

## 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 <sub>14</sub> H <sub>17</sub> N <sub>3</sub> O <sub>3</sub> S	C <sub>13</sub> H <sub>15</sub> FN <sub>2</sub> S	C <sub>13</sub> H <sub>14</sub> ClN <sub>3</sub> O <sub>2</sub> S	C <sub>13</sub> H <sub>15</sub> BrN <sub>2</sub> S	C <sub>13</sub> H <sub>13</sub> Cl <sub>3</sub> N <sub>2</sub> S
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)
$\alpha$ (°)	90	90	91.338(4)	90	90
$\beta$ (°)	107.574(3)	91.594(5)	98.933(3)	114.046(3)	90
$\gamma$ (°)	90	90	99.800(4)	90	90
V(Å <sup>3</sup> ), Z	1560.4(3), 4	1310.96(17), 4	744.59(10), 2	1425.73(15), 4	3086.8(4), 8
D <sub>c</sub> (Mg/m <sup>3</sup> ), $\mu$ (mm <sup>-1</sup> )	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 <sup>3</sup> )	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
$\theta$ 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 to $\theta$ (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 <sup>2</sup>	1.014	1.060	1.047	1.032	1.033
Final R indices [ $I > 2\sigma(I)$ ]	R1 = 0.0587, wR2 = 0.1314	R1 = 0.0594, wR2 = 0.1647	R <sub>1</sub> = 0.0485, wR <sub>2</sub> = 0.1248	R <sub>1</sub> = 0.0594, wR <sub>2</sub> = 0.1457	R <sub>1</sub> = 0.0284, wR <sub>2</sub> = 0.0741
R indices (all data)	R1 = 0.0587, wR2 = 0.1612	R1 = 0.0904, wR2 = 0.1838	R <sub>1</sub> = 0.0721, wR <sub>2</sub> = 0.1387	R <sub>1</sub> = 0.1158, wR <sub>2</sub> = 0.1729	R <sub>1</sub> = 0.0364, wR <sub>2</sub> = 0.0809
Largest peak and hole (e Å <sup>-3</sup> )	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).

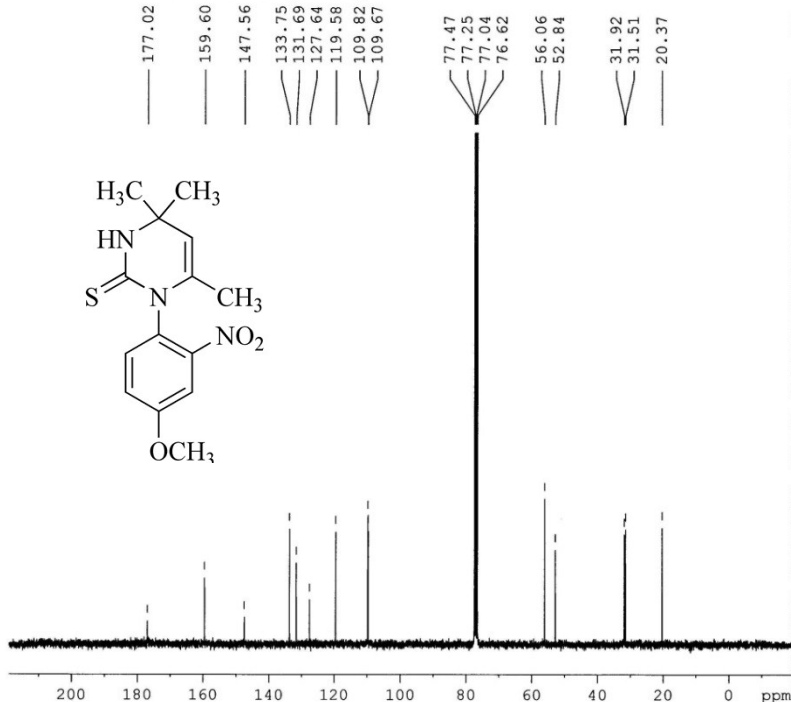
(1)				(2)			
S(1)-C(8)	1.693(3)	O(1)-N(1)-O(2)	124.2(4)	S(1)-C(7)	1.681(3)	C(7)-N(1)-C(10)	121.3(2)
O(1)-N(1)	1.185(4)	O(1)-N(1)-C(2)	119.4(3)	F(1)-C(2)	1.352(3)	C(2)-C(1)-N(1)	121.0(3)
O(2)-N(1)	1.216(4)	C(8)-N(2)-C(1)	118.7(2)	N(2)-C(7)	1.326(4)	F(1)-C(2)-C(3)	119.1(3)
N(3)-C(8)	1.317(3)	C(11)-N(2)-C(1)	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)-C(7)-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, °.

<i>D-H...A</i>	<i>D-H</i>	<i>H...A</i>	<i>D...A</i>	<i>D-H...A</i>	<i>D-H...A</i>	<i>D-H</i>	<i>H...A</i>	<i>D...A</i>	<i>D-H...A</i>
<b>(1)</b>					<b>(2)</b>				
N(3)-H(3A)···S(1) <sup>i</sup>	0.86	2.50	3.337(3)	165.0	N(2)-H(2)···S(1) <sup>i</sup>	0.86	2.64	3.466(3)	162.0
C(5)-H(5)···S(1) <sup>ii</sup>	0.93	3.01	3.752(4)	138.4	C(6)-H(6)···S(1) <sup>ii</sup>	0.93	2.97	3.860(3)	159.6
<b>(3)</b>					<b>(4)</b>				
N(3)-H(3A)···S(1) <sup>i</sup>	0.86	2.60	3.437(2)	164.8	N(2)-H(2)···S(1) <sup>i</sup>	0.86	2.53	3.371(3)	164.4
C(11)-H(11C)···O(1) <sup>ii</sup>	0.96	2.39	3.345(5)	172.5	C(6)-H(6)···S(1) <sup>ii</sup>	0.93	3.00	3.753(6)	139.7
<b>(7)</b>					C(9)-H(9)···S(1) <sup>iii</sup>				
N(2)-H(2)···S(1) <sup>i</sup>	0.86	2.59	3.4219(14)	162.2	C(11)-H(11C)···Br(1) <sup>iv</sup>	0.96	3.02	3.663(5)	125.4
C(5)-H(5)···S(1) <sup>ii</sup>	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) $-x+1, -y+1, -z+1$ <b>(1)</b> ; (i) $-x, -y, -z+1$ ; (ii) $-x, -y+1, -z+1$ <b>(2)</b> ; (i) $-x+1, -y, -z$ ; (ii) $x-1, y, z$ <b>(3)</b> ; (i) $-x, -y+1, -z+1$ ; (ii) $-x, -y, -z+1$ ; (iii) $x-1/2, -y+1/2, z-1/2$ ; (iv) $-x+1/2, y-1/2, -z+1/2$ . <b>(4)</b> ; (i) $-x+1, -y+1, -z+1$ ; (ii) $-x+1, y-1/2, -z+1/2$ <b>(7)</b>									

NMR ( $^1\text{H}$  and  $^{13}\text{C}$ ) spectra for representative compounds*1-(4-methoxy-2-nitrophenyl)-4,4,6-trimethyl-3,4-dihydropyrimidine-2(1H)-thione (1)*

DR.IMTIAZ-UD-DIN/SOHAJLA/TH4\_13CNMR\_CDCL3



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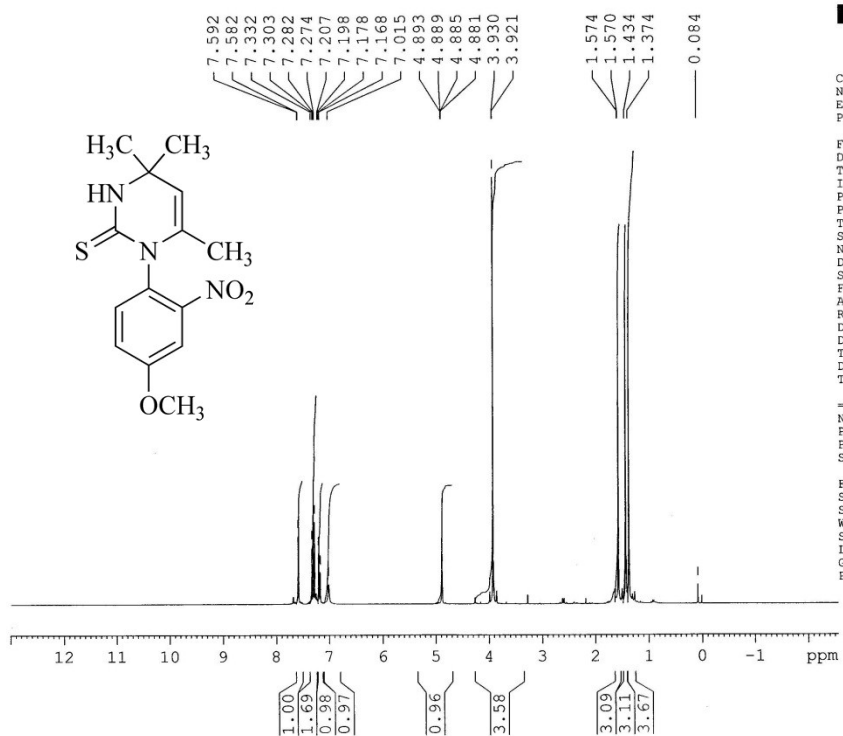
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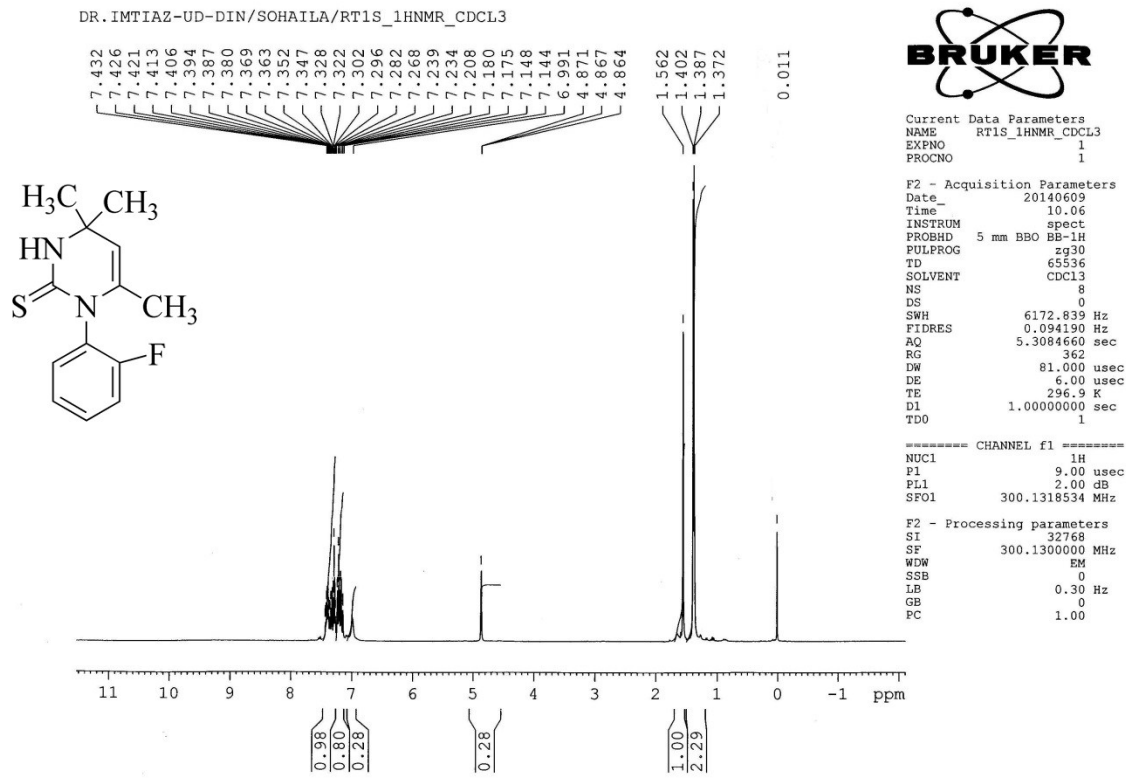
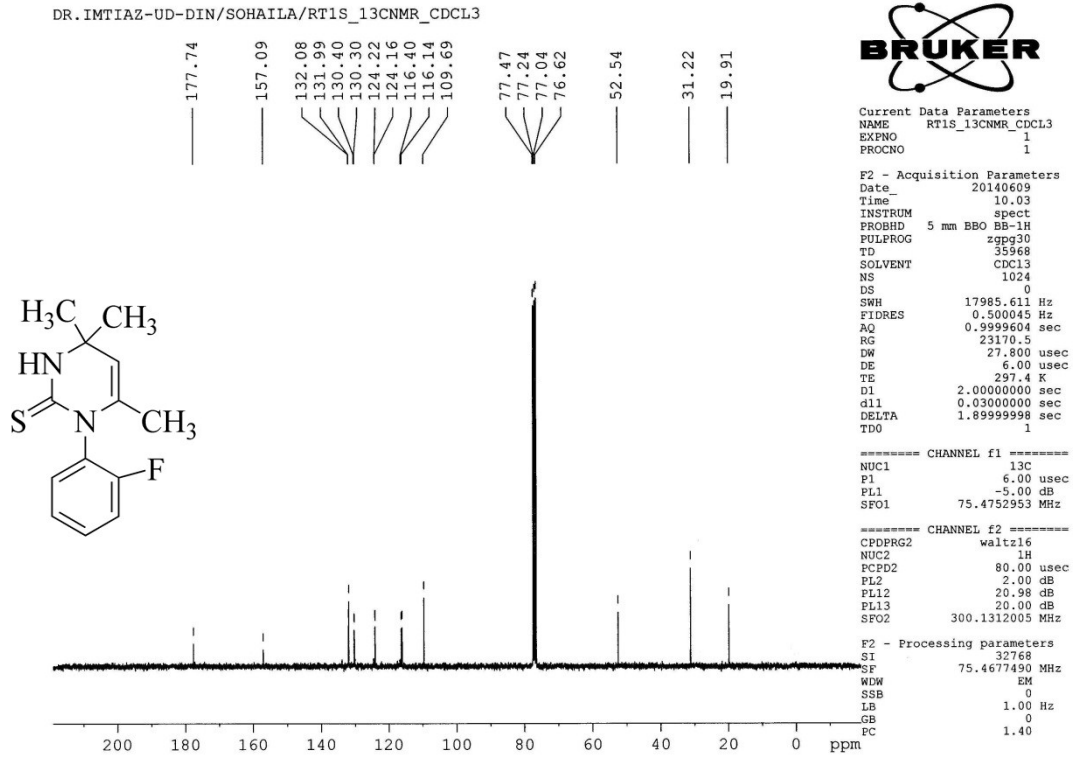
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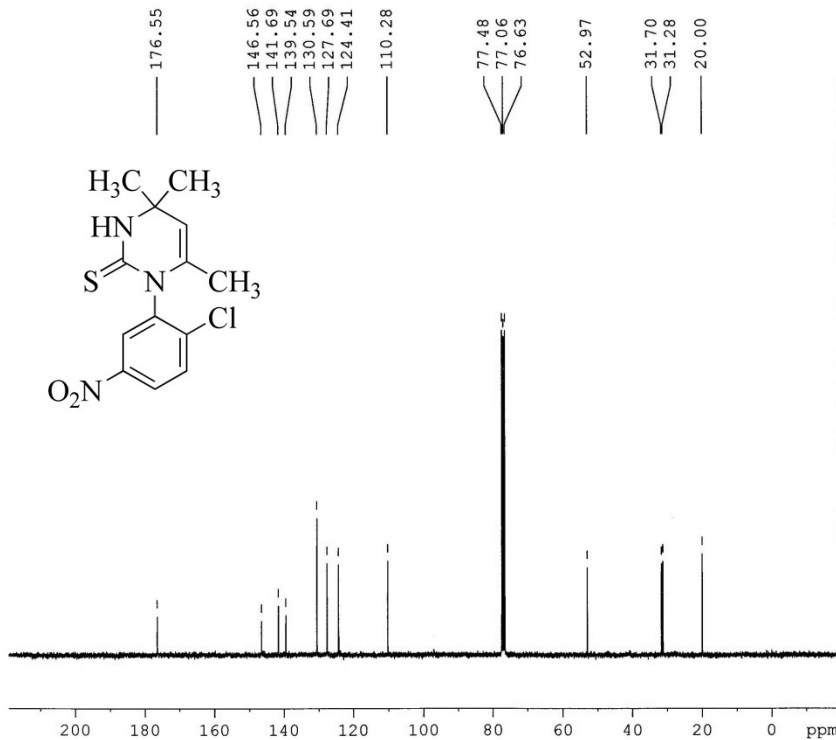
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1-(2-Fluorophenyl)-4,4,6-trimethyl-3,4-dihydropyrimidine-2(1H)-thione(2)



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

DR. IMTIAZ-UD-DIN/SOHAILA/TH1\_13CNMR\_CDCL3



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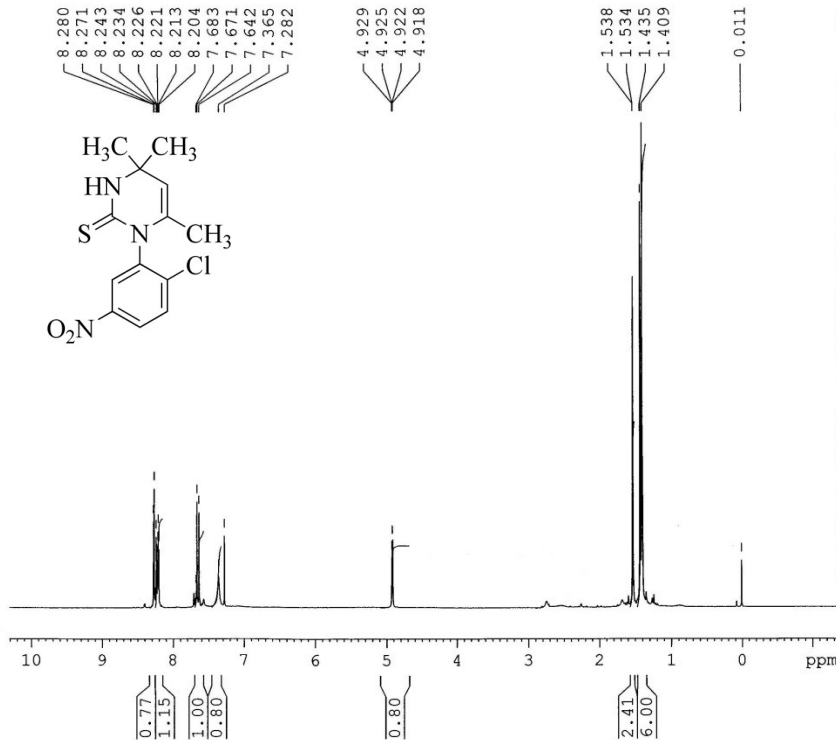
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DR. IMTIAZ-UD-DIN/SOHAILA/TH1\_1HNMR\_CDCL3



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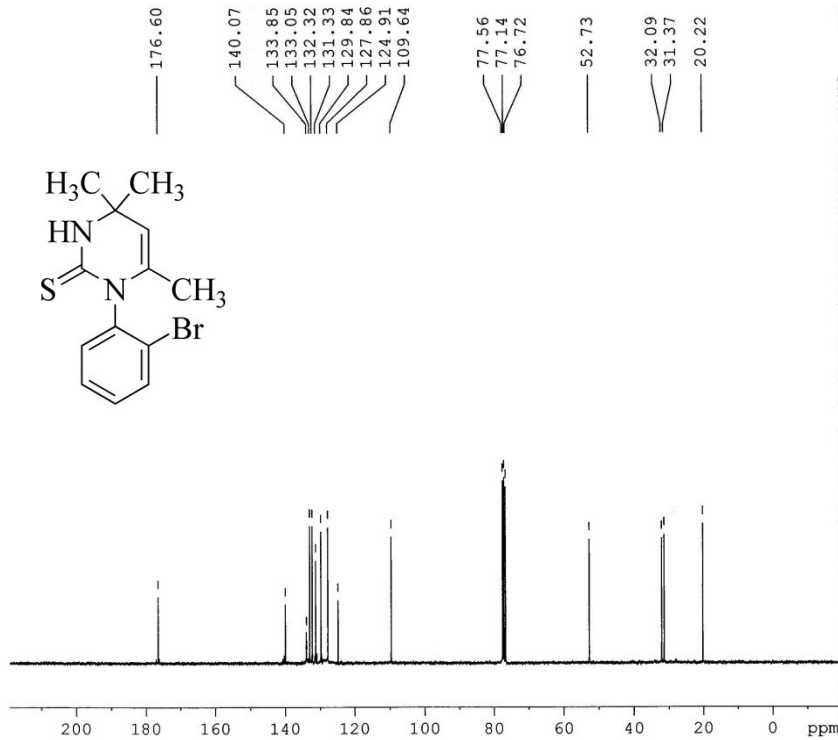
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*1-(2-Bromophenyl)-4,4,6-trimethyl-3,4-dihydropyrimidine-2(1H)-thione(4)*

DR. IMTIAZ-UD-DIN/SOHAILA/RT4\_13CNMR\_CDCL3



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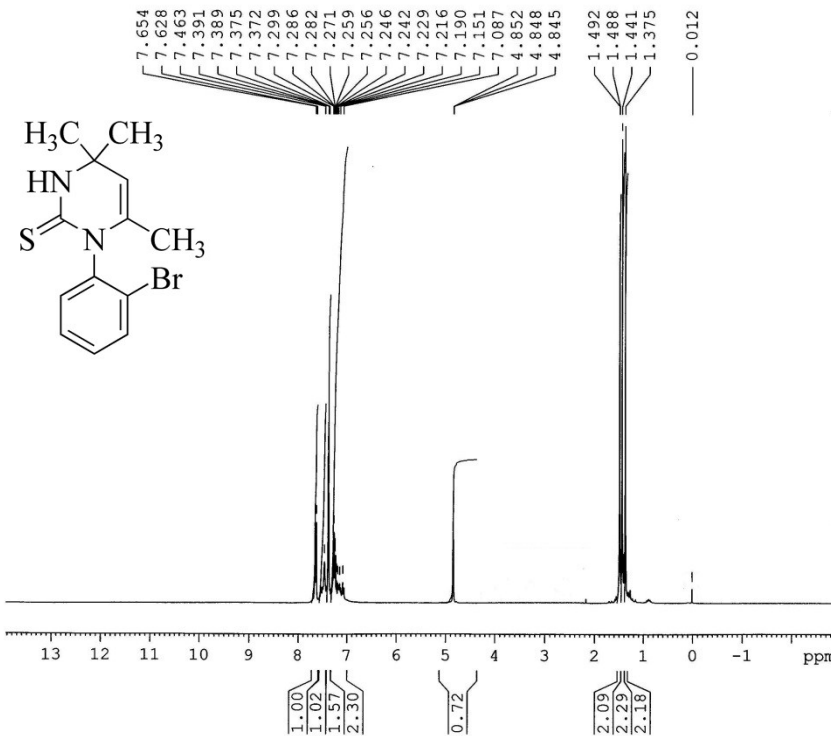
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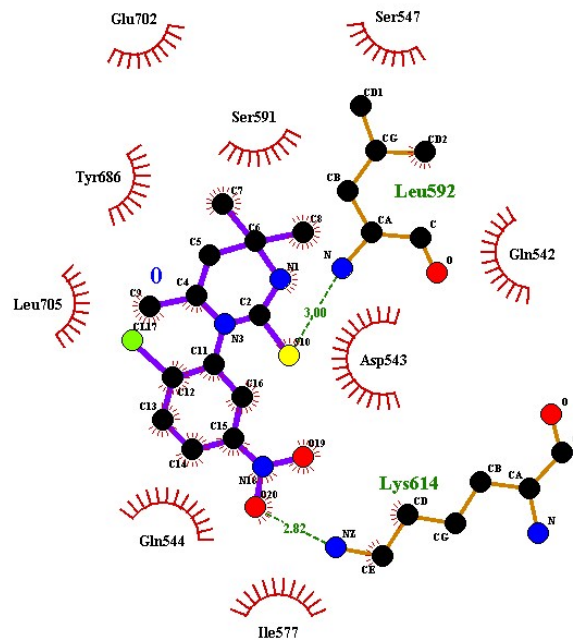


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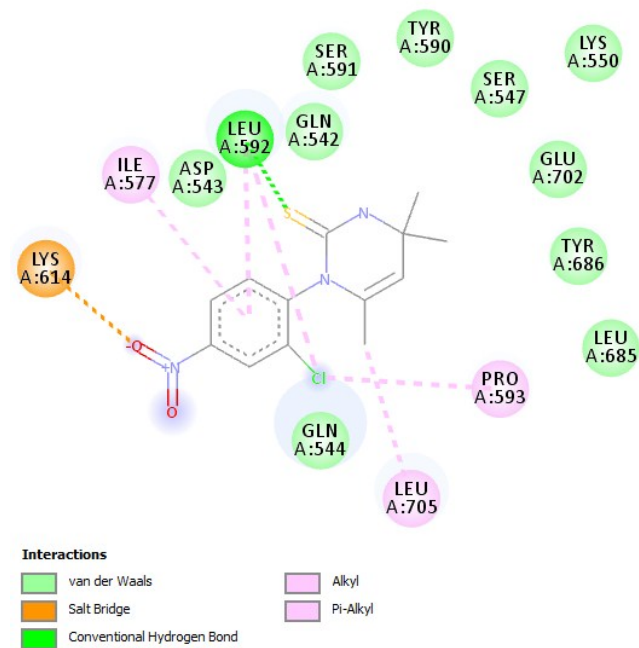
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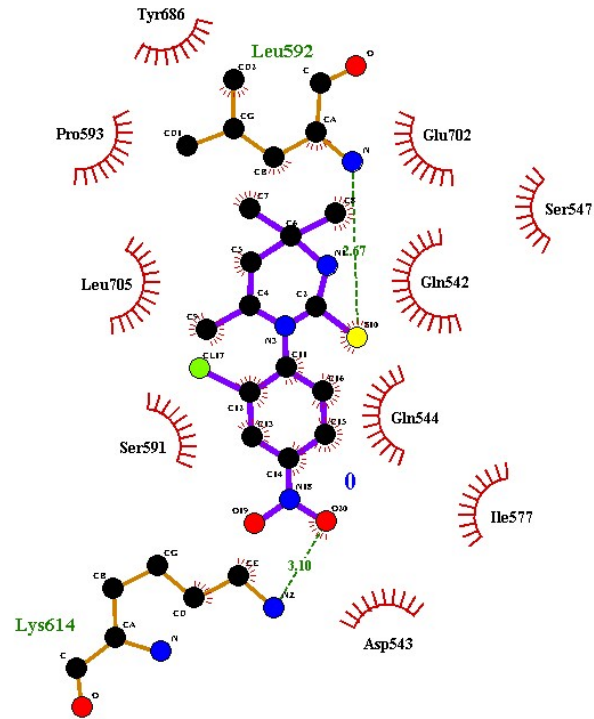


**Supplementary Fig. 1.** Interaction diagram of **3** with Human topoisomerase II alpha (4fm9) using LigPlot

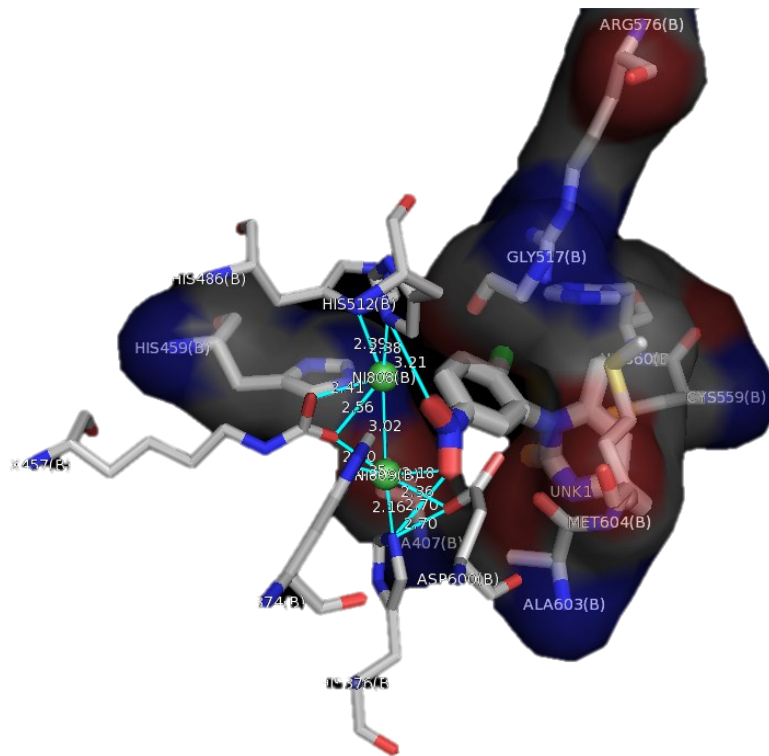


**Supplementary Fig. 2.** Interaction diagram of **8** with Human topoisomerase II alpha (4fm9) using Discovery Studio

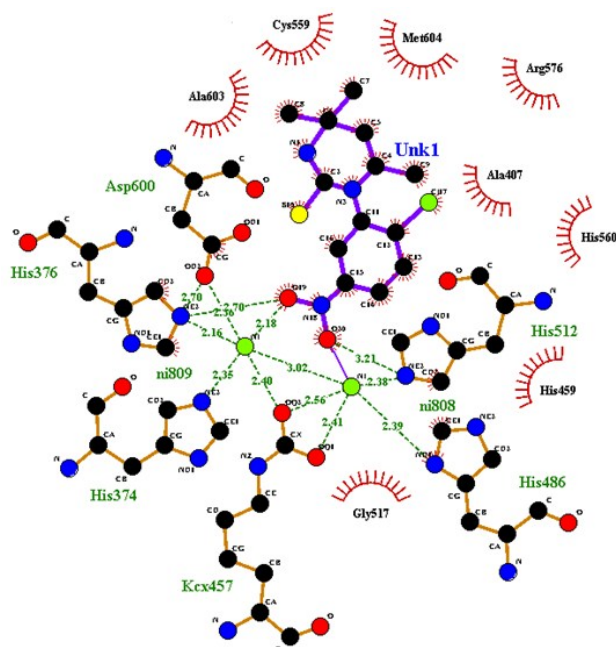




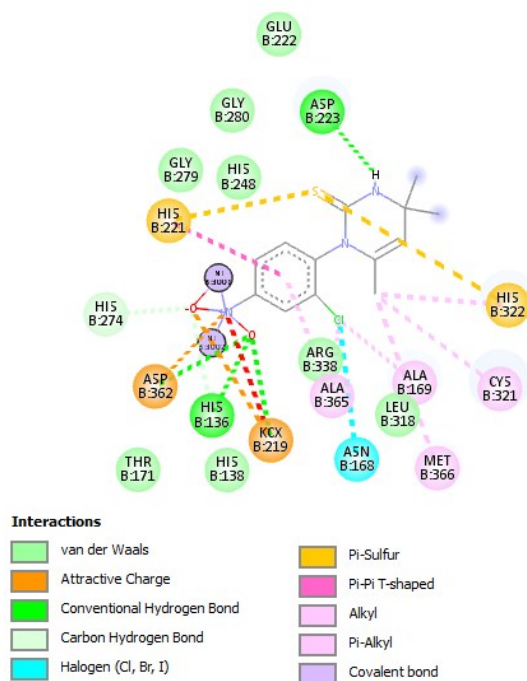
**Supplementary Fig. 3.** Interaction diagram of **8** with Human topoisomerase II alpha (4fm9) using LigPlot



**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.

