Supplementary Materials: Synthesis, Crystal Structure and DFT Studies of 1,3-Dimethyl-5-propionylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione

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Table S1. The calculated bond distances and bond angles compared to the experimental data of title compound.

Parameter	Bond Length		Parameter	Bond Angles	
	Experimental	Theoretical		Experimental	Theoretical
R (1,7)	1.218 (2)	1.2215	A (19,4,27)	103 (2)	107.1839
R (2,12)	1.213 (3)	1.2142	A (7,5,8)	118.1 (2)	118.7543
R (3,17)	1.264 (3)	1.2489	A (7,5,12)	125.7 (2)	125.5948
R (4,19)	1.310 (3)	1.3082	A (8,5,12)	116.2 (2)	115.6509
R (4,27)	1.110 (3)	1.0189	A (12,6,13)	117.8 (2)	118.4499
R (5,7)	1.404 (2)	1.4113	A (12,6,17)	123.3 (2)	123.7612
R (5,8)	1.476 (4)	1.4706	A (13,6,17)	118.9 (2)	117.7889
R (5,12)	1.383 (3)	1.3878	A (1,7,5)	119.4 (2)	119.8531
R (6,12)	1.391 (3)	1.4038	A (1,7,18)	125.6 (2)	124.7365
R (6,13)	1.472 (3)	1.4708	A (5,7,18)	115.0 (2)	115.4104
R (6,17)	1.372 (2)	1.3781	A (5,8,9)	109.5	109.8901
R (7,18)	1.451 (3)	1.4593	A (5,8,10)	109.4	107.4694
R (8,9)	0.980	1.0900	A (5,8,11)	109.4	109.8914
R (8,10)	0.979	1.0853	A (9,8,10)	109.6	110.486
R (8,11)	0.980	1.0900	A (9,8,11)	109.5	108.6143
R (13,14)	0.980	1.0899	A (10,8,11)	109.5	110.4854
R (13,15)	0.980	1.0899	A (2,12,5)	122.0 (2)	121.6725
R (13,16)	0.980	1.0851	A (2,12,6)	121.3 (2)	121.7421
R (17,18)	1.428 (3)	1.4486	A (5,12,6)	116.6 (2)	116.5854
R (18,19)	1.410 (2)	1.4025	A (6,13,14)	109.4	109.7358
R (19,20)	1.490 (3)	1.5016	A (6,13,15)	109.5	109.7356
R (20,21)	0.990	1.0942	A (6,13,16)	109.5	107.6712
R (20,22)	0.990	1.0942	A (14,13,15)	109.5	108.676
R (20,23)	1.517 (3)	1.5288	A (14,13,16)	109.4	110.5068
R (23,24)	0.980	1.0922	A (15,13,16)	109.5	110.507
R (23,25)	0.980	1.0915	A (3,17,6)	118.0 (2)	118.5799
R (23,26)	0.980	1.0915	A (3,17,18)	122.9 (2)	122.9107
			A (6,17,18)	119.1 (2)	118.5094
			A (7,18,17)	120.3 (2)	120.1389
			A (7,18,19)	121.9 (2)	121.8316
			A (17,18,19)	117.8 (2)	118.0295
			A (4,19,18)	119.2 (2)	120.1114
			A (4,19,20)	115.0 (2)	114.661
			A (18,19,20)	125.8 (2)	125.2277
			A (19,20,21)	108.6	107.6702
			A (19,20,22)	108.7	107.6708
			A (19,20,23)	114.2 (2)	114.6173
			A (21,20,22)	107.7	103.2987
			A (21,20,23)	108.7	111.4397
			A (22,20,23)	108.7	111.4403
			A (20,23,24)	109.5	109.214
			A (20,23,25)	109.4	111.7744
			A (20,23,26)	109.5	111.7744
			A (24,23,25)	109.5	108.1569
			A (24,23,26)	109.5	108.1571
			A (25,23,26)	109.4	107.6318

Theoretical Calculations

According to the above crystal structure, a crystal unit was selected as the initial structure, while DFT-B3LYP/6-311G++(d,p) methods in Gaussian09 was used to optimize the structure of the title compound. Further, keto form of title compound was also optimized using Gaussian09. No solvent corrections were made with these calculations. Vibration analysis showed that the optimized structure indeed represents a minimum on the potential energy surface (no negative eigenvalues). A four-membered ring transition state was calculated which was confirmed using IRC calculations.

Table S2. Optimized Cartesian Coordinates (Å) of enol form for title compound.

# opt b3lyp/6-311++g(d,p) (HF = −760.87486944 a.u.)			
0 1			
O	−0.61415600	2.28424300	−0.00000500
O	3.47762000	0.28492700	−0.00021300
O	−0.17101600	−2.43068900	0.00015600
O	−2.45406100	−1.49715100	0.00006600
N	1.43203200	1.27760900	0.00012000
N	1.64613100	−1.08770900	−0.00002300
C	0.02118200	1.24096900	0.00004000
C	2.10576300	2.58480300	0.00012800
H	2.73500300	2.67767400	0.88528700
H	1.33481900	3.34867600	0.00030500
H	2.73474700	2.67784400	−0.88519400
C	2.26883400	0.17045200	−0.00006100
C	2.49429800	−2.28926800	−0.00008100
H	2.28334500	−2.88863100	−0.88559600
H	2.28340400	−2.88867000	0.88542100
H	3.52892800	−1.96212400	−0.00011100
C	0.27963200	−1.26589000	0.00008400
C	−0.57059000	−0.09300800	0.00003900
C	−1.95973200	−0.28598700	−0.00000100
C	−2.98645500	0.80979300	−0.00009400
H	−2.78143300	1.45696600	−0.85823500
H	−2.78148000	1.45707700	0.85796200
C	−4.43608700	0.32421300	−0.00010900
H	−5.10447400	1.18796900	−0.00018700
H	−4.66082000	−0.27969300	0.88091200
H	−4.66076100	−0.27981000	−0.88106400
H	−1.66659400	−2.14367100	0.00013000

Table S3. Optimized Cartesian Coordinates (Å) of keto form for title compound.

# opt b3lyp/6-311++g(d,p) (HF = −760.84960093 a.u.)			
0 1			
C	–0.03595400	1.30960200	–0.35734600
C	2.01450200	–0.02425000	0.00028000
C	–0.09232900	–1.26557800	–0.37034900
C	–0.74078600	0.04089700	–0.79630600
C	2.11535800	2.40799300	0.15313700
H	2.42217400	2.44549200	1.19911400
H	1.48604800	3.26201100	–0.07852300
C	2.01335700	–2.45974100	0.11210600
H	2.29889000	–2.53578100	1.16217700
H	1.35548400	–3.28243000	–0.15135200
N	1.32582300	1.19183500	–0.10513900
N	1.27717200	–1.20710500	–0.12981800
O	3.20263900	–0.04950100	0.23309500
O	–0.71657600	–2.30061500	–0.30843800
O	–0.61673100	2.37205100	–0.29739400
C	–2.26607700	0.05265400	–0.49060000
C	–2.74063400	0.35126900	0.91971700
H	–2.73613500	1.44463300	1.00338800
H	–3.78394400	0.03268200	0.96054500
O	–3.03274500	–0.14073500	–1.40006300
C	–1.93304000	–0.25699900	2.07250100
H	–2.38373800	0.02832400	3.02554800
H	–1.91437600	–1.34677900	2.01917100
H	–0.90000600	0.10364500	2.09370800
H	–0.68308100	0.04116300	–1.89288300
H	3.00501100	2.40033700	–0.47366800
H	2.91362900	–2.47108500	–0.49896100

Table S4. Optimized Cartesian Coordinates (Å) of transition state.

# opt = (calcfc,ts,noeigentest) b3lyp/6-311++g(d,p) (HF = −760.780416598 a.u.)			
0 1			
C	−0.06295000	−1.31148200	−0.13255000
C	−2.10326300	0.06710400	0.06433000
C	−2.10326300	0.06710400	0.06433000
C	0.06554400	1.22165200	−0.22232600
C	−2.27397400	−2.35820700	0.24336600
H	−2.69765500	−2.35219300	1.24860000
H	−1.63384700	−3.22651400	0.11619300
C	−2.03135400	2.50246100	0.07758100
H	−2.46131100	2.60072400	1.07521900
H	−1.30632700	3.29278400	−0.09417000
N	1.44419600	−1.16519700	0.03067000
N	−1.32405900	1.22128900	−0.05005500
O	−3.30678200	0.13255500	0.21668000
O	0.72499000	2.25141600	−0.17698600
O	0.49597500	−2.39371800	−0.00581400
C	2.12776100	−0.15961200	−0.56453100
C	3.12239000	−0.35632200	0.51128000
H	3.07264300	−1.43685100	0.71451500
H	4.11645500	−0.14714000	0.10947700
O	2.44068400	−0.08001100	−1.78113400
C	2.83189800	0.42274900	1.80238800
H	3.60660100	0.20459100	2.53933100
H	2.81428400	1.49737700	1.61905700
H	1.86966800	0.13200100	2.22872300
H	1.19942800	−0.04937600	−1.91507600
H	−3.08976700	−2.36982900	−0.47832800
H	−2.83638900	2.55082700	−0.65478700

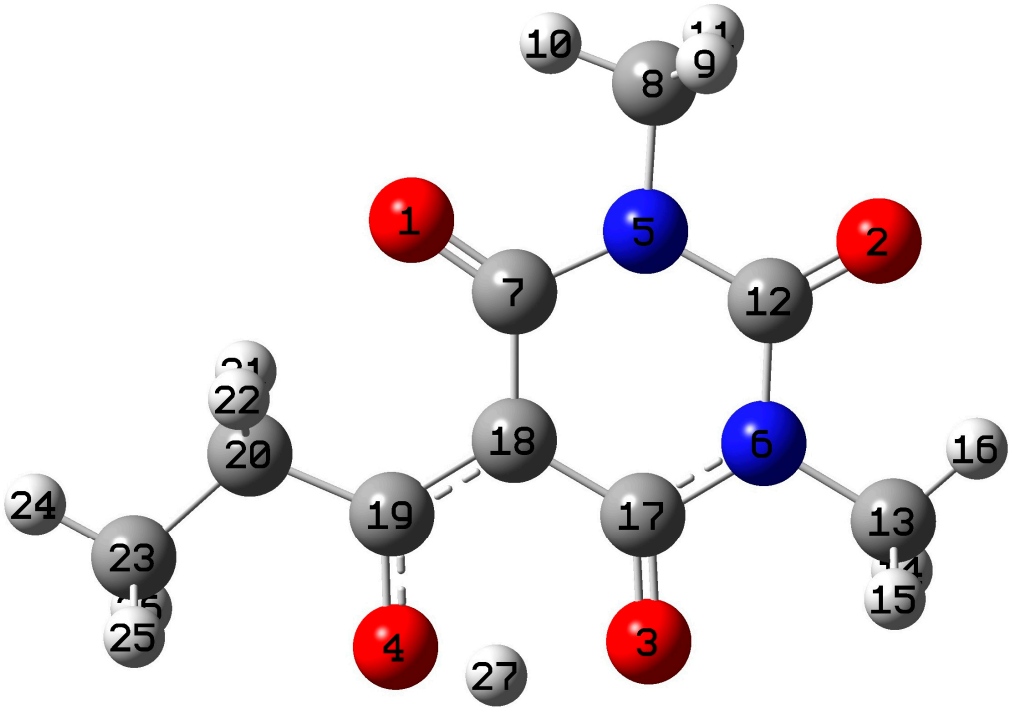
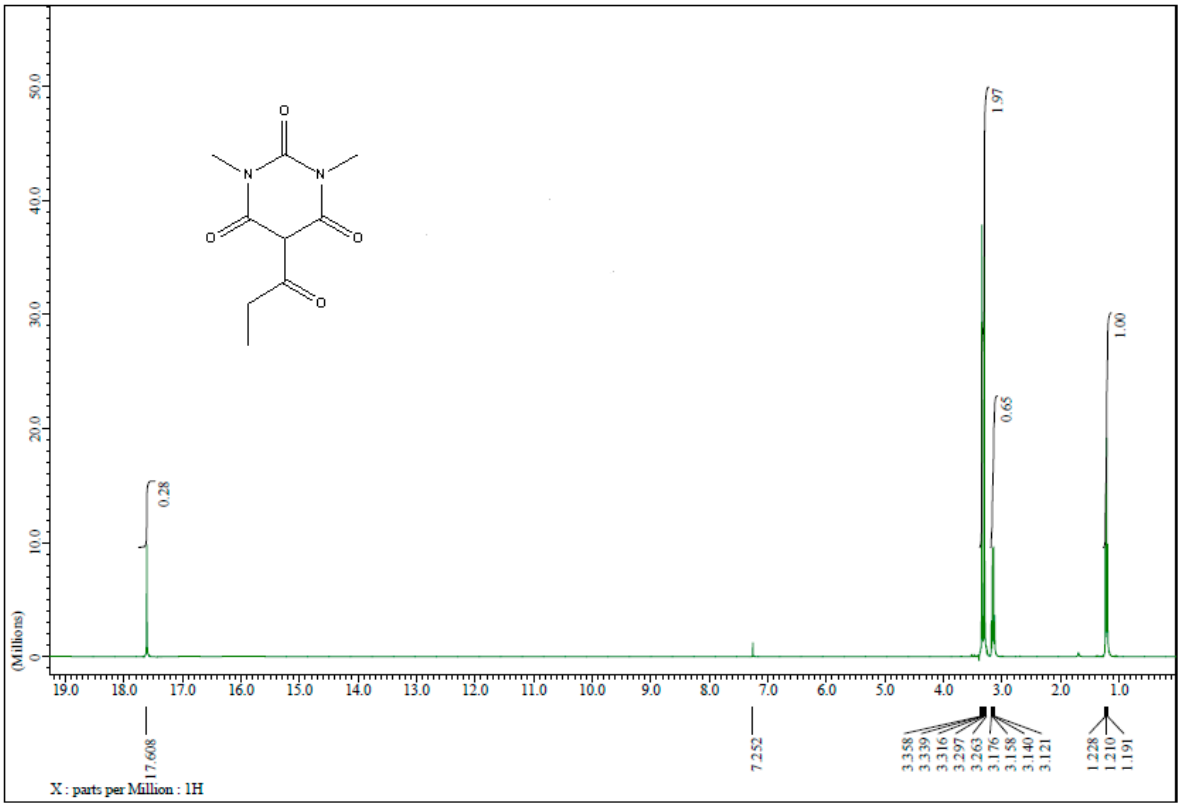


Figure S1. Optimized geometry of the title compound (B3LYP/6-311++G(d,p)).



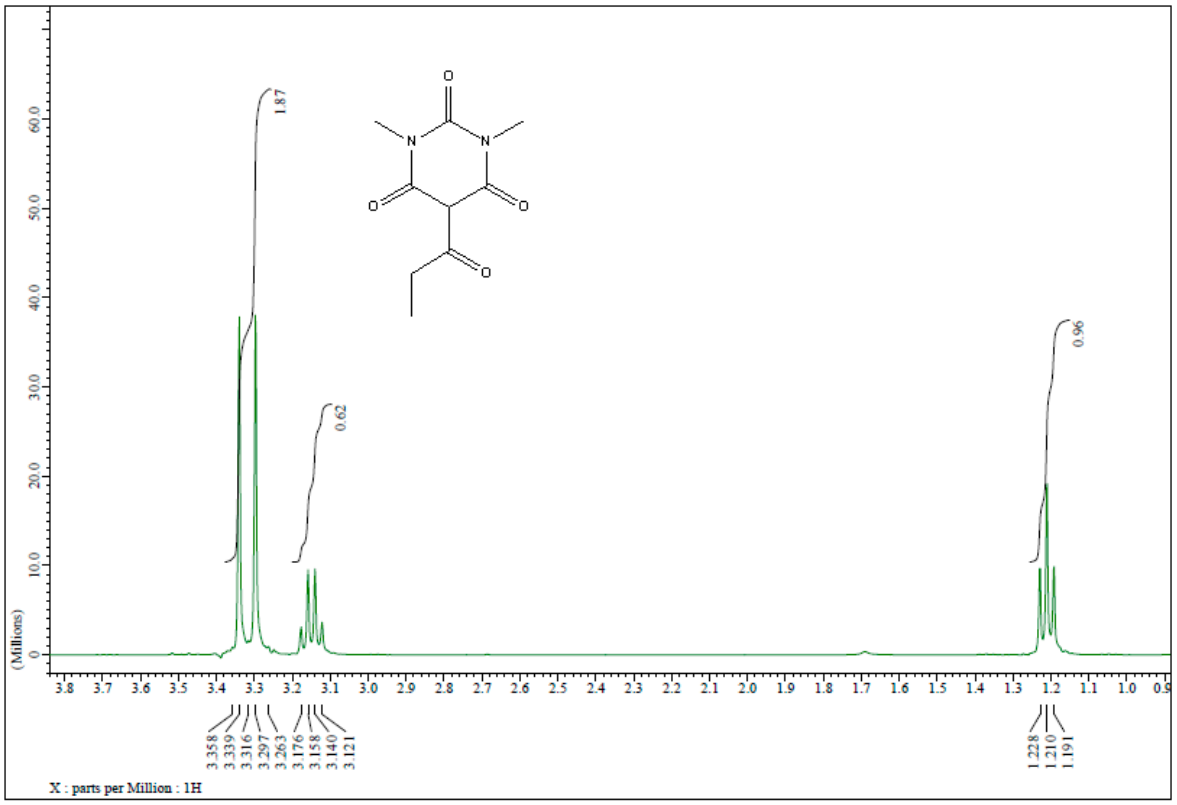
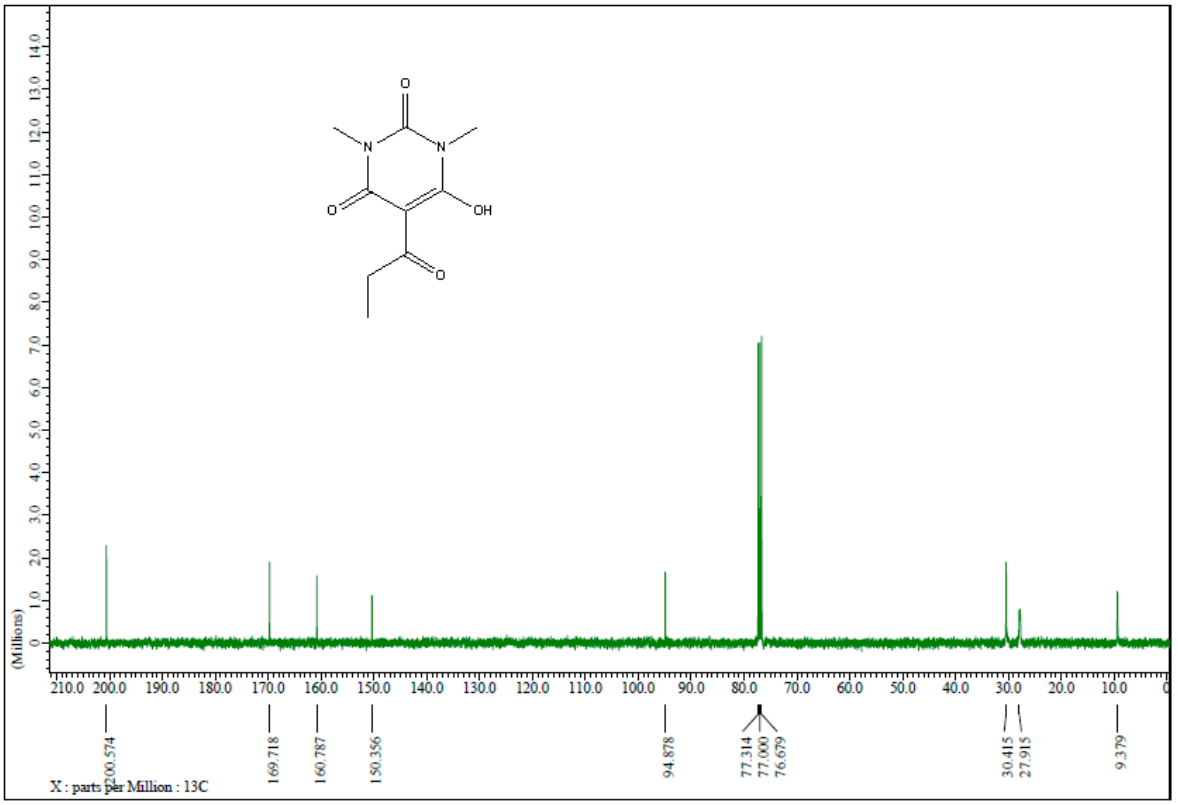


Figure S2. ^{1}H NMR of title compound in $CDCl_3$.



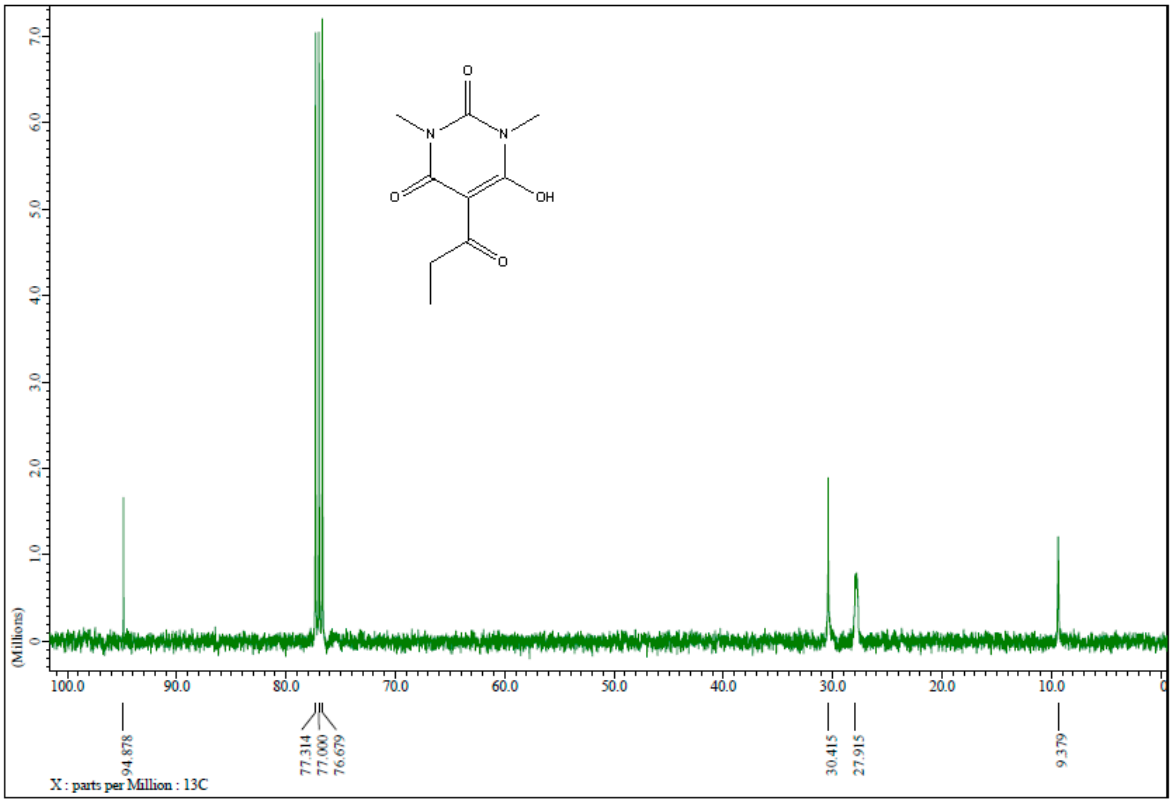
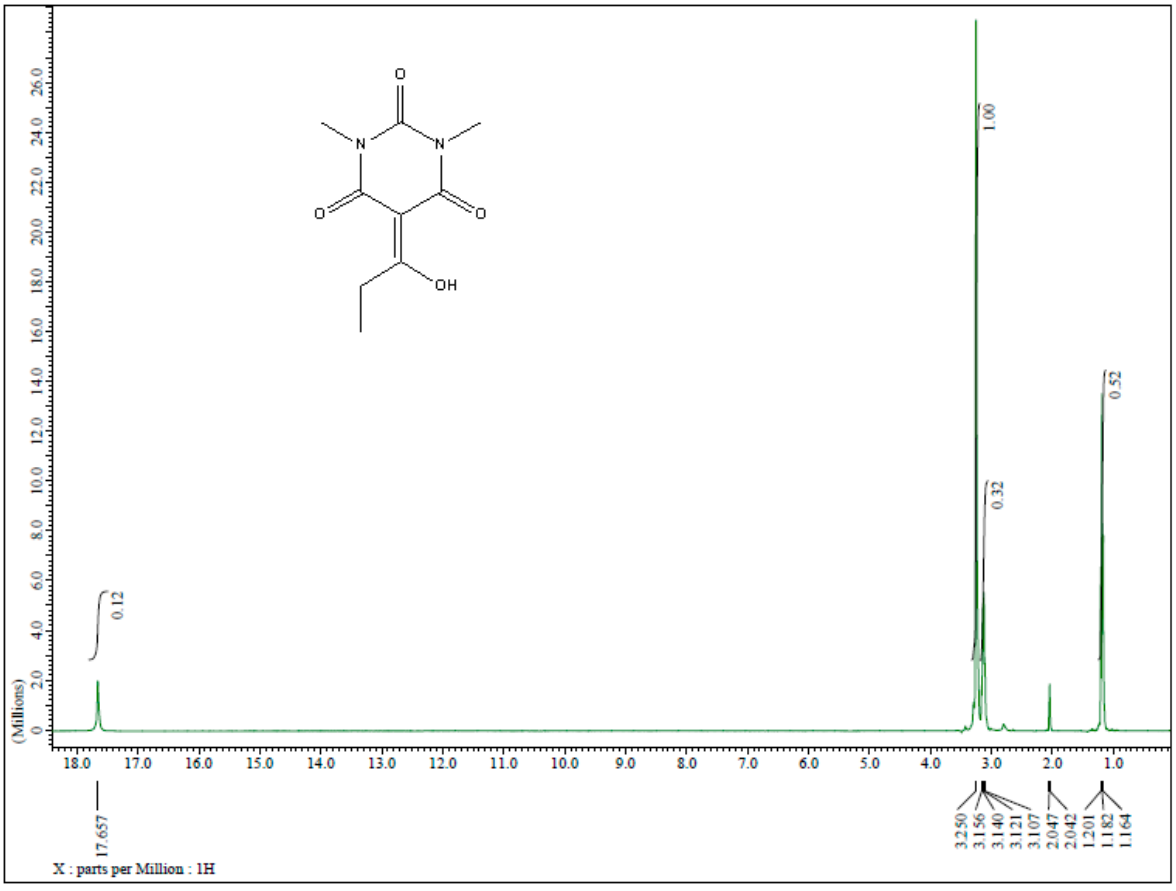


Figure S3. ^{13}C NMR of title compound in $CDCl_3$.



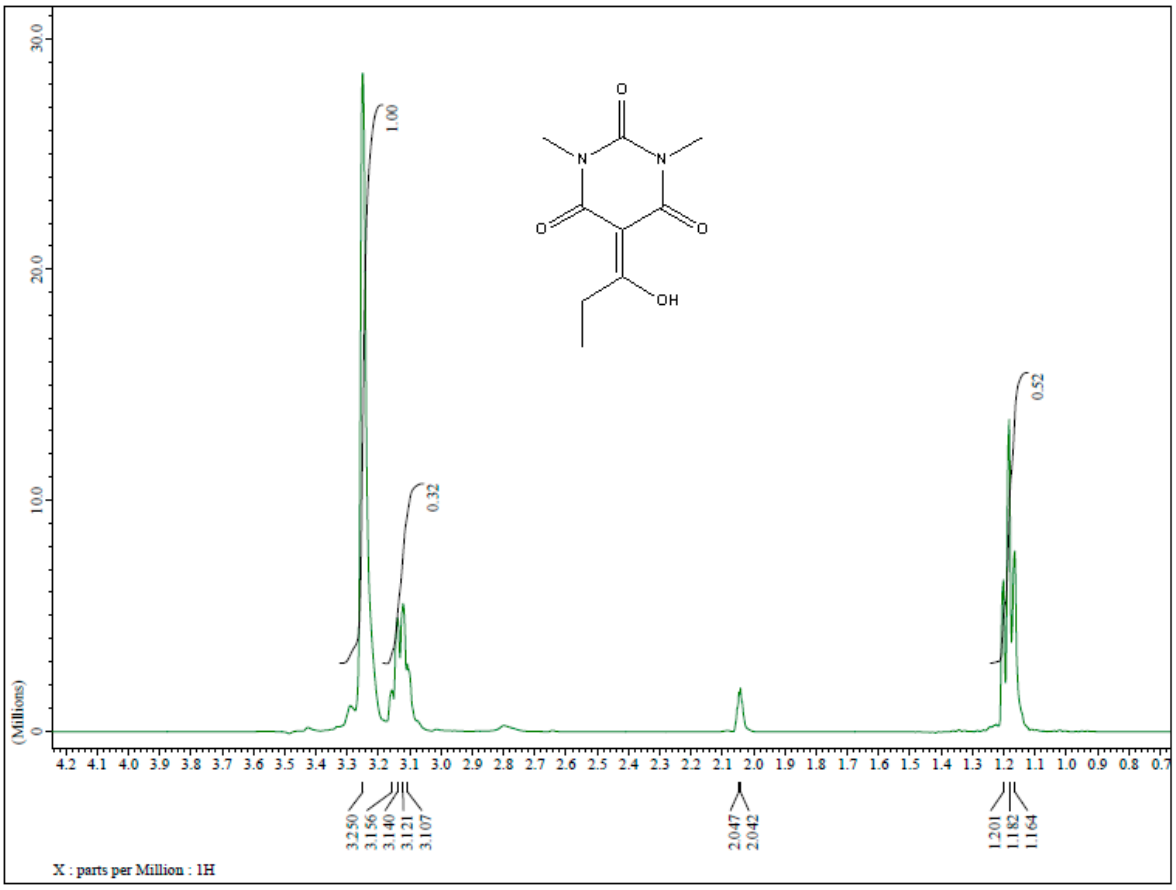
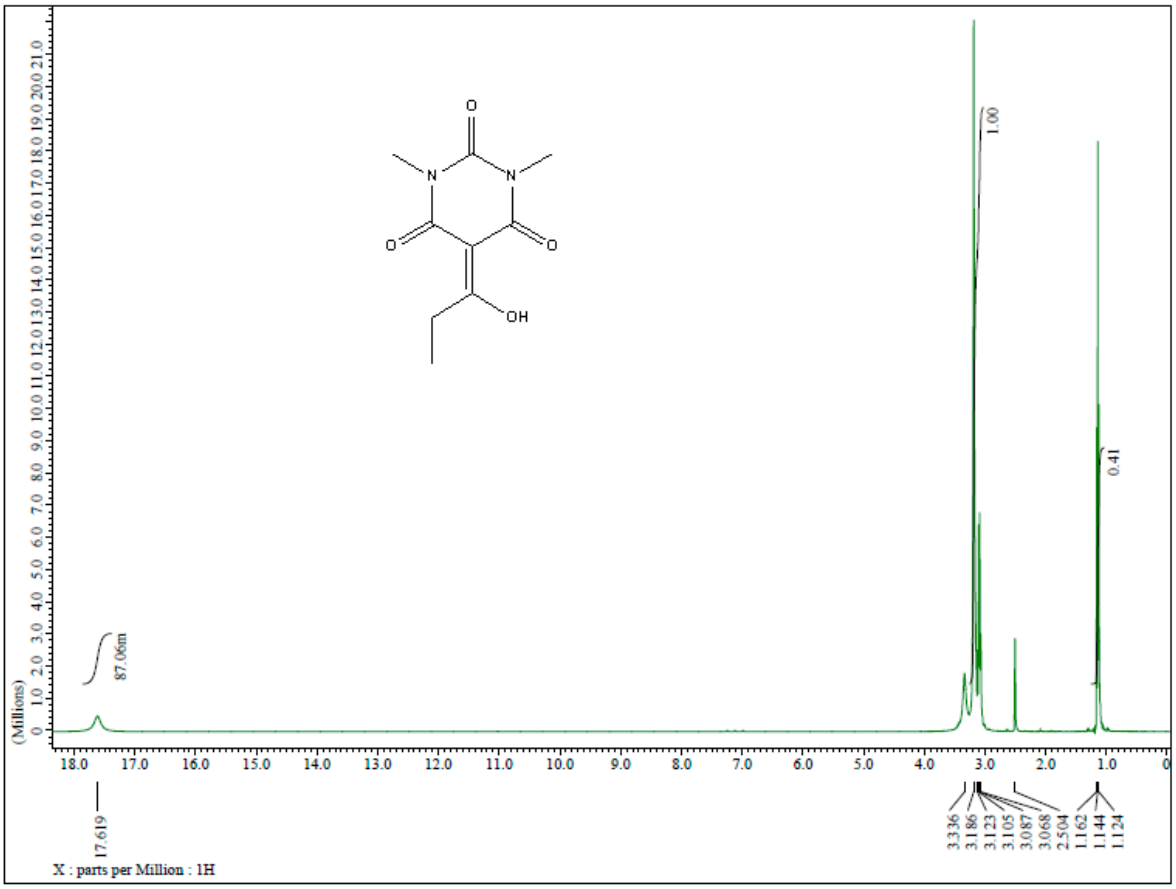


Figure S4. ^{1}H NMR of title compound in Acetone-d_6.



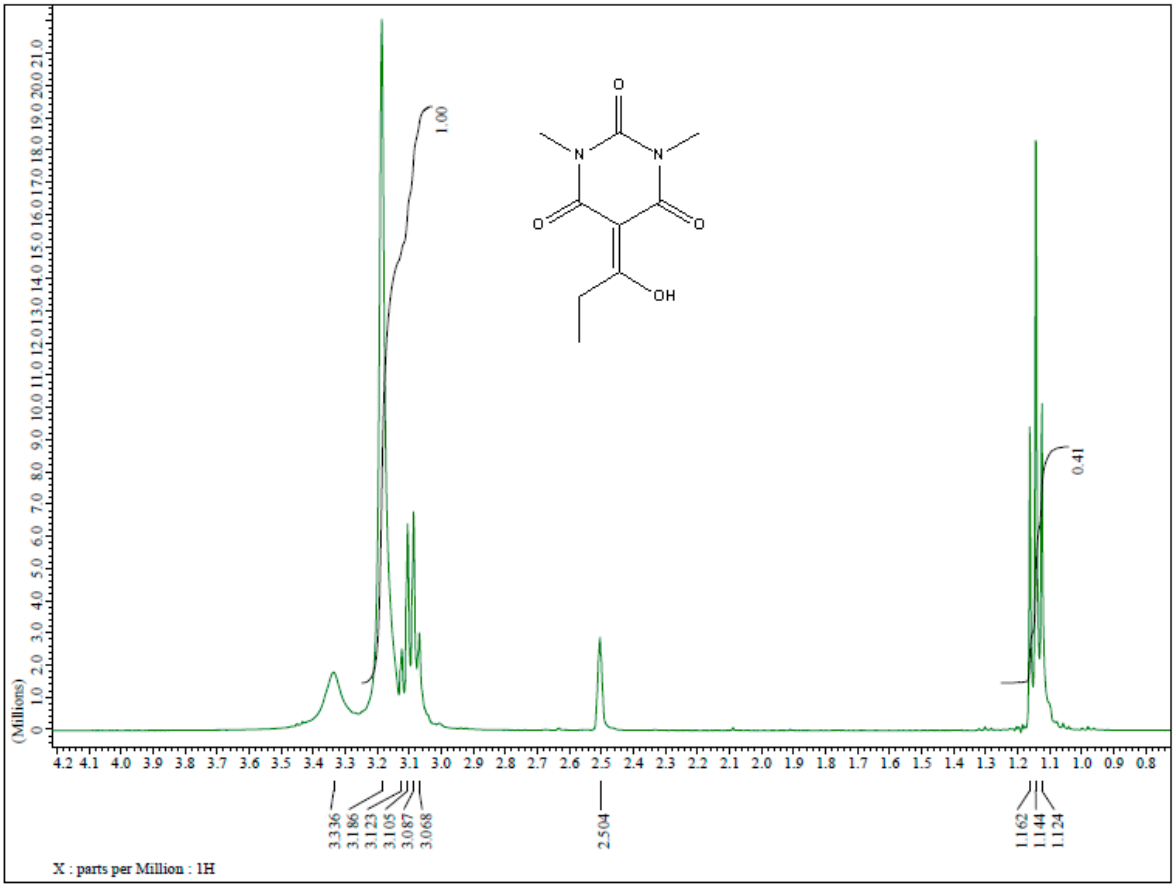


Figure S5. ^{1}H NMR of title compound in DMSO-d_6 at 20 °C.

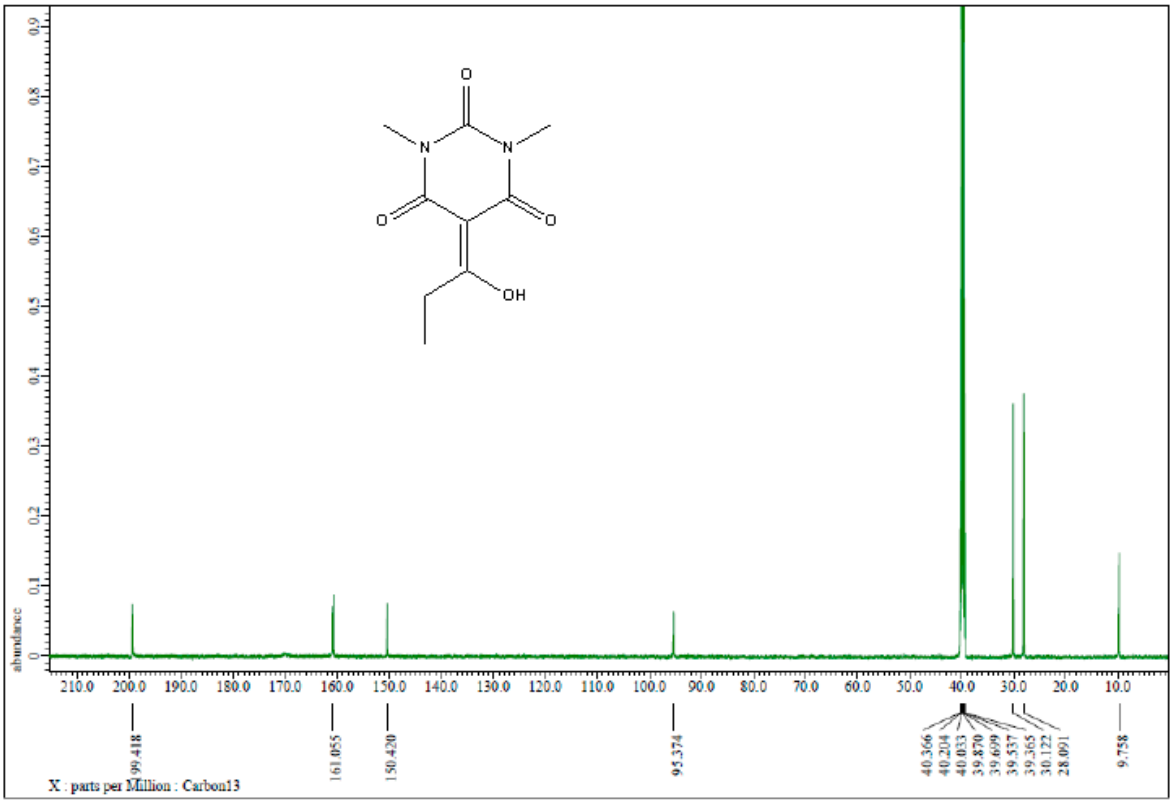


Figure S6. ^{13}C NMR of title compound in DMSO-d_6 at 20 °C

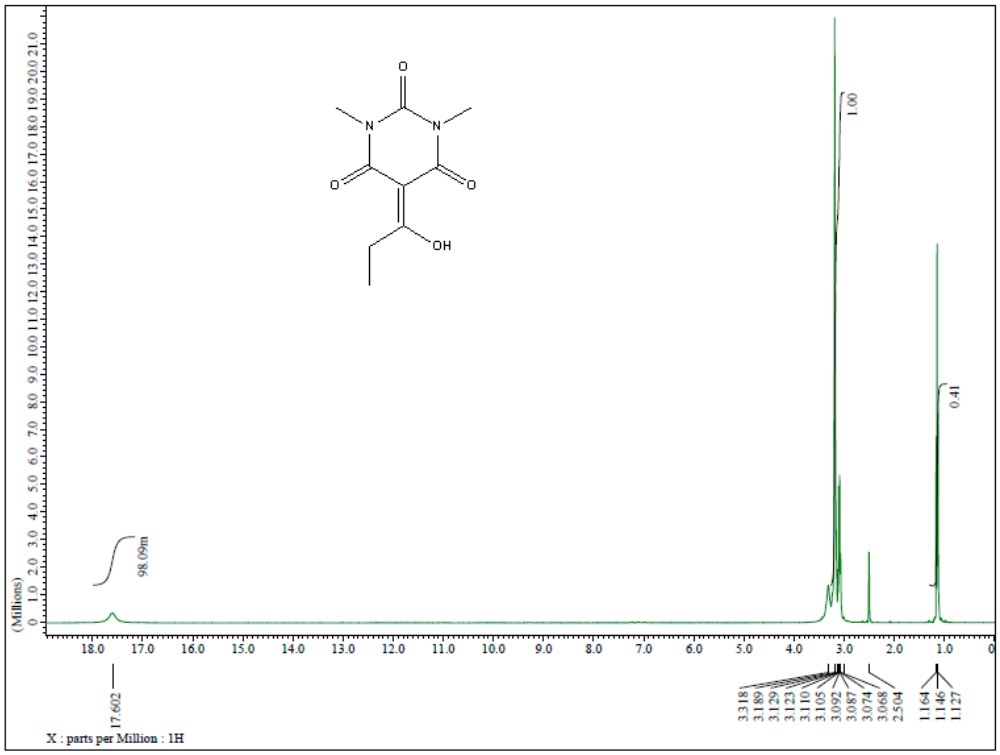


Figure S7. ^{1}H NMR of title compound in DMSO-d_6 at 30 °C.

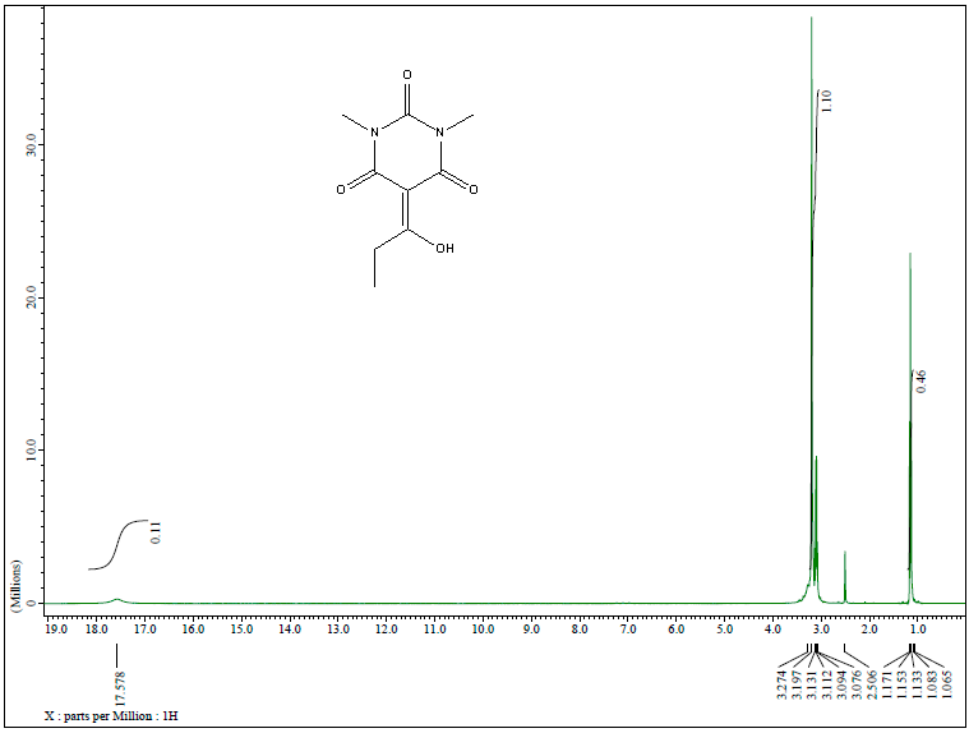


Figure S8. ^{1}H NMR of title compound in DMSO-d_6 at 40 °C.