

Synthesis of 6-(2-Furyl) and 6-(2-Thienyl)-4-trifluoromethylpyrimidinones and -pyrimidines from 4-(2-Heteroaryl)-4-methoxy-1,1,1-trifluoro-3-buten-2-ones

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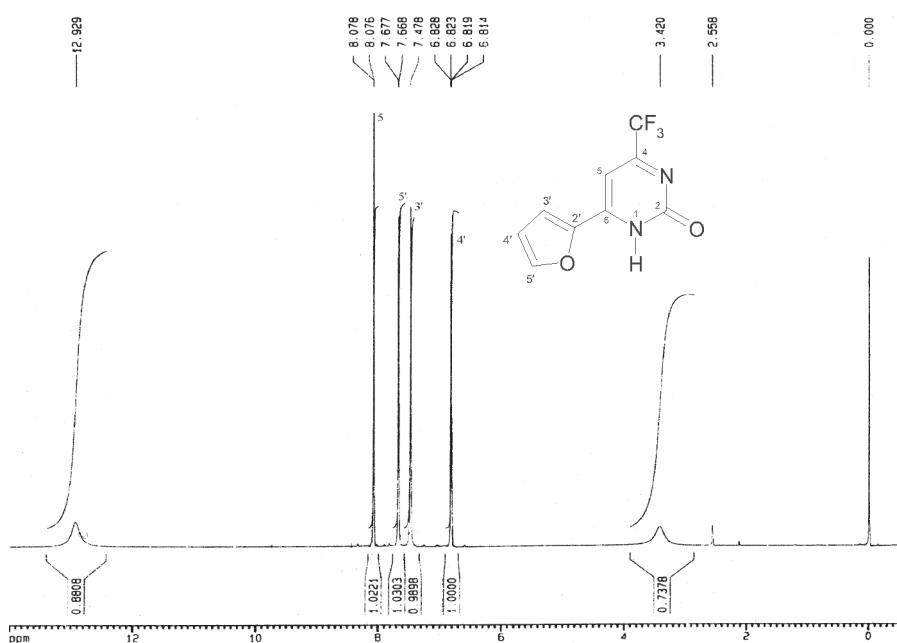
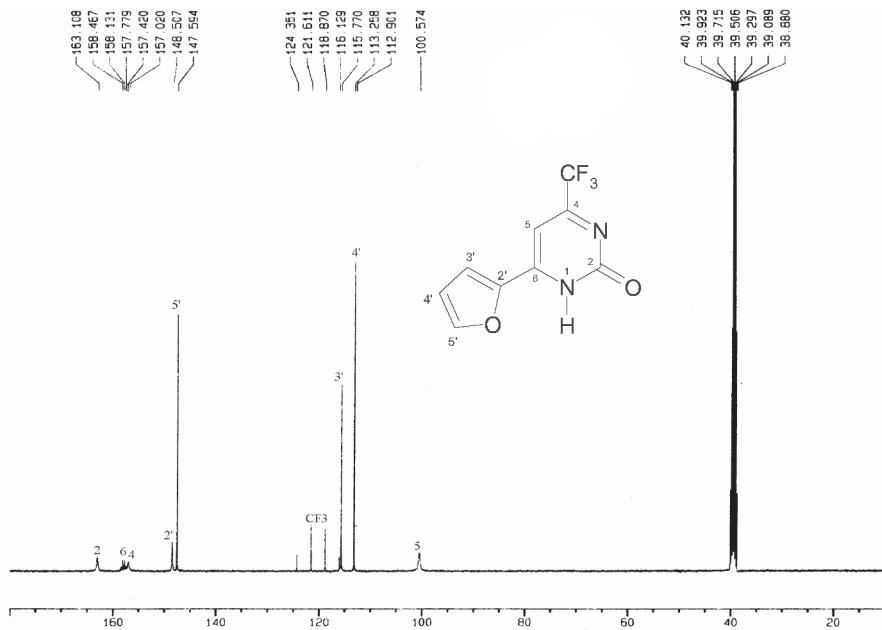
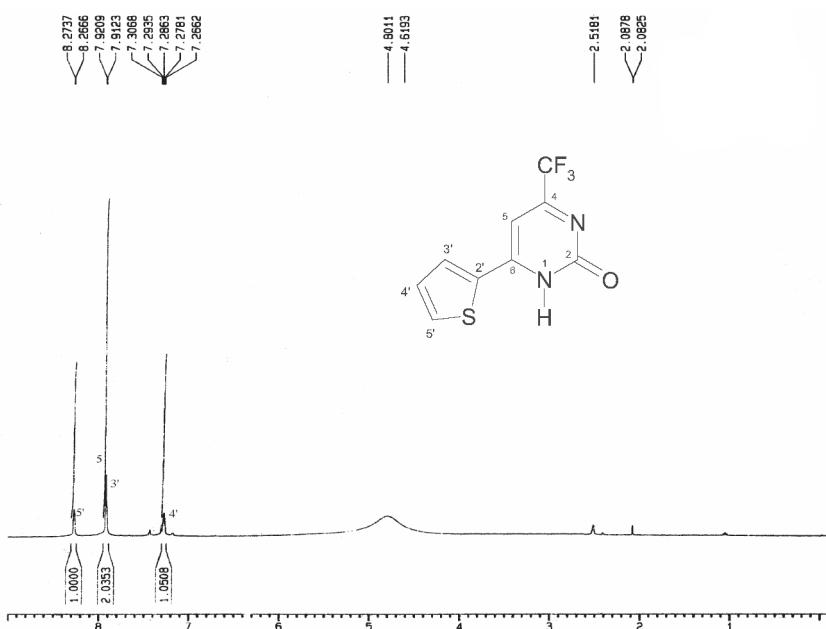


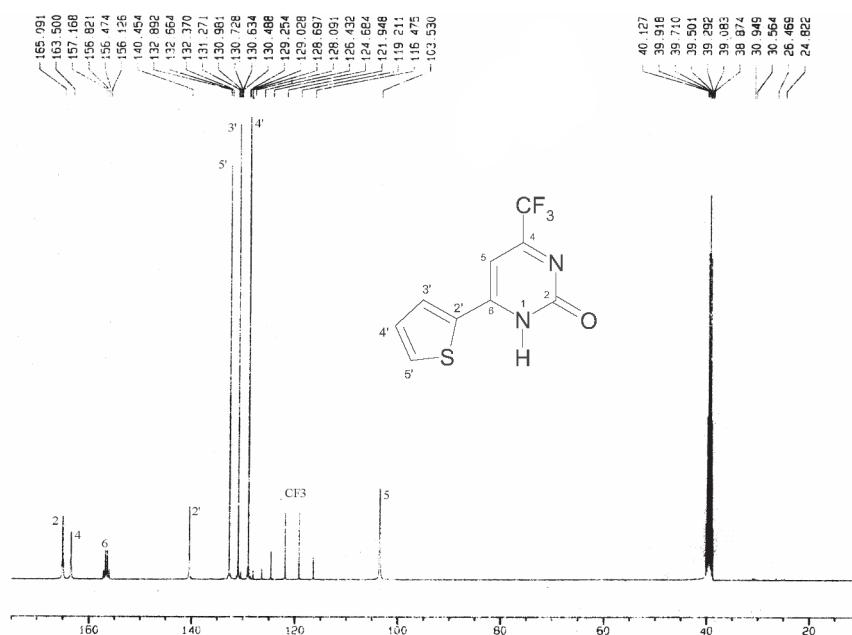
Figure S1. <sup>1</sup>H NMR spectrum of the 6-(2-furyl)-4-trifluoromethyl-1*H*-pyrimidin-2-one (2a), DMSO-d<sub>6</sub>.



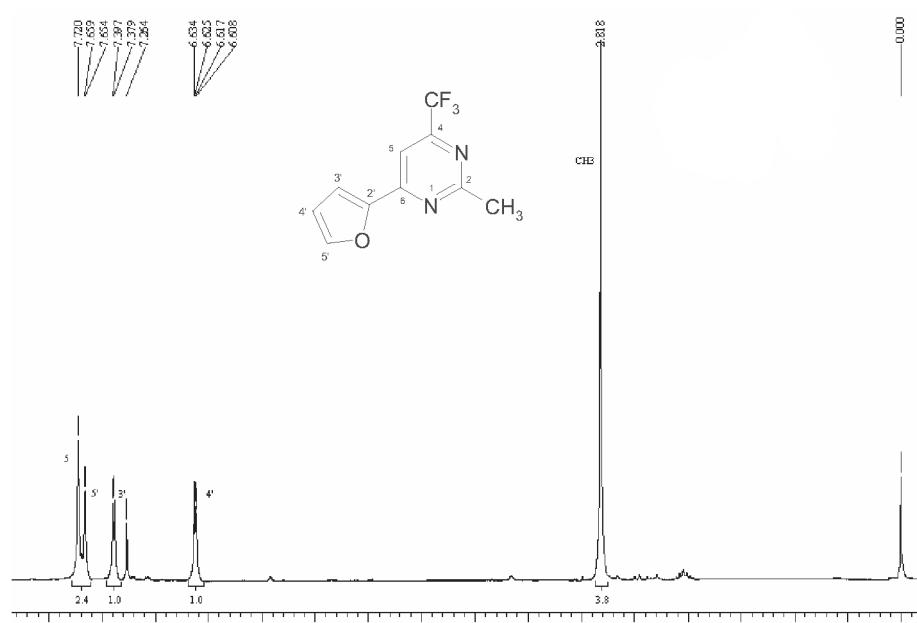
**Figure S2.**  $^{13}\text{C}[\text{H}]$  NMR spectrum of the 6-(2-furyl)-4-trifluoromethyl-1*H*-pyrimidin-2-one (**2a**), DMSO- $d_6$ .



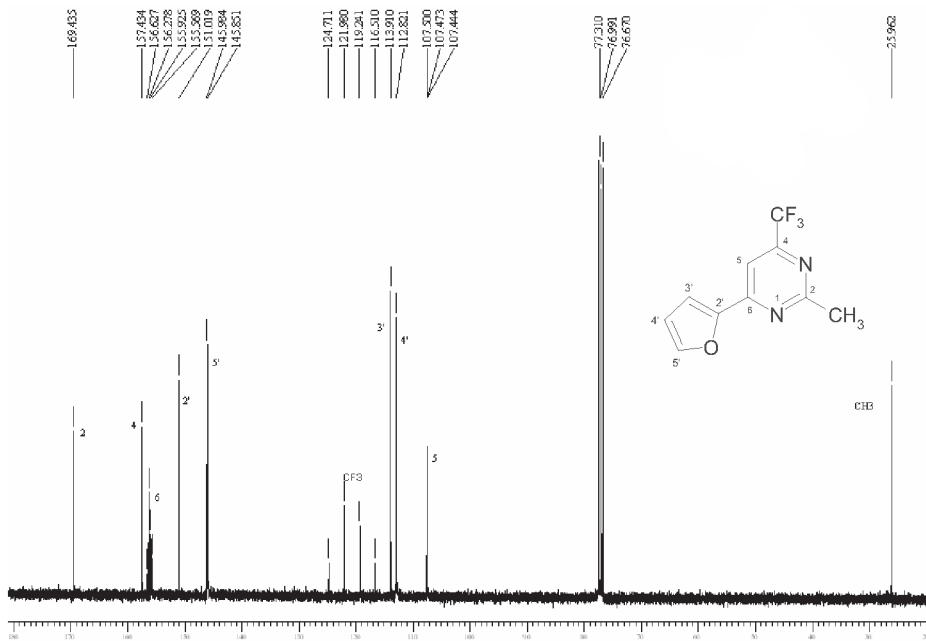
**Figure S3.**  $^1\text{H}$  NMR spectrum of the 6-(2-thienyl)-4-trifluoromethyl-1*H*-pyrimidin-2-one (**2b**), DMSO- $d_6$ .



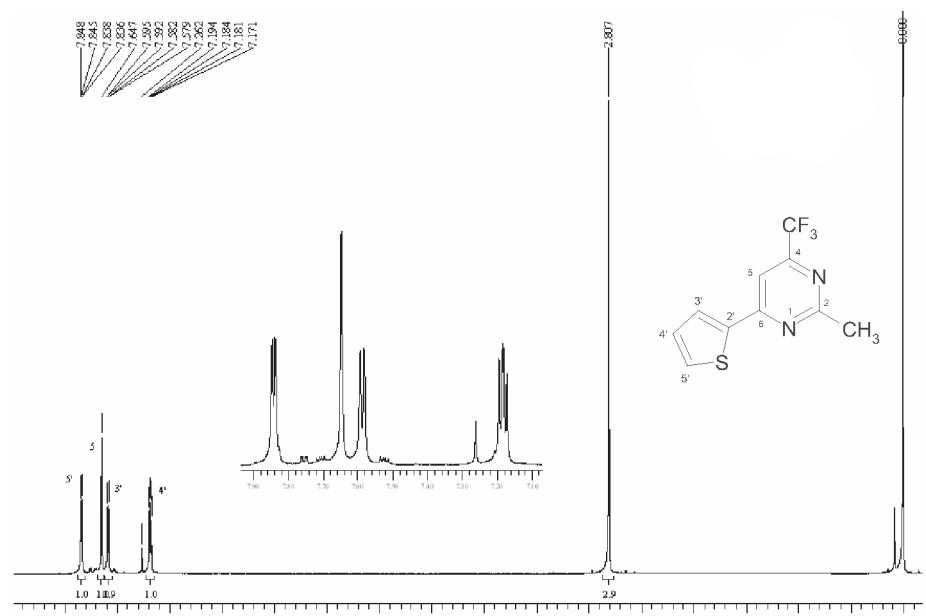
**Figure S4.**  $^{13}\text{C}$  NMR spectrum of the 6-(2-thienyl)-4-trifluoromethyl-1*H*-pyrimidin-2-one (**2b**), DMSO- $d_6$ .



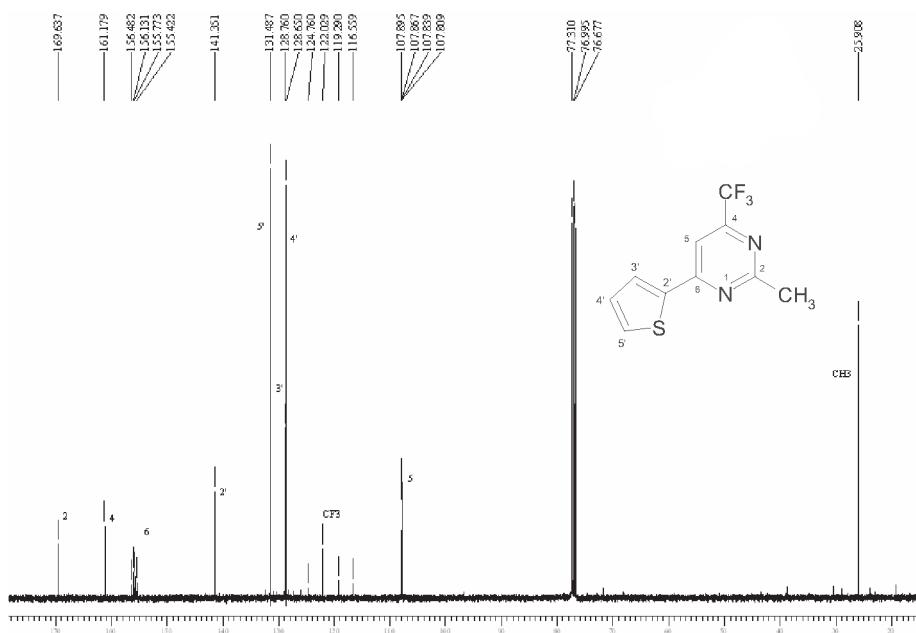
**Figura S5.**  $^1\text{H}$  NMR spectrum of the 6-(2-furyl)-2-methyl-4-trifluoromethylpyrimidine (**3a**),  $\text{CDCl}_3$ .



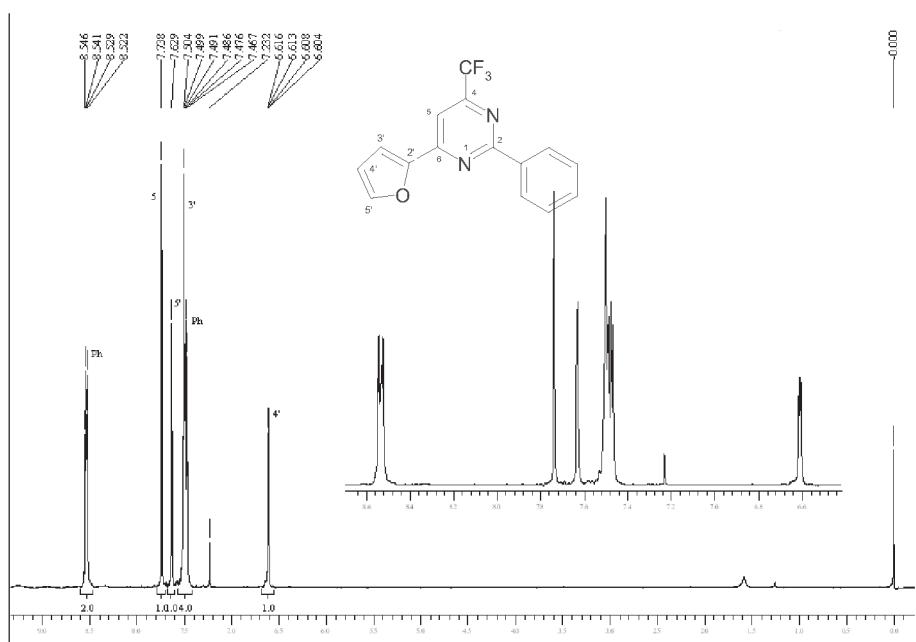
**Figure S6.** <sup>13</sup>C NMR spectrum of the 6-(2-furyl)-2-methyl-4-trifluoromethylpyrimidine (**3a**),  $\text{CDCl}_3$ .



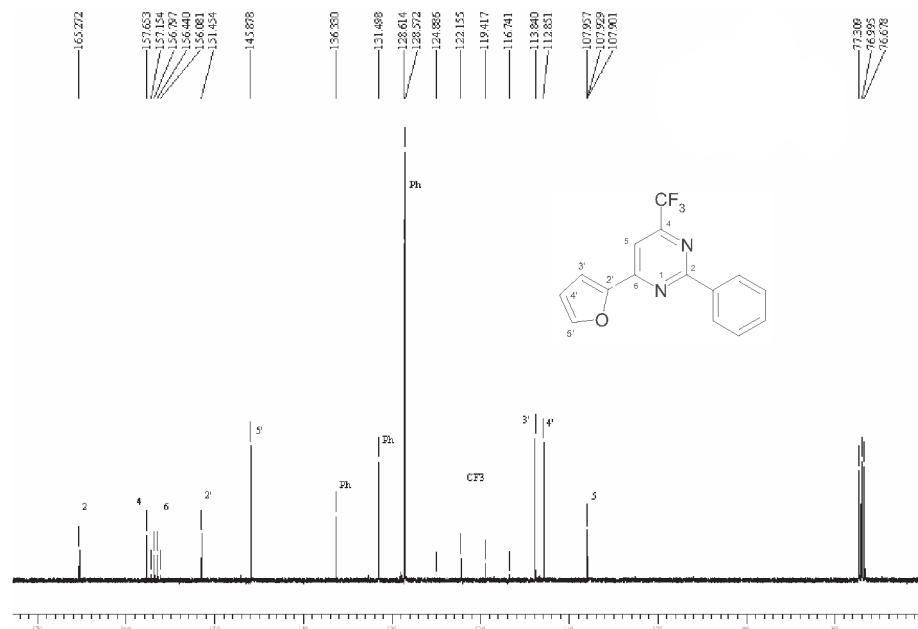
**Figure S7.** <sup>1</sup>H NMR spectrum of the 2-methyl-6-(2-thienyl)-4-trifluoromethylpyrimidine (**3b**),  $\text{CDCl}_3$ .



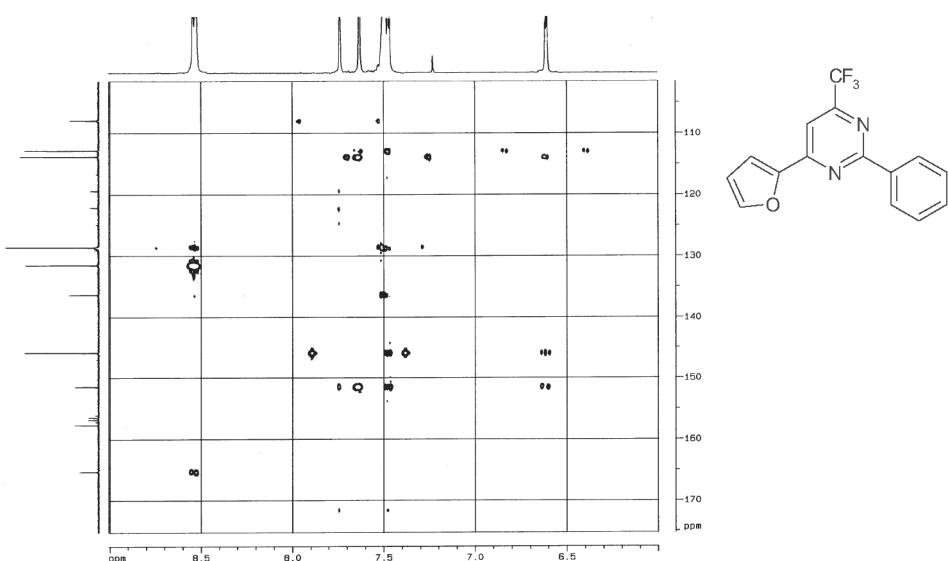
**Figure S8.**  $^{13}\text{C}[\text{H}]$  NMR spectrum of the 6-(2-thienyl)-2-methyl-4-trifluoromethylpyrimidine **3b**,  $\text{CDCl}_3$ .



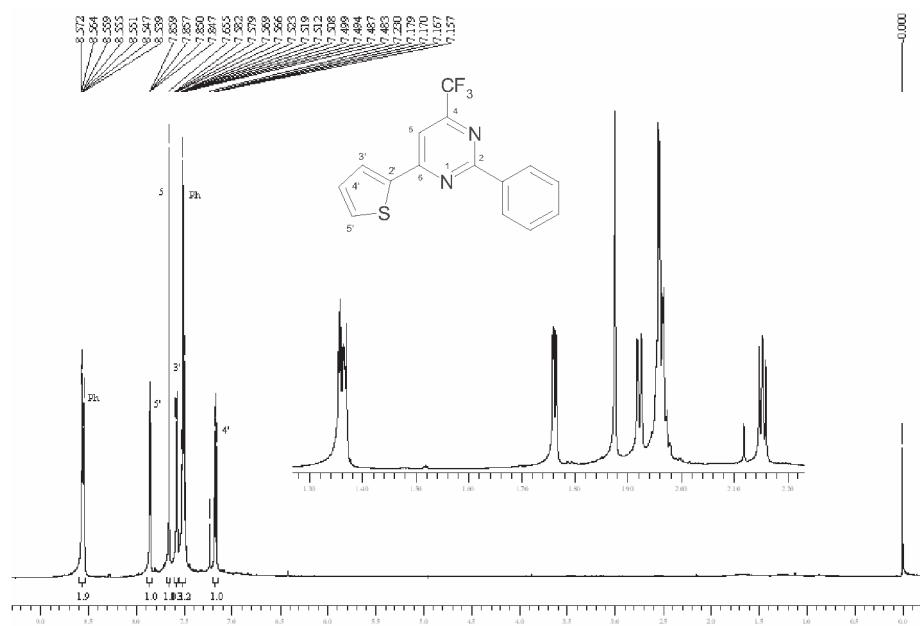
**Figure S9.**  $^1\text{H}$  NMR spectrum of the 6-(2-furyl)- 2-phenyl-4-trifluoromethylpyrimidine **4a**,  $\text{CDCl}_3$ ,



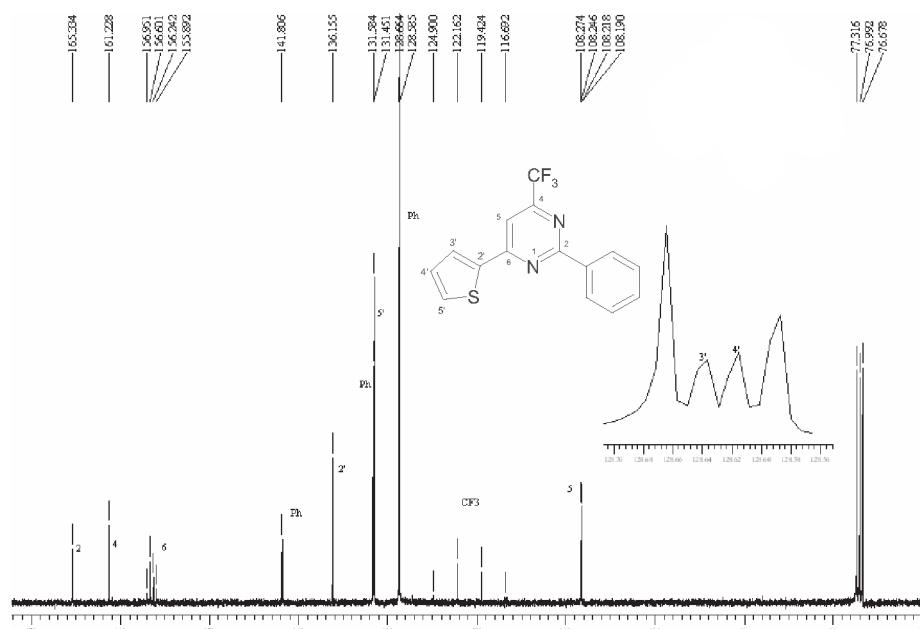
**Figure S10.** <sup>13</sup>C NMR spectrum of the 6-(2-furyl)-2-phenyl-4-trifluoromethylpyrimidine **4a**, CDCl<sub>3</sub>.



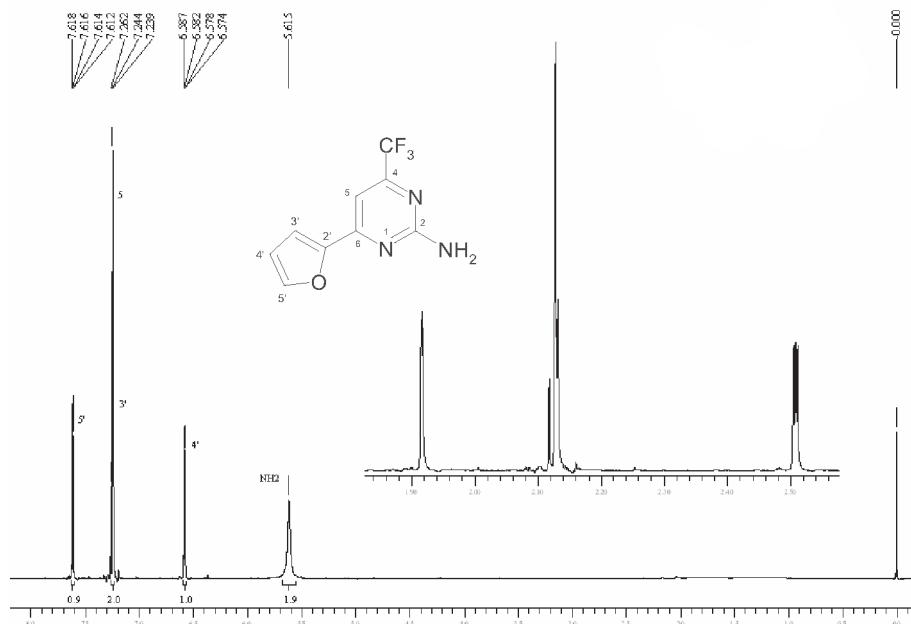
**Figure S11.** HMBC spectrum of the 6-(2-furyl)-2-phenyl-4-trifluoromethylpyrimidine **3b**, CDCl<sub>3</sub>.



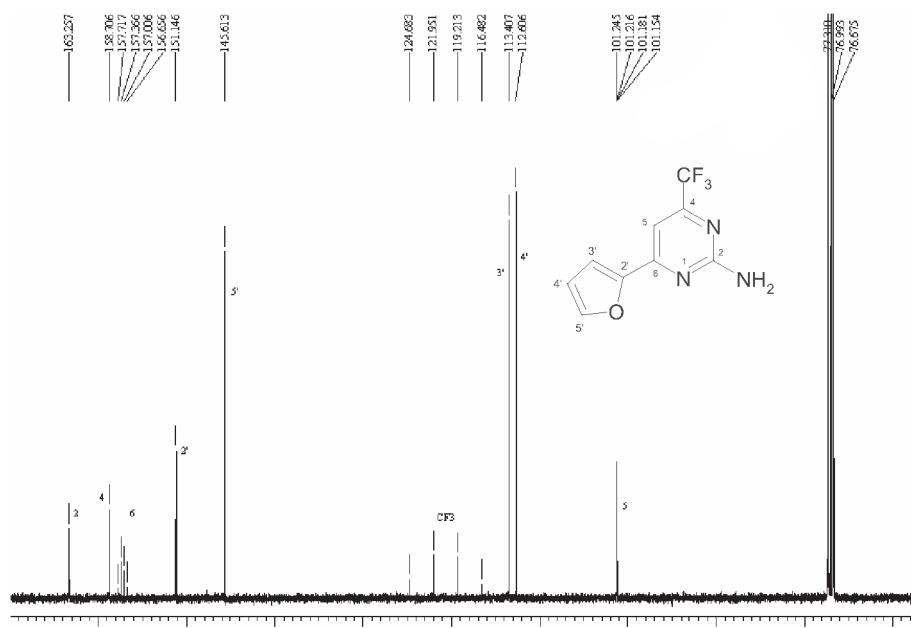
**Figure S12.** <sup>1</sup>H NMR spectrum of the 2-phenyl-6-(2-thienyl)-4-trifluoromethylpyrimidine **4b**, CDCl<sub>3</sub>.



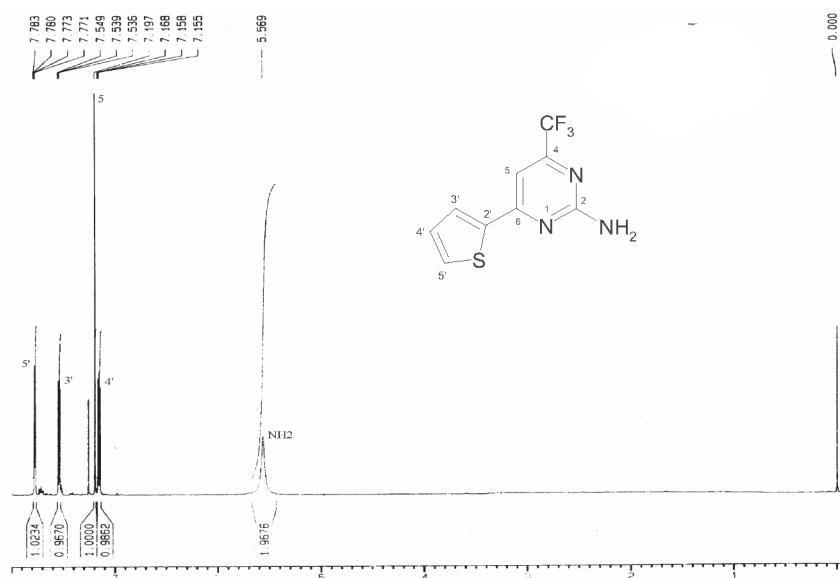
**Figure S13.** <sup>13</sup>C{H} NMR spectrum of the 2-phenyl-6-(2-thienyl)-4-trifluoromethylpyrimidine **4b**, CDCl<sub>3</sub>.



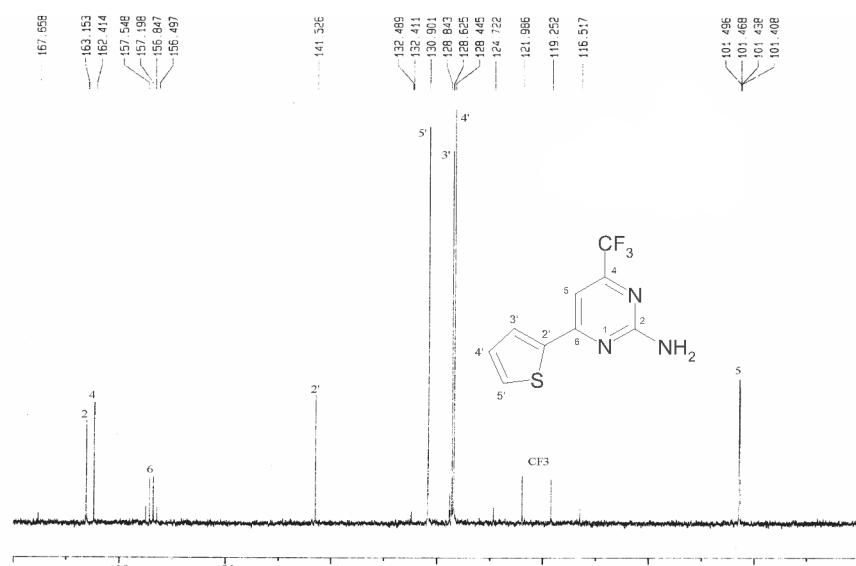
**Figure S14.**  $^1\text{H}$  NMR spectrum of the 2-amino-6-(2-furyl)-4-trifluoromethylpyrimidine **5a**,  $\text{CDCl}_3$ .



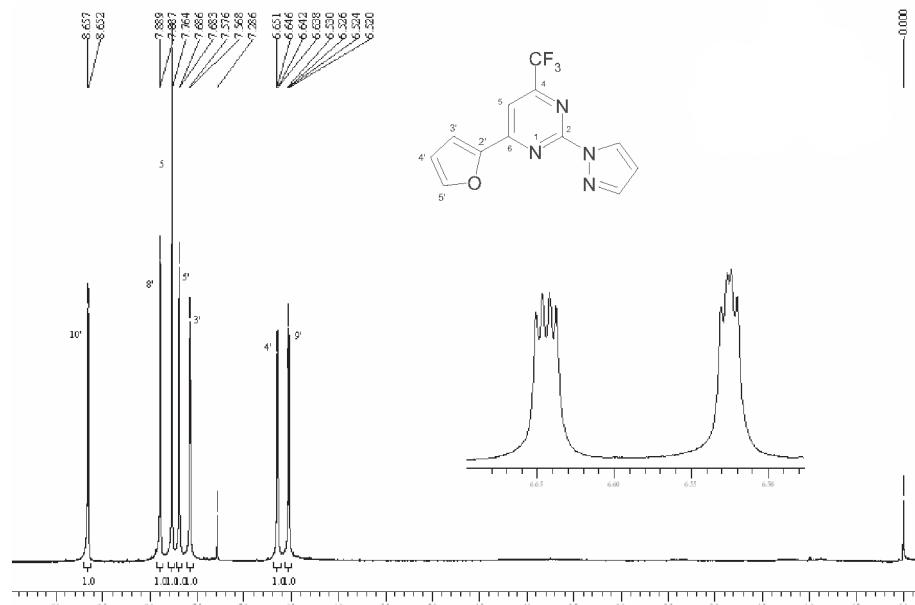
**Figure S15.**  $^{13}\text{C}$  [H] NMR spectrum of the 2-amino-6-(2-furyl)-4-trifluoromethylpyrimidine **5a**,  $\text{CDCl}_3$ .



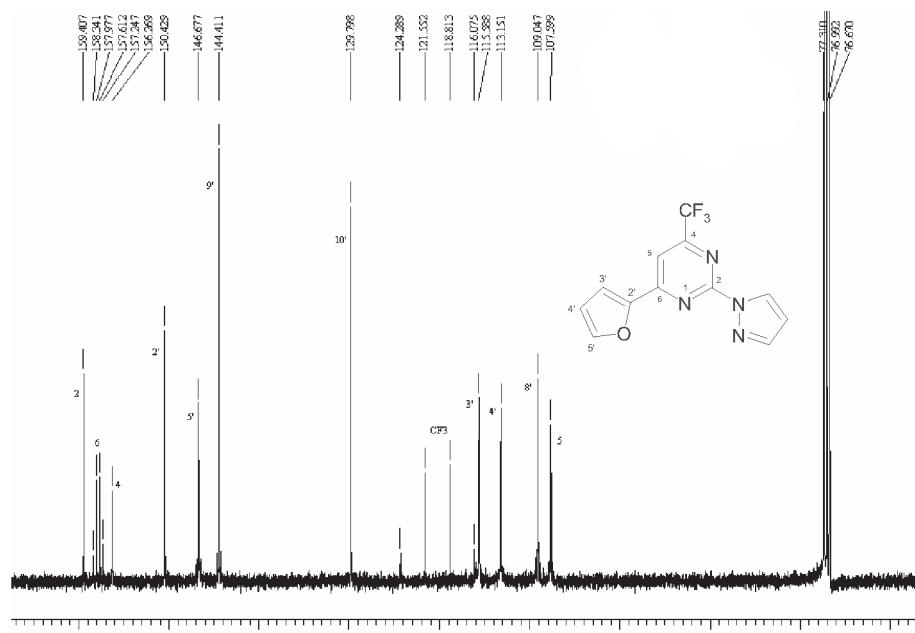
**Figure S16.** <sup>1</sup>H NMR spectrum of the 2-amino-6-(2-thienyl)-4-trifluoromethylpyrimidine **5b**, CDCl<sub>3</sub>.



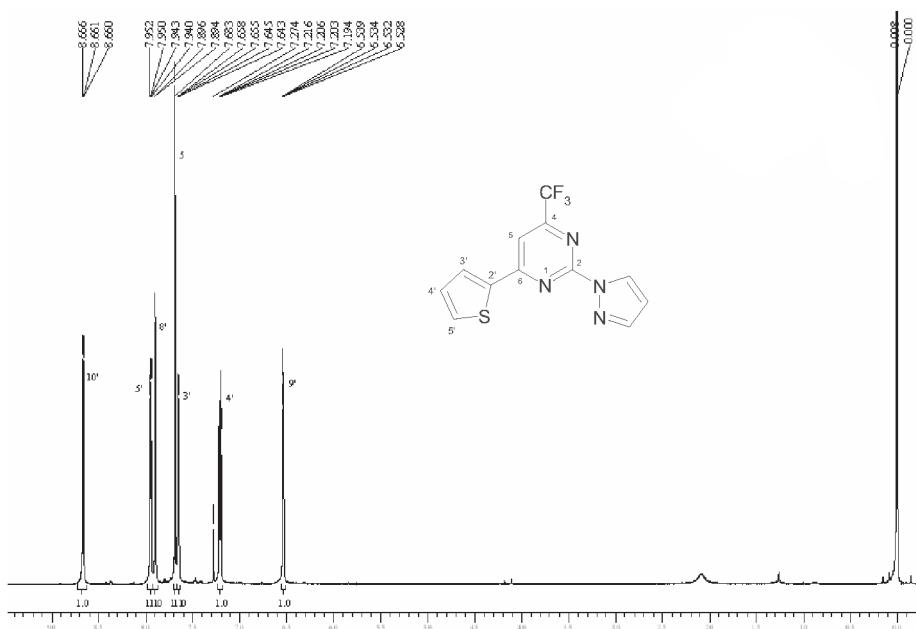
**Figure S17.** <sup>13</sup>C{H} NMR spectrum of the 2-amino-6-(2-thienyl)-4-trifluoromethylpyrimidine **5b**, CDCl<sub>3</sub>.



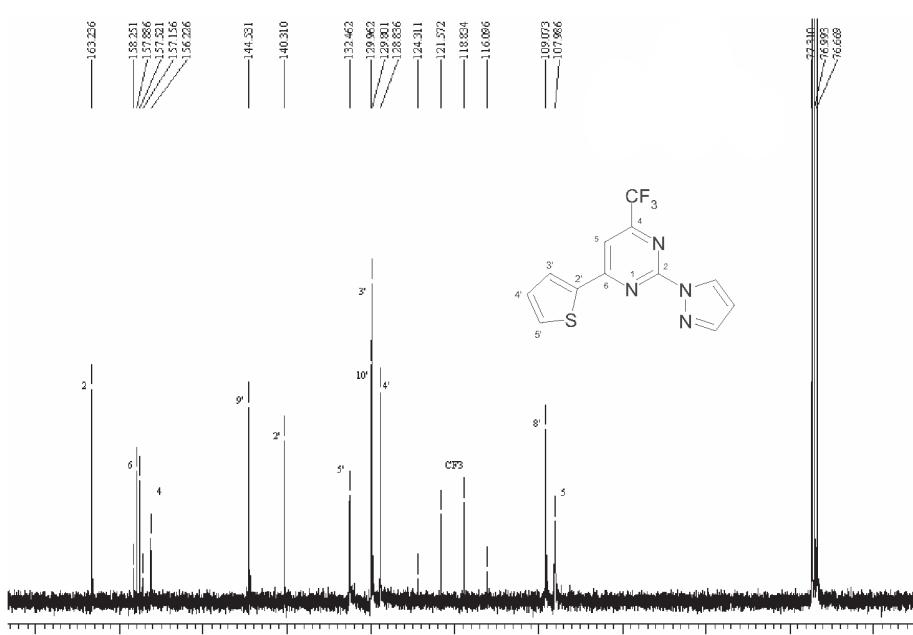
**Figure S18.**  $^1\text{H}$  NMR spectrum of the 6-(2-furyl)-2-(1*H*-pyrazol-1-yl)-4-trifluoromethyl-pyrimidine **6a**,  $\text{CDCl}_3$ .



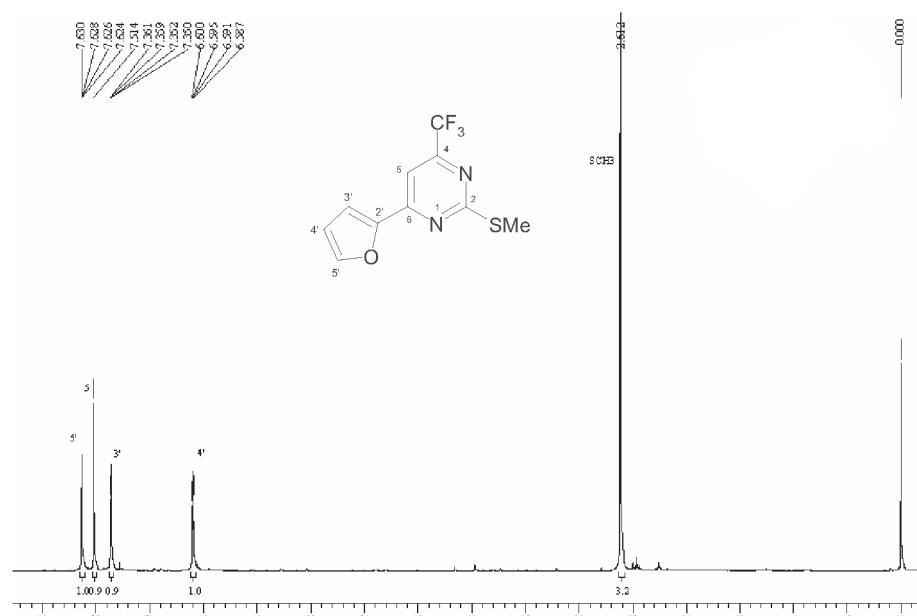
**Figure S19.**  $^{13}\text{C}[\text{H}]$  NMR spectrum of 6-(2-furyl)-2-(1*H*-pyrazol-1-yl)-4-trifluoromethyl-pyrimidine **6a**,  $\text{CDCl}_3$ .



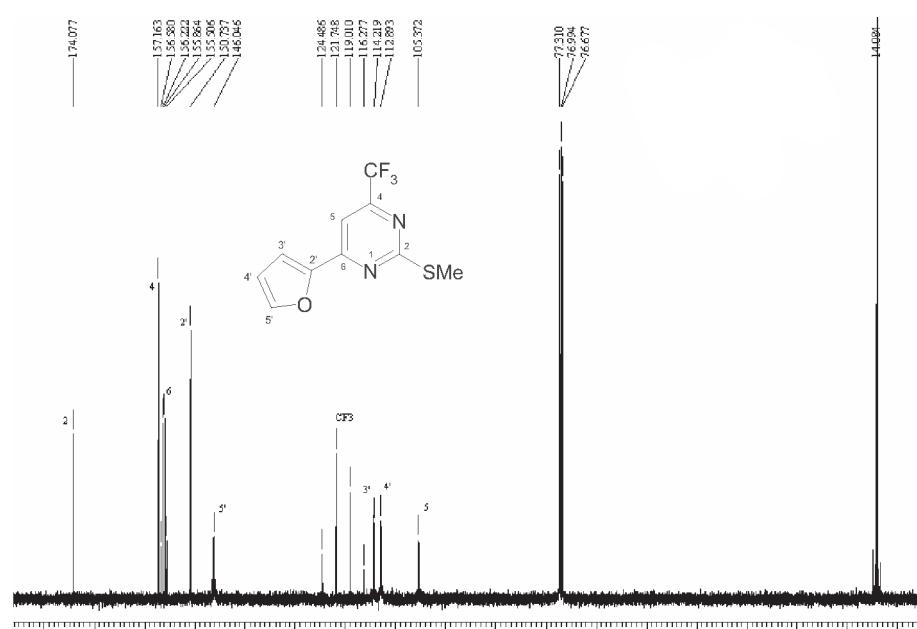
**Figure S20.**  $^1\text{H}$  NMR spectrum of the 2-(1*H*-pyrazol-1-yl)-6-(2-thienyl) 4-trifluoromethylpyrimidine **6b**,  $\text{CDCl}_3$ .



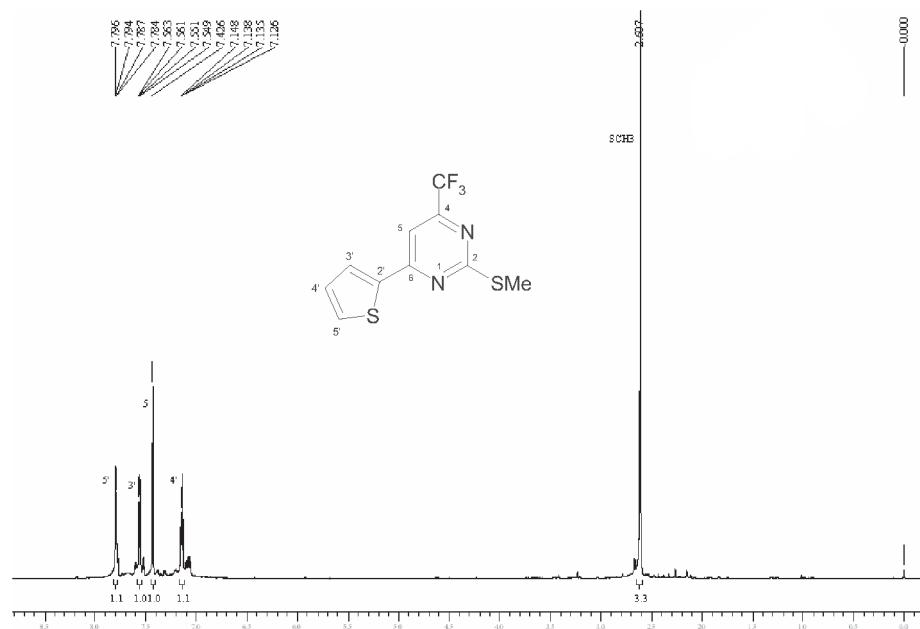
**Figure S21.**  $^{13}\text{C}[\text{H}]$  NMR spectrum of the 2-(1*H*-pyrazol-1-yl)-6-(2-thienyl)-4-trifluoromethylpyrimidine **6b**,  $\text{CDCl}_3$ .



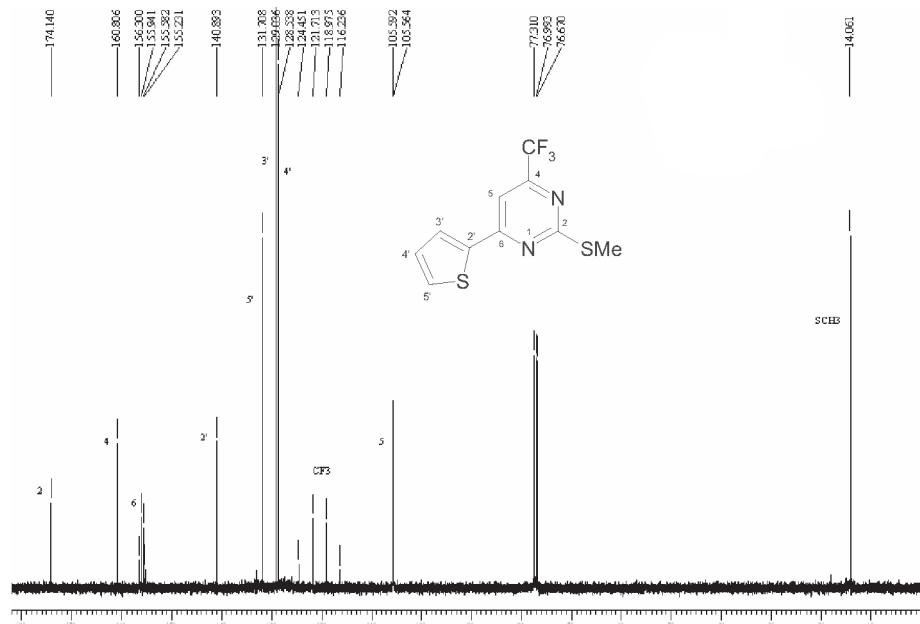
**Figure S22.**  $^1\text{H}$  NMR spectrum of the 6-(2-furyl)-2-tiomethyl-4-trifluoromethylpyrimidine **7a**,  $\text{CDCl}_3$ .



**Figure S23.**  $^{13}\text{C}[\text{H}]$  NMR spectrum of the 6-(2-furyl)-2-tiomethyl-4-trifluoromethylpyrimidine **7a**,  $\text{CDCl}_3$ .



**Figure S24.** <sup>1</sup>H NMR spectrum of the 6-(2-thienyl)-2-tiomethyl-4-trifluoromethylpyrimidine **7b**, CDCl<sub>3</sub>.



**Figure S25.** <sup>13</sup>C{H} NMR spectrum of the 6-(2-thienyl)-2-tiomethyl-4-trifluoromethylpyrimidine **7b**, CDCl<sub>3</sub>.

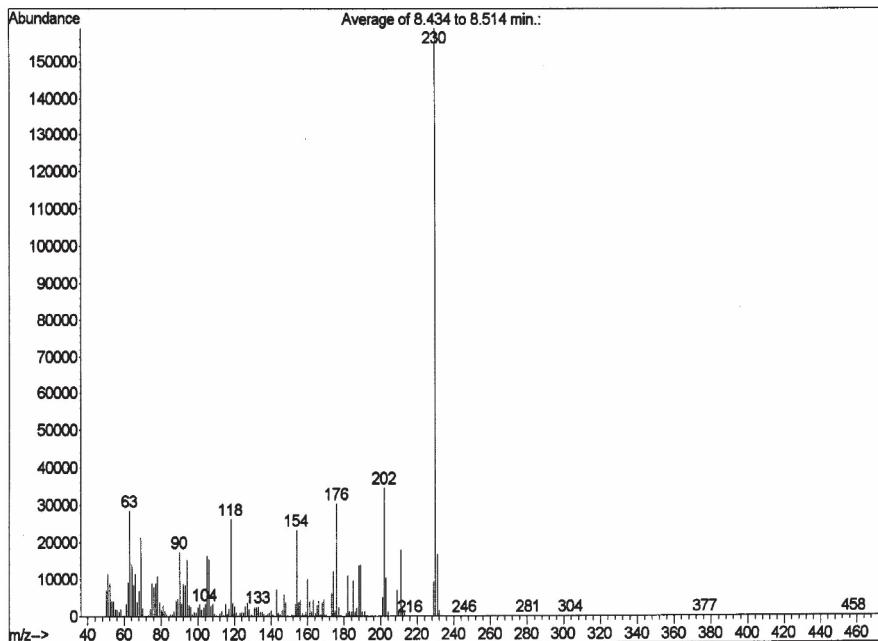


Figure S26. MS of 6-(2-furyl)-4-trifluoromethyl-1*H*-pyrimidin-2-one (**2a**).

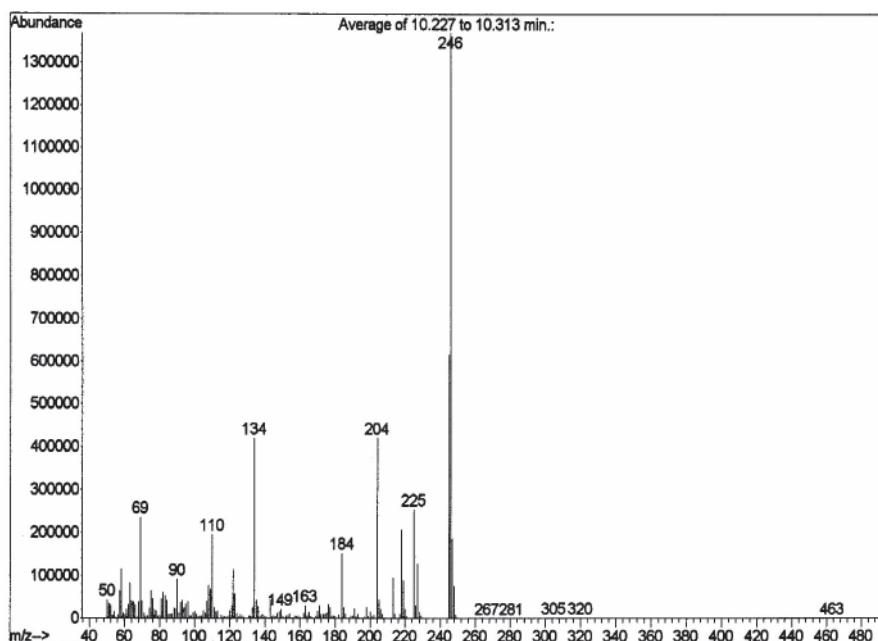


Figure S27. MS of 6-(2-thienyl)-4-trifluoromethyl-1*H*-pyrimidin-2-one (**2b**).

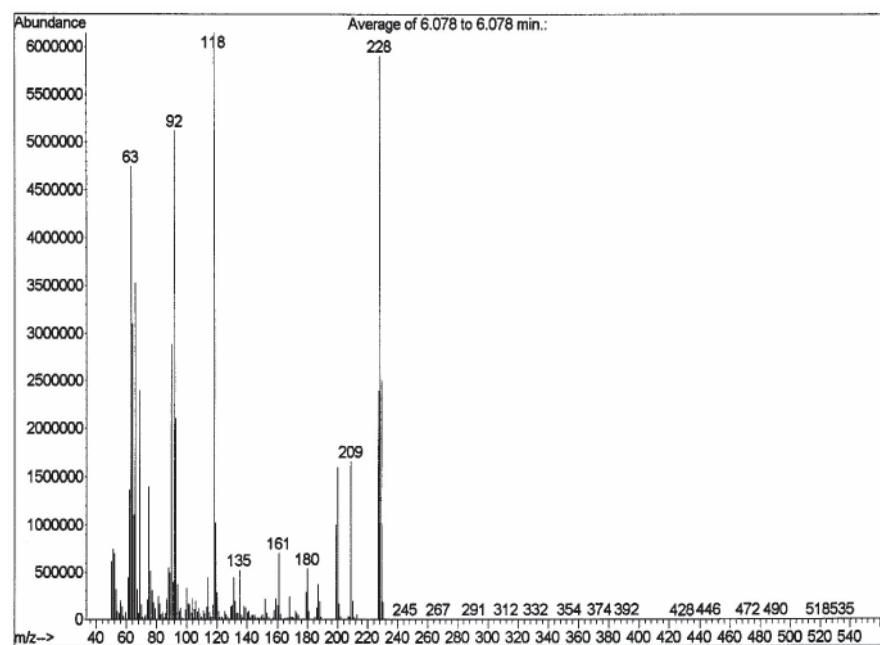


Figure S28. MS of 6-(2-furyl)-2-methyl-4-trifluoromethylpyrimidine (3a).

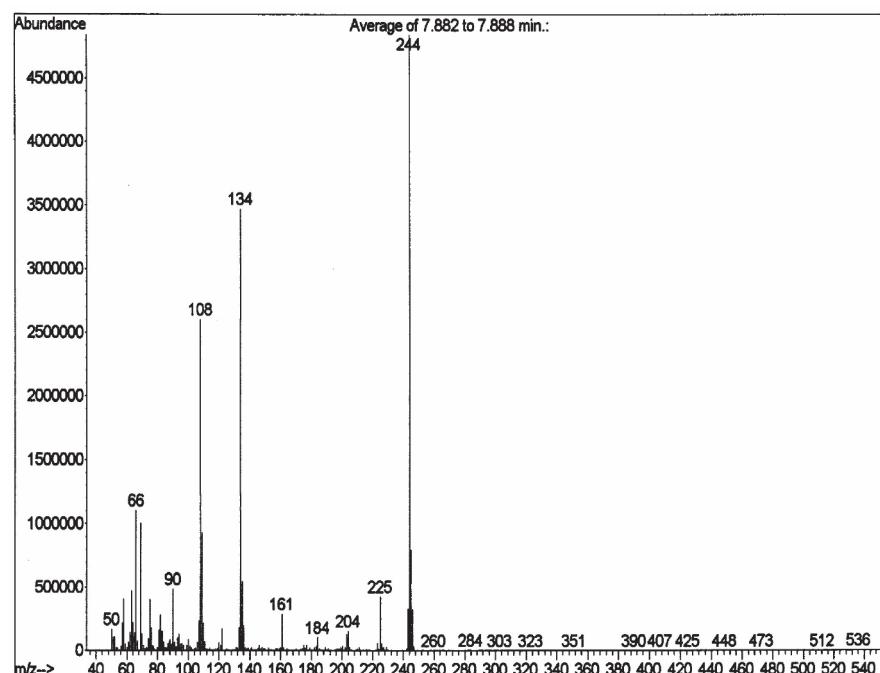


Figure S29. MS of 2-methyl-6-(2-thienyl)-4-trifluoromethylpyrimidine (3b).

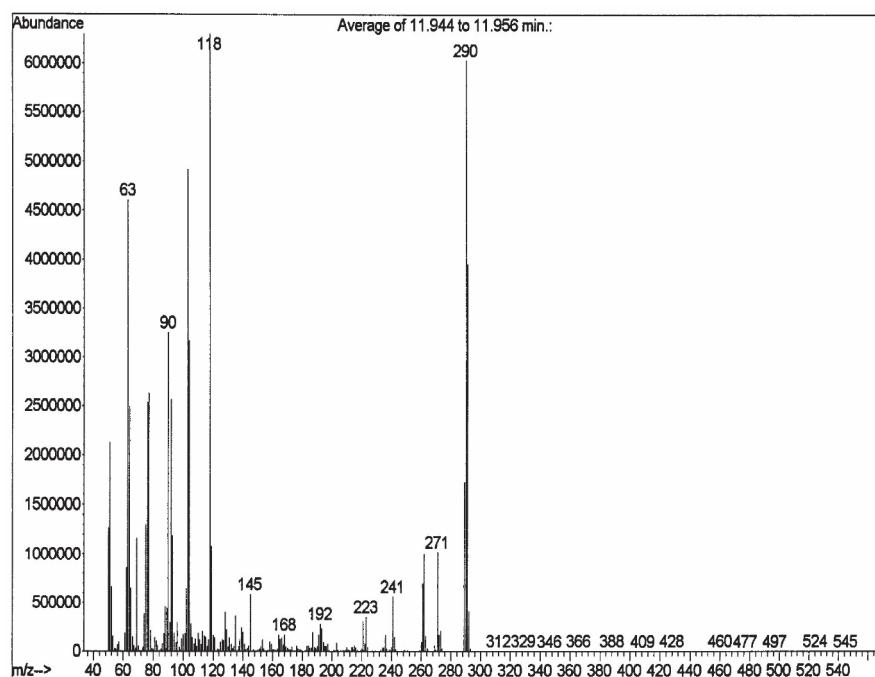


Figure S30. MS of 6-(2-furyl)-2-phenyl-4-trifluoromethyl-pyrimidine (**4a**).

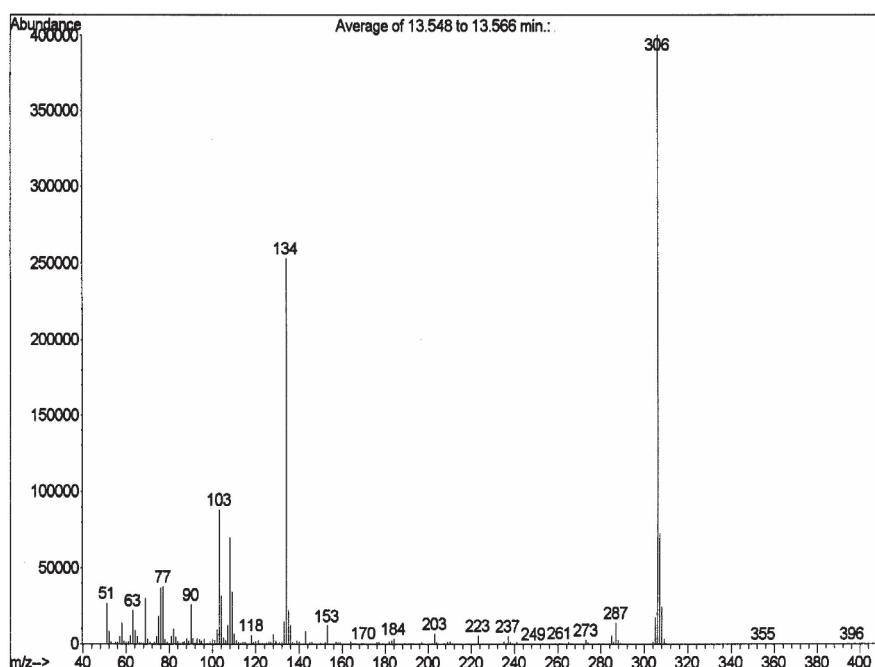


Figure S31. MS of 2-phenyl-6-(2-thienyl)-4-trifluoromethylpyrimidine (**4b**).