J. Braz. Chem. Soc., Vol. 26, No. 11, S1-S30, 2015.
Printed in Brazil - ©2015 Sociedade Brasileira de Química
0103 - 5053 $6.00+0.00

Supplementary Information

Synthesis, Structure Elucidation, Antioxidant and Antimicrobial Activity of Novel 2-(5-Trifluoromethyl-1*H*-pyrazol-1-yl)-5-(5-trihalomethyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridines

Helio G. Bonacorso,*,[a] Susiane Cavinatto,[a] Maiara C. Moraes,[a] Everton P. Pittaluga,[a] Luis R. Peroza,[b] Tarcieli Venturini,[c] Sydney H. Alves,[c] Sílvio T. Stefanello,[d] Félix A. A. Soares,[d] Marcos A. P. Martins,[a] Nilo Zanatta[a] and Clarissa P. Frizzo[a]

[a]NUQUIMHE, Departamento de Química, [b]NEUROTOX, Departamento de Toxicologia Bioquímica, [c]LAPEMI, Departamento de Parasitologia e Microbiologia and [d]Departmento de Bioquímica e Biologia Molecular, Universidade Federal de Santa Maria, 97105-900 Santa Maria-RS, Brazil

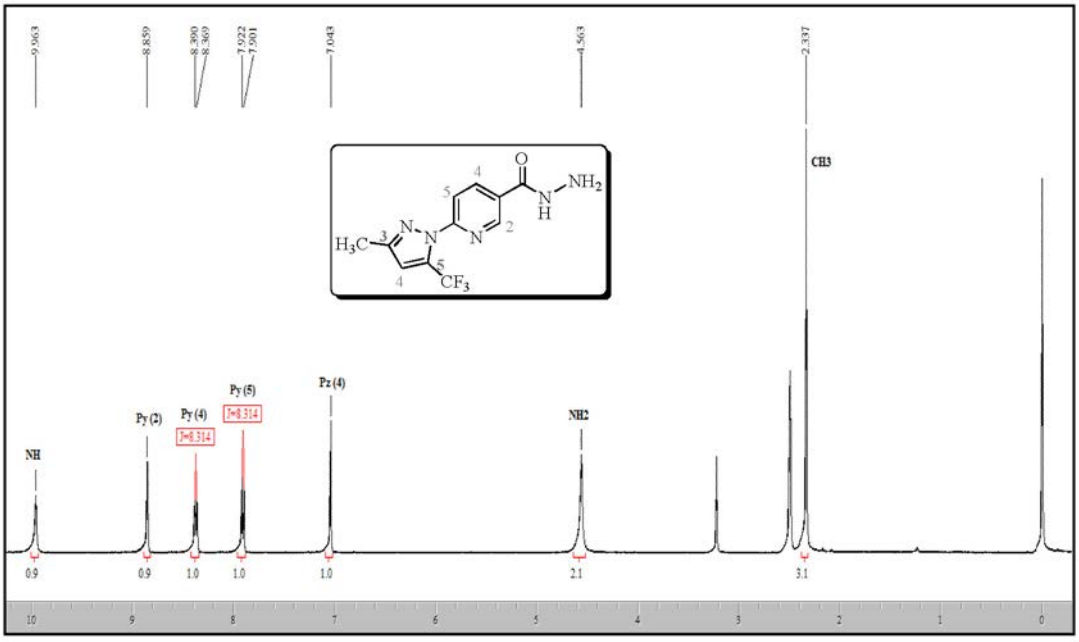

Figure S1. ^{1}H NMR spectrum (400.13 MHz, DMSO-d_6) of 6-(5-trifluoromethyl-3-methyl-1*H*-pyrazol-1-yl) nicotinohydrazide (**1**).

*e-mail: helio.bonacorso@ufsm.br

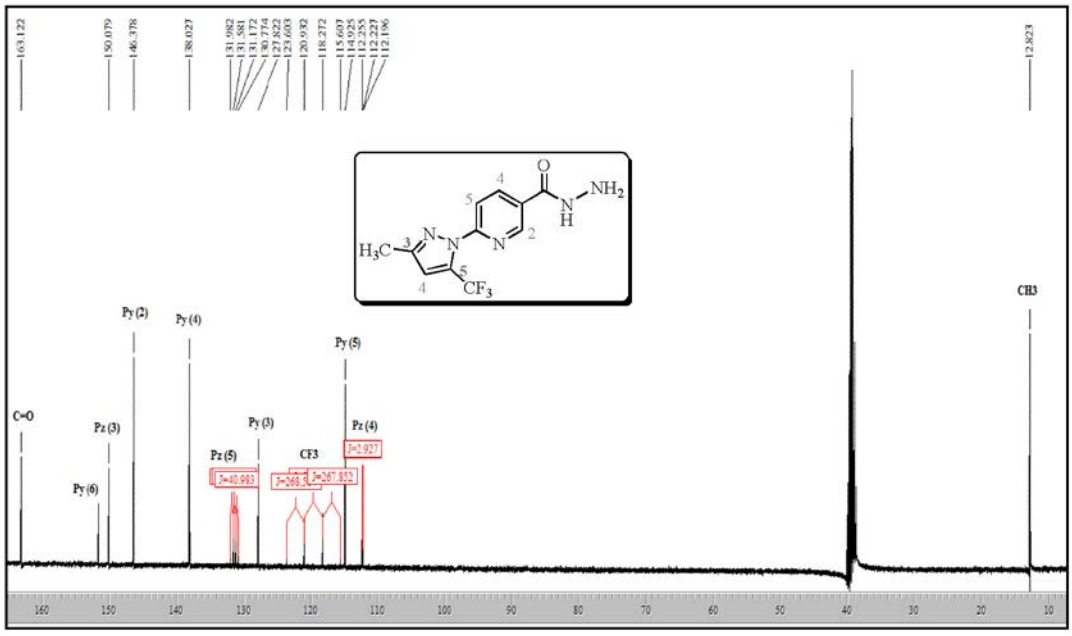

Figure S2. ^{13}C {^{1}H} NMR spectrum (100.61 MHz, DMSO-d_6) of 6-(5-trifluoromethyl-3-methyl-1*H*-pyrazol-1-yl) nicotinohydrazide (**1**).

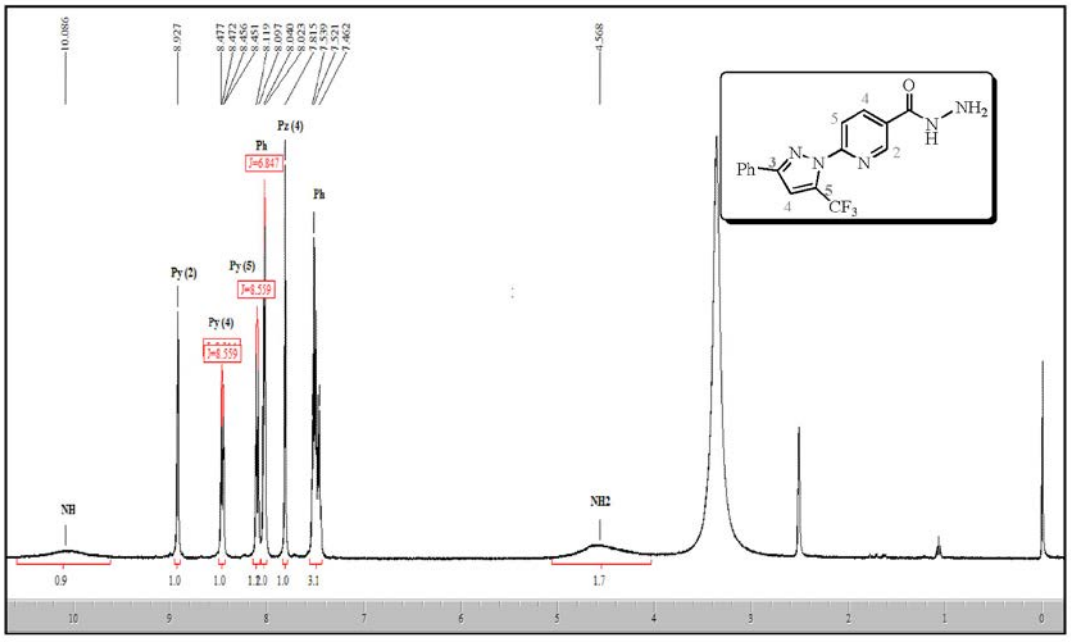

Figure S3. ^{1}H NMR spectrum (400.13 MHz, DMSO-d_6) of 6-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl) nicotinohydrazide (**2**).

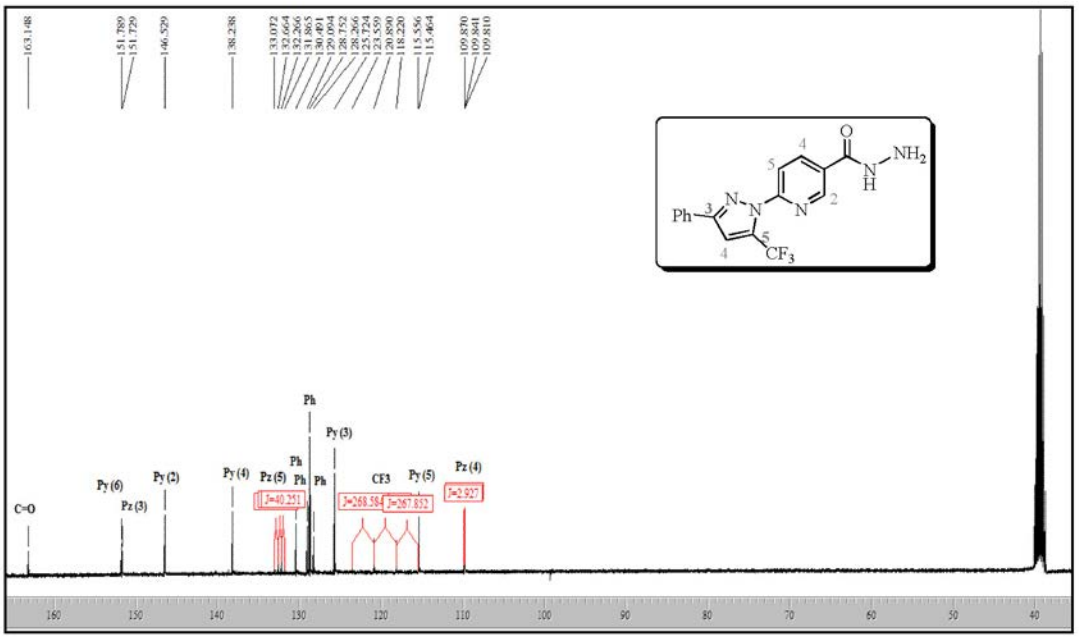

Figure S4. ^{13}C {^{1}H} NMR spectrum (100.61 MHz, DMSO-d_6) of 6-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl) nicotinohydrazide (**2**).

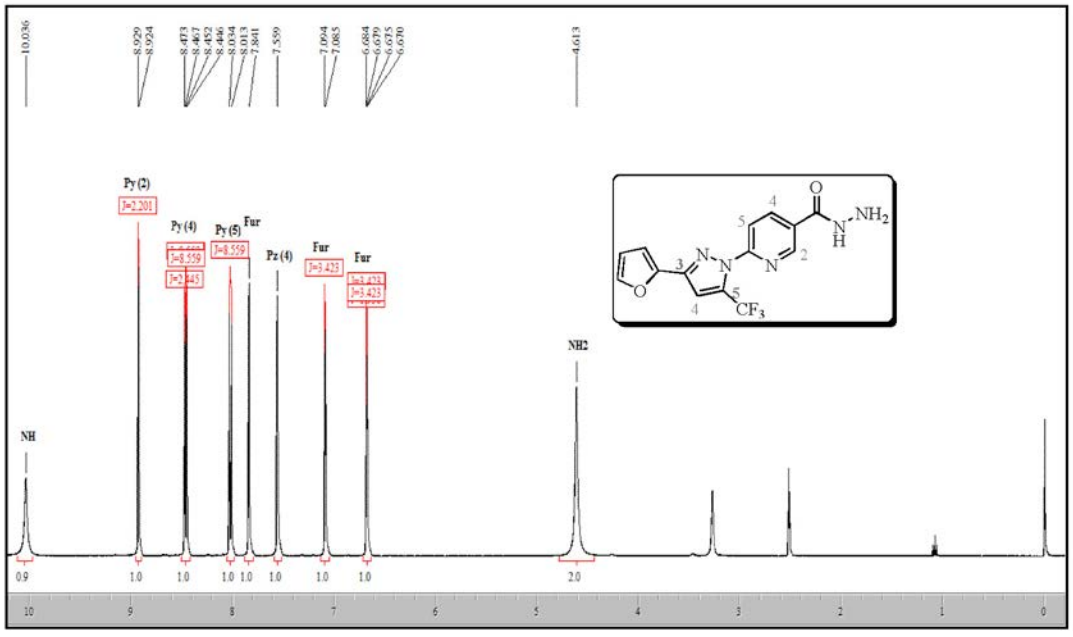

Figure S5. ^{1}H NMR spectrum (400.13 MHz, DMSO-d_6) of 6-(5-trifluoromethyl-3-(fur-2-yl)-1*H*-pyrazol-1-yl) nicotinohydrazide (**3**).

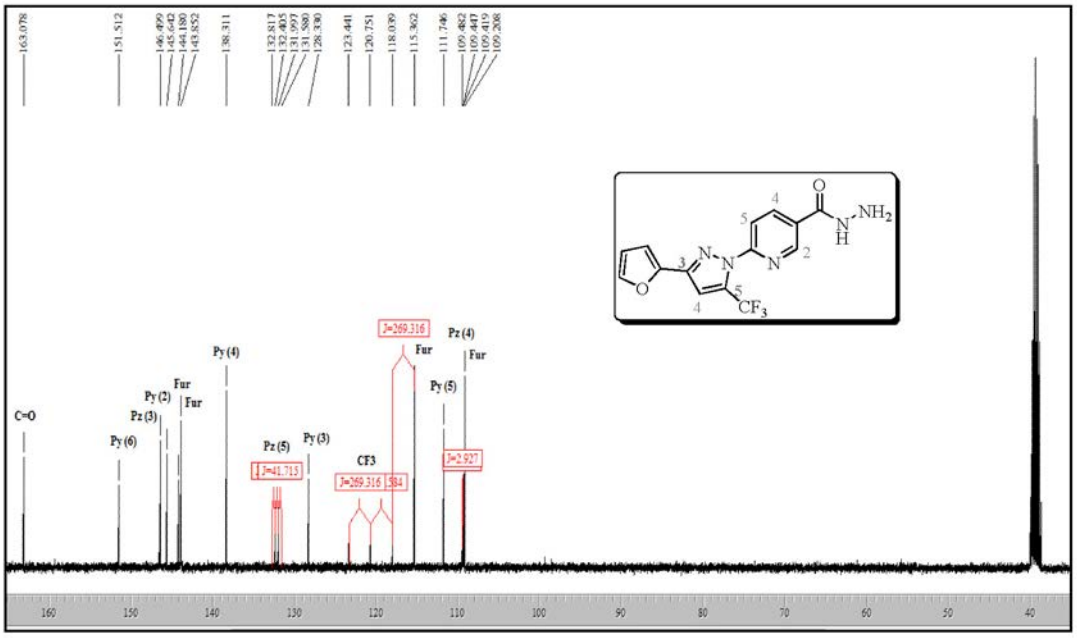

Figure S6. ^{13}C {^{1}H} NMR spectrum (100.61 MHz, DMSO-d_6) of 6-(5-trifluoromethyl-3-(fur-2-yl)-1*H*-pyrazol-1-yl) nicotinohydrazide (**3**).

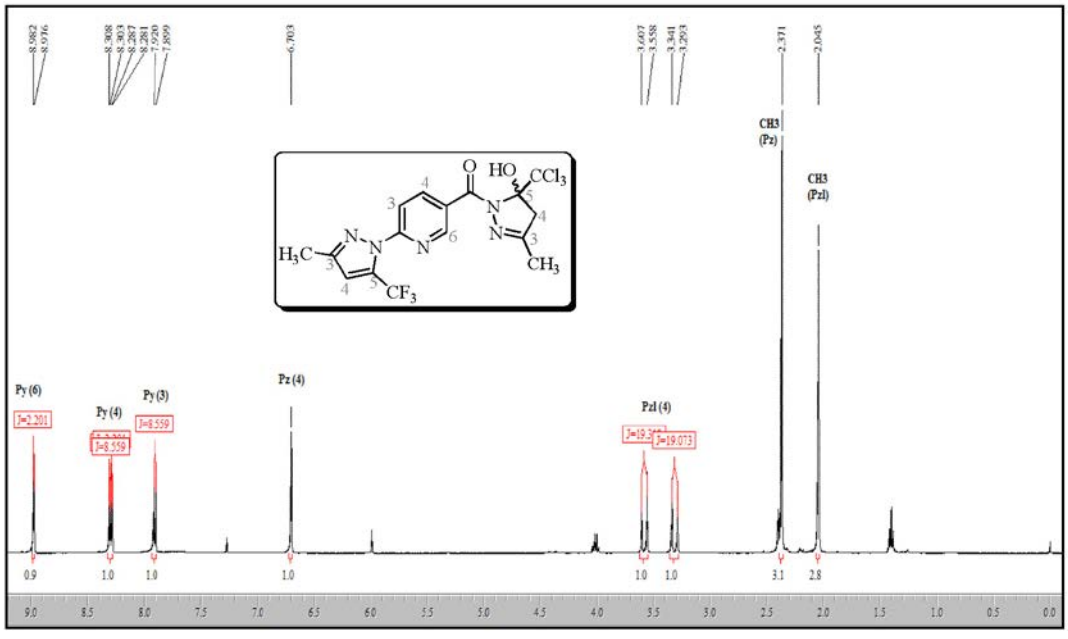

Figure S7. ^{1}H NMR spectrum (400.13 MHz, $CDCl_3$) of 2-(5-trifluoromethyl-3-methyl-1*H*-pyrazol-1-yl)-5-(5-trichloromethyl-4,5-dihydro-5-hydroxy-3-methyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**6a**).

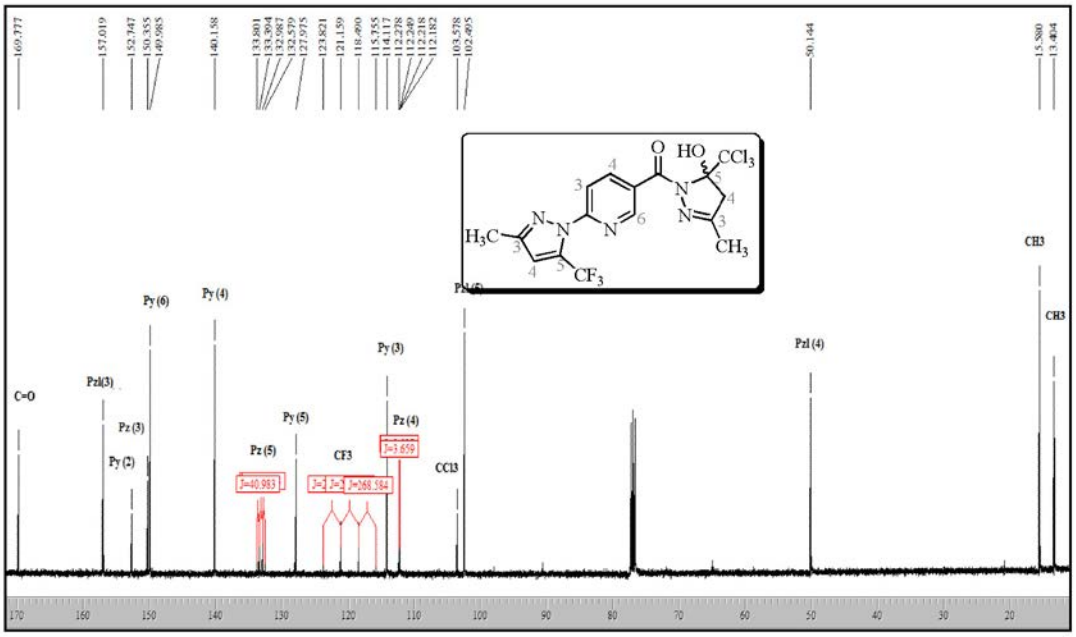

Figure S8. ^{13}C {^{1}H} NMR spectrum (100.61 MHz, $CDCl_3$) of 2-(5-trifluoromethyl-3-methyl-1*H*-pyrazol-1-yl)-5-(5-trichloromethyl-4,5-dihydro-5-hydroxy-3-methyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**6a**).

Figure S9. ^{19}F NMR spectrum (564.68 MHz, $CDCl_3$) of 2-(5-trifluoromethyl-3-methyl-1*H*-pyrazol-1-yl)-5-(5-trichloromethyl-4,5-dihydro-5-hydroxy-3-methyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**6a**).

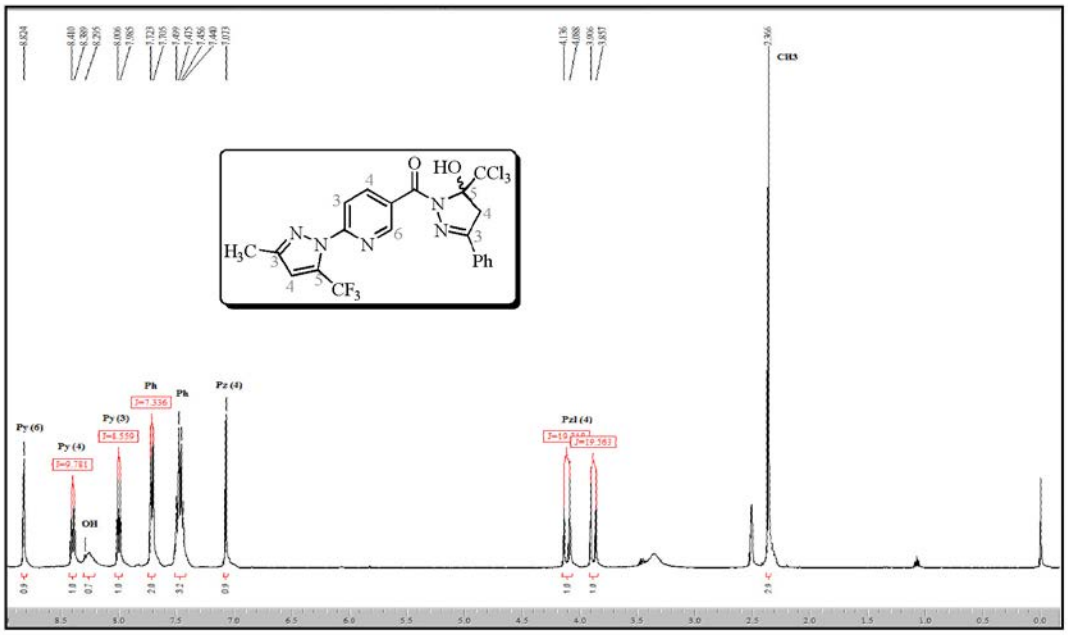

Figure S10. ^{1}H NMR spectrum (400.13 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-methyl-1*H*-pyrazol-1-yl)-5-(5-trichloromethyl-4,5-dihydro-5-hydroxy-3-phenyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**6b**).

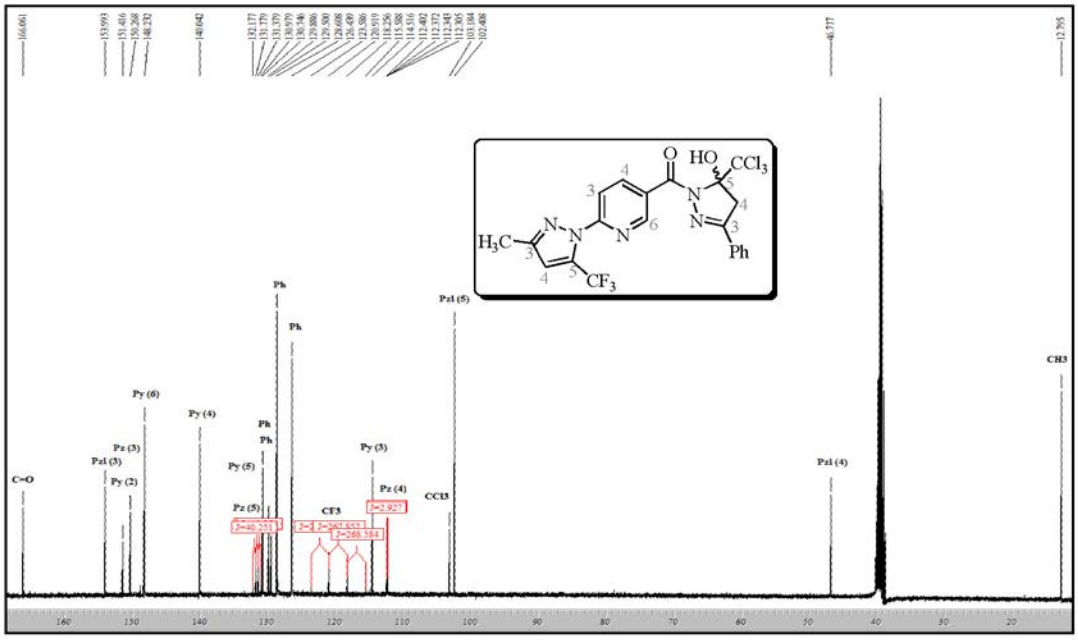

Figure S11. ^{13}C {^{1}H} NMR spectrum (100.61 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-methyl-1*H*-pyrazol-1-yl)-5-(5-trichloromethyl-4,5-dihydro-5-hydroxy-3-phenyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**6b**).

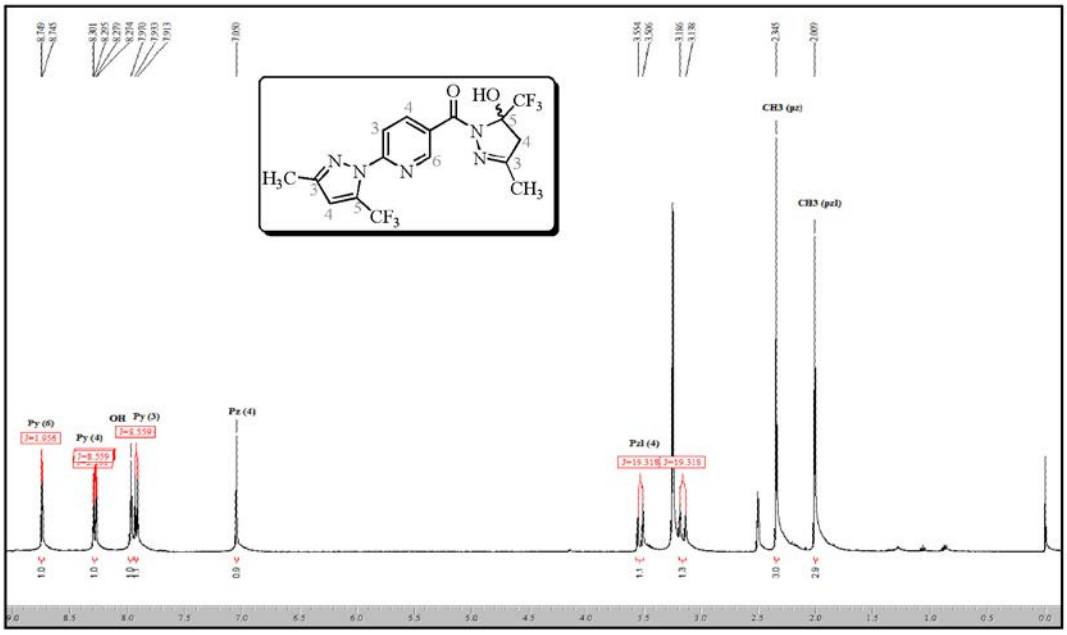

Figure S12. ^{1}H NMR spectrum (400.13 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-methyl-1*H*-pyrazol-1-yl)-5-(5-trifluoromethyl-4,5-dihydro-5-hydroxy-3-methyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**7a**).

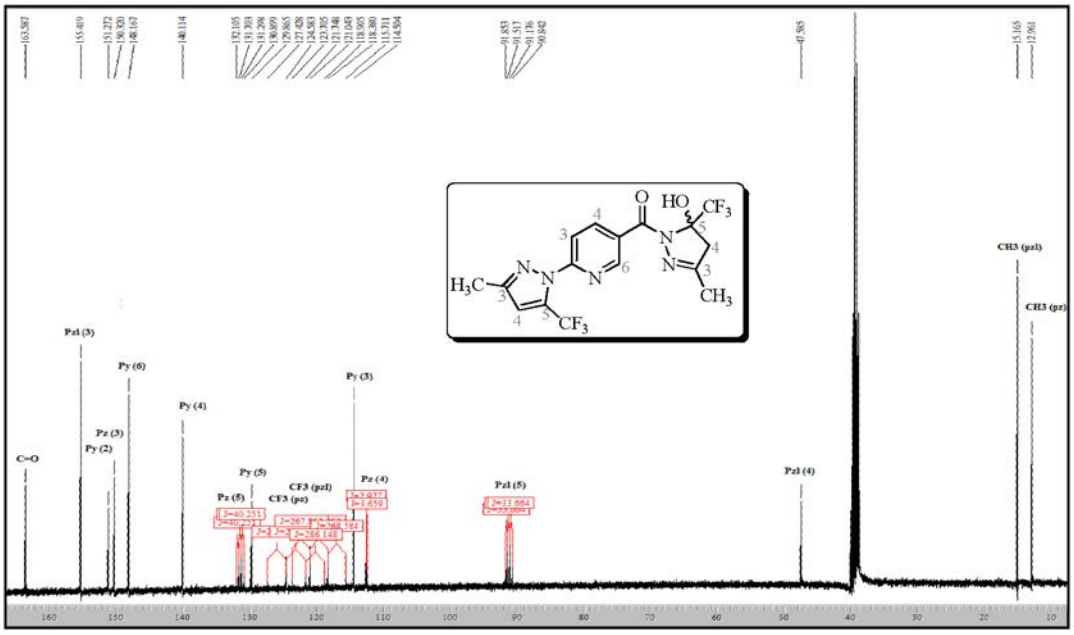

Figure S13. ^{13}C {^{1}H} NMR spectrum (100.61 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-methyl-1*H*-pyrazol-1-yl)-5-(5-trifluoromethyl-4,5-dihydro-5-hydroxy-3-methyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**7a**).

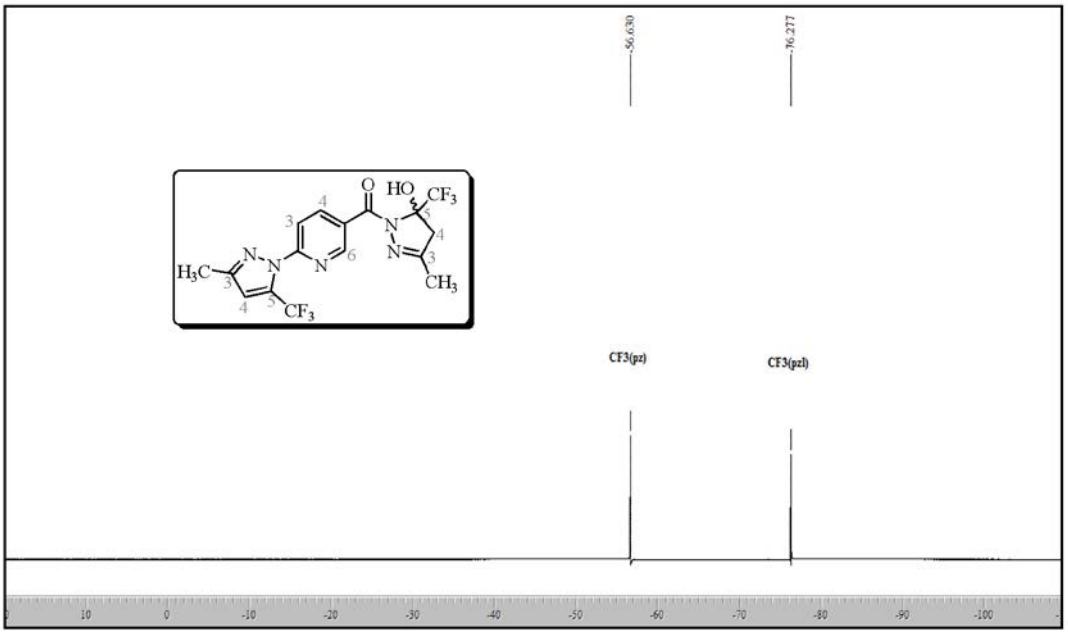

Figure S14. ^{19}F NMR spectrum (564.68 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-methyl-1*H*-pyrazol-1-yl)-5-(5-trifluoromethyl-4,5-dihydro-5-hydroxy-3-methyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**7a**).

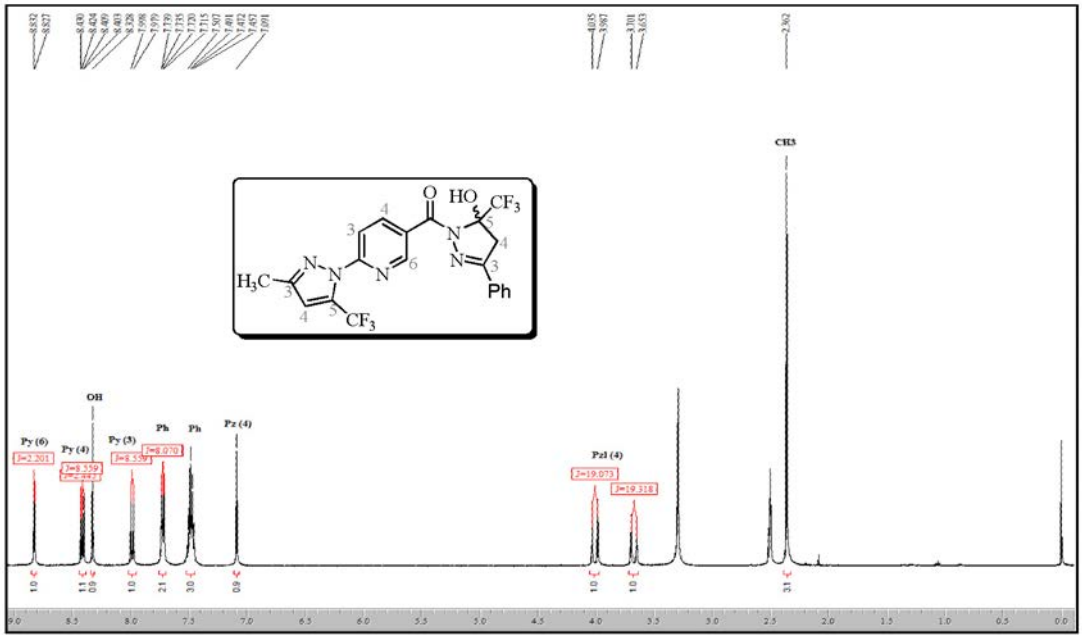

Figure S15. ^{1}H NMR spectrum (400.13 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-methyl-1*H*-pyrazol-1-yl)-5-(5-trifluoromethyl-4,5-dihydro-5-hydroxy-3-phenyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**7b**).

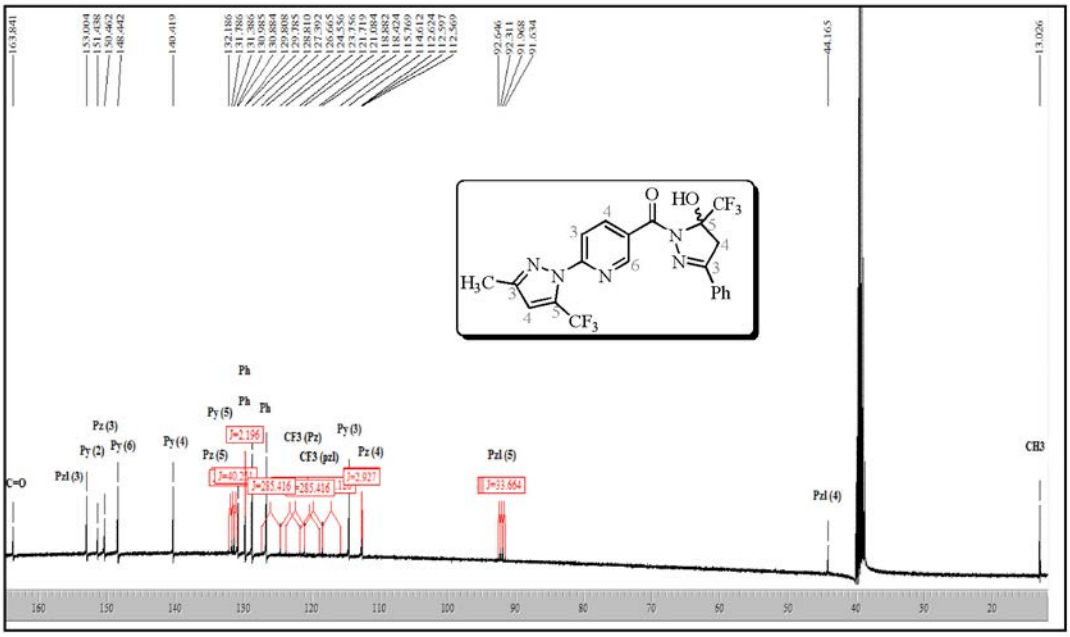

Figure S16. ^{13}C {^{1}H} NMR spectrum (100.61 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-methyl-1*H*-pyrazol-1-yl)-5-(5-trifluoromethyl-4,5-dihydro-5-hydroxy-3-phenyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**7b**).

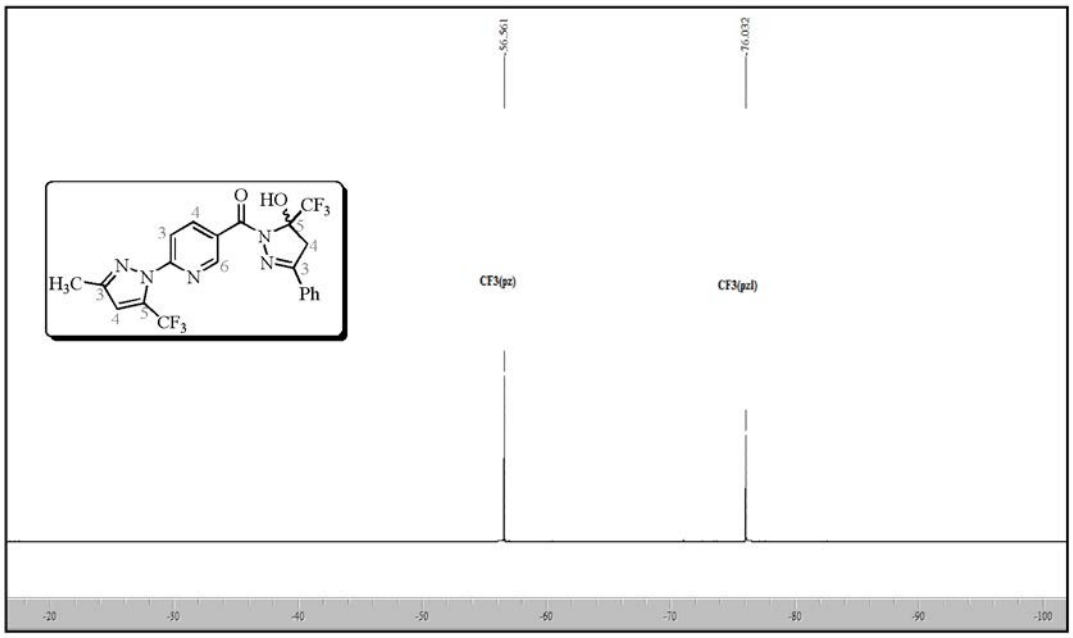

Figure S17. ^{19}F NMR spectrum (564.68 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-methyl-1*H*-pyrazol-1-yl)-5-(5-trifluoromethyl-4,5-dihydro-5-hydroxy-3-phenyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**7b**).

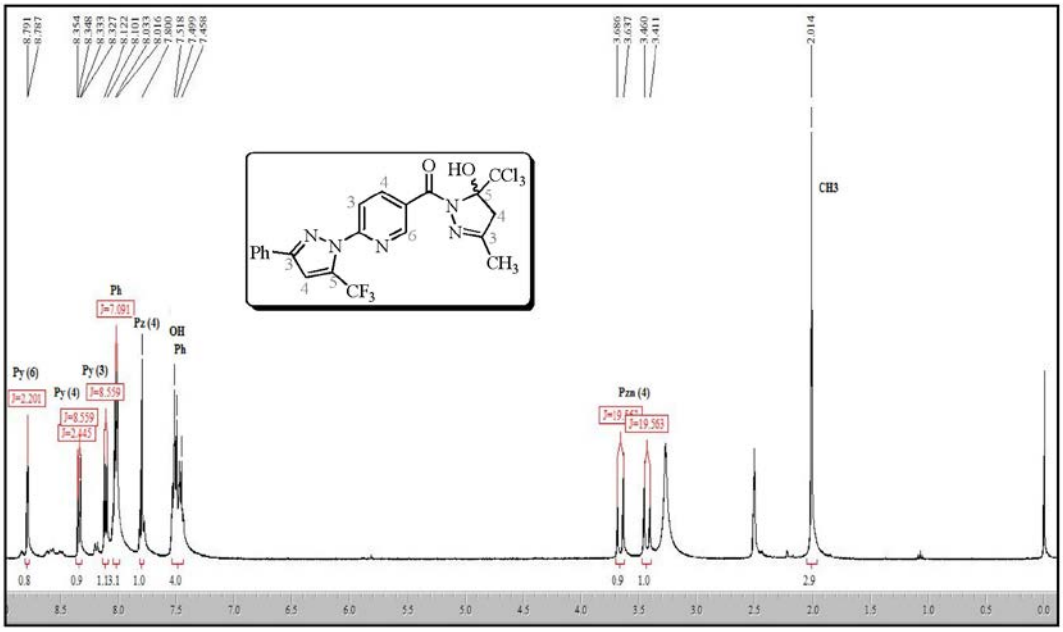

Figure S18. ^{1}H NMR spectrum (400.13 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(5-trichloromethyl-4,5-dihydro-5-hydroxy-3-methyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**8c**).

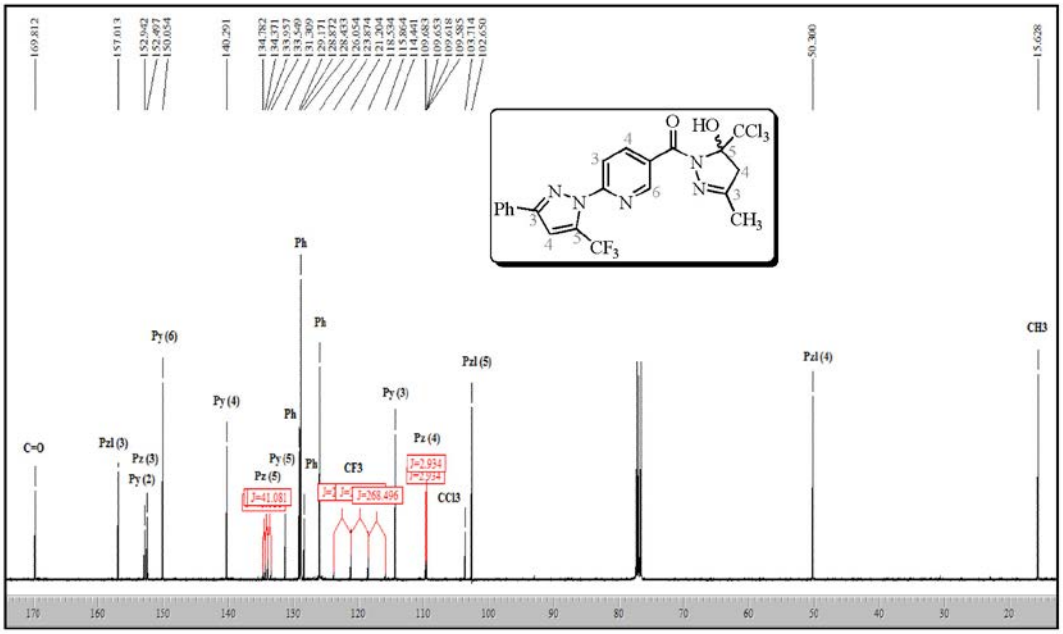

Figure S19. ^{13}C {^{1}H} NMR spectrum (100.61 MHz, $CDCl_3$) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(5-trichloromethyl-4,5-dihydro-5-hydroxy-3-methyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**8c**).

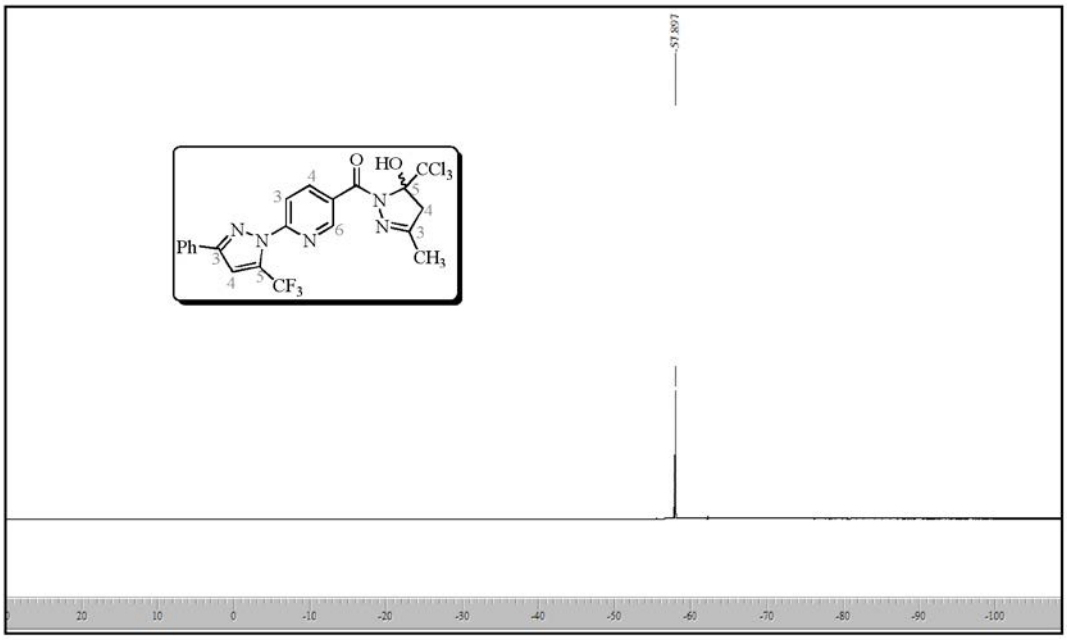

Figure S20. [19]F NMR spectrum (564.68 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(5-trichloromethyl-4,5-dihydro-5-hydroxy-3-methyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**8c**).

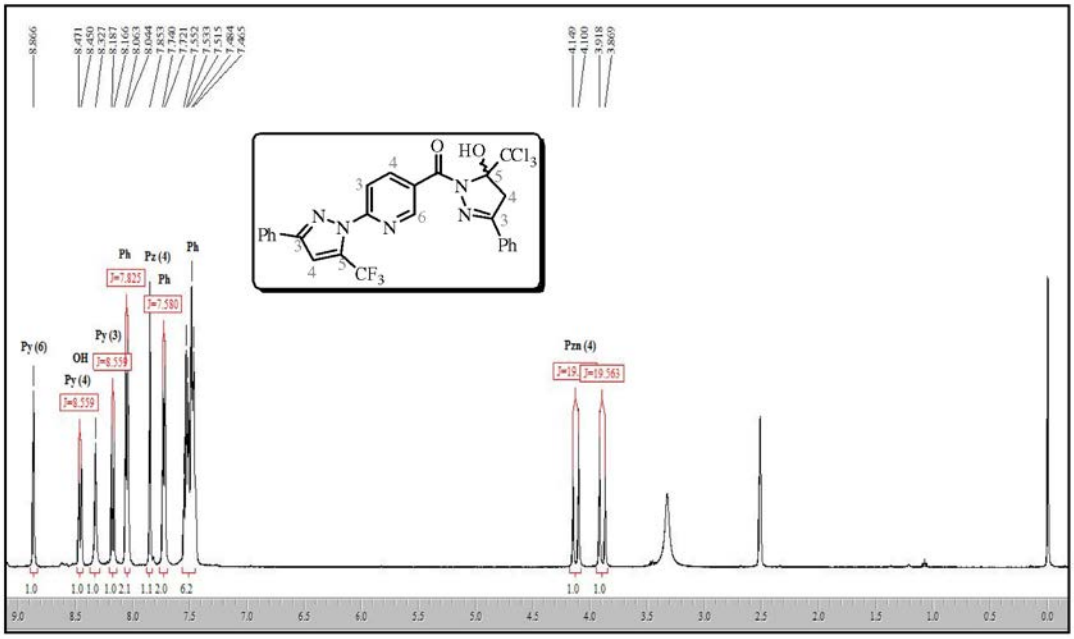

Figure S21. [1]H NMR spectrum (400.13 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(5-trichloromethyl-4,5-dihydro-5-hydroxy-3-phenyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**8d**).

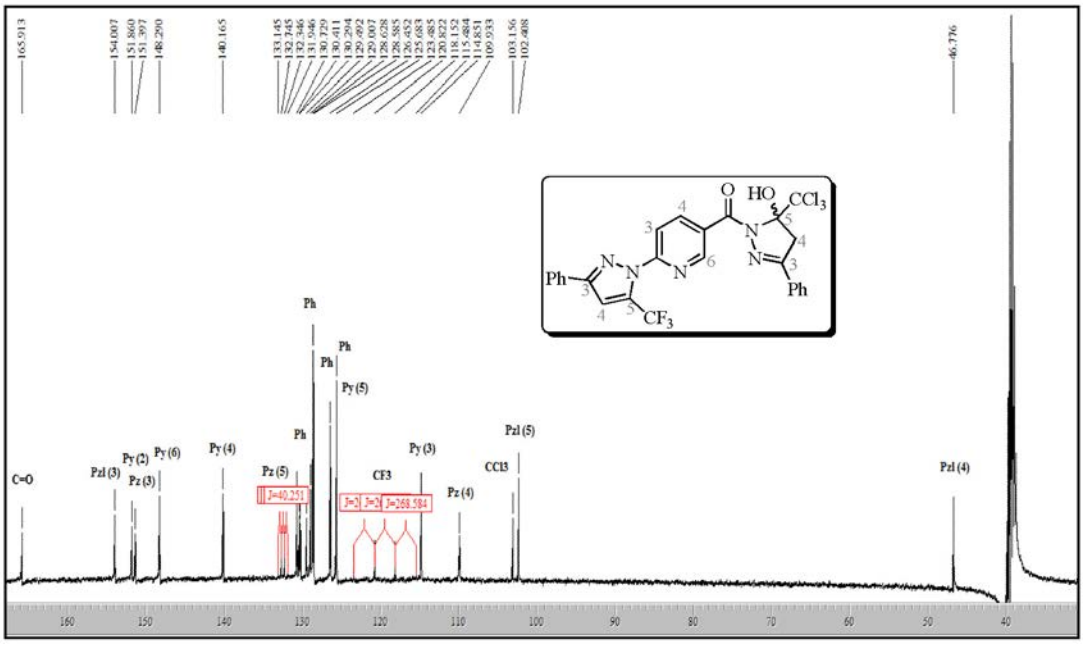

Figure S22. ^{13}C {^{1}H} NMR spectrum (100.61 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(5-trichloromethyl-4,5-dihydro-5-hydroxy-3-phenyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**8d**).

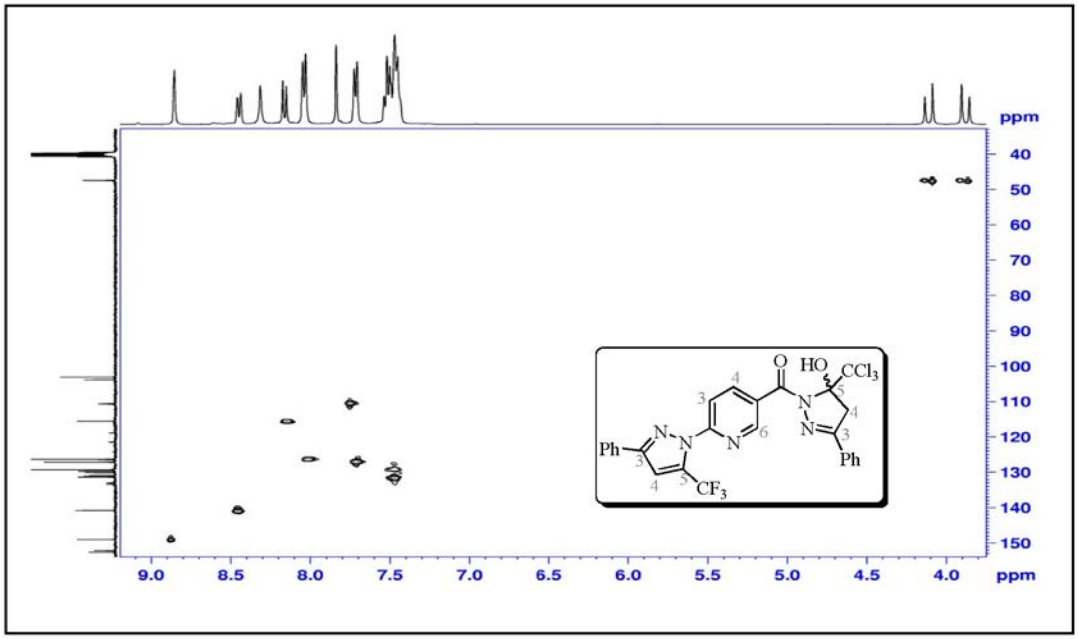

Figure S23. 2D HSQC spectrum (100.61 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(5-trichloromethyl-4,5-dihydro-5-hydroxy-3-phenyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**8d**).

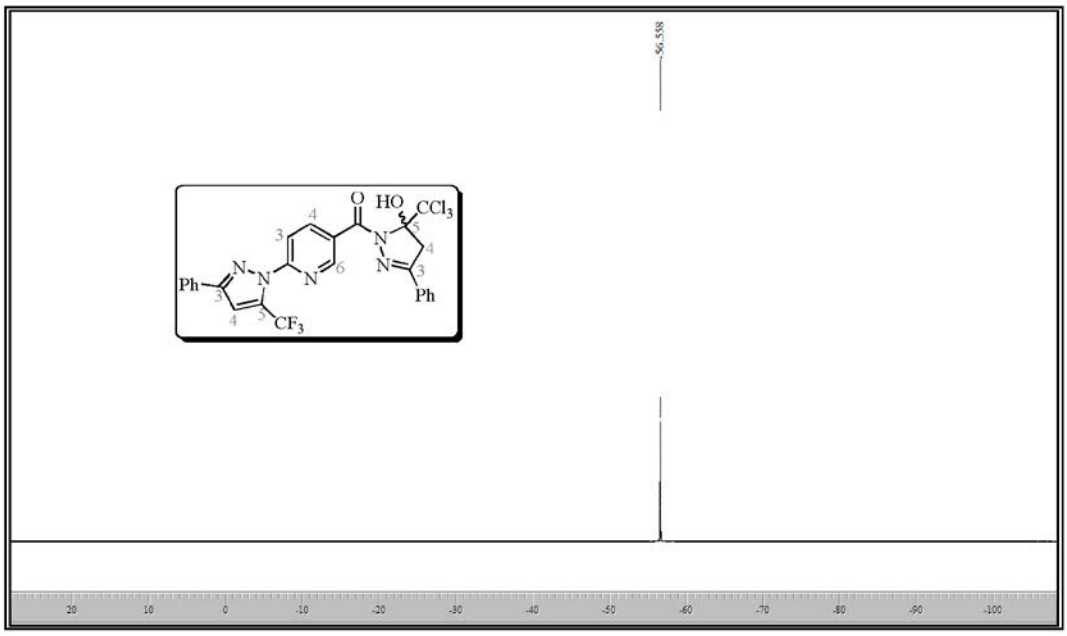

Figure S24. [19]F NMR spectrum (564.68 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(5-trichloromethyl-4,5-dihydro-5-hydroxy-3-phenyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**8d**).

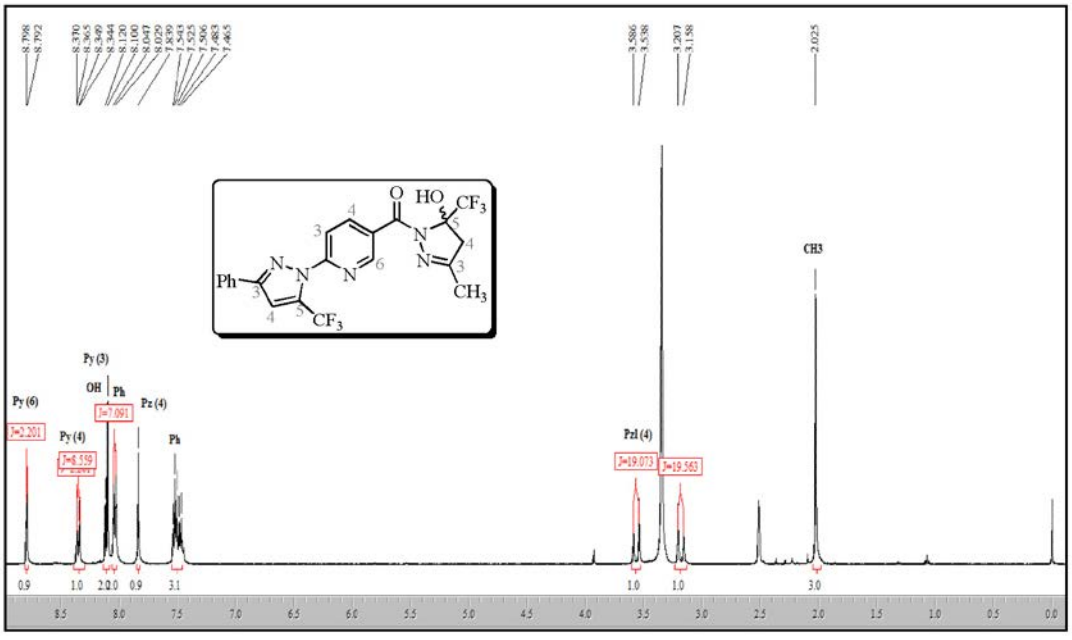

Figure S25. [1]H NMR spectrum (400.13 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(5-trifluoromethyl-4,5-dihydro-5-hydroxy-3-methyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**9c**).

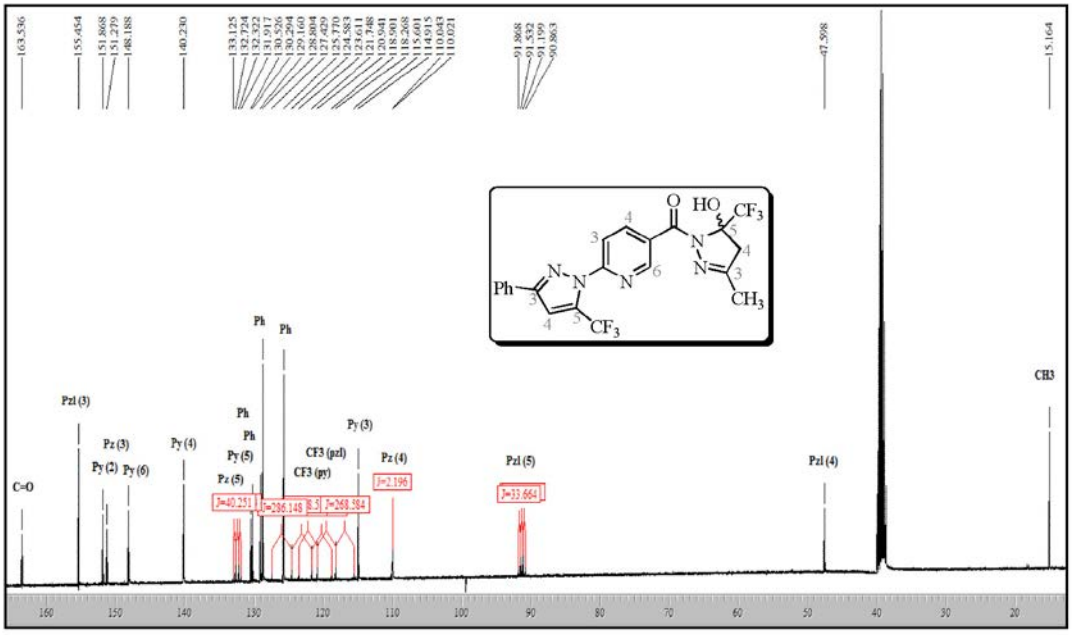

Figure S26. ^{13}C {^{1}H} NMR spectrum (100.61 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(5-trifluoromethyl-4,5-dihydro-5-hydroxy-3-methyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**9c**).

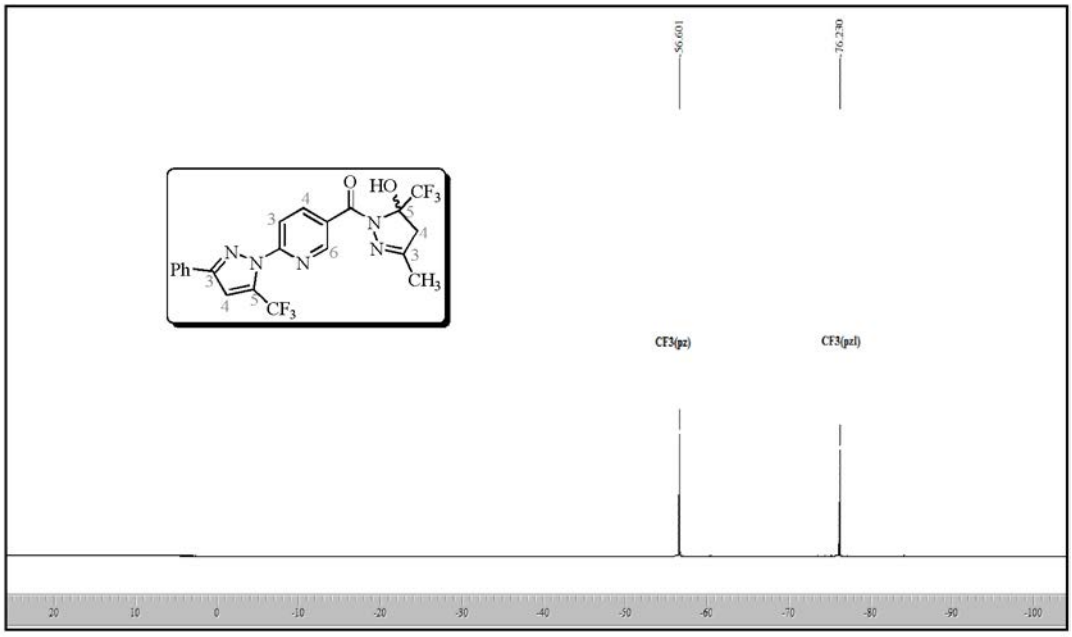

Figure S27. ^{19}F NMR spectrum (564.68 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(5-trifluoromethyl-4,5-dihydro-5-hydroxy-3-methyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**9c**).

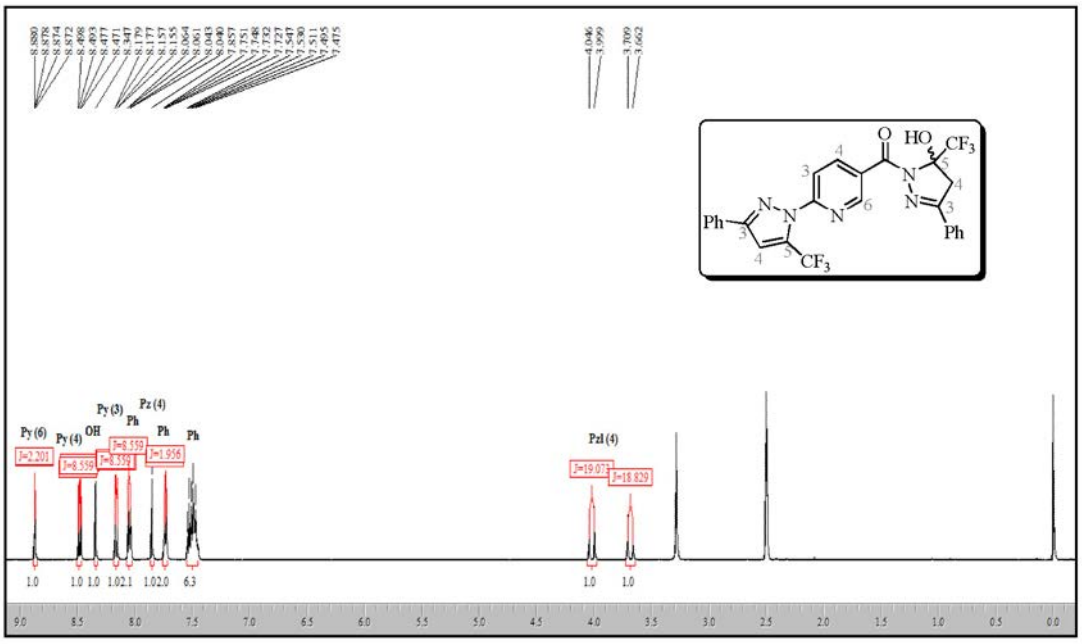

Figure S28. [1]H NMR spectrum (400.13 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(5-trifluoromethyl-4,5-dihydro-5-hydroxy-3-phenyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**9d**).

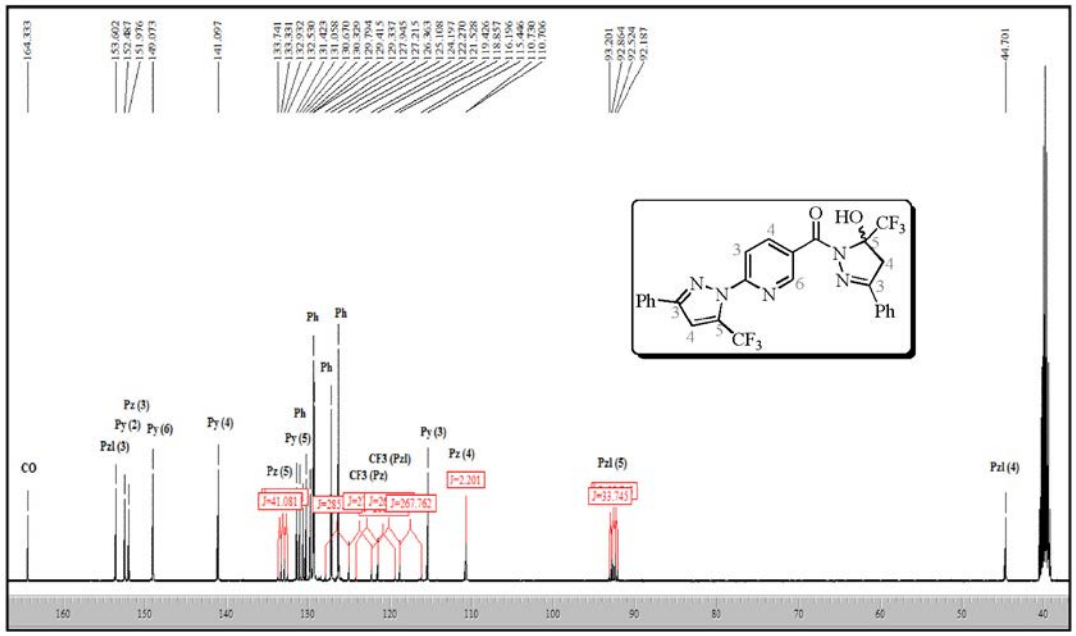

Figure S29. [13]C {[1]H} NMR spectrum (100.61 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(5-trifluoromethyl-4,5-dihydro-5-hydroxy-3-phenyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**9d**).

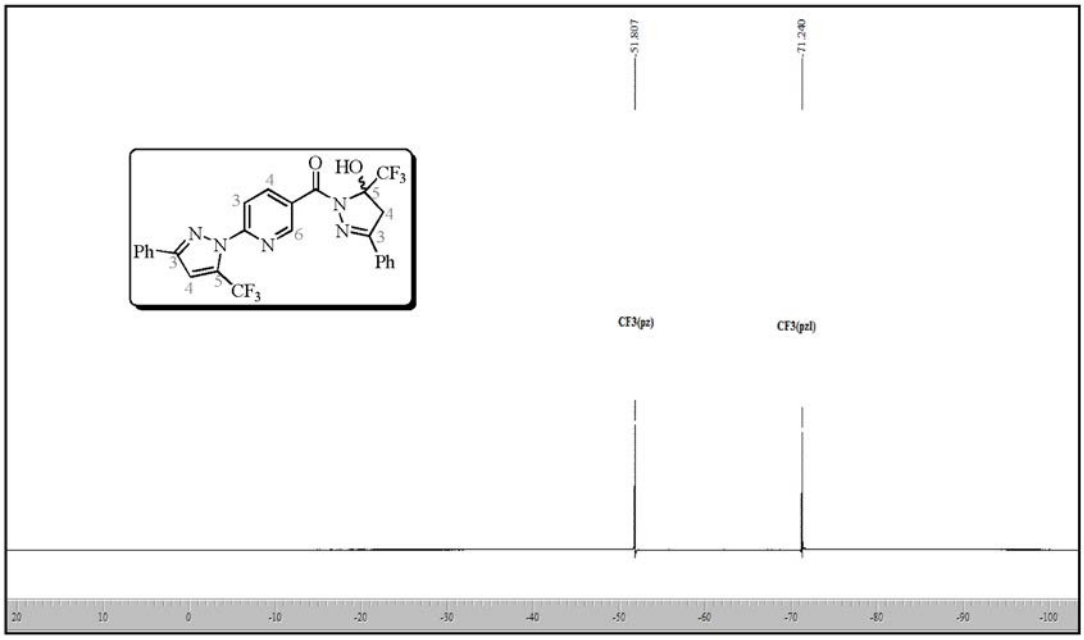

Figure S30. [19]F NMR spectrum (564.68 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(5-trifluoromethyl-4,5-dihydro-5-hydroxy-3-phenyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**9d**).

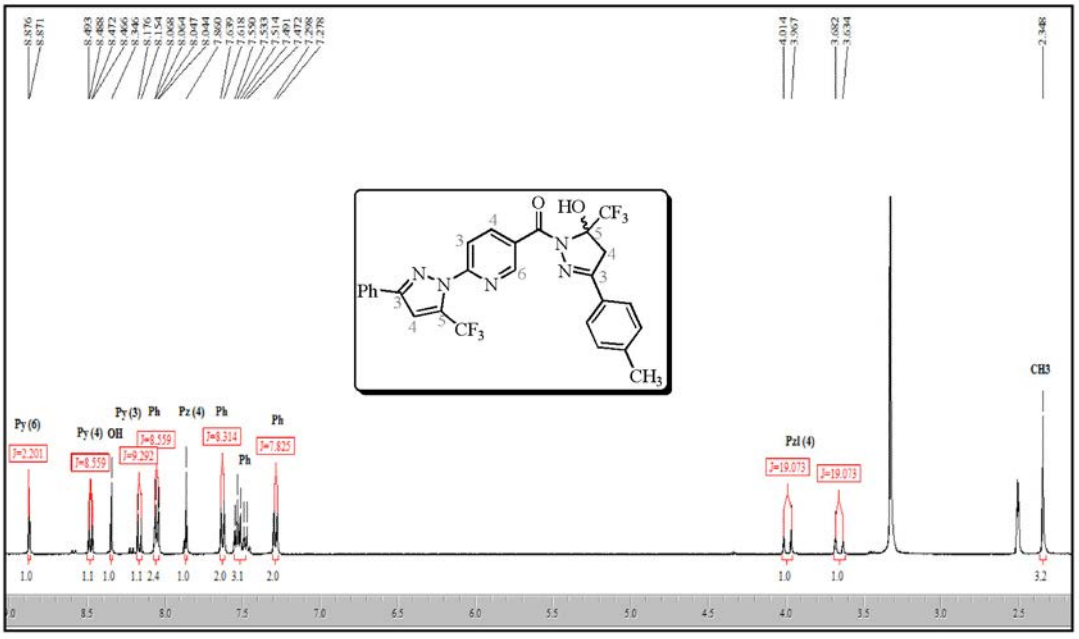

Figure S31. [1]H NMR spectrum (400.13 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(5-trifluoromethyl-4,5-dihydro-5-hydroxy-3-(4-methylphenyl)-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**9e**).

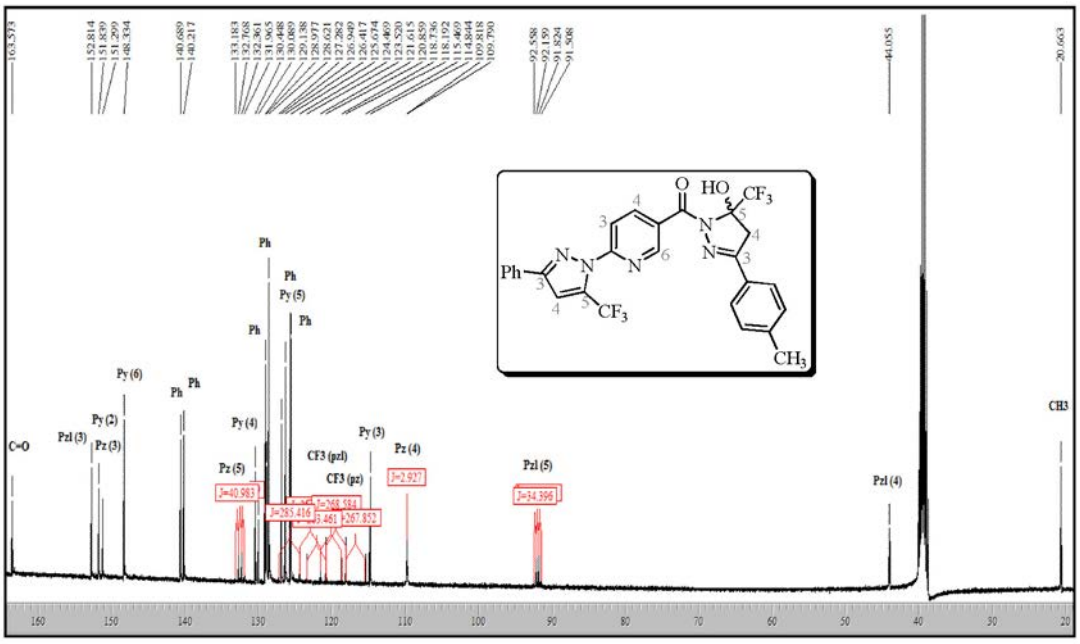

Figure S32. ^{13}C {^{1}H} NMR spectrum (100.61 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(5-trifluoromethyl-4,5-dihydro-5-hydroxy-3-(4-methylphenyl)-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**9e**).

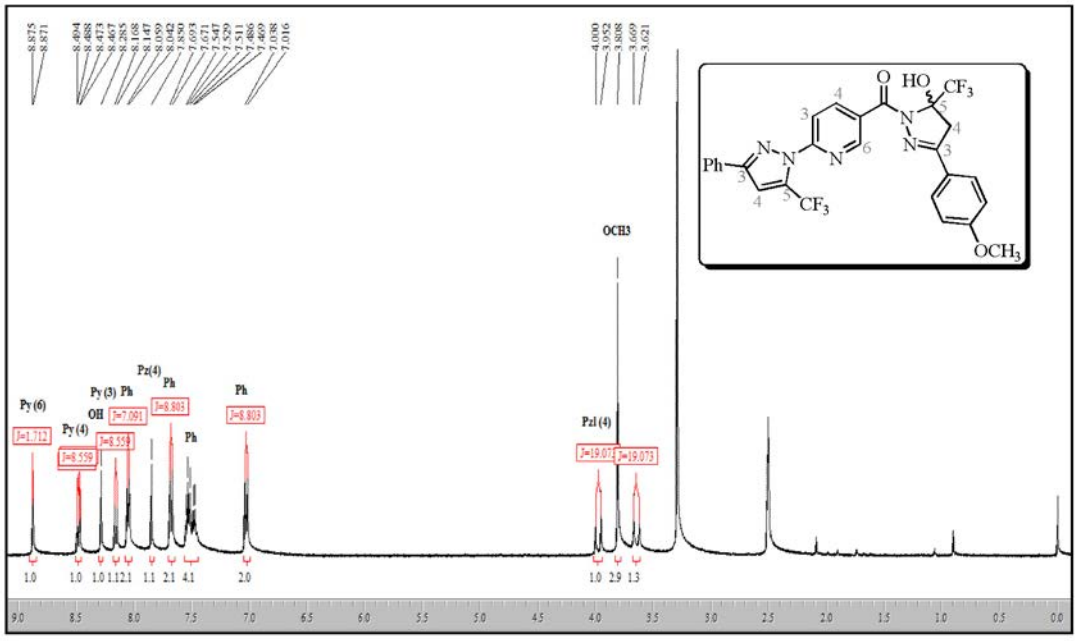

Figure S33. ^{1}H NMR spectrum (400.13 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(5-trifluoromethyl-4,5-dihydro-5-hydroxy-3-(4-methoxyphenyl)-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**9f**).

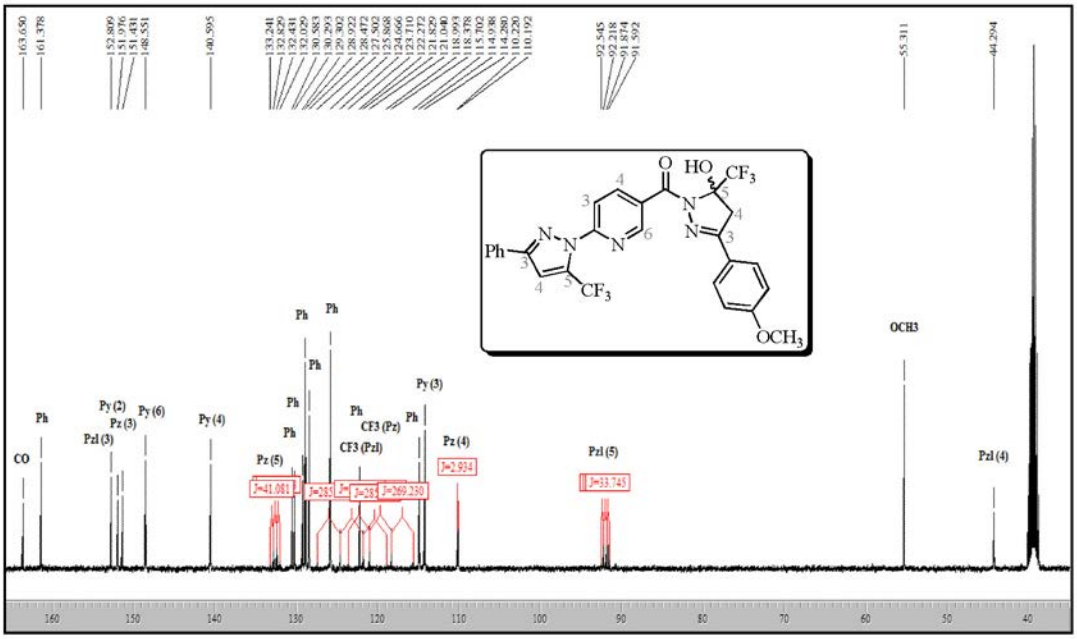

Figure S34. ^{13}C {^{1}H} NMR spectrum (100.61 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(5-trifluoromethyl-4,5-dihydro-5-hydroxy-3-(4-methoxyphenyl)-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**9f**).

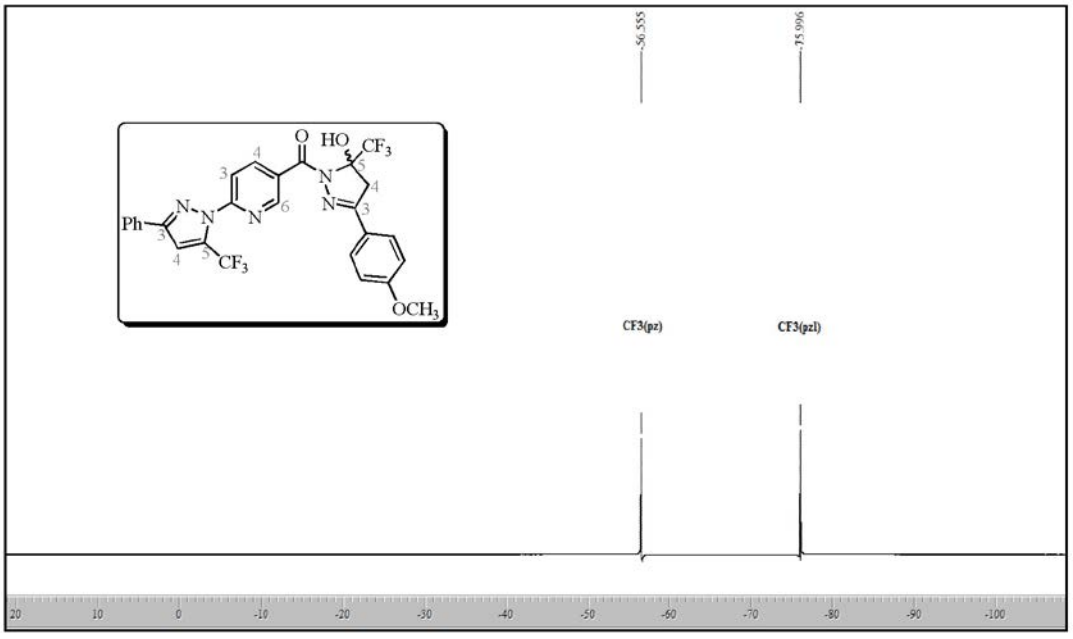

Figure S35. ^{19}F NMR spectrum (564.68 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(5-trifluoromethyl-4,5-dihydro-5-hydroxy-3-(4-methoxyphenyl)-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**9f**).

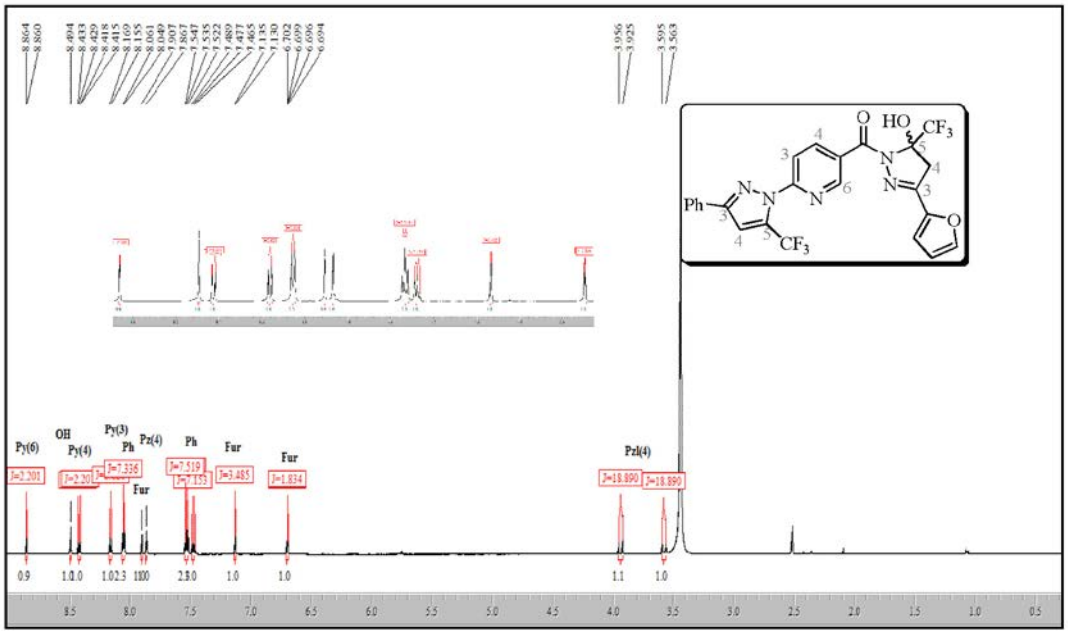

Figure S36. ^{1}H NMR spectrum (400.13 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(3-(fur-2-yl)-5-trifluoromethyl-4,5-dihydro-5-hydroxy-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**9g**).

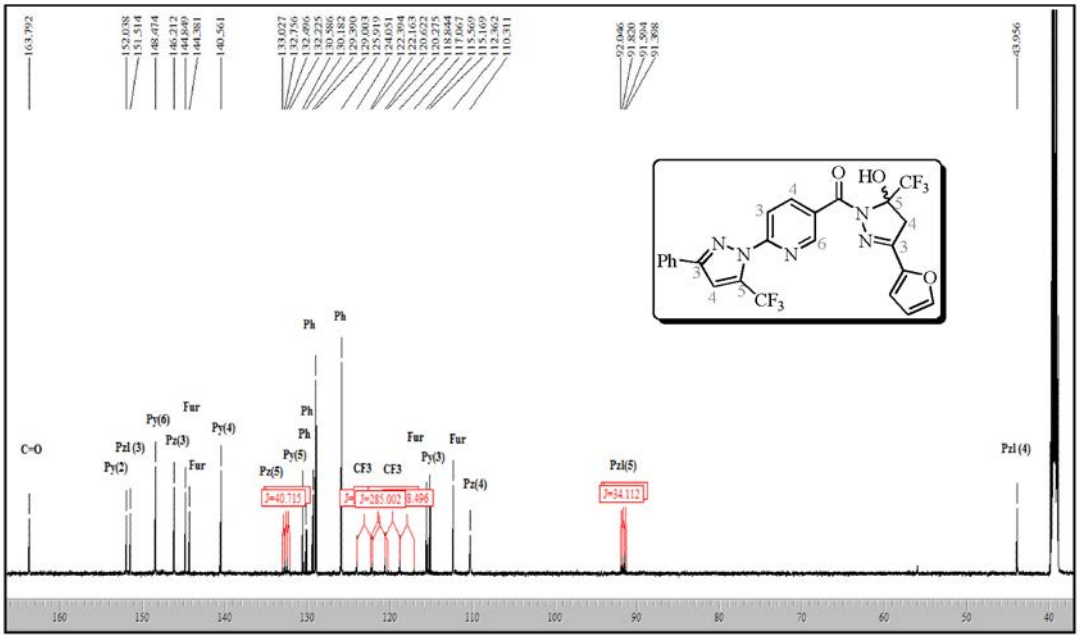

Figure S37. ^{13}C {^{1}H} NMR spectrum (100.61 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(3-(fur-2-yl)-5-trifluoromethyl-4,5-dihydro-5-hydroxy-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**9g**).

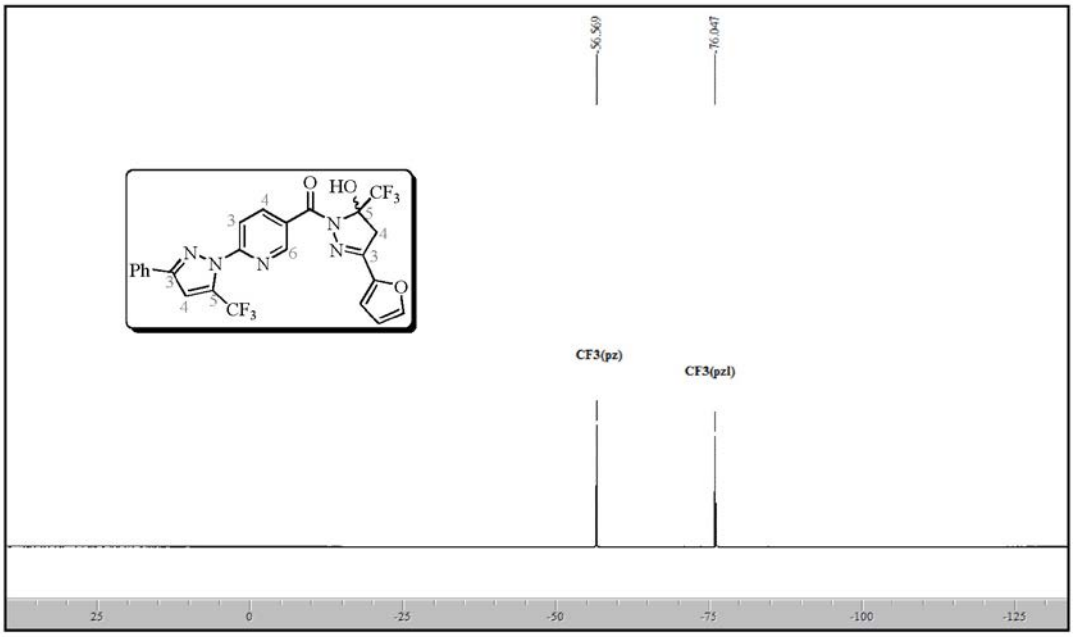

Figure S38. [19]F NMR spectrum (564.68 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(3-(fur-2-yl)-5-trifluoromethyl-4,5-dihydro-5-hydroxy-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**9g**).

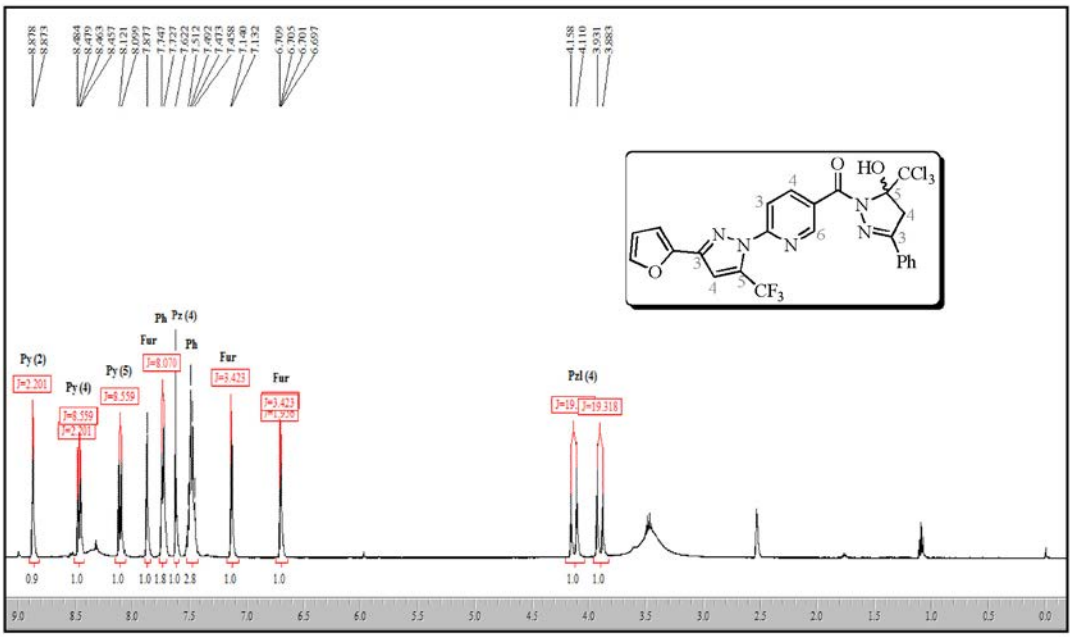

Figure S39. [1]H NMR spectrum (400.13 MHz, DMSO-d_6) of 2-(3-(fur-2-yl)-5-trifluoromethyl-1*H*-pyrazol-1-yl)-5-(5-trichloromethyl-4,5-dihydro-5-hydroxy-3-phenyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**10h**).

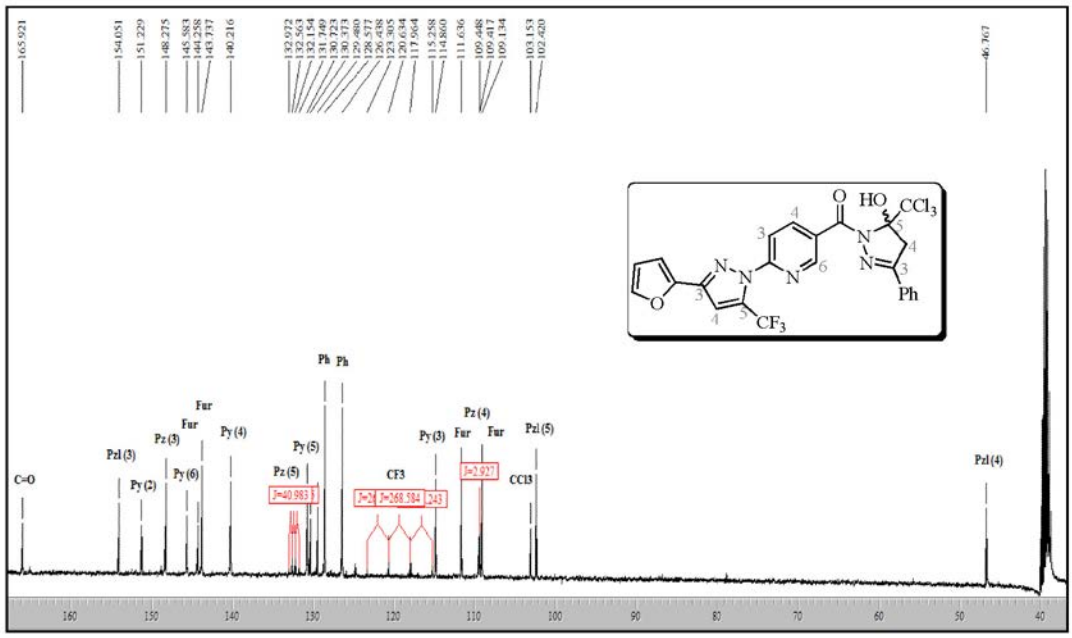

Figure S40. ^{13}C {^{1}H} NMR spectrum (100.61 MHz, DMSO-d_6) of 2-(3-(fur-2-yl)-5-trifluoromethyl-1*H*-pyrazol-1-yl)-5-(5-trichloromethyl-4,5-dihydro-5-hydroxy-3-phenyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**10h**).

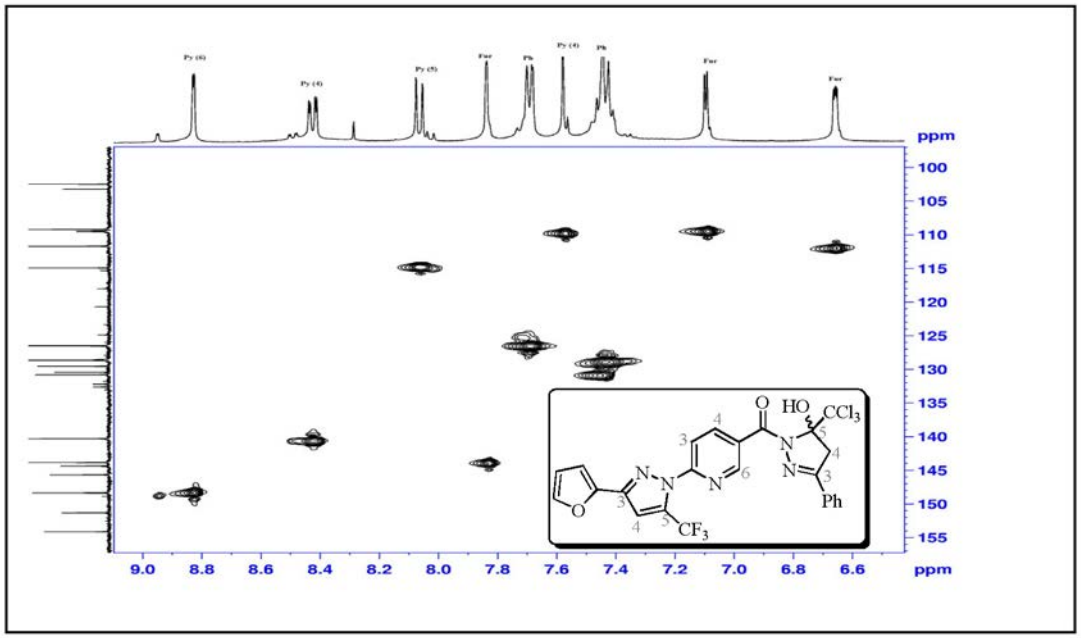

Figure S41. 2D HSQC spectrum (100.61 MHz, DMSO-d_6) of 2-(3-(fur-2-yl)-5-trifluoromethyl-1*H*-pyrazol-1-yl)-5-(5-trichloromethyl-4,5-dihydro-5-hydroxy-3-phenyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**10h**).

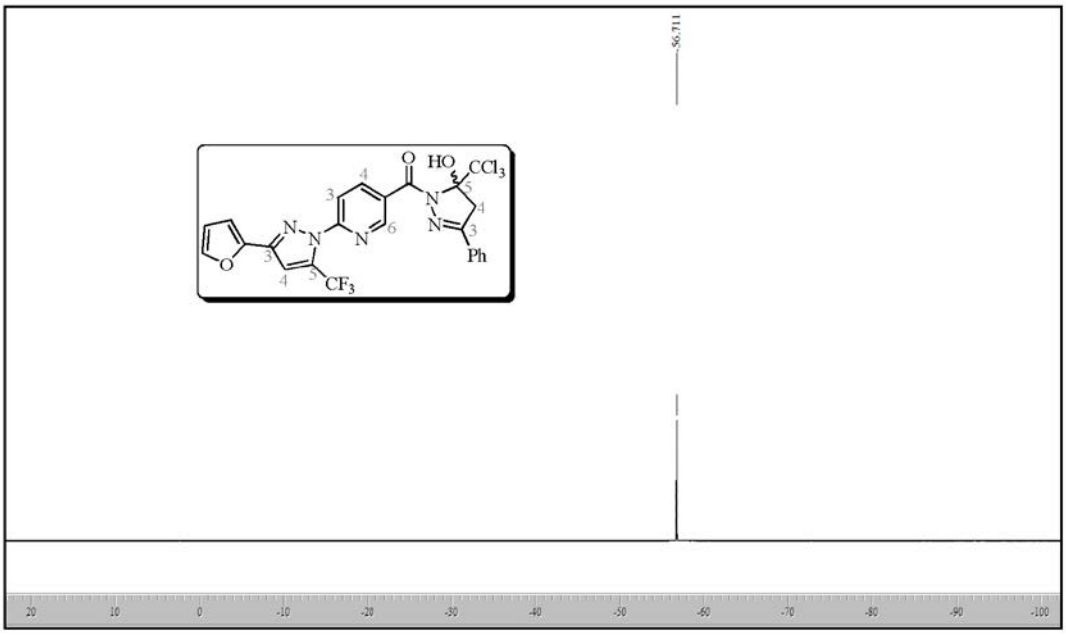

Figure S42. ^{19}F NMR spectrum (564.68 MHz, DMSO-d_6) of 2-(3-(fur-2-yl)-5-trifluoromethyl-1*H*-pyrazol-1-yl)-5-(5-trichloromethyl-4,5-dihydro-5-hydroxy-3-phenyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**10h**).

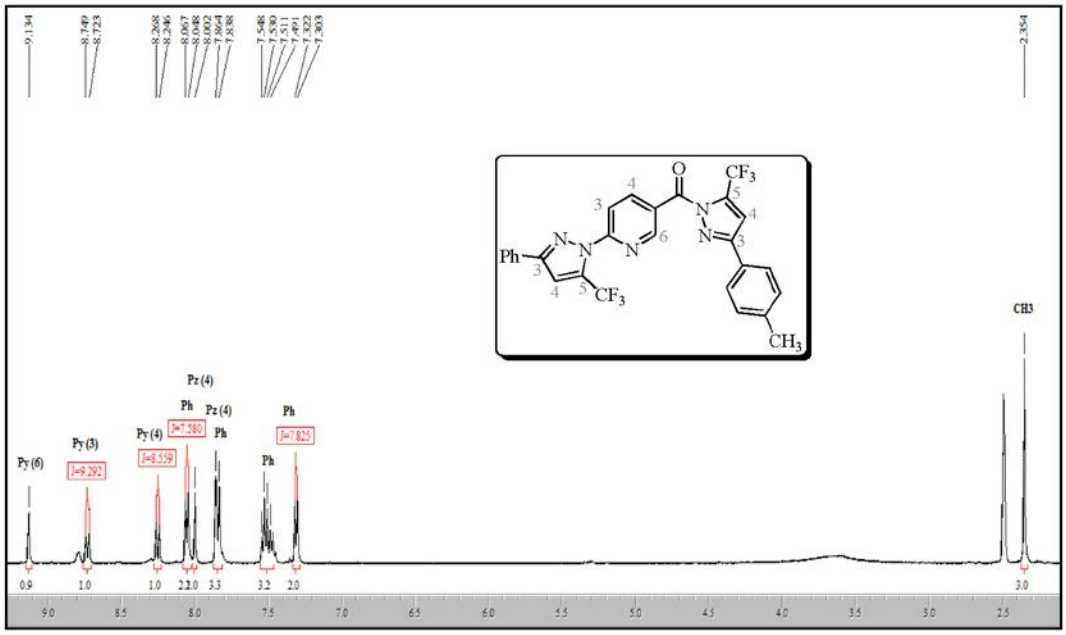

Figure S43. ^{1}H NMR spectrum (400.13 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(5-trifluoromethyl-3-(4-methylphenyl)-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**11e**).

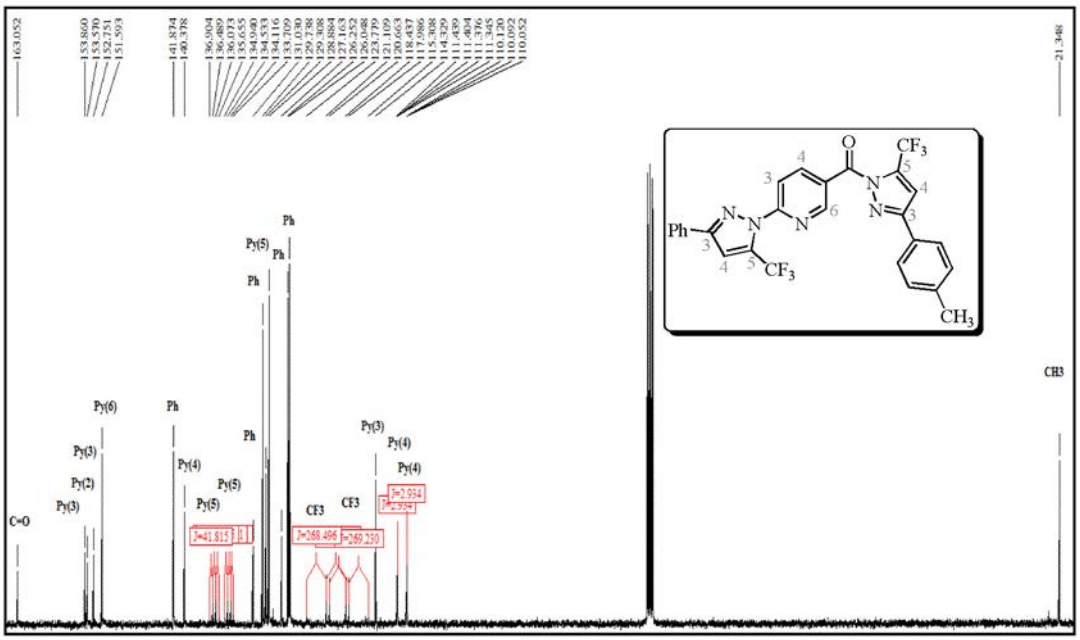

Figure S44. ^{13}C {^{1}H} NMR spectrum (100.61 MHz, $CDCl_3$) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(5-trifluoromethyl-3-(4-methylphenyl)-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**11e**).

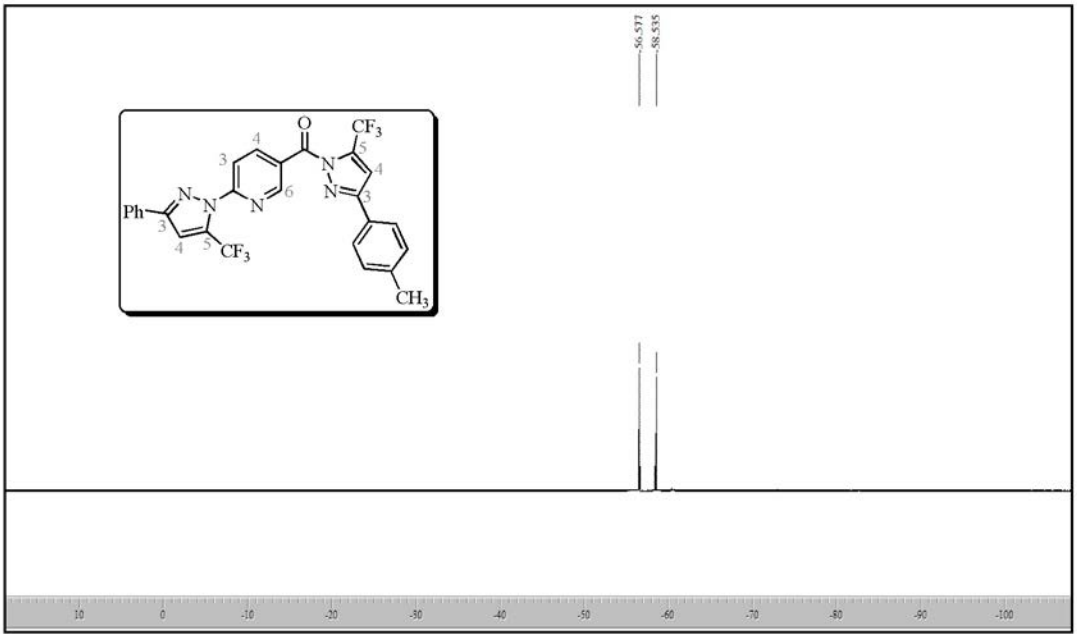

Figure S45. ^{19}F NMR spectrum (564.68 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(5-trifluoromethyl-3-(4-methylphenyl)-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**11e**).

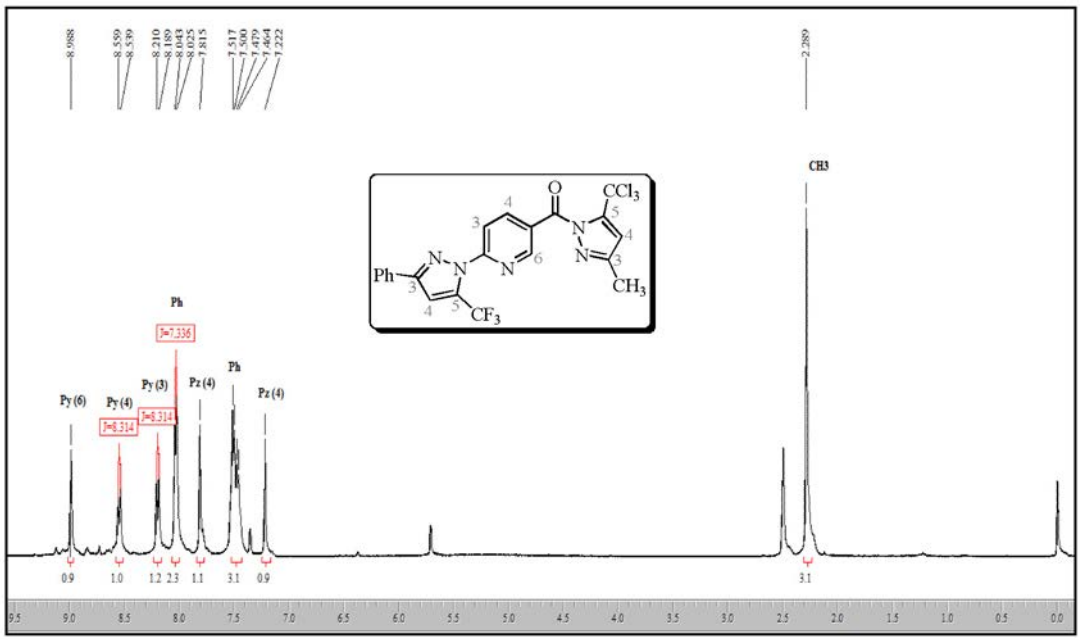

Figure S46. ^{1}H NMR spectrum (400.13 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(5-trichloromethyl-3-methyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**12c**).

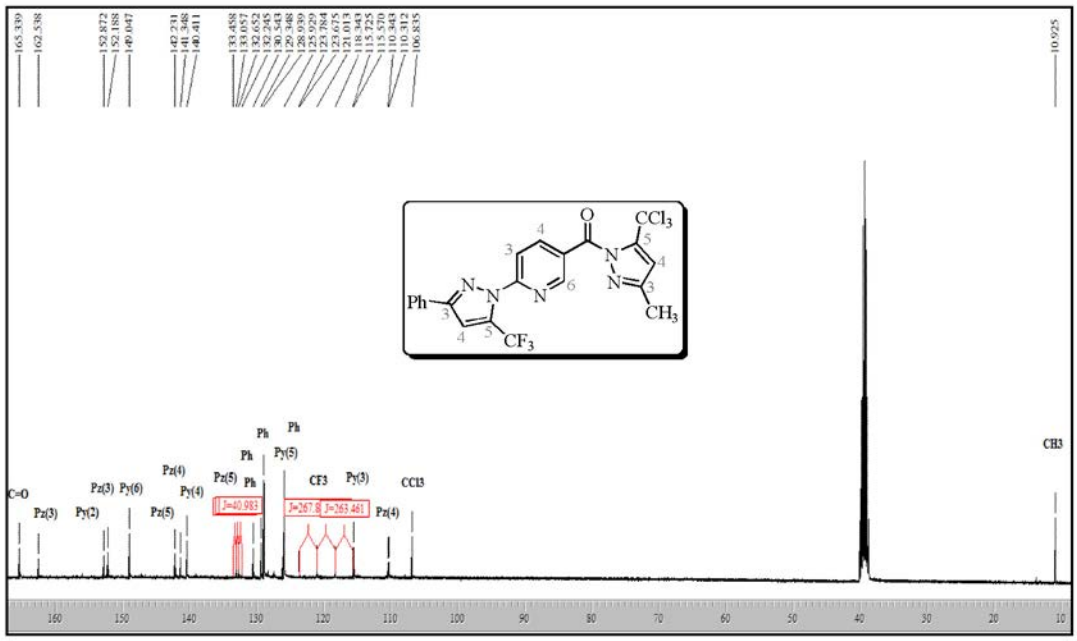

Figure S47. ^{13}C {^{1}H} NMR spectrum (100.61 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(5-trichloromethyl-3-methyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**12c**).

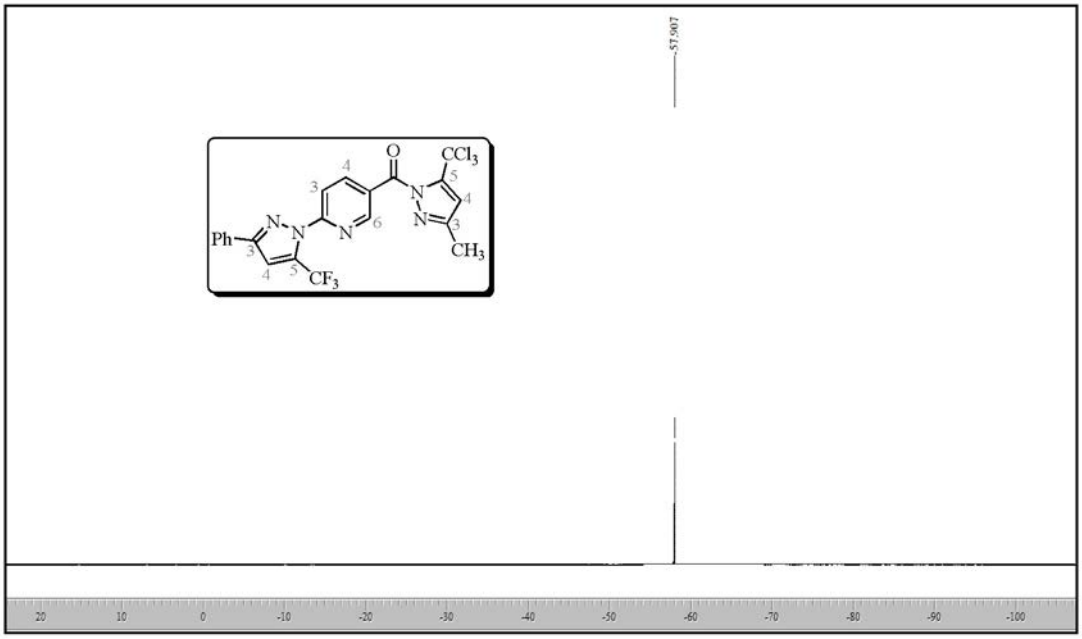

Figure S48. [19]F NMR spectrum (564.68 MHz, $CDCl_3$) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(5-trichloromethyl-3-methyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**12c**).

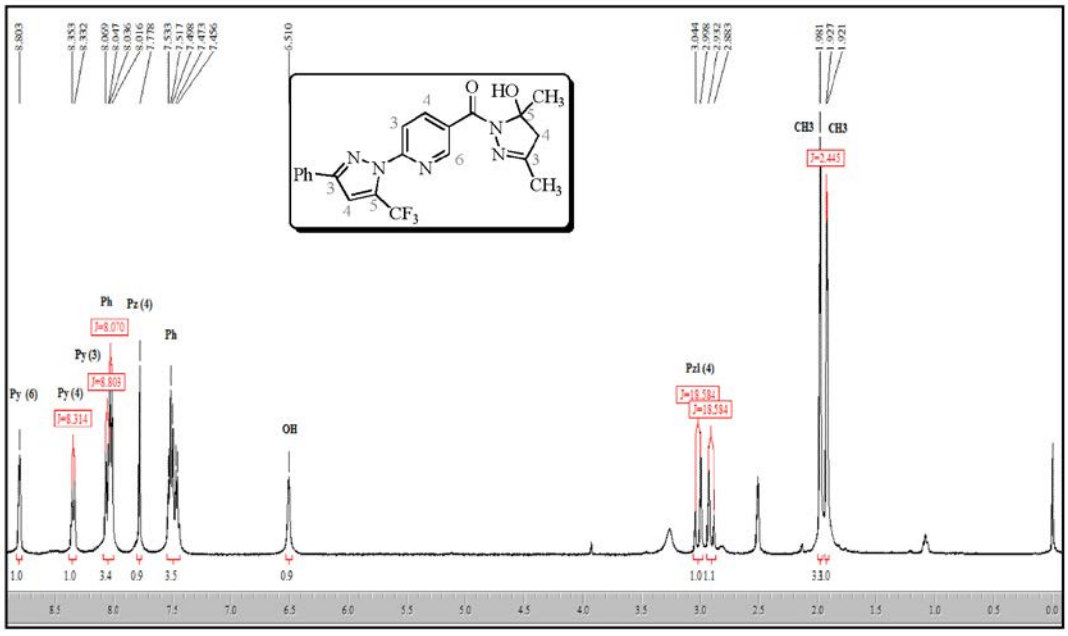

Figure S49. [1]H NMR spectrum (400.13 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(4,5-dihydro-5-hydroxy-3,5-dimethyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**13**).

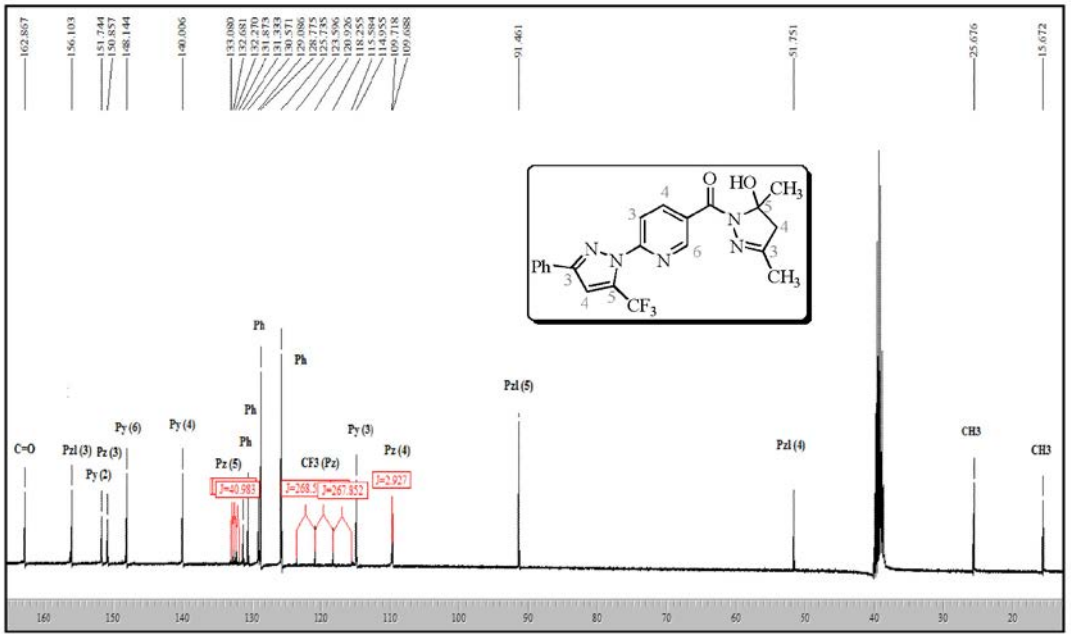

Figure S50. ^{13}C {^{1}H} NMR spectrum (100.61 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(4,5-dihydro-5-hydroxy-3,5-dimethyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**13**).

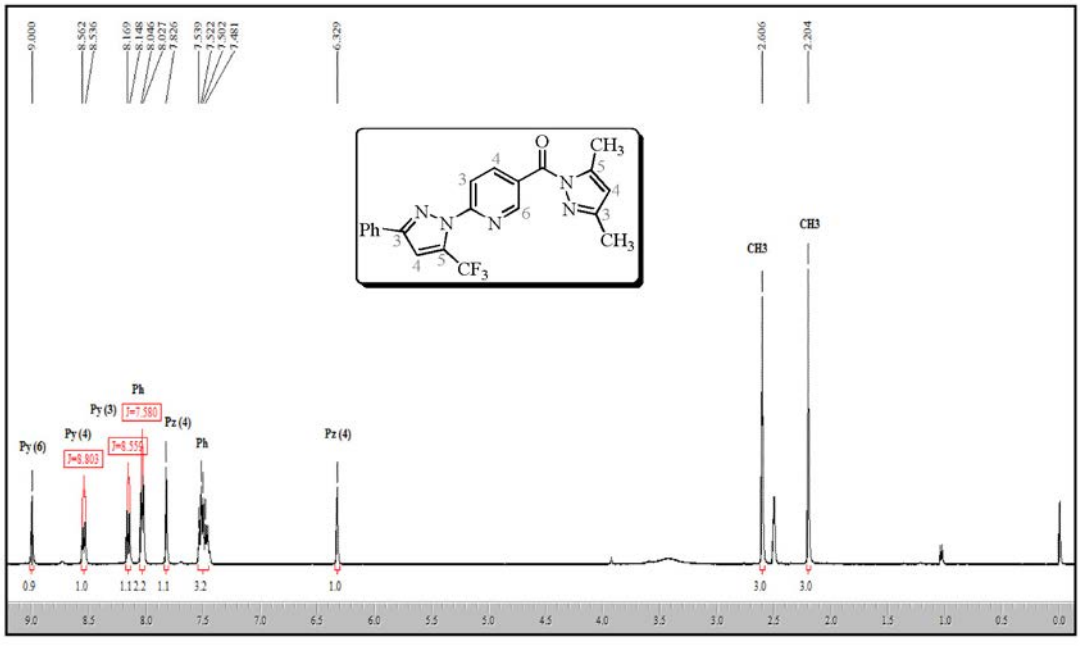

Figure S51. ^{1}H NMR spectrum (400.13 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(3,5-dimethyl-1*H*-pyrazol-1-yl-1-carbonyl) pyridine (**14**).

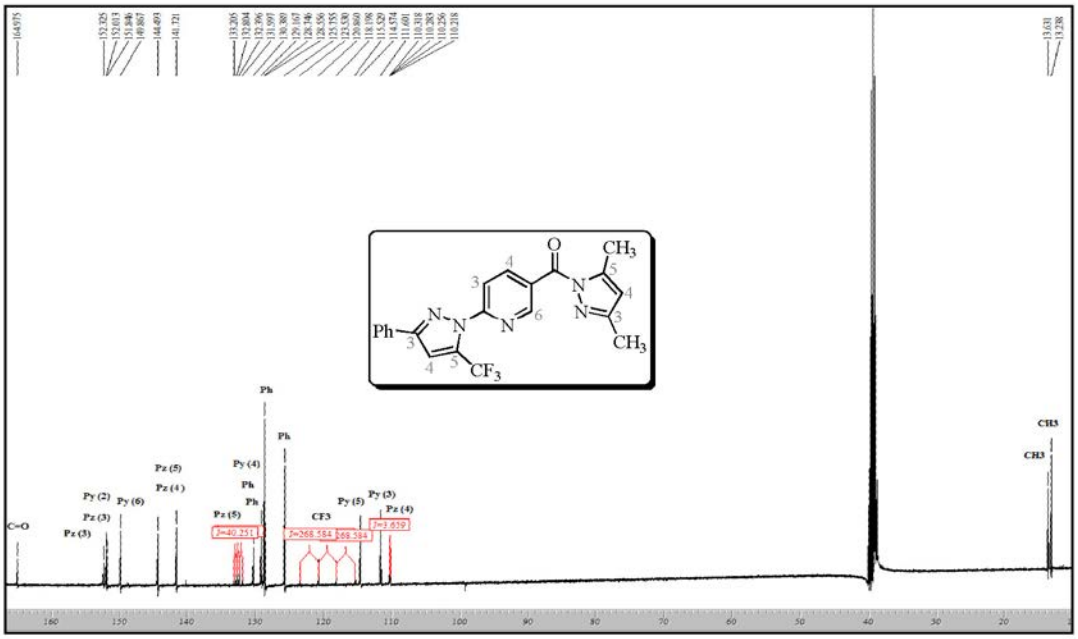

Figure S52. ^{13}C {^{1}H} NMR spectrum (100.61 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(3,5-dimethyl-1*H*-pyrazol-1-yl-1-carbonyl)pyridine (**14**).

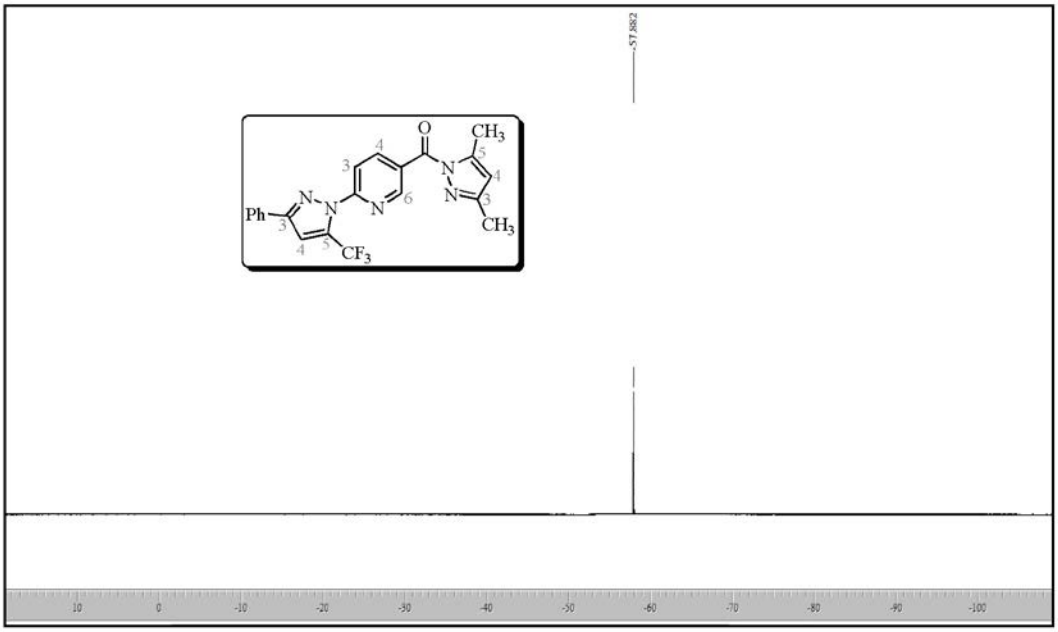

Figure S53. ^{19}F NMR spectrum (564.68 MHz, DMSO-d_6) of 2-(5-trifluoromethyl-3-phenyl-1*H*-pyrazol-1-yl)-5-(3,5-dimethyl-1*H*-pyrazol-1-yl-1-carbonyl) pyridine (**14**).

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: p21c

Bond precision: C-C = 0.0037 A Wavelength=0.71073

Cell: a=10.3520(4) b=9.3002(3) c=21.0663(7)
alpha=90 beta=99.887(2) gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	1998.05(12)	1998.05(12)
Space group	P 21/c	P21/c
Hall group	-P 2ybc	-P2ybc
Moiety formula	C16 H12 Cl3 F3 N5 O2	C16 H12 Cl3 F3 N5 O2
Sum formula	C16 H12 Cl3 F3 N5 O2	C16 H12 Cl3 F3 N5 O2
Mr	469.66	469.66
Dx,g cm-3	1.561	1.561
Z	4	4
Mu (mm-1)	0.509	0.509
F000	948.0	948.0
F000'	950.24	
h,k,lmax	13,11,27	13,11,26
Nref	4439	4429
Tmin,Tmax	0.650,0.750	0.889,0.968
Tmin'	0.610	

Correction method= GAUSSIAN

Data completeness= 0.998 Theta(max)= 27.180

R(reflections)= 0.0512(3547) wR2(reflections)= 0.1538(4429)

S = 1.047 Npar= 262

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.

Figure S54. Crystallographic data of compound **6a**.

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: p-1

Bond precision: C-C = 0.0028 A Wavelength=0.71073

Cell: a=6.9665(19) b=11.405(3) c=12.857(3)
alpha=115.584(14) beta=101.254(14) gamma=94.123(14)
Temperature: 293 K

	Calculated	Reported
Volume	889.5(4)	889.5(4)
Space group	P -1	P-1
Hall group	-P 1	-P1
Moiety formula	C16 H13 F6 N5 O2	C8 H6.50 F3 N2.50 O
Sum formula	C16 H13 F6 N5 O2	C8 H6.50 F3 N2.50 O
Mr	421.31	210.66
Dx,g cm-3	1.573	1.573
Z	2	4
Mu (mm-1)	0.149	0.149
F000	428.0	428.0
F000'	428.32	
h,k,lmax	8,14,16	8,14,16
Nref	4004	3982
Tmin,Tmax	0.954,0.967	0.999,0.999
Tmin'	0.950	

Correction method= GAUSSIAN

Data completeness= 0.995 Theta(max)= 27.310

R(reflections)= 0.0401(3013) wR2(reflections)= 0.1099(3982)

S = 1.028 Npar= Npar = 262

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.

Figure S55. Crystallographic data of compound **7a**.

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: teste2

Bond precision: C-C = 0.0035 A Wavelength=0.71073

Cell: a=17.7171(12) b=13.4853(10) c=8.2053(6)
alpha=90 beta=92.483(3) gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	1958.6(2)	1958.6(2)
Space group	P 21/c	P21/c
Hall group	-P 2ybc	-P2ybc
Moiety formula	C21 H16 F3 N5 O	C21 H16 F3 N5 O
Sum formula	C21 H16 F3 N5 O	C21 H16 F3 N5 O
Mr	411.39	411.39
Dx,g cm-3	1.395	1.395
Z	4	4
Mu (mm-1)	0.110	0.110
F000	848.0	848.0
F000'	848.46	
h,k,lmax	22,17,10	22,17,10
Nref	4437	4379
Tmin,Tmax	0.968,0.984	0.958,0.975
Tmin'	0.931	

Correction method= GAUSSIAN

Data completeness= 0.987 Theta(max)= 27.330

R(reflections)= 0.0499(3085) wR2(reflections)= 0.1947(4379)

S = 1.073 Npar= Npar = 271

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.

Figure S56. Crystallographic data of compound **14**.