

## Supplementary Information

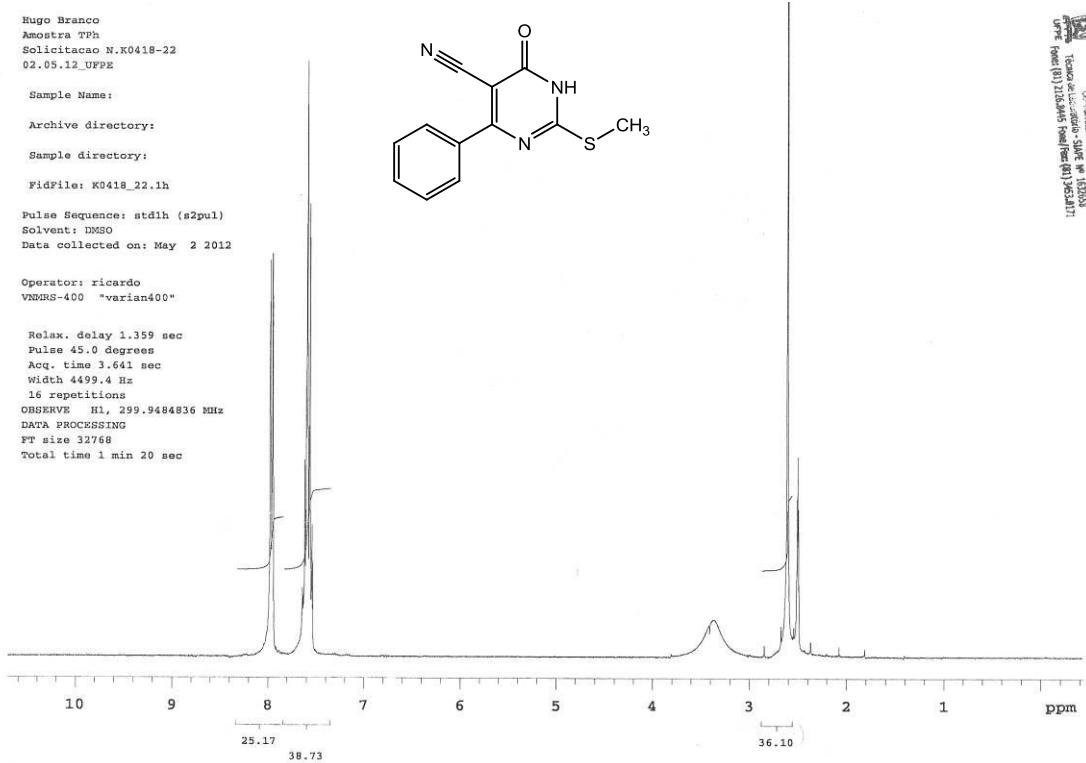
### Vasoactive Thiomethyl-Pyrimidines: Promising Drug Candidates with Vascular Activity

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50740-560 Recife-PE, Brazil

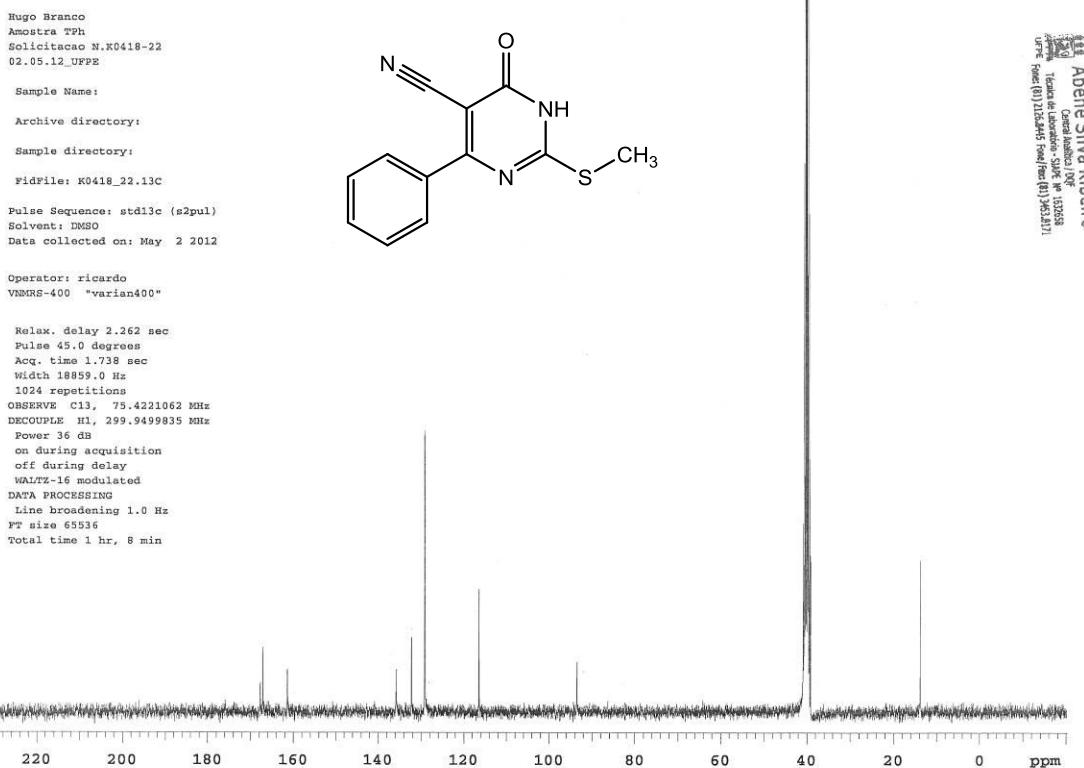
<sup>b</sup>Núcleo de Nutrição, Universidade Federal de Pernambuco,  
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<sup>c</sup>Departamento de Fisiologia e Farmacologia, Universidade Federal de Pernambuco,  
50670-901, Recife-PE, Brazil

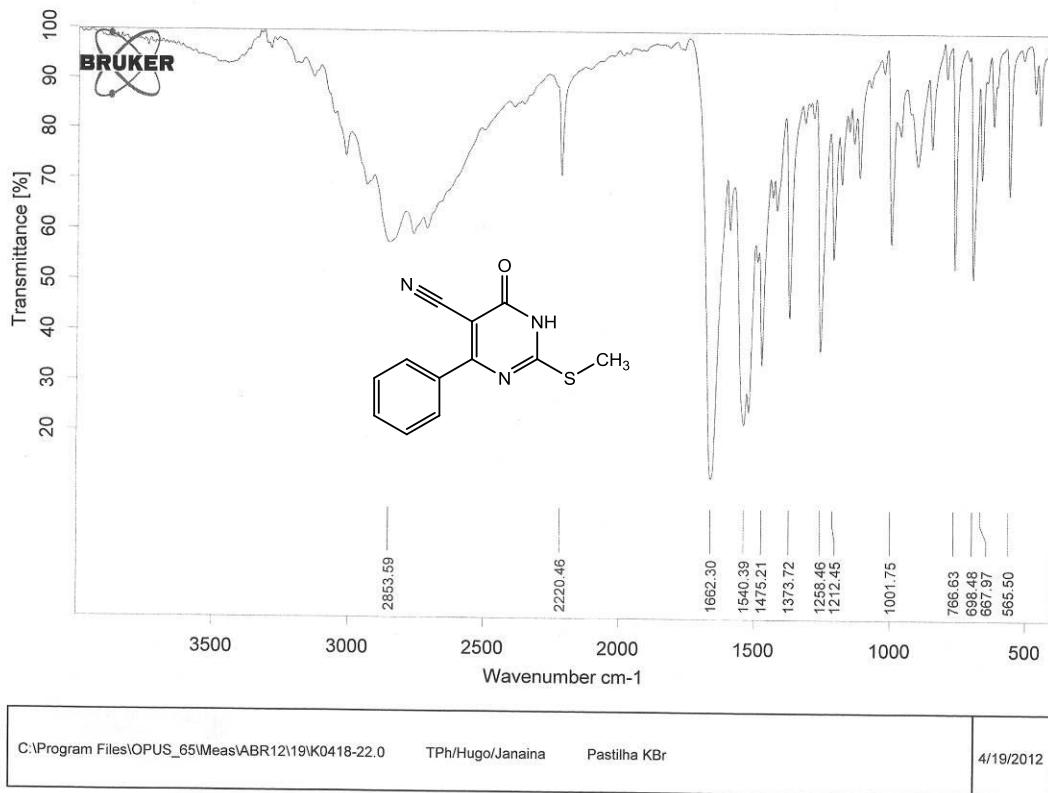


**Figure S1.** <sup>1</sup>H NMR spectrum (400 MHz, DMSO-*d*<sub>6</sub>) of compound 4a.

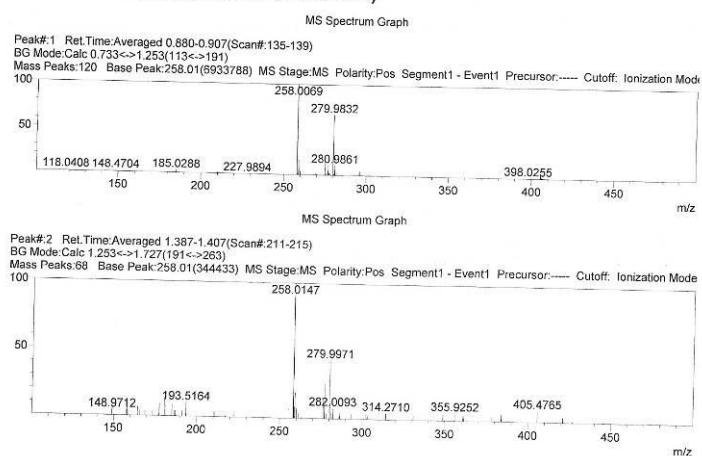
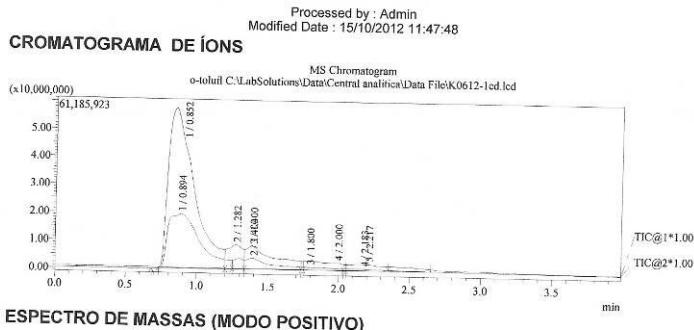
\*e-mail: omlmalta@gmail.com, janaina.anjos@ufpe.br



**Figure S2.**  $^{13}\text{C}$  NMR spectrum (100 MHz,  $\text{DMSO}-d_6$ ) of compound **4a**.



**Figure S3.** FTIR (KBr) spectrum of compound **4a**.



**Figure S4.** Mass spectrum of compound **4b**.

Hugo Branco  
Amostra: o-Toluil  
Solicitação N. K0612-1  
28.06.2012 UFPE

Sample Name:

Data Collected on:  
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Archive directory:

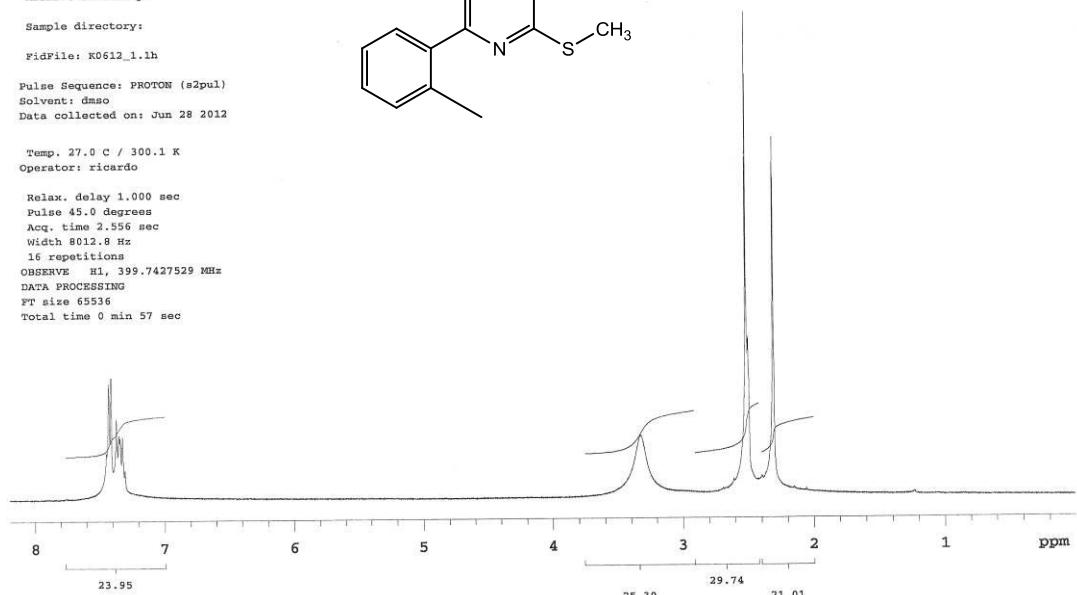
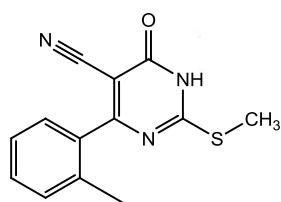
Sample directory:

FidFile: K0612\_1.fid

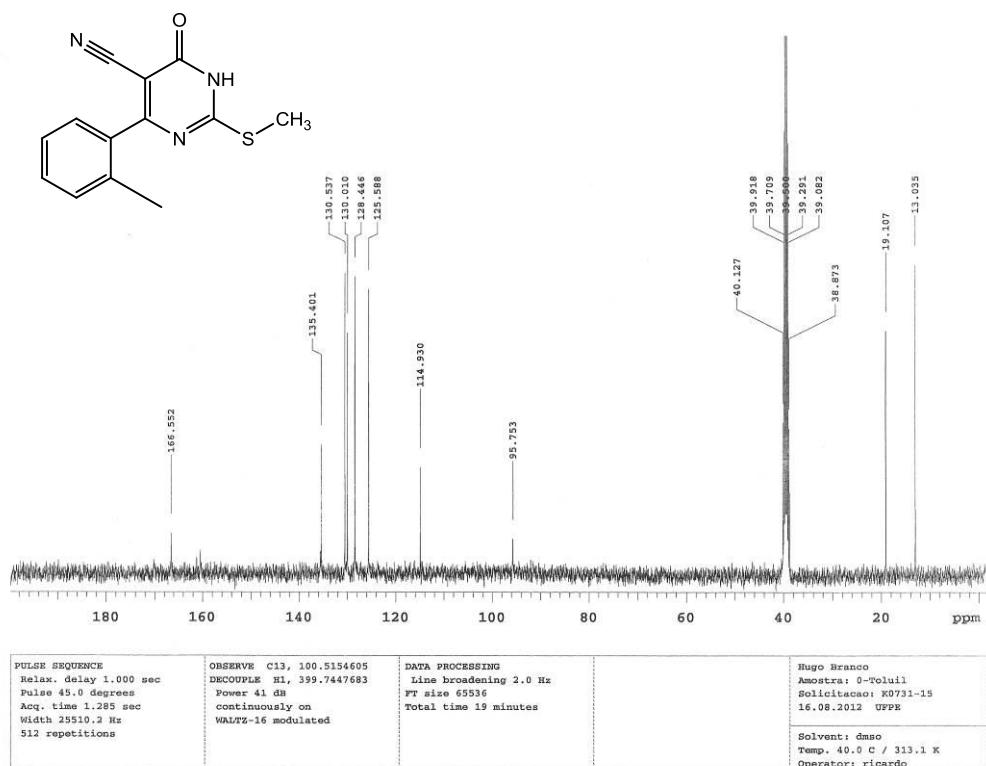
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Solvent: dmso  
Data collected on: Jun 28 2012

Temp. 27.0 C / 300.1 K  
Operator: ricardo

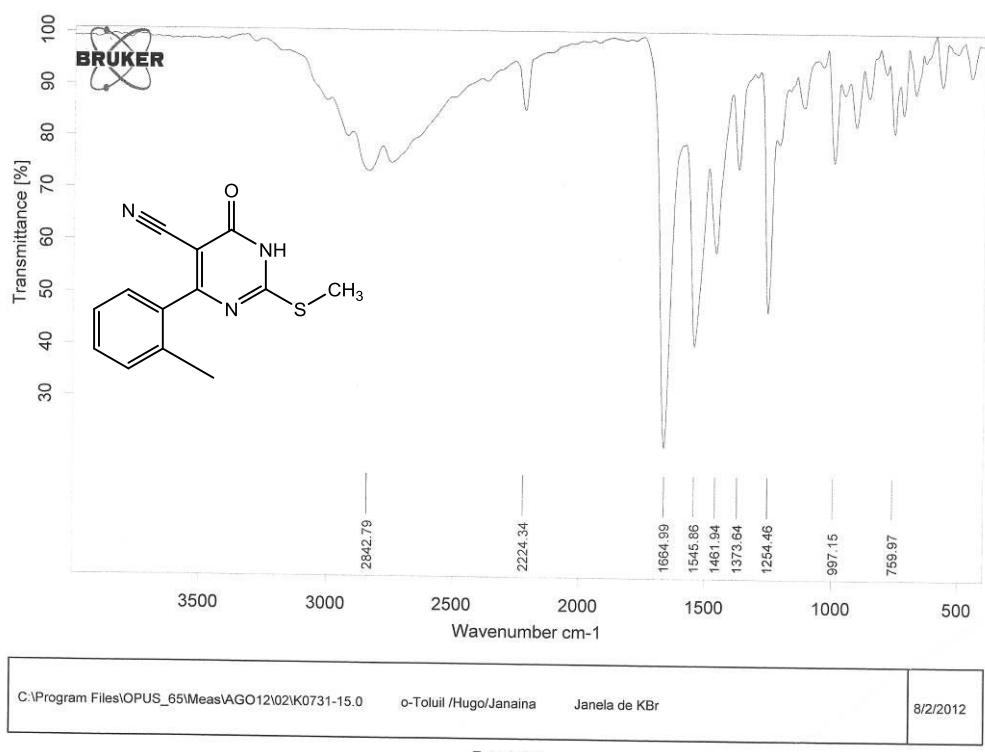
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Pulse 45.0 degrees  
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16 repetitions  
OBSERVE H1, 399.7427529 MHz  
DATA PROCESSING  
FT size 65536  
Total time 0 min 57 sec



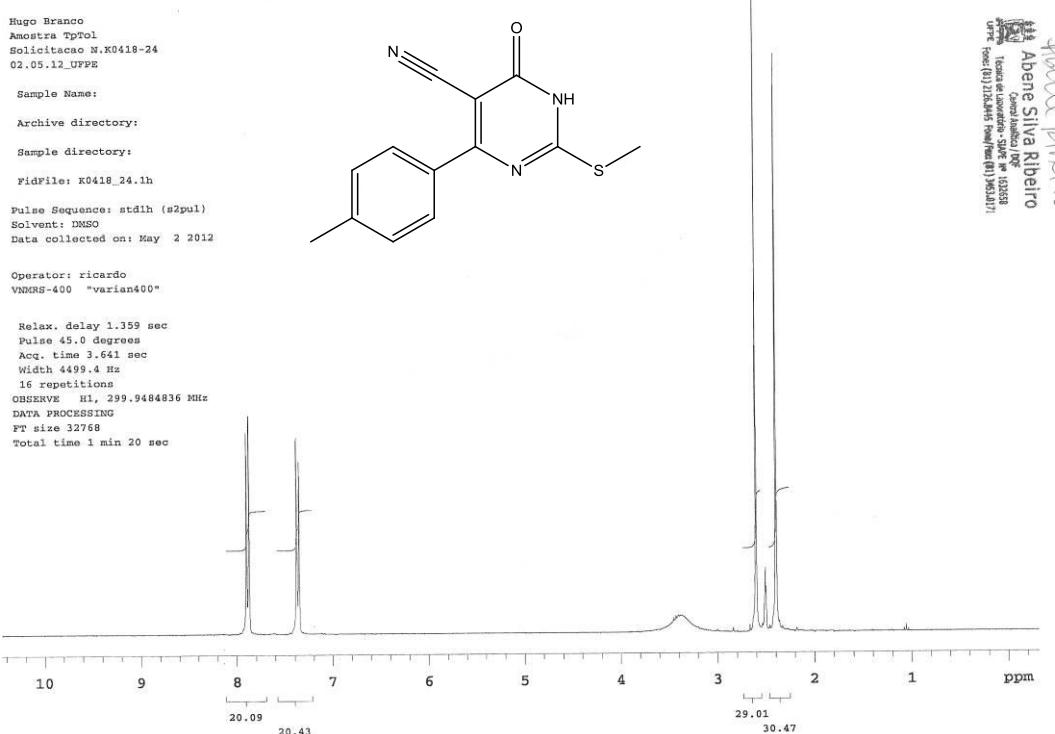
**Figure S5.**  $^1\text{H}$  NMR spectrum (400 MHz, DMSO- $d_6$ ) of compound **4b**.



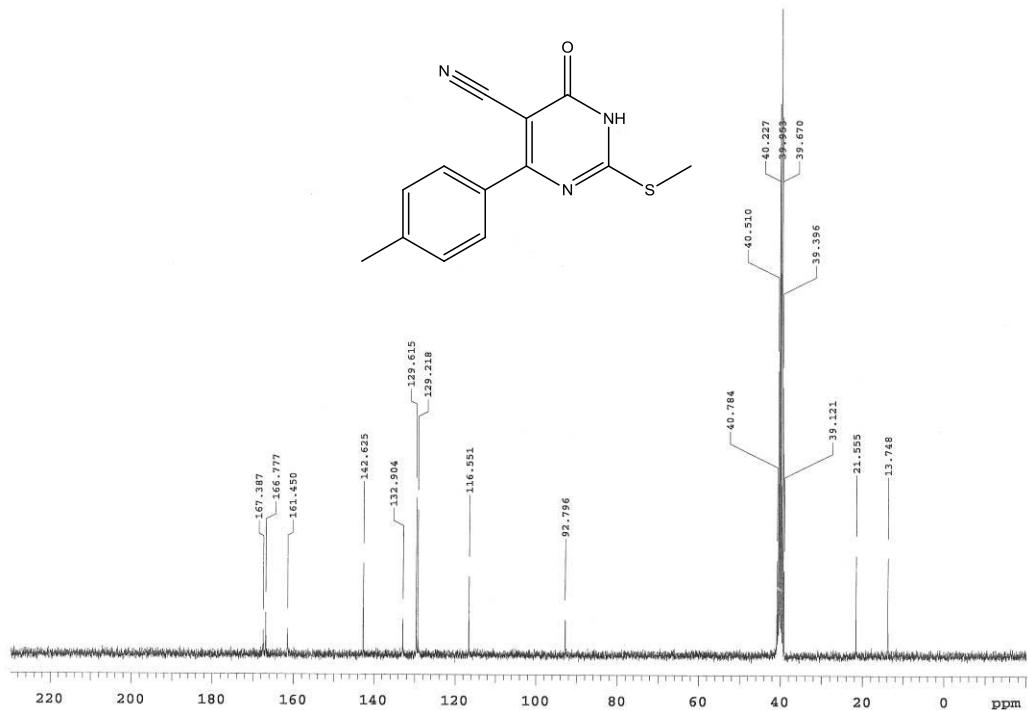
**Figure S6.**  $^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ ) of compound **4b**.



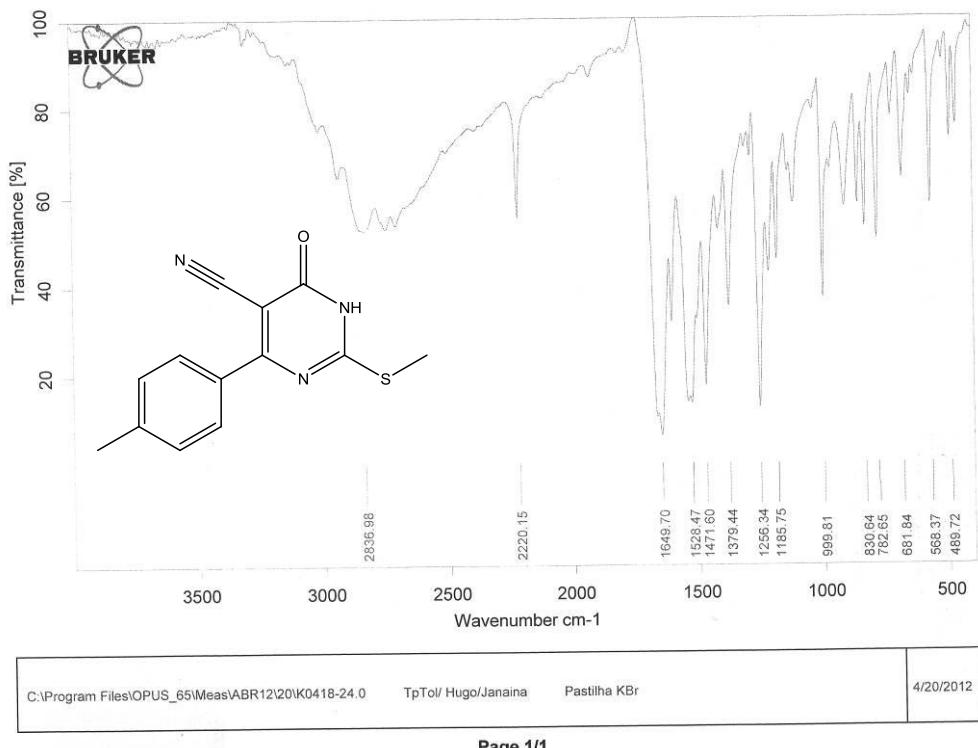
**Figure S7.** FTIR (KBr) spectrum of compound **4b**.



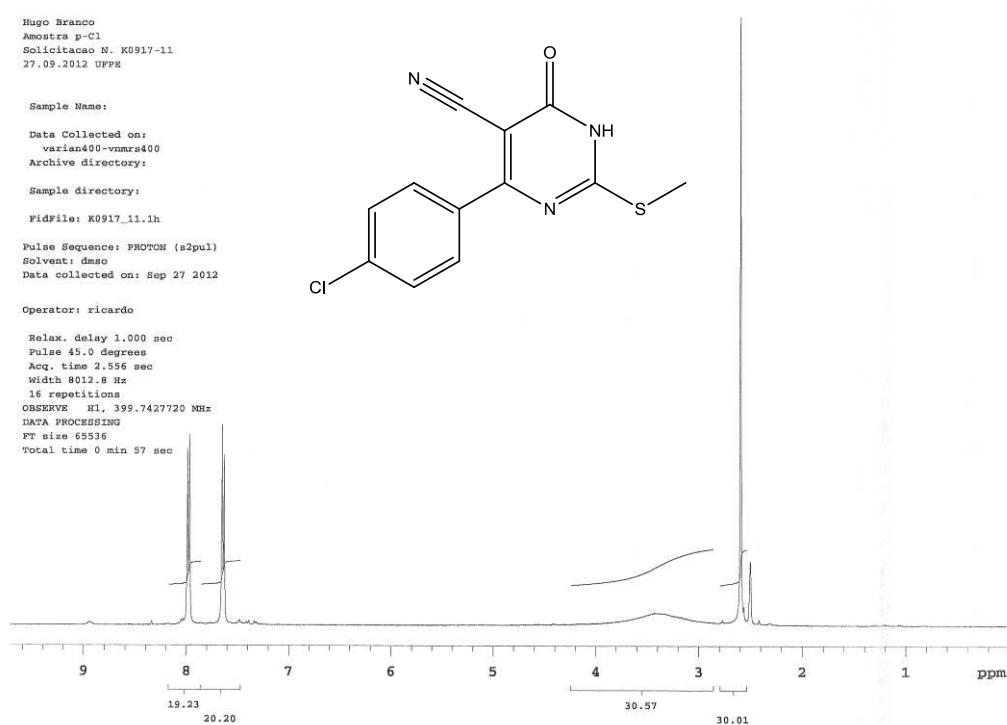
**Figure S8.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{DMSO}-d_6$ ) of compound **4c**.



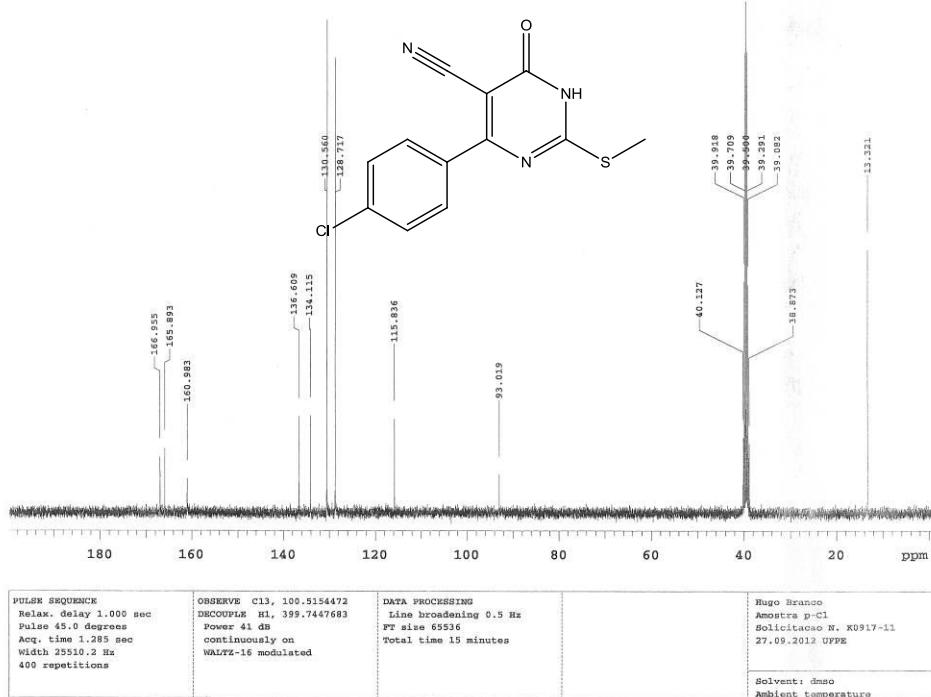
**Figure S9.**  $^{13}\text{C}$  NMR spectrum (100 MHz,  $\text{DMSO}-d_6$ ) of compound **4c**.



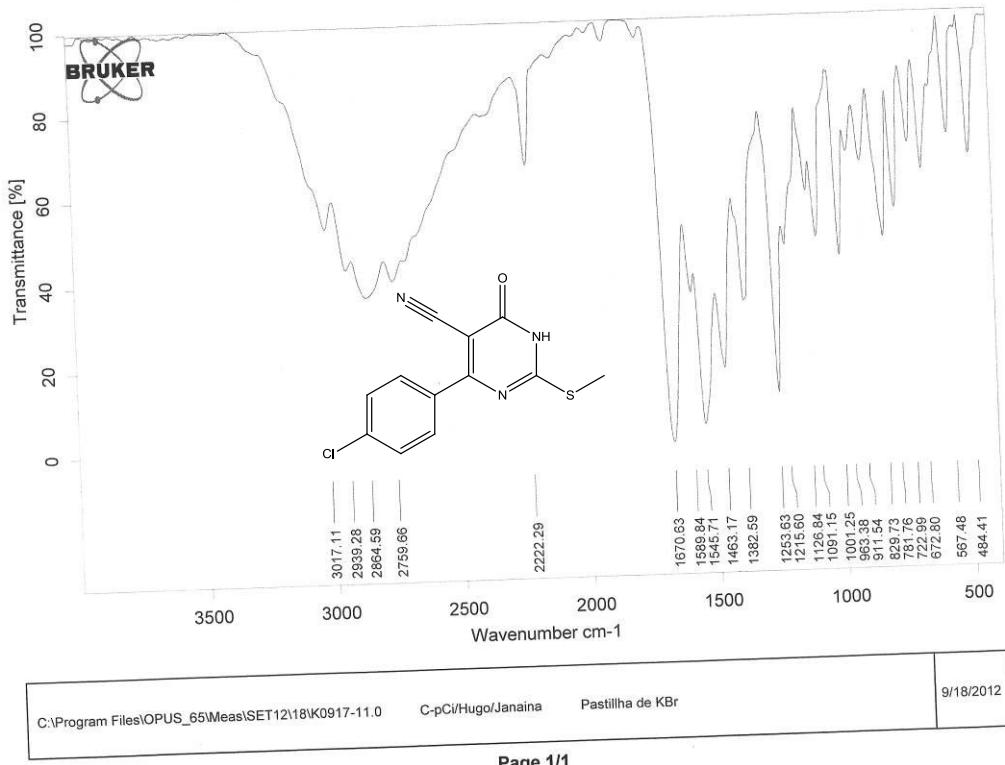
**Figure S10.** FTIR (KBr) spectrum of compound **4c**.



**Figure S11.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{DMSO}-d_6$ ) of compound **4d**.



**Figure S12.**  $^{13}\text{C}$  NMR spectrum (100 MHz, DMSO- $d_6$ ) of compound **4d**.



**Figure S13.** FTIR (KBr) spectrum of compound **4d**.

Hugo Branco  
Amostra: p-Br  
Solicitacao N. K0612-5  
28.06.2012 UFPE

Sample Name:

Data Collected on:  
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Archive directory:

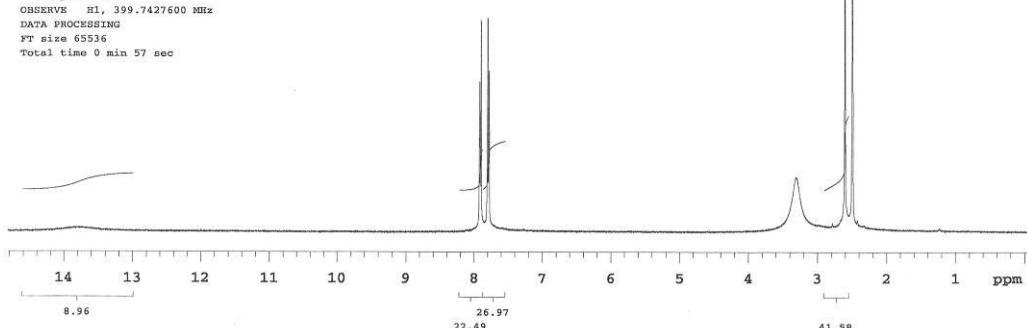
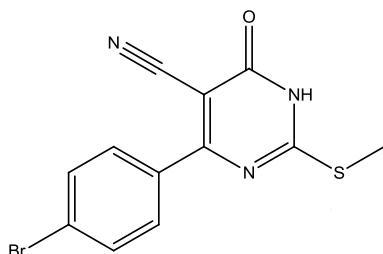
Sample directory:

FidFile: K0612\_5.lh

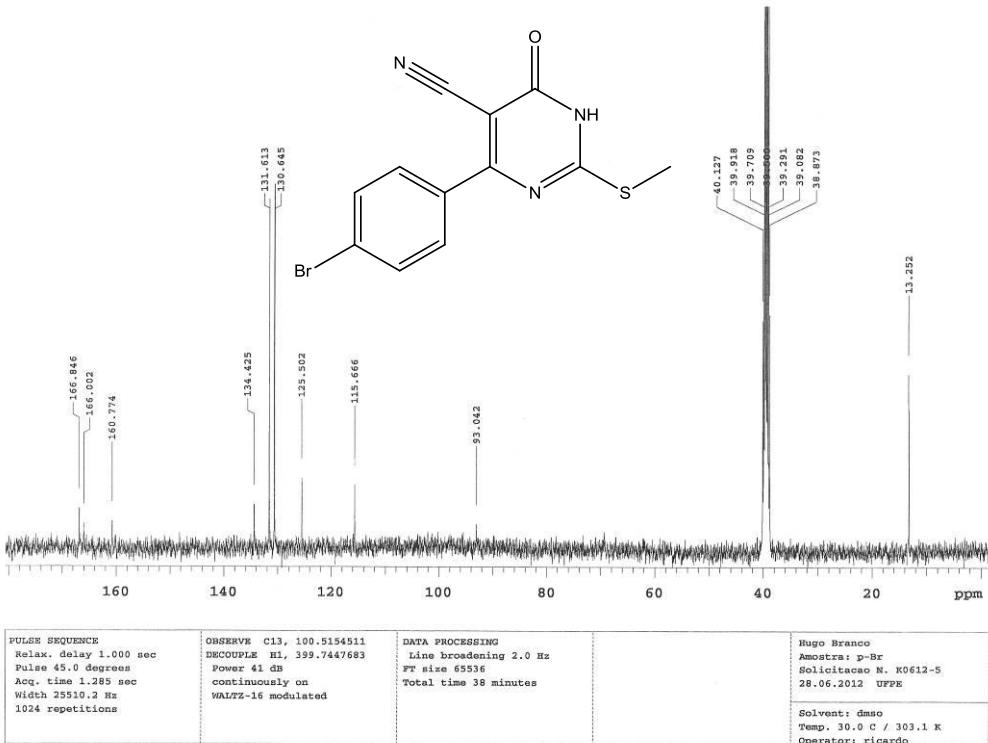
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Solvent: dmo  
Data collected on: Jun 28 2012

Temp. 30.0 C / 303.1 K  
Operator: ricardo

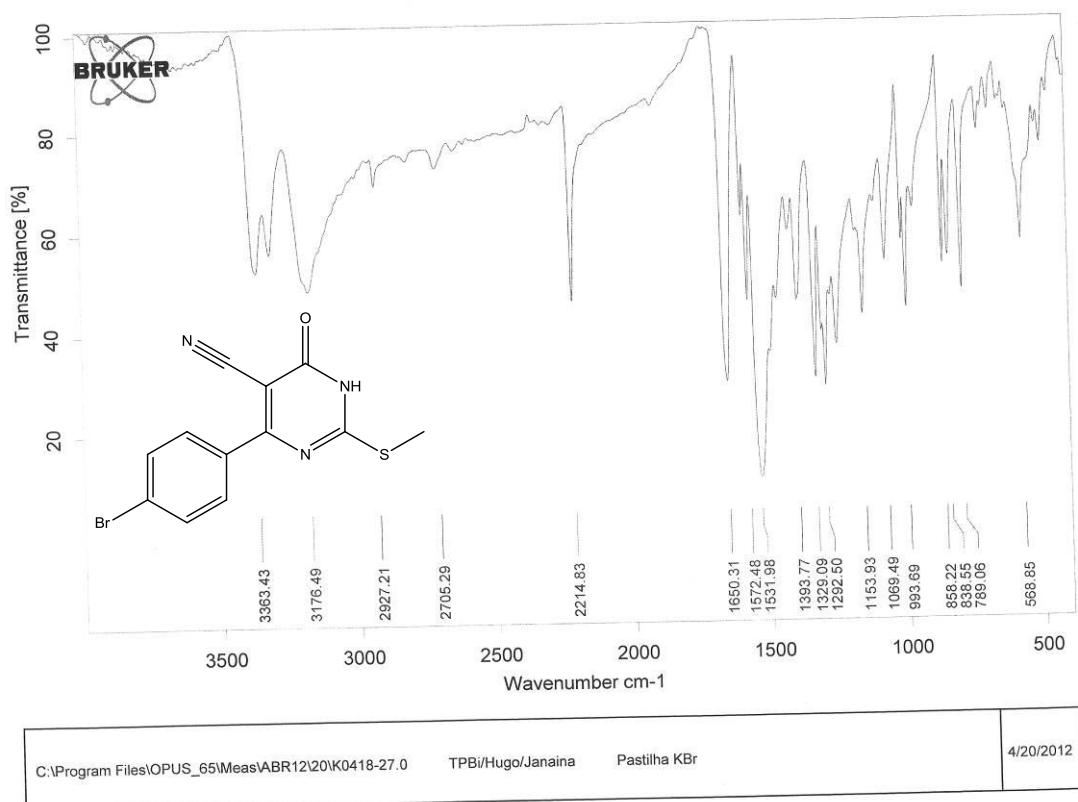
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Pulse 45.0 degrees  
Acq. time 2.556 sec  
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16 repetitions  
OBSERVE H1, 399.7427600 MHz  
DATA PROCESSING  
FT size 65536  
Total time 0 min 57 sec



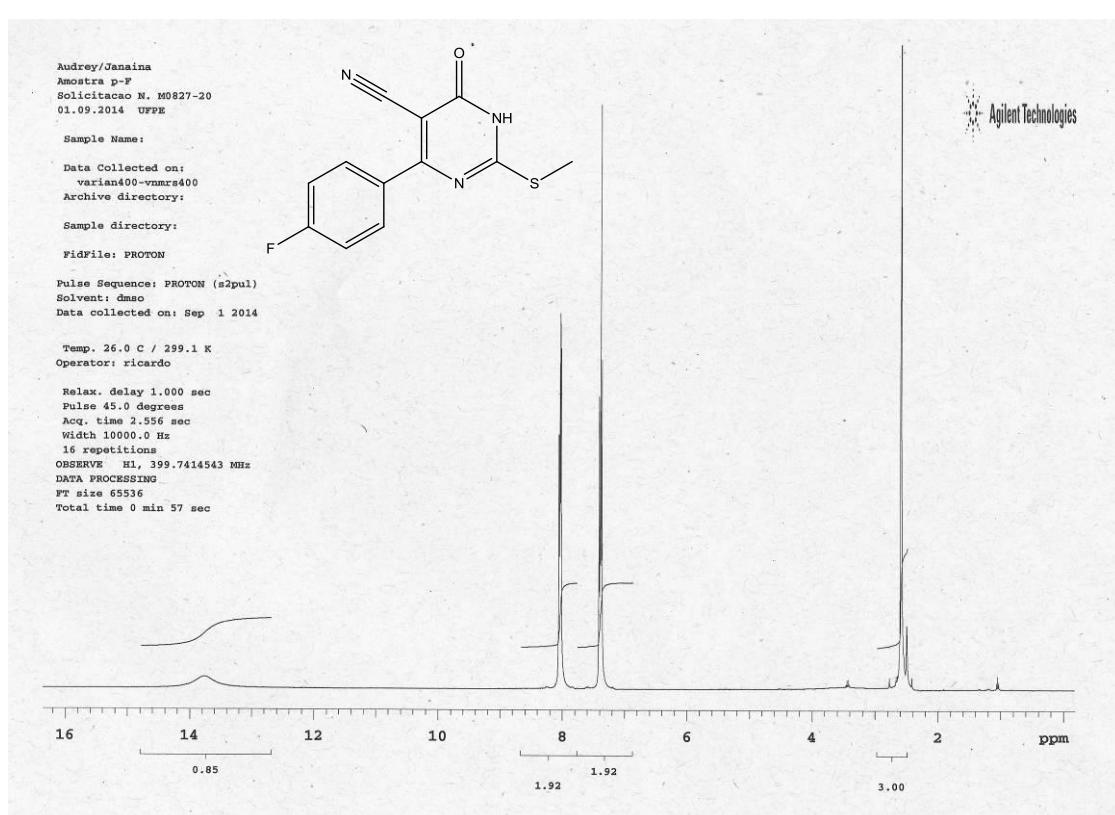
**Figure S14.** <sup>1</sup>H NMR spectrum (400 MHz, DMSO-*d*<sub>6</sub>) of compound 4e.



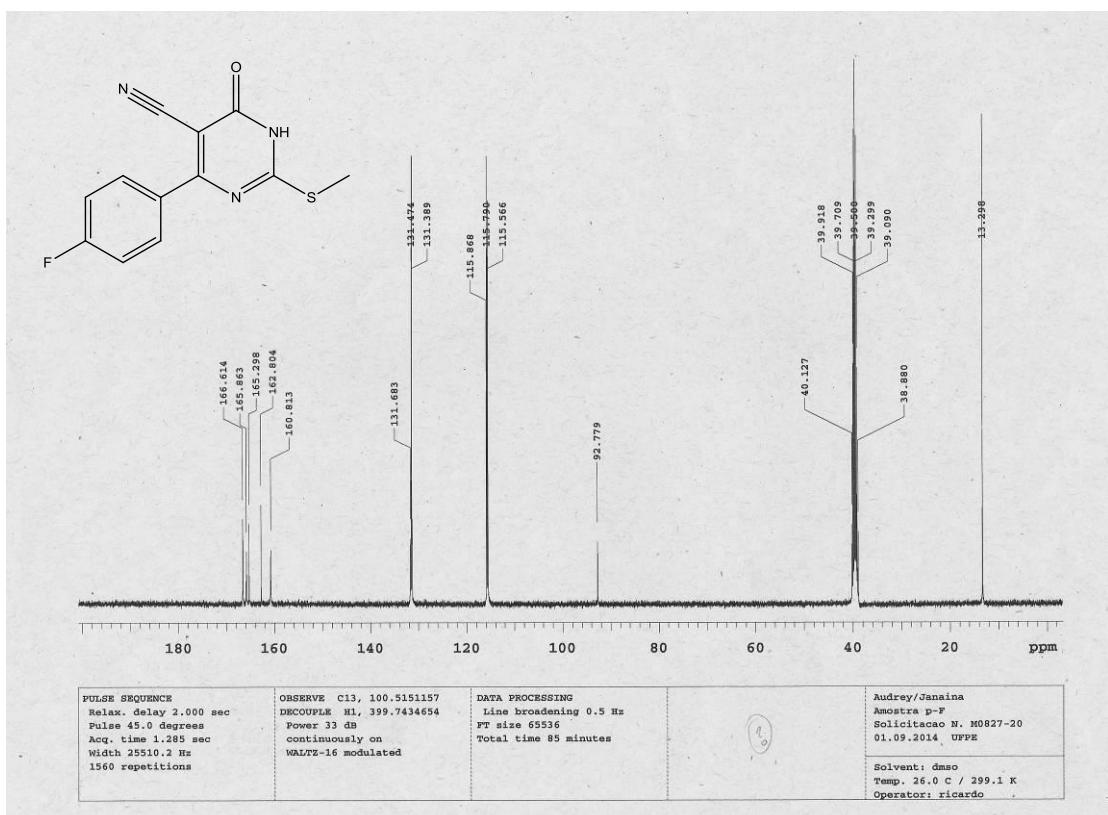
**Figure S15.** <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) of compound 4e.



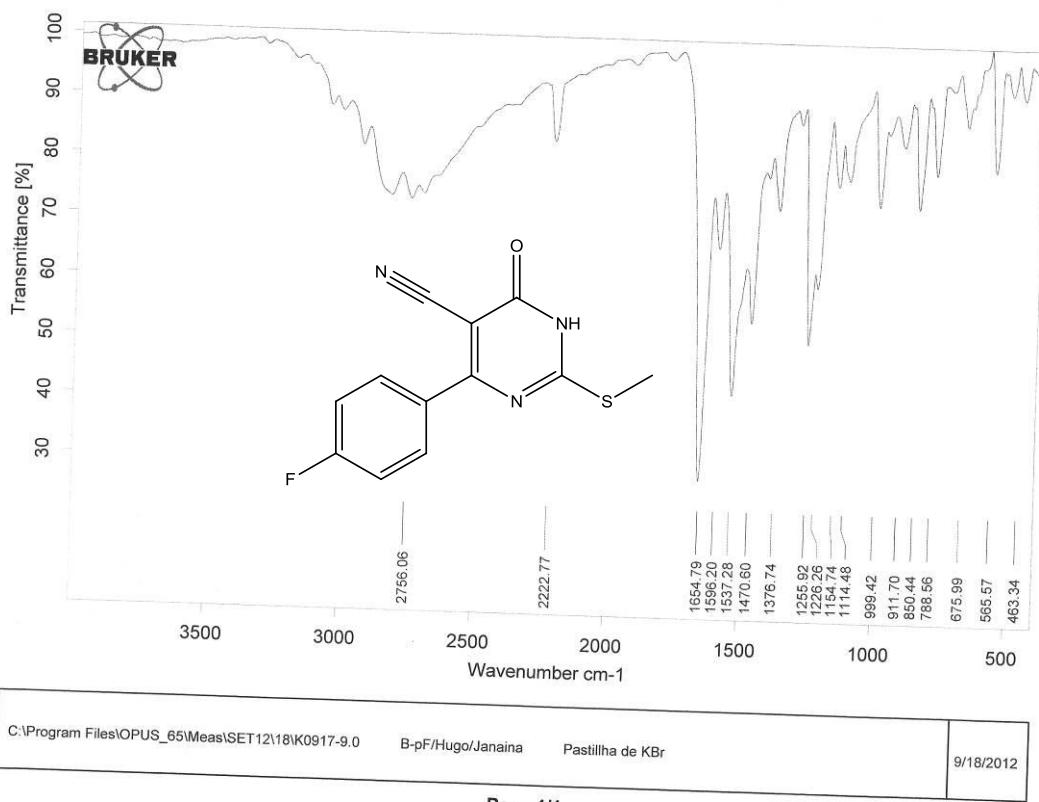
**Figure S16.** FTIR (KBr) spectrum of compound 4e.



**Figure S17.**  $^1\text{H}$  NMR spectrum (300 MHz,  $\text{DMSO}-d_6$ ) of compound 4f.



**Figure S18.**  $^{13}\text{C}$  NMR spectrum (100 MHz, DMSO- $d_6$ ) of compound **4f**.



**Figure S19.** FTIR (KBr) spectrum of compound **4f**.

Hugo Branco  
 Amostra TSGH3  
 Solicitud N.K0418\_25  
 02.05.12\_UFPE

Sample Name:

Archive directory:

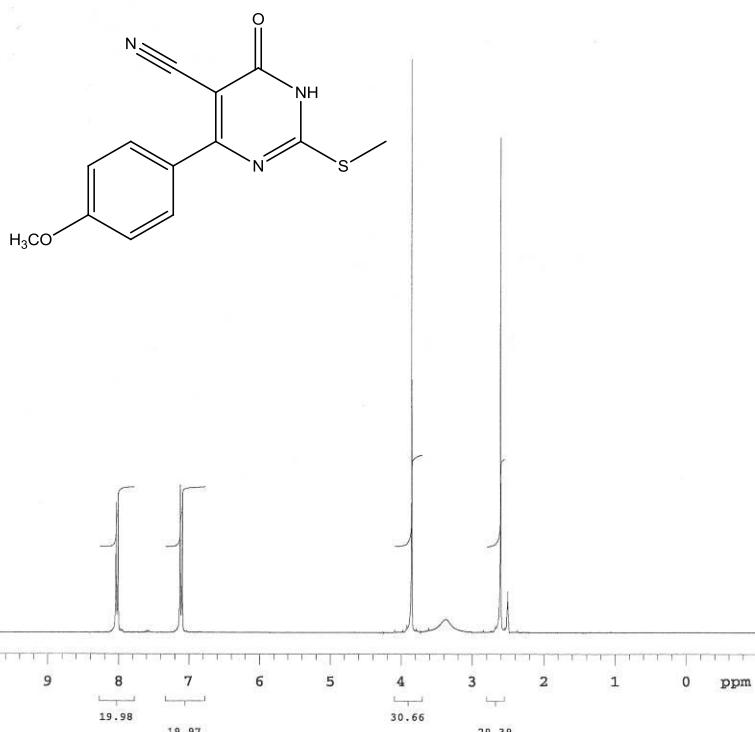
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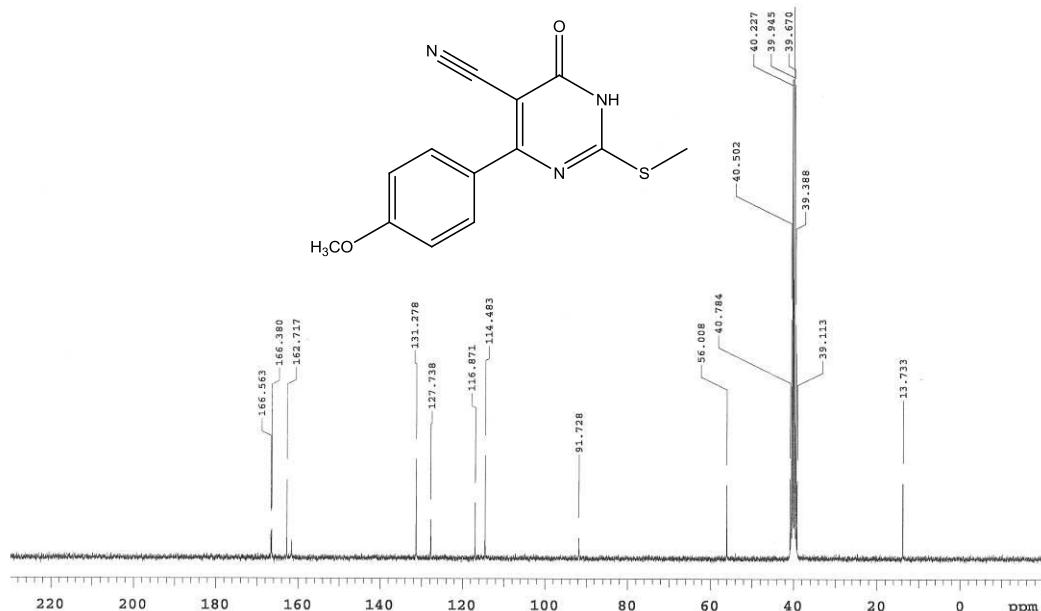
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 Data collected on: May 2 2012

Operator: ricardo  
 VNMR-S-400 "varian400"

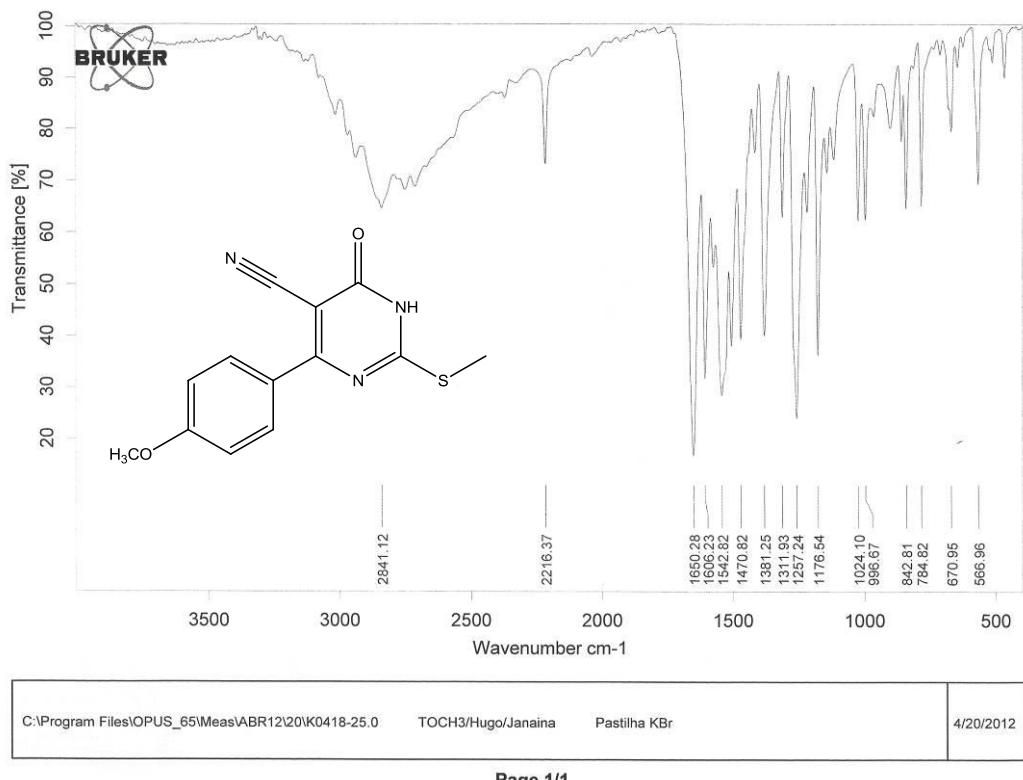
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 Pulse 45.0 degrees  
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 Total time 1 min 20 sec



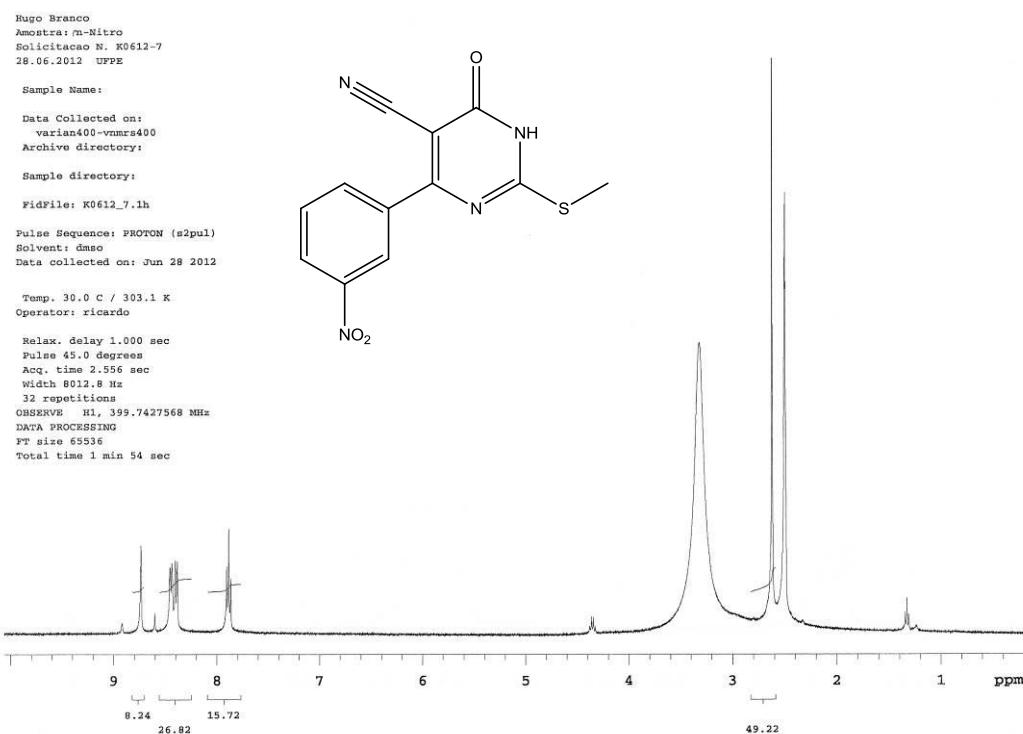
**Figure S20.** <sup>1</sup>H NMR spectrum (400 MHz, DMSO-*d*<sub>6</sub>) of compound 4g.



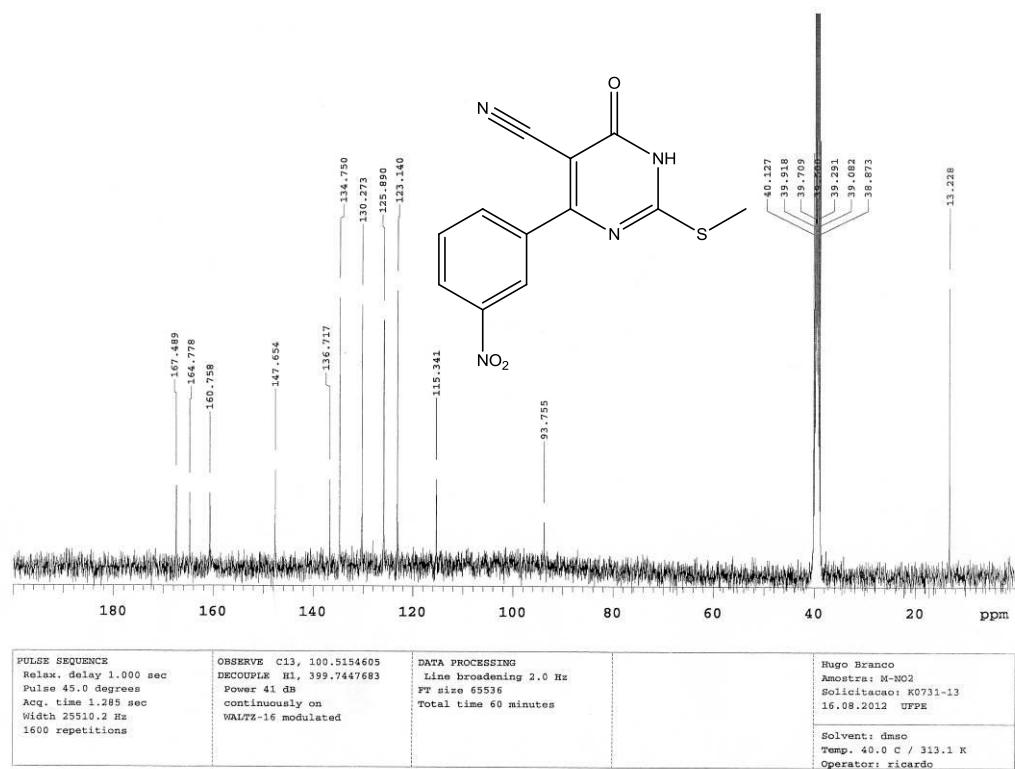
**Figure S21.** <sup>13</sup>C NMR spectrum (100 MHz, DMSO-*d*<sub>6</sub>) of compound 4g.



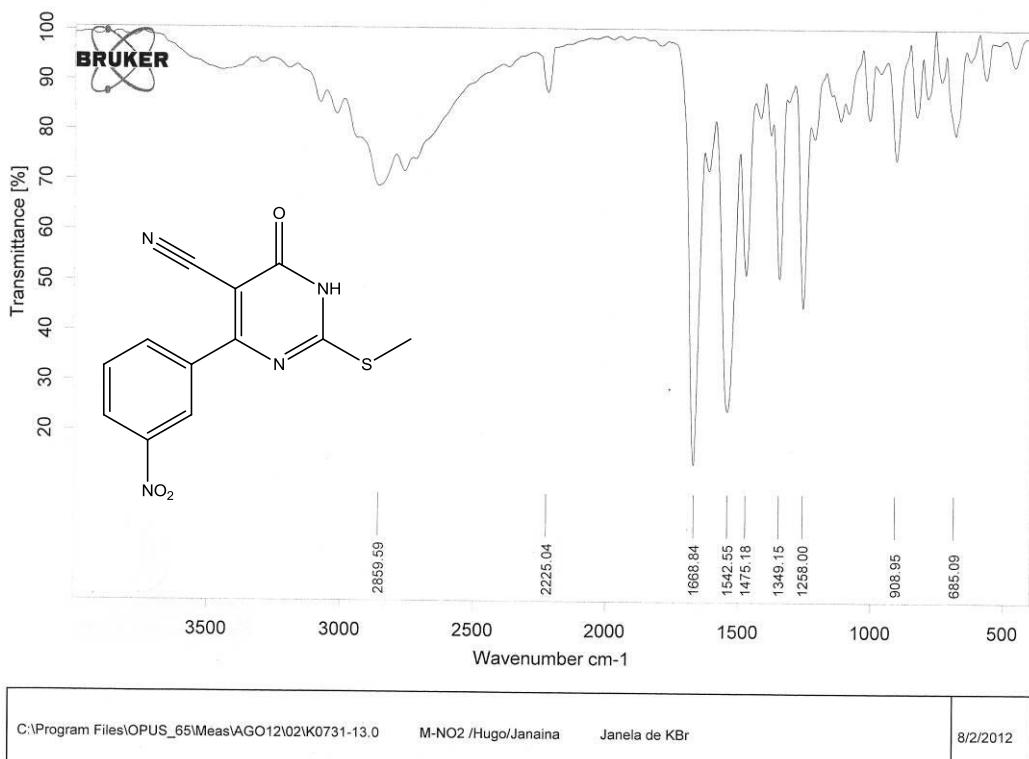
**Figure S22.** FTIR (KBr) spectrum of compound **4g**.



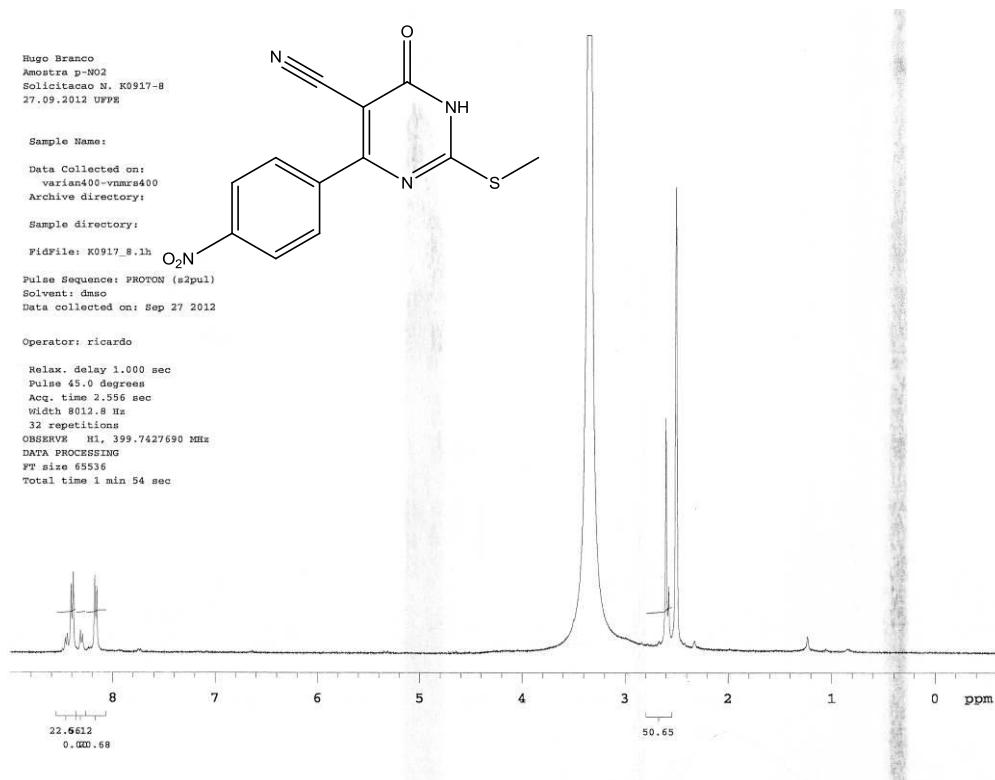
**Figure S23.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{DMSO}-d_6$ ) of compound **4h**.



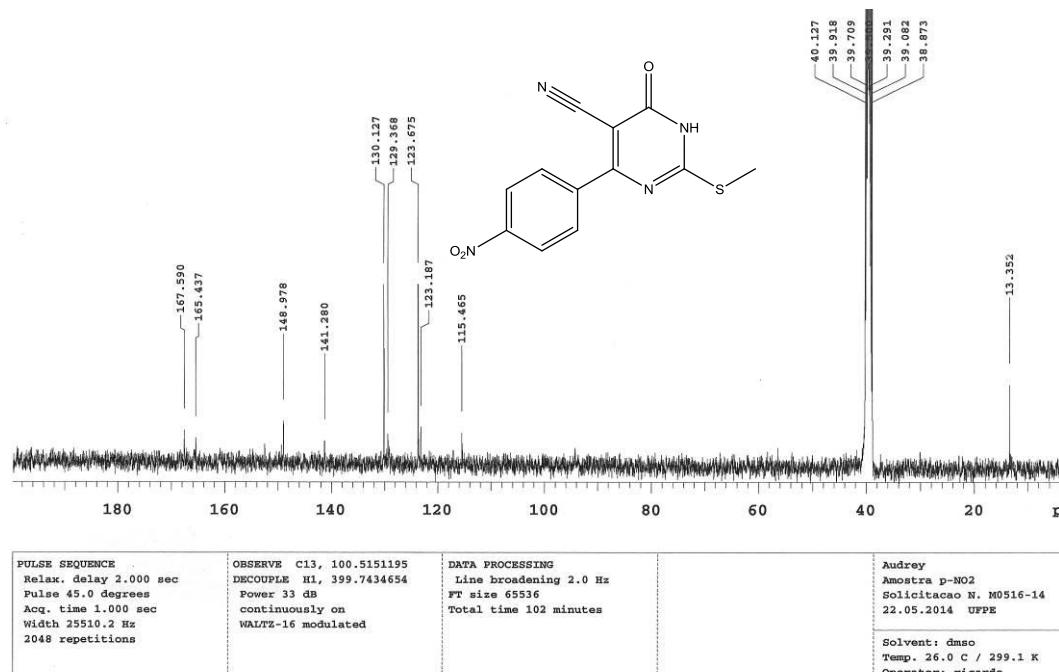
**Figure S24.**  $^{13}\text{C}$  NMR spectrum (100 MHz, DMSO- $d_6$ ) of compound **4h**.



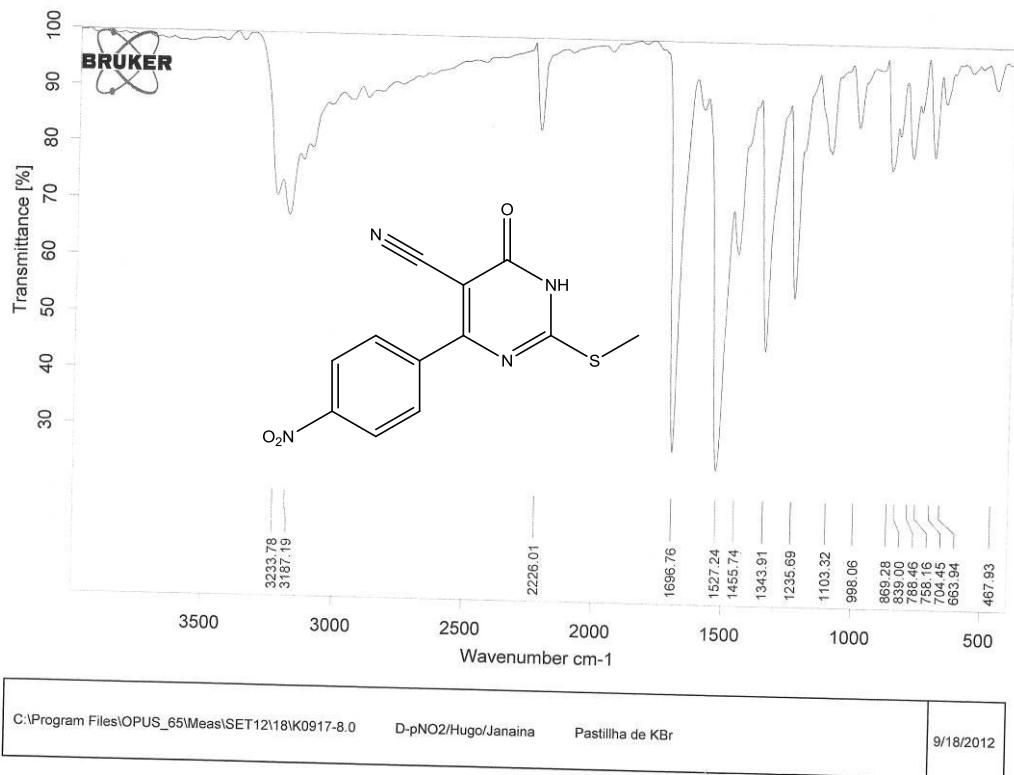
**Figure S25.** FTIR (KBr) spectrum of compound **4h**.



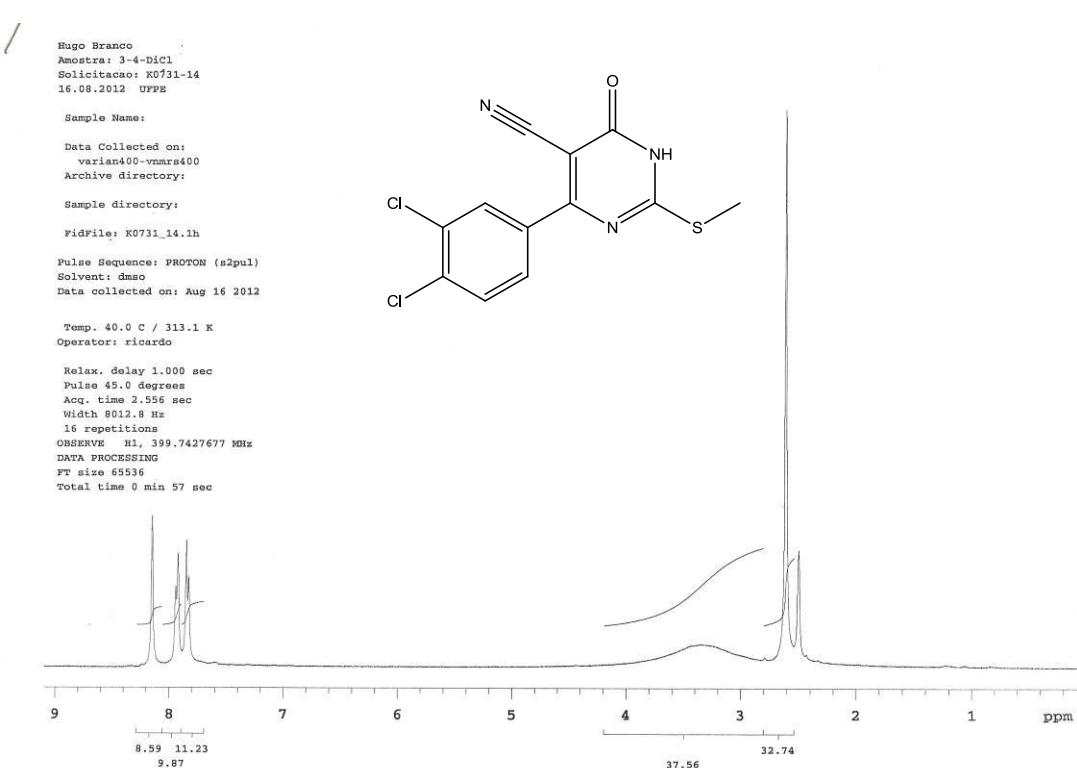
**Figure S26.** <sup>1</sup>H NMR spectrum (400 MHz, DMSO-*d*<sub>6</sub>) of compound **4i**.



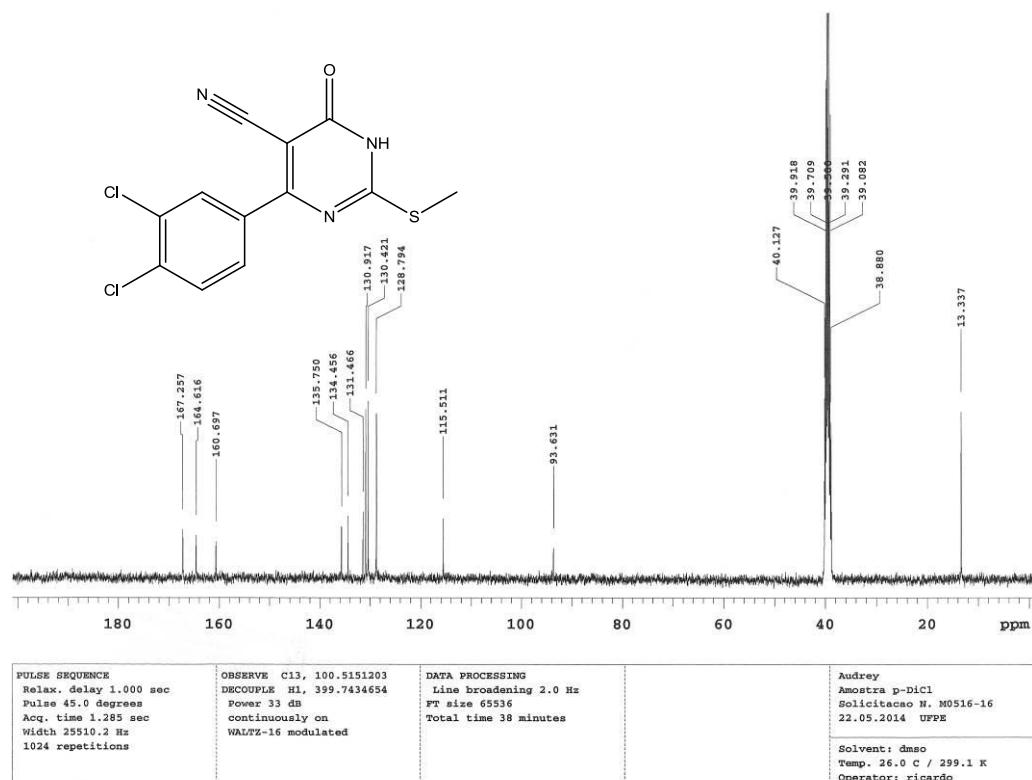
**Figure S27.** <sup>13</sup>C NMR spectrum (100 MHz, DMSO-*d*<sub>6</sub>) of compound **4i**.



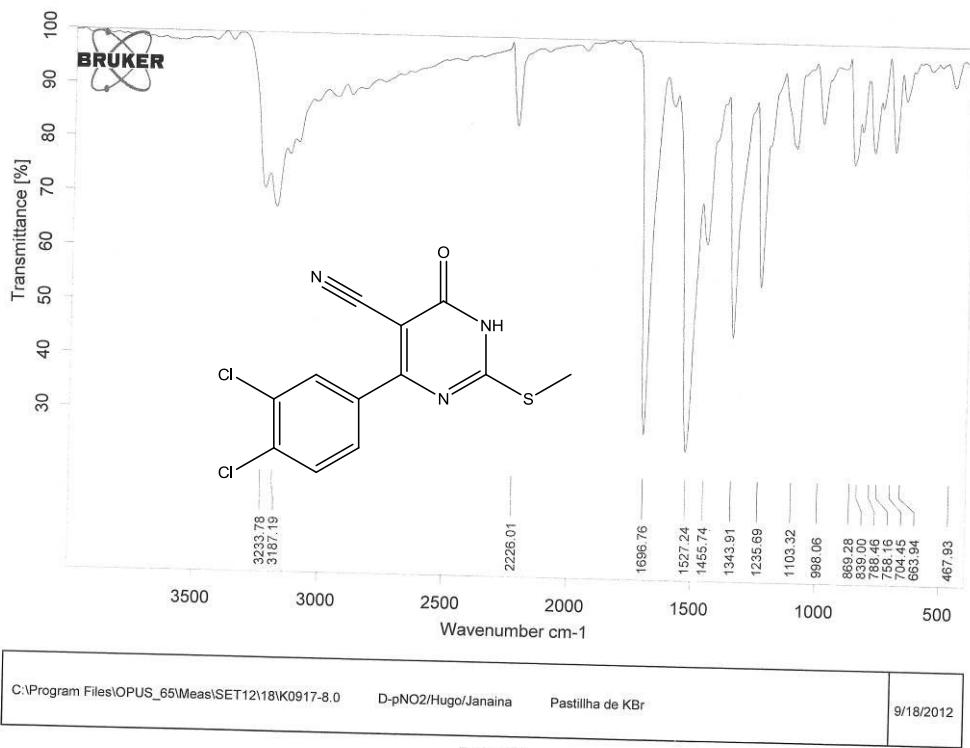
**Figure S28.** FTIR (KBr) spectrum of compound **4i**.



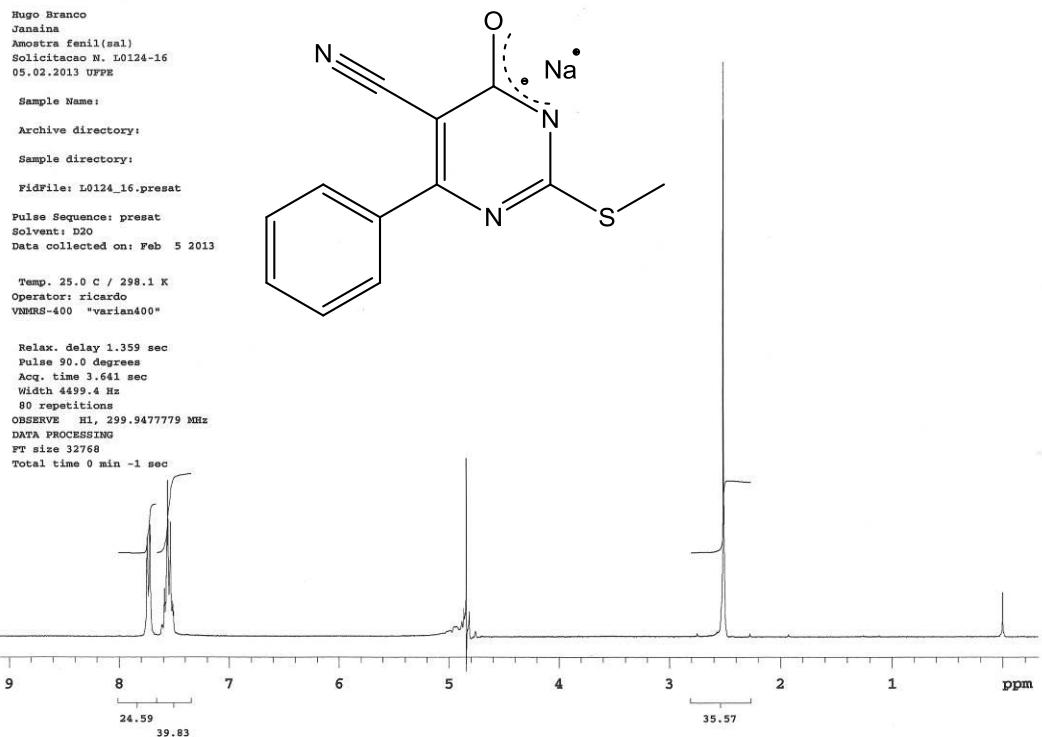
**Figure S29.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{DMSO}-d_6$ ) of compound **4j**.



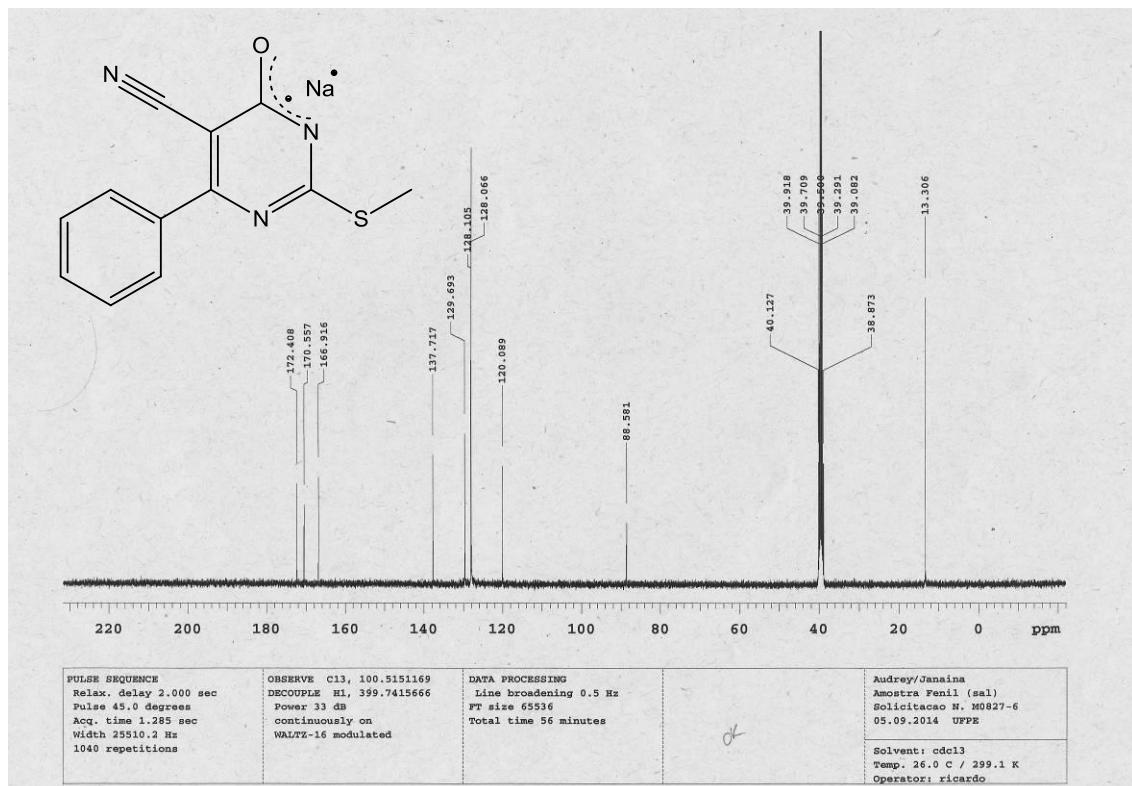
**Figure S30.** <sup>13</sup>C NMR spectrum (100 MHz, DMSO-*d*<sub>6</sub>) of compound **4j**.



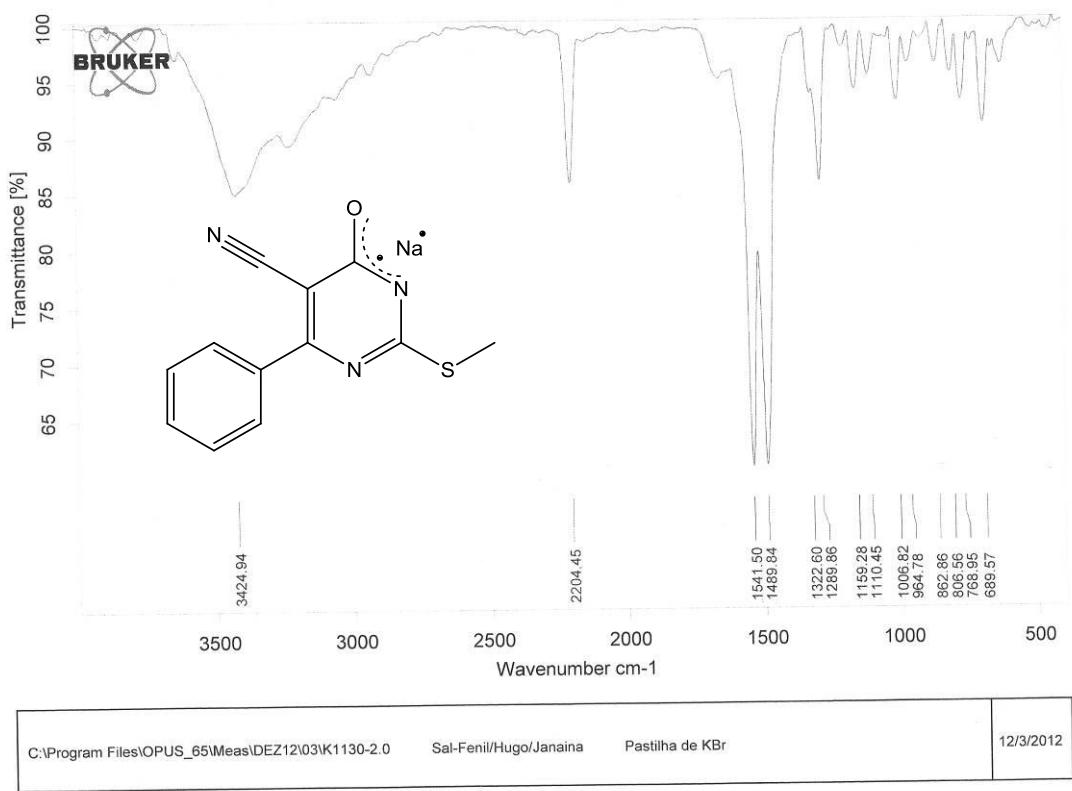
**Figure S31.** FTIR (KBr) spectrum of compound **4j**.



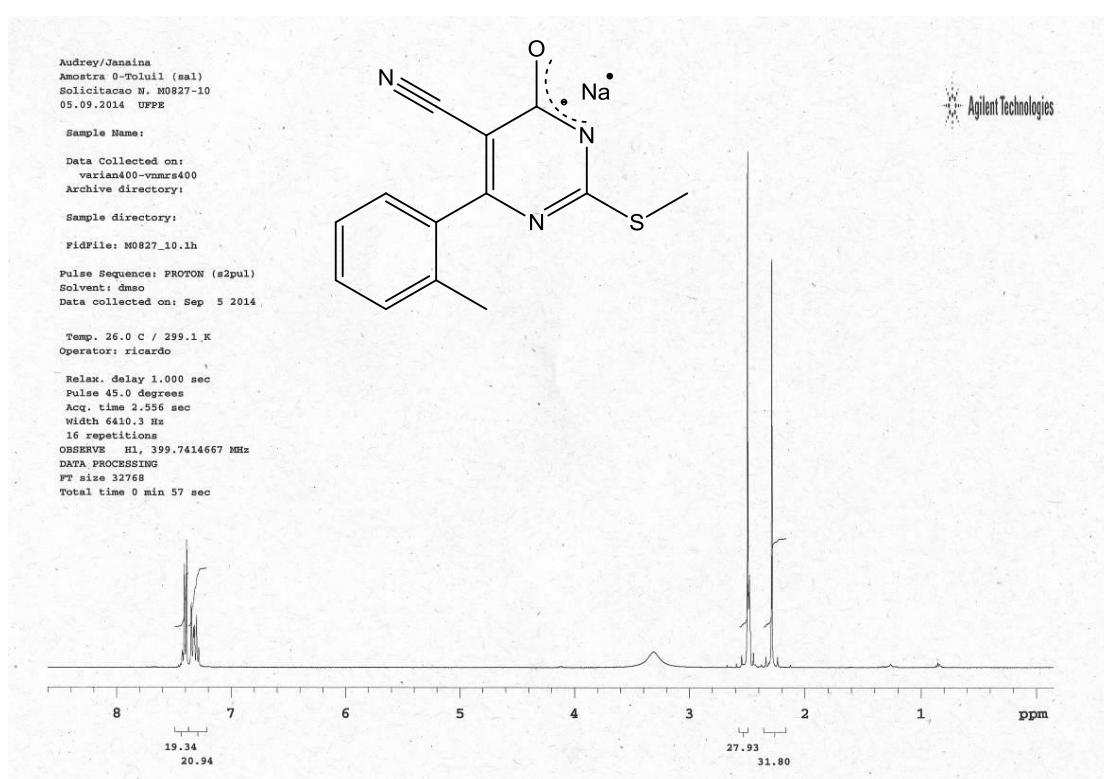
**Figure S32.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{D}_2\text{O}$ ) of compound **5a**.



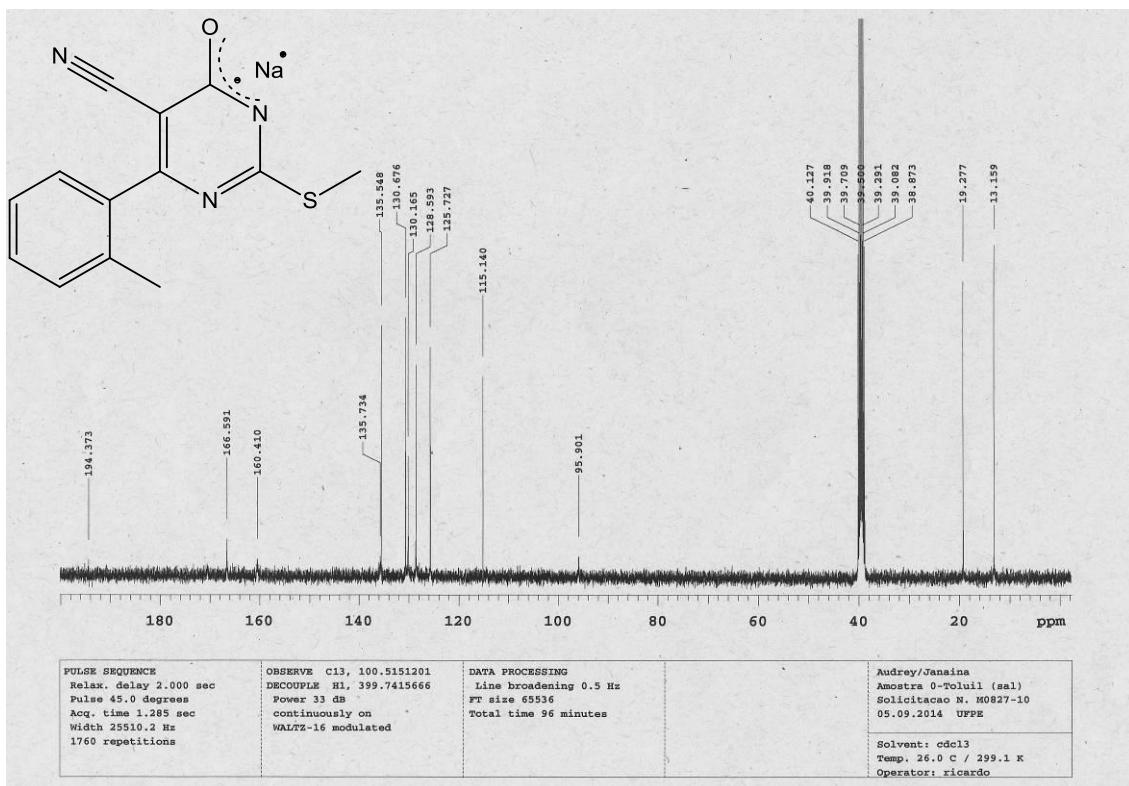
**Figure S33.**  $^{13}\text{C}$  NMR spectrum (100 MHz,  $\text{DMSO}-d_6$ ) of compound **5a**.



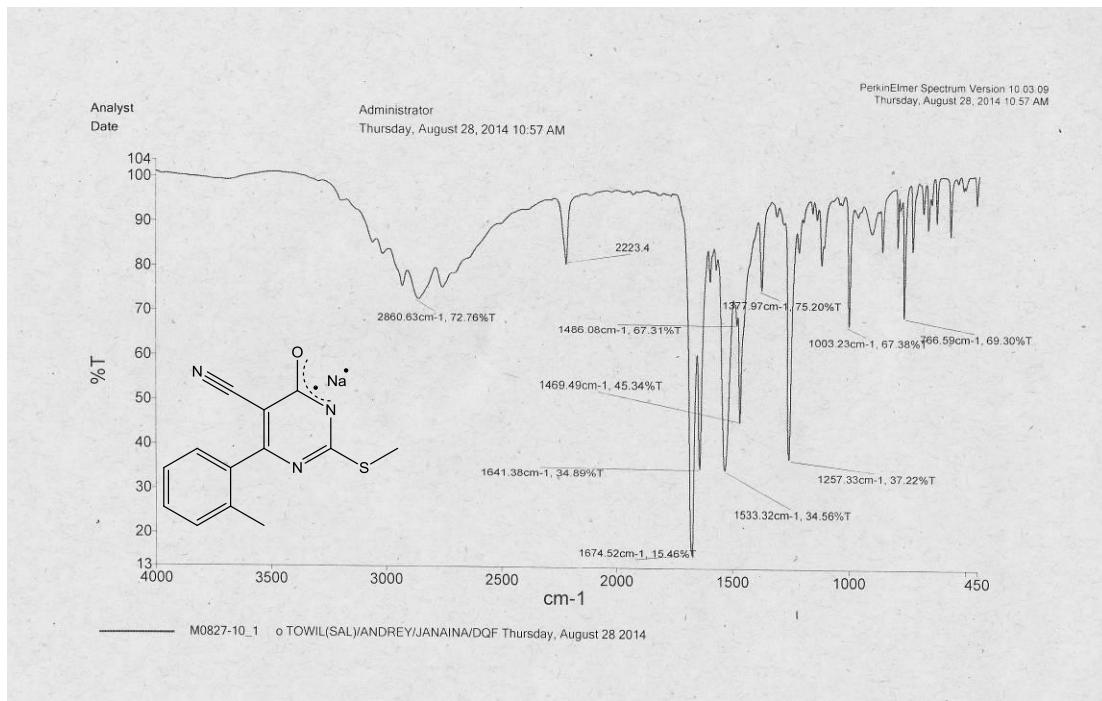
**Figure S34.** FTIR (KBr) spectrum of compound **5a**.



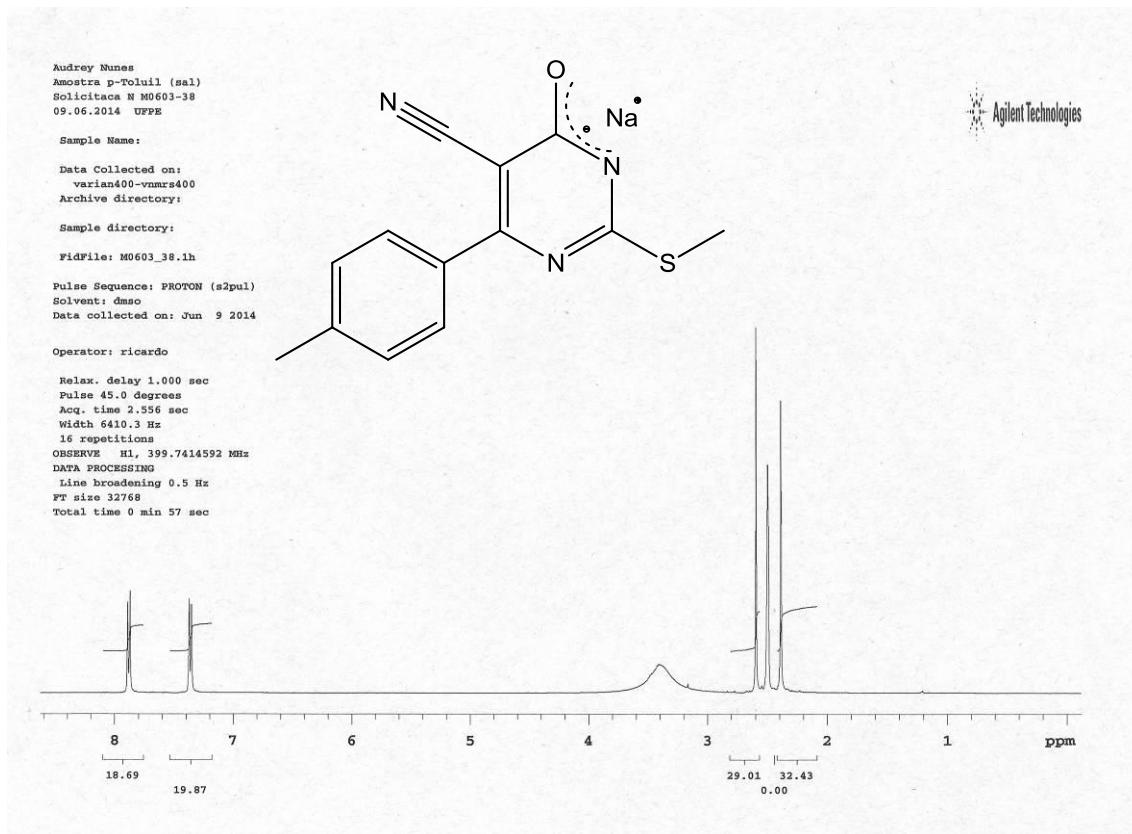
**Figure S35.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{DMSO}-d_6$ ) of compound **5b**.



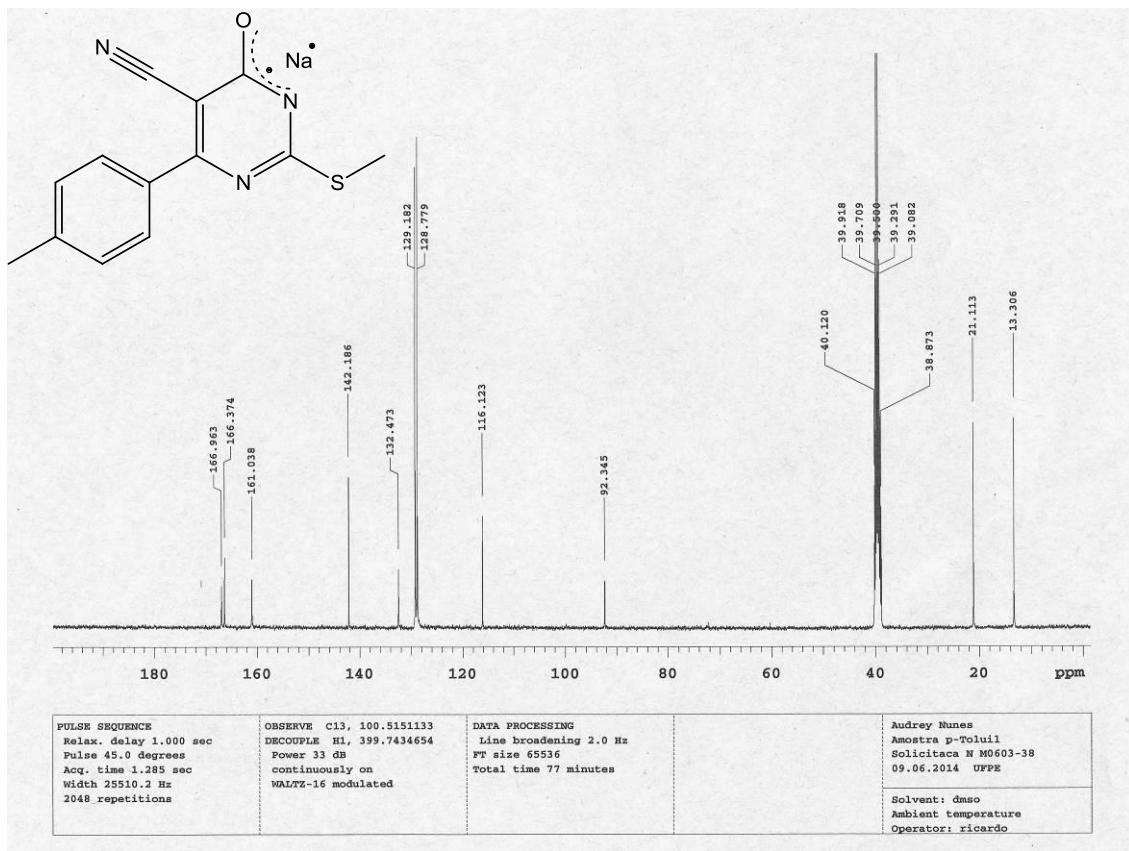
**Figure S36.**  $^{13}\text{C}$  NMR spectrum (100 MHz, DMSO- $d_6$ ) of compound **5b**.



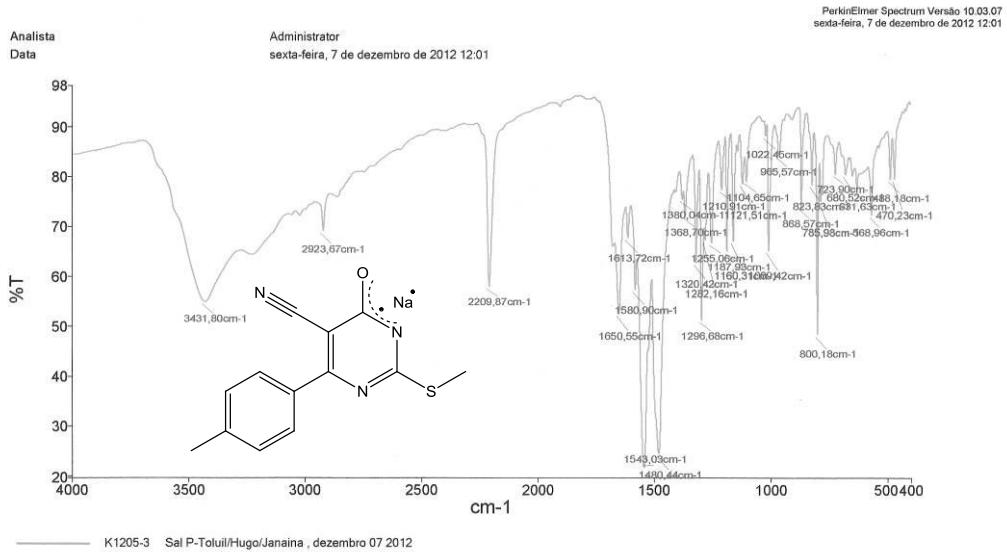
**Figure S37.** FTIR (KBr) spectrum of compound **5b**.



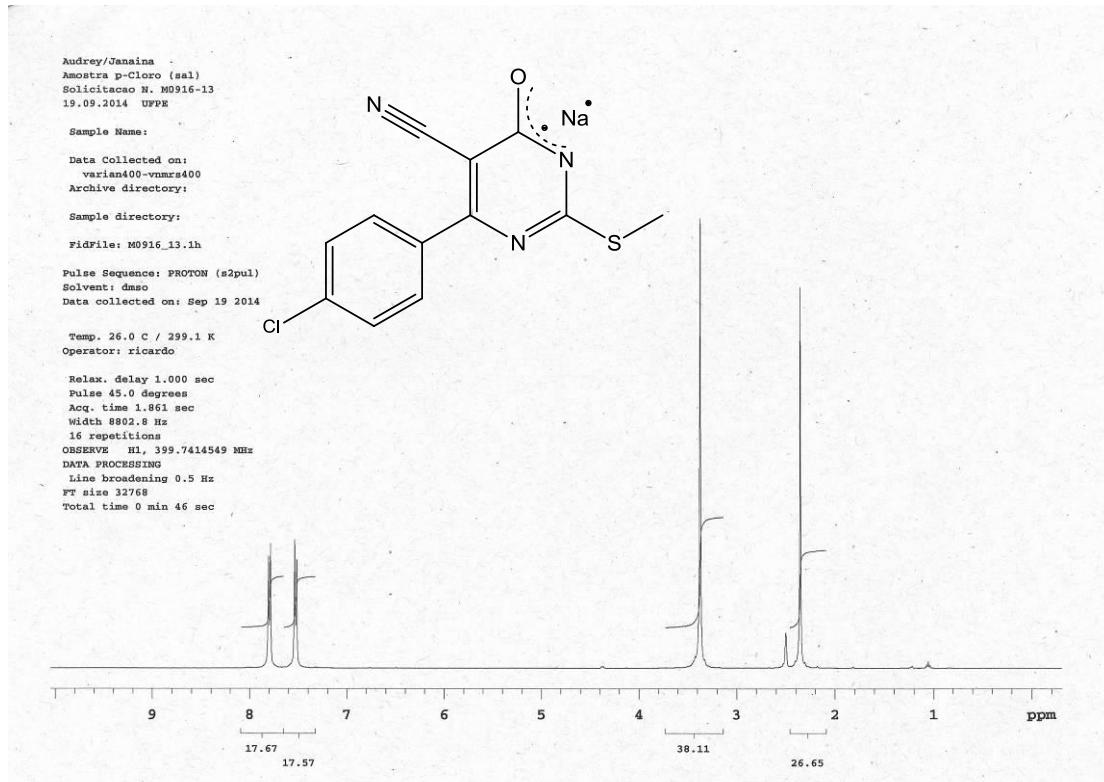
**Figure S38.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{DMSO}-d_6$ ) of compound **5c**.



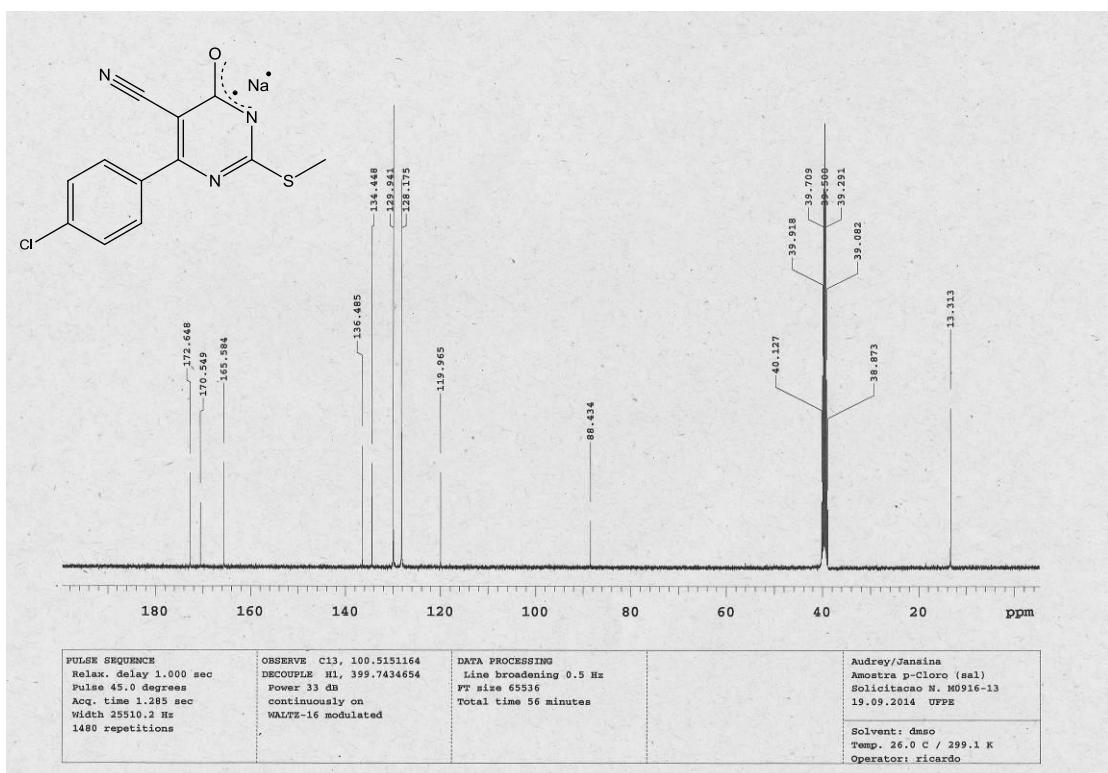
**Figure S39.**  $^{13}\text{C}$  NMR spectrum (100 MHz,  $\text{DMSO}-d_6$ ) of compound **5c**.



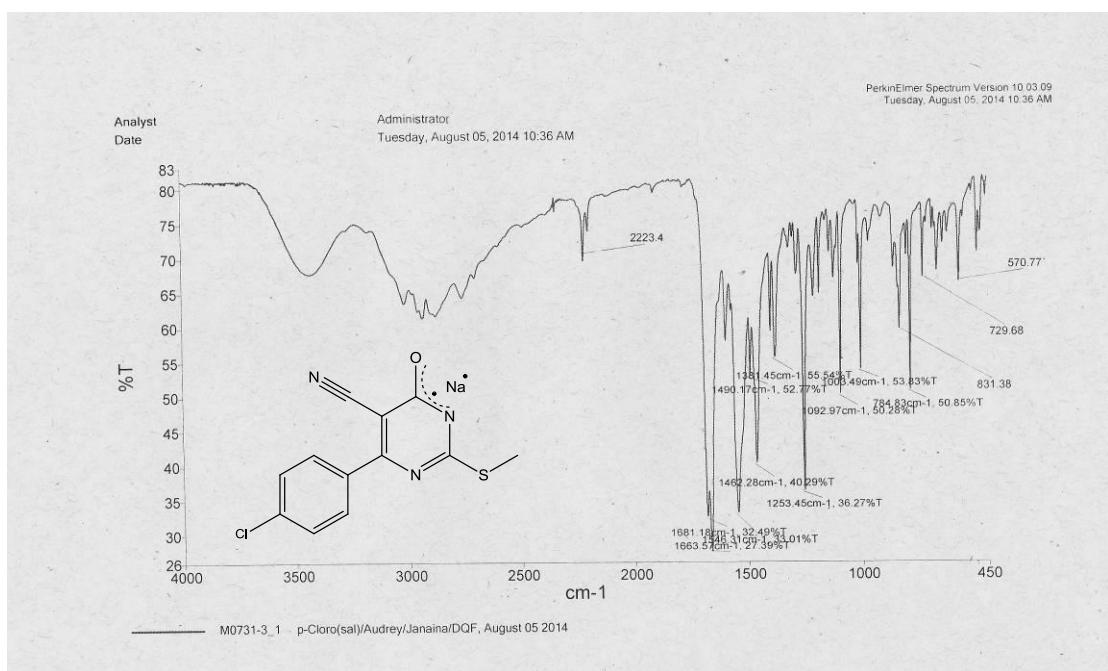
**Figure S40.** FTIR (KBr) spectrum of compound **5c**.



**Figure S41.** <sup>1</sup>H NMR spectrum (400 MHz, DMSO-*d*<sub>6</sub>) of compound **5d**.

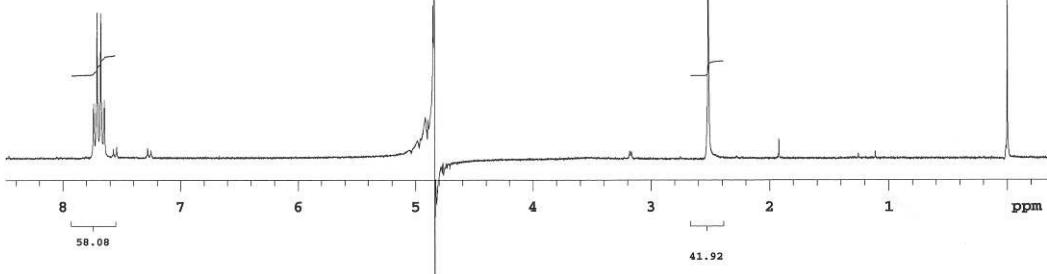


**Figure S42.**  $^{13}\text{C}$  NMR spectrum (100 MHz, DMSO- $d_6$ ) of compound **5d**.

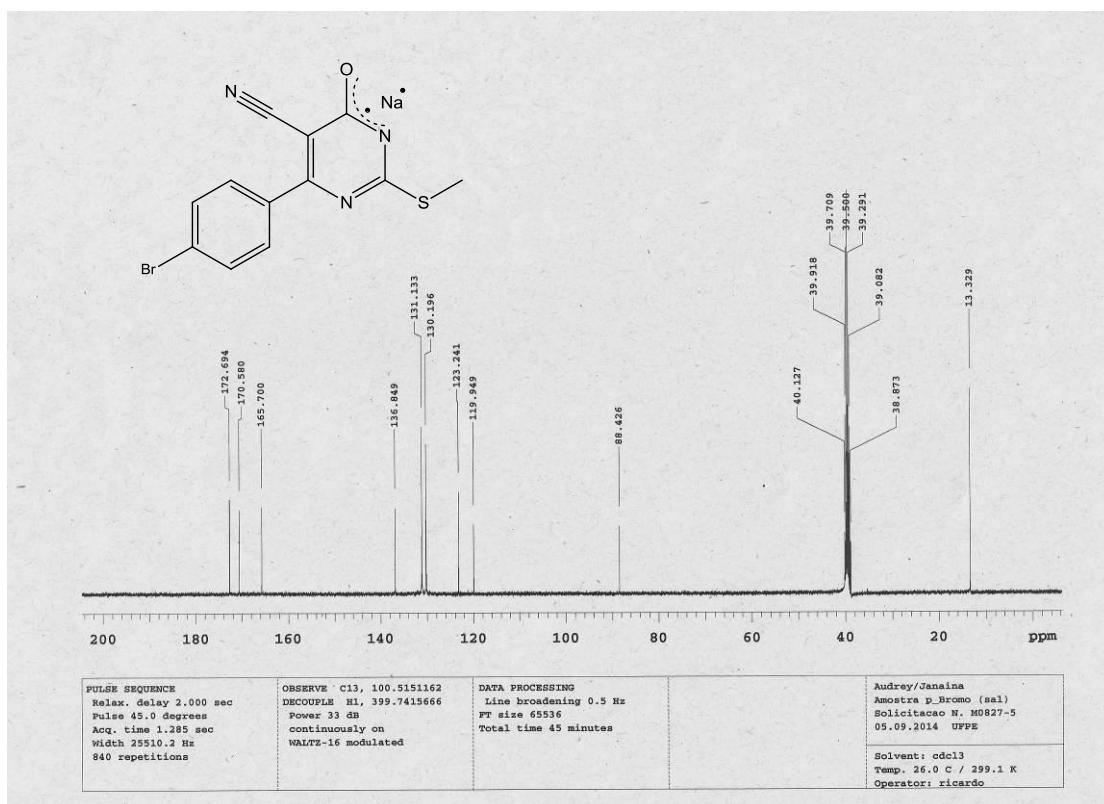


**Figure S43.** FTIR (KBr) spectrum of compound **5d**.

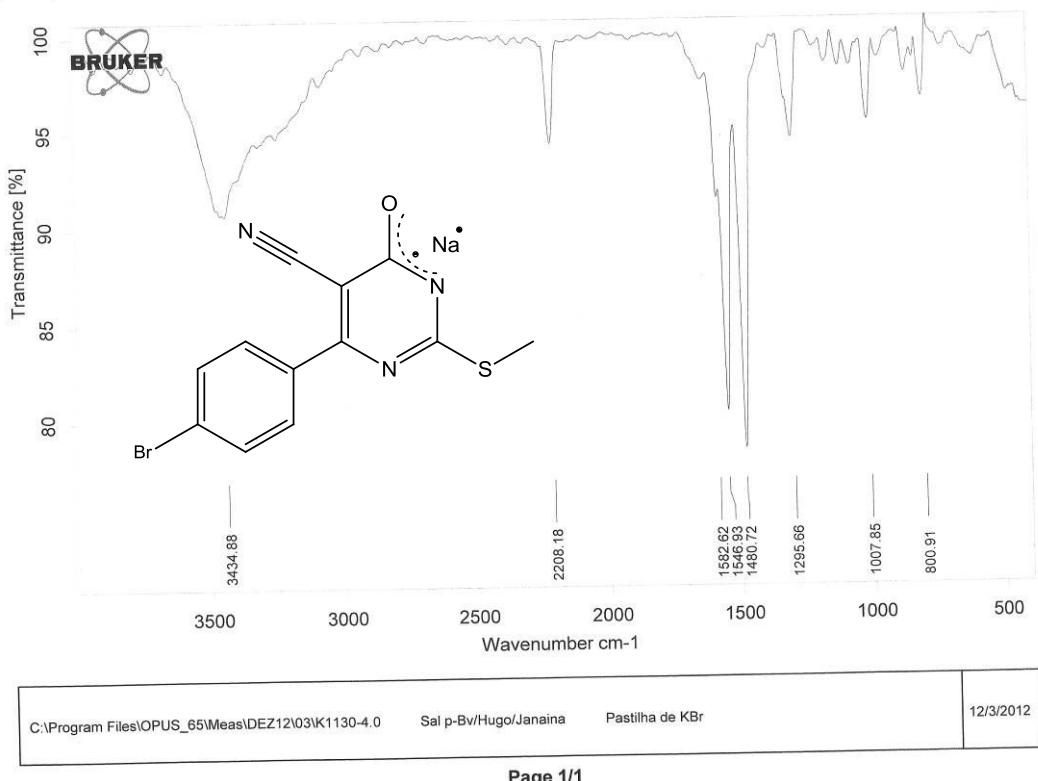
Hugo Branco  
 Janaina  
 Amostra pBr(sal)  
 Solicitacao N. L0124-15  
 05.02.2013 UFPE  
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 Pulse 90.0 degrees  
 Acc. time 3.641 sec  
 Width 4499.4 Hz  
 80 repetitions  
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 DATA PROCESSING  
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 Total time 0 min -1 sec



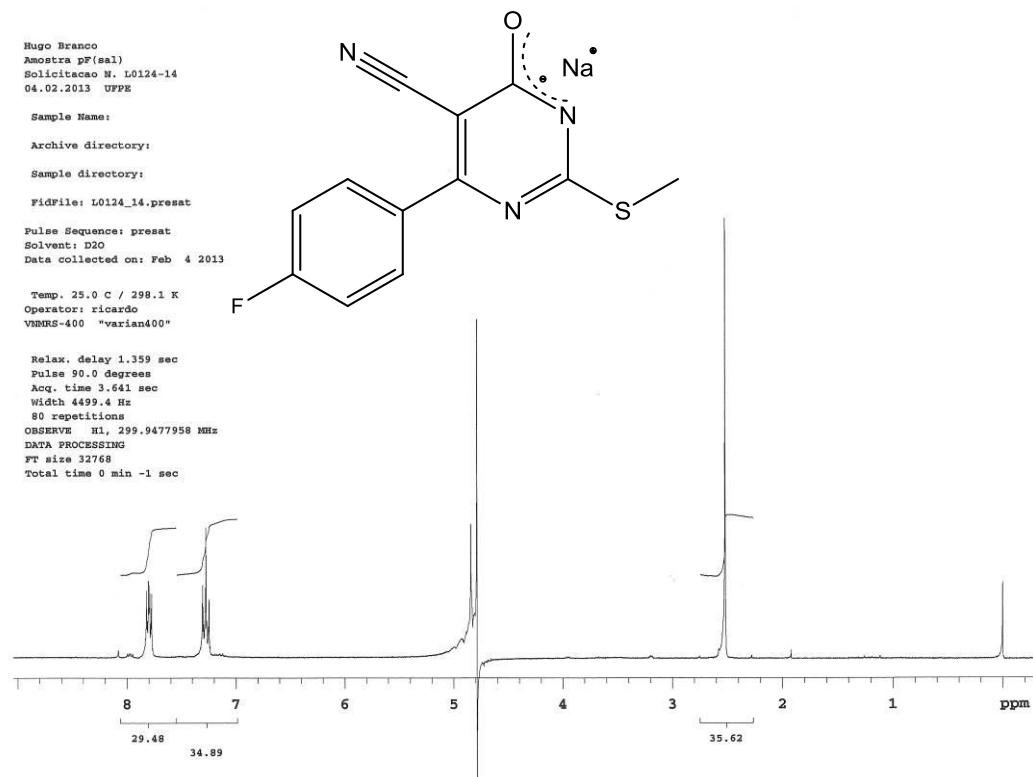
**Figure S44.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{D}_2\text{O}$ ) of compound **5e**.



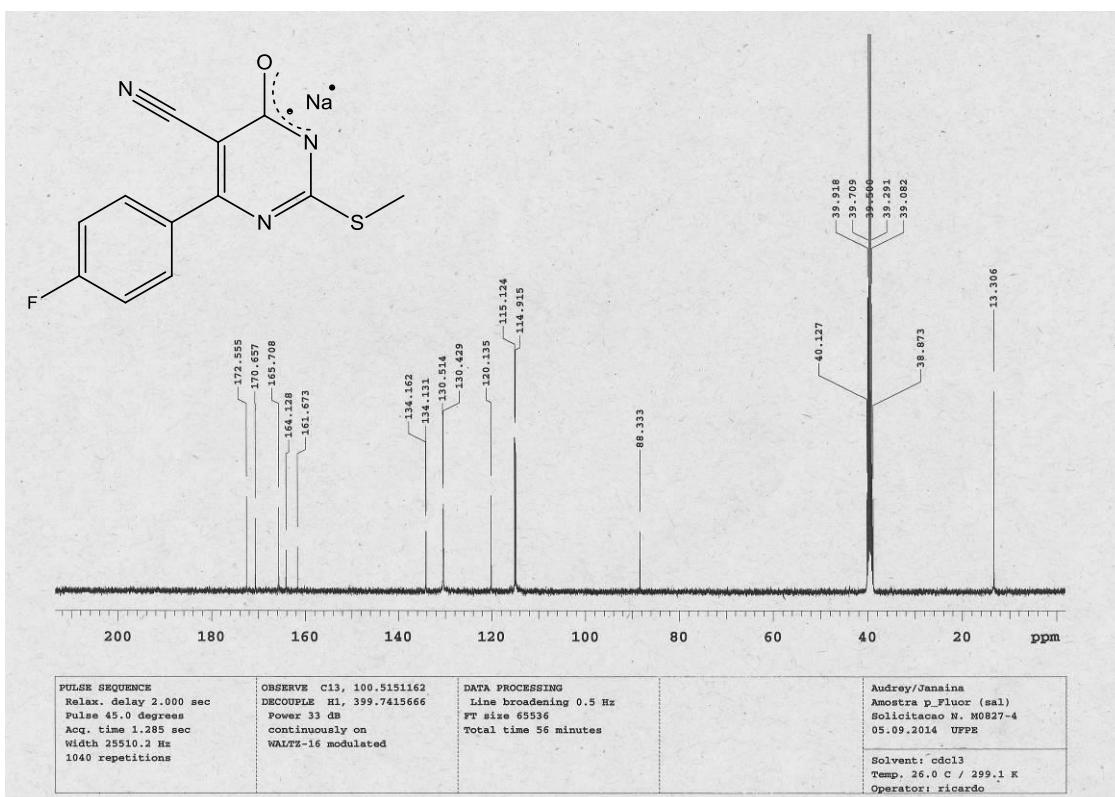
**Figure S45.**  $^{13}\text{C}$  NMR spectrum (100 MHz,  $\text{DMSO}-d_6$ ) of compound **5e**.



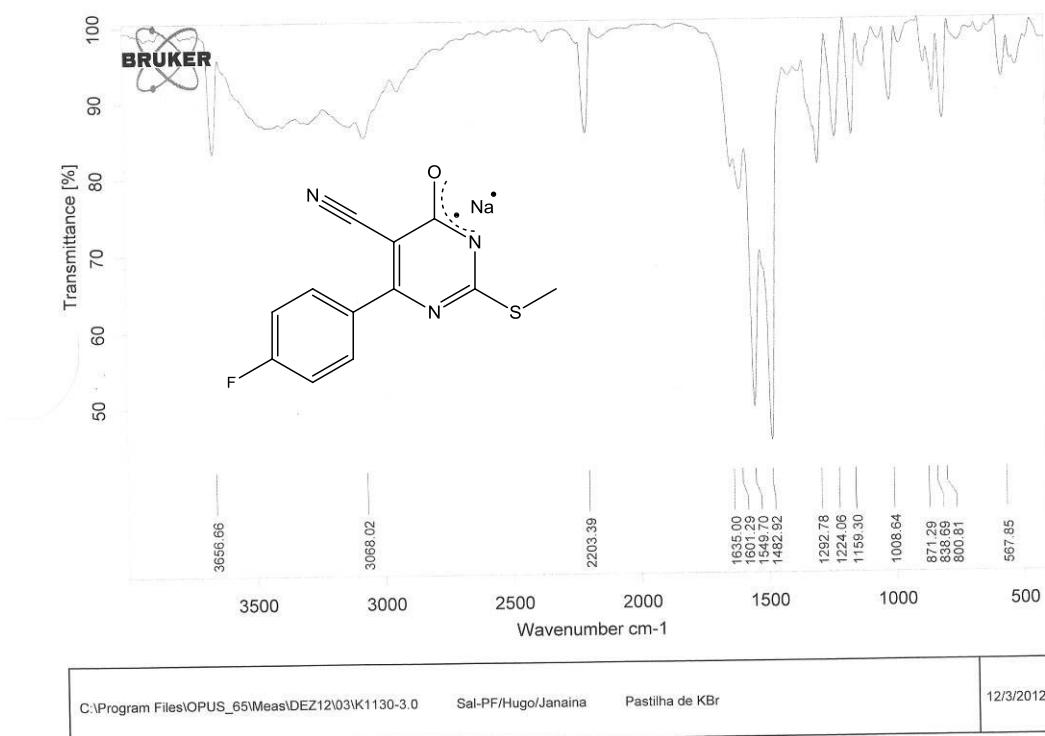
**Figure S46.** FTIR (KBr) spectrum of compound **5e**.



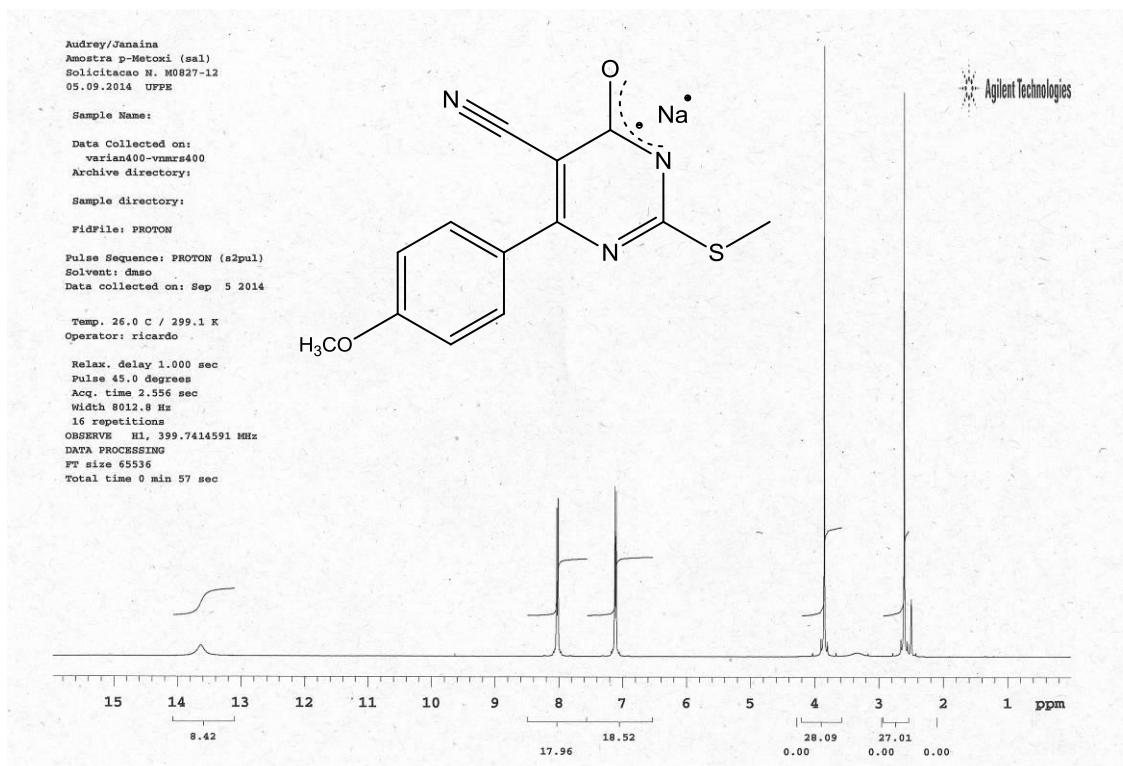
**Figure S47.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{D}_2\text{O}$ ) of compound **5f**.



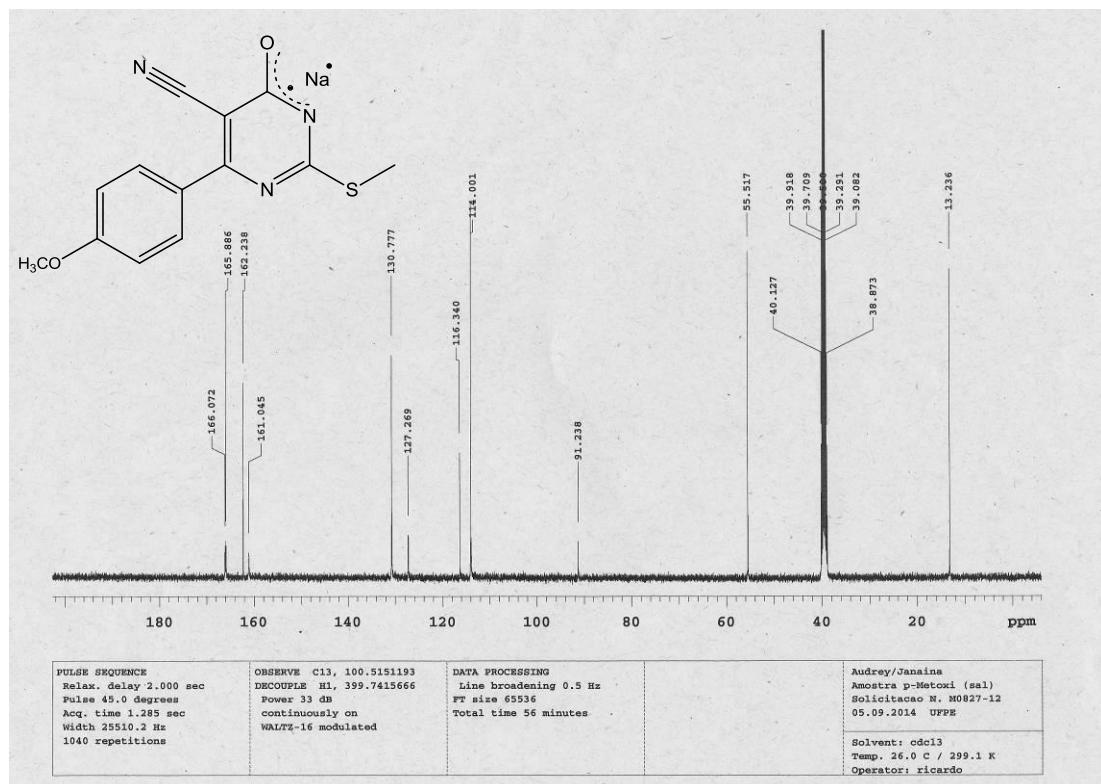
**Figure S48.**  $^{13}\text{C}$  NMR spectrum (100 MHz, DMSO- $d_6$ ) of compound **5f**.



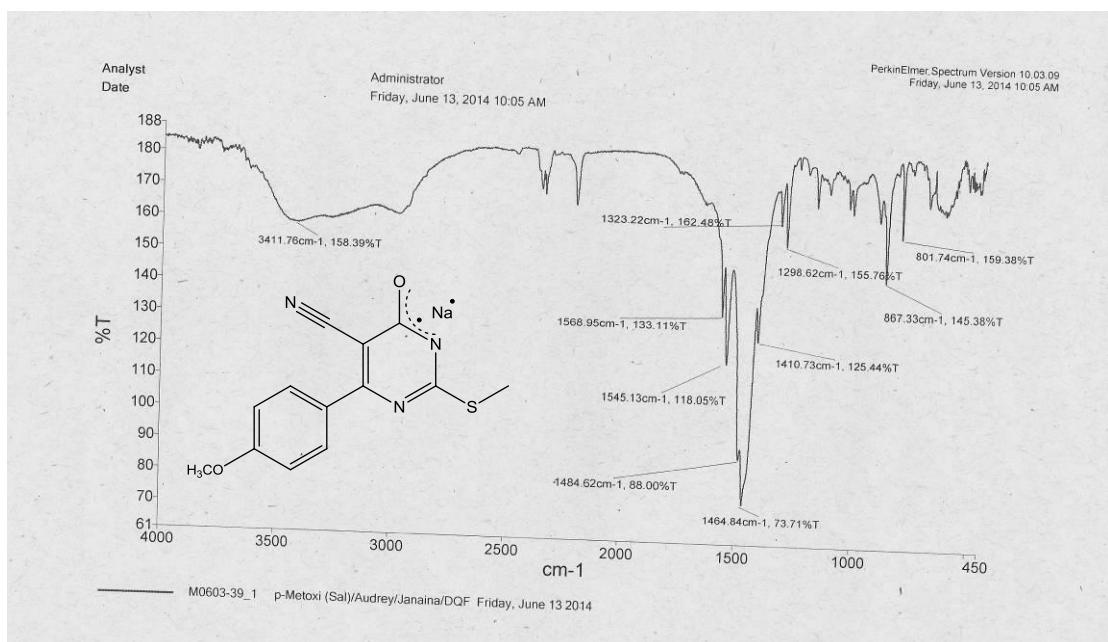
**Figure S49.** FTIR (KBr) spectrum of compound **5f**.



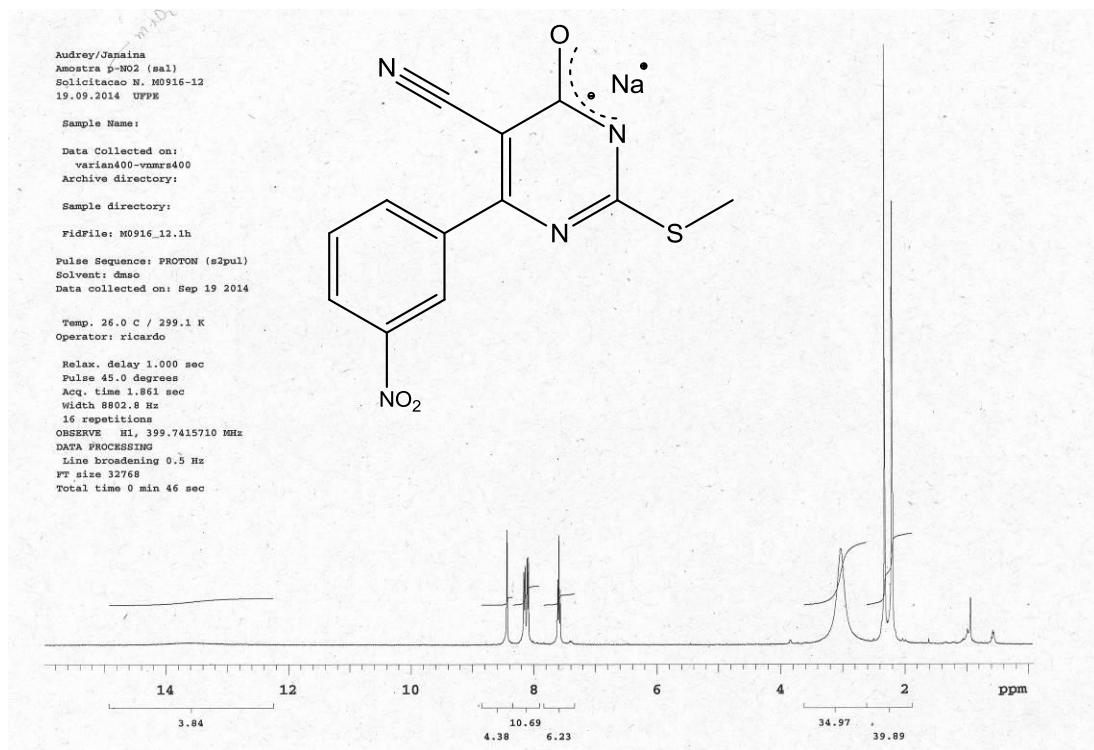
**Figure S50.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{DMSO}-d_6$ ) of compound **5g**.



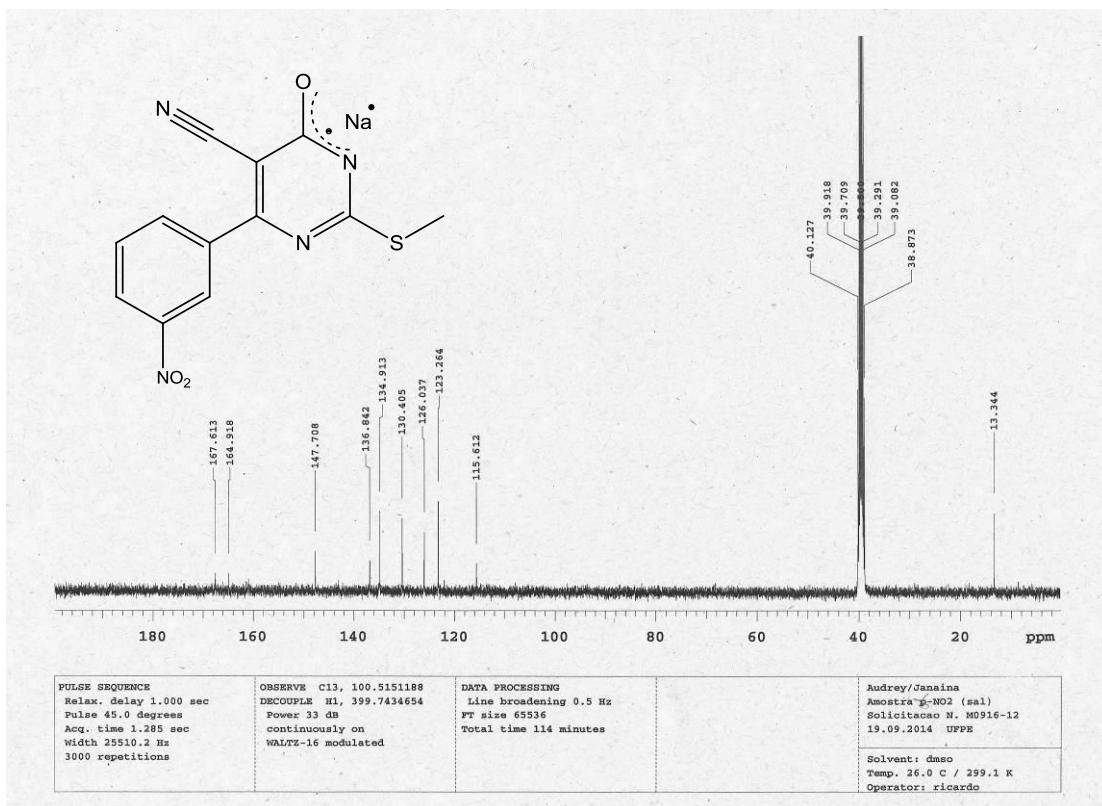
**Figure S51.**  $^{13}\text{C}$  NMR spectrum (100 MHz,  $\text{DMSO}-d_6$ ) of compound **5g**.



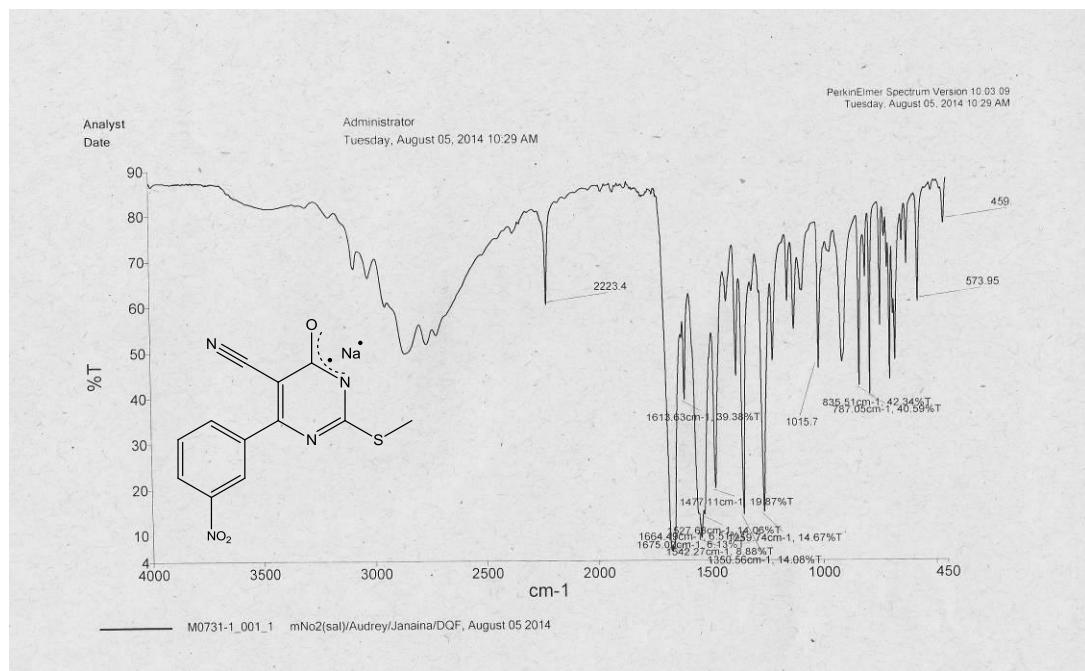
**Figure S52.** FTIR (KBr) spectrum of compound 5g.



**Figure S53.** <sup>1</sup>H NMR spectrum (400 MHz, DMSO-*d*<sub>6</sub>) of compound 5h.



**Figure S54.**  $^{13}\text{C}$  NMR spectrum (100 MHz, DMSO- $d_6$ ) of compound **5h**.



**Figure S55.** FTIR (KBr) spectrum of compound **5h**.

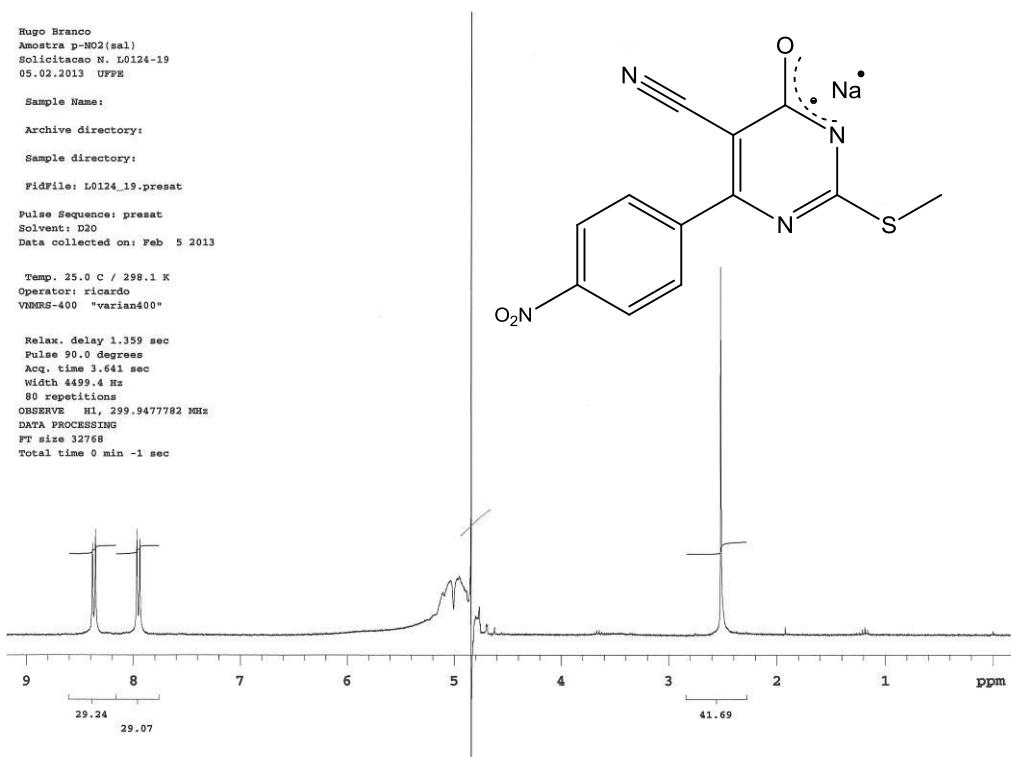
Rugo Branco  
Amostra p-N02(sal)  
Solicitacao N. L0124-19  
05.02.2013 UFPE

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Archive directory:  
Sample directory:  
FidFile: L0124\_19.preset

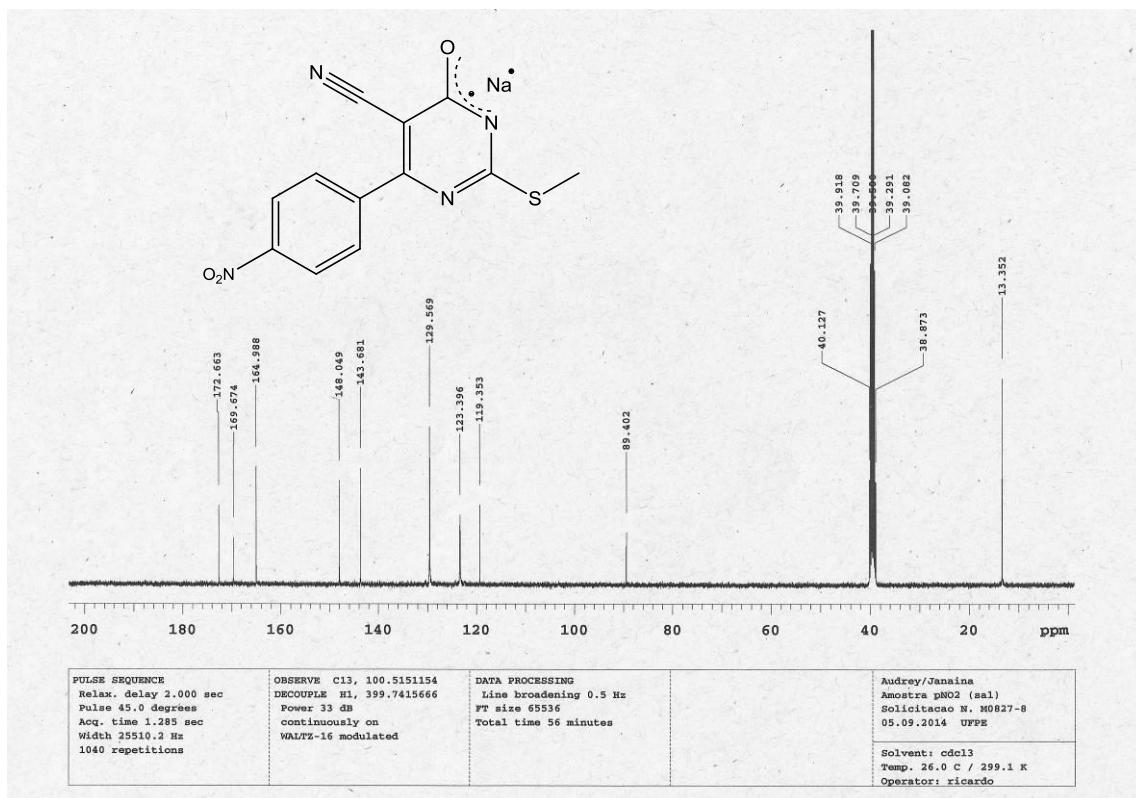
Pulse Sequence: preset  
Solvent: D2O  
Data collected on: Feb 5 2013

Temp. 25.0 C / 298.1 K  
Operator: ricardo  
VNMR-S-400 "varian400"

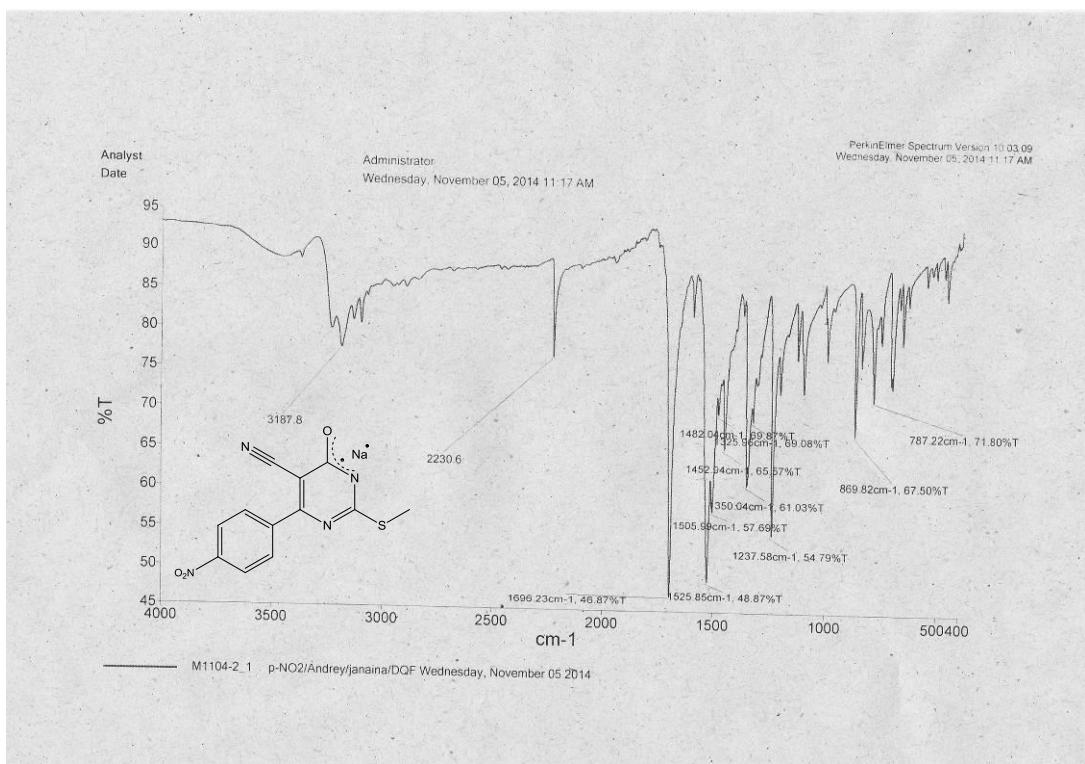
Relax. delay 1.359 sec  
Pulse 90.0 degrees  
Acq. time 3.641 sec  
Width 4499.4 Hz  
80 repetitions  
OBSERVE H1, 299.9477782 MHz  
DATA PROCESSING  
FT size 32768  
Total time 0 min -1 sec



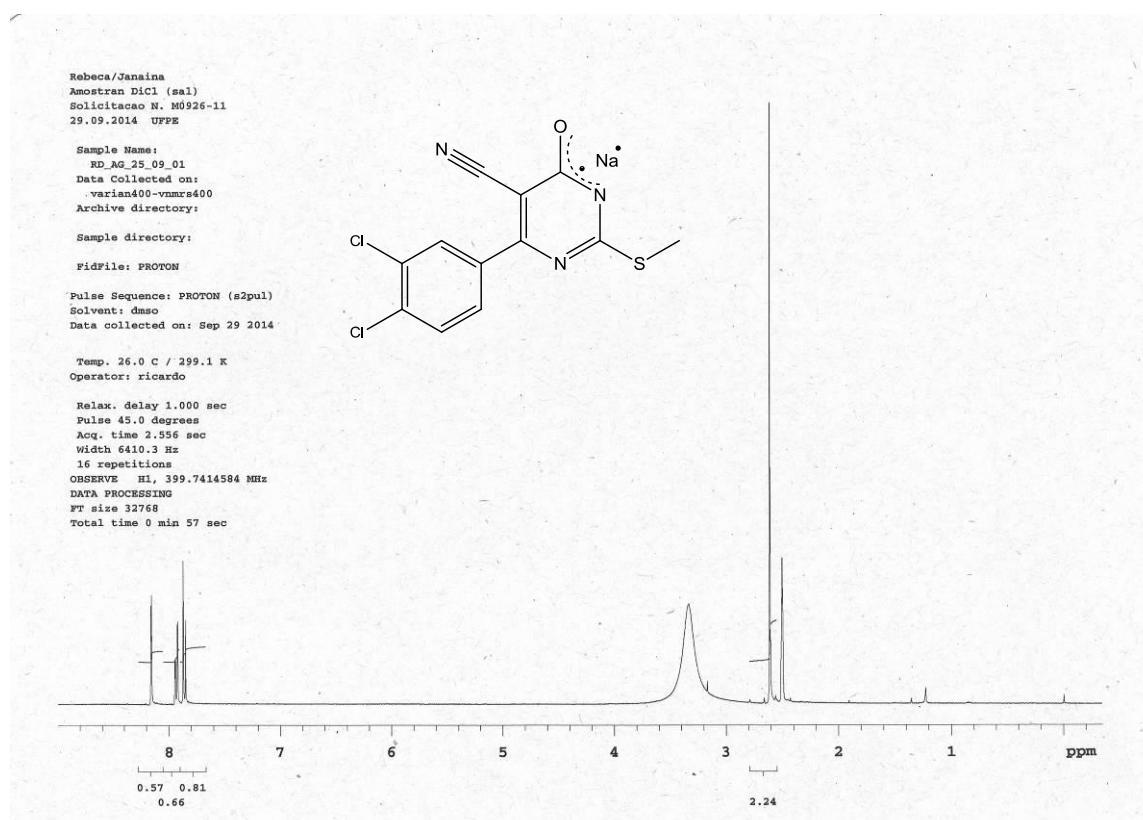
**Figure S56.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{D}_2\text{O}$ ) of compound **5i**.



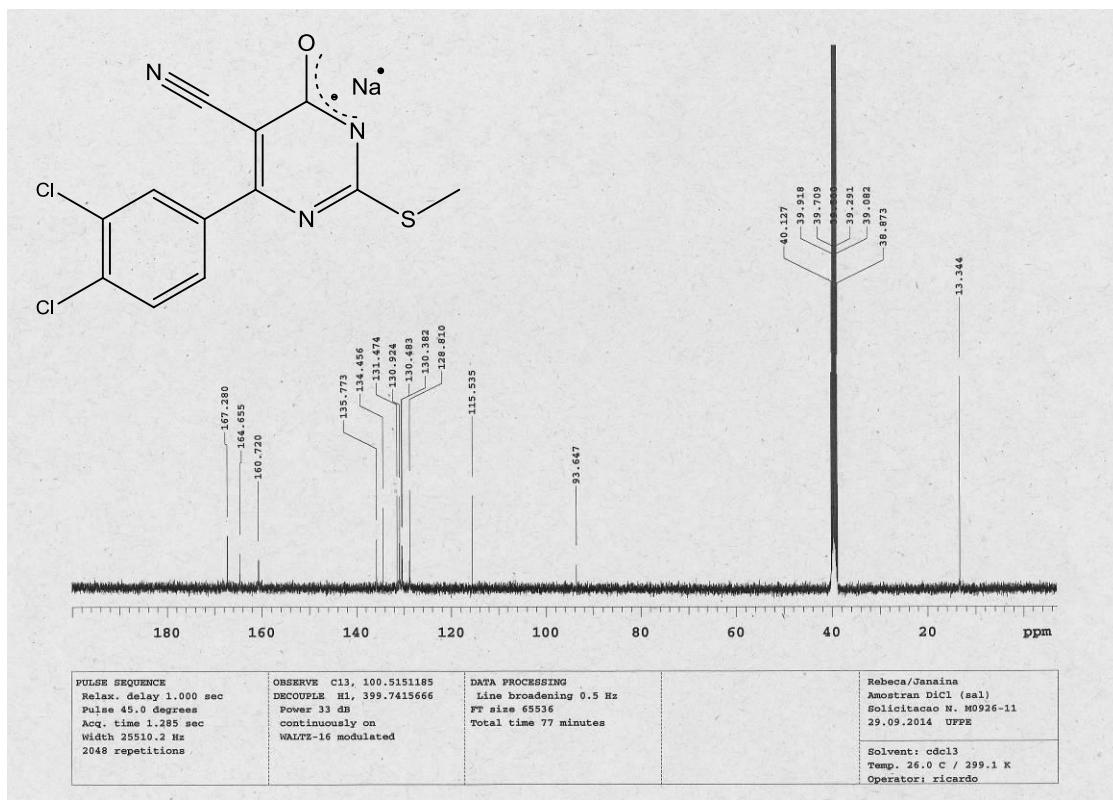
**Figure S57.**  $^{13}\text{C}$  NMR spectrum (100 MHz,  $\text{DMSO}-d_6$ ) of compound **5i**.



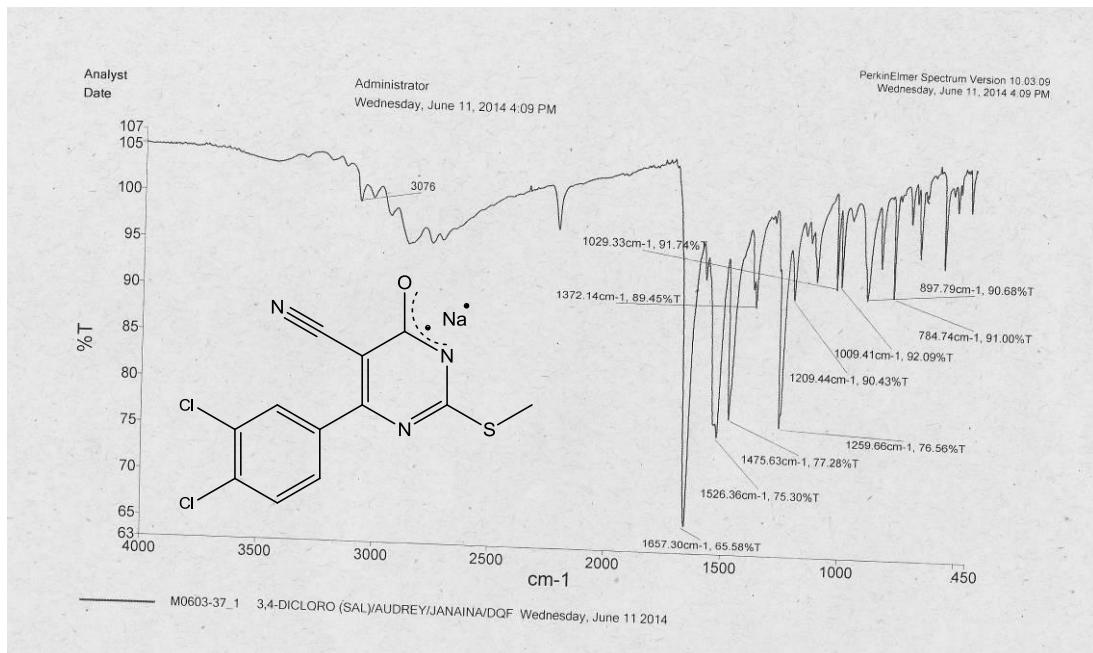
**Figure S58.** FTIR (KBr) spectrum of compound **5i**.



**Figure S59.** <sup>1</sup>H NMR spectrum (400 MHz, DMSO-*d*<sub>6</sub>) of compound **5j**.



**Figure S60.**  $^{13}\text{C}$  NMR spectrum (100 MHz, DMSO- $d_6$ ) of compound **5j**.



**Figure S61.** FTIR (KBr) spectrum of compound **5j**.