A One-pot Multi-component Facile Synthesis of Dihydropyrimidin-2(*1H*)-thione Derivatives using Triphenylgermane as a Catalyst and its Binding Pattern Validation

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Supporting Information

Supplementary Table 1. Crystallographic data and structure refinement for compounds (**1**-**4**) and (**7**).

	(**1**)	(**2**)	(**3**)	(**4**)	(**7**)
Formula	$C_{14}H_{17}N_3O_3S$	$C_{13}H_{15}FN_2S$	$C_{13}H_{14}ClN_3O_2S$	$C_{13}H_{15}BrN_2S$	$C_{13}H_{13}Cl_3N_2S$
FW	307.36	250.33	311.78	311.24	335.66
T (K)	296(2)	296(2)	296(2)	296(2)	296(2)
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system	monoclinic	Monoclinic	triclinic	monoclinic	orthorhombic
Space group	P 21/n	P 21/n	P -1	P 21/n	P b c a
a(Å)	12.0474(15)	9.7432(8)	6.3088(5)	12.3156(7)	15.2154(11)
b(Å)	9.4787(9)	7.1550(5)	10.1010(8)	8.5081(5)	11.9065(9)
c(Å)	14.3337(17)	18.8125(14)	12.0187(10)	14.8996(9)	17.0387(14)
α (°)	90	90	91.338(4)	90	90
β (°)	107.574(3)	91.594(5)	98.933(3)	114.046(3)	90
γ (°)	90	90	99.800(4)	90	90
V(Å^3), Z	1560.4(3), 4	1310.96(17), 4	744.59(10), 2	1425.73(15), 4	3086.8(4), 8
D_C (Mg/m^3), μ (mm^{-1})	1.308, 0.220	1.268, 0.238	1.391, 0.401	1.450, 3.010	1.445, 0.716
F(000)	648	528	324	632	1376
Crystal size (mm^3)	0.40×0.22×0.20	0.35×0.24×0.22	0.38×0.32×0.28	0.36×0.24×0.22	0.38×0.30×0.26
θ range (°)	2.615-27.00	2.166-27.587	1.717-27.00	2.780 -27.513	2.391-27.00
Index ranges	-15 ≤ h ≤ 15 -12 ≤ k ≤ 8 -18≤ l ≤ 18	-12 ≤ h ≤ 12 -8 ≤ k ≤ 9 -24≤ l ≤24	-8 ≤ h ≤ 7 -12 ≤ k ≤ 12 -15≤ l ≤ 15	-15 ≤ h ≤ 15 -10 ≤ k ≤ 11 -19 ≤ l ≤ 16	-15 ≤ h ≤ 19 -15 ≤ k ≤ 12 -21 ≤ l ≤ 17
Total reflections	12620	11164	11708	11792	14207
Indept. Reflect.[R(int)]	3398 (0.0533)	3023 (0.0295)	3177 (0.0298)	3266 (0.0310)	3366 (0.0209)
Completeness toθ(25.00°)	99.8%	99.4%	97.9%	99.6%	99.9%

Max. and min.transmission	0.918& 0.960	0.921& 0.949	0.865 & 0.898	0.410 &0.557	0.775&0.835
Data/restraints/parameters	3398/0/194	3023/39/178	3177/0/184	3266 /0/157	3366 /0/175
Goodness-of-fit on F^2	1.014	1.060	1.047	1.032	1.033
Final R indices [I>2σ(I)]	R1 = 0.0587, wR2 = 0.1314	R1 = 0.0594, wR2 = 0.1647	R_1 = 0.0485, wR_2 = 0.1248	R_1 = 0.0594, wR_2 = 0.1457	R_1 = 0.0284, wR_2 = 0.0741
R indices (all data)	R1 = 0.0587, wR2 = 0.1612	R1 = 0.0904, wR2 = 0.1838	R_1 = 0.0721, wR_2 = 0.1387	R_1 = 0.1158, wR_2 = 0.1729	R_1 = 0.0364, wR_2 = 0.0809
Largest peak and hole (e A^{-3})	0.217 and -0.196	0.916 and -0.382	0.794 and -0.268	0.773 and -0.809	0.22 5and -0.212

Supplementary Table 2. Selected bond lengths (Å) and angles (˚) for compounds (**1**-**4**) and (**7**).

(**1**)				(**2**)			
S(1)-C(8)	1.693(3)	O(1)-N(1)-O(2)	124.2(4)	S(1)-C(7)	1.681(3)	C(7)-N(1)-C(10)	121.3(2)
O(1)-N(1)	1.185(4)	O(1)-N(1)-C(2)	119.4(3)	F(1)-C(2)	1.352(3)	C(2)-C(1)-N(1)	121.0(3)
O(2)-N(1)	1.216(4)	C(8)-N(2)-C(1)	118.7(2)	N(2)-C(7)	1.326(4)	F(1)-C(2)-C(3)	119.1(3)
N(3)-C(8)	1.317(3)	C(11)-N(2)-C(1)	120.1(2)	N(2)-C(8)	1.452(4)	N(2)-C(7)-N(1)	117.2(2)
N(1)-C(2)	1.479(4)	N(3)-C(8)-N(2)	117.3(2)	C(1)-C(2)	1.373(4)	N(2)-(C7)-S(1)	121.2(2)
(**3**)				(**4**)			
S(1)- C(7)	1.680(3)	O(2)-N(1)-O(1)	123.1(3)	Br(1)-C(2)	1.877(5)	C(7)-N(1)-C(1)	119.2(3)
O(1)-N(1)	1.214(3)	O(2)-N(1)-C(5)	117.5(3)	S(1)-C(7)	1.686(4)	C(2)-C(1)-N(1)	120.4(4)
O(2)-N(1)	1.208(3)	O(1)-N(1)-C(5)	119.4(2)	N(2)-C(7)	1.322(5)	C(1)-C(2)-Br(1)	120.0(4)
N(3)-C(7)	1.325(3)	N(3)-C(7)-N(2)	116.6(2)	N(2)-C(8)	1.462(5)	N(2)-C(7)-N(1)	117.7(3)
N(1)-C(5)	1.470(4)	N(3)-C(7)-S(1)	121.50(19)	C(1)-C(2)	1.382(6)	N(2)-C(7)-S(1)	121.1(3)
(**7**)							
S(1)-C(7)	1.6886(15)	C(7)-N(1)-C(1)	118.01(12)	Cl(1)-C(2)	1.7265(15)	N(1)-C(7)-S(1)	120.99(11)
N(2)-C(7)	1.3224(19)	N(2)-C(7)-N(1)	116.97(13	Cl(2)-C(4)	1.7417(16)	N(2)-C(8)-C(9)	108.01(12)
N(2)-C(8)	1.472(2)	N(2)-C(7)-S(1)	122.04(11)	Cl(3)-C(6)	1.7291(16)	C(5)-C(6)-Cl(3)	119.21(12)

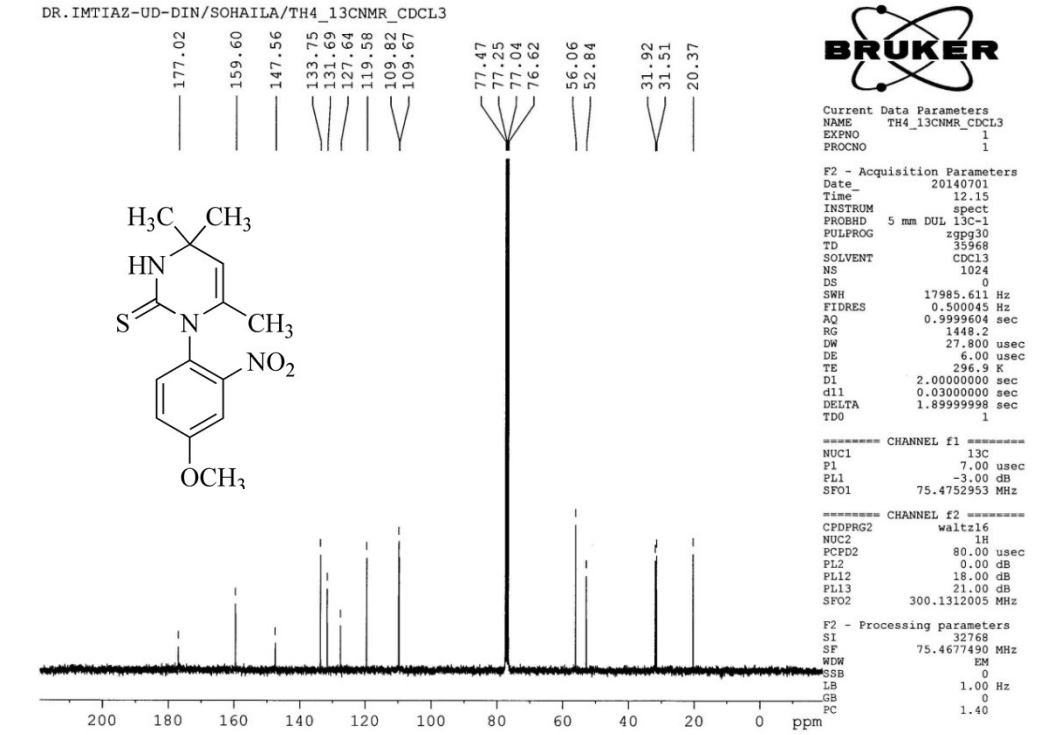
Supplementary Table 3. The intermolecular and intramolecular hydrogen bonds for compounds (**1**-**4**) and (**7**).Hydrogen-bond geometry: Distance, Å; angle,˚.

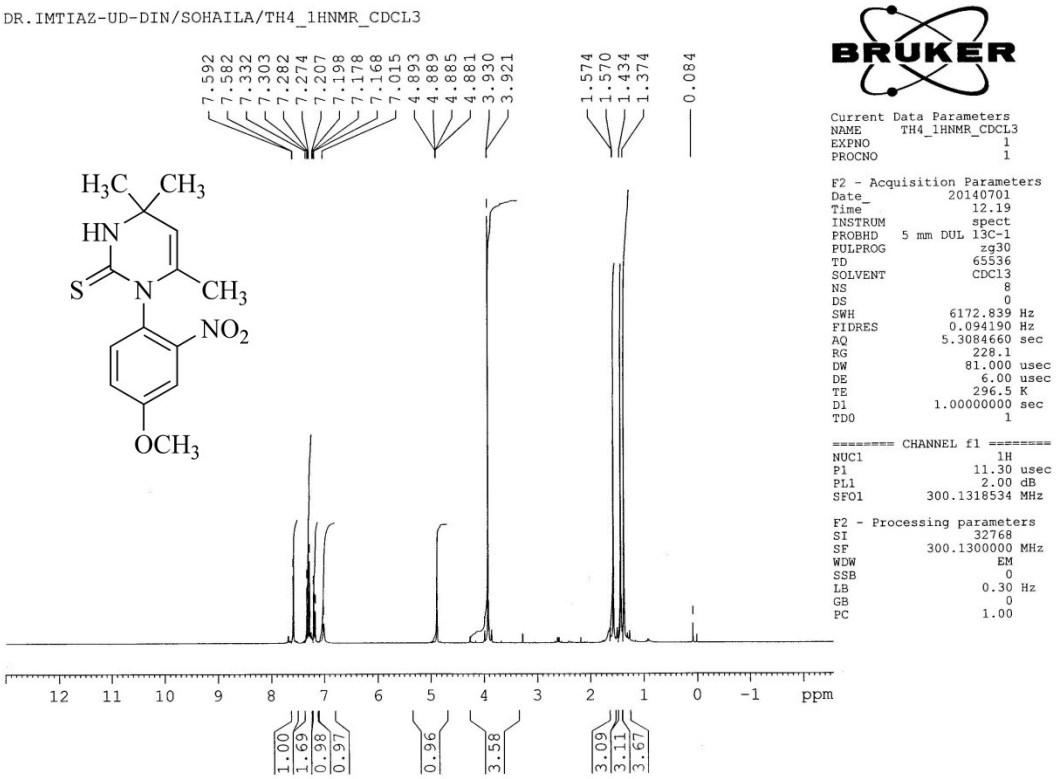
D*-H···*A	***D*-H**	**H···*A***	***D*···*A***	***D*-H···*A***	***D*-H···*A***	***D*-H**	**H···*A***	***D*···*A***	***D*-H···*A***
(**1**)					(**2**)				
N(3)-H(3A)···S(1)^{i}	0.86	2.50	3.337(3)	165.0	N(2)-H(2)···S(1)^{i}	0.86	2.64	3.466(3)	162.0
C(5)-H(5)···S(1)^{ii}	0.93	3.01	3.752(4)	138.4	C(6)-H(6)···S(1)^{ii}	0.93	2.97	3.860(3)	159.6
(**3**)					(**4**)				
N(3)-H(3A)···S(1)^{i}	0.86	2.60	3.437(2)	164.8	N(2)-H(2)···S(1)^{i}	0.86	2.53	3.371(3)	164.4
C(11)-H(11C)···O(1)^{ii}	0.96	2.39	3.345(5)	172.5	C(6)-H(6)···S(1)^{ii}	0.93	3.00	3.753(6)	139.7
(**7**)					C(9)-H(9)···S(1)^{iii}	0.93	3.00	3.637(4)	127.3
N(2)-H(2)···S(1)^{i}	0.86	2.59	3.4219(14)	162.2	C(11)-H(11C)···Br(1)^{iv}	0.96	3.02	3.663(5)	125.4
C(5)-H(5)···S(1)^{ii}	0.93	2.87	3.8017(17)	176.3					
C(11)-H(11C)···Cl(3)	0.96	2.98	3.658(2)	128.9					

Symmetry codes: (i) −*x*+1, −*y*+2, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*+1 (**1**); (i) −*x*, −*y*, −*z*+1; (ii) −*x*, −*y*+1, −*z*+1 (**2**); (i) −*x*+1, −*y*, −*z*; (ii) *x*−1, *y*, *z*. (**3**); (i) −*x*, −*y*+1, −*z*+1; (ii) −*x*, −*y*, −*z*+1; (iii) *x*−1/2, −*y*+1/2, *z*−1/2; (iv) −*x*+1/2, *y*−1/2, −*z*+1/2. (**4**);(i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+1, *y*−1/2, −*z*+1/2 (**7**)

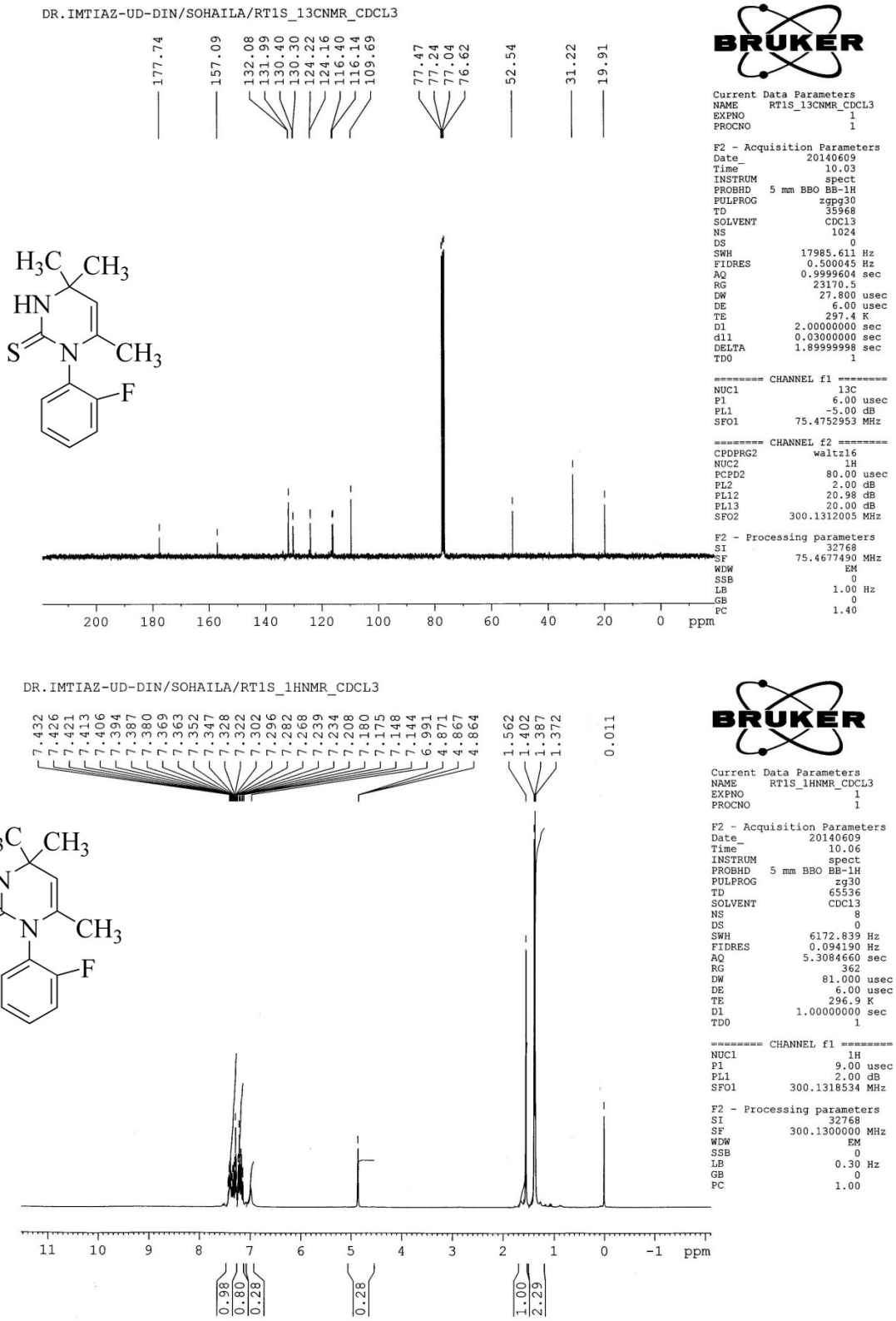
NMR (^{1}H and ^{13}C) spectra for representative compounds

1-(4-methoxy-2-nitrophenyl)-4,4,6-trimethyl-3,4-dihydropyrimidine-2(1H)-thione **(1)**

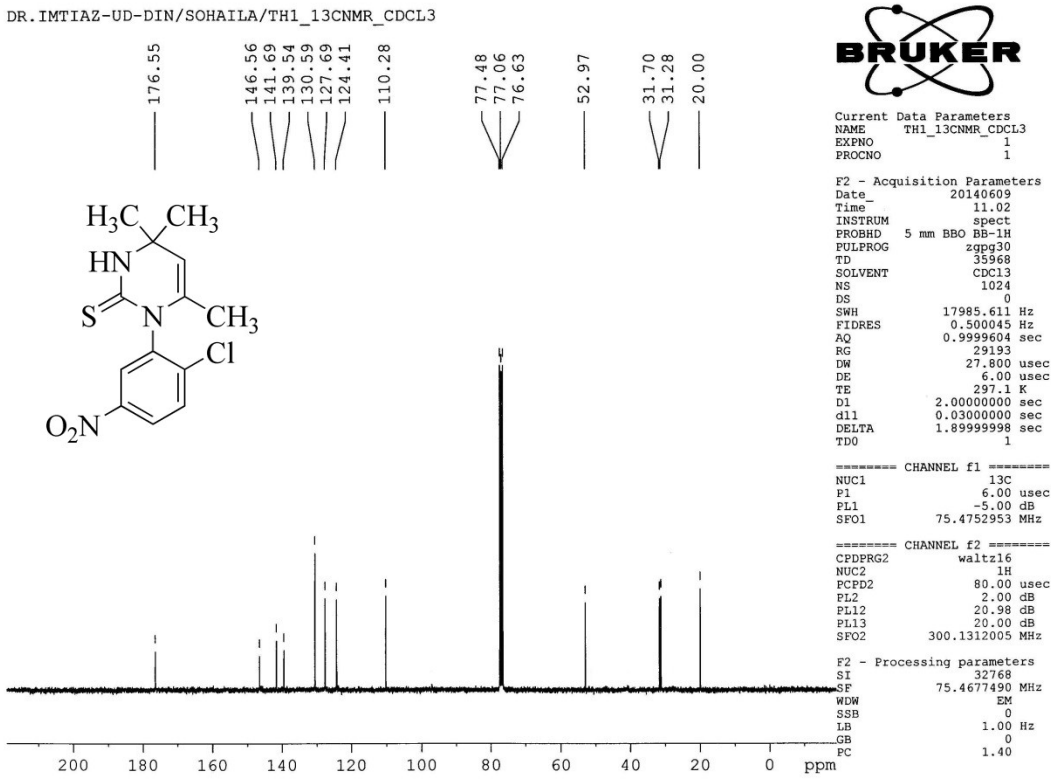


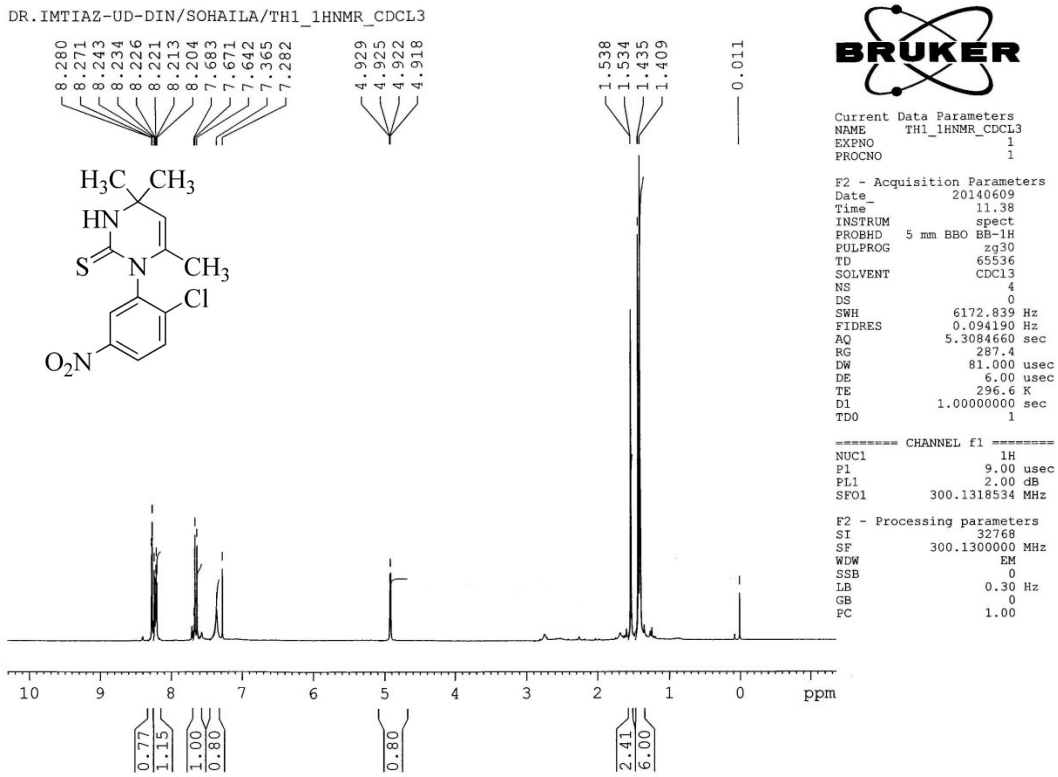


*1-(2-Fluorophenyl)-4,4,6-trimethyl-3,4-dihydropyrimidine-2(1H)-thione***(2)**

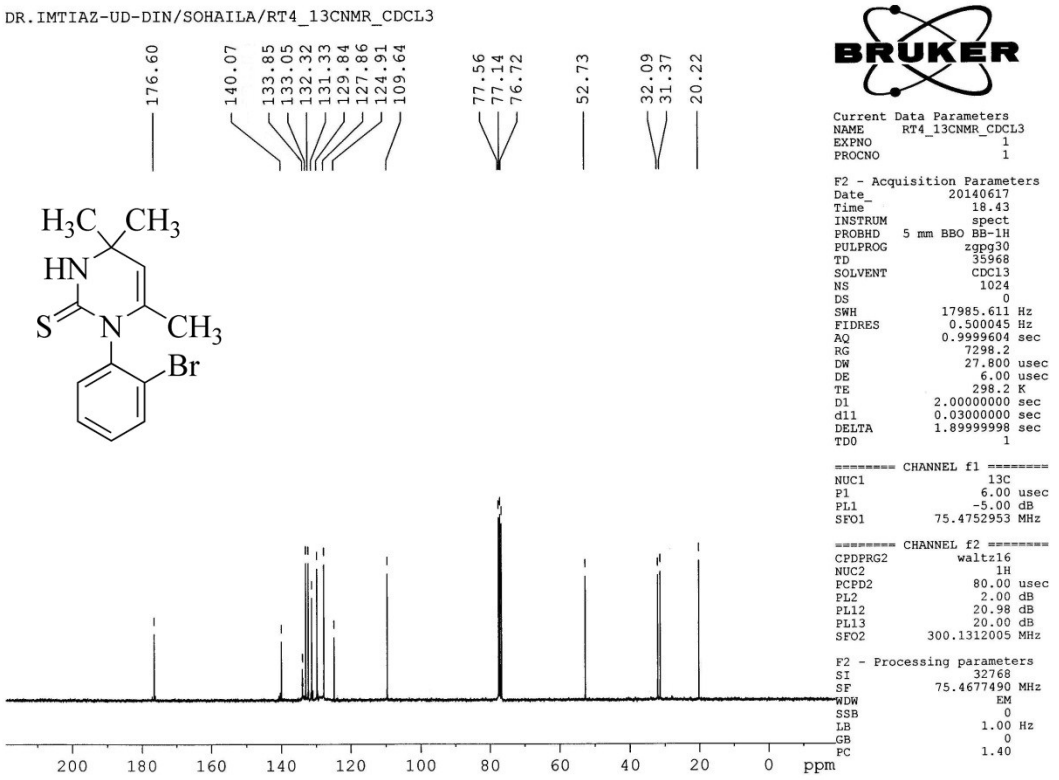


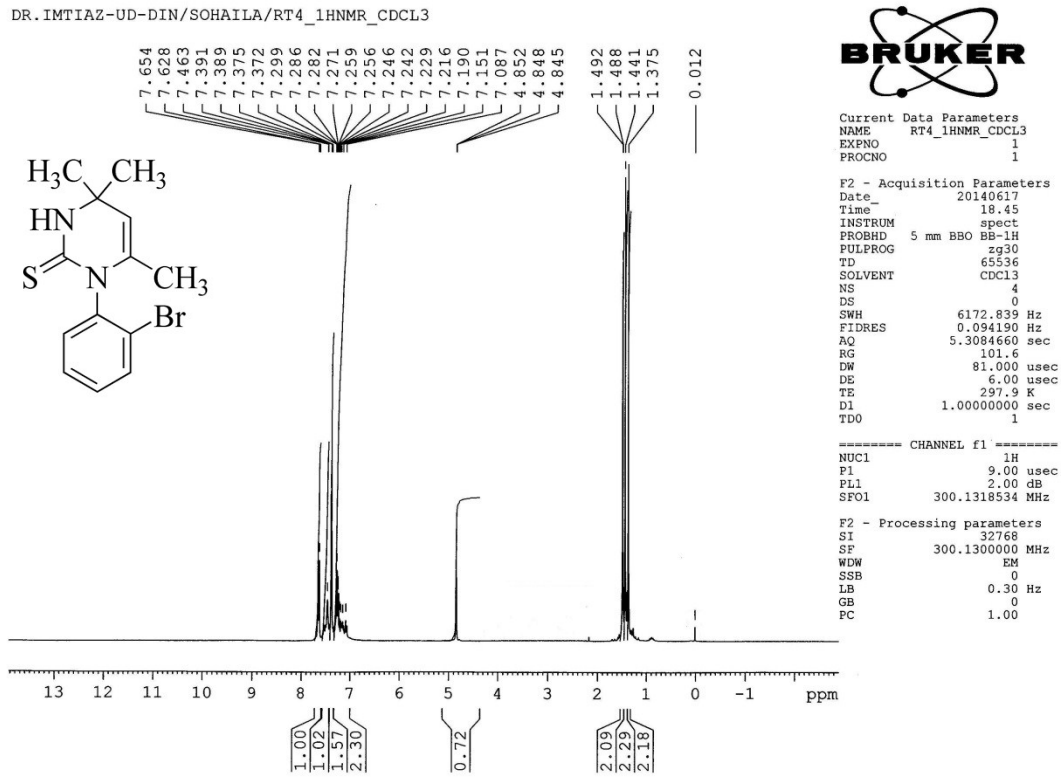
*1-(2-Chloro-5-nitrophenyl)-4,4,6-trimethyl-3,4-dihydropyrimidine-2(1H)-thione***(3)**

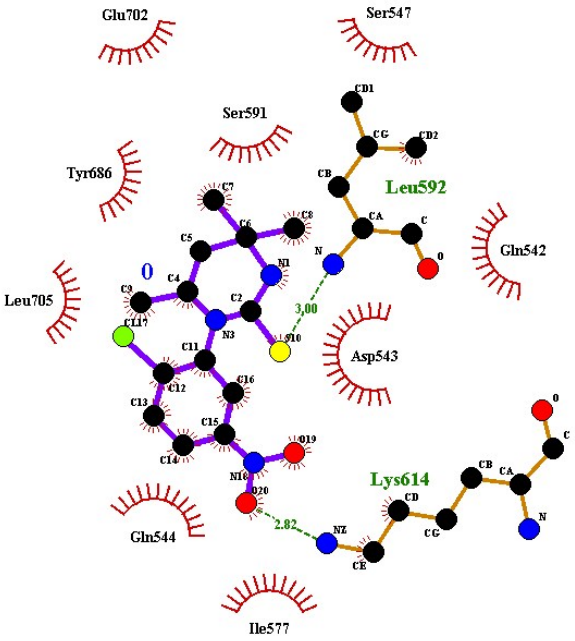




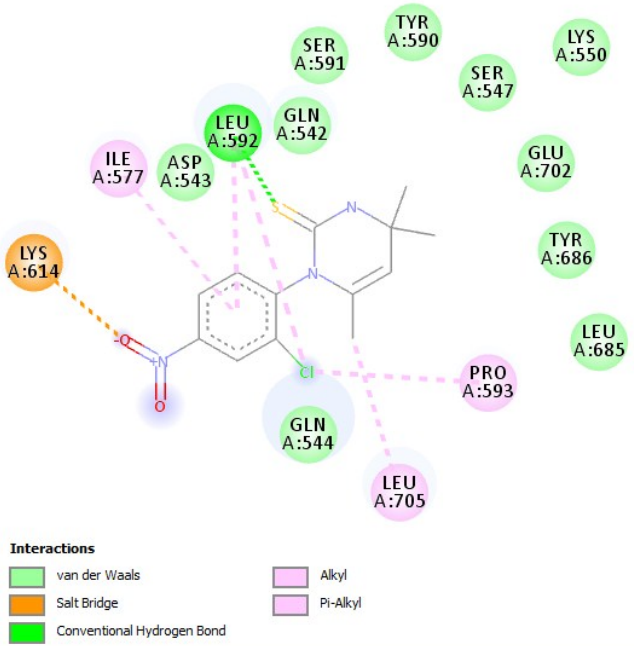
*1-(2-Bromophenyl)-4,4,6-trimethyl-3,4-dihydropyrimidine-2(1H)-thione***(4)**



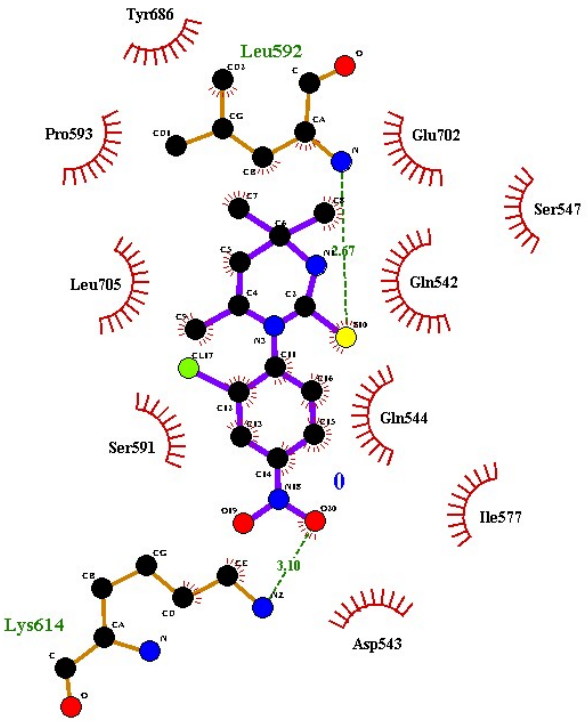




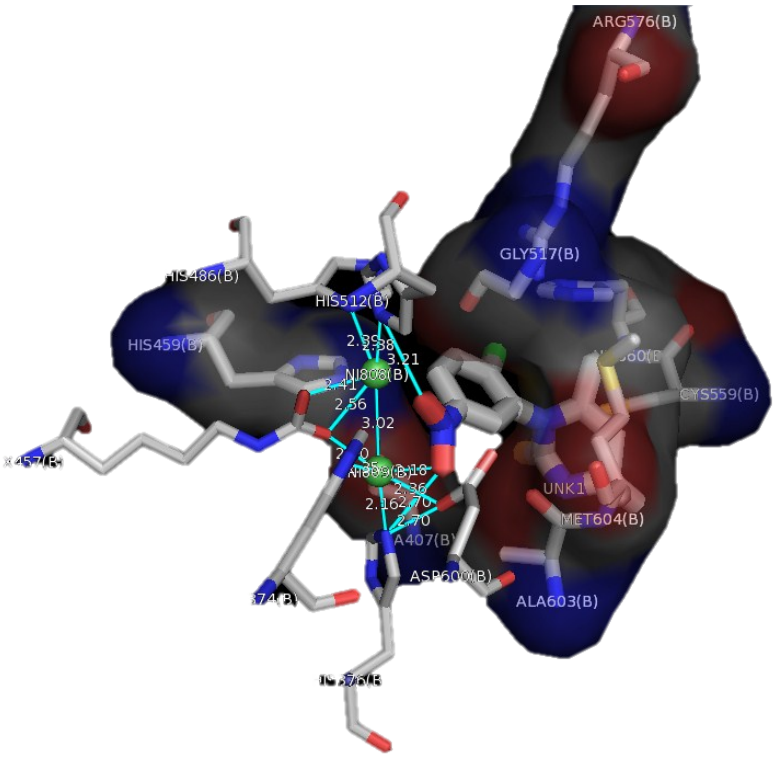
Supplementary Fig. 1. Interaction diagram of **3** with Human topoisomerase II alpha (4fm9) using LigPlot



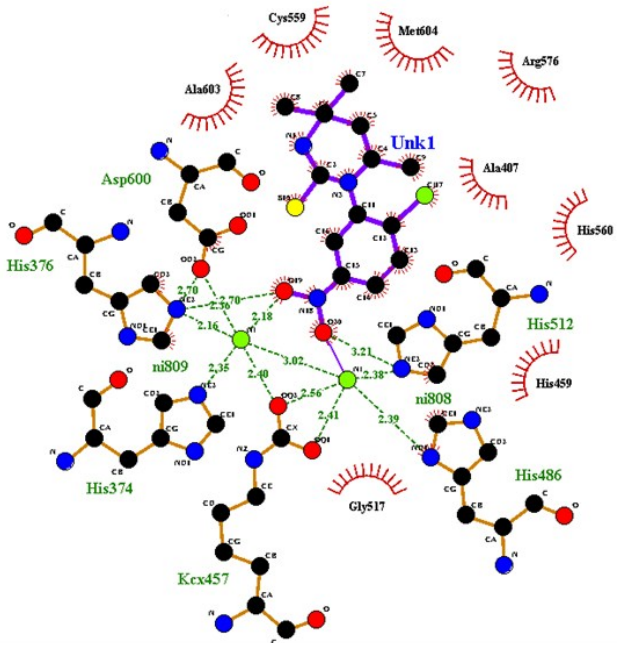
Supplementary Fig. 2. Interaction diagram of **8** with Human topoisomerase II alpha (4fm9) using Discovery Studio



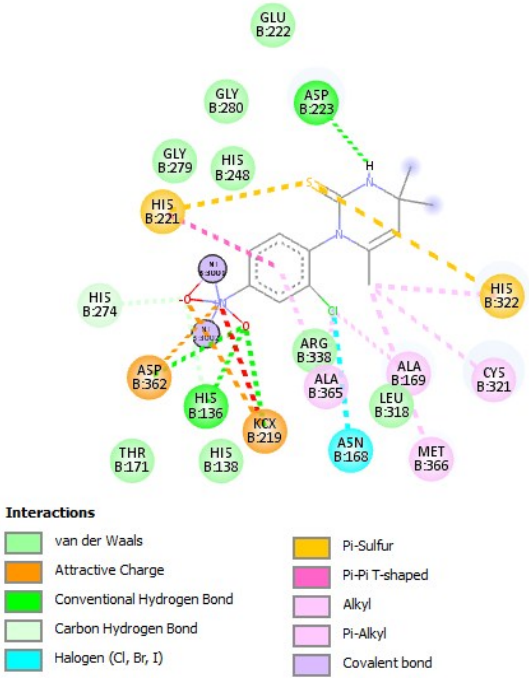
Supplementary Fig. 3. Interaction diagram of **8** with Human topoisomerase II alpha (4fm9) uisng LigPlot



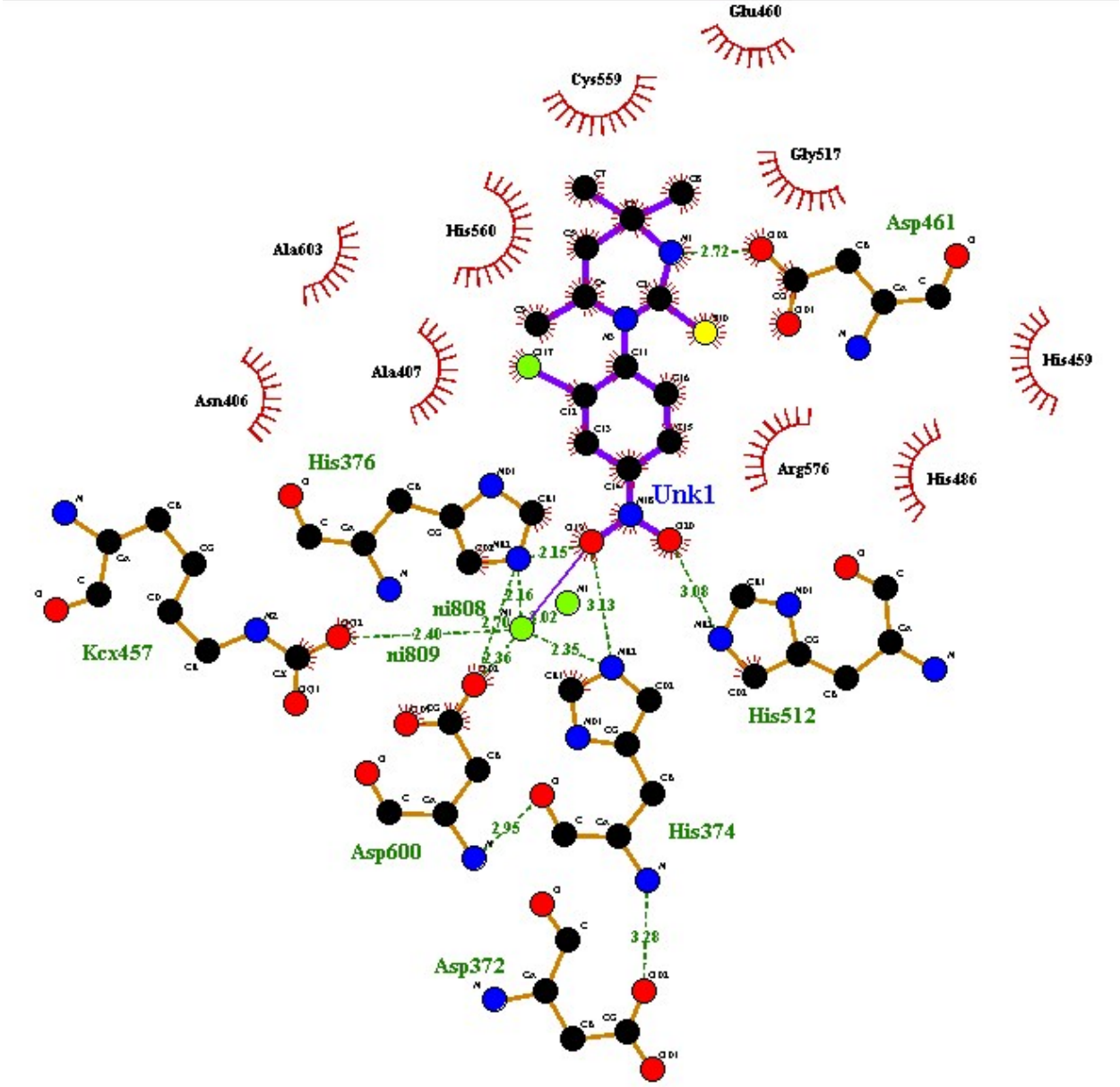
Supplementary Fig. 4. Interaction diagram of **3** with *Helicobacter pylori* Urease (1e9y) using PyMol.



Supplementary Fig. 5. Interaction diagram of **3** with *Helicobacter pylori* Urease (1e9y) using LigPlot.



Supplementary Fig. 6. Interaction diagram of **8** with *Helicobacter pylori* Urease (1e9y) using Discovery Studio.



Supplementary Fig. 7. Interaction diagram of **8** with *Helicobacter pylori* Urease (1e9y) using LigPlot.