SUPPLEMENTARY INFORMATION

Synthesis and cytotoxic evaluation of some substituted 5-pyrazolones and their urea derivatives

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FT-IR spectra

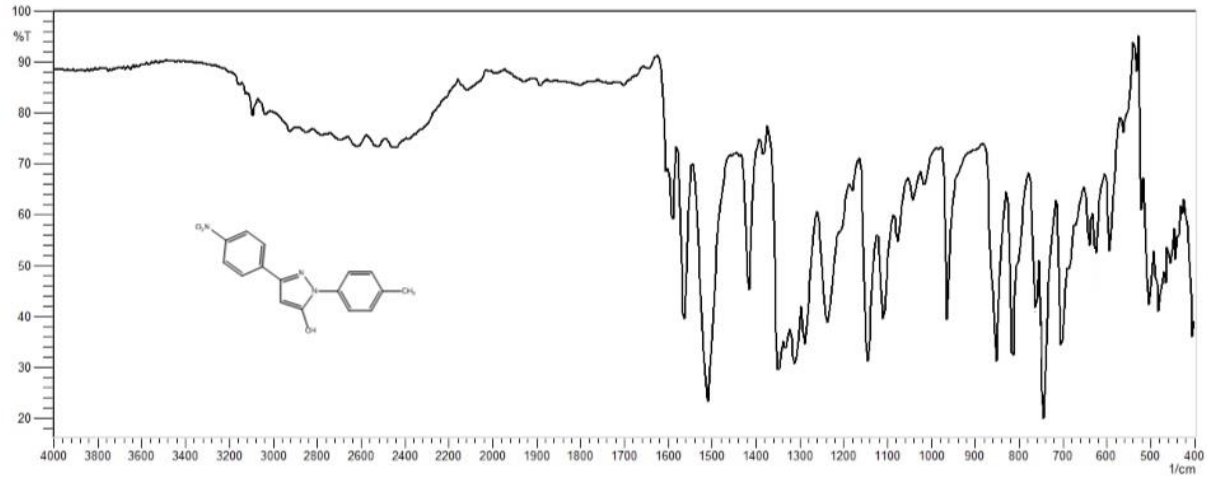


Figure S1. FTIR spectrum of 5-hydroxy-3-(4-nitrophenyl)-1-(p-tolyl)-1*H*-pyrazole **3e**.

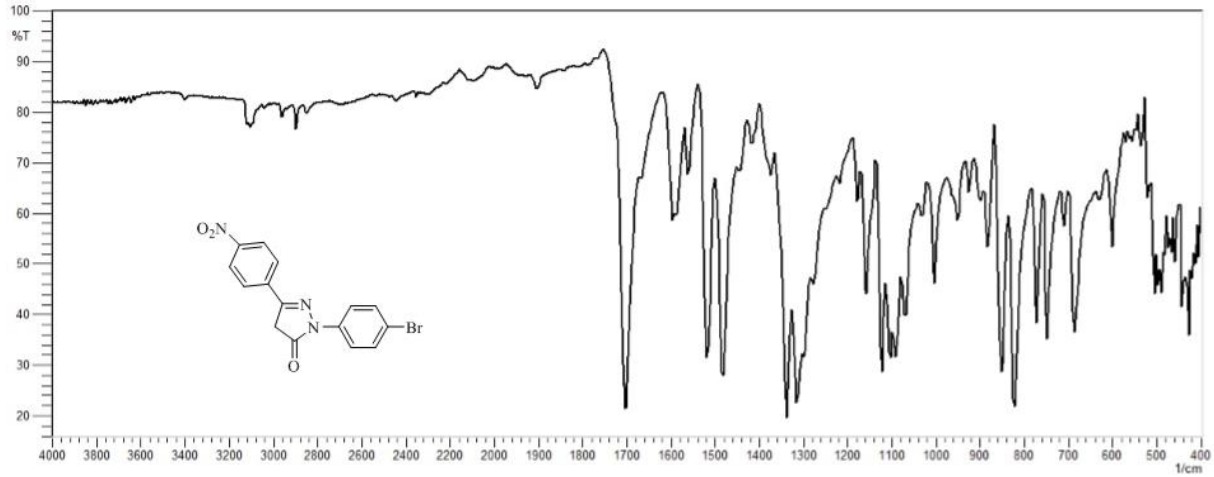


Figure S2. FTIR spectrum of 1-(4-bromophenyl)-3-(4-nitrophenyl)-1*H*-pyrazole-5(4*H*)-one **3f**.

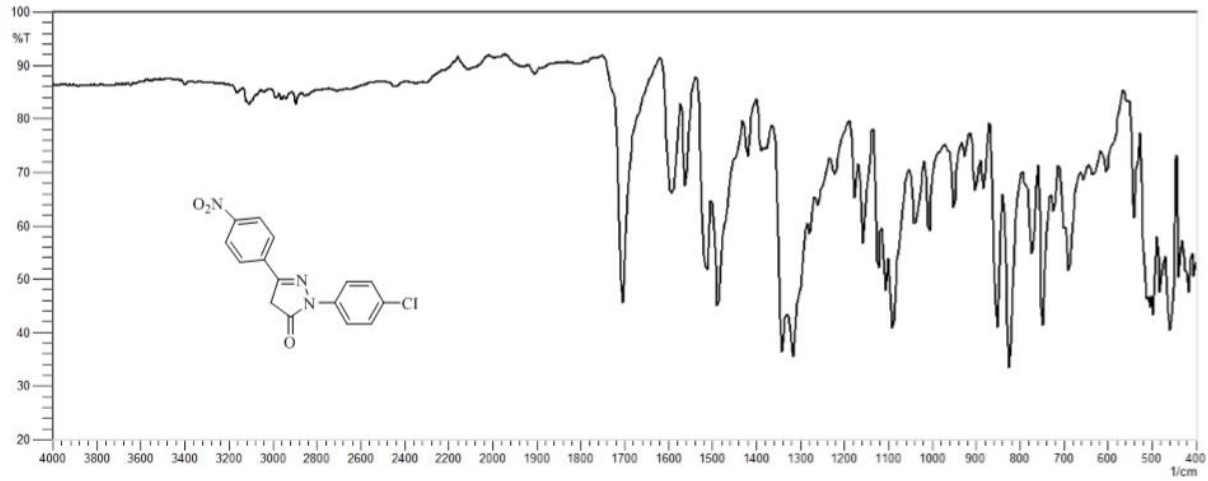


Figure S3. FTIR spectrum of 1-(4-chlorophenyl)-3-(4-nitrophenyl)-1*H*-pyrazole-5(4*H*)-one **3g**.

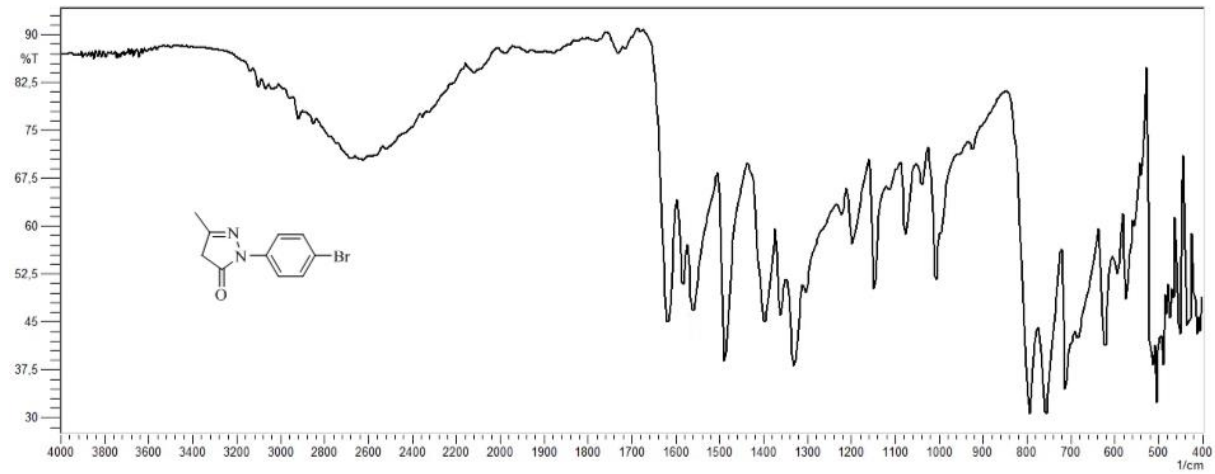


Figure S4. FTIR spectrum of 1-(4-bromophenyl)-3-methyl-1*H*-pyrazole-5(4*H*)-one **3h**.

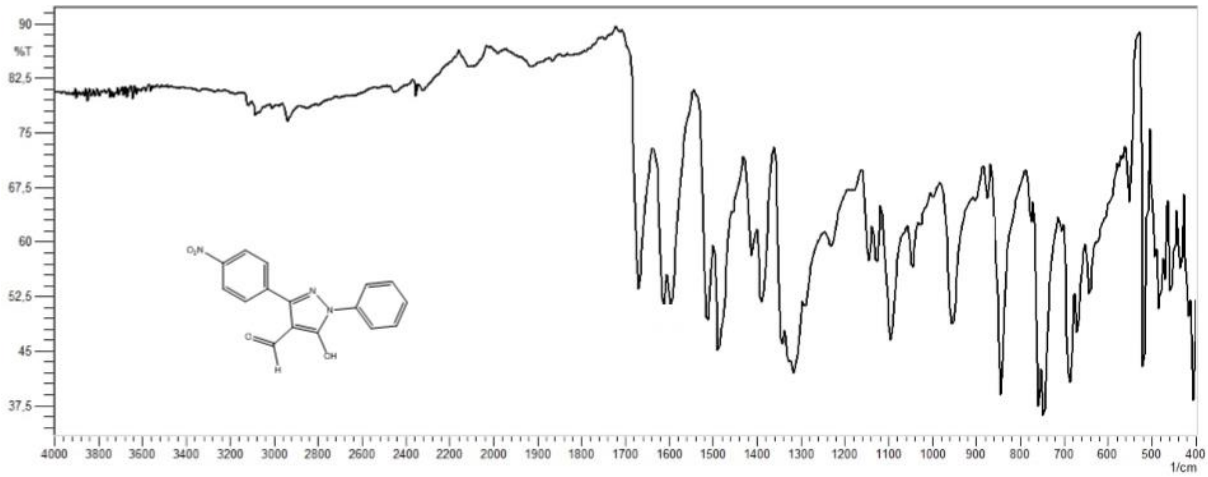


Figure S5. FTIR spectrum of 5-hydroxy-3-(4-nitrophenyl)-1-phenyl-4-formyl-1*H*-pyrazole **4d**.

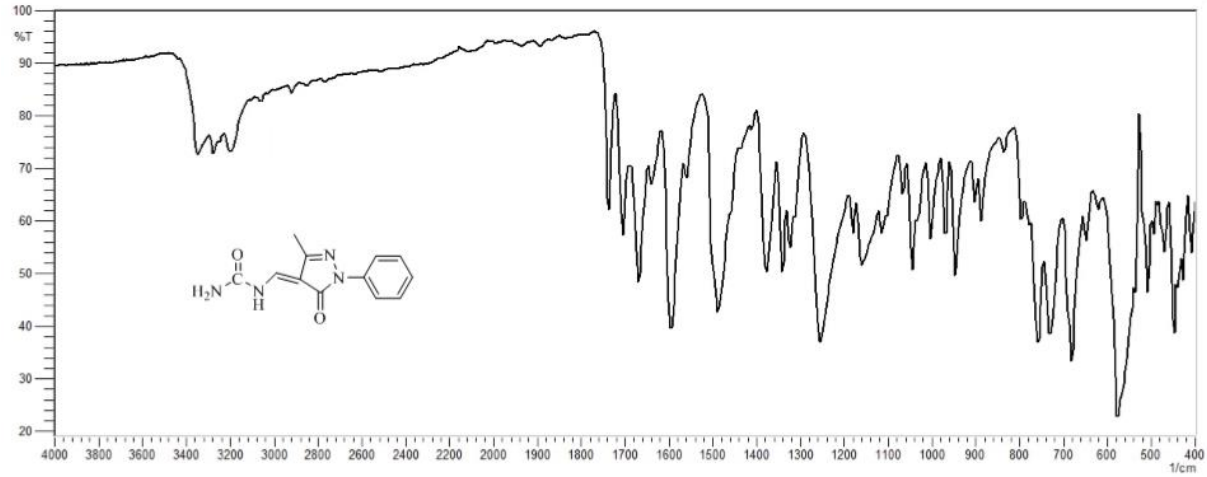


Figure S6. FTIR spectrum of N-[(1,5-dihydro-3-methyl-5-oxo-1-phenyl-4*H*-pyrazole-4-ylidene)methyl]urea **5a**.

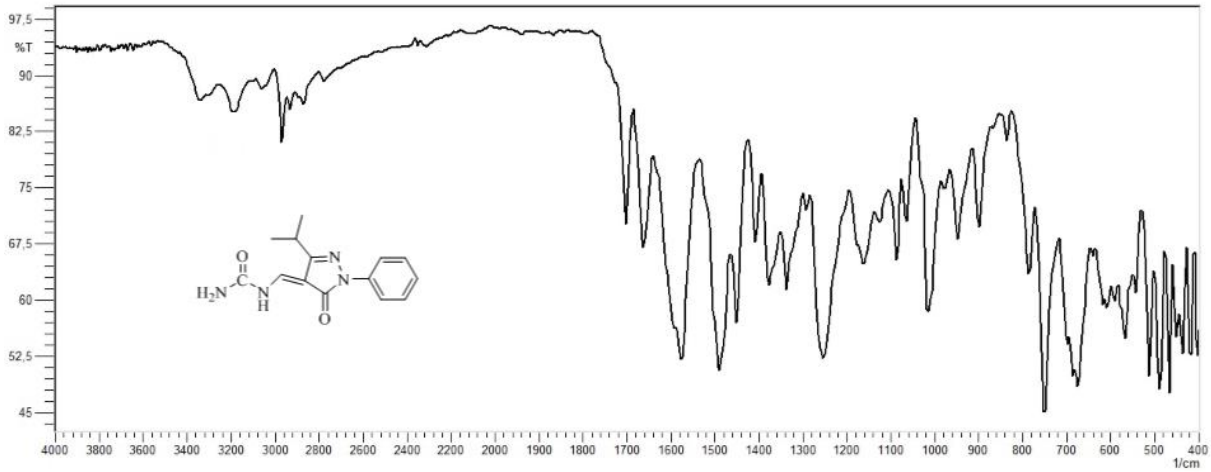


Figure 7. FTIR spectrum of N-[(1,5-dihydro-1-phenyl-5-oxo-3-(isopropyl)-4*H*-pyrazole-4-ylidene)methyl]urea **5b**.

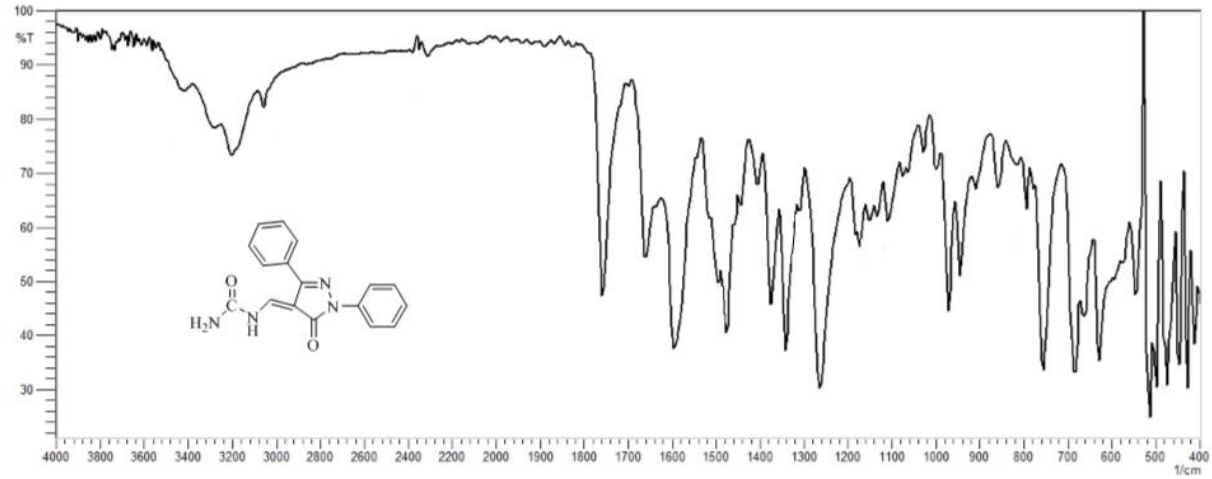


Figure 8. FTIR spectrum of N-[(1,5-dihydro-1,3-diphenyl-5-oxo-4*H*-pyrazole-4-ylidene)methyl]urea **5c**.

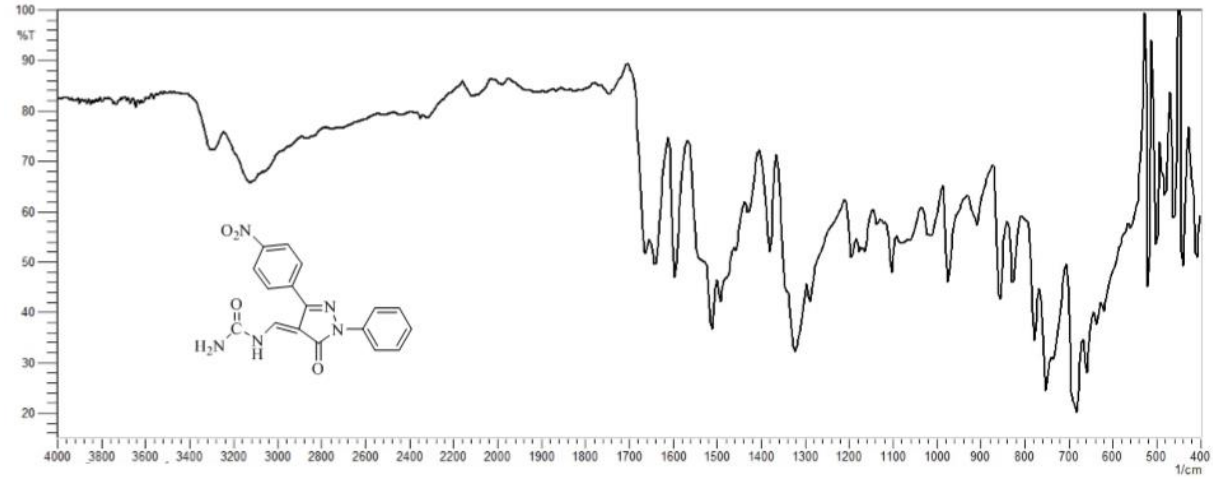


Figure 9. FTIR spectrum of N-[(1,5-dihydro-1-phenyl-5-oxo-3-(4-nitrophenyl)-4*H*-pyrazole-4-ylidene)methyl]urea **5d**.

^{1}H NMR spectra

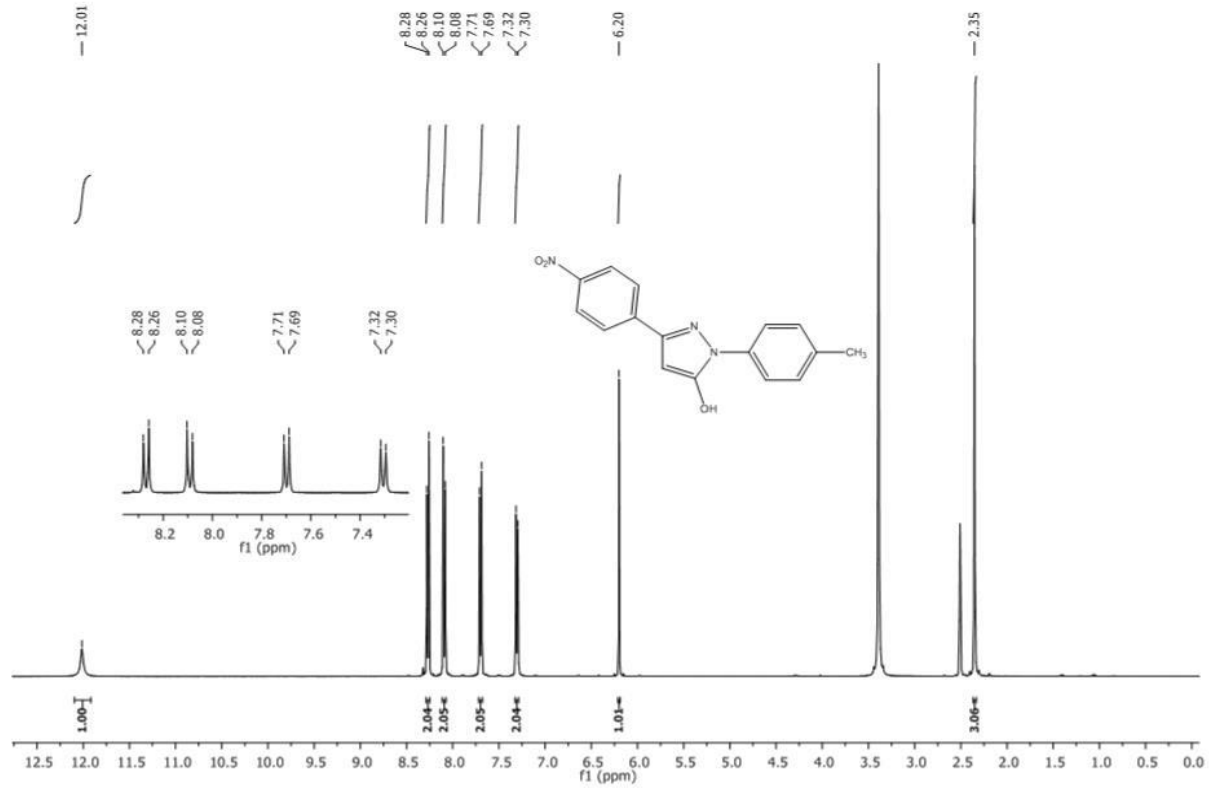


Figure S10. ^{1}H NMR spectrum in DMSO-d_6 of 5-hydroxy-3-(4-nitrophenyl)-1-(p-tolyl)-1*H*-pyrazole **3e**.

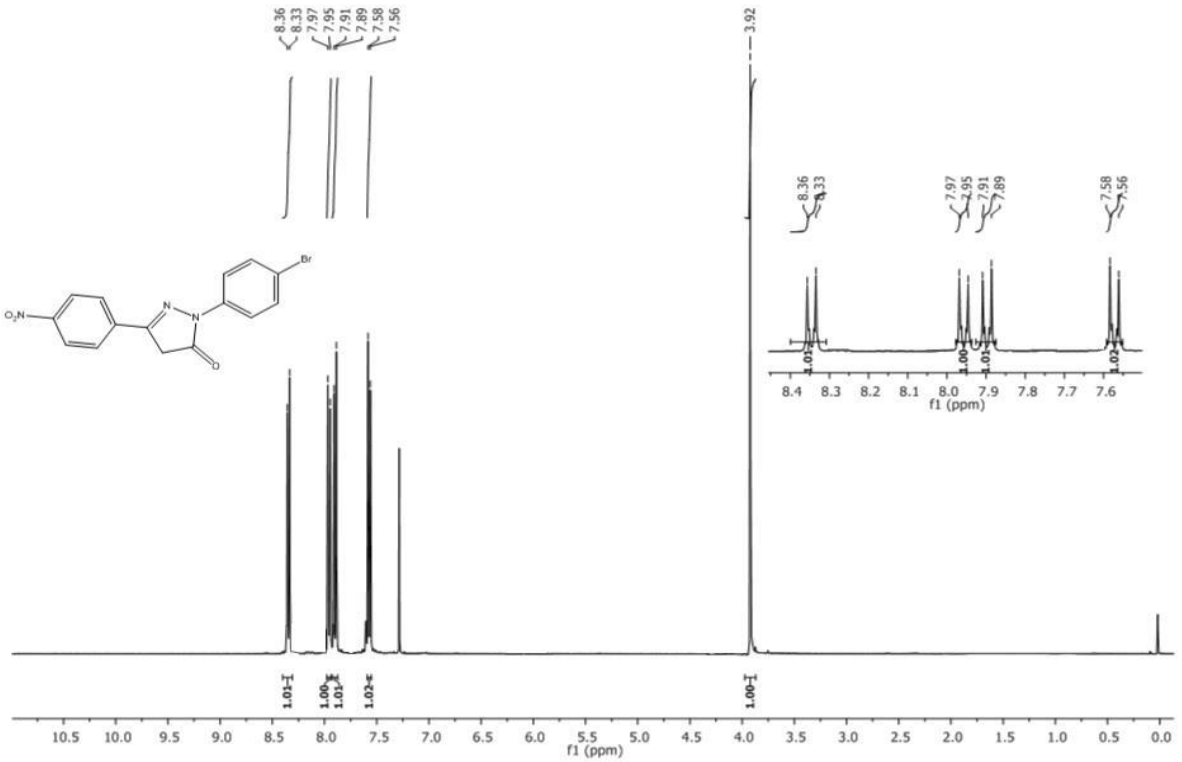


Figure S11. ^{1}H NMR spectrum in $CDCl_3$ of 1-(4-bromophenyl)-3-(4-nitrophenyl)-1*H*-pyrazole-5(4*H*)-one **3f**.

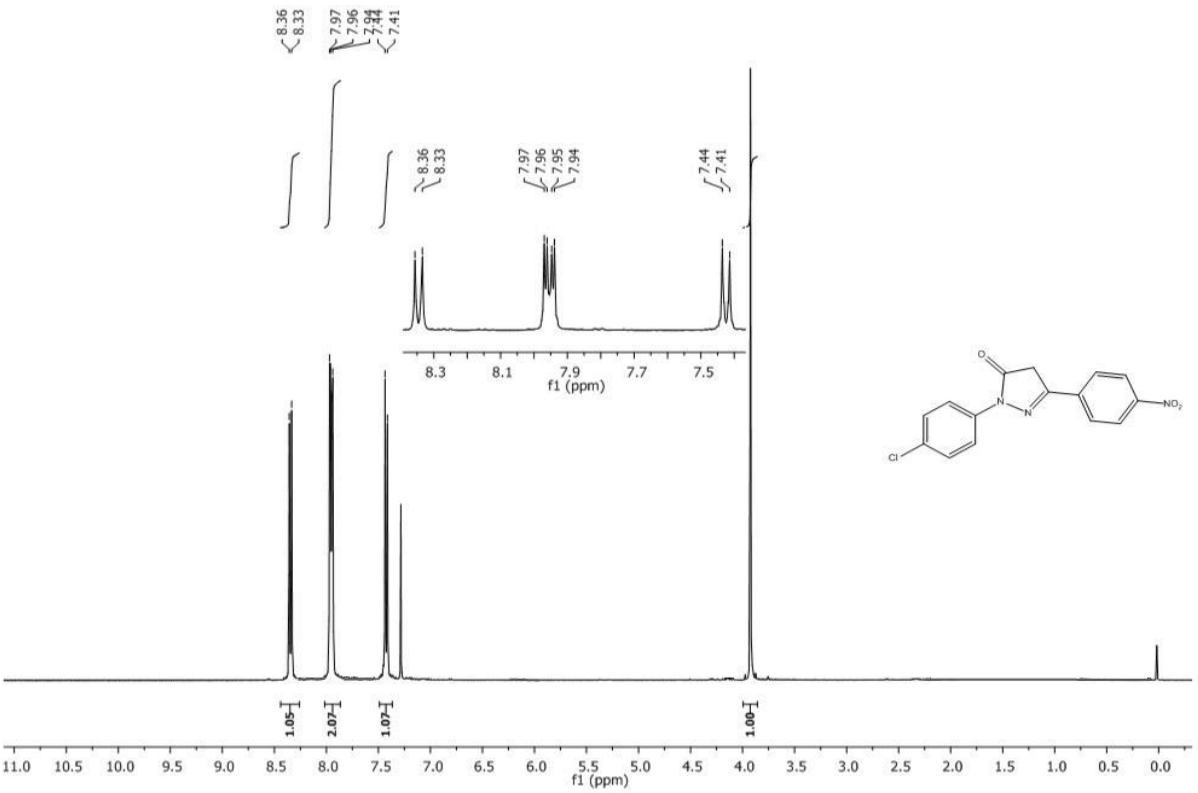


Figure S12. ^{1}H NMR spectrum in $CDCl_3$ of 1-(4-chlorophenyl)-3-(4-nitrophenyl)-1*H*-pyrazole-5(4*H*)-one **3g**.

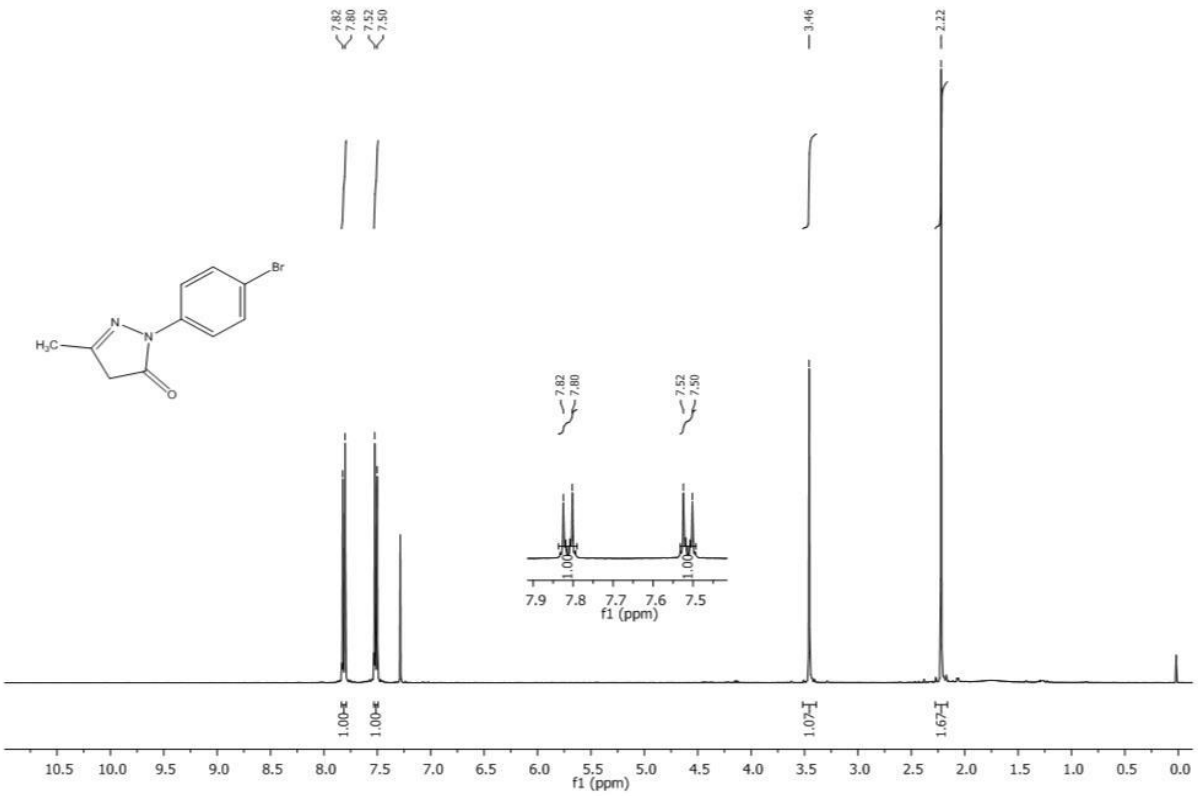


Figure S13. ^{1}H NMR spectrum in $CDCl_3$ of 1-(4-bromophenyl)-3-methyl-1*H*-pyrazole-5(4*H*)-one **3h**.

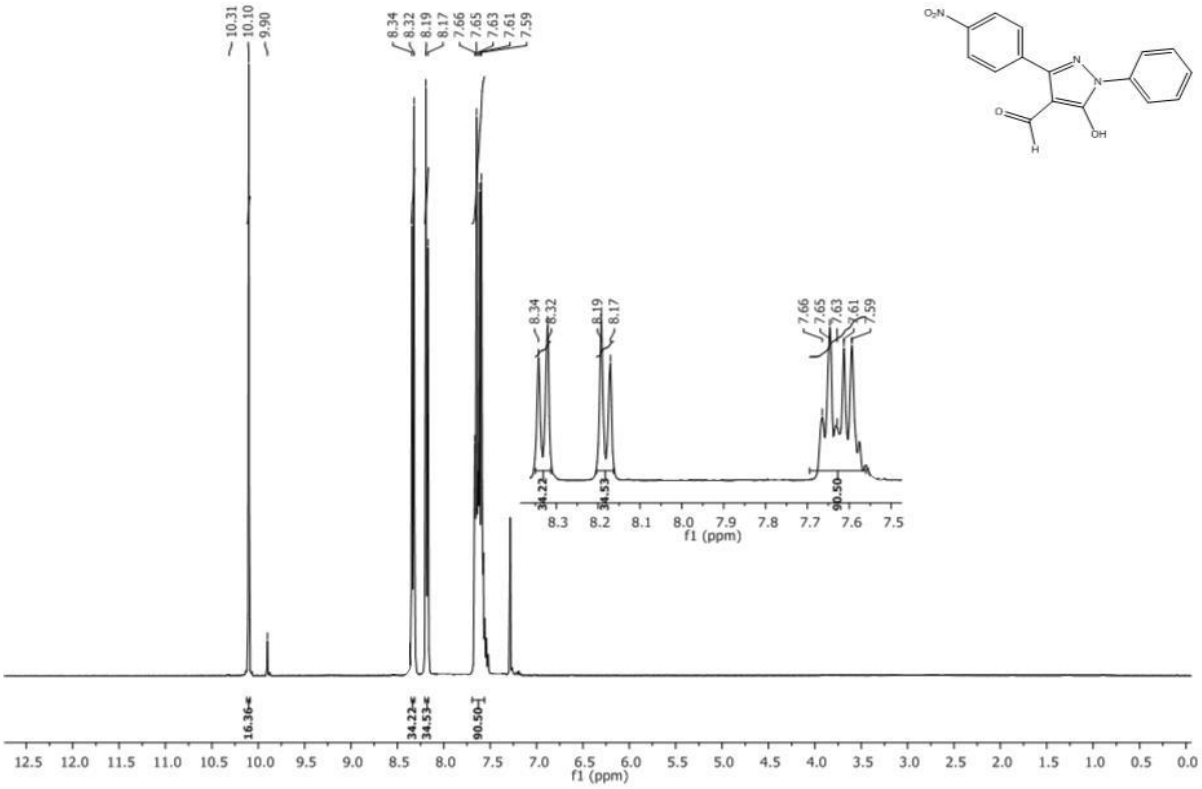


Figure S14. [1]H NMR spectrum in $CDCl_3$ of 5-hydroxy-3-(4-nitrophenyl)-1-phenyl-4-formyl-1*H*-pyrazole **4d**.

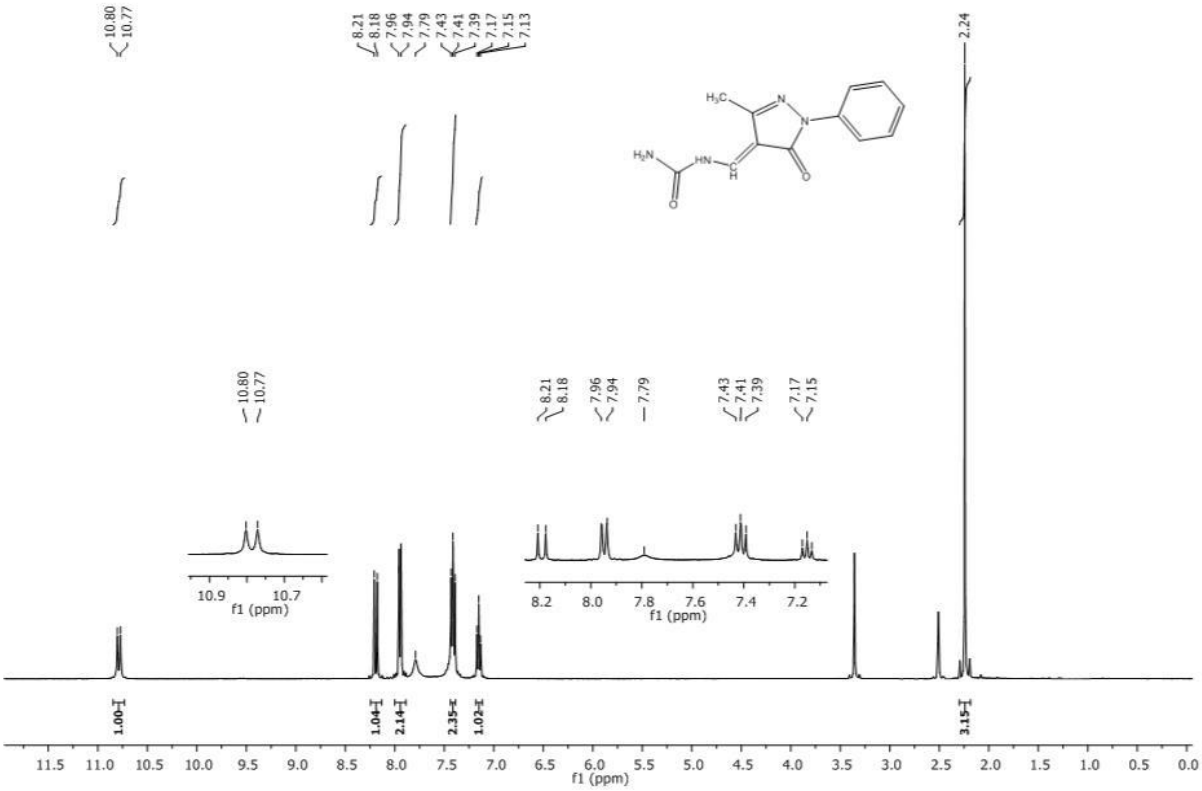


Figure S15. [1]H NMR spectrum in DMSO-d_6 of N-[(1,5-dihydro-3-methyl-5-oxo-1-phenyl-4*H*-pyrazole-4-ylidene)methyl]urea **5a**.

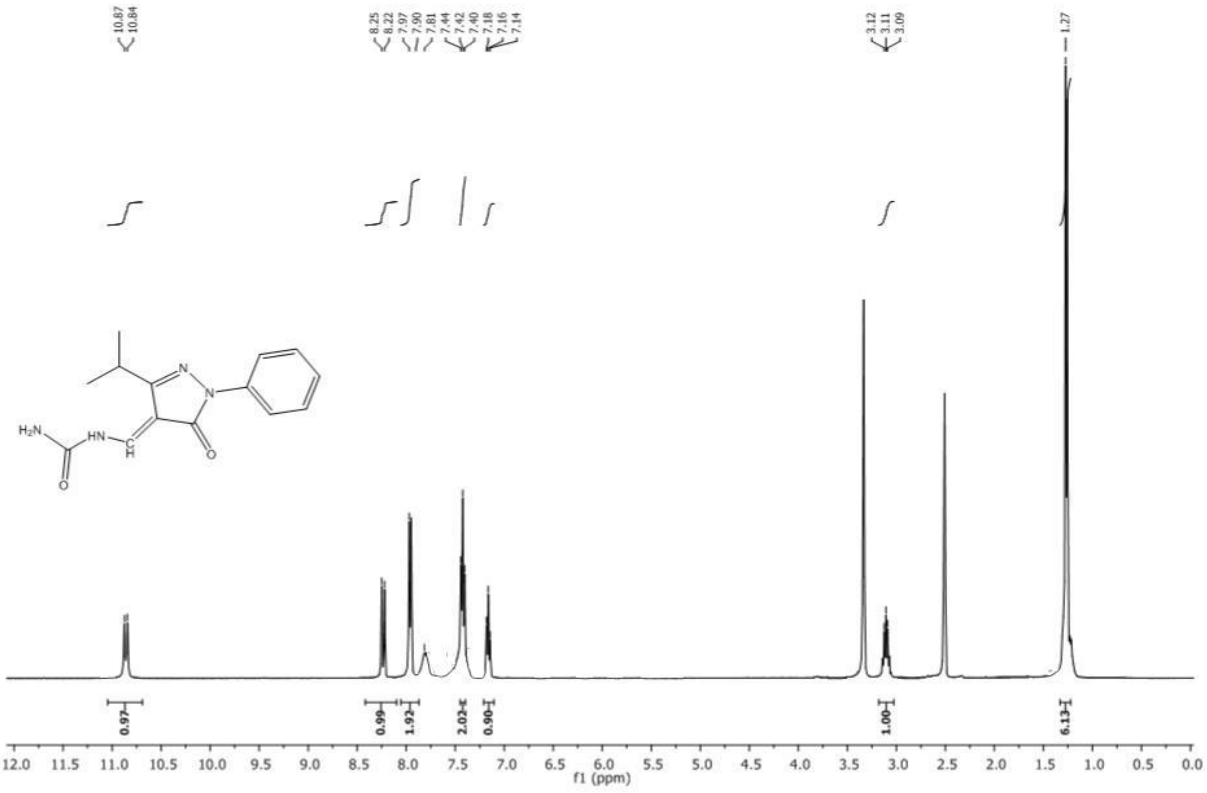


Figure S16. [1]H NMR spectrum in DMSO-*d*$_6$ of N-[(1,5-dihydro-1-phenyl-5-oxo-3-(isopropyl)-4*H*-pyrazole-4-ylidene)methyl]urea **5b**.

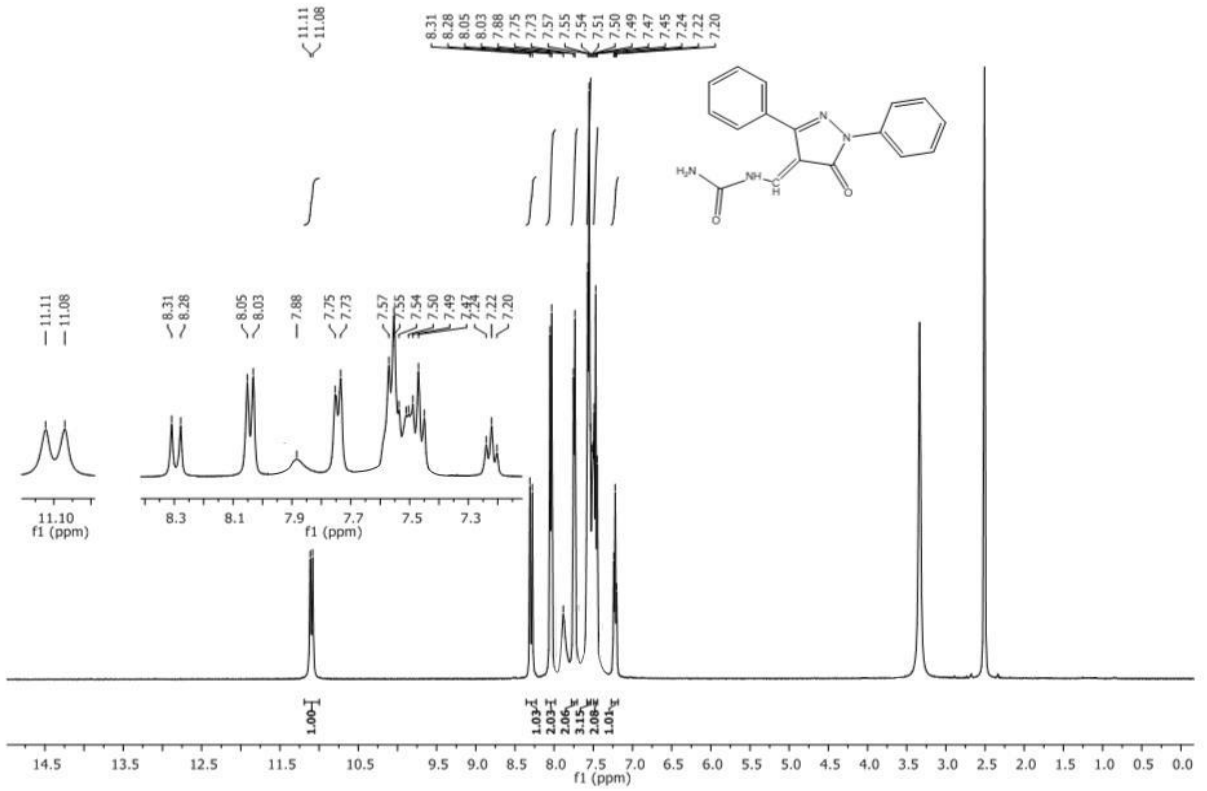


Figure S17. [1]H NMR spectrum in DMSO-*d*$_6$ of N-[(1,5-dihydro-1,3-diphenyl-5-oxo-4*H*-pyrazole-4-ylidene)methyl]urea **5c**.

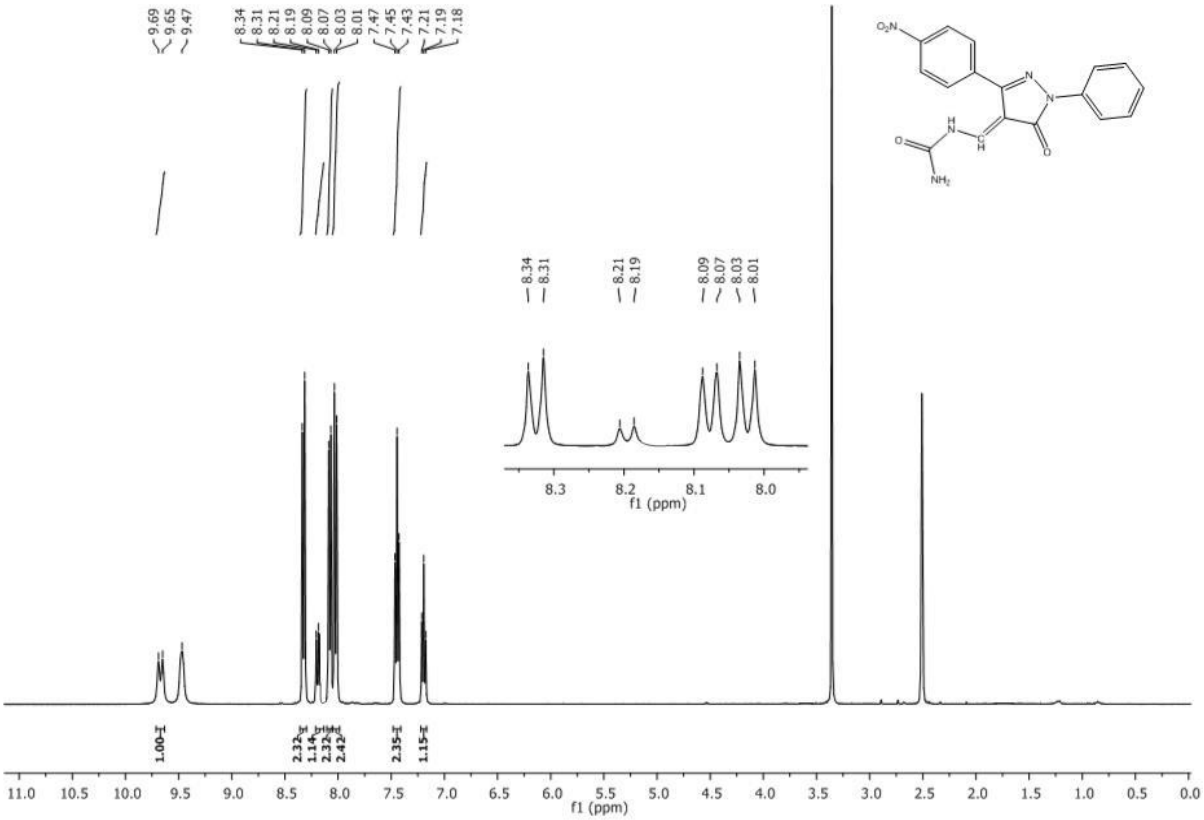


Figure S18. ^{1}H NMR spectrum in DMSO-d_6 of N-[(1,5-dihydro-1-phenyl-5-oxo-3-(4-nitrophenyl)-4*H*-pyrazole-4-ylidene)methyl]urea **5d**.

^{13}C NMR spectra

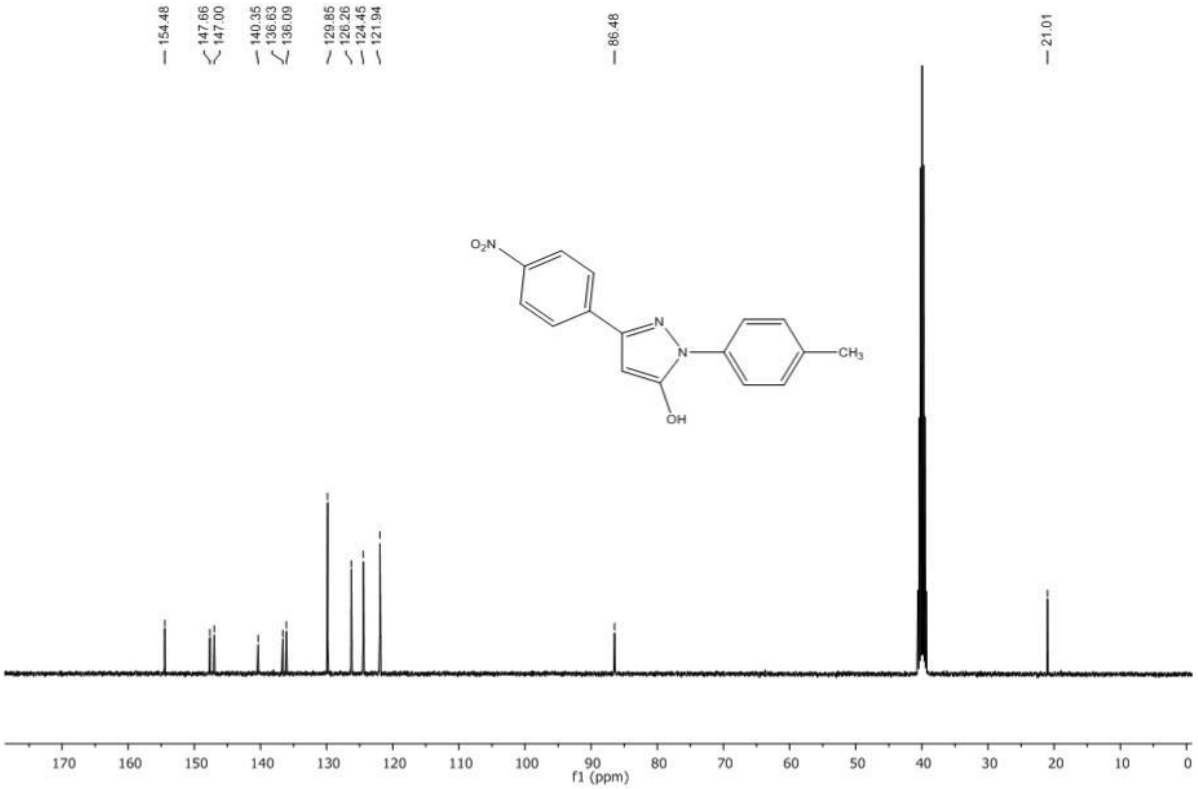


Figure S19. ^{13}C NMR spectrum in DMSO-d_6 of 5-hydroxy-3-(4-nitrophenyl)-1-(p-tolyl)-1*H*-pyrazole **3e**.

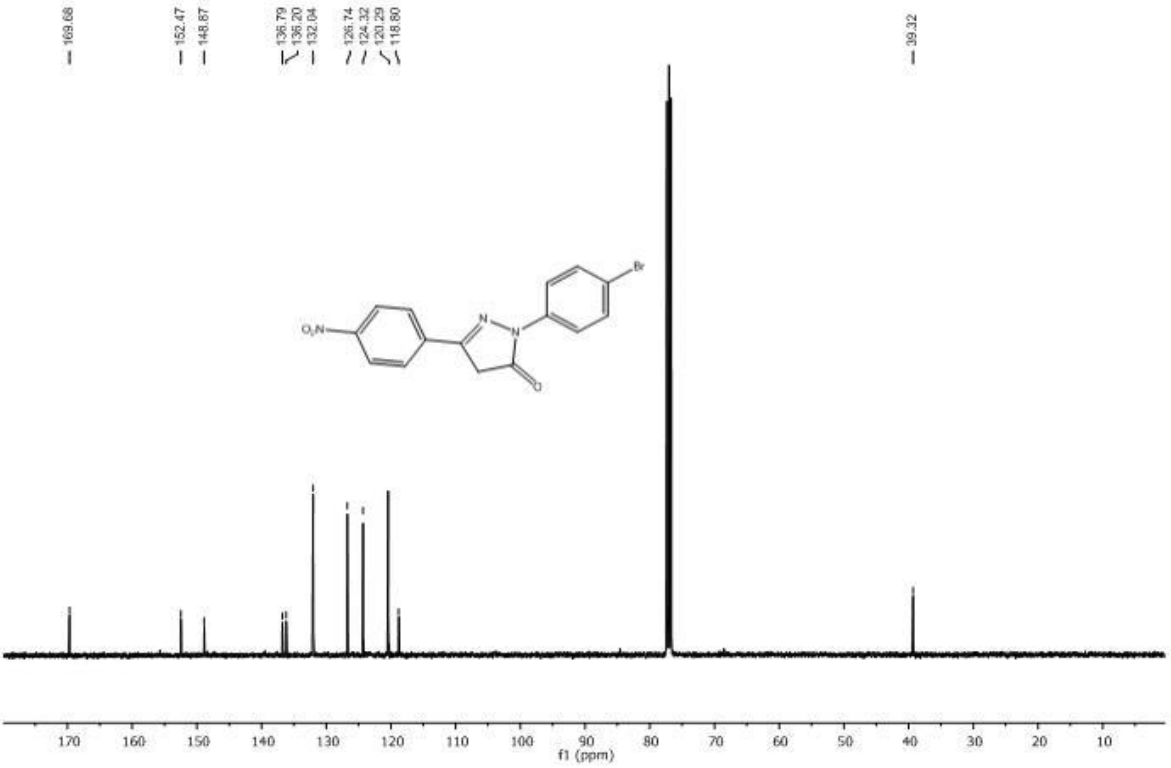


Figure S20. ^{13}C NMR spectrum in $CDCl_3$ of 1-(4-bromophenyl)-3-(4-nitrophenyl)-1*H*-pyrazole-5(4*H*)-one **3f**.

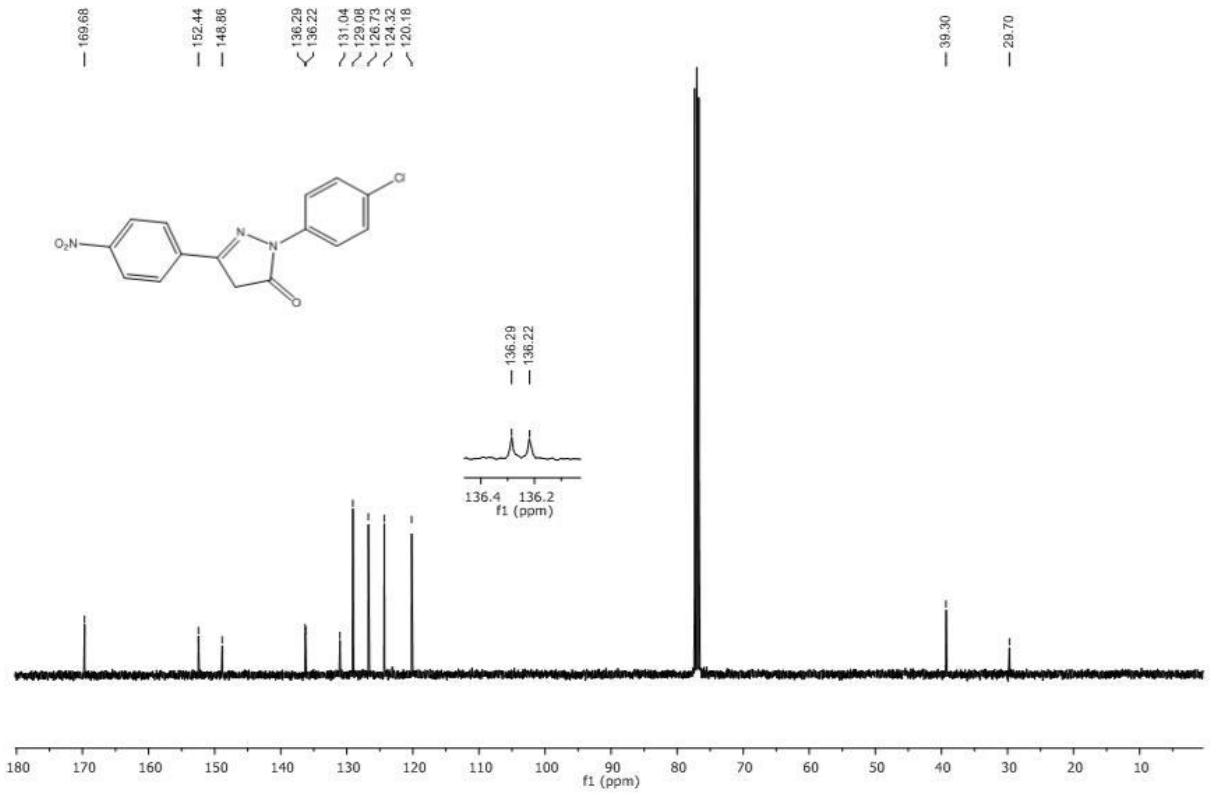


Figure S21. ^{13}C NMR spectrum in $CDCl_3$ of 1-(4-chlorophenyl)-3-(4-nitrophenyl)-1*H*-pyrazole-5(4*H*)-one **3g**.

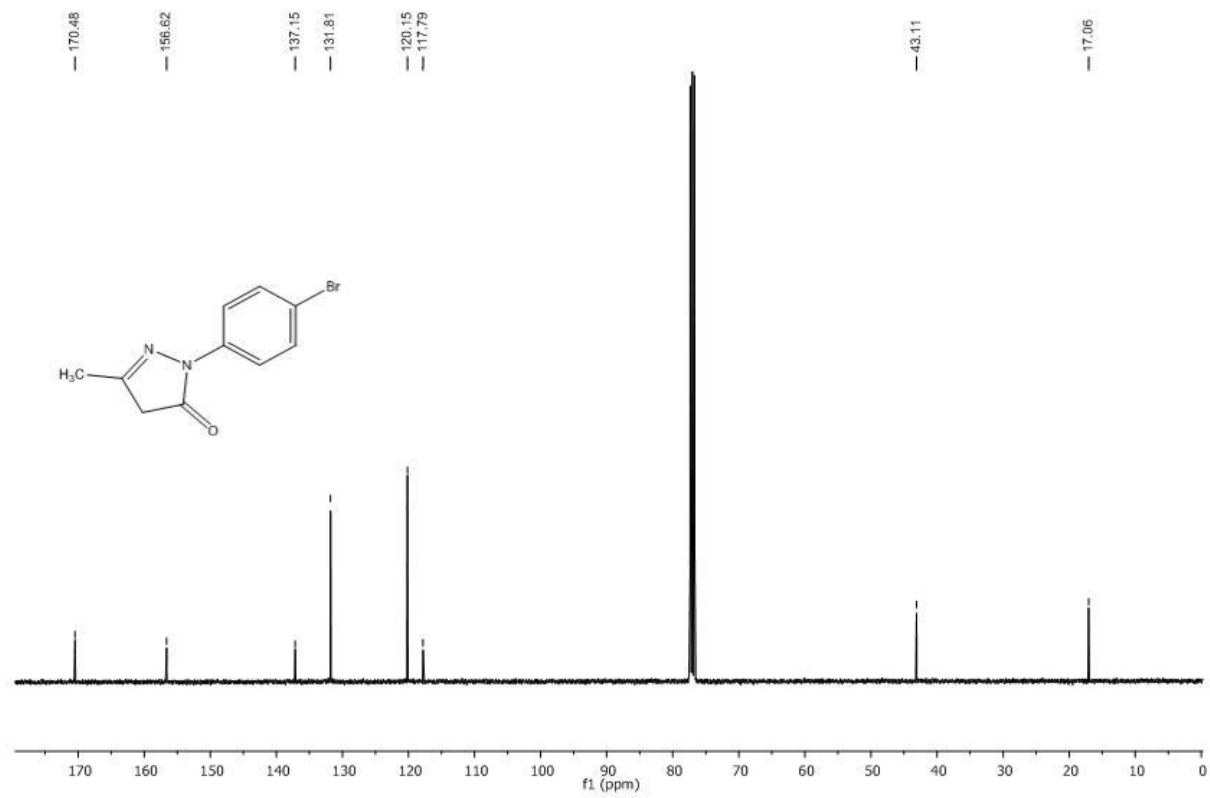


Figure S22. ^{13}C NMR spectrum in $CDCl_3$ of 1-(4-bromophenyl)-3-methyl-1*H*-pyrazole-5(4*H*)-one **3h**.

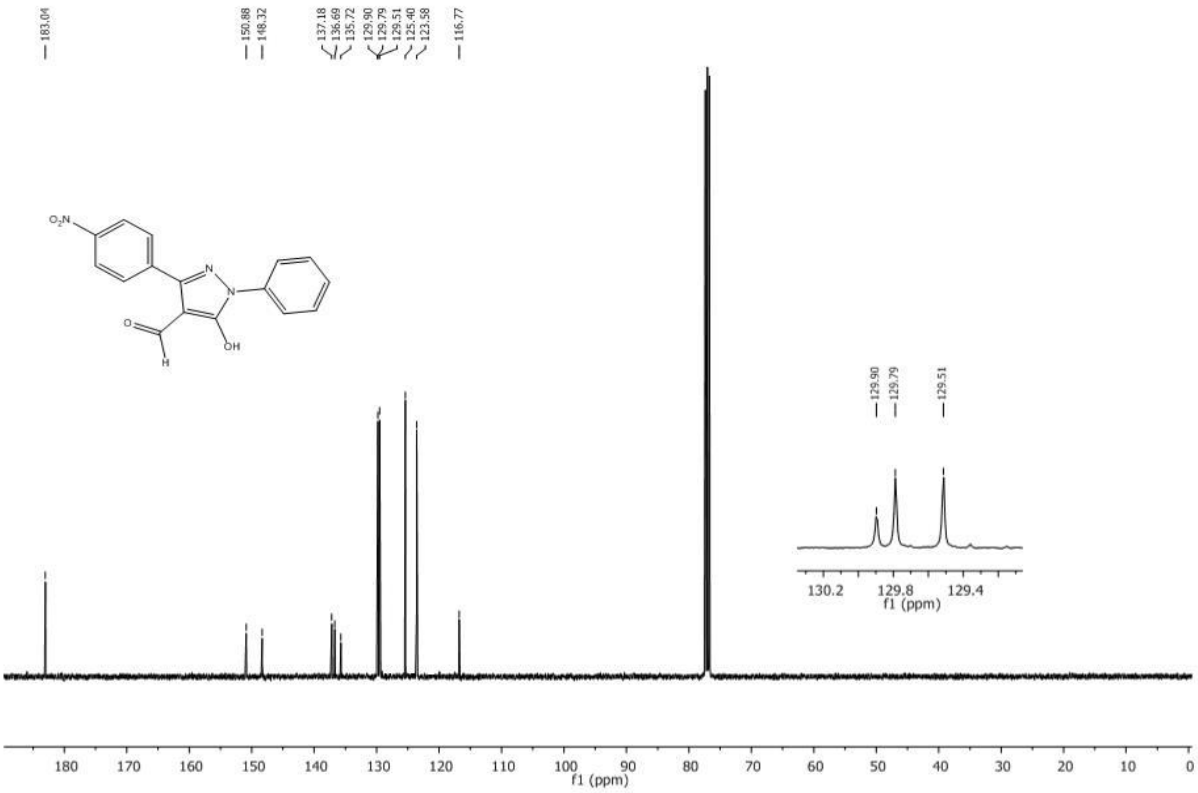


Figure S23. ^{13}C NMR spectrum in $CDCl_3$ of 5-hydroxy-3-(4-nitrophenyl)-1-phenyl-4-formyl-1*H*-pyrazole **4d**.

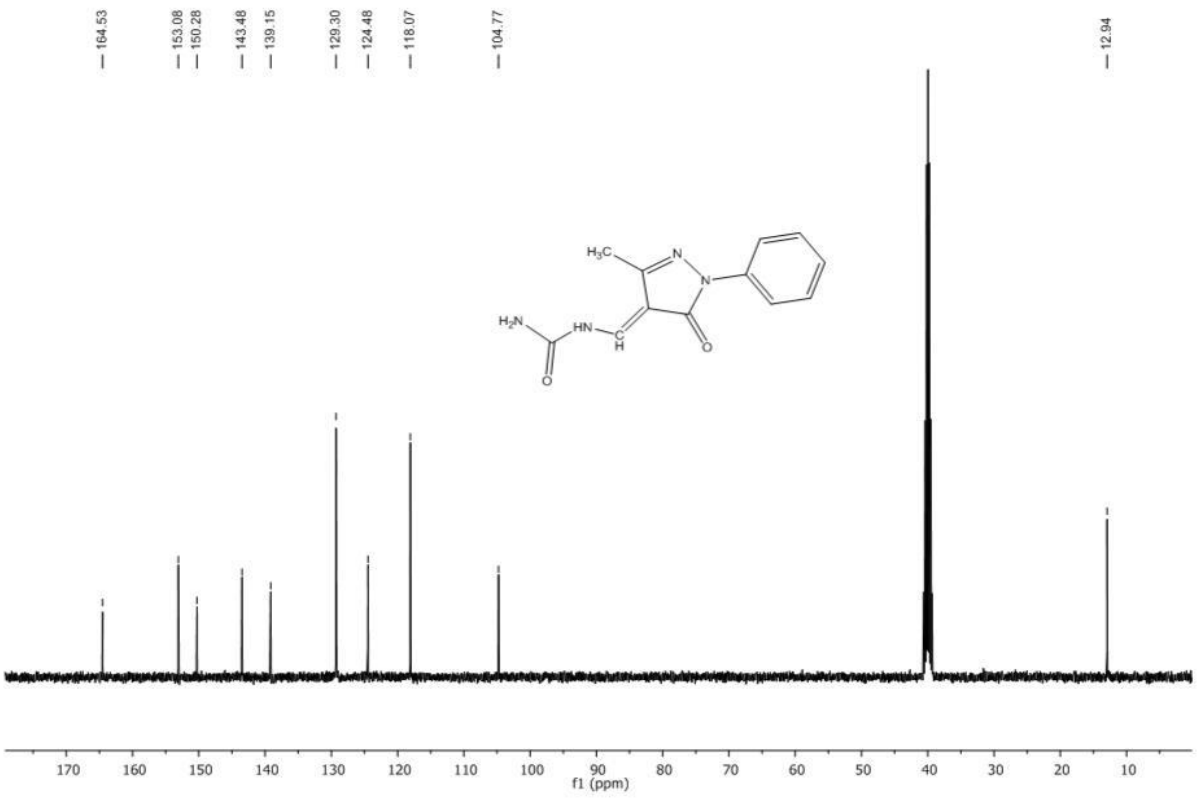


Figure S24. ^{13}C NMR spectrum in DMSO-d_6 of N-[(1,5-dihydro-3-methyl-5-oxo-1-phenyl-4*H*-pyrazole-4-ylidene)methyl]urea **5a**.

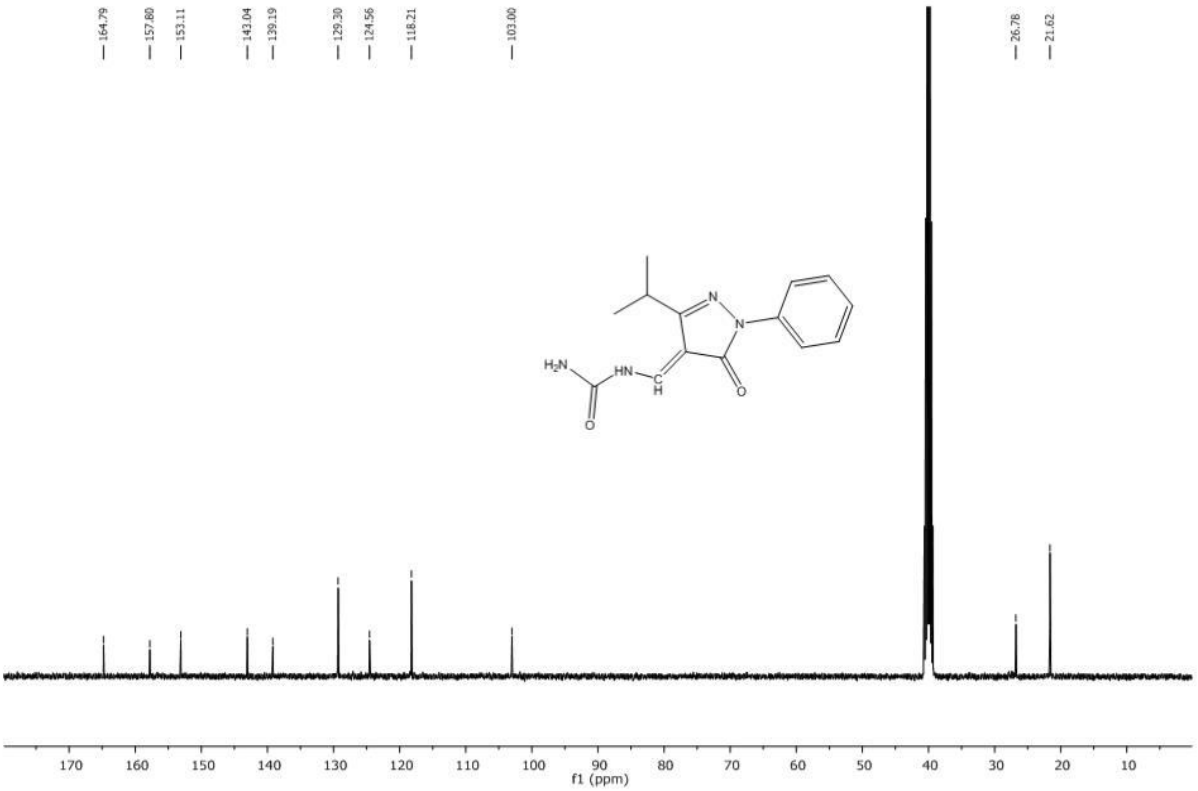


Figure S25. ^{13}C NMR spectrum in DMSO-d_6 of N-[(1,5-dihydro-1-phenyl-5-oxo-3-(isopropyl)-4*H*-pyrazole-4-ylidene)methyl]urea **5b**.

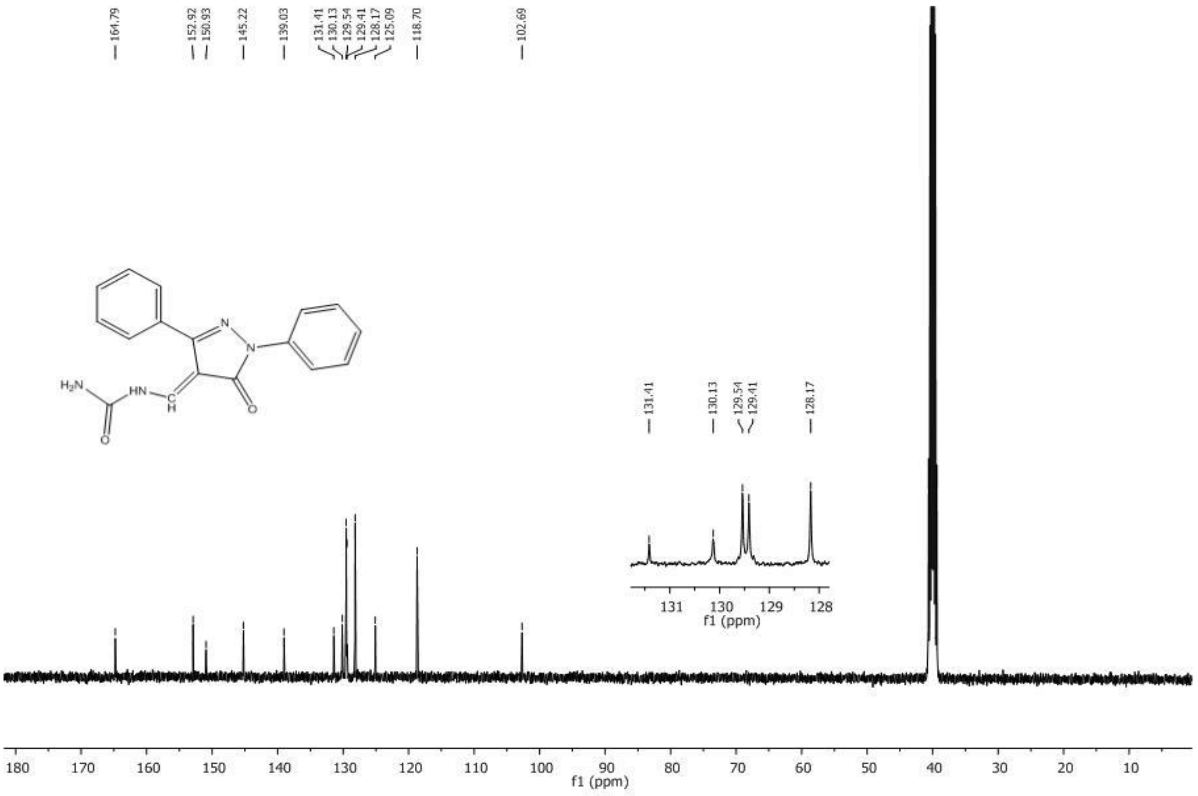


Figure S26. ^{13}C NMR spectrum in DMSO-d_6 of N-[(1,5-dihydro-1,3-diphenyl-5-oxo-4*H*-pyrazole-4-ylidene)methyl]urea **5c**.

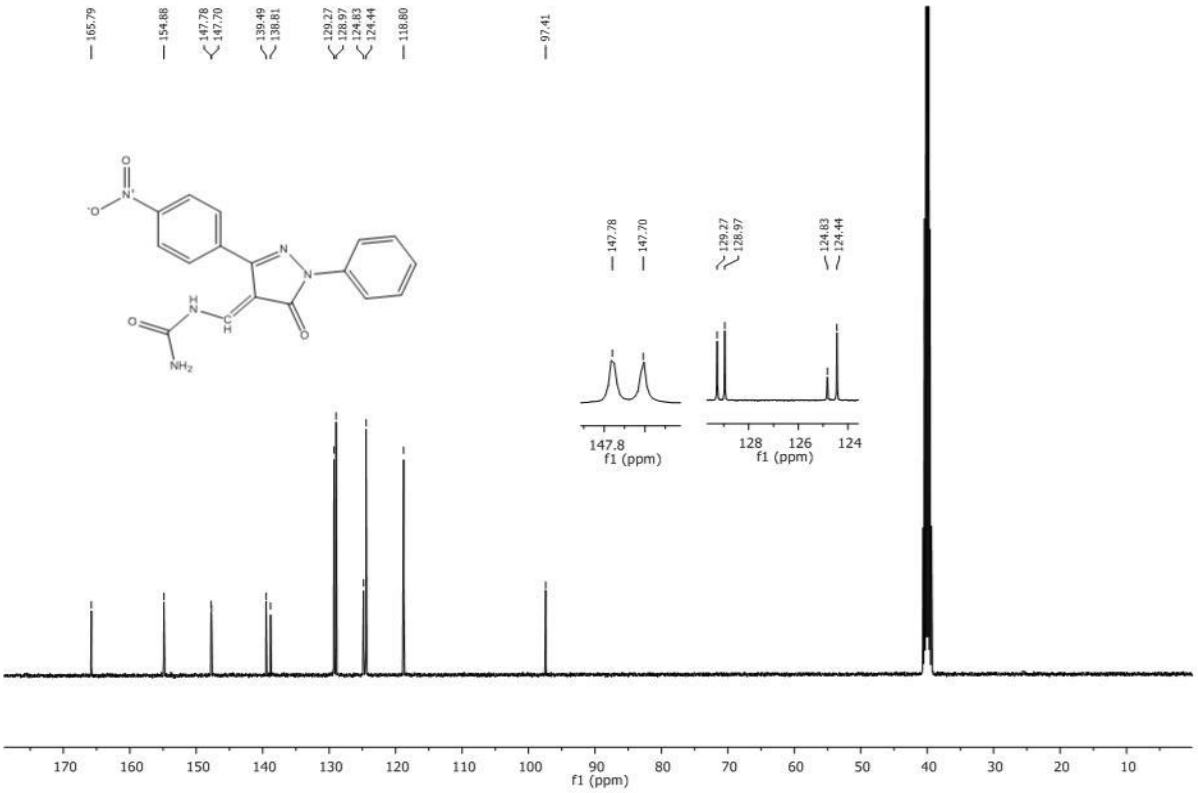


Figure S27. ^{13}C NMR spectrum in DMSO-d_6 of N-[(1,5-dihydro-1-phenyl-5-oxo-3-(4-nitrophenyl)-4*H*-pyrazole-4-ylidene)methyl]urea **5d**.

LC-MS/MS spectra

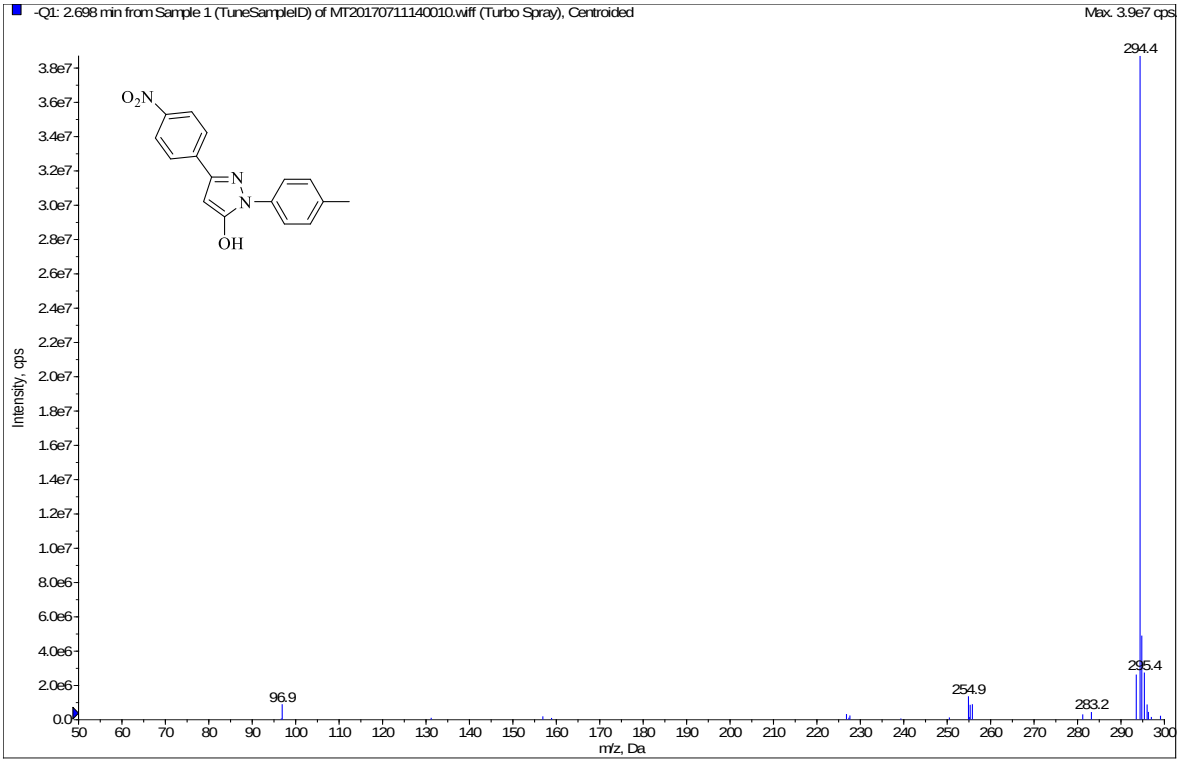


Figure S28. LC-MS/MS spectrum of 5-hydroxy-3-(4-nitrophenyl)-1-(p-tolyl)-1*H*-pyrazole **3e**.

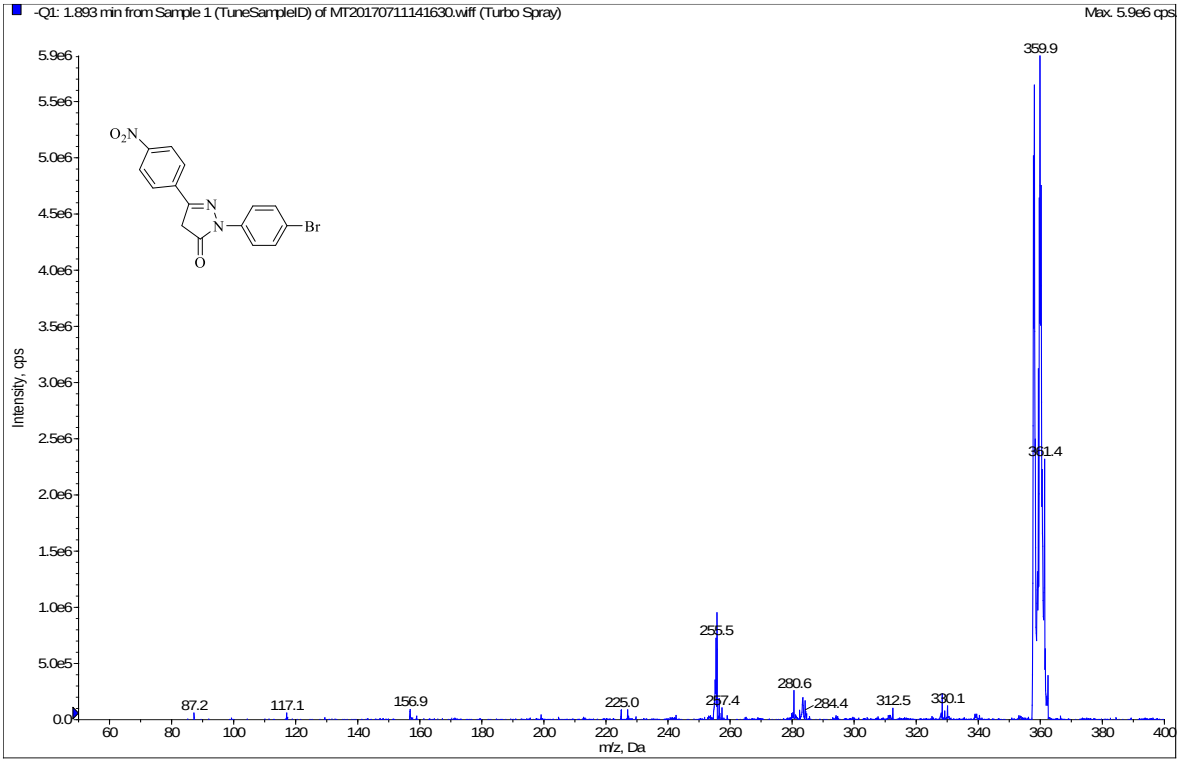


Figure S29. LC-MS/MS spectrum of 1-(4-bromophenyl)-3-(4-nitrophenyl)-1*H*-pyrazole-5(4*H*)-one **3f**.

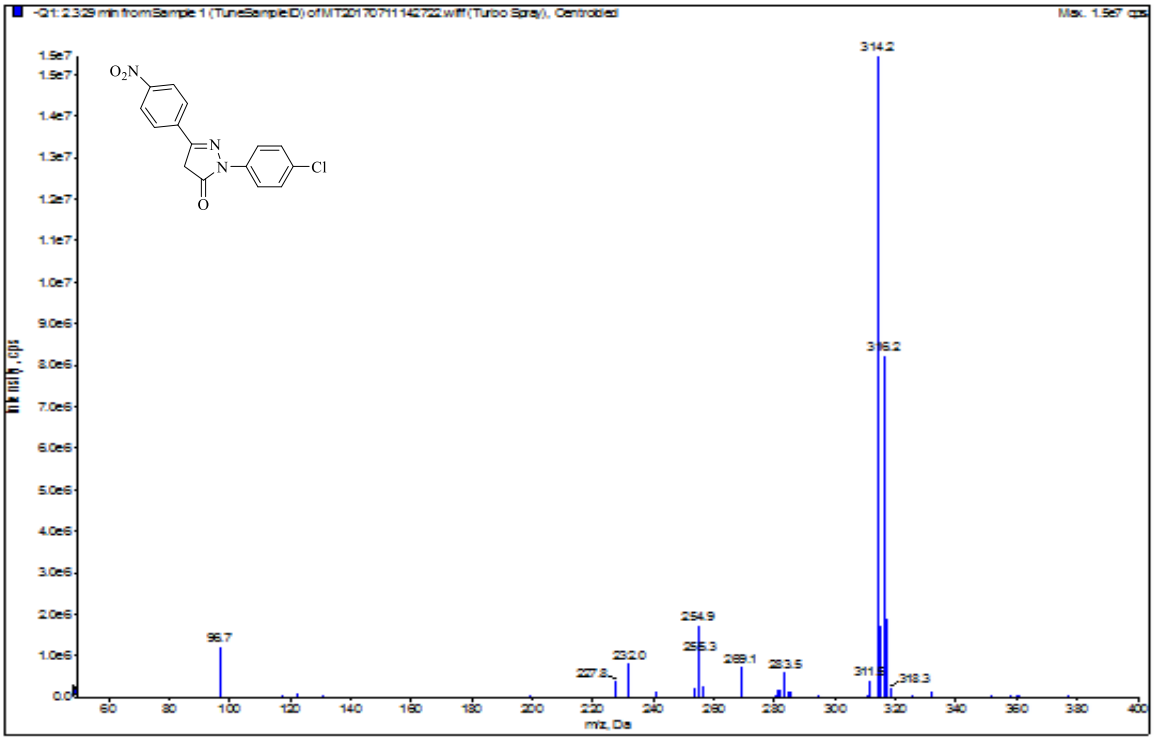


Figure S30. LC-MS/MS spectrum of 1-(4-chlorophenyl)-3-(4-nitrophenyl)-1*H*-pyrazole-5(4*H*)-one **3g**.

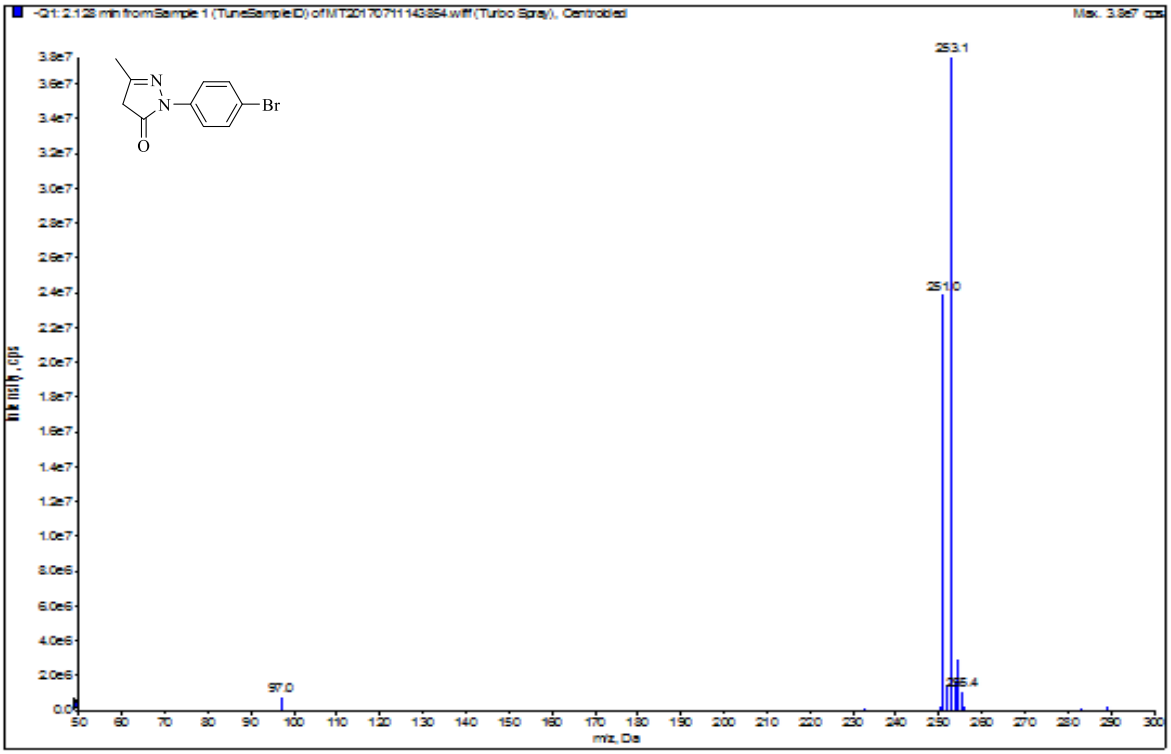


Figure S31. LC-MS/MS spectrum of 1-(4-bromophenyl)-3-methyl-1*H*-pyrazole-5(4*H*)-one **3h**.

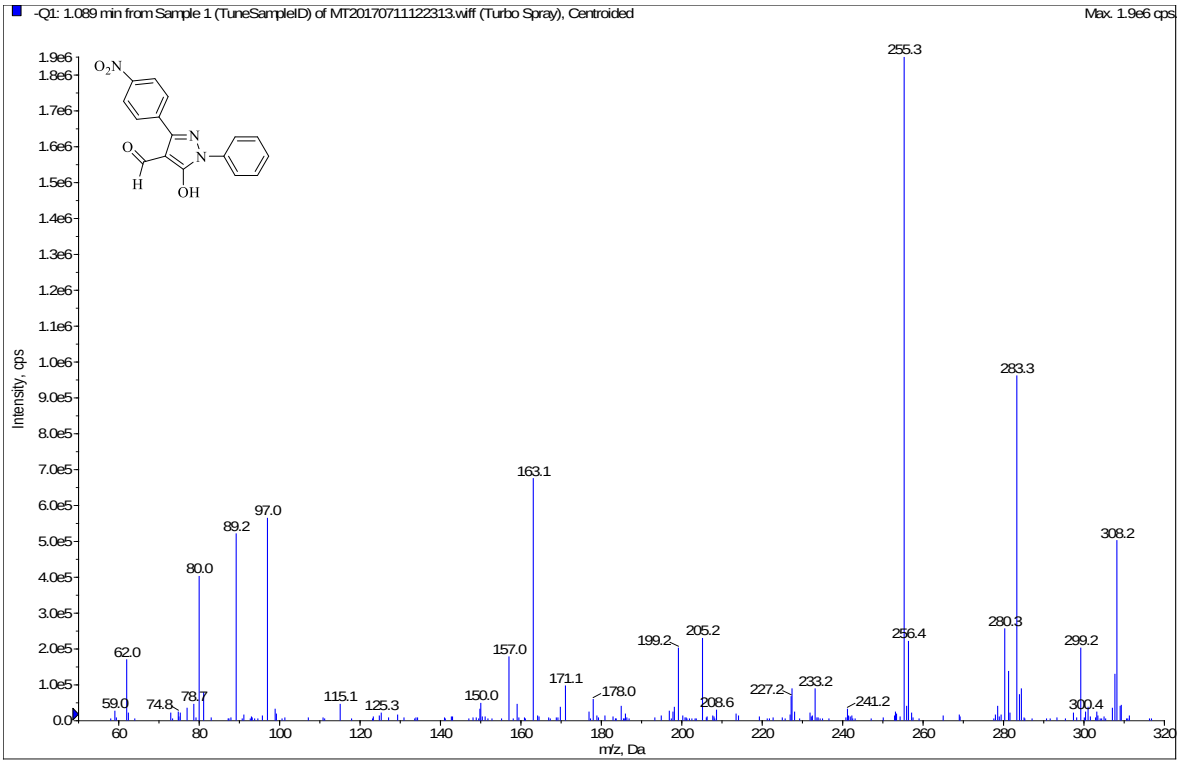


Figure S32. LC-MS/MS spectrum of 5-hydroxy-3-(4-nitrophenyl)-1-phenyl-4-formyl-1*H*-pyrazole **4d**.

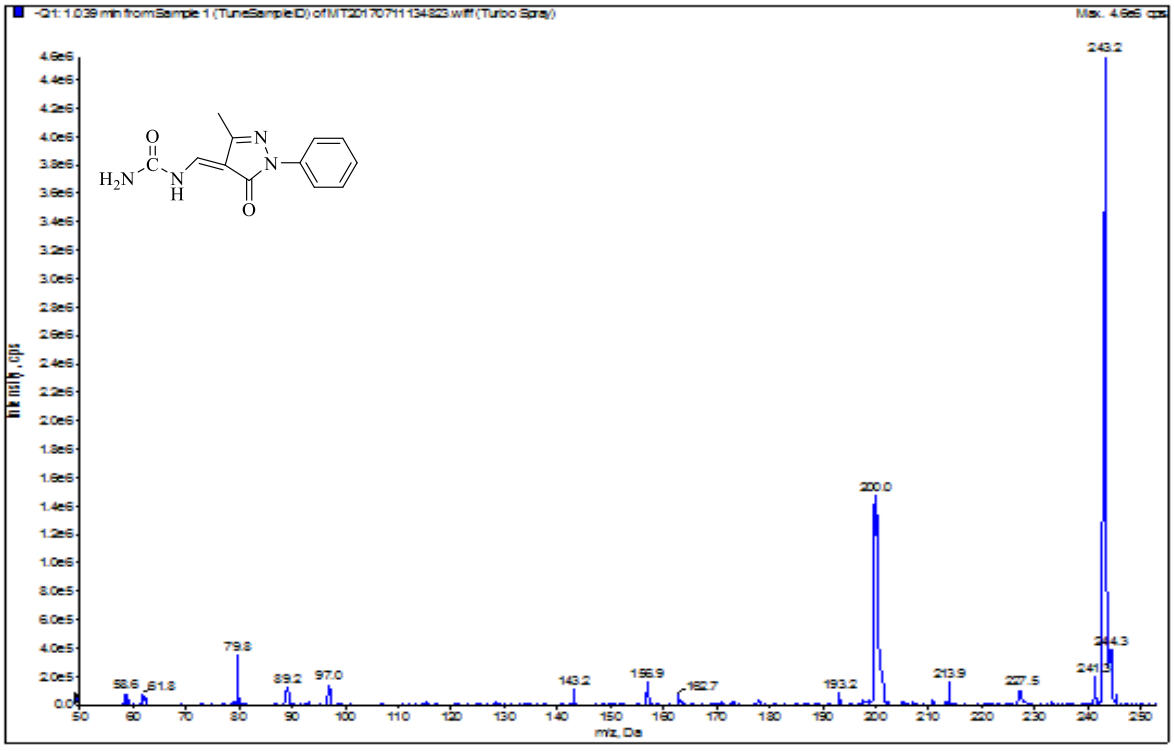


Figure S33. LC-MS/MS spectrum of N-[(1,5-dihydro-3-methyl-5-oxo-1-phenyl-4*H*-pyrazole-4-ylidene)methyl]urea **5a**.

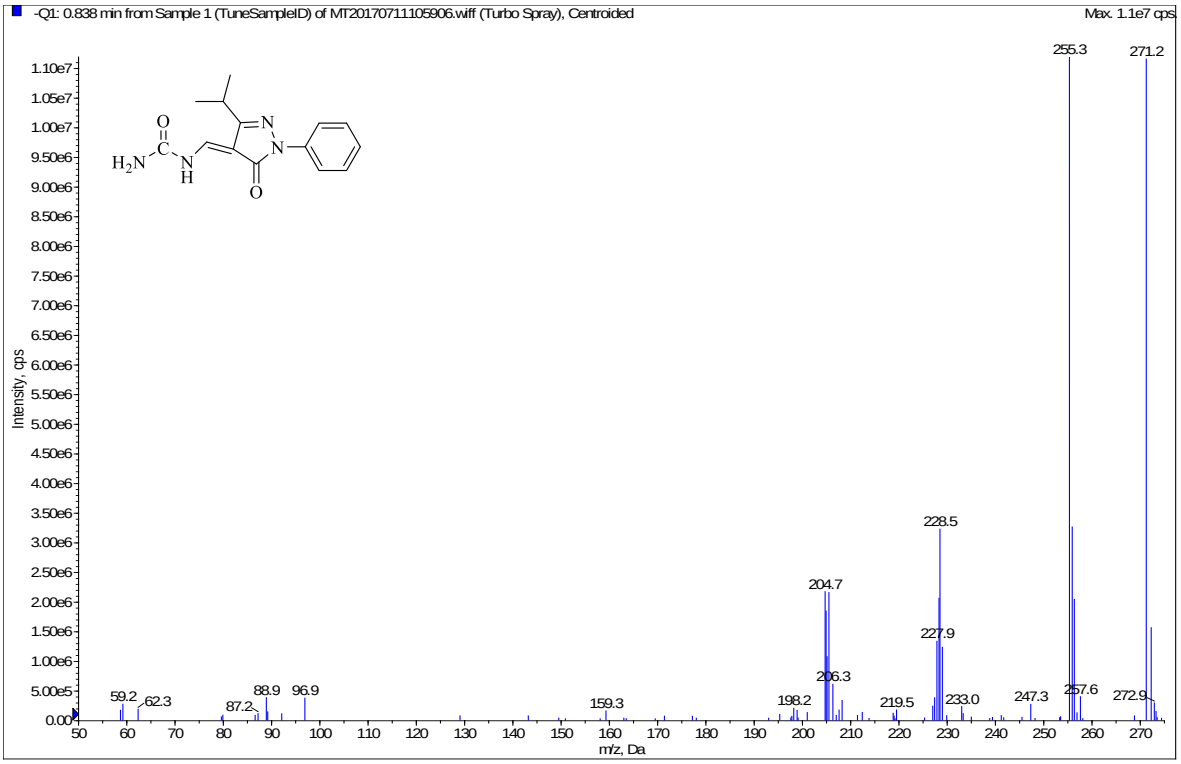


Figure S34. LC-MS/MS spectrum of N-[(1,5-dihydro-1-phenyl-5-oxo-3-(isopropyl)-4*H*-pyrazole-4-ylidene)methyl]urea **5b**.

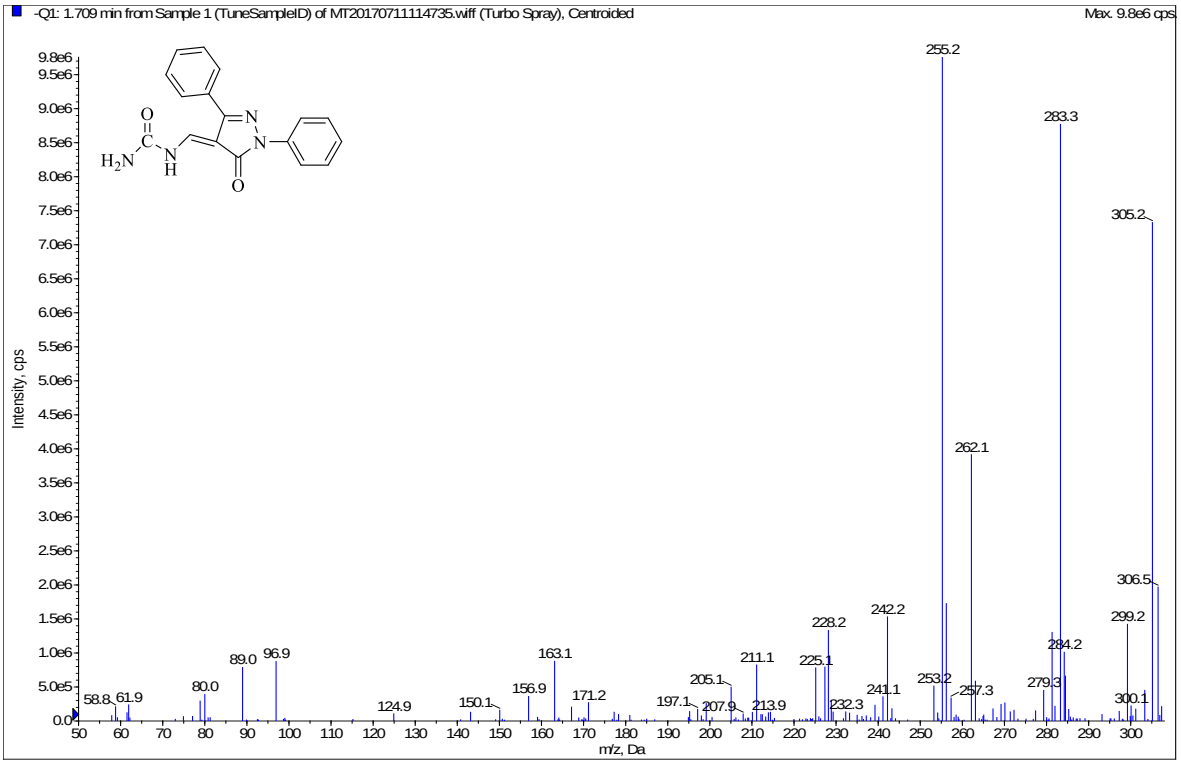


Figure S35. LC-MS/MS spectrum of N-[(1,5-dihydro-1,3-diphenyl-5-oxo-4*H*-pyrazole-4-ylidene)methyl]urea **5c**.

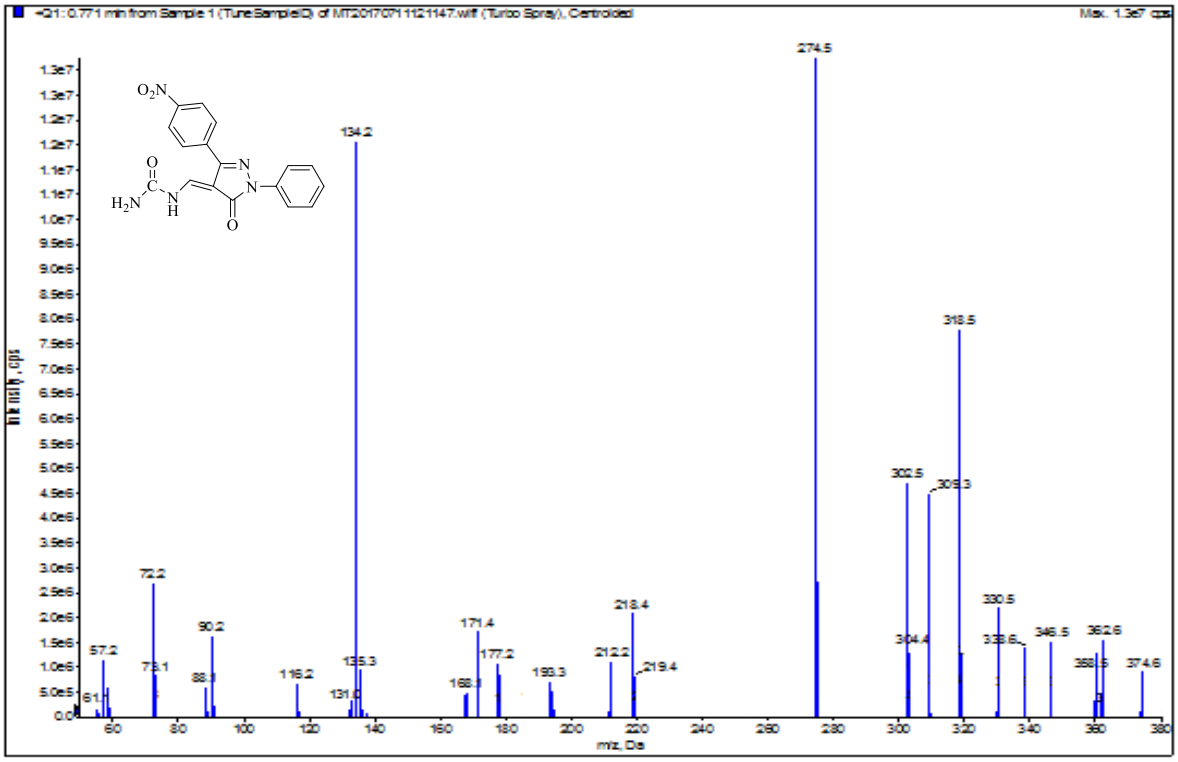
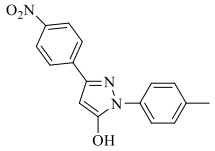
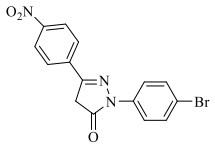
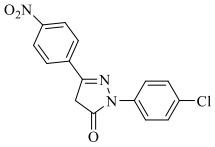
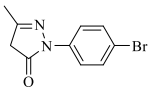
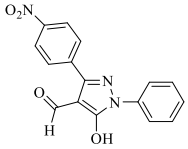
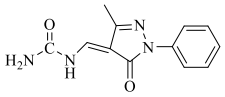
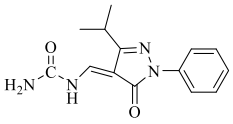
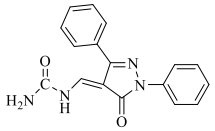
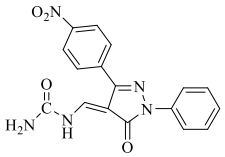


Figure S36. LC-MS/MS spectrum of N-[(1,5-dihydro-1-phenyl-5-oxo-3-(4-nitrophenyl)-4*H*-pyrazole-4-ylidene)methyl]urea **5d**.

Elemental analysis results

Table 1. Elemental analysis results of compounds.

No	Compounds	Formula	Results		
			Element	Calculated [%]	Found [%]
3e		$C_{16}H_{13}N_3O_3$	C	65.08	64.97
			H	4.44	4.54
			N	14.23	14.17
3f		$C_{15}H_{10}BrN_3O_3$	C	50.02	49.86
			H	2.80	2.83
			N	11.67	11.55
3g		$C_{15}H_{10}ClN_3O_3$	C	57.07	56.79
			H	3.19	3.29
			N	13.31	13.87
3h		$C_{10}H_9BrN_2O$	C	47.46	47.54
			H	3.58	3.54
			N	11.07	11.14
4d		$C_{16}H_{11}N_3O_4$	C	62.14	62.06
			H	3.59	3.50
			N	13.59	13.65
5a		$C_{12}H_{12}N_4O_2$	C	59.01	58.93
			H	4.95	4.81
			N	22.94	23.07
5b		$C_{14}H_{16}N_4O_2$	C	61.75	61.88
			H	5.92	5.86
			N	20.58	20.77
5c		$C_{17}H_{14}N_4O_2$	C	66.66	66.9
			H	4.61	4.50
			N	18.29	18.50
5d		$C_{17}H_{13}N_5O_4$	C	58.12	58.26
			H	3.73	3.70
			N	19.93	20.16

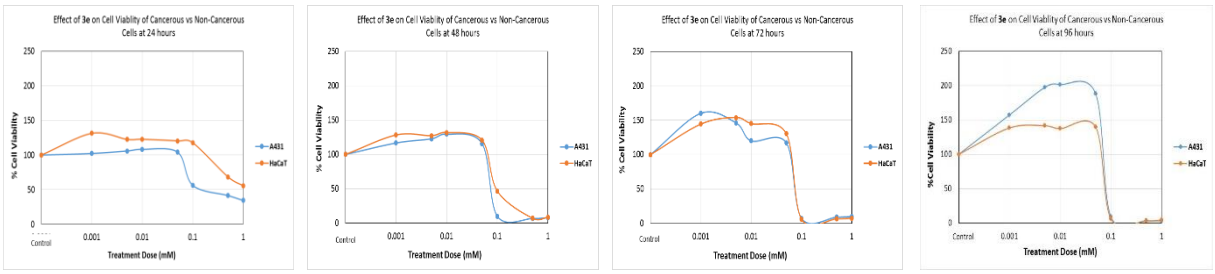


Figure S37. Effects of **3e** on Cell Viability of Cancerous vs Non-Cancerous Cells at 24, 48, 72, and 96 Hours.

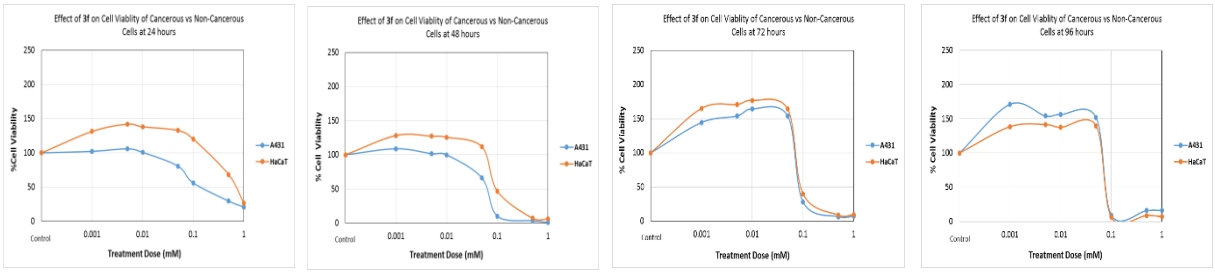


Figure S38. Effects of **3f** on Cell Viability of Cancerous vs Non-Cancerous Cells at 24, 48, 72, and 96 Hours.

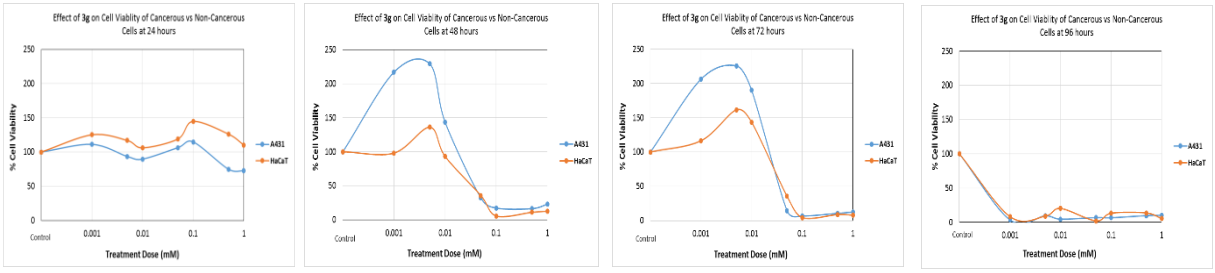


Figure S39. Effects of **3g** on Cell Viability of Cancerous vs Non-Cancerous Cells at 24, 48, 72, and 96 Hours.

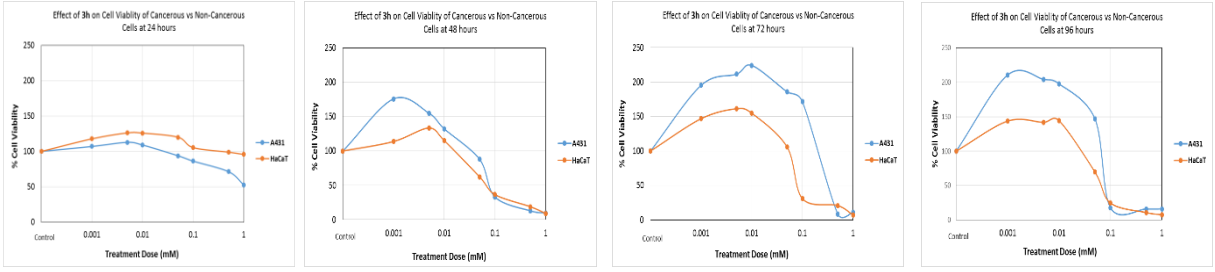


Figure S40. Effects of **3h** on Cell Viability of Cancerous vs Non-Cancerous Cells at 24, 48, 72, and 96 Hours.

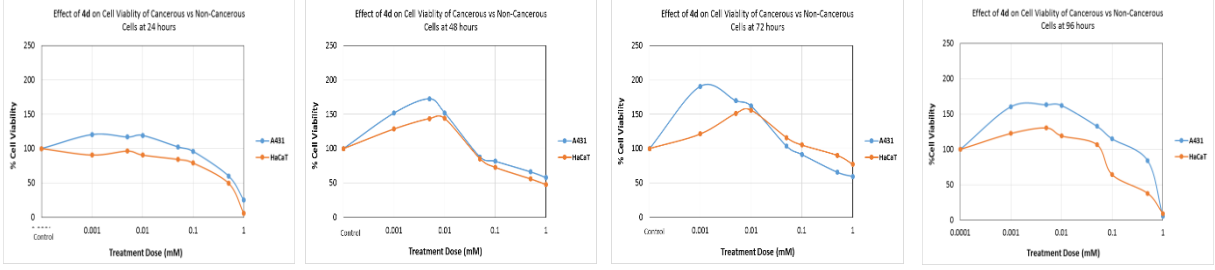


Figure S41. Effects of **4d** on Cell Viability of Cancerous vs Non-Cancerous Cells at 24, 48, 72, and 96 Hours.

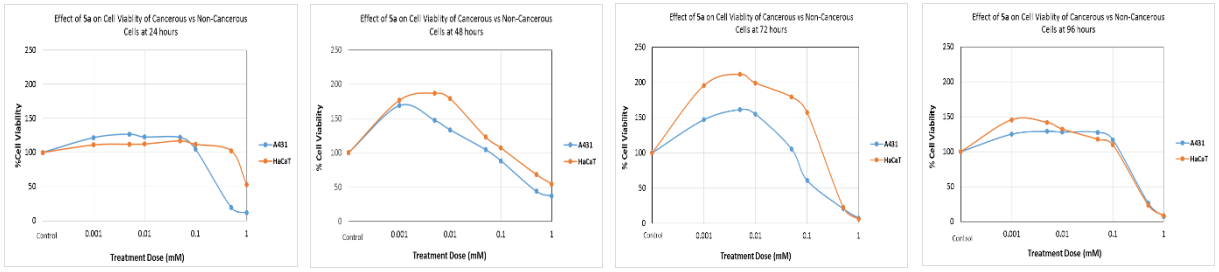


Figure S42. Effects of **5a** on Cell Viability of Cancerous vs Non-Cancerous Cells at 24, 48, 72, and 96 Hours.

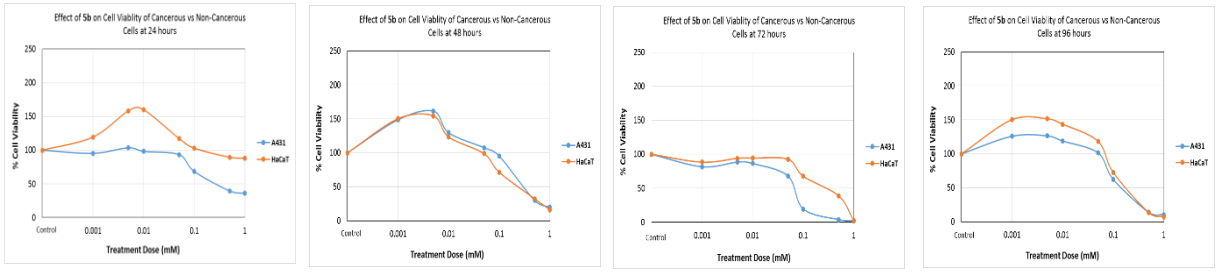


Figure S43. Effects of **5b** on Cell Viability of Cancerous vs Non-Cancerous Cells at 24, 48, 72, and 96 Hours.

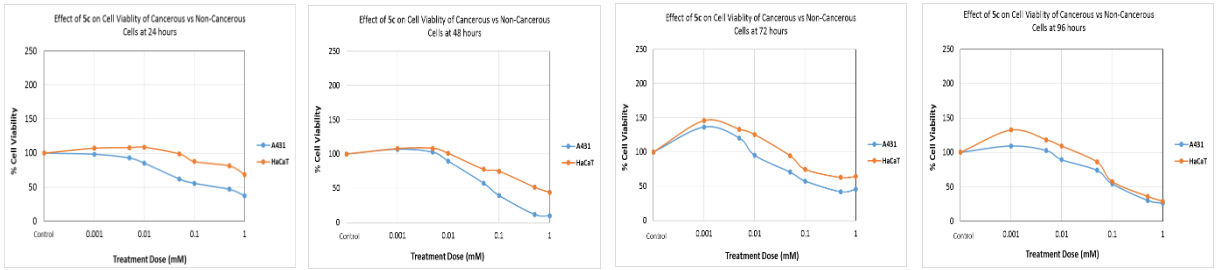


Figure S44. Effects of **5c** on Cell Viability of Cancerous vs Non-Cancerous Cells at 24, 48, 72, and 96 Hours.

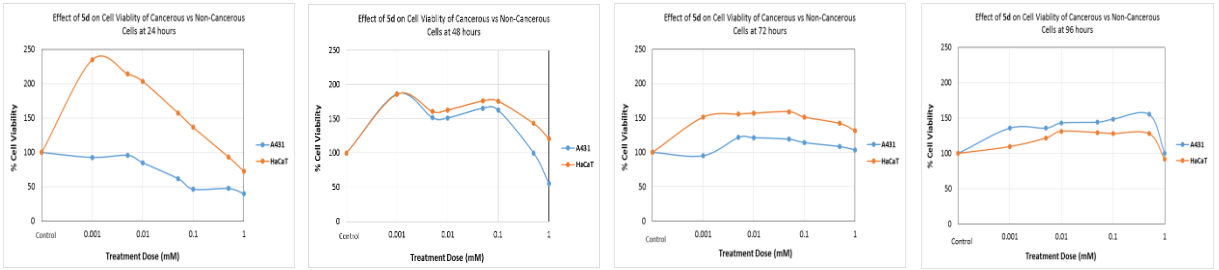
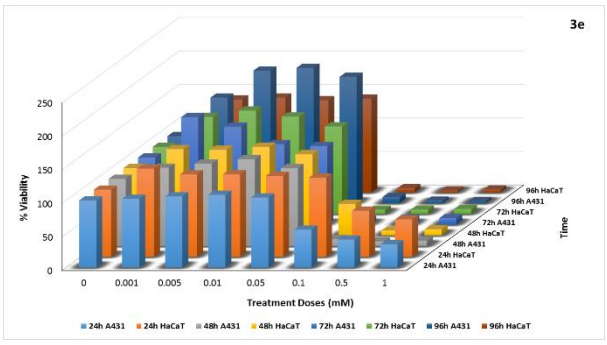
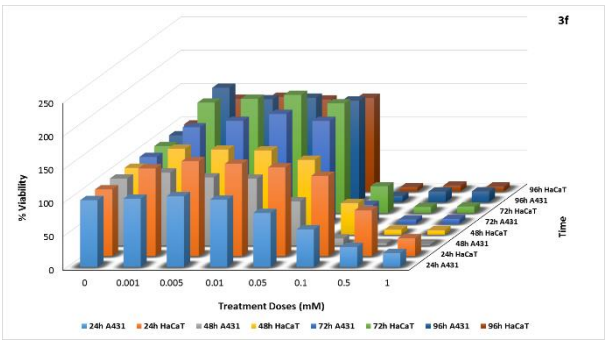
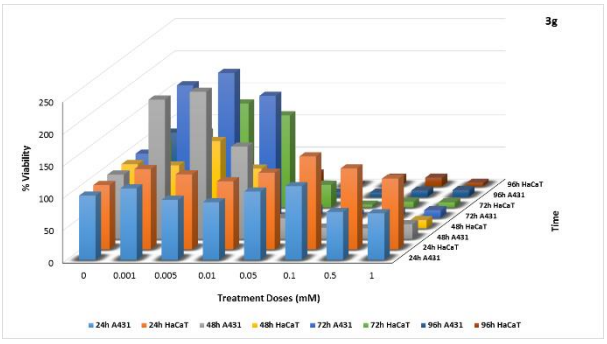
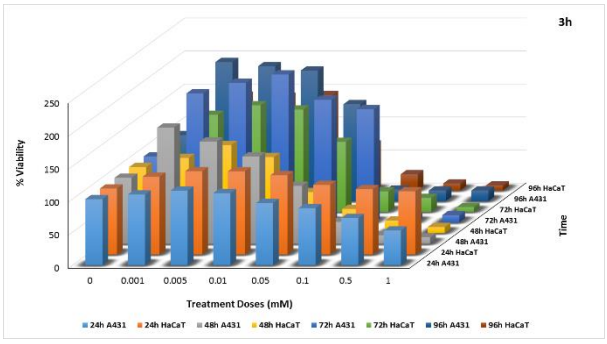


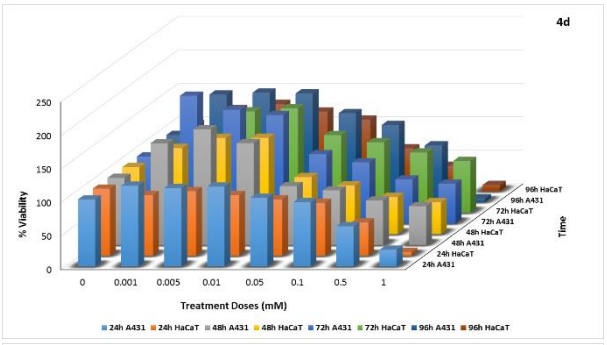
Figure S45. Effects of **5d** on Cell Viability of Cancerous vs Non-Cancerous Cells at 24, 48, 72, and 96 Hours.

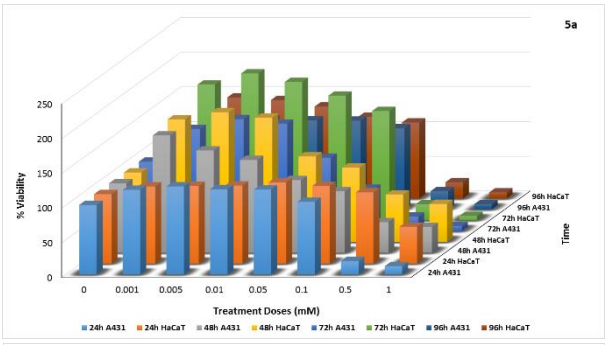

3e
% Viability
Treatment Doses (mM)
Time
24h A431 24h HaCaT 48h A431 48h HaCaT 72h A431 72h HaCaT 96h A431 96h HaCaT

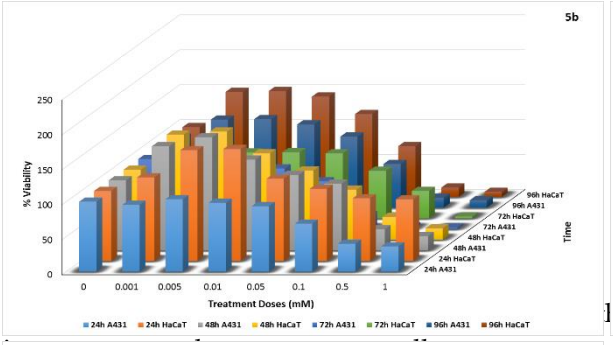

3f
% Viability
Treatment Doses (mM)
Time
24h A431 24h HaCaT 48h A431 48h HaCaT 72h A431 72h HaCaT 96h A431 96h HaCaT

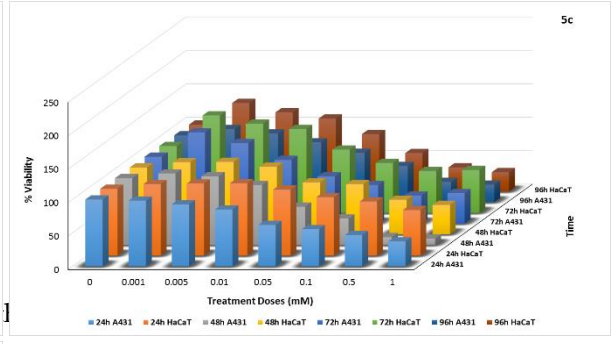

3g
% Viability
Treatment Doses (mM)
Time
24h A431 24h HaCaT 48h A431 48h HaCaT 72h A431 72h HaCaT 96h A431 96h HaCaT

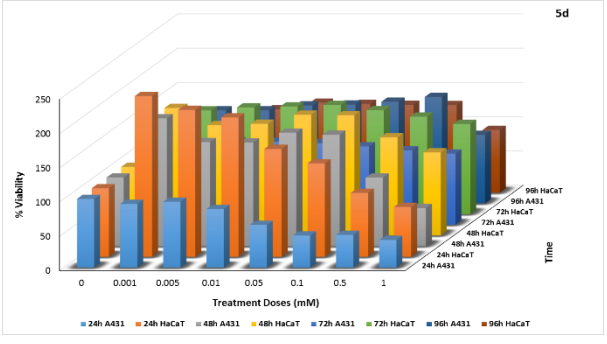

3h
% Viability
Treatment Doses (mM)
Time
24h A431 24h HaCaT 48h A431 48h HaCaT 72h A431 72h HaCaT 96h A431 96h HaCaT


4d
% Viability
Treatment Doses (mM)
Time
24h A431 24h HaCaT 48h A431 48h HaCaT 72h A431 72h HaCaT 96h A431 96h HaCaT


5a
% Viability
Treatment Doses (mM)
Time
24h A431 24h HaCaT 48h A431 48h HaCaT 72h A431 72h HaCaT 96h A431 96h HaCaT


5b
% Viability
Treatment Doses (mM)
Time
24h A431 24h HaCaT 48h A431 48h HaCaT 72h A431 72h HaCaT 96h A431 96h HaCaT


5c
% Viability
Treatment Doses (mM)
Time
24h A431 24h HaCaT 48h A431 48h HaCaT 72h A431 72h HaCaT 96h A431 96h HaCaT


5d
% Viability
Treatment Doses (mM)
Time
24h A431 24h HaCaT 48h A431 48h HaCaT 72h A431 72h HaCaT 96h A431 96h HaCaT