Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Janus head type lone pair–π–lone pair and S···F···S interactions in retaining hexafluorobenzene

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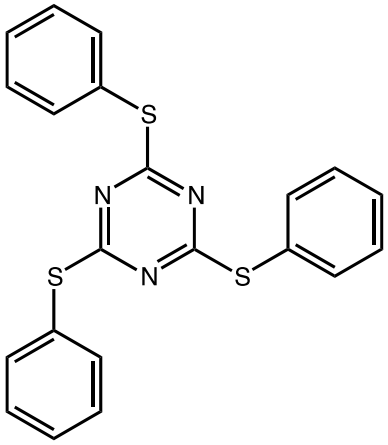
Figure S 1. **^{1}H NMR spectrum of 2,4,6-tris(phenylthio)-1,3,5-triazine (1) in $CDCl_3$.**



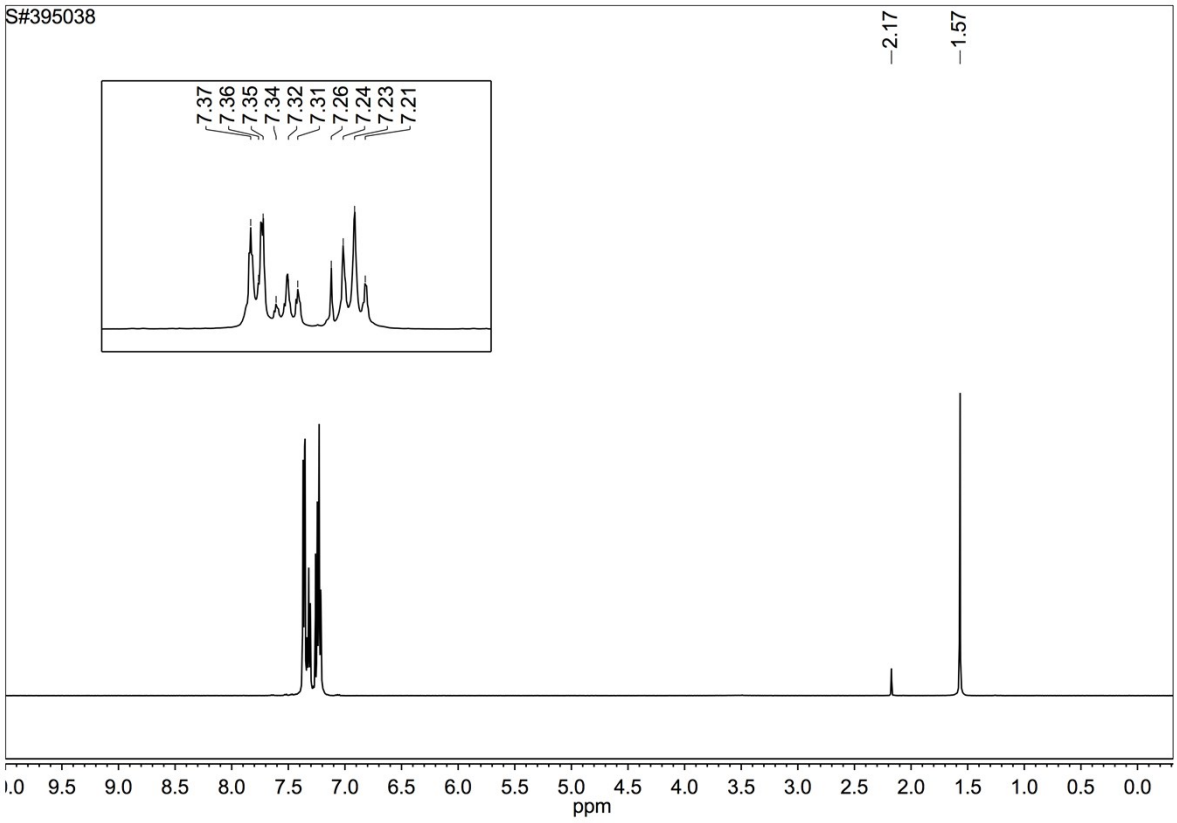
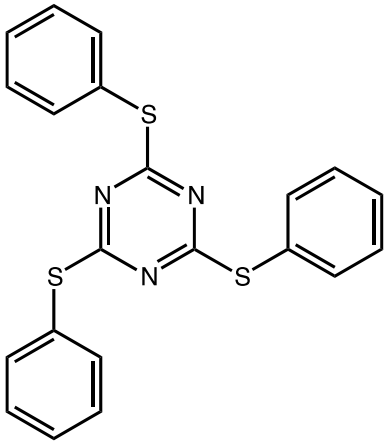


Figure S 2. **^{13}C NMR spectrum of 2,4,6-tris(phenylthio)-1,3,5-triazine (1) in $CDCl_3$.**



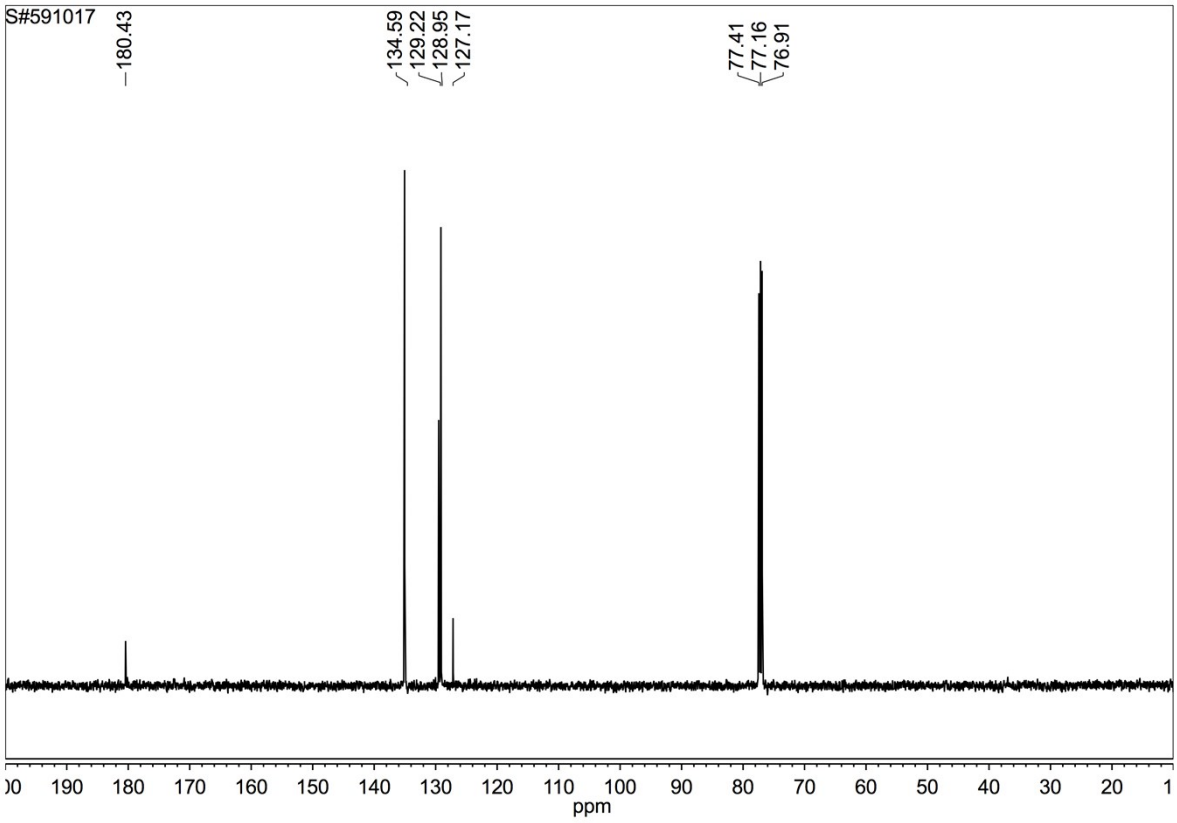
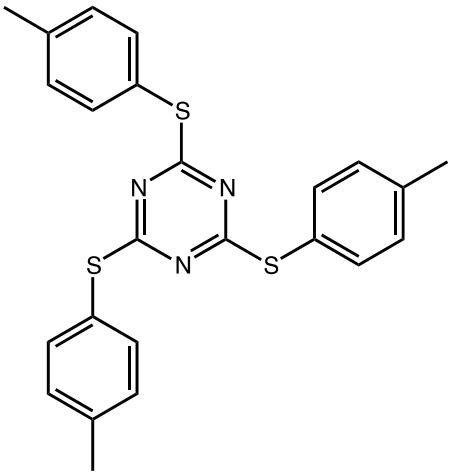


Figure S 3. **^{1}H NMR spectrum of 2,4,6-tris(p-tolylthio)-1,3,5-triazine (2) in $CDCl_3$.**



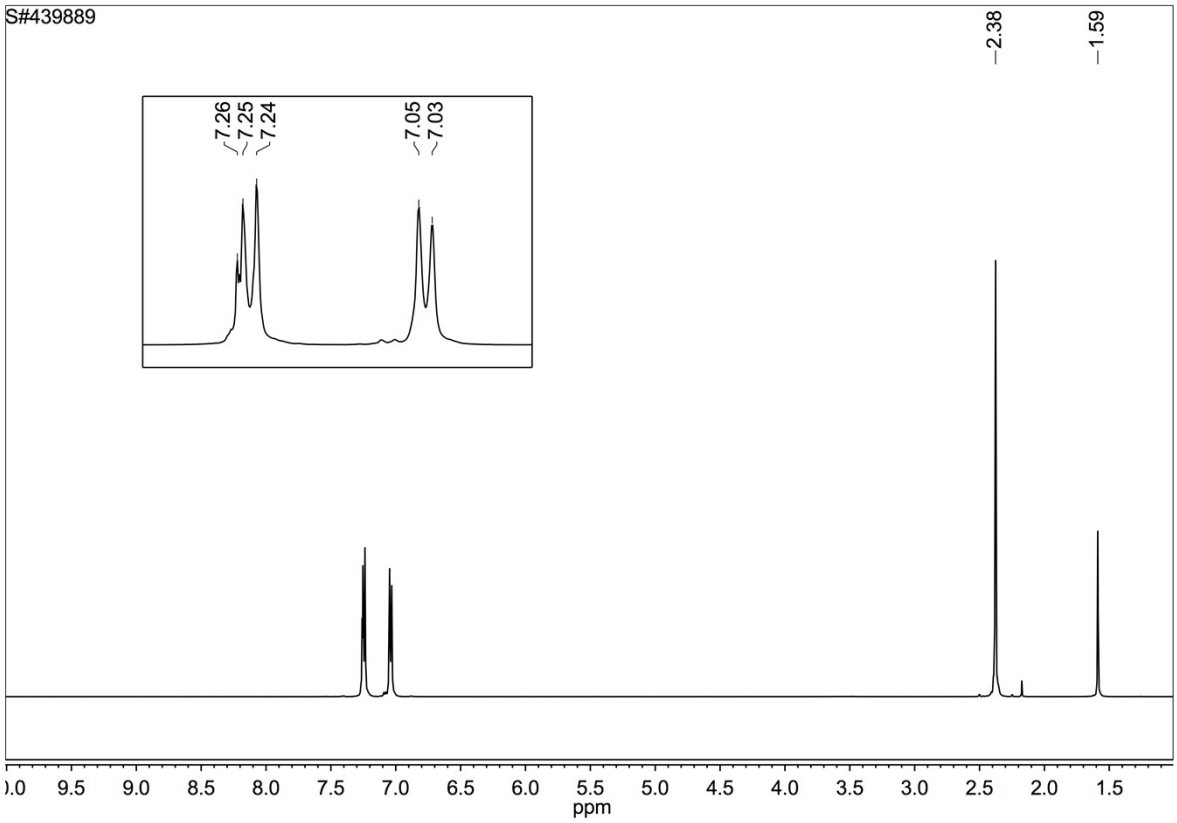
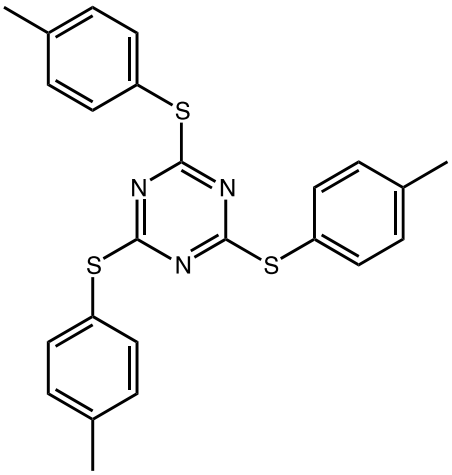


Figure S 4. **^{13}C NMR spectrum of 2,4,6-tris(p-tolylthio)-1,3,5-triazine (2) in $CDCl_3$.**



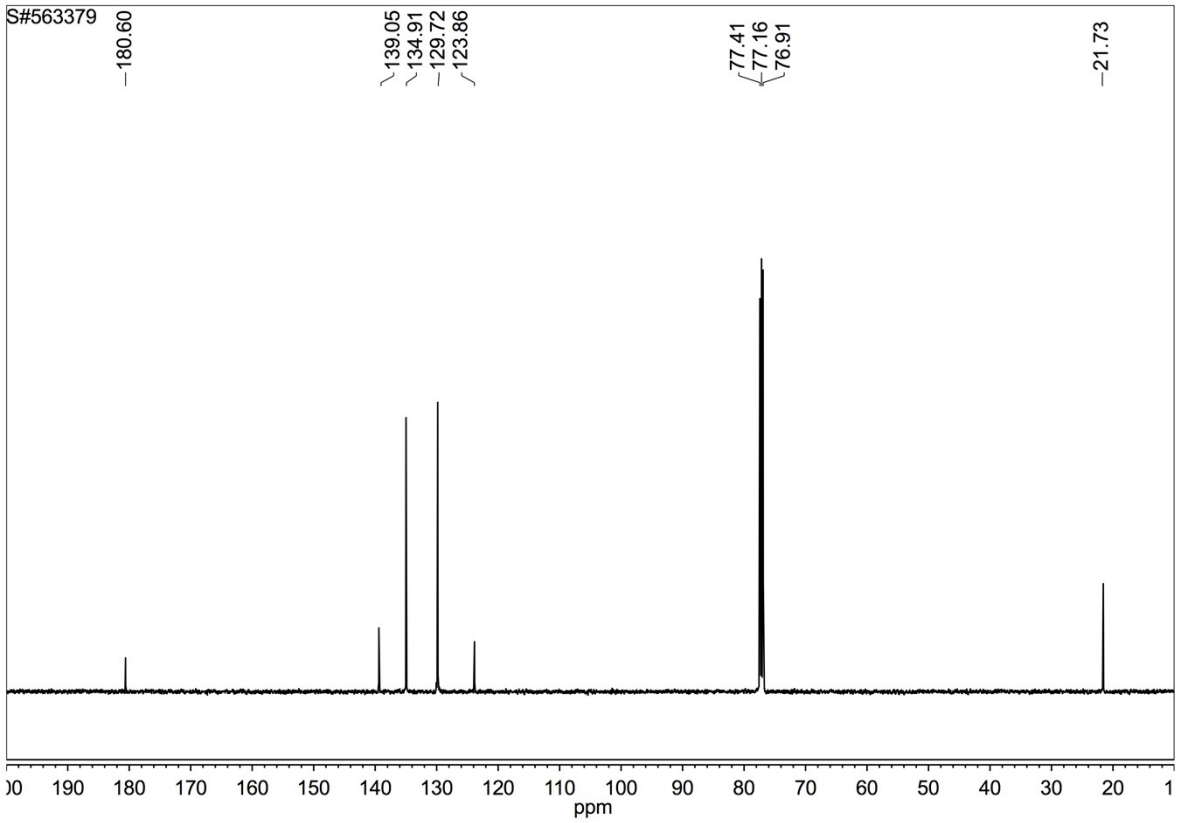
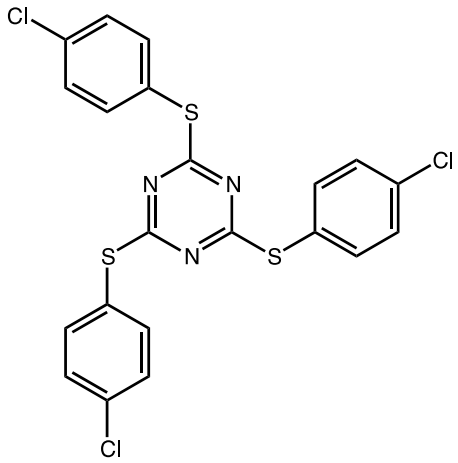


Figure S 5. **^{1}H NMR spectrum of 2,4,6-tris((4-chlorophenyl)thio)-1,3,5-triazine (3) in $CDCl_3$.**



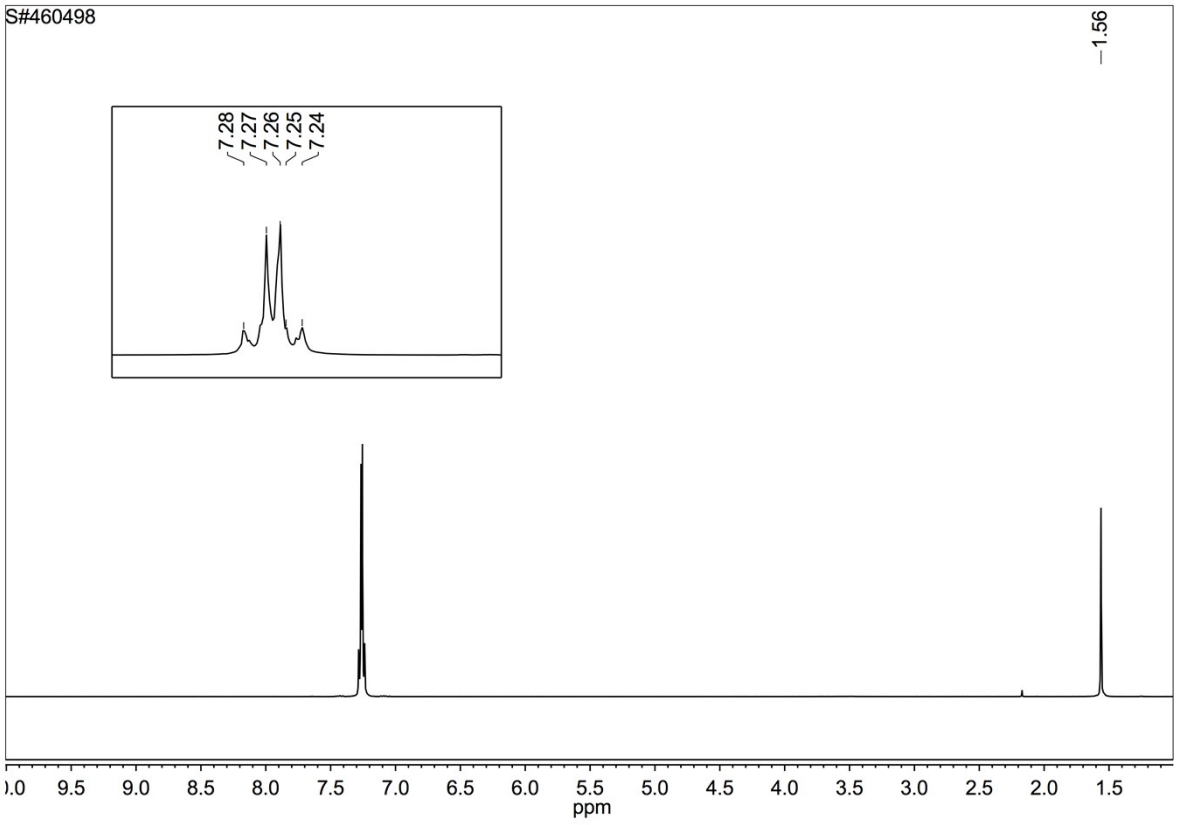


Figure S 6. **^{13}C NMR spectrum of 2,4,6-tris((4-chlorophenyl)thio)-1,3,5-triazine (3) in $CDCl_3$.**

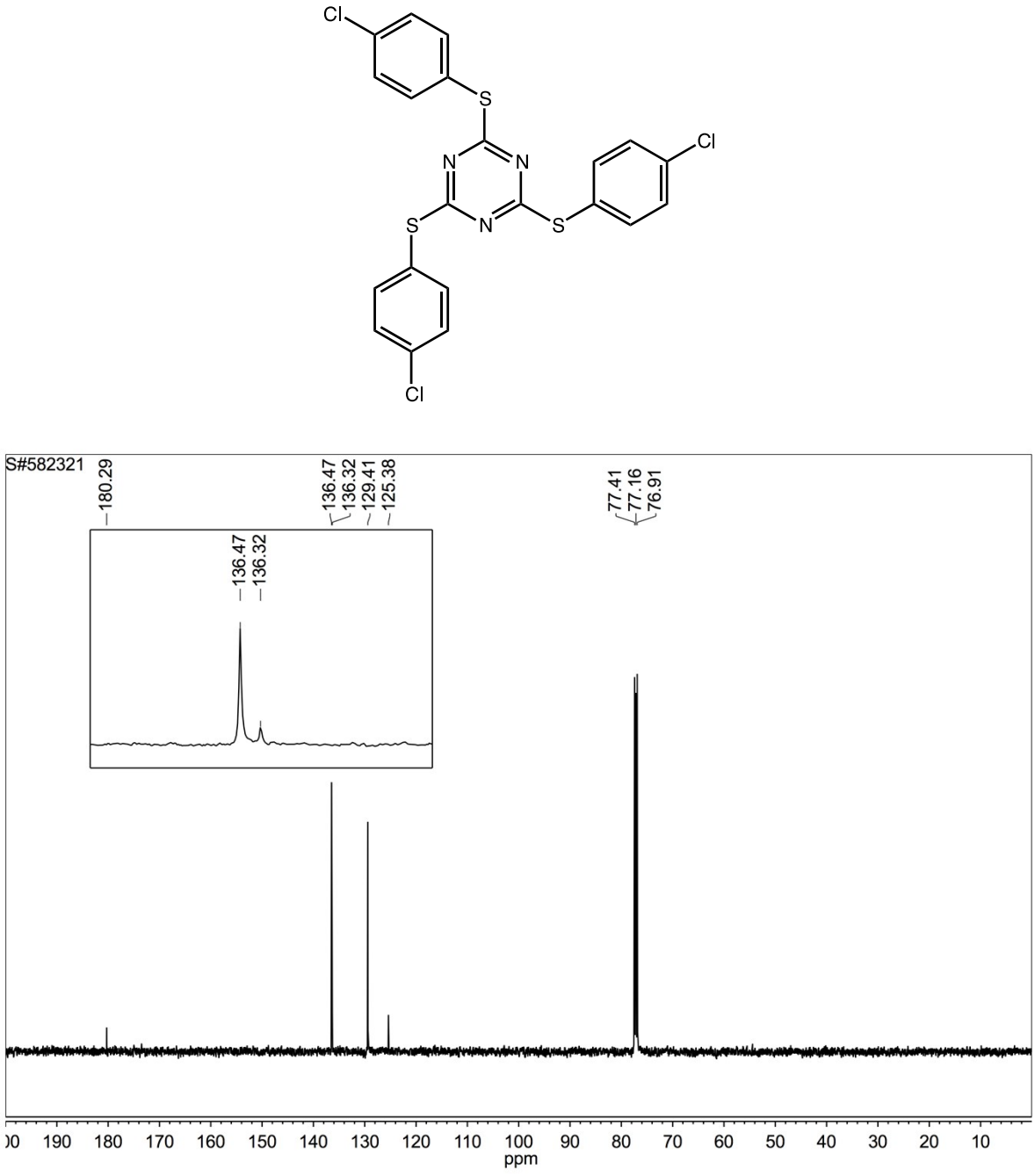


Figure S 7. **^{1}H NMR spectrum of 3-nitrobenzene-1-sulfonyl chloride in $CDCl_3$.**

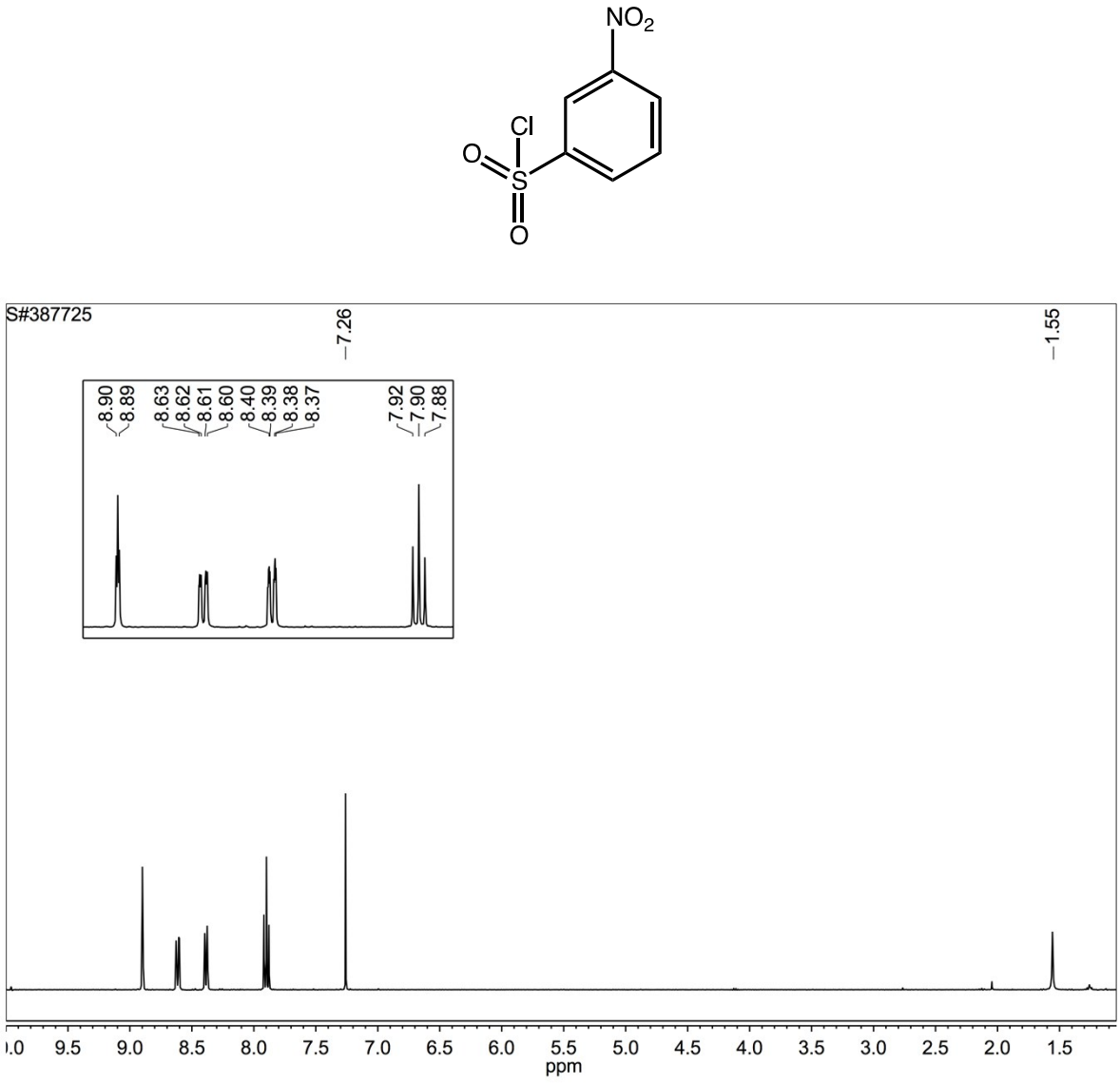


Figure S 8. **^{13}C NMR spectrum of 3-nitrobenzene-1-sulfonyl chloride in $CDCl_3$.**

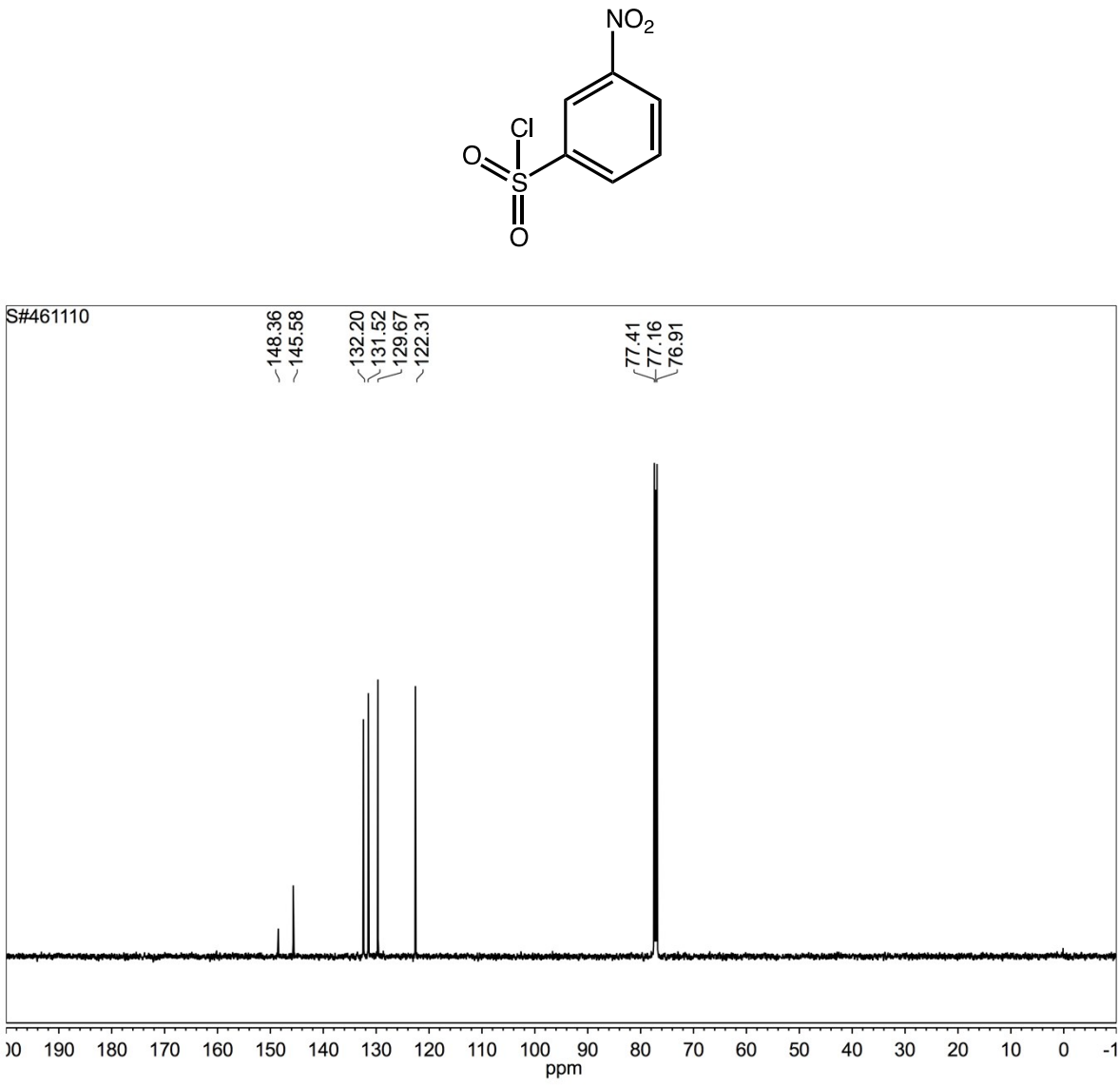


Figure S 9. **^{1}H NMR spectrum of 3-nitrobenzenethiol in $CDCl_3$.**

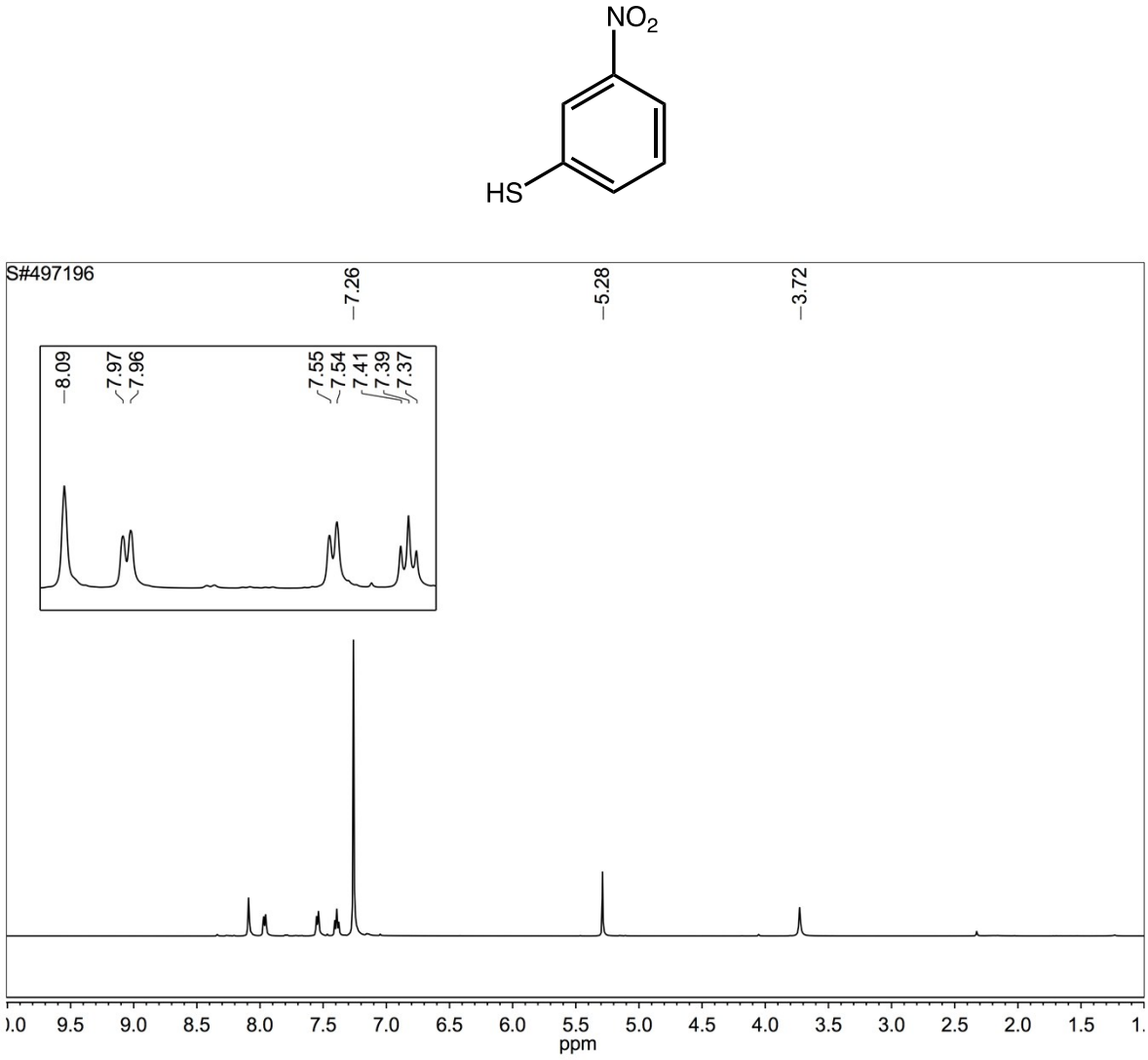


Figure S 10. **^{13}C NMR spectrum of 3-nitrobenzenethiol in $CDCl_3$.**

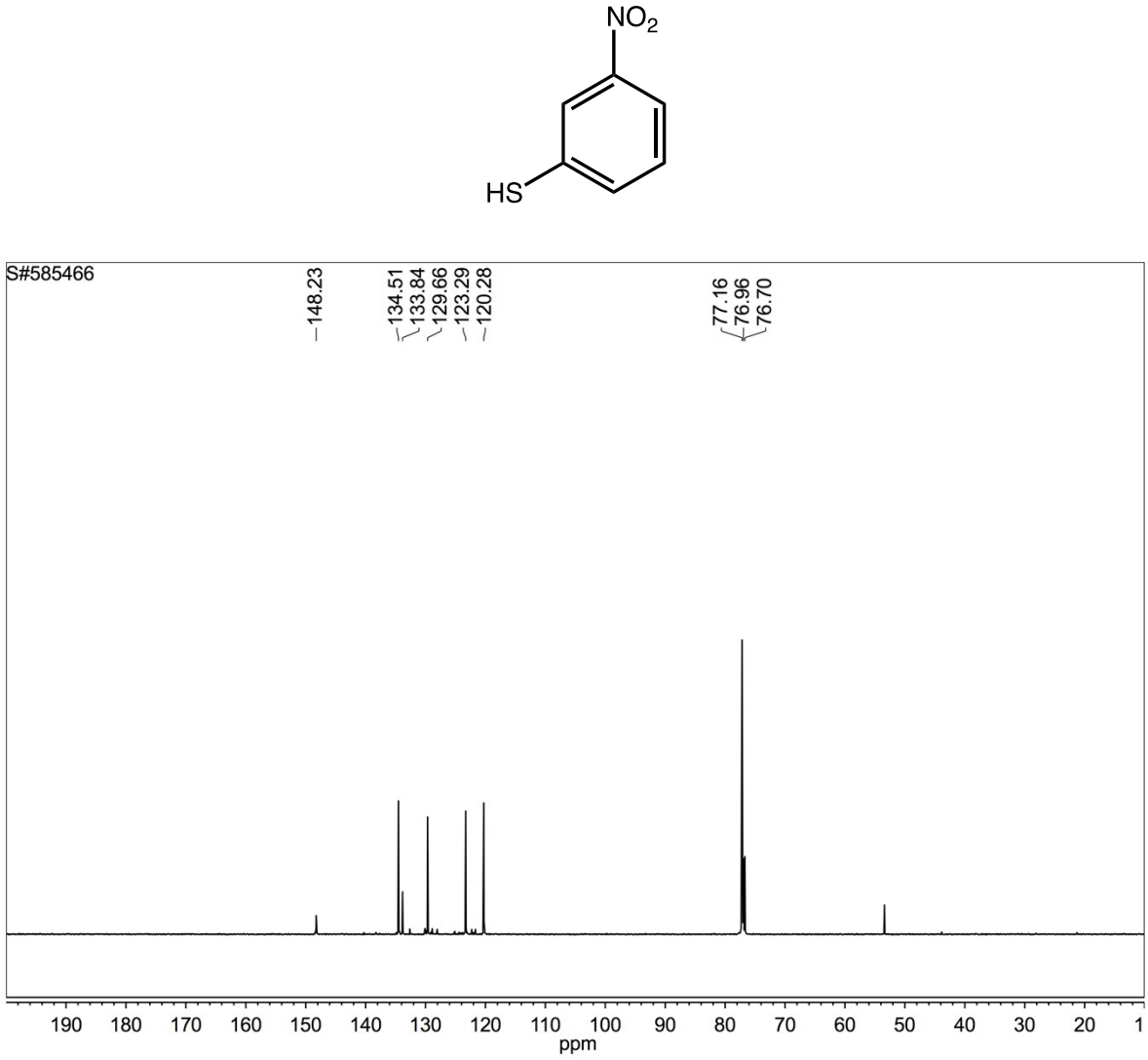
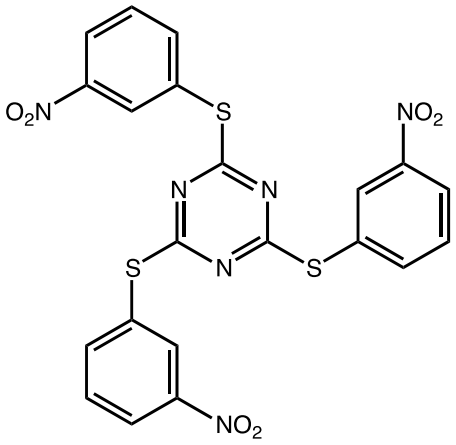


Figure S 11. **^{1}H NMR spectrum of 2,4,6-tris((3-nitrophenyl)thio)-1,3,5-triazine (4) in DMSO-d6.**



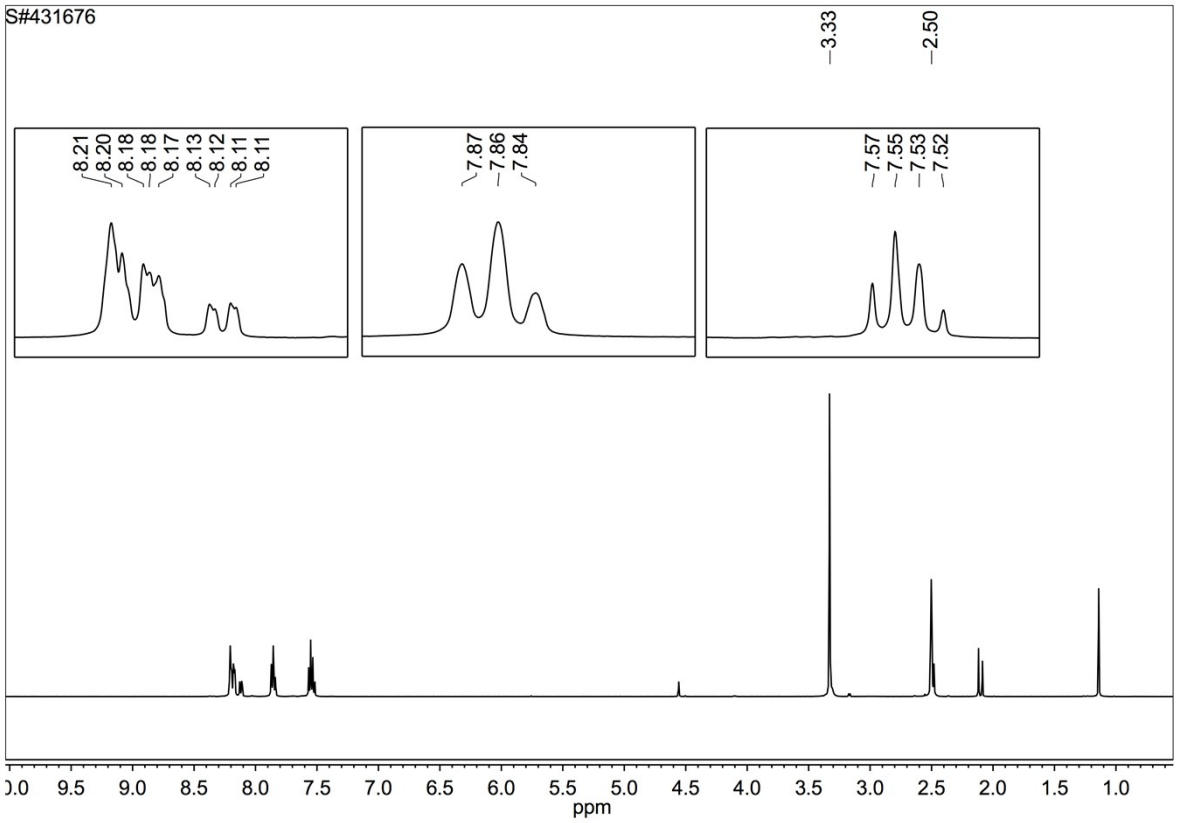
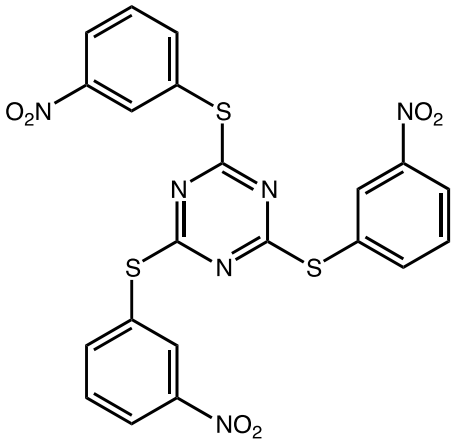


Figure S 12. **^{13}C NMR spectrum of 2,4,6-tris((3-nitrophenyl)thio)-1,3,5-triazine (4) in DMSO-d6.**



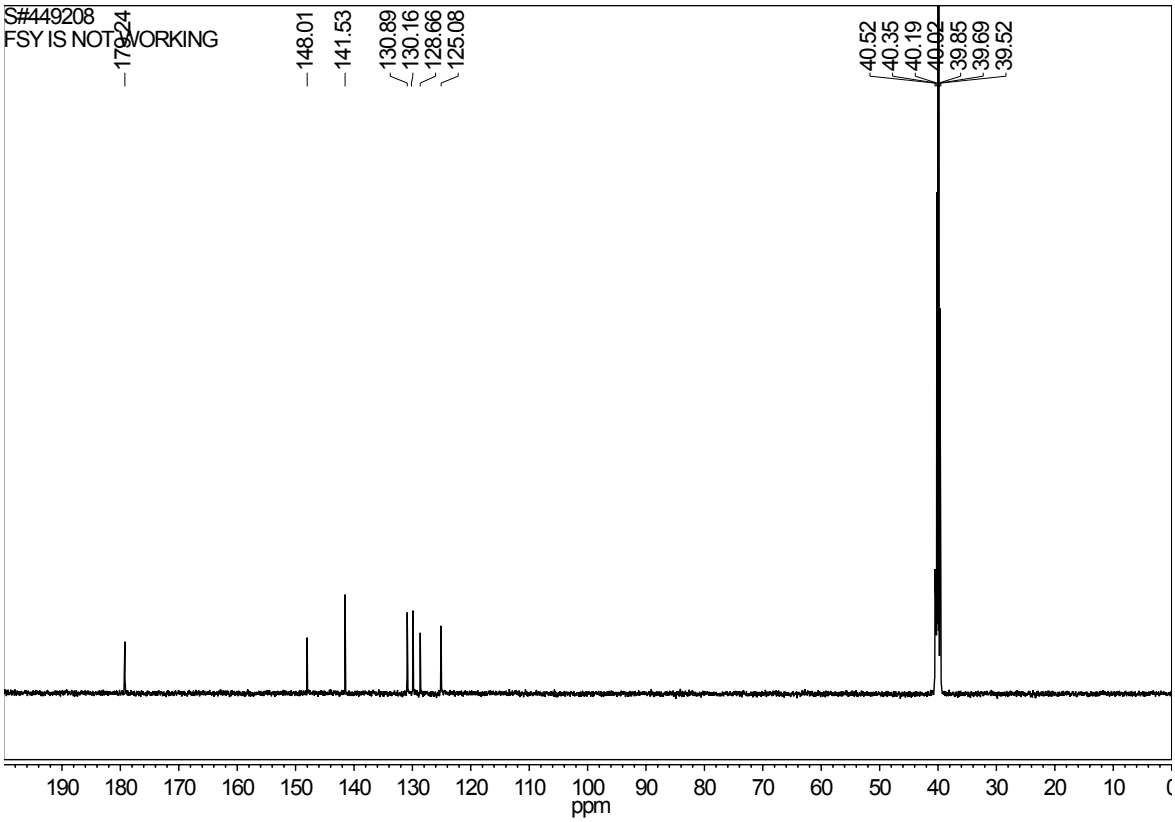
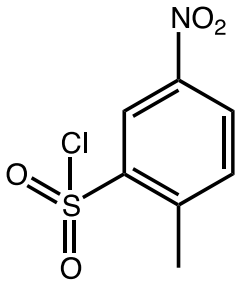


Figure S 13. **^{1}H NMR spectrum of 2-methyl-5-nitrobenzene-1-sulfonyl chloride in DMSO-d6.**



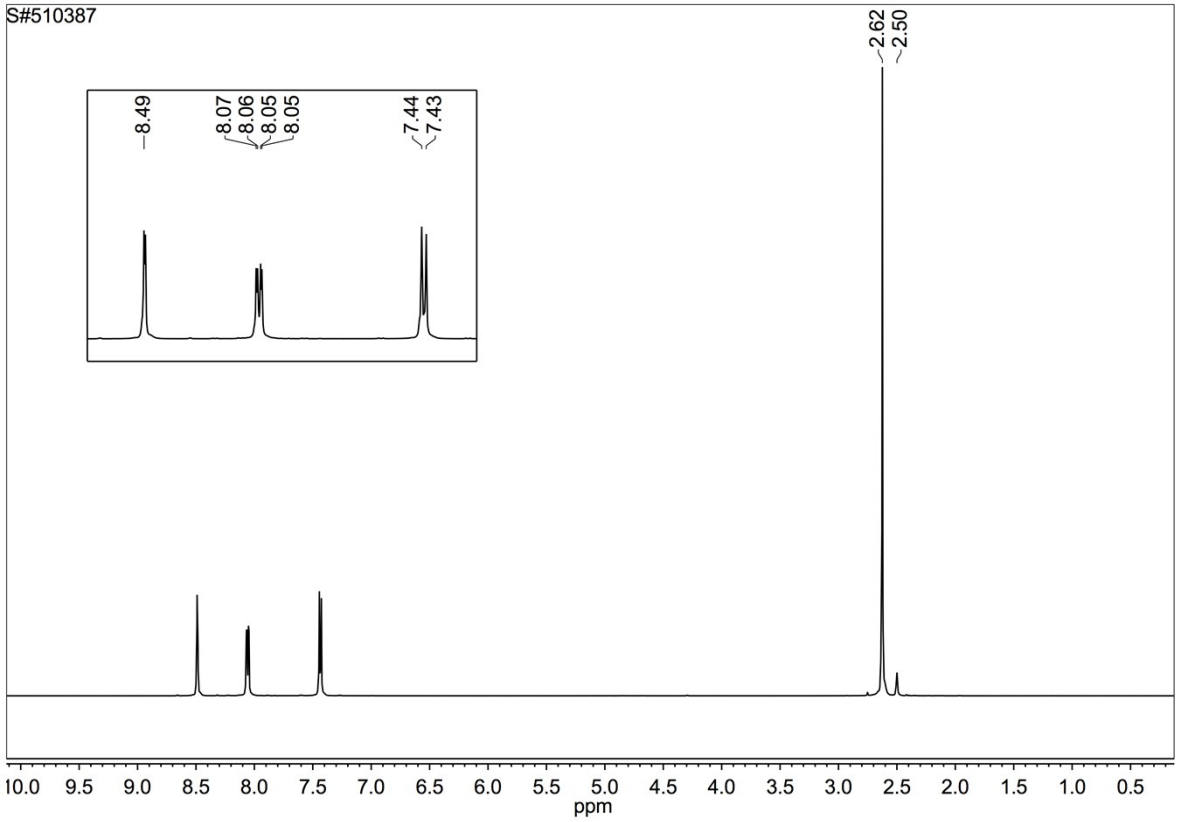


Figure S 14. **^{13}C NMR spectrum of 2-methyl-5-nitrobenzene-1-sulfonyl chloride in DMSO-d6.**

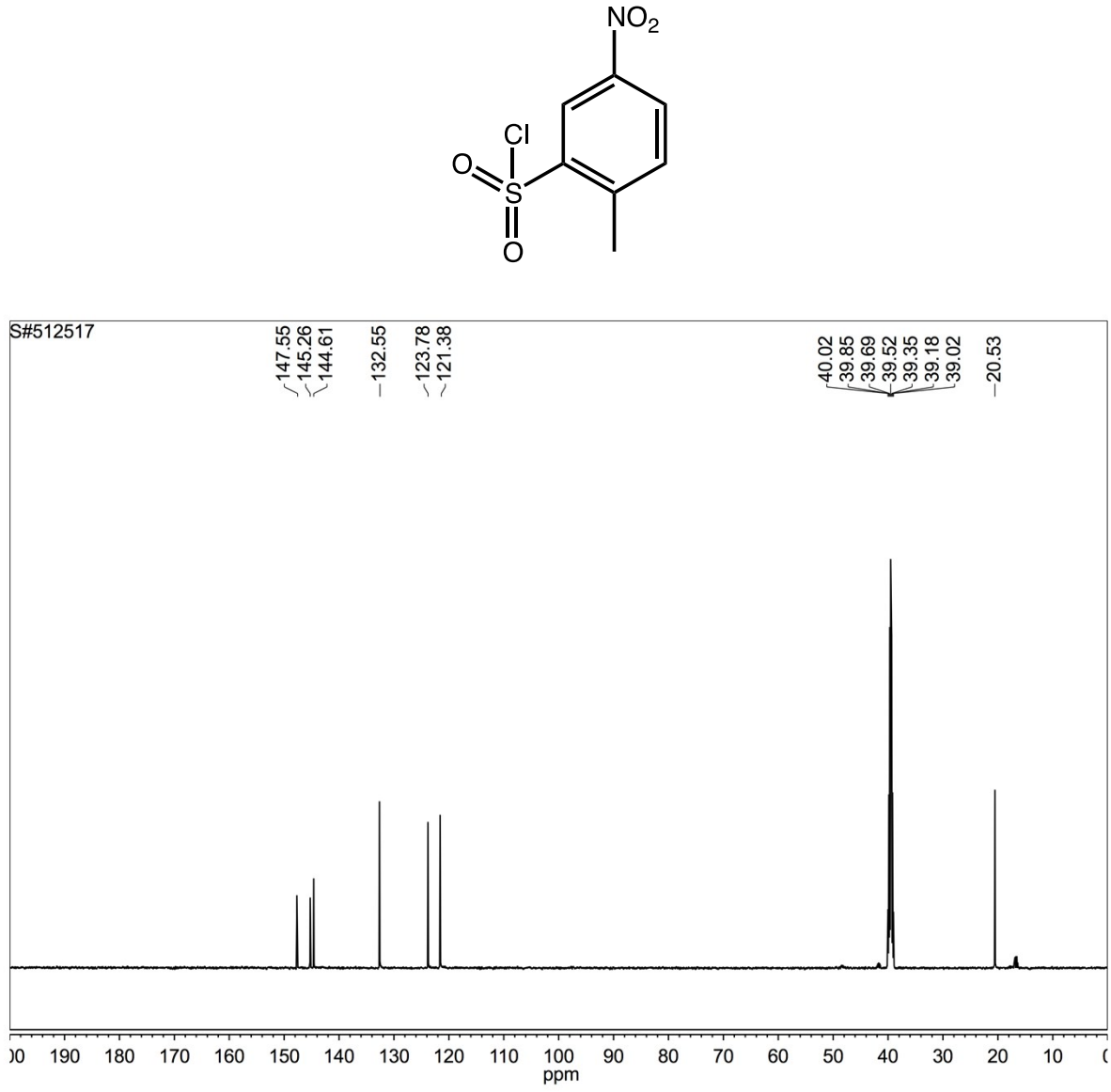


Figure S 15. **^{1}H NMR spectrum of 2-methyl-5-nitrobenzenethiol in $CDCl_3$.**

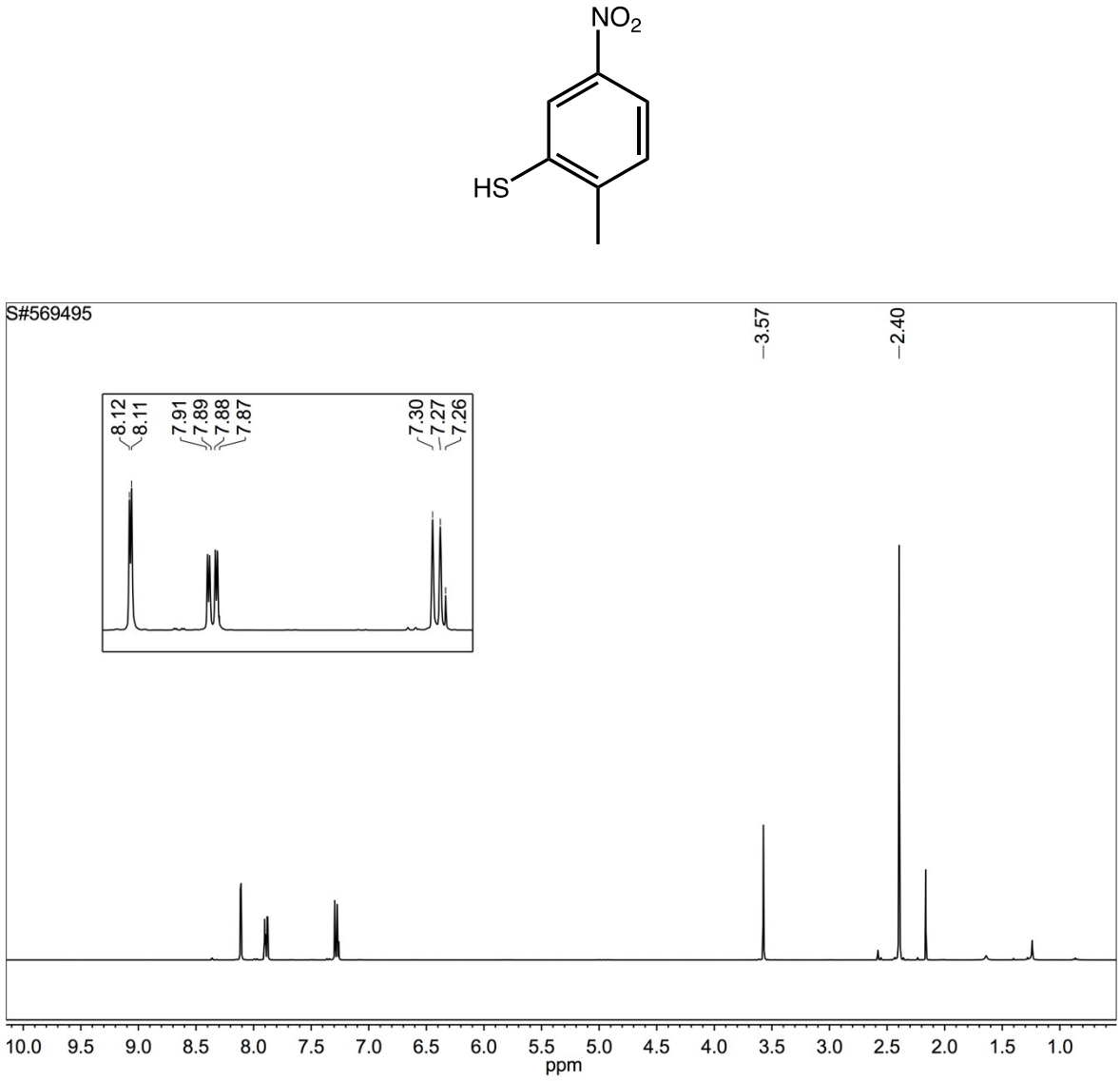


Figure S 16. **^{13}C NMR spectrum of 2-methyl-5-nitrobenzenethiol in $CDCl_3$.**

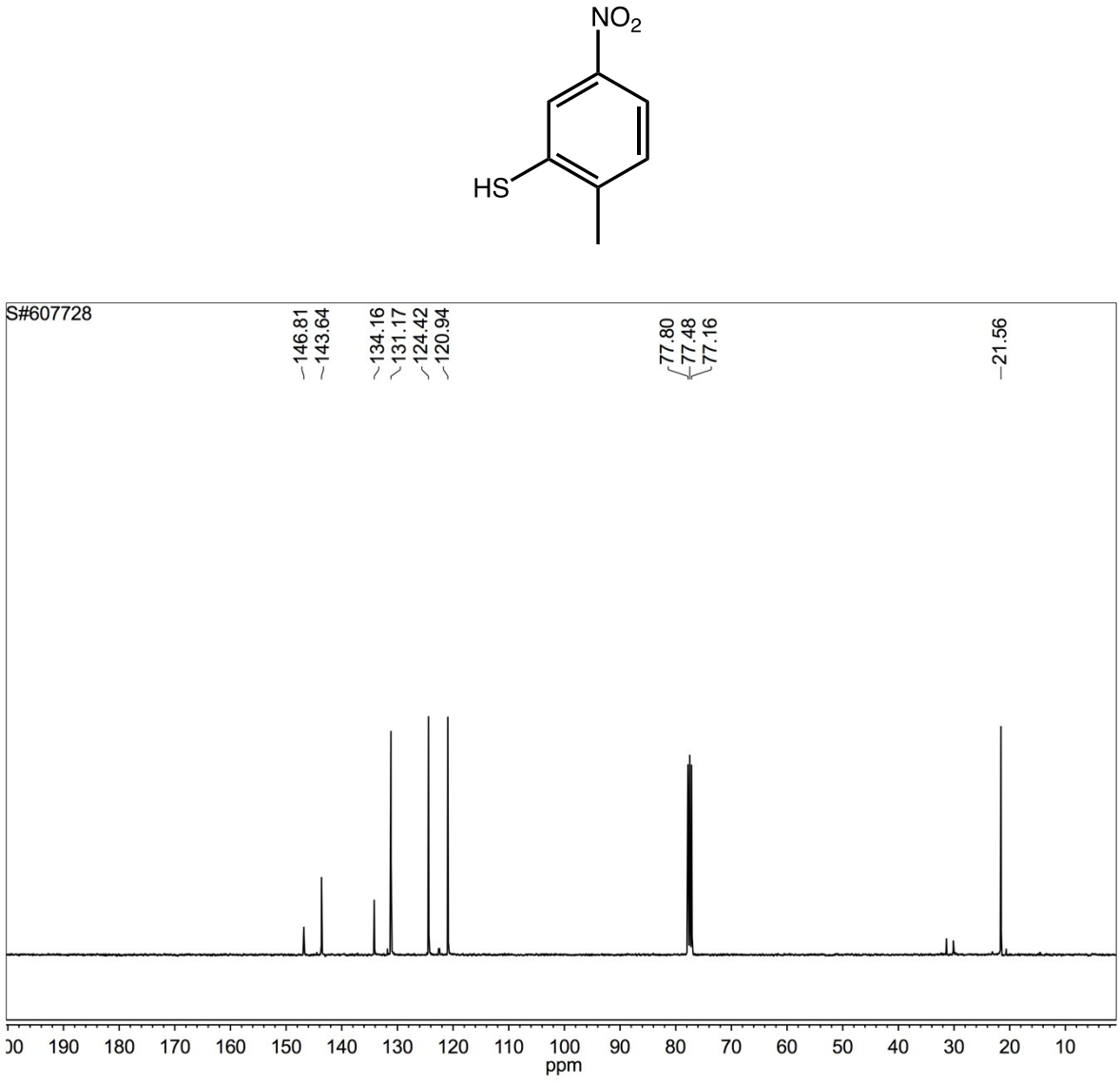
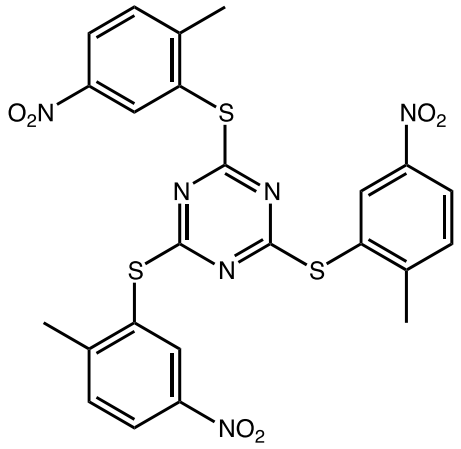


Figure S 17. **^{1}H NMR spectrum of 2,4,6-tris((2-methyl-5-nitrophenyl)thio)-1,3,5-triazine (5) in DMSO-d6.**



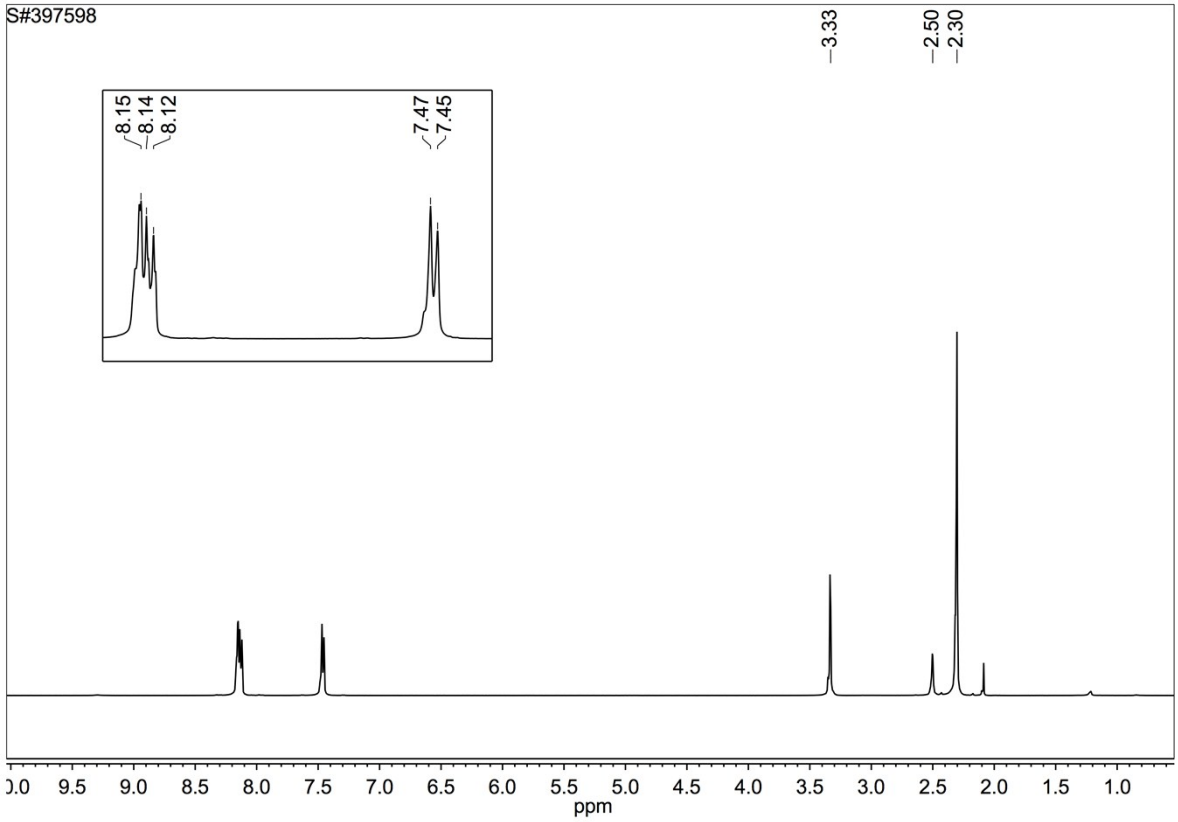
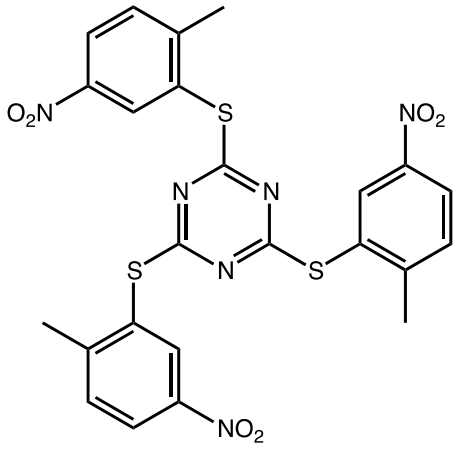


Figure S 18. **^{13}C NMR spectrum of 2,4,6-tris((2-methyl-5-nitrophenyl)thio)-1,3,5-triazine (5): in DMSO-d6.**



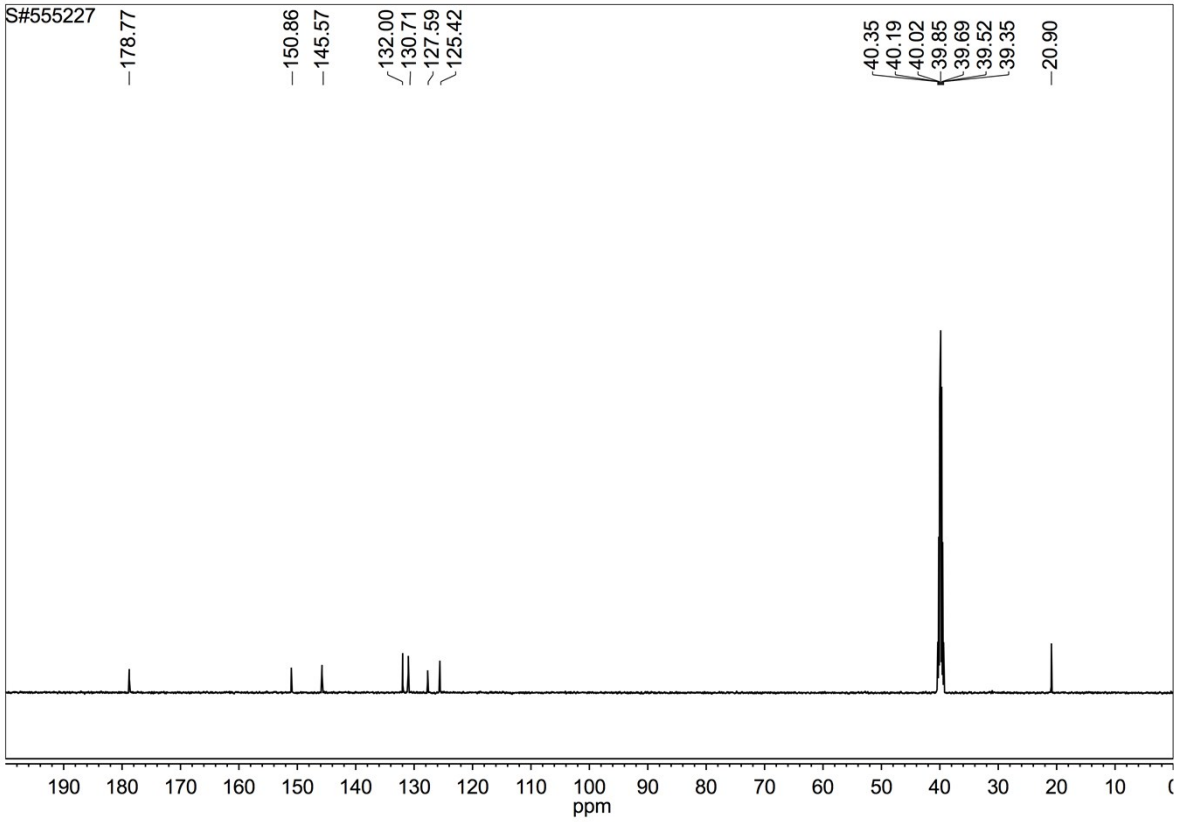


Figure S 19. **^{1}H NMR spectrum of 2,4,6-tris(2,6-dimethylphenylthio)-1,3,5-triazine (6)**

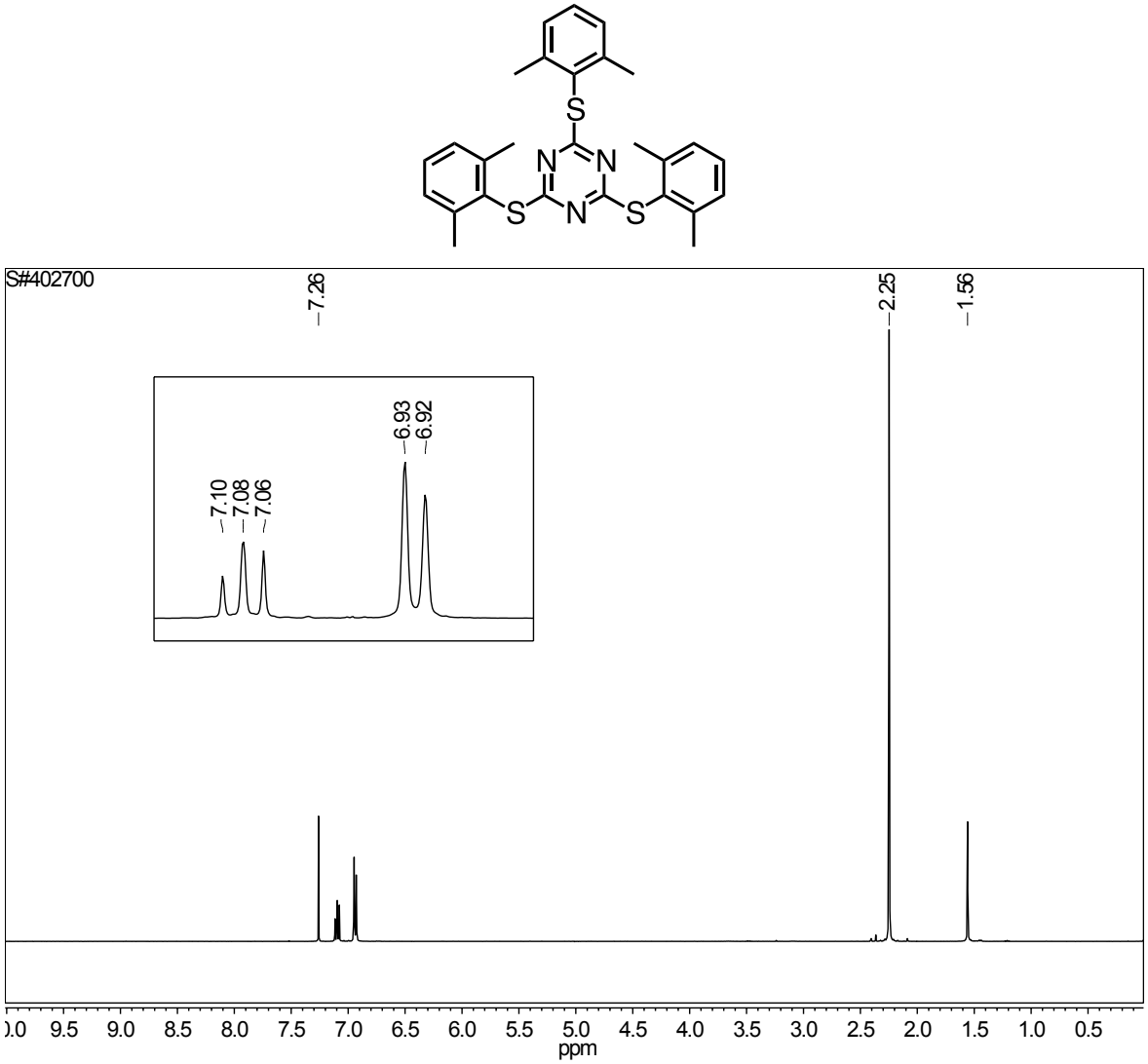


Figure S 20. **^{13}C NMR spectrum of 2,4,6-tris(2,6-dimethylphenylthio)-1,3,5-triazine (6)**

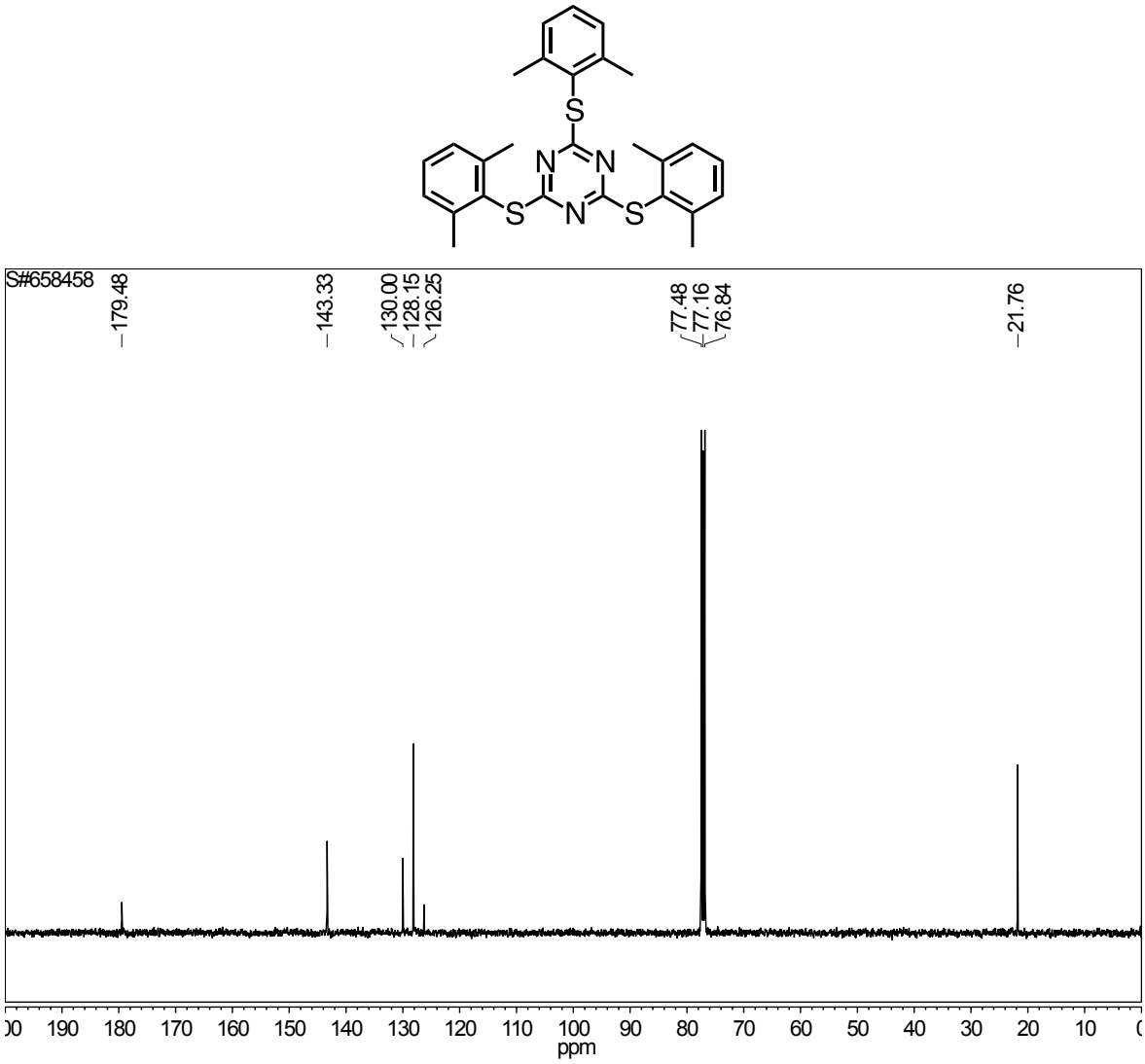


Figure S 21. **^{1}H NMR spectrum of 2,3,4,5,6-pentamethylbenzenethiol**

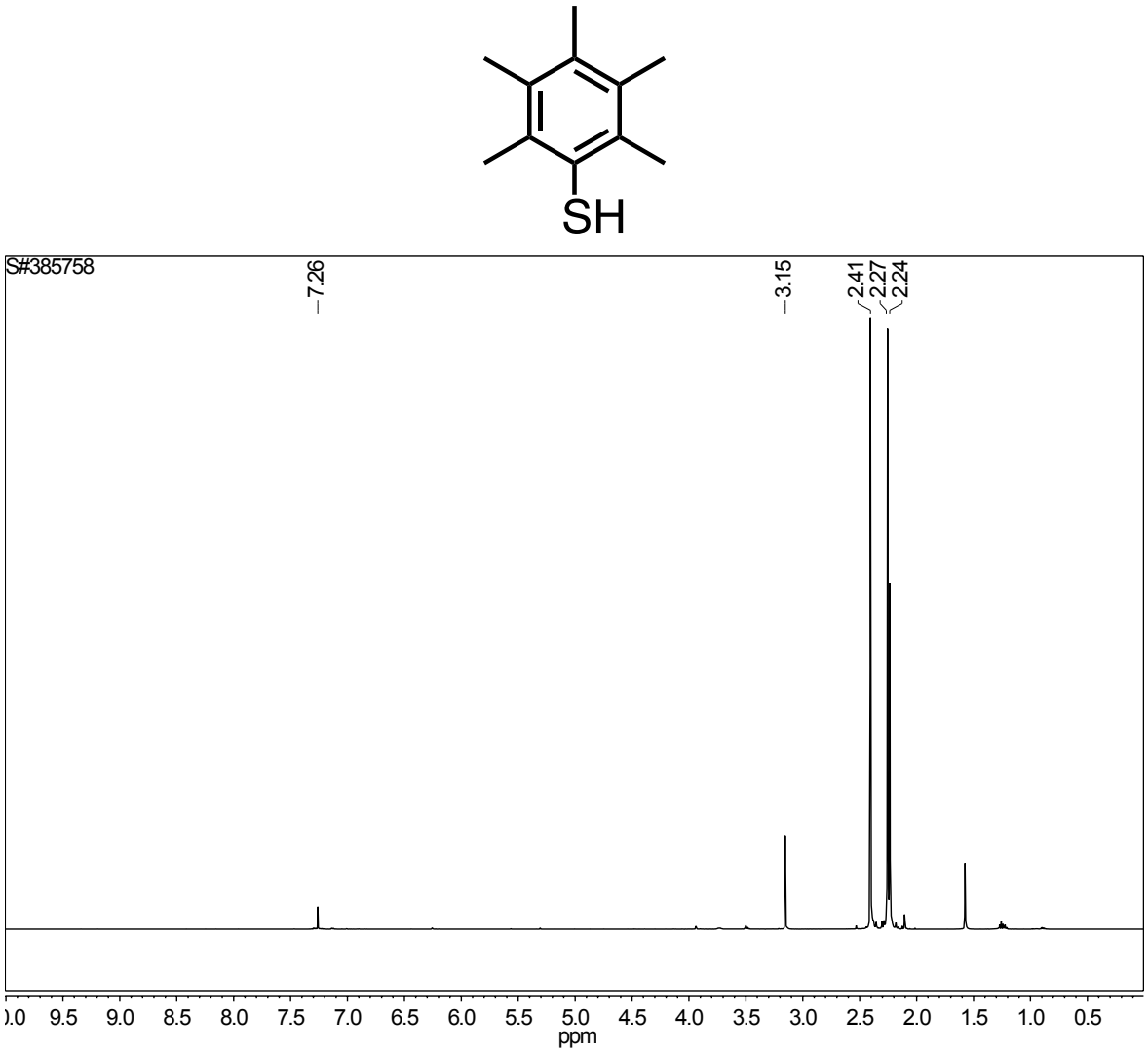


Figure S 22. **^{13}C NMR spectrum of 2,3,4,5,6-pentamethylbenzenethiol**

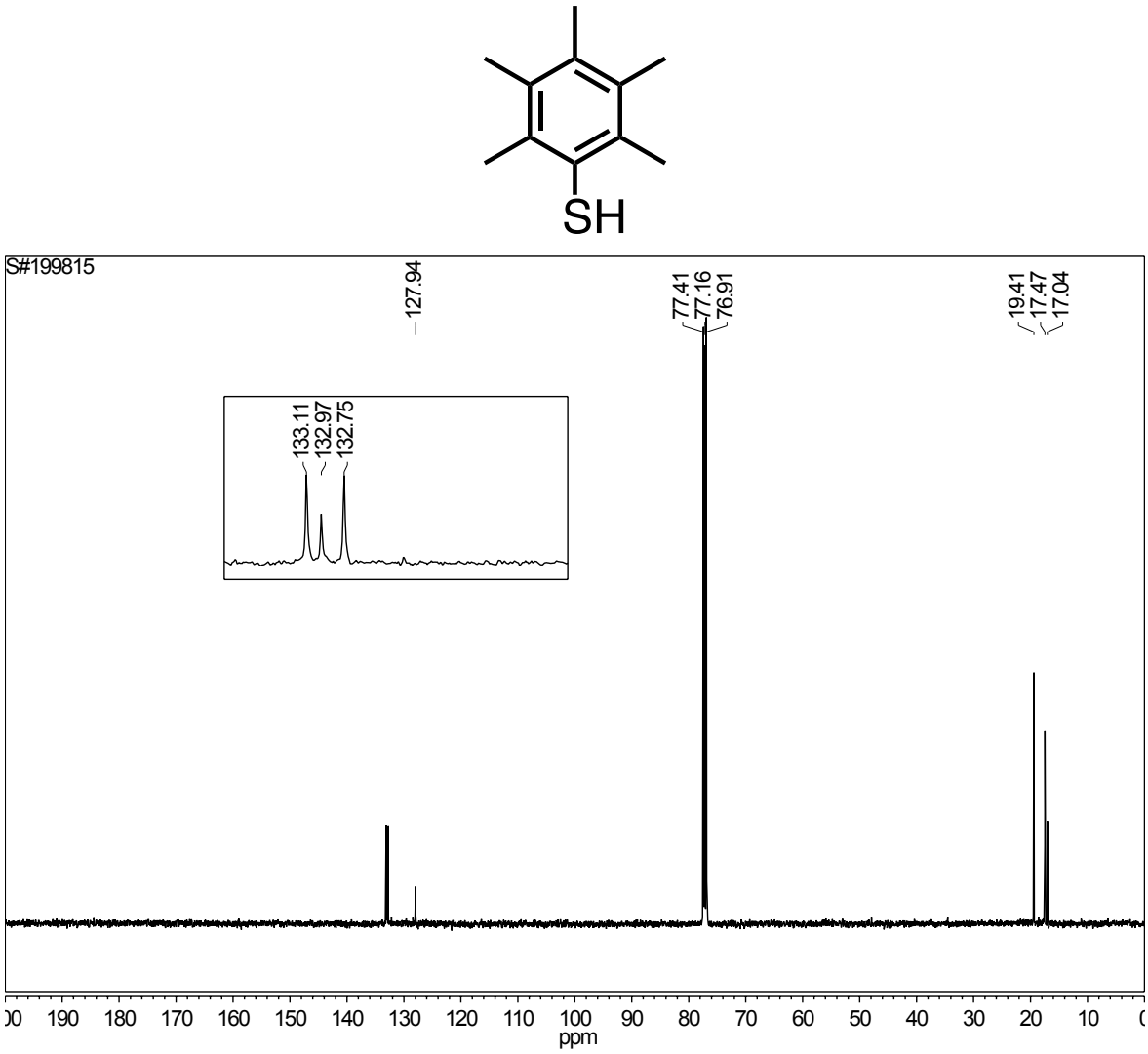


Figure S 23. **^{1}H NMR spectrum of 2,4,6-tris(2,3,4,5,6-pentamethyl phenylthio)-1,3,5-triazine (7)**

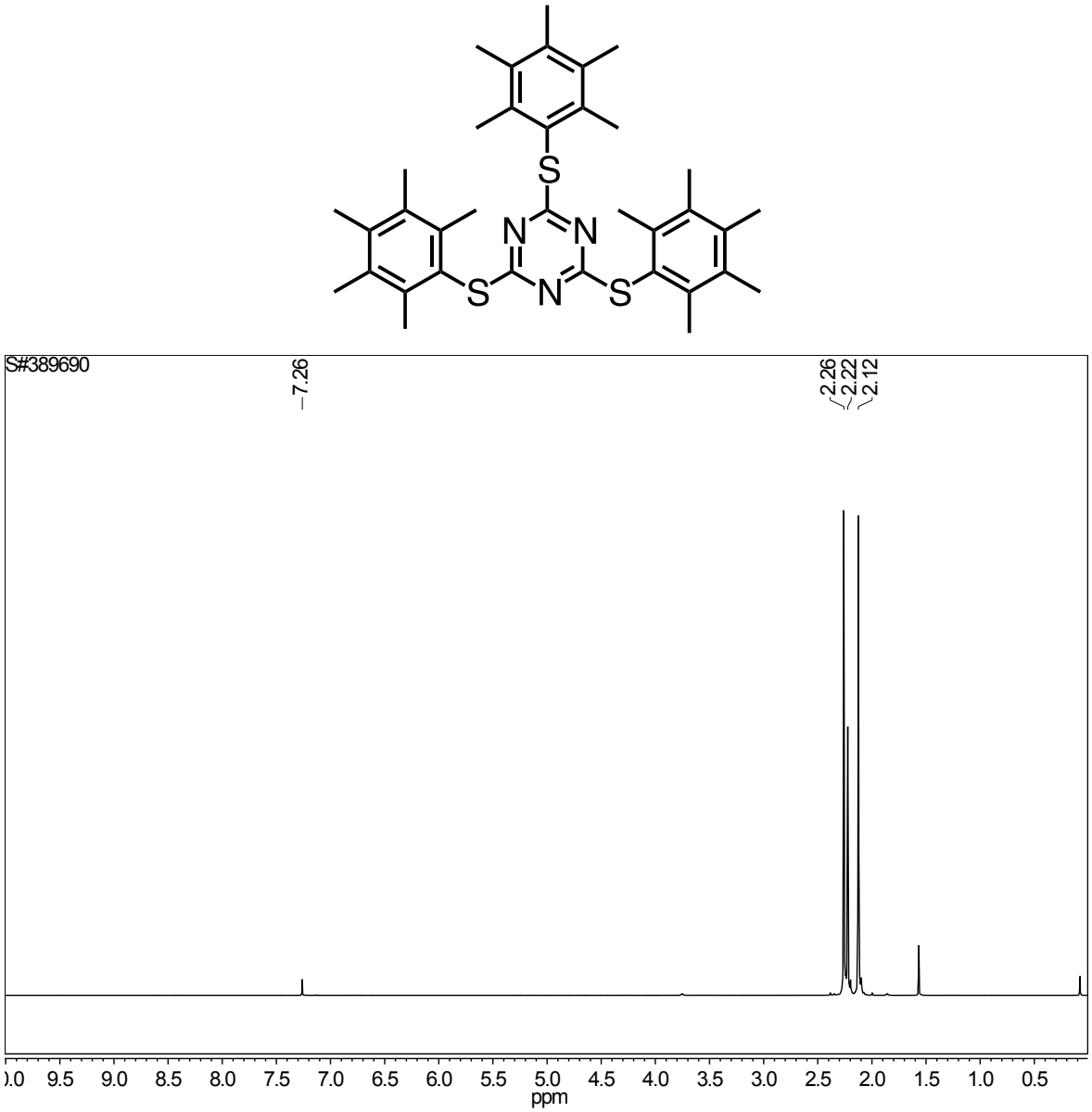


Figure S 24. **^{13}C NMR spectrum of 2,4,6-tris(2,3,4,5,6-pentamethyl phenylthio)-1,3,5-triazine (7)**

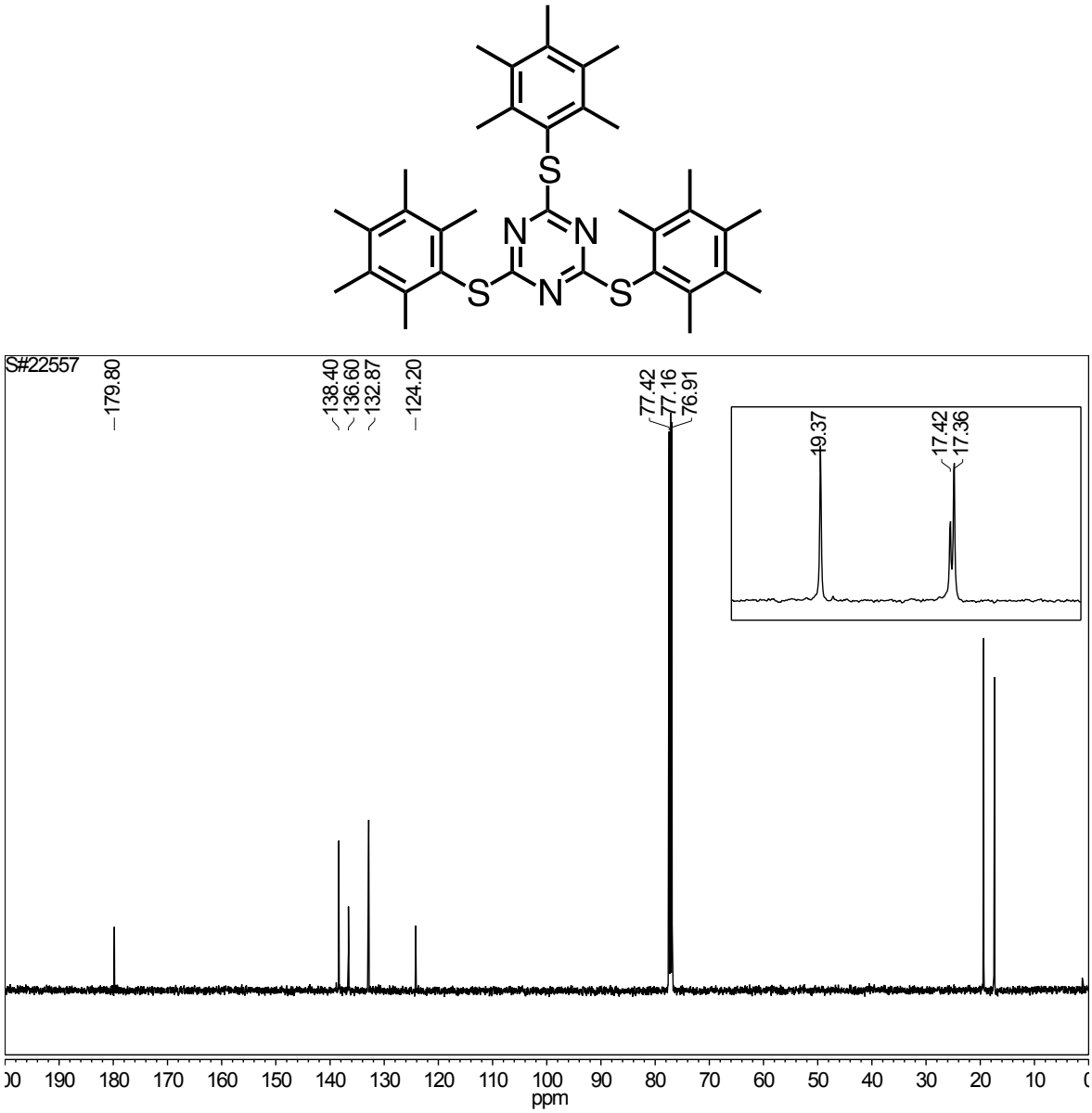
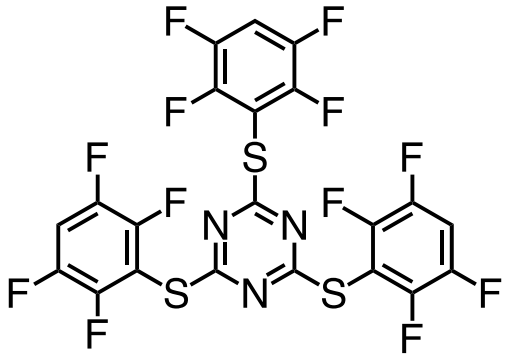


Figure S 25. **^{1}H NMR spectrum of 2,4,6-tris((2,3,5,6-tetrafluorophenyl)thio)-1,3,5-triazine (8).**



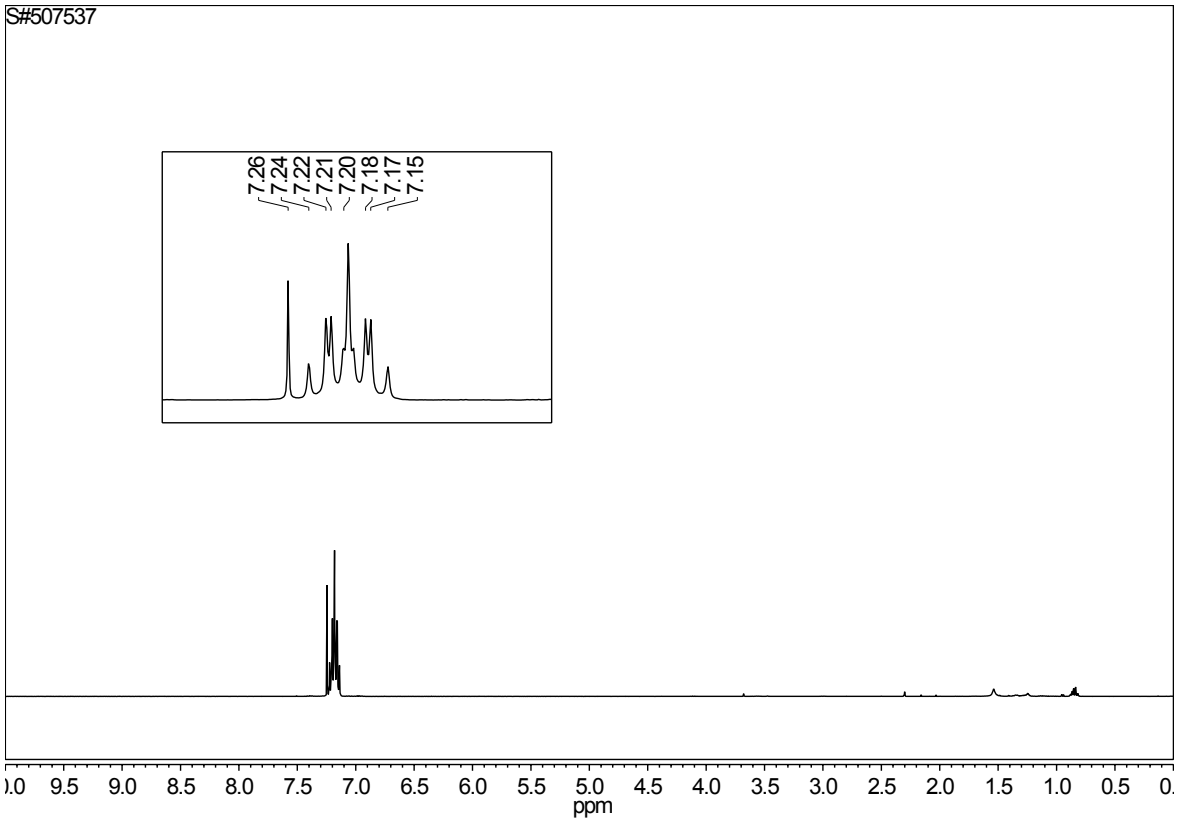
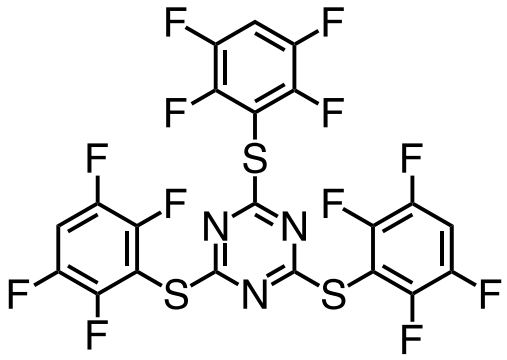


Figure S 26. **^{13}C NMR spectrum of 2,4,6-tris((2,3,5,6-tetrafluorophenyl)thio)-1,3,5-triazine (8).**



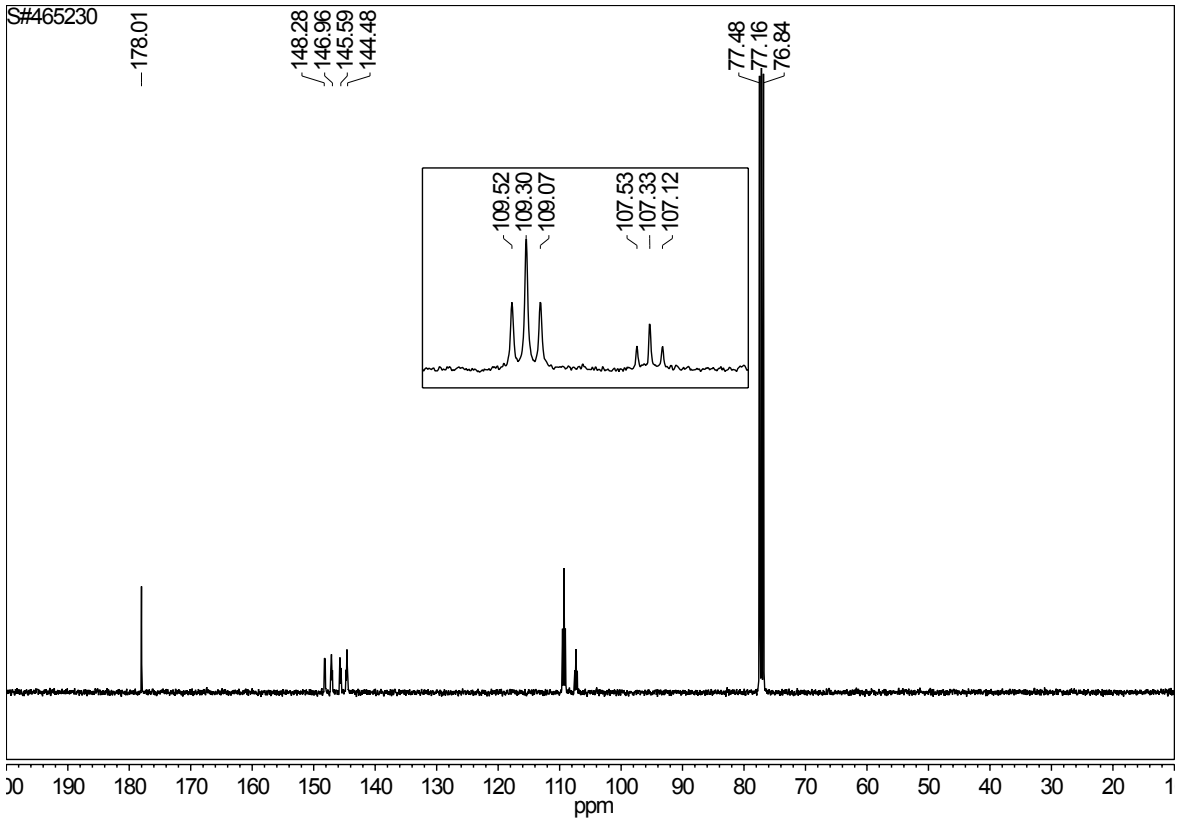
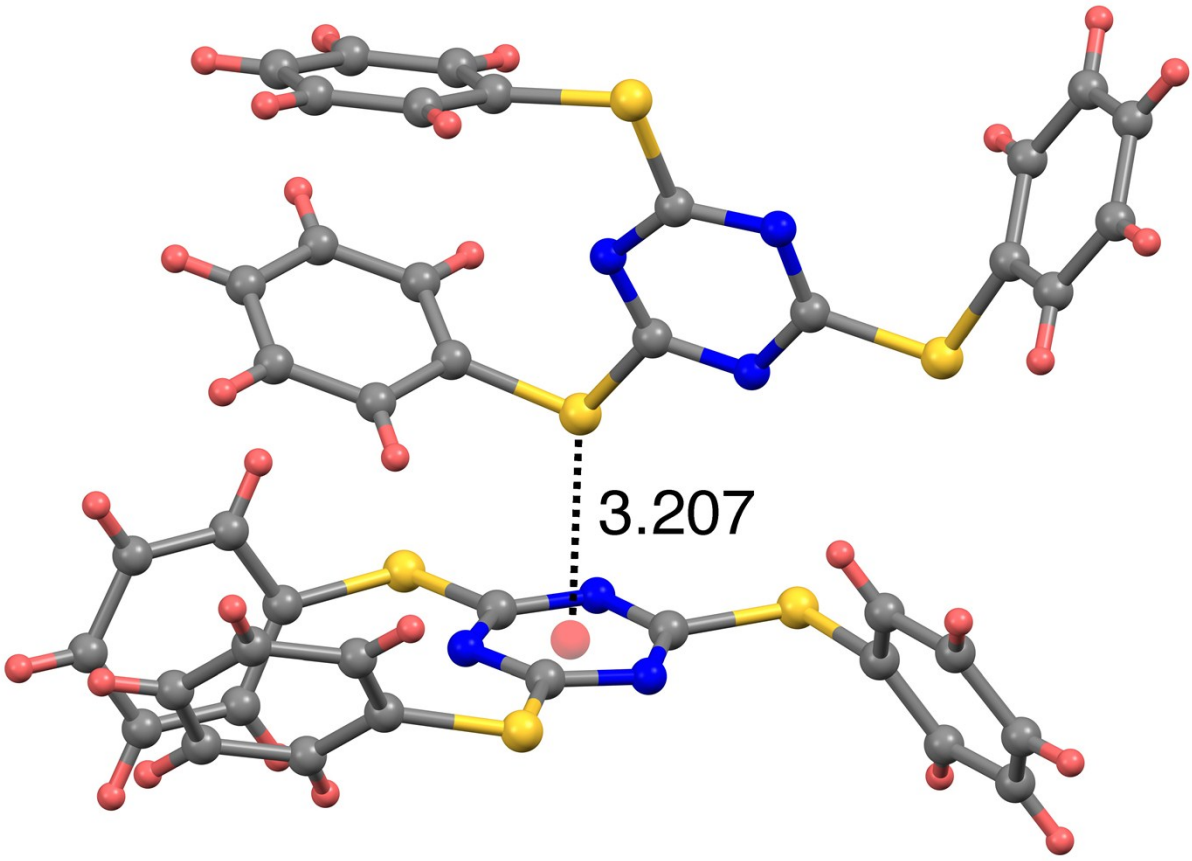
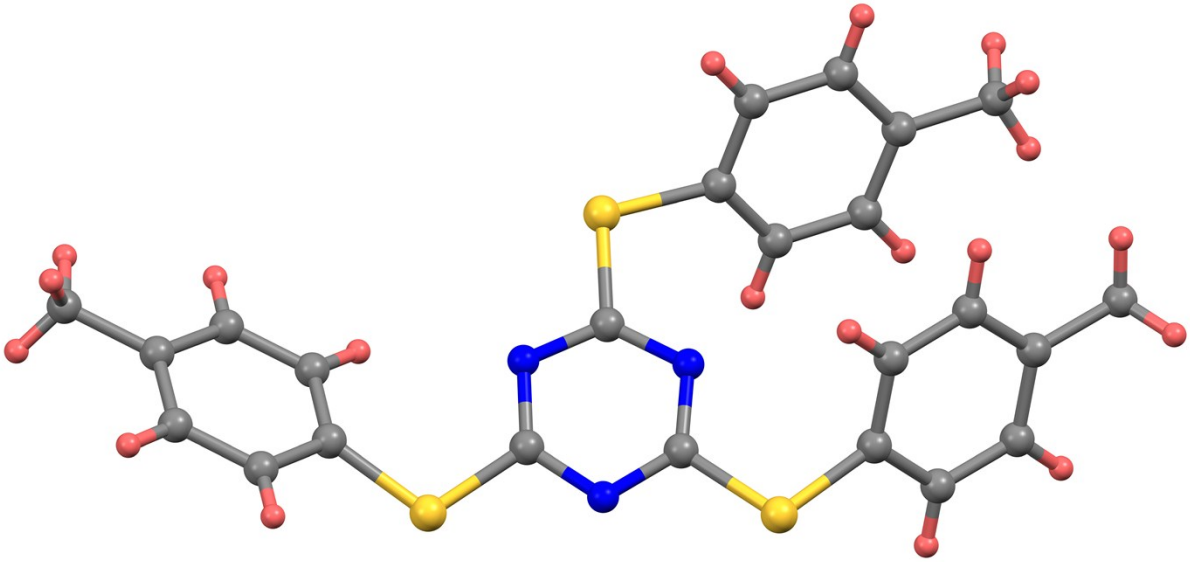


Figure S 27. SCXRD structure of 2,4,6-tris(phenylthio)-1,3,5-triazine (1): CCDC-1403546



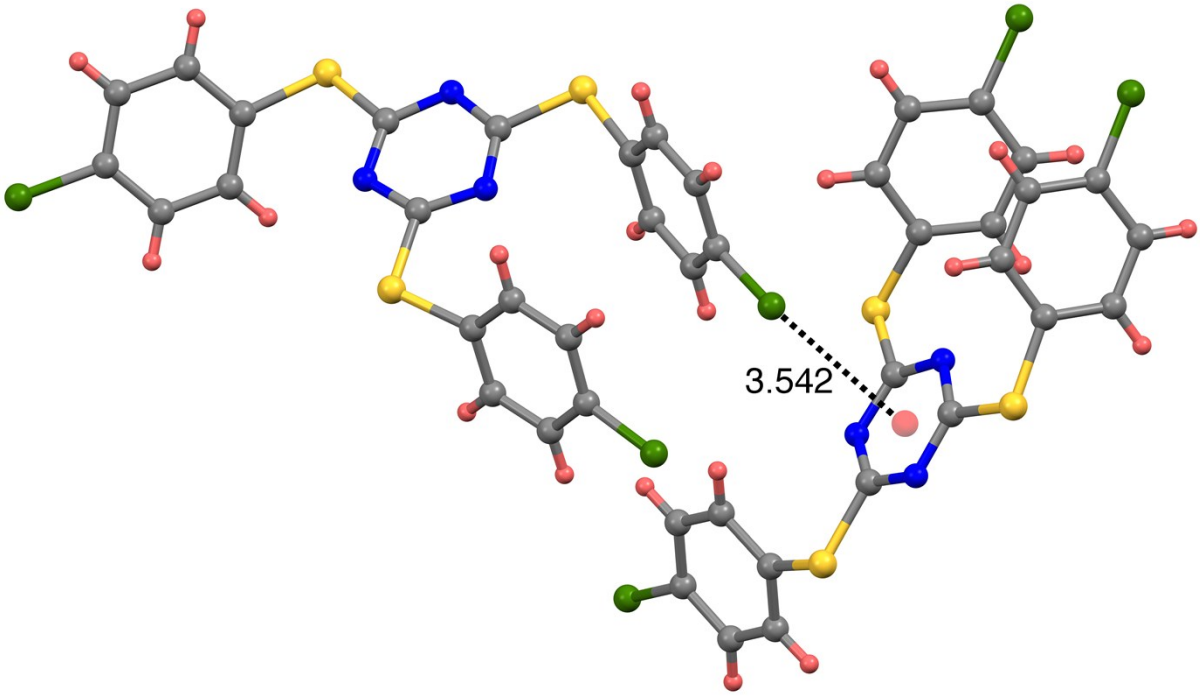
Color code: S, yellow; C, grey; H, salmon; N, blue. Selected distances (Å): S(1A)-C(1A), 1.749(3); S(1A)-C(4A), 1.772(3); S(2A)-C(2A), 1.761(3); S(2A)-C(10A), 1.774(3); S(3A)-C(3A), 1.749(3); S(3A)-C(16A), 1.767(3); N(1A)-C(3A), 1.333(4); N(1A)-C(1A), 1.333(4); N(2A)-C(2A), 1.329(4); N(2A)-C(1A), 1.349(4); N(3A)-C(3A), 1.331(4); N(3A)-C(2A), 1.341(4). Selected angles (deg): C(1A)-S(1A)-C(4A), 103.64(14); C(2A)-S(2A)-C(10A), 104.88(15); C(3A)-S(3A)-C(16A), 104.20(15); C(3A)-N(1A)-C(1A), 113.2(3); C(2A)-N(2A)-C(1A), 112.6(3); C(3A)-N(3A)-C(2A), 113.6(3); N(1A)-C(1A)-N(2A), 127.0(3); N(1A)-C(1A)-S(1A), 120.4(2); N(2A)-C(1A)-S(1A), 112.6(2); N(2A)-C(2A)-N(3A), 126.9(3); N(2A)-C(2A)-S(2A), 121.4(2); N(3A)-C(2A)-S(2A), 111.7(2); N(3A)-C(3A)-N(1A), 126.6(3); N(3A)-C(3A)-S(3A), 112.2(2); N(1A)-C(3A)-S(3A), 121.2(2).

Figure S 28. SCXRD structure of 2,4,6-tris(p-tolylthio)-1,3,5-triazine (2): CCDC-1403547



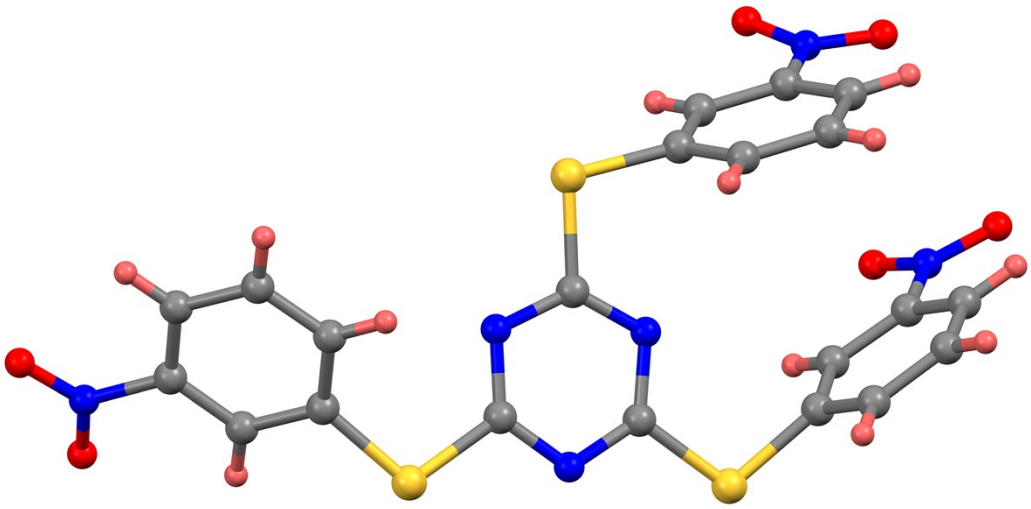
Color code: S, yellow; C, grey; H, salmon; N, blue. Selected distances (Å): S(1)-C(1), 1.746(3); S(1)-C(4), 1.777(2); S(2)-C(2), 1.756(2); S(2)-C(11), 1.774(3); S(3)-C(3), 1.755(3); S(3)-C(18), 1.774(3); N(1)-C(1), 1.338(3); N(1)-C(3), 1.343(3); N(2)-C(2), 1.333(3); N(2)-C(1), 1.343(3); N(3)-C(3), 1.335(3); N(3)-C(2), 1.339(3). Selected angles (deg): C(1)-S(1)-C(4), 109.89(12); C(2)-S(2)-C(11), 105.28(12); C(3)-S(3)-C(18), 104.05(12); C(1)-N(1)-C(3), 112.9(2); C(2)-N(2)-C(1), 113.9(2); C(3)-N(3)-C(2), 113.3(2); N(1)-C(1)-N(2), 126.4(2); N(1)-C(1)-S(1), 122.70(19); N(2)-C(1)-S(1), 110.83(18); N(2)-C(2)-N(3), 126.3(2); N(2)-C(2)-S(2), 112.64(18); N(3)-C(2)-S(2), 120.99(19); N(3)-C(3)-N(1), 127.1(2); N(3)-C(3)-S(3), 120.40(18); N(1)-C(3)-S(3), 112.46(18).

Figure S 29. SCXRD structure of 2,4,6-tris((4-chlorophenyl)thio)-1,3,5-triazine (3): CCDC-1403548



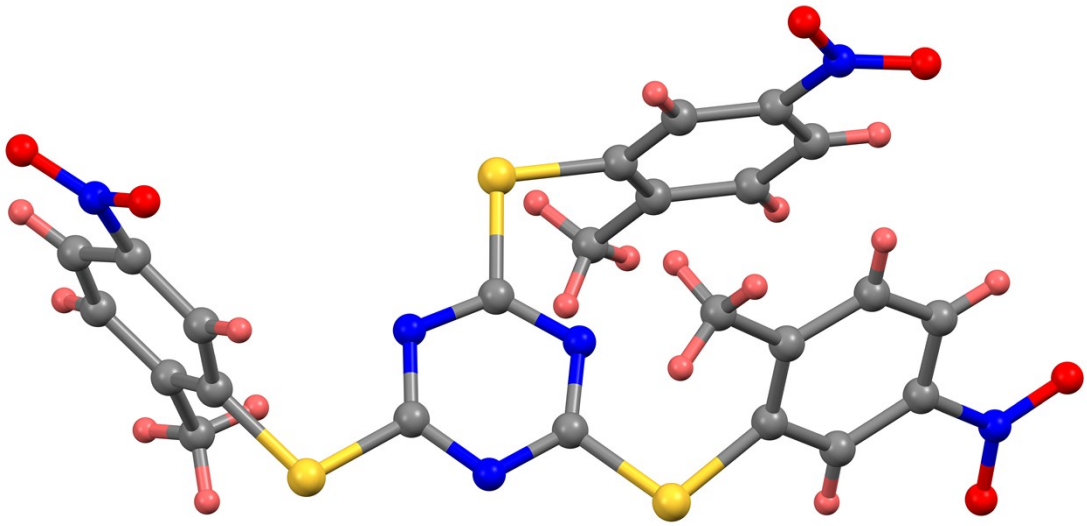
Color code: S, yellow; Cl, green; C, grey; H, salmon; N, blue. Selected distances (Å): Cl(1)-C(7), 1.740(3); Cl(2)-C(13), 1.741(3); Cl(3)-C(19), 1.741(3); S(1)-C(1), 1.753(3); S(1)-C(4), 1.778(3); S(2)-C(2), 1.751(3); S(2)-C(10), 1.776(3); S(3)-C(3), 1.752(3); S(3)-C(16), 1.772(3); N(1)-C(1), 1.329(4); N(1)-C(3), 1.336(3); N(2)-C(2), 1.336(4); N(2)-C(1), 1.346(3); N(3)-C(2), 1.331(4); N(3)-C(3), 1.336(3). Selected angles (deg): C(1)-S(1)-C(4), 105.44(13); C(2)-S(2)-C(10), 102.15(13); C(3)-S(3)-C(16), 104.02(13); C(1)-N(1)-C(3), 112.9(2); C(2)-N(2)-C(1), 113.5(2); C(2)-N(3)-C(3), 112.9(2); N(1)-C(1)-N(2), 126.4(3); N(1)-C(1)-S(1), 121.6(2); N(2)-C(1)-S(1), 112.0(2); N(3)-C(2)-N(2), 126.7(3); N(3)-C(2)-S(2), 119.8(2); N(2)-C(2)-S(2), 113.5(2); N(3)-C(3)-N(1), 127.5(3); N(3)-C(3)-S(3), 119.5(2); N(1)-C(3)-S(3), 113.0(2).

Figure S 30. SCXRD structure of 2,4,6-tris((3-nitrophenyl)thio)-1,3,5-triazine (4): CCDC-1403549



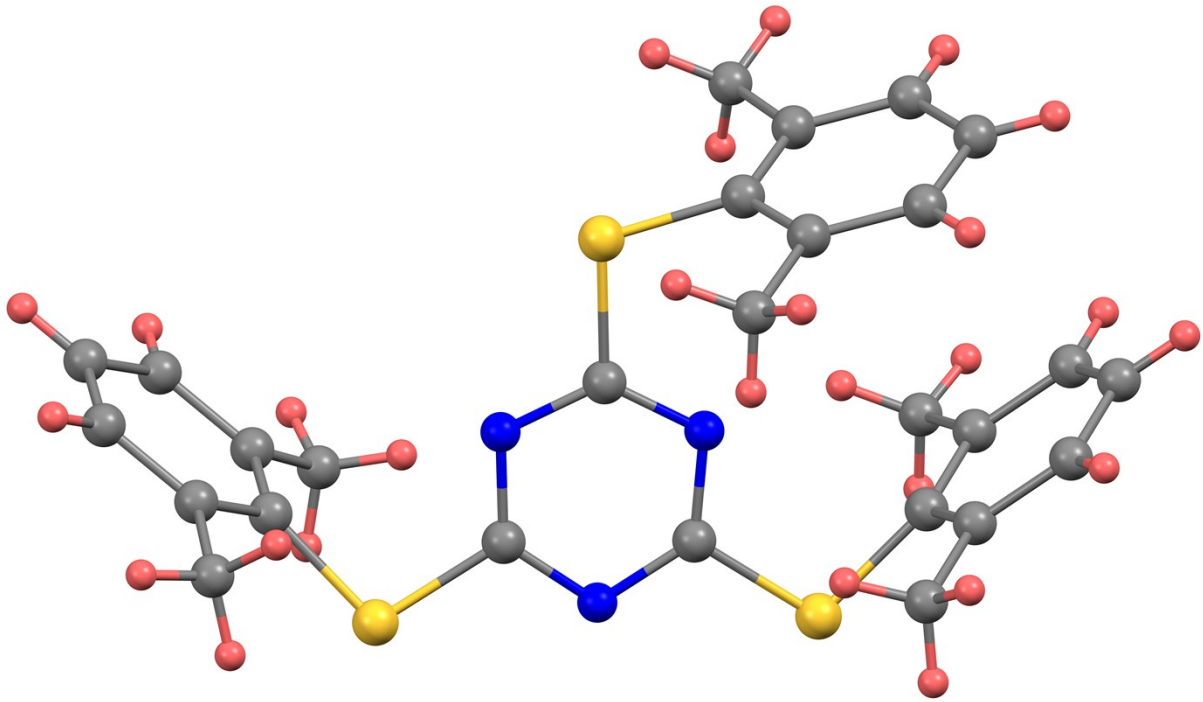
Color code: S, yellow; O, red; C, grey; H, salmon; N, blue. Selected distances (Å): S(1)-C(1), 1.756(3); S(1)-C(4), 1.758(3); S(2)-C(2), 1.746(3); S(2)-C(10), 1.774(3); S(3)-C(3), 1.741(3); S(3)-C(16), 1.770(4); O(1)-N(4), 1.205(4); O(2)-N(4), 1.216(4); O(3)-N(5), 1.211(4); O(4)-N(5), 1.183(4); O(5)-N(6), 1.206(5); O(6)-N(6), 1.194(5); N(1)-C(1), 1.323(4); N(1)-C(3), 1.345(4); N(2)-C(1), 1.325(4); N(2)-C(2), 1.330(4); N(3)-C(3), 1.320(4); N(3)-C(2), 1.326(4); N(4)-C(6), 1.468(4); N(5)-C(14), 1.460(5); N(6)-C(20), 1.458(5). Selected angles (deg): C(1)-S(1)-C(4), 105.77(16); C(2)-S(2)-C(10), 103.26(17); C(3)-S(3)-C(16), 101.88(17); C(1)-N(1)-C(3), 112.5(3); C(1)-N(2)-C(2), 112.9(3); C(3)-N(3)-C(2), 113.2(3); O(1)-N(4)-O(2), 123.9(4); O(1)-N(4)-C(6), 118.0(4); O(2)-N(4)-C(6), 118.2(4); O(4)-N(5)-O(3), 122.7(4); O(4)-N(5)-C(14), 118.4(4); O(3)-N(5)-C(14), 118.9(4); O(6)-N(6)-O(5), 123.5(5); O(6)-N(6)-C(20), 119.0(5); O(5)-N(6)-C(20), 117.3(5); N(1)-C(1)-N(2), 127.5(3); N(1)-C(1)-S(1), 121.5(3); N(2)-C(1)-S(1), 110.9(2); N(3)-C(2)-N(2), 127.0(3); N(3)-C(2)-S(2), 120.2(3); N(2)-C(2)-S(2), 112.8(3); N(3)-C(3)-N(1), 126.9(3); N(3)-C(3)-S(3), 120.4(3); N(1)-C(3)-S(3), 112.7(3).

Figure S 31. SCXRD structure of 2,4,6-tris((2-methyl-5-nitrophenyl)thio)-1,3,5-triazine (5): CCDC-1403550



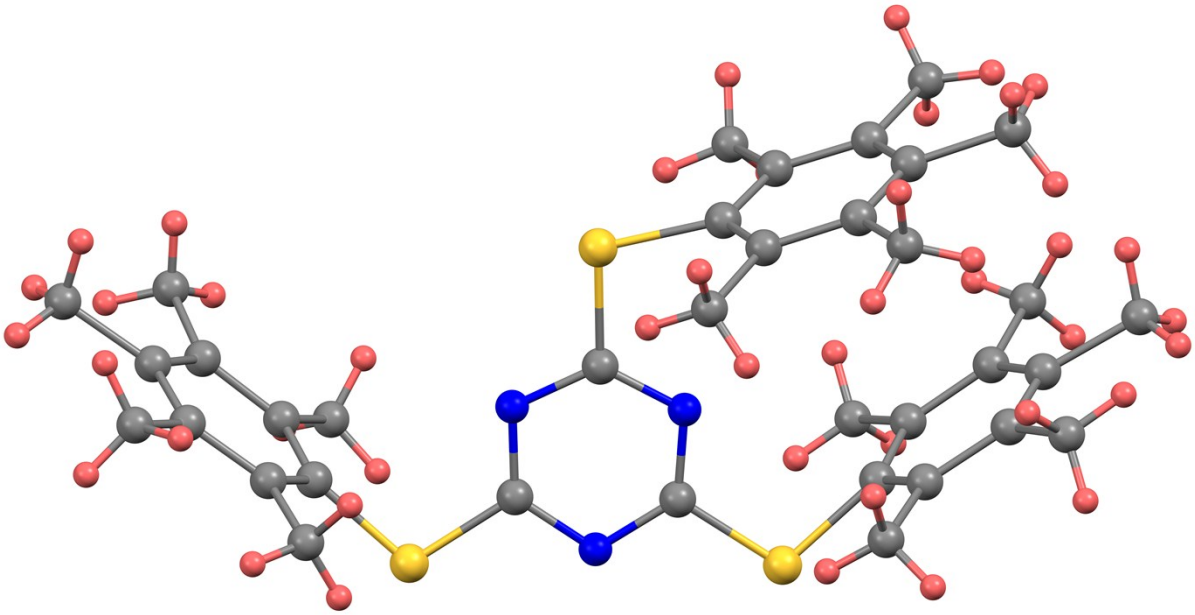
Color code: S, yellow; O, red; C, grey; H, salmon; N, blue. Selected distances (Å): S(1)-C(1), 1.749(3); S(1)-C(4), 1.774(3); S(1)-C(4B), 1.776(5); S(2)-C(2), 1.753(2); S(2)-C(11), 1.776(3); S(3)-C(3), 1.751(3); S(3)-C(18), 1.777(3); N(5)-O(3), 1.213(3); N(5)-O(4), 1.214(3); N(5)-C(16), 1.471(3); N(6)-O(6), 1.210(3); N(6)-O(5), 1.212(2); N(6)-C(23), 1.471(3); N(1)-C(1), 1.327(3); N(1)-C(3), 1.331(3); N(2)-C(2), 1.330(3); N(2)-C(1), 1.337(3); N(3)-C(2), 1.322(3); N(3)-C(3), 1.330(3); N(4)-O(1), 1.210(4); N(4)-O(2), 1.214(4); N(4)-C(9), 1.461(5). Selected angles (deg): C(1)-S(1)-C(4), 106.2(2); C(1)-S(1)-C(4B), 96.9(3); C(2)-S(2)-C(11), 104.15(12); C(3)-S(3)-C(18), 100.59(11); O(3)-N(5)-O(4), 123.8(2); O(3)-N(5)-C(16), 118.2(2); O(4)-N(5)-C(16), 118.0(2); O(6)-N(6)-O(5), 123.6(3); O(6)-N(6)-C(23), 118.0(2); O(5)-N(6)-C(23), 118.4(2); C(1)-N(1)-C(3), 113.0(2); C(2)-N(2)-C(1), 113.0(2); C(2)-N(3)-C(3), 113.0(2); N(1)-C(1)-N(2), 126.7(2); N(1)-C(1)-S(1), 121.16(18); N(2)-C(1)-S(1), 112.2(2); N(3)-C(2)-N(2), 127.1(2); N(3)-C(2)-S(2), 120.38(19); N(2)-C(2)-S(2), 112.48(19); N(3)-C(3)-N(1), 127.1(2); N(3)-C(3)-S(3), 118.58(19); N(1)-C(3)-S(3), 114.29(17); O(1)-N(4)-O(2), 124.5(5); O(1)-N(4)-C(9), 112.7(4); O(2)-N(4)-C(9), 122.9(5).

Figure S 32. SCXRD structure of 2,4,6-tris(2,6-dimethylphenylthio)-1,3,5-triazine (6): CCDC-1436792



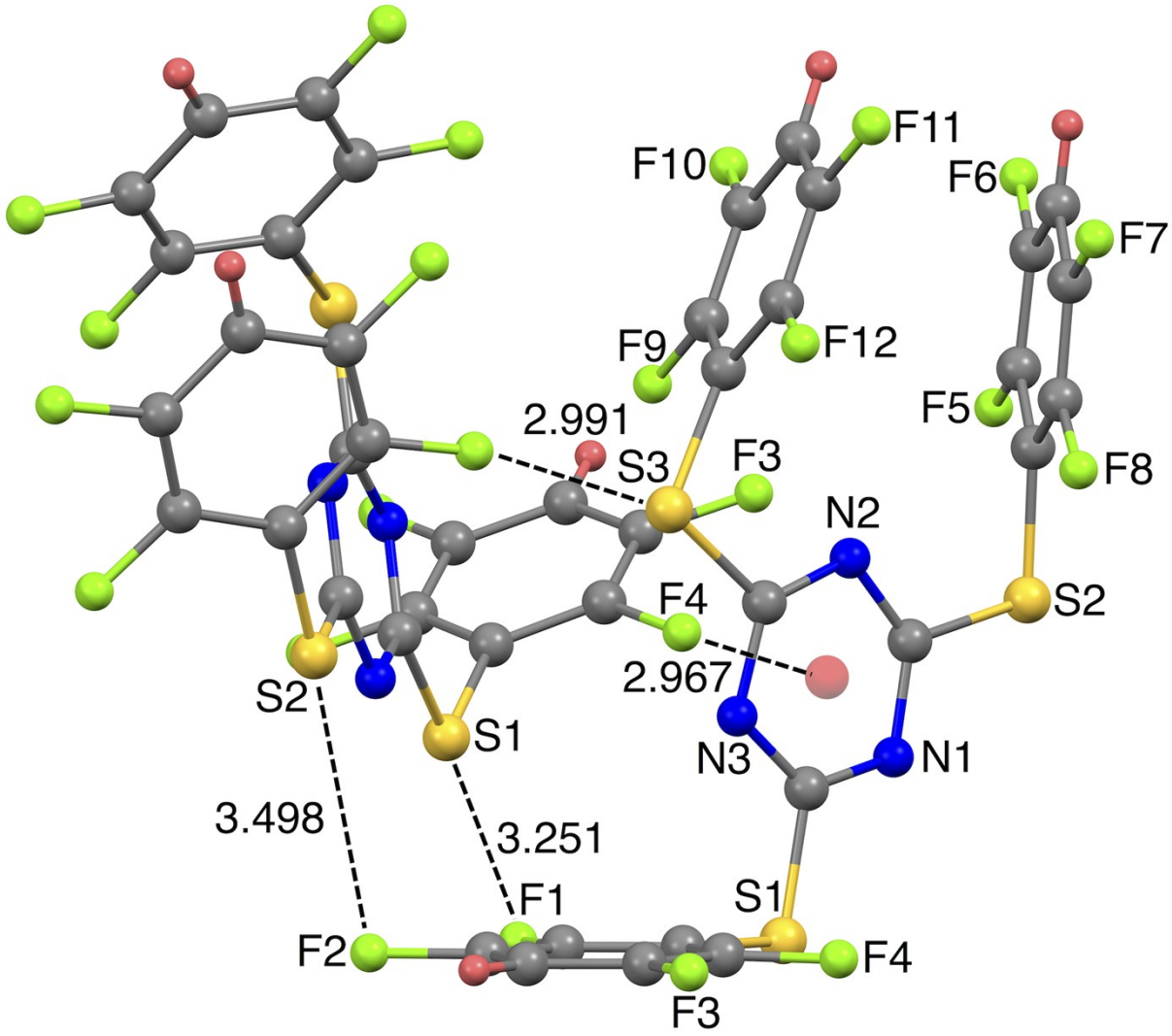
Color code: S, yellow; C, grey; H, salmon; N, blue. Selected distances (Å): S(1)-C(4), 1.722(7); S(1)-C(1), 1.740(3); S(1)-C(4A), 1.829(10); S(2)-C(2), 1.752(3); S(2)-C(12), 1.755(7); S(2)-C(12A), 1.757(10); S(3)-C(20A), 1.718(8); S(3)-C(3), 1.750(3); S(3)-C(20), 1.781(5); N(1)-C(2), 1.327(3); N(1)-C(1), 1.334(3); N(2)-C(3), 1.333(3); N(2)-C(2), 1.333(3); N(3)-C(1), 1.324(3); N(3)-C(3), 1.326(3). Selected angles (deg): C(4)-S(1)-C(1), 106.8(4); C(1)-S(1)-C(4A), 97.2(6); C(2)-S(2)-C(12), 101.5(6); C(2)-S(2)-C(12A), 106.7(9); C(20A)-S(3)-C(3), 104.7(10); C(3)-S(3)-C(20), 100.5(7); C(2)-N(1)-C(1), 113.3(2); C(3)-N(2)-C(2), 112.9(2); C(1)-N(3)-C(3), 113.4(2); N(3)-C(1)-N(1), 126.6(2); N(3)-C(1)-S(1), 119.69(18); N(1)-C(1)-S(1), 113.68(19); N(1)-C(2)-N(2), 126.8(2); N(1)-C(2)-S(2), 119.8(2); N(2)-C(2)-S(2), 113.4(2); N(3)-C(3)-N(2), 126.9(2); N(3)-C(3)-S(3), 118.9(2); N(2)-C(3)-S(3), 114.2(2); C(5)-C(4)-C(9), 120.0; C(5)-C(4)-S(1), 118.2(6); C(9)-C(4)-S(1), 121.7(6);

Figure S 33. SCXRD structure of 2,4,6-tris(2,3,4,5,6-pentamethyl phenylthio)-1,3,5-triazine (7): CCDC-1436793



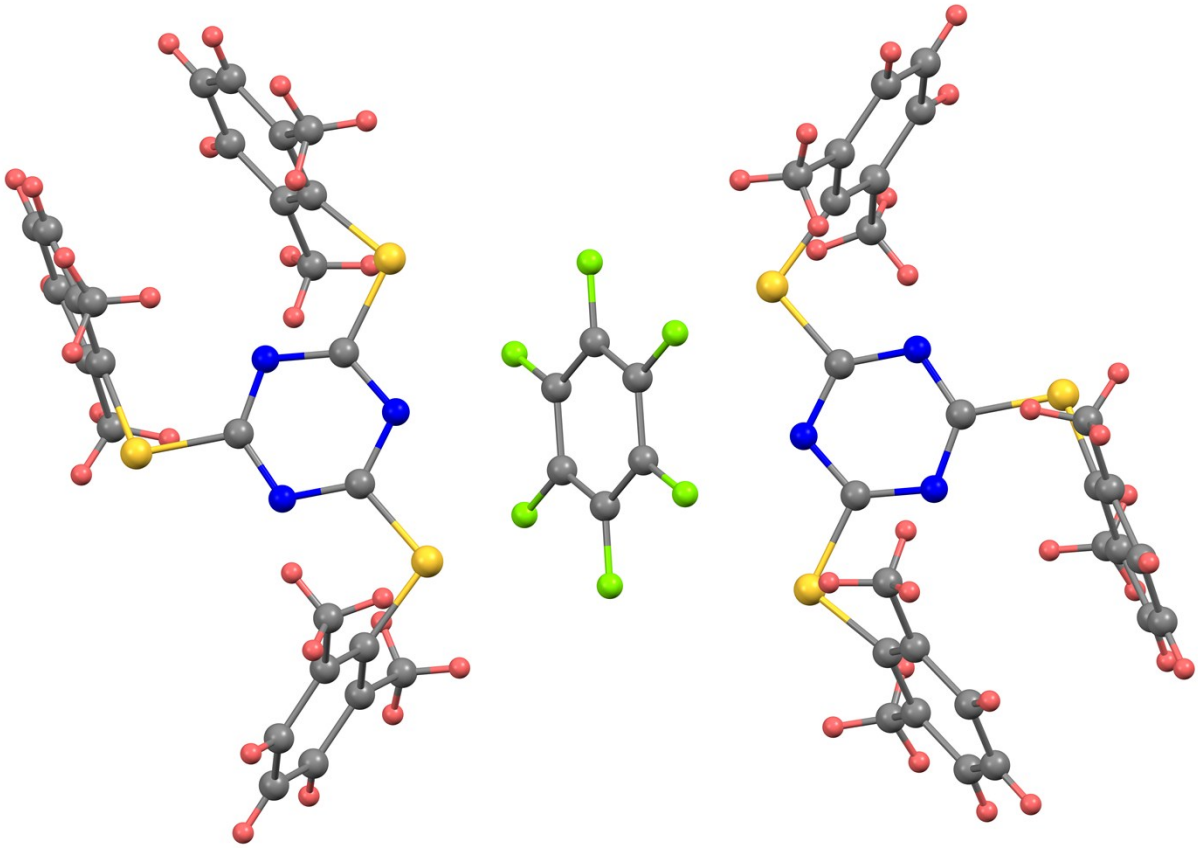
Color code: S, yellow; C, grey; H, salmon; N, blue. Selected distances (Å): S(1)-C(1), 1.749(5); S(1)-C(4), 1.774(6); S(2)-C(2), 1.745(6); S(2)-C(15), 1.784(5); S(3)-C(3), 1.734(5); S(3)-C(26), 1.788(5); N(1)-C(2), 1.345(6); N(1)-C(1), 1.348(6); N(2)-C(2), 1.310(6); N(2)-C(3), 1.326(6); N(3)-C(1), 1.309(7); N(3)-C(3), 1.348(6). Selected angles (deg): C(1)-S(1)-C(4), 104.3(3); C(2)-S(2)-C(15), 103.4(3); C(3)-S(3)-C(26), 103.9(3); C(2)-N(1)-C(1), 113.0(5); C(2)-N(2)-C(3), 114.3(4); C(1)-N(3)-C(3), 114.1(5); N(3)-C(1)-N(1), 126.2(5); N(3)-C(1)-S(1), 122.0(5); N(1)-C(1)-S(1), 111.8(5); N(2)-C(2)-N(1), 126.6(5); N(2)-C(2)-S(2), 119.8(4); N(1)-C(2)-S(2), 113.6(5); N(2)-C(3)-N(3), 125.7(5); N(2)-C(3)-S(3), 119.4(4); N(3)-C(3)-S(3), 114.9(4); C(5)-C(4)-C(9), 121.2(6); C(5)-C(4)-S(1), 120.0(5); C(9)-C(4)-S(1), 118.7(5).

Figure S 34. SCXRD structure of **2,4,6-tris((2,3,5,6-tetrafluorophenyl)thio)-1,3,5-triazine** (8): CCDC-1452878



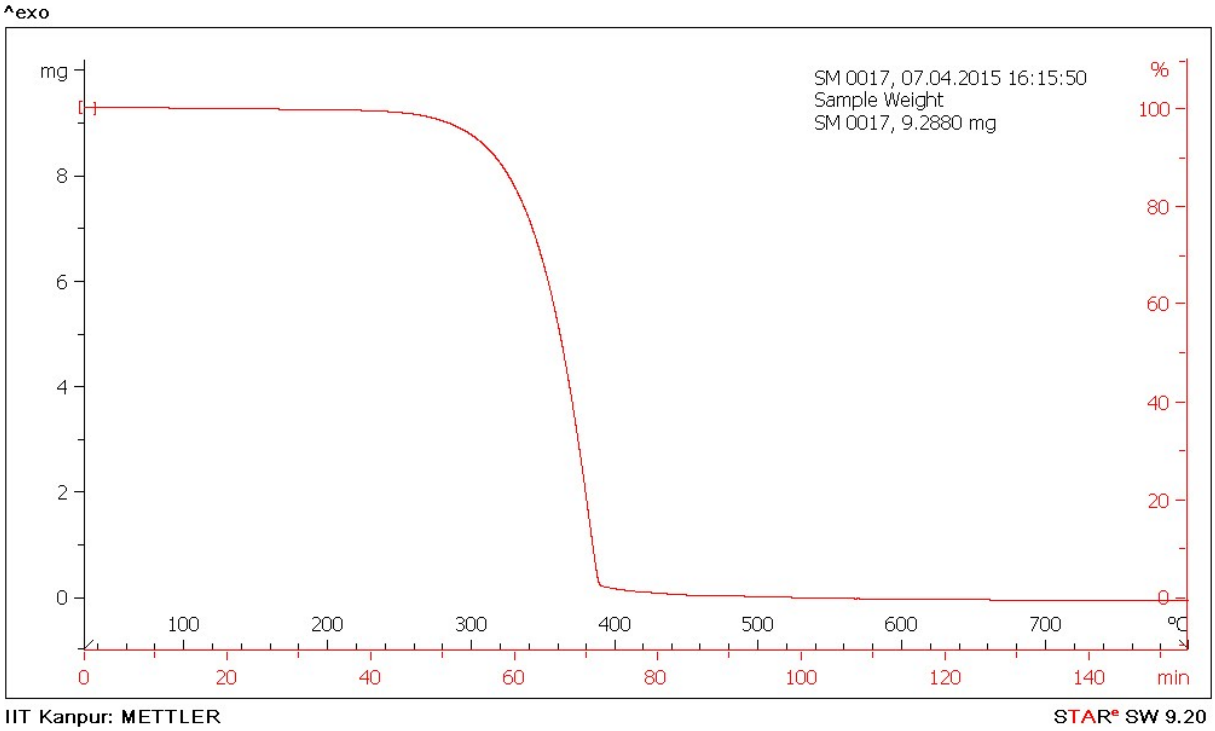
Color code: S, yellow; C, grey; H, salmon; N, blue; F, green. Selected distances (Å): S(1)-C(1), 1.747(6); S(1)-C(4), 1.757(6); S(2)-C(10), 1.753(6); S(2)-C(2), 1.754(6); S(3)-C(3), 1.750(6); S(3)-C(16), 1.768(7); N(1)-C(2), 1.334(7); N(1)-C(1), 1.336(7); N(2)-C(3), 1.326(7); N(2)-C(2), 1.330(7); N(3)-C(1), 1.327(7); N(3)-C(3), 1.338(7). Selected angles (deg): C(1)-S(1)-C(4), 100.9(3); C(10)-S(2)-C(2), 101.5(3); C(3)-S(3)-C(16), 101.9(3); C(2)-N(1)-C(1), 113.2(5); C(3)-N(2)-C(2), 112.5(5); C(1)-N(3)-C(3), 113.4(5); N(3)-C(1)-N(1), 126.2(5); N(3)-C(1)-S(1), 119.3(4); N(1)-C(1)-S(1), 114.5(5); N(2)-C(2)-N(1), 127.3(5); N(2)-C(2)-S(2), 119.4(5); N(1)-C(2)-S(2), 113.3(5); N(2)-C(3)-N(3), 127.3(5); N(2)-C(3)-S(3), 120.6(5); N(3)-C(3)-S(3), 112.1(4); C(9)-C(4)-C(5), 117.8(6); C(9)-C(4)-S(1), 120.5(6); C(5)-C(4)-S(1), 121.7(6).

Figure S 35. SCXRD structure of 2,4,6-tris(2,6-dimethylphenylthio)-1,3,5-triazine ($6 \cdot 0.5C_6F_6$): CCDC-1436791



Color code: S, yellow; F, green; C, grey; H, salmon; N, blue. Selected distances (Å): S(1)-C(1), 1.751(3); S(1)-C(4), 1.784(3); S(2)-C(2), 1.757(3); S(2)-C(12), 1.776(3); S(3)-C(3), 1.749(3); S(3)-C(20), 1.777(3); F(1)-C(28), 1.343(4); F(2)-C(29), 1.340(4); F(3)-C(30), 1.334(4); N(1)-C(2), 1.344(4); N(1)-C(1), 1.353(4); N(2)-C(2), 1.325(4); N(2)-C(3), 1.335(3); N(3)-C(1), 1.326(4); N(3)-C(3), 1.341(4). Selected angles (deg): C(1)-S(1)-C(4), 102.66(15); C(2)-S(2)-C(12), 103.74(14); C(3)-S(3)-C(20), 101.66(14); C(2)-N(1)-C(1), 112.8(3); C(2)-N(2)-C(3), 113.6(3); C(1)-N(3)-C(3), 113.4(2); N(3)-C(1)-N(1), 126.6(3); N(3)-C(1)-S(1), 120.3(2); N(1)-C(1)-S(1), 113.1(2); N(2)-C(2)-N(1), 126.8(3); N(2)-C(2)-S(2), 120.0(2); N(1)-C(2)-S(2), 113.2(2); N(2)-C(3)-N(3), 126.7(3); N(2)-C(3)-S(3), 119.9(2); N(3)-C(3)-S(3), 113.4(2).

Figure S 36. TGA of 1.



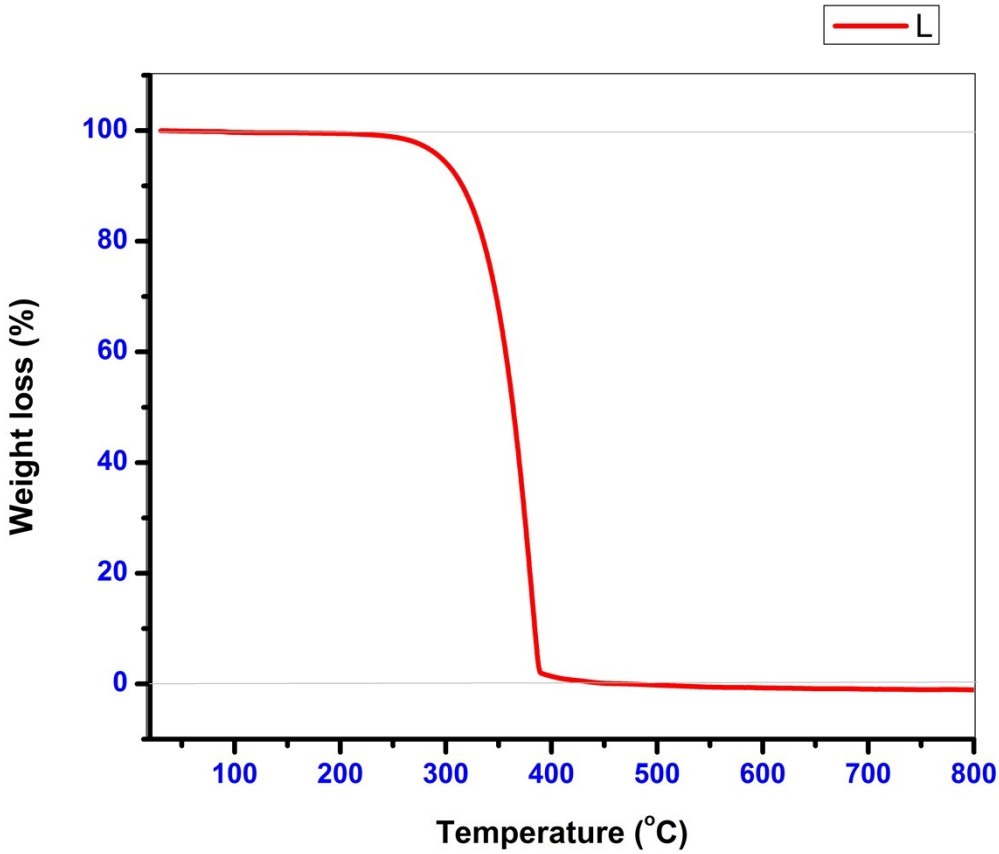
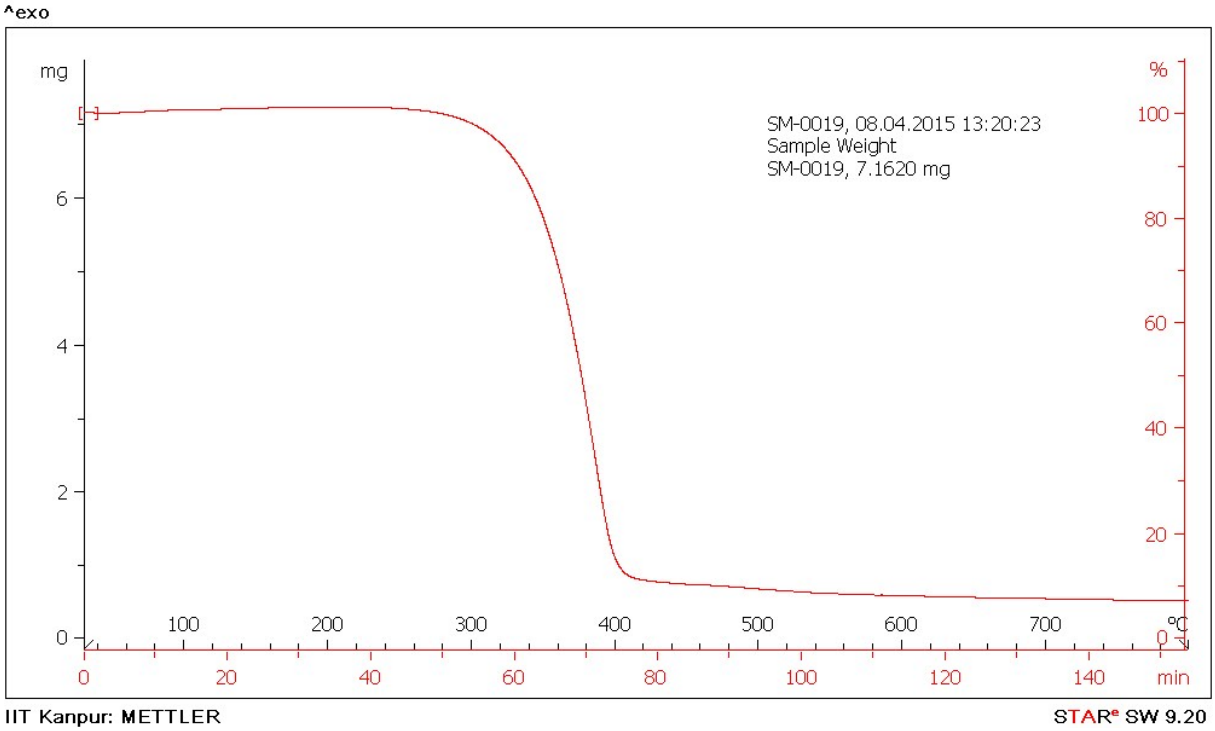


Figure S 37. TGA of 2.



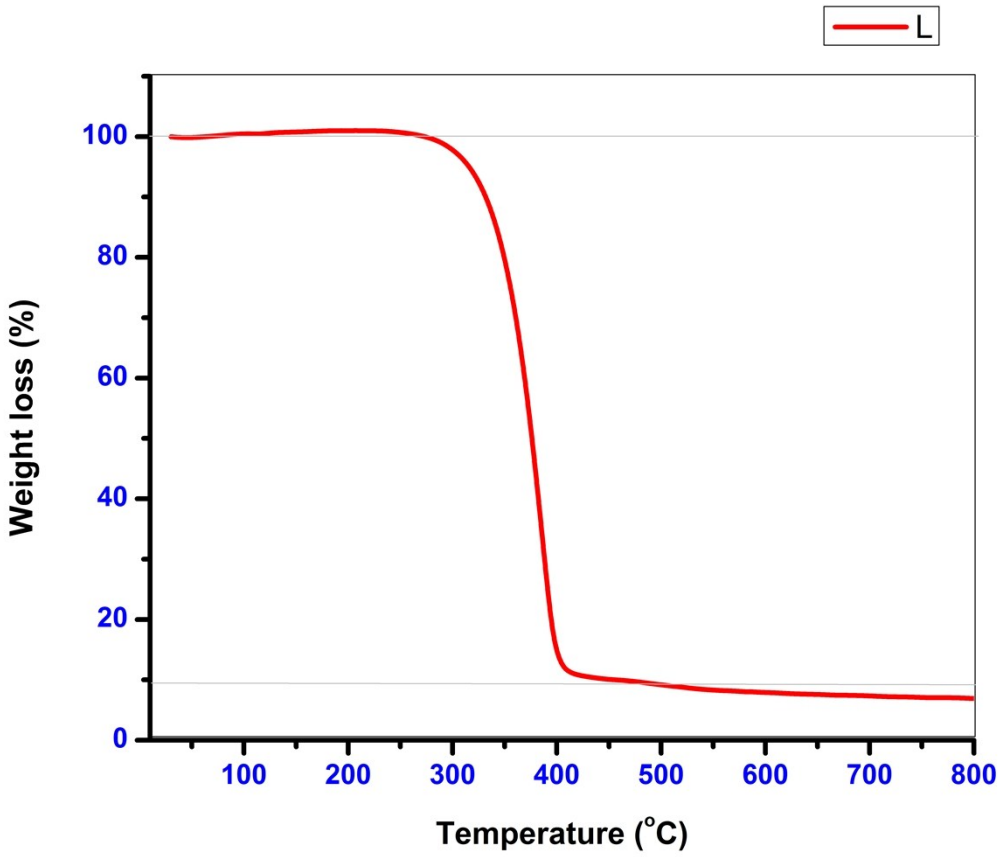
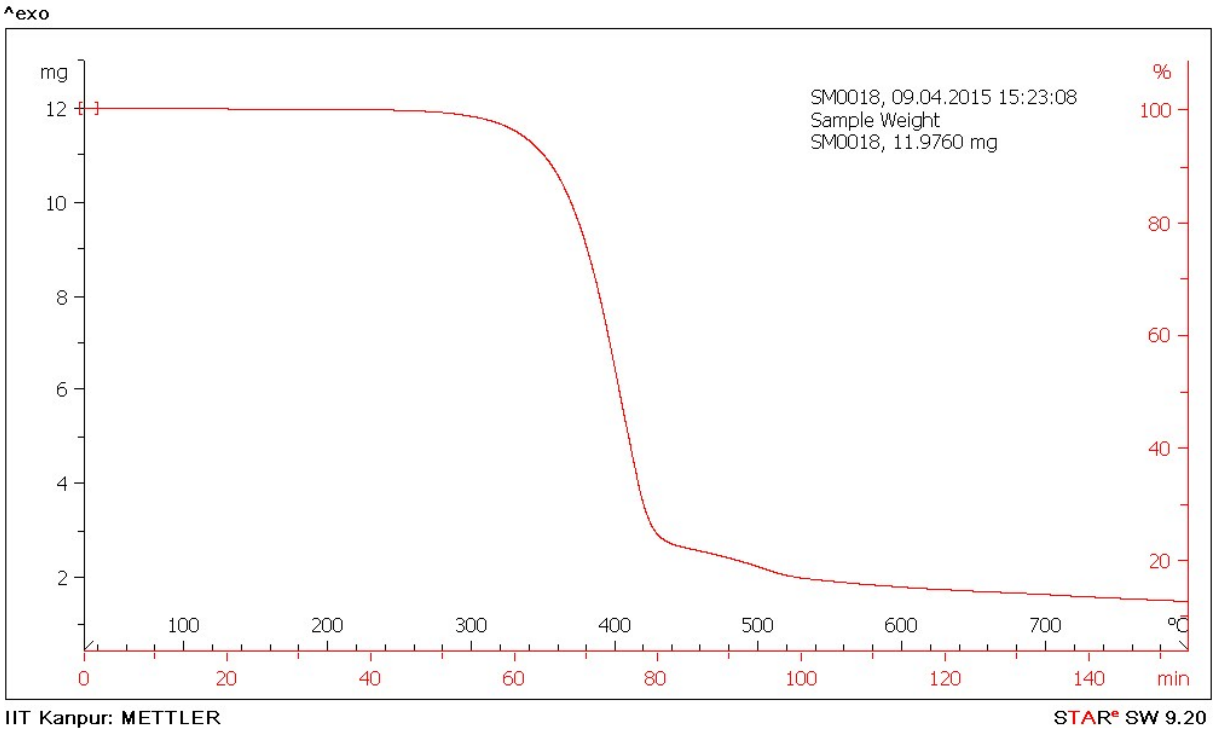


Figure S 38. TGA of 3.



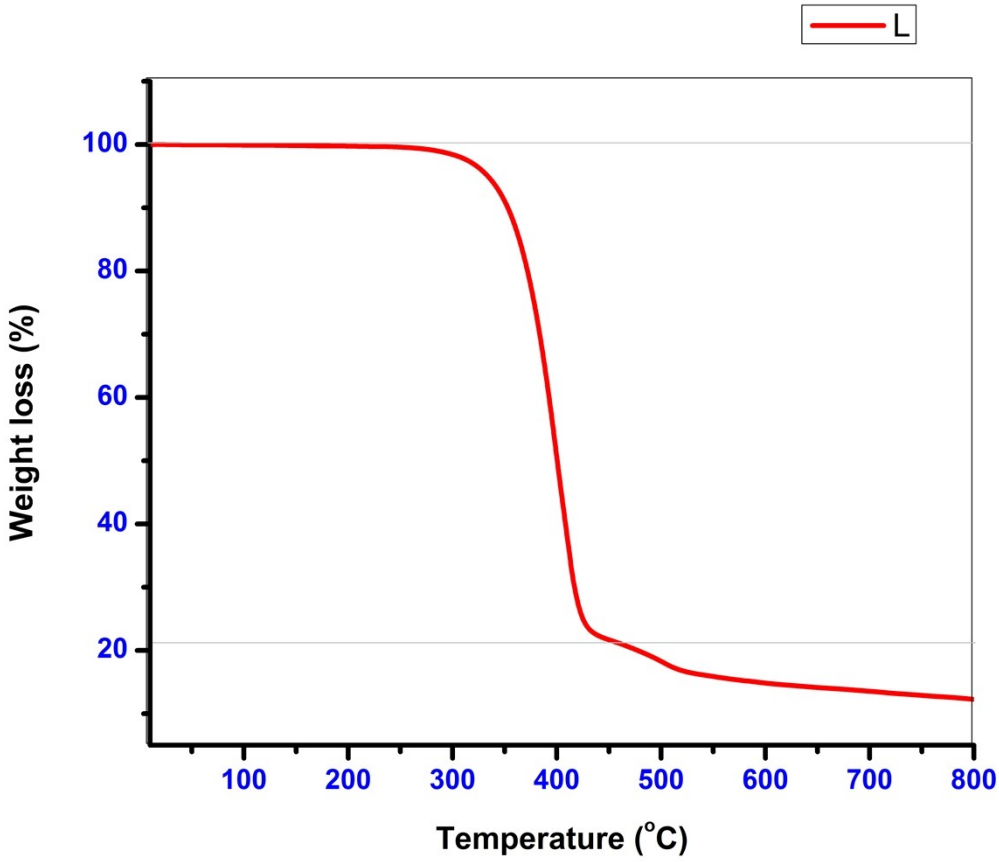
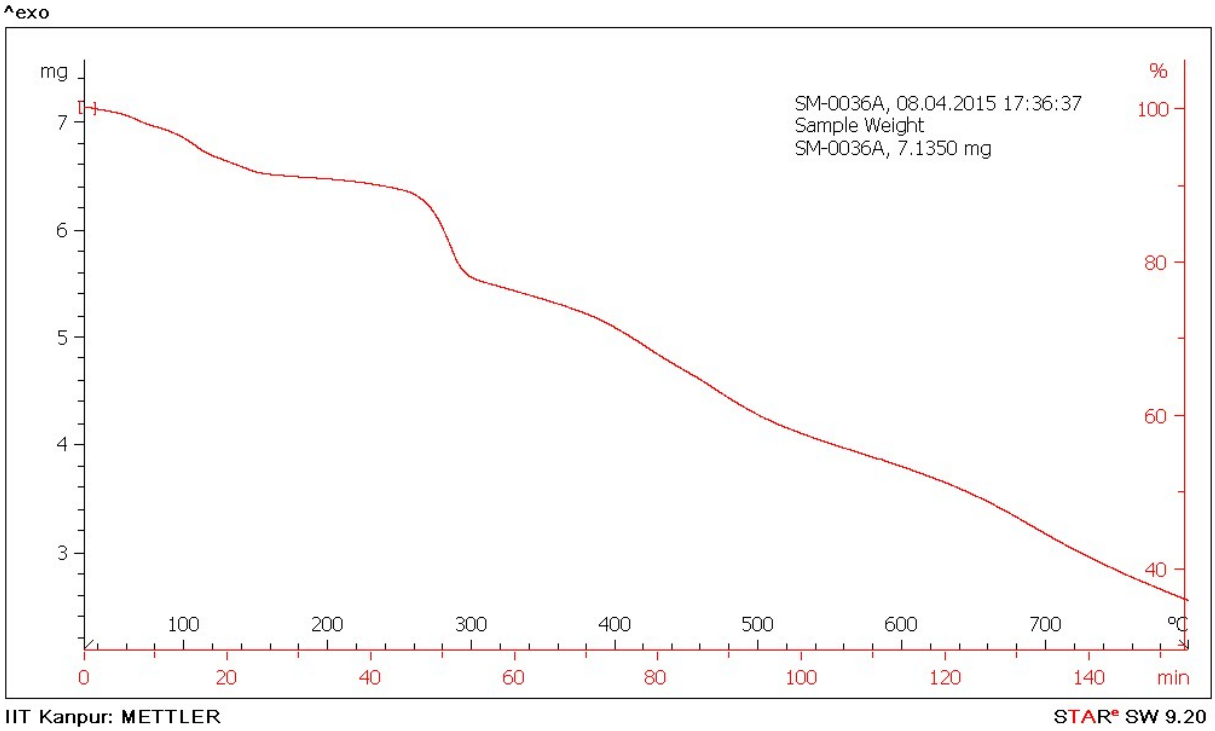


Figure S 39. TGA of 4.



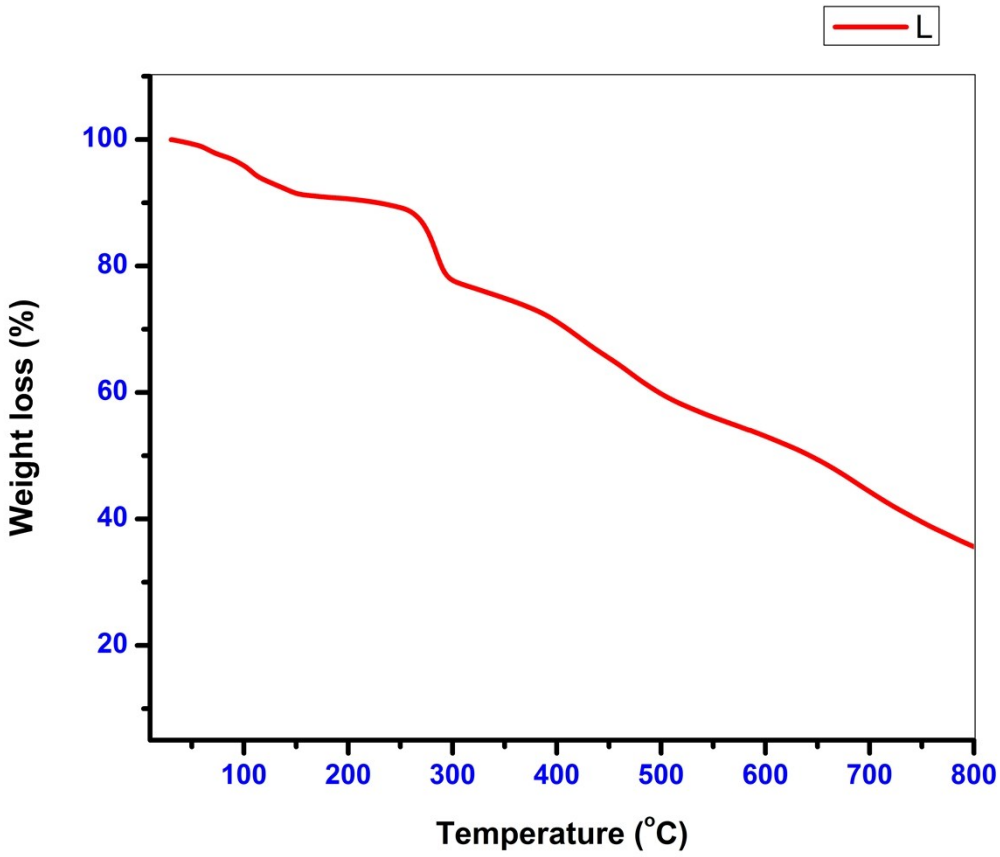
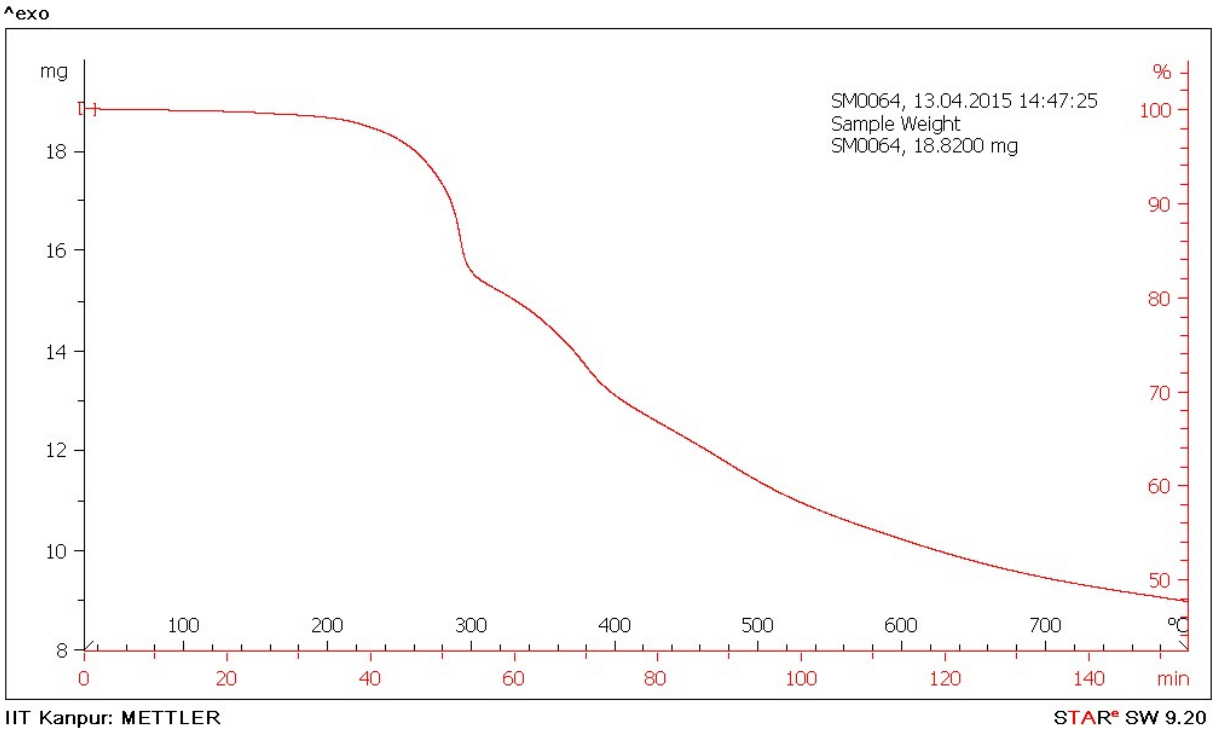


Figure S 40. TGA of 5.



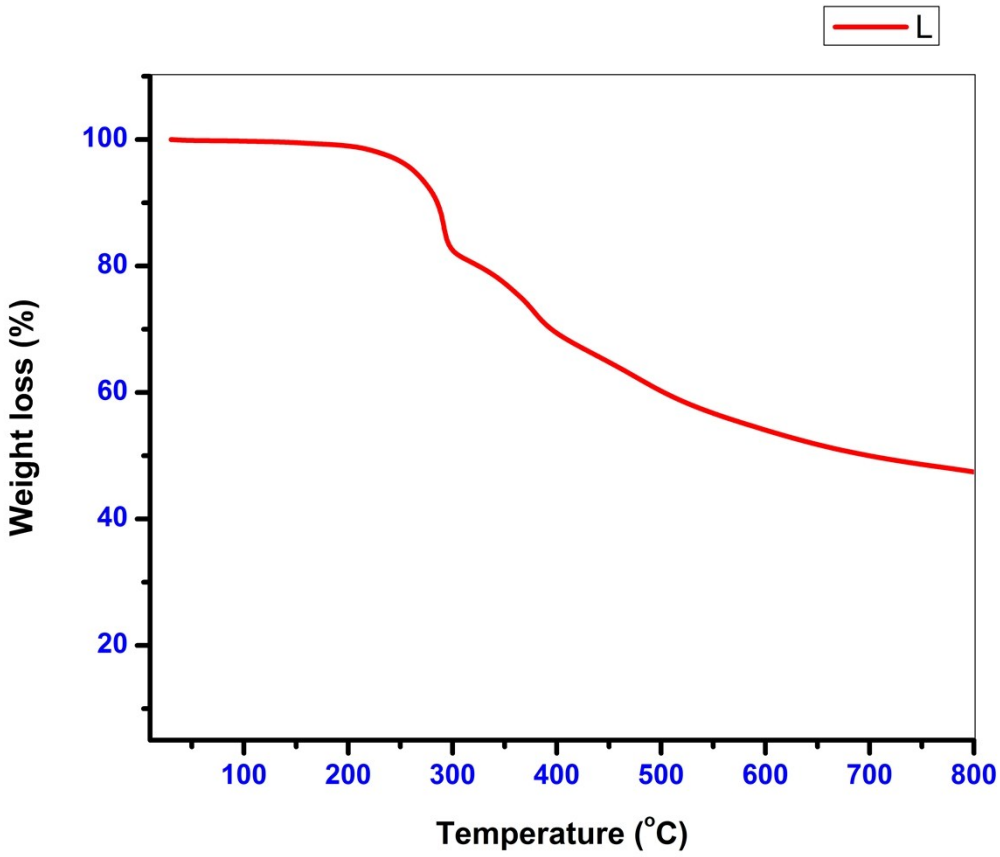
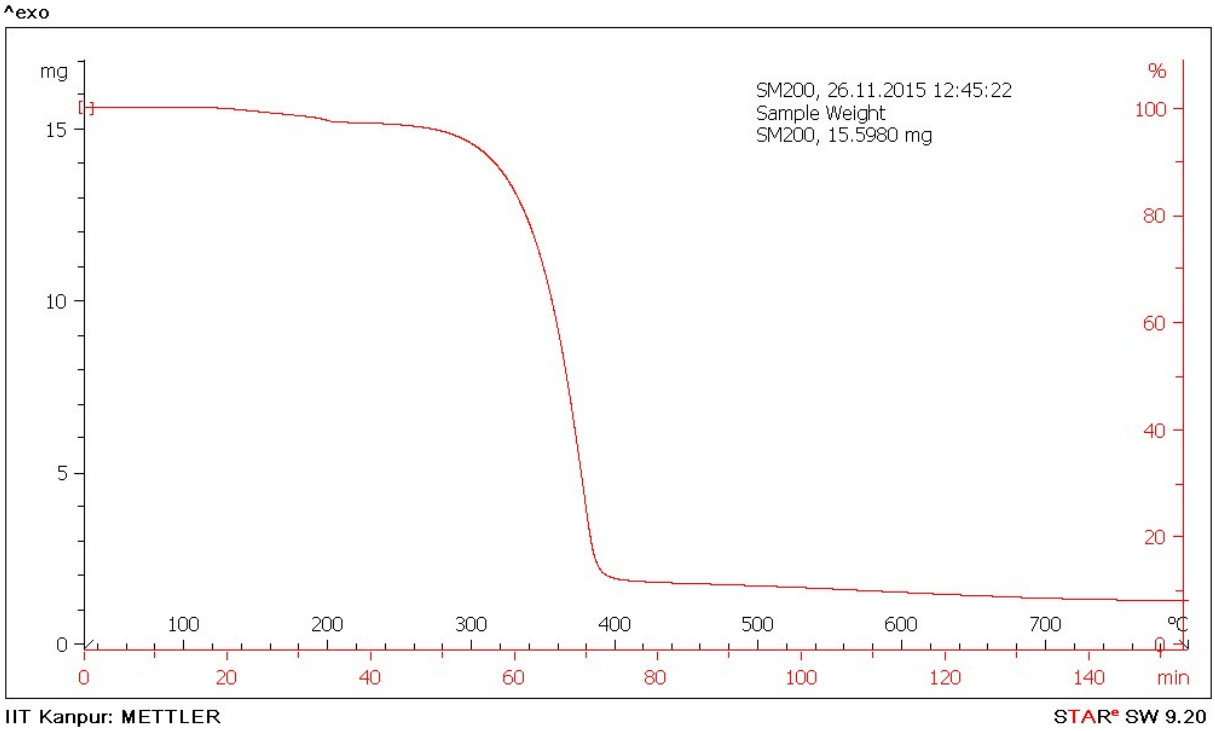


Figure S 41. TGA of 6.



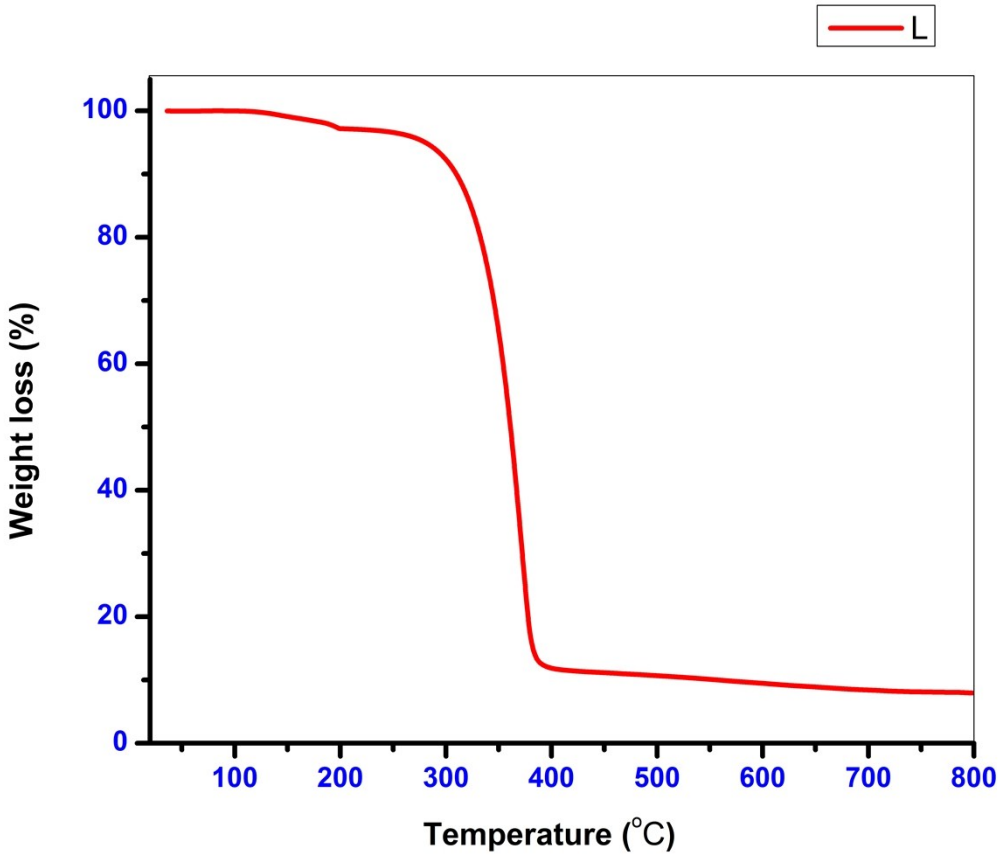
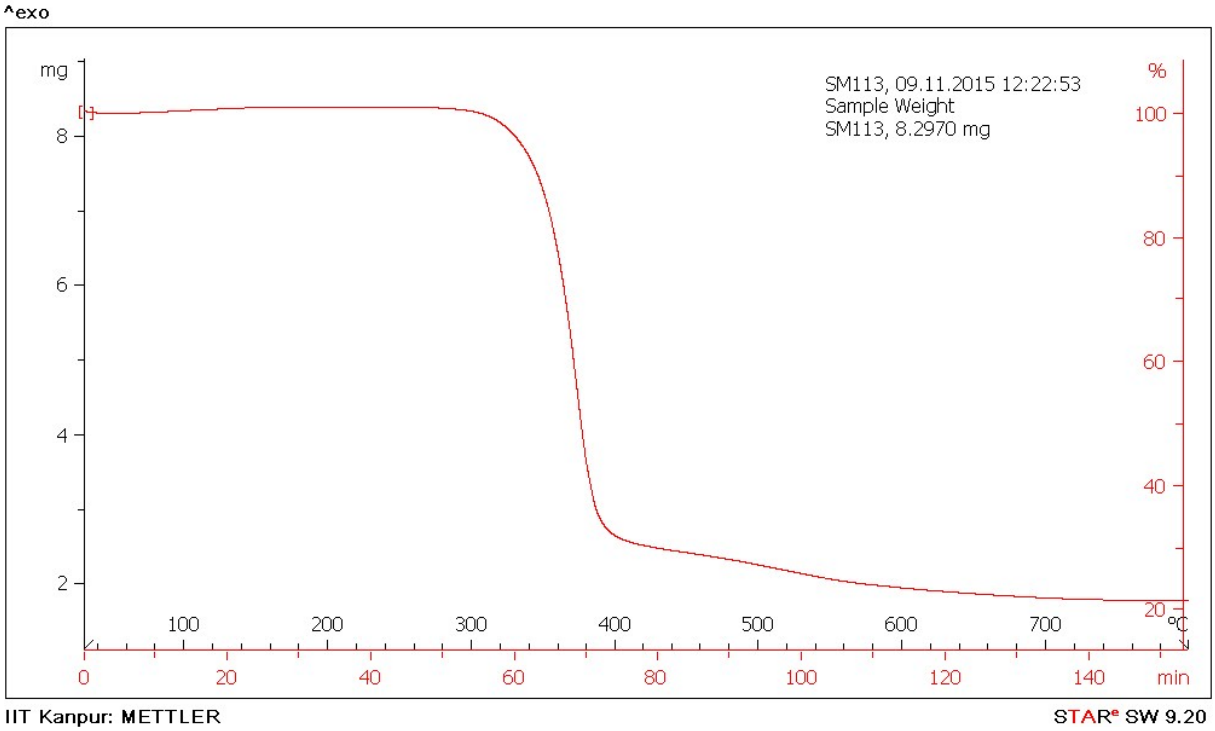


Figure S 42. TGA of 7.



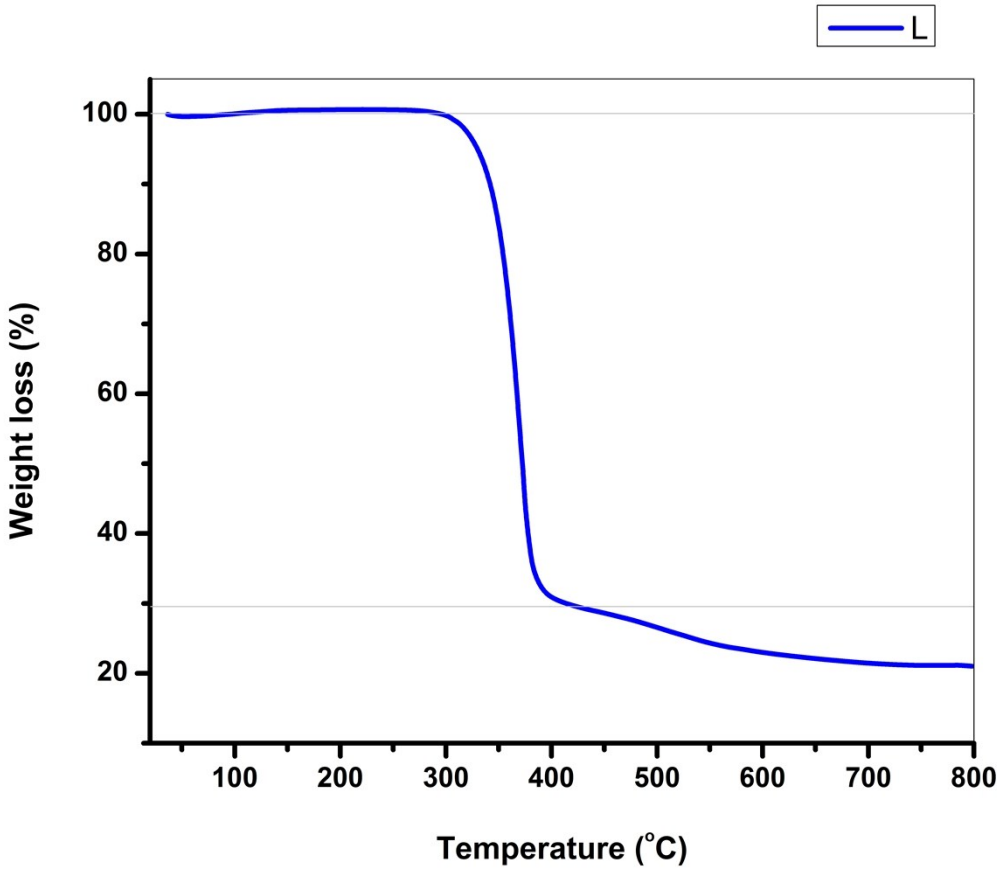
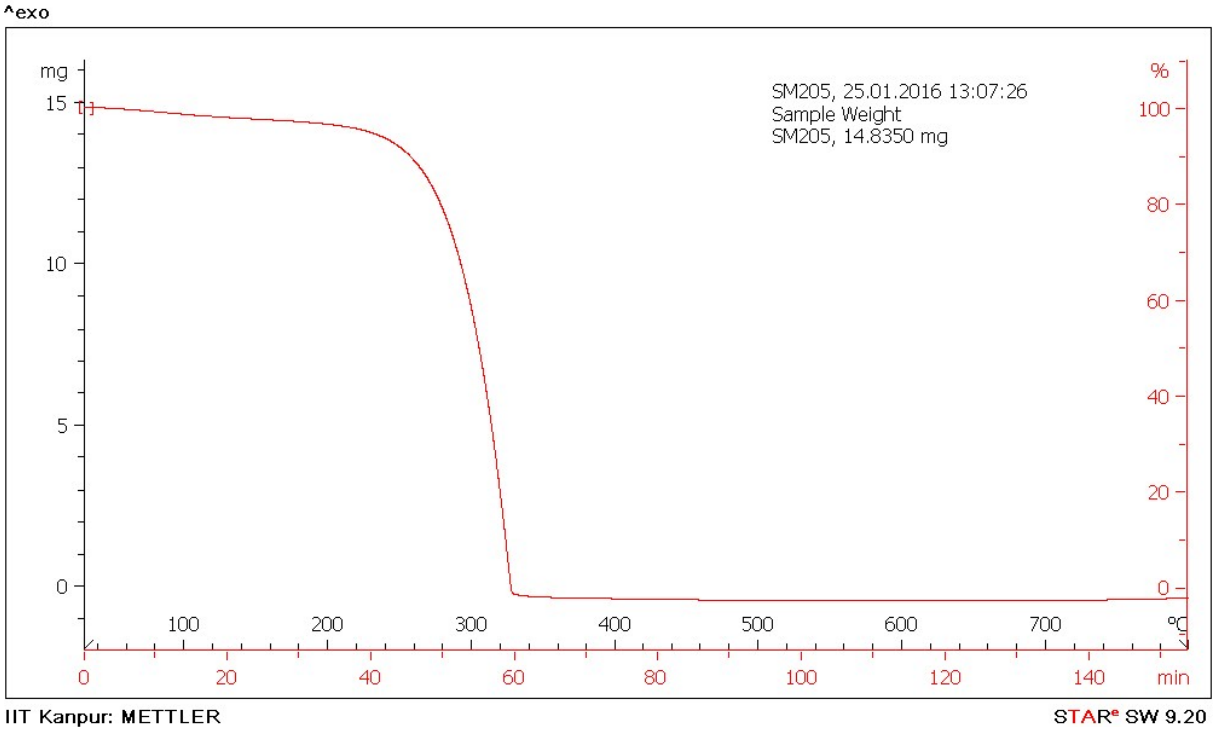


Figure S 43. TGA of 8.



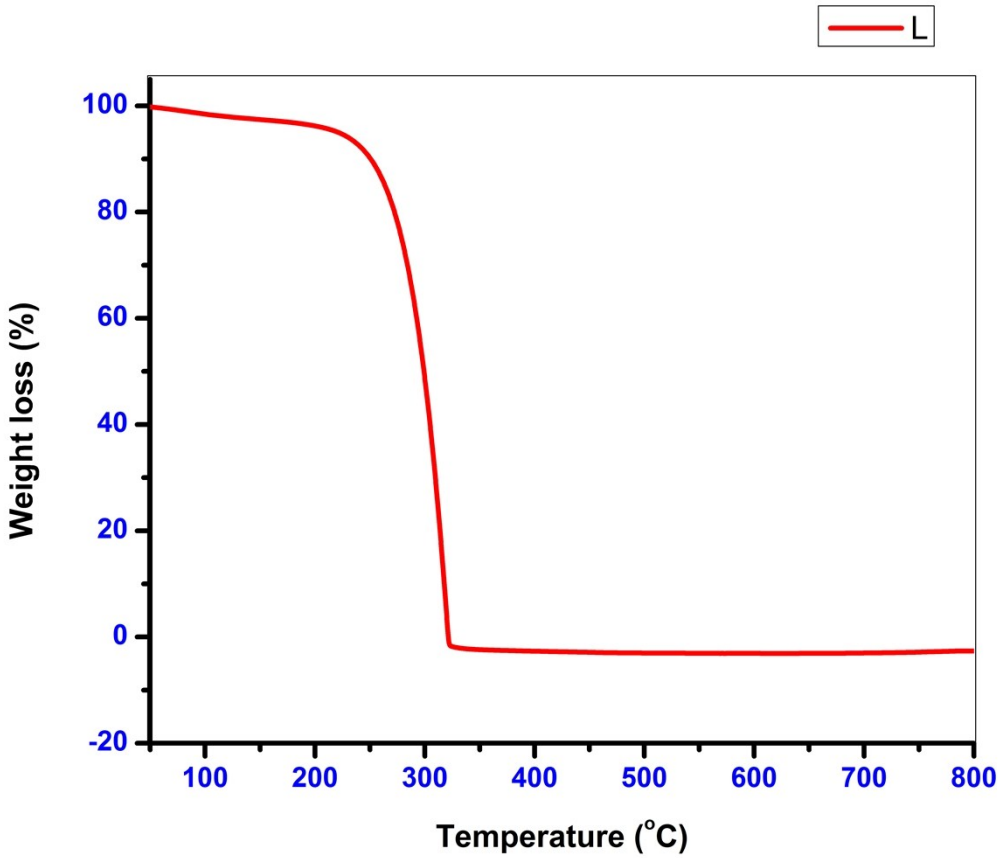
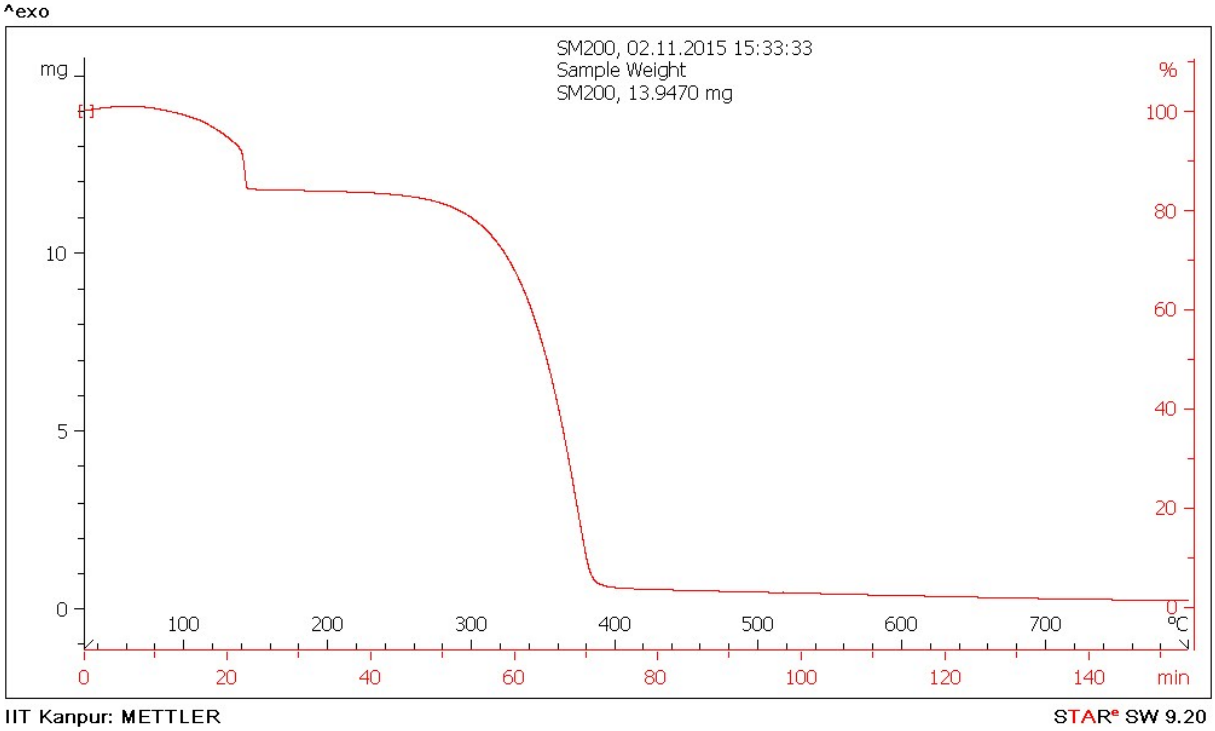


Figure S 44. TGA of $6 \cdot 0.5C_6F_6$.



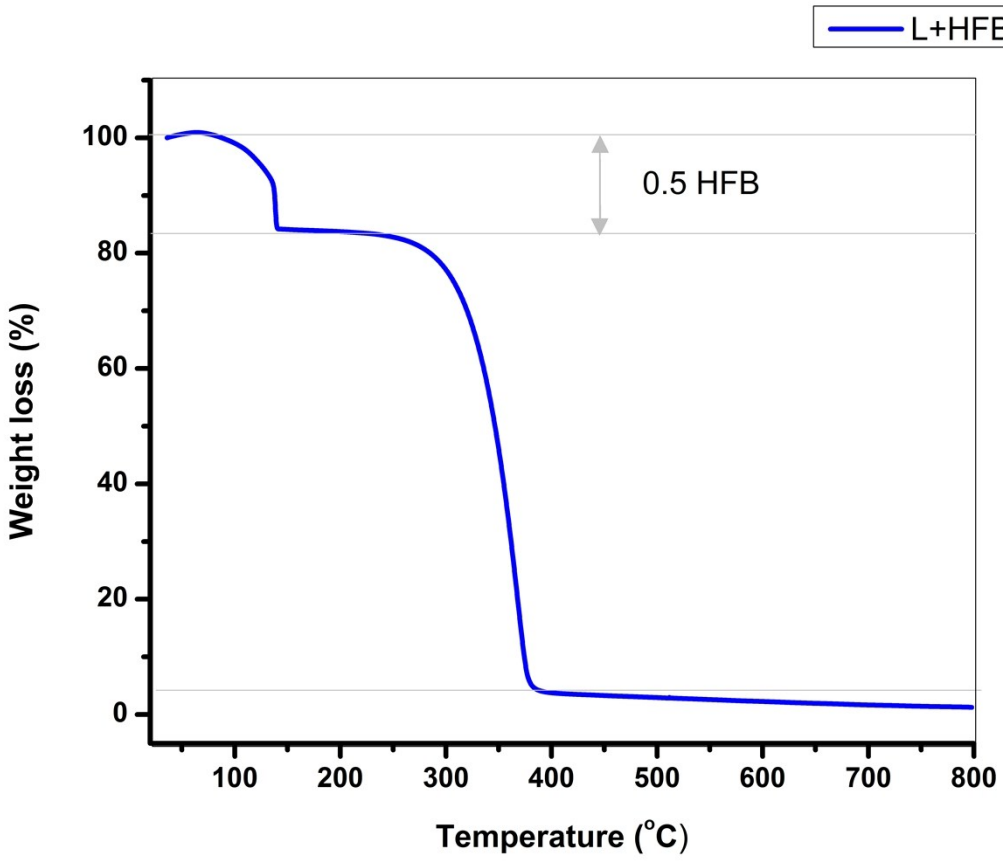


Table S 1. Crystallographic data for 2,4,6-tris(phenylthio)-1,3,5-triazine (1): CCDC-1403546

Identification code	23janb_sq	
Empirical formula	C21 H15 N3 S3	
Formula weight	405.54	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 33.368(9) Å	alpha= 90°.
	b = 13.694(3) Å	beta= 133.022(10)°.
	c = 23.569(7) Å	gamma = 90°.
Volume	7873(4) $Å^3$	
Z	16	
Density (calculated)	1.369 Mg/m^3	
Absorption coefficient	0.387 mm^{-1}	
F(000)	3360	
Crystal size	0.32 x 0.23 x 0.08 mm^3	
Theta range for data collection	1.705 to 25.260°.	
Index ranges	-40<=h<=39, -16<=k<=16, -28<=l<=27	
Reflections collected	20642	
Independent reflections	7104 [R(int) = 0.0645]	
Completeness to theta = 25.260°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.369	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7104 / 0 / 487	
Goodness-of-fit on F^2	1.006	
Final R indices [I>2sigma(I)]	R1 = 0.0523, wR2 = 0.1161	
R indices (all data)	R1 = 0.0847, wR2 = 0.1345	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.487 and -0.317 $e.Å^{-3}$	

Table S 2. Crystallographic data for 2,4,6-tris(p-tolylthio)-1,3,5-triazine (2): CCDC-1403547

Identification code	2janc	
Empirical formula	C24 H21 N3 S3	
Formula weight	447.62	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 7.5595(16) Å	alpha= 90°.
	b = 9.694(2) Å	beta= 96.753(4)°.
	c = 29.683(6) Å	gamma = 90°.
Volume	2160.2(8) $Å^3$	
Z	4	
Density (calculated)	1.376 Mg/m^3	
Absorption coefficient	0.360 mm^{-1}	
F(000)	936	
Crystal size	0.32 x 0.19 x 0.12 mm^3	
Theta range for data collection	2.21 to 28.37°.	
Index ranges	-9<=h<=9, -12<=k<=12, -25<=l<=39	
Reflections collected	13058	
Independent reflections	4982 [R(int) = 0.0496]	
Completeness to theta = 25.50°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.772	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4982 / 0 / 274	
Goodness-of-fit on F^2	1.083	
Final R indices [I>2sigma(I)]	R1 = 0.0514, wR2 = 0.1233	
R indices (all data)	R1 = 0.0770, wR2 = 0.1545	
Largest diff. peak and hole	0.503 and -0.373 $e.Å^{-3}$	

Table S 3. Crystallographic data for 2,4,6-tris((4-chlorophenyl)thio)-1,3,5-triazine (3): CCDC-1403548

Identification code	19jana	
Empirical formula	C21 H12 Cl3 N3 S3	
Formula weight	508.87	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 10.233(3) Å	alpha= 90°.
	b = 14.350(4) Å	beta= 90.980(5)°.
	c = 14.563(4) Å	gamma = 90°.
Volume	2138.1(10) $Å^3$	
Z	4	
Density (calculated)	1.581 Mg/m^3	
Absorption coefficient	0.737 mm^{-1}	
F(000)	1032	
Crystal size	0.17 x 0.15 x 0.08 mm^3	
Theta range for data collection	1.993 to 28.391°.	
Index ranges	-9<=h<=13, -18<=k<=19, -19<=l<=19	
Reflections collected	12975	
Independent reflections	4952 [R(int) = 0.0623]	
Completeness to theta = 25.500°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4952 / 0 / 271	
Goodness-of-fit on F^2	1.060	
Final R indices [I>2sigma(I)]	R1 = 0.0461, wR2 = 0.1043	
R indices (all data)	R1 = 0.0800, wR2 = 0.1298	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.739 and -0.474 $e.Å^{-3}$	

Table S 4. Crystallographic data for 2,4,6-tris((3-nitrophenyl)thio)-1,3,5-triazine (4): CCDC-1403549

Identification code	1julc	
Empirical formula	C21 H12 N6 O6 S3	
Formula weight	540.55	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 20.799(4) Å	alpha= 90°.
	b = 7.8317(15) Å	beta= 109.382(5)°.
	c = 15.126(3) Å	gamma = 90°.
Volume	2324.1(8) $Å^3$	
Z	4	
Density (calculated)	1.545 Mg/m^3	
Absorption coefficient	0.371 mm^{-1}	
F(000)	1104	
Crystal size	0.17 x 0.15 x 0.08 mm^3	
Theta range for data collection	2.800 to 28.411°.	
Index ranges	-27<=h<=18, -10<=k<=10, -19<=l<=20	
Reflections collected	15610	
Independent reflections	5801 [R(int) = 0.0774]	
Completeness to theta = 25.500°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.6666	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5801 / 0 / 325	
Goodness-of-fit on F^2	0.964	
Final R indices [I>2sigma(I)]	R1 = 0.0756, wR2 = 0.1106	
R indices (all data)	R1 = 0.2272, wR2 = 0.1432	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.297 and -0.193 $e.Å^{-3}$	

Table S 5. Crystallographic data for 2,4,6-tris((2-methyl-5-nitrophenyl)thio)-1,3,5-triazine (5): CCDC-1403550

Identification code	13apra	
Empirical formula	C24 H18 N6 O6 S3	
Formula weight	582.62	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 12.642(3) Å	alpha= 90°.
	b = 8.916(2) Å	beta= 97.804(6)°.
	c = 23.281(5) Å	gamma = 90°.
Volume	2599.9(10) $Å^3$	
Z	4	
Density (calculated)	1.488 Mg/m^3	
Absorption coefficient	0.338 mm^{-1}	
F(000)	1200	
Crystal size	0.23 x 0.18 x 0.15 mm^3	
Theta range for data collection	2.449 to 25.250°.	
Index ranges	-15<=h<=15, -9<=k<=10, -26<=l<=27	
Reflections collected	18042	
Independent reflections	4706 [R(int) = 0.0547]	
Completeness to theta = 25.250°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.6369	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4706 / 77 / 391	
Goodness-of-fit on F^2	1.007	
Final R indices [I>2sigma(I)]	R1 = 0.0495, wR2 = 0.0995	
R indices (all data)	R1 = 0.1009, wR2 = 0.1167	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.306 and -0.251 $e.Å^{-3}$	

Table S 6. Crystallographic data for 2,4,6-tris(2,6-dimethylphenylthio)-1,3,5-triazine (6): CCDC-1436792

Identification code	24jula	
Empirical formula	C27 H27 N3 S3	
Formula weight	489.69	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 11.446(2) Å	alpha = 90°.
	b = 9.9569(18) Å	beta = 93.964(8)°.
	c = 22.647(4) Å	gamma = 90°.
Volume	2574.9(8) $Å^3$	
Z	4	
Density (calculated)	1.263 Mg/m^3	
Absorption coefficient	0.308 mm^{-1}	
F(000)	1032	
Crystal size	0.26 x 0.17 x 0.15 mm^3	
Theta range for data collection	2.235 to 25.252°.	
Index ranges	-13<=h<=9, -11<=k<=11, -27<=l<=27	
Reflections collected	20447	
Independent reflections	4651 [R(int) = 0.0578]	
Completeness to theta = 25.252°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.6065	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4651 / 198 / 312	
Goodness-of-fit on F^2	1.022	
Final R indices [I>2sigma(I)]	R1 = 0.0508, wR2 = 0.1135	
R indices (all data)	R1 = 0.0946, wR2 = 0.1324	
Extinction coefficient	0.0082(14)	
Largest diff. peak and hole	0.262 and -0.284 $e.Å^{-3}$	

Table S 7. Crystallographic data for 2,4,6-tris(2,3,4,5,6-pentamethyl phenylthio)-1,3,5-triazine (7): CCDC-1436793

Identification code	1julam	
Empirical formula	C36 H45 N3 S3	
Formula weight	615.93	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 13.491(5) Å	alpha = 90°.
	b = 10.406(4) Å	beta = 94.092(7)°.
	c = 23.955(9) Å	gamma = 90°.
Volume	3354(2) $Å^3$	
Z	4	
Density (calculated)	1.220 Mg/m^3	
Absorption coefficient	0.250 mm^{-1}	
F(000)	1320	
Crystal size	0.21 x 0.17 x 0.08 mm^3	
Theta range for data collection	1.683 to 25.252°.	
Index ranges	-9<=h<=16, -12<=k<=12, -28<=l<=28	
Reflections collected	17498	
Independent reflections	6079 [R(int) = 0.2114]	
Completeness to theta = 25.252°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.273	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6079 / 18 / 394	
Goodness-of-fit on F^2	0.906	
Final R indices [I>2sigma(I)]	R1 = 0.0807, wR2 = 0.1270	
R indices (all data)	R1 = 0.2417, wR2 = 0.1836	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.274 and -0.312 $e.Å^{-3}$	

Table S 8. Crystallographic data for 2,4,6-tris(2,3,4,5,6-pentamethyl phenylthio)-1,3,5-triazine (8): CCDC-1452878

Identification code	30juld	
Empirical formula	C21 H3 F12 N3 S3	
Formula weight	621.44	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P n a 21	
Unit cell dimensions	a = 9.899(3) Å	alpha = 90°.
	b = 12.113(3) Å	beta = 90°.
	c = 20.030(5) Å	gamma = 90°.
Volume	2401.8(11) $Å^3$	
Z	4	
Density (calculated)	1.719 Mg/m^3	
Absorption coefficient	0.419 mm^{-1}	
F(000)	1224	
Crystal size	0.29 x 0.23 x 0.17 mm^3	
Theta range for data collection	2.845 to 28.240°.	
Index ranges	?<=h<=?, ?<=k<=?, ?<=l<=?	
Reflections collected	4627	
Independent reflections	4627 [R(int) = ?]	
Completeness to theta = 25.500°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.5868	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4627 / 1 / 352	
Goodness-of-fit on F^2	1.001	
Final R indices [I>2sigma(I)]	R1 = 0.0450, wR2 = 0.0761	
R indices (all data)	R1 = 0.1336, wR2 = 0.1014	
Absolute structure parameter	0.09(5)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.216 and -0.257 $e.Å^{-3}$	

Table S 9. Crystallographic data for 2,4,6-tris(2,6-dimethylphenylthio)-1,3,5-triazine ($6 \cdot 0.5C_6F_6$): CCDC-1436791

Identification code	6sepam	
Empirical formula	C30 H27 F3 N3 S3	
Formula weight	582.72	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.411(2) Å	alpha = 108.662(4)°.
	b = 12.295(3) Å	beta = 108.819(3)°.
	c = 13.934(3) Å	gamma = 92.389(4)°.
Volume	1426.8(5) $Å^3$	
Z	2	
Density (calculated)	1.356 Mg/m^3	
Absorption coefficient	0.304 mm^{-1}	
F(000)	606	
Crystal size	0.27 x 0.21 x 0.14 mm^3	
Theta range for data collection	1.771 to 28.254°.	
Index ranges	-8<=h<=12, -16<=k<=16, -18<=l<=18	
Reflections collected	8482	
Independent reflections	6145 [R(int) = 0.0232]	
Completeness to theta = 25.500°	97.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.573	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6145 / 0 / 358	
Goodness-of-fit on F^2	1.163	
Final R indices [I>2sigma(I)]	R1 = 0.0930, wR2 = 0.2450	
R indices (all data)	R1 = 0.1076, wR2 = 0.2863	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.346 and -1.416 $e.Å^{-3}$	