

Supplementary Materials

Table S1: Raw replicate inhibition zone diameters (mm) of chalcone and pyrazoline derivatives against *Escherichia coli* (disc diffusion, n = 3)

Compound	Conc. (µg/disc)	Replicate 1	Replicate 2	Replicate 3	Mean ± SD
5a	2	NG	NG	NG	NG
5a	4	24.0	24.8	24.2	24.3 ± 0.6
5a	6	31.8	32.0	32.5	32.1 ± 0.5
5a	8	34.6	35.1	35.2	35.0 ± 0.7
5b	2	9.8	10.5	10.3	10.2 ± 0.5
5b	4	15.4	16.0	16.6	16.0 ± 0.6
5b	6	9.8	10.2	10.4	10.1 ± 0.3
5b	8	7.6	8.0	8.4	8.0 ± 0.4
5c	2	NG	NG	NG	NG
5c	4	19.8	20.3	20.5	20.2 ± 0.4
5c	6	32.6	33.3	34.2	33.4 ± 0.8
5c	8	34.2	35.3	35.6	35.0 ± 0.9
5d	2	19.6	20.2	20.3	20.0 ± 0.5
5d	4	20.4	21.2	21.7	21.1 ± 0.7
5d	6	20.5	21.0	21.5	21.0 ± 0.6
5d	8	22.2	23.1	23.7	23.0 ± 0.8
5e	2	16.6	17.0	17.4	17.0 ± 0.4
5e	4	4.8	5.0	5.2	5.0 ± 0.2
5e	6	NG	NG	NG	NG
5e	8	17.6	18.0	18.4	18.0 ± 0.5
5f	2	NG	NG	NG	NG
5f	4	12.0	12.3	12.4	12.2 ± 0.3
5f	6	12.6	13.0	13.4	13.0 ± 0.4
5f	8	32.4	33.2	33.5	33.0 ± 0.8
5g	2	NG	NG	NG	NG
5g	4	7.9	8.0	8.4	8.1 ± 0.2
5g	6	21.5	22.0	22.6	22.0 ± 0.6
5g	8	30.4	31.0	31.6	31.0 ± 0.7
5h	2	NG	NG	NG	NG
5h	4	NG	NG	NG	NG
5h	6	NG	NG	NG	NG
5h	8	NG	NG	NG	NG
5i	2	NG	NG	NG	NG
5i	4	NG	NG	NG	NG
5i	6	9.7	10.0	10.3	10.0 ± 0.3
5i	8	20.4	21.0	21.6	21.0 ± 0.6
4a	2	NG	NG	NG	NG
4a	4	NG	NG	NG	NG
4a	6	NG	NG	NG	NG
4a	8	7.6	8.0	8.4	8.0 ± 0.4
Amoxicillin	2	9.7	10.0	10.3	10.0 ± 0.3
Amoxicillin	4	12.6	13.0	13.4	13.0 ± 0.4
Amoxicillin	6	14.5	15.0	15.5	15.0 ± 0.5
Amoxicillin	8	17.5	18.0	18.5	18.0 ± 0.5

Table S2: Raw replicate inhibition zone diameters (mm) of chalcone and pyrazoline derivatives against *Staphylococcus aureus*
(disc diffusion, n = 3)

Compound	Conc. (µg/disc)	Replicate 1	Replicate 2	Replicate 3	Mean ± SD
5a	2	NG	NG	NG	NG
5a	4	23.6	24.1	24.4	24.0 ± 0.6
5a	6	31.4	32.0	32.6	32.0 ± 0.7
5a	8	34.2	35.0	35.8	35.0 ± 0.8
5b	2	NG	NG	NG	NG
5b	4	24.3	25.0	25.7	25.0 ± 0.7
5b	6	25.4	26.0	26.6	26.0 ± 0.6
5b	8	NG	NG	NG	NG
5c	2	NG	NG	NG	NG
5c	4	NG	NG	NG	NG
5c	6	34.2	35.0	35.8	35.0 ± 0.9
5c	8	37.1	38.0	38.9	38.0 ± 1.0
5d	2	NG	NG	NG	NG
5d	4	NG	NG	NG	NG
5d	6	23.4	24.0	24.6	24.0 ± 0.6
5d	8	33.2	34.0	34.8	34.0 ± 0.8
5e	2	NG	NG	NG	NG
5e	4	NG	NG	NG	NG
5e	6	19.6	20.0	20.4	20.0 ± 0.5
5e	8	29.4	30.0	30.6	30.0 ± 0.7
5f	2	NG	NG	NG	NG
5f	4	22.4	23.0	23.6	23.0 ± 0.6
5f	6	24.3	25.0	25.7	25.0 ± 0.7
5f	8	29.1	30.0	30.9	30.0 ± 0.9
5g	2	12.0	12.4	12.8	12.4 ± 0.5
5g	4	11.9	12.3	12.7	12.3 ± 0.5
5g	6	11.8	12.2	12.6	12.2 ± 0.4
5g	8	11.6	12.0	12.4	12.0 ± 0.4
5h	2	NG	NG	NG	NG
5h	4	NG	NG	NG	NG
5h	6	NG	NG	NG	NG
5h	8	16.6	17.0	17.4	17.0 ± 0.6
5i	2	21.3	22.0	22.7	22.0 ± 0.7
5i	4	32.4	33.0	33.6	33.0 ± 0.8
5i	6	33.1	34.0	34.9	34.0 ± 0.9
5i	8	34.2	35.0	35.8	35.0 ± 0.8
4a	2	NG	NG	NG	NG
4a	4	NG	NG	NG	NG
4a	6	NG	NG	NG	NG
4a	8	19.4	20.0	20.6	20.0 ± 0.6
Amoxicillin	2	19.4	20.0	20.6	20.0 ± 0.6
Amoxicillin	4	22.3	23.0	23.7	23.0 ± 0.7
Amoxicillin	6	28.2	29.0	29.8	29.0 ± 0.8
Amoxicillin	8	29.1	30.0	30.9	30.0 ± 0.9

Table S3: Correlation of ABX protons (H_a, H_b, H_x) with their corresponding carbons for pyrazoline derivatives 5a–5i, based on exact ¹³C chemical shifts from the characterization data.

Compound	H _a → C _{CH2}	H _b → C _{CH2}	H _x → C _{Hx}	O–CH ₂	O–CH ₂ carbon(s) δC
5a	3.04 (dd, 1H) → 44.26	3.77 (dd, 1H) → 44.26	5.21 (dd, 1H) → 64.41	5.06 (s, 2H)	69.96
5b	3.16 (dd, 1H) → 42.60	4.02 (dd, 1H) → 42.60	5.53 (dd, 1H) → 62.17	5.22 (s, 2H)	69.90
5c	3.21 (dd, 1H) → 43.84	4.06 (dd, 1H) → 43.84	5.29 (dd, 1H) → 64.28	5.21 (s, 2H) + 5.21 (s, 2H)	69.45, 70.29
5d	3.11 (dd, 1H) → 43.90	3.83 (dd, 1H) → 43.90	5.22 (dd, 1H) → 64.07	5.08 (s, 2H)	69.45
5e	3.07 (dd, 1H) → 44.21	3.61 (dd, 1H) → 44.21	5.31 (dd, 1H) → 60.74	4.88 (s, 2H)	69.50
5f	3.01 (dd, 1H) → 43.53	3.73 (dd, 1H) → 43.53	5.11 (dd, 1H) → 63.95	5.00 (s, 2H) ×3	69.16, 70.20, 70.43
5g	3.08 (dd, 1H) → 43.82	3.78 (dd, 1H) → 43.82	5.20 (dd, 1H) → 63.98	4.98 (s, 2H)	69.40 (also 72.72 for additional benzylic site)
5h	3.08 (dd, 1H) → 43.85	3.79 (dd, 1H) → 43.85	5.22 (dd, 1H) → 64.22	5.05 (s, 2H)	69.52
5i	3.19 (dd, 1H) → 44.27	3.89 (dd, 1H) → 44.27	5.31 (dd, 1H) → 64.72	5.17 (s, 2H)	69.81

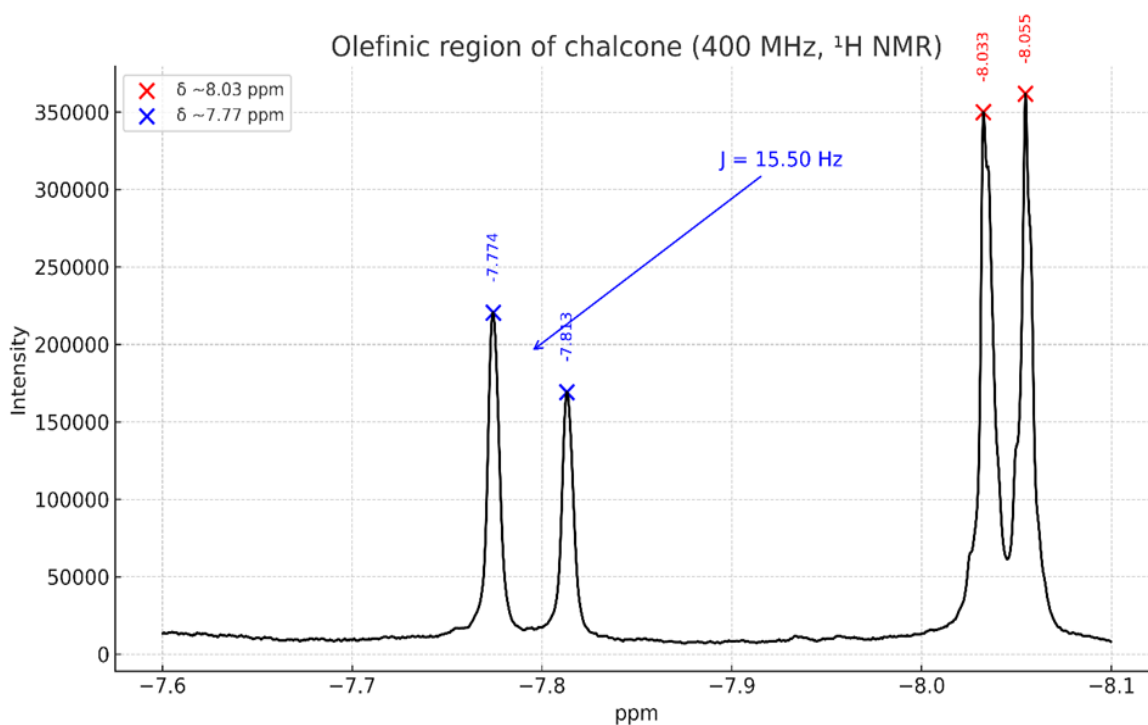


Figure S1: Olefinic region of the ¹H NMR spectrum (400 MHz, CDCl₃) of the representative chalcone (4a) derivative. The trans-coupled olefinic protons appear at δ 7.77 and 8.03 ppm with a coupling constant of J = 15.5 Hz, confirming the E-configuration of the double bond.

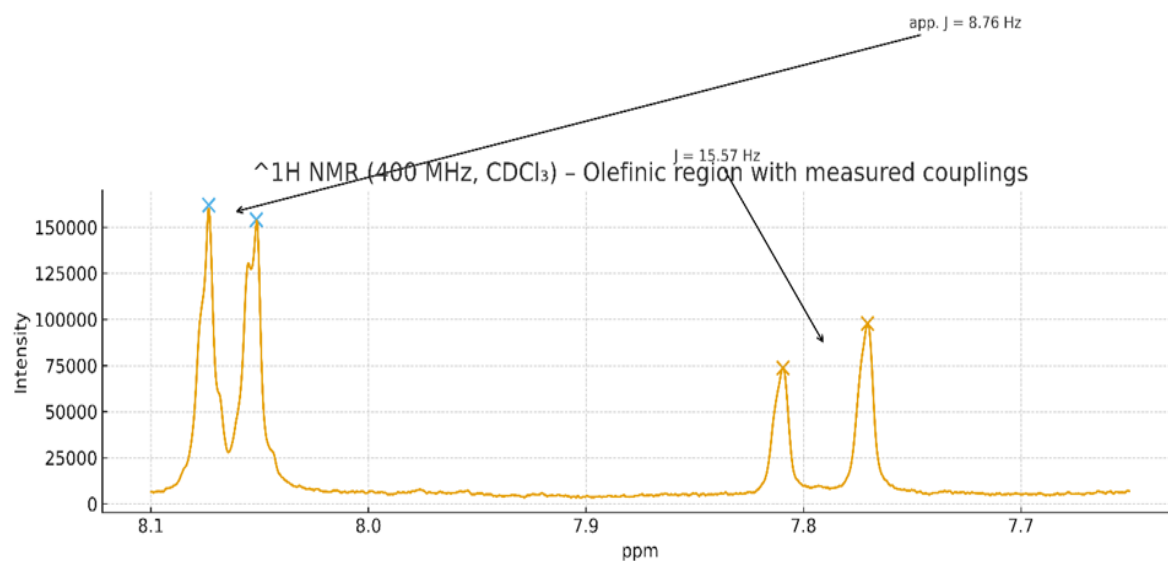


Figure S2: Olefinic region of the ¹H NMR spectrum (400 MHz, CDCl₃) of the chalcone(4b) derivative, highlighting the measured coupling constants. The trans-vinylic protons resonate at $\delta \sim 7.8$ and ~ 8.1 ppm with a coupling constant of $J = 15.6 \text{ Hz}$, confirming the E-configuration of the double bond. An additional vicinal coupling ($J \approx 8.8 \text{ Hz}$) is also observed.

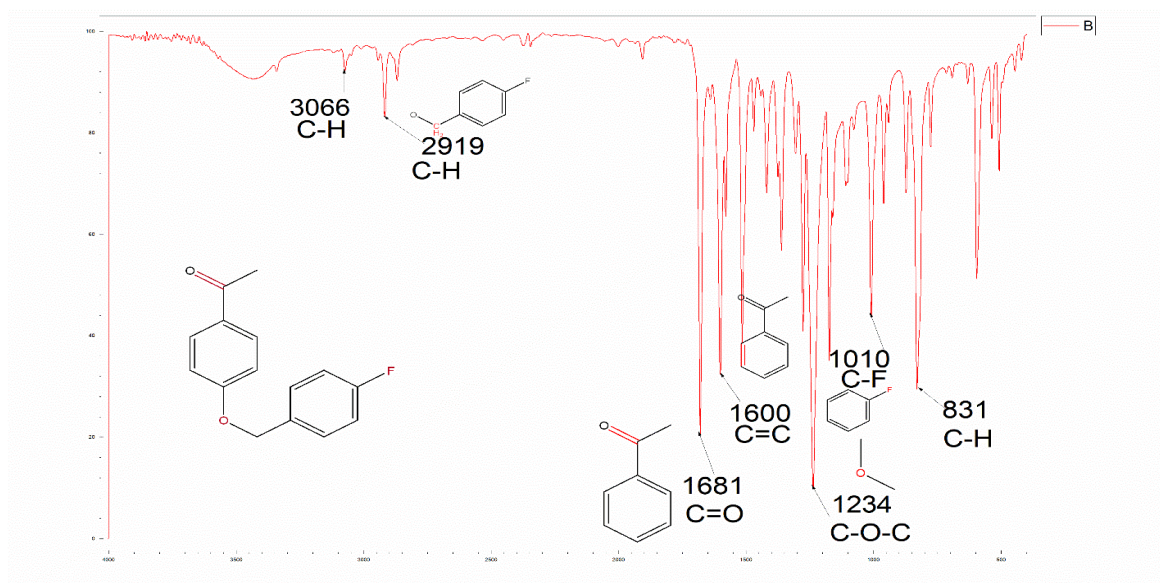


Figure S3: FTIR of 4-(4-Fluorobenzyl)oxyacetophenone (1).

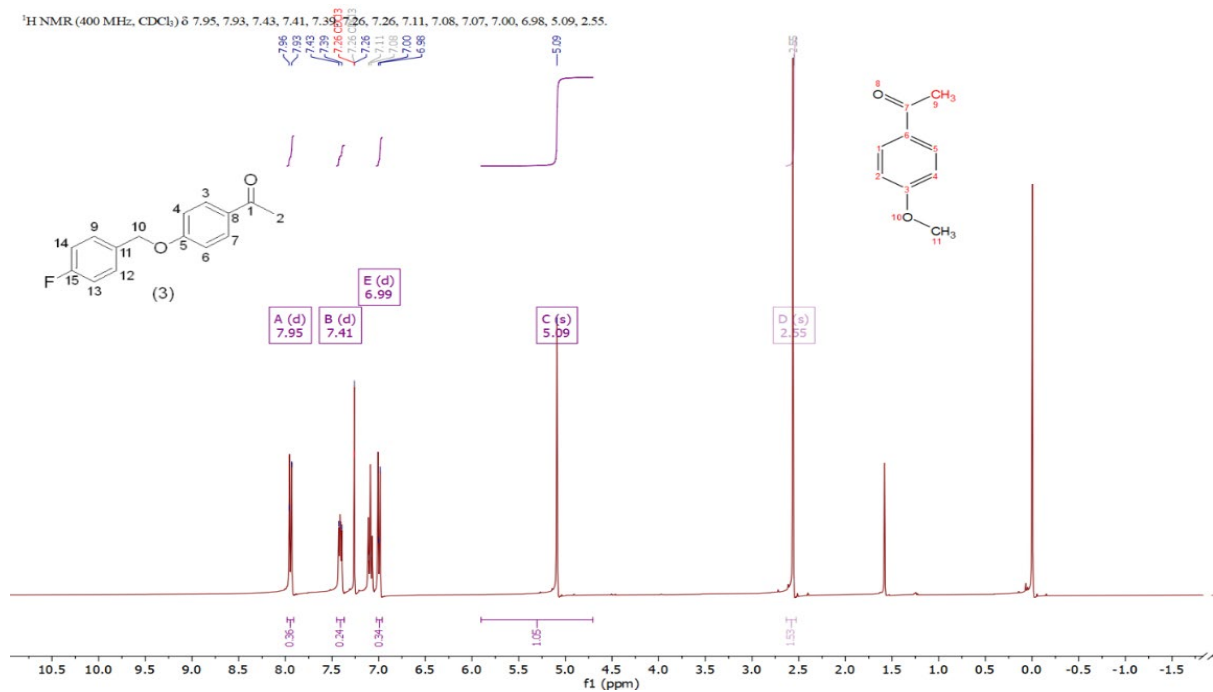


Figure S4: ^1H -NMR of 4-(4-Fluorobenzyl) oxyacetophenone (1).

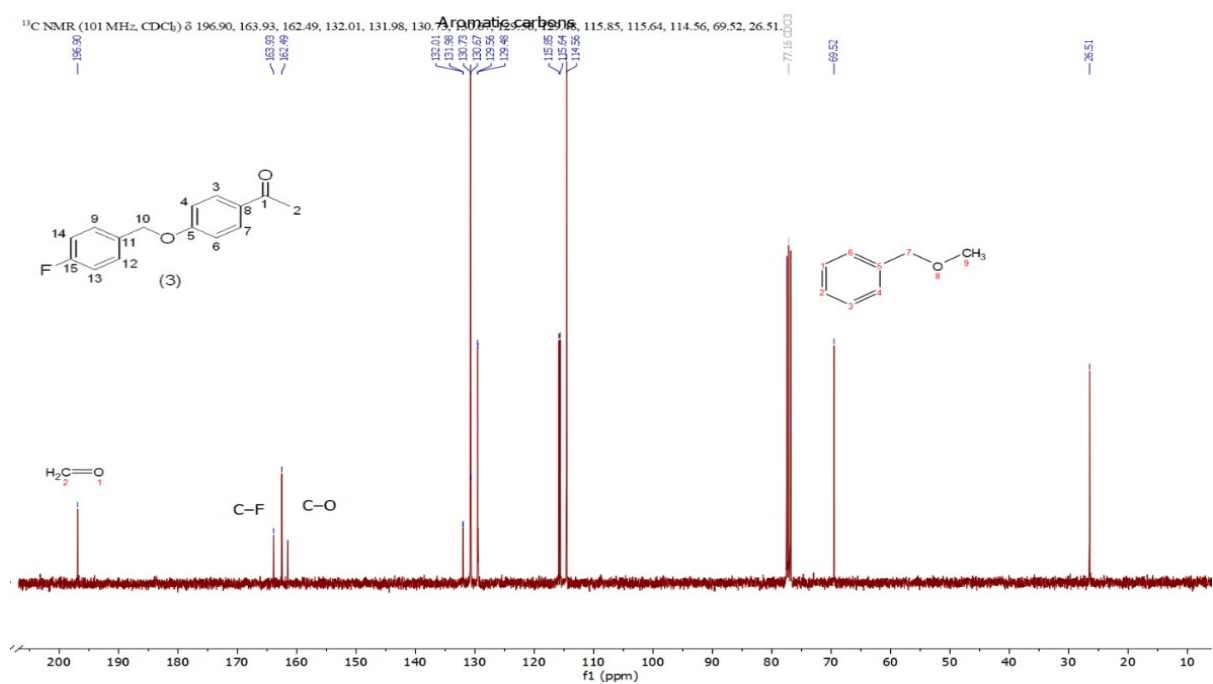


Figure S5: ^{13}C -NMR of 4-(4-Fluorobenzyl) oxyacetophenone(1).

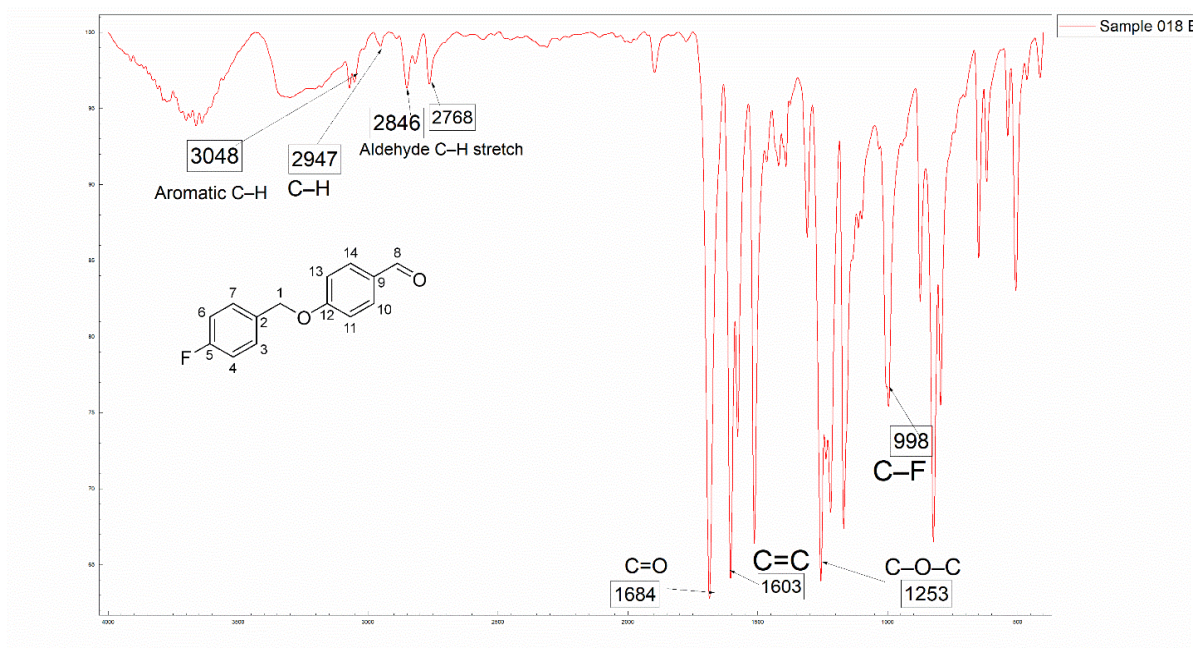


Figure S6: FTIR 4-((4-fluorobenzyl) oxy) benzaldehyde (2).

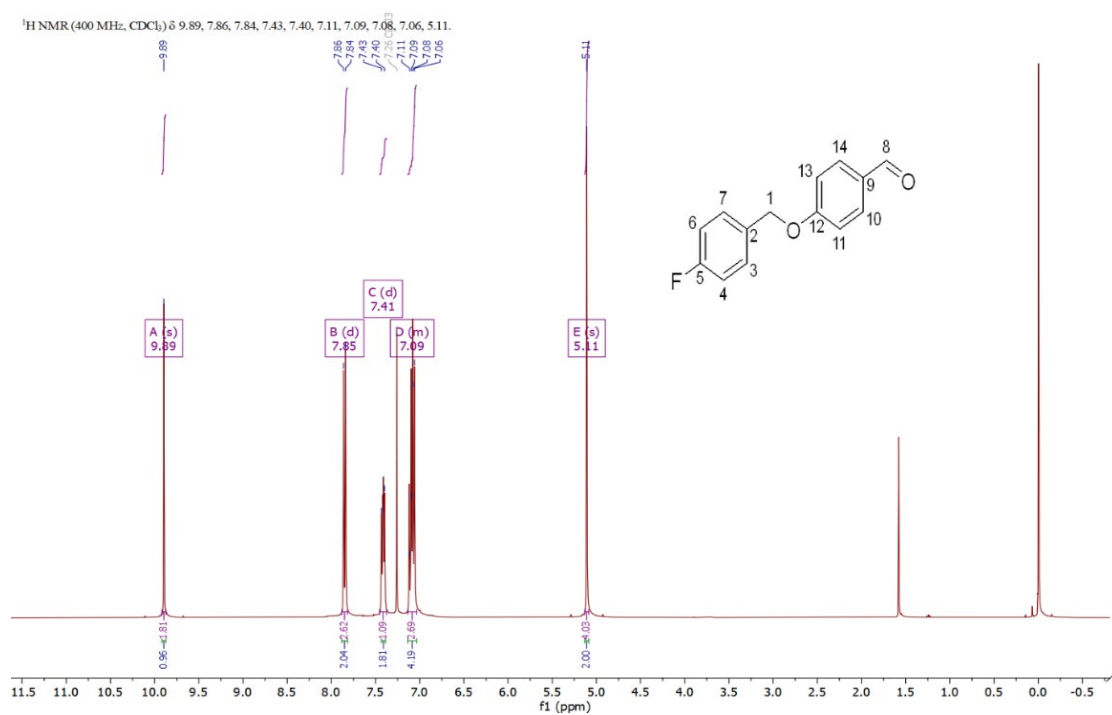


Figure S7: ¹H-NMR of 4-((4-fluorobenzyl) oxy) benzaldehyde (2).

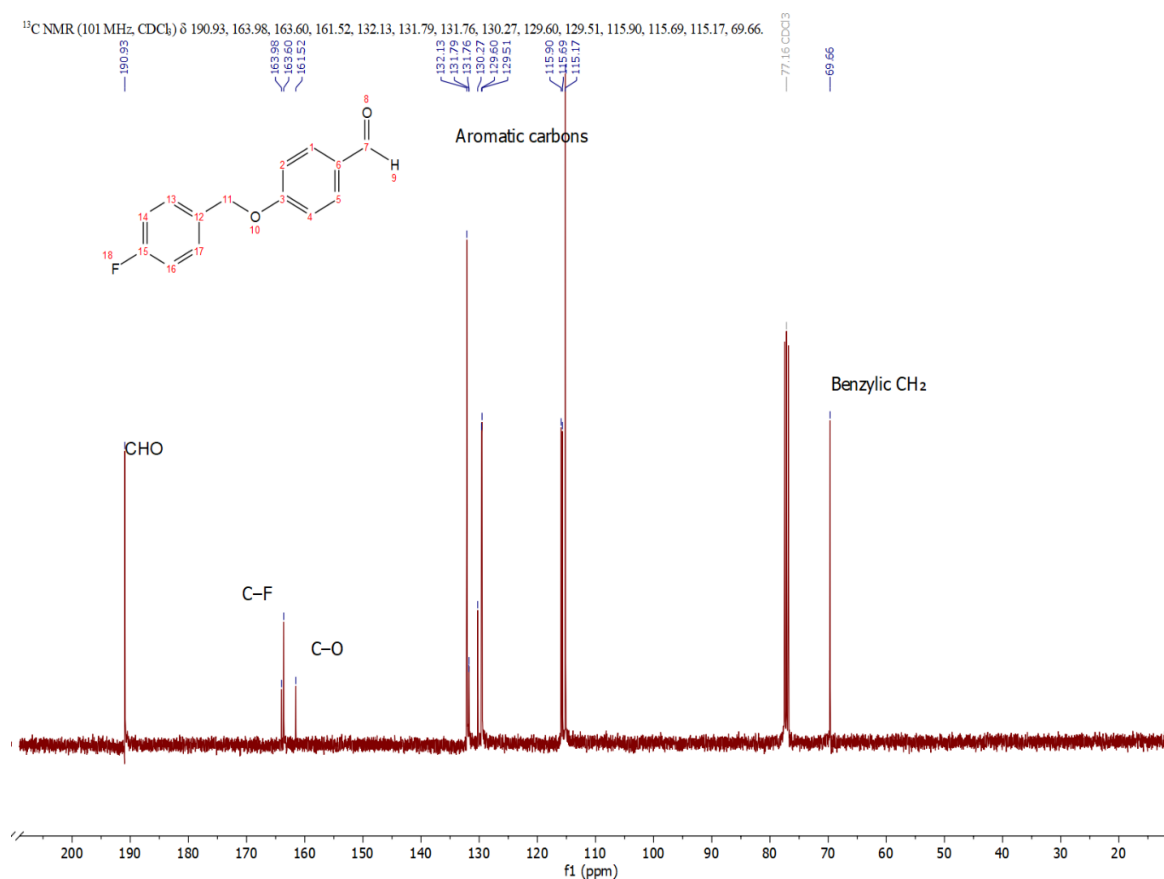


Figure S8: ¹³C-NMR of 4-((4-fluorobenzyl) oxy) benzaldehyde (2).

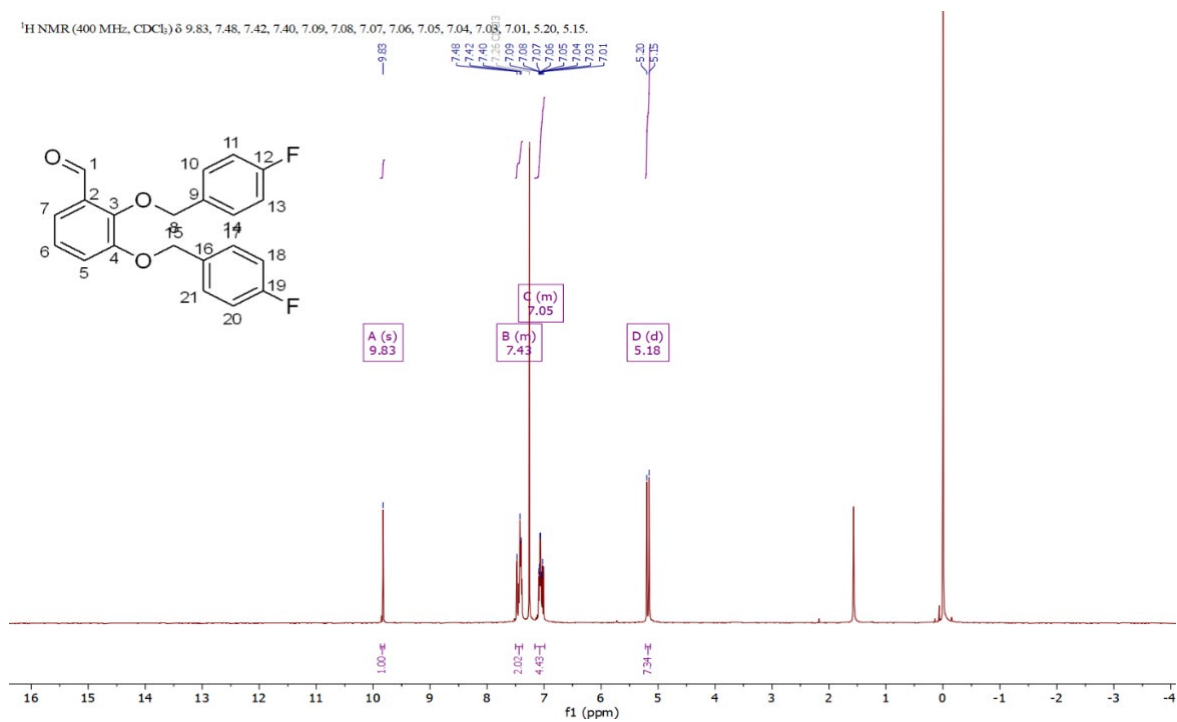


Figure S9: ¹H-NMR of 2,3-bis(4-fluorobenzyl)oxy benzaldehyde (3).

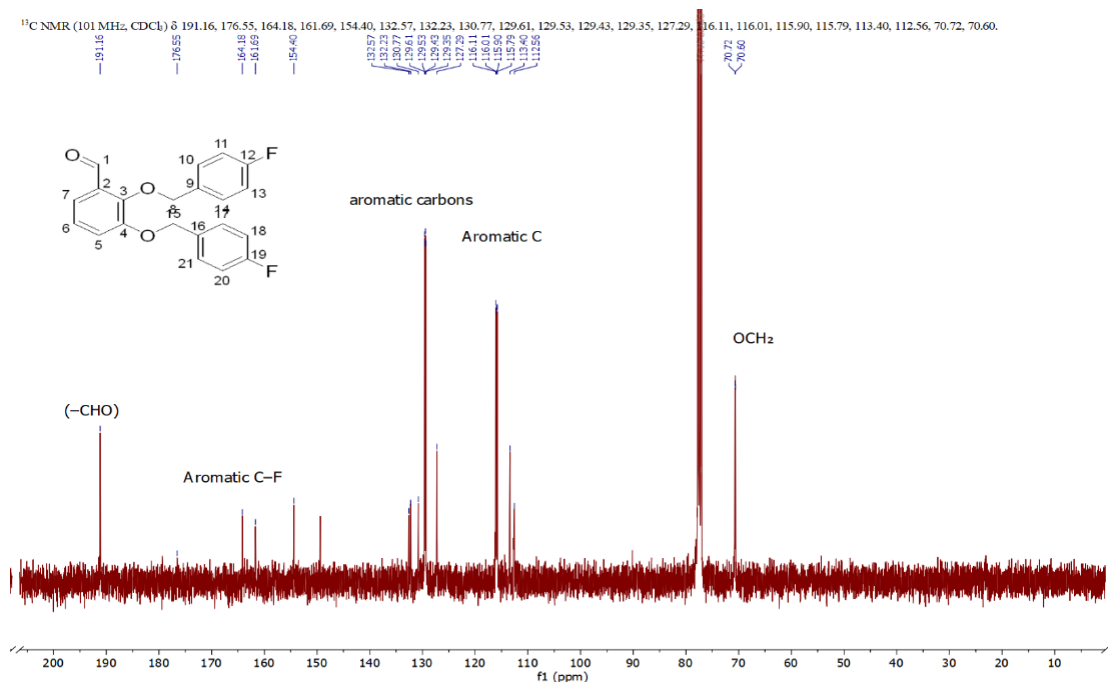


Figure S10: ¹³C-NMR of 2,3-bis(4-fluorobenzoyloxy) benzaldehyde (3).

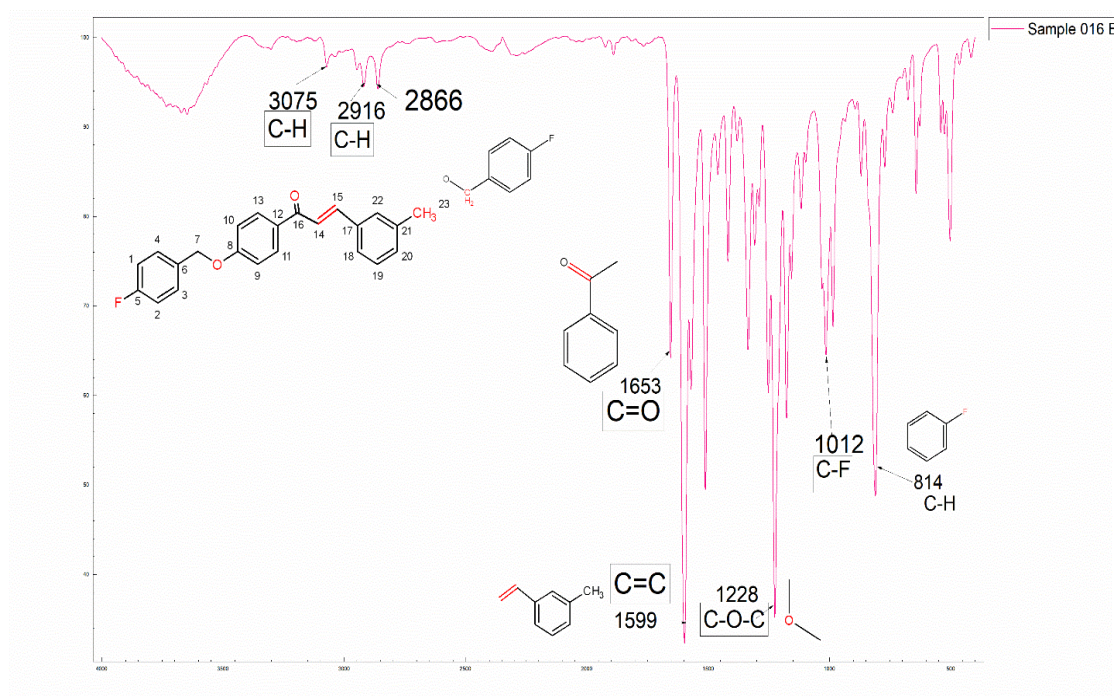


Figure S11: FTIR of (4)(E)-1-4-((4-fluorobenzyl) oxy) phenyl)-3-(m-tolyl) prop-2-en-1-one(4a)

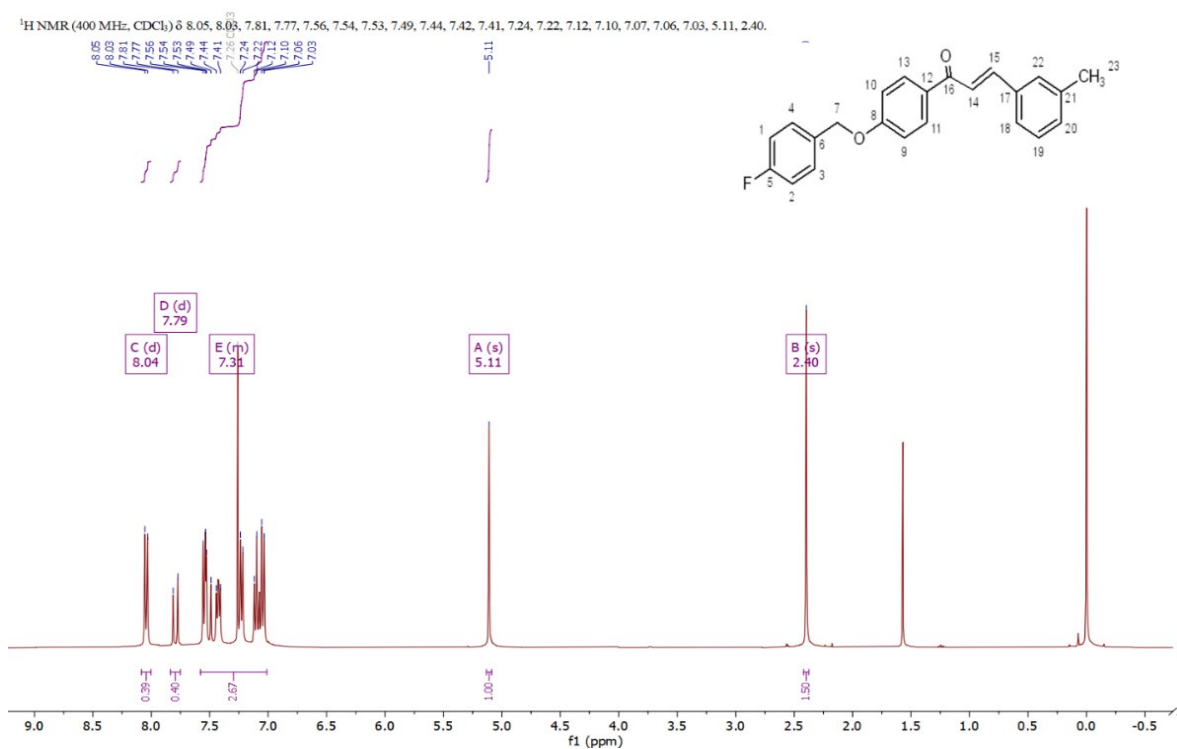


Figure S12: ¹H-NMR of (4)(E)-1-(4-((4-fluorobenzyl) oxy) phenyl)-3-(m-tolyl) prop-2-en-1-one(4a).

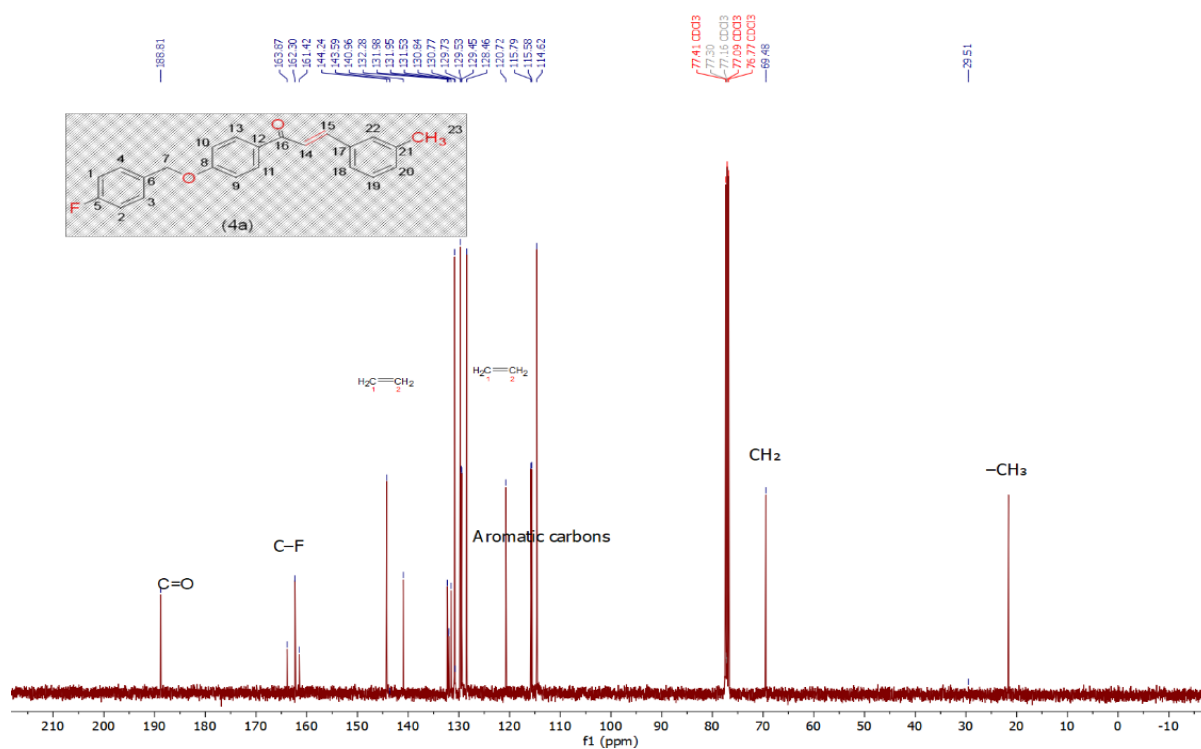


Figure S13: ¹³C-NMR of (4)(E)-1-(4-((4-fluorobenzyl) oxy) phenyl)-3-(m-tolyl) prop-2-en-1-one(4a).

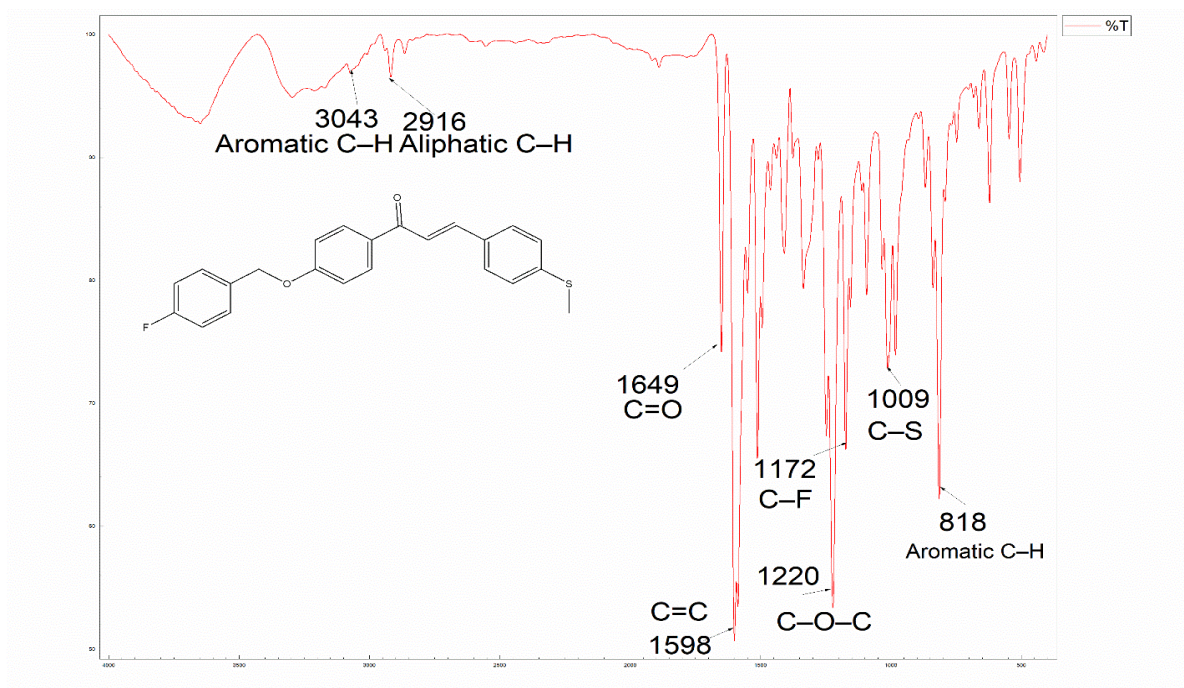


Figure S14: FTIR of (E)-1-(4-((4-fluorobenzyl)oxy)phenyl)-3-(4-(methylthio)phenyl)prop-2-en-1-one (**4b**).

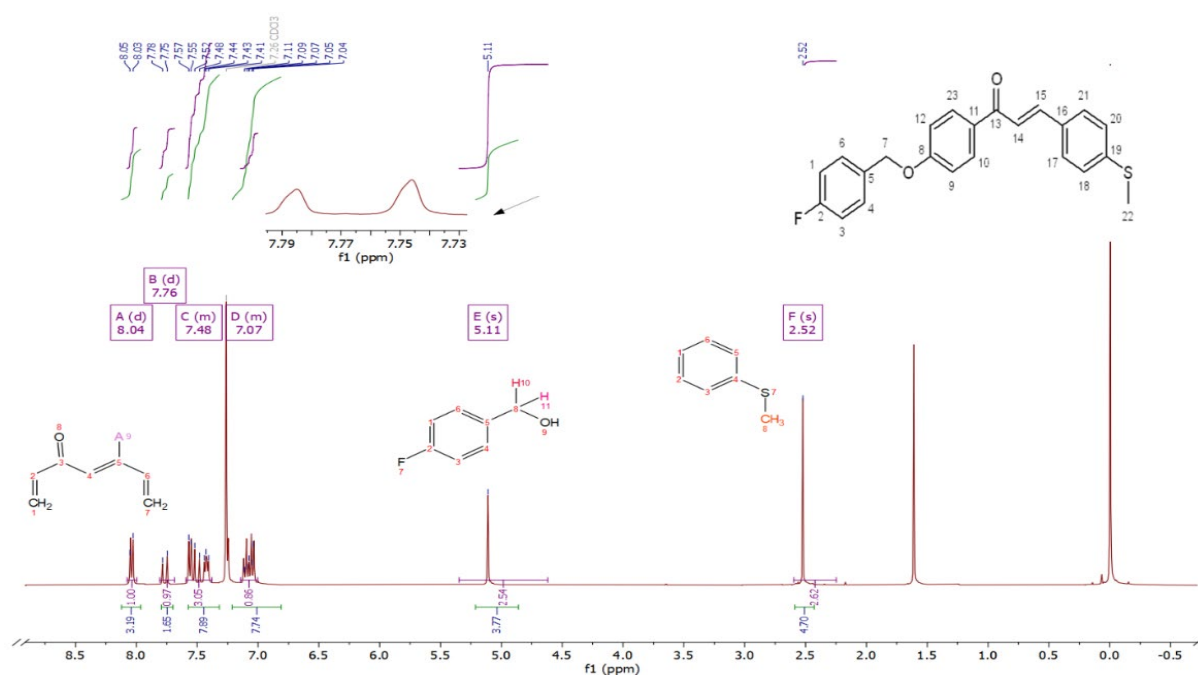


Figure S15: ¹H-NMR of (E)-1-(4-((4-fluorobenzyl)oxy)phenyl)-3-(4-(methylthio)phenyl)prop-2-en-1-one (**4b**).

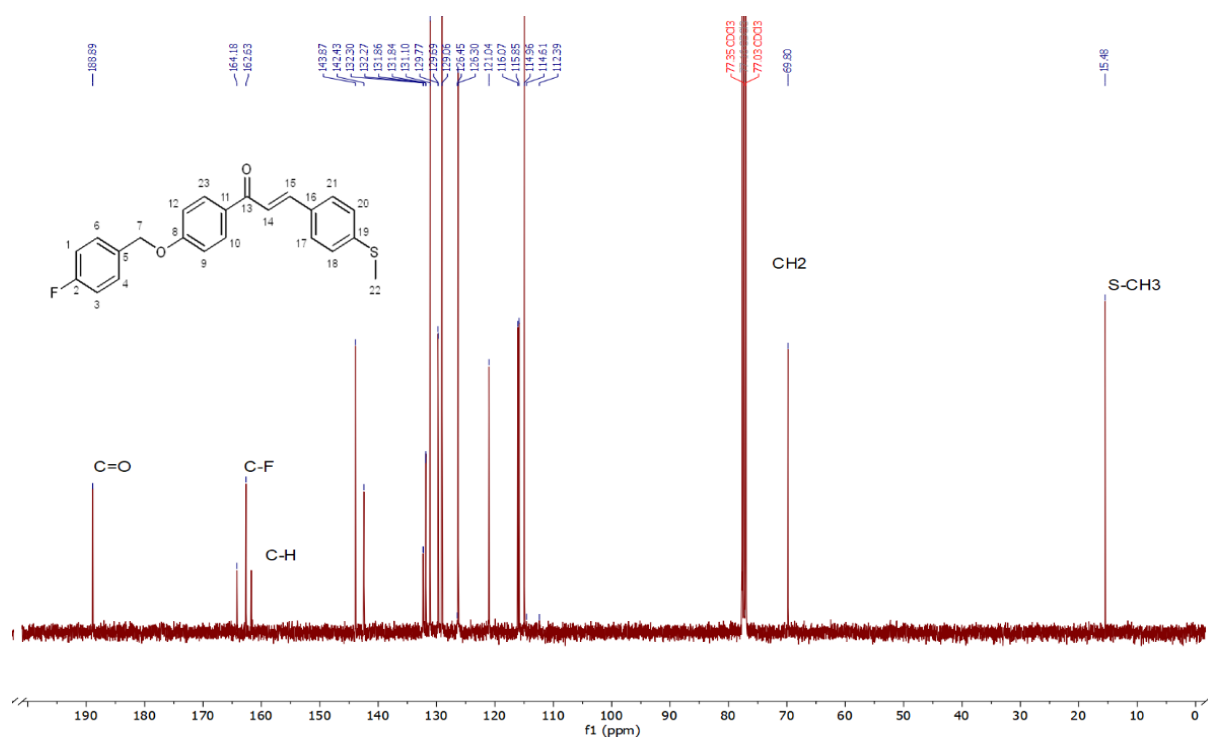


Figure S1: ^{13}C -NMR of (E)-1-(4-((4-fluorobenzyl)oxy)phenyl)-3-(4-(methylthio)phenyl)prop-2-en-1-one (**4b**).

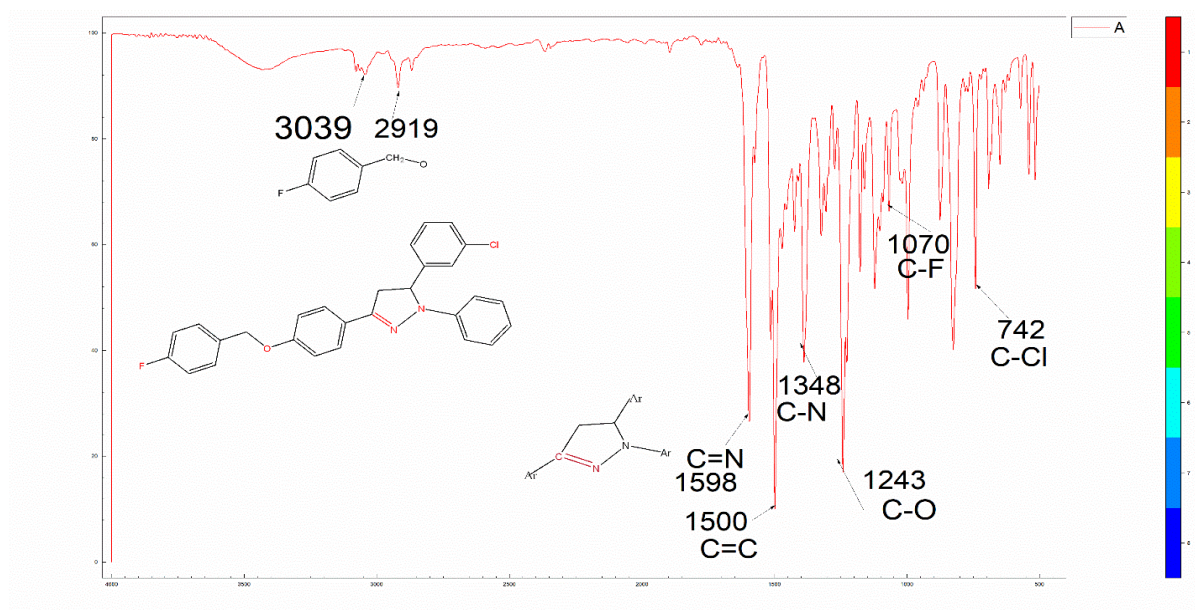


Figure S17: FTIR of 5-(3-chlorophenyl)-3-(4-((4-fluorobenzyl)oxy)phenyl)-1-phenyl-4,5-dihydro-1H-pyrazole (**5a**).

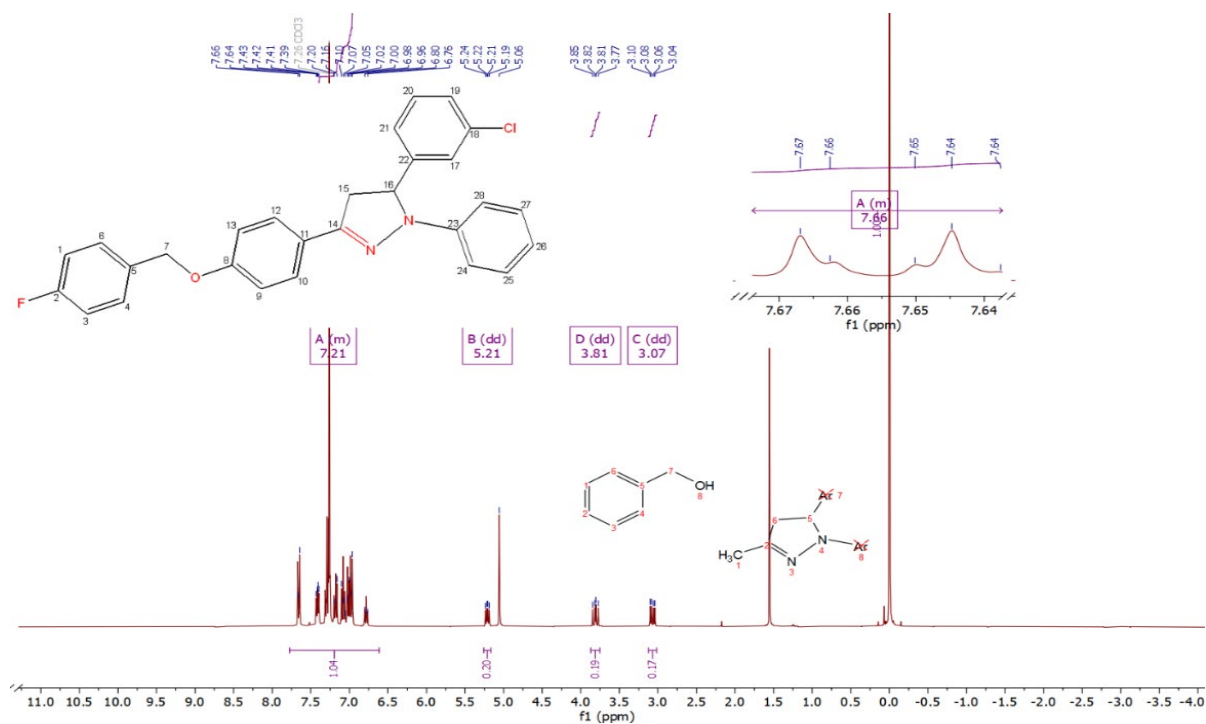


Figure S2: ¹H-NMR of 5-(3-chlorophenyl)-3-(4-((4-fluorobenzyl)oxy)phenyl)-1-phenyl-4,5-dihydro-1H-pyrazole (**5a**).

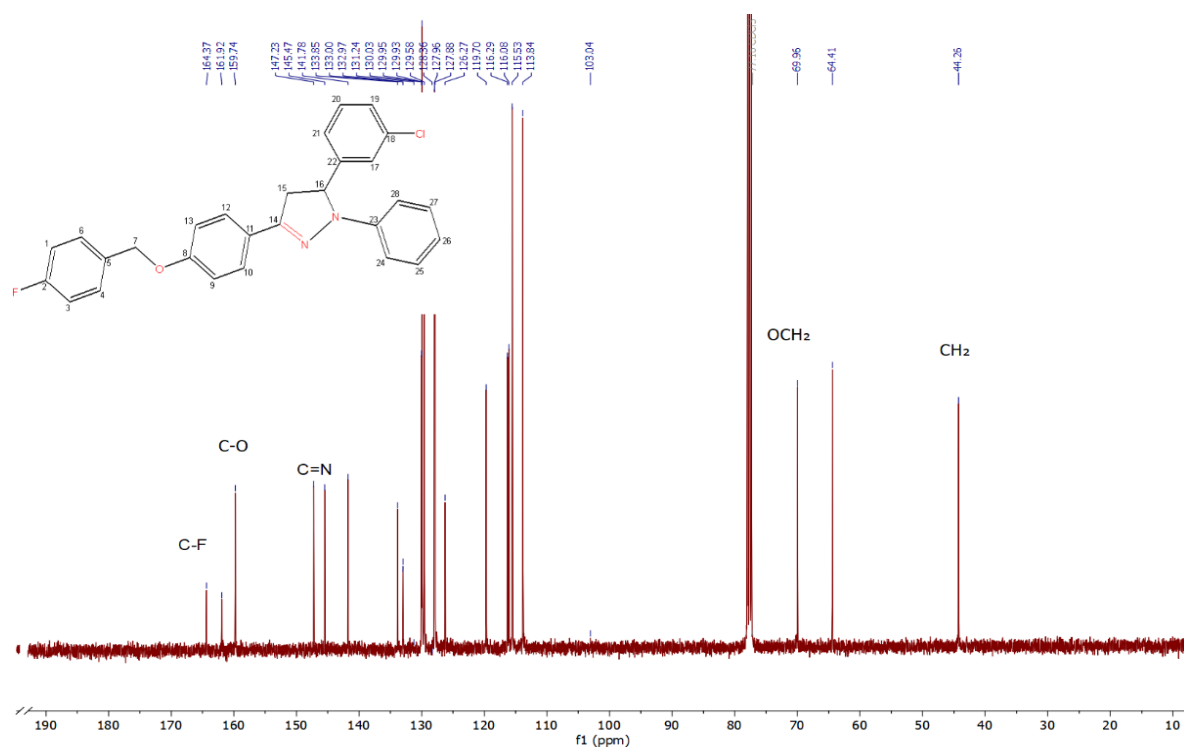


Figure S19: ¹³C-NMR of 5-(3-chlorophenyl)-3-(4-((4-fluorobenzyl)oxy)phenyl)-1-phenyl-4,5-dihydro-1H-pyrazole (**5a**).

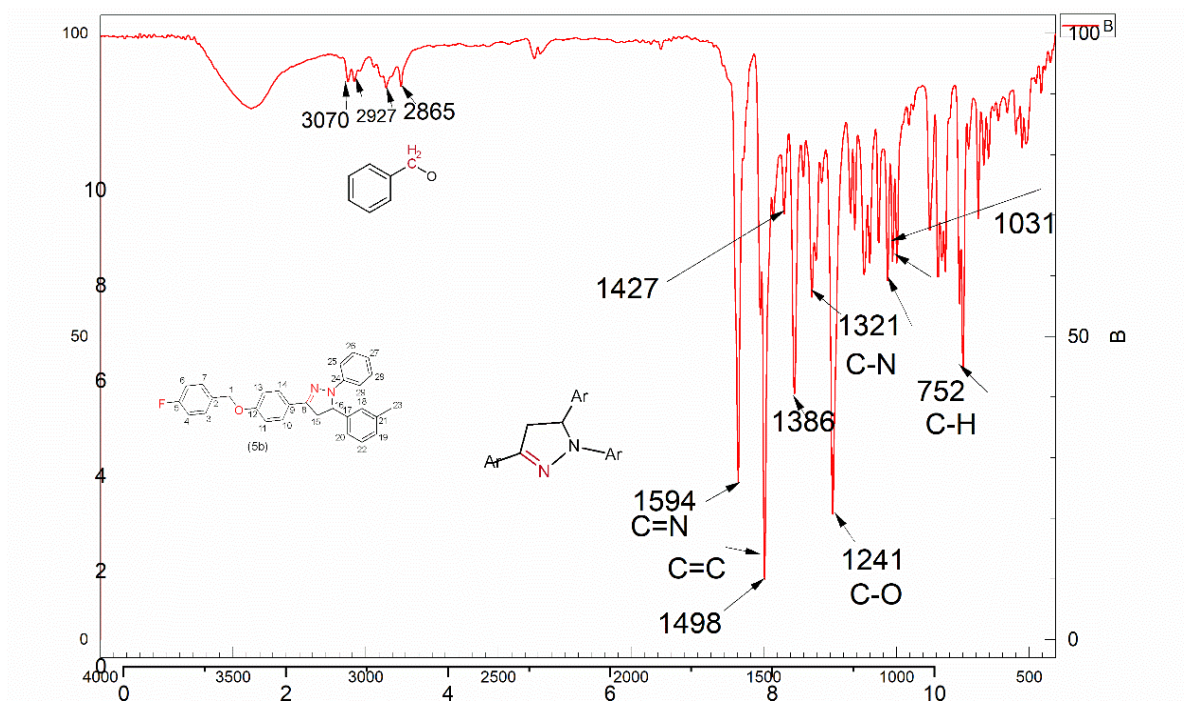


Figure S20: FTIR of 3-(4-((4-fluorobenzyl)oxy)phenyl)-1-phenyl-5-(m-tolyl)-4,5-dihydro-1H-pyrazole (**5b**).

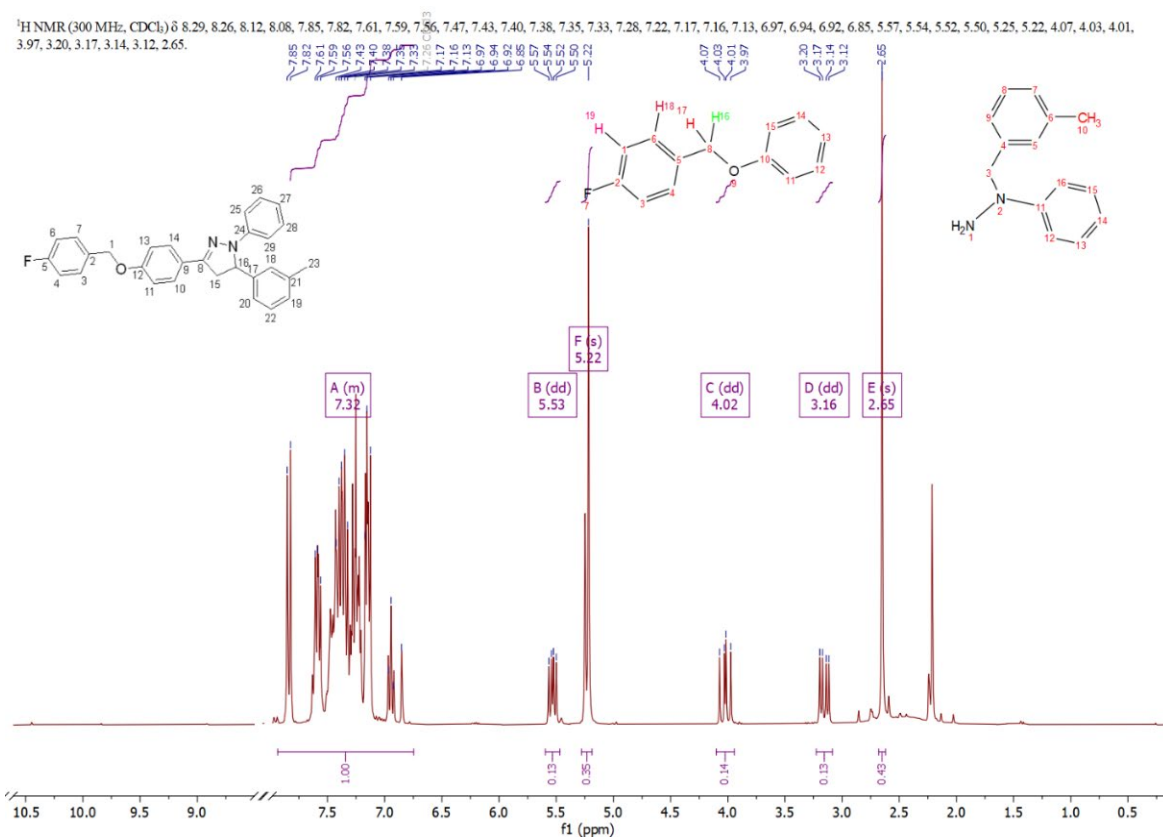


Figure S3: ¹H-NMR of 3-(4-((4-fluorobenzyl)oxy)phenyl)-1-phenyl-5-(m-tolyl)-4,5-dihydro-1H-pyrazole (**5b**).

^{13}C NMR (75 MHz, CDCl_3) δ 164.72, 161.45, 159.58, 147.09, 145.58, 140.70, 137.69, 134.35, 132.97, 131.43, 131.04, 129.97, 129.87, 129.49, 129.40, 128.63, 128.04, 127.87, 127.76, 127.42, 126.50, 124.47, 119.32, 115.96, 115.44, 113.55, 106.31, 69.90, 62.17, 42.60, 20.09.

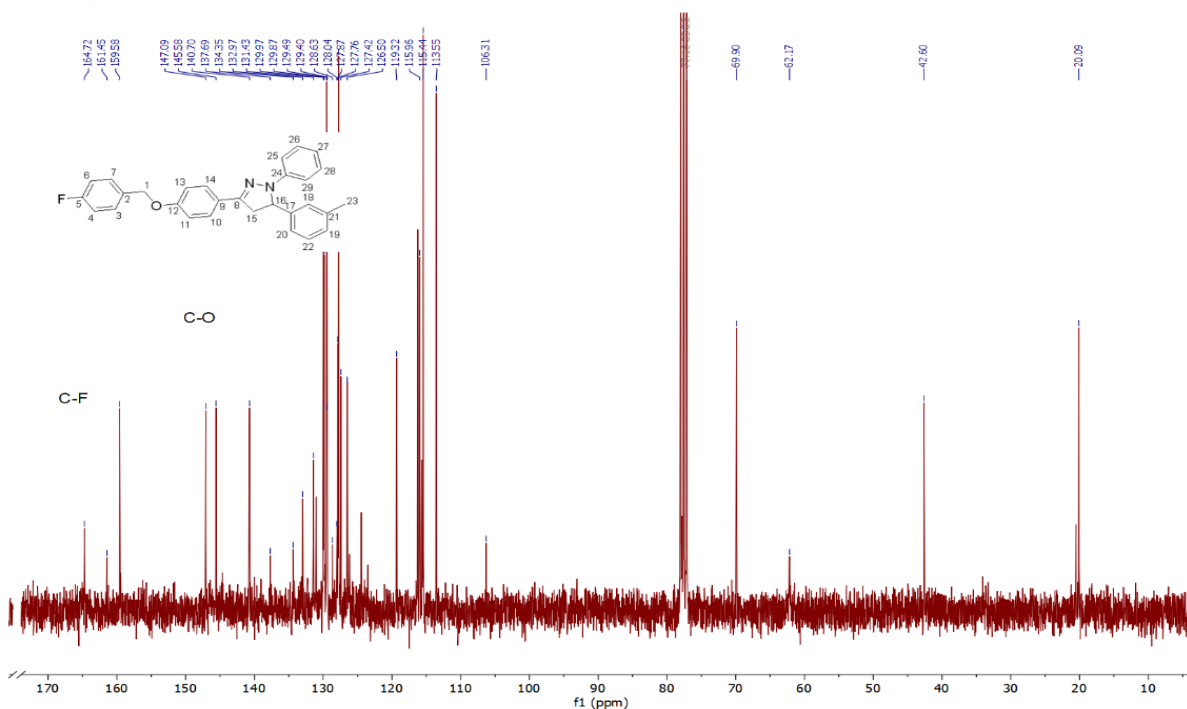


Figure S4: ^{13}C -NMR of 3-4-((4-fluorobenzyl)oxy)phenyl)-1-phenyl-5-(m-tolyl)-4,5-dihydro-1H-pyrazole (**5b**).

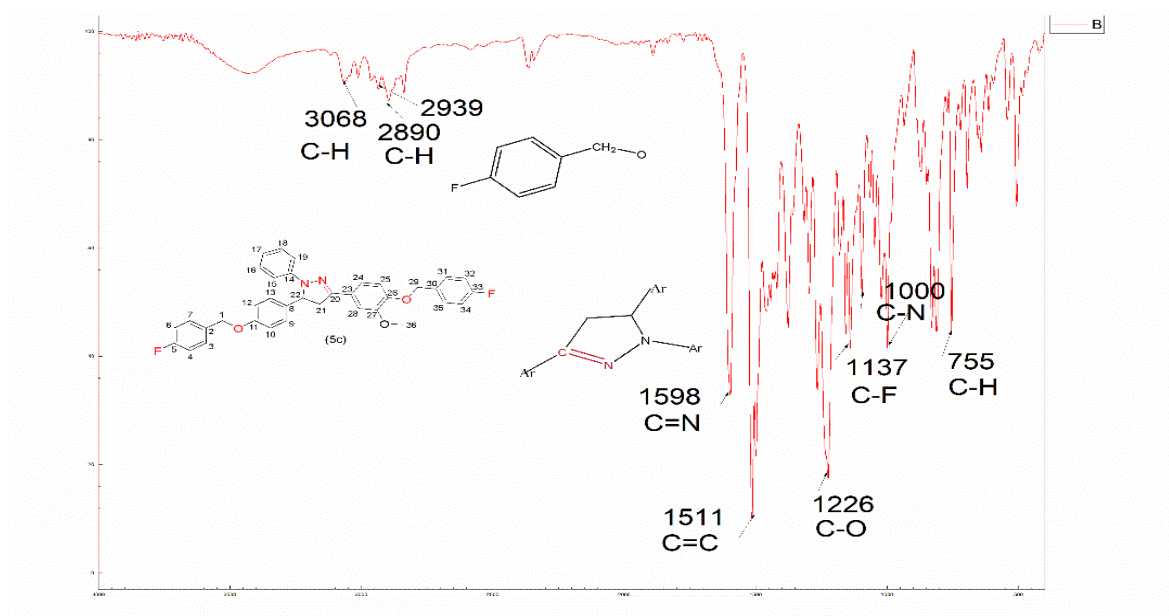


Figure S5: FTIR of 3-4-((4-fluorobenzyl)oxy)-3-methoxyphenyl)-5-4-((4-fluorobenzyl)oxy)phenyl)-1-phenyl-4,5-dihydro-1H-pyrazole (**5c**).

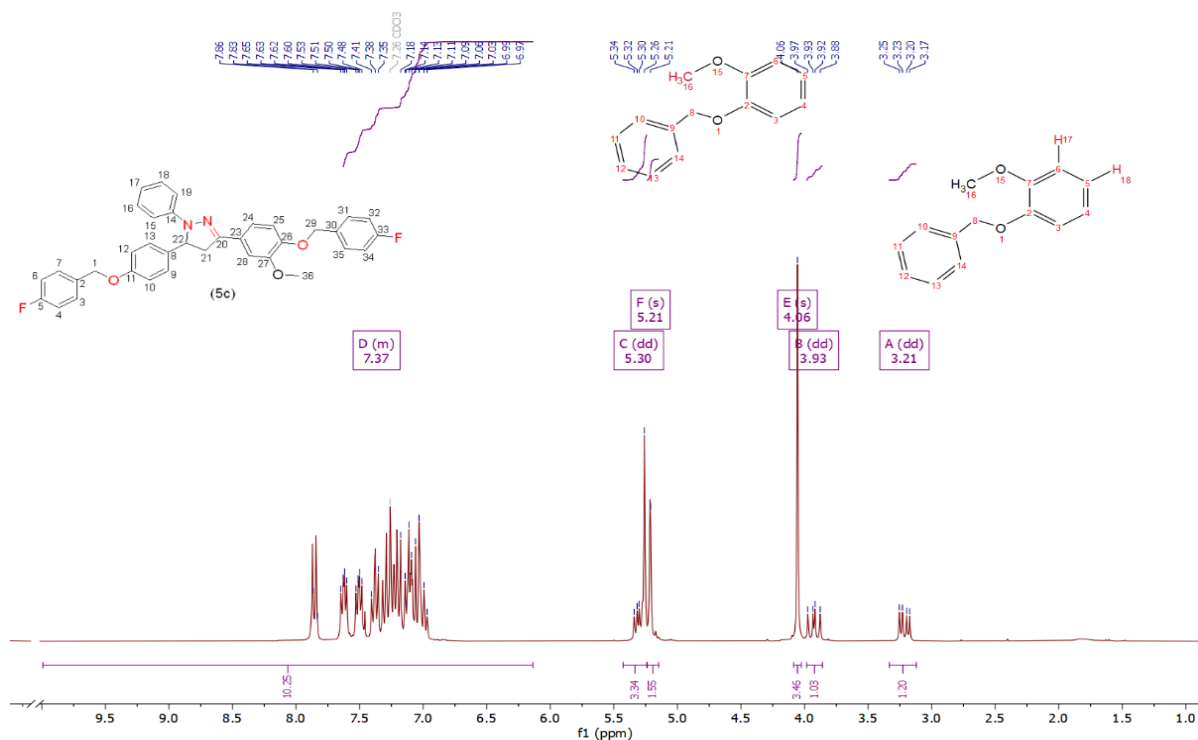


Figure S24: ^1H -NMR of 3-(4-((4-fluorobenzyl)oxy)-3-methoxyphenyl)-5-(4-((4-fluorobenzyl)oxy)phenyl)-1-phenyl-4,5-dihydro-1H-pyrazole (**5c**).

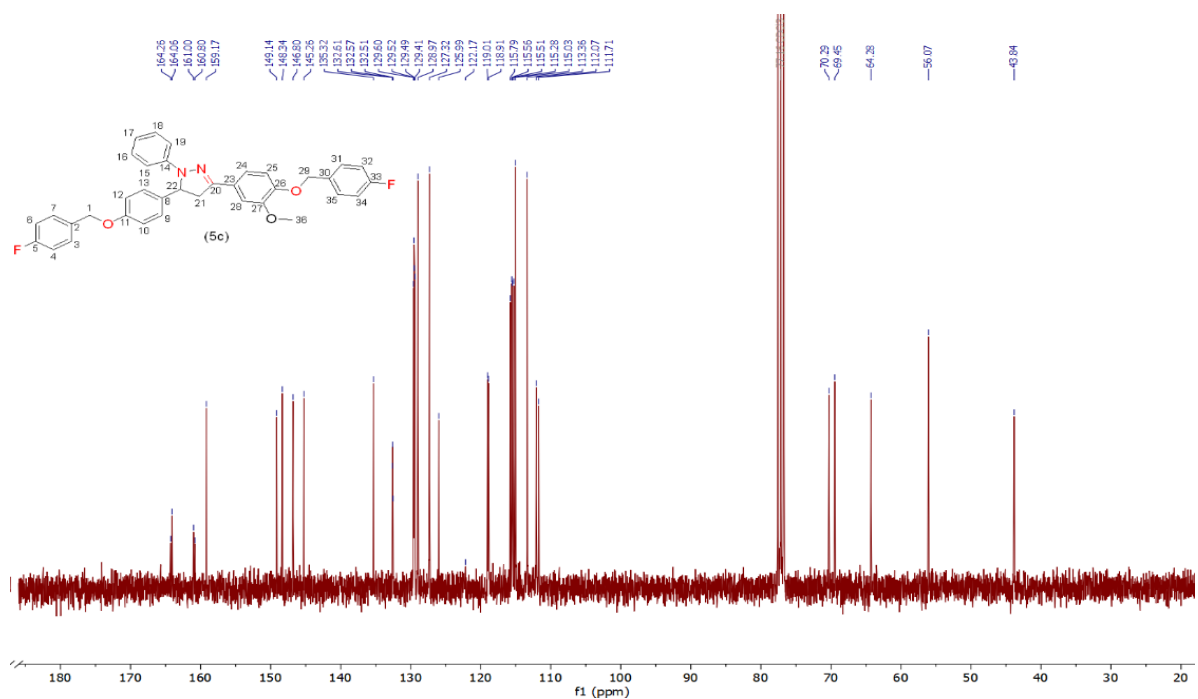
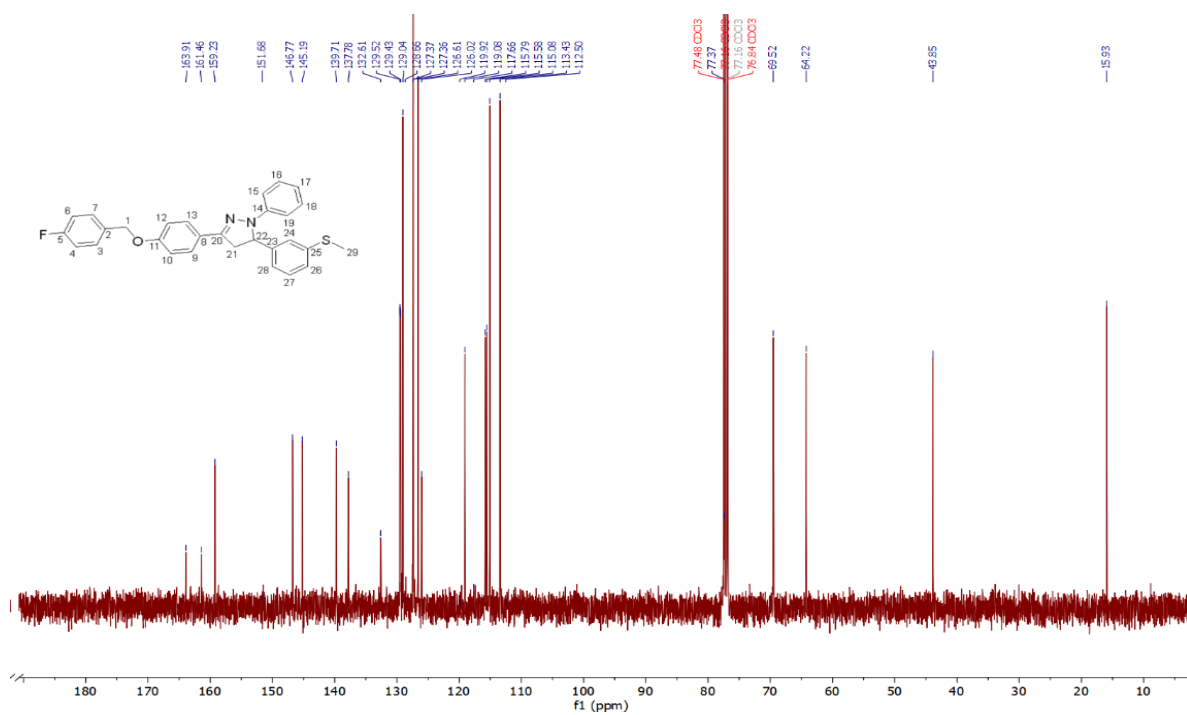
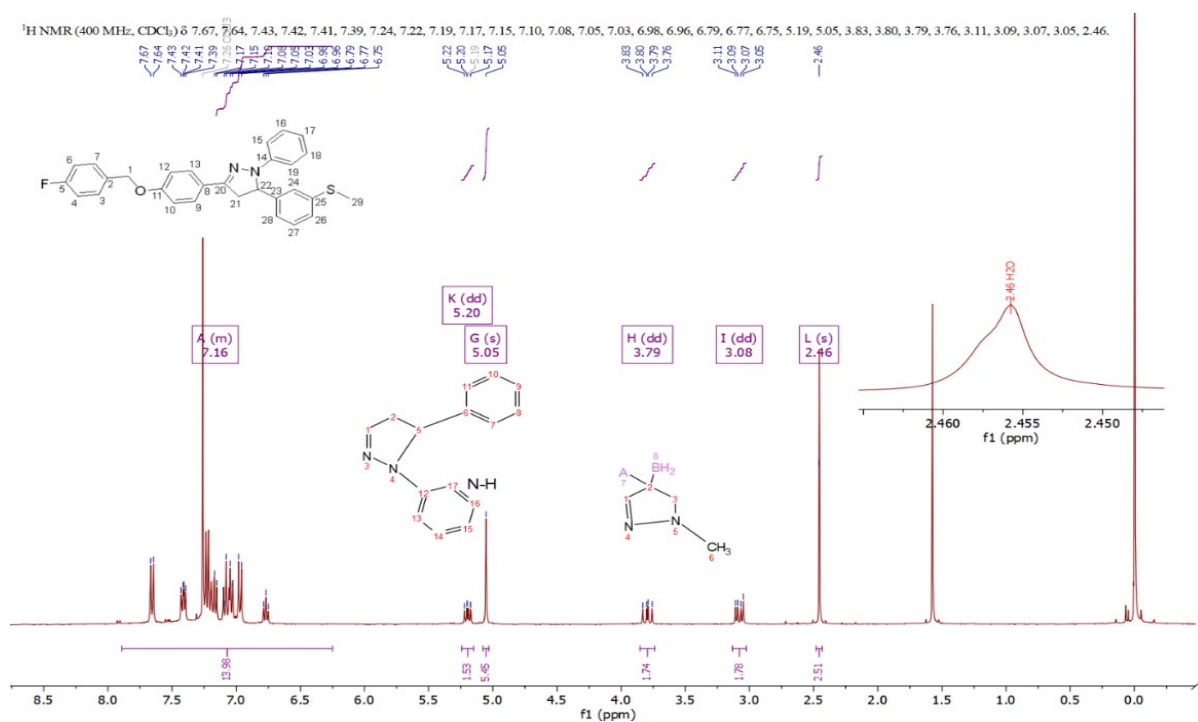


Figure S25: ^{13}C -NMR of 3-(4-((4-fluorobenzyl)oxy)-3-methoxyphenyl)-5-(4-((4-fluorobenzyl)oxy)phenyl)-1-phenyl-4,5-dihydro-1H-pyrazole (**5c**).



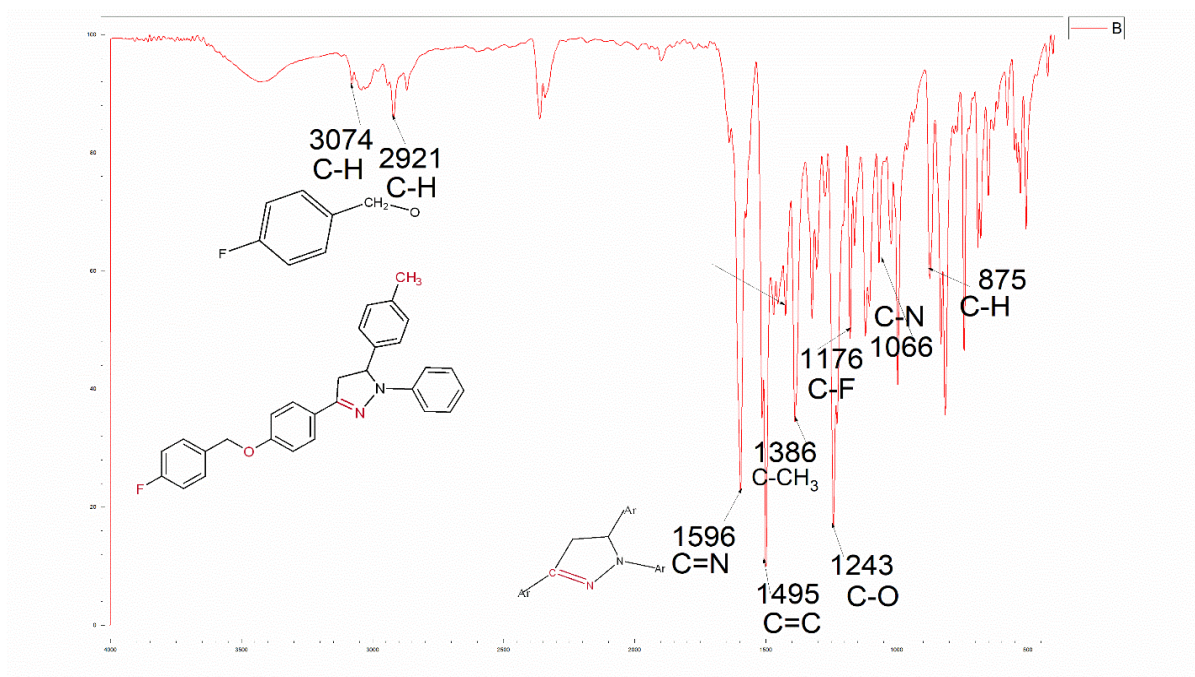


Figure S7: FTIR of 3-(4-((4-fluorobenzyl)oxy)phenyl)-1-phenyl-5-(p-tolyl)-4,5-dihydro-1H-pyrazole (**5i**).

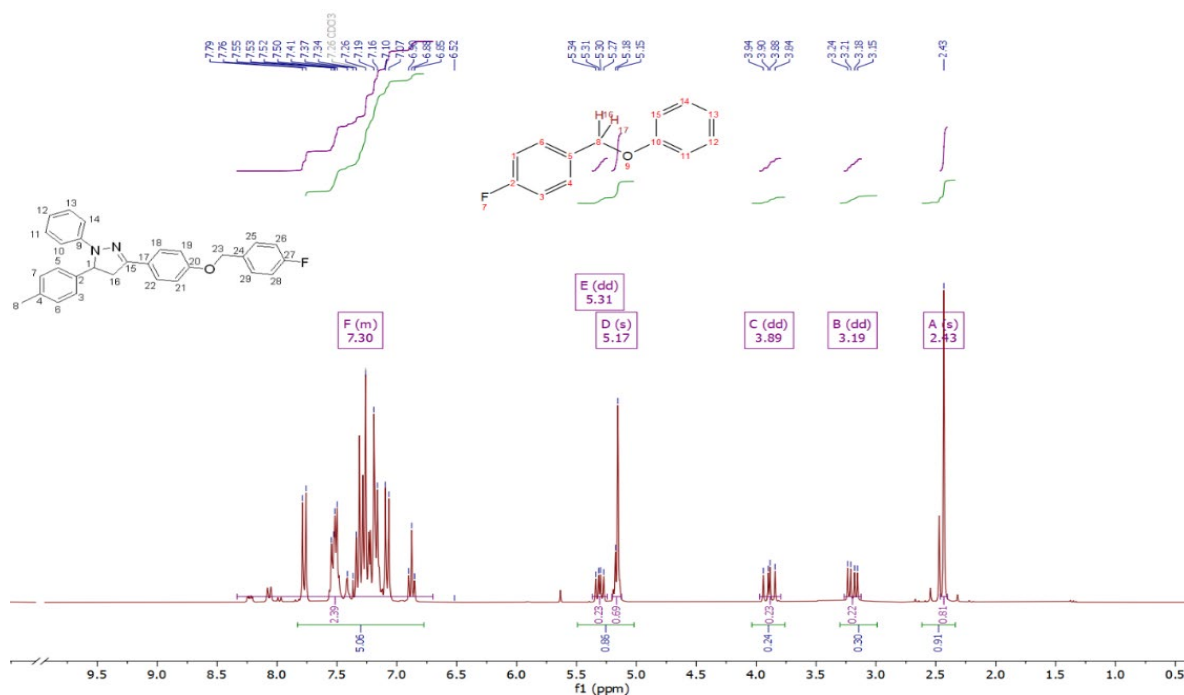


Figure S8: ¹H-NMR of 3-(4-((4-fluorobenzyl)oxy)phenyl)-1-phenyl-5-(p-tolyl)-4,5-dihydro-1H-pyrazole (**5i**).

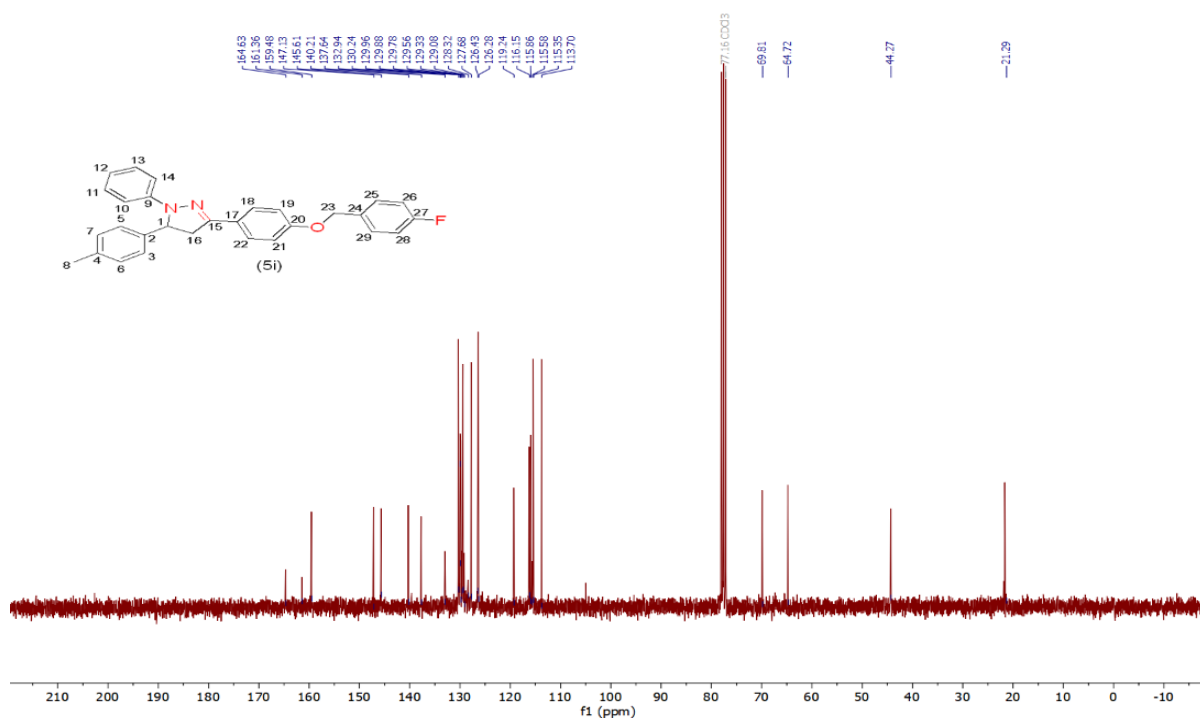


Figure S30: ¹³C-NMR of 3-4-((4-fluorobenzyl)oxy)phenyl-1-phenyl-5-(p-tolyl)-4,5-dihydro-1H-pyrazole (5i).

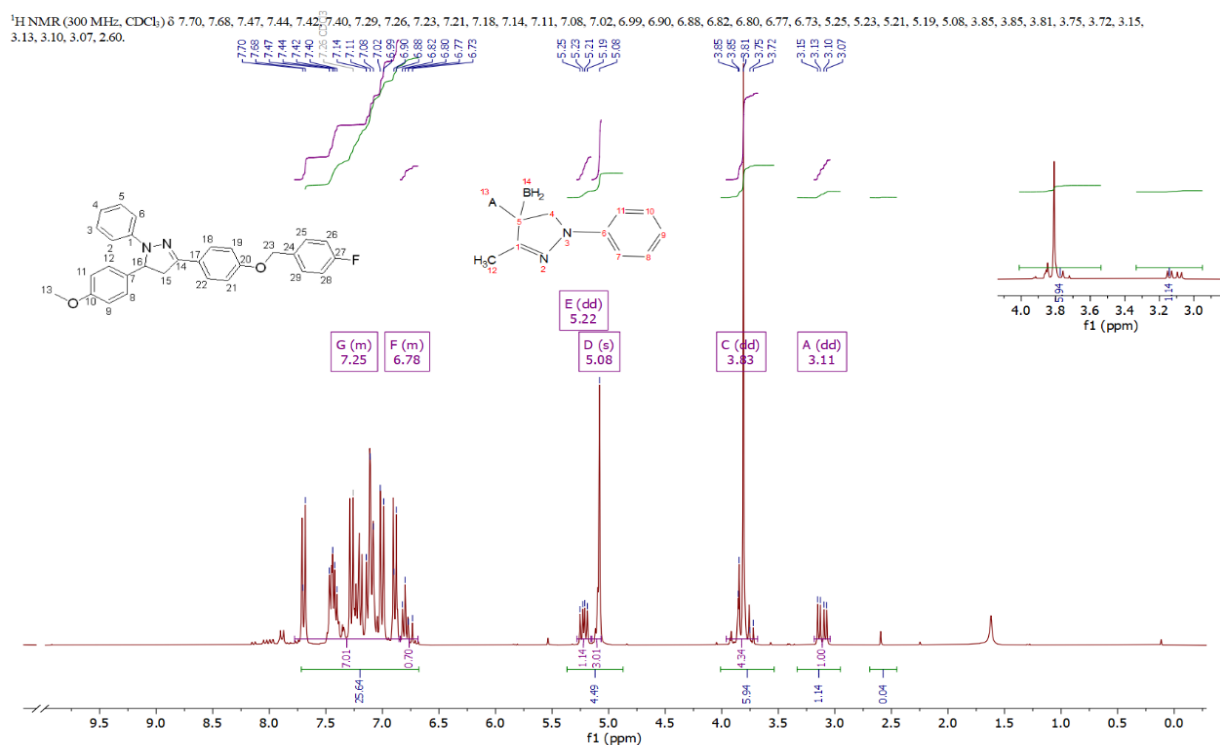


Figure S9: ¹H-NMR of 3-4-((4-fluorobenzyl)oxy)phenyl-5-(4-methoxyphenyl)-1-phenyl-4,5-dihydro-1H-pyrazole (5d).

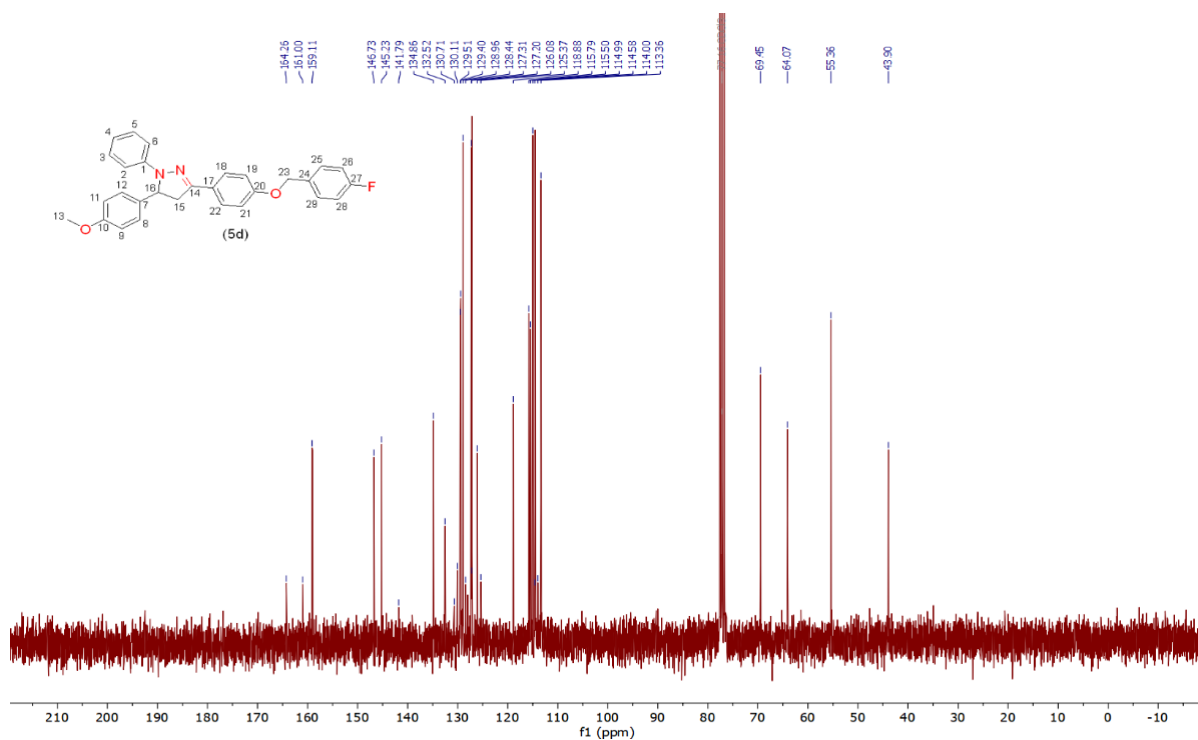


Figure S32: ^{13}C -NMR of 3-(4-((4-fluorobenzyl)oxy)phenyl)-5-(4-methoxyphenyl)-1-phenyl-4,5-dihydro-1H-pyrazole (**5d**).

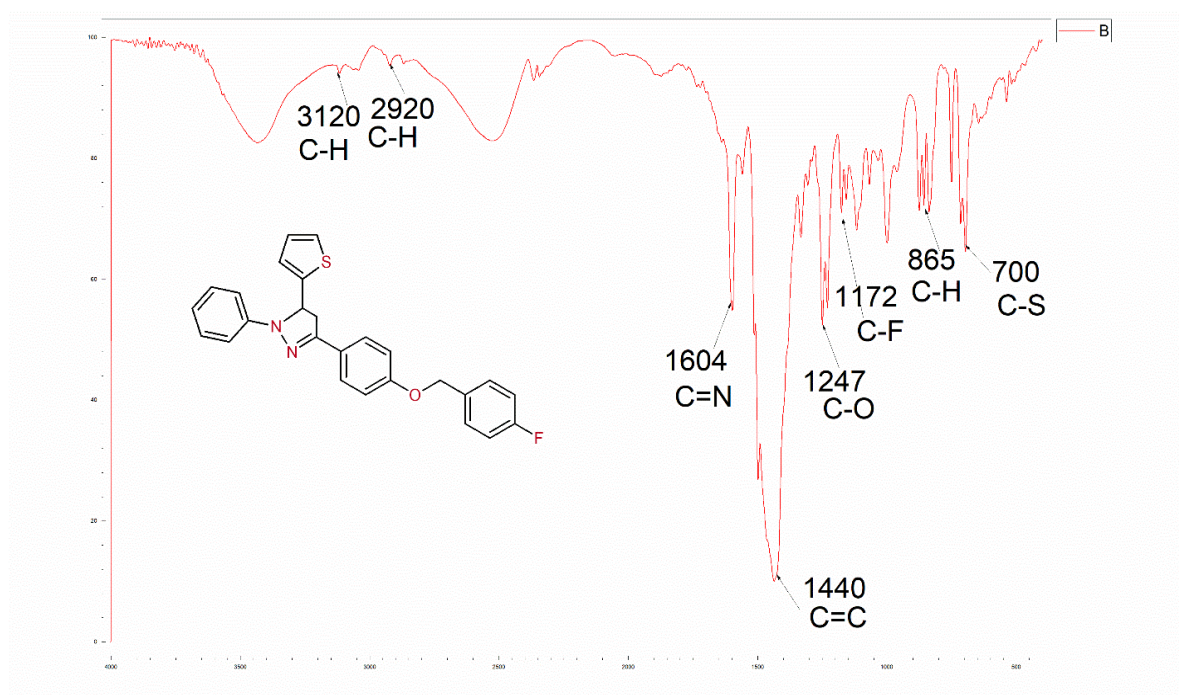


Figure S10: FTIR of 3-(4-((4-fluorobenzyl)oxy)phenyl)-1-phenyl-5-(thiophen-2-yl)-4,5-dihydro-1H-pyrazole (**5e**).

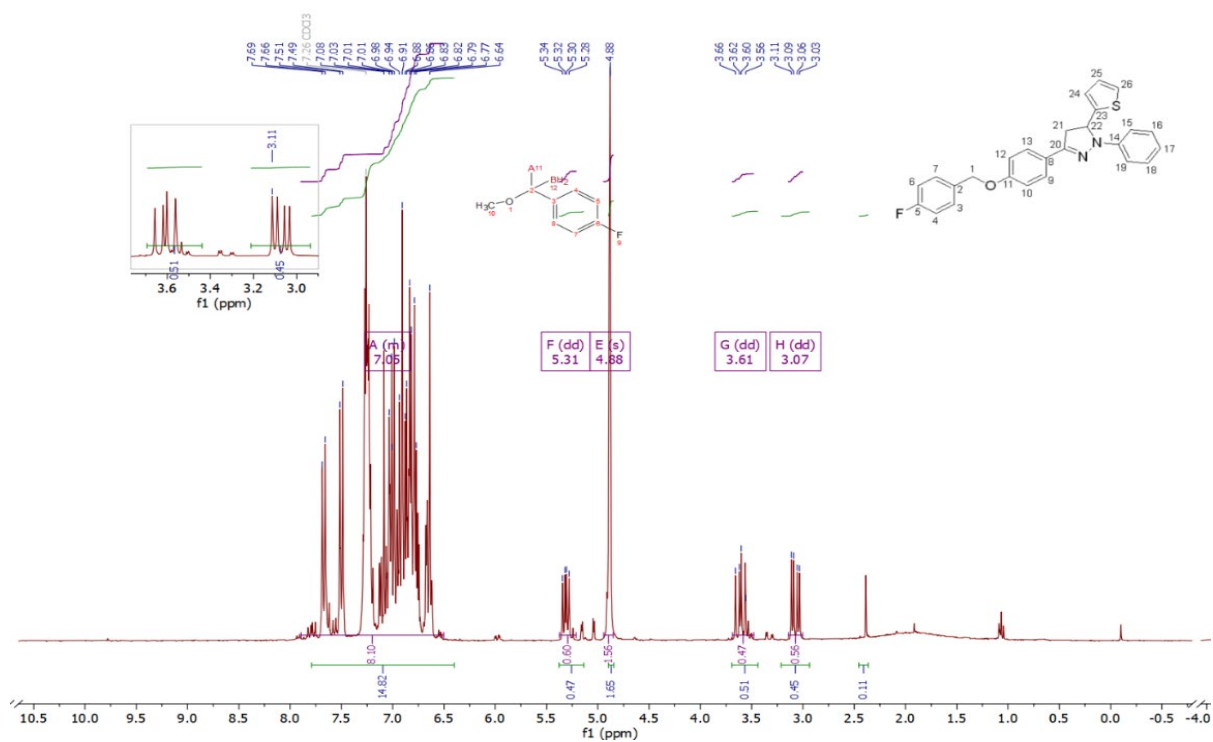


Figure S11: ¹H-NMR of 3-(4-((4-fluorobenzyl)oxy)phenyl)-1-phenyl-5-(thiophen-2-yl)-4,5-dihydro-1H-pyrazole (**5e**).

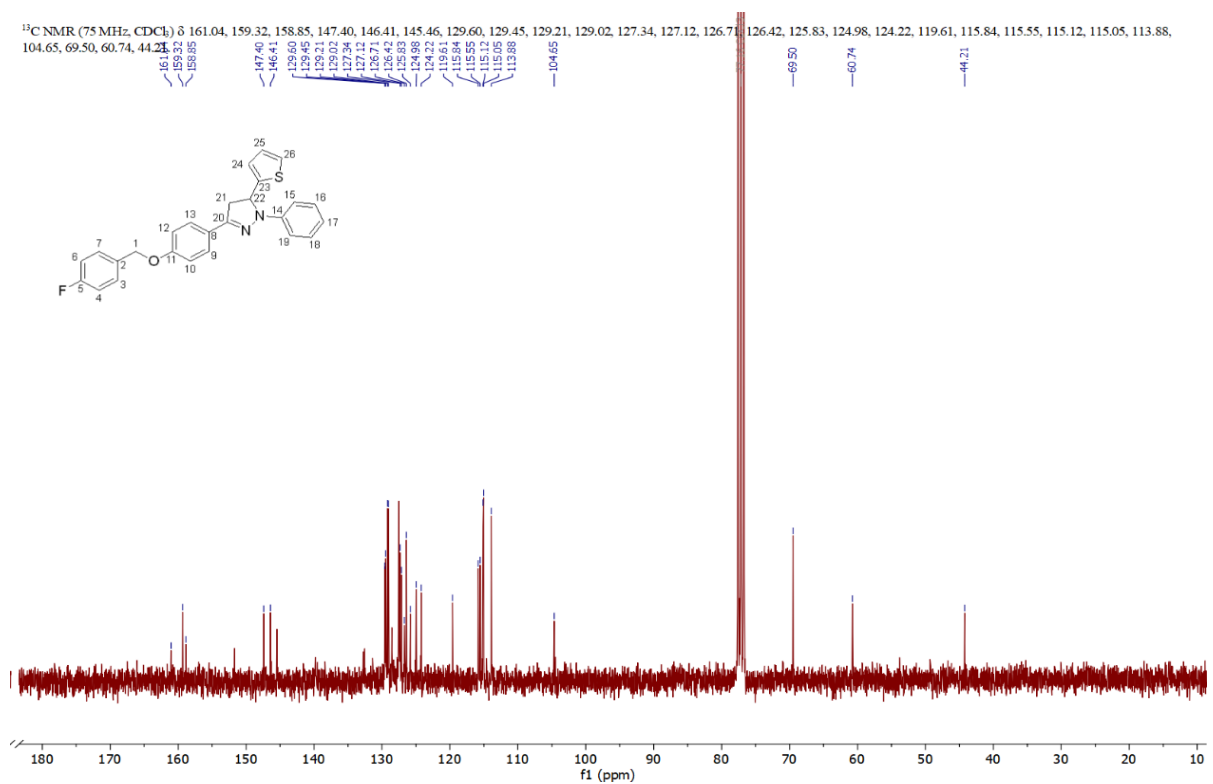


Figure S12: ¹³C-NMR of 3-(4-((4-fluorobenzyl)oxy)phenyl)-1-phenyl-5-(thiophen-2-yl)-4,5-dihydro-1H-pyrazole (**5e**).

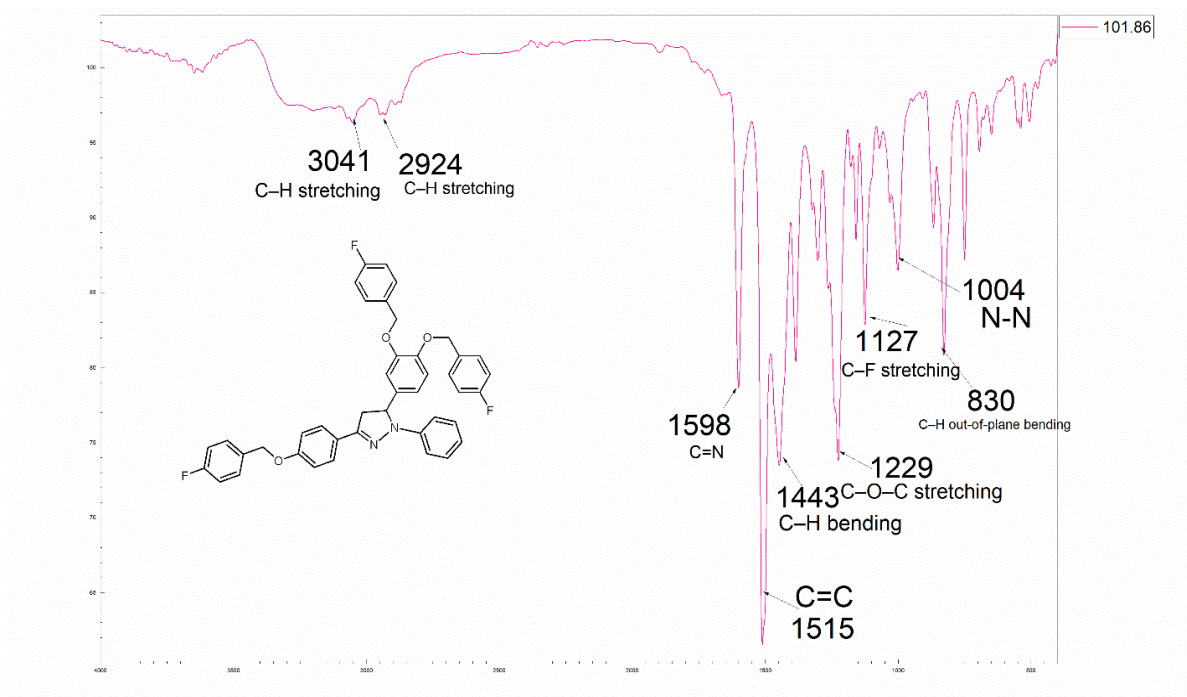


Figure S13: FTIR of 5-(3,4-bis((4-fluorobenzyl)oxy)phenyl)-3-(4-((4-fluorobenzyl)oxy)phenyl)-1-phenyl-4,5-dihydro-1H-pyrazole (5f).

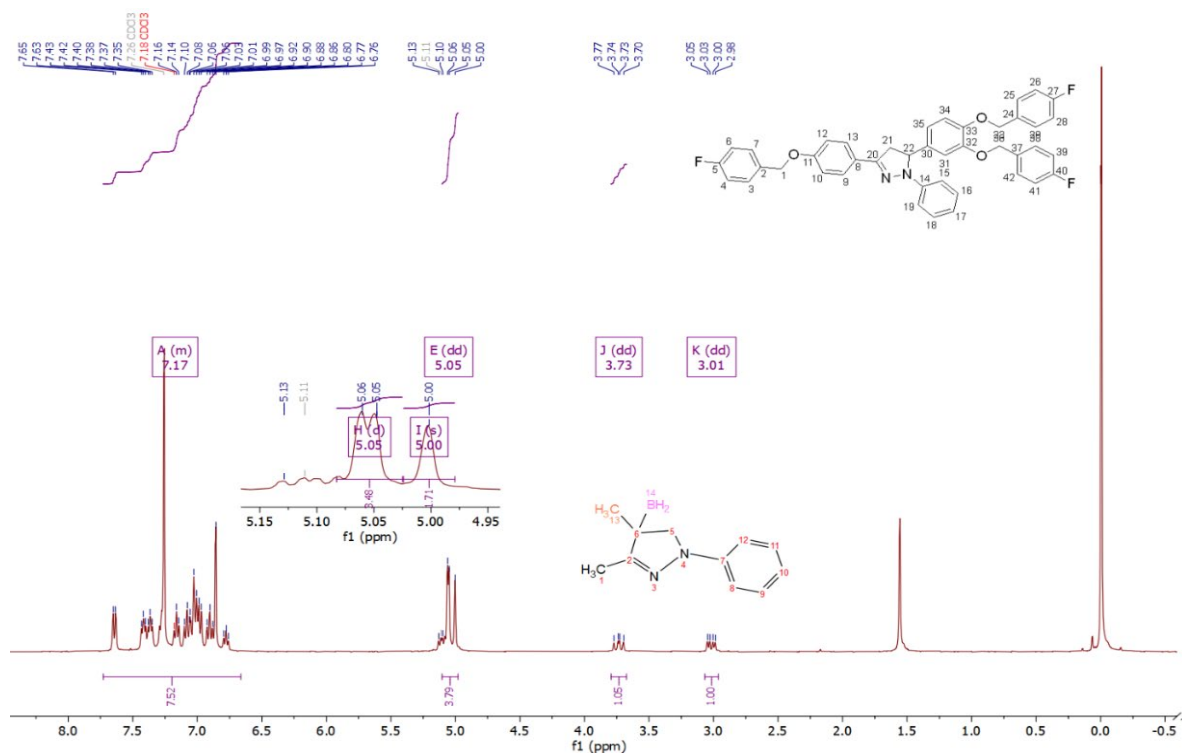


Figure S14: ¹H-NMR of 5-(3,4-bis((4-fluorobenzyl)oxy)phenyl)-3-(4-((4-fluorobenzyl)oxy)phenyl)-1-phenyl-4,5-dihydro-1H-pyrazole (5f).

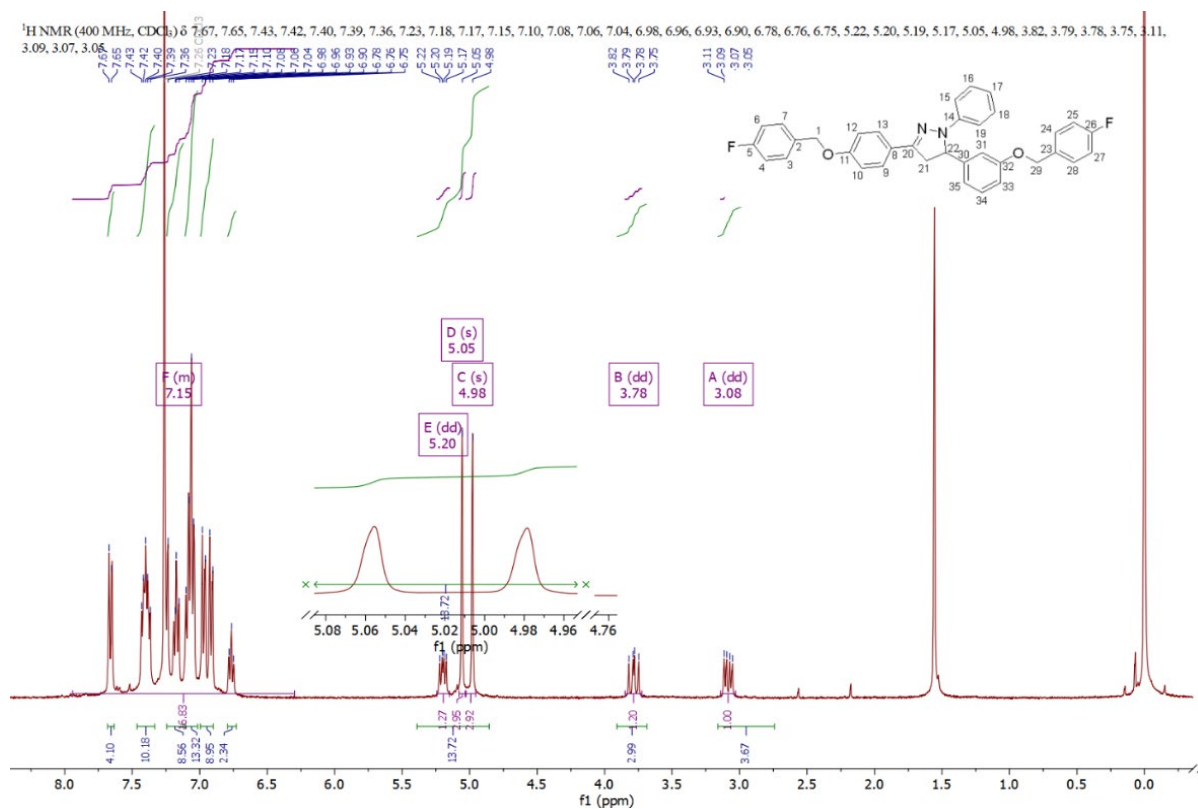


Figure S40: ¹H-NMR of 5-(3-((4-fluorobenzyl)oxy)phenyl)-3-(4-((4-fluorobenzyl)oxy)phenyl)-1-phenyl-4,5-dihydro-1H-pyrazole (5g).

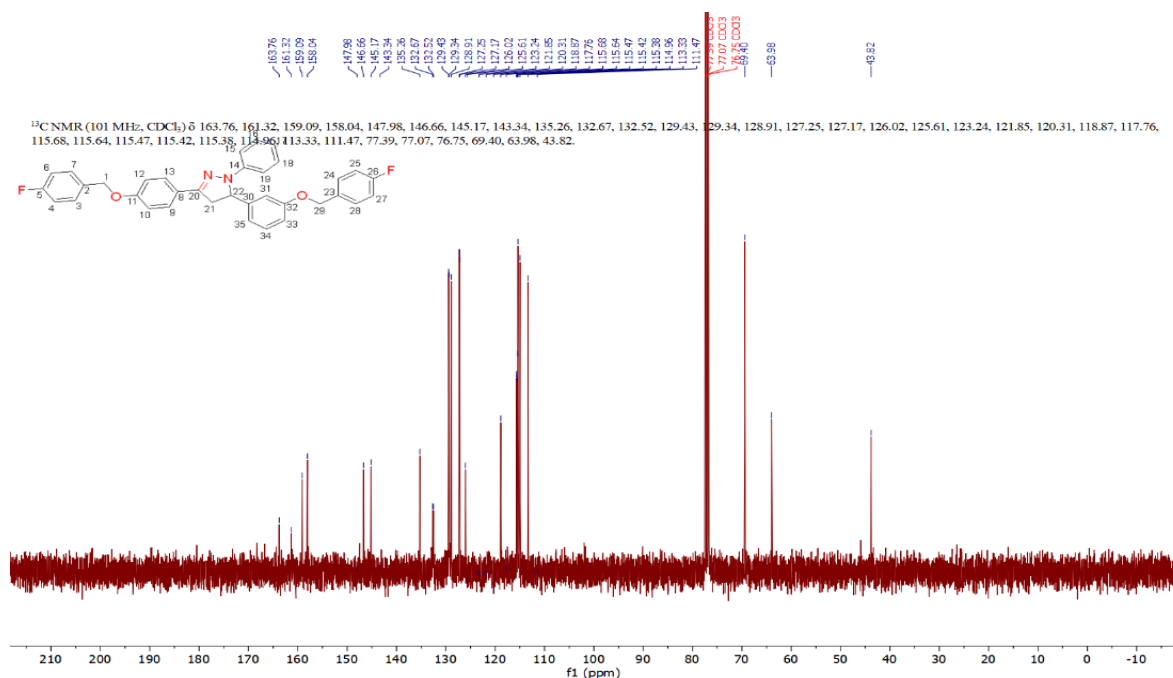


Figure S41: ¹³C-NMR of 5-(3-((4-fluorobenzyl)oxy)phenyl)-3-(4-((4-fluorobenzyl)oxy)phenyl)-1-phenyl-4,5-dihydro-1H-pyrazole (5g).

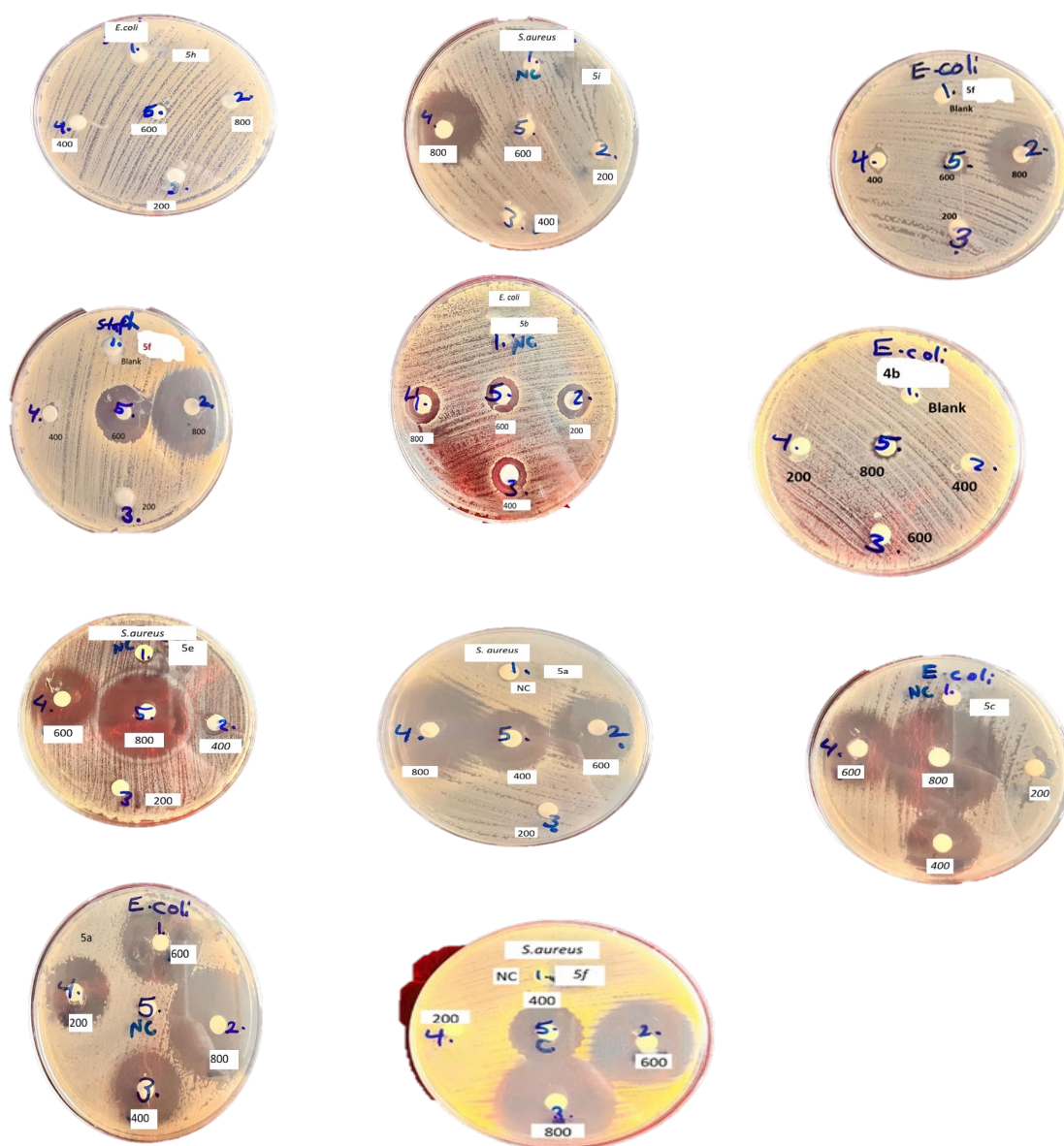


Figure S42: Inhibition zone of Chalcone and Pyrazoline compounds at concentration (200,400,600,800 and 1000) on *E. coli* and *Aureus* microorganism.