

Electronic Supplementary Information

for

Synthesis and SAR Studies of Pyrazole-3–Carboxamides and –Thioureides Including Chiral Moiety: Novel Candidates as Antibacterial Agents

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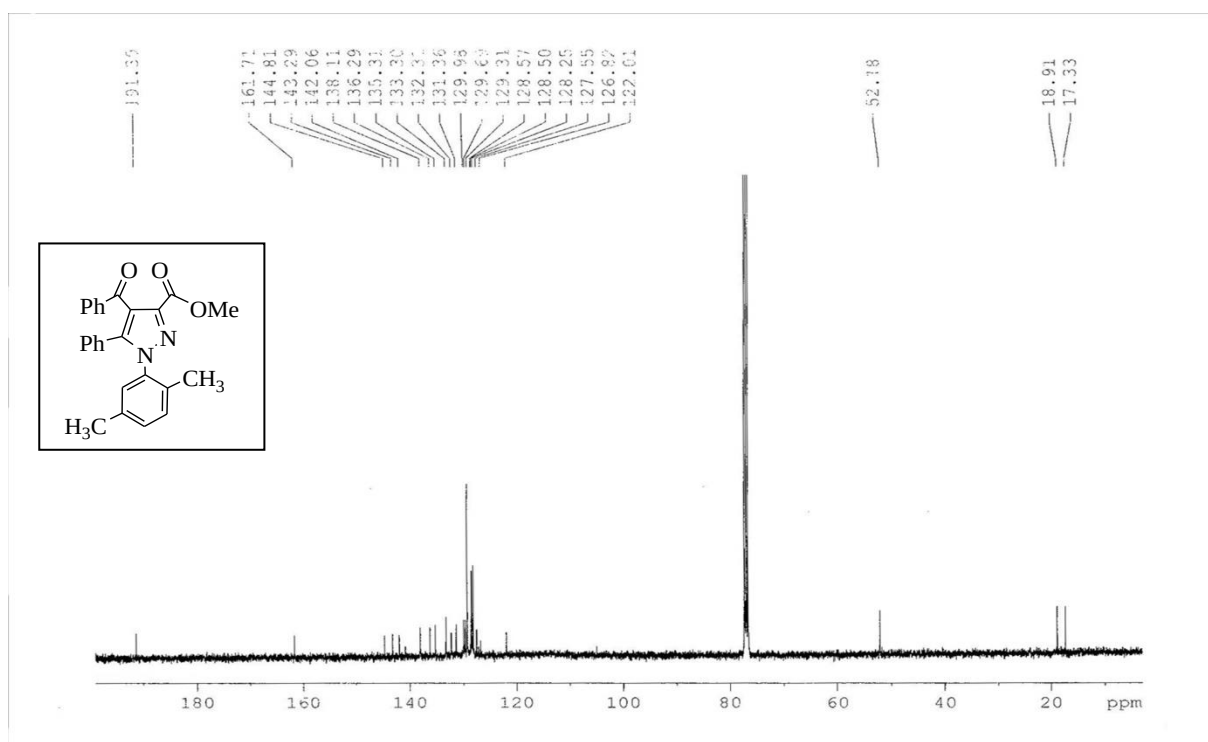
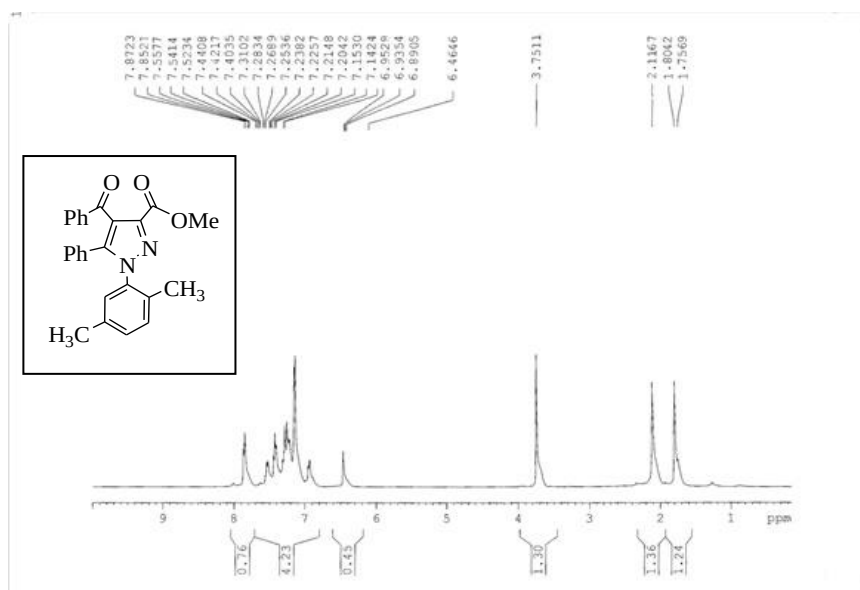
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Figure S2. ^1H and ^{13}C NMR Spectra of 4-Benzoyl-1-(2,5-dimethylphenyl)-5-phenyl-1H-pyrazole-3- carboxylate (2)



28 **Figure S3.** (R)-4-benzoyl-1-(2,5-dimethylphenyl)-N-(2-hydroxy-1-phenylethyl)-5-phenyl-1H-pyrazole-3-
 29 carboxamide (**3a**)

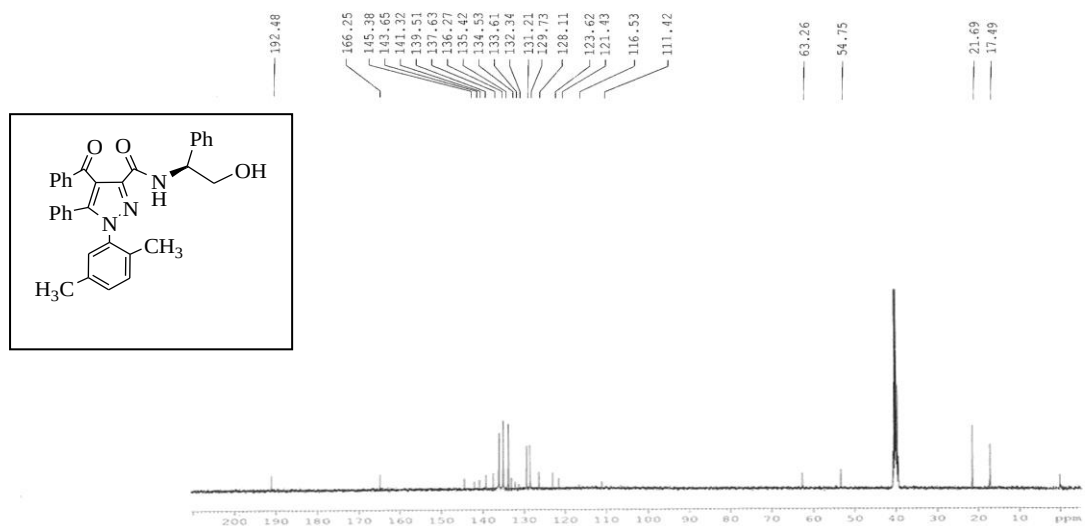
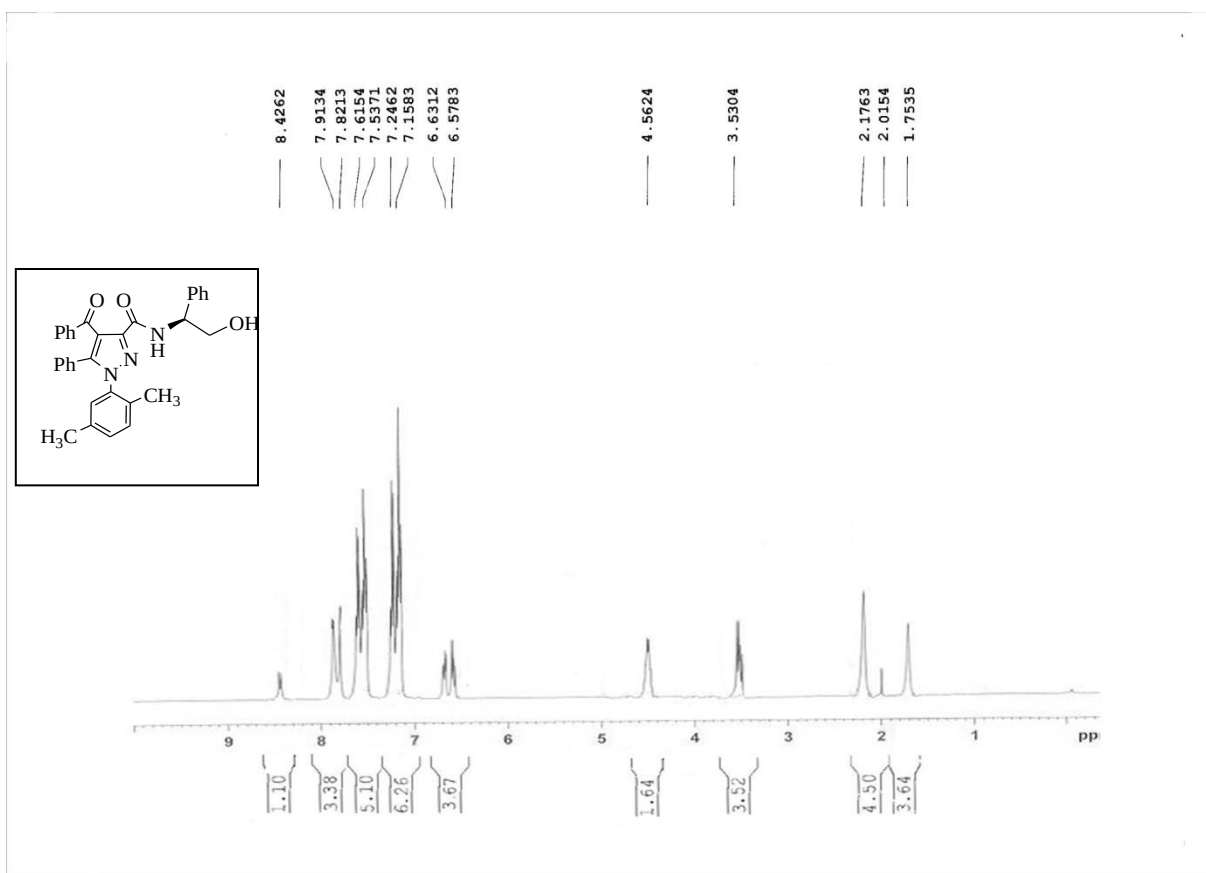


Figure S4. ^1H and ^{13}C NMR Spectra of 4-benzoyl-1-(2,5-dimethylphenyl)-N-(1-hydroxy-3-methylbutan-2-yl)-5-phenyl-1*H*-pyrazole-3-carboxamide (**3b**)

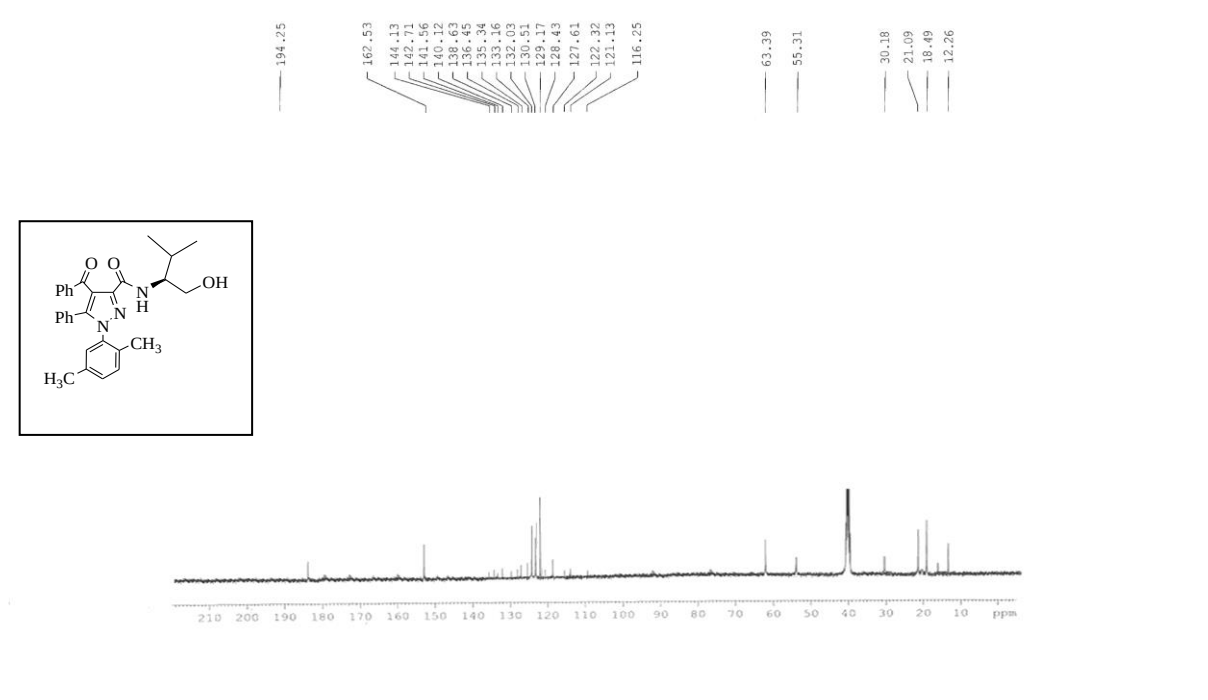
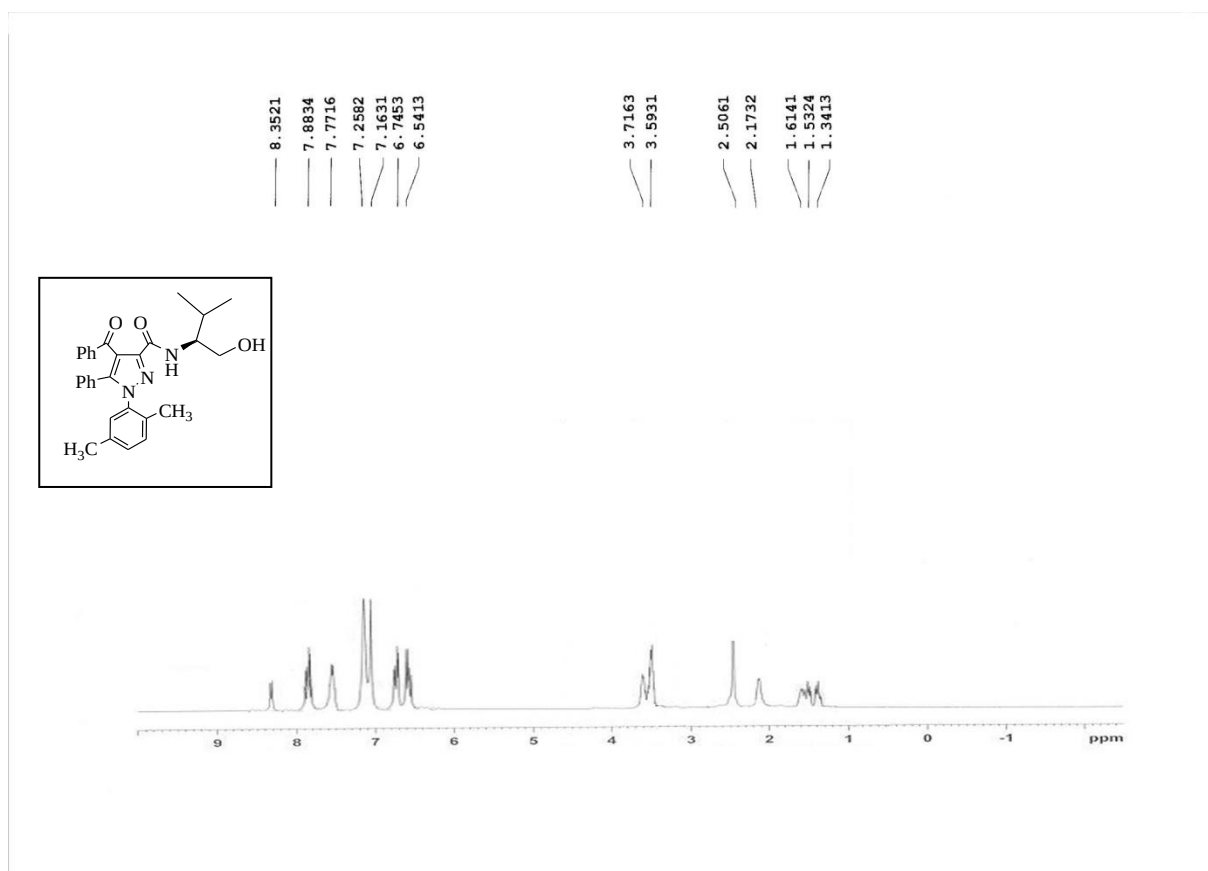
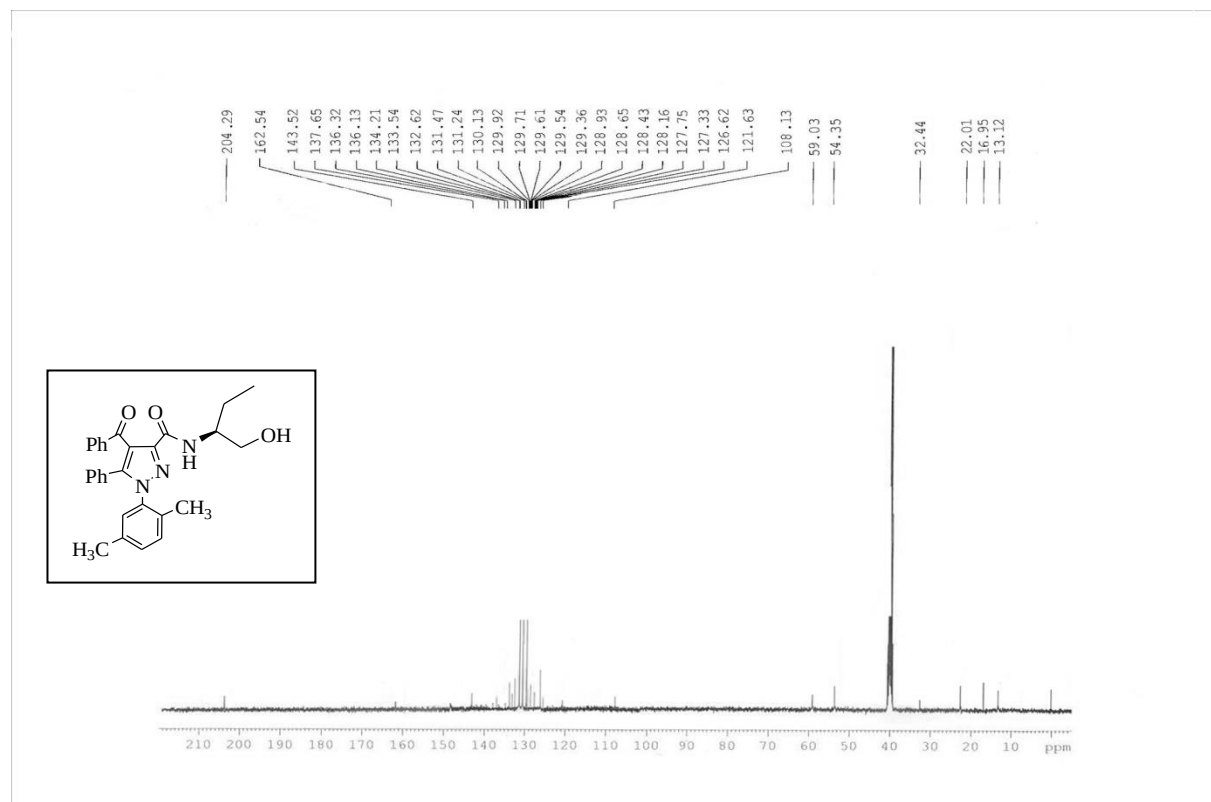
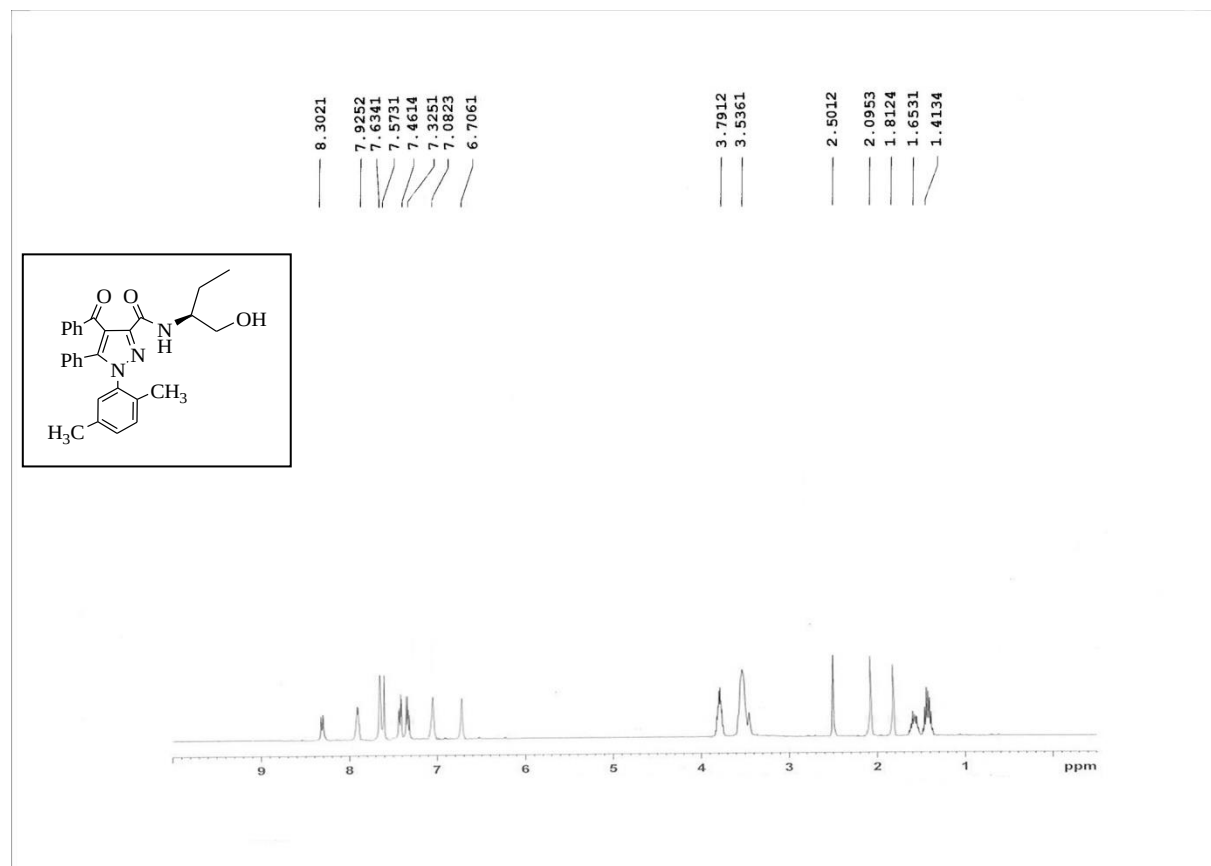
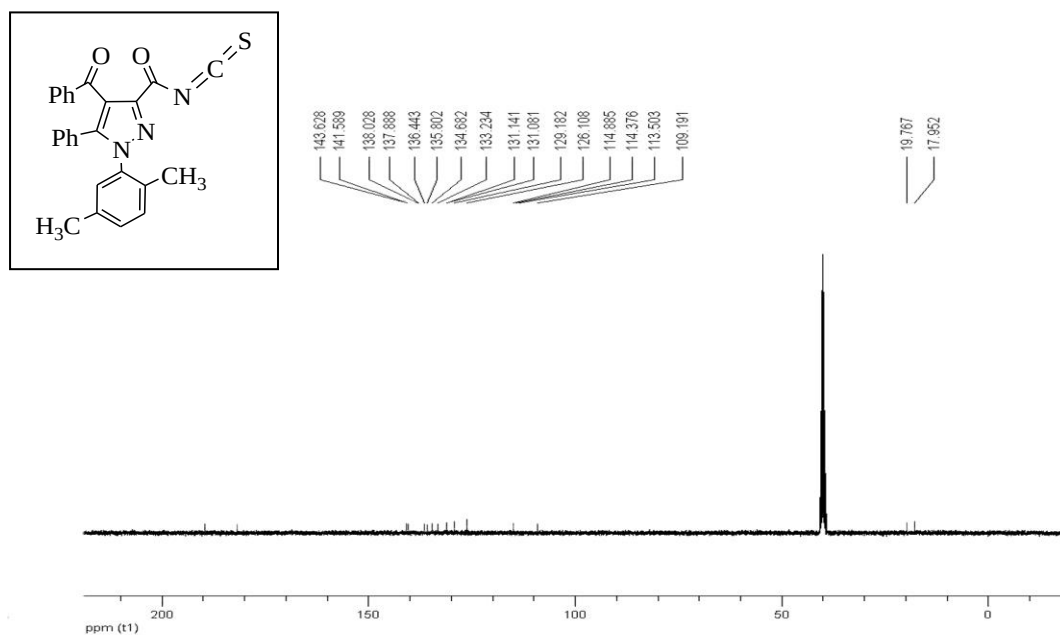


Figure S5. ^1H and ^{13}C NMR Spectra of 4-benzoyl-1-(2,5-dimethylphenyl)-N-(1-hydroxy-butan-2-yl)-5-phenyl-1H-pyrazole-3-carboxamide (**3c**)

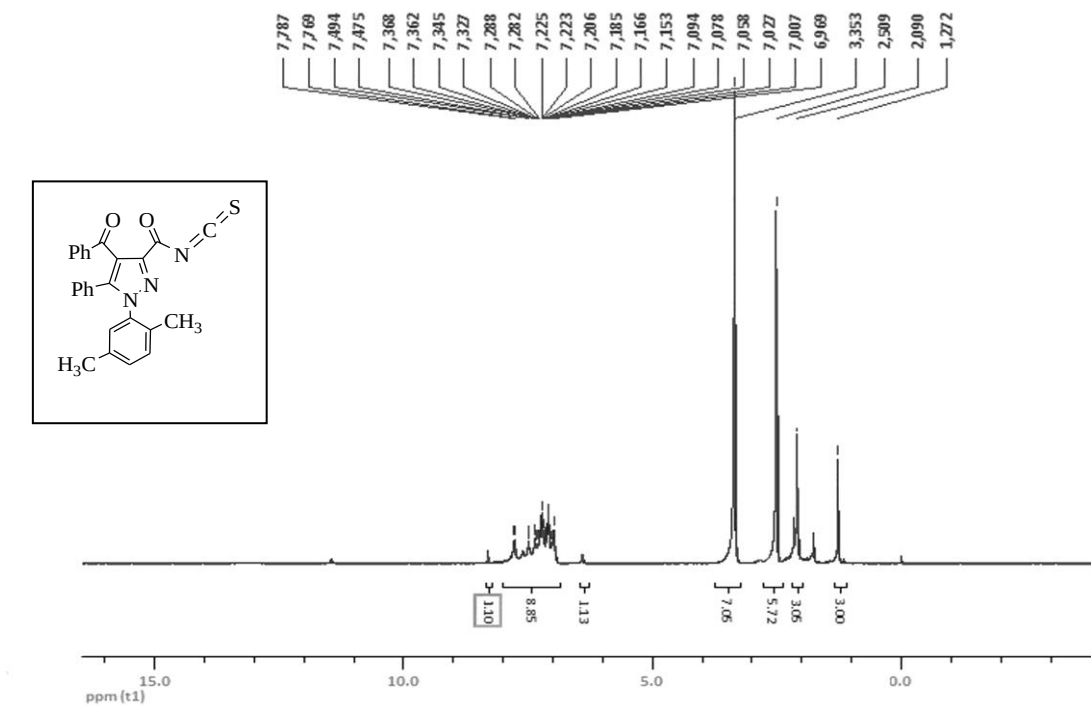


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43 **Figure S6.** ^1H and ^{13}C NMR Spectra of 4-benzoyl-1-(2,5-dimethylphenyl)-5-phenyl-1*H*-pyrazole-3-carbonyl-
44 isothiocyanate (**4**)



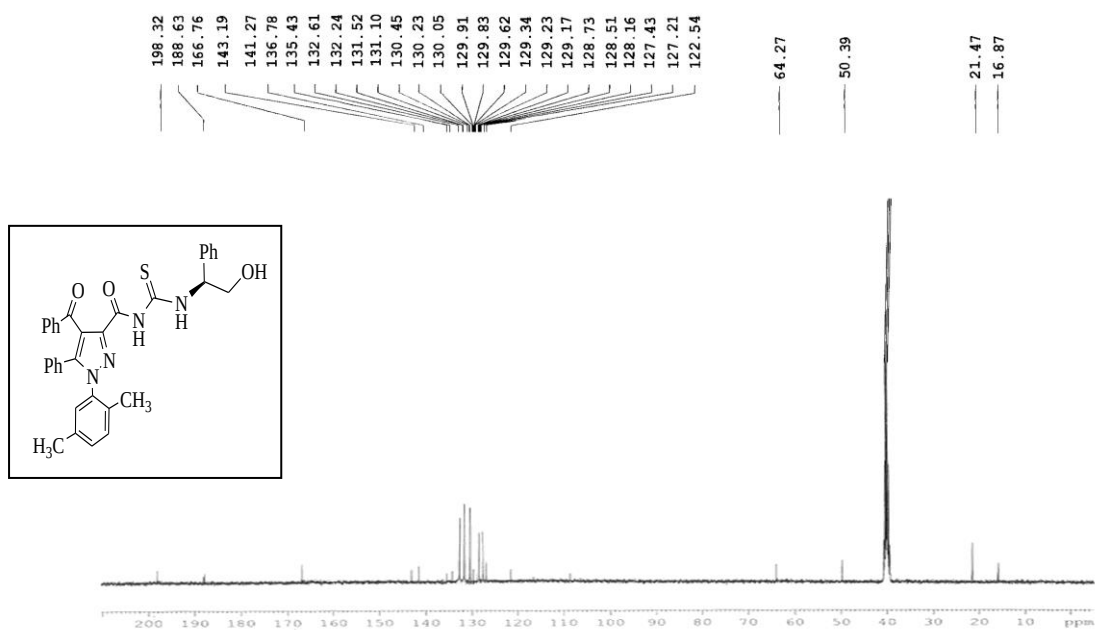
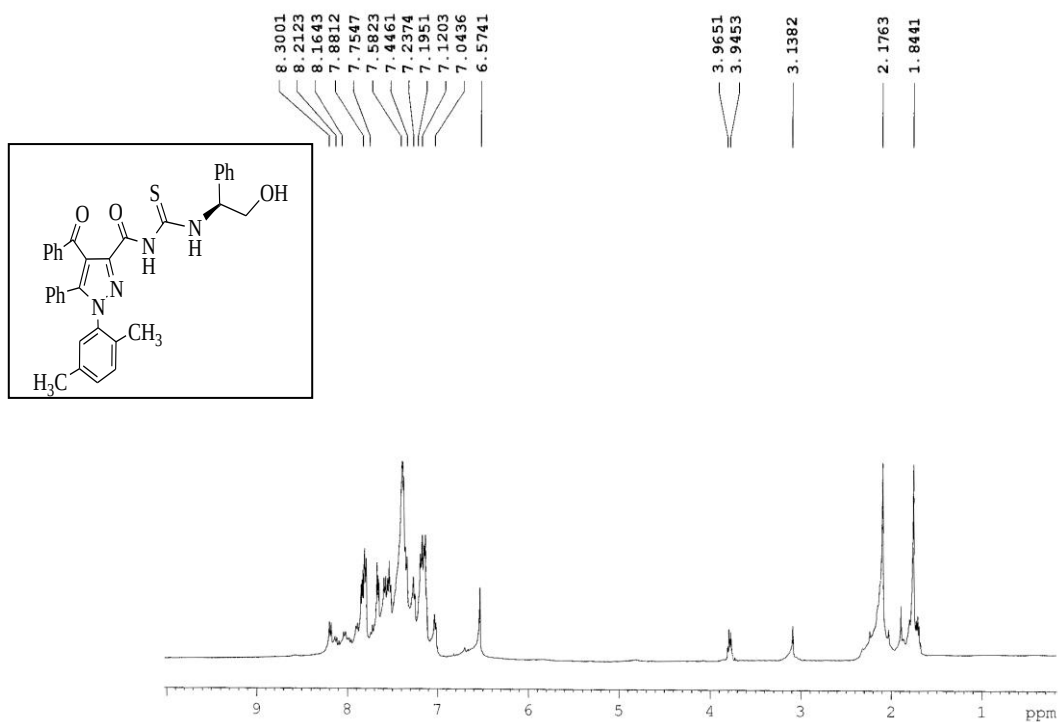
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49 **Figure S7.** ^1H and ^{13}C NMR Spectra of 1-(4-Benzoyl-1-(2,5-dimethylphenyl)-5-phenyl-1*H*-pyrazole-3-
50 carbonyl)-3-(2-hydroxy-1-phenylethyl)-thiourea (**5a**)



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60 **Figure S9.** ^1H and ^{13}C NMR Spectra of 1-(4-Benzoyl-1-(2,5-dimethylphenyl)-5-phenyl-1*H*-pyrazole-3-
 61 carbonyl)-3-(1-hydroxy propan-2-yl)-thiourea (**5c**)

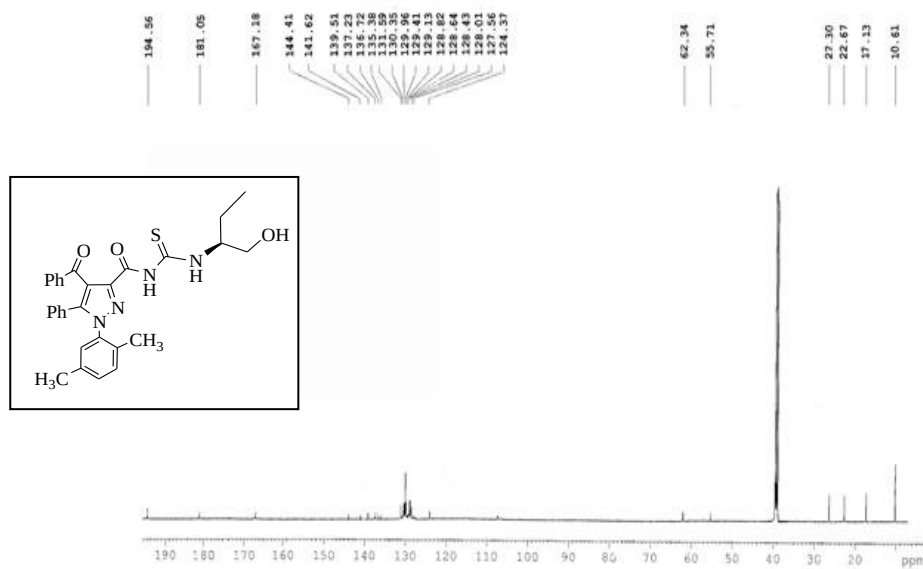
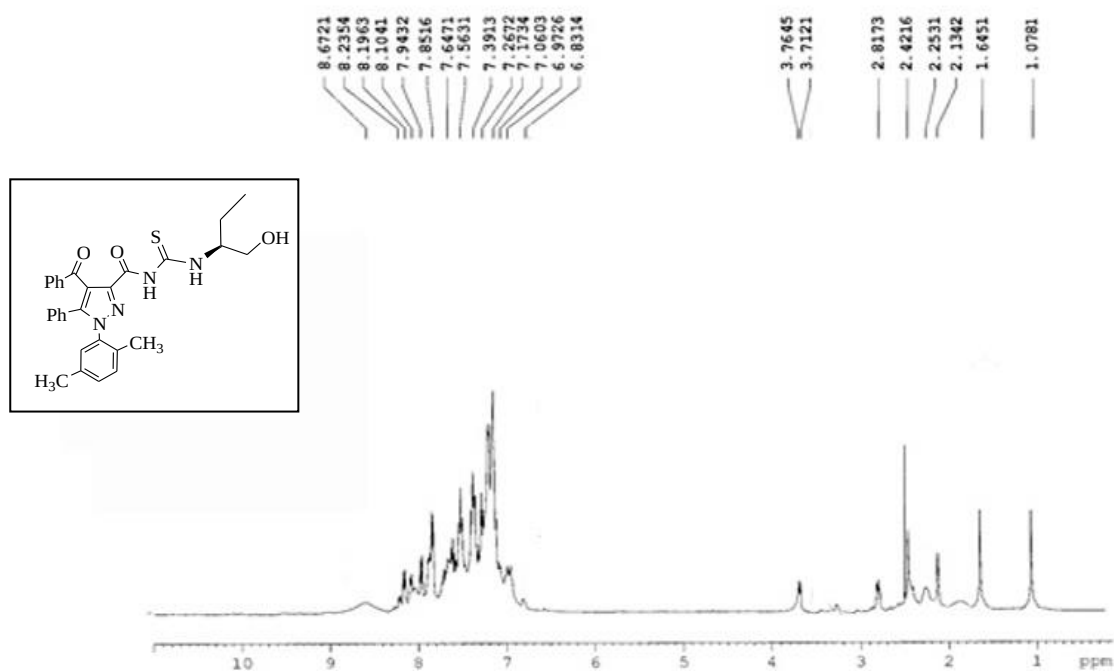


Table 1. Geometric optimization was done by means of Gaussian 09 with DFT/B3LYP 6-311G
Coordinates for compound 3a

	Center	Atomic	Atomic	Coordinates (Angstroms)		
	Number	Number	Type	X	Y	Z

73	1	6	C	1.886164	0.182310	0.387761
74	2	6	C	0.815864	1.067826	0.490730
75	3	6	C	-0.311698	0.321007	0.073428
76	4	7	N	1.352732	-1.001579	0.074996
77	5	7	N	0.020381	-0.922917	0.257937
78	6	6	C	-1.733583	0.771618	0.058274
79	7	7	N	-2.601688	-0.142755	0.461464
80	8	1	H	-2.204126	-1.019508	0.767333
81	9	6	C	-4.038832	0.068571	0.513621
82	10	1	H	-4.197588	1.096045	0.179523
83	11	6	C	-4.489919	-0.009421	1.984974
84	12	1	H	-4.402315	-1.047914	2.336405
85	13	1	H	-3.810929	0.617868	2.576822
86	14	8	O	-5.829246	0.456676	2.077350
87	15	1	H	-6.166408	0.241696	2.950967
88	16	6	C	-4.824462	-0.873797	0.394263
89	17	6	C	-4.273670	-2.055062	0.897675
90	18	6	C	-6.148309	-0.560315	0.726002
91	19	6	C	-5.027405	-2.908686	1.702377
92	20	1	H	-3.240996	-2.308568	0.688846
93	21	6	C	-6.901028	-1.411384	1.529307
94	22	1	H	-6.588670	0.350302	0.340795
95	23	6	C	-6.344504	-2.591568	2.019560
96	24	1	H	-4.578337	-3.818053	2.086572
97	25	1	H	-7.923228	-1.148303	1.778727
98	26	1	H	-6.929760	-3.252410	2.649274
99	27	8	O	-2.054630	1.869538	0.484301
100	28	6	C	0.858672	2.492137	0.961191
101	29	6	C	0.549206	3.584426	0.009477
102	30	6	C	0.395199	4.886137	0.483962
103	31	6	C	0.456673	3.358701	1.386761
104	32	6	C	0.142197	5.939544	0.383868
105	33	1	H	0.474180	5.043631	1.552193
106	34	6	C	0.213594	4.417021	2.257364
107	35	1	H	0.582518	2.356515	1.777708
108	36	6	C	0.052275	5.707100	1.757413
109	37	1	H	0.013837	6.943088	0.005783
110	38	1	H	0.148526	4.235807	3.324333
111	39	1	H	-0.143434	6.530682	2.435263
112	40	6	C	3.326781	0.388513	0.630504
113	41	6	C	3.757209	1.005177	1.815445
114	42	6	C	4.285059	-0.005154	0.315680
115	43	6	C	5.114068	1.215109	2.044587
116	44	1	H	3.022101	1.326393	2.541334
117	45	6	C	5.639292	0.205689	0.078958
118	46	1	H	3.969905	-0.466895	1.242860
119	47	6	C	6.058517	0.814305	1.102551
120	48	1	H	5.431324	1.693881	2.963977
121	49	1	H	6.367133	-0.100175	0.821931

122	50	1	H	7.114527	0.978993	1.284788
123	51	6	C	2.006901	-2.257865	0.325938
124	52	6	C	2.511389	-3.020235	0.732891
125	53	6	C	2.070626	-2.700751	1.647262
126	54	6	C	3.119652	-4.235089	0.393891
127	55	6	C	2.668428	-3.916626	1.970104
128	56	1	H	1.638241	-2.078773	2.422823
129	57	6	C	3.202307	-4.673704	0.921021
130	58	1	H	3.523617	-4.854024	1.187999
131	59	1	H	3.678602	-5.625078	1.135985
132	60	6	C	2.399505	-2.586885	2.171709
133	61	1	H	1.420332	-2.151899	2.383183
134	62	1	H	3.151851	-1.833663	2.422297
135	63	1	H	2.545113	-3.439158	2.837537
136	64	6	C	2.733450	-4.407195	3.396130
137	65	1	H	2.145558	-5.321255	3.525555
138	66	1	H	3.761621	-4.638945	3.689139
139	67	1	H	2.345910	-3.661276	4.092470
140	68	8	O	1.188026	2.742913	2.106971

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