J. Braz. Chem. Soc., Vol. 22, No. 10, 1939-1943, 2011.
Printed in Brazil - ©2011 Sociedade Brasileira de Química
0103 - 5053 $6.00+0.00

Article

A Concise Synthetic Method for 1,3,5-Triazinane-2,4-Dithiones

Zheng Li,* Hongfang Cai, Jingya Yang, Pengxian Niu and Chenhui Liu

College of Chemistry and Chemical Engineering, Northwest Normal University, Lanzhou, Gansu, 730070, P. R. China

1,3,5-Triazinane-2,4-ditionas foram sintetizadas eficientemente via condensação de 2 equiv. de 1-aril-tiouréa com 1 equiv. de ácidos carboxílicos alifáticos usando cloreto férrico hexahidratado como catalisador. Este protocolo tem as vantagens de alto rendimento, condições brandas e procedimento simples.

1,3,5-Triazinane-2,4-dithiones were efficiently synthesized via condensation of 2 equiv. of 1-arylthioureas with 1 equiv. of aliphatic carboxylic acids using ferric chloride hexahydrate as a catalyst. This protocol has the advantages of high yield, mild condition and simple procedure.

Keywords: 1,3,5-triazinane-2,4-dithione, 1,3,5-triazinane, thiourea, carboxylic acid, synthesis

Introduction

Heterocyclic compounds have long been known to exhibit remarkable biological and pharmacological properties.[1] Among the heterocycles, triazine derivatives have attracted much attention because they can connect with other molecules by hydrogen or coordination bond to form network supramolecular materials,[2] and they can serve as luminescent or n-type electron-carrying materials after connected with some substituents like diphenylacetylene, naphthalene and anthracene.[3] Triazine derivatives constitute well-known compounds that have been used as fungicidal,[4] antiplasmodial,[5] anti-HIV [6] and herbicidal agents,[7] and chiral discriminators,[8] hydrogen sulfide scavengers[9] and low-toxicity drug deliverers.[10] They were also applied in organic synthesis,[11] enantiodifferentiating coupling reagents,[12] catalysis,[13] molecular tectonics,[14] and polymeric materials.[15] Meanwhile, heterocycles containing a thiourea structural unit have a special place among pharmaceutically important natural and synthetic materials, showing powerful antiproliferative action,[16] antibacterial properties[17] and anticancer activity.[18] For these reasons, 1,3,5-triazinane derivatives incorporating thiourea unit may be important in many fields.

The general synthetic methods for 1,3,5-triazinane derivatives involve the reactions of *N*,*N'*-bis(arylmethylidene)arylmethane diimines with thioureas,[19] the multi-component reactions of phosphonates, nitriles, aldehydes and isocyanates,[20] the condensation of trifluoromethanesulfonamide with formaldehyde,[21] and the reactions of thiosemicarbazones with potassium thiocyanate and benzoyl chloride.[22] However, some methods use expensive reagents, toxic organic solvents, rigorous conditions, tedious workup procedure and long reaction time. Therefore, it is necessary to develop simple and efficient synthetic methods to 1,3,5-triazinane derivatives.

In this article, we report the synthesis of 1,3,5-triazinane-2,4-dithiones by reactions of 2 equiv. of 1-arylthioureas with 1 equiv. of aliphatic carboxylic acids using ferric chloride hexahydrate as a catalyst.

Results and Discussion

Initially, the synthesis of 1,3,5-triazinane-2,4-dithione was attempted by reaction of 1-phenylthiourea with acetic acid at room temperature under catalyst-free condition, however, no product was observed. Subsequently, the mixture of 1-phenylthiourea and acetic acid was heated at 80 °C for several hours, a new compound was isolated in low yield, which was identified to be a novel heterocyclic compound, 6-hydroxy-6-methyl-1,5-diphenyl-1,3,5-triazinane-2,4-dithione. In our further research, it was found that some Brønsted acids, such as *p*-toluenesulfonic acid (PTSA) and trichloroacetic acid (TCA), and Lewis acids, such as $AlCl_3$, $CuCl_2$, $NiCl_2$, $FeCl_3$ and $FeCl_3{\cdot}6H_2O$,

*e-mail: lizheng@nwnu.edu.cn

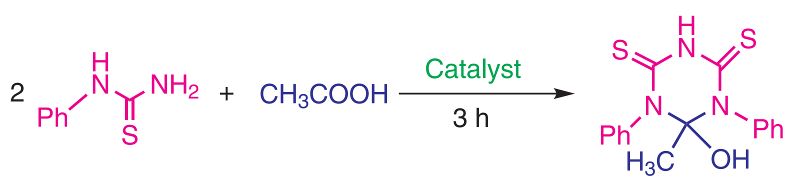
could efficiently catalyze the reaction (Table 1). Among them, $FeCl_3{\cdot}6H_2O$ could give the best yield if the reaction was carried out at 80 °C using 10 mol% amount of catalyst (Table 1, entry 8). In addition, in this reaction, acetic acid was acted as a reactant and solvent.

To explore the generality and scope of the synthetic reactions, and synthesis of a series of 6-hydroxy-6-alkyl-1,5-diaryl-1,3,5-triazinane-2,4-dithiones (Scheme 1), different 1-arylthioureas and aliphatic carboxylic acids as substrates were examined under optimal conditions (Table 2). It was found that various 1-arylthioureas could efficiently react with aliphatic carboxylic acids at 80 °C in the presence of $FeCl_3{\cdot}6H_2O$ to give the corresponding products in high yield. In comparison with 1-phenylthiourea, it was found that 1-arylthioureas including electron-donating groups, such as methyl and methoxyl, on the aromatic rings gave the corresponding products in higher yield and in faster rate (Table 2, entries 7-18). 1-Arylthioureas bearing electron-withdrawing substituents, such as chloro, on aromatic rings gave the corresponding product in slightly lower yield under similar conditions (Table 1, entry 19). Aliphatic carboxylic acids from C_2-C_7 were examined for the reactions, and afforded the corresponding products in high yield. In addition, aromatic carboxylic acids, such as various (un)substituted benzoic acids, were also attempted for the similar reactions, but no desired products were observed.

The resulting compounds 6-hydroxy-6-alkyl-1,5-diaryl-1,3,5-triazinane-2,4-dithiones are highly soluble in polar organic solvents including $CHCl_3$, CH_2Cl_2, DMSO, DMF and EtOH, but insoluble in toluene, benzene, ether and *n*-hexane. The structures of all compounds were identified by infrared (IR), ^1H and ^{13}C nuclear magnetic resonance (NMR) spectroscopies and elemental analysis. The ^1H NMR spectra of 6-hydroxy-6-alkyl-1,5-diaryl-1,3,5-triazinane-2,4-dithiones show the singlets of hydroxyls at 5.89-6.12 ppm and the multiplets of aromatic rings at 6.84-8.12 ppm. The IR spectra show the characteristic adsorption of hydroxyls at 3359-3450 cm^{-1}.

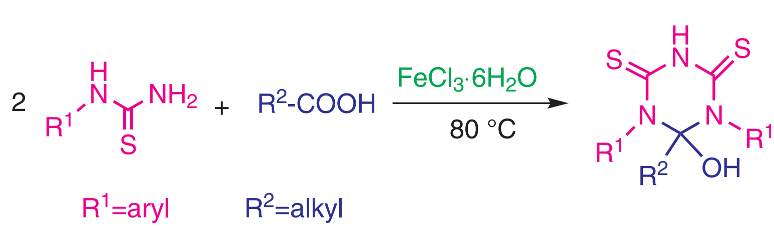
A possible mechanism for the synthesis of 1,3,5-triazinane-2,4-dithione is shown in Scheme 2.

Table 1. Synthesis of 6-hydroxy-6-methyl-1,5-diphenyl-1,3,5-triazinane-2,4-dithione under different conditions[a]



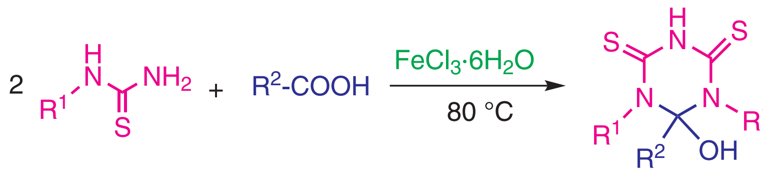
entry	Catalyst	Amount of catalyst / (mol%)	Temperature / °C	Yield / %[b]
1	–	0	80	10
2	PTSA	10	80	48
3	TCA	10	80	56
4	$AlCl_3$	10	80	51
5	$CuCl_2$	10	80	60
6	$NiCl_2$	10	80	70
7	$FeCl_3$	10	80	74
8	$FeCl_3{\cdot}6H_2O$	10	80	88
9	$FeCl_3{\cdot}6H_2O$	10	20	20
10	$FeCl_3{\cdot}6H_2O$	10	40	46
11	$FeCl_3{\cdot}6H_2O$	10	60	70
12	$FeCl_3{\cdot}6H_2O$	10	100	60
13	$FeCl_3{\cdot}6H_2O$	5	80	85
14	$FeCl_3{\cdot}6H_2O$	15	80	86

[a]Reaction conditions: 1-phenylthiourea (2 mmol), acetic acid (3 mmol) under different conditions; [b]isolated yields.



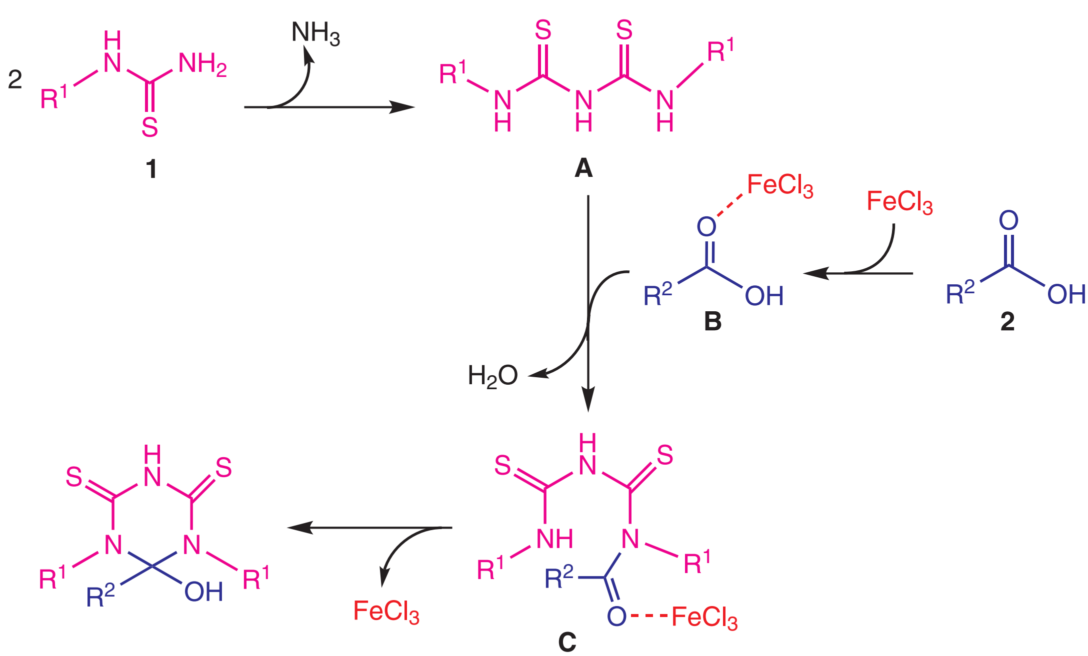
Scheme 1. Synthesis of 6-hydroxy-6-alkyl-1,5-diaryl-1,3,5-triazinane-2,4-dithiones.

Table 2 Synthesis of 6-hydroxy-6-alkyl-1,5-diaryl-1,3,5-triazinane-2,4-dithiones[a]



entry	R^1	R^2	time / h	mp / °C	Yield / %[b]
1	C_6H_5	CH_3	3	254-256	87
2	C_6H_5	C_2H_5	3	197-198	85
3	C_6H_5	*n*-C_3H_7	3	133-135	84
4	C_6H_5	*n*-C_4H_9	4	155-157	80
5	C_6H_5	*n*-C_5H_{11}	4	124-126	80
6	C_6H_5	*n*-C_6H_{13}	4	105-106	79
7	2-$CH_3C_6H_4$	CH_3	3	239-241	82
8	2-$CH_3C_6H_4$	C_2H_5	3	160-162	88
9	2-$CH_3C_6H_4$	*n*-C_3H_7	3	154-155	83
10	2-$CH_3C_6H_4$	*n*-C_4H_9	4	123-124	85
11	4-$CH_3C_6H_4$	C_2H_5	2	119-121	88
12	4-$CH_3C_6H_4$	*n*-C_3H_7	2	127-129	90
13	4-$CH_3C_6H_4$	*n*-C_4H_9	2	126-127	86
14	4-$CH_3C_6H_4$	*n*-C_5H_{11}	3	111-113	80
15	4-$CH_3C_6H_4$	*n*-C_6H_{13}	3	103-104	81
16	4-$CH_3OC_6H_4$	CH_3	3	218-219	80
17	4-$CH_3OC_6H_4$	C_2H_5	4	243-245	84
18	4-$CH_3OC_6H_4$	*n*-C_3H_7	4	219-221	78
19	4-ClC_6H_4	CH_3	4	208-210	66

[a]Reaction conditions: 1-arylthiourea (2 mmol), aliphatic carboxylic acid (3 mmol) and ferric chloride hexahydrate (0.2 mmol) at 80 °C; [b]isolated yields.



Scheme 2. The possible mechanism for the synthesis of 1,3,5-triazinane-2,4-dithiones.

Presumably, condensation of 2 equiv. of 1-arylthiourea **1** releasing a mole of ammonia first generates an intermediate **A**. One of amino groups of **A** subsequent reacts with a mole of complex **B**, which is formed from aliphatic carboxylic acid **2** and ferric chloride in the solution, to give intermediate **C** by loss of water. Subsequently the carbonyl group of **C** undergoes the nuleophilic addition of its amino group by releasing ferric chloride to form a six-membered heterocyclic compound, 1,3,5-triazinane-2,4-dithione **3**.

Conclusion

An efficient and concise method has been developed for the synthesis of 1,3,5-triazinane-2,4-dithiones via condensation of 2 equiv. of 1-arylthioureas with 1 equiv. of aliphatic carboxylic acids using ferric chloride hexahydrate as a catalyst. This protocol has the advantages of high yield, mild condition and simple procedure.

Experimental

IR spectra were recorded using KBr pellets on an Alpha Centauri FTIR spectrophotometer and ^{1}H and ^{13}C NMR spectra on a Mercury-400BB instrument using $CDCl_3$ or DMSO-d_6 as solvents and Me_4Si as internal standard. Melting points (mp) were observed in an electrothermal melting point apparatus. Flash column chromatography was carried out using 200-300 mesh silica gel at increased pressure. Aromatic thioureas were synthesized according to the literature methods.[23]

General procedure for the preparation of 6-hydroxy-6-alkyl-1,5-diaryl-1,3,5-triazinane-2,4-dithiones

The mixture of 1-arylthioureas (2 mmol), aliphatic carboxylic acids (3 mmol) and ferric chloride hexahydrate (0.2 mmol) was heated at 80 °C for appropriate time according to Table 2. The progress of the reactions was monitored by TLC (thin layer chromatography). After the completion of the reactions, the systems were cooled to room temperature, and the mixture was subjected to silica gel flash column chromatography (ethyl acetate, petroleum ether, 1:6) to obtain pure products.

Supplementary Information

Full set of characterization data (IR, ^{1}H and ^{13}C NMR spectra) are available free of charge at http://jbcs.sbq.org.br as PDF file.

Acknowledgements

The authors thank the National Natural Science Foundation of China (20772096) and Key Laboratory of Polymer Materials of Gansu Province for the financial support of this work.

References

1. Menicagli, R.; Samaritani, S.; Signore, G.; Vaglini, F.; Via, L. D.; *J. Med. Chem.* **2004**, *47*, 4649; Franzen, R. G.; *J. Comb. Chem.* **2000**, *2*, 195; Nefzi, A.; Ostresh, J. M.; Houghten, R. A.; *Chem. Rev.* **1997**, *97*, 449.
2. Cai, Y. Q.; Wu, W.; Wang, H.; Miyake, J.; Qian, D. J.; *Surf. Sci.* **2011**, *605*, 321.
3. Kostas, I. D.; Andreadaki, F. J.; Medlycott, E. A.; Hanan, G. S.; Monflier, E.; *Tetrahedron Lett.* **2009**, *50*, 1851; Lee, C. H.; Yamamoto, T.; *Tetrahedron Lett.* **2001**, *42*, 3993.
4. Ibrahim, M. A.; Abdel-Rahman, R. M.; Abdel-Halim, A. M.; Ibrahim, S. S.; Allimony, H. A.; *J. Braz. Chem. Soc.* **2009**, *20*, 1275.
5. Klenke, B.; Barrett, M. P.; Brun, R.; Gilbert, I. H.; *J. Antimicrob. Chemother.* **2003**, *52*, 290.
6. Patel, R. B.; Chikhalia, K. H.; Pannecouque, C.; Clercq, E.; *J. Braz. Chem. Soc.* **2007**, *18*, 312.
7. Soong, C. L.; Ogawa, J.; Sakuradani, E.; Shimizu, S.; *J. Biol. Chem.* **2002**, *227*, 7051.
8. Sugimoto, H.; Yamane, Y.; Inoue, S.; *Tetrahedron: Asymmetry* **2000**, *11*, 2067.
9. Bakke, J. M.; Buhaug, J. B.; *Ind. Eng. Chem. Res.* **2004**, *43*, 1962.
10. Murray, A. P.; Miller, M. J.; *J. Org. Chem.* **2003**, *68*, 191; Ghosh, M.; Miller, M. J.; *J. Org. Chem.* **1994**, *59*, 1020.
11. Falorni, M.; Porcheddu, A.; Taddei, M.; *Tetrahedron Lett.* **1999**, *40*, 4395; Luca, L. D.; Giacomelli, G.; Taddei, M.; *J. Org. Chem.* **2001**, *66*, 2534; Babak, K.; Hazarkhani, H.; *Synthesis* **2003**, 2547; Dang, Q.; Gomez-Galeno, J. E.; *J. Org. Chem.* **2002**, *67*, 8703.
12. Kaminski, Z. J.; Kolesinska, B.; Kaminska, J. E.; Gora, J.; *J. Org. Chem.* **2001**, *66*, 6276.
13. Omotowa, B. A.; Shreeve, J. M.; *Organometallics* **2004**, *23*, 783; Graeme, C.; Cremiers, H. A.; Rotello, V. M.; Tarbitc, B.; Vanderstraetena, P. E.; *Tetrahedron* **2001**, *57*, 2787.
14. Fournier, J. H.; Maris, T.; Wuest, J. D.; *J. Org. Chem.* **2004**, *69*, 1762; Laliberte, D.; Maris, T.; Wuest, J. D.; *J. Org. Chem.* **2004**, *69*, 1776.
15. Brunsveld, L.; Vekemans, J. A. J. M.; Hirschberg, J. H. K. K.; Sijbesma, R. P.; Meijer, E. W.; *Proc. Natl. Acad. Sci. U.S.A.* **2002**, *99*, 4977.
16. Figueiredo, I. M.; Santos, L. V.; Costa, W. F.; Carvalho, J. E.; Silva, C. C.; Sacoman, J. L.; Kohn, L. K.; Sarragiotto, M. H.; *J. Braz. Chem. Soc.* **2006**, *17*, 954.
17. Han, T.; Cho, J. H.; Oh, C. H.; *Eur. J. Med. Chem.* **2006**, *41*, 825.
18. Yan, K.; Lok, C. N.; Bierla, K.; Che, C. M.; *Chem. Commun.* **2010**, *46*, 7691.
19. Kaboudin, B.; Ghasemi, T.; Yokomatsu, T.; *Synthesis* **2009**, 3089.

20. Groenendaal, B.; Vugts, D. J.; Schmitz, R. F.; Kanter, F. J. J.; Ruijter, E.; Groen, M. B.; Orru, R. V. A.; *J. Org. Chem.* **2008**, *73*, 719.
21. Meshcheryakov, V. I.; Albanov, A. I.; Shainyan, B. A.; *Russ. J. Org. Chem. (Engl. Transl.)* **2005**, *41*, 1381.
22. Ali, T. E. S.; Abdel-Monem, W. R.; *Phosphorus, Sulfur, Silicon Relat. Elem.* **2008**, *183*, 2161.
23. Thanigaimalai, P.; Hoang, T. A. L.; Lee, K. C.; Bang, S. C.; Sharma, V. K.; Yun, C. Y.; Roh, E.; Hwang, B. Y.; Kim, Y.; Jung, S. H.; *Bioorg. Med. Chem. Lett.* **2010**, *20*, 2991; Ubarhande, S. S.; Thakare, V. G.; Berad, B. N.; *J. Indian Chem. Soc.* **2010**, *87*, 1137.

Submitted: May 13, 2011
Published online: August 11, 2011

J. Braz. Chem. Soc., Vol. 22, No. 10, S1-S32, 2011.
Printed in Brazil - ©2011 Sociedade Brasileira de Química
0103 - 5053 $6.00+0.00

Supplementary Information

SI

A Concise Synthetic Method for 1,3,5-Triazinane-2,4-Dithiones

Zheng Li,* Hongfang Cai, Jingya Yang, Pengxian Niu and Chenhui Liu

College of Chemistry and Chemical Engineering, Northwest Normal University, Lanzhou, Gansu, 730070, P. R. China

General procedure for the preparation of 6-hydroxy-6-alkyl-1,5-diaryl-1,3,5-triazinane-2,4-dithiones

The mixture of 1-arylthioureas (2 mmol), aliphatic carboxylic acids (3 mmol) and ferric chloride hexahydrate (0.2 mmol) was heated at 80 °C for appropriate time according to Table 2. The progress of the reactions was monitored by TLC (thin layer chromatography). After the completion of the reactions, the systems were cooled to room temperature, and the mixture was subjected to silica gel flash column chromatography (ethyl acetate, petroleum ether, 1:6) to obtain pure products. The spectral data and scanned spectra for products are given below.

*6-Hydroxy-6-methyl-1,5-diphenyl-1,3,5-triazinane-2,4-dithione (**1**)*

White solid, mp 254-256 °C; IR (KBr) ν_{max}/cm^{-1} 3409, 2925, 2861, 1614, 1582, 1533, 1473, 1442, 1301, 1251, 1157, 759, 697; ^{1}H NMR ($CDC1_3$, 400 MHz) δ 7.06-7.71 (m, 10H, Ph-H), 6.10 (s, 1H, OH), 2.24 (s, 3H, CH_3); ^{13}C NMR (DMSO-d_6, 100 MHz) δ 181.6, 177.4, 147.8, 139.3, 134.2, 130.0, 129.9 (2C), 128.7 (2C), 128.4 (2C), 122.7, 120.0 (2C), 25.9; Anal. calcd. for $C_{16}H_{15}N_3OS_2$: C, 58.33; H, 4.59; N, 12.76; Found: C, 58.22; H, 4.57; N, 12.73.

*6-Hydroxy-6-ethyl-1,5-diphenyl-1,3,5-triazinane-2,4-dithione (**2**)*

White solid, mp 197-198 °C; IR (KBr) ν_{max}/cm^{-1} 3359, 3064, 2986, 2915, 1616, 1579, 1539, 1483, 1443, 1350, 1216, 1060, 750, 690; ^{1}H NMR ($CDC1_3$, 400 MHz) δ 7.05-7.71 (m, 10H, Ph-H), 6.11 (s, 1H, OH), 2.51 (q, 2H, *J* 7.6 Hz, CH_2), 1.13 (t, 3H, *J* 7.6 Hz, CH_3); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 186.7, 177.3, 145.7, 137.8, 133.8, 130.8 (3C), 129.2 (2C), 128.2 (2C), 123.7, 118.8 (2C), 32.30, 9.50; Anal. calcd. for $C_{17}H_{17}N_3OS_2$: C, 59.45; H, 4.99; N, 12.23; Found: C, 59.54; H, 4.98; N, 12.19.

*e-mail: lizheng@nwnu.edu.cn

*6-Hydroxy-6-propyl-1,5-diphenyl-1,3,5-triazinane-2,4-dithione (**3**)*

White solid, mp 133-135 °C; IR (KBr) ν_{max}/cm^{-1} 3410, 3054, 2960, 2927, 2862, 1601, 1586, 1543, 1475, 1442, 1377, 1349, 1282, 1231, 1210, 1157, 751, 690; ^{1}H NMR ($CDC1_3$, 400 MHz) δ 7.05-7.71 (m, 10H, Ph-H), 6.11 (s, 1H, OH), 2.47 (t, 2H, *J* 7.4 Hz, CH_2), 1.60-1.68 (m, 2H, CH_2), 0.90 (t, 3H, *J* 7.4 Hz, CH_3); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 185.9, 177.2, 145.7, 137.7, 133.8, 130.7 (3C), 129.1 (2C), 128.1 (2C), 123.7, 118.8 (2C), 41.0, 18.8, 13.9; Anal. calcd. for $C_{18}H_{19}N_3OS_2$: C, 60.47; H, 5.36; N, 11.75; Found C, 60.50; H, 5.35; N, 11.74.

*6-Hydroxy-6-butyl-1,5-diphenyl-1,3,5-triazinane-2,4-dithione (**4**)*

White solid, mp 155-157 °C; IR (KBr) ν_{max}/cm^{-1} 3418, 3059, 2949, 2864, 1617, 1602, 1585, 1541, 1477, 1443, 1349, 1290, 1204, 752, 694; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.05-7.71 (m, 10H, Ph-H), 6.11 (s, 1H, OH), 2.49 (t, 2H, *J* 7.4 Hz, CH_2), 1.57-1.64 (m, 2H, CH_2), 1.26-1.33 (m, 2H, CH_2), 0.87 (t, 3H, *J* 7.4 Hz, CH_3); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 186.1, 177.2, 145.7, 137.7, 133.8, 130.7 (3C), 129.1 (2C), 128.1 (2C), 123.7, 118.8 (2C), 38.8, 27.5, 22.4, 13.9; Anal. calcd. for $C_{19}H_{21}N_3OS_2$: C, 61.42; H, 5.70; N, 11.31; Found C, 61.54; H, 5.71; N, 11.29.

*6-Hydroxy-6-pentyl-1,5-diphenyl-1,3,5-triazinane-2,4-dithione (**5**)*

White solid, mp 124-126 °C; IR (KBr) ν_{max}/cm^{-1} 3448, 2955, 2927, 2864, 1616, 1578, 1539, 1513, 1480, 1441, 1350, 1245, 1201, 752, 692; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.05-7.70 (m, 10H, Ph-H), 6.12 (s, 1H, OH), 2.48 (t, 2H, *J* 7.4 Hz, CH_2), 1.60-1.64 (m, 2H, CH_2), 1.26-1.27 (m, 4H, CH_2), 0.85 (t, 3H, *J* 7.4 Hz, CH_3); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 186.1, 177.2, 145.7, 137.7, 133.8, 130.7 (3C), 129.1 (2C), 128.1 (2C), 123.7, 118.8 (2C), 39.0, 31.5, 25.0, 22.4, 13.9; Anal. calcd. for $C_{20}H_{23}N_3OS_2$: C, 62.30; H, 6.01; N, 10.90; Found C, 62.22; H, 5.99; N, 10.88.

*6-Hydroxy-6-hexyl-1,5-diphenyl-1,3,5-triazinane-2,4-dithione (**6**)*

White solid, mp 105-106 °C; IR (KBr) ν_{max}/cm^{-1}: 3450, 2945, 2921, 2850, 1614, 1577, 1539, 1481, 1439, 1348, 1299, 1240, 1199, 752, 692; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.05-7.71 (m, 10H, Ph-H), 6.11 (s, 1H, OH), 2.48 (t, 2H, *J* 7.4 Hz, CH_2), 1.58-1.63 (m, 2H, CH_2), 1.22-1.31 (m, 6H, CH_2), 0.85 (t, 3H, *J* 7.4 Hz, CH_3); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 186.1, 177.2, 145.7, 137.7, 133.8, 130.7 (2C), 129.1 (2C), 128.5 (2C), 128.1, 123.7, 118.8 (2C), 39.1, 31.6, 29.0, 25.3, 22.5, 14.0; Anal. calcd. for $C_{21}H_{25}N_3OS_2$: C, 63.12; H, 6.31; N,10.52; Found C, 63.01; H, 6.30; N, 10.47.

*6-Hydroxy-6-methyl-1,5-di(2-methylphenyl)-1,3,5-triazinane-2,4-dithione (**7**)*

White solid, mp 239-241 °C; IR (KBr) ν_{max}/cm^{-1} 3415, 2961, 2925, 2856, 1617, 1587, 1544, 1484, 1455, 1363, 1300, 1256, 752; ^{1}H NMR ($CDC1_3$, 400 MHz) δ 8.11 (d, 1H, *J* 8.4 Hz, Ph-H), 7.00-7.59 (m, 7H, Ph-H), 5.89 (s, 1H, OH), 2.24 (s, 3H, CH_3), 2.20 (s, 3H, CH_3), 1.88 (s, 3H, CH_3); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 183.3, 176.9, 145.8, 136.9, 135.9, 132.7, 132.4, 131.3, 130.5, 128.3, 128.1, 127.2, 126.7, 124.1, 119.9, 26.1, 17.5, 16.9; Anal. calcd. for $C_{18}H_{19}N_3OS_2$: C, 60.47; H, 5.36; N, 11.75; Found C, 60.53; H, 5.35; N, 11.71.

*6-Hydroxy-6-ethyl-1,5-di(2-methylphenyl)-1,3,5-triazinane-2,4-dithione (**8**)*

White solid, mp 160-162 °C; IR (KBr) ν_{max}/cm^{-1} 3413, 3061, 2972, 2925, 2860, 1618, 1587, 1549, 1489, 1456, 1371, 1226, 748; ^{1}H NMR ($CDC1_3$, 400 MHz) δ 8.10 (d, 1H, *J* 8.0 Hz, Ph-H), 6.97-7.58 (m, 7H, Ph-H), 5.90 (s, 1H, OH), 2.53 (q, 2H, *J* 7.4 Hz, CH_2), 2.17 (s, 3H, CH_3), 1.88 (s, 3H, CH_3), 1.13 (t, 3H, *J* 7.4 Hz, CH_3); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 186.7, 176.6, 145.8, 137.0, 135.9, 132.7, 132.3, 131.2, 130.5, 128.2, 128.1, 127.2, 126.7, 124.1, 119.9, 32.3, 17.5, 16.9, 9.5; Anal. calcd. for $C_{19}H_{21}N_3OS_2$: C, 61.42; H, 5.70; N, 11.31; Found C, 61.47; H, 5.69; N, 11.28.

*6-Hydroxy-6-propyl-1,5-di(2-methylphenyl)-1,3,5-triazinane-2,4-dithione (**9**)*

White solid, mp 154-155 °C; IR (KBr) ν_{max}/cm^{-1} 3409, 3009, 2963, 2928, 2841, 1609, 1547, 1511, 1468, 1366, 1300, 1254, 668; ^{1}H NMR ($CDC1_3$, 400 MHz) δ 8.10 (d, 1H, *J* 8.4 Hz, Ph-H), 7.00-7.56 (m, 7H, Ph-H), 5.89 (s, 1H, OH), 2.47 (t, 2H, *J* 7.6 Hz, CH_2), 2.20 (s, 3H, CH_3), 1.88 (s, 3H, CH_3), 1.62-1.68 (m, 2H, CH_2), 0.90 (t, 3H, *J* 7.2 Hz, CH_3); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 186.0, 176.6, 145.8, 137.0, 135.9, 132.7, 132.3, 131.2, 130.5, 128.2, 128.1, 127.2, 126.7, 124.1, 119.9, 41.0, 18.9, 17.5, 16.9, 13.8; Anal. calcd. for $C_{20}H_{23}N_3OS_2$: C, 62.30; H, 6.01; N, 10.90; Found C, 62.15; H, 5.99; N, 10.87.

*6-Hydroxy-6-butyl-1,5-di(2-methylphenyl)-1,3,5-triazinane-2,4-dithione (**10**)*

White solid, mp 123-124 °C; IR (KBr) ν_{max}/cm^{-1} 3383, 2961, 2924, 2857, 1600, 1535, 1512, 1471, 1408, 1341, 1240, 1201, 1070, 804; ^{1}H NMR ($CDC1_3$, 400 MHz) δ 8.09 (d, 1H, *J* 8.0 Hz, Ph-H), 6.99-7.56 (m, 7H, Ph-H), 5.90 (s, 1H, OH), 2.49 (t, 2H, *J* 7.6 Hz, CH_2), 2.20 (s, 3H, CH_3), 1.88 (s, 3H, CH_3), 1.57-1.65 (m, 2H, CH_2), 1.26-1.33 (m, 2H, CH_2), 0.87 (t, 3H, *J* 7.2 Hz, CH_3); ^{13}C NMR ($CDCl_3$, 100 MHz) 186.1, 176.5, 145.8, 137.0, 135.9, 132.6, 132.3, 131.2, 130.4, 128.2, 128.0, 127.1, 126.7, 124.1, 119.9, 38.8, 27.5, 22.4, 17.4, 16.9, 13.8; Anal. calcd. for $C_{21}H_{25}N_3OS_2$: C, 63.12; H, 6.31; N, 10.52; Found C, 63.05; H, 6.30; N, 10.49.

*6-Hydroxy-6-ethyl-1,5-di(4-methylphenyl)-1,3,5-triazinane-2,4-dithione (**11**)*

White solid, mp 119-121 °C; IR (KBr) ν_{max}/cm^{-1} 3396, 3264, 3041, 2962, 2925, 2857, 1600, 1583, 1534, 1513, 1472, 1454, 1370, 1223, 1062, 810; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.44 (d, 2H, *J* 8.0 Hz, Ph-H), 7.26-7.33 (m, 4H, Ph-H), 7.10 (d, 2H, *J* 8.0 Hz, Ph-H), 6.07 (s, 1H, OH), 2.51 (s, 3H, CH_3), 2.51 (q, 2H, *J* 7.4 Hz, CH_2), 2.29 (s, 3H, CH_3), 1.12 (t, 3H, *J* 7.4 Hz, CH_3); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 186.5, 177.5, 146.2, 141.0, 135.2, 133.3, 131.3 (2C), 131.0, 129.6 (2C), 127.8 (2C), 119.1 (2C), 32.3, 21.4, 20.7, 9.5; Anal. calcd. for $C_{19}H_{21}N_3OS_2$: C, 61.42; H, 5.70; N, 11.31; Found C, 61.38; H, 5.70; N, 11.29.

*6-Hydroxy-6-propyl-1,5-di(4-methylphenyl)-1,3,5-triazinane-2,4-dithione (**12**)*

White solid, mp 127-129 °C; IR (KBr) ν_{max}/cm^{-1} 3412, 3321, 3035, 2961, 2925, 2870, 1604, 1539, 1512, 1459, 1409, 1377, 1279, 1208, 1067, 813; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.44 (d, 2H, *J* 8.0 Hz, Ph-H), 7.26-7.33 (m, 4H, Ph-H), 7.10 (d, 2H, *J* 8.0 Hz, Ph-H), 6.09 (s, 1H, OH), 2.49 (s, 3H, CH_3), 2.46 (t, 2H, *J* 7.4 Hz, CH_2), 2.29 (s, 3H, CH_3), 1.61-1.67 (m, 2H, CH_2), 0.89 (t, 3H, *J* 7.4 Hz, CH_3); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 185.7, 177.4, 146.2, 141.0, 135.2, 133.3, 131.3 (2C), 131.0, 129.5 (2C), 127.7 (2C), 119.1 (2C), 41.0, 21.4, 20.7, 18.8, 13.8; Anal. calcd. for $C_{20}H_{23}N_3OS_2$: C, 62.30; H, 6.01; N, 10.90; Found C, 62.37; H, 6.00; N, 10.87.

*6-Hydroxy-6-butyl-1,5-di(4-methylphenyl)-1,3,5-triazinane-2,4-dithione (**13**)*

White solid, mp 126-127 °C; IR (KBr) ν_{max}/cm^{-1} 3425, 3032, 2958, 2924, 2857, 1599, 1581, 1533, 1508, 1458, 1350, 1282, 1244, 1209, 810; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.43 (d, 2H, *J* 8.0 Hz, Ph-H), 7.25-7.33 (m, 4H, Ph-H), 7.09 (d, 2H, *J* 8.0 Hz, Ph-H), 6.08 (s, 1H, OH), 2.48 (t, 2H, *J* 7.6 Hz, CH_2), 2.48 (s, 3H, CH_3), 2.29 (s, 3H, CH_3), 1.56-1.64 (m, 2H, CH_2), 1.25-1.32 (m, 2H, CH_2), 0.86 (t, 3H, *J* 7.4 Hz, CH_3); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 185.9, 177.4, 146.2, 141.0, 135.2, 133.3, 131.3 (2C), 131.0, 129.5 (2C), 127.7 (2C), 119.1 (2C), 38.8, 27.4, 22.4, 21.4, 20.8, 13.8; Anal. calcd. for $C_{21}H_{25}N_3OS_2$: C, 63.12; H, 6.31; N, 10.52; Found C, 63.18; H, 6.29; N, 10.48.

*6-Hydroxy-6-pentyl-1,5-di(4-methylphenyl)-1,3,5-triazinane-2,4-dithione (**14**)*

Yellowish solid, mp 111-113 °C; IR (KBr) ν_{max}/cm^{-1} 3407, 2953, 2929, 2862, 1622, 1588, 1543, 1486, 1456, 1381, 1348, 1287, 1258, 1198, 753; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.45 (d, 2H, *J* 8.4 Hz, Ph-H), 7.26-7.33 (m, 4H, Ph-H), 7.10 (d, 2H, *J* 8.4 Hz, Ph-H), 6.07 (s, 1H, OH), 2.50 (s, 3H, CH_3), 2.48 (t, 2H, *J* 7.6 Hz, CH_2), 2.30 (s, 3H, CH_3), 1.52-1.63 (m, 2H, CH_2), 1.25-1.31 (m, 4H, CH_2), 0.85 (t, 3H, *J* 7.0 Hz, CH_3); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 186.0, 177.4, 146.2, 141.0, 135.2, 133.3, 131.3 (2C), 131.1, 129.6 (2C), 127.8 (2C), 119.1 (2C), 39.0, 31.5, 25.1, 22.4, 21.4, 20.7, 13.9; Anal. calcd. for $C_{22}H_{27}N_3OS_2$: C, 63.89; H, 6.58; N, 10.16; Found C, 63.97; H, 6.59; N, 10.12.

*6-Hydroxy-6-hexyl-1,5-di(4-methylphenyl)-1,3,5-triazinane-2,4-dithione (**15**)*

White solid, mp 103-104 °C; IR (KBr) ν_{max}/cm^{-1} 3387, 3063, 2929, 2862, 1600, 1539, 1513, 1476, 1382, 1348, 1298, 1241, 1199, 815; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.43 (d, 2H, *J* 8.4 Hz, Ph-H), 7.26-7.33 (m, 4H, Ph-H), 7.10 (d, 2H, *J* 8.4 Hz, Ph-H), 6.07 (s, 1H, OH), 2.49 (s, 3H, CH_3), 2.47 (t, 2H, *J* 7.6 Hz, CH_2), 2.29 (s, 3H, CH_3), 1.59-1.63 (m, 2H, CH_2), 1.21-1.28 (m, 6H, CH_2), 0.85 (t, 3H, *J* 7.4 Hz, CH_3); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 186.0, 177.4, 146.2, 141.0, 135.2, 133.3, 131.3 (2C), 131.0, 129.6 (2C), 127.8 (2C), 119.1 (2C), 39.1, 31.6, 29.0, 25.3, 22.5, 21.4, 20.7, 14.1; Anal. calcd. for $C_{23}H_{29}N_3OS_2$: C, 64.60; H, 6.84; N, 9.83; Found C, 64.43; H, 6.83; N, 9.79.

*6-Hydroxy-6-methyl-1,5-di(4-methoxyphenyl)-1,3,5-triazinane-2,4-dithione (**16**)*

White solid, mp 218-219 °C; IR (KBr) ν_{max}/cm^{-1} 3414, 2959, 2930, 2863, 1619, 1588, 1531, 1456, 1251, 1193, 754; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.33-7.38 (m, 4H, Ph-H), 7.13 (d, 2H, *J* 8.8 Hz, Ph-H), 6.85 (d, 2H, *J* 8.8 Hz, Ph-H), 6.01 (s, 1H, OH), 3.91 (s, 3H, OCH_3), 3.78 (s, 3H, OCH_3), 2.22 (s, 3H, CH_3); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 183.1, 178.0, 161.0, 156.2, 147.0, 130.8, 129.3 (2C), 126.0, 121.4 (2C) (2C), 116.0 (2C), 114.3 (2C), 55.6, 55.5, 26.1; Anal. calcd. for $C_{18}H_{19}N_3O_3S_2$: C, 55.51; H, 4.92; N, 10.79; Found C, 55.60; H, 4.90; N, 10.74.

*6-Hydroxy-6-ethyl-1,5-di(4-methoxyphenyl)-1,3,5-triazinane-2,4-dithione (**17**)*

White solid, mp 243-245 °C; IR (KBr) ν_{max}/cm^{-1} 3410, 3007, 2963, 2932, 2837, 1606, 1548, 1511, 1469, 1366, 1301, 1252, 824; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.33-7.36 (m, 4H, Ph-H), 7.13 (d, 2H, *J* 8.8 Hz, Ph-H), 6.85 (d, 2H, *J* 8.8 Hz, Ph-H), 5.98 (s, 1H, OH), 3.92 (s, 3H, OCH_3), 3.78 (s, 3H, OCH_3), 2.51 (q, 2H, *J* 7.4 Hz, CH_2), 1.13 (t, 3H, *J* 7.4 Hz, CH_3); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 186.6, 177.8, 160.9, 156.2, 147.0, 130.8, 129.3 (2C), 126.0, 121.4 (2C), 115.9 (2C), 114.3 (2C), 55.6, 55.5, 32.3, 9.5; Anal. calcd. for $C_{19}H_{21}N_3O_3S_2$: C, 56.55; H, 5.25; N, 10.41; Found C, 56.46; H, 5.26; N, 10.37.

*6-Hydroxy-6-propyl-1,5-di(4-methoxyphenyl)-1,3,5-triazinane-2,4-dithione (**18**)*

White solid, mp 219-221 °C; IR (KBr) ν_{max}/cm^{-1} 3369, 3008, 2961, 2835, 1599, 1543, 1510, 1471, 1379, 1246, 1170, 820; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.32-7.36 (m, 4H, Ph-H), 7.13 (d, 2H, *J* 8.8 Hz, Ph-H), 6.85 (d, 2H, *J* 8.8 Hz, Ph-H), 6.01 (s, 1H, OH), 3.91 (s, 3H, OCH_3), 3.78 (s, 3H, OCH_3), 2.46 (t, 2H, *J* 7.2 Hz, CH_2), 1.62-1.67 (m, 2H, CH_2), 0.89 (t, 3H, *J* 7.4 Hz, CH_3); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 185.8, 177.7, 160.9, 156.2, 147.0, 130.8, 129.3 (2C), 126.0, 121.4 (2C), 115.8 (2C), 114.3 (2C), 55.6, 55.5, 41.0, 18.8, 13.8; Anal. calcd. for $C_{20}H_{23}N_3O_3S_2$: C, 57.53; H, 5.55; N, 10.06; Found C, 57.58; H, 5.57; N, 10.01.

*6-Hydroxy-6-methyl-1,5-di(4-chlorophenyl)-1,3,5-triazinane-2,4-dithione (**19**)*

White solid, mp 208-210 °C; IR (KBr) ν_{max}/cm^{-1} 3449, 3286, 2960, 2925, 2856, 1605, 1539, 1491, 1450, 1373, 1300, 1250, 1090, 825; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.66 (d, 2H, *J* 8.4 Hz, Ph-H), 7.39-7.45 (m, 4H, Ph-H), 7.27 (d, 2H, *J* 8.4 Hz, Ph-H), 6.09 (s, 1H, OH), 2.23 (s, 3H, CH_3); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 183.3, 177.3, 145.1, 137.2, 136.2, 131.9, 131.2 (2C), 129.6 (2C), 129.2 (2C), 128.8, 120.1 (2C), 26.1; Anal. calcd. for $C_{16}H_{13}Cl_2N_3OS_2$: C, 48.24; H, 3.29; N, 10.55; Found C, 48.10; H, 3.30; N, 10.58.

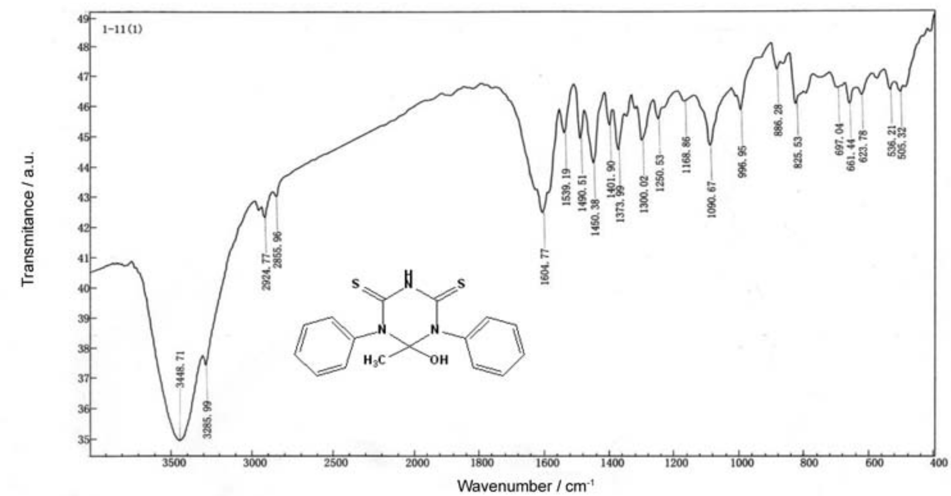


Figure S1. IR (KBr) spectrum of 6-hydroxy-6-methyl-1,5-diphenyl-1,3,5-triazinane-2,4-dithione (**1**).

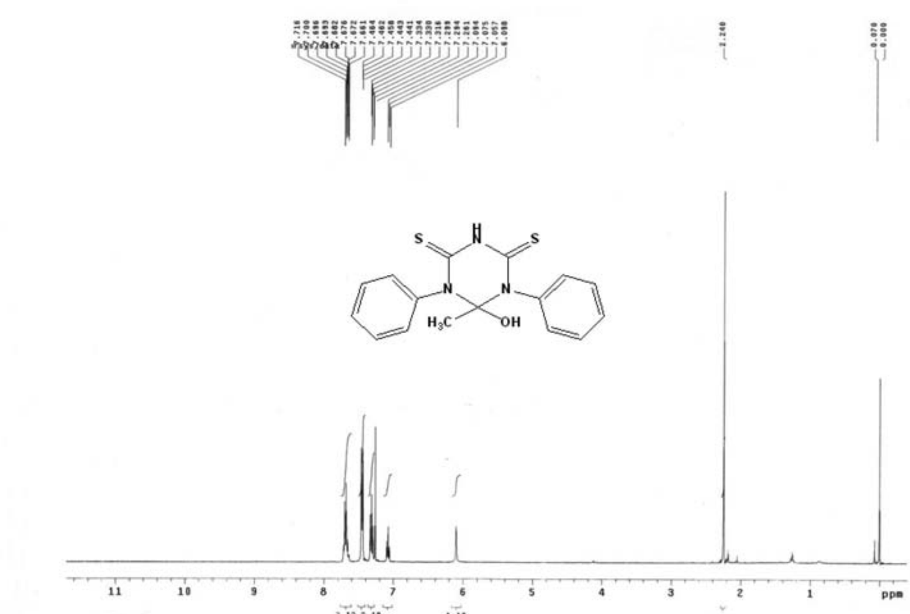


Figure S2. ^{1}H NMR ($CDCl_3$) spectrum of 6-hydroxy-6-methyl-1,5-diphenyl-1,3,5-triazinane-2,4-dithione (**1**).

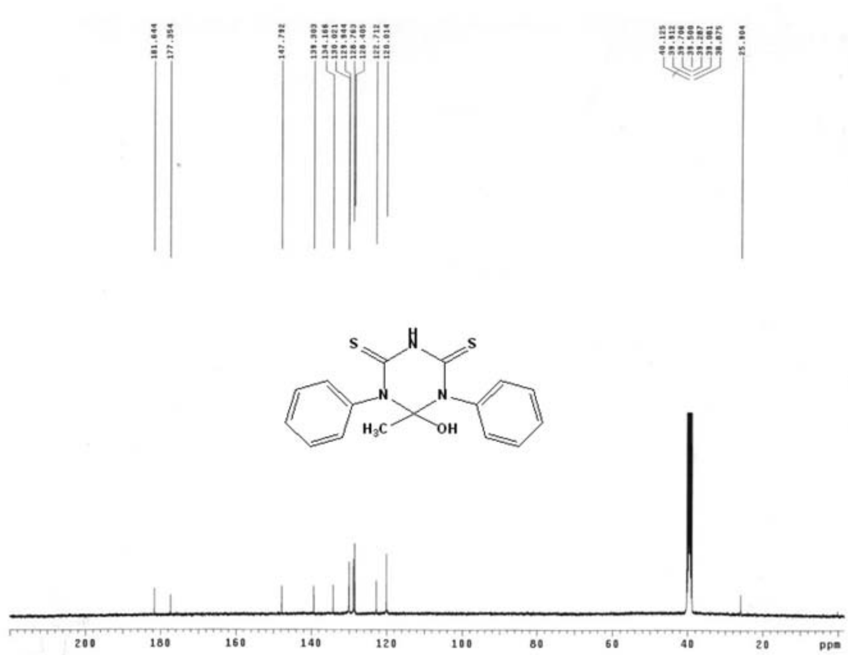


Figure S3. ^{13}C NMR (DMSO-d_6) spectrum of 6-hydroxy-6-methyl-1,5-diphenyl-1,3,5-triazinane-2,4-dithione (**1**).

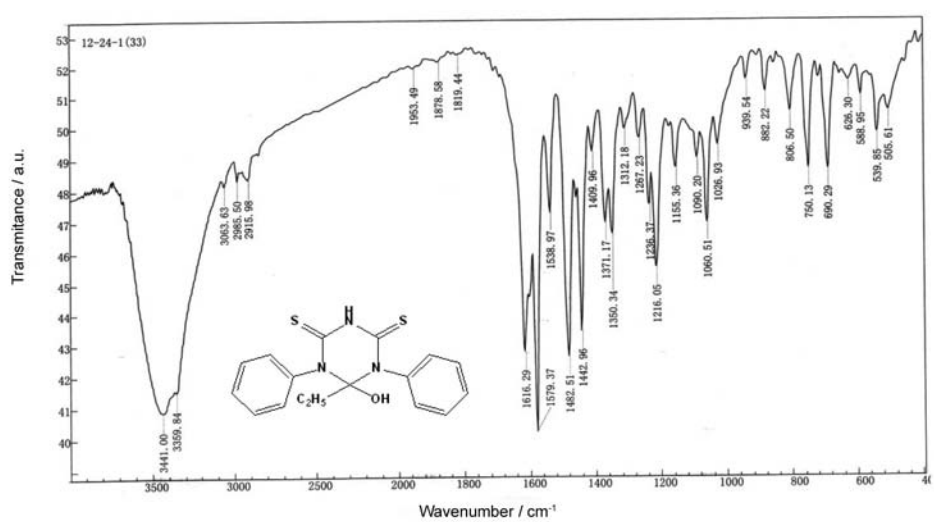


Figure S4. IR (KBr) spectrum of 6-hydroxy-6-ethyl-1,5-diphenyl-1,3,5-triazinane-2,4-dithione (**2**).

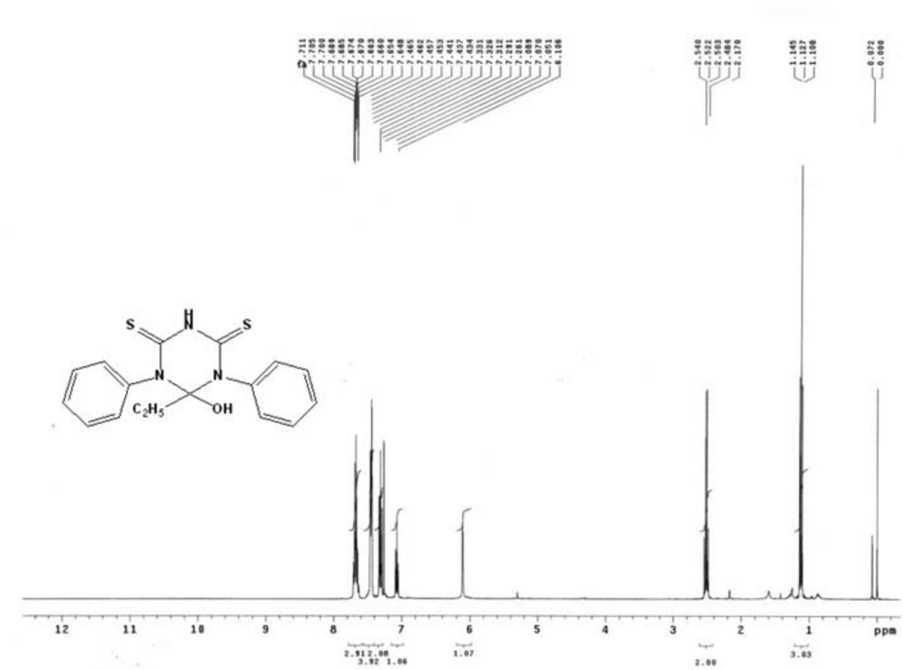


Figure S5. ^{1}H NMR ($CDCl_3$) spectrum of 6-hydroxy-6-ethyl-1,5-diphenyl-1,3,5-triazinane-2,4-dithione (**2**).

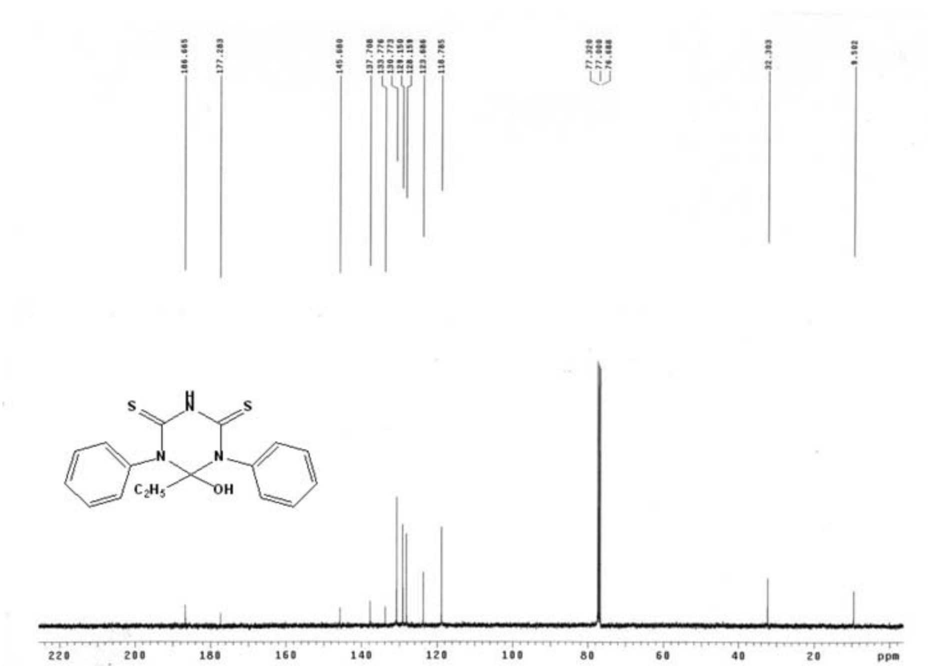


Figure S6. ^{13}C NMR ($CDCl_3$) spectrum of 6-hydroxy-6-ethyl-1,5-diphenyl-1,3,5-triazinane-2,4-dithione (**2**).

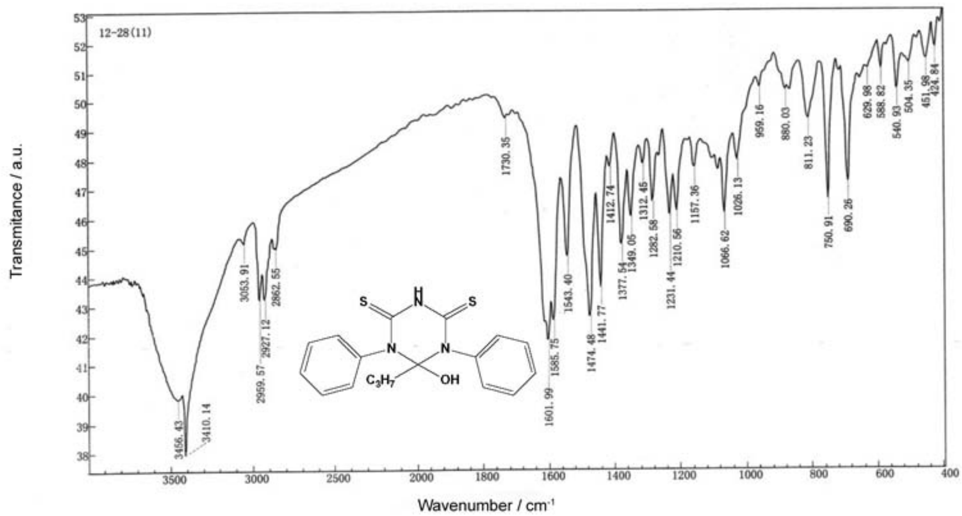


Figure S7. IR (KBr) spectrum of 6-hydroxy-6-propyl-1,5-diphenyl-1,3,5-triazinane-2,4-dithione (**3**).

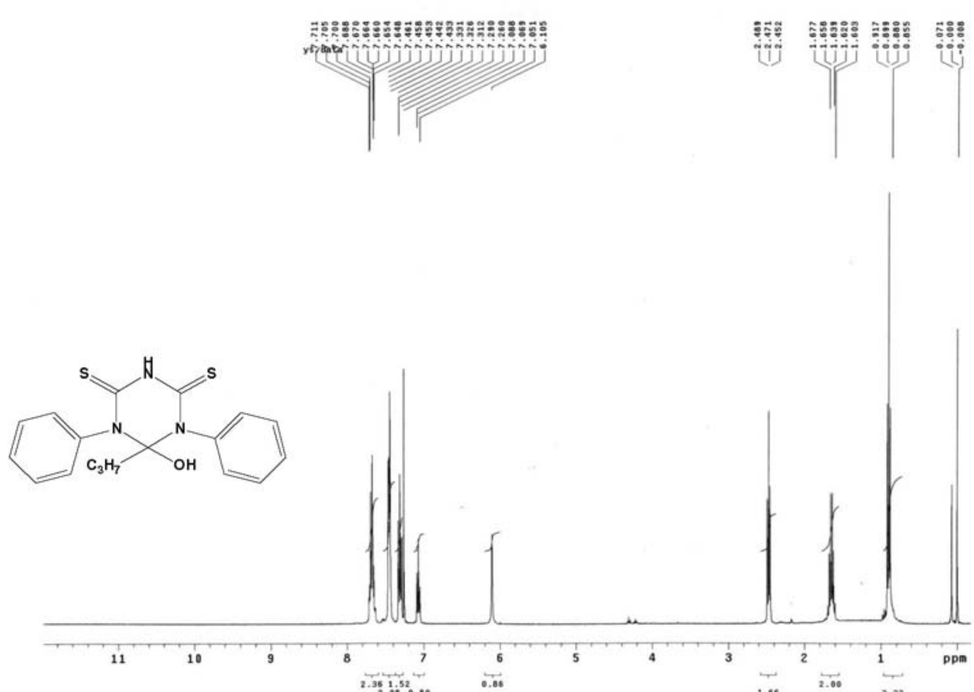


Figure S8. ^{1}H NMR ($CDCl_3$) spectrum of 6-hydroxy-6-propyl-1,5-diphenyl-1,3,5-triazinane-2,4-dithione (**3**).

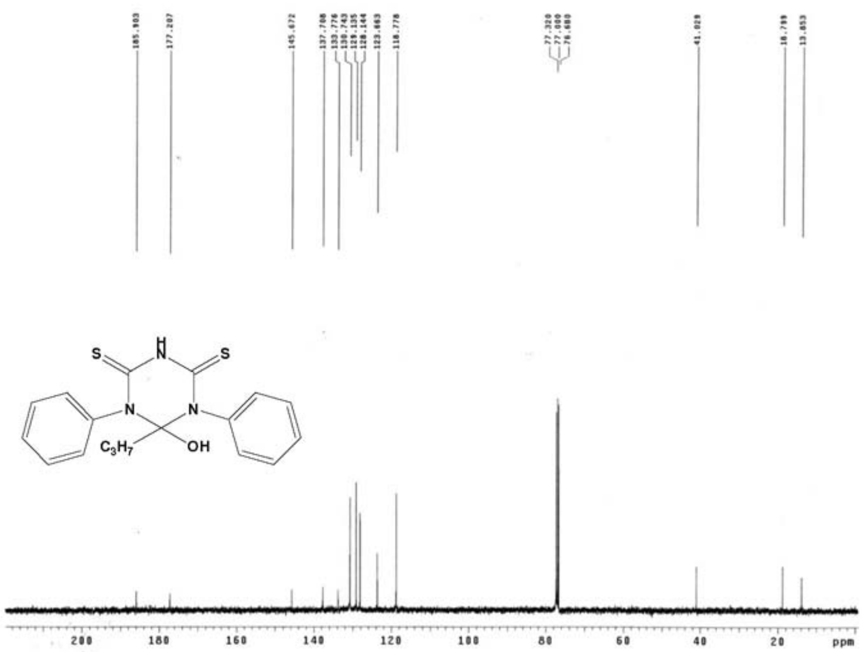


Figure S9. ^{13}C NMR ($CDCl_3$) spectrum of 6-hydroxy-6-propyl-1,5-diphenyl-1,3,5-triazinane-2,4-dithione (**3**).

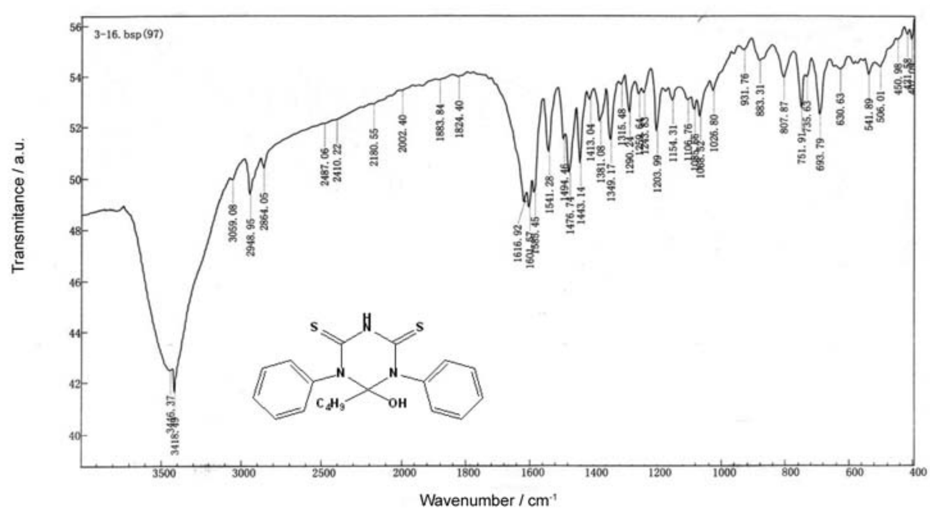


Figure S10. IR (KBr) spectrum of 6-hydroxy-6-butyl-1,5-diphenyl-1,3,5-triazinane-2,4-dithione (**4**).

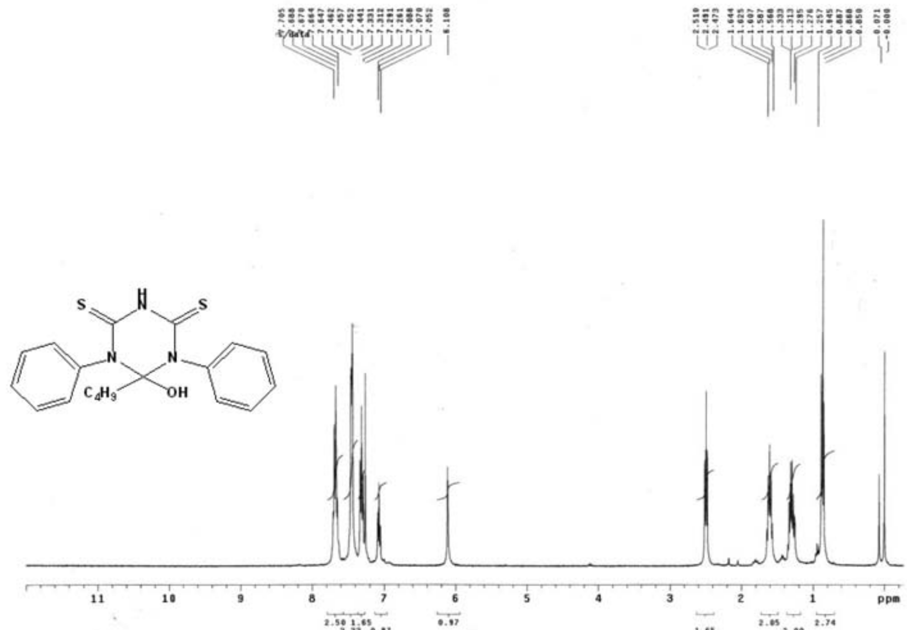


Figure S11. ^{1}H NMR ($CDCl_3$) spectrum of 6-hydroxy-6-butyl-1,5-diphenyl-1,3,5-triazinane-2,4-dithione (**4**).

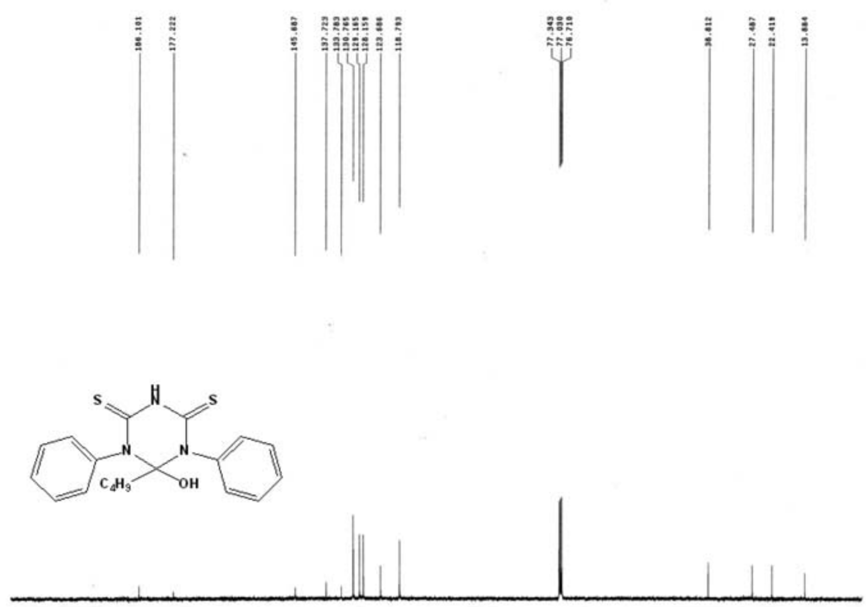


Figure S12. ^{13}C NMR ($CDCl_3$) spectrum of 6-hydroxy-6-butyl-1,5-diphenyl-1,3,5-triazinane-2,4-dithione (**4**).

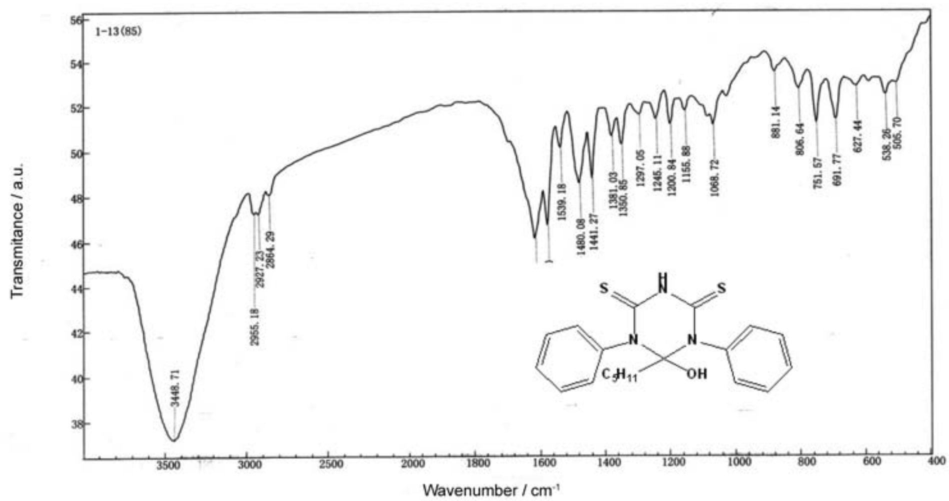


Figure S13. IR (KBr) spectrum of 6-hydroxy-6-pentyl-1,5-diphenyl-1,3,5-triazinane-2,4-dithione (**5**).

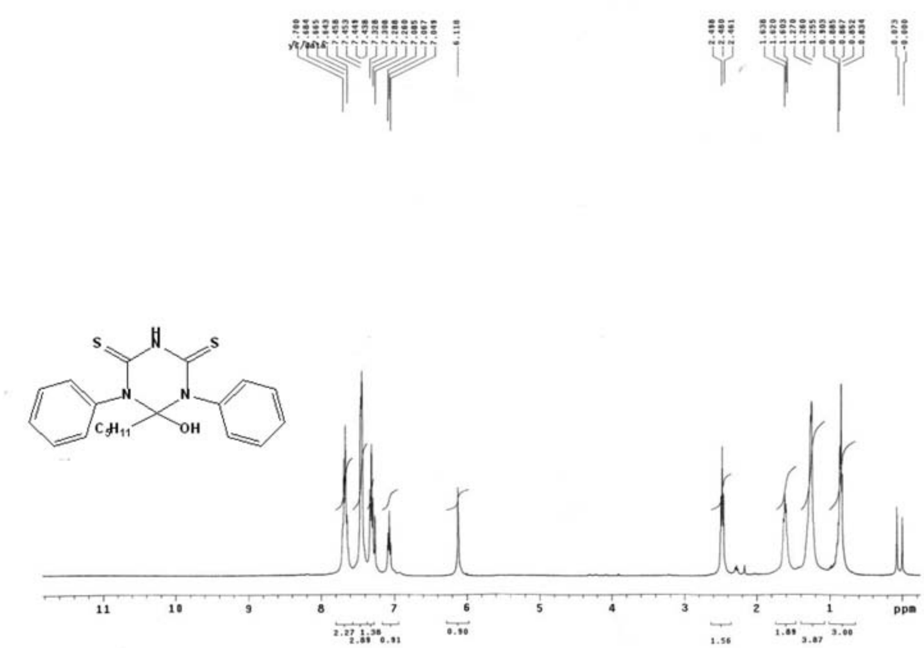


Figure S14. ^{1}H NMR ($CDCl_3$) spectrum of 6-hydroxy-6-pentyl-1,5-diphenyl-1,3,5-triazinane-2,4-dithione (**5**).

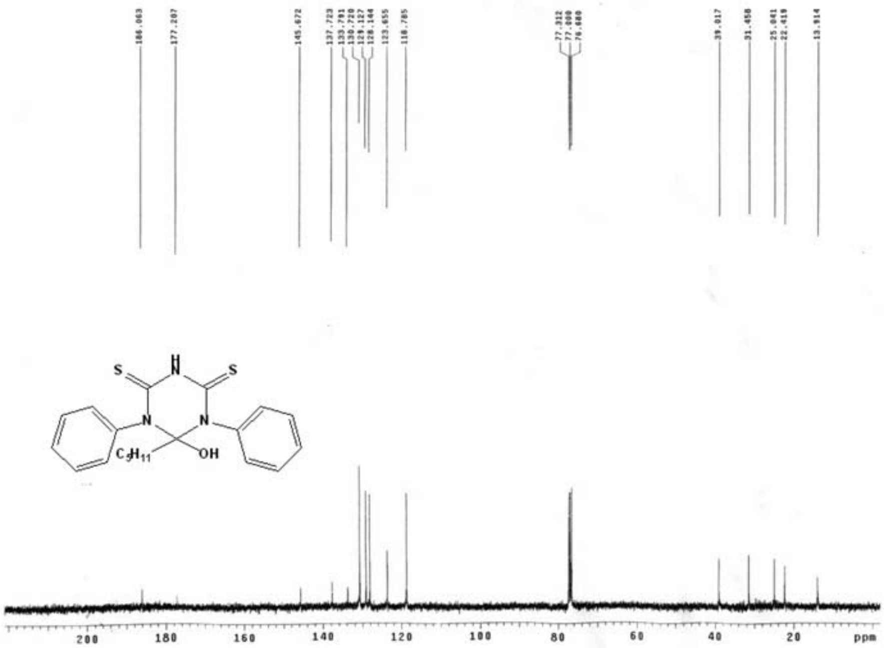


Figure S15. ^{13}C NMR ($CDCl_3$) spectrum of 6-hydroxy-6-pentyl-1,5-diphenyl-1,3,5-triazinane-2,4-dithione (**5**).

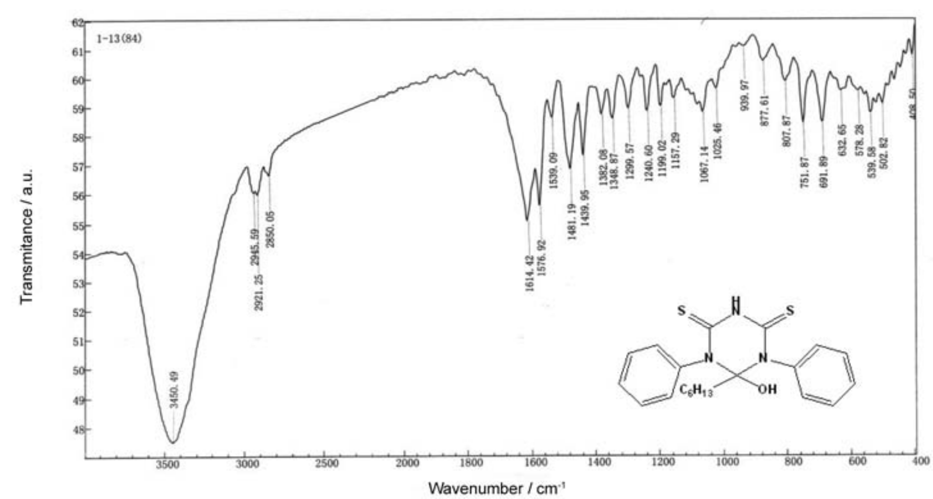


Figure S16. IR (KBr) spectrum of 6-hydroxy-6-hexyl-1,5-diphenyl-1,3,5-triazinane-2,4-dithione (**6**).

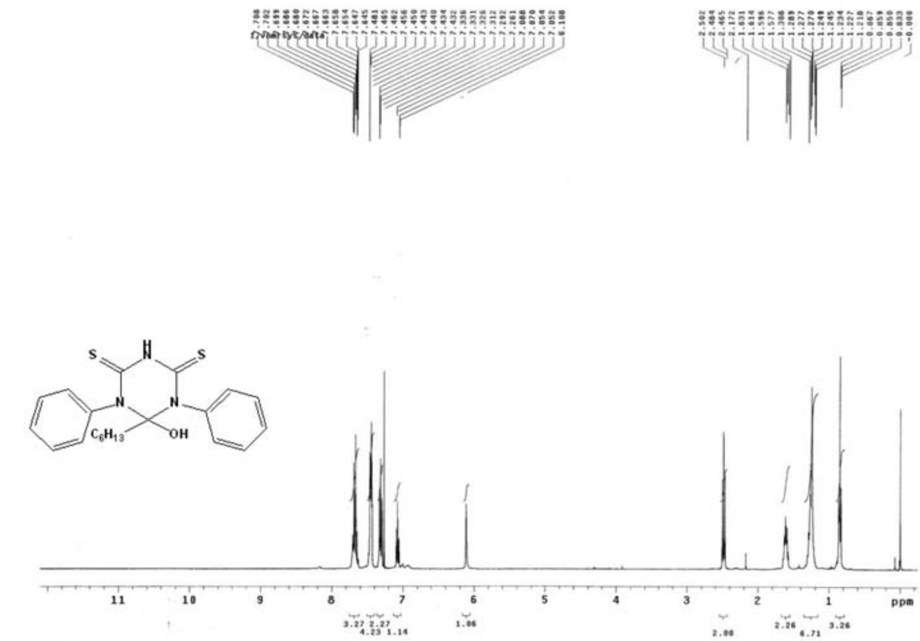


Figure S17. ^{1}H NMR ($CDCl_3$) spectrum of 6-hydroxy-6-hexyl-1,5-diphenyl-1,3,5-triazinane-2,4-dithione (**6**).

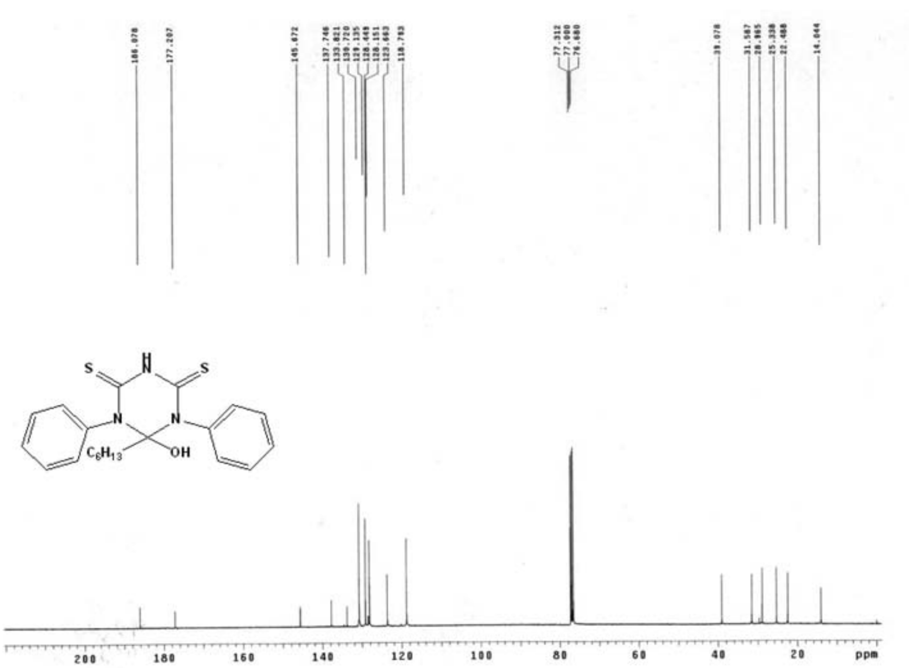


Figure S18. ^{13}C NMR ($CDCl_3$) spectrum of 6-hydroxy-6-hexyl-1,5-diphenyl-1,3,5-triazinane-2,4-dithione (**6**).

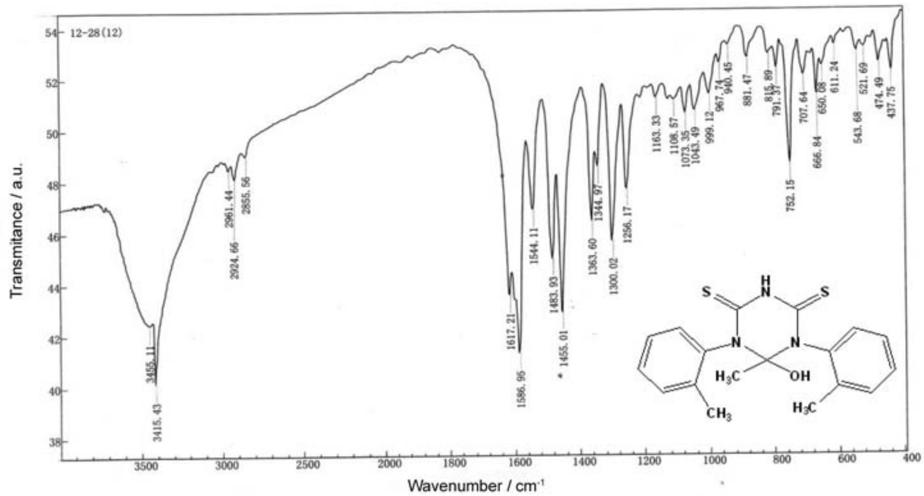


Figure S19. IR (KBr) spectrum of 6-hydroxy-6-methyl-1,5-di(2-methylphenyl)-1,3,5-triazinane-2,4-dithione (**7**).

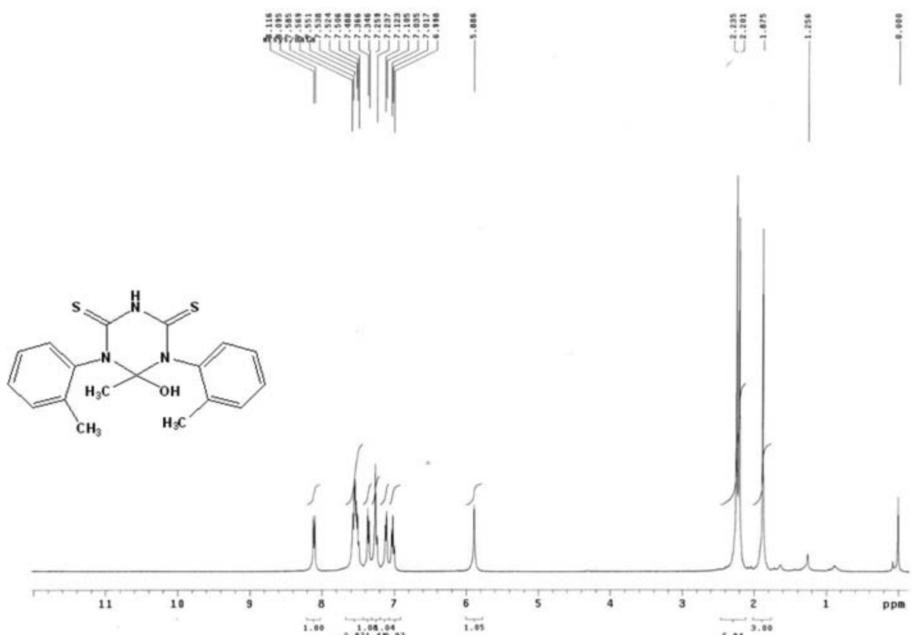


Figure S20. ^{1}H NMR ($CDCl_3$) spectrum of 6-hydroxy-6-methyl-1,5-di(2-methylphenyl)-1,3,5-triazinane-2,4-dithione (**7**).

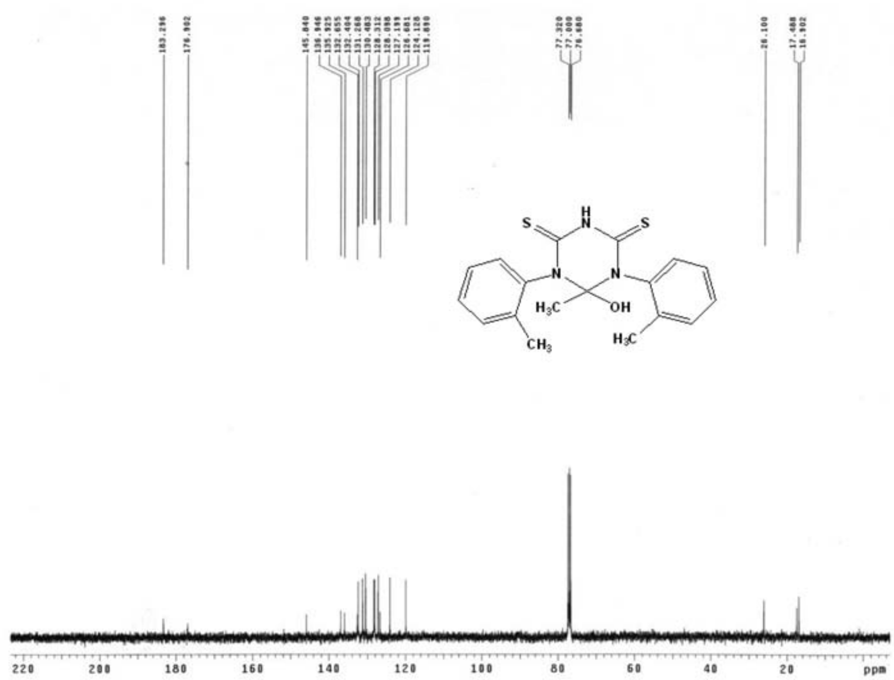


Figure S21. ^{13}C NMR ($CDCl_3$) spectrum of 6-hydroxy-6-methyl-1,5-di(2-methylphenyl)-1,3,5-triazinane-2,4-dithione (**7**).

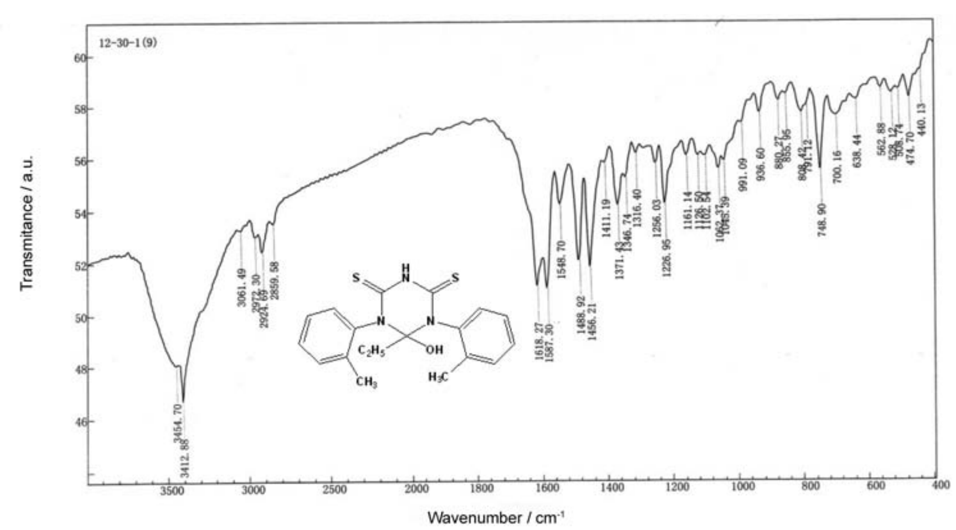


Figure S22. IR (KBr) spectrum of 6-hydroxy-6-ethyl-1,5-di(2-methylphenyl)-1,3,5-triazinane-2,4-dithione (**8**).

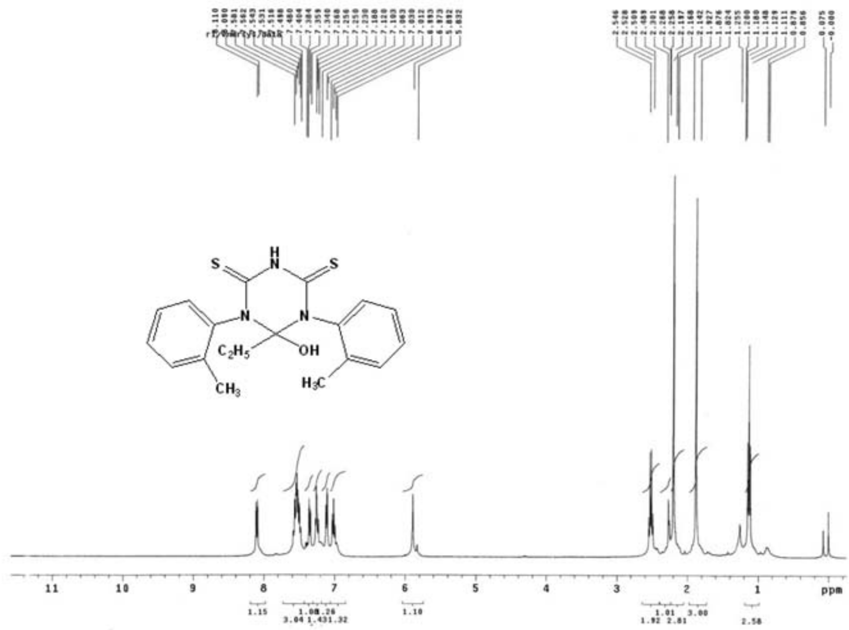


Figure S23. ^{1}H NMR ($CDCl_3$) spectrum of 6-hydroxy-6-ethyl-1,5-di(2-methylphenyl)-1,3,5-triazinane-2,4-dithione (**8**).

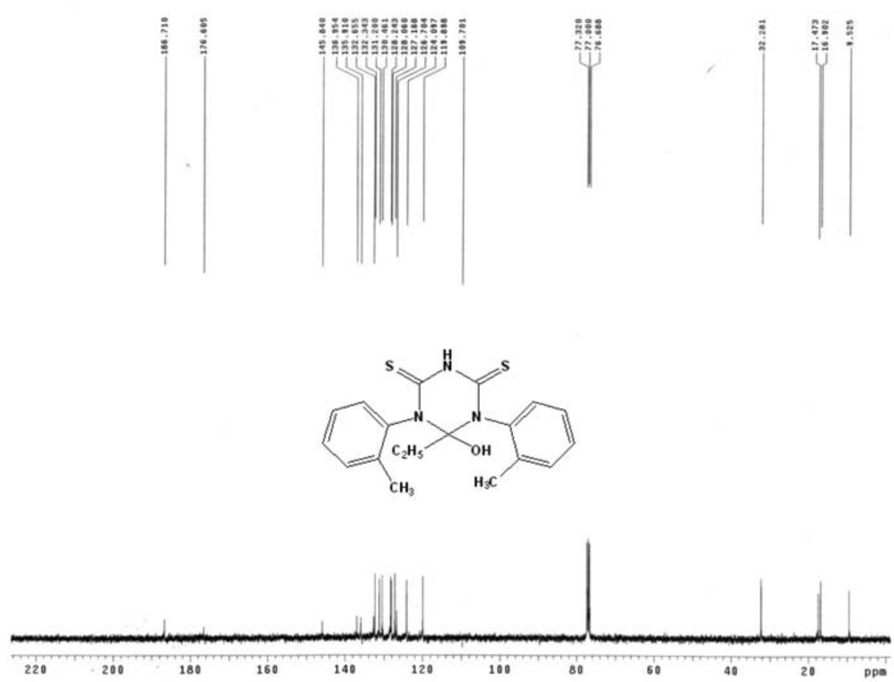


Figure S24. ^{13}C NMR ($CDCl_3$) spectrum of 6-hydroxy-6-ethyl-1,5-di(2-methylphenyl)-1,3,5-triazinane-2,4-dithione (**8**).

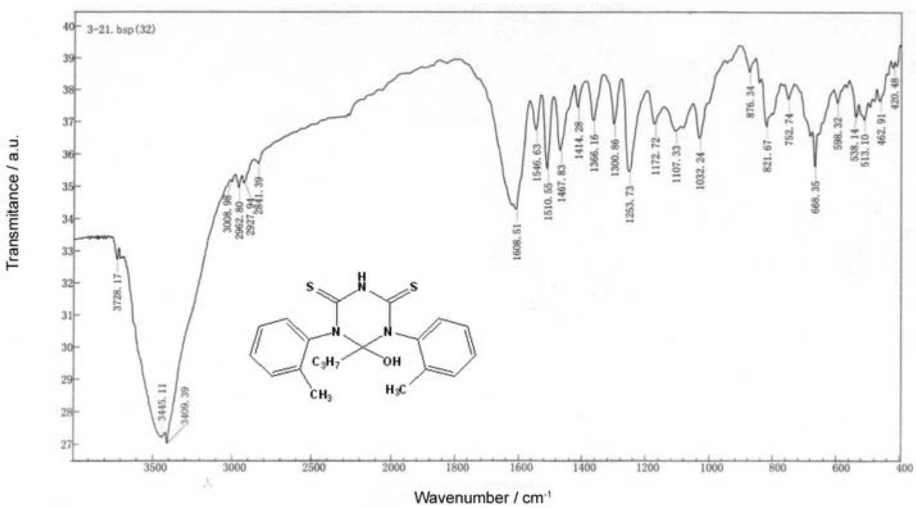


Figure S25. IR (KBr) spectrum of 6-hydroxy-6-propyl-1,5-di(2-methylphenyl)-1,3,5-triazinane-2,4-dithione (**9**).

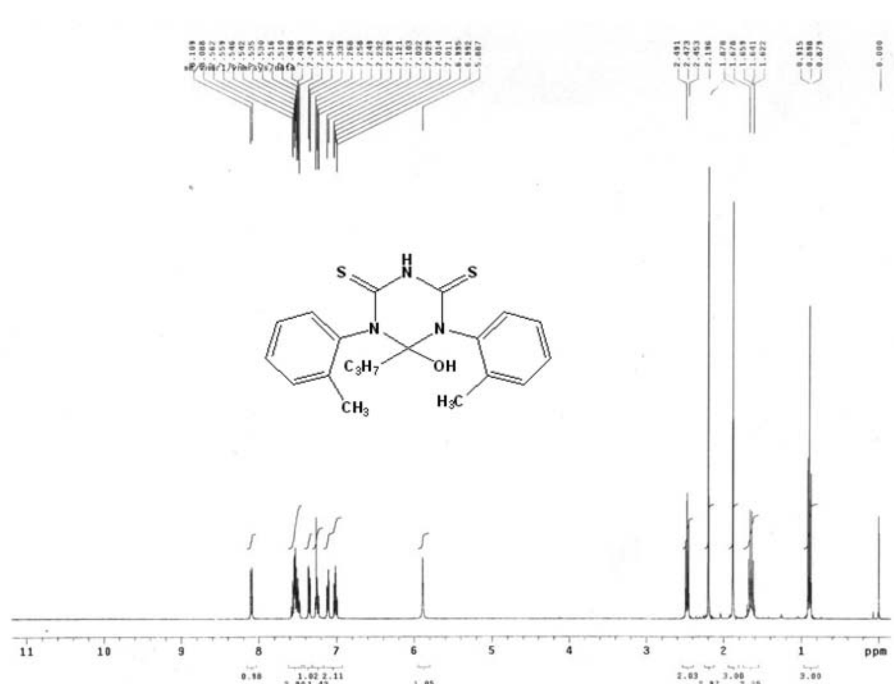


Figure S26. [1]H NMR ($CDCl_3$) spectrum of 6-hydroxy-6-propyl-1,5-di(2-methylphenyl)-1,3,5-triazinane-2,4-dithione (**9**).

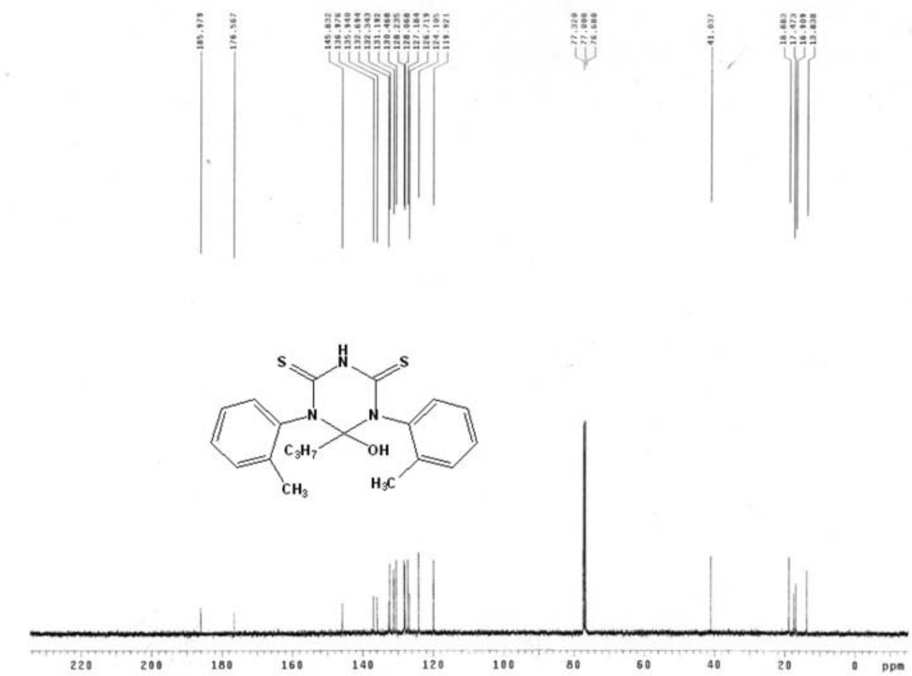


Figure S27. ^{13}C NMR ($CDCl_3$) spectrum of 6-hydroxy-6-propyl-1,5-di(2-methylphenyl)-1,3,5-triazinane-2,4-dithione (**9**).

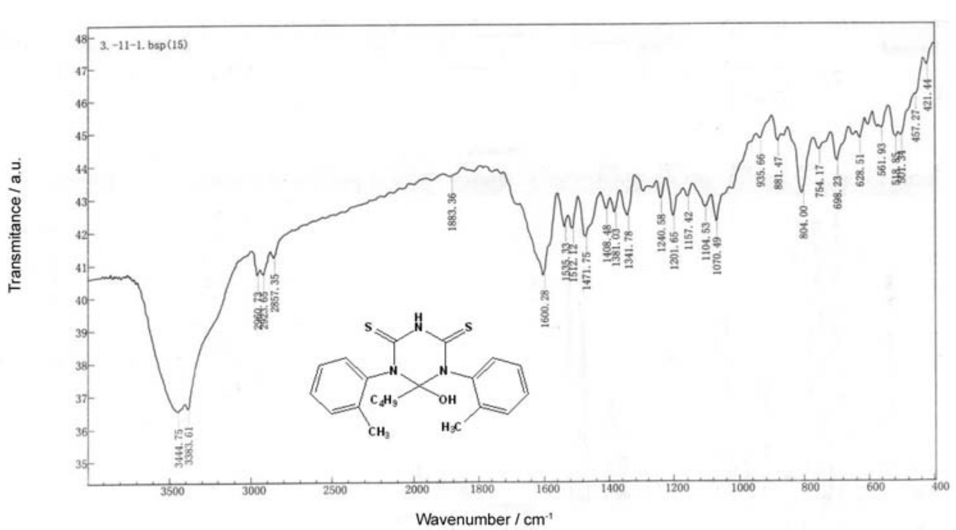


Figure S28. IR (KBr) spectrum of 6-hydroxy-6-butyl-1,5-di(2-methylphenyl)-1,3,5-triazinane-2,4-dithione (**10**).

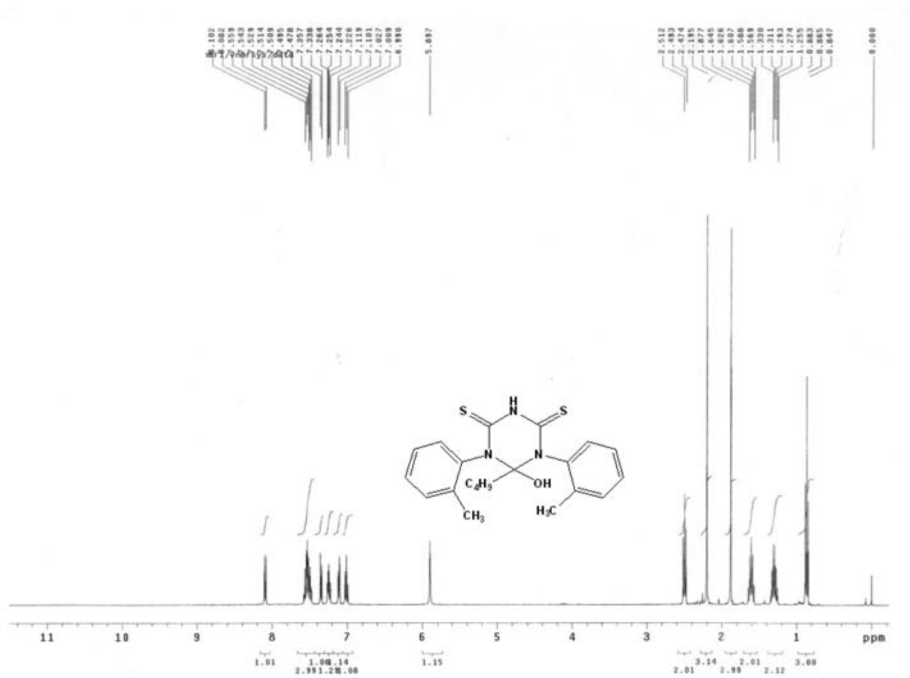


Figure S29. ^{1}H NMR ($CDCl_3$) spectrum of 6-hydroxy-6-butyl-1,5-di(2-methylphenyl)-1,3,5-triazinane-2,4-dithione (**10**).

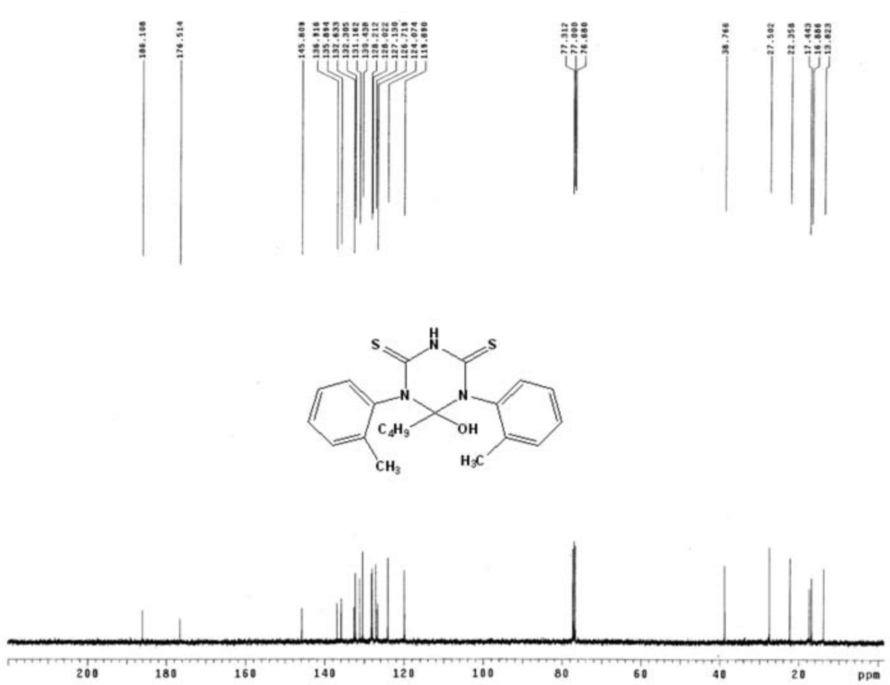


Figure S30. ^{13}C NMR ($CDCl_3$) spectrum of 6-hydroxy-6-butyl-1,5-di(2-methylphenyl)-1,3,5-triazinane-2,4-dithione (**10**).

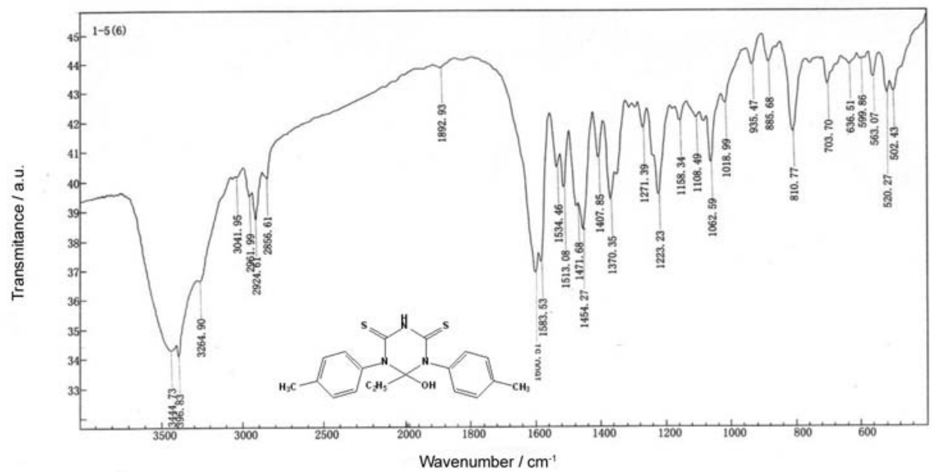


Figure S31. IR (KBr) spectrum of 6-hydroxy-6-ethyl-1,5-di(4-methylphenyl)-1,3,5-triazinane-2,4-dithione (**11**).

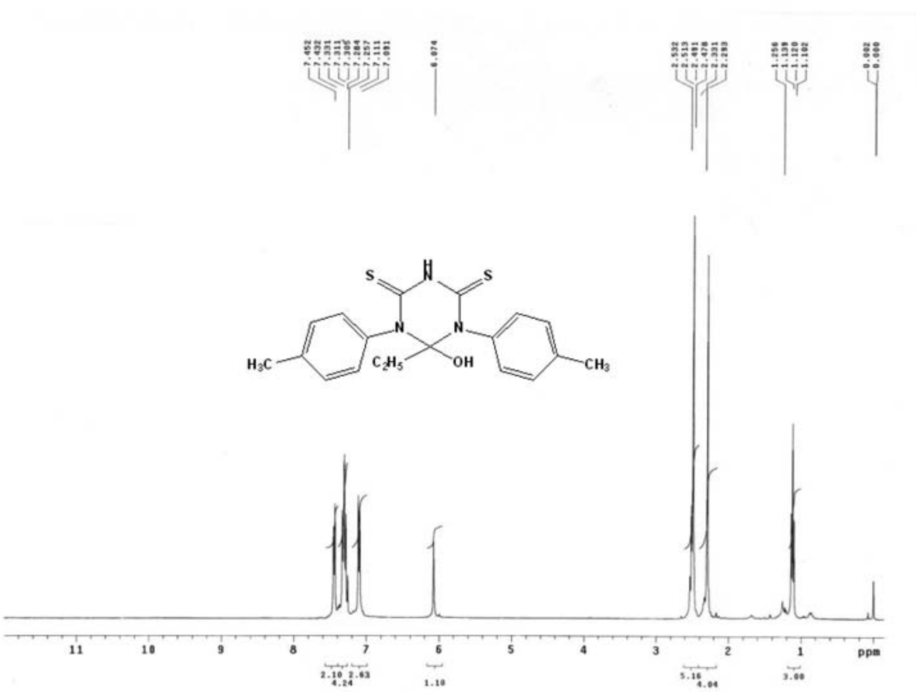


Figure S32. ^{1}H NMR ($CDCl_3$) spectrum of 6-hydroxy-6-ethyl-1,5-di(4-methylphenyl)-1,3,5-triazinane-2,4-dithione (**11**).

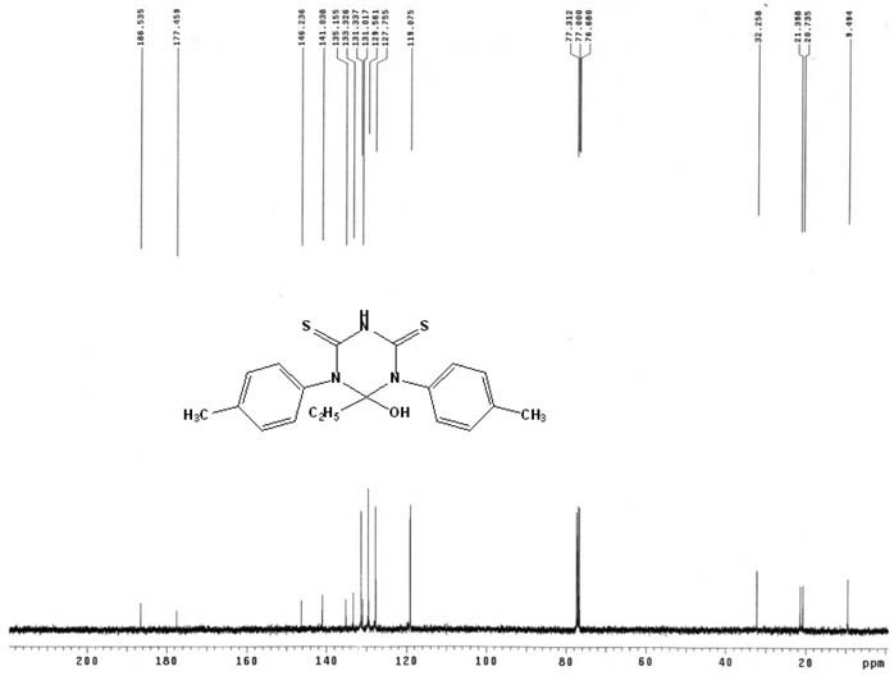


Figure S33. ^{13}C NMR ($CDCl_3$) spectrum of 6-hydroxy-6-ethyl-1,5-di(4-methylphenyl)-1,3,5-triazinane-2,4-dithione (**11**).

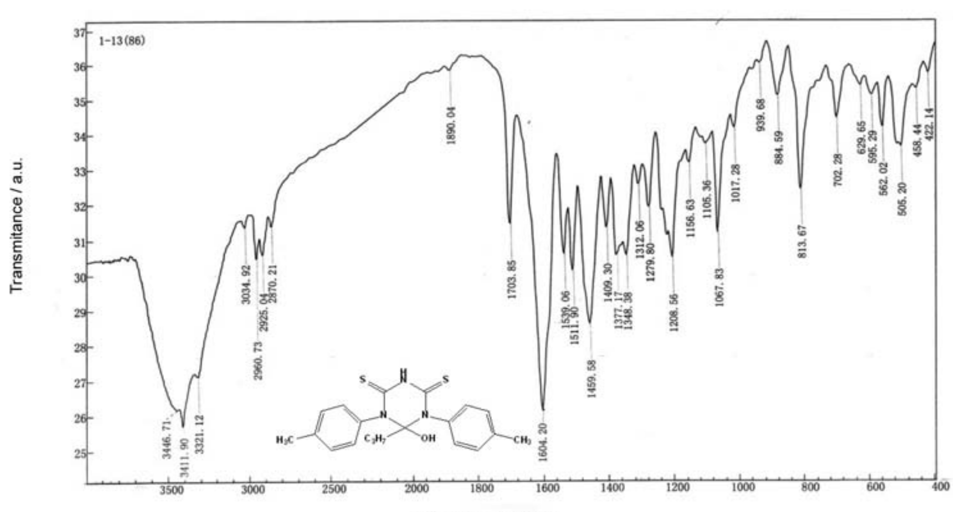


Figure S34. IR (KBr) spectrum of 6-hydroxy-6-propyl-1,5-di(4-methylphenyl)-1,3,5-triazinane-2,4-dithione (**12**).

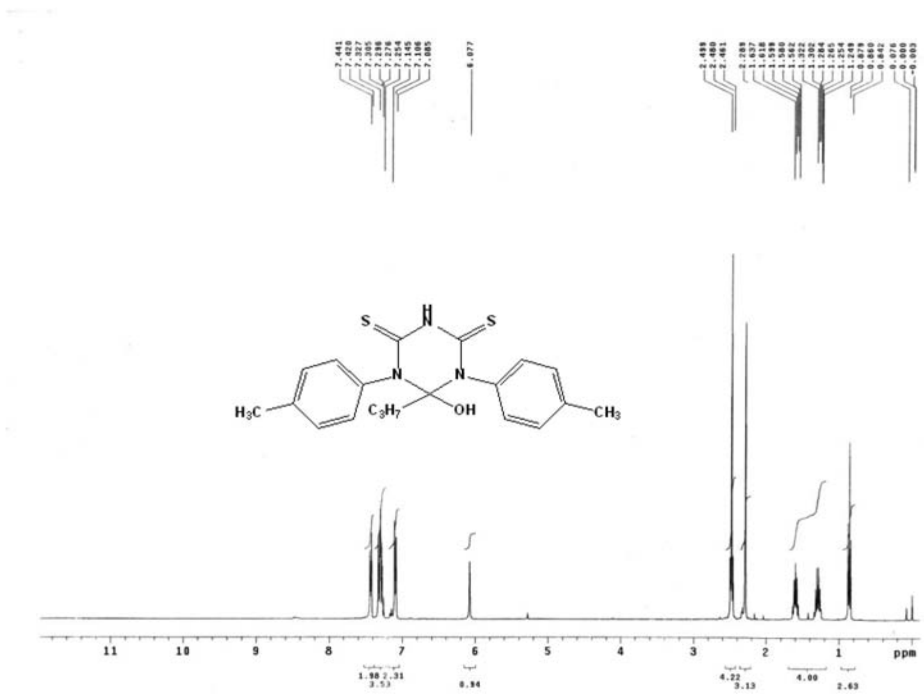


Figure S35. ^{1}H NMR ($CDCl_3$) spectrum of 6-hydroxy-6-propyl-1,5-di(4-methylphenyl)-1,3,5-triazinane-2,4-dithione (**12**).

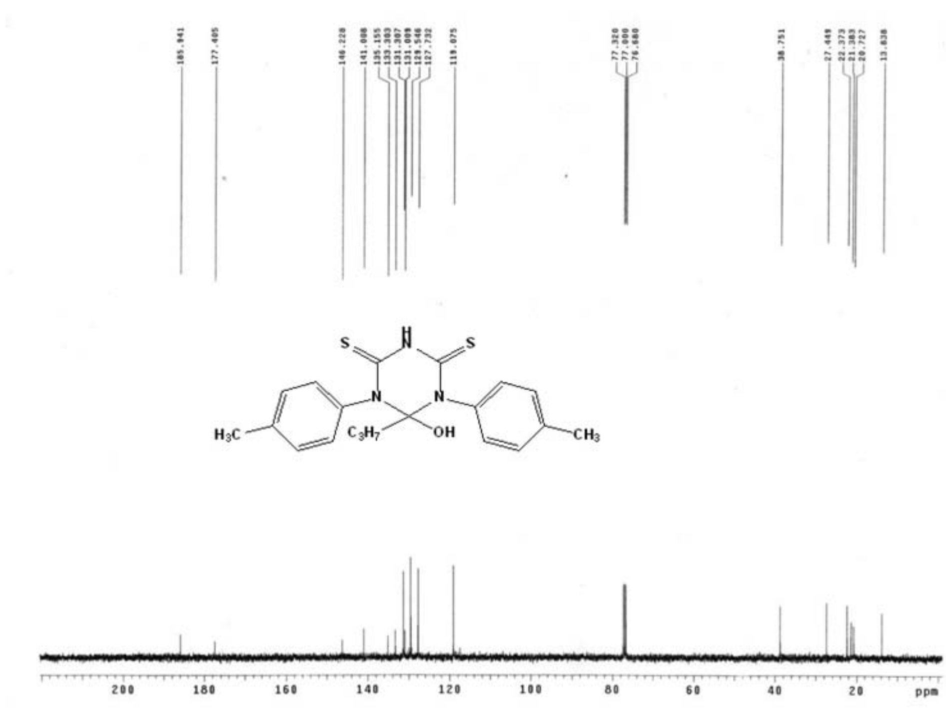


Figure S36. ^{13}C NMR ($CDCl_3$) spectrum of 6-hydroxy-6-propyl-1,5-di(4-methylphenyl)-1,3,5-triazinane-2,4-dithione (**12**).

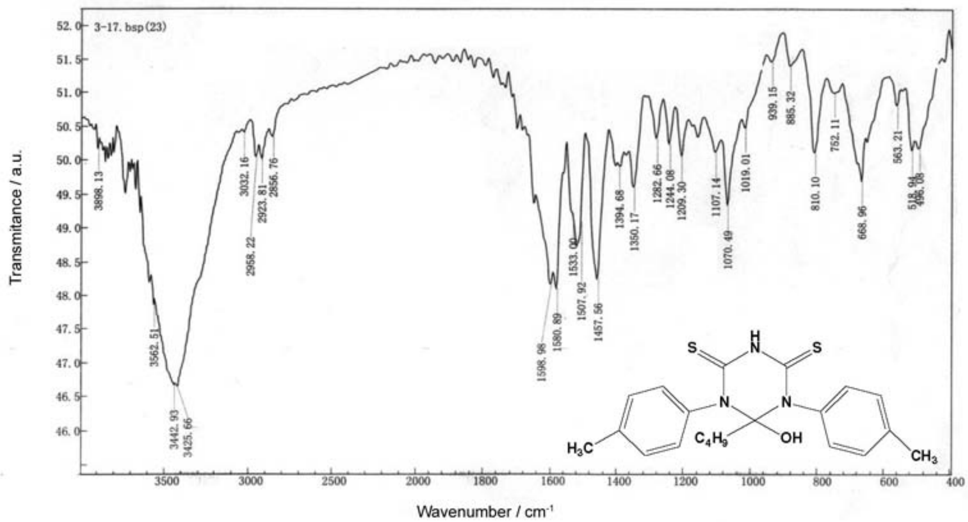


Figure S37. IR (KBr) spectrum of 6-hydroxy-6-butyl-1,5-di(4-methylphenyl)-1,3,5-triazinane-2,4-dithione (**13**).

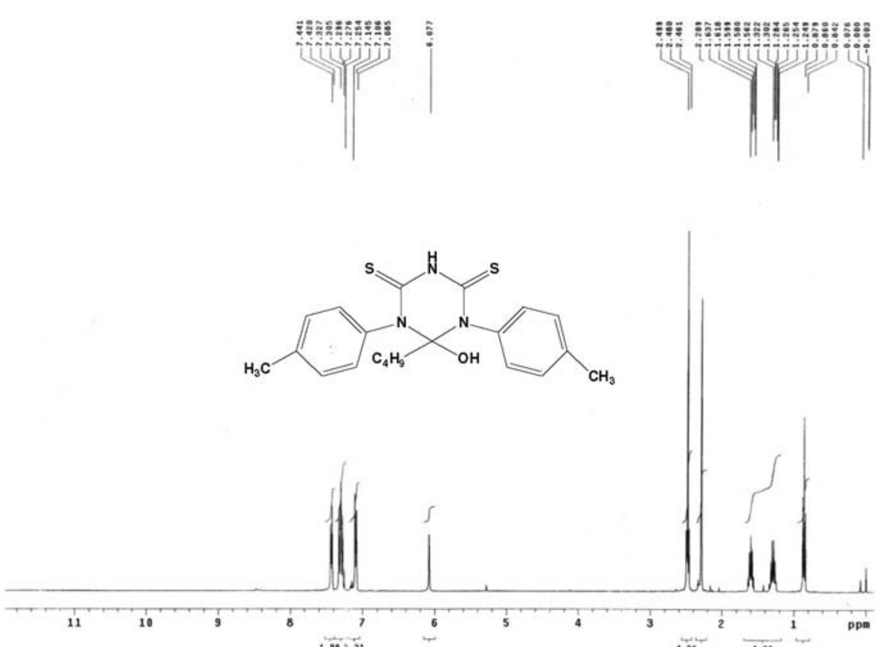


Figure S38. ^{1}H NMR ($CDCl_3$) spectrum of 6- ydroxyl-6-butyl-1,5-di(4-methylphenyl)-1,3,5-triazinane-2,4-dithione (**13**).

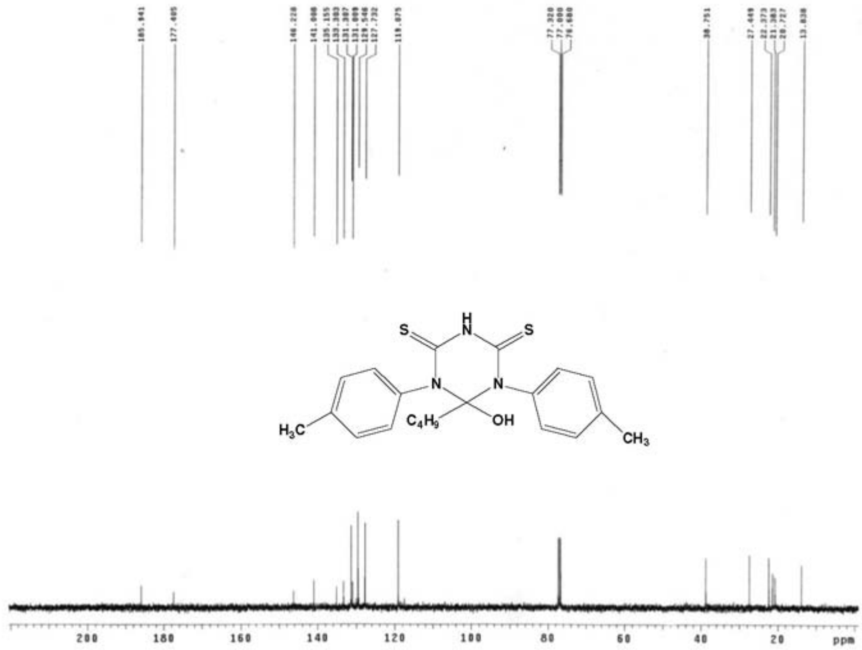


Figure S39. ^{13}C NMR ($CDCl_3$) spectrum of 6-hydroxy-6-butyl-1,5-di(4-methylphenyl)-1,3,5-triazinane-2,4-dithione (**13**).

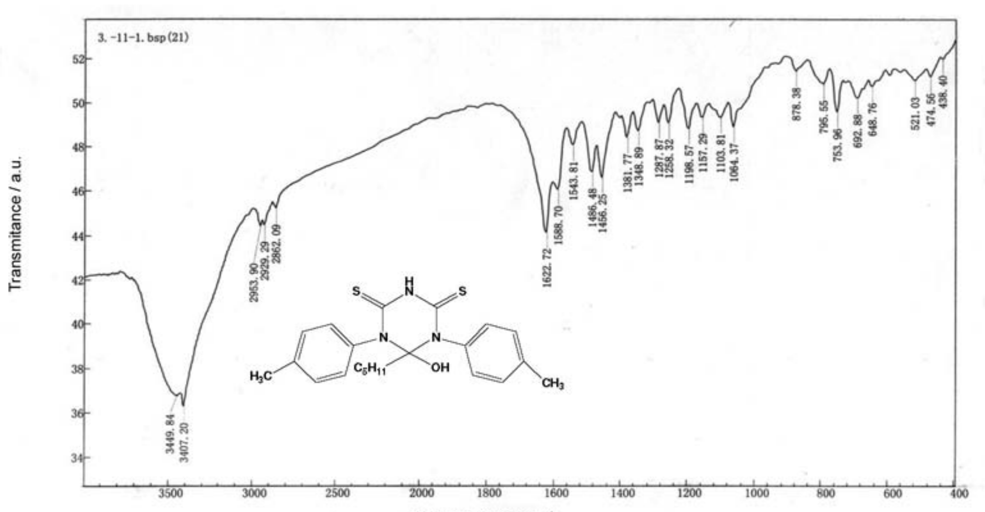


Figure S40. IR (KBr) spectrum of 6-hydroxy-6-pentyl-1,5-di(4-methylphenyl)-1,3,5-triazinane-2,4-dithione (**14**).

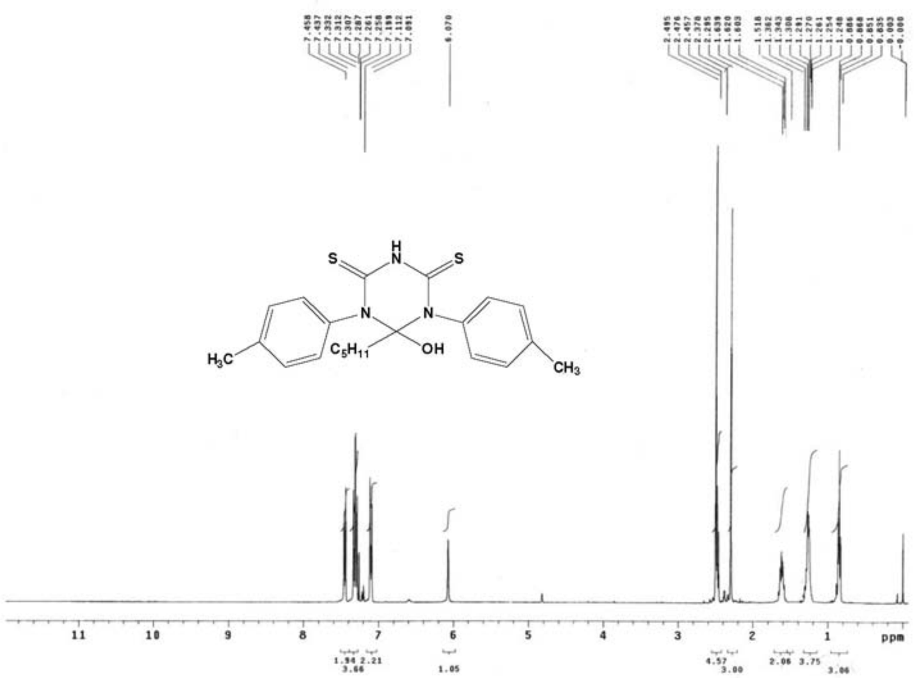


Figure S41. ^{1}H NMR ($CDCl_3$) spectrum of 6-hydroxy-6-pentyl-1,5-di(4-methylphenyl)-1,3,5-triazinane-2,4-dithione (**14**).

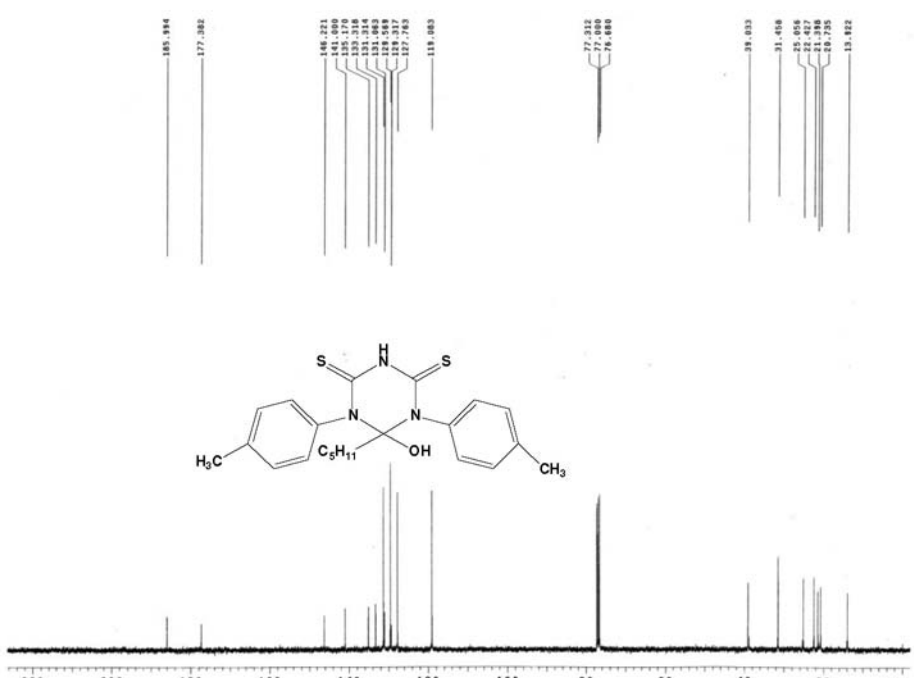


Figure S42. ^{13}C NMR ($CDCl_3$) spectrum of 6-hydroxy-6-pentyl-1,5-di(4-methylphenyl)-1,3,5-triazinane-2,4-dithione (**14**).

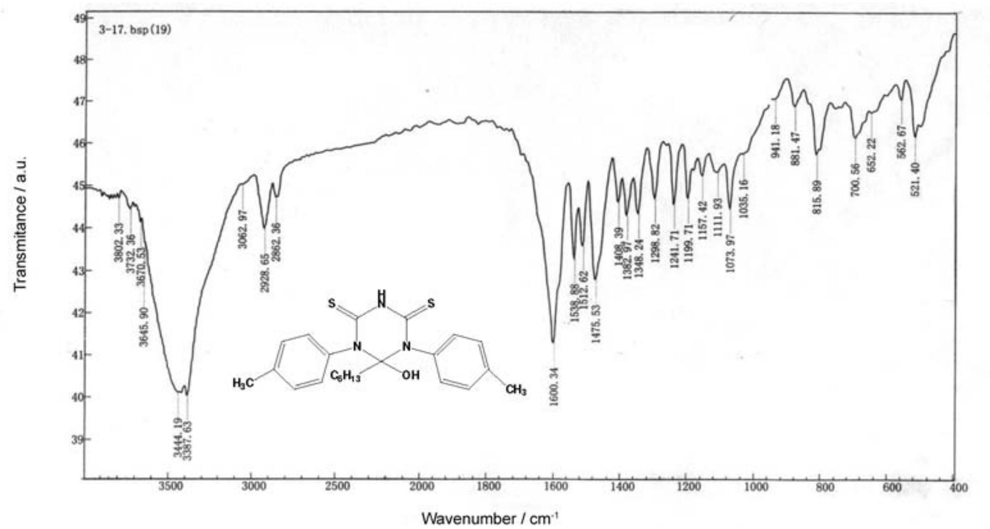


Figure S43. IR (KBr) spectrum of 6-hydroxy-6-hexyl-1,5-di(4-methylphenyl)-1,3,5-triazinane-2,4-dithione (**15**).

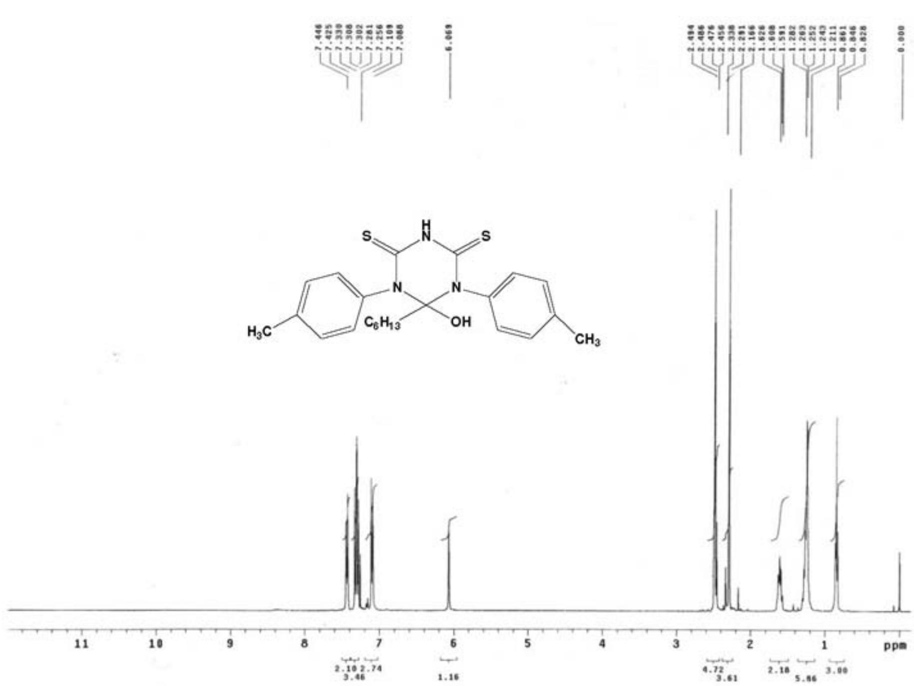


Figure S44. [1]H NMR ($CDCl_3$) spectrum of 6-hydroxy-6-hexyl-1,5-di(4-methylphenyl)-1,3,5-triazinane-2,4-dithione (**15**).

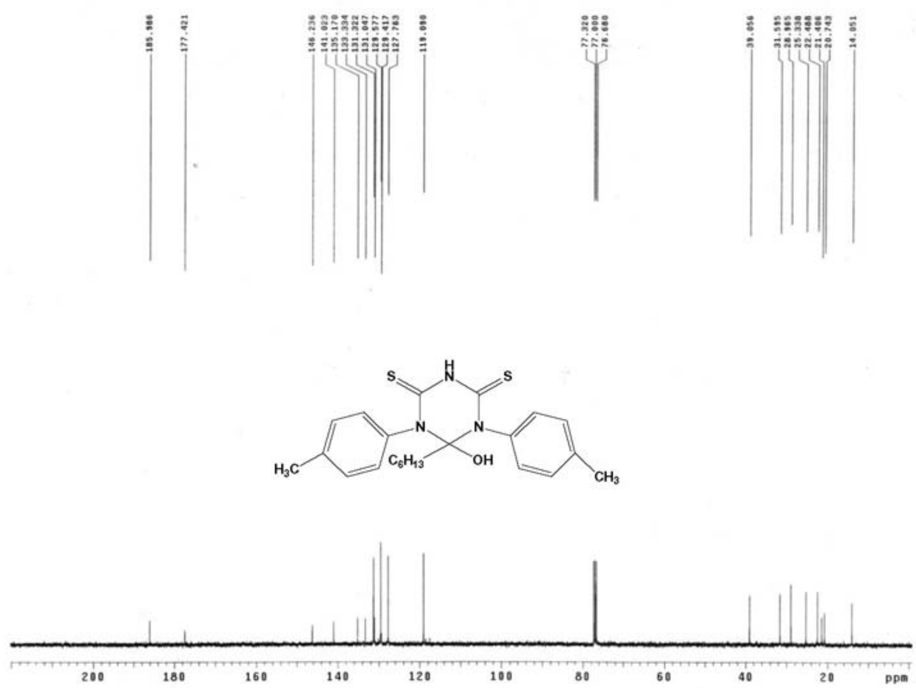


Figure S45. ^{13}C NMR ($CDCl_3$) spectrum of 6-hydroxy-6-hexyl-1,5-di(4-methylphenyl)-1,3,5-triazinane-2,4-dithione (**15**).

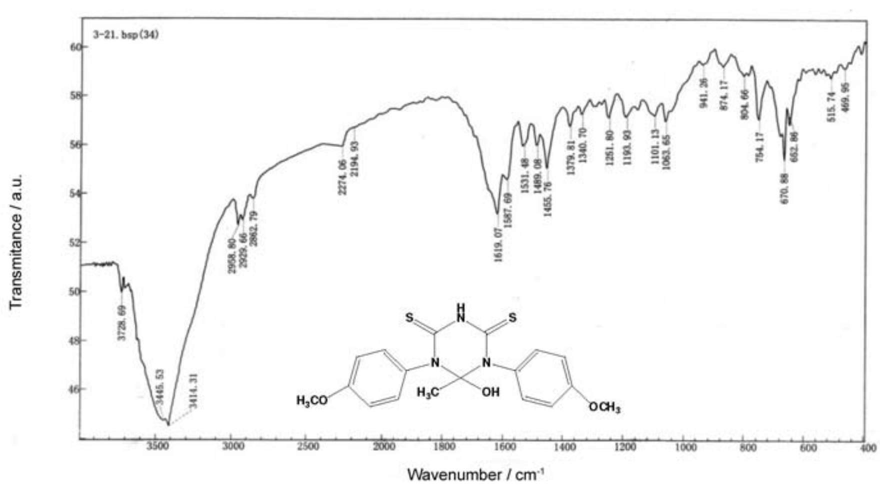


Figure S46. IR (KBr) spectrum of 6-hydroxy-6-methyl-1,5-di(4-methoxyphenyl)-1,3,5-triazinane-2,4-dithione (**16**).

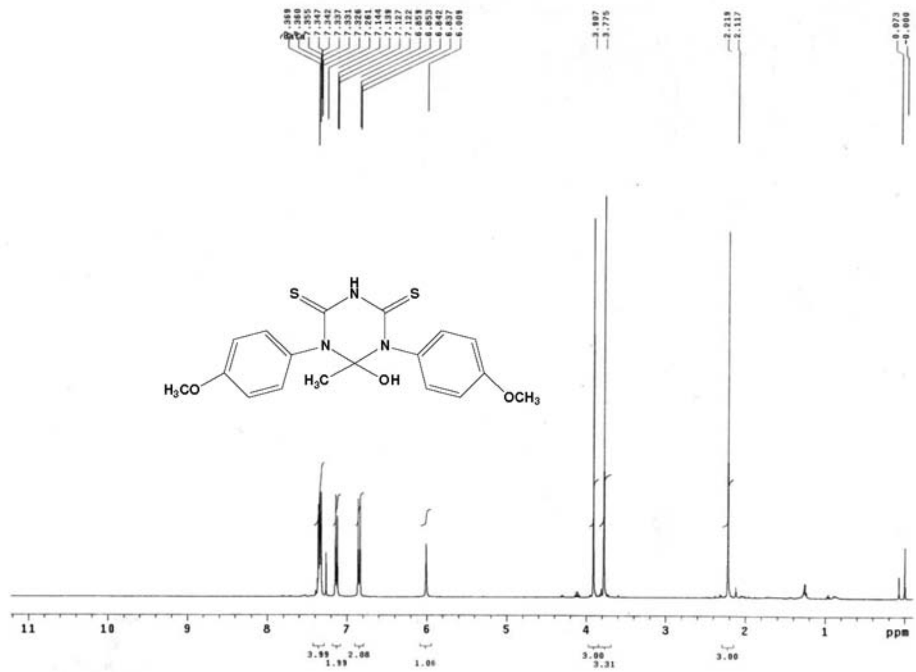


Figure S47. ¹H NMR ($CDCl_3$) spectrum of 6-hydroxy-6-methyl-1,5-di(4-methoxyphenyl)-1,3,5-triazinane-2,4-dithione (**16**).

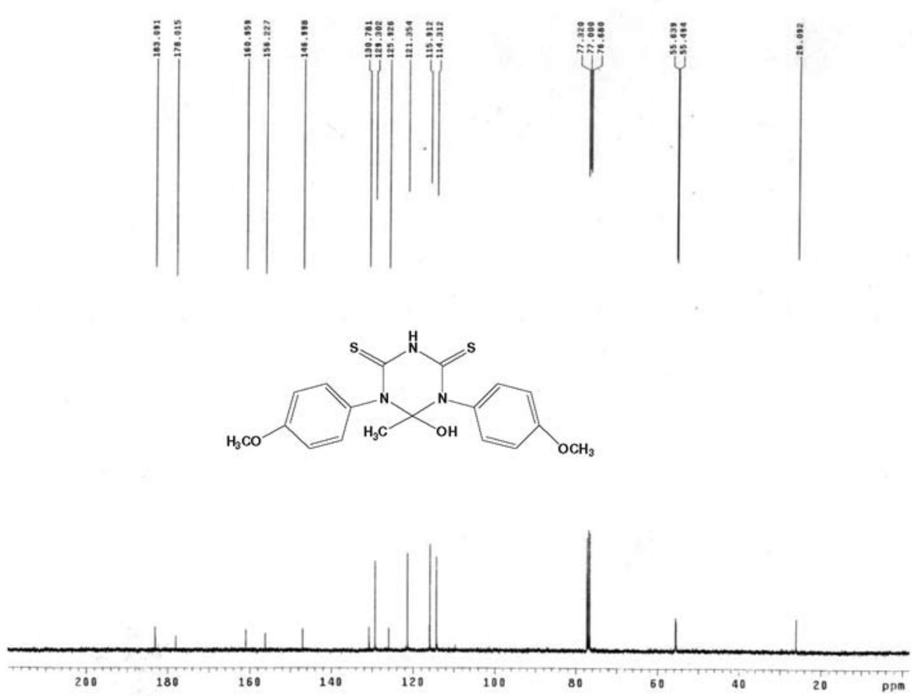


Figure S48. ¹³C NMR ($CDCl_3$) spectrum of 6-hydroxy-6-methyl-1,5-di(4-methoxyphenyl)-1,3,5-triazinane-2,4-dithione (**16**).

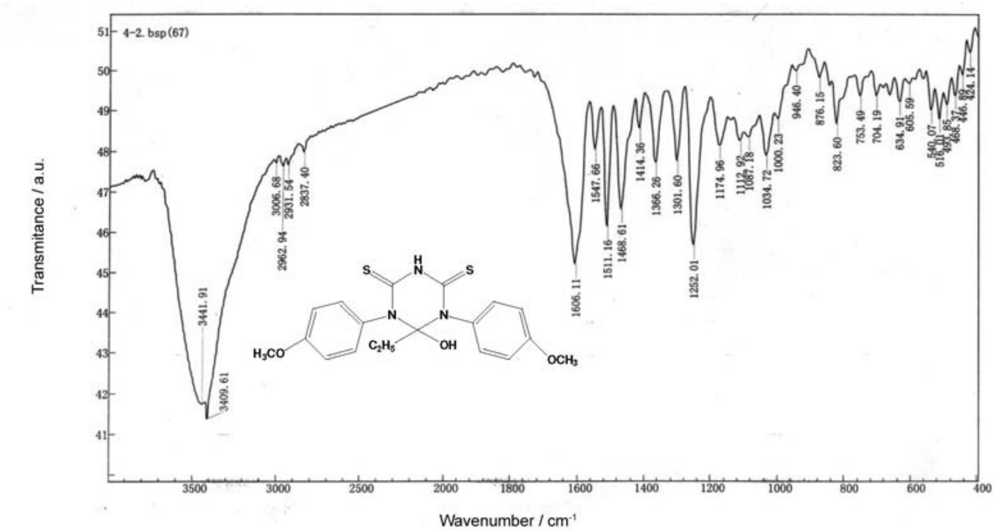


Figure S49. IR (KBr) spectrum of 6-hydroxy-6-ethyl-1,5-di(4-methoxyphenyl)-1,3,5-triazinane-2,4-dithione (**17**).

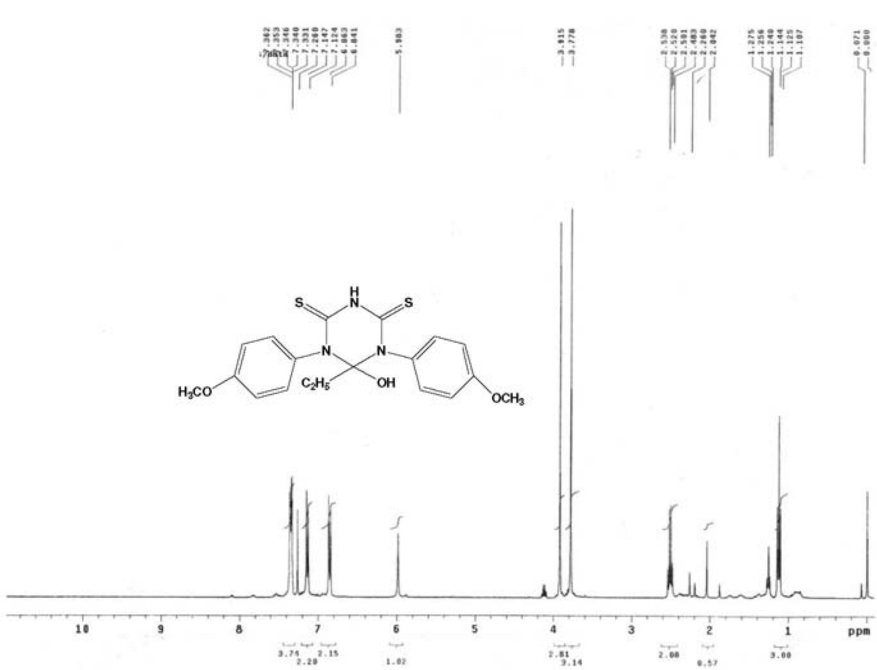


Figure S50. ^{1}H NMR ($CDCl_3$) spectrum of 6-hydroxy-6-ethyl-1,5-di(4-methoxyphenyl)-1,3,5-triazinane-2,4-dithione (**17**).

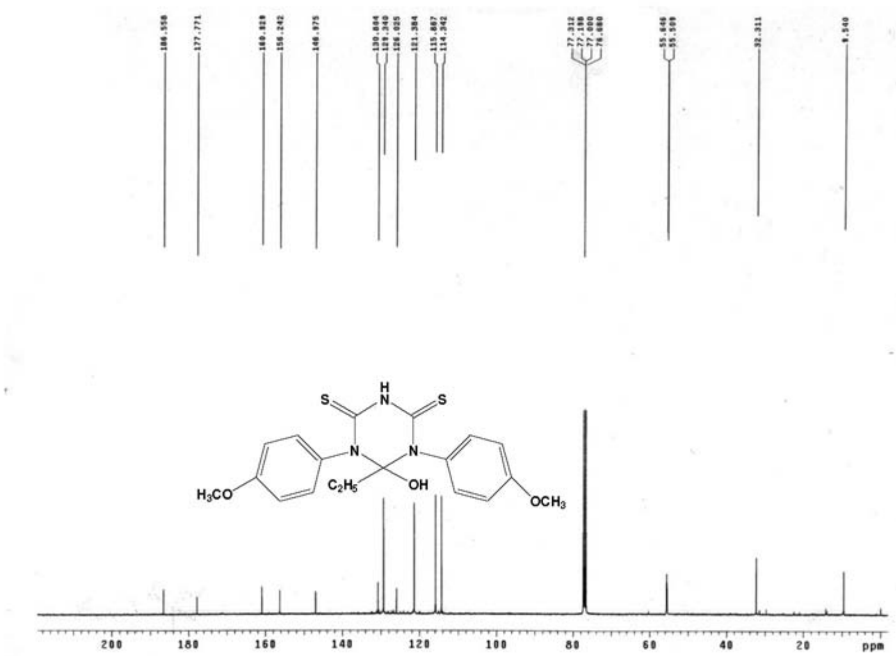


Figure S51. ^{13}C NMR ($CDCl_3$) spectrum of 6-hydroxy-6-ethyl-1,5-di(4-methoxyphenyl)-1,3,5-triazinane-2,4-dithione (**17**).

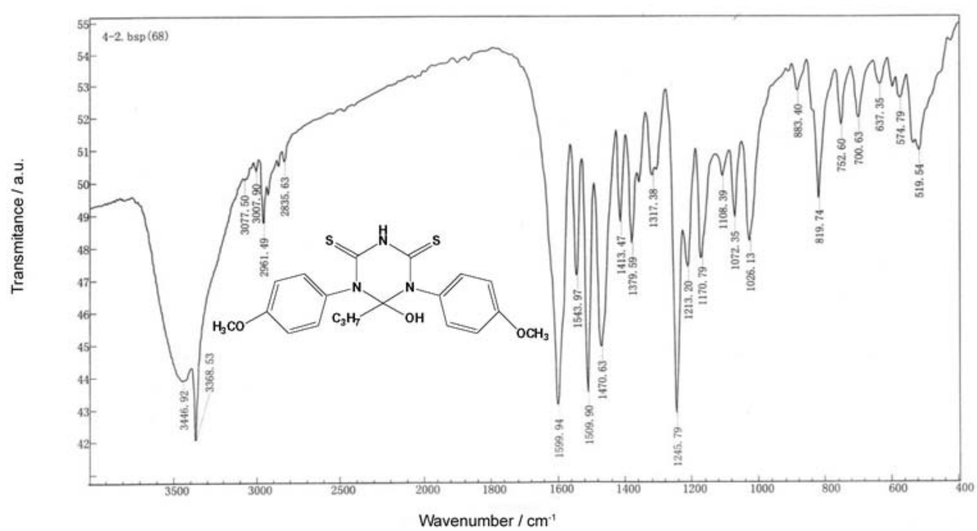


Figure S52. IR (KBr) spectrum of 6-hydroxy-6-propyl-1,5-di(4-methoxyphenyl)-1,3,5-triazinane-2,4-dithione (**18**).

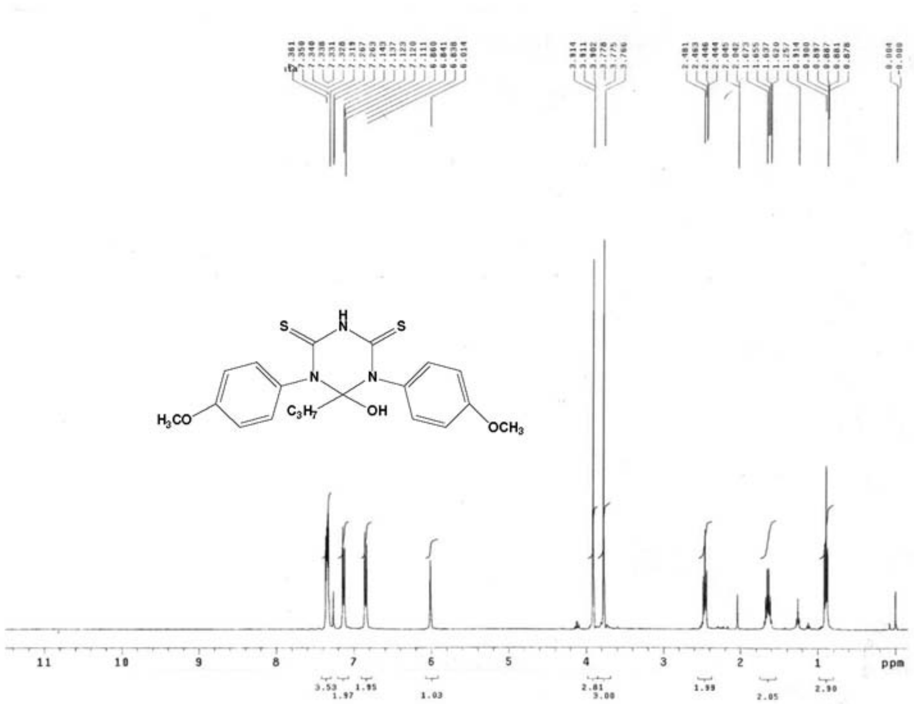


Figure S53. [1]H NMR ($CDCl_3$) spectrum of 6-hydroxy-6-propyl-1,5-di(4-methoxyphenyl)-1,3,5-triazinane-2,4-dithione (**18**).

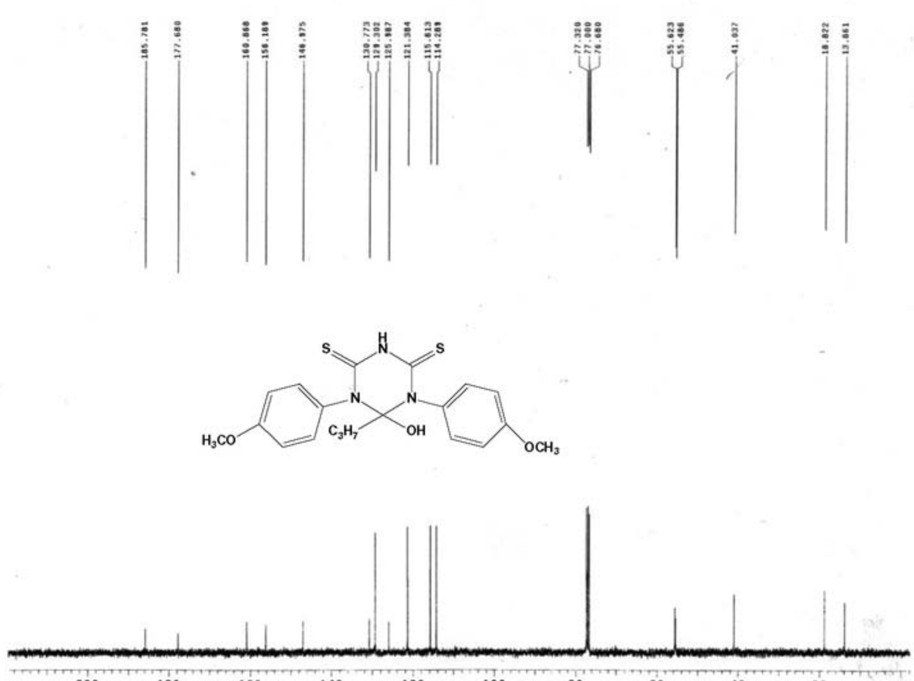


Figure S54. [13]C NMR ($CDCl_3$) spectrum of 6-hydroxy-6-propyl-1,5-di(4-methoxyphenyl)-1,3,5-triazinane-2,4-dithione (**18**).

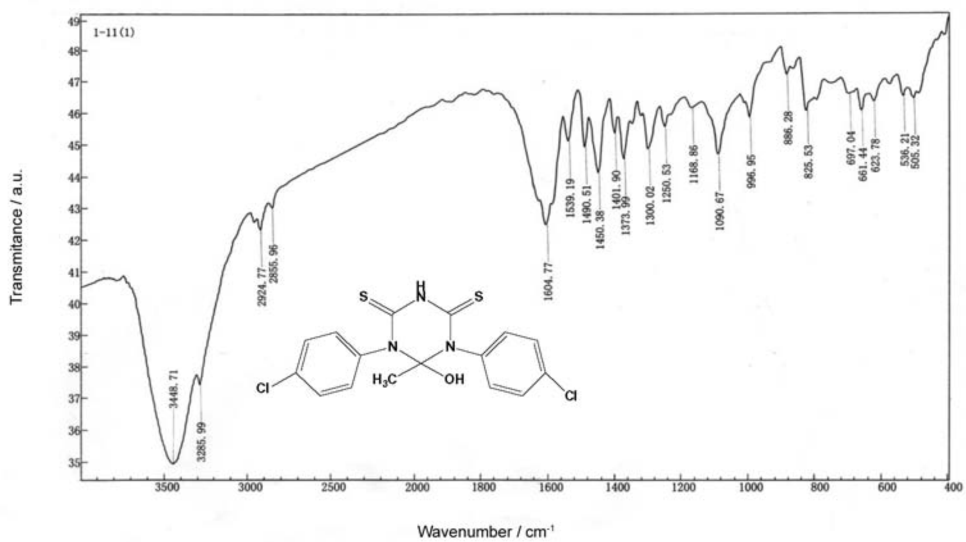


Figure S55. IR (KBr) spectrum of 6-hydroxy-6-methyl-1,5-di(4-chlorophenyl)-1,3,5-triazinane-2,4-dithione (**19**).

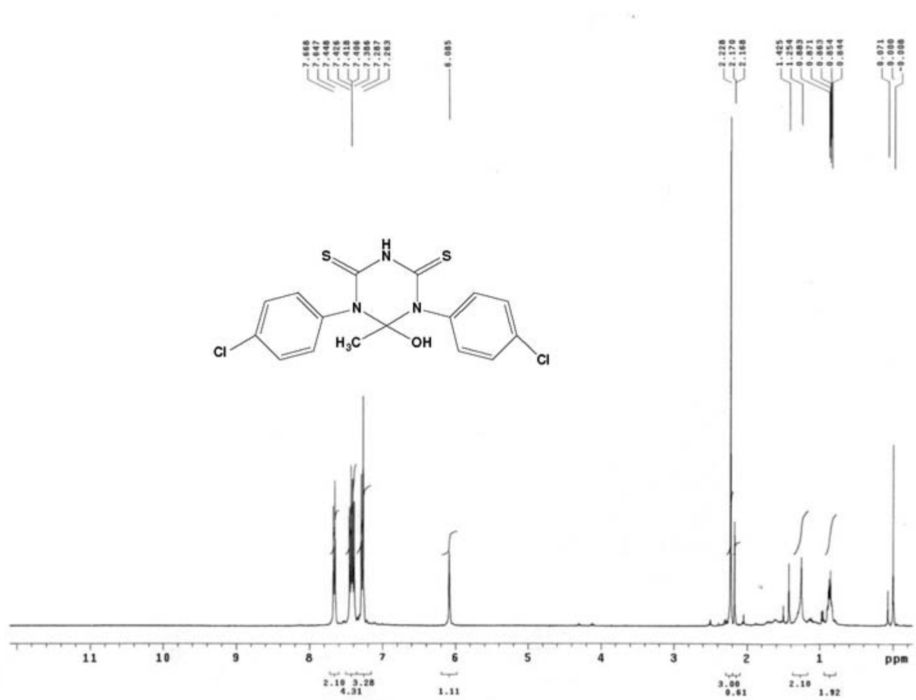


Figure S56. ^{1}H NMR ($CDCl_3$) spectrum of 6-hydroxy-6-methyl-1,5-di(4-chlorophenyl)-1,3,5-triazinane-2,4-dithione (**19**).

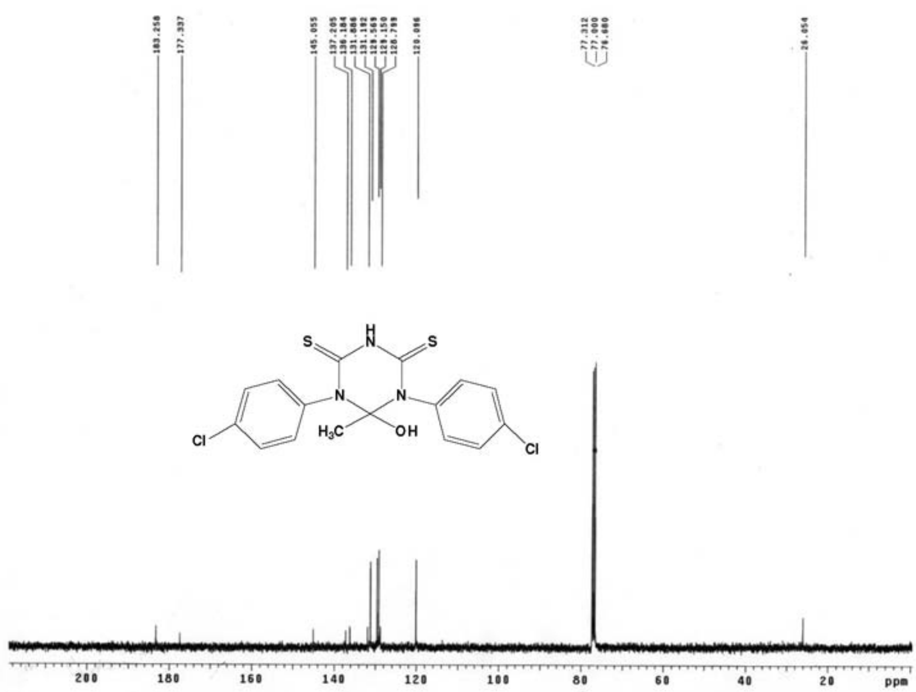


Figure S57. ^{13}C NMR ($CDCl_3$) spectrum of 6- ydroxyl-6-methyl-1,5-di(4-chlorophenyl)-1,3,5-triazinane-2,4-dithione (**19**).