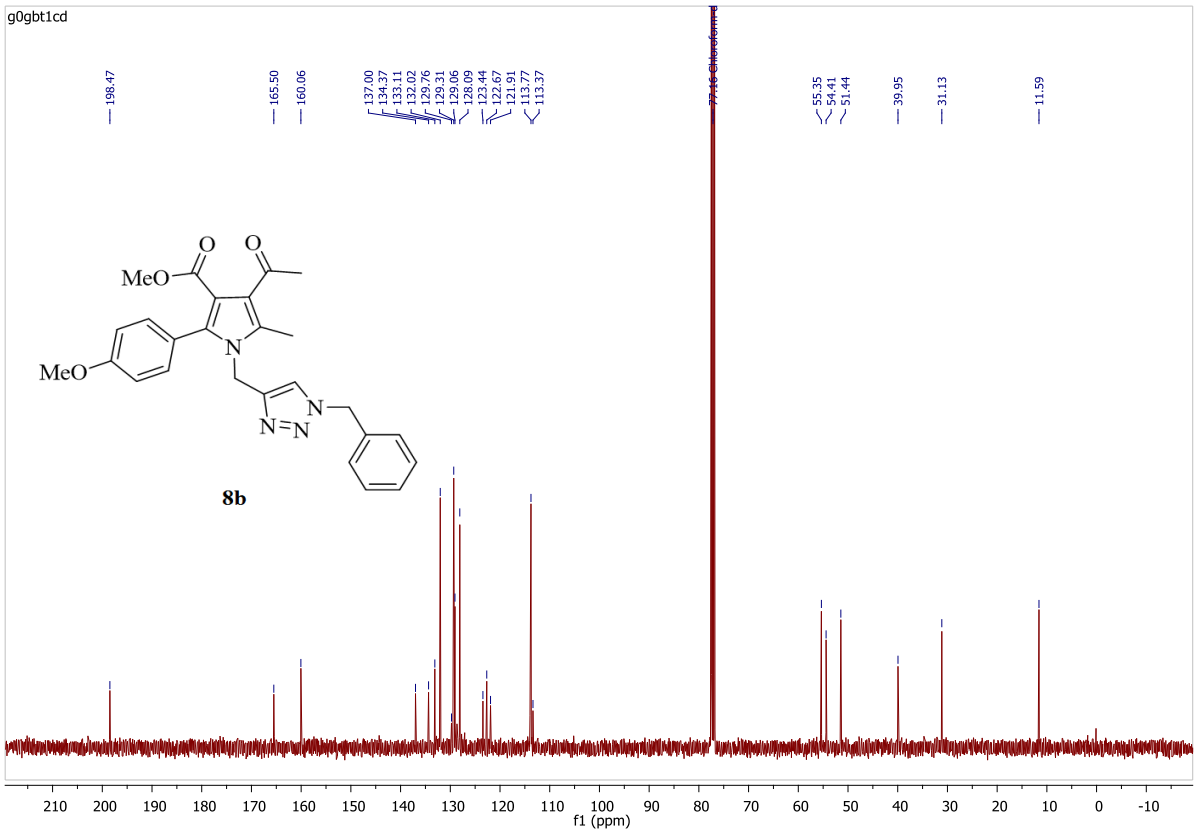


Figure S22. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **8b**.

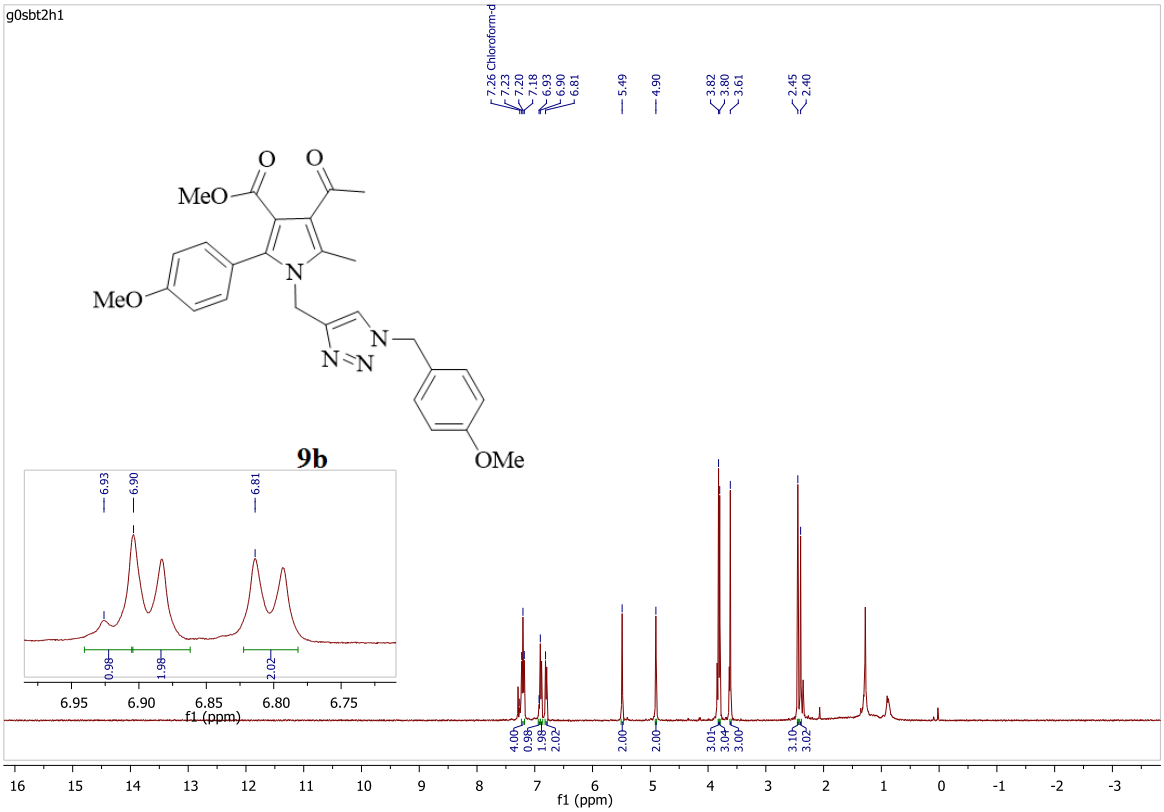


Figure S23. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **9b**.

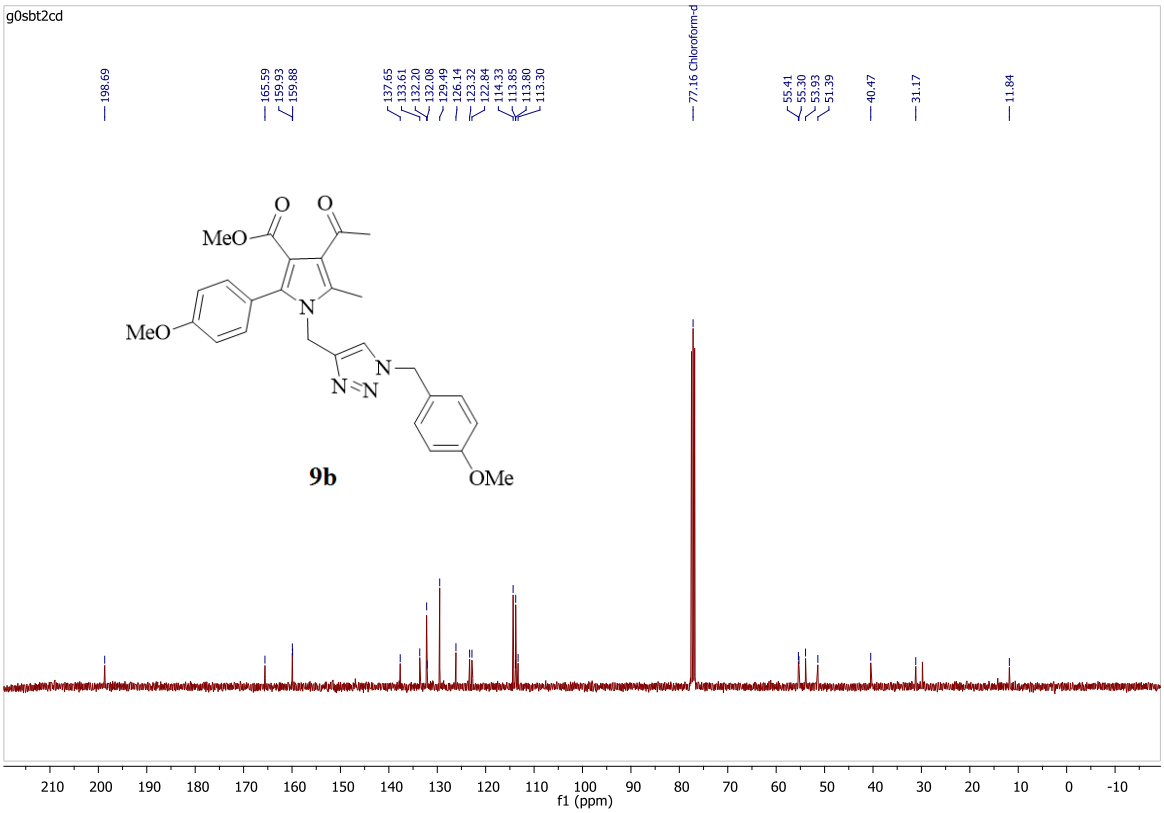


Figure S24. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **9b**.

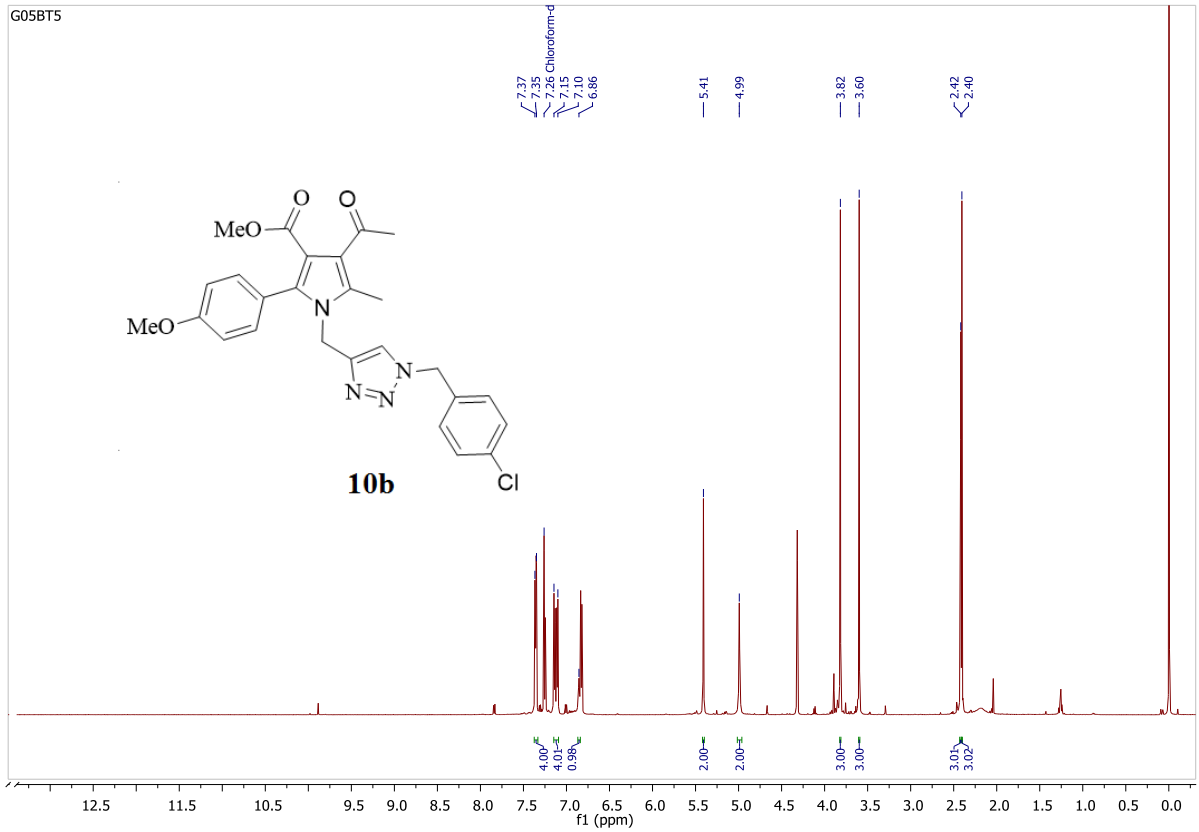


Figure S25. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **10b**.

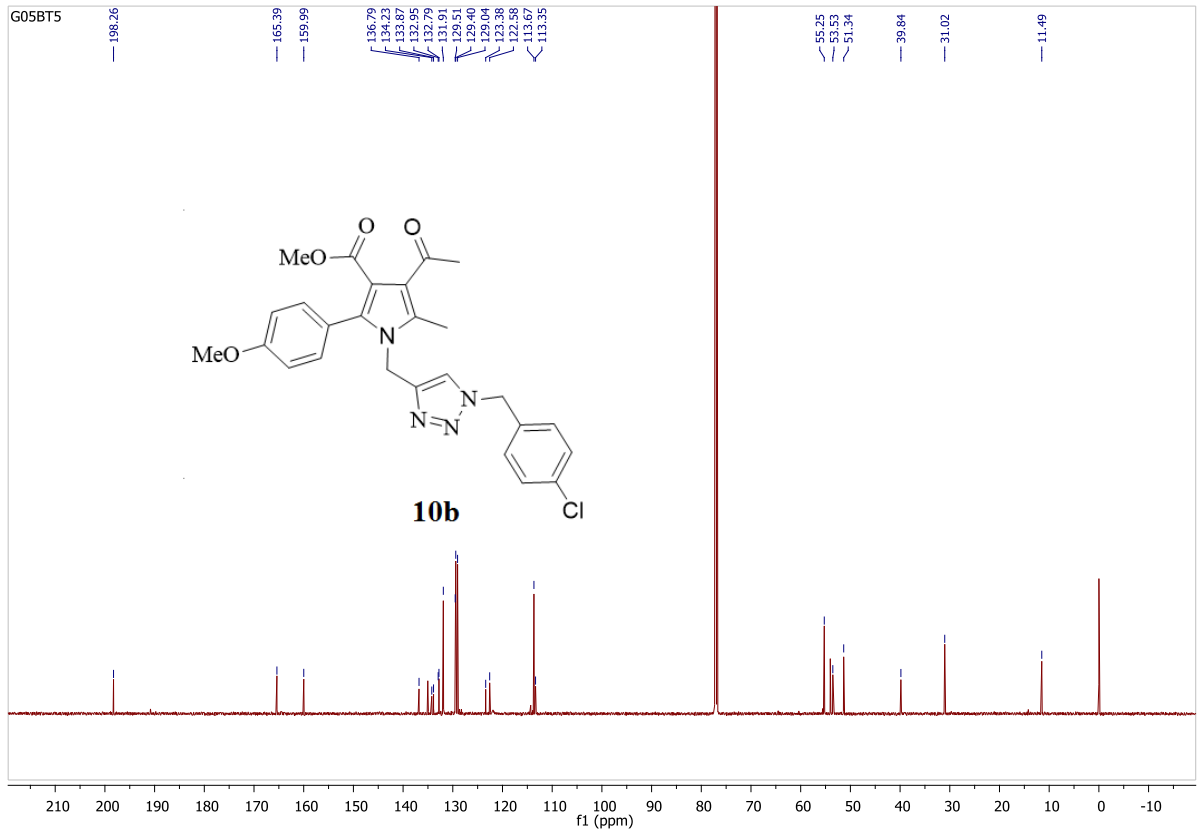


Figure S26. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **10b**.

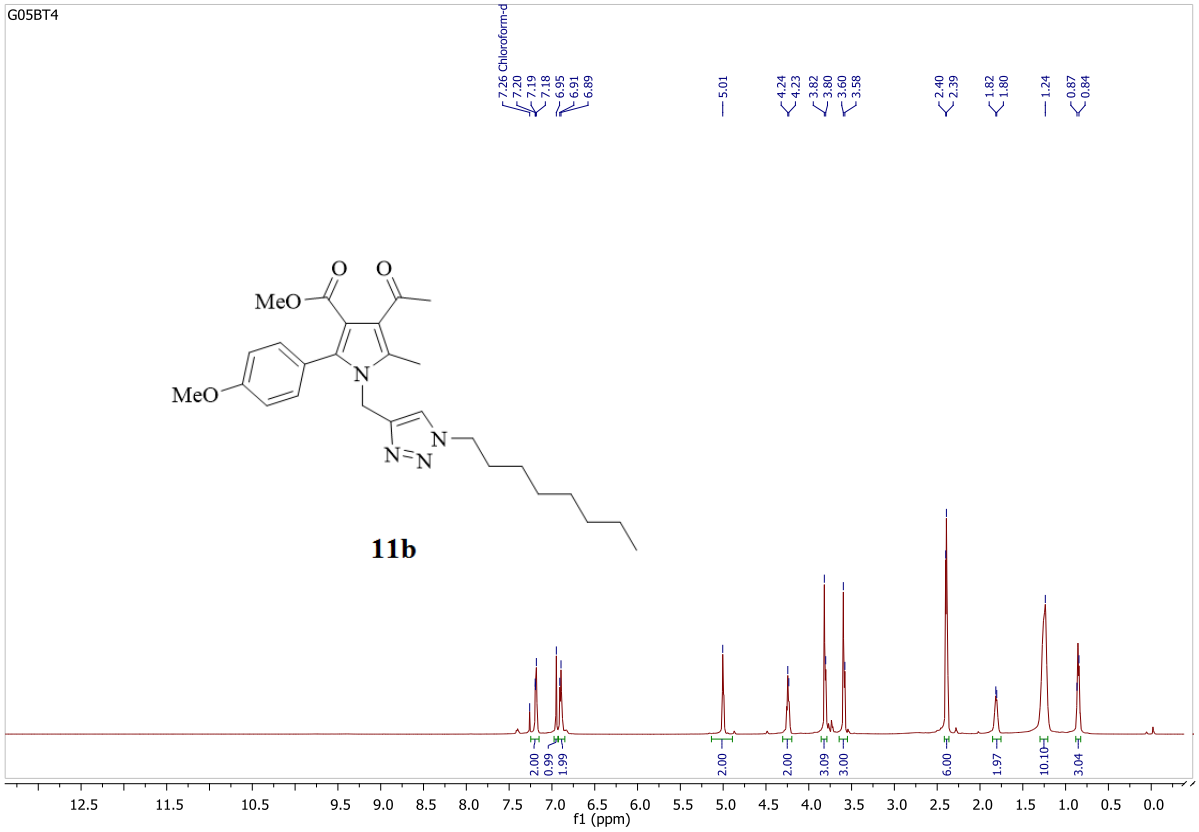


Figure S27. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **11b**.

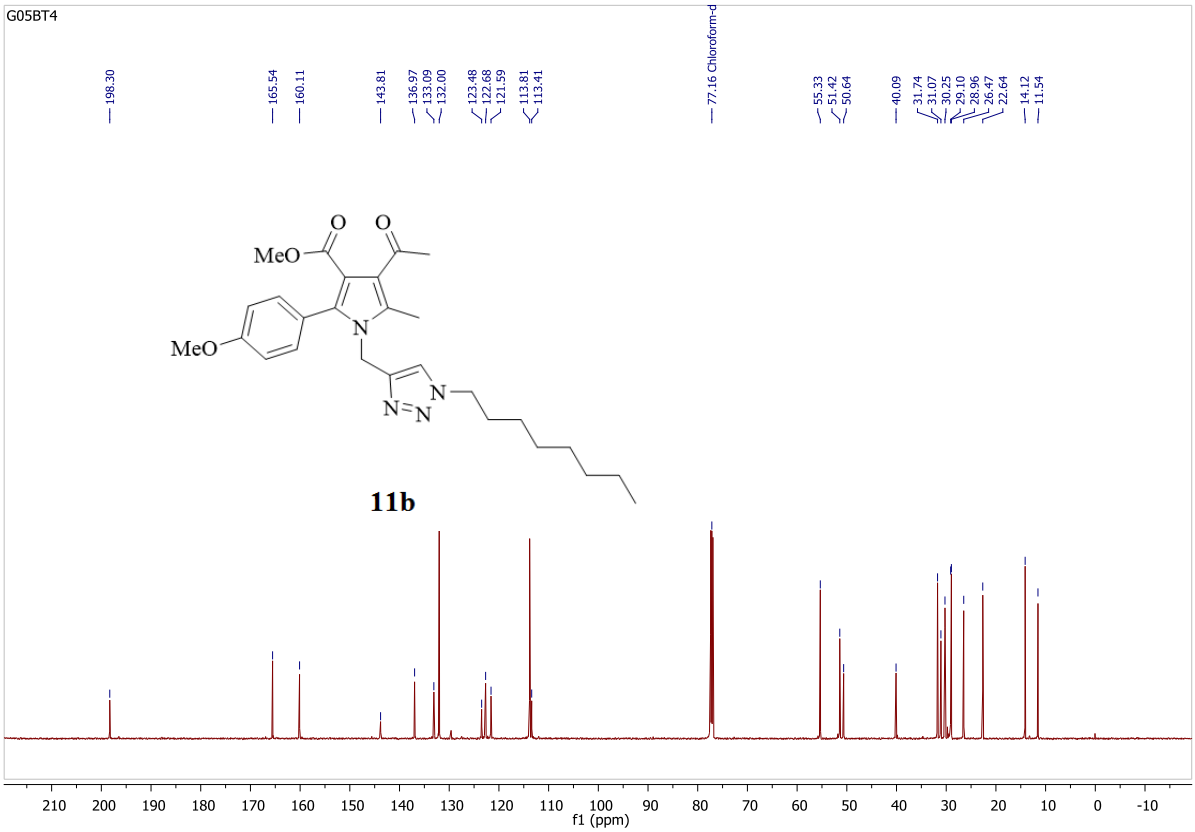


Figure S28. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **11b**.

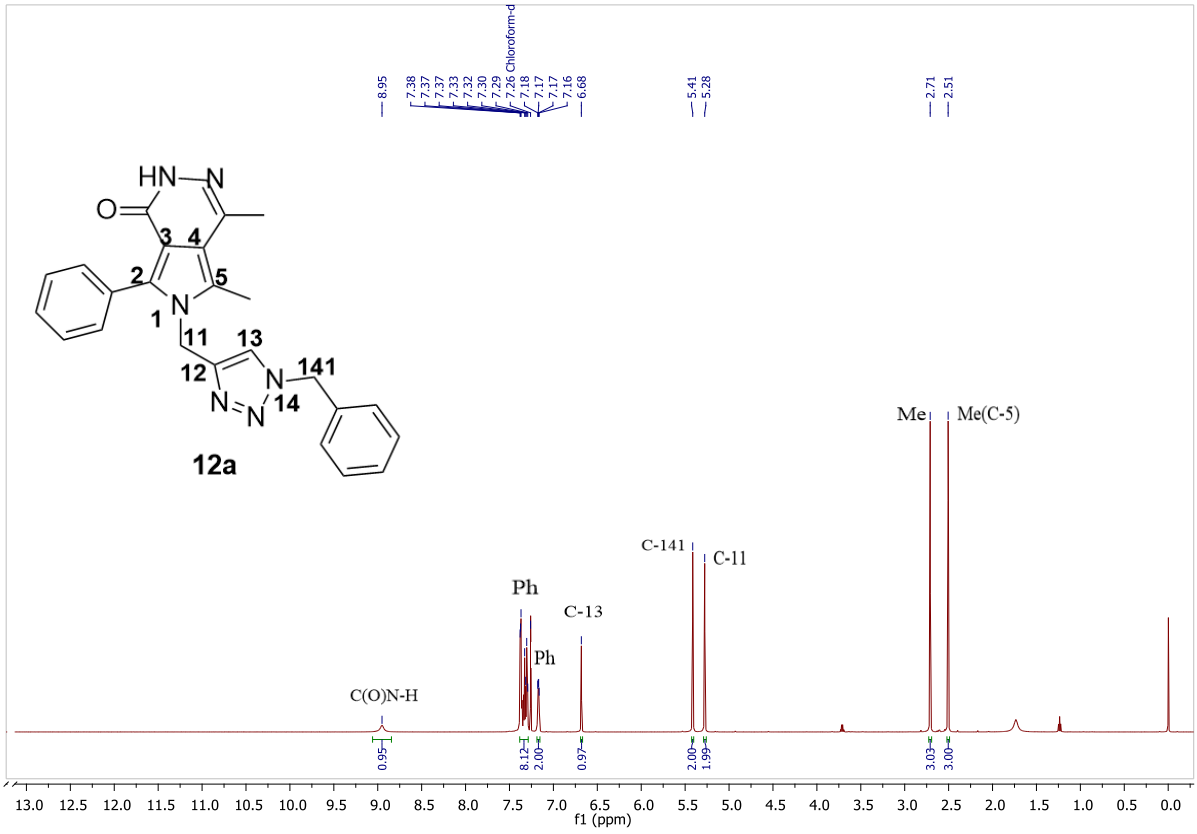


Figure S29. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **12a**.

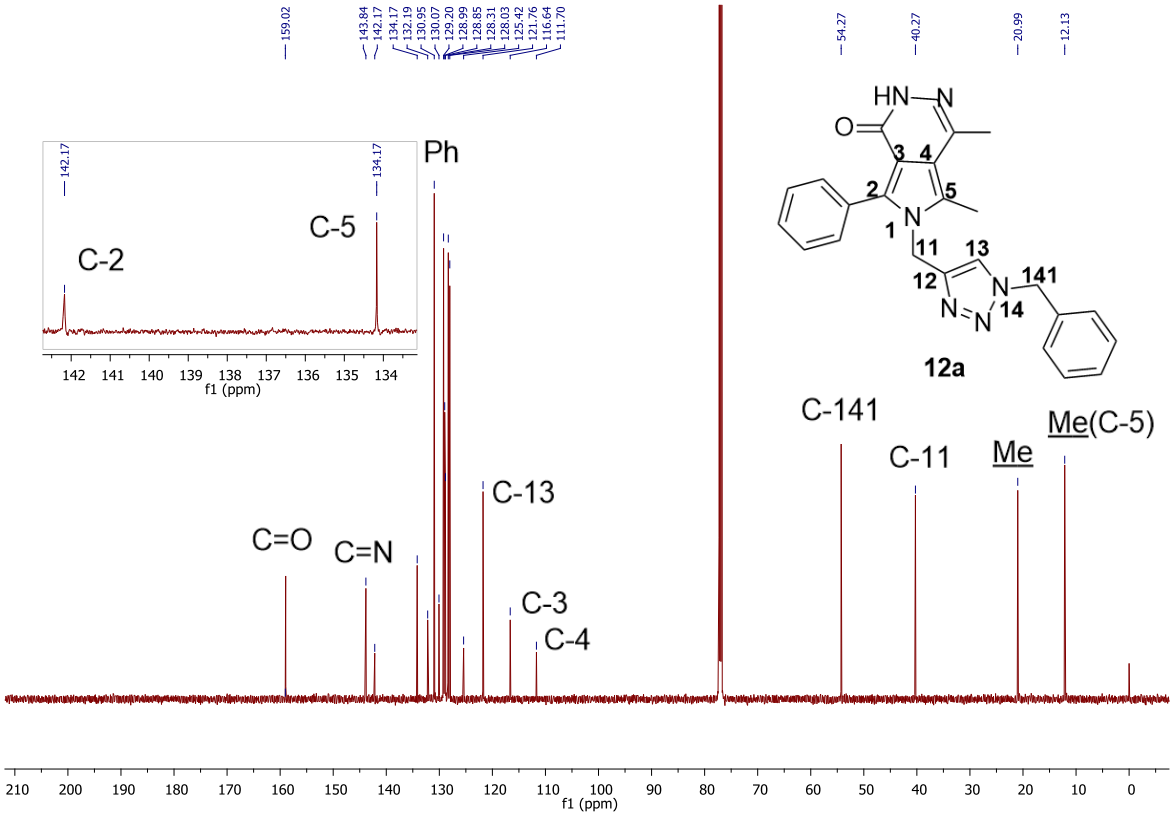


Figure S30. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **12a**.

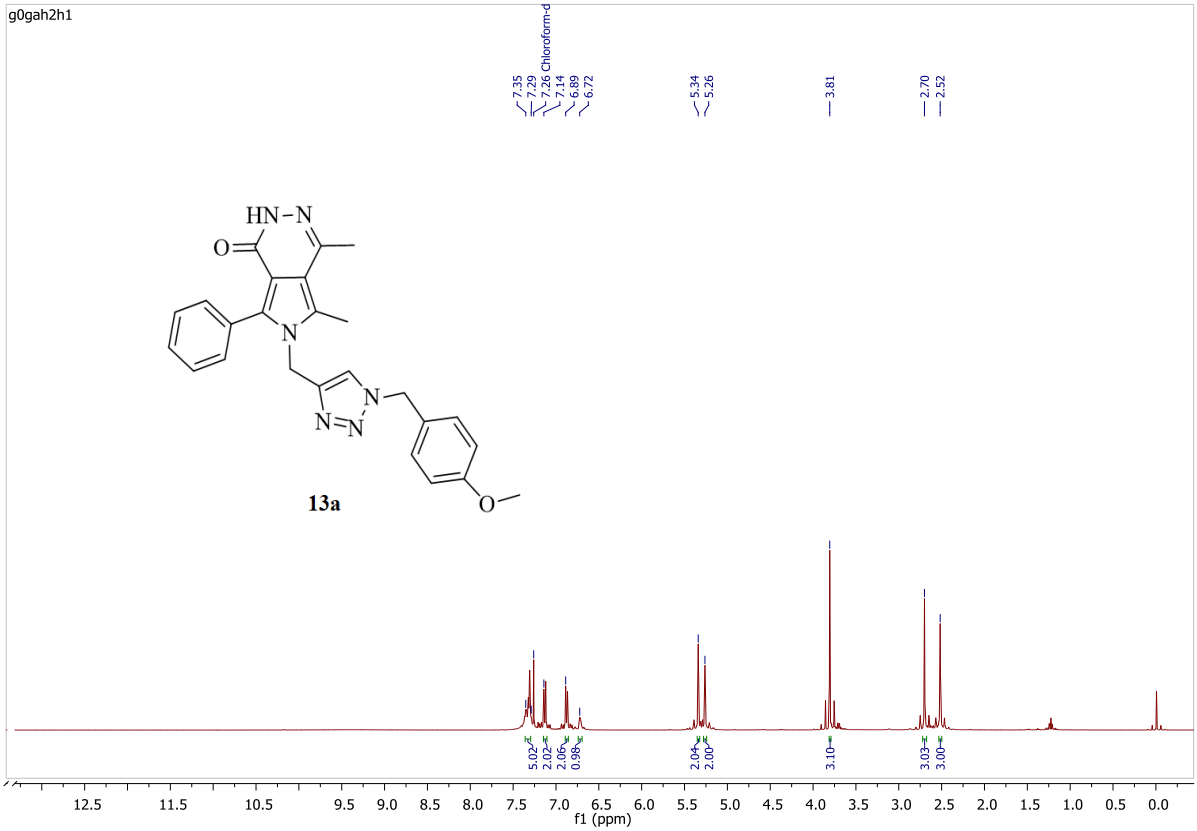


Figure S31. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **13a**.

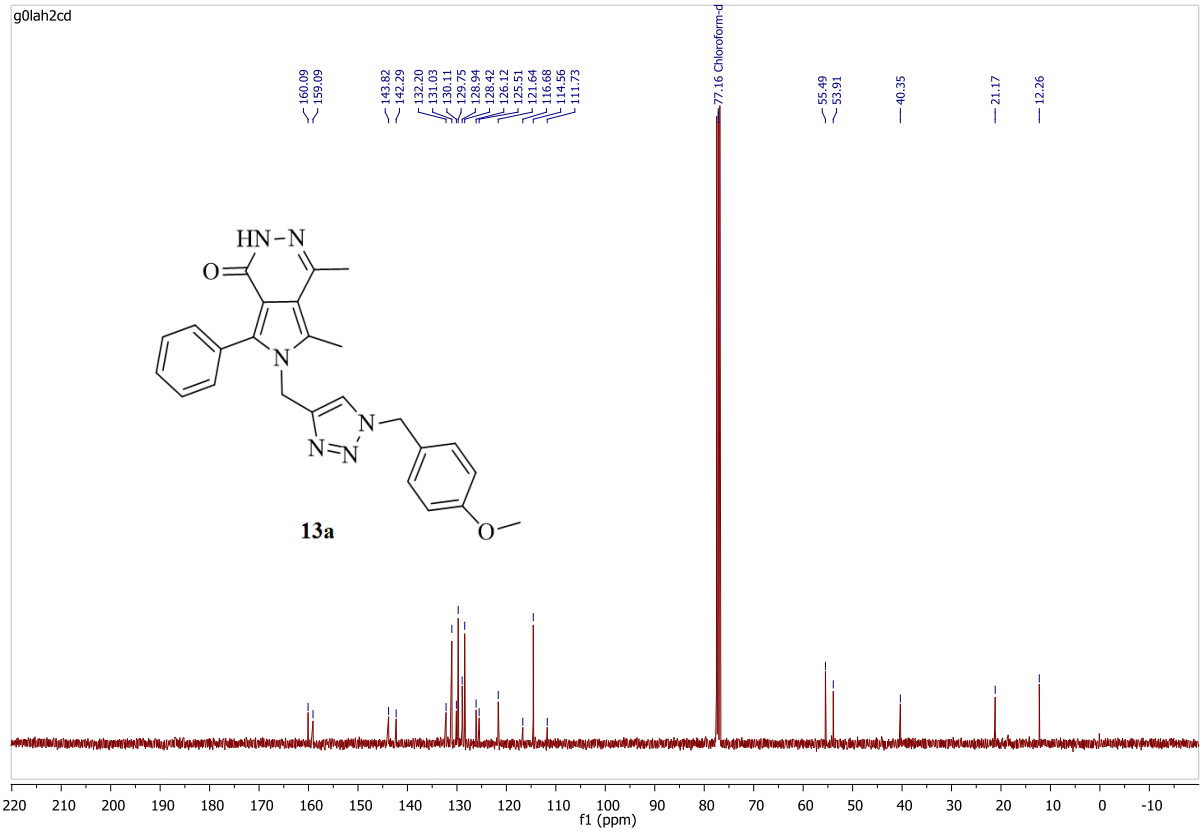


Figure S32. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **13a**.

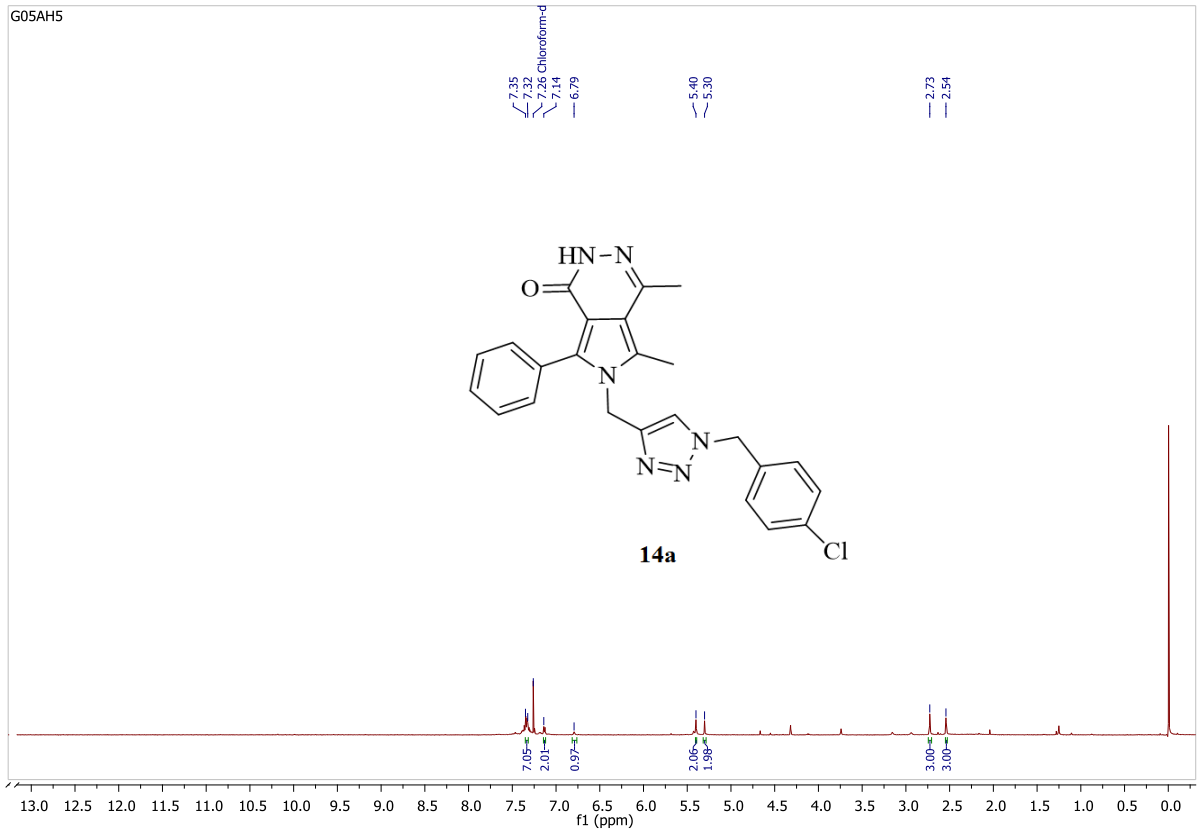


Figure S33. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **14a**.

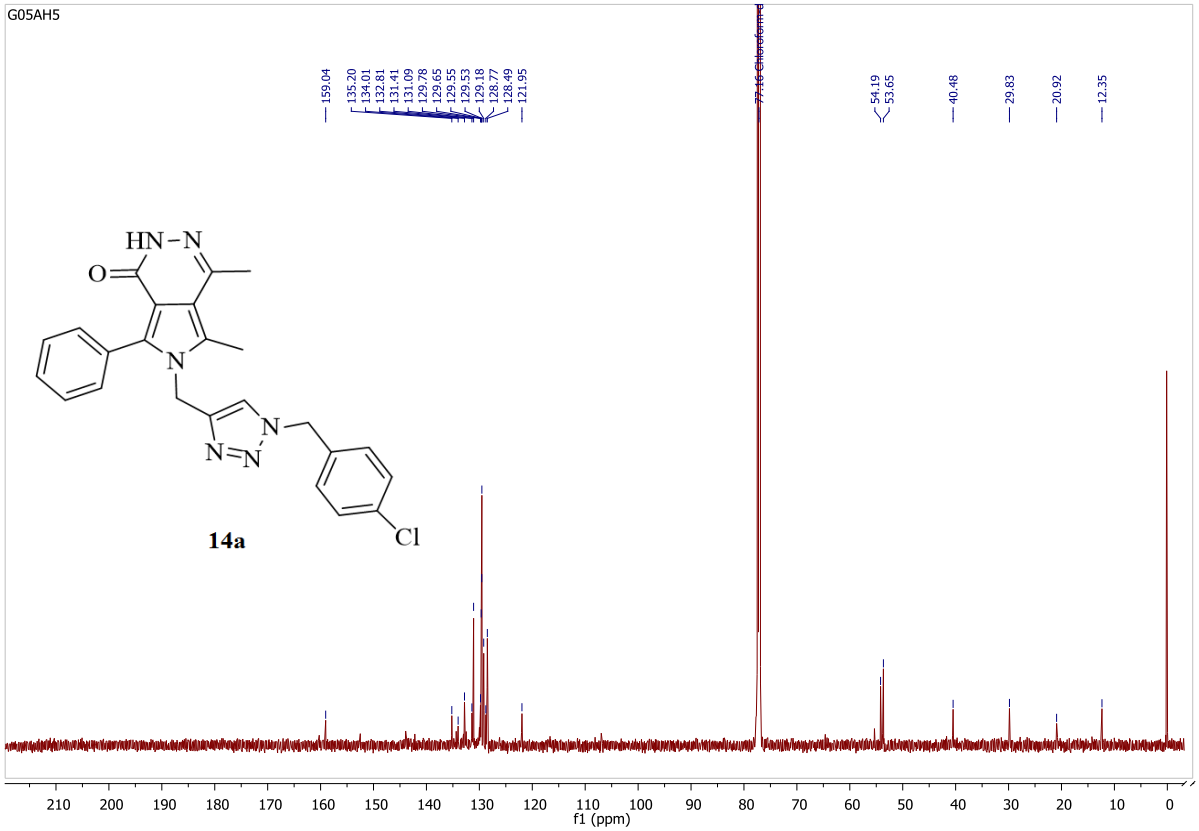


Figure S34. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **14a**.

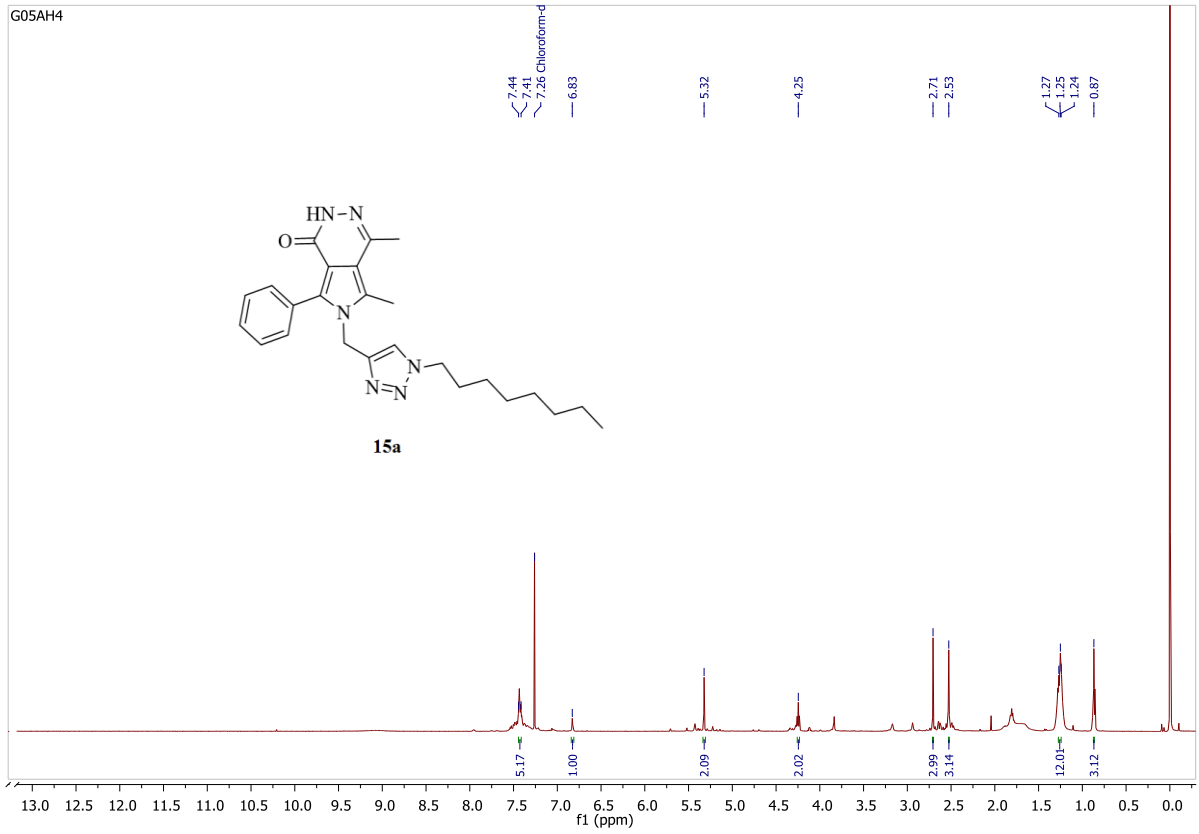


Figure S35. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **15a**.

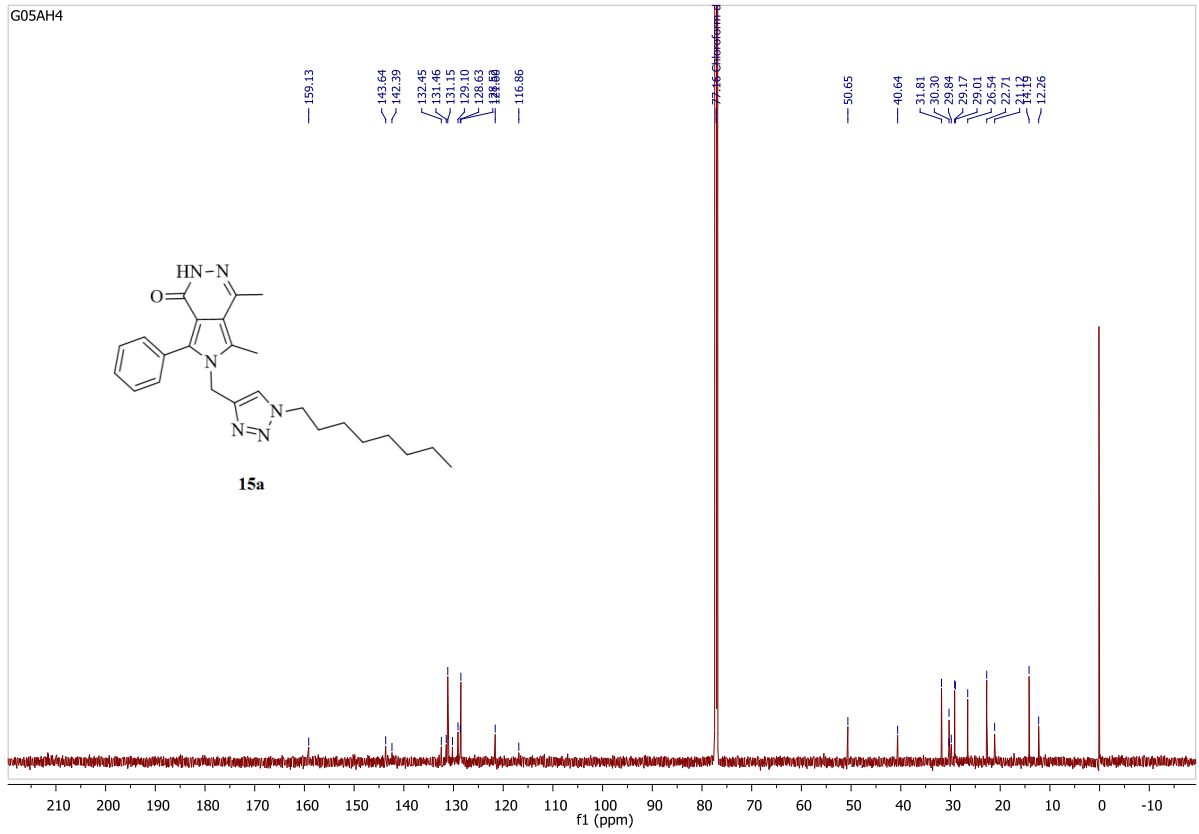


Figure S36. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **15a**.

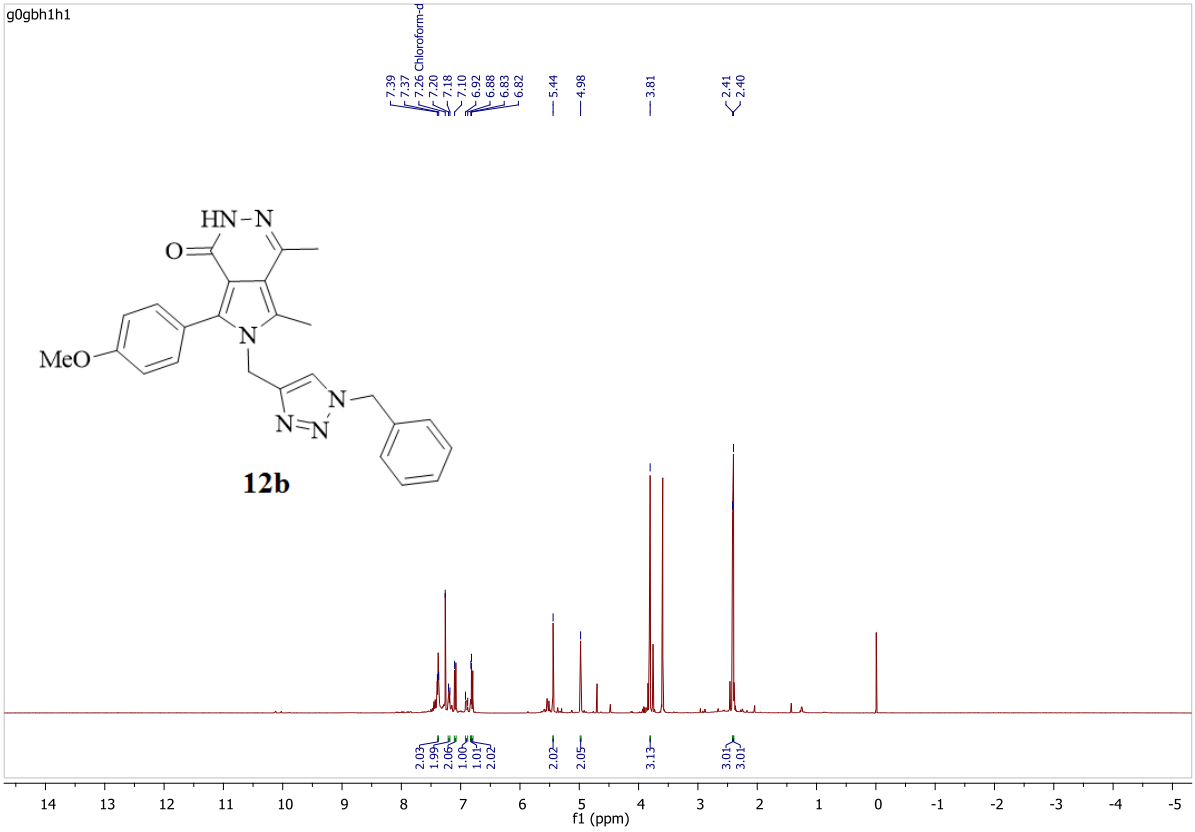


Figure S37. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **12b**.

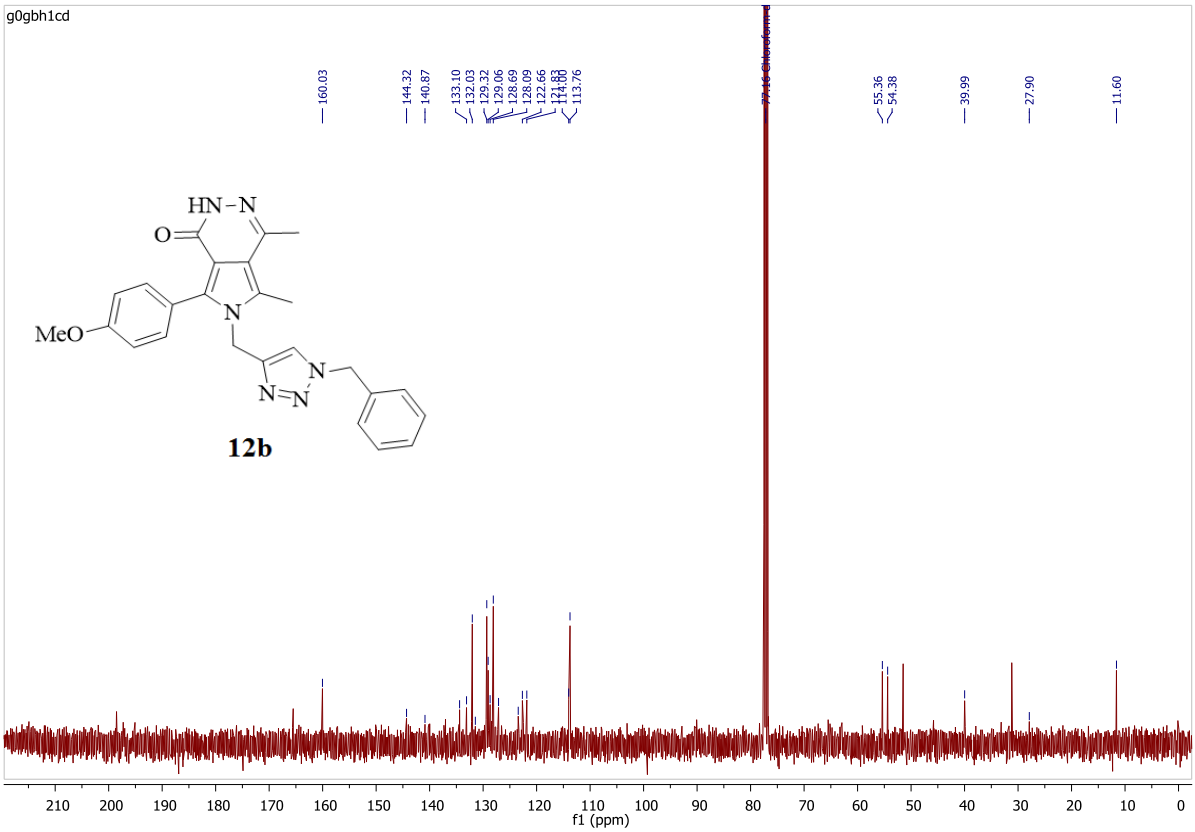


Figure S38. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **12b**.

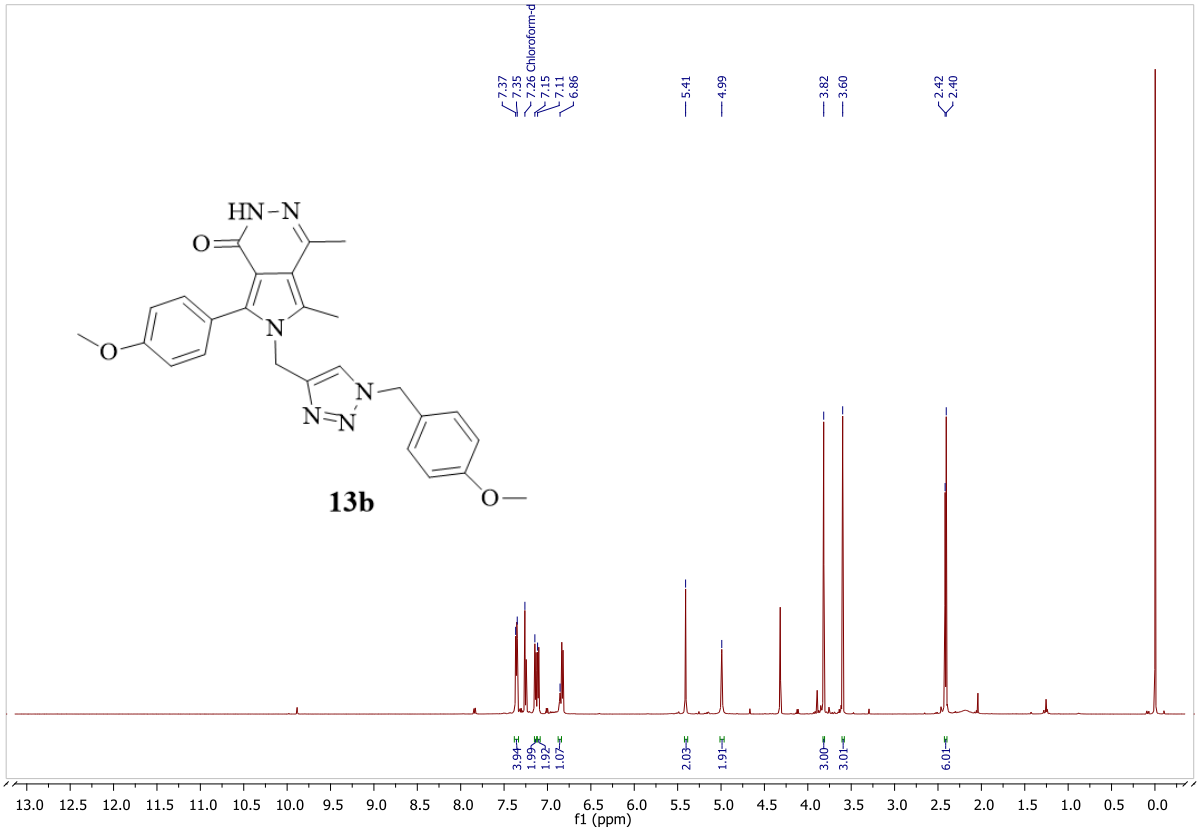


Figure S39. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **13b**.

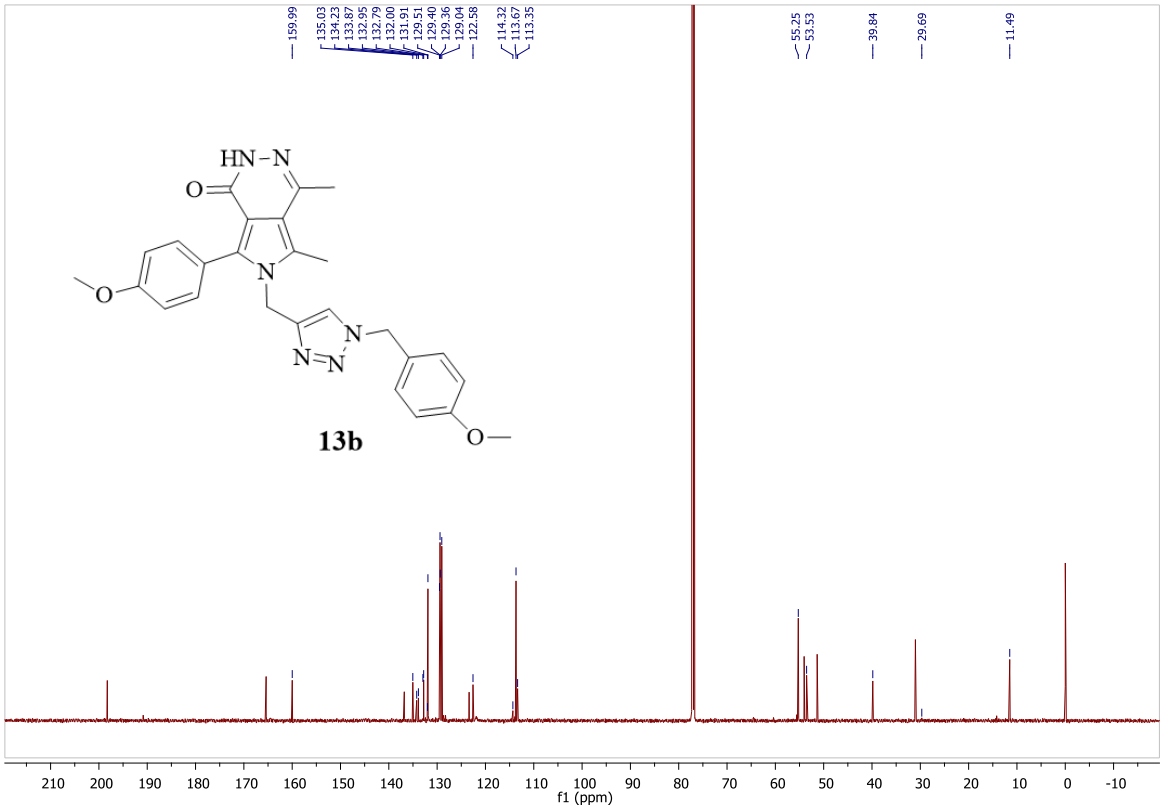


Figure S40. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **13b**.

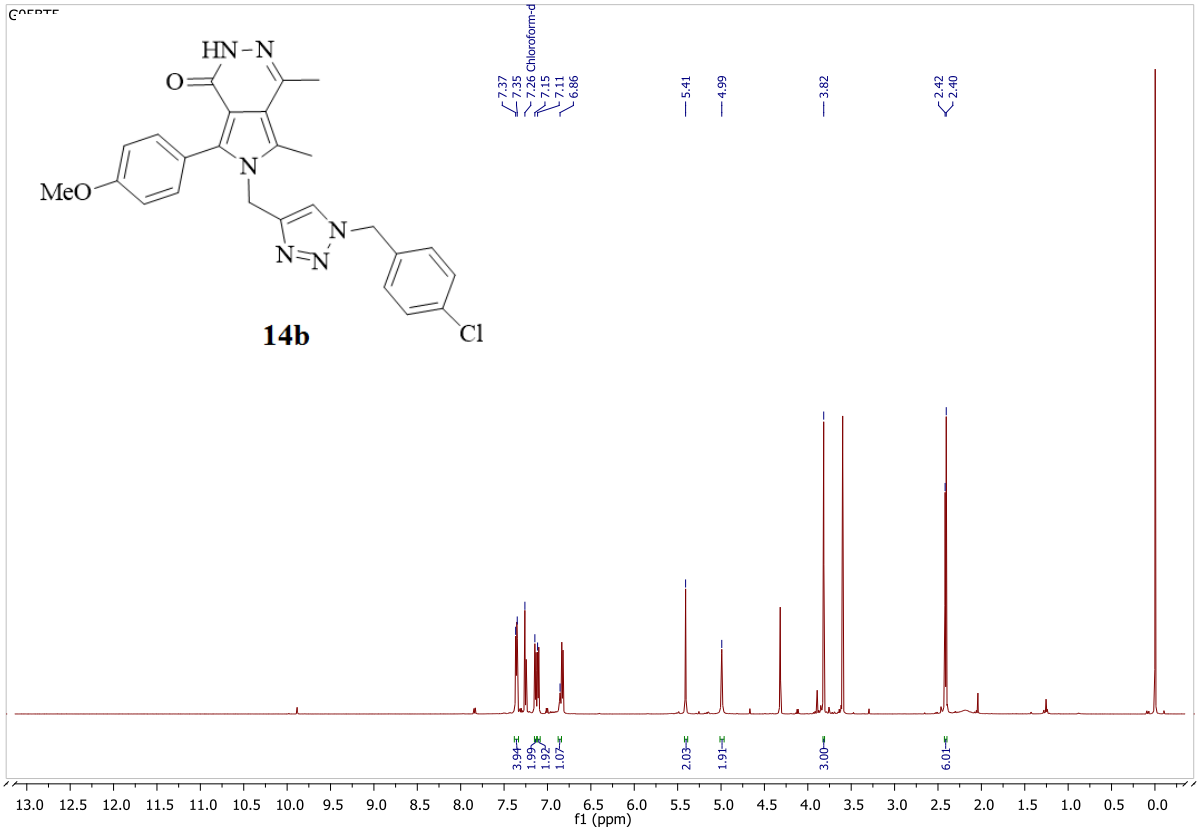


Figure S41. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **14b**.

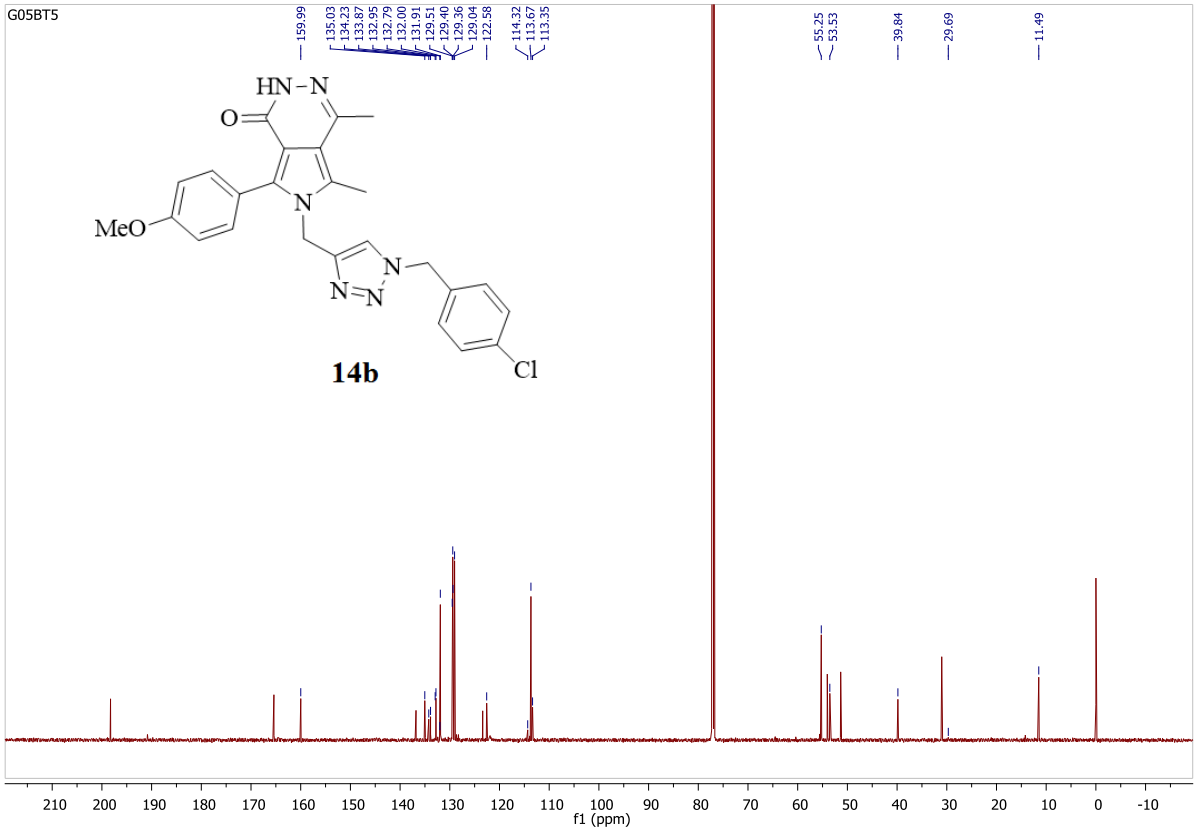


Figure S42. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **14b**.

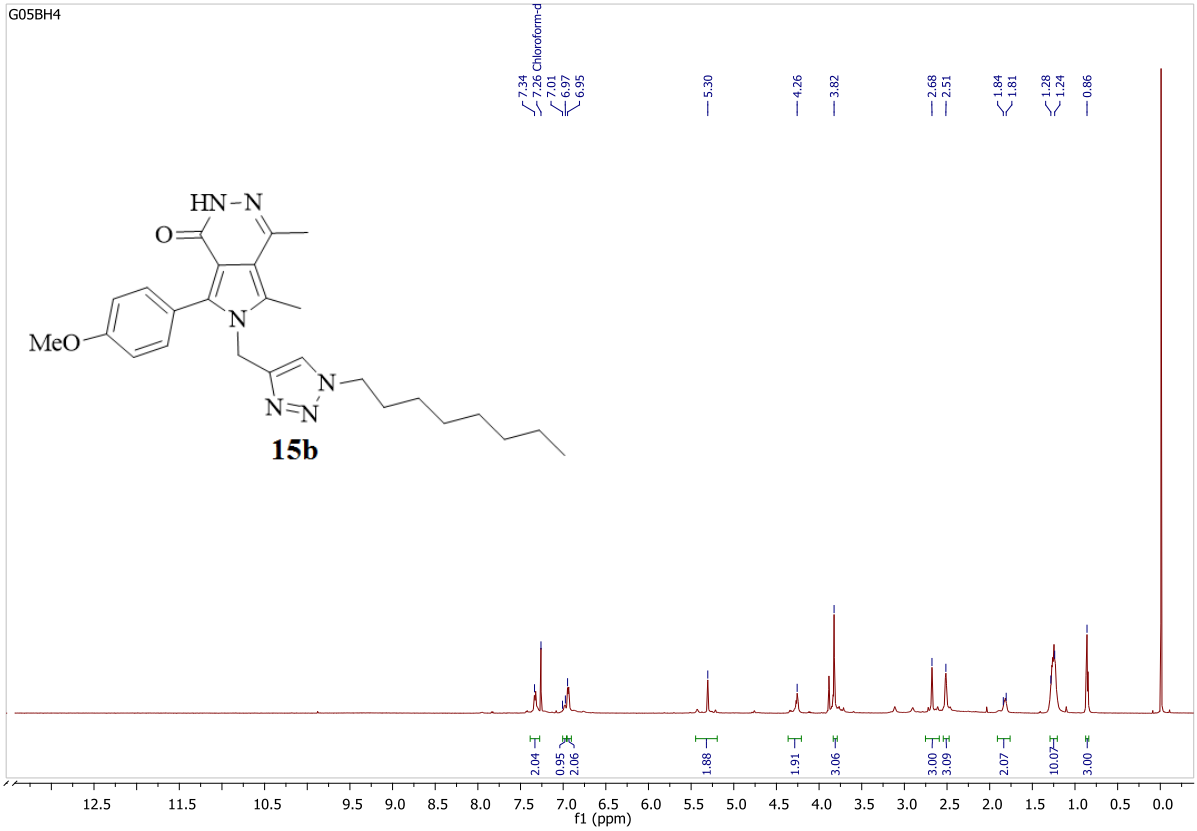


Figure S43. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **15b**.

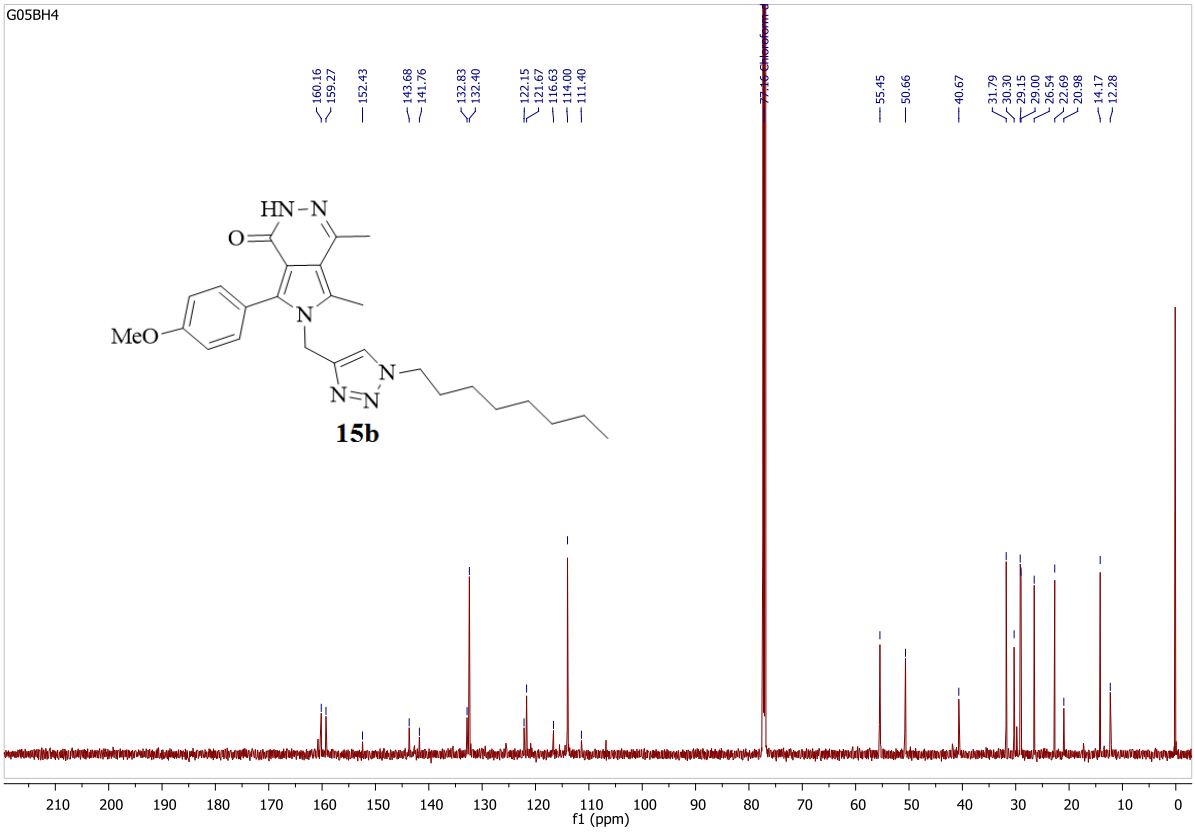


Figure S44. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of **15b**.

CheckCIF **3a**

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: shelx

```
Bond precision:  C-C = 0.0033 A          Wavelength=1.54178

Cell:            a=10.3244(3)     b=19.9176(6)        c=8.2093(2)
                 alpha=90         beta=111.090(1)     gamma=90
Temperature:     293 K
```

	Calculated	Reported
Volume	1575.06(8)	1575.06(8)
Space group	C c	C c
Hall group	C -2yc	C -2yc
Moiety formula	C18 H15 N O3	?
Sum formula	C18 H15 N O3	C18 H15 N O3
Mr	293.31	293.31
Dx,g cm-3	1.237	1.237
Z	4	4
Mu (mm-1)	0.689	0.689
F000	616.0	616.0
F000'	617.93	
h,k,lmax	12,23,9	12,23,9
Nref	2889[1450]	2375
Tmin,Tmax		
Tmin'		

```
Correction method= Not given

Data completeness= 1.64/0.82      Theta(max)= 68.237

R(reflections)= 0.0312( 2369)     wR2(reflections)= 0.0882( 2375)

S = 1.088                 Npar= 203
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given     Please Do !
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...     Please Check
PLAT054_ALERT_1_C Medium  Crystal Dimension Missing (or Error) ...     Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...     Please Check
PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) ........      6.79 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600       68 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....       25 Note
PLAT915_ALERT_3_C No Flack x Check Done: Low Friedel Pair Coverage       69 %
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.       0 Info
```

Alert level G

```
PLAT019_ALERT_1_G _diffrn_measured_fraction_theta_full/*_max < 1.0     0.663 Report
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High .     0.300 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)       293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)       293 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C11 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        33 Check
             O411 -C25  -H25     1.655   1.555   1.555          40.60 Deg.
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).        2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        2 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...        5 Note
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   9 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   9 ALERT level G = General information/check it is not something unexpected

   7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 ALERT type 2 Indicator that the structure model may be wrong or deficient
   5 ALERT type 3 Indicator that the structure quality may be low
   3 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

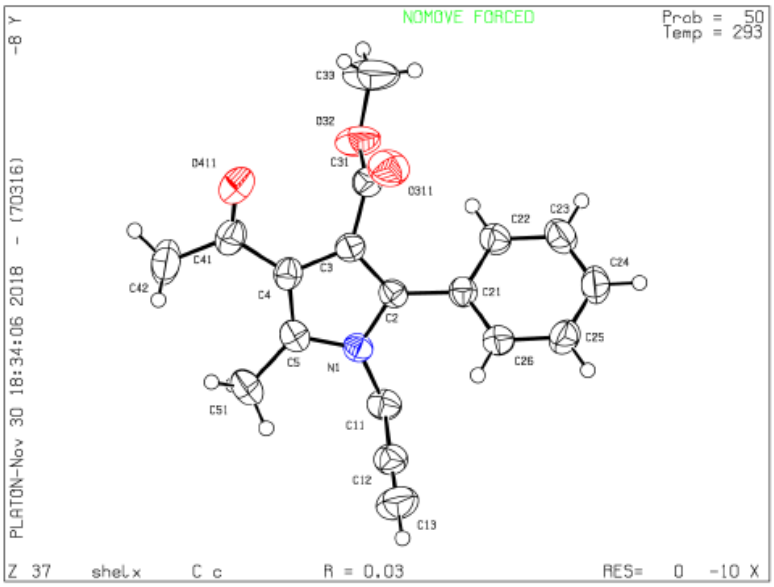
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 19/10/2018; check.def file version of 15/10/2018

Datablock shelx - ellipsoid plot



CheckCIF **8a**

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: shelx

```
Bond precision:  C-C = 0.0020 A          Wavelength=0.56086

Cell:          a=9.5258(4)        b=10.2250(4)     c=12.4371(5)
               alpha=107.545(1)   beta=91.326(1)   gamma=111.849(1)
Temperature:   273 K
```

	Calculated	Reported
Volume	1059.46(8)	1059.46(7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C25 H24 N4 O3	?
Sum formula	C25 H24 N4 O3	C25 H24 N4 O3
Mr	428.48	428.48
Dx,g cm-3	1.343	1.343
Z	2	2
Mu (mm-1)	0.057	0.057
F000	452.0	452.0
F000'	452.04	
h,k,lmax	15,16,20	15,16,20
Nref	9816	9775
Tmin,Tmax	0.985,0.990	
Tmin'	0.978	

```
Correction method= Not given

Data completeness= 0.996          Theta(max)= 27.405

R(reflections)= 0.0608( 6010)     wR2(reflections)= 0.1488( 9775)

S = 1.043                 Npar= 289
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given     Please Do !
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      5.376 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).          6 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         18 Report
```

Alert level G

```
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.001 Degree
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        273 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        273 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C51 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....      C411 Check
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C2       --C155           3.41 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C3       --C155           3.47 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C22      --C156           3.49 Ang.
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         17 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         24 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         17 Info
```

```
  0 ALERT level A = Most likely a serious problem - resolve or explain
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  0 ALERT type 5 Informative message, check
```

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PLATON version of 19/10/2018; check.def file version of 15/10/2018

Datablock shelx - ellipsoid plot