

Figure 1. ATR-FTIR: 1H-Benzimidazole-5-carboxylic acid (1-C1).

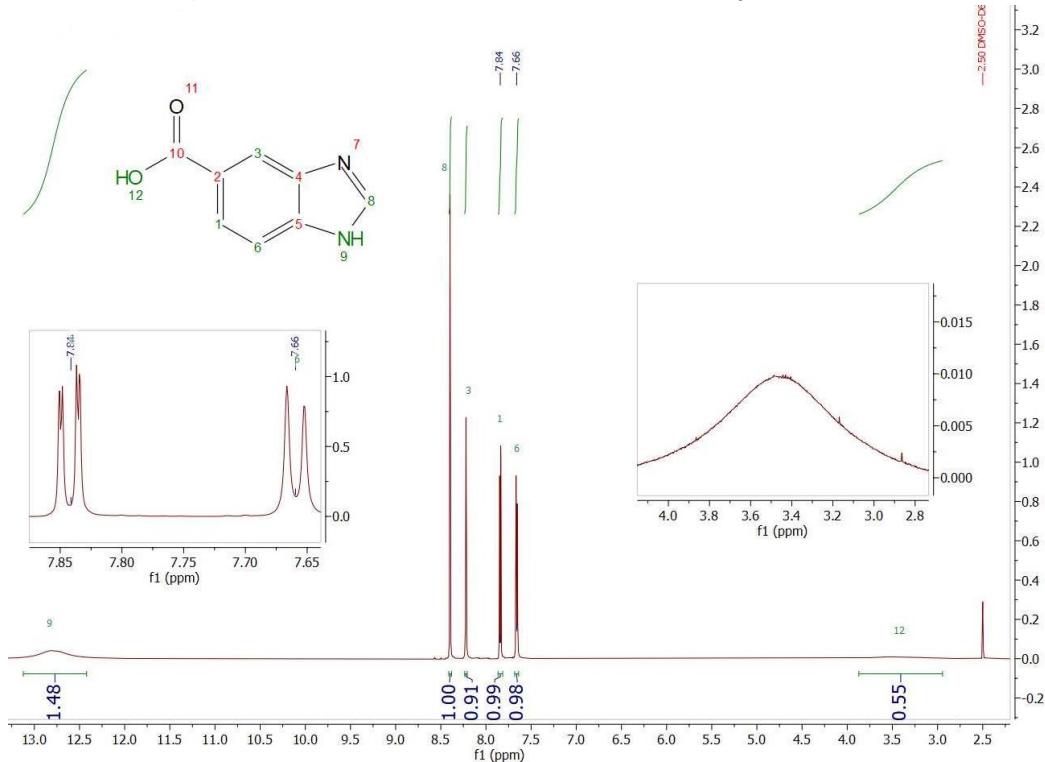
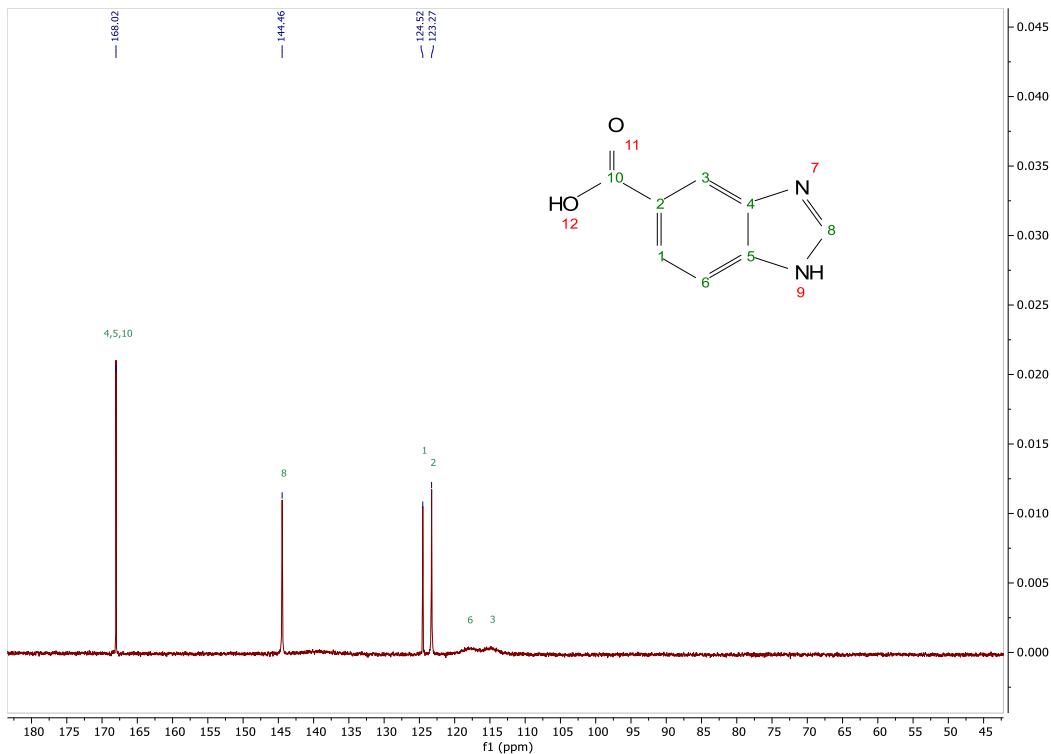
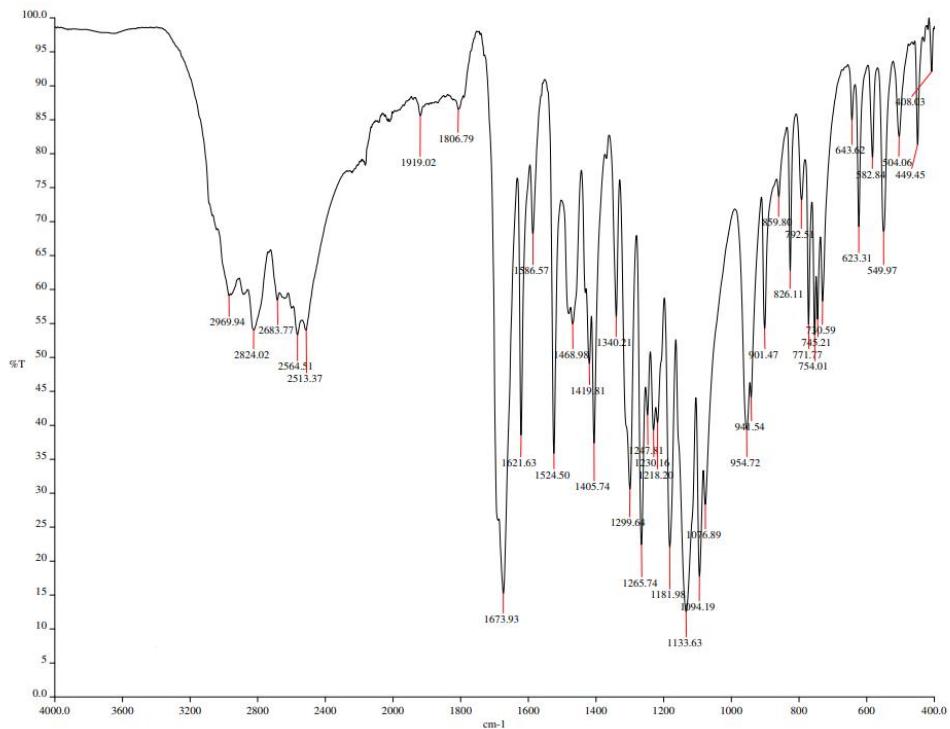


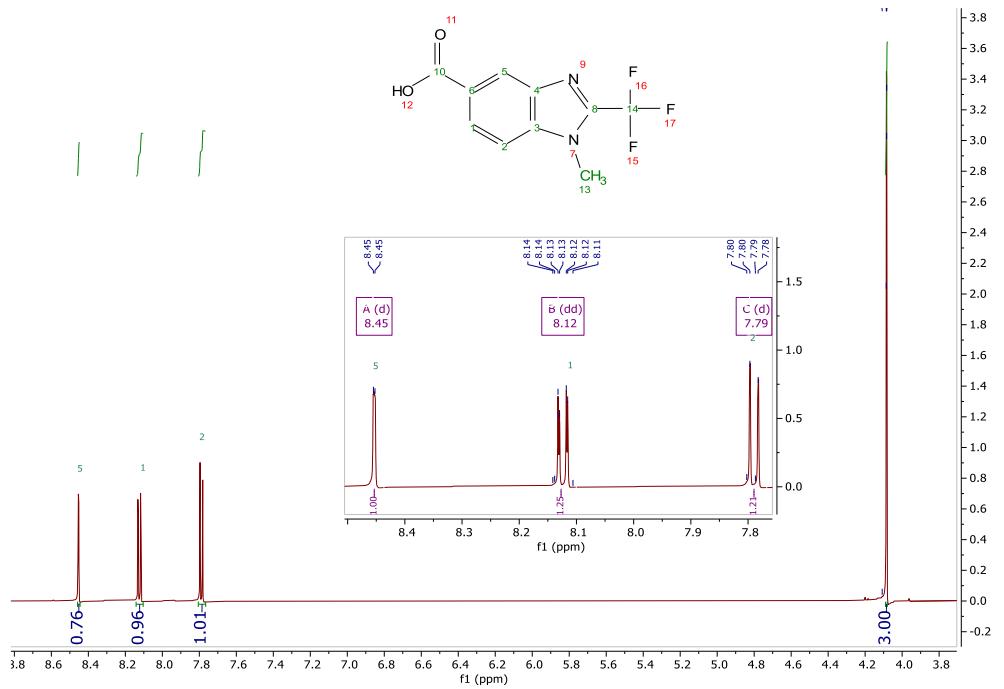
Figure 2. <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 600 MHz): 1H-Benzimidazole-5-carboxylic acid (1-C1).



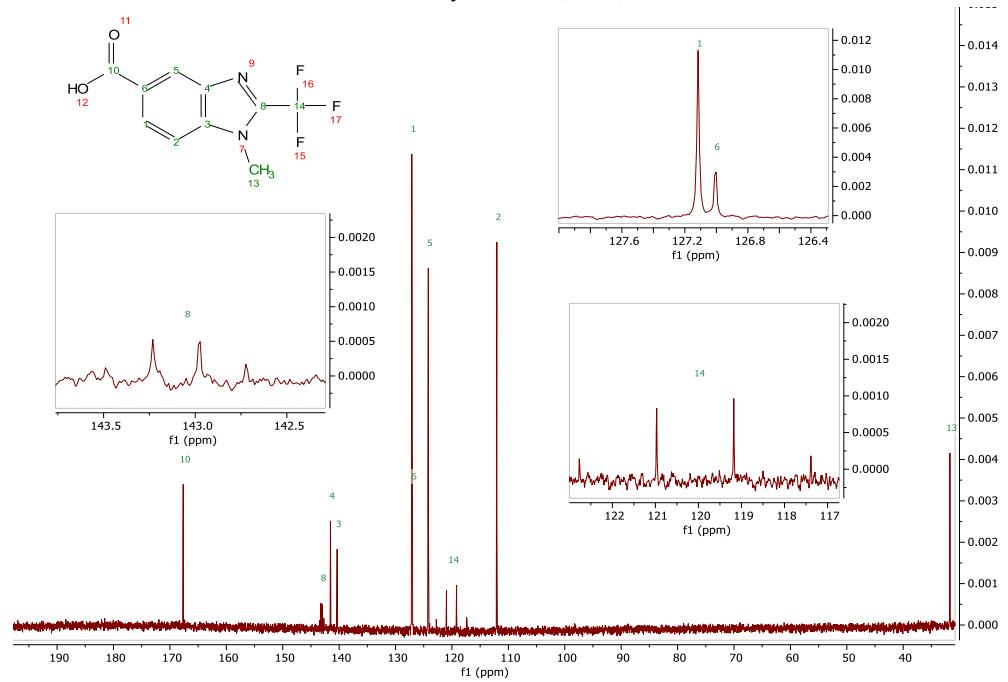
**Figure 3.** <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 151 MHz): 1*H*-Benzimidazole-5-carboxylic acid (**1-C1**).



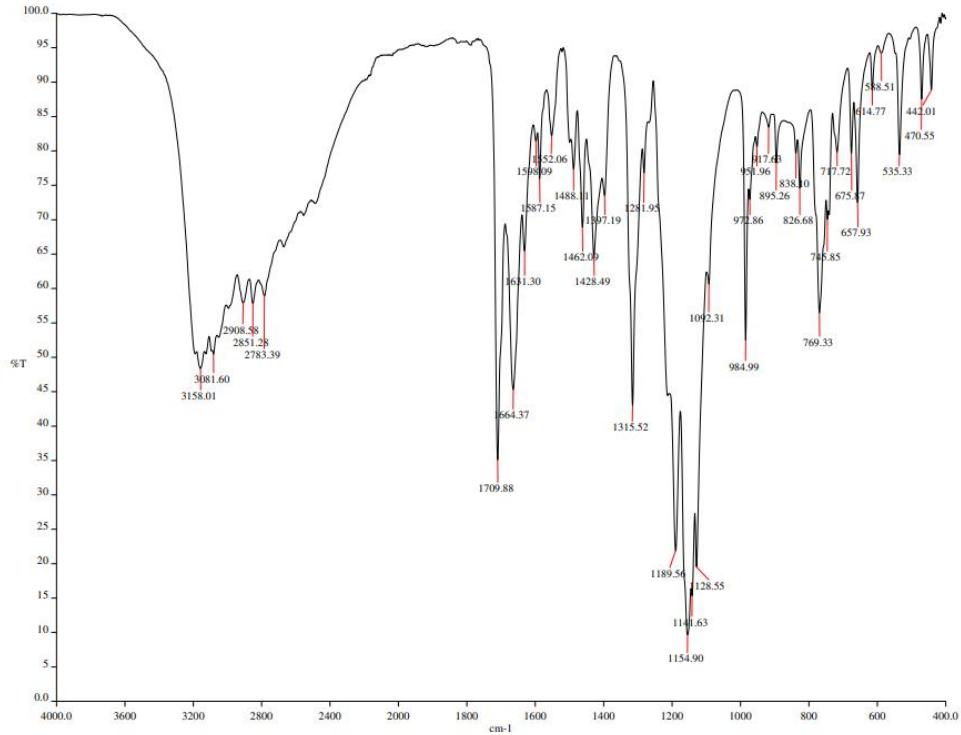
**Figure 4.** ATR-FTIR: 1-Methyl-2-trifluoromethyl-1*H*-benzimidazole-5-carboxylic acid (**1-C2**).



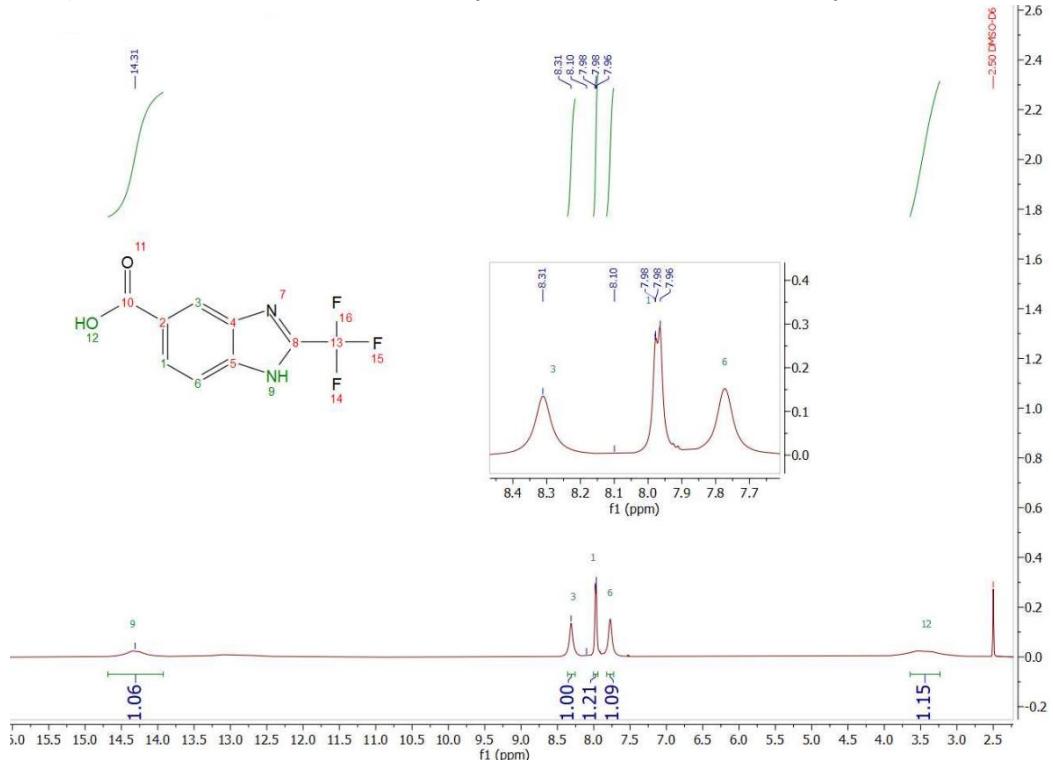
**Figure 5.**  $^1\text{H}$  NMR (DMSO- $d_6$ , 600 MHz): 1-Methyl-2-trifluoromethyl-1*H*-benzimidazole-5-carboxylic acid (**1-C2**).



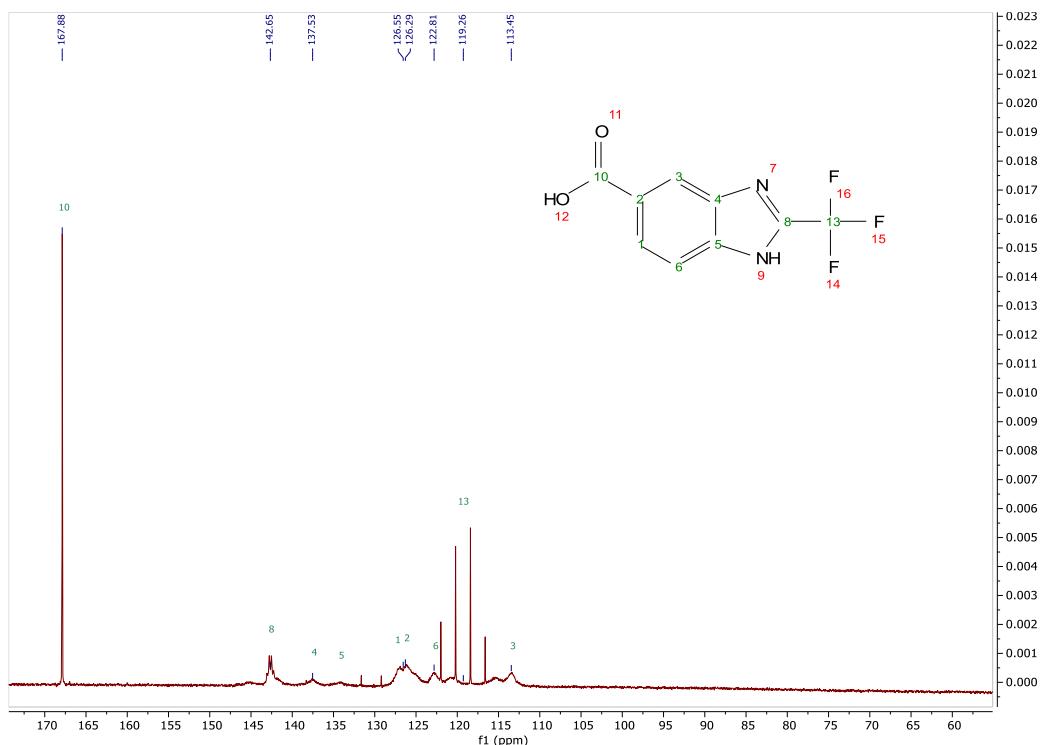
**Figure 6.**  $^{13}\text{C}$  NMR (DMSO- $d_6$ , 151 MHz): 1-Methyl-2-trifluoromethyl-1*H*-benzimidazole-5-carboxylic acid (**1-C2**).



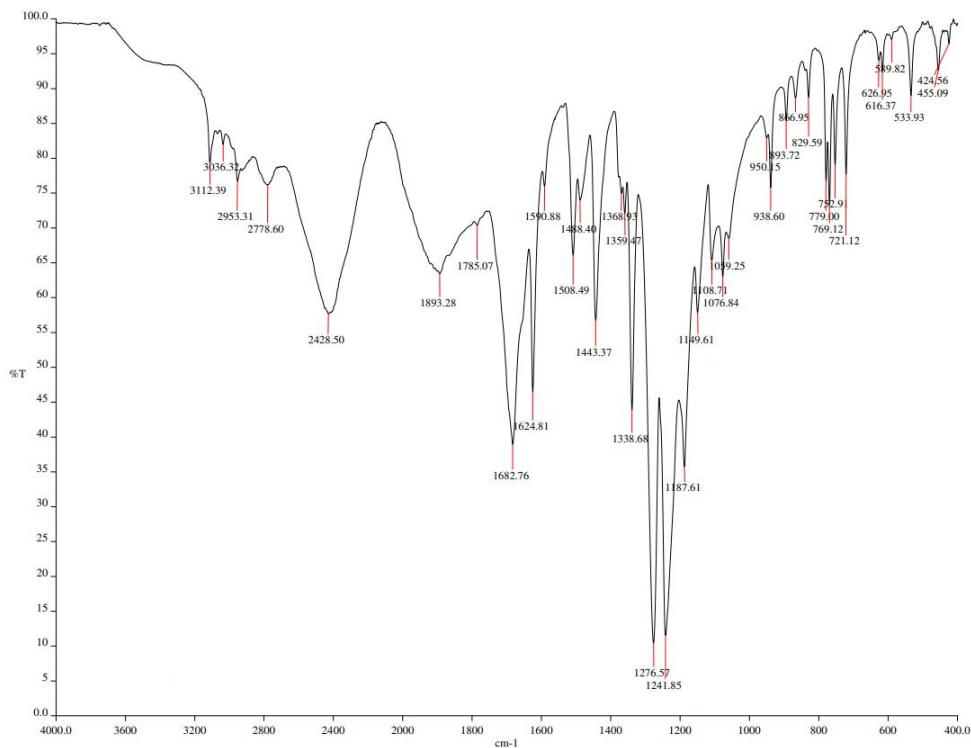
**Figure 7.** ATR-FTIR: 2-Trifluoromethyl-1*H*-benzimidazole-5-carboxylic acid (**1-C3**).



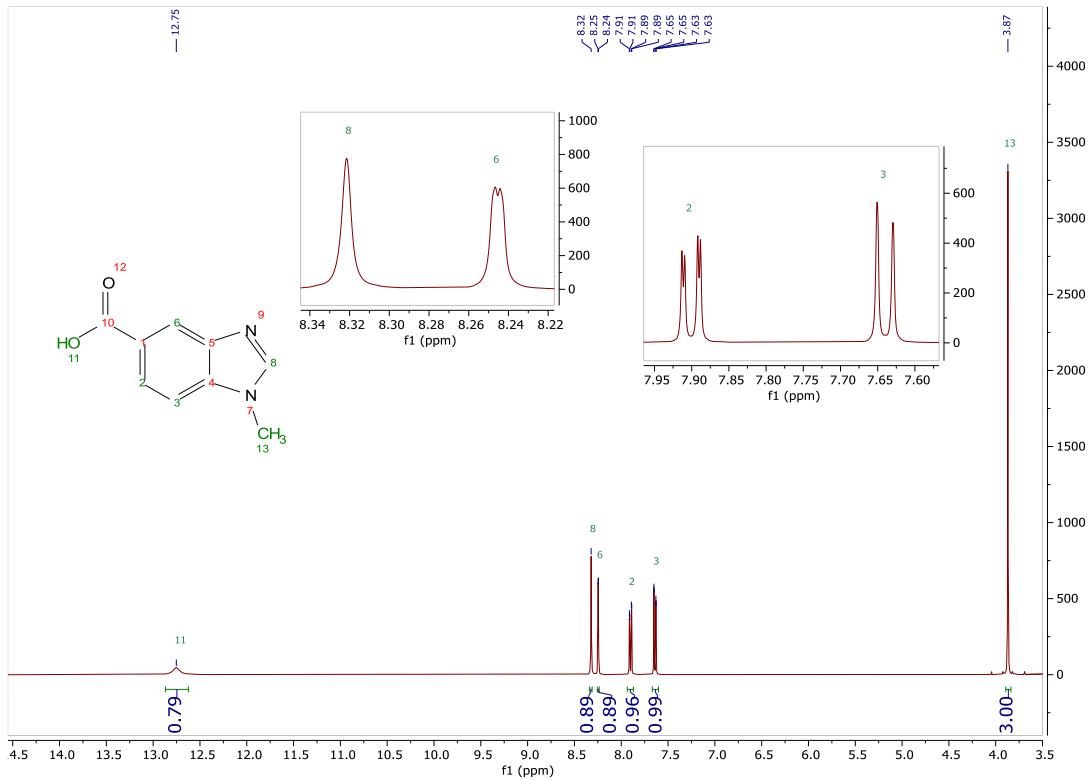
**Figure 8.**  $^1\text{H}$  NMR ( $\text{DMSO}-d_6$ , 600 MHz): 2-Trifluoromethyl-1*H*-benzimidazole-5-carboxylic acid (**1-C3**).



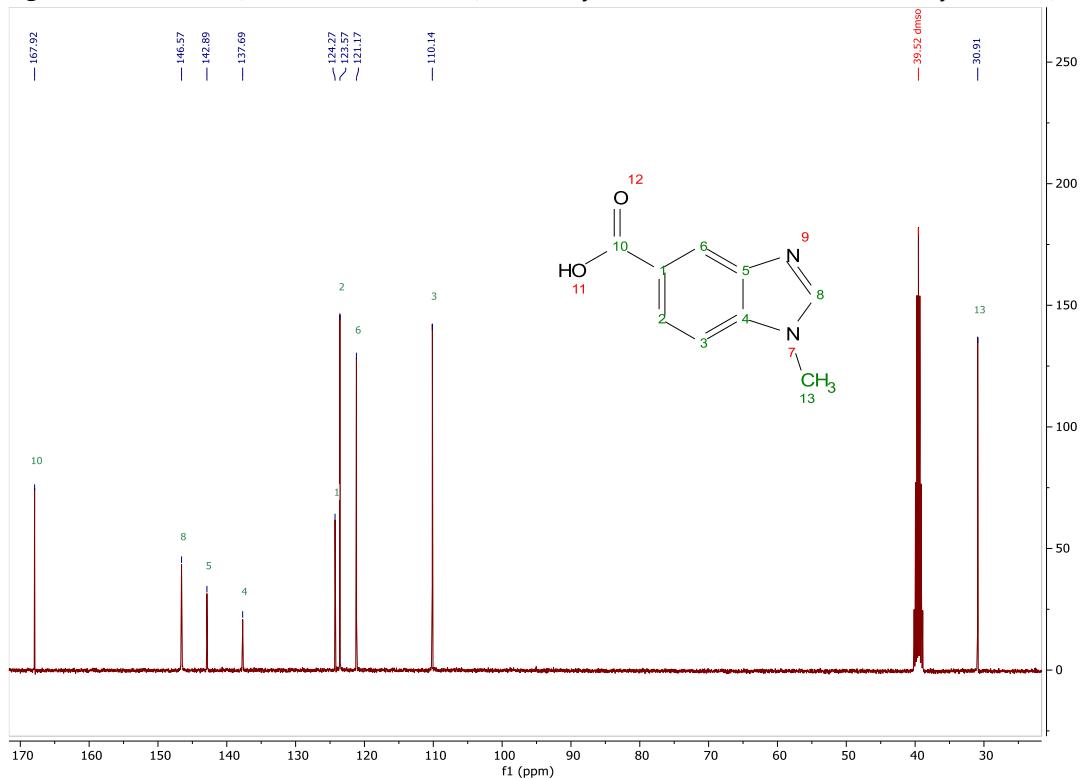
**Figure 9.**  $^{13}\text{C}$  NMR ( $\text{DMSO}-d_6$ , 151 MHz): 2-Trifluoromethyl-1*H*-benzimidazole-5-carboxylic acid (1-C3).



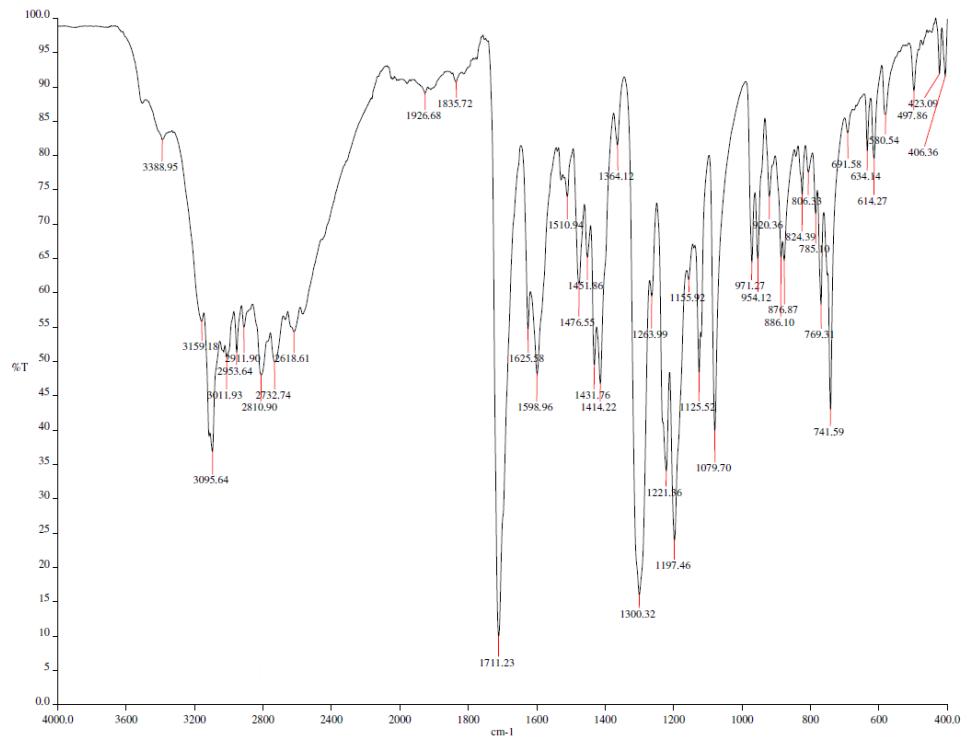
**Figure 10.** ATR-FTIR: 1-Methyl-1*H*-benzimidazole-5-carboxylic acid (1-C4).



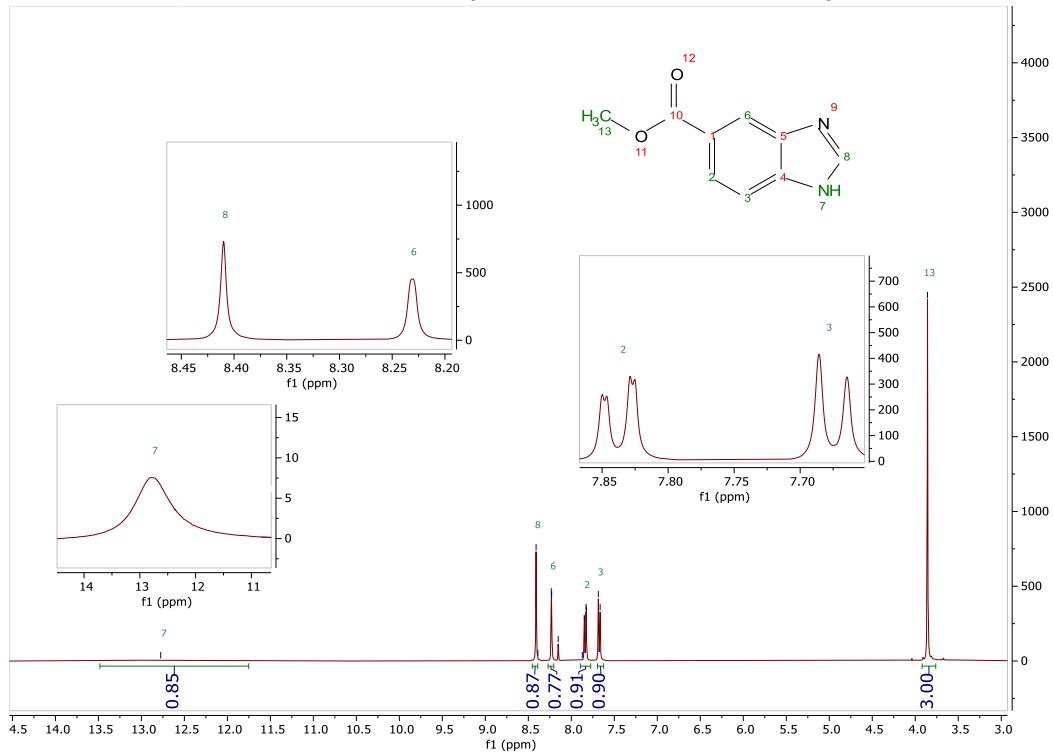
**Figure 11.** <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 400 MHz): 1-Methyl-1*H*-benzimidazole-5-carboxylic acid (**1-C4**).



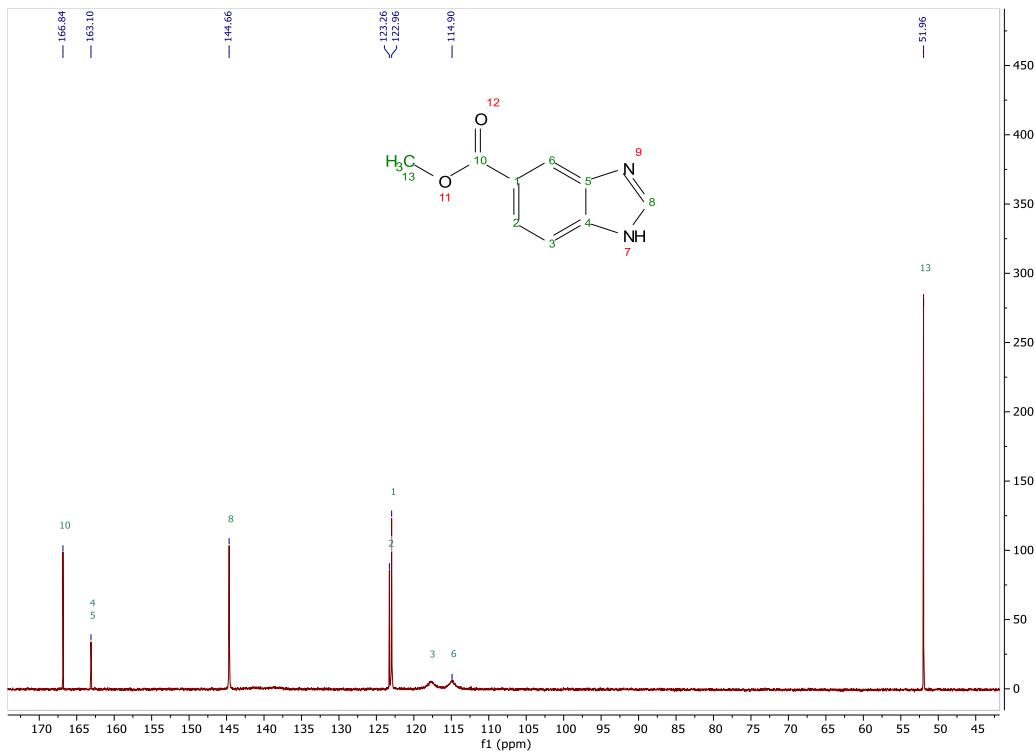
**Figure 12.** <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 101 MHz): 1-Methyl-1*H*-benzimidazole-5-carboxylic acid (**1-C4**).



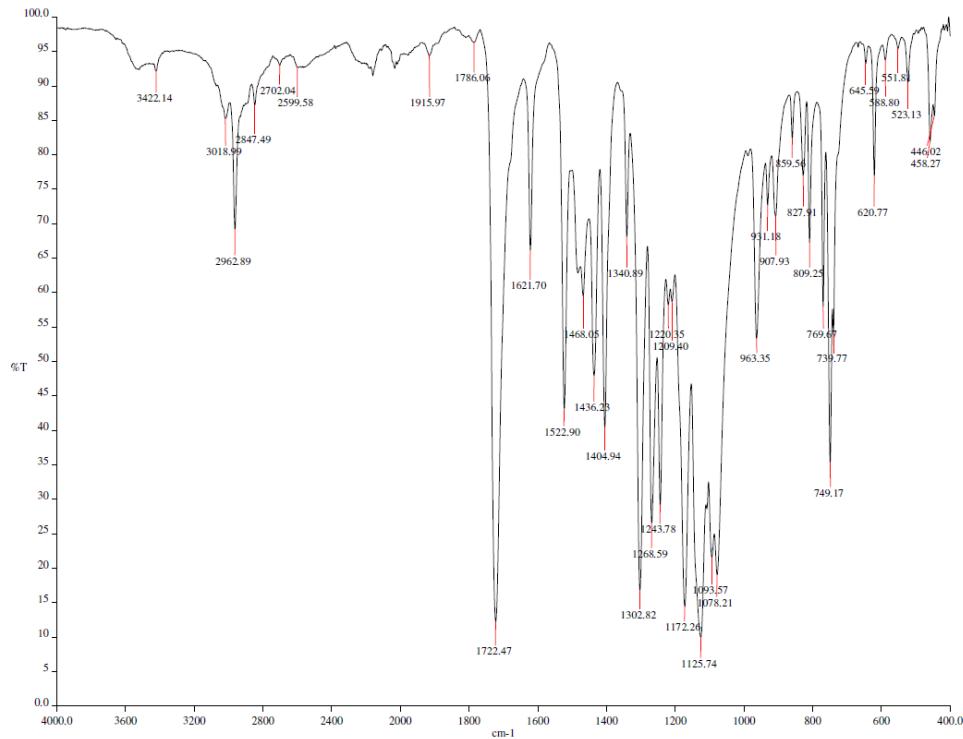
**Figure 13.** ATR-FTIR: Methyl 1*H*-benzimidazole-5-carboxylate (**2-C1**).



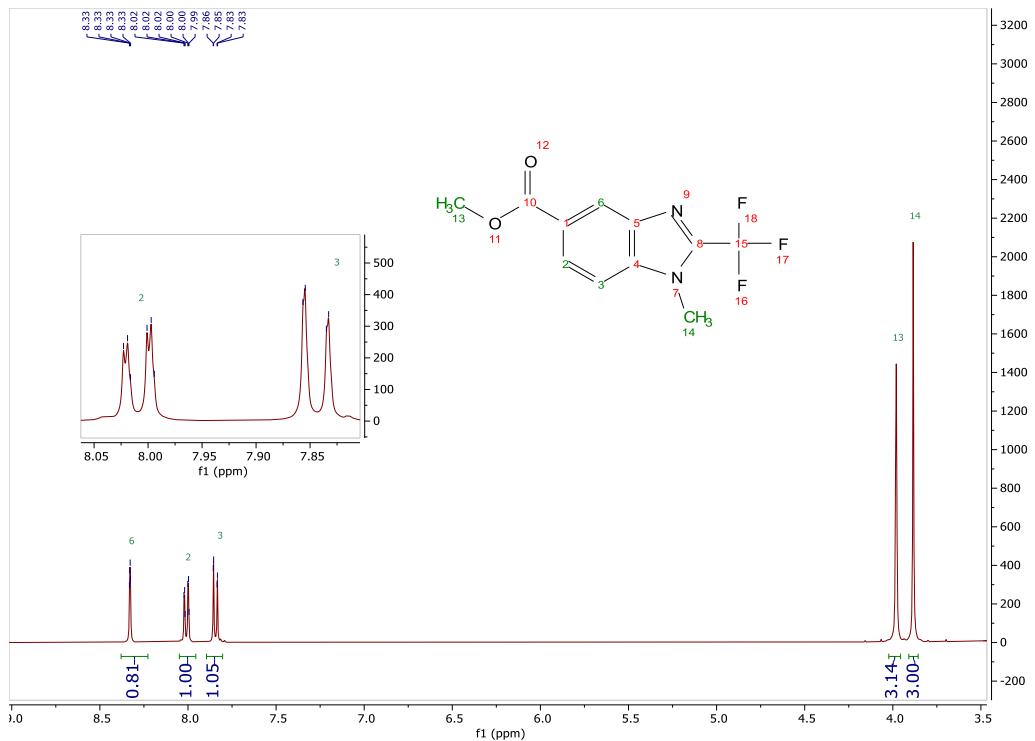
**Figure 14.**  $^1\text{H}$  NMR (DMSO- $d_6$ , 400 MHz): Methyl 1*H*-benzimidazole-5-carboxylate (**2-C1**).



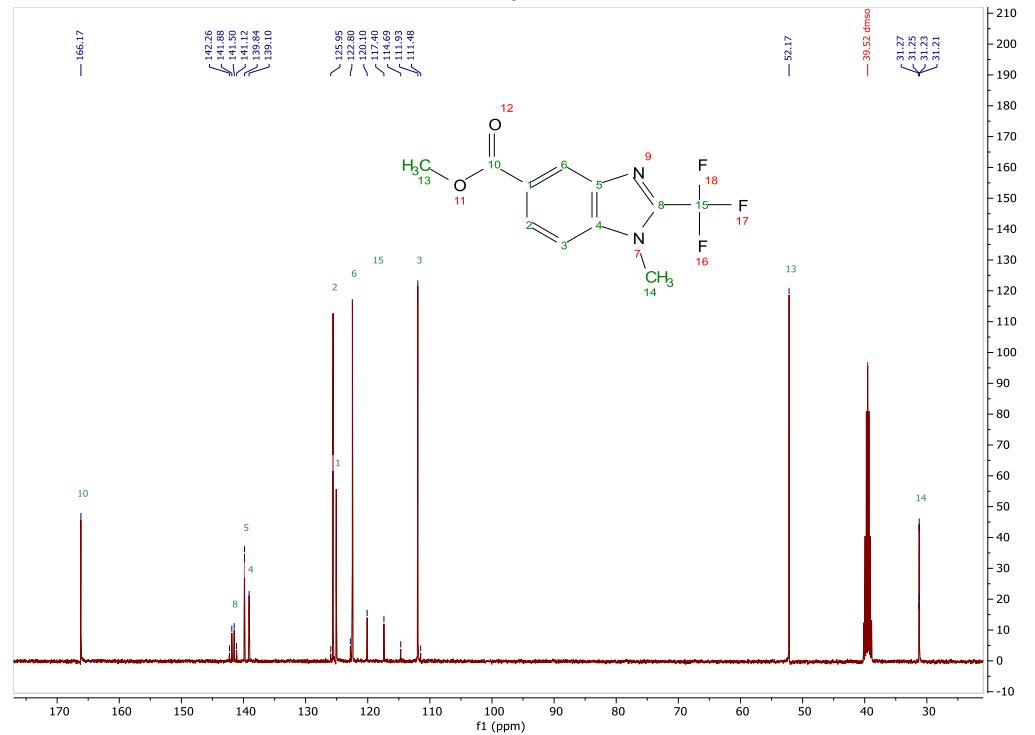
**Figure 15.**  $^{13}\text{C}$  NMR ( $\text{DMSO}-d_6$ , 400 MHz): Methyl 1*H*-benzimidazole-5-carboxylate (**2-C1**).



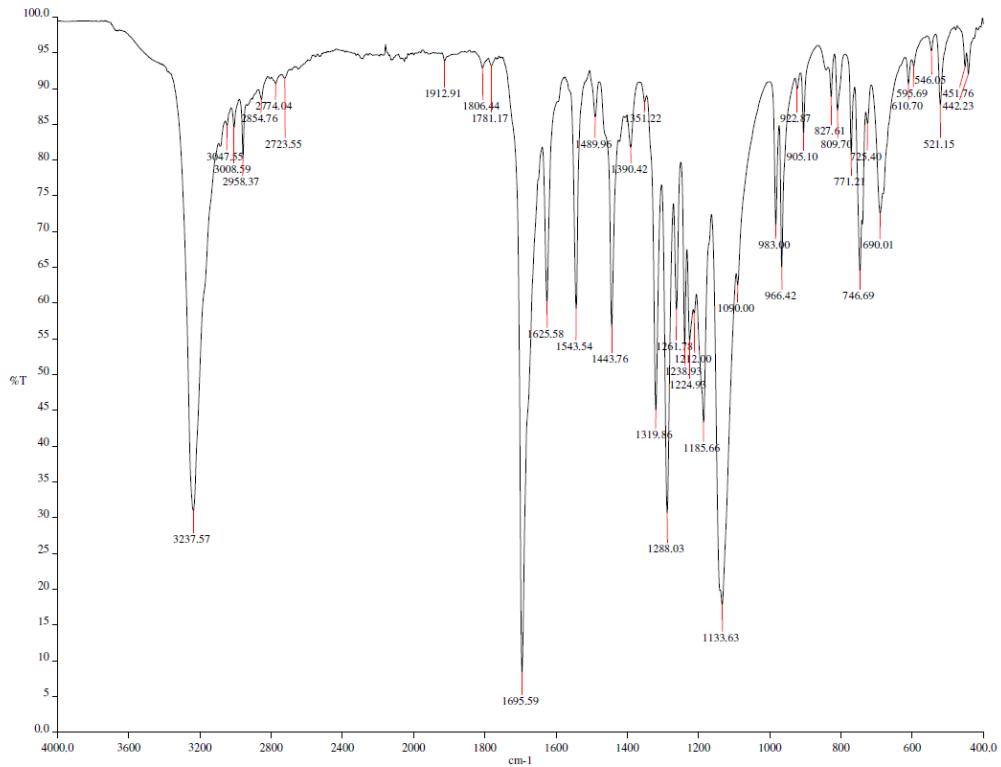
**Figure 16.** ATR-FTIR: Methyl 1-methyl-2-trifluoromethyl-1*H*-benzimidazole-5-carboxylate (**2-C2**).



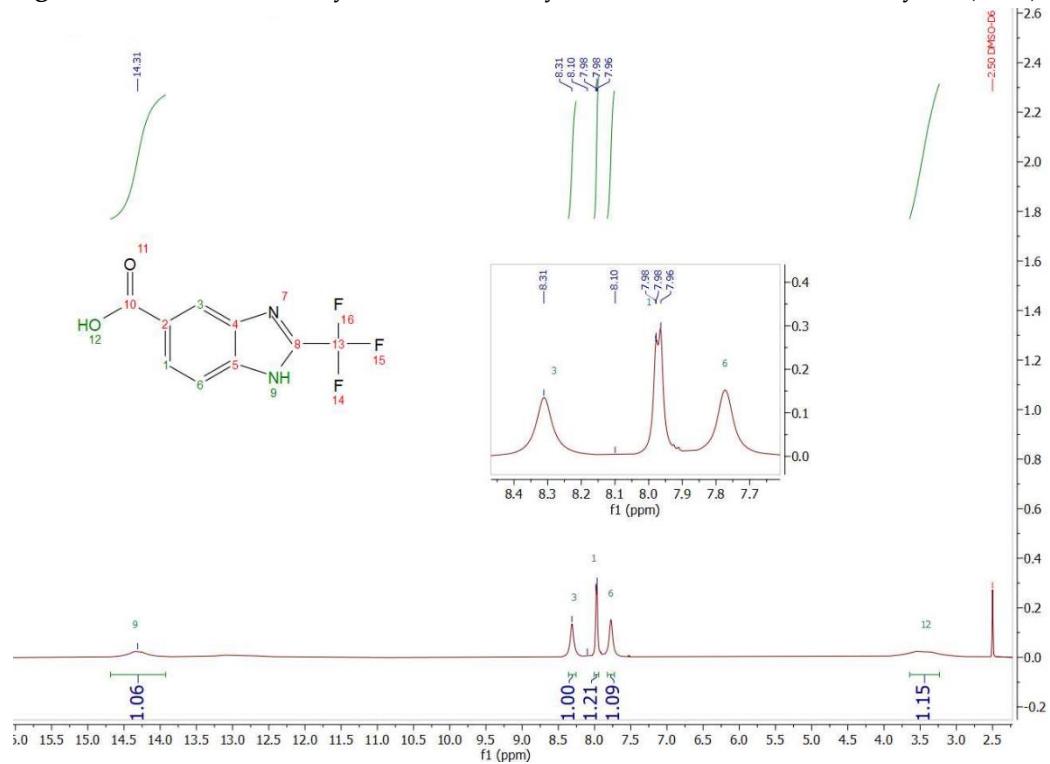
**Figure 17.**  $^1\text{H}$  NMR (DMSO- $d_6$ , 600 MHz): Methyl 1-methyl-2-trifluoromethyl-1*H*-benzimidazole-5-carboxylate (**2-C2**).



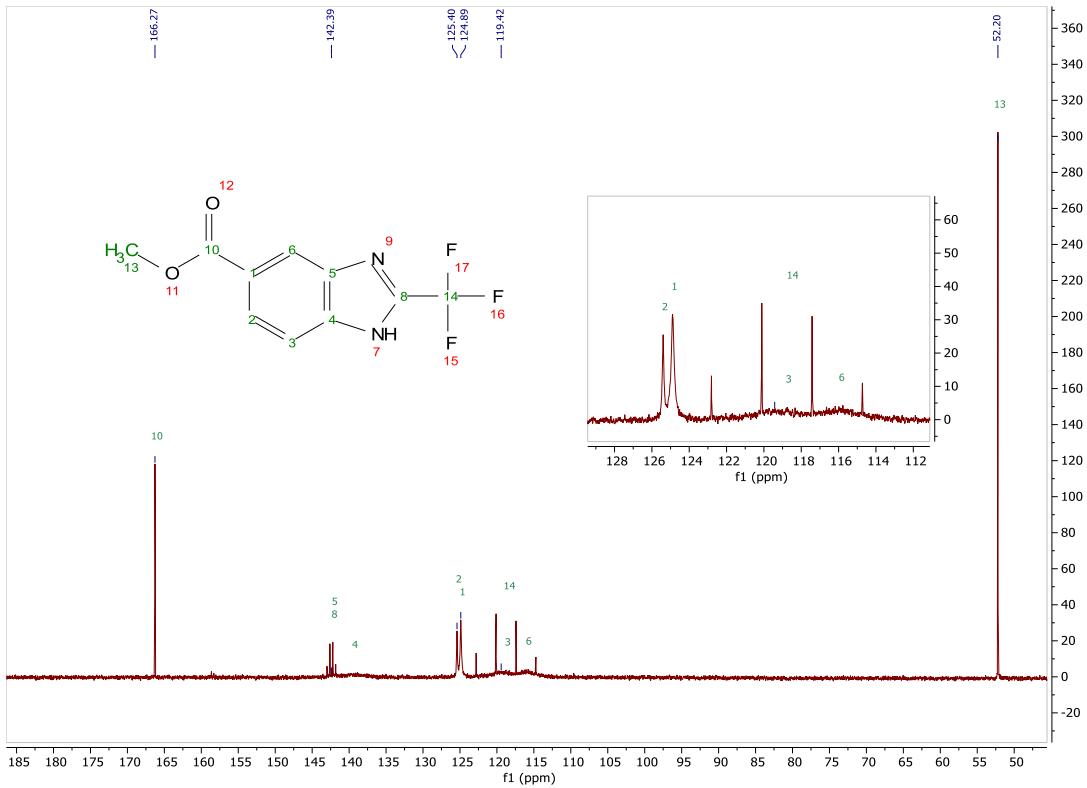
**Figure 18.**  $^{13}\text{C}$  NMR (DMSO- $d_6$ , 151 MHz): Methyl 1-methyl-2-trifluoromethyl-1*H*-benzimidazole-5-carboxylate (**2-C2**).



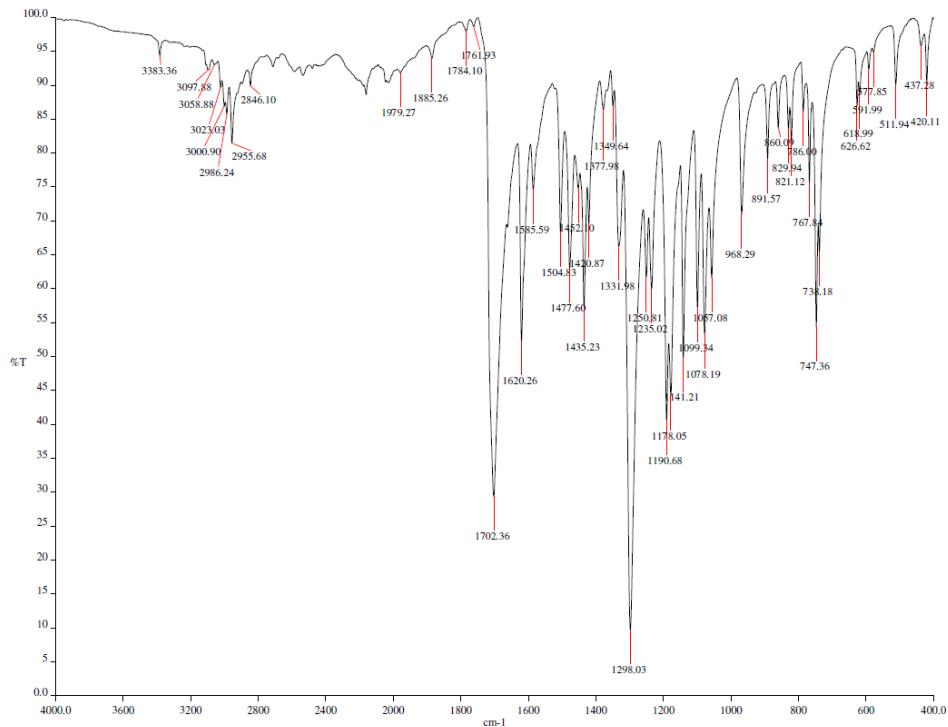
**Figure 19.** ATR-FTIR: Methyl 2-trifluoromethyl-1*H*-benzimidazole-5-carboxylate (2-C3).



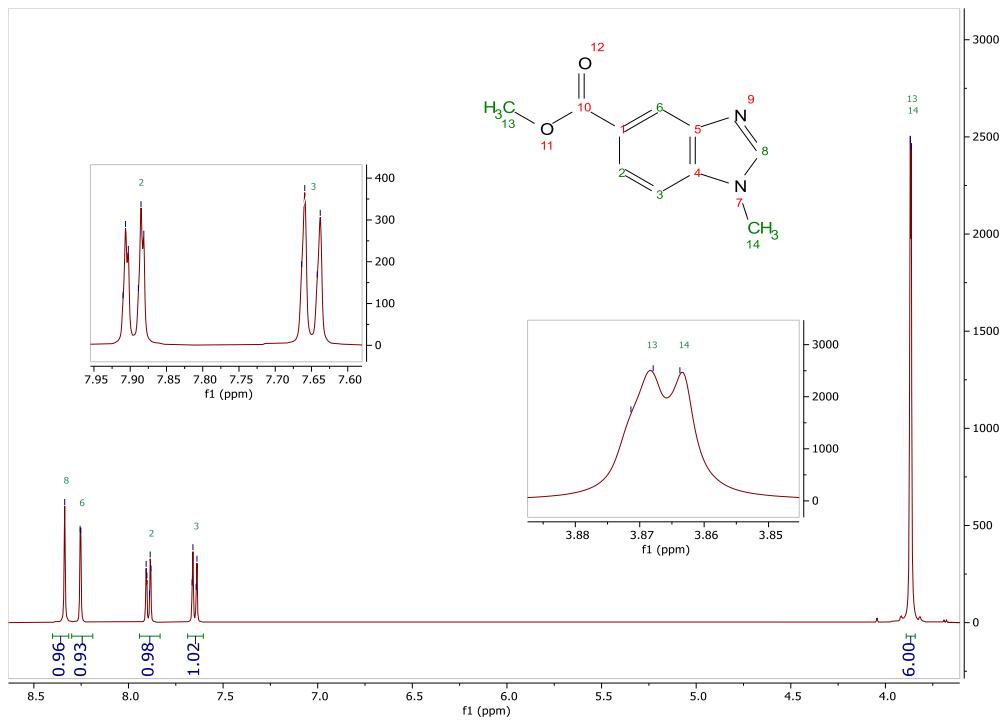
**Figure 20.** <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 600 MHz): Methyl 2-trifluoromethyl-1*H*-benzimidazole-5-carboxylate (2-C3).



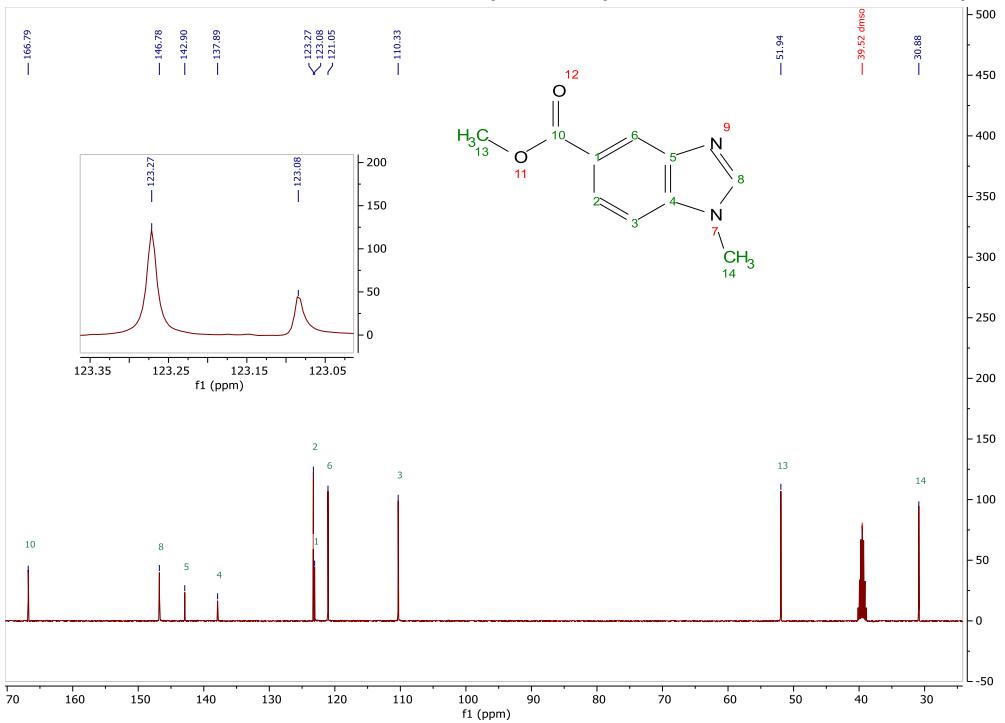
**Figure 21.**  $^{13}\text{C}$  NMR (DMSO- $d_6$ , 101 MHz): Methyl 2-trifluoromethyl-1*H*-benzimidazole-5-carboxylate (2-C3).



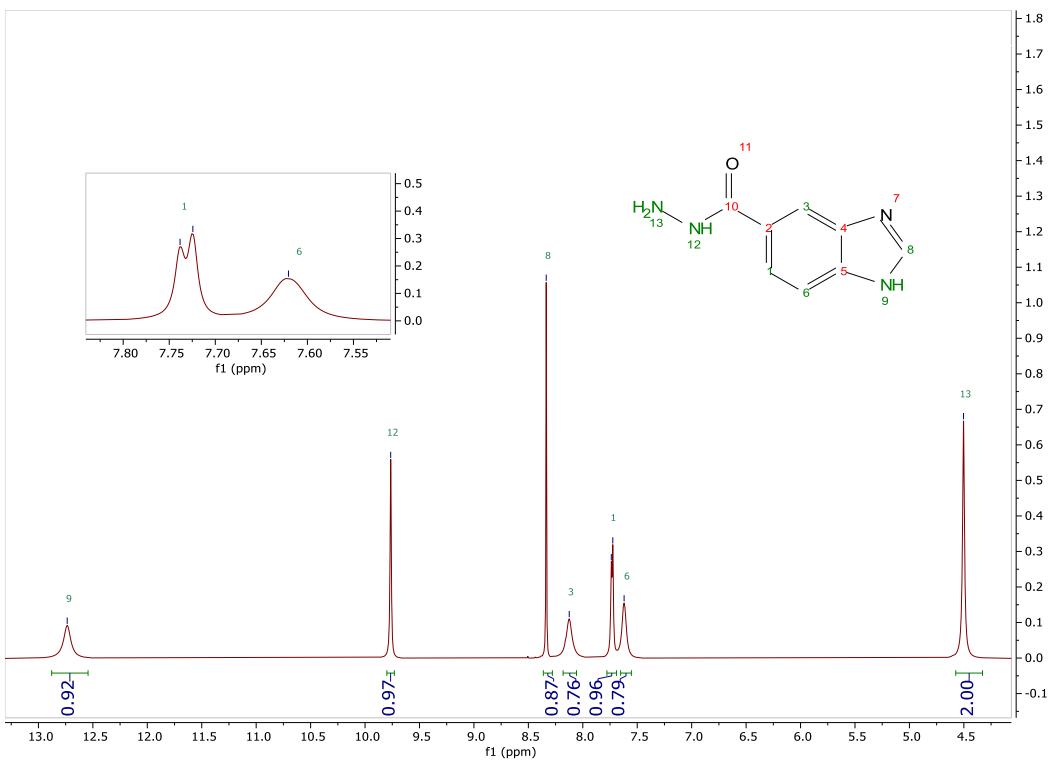
**Figure 22.** ATR-FTIR: Methyl 1-methyl-1*H*-benzimidazole-5-carboxylate (2-C4).



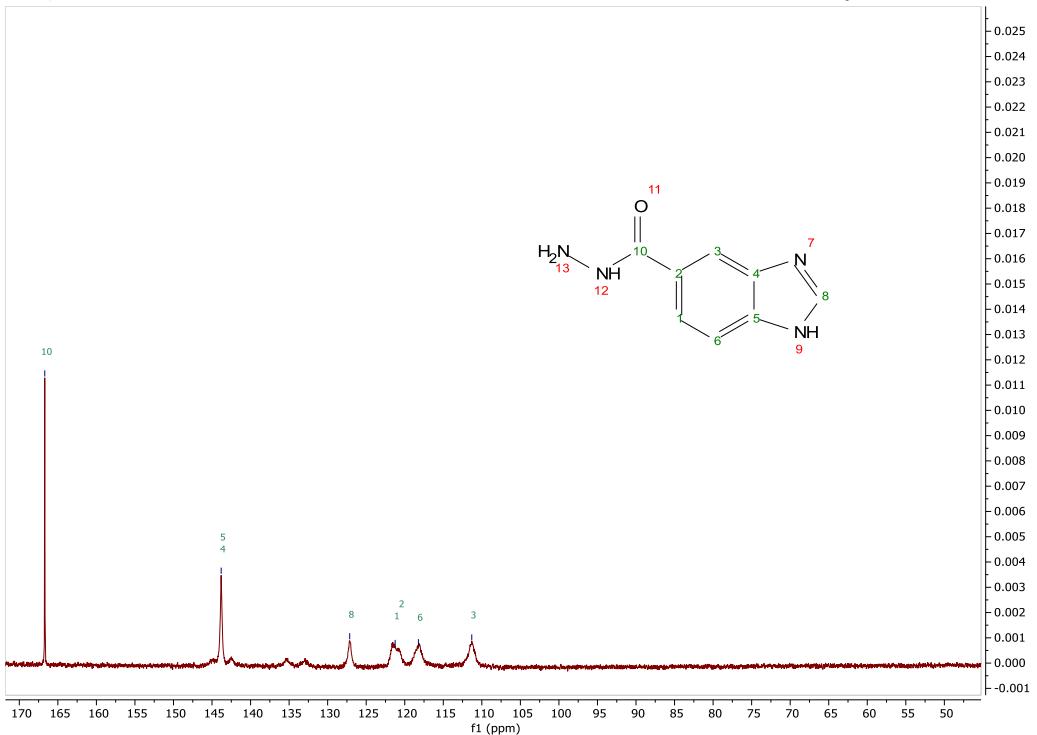
**Figure 23.** <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 400 MHz): Methyl 1-methyl-1*H*-benzimidazole-5-carboxylate (**2-C4**).



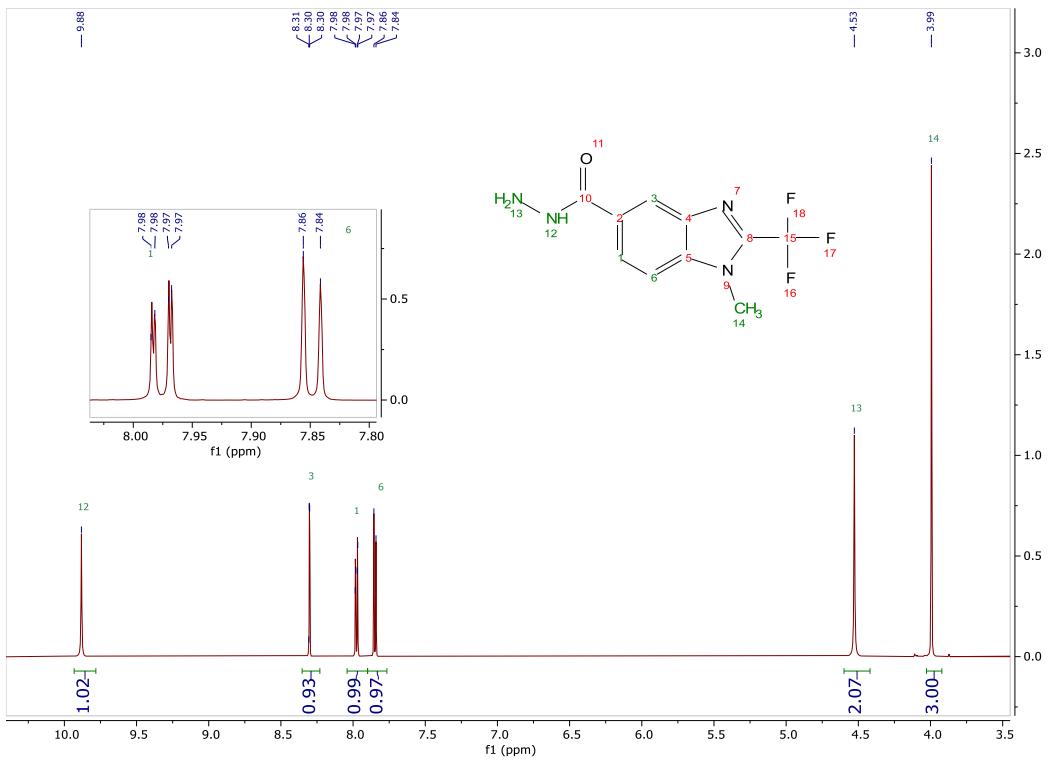
**Figure 24.** <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 101 MHz): Methyl 1-methyl-1*H*-benzimidazole-5-carboxylate (**2-C4**).



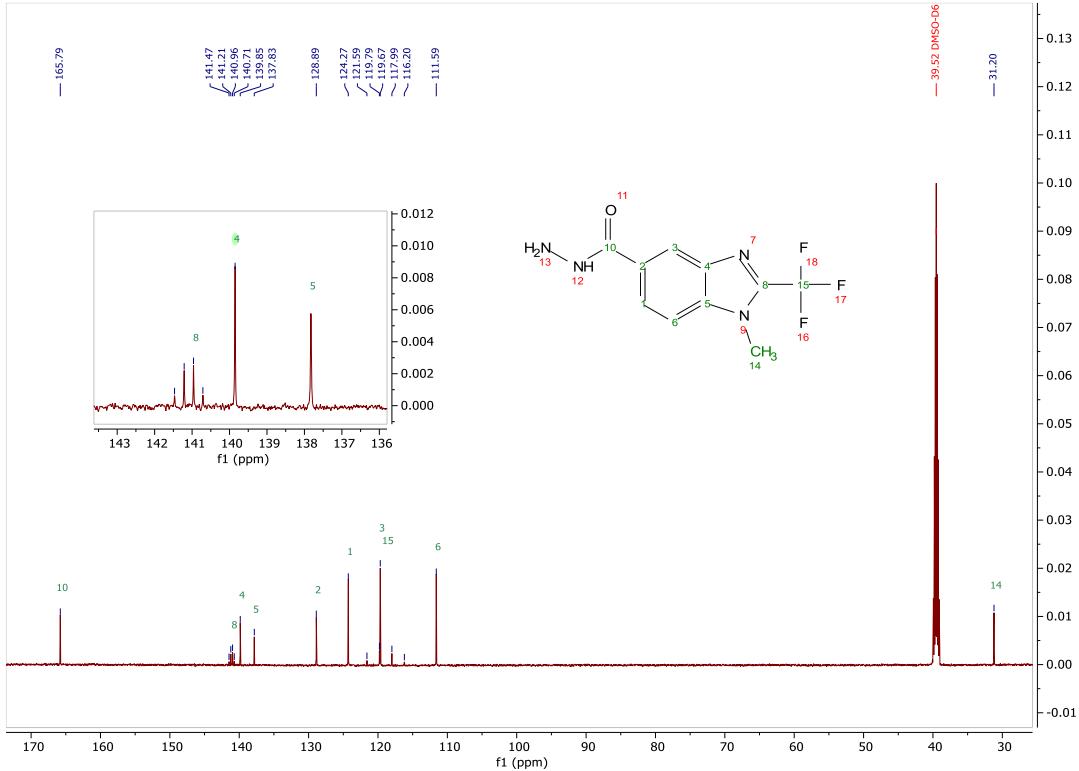
**Figure 25.**  $^1\text{H}$  NMR ( $\text{DMSO}-d_6$ , 600 MHz): 1*H*-benzimidazole-5-carbohydrazide (3-C1).



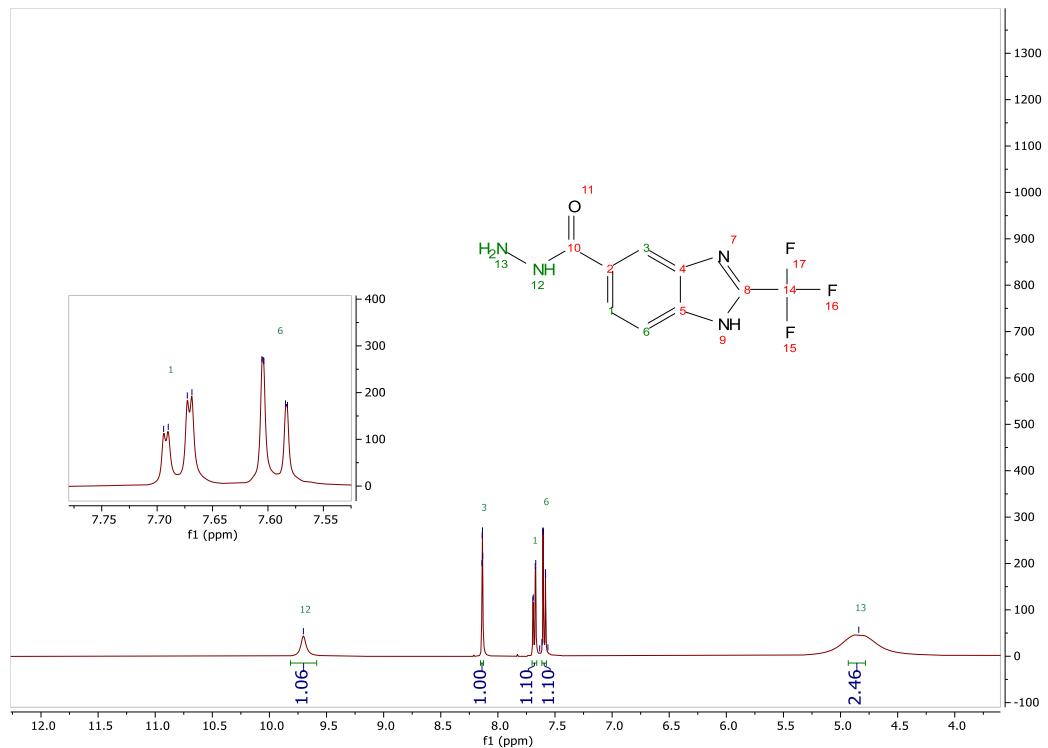
**Figure 26.**  $^{13}\text{C}$  NMR ( $\text{DMSO}-d_6$ , 151 MHz): 1*H*-benzimidazole-5-carbohydrazide (3-C1).



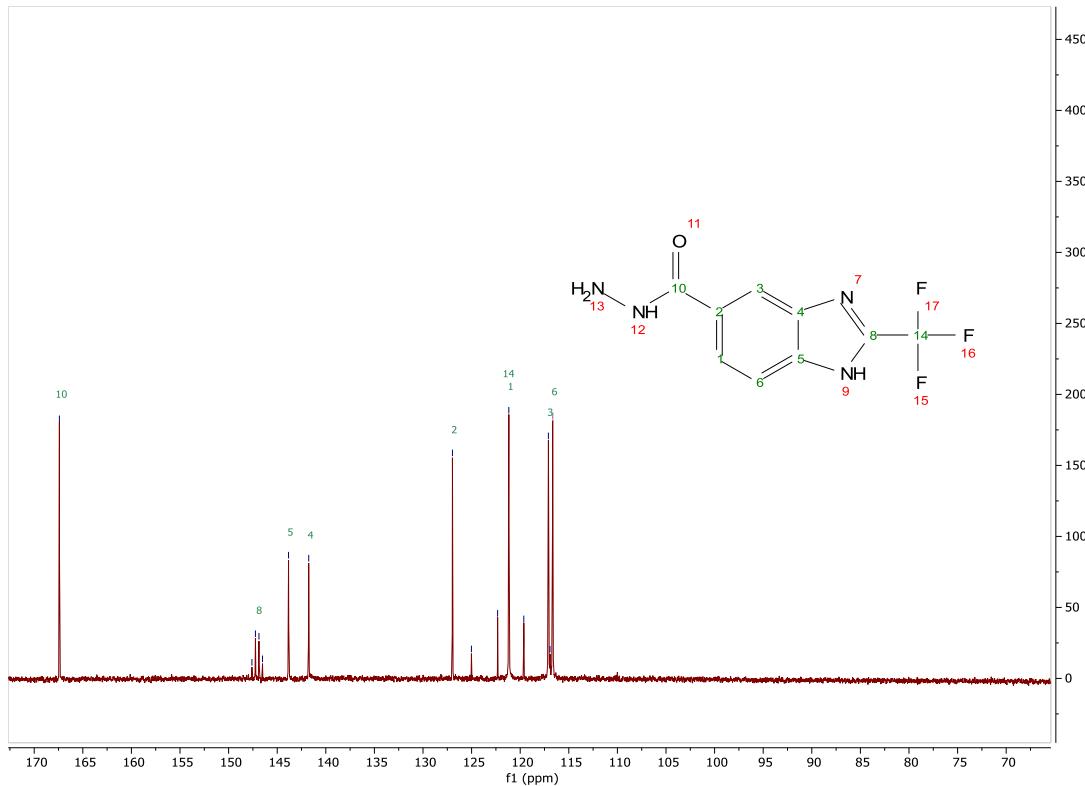
**Figure 27.** <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 600 MHz): 1-Methyl-2-(trifluoromethyl)-1*H*-benzimidazole-5-carbohydrazide (3-C2).



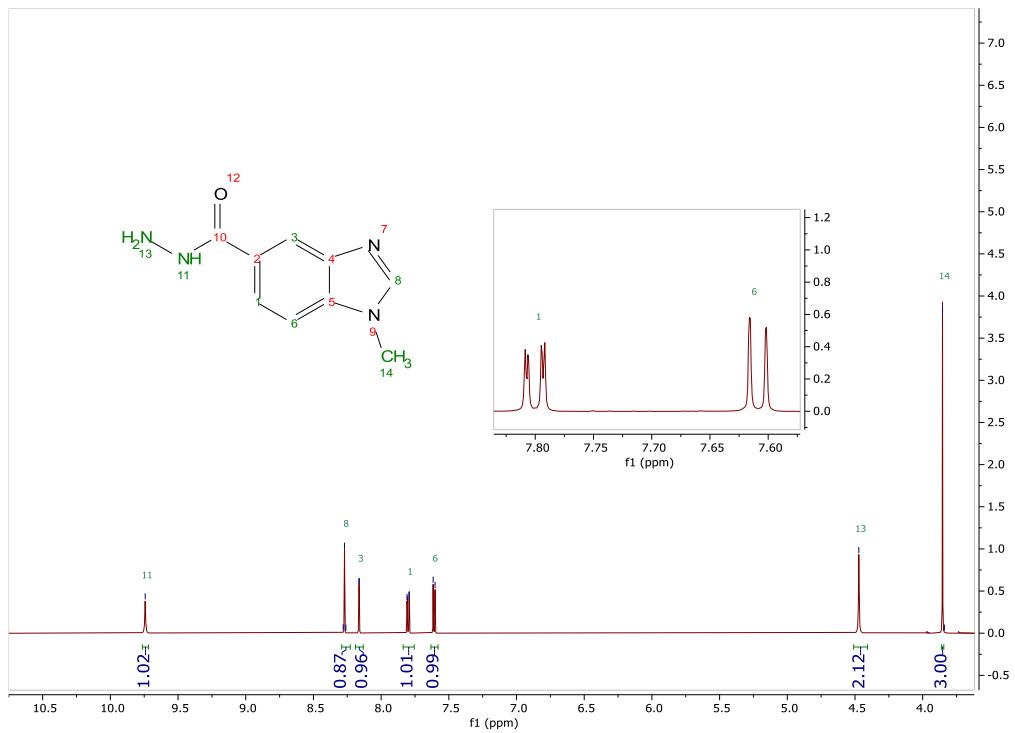
**Figure 28.** <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 151 MHz): 1-Methyl-2-(trifluoromethyl)-1*H*-benzimidazole-5-carbohydrazide (3-C2).



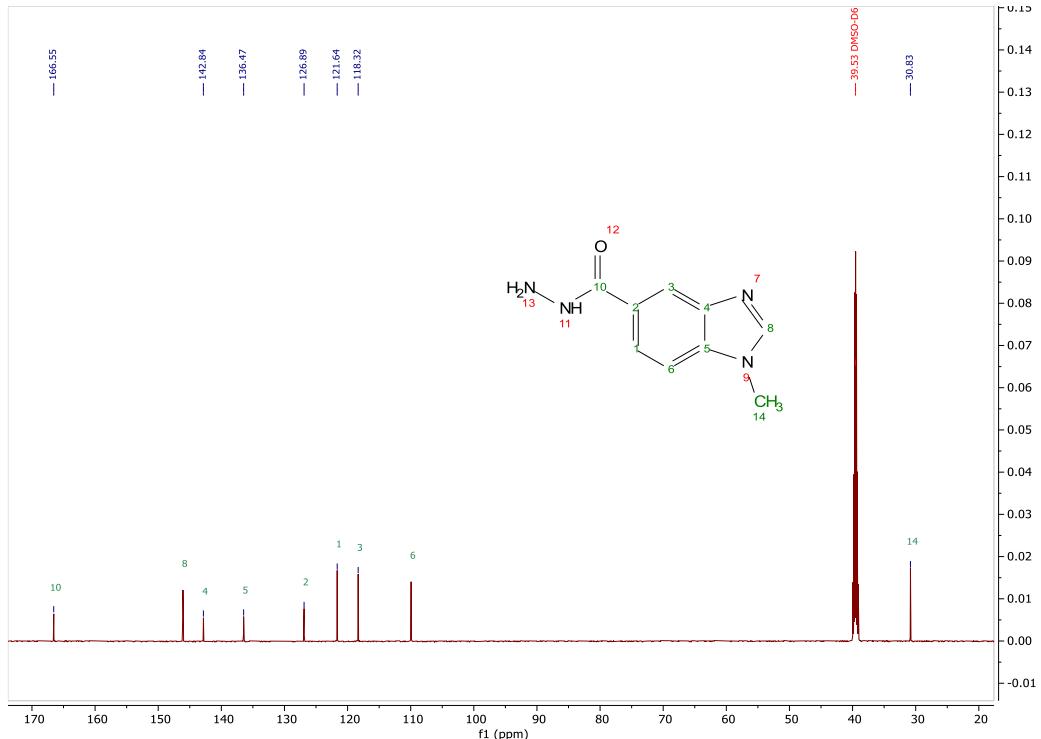
**Figure 29.** <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 400 MHz): 2-(Trifluoromethyl)-1*H*-benzimidazole-5-carbohydrazide (3-C3).



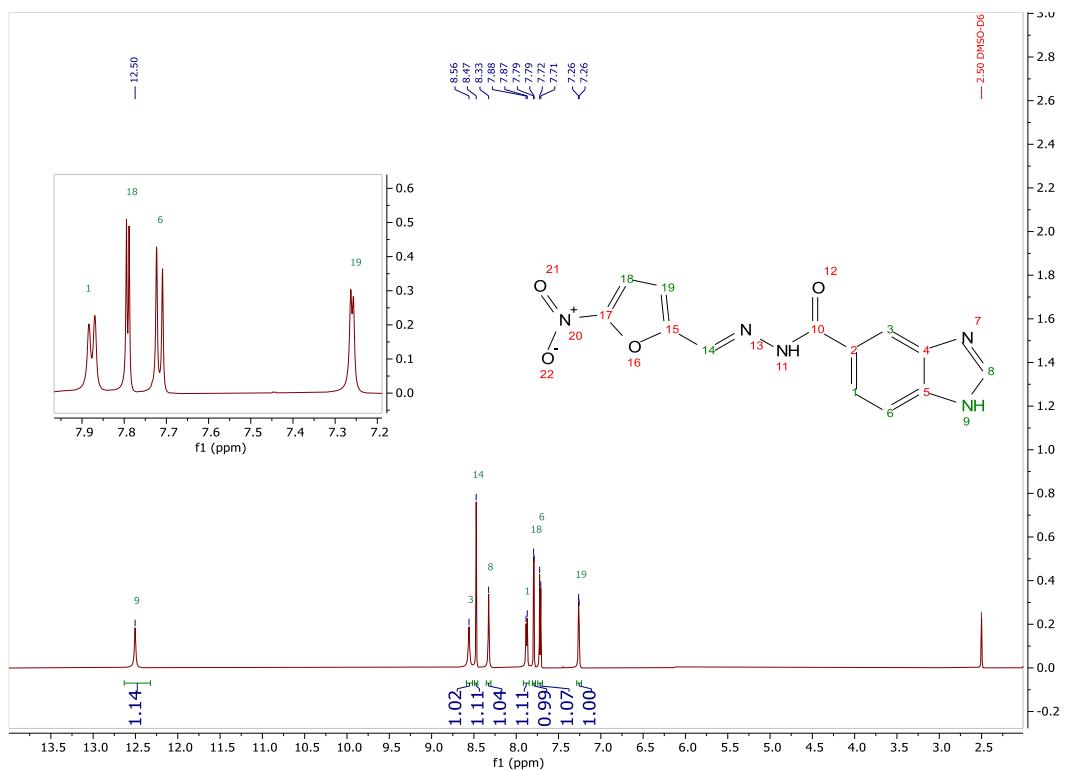
**Figure 30.** <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 101 MHz): 2-(Trifluoromethyl)-1*H*-benzimidazole-5-carbohydrazide (3-C3).



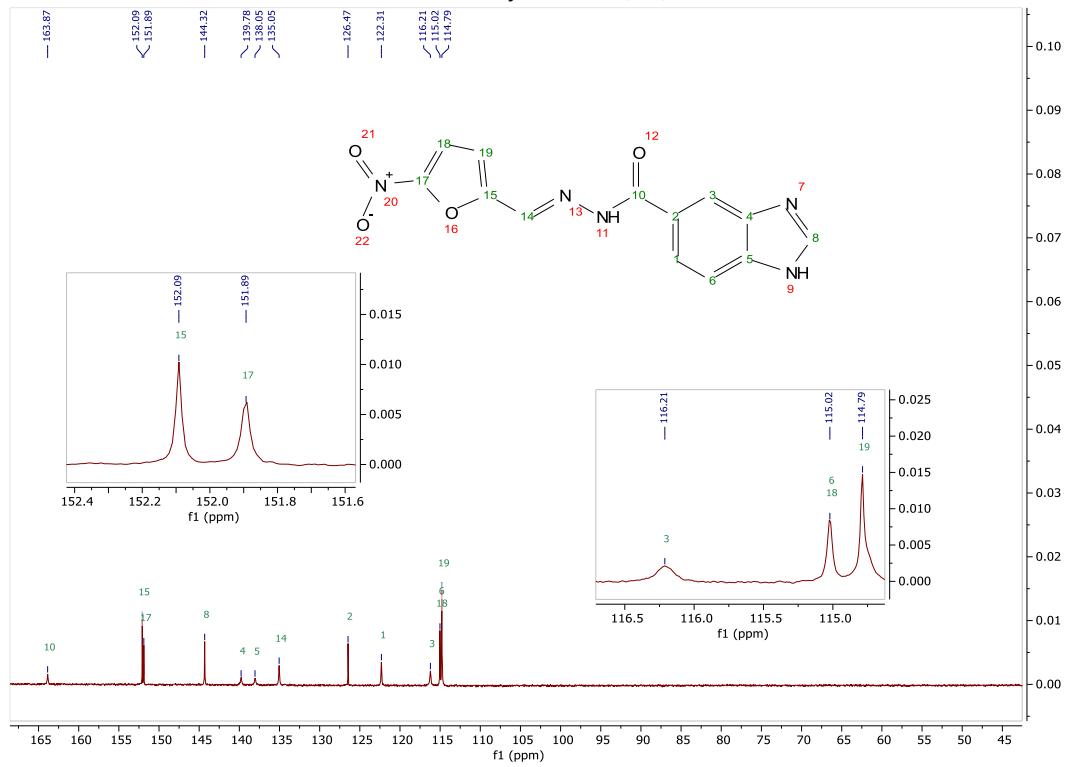
**Figure 31.**  $^1\text{H}$  NMR ( $\text{DMSO}-d_6$ , 600 MHz): 1-Methyl-1*H*-benzimidazole-5-carbohydrazide (3-C4).



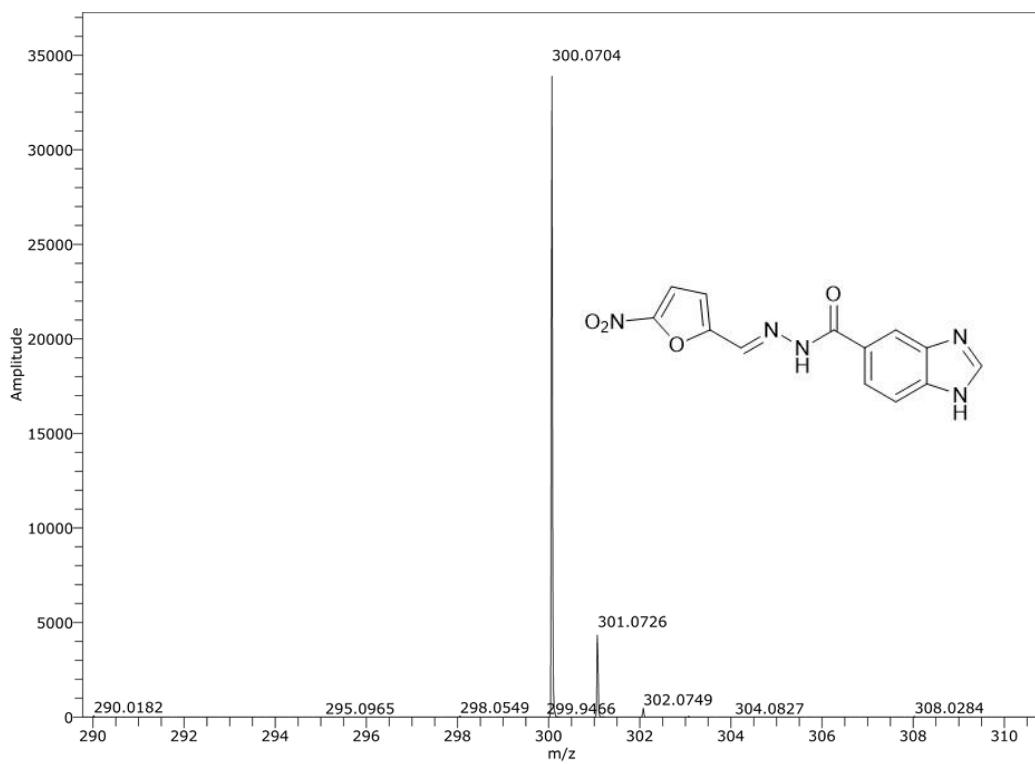
**Figure 32.**  $^{13}\text{C}$  NMR ( $\text{DMSO}-d_6$ , 151 MHz): 1-Methyl-1*H*-benzimidazole-5-carbohydrazide (3-C4).



**Figure 33.**  $^1\text{H}$  NMR (DMSO- $d_6$ , 600 MHz):  $\text{N}'$ -[(5-Nitrofuran-2-yl)methylene]-1*H*-benzimidazole-5-carbohydrazide (**C1**).

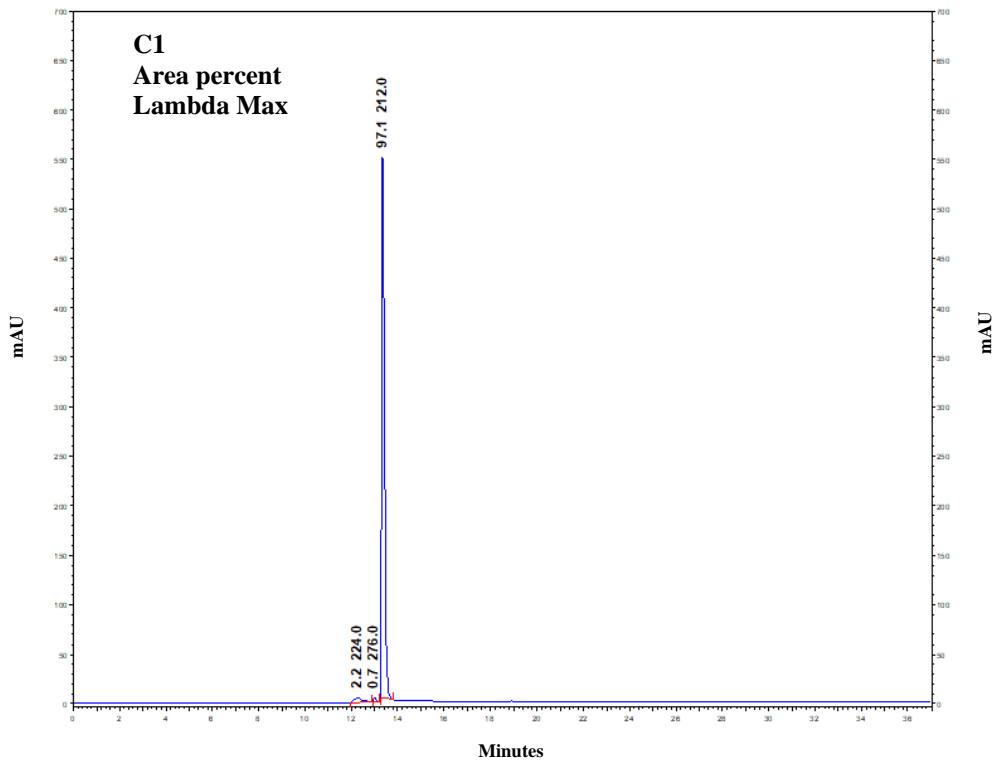


**Figure 34.**  $^{13}\text{C}$  NMR (DMSO- $d_6$ , 151 MHz):  $\text{N}'$ -[(5-Nitrofuran-2-yl)methylene]-1*H*-benzimidazole-5-carbohydrazide (**C1**).

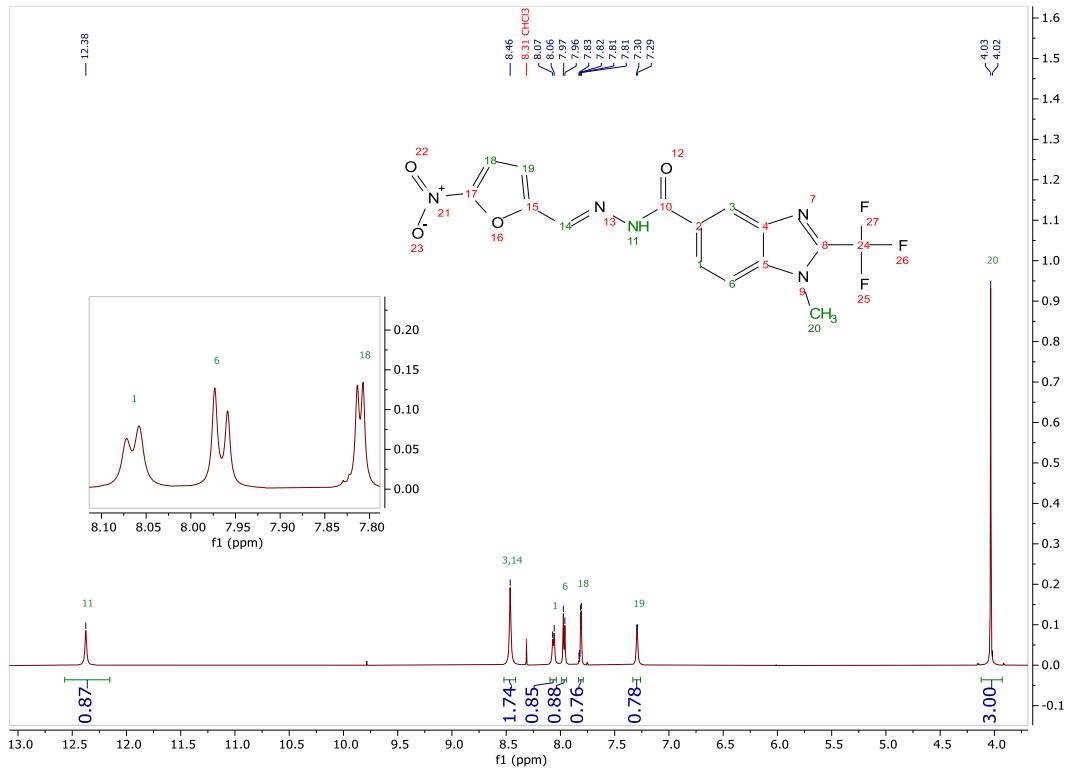


Formula	Calculated	Obtained	Obtained formula	%	ppM error	Score
C <sub>13</sub> H <sub>9</sub> N <sub>5</sub> O <sub>4</sub>	300.07273	300.0704	C <sub>13</sub> H <sub>9</sub> N <sub>5</sub> O <sub>4</sub> + H <sup>+</sup>	300.0704 (100), 301.0726 (18), 302.0749 (2)	-3.23	0.84

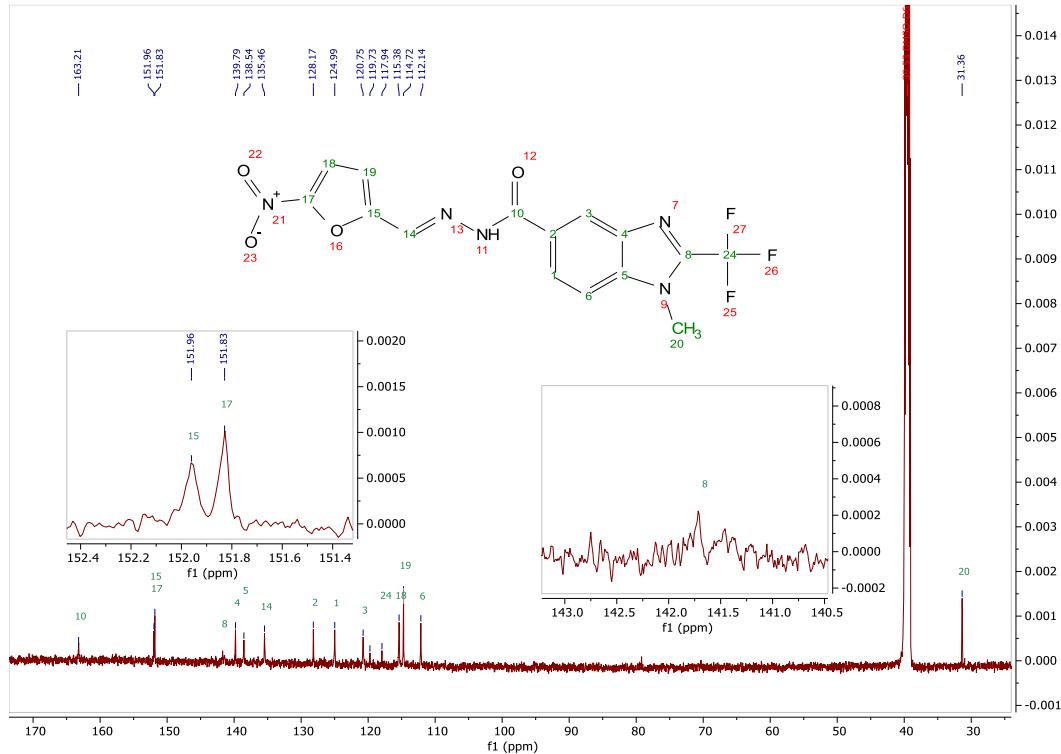
**Figure 35.** HRMS (APCI):  $m/z$  300.0704 [ $M^+ + H$ ]  $N'$ -(5-Nitrofuran-2-yl)methylene]-1*H*-benzimidazole-5-carbohydrazide (**C1**).



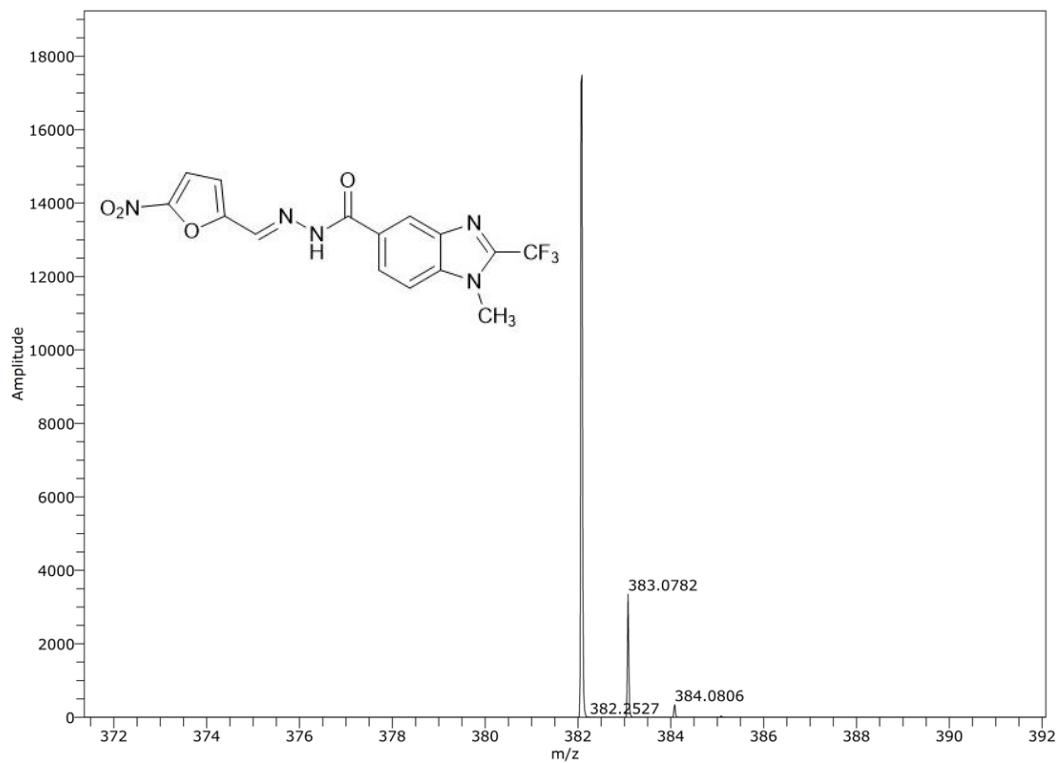
**Figure 36.** HPLC-DAD: 97.1% purity, with a  $\lambda_{\text{max}}$  of 212.0 nm as a result of scanning from 190 to 600 nm of *N'*-[(5-Nitrofuran-2-yl)methylene]-1*H*-benzimidazole-5-carbohydrazide (**C1**).



**Figure 37.**  $^1\text{H}$  NMR (DMSO- $d_6$ , 600 MHz): 1-Methyl- $N'$ -[(5-nitrofuran-2-yl)methylene]-2-(trifluoromethyl)-1*H*-benzimidazole-5-carbohydrazide (C2).

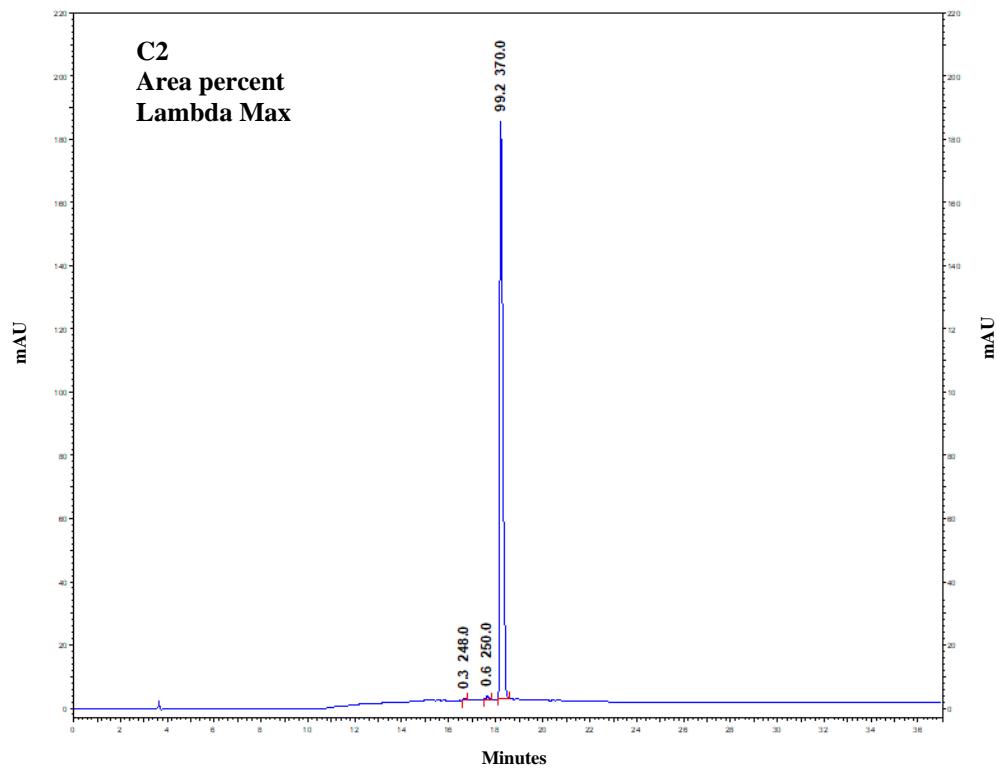


**Figure 38.**  $^{13}\text{C}$  NMR (DMSO- $d_6$ , 151 MHz): 1-Methyl- $N'$ -[(5-nitrofuran-2-yl)methylene]-2-(trifluoromethyl)-1*H*-benzimidazole-5-carbohydrazide (C2).

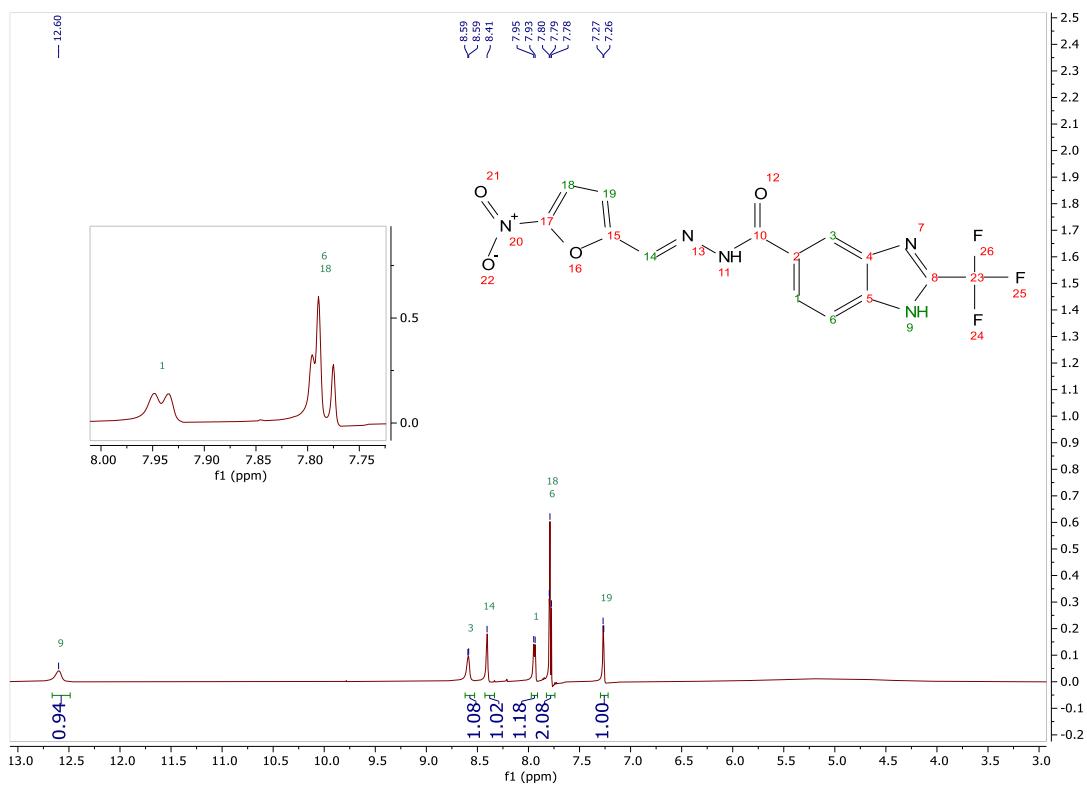


Formula	Calculated	Obtained	Obtained formula	%	ppM error	Score
C <sub>15</sub> H <sub>10</sub> F <sub>3</sub> N <sub>5</sub> O <sub>4</sub>	382.07577	382.0761	C <sub>15</sub> H <sub>10</sub> F <sub>3</sub> N <sub>5</sub> O <sub>4</sub> + H <sup>+</sup>	382.0761 (100), 383.0782 (18), 384.0806 (2)	-0.87	0.849

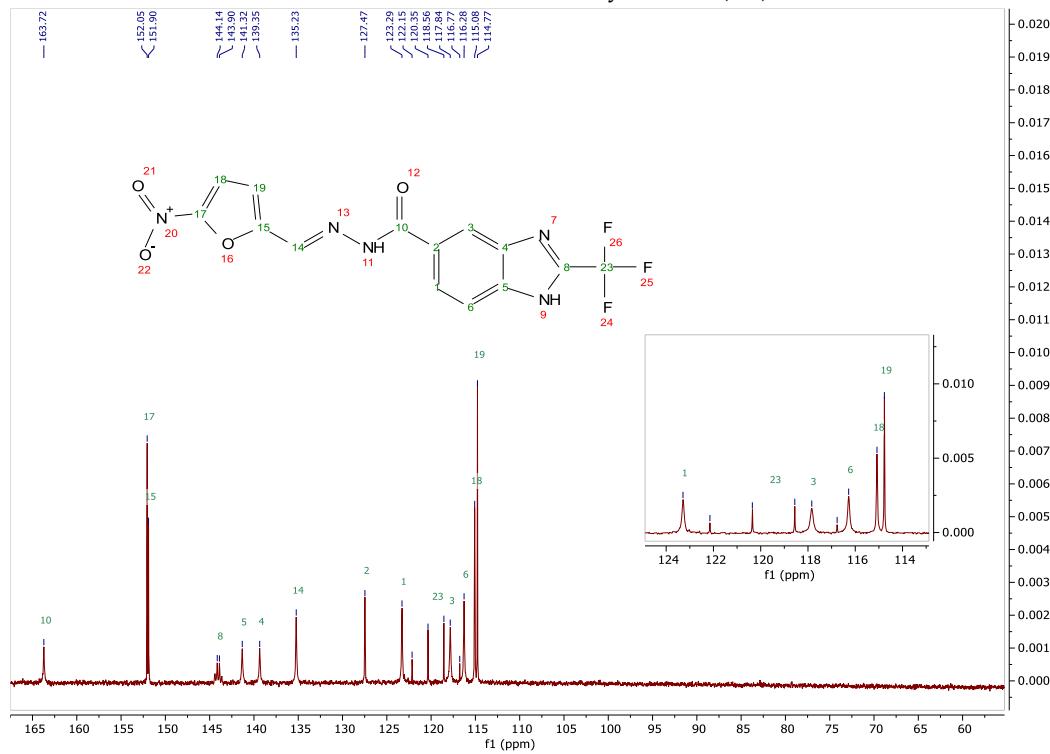
**Figure 39.** HRMS (APCI):  $m/z$  382.0761 [ $M^+ + H$ ] 1-Methyl- $N'$ -[(5-nitrofuran-2-yl)methylene]-2-(trifluoromethyl)-1*H*-benzimidazole-5-carbohydrazide (**C2**).



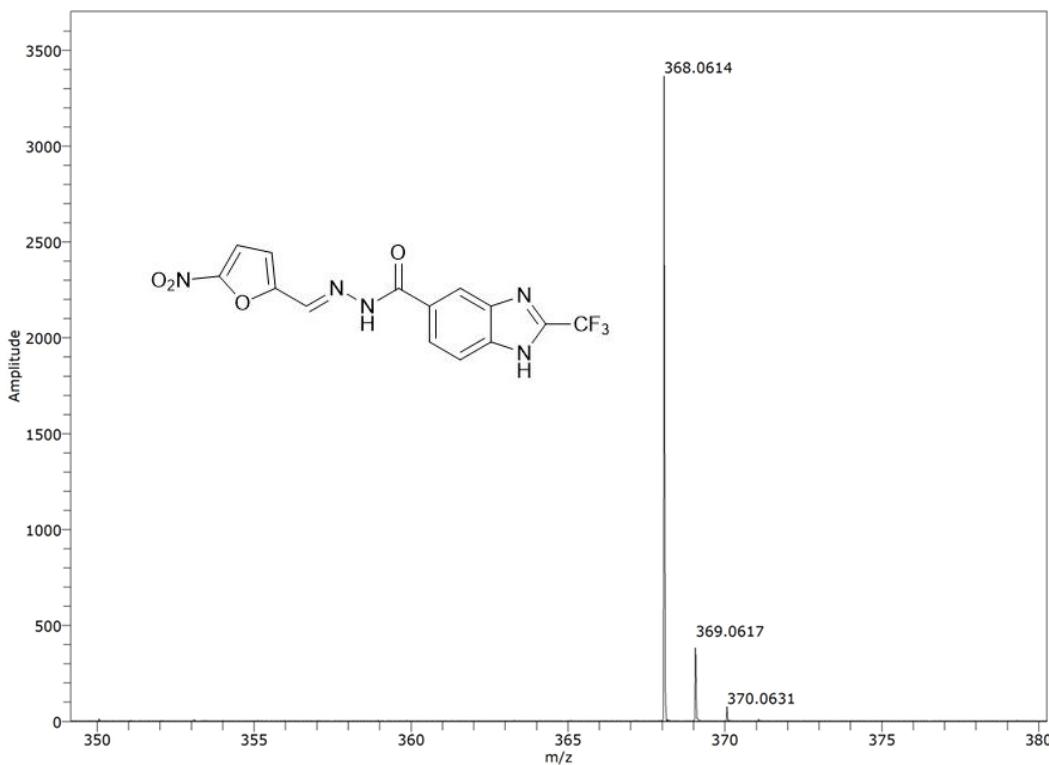
**Figure 40.** HPLC-DAD: 99.2% purity, with a  $\lambda_{\text{max}}$  of 370.0 nm as a result of scanning from 190 to 600 nm of 1-Methyl-*N*'-[5-nitrofuran-2-yl)methylene]-2-(trifluoromethyl)-1*H*-benzimidazole-5-carbohydrazide (**C2**).



**Figure 41.**  $^1\text{H}$  NMR (DMSO- $d_6$ , 600 MHz):  $N'-(5\text{-Nitrofuran-2-yl)methylene]-2-(trifluoromethyl)-1H\text{-benzimidazole-5-carbohydrazide (C3)}$ .

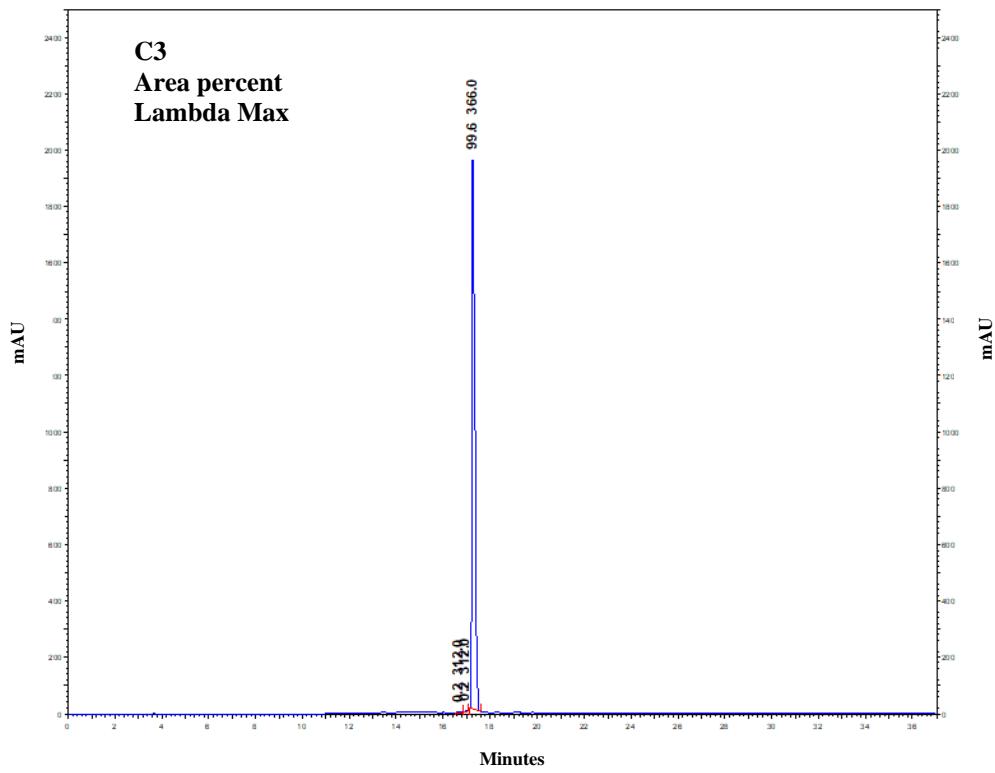


**Figure 42.**  $^{13}\text{C}$  NMR (DMSO- $d_6$ , 151 MHz):  $N'-(5\text{-Nitrofuran-2-yl)methylene]-2-(trifluoromethyl)-1H\text{-benzimidazole-5-carbohydrazide (C3)}$ .

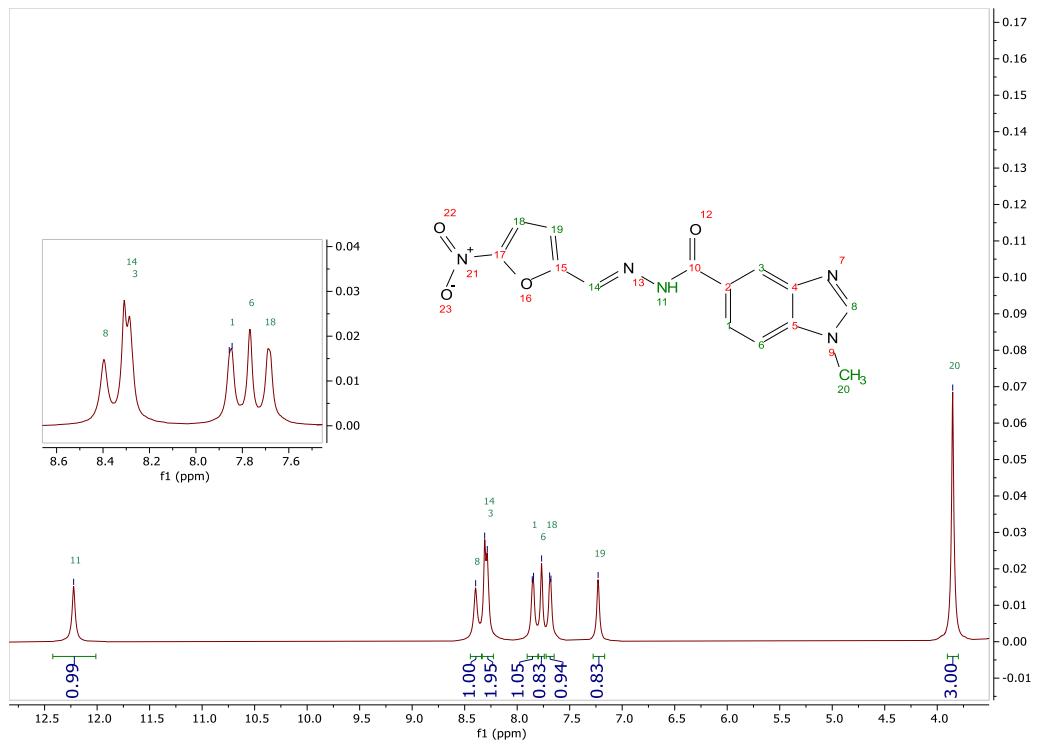


Formula	Calculated	Obtained	Obtained formula	%	ppM error	Score
$C_{14}H_8F_3N_5O_4$	368.06012	368.0614	$C_{14}H_8F_3N_5O_4 + H^+$	368.0614 (100), 369.0617 (18), 370.0631 (2)	-3.08	0.804

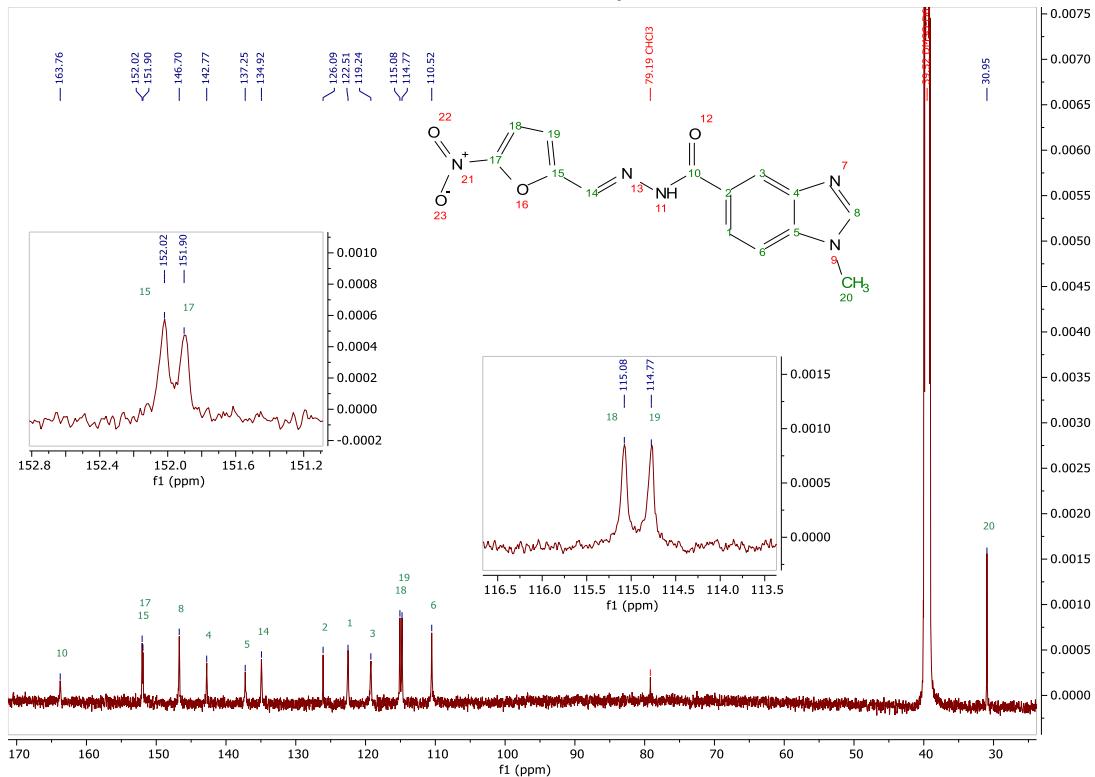
**Figure 43.** HRMS (APCI):  $m/z$  368.0614 [ $M^+ + H$ ]  $N'-(5\text{-Nitrofuran-2-yl})\text{methylene}-2\text{-}(trifluoromethyl)-1H\text{-benzimidazole-5-carbohydrazide}$  (**C3**).



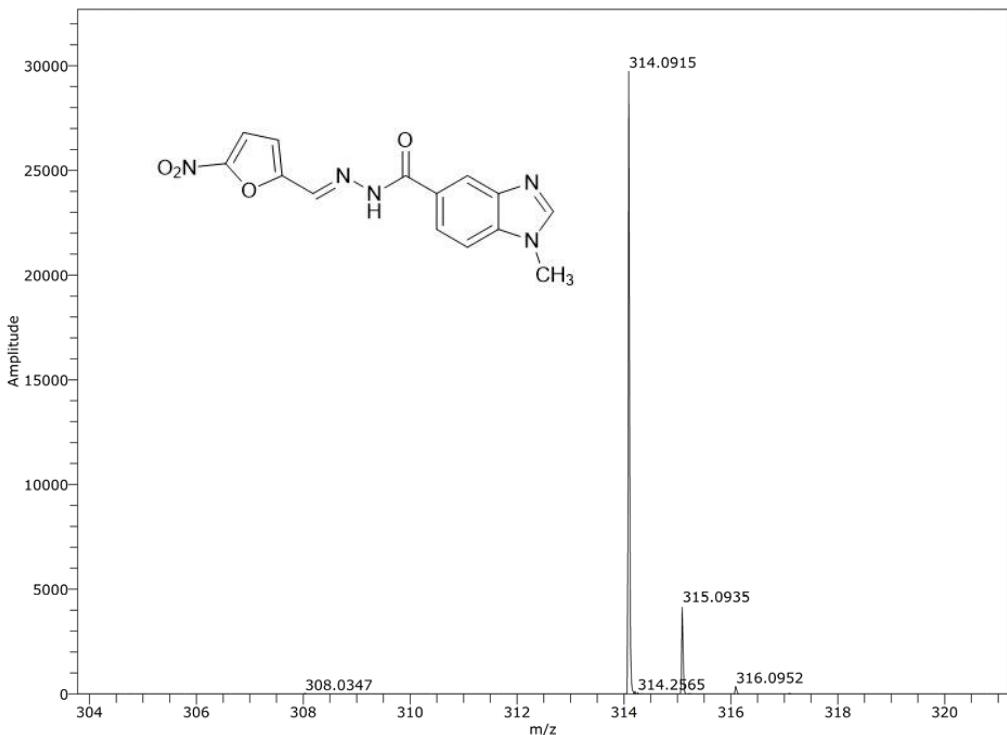
**Figure 44.** HPLC-DAD: 99.6% purity, with a  $\lambda_{\text{max}}$  of 366.0 nm as a result of scanning from 190 to 600 nm of *N'*-[(5-Nitrofuran-2-yl)methylene]-2-(trifluoromethyl)-1*H*-benzimidazole-5-carbohydrazide (C3).



**Figure 45.** <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 600 MHz): 1-Methyl-*N'*-(5-nitrofuran-2-yl)methylene-1*H*-benzimidazole-5-carbohydrazide (**C4**).

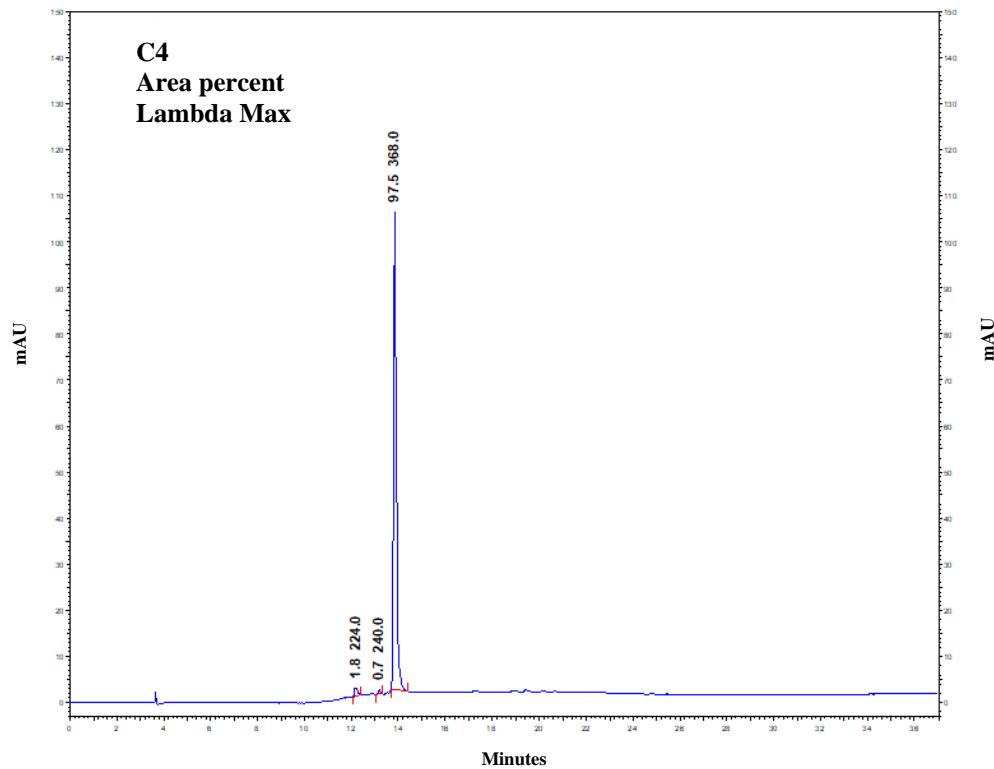


**Figure 46.** <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 151 MHz): 1-Methyl-*N'*-(5-nitrofuran-2-yl)methylene-1*H*-benzimidazole-5-carbohydrazide (**C4**).



Formula	Calculated	Obtained	Obtained formula	%	ppM error	Score
$C_{14}H_{11}N_5O_4$	314.0915	314.08838	$C_{14}H_{11}N_5O_4 + H^+$	314.0915 (100), 315.0935 (18), 316.0952 (2)	-10	0.753

**Figure 47.** HRMS (APCI):  $m/z$  314.0915 [ $M^+ + H$ ] 1-Methyl-N'-(5-nitrofuran-2-yl)methylene]-1*H*-benzimidazole-5-carbohydrazide (**C4**).



**Figure 48.** HPLC-DAD: 97.5% purity, with a  $\lambda_{\text{max}}$  of 368.0 nm as a result of scanning from 190 to 600 nm of 1-Methyl-*N'*-[(5-nitrofuran-2-yl)methylene]-1*H*-benzimidazole-5-carbohydrazide (**C4**).